



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 07:07 AM EDT

PDB ID : 7KSQ / pdb_00007ksq
EMDB ID : EMD-23023
Title : The Structure of the moss PSI-LHCI reveals the evolution of the LHCI antenna
Authors : Riddle, R.; Gorski, C.; Toporik, H.; Dobson, Z.; Da, Z.; Williams, D.; Mazor, Y.
Deposited on : 2020-11-23
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

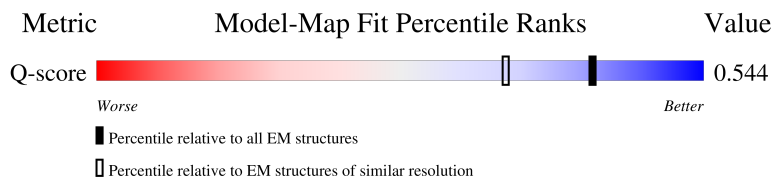
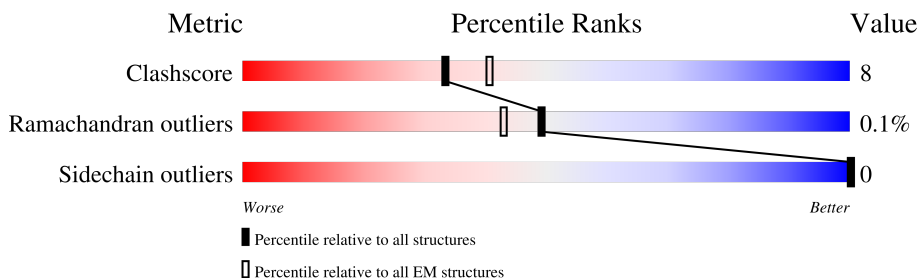
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

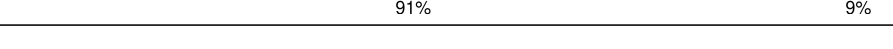
The reported resolution of this entry is 2.80 Å.

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



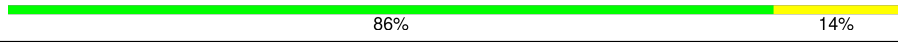
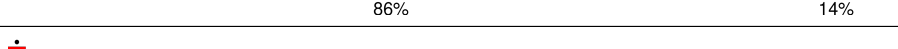
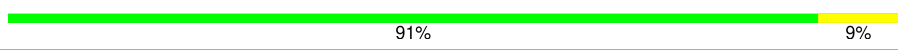
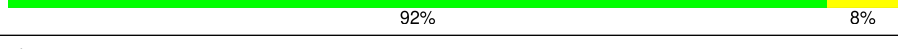
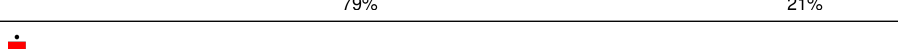
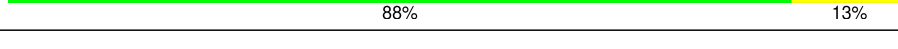
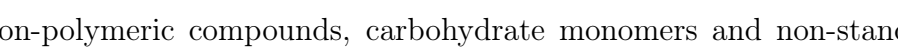
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	742	
2	B	732	
3	1	192	
4	2	203	

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Mol	Chain	Length	Quality of chain
5	3	218	
6	4	203	
7	C	80	
8	D	142	
9	E	63	
10	F	160	
11	G	91	
12	H	87	
13	I	34	
14	J	41	
15	K	81	
16	L	160	
17	M	30	
18	O	88	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	LUT	2	623	X	-	-	-
29	LUT	4	623	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 36553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5837	3827	993	998	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5845	3836	995	998	16		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	192	Total	C	N	O	S	0	0
			1473	961	247	264	1		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	203	Total	C	N	O	S	0	0
			1567	1021	262	280	4		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	218	Total	C	N	O	S	0	0
			1678	1099	272	300	7		

- Molecule 6 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	203	Total	C	N	O	S	0	0
			1574	1024	264	281	5		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			596	365	103	117	11		

- Molecule 8 is a protein called PsuD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	142	Total	C	N	O	S	0	0
			1109	711	195	200	3		

- Molecule 9 is a protein called PsuE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			500	317	89	94		

- Molecule 10 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	160	Total	C	N	O	S	0	0
			1239	801	215	220	3		

- Molecule 11 is a protein called PSI-G.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	91	Total	C	N	O	0	0
			689	444	119	126		

- Molecule 12 is a protein called PsuH.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	87	Total	C	N	O	S	0	0
			659	418	114	126	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	34	Total	C	N	O	S	0	0
			266	181	35	48	2		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	41	Total	C	N	O	S	0	0
			325	222	48	54	1		

- Molecule 15 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	81	Total	C	N	O	S	0	0
			561	352	97	108	4		

- Molecule 16 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	160	Total	C	N	O	S	0	0
			1171	771	188	210	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	30	Total	C	N	O	0	0
			223	146	36	41		

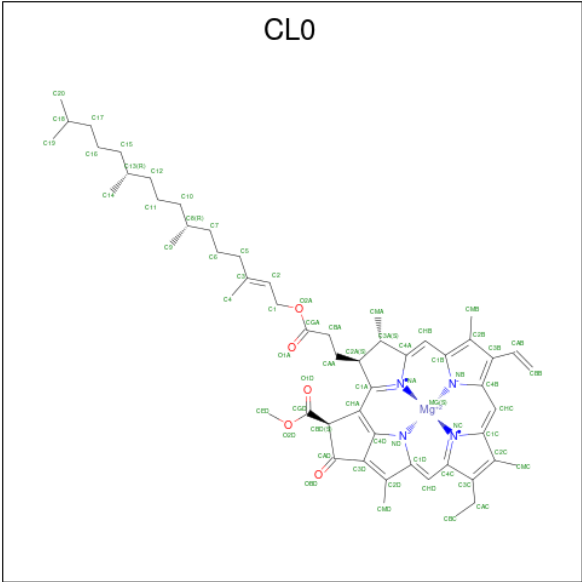
- Molecule 18 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	88	Total	C	N	O	S	0	0
			655	432	113	109	1		

There are 2 discrepancies between the modelled and reference sequences:

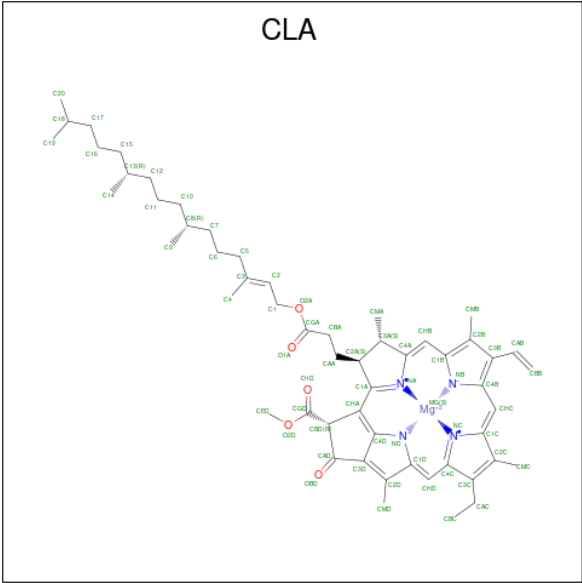
Chain	Residue	Modelled	Actual	Comment	Reference
O	62	ARG	LYS	conflict	UNP A0A2K1JDE1
O	130	PHE	LEU	conflict	UNP A0A2K1JDE1

- Molecule 19 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 27	C 22	Mg 1	N 4		0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0

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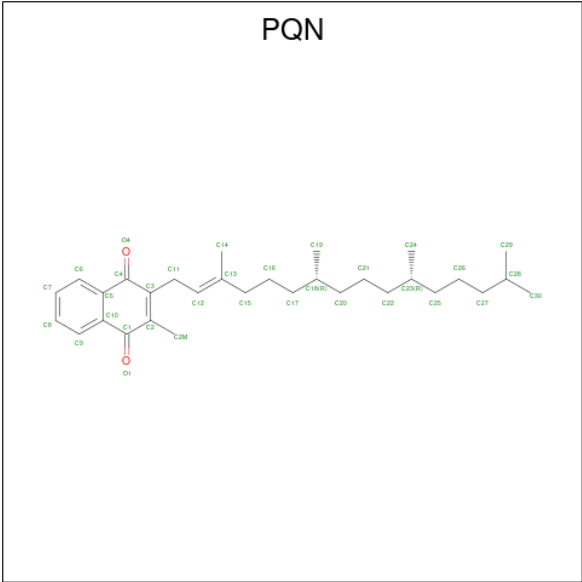
Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	F	1	Total	C	Mg	N		0
			27	22	1	4		

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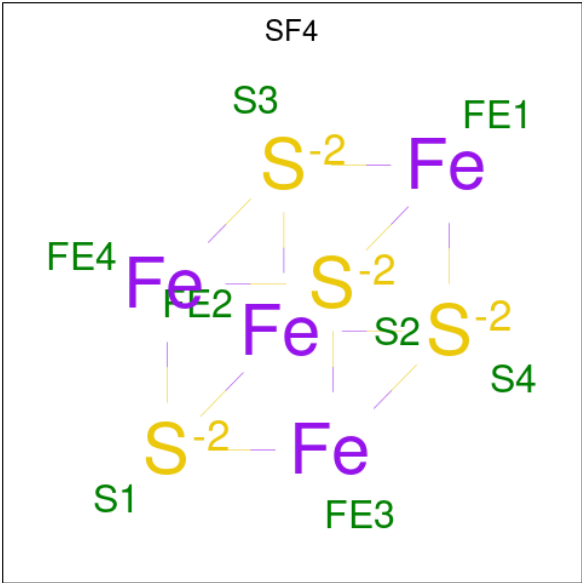
Mol	Chain	Residues	Atoms					AltConf
20	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	K	1	Total	C	Mg	N		0
			27	22	1	4		
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	O	1	Total	C	Mg	N		0
			27	22	1	4		
20	O	1	Total	C	Mg	N		0
			27	22	1	4		
20	O	1	Total	C	Mg	N		0
			27	22	1	4		

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



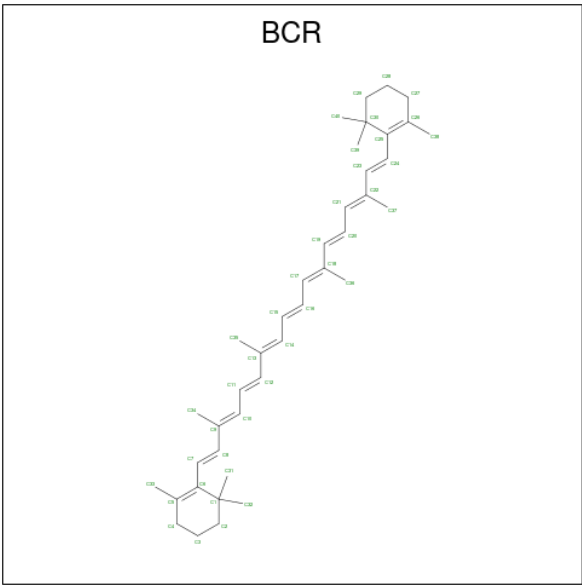
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



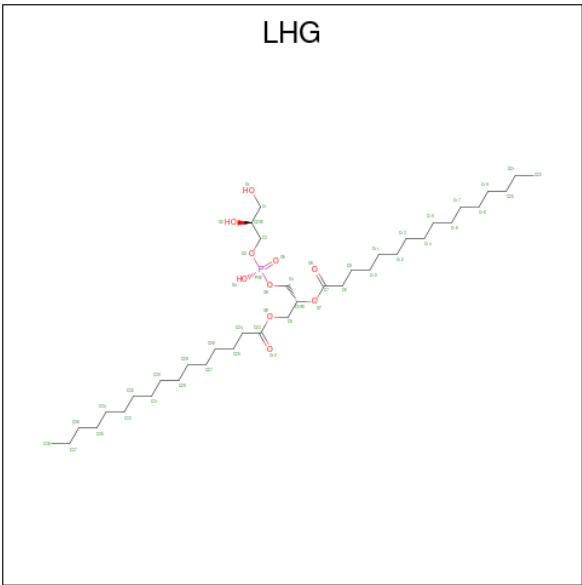
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	

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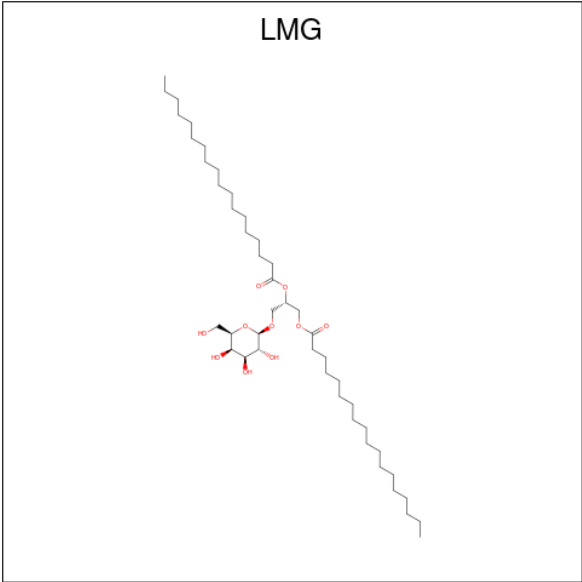
Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	1	1	Total C 25 25	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	M	1	Total C 40 40	0
23	O	1	Total C 14 14	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



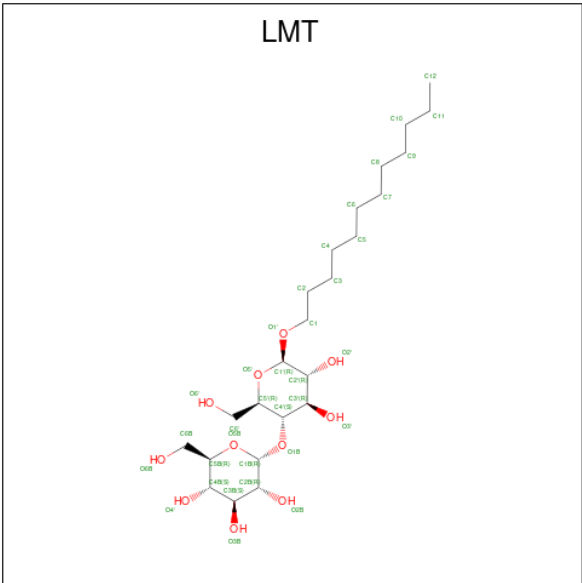
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			31	20	10	1	
24	B	1	Total	C	O	P	0
			35	24	10	1	
24	1	1	Total	C	O	P	0
			37	26	10	1	
24	2	1	Total	C	O	P	0
			32	21	10	1	
24	3	1	Total	C	O	P	0
			34	23	10	1	
24	4	1	Total	C	O	P	0
			38	27	10	1	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



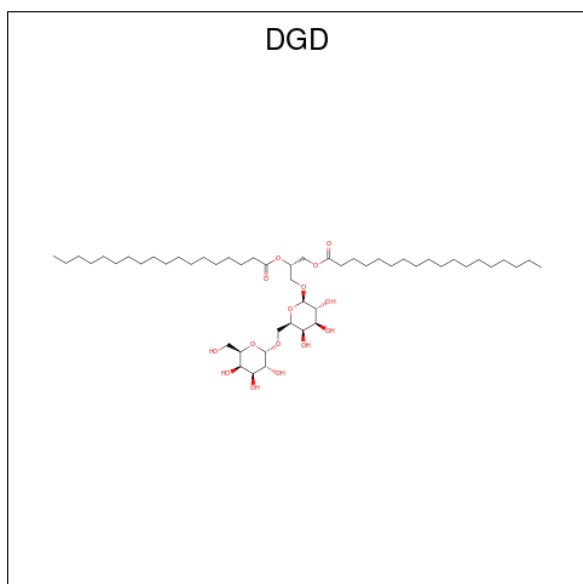
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			34	24	10	
25	2	1	Total	C	O	0
			36	26	10	
25	J	1	Total	C	O	0
			49	39	10	
25	J	1	Total	C	O	0
			26	16	10	

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



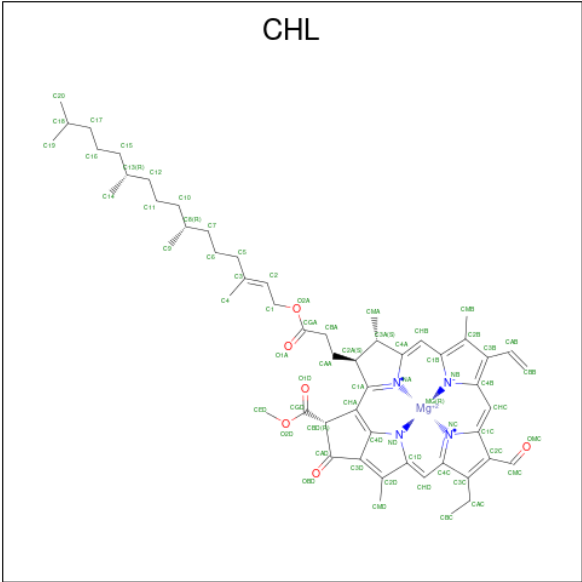
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	22	11	
26	B	1	Total	C	O	0
			31	20	11	
26	1	1	Total	C	O	0
			35	24	11	
26	4	1	Total	C	O	0
			35	24	11	
26	G	1	Total	C	O	0
			35	24	11	
26	G	1	Total	C	O	0
			31	20	11	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



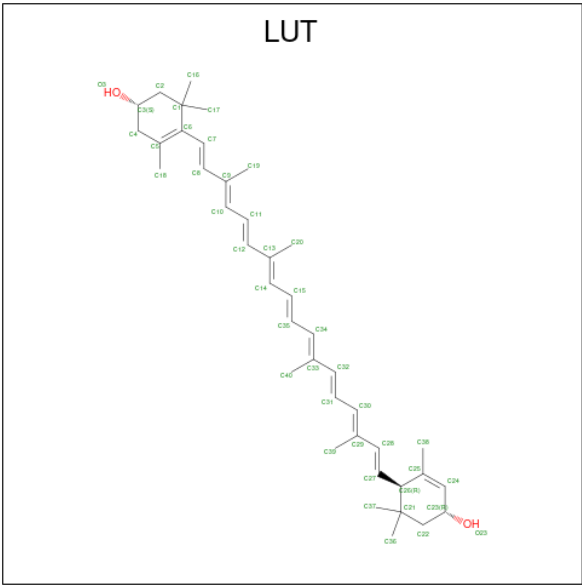
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			61	46	15	

- Molecule 28 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	1	1	Total 56	C 45	Mg 1	N 4	O 6	0
28	2	1	Total 56	C 45	Mg 1	N 4	O 6	0
28	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
28	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	2	1	Total 48	C 37	Mg 1	N 4	O 6	0
28	2	1	Total 56	C 45	Mg 1	N 4	O 6	0
28	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
28	3	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	4	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	4	1	Total 47	C 36	Mg 1	N 4	O 6	0
28	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
28	4	1	Total 43	C 34	Mg 1	N 4	O 4	0

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	

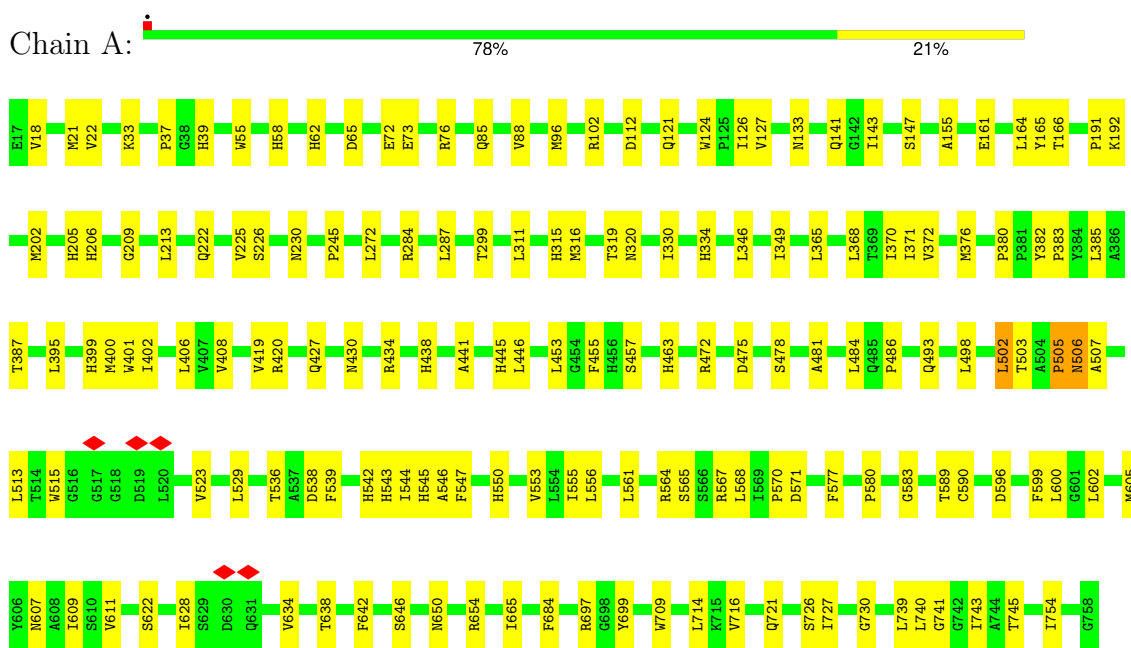
- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	A	15	Total 15	O 15	0
30	B	23	Total 23	O 23	0
30	3	1	Total 1	O 1	0
30	4	1	Total 1	O 1	0
30	C	2	Total 2	O 2	0
30	D	1	Total 1	O 1	0
30	F	1	Total 1	O 1	0
30	G	1	Total 1	O 1	0

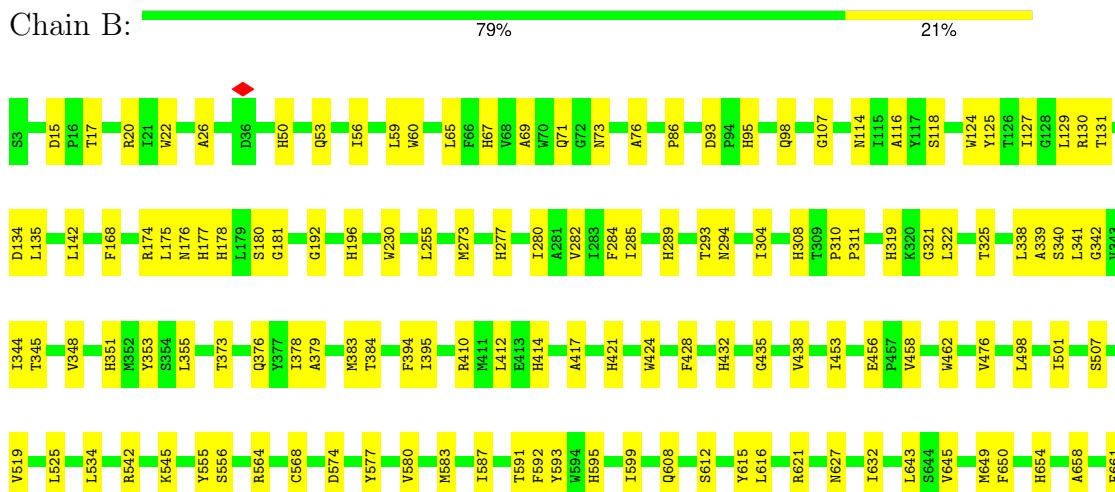
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

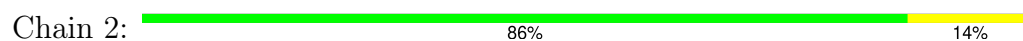




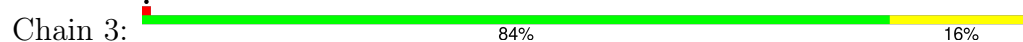
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



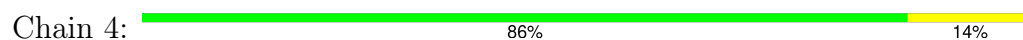
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic



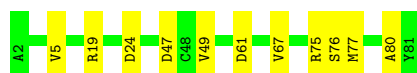
- Molecule 5: Chlorophyll a-b binding protein, chloroplastic



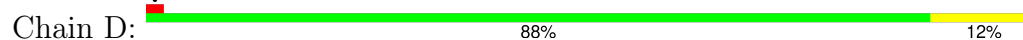
- Molecule 6: Chlorophyll a-b binding protein, chloroplastic



- Molecule 7: Photosystem I iron-sulfur center

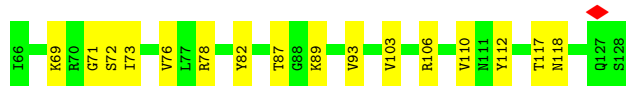


- Molecule 8: Psad



- Molecule 9: PsaE

Chain E:  75% 25%



- Molecule 10: PSI-F

Chain F:  85% 15%

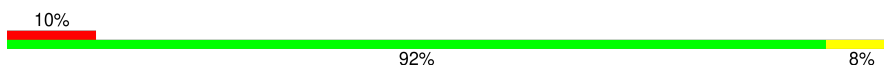


- Molecule 11: PSI-G

Chain G:  91% 9%



- Molecule 12: PsaH

Chain H:  10% 92% 8%



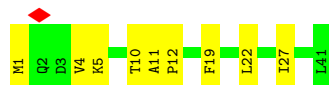
- Molecule 13: Photosystem I reaction center subunit VIII

Chain I:  79% 21%



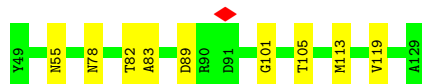
- Molecule 14: Photosystem I reaction center subunit IX

Chain J:  78% 22%



- Molecule 15: PsaK

Chain K:  89% 11%



- Molecule 16: PSI subunit V

Chain L:  89% 11%



- Molecule 17: Photosystem I reaction center subunit XII

Chain M:  87% 13%



- Molecule 18: PsaO

Chain O:  88% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114608	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 ($e^-/\text{\AA}^2$)	1.6	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	33.849	Depositor
Minimum map value	-23.604	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.825	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	291.2, 291.2, 291.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0400001, 1.0400001, 1.0400001	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, CL0, CLA, PQN, LMG, SF4, LHG, LMT, LUT, DGD, CHL

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	0.30	0/6032	0.61	3/8227 (0.0%)
2	B	0.30	0/6059	0.64	0/8267
3	1	0.22	0/1522	0.51	0/2081
4	2	0.18	0/1618	0.42	0/2218
5	3	0.20	0/1729	0.46	0/2349
6	4	0.24	0/1623	0.57	0/2219
7	C	0.23	0/606	0.57	0/821
8	D	0.17	0/1136	0.46	0/1538
9	E	0.15	0/511	0.37	0/694
10	F	0.30	1/1265 (0.1%)	0.54	0/1710
11	G	0.16	0/704	0.40	0/960
12	H	0.19	0/673	0.48	0/909
13	I	0.29	0/273	0.61	0/373
14	J	0.20	0/334	0.46	0/457
15	K	0.16	0/567	0.41	0/768
16	L	0.22	0/1202	0.57	0/1645
17	M	0.16	0/224	0.46	0/302
18	O	0.30	0/680	0.76	0/933
All	All	0.26	1/26758 (0.0%)	0.56	3/36471 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	213	TRP	C-N	6.98	1.42	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	LEU	CA-CB-CG	5.62	135.98	116.30
1	A	502	LEU	CA-CB-CG	5.19	134.46	116.30
1	A	506	ASN	N-CA-C	5.11	121.67	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	667	TRP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5837	0	5725	125	0
2	B	5845	0	5618	120	0
3	1	1473	0	1448	15	0
4	2	1567	0	1527	22	0
5	3	1678	0	1638	31	0
6	4	1574	0	1549	22	0
7	C	596	0	573	9	0
8	D	1109	0	1111	14	0
9	E	500	0	494	10	0
10	F	1239	0	1288	21	0
11	G	689	0	681	6	0
12	H	659	0	636	6	0
13	I	266	0	274	7	0
14	J	325	0	341	9	0
15	K	561	0	574	7	0
16	L	1171	0	1186	15	0
17	M	223	0	244	4	0
18	O	655	0	599	6	0
19	A	65	0	72	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	1	614	0	508	9	0
20	2	378	0	334	4	0
20	3	648	0	530	14	0
20	4	527	0	448	9	0
20	A	2384	0	2226	105	0
20	B	2177	0	1998	104	0
20	F	118	0	69	4	0
20	G	151	0	121	0	0
20	H	45	0	33	2	0
20	I	65	0	72	7	0
20	J	45	0	33	0	0
20	K	173	0	118	3	0
20	L	155	0	131	9	0
20	O	81	0	9	0	0
21	A	33	0	46	2	0
21	B	33	0	46	5	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	1	25	0	33	0	0
23	3	80	0	112	4	0
23	A	240	0	336	8	0
23	B	280	0	392	29	0
23	F	40	0	56	2	0
23	G	40	0	56	3	0
23	I	80	0	112	5	0
23	J	80	0	112	4	0
23	K	40	0	56	1	0
23	L	80	0	112	7	0
23	M	40	0	56	5	0
23	O	14	0	20	0	0
24	1	37	0	44	1	0
24	2	32	0	34	2	0
24	3	34	0	38	1	0
24	4	38	0	46	2	0
24	A	80	0	106	4	0
24	B	35	0	40	0	0
25	2	36	0	42	0	0
25	A	34	0	38	2	0
25	J	75	0	90	4	0
26	1	35	0	46	2	0
26	4	35	0	45	3	0
26	A	33	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	31	0	35	0	0
26	G	66	0	80	3	0
27	B	61	0	83	5	0
28	1	103	0	78	2	0
28	2	366	0	290	11	0
28	3	47	0	31	2	0
28	4	188	0	128	1	0
29	1	84	0	112	8	0
29	2	126	0	165	9	0
29	3	84	0	110	9	0
29	4	126	0	166	7	0
30	3	1	0	0	0	0
30	4	1	0	0	0	0
30	A	15	0	0	0	0
30	B	23	0	0	0	0
30	C	2	0	0	0	0
30	D	1	0	0	0	0
30	F	1	0	0	0	0
30	G	1	0	0	0	0
All	All	36553	0	35639	601	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 601 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)
20:A:1134:CLA:H2A	20:A:1134:CLA:HED3	1.63	0.80
20:4:601:CLA:HBB2	20:4:602:CLA:HHD	1.64	0.79
20:3:610:CLA:HAB	29:3:620:LUT:H32	1.67	0.75
20:4:610:CLA:HAB	29:4:620:LUT:H32	1.69	0.75
1:A:209:GLY:HA3	20:A:1111:CLA:HBB1	1.71	0.72

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	740/742 (100%)	699 (94%)	38 (5%)	3 (0%)	30	60
2	B	730/732 (100%)	708 (97%)	22 (3%)	0	100	100
3	1	190/192 (99%)	182 (96%)	8 (4%)	0	100	100
4	2	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
5	3	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
6	4	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
7	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
8	D	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
9	E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
10	F	158/160 (99%)	153 (97%)	5 (3%)	0	100	100
11	G	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
12	H	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
13	I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
14	J	39/41 (95%)	39 (100%)	0	0	100	100
15	K	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
16	L	158/160 (99%)	149 (94%)	9 (6%)	0	100	100
17	M	28/30 (93%)	28 (100%)	0	0	100	100
18	O	86/88 (98%)	75 (87%)	11 (13%)	0	100	100
All	All	3311/3347 (99%)	3179 (96%)	129 (4%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	506	ASN
1	A	505	PRO
1	A	284	ARG

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	603/603 (100%)	603 (100%)	0	100	100
2	B	595/595 (100%)	595 (100%)	0	100	100
3	1	148/148 (100%)	148 (100%)	0	100	100
4	2	160/160 (100%)	160 (100%)	0	100	100
5	3	169/171 (99%)	169 (100%)	0	100	100
6	4	161/162 (99%)	161 (100%)	0	100	100
7	C	67/67 (100%)	67 (100%)	0	100	100
8	D	114/115 (99%)	114 (100%)	0	100	100
9	E	55/55 (100%)	55 (100%)	0	100	100
10	F	130/131 (99%)	130 (100%)	0	100	100
11	G	72/72 (100%)	72 (100%)	0	100	100
12	H	66/68 (97%)	66 (100%)	0	100	100
13	I	30/30 (100%)	30 (100%)	0	100	100
14	J	35/35 (100%)	35 (100%)	0	100	100
15	K	57/58 (98%)	57 (100%)	0	100	100
16	L	116/118 (98%)	116 (100%)	0	100	100
17	M	25/25 (100%)	25 (100%)	0	100	100
18	O	60/72 (83%)	60 (100%)	0	100	100
All	All	2663/2685 (99%)	2663 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
10	F	97	GLN
18	O	56	ASN
17	M	7	GLN

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Mol	Chain	Res	Type
3	1	55	ASN
9	E	127	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

219 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
20	CLA	B	1224	-	65,69,73	1.22	10 (15%)	77,108,113	1.46	10 (12%)
20	CLA	B	1226	-	59,63,73	1.31	9 (15%)	70,101,113	1.71	11 (15%)
20	CLA	4	611	-	59,63,73	1.26	9 (15%)	70,101,113	1.47	7 (10%)
20	CLA	3	610	-	59,63,73	1.25	8 (13%)	70,101,113	1.24	7 (10%)
28	CHL	4	607	-	51,55,74	2.17	18 (35%)	56,91,114	2.90	22 (39%)
20	CLA	A	1102	-	49,53,73	1.36	9 (18%)	58,89,113	1.35	7 (12%)
23	BCR	B	4017	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	5 (8%)
23	BCR	F	416	-	41,41,41	1.02	2 (4%)	56,56,56	1.36	10 (17%)
25	LMG	2	631	-	36,36,55	0.94	0	44,44,63	1.21	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	1107	-	49,53,73	1.39	8 (16%)	58,89,113	1.60	7 (12%)
23	BCR	B	4006	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	5 (8%)
20	CLA	A	1105	-	54,58,73	1.31	8 (14%)	64,95,113	1.63	7 (10%)
20	CLA	B	1209	-	49,53,73	1.41	7 (14%)	58,89,113	1.54	6 (10%)
23	BCR	3	624	-	41,41,41	0.99	2 (4%)	56,56,56	1.36	9 (16%)
20	CLA	B	1220	-	49,53,73	1.38	8 (16%)	58,89,113	1.39	6 (10%)
20	CLA	2	610	-	64,68,73	1.21	7 (10%)	76,107,113	1.16	5 (6%)
20	CLA	4	614	-	50,54,73	1.37	8 (16%)	59,90,113	1.38	5 (8%)
29	LUT	4	623	-	42,43,43	2.42	1 (2%)	51,60,60	1.79	8 (15%)
23	BCR	B	4010	-	41,41,41	1.08	1 (2%)	56,56,56	1.70	13 (23%)
20	CLA	F	302	-	50,54,73	1.36	8 (16%)	59,90,113	1.38	5 (8%)
24	LHG	A	5001	-	48,48,48	0.68	1 (2%)	51,54,54	1.29	6 (11%)
20	CLA	A	1022	-	69,73,73	1.19	7 (10%)	82,113,113	1.27	6 (7%)
20	CLA	A	1130	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	9 (11%)
20	CLA	B	1212	-	49,53,73	1.37	9 (18%)	58,89,113	1.54	7 (12%)
20	CLA	B	1237	-	69,73,73	1.21	8 (11%)	82,113,113	1.32	7 (8%)
20	CLA	3	611	-	45,49,73	1.43	8 (17%)	54,84,113	1.37	3 (5%)
20	CLA	A	1136	-	69,73,73	1.18	8 (11%)	82,113,113	1.40	9 (10%)
20	CLA	A	1116	-	58,62,73	1.27	10 (17%)	68,99,113	1.33	7 (10%)
23	BCR	A	4008	-	41,41,41	1.01	1 (2%)	56,56,56	1.86	15 (26%)
20	CLA	B	1227	-	49,53,73	1.40	10 (20%)	58,89,113	1.71	10 (17%)
20	CLA	1	611	-	50,54,73	1.36	7 (14%)	59,90,113	1.28	4 (6%)
29	LUT	4	621	-	42,43,43	2.53	4 (9%)	51,60,60	3.06	14 (27%)
20	CLA	B	1228	-	53,57,73	1.31	9 (16%)	61,93,113	1.42	7 (11%)
20	CLA	2	604	-	54,58,73	1.32	8 (14%)	64,95,113	1.36	6 (9%)
20	CLA	B	1205	-	69,73,73	1.18	9 (13%)	82,113,113	1.47	10 (12%)
20	CLA	B	1211	-	60,64,73	1.25	7 (11%)	71,102,113	1.45	7 (9%)
29	LUT	3	621	-	42,43,43	2.44	1 (2%)	51,60,60	1.85	10 (19%)
20	CLA	A	1121	-	55,59,73	1.32	8 (14%)	64,96,113	1.54	8 (12%)
26	LMT	4	631	-	36,36,36	1.18	5 (13%)	47,47,47	0.95	1 (2%)
20	CLA	B	1234	-	55,59,73	1.30	9 (16%)	64,96,113	1.49	8 (12%)
26	LMT	1	631	-	36,36,36	1.15	4 (11%)	47,47,47	0.97	2 (4%)
28	CHL	2	615	-	51,55,74	2.17	17 (33%)	56,91,114	2.92	23 (41%)
23	BCR	A	4002	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	5 (8%)
29	LUT	1	620	-	42,43,43	2.72	2 (4%)	51,60,60	2.30	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	5005	-	54,58,73	1.31	8 (14%)	64,95,113	1.39	8 (12%)
20	CLA	3	607	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	4 (5%)
20	CLA	3	612	-	49,53,73	1.39	7 (14%)	58,89,113	1.34	5 (8%)
23	BCR	B	4005	-	41,41,41	1.04	2 (4%)	56,56,56	1.20	5 (8%)
23	BCR	1	623	-	25,25,41	1.04	2 (8%)	33,33,56	1.29	5 (15%)
20	CLA	B	1012	-	59,63,73	1.30	8 (13%)	70,101,113	1.45	10 (14%)
20	CLA	B	1230	-	49,53,73	1.39	8 (16%)	58,89,113	1.36	5 (8%)
20	CLA	3	606	-	50,54,73	1.38	9 (18%)	59,90,113	1.30	3 (5%)
20	CLA	A	1108	-	49,53,73	1.36	8 (16%)	58,89,113	1.66	6 (10%)
23	BCR	A	4007	-	41,41,41	1.11	3 (7%)	56,56,56	1.88	18 (32%)
20	CLA	A	1119	-	69,73,73	1.16	9 (13%)	82,113,113	1.49	8 (9%)
28	CHL	2	608	-	52,56,74	2.09	15 (28%)	57,92,114	2.96	22 (38%)
20	CLA	A	1135	-	55,59,73	1.33	8 (14%)	64,96,113	1.44	7 (10%)
20	CLA	1	602	-	64,68,73	1.22	8 (12%)	76,107,113	1.45	7 (9%)
28	CHL	2	607	-	51,55,74	2.17	16 (31%)	56,91,114	2.95	25 (44%)
20	CLA	B	1240	-	69,73,73	1.19	9 (13%)	82,113,113	1.37	9 (10%)
20	CLA	B	1202	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	7 (8%)
20	CLA	1	603	-	59,63,73	1.26	8 (13%)	70,101,113	1.38	8 (11%)
25	LMG	J	302	-	26,26,55	1.12	2 (7%)	34,34,63	1.16	4 (11%)
20	CLA	B	1023	-	65,69,73	1.20	9 (13%)	77,108,113	1.52	12 (15%)
28	CHL	4	608	-	55,59,74	2.08	19 (34%)	61,96,114	2.80	23 (37%)
20	CLA	A	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.42	7 (10%)
20	CLA	A	1132	-	69,73,73	1.14	8 (11%)	82,113,113	1.63	14 (17%)
20	CLA	A	1134	-	49,53,73	1.38	8 (16%)	58,89,113	1.62	6 (10%)
20	CLA	A	1140	-	55,59,73	1.31	8 (14%)	64,96,113	1.39	9 (14%)
28	CHL	1	607	-	51,55,74	2.20	18 (35%)	56,91,114	3.00	27 (48%)
23	BCR	A	4001	-	41,41,41	1.04	2 (4%)	56,56,56	1.37	7 (12%)
23	BCR	I	120	-	41,41,41	1.06	3 (7%)	56,56,56	1.77	15 (26%)
24	LHG	A	5003	-	30,30,48	0.78	1 (3%)	33,36,54	1.28	3 (9%)
23	BCR	L	420	-	41,41,41	0.99	1 (2%)	56,56,56	1.50	10 (17%)
20	CLA	B	1213	-	59,63,73	1.22	8 (13%)	70,101,113	1.48	9 (12%)
23	BCR	G	311	-	41,41,41	0.99	2 (4%)	56,56,56	1.36	9 (16%)
29	LUT	2	621	-	42,43,43	2.38	1 (2%)	51,60,60	1.58	6 (11%)
20	CLA	I	121	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
28	CHL	2	601	-	70,74,74	1.84	16 (22%)	79,114,114	2.62	30 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	L	419	-	41,41,41	0.97	1 (2%)	56,56,56	1.59	12 (21%)
20	CLA	B	1222	-	50,54,73	1.34	8 (16%)	59,90,113	1.57	9 (15%)
23	BCR	B	4009	-	41,41,41	0.99	1 (2%)	56,56,56	1.56	11 (19%)
20	CLA	A	1128	-	69,73,73	1.21	9 (13%)	82,113,113	1.41	14 (17%)
20	CLA	3	613	-	59,63,73	1.29	8 (13%)	70,101,113	1.32	3 (4%)
20	CLA	K	202	-	50,54,73	1.37	8 (16%)	59,90,113	1.36	6 (10%)
20	CLA	K	203	-	27,35,73	1.85	6 (22%)	32,60,113	1.60	5 (15%)
20	CLA	O	203	-	27,35,73	1.86	7 (25%)	32,60,113	1.65	5 (15%)
28	CHL	2	606	-	50,54,74	2.19	17 (34%)	55,90,114	2.95	21 (38%)
20	CLA	A	1013	-	60,64,73	1.23	10 (16%)	71,102,113	1.82	14 (19%)
29	LUT	2	623	-	42,43,43	2.55	1 (2%)	51,60,60	1.76	9 (17%)
20	CLA	G	218	-	59,63,73	1.27	7 (11%)	70,101,113	1.28	4 (5%)
20	CLA	A	1118	-	59,63,73	1.28	6 (10%)	70,101,113	1.25	6 (8%)
20	CLA	A	1110	-	59,63,73	1.28	9 (15%)	70,101,113	1.45	6 (8%)
20	CLA	B	1232	-	49,53,73	1.44	8 (16%)	58,89,113	1.78	7 (12%)
23	BCR	J	213	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	7 (12%)
29	LUT	1	621	-	42,43,43	2.66	2 (4%)	51,60,60	2.23	9 (17%)
20	CLA	3	614	-	52,56,73	1.35	7 (13%)	61,92,113	1.53	6 (9%)
20	CLA	K	204	-	49,53,73	1.40	9 (18%)	58,89,113	1.49	9 (15%)
20	CLA	A	1127	-	69,73,73	1.18	11 (15%)	82,113,113	1.56	11 (13%)
23	BCR	K	301	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	6 (10%)
20	CLA	A	1114	-	49,53,73	1.39	6 (12%)	58,89,113	1.70	9 (15%)
20	CLA	4	613	-	59,63,73	1.27	9 (15%)	70,101,113	1.35	5 (7%)
23	BCR	A	4011	-	41,41,41	1.03	2 (4%)	56,56,56	1.23	6 (10%)
20	CLA	A	1109	-	69,73,73	1.18	10 (14%)	82,113,113	1.31	7 (8%)
23	BCR	J	212	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
24	LHG	3	630	-	33,33,48	0.75	1 (3%)	36,39,54	1.30	4 (11%)
20	CLA	1	604	-	54,58,73	1.30	8 (14%)	64,95,113	1.49	7 (10%)
20	CLA	A	1112	-	49,53,73	1.38	9 (18%)	58,89,113	1.31	8 (13%)
20	CLA	2	603	-	50,54,73	1.34	8 (16%)	59,90,113	1.38	4 (6%)
23	BCR	B	4004	-	41,41,41	1.05	2 (4%)	56,56,56	1.29	5 (8%)
20	CLA	1	606	-	49,53,73	1.39	9 (18%)	58,89,113	1.53	8 (13%)
20	CLA	O	202	-	27,35,73	1.85	7 (25%)	32,60,113	1.62	5 (15%)
20	CLA	A	1138	-	64,68,73	1.20	8 (12%)	76,107,113	1.42	7 (9%)
25	LMG	A	5002	-	34,34,55	0.95	0	42,42,63	1.23	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	1137	-	49,53,73	1.40	7 (14%)	58,89,113	1.41	5 (8%)
20	CLA	1	613	-	59,63,73	1.27	9 (15%)	70,101,113	1.31	6 (8%)
21	PQN	A	2001	-	34,34,34	0.41	0	43,45,45	1.04	1 (2%)
21	PQN	B	2002	-	34,34,34	0.42	0	43,45,45	1.07	1 (2%)
29	LUT	2	620	-	42,43,43	2.47	1 (2%)	51,60,60	2.11	19 (37%)
20	CLA	1	610	-	59,63,73	1.24	7 (11%)	70,101,113	1.65	9 (12%)
20	CLA	1	615	-	50,54,73	1.38	8 (16%)	59,90,113	1.45	5 (8%)
22	SF4	C	1003	7	0,12,12	-	-	-		
24	LHG	B	5101	-	34,34,48	0.75	1 (2%)	37,40,54	1.29	4 (10%)
20	CLA	A	1111	-	69,73,73	1.19	9 (13%)	82,113,113	1.34	6 (7%)
20	CLA	4	612	-	50,54,73	1.37	7 (14%)	59,90,113	1.28	4 (6%)
20	CLA	B	1223	-	69,73,73	1.15	7 (10%)	82,113,113	1.33	10 (12%)
23	BCR	O	301	-	14,14,41	1.09	1 (7%)	20,20,56	1.06	1 (5%)
20	CLA	B	1236	-	51,55,73	1.33	8 (15%)	60,91,113	1.41	5 (8%)
20	CLA	1	609	-	64,68,73	1.24	8 (12%)	76,107,113	1.59	3 (3%)
20	CLA	3	617	-	50,54,73	1.36	8 (16%)	59,90,113	1.33	5 (8%)
20	CLA	3	609	-	64,68,73	1.21	8 (12%)	76,107,113	1.31	8 (10%)
22	SF4	C	1002	7	0,12,12	-	-	-		
27	DGD	B	5002	-	62,62,67	0.97	4 (6%)	76,76,81	1.26	8 (10%)
20	CLA	L	302	-	64,68,73	1.21	7 (10%)	76,107,113	1.21	7 (9%)
24	LHG	2	630	-	31,31,48	0.79	2 (6%)	34,37,54	1.24	3 (8%)
20	CLA	B	1225	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	8 (9%)
20	CLA	B	1221	-	58,62,73	1.30	10 (17%)	68,99,113	1.64	9 (13%)
28	CHL	4	606	-	51,55,74	2.16	17 (33%)	56,91,114	2.92	23 (41%)
24	LHG	4	630	-	37,37,48	0.83	2 (5%)	40,43,54	1.26	3 (7%)
20	CLA	A	1126	-	64,68,73	1.19	9 (14%)	76,107,113	1.81	16 (21%)
20	CLA	B	1201	-	54,58,73	1.30	8 (14%)	64,95,113	1.40	10 (15%)
20	CLA	O	201	-	27,35,73	1.84	7 (25%)	32,60,113	1.62	5 (15%)
24	LHG	1	630	-	36,36,48	0.68	1 (2%)	39,42,54	1.26	4 (10%)
20	CLA	A	1131	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	6 (7%)
20	CLA	A	8895	-	69,73,73	1.19	9 (13%)	82,113,113	1.46	5 (6%)
28	CHL	2	611	-	60,64,74	1.99	18 (30%)	67,102,114	2.72	26 (38%)
28	CHL	3	608	-	51,55,74	2.12	16 (31%)	56,91,114	2.91	24 (42%)
25	LMG	J	301	-	49,49,55	0.81	1 (2%)	57,57,63	1.27	5 (8%)
20	CLA	A	1125	-	64,68,73	1.22	9 (14%)	76,107,113	1.69	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	4	610	-	59,63,73	1.26	10 (16%)	70,101,113	1.55	8 (11%)
20	CLA	G	201	-	54,58,73	1.33	8 (14%)	64,95,113	1.36	5 (7%)
20	CLA	2	613	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	6 (7%)
26	LMT	A	5004	-	34,34,36	1.20	4 (11%)	45,45,47	1.05	1 (2%)
23	BCR	I	118	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	8 (14%)
20	CLA	H	200	-	49,53,73	1.39	6 (12%)	58,89,113	1.33	6 (10%)
20	CLA	1	612	-	50,54,73	1.37	8 (16%)	59,90,113	1.30	7 (11%)
20	CLA	B	1203	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	9 (10%)
28	CHL	1	601	-	60,64,74	1.96	17 (28%)	67,102,114	2.86	28 (41%)
20	CLA	A	1139	-	54,58,73	1.31	9 (16%)	64,95,113	1.45	6 (9%)
20	CLA	B	1208	-	49,53,73	1.38	8 (16%)	58,89,113	1.56	7 (12%)
20	CLA	B	1217	-	49,53,73	1.38	7 (14%)	58,89,113	1.37	6 (10%)
20	CLA	3	603	-	59,63,73	1.28	9 (15%)	70,101,113	1.39	5 (7%)
20	CLA	F	301	-	49,53,73	1.38	8 (16%)	58,89,113	1.47	4 (6%)
23	BCR	M	4021	-	41,41,41	0.99	2 (4%)	56,56,56	1.31	9 (16%)
26	LMT	G	401	-	36,36,36	1.15	5 (13%)	47,47,47	1.04	1 (2%)
20	CLA	F	303	-	27,35,73	1.85	6 (22%)	32,60,113	1.62	5 (15%)
20	CLA	A	1115	-	58,62,73	1.26	8 (13%)	68,99,113	1.41	10 (14%)
20	CLA	G	202	-	50,54,73	1.36	7 (14%)	59,90,113	1.34	4 (6%)
20	CLA	3	605	-	27,35,73	1.85	7 (25%)	32,60,113	1.64	6 (18%)
20	CLA	B	1231	-	49,53,73	1.40	7 (14%)	58,89,113	1.46	6 (10%)
20	CLA	L	303	-	49,53,73	1.37	8 (16%)	58,89,113	1.61	8 (13%)
20	CLA	A	1801	-	54,58,73	1.32	9 (16%)	64,95,113	1.46	5 (7%)
20	CLA	J	102	-	49,53,73	1.39	8 (16%)	58,89,113	1.51	4 (6%)
20	CLA	B	1239	-	49,53,73	1.38	7 (14%)	58,89,113	1.58	9 (15%)
20	CLA	4	602	-	64,68,73	1.19	7 (10%)	76,107,113	1.37	8 (10%)
20	CLA	B	1206	-	51,55,73	1.34	9 (17%)	60,91,113	1.49	6 (10%)
20	CLA	3	602	-	64,68,73	1.22	8 (12%)	76,107,113	1.53	9 (11%)
20	CLA	A	1133	-	49,53,73	1.41	6 (12%)	58,89,113	1.18	4 (6%)
20	CLA	4	601	-	54,58,73	1.32	7 (12%)	64,95,113	1.43	5 (7%)
20	CLA	B	1238	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	7 (8%)
20	CLA	K	201	-	59,63,73	1.27	8 (13%)	70,101,113	1.35	6 (8%)
20	CLA	3	604	-	54,58,73	1.33	8 (14%)	64,95,113	1.45	8 (12%)
28	CHL	2	602	-	60,64,74	2.03	21 (35%)	67,102,114	2.77	26 (38%)
20	CLA	B	1210	-	69,73,73	1.18	8 (11%)	82,113,113	1.50	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LUT	3	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.58	5 (9%)
20	CLA	A	1103	-	69,73,73	1.19	9 (13%)	82,113,113	1.22	6 (7%)
20	CLA	A	1124	-	61,65,73	1.23	7 (11%)	72,103,113	1.27	5 (6%)
20	CLA	B	1219	-	49,53,73	1.40	9 (18%)	58,89,113	1.62	9 (15%)
23	BCR	B	4014	-	41,41,41	1.03	2 (4%)	56,56,56	1.41	9 (16%)
20	CLA	A	1104	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	9 (10%)
20	CLA	4	609	-	59,63,73	1.26	8 (13%)	70,101,113	1.69	9 (12%)
20	CLA	4	603	-	59,63,73	1.25	8 (13%)	70,101,113	1.32	7 (10%)
20	CLA	B	1235	-	59,63,73	1.26	9 (15%)	70,101,113	1.32	5 (7%)
20	CLA	A	1117	-	69,73,73	1.17	9 (13%)	82,113,113	1.48	13 (15%)
20	CLA	B	1204	-	65,69,73	1.19	8 (12%)	77,108,113	1.13	6 (7%)
20	CLA	A	1122	-	64,68,73	1.22	9 (14%)	76,107,113	1.42	5 (6%)
20	CLA	B	1229	-	59,63,73	1.28	8 (13%)	70,101,113	1.31	7 (10%)
20	CLA	2	609	-	59,63,73	1.26	7 (11%)	70,101,113	1.63	6 (8%)
22	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
23	BCR	3	623	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	7 (12%)
20	CLA	A	1113	-	49,53,73	1.38	8 (16%)	58,89,113	1.57	10 (17%)
20	CLA	A	1120	-	49,53,73	1.37	8 (16%)	58,89,113	1.45	4 (6%)
20	CLA	B	1021	-	69,73,73	1.16	10 (14%)	82,113,113	1.27	9 (10%)
26	LMT	B	5001	-	32,32,36	1.24	6 (18%)	43,43,47	0.96	0
26	LMT	G	402	-	32,32,36	1.23	5 (15%)	43,43,47	0.91	0
20	CLA	4	604	-	54,58,73	1.31	8 (14%)	64,95,113	1.39	7 (10%)
20	CLA	1	614	-	50,54,73	1.37	8 (16%)	59,90,113	1.50	7 (11%)
20	CLA	1	608	-	54,58,73	1.31	7 (12%)	64,95,113	1.44	7 (10%)
28	CHL	4	615	-	47,51,74	2.18	16 (34%)	50,86,114	3.03	22 (44%)
20	CLA	2	612	-	56,60,73	1.31	7 (12%)	65,97,113	1.42	6 (9%)
20	CLA	L	301	-	54,58,73	1.35	8 (14%)	64,95,113	1.63	9 (14%)
20	CLA	B	1215	-	64,68,73	1.22	9 (14%)	76,107,113	1.70	11 (14%)
23	BCR	A	4003	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
19	CL0	A	1011	-	69,73,73	1.18	10 (14%)	82,113,113	1.28	7 (8%)
20	CLA	A	1106	-	59,63,73	1.25	9 (15%)	70,101,113	1.60	6 (8%)
20	CLA	B	1216	-	59,63,73	1.27	10 (16%)	70,101,113	1.72	11 (15%)
20	CLA	2	614	-	54,58,73	1.31	8 (14%)	64,95,113	1.51	7 (10%)
20	CLA	B	1214	-	63,67,73	1.24	10 (15%)	74,105,113	1.51	11 (14%)
29	LUT	4	620	-	42,43,43	2.51	2 (4%)	51,60,60	2.04	12 (23%)

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
20	CLA	B	1224	-	-	11/35/111/115	-
20	CLA	B	1226	-	-	6/27/103/115	-
20	CLA	4	611	-	-	6/27/103/115	-
20	CLA	3	610	-	-	9/27/103/115	-
28	CHL	4	607	-	-	9/19/95/117	-
20	CLA	A	1102	-	-	8/15/91/115	-
23	BCR	B	4017	-	-	17/29/63/63	0/2/2/2
23	BCR	F	416	-	-	17/29/63/63	0/2/2/2
25	LMG	2	631	-	-	6/31/51/70	0/1/1/1
20	CLA	A	1107	-	-	9/15/91/115	-
23	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
20	CLA	A	1105	-	-	0/21/97/115	-
20	CLA	B	1209	-	-	2/15/91/115	-
23	BCR	3	624	-	-	16/29/63/63	0/2/2/2
20	CLA	B	1220	-	-	4/15/91/115	-
29	LUT	4	623	-	1/1/12/27	12/29/67/67	0/2/2/2
20	CLA	2	610	-	-	10/33/109/115	-
20	CLA	4	614	-	-	7/17/93/115	-
23	BCR	B	4010	-	-	6/29/63/63	0/2/2/2
20	CLA	F	302	-	-	7/17/93/115	-
24	LHG	A	5001	-	-	20/53/53/53	-
20	CLA	A	1022	-	-	9/39/115/115	-
20	CLA	A	1130	-	-	6/33/109/115	-
20	CLA	B	1212	-	-	3/15/91/115	-
20	CLA	B	1237	-	-	11/39/115/115	-
20	CLA	3	611	-	-	4/10/86/115	-
20	CLA	A	1136	-	-	10/39/115/115	-
20	CLA	A	1116	-	-	8/26/102/115	-
23	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
20	CLA	B	1227	-	-	1/15/91/115	-
20	CLA	1	611	-	-	4/17/93/115	-
29	LUT	4	621	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1228	-	-	9/20/96/115	-
20	CLA	2	604	-	-	5/21/97/115	-
20	CLA	B	1205	-	-	9/39/115/115	-
20	CLA	B	1211	-	-	9/29/105/115	-
29	LUT	3	621	-	-	8/29/67/67	0/2/2/2
20	CLA	A	1121	-	-	9/23/99/115	-
26	LMT	4	631	-	-	4/21/61/61	0/2/2/2
20	CLA	B	1234	-	-	6/23/99/115	-
26	LMT	1	631	-	-	6/21/61/61	0/2/2/2
28	CHL	2	615	-	-	13/19/95/117	-
23	BCR	A	4002	-	-	9/29/63/63	0/2/2/2
29	LUT	1	620	-	-	5/29/67/67	0/2/2/2
20	CLA	A	5005	-	-	6/21/97/115	-
20	CLA	3	607	-	-	18/33/109/115	-
20	CLA	3	612	-	-	5/15/91/115	-
23	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
23	BCR	1	623	-	-	5/18/35/63	0/1/1/2
20	CLA	B	1012	-	-	14/27/103/115	-
20	CLA	B	1230	-	-	8/15/91/115	-
20	CLA	3	606	-	-	11/17/93/115	-
20	CLA	A	1108	-	-	5/15/91/115	-
23	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
20	CLA	A	1119	-	-	10/39/115/115	-
28	CHL	2	608	-	-	11/20/96/117	-
20	CLA	A	1135	-	-	8/23/99/115	-
20	CLA	1	602	-	-	2/33/109/115	-
28	CHL	2	607	-	-	10/19/95/117	-
20	CLA	B	1240	-	-	13/39/115/115	-
20	CLA	B	1202	-	-	10/39/115/115	-
20	CLA	1	603	-	-	14/27/103/115	-
25	LMG	J	302	-	-	6/21/41/70	0/1/1/1
20	CLA	B	1023	-	-	8/35/111/115	-
28	CHL	4	608	-	-	10/23/99/117	-
20	CLA	A	1101	-	-	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1132	-	-	8/39/115/115	-
20	CLA	A	1134	-	-	6/15/91/115	-
20	CLA	A	1140	-	-	8/23/99/115	-
28	CHL	1	607	-	-	8/19/95/117	-
23	BCR	A	4001	-	-	15/29/63/63	0/2/2/2
23	BCR	I	120	-	-	14/29/63/63	0/2/2/2
24	LHG	A	5003	-	-	11/35/35/53	-
23	BCR	L	420	-	-	7/29/63/63	0/2/2/2
20	CLA	B	1213	-	-	6/27/103/115	-
23	BCR	G	311	-	-	7/29/63/63	0/2/2/2
29	LUT	2	621	-	-	2/29/67/67	0/2/2/2
20	CLA	I	121	-	-	12/39/115/115	-
28	CHL	2	601	-	-	22/41/117/117	-
23	BCR	L	419	-	-	4/29/63/63	0/2/2/2
20	CLA	B	1222	-	-	6/17/93/115	-
23	BCR	B	4009	-	-	3/29/63/63	0/2/2/2
20	CLA	A	1128	-	-	12/39/115/115	-
20	CLA	3	613	-	-	10/27/103/115	-
20	CLA	K	202	-	-	8/17/93/115	-
28	CHL	2	606	-	-	9/17/93/117	-
20	CLA	A	1013	-	-	3/29/105/115	-
29	LUT	2	623	-	1/1/12/27	9/29/67/67	0/2/2/2
20	CLA	G	218	-	-	10/27/103/115	-
20	CLA	A	1118	-	-	13/27/103/115	-
20	CLA	A	1110	-	-	7/27/103/115	-
20	CLA	B	1232	-	-	6/15/91/115	-
23	BCR	J	213	-	-	8/29/63/63	0/2/2/2
29	LUT	1	621	-	-	5/29/67/67	0/2/2/2
20	CLA	3	614	-	-	9/19/95/115	-
20	CLA	K	204	-	-	8/15/91/115	-
20	CLA	A	1127	-	-	18/39/115/115	-
23	BCR	K	301	-	-	14/29/63/63	0/2/2/2
20	CLA	A	1114	-	-	6/15/91/115	-
20	CLA	4	613	-	-	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A	4011	-	-	18/29/63/63	0/2/2/2
20	CLA	A	1109	-	-	10/39/115/115	-
23	BCR	J	212	-	-	14/29/63/63	0/2/2/2
24	LHG	3	630	-	-	12/38/38/53	-
20	CLA	1	604	-	-	4/21/97/115	-
20	CLA	A	1112	-	-	6/15/91/115	-
20	CLA	2	603	-	-	7/17/93/115	-
23	BCR	B	4004	-	-	14/29/63/63	0/2/2/2
20	CLA	1	606	-	-	6/15/91/115	-
25	LMG	A	5002	-	-	13/29/49/70	0/1/1/1
20	CLA	A	1138	-	-	9/33/109/115	-
20	CLA	A	1137	-	-	5/15/91/115	-
20	CLA	1	613	-	-	9/27/103/115	-
21	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
21	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
29	LUT	2	620	-	-	6/29/67/67	0/2/2/2
20	CLA	1	610	-	-	6/27/103/115	-
20	CLA	1	615	-	-	8/17/93/115	-
24	LHG	B	5101	-	-	9/39/39/53	-
22	SF4	C	1003	7	-	-	0/6/5/5
20	CLA	A	1111	-	-	15/39/115/115	-
20	CLA	4	612	-	-	10/17/93/115	-
20	CLA	B	1223	-	-	6/39/115/115	-
23	BCR	O	301	-	-	3/5/22/63	0/1/1/2
20	CLA	B	1236	-	-	6/18/94/115	-
20	CLA	1	609	-	-	6/33/109/115	-
20	CLA	3	617	-	-	6/17/93/115	-
20	CLA	3	609	-	-	10/33/109/115	-
22	SF4	C	1002	7	-	-	0/6/5/5
27	DGD	B	5002	-	-	18/50/90/95	0/2/2/2
20	CLA	L	302	-	-	12/33/109/115	-
24	LHG	2	630	-	-	10/36/36/53	-
20	CLA	B	1225	-	-	15/39/115/115	-
20	CLA	B	1221	-	-	1/26/102/115	-
28	CHL	4	606	-	-	11/19/95/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	4	630	-	-	15/42/42/53	-
20	CLA	A	1126	-	-	11/33/109/115	-
20	CLA	B	1201	-	-	10/21/97/115	-
24	LHG	1	630	-	-	14/41/41/53	-
20	CLA	A	1131	-	-	6/39/115/115	-
20	CLA	A	8895	-	-	9/39/115/115	-
28	CHL	2	611	-	-	8/29/105/117	-
28	CHL	3	608	-	-	5/19/95/117	-
25	LMG	J	301	-	-	15/44/64/70	0/1/1/1
20	CLA	A	1125	-	-	13/33/109/115	-
20	CLA	4	610	-	-	7/27/103/115	-
20	CLA	G	201	-	-	6/21/97/115	-
20	CLA	2	613	-	-	13/39/115/115	-
26	LMT	A	5004	-	-	7/19/59/61	0/2/2/2
23	BCR	I	118	-	-	11/29/63/63	0/2/2/2
20	CLA	H	200	-	-	5/15/91/115	-
20	CLA	1	612	-	-	8/17/93/115	-
20	CLA	B	1203	-	-	13/39/115/115	-
28	CHL	1	601	-	-	10/29/105/117	-
20	CLA	A	1139	-	-	6/21/97/115	-
20	CLA	B	1208	-	-	3/15/91/115	-
20	CLA	B	1217	-	-	5/15/91/115	-
20	CLA	3	603	-	-	12/27/103/115	-
20	CLA	F	301	-	-	3/15/91/115	-
23	BCR	M	4021	-	-	5/29/63/63	0/2/2/2
26	LMT	G	401	-	-	5/21/61/61	0/2/2/2
20	CLA	A	1115	-	-	6/26/102/115	-
20	CLA	G	202	-	-	8/17/93/115	-
20	CLA	B	1231	-	-	7/15/91/115	-
20	CLA	L	303	-	-	7/15/91/115	-
20	CLA	A	1801	-	-	7/21/97/115	-
20	CLA	J	102	-	-	9/15/91/115	-
20	CLA	B	1239	-	-	6/15/91/115	-
20	CLA	4	602	-	-	3/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1206	-	-	7/18/94/115	-
20	CLA	3	602	-	-	8/33/109/115	-
20	CLA	A	1133	-	-	7/15/91/115	-
20	CLA	4	601	-	-	9/21/97/115	-
20	CLA	B	1238	-	-	16/39/115/115	-
20	CLA	K	201	-	-	7/27/103/115	-
20	CLA	3	604	-	-	6/21/97/115	-
28	CHL	2	602	-	-	15/29/105/117	-
20	CLA	B	1210	-	-	22/39/115/115	-
29	LUT	3	620	-	-	2/29/67/67	0/2/2/2
20	CLA	A	1103	-	-	17/39/115/115	-
20	CLA	A	1124	-	-	11/30/106/115	-
20	CLA	B	1219	-	-	3/15/91/115	-
23	BCR	B	4014	-	-	19/29/63/63	0/2/2/2
20	CLA	A	1104	-	-	19/39/115/115	-
20	CLA	4	609	-	-	10/27/103/115	-
20	CLA	4	603	-	-	12/27/103/115	-
20	CLA	B	1235	-	-	9/27/103/115	-
20	CLA	A	1117	-	-	10/39/115/115	-
20	CLA	B	1204	-	-	8/35/111/115	-
20	CLA	A	1122	-	-	14/33/109/115	-
20	CLA	B	1229	-	-	9/27/103/115	-
20	CLA	2	609	-	-	3/27/103/115	-
23	BCR	3	623	-	-	14/29/63/63	0/2/2/2
22	SF4	A	3001	2,1	-	-	0/6/5/5
20	CLA	A	1113	-	-	4/15/91/115	-
20	CLA	A	1120	-	-	3/15/91/115	-
20	CLA	B	1021	-	-	16/39/115/115	-
26	LMT	B	5001	-	-	4/17/57/61	0/2/2/2
26	LMT	G	402	-	-	6/17/57/61	0/2/2/2
20	CLA	4	604	-	-	6/21/97/115	-
20	CLA	1	614	-	-	8/17/93/115	-
20	CLA	1	608	-	-	3/21/97/115	-
28	CHL	4	615	-	-	4/14/90/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	2	612	-	-	7/24/100/115	-
20	CLA	L	301	-	-	7/21/97/115	-
20	CLA	B	1215	-	-	11/33/109/115	-
23	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
19	CL0	A	1011	-	-	7/39/115/115	-
20	CLA	A	1106	-	-	8/27/103/115	-
20	CLA	B	1216	-	-	9/27/103/115	-
20	CLA	2	614	-	-	5/21/97/115	-
20	CLA	B	1214	-	-	8/32/108/115	-
29	LUT	4	620	-	-	9/29/67/67	0/2/2/2

The worst 5 of 1536 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	620	LUT	C24-C25	16.76	1.53	1.33
29	1	621	LUT	C24-C25	16.27	1.52	1.33
29	2	623	LUT	C24-C25	15.79	1.51	1.33
29	4	620	LUT	C24-C25	15.47	1.51	1.33
29	2	620	LUT	C24-C25	15.22	1.51	1.33

The worst 5 of 1773 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	621	LUT	O23-C23-C22	-11.92	88.94	110.06
20	2	609	CLA	C4A-NA-C1A	10.10	111.29	106.68
20	4	609	CLA	C4A-NA-C1A	9.85	111.17	106.68
20	1	609	CLA	C4A-NA-C1A	9.25	110.90	106.68
20	A	1106	CLA	C4A-NA-C1A	9.16	110.86	106.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	2	623	LUT	C26
29	4	623	LUT	C26

5 of 1828 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1013	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	1022	CLA	C1A-C2A-CAA-CBA
20	A	1022	CLA	C3A-C2A-CAA-CBA
20	A	1101	CLA	CHA-CBD-CGD-O1D
20	A	1101	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

