



wwPDB EM Validation Summary Report ⓘ

Sep 9, 2026 – 11:59 PM JST

PDB ID : 6IJO / pdb_00006ijo
EMDB ID : EMD-9680
Title : Photosystem I of Chlamydomonas reinhardtii
Authors : Pan, X.; Ma, J.; Su, X.; Liu, Z.; Zhang, X.; Li, M.
Deposited on : 2018-10-10
Resolution : 3.30 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:

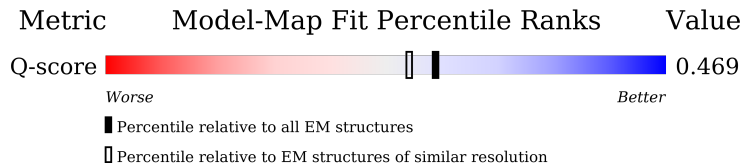
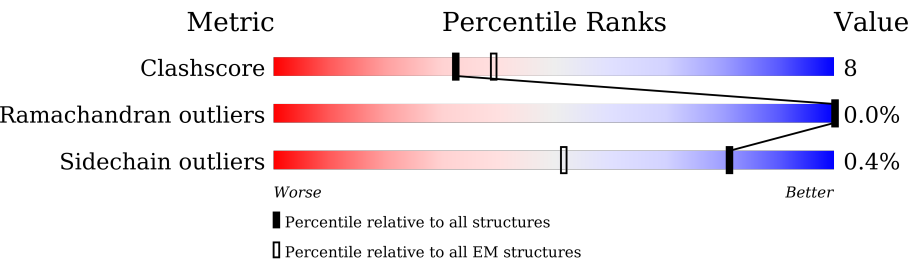
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	7% 83% 15% .
2	B	735	7% 84% 16% .
3	C	81	7% 79% 20% .
4	D	247	7% 46% 12% 42%

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Mol	Chain	Length	Quality of chain
5	E	143	
6	F	227	
7	G	159	
8	H	155	
9	I	106	
10	J	41	
11	K	160	
12	L	258	
13	1	248	
13	a	248	
14	3	298	
15	4	290	
16	5	274	
17	6	318	
18	7	241	
19	8	272	
20	2	227	
21	9	213	
22	X	26	

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 49685 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5819	3805	993	999	22		

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5812	3818	975	1001	18		

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	116	12		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1129	722	200	200	7		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			505	322	89	94		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	164	Total	C	N	O	S	0	0
			1254	811	209	231	3		

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	70	Total	C	N	O	0	0
			514	334	89	91		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	51	Total	C	N	O	0	0
			357	223	66	68		

- Molecule 9 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	32	Total	C	N	O	S	0	0
			242	166	34	41	1		

- Molecule 10 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			337	231	47	58	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	85	Total	C	N	O	S	0	0
			578	368	99	109	2		

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	106	Total	C	N	O	S	0	0
			768	507	123	136	2		

- Molecule 13 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1433	932	239	259	3		
13	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

- Molecule 14 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	221	Total	C	N	O	S	0	0
			1683	1099	271	305	8		

- Molecule 15 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4	210	Total	C	N	O	S	0	0
			1631	1071	263	292	5		

- Molecule 16 is a protein called Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	5	226	Total	C	N	O	S	0	0
			1765	1149	295	313	8		

- Molecule 17 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

- Molecule 18 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	7	213	Total	C	N	O	S	0	0
			1649	1072	274	297	6		

- Molecule 19 is a protein called Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	8	215	Total	C	N	O	S	0	0
			1630	1058	278	290	4		

- Molecule 20 is a protein called Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	173	Total	C	N	O	S	0	0
			1346	874	223	241	8		

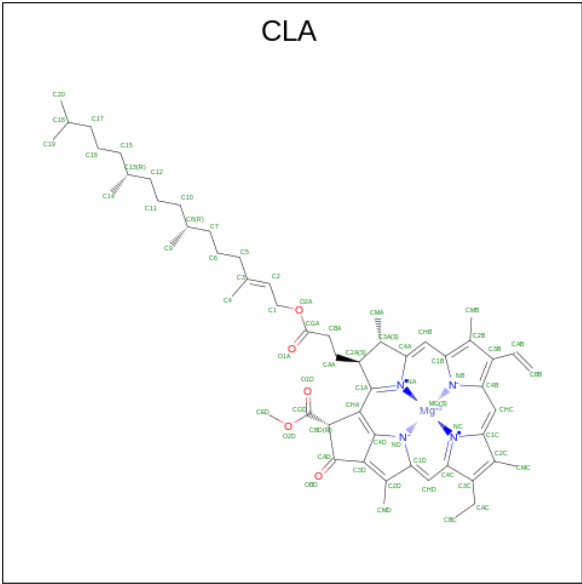
- Molecule 21 is a protein called Lhca9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	9	172	Total	C	N	O	S	0	0
			1302	840	220	235	7		

- Molecule 22 is a protein called ChainX.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
23	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
23	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
23	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
23	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
23	F	1	Total 57	C 47	Mg 1	N 4	O 5	0
23	F	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	K	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	1	1	Total 53	C 44	Mg 1	N 4	O 4	0
23	1	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	1	1	Total 39	C 32	Mg 1	N 4	O 2	0
23	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
23	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
23	1	1	Total 39	C 31	Mg 1	N 4	O 3	0
23	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	1	1	Total 37	C 29	Mg 1	N 4	O 3	0
23	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
23	a	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	a	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	a	1	Total 44	C 35	Mg 1	N 4	O 4	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	a	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	a	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	a	1	Total 38	C 30	Mg 1	N 4	O 3	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	3	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
23	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
23	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
23	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
23	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	6	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	6	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
23	6	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	7	1	Total 44	C 35	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
23	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	7	1	Total 42	C 33	Mg 1	N 4	O 4	0
23	7	1	Total 43	C 33	Mg 1	N 4	O 5	0
23	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	8	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	8	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	8	1	Total 43	C 33	Mg 1	N 4	O 5	0

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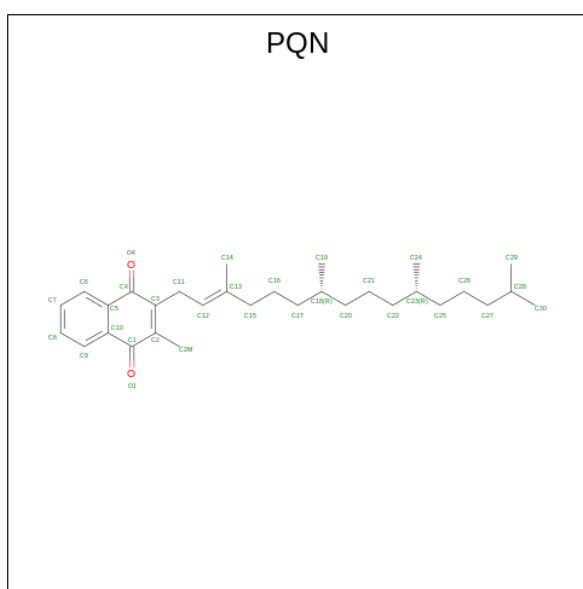
Mol	Chain	Residues	Atoms				AltConf
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			26	21	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	2	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	

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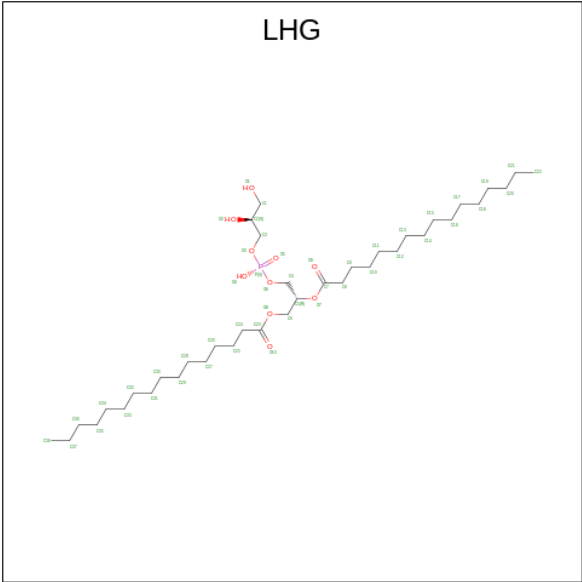
Mol	Chain	Residues	Atoms				AltConf
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	

- Molecule 24 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O		0
			33	31	2		
24	B	1	Total	C	O		0
			33	31	2		

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



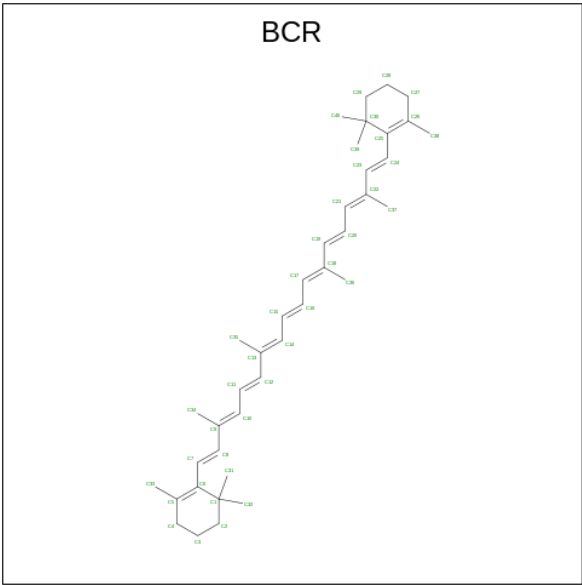
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			30	19	10	1	
25	B	1	Total	C	O	P	0
			38	27	10	1	
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	a	1	Total	C	O	P	0
			49	38	10	1	
25	3	1	Total	C	O	P	0
			45	34	10	1	
25	3	1	Total	C	O	P	0
			49	38	10	1	
25	4	1	Total	C	O	P	0
			49	38	10	1	
25	5	1	Total	C	O	P	0
			49	38	10	1	
25	5	1	Total	C	O	P	0
			49	38	10	1	
25	6	1	Total	C	O	P	0
			48	37	10	1	
25	7	1	Total	C	O	P	0
			37	26	10	1	
25	8	1	Total	C	O	P	0
			49	38	10	1	
25	8	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
25	2	1	Total	C	O	P	0
			37	26	10	1	
25	9	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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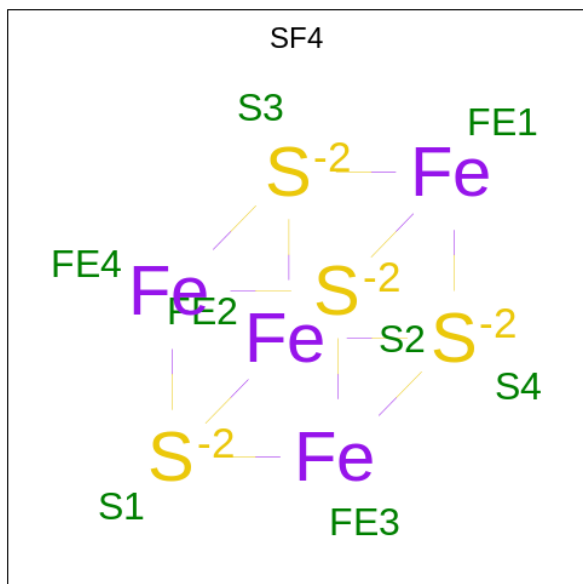
Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	F	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	1	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	4	1	Total C 40 40	0
26	5	1	Total C 40 40	0
26	6	1	Total C 40 40	0
26	7	1	Total C 40 40	0
26	7	1	Total C 40 40	0

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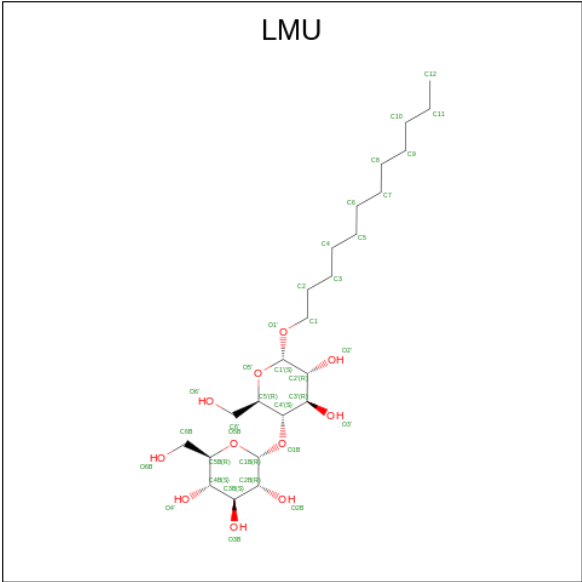
Mol	Chain	Residues	Atoms		AltConf
26	8	1	Total	C	0
			40	40	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



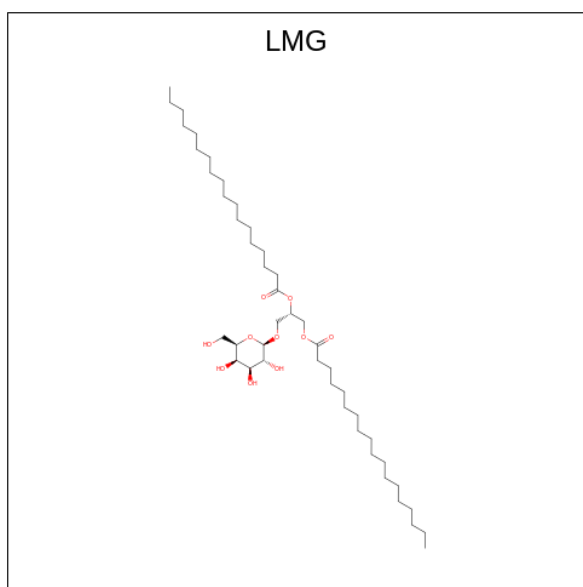
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 28 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



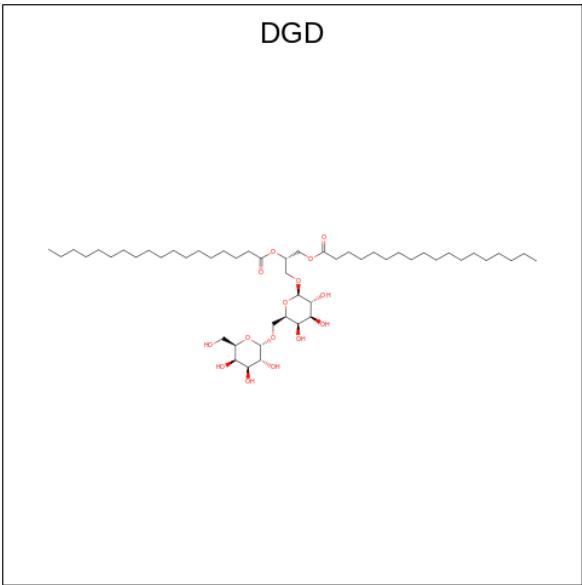
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	
28	A	1	Total	C	O	0
			34	24	10	
28	A	1	Total	C	O	0
			34	24	10	
28	K	1	Total	C	O	0
			35	24	11	
28	5	1	Total	C	O	0
			33	22	11	
28	8	1	Total	C	O	0
			35	24	11	
28	8	1	Total	C	O	0
			35	24	11	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



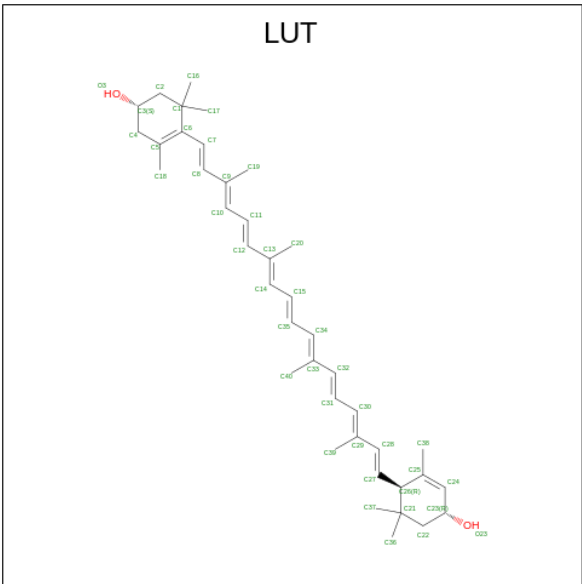
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			40	30	10	
29	J	1	Total	C	O	0
			40	30	10	
29	4	1	Total	C	O	0
			40	30	10	
29	4	1	Total	C	O	0
			40	30	10	
29	5	1	Total	C	O	0
			40	30	10	
29	5	1	Total	C	O	0
			40	30	10	
29	7	1	Total	C	O	0
			44	34	10	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			62	47	15	
30	J	1	Total	C	O	0
			58	43	15	

- Molecule 31 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



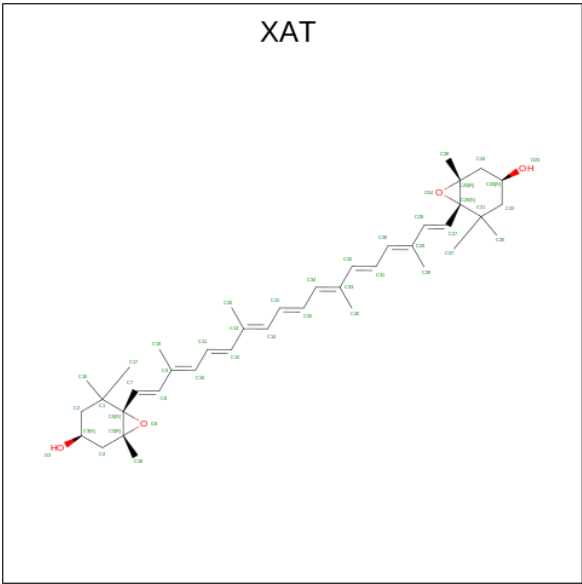
Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	2	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	

- Molecule 32 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



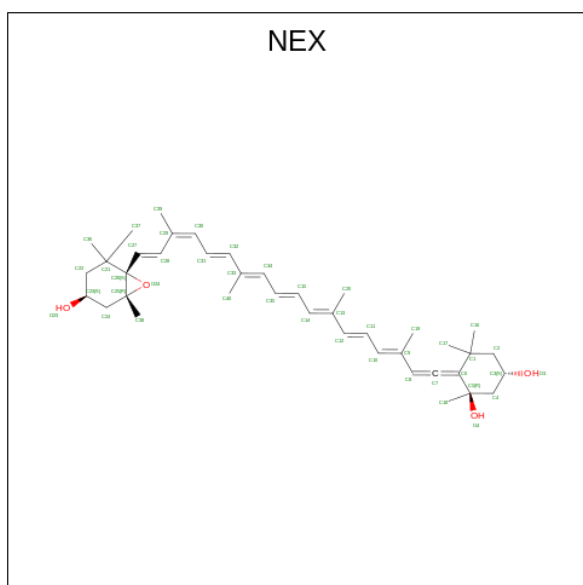
Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			44	40	4	
32	a	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
32	3	1	Total	C	O	0
			44	40	4	
32	4	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	6	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	
32	8	1	Total	C	O	0
			44	40	4	
32	2	1	Total	C	O	0
			44	40	4	
32	9	1	Total	C	O	0
			44	40	4	

- Molecule 33 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).

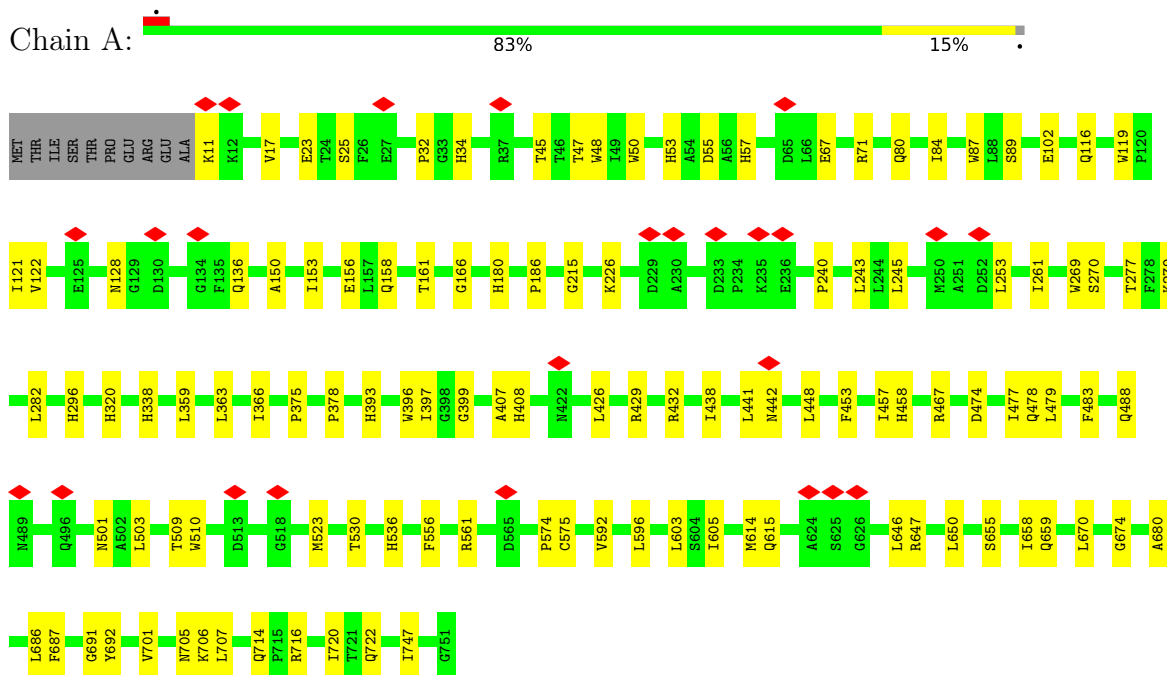


Mol	Chain	Residues	Atoms			AltConf
33	5	1	Total	C	O	0
			44	40	4	
33	6	1	Total	C	O	0
			44	40	4	

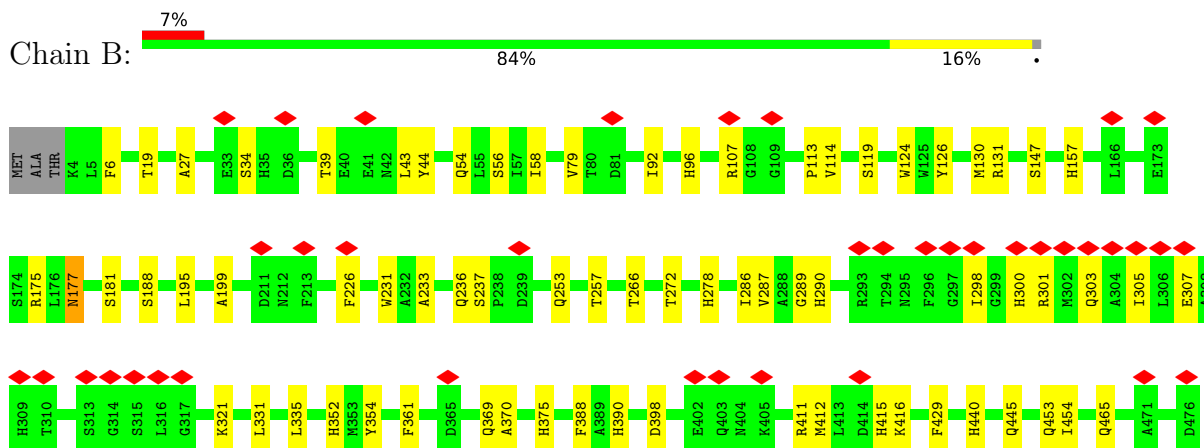
3 Residue-property plots

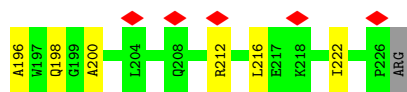
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: PsaA

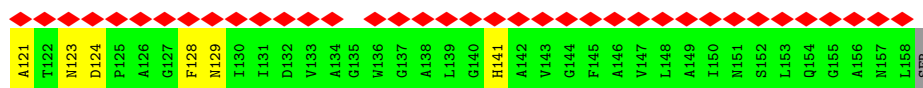
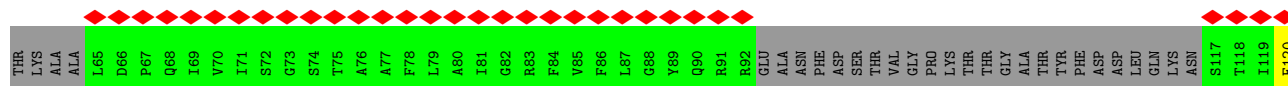
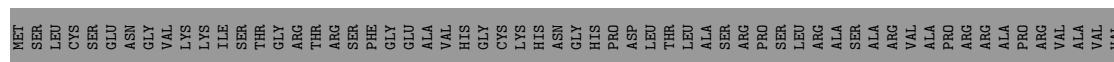
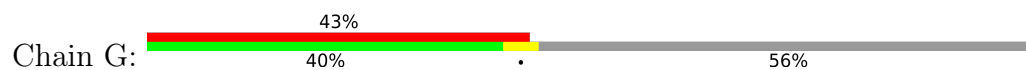


• Molecule 2: PsaB

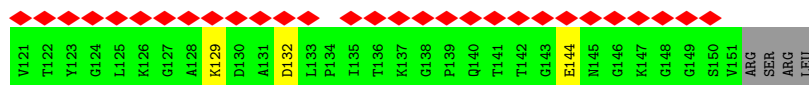
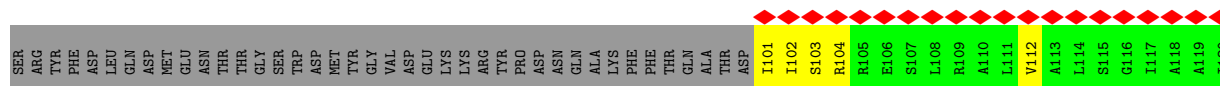




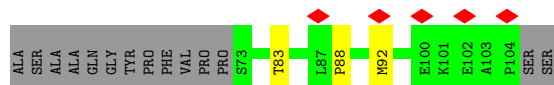
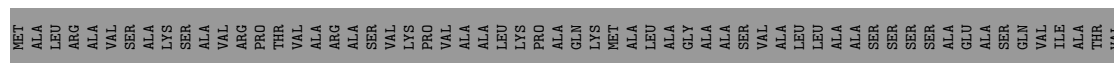
• Molecule 7: PsaG



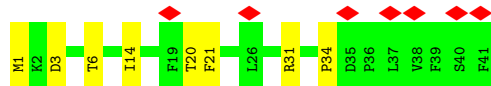
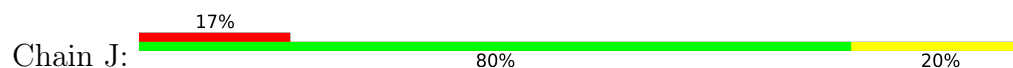
• Molecule 8: PsaH



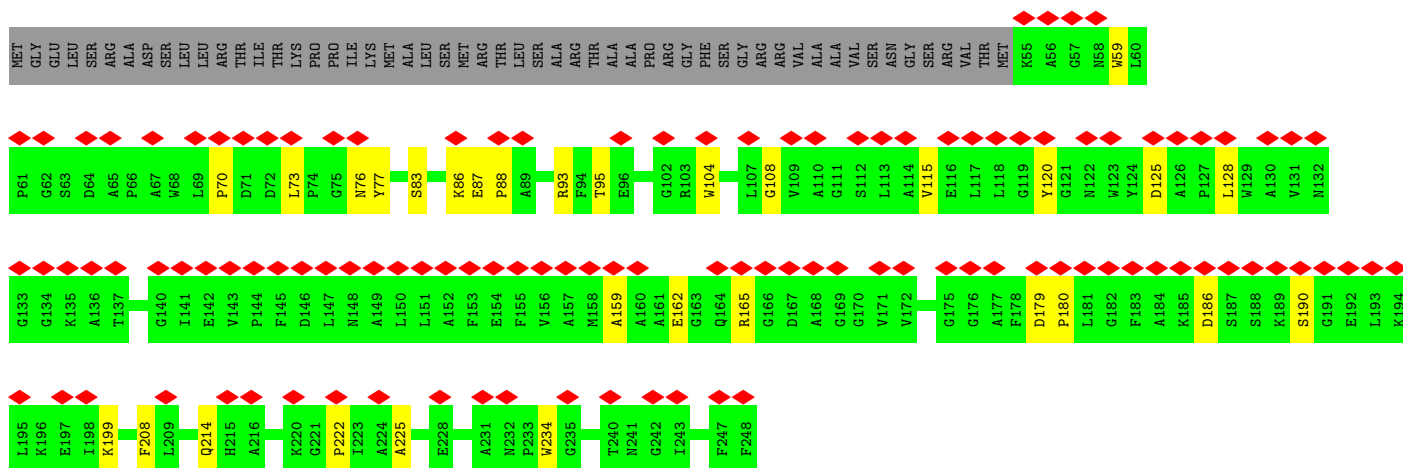
• Molecule 9: PsaI



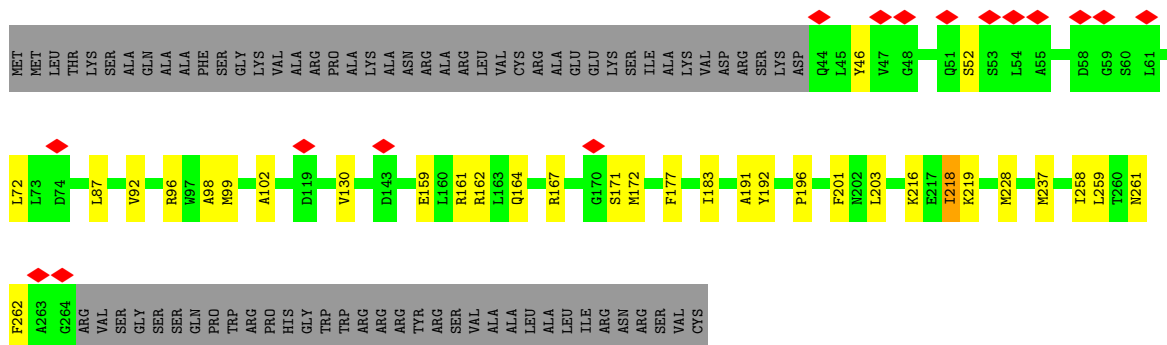
• Molecule 10: PsaJ



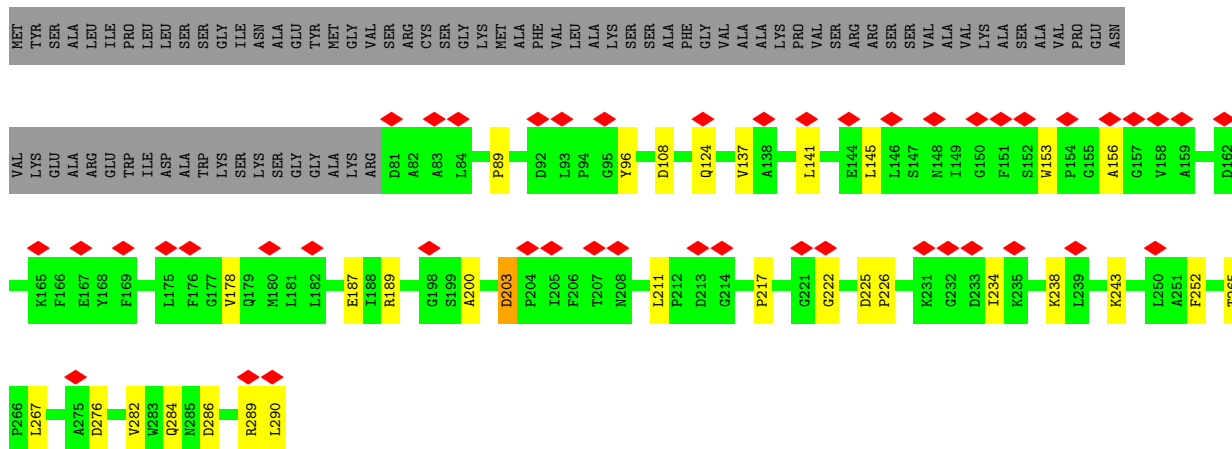
• Molecule 11: PsaK



• Molecule 14: Lhca3

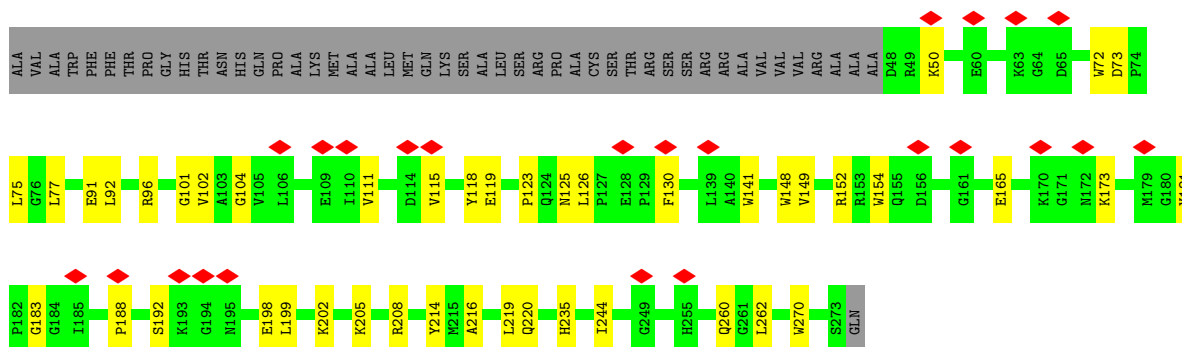


• Molecule 15: Lhca4

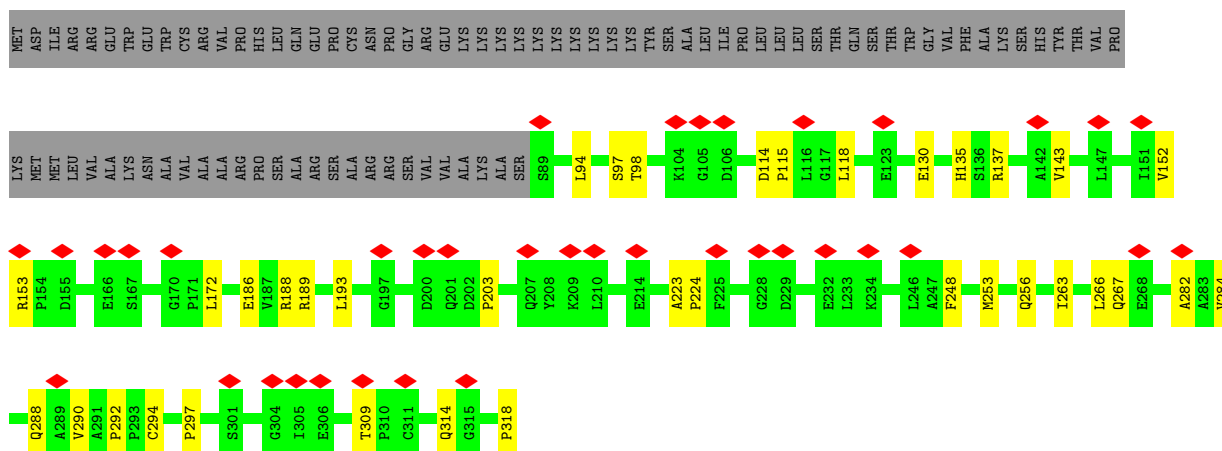


• Molecule 16: Lhca5

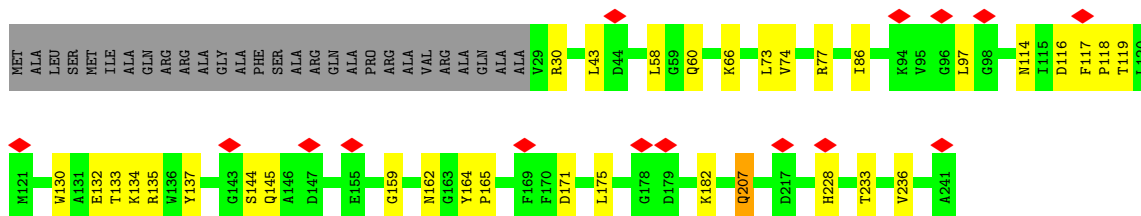
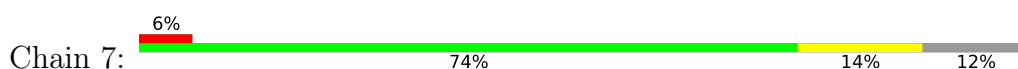




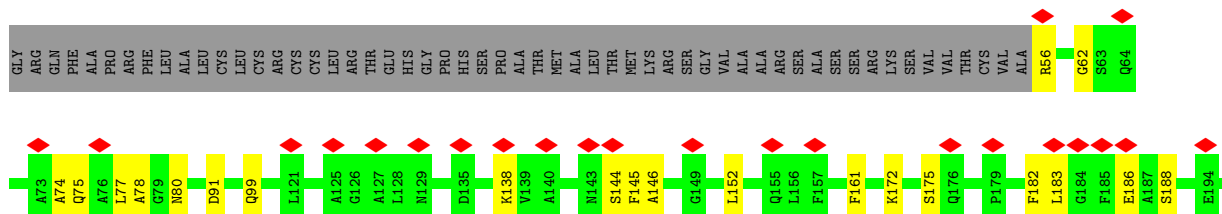
• Molecule 17: Lhca6

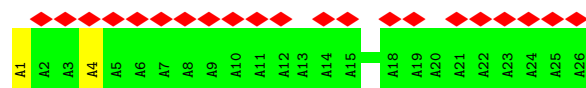


• Molecule 18: Lhca7



• Molecule 19: Lhca8





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.400	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LMU, DGD, SF4, PQN, NEX, CLA, XAT, LUT, LMG, BCR

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	0.47	0/6015	0.54	0/8201
2	B	0.44	0/6024	0.56	2/8225 (0.0%)
3	C	0.43	0/610	0.71	2/826 (0.2%)
4	D	0.36	0/1157	0.62	0/1563
5	E	0.33	0/515	0.52	0/700
6	F	0.34	0/1280	0.54	0/1733
7	G	0.31	0/524	0.69	1/711 (0.1%)
8	H	0.25	0/359	0.56	0/483
9	I	0.37	0/250	0.61	0/345
10	J	0.34	0/349	0.56	0/478
11	K	0.27	0/583	0.64	2/790 (0.3%)
12	L	0.28	0/787	0.54	0/1074
13	1	0.33	0/1478	0.51	0/2012
13	a	0.33	0/1490	0.51	0/2028
14	3	0.43	0/1731	0.65	0/2349
15	4	0.29	0/1686	0.51	0/2300
16	5	0.36	0/1820	0.58	0/2480
17	6	0.32	0/1833	0.56	0/2505
18	7	0.41	0/1701	0.61	1/2310 (0.0%)
19	8	0.38	0/1680	0.62	1/2288 (0.0%)
20	2	0.22	0/1382	0.57	2/1870 (0.1%)
21	9	0.27	0/1337	0.67	0/1814
22	X	0.12	0/129	0.25	0/179
All	All	0.38	0/34720	0.57	11/47264 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	124	ASP	N-CA-C	-7.14	101.75	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	7	236	VAL	N-CA-C	-6.41	106.55	112.96
3	C	62	PHE	CA-C-N	5.63	129.70	121.31
3	C	62	PHE	C-N-CA	5.63	129.70	121.31
19	8	238	GLN	CB-CG-CD	5.44	121.86	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5672	92	0
2	B	5812	0	5569	88	0
3	C	600	0	589	9	0
4	D	1129	0	1144	23	0
5	E	505	0	504	5	0
6	F	1254	0	1288	15	0
7	G	514	0	509	6	0
8	H	357	0	382	6	0
9	I	242	0	252	2	0
10	J	337	0	336	9	0
11	K	578	0	617	8	0
12	L	768	0	776	20	0
13	1	1433	0	1387	23	0
13	a	1444	0	1396	22	0
14	3	1683	0	1641	26	0
15	4	1631	0	1587	26	0
16	5	1765	0	1738	41	0
17	6	1771	0	1770	31	0
18	7	1649	0	1589	29	0
19	8	1630	0	1609	28	0
20	2	1346	0	1330	18	0
21	9	1302	0	1275	30	0
22	X	130	0	132	3	0
23	1	674	0	541	15	0
23	2	350	0	39	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	3	724	0	628	18	0
23	4	782	0	686	24	0
23	5	878	0	758	35	0
23	6	912	0	845	35	0
23	7	760	0	643	19	0
23	8	727	0	635	15	0
23	9	324	0	36	12	0
23	A	2625	0	2614	115	0
23	B	2270	0	2210	80	0
23	F	140	0	113	6	0
23	G	87	0	64	4	0
23	J	42	0	31	2	0
23	K	201	0	171	2	0
23	L	135	0	99	5	0
23	a	709	0	597	12	0
24	A	33	0	46	4	0
24	B	33	0	46	6	0
25	1	49	0	74	6	0
25	2	37	0	44	1	0
25	3	94	0	137	3	0
25	4	49	0	74	6	0
25	5	98	0	148	7	0
25	6	48	0	69	3	0
25	7	37	0	44	2	0
25	8	96	0	141	5	0
25	9	49	0	74	5	0
25	A	79	0	104	3	0
25	B	38	0	46	2	0
25	a	49	0	74	4	0
26	1	40	0	56	2	0
26	3	120	0	168	9	0
26	4	40	0	56	2	0
26	5	40	0	56	3	0
26	6	40	0	56	4	0
26	7	80	0	112	3	0
26	8	40	0	56	3	0
26	A	240	0	336	26	0
26	B	280	0	392	13	0
26	F	40	0	56	4	0
26	G	40	0	56	5	0
26	J	40	0	56	5	0
26	K	80	0	112	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	L	80	0	112	6	0
26	a	40	0	56	4	0
27	A	8	0	0	0	0
27	C	16	0	0	0	0
28	5	33	0	39	3	0
28	8	70	0	92	3	0
28	A	103	0	134	3	0
28	K	35	0	46	0	0
29	4	80	0	100	1	0
29	5	80	0	100	4	0
29	7	44	0	61	1	0
29	A	40	0	50	2	0
29	J	40	0	50	1	0
30	B	62	0	84	5	0
30	J	58	0	77	1	0
31	1	42	0	56	3	0
31	2	42	0	56	3	0
31	3	42	0	56	1	0
31	4	42	0	56	5	0
31	5	42	0	56	5	0
31	6	42	0	56	4	0
31	7	42	0	56	5	0
31	8	42	0	56	6	0
31	9	42	0	56	1	0
31	a	42	0	56	5	0
32	1	44	0	56	4	0
32	2	44	0	56	3	0
32	3	44	0	56	3	0
32	4	44	0	56	3	0
32	5	44	0	56	9	0
32	6	44	0	56	1	0
32	7	44	0	56	1	0
32	8	44	0	56	1	0
32	9	44	0	56	3	0
32	a	44	0	56	3	0
33	5	44	0	56	3	0
33	6	44	0	56	4	0
All	All	49685	0	48724	835	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 835 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)
21:9:182:GLN:CB	21:9:183:PRO:HD2	1.85	1.05
1:A:11:LYS:N	14:3:52:SER:HG	1.56	1.02
12:L:223:LEU:HD12	12:L:223:LEU:O	1.78	0.82
23:9:611:CLA:NB	25:9:622:LHG:O4	2.20	0.75
23:A:830:CLA:H2	26:A:849:BCR:HC7	1.68	0.74

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	708 (96%)	31 (4%)	0	100	100
2	B	729/735 (99%)	694 (95%)	35 (5%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	D	142/247 (58%)	131 (92%)	11 (8%)	0	100	100
5	E	62/143 (43%)	56 (90%)	6 (10%)	0	100	100
6	F	162/227 (71%)	149 (92%)	13 (8%)	0	100	100
7	G	66/159 (42%)	59 (89%)	7 (11%)	0	100	100
8	H	49/155 (32%)	41 (84%)	8 (16%)	0	100	100
9	I	30/106 (28%)	28 (93%)	2 (7%)	0	100	100
10	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
11	K	83/160 (52%)	74 (89%)	9 (11%)	0	100	100
12	L	102/258 (40%)	94 (92%)	8 (8%)	0	100	100
13	1	191/248 (77%)	177 (93%)	14 (7%)	0	100	100
13	a	192/248 (77%)	177 (92%)	15 (8%)	0	100	100
14	3	219/298 (74%)	199 (91%)	20 (9%)	0	100	100
15	4	208/290 (72%)	195 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	5	224/274 (82%)	198 (88%)	26 (12%)	0	100	100
17	6	228/318 (72%)	209 (92%)	19 (8%)	0	100	100
18	7	211/241 (88%)	192 (91%)	19 (9%)	0	100	100
19	8	213/272 (78%)	198 (93%)	15 (7%)	0	100	100
20	2	171/227 (75%)	145 (85%)	26 (15%)	0	100	100
21	9	168/213 (79%)	143 (85%)	23 (14%)	2 (1%)	10	37
22	X	24/26 (92%)	23 (96%)	1 (4%)	0	100	100
All	All	4330/5718 (76%)	3999 (92%)	329 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	9	184	ILE
21	9	183	PRO

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	601/610 (98%)	601 (100%)	0	100	100
2	B	595/597 (100%)	593 (100%)	2 (0%)	86	86
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/197 (61%)	120 (100%)	0	100	100
5	E	55/123 (45%)	55 (100%)	0	100	100
6	F	126/169 (75%)	125 (99%)	1 (1%)	73	79
7	G	50/121 (41%)	50 (100%)	0	100	100
8	H	36/126 (29%)	36 (100%)	0	100	100
9	I	26/76 (34%)	26 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/123 (48%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	75/198 (38%)	74 (99%)	1 (1%)	61	74
13	1	136/180 (76%)	136 (100%)	0	100	100
13	a	137/180 (76%)	137 (100%)	0	100	100
14	3	167/230 (73%)	166 (99%)	1 (1%)	78	81
15	4	165/226 (73%)	164 (99%)	1 (1%)	78	81
16	5	183/219 (84%)	182 (100%)	1 (0%)	81	83
17	6	184/260 (71%)	184 (100%)	0	100	100
18	7	164/181 (91%)	162 (99%)	2 (1%)	63	75
19	8	161/207 (78%)	160 (99%)	1 (1%)	78	81
20	2	134/183 (73%)	133 (99%)	1 (1%)	76	80
21	9	127/159 (80%)	124 (98%)	3 (2%)	43	65
All	All	3407/4472 (76%)	3393 (100%)	14 (0%)	81	84

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	7	86	ILE
18	7	207	GLN
21	9	184	ILE
21	9	131	LYS
21	9	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	154	GLN
16	5	260	GLN
13	1	214	GLN
15	4	284	GLN
17	6	240	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

333 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	$\# Z > 2$
23	CLA	A	813	1	58,62,73	1.35	11 (18%)	69,99,113	1.49	8 (11%)
25	LHG	5	625	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
32	XAT	1	618	-	39,47,47	0.93	2 (5%)	54,74,74	2.58	18 (33%)
26	BCR	J	102	-	41,41,41	0.84	1 (2%)	56,56,56	2.15	16 (28%)
33	NEX	6	624	-	38,46,46	1.01	2 (5%)	50,70,70	2.27	17 (34%)
23	CLA	4	610	15	65,69,73	1.27	10 (15%)	78,108,113	1.33	6 (7%)
23	CLA	7	608	-	54,58,73	1.40	11 (20%)	65,95,113	1.44	7 (10%)
23	CLA	B	840	2	69,73,73	1.25	10 (14%)	83,113,113	1.36	6 (7%)
25	LHG	8	622	23	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
23	CLA	7	610	18	69,73,73	1.22	11 (15%)	83,113,113	1.35	7 (8%)
26	BCR	B	847	-	41,41,41	0.89	1 (2%)	56,56,56	2.01	19 (33%)
23	CLA	5	618	16	43,48,73	1.61	9 (20%)	54,83,113	1.60	10 (18%)
23	CLA	9	604	-	28,35,73	1.90	8 (28%)	32,60,113	1.72	6 (18%)
23	CLA	8	611	25	46,50,73	1.49	11 (23%)	55,85,113	1.53	8 (14%)
31	LUT	a	617	-	42,43,43	0.79	0	51,60,60	1.56	12 (23%)
23	CLA	3	610	14	69,73,73	1.22	10 (14%)	83,113,113	1.44	10 (12%)
23	CLA	B	839	-	69,73,73	1.25	10 (14%)	83,113,113	1.40	10 (12%)
23	CLA	8	616	19	47,51,73	1.60	8 (17%)	60,87,113	1.71	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	829	1	69,73,73	1.23	11 (15%)	83,113,113	1.40	9 (10%)
23	CLA	8	603	19	48,52,73	1.59	11 (22%)	61,88,113	1.55	11 (18%)
23	CLA	6	611	25	46,50,73	1.47	10 (21%)	55,85,113	1.45	5 (9%)
23	CLA	6	616	17	69,73,73	1.25	10 (14%)	83,113,113	1.52	15 (18%)
25	LHG	2	622	23	36,36,48	0.78	1 (2%)	39,42,54	1.29	5 (12%)
23	CLA	A	836	1	69,73,73	1.24	11 (15%)	83,113,113	1.42	7 (8%)
23	CLA	1	616	13	47,51,73	1.58	11 (23%)	60,87,113	1.48	7 (11%)
23	CLA	B	821	2	47,51,73	1.59	10 (21%)	55,86,113	1.64	7 (12%)
23	CLA	2	604	-	28,35,73	1.90	7 (25%)	32,60,113	1.75	6 (18%)
23	CLA	6	603	17	58,62,73	1.45	11 (18%)	73,100,113	1.44	7 (9%)
23	CLA	A	854	-	69,73,73	1.26	12 (17%)	83,113,113	1.38	12 (14%)
23	CLA	4	614	15	60,64,73	1.35	9 (15%)	72,102,113	1.34	7 (9%)
23	CLA	B	830	2	47,51,73	1.48	10 (21%)	56,86,113	1.60	6 (10%)
26	BCR	B	846	-	41,41,41	0.88	2 (4%)	56,56,56	2.17	25 (44%)
29	LMG	J	104	-	40,40,55	0.89	2 (5%)	48,48,63	1.26	5 (10%)
23	CLA	A	833	1	49,53,73	1.46	11 (22%)	59,89,113	1.56	8 (13%)
32	XAT	a	618	-	39,47,47	0.94	2 (5%)	54,74,74	2.57	18 (33%)
23	CLA	B	818	2	64,68,73	1.29	10 (15%)	77,107,113	1.48	9 (11%)
23	CLA	a	609	13	67,72,73	1.24	8 (11%)	80,112,113	1.30	6 (7%)
23	CLA	9	611	25	28,35,73	1.93	8 (28%)	32,60,113	1.72	7 (21%)
31	LUT	8	619	-	42,43,43	0.87	1 (2%)	51,60,60	1.82	14 (27%)
23	CLA	B	810	2	68,72,73	1.26	10 (14%)	81,111,113	1.33	6 (7%)
23	CLA	B	812	2	47,51,73	1.47	9 (19%)	56,86,113	1.55	5 (8%)
23	CLA	B	825	-	66,70,73	1.29	10 (15%)	79,109,113	1.35	10 (12%)
23	CLA	3	614	14	43,48,73	1.54	9 (20%)	51,83,113	1.52	8 (15%)
23	CLA	8	608	-	55,59,73	1.38	10 (18%)	66,96,113	1.51	6 (9%)
23	CLA	8	607	-	45,49,73	1.57	12 (26%)	57,84,113	1.59	7 (12%)
23	CLA	6	609	17	49,53,73	1.46	10 (20%)	59,89,113	1.56	9 (15%)
23	CLA	8	612	19	44,49,73	1.50	11 (25%)	52,84,113	1.61	10 (19%)
26	BCR	B	848	-	41,41,41	0.87	0	56,56,56	1.79	12 (21%)
23	CLA	B	816	2	58,62,73	1.32	10 (17%)	69,99,113	1.50	6 (8%)
23	CLA	B	815	2	47,51,73	1.47	10 (21%)	56,86,113	1.57	5 (8%)
23	CLA	7	606	-	45,49,73	1.54	11 (24%)	54,84,113	1.54	10 (18%)
23	CLA	6	612	17	44,49,73	1.53	9 (20%)	52,84,113	1.57	7 (13%)
23	CLA	B	819	-	59,63,73	1.37	9 (15%)	71,101,113	1.42	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	4	606	-	43,48,73	1.56	10 (23%)	51,83,113	1.52	8 (15%)
23	CLA	A	828	1	69,73,73	1.27	11 (15%)	83,113,113	1.34	6 (7%)
23	CLA	9	614	21	28,35,73	1.91	8 (28%)	32,60,113	1.75	6 (18%)
23	CLA	6	601	17	69,73,73	1.25	11 (15%)	83,113,113	1.40	11 (13%)
23	CLA	5	619	-	47,51,73	1.58	12 (25%)	60,87,113	1.84	13 (21%)
23	CLA	5	609	16	69,73,73	1.25	11 (15%)	83,113,113	1.30	10 (12%)
23	CLA	B	832	2	64,68,73	1.28	11 (17%)	77,107,113	1.44	11 (14%)
26	BCR	3	620	-	41,41,41	0.83	0	56,56,56	2.17	20 (35%)
32	XAT	9	620	-	39,47,47	0.92	0	54,74,74	2.63	16 (29%)
23	CLA	A	845	25	54,58,73	1.39	11 (20%)	65,95,113	1.53	5 (7%)
23	CLA	3	617	14	43,48,73	1.54	12 (27%)	51,83,113	1.62	7 (13%)
26	BCR	A	852	-	41,41,41	0.73	0	56,56,56	1.90	12 (21%)
23	CLA	L	304	-	49,53,73	1.47	7 (14%)	59,89,113	1.50	7 (11%)
31	LUT	9	619	-	42,43,43	0.76	0	51,60,60	1.67	11 (21%)
23	CLA	K	204	11	50,54,73	1.48	9 (18%)	60,90,113	1.46	7 (11%)
23	CLA	3	606	-	57,62,73	1.37	9 (15%)	68,100,113	1.38	6 (8%)
23	CLA	2	614	20	28,35,73	1.92	8 (28%)	32,60,113	1.69	6 (18%)
23	CLA	9	610	21	28,35,73	1.91	9 (32%)	32,60,113	1.60	5 (15%)
25	LHG	3	623	-	44,44,48	0.66	2 (4%)	47,50,54	1.26	6 (12%)
31	LUT	5	620	-	42,43,43	0.80	0	51,60,60	1.70	13 (25%)
23	CLA	9	612	21	28,35,73	1.94	8 (28%)	32,60,113	1.61	4 (12%)
26	BCR	F	305	-	41,41,41	0.83	1 (2%)	56,56,56	2.26	23 (41%)
23	CLA	B	837	2	69,73,73	1.27	11 (15%)	83,113,113	1.37	6 (7%)
23	CLA	B	808	2	69,73,73	1.25	11 (15%)	83,113,113	1.56	9 (10%)
23	CLA	G	204	7	49,53,73	1.51	8 (16%)	59,89,113	1.61	11 (18%)
23	CLA	K	206	11	49,53,73	1.46	9 (18%)	59,89,113	1.52	6 (10%)
23	CLA	4	616	15	47,51,73	1.57	12 (25%)	60,87,113	1.53	7 (11%)
23	CLA	7	616	18	47,51,73	1.56	10 (21%)	60,87,113	1.57	10 (16%)
23	CLA	A	823	1	46,50,73	1.48	9 (19%)	55,85,113	1.70	7 (12%)
30	DGD	B	850	-	63,63,67	1.06	5 (7%)	77,77,81	1.55	10 (12%)
23	CLA	8	613	19	69,73,73	1.24	10 (14%)	83,113,113	1.53	8 (9%)
23	CLA	A	809	1	69,73,73	1.25	12 (17%)	83,113,113	1.38	8 (9%)
23	CLA	A	826	-	68,72,73	1.27	11 (16%)	81,111,113	1.41	11 (13%)
23	CLA	B	836	2	54,58,73	1.44	11 (20%)	65,95,113	1.54	12 (18%)
23	CLA	F	304	-	45,49,73	1.50	9 (20%)	54,84,113	1.56	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	K	203	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
28	LMU	5	628	-	34,34,36	1.24	3 (8%)	45,45,47	1.50	8 (17%)
23	CLA	G	203	7	46,50,73	1.50	7 (15%)	55,85,113	1.56	4 (7%)
23	CLA	6	606	-	43,48,73	1.56	10 (23%)	51,83,113	1.55	9 (17%)
23	CLA	A	843	-	68,72,73	1.29	11 (16%)	81,111,113	1.40	7 (8%)
23	CLA	B	834	2	64,68,73	1.29	9 (14%)	77,107,113	1.34	6 (7%)
30	DGD	J	103	-	59,59,67	0.99	3 (5%)	73,73,81	1.48	8 (10%)
23	CLA	a	611	25	41,46,73	1.60	11 (26%)	52,81,113	1.63	9 (17%)
23	CLA	B	824	-	69,73,73	1.26	11 (15%)	83,113,113	1.47	12 (14%)
23	CLA	A	815	1	54,58,73	1.40	9 (16%)	65,95,113	1.53	12 (18%)
23	CLA	3	615	-	43,48,73	1.52	9 (20%)	51,83,113	1.56	6 (11%)
23	CLA	6	620	-	68,72,73	1.24	11 (16%)	81,111,113	1.37	8 (9%)
26	BCR	G	205	-	41,41,41	0.75	0	56,56,56	2.06	21 (37%)
26	BCR	A	849	-	41,41,41	0.89	1 (2%)	56,56,56	2.03	17 (30%)
23	CLA	6	610	17	69,73,73	1.22	9 (13%)	83,113,113	1.33	10 (12%)
23	CLA	5	610	16	58,62,73	1.37	11 (18%)	69,99,113	1.44	10 (14%)
26	BCR	A	856	-	41,41,41	0.70	0	56,56,56	1.99	19 (33%)
24	PQN	B	842	-	34,34,34	2.91	11 (32%)	42,45,45	2.04	5 (11%)
23	CLA	L	302	12	49,53,73	1.47	6 (12%)	59,89,113	1.49	5 (8%)
23	CLA	6	602	17	69,73,73	1.25	9 (13%)	83,113,113	1.37	5 (6%)
23	CLA	A	802	2	69,73,73	1.27	11 (15%)	83,113,113	1.57	11 (13%)
26	BCR	8	621	-	41,41,41	0.74	0	56,56,56	1.98	18 (32%)
25	LHG	4	622	23	48,48,48	0.60	0	51,54,54	1.29	6 (11%)
23	CLA	1	602	13	65,69,73	1.27	10 (15%)	78,108,113	1.39	7 (8%)
23	CLA	2	602	20	28,35,73	1.91	8 (28%)	32,60,113	1.64	3 (9%)
26	BCR	B	844	-	41,41,41	0.79	1 (2%)	56,56,56	1.95	15 (26%)
26	BCR	B	843	-	41,41,41	0.79	0	56,56,56	1.92	14 (25%)
23	CLA	A	805	1	56,60,73	1.40	11 (19%)	67,97,113	1.51	8 (11%)
23	CLA	A	842	1	69,73,73	1.24	10 (14%)	83,113,113	1.36	7 (8%)
23	CLA	3	602	14	64,68,73	1.28	10 (15%)	77,107,113	1.39	7 (9%)
29	LMG	A	860	-	40,40,55	0.95	3 (7%)	48,48,63	1.32	5 (10%)
23	CLA	6	618	17	43,48,73	1.62	12 (27%)	54,83,113	1.65	9 (16%)
23	CLA	4	602	15	64,68,73	1.29	10 (15%)	77,107,113	1.45	9 (11%)
23	CLA	7	609	18	47,52,73	1.43	9 (19%)	55,87,113	1.67	8 (14%)
23	CLA	a	603	13	46,50,73	1.49	11 (23%)	55,85,113	1.68	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	1	609	13	44,48,73	1.56	9 (20%)	56,83,113	1.66	11 (19%)
23	CLA	A	817	-	49,53,73	1.49	11 (22%)	59,89,113	1.60	8 (13%)
32	XAT	6	621	-	39,47,47	0.93	2 (5%)	54,74,74	2.61	20 (37%)
27	SF4	C	102	-	0,12,12	-	-	-		
23	CLA	8	602	19	64,68,73	1.31	10 (15%)	77,107,113	1.45	11 (14%)
23	CLA	2	601	20	28,35,73	1.89	8 (28%)	32,60,113	1.72	7 (21%)
23	CLA	A	808	1	54,58,73	1.40	10 (18%)	65,95,113	1.53	11 (16%)
23	CLA	A	827	-	63,67,73	1.36	10 (15%)	75,105,113	1.44	11 (14%)
26	BCR	L	305	-	41,41,41	0.80	0	56,56,56	1.88	14 (25%)
28	LMU	8	625	-	36,36,36	1.16	2 (5%)	47,47,47	1.41	7 (14%)
23	CLA	a	612	13	49,53,73	1.46	10 (20%)	59,89,113	1.49	8 (13%)
23	CLA	2	603	20	28,35,73	1.92	8 (28%)	32,60,113	1.73	6 (18%)
23	CLA	5	614	16	48,52,73	1.49	10 (20%)	55,87,113	1.46	5 (9%)
23	CLA	B	814	2	68,72,73	1.24	10 (14%)	81,111,113	1.38	8 (9%)
23	CLA	B	838	2	51,55,73	1.39	10 (19%)	61,91,113	1.63	6 (9%)
26	BCR	a	619	-	41,41,41	0.69	0	56,56,56	2.01	16 (28%)
23	CLA	1	611	25	69,73,73	1.20	10 (14%)	83,113,113	1.30	6 (7%)
32	XAT	2	620	-	39,47,47	0.89	0	54,74,74	2.65	14 (25%)
23	CLA	a	616	13	49,53,73	1.48	10 (20%)	59,89,113	1.41	5 (8%)
23	CLA	8	609	19	49,53,73	1.43	10 (20%)	59,89,113	1.51	8 (13%)
23	CLA	8	610	19	64,68,73	1.25	10 (15%)	77,107,113	1.35	8 (10%)
23	CLA	A	814	1	69,73,73	1.27	11 (15%)	83,113,113	1.46	10 (12%)
23	CLA	2	609	20	28,35,73	1.92	7 (25%)	32,60,113	1.70	6 (18%)
23	CLA	A	840	1	56,60,73	1.39	10 (17%)	67,97,113	1.53	11 (16%)
23	CLA	1	603	13	56,61,73	1.38	11 (19%)	66,98,113	1.54	6 (9%)
23	CLA	B	829	2	69,73,73	1.34	10 (14%)	83,113,113	1.57	11 (13%)
23	CLA	B	813	2	69,73,73	1.26	12 (17%)	83,113,113	1.35	8 (9%)
23	CLA	B	823	2	49,53,73	1.48	10 (20%)	59,89,113	1.54	8 (13%)
29	LMG	7	624	-	44,44,55	0.83	1 (2%)	52,52,63	1.26	6 (11%)
23	CLA	5	608	-	54,58,73	1.42	13 (24%)	65,95,113	1.44	7 (10%)
23	CLA	A	820	1	69,73,73	1.31	11 (15%)	83,113,113	1.54	16 (19%)
23	CLA	B	809	2	69,73,73	1.25	11 (15%)	83,113,113	1.44	9 (10%)
26	BCR	5	622	-	41,41,41	0.71	0	56,56,56	2.17	19 (33%)
23	CLA	5	606	-	43,48,73	1.55	10 (23%)	51,83,113	1.51	6 (11%)
25	LHG	A	847	23	29,29,48	0.95	1 (3%)	32,35,54	1.37	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	834	1	69,73,73	1.23	11 (15%)	83,113,113	1.40	6 (7%)
23	CLA	6	617	17	49,53,73	1.46	10 (20%)	59,89,113	1.37	6 (10%)
31	LUT	3	618	-	42,43,43	0.88	0	51,60,60	1.73	13 (25%)
23	CLA	5	617	16	54,58,73	1.42	11 (20%)	65,95,113	1.48	6 (9%)
23	CLA	2	612	20	28,35,73	1.93	7 (25%)	32,60,113	1.65	4 (12%)
25	LHG	6	623	23	47,47,48	0.64	1 (2%)	50,53,54	1.24	5 (10%)
28	LMU	A	857	-	36,36,36	1.20	3 (8%)	47,47,47	1.33	4 (8%)
23	CLA	A	818	1	64,68,73	1.28	11 (17%)	77,107,113	1.44	8 (10%)
28	LMU	A	858	-	34,35,36	1.29	2 (5%)	42,45,47	1.28	6 (14%)
23	CLA	3	608	-	59,63,73	1.42	11 (18%)	71,101,113	1.52	10 (14%)
23	CLA	2	616	-	28,35,73	1.89	8 (28%)	32,60,113	1.74	8 (25%)
23	CLA	7	613	18	69,73,73	1.25	9 (13%)	83,113,113	1.35	7 (8%)
31	LUT	4	619	-	42,43,43	0.82	0	51,60,60	1.70	11 (21%)
23	CLA	7	607	-	46,50,73	1.48	12 (26%)	55,85,113	1.66	10 (18%)
23	CLA	a	606	13	47,52,73	1.48	9 (19%)	55,87,113	1.46	5 (9%)
23	CLA	7	612	18	48,52,73	1.54	11 (22%)	58,88,113	1.50	8 (13%)
23	CLA	A	841	1	69,73,73	1.23	10 (14%)	83,113,113	1.46	8 (9%)
23	CLA	1	613	-	69,73,73	1.24	9 (13%)	83,113,113	1.43	7 (8%)
23	CLA	1	607	-	43,48,73	1.54	8 (18%)	51,83,113	1.55	5 (9%)
23	CLA	1	612	13	49,53,73	1.47	10 (20%)	59,89,113	1.49	8 (13%)
23	CLA	6	607	-	45,49,73	1.57	12 (26%)	57,84,113	1.69	11 (19%)
23	CLA	4	607	-	49,53,73	1.48	10 (20%)	59,89,113	1.48	4 (6%)
31	LUT	2	619	-	42,43,43	0.75	0	51,60,60	1.77	13 (25%)
23	CLA	B	802	2	69,73,73	1.25	10 (14%)	83,113,113	1.29	7 (8%)
26	BCR	4	621	-	41,41,41	0.73	0	56,56,56	2.10	22 (39%)
23	CLA	K	201	11	49,53,73	1.48	8 (16%)	59,89,113	1.65	9 (15%)
23	CLA	3	609	14	64,68,73	1.29	9 (14%)	77,107,113	1.44	9 (11%)
23	CLA	6	613	-	67,72,73	1.25	11 (16%)	80,112,113	1.35	8 (10%)
26	BCR	B	801	-	41,41,41	0.77	0	56,56,56	2.05	13 (23%)
25	LHG	5	623	23	48,48,48	0.62	1 (2%)	51,54,54	1.21	5 (9%)
23	CLA	B	831	2	69,73,73	1.21	8 (11%)	83,113,113	1.44	5 (6%)
23	CLA	5	611	25	46,50,73	1.48	9 (19%)	55,85,113	1.48	6 (10%)
23	CLA	a	602	13	65,69,73	1.28	10 (15%)	78,108,113	1.39	7 (8%)
23	CLA	7	602	18	69,73,73	1.27	11 (15%)	83,113,113	1.31	7 (8%)
23	CLA	7	611	25	63,67,73	1.27	10 (15%)	75,105,113	1.40	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	601	13	57,62,73	1.38	10 (17%)	68,100,113	1.36	6 (8%)
23	CLA	a	613	-	69,73,73	1.24	10 (14%)	83,113,113	1.43	7 (8%)
23	CLA	a	607	-	49,53,73	1.47	8 (16%)	59,89,113	1.50	5 (8%)
23	CLA	A	812	1	69,73,73	1.25	11 (15%)	83,113,113	1.41	9 (10%)
23	CLA	A	822	-	69,73,73	1.25	11 (15%)	83,113,113	1.39	9 (10%)
26	BCR	B	845	-	41,41,41	0.84	0	56,56,56	2.06	19 (33%)
28	LMU	8	624	-	36,36,36	1.19	2 (5%)	47,47,47	0.93	1 (2%)
26	BCR	L	301	-	41,41,41	0.84	0	56,56,56	1.78	16 (28%)
28	LMU	A	859	-	35,35,36	1.33	3 (8%)	43,45,47	1.27	6 (13%)
23	CLA	3	607	14	60,64,73	1.37	12 (20%)	75,102,113	1.44	10 (13%)
23	CLA	1	604	-	53,57,73	1.40	9 (16%)	62,93,113	1.54	4 (6%)
23	CLA	7	603	18	47,52,73	1.53	11 (23%)	56,88,113	1.52	7 (12%)
23	CLA	A	825	1	69,73,73	1.25	11 (15%)	83,113,113	1.37	9 (10%)
26	BCR	3	621	-	41,41,41	0.72	0	56,56,56	2.28	19 (33%)
23	CLA	B	817	2	63,67,73	1.32	10 (15%)	75,105,113	1.48	9 (12%)
23	CLA	2	607	-	28,35,73	1.92	8 (28%)	32,60,113	1.72	6 (18%)
23	CLA	8	601	19	69,73,73	1.26	11 (15%)	83,113,113	1.42	11 (13%)
28	LMU	K	208	-	36,36,36	1.19	3 (8%)	47,47,47	1.30	5 (10%)
32	XAT	4	620	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	20 (37%)
32	XAT	7	620	-	39,47,47	1.04	2 (5%)	54,74,74	2.59	18 (33%)
23	CLA	A	801	1	69,73,73	1.28	11 (15%)	83,113,113	1.37	6 (7%)
23	CLA	B	827	2	66,70,73	1.29	11 (16%)	79,109,113	1.36	8 (10%)
23	CLA	a	604	-	53,57,73	1.40	9 (16%)	62,93,113	1.53	5 (8%)
23	CLA	A	832	1	54,58,73	1.41	11 (20%)	65,95,113	1.53	7 (10%)
23	CLA	9	601	21	28,35,73	1.89	8 (28%)	32,60,113	1.67	5 (15%)
23	CLA	1	601	13	57,62,73	1.37	10 (17%)	68,100,113	1.36	6 (8%)
26	BCR	1	619	-	41,41,41	0.68	0	56,56,56	2.01	16 (28%)
27	SF4	C	101	-	0,12,12	-	-	-	-	-
23	CLA	6	604	-	69,73,73	1.24	11 (15%)	83,113,113	1.33	7 (8%)
23	CLA	a	614	13	58,62,73	1.35	9 (15%)	67,99,113	1.35	5 (7%)
23	CLA	5	603	16	58,62,73	1.46	13 (22%)	73,100,113	1.50	9 (12%)
23	CLA	2	613	20	28,35,73	1.92	8 (28%)	32,60,113	1.64	6 (18%)
25	LHG	A	846	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	6 (11%)
23	CLA	F	303	-	46,50,73	1.53	11 (23%)	55,85,113	1.55	10 (18%)
29	LMG	5	627	-	40,40,55	0.91	2 (5%)	48,48,63	1.20	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	3	622	-	41,41,41	0.79	0	56,56,56	2.67	21 (37%)
29	LMG	4	624	-	40,40,55	1.01	4 (10%)	48,48,63	1.29	6 (12%)
24	PQN	A	844	-	34,34,34	2.89	11 (32%)	42,45,45	2.11	5 (11%)
23	CLA	B	820	2	54,58,73	1.37	8 (14%)	65,95,113	1.46	5 (7%)
23	CLA	4	618	15	43,48,73	1.62	12 (27%)	54,83,113	1.57	9 (16%)
32	XAT	5	621	-	39,47,47	1.02	2 (5%)	54,74,74	2.89	23 (42%)
23	CLA	B	805	2	69,73,73	1.26	10 (14%)	83,113,113	1.49	8 (9%)
23	CLA	5	602	16	69,73,73	1.27	10 (14%)	83,113,113	1.42	10 (12%)
23	CLA	F	301	-	61,65,73	1.32	10 (16%)	73,103,113	1.47	7 (9%)
23	CLA	4	611	25	46,50,73	1.48	9 (19%)	55,85,113	1.49	7 (12%)
23	CLA	B	828	2	69,73,73	1.28	12 (17%)	83,113,113	1.37	11 (13%)
23	CLA	A	807	1	69,73,73	1.31	11 (15%)	83,113,113	1.34	8 (9%)
23	CLA	a	610	13	63,67,73	1.32	10 (15%)	76,106,113	1.32	6 (7%)
23	CLA	B	807	2	56,60,73	1.38	10 (17%)	67,97,113	1.41	6 (8%)
23	CLA	J	101	10	46,50,73	1.47	9 (19%)	55,85,113	1.57	6 (10%)
23	CLA	5	612	16	44,49,73	1.51	11 (25%)	52,84,113	1.58	9 (17%)
31	LUT	7	619	-	42,43,43	0.95	2 (4%)	51,60,60	1.79	16 (31%)
23	CLA	7	614	18	46,50,73	1.47	11 (23%)	55,85,113	1.52	7 (12%)
23	CLA	2	611	25	29,33,73	3.04	10 (34%)	28,56,113	1.09	2 (7%)
23	CLA	1	614	13	40,45,73	1.68	11 (27%)	50,79,113	1.60	7 (14%)
23	CLA	A	819	1	63,67,73	1.36	11 (17%)	75,105,113	1.44	8 (10%)
32	XAT	8	620	-	39,47,47	1.00	2 (5%)	54,74,74	2.70	19 (35%)
23	CLA	8	606	-	68,72,73	1.27	11 (16%)	82,112,113	1.37	9 (10%)
26	BCR	A	850	-	41,41,41	0.82	1 (2%)	56,56,56	2.02	18 (32%)
23	CLA	1	608	-	47,52,73	1.48	7 (14%)	56,88,113	1.51	6 (10%)
33	NEX	5	624	-	38,46,46	0.93	0	50,70,70	2.49	19 (38%)
23	CLA	B	841	25	47,51,73	1.52	10 (21%)	56,86,113	1.57	6 (10%)
26	BCR	7	621	-	41,41,41	0.80	0	56,56,56	2.04	18 (32%)
23	CLA	B	806	2	69,73,73	1.28	12 (17%)	83,113,113	1.30	4 (4%)
23	CLA	3	611	25	41,46,73	1.63	11 (26%)	52,81,113	1.67	9 (17%)
23	CLA	6	614	17	64,68,73	1.29	10 (15%)	77,107,113	1.34	5 (6%)
23	CLA	9	602	21	28,35,73	1.89	8 (28%)	32,60,113	1.70	4 (12%)
23	CLA	A	824	1	45,49,73	1.51	9 (20%)	54,84,113	1.64	8 (14%)
23	CLA	A	816	1	47,52,73	1.49	10 (21%)	55,87,113	1.62	4 (7%)
25	LHG	9	622	23	48,48,48	0.62	0	51,54,54	1.23	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	5	616	16	45,50,73	1.61	11 (24%)	56,85,113	1.51	8 (14%)
23	CLA	7	604	-	58,62,73	1.37	12 (20%)	70,100,113	1.50	11 (15%)
32	XAT	3	619	-	39,47,47	1.02	2 (5%)	54,74,74	2.60	22 (40%)
23	CLA	3	603	14	59,63,73	1.40	12 (20%)	71,101,113	1.58	9 (12%)
23	CLA	4	608	-	69,73,73	1.23	10 (14%)	83,113,113	1.42	9 (10%)
23	CLA	1	610	13	42,47,73	1.56	10 (23%)	51,81,113	1.60	7 (13%)
23	CLA	A	821	1	57,61,73	1.36	11 (19%)	68,98,113	1.48	5 (7%)
23	CLA	B	803	-	69,73,73	1.27	11 (15%)	83,113,113	1.67	14 (16%)
23	CLA	4	604	-	58,62,73	1.42	12 (20%)	73,100,113	1.41	6 (8%)
31	LUT	6	619	-	42,43,43	0.81	0	51,60,60	1.69	13 (25%)
23	CLA	4	603	15	48,52,73	1.57	12 (25%)	61,88,113	1.54	9 (14%)
23	CLA	B	822	2	46,50,73	1.48	8 (17%)	55,85,113	1.48	7 (12%)
23	CLA	A	804	1	69,73,73	1.23	11 (15%)	83,113,113	1.52	9 (10%)
23	CLA	B	826	2	59,63,73	1.37	11 (18%)	71,101,113	1.40	9 (12%)
23	CLA	1	606	13	41,47,73	1.56	9 (21%)	48,80,113	1.60	6 (12%)
23	CLA	2	610	20	28,35,73	1.88	7 (25%)	32,60,113	1.74	6 (18%)
23	CLA	A	839	1	59,63,73	1.37	9 (15%)	71,101,113	1.42	6 (8%)
23	CLA	6	608	-	55,59,73	1.41	10 (18%)	66,96,113	1.52	10 (15%)
26	BCR	K	207	-	41,41,41	0.75	0	56,56,56	1.86	16 (28%)
23	CLA	4	612	15	44,49,73	1.51	9 (20%)	52,84,113	1.56	7 (13%)
27	SF4	A	853	-	0,12,12	-	-	-	-	-
25	LHG	8	623	-	46,46,48	0.66	1 (2%)	49,52,54	1.24	5 (10%)
23	CLA	4	609	15	65,69,73	1.29	7 (10%)	78,108,113	1.41	6 (7%)
23	CLA	B	833	2	69,73,73	1.26	10 (14%)	83,113,113	1.44	9 (10%)
23	CLA	4	601	15	69,73,73	1.24	9 (13%)	83,113,113	1.40	9 (10%)
23	CLA	3	604	-	69,73,73	1.25	11 (15%)	83,113,113	1.33	7 (8%)
23	CLA	5	601	16	60,64,73	1.36	10 (16%)	72,102,113	1.33	8 (11%)
23	CLA	a	608	-	47,52,73	1.48	8 (17%)	56,88,113	1.50	6 (10%)
26	BCR	A	851	-	41,41,41	0.88	2 (4%)	56,56,56	1.97	16 (28%)
29	LMG	5	626	-	40,40,55	0.94	1 (2%)	48,48,63	1.33	5 (10%)
23	CLA	8	614	19	60,64,73	1.33	11 (18%)	72,102,113	1.40	10 (13%)
23	CLA	9	609	21	28,35,73	1.89	7 (25%)	32,60,113	1.71	4 (12%)
23	CLA	A	831	1	69,73,73	1.37	11 (15%)	83,113,113	1.60	15 (18%)
23	CLA	5	613	16	68,72,73	1.28	10 (14%)	81,111,113	1.42	5 (6%)
23	CLA	5	607	-	69,73,73	1.27	11 (15%)	83,113,113	1.48	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	3	612	14	47,51,73	1.52	11 (23%)	56,86,113	1.52	6 (10%)
25	LHG	7	622	23	36,36,48	0.70	0	39,42,54	1.23	4 (10%)
25	LHG	1	620	23	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
23	CLA	A	835	1	65,69,73	1.28	9 (13%)	78,108,113	1.48	6 (7%)
23	CLA	B	835	-	49,53,73	1.50	9 (18%)	59,89,113	1.59	10 (16%)
23	CLA	9	603	21	28,35,73	1.95	8 (28%)	32,60,113	1.60	5 (15%)
23	CLA	A	806	1	69,73,73	1.30	13 (18%)	83,113,113	1.57	11 (13%)
23	CLA	7	601	18	64,68,73	1.32	12 (18%)	77,107,113	1.42	7 (9%)
23	CLA	A	803	-	69,73,73	1.31	11 (15%)	83,113,113	1.35	5 (6%)
25	LHG	B	851	23	37,37,48	0.63	0	40,43,54	1.22	4 (10%)
23	CLA	A	810	1	54,58,73	1.41	12 (22%)	65,95,113	1.49	6 (9%)
23	CLA	B	811	2	56,61,73	1.43	11 (19%)	70,99,113	1.44	8 (11%)
23	CLA	A	830	1	69,73,73	1.26	10 (14%)	83,113,113	1.49	9 (10%)
23	CLA	5	604	-	67,71,73	1.32	12 (17%)	84,111,113	1.37	8 (9%)
26	BCR	A	848	-	41,41,41	0.92	1 (2%)	56,56,56	2.07	17 (30%)
23	CLA	8	604	-	54,58,73	1.40	10 (18%)	65,95,113	1.46	9 (13%)
25	LHG	a	620	23	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
23	CLA	7	615	-	45,50,73	1.59	10 (22%)	56,85,113	1.60	8 (14%)
23	CLA	3	613	14	56,61,73	1.36	10 (17%)	66,98,113	1.43	6 (9%)
25	LHG	3	624	23	48,48,48	0.66	0	51,54,54	1.24	5 (9%)
23	CLA	A	838	1	54,58,73	1.38	9 (16%)	65,95,113	1.62	13 (20%)
23	CLA	A	811	1	69,73,73	1.24	11 (15%)	83,113,113	1.39	11 (13%)
23	CLA	4	613	15	69,73,73	1.26	10 (14%)	83,113,113	1.37	6 (7%)
23	CLA	B	804	2	45,49,73	1.52	11 (24%)	54,84,113	1.67	9 (16%)
29	LMG	4	623	-	40,40,55	0.90	1 (2%)	48,48,63	1.28	5 (10%)
26	BCR	K	202	-	41,41,41	0.79	0	56,56,56	2.26	20 (35%)
31	LUT	1	617	-	42,43,43	0.79	0	51,60,60	1.56	12 (23%)
26	BCR	6	622	-	41,41,41	0.69	0	56,56,56	1.94	17 (30%)
26	BCR	7	623	-	41,41,41	0.68	0	56,56,56	1.81	13 (23%)
23	CLA	A	837	1	49,53,73	1.48	9 (18%)	59,89,113	1.52	6 (10%)
23	CLA	L	303	12	49,53,73	1.44	11 (22%)	59,89,113	1.54	5 (8%)
23	CLA	2	606	20	28,35,73	1.93	7 (25%)	32,60,113	1.58	4 (12%)
23	CLA	9	613	21	28,35,73	1.89	7 (25%)	32,60,113	1.69	5 (15%)
23	CLA	9	606	21	28,35,73	1.92	7 (25%)	32,60,113	1.68	6 (18%)
23	CLA	9	607	-	28,35,73	1.88	8 (28%)	32,60,113	1.74	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	813	1	-	7/26/102/115	-
25	LHG	5	625	-	-	23/53/53/53	-
32	XAT	1	618	-	-	1/31/93/93	0/4/4/4
26	BCR	J	102	-	-	5/29/63/63	0/2/2/2
33	NEX	6	624	-	-	4/27/83/83	0/3/3/3
23	CLA	4	610	15	-	14/35/111/115	-
23	CLA	7	608	-	-	6/21/97/115	-
23	CLA	B	840	2	-	11/39/115/115	-
25	LHG	8	622	23	-	26/53/53/53	-
23	CLA	7	610	18	-	8/39/115/115	-
26	BCR	B	847	-	-	1/29/63/63	0/2/2/2
23	CLA	5	618	16	-	2/8/84/115	-
23	CLA	8	611	25	-	6/12/88/115	-
31	LUT	a	617	-	-	2/29/67/67	0/2/2/2
23	CLA	3	610	14	-	18/39/115/115	-
23	CLA	B	839	-	-	14/39/115/115	-
23	CLA	8	616	19	-	7/11/87/115	-
23	CLA	A	829	1	-	11/39/115/115	-
23	CLA	8	603	19	-	8/13/89/115	-
23	CLA	6	611	25	-	5/12/88/115	-
23	CLA	6	616	17	-	18/39/115/115	-
25	LHG	2	622	23	-	19/41/41/53	-
23	CLA	A	836	1	-	13/39/115/115	-
23	CLA	1	616	13	-	4/11/87/115	-
23	CLA	B	821	2	-	5/13/89/115	-
23	CLA	6	603	17	-	4/25/101/115	-
23	CLA	A	854	-	-	13/39/115/115	-
23	CLA	4	614	15	-	9/29/105/115	-
23	CLA	B	830	2	-	4/13/89/115	-
26	BCR	B	846	-	-	5/29/63/63	0/2/2/2
29	LMG	J	104	-	-	19/35/55/70	0/1/1/1
23	CLA	A	833	1	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	XAT	a	618	-	-	1/31/93/93	0/4/4/4
23	CLA	B	818	2	-	16/33/109/115	-
23	CLA	a	609	13	-	21/37/113/115	-
31	LUT	8	619	-	-	2/29/67/67	0/2/2/2
23	CLA	B	810	2	-	17/37/113/115	-
23	CLA	B	812	2	-	8/13/89/115	-
23	CLA	B	825	-	-	11/36/112/115	-
23	CLA	3	614	14	-	2/8/84/115	-
23	CLA	8	608	-	-	6/23/99/115	-
23	CLA	8	607	-	-	3/10/86/115	-
23	CLA	6	609	17	-	6/15/91/115	-
23	CLA	8	612	19	-	2/10/86/115	-
26	BCR	B	848	-	-	4/29/63/63	0/2/2/2
23	CLA	B	816	2	-	11/25/101/115	-
23	CLA	B	815	2	-	4/13/89/115	-
23	CLA	7	606	-	-	4/10/86/115	-
23	CLA	6	612	17	-	3/10/86/115	-
23	CLA	B	819	-	-	13/27/103/115	-
23	CLA	4	606	-	-	5/8/84/115	-
23	CLA	A	828	1	-	11/39/115/115	-
23	CLA	6	601	17	-	14/39/115/115	-
23	CLA	5	619	-	-	7/11/87/115	-
23	CLA	5	609	16	-	15/39/115/115	-
23	CLA	B	832	2	-	7/33/109/115	-
26	BCR	3	620	-	-	4/29/63/63	0/2/2/2
32	XAT	9	620	-	-	0/31/93/93	0/4/4/4
23	CLA	A	845	25	-	11/21/97/115	-
23	CLA	3	617	14	-	2/8/84/115	-
26	BCR	A	852	-	-	11/29/63/63	0/2/2/2
23	CLA	L	304	-	-	8/15/91/115	-
31	LUT	9	619	-	-	3/29/67/67	0/2/2/2
23	CLA	K	204	11	-	9/17/93/115	-
23	CLA	3	606	-	-	12/25/101/115	-
25	LHG	3	623	-	-	26/49/49/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LUT	5	620	-	-	2/29/67/67	0/2/2/2
26	BCR	F	305	-	-	2/29/63/63	0/2/2/2
23	CLA	B	837	2	-	17/39/115/115	-
23	CLA	B	808	2	-	16/39/115/115	-
23	CLA	G	204	7	-	8/15/91/115	-
23	CLA	K	206	11	-	7/15/91/115	-
23	CLA	4	616	15	-	6/11/87/115	-
23	CLA	7	616	18	-	7/11/87/115	-
23	CLA	A	823	1	-	7/12/88/115	-
30	DGD	B	850	-	-	22/51/91/95	0/2/2/2
23	CLA	8	613	19	-	18/39/115/115	-
23	CLA	A	809	1	-	14/39/115/115	-
23	CLA	A	826	-	-	12/37/113/115	-
23	CLA	B	836	2	-	6/21/97/115	-
23	CLA	F	304	-	-	4/10/86/115	-
23	CLA	K	203	-	-	12/39/115/115	-
28	LMU	5	628	-	-	11/19/59/61	0/2/2/2
23	CLA	G	203	7	-	5/12/88/115	-
23	CLA	6	606	-	-	0/8/84/115	-
23	CLA	A	843	-	-	18/37/113/115	-
23	CLA	B	834	2	-	15/33/109/115	-
30	DGD	J	103	-	-	25/47/87/95	0/2/2/2
23	CLA	a	611	25	-	0/4/80/115	-
23	CLA	B	824	-	-	9/39/115/115	-
23	CLA	A	815	1	-	8/21/97/115	-
23	CLA	3	615	-	-	3/8/84/115	-
23	CLA	6	620	-	-	16/37/113/115	-
26	BCR	G	205	-	-	0/29/63/63	0/2/2/2
26	BCR	A	849	-	-	5/29/63/63	0/2/2/2
23	CLA	6	610	17	-	10/39/115/115	-
23	CLA	5	610	16	-	7/26/102/115	-
26	BCR	A	856	-	-	8/29/63/63	0/2/2/2
24	PQN	B	842	-	-	7/23/43/43	0/2/2/2
23	CLA	L	302	12	-	5/15/91/115	-
23	CLA	6	602	17	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	802	2	-	9/39/115/115	-
26	BCR	8	621	-	-	6/29/63/63	0/2/2/2
25	LHG	4	622	23	-	21/53/53/53	-
23	CLA	1	602	13	-	8/35/111/115	-
26	BCR	B	844	-	-	9/29/63/63	0/2/2/2
26	BCR	B	843	-	-	8/29/63/63	0/2/2/2
23	CLA	A	805	1	-	7/24/100/115	-
23	CLA	A	842	1	-	12/39/115/115	-
23	CLA	3	602	14	-	10/33/109/115	-
29	LMG	A	860	-	-	18/35/55/70	0/1/1/1
23	CLA	6	618	17	-	2/8/84/115	-
23	CLA	4	602	15	-	10/33/109/115	-
23	CLA	7	609	18	-	4/12/88/115	-
23	CLA	a	603	13	-	5/12/88/115	-
23	CLA	1	609	13	-	5/8/84/115	-
23	CLA	A	817	-	-	7/15/91/115	-
32	XAT	6	621	-	-	2/31/93/93	0/4/4/4
27	SF4	C	102	-	-	-	0/6/5/5
23	CLA	8	602	19	-	10/33/109/115	-
23	CLA	A	808	1	-	2/21/97/115	-
23	CLA	A	827	-	-	5/32/108/115	-
26	BCR	L	305	-	-	10/29/63/63	0/2/2/2
28	LMU	8	625	-	-	10/21/61/61	0/2/2/2
23	CLA	a	612	13	-	6/15/91/115	-
23	CLA	5	614	16	-	9/15/87/115	-
23	CLA	B	814	2	-	12/38/114/115	-
23	CLA	B	838	2	-	5/18/94/115	-
26	BCR	a	619	-	-	4/29/63/63	0/2/2/2
23	CLA	1	611	25	-	13/39/115/115	-
32	XAT	2	620	-	-	0/31/93/93	0/4/4/4
23	CLA	a	616	13	-	6/15/91/115	-
23	CLA	8	609	19	-	4/15/91/115	-
23	CLA	8	610	19	-	7/33/109/115	-
23	CLA	A	814	1	-	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	840	1	-	5/24/100/115	-
23	CLA	1	603	13	-	13/23/99/115	-
23	CLA	B	829	2	-	8/39/115/115	-
23	CLA	B	813	2	-	22/39/115/115	-
23	CLA	B	823	2	-	4/15/91/115	-
29	LMG	7	624	-	-	19/39/59/70	0/1/1/1
23	CLA	5	608	-	-	9/21/97/115	-
23	CLA	A	820	1	-	17/39/115/115	-
23	CLA	B	809	2	-	15/39/115/115	-
26	BCR	5	622	-	-	3/29/63/63	0/2/2/2
23	CLA	5	606	-	-	4/8/84/115	-
25	LHG	A	847	23	-	11/34/34/53	-
23	CLA	A	834	1	-	19/39/115/115	-
23	CLA	6	617	17	-	9/15/91/115	-
31	LUT	3	618	-	-	2/29/67/67	0/2/2/2
23	CLA	5	617	16	-	8/21/97/115	-
25	LHG	6	623	23	-	23/52/52/53	-
28	LMU	A	857	-	-	11/21/61/61	0/2/2/2
23	CLA	A	818	1	-	12/33/109/115	-
28	LMU	A	858	-	-	6/21/57/61	0/2/2/2
23	CLA	3	608	-	-	11/27/103/115	-
23	CLA	7	613	18	-	19/39/115/115	-
31	LUT	4	619	-	-	4/29/67/67	0/2/2/2
23	CLA	7	607	-	-	6/12/88/115	-
23	CLA	a	606	13	-	5/12/88/115	-
23	CLA	7	612	18	-	6/13/89/115	-
23	CLA	A	841	1	-	20/39/115/115	-
23	CLA	1	613	-	-	14/39/115/115	-
23	CLA	1	607	-	-	5/8/84/115	-
23	CLA	1	612	13	-	6/15/91/115	-
23	CLA	6	607	-	-	6/10/86/115	-
23	CLA	4	607	-	-	7/15/91/115	-
31	LUT	2	619	-	-	2/29/67/67	0/2/2/2
23	CLA	B	802	2	-	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	4	621	-	-	1/29/63/63	0/2/2/2
23	CLA	K	201	11	-	8/15/91/115	-
23	CLA	3	609	14	-	18/33/109/115	-
23	CLA	6	613	-	-	15/37/113/115	-
26	BCR	B	801	-	-	4/29/63/63	0/2/2/2
25	LHG	5	623	23	-	23/53/53/53	-
23	CLA	B	831	2	-	13/39/115/115	-
23	CLA	5	611	25	-	5/12/88/115	-
23	CLA	a	602	13	-	8/35/111/115	-
23	CLA	7	602	18	-	17/39/115/115	-
23	CLA	7	611	25	-	10/31/107/115	-
23	CLA	a	601	13	-	7/25/101/115	-
23	CLA	a	613	-	-	14/39/115/115	-
23	CLA	a	607	-	-	8/15/91/115	-
23	CLA	A	812	1	-	13/39/115/115	-
23	CLA	A	822	-	-	15/39/115/115	-
26	BCR	B	845	-	-	5/29/63/63	0/2/2/2
28	LMU	8	624	-	-	6/21/61/61	0/2/2/2
26	BCR	L	301	-	-	6/29/63/63	0/2/2/2
28	LMU	A	859	-	-	13/21/57/61	0/2/2/2
23	CLA	3	607	14	-	9/28/104/115	-
23	CLA	1	604	-	-	12/20/96/115	-
23	CLA	7	603	18	-	4/13/89/115	-
23	CLA	A	825	1	-	20/39/115/115	-
26	BCR	3	621	-	-	6/29/63/63	0/2/2/2
23	CLA	B	817	2	-	12/32/108/115	-
23	CLA	8	601	19	-	20/39/115/115	-
28	LMU	K	208	-	-	10/21/61/61	0/2/2/2
32	XAT	4	620	-	-	1/31/93/93	0/4/4/4
32	XAT	7	620	-	-	1/31/93/93	0/4/4/4
23	CLA	A	801	1	-	12/39/115/115	-
23	CLA	B	827	2	-	14/36/112/115	-
23	CLA	a	604	-	-	12/20/96/115	-
23	CLA	A	832	1	-	9/21/97/115	-
23	CLA	1	601	13	-	7/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	1	619	-	-	4/29/63/63	0/2/2/2
27	SF4	C	101	-	-	-	0/6/5/5
23	CLA	6	604	-	-	24/39/115/115	-
23	CLA	a	614	13	-	12/27/99/115	-
23	CLA	5	603	16	-	10/25/101/115	-
25	LHG	A	846	-	-	25/53/53/53	-
23	CLA	F	303	-	-	7/12/88/115	-
29	LMG	5	627	-	-	13/35/55/70	0/1/1/1
26	BCR	3	622	-	-	8/29/63/63	0/2/2/2
29	LMG	4	624	-	-	15/35/55/70	0/1/1/1
24	PQN	A	844	-	-	8/23/43/43	0/2/2/2
23	CLA	B	820	2	-	9/21/97/115	-
23	CLA	4	618	15	-	0/8/84/115	-
32	XAT	5	621	-	-	2/31/93/93	0/4/4/4
23	CLA	B	805	2	-	16/39/115/115	-
23	CLA	5	602	16	-	11/39/115/115	-
23	CLA	F	301	-	-	11/30/106/115	-
23	CLA	4	611	25	-	6/12/88/115	-
23	CLA	B	828	2	-	18/39/115/115	-
23	CLA	A	807	1	-	15/39/115/115	-
23	CLA	a	610	13	-	7/31/107/115	-
23	CLA	B	807	2	-	6/24/100/115	-
23	CLA	J	101	10	-	7/12/88/115	-
23	CLA	5	612	16	-	3/10/86/115	-
31	LUT	7	619	-	-	5/29/67/67	0/2/2/2
23	CLA	7	614	18	-	5/12/88/115	-
23	CLA	1	614	13	-	0/4/76/115	-
23	CLA	A	819	1	-	10/32/108/115	-
32	XAT	8	620	-	-	2/31/93/93	0/4/4/4
23	CLA	8	606	-	-	16/37/113/115	-
26	BCR	A	850	-	-	1/29/63/63	0/2/2/2
23	CLA	1	608	-	-	6/13/89/115	-
33	NEX	5	624	-	-	2/27/83/83	0/3/3/3
23	CLA	B	841	25	-	3/13/89/115	-
26	BCR	7	621	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	806	2	-	15/39/115/115	-
23	CLA	3	611	25	-	2/4/80/115	-
23	CLA	6	614	17	-	9/33/109/115	-
23	CLA	A	824	1	-	2/10/86/115	-
23	CLA	A	816	1	-	3/12/88/115	-
25	LHG	9	622	23	-	23/53/53/53	-
23	CLA	5	616	16	-	4/8/84/115	-
23	CLA	7	604	-	-	8/25/101/115	-
32	XAT	3	619	-	-	1/31/93/93	0/4/4/4
23	CLA	3	603	14	-	11/27/103/115	-
23	CLA	4	608	-	-	11/39/115/115	-
23	CLA	1	610	13	-	3/8/80/115	-
23	CLA	A	821	1	-	14/25/101/115	-
23	CLA	B	803	-	-	17/39/115/115	-
23	CLA	4	604	-	-	6/25/101/115	-
31	LUT	6	619	-	-	2/29/67/67	0/2/2/2
23	CLA	4	603	15	-	7/13/89/115	-
23	CLA	B	822	2	-	6/12/88/115	-
23	CLA	A	804	1	-	13/39/115/115	-
23	CLA	B	826	2	-	8/27/103/115	-
23	CLA	1	606	13	-	3/7/79/115	-
23	CLA	A	839	1	-	7/27/103/115	-
23	CLA	6	608	-	-	10/23/99/115	-
26	BCR	K	207	-	-	3/29/63/63	0/2/2/2
23	CLA	4	612	15	-	2/10/86/115	-
27	SF4	A	853	-	-	-	0/6/5/5
25	LHG	8	623	-	-	24/51/51/53	-
23	CLA	4	609	15	-	13/35/111/115	-
23	CLA	B	833	2	-	21/39/115/115	-
23	CLA	4	601	15	-	18/39/115/115	-
23	CLA	3	604	-	-	13/39/115/115	-
23	CLA	5	601	16	-	8/29/105/115	-
23	CLA	a	608	-	-	6/13/89/115	-
26	BCR	A	851	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	5	626	-	-	23/35/55/70	0/1/1/1
23	CLA	8	614	19	-	12/29/105/115	-
23	CLA	A	831	1	-	14/39/115/115	-
23	CLA	5	613	16	-	21/37/113/115	-
23	CLA	5	607	-	-	17/39/115/115	-
23	CLA	3	612	14	-	5/13/89/115	-
25	LHG	7	622	23	-	24/41/41/53	-
25	LHG	1	620	23	-	24/53/53/53	-
23	CLA	A	835	1	-	15/35/111/115	-
23	CLA	B	835	-	-	10/15/91/115	-
23	CLA	A	806	1	-	15/39/115/115	-
23	CLA	7	601	18	-	15/33/109/115	-
23	CLA	A	803	-	-	9/39/115/115	-
25	LHG	B	851	23	-	22/42/42/53	-
23	CLA	A	810	1	-	7/21/97/115	-
23	CLA	B	811	2	-	8/23/99/115	-
23	CLA	A	830	1	-	16/39/115/115	-
23	CLA	5	604	-	-	13/35/111/115	-
26	BCR	A	848	-	-	4/29/63/63	0/2/2/2
23	CLA	8	604	-	-	5/21/97/115	-
25	LHG	a	620	23	-	24/53/53/53	-
23	CLA	7	615	-	-	4/8/84/115	-
23	CLA	3	613	14	-	7/23/99/115	-
25	LHG	3	624	23	-	26/53/53/53	-
23	CLA	A	838	1	-	7/21/97/115	-
23	CLA	A	811	1	-	17/39/115/115	-
23	CLA	4	613	15	-	14/39/115/115	-
23	CLA	B	804	2	-	4/10/86/115	-
29	LMG	4	623	-	-	11/35/55/70	0/1/1/1
26	BCR	K	202	-	-	4/29/63/63	0/2/2/2
31	LUT	1	617	-	-	2/29/67/67	0/2/2/2
26	BCR	6	622	-	-	7/29/63/63	0/2/2/2
26	BCR	7	623	-	-	0/29/63/63	0/2/2/2
23	CLA	A	837	1	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	L	303	12	-	7/15/91/115	-

The worst 5 of 2531 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	611	CLA	C1A-NA	12.76	1.40	1.29
24	A	844	PQN	C12-C13	8.62	1.53	1.33
24	B	842	PQN	C12-C13	8.55	1.53	1.33
24	A	844	PQN	O1-C1	7.91	1.40	1.23
24	B	842	PQN	O1-C1	7.62	1.39	1.23

The worst 5 of 2930 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	621	XAT	O24-C25-C24	10.95	121.61	113.38
32	2	620	XAT	O24-C25-C24	10.87	121.55	113.38
32	9	620	XAT	O4-C5-C4	10.55	121.31	113.38
23	B	803	CLA	C4A-NA-C1A	9.04	110.77	106.71
23	8	613	CLA	C4A-NA-C1A	8.99	110.75	106.71

There are no chirality outliers.

5 of 2885 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	801	CLA	C2B-C3B-CAB-CBB
23	A	801	CLA	C4B-C3B-CAB-CBB
23	A	801	CLA	CBD-CGD-O2D-CED
23	A	804	CLA	C1A-C2A-CAA-CBA
23	A	804	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

264 monomers are involved in 558 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	813	CLA	2	0
25	5	625	LHG	5	0
32	1	618	XAT	4	0
26	J	102	BCR	5	0
33	6	624	NEX	4	0
23	4	610	CLA	2	0
23	7	608	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	840	CLA	2	0
25	8	622	LHG	2	0
23	7	610	CLA	5	0
26	B	847	BCR	2	0
31	a	617	LUT	5	0
23	3	610	CLA	3	0
23	B	839	CLA	3	0
23	8	616	CLA	1	0
23	A	829	CLA	9	0
23	8	603	CLA	1	0
23	6	616	CLA	4	0
25	2	622	LHG	1	0
23	A	836	CLA	4	0
23	B	821	CLA	2	0
23	6	603	CLA	1	0
23	A	854	CLA	5	0
23	4	614	CLA	1	0
23	B	830	CLA	5	0
26	B	846	BCR	1	0
29	J	104	LMG	1	0
32	a	618	XAT	3	0
23	B	818	CLA	2	0
23	a	609	CLA	2	0
23	9	611	CLA	7	0
31	8	619	LUT	6	0
23	B	810	CLA	3	0
23	B	825	CLA	4	0
23	8	608	CLA	3	0
23	8	607	CLA	2	0
23	6	609	CLA	1	0
26	B	848	BCR	1	0
23	B	815	CLA	1	0
23	6	612	CLA	1	0
23	B	819	CLA	1	0
23	A	828	CLA	1	0
23	9	614	CLA	1	0
23	6	601	CLA	5	0
23	5	619	CLA	1	0
23	5	609	CLA	4	0
23	B	832	CLA	4	0
26	3	620	BCR	3	0
32	9	620	XAT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	845	CLA	1	0
23	3	617	CLA	2	0
26	A	852	BCR	5	0
23	L	304	CLA	2	0
31	9	619	LUT	1	0
23	K	204	CLA	1	0
23	3	606	CLA	1	0
23	2	614	CLA	1	0
25	3	623	LHG	1	0
31	5	620	LUT	5	0
26	F	305	BCR	4	0
23	B	837	CLA	3	0
23	B	808	CLA	2	0
23	G	204	CLA	2	0
23	4	616	CLA	1	0
23	7	616	CLA	1	0
23	A	823	CLA	1	0
30	B	850	DGD	5	0
23	8	613	CLA	1	0
23	A	809	CLA	4	0
23	A	826	CLA	1	0
23	B	836	CLA	1	0
23	F	304	CLA	1	0
28	5	628	LMU	3	0
23	G	203	CLA	2	0
23	6	606	CLA	1	0
23	A	843	CLA	4	0
23	B	834	CLA	2	0
30	J	103	DGD	1	0
23	B	824	CLA	3	0
23	6	620	CLA	5	0
26	G	205	BCR	5	0
26	A	849	BCR	4	0
23	6	610	CLA	4	0
23	5	610	CLA	5	0
26	A	856	BCR	7	0
24	B	842	PQN	6	0
23	L	302	CLA	1	0
23	6	602	CLA	6	0
23	A	802	CLA	7	0
26	8	621	BCR	3	0
25	4	622	LHG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	844	BCR	3	0
26	B	843	BCR	1	0
23	A	805	CLA	4	0
23	A	842	CLA	5	0
23	3	602	CLA	1	0
29	A	860	LMG	2	0
23	4	602	CLA	1	0
23	a	603	CLA	1	0
23	1	609	CLA	1	0
23	A	817	CLA	1	0
32	6	621	XAT	1	0
23	A	808	CLA	1	0
23	A	827	CLA	2	0
26	L	305	BCR	4	0
23	B	814	CLA	3	0
23	B	838	CLA	3	0
26	a	619	BCR	4	0
23	1	611	CLA	5	0
32	2	620	XAT	3	0
23	8	609	CLA	1	0
23	8	610	CLA	2	0
23	A	814	CLA	4	0
23	2	609	CLA	1	0
23	A	840	CLA	2	0
23	1	603	CLA	1	0
23	B	829	CLA	7	0
23	B	813	CLA	5	0
23	B	823	CLA	1	0
29	7	624	LMG	1	0
23	5	608	CLA	2	0
23	A	820	CLA	4	0
23	B	809	CLA	1	0
26	5	622	BCR	3	0
23	5	606	CLA	4	0
25	A	847	LHG	1	0
23	A	834	CLA	4	0
31	3	618	LUT	1	0
25	6	623	LHG	3	0
28	A	857	LMU	1	0
23	A	818	CLA	4	0
23	3	608	CLA	2	0
23	7	613	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	4	619	LUT	5	0
23	7	607	CLA	2	0
23	a	606	CLA	2	0
23	A	841	CLA	5	0
23	1	607	CLA	1	0
23	1	612	CLA	1	0
31	2	619	LUT	3	0
23	B	802	CLA	1	0
26	4	621	BCR	2	0
23	K	201	CLA	1	0
23	3	609	CLA	6	0
23	6	613	CLA	4	0
26	B	801	BCR	4	0
25	5	623	LHG	2	0
23	B	831	CLA	2	0
23	5	611	CLA	1	0
23	7	602	CLA	1	0
23	7	611	CLA	2	0
23	a	601	CLA	1	0
23	a	613	CLA	3	0
23	a	607	CLA	1	0
23	A	812	CLA	3	0
23	A	822	CLA	3	0
26	B	845	BCR	2	0
28	8	624	LMU	3	0
26	L	301	BCR	2	0
28	A	859	LMU	2	0
23	3	607	CLA	1	0
23	7	603	CLA	1	0
23	A	825	CLA	5	0
26	3	621	BCR	2	0
23	B	817	CLA	2	0
23	8	601	CLA	4	0
32	4	620	XAT	3	0
32	7	620	XAT	1	0
23	A	801	CLA	4	0
23	B	827	CLA	6	0
23	A	832	CLA	1	0
23	9	601	CLA	1	0
23	1	601	CLA	5	0
26	1	619	BCR	2	0
23	6	604	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2	613	CLA	1	0
25	A	846	LHG	2	0
23	F	303	CLA	2	0
29	5	627	LMG	3	0
26	3	622	BCR	4	0
29	4	624	LMG	1	0
24	A	844	PQN	4	0
23	B	820	CLA	1	0
23	4	618	CLA	1	0
32	5	621	XAT	9	0
23	B	805	CLA	4	0
23	5	602	CLA	5	0
23	F	301	CLA	3	0
23	B	828	CLA	1	0
23	A	807	CLA	1	0
23	a	610	CLA	2	0
23	B	807	CLA	2	0
23	J	101	CLA	2	0
31	7	619	LUT	5	0
23	A	819	CLA	2	0
32	8	620	XAT	1	0
26	A	850	BCR	3	0
23	1	608	CLA	1	0
33	5	624	NEX	3	0
23	B	841	CLA	3	0
26	7	621	BCR	3	0
23	B	806	CLA	1	0
23	6	614	CLA	4	0
23	A	824	CLA	1	0
23	A	816	CLA	1	0
25	9	622	LHG	5	0
23	5	616	CLA	1	0
32	3	619	XAT	3	0
23	3	603	CLA	2	0
23	4	608	CLA	3	0
23	A	821	CLA	1	0
23	B	803	CLA	3	0
23	4	604	CLA	1	0
31	6	619	LUT	4	0
23	4	603	CLA	1	0
23	B	822	CLA	1	0
23	A	804	CLA	2	0

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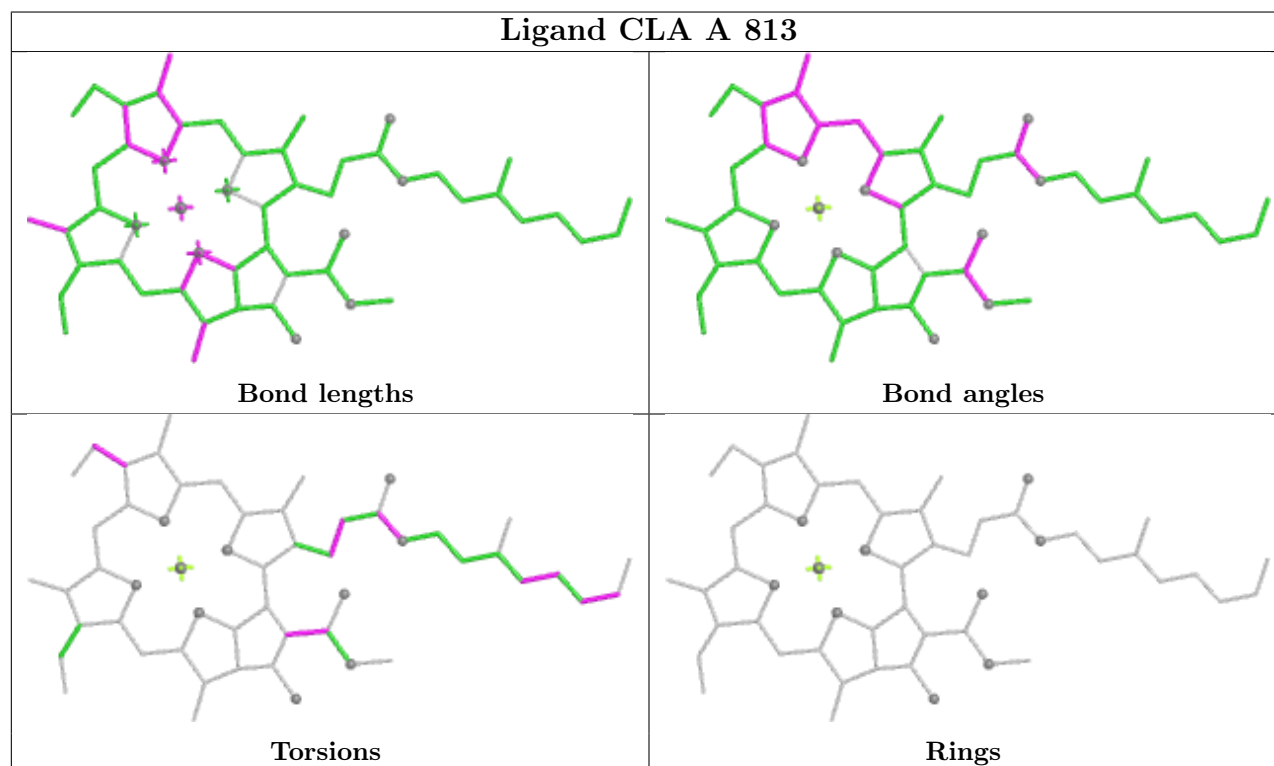
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	826	CLA	2	0
23	1	606	CLA	1	0
23	2	610	CLA	1	0
23	A	839	CLA	2	0
23	6	608	CLA	2	0
26	K	207	BCR	3	0
23	4	612	CLA	1	0
25	8	623	LHG	3	0
23	4	609	CLA	4	0
23	B	833	CLA	2	0
23	4	601	CLA	6	0
23	3	604	CLA	1	0
23	5	601	CLA	1	0
23	a	608	CLA	1	0
26	A	851	BCR	3	0
29	5	626	LMG	1	0
23	8	614	CLA	1	0
23	9	609	CLA	1	0
23	A	831	CLA	4	0
23	5	613	CLA	5	0
23	5	607	CLA	5	0
23	3	612	CLA	1	0
25	7	622	LHG	2	0
25	1	620	LHG	6	0
23	A	835	CLA	4	0
23	B	835	CLA	1	0
23	A	806	CLA	3	0
23	7	601	CLA	4	0
23	A	803	CLA	5	0
25	B	851	LHG	2	0
23	A	810	CLA	1	0
23	B	811	CLA	2	0
23	A	830	CLA	6	0
23	5	604	CLA	5	0
26	A	848	BCR	5	0
25	a	620	LHG	4	0
25	3	624	LHG	2	0
23	A	838	CLA	2	0
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23	4	613	CLA	5	0
26	K	202	BCR	3	0
31	1	617	LUT	3	0

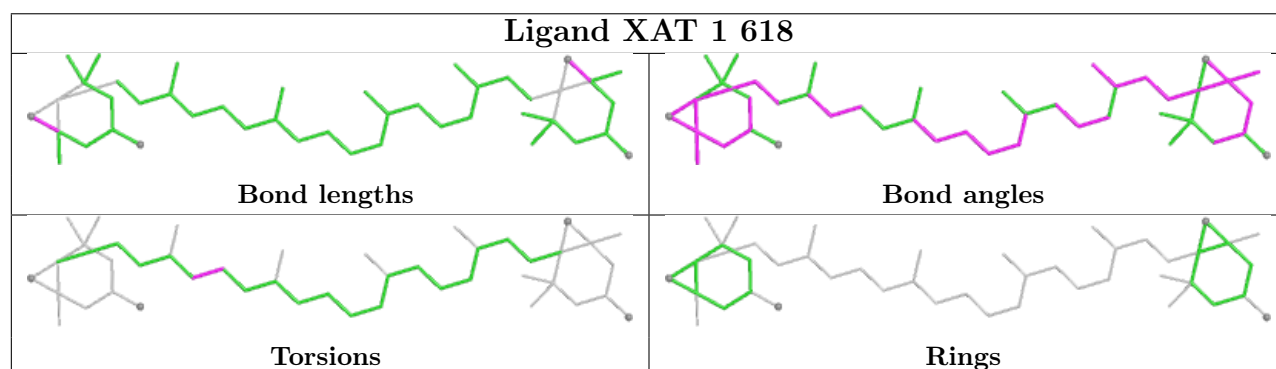
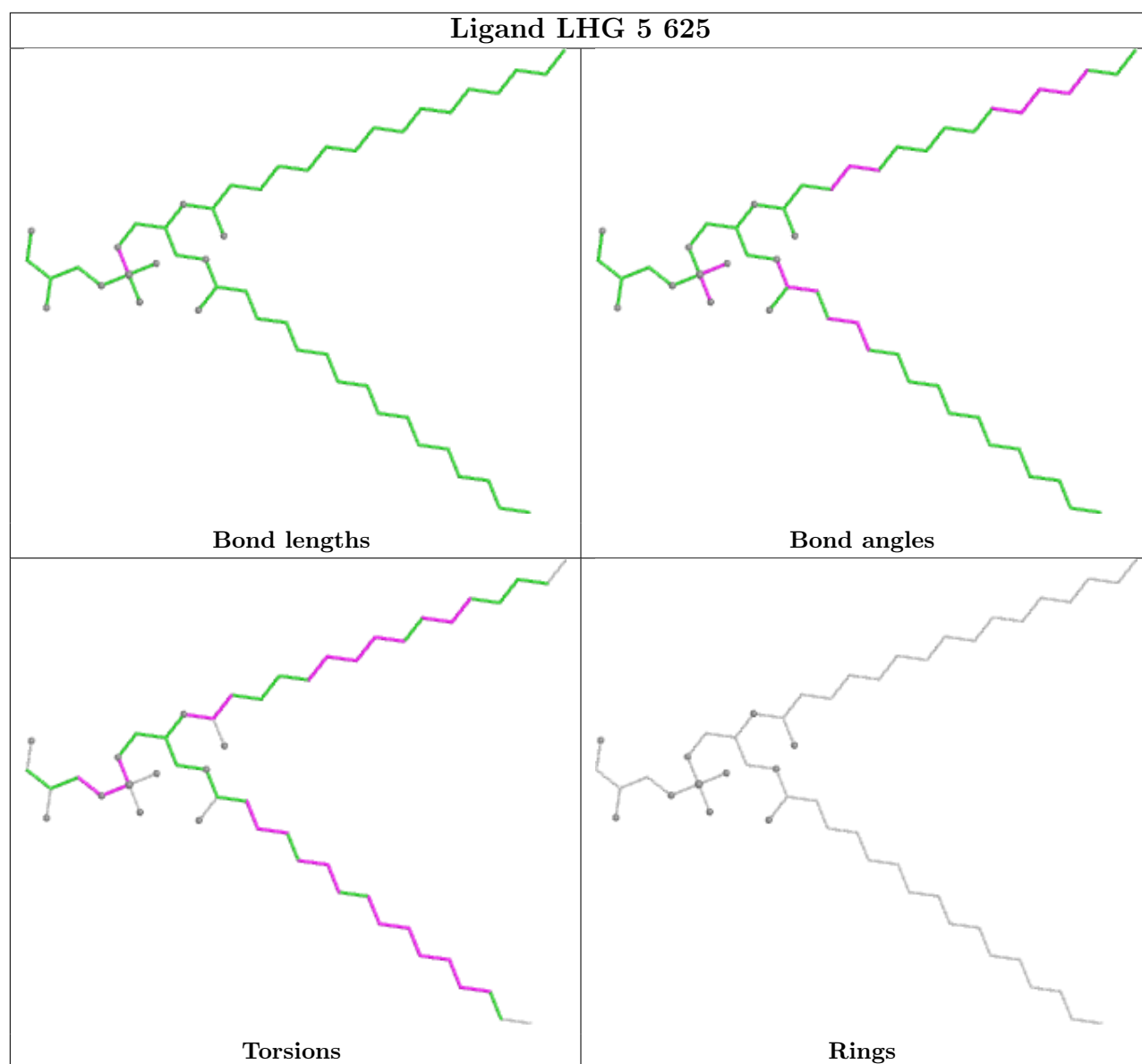
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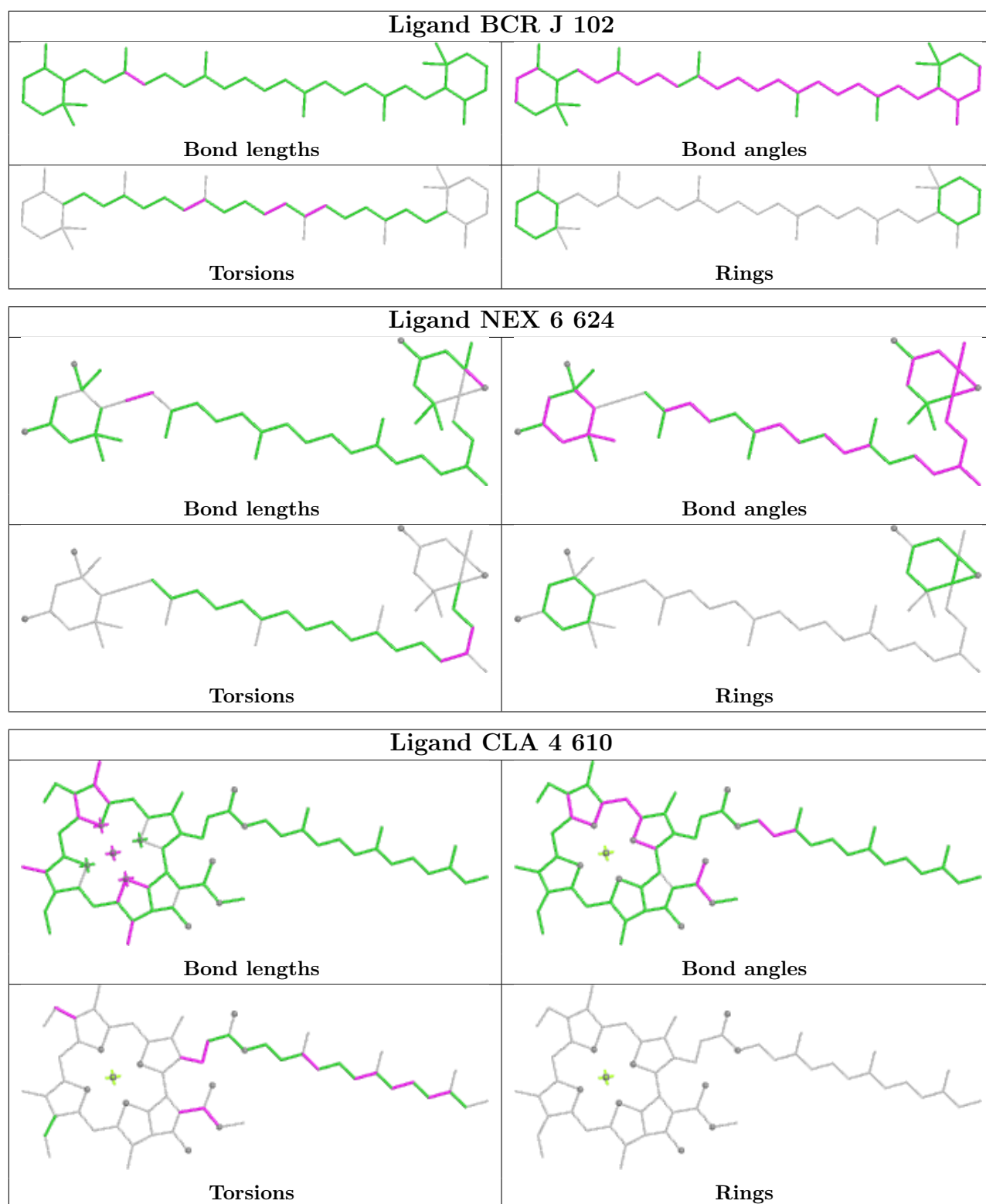
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	6	622	BCR	4	0
23	A	837	CLA	2	0
23	L	303	CLA	2	0
23	9	613	CLA	1	0
23	9	606	CLA	1	0

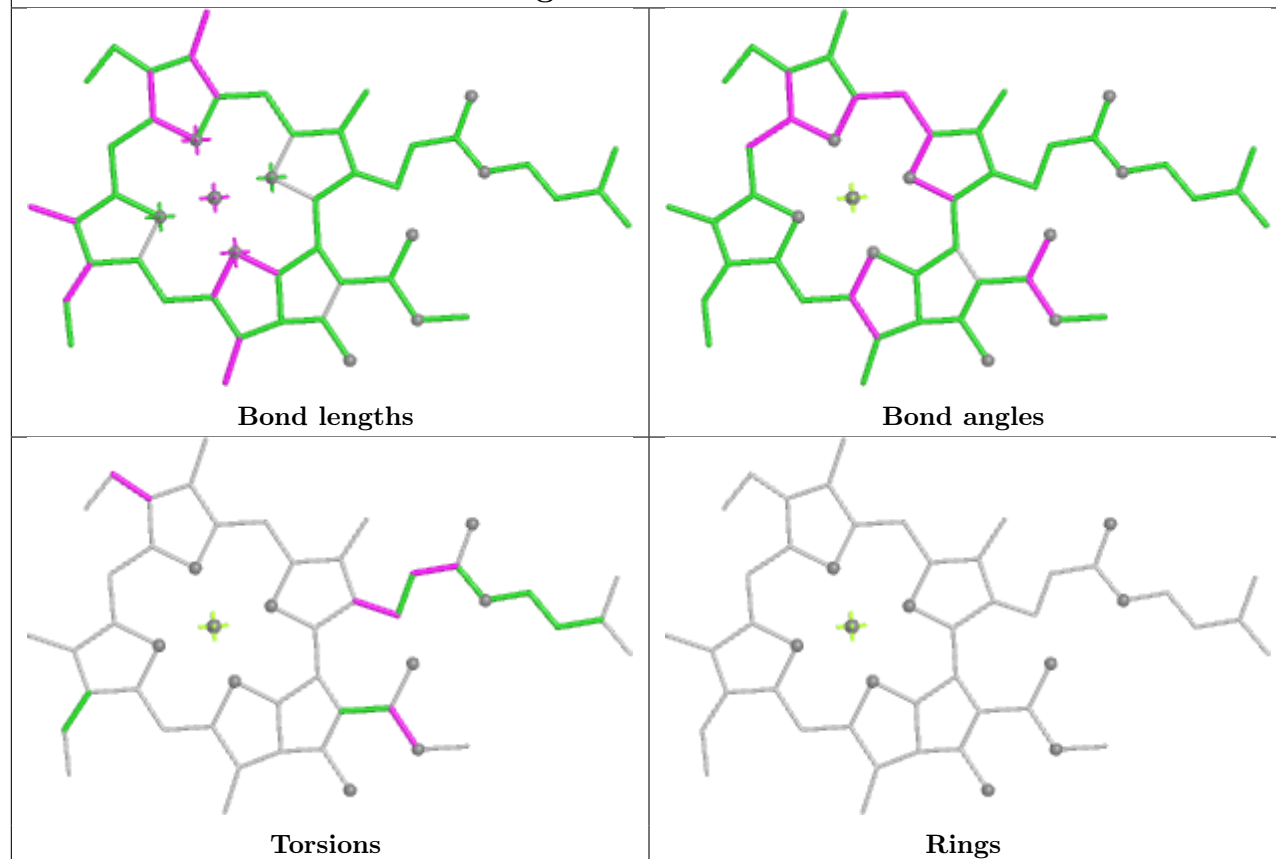
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