163 monomers are involved in 359 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1224	CLA	4	0
20	B	1226	CLA	3	0
20	3	610	CLA	4	0
20	A	1102	CLA	4	0
23	B	4017	BCR	7	0
23	F	416	BCR	2	0
20	A	1107	CLA	1	0
23	B	4006	BCR	4	0
20	A	1105	CLA	1	0
20	B	1209	CLA	2	0
23	3	624	BCR	3	0
20	B	1220	CLA	2	0
20	2	610	CLA	2	0
29	4	623	LUT	1	0
23	B	4010	BCR	5	0
24	A	5001	LHG	3	0
20	A	1022	CLA	8	0
20	A	1130	CLA	3	0
20	B	1212	CLA	1	0
20	B	1237	CLA	8	0
20	A	1136	CLA	3	0
20	A	1116	CLA	4	0
23	A	4008	BCR	2	0
20	B	1227	CLA	2	0
29	4	621	LUT	2	0
20	B	1228	CLA	3	0
20	B	1205	CLA	5	0
29	3	621	LUT	2	0
26	4	631	LMT	3	0
26	1	631	LMT	2	0
29	1	620	LUT	3	0
20	A	5005	CLA	4	0
20	3	607	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	612	CLA	1	0
23	B	4005	BCR	3	0
20	B	1012	CLA	6	0
20	B	1230	CLA	3	0
20	A	1108	CLA	3	0
23	A	4007	BCR	2	0
20	A	1119	CLA	2	0
28	2	608	CHL	3	0
20	A	1135	CLA	2	0
20	1	602	CLA	2	0
20	B	1240	CLA	2	0
20	B	1202	CLA	6	0
20	1	603	CLA	4	0
25	J	302	LMG	1	0
20	B	1023	CLA	5	0
28	4	608	CHL	1	0
20	A	1101	CLA	2	0
20	A	1132	CLA	4	0
20	A	1134	CLA	2	0
20	A	1140	CLA	4	0
28	1	607	CHL	1	0
23	A	4001	BCR	1	0
23	I	120	BCR	5	0
24	A	5003	LHG	1	0
23	L	420	BCR	4	0
20	B	1213	CLA	3	0
23	G	311	BCR	3	0
29	2	621	LUT	2	0
20	I	121	CLA	7	0
28	2	601	CHL	7	0
23	L	419	BCR	3	0
23	B	4009	BCR	2	0
20	A	1128	CLA	5	0
20	3	613	CLA	2	0
20	A	1013	CLA	2	0
29	2	623	LUT	1	0
20	A	1118	CLA	4	0
20	A	1110	CLA	2	0
20	B	1232	CLA	1	0
23	J	213	BCR	3	0
29	1	621	LUT	5	0
20	K	204	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1127	CLA	6	0
23	K	301	BCR	1	0
20	A	1114	CLA	2	0
23	A	4011	BCR	1	0
20	A	1109	CLA	2	0
23	J	212	BCR	1	0
24	3	630	LHG	1	0
23	B	4004	BCR	1	0
20	1	606	CLA	1	0
20	A	1138	CLA	5	0
25	A	5002	LMG	2	0
20	A	1137	CLA	3	0
21	A	2001	PQN	2	0
21	B	2002	PQN	5	0
29	2	620	LUT	6	0
20	A	1111	CLA	6	0
20	B	1223	CLA	6	0
20	B	1236	CLA	1	0
20	1	609	CLA	3	0
20	3	617	CLA	1	0
20	3	609	CLA	2	0
27	B	5002	DGD	5	0
20	L	302	CLA	5	0
24	2	630	LHG	2	0
20	B	1225	CLA	5	0
20	B	1221	CLA	5	0
24	4	630	LHG	2	0
20	A	1126	CLA	5	0
20	B	1201	CLA	2	0
24	1	630	LHG	1	0
20	A	1131	CLA	2	0
20	A	8895	CLA	4	0
28	3	608	CHL	2	0
25	J	301	LMG	3	0
20	A	1125	CLA	2	0
20	4	610	CLA	3	0
20	2	613	CLA	1	0
26	A	5004	LMT	1	0
23	I	118	BCR	1	0
20	H	200	CLA	2	0
20	B	1203	CLA	4	0
28	1	601	CHL	1	0

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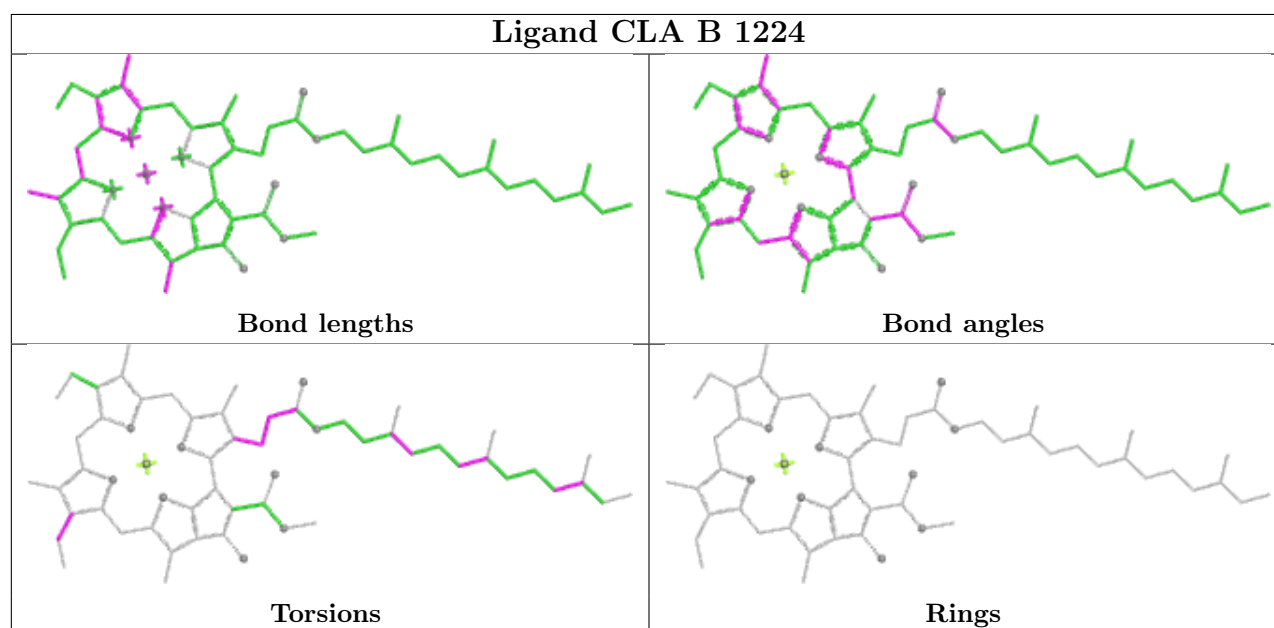
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1139	CLA	2	0
20	B	1208	CLA	4	0
20	B	1217	CLA	4	0
20	F	301	CLA	4	0
23	M	4021	BCR	5	0
26	G	401	LMT	3	0
20	A	1115	CLA	1	0
20	B	1231	CLA	1	0
20	L	303	CLA	4	0
20	A	1801	CLA	1	0
20	B	1239	CLA	2	0
20	4	602	CLA	2	0
20	B	1206	CLA	4	0
20	3	602	CLA	3	0
20	A	1133	CLA	2	0
20	4	601	CLA	1	0
20	B	1238	CLA	7	0
20	K	201	CLA	1	0
20	3	604	CLA	1	0
28	2	602	CHL	2	0
20	B	1210	CLA	6	0
29	3	620	LUT	7	0
20	A	1103	CLA	4	0
20	A	1124	CLA	3	0
20	B	1219	CLA	1	0
23	B	4014	BCR	7	0
20	A	1104	CLA	5	0
20	4	603	CLA	4	0
20	B	1235	CLA	2	0
20	A	1117	CLA	7	0
20	B	1204	CLA	5	0
20	A	1122	CLA	3	0
20	B	1229	CLA	1	0
20	2	609	CLA	1	0
23	3	623	BCR	1	0
20	A	1113	CLA	1	0
20	A	1120	CLA	1	0
20	B	1021	CLA	2	0
20	L	301	CLA	1	0
20	B	1215	CLA	1	0
23	A	4003	BCR	2	0
19	A	1011	CL0	5	0

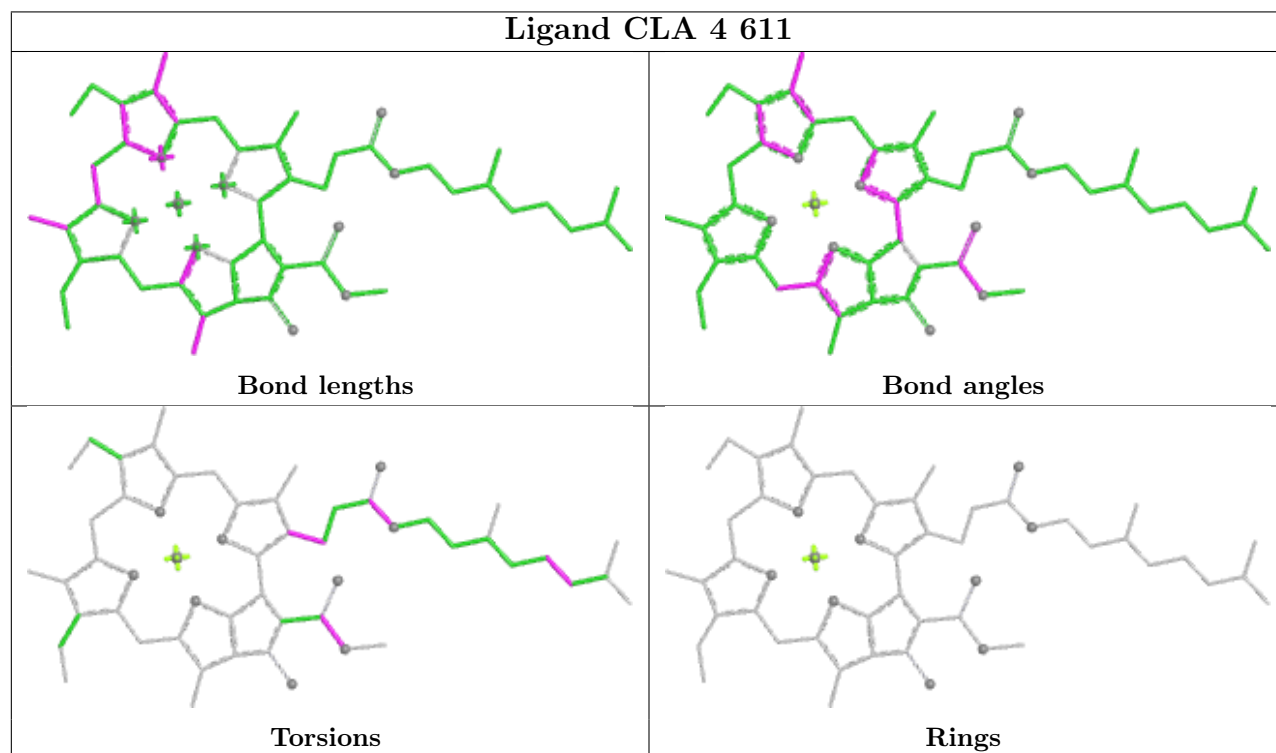
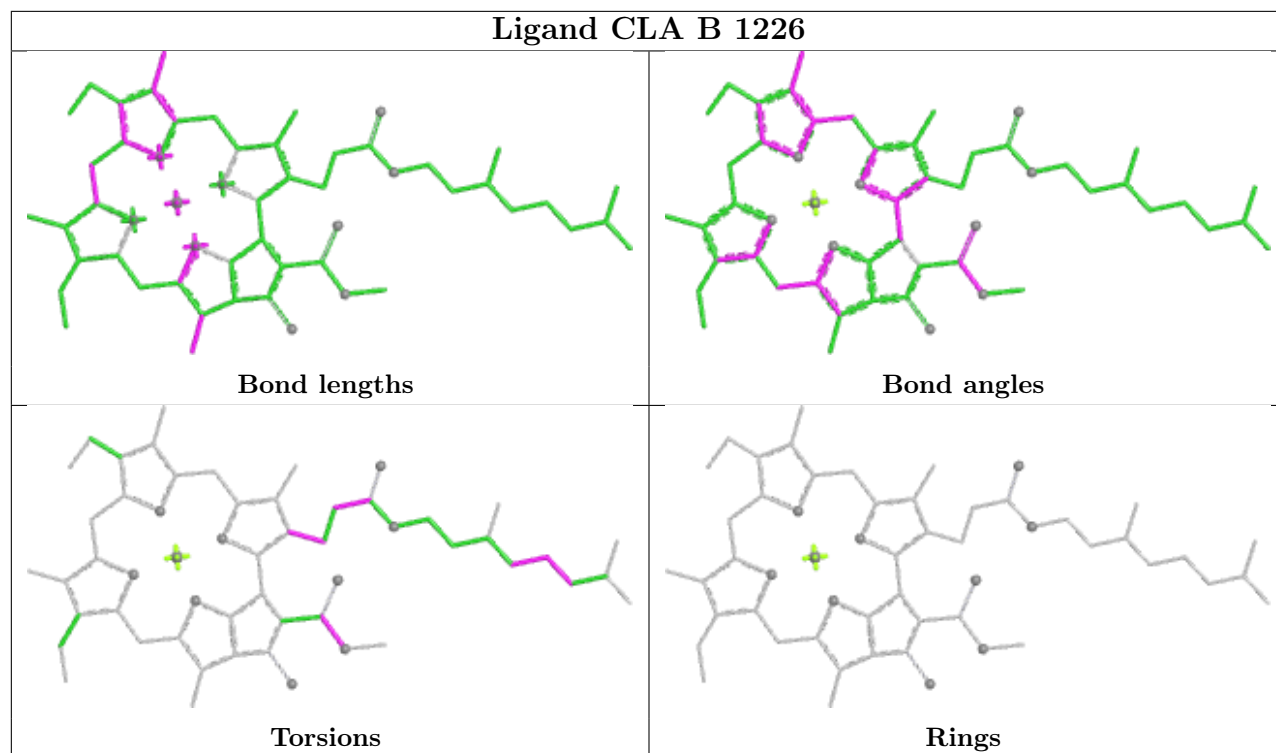
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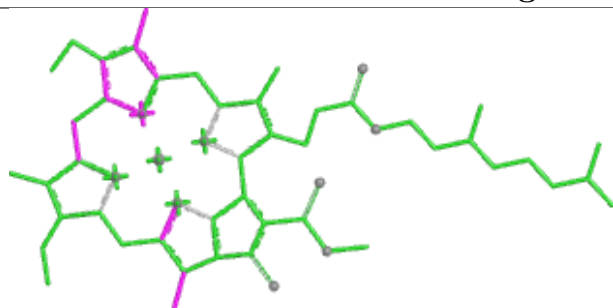
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1106	CLA	3	0
20	B	1216	CLA	2	0
20	B	1214	CLA	3	0
29	4	620	LUT	4	0

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

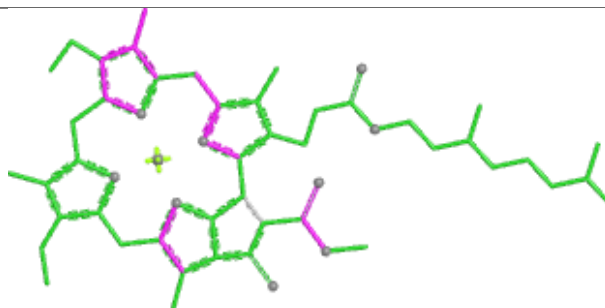




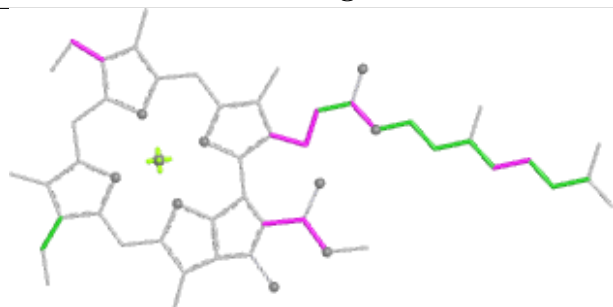
Ligand CLA 3 610



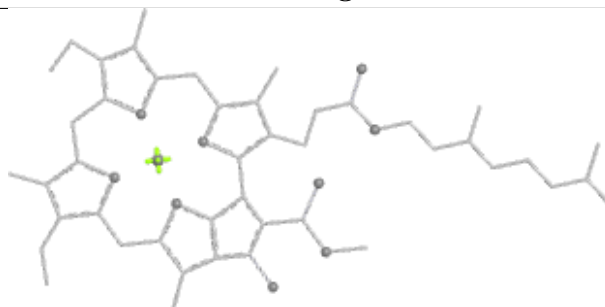
Bond lengths



Bond angles

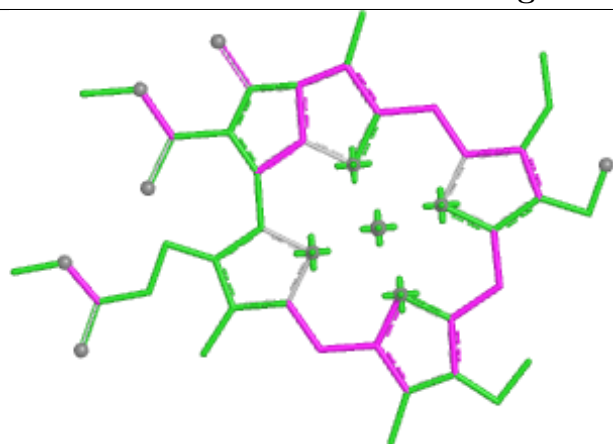


Torsions

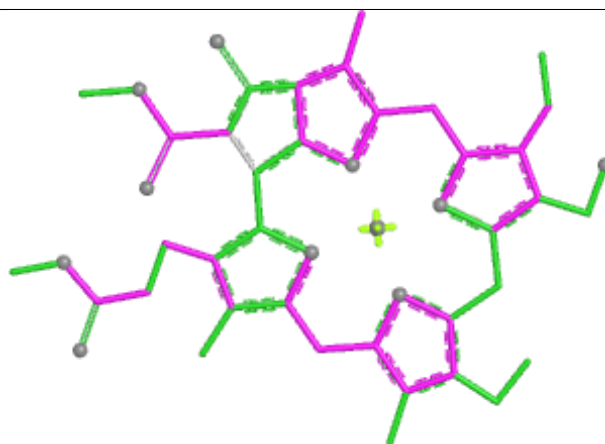


Rings

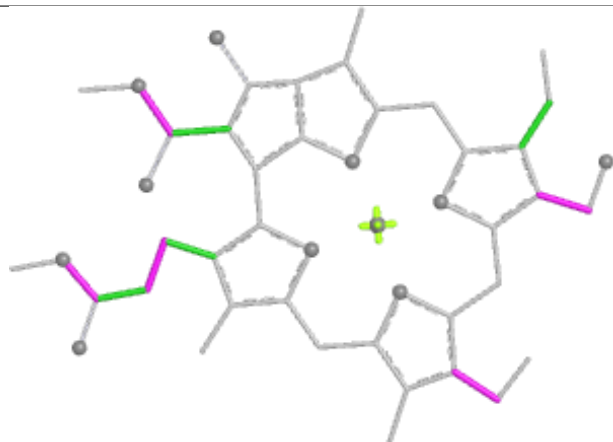
Ligand CHL 4 607



Bond lengths



Bond angles

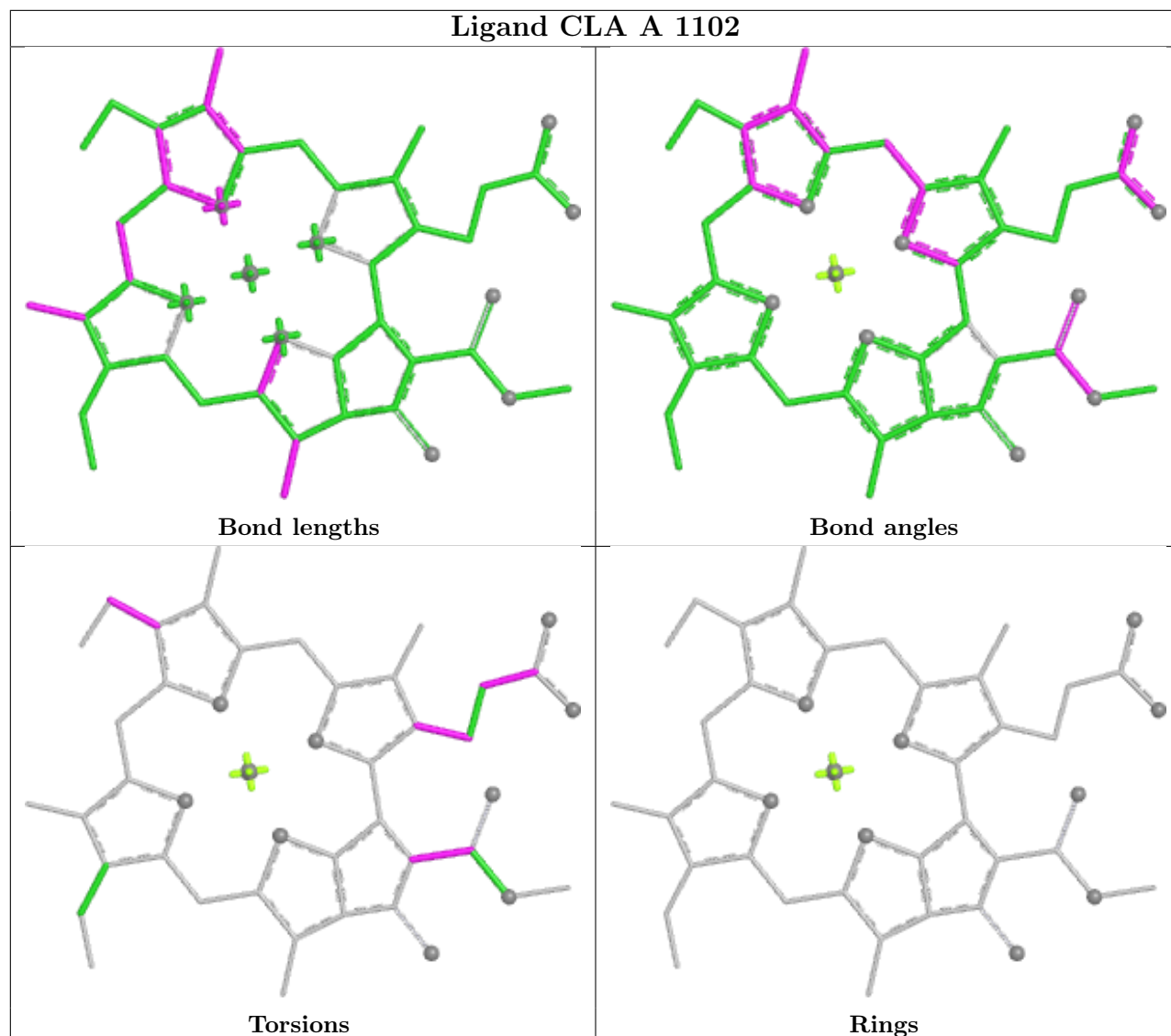


Torsions

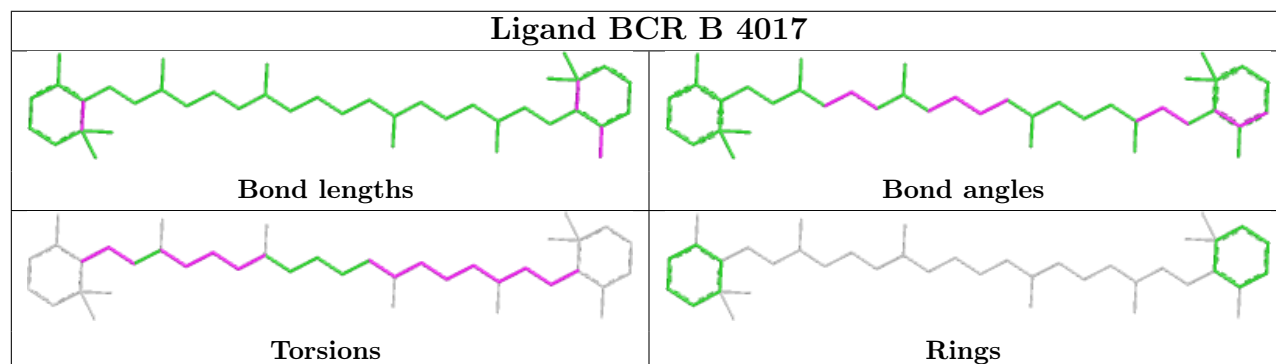


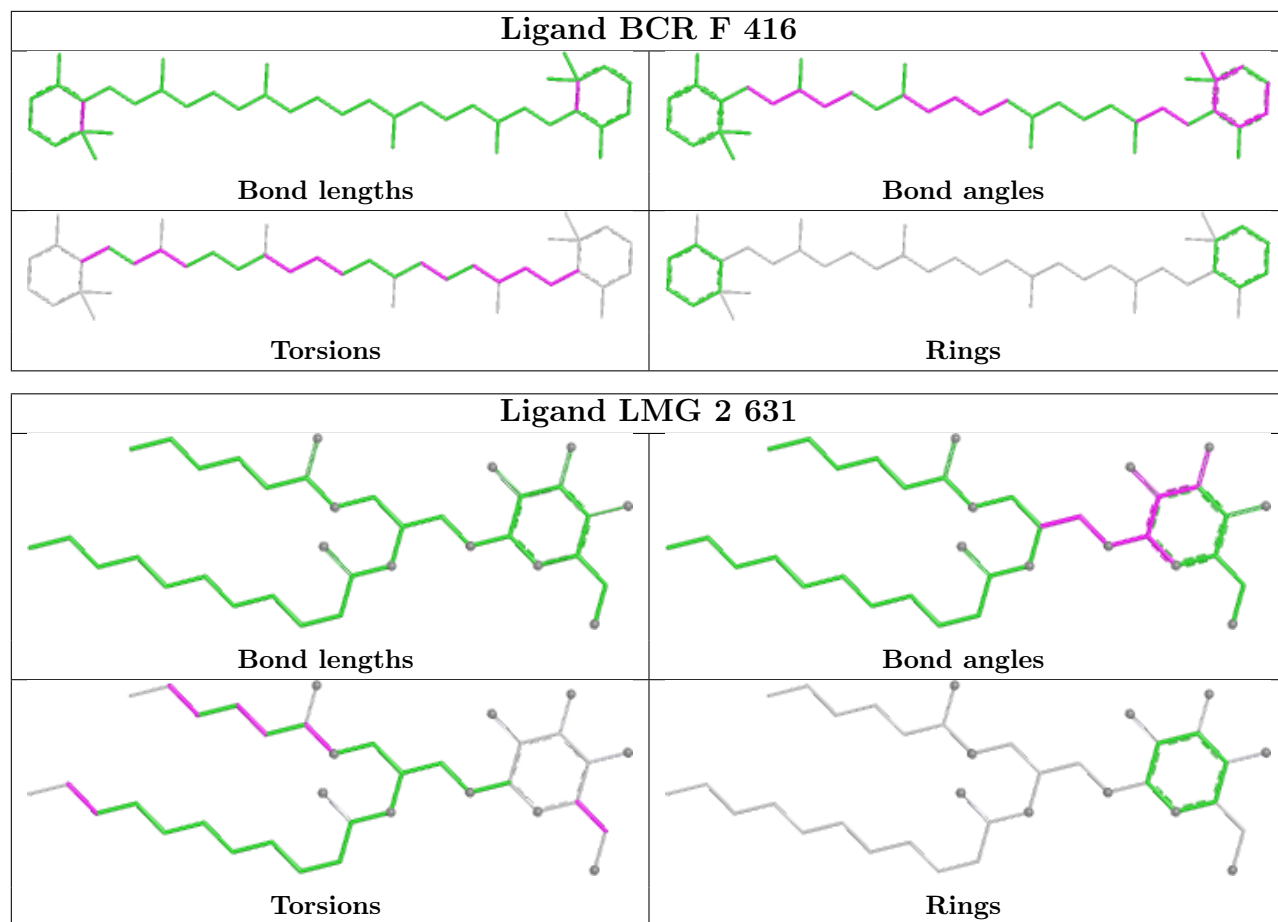
Rings

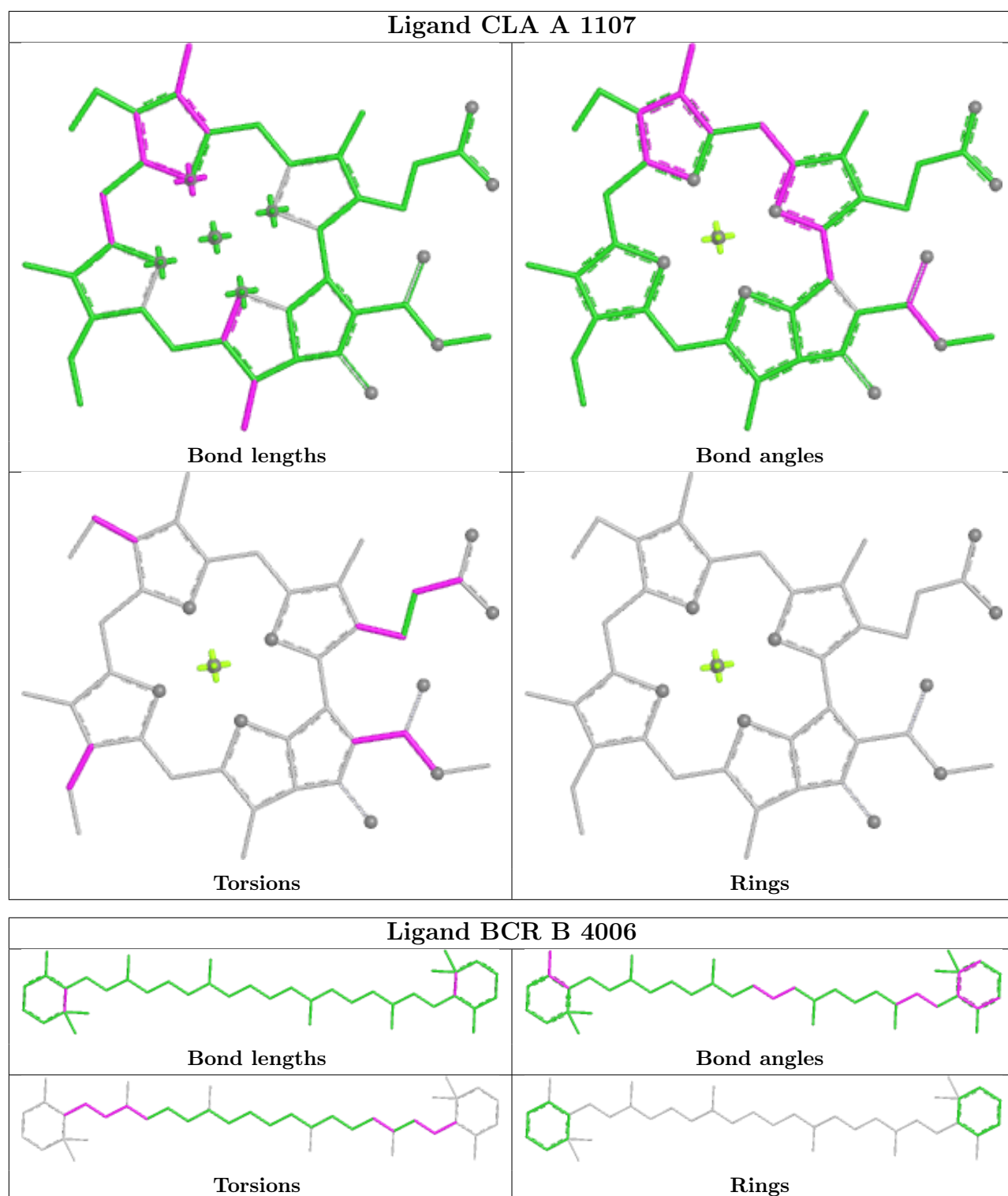
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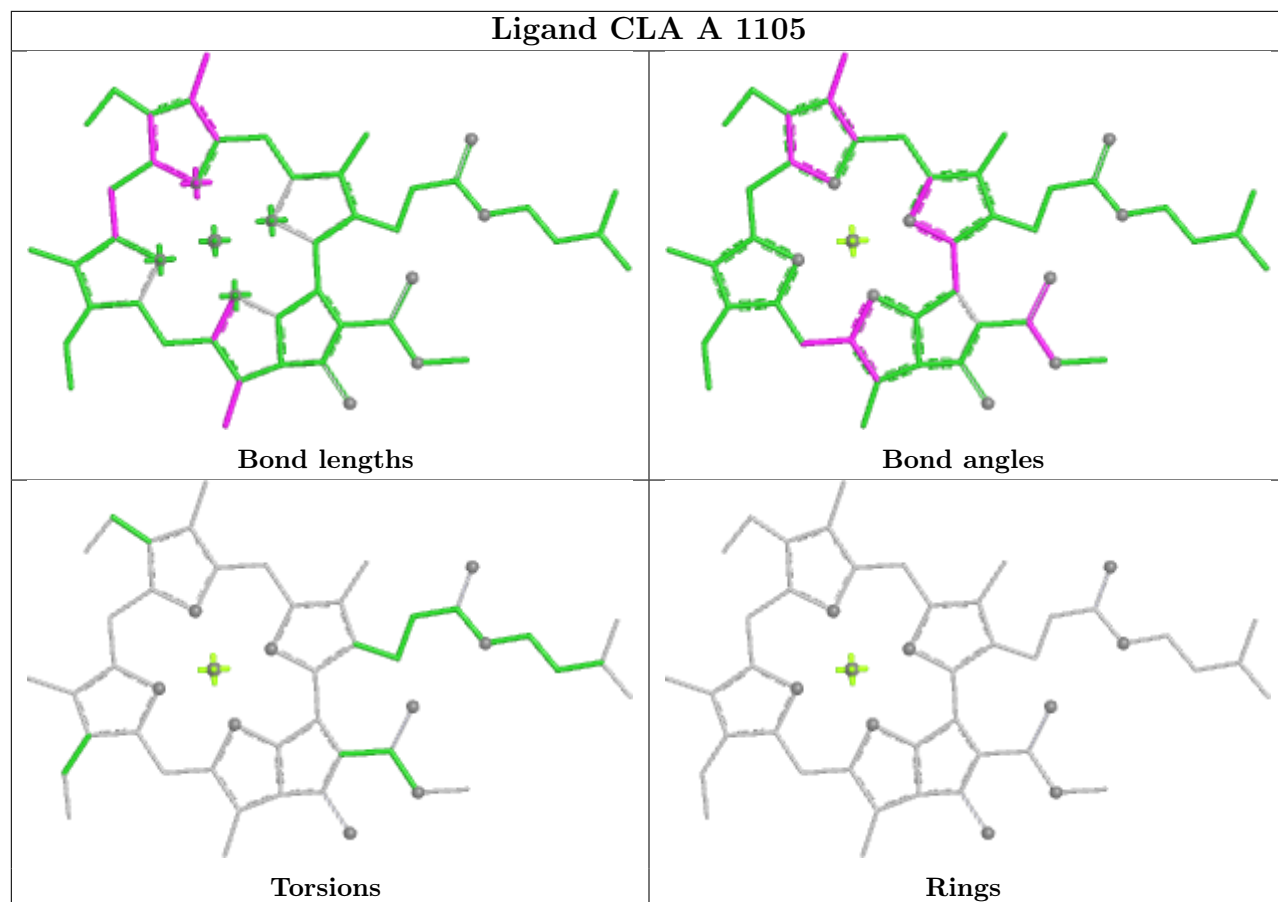


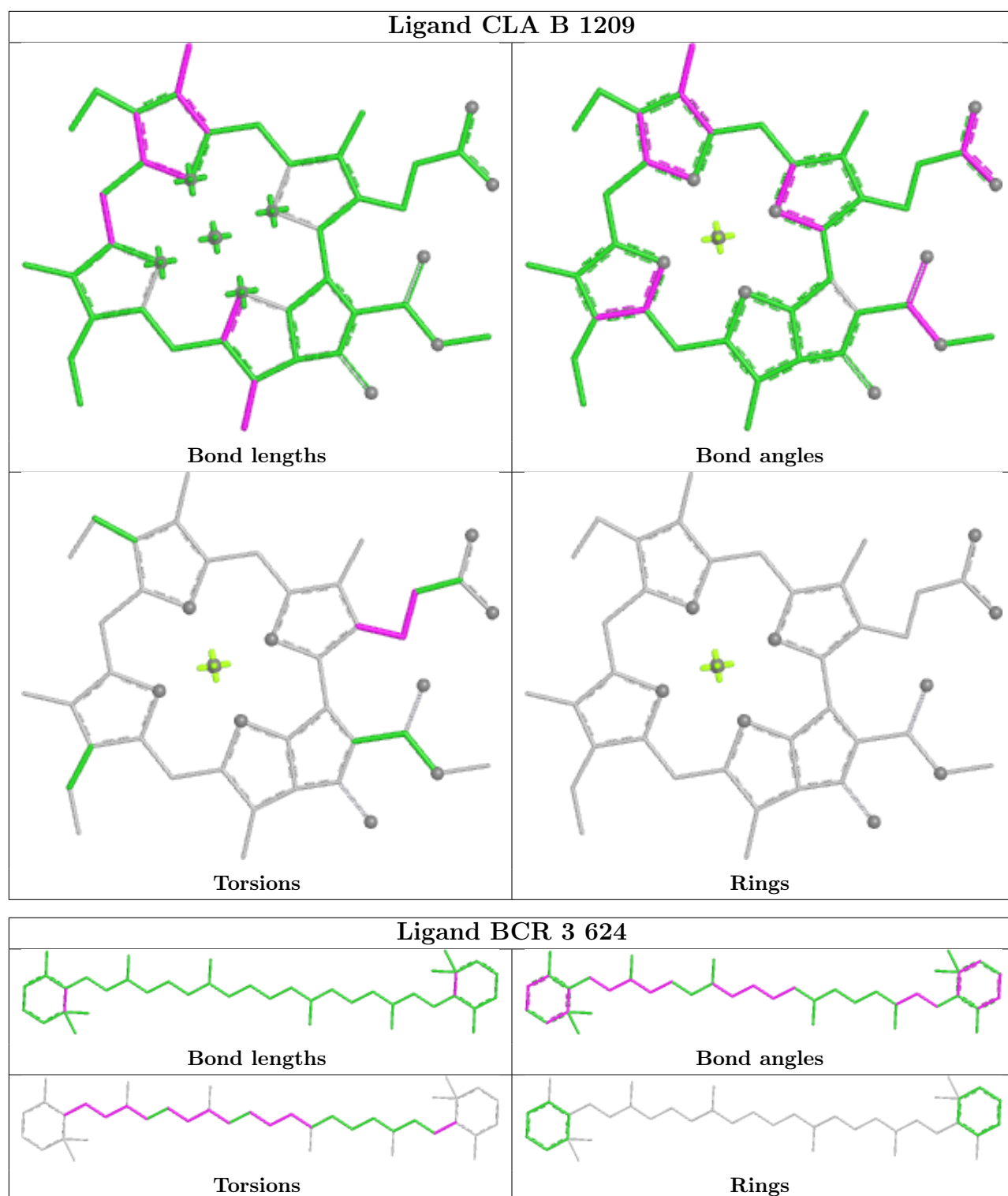
Ligand BCR B 4017



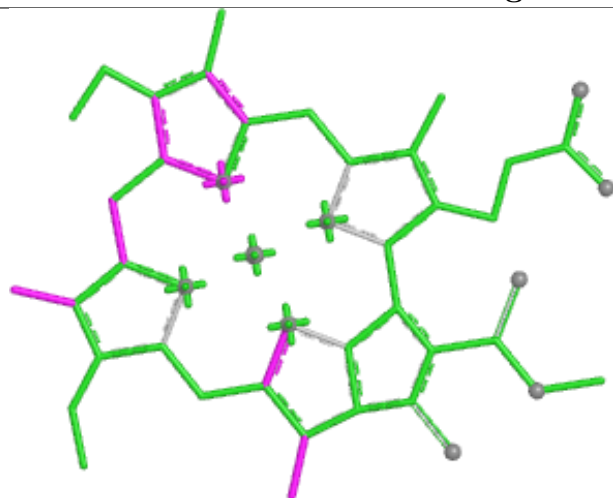




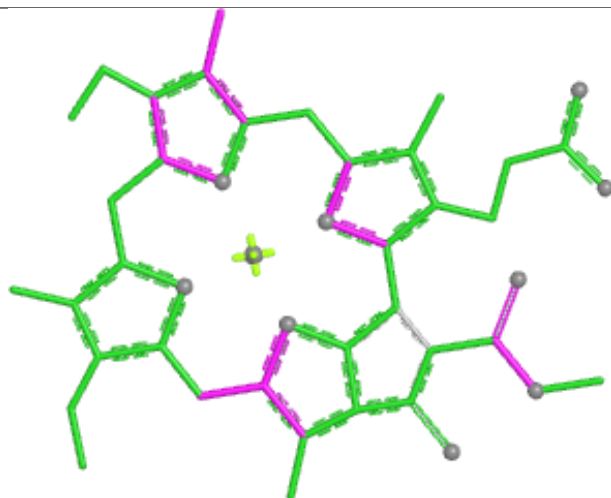




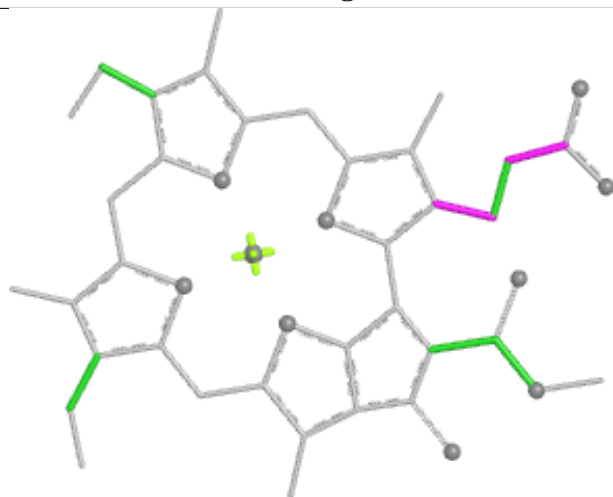
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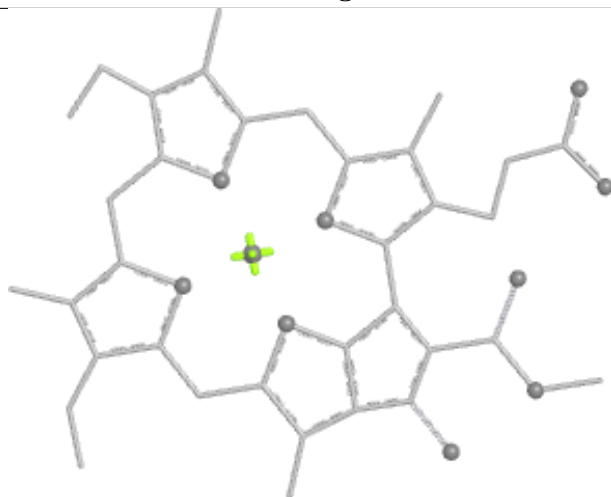
Bond lengths



Bond angles

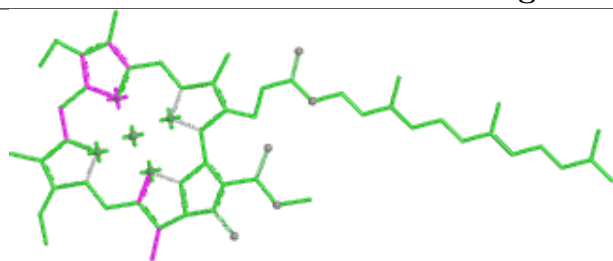


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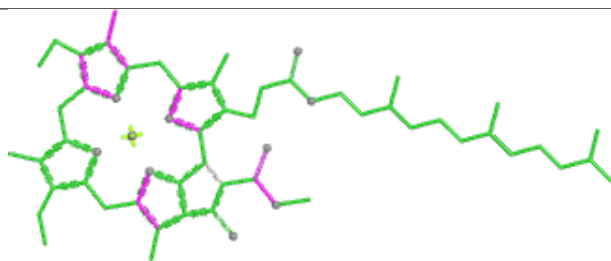


Rings

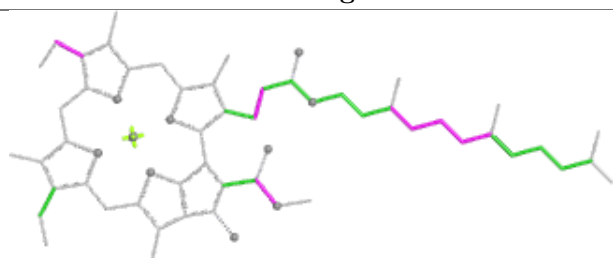
Ligand CLA 2 610



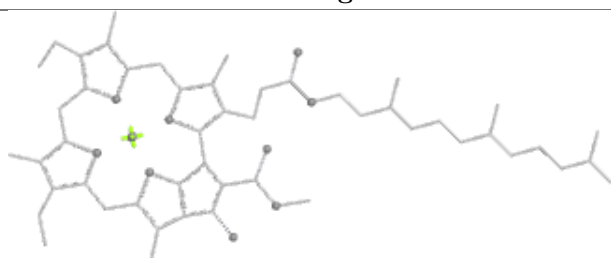
Bond lengths



Bond angles

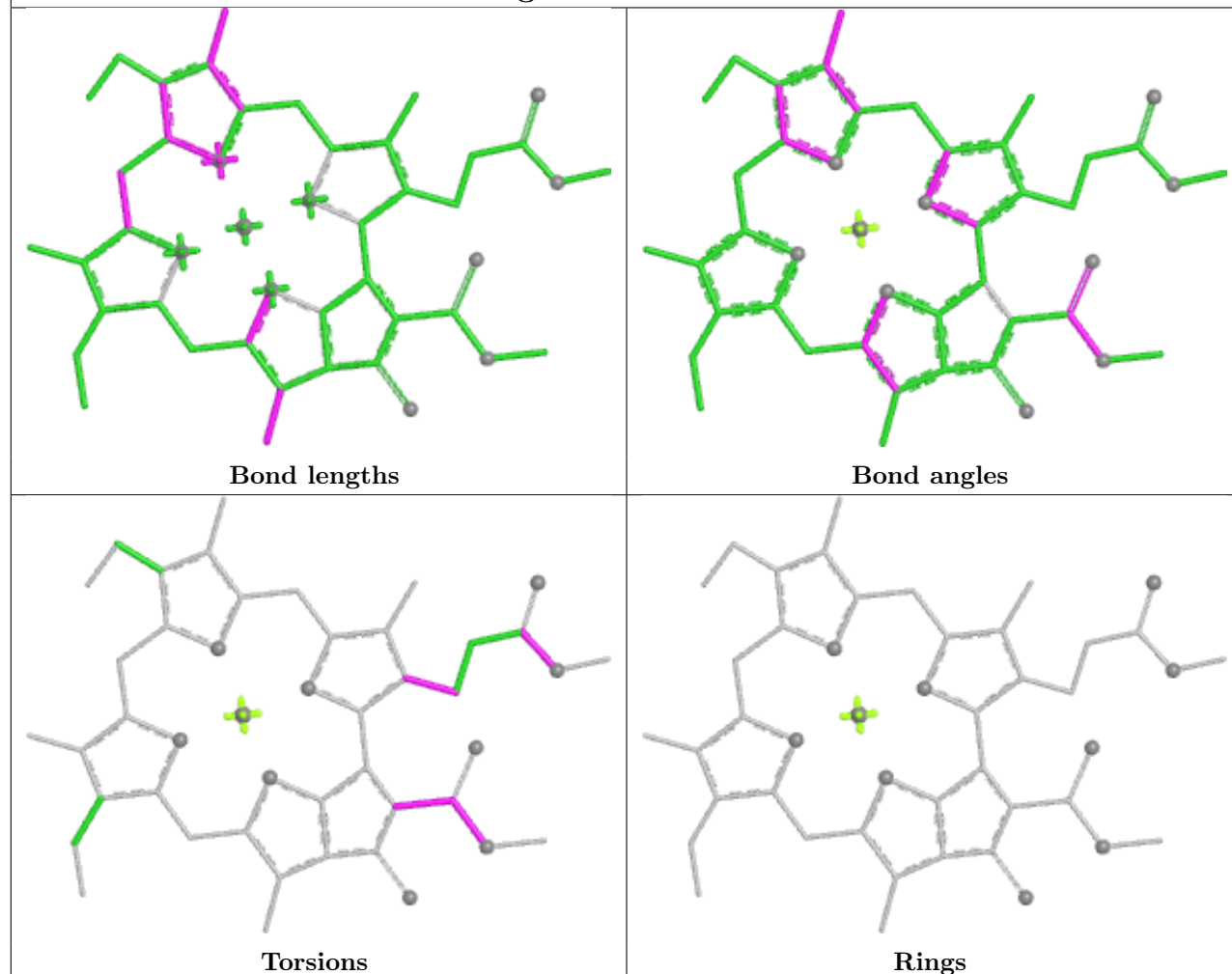


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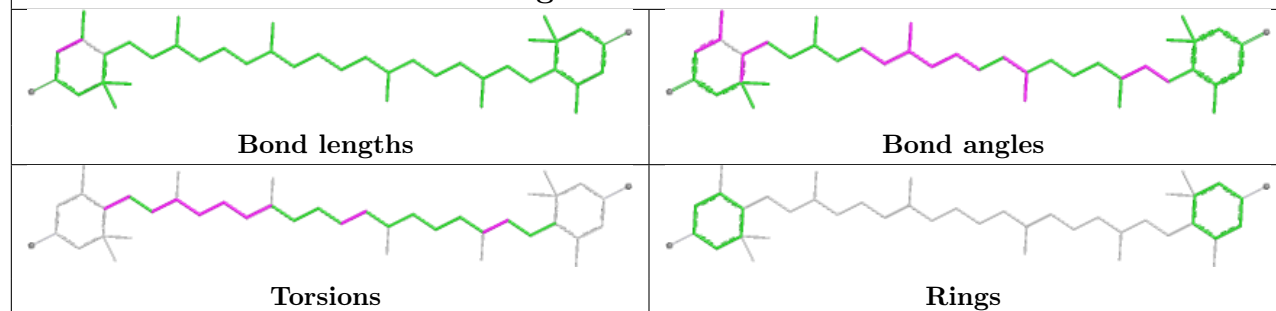


Rings

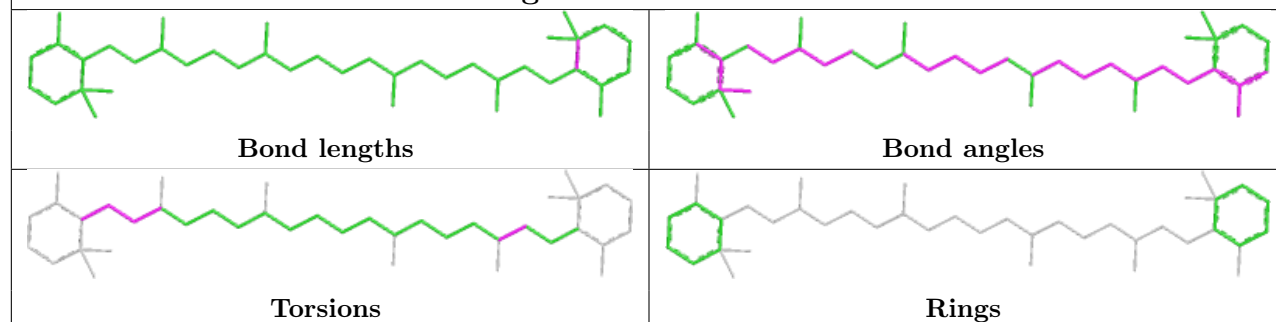
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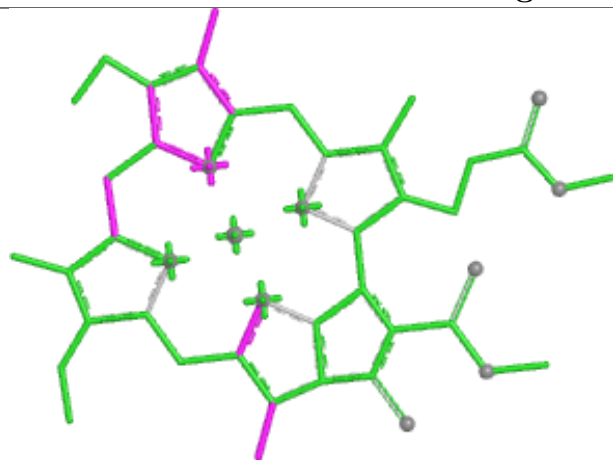
Ligand LUT 4 623



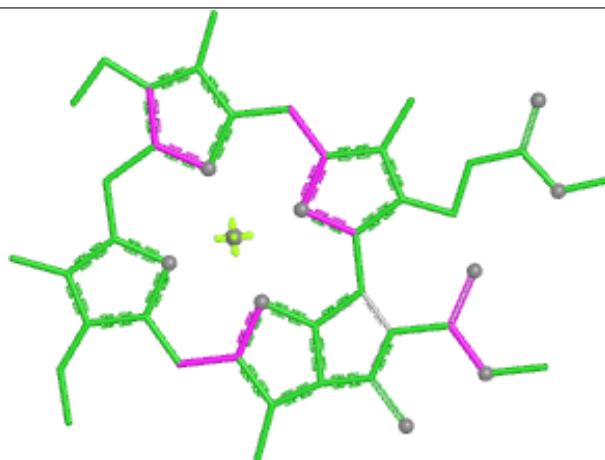
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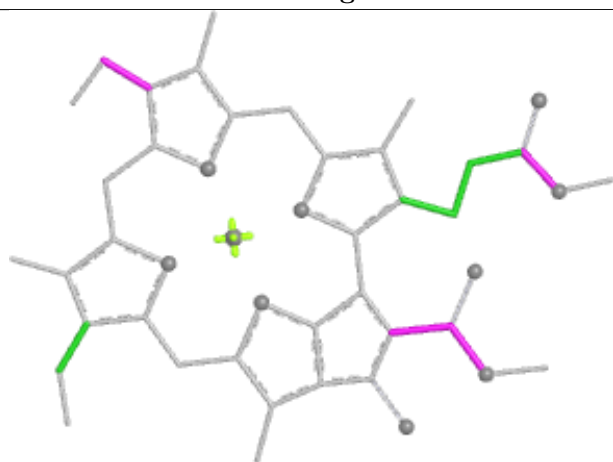
Ligand CLA F 302



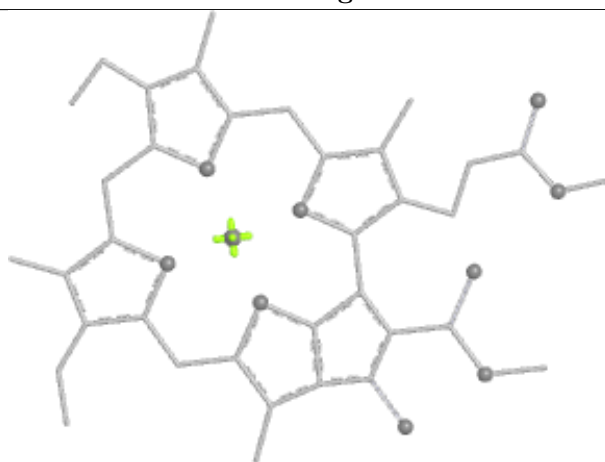
Bond lengths



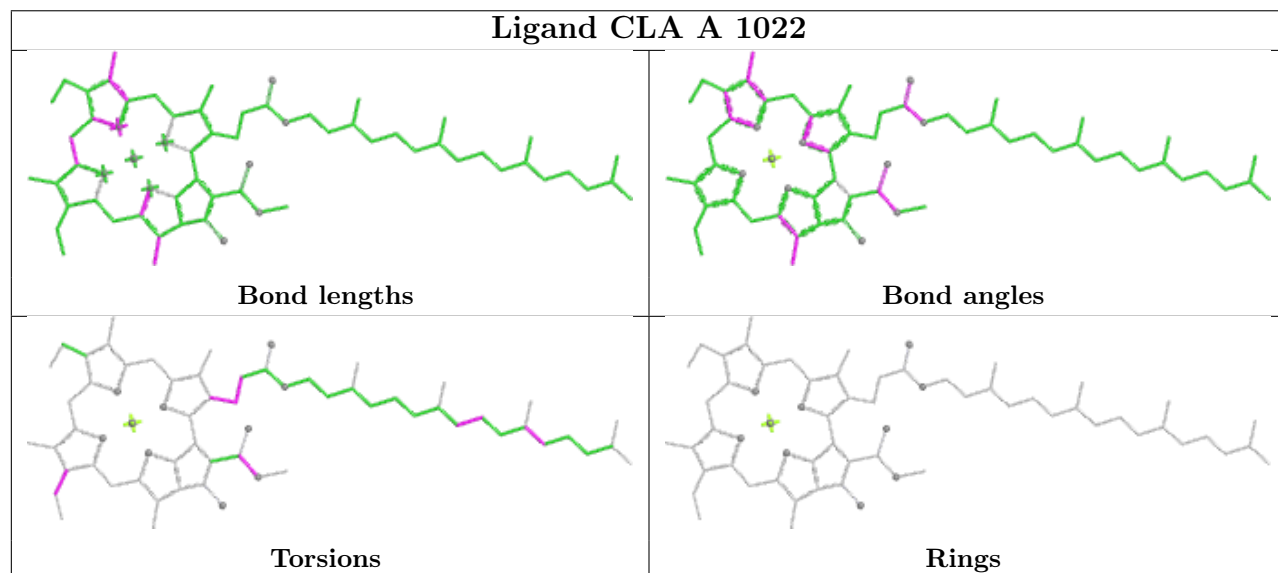
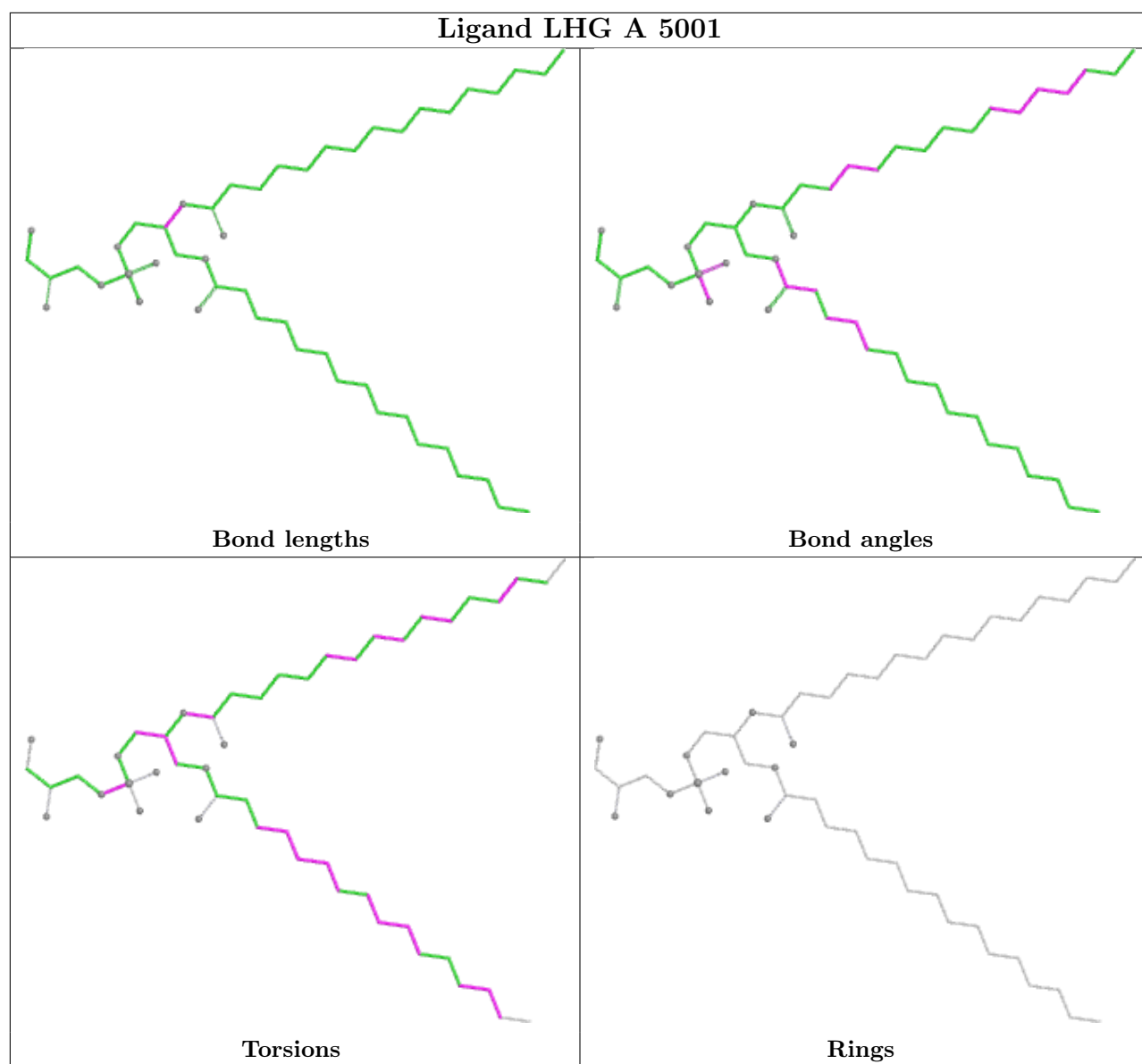
Bond angles



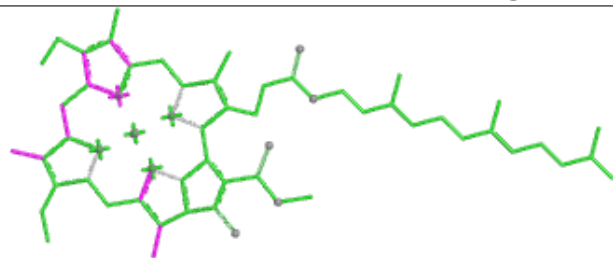
Torsions



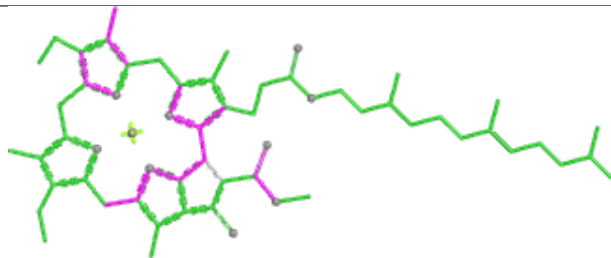
Rings



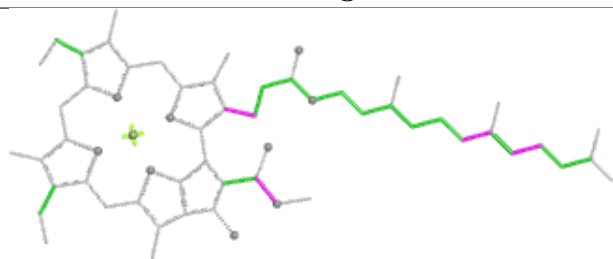
Ligand CLA A 1130



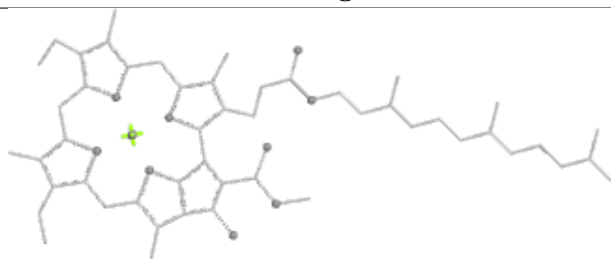
Bond lengths



Bond angles

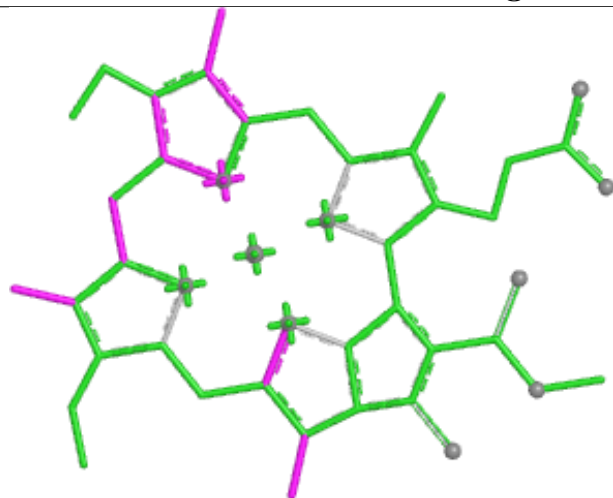


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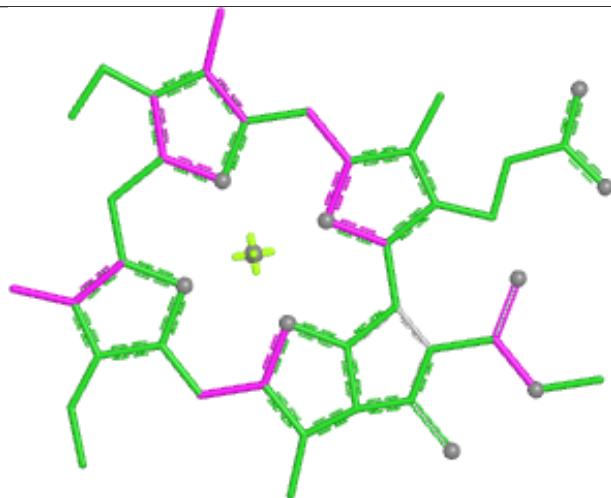


Rings

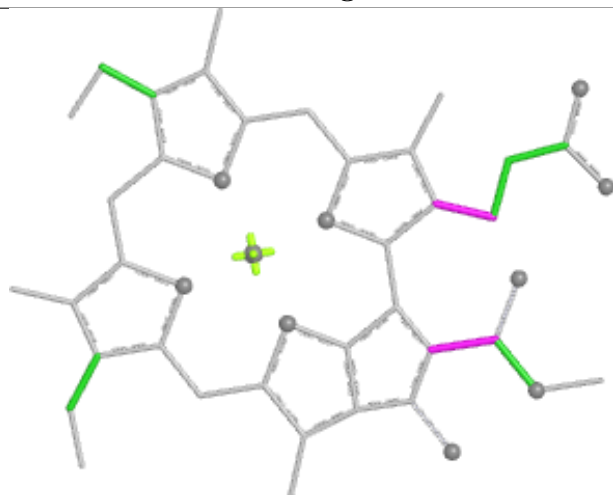
Ligand CLA B 1212



Bond lengths



Bond angles

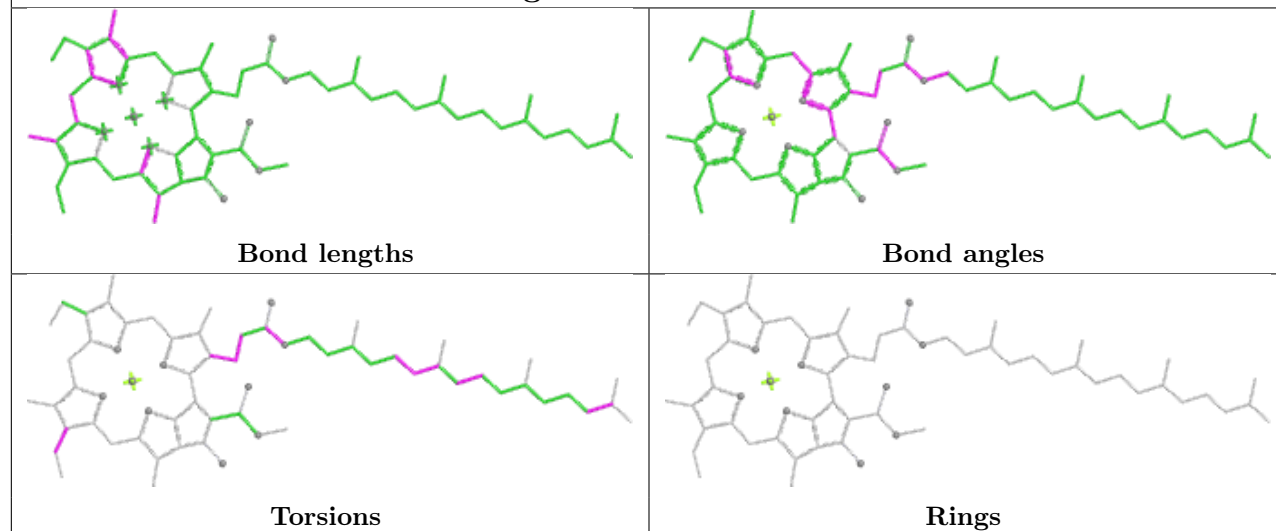


Torsions

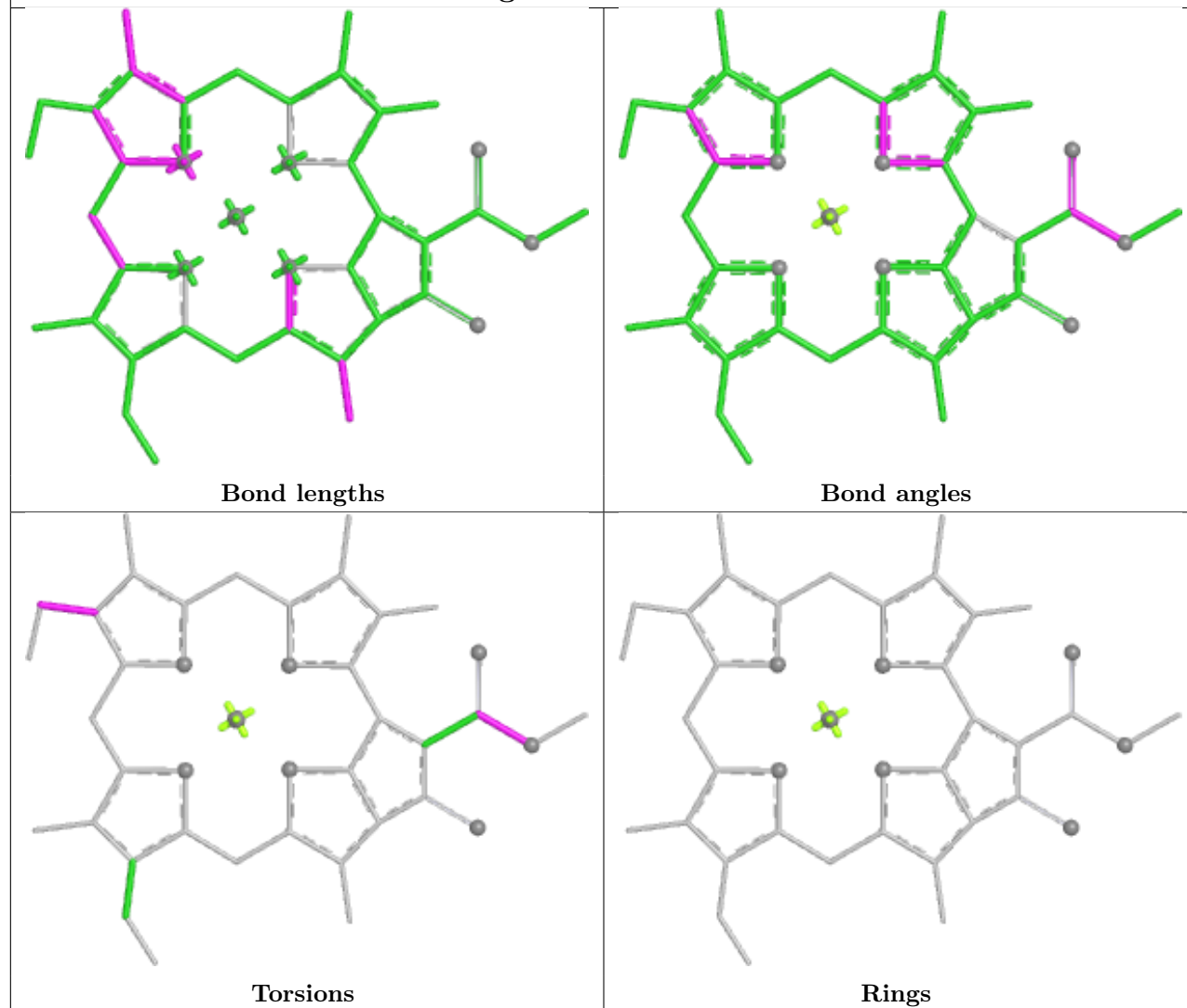


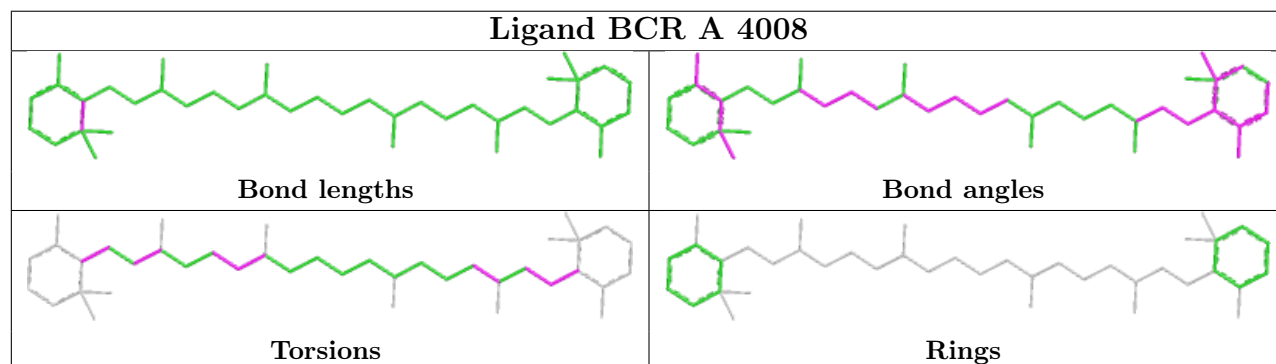
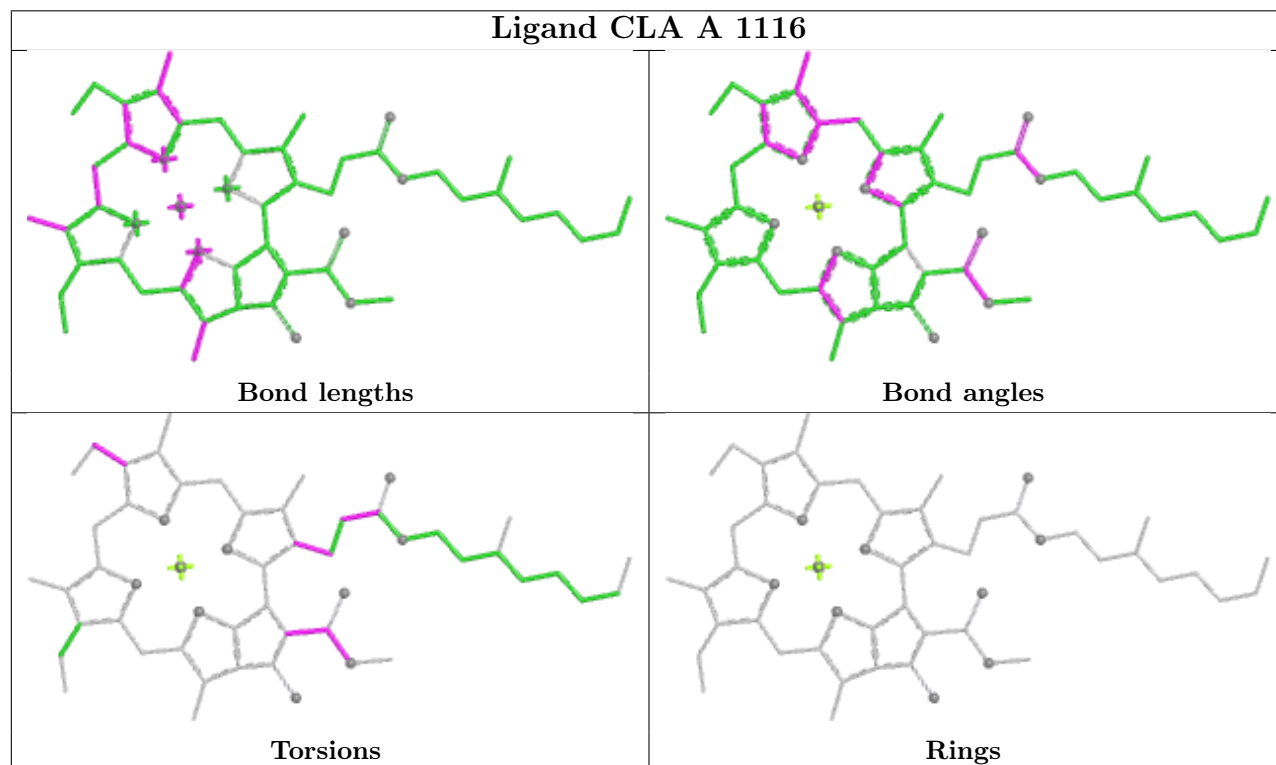
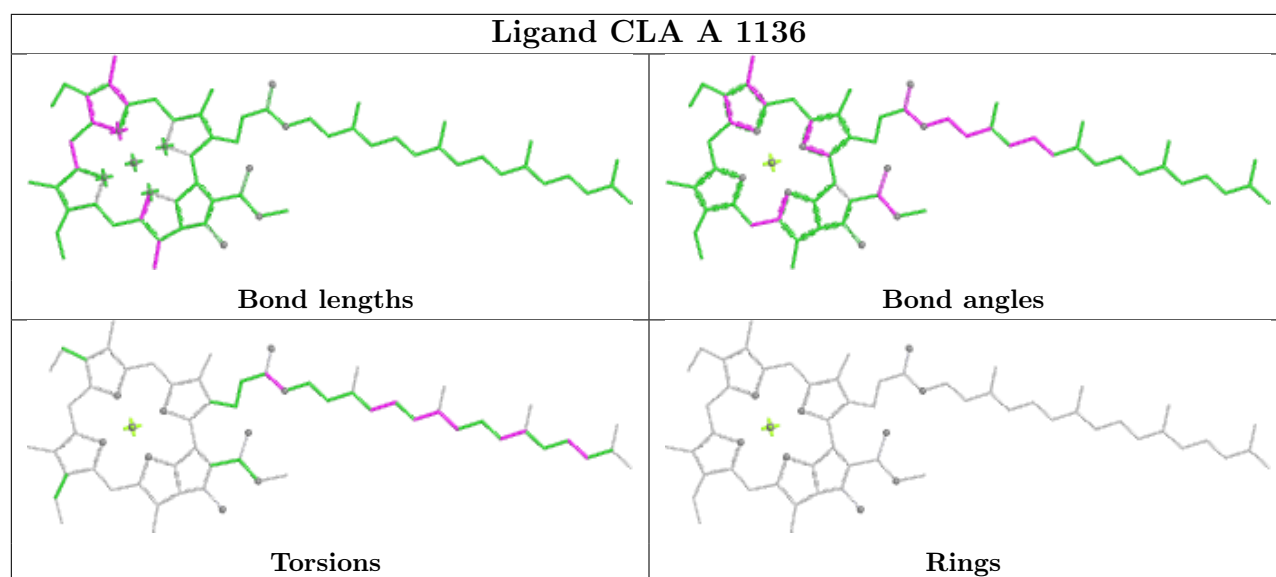
Rings

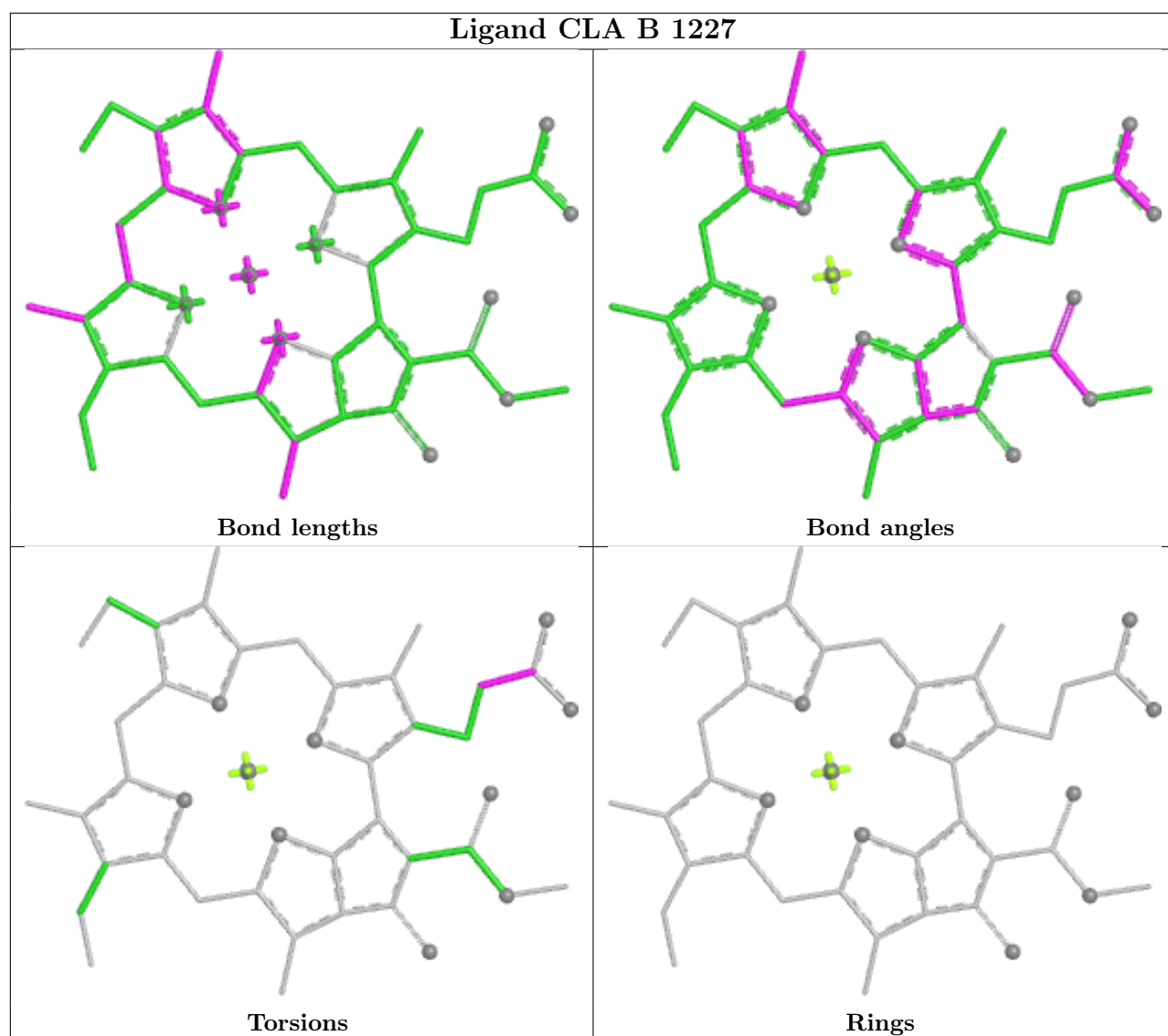
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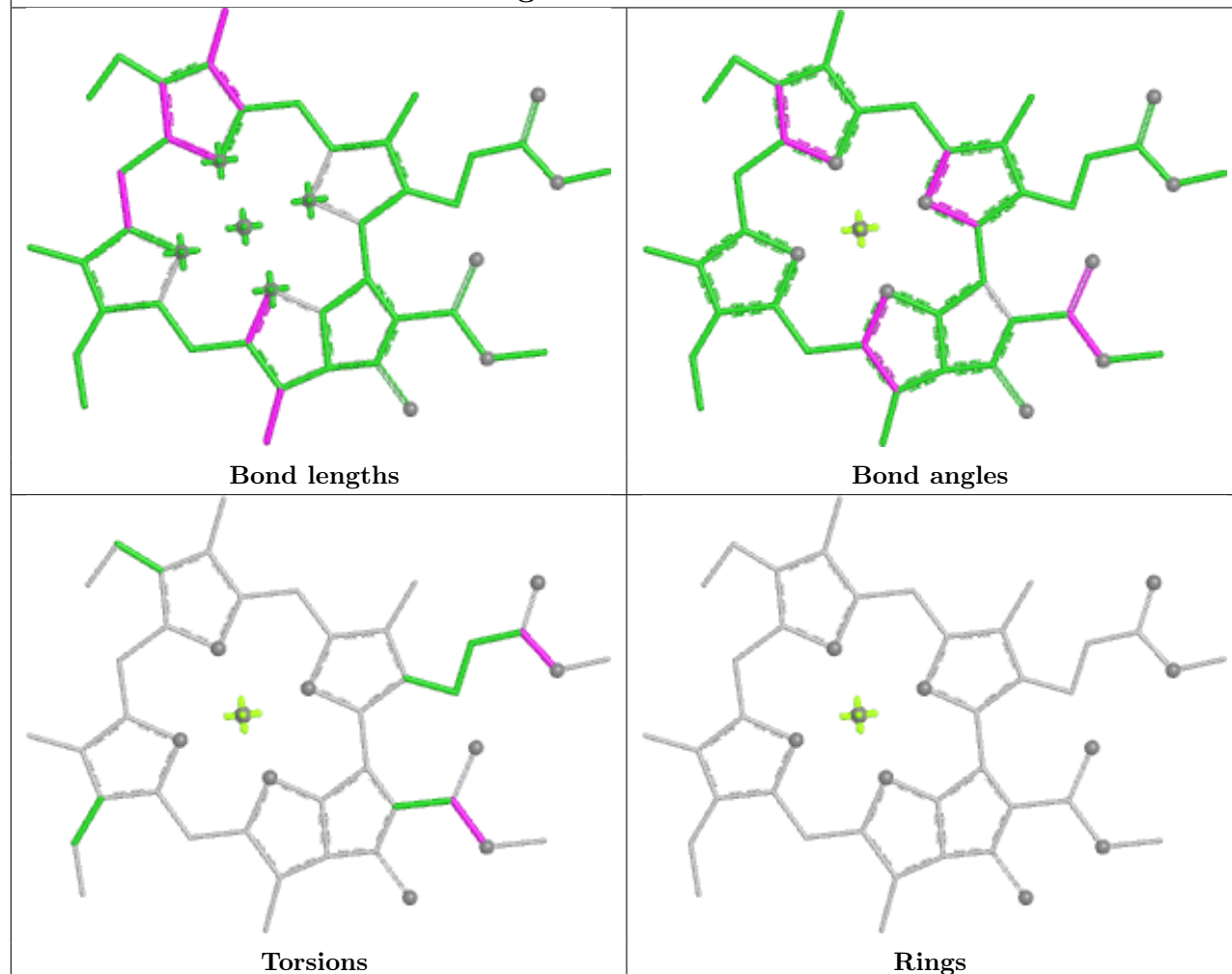
Ligand CLA 3 611



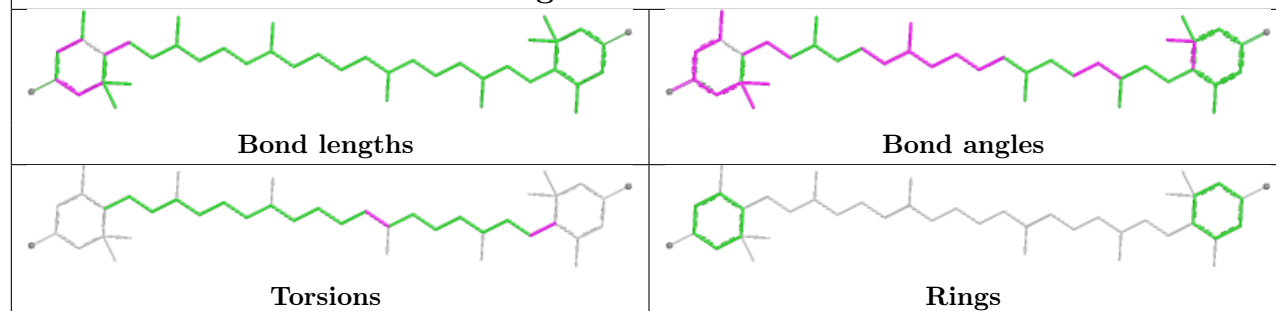


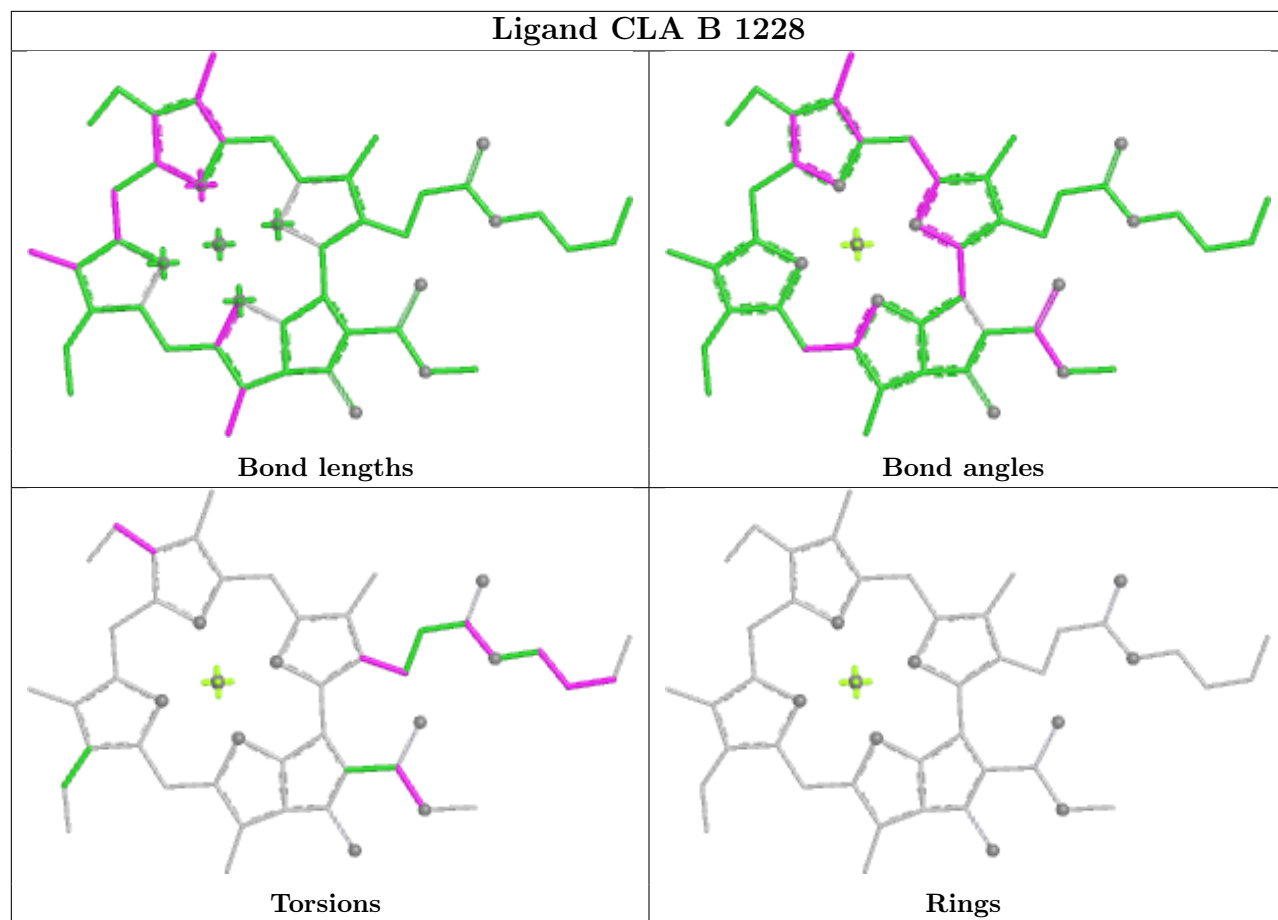


Ligand CLA 1 611

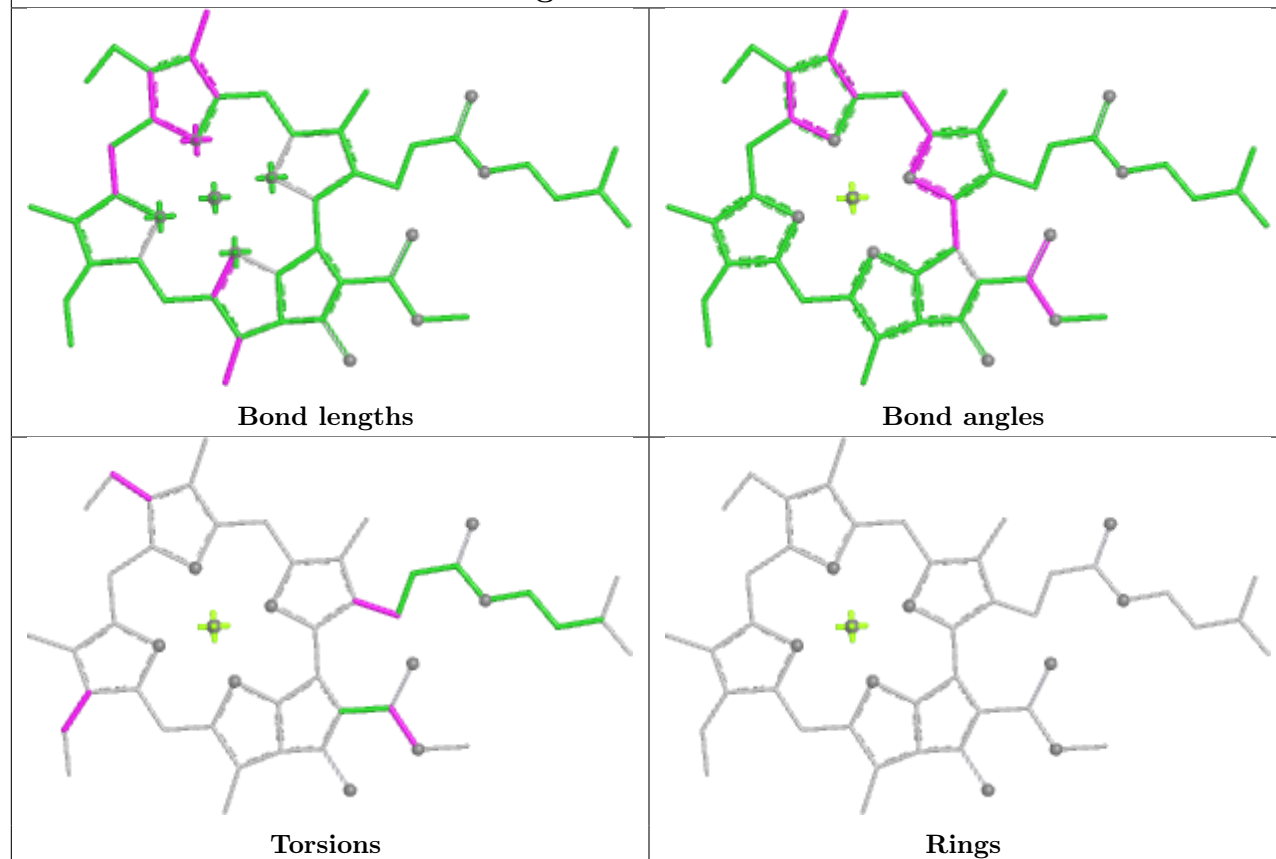


Ligand LUT 4 621

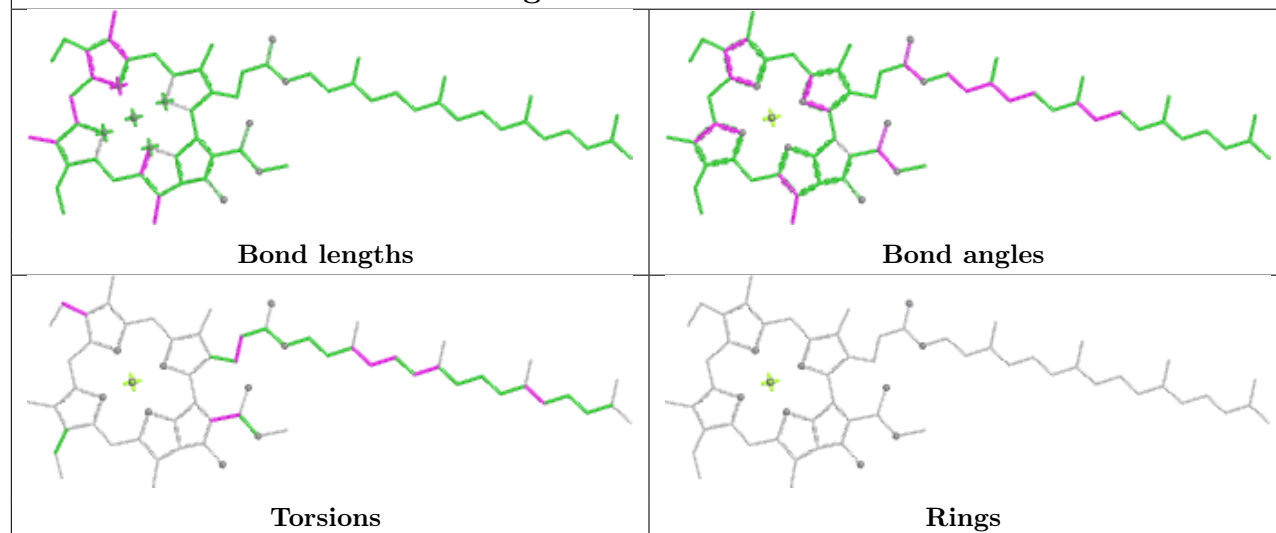


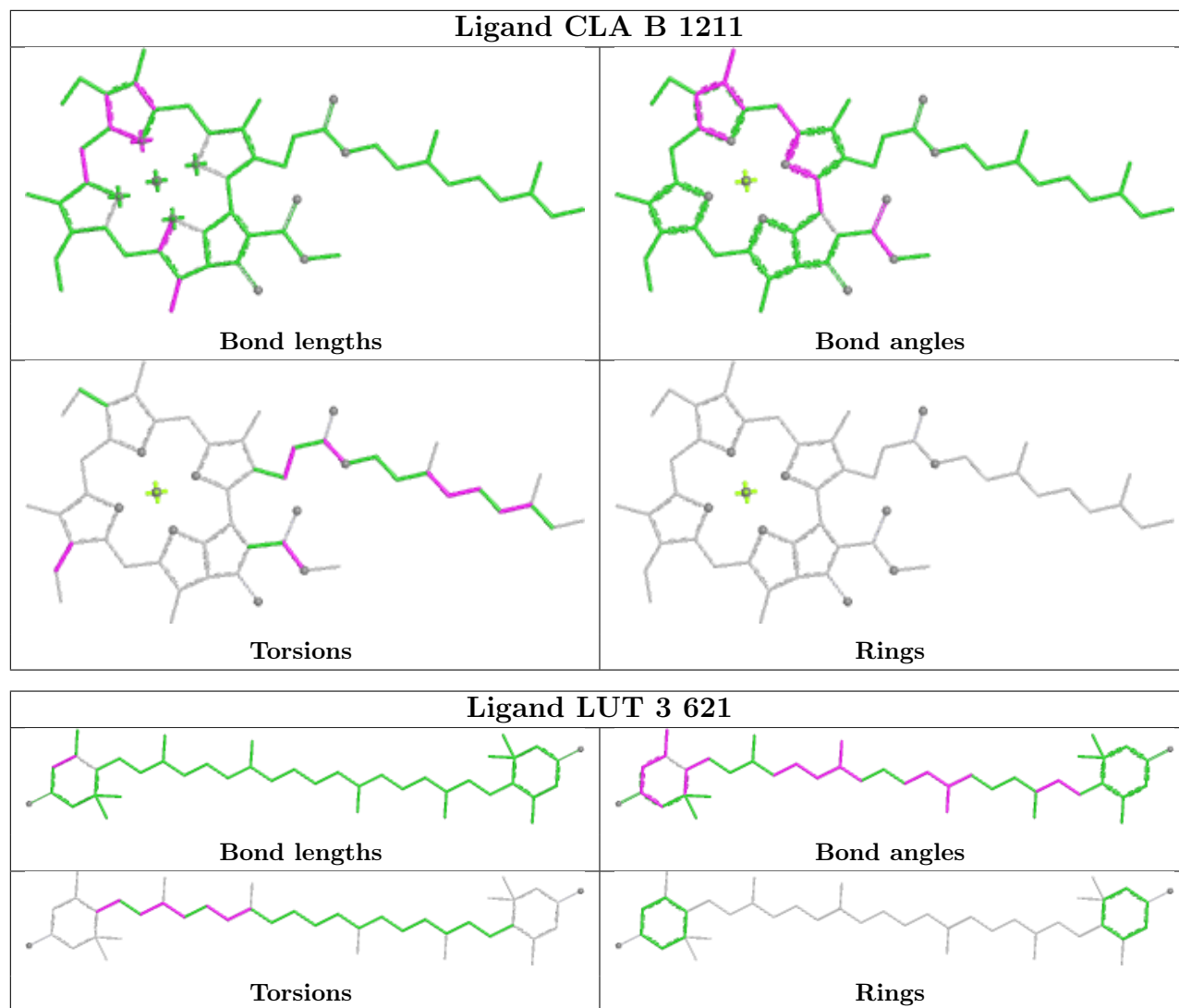


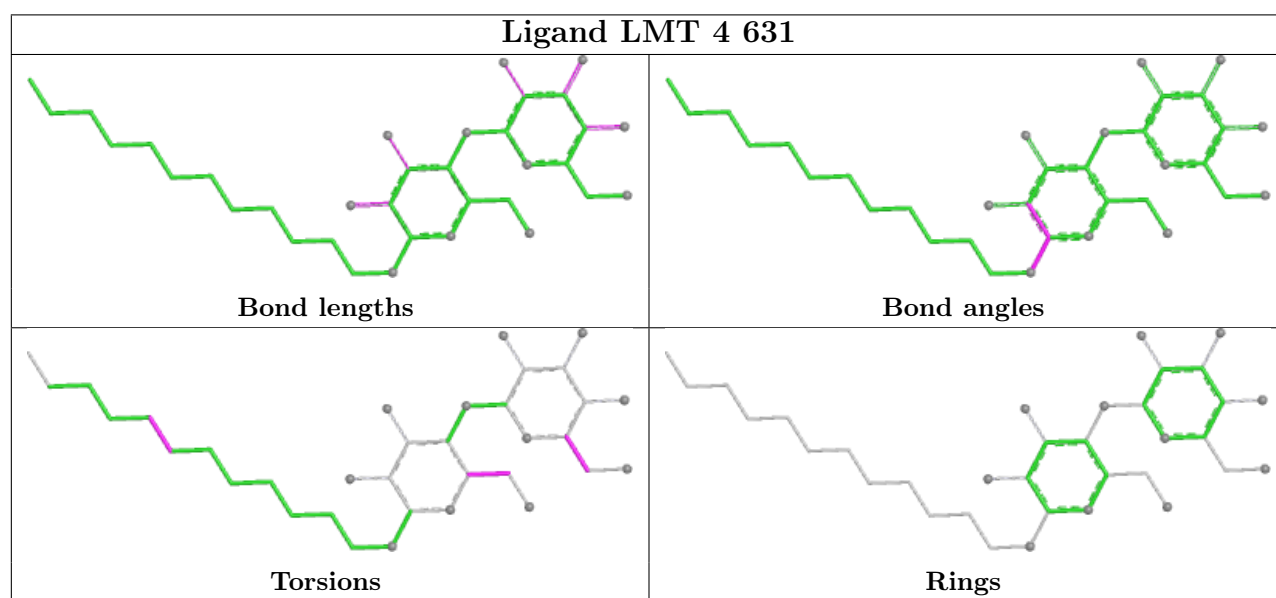
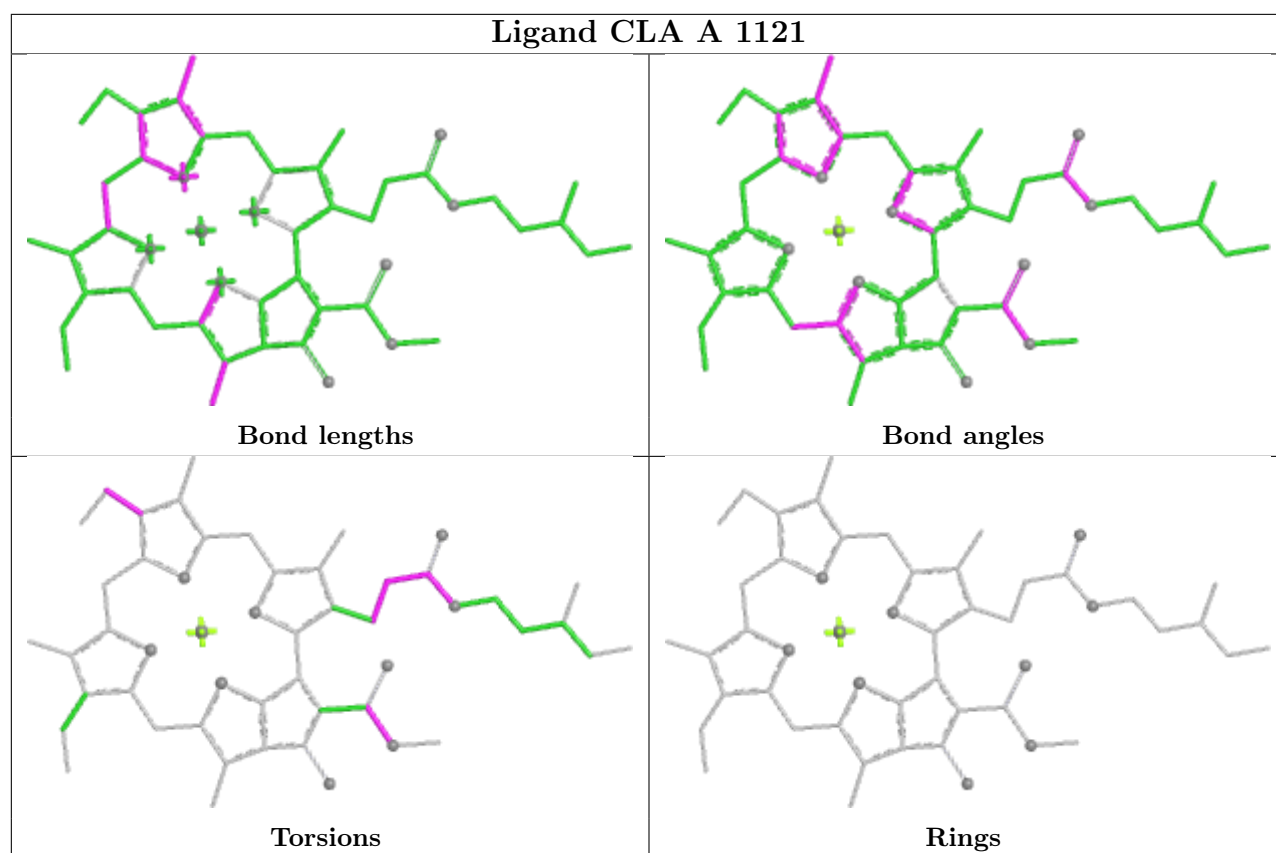
Ligand CLA 2 604



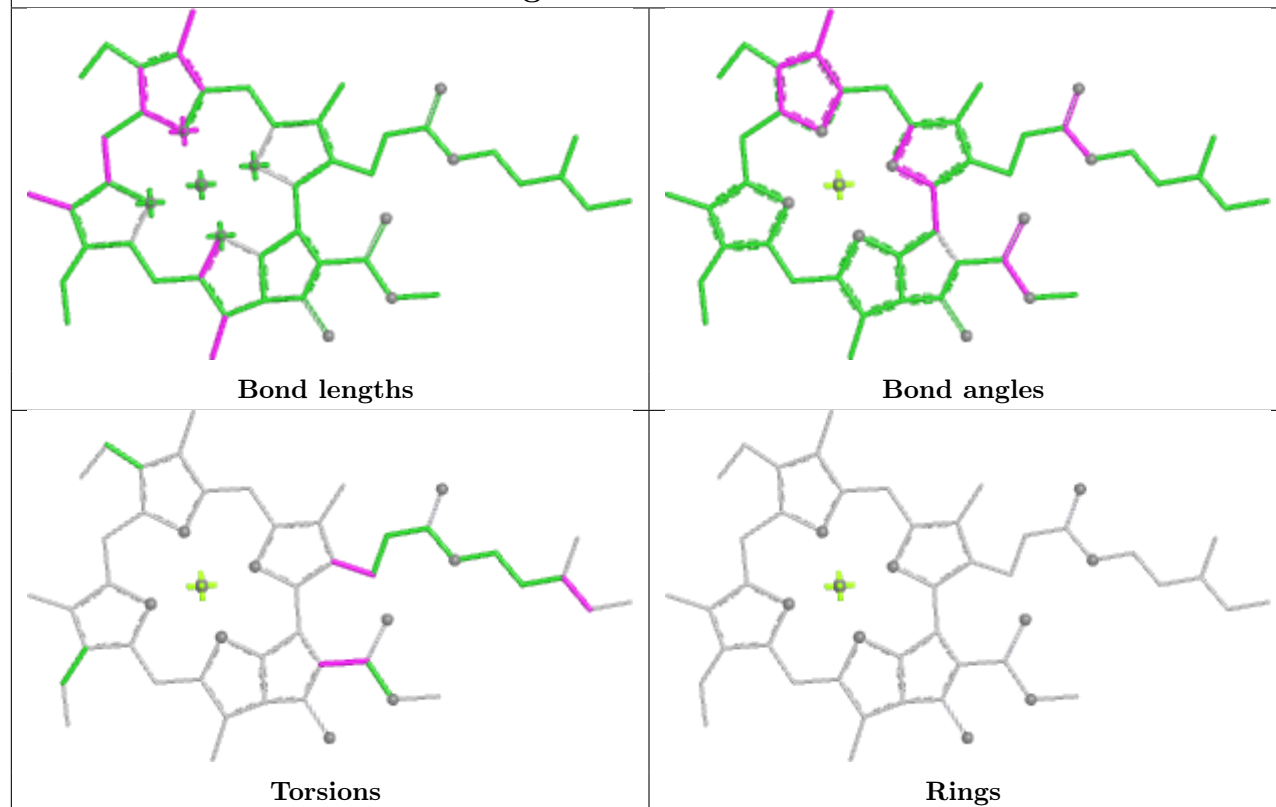
Ligand CLA B 1205



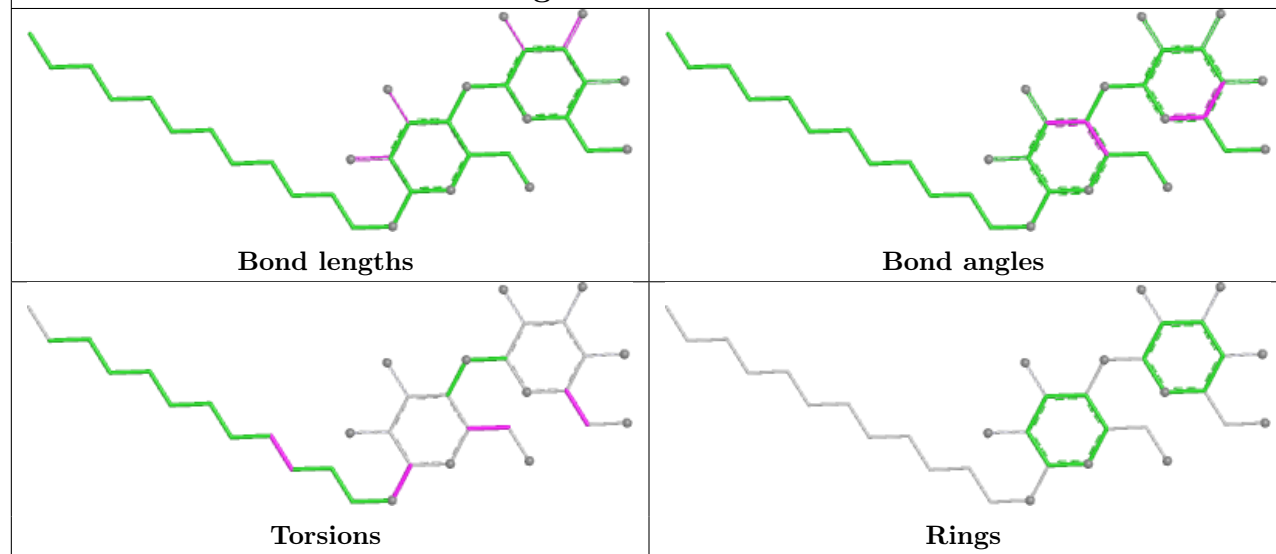


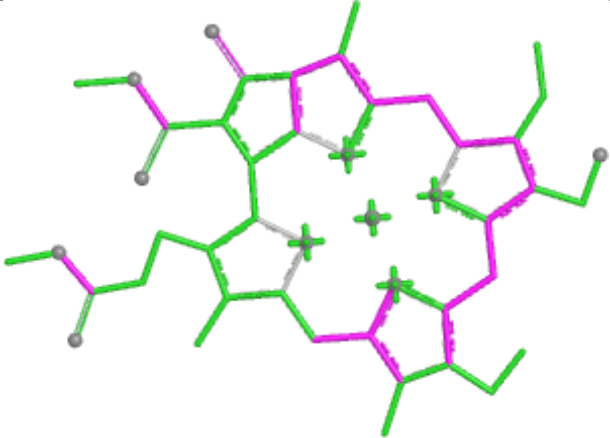
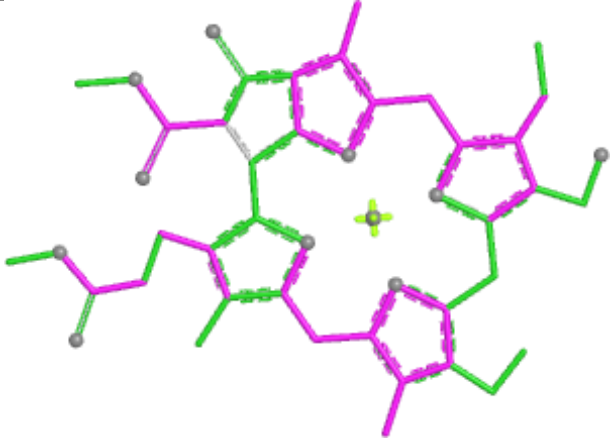
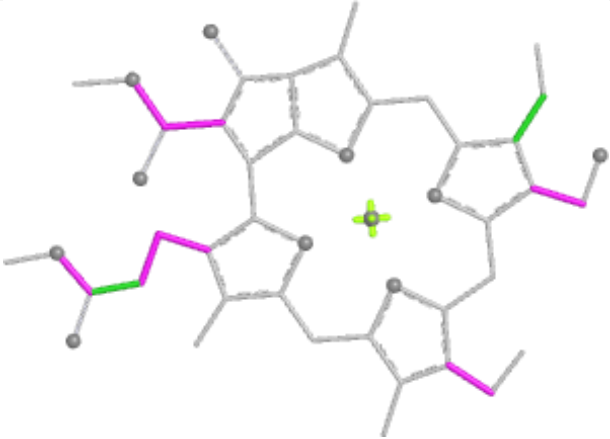
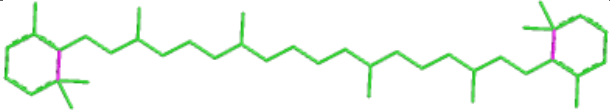
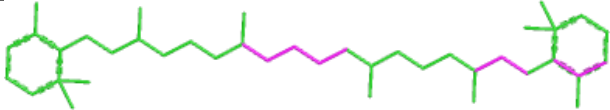
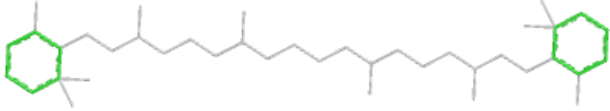
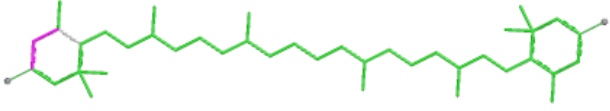
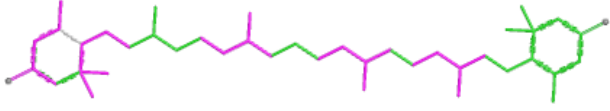
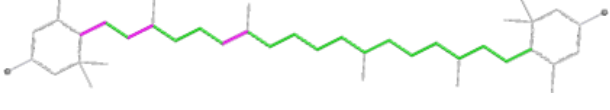
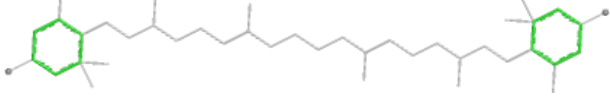


Ligand CLA B 1234

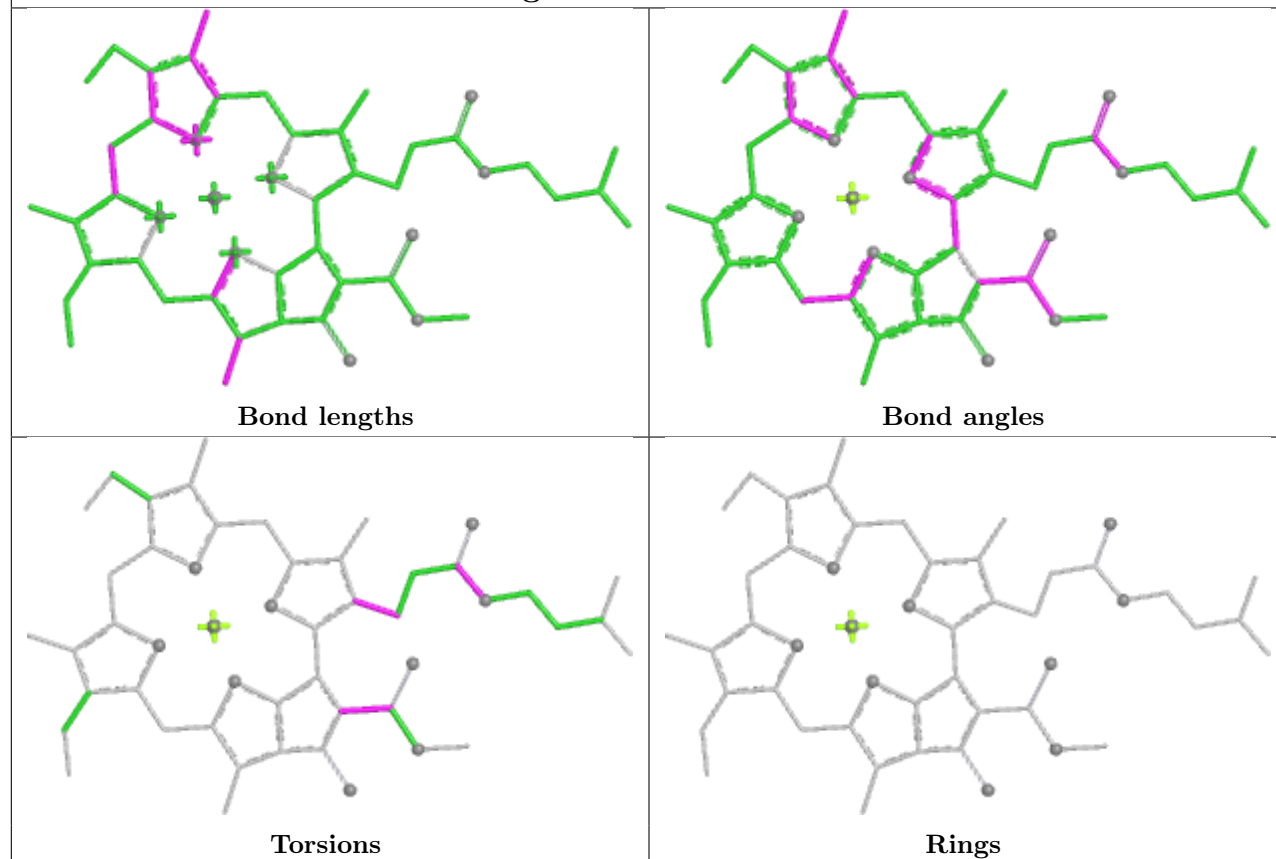


Ligand LMT 1 631

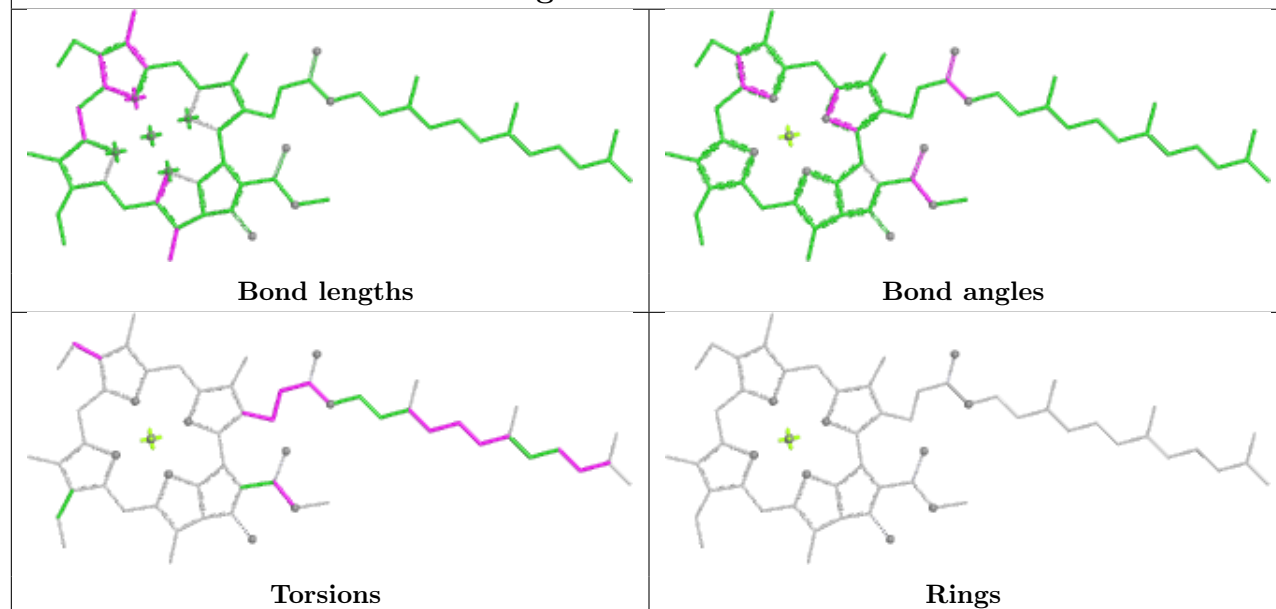


Ligand CHL 2 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 4002	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 1 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

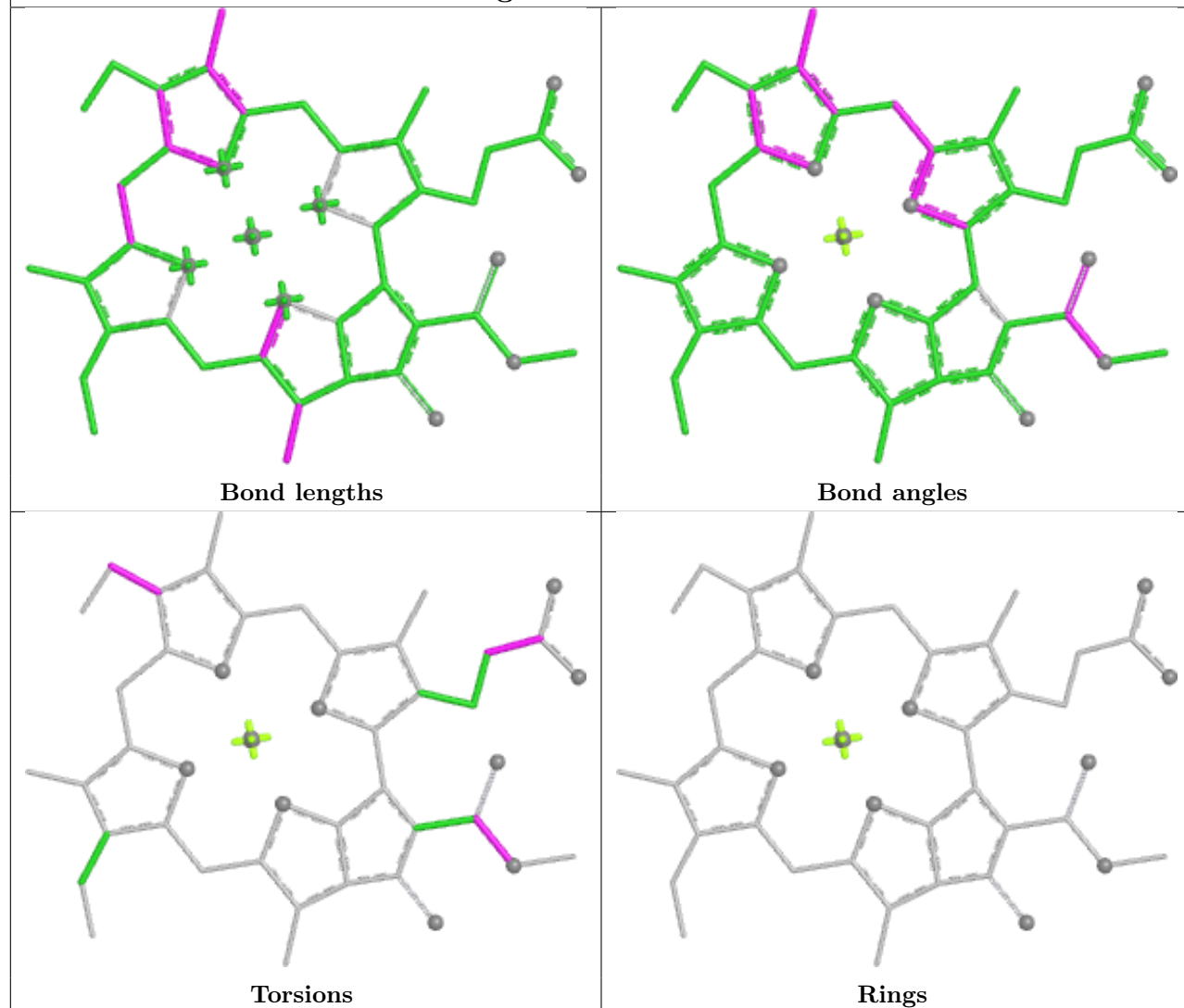
Ligand CLA A 5005



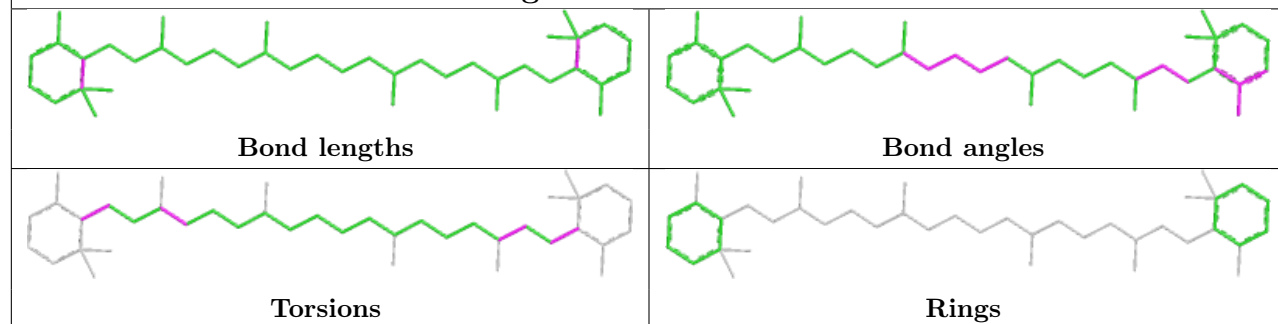
Ligand CLA 3 607

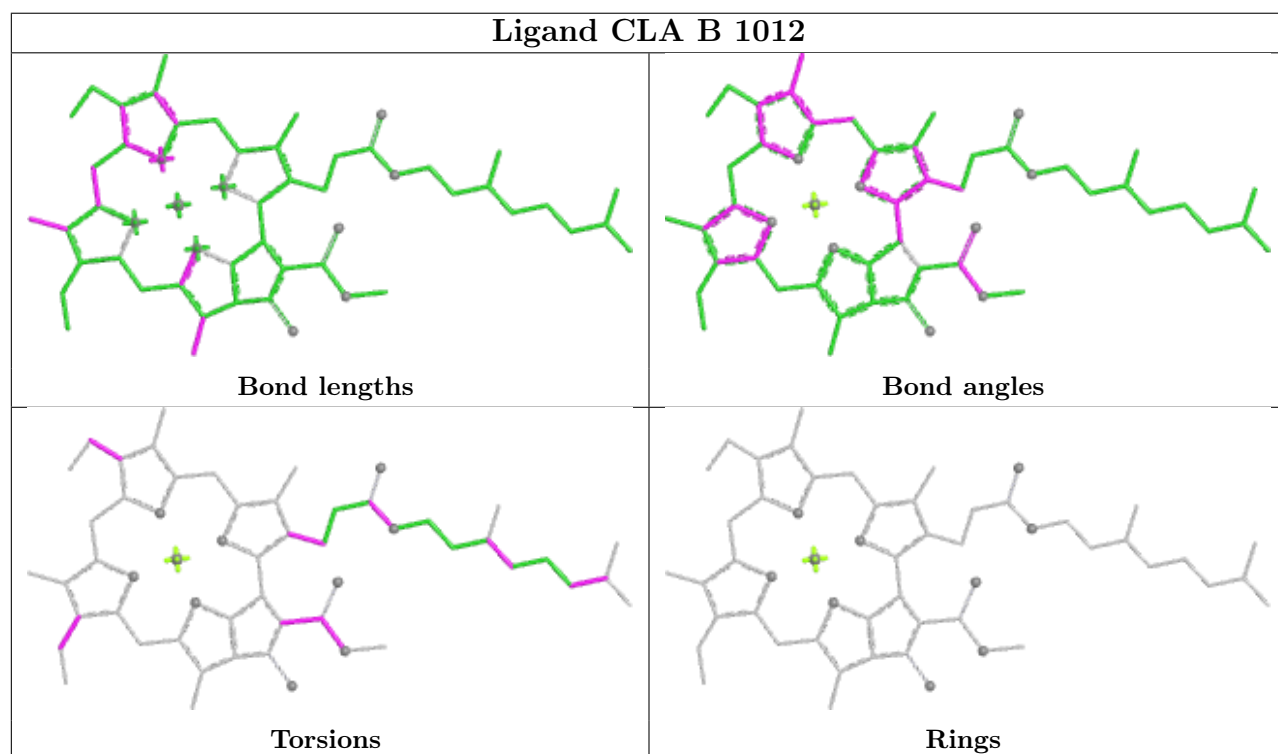
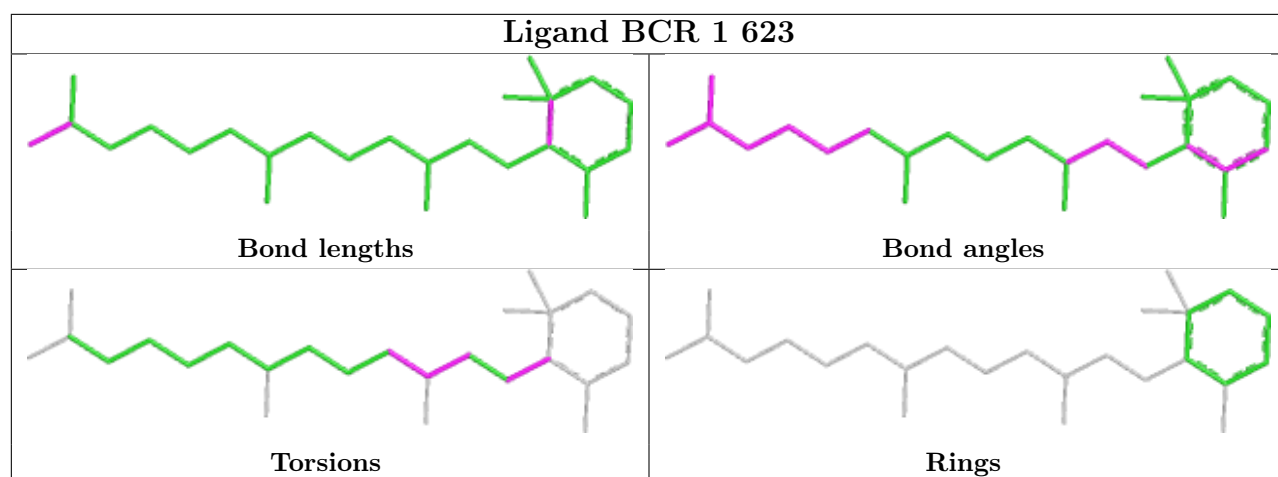


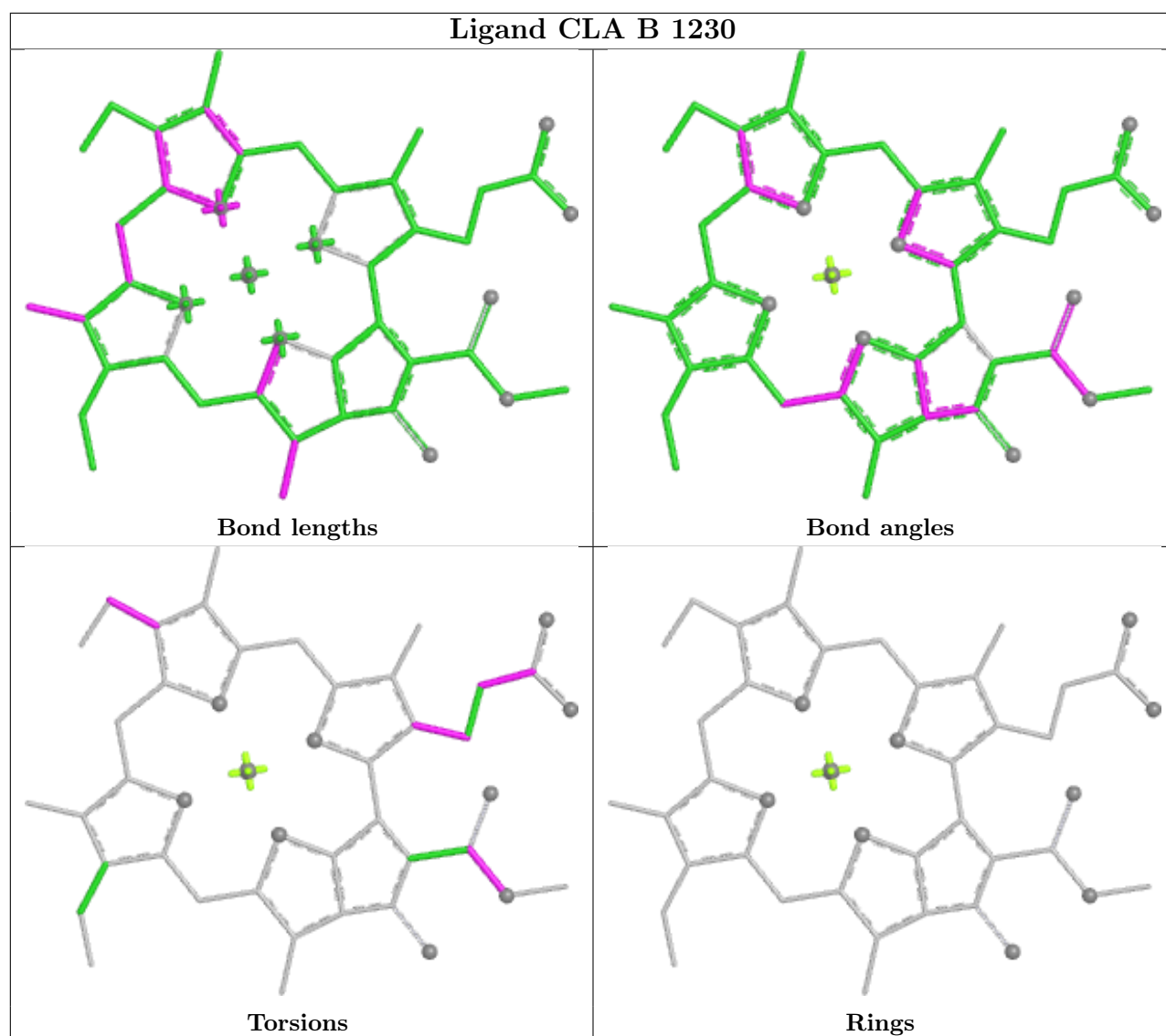
Ligand CLA 3 612



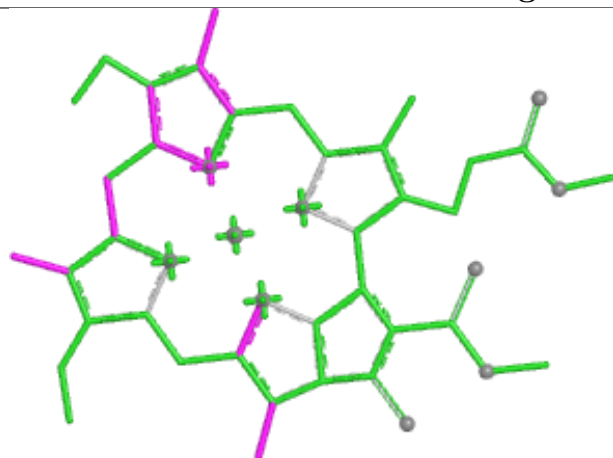
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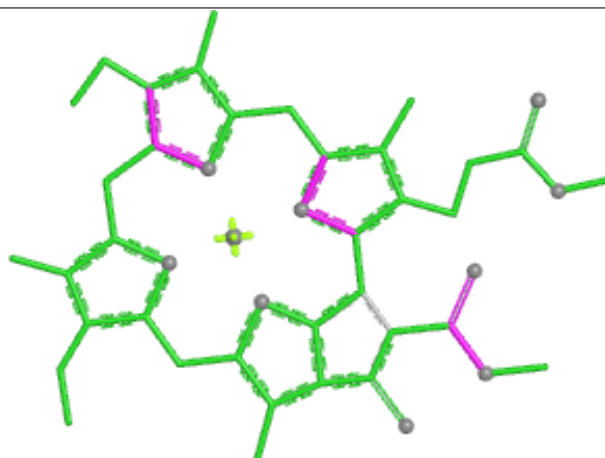