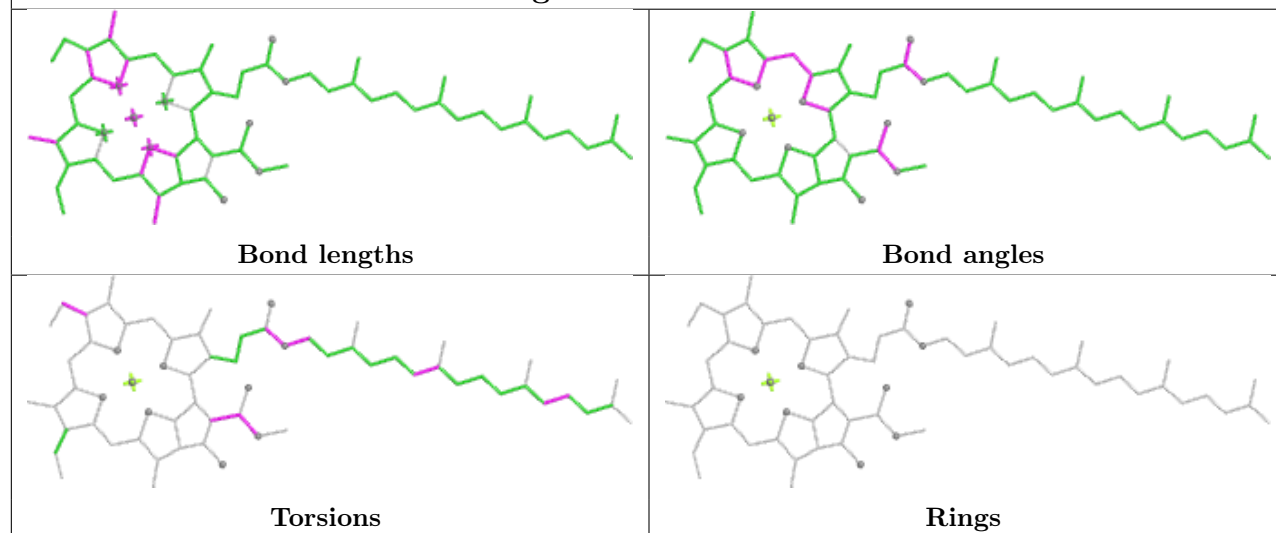


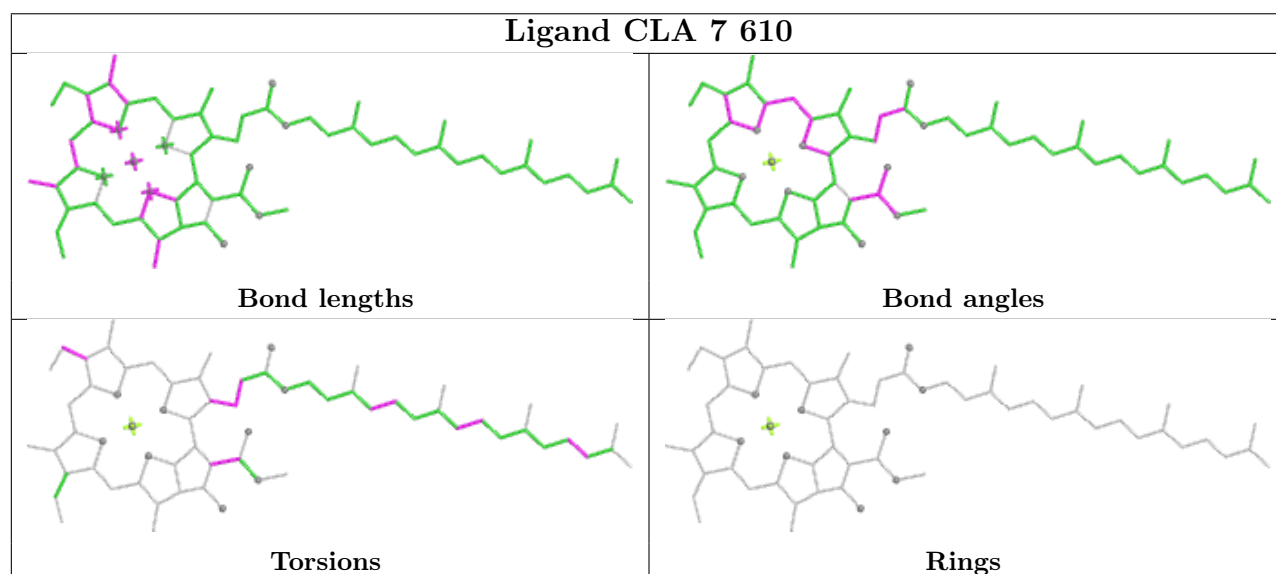
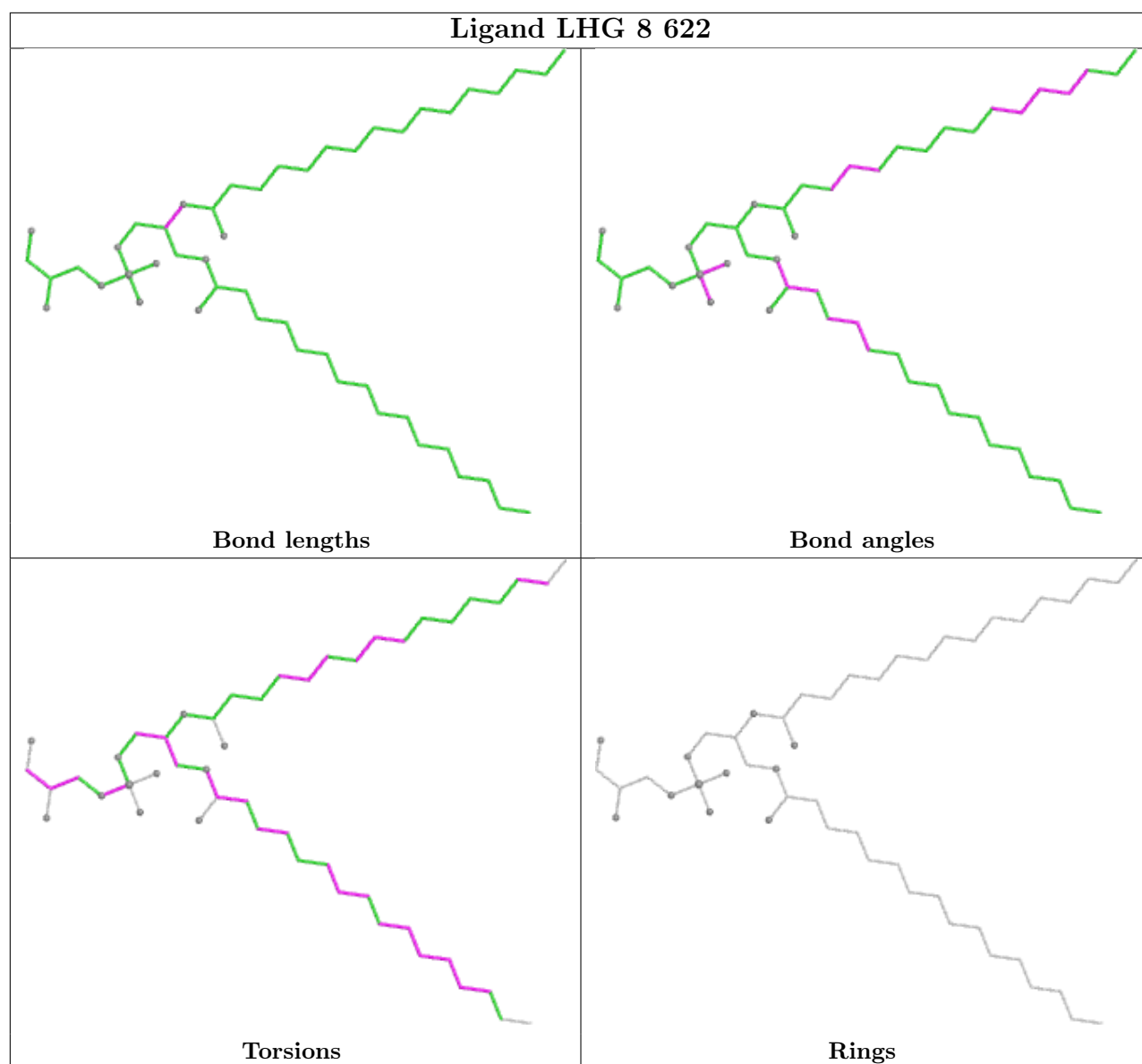


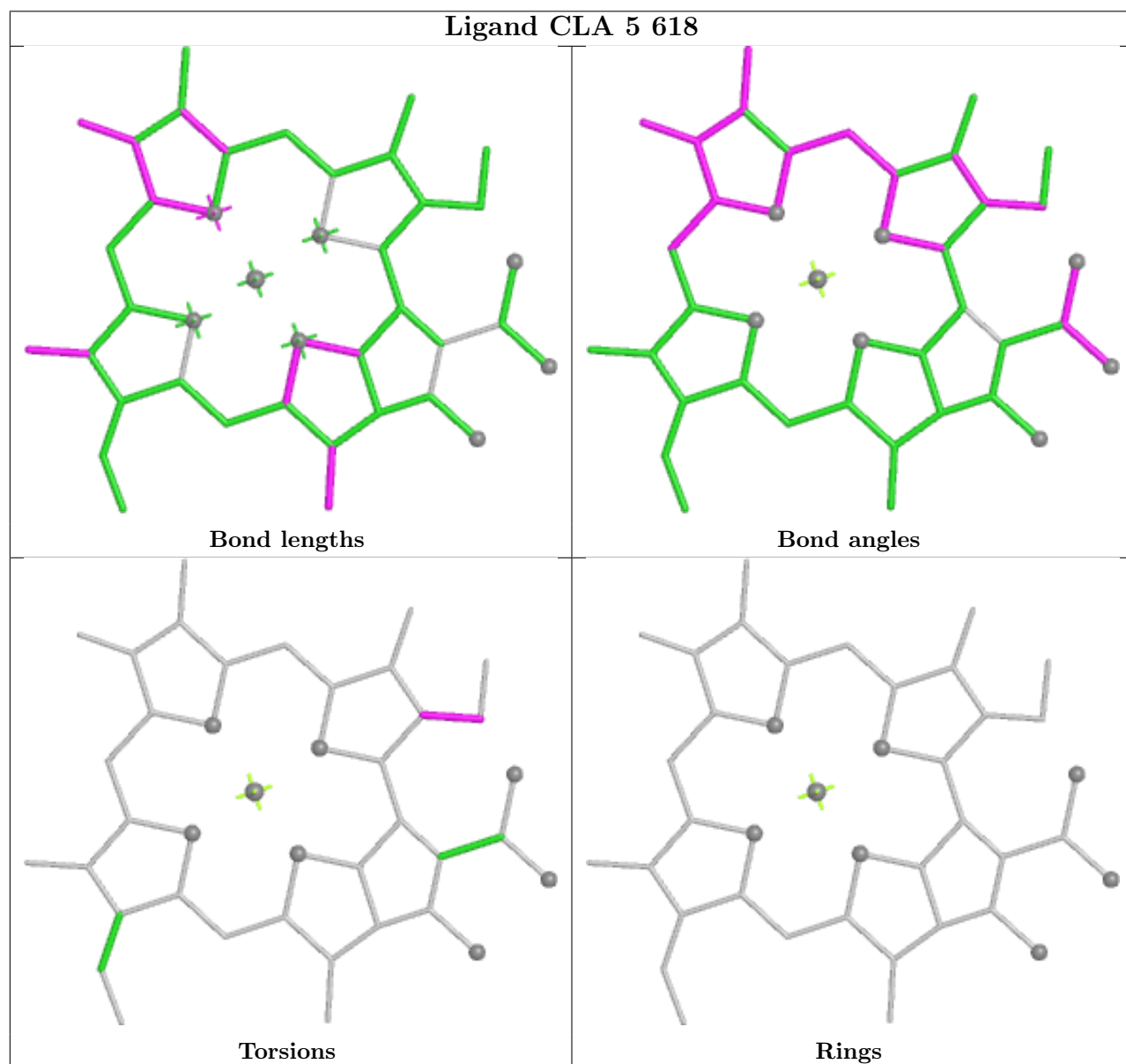
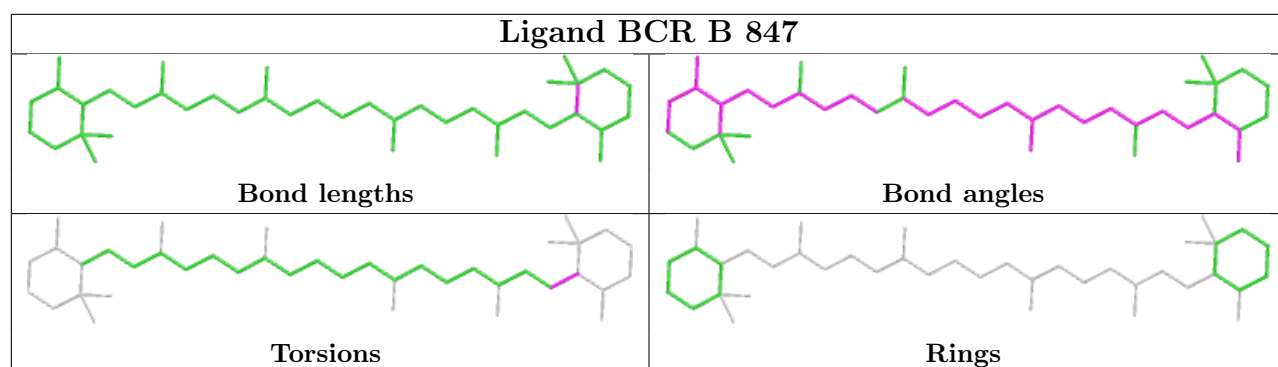
Ligand CLA 7 608



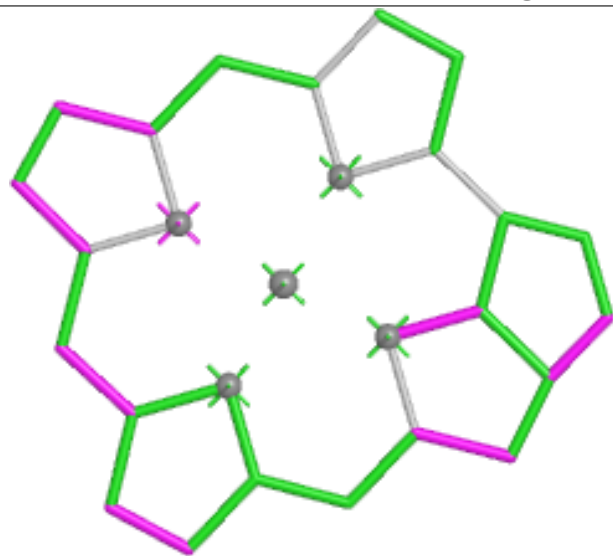
Ligand CLA B 840



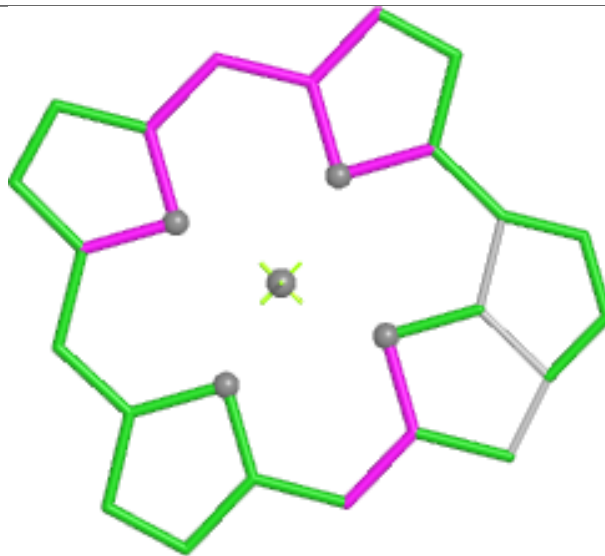




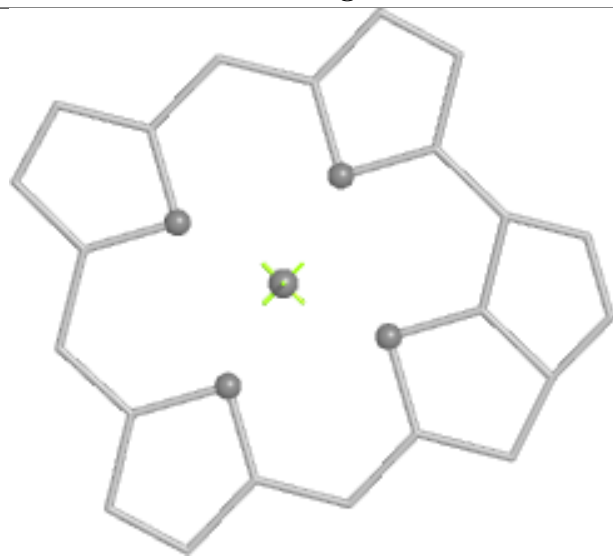
Ligand CLA 9 604



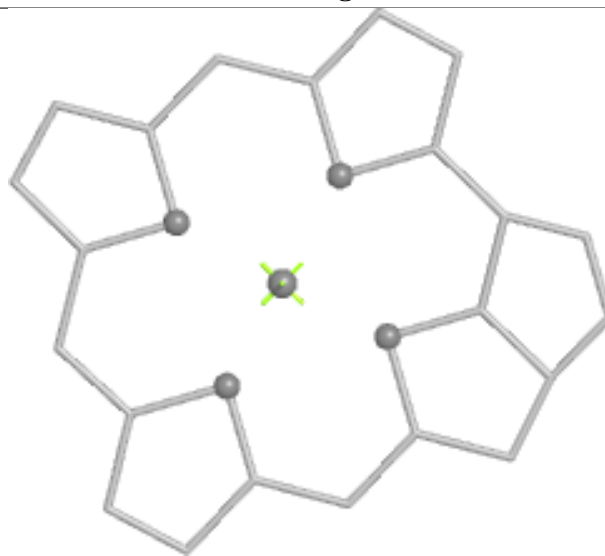
Bond lengths



Bond angles

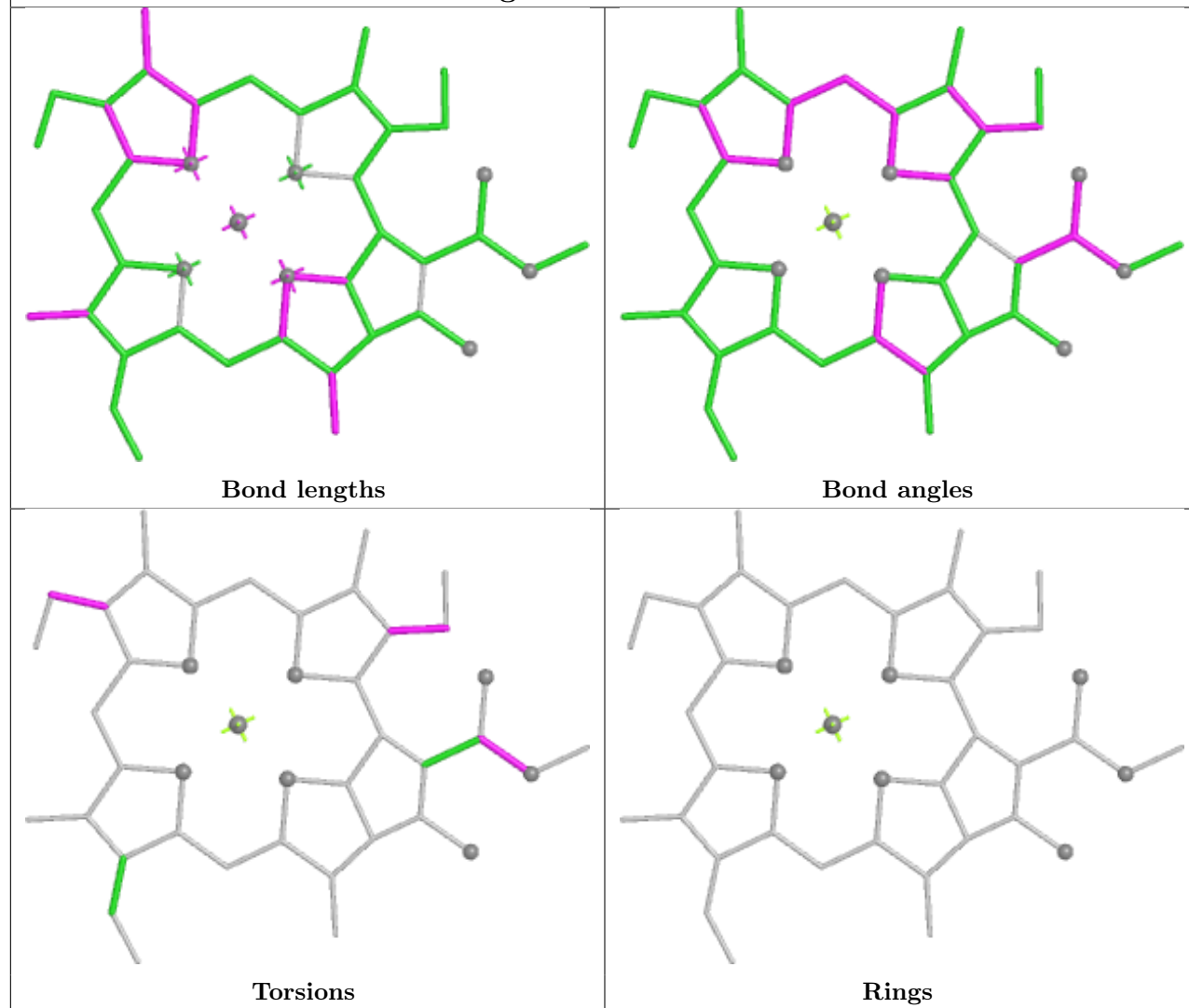


Torsions

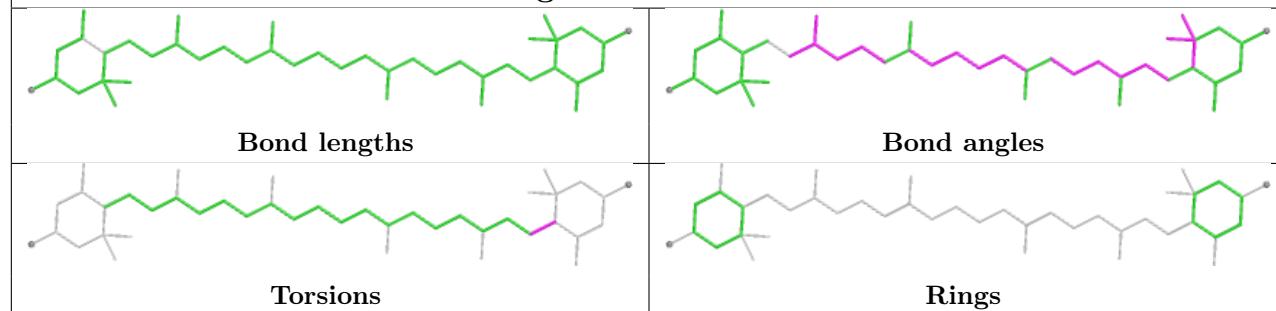


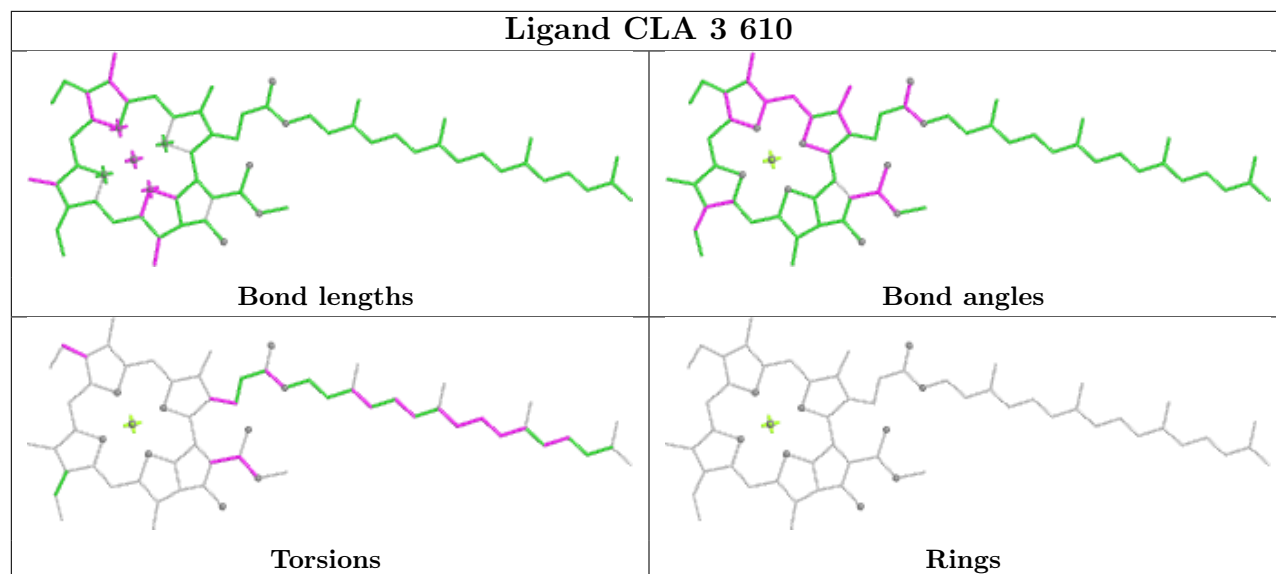
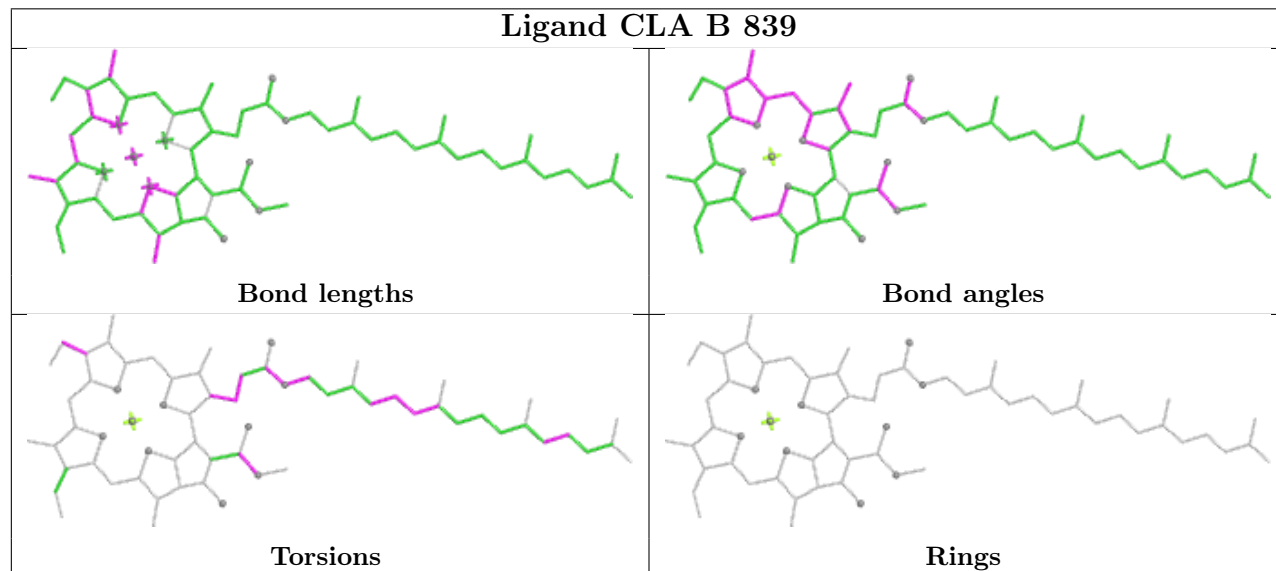
Rings

Ligand CLA 8 611

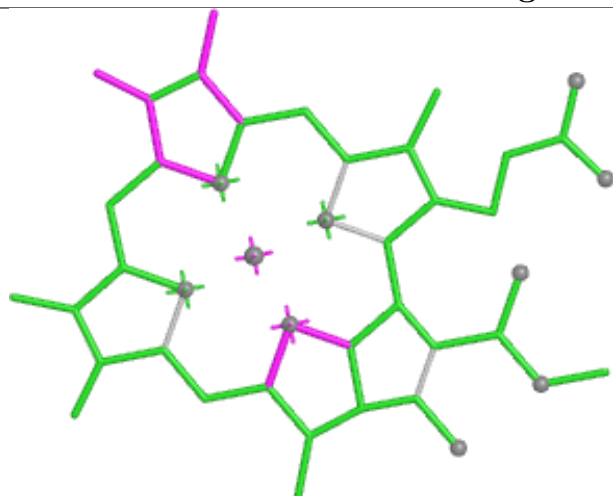


Ligand LUT a 617

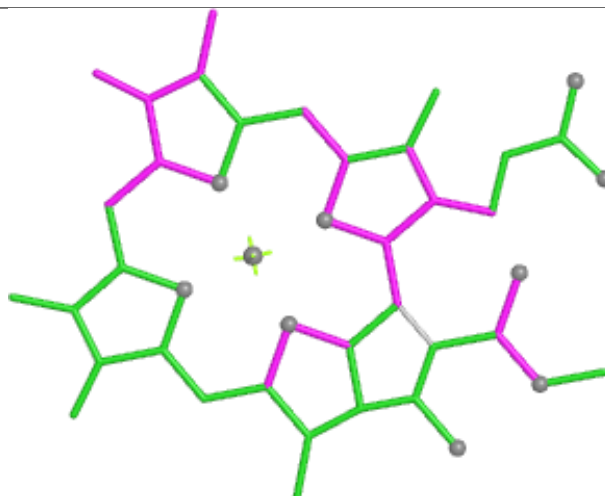


Ligand CLA 3 610**Ligand CLA B 839**

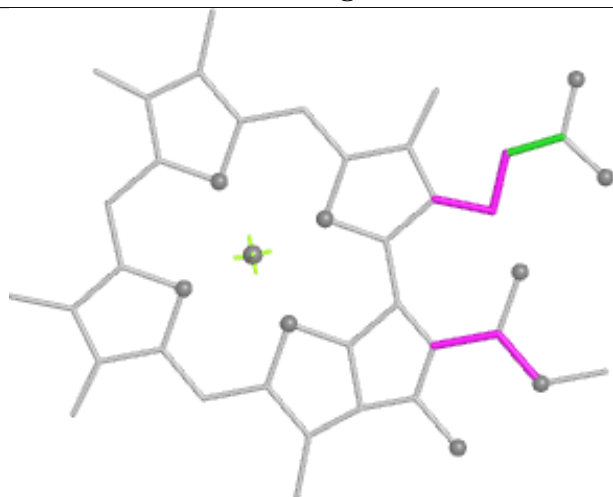
Ligand CLA 8 616



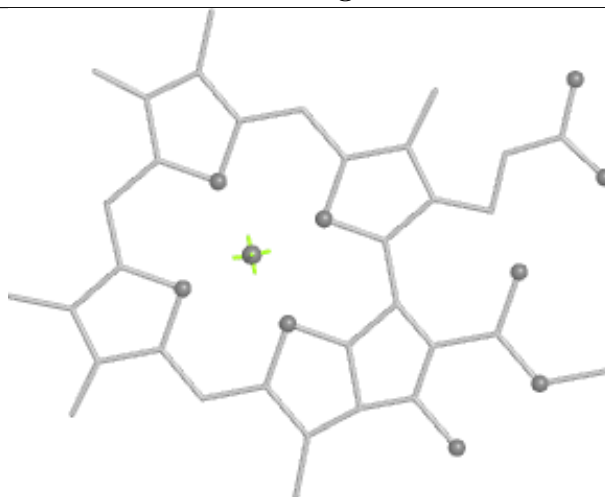
Bond lengths



Bond angles

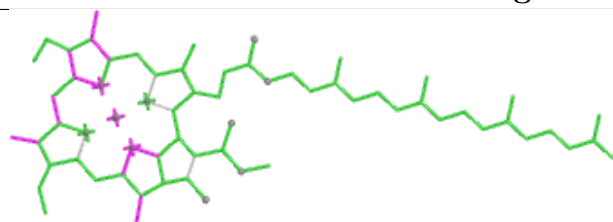


Torsions

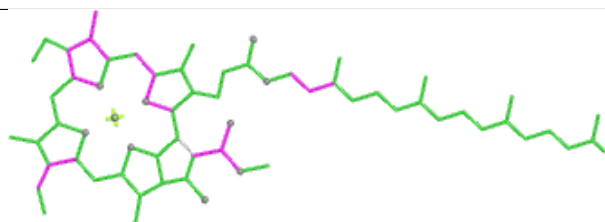


Rings

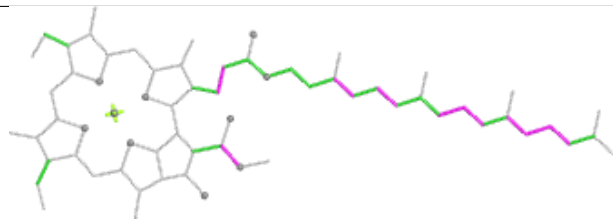
Ligand CLA A 829



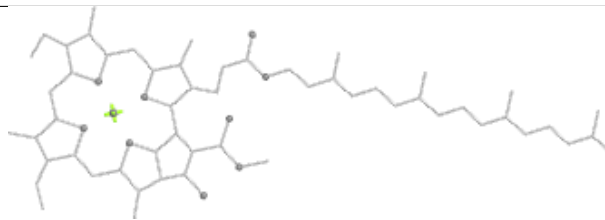
Bond lengths



Bond angles

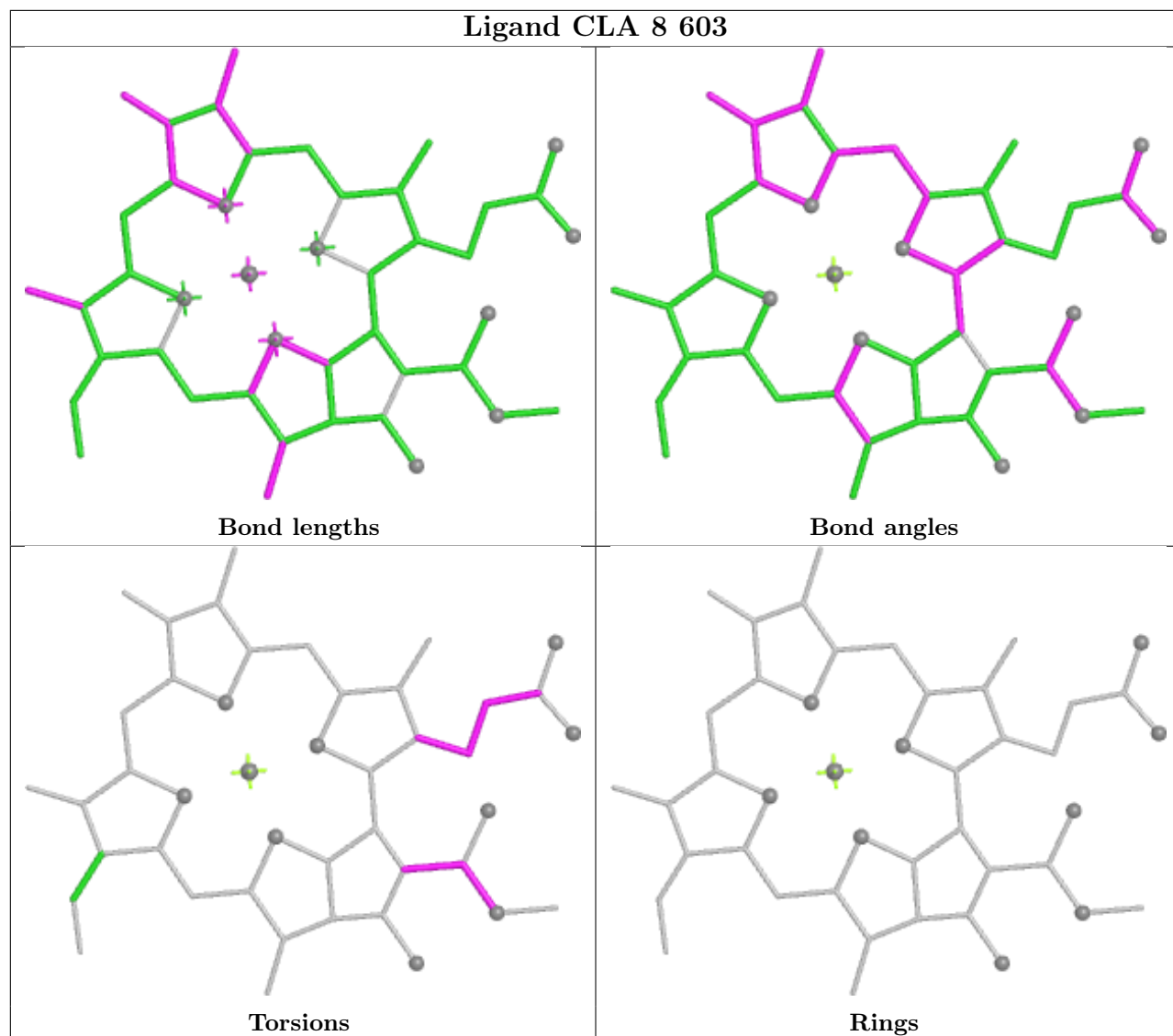


Torsions

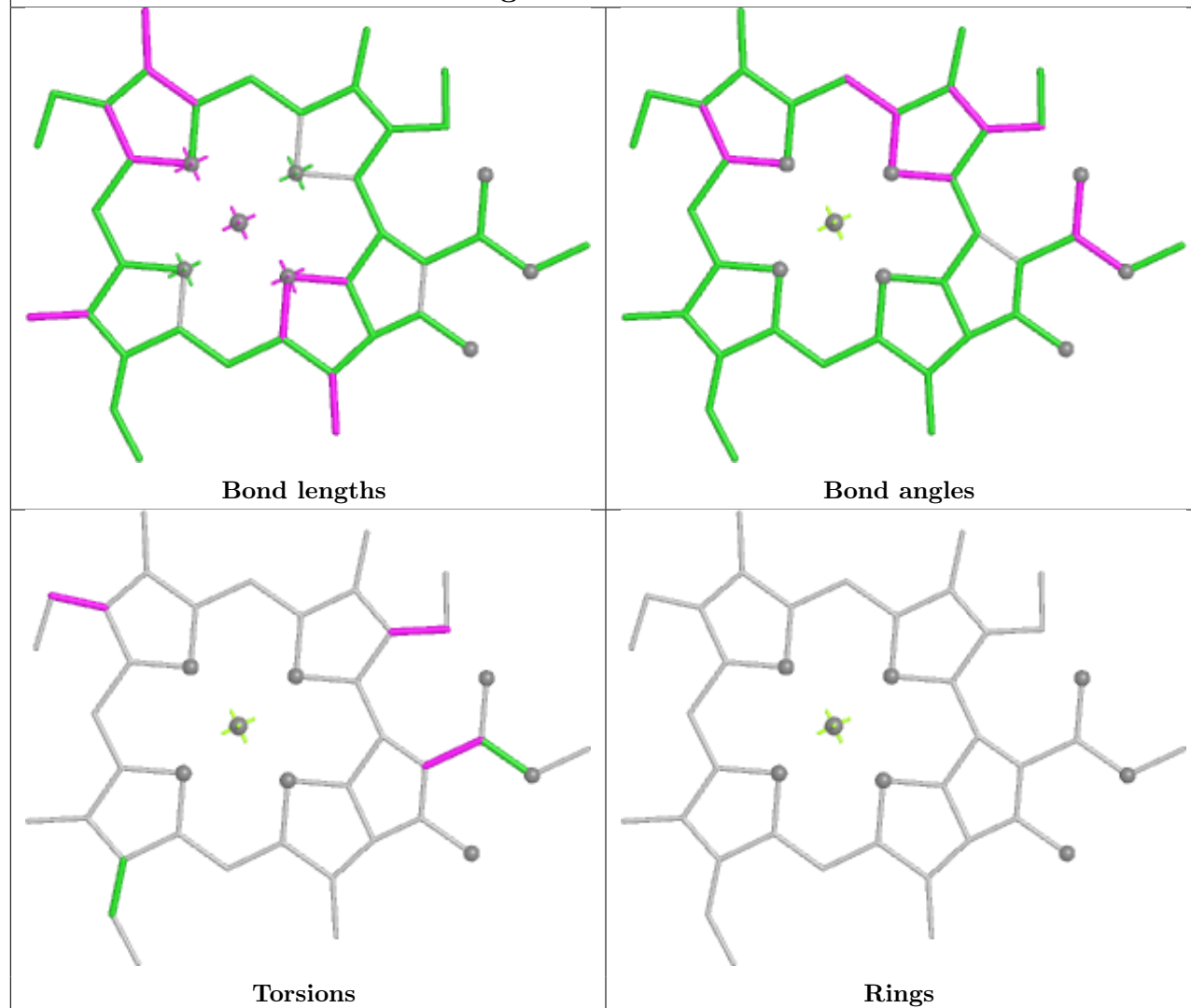


Rings

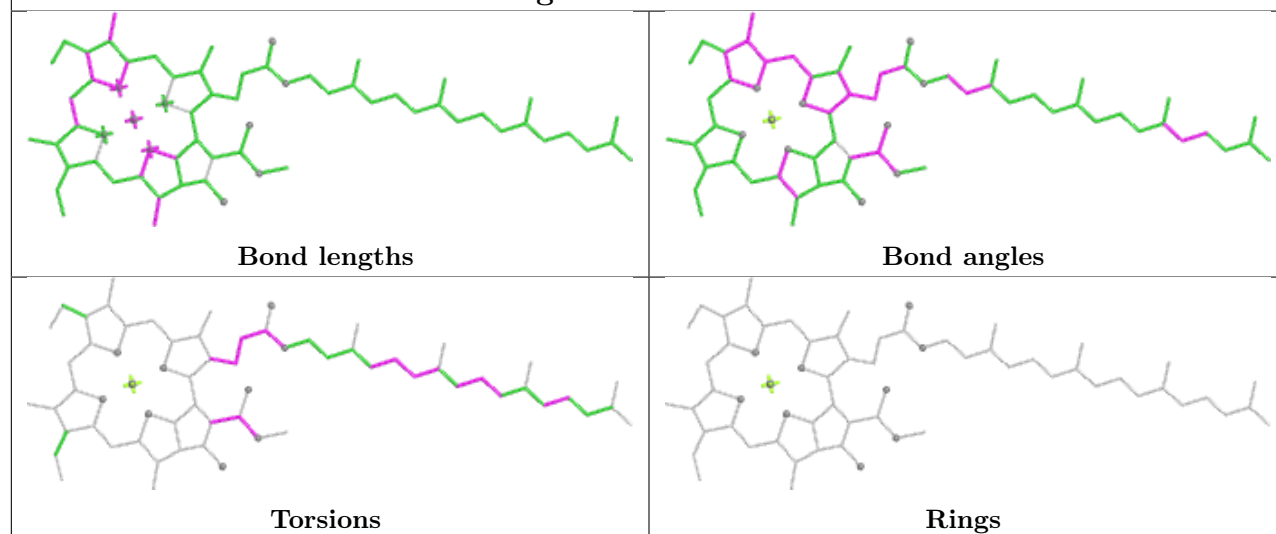
Ligand CLA 8 603

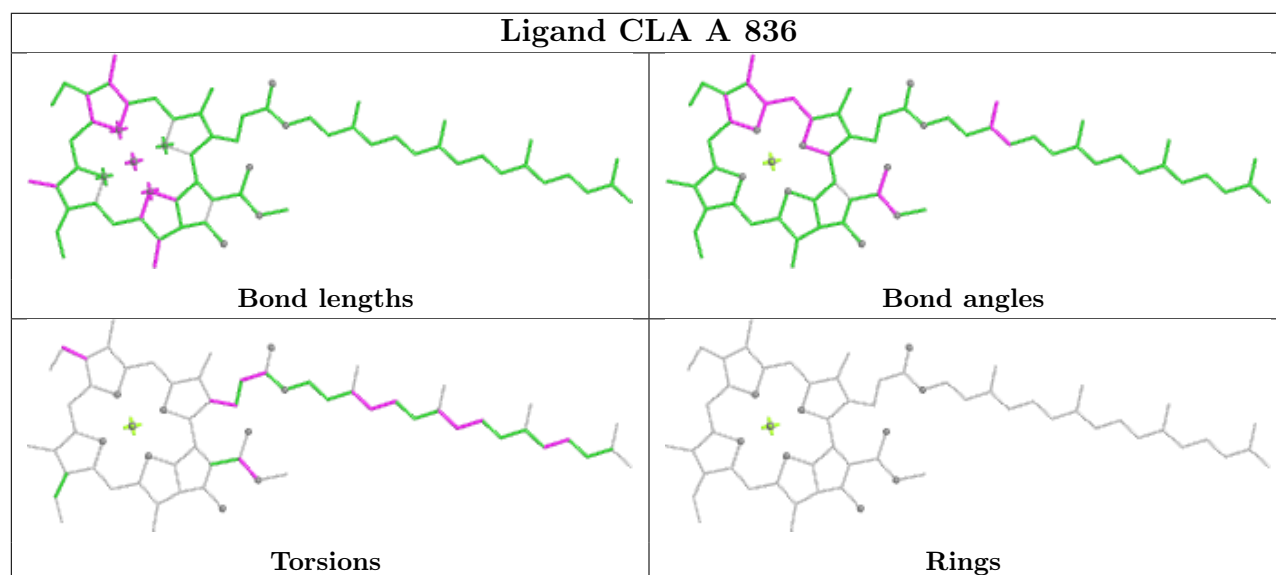
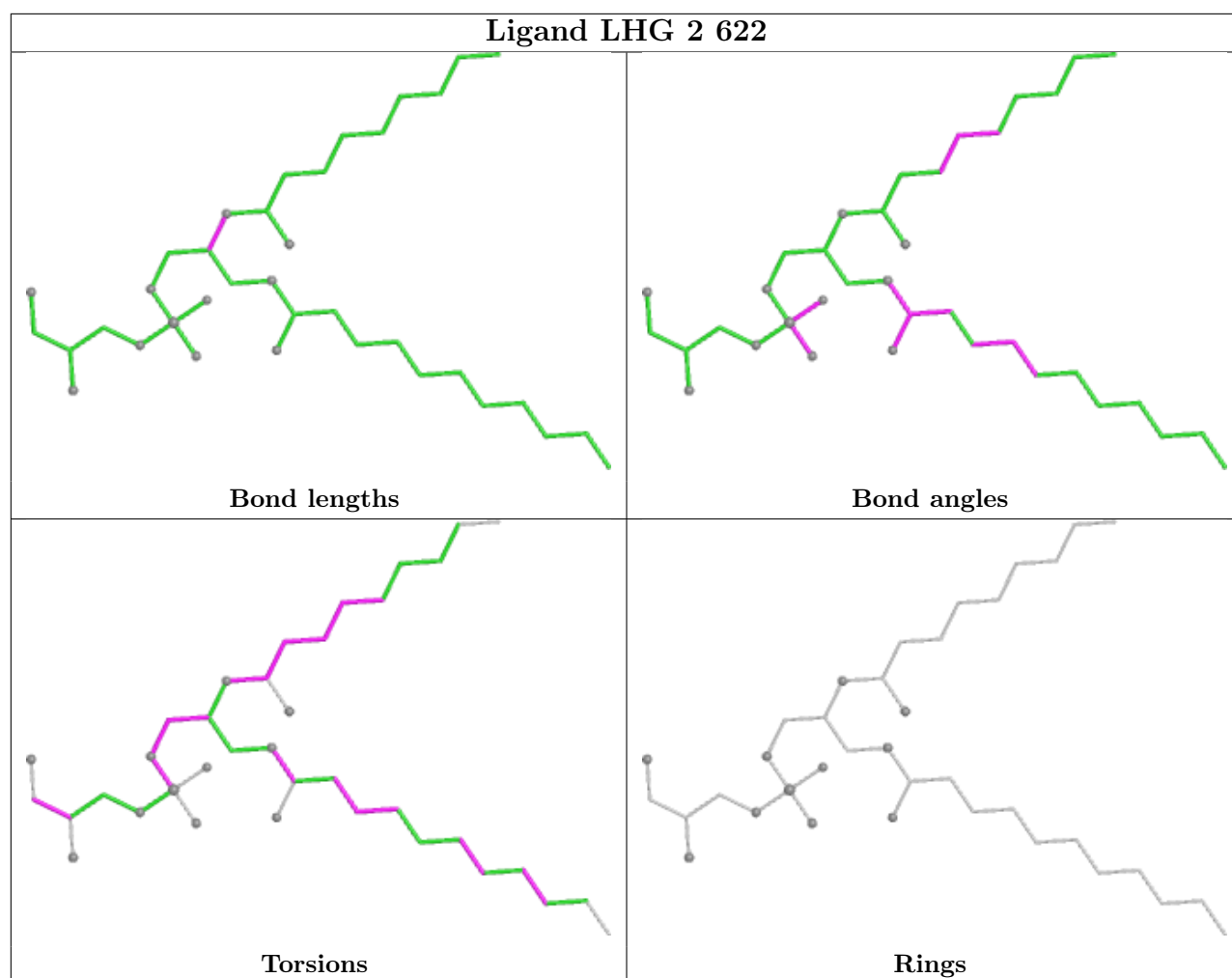


Ligand CLA 6 611

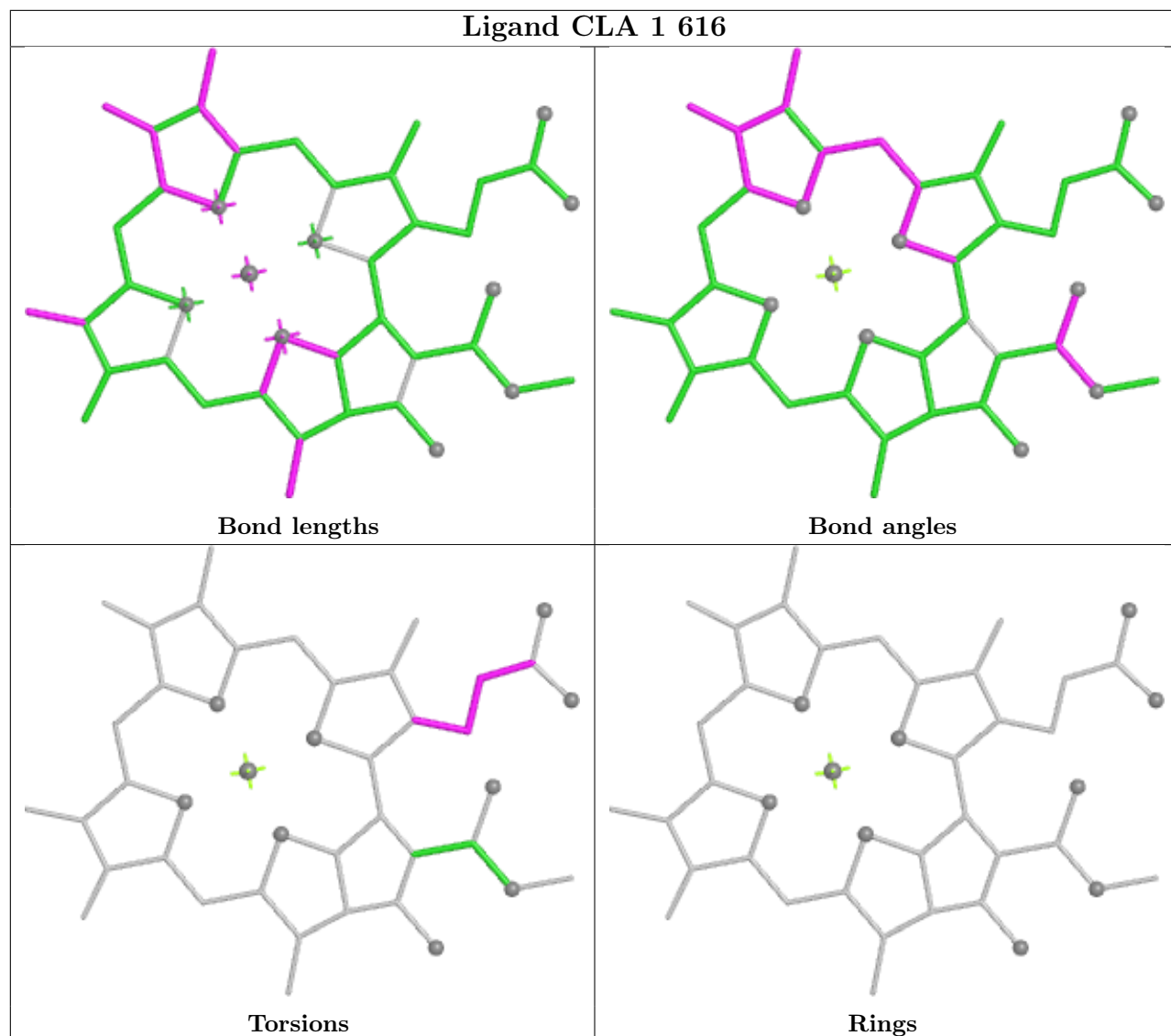


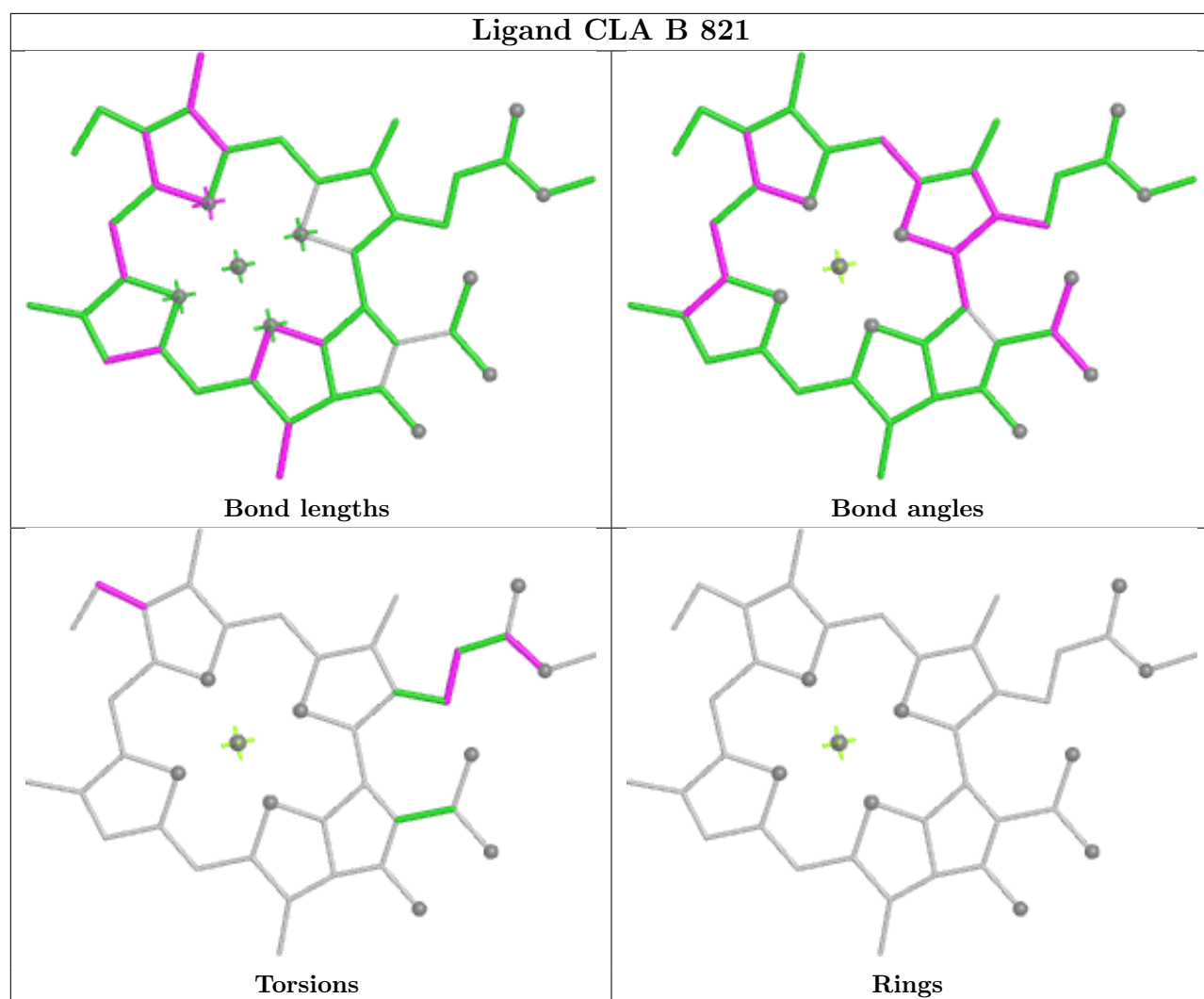
Ligand CLA 6 616



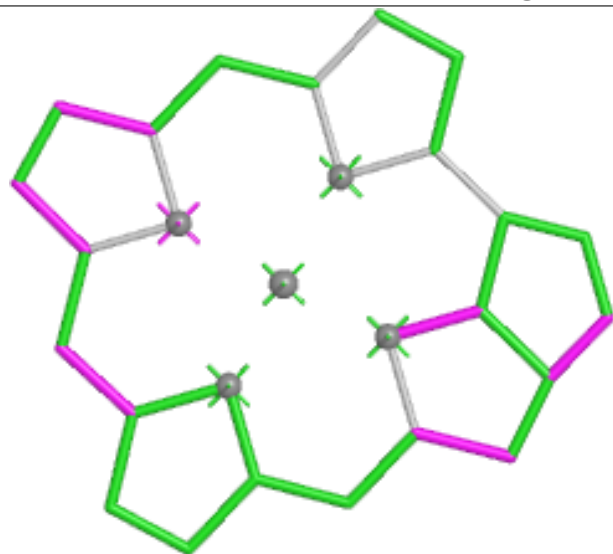


Ligand CLA 1 616

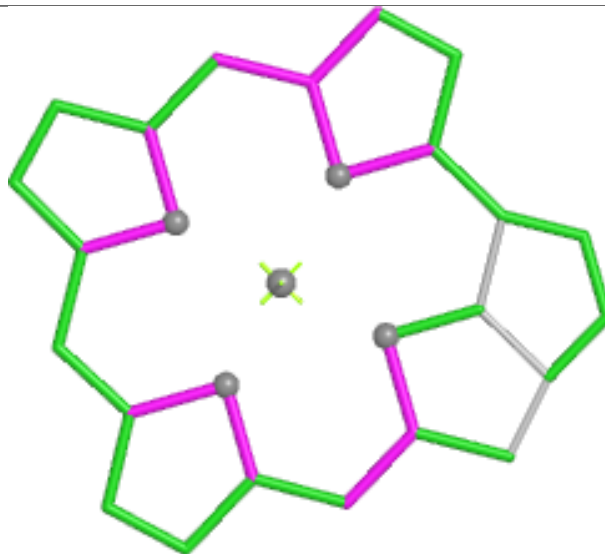




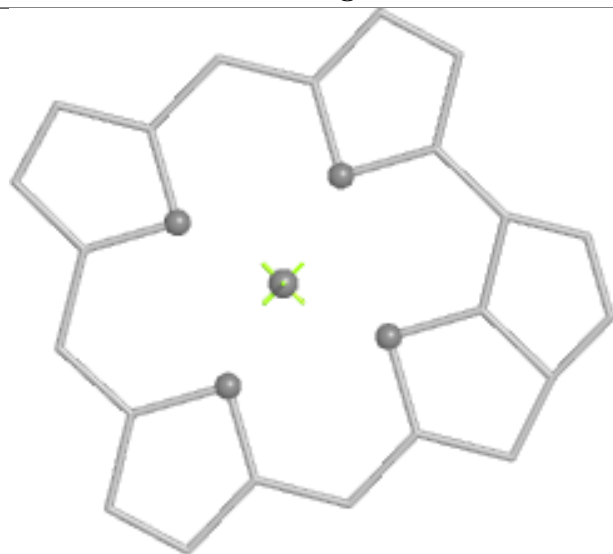
Ligand CLA 2 604



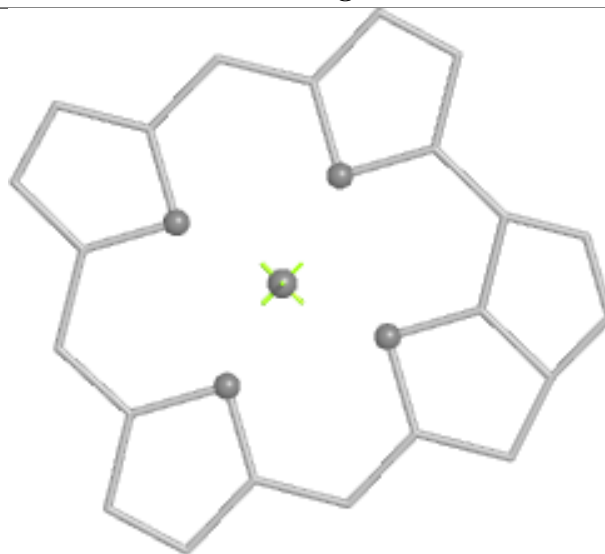
Bond lengths



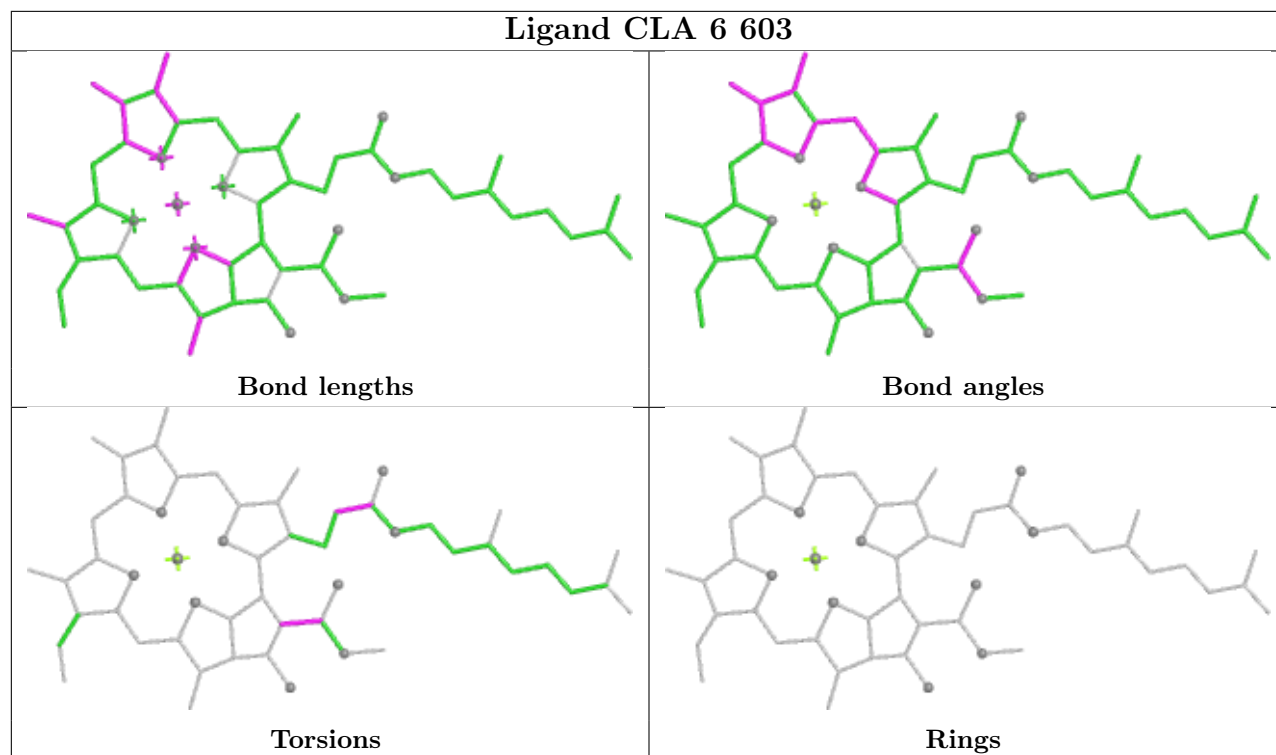
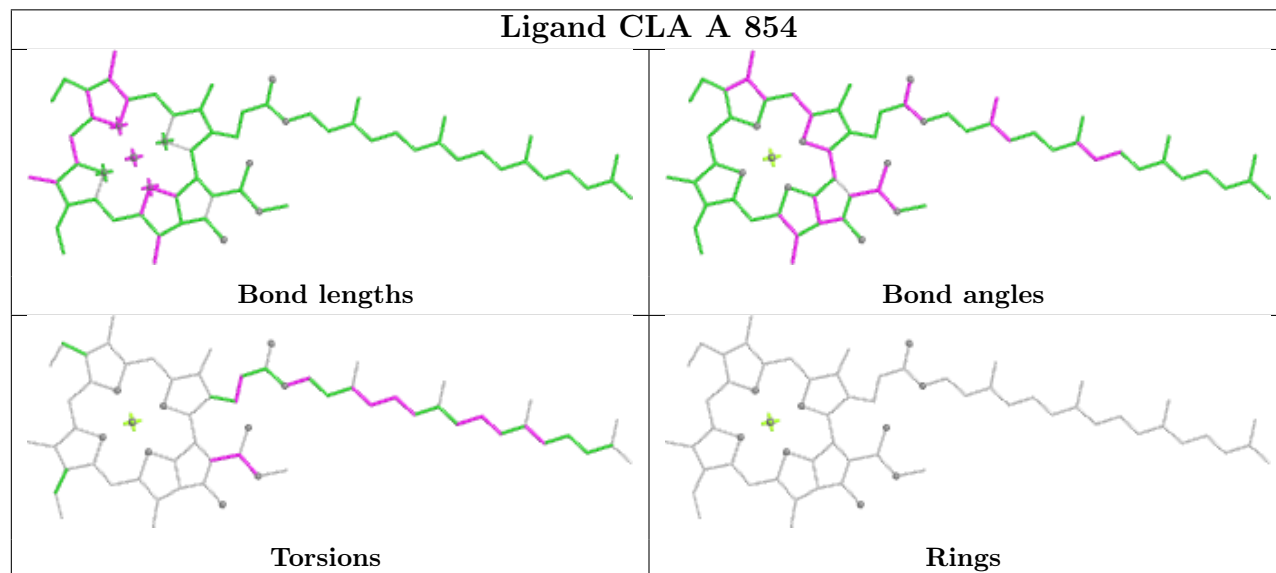
Bond angles

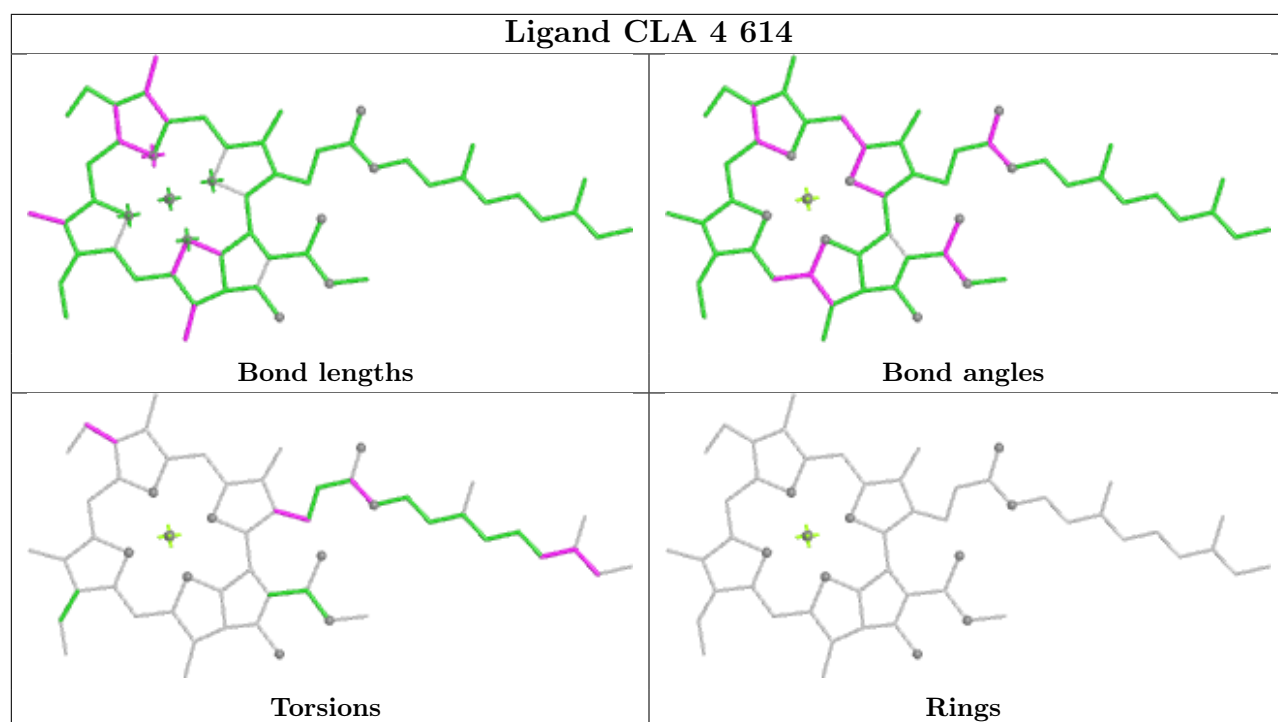


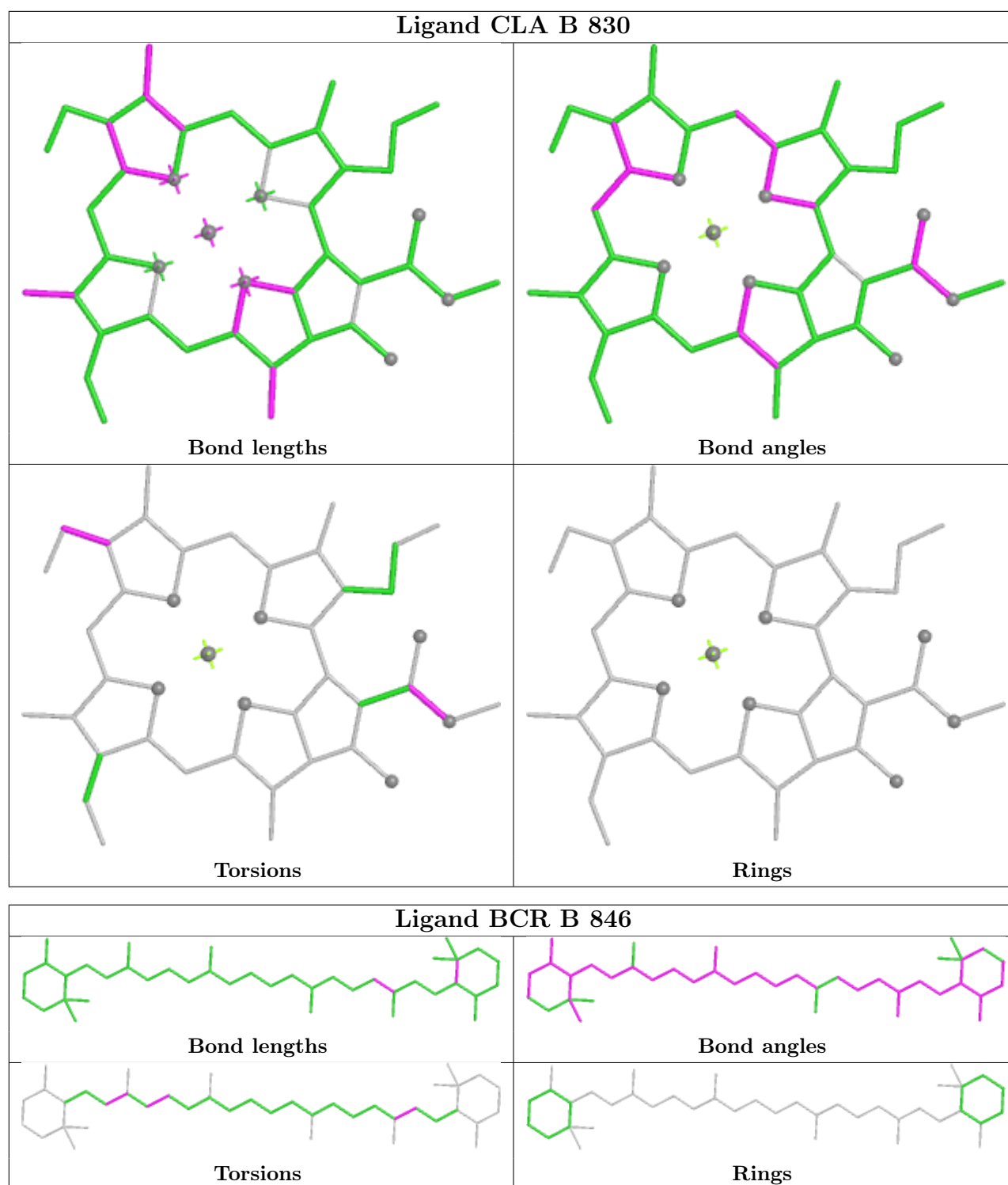
Torsions

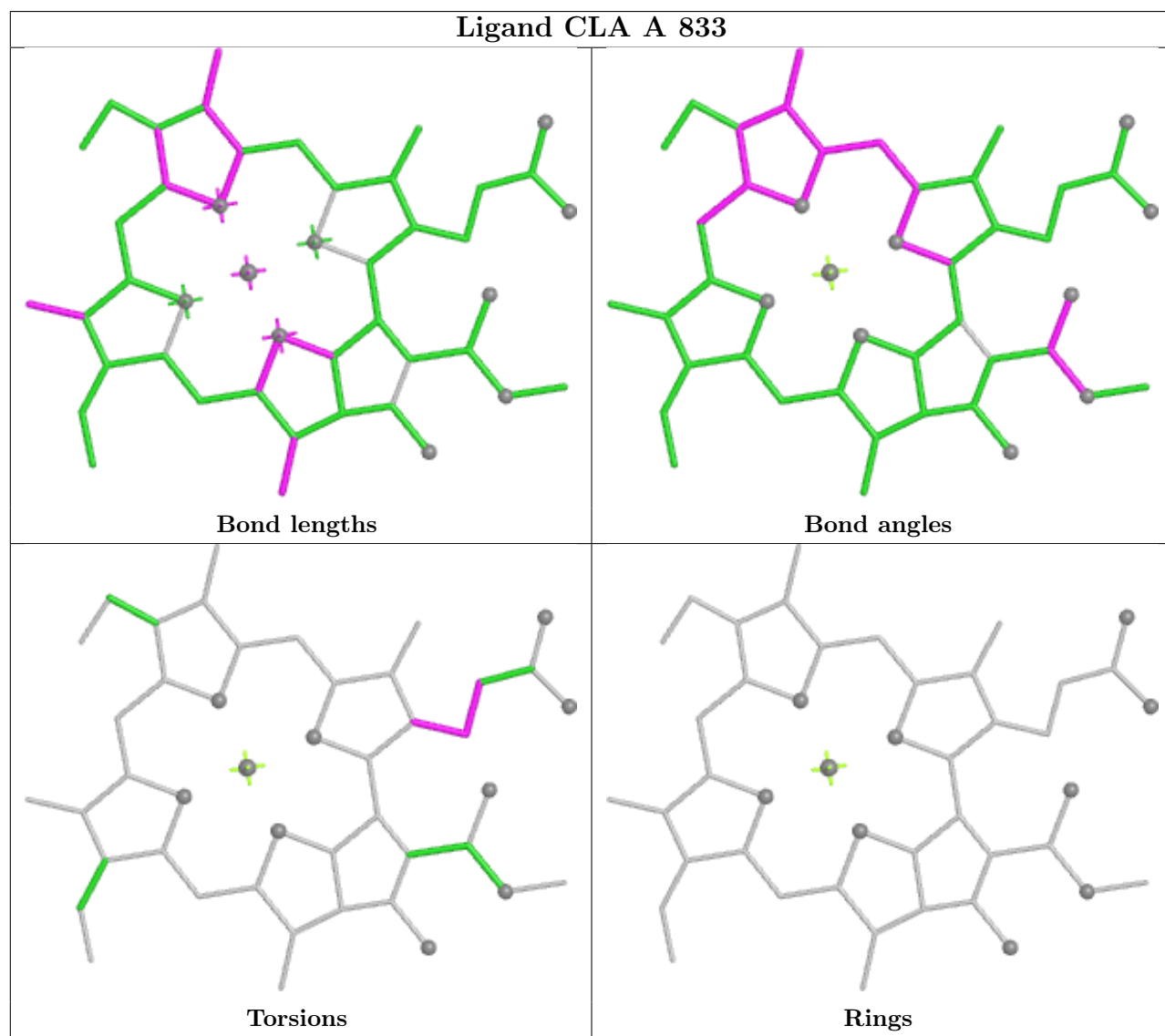
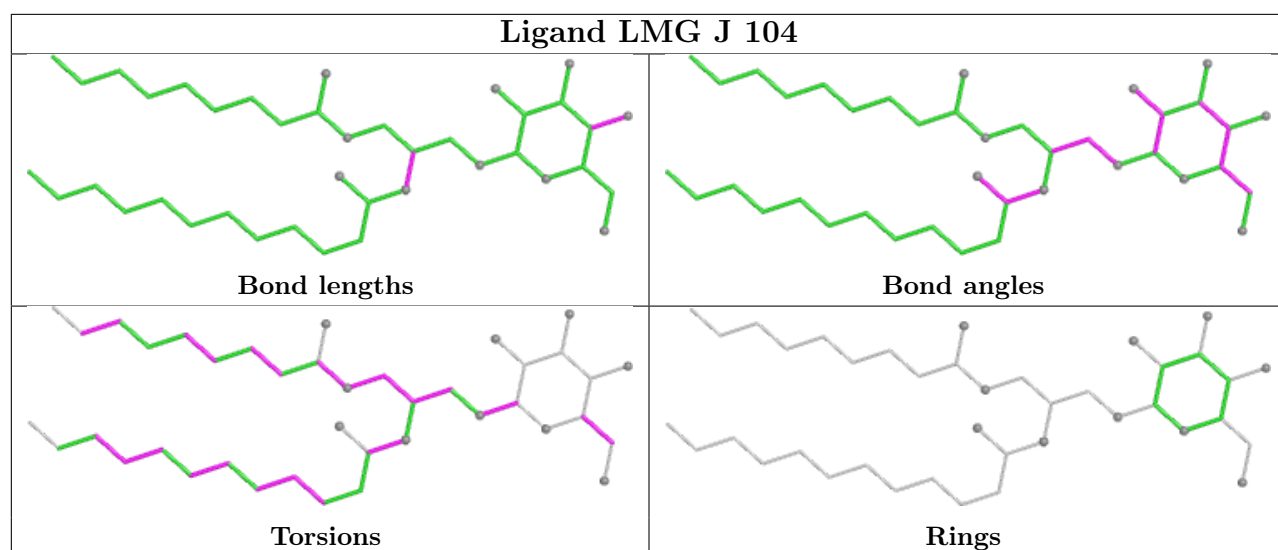


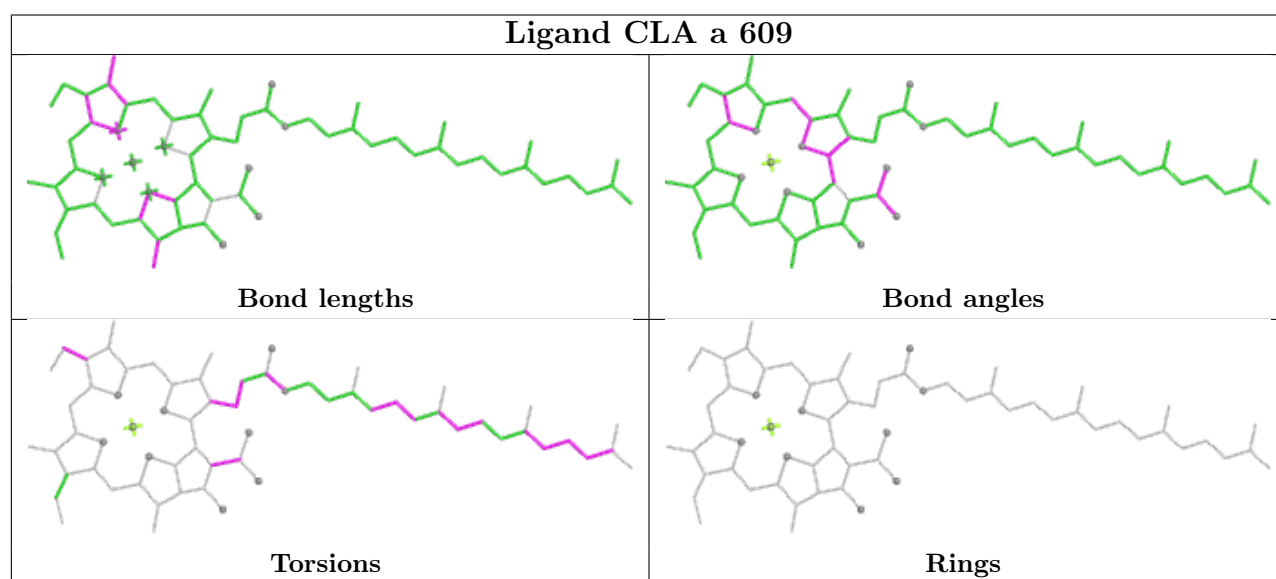
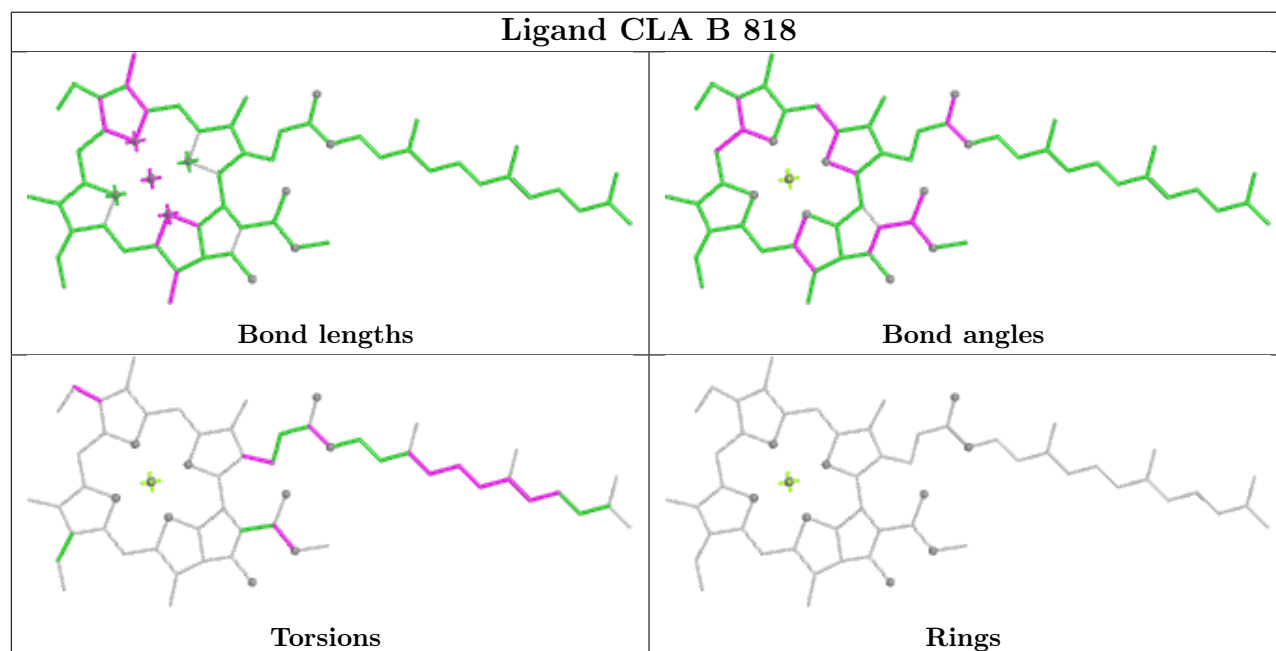
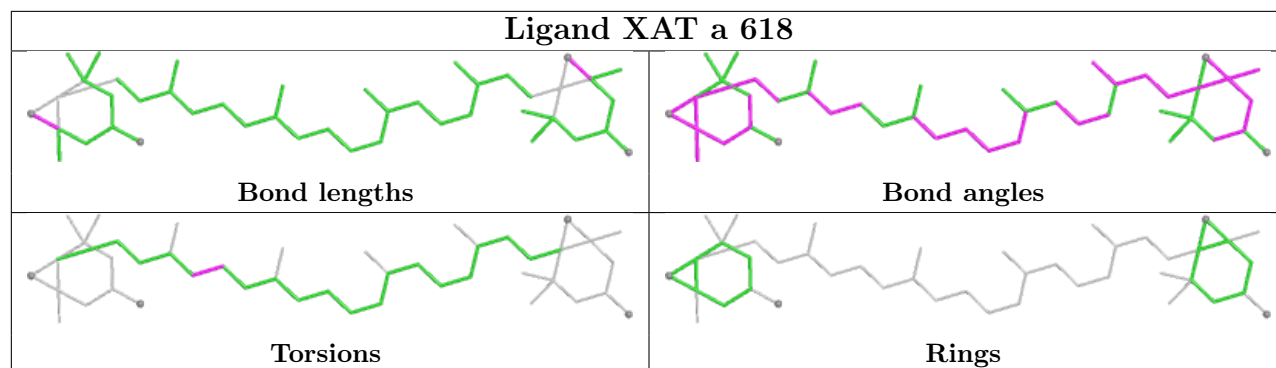
Rings

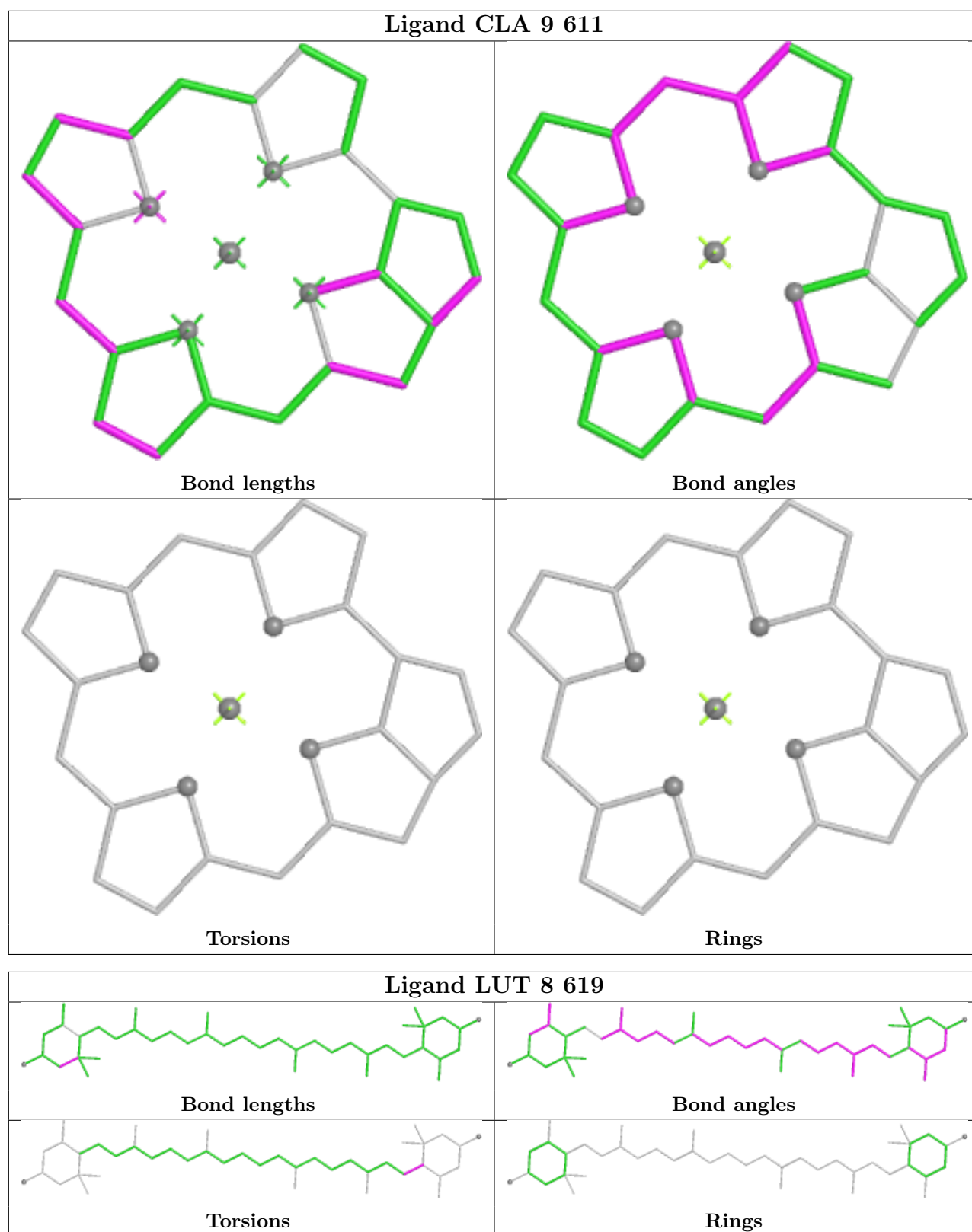
Ligand CLA 6 603**Ligand CLA A 854**



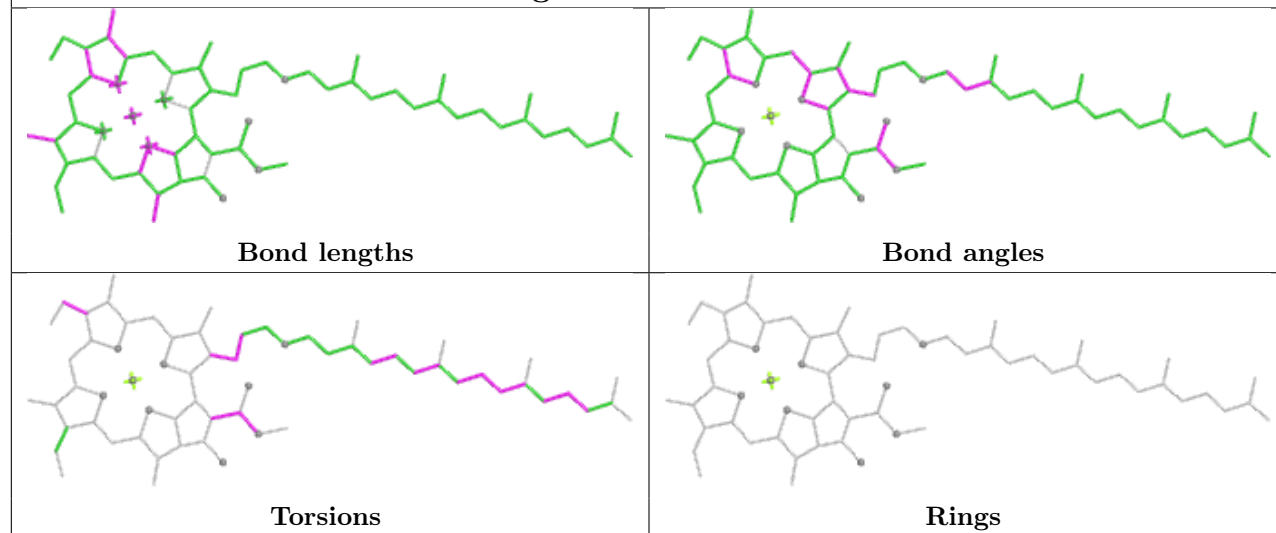




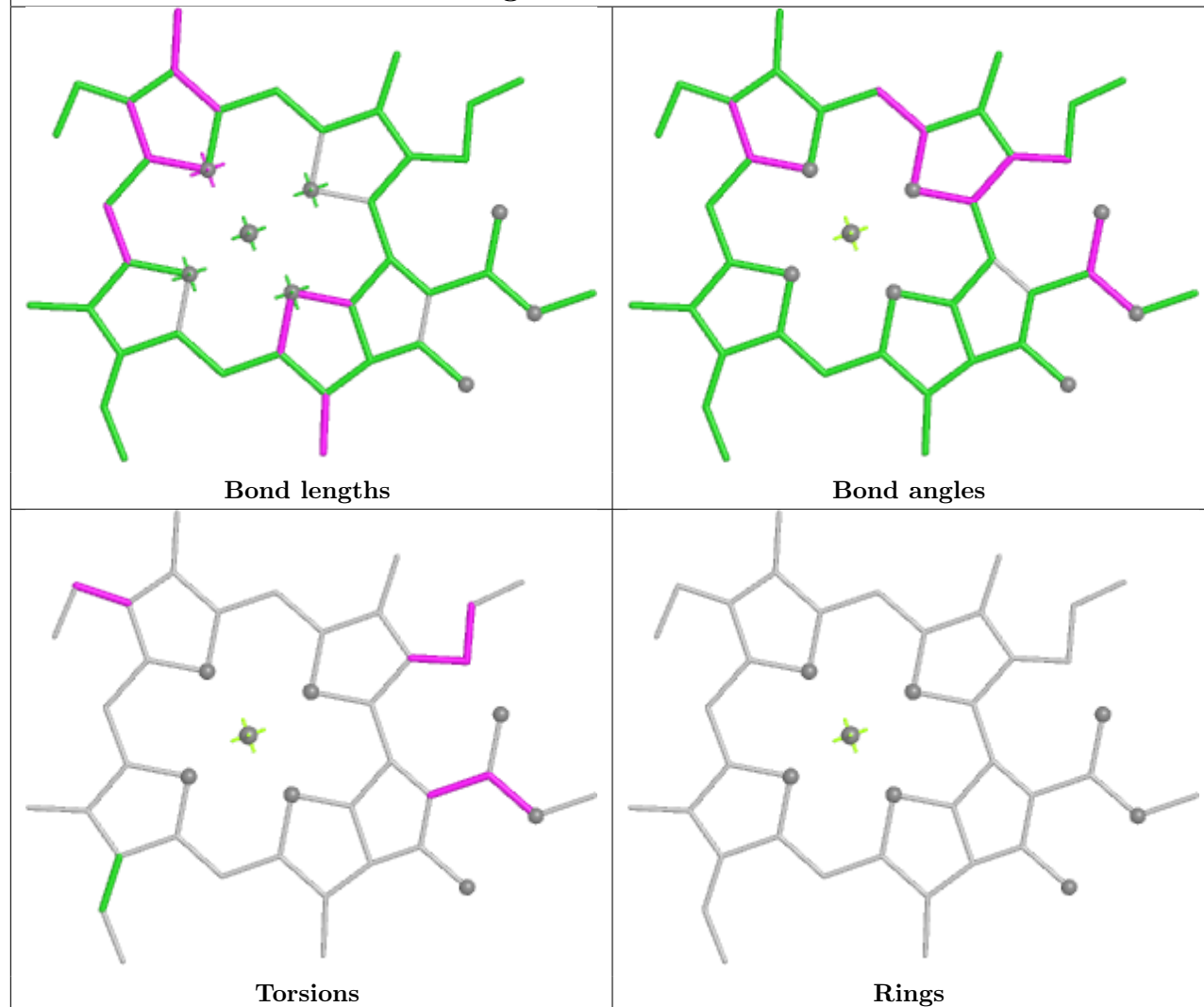


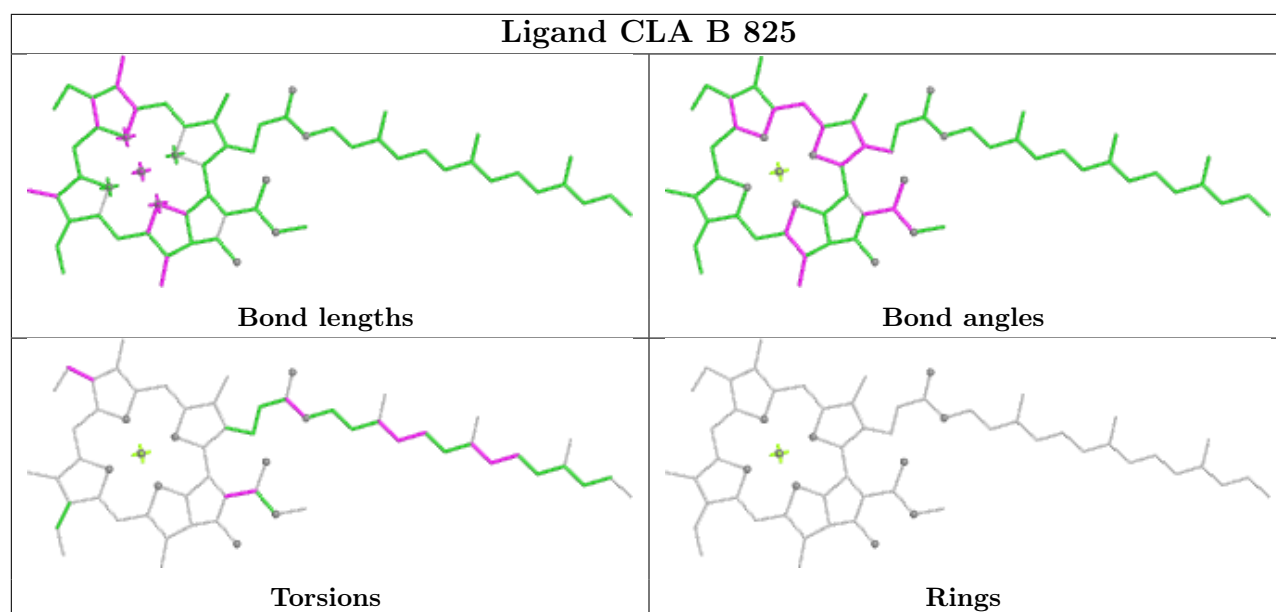


Ligand CLA B 810

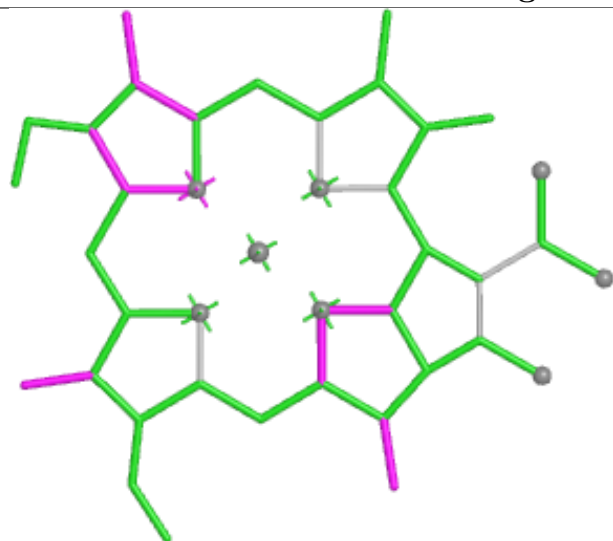


Ligand CLA B 812

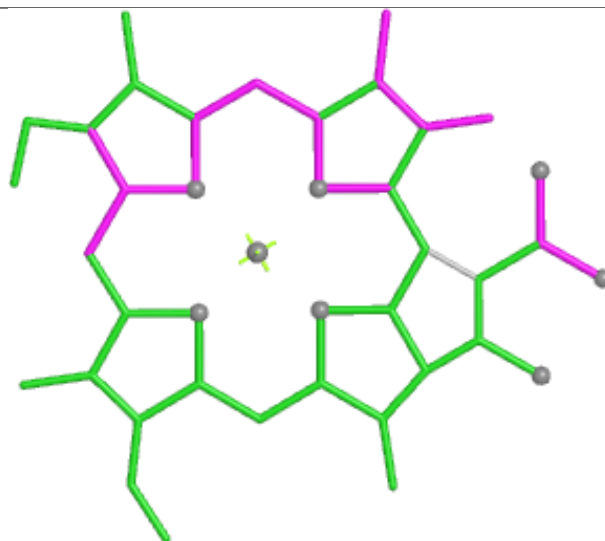




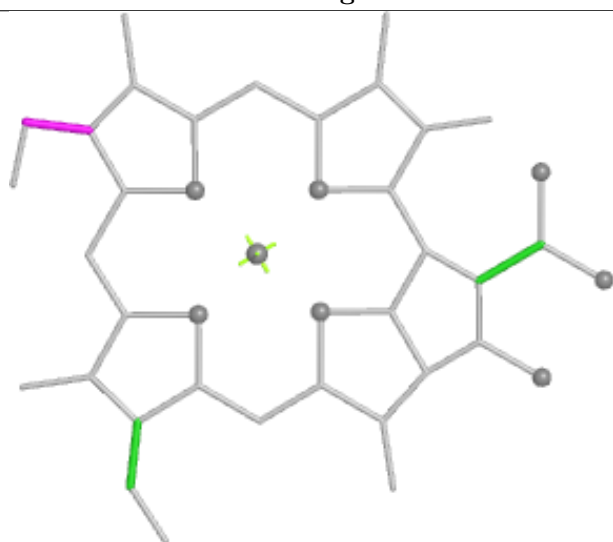
Ligand CLA 3 614



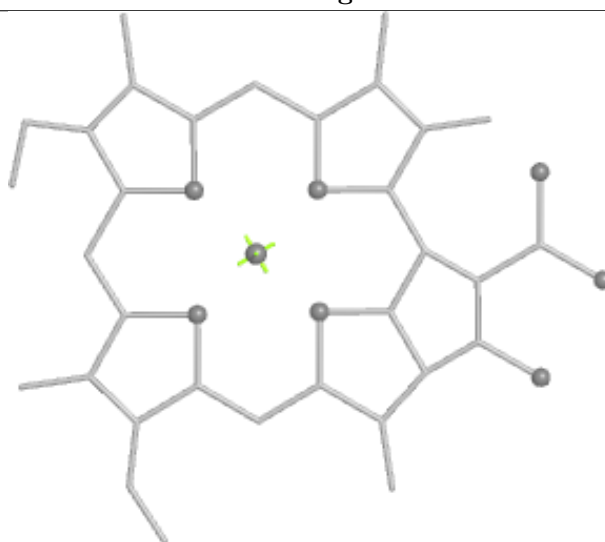
Bond lengths



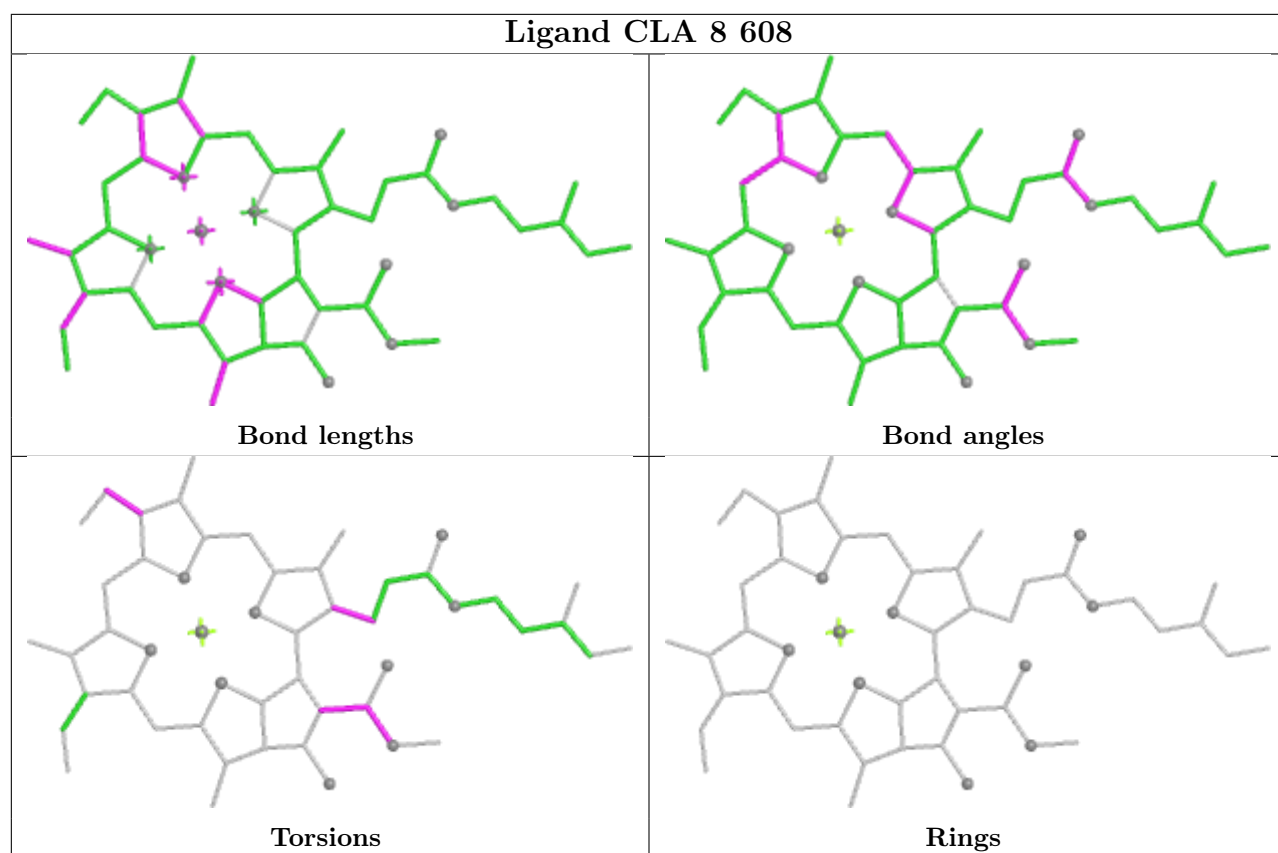
Bond angles



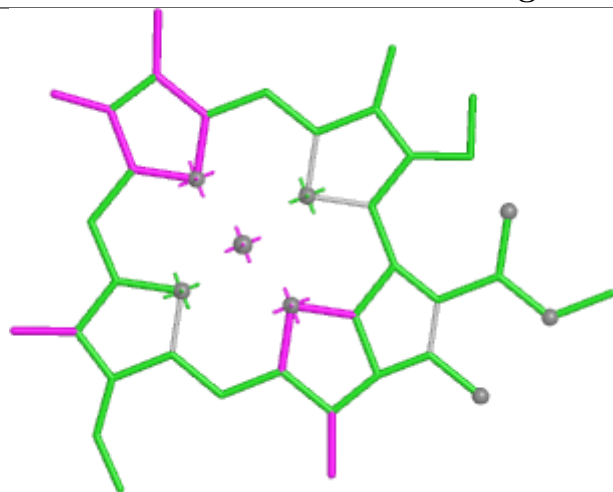
Torsions



Rings



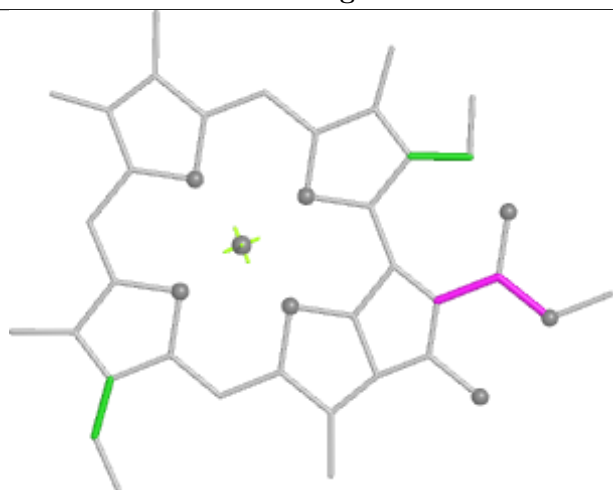
Ligand CLA 8 607



Bond lengths



Bond angles

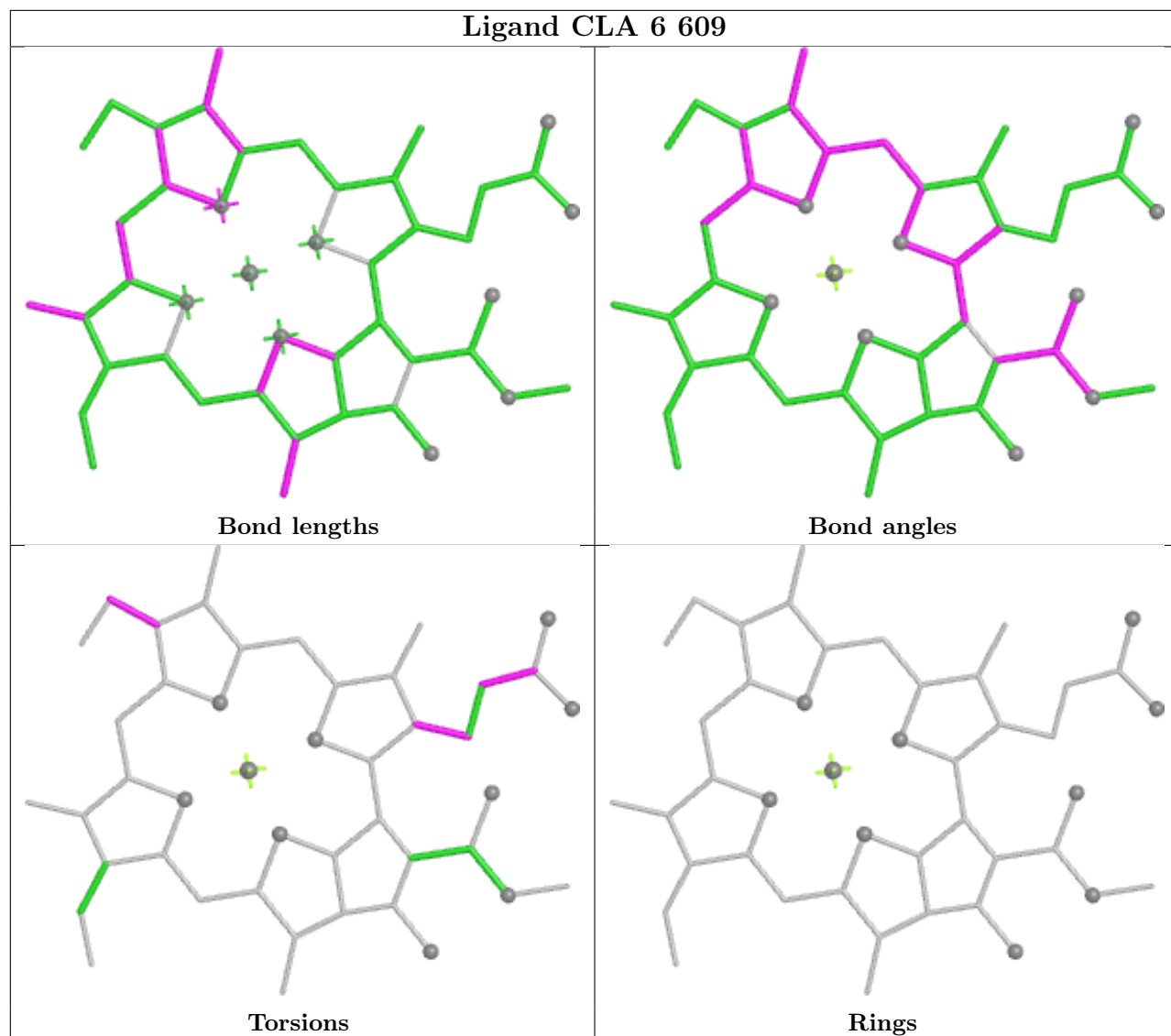


Torsions

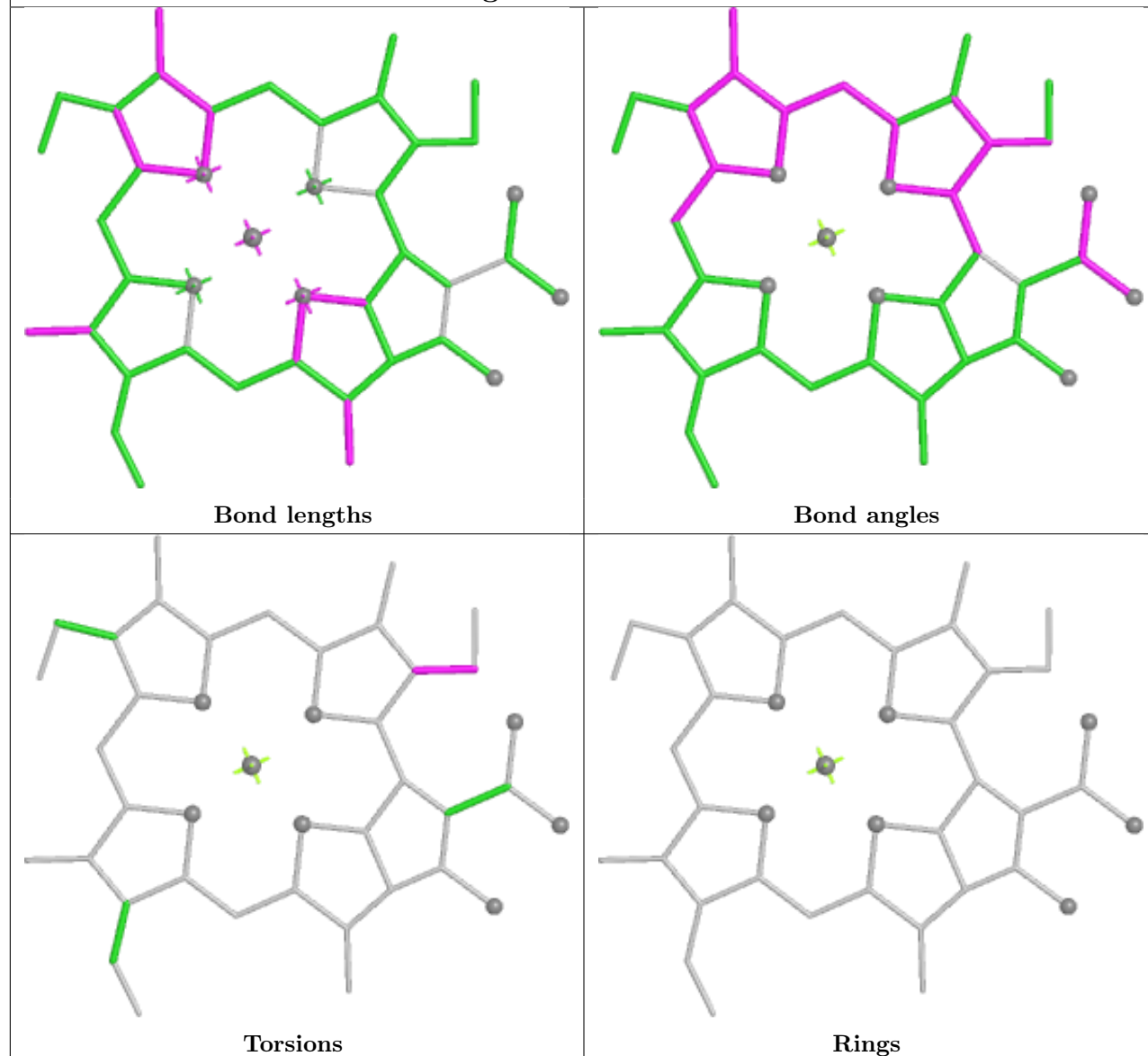


Rings

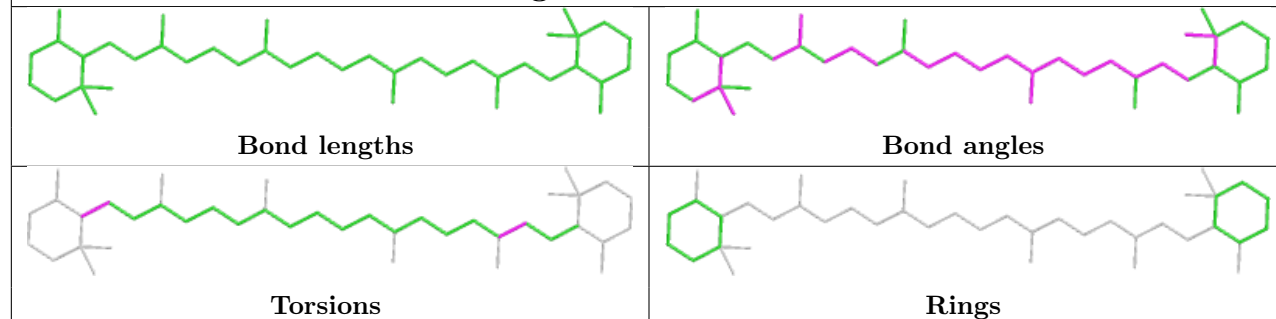
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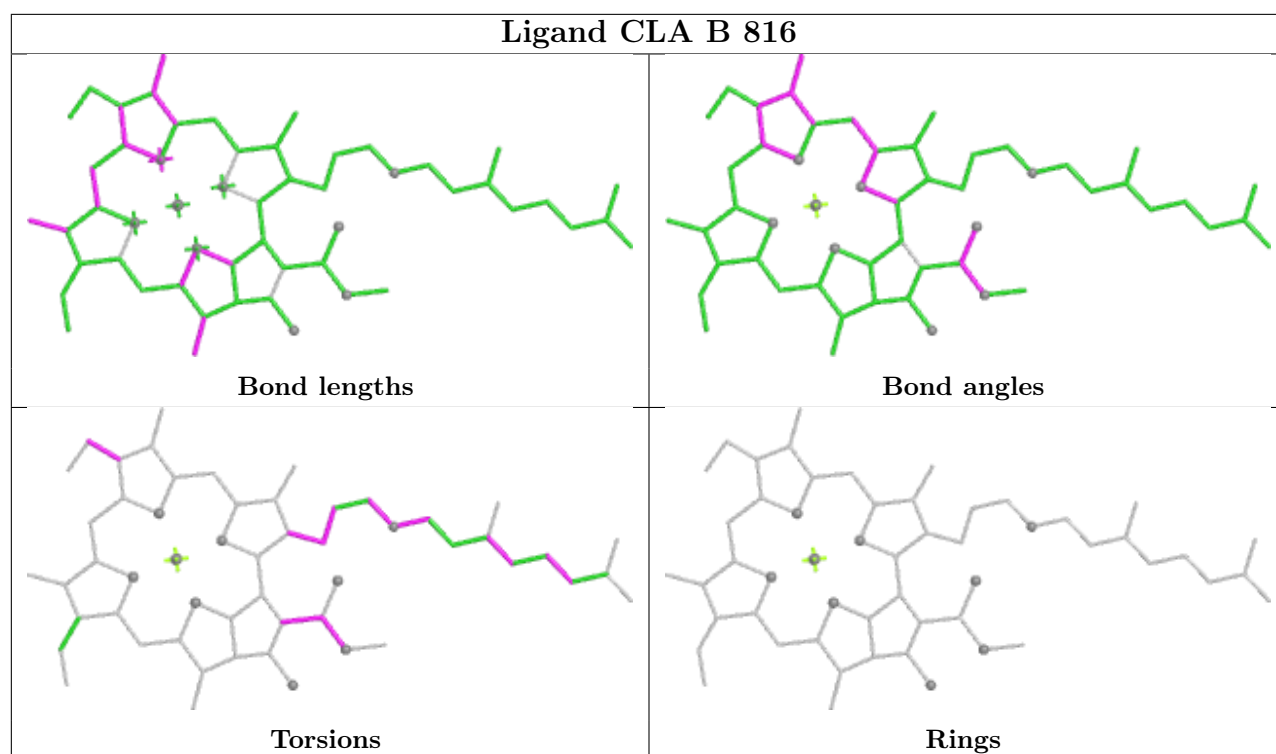


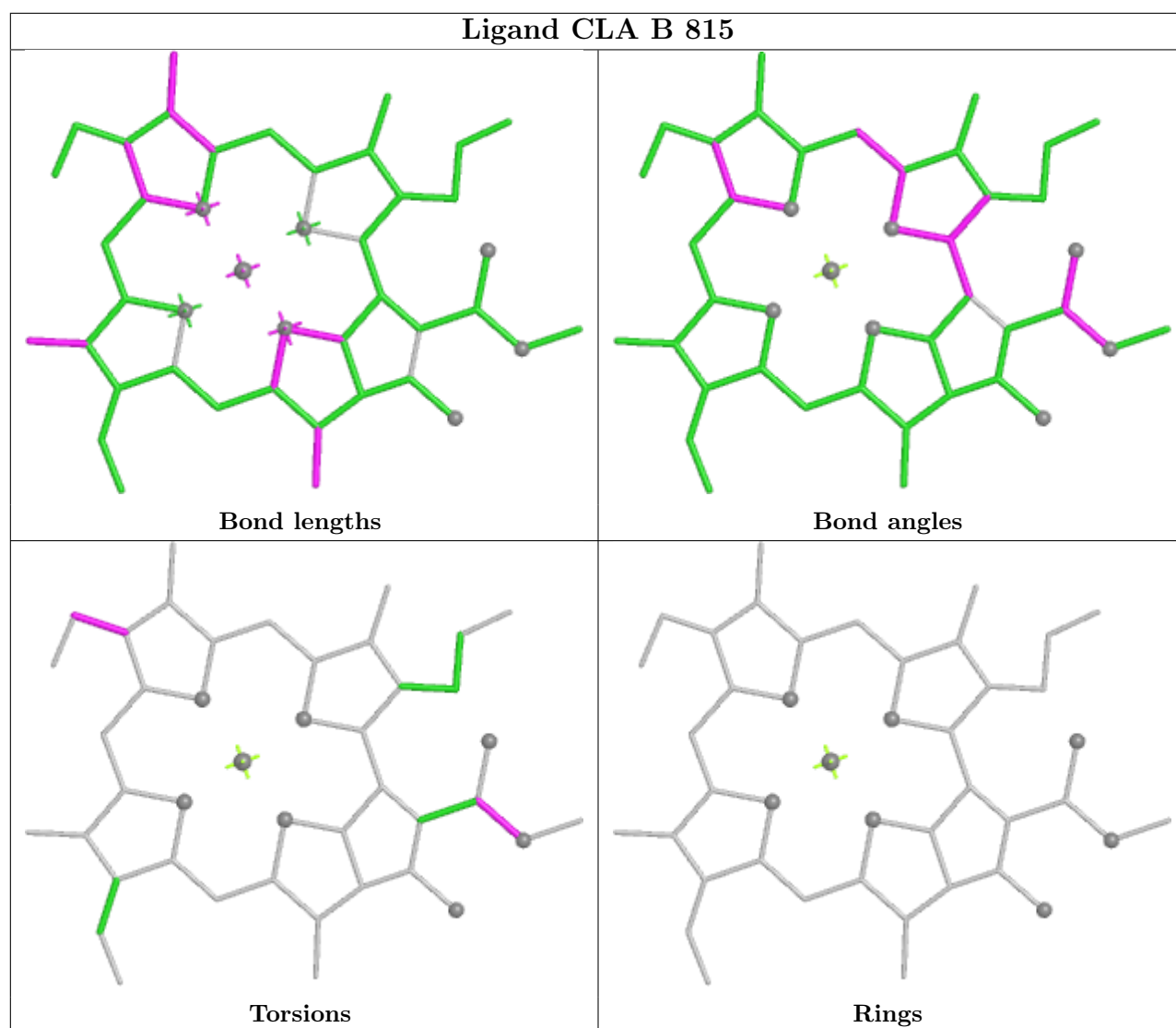
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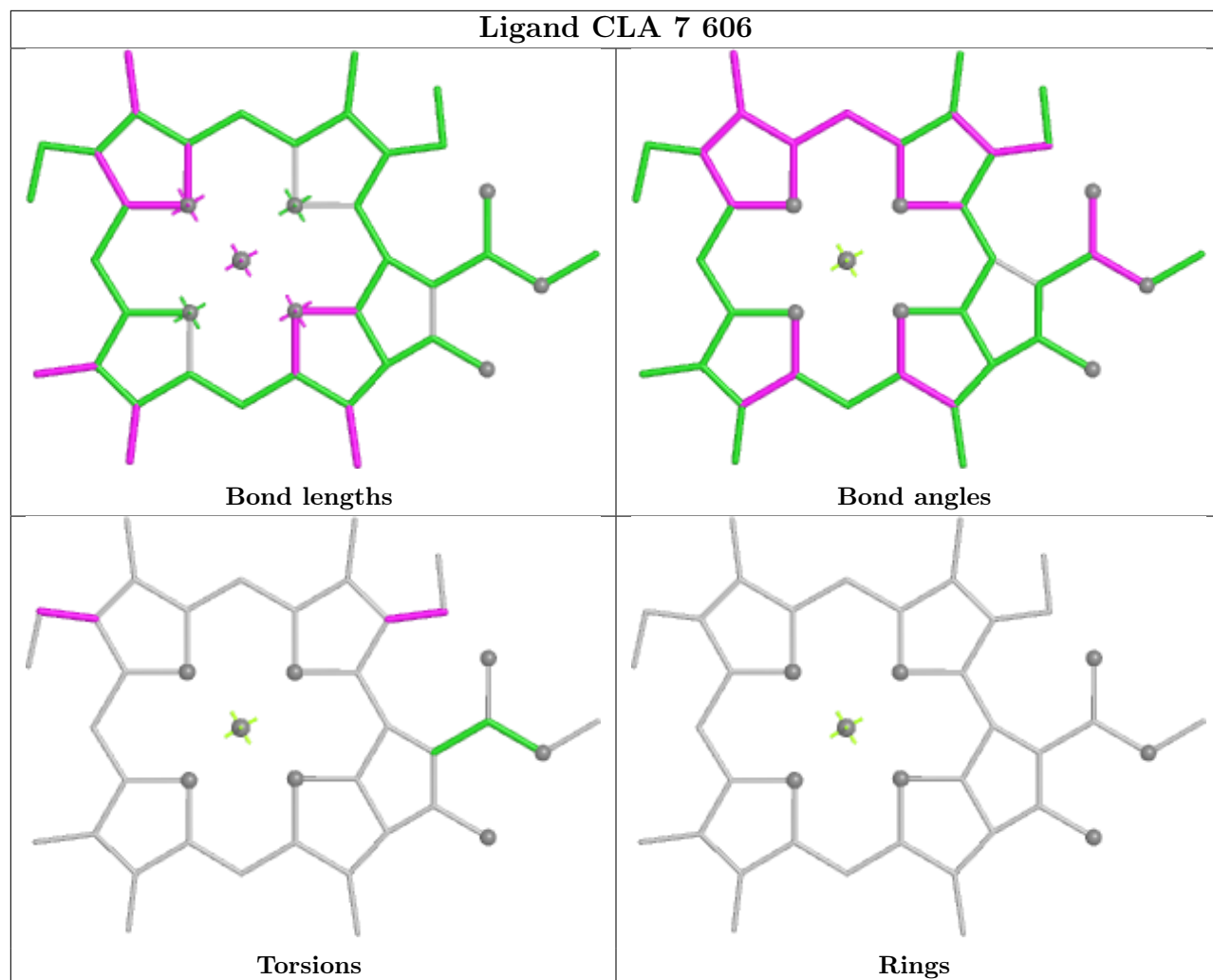
Ligand BCR B 848