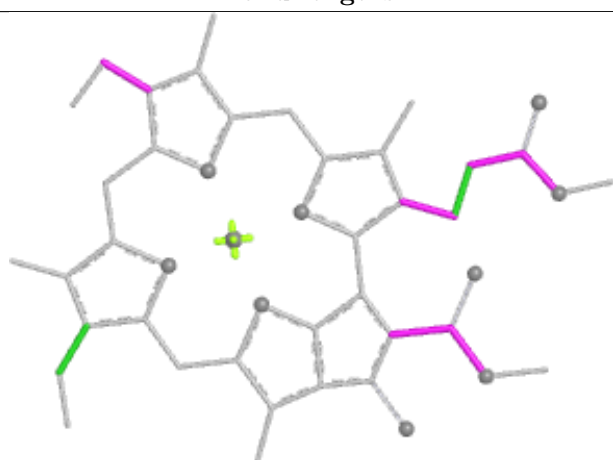
Ligand CLA 3 606



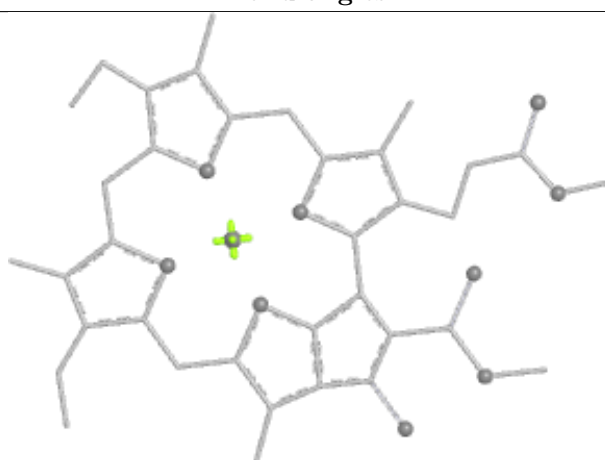
Bond lengths



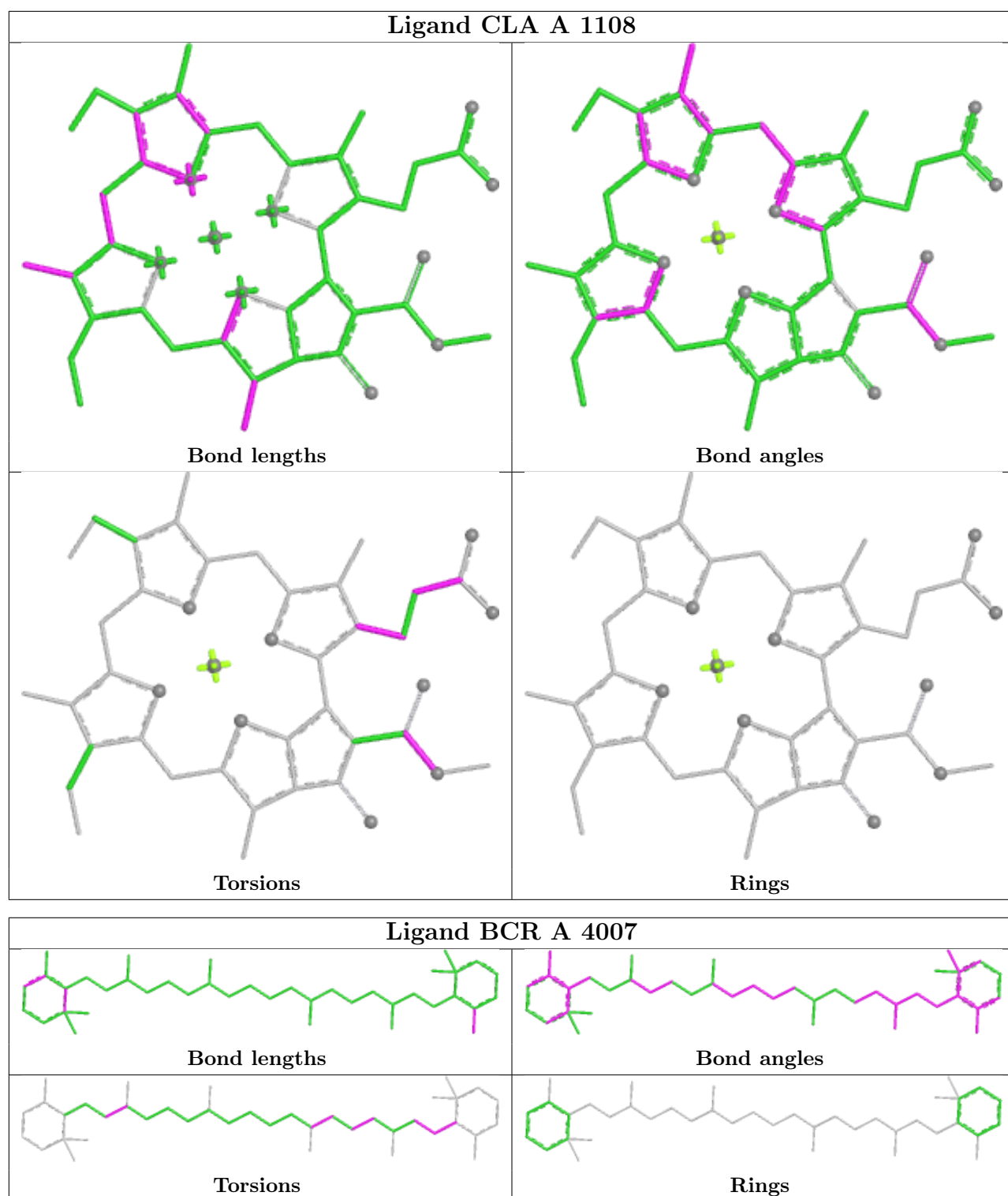
Bond angles

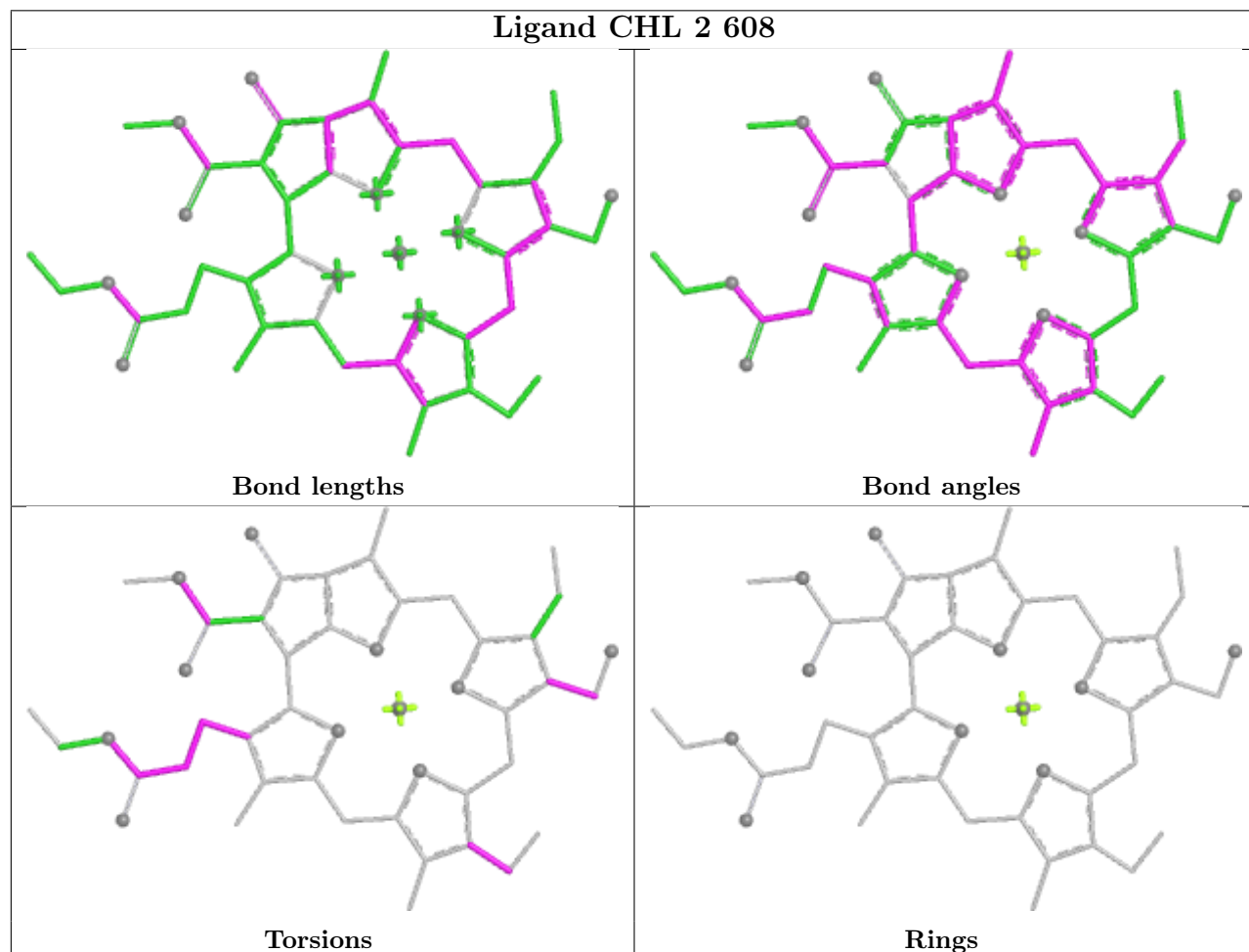
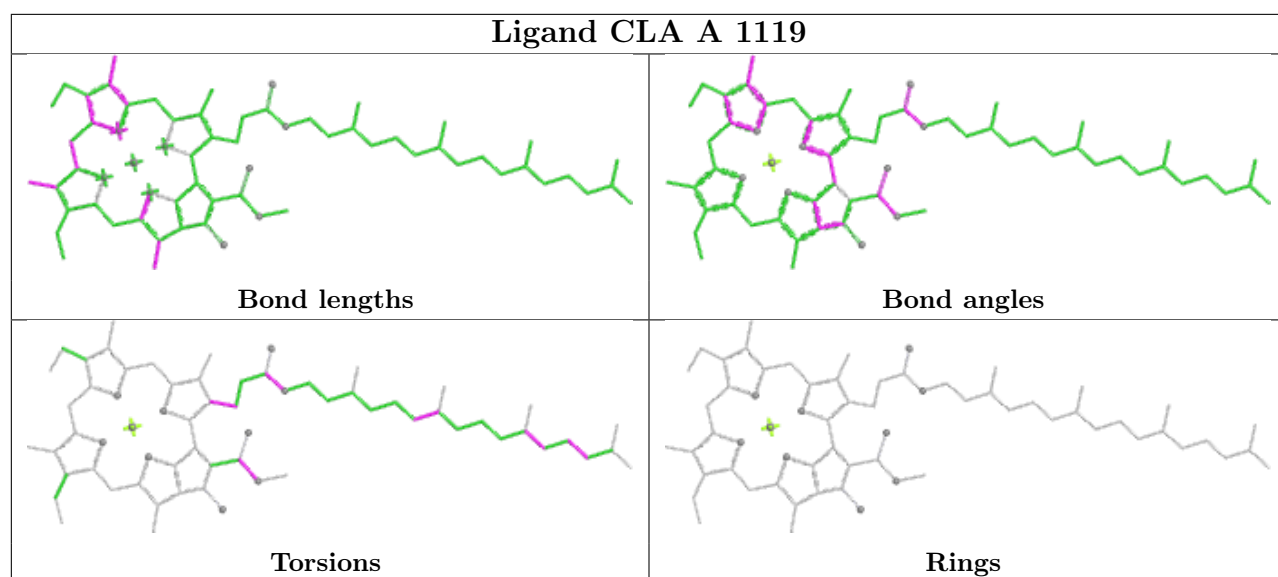


Torsions

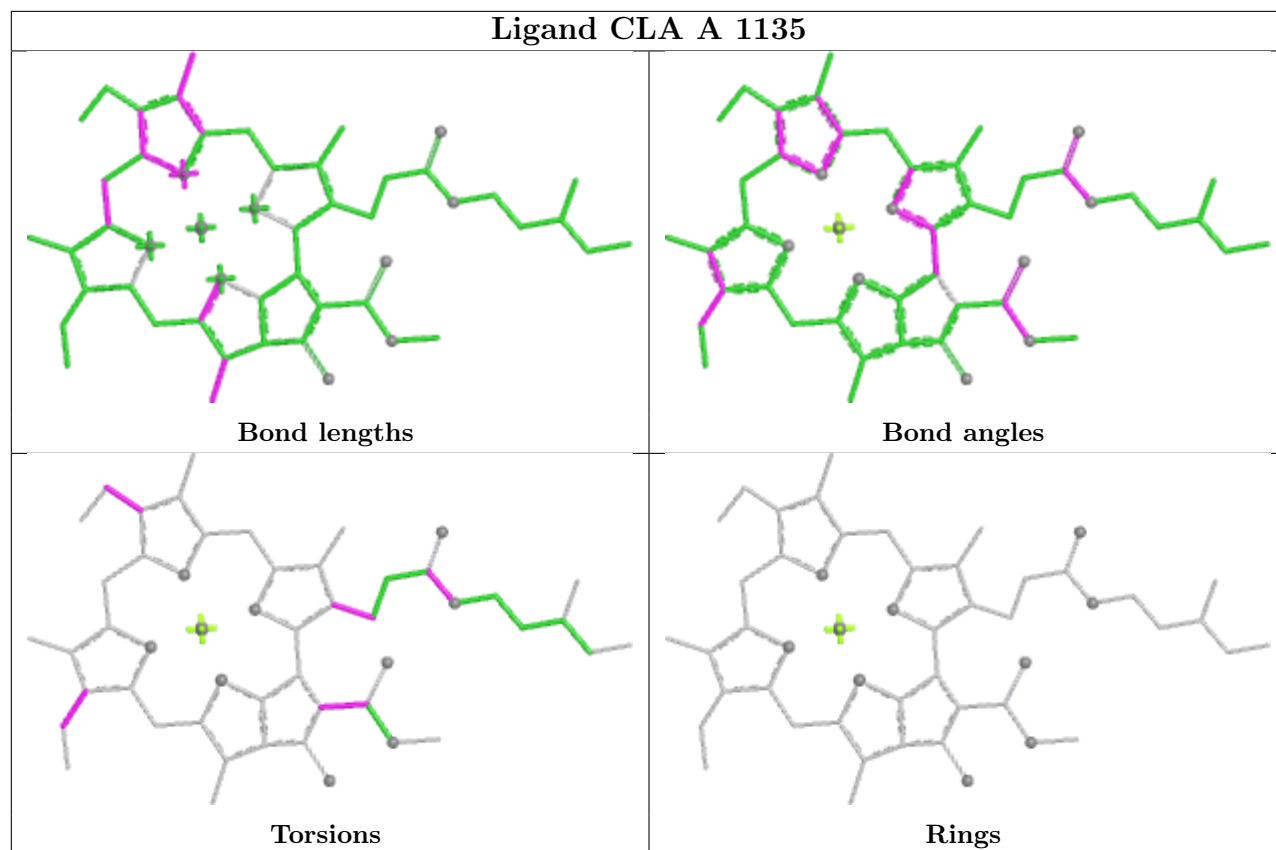


Rings

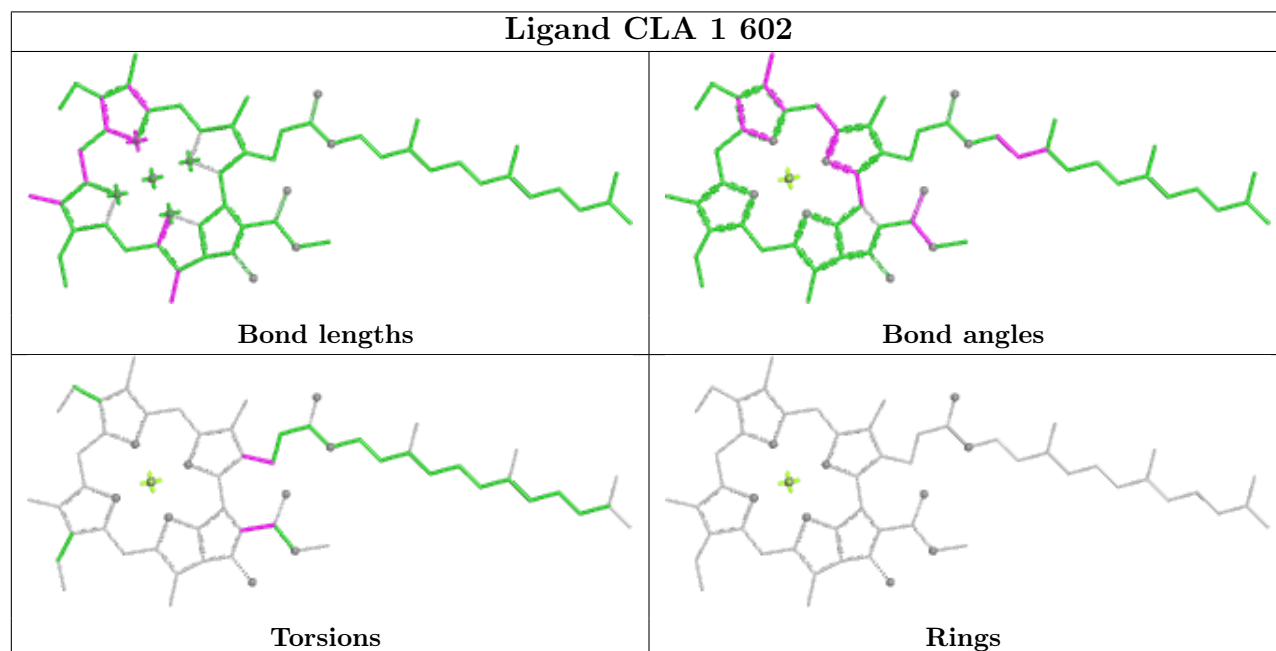




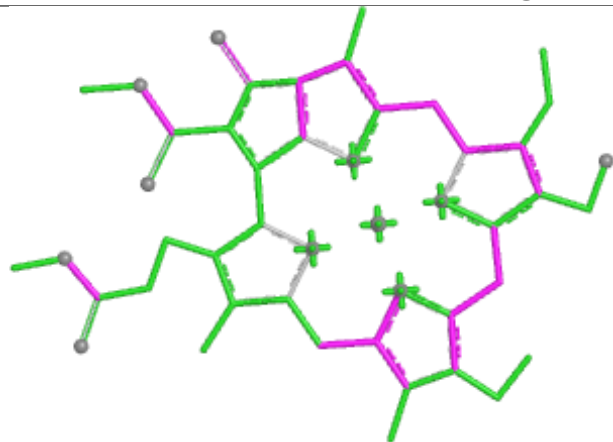
Ligand CLA A 1135



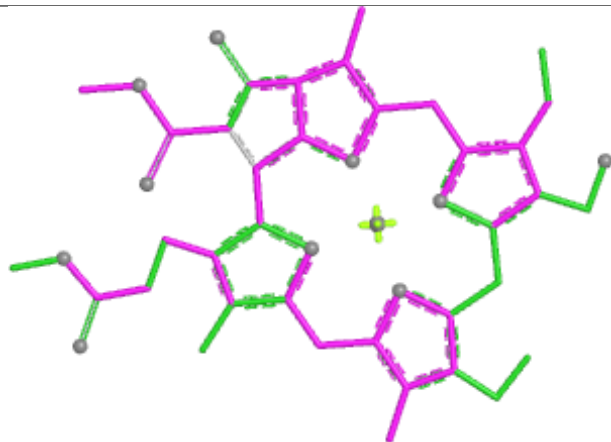
Ligand CLA 1 602



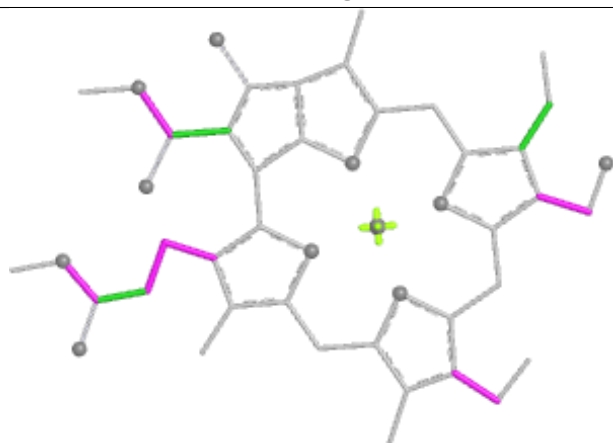
Ligand CHL 2 607



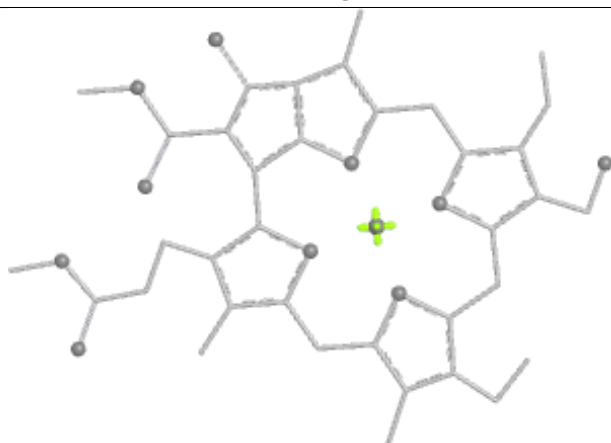
Bond lengths



Bond angles

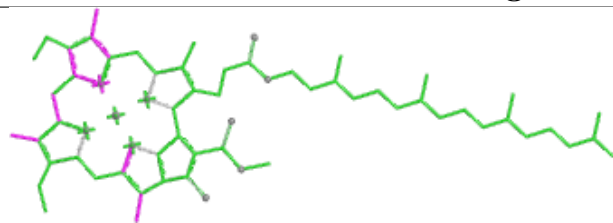


Torsions

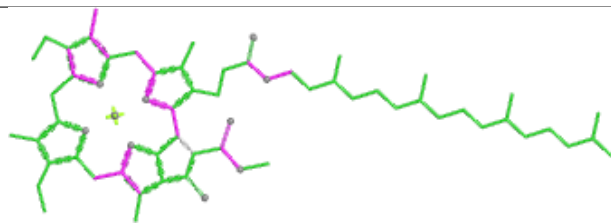


Rings

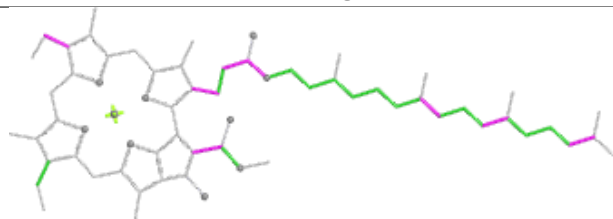
Ligand CLA B 1240



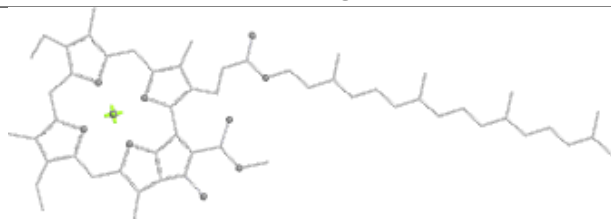
Bond lengths



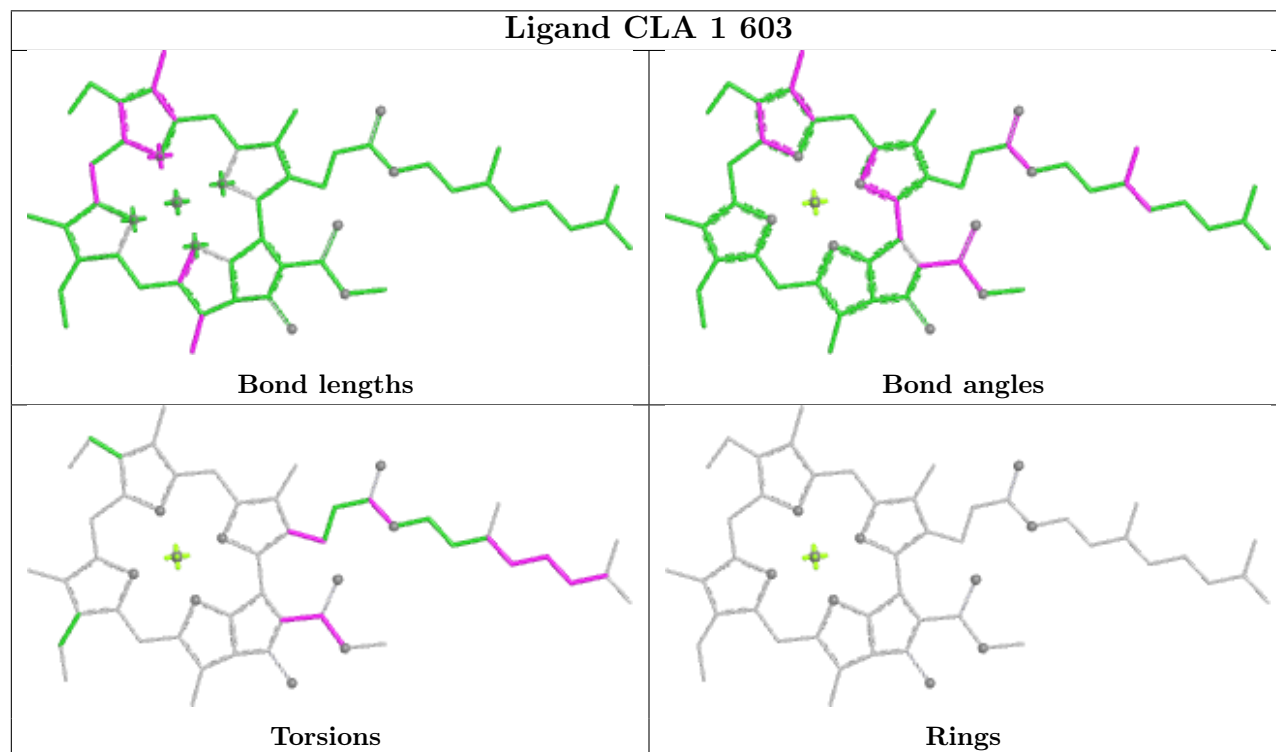
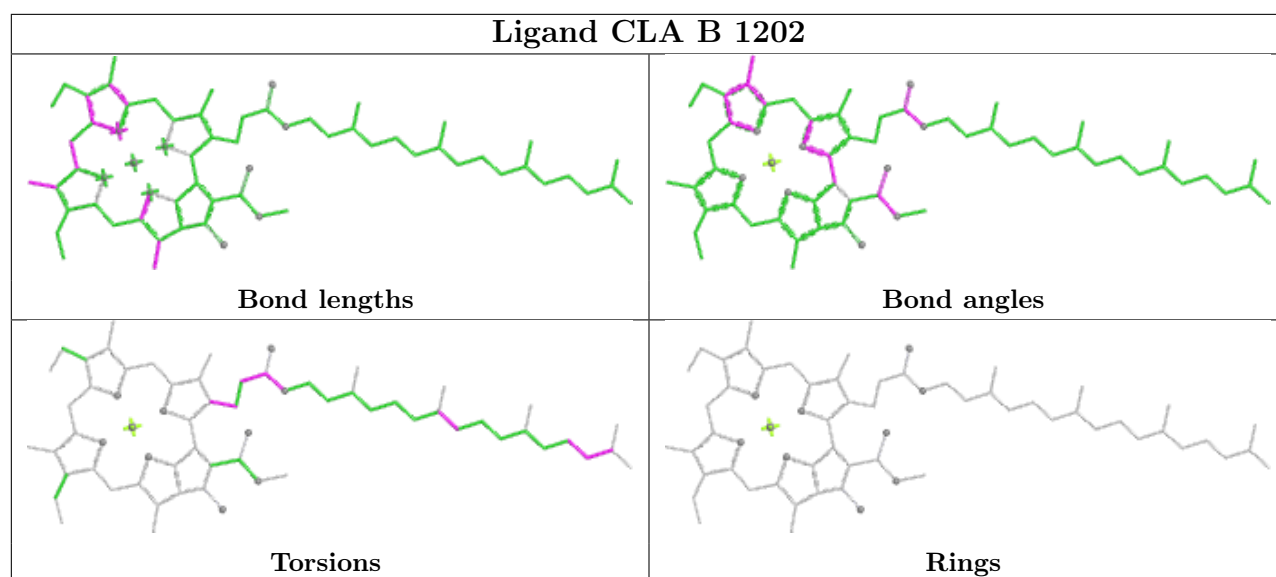
Bond angles

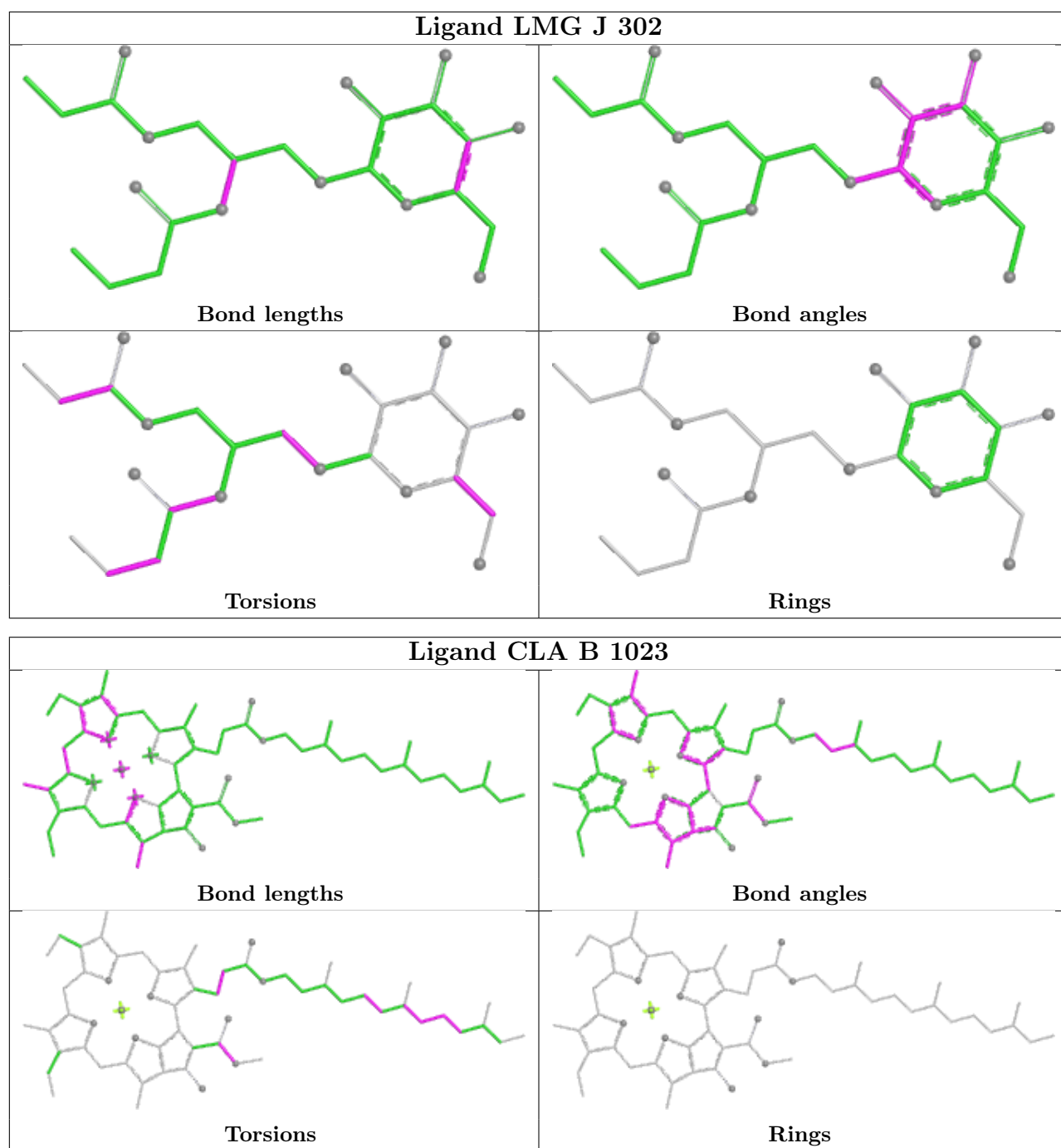


Torsions

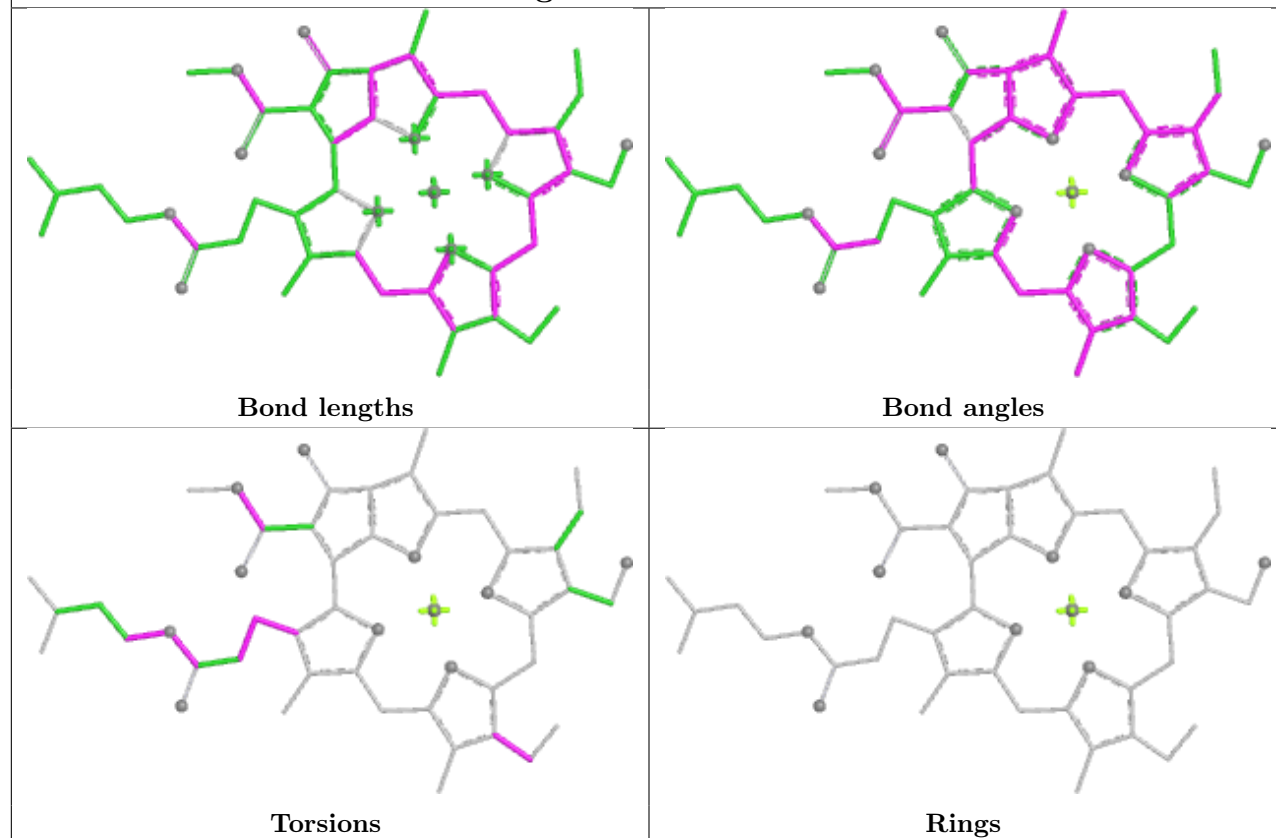


Rings

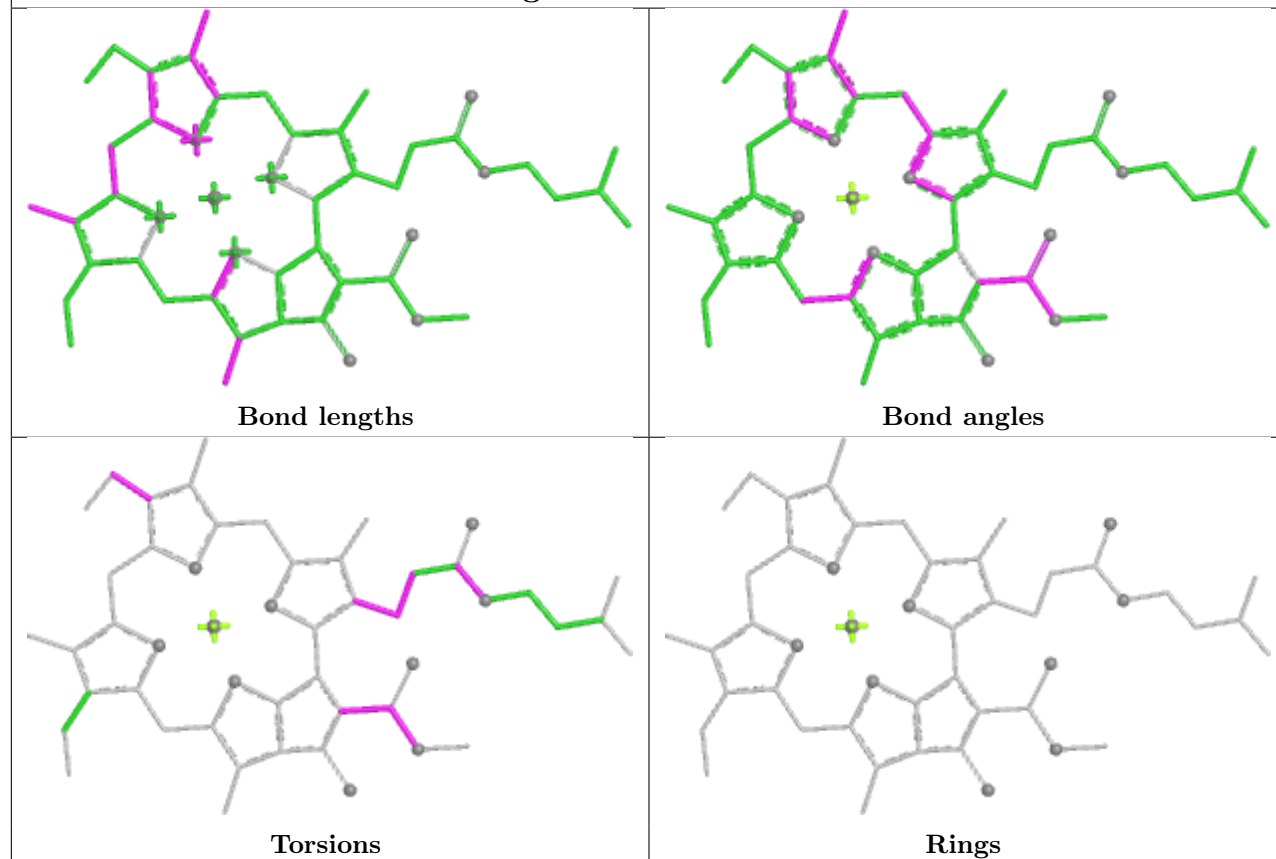


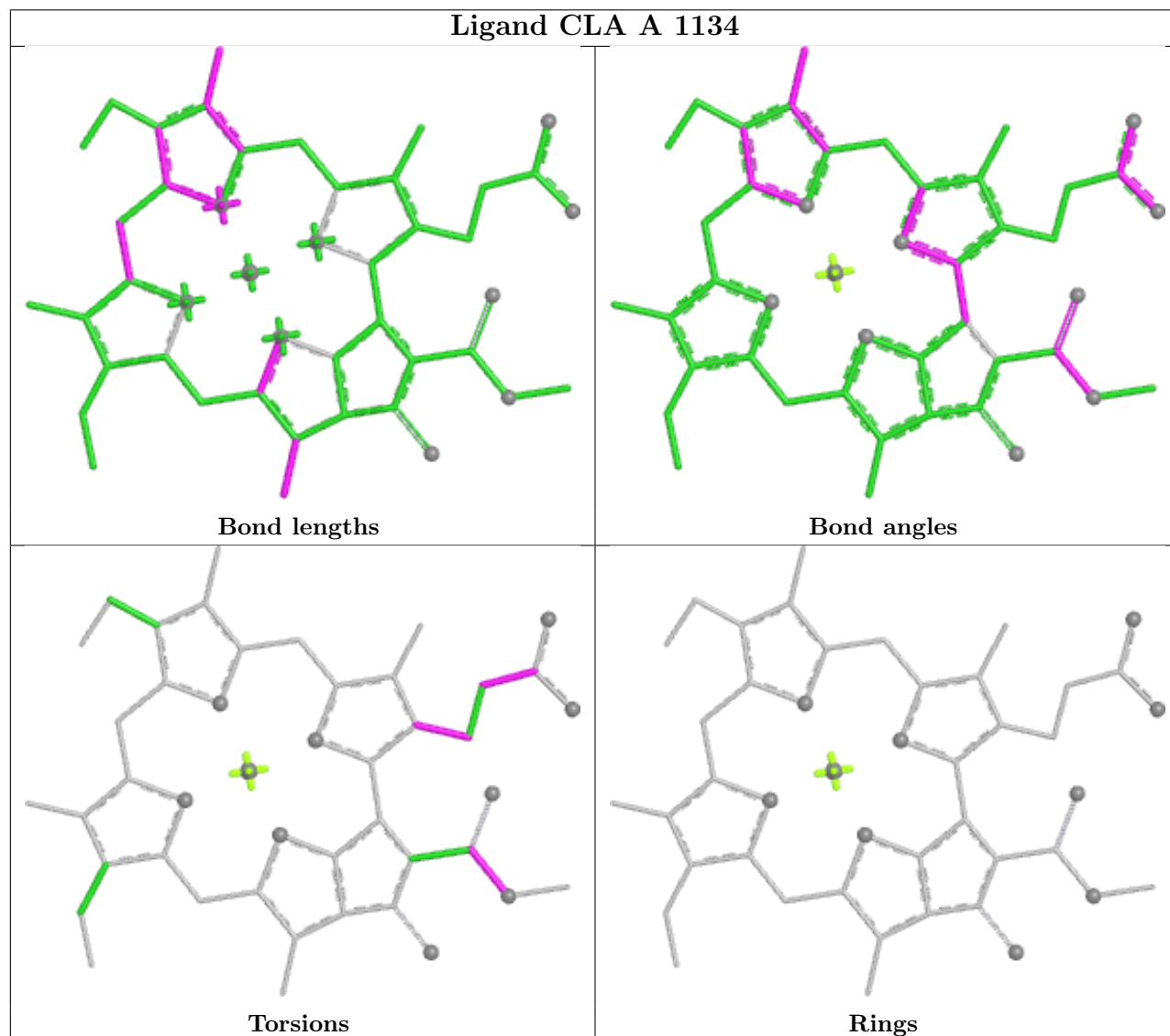
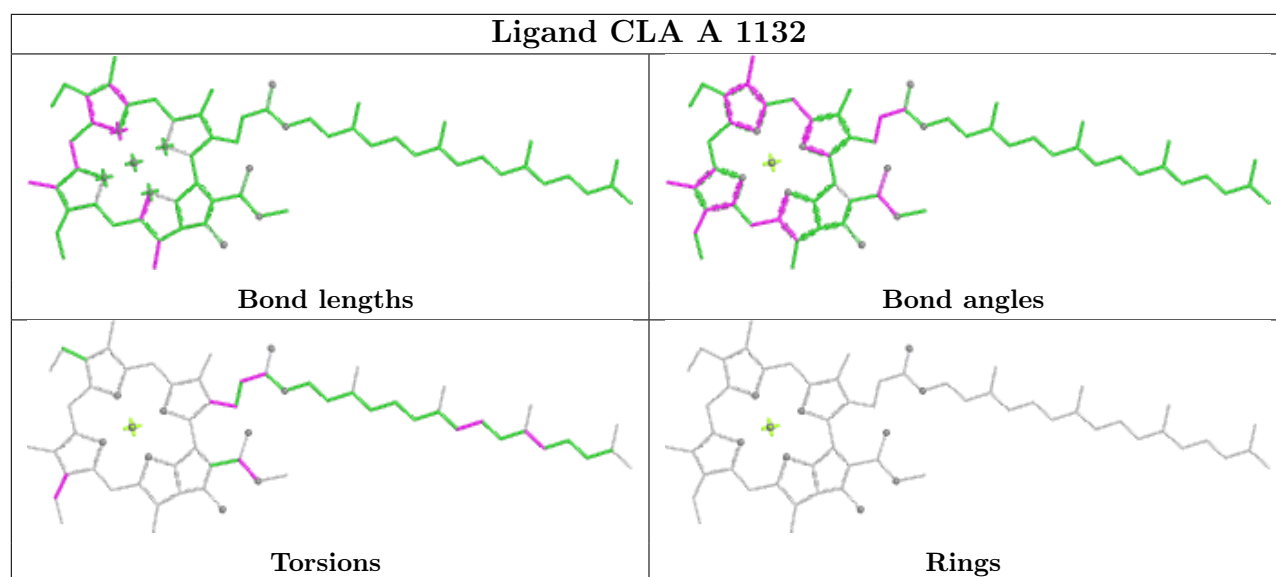


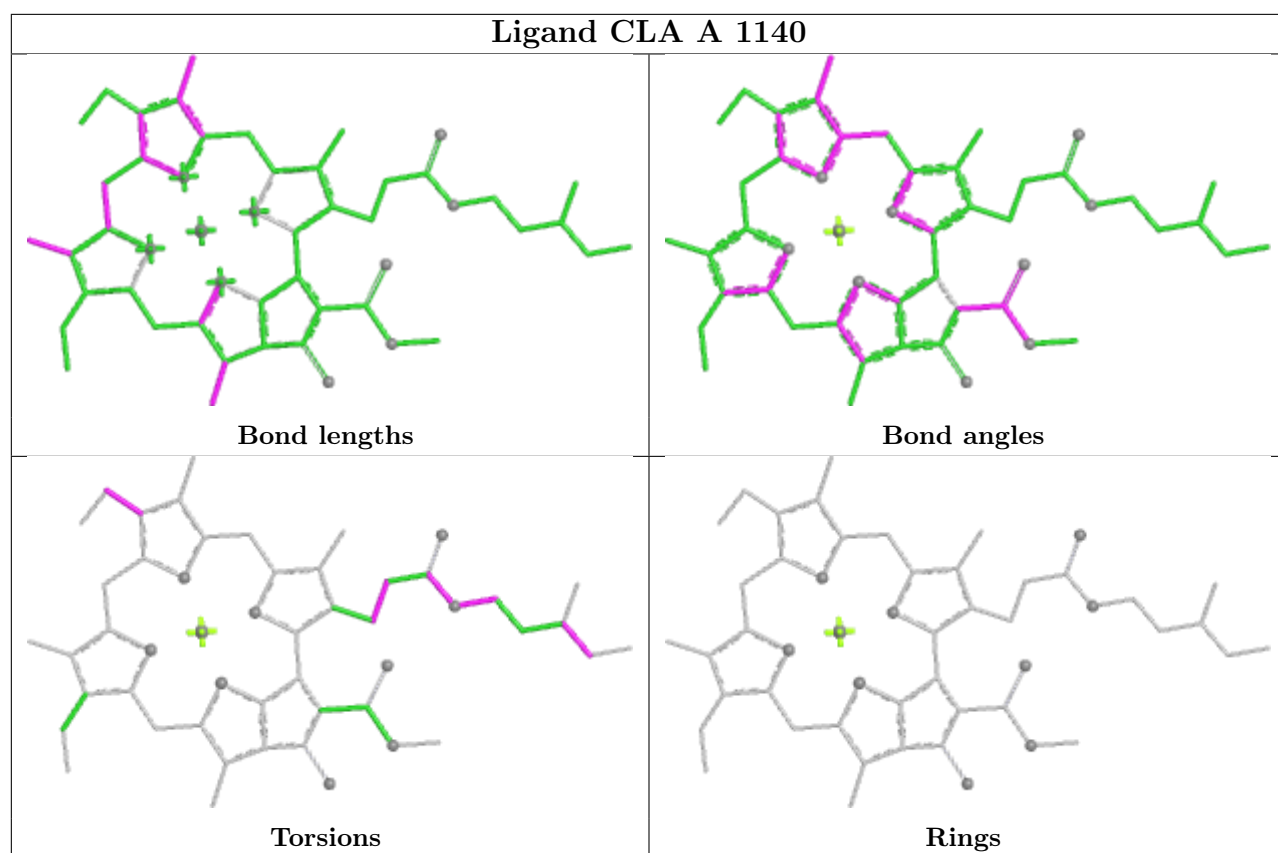
Ligand CHL 4 608

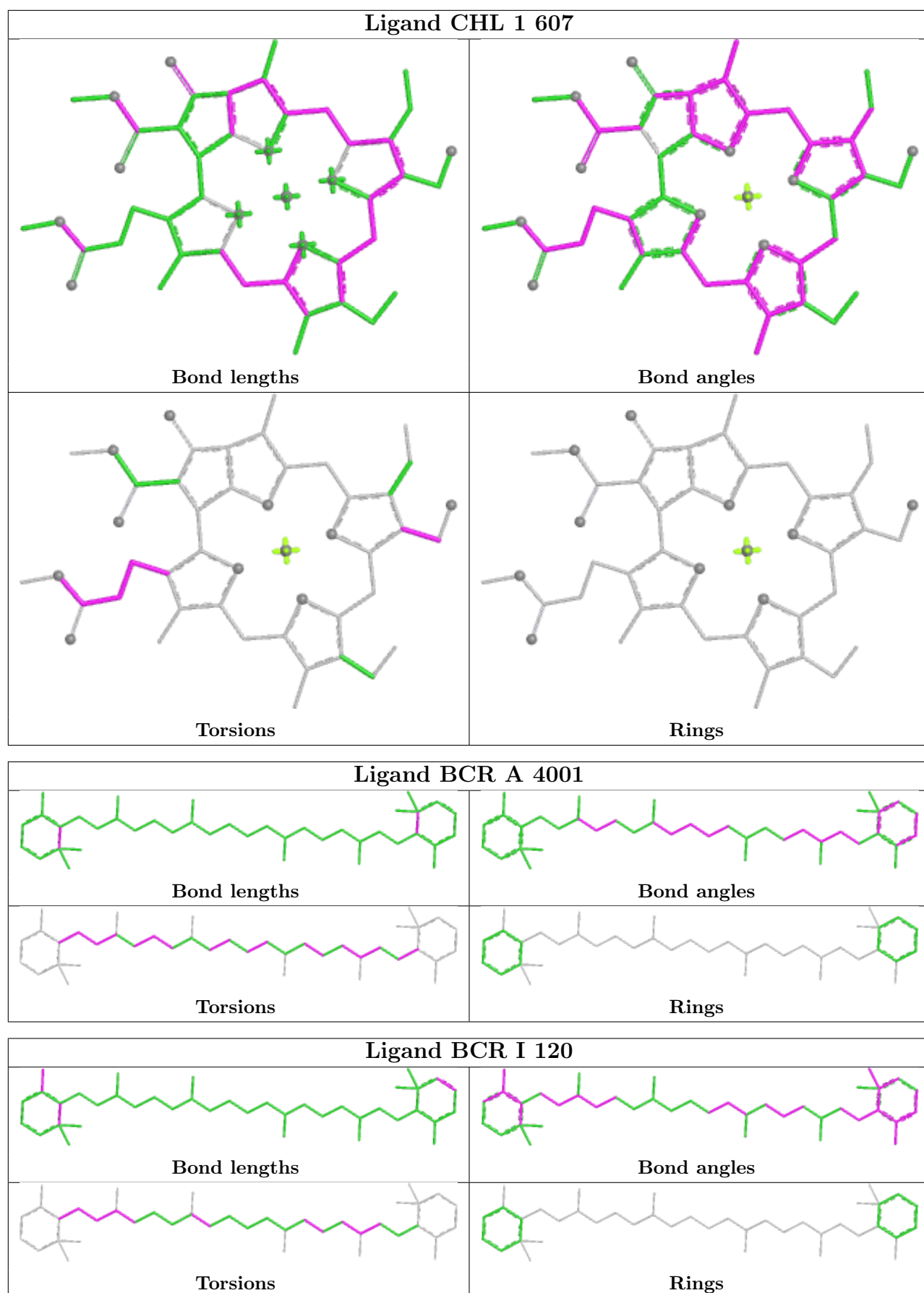


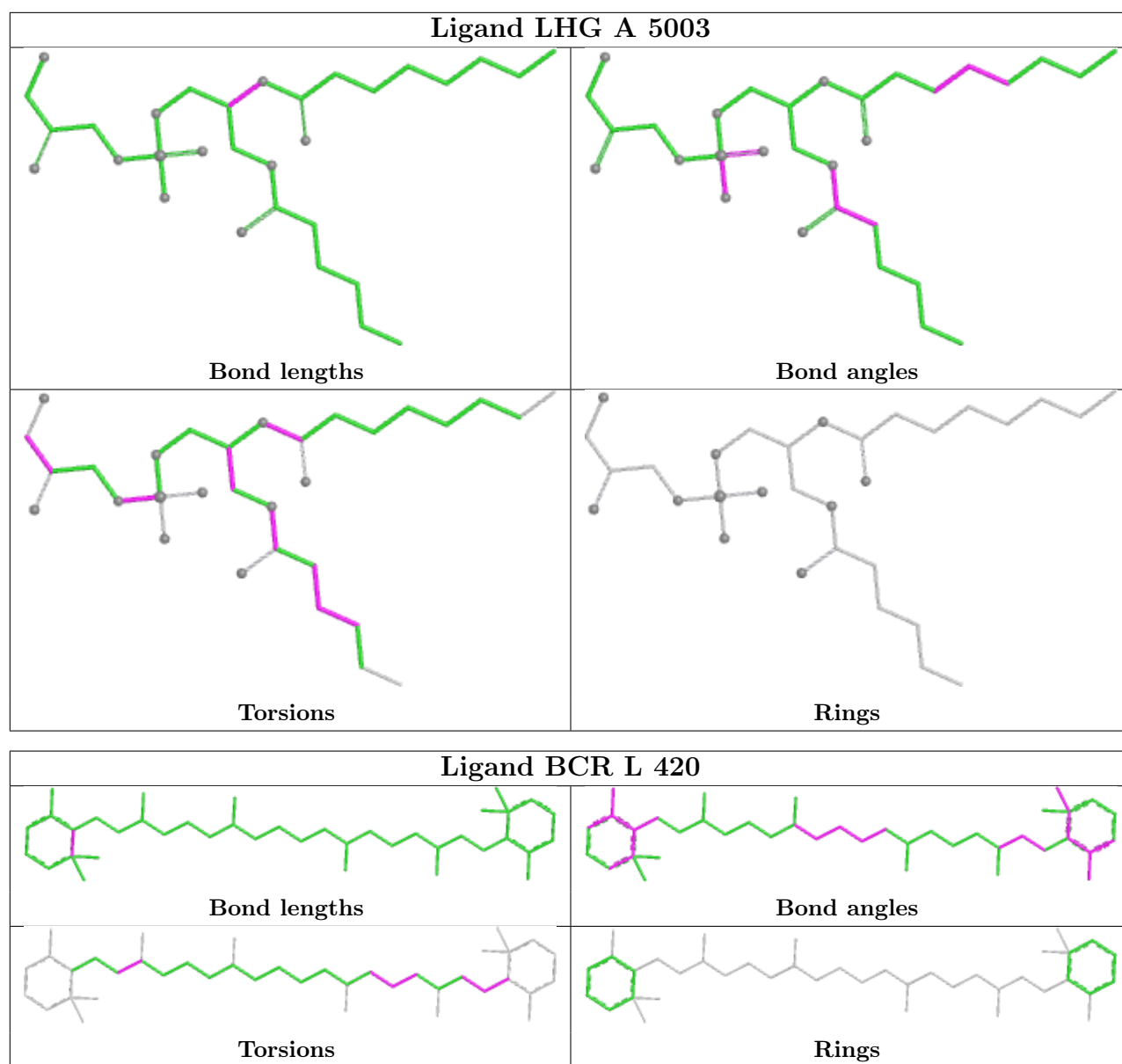
Ligand CLA A 1101

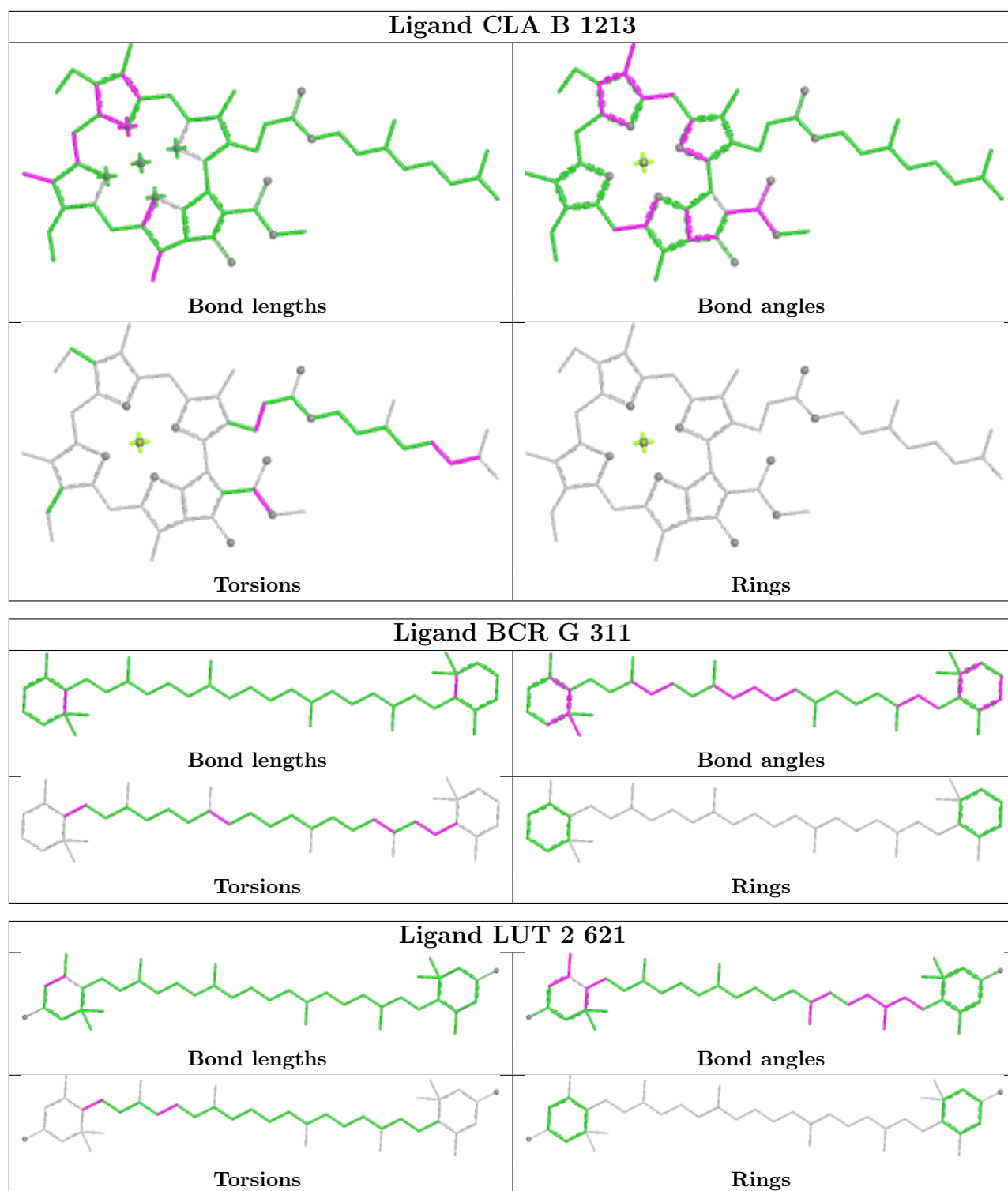


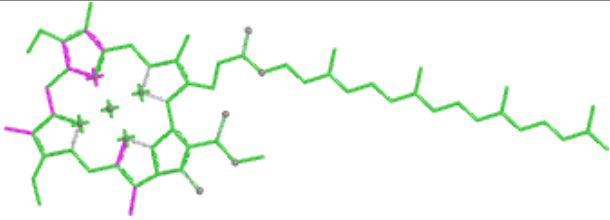
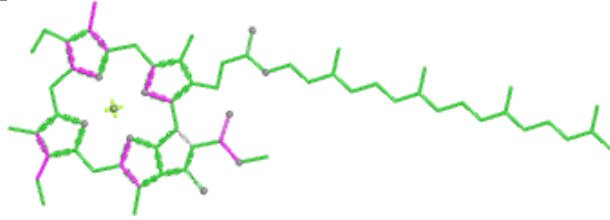
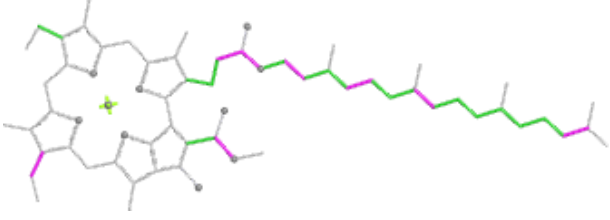
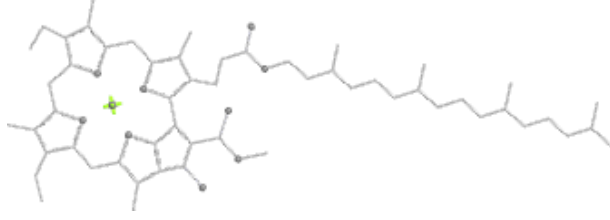
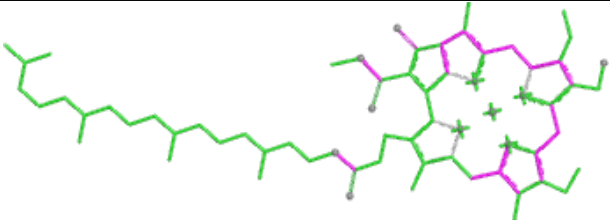
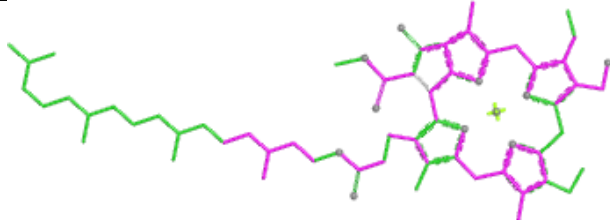
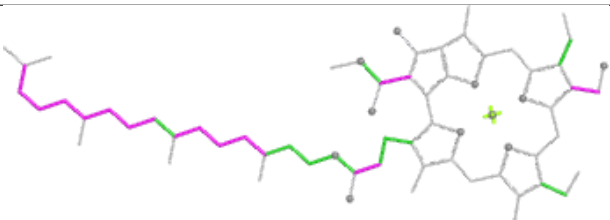
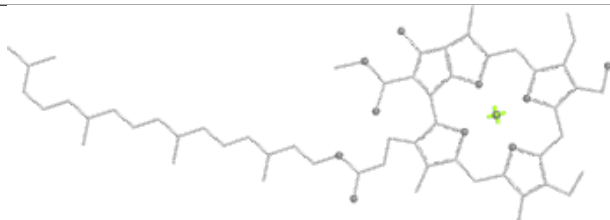
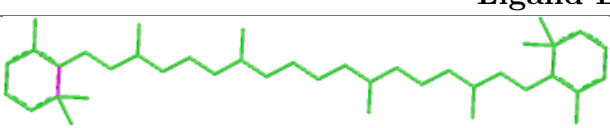
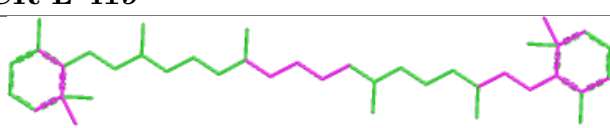
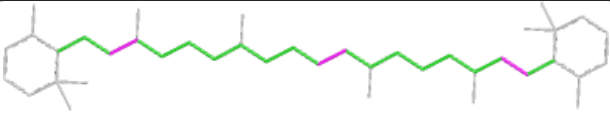
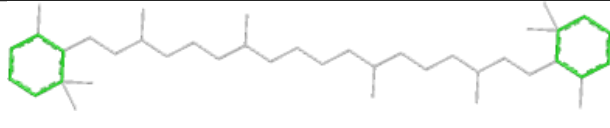


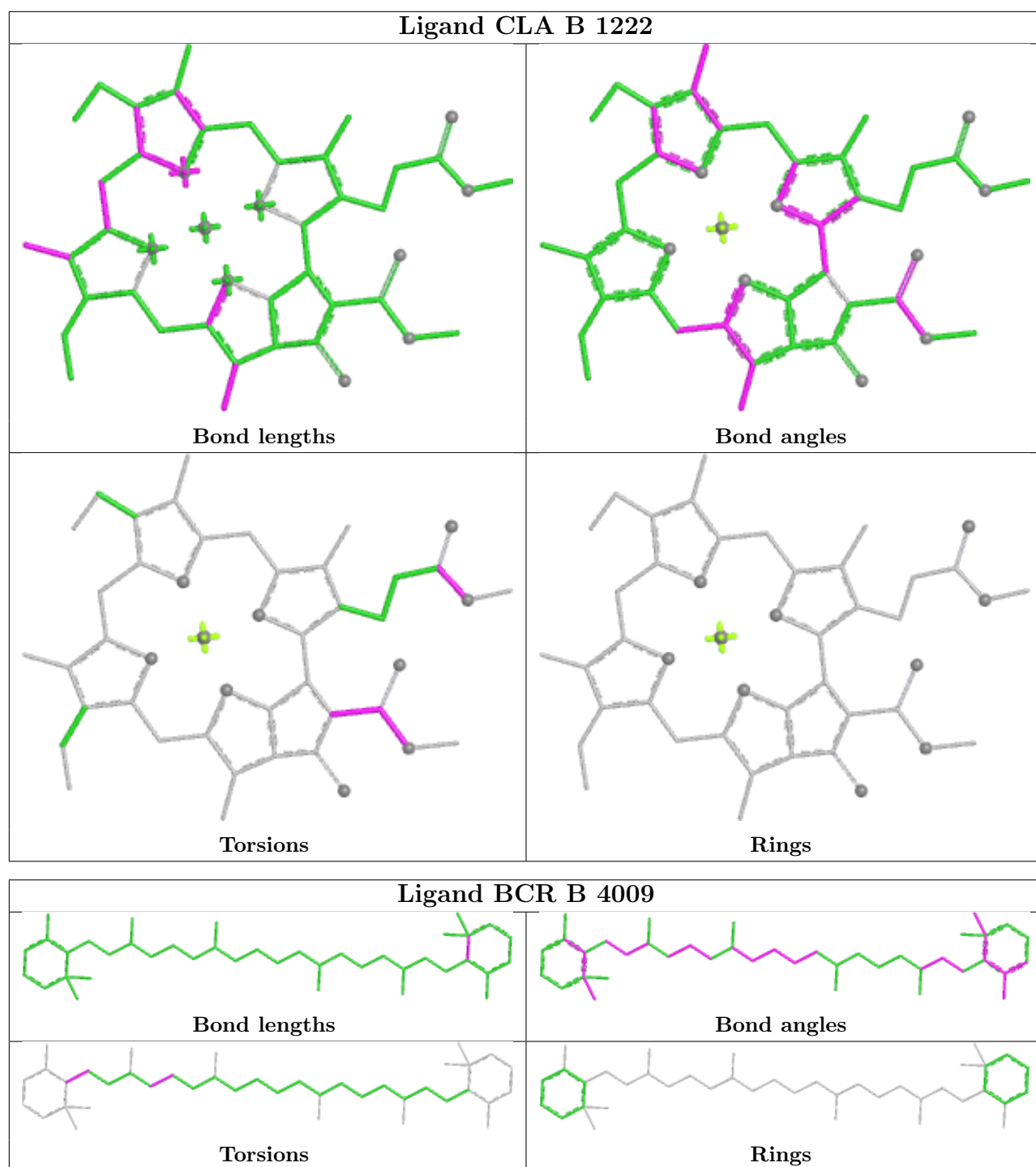


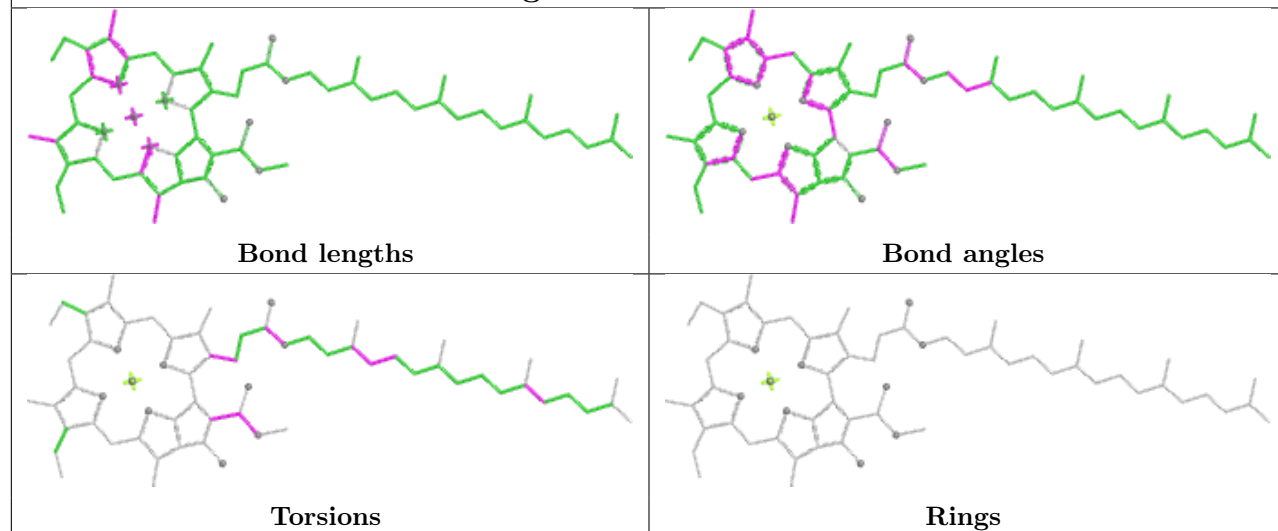
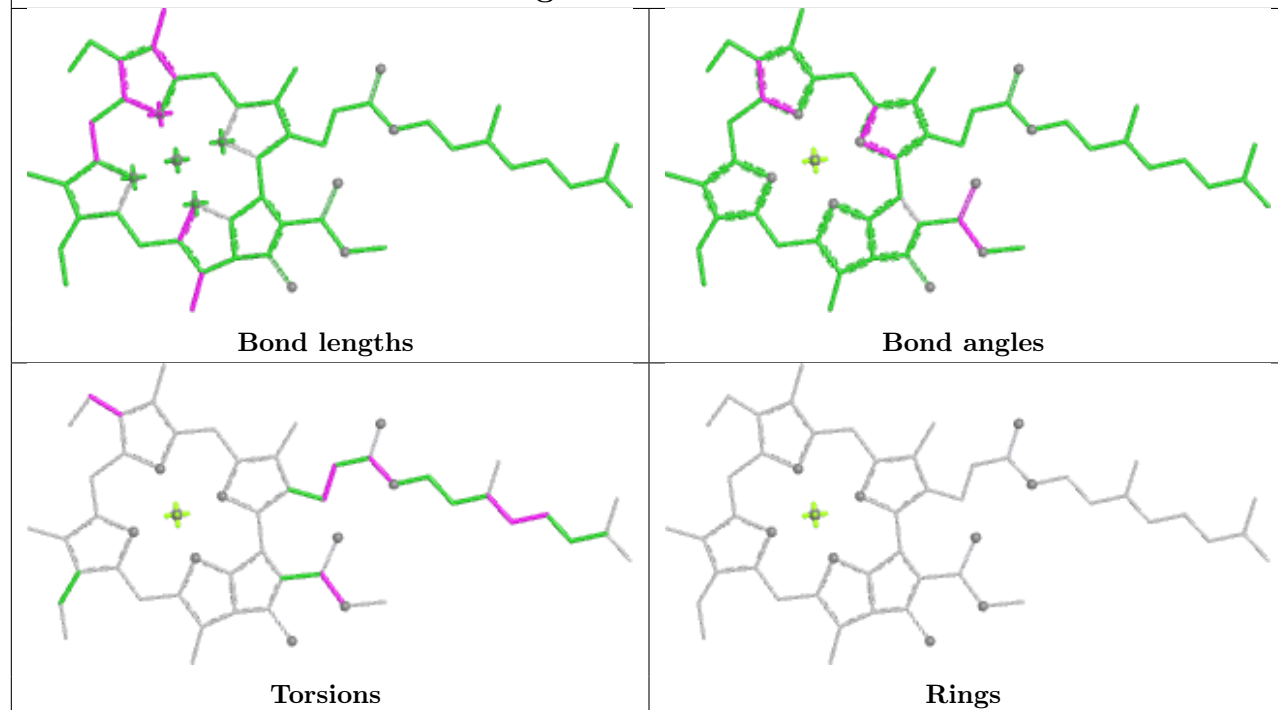


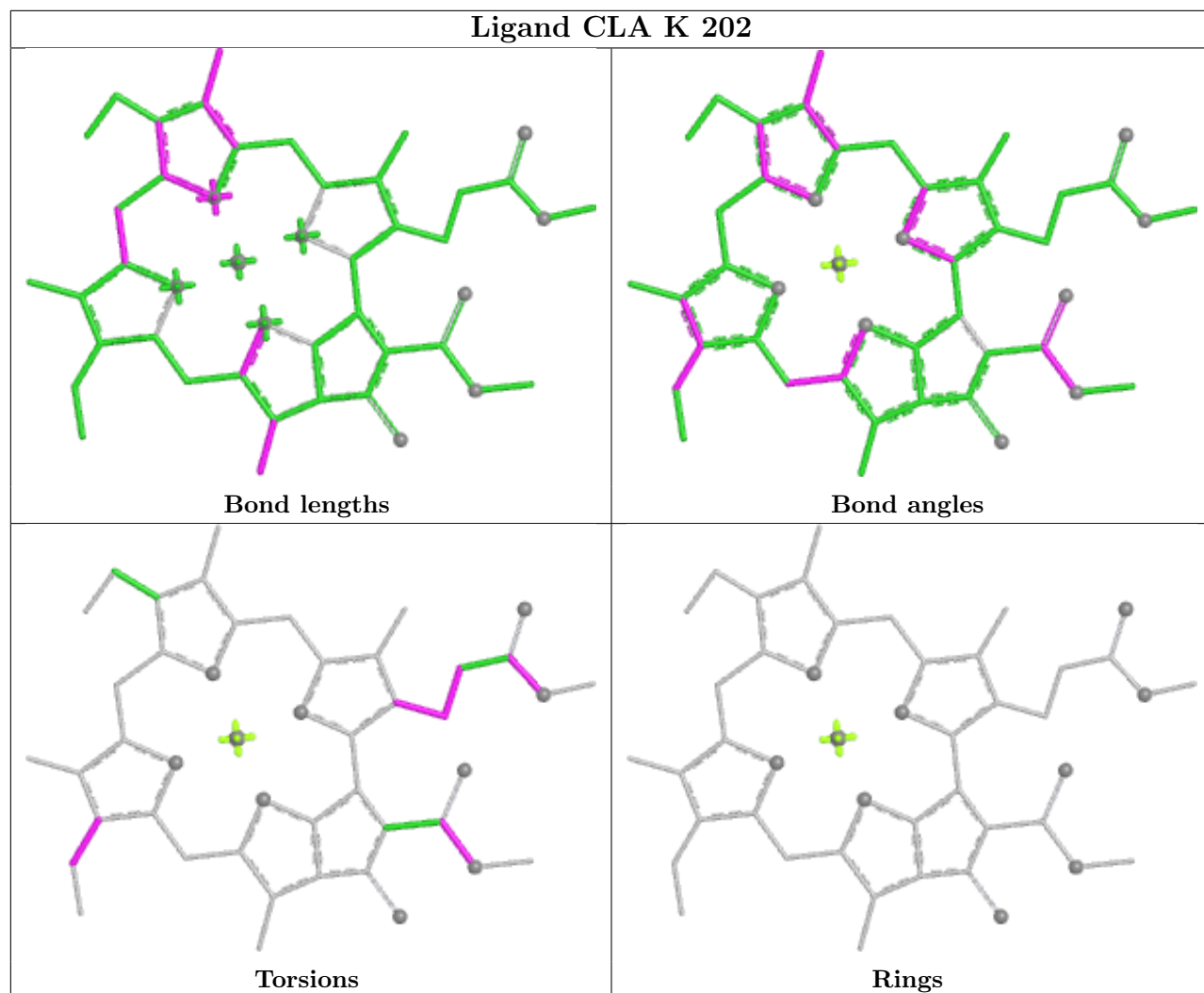




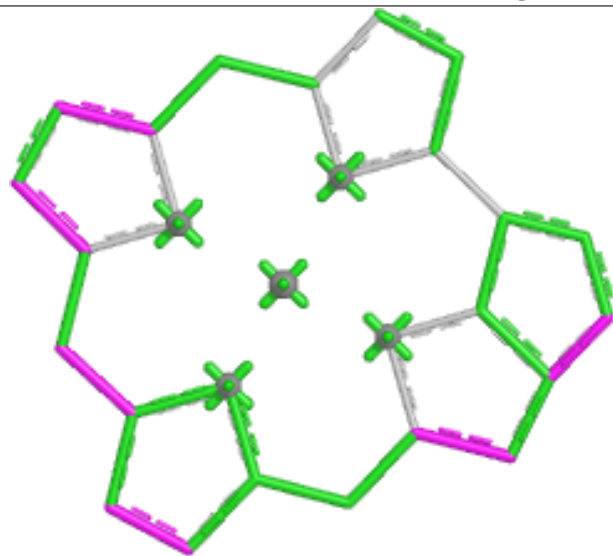
Ligand CLA I 121	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL 2 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR L 419	
 Bond lengths	 Bond angles
 Torsions	 Rings



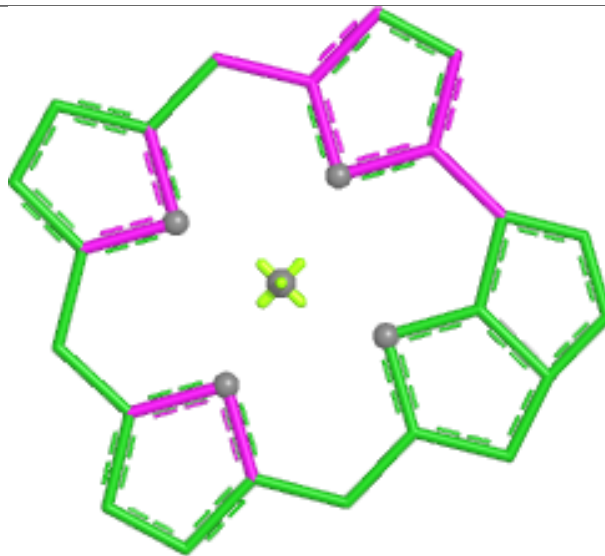
Ligand CLA A 1128**Ligand CLA 3 613**



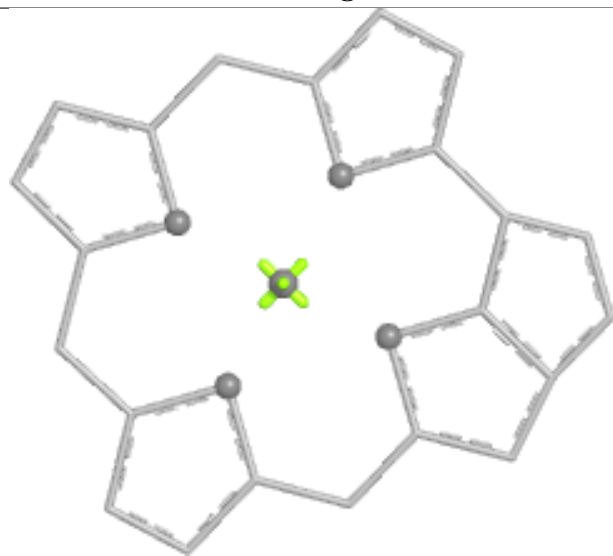
Ligand CLA K 203



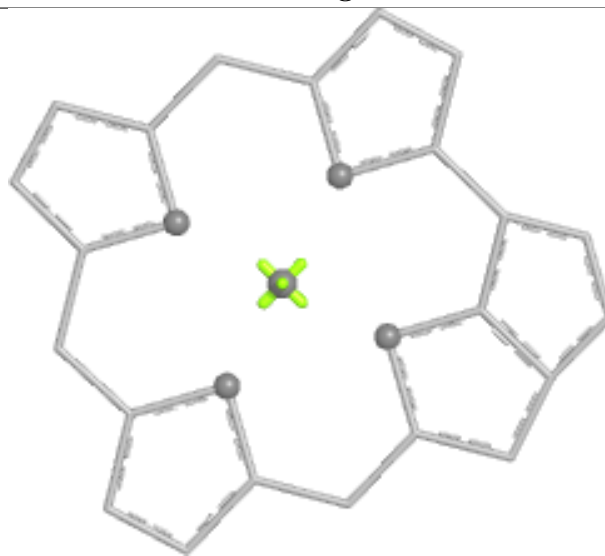
Bond lengths



Bond angles

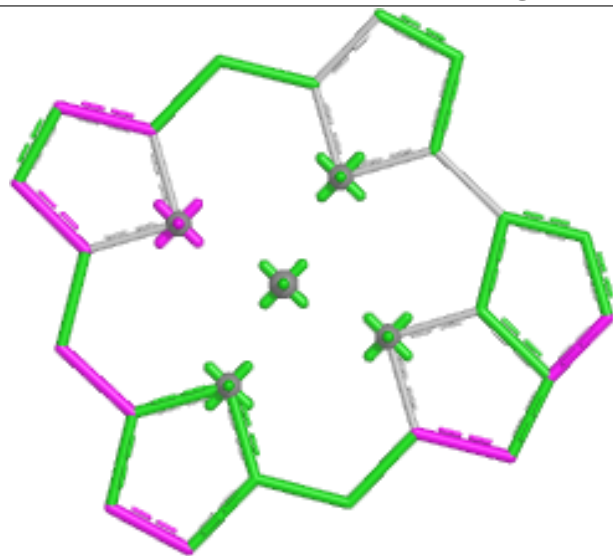


Torsions

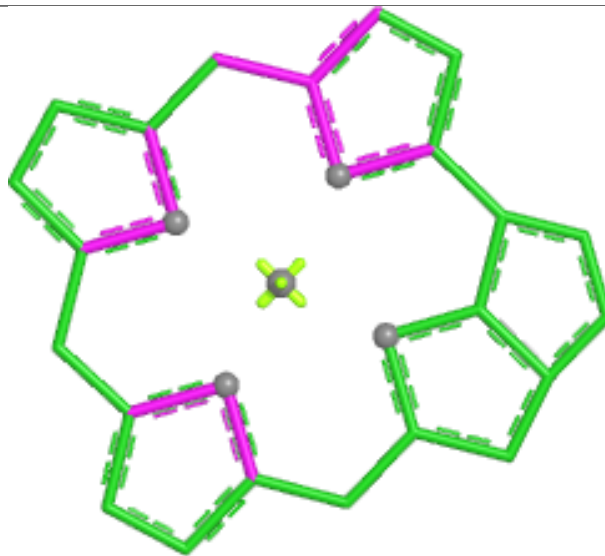


Rings

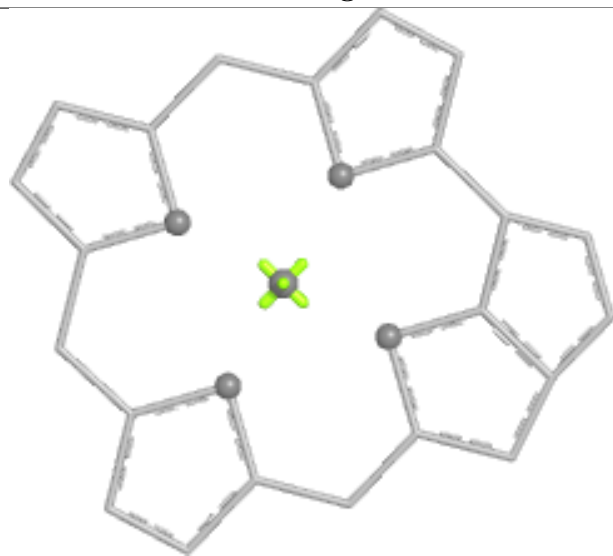
Ligand CLA O 203



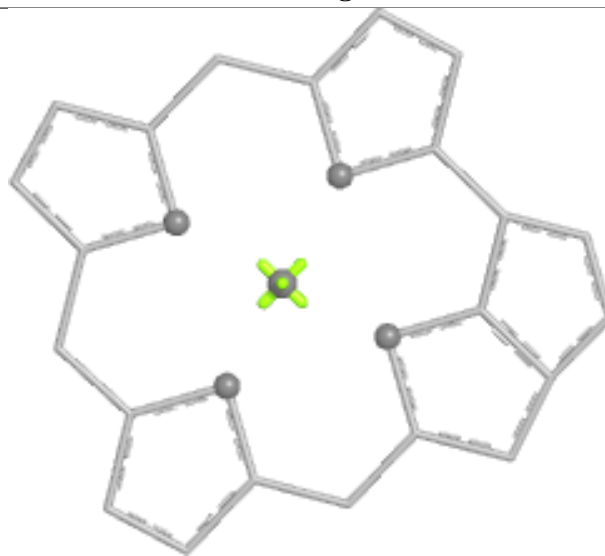
Bond lengths



Bond angles

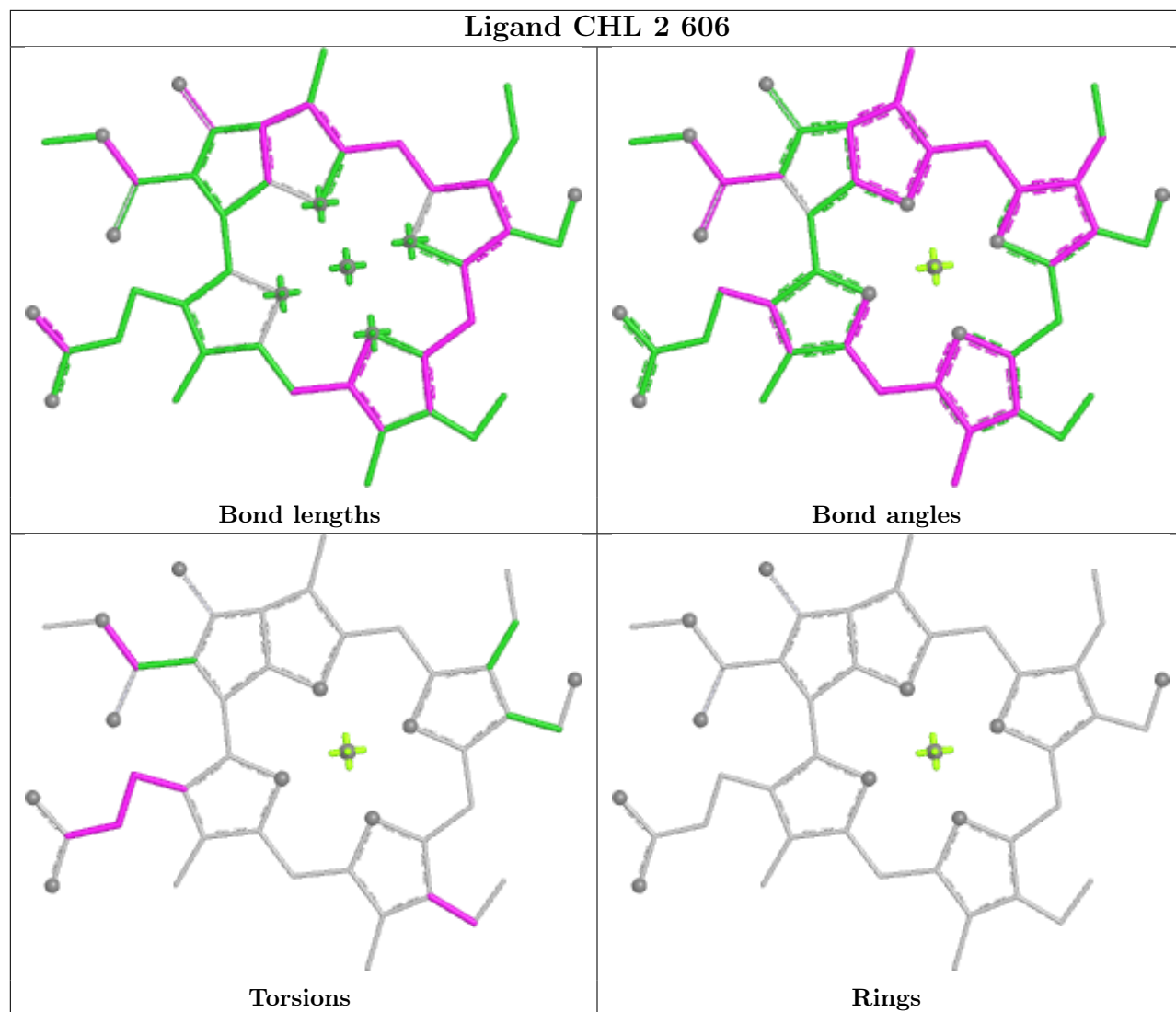


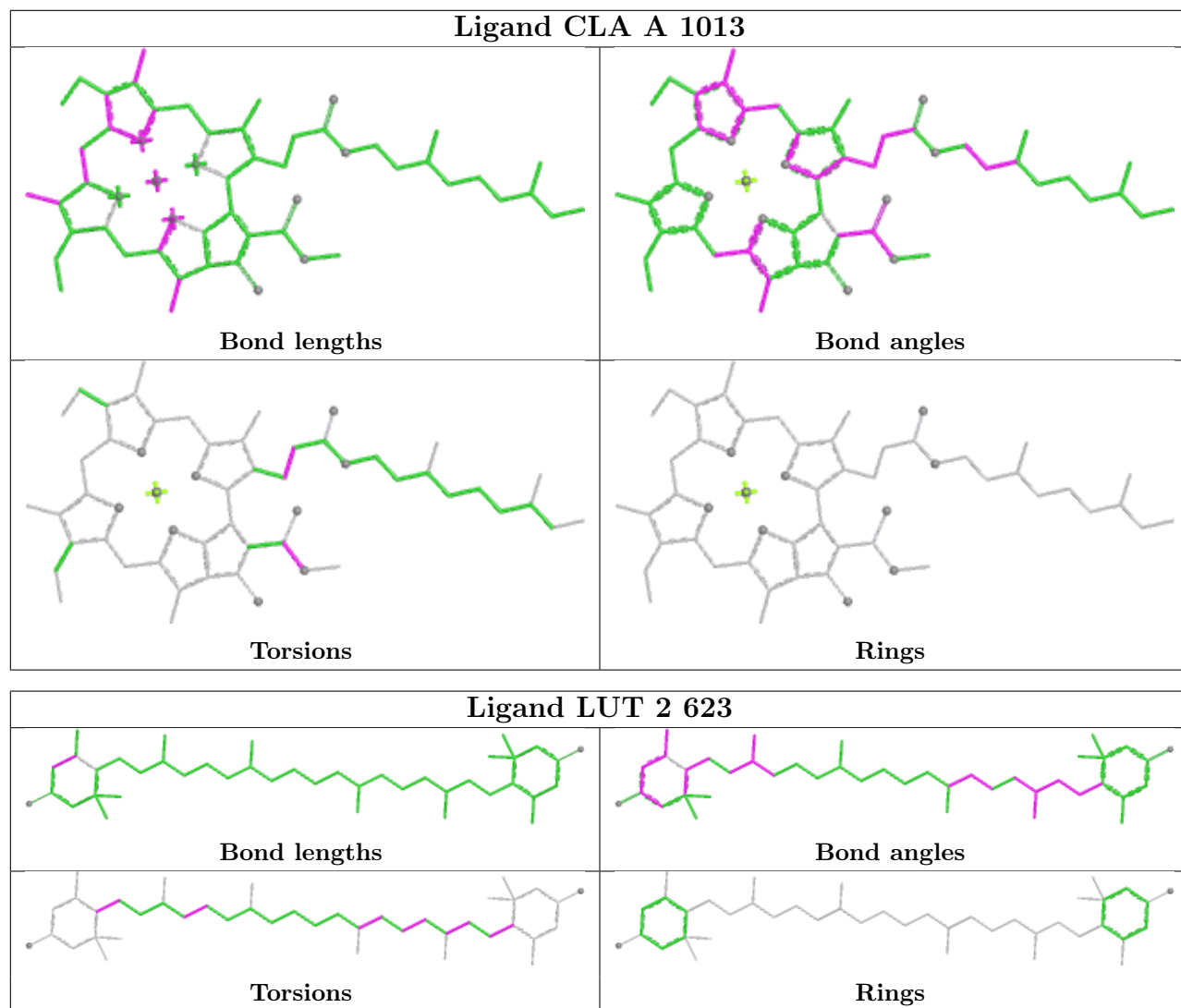
Torsions



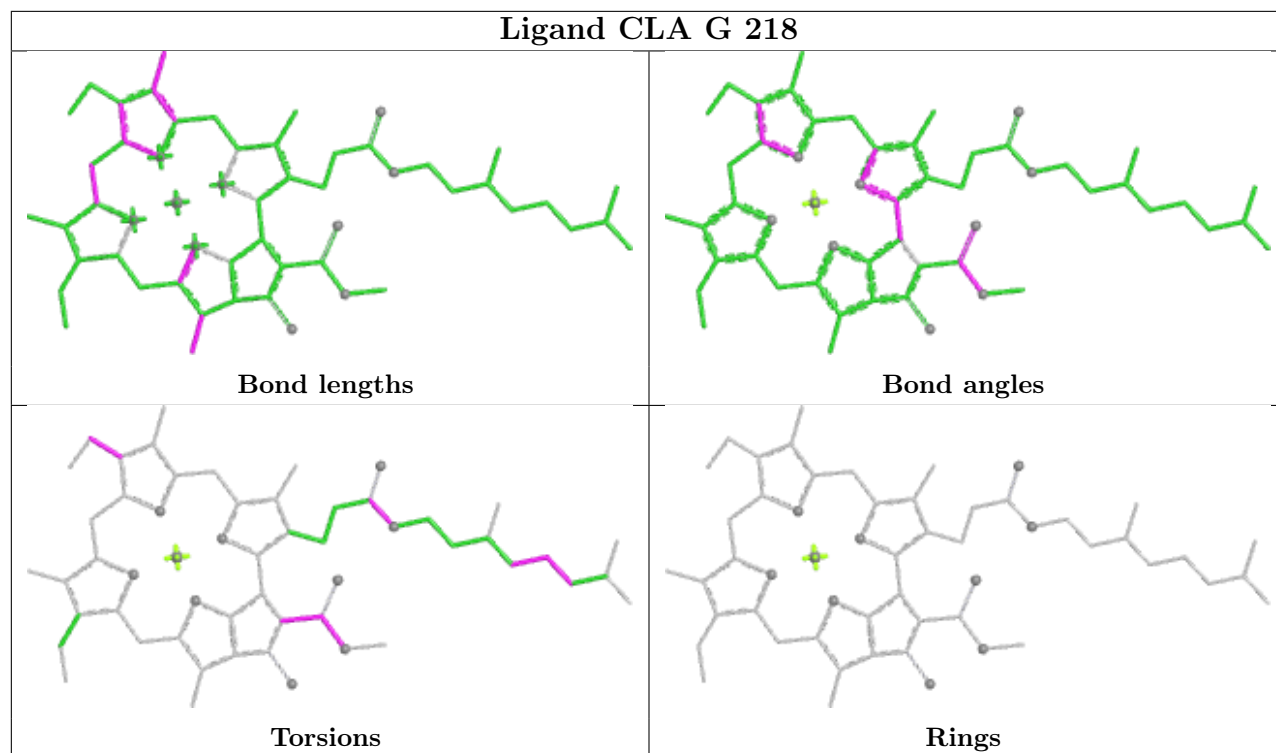
Rings

Ligand CHL 2 606

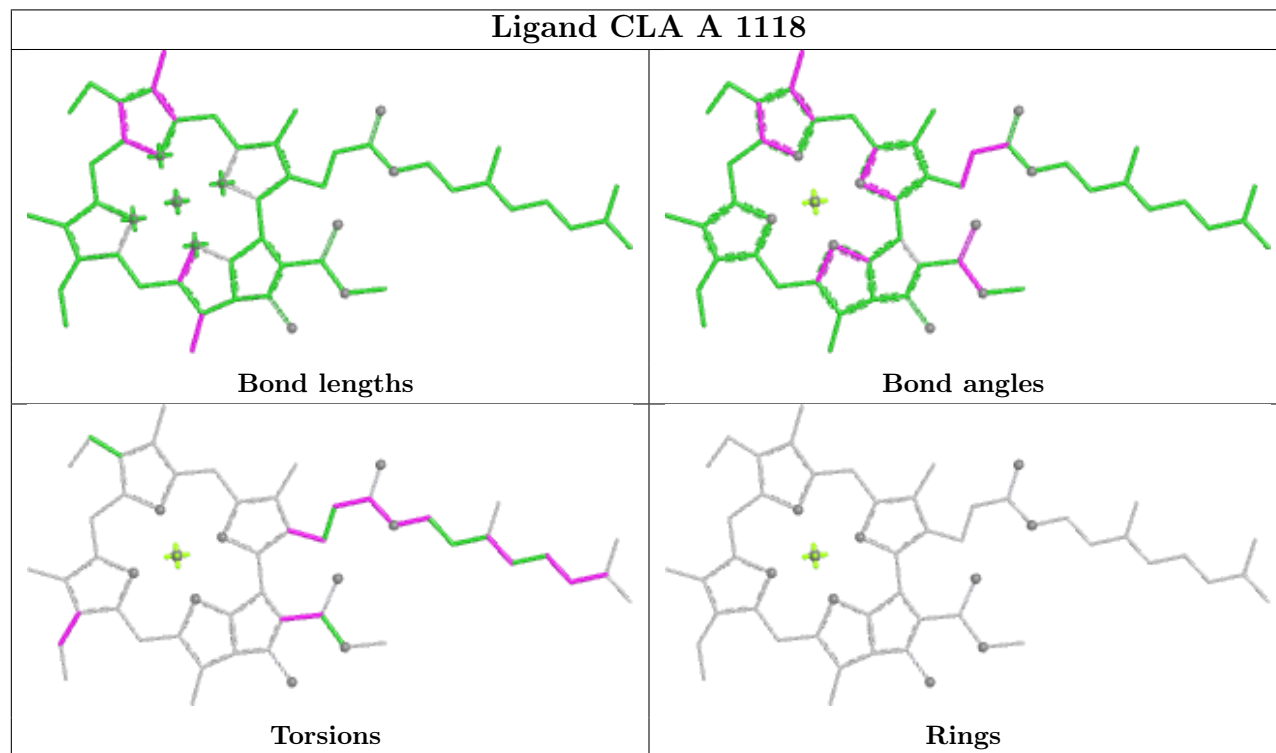


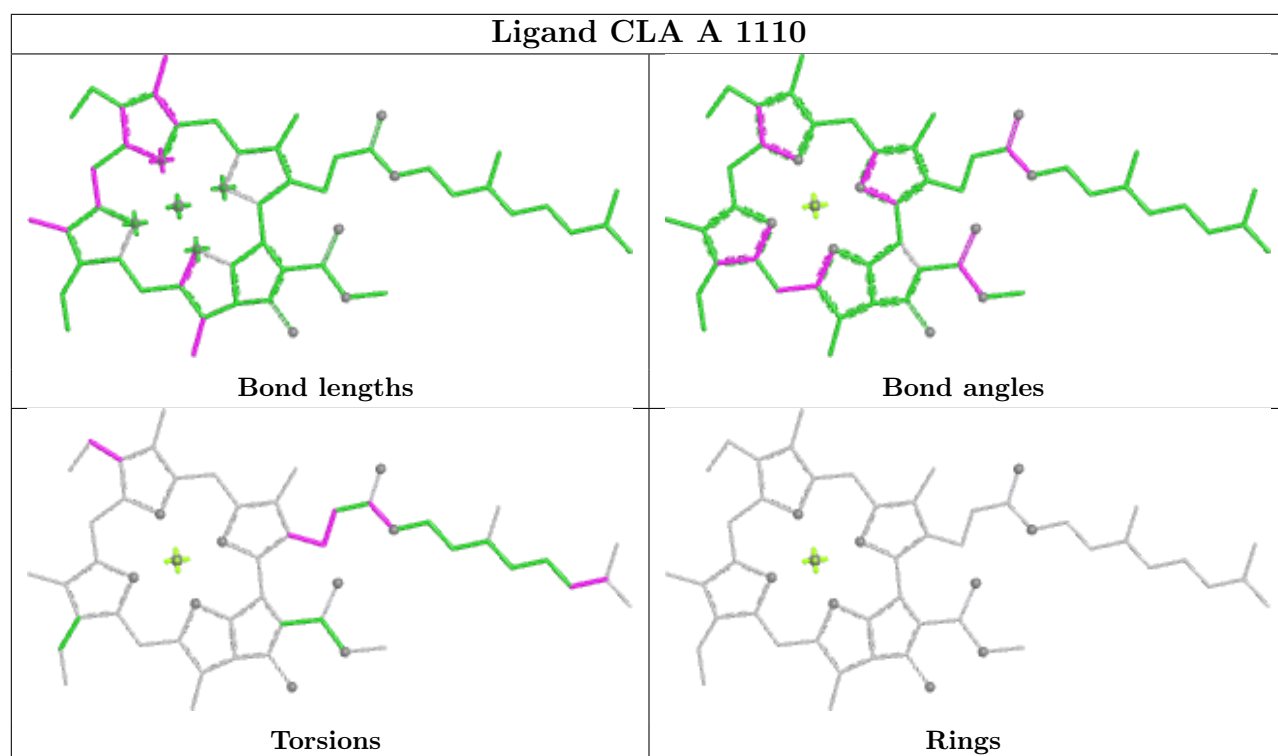


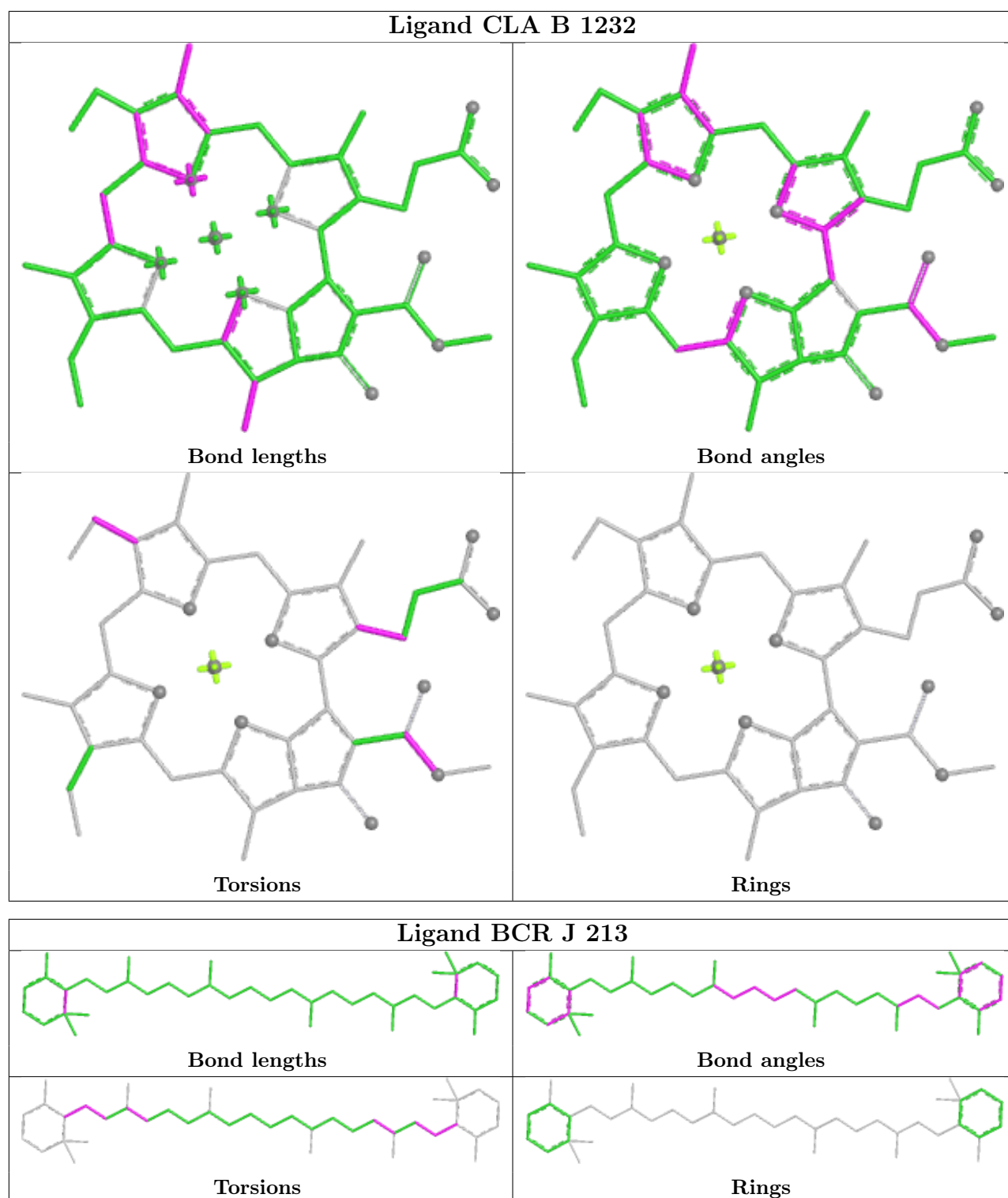
Ligand CLA G 218

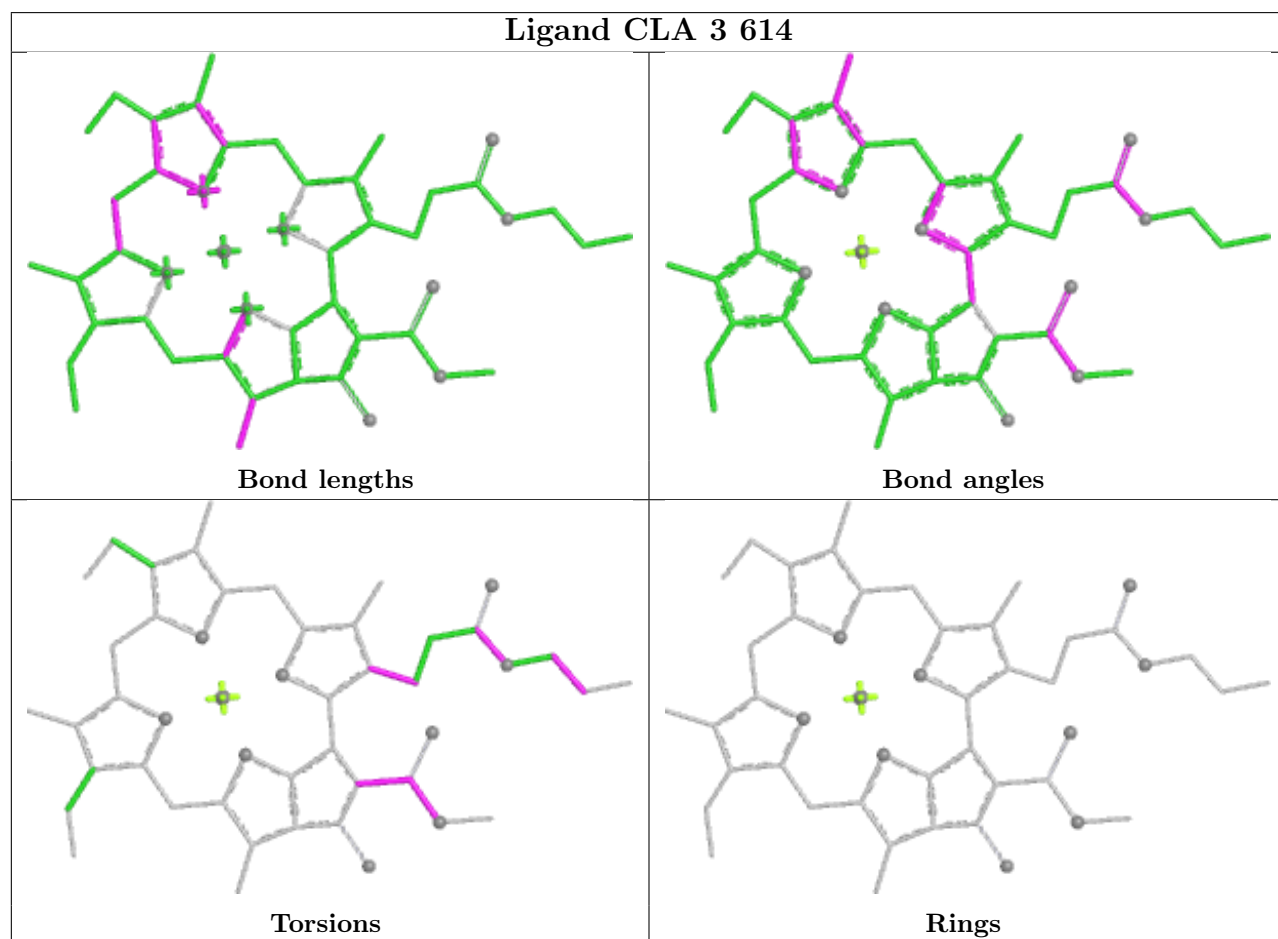
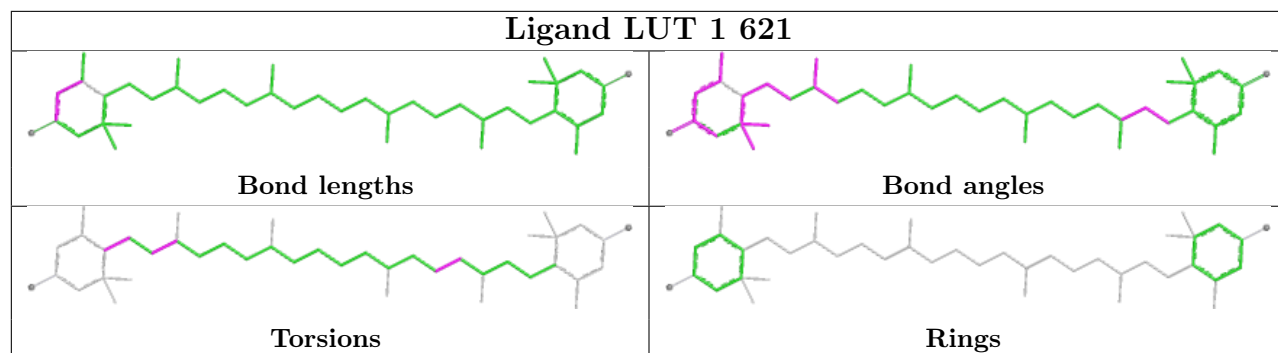


Ligand CLA A 1118

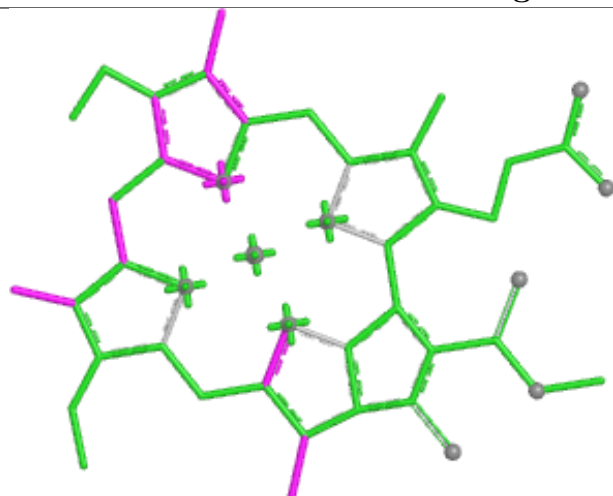




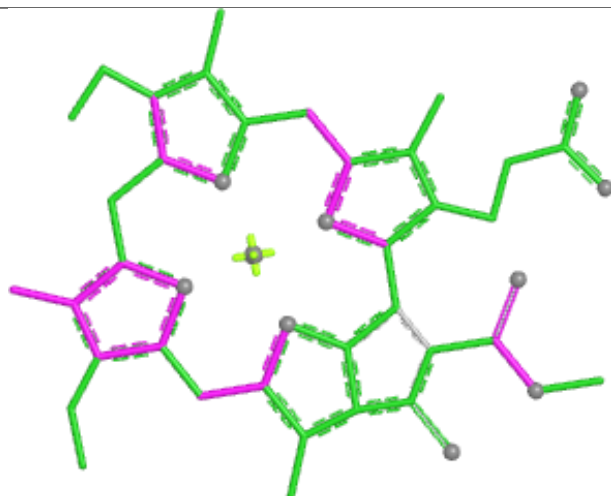




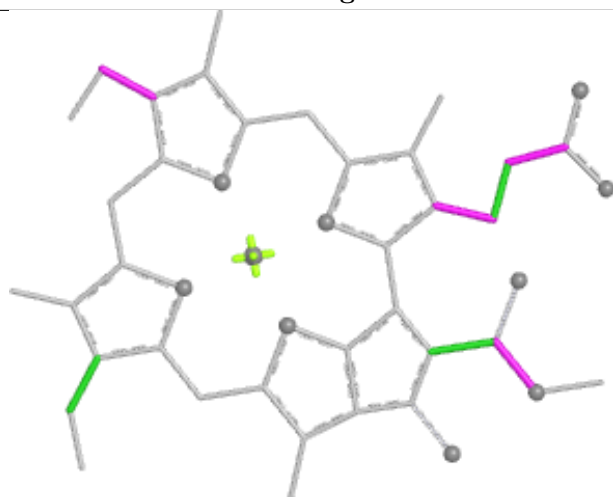
Ligand CLA K 204



Bond lengths



Bond angles

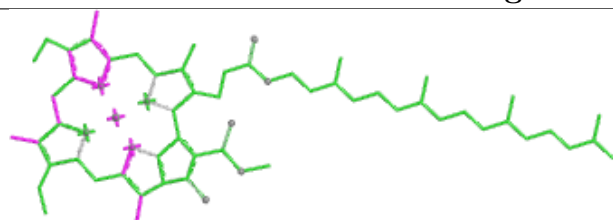


Torsions

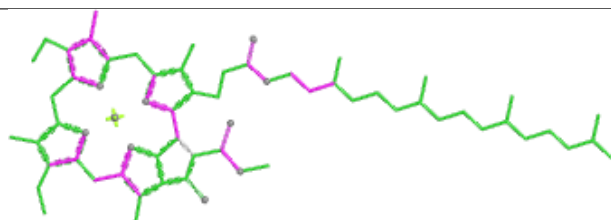


Rings

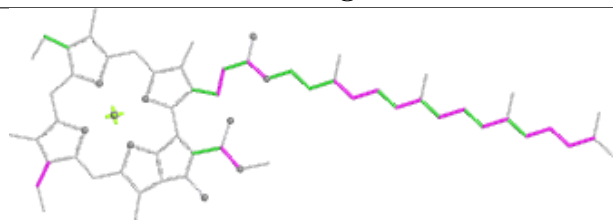
Ligand CLA A 1127



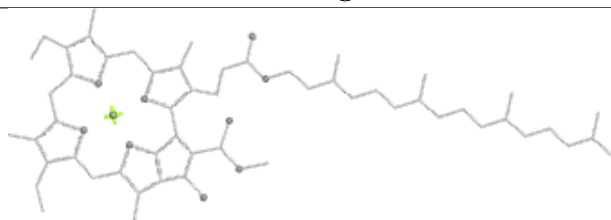
Bond lengths



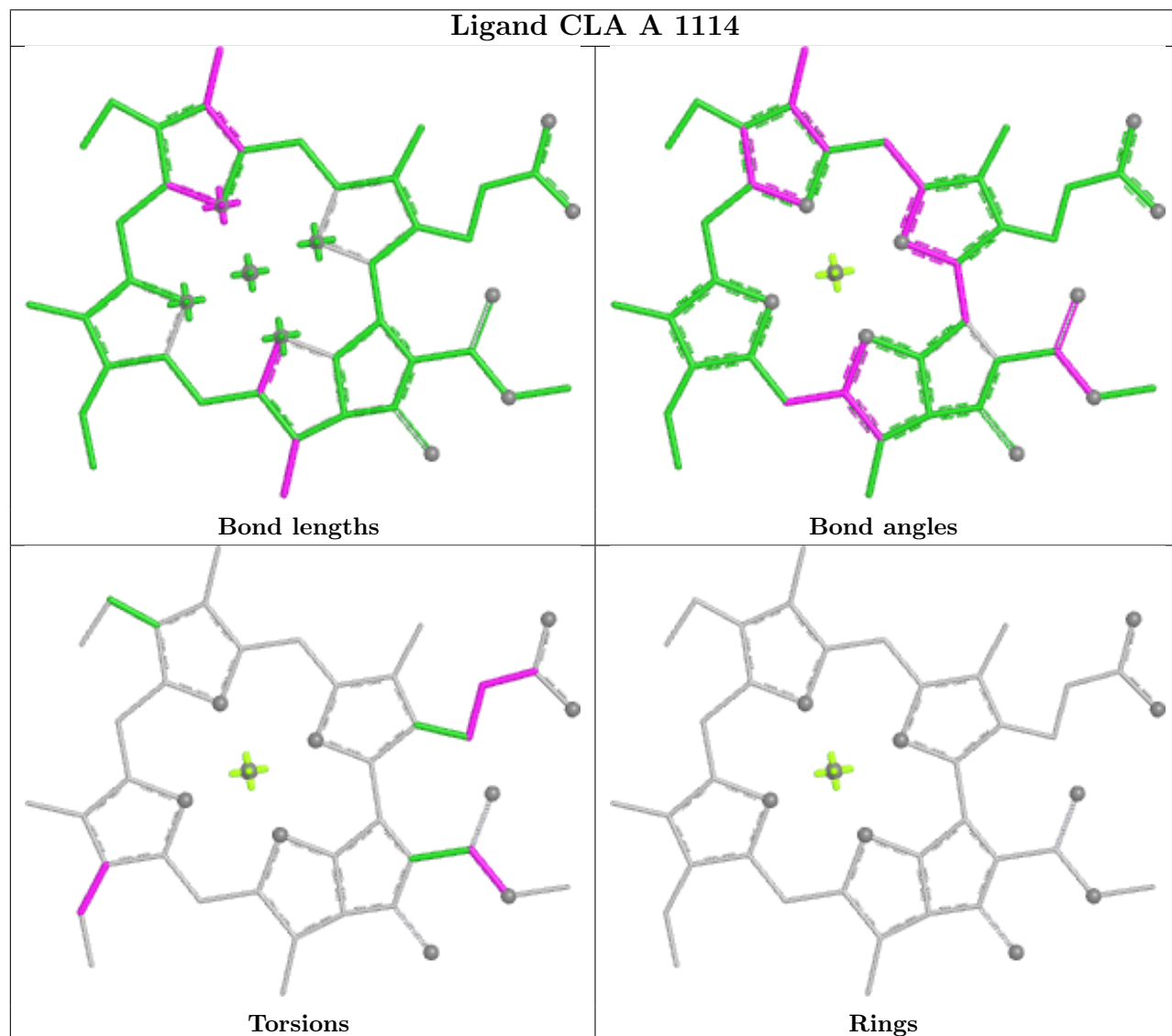
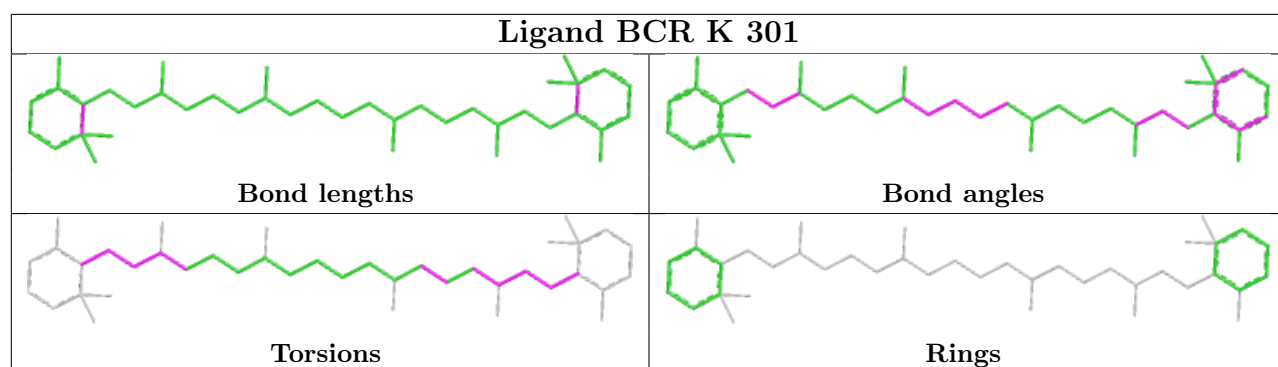
Bond angles

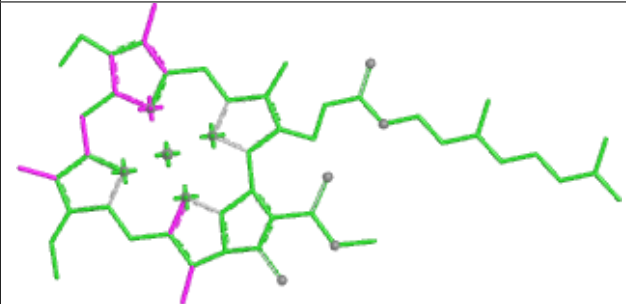
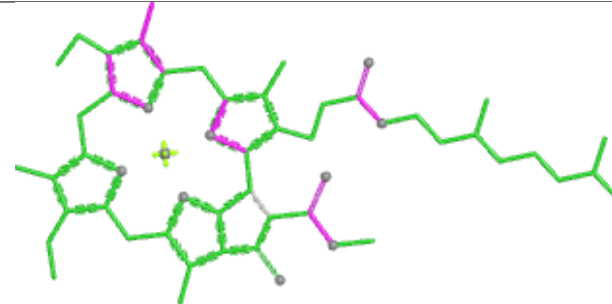
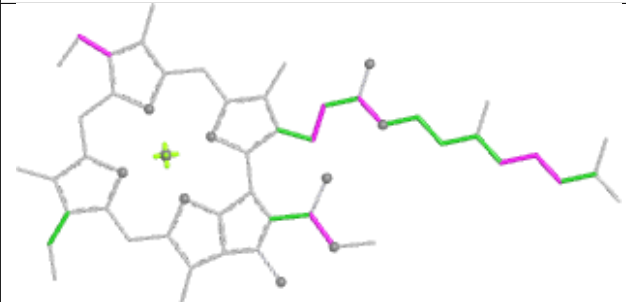
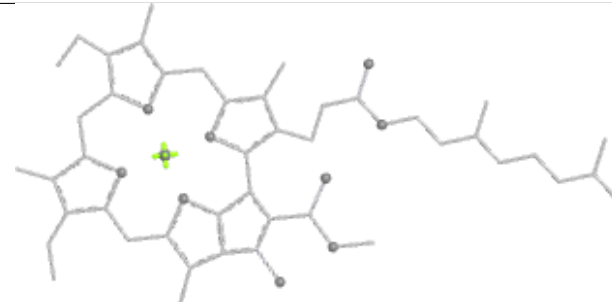


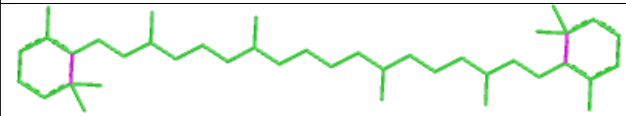
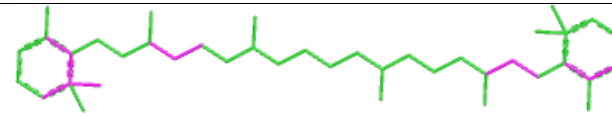
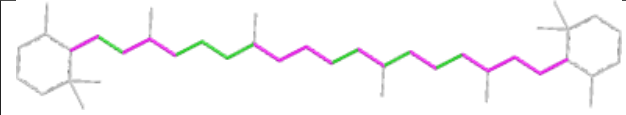
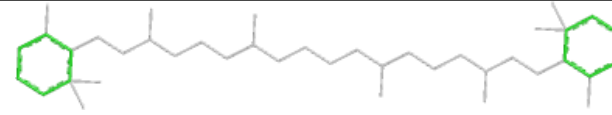
Torsions

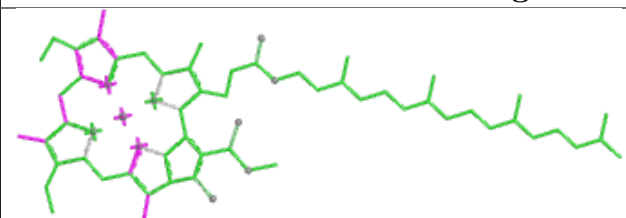
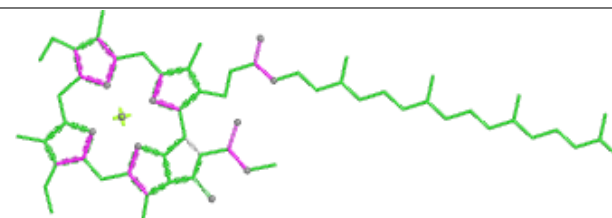
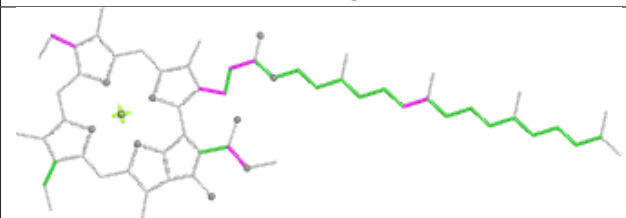
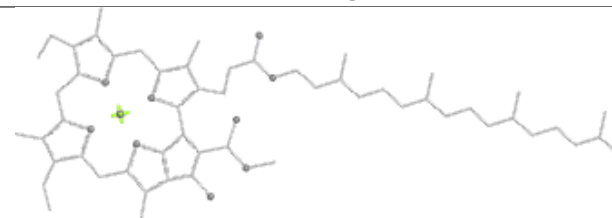


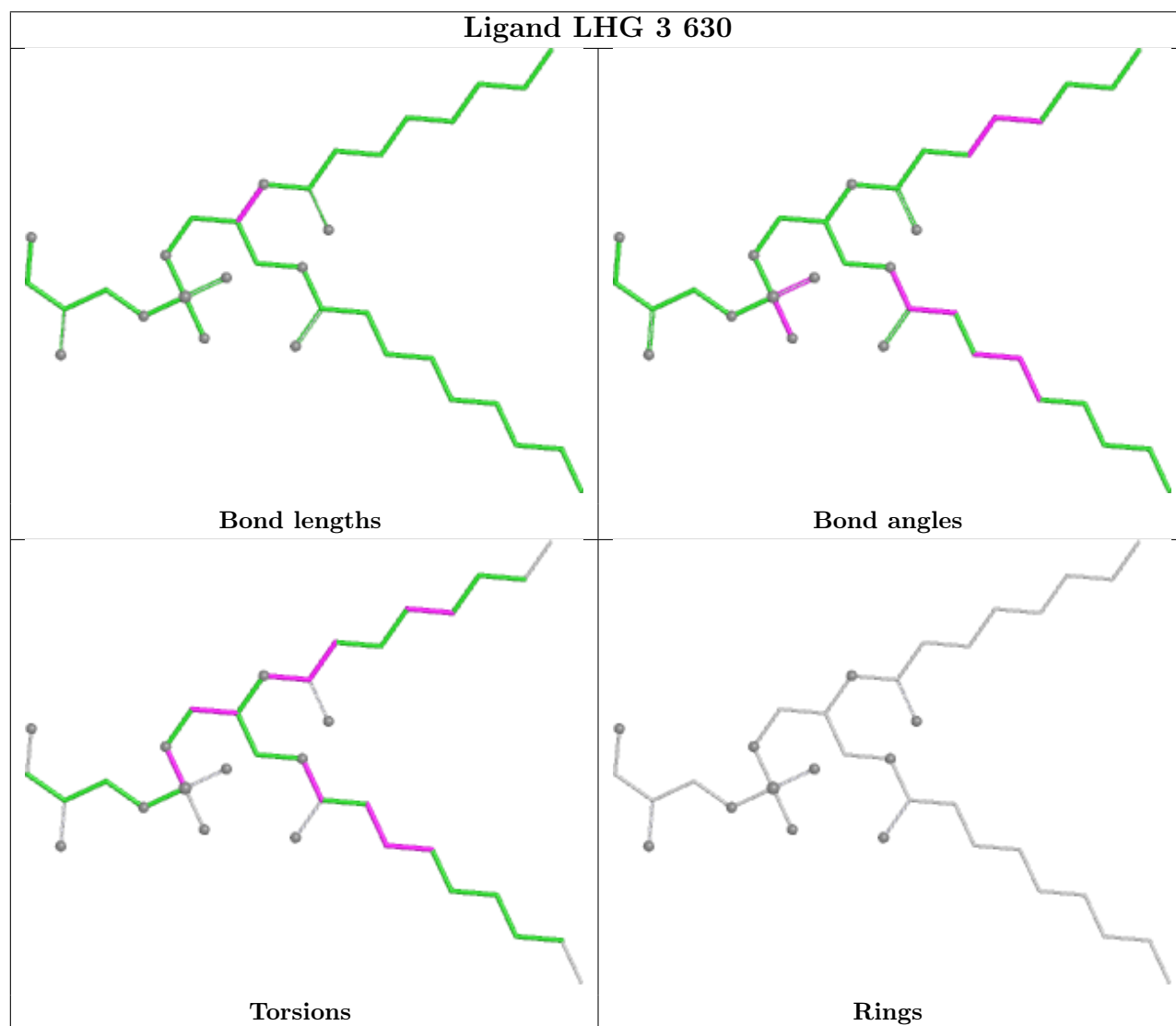
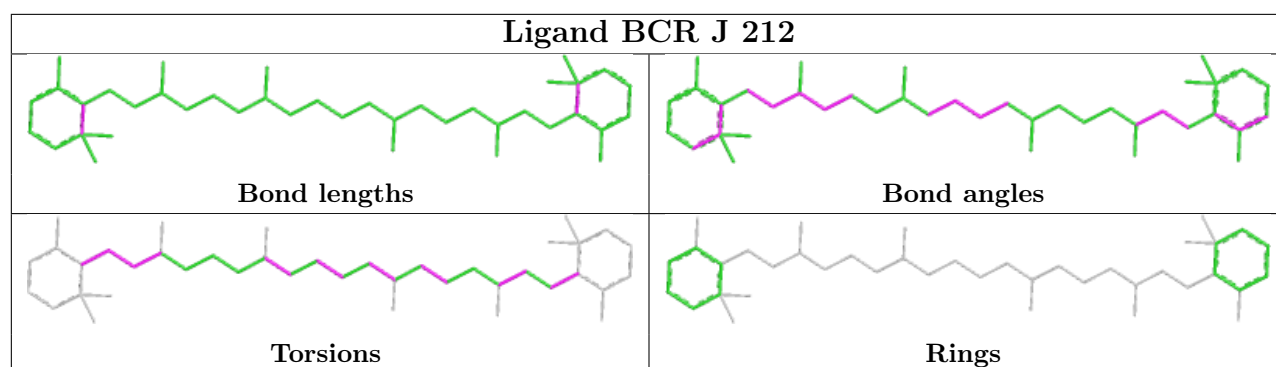
Rings



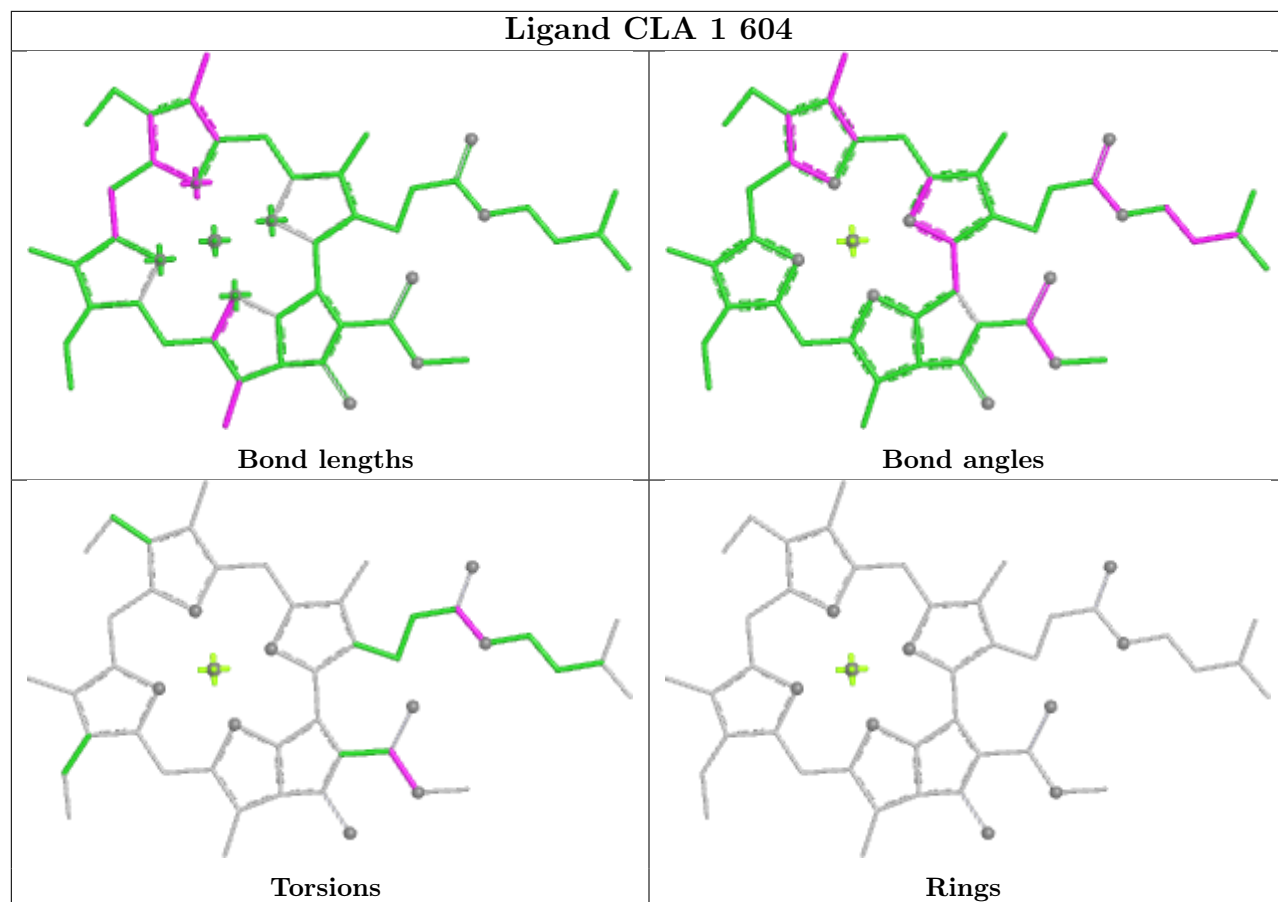
Ligand CLA 4 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 4011	
	