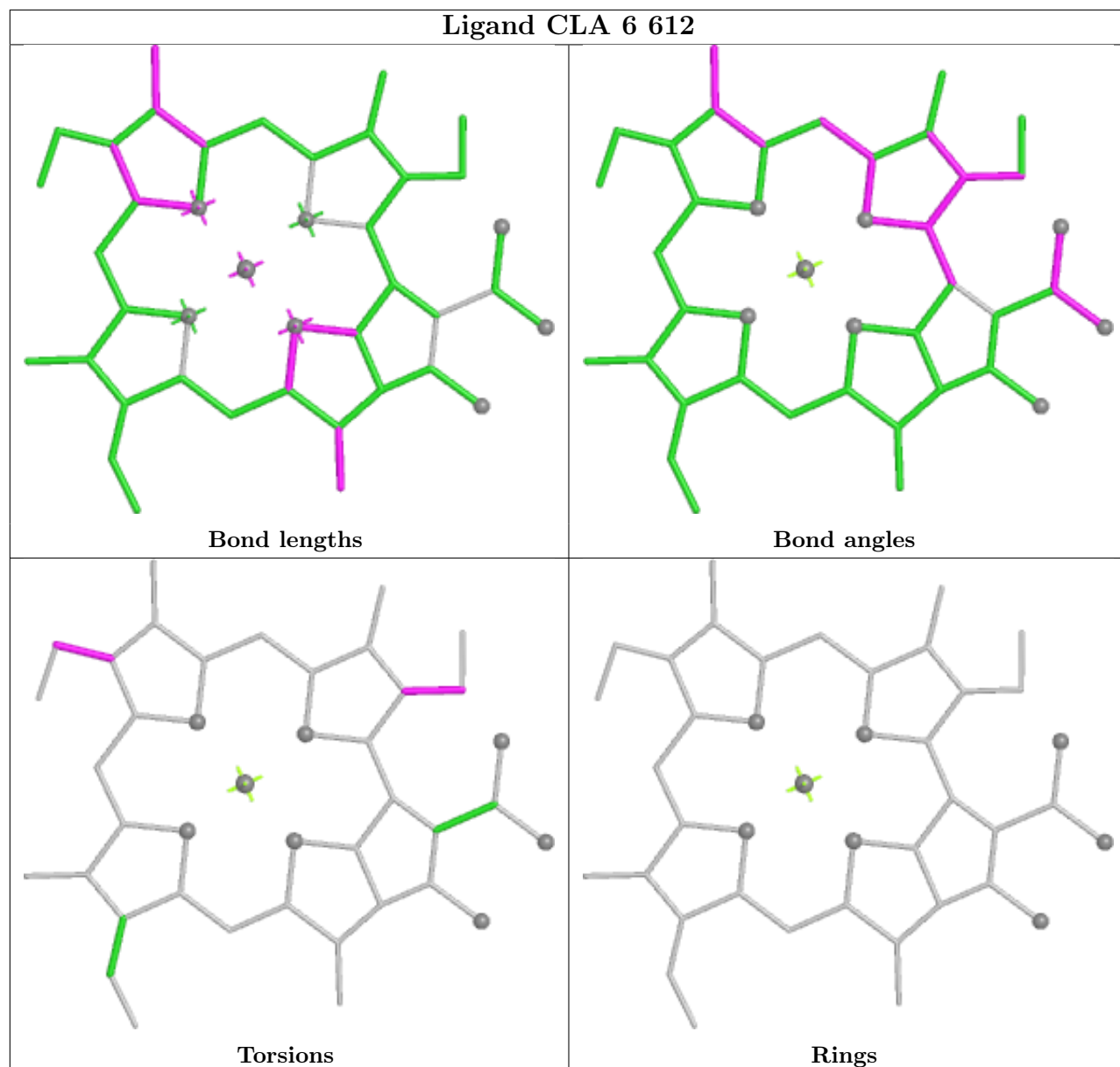


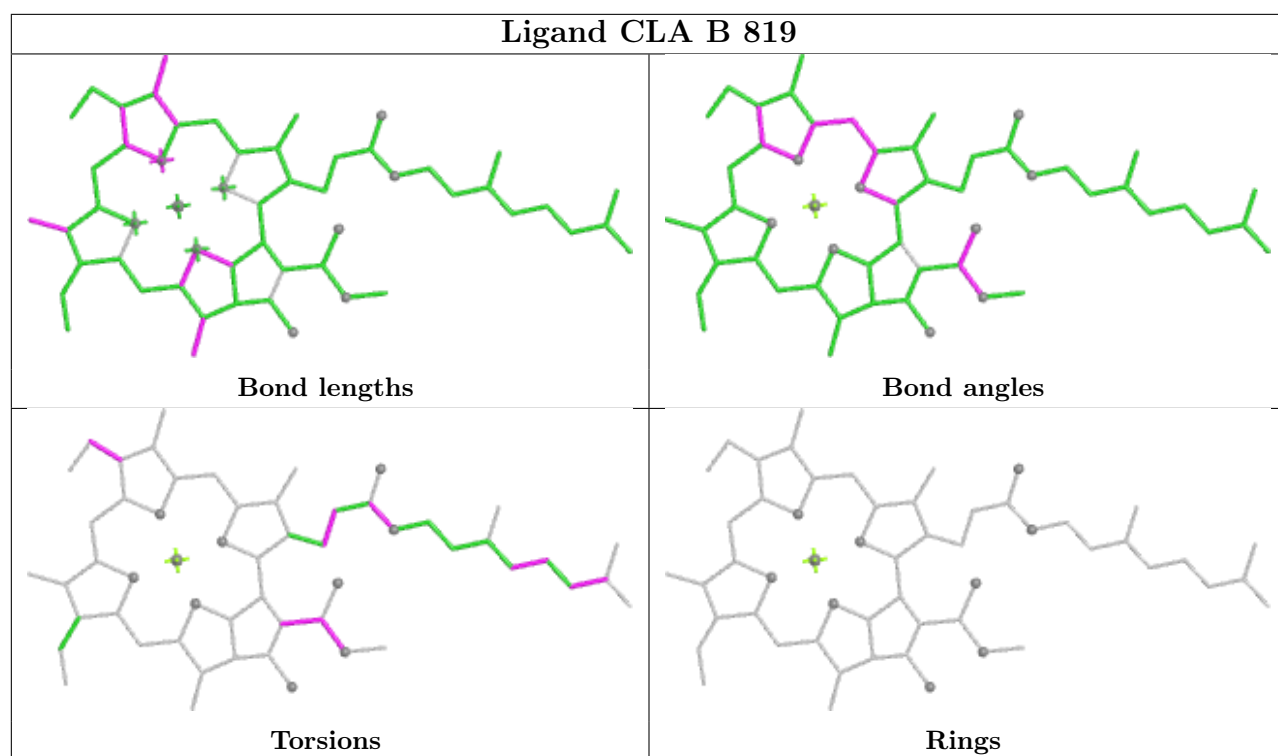


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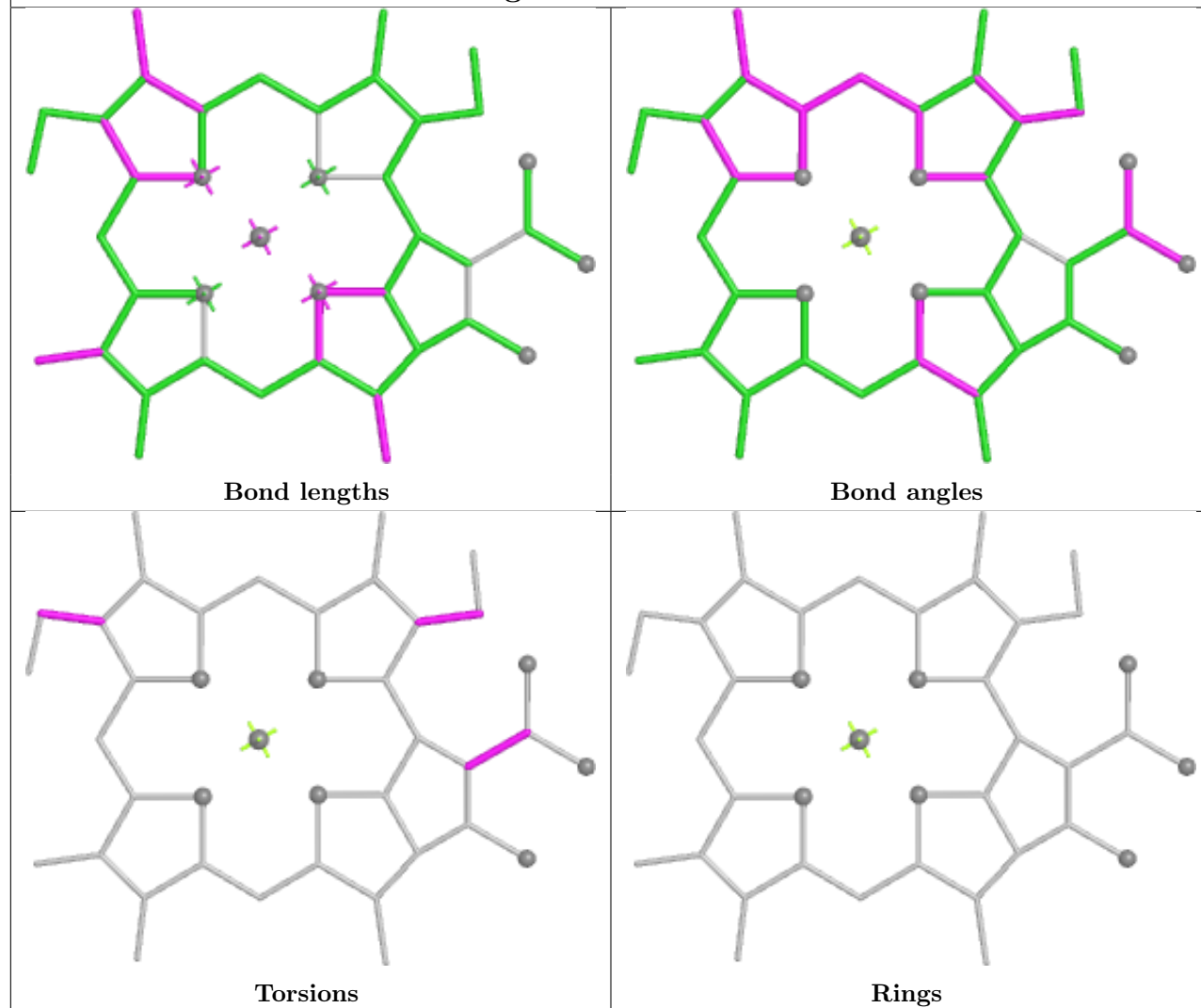


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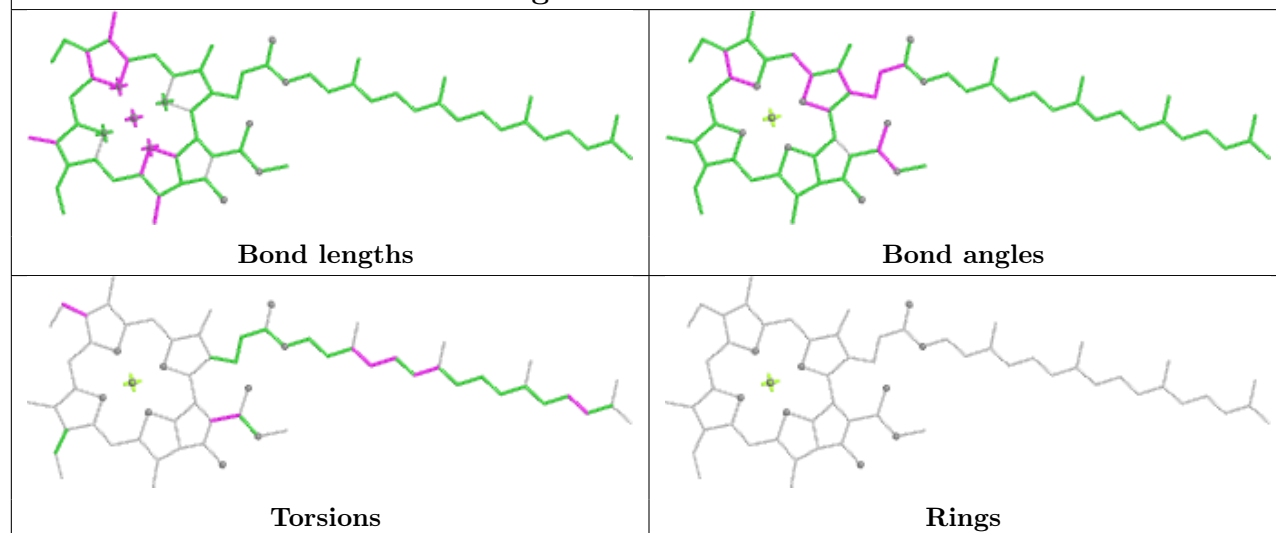




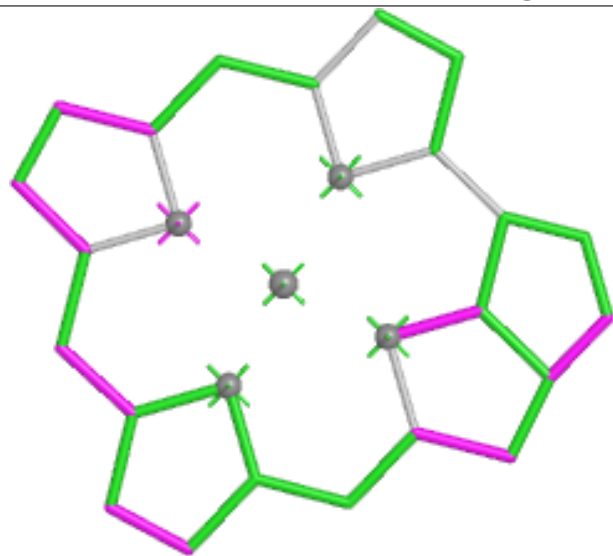
Ligand CLA 4 606



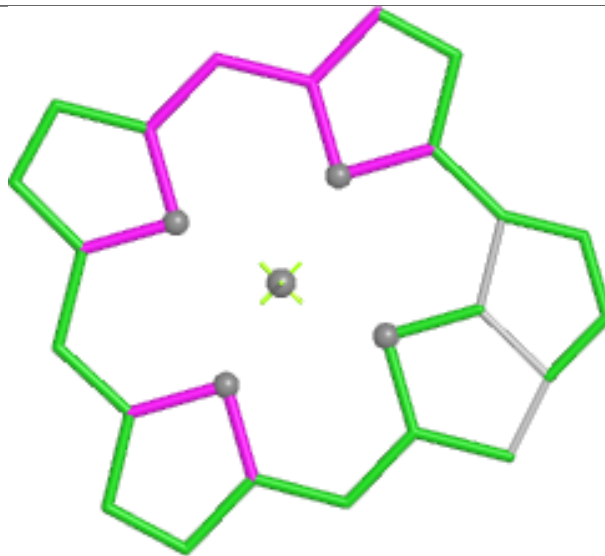
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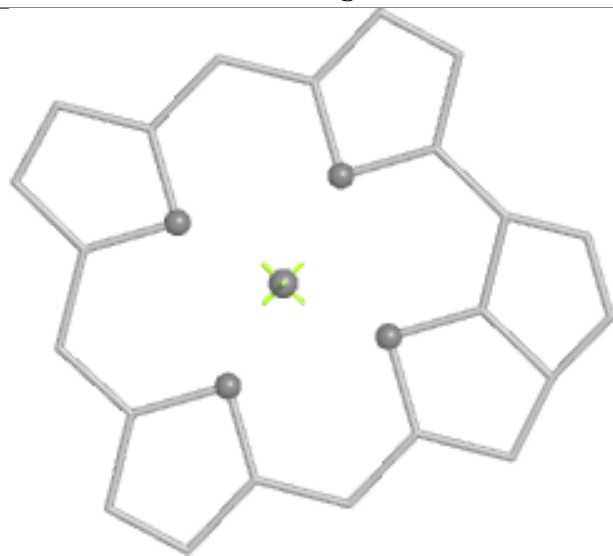
Ligand CLA 9 614



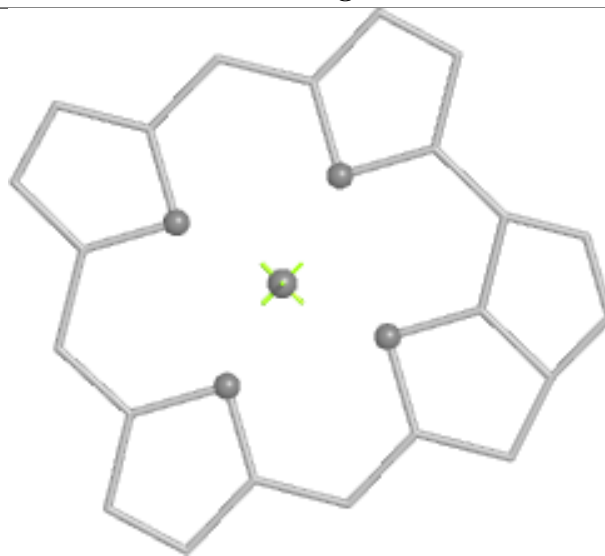
Bond lengths



Bond angles

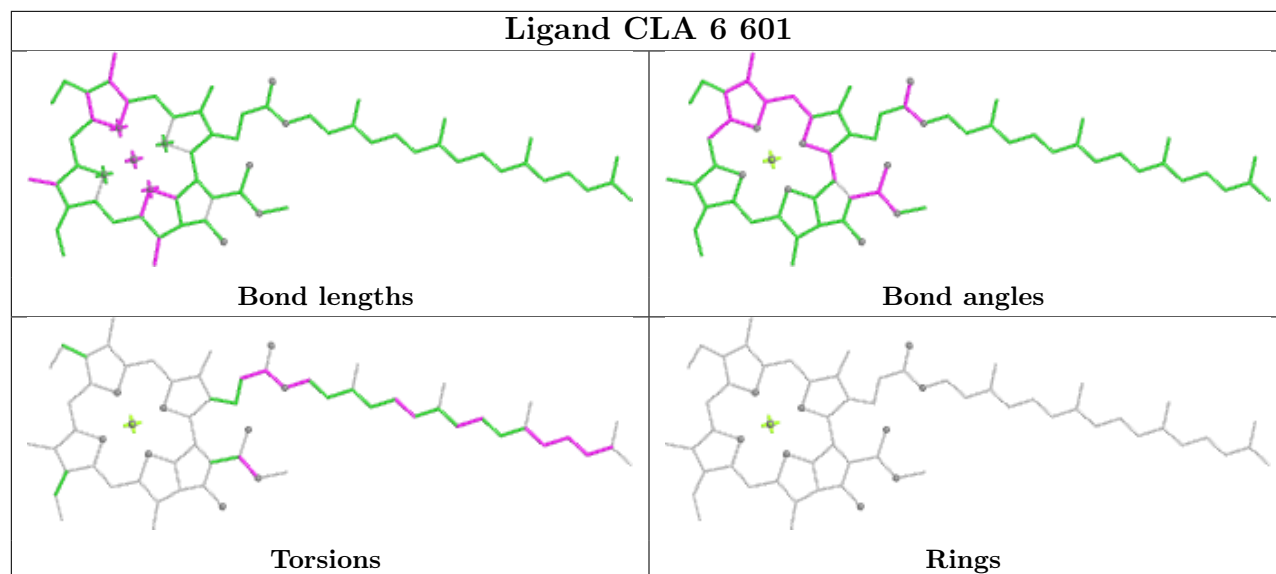


Torsions

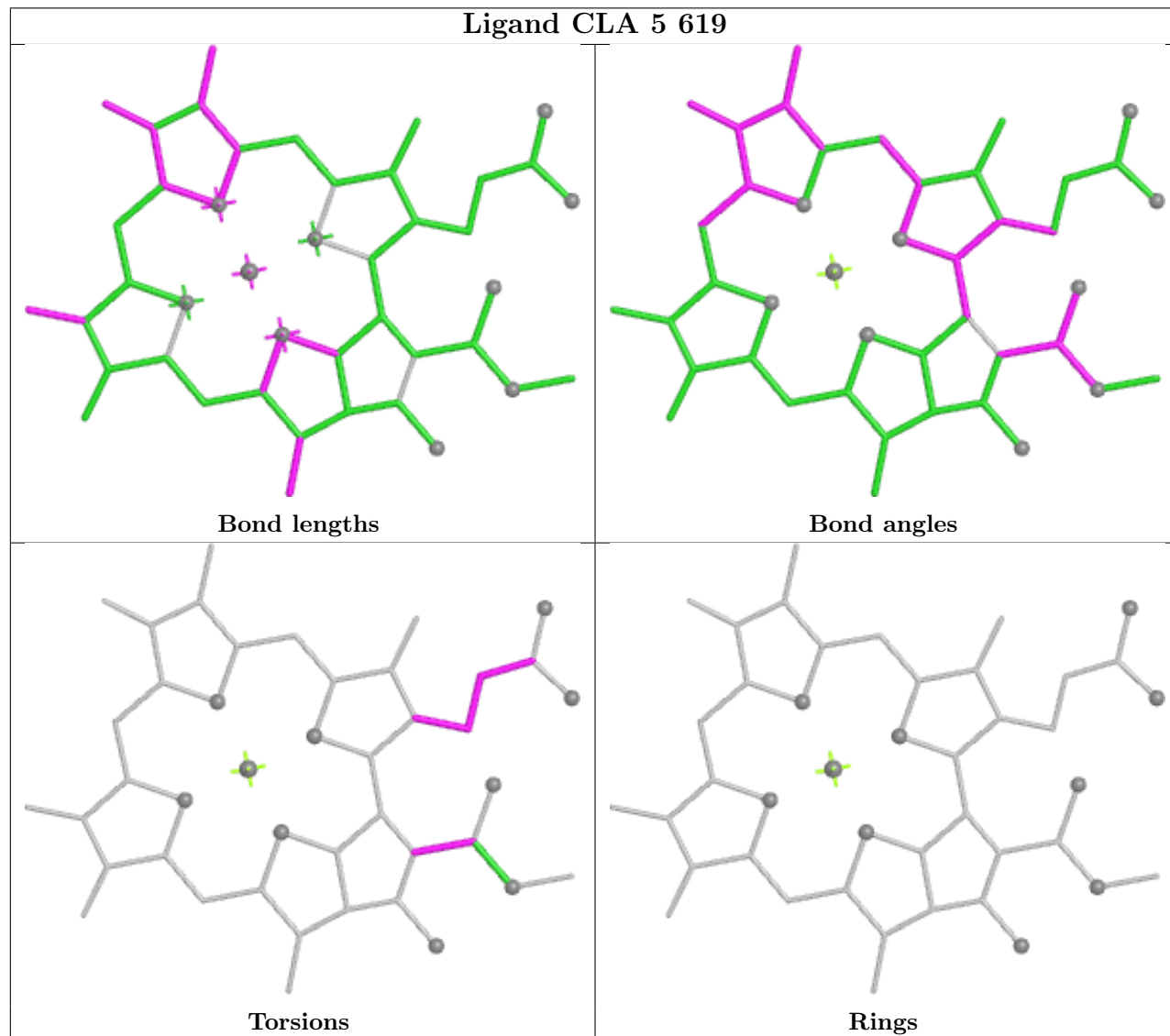


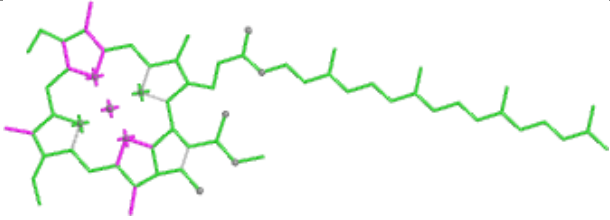
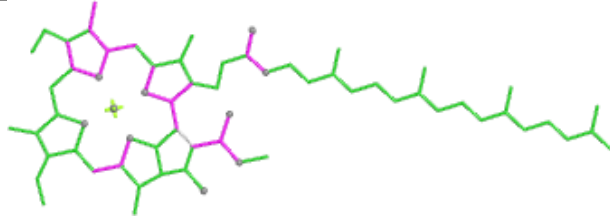
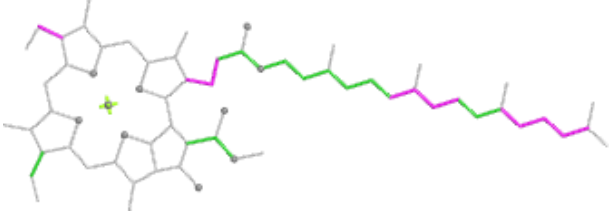
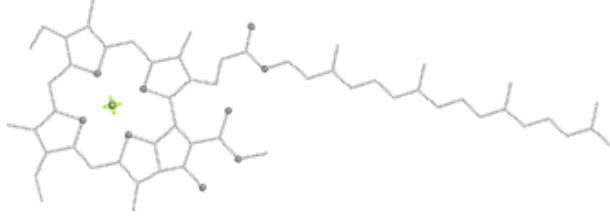
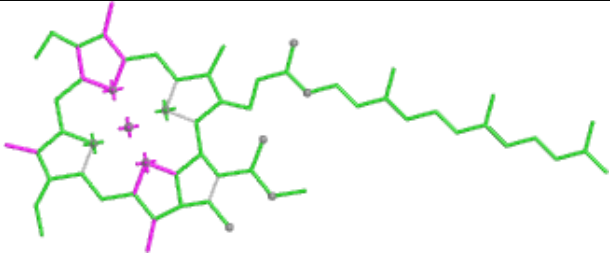
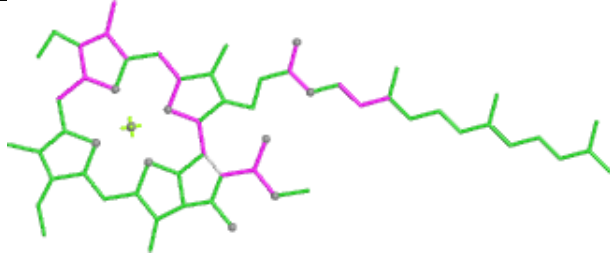
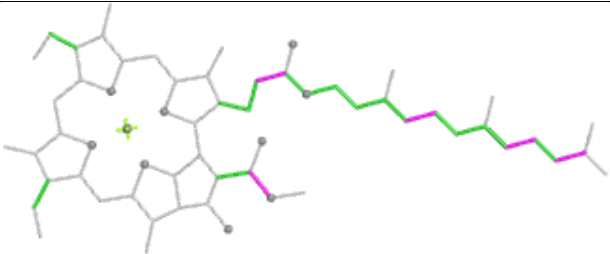
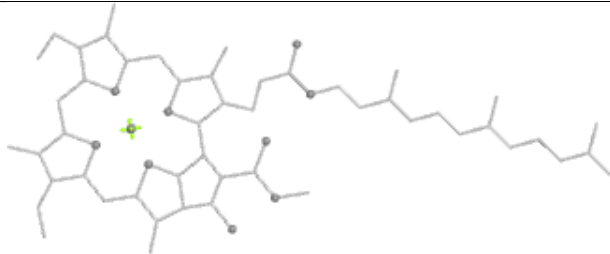
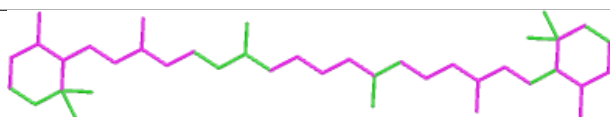
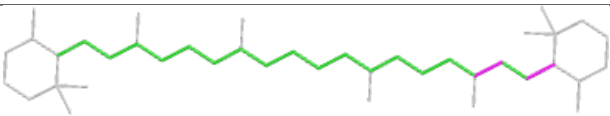
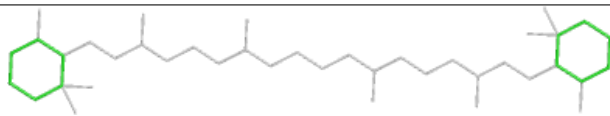
Rings

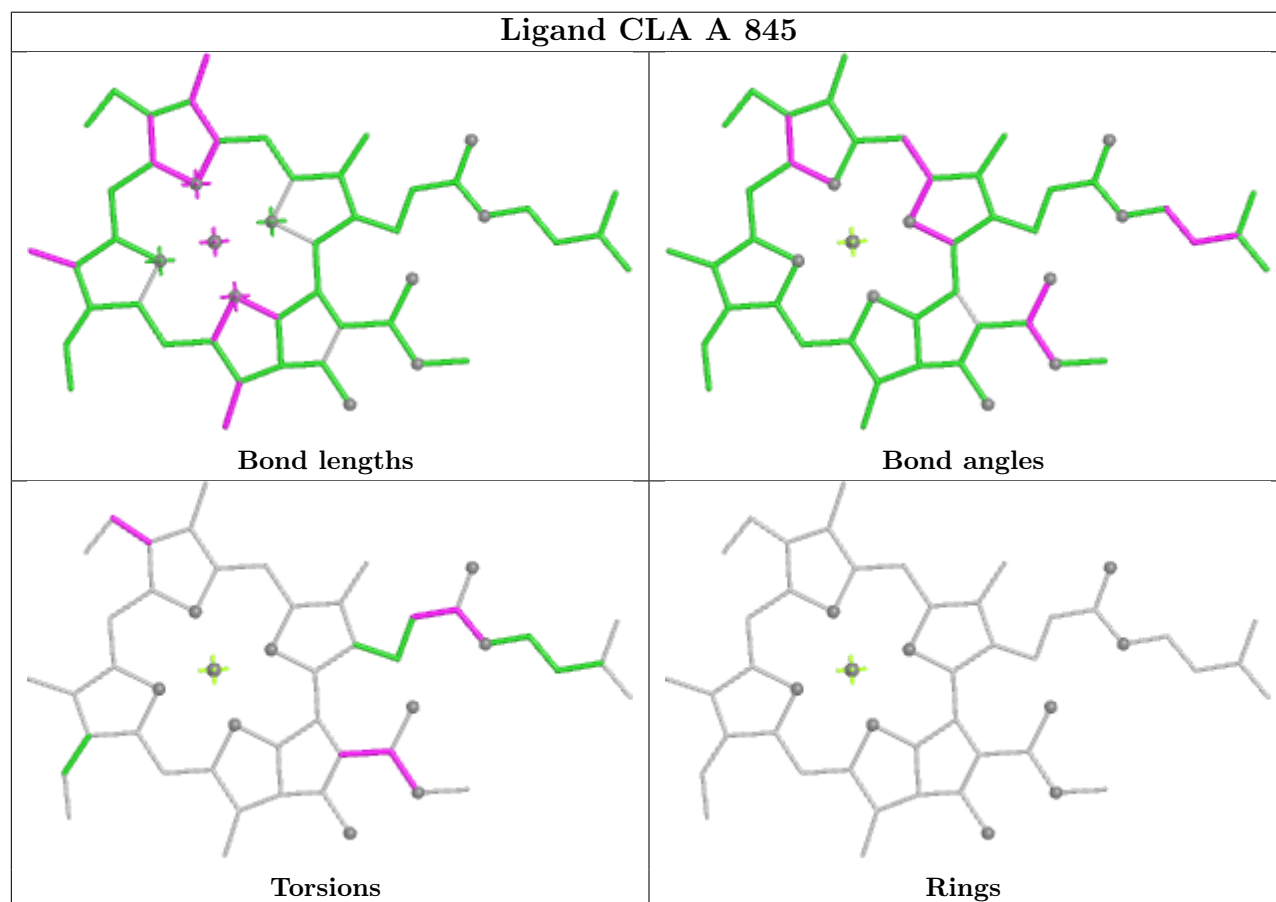
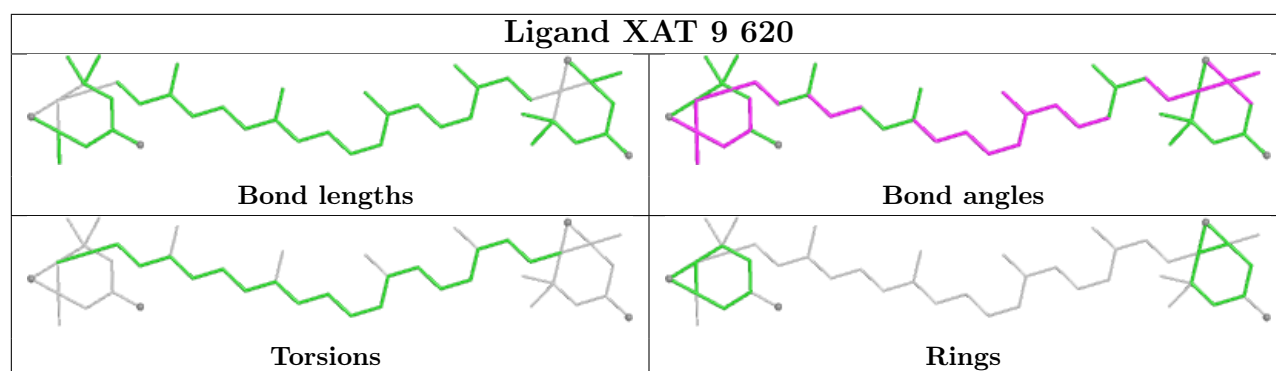
Ligand CLA 6 601

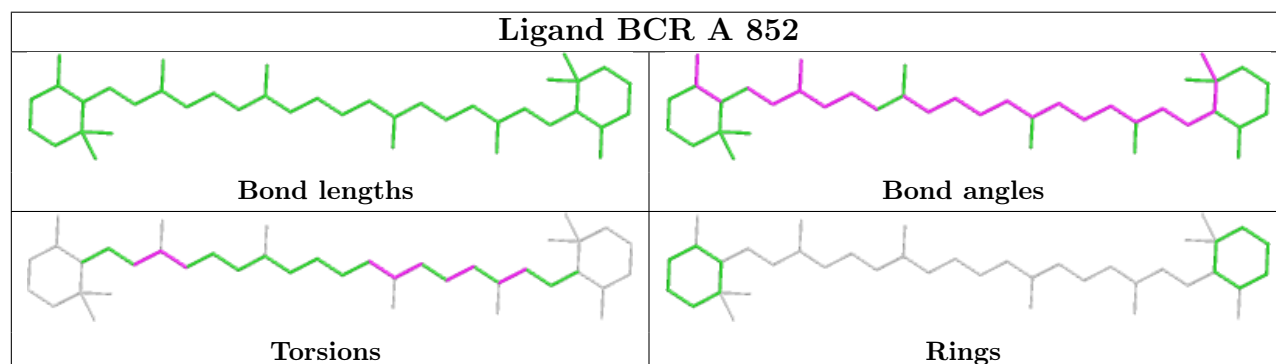
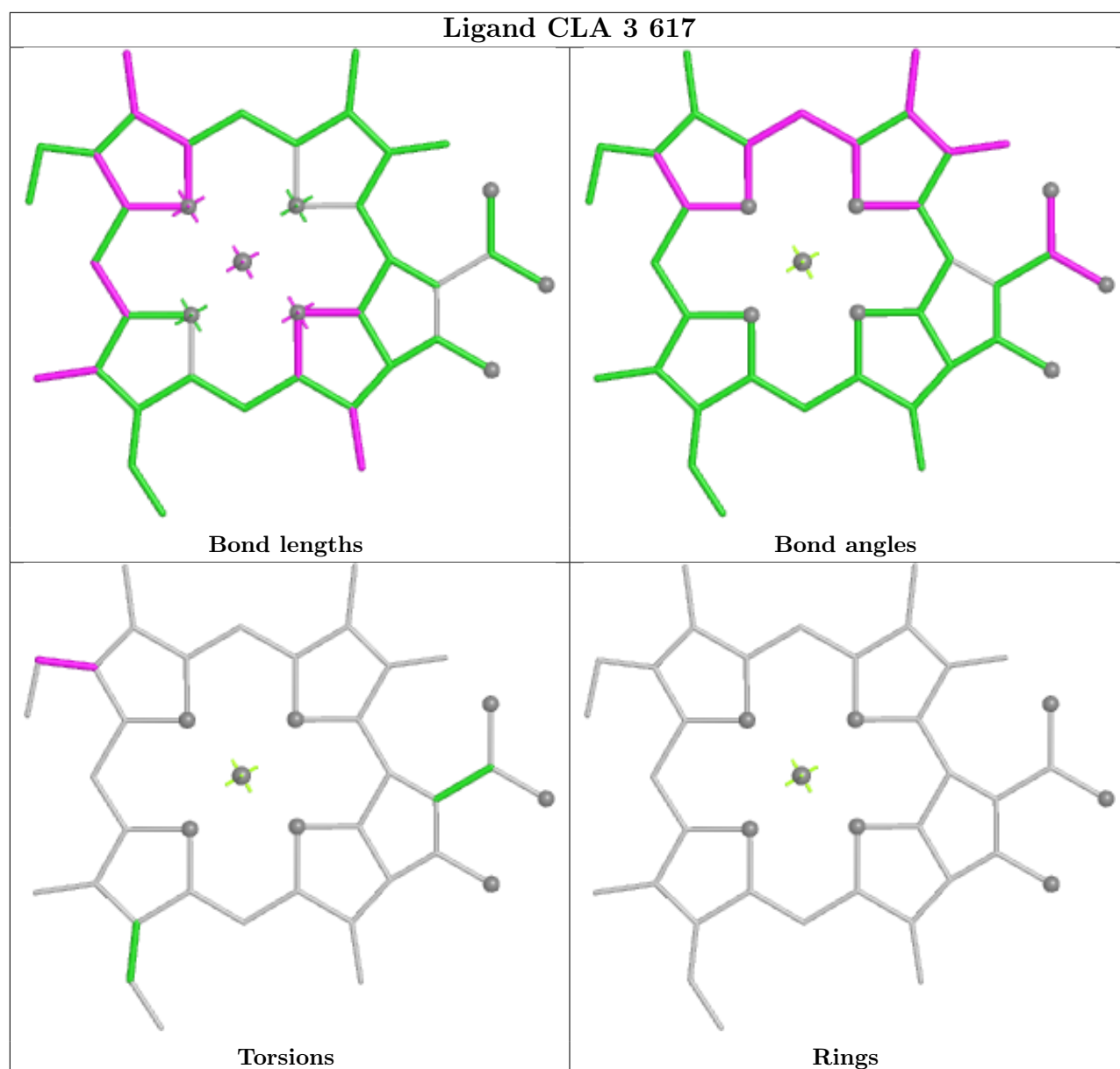


Ligand CLA 5 619

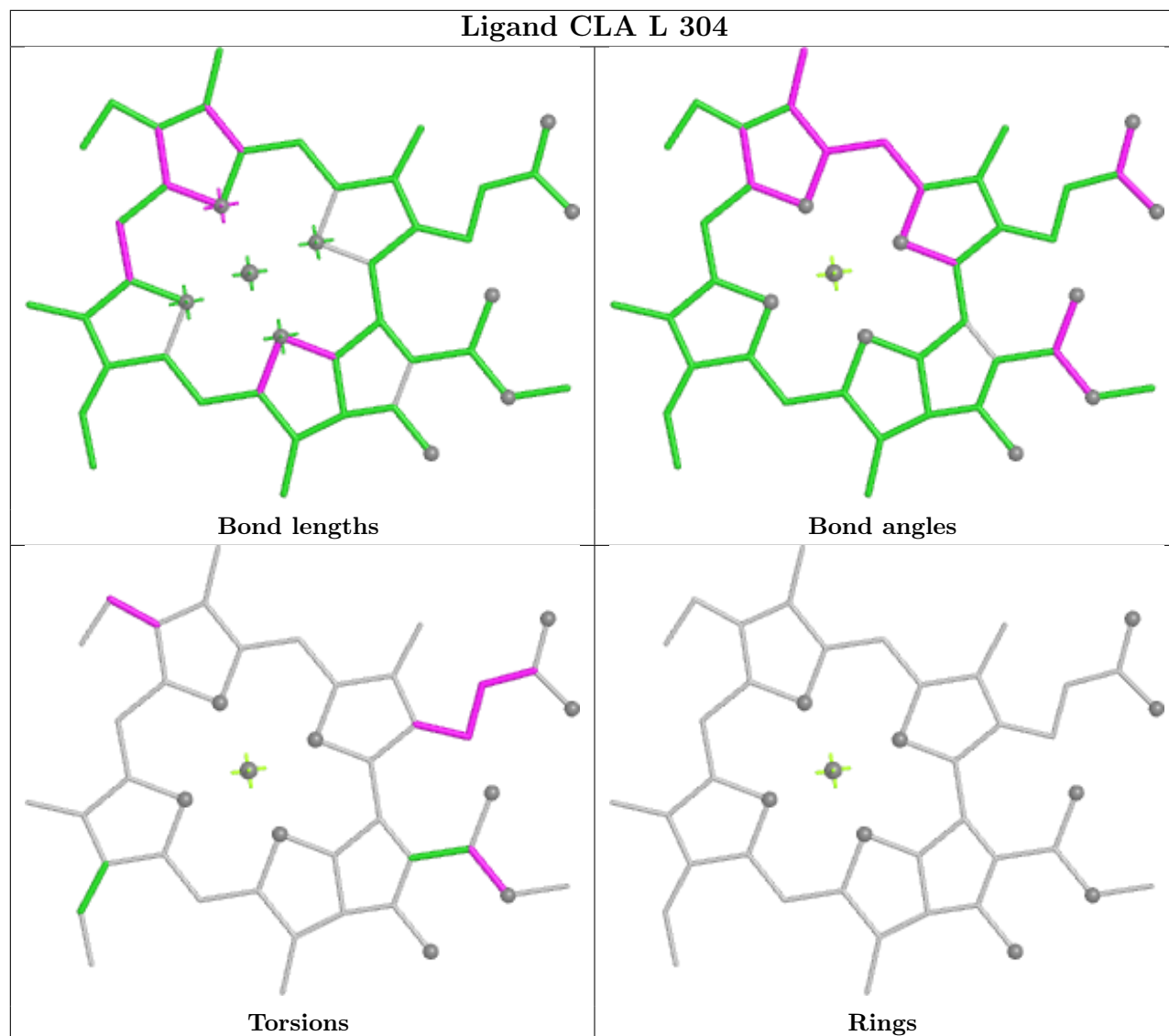


Ligand CLA 5 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 832	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 3 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

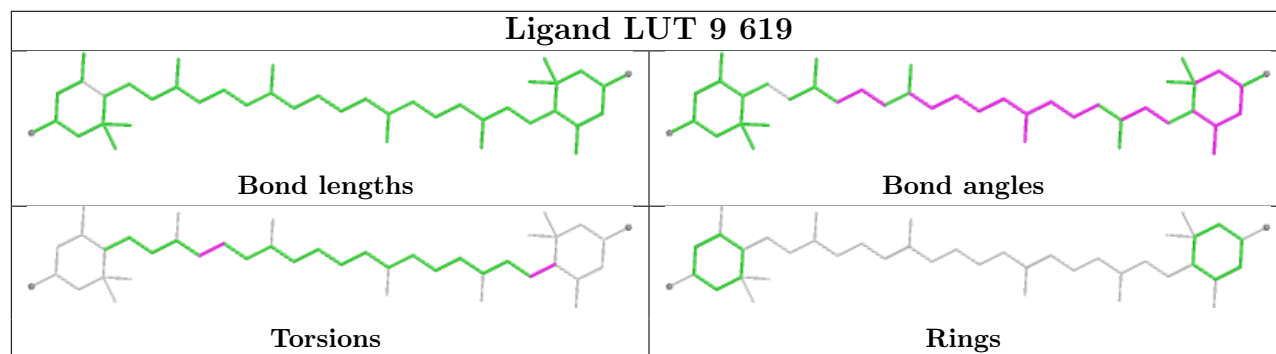


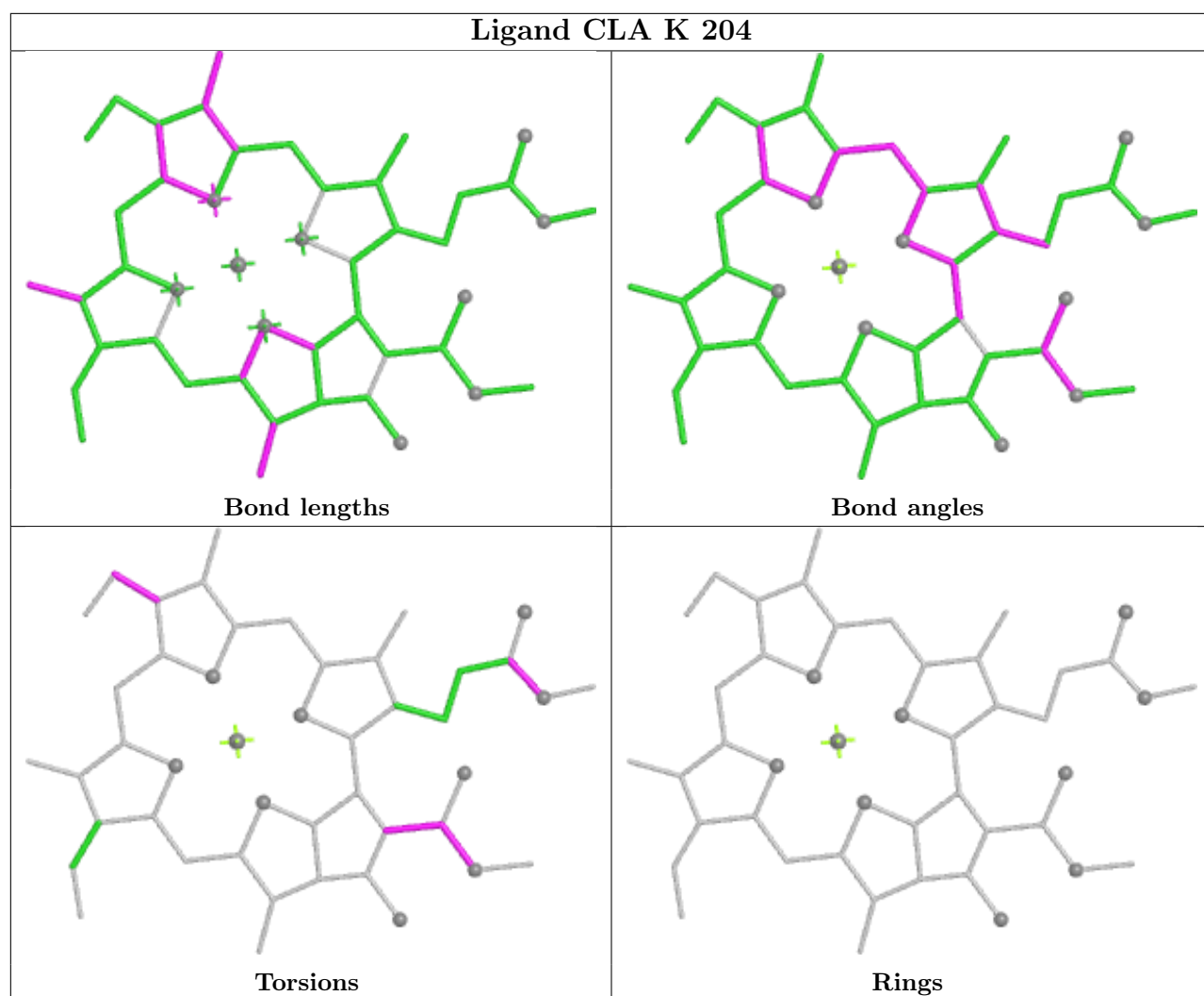


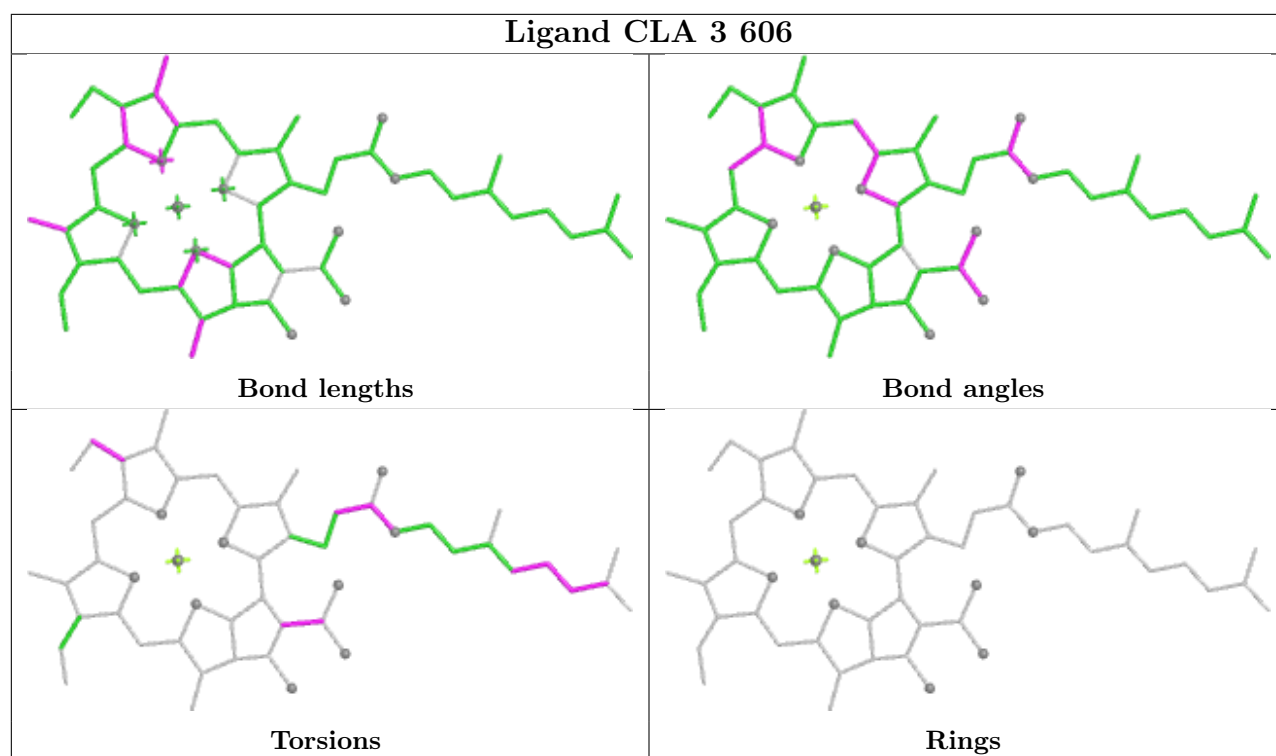
Ligand CLA L 304



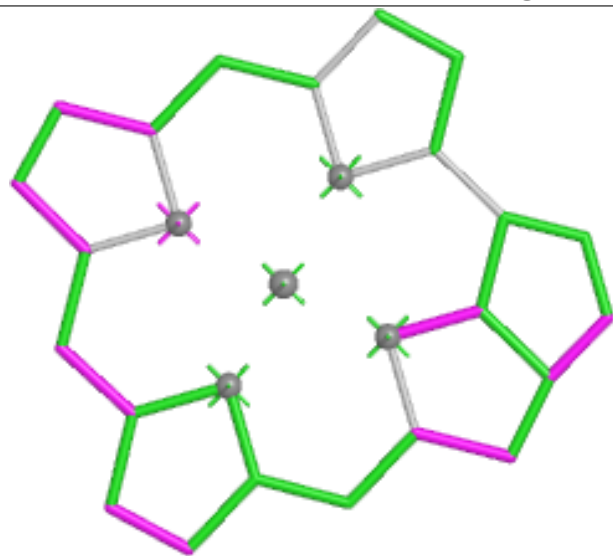
Ligand LUT 9 619



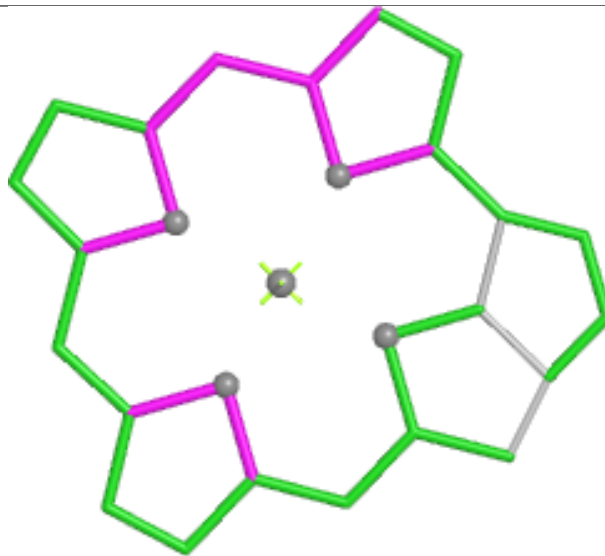




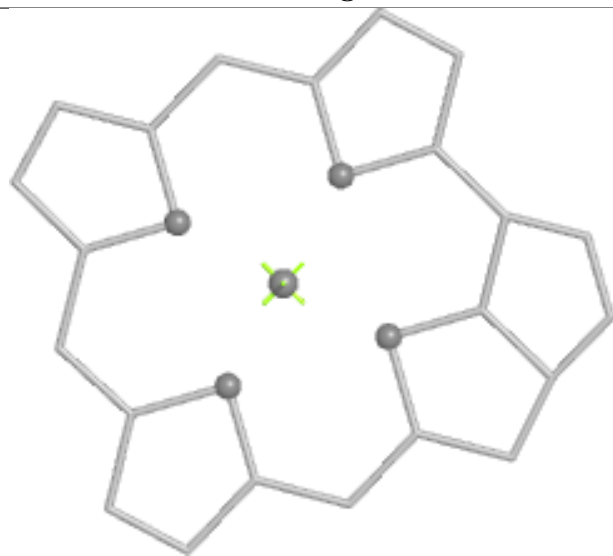
Ligand CLA 2 614



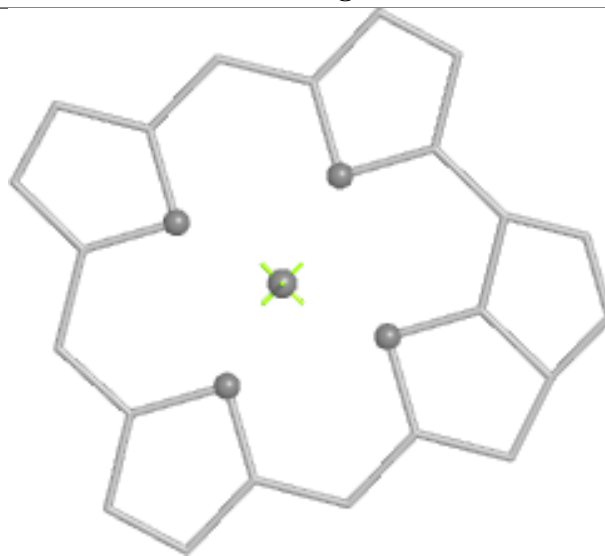
Bond lengths



Bond angles

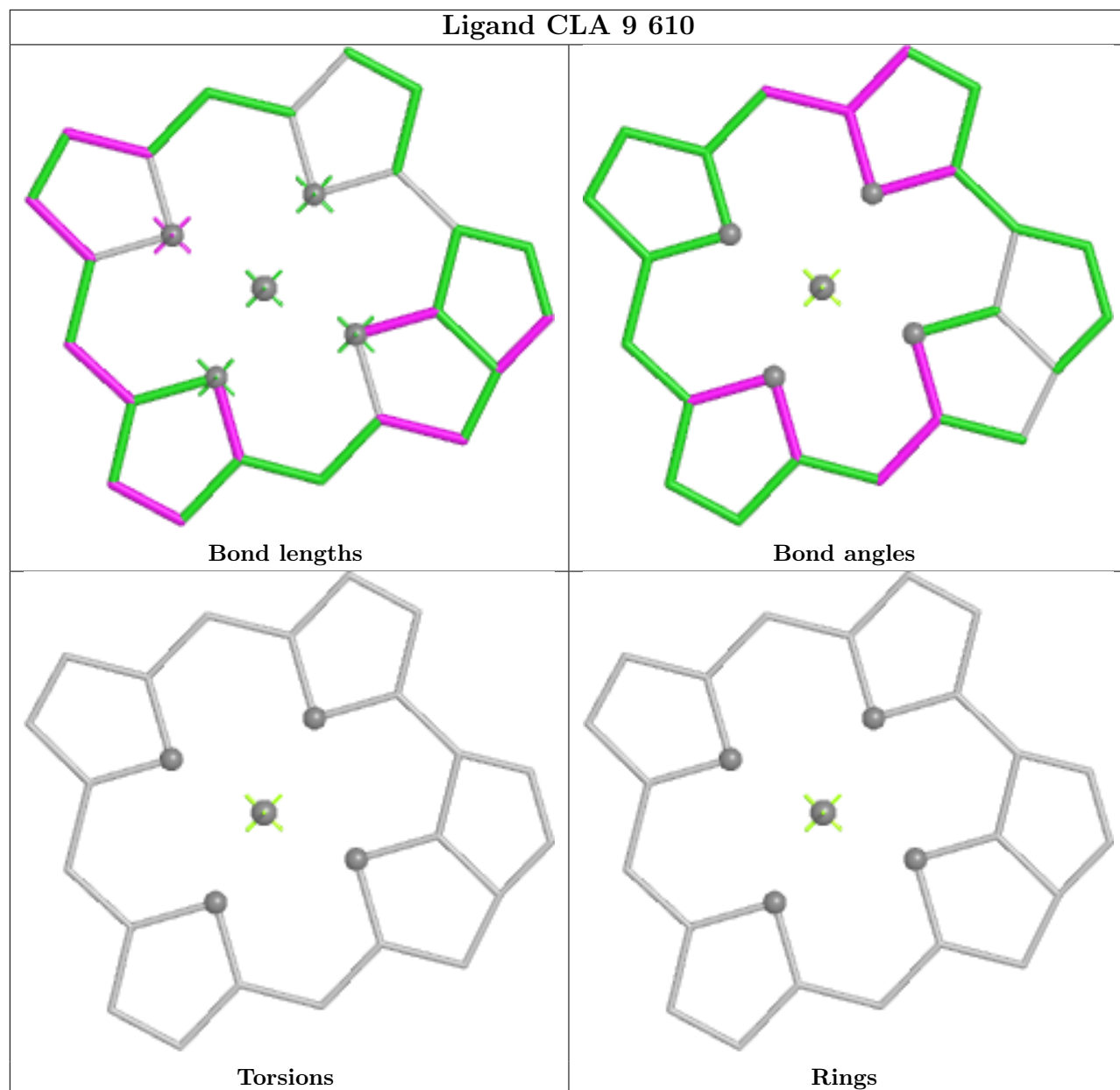


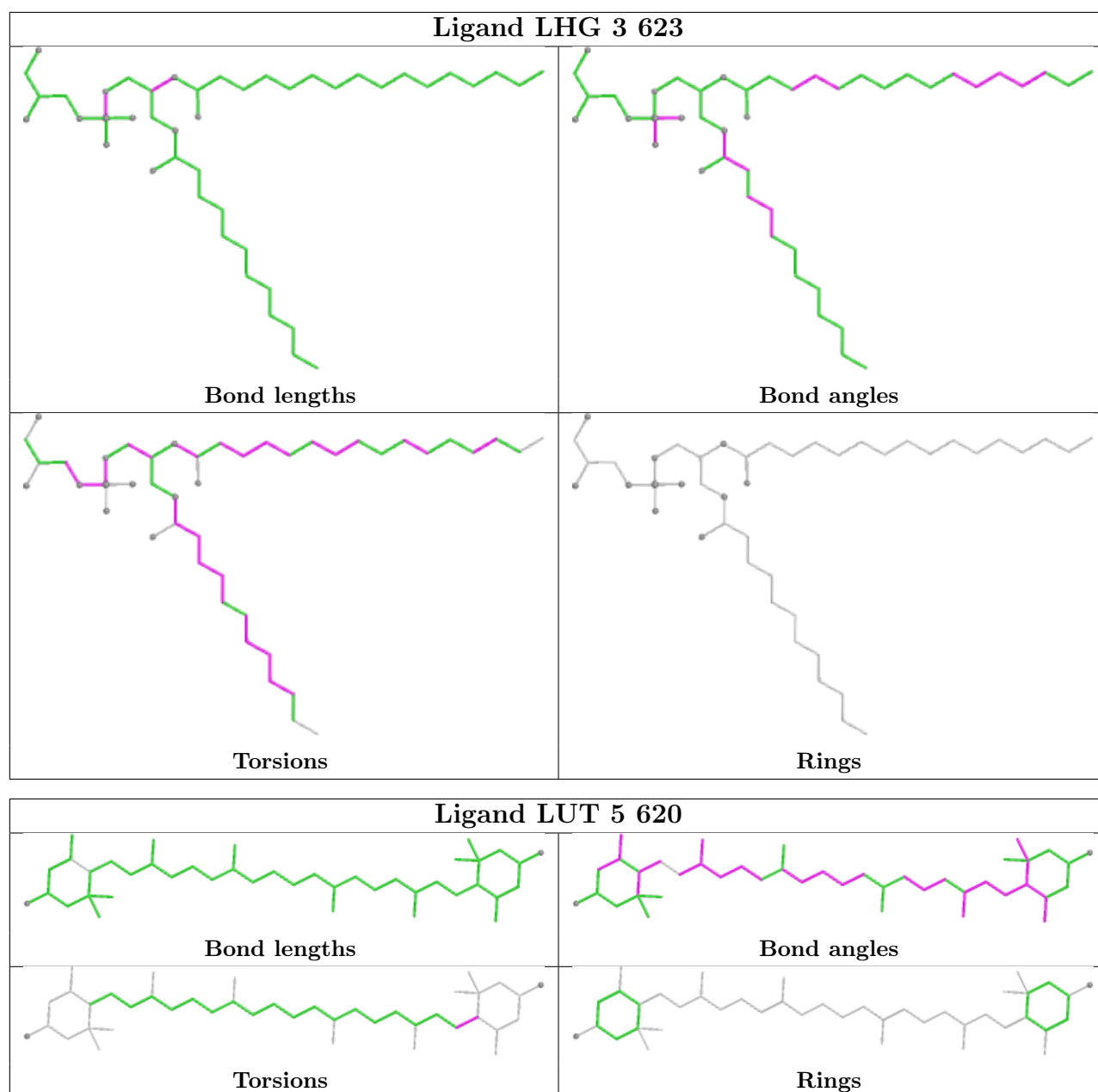
Torsions

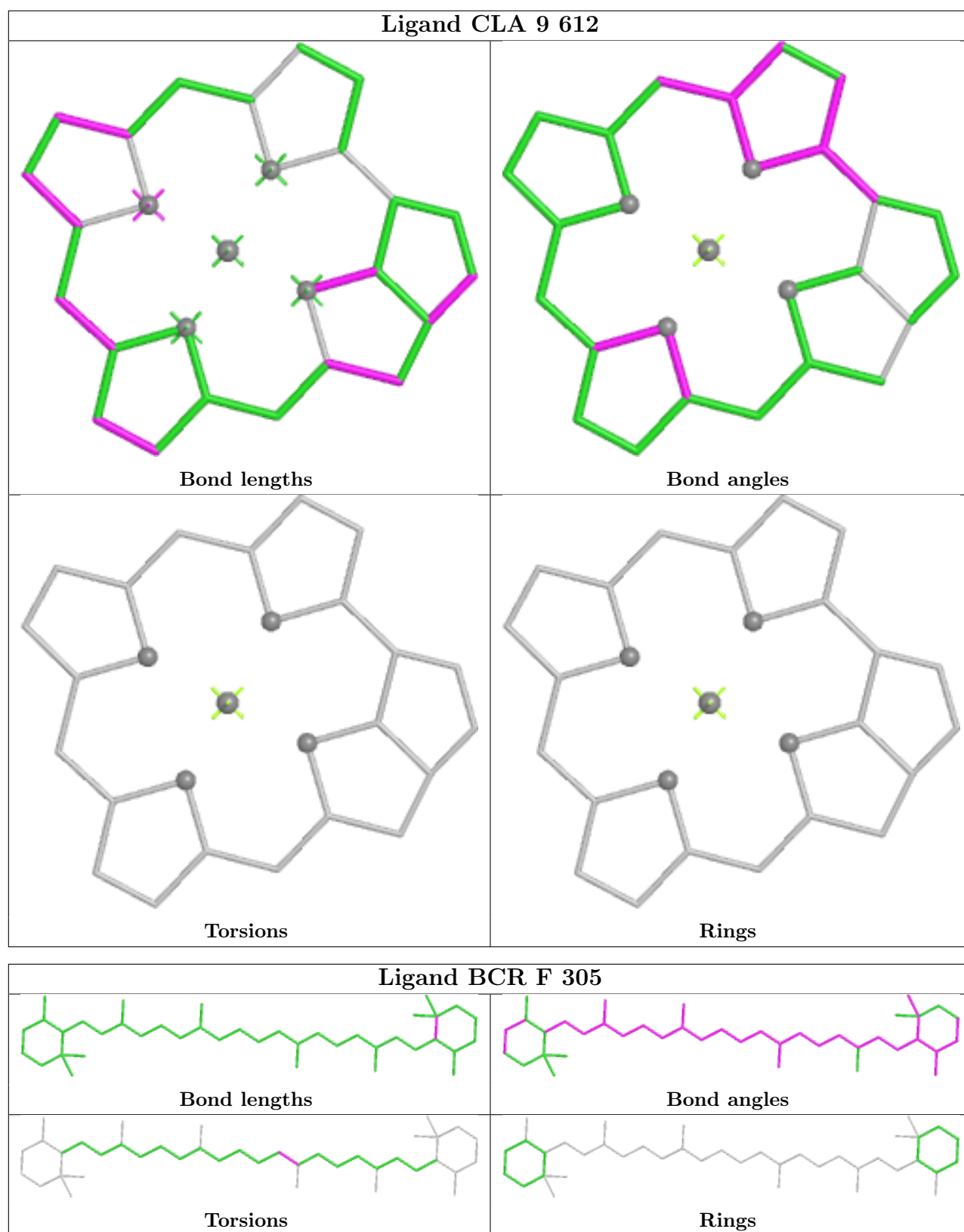


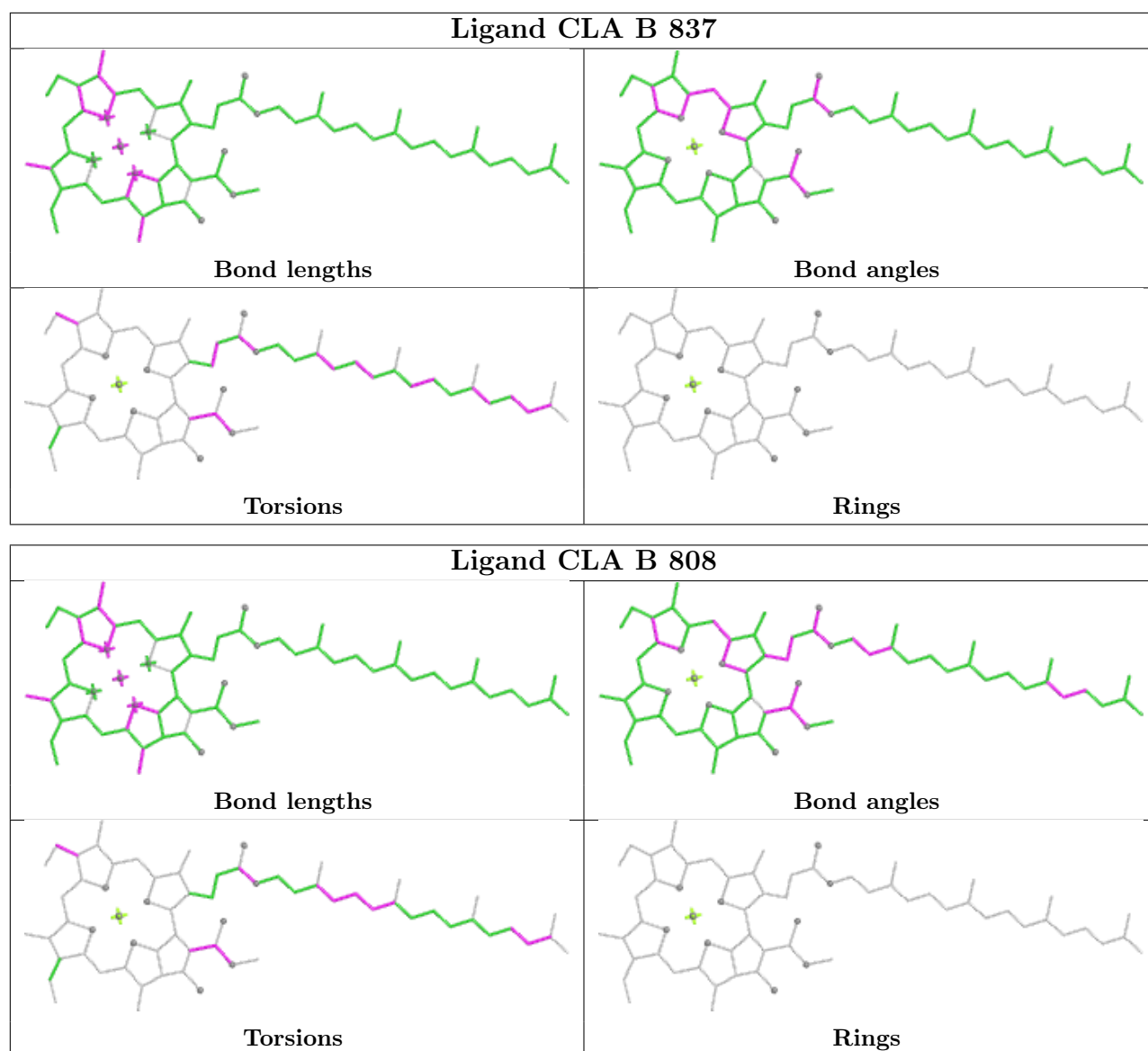
Rings

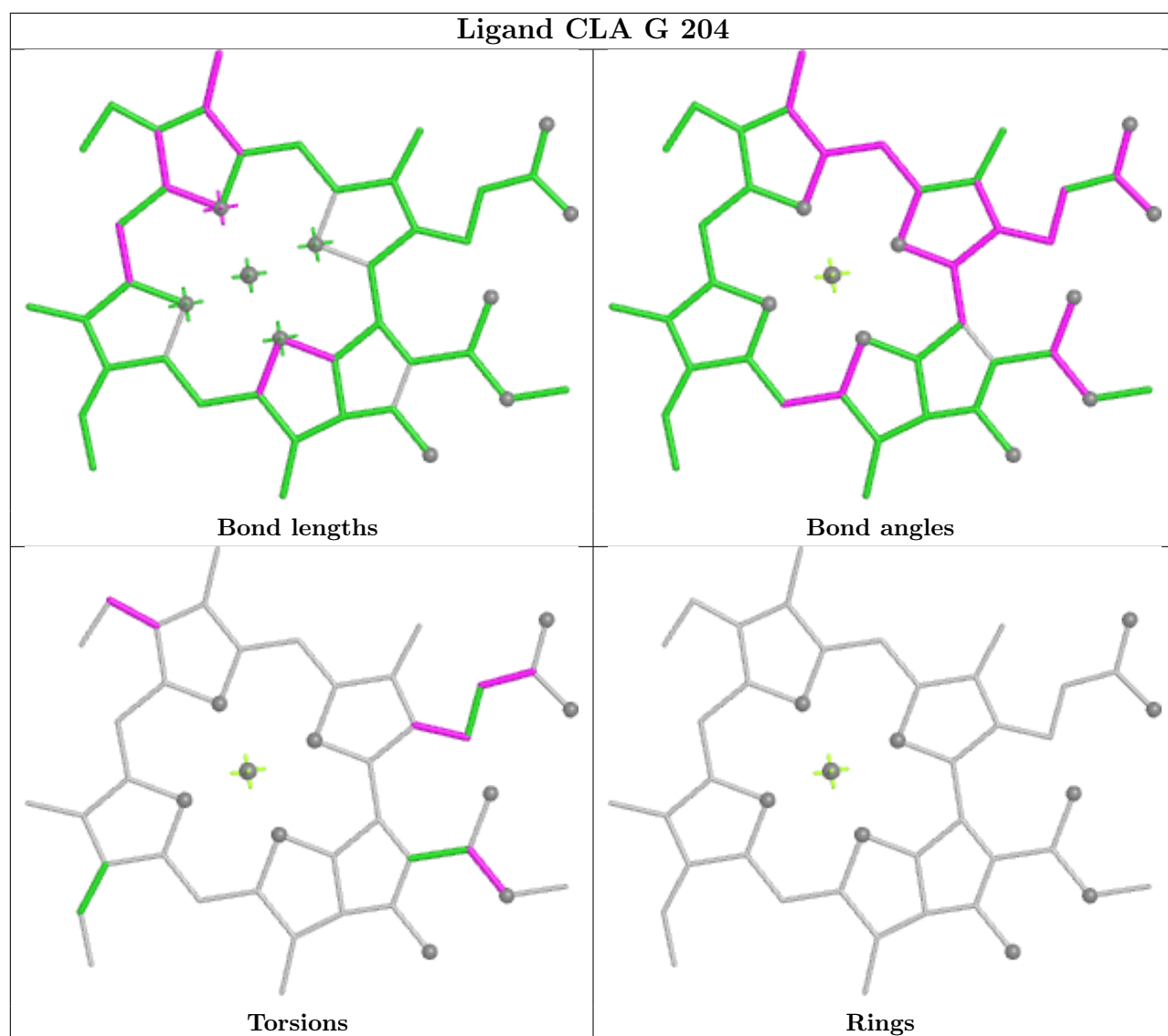
Ligand CLA 9 610



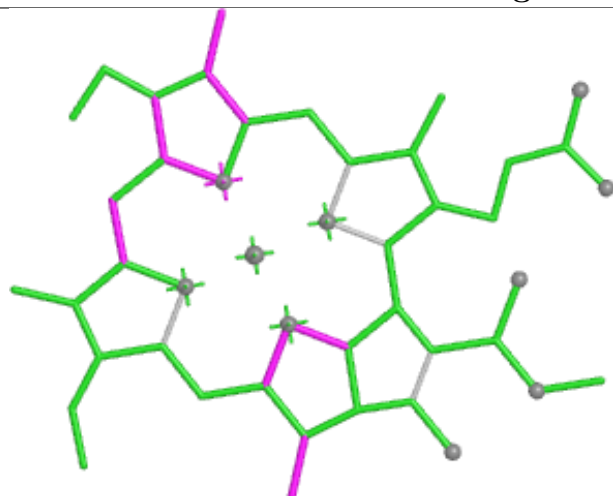




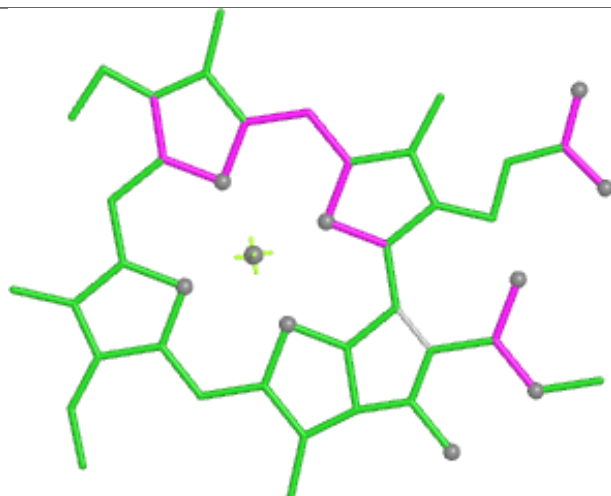




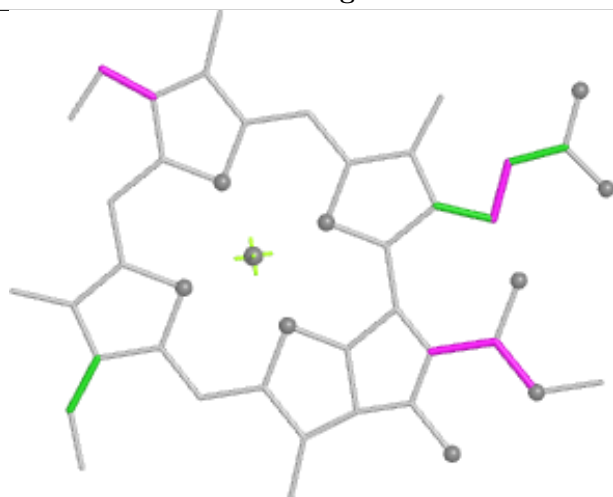
Ligand CLA K 206



Bond lengths



Bond angles

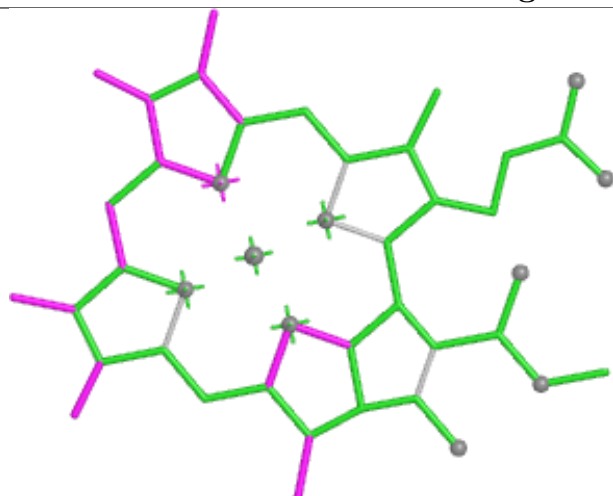


Torsions

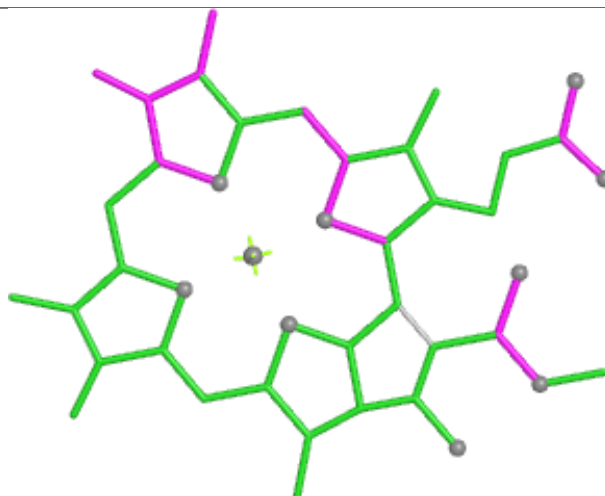


Rings

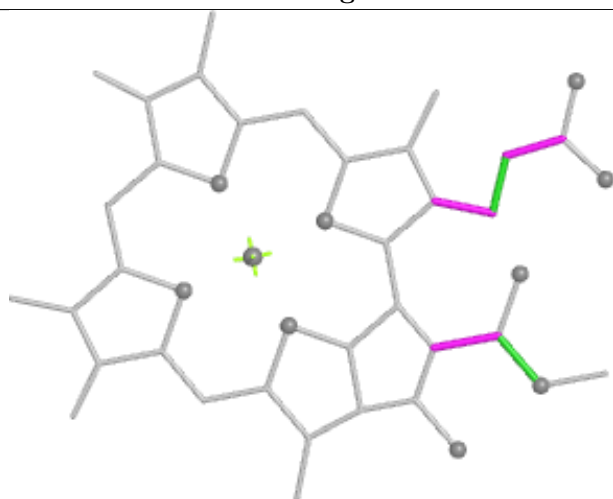
Ligand CLA 4 616



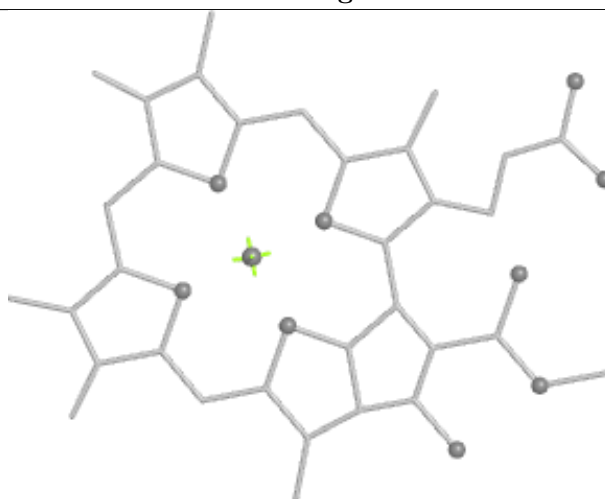
Bond lengths



Bond angles

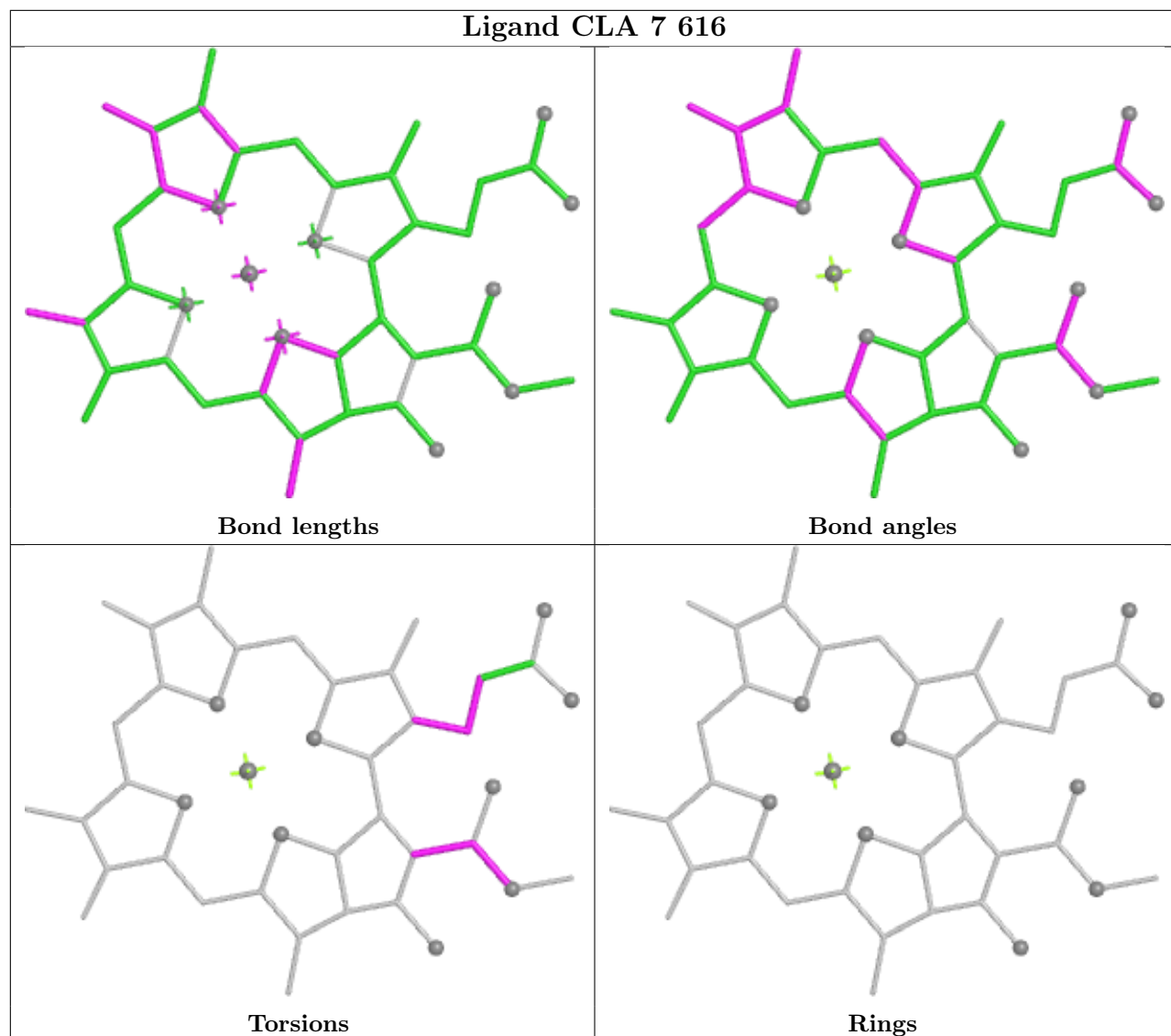


Torsions

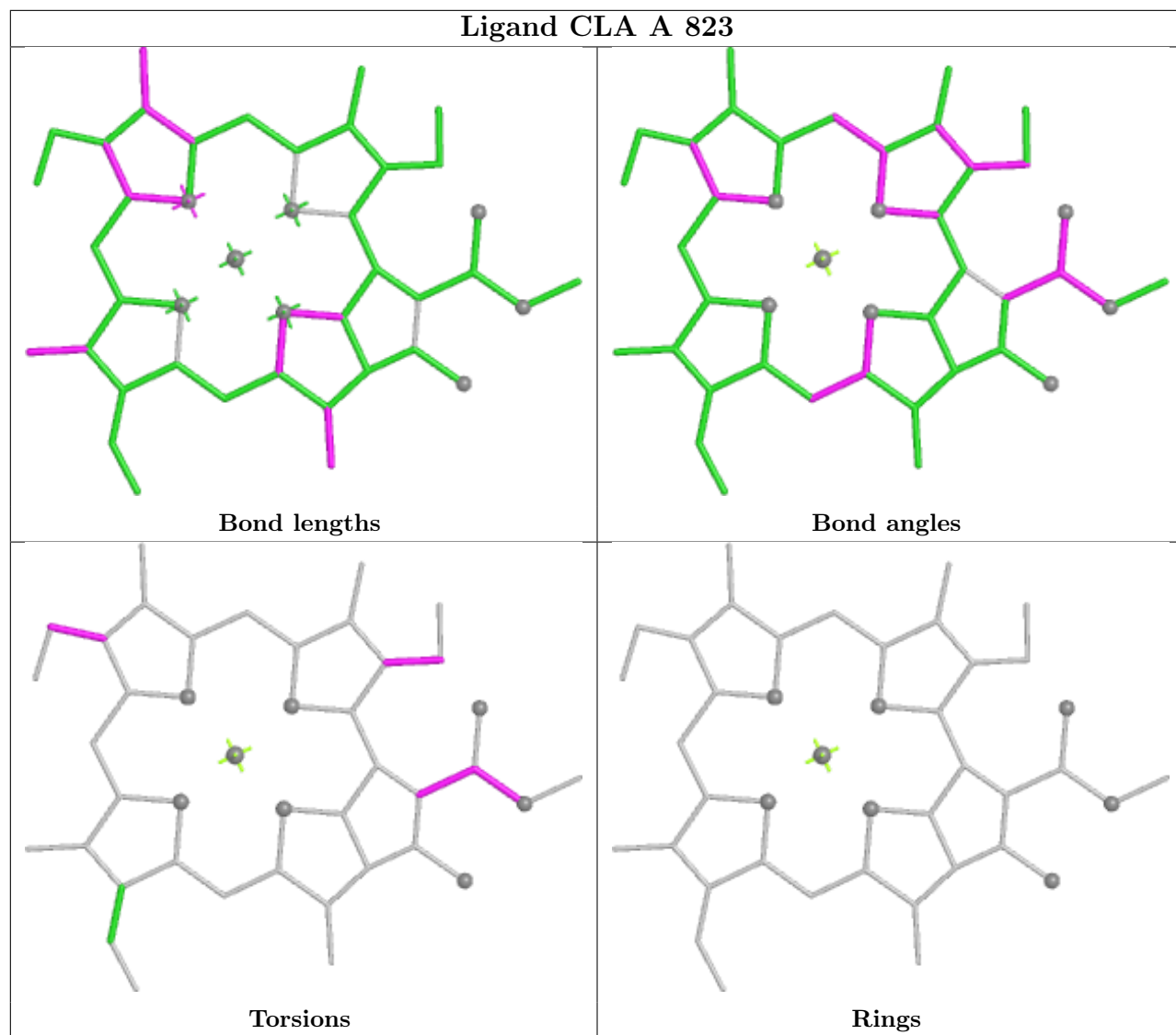


Rings

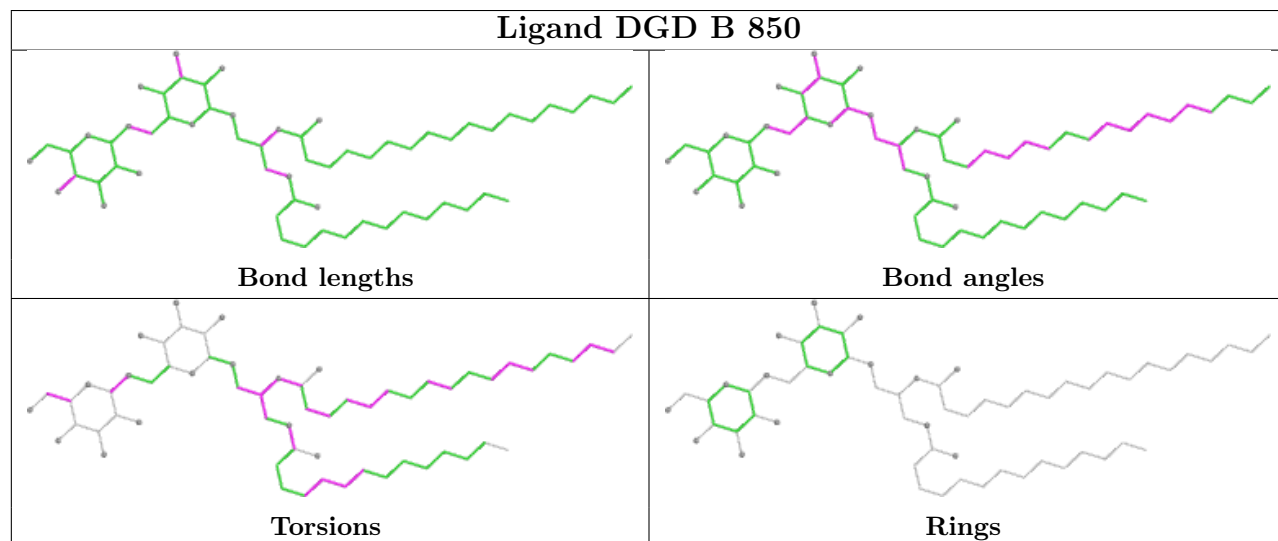
Ligand CLA 7 616

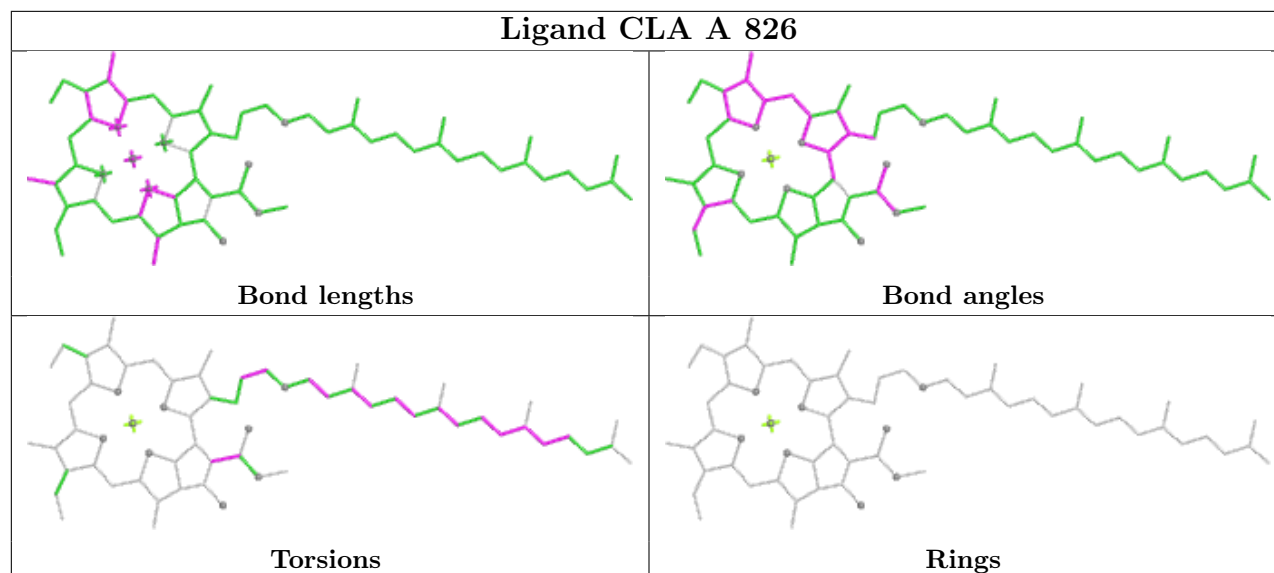
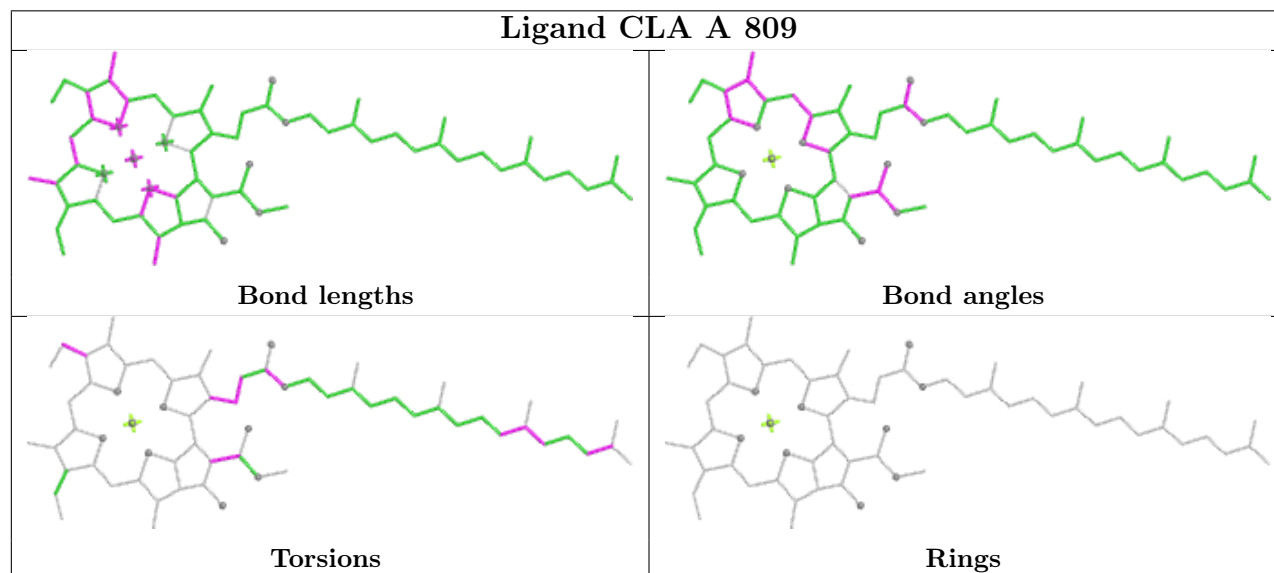
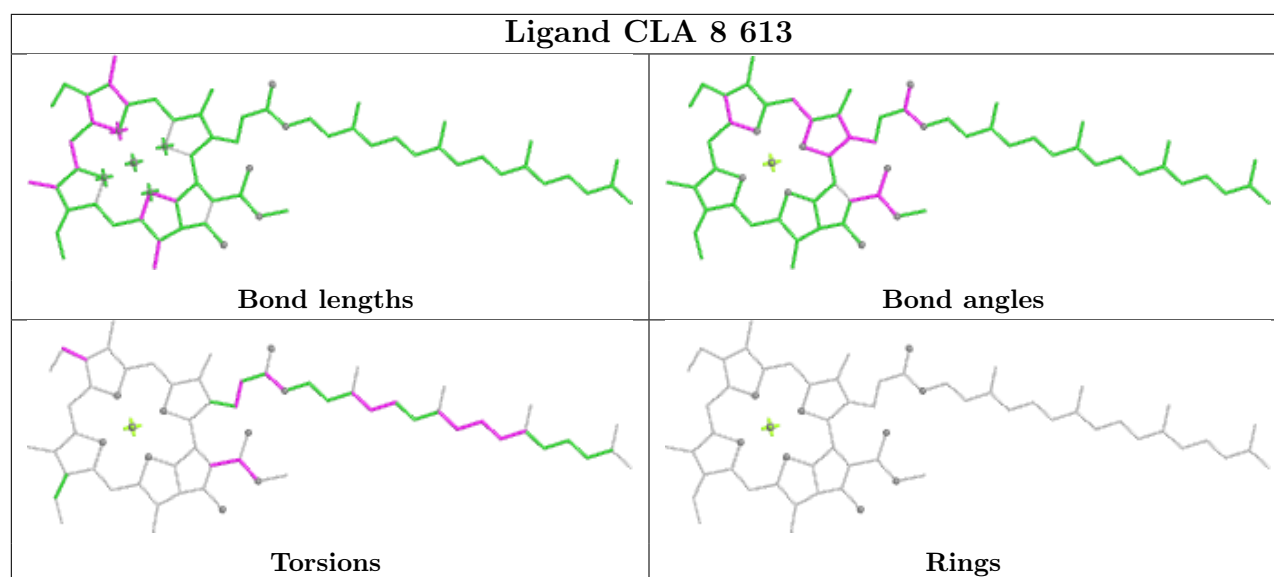


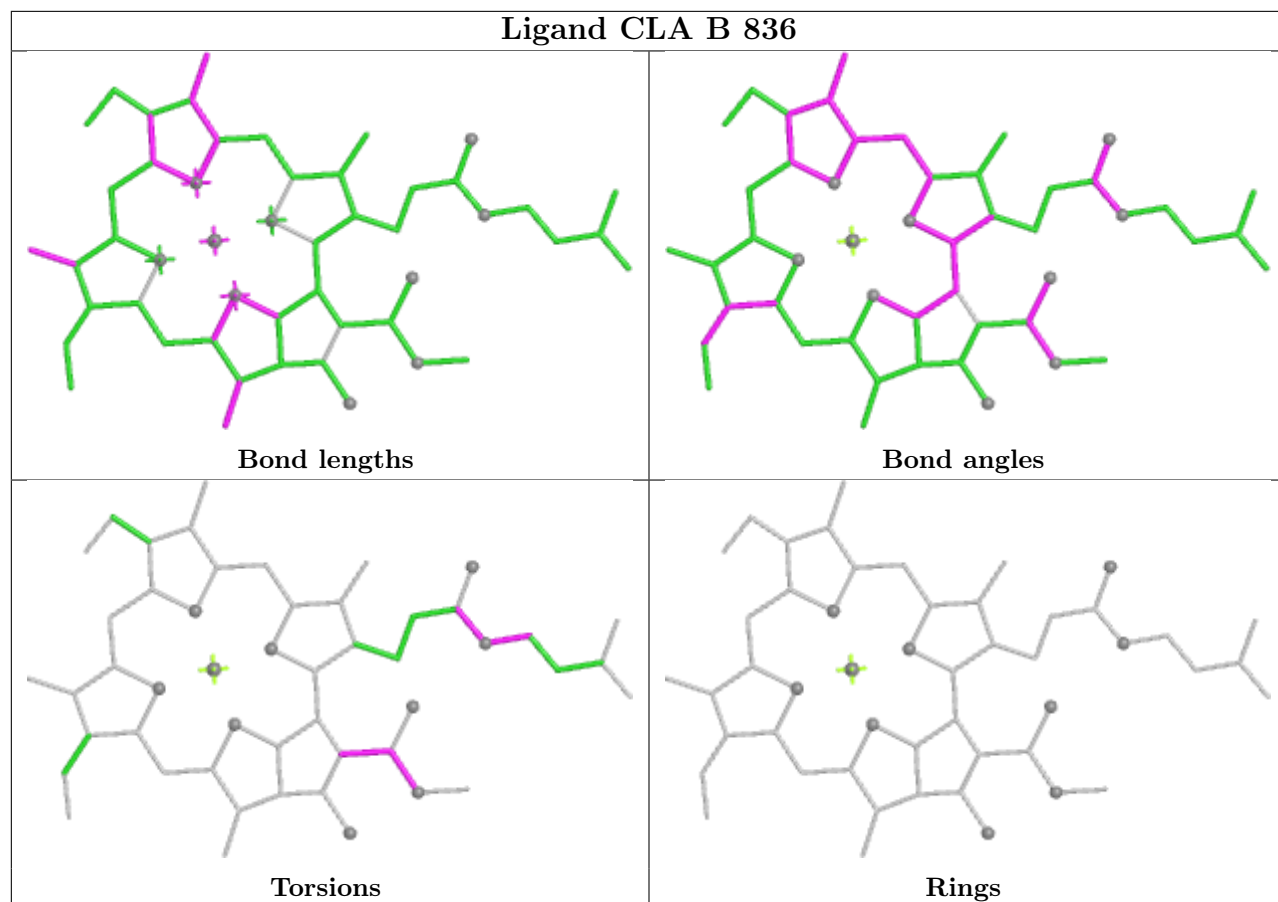
Ligand CLA A 823



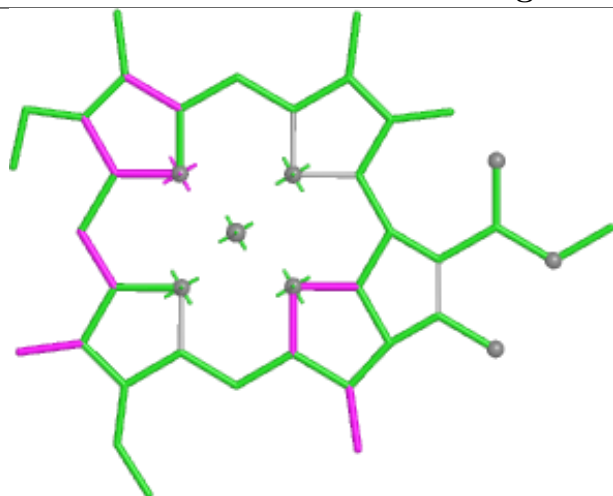
Ligand DGD B 850



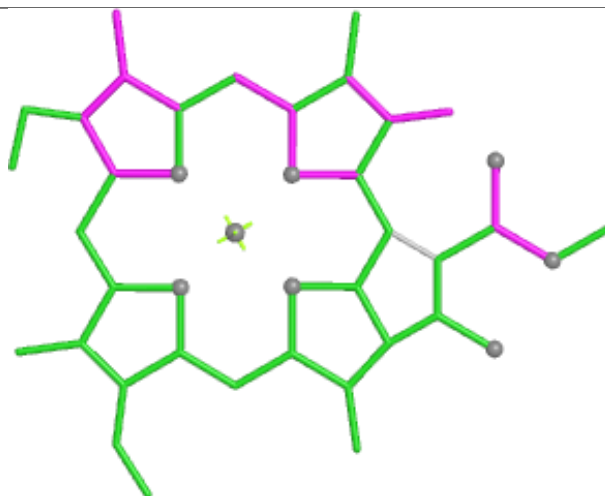




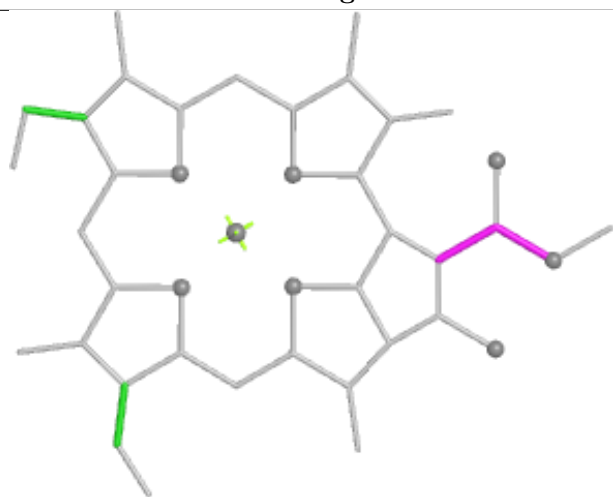
Ligand CLA F 304



Bond lengths



Bond angles

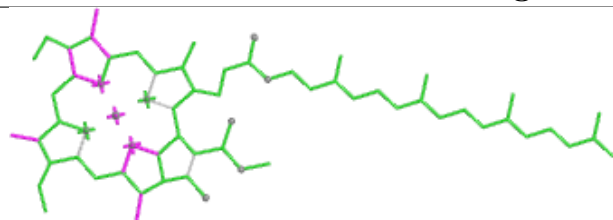


Torsions

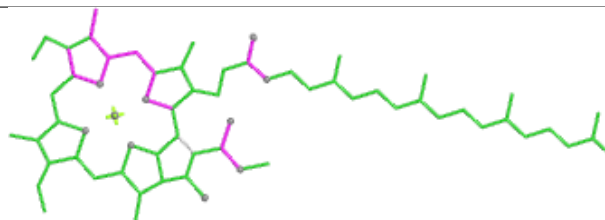


Rings

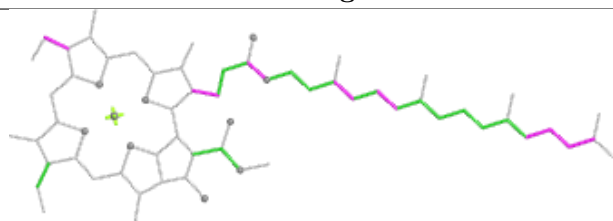
Ligand CLA K 203



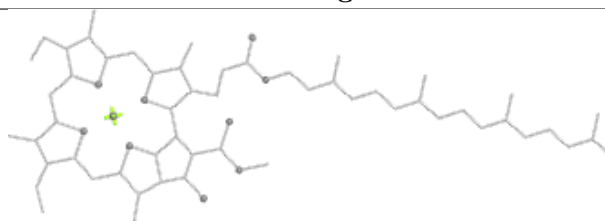
Bond lengths



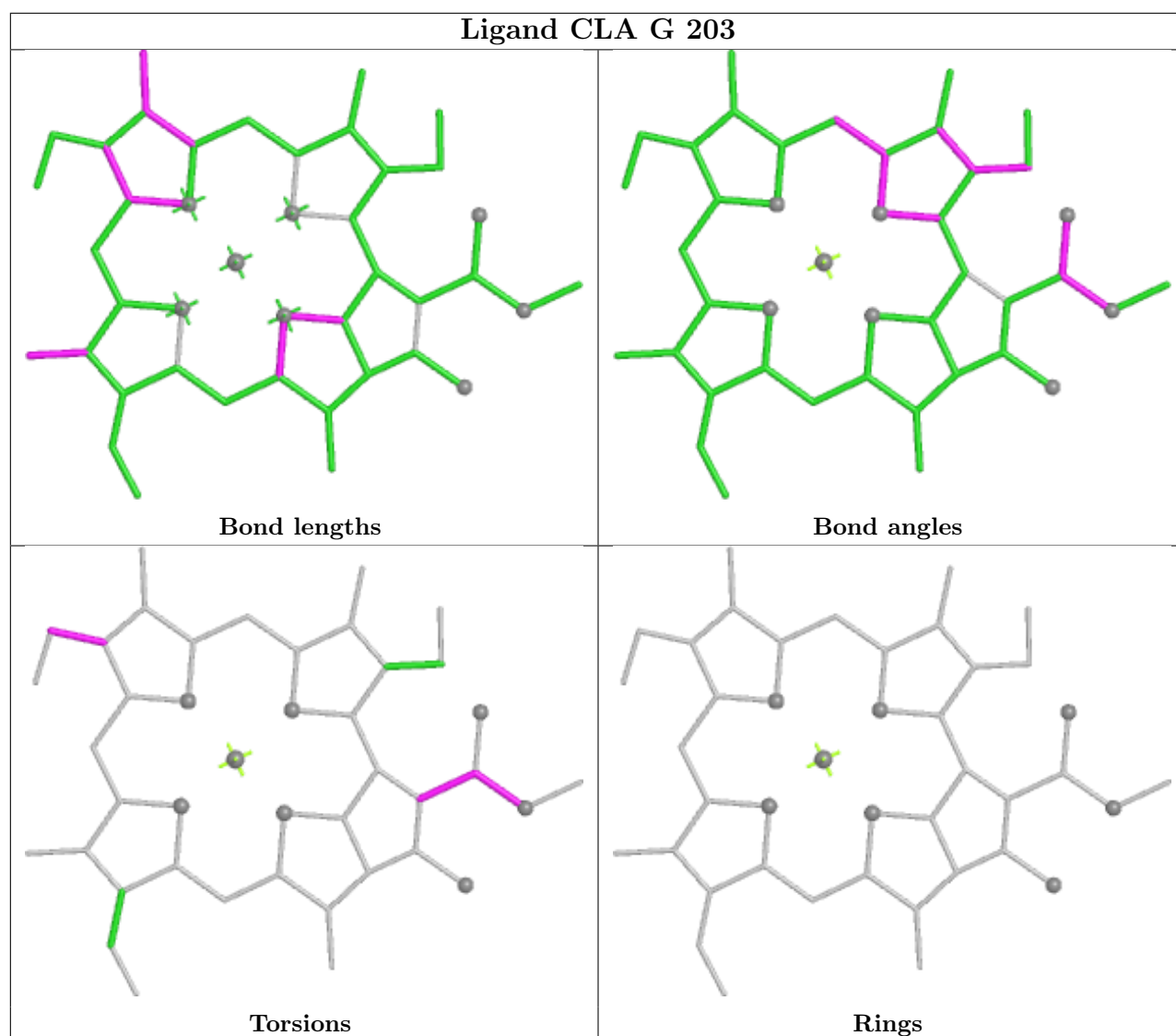
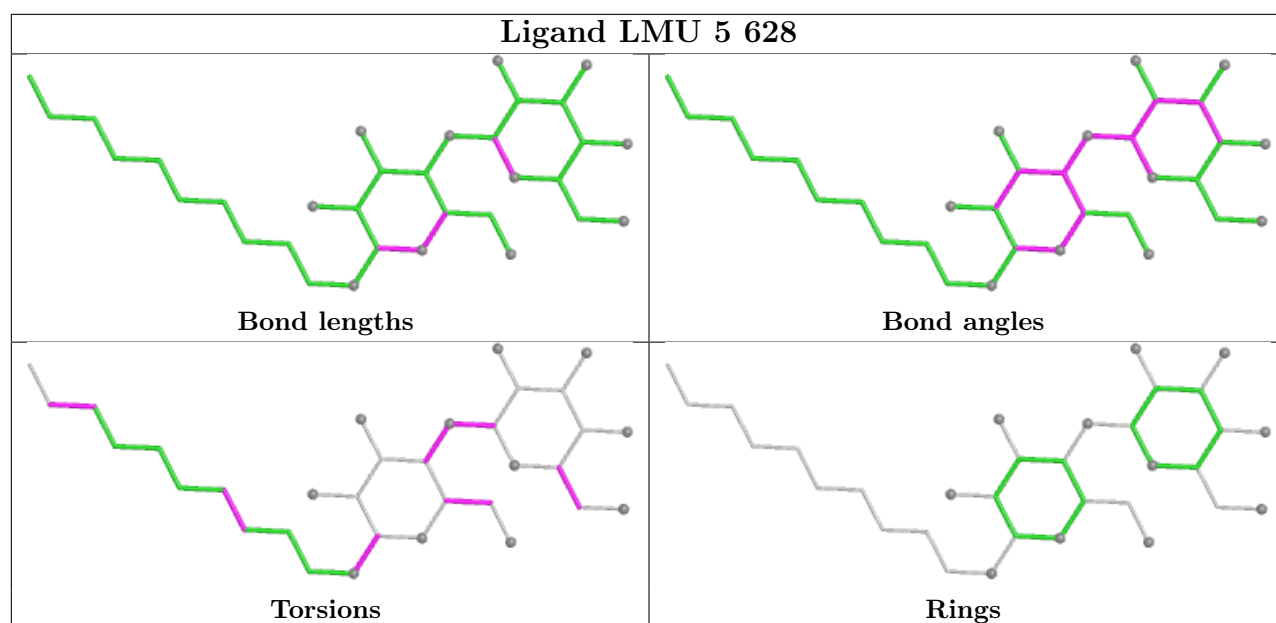
Bond angles



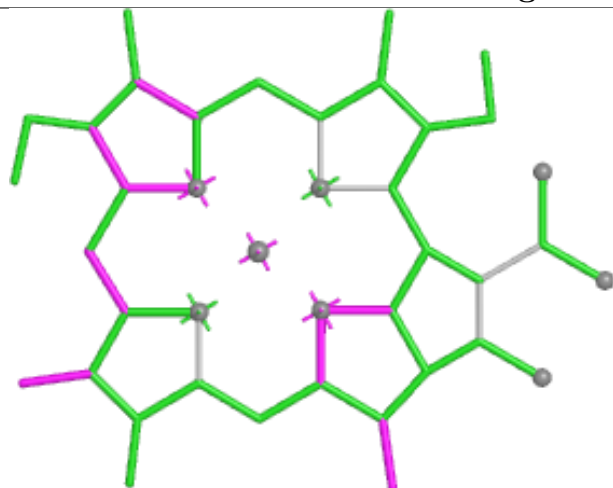
Torsions



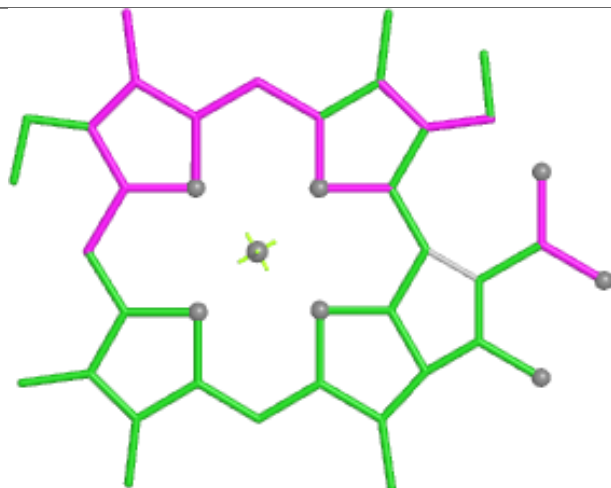
Rings



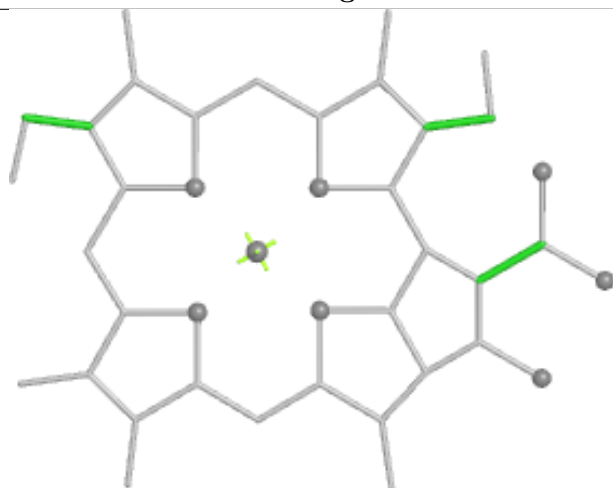
Ligand CLA 6 606



Bond lengths



Bond angles

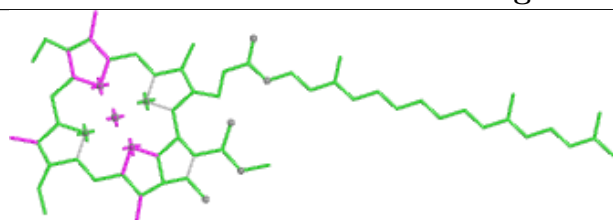


Torsions

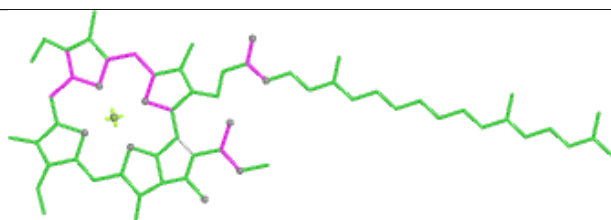


Rings

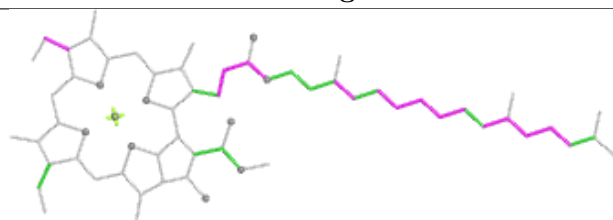
Ligand CLA A 843



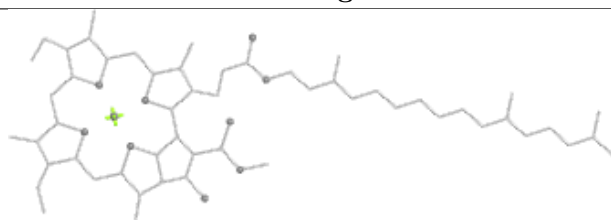
Bond lengths



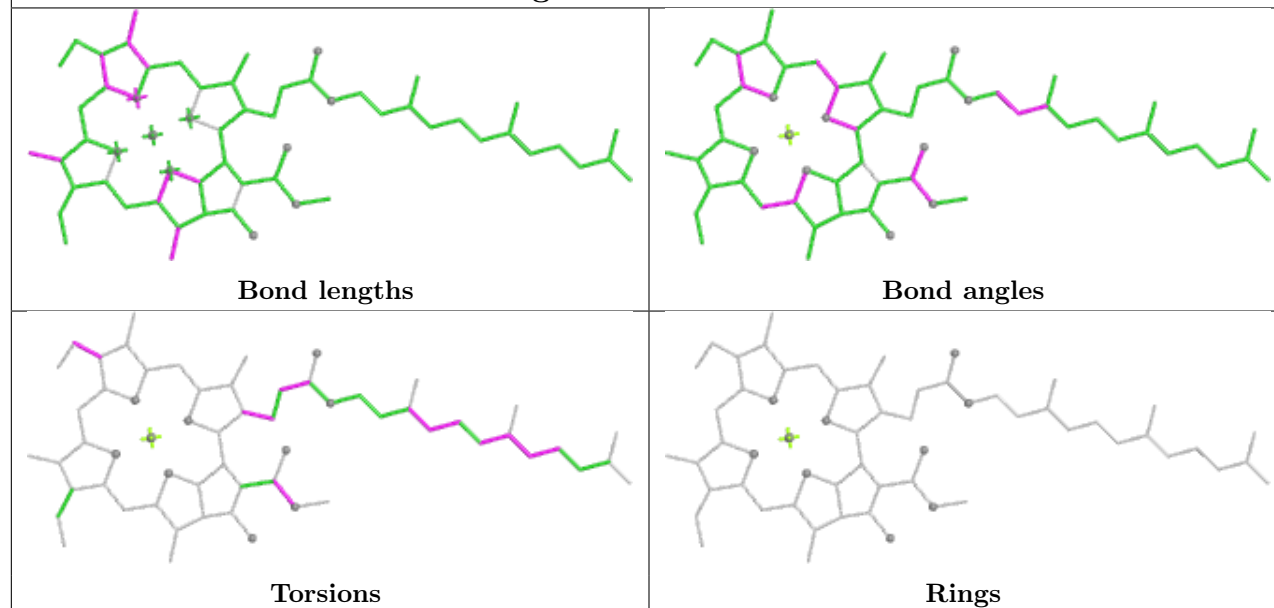
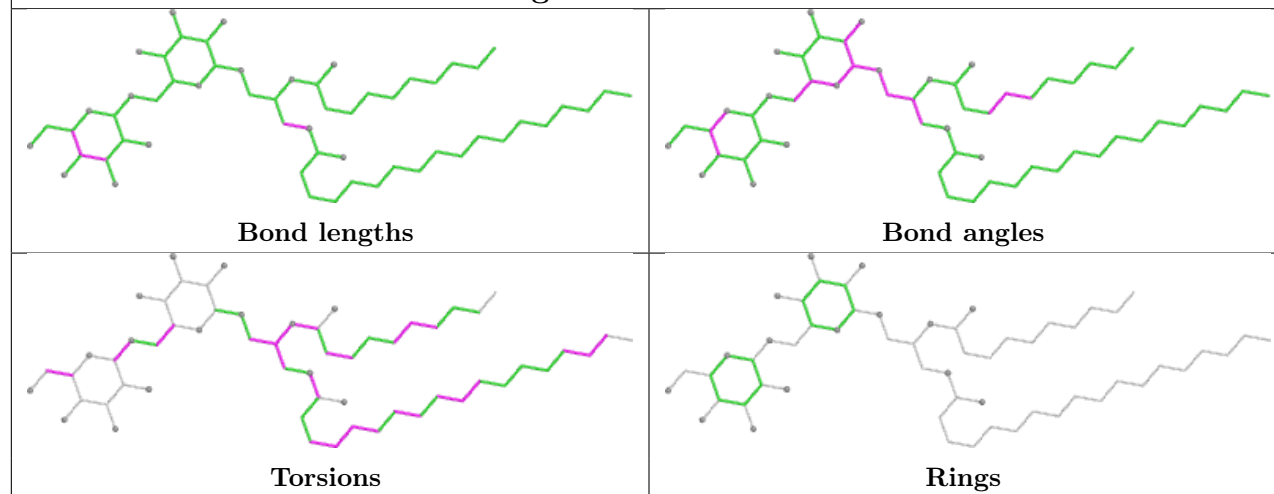
Bond angles



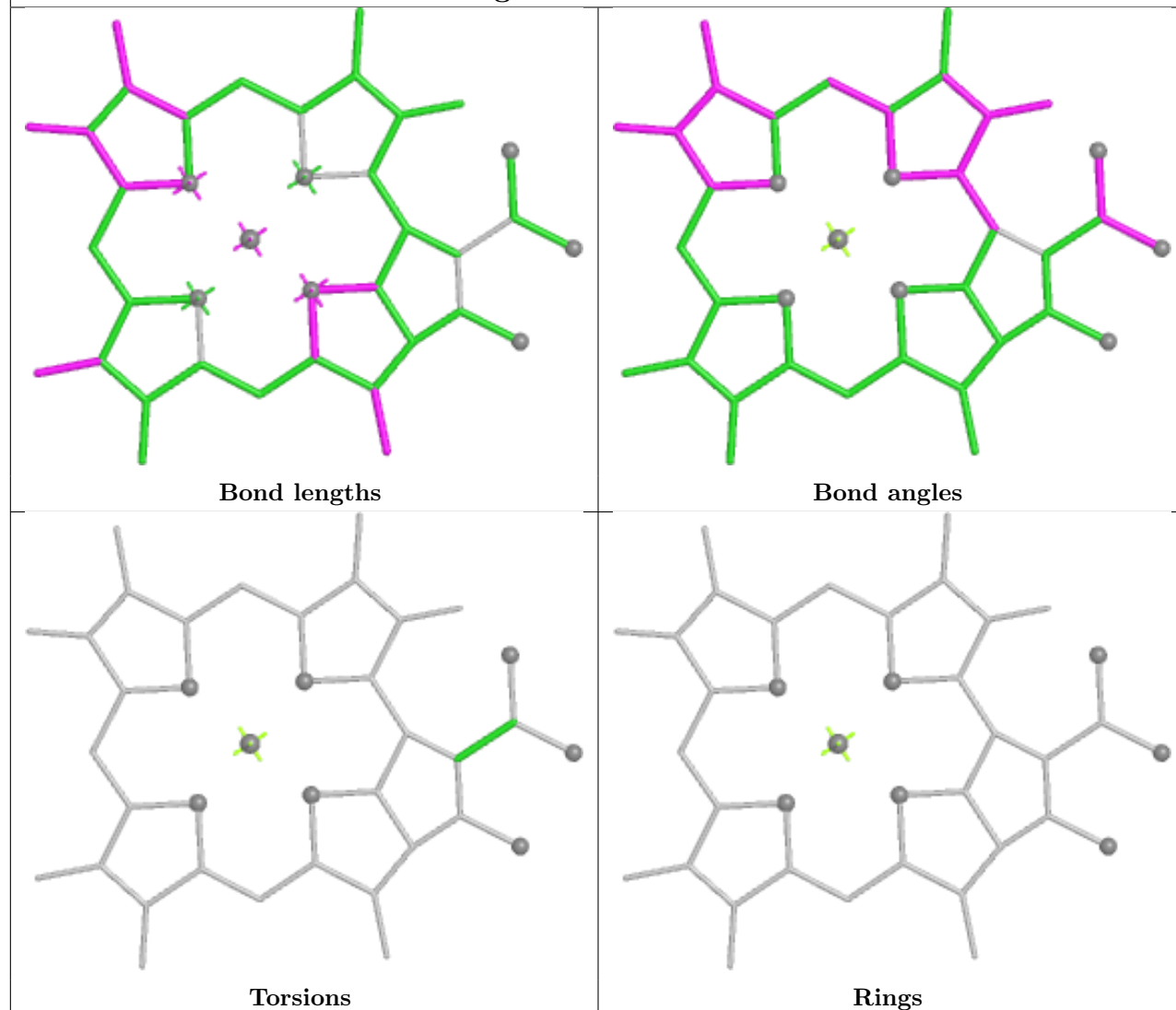
Torsions



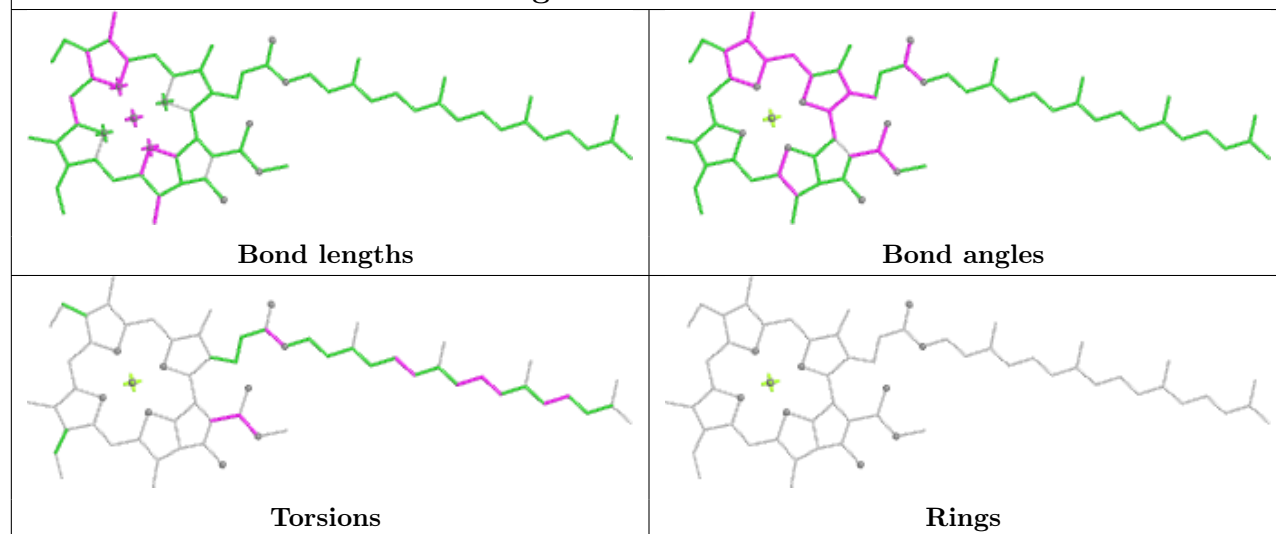
Rings

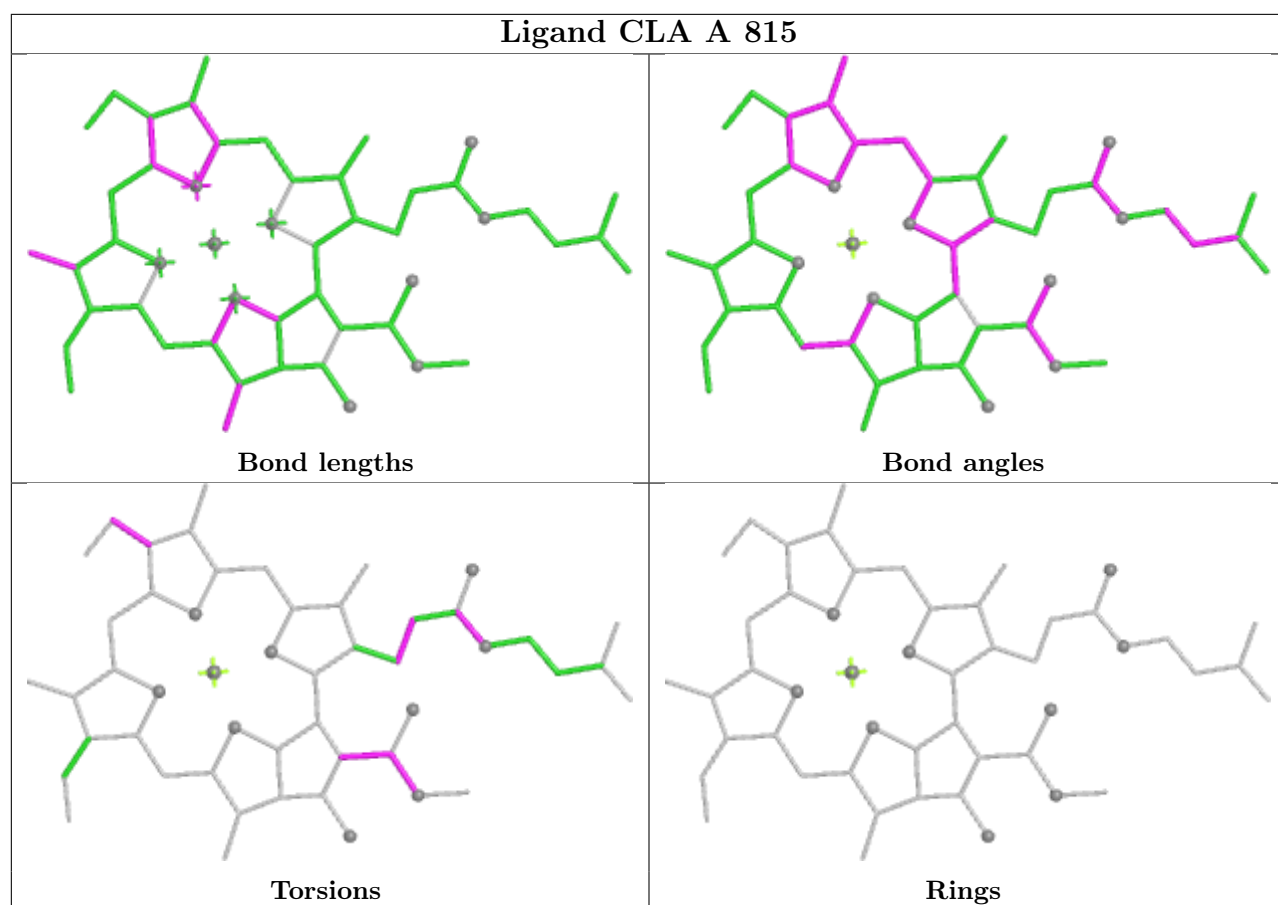
Ligand CLA B 834**Ligand DGD J 103**

Ligand CLA a 611

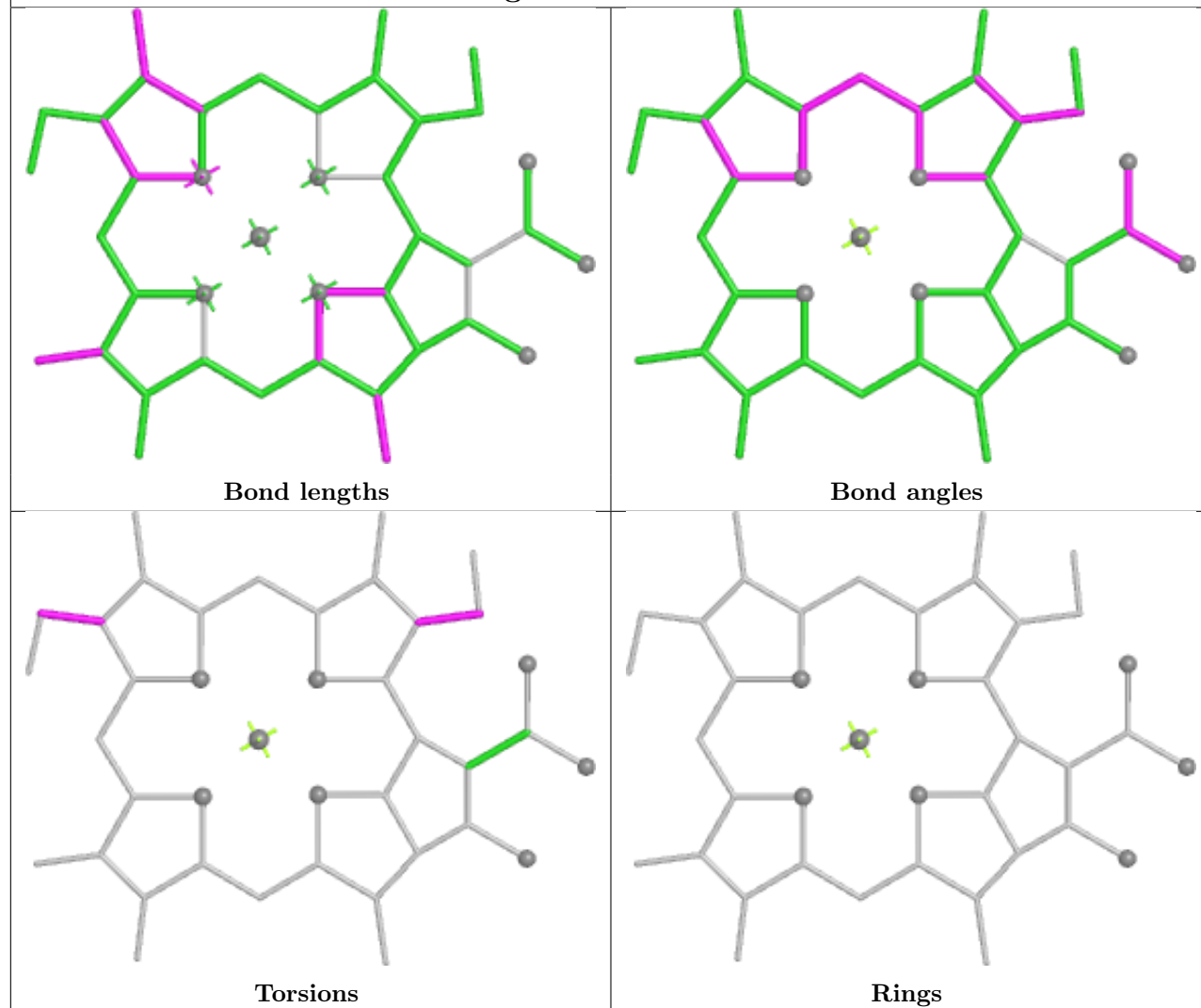


Ligand CLA B 824

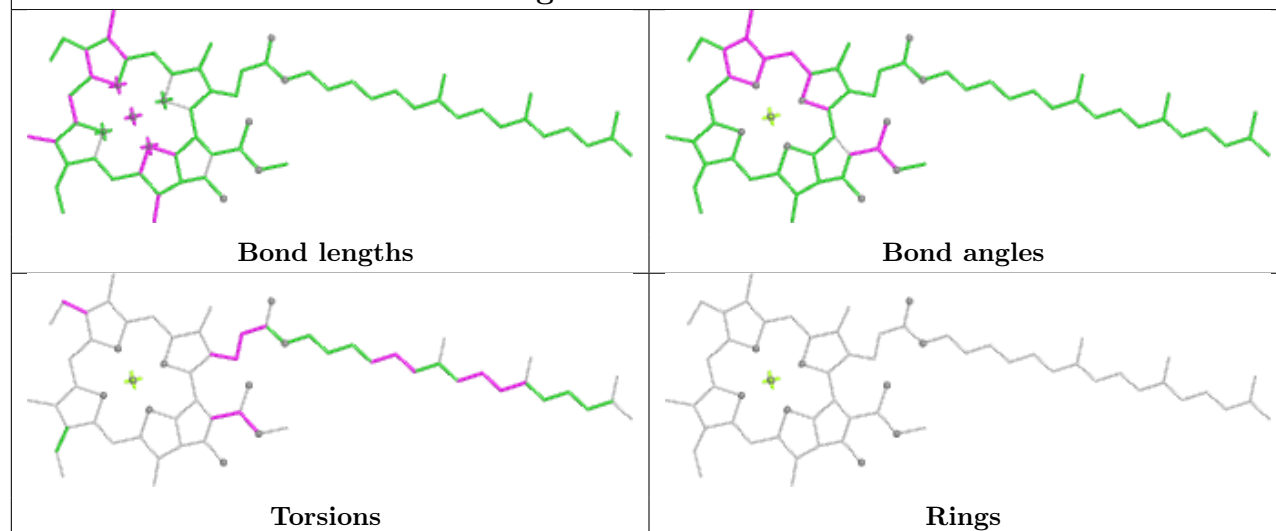


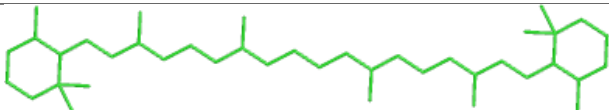
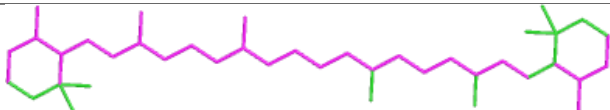
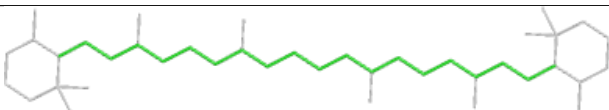
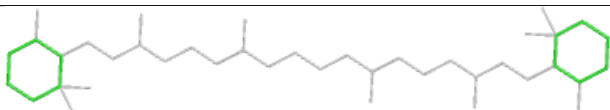