Bond lengths	Bond angles
	
Torsions	Rings

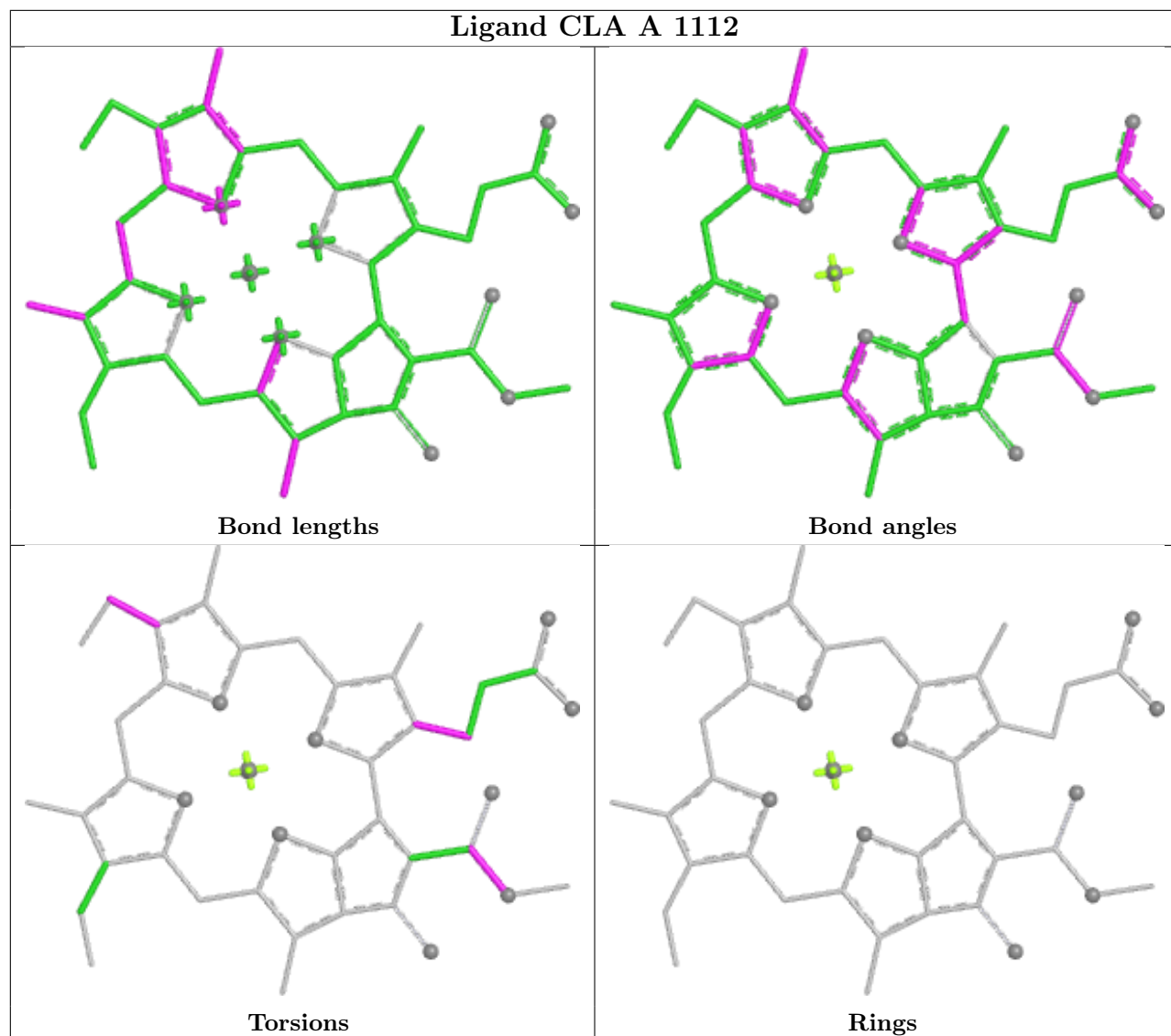
Ligand CLA A 1109	
	
Bond lengths	Bond angles
	
Torsions	Rings

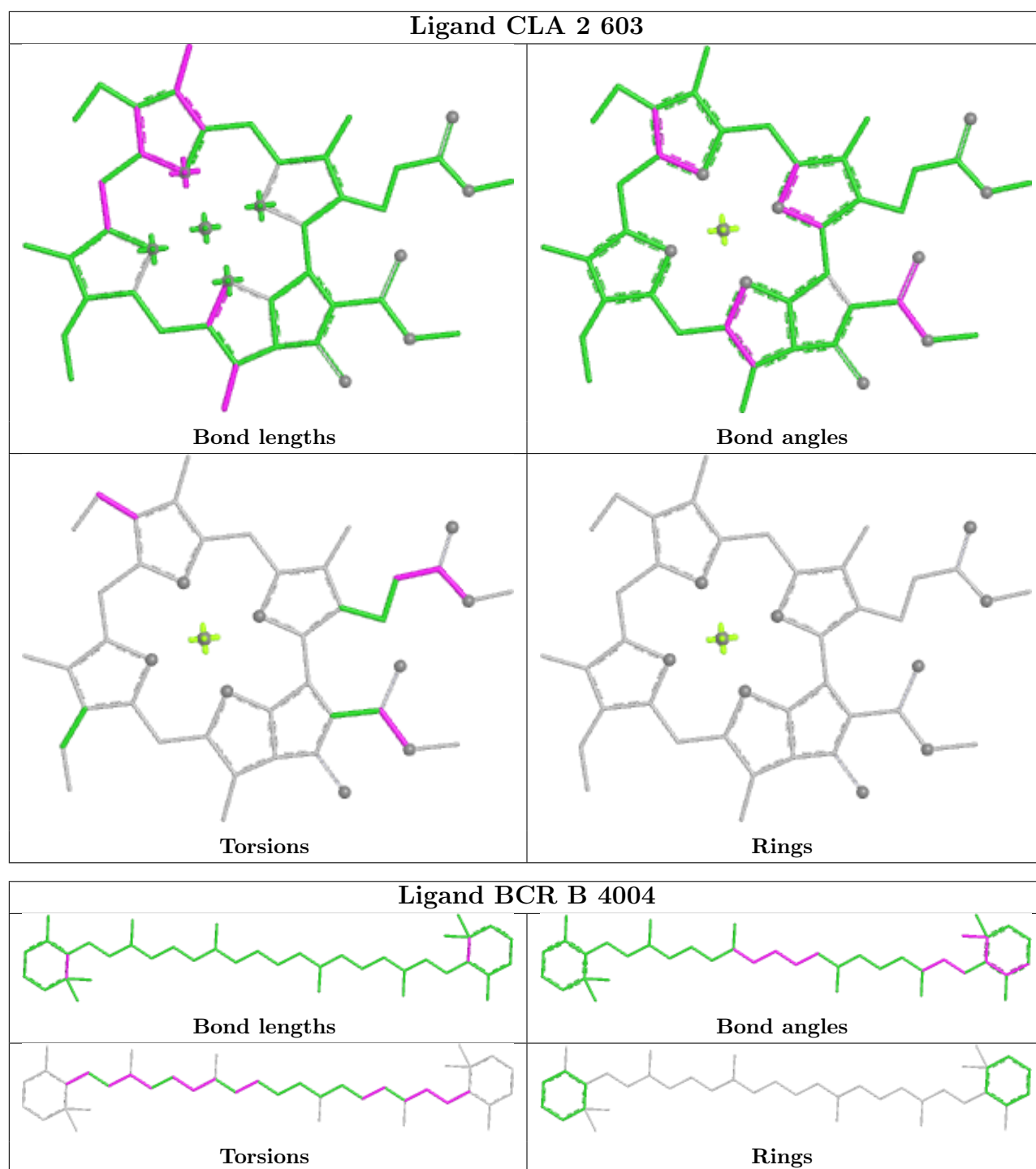


Ligand CLA 1 604

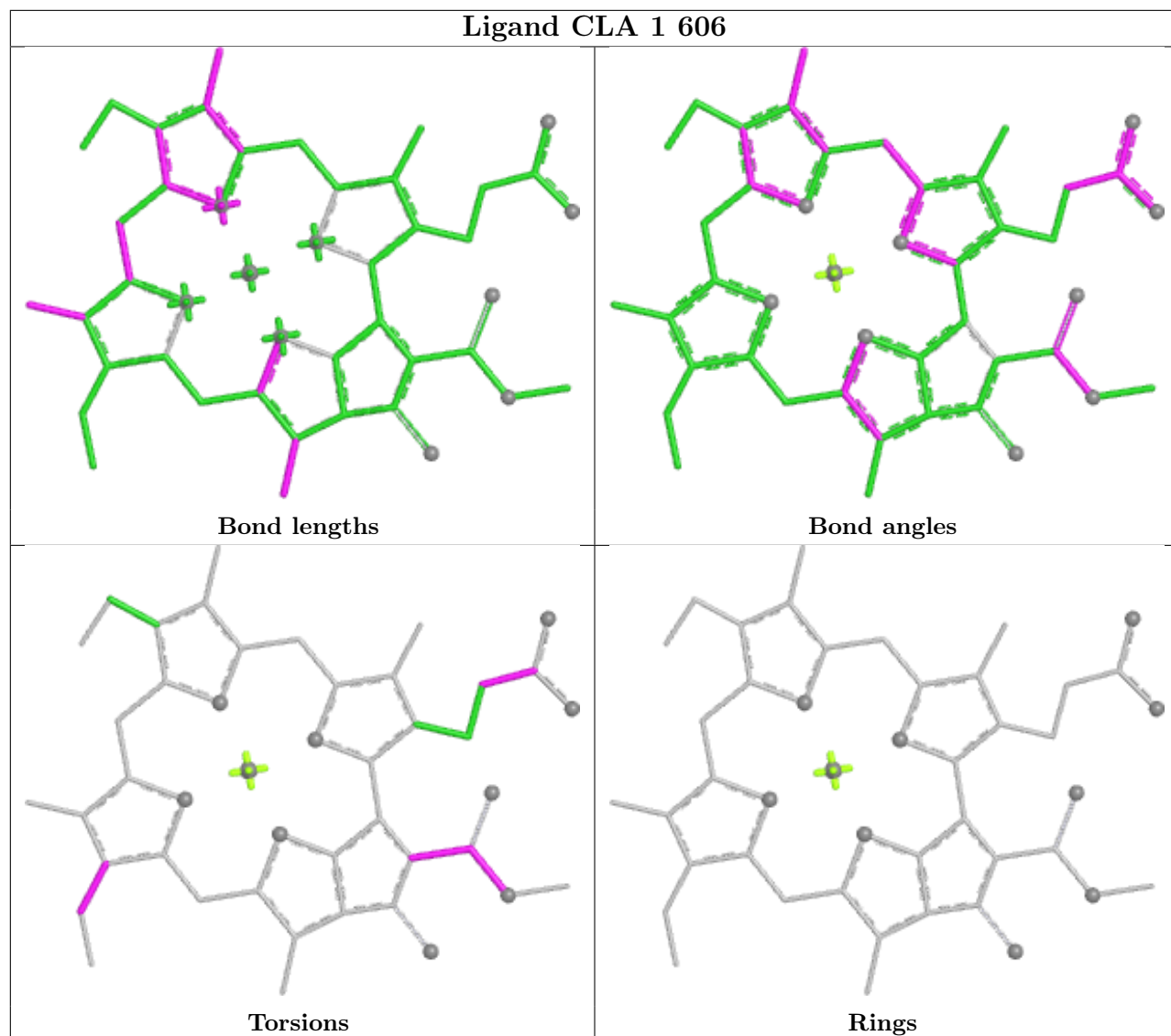


Ligand CLA A 1112

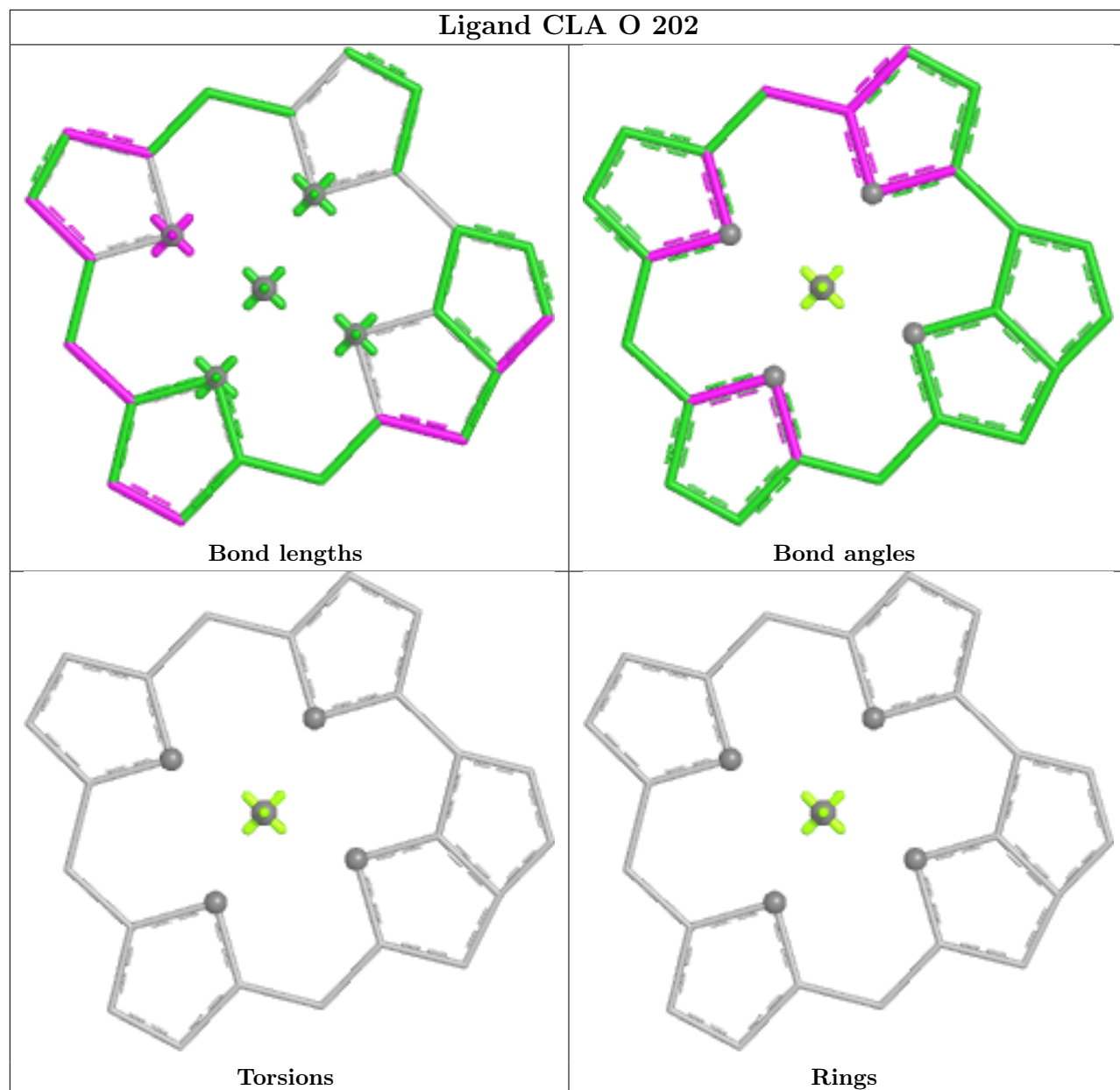


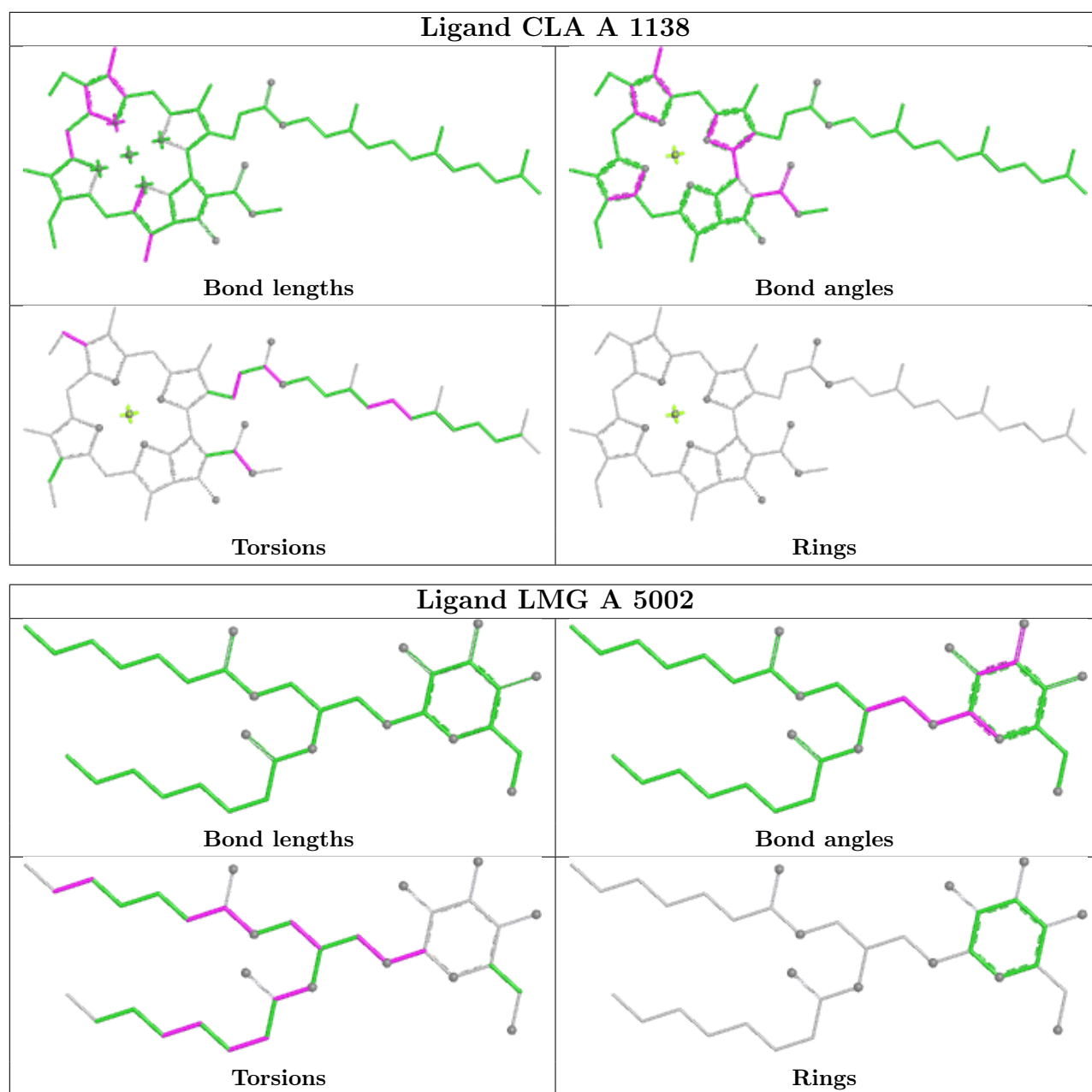


Ligand CLA 1 606

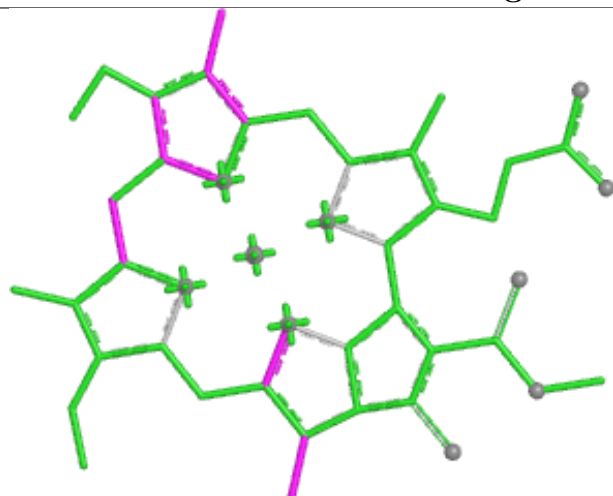


Ligand CLA O 202

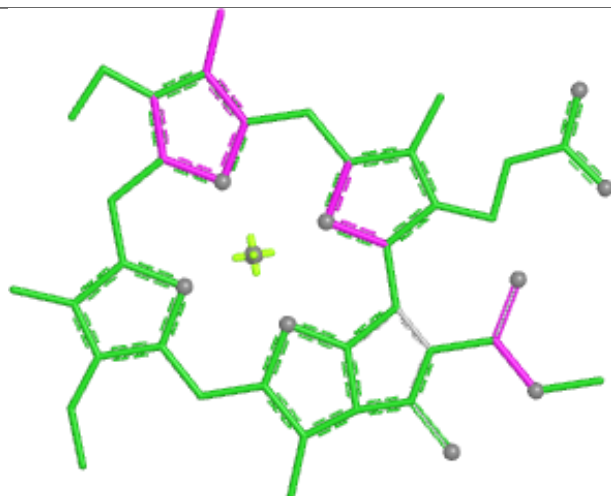




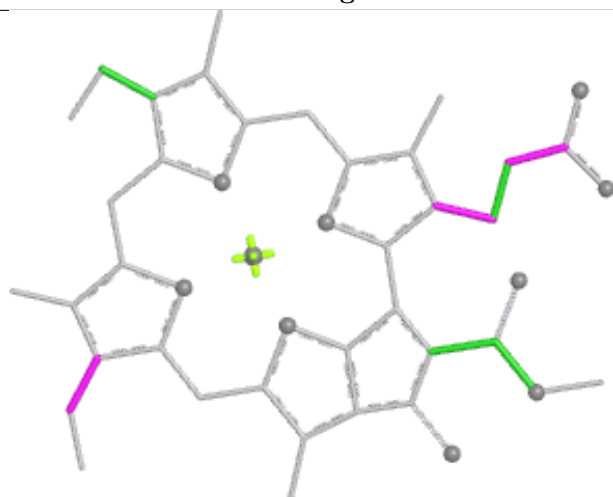
Ligand CLA A 1137



Bond lengths



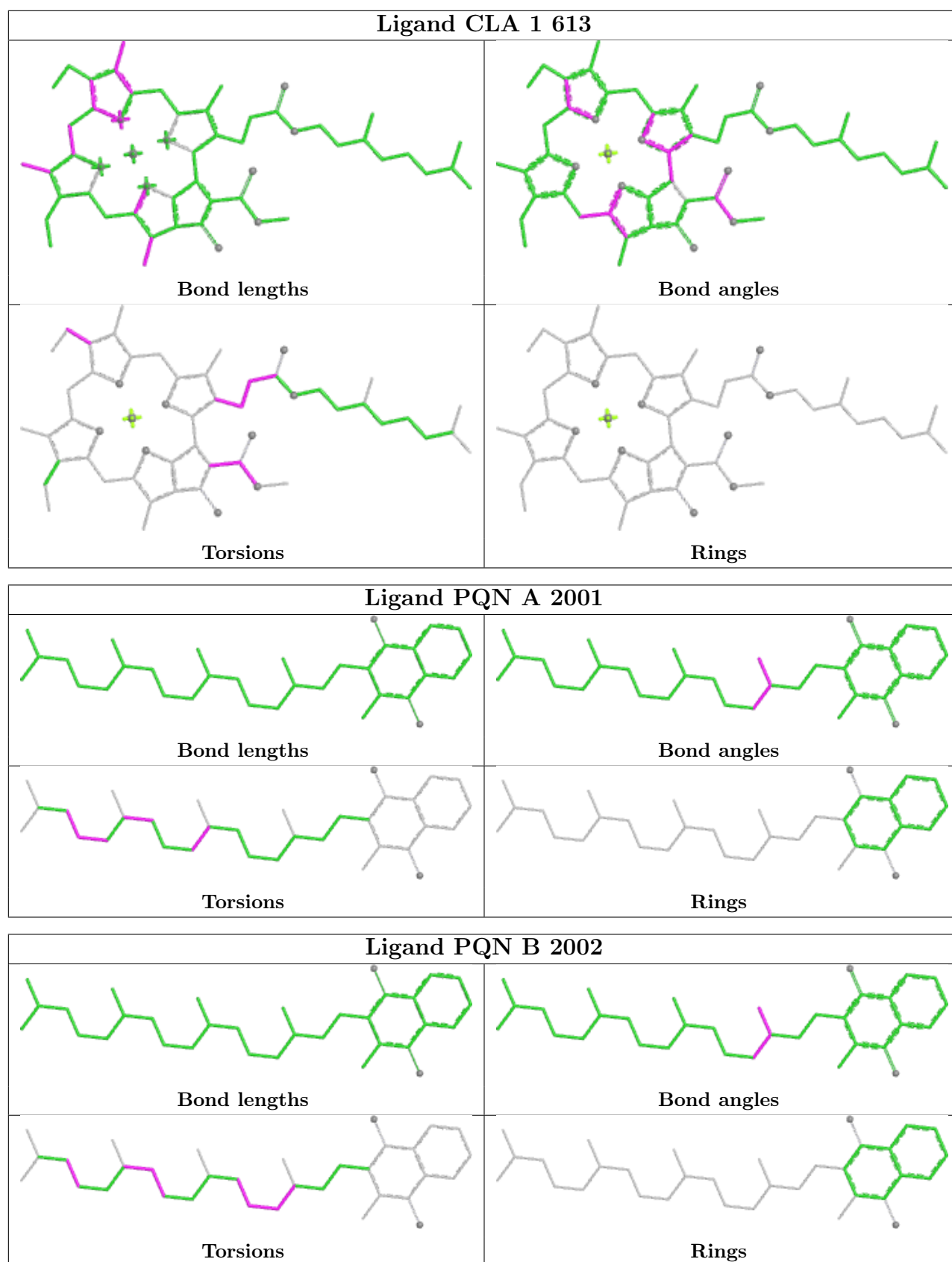
Bond angles

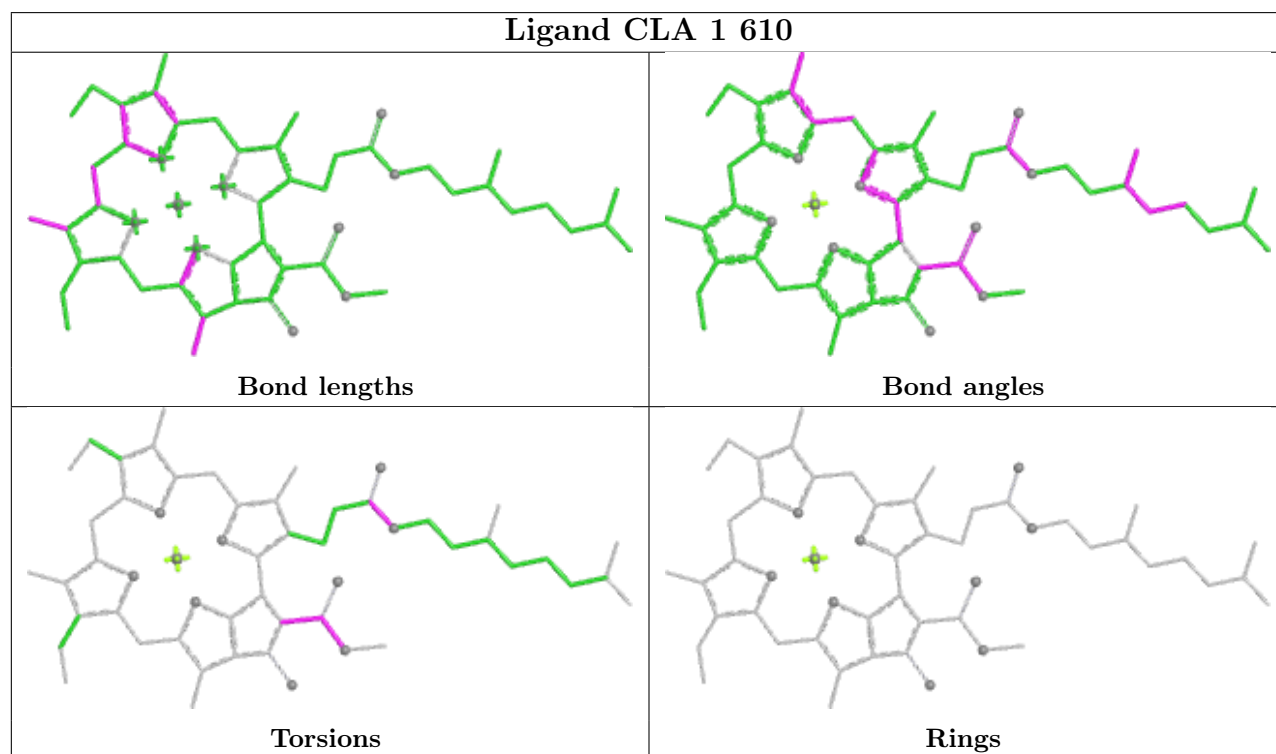
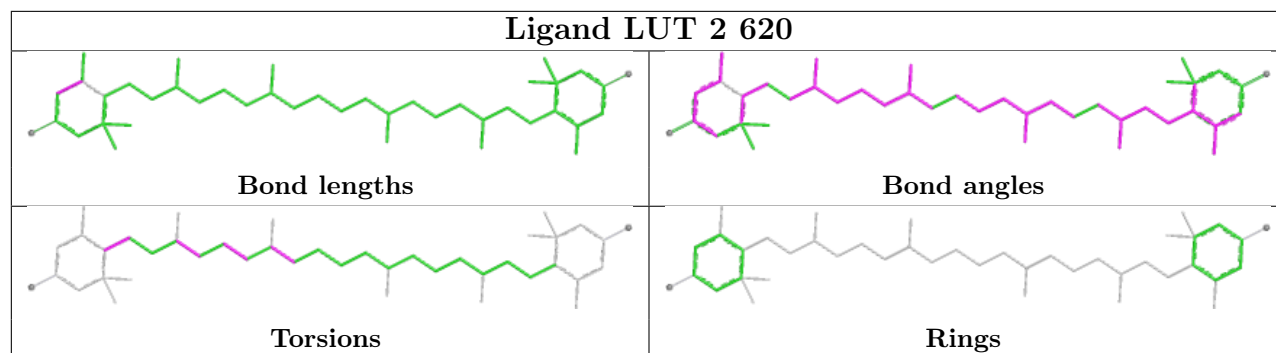


Torsions

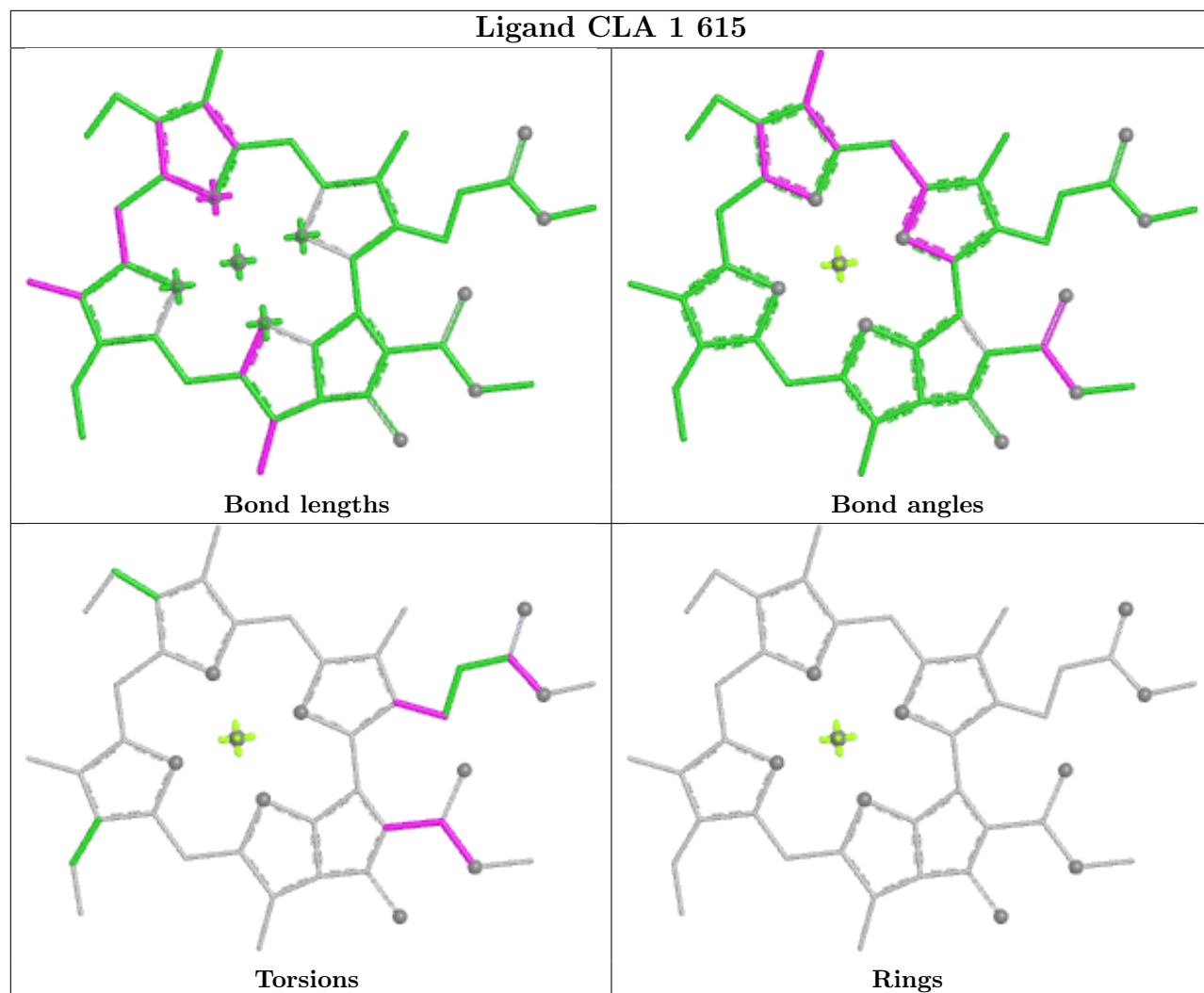


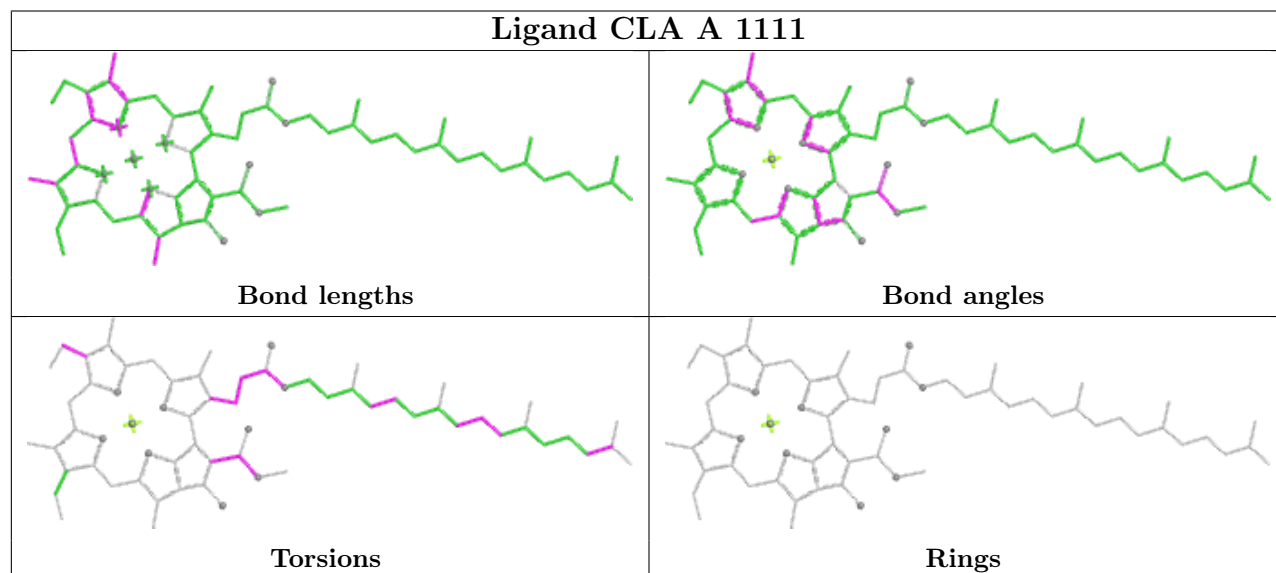
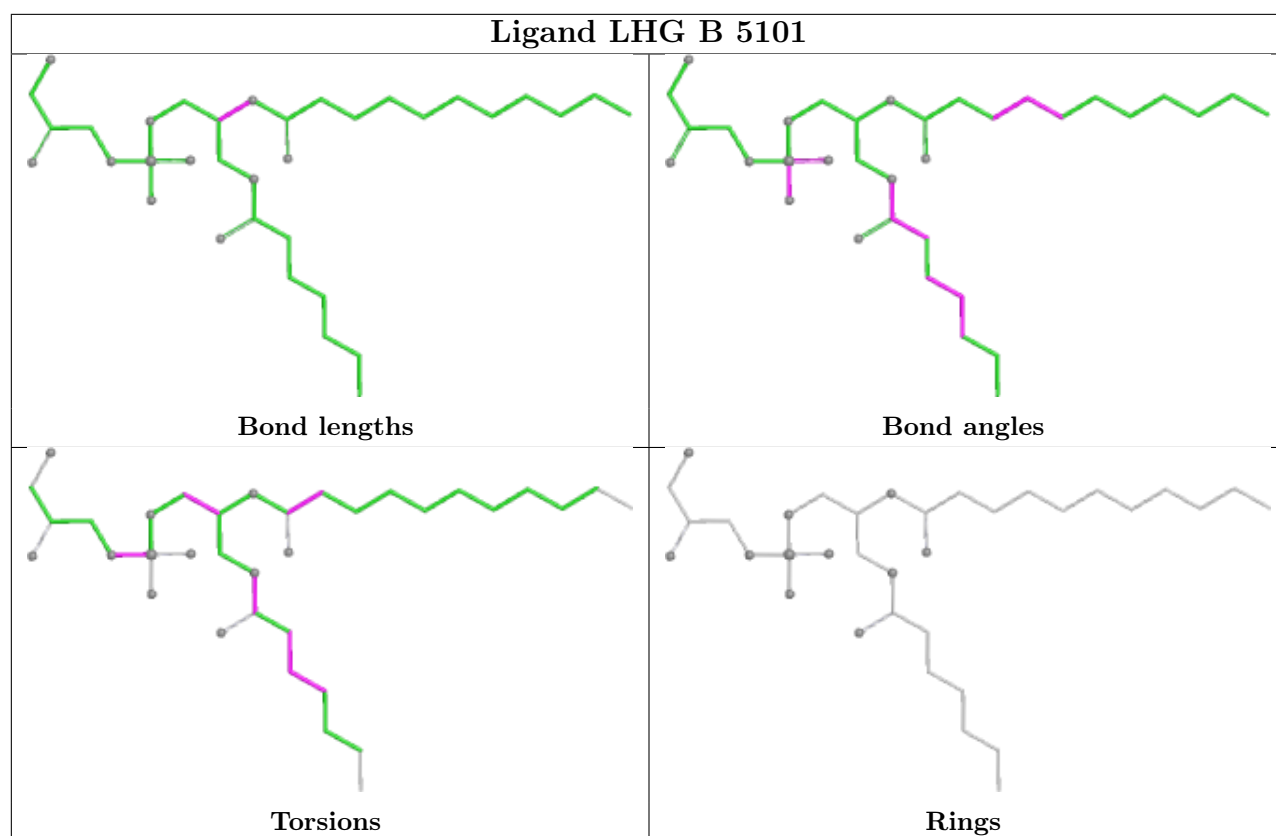
Rings



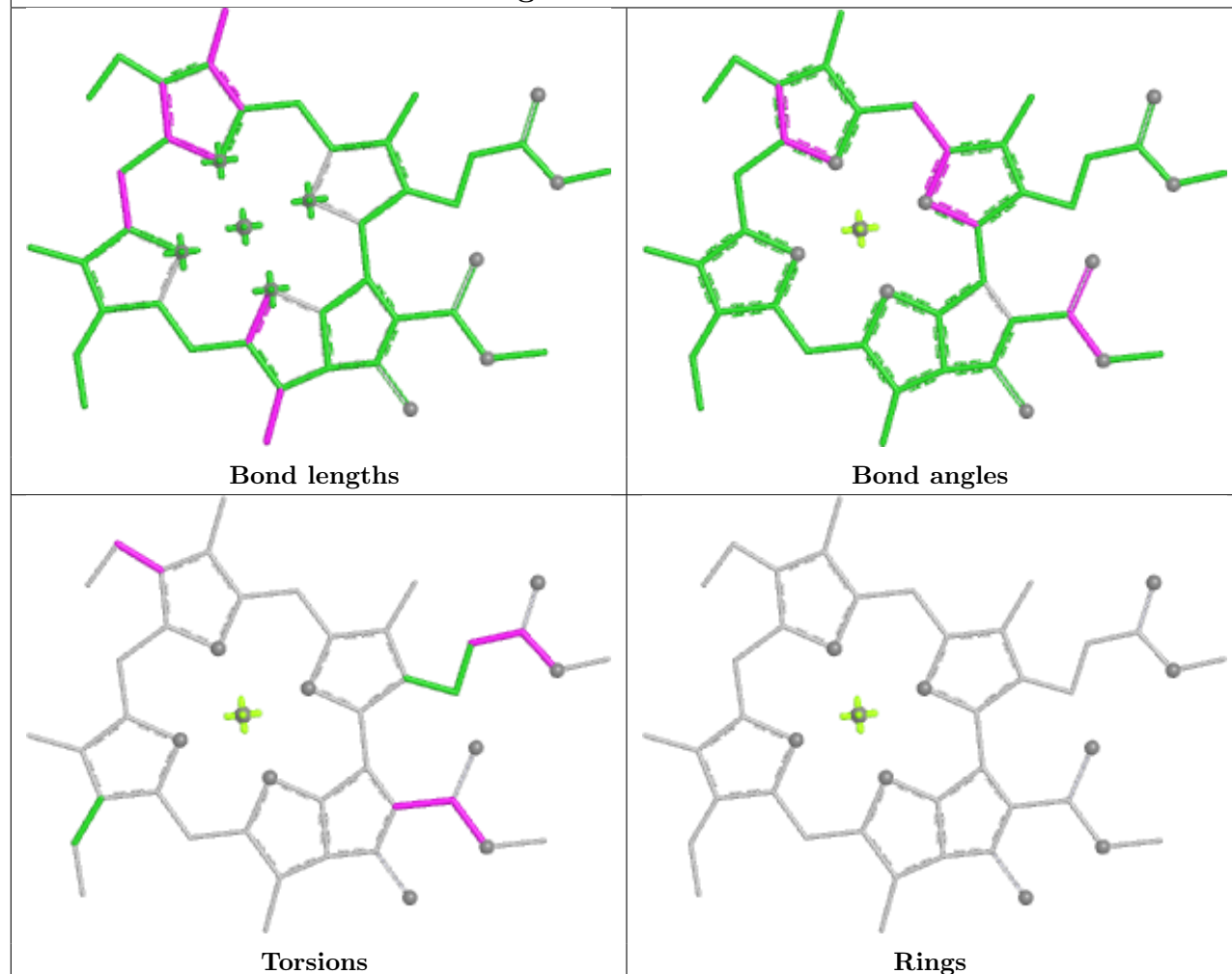


Ligand CLA 1 615

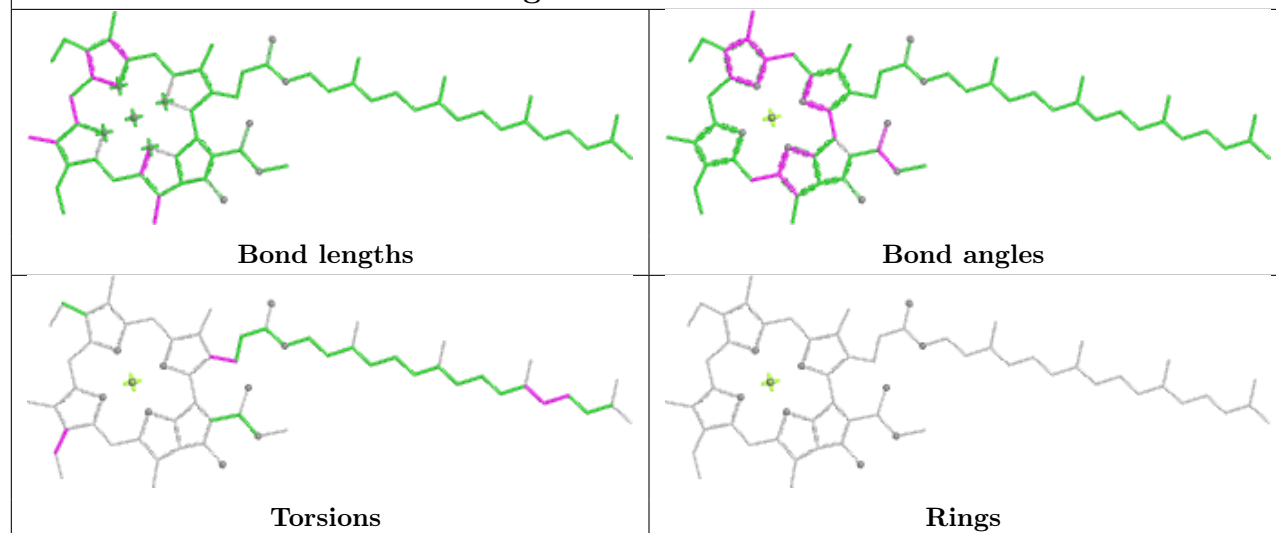


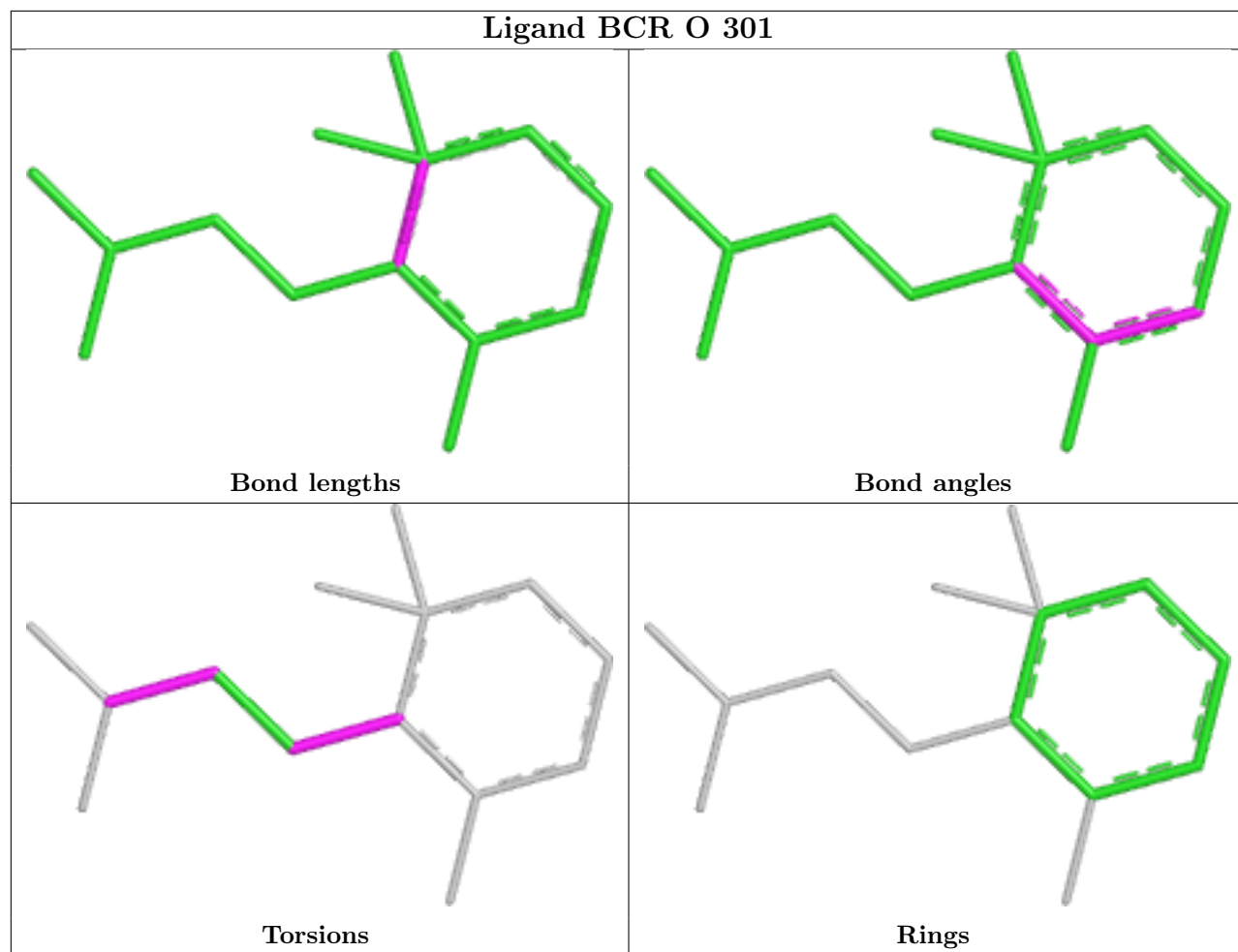


Ligand CLA 4 612

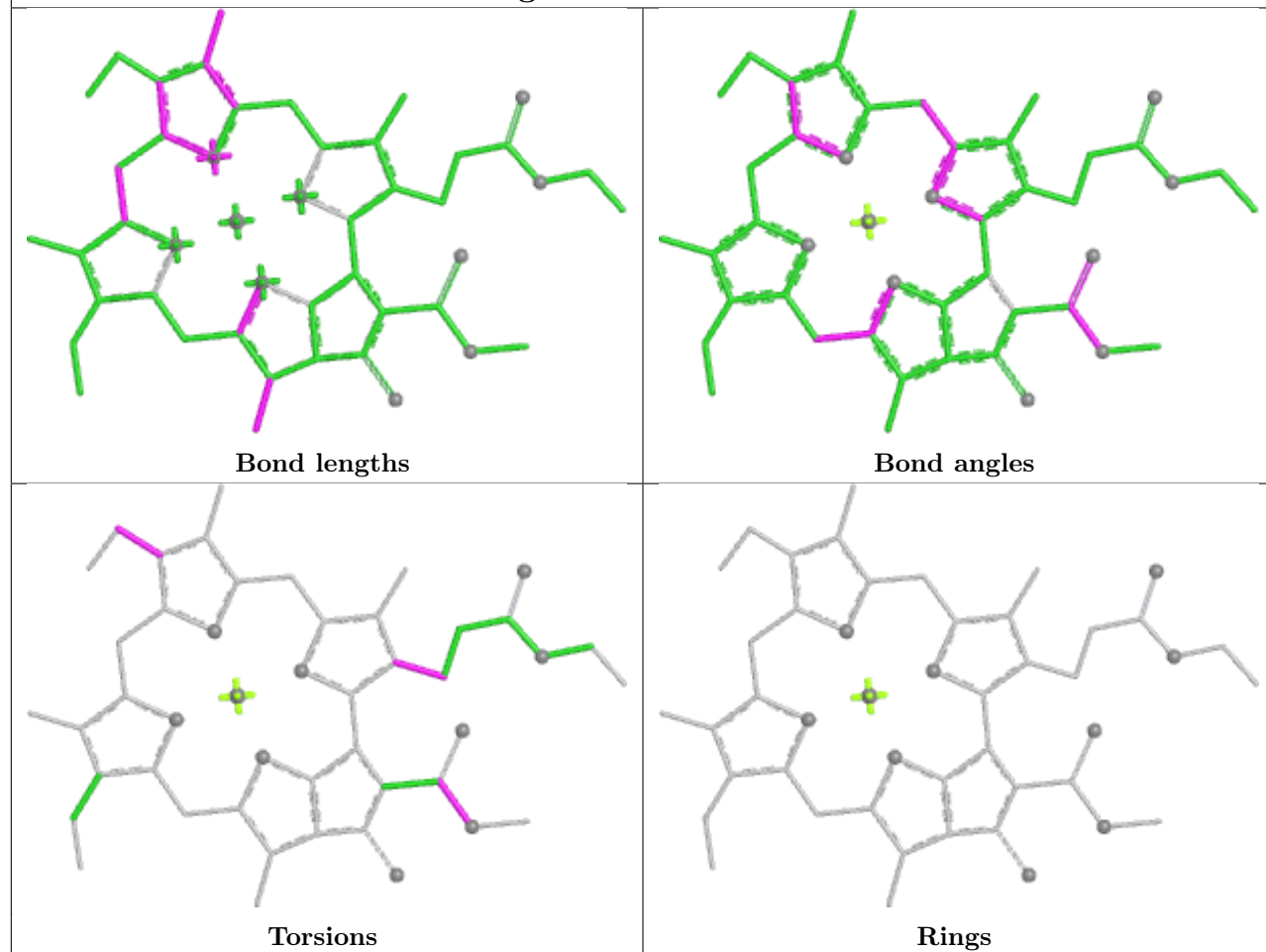


Ligand CLA B 1223

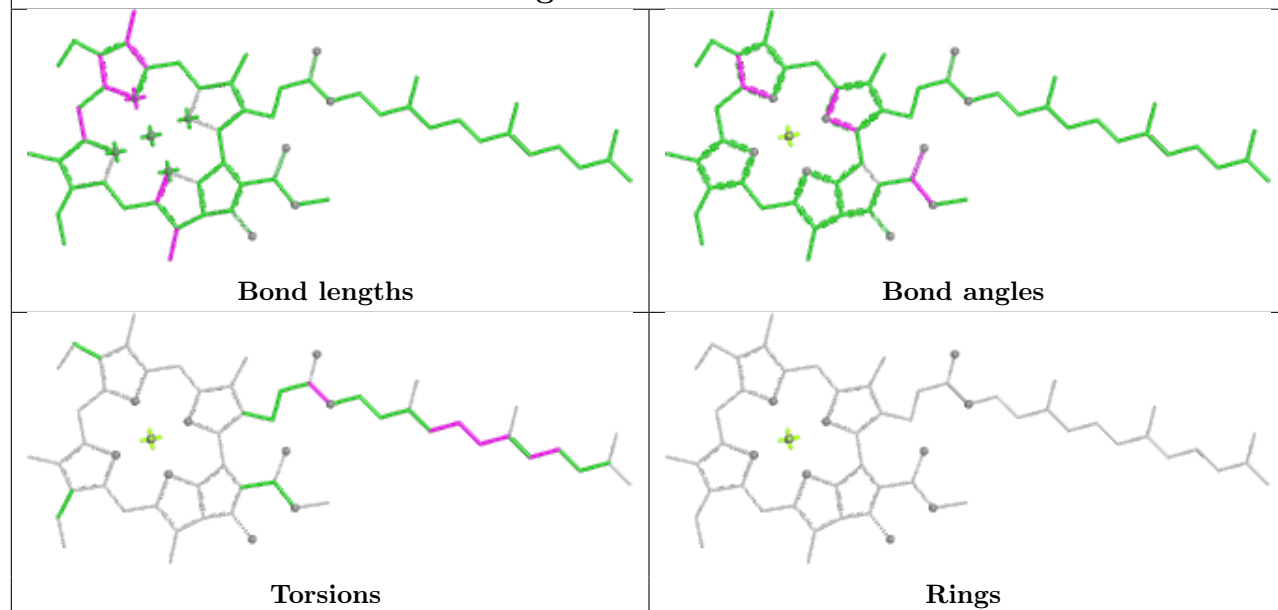




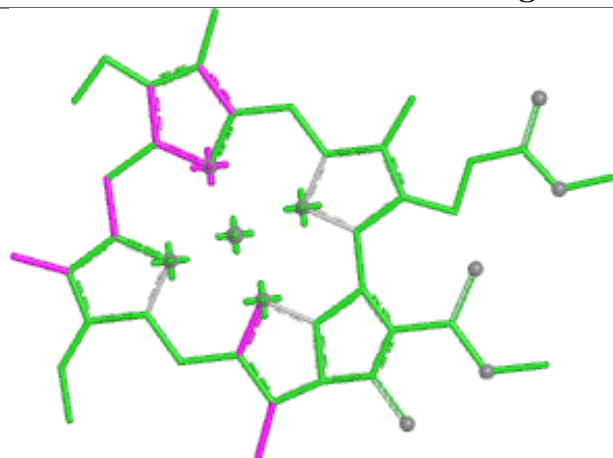
Ligand CLA B 1236



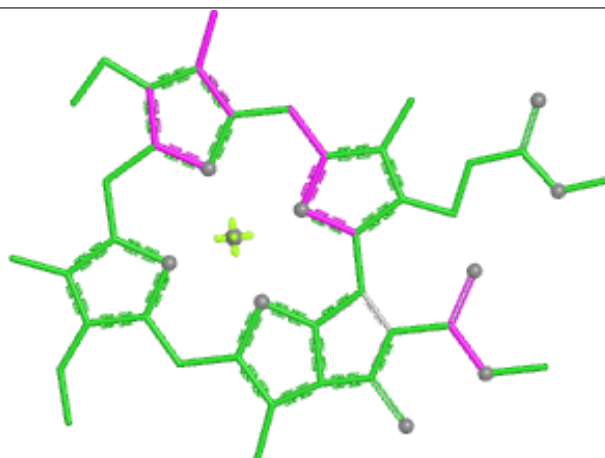
Ligand CLA 1 609



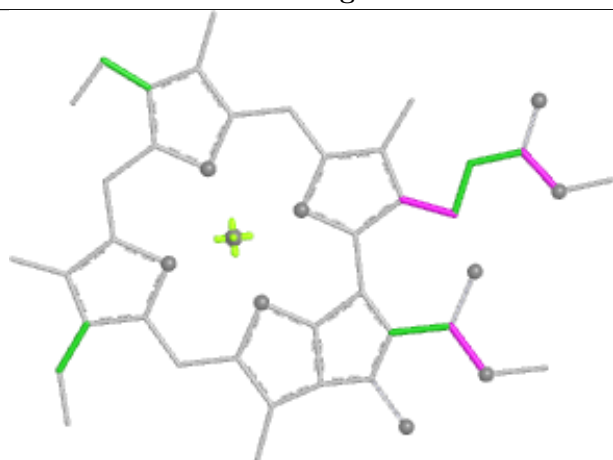
Ligand CLA 3 617



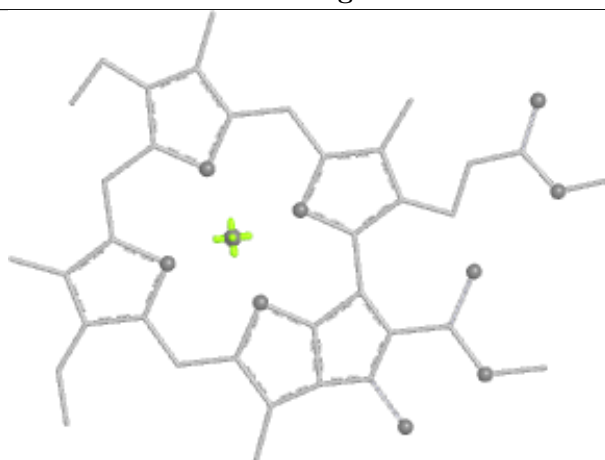
Bond lengths



Bond angles

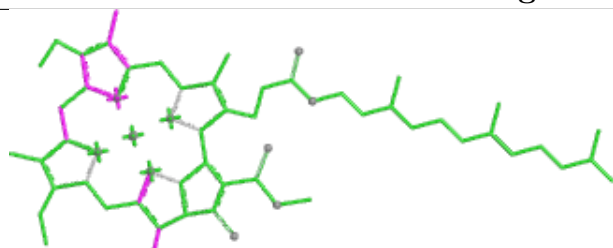


Torsions

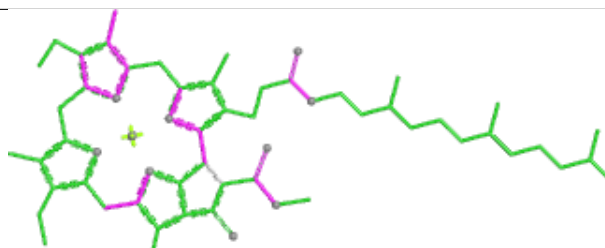


Rings

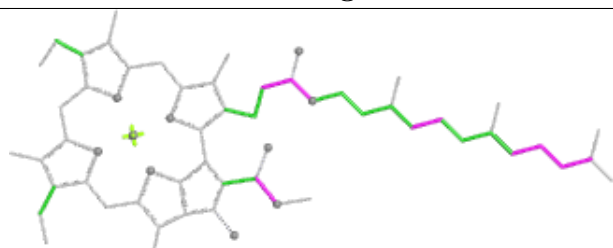
Ligand CLA 3 609



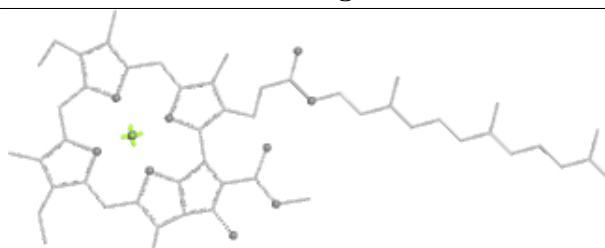
Bond lengths



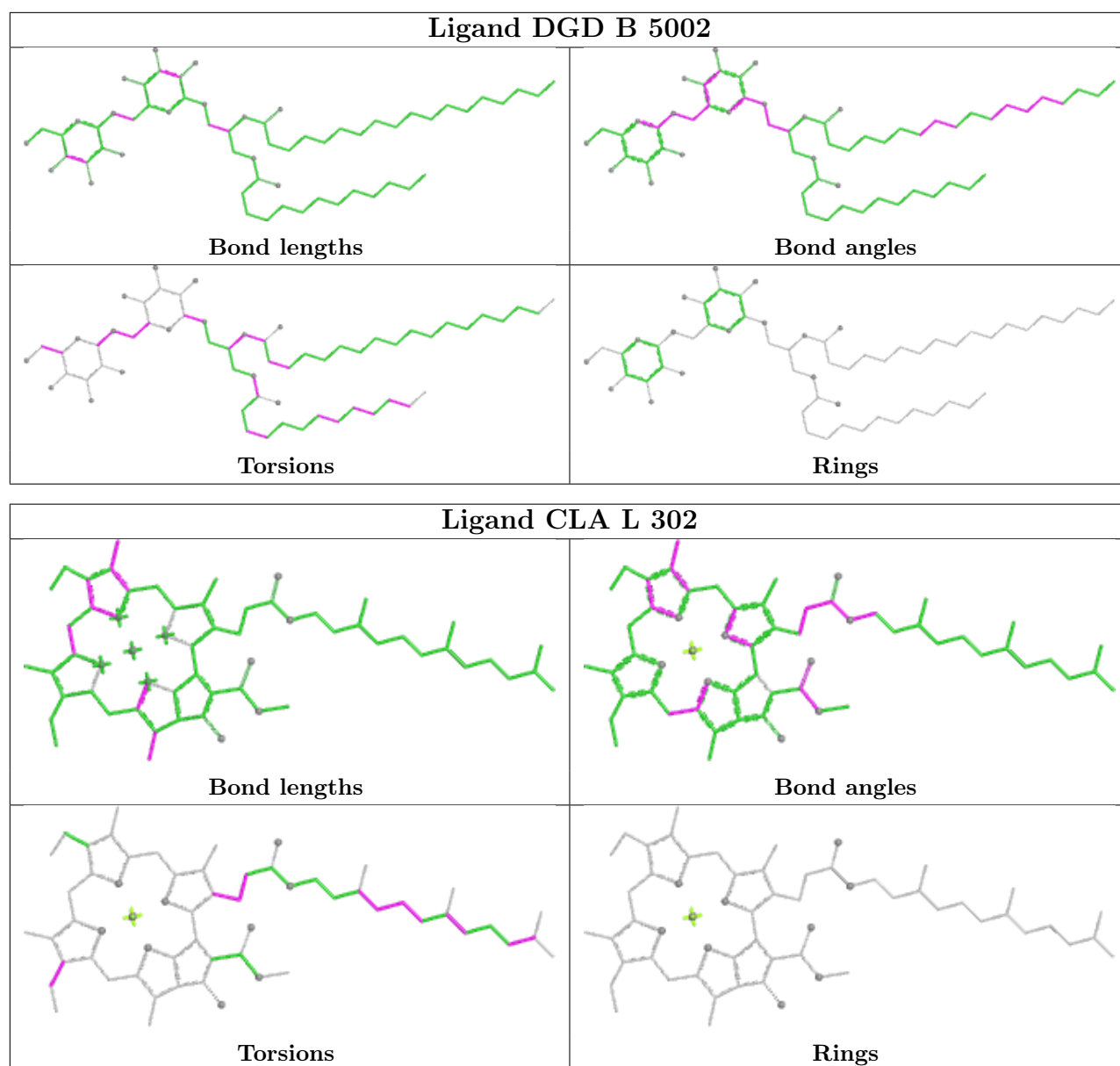
Bond angles



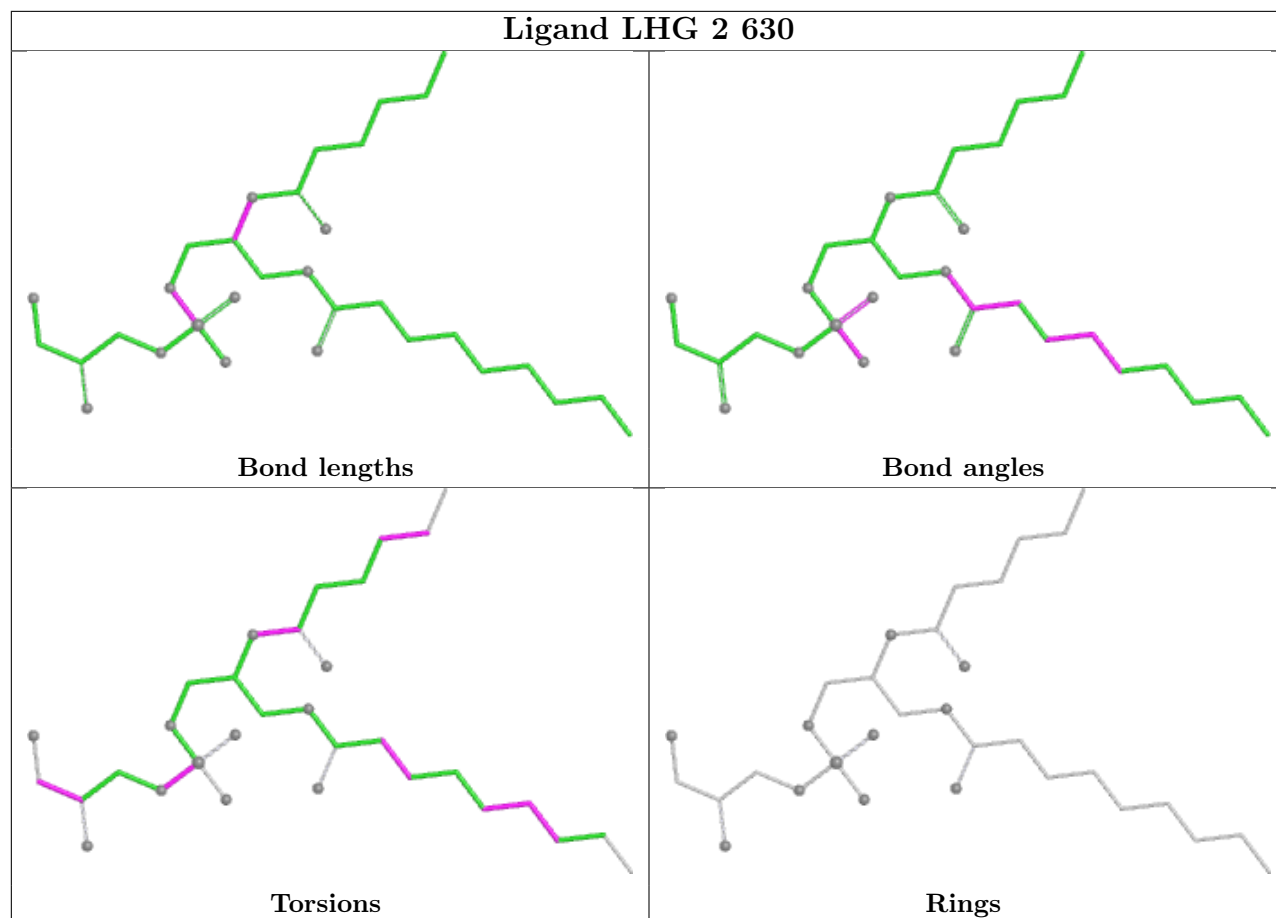
Torsions



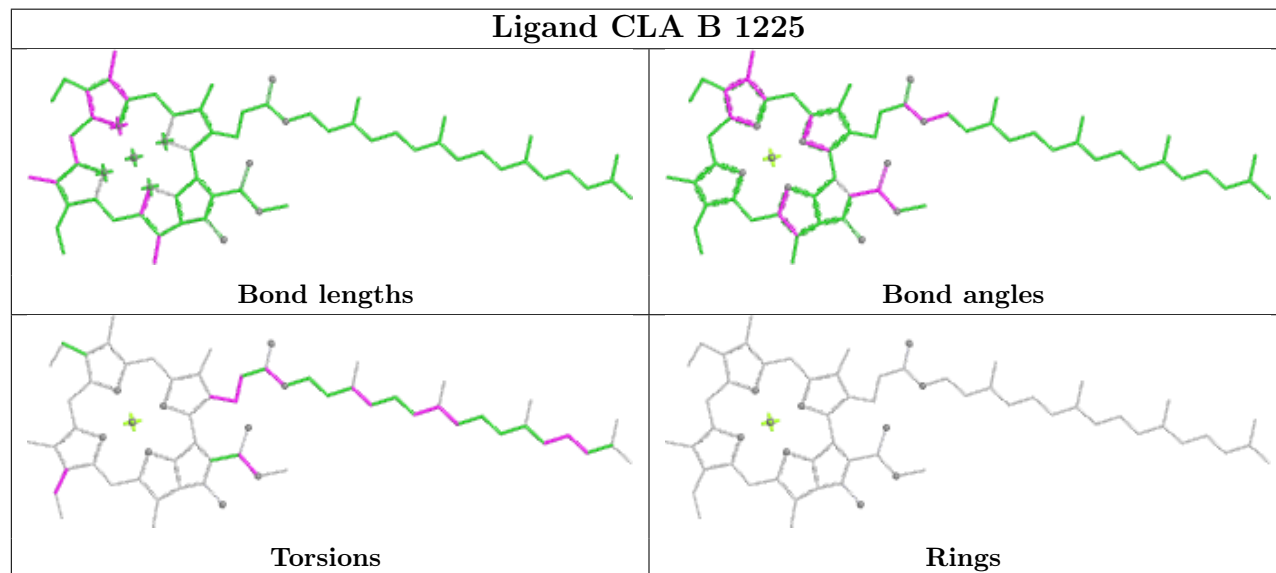
Rings

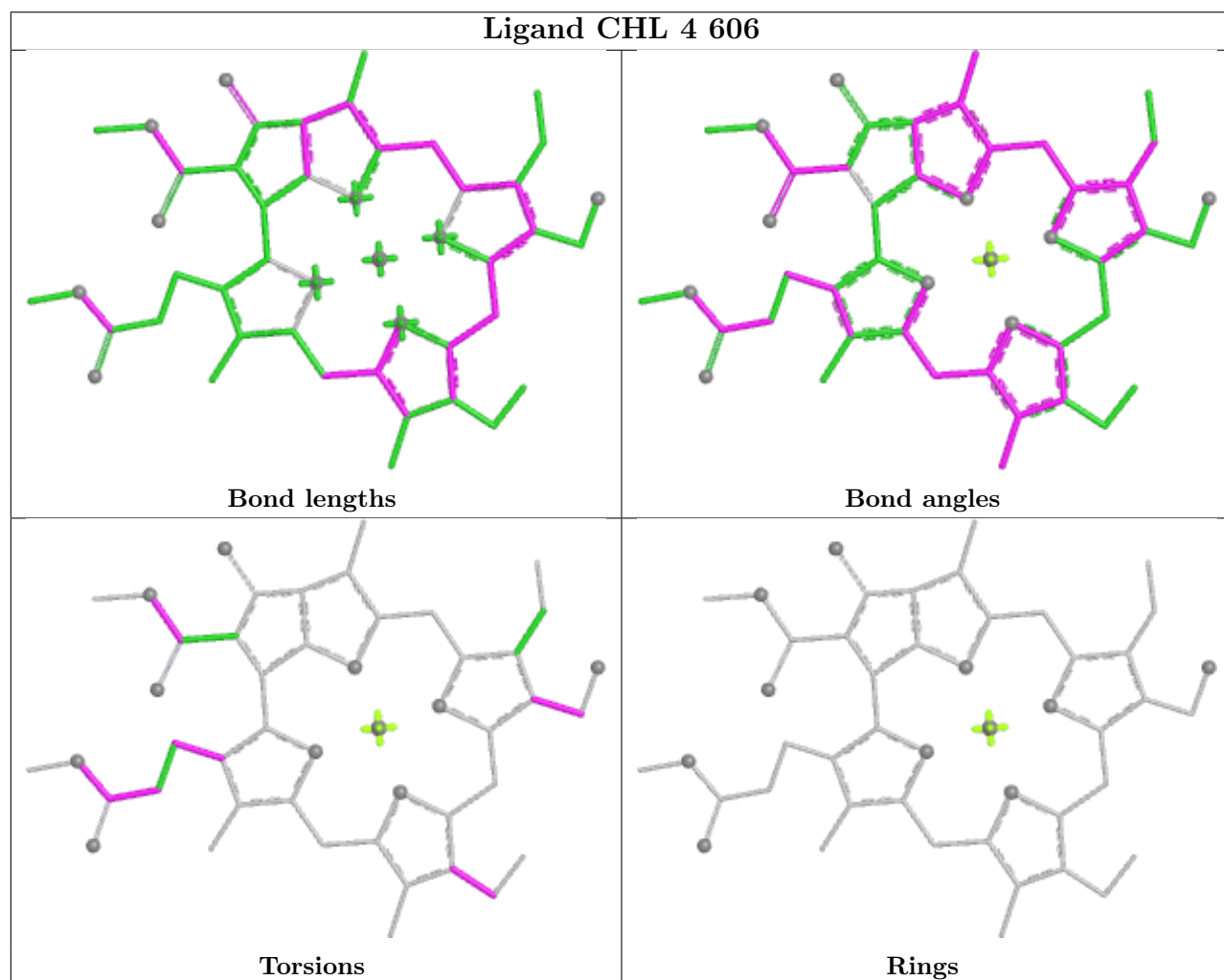
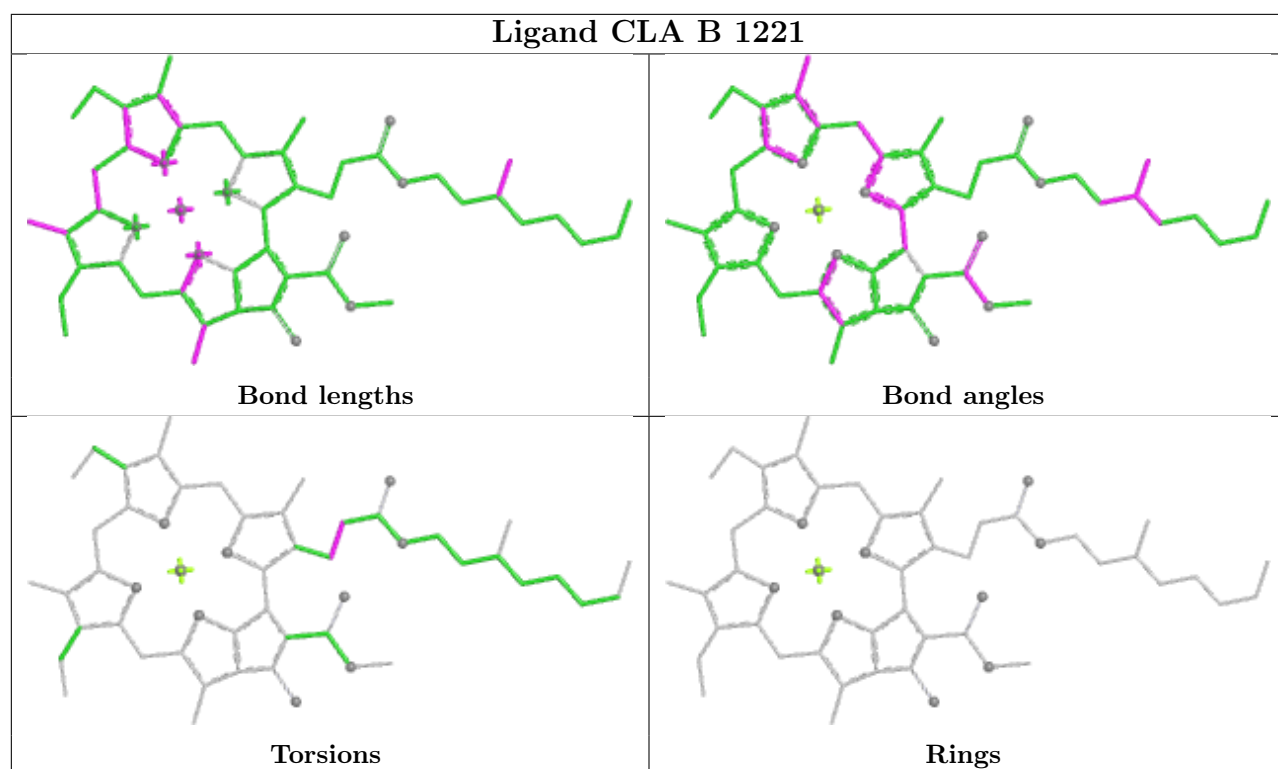


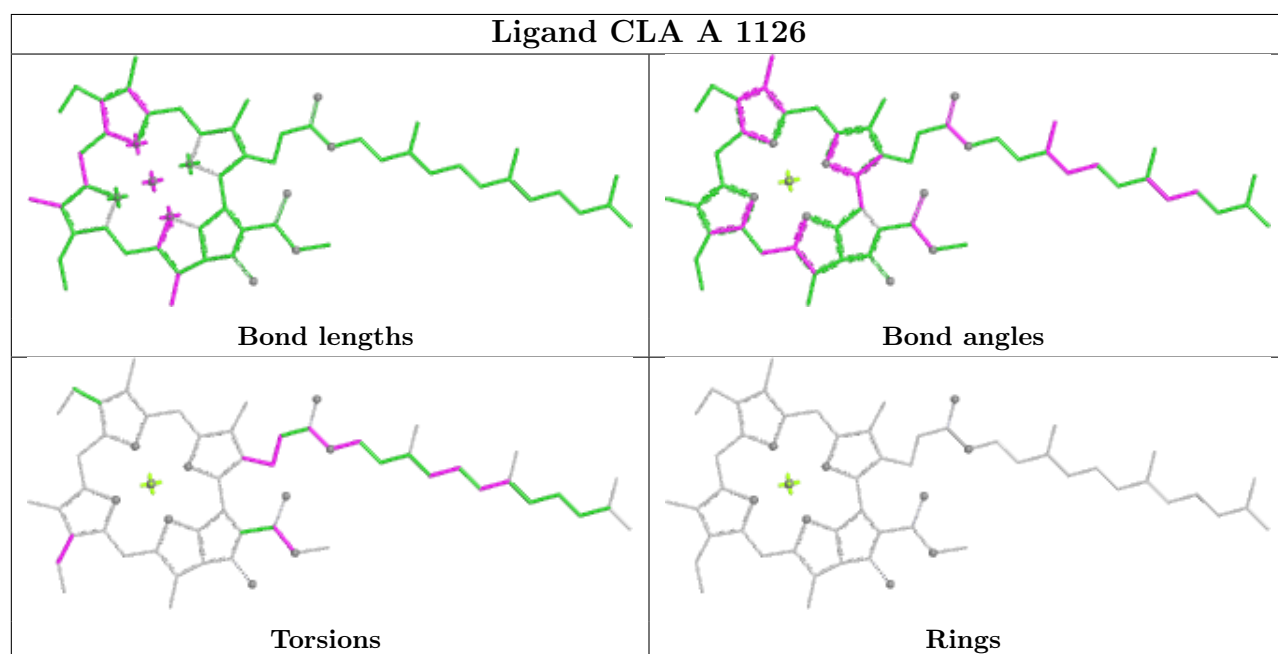
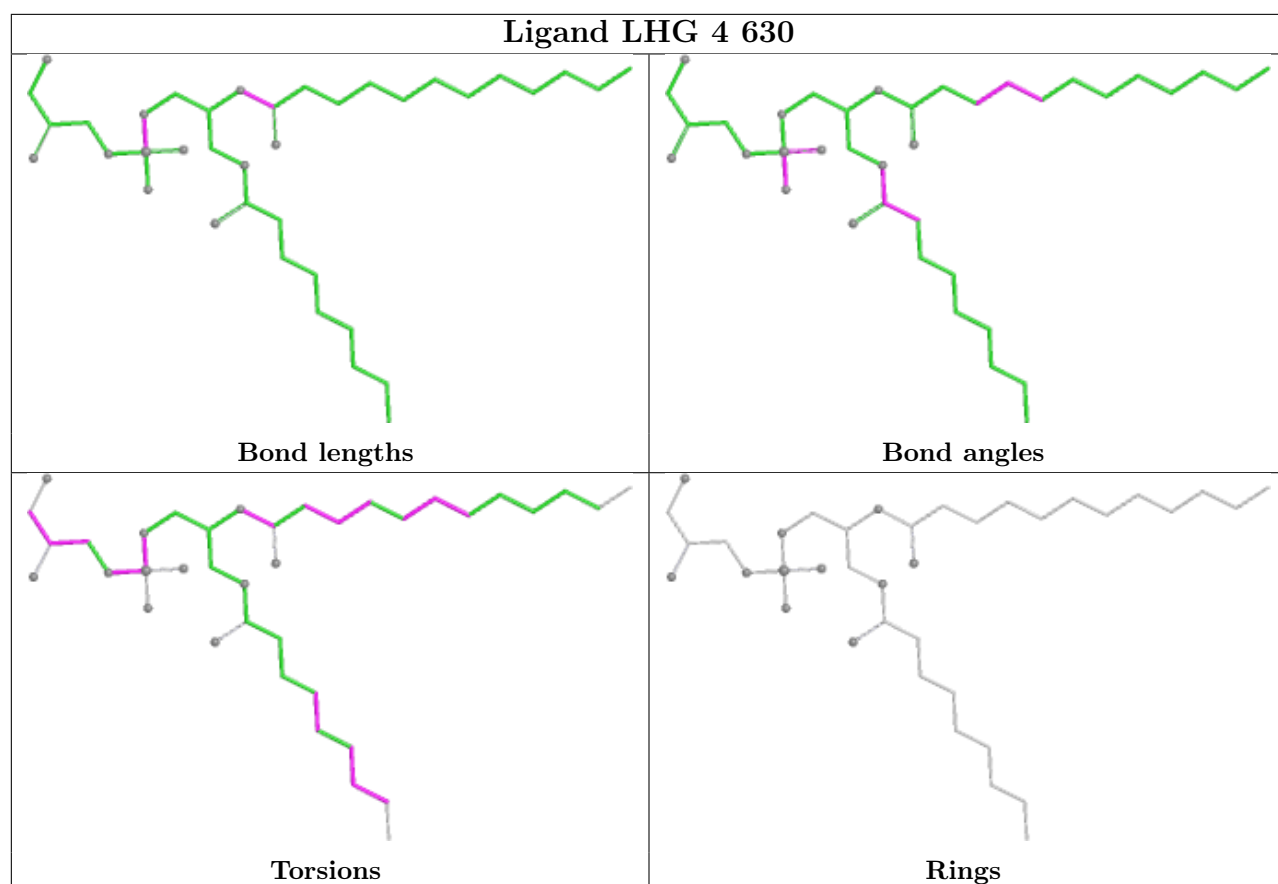
Ligand LHG 2 630

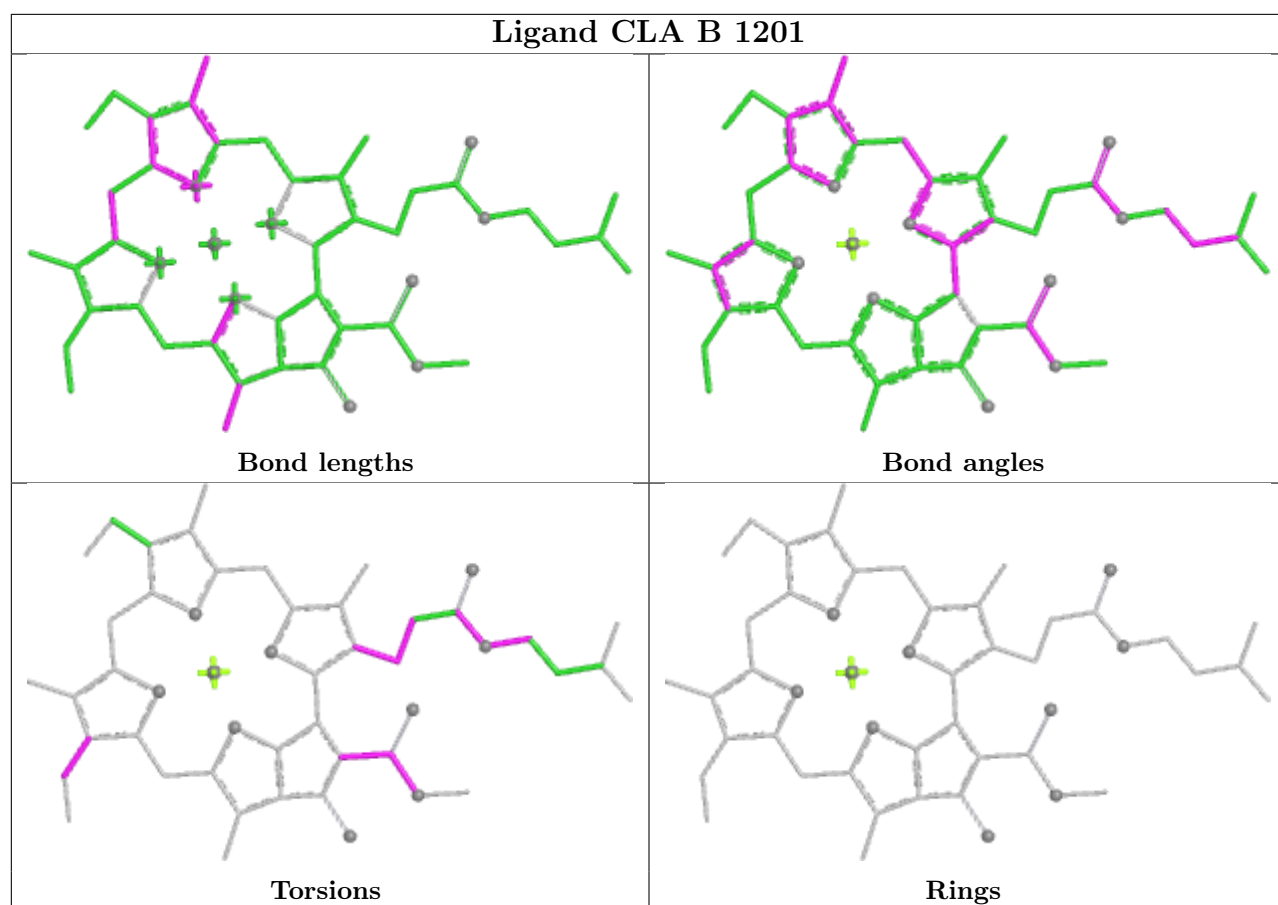


Ligand CLA B 1225

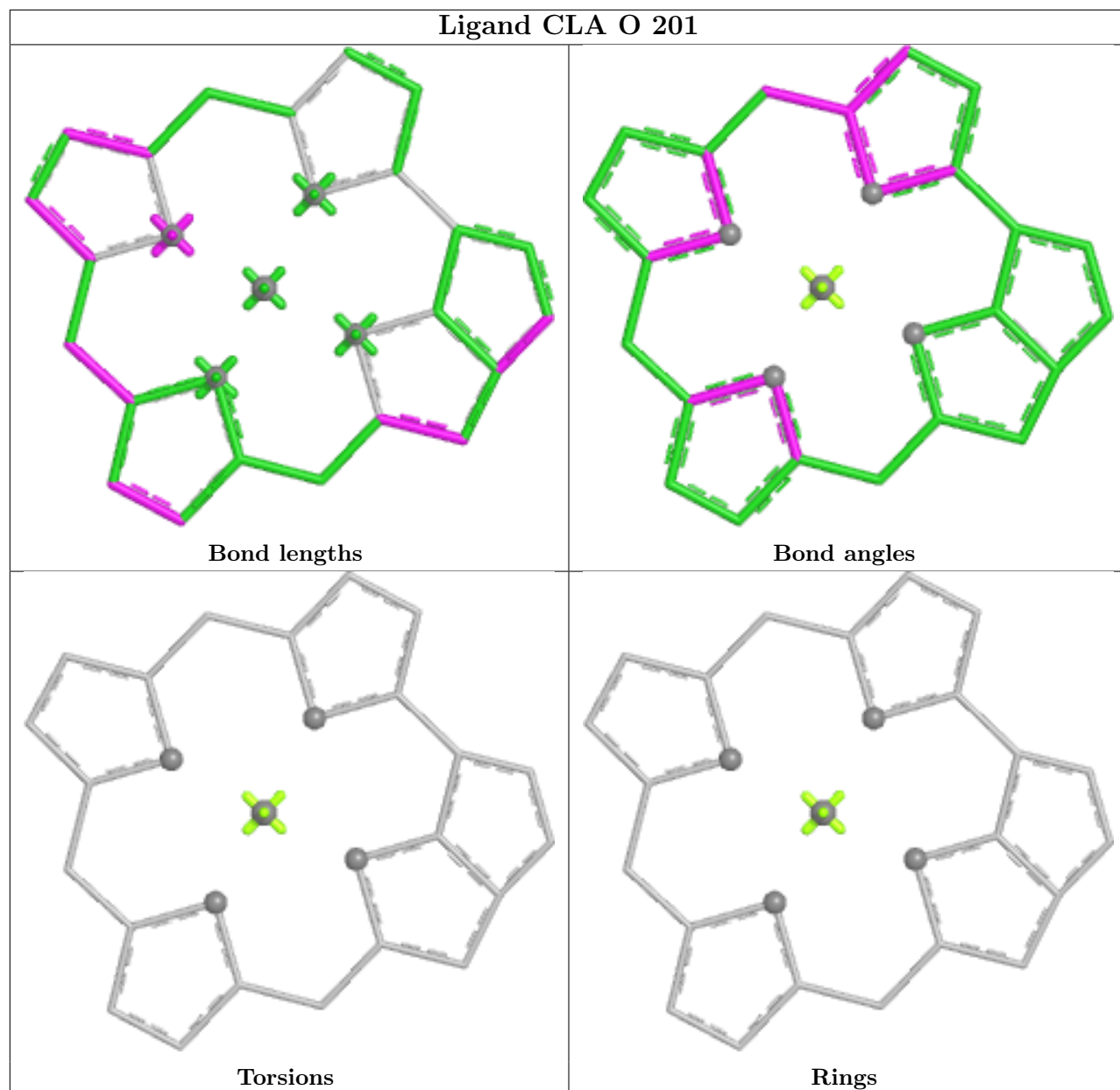


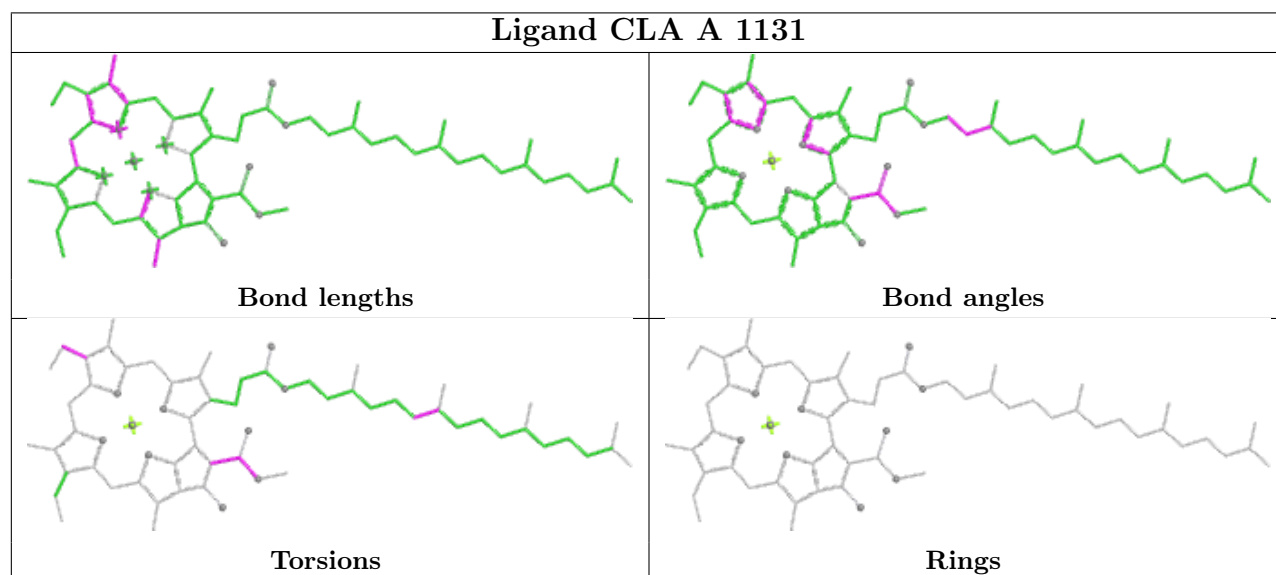
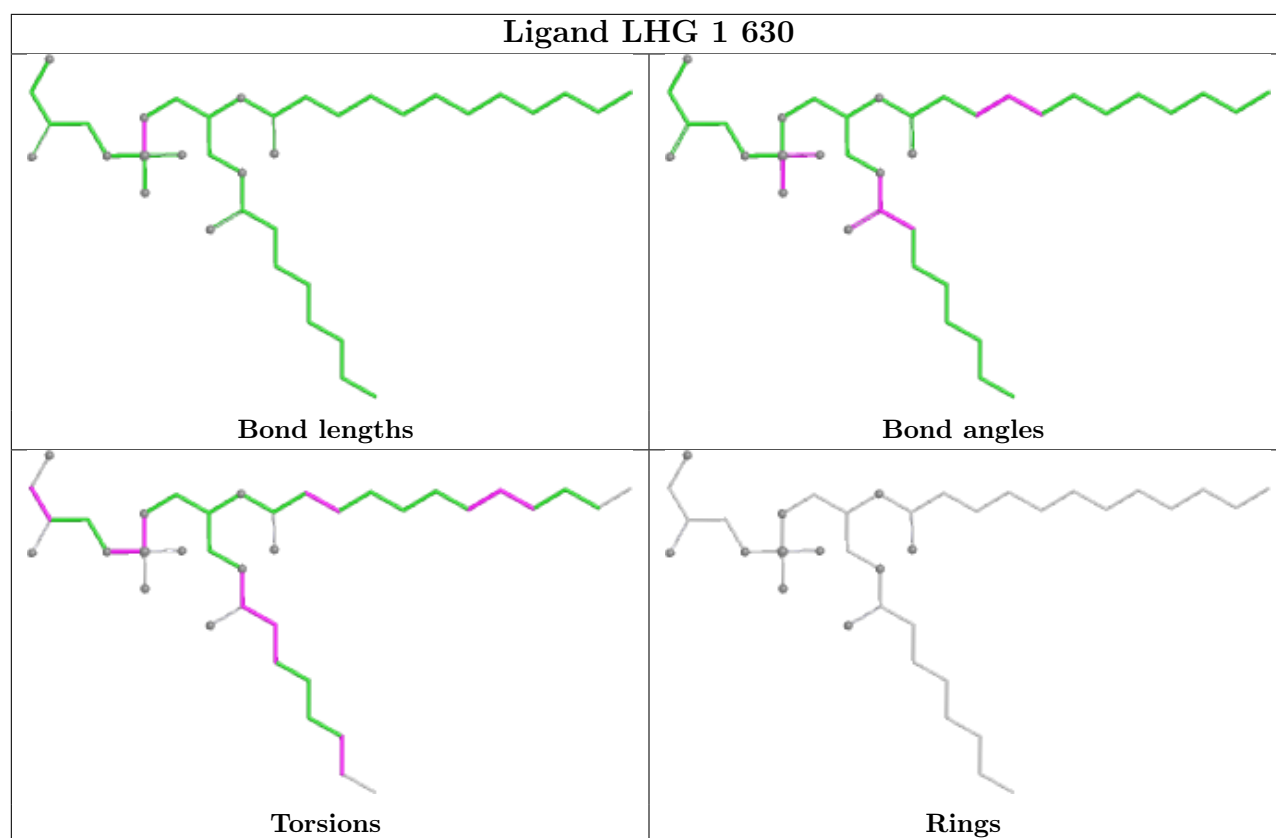


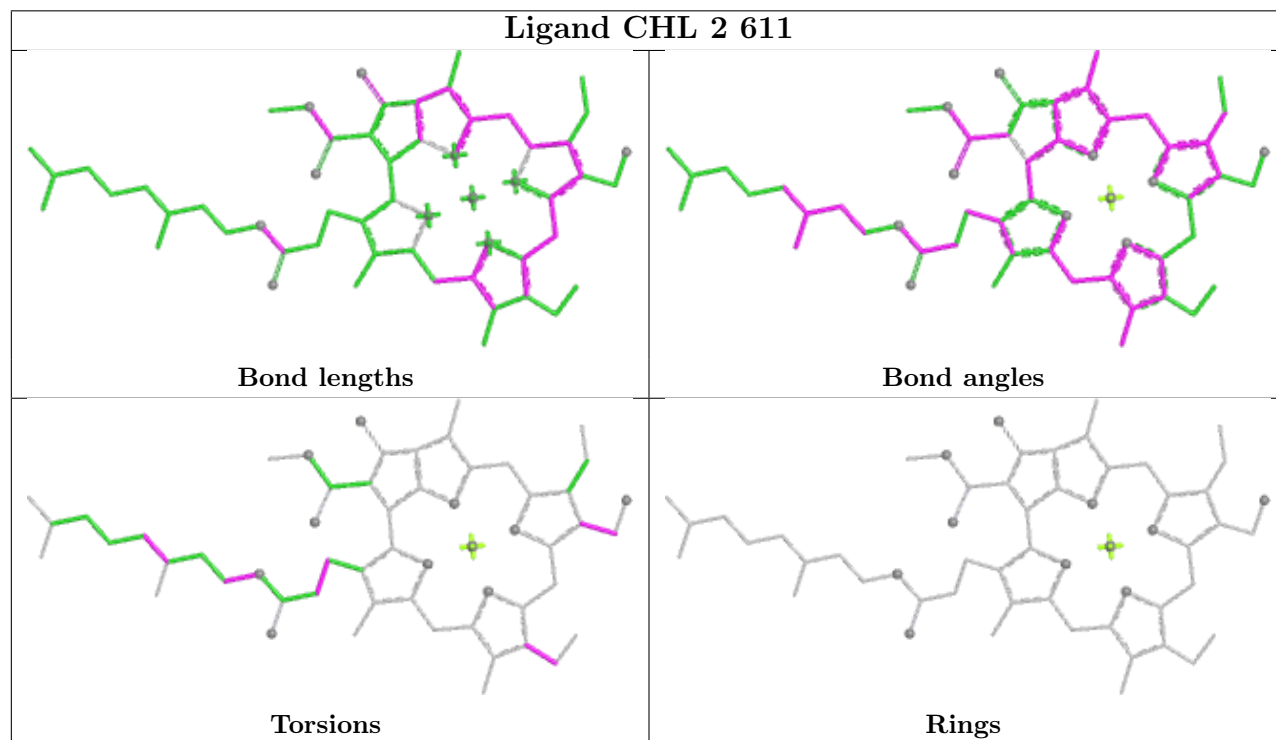
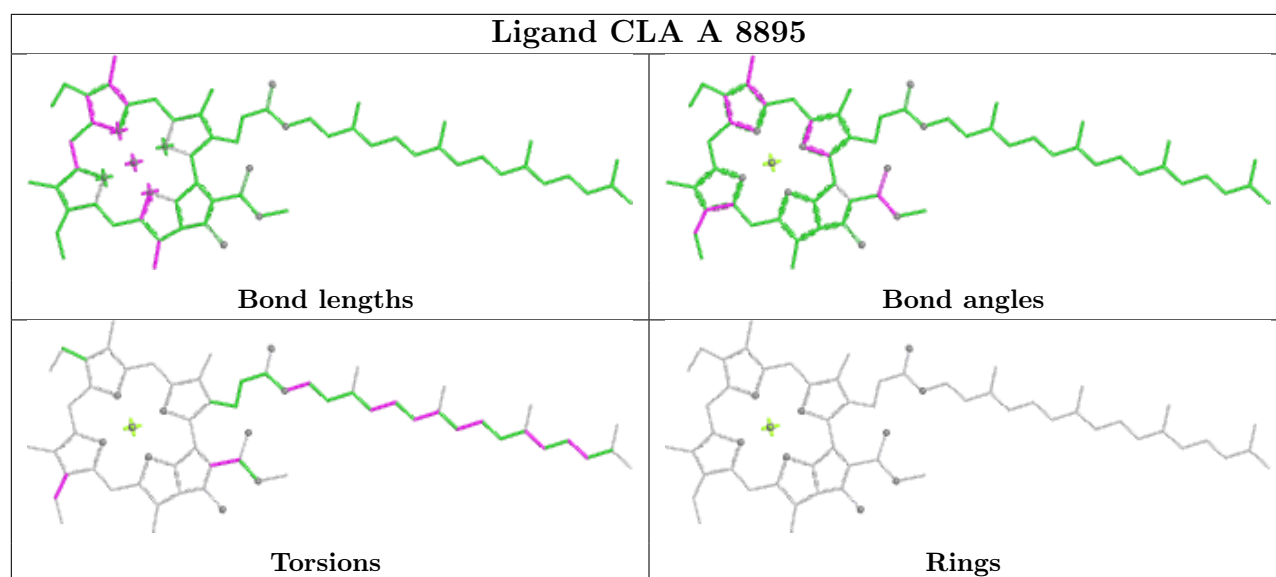


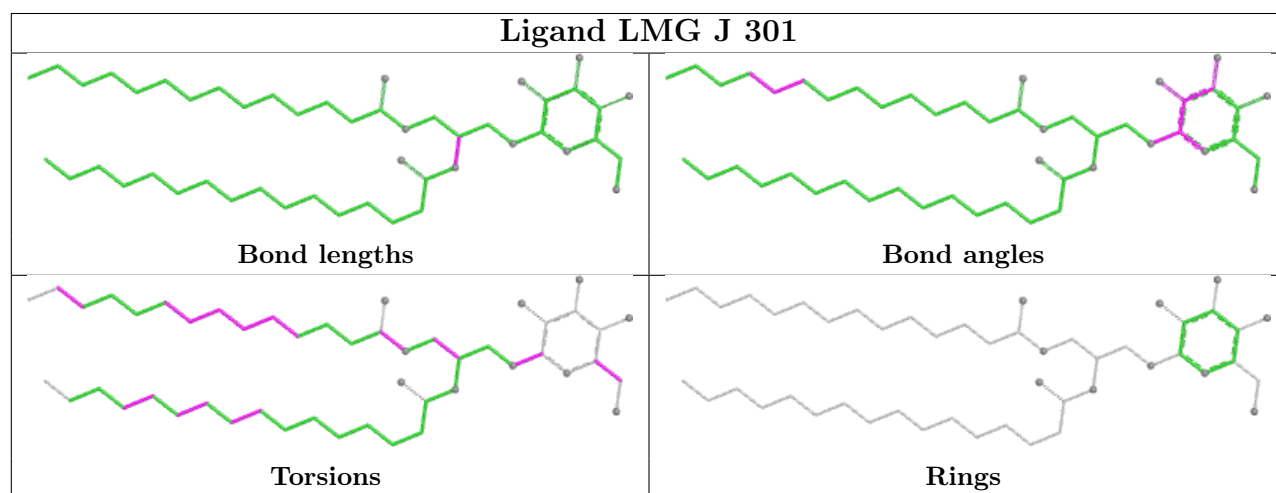
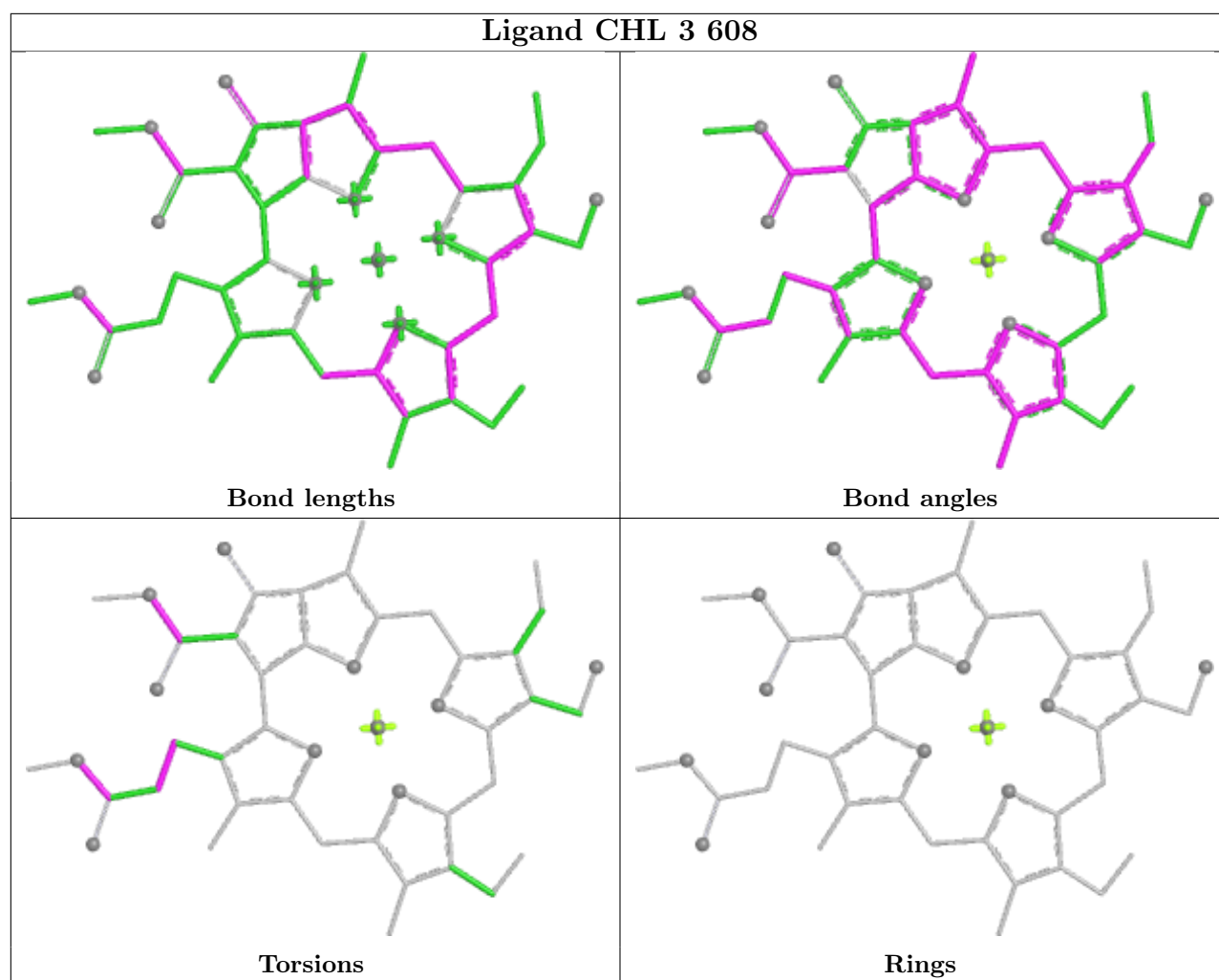


Ligand CLA O 201

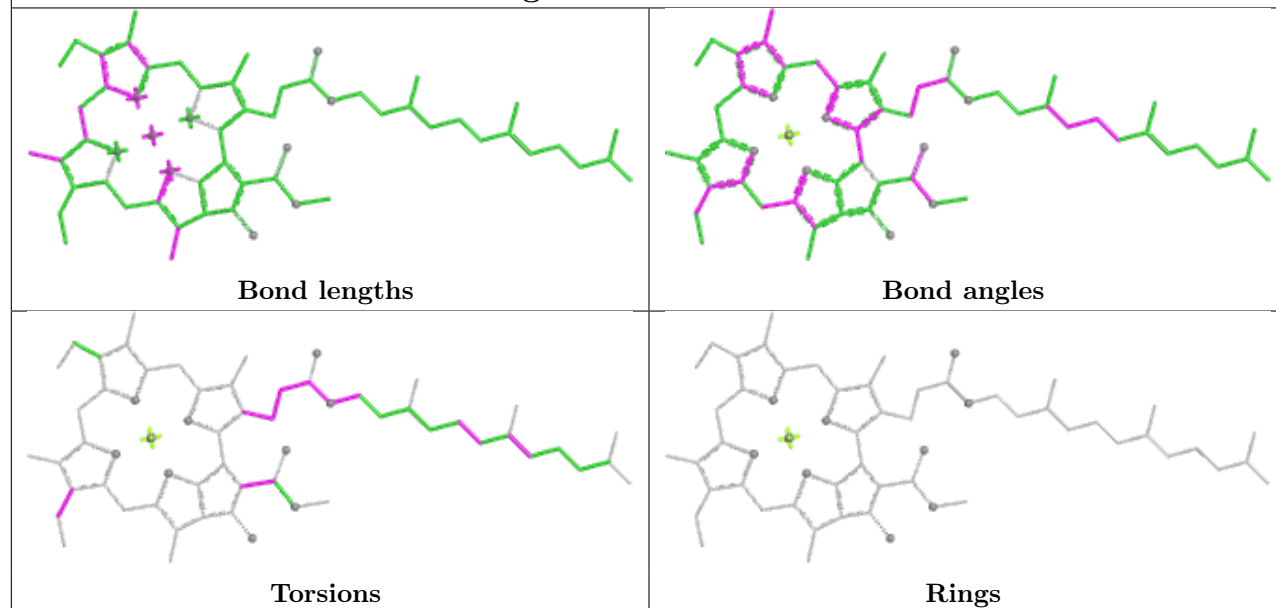




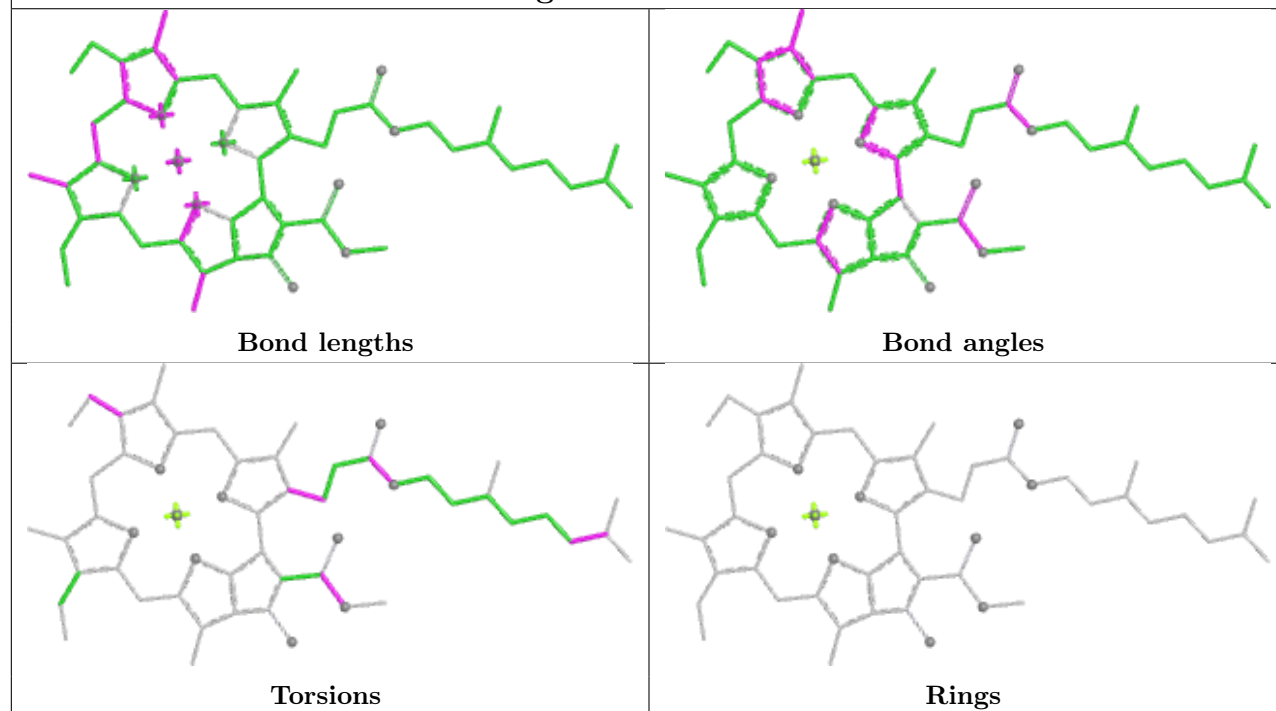




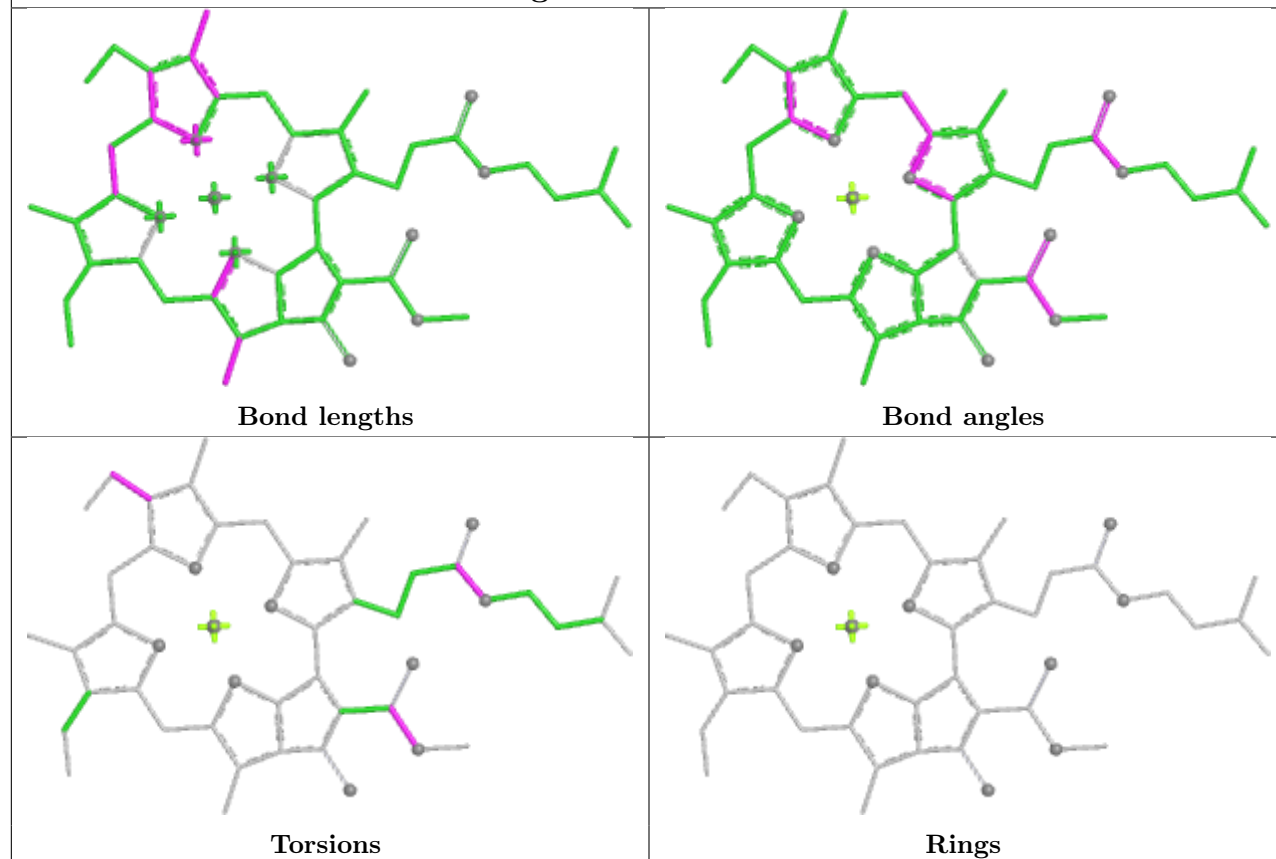
Ligand CLA A 1125



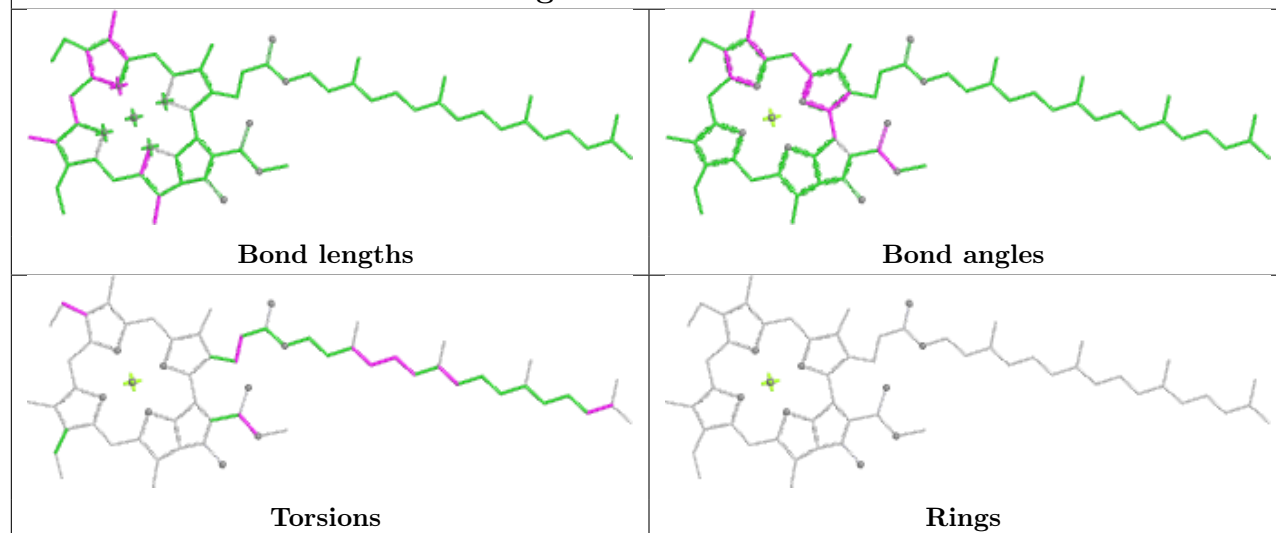
Ligand CLA 4 610

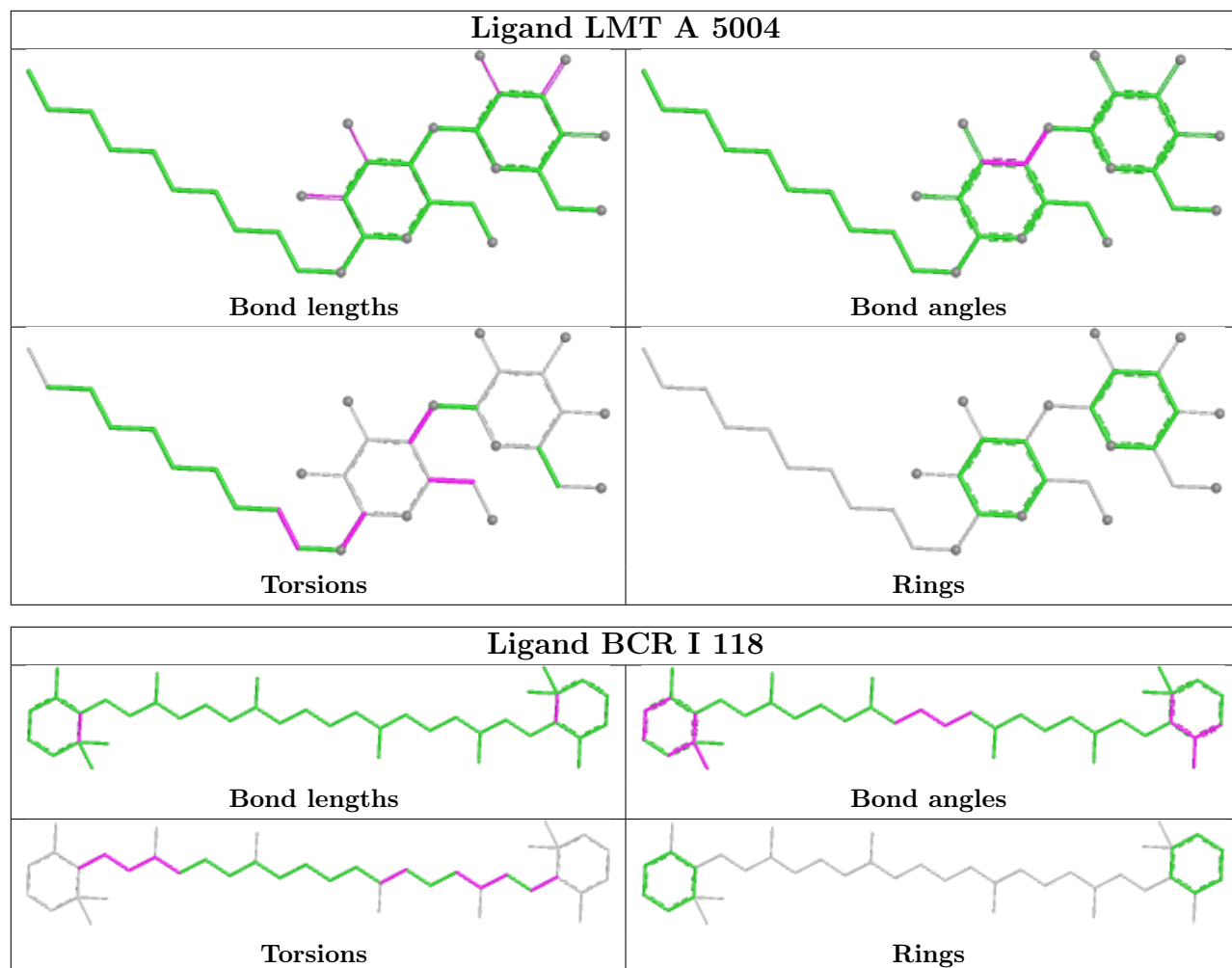


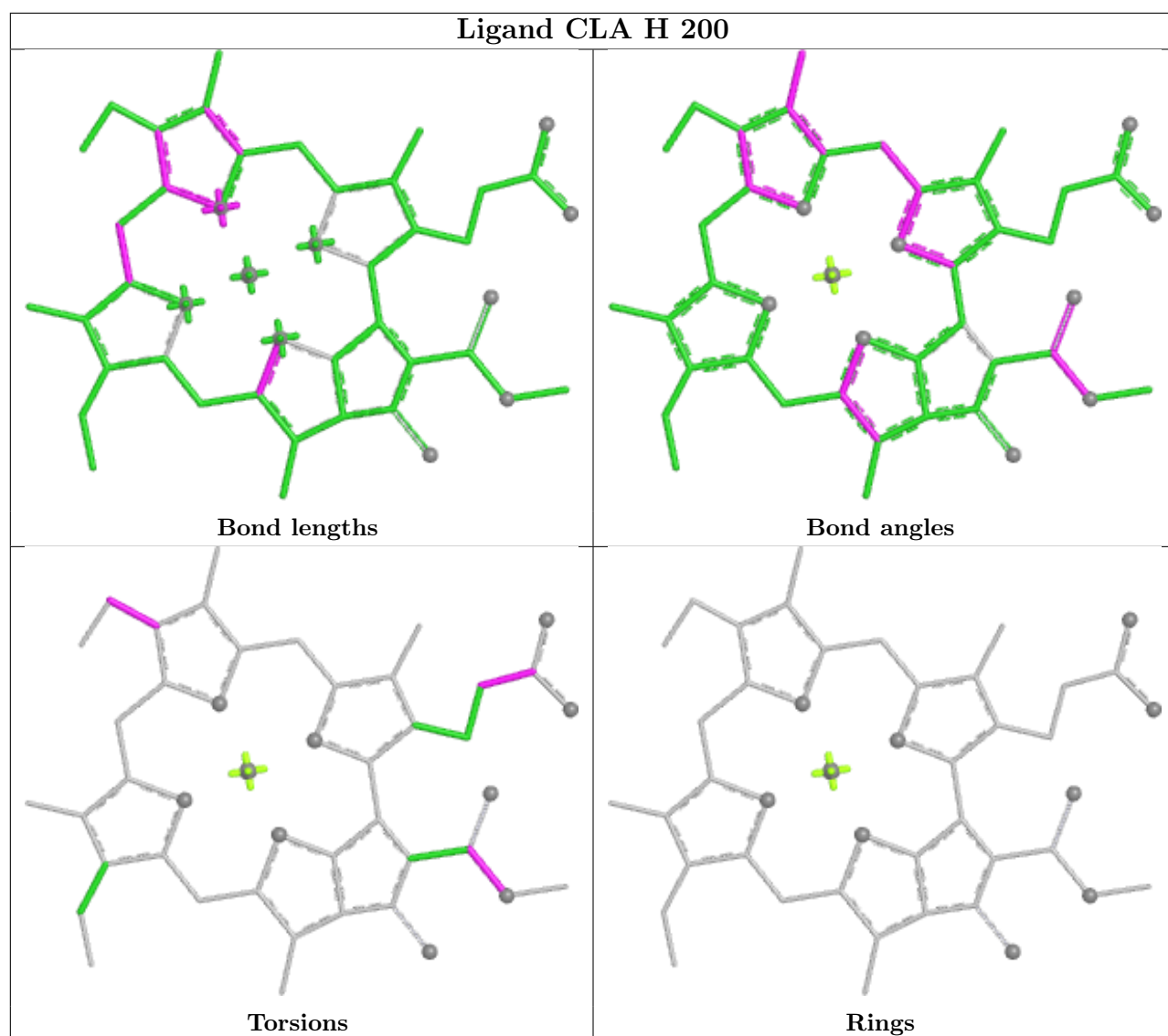
Ligand CLA G 201



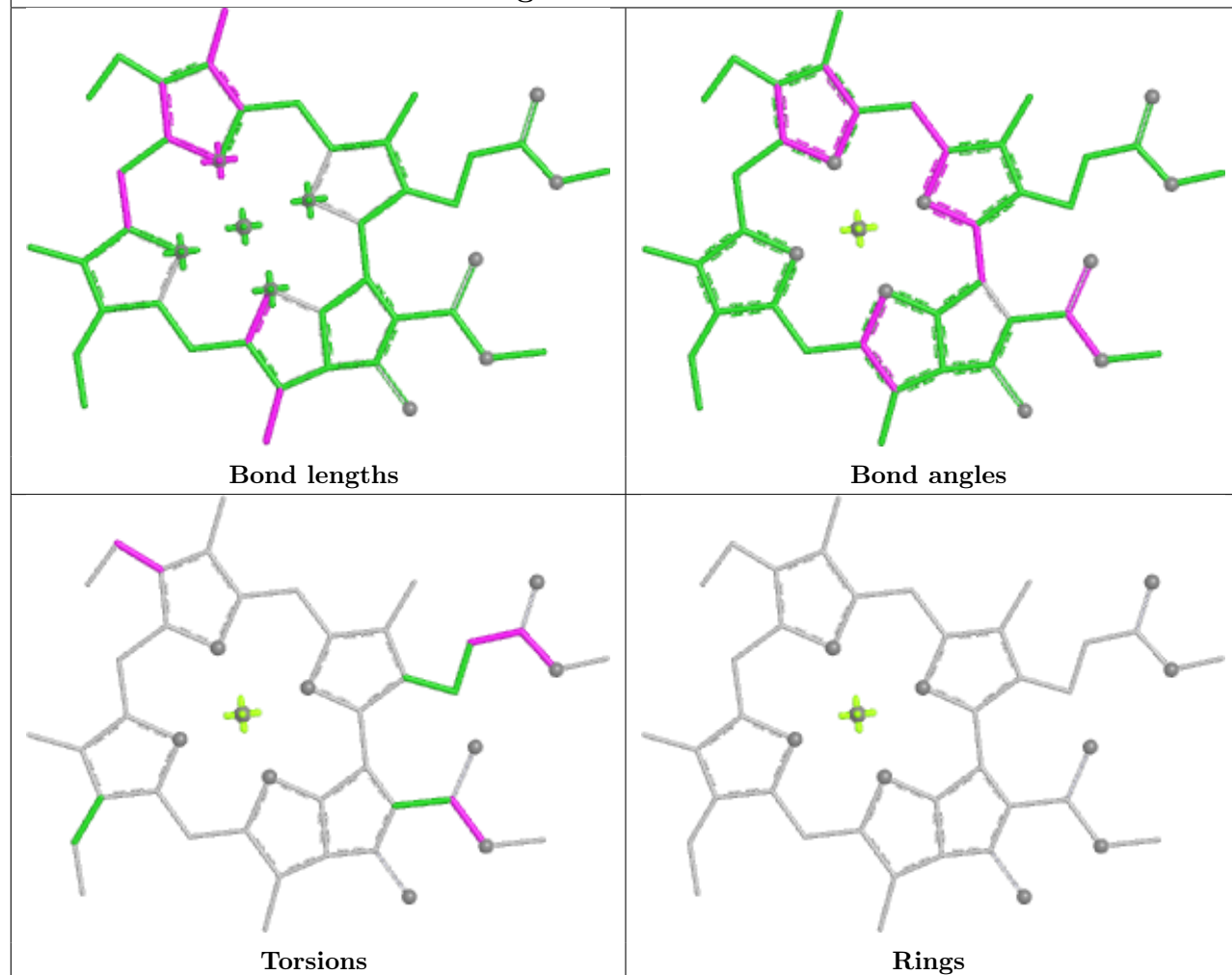
Ligand CLA 2 613



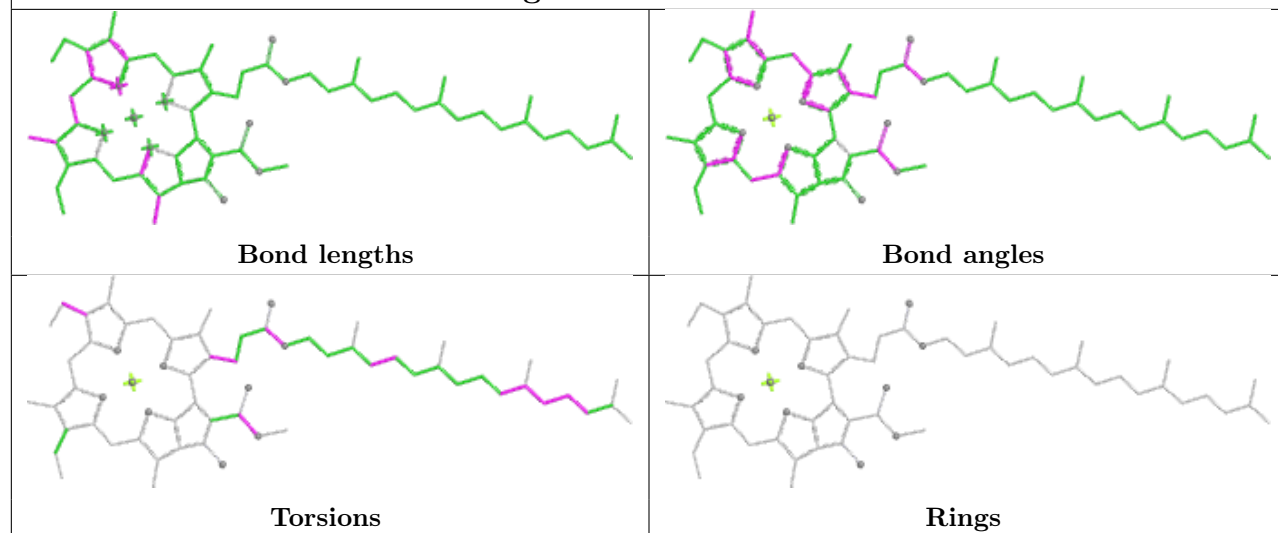


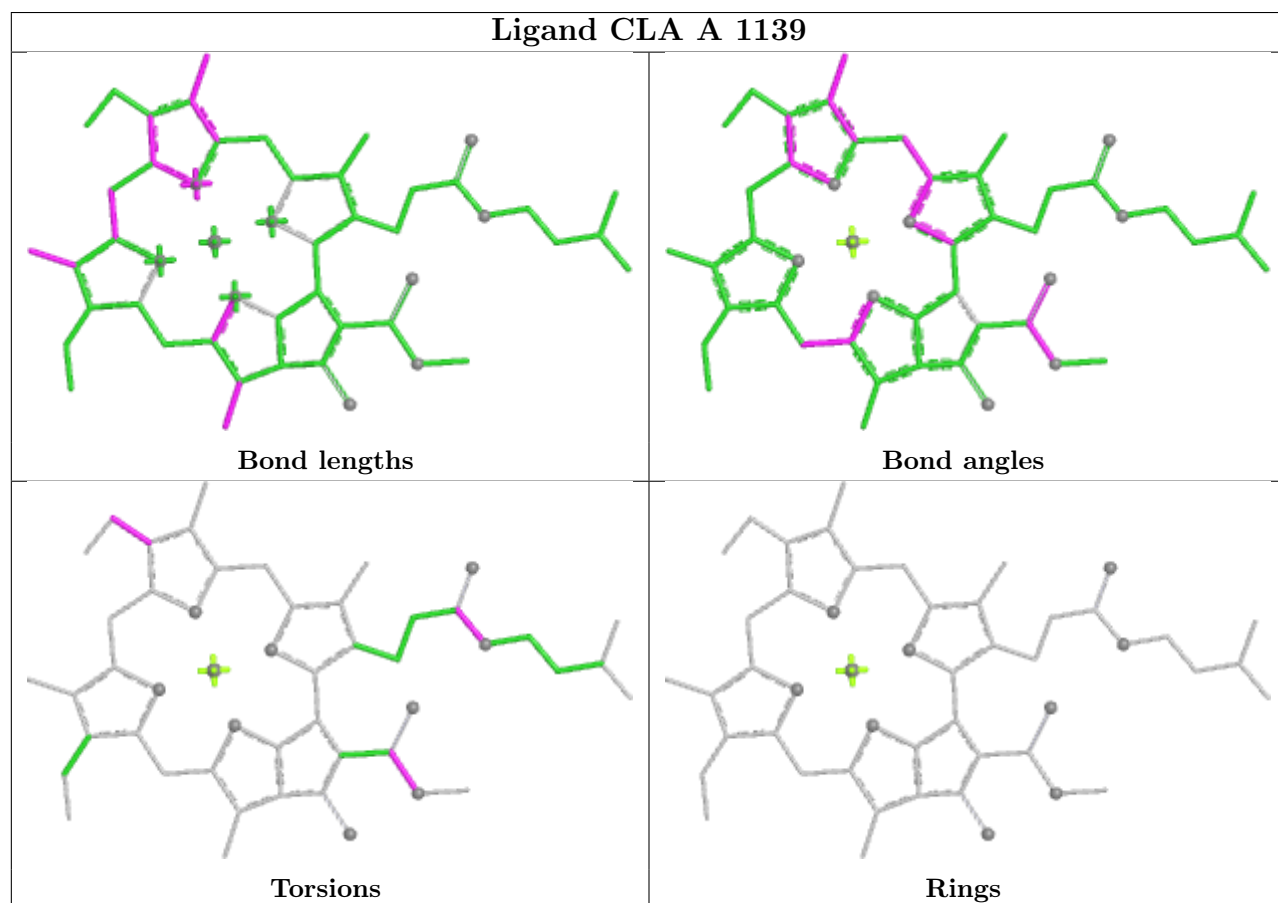
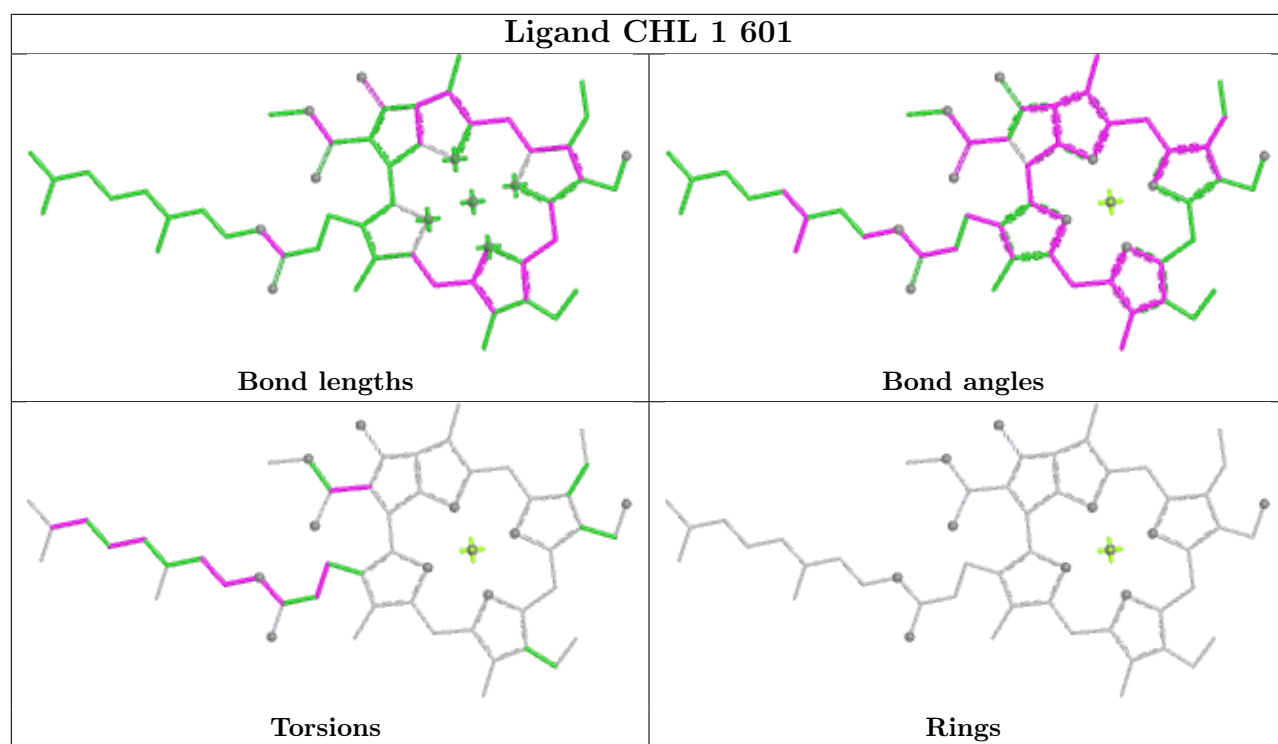