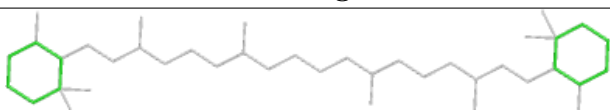
Ligand CLA 3 615

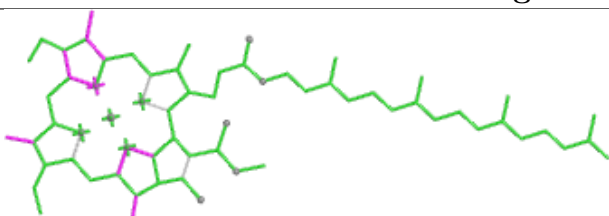
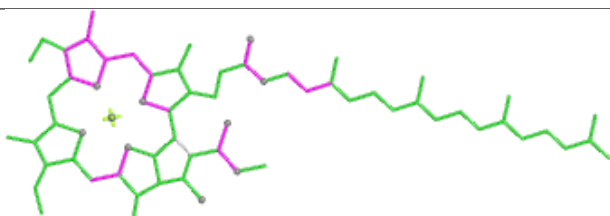
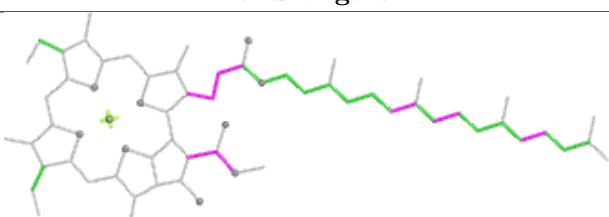
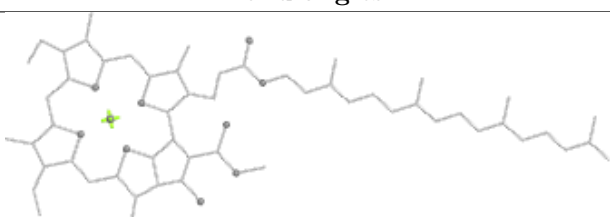


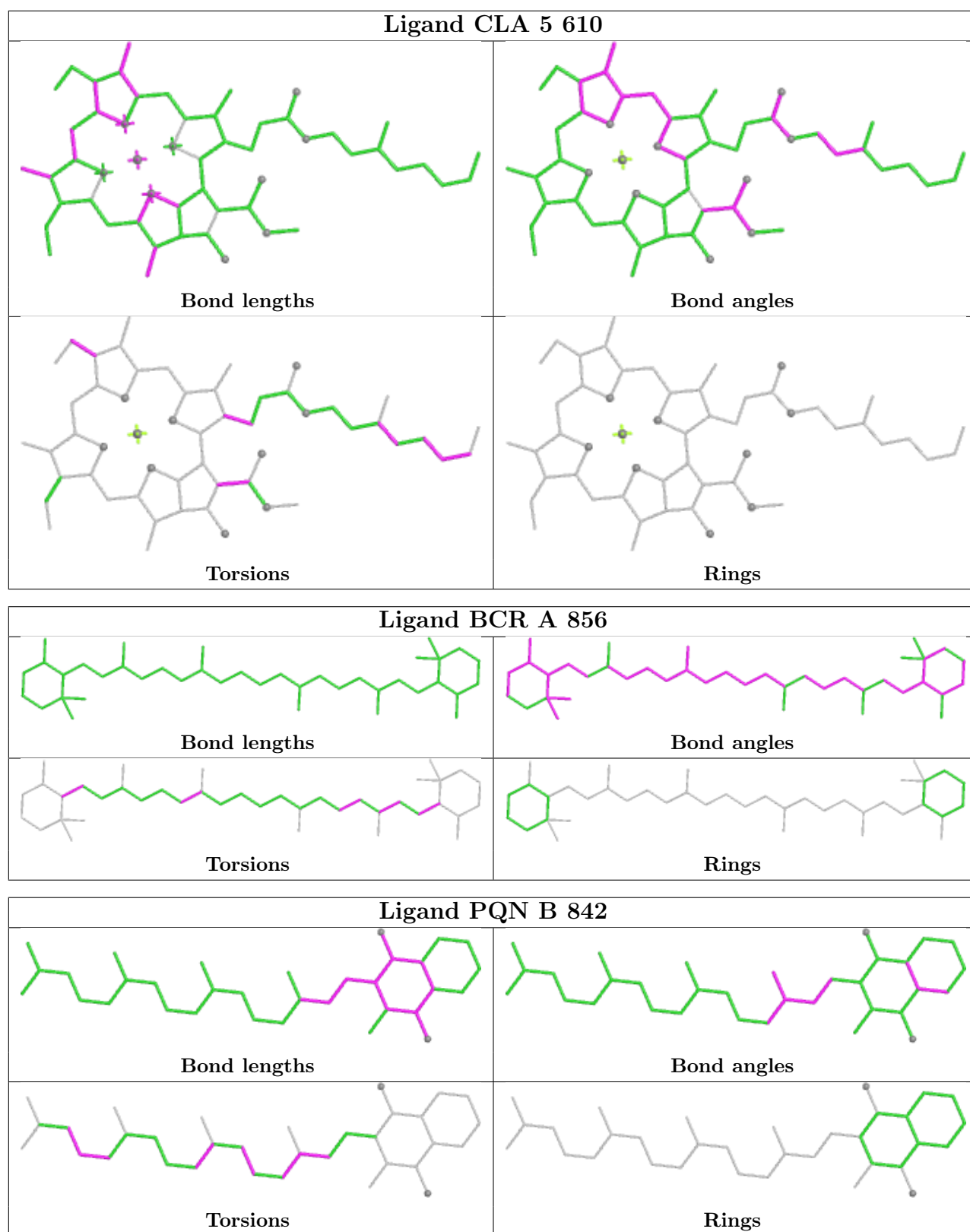
Ligand CLA 6 620



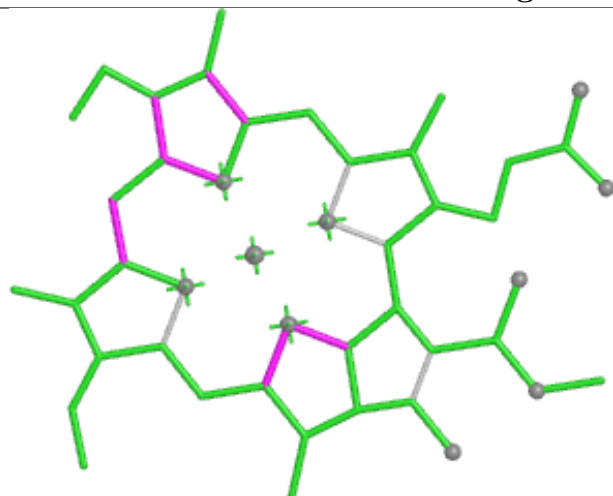
Ligand BCR G 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

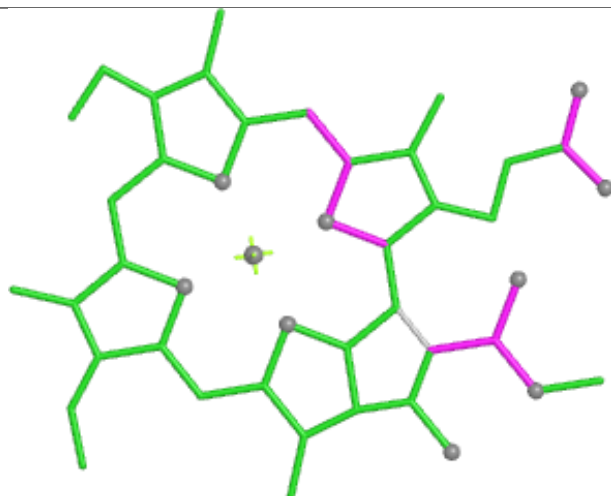
Ligand CLA 6 610	
	
Bond lengths	Bond angles
	
Torsions	Rings



Ligand CLA L 302



Bond lengths



Bond angles

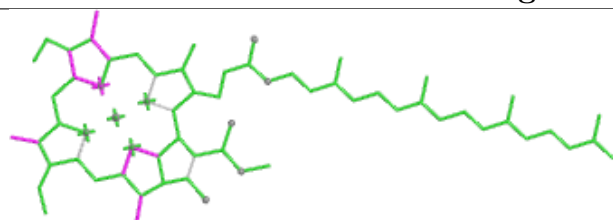


Torsions

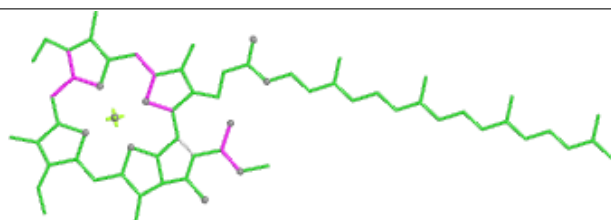


Rings

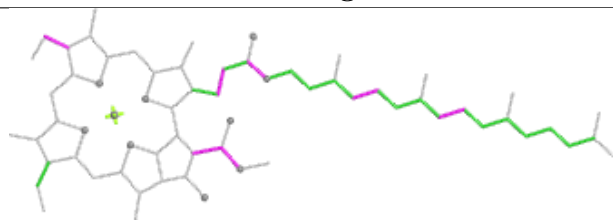
Ligand CLA 6 602



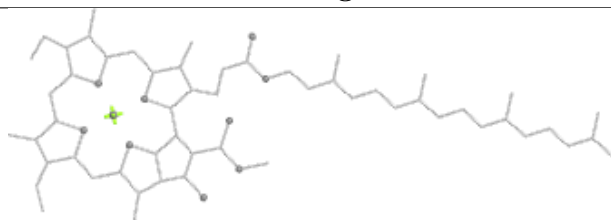
Bond lengths



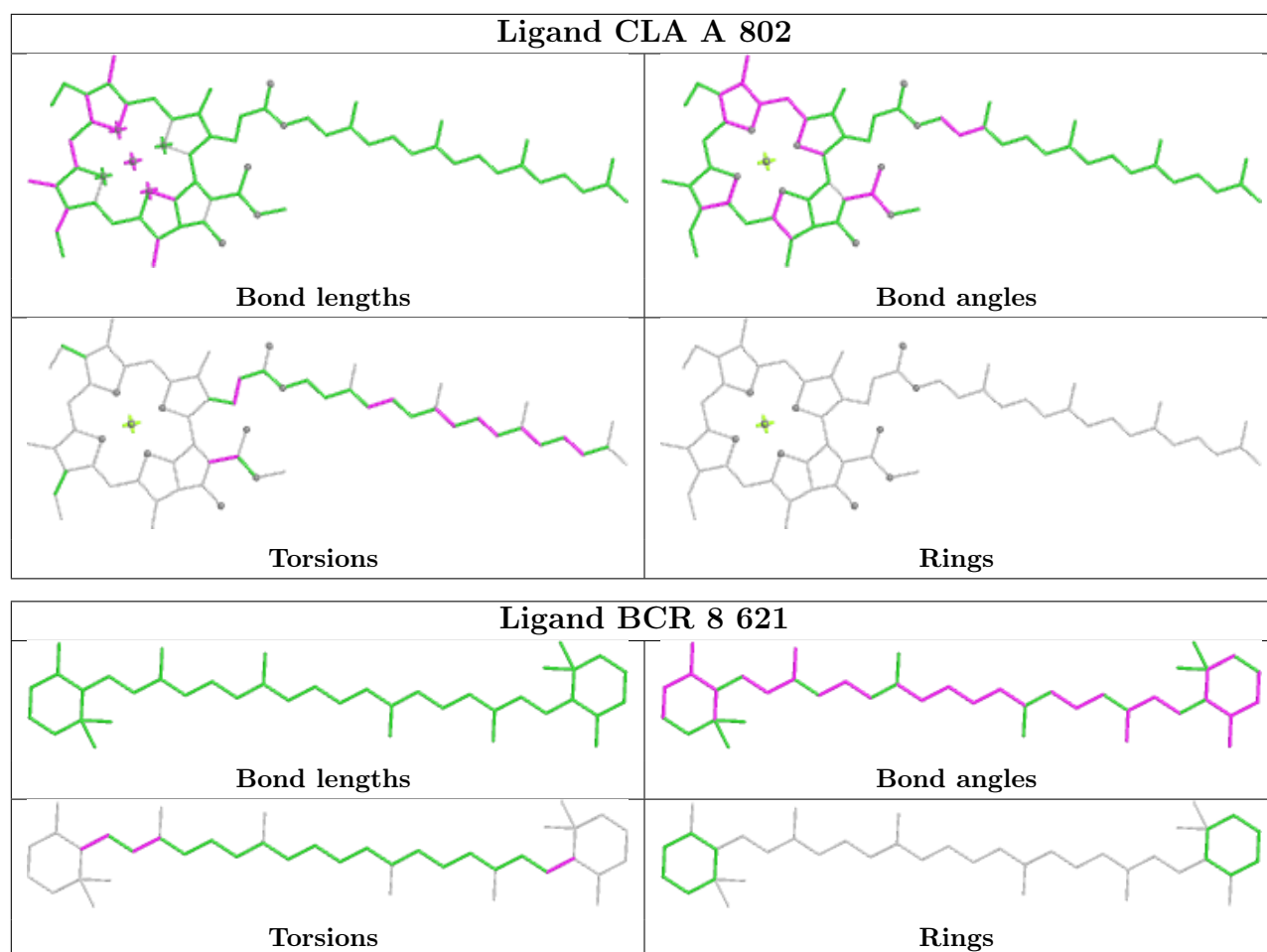
Bond angles

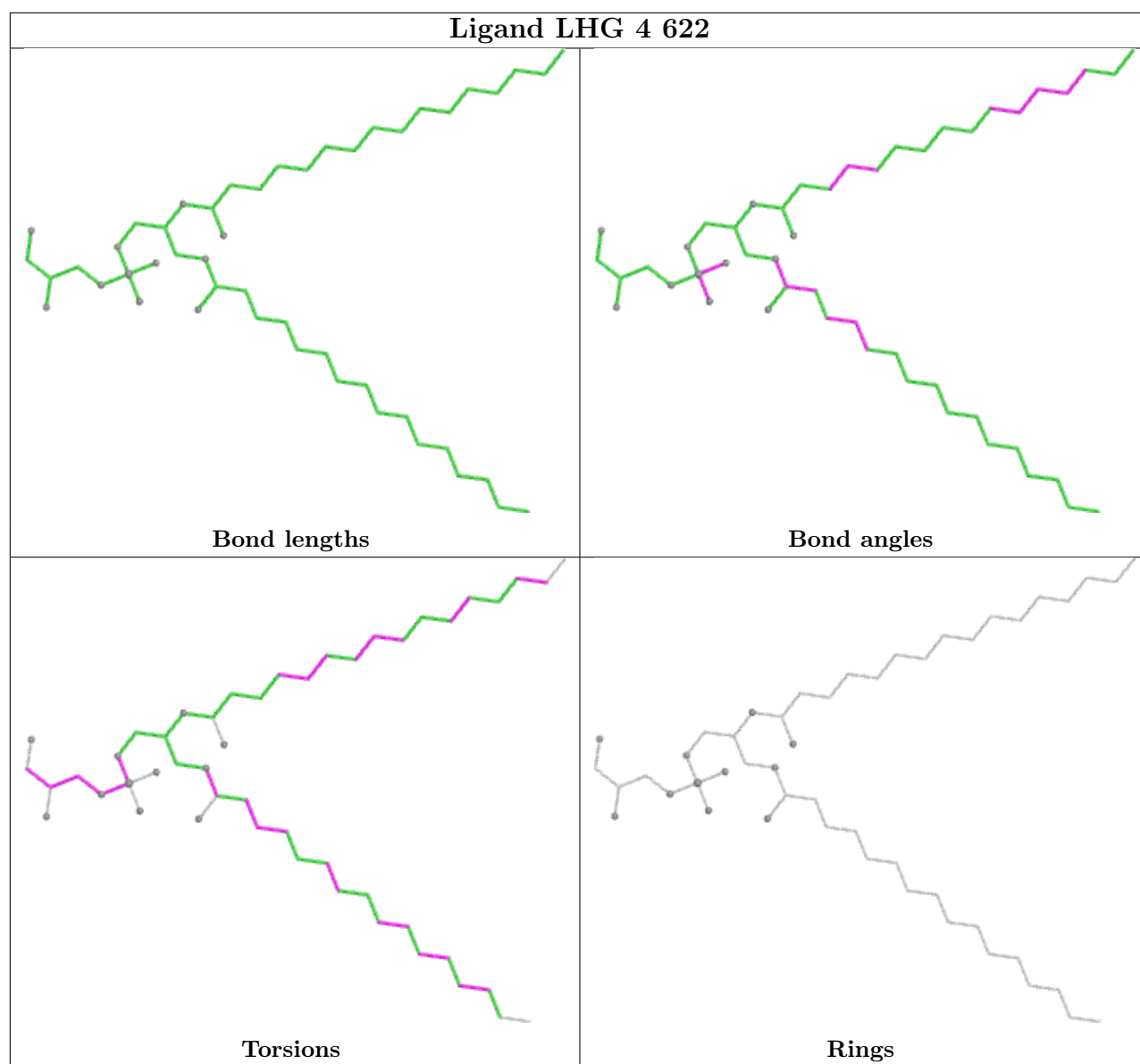


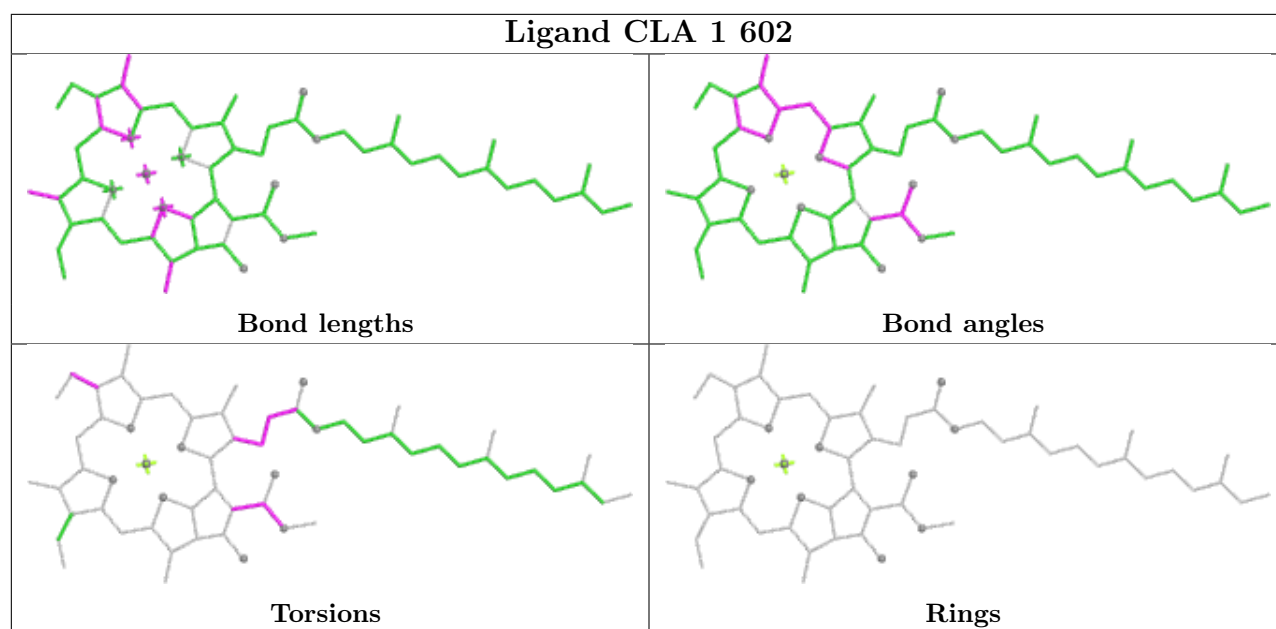
Torsions

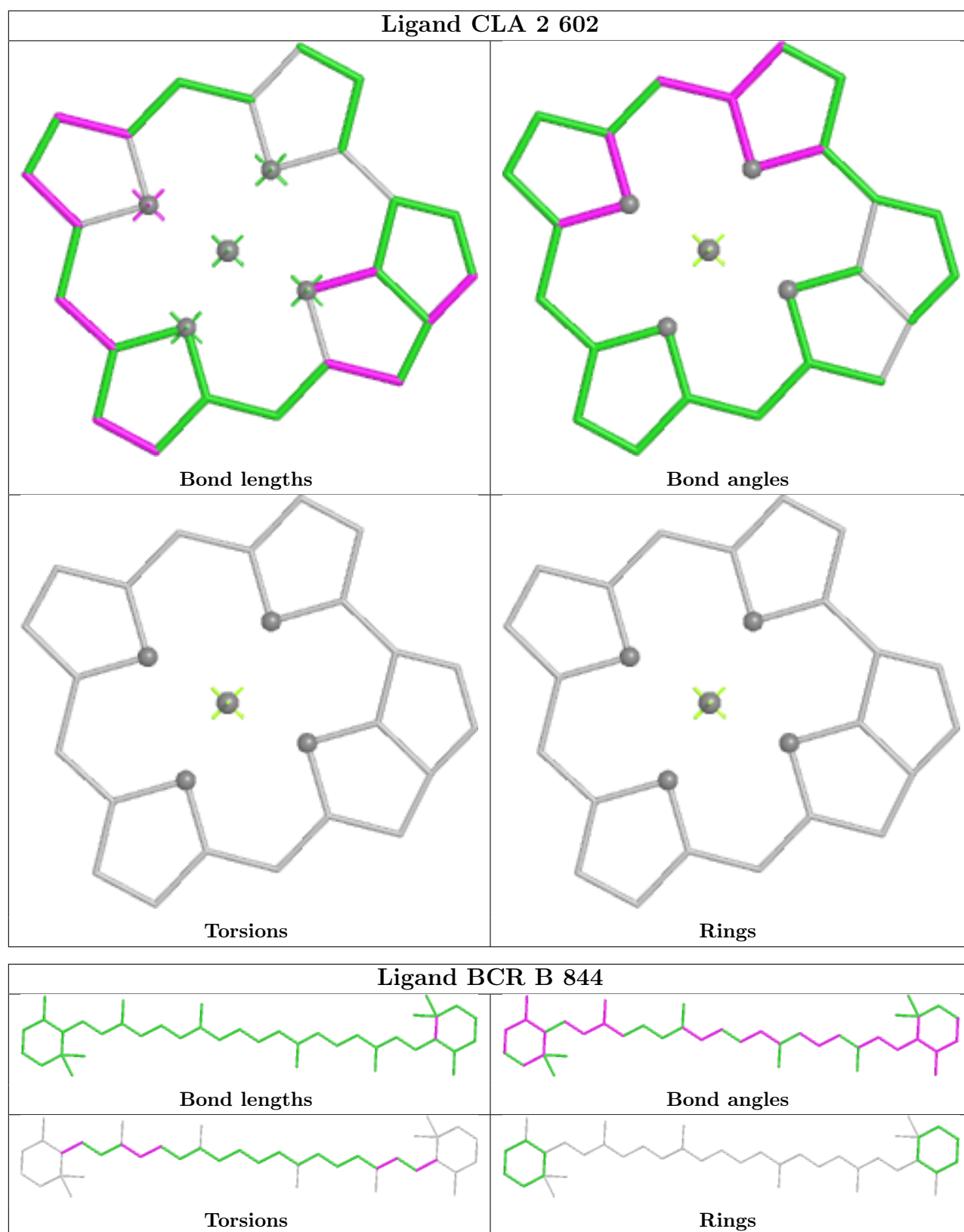


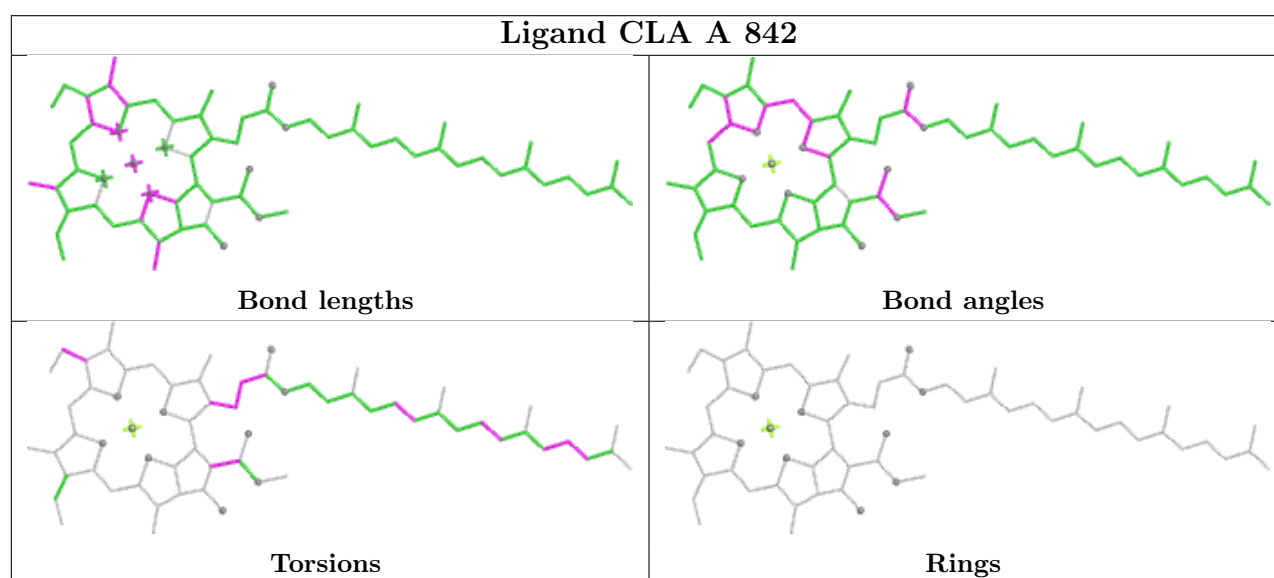
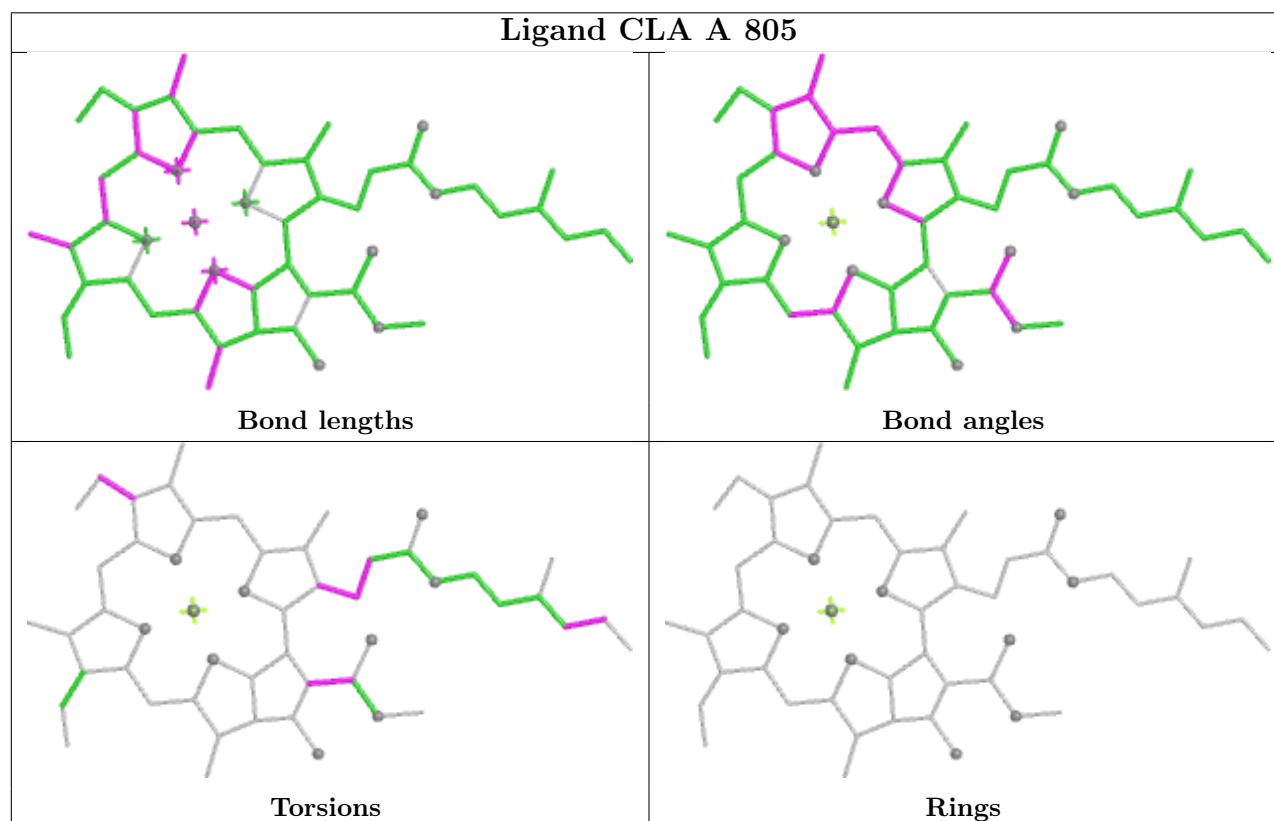
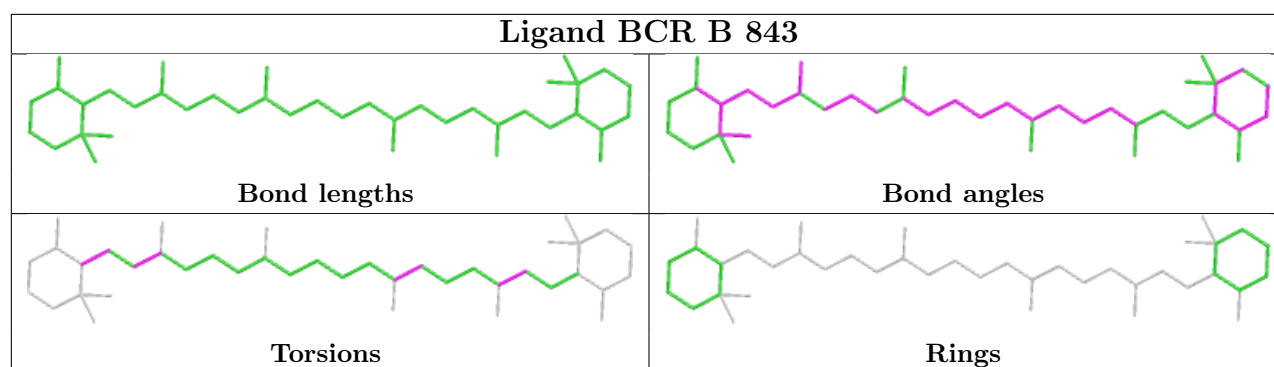
Rings

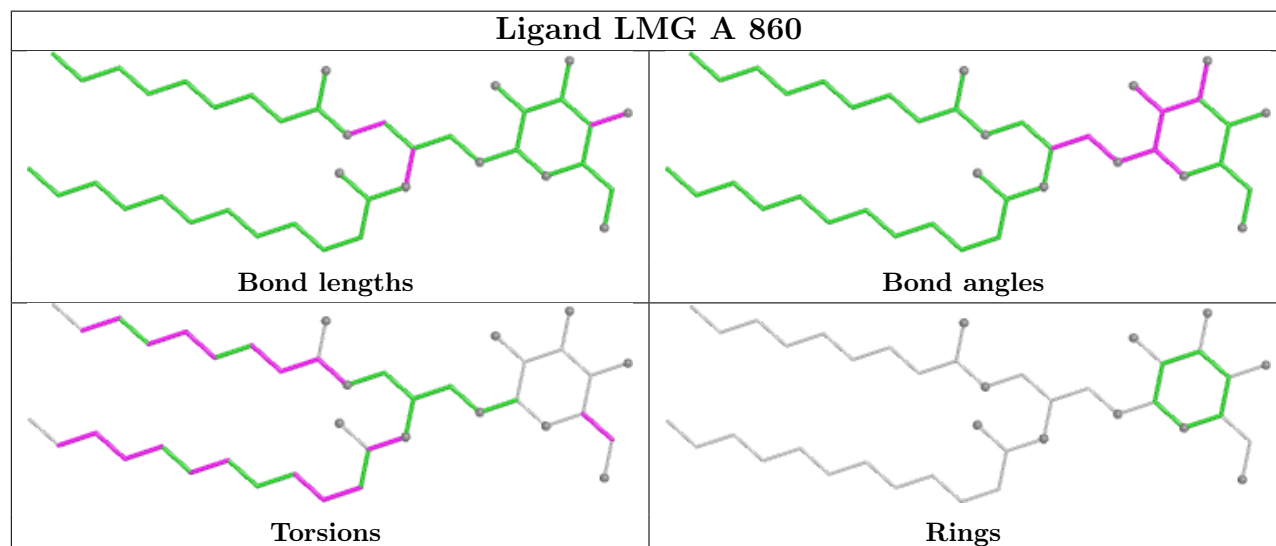
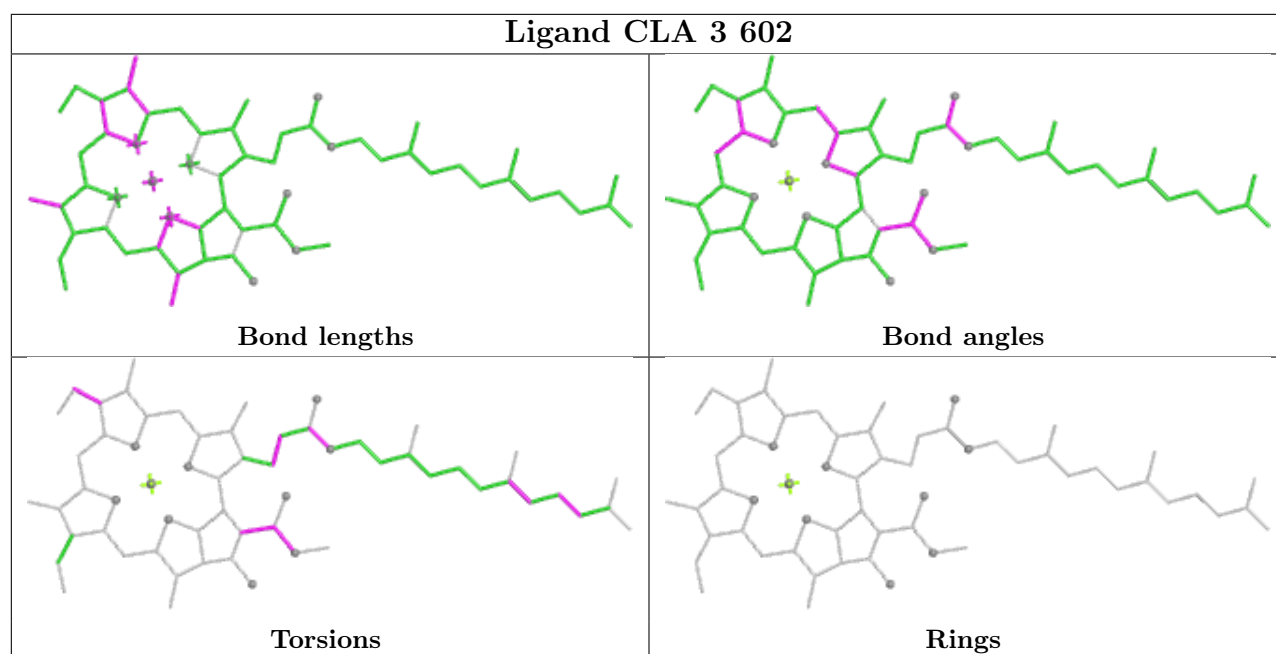




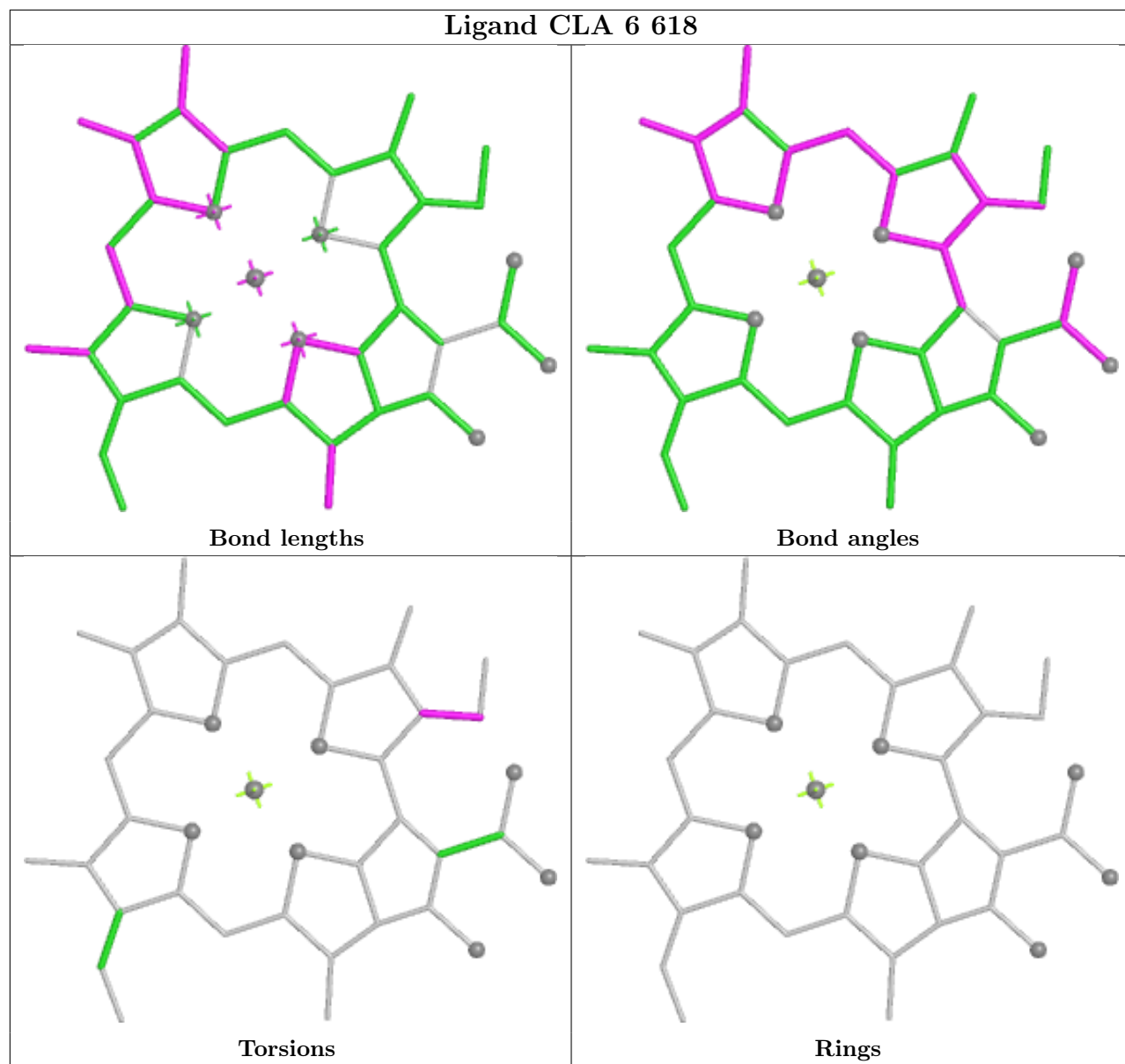




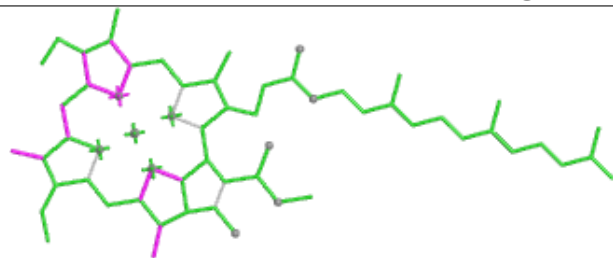




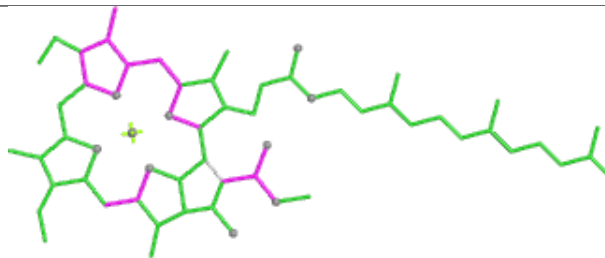
Ligand CLA 6 618



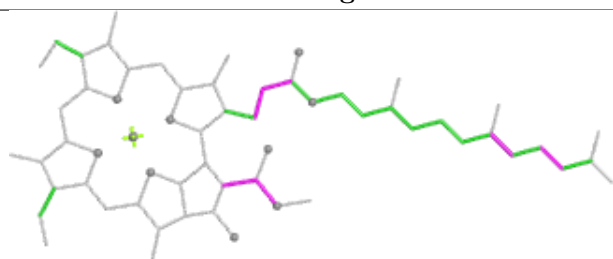
Ligand CLA 4 602



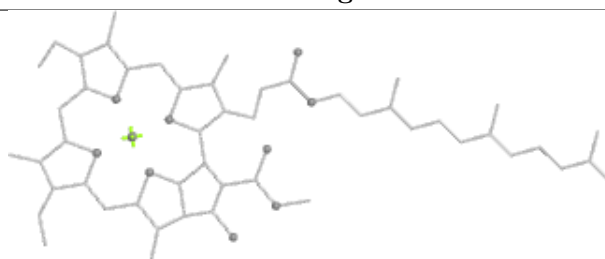
Bond lengths



Bond angles

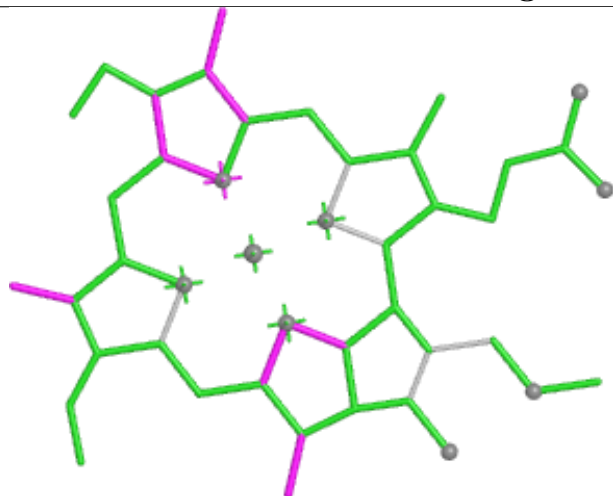


Torsions

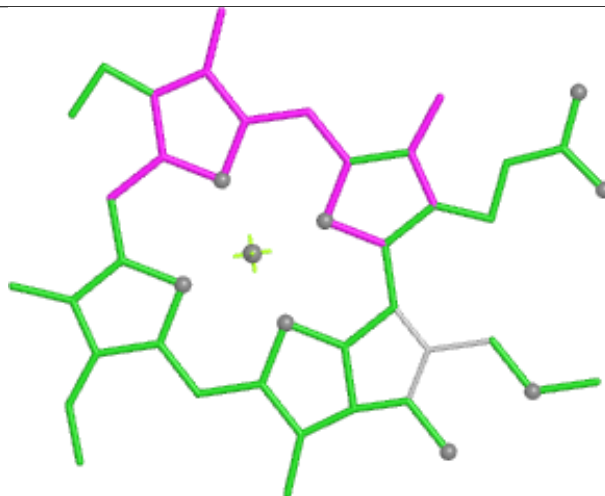


Rings

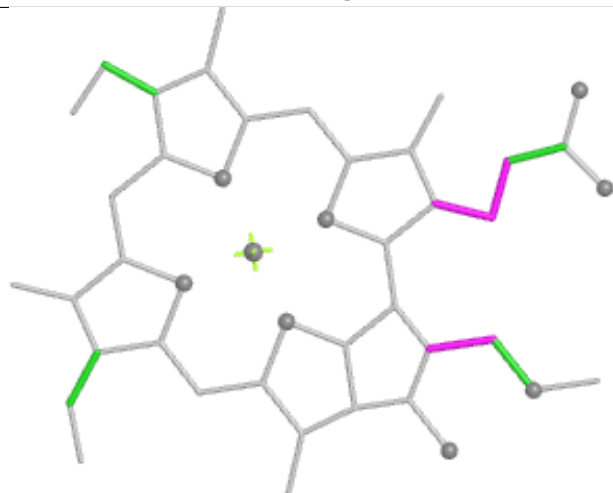
Ligand CLA 7 609



Bond lengths



Bond angles

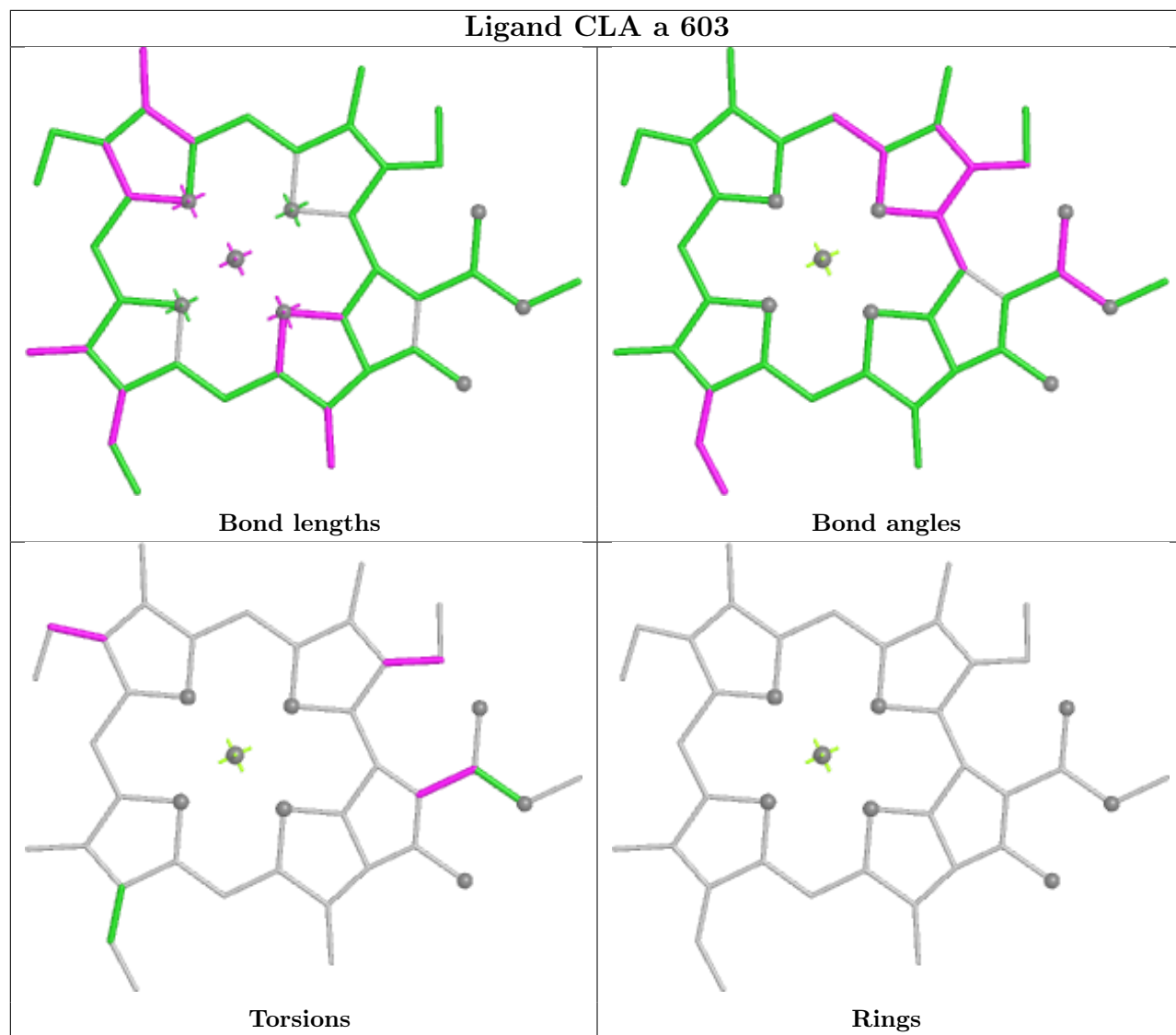


Torsions

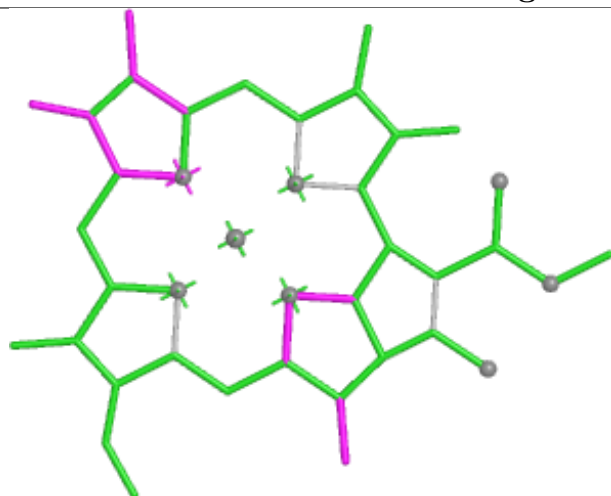


Rings

Ligand CLA a 603



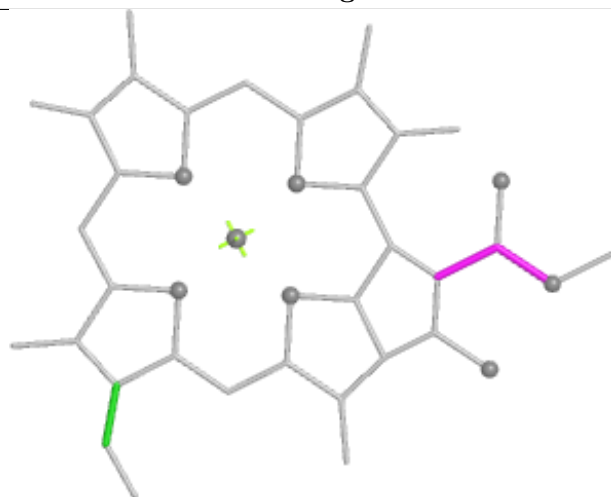
Ligand CLA 1 609



Bond lengths



Bond angles

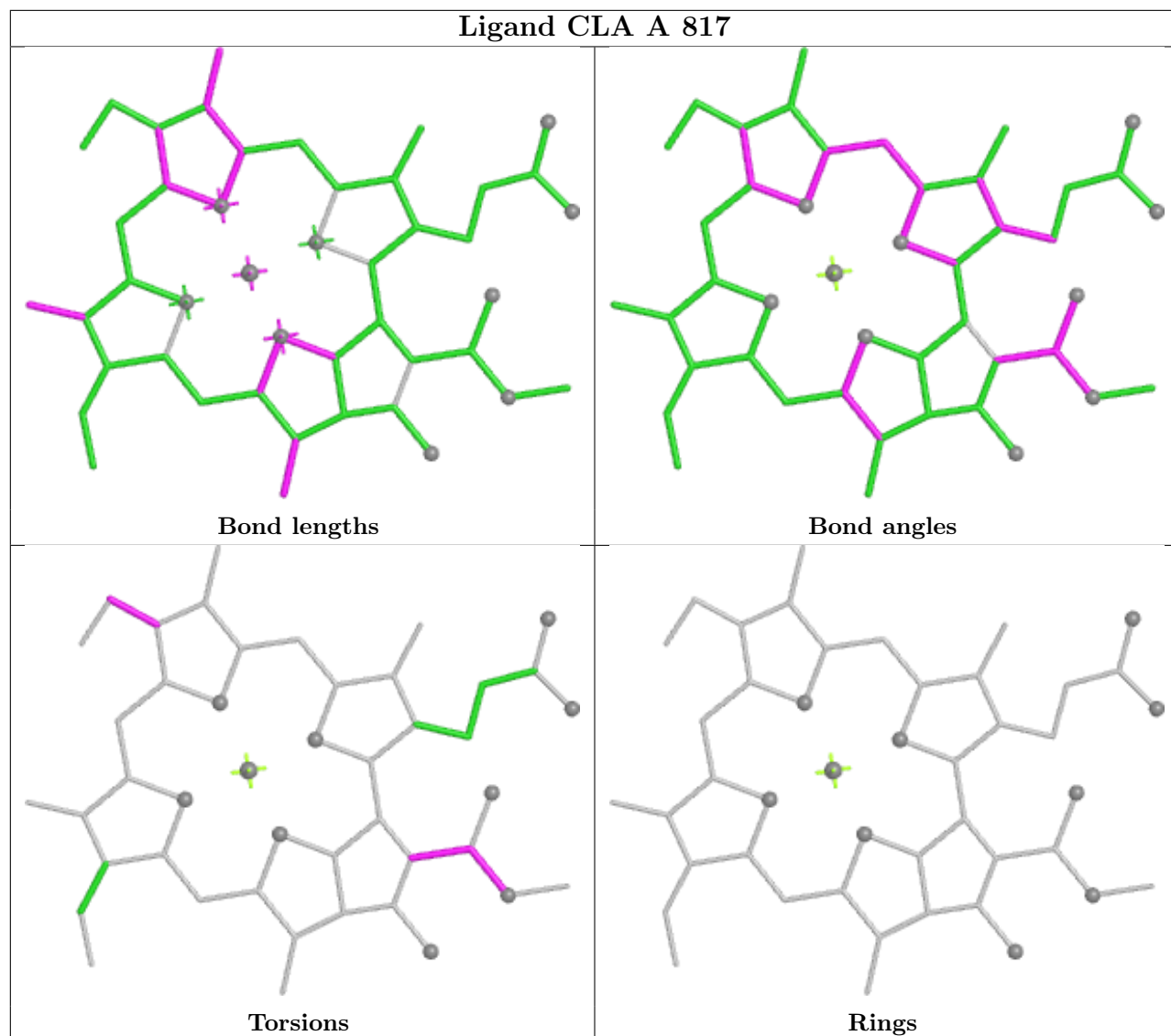


Torsions

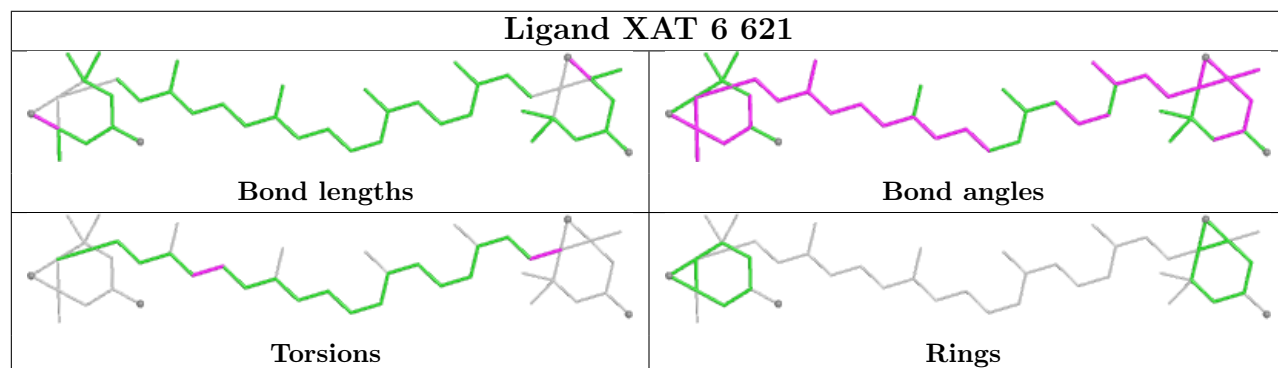


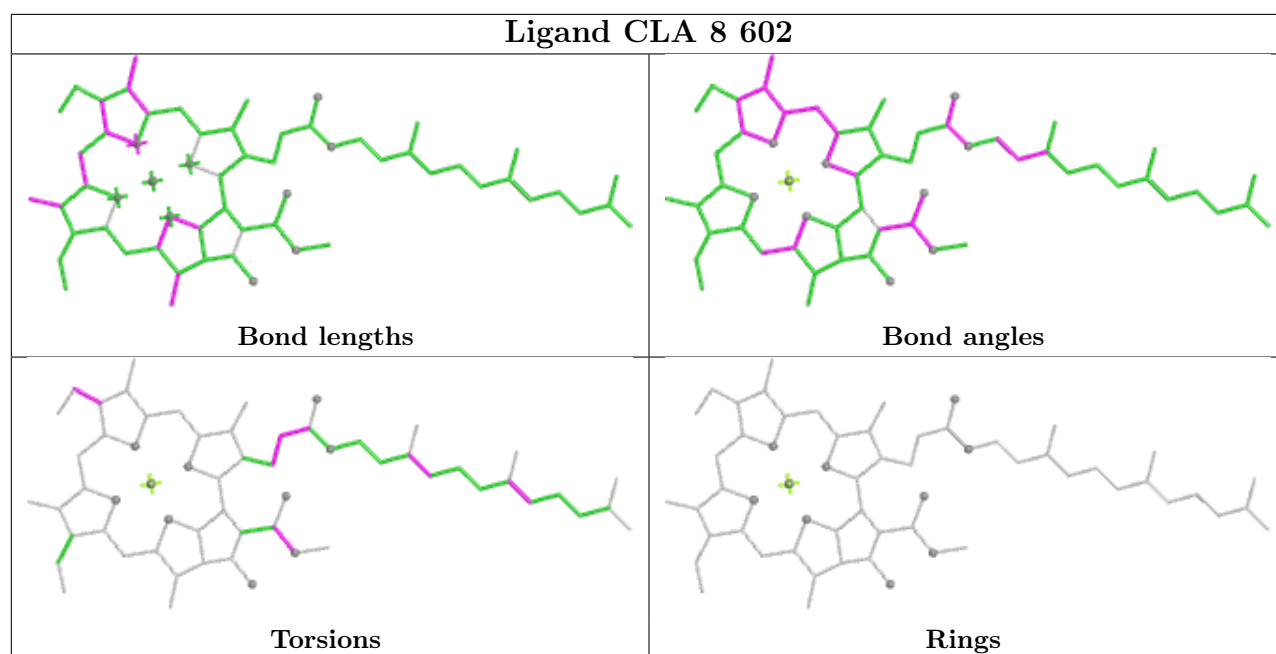
Rings

Ligand CLA A 817

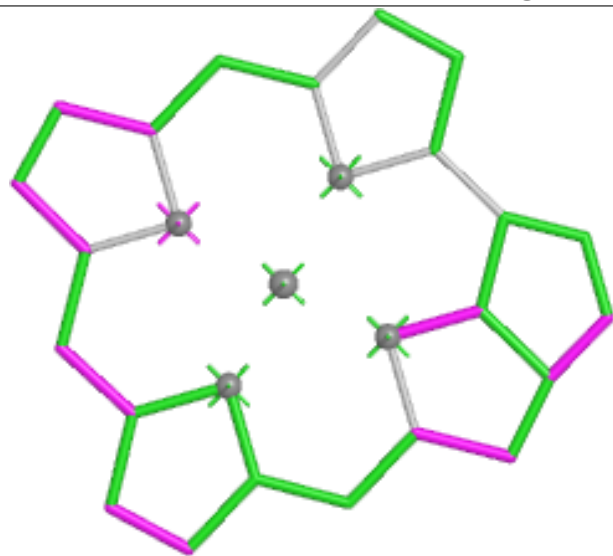


Ligand XAT 6 621

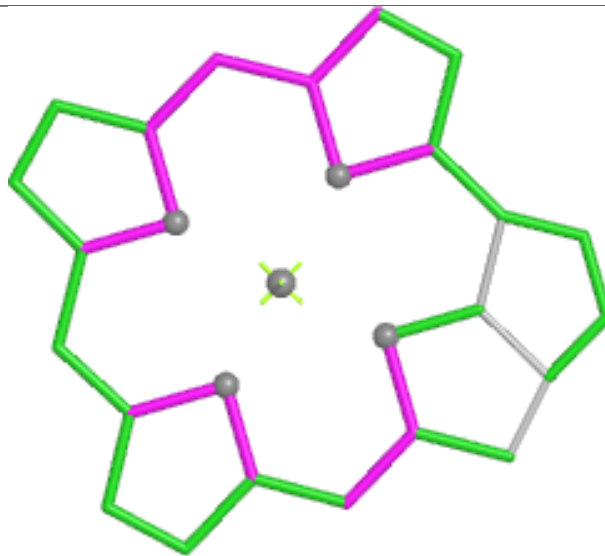




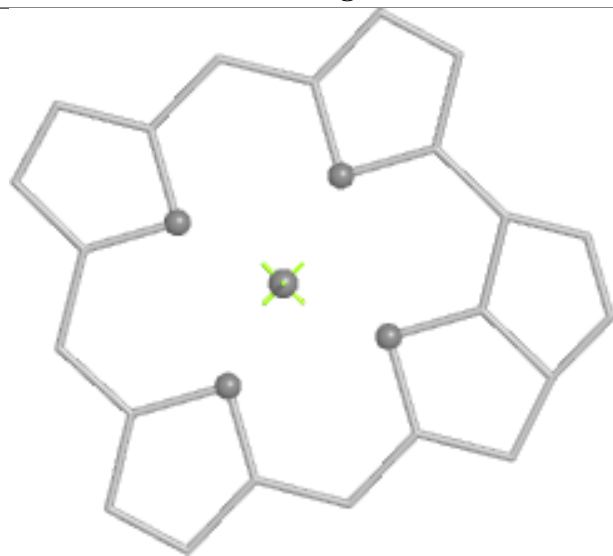
Ligand CLA 2 601



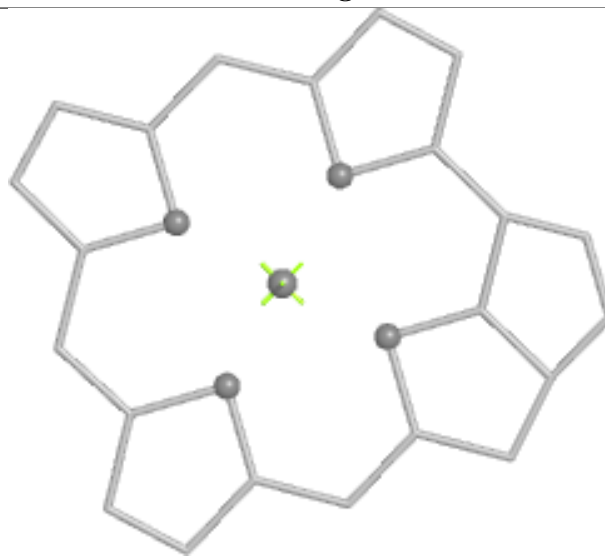
Bond lengths



Bond angles

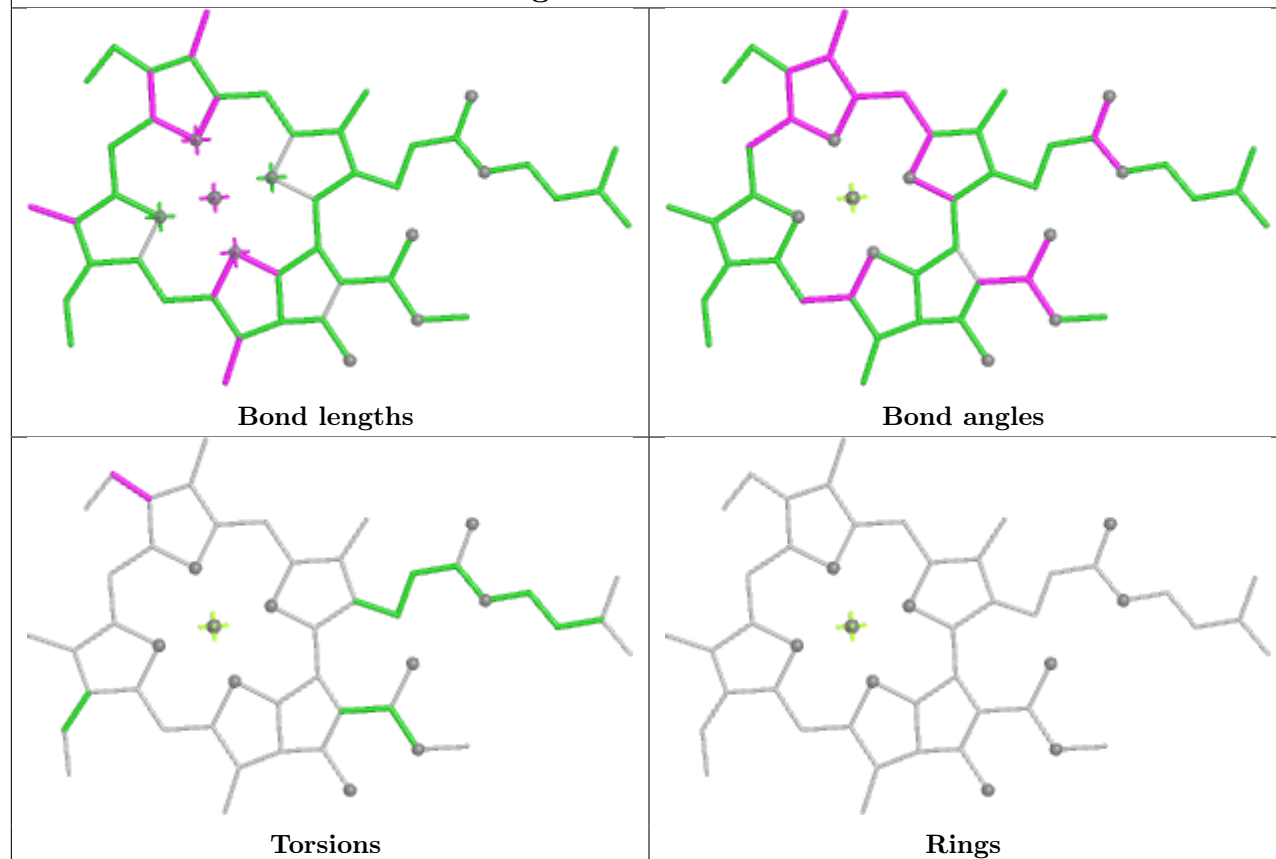


Torsions

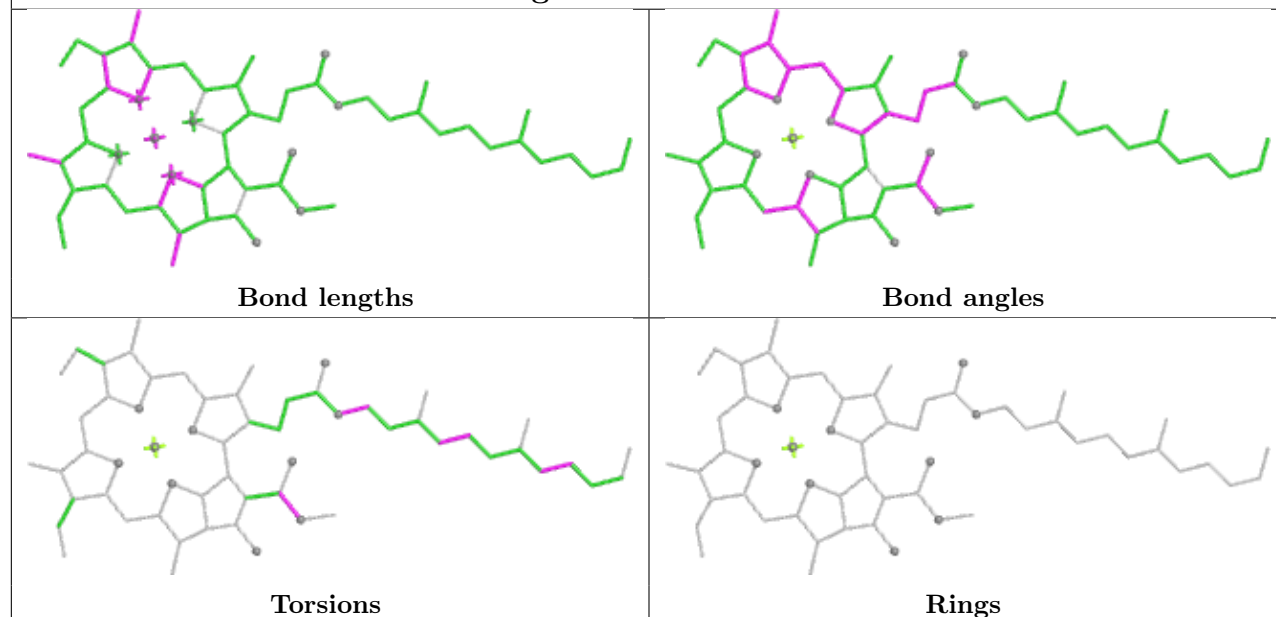


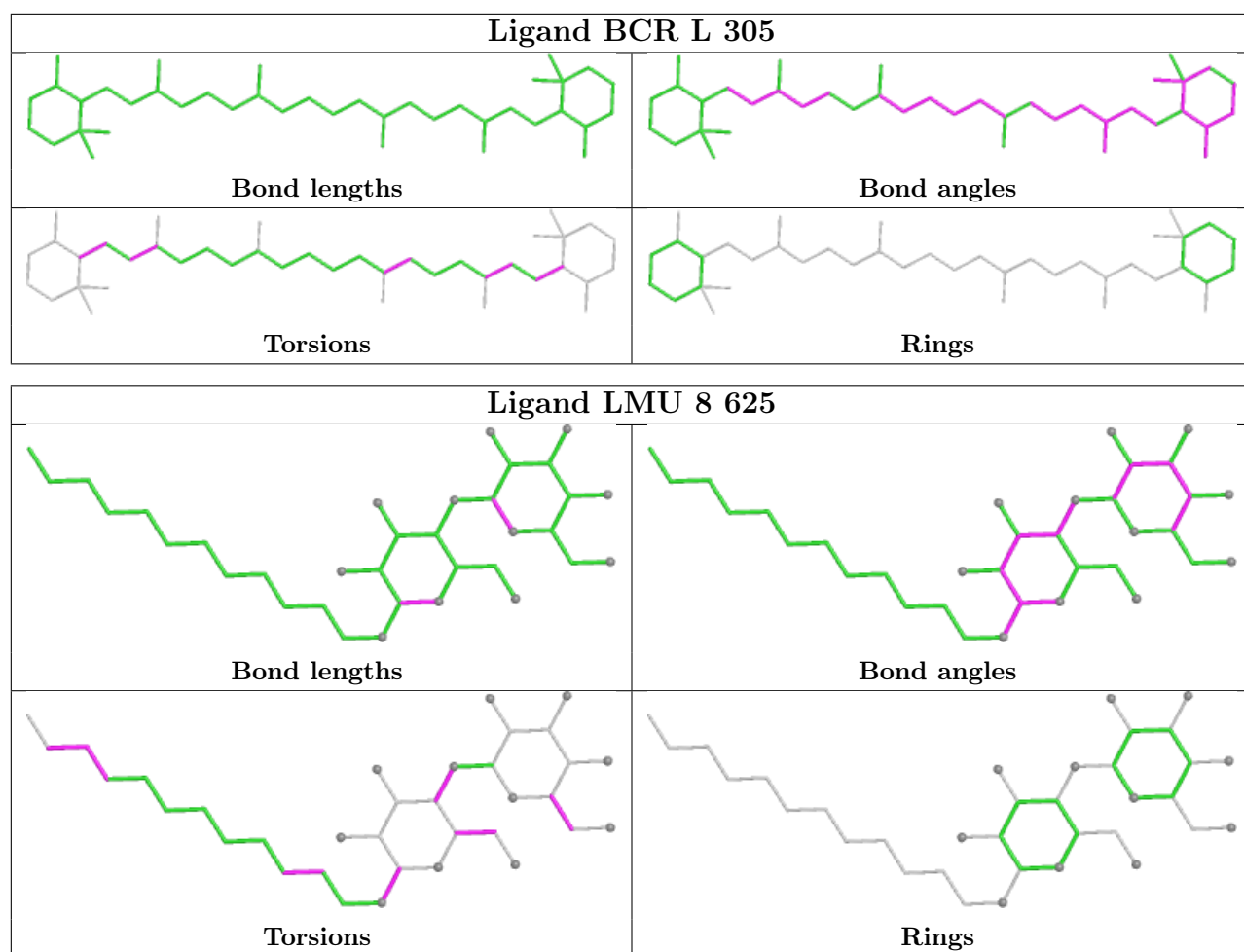
Rings

Ligand CLA A 808

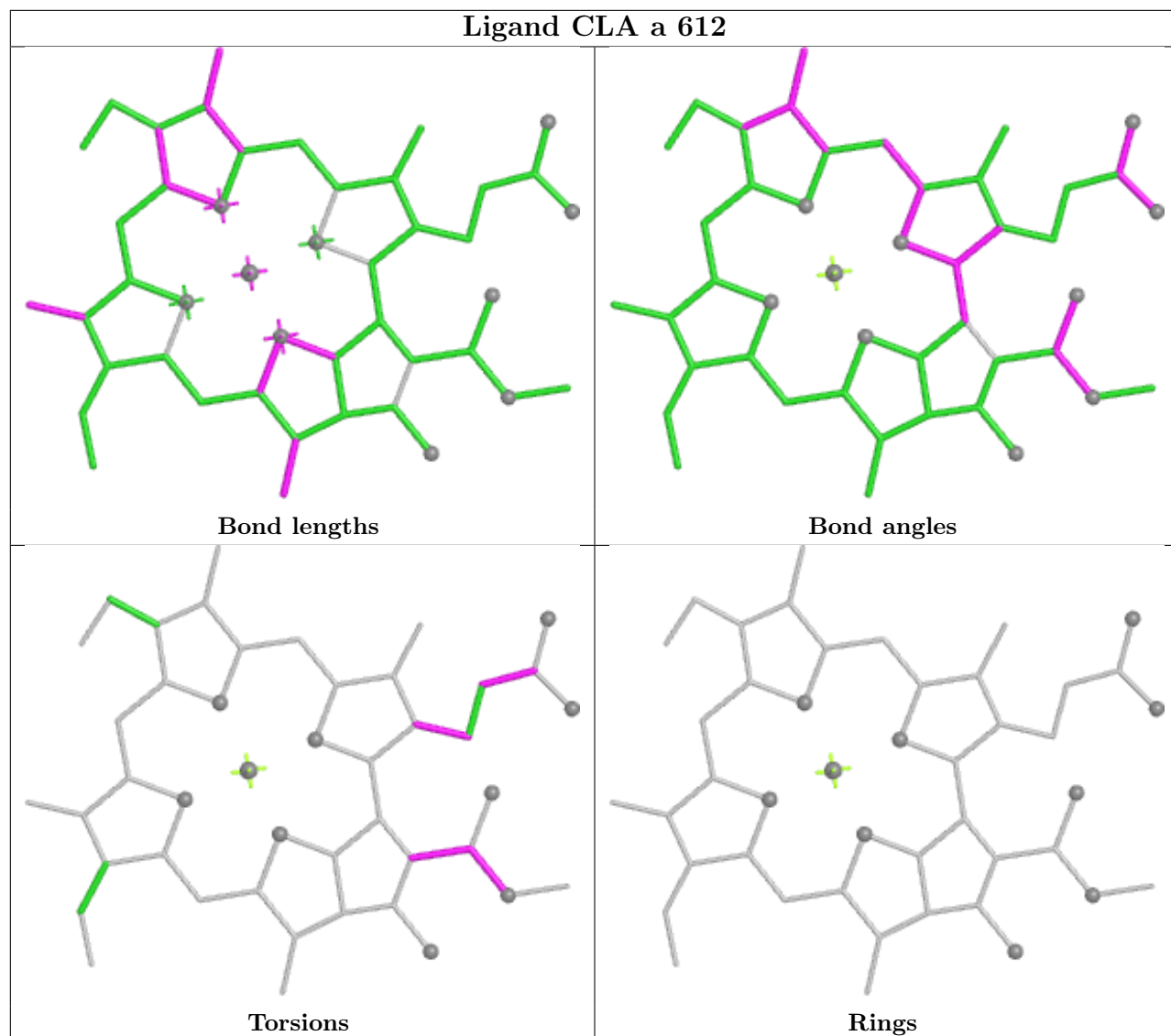


Ligand CLA A 827

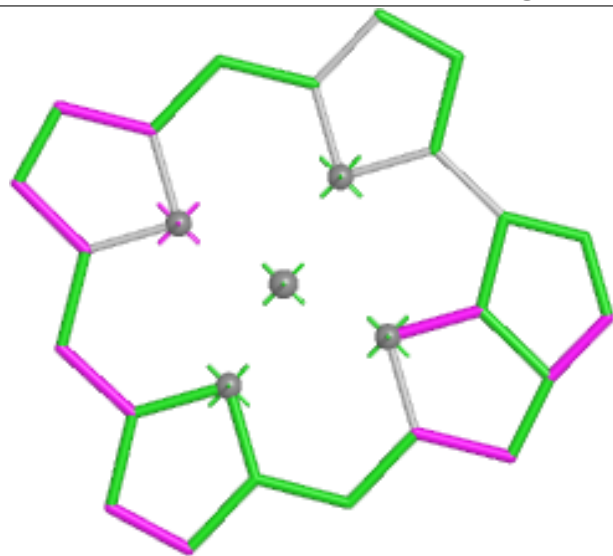




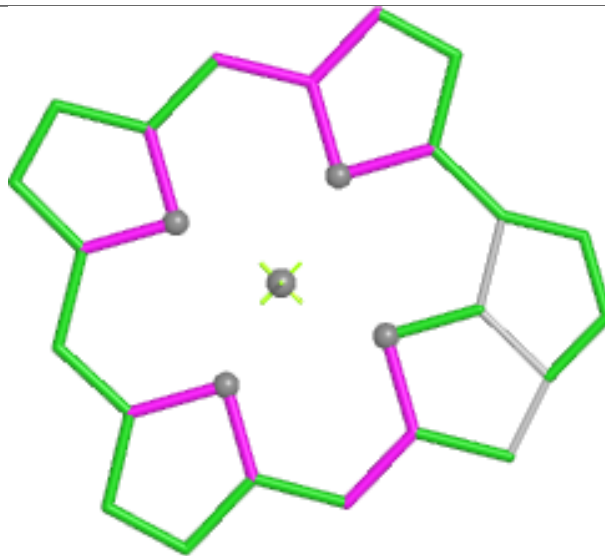
Ligand CLA a 612



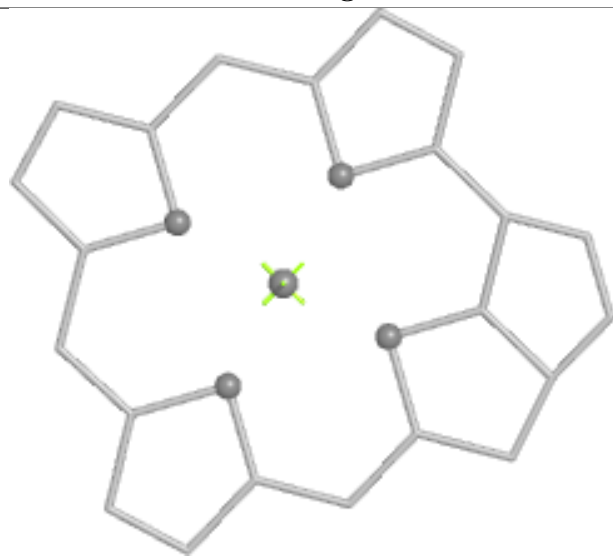
Ligand CLA 2 603



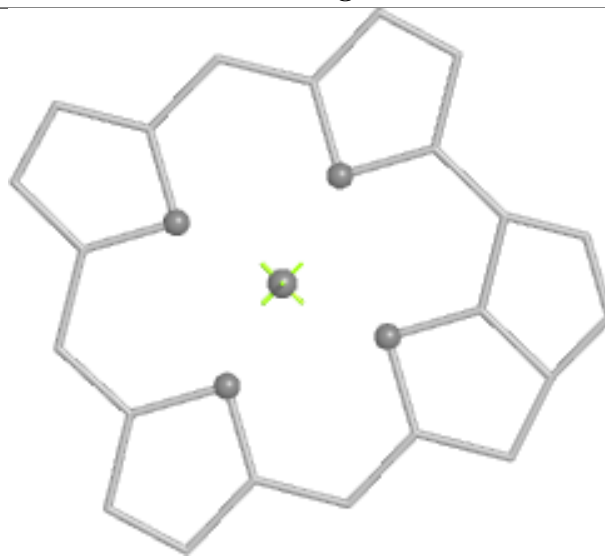
Bond lengths



Bond angles

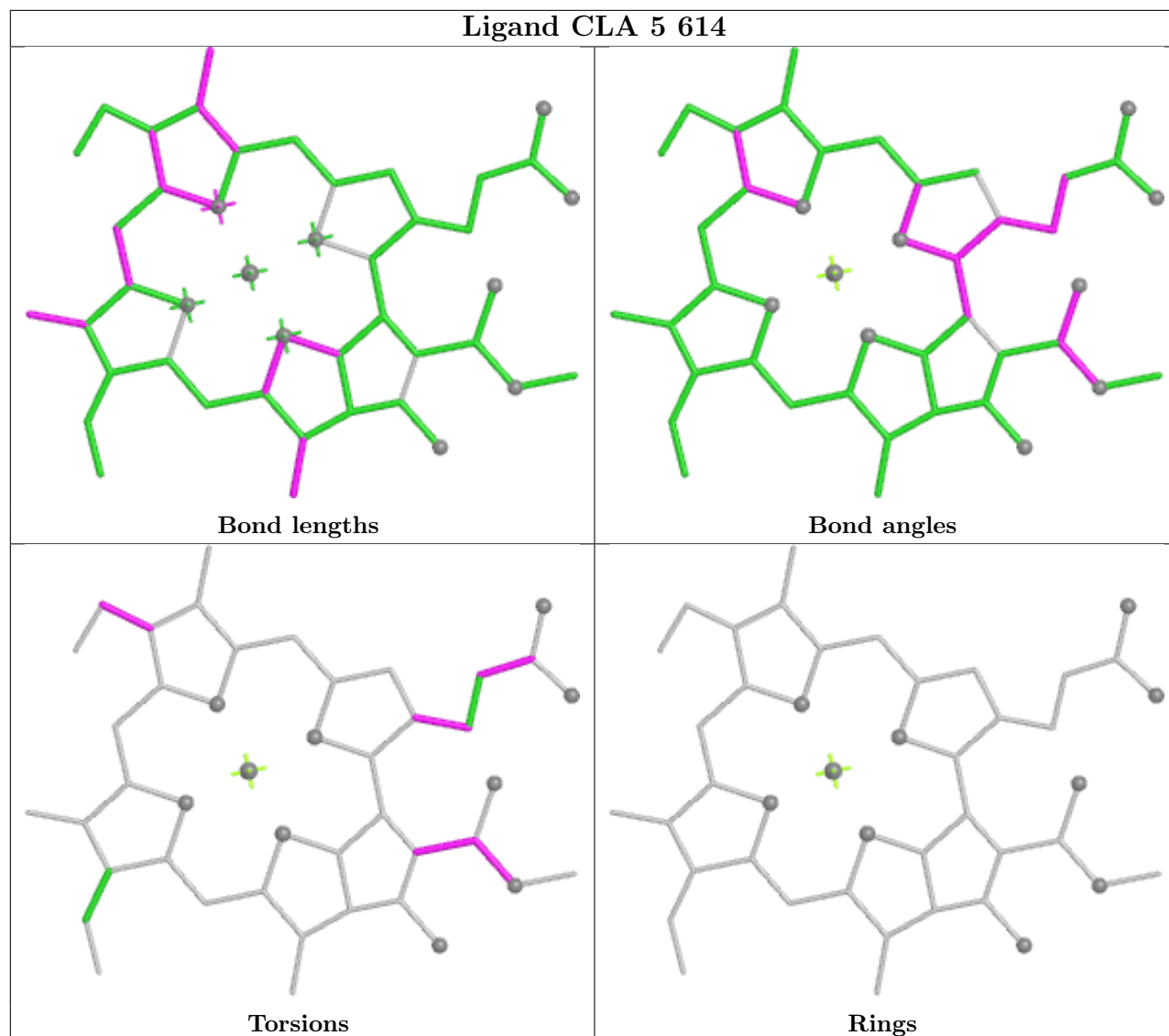


Torsions

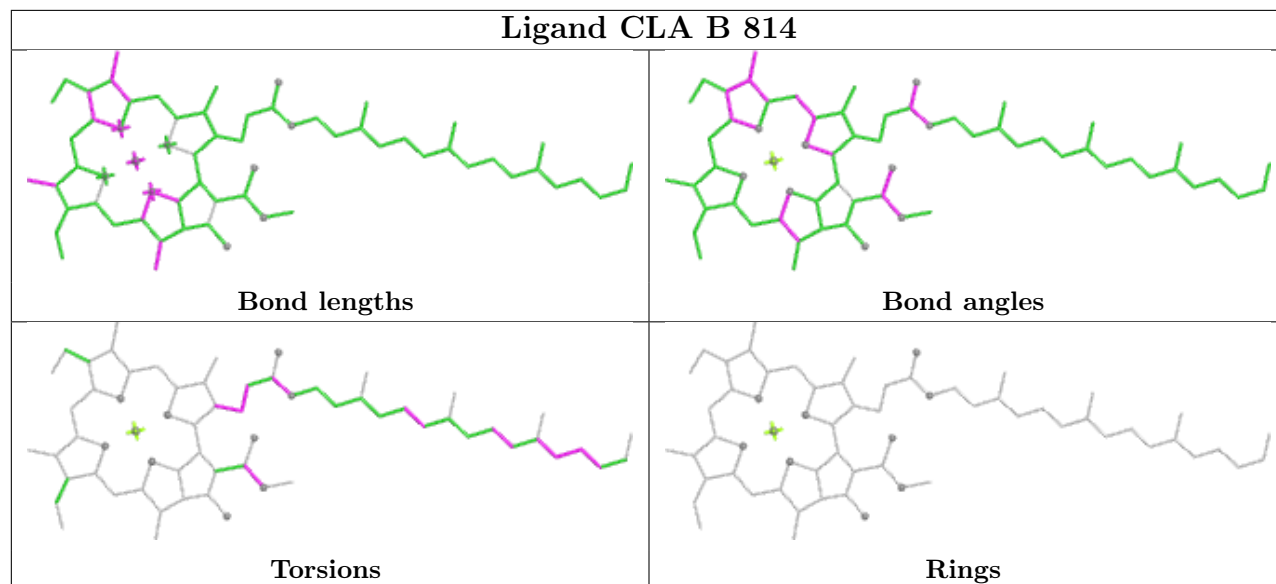


Rings

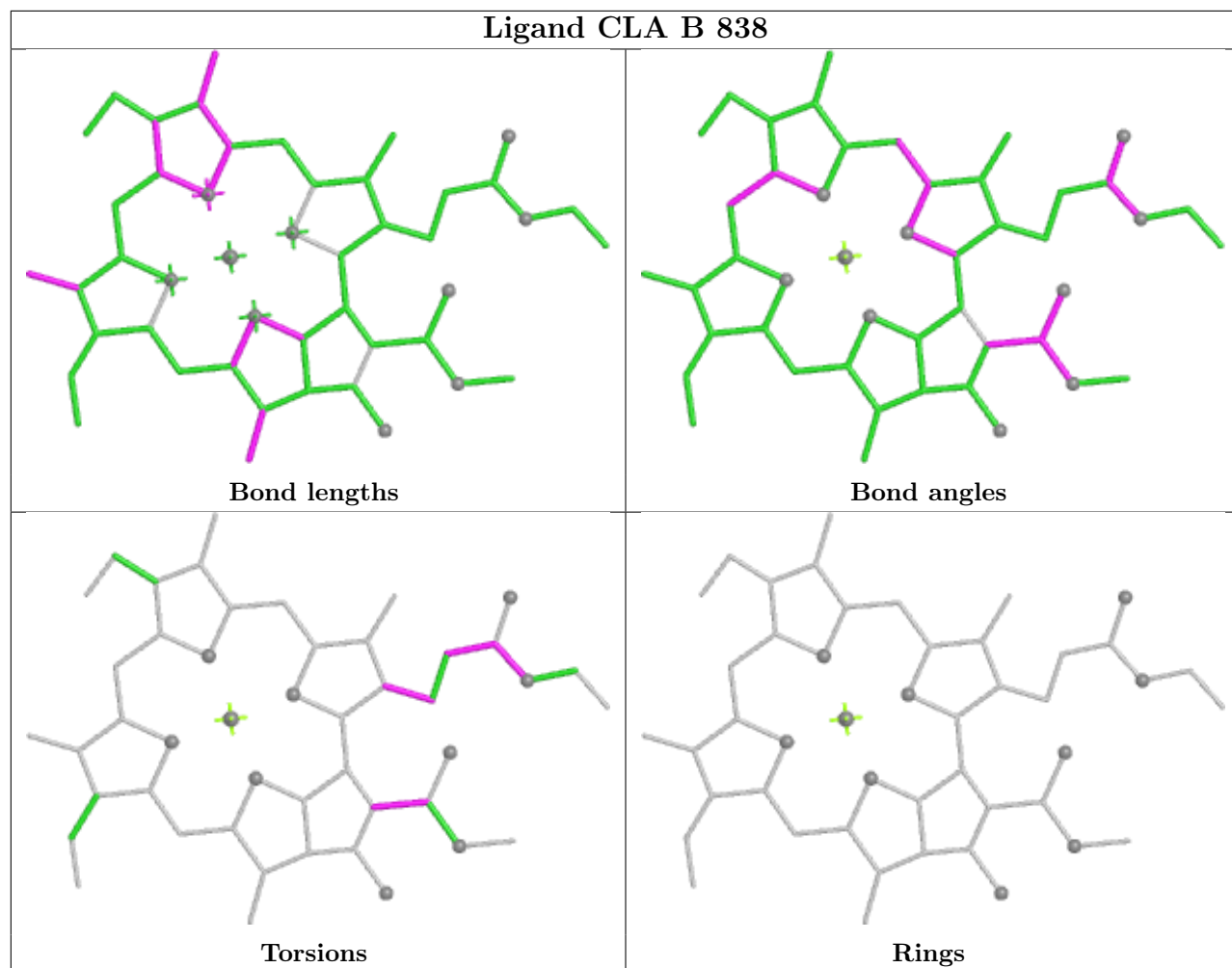
Ligand CLA 5 614



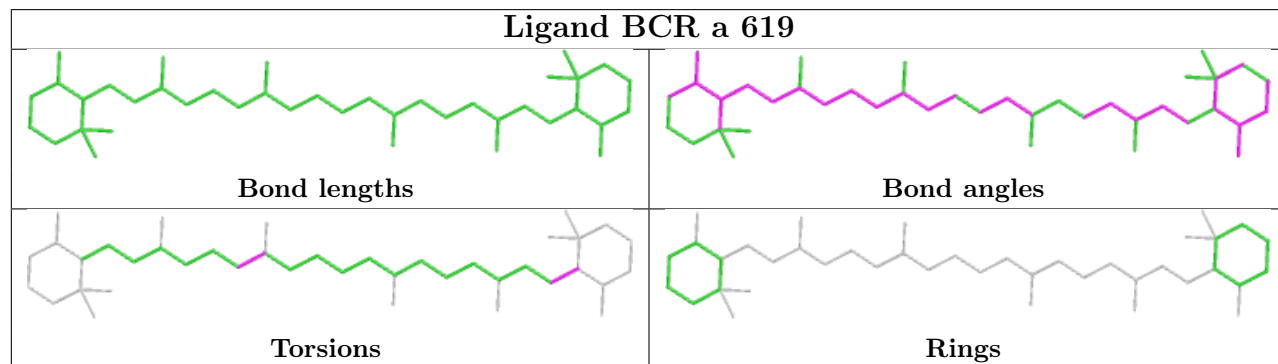
Ligand CLA B 814

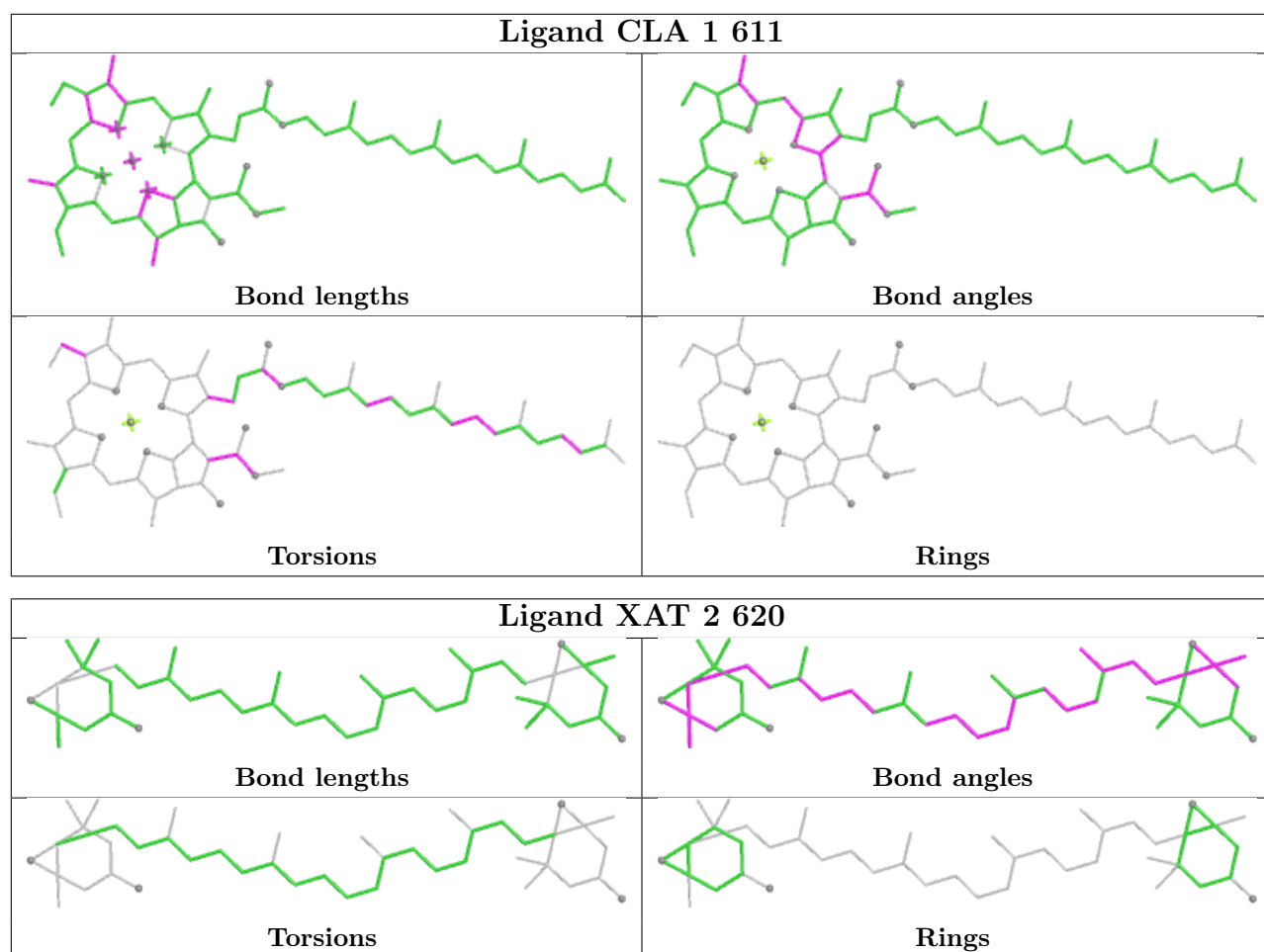


Ligand CLA B 838

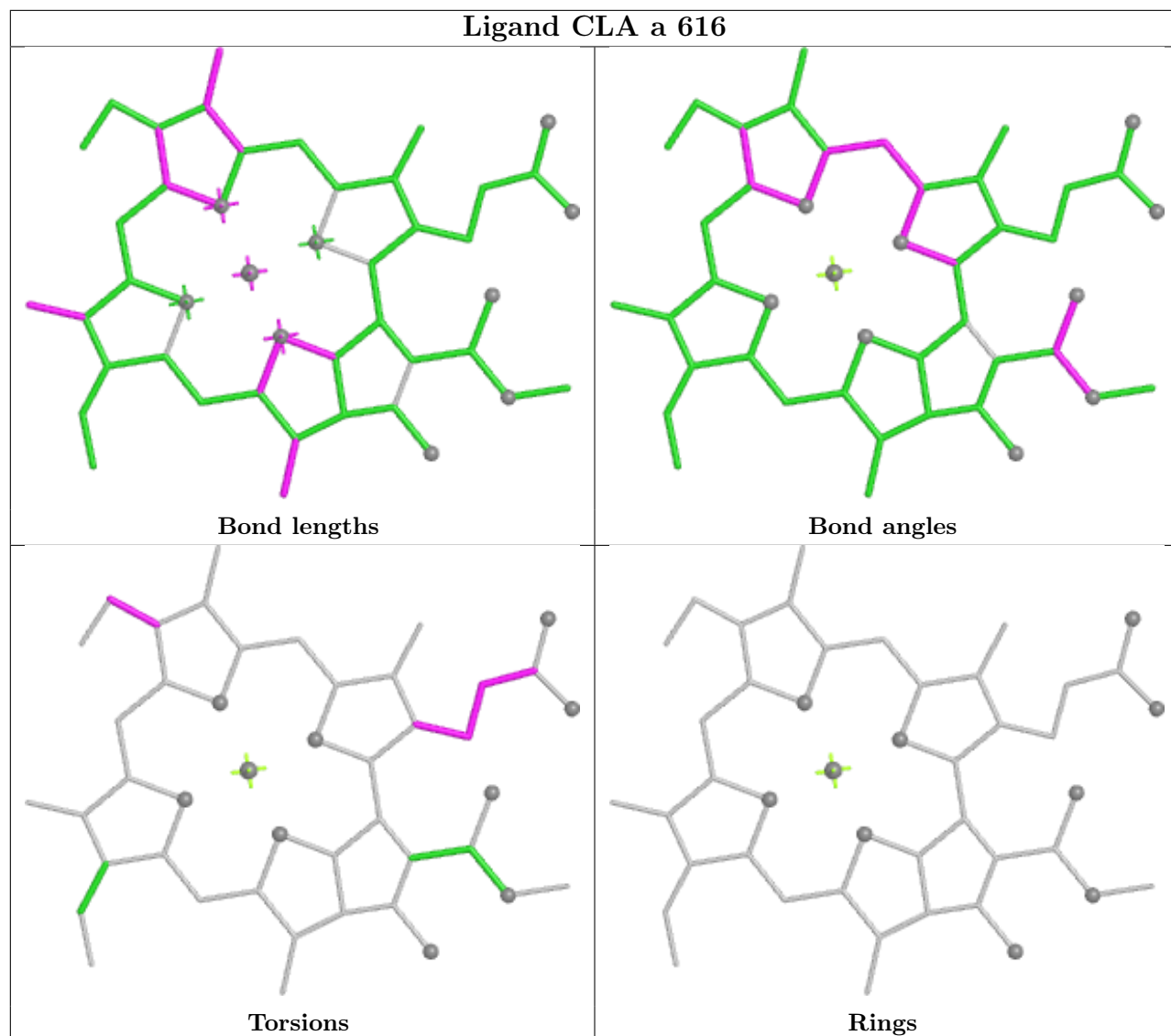


Ligand BCR a 619

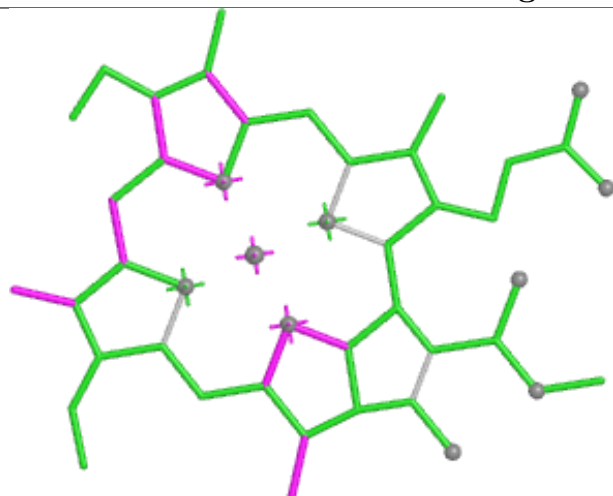




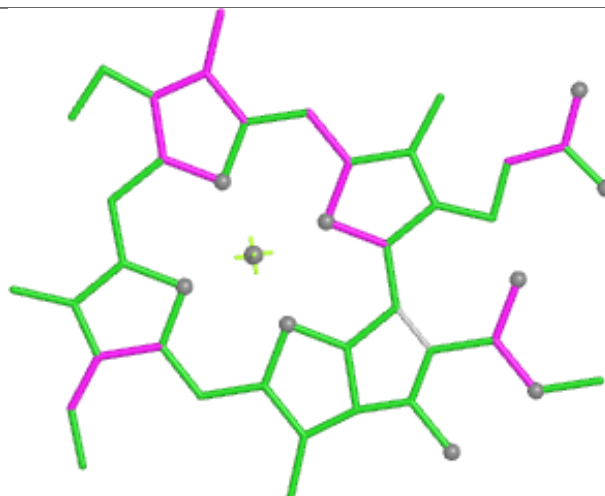
Ligand CLA a 616



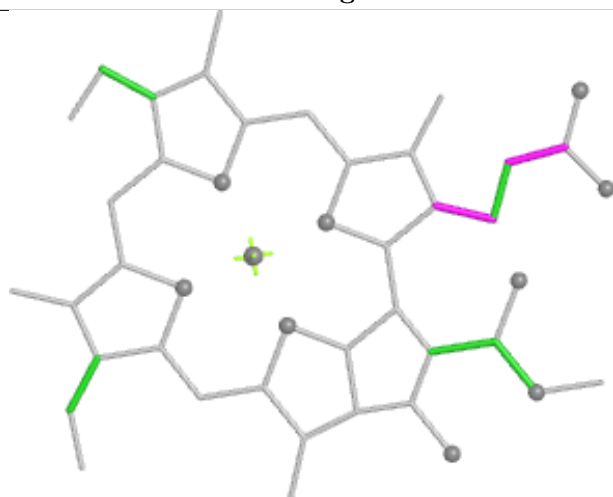
Ligand CLA 8 609



Bond lengths



Bond angles

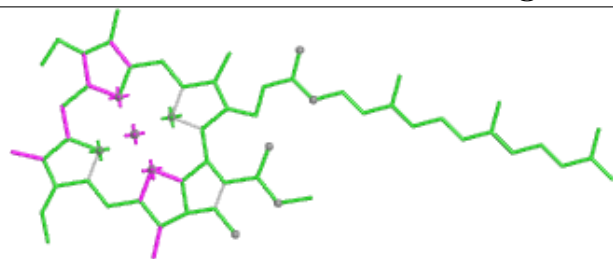


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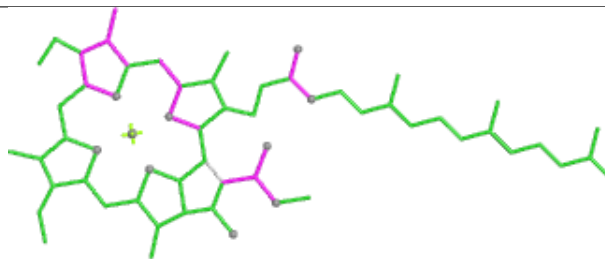


Rings

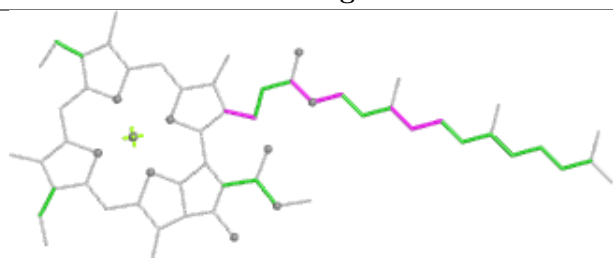
Ligand CLA 8 610



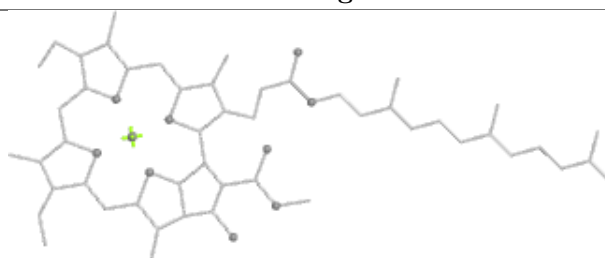
Bond lengths



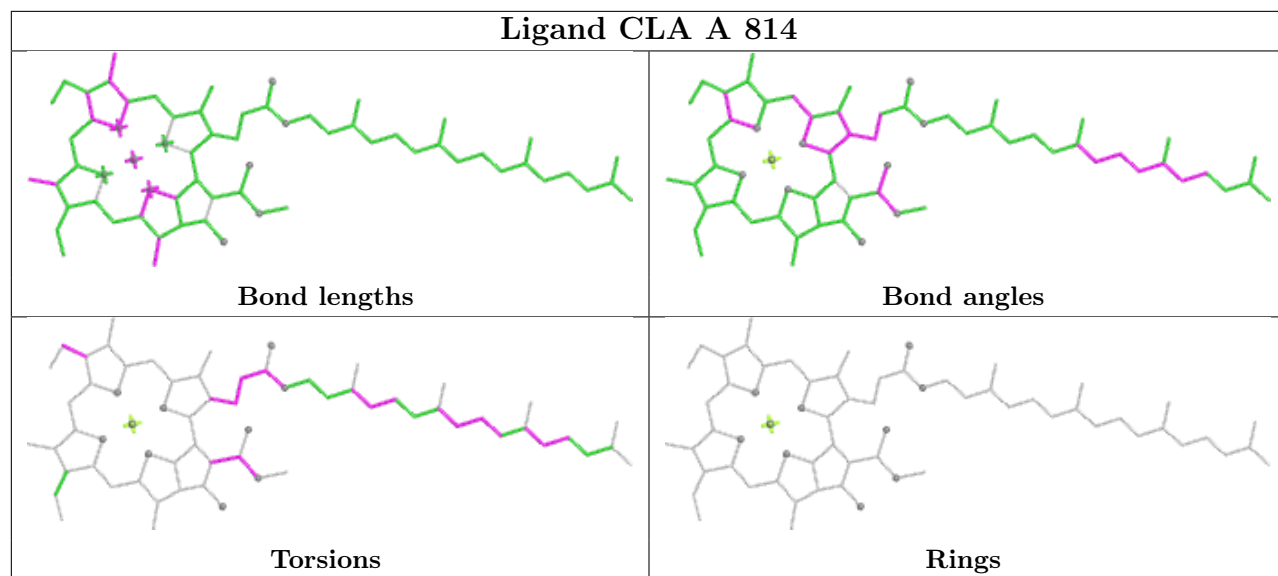
Bond angles



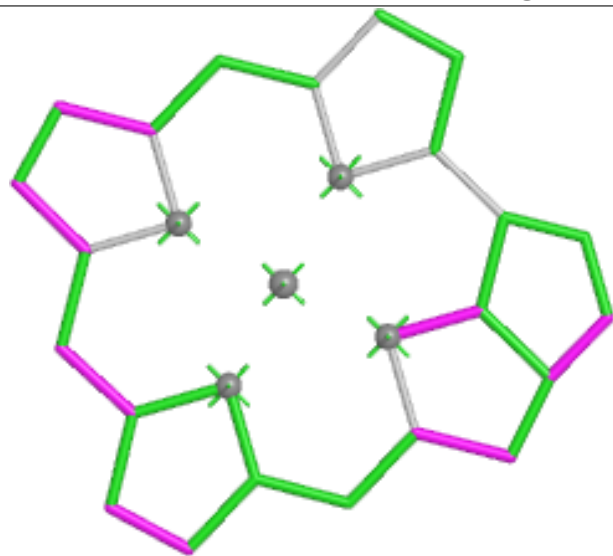
Torsions



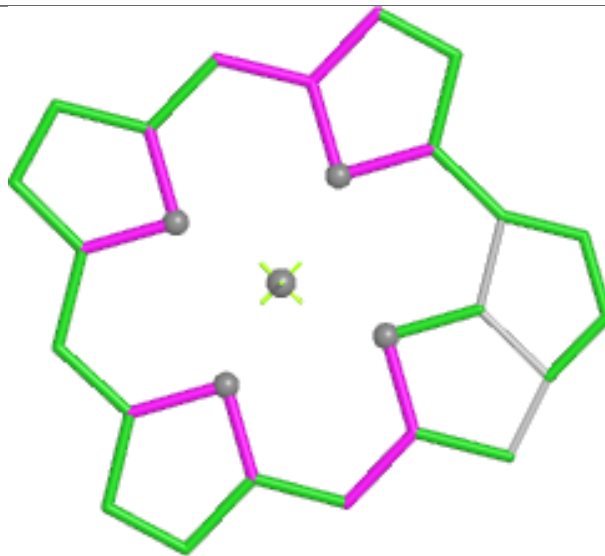
Rings



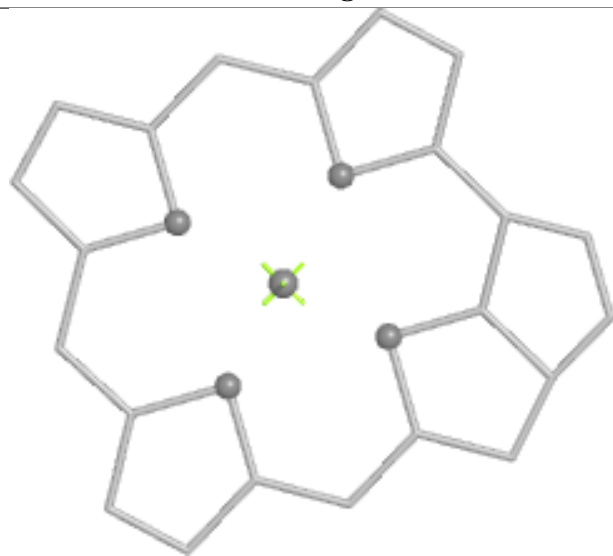
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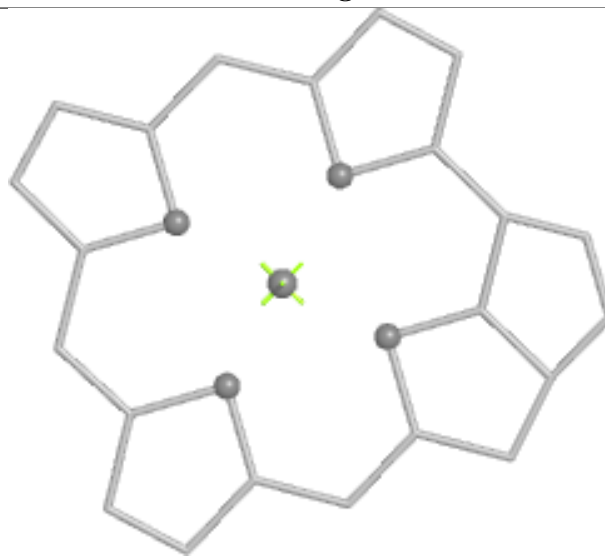
Bond lengths



Bond angles

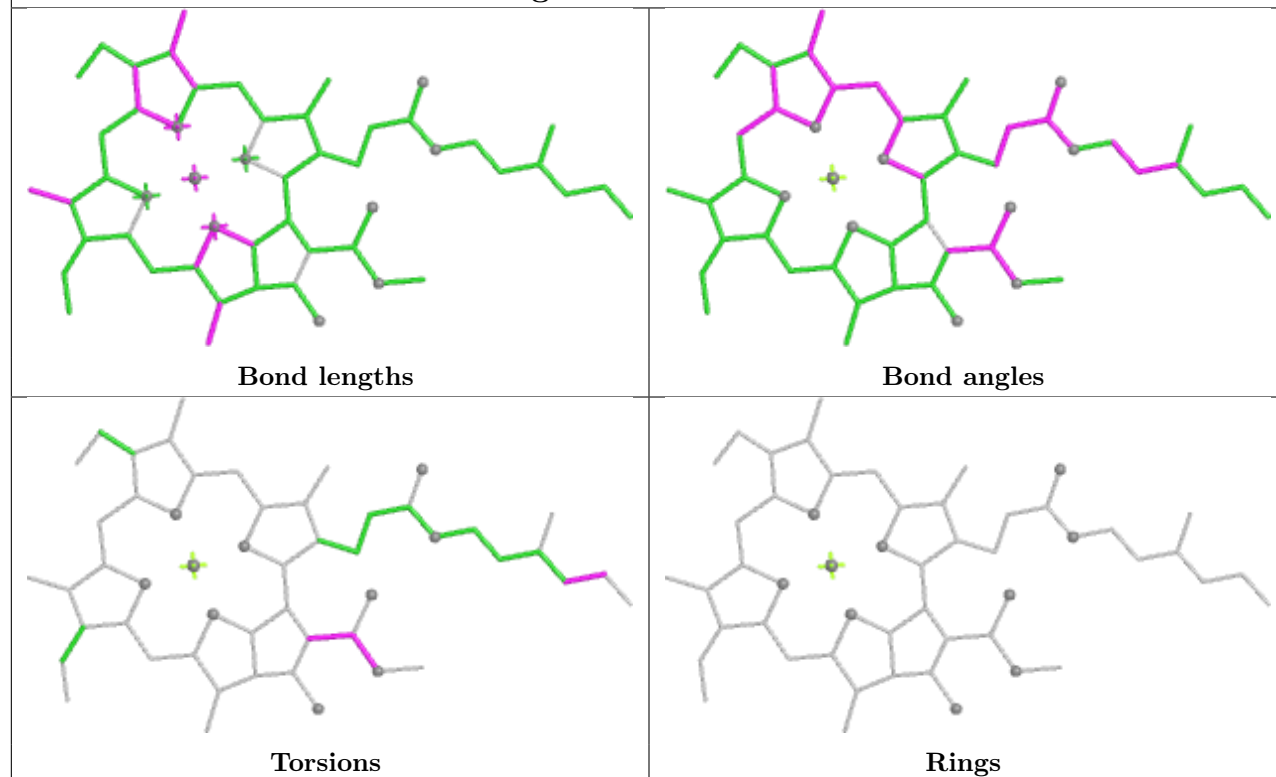


Torsions

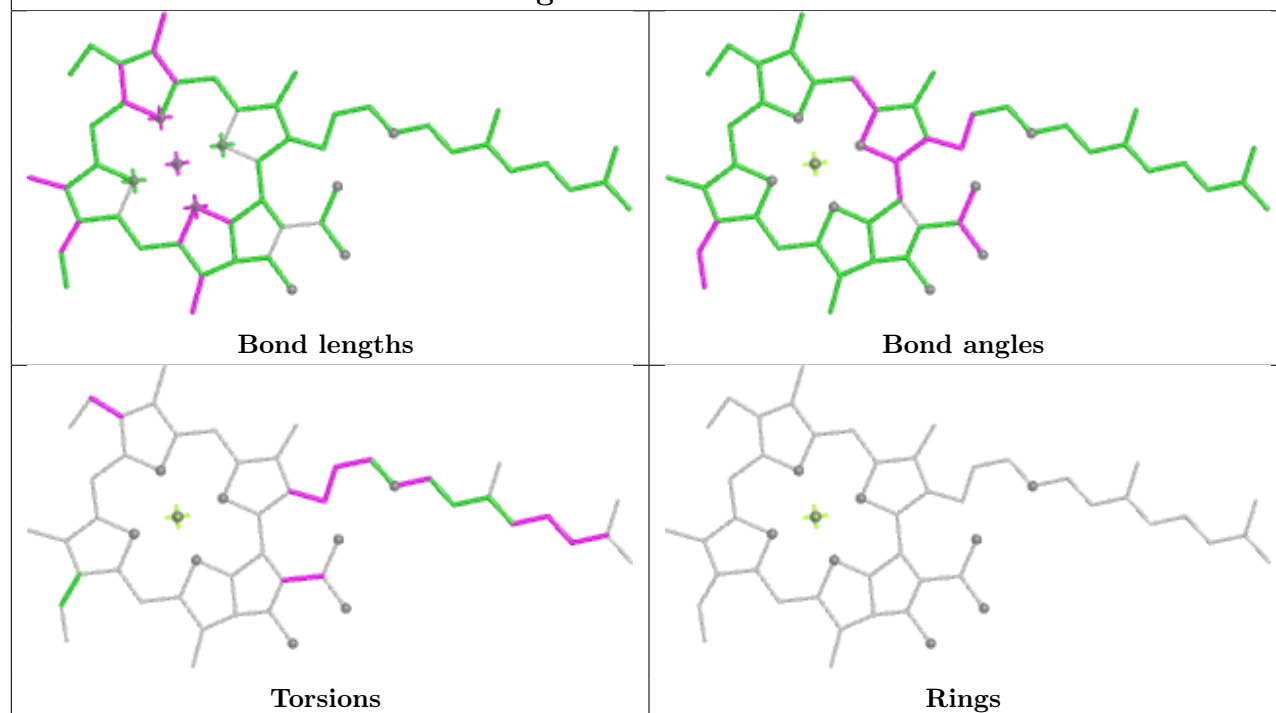


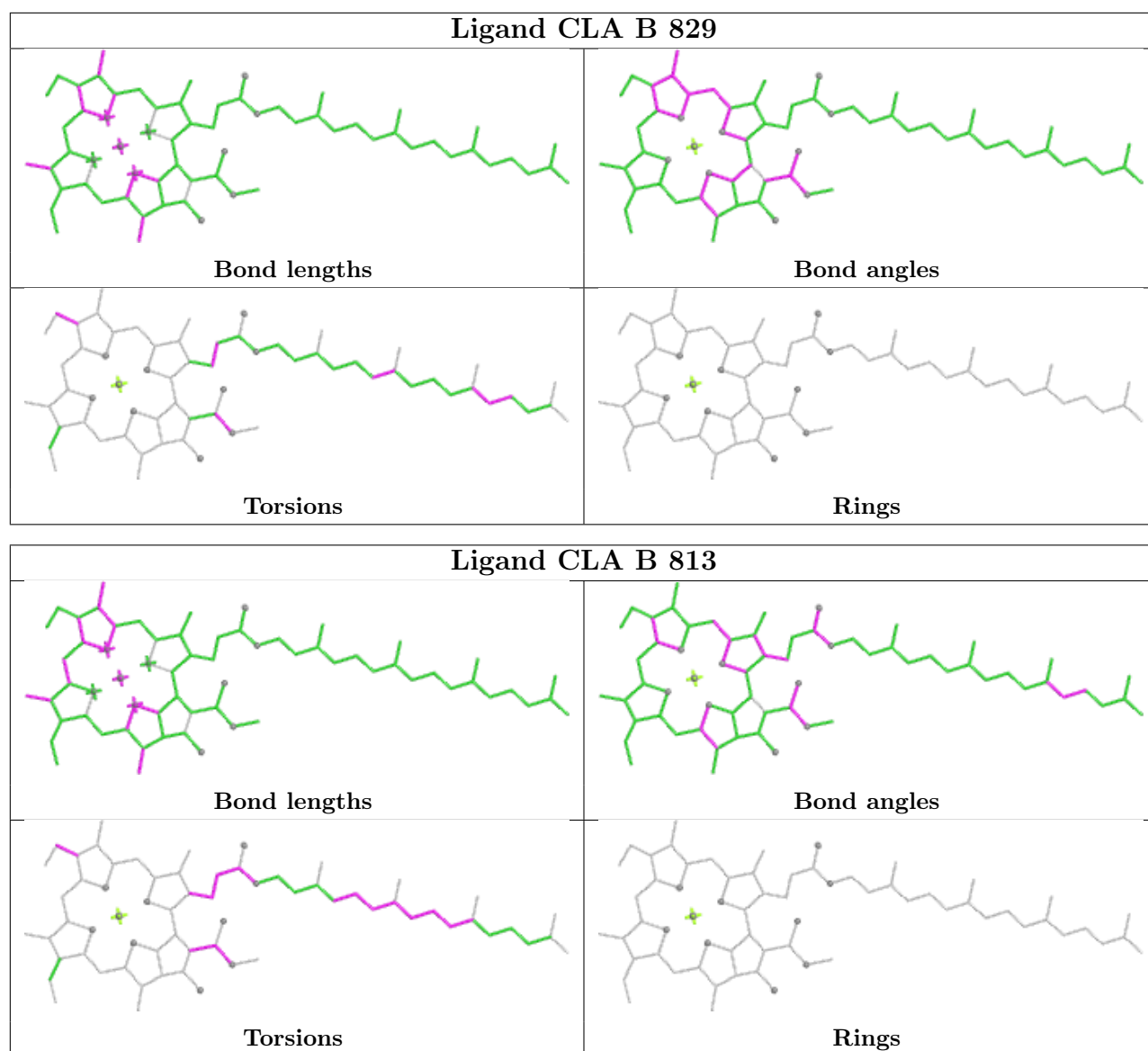
Rings

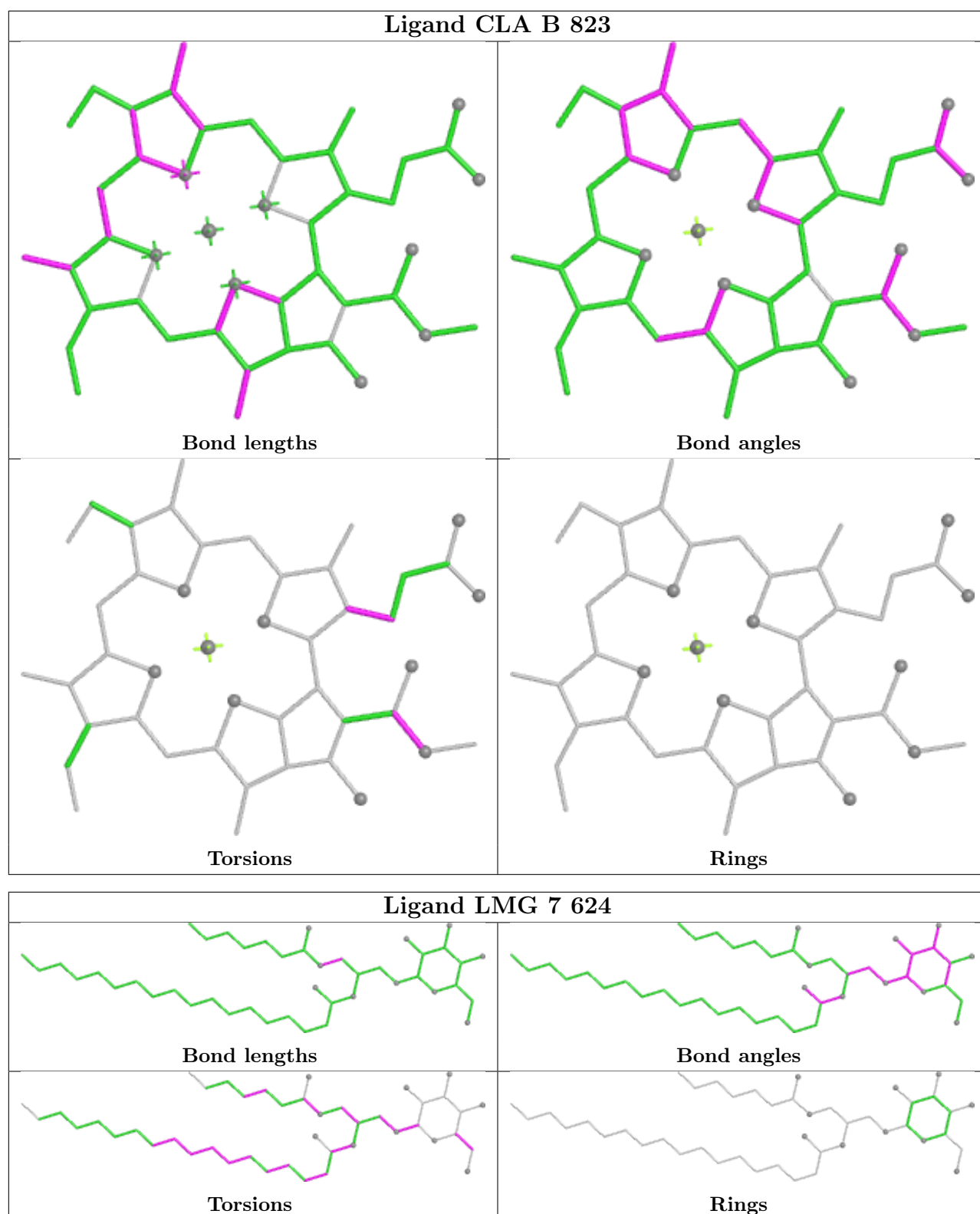
Ligand CLA A 840



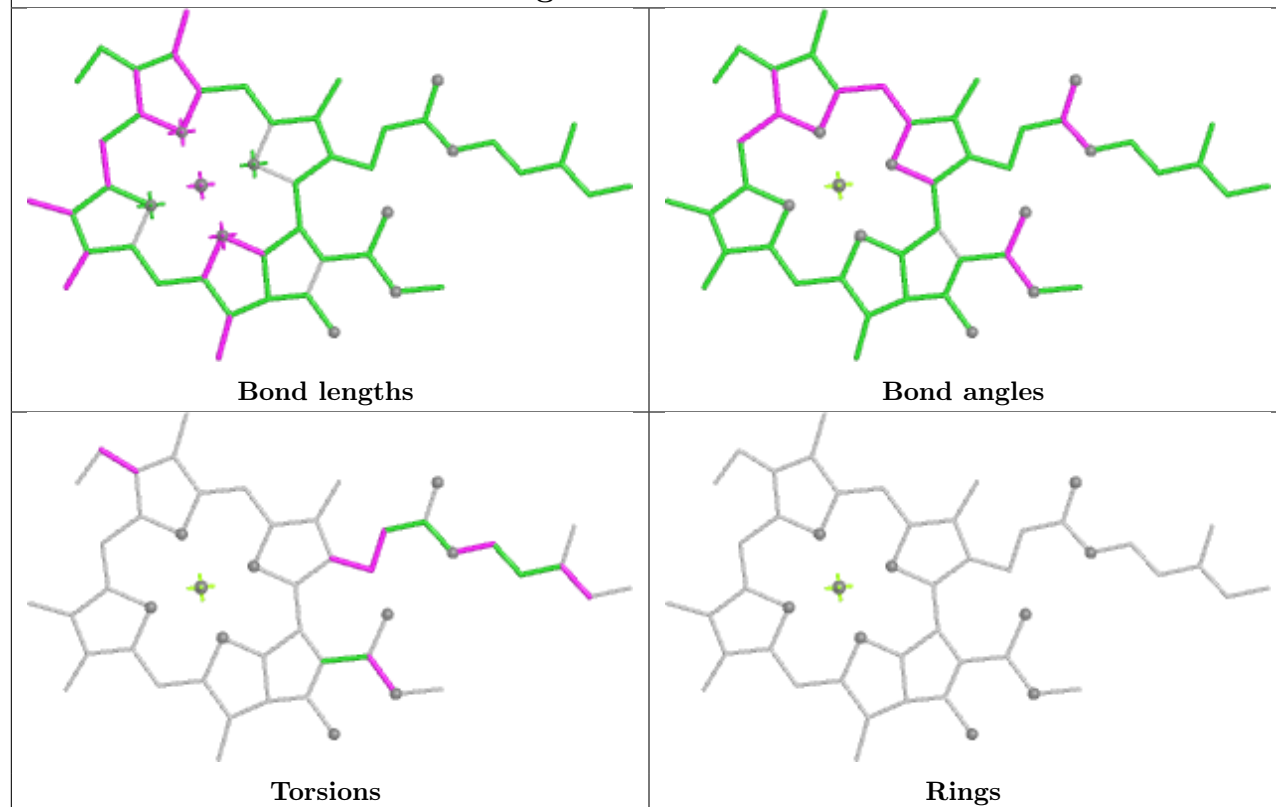
Ligand CLA 1 603



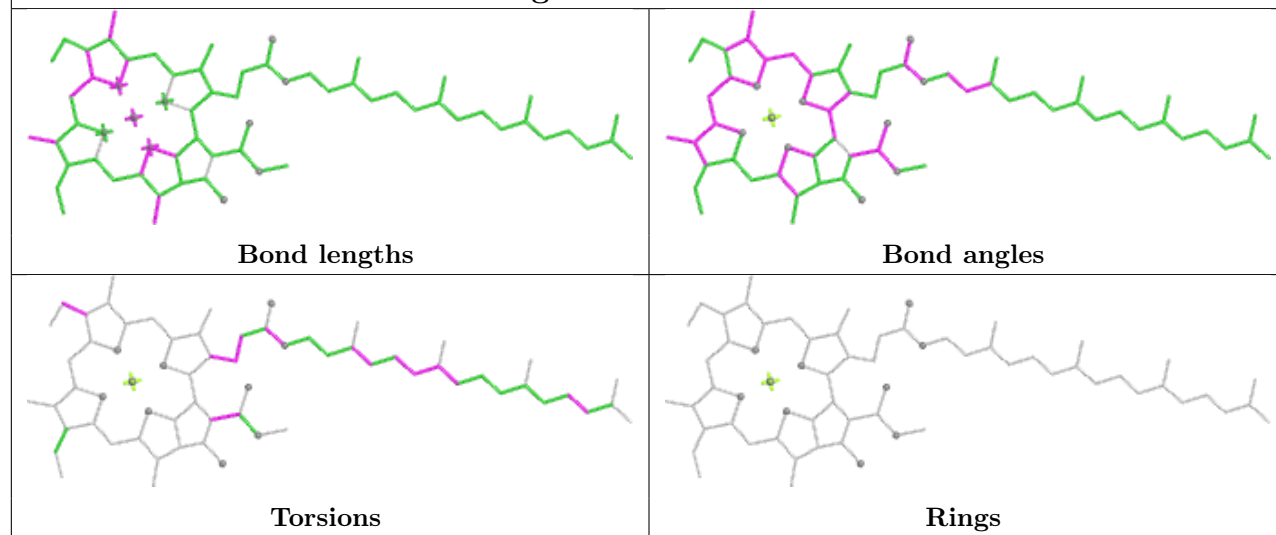


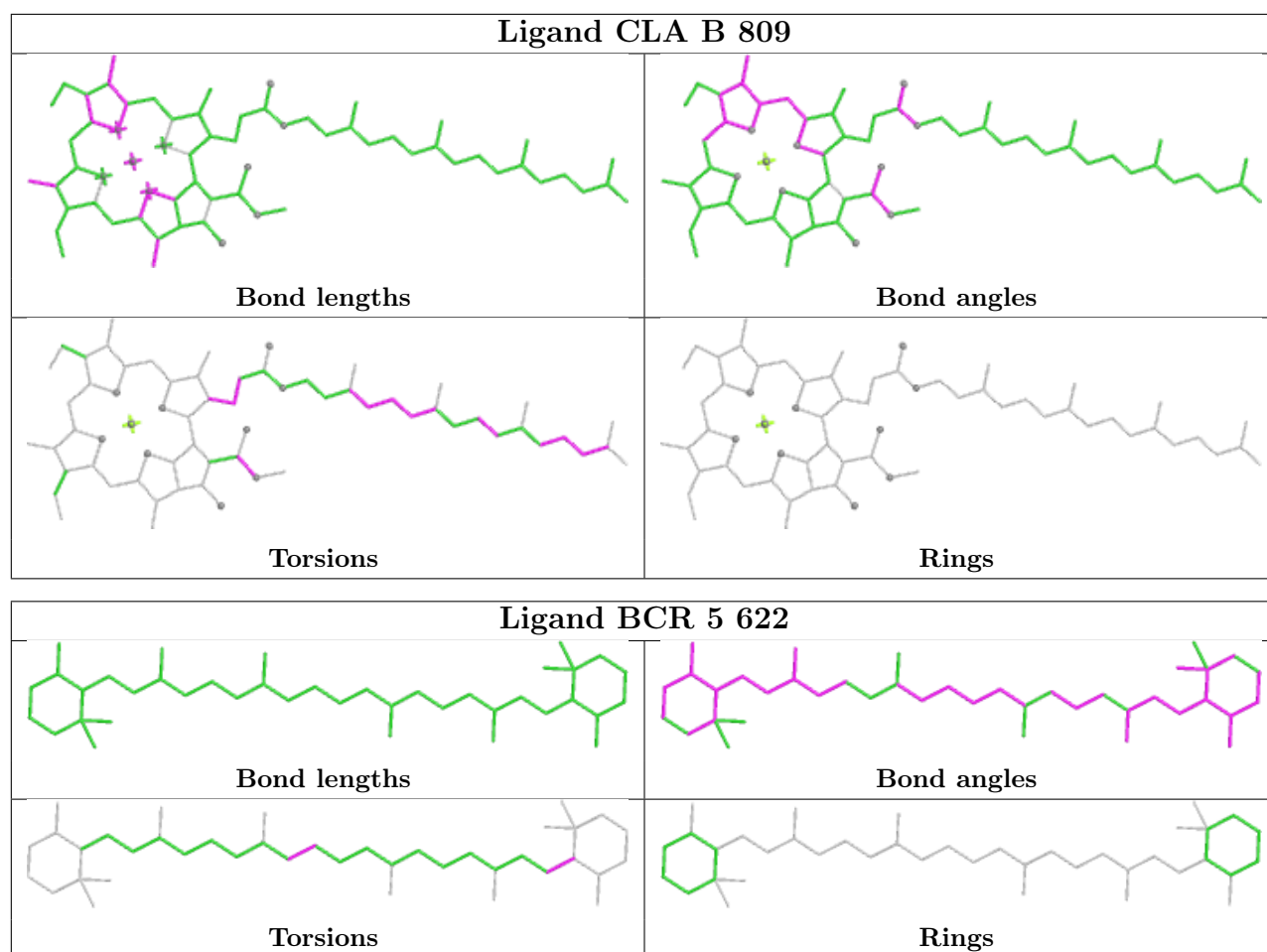


Ligand CLA 5 608

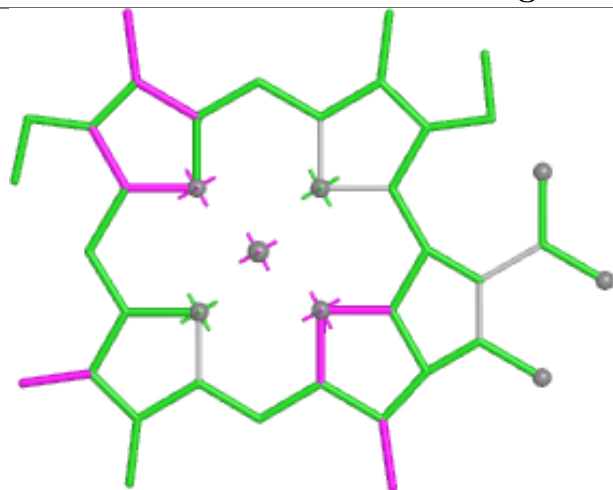


Ligand CLA A 820

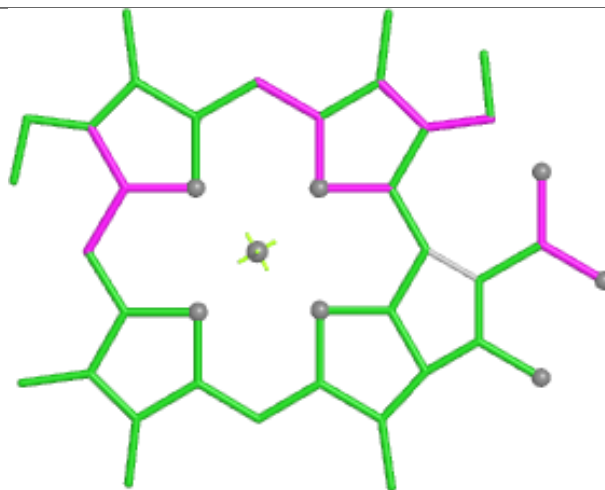




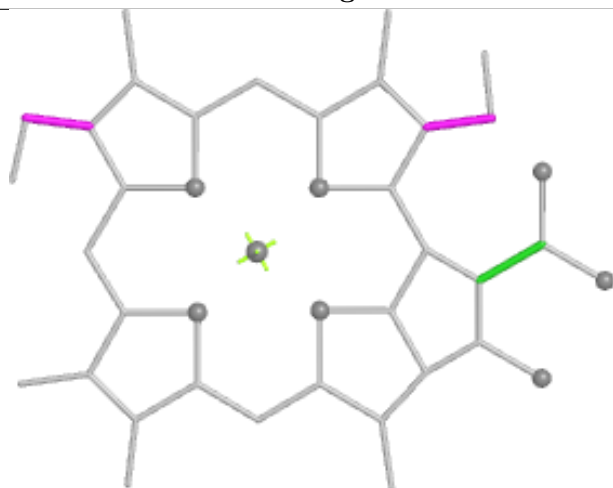
Ligand CLA 5 606



Bond lengths



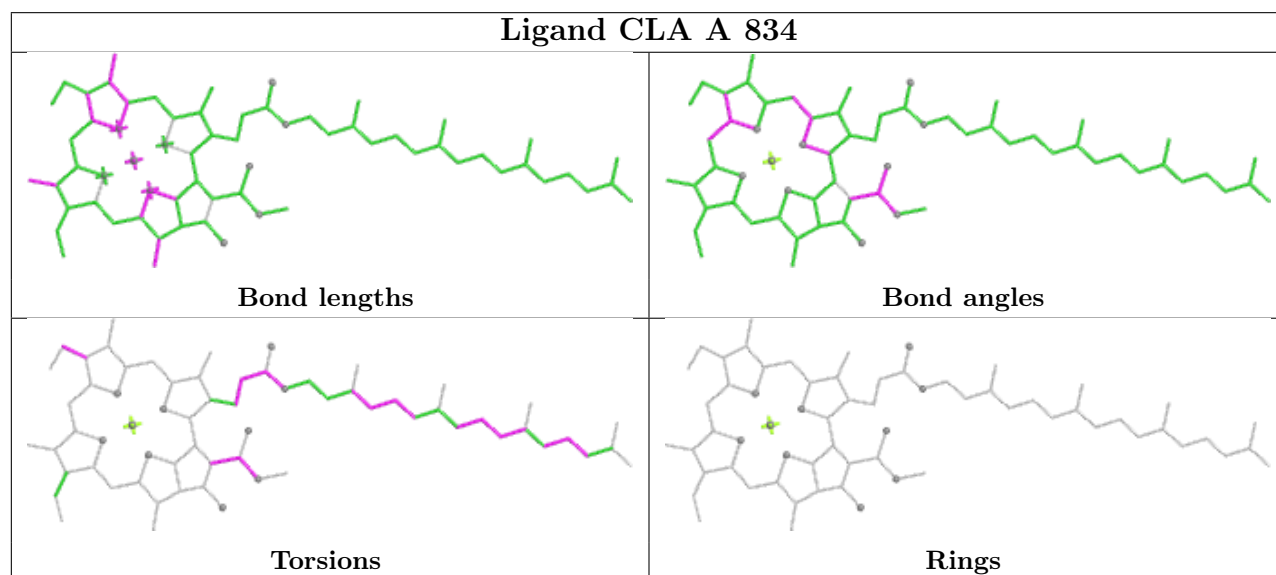
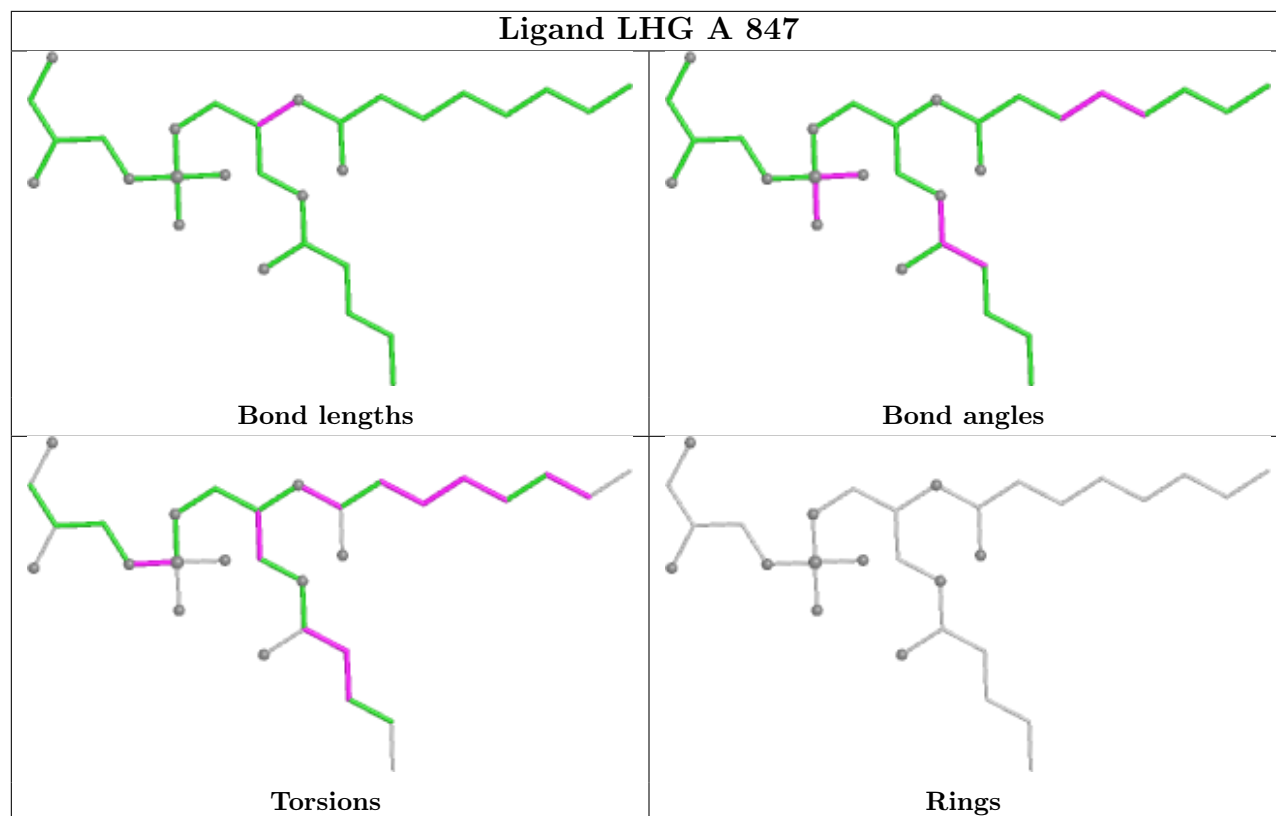
Bond angles



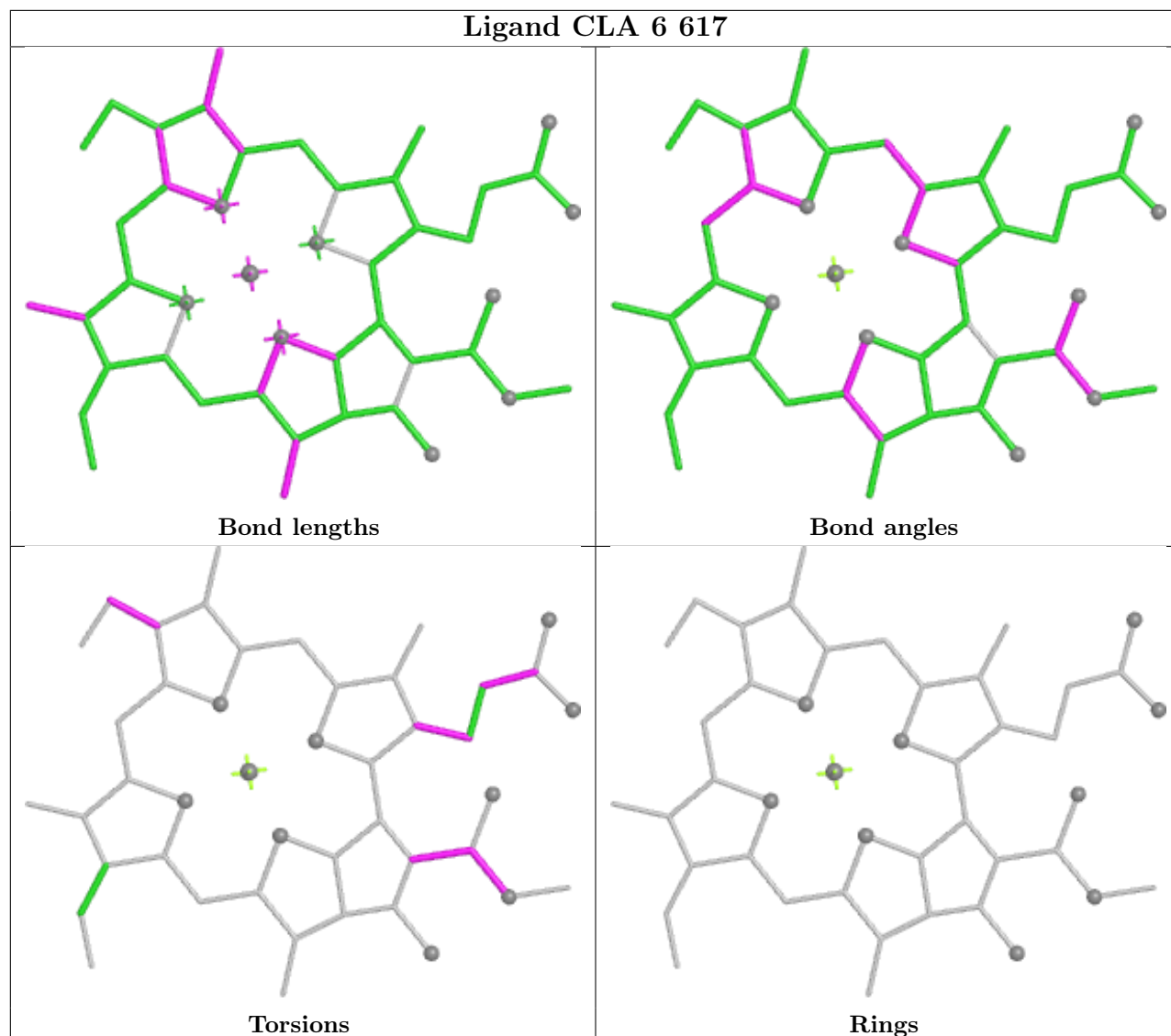
Torsions



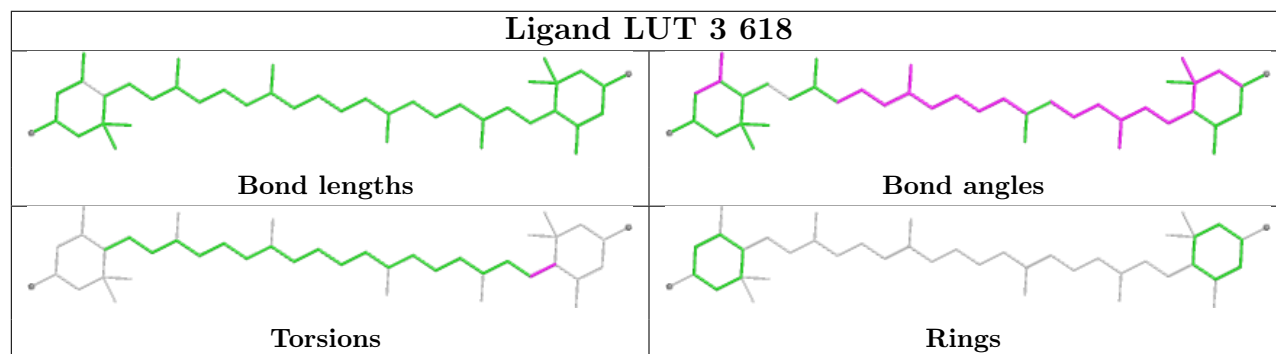
Rings



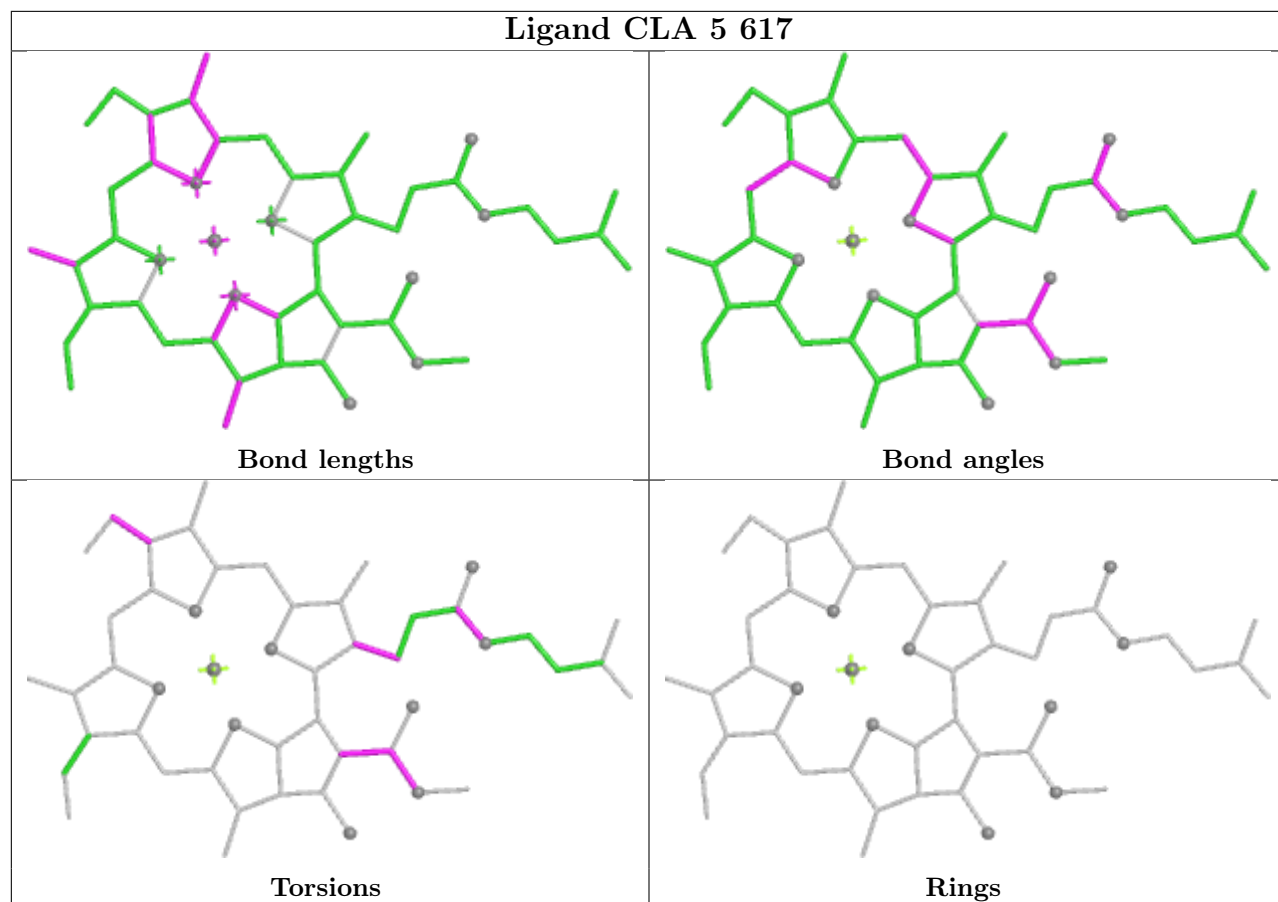
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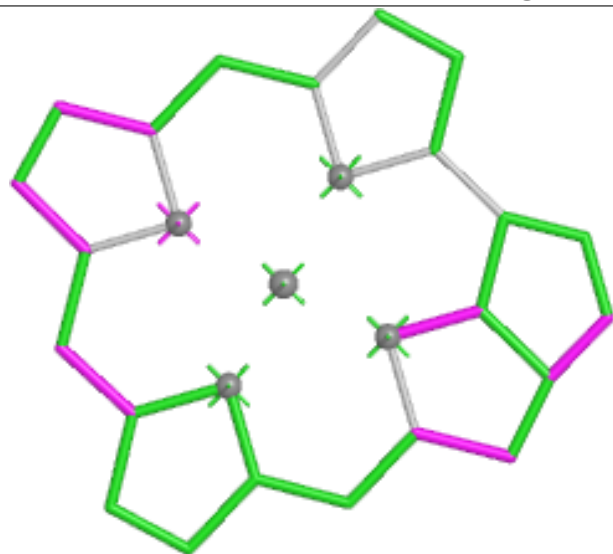
Ligand LUT 3 618



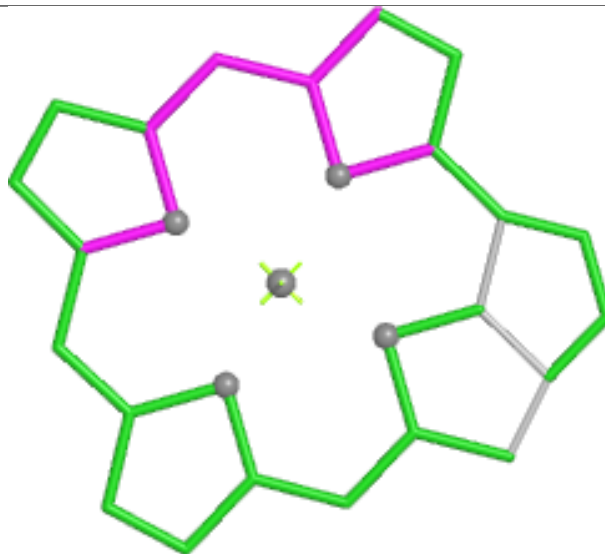
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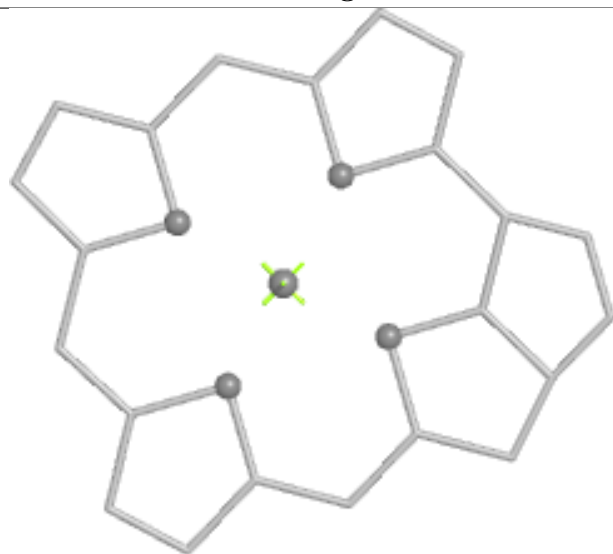
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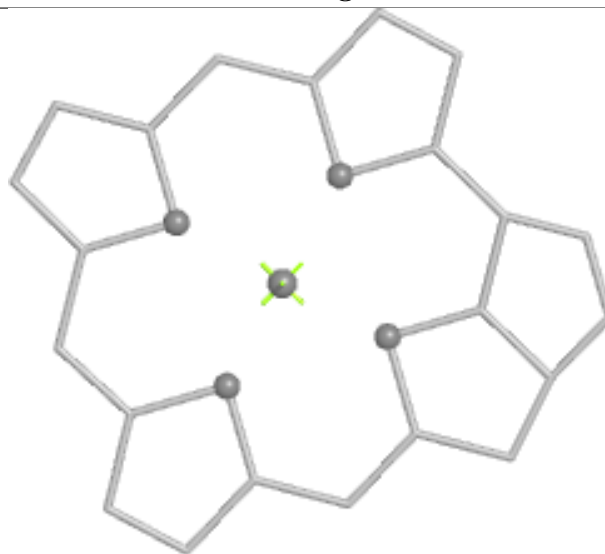
Bond lengths



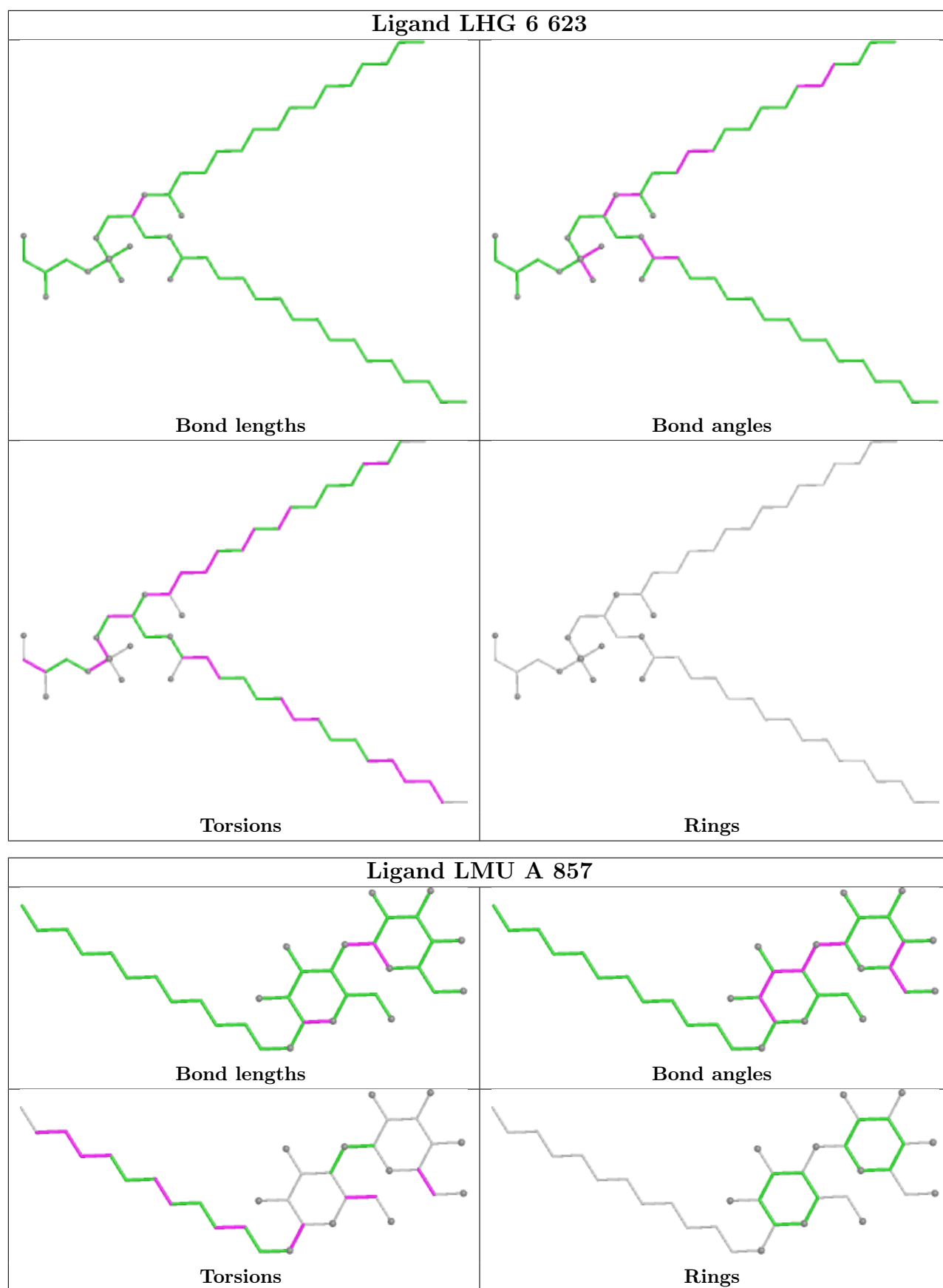
Bond angles

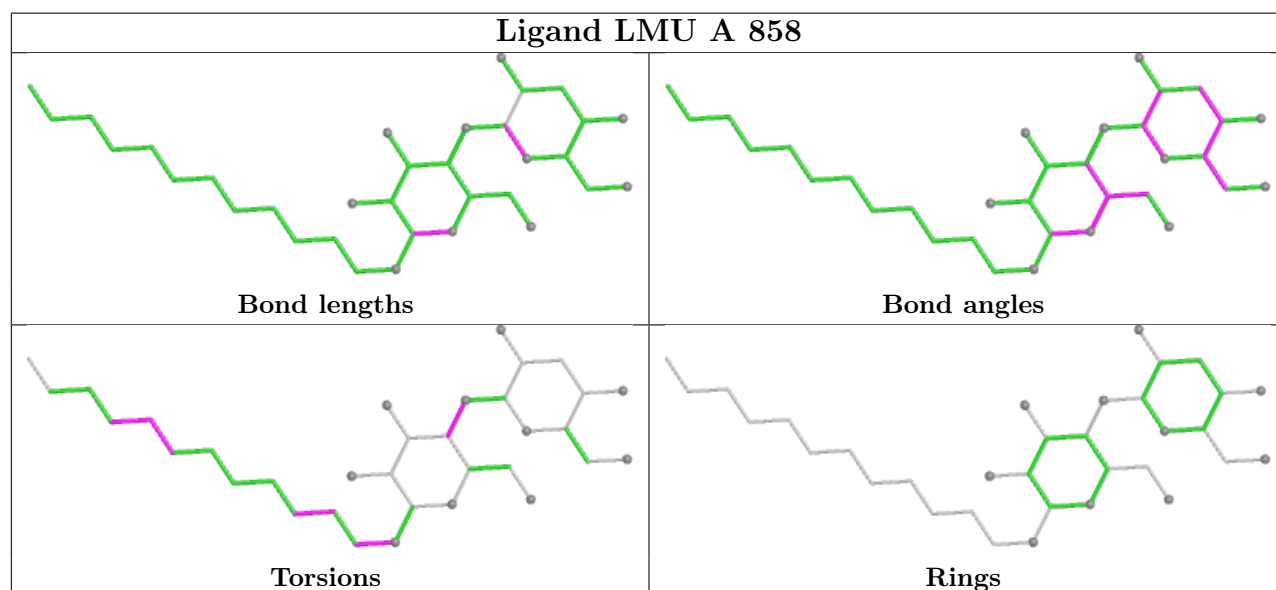
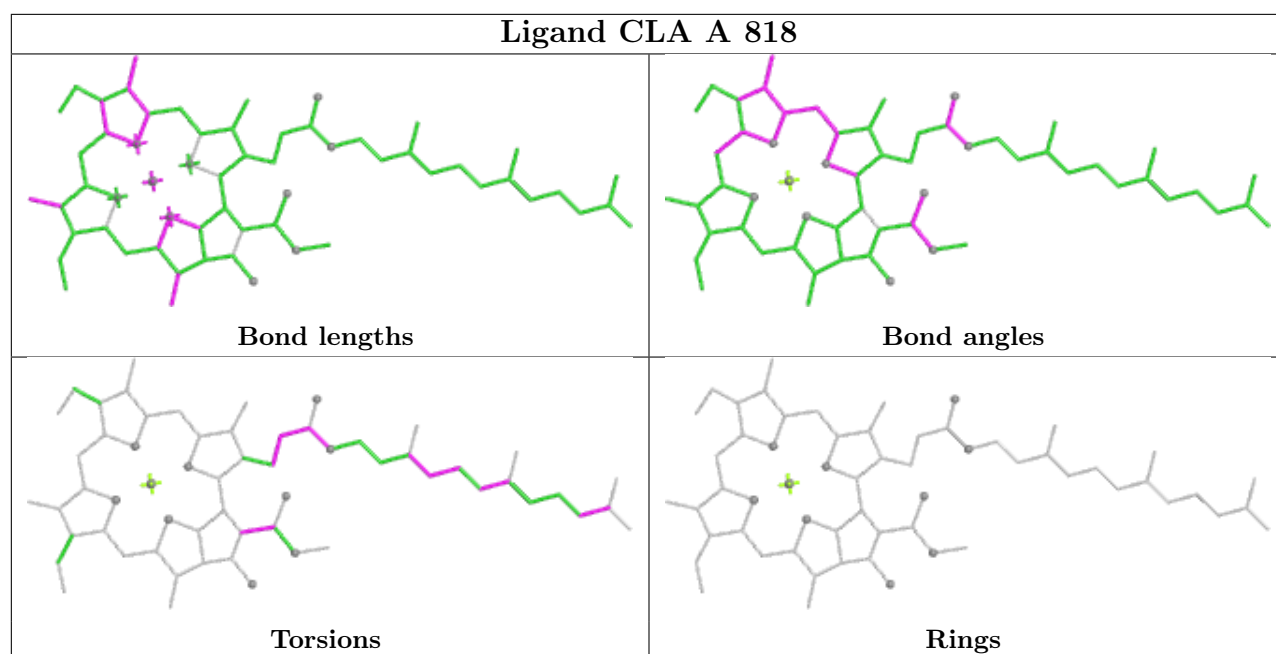


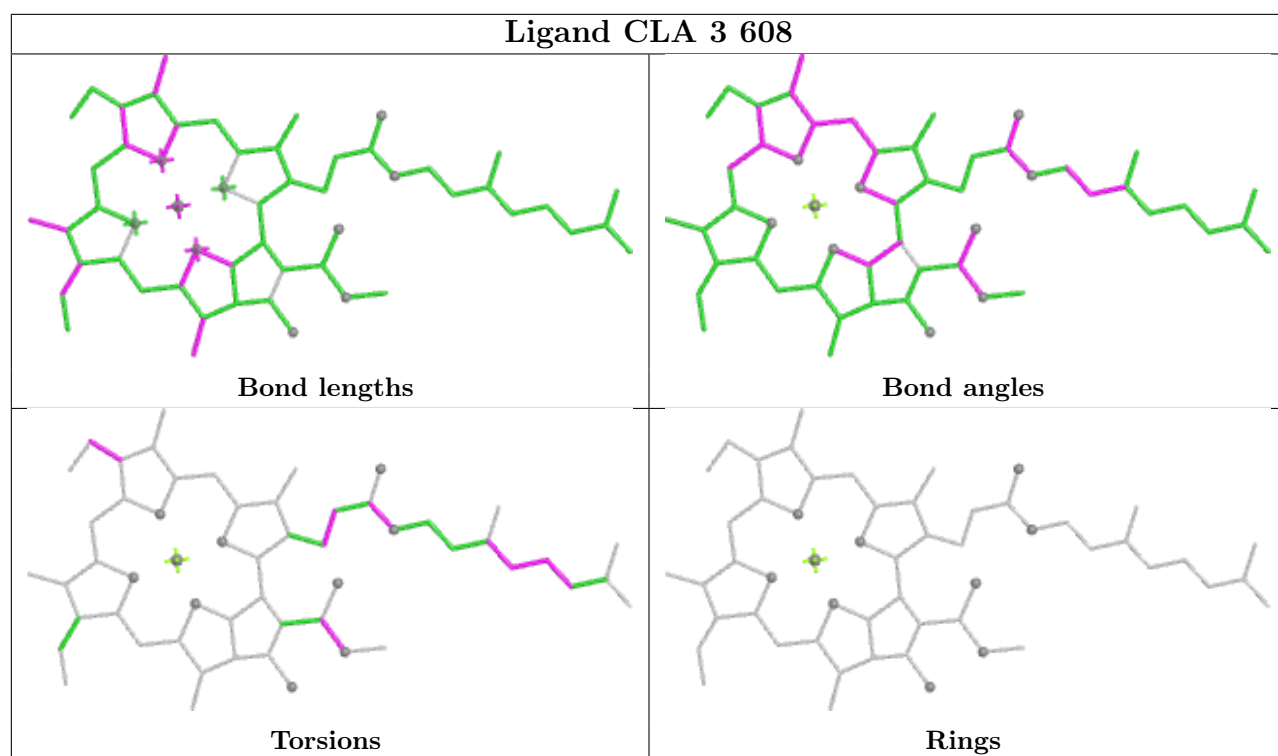
Torsions



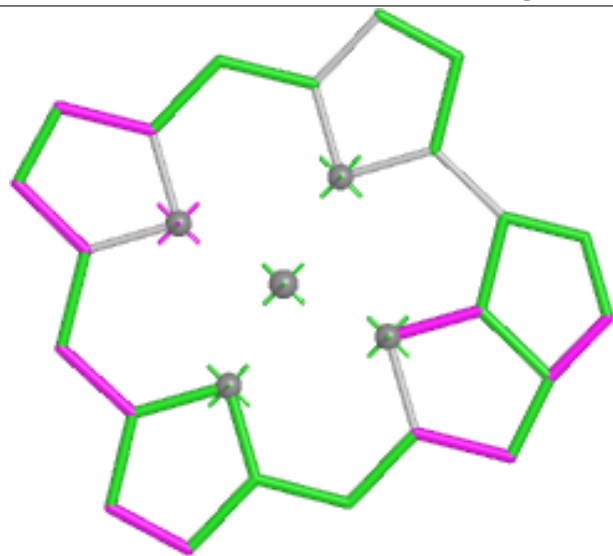
Rings



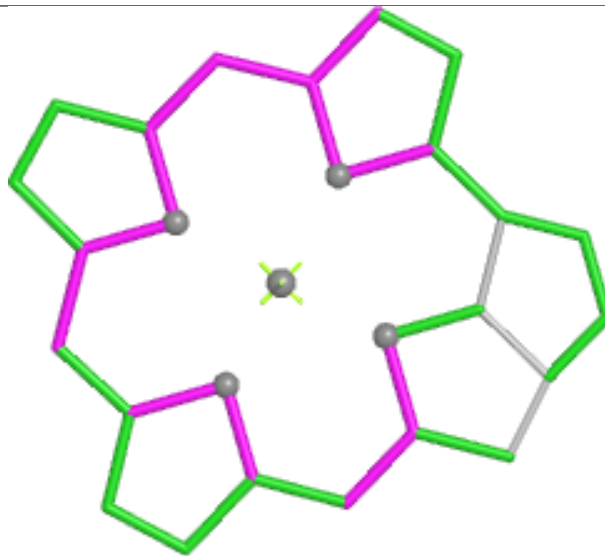




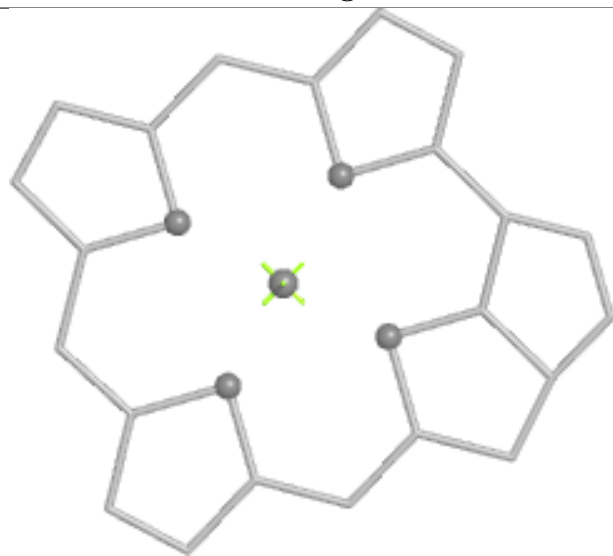
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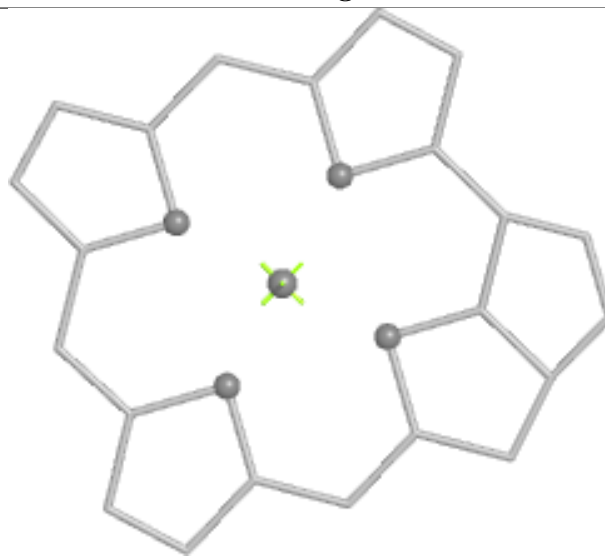
Bond lengths



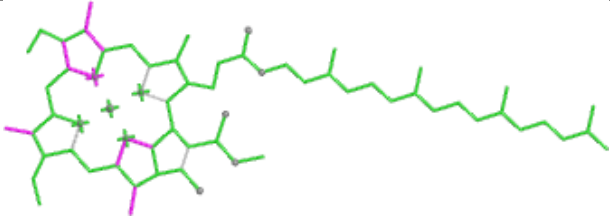
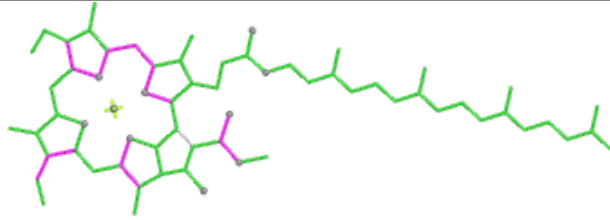
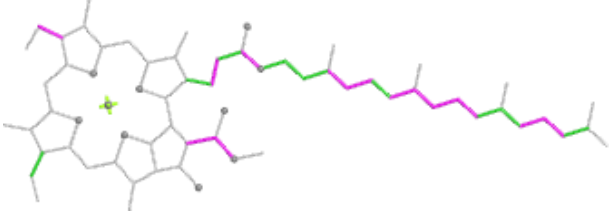
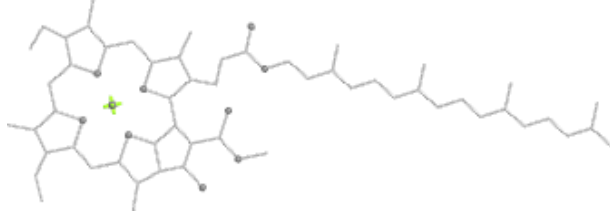
Bond angles

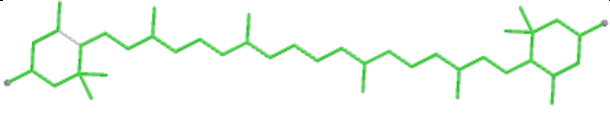
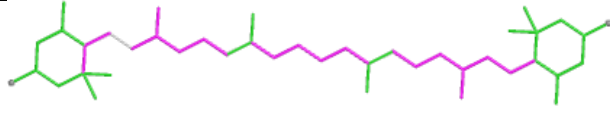
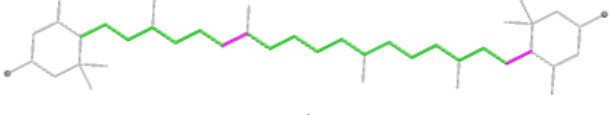
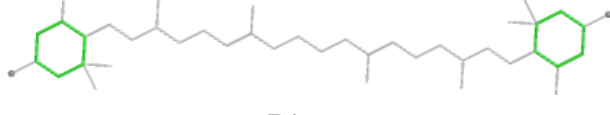


Torsions

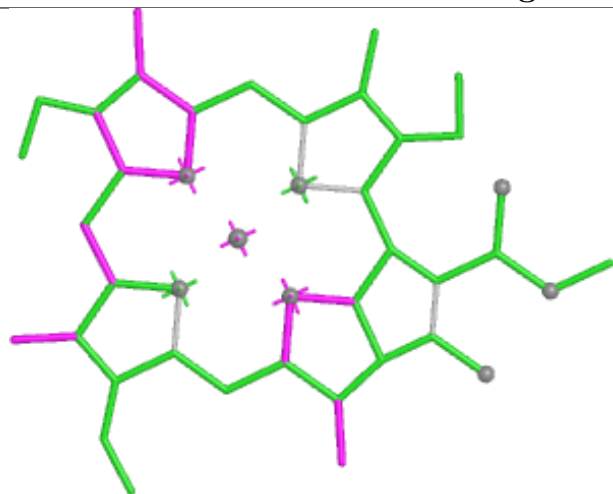


Rings

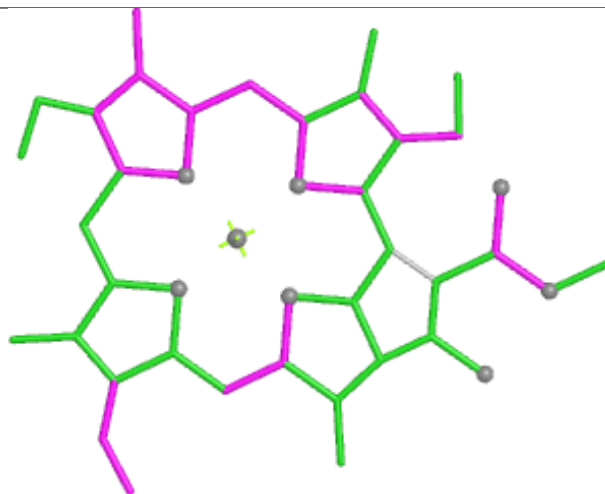
Ligand CLA 7 613			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand LUT 4 619			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

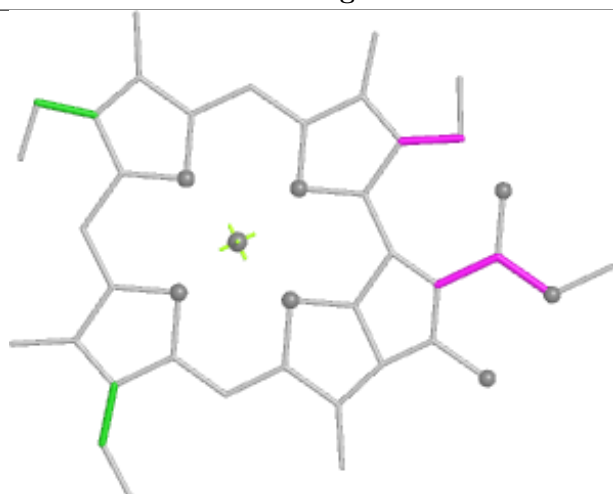
Ligand CLA 7 607



Bond lengths



Bond angles

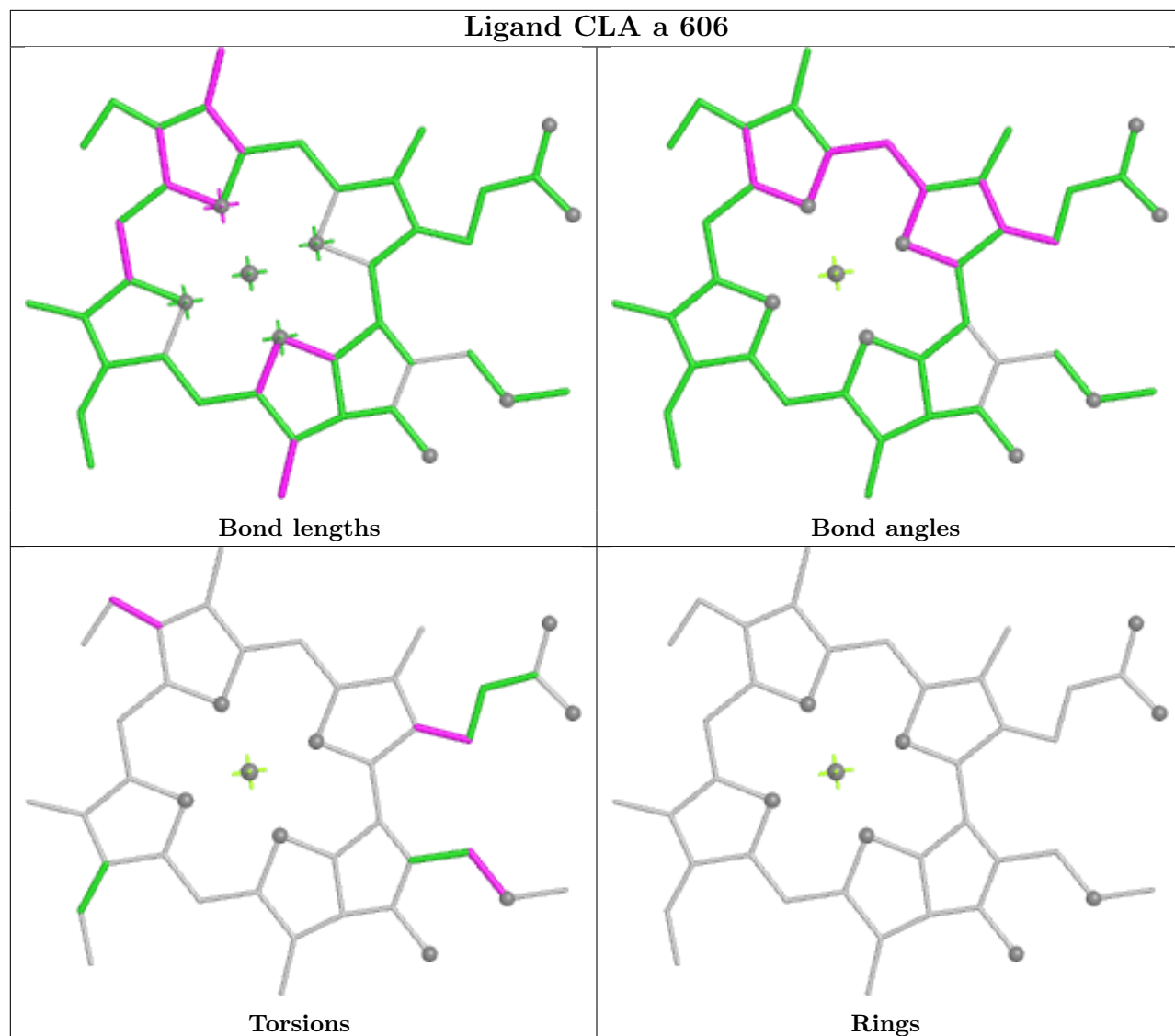


Torsions

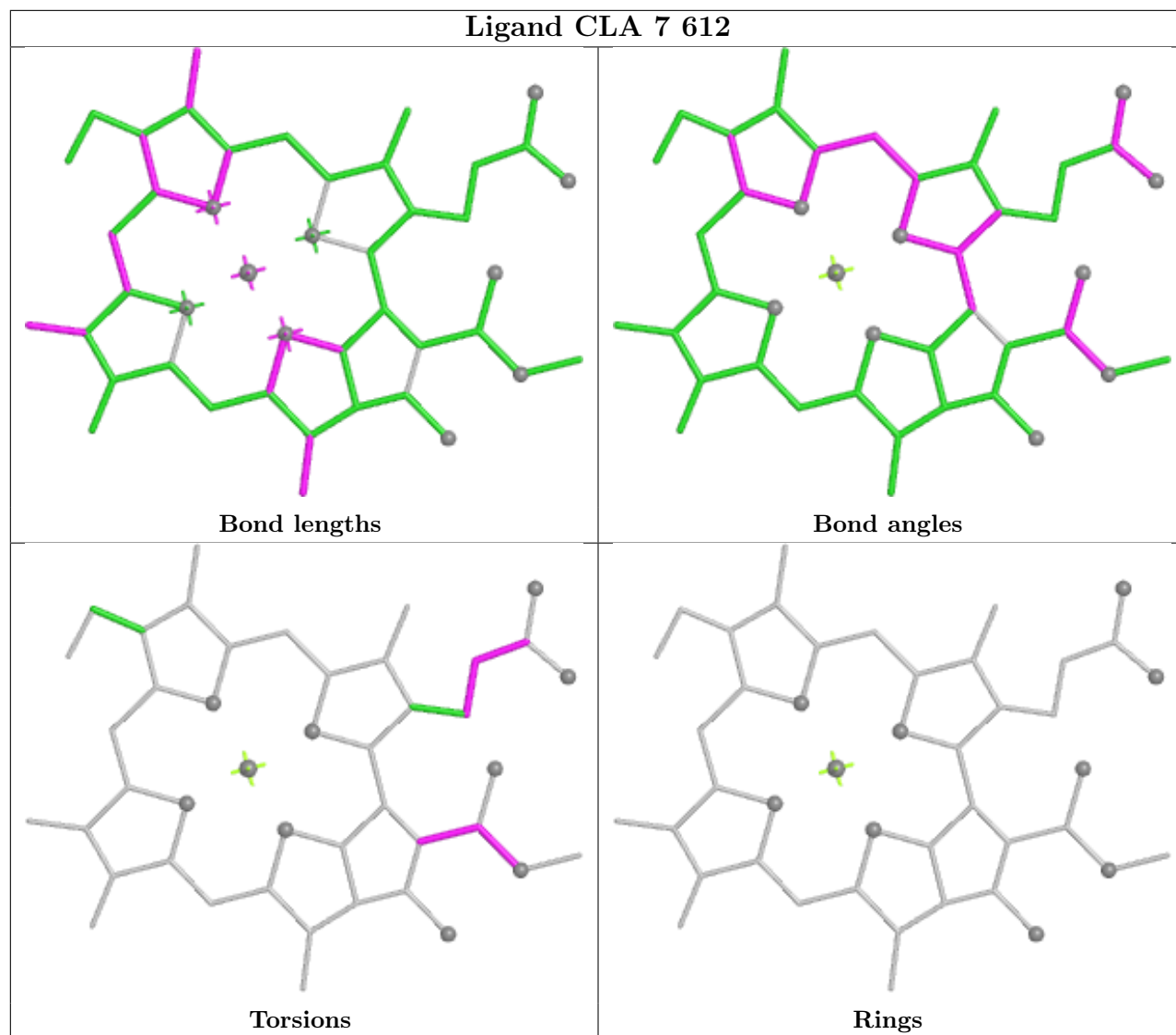


Rings

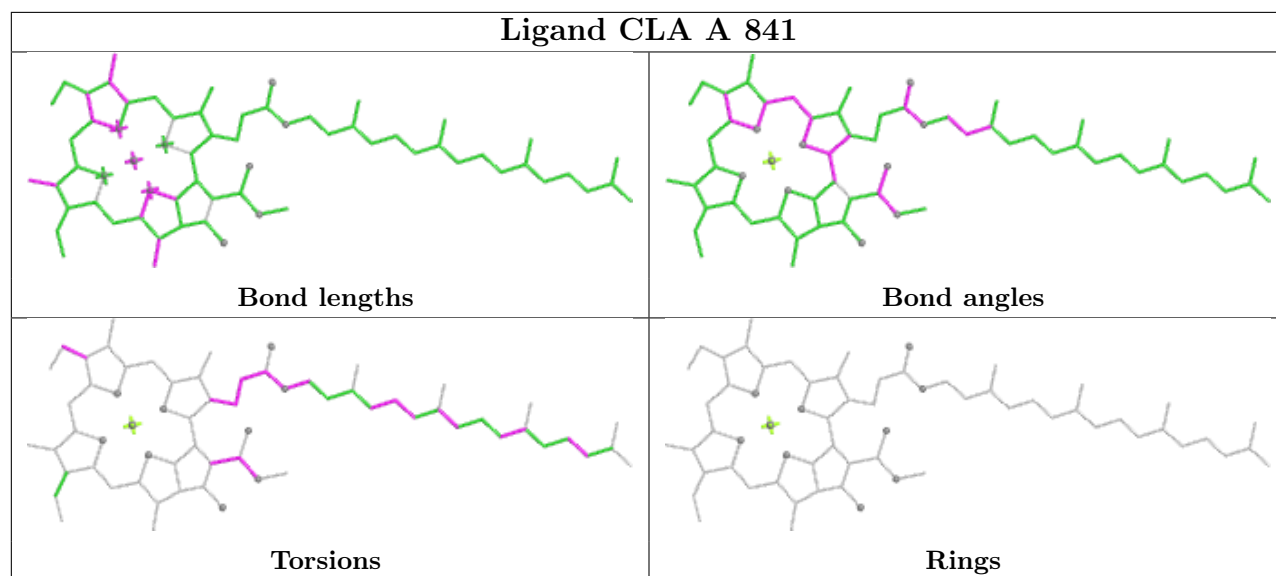
Ligand CLA a 606



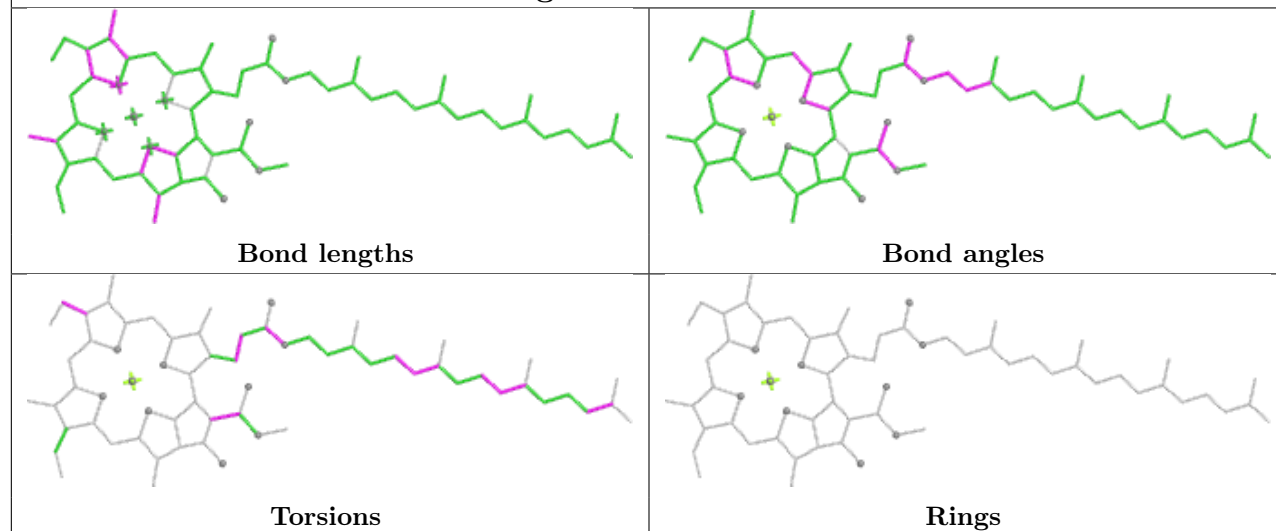
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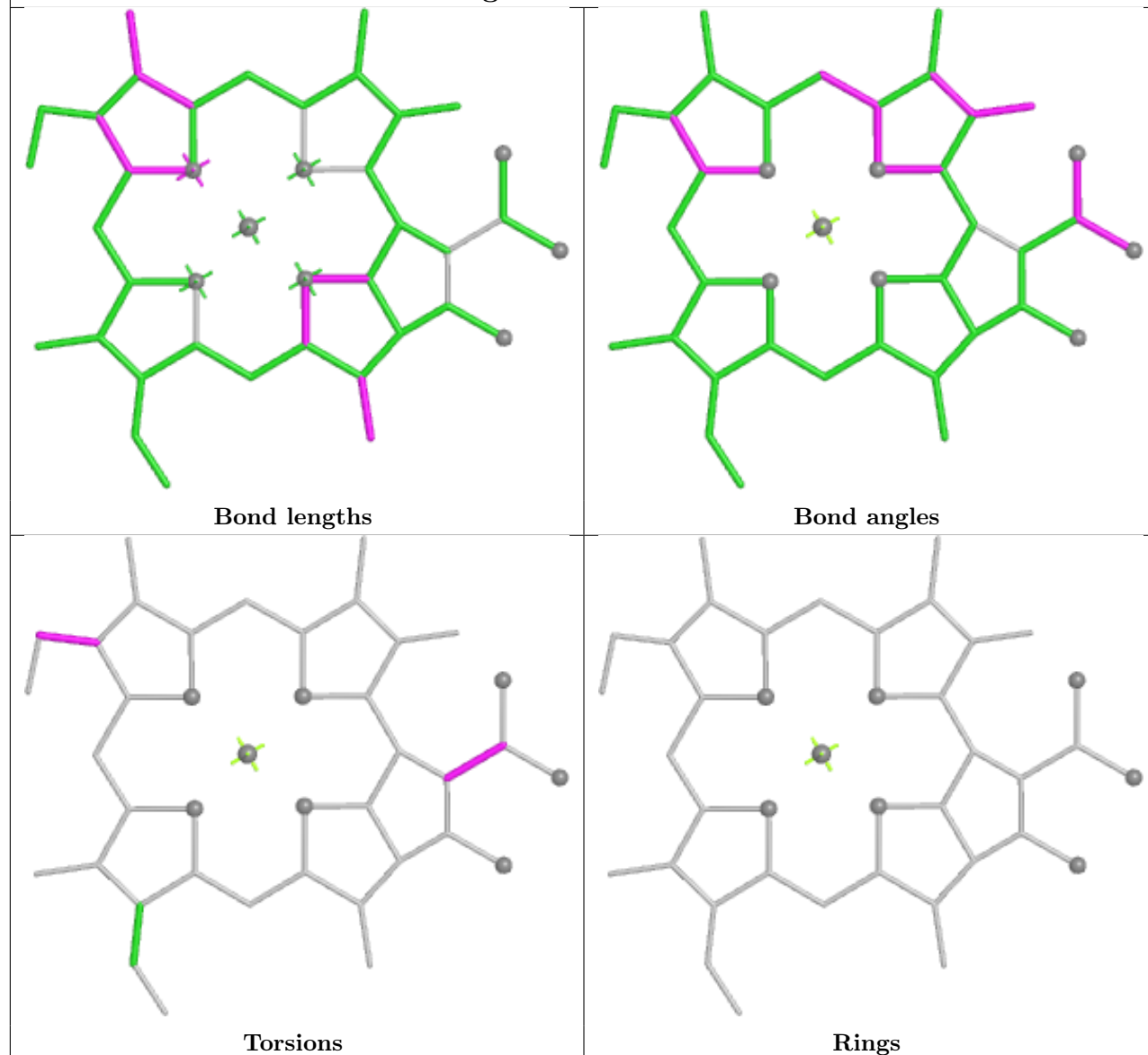
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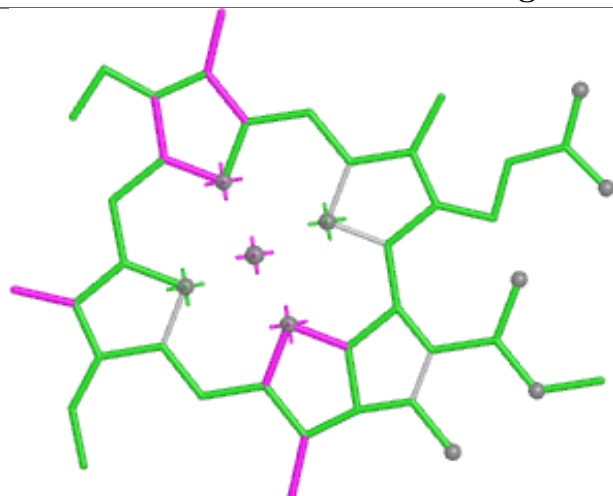
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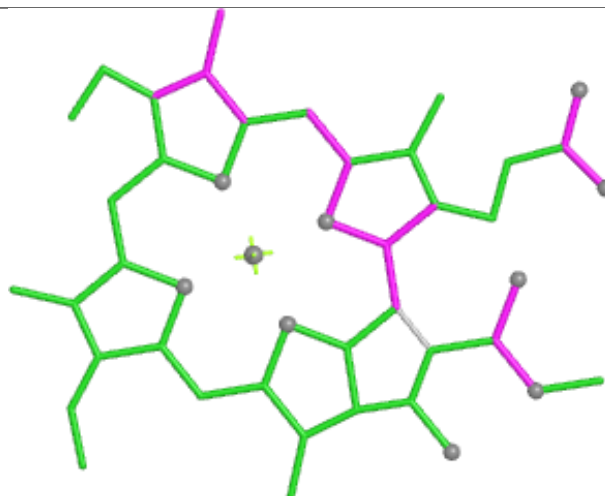
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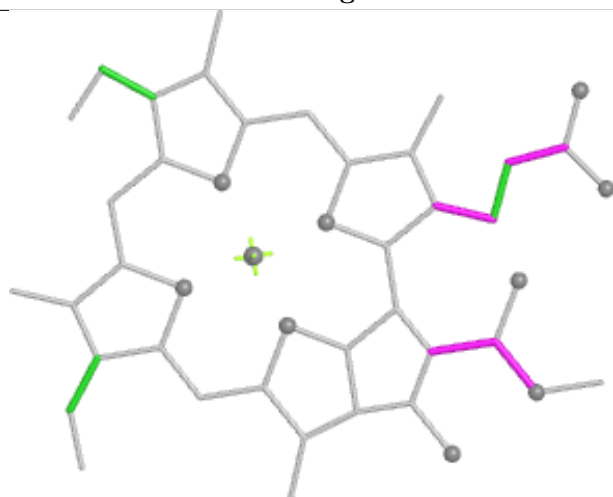
Ligand CLA 1 612



Bond lengths



Bond angles

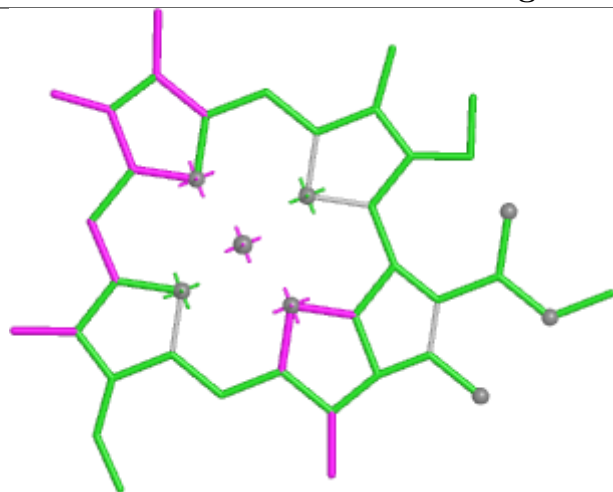


Torsions



Rings

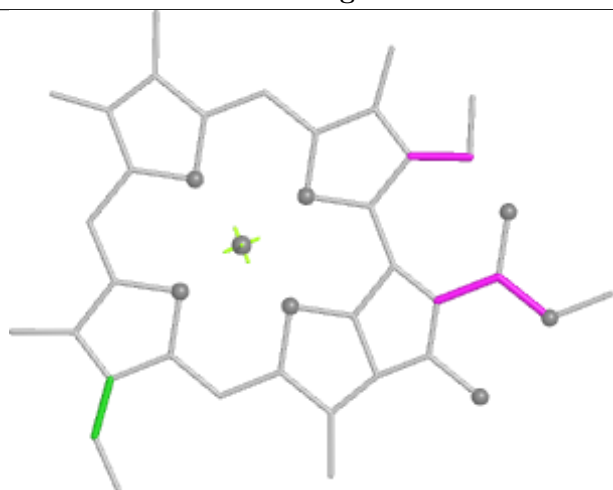
Ligand CLA 6 607



Bond lengths



Bond angles

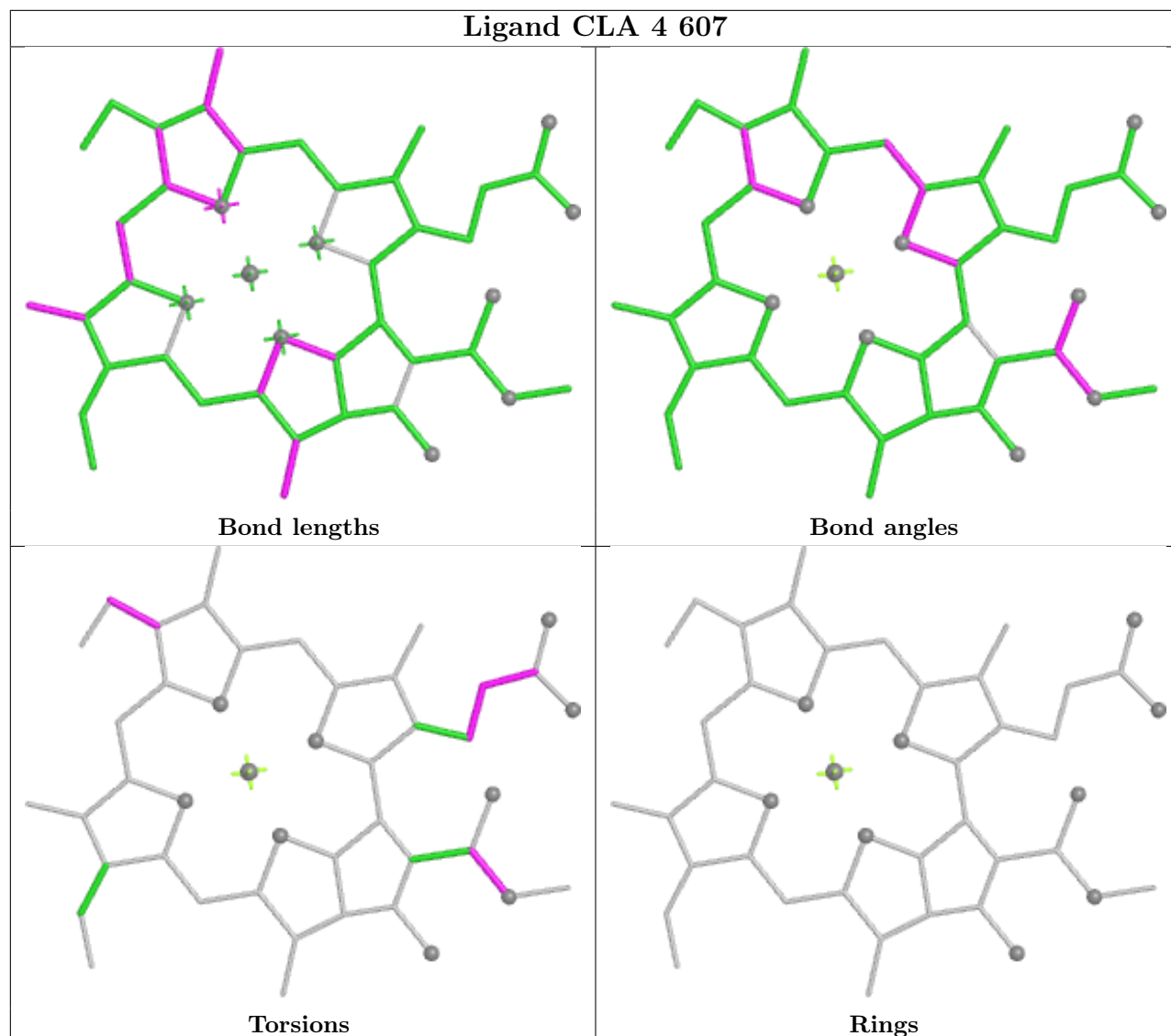


Torsions

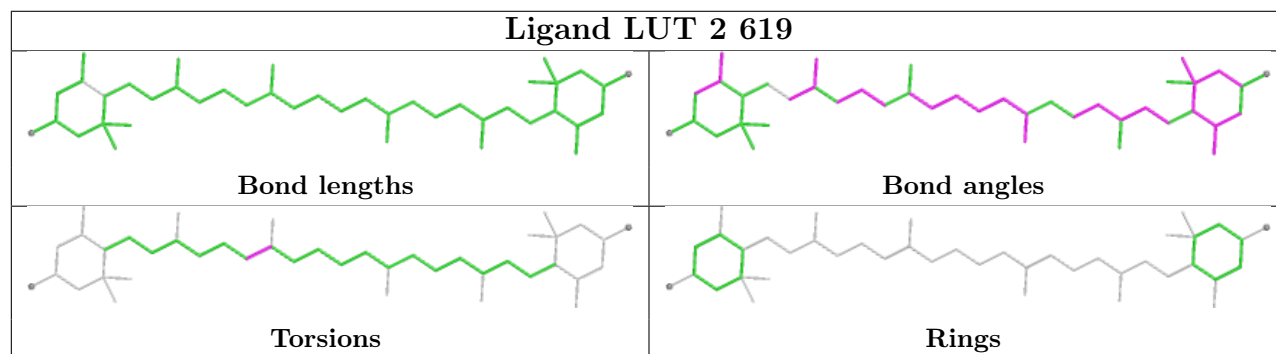


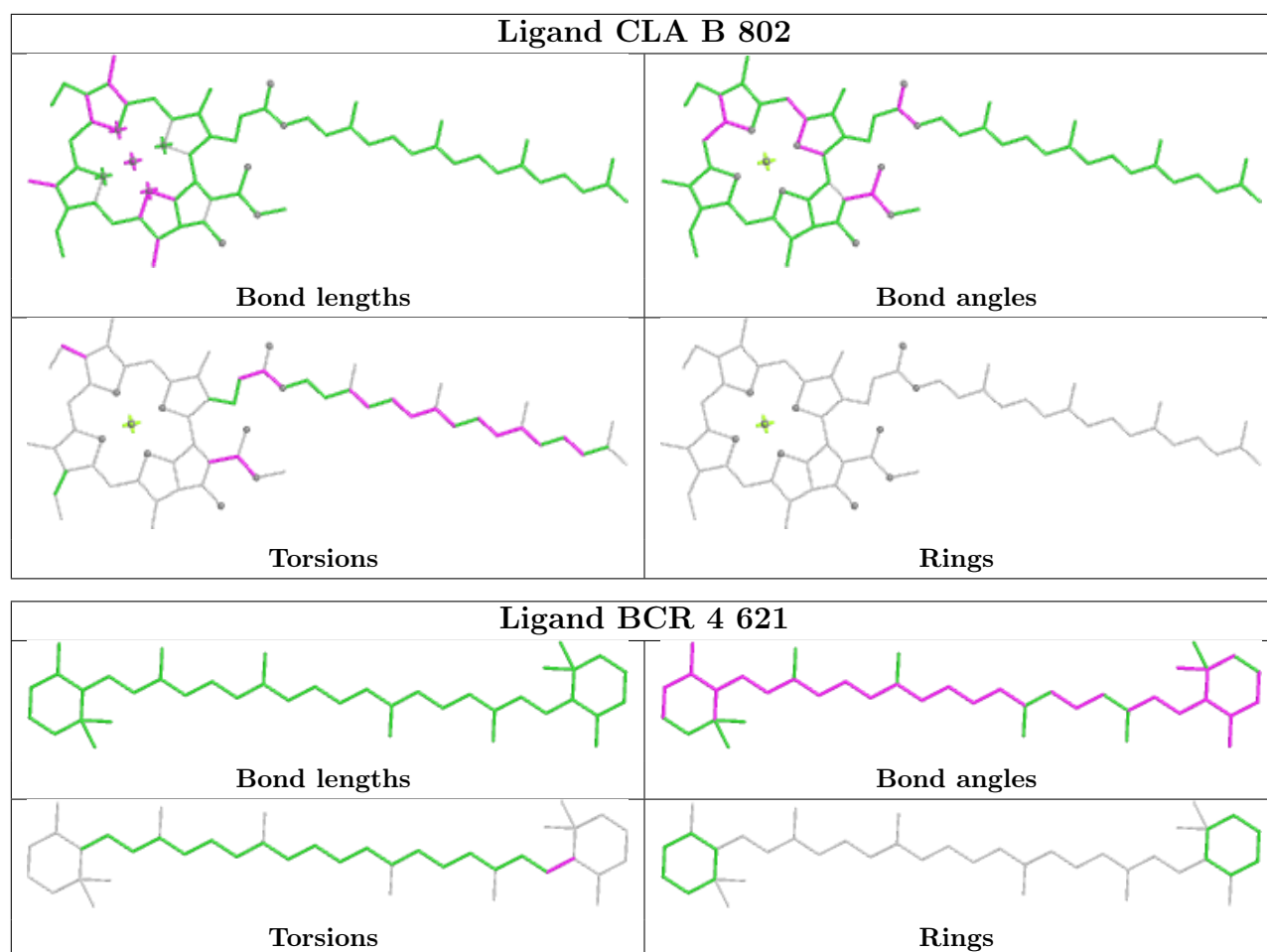
Rings

Ligand CLA 4 607

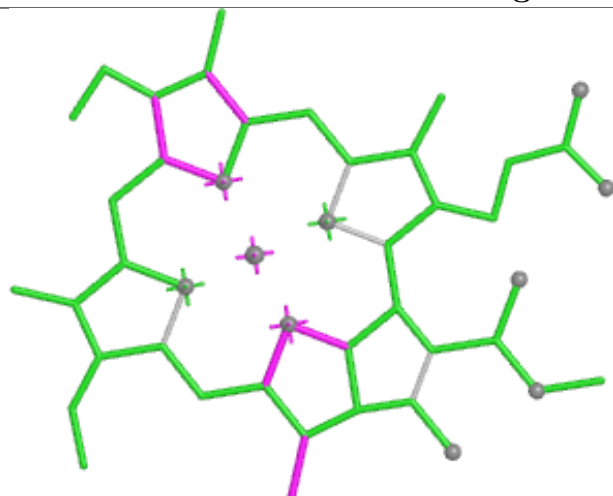


Ligand LUT 2 619

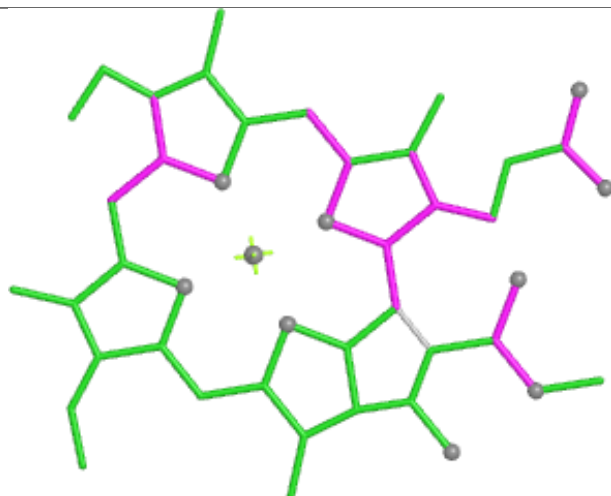




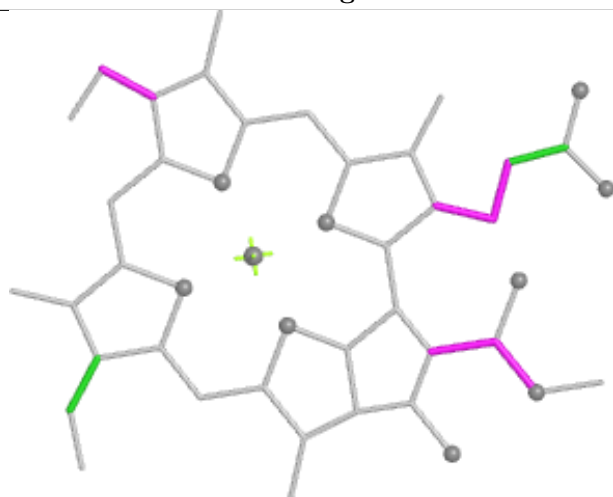
Ligand CLA K 201



Bond lengths



Bond angles

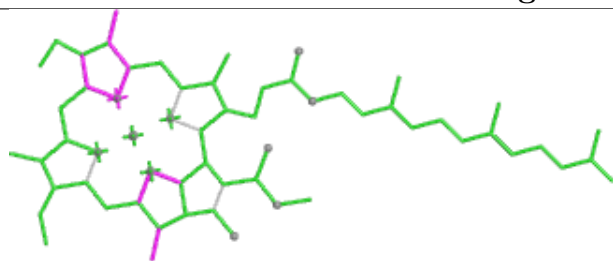


Torsions

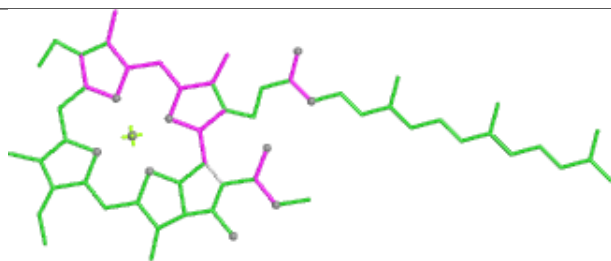


Rings

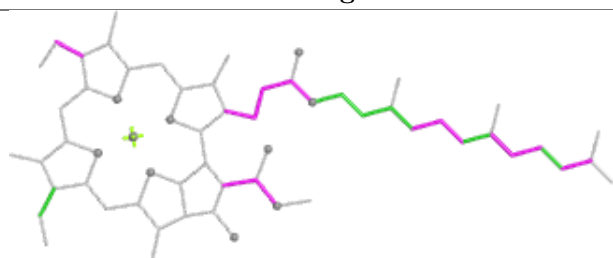
Ligand CLA 3 609



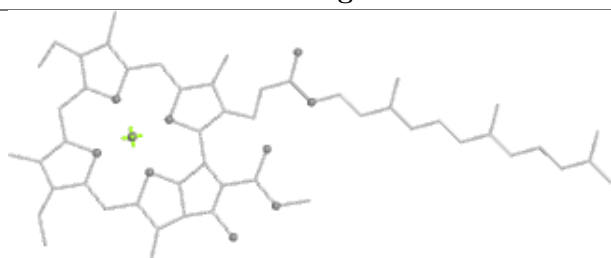
Bond lengths



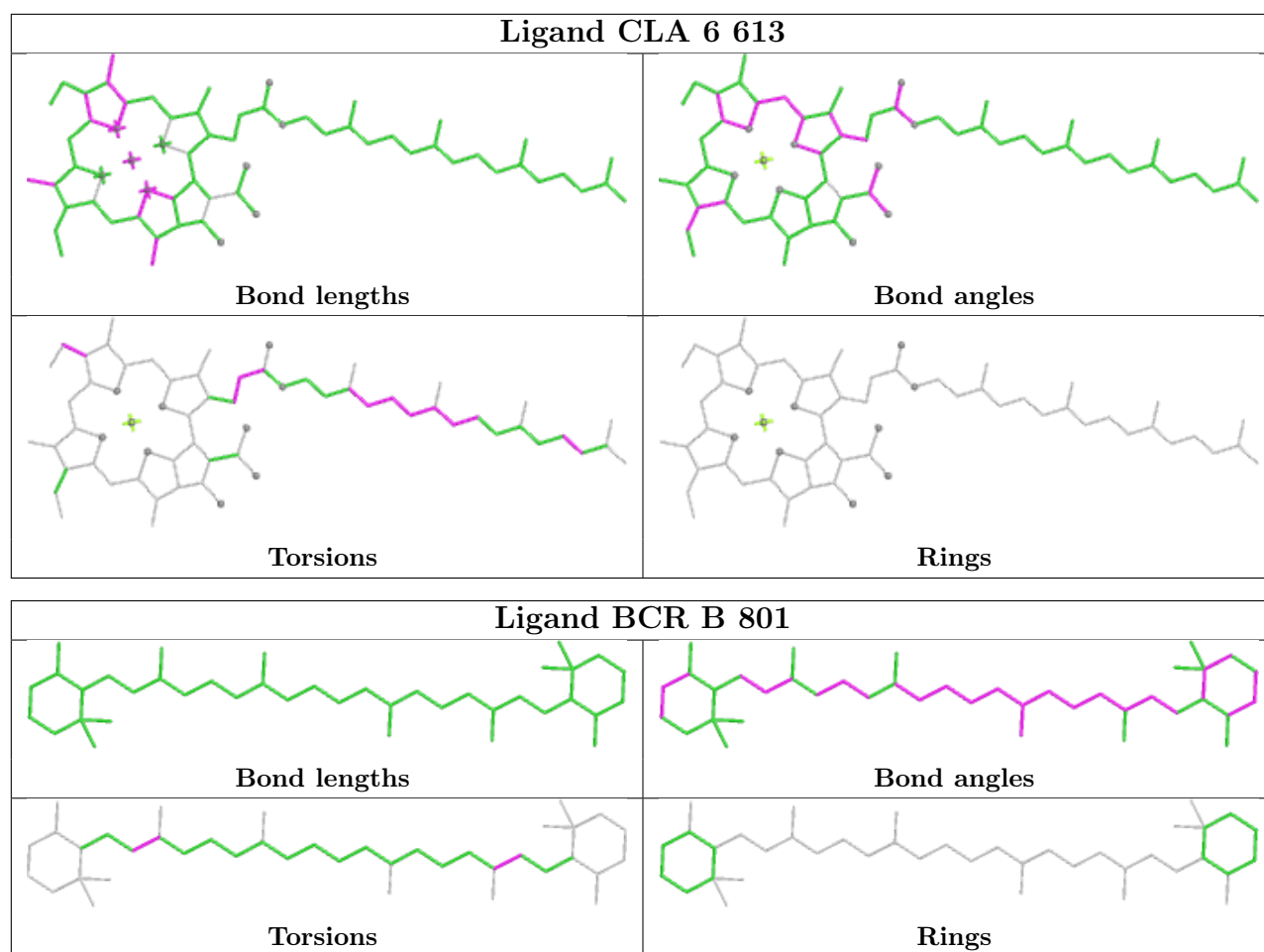
Bond angles

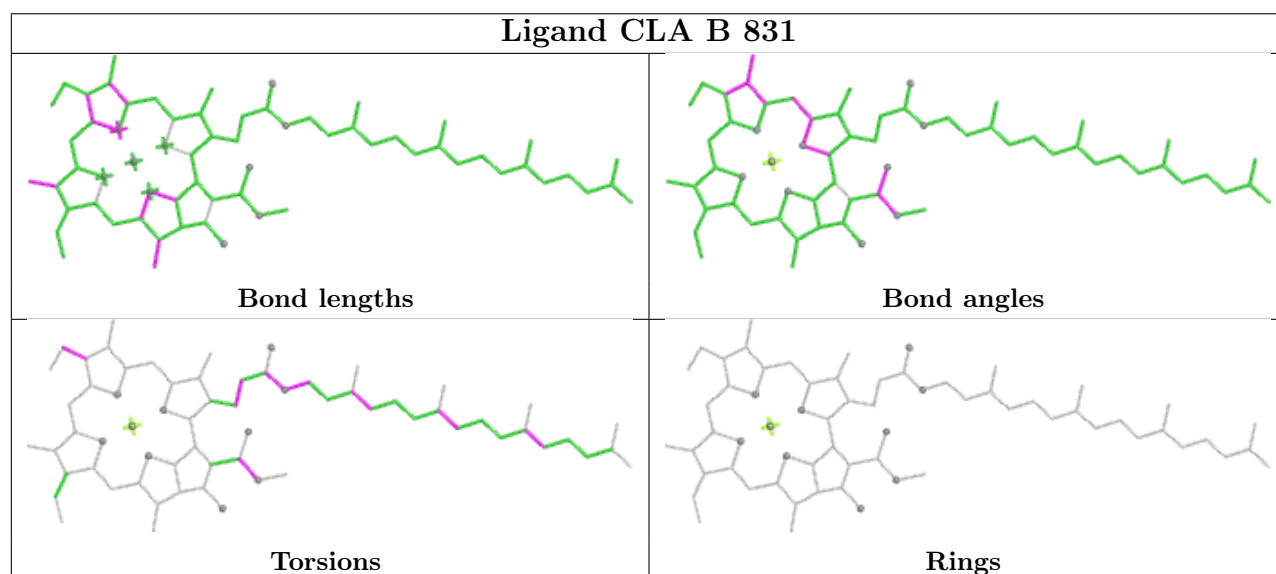
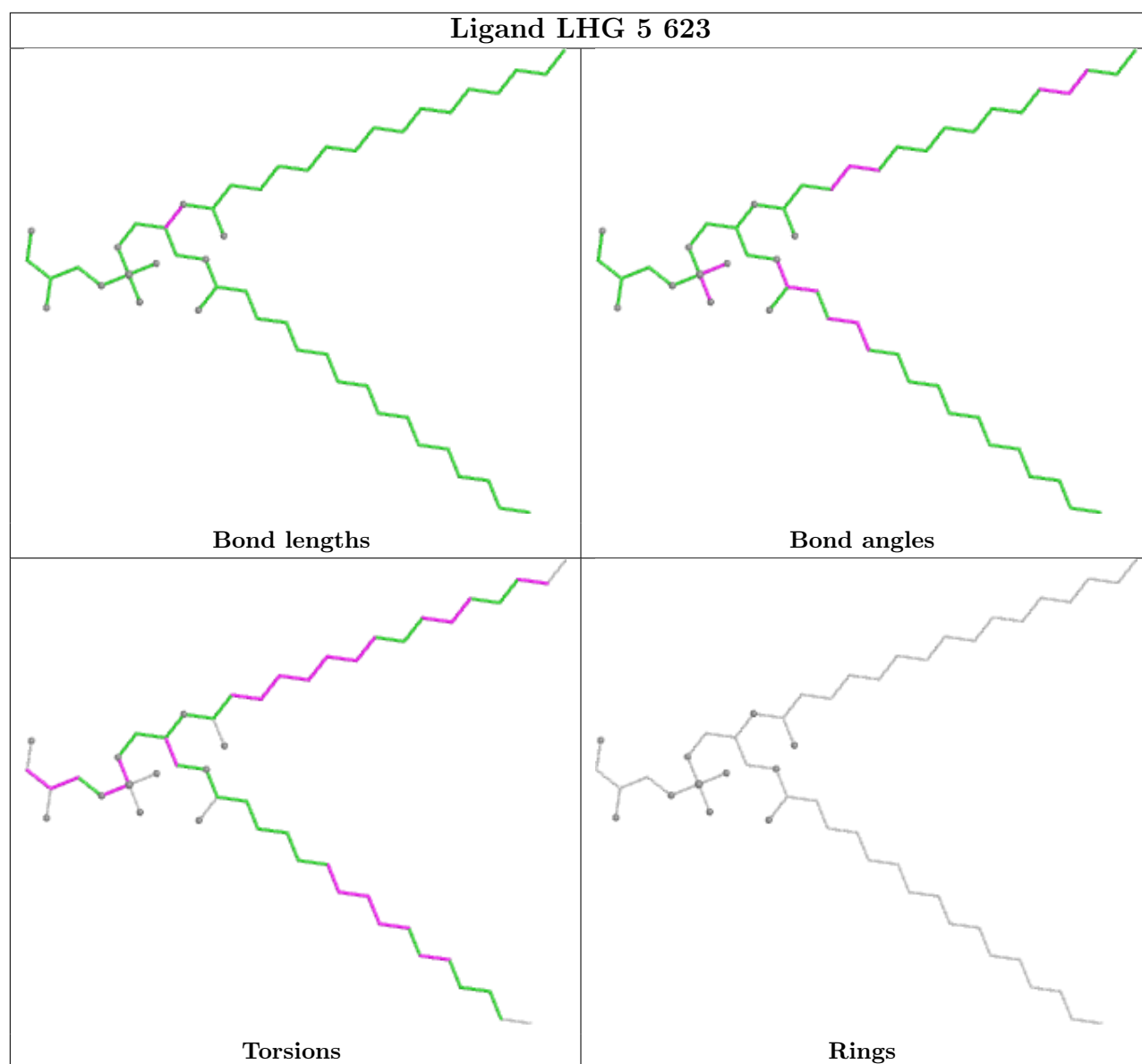


Torsions

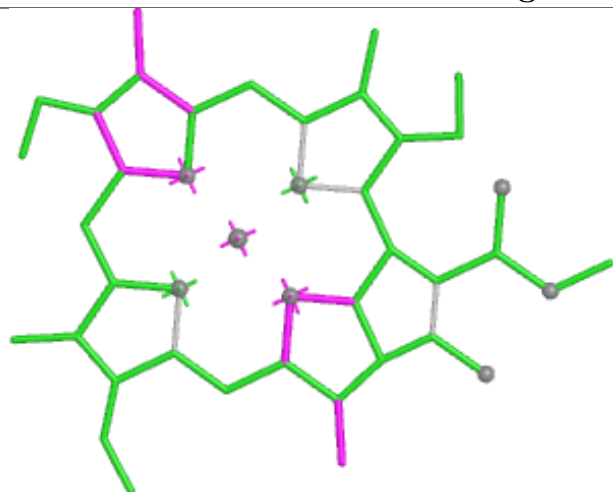


Rings

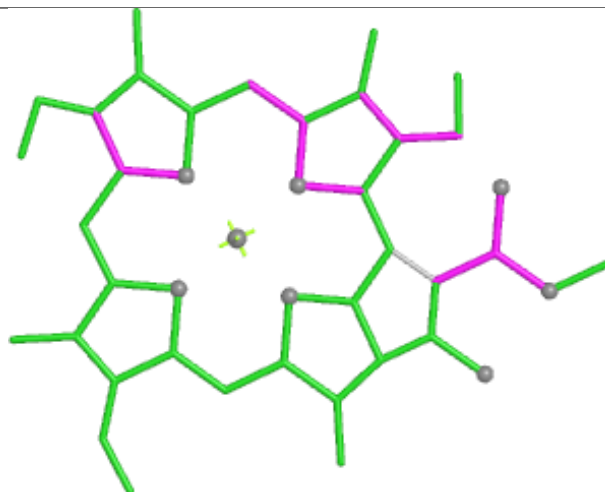




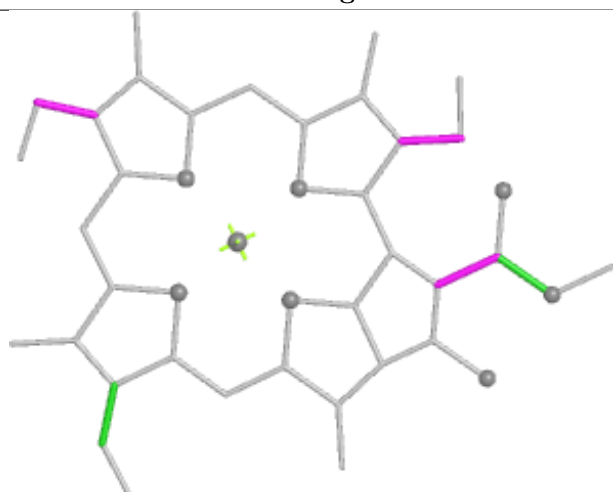
Ligand CLA 5 611



Bond lengths



Bond angles

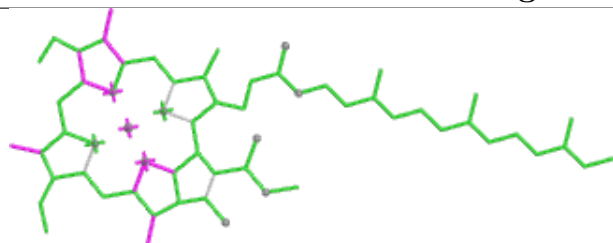


Torsions

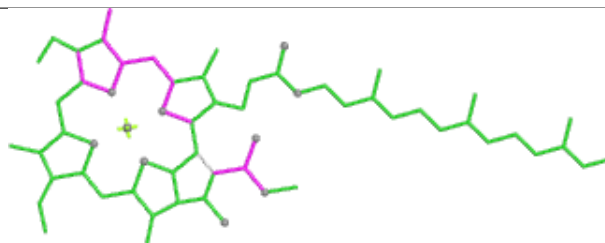


Rings

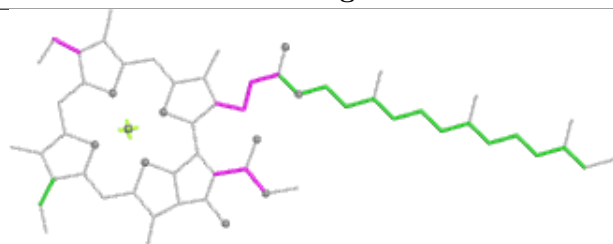
Ligand CLA a 602



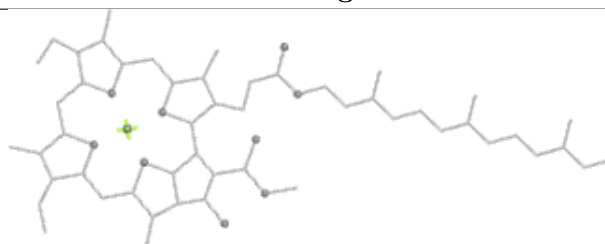
Bond lengths



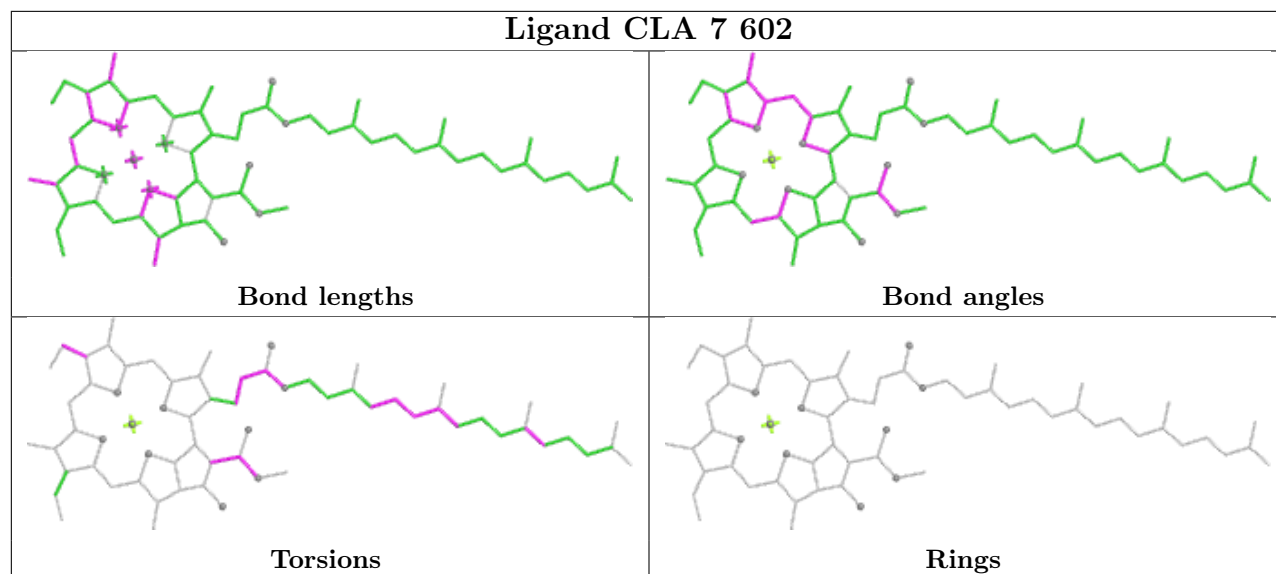
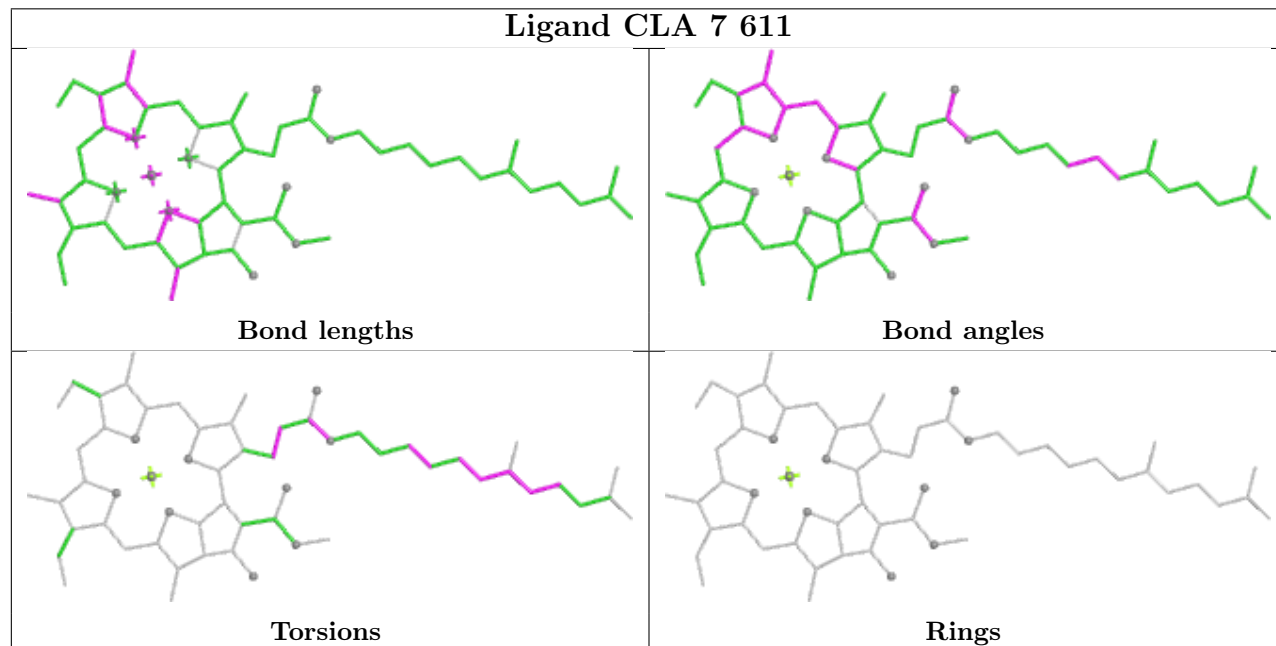
Bond angles

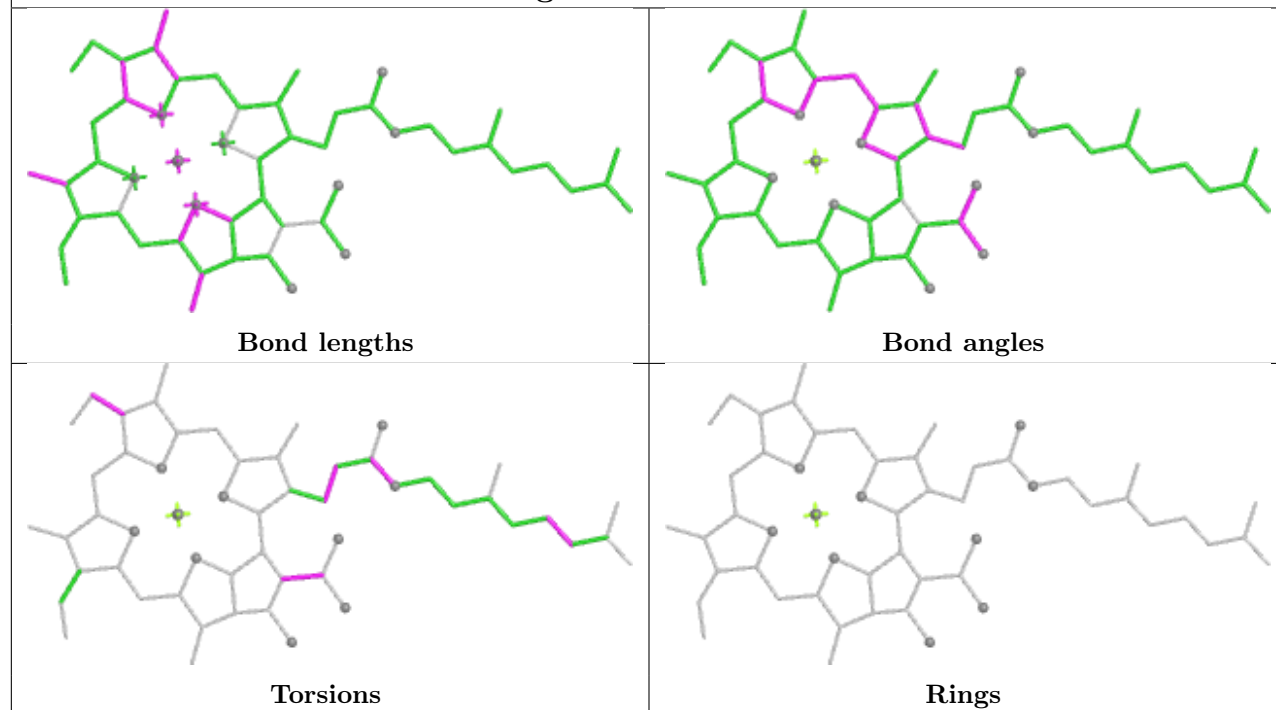
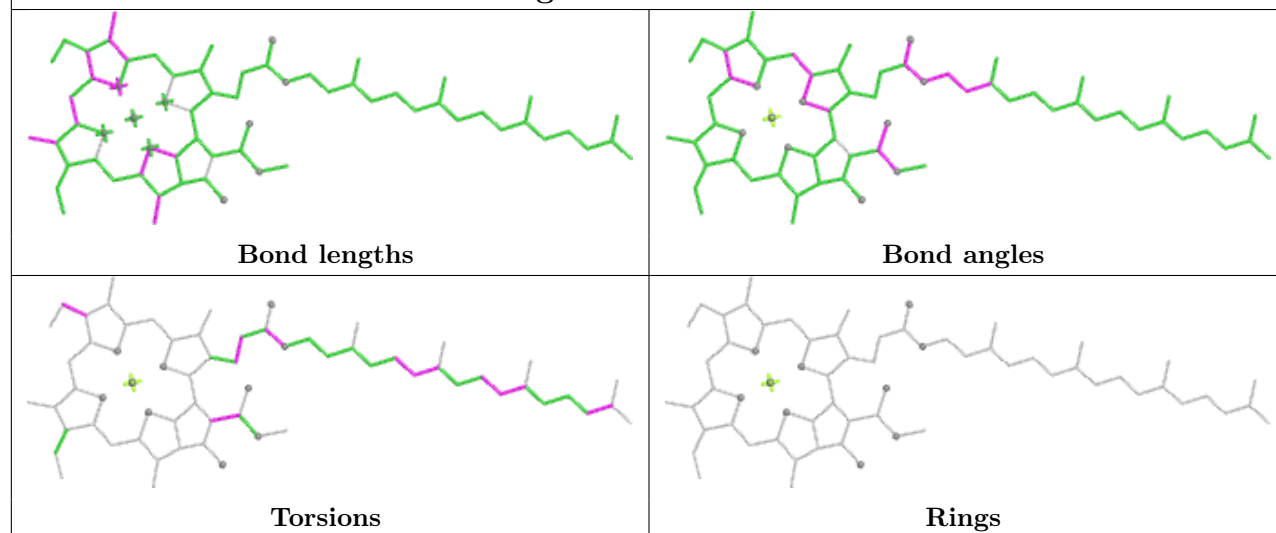


Torsions

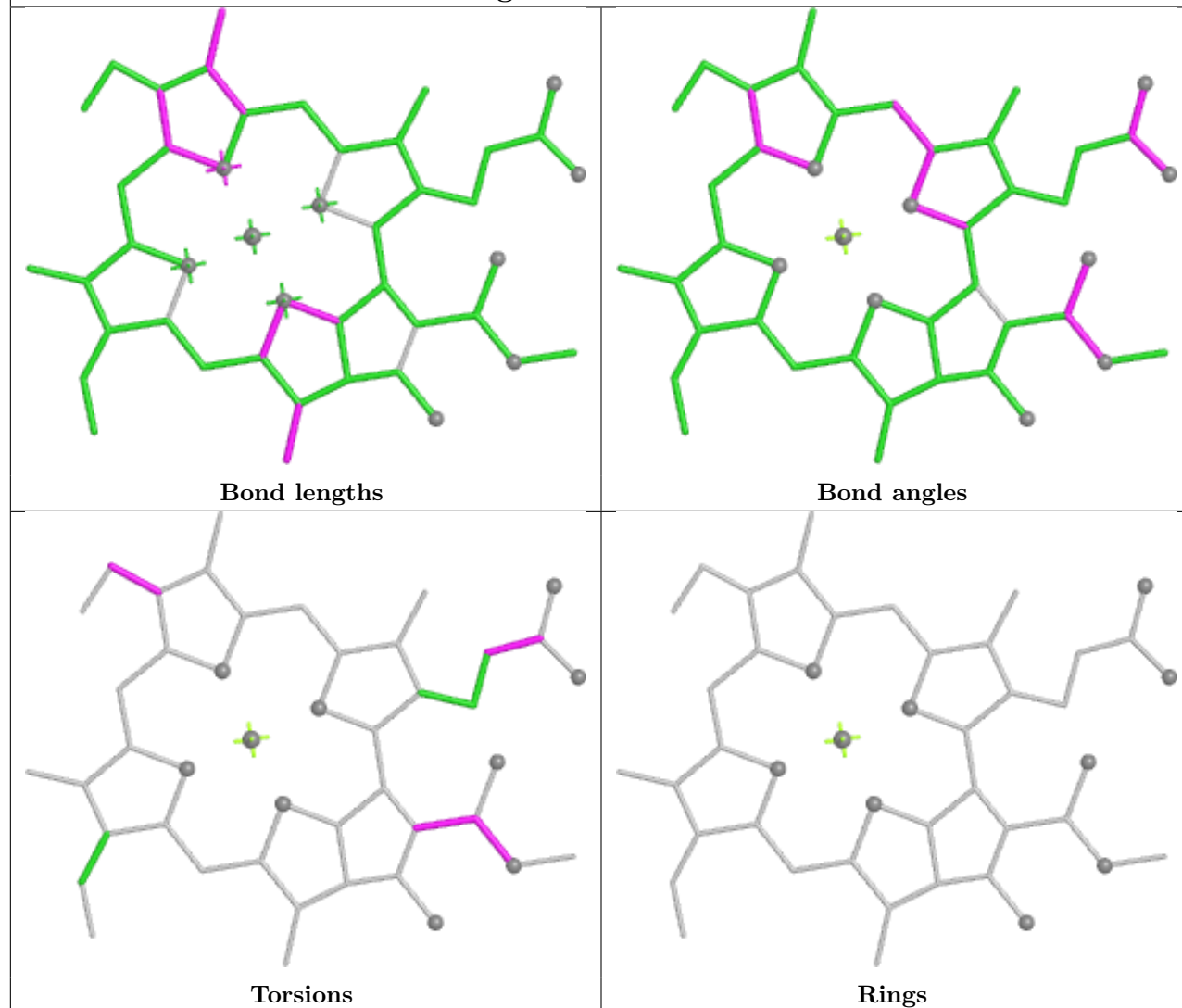


Rings

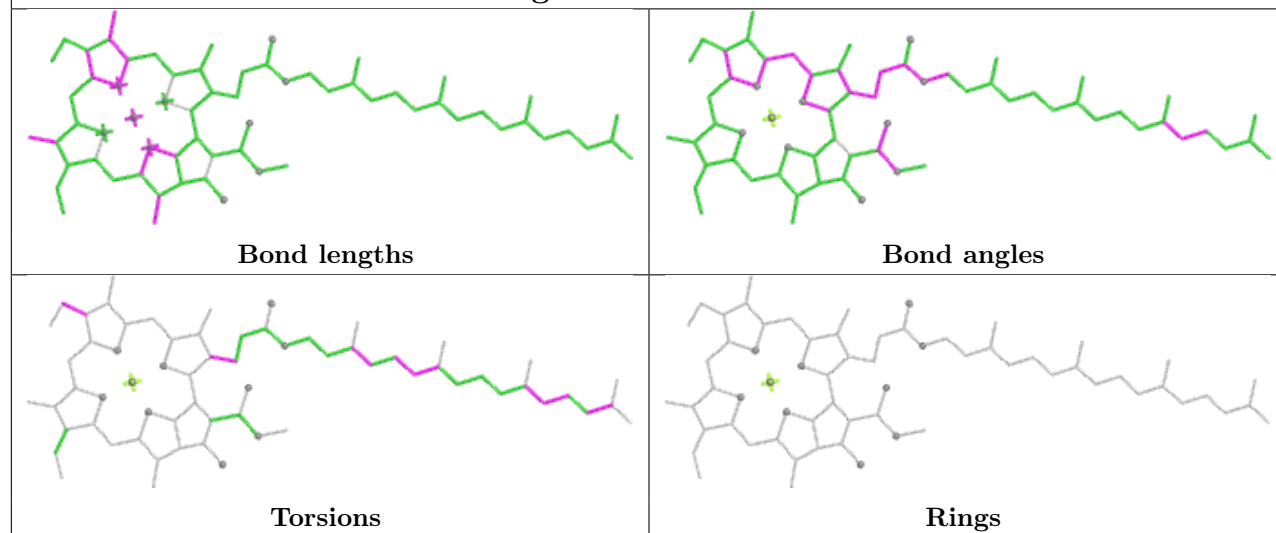
Ligand CLA 7 602**Ligand CLA 7 611**

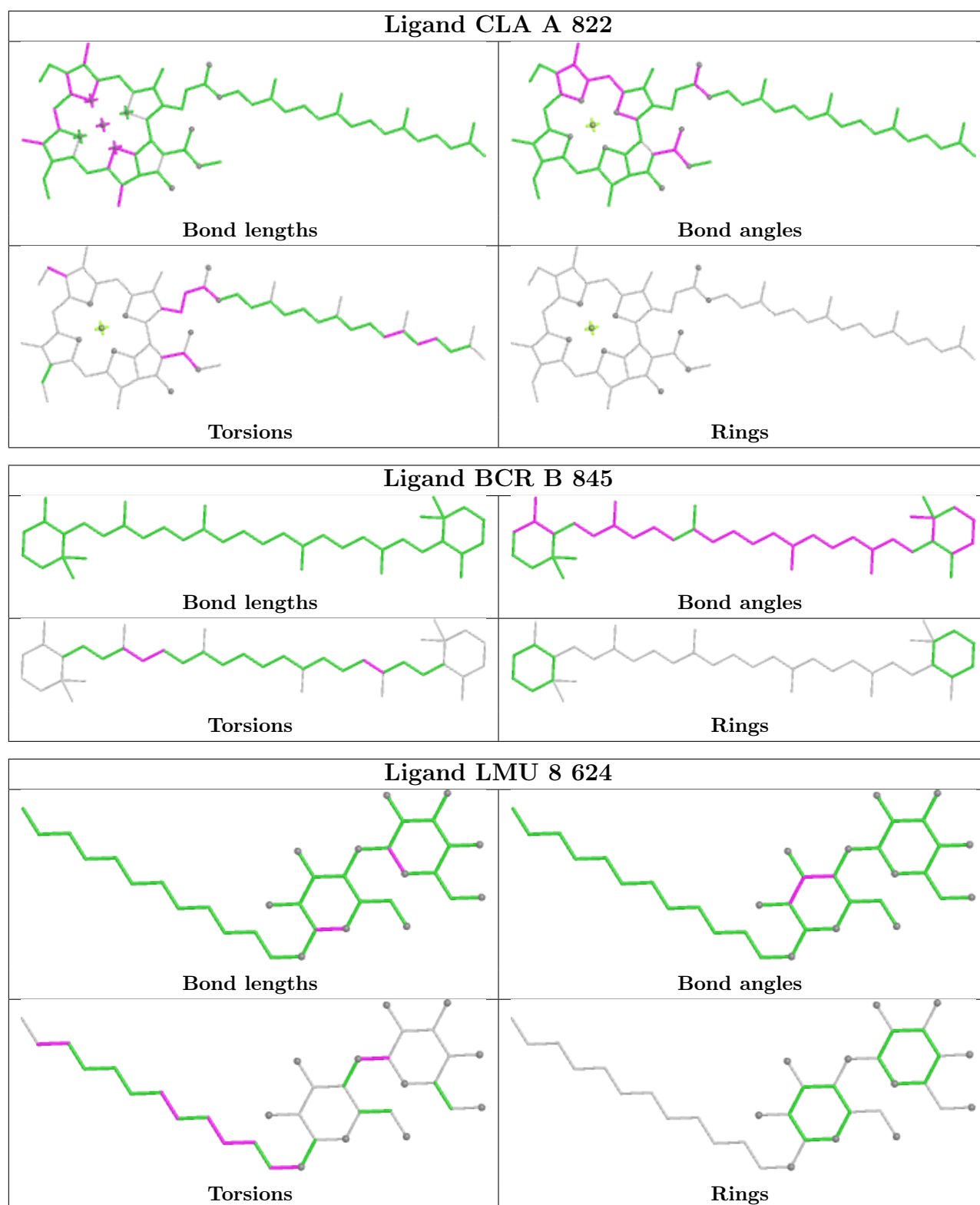
Ligand CLA a 601**Ligand CLA a 613**

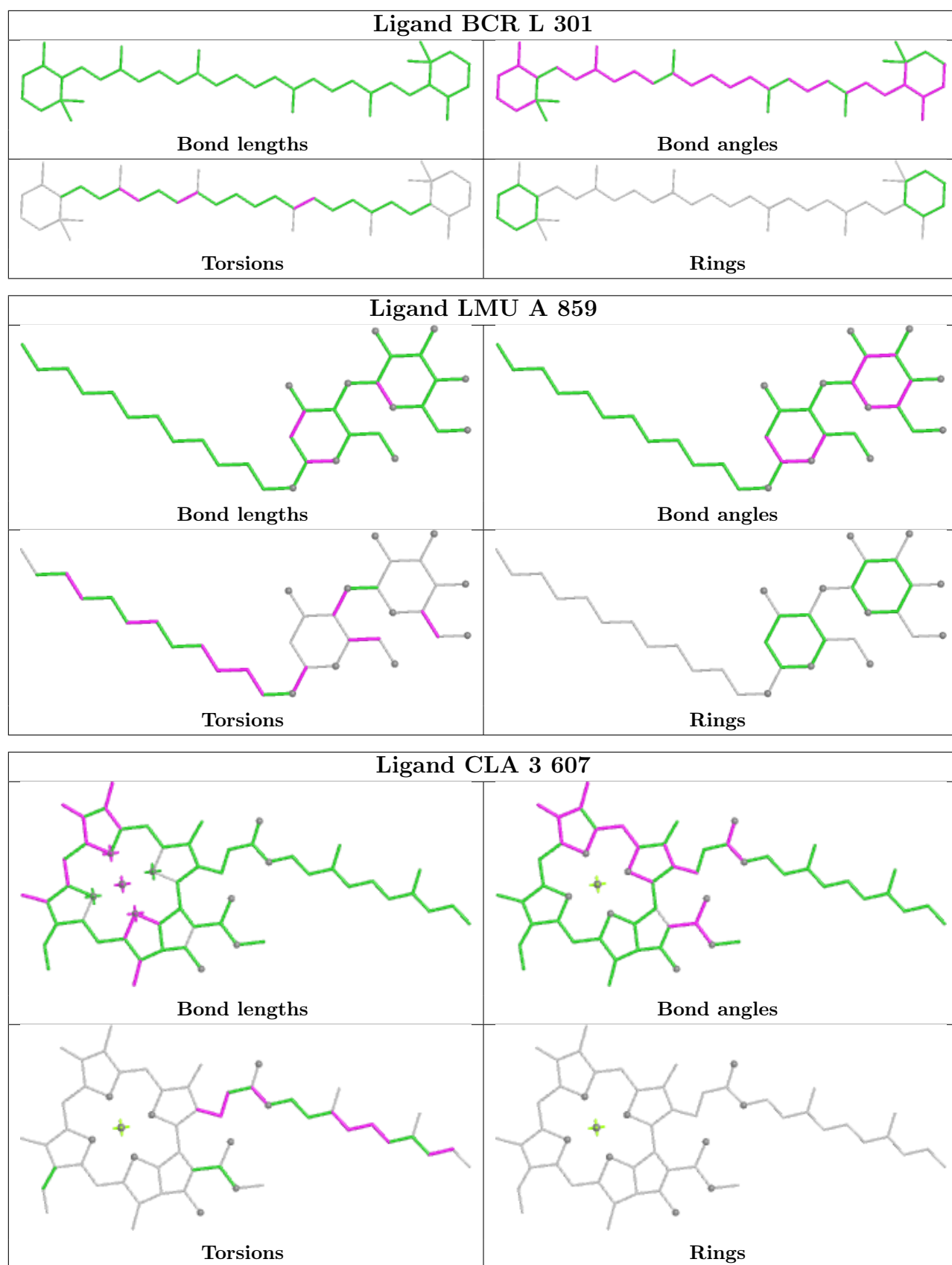
Ligand CLA a 607



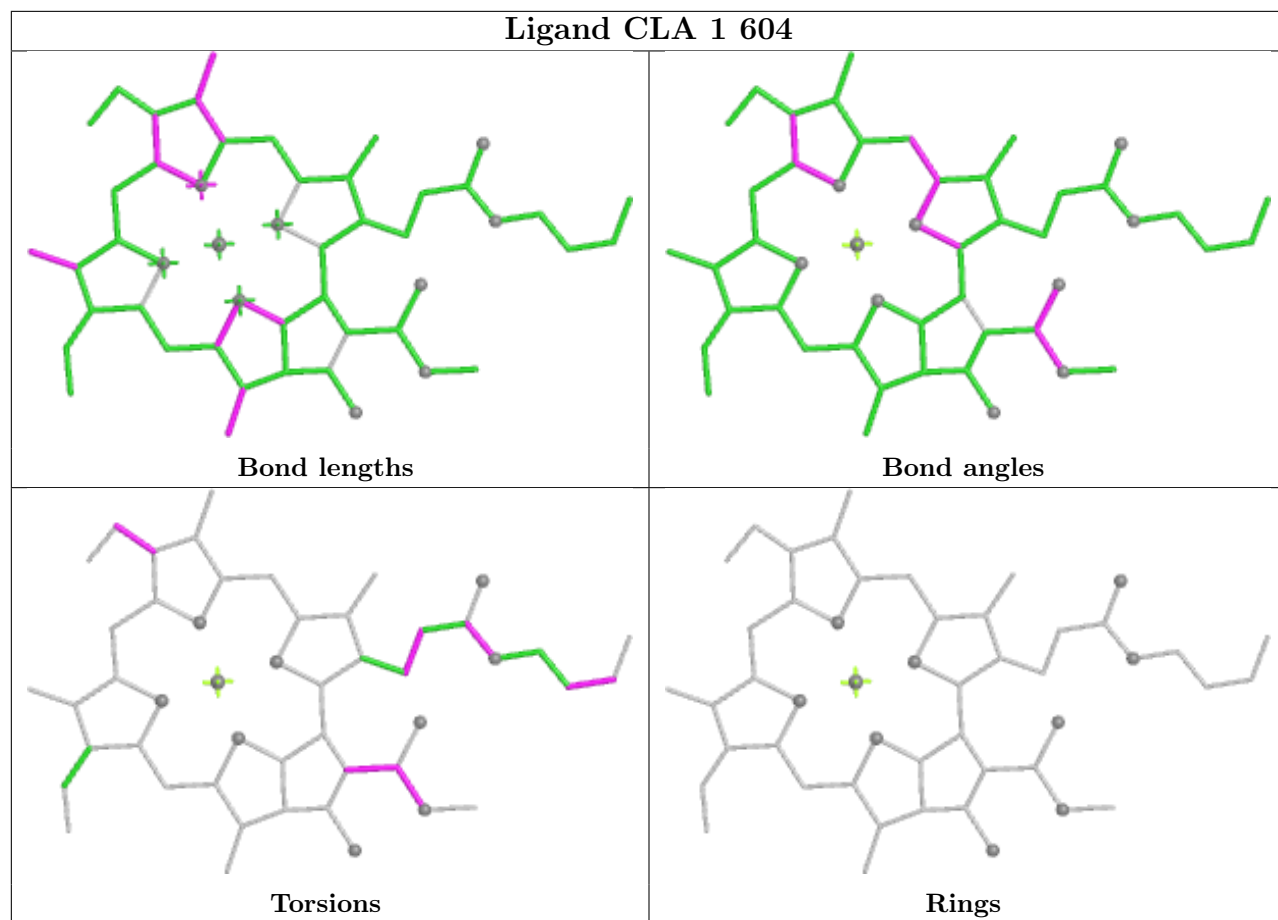
Ligand CLA A 812



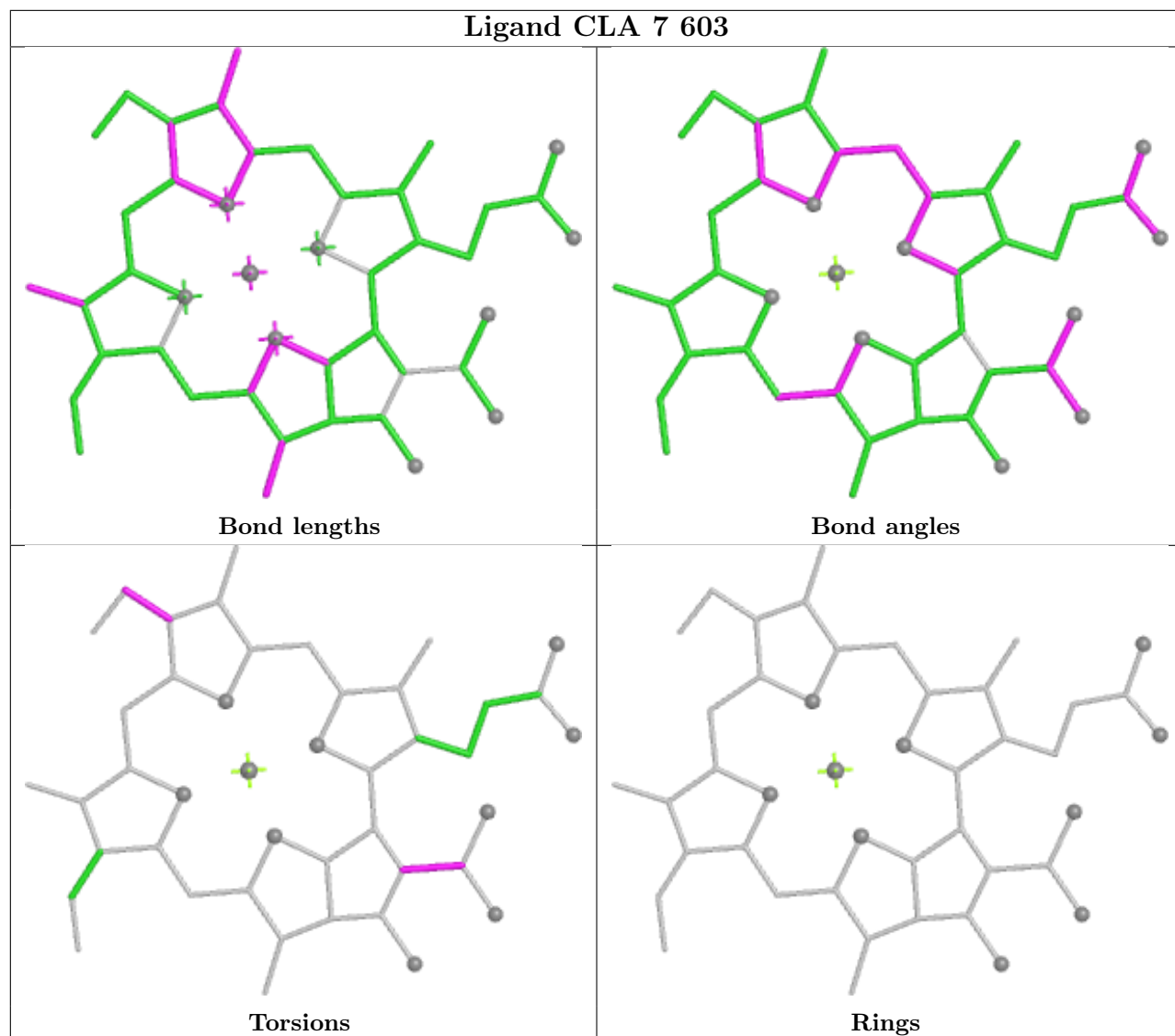




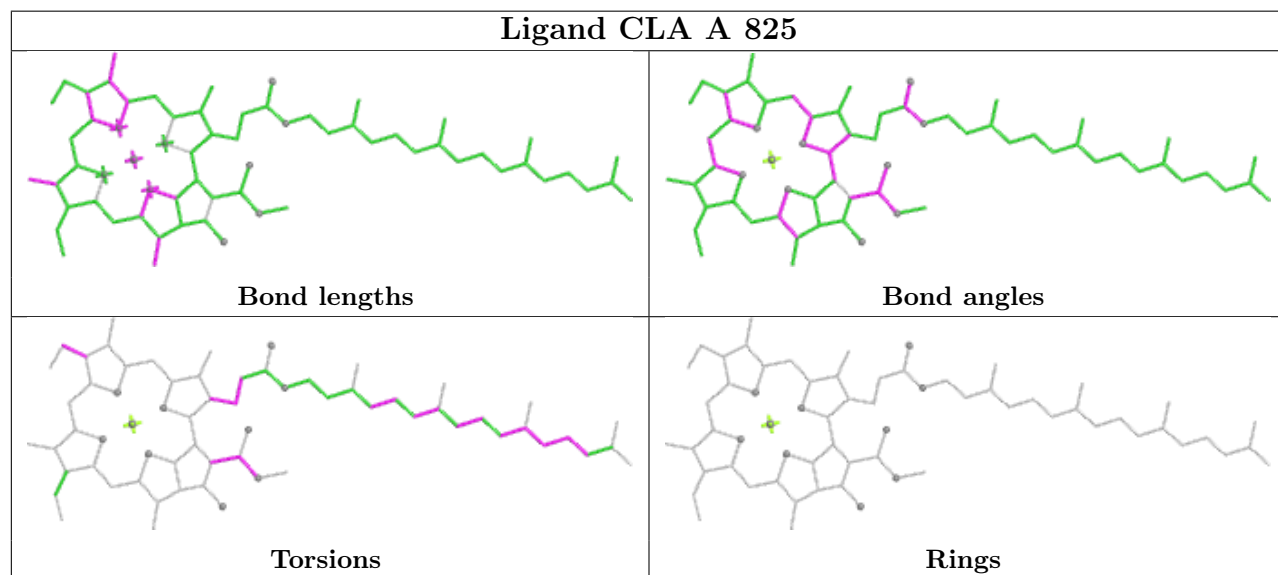
Ligand CLA 1 604

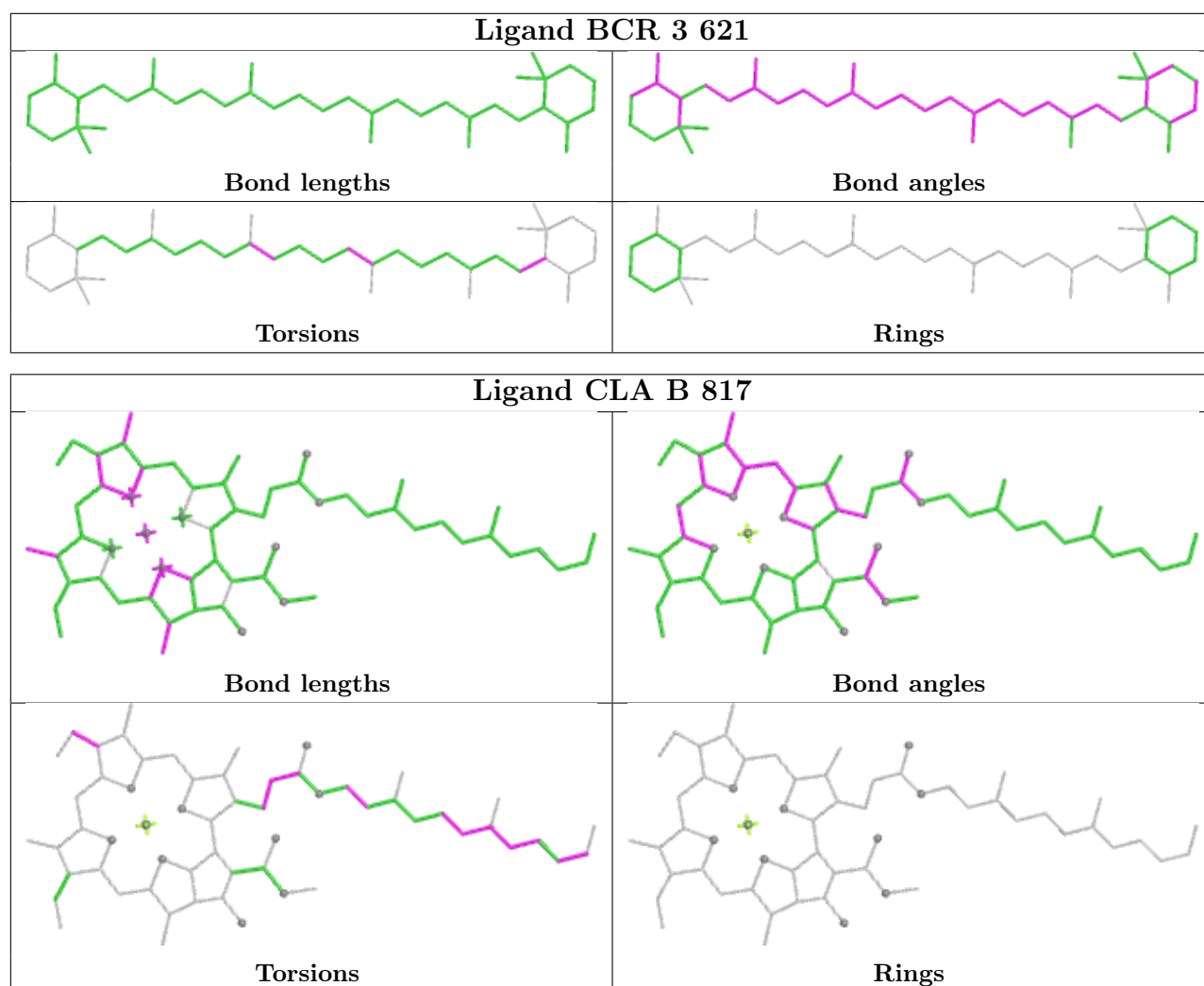


Ligand CLA 7 603

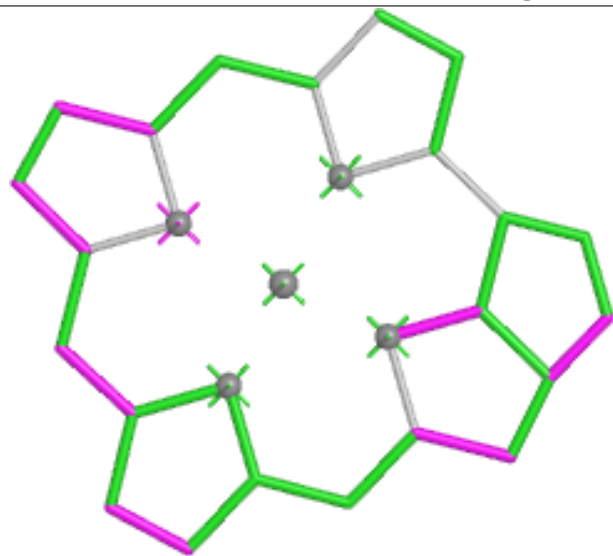


Ligand CLA A 825

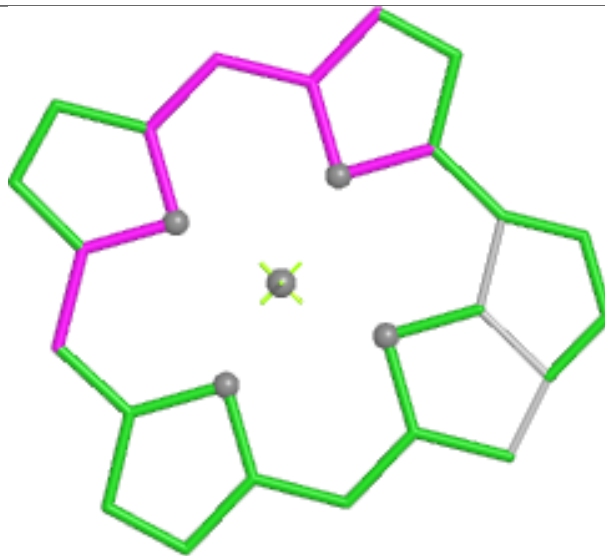




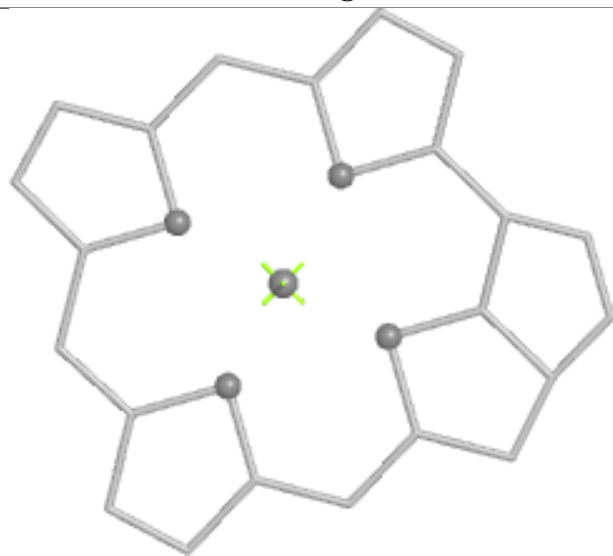
Ligand CLA 2 607



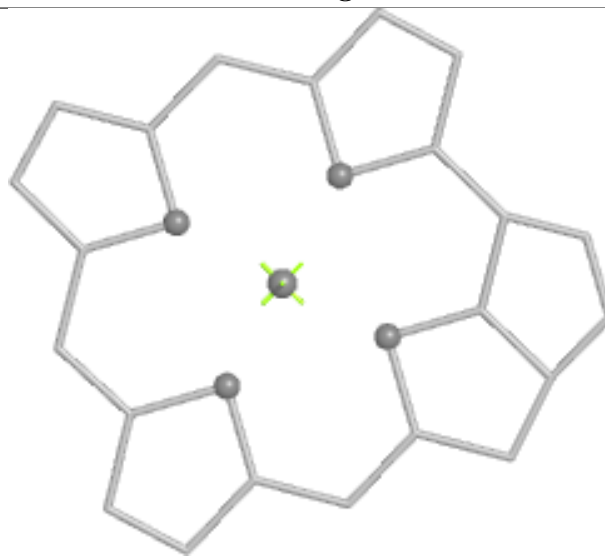
Bond lengths



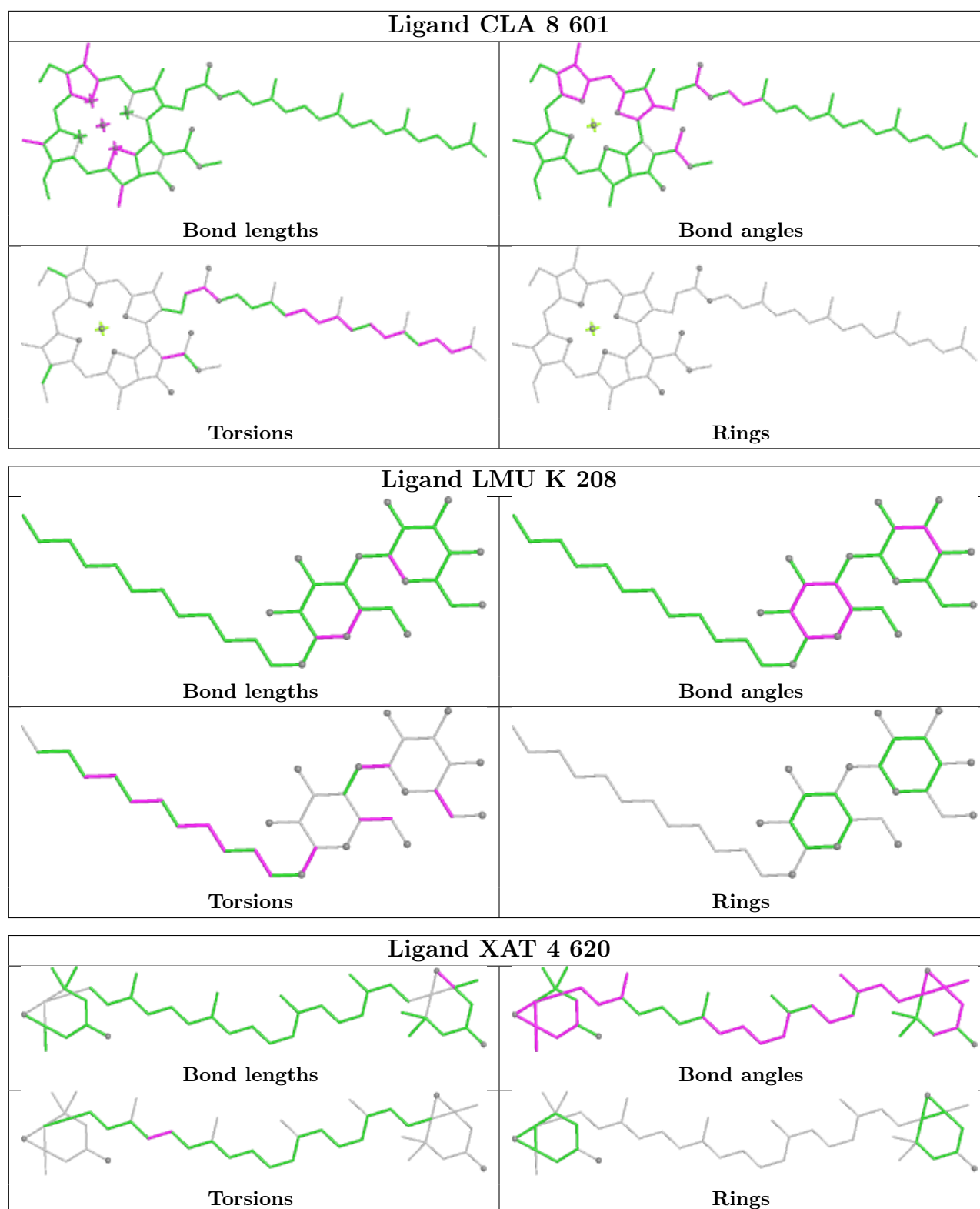
Bond angles

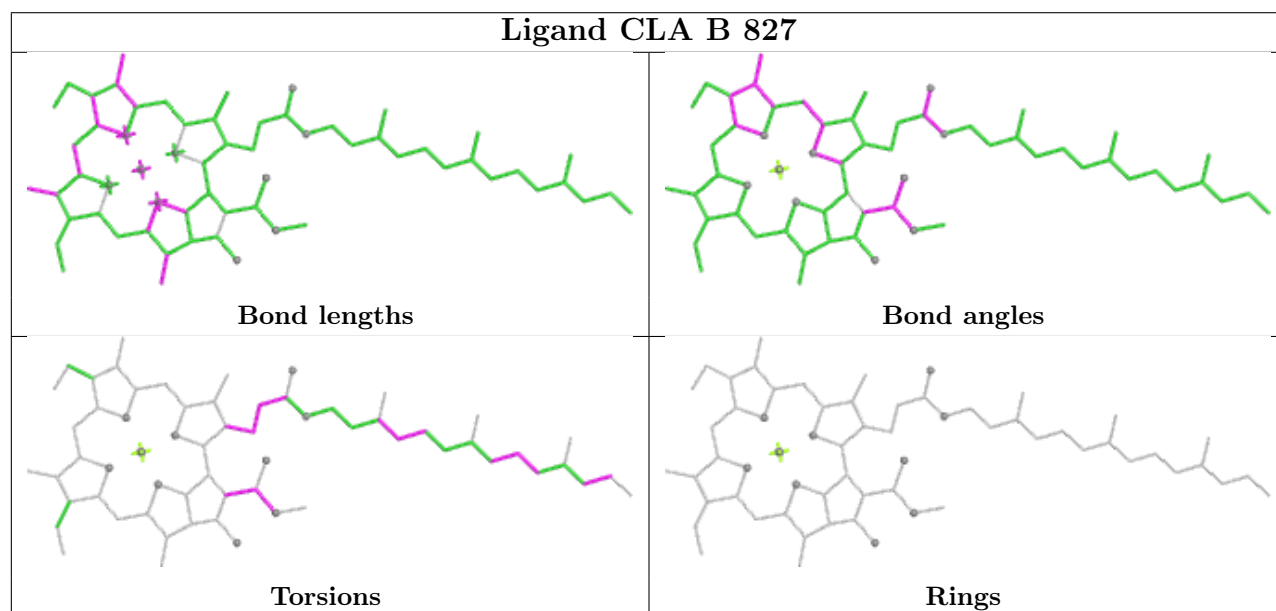
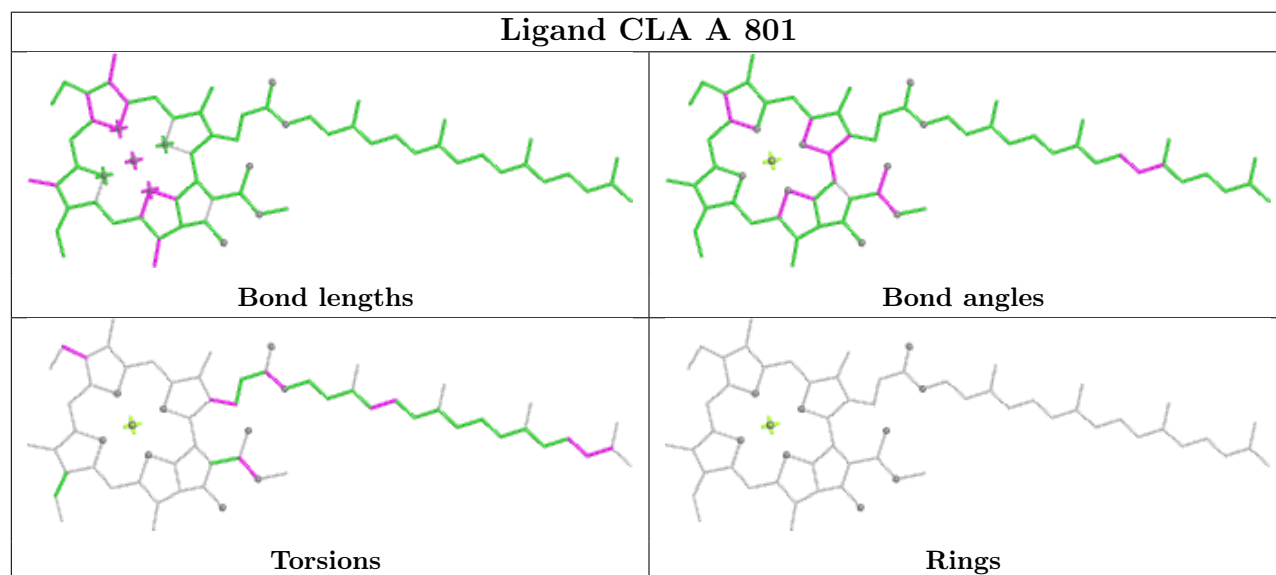
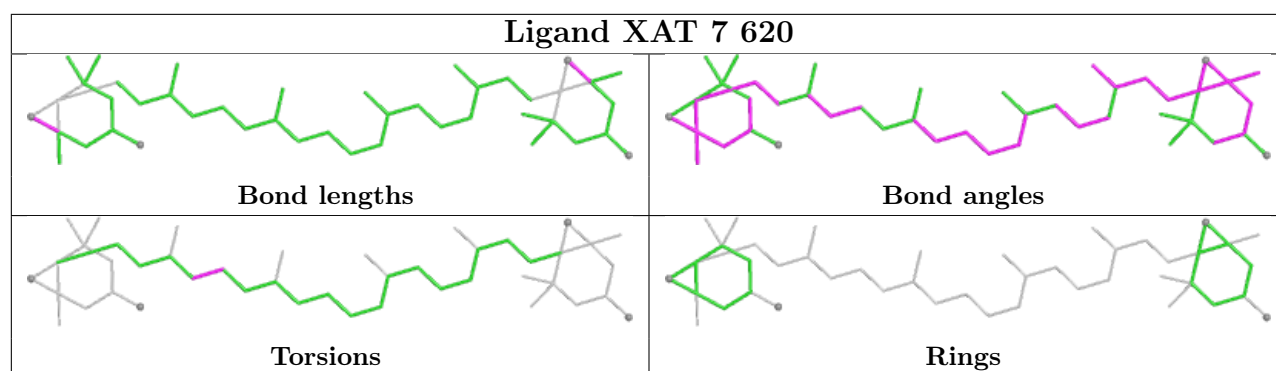


Torsions

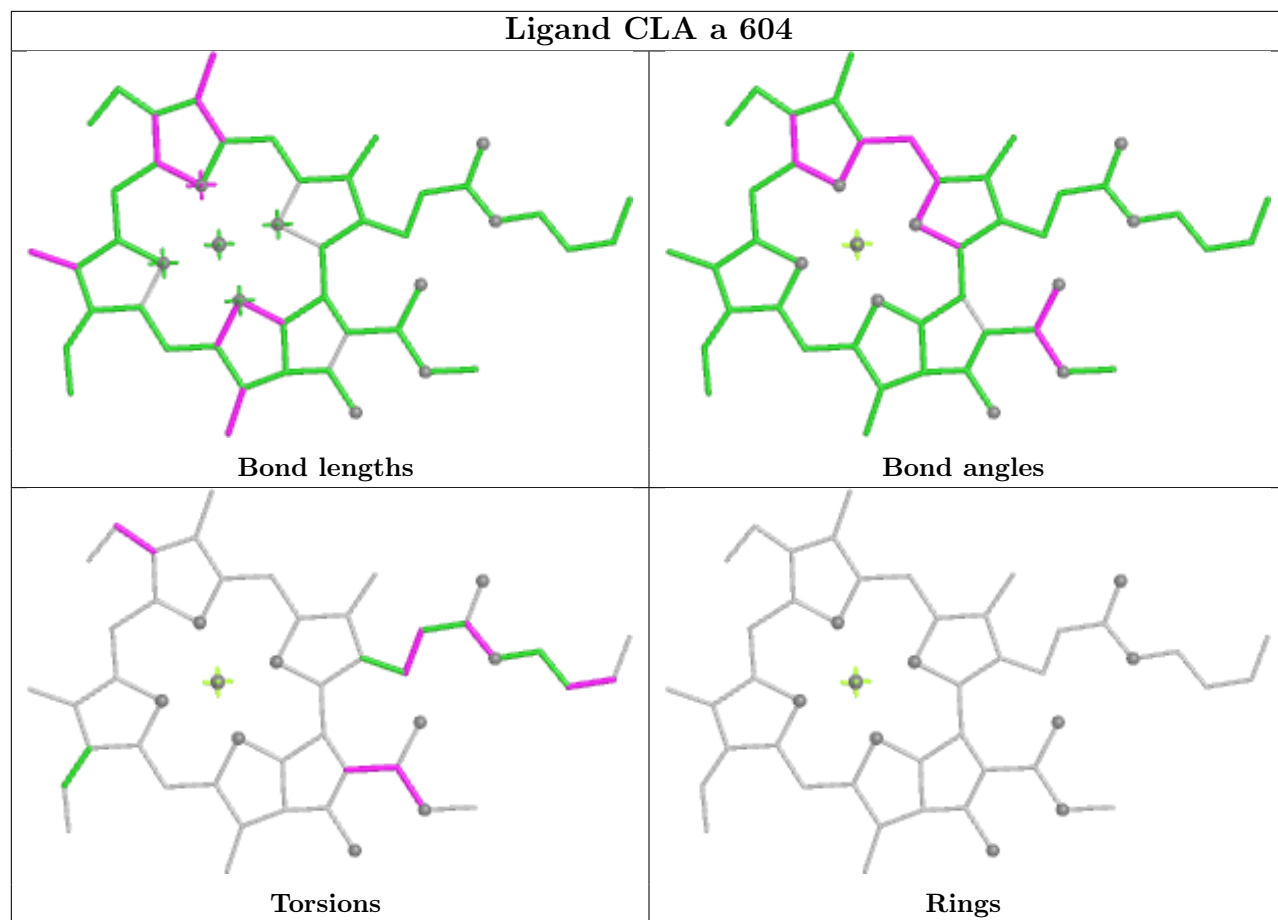


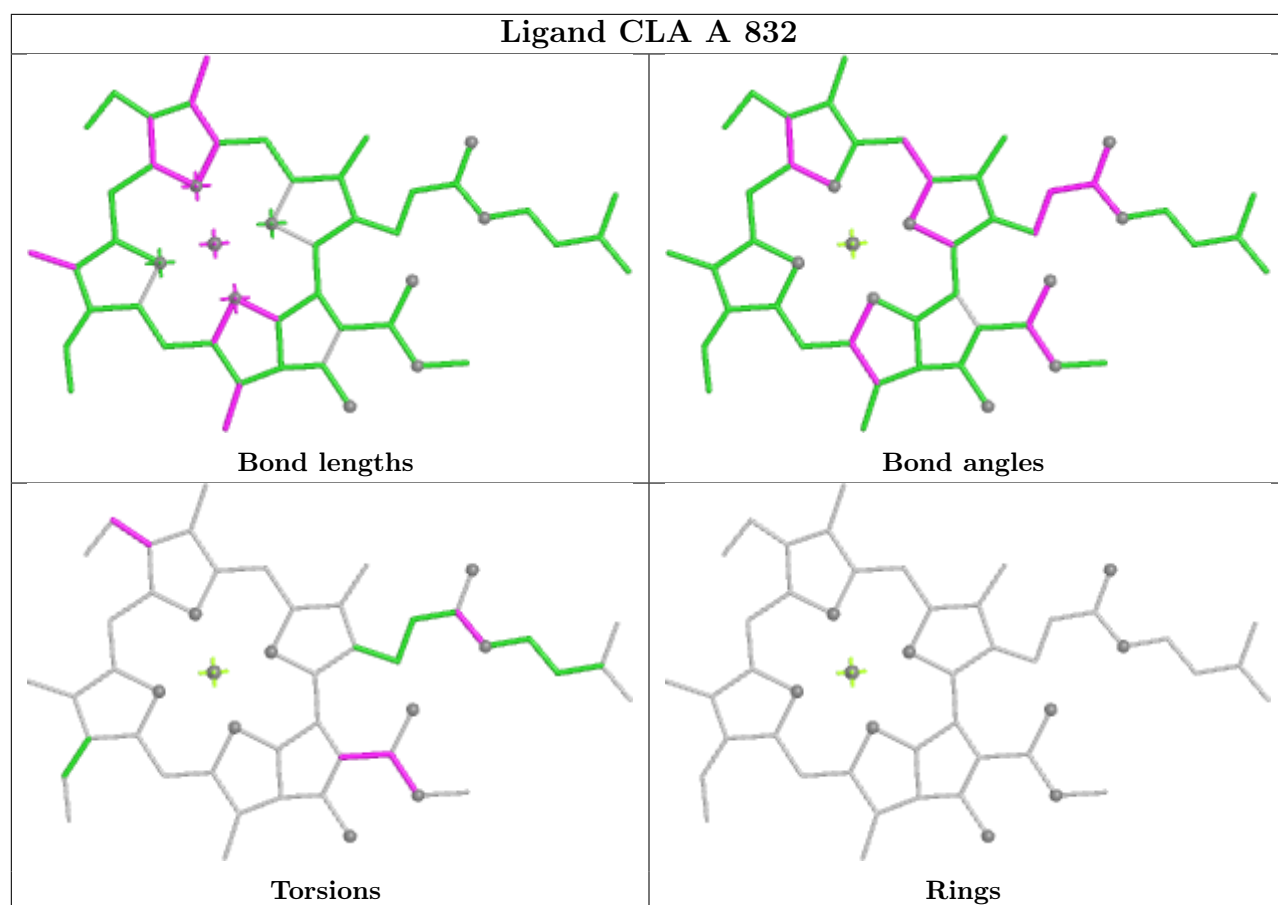
Rings



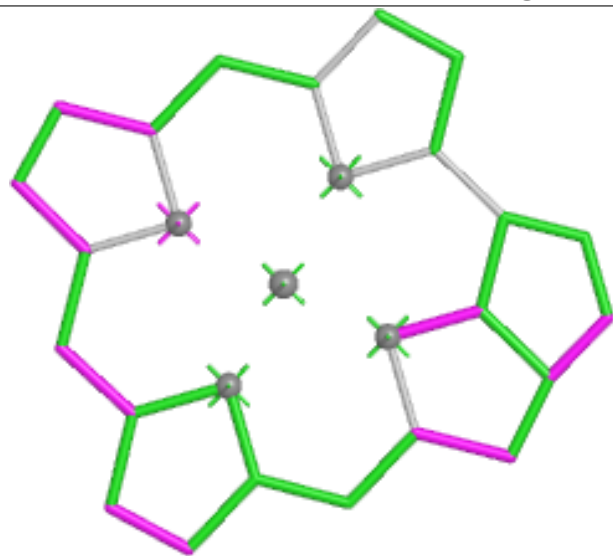


Ligand CLA a 604

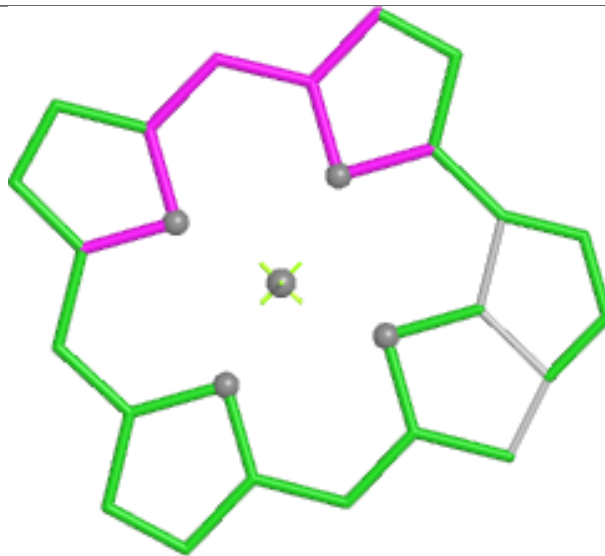




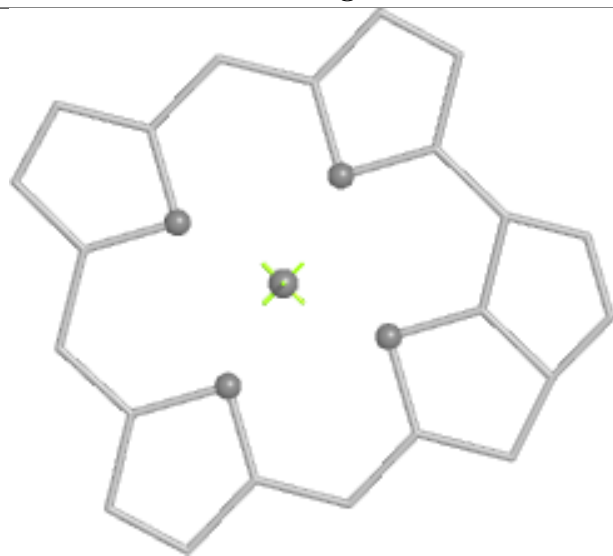
Ligand CLA 9 601



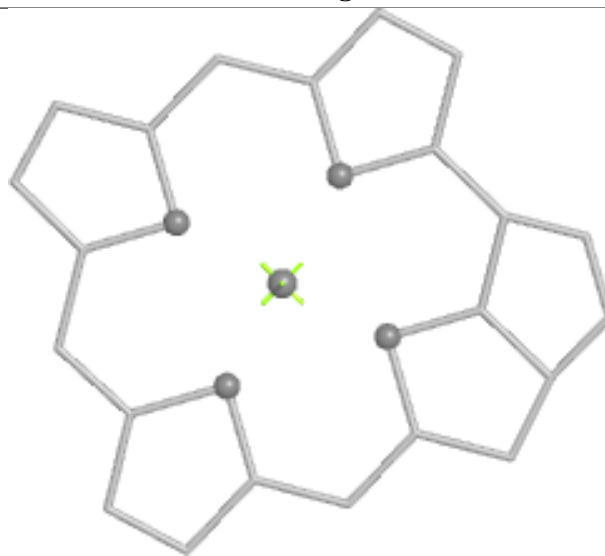
Bond lengths



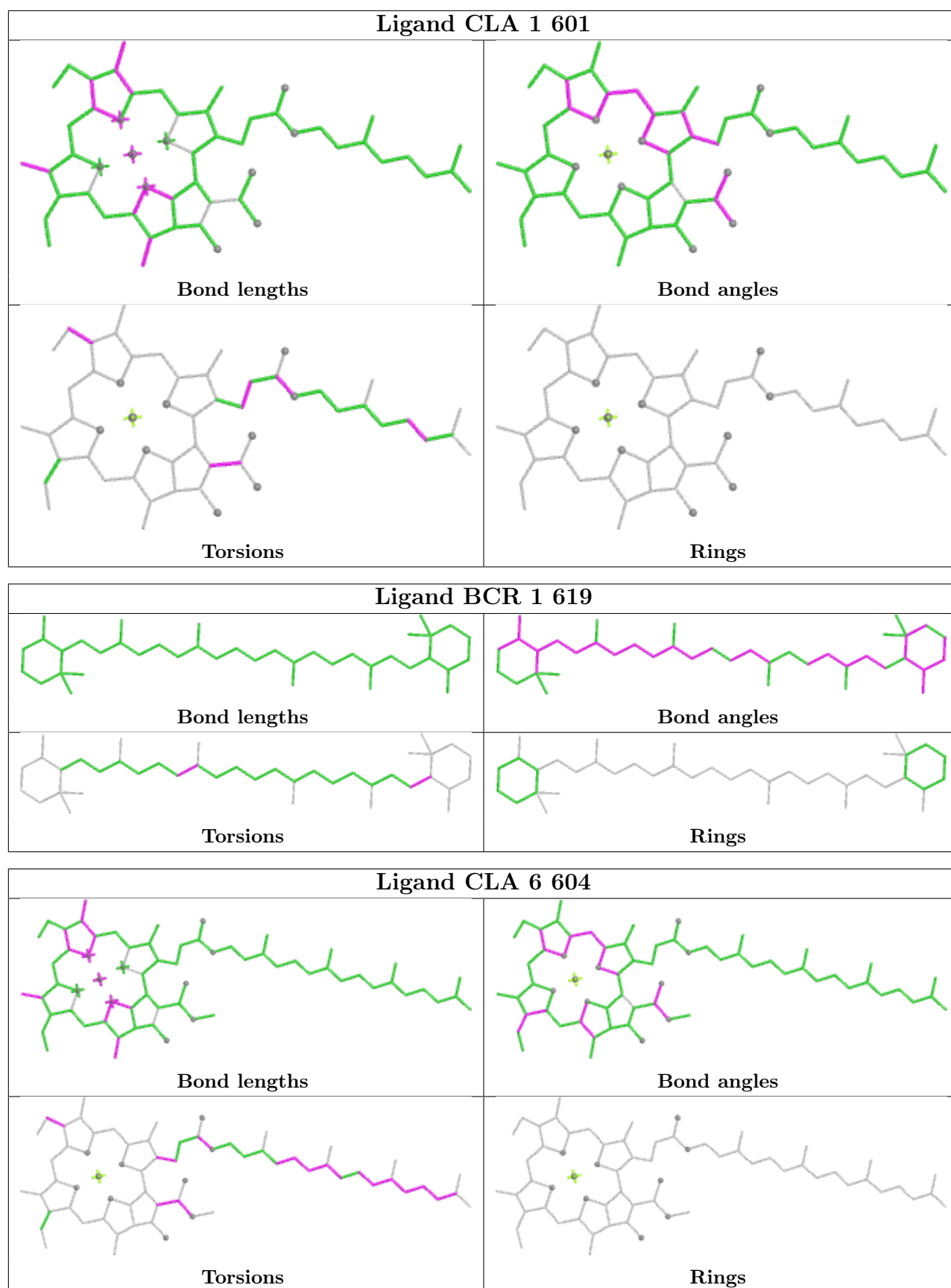
Bond angles

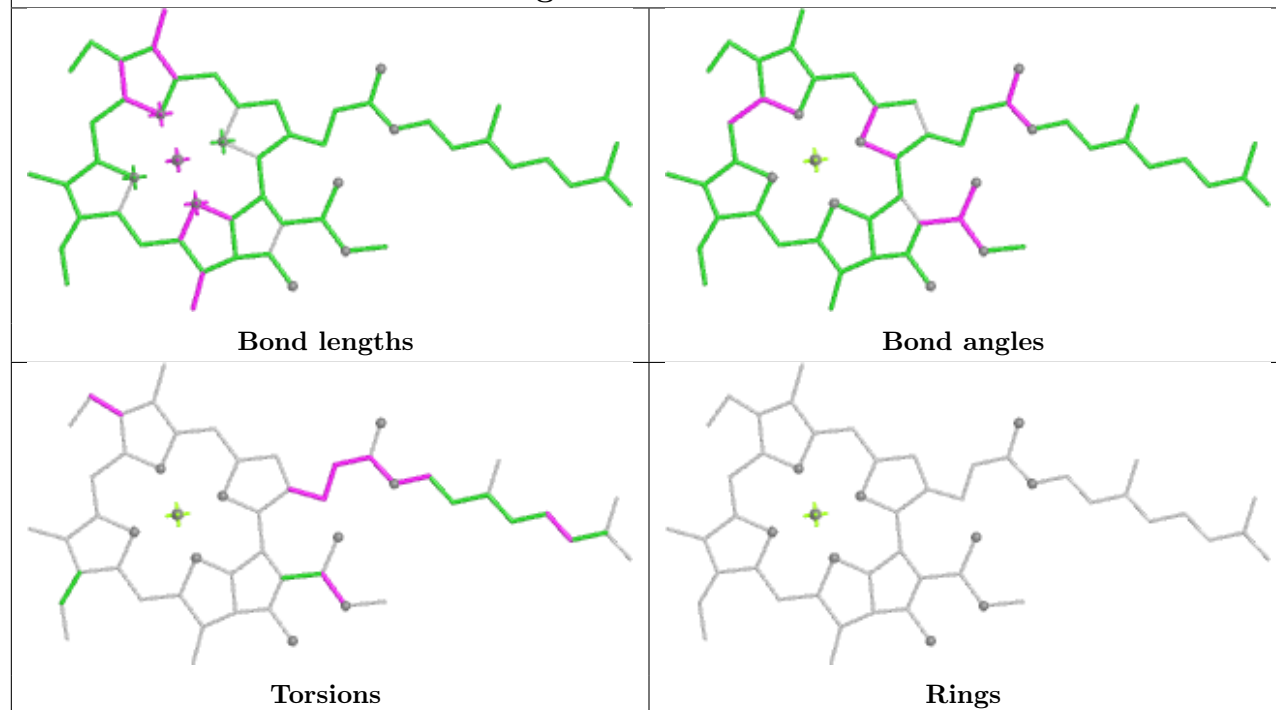
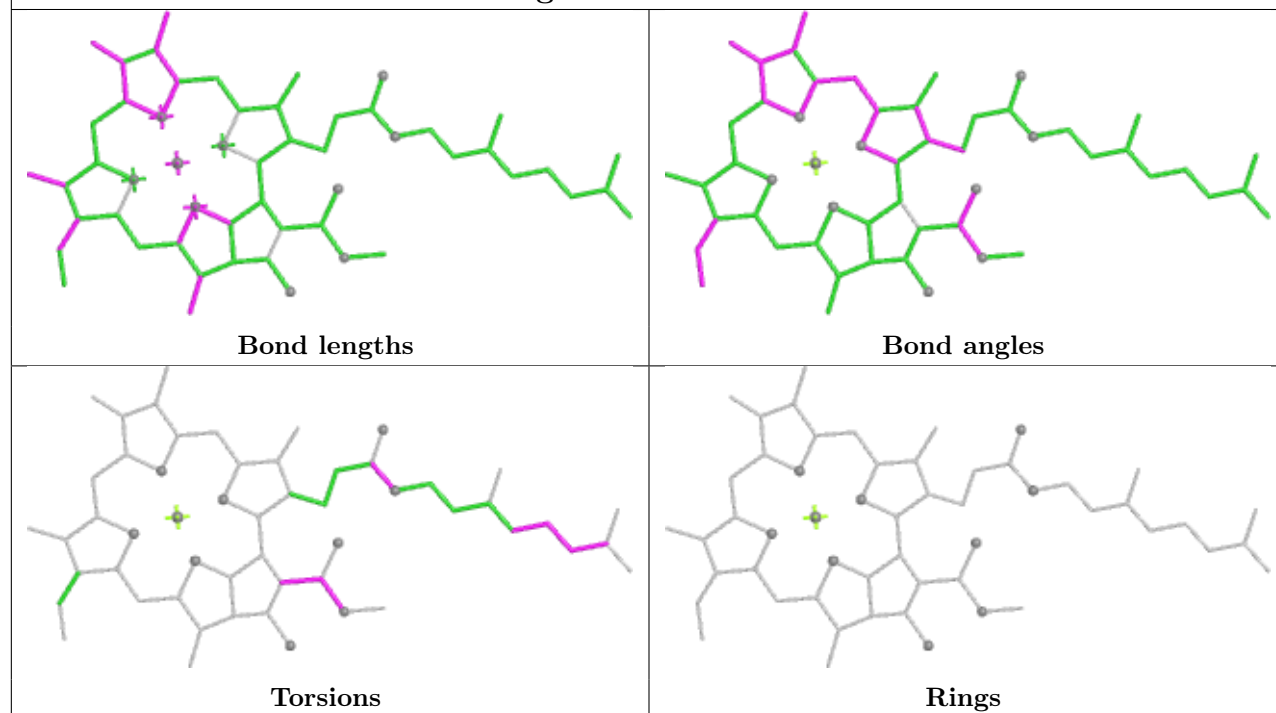


Torsions

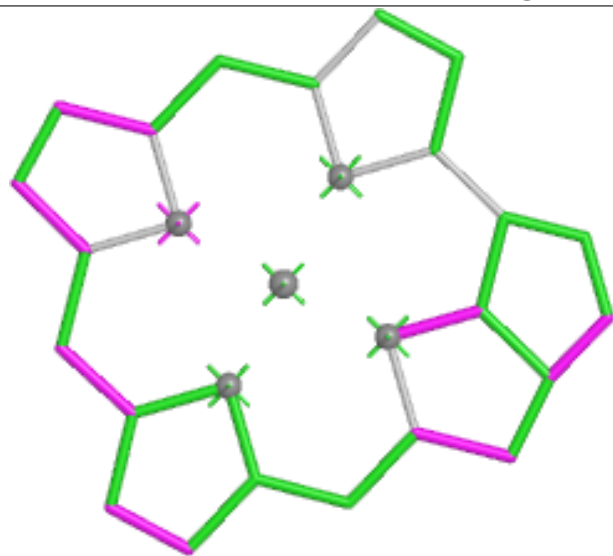


Rings

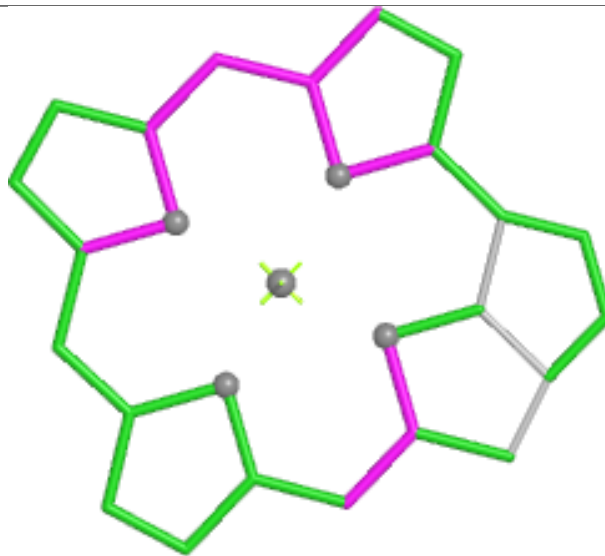


Ligand CLA a 614**Ligand CLA 5 603**

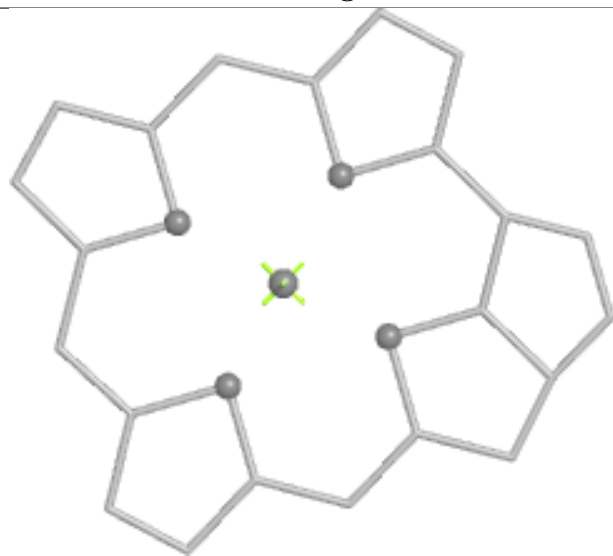
Ligand CLA 2 613



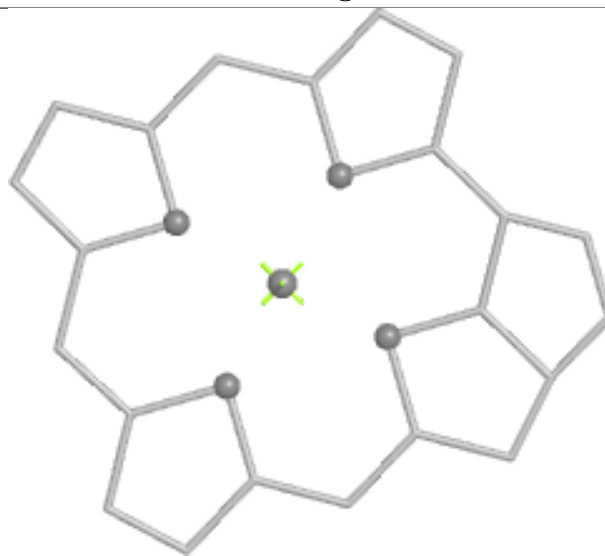
Bond lengths



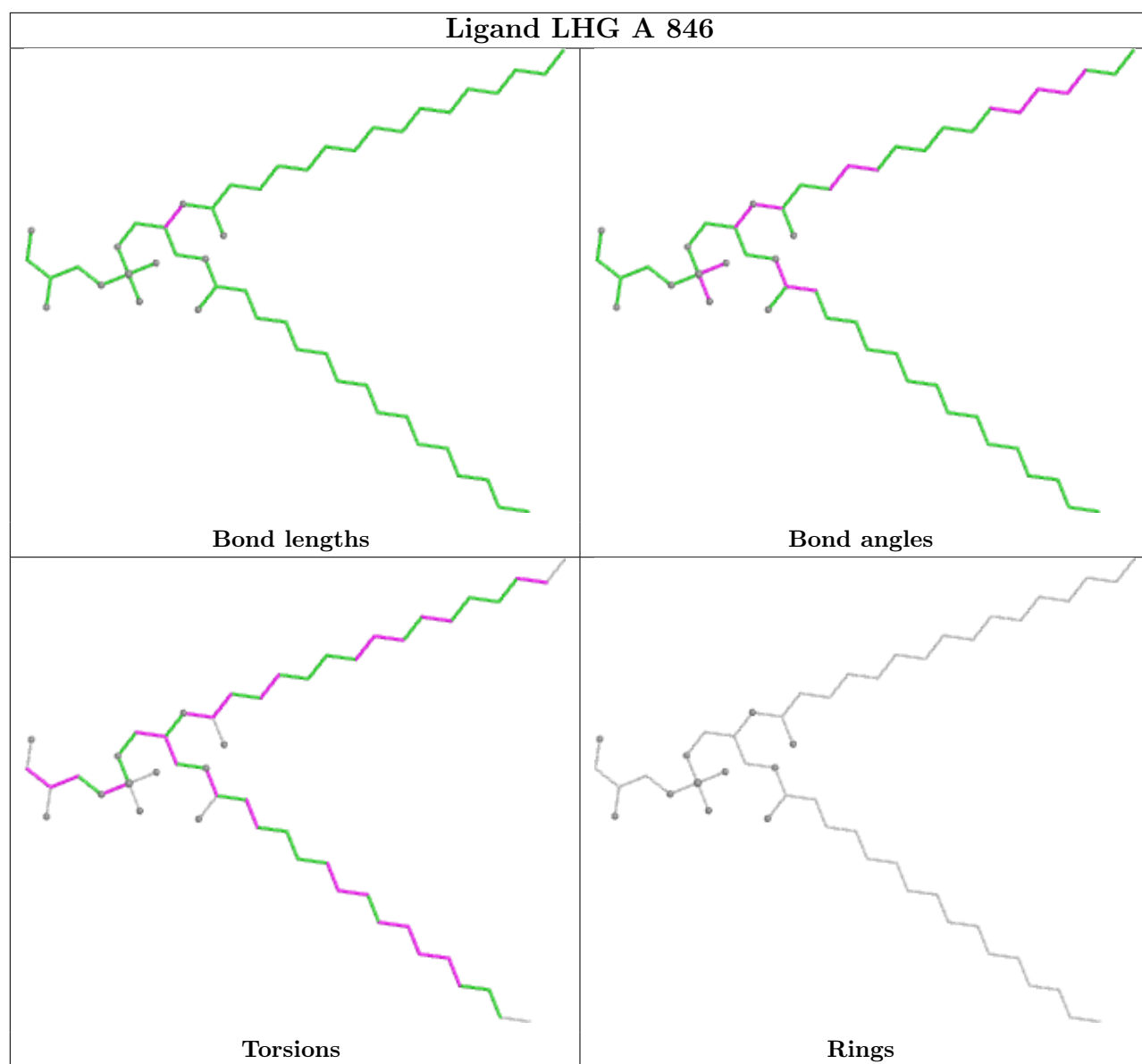
Bond angles



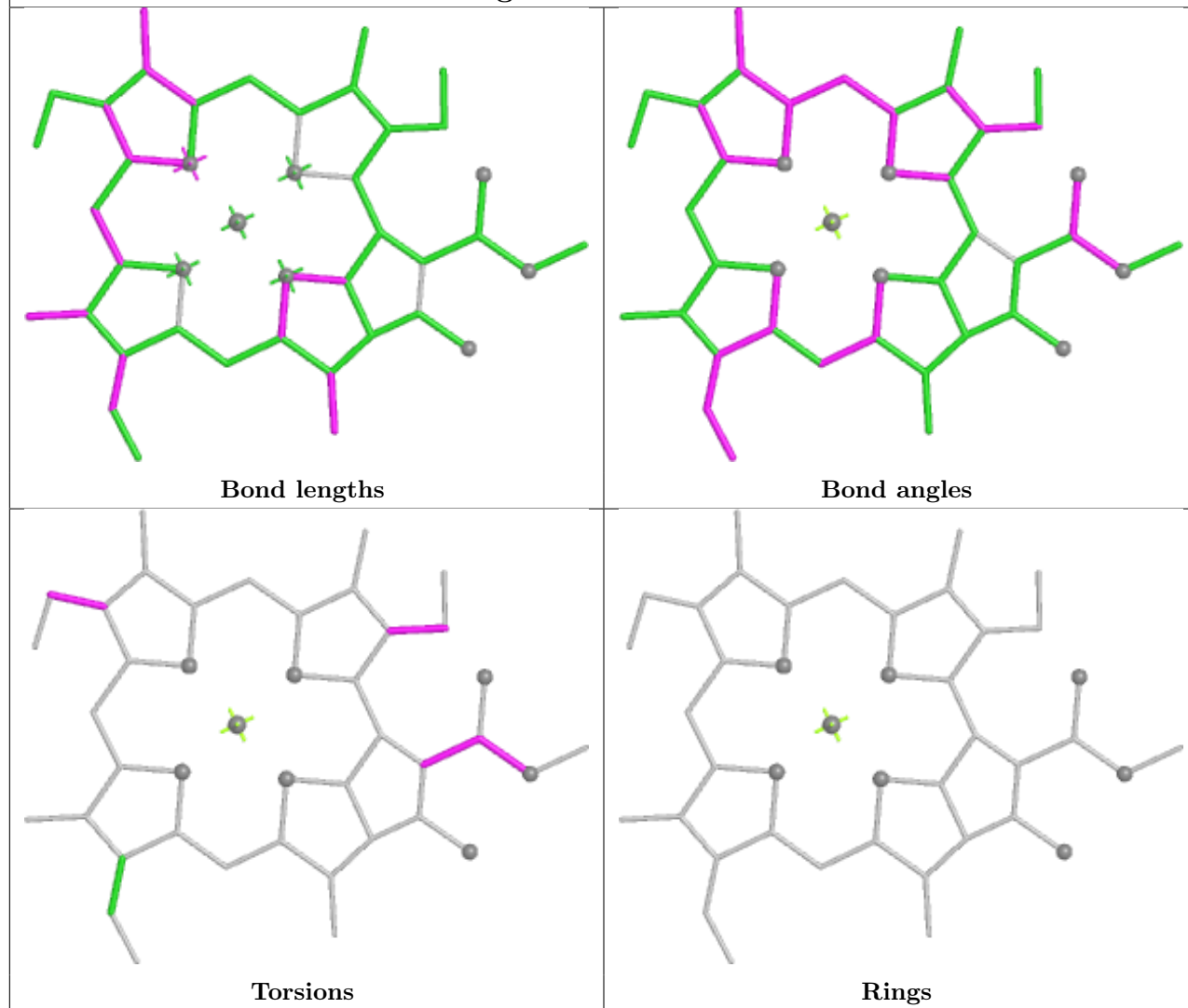
Torsions



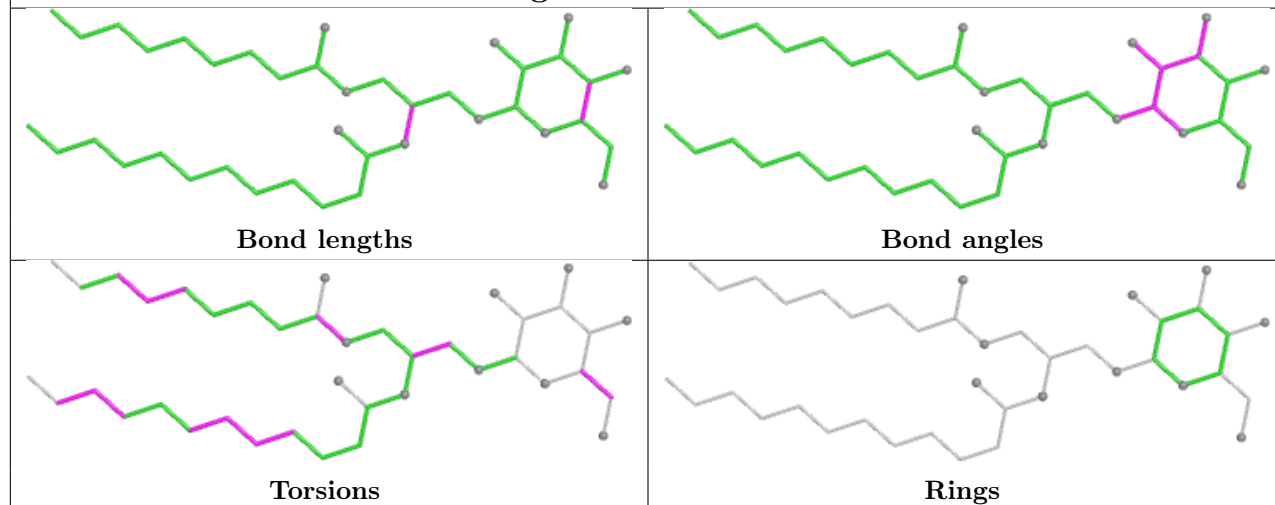
Rings

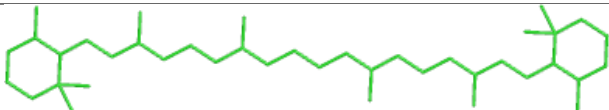
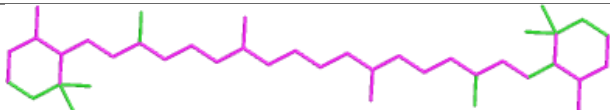
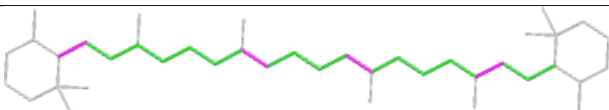
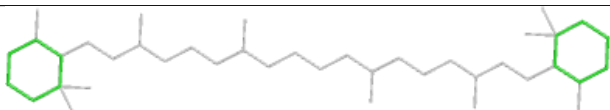


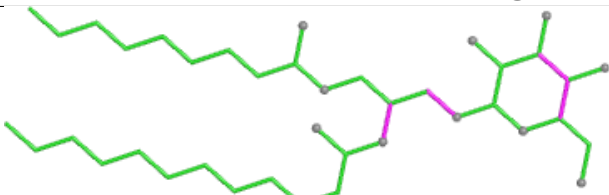
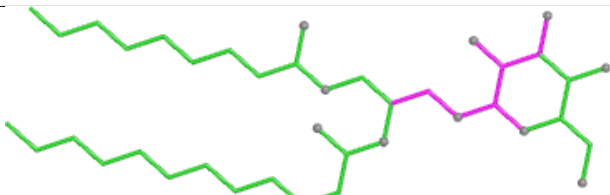
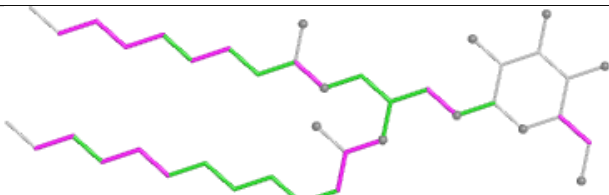
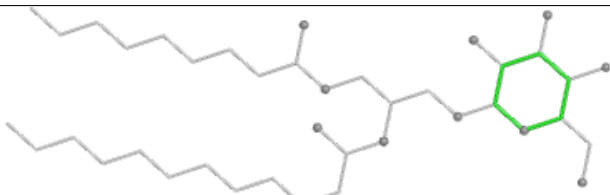
Ligand CLA F 303

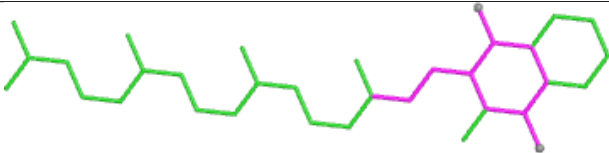
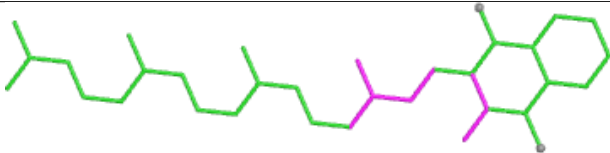
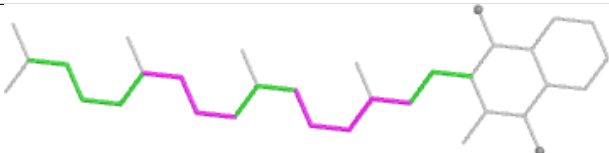
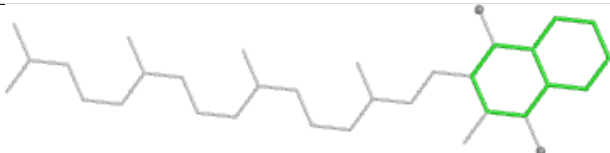


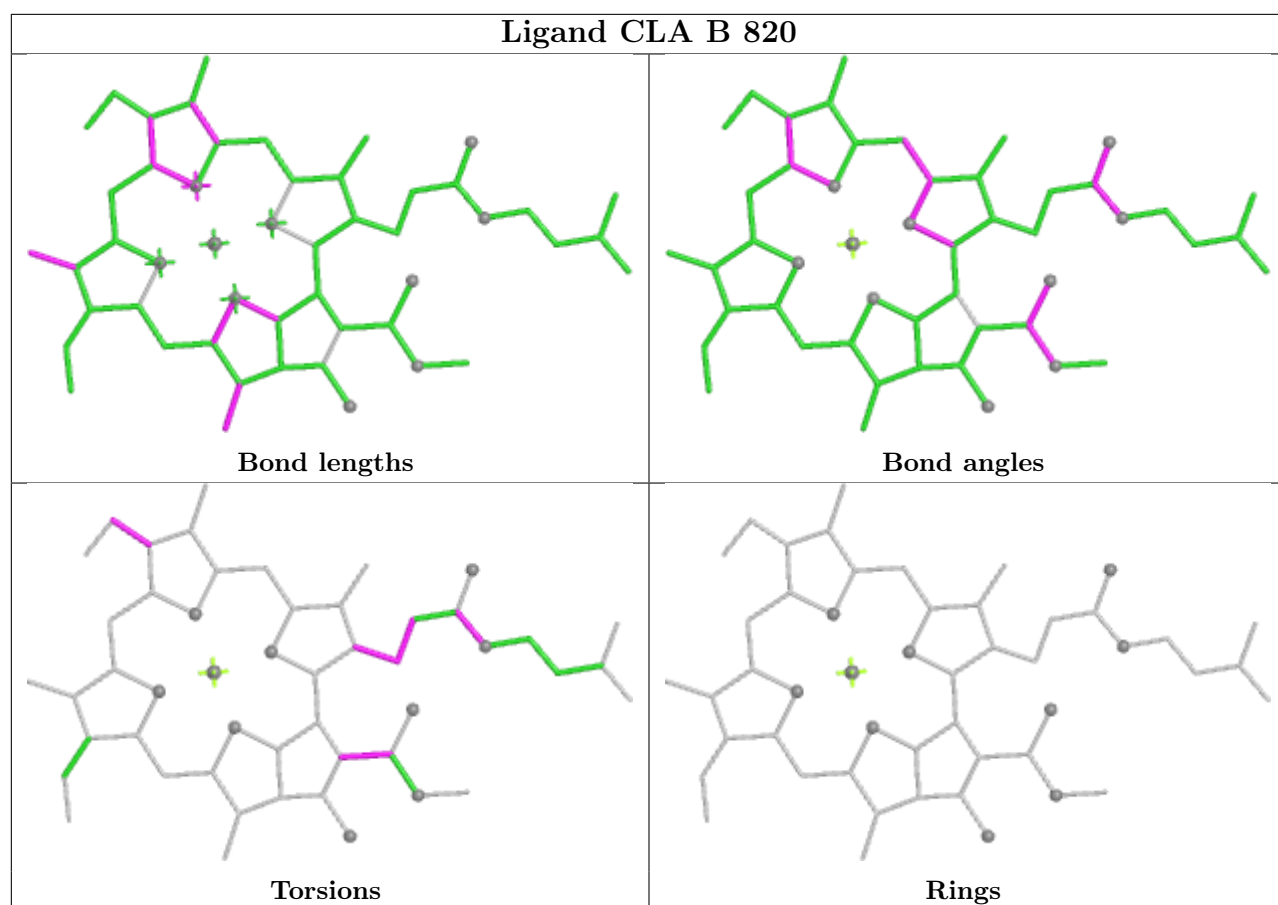
Ligand LMG 5 627



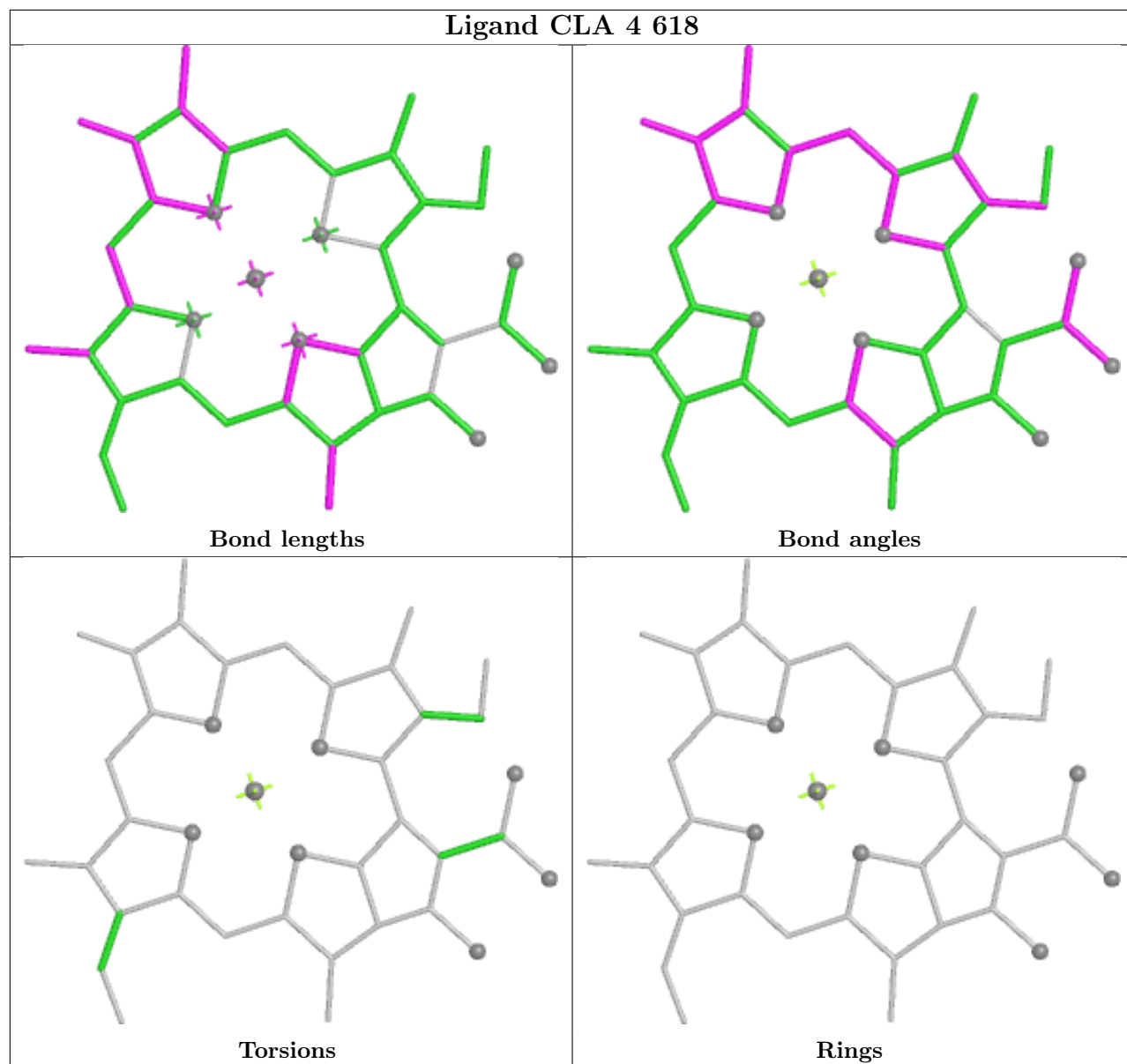
Ligand BCR 3 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG 4 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

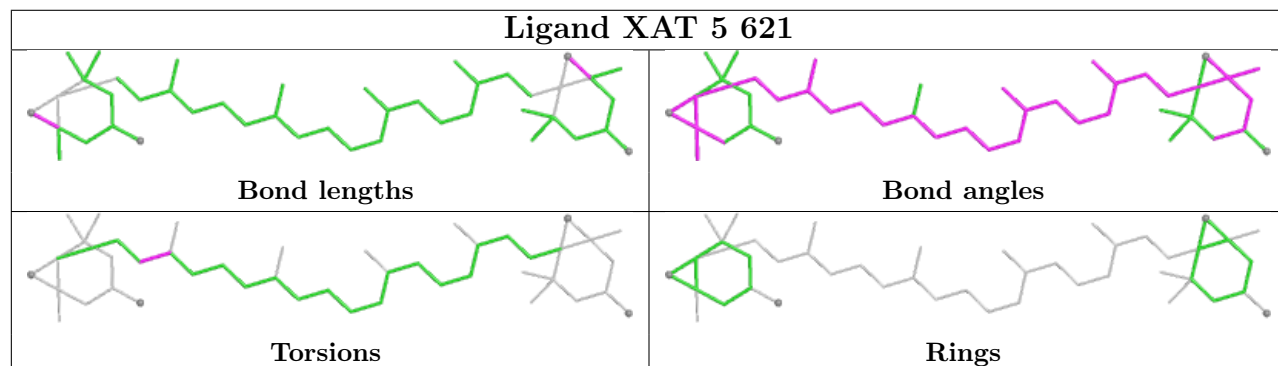
Ligand PQN A 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

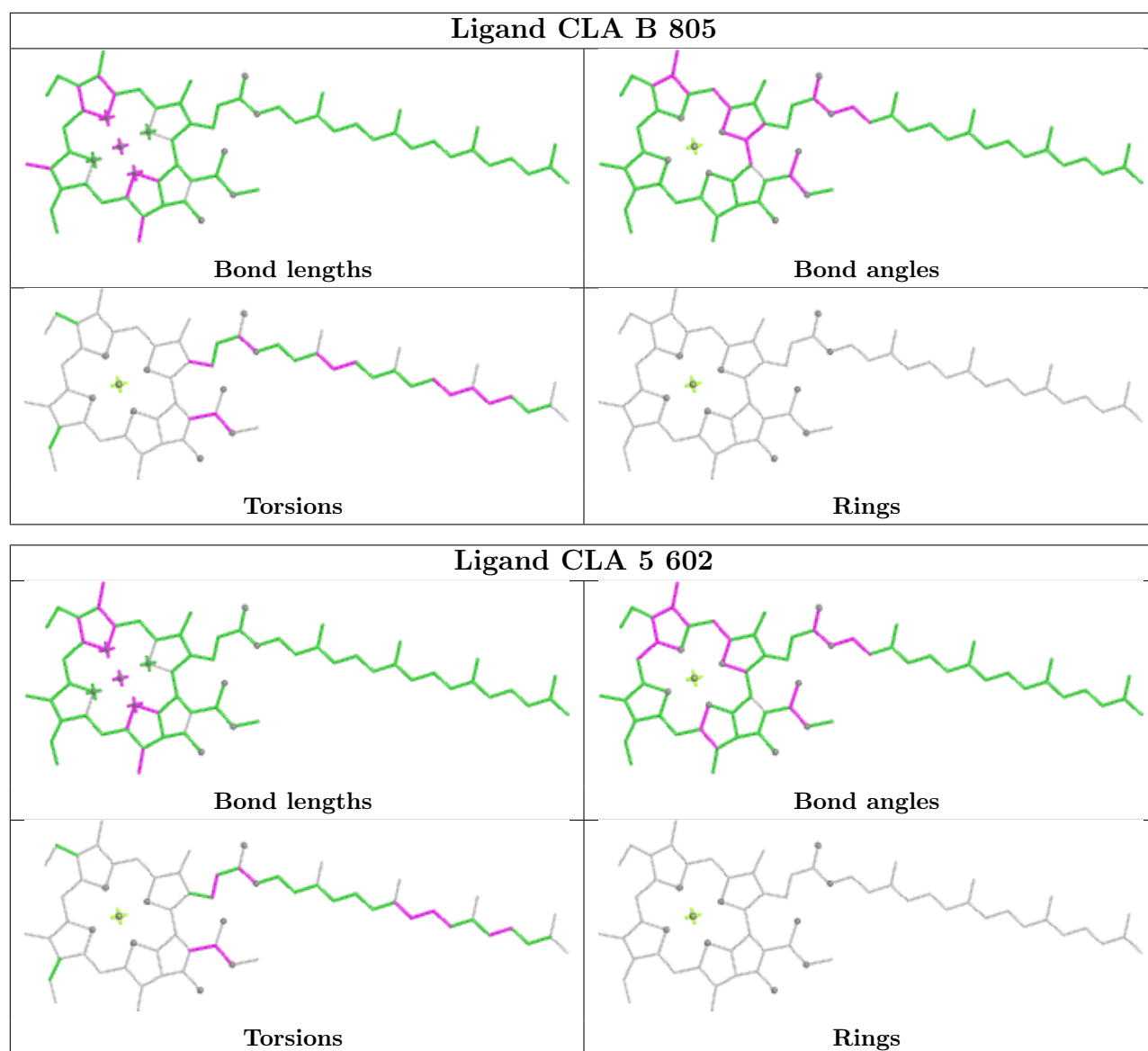


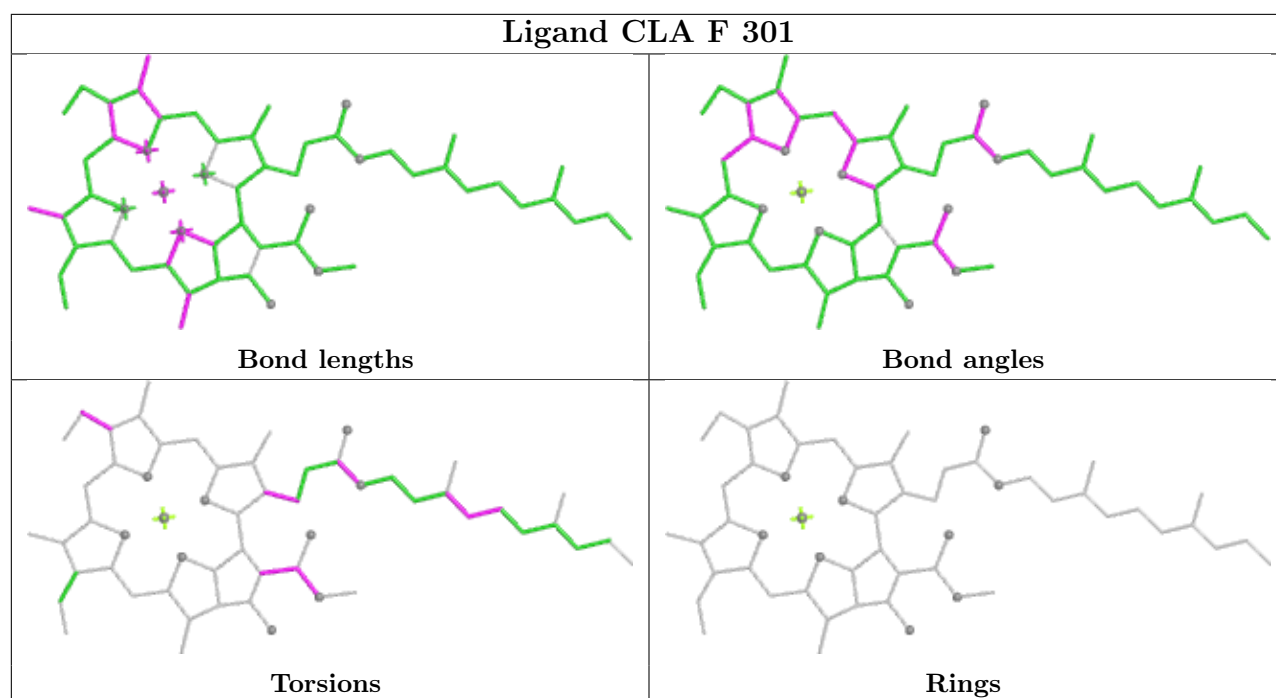
Ligand CLA 4 618



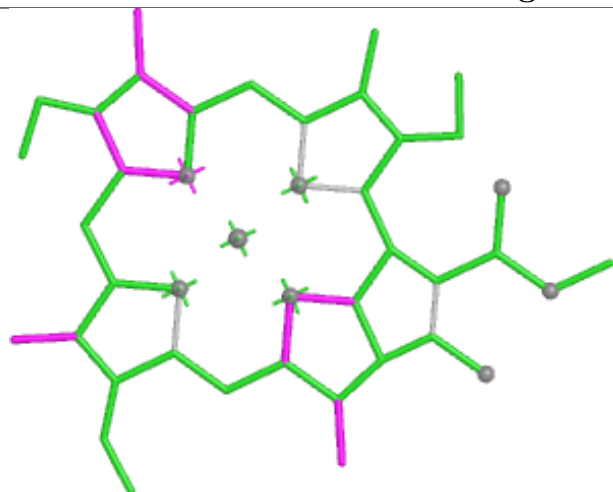
Ligand XAT 5 621



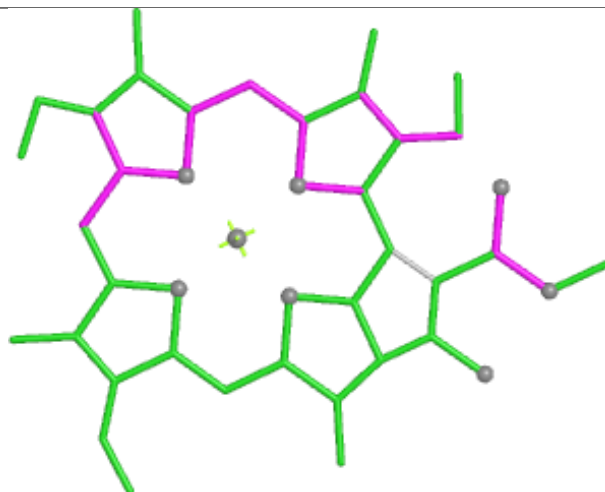




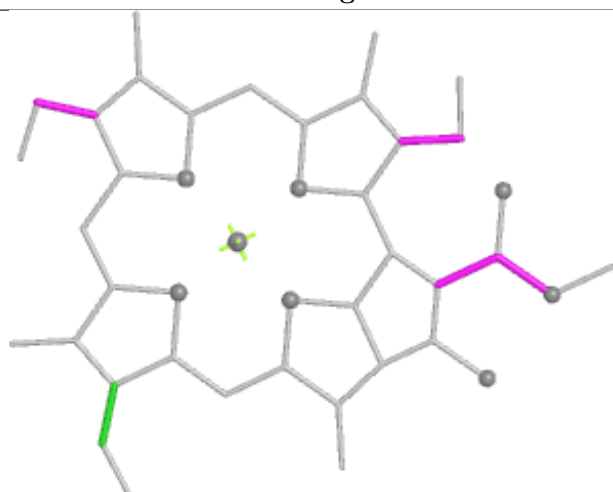
Ligand CLA 4 611



Bond lengths



Bond angles

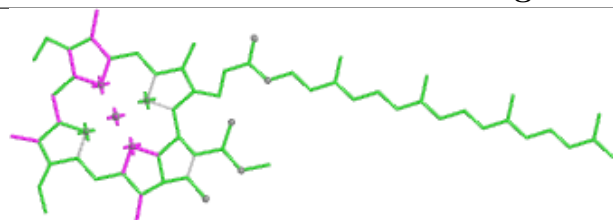


Torsions

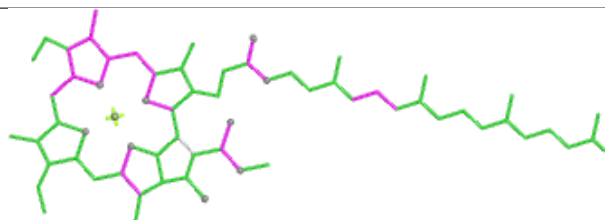


Rings

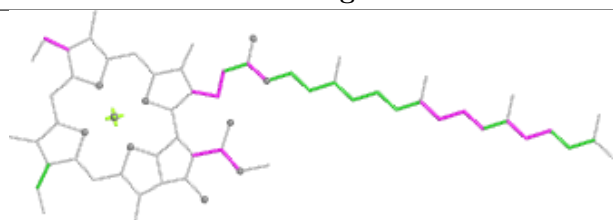
Ligand CLA B 828



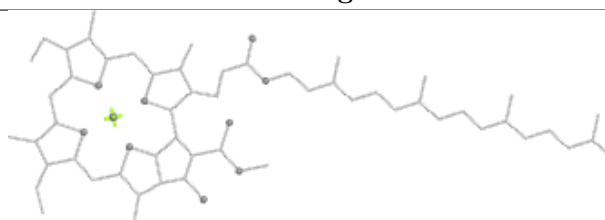
Bond lengths



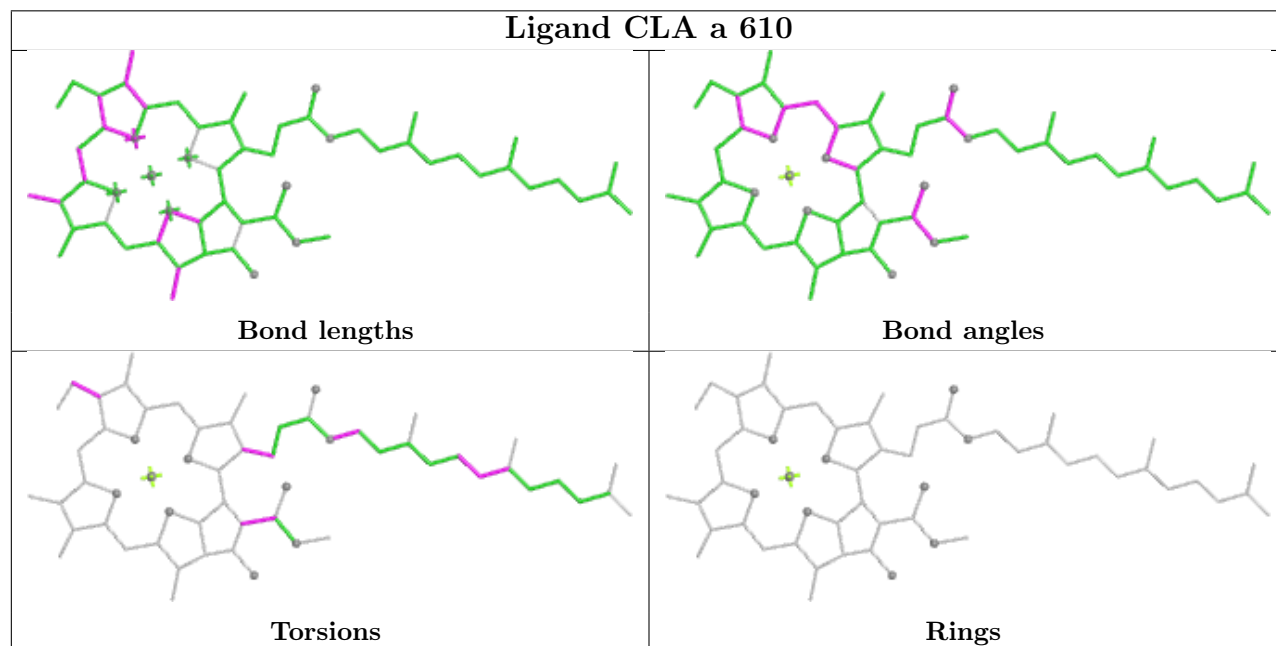
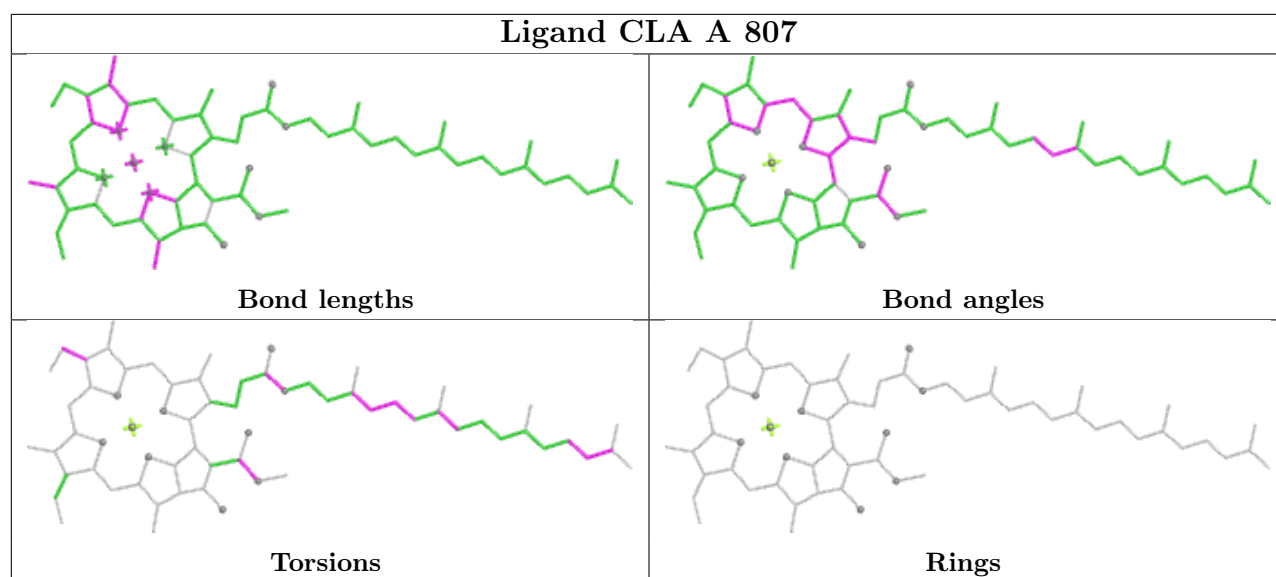
Bond angles

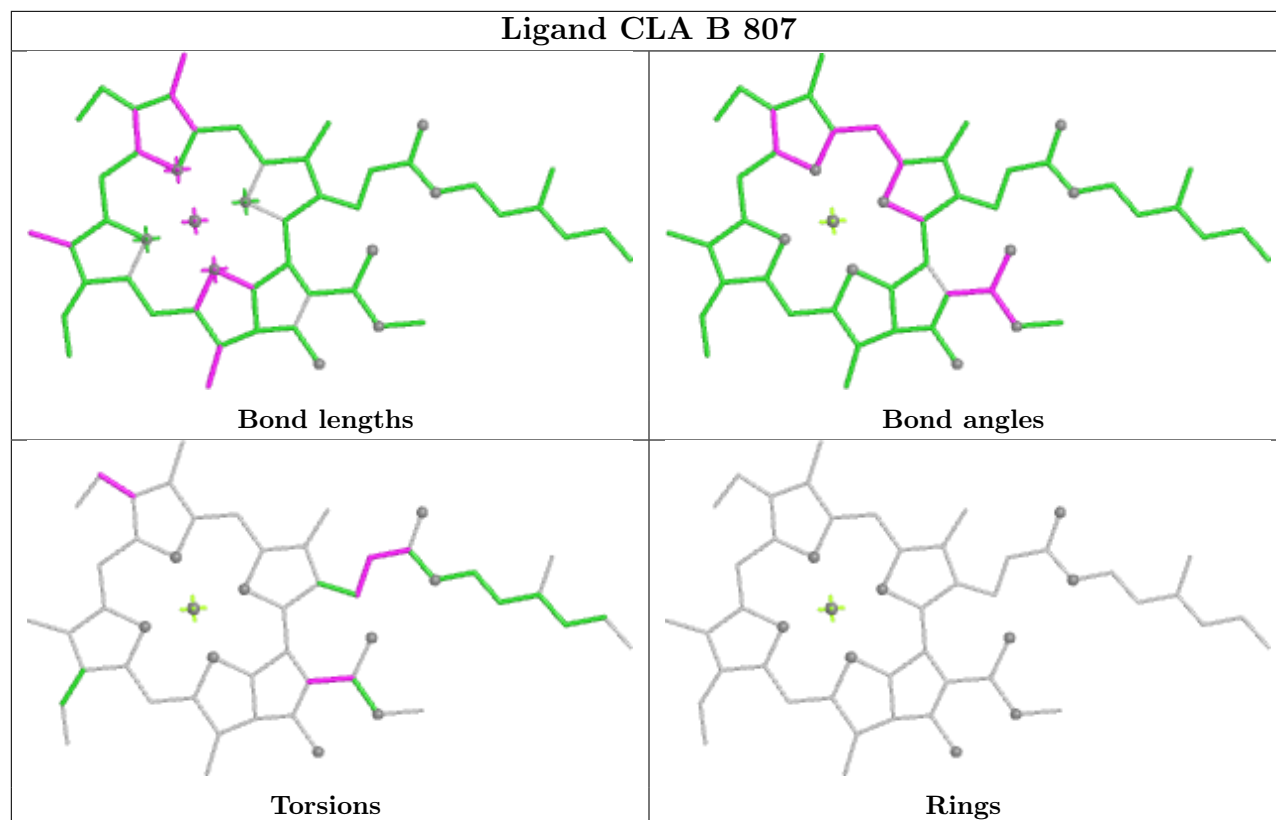


Torsions

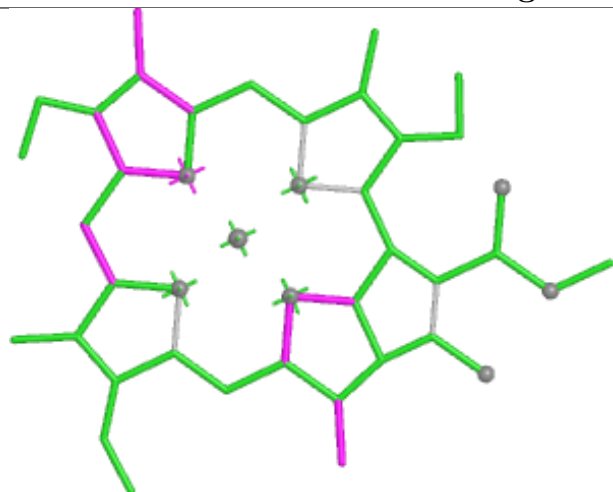


Rings

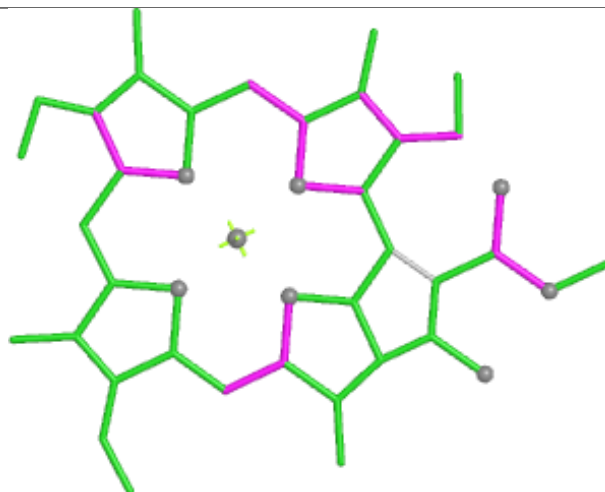




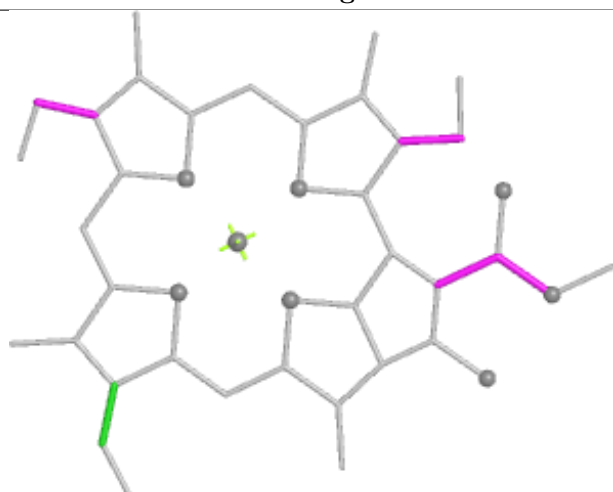
Ligand CLA J 101



Bond lengths



Bond angles

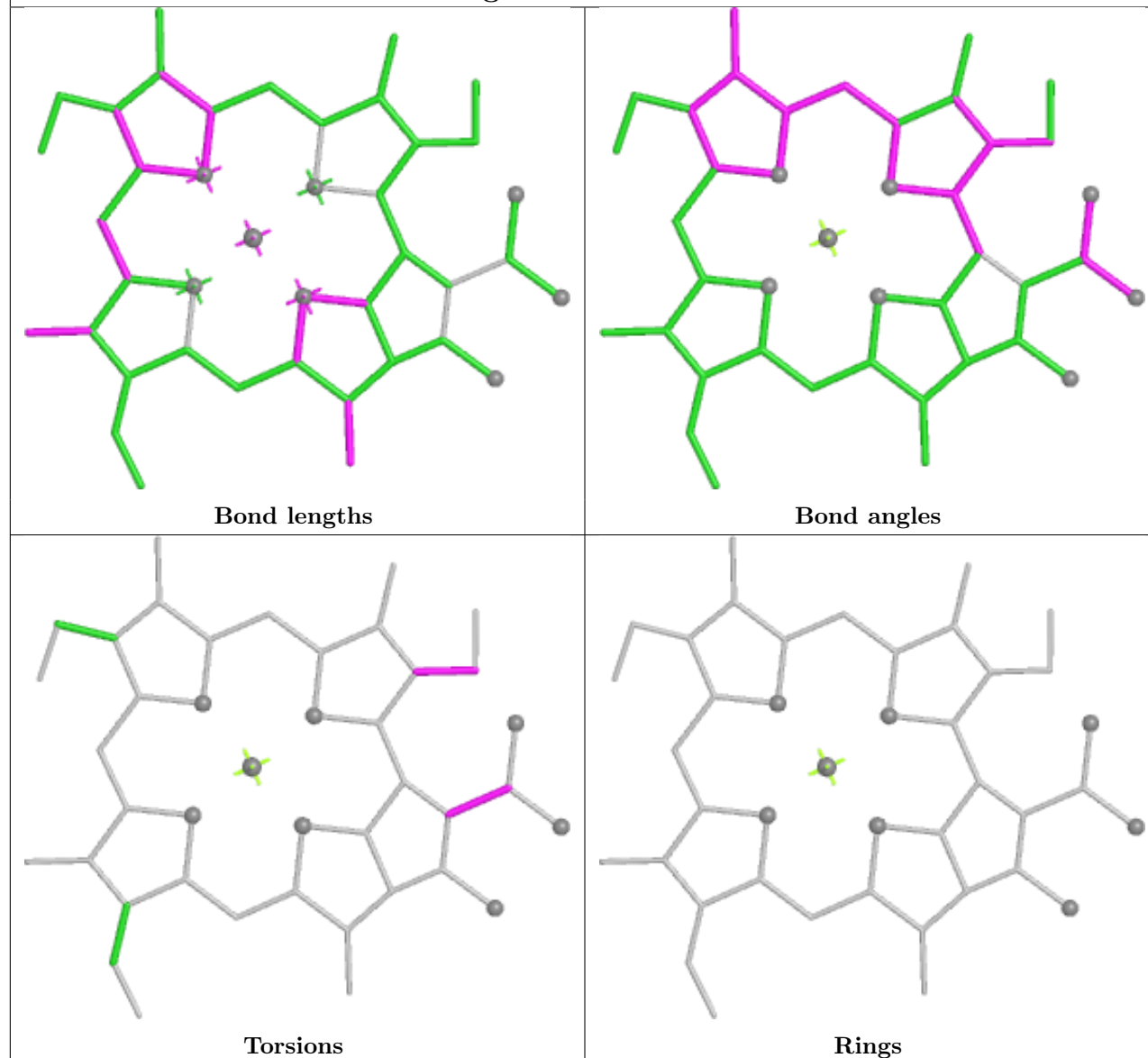


Torsions

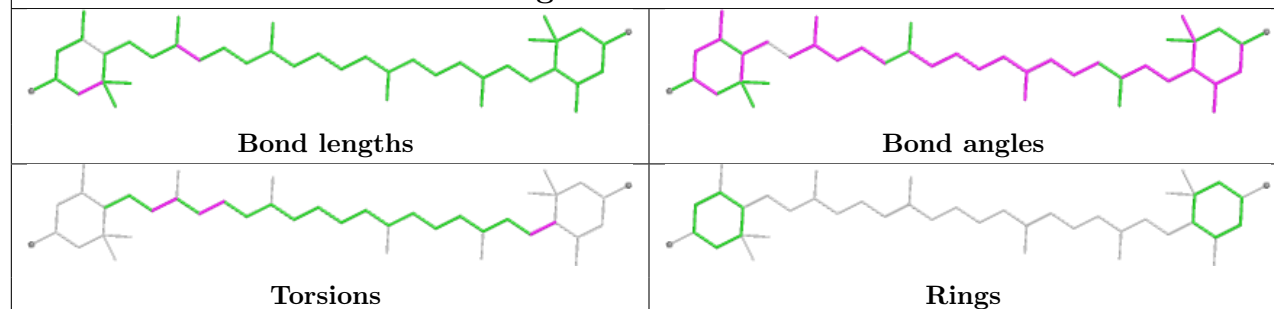


Rings

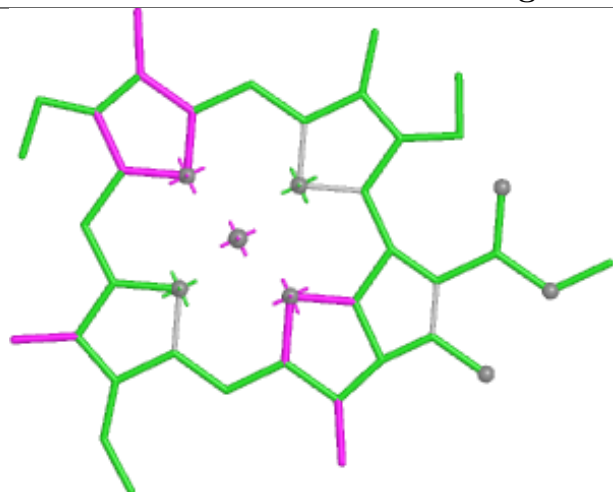
Ligand CLA 5 612



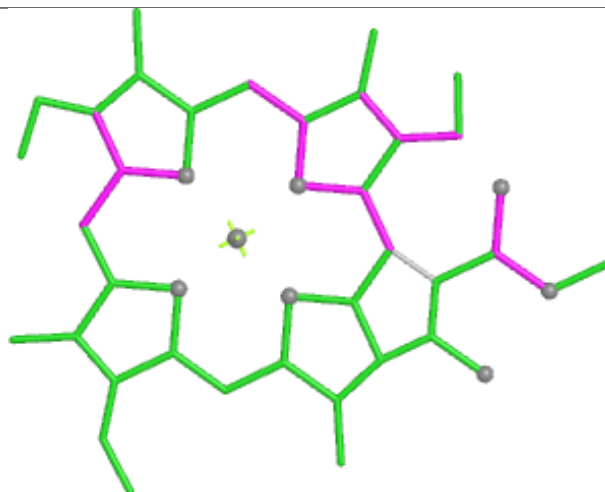
Ligand LUT 7 619



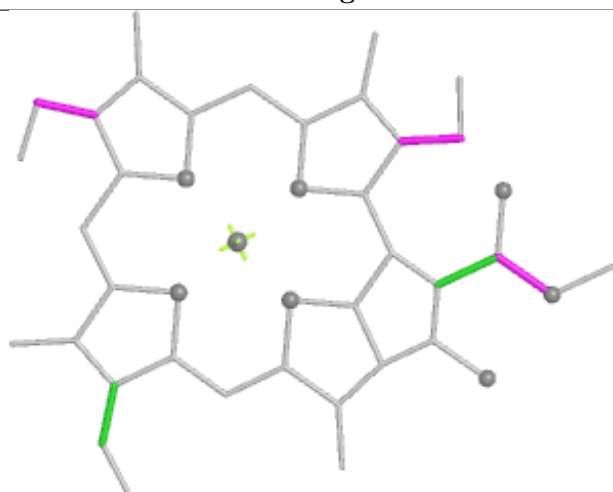
Ligand CLA 7 614



Bond lengths



Bond angles

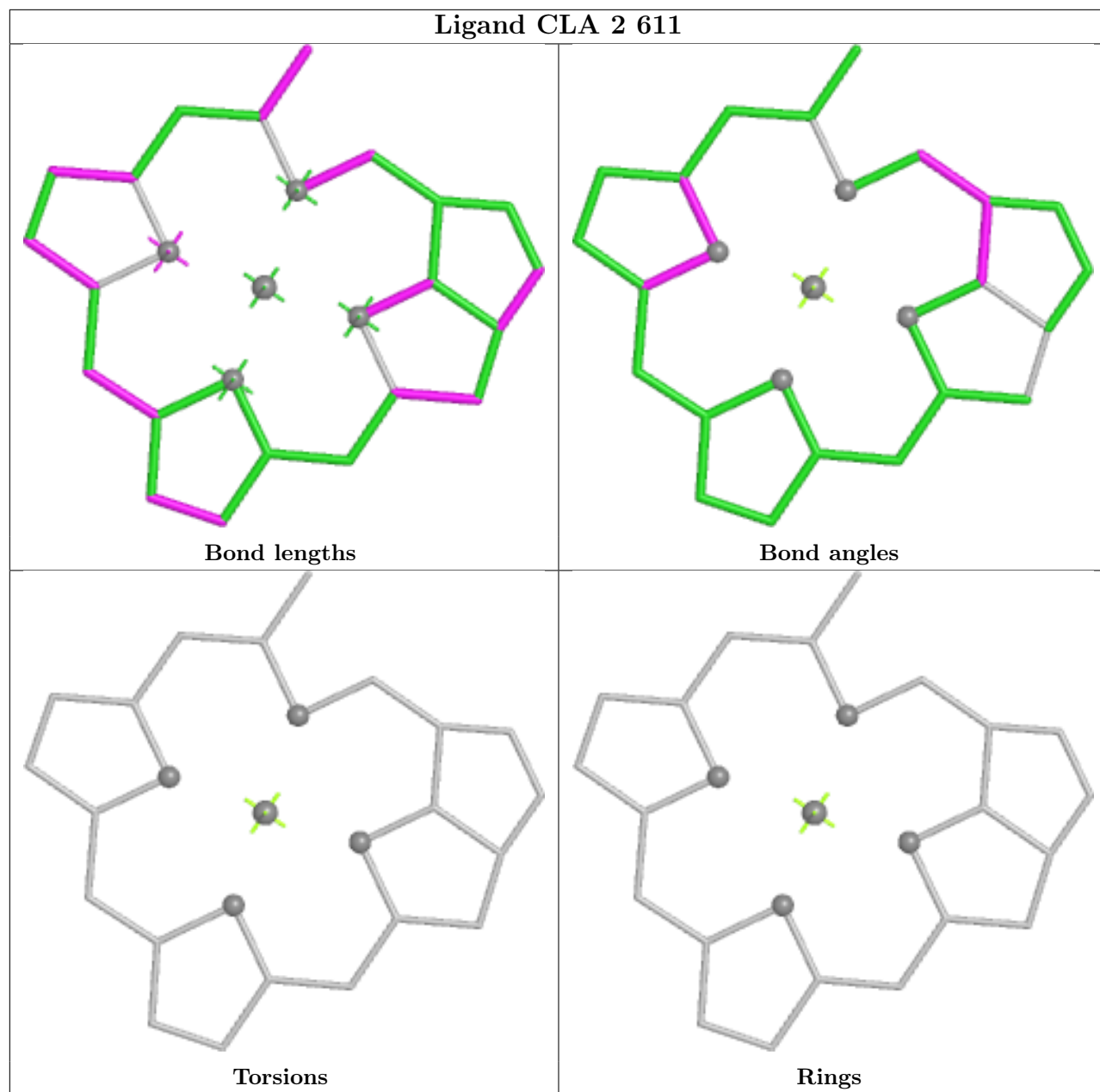


Torsions

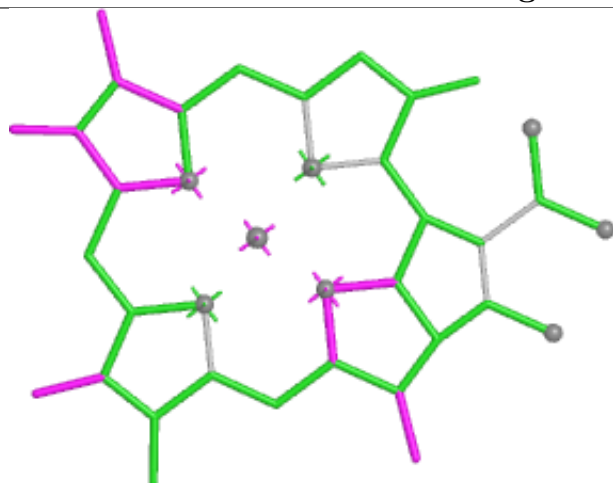


Rings

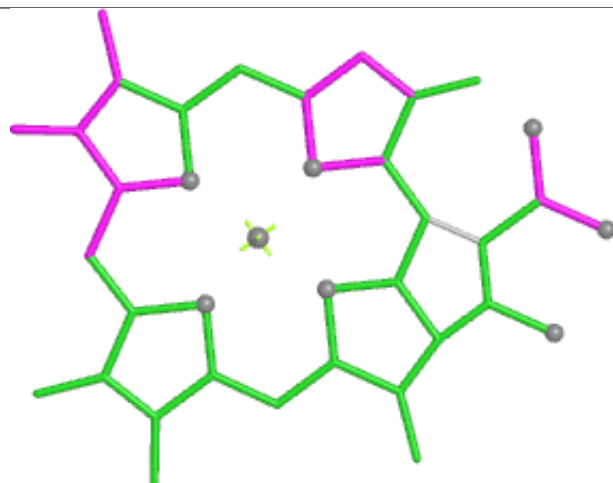
Ligand CLA 2 611



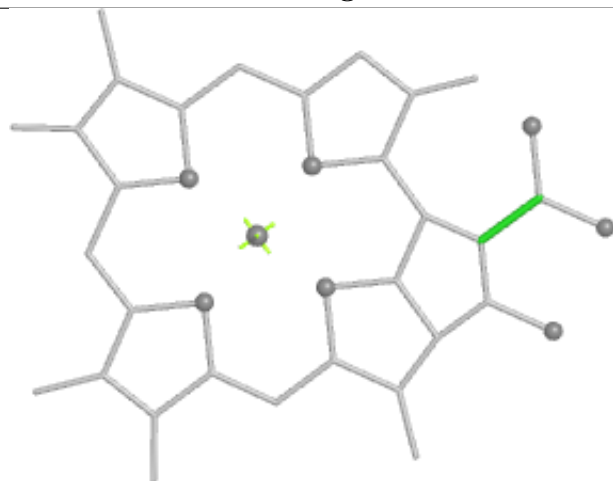
Ligand CLA 1 614



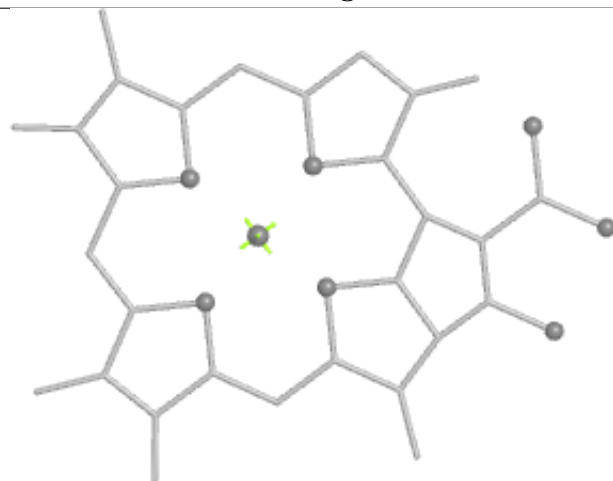
Bond lengths



Bond angles

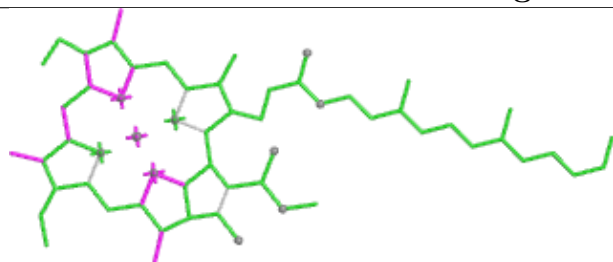


Torsions

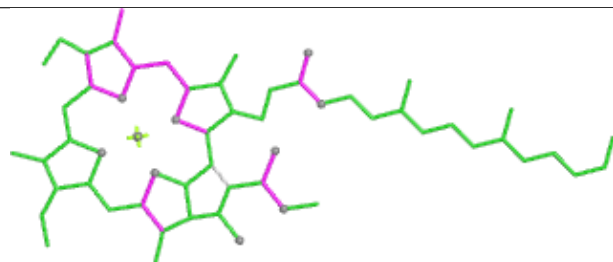


Rings

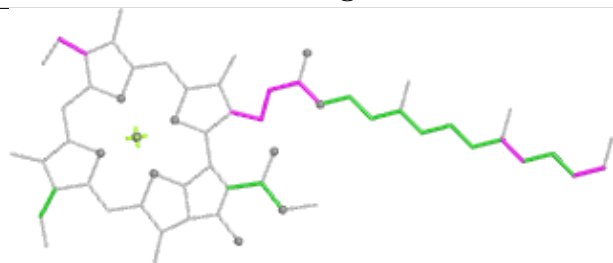
Ligand CLA A 819



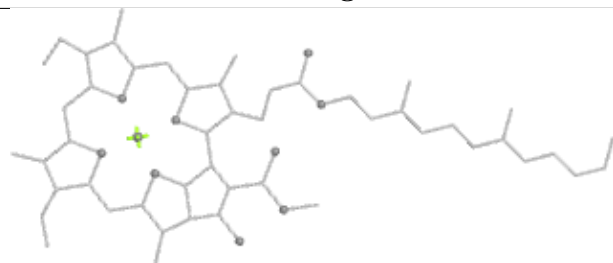
Bond lengths



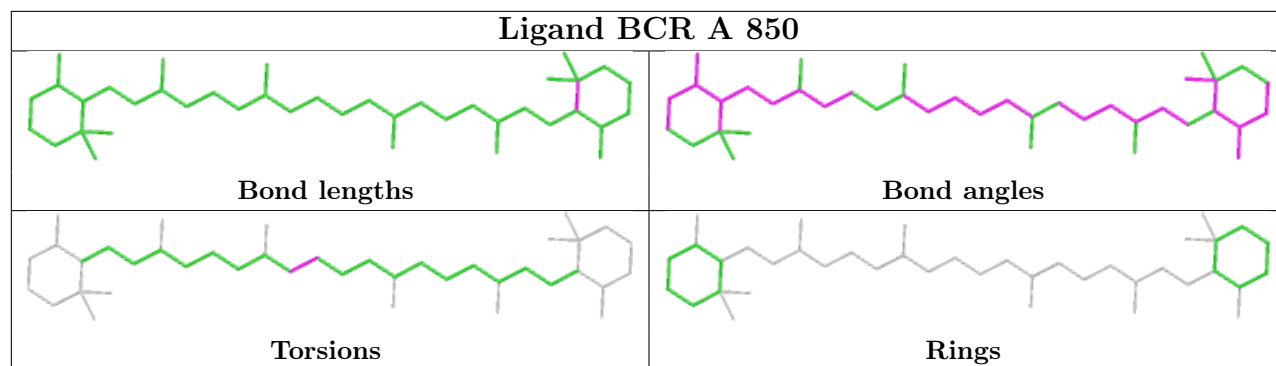
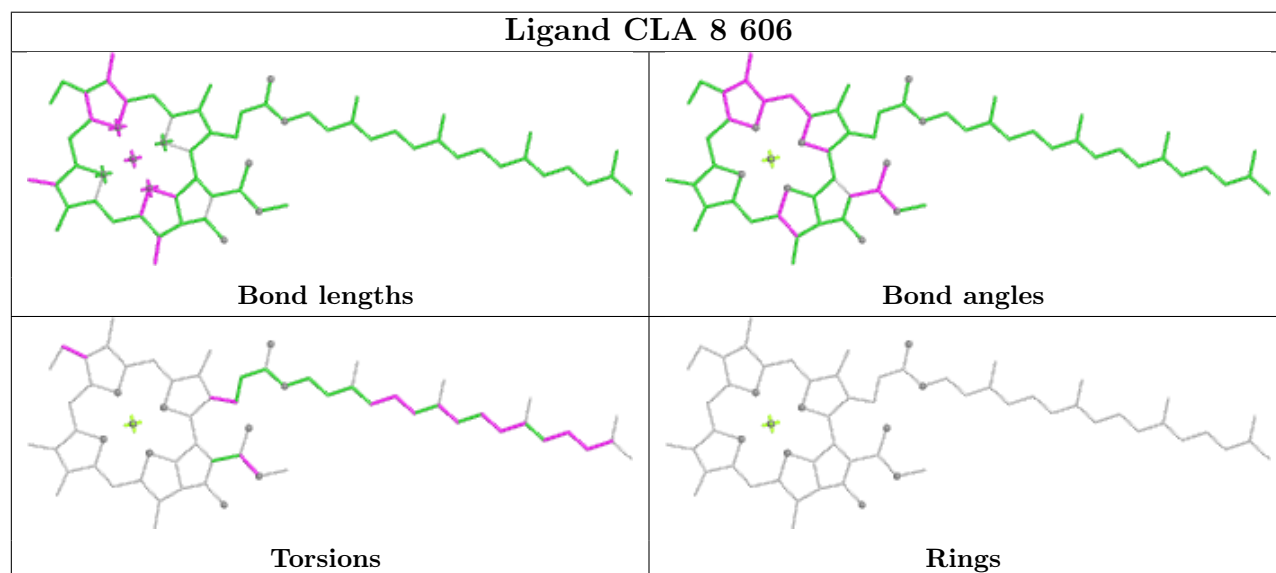
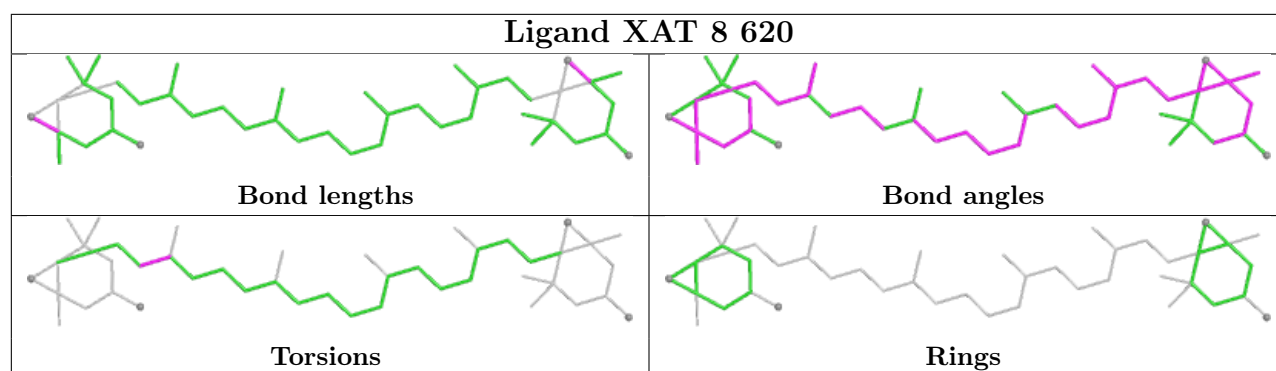
Bond angles



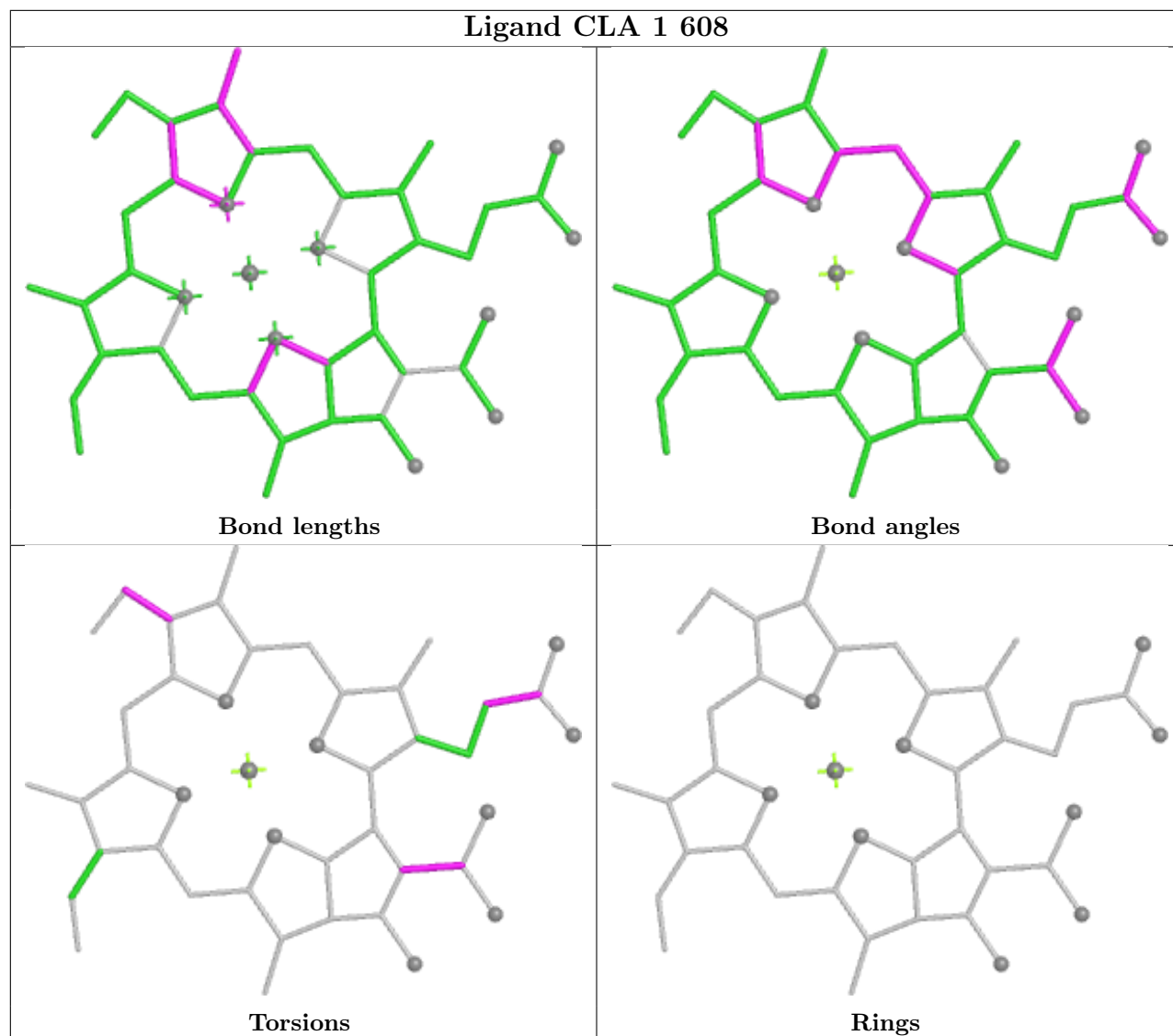
Torsions



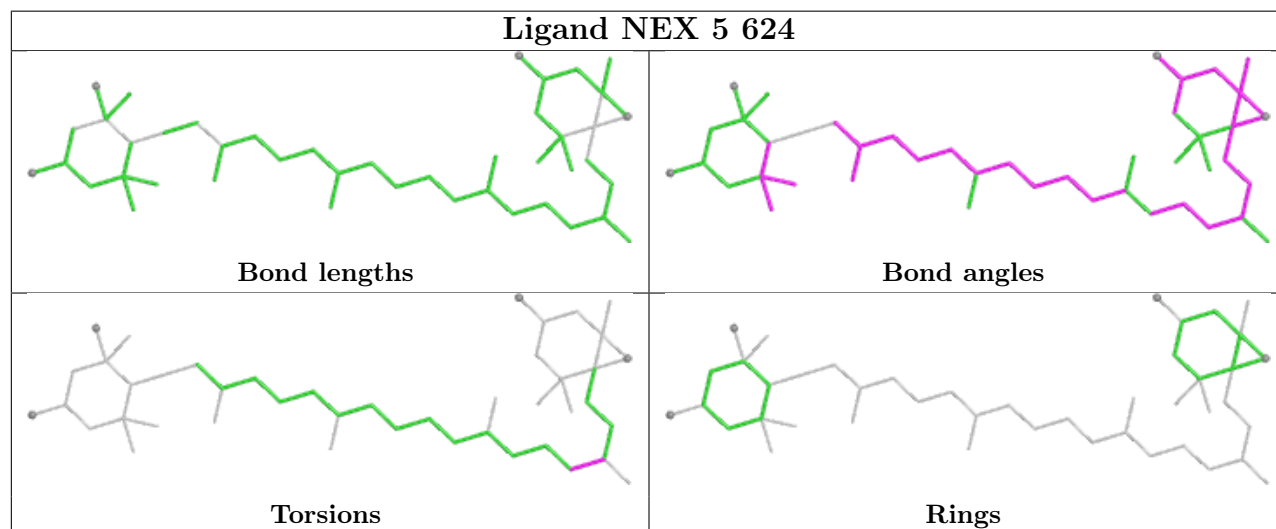
Rings

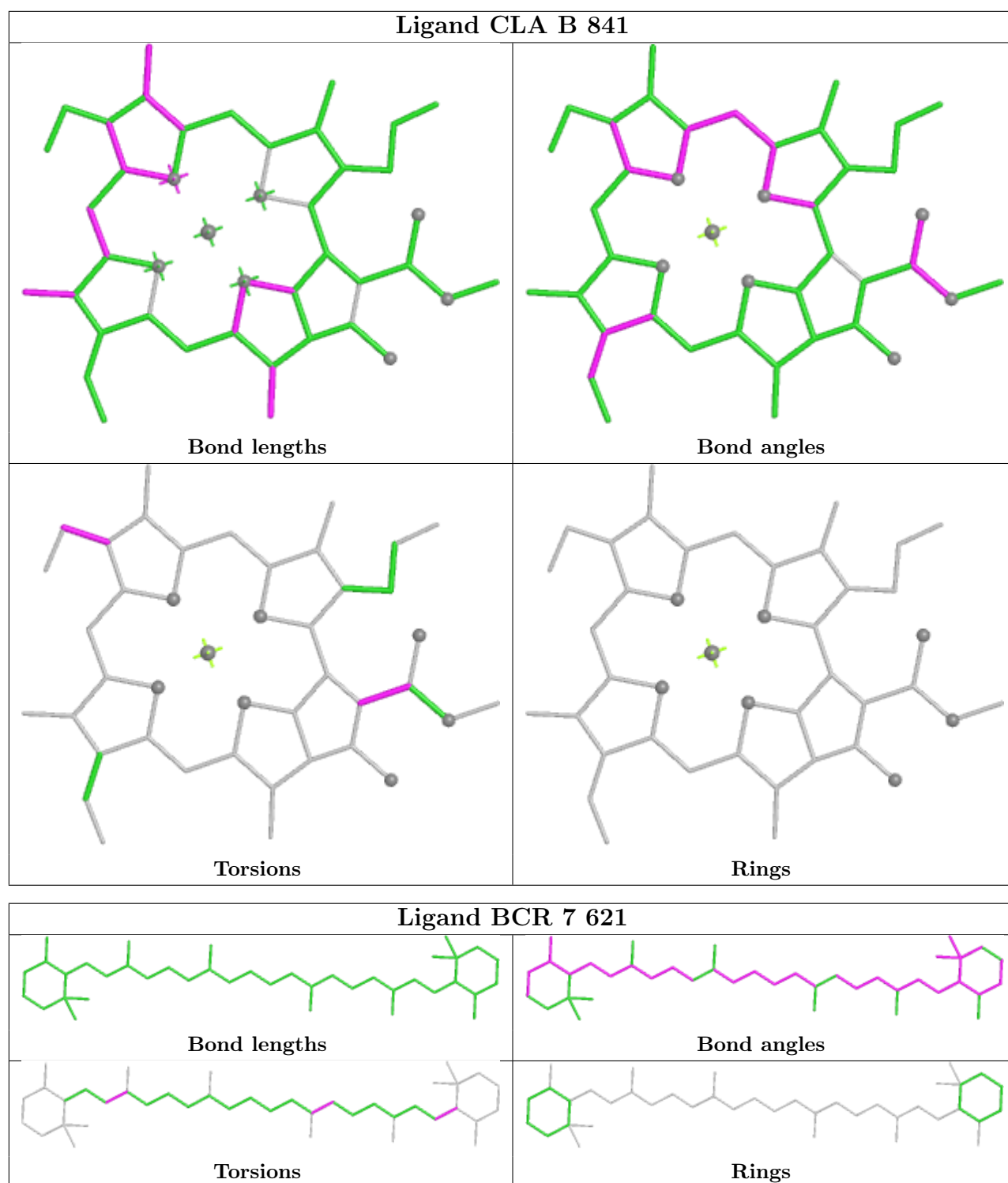


Ligand CLA 1 608

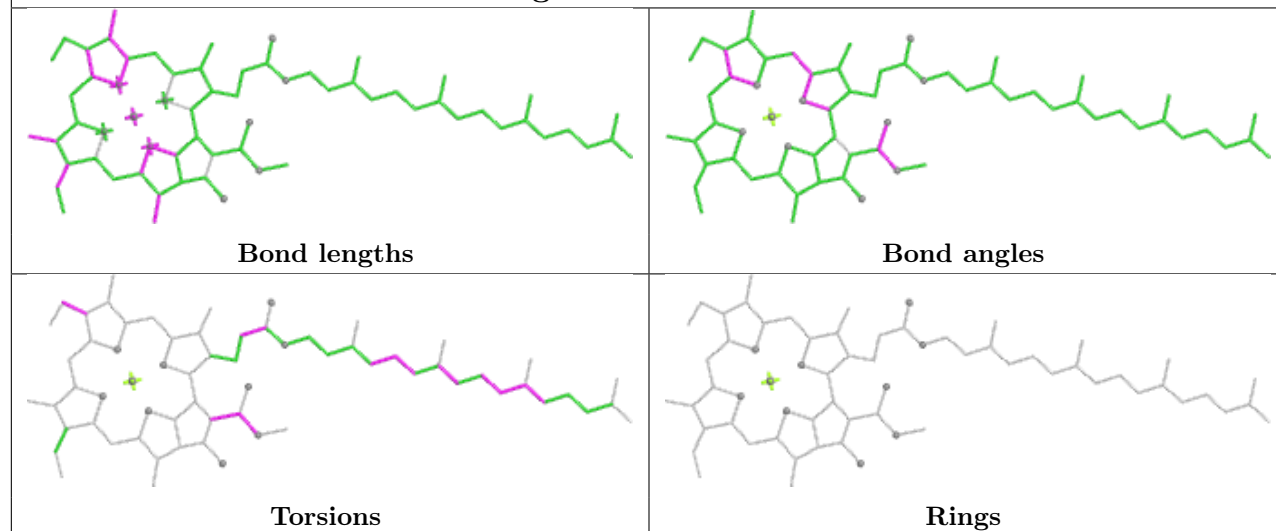


Ligand NEX 5 624

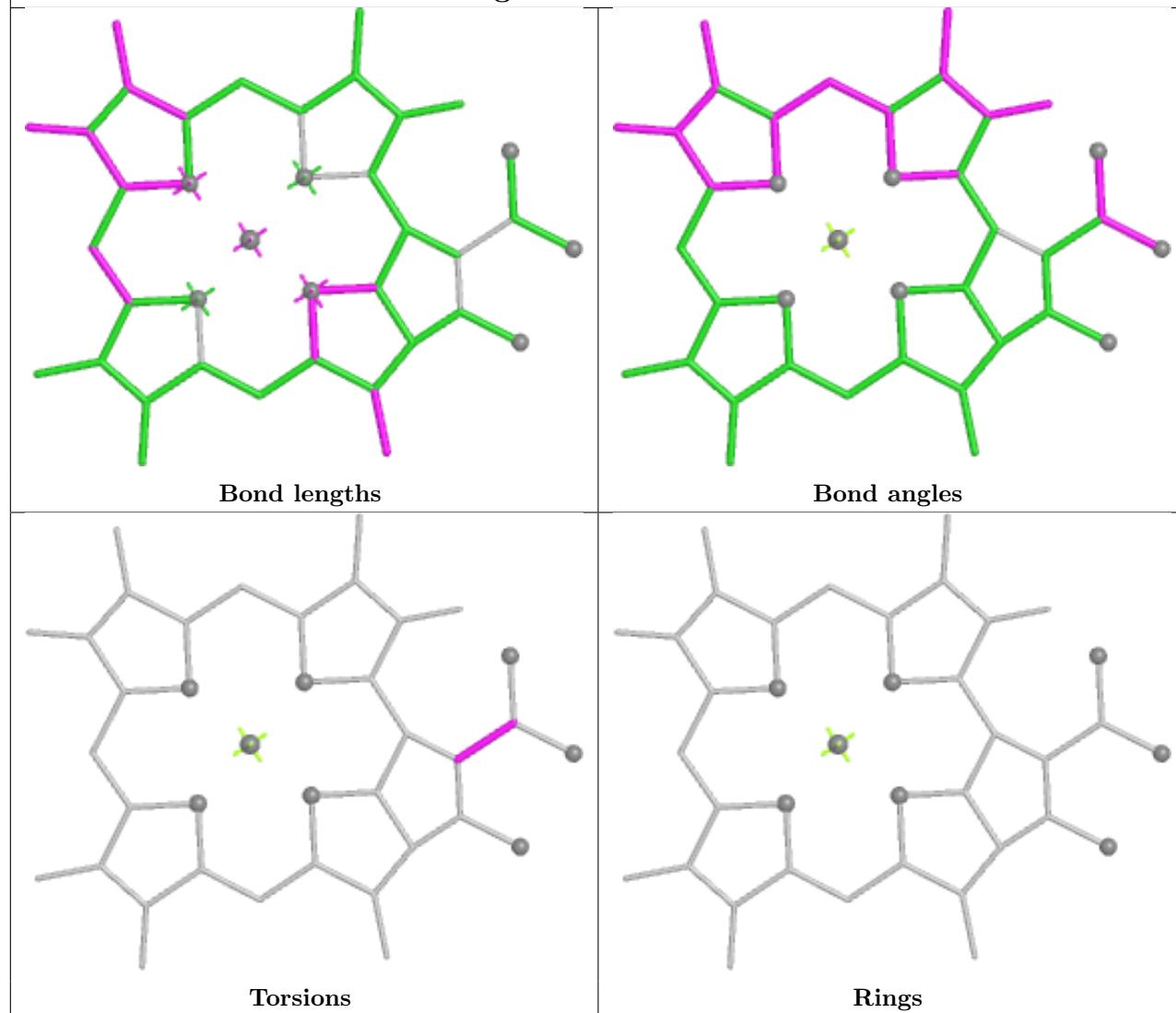


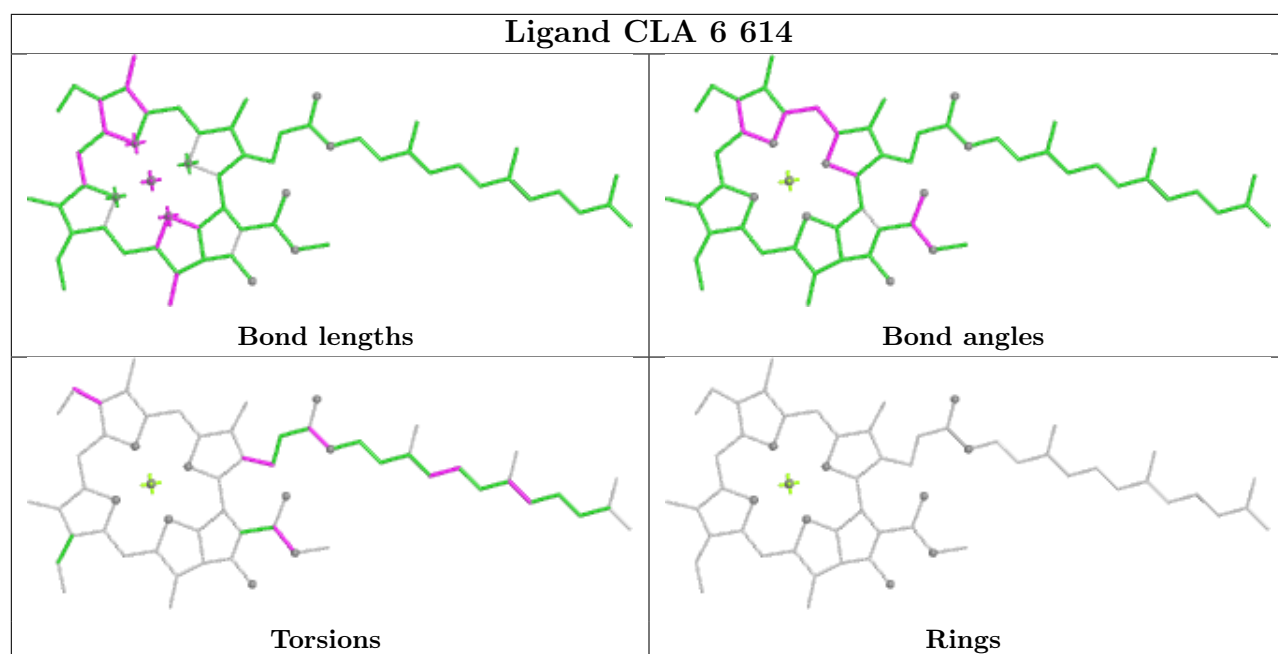


Ligand CLA B 806

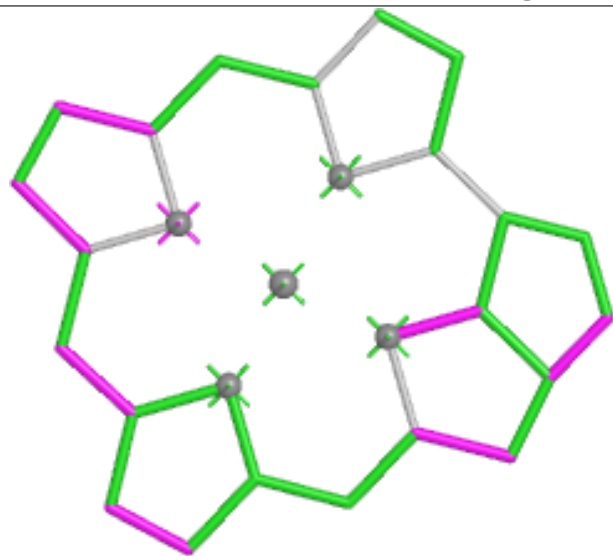


Ligand CLA 3 611

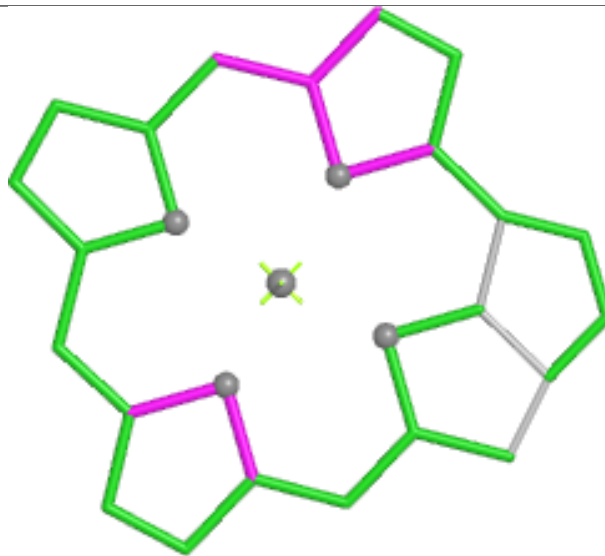




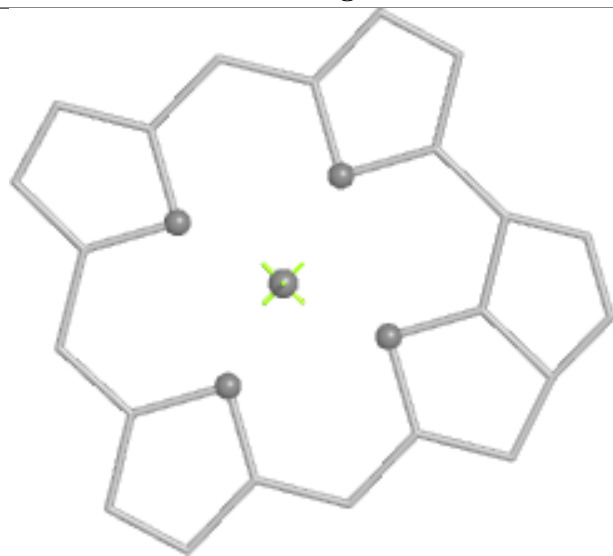
Ligand CLA 9 602



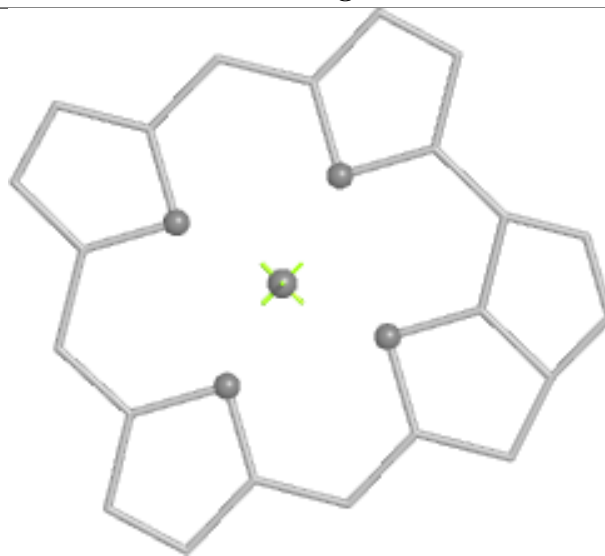
Bond lengths



Bond angles

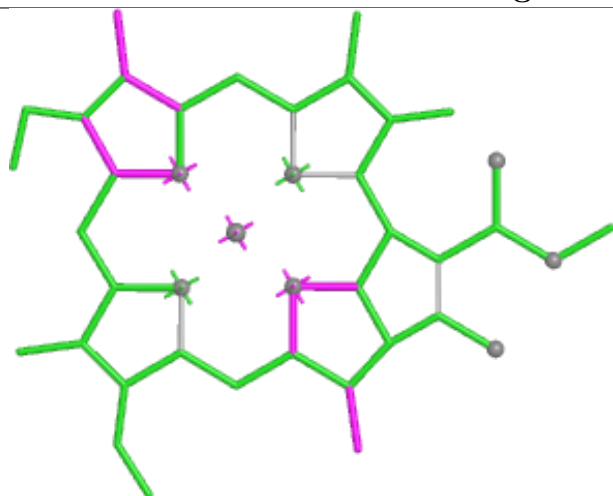


Torsions



Rings

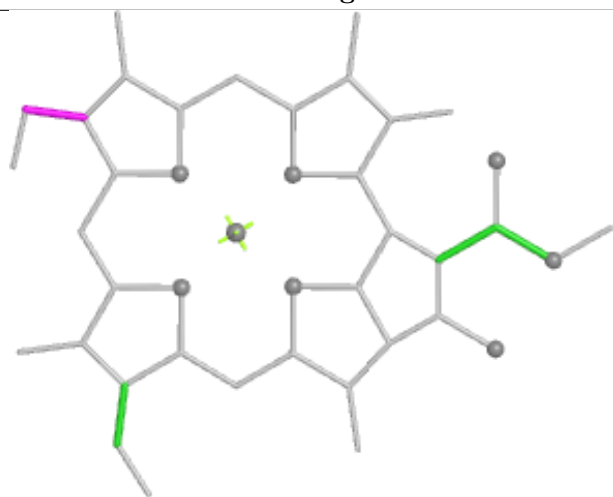
Ligand CLA A 824



Bond lengths



Bond angles

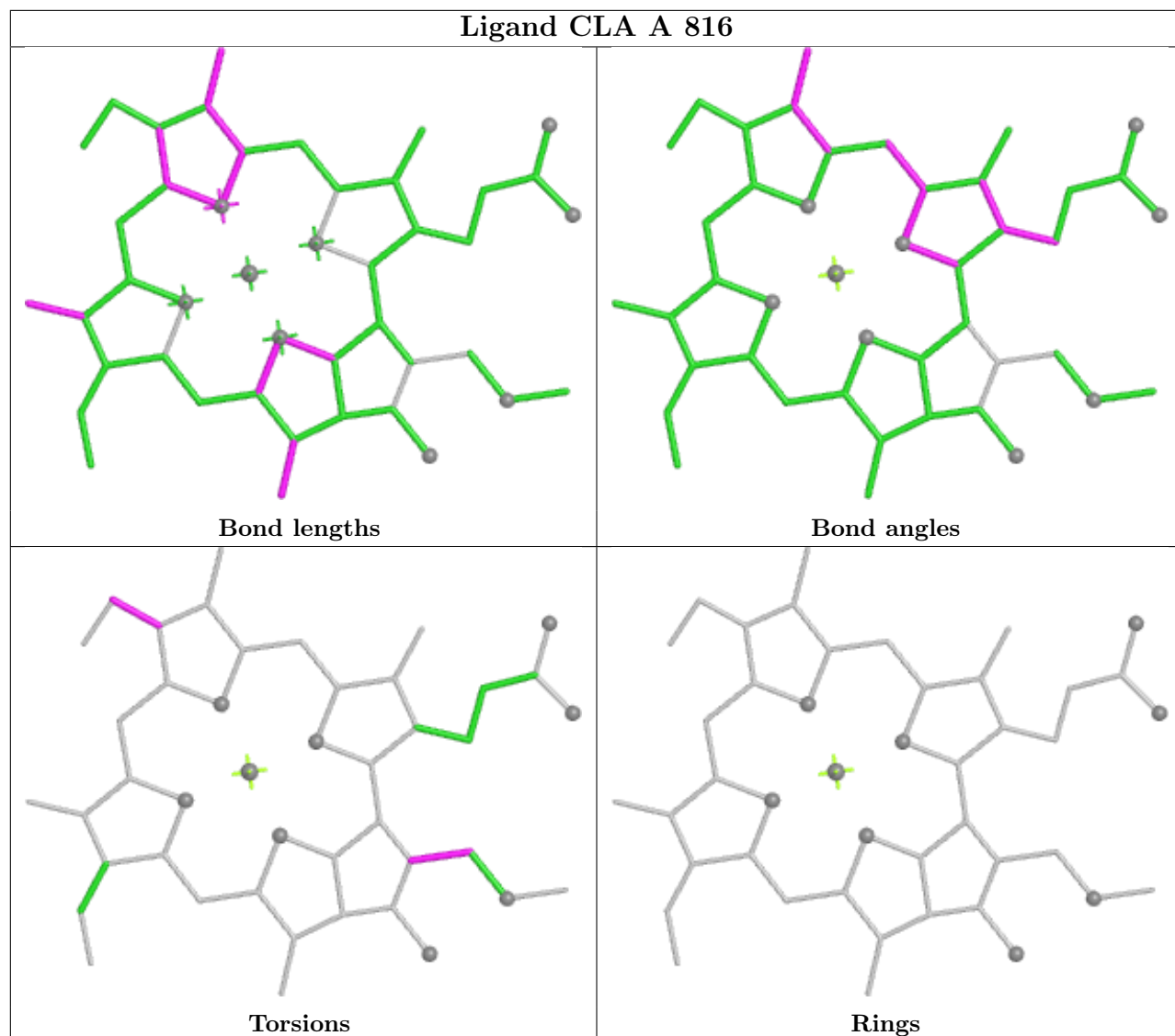


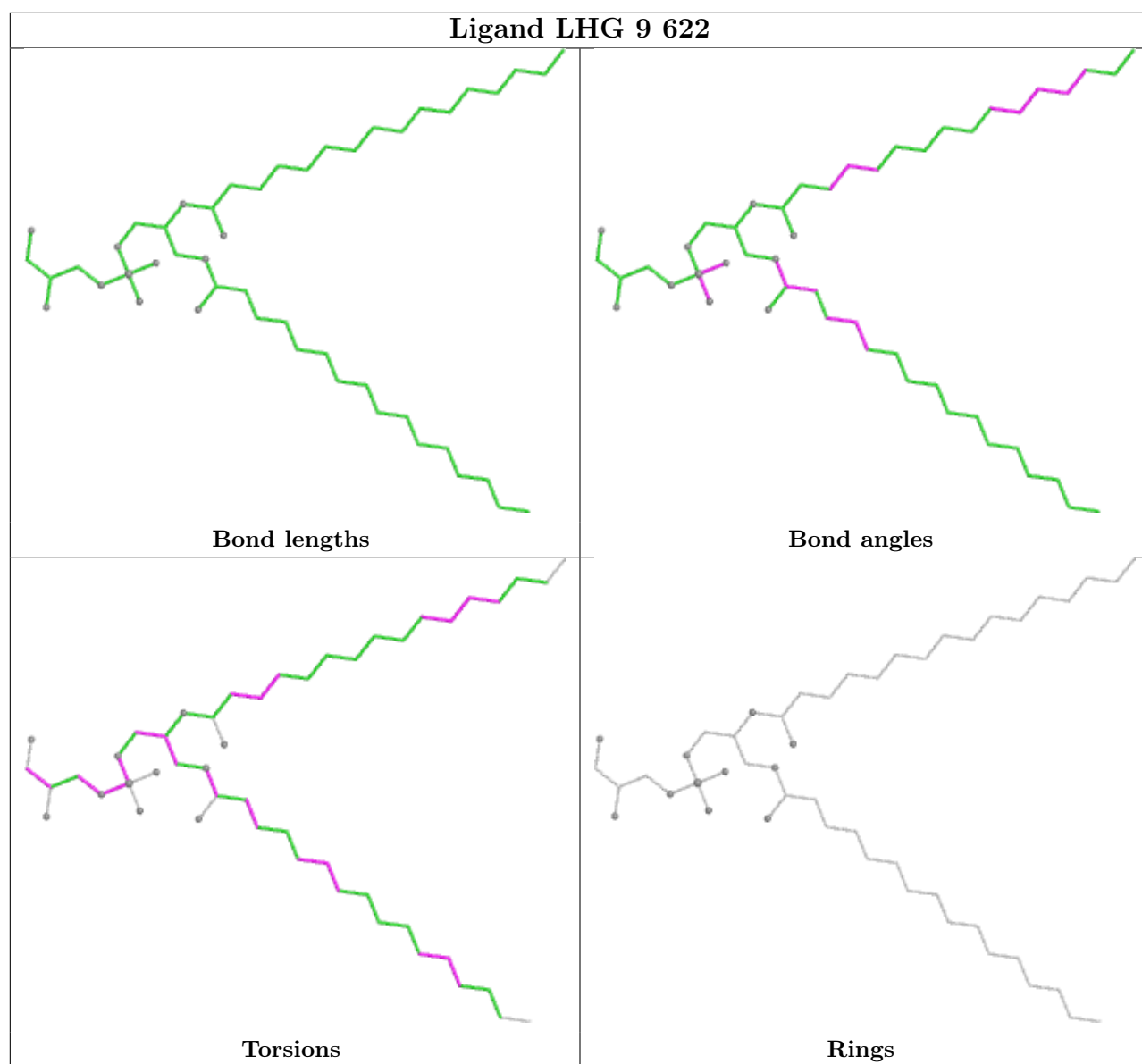
Torsions



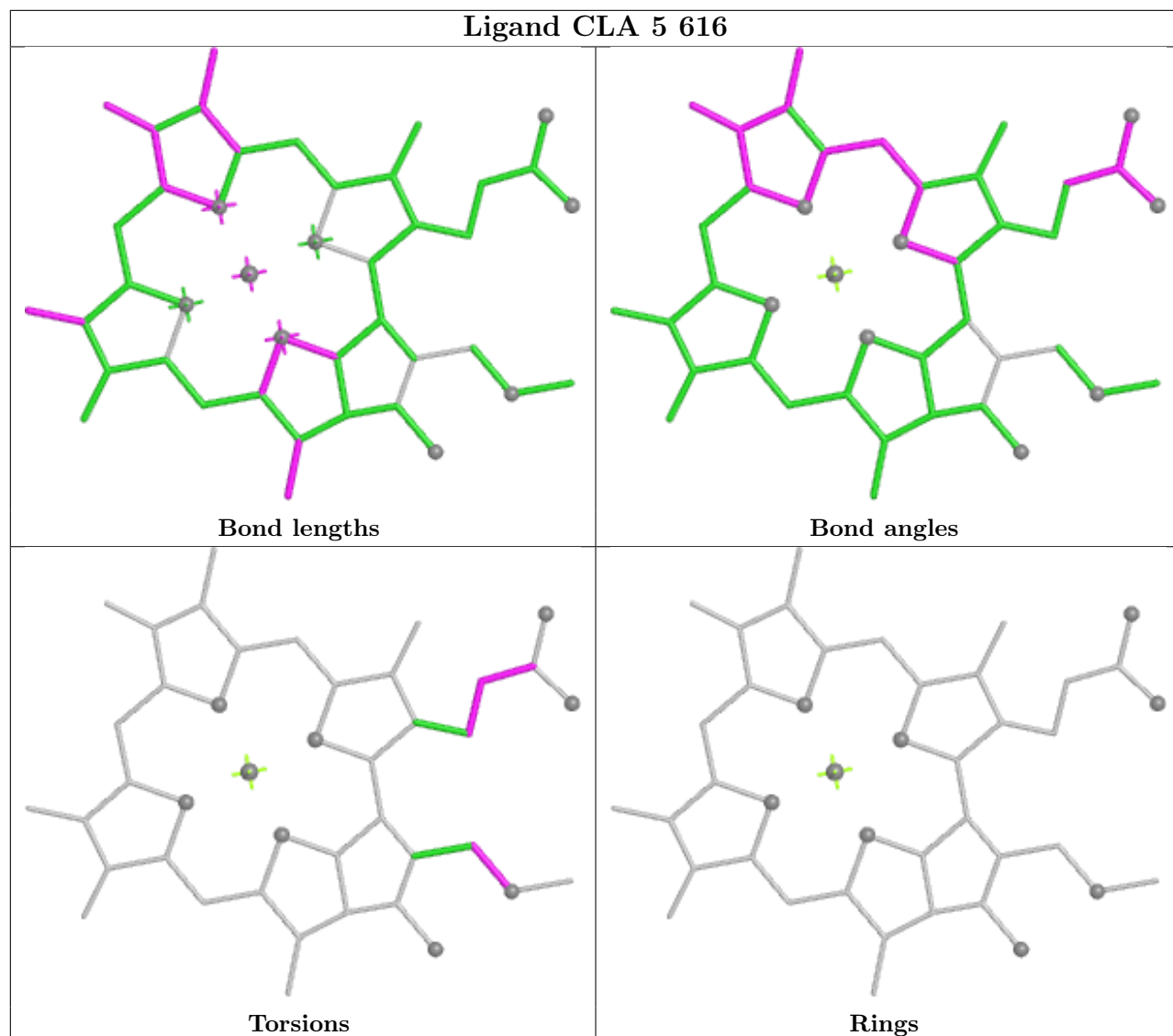
Rings

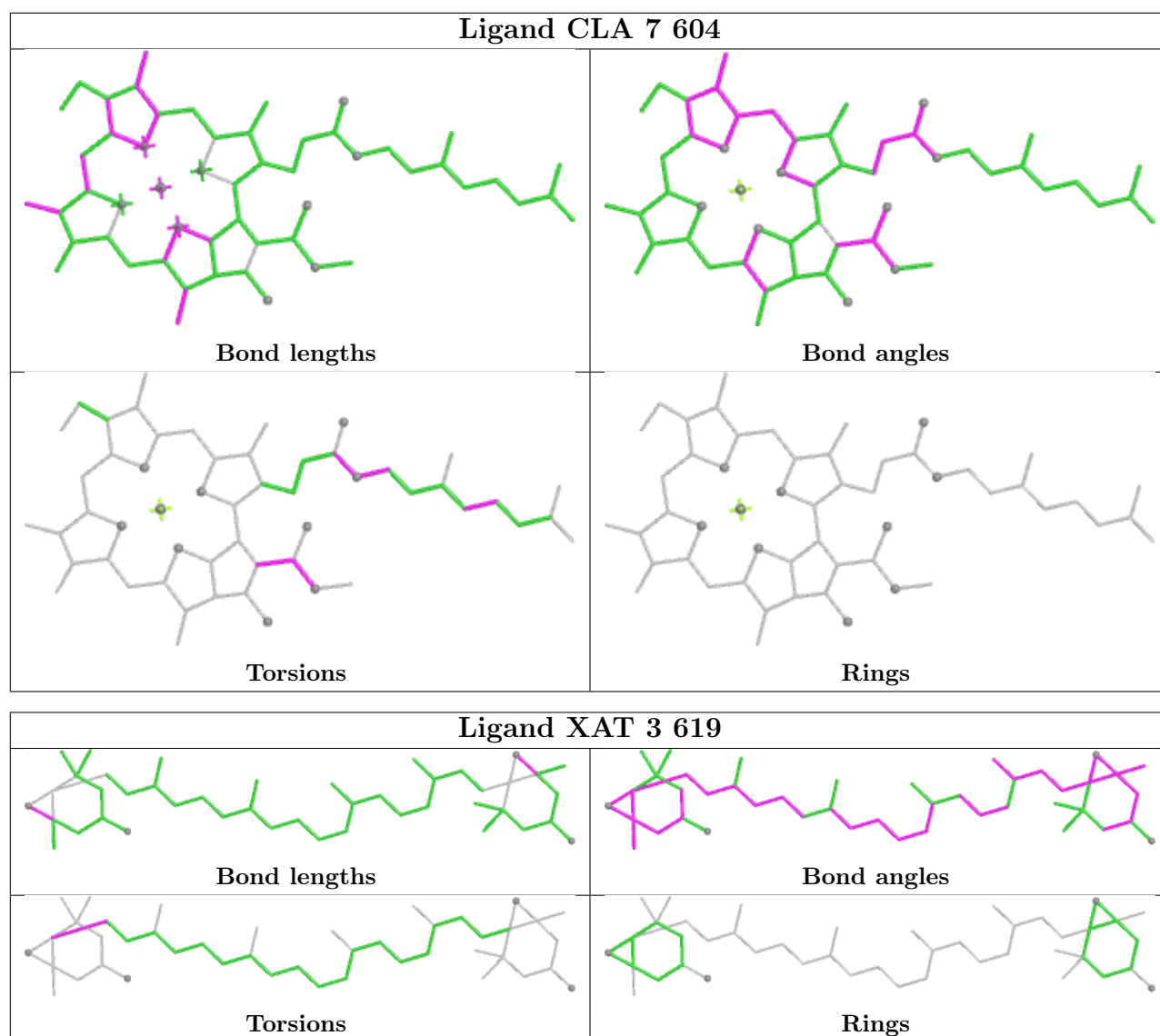
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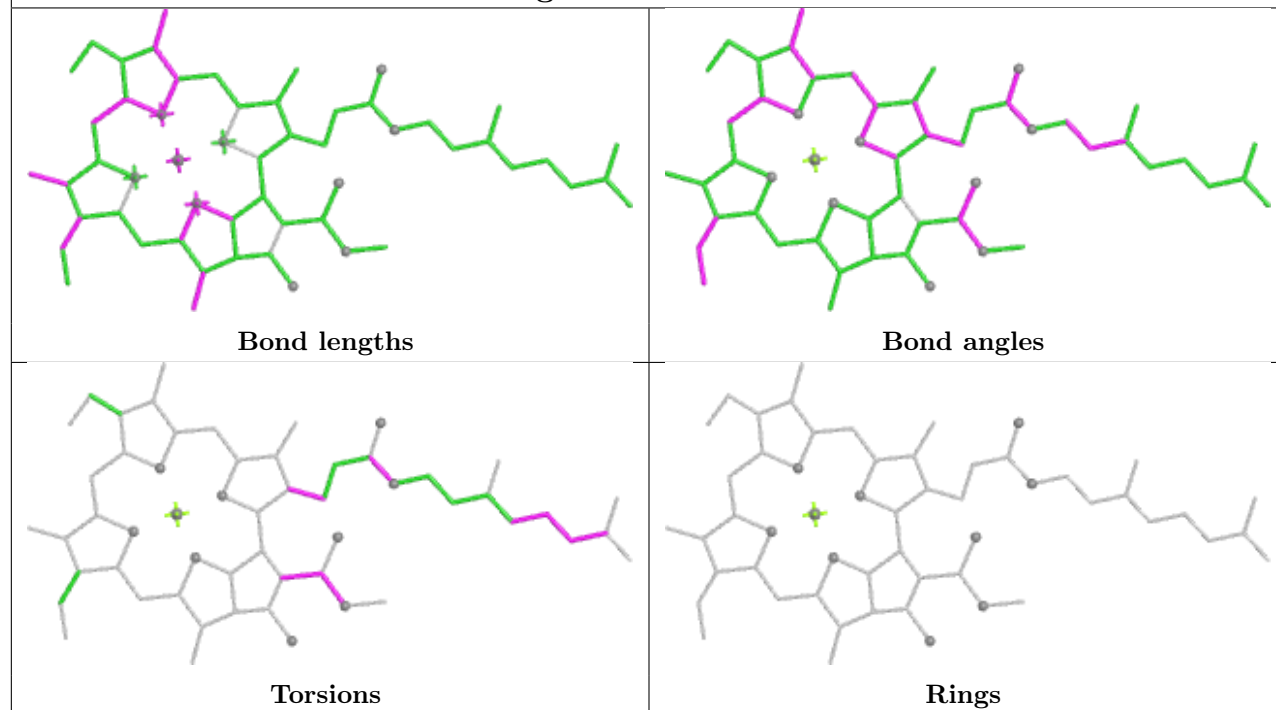
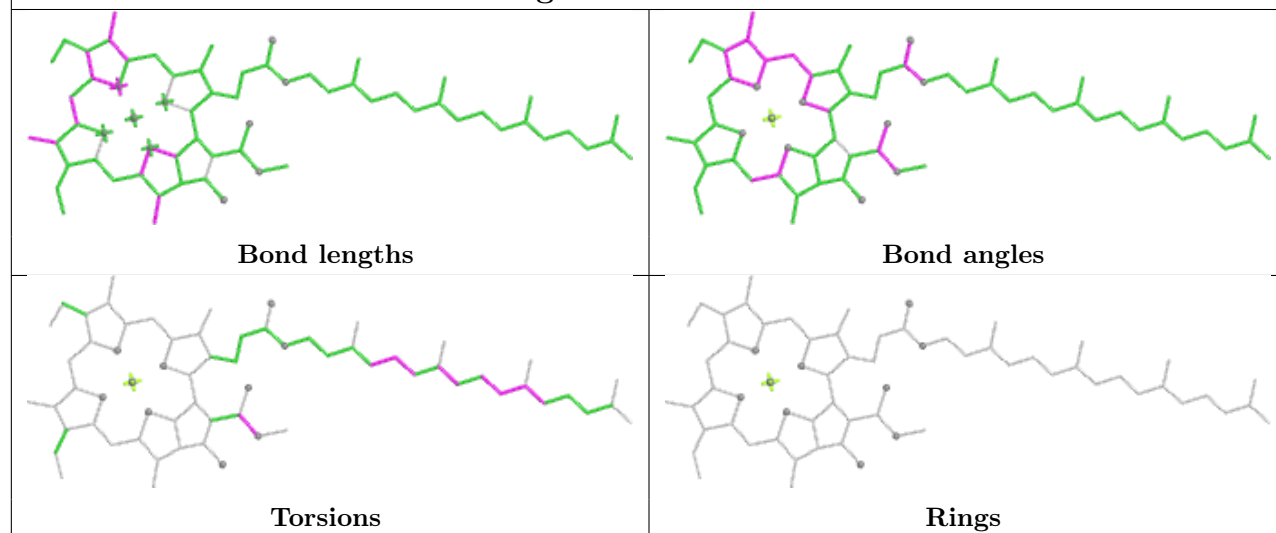




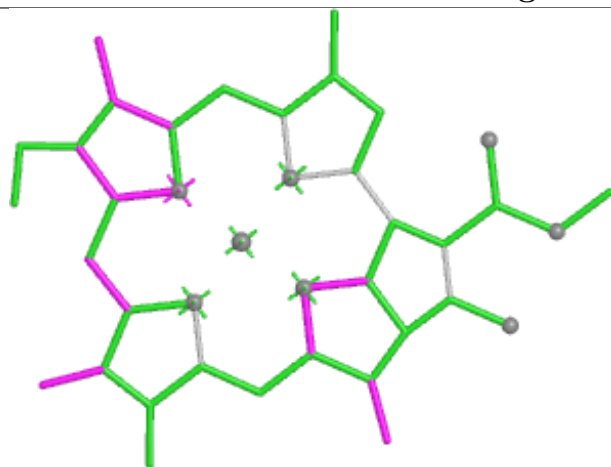
Ligand CLA 5 616





Ligand CLA 3 603**Ligand CLA 4 608**

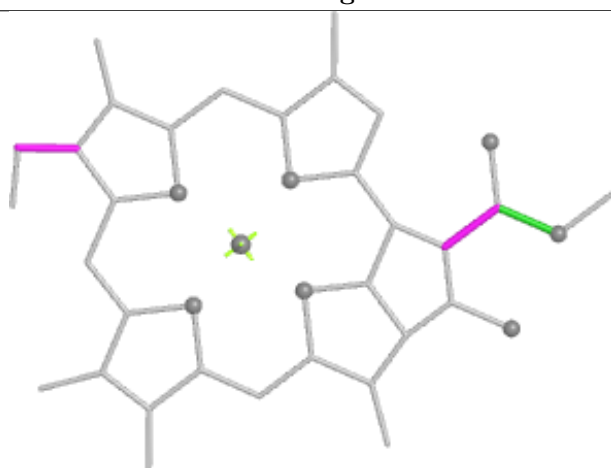
Ligand CLA 1 610



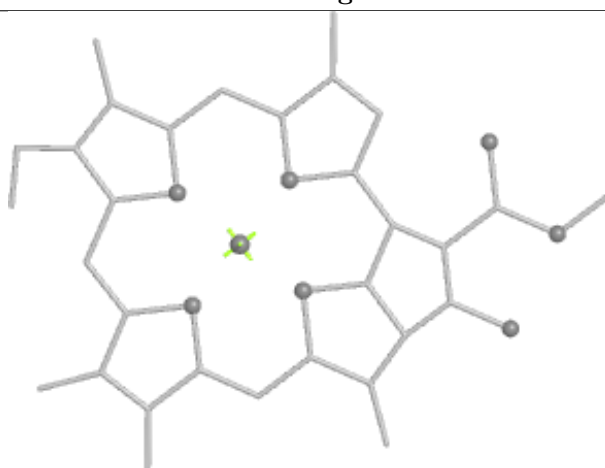
Bond lengths



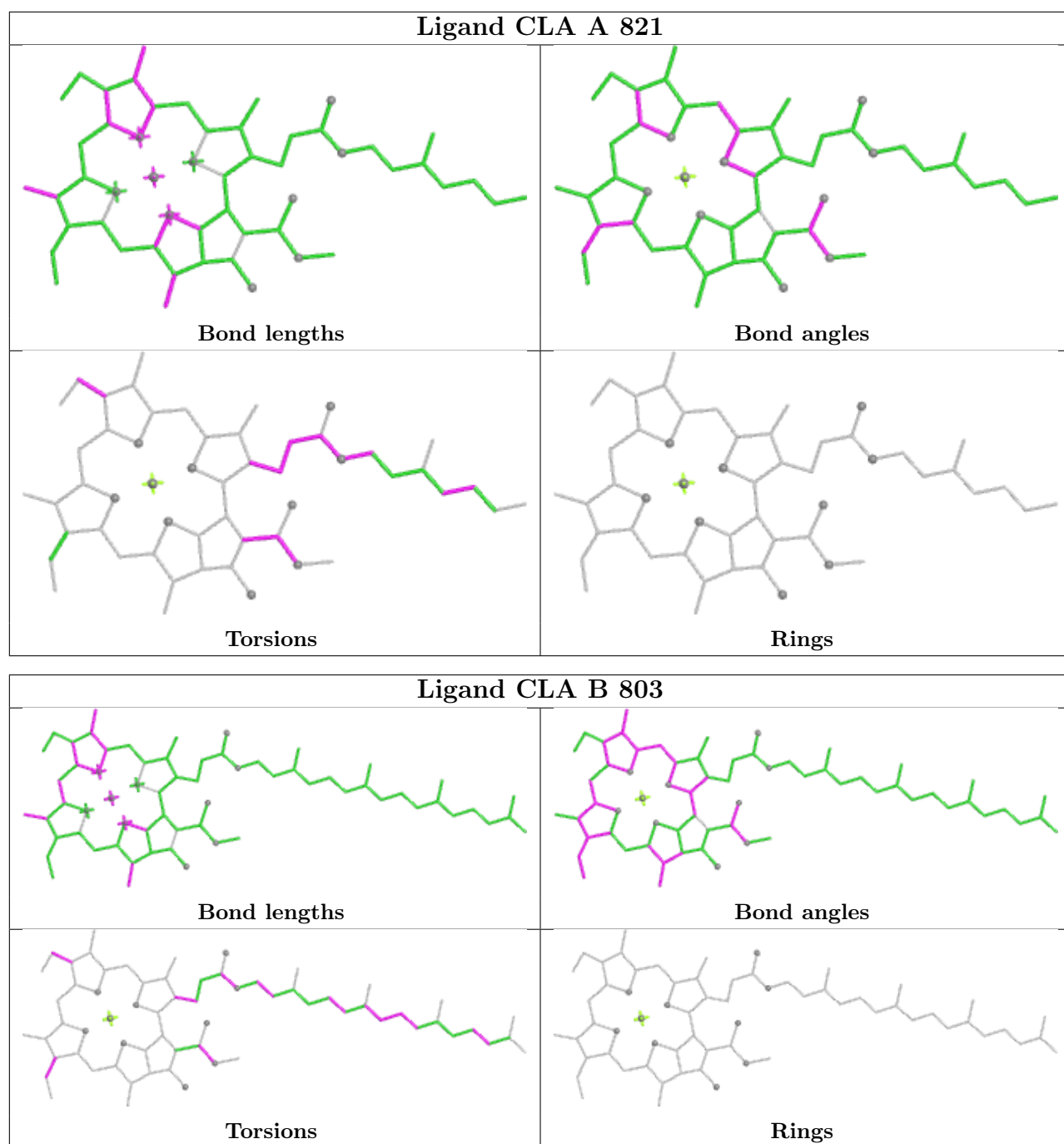
Bond angles

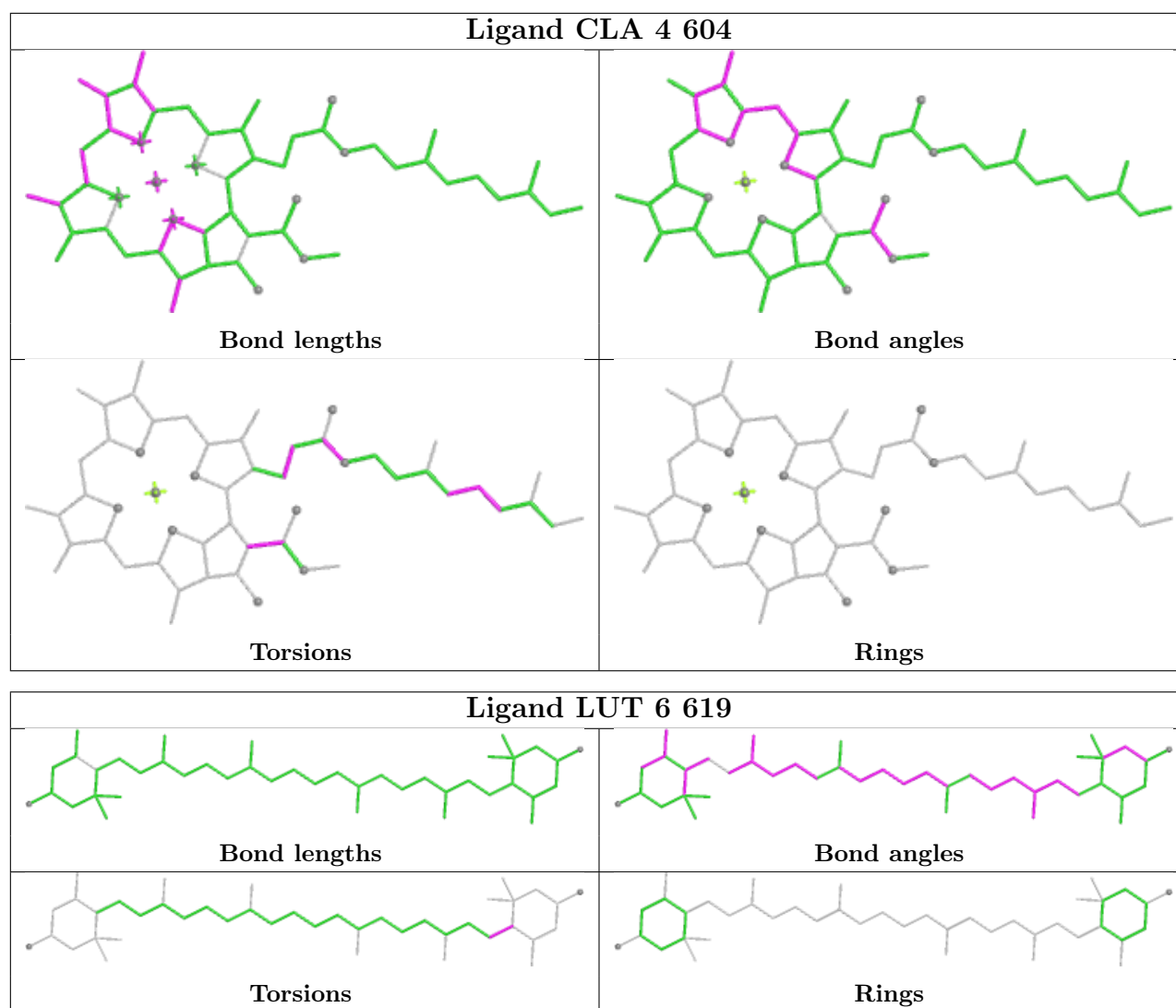


Torsions

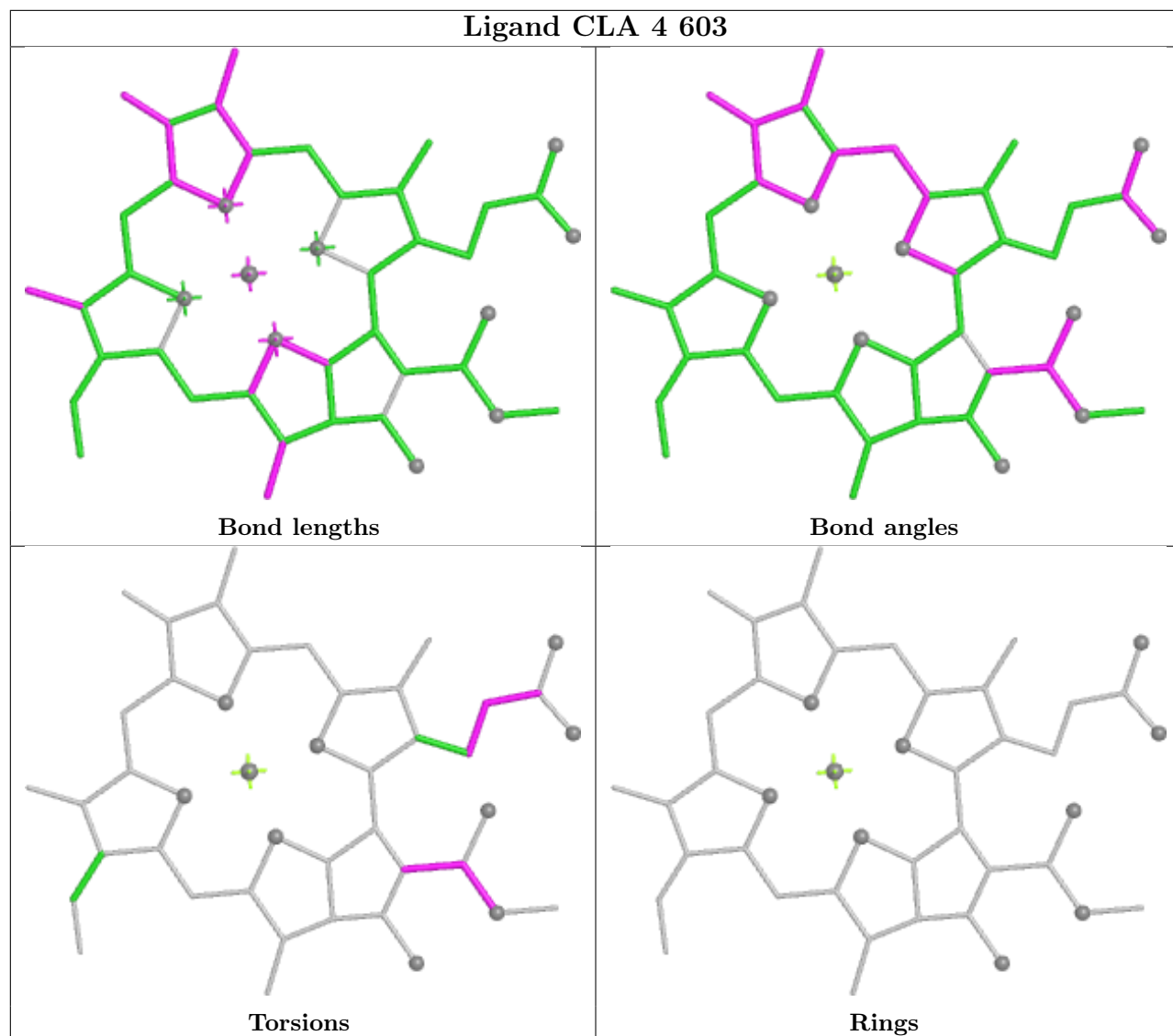


Rings

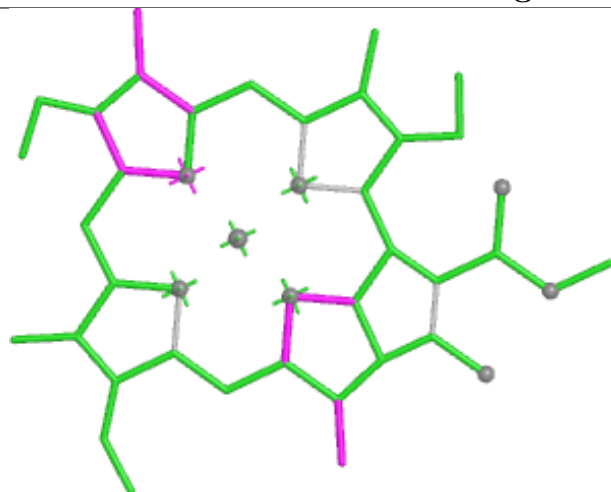




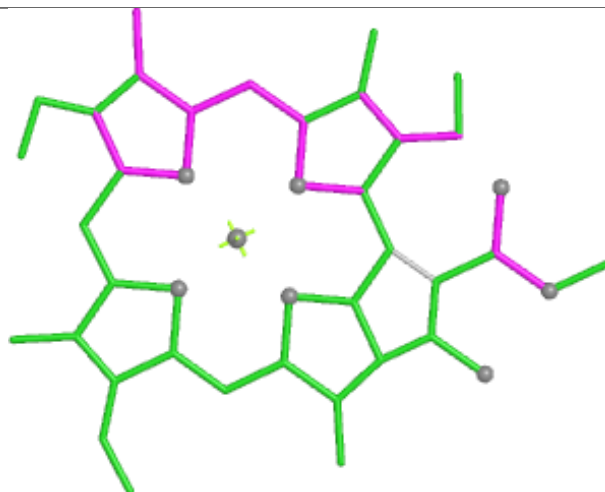
Ligand CLA 4 603



Ligand CLA B 822



Bond lengths



Bond angles

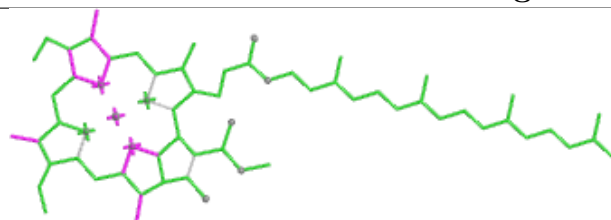


Torsions

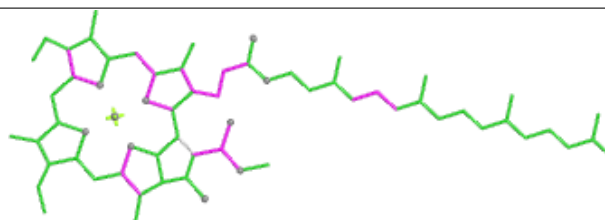


Rings

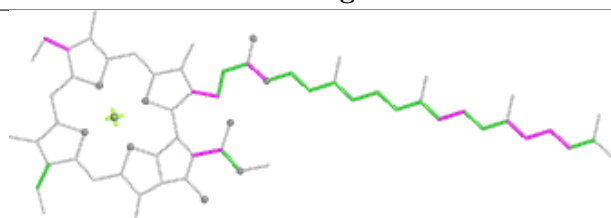
Ligand CLA A 804



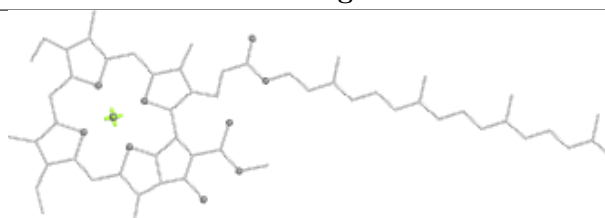
Bond lengths



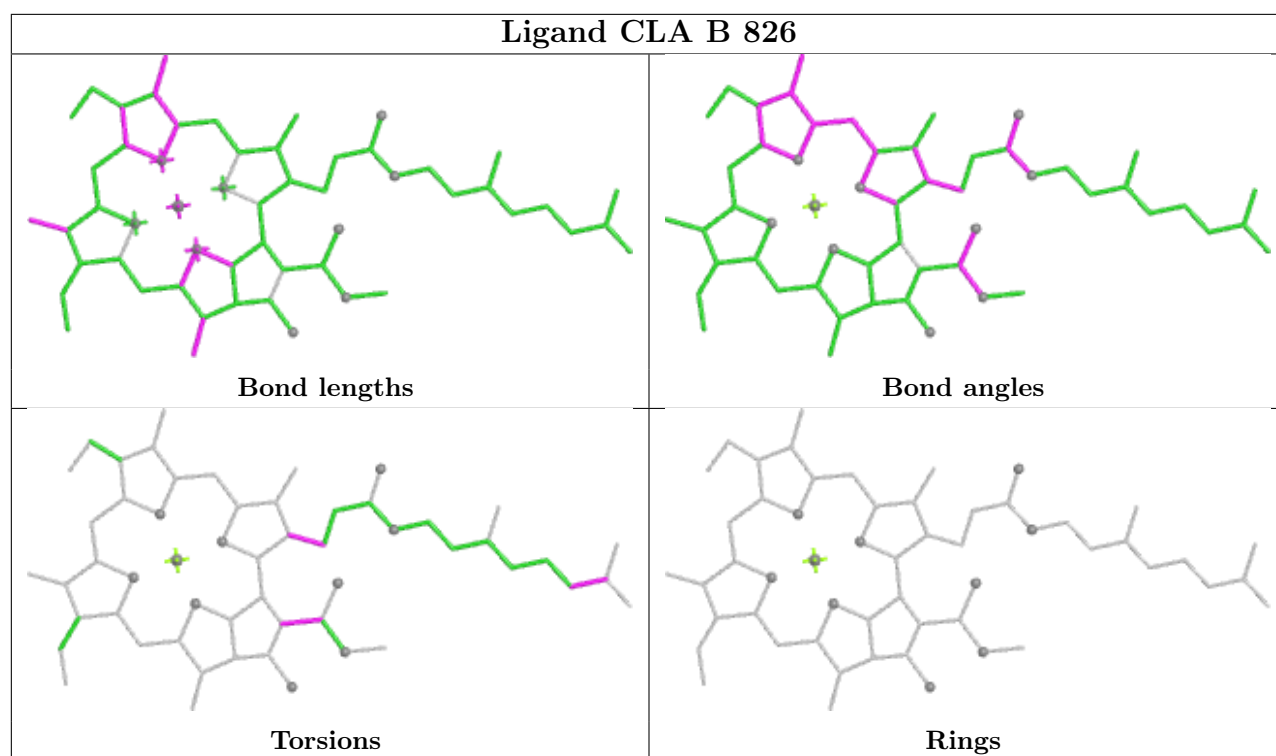
Bond angles



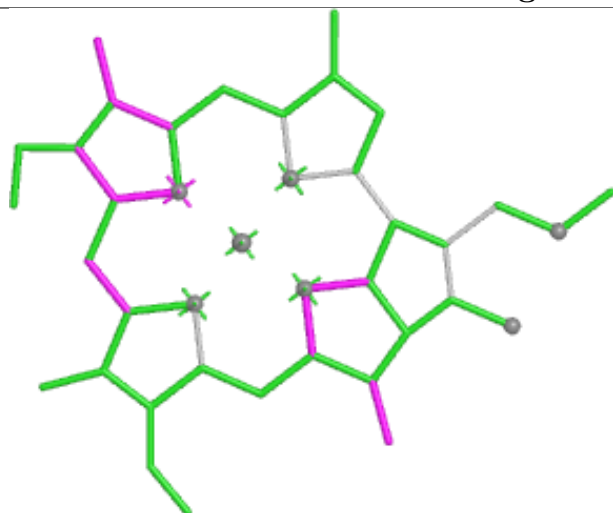
Torsions



Rings



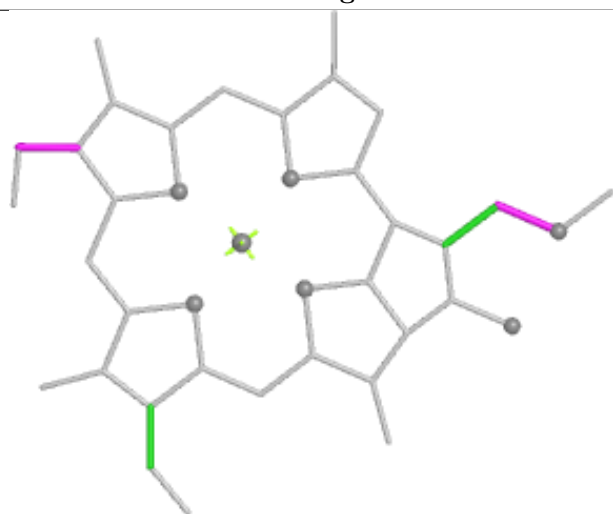
Ligand CLA 1 606



Bond lengths



Bond angles

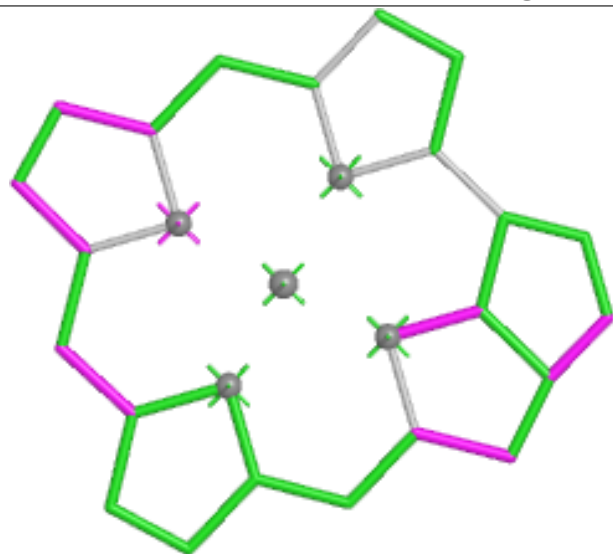


Torsions

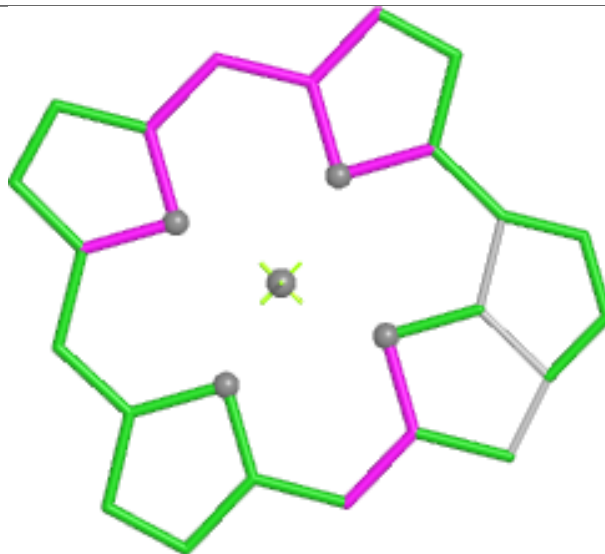


Rings

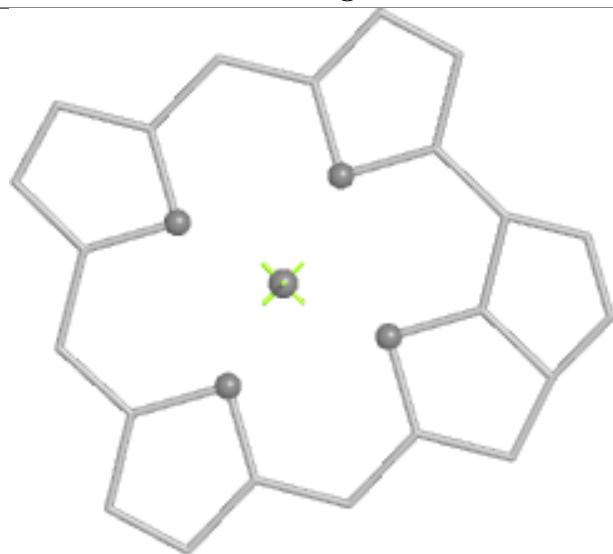
Ligand CLA 2 610



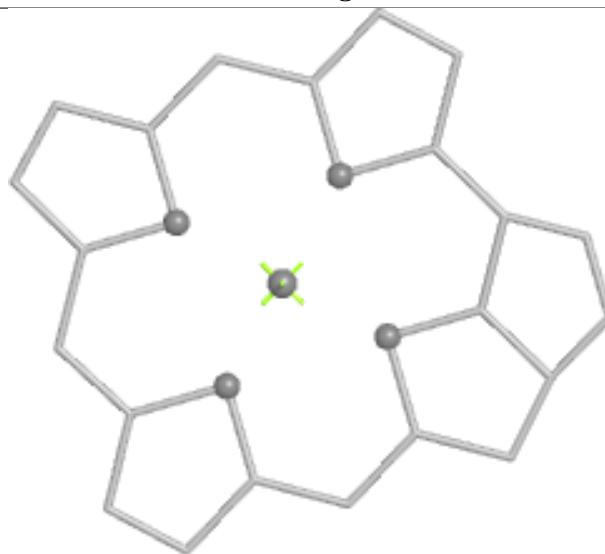
Bond lengths



Bond angles

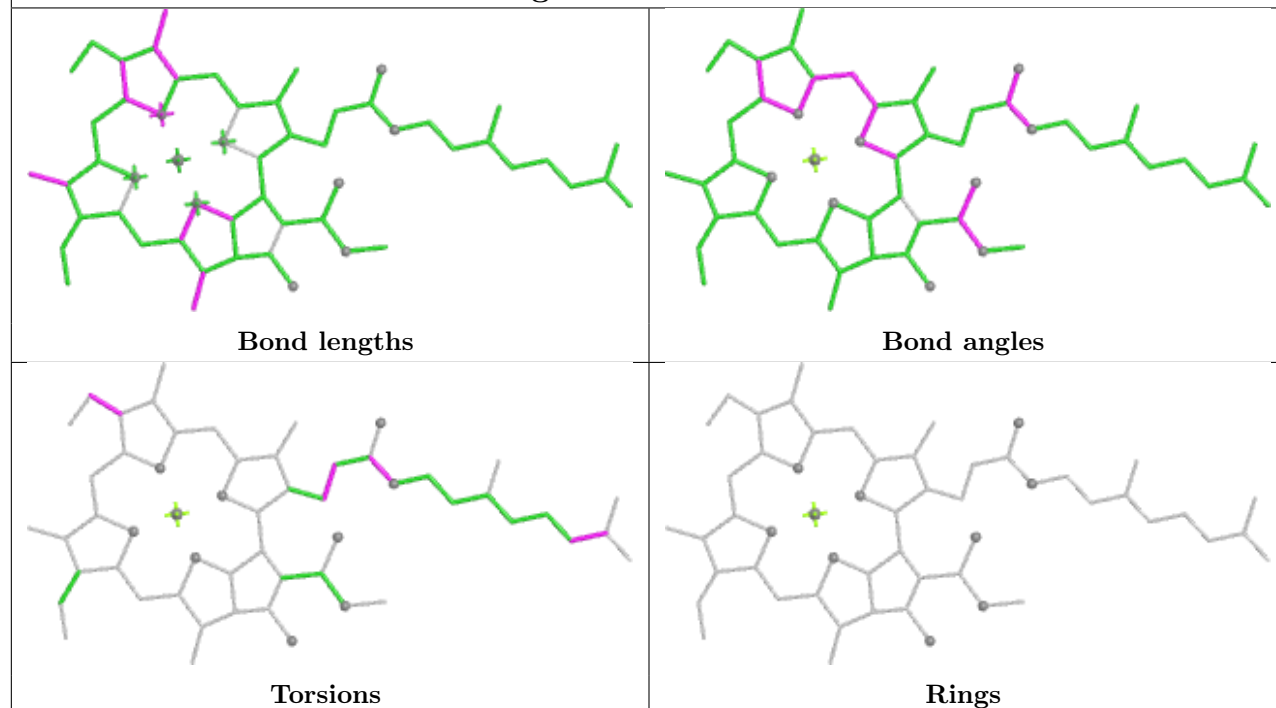


Torsions

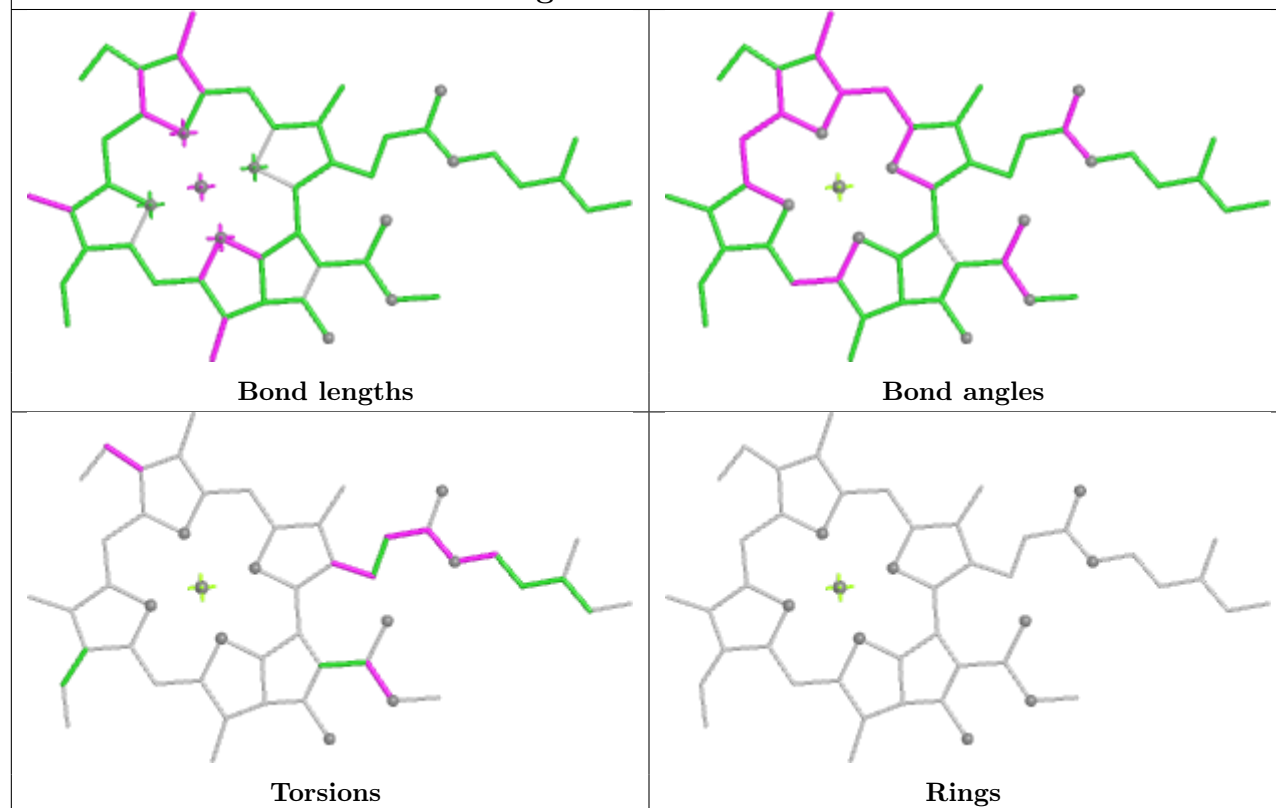


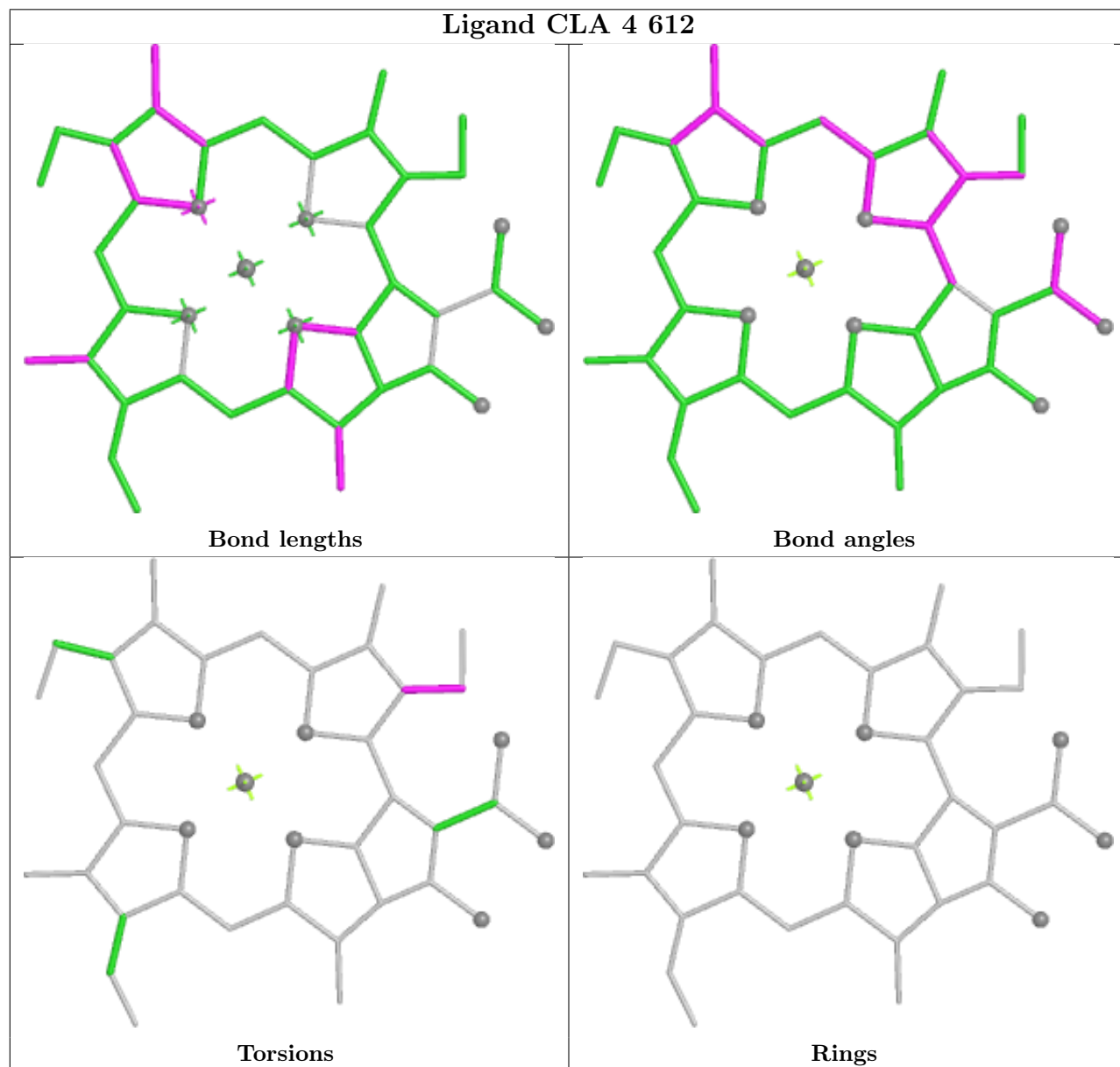
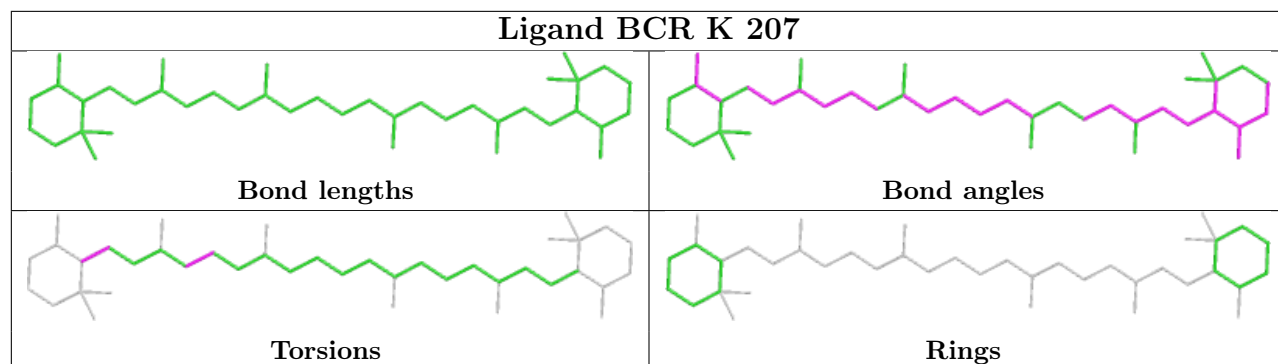
Rings

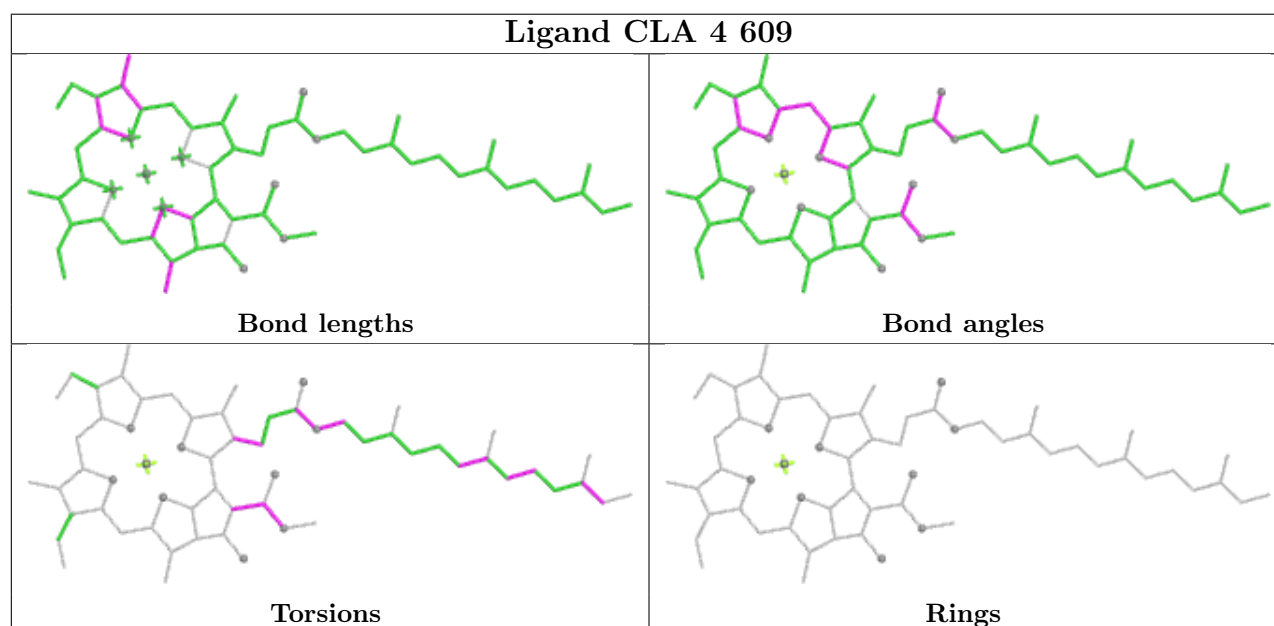
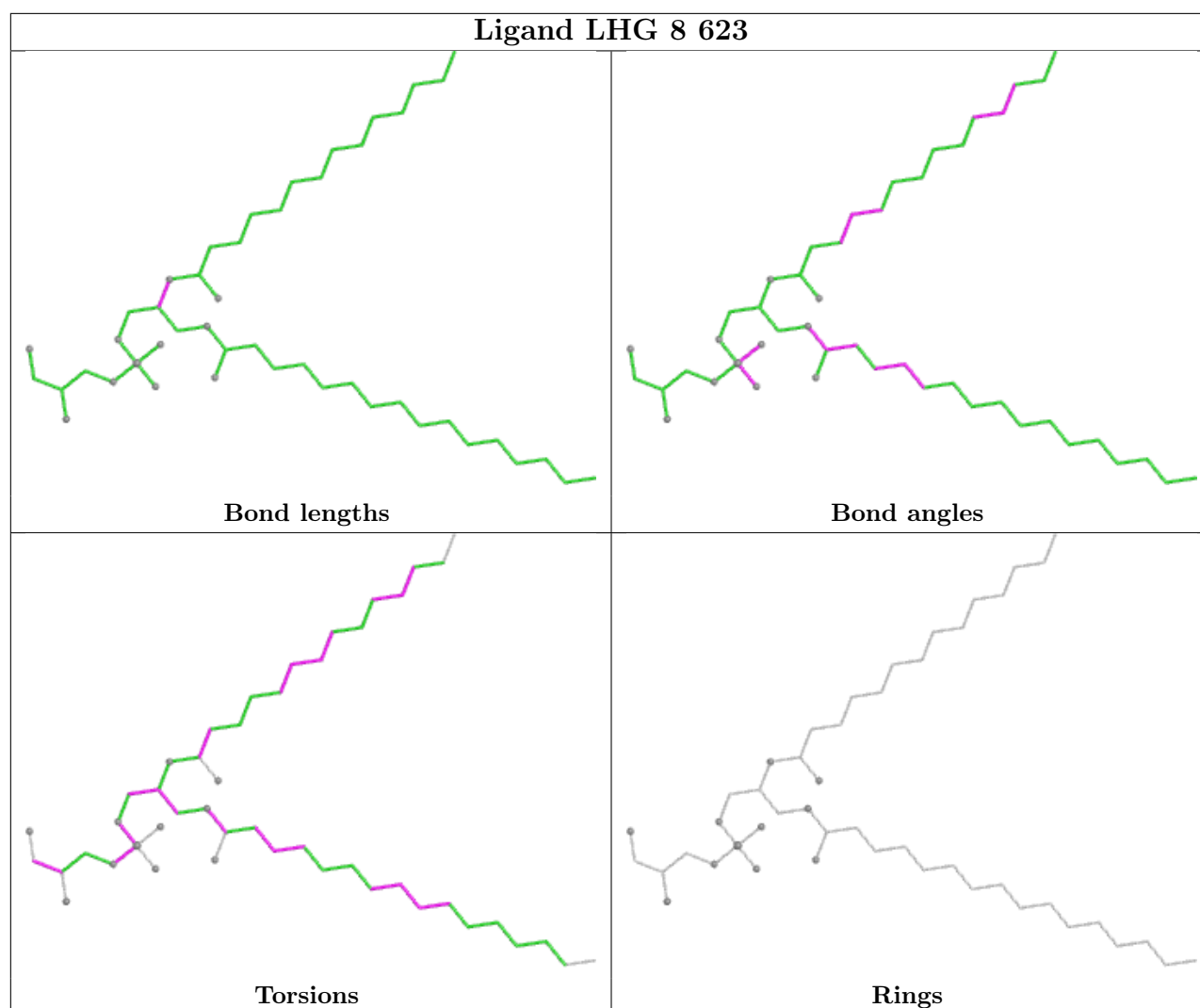
Ligand CLA A 839

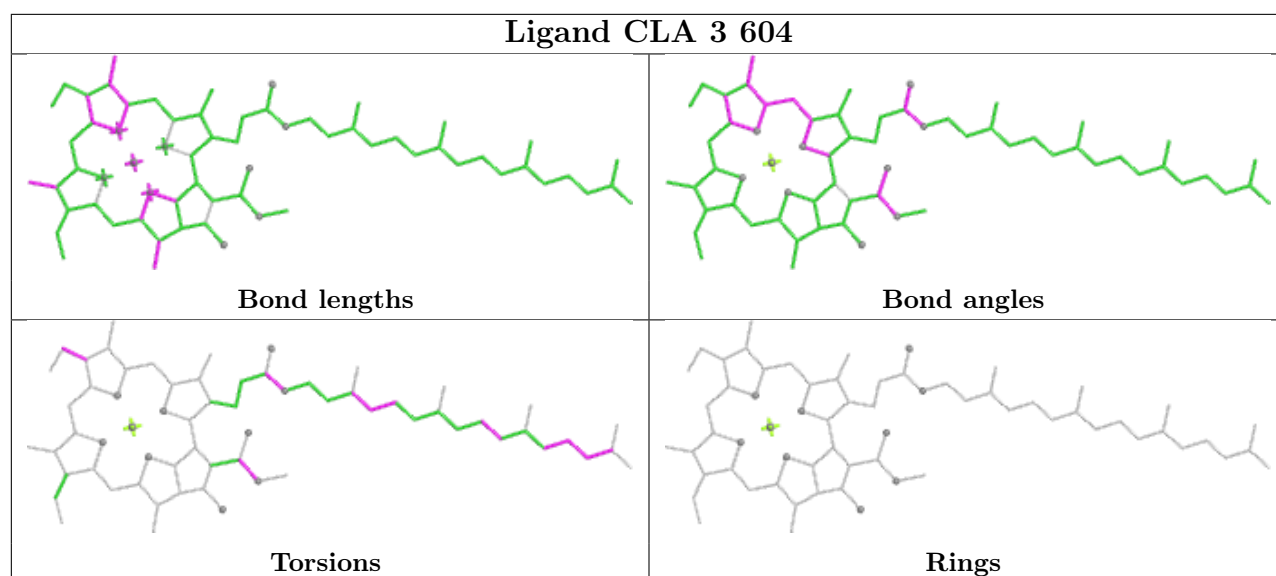
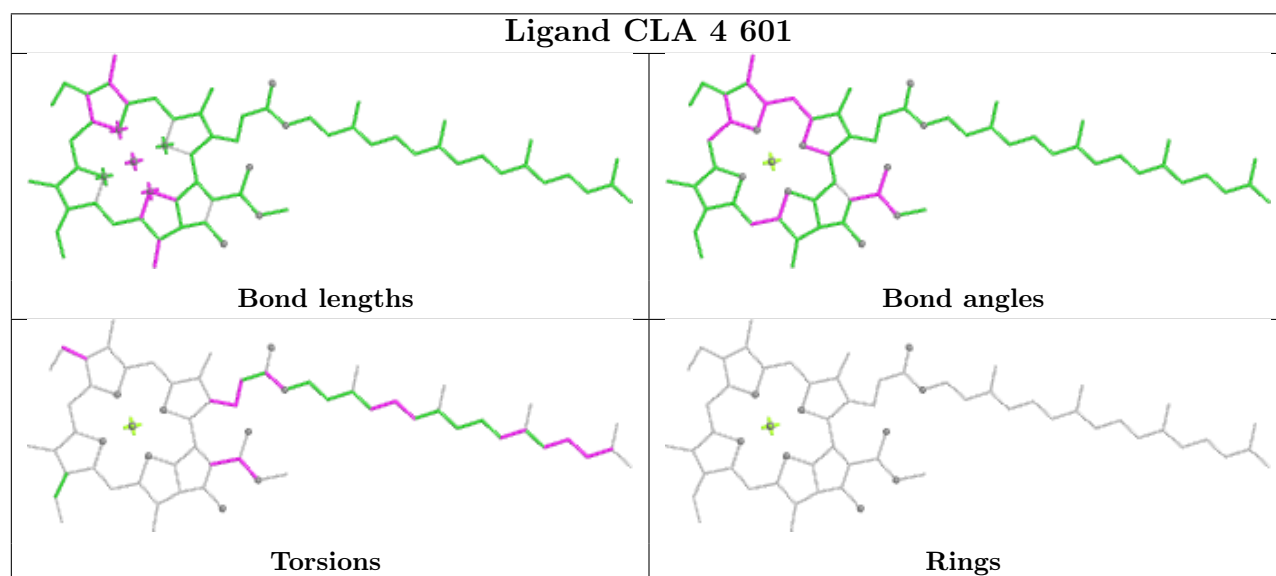
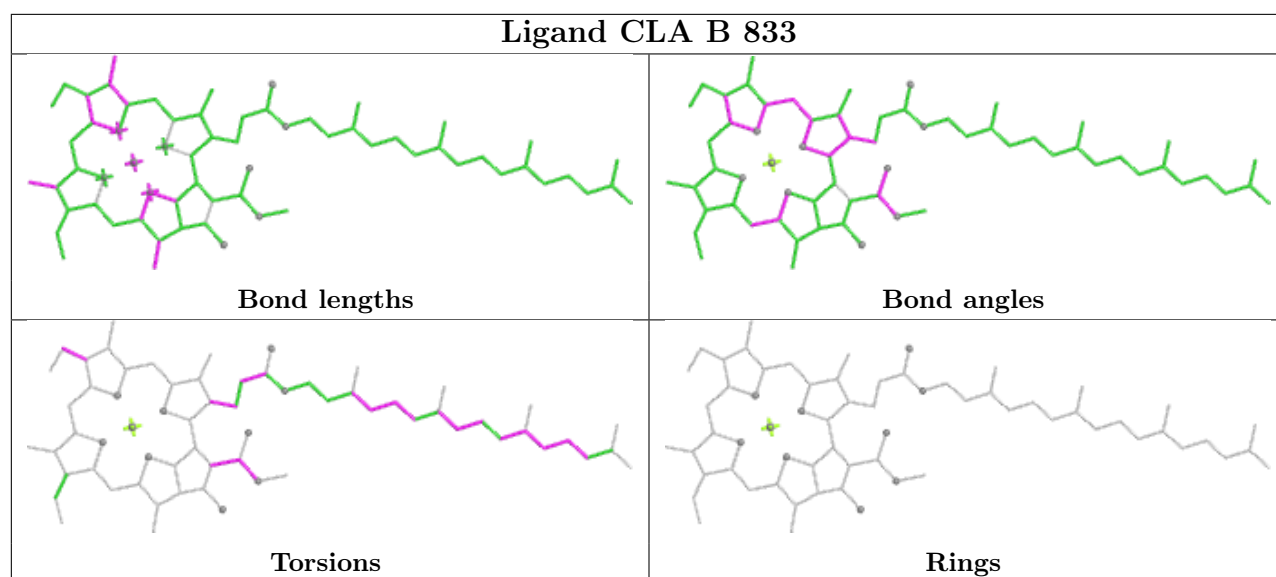


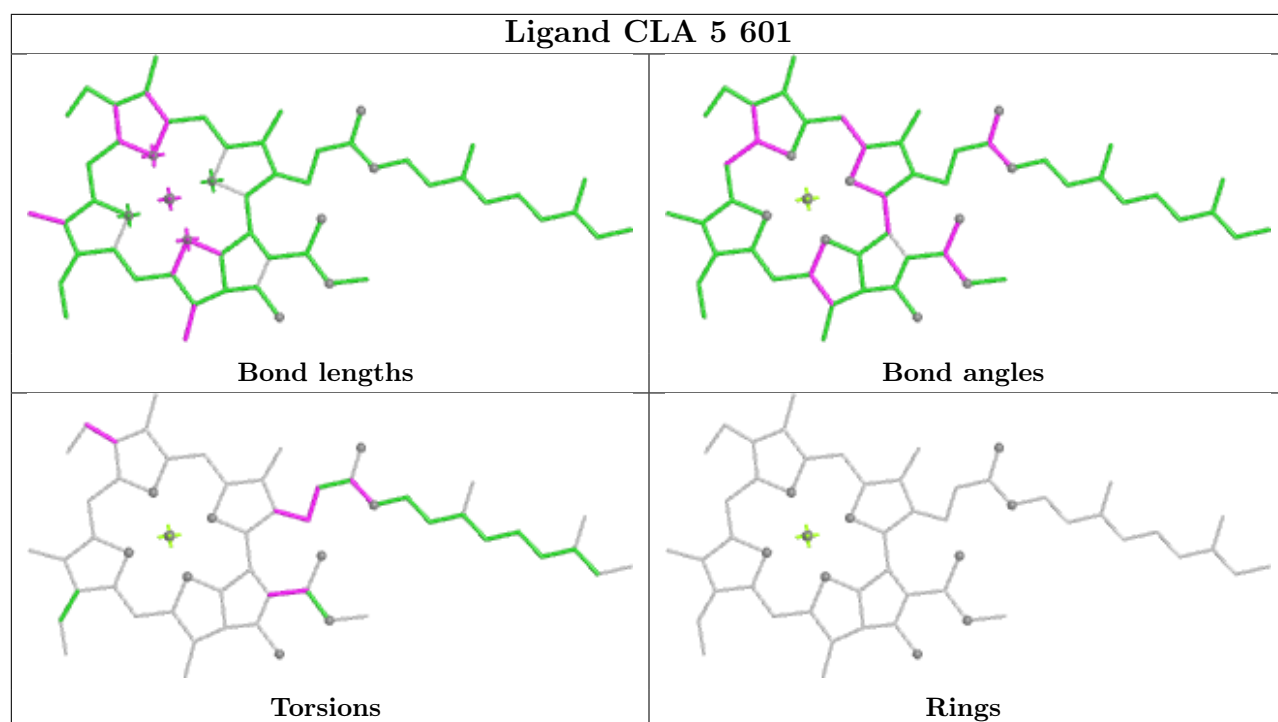
Ligand CLA 6 608



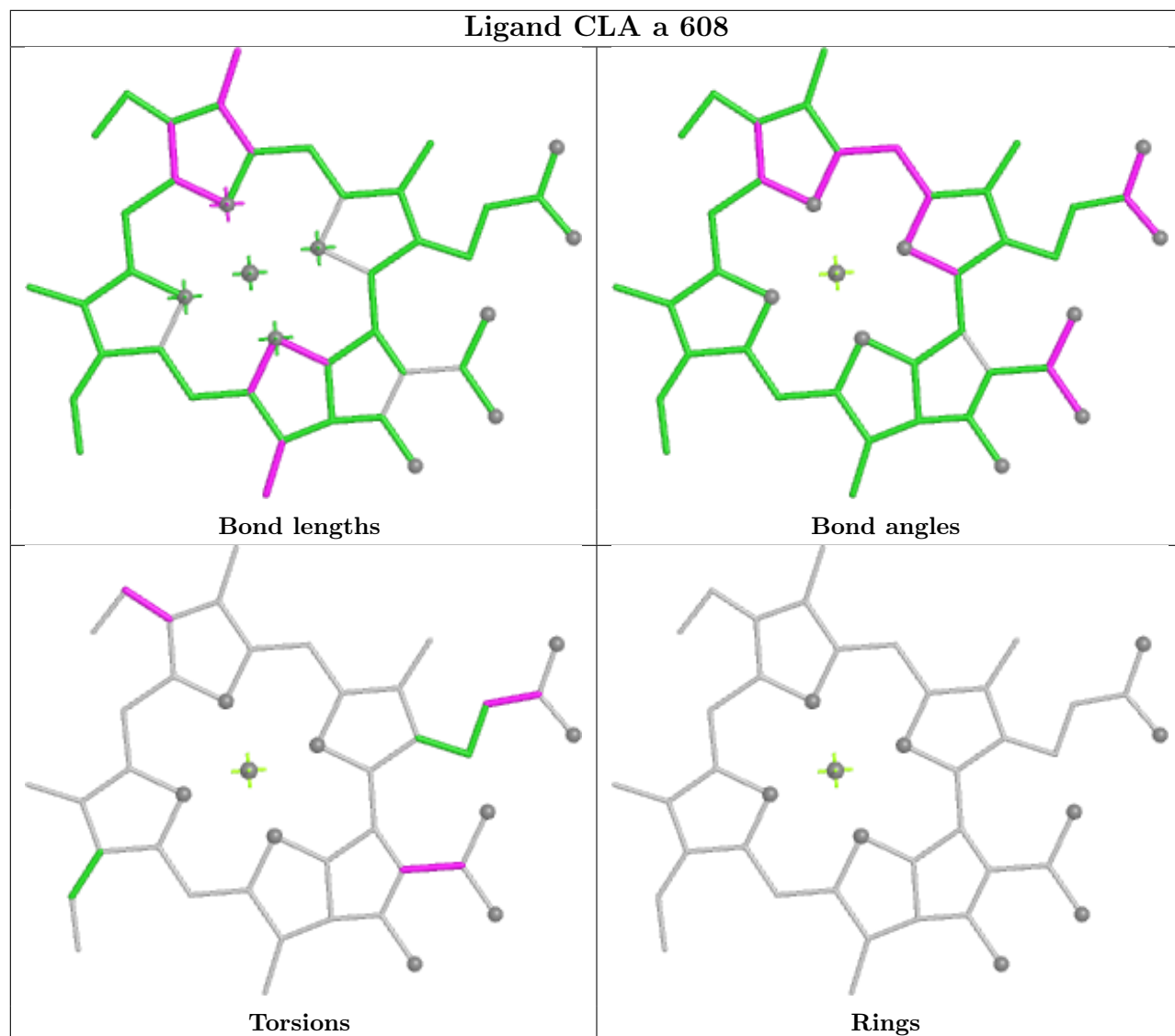




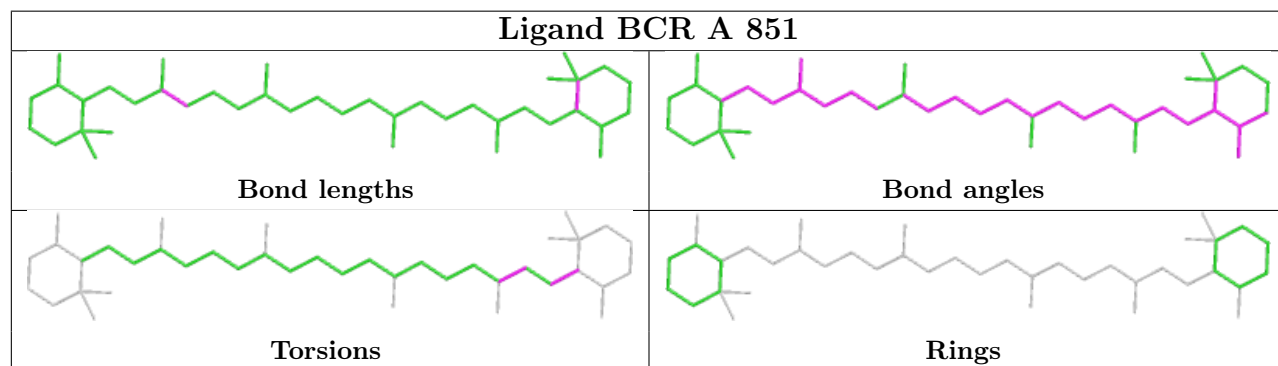


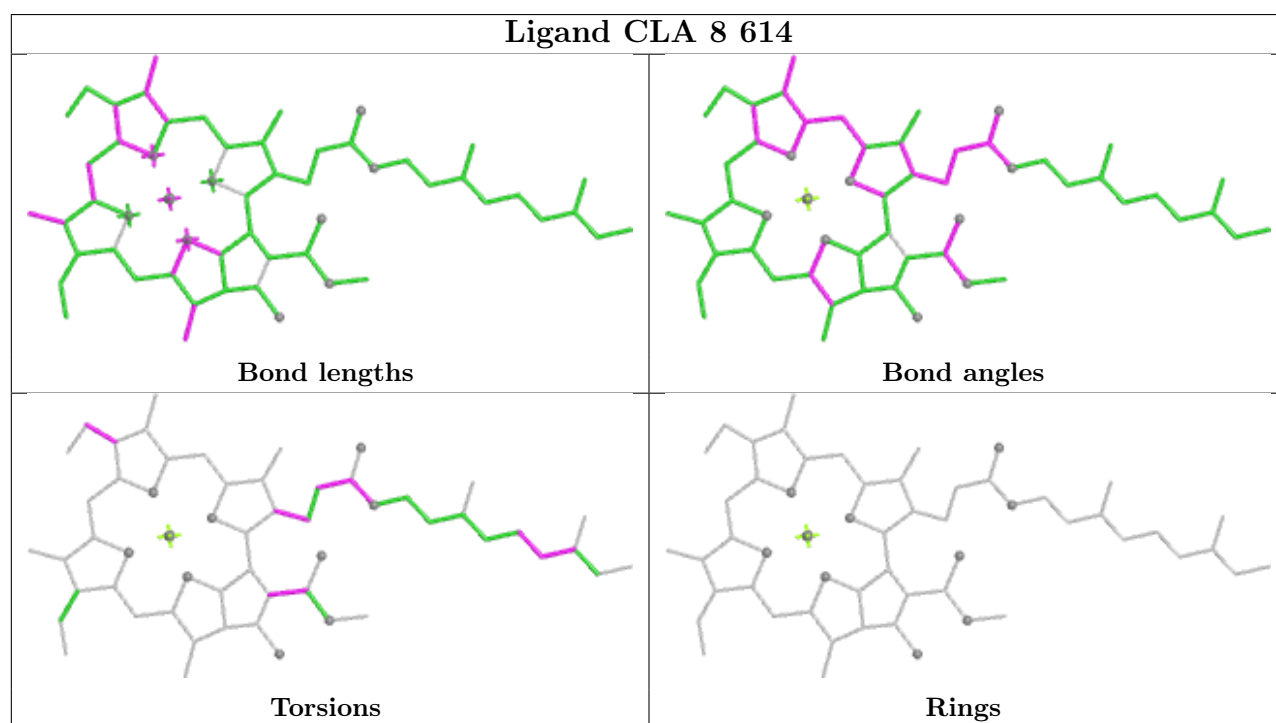
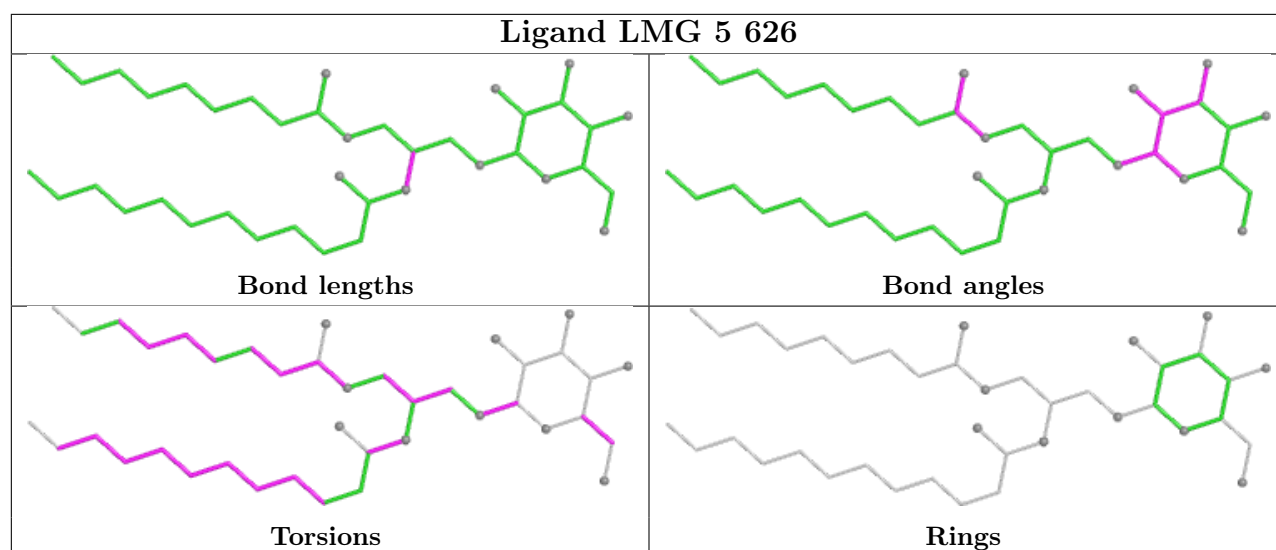


Ligand CLA a 608

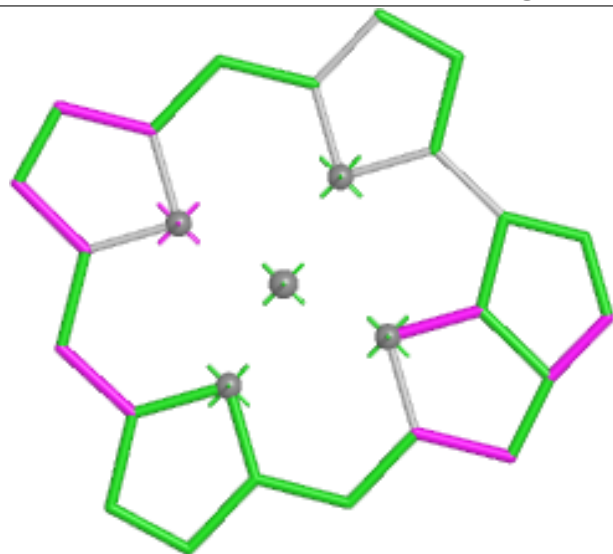


Ligand BCR A 851

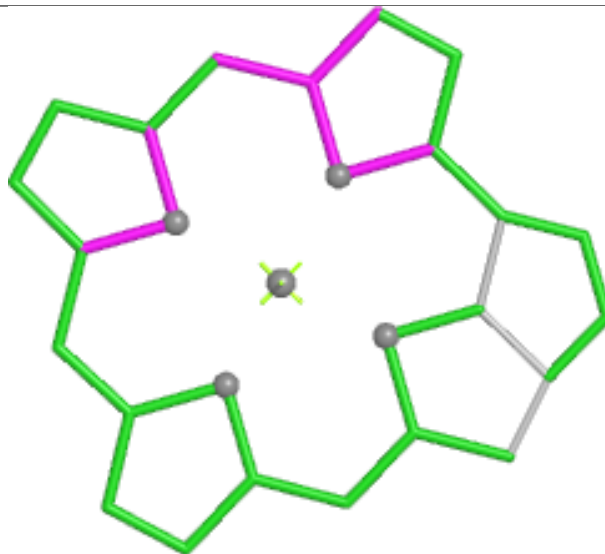




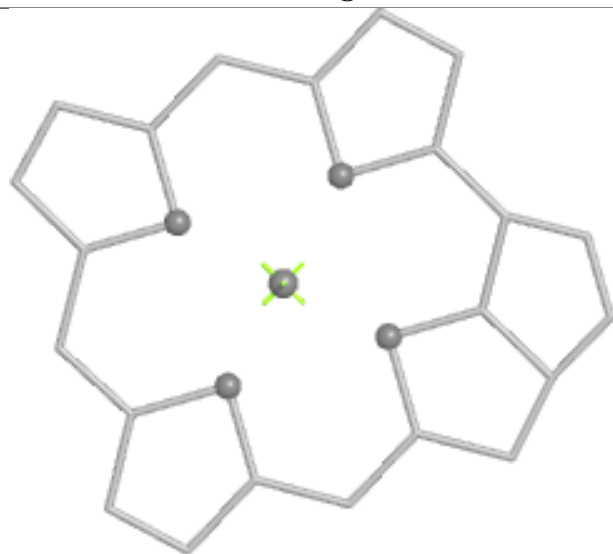
Ligand CLA 9 609



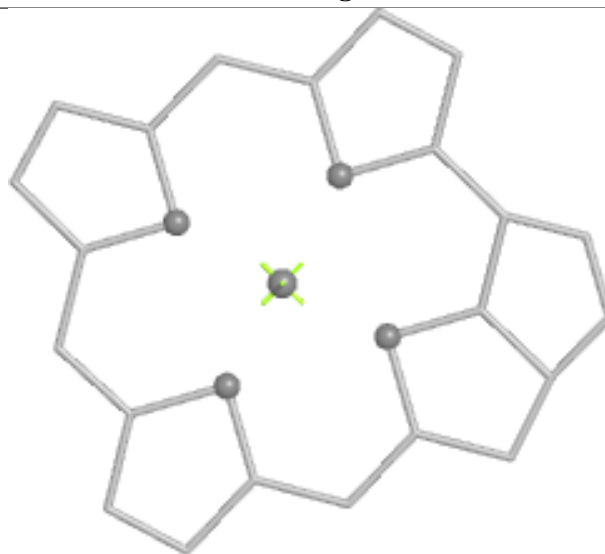
Bond lengths



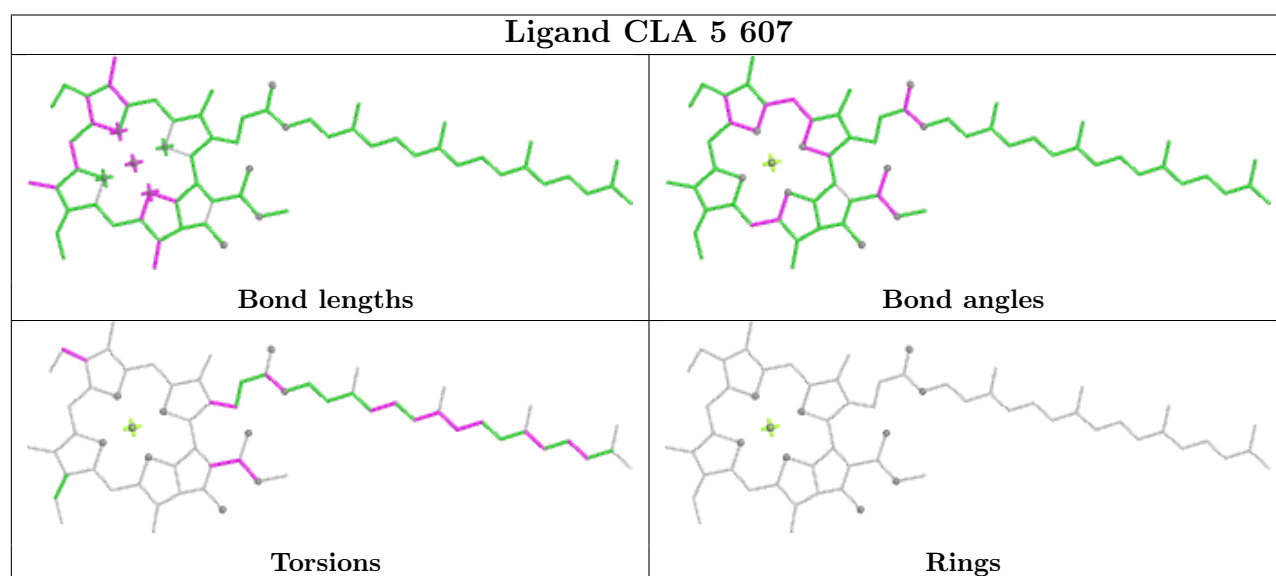
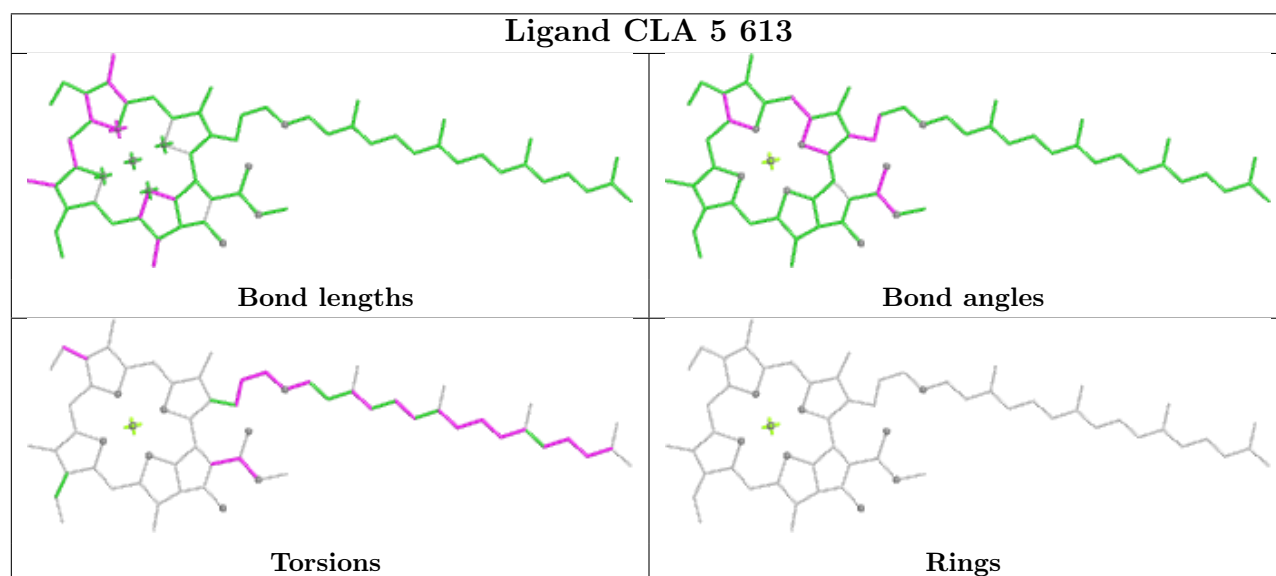
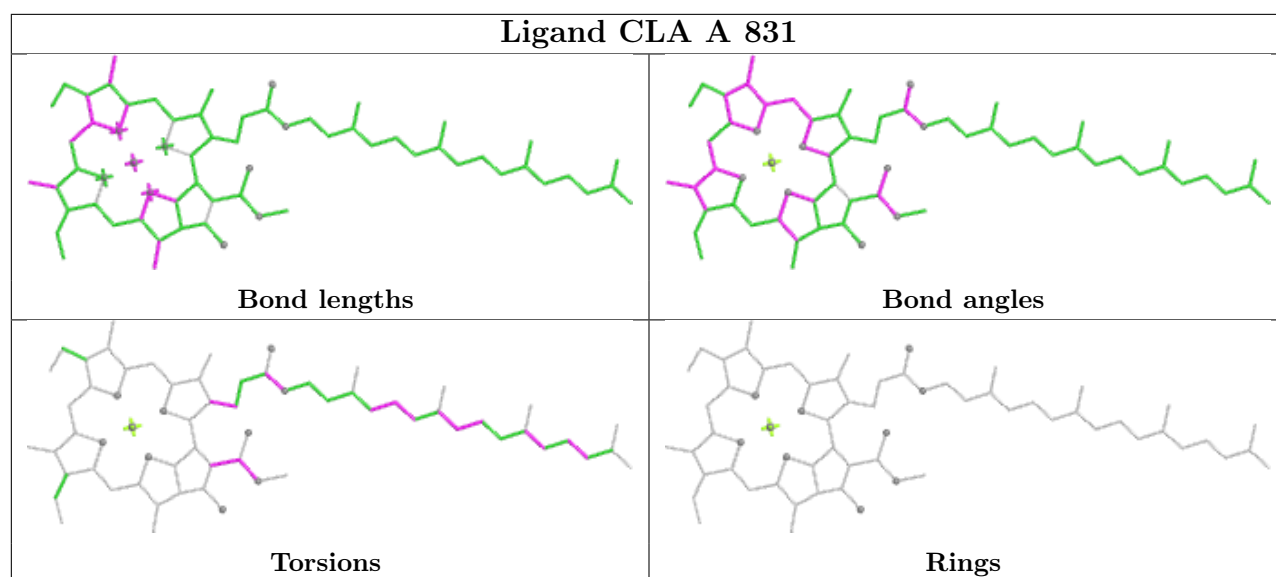
Bond angles



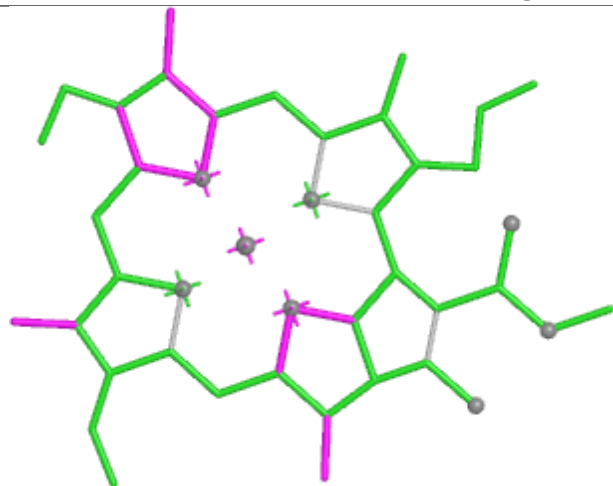
Torsions



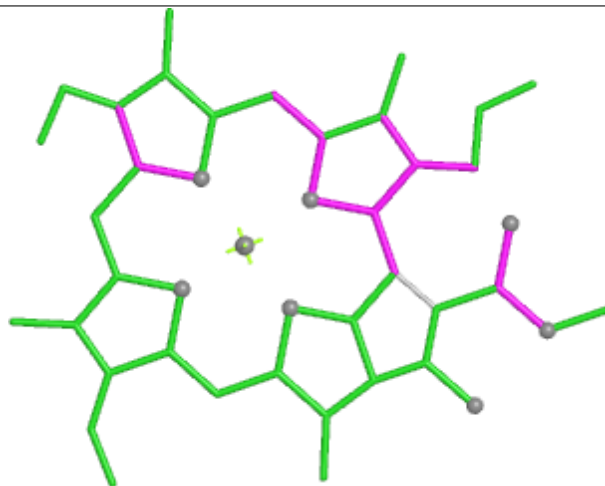
Rings



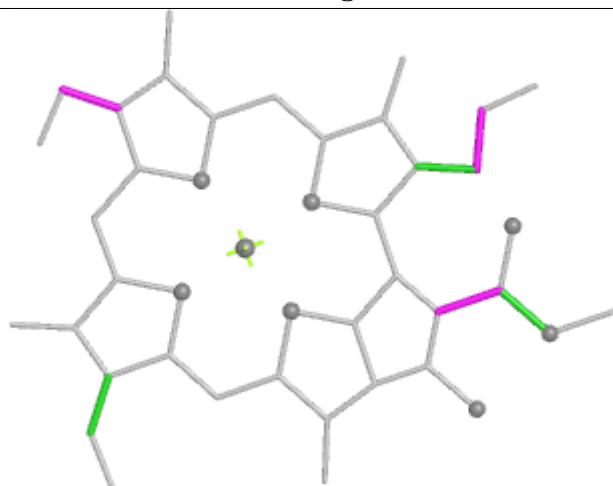
Ligand CLA 3 612



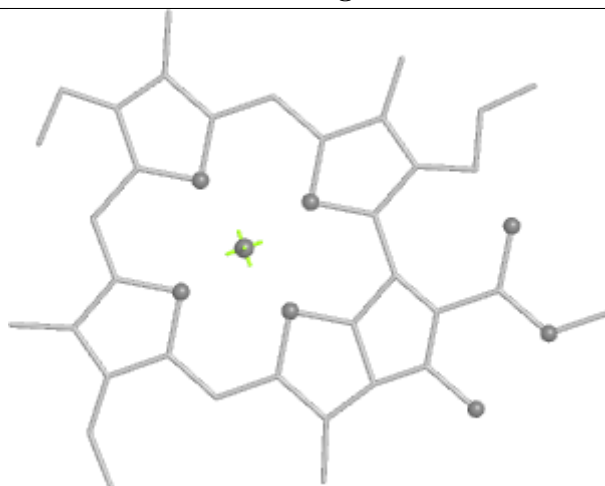
Bond lengths



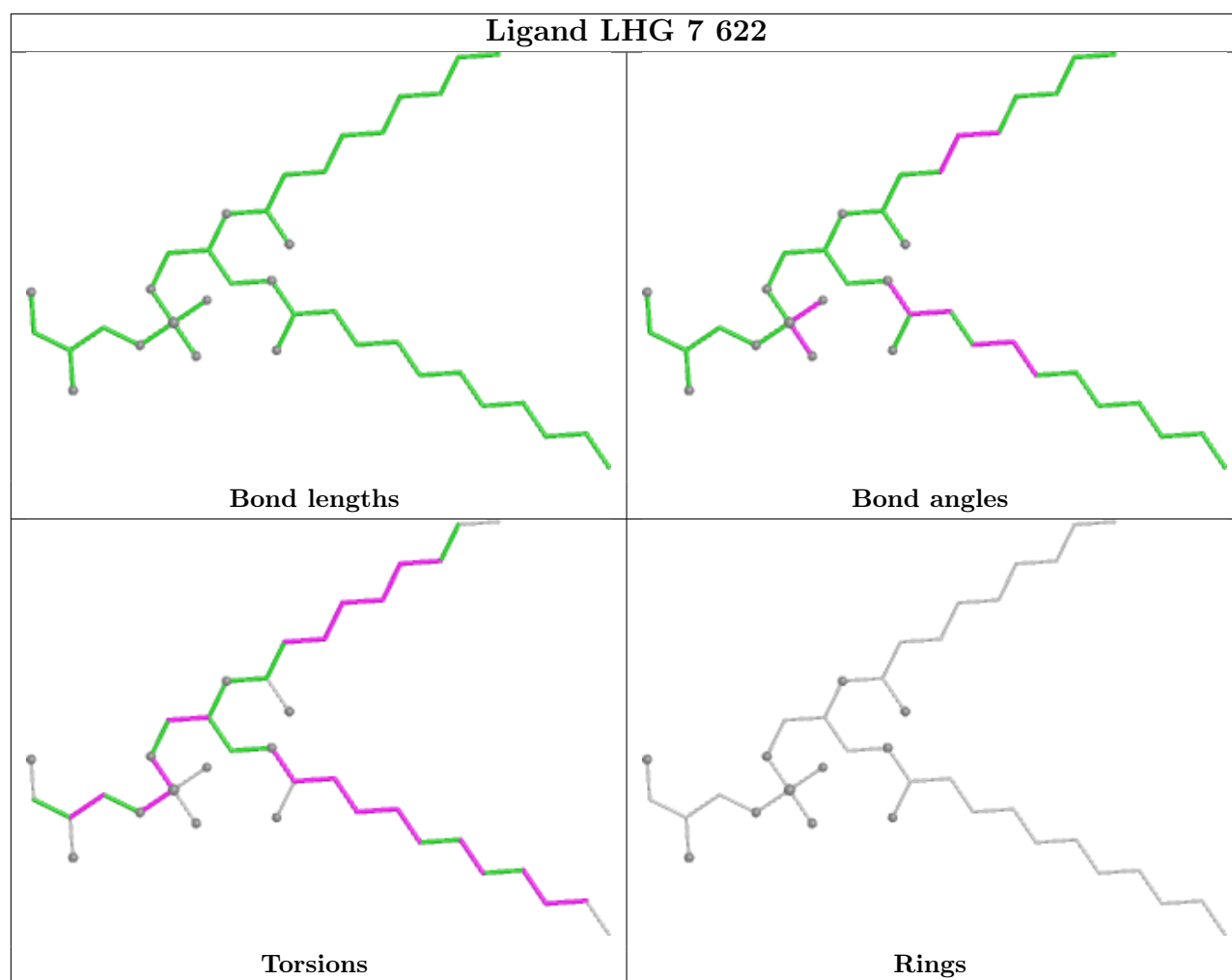
Bond angles

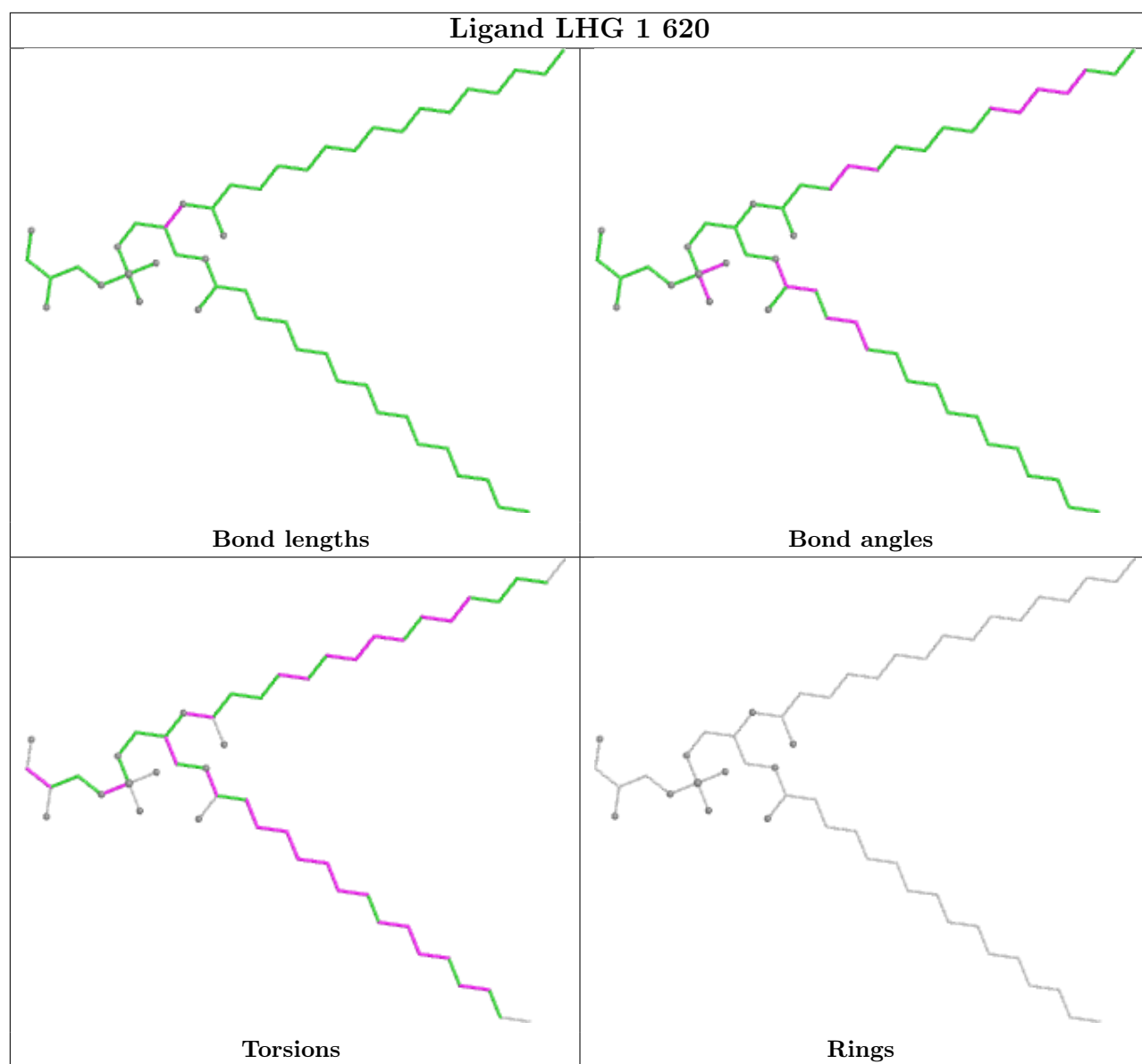


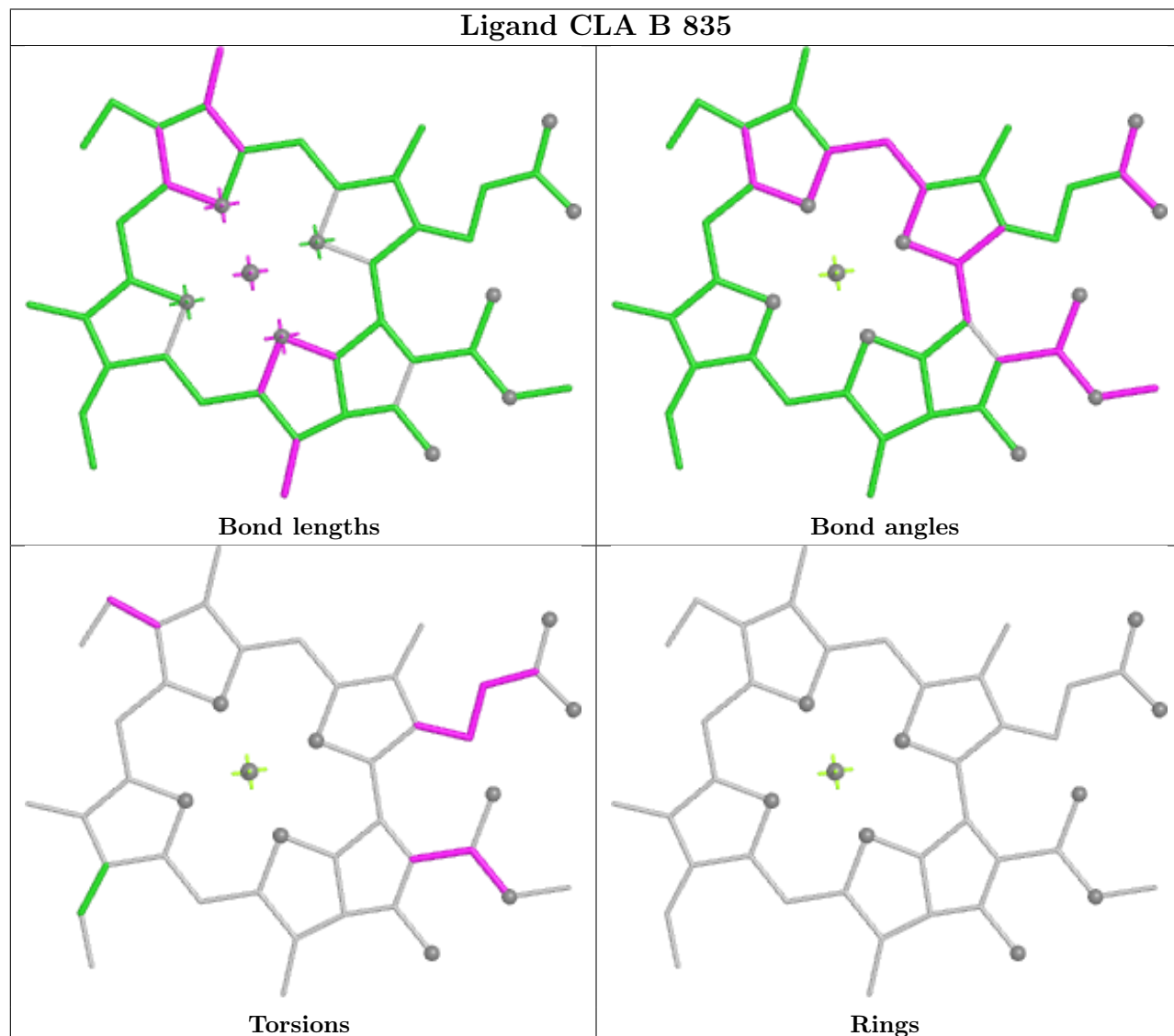
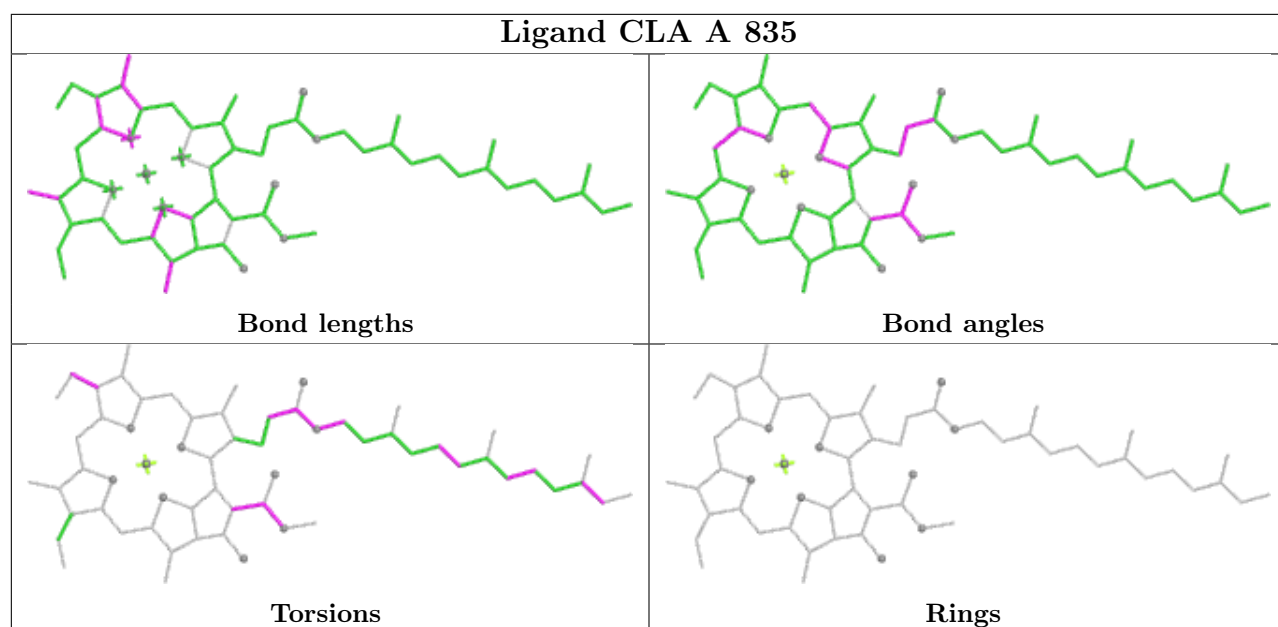
Torsions



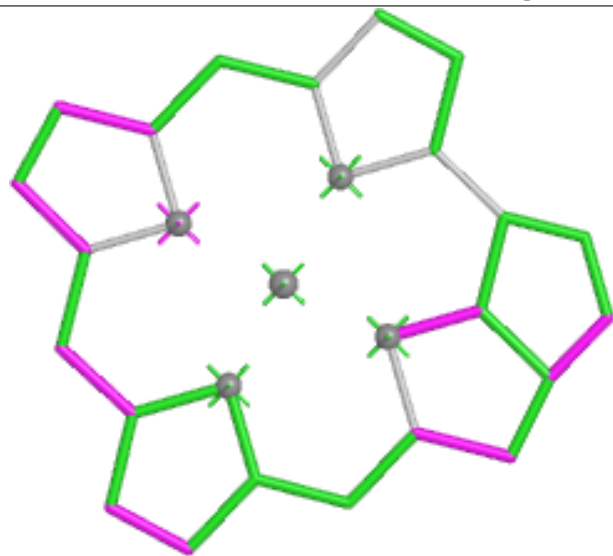
Rings



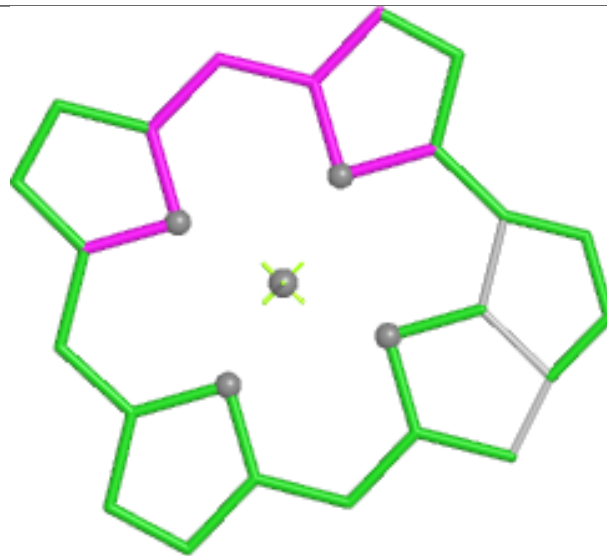




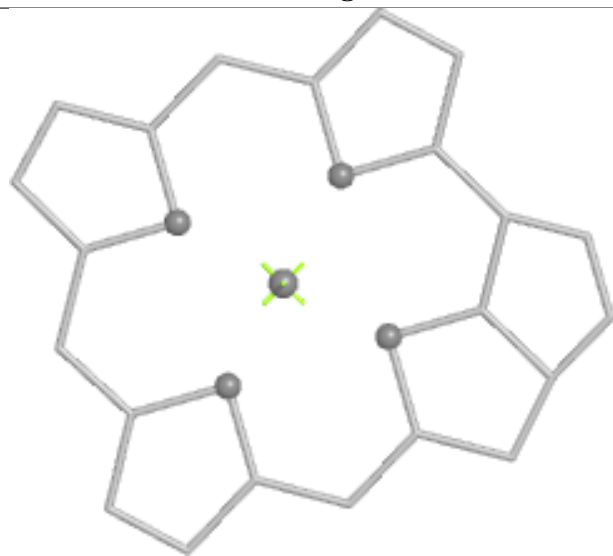
Ligand CLA 9 603



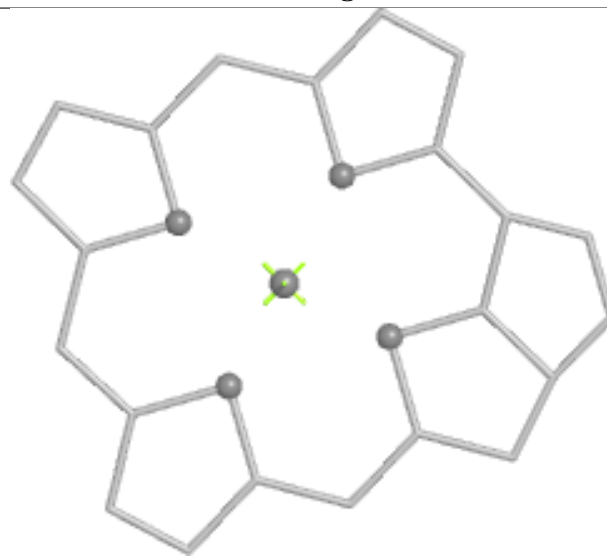
Bond lengths



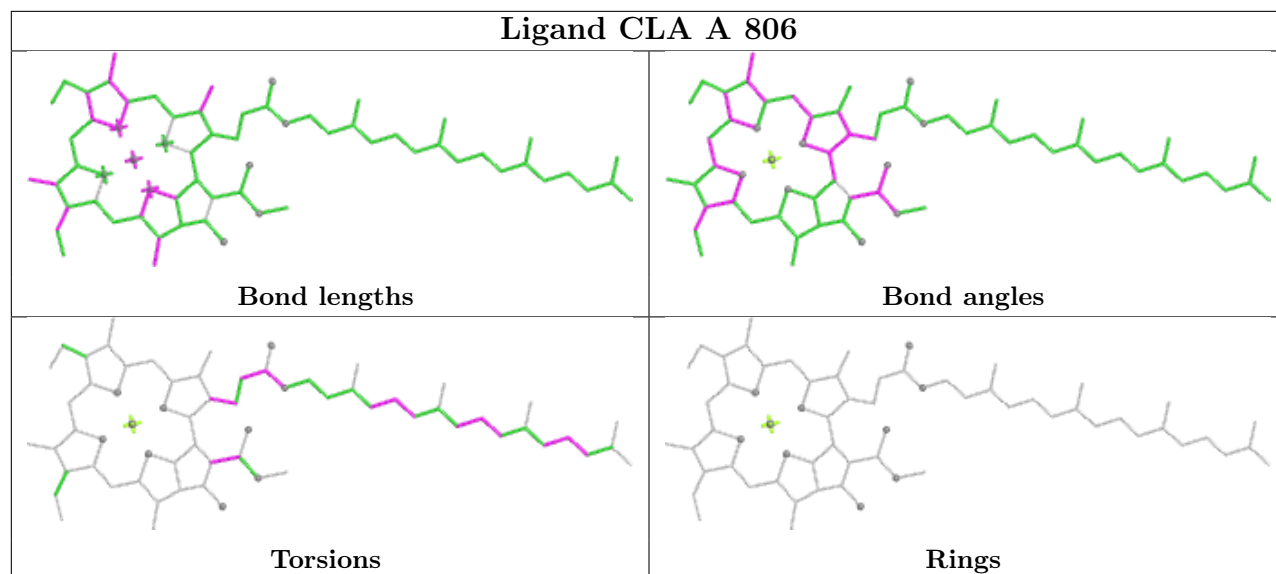
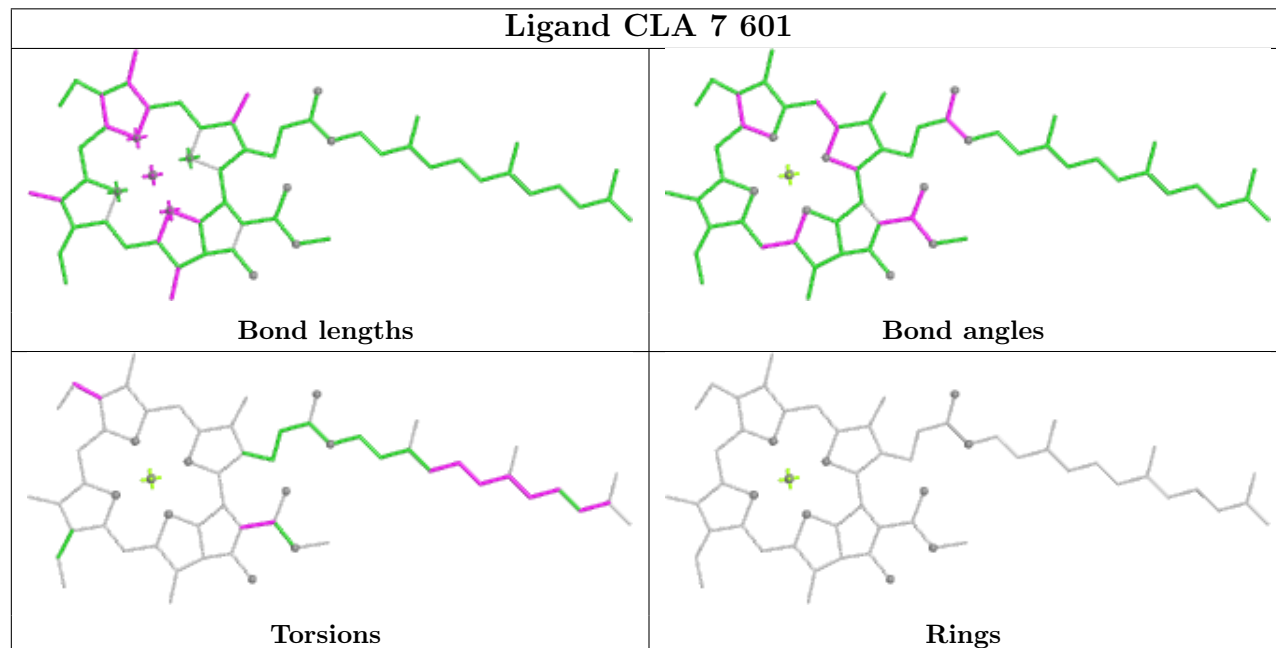
Bond angles

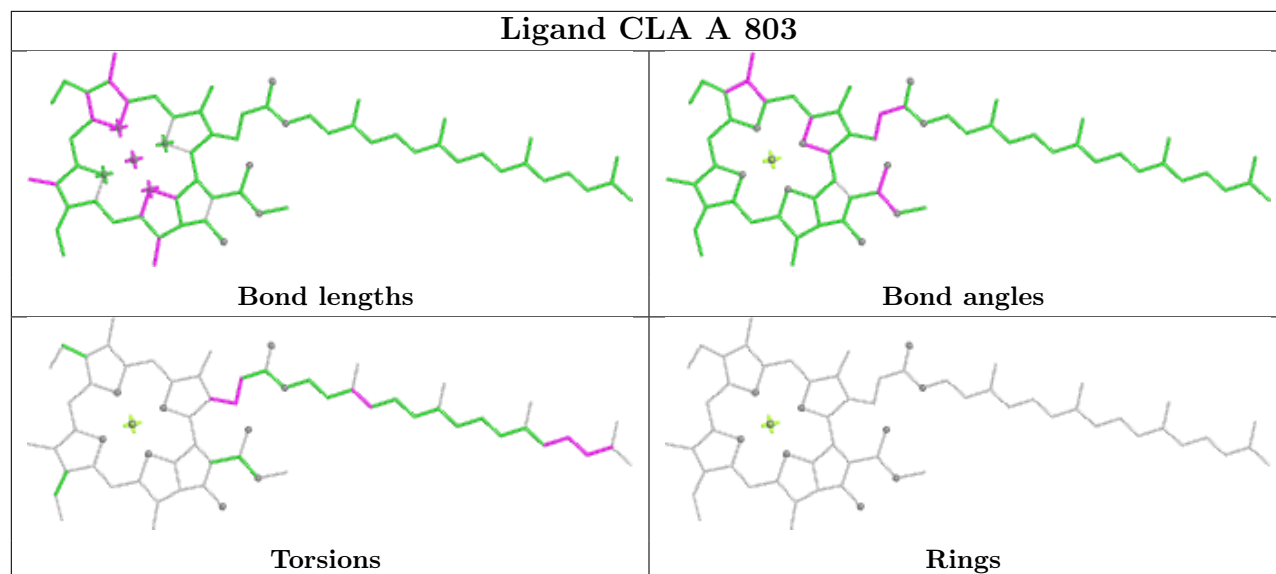
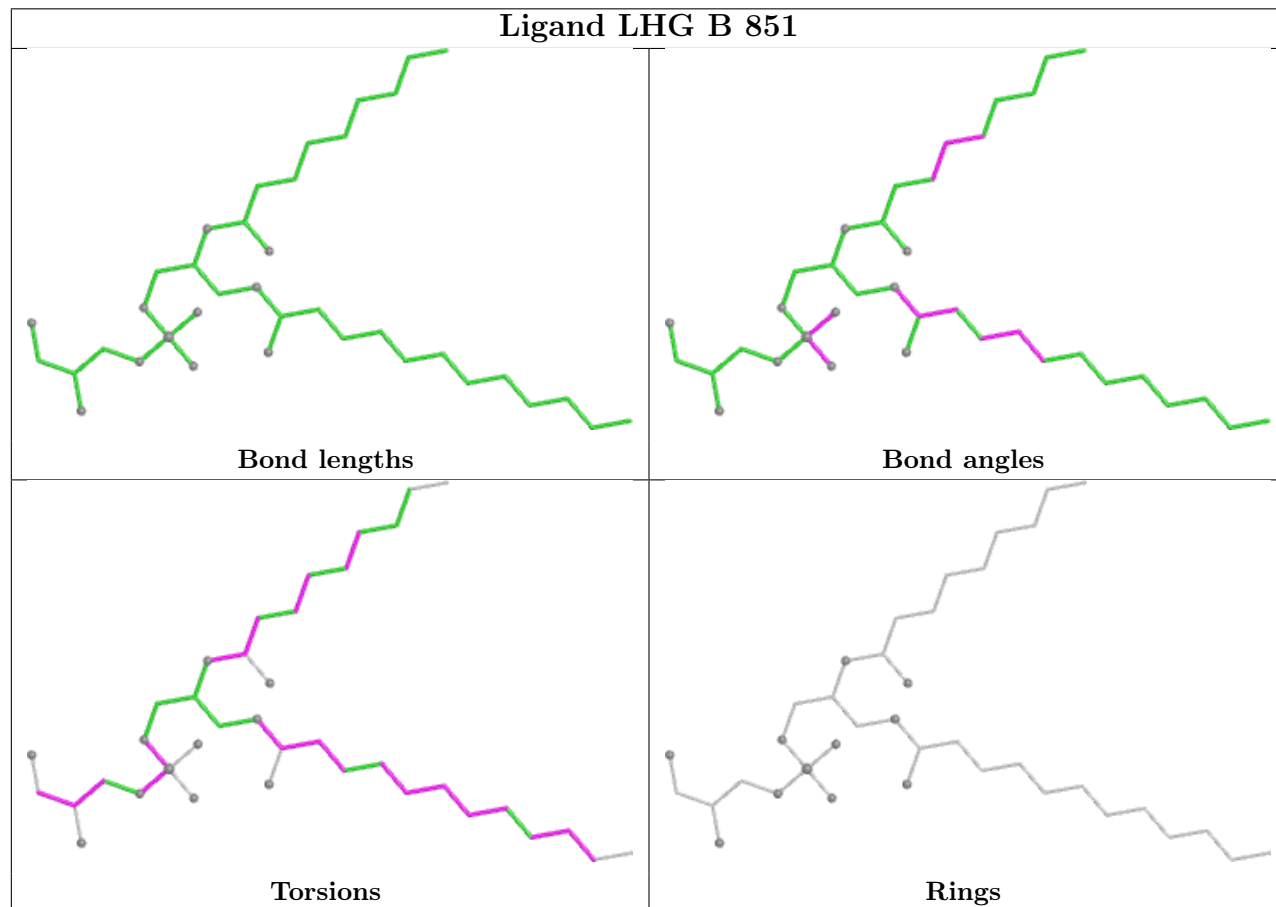


Torsions

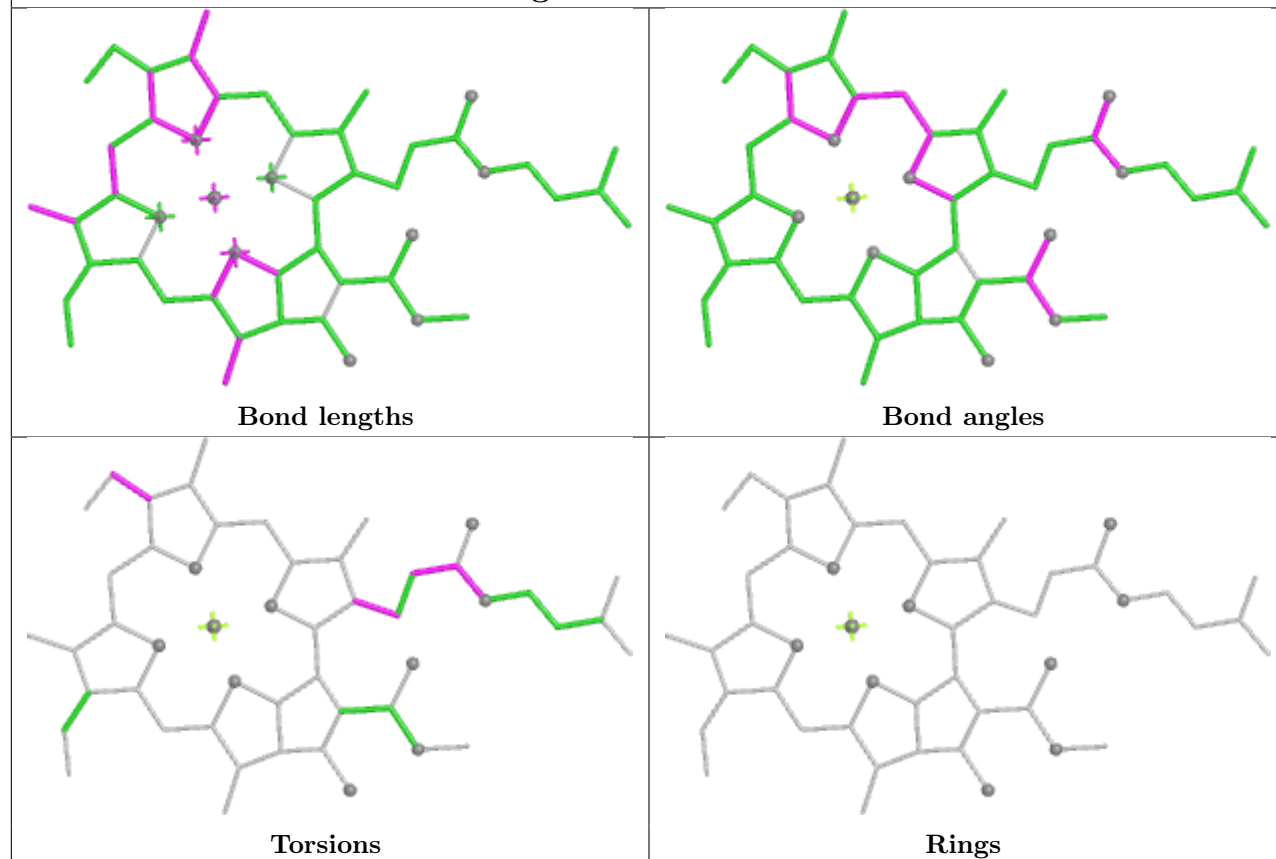


Rings

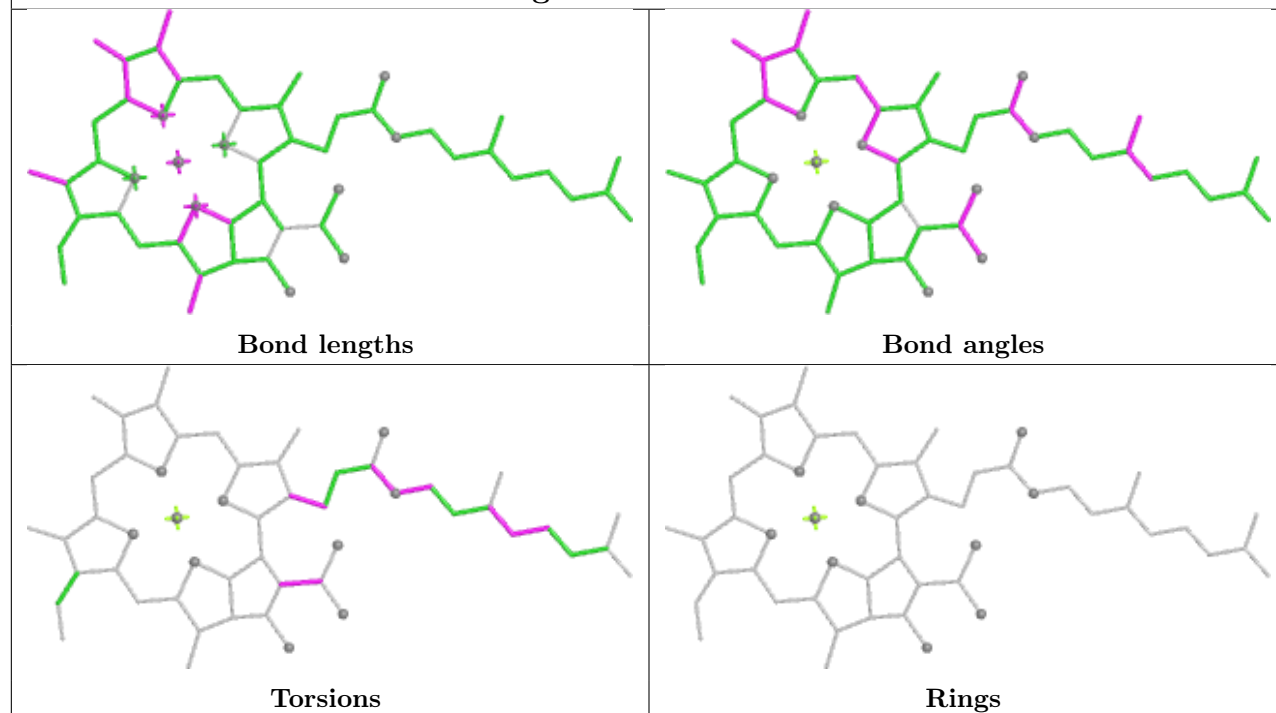
Ligand CLA A 806**Ligand CLA 7 601**

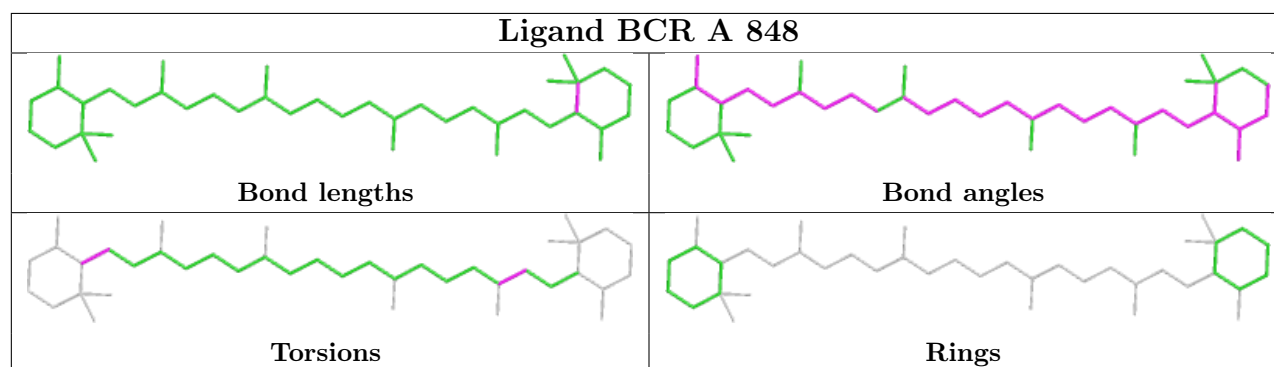
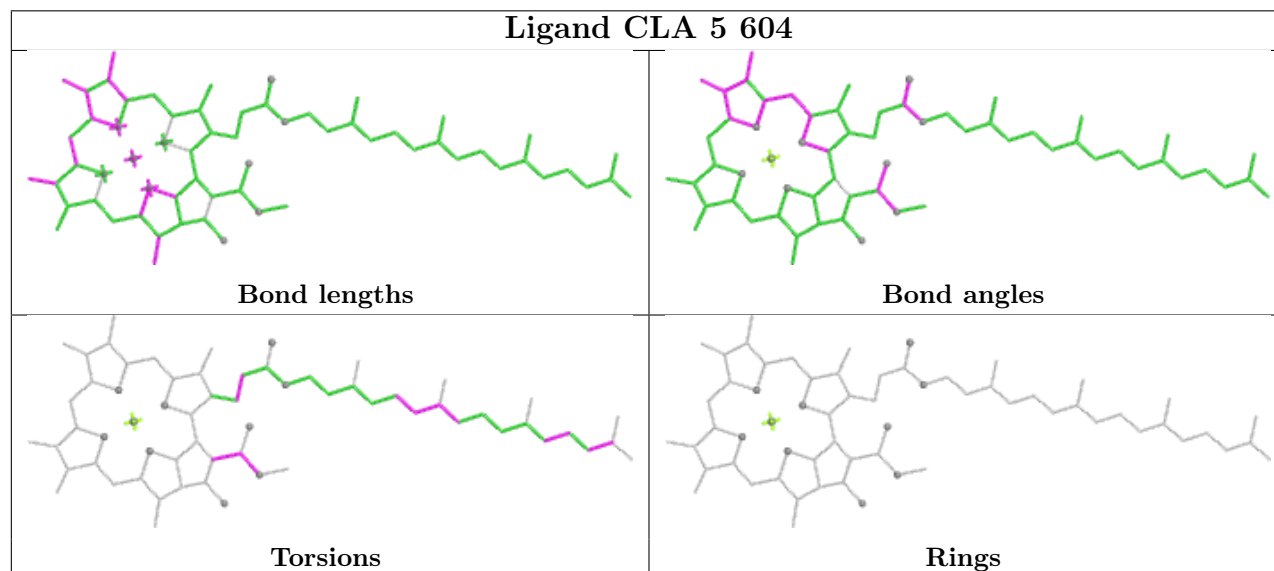
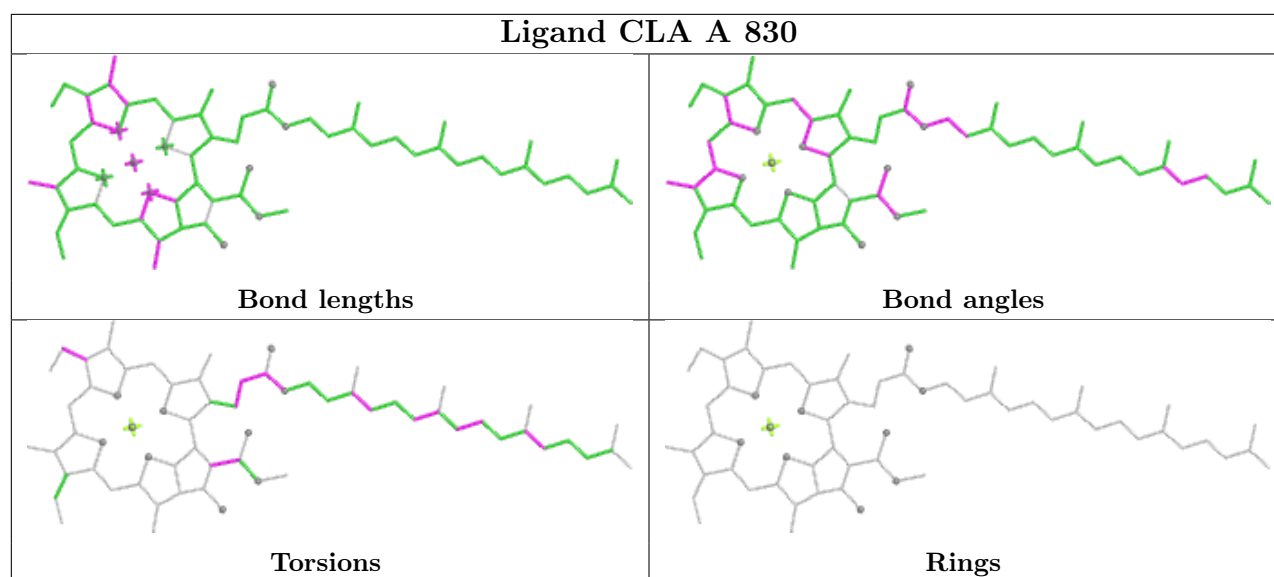
Ligand CLA A 803**Ligand LHG B 851**

Ligand CLA A 810

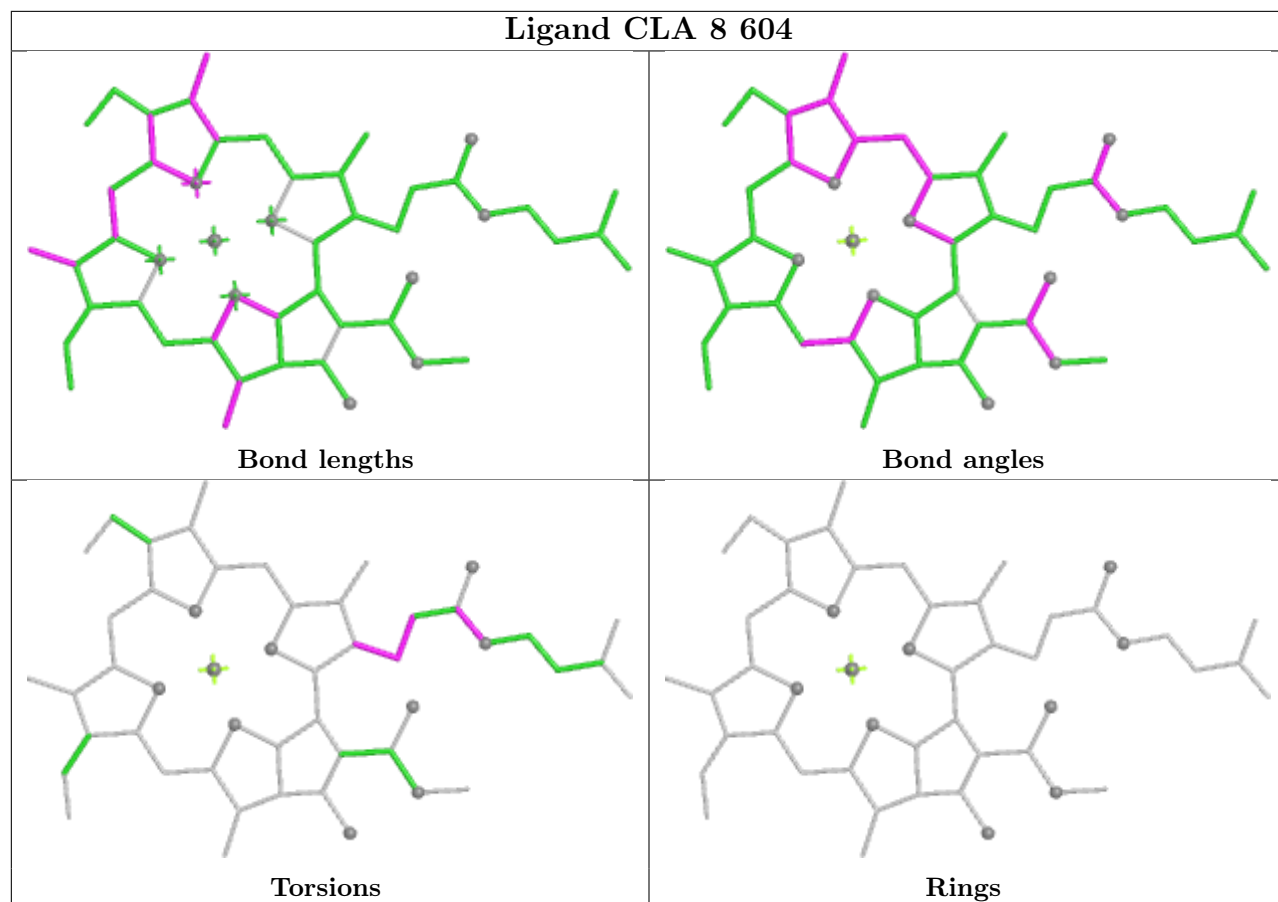


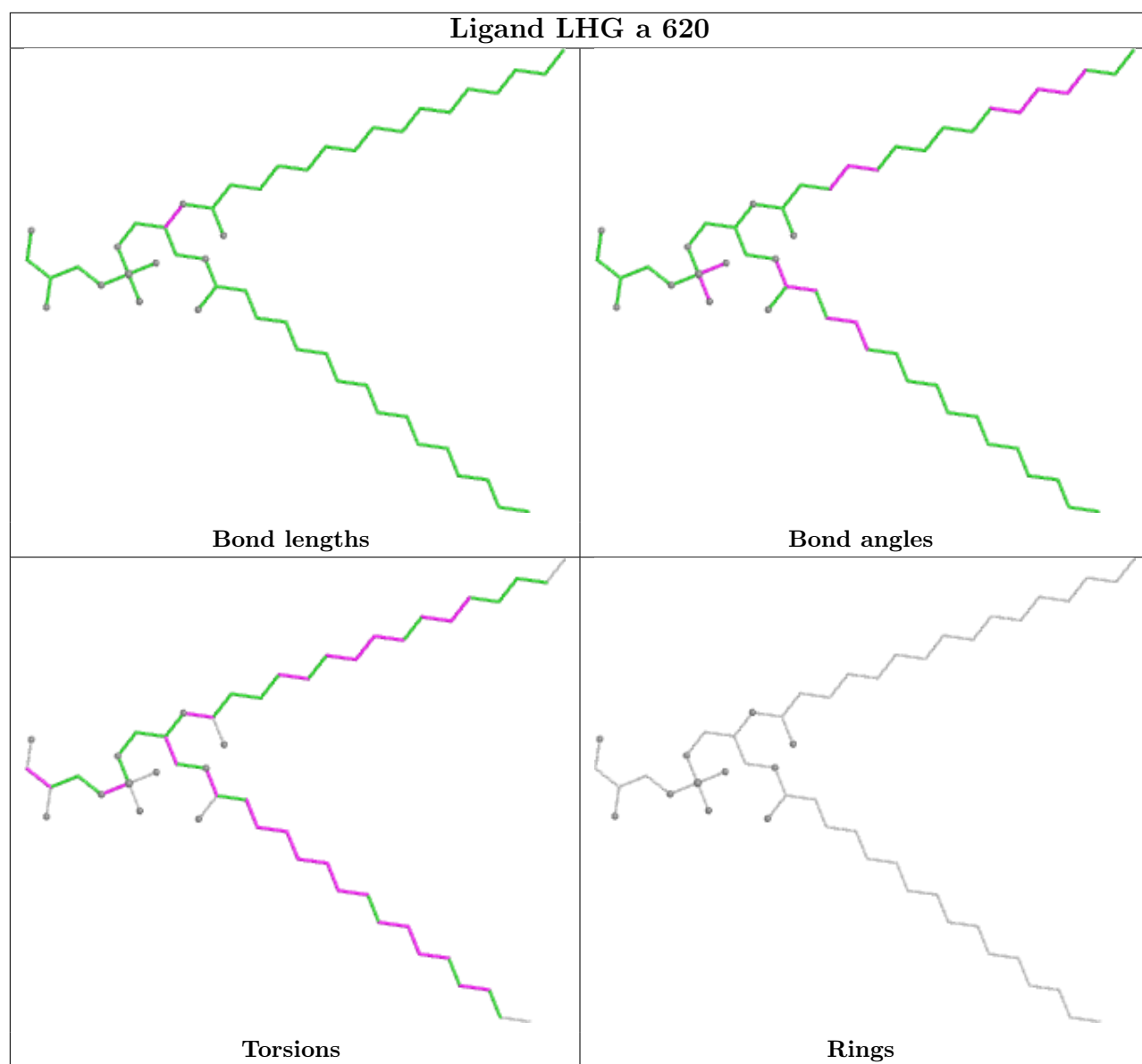
Ligand CLA B 811



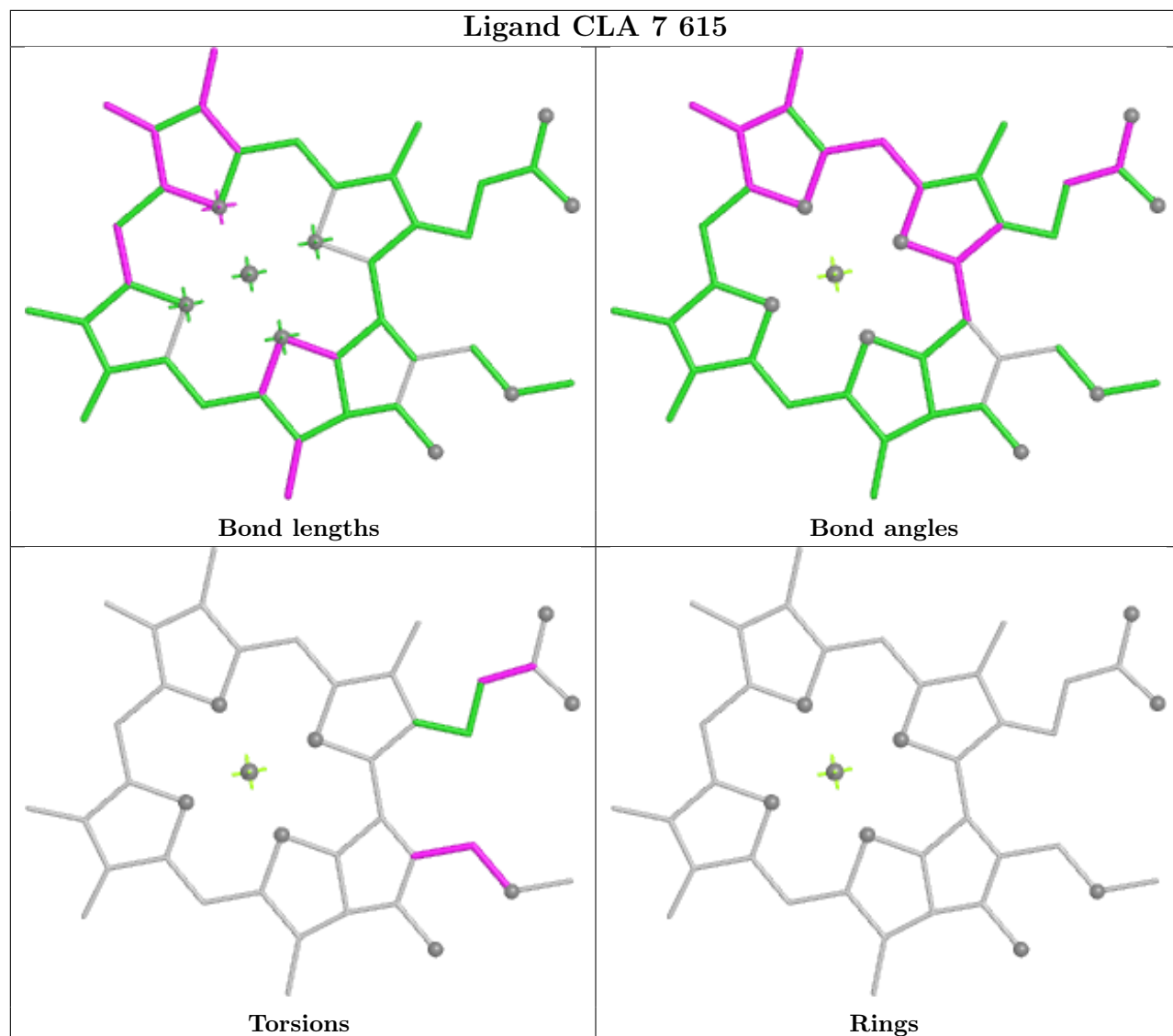


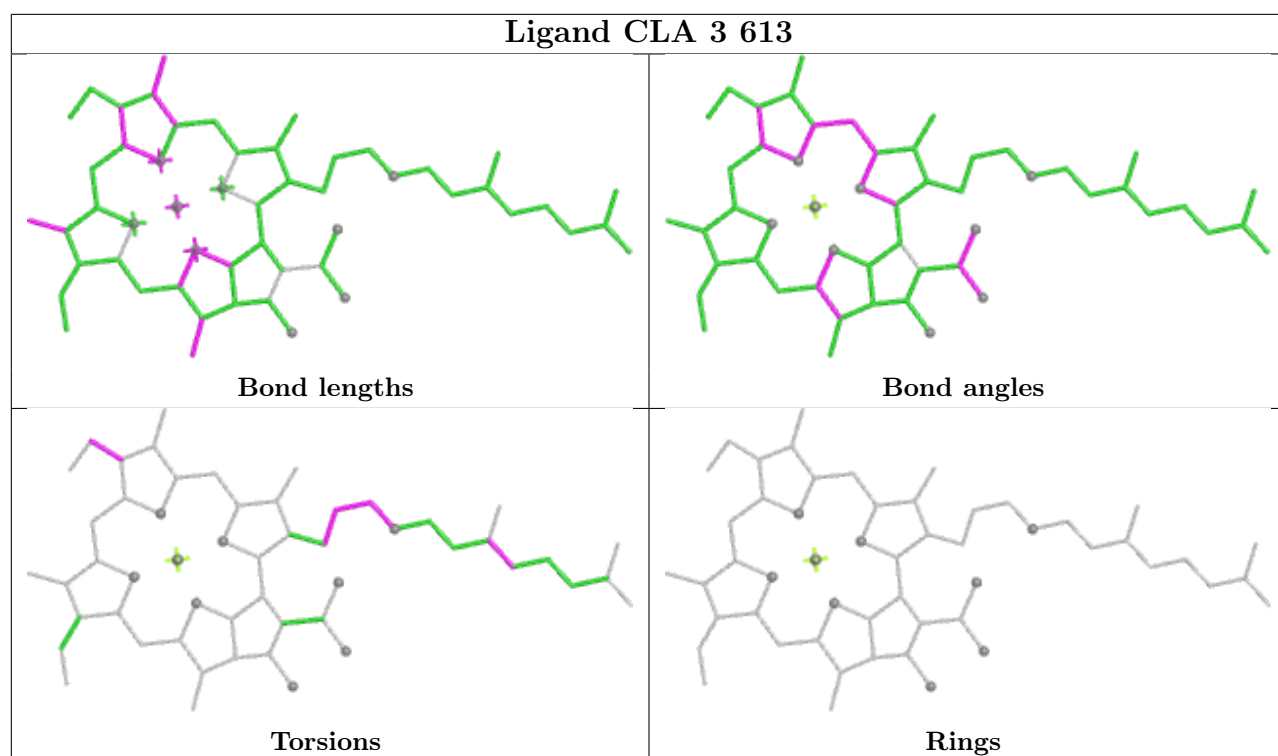
Ligand CLA 8 604

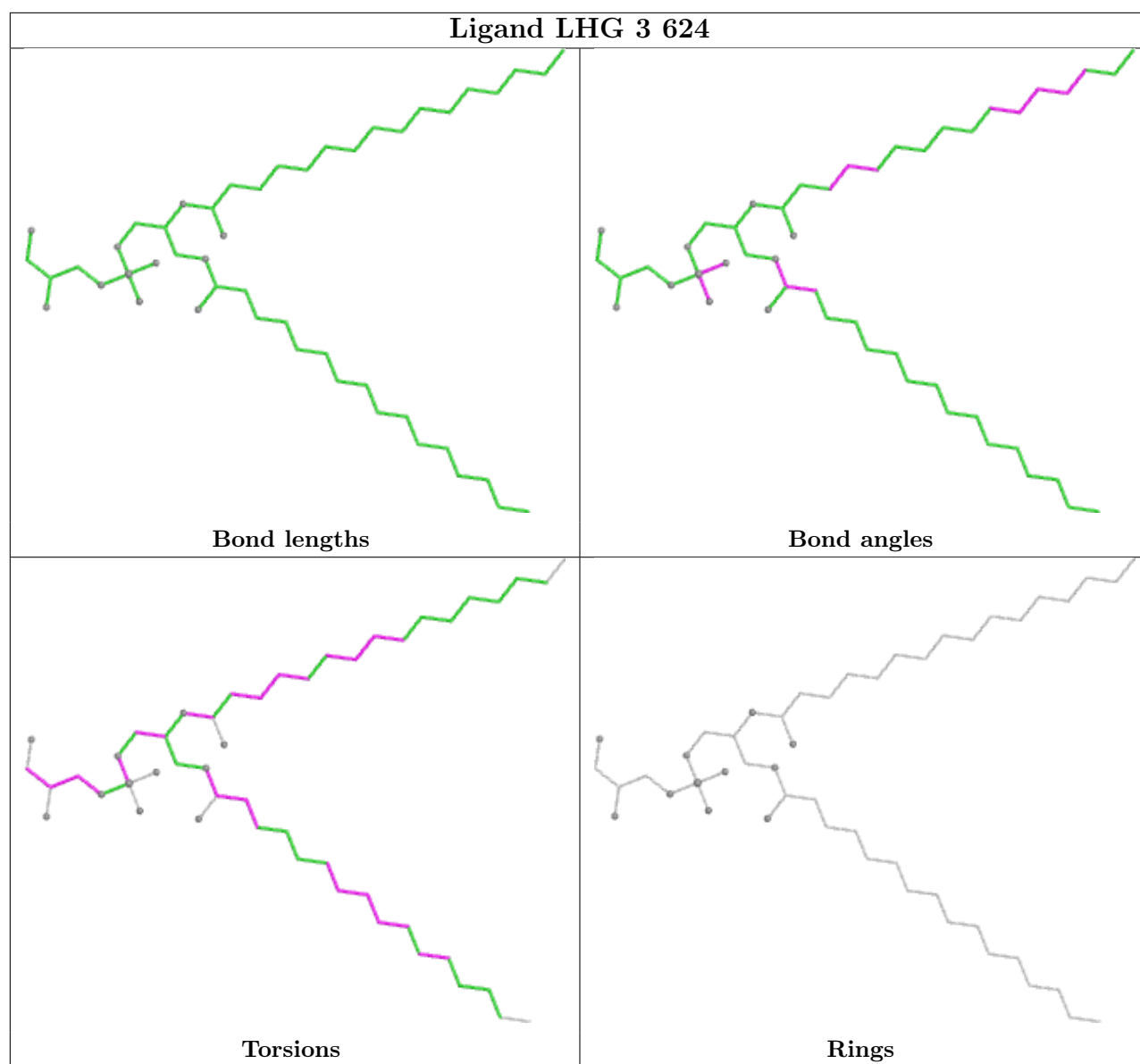




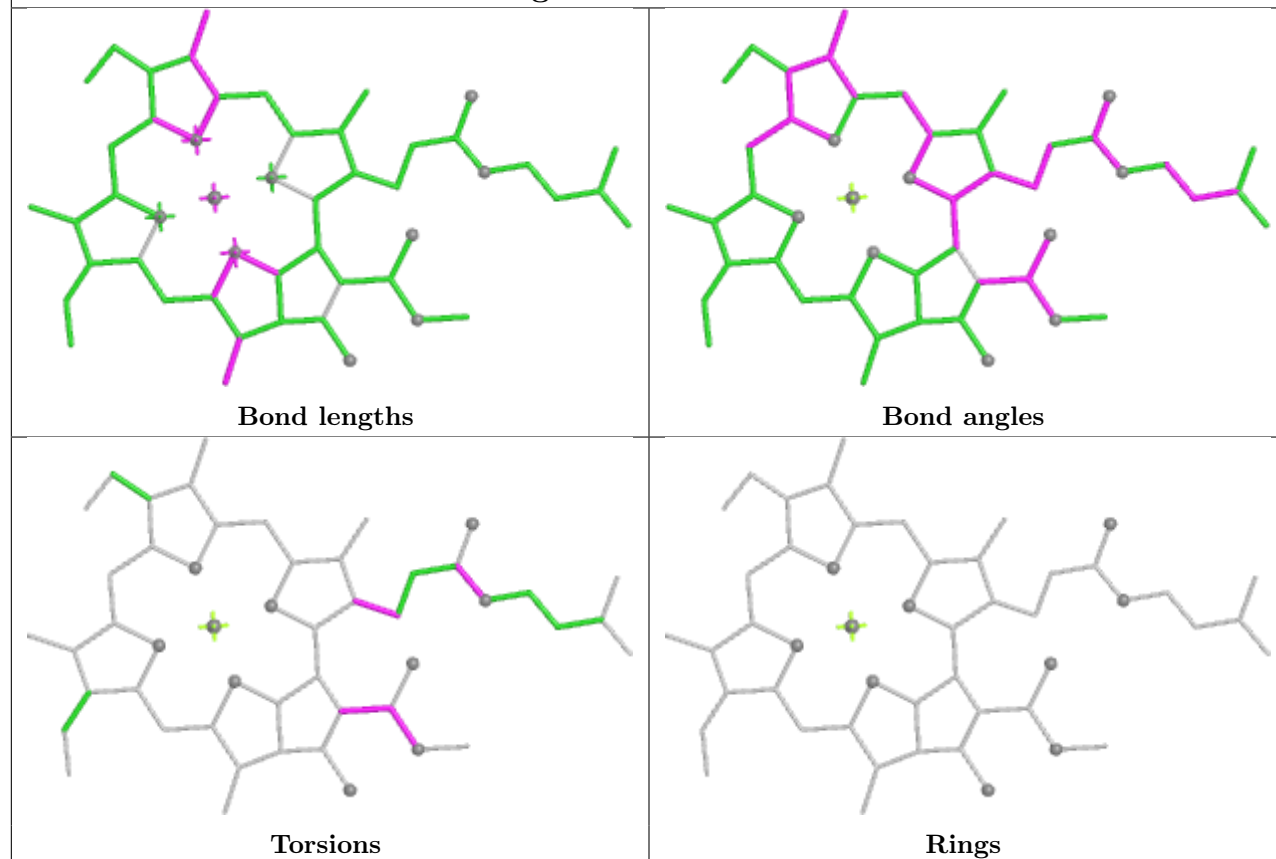
Ligand CLA 7 615



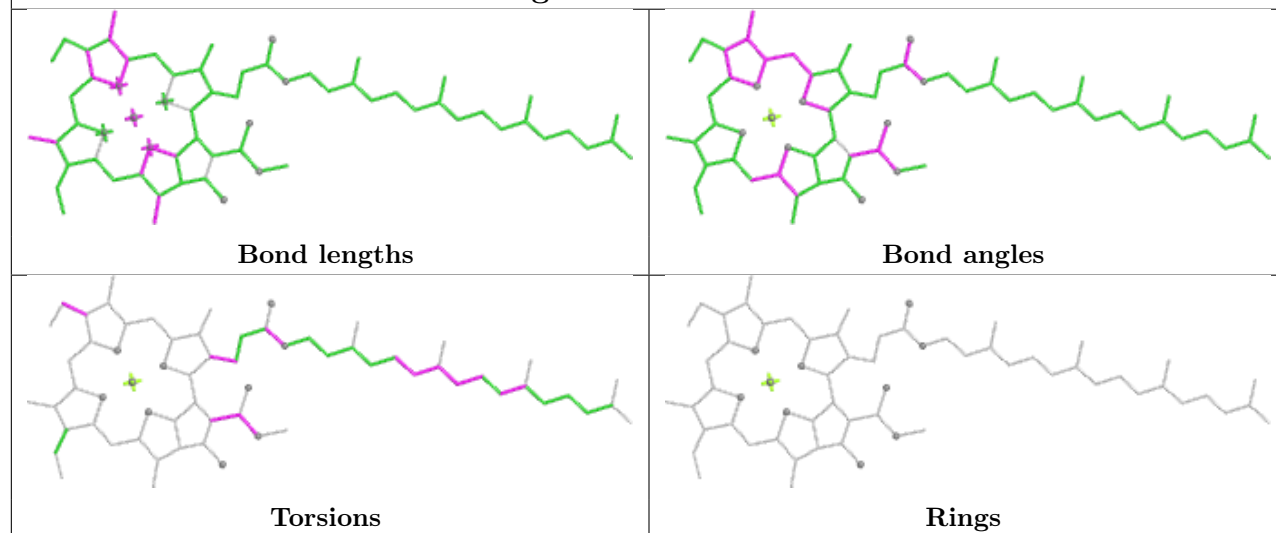




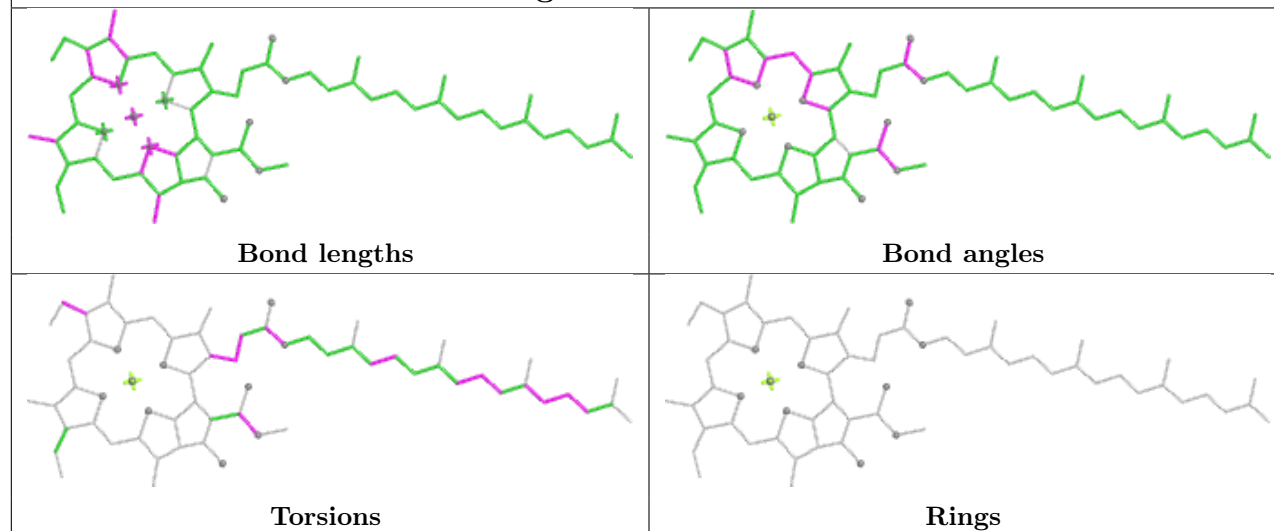
Ligand CLA A 838



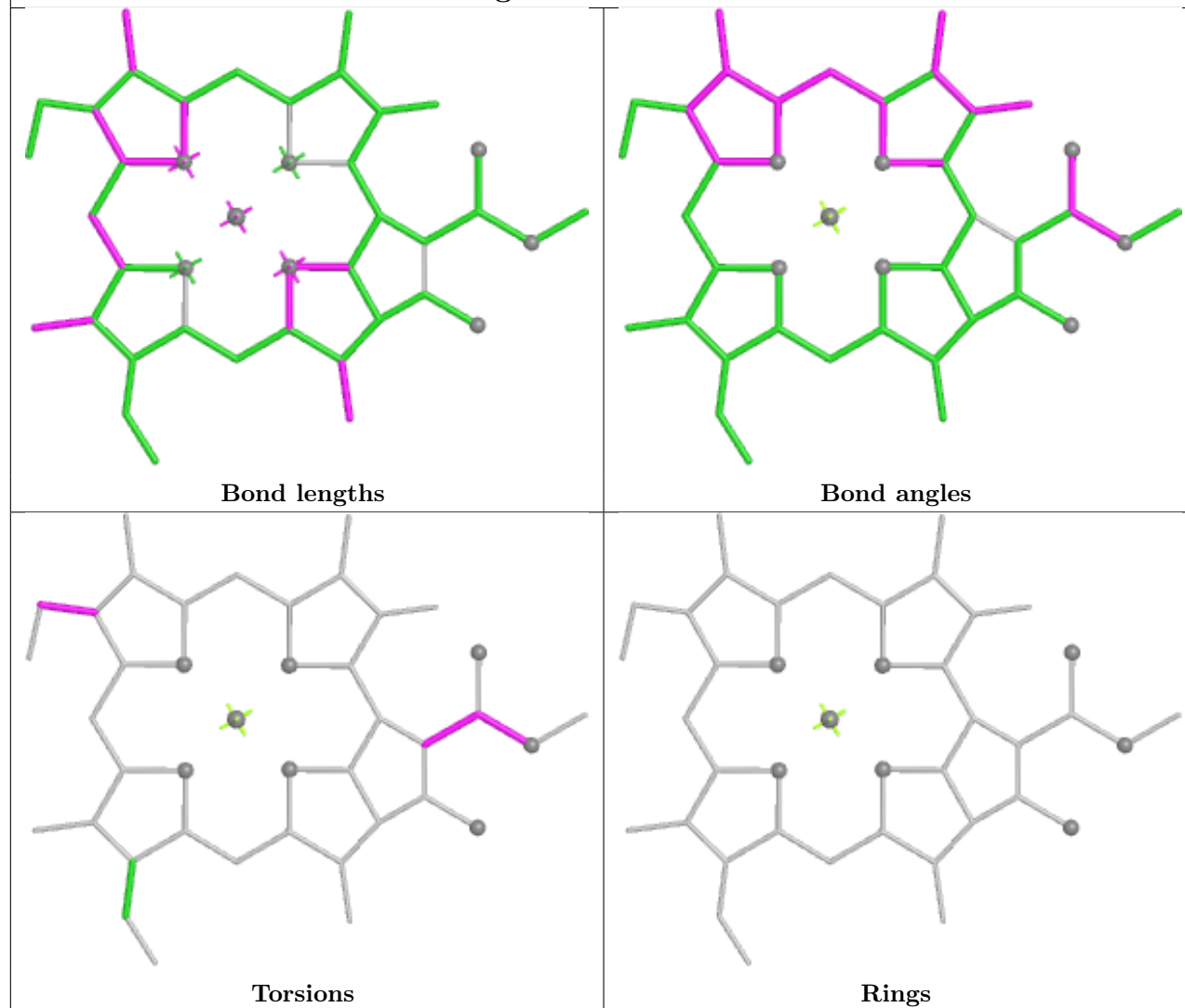
Ligand CLA A 811

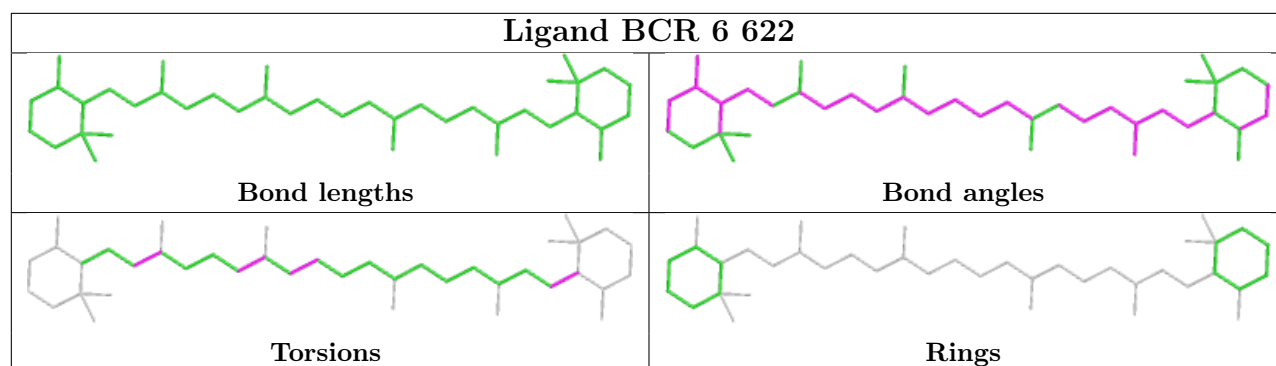
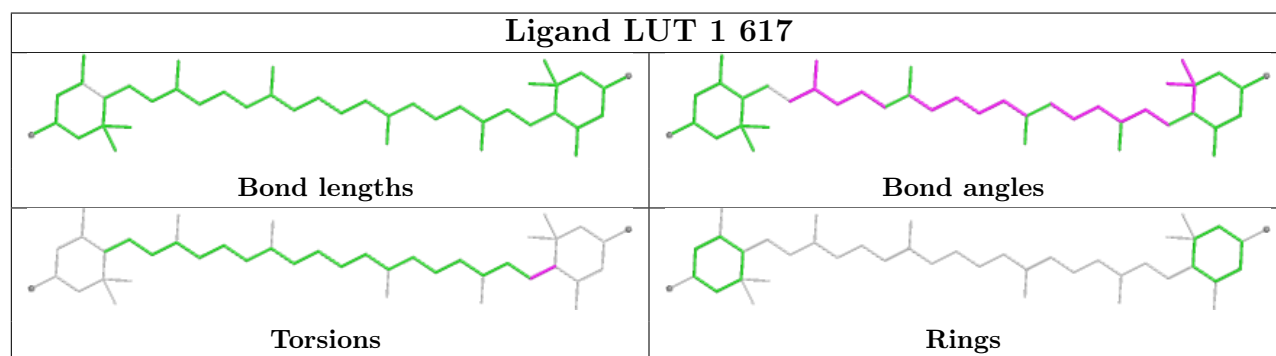
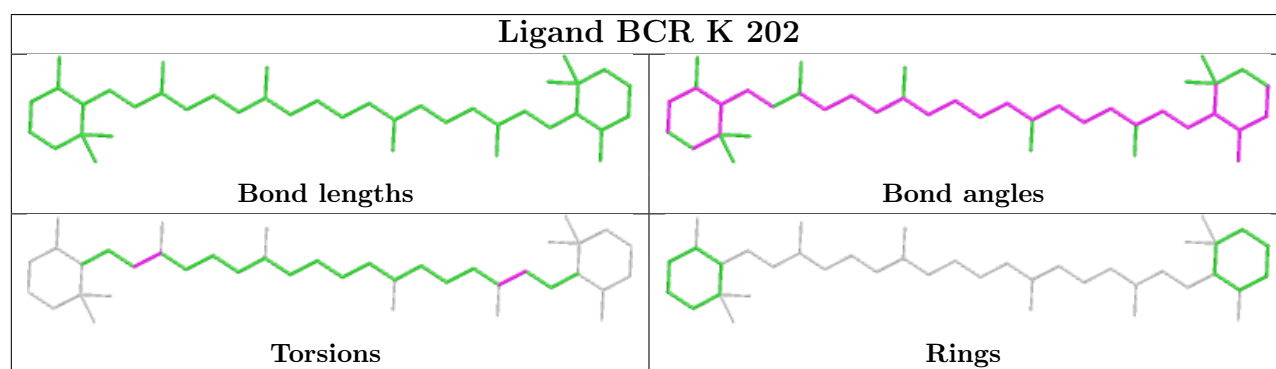
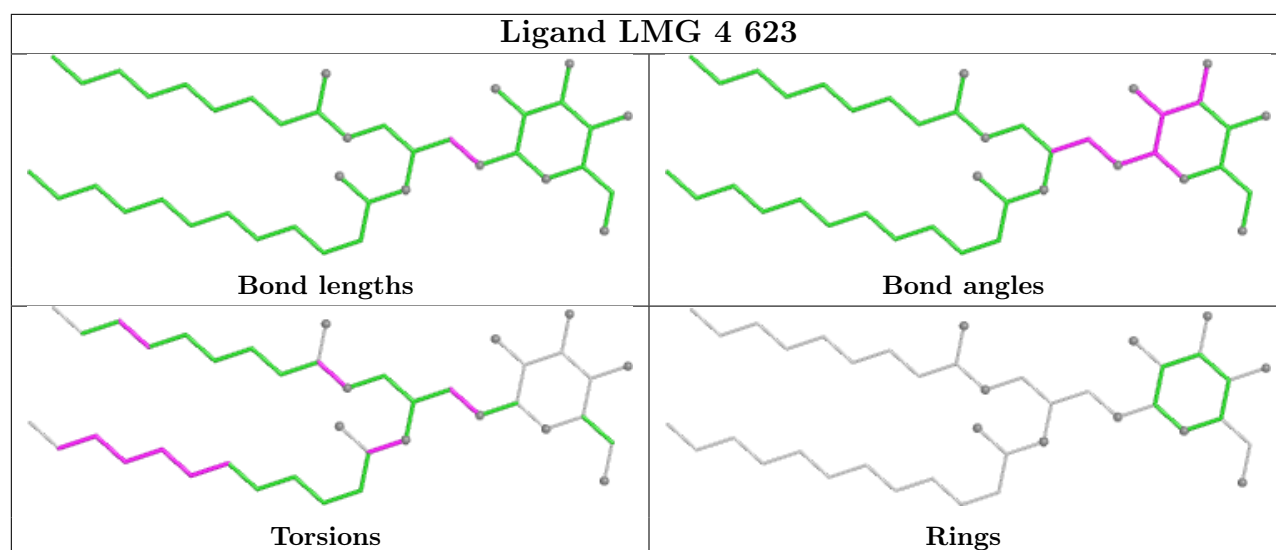


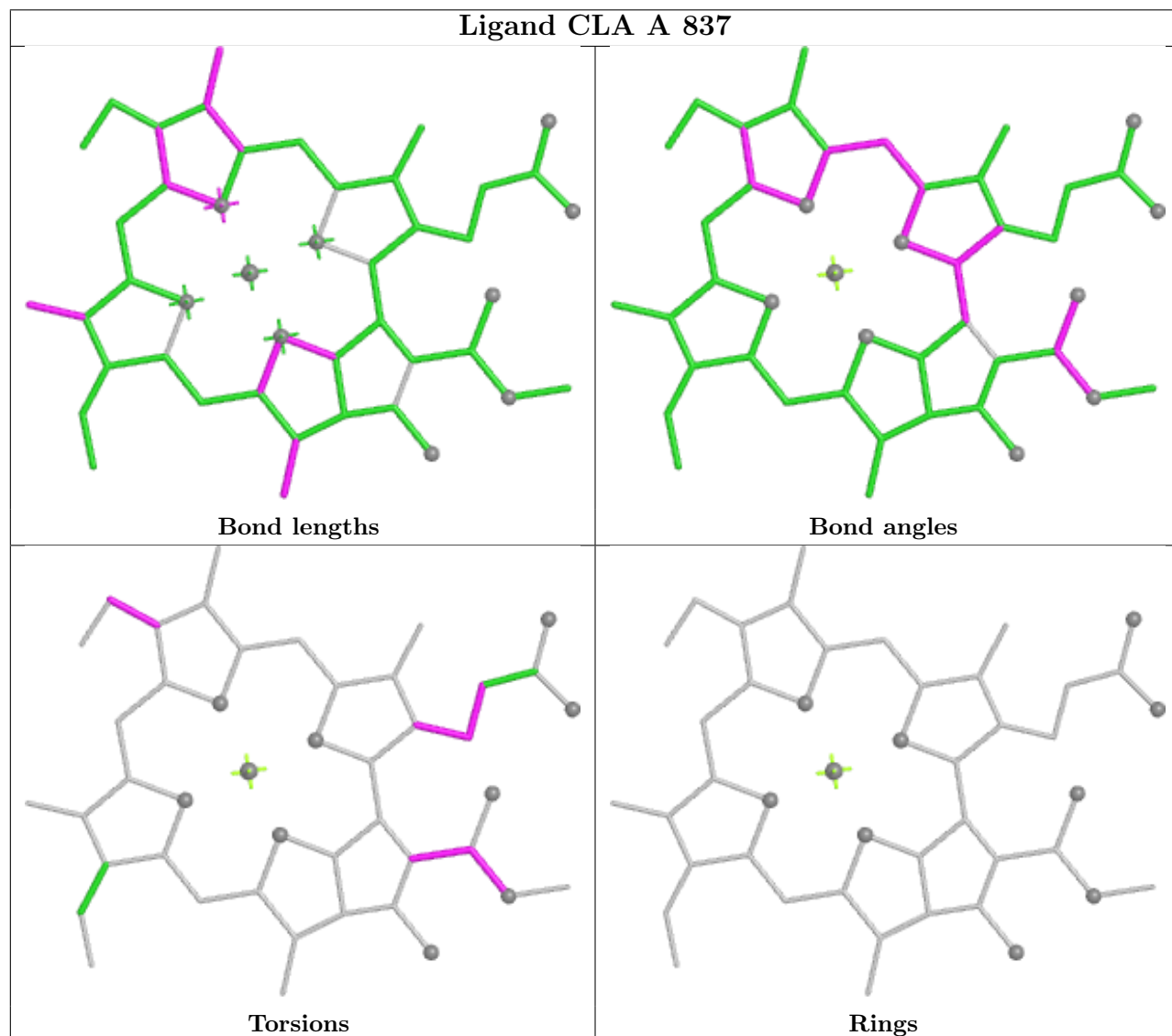
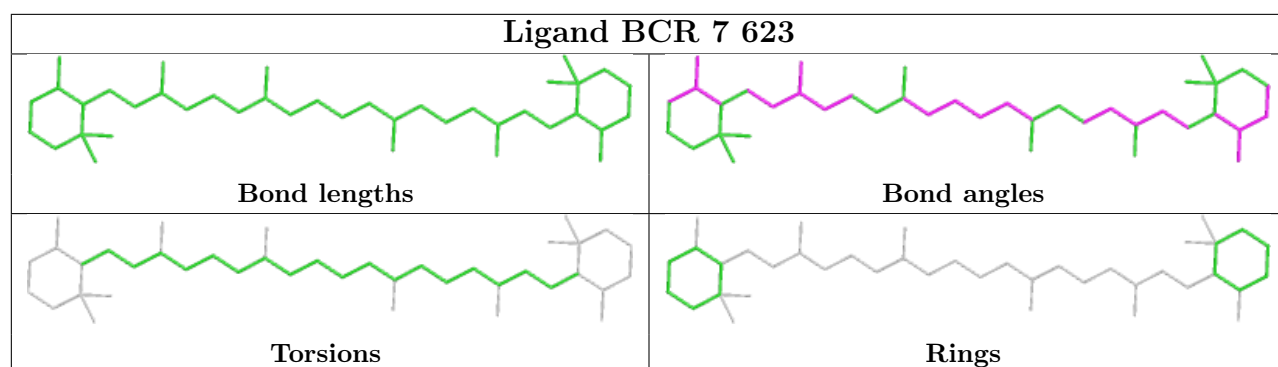
Ligand CLA 4 613



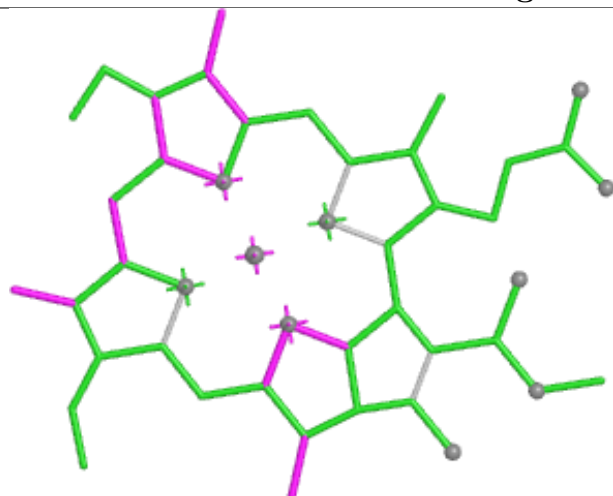
Ligand CLA B 804



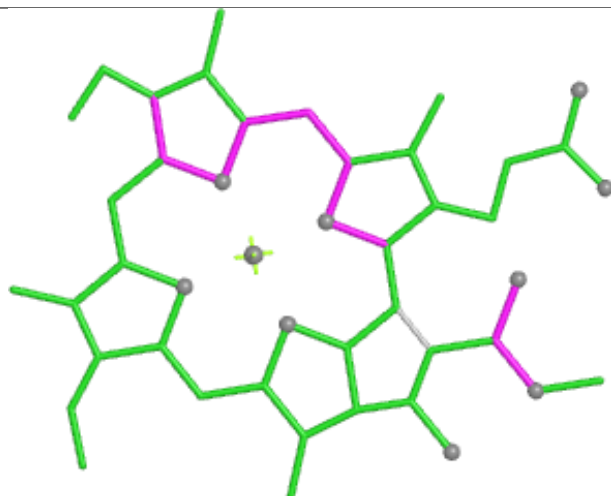




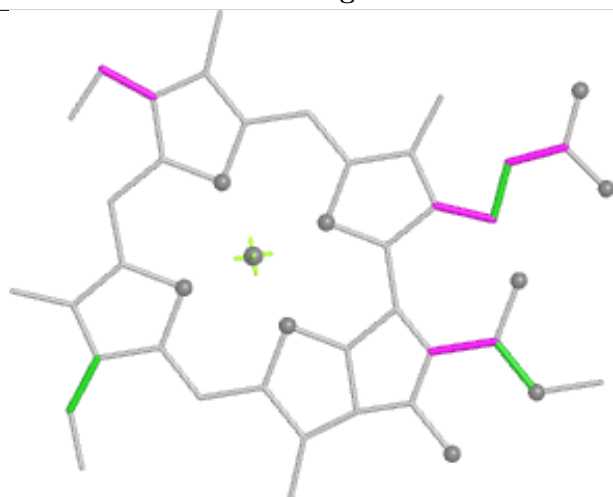
Ligand CLA L 303



Bond lengths



Bond angles

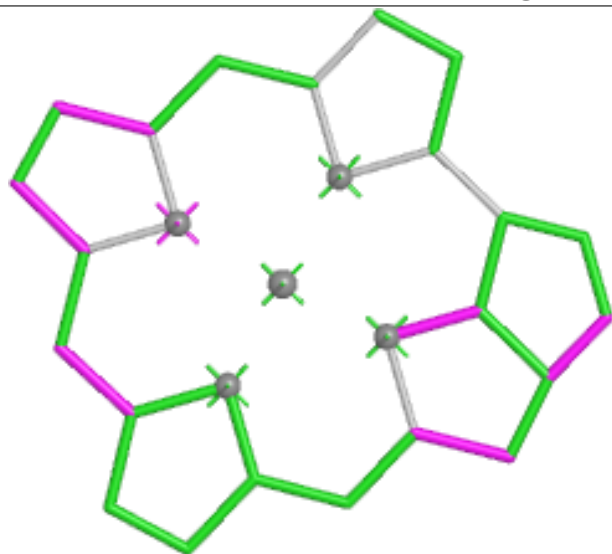


Torsions

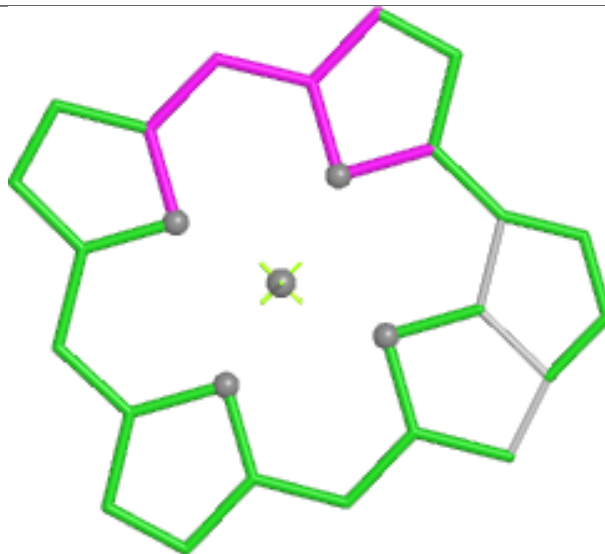


Rings

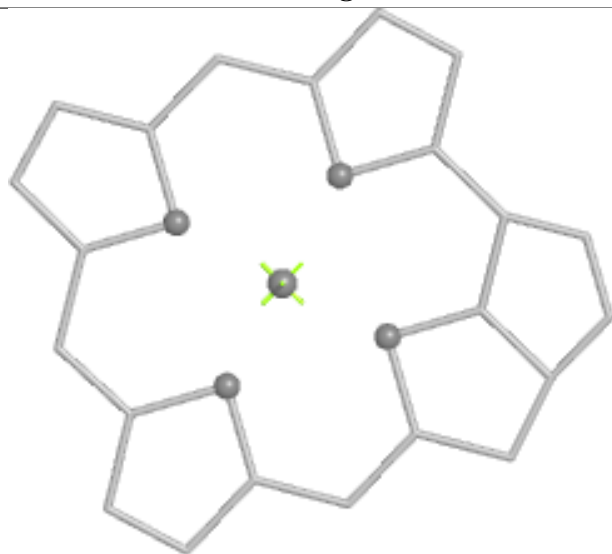
Ligand CLA 2 606



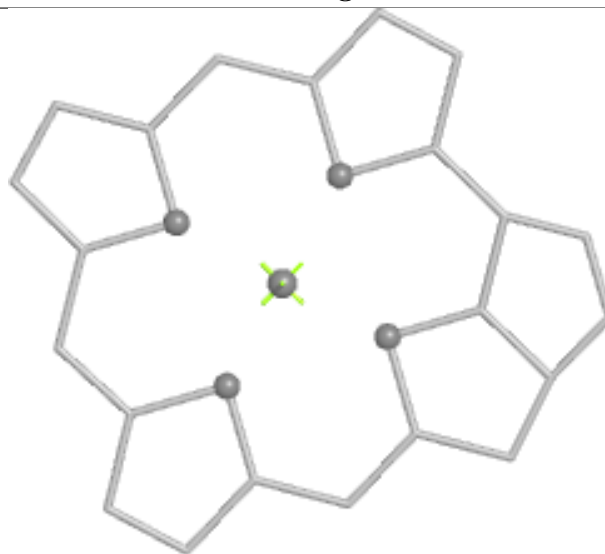
Bond lengths



Bond angles

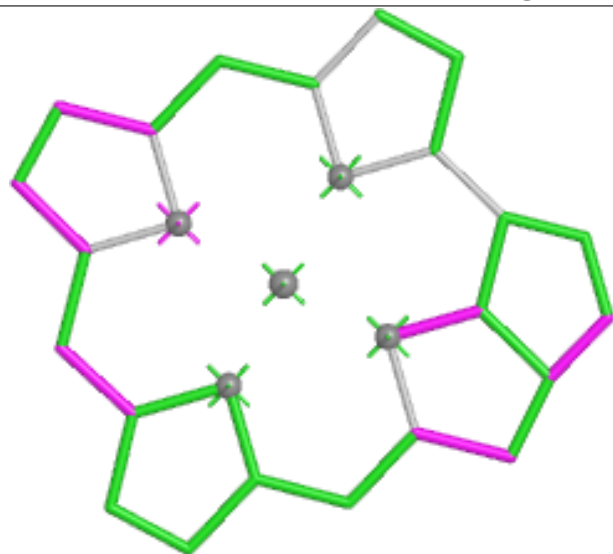


Torsions

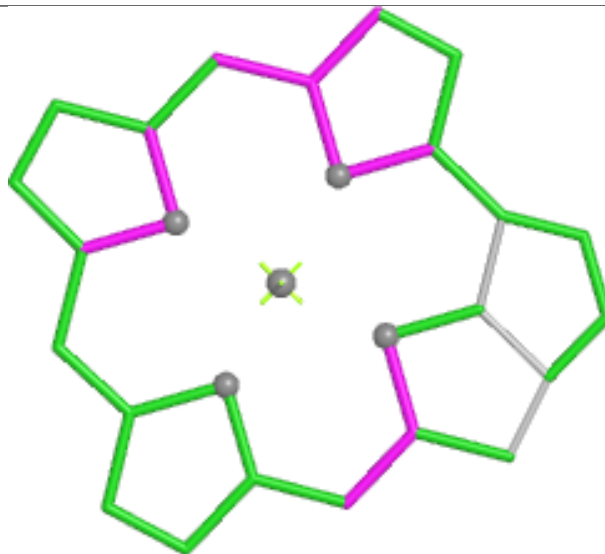


Rings

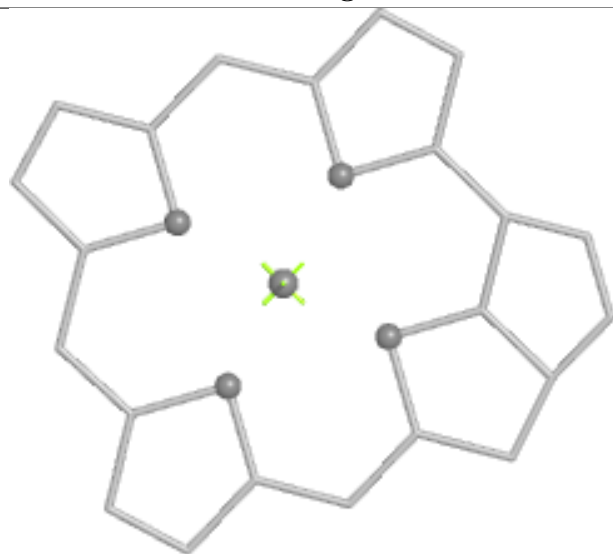
Ligand CLA 9 613



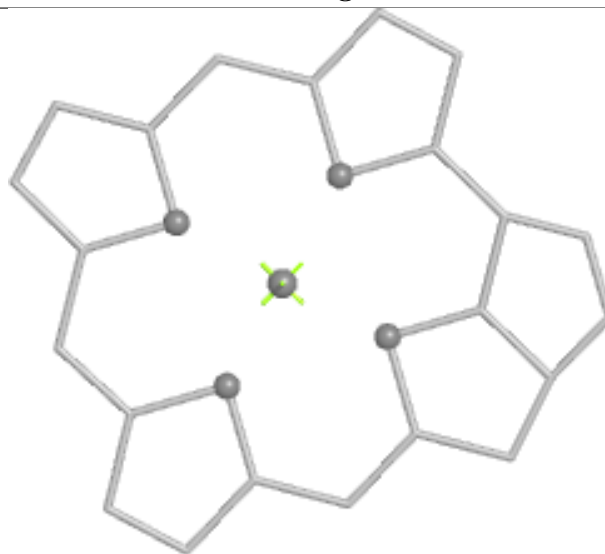
Bond lengths



Bond angles

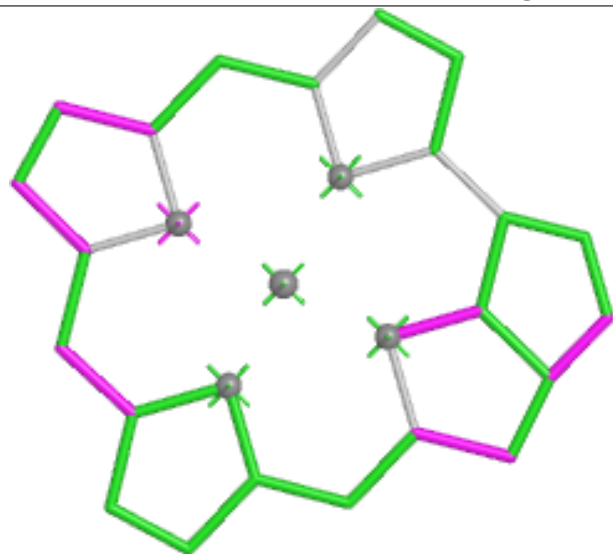


Torsions

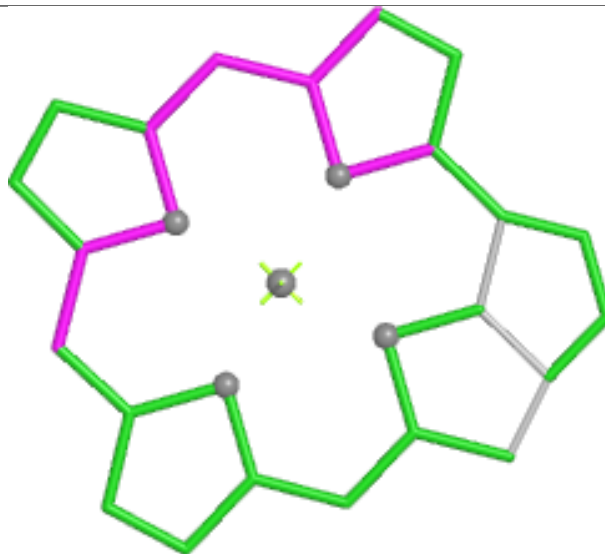


Rings

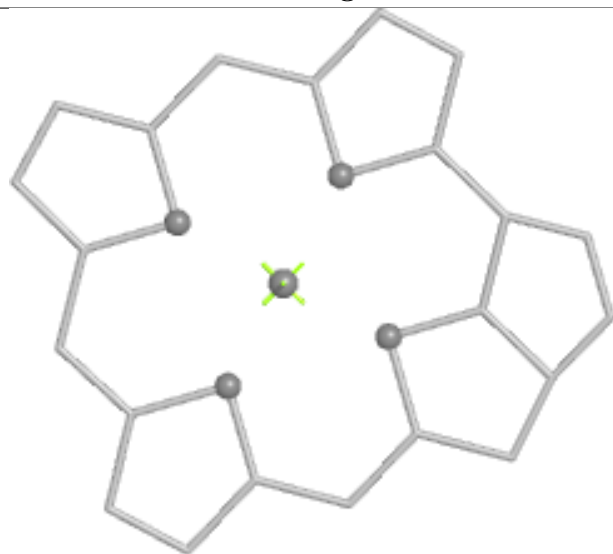
Ligand CLA 9 606



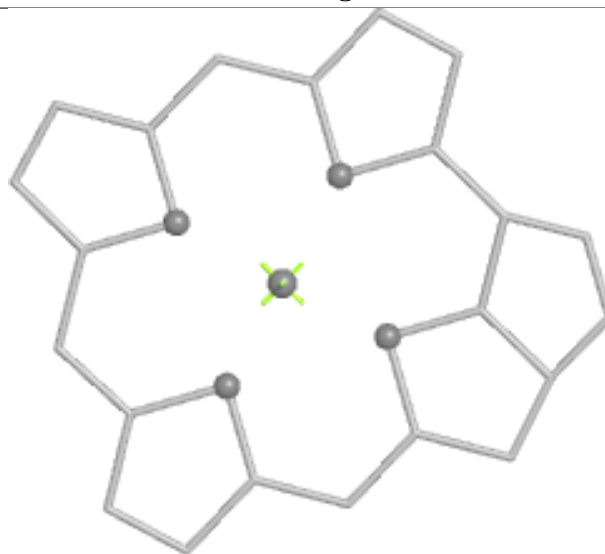
Bond lengths



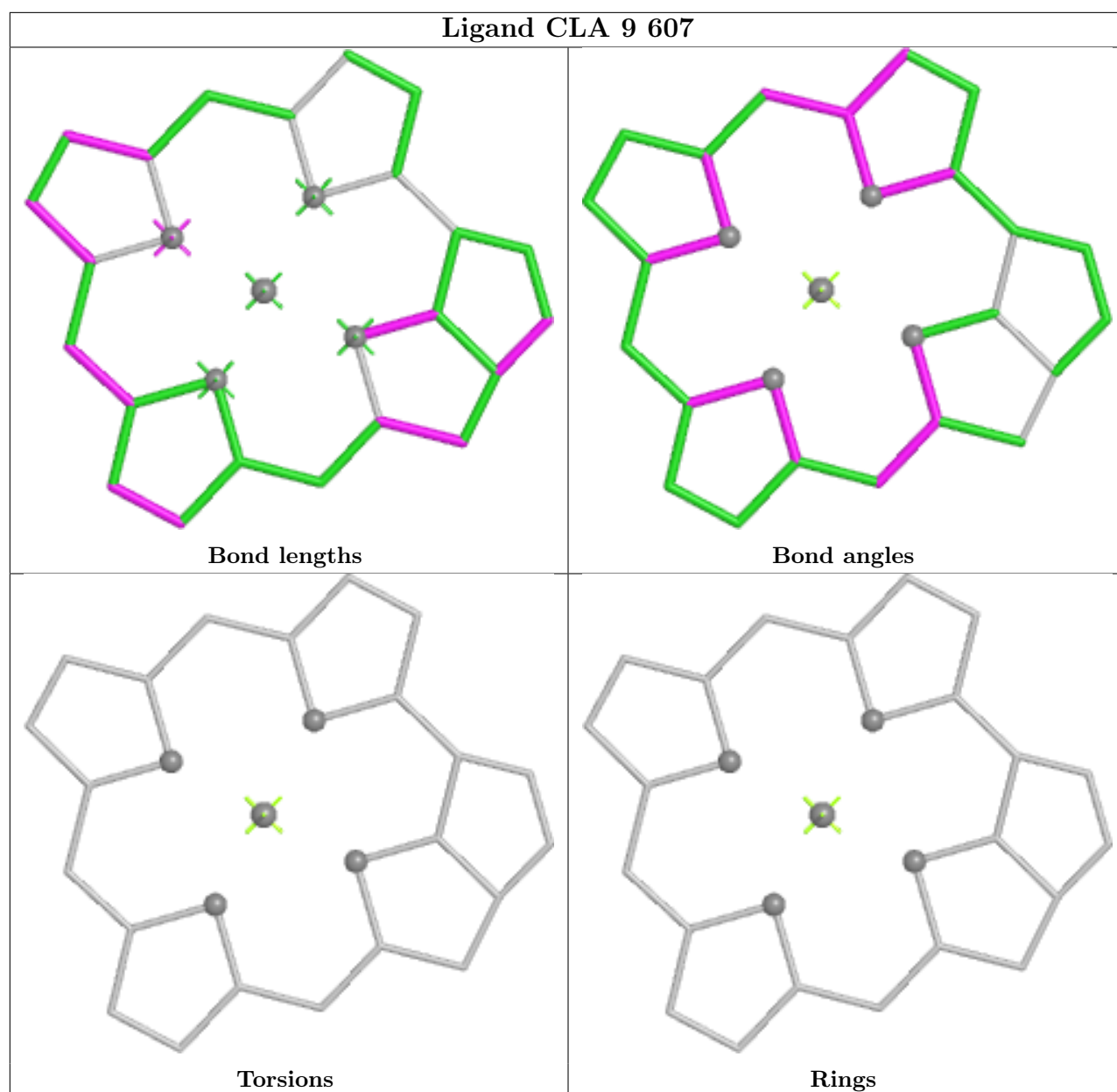
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

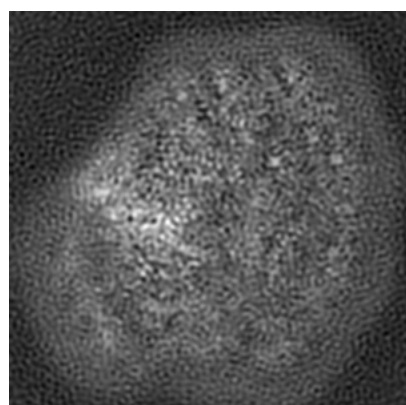
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9680. These allow visual inspection of the internal detail of the map and identification of artifacts.

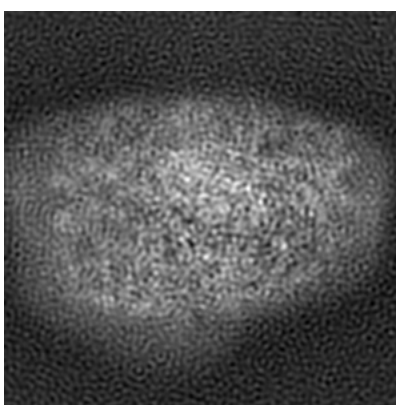
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

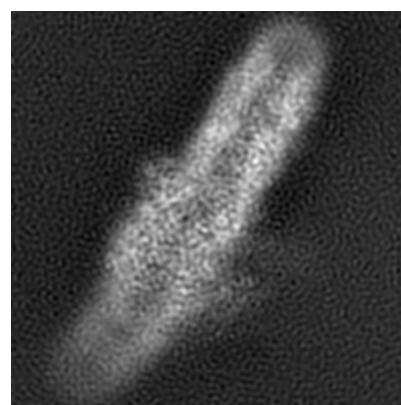
6.1.1 Primary map



X



Y

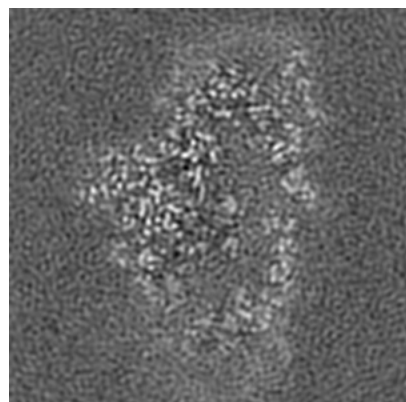


Z

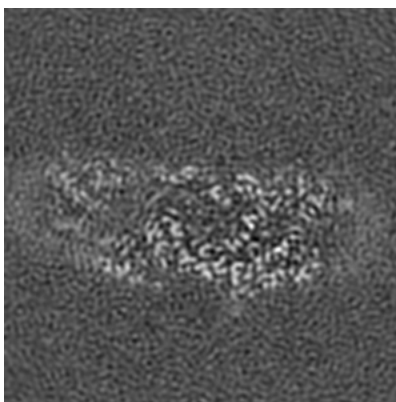
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

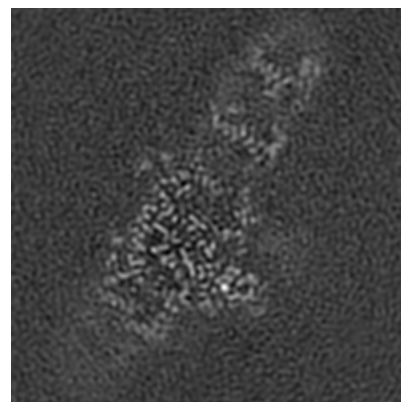
6.2.1 Primary map



X Index: 100



Y Index: 100

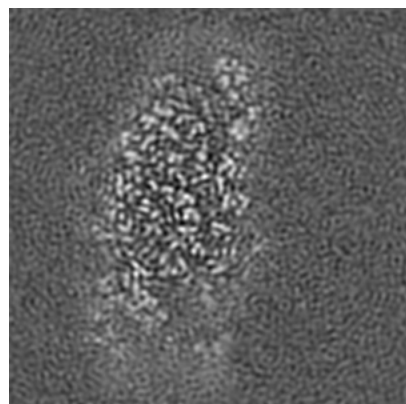


Z Index: 100

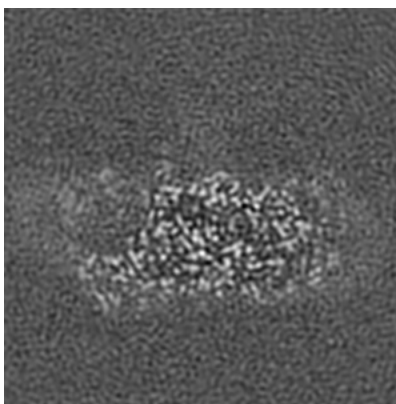
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

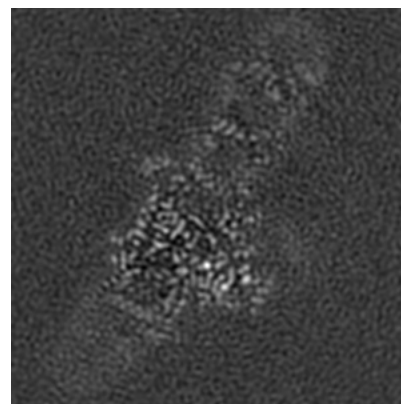
6.3.1 Primary map



X Index: 84



Y Index: 88

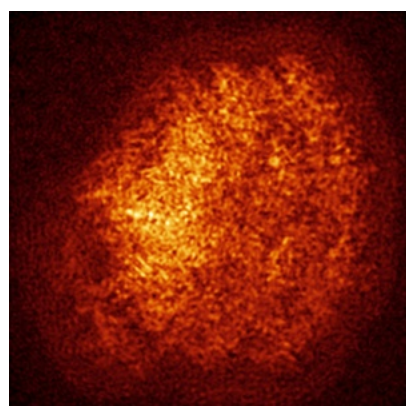


Z Index: 98

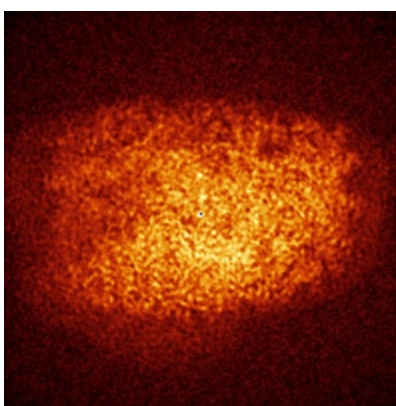
The images above show the largest variance slices of the map in three orthogonal directions.

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

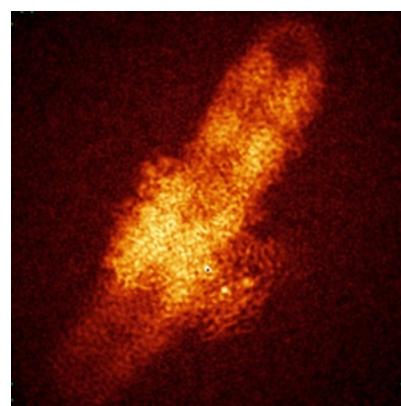
6.4.1 Primary map



X



Y

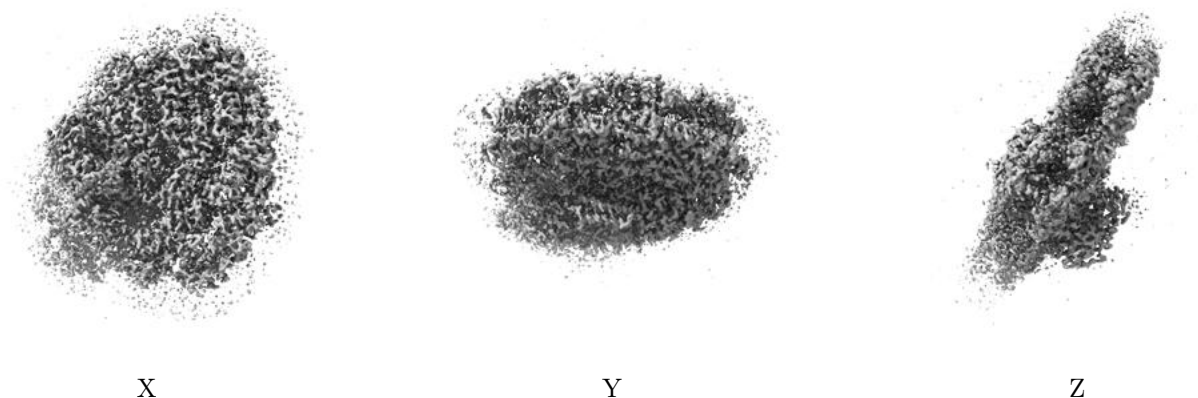


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

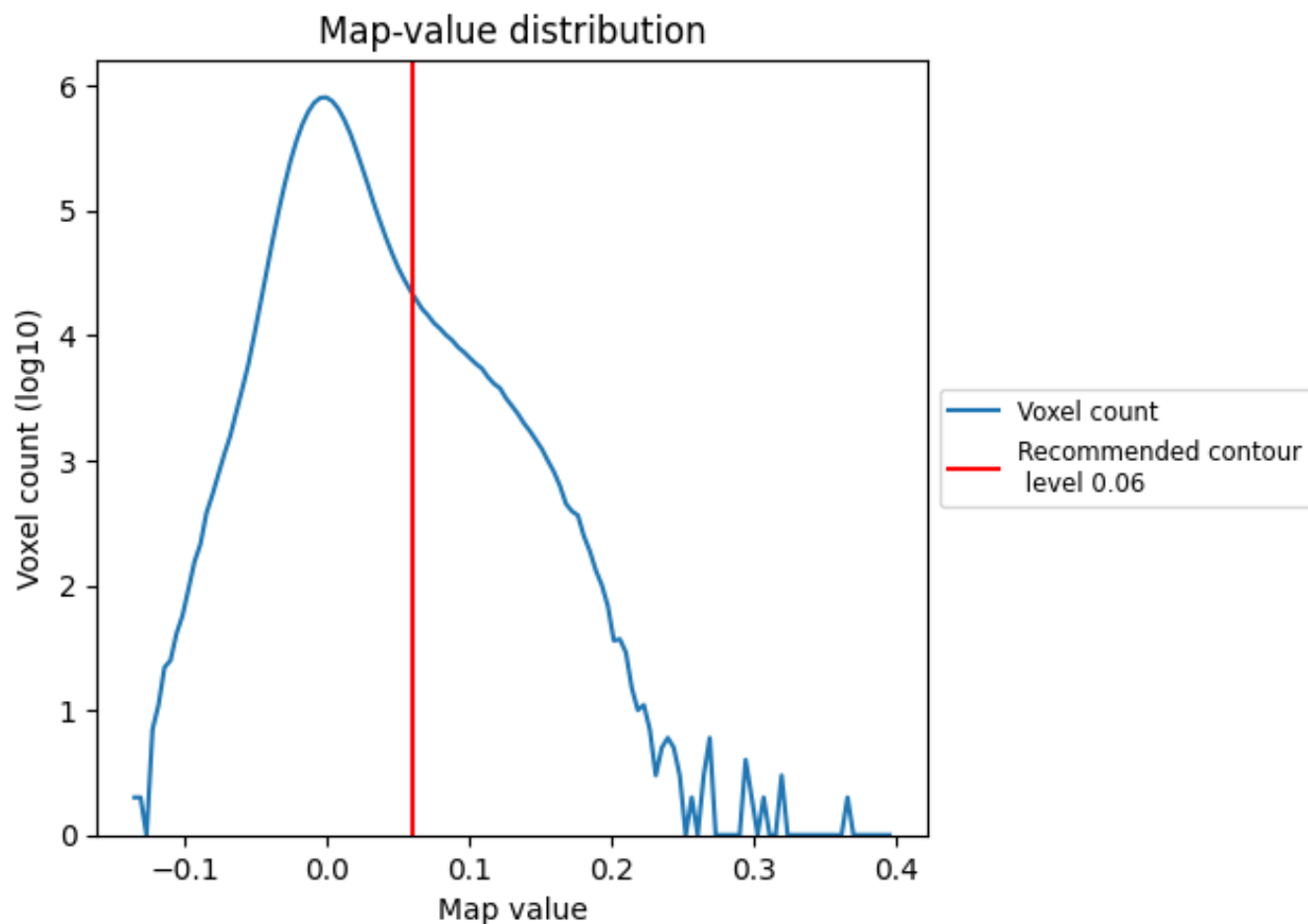
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

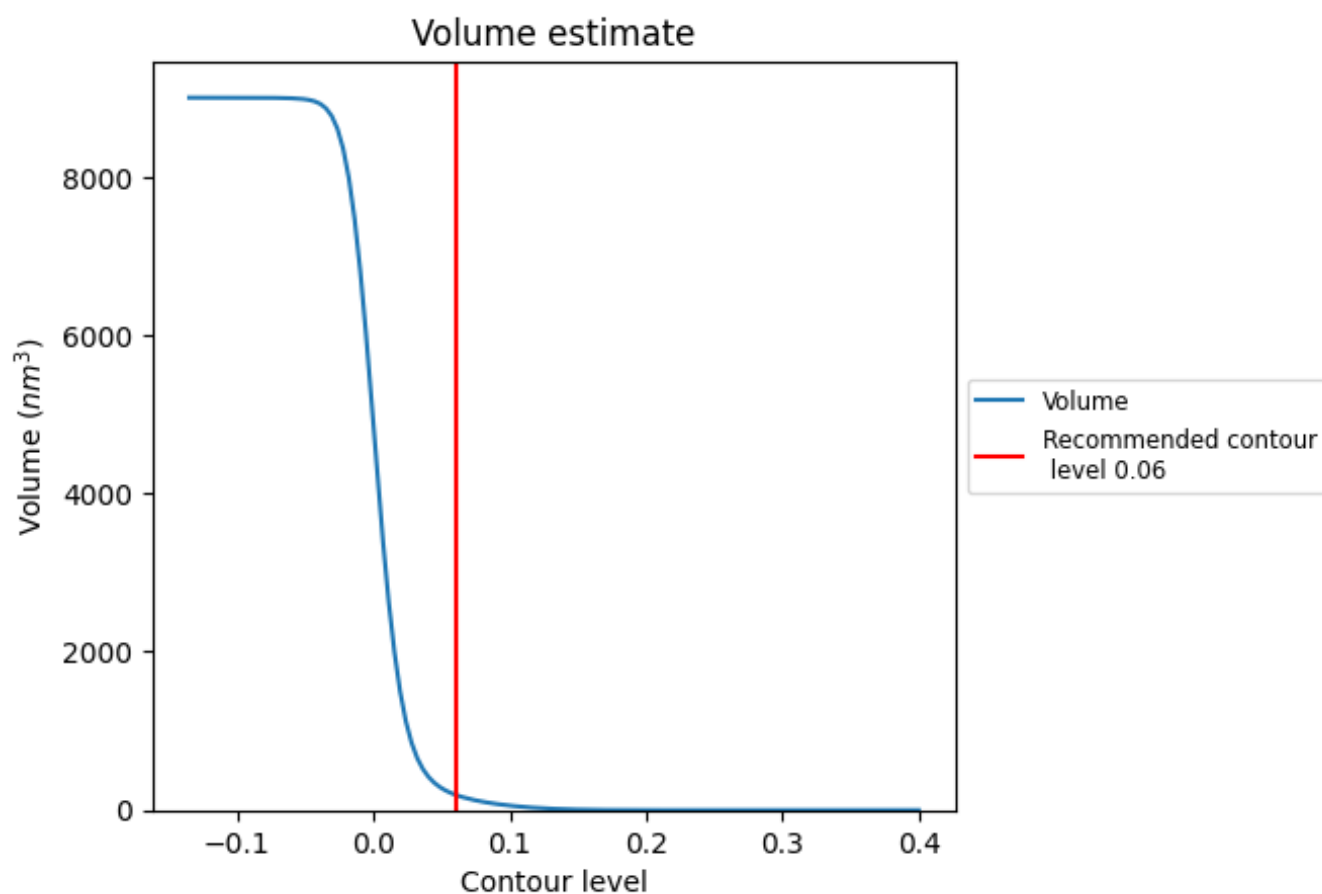
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

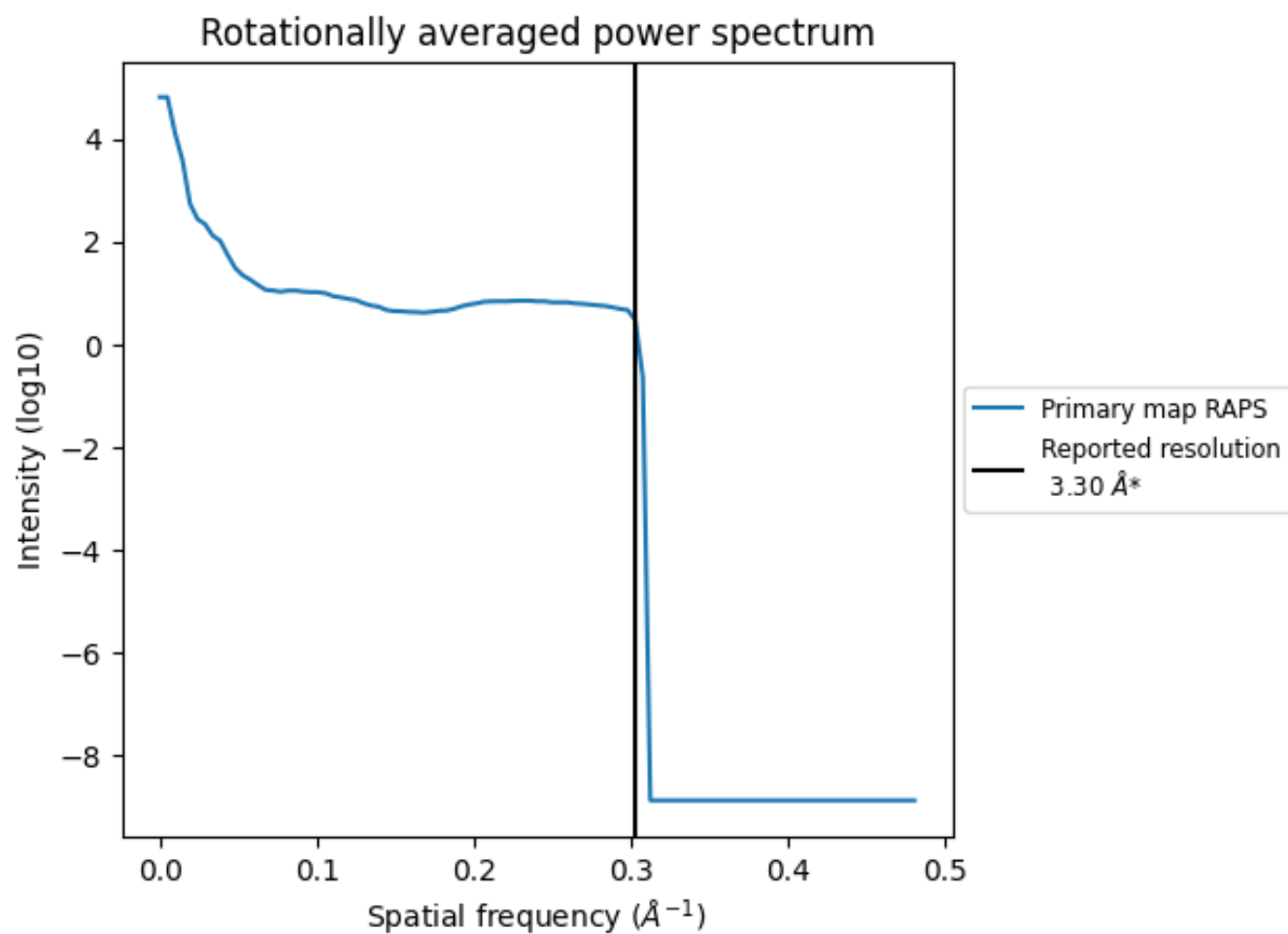
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm³; this corresponds to an approximate mass of 177 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 0.303 Å⁻¹

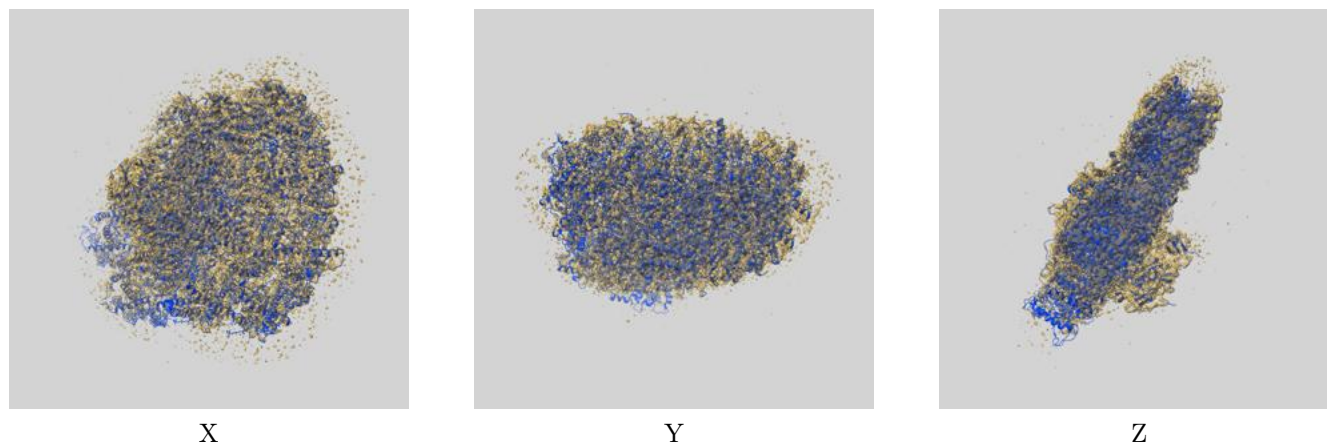
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

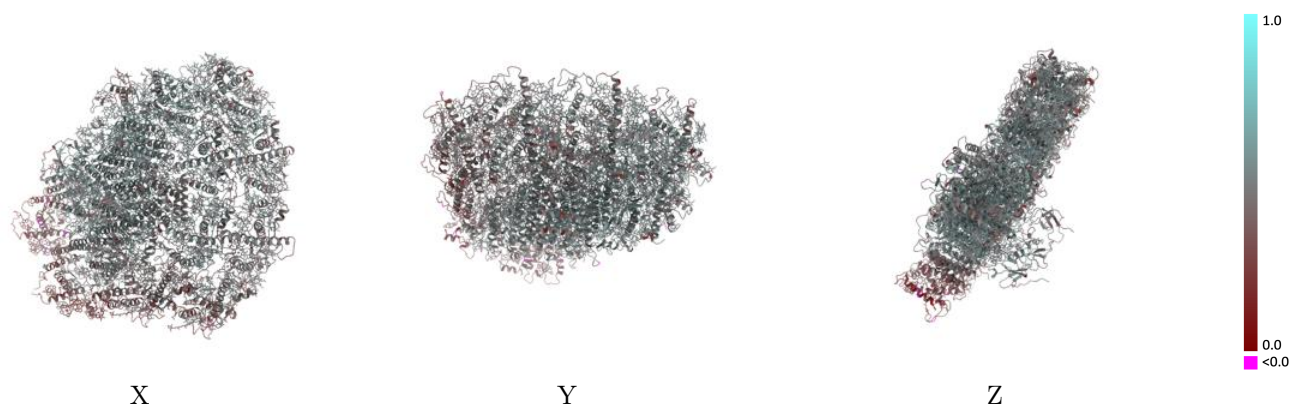
This section contains information regarding the fit between EMDB map EMD-9680 and PDB model 6IJO. Per-residue inclusion information can be found in section 3 on page 29.

9.1 Map-model overlay [i](#)



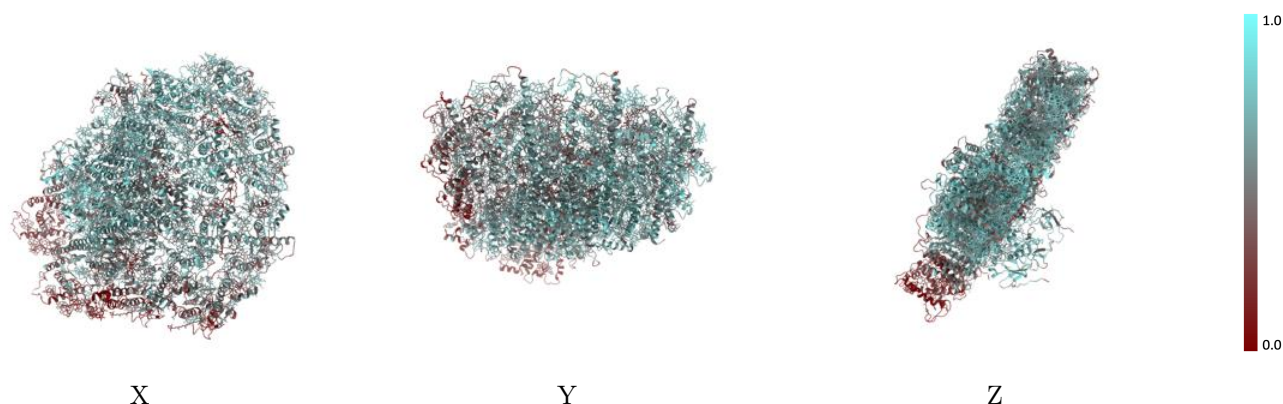
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



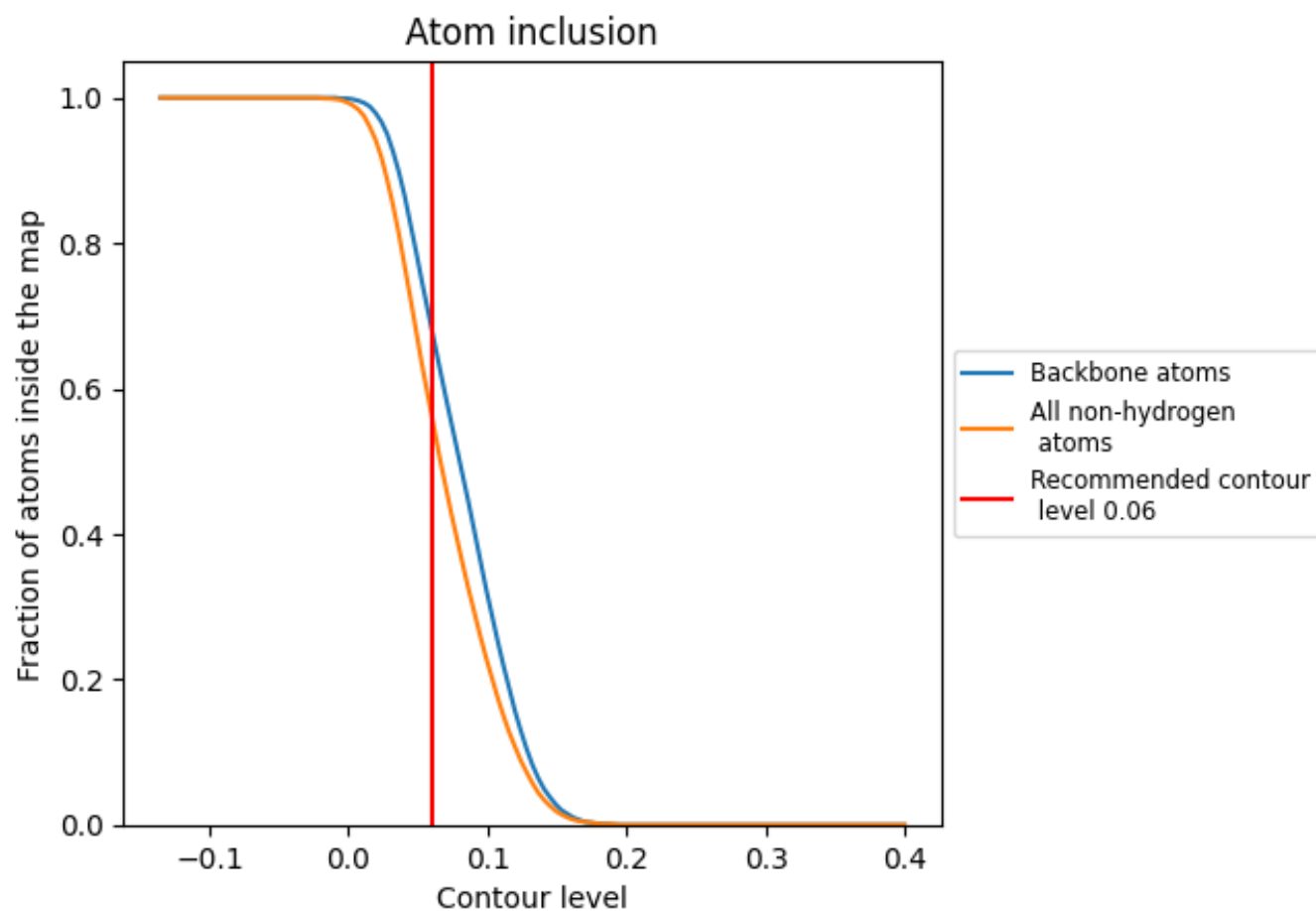
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 56% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5620	 0.4690
1	 0.4300	 0.3900
2	 0.0930	 0.2380
3	 0.6630	 0.5120
4	 0.5190	 0.4540
5	 0.5820	 0.4790
6	 0.5810	 0.4770
7	 0.6370	 0.4970
8	 0.5960	 0.4870
9	 0.2720	 0.2900
A	 0.7080	 0.5400
B	 0.6440	 0.5150
C	 0.7140	 0.4870
D	 0.6490	 0.4900
E	 0.6160	 0.4570
F	 0.5690	 0.4590
G	 0.0740	 0.3300
H	 0.0910	 0.3340
I	 0.5670	 0.4660
J	 0.4220	 0.4370
K	 0.4790	 0.4470
L	 0.4380	 0.4150
X	 0.2620	 0.2840
a	 0.4000	 0.4140