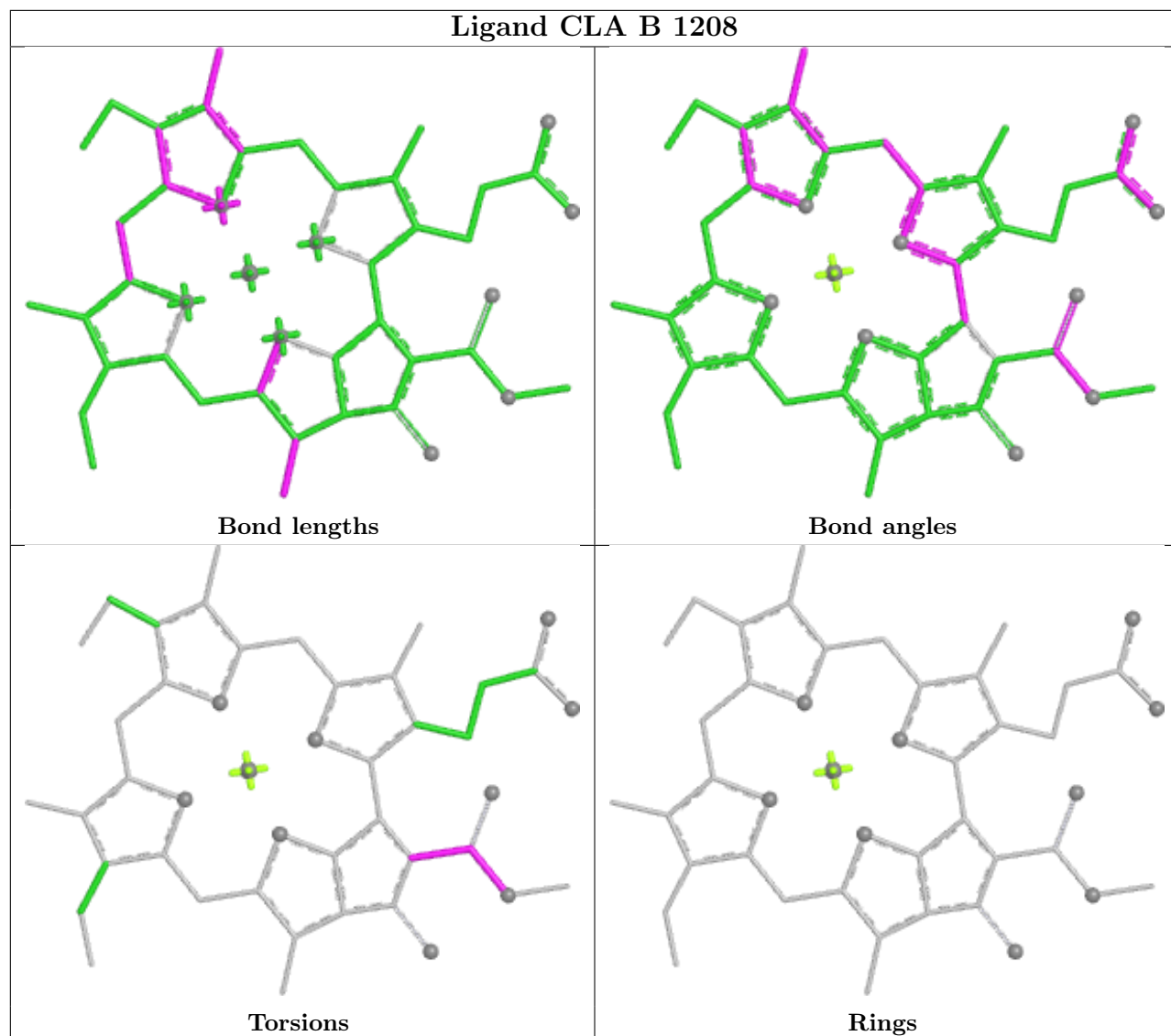
Ligand CLA 1 612

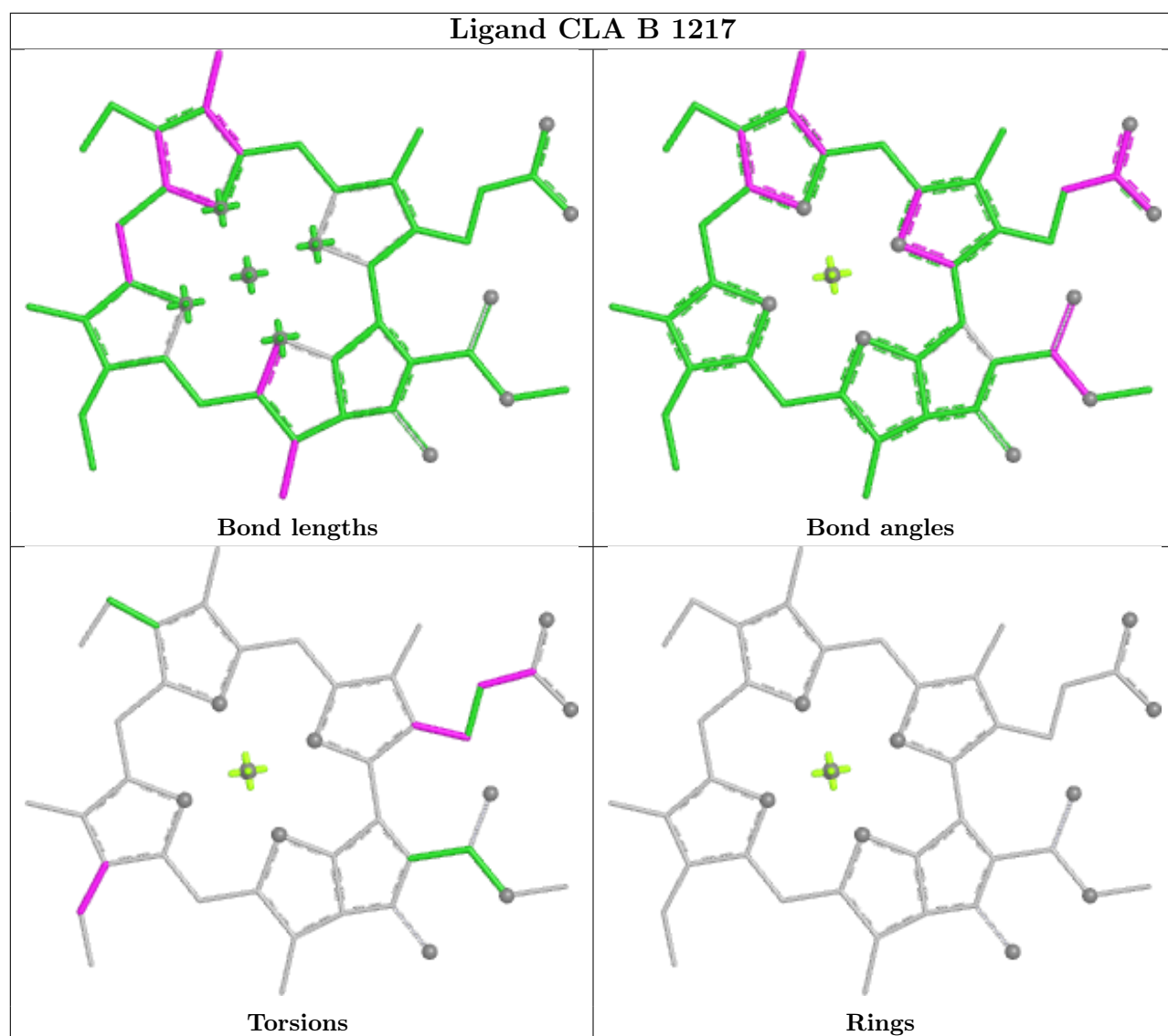


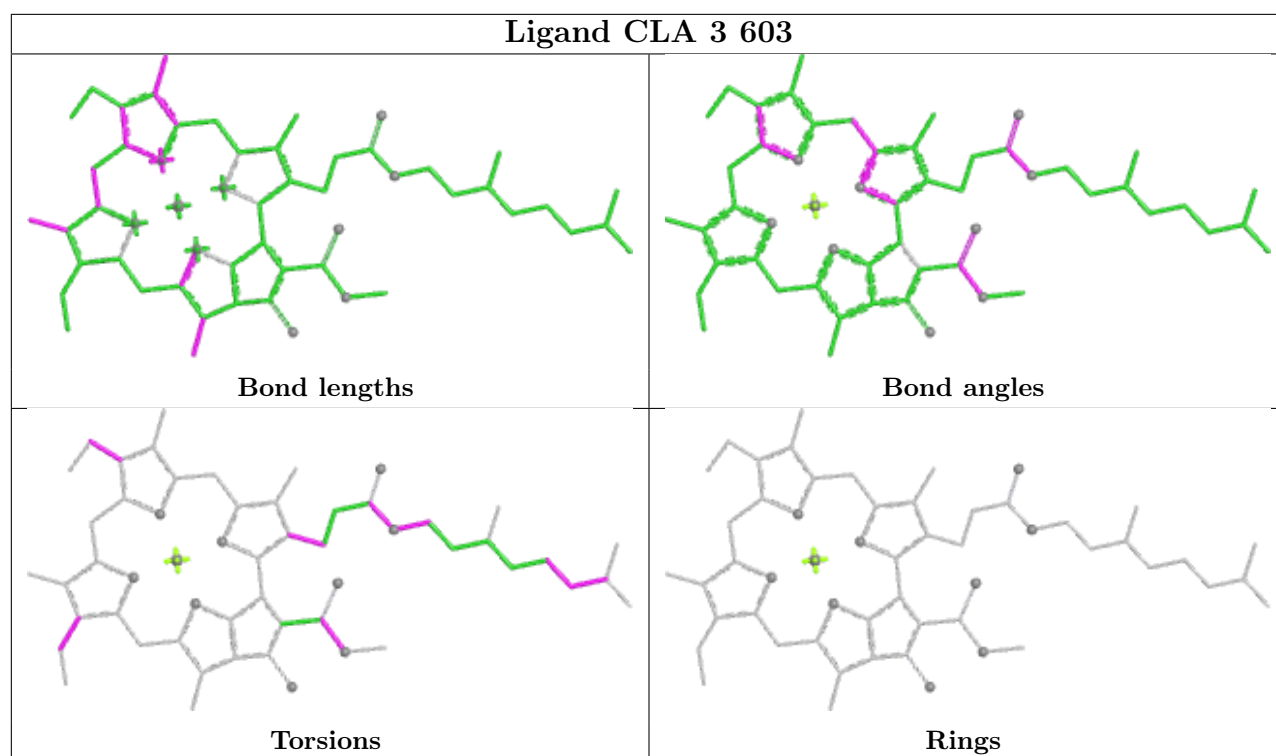
Ligand CLA B 1203



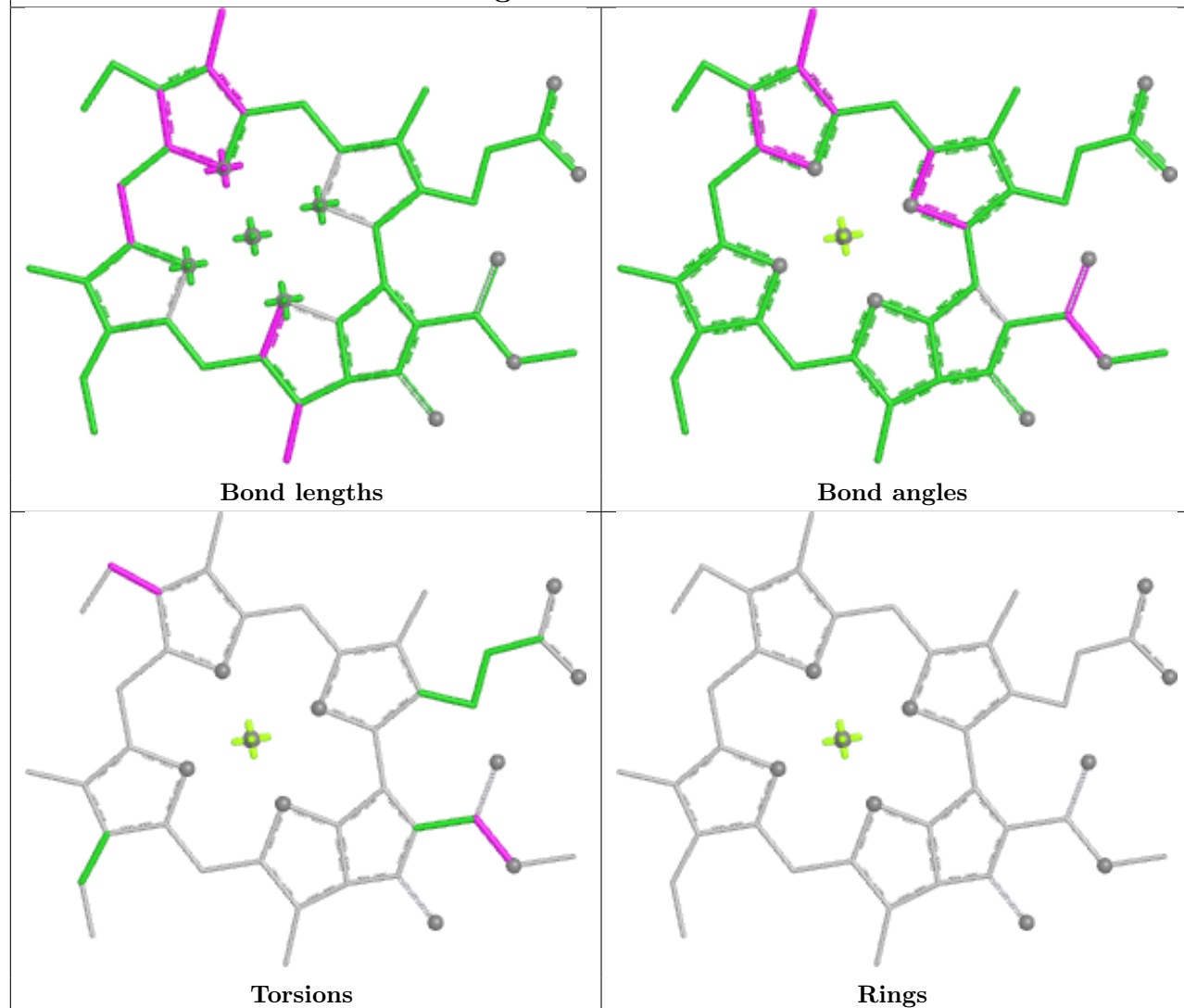




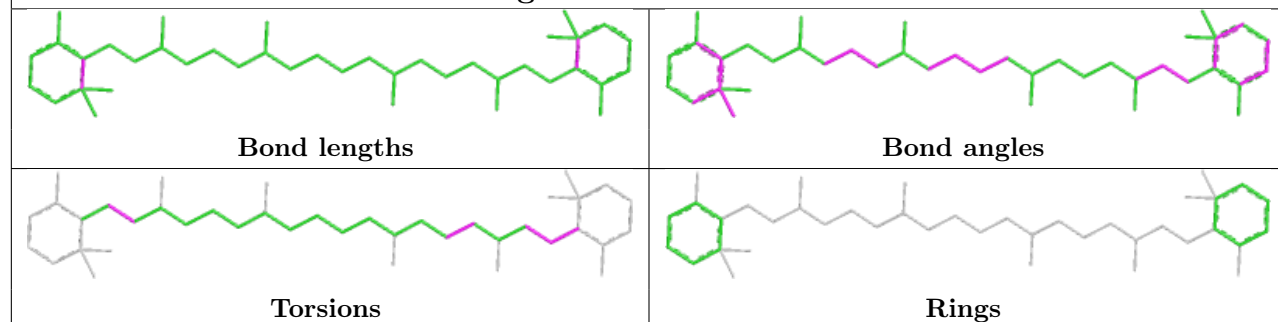


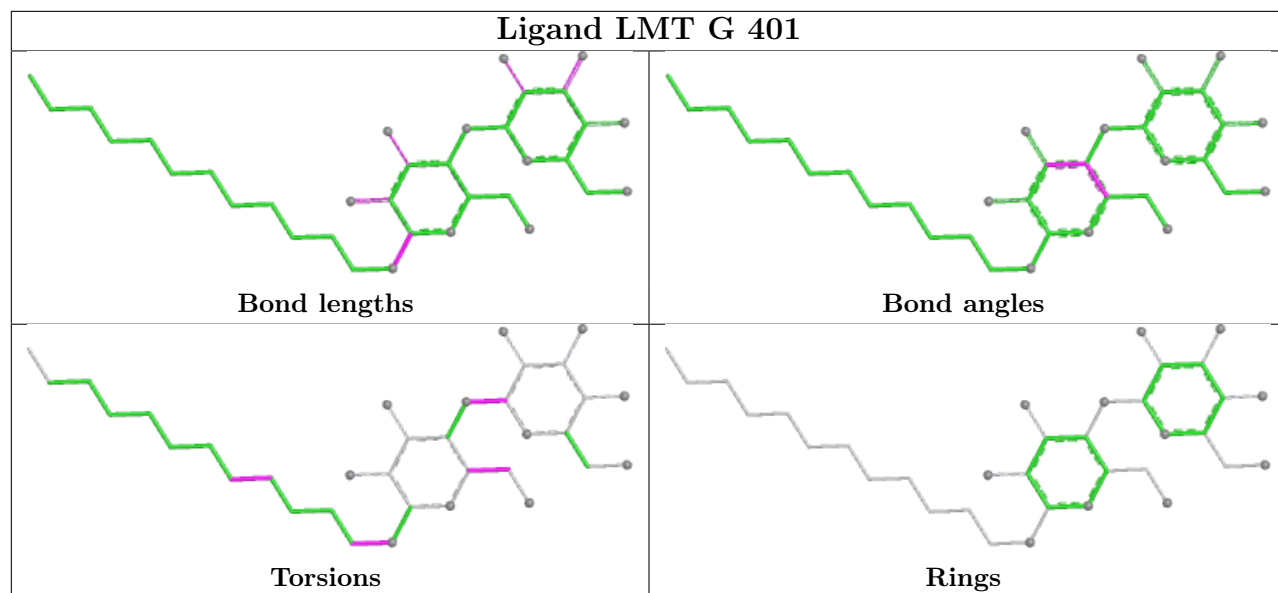


Ligand CLA F 301

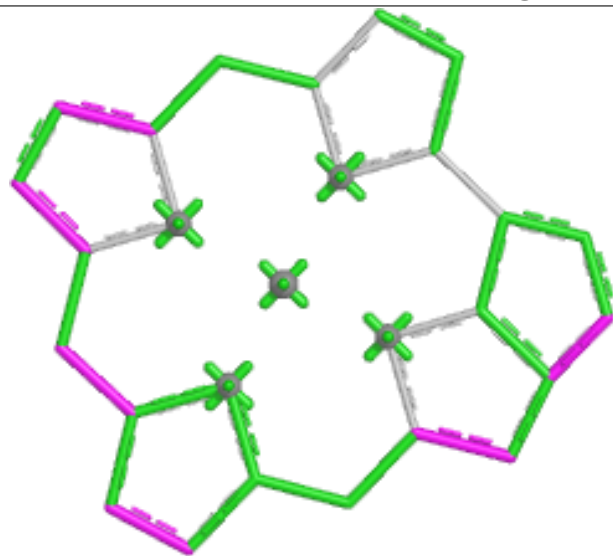


Ligand BCR M 4021

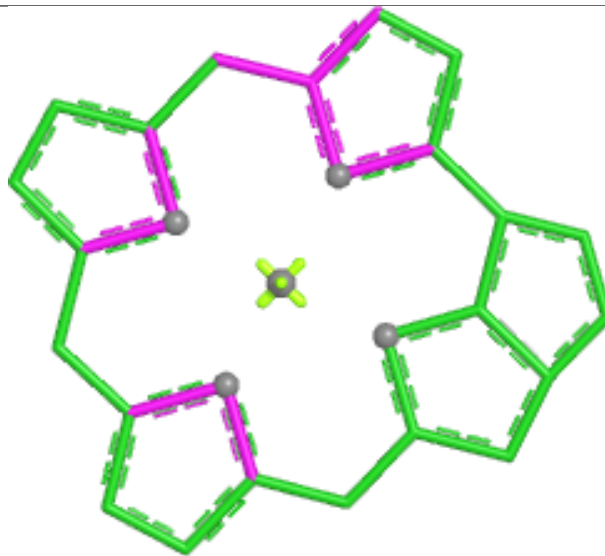




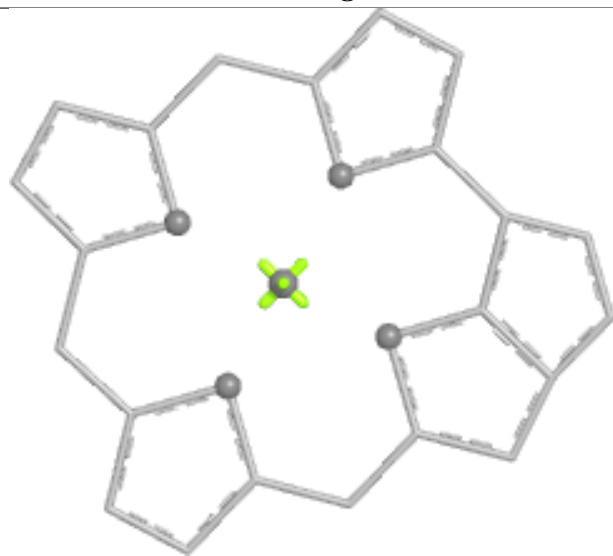
Ligand CLA F 303



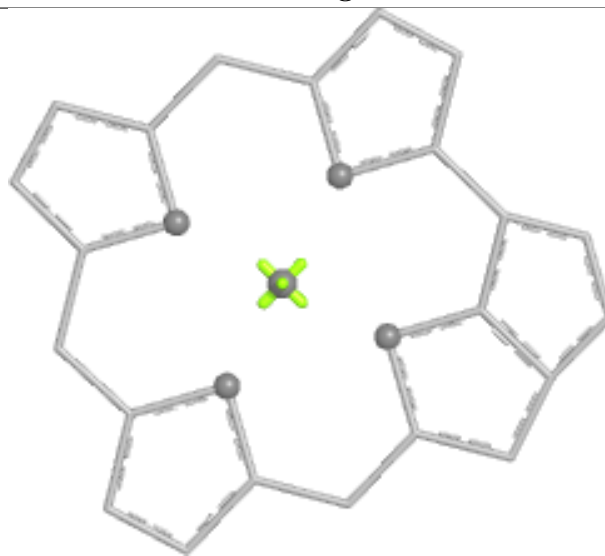
Bond lengths



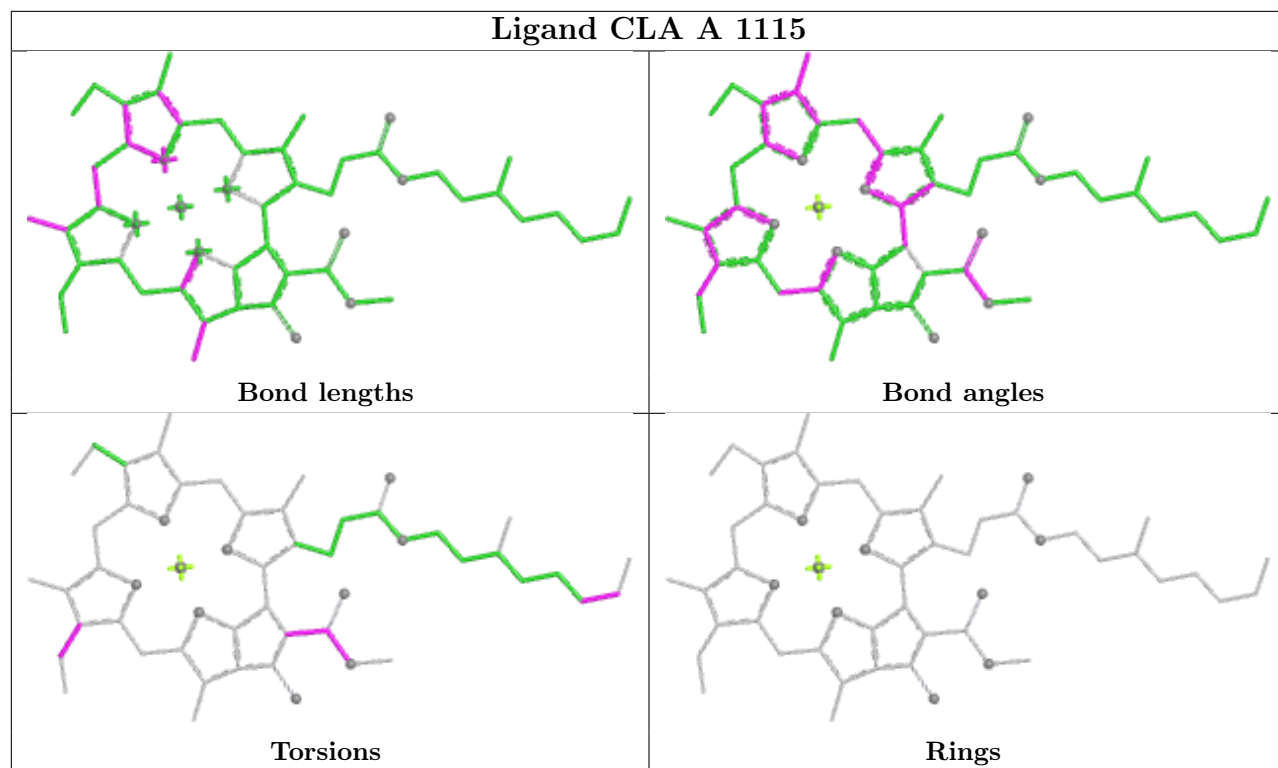
Bond angles

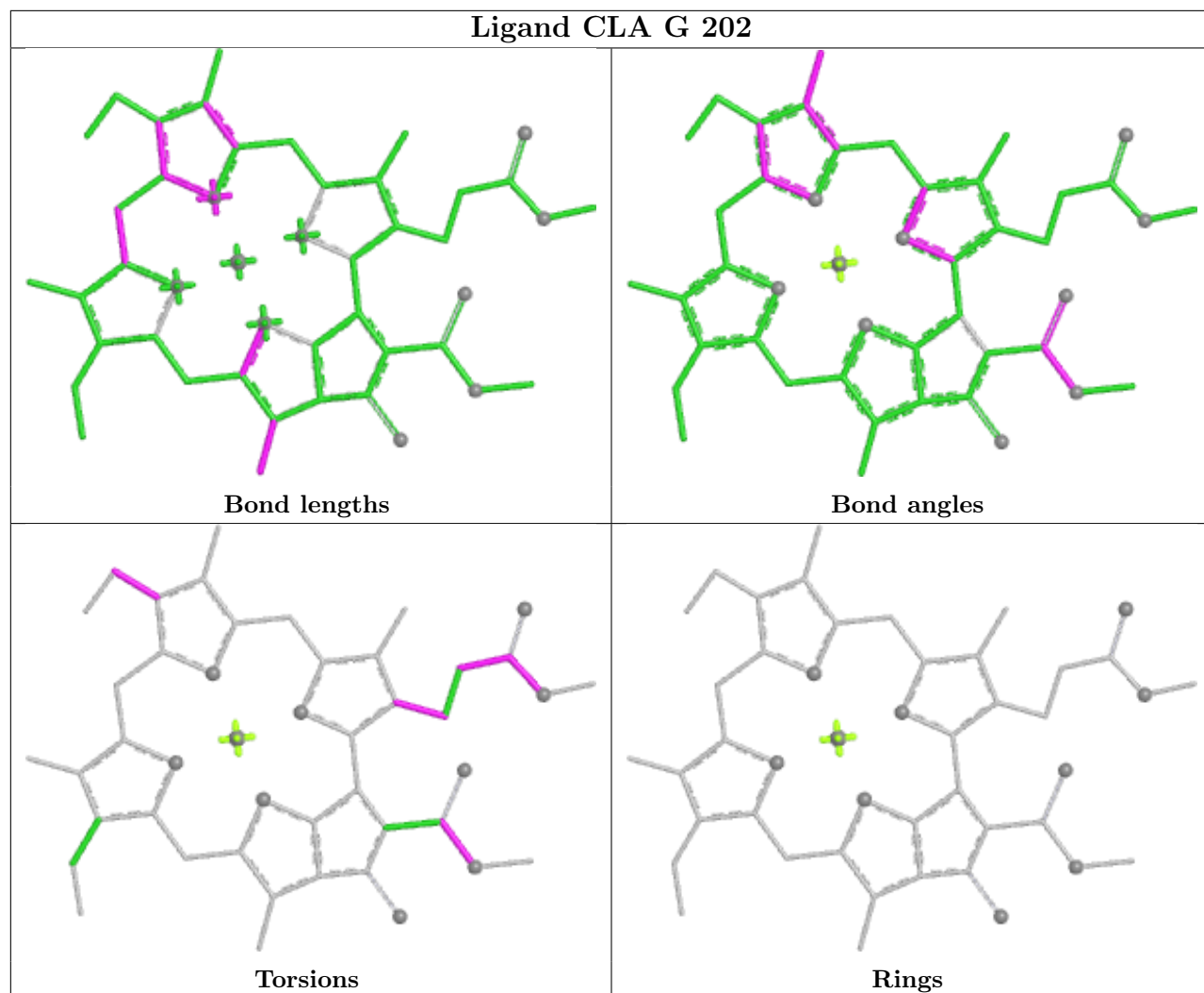


Torsions

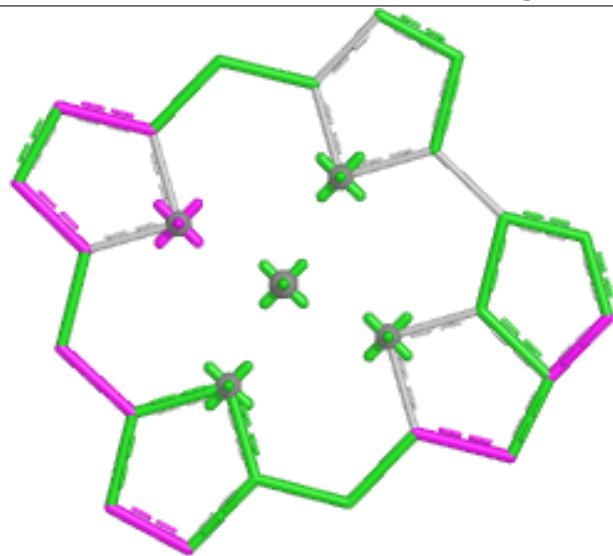


Rings

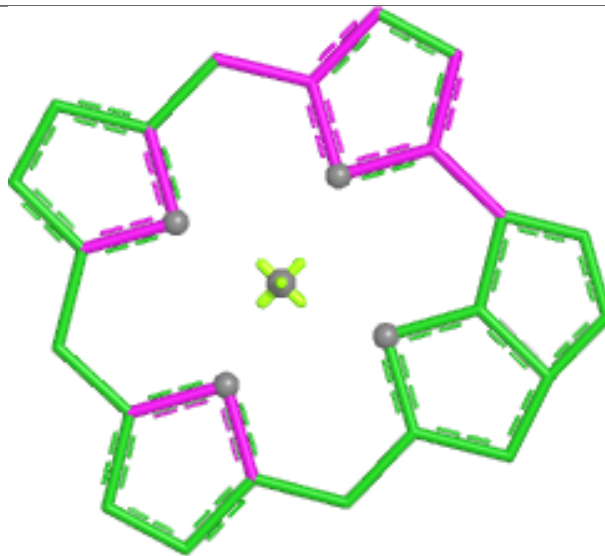




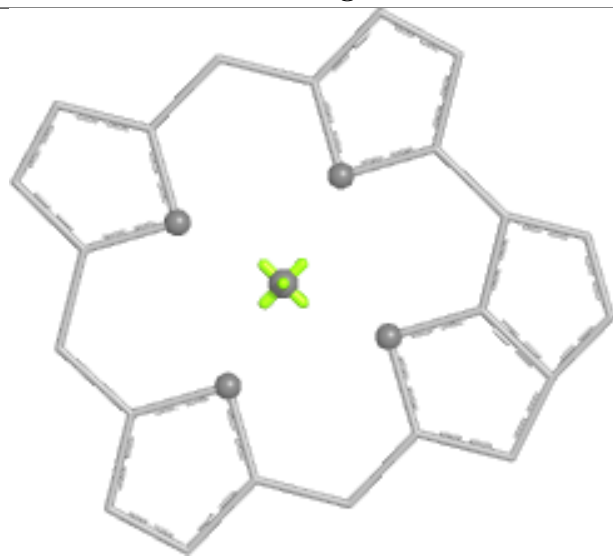
Ligand CLA 3 605



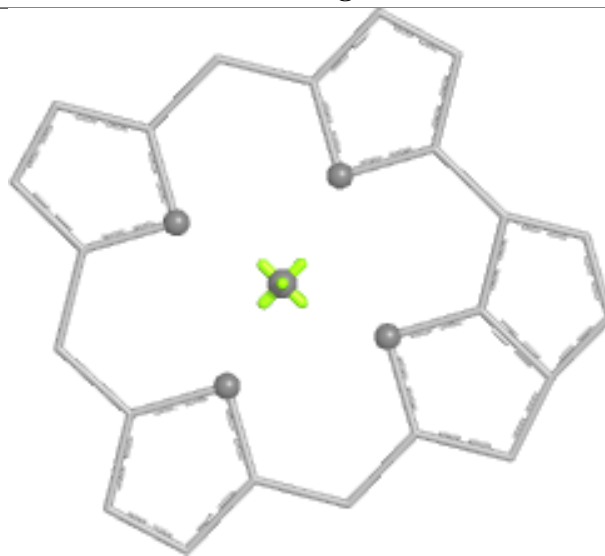
Bond lengths



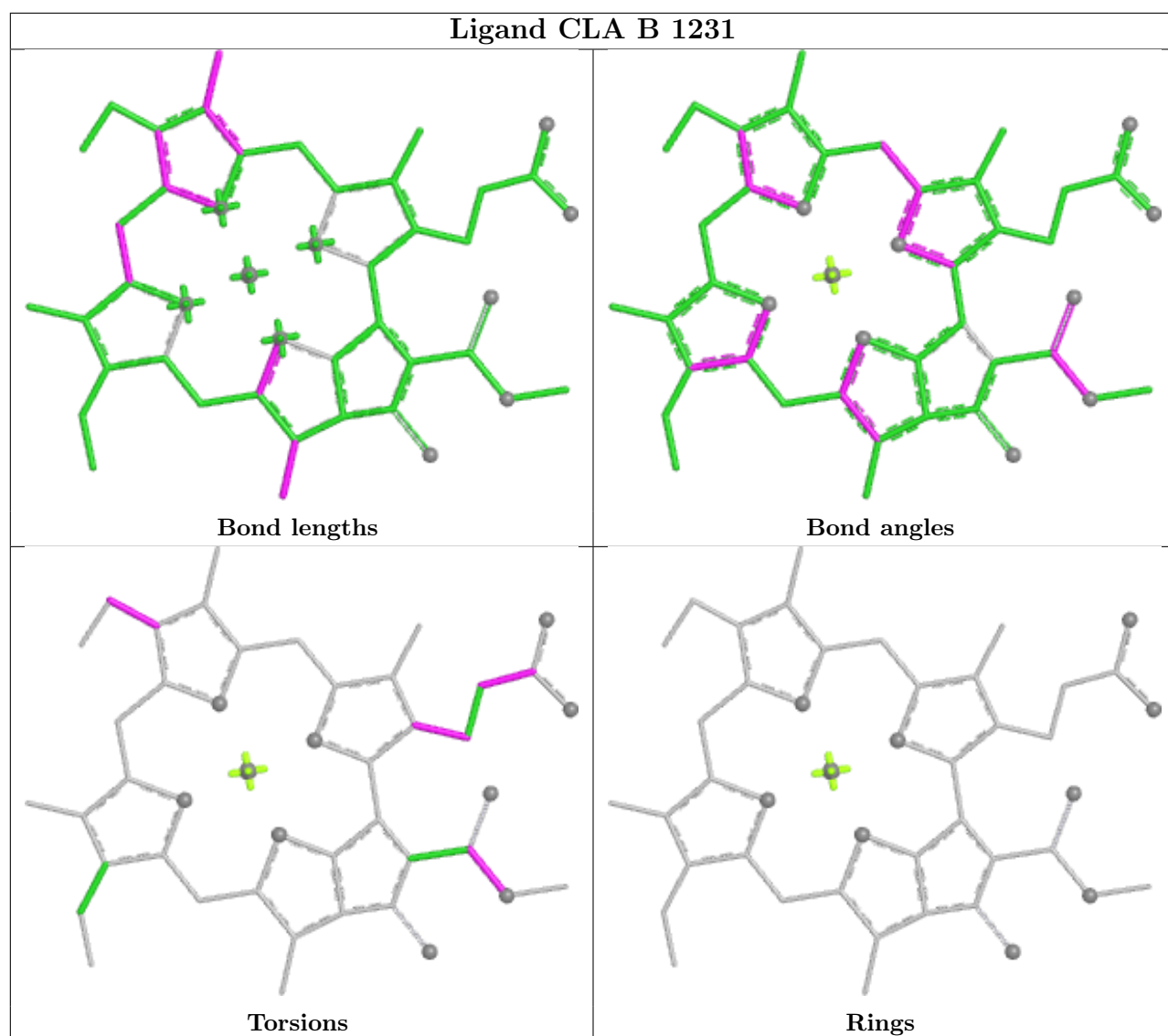
Bond angles



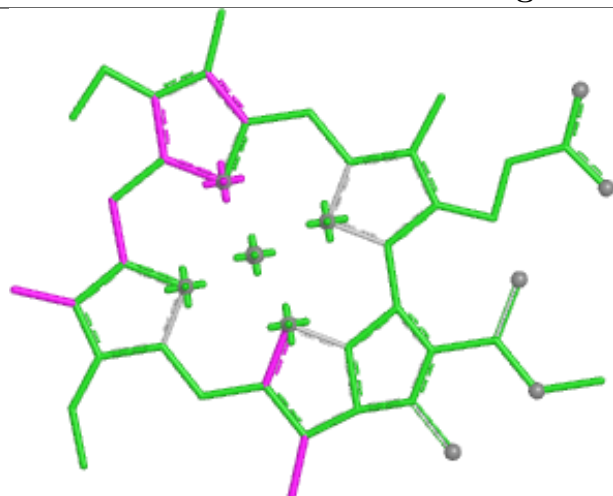
Torsions



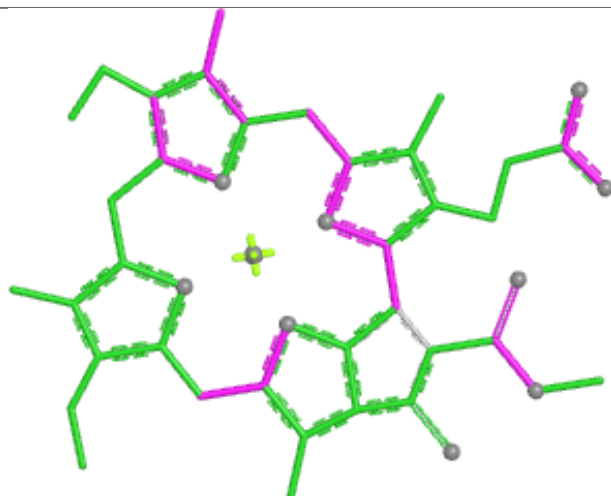
Rings



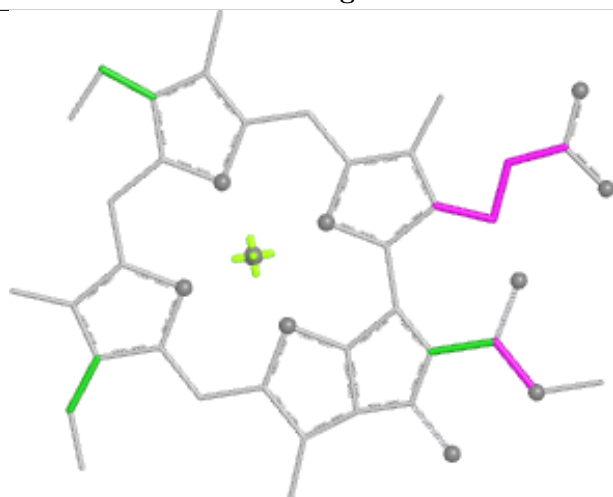
Ligand CLA L 303



Bond lengths



Bond angles

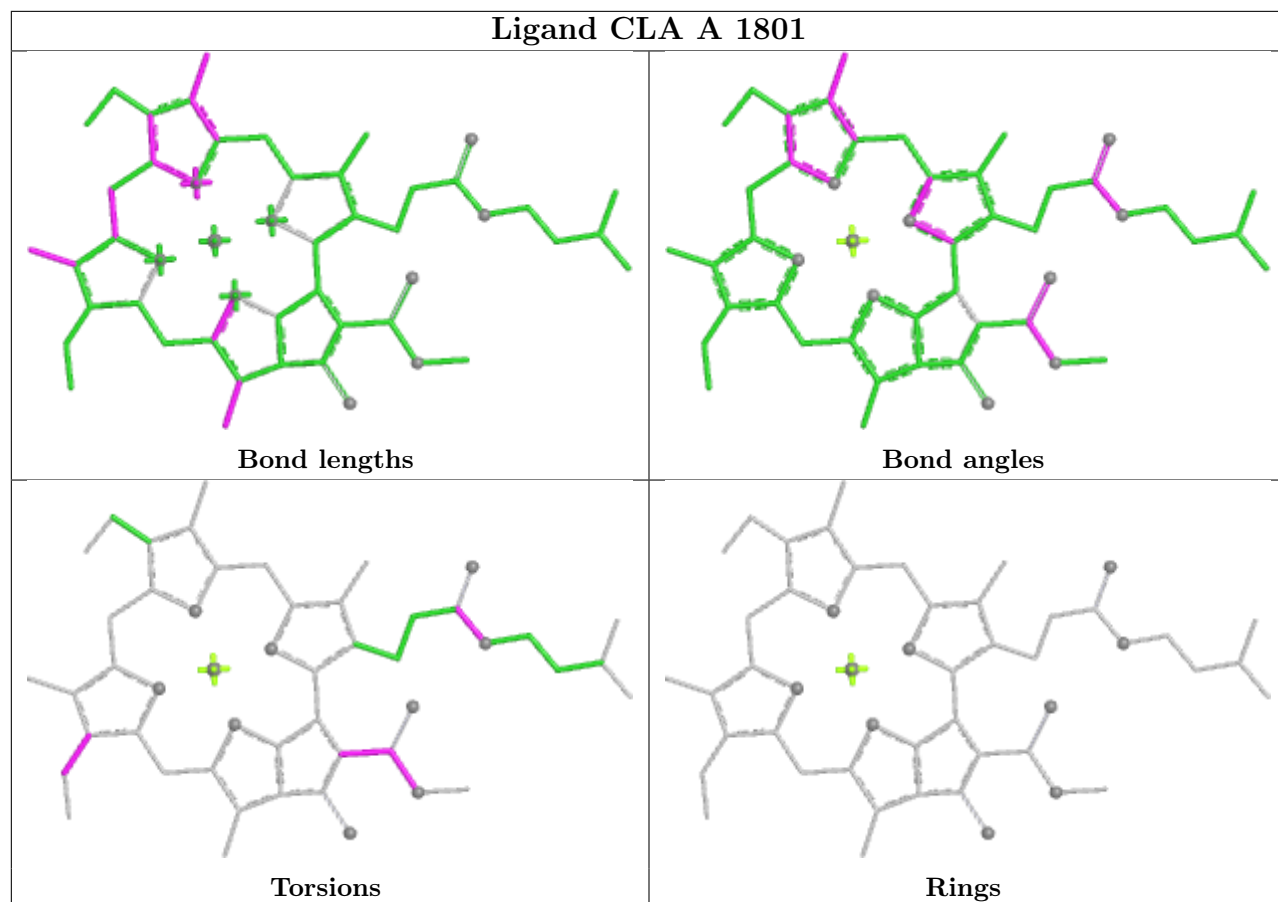


Torsions

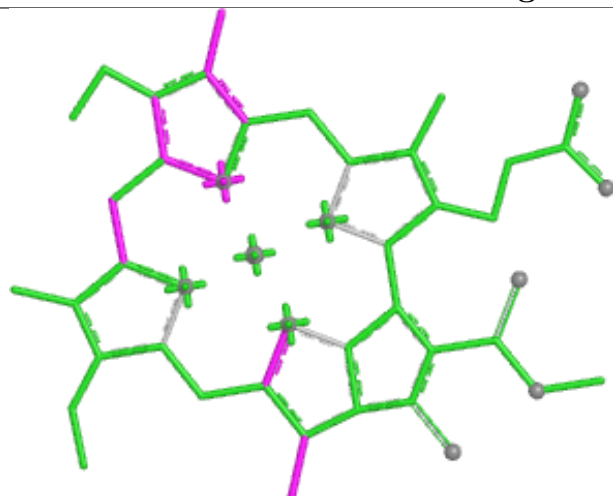


Rings

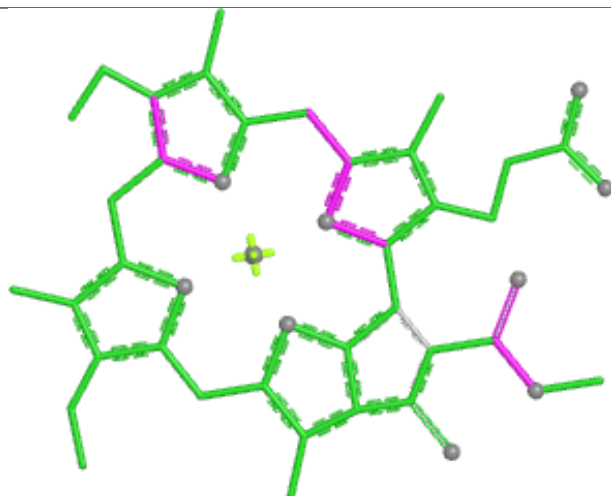
Ligand CLA A 1801



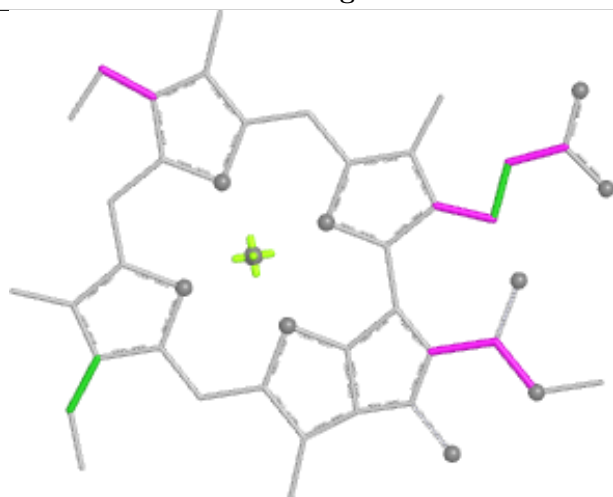
Ligand CLA J 102



Bond lengths



Bond angles

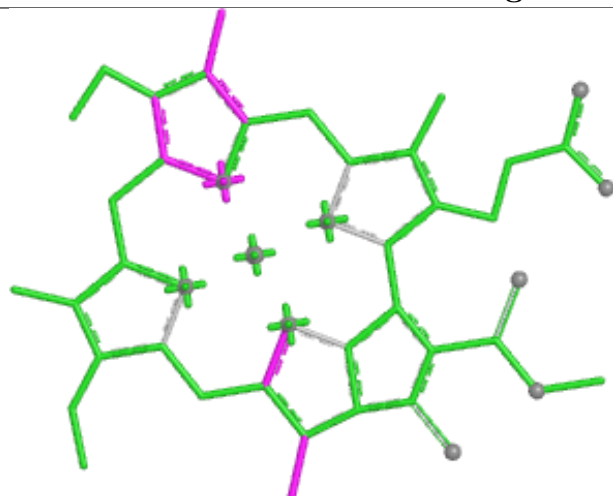


Torsions

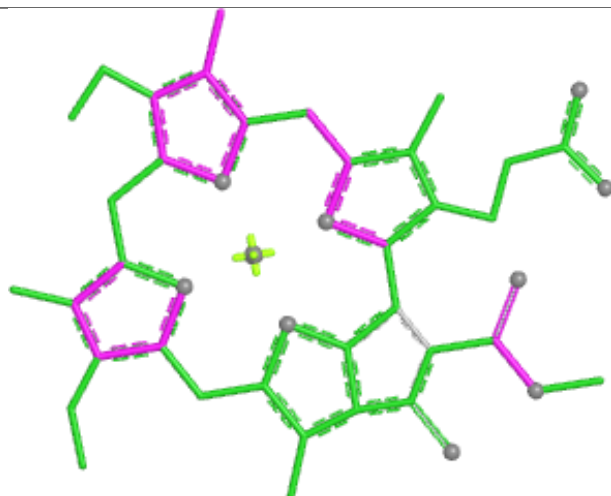


Rings

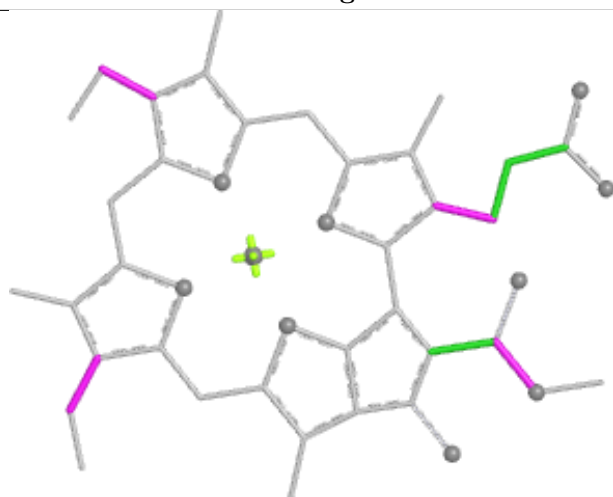
Ligand CLA B 1239



Bond lengths



Bond angles

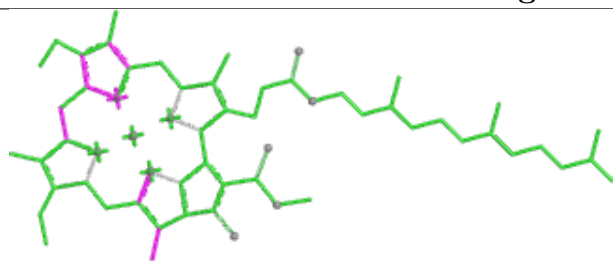


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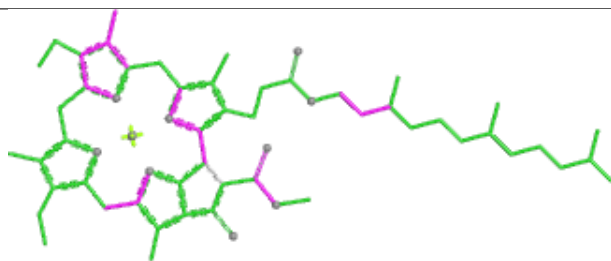


Rings

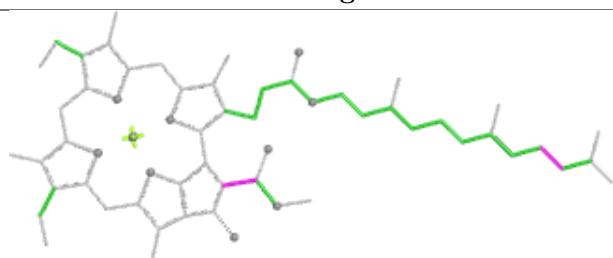
Ligand CLA 4 602



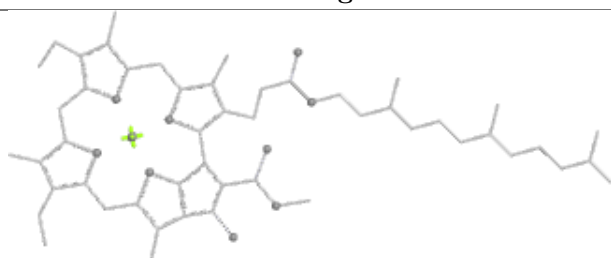
Bond lengths



Bond angles

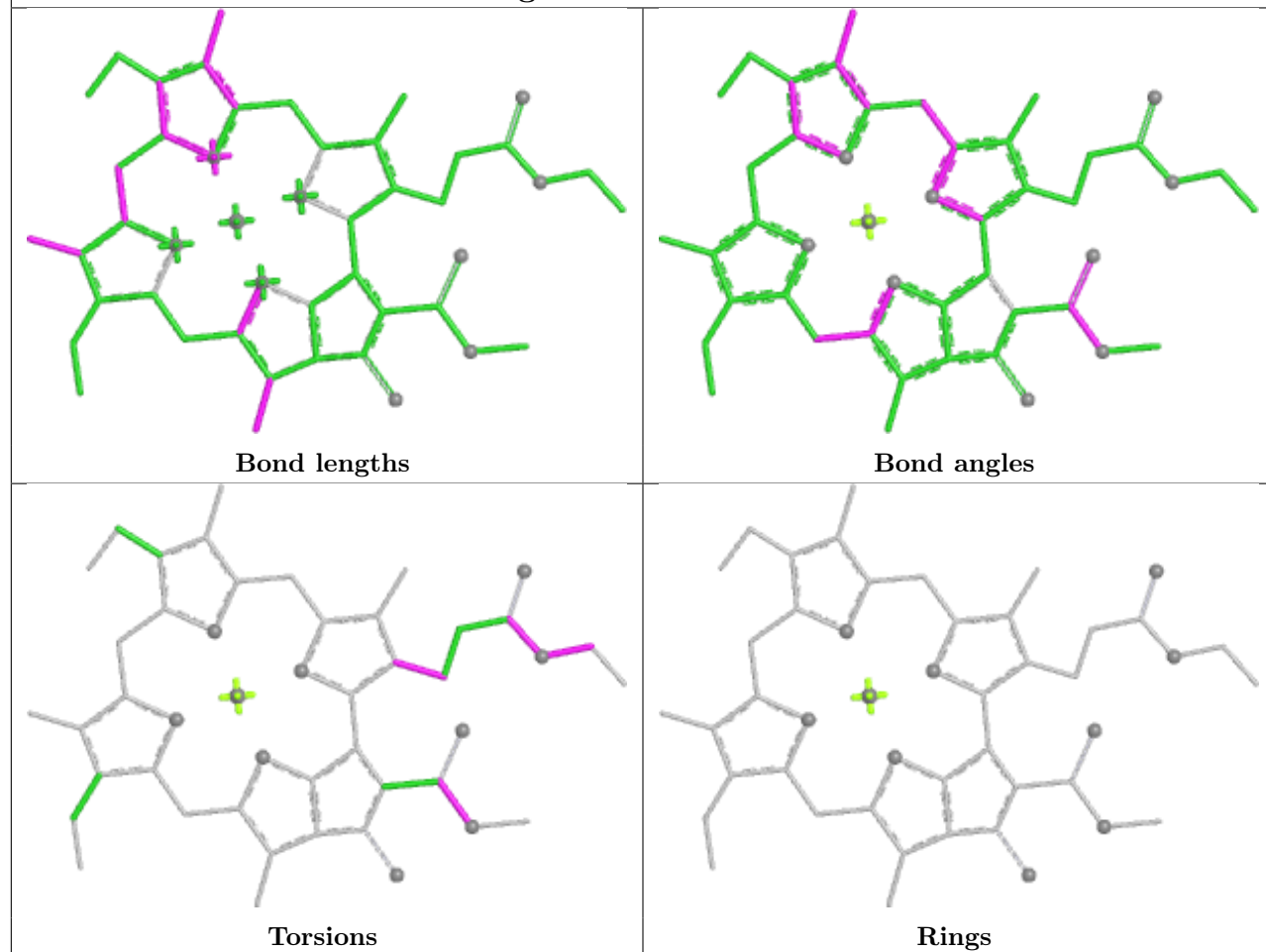


Torsions

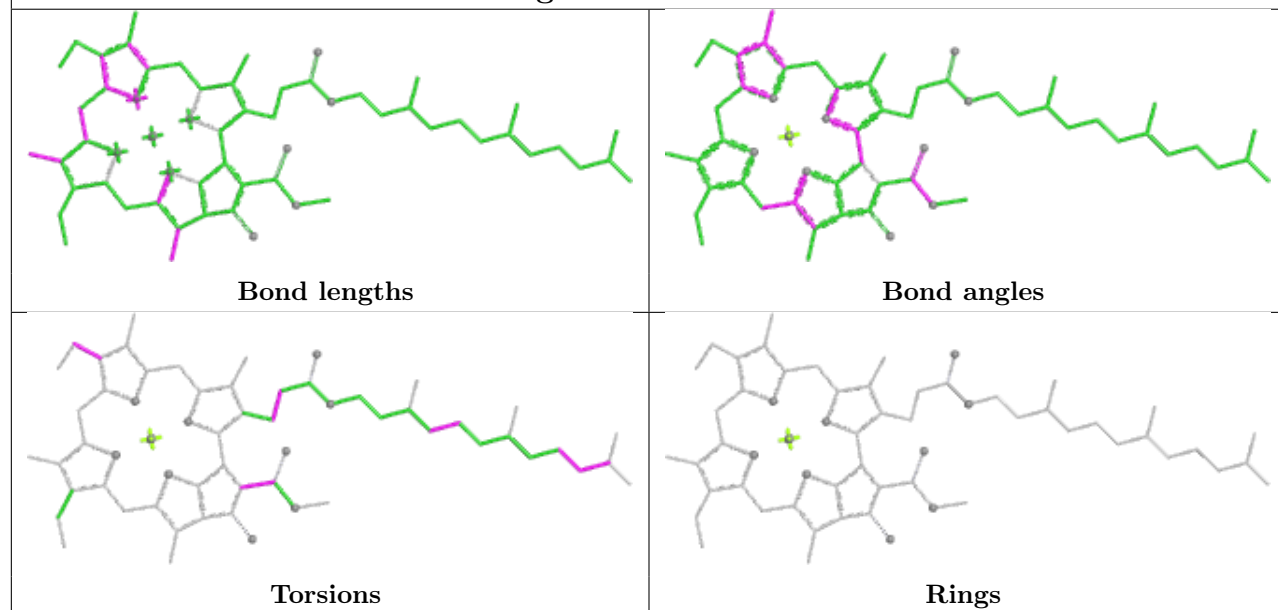


Rings

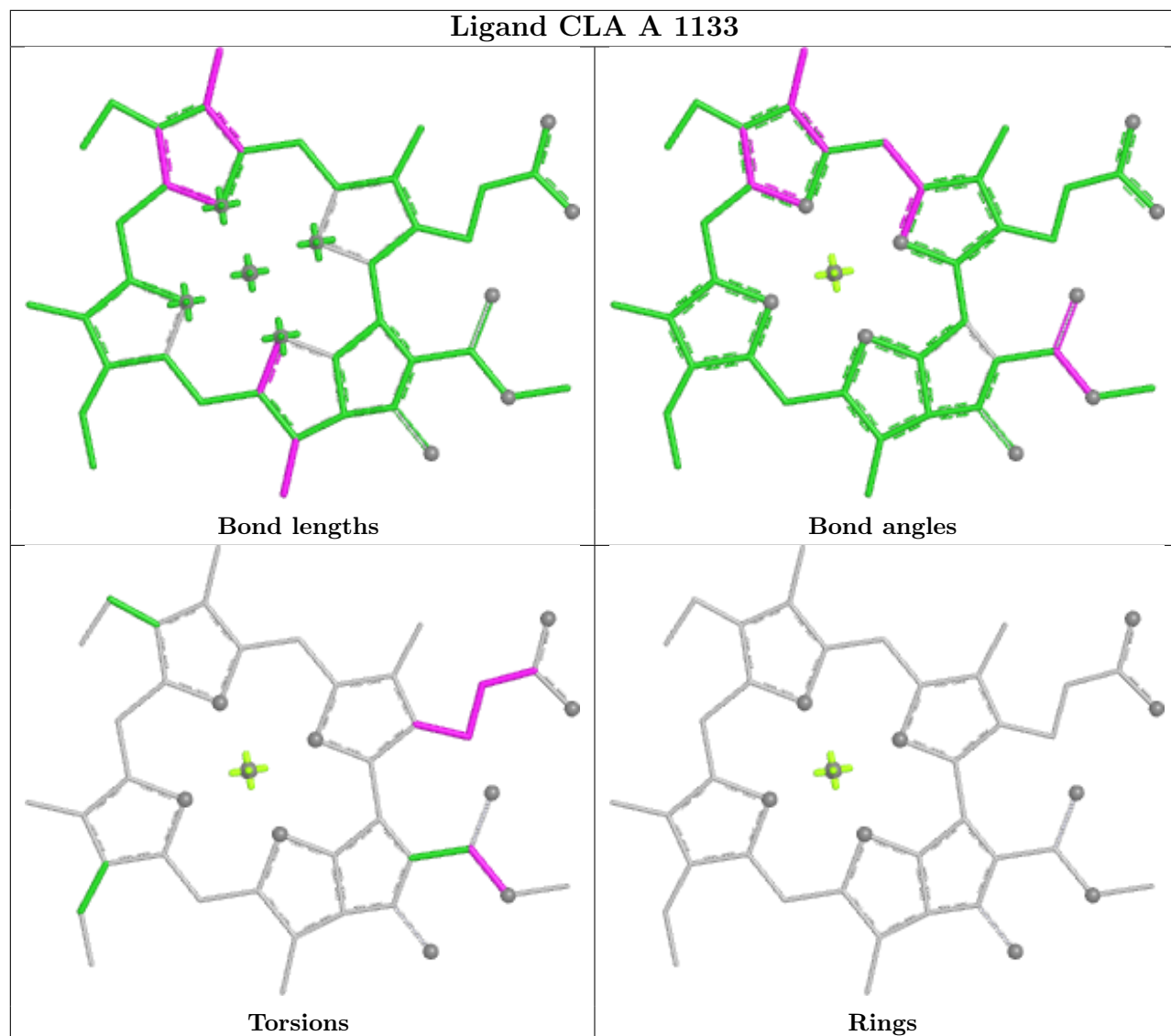
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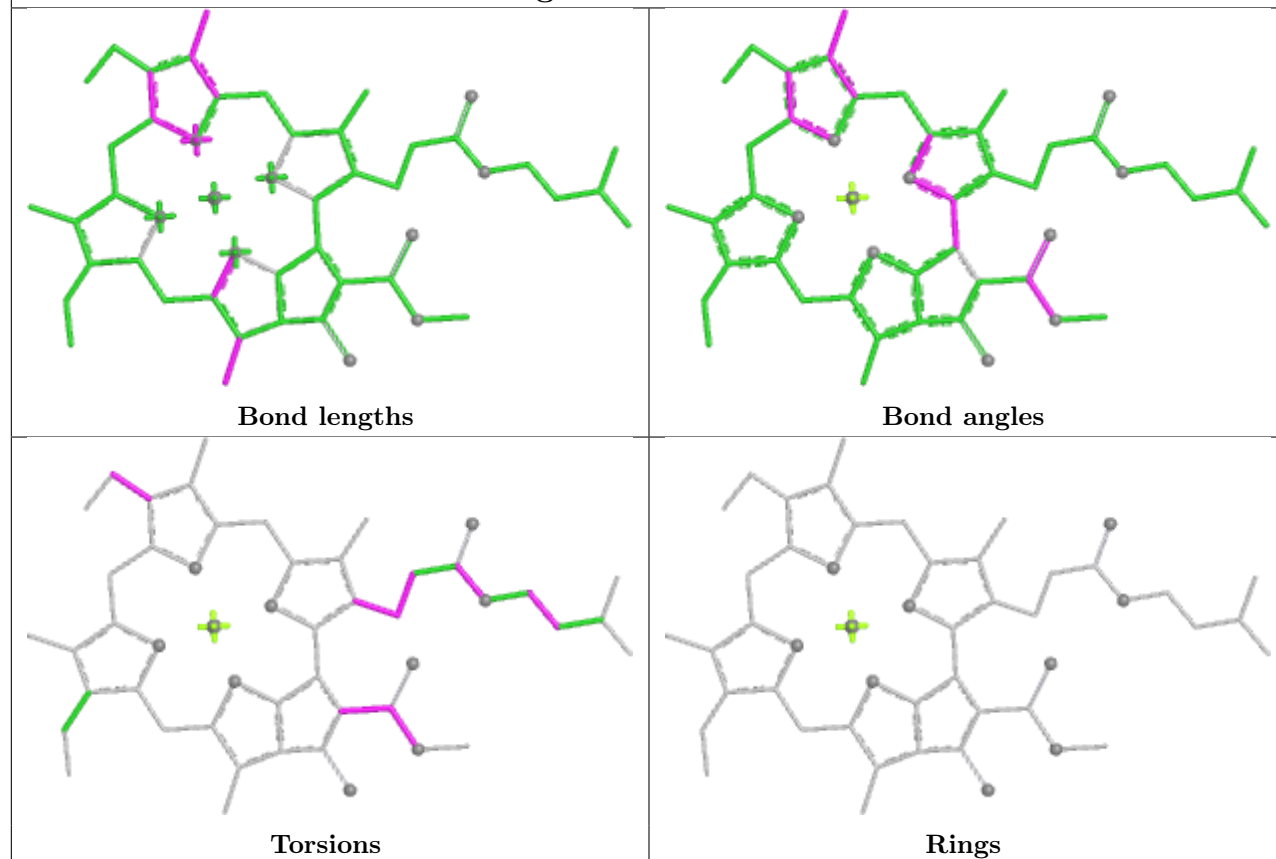
Ligand CLA 3 602



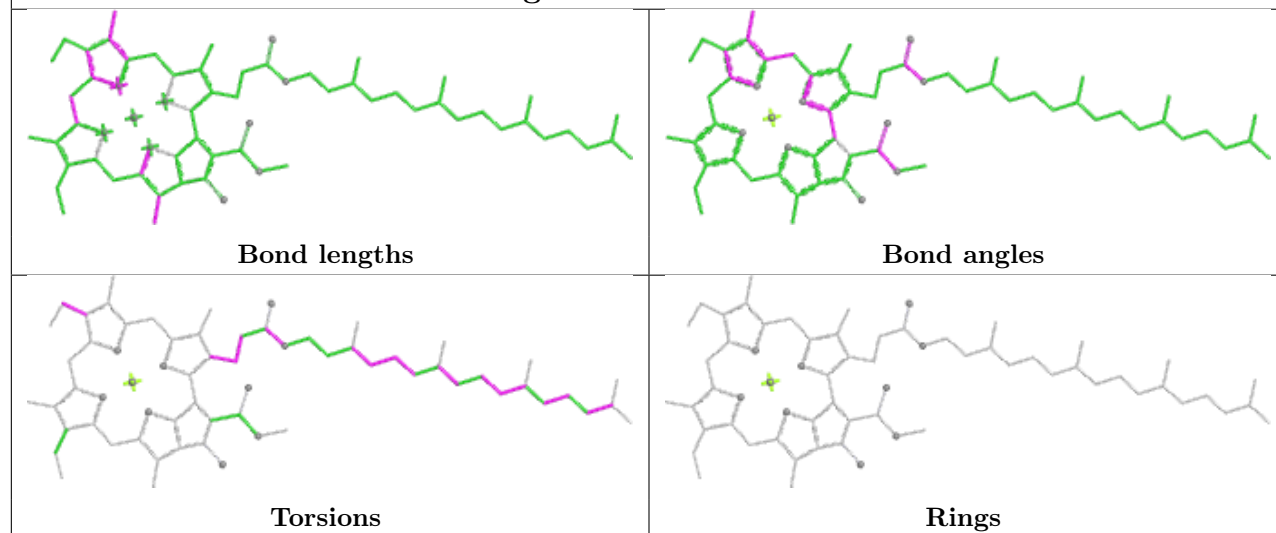
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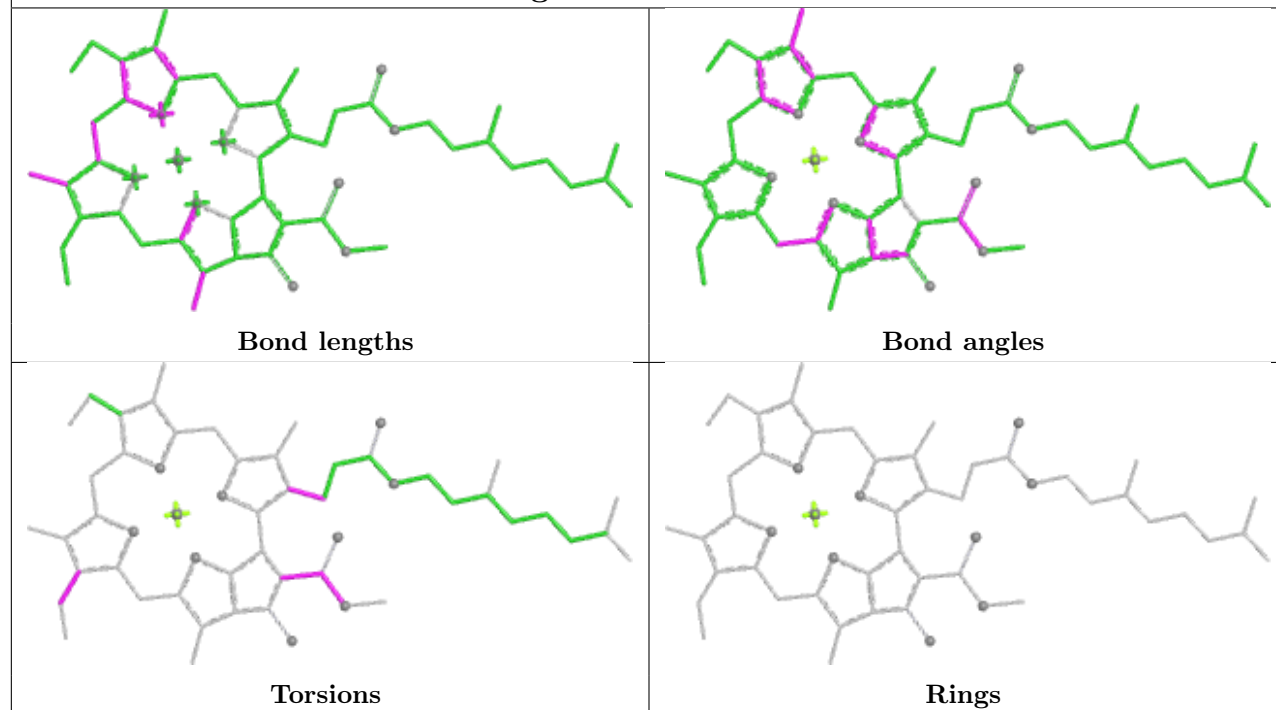
Ligand CLA 4 601



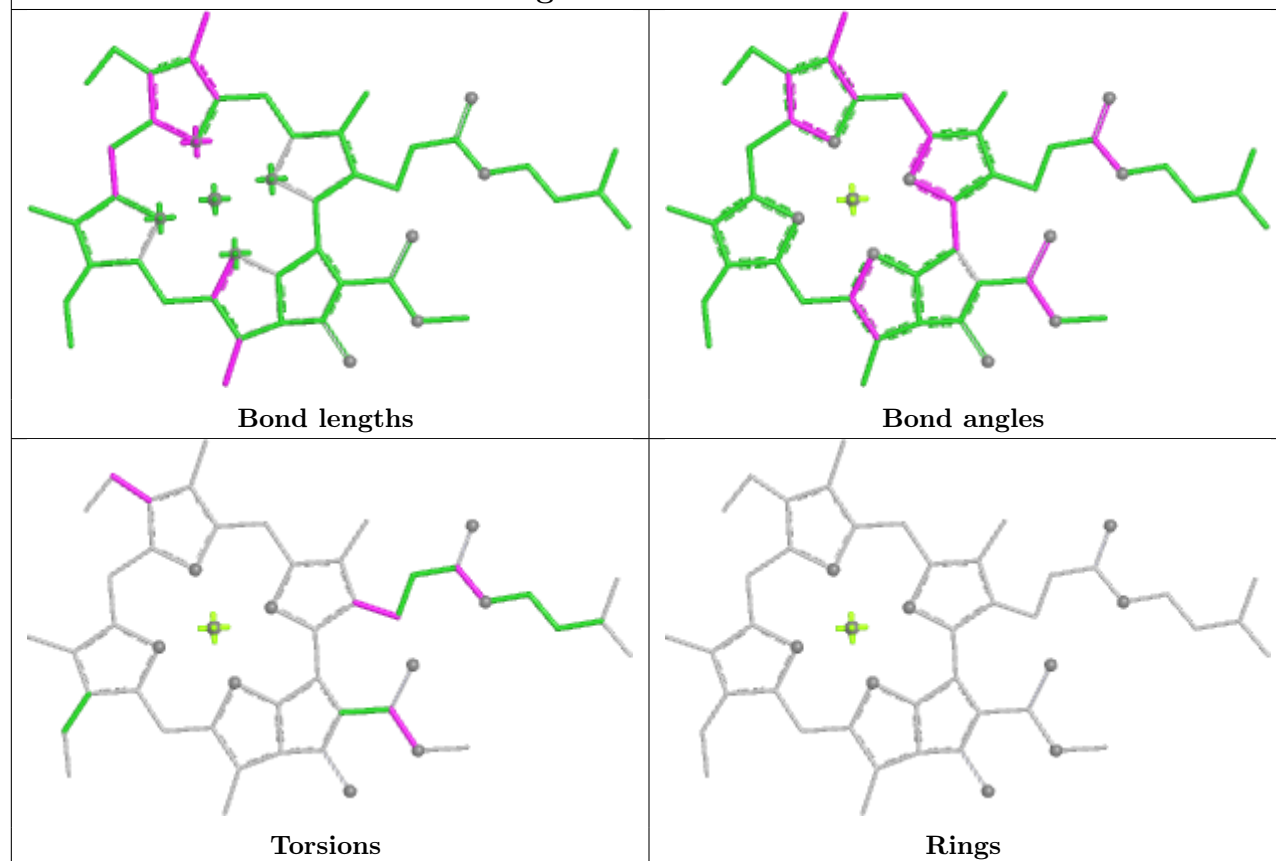
Ligand CLA B 1238

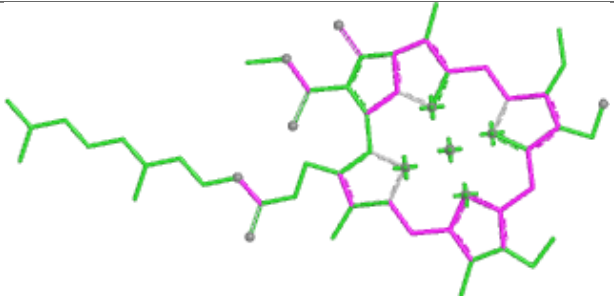
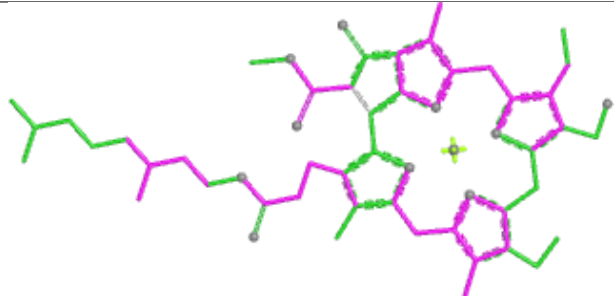
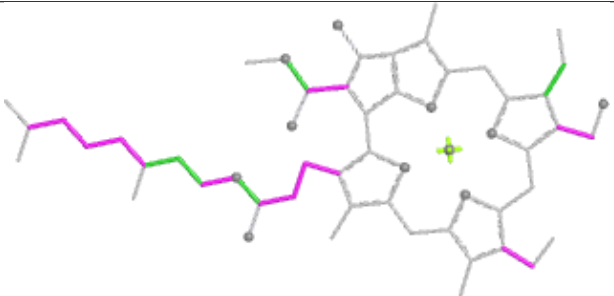
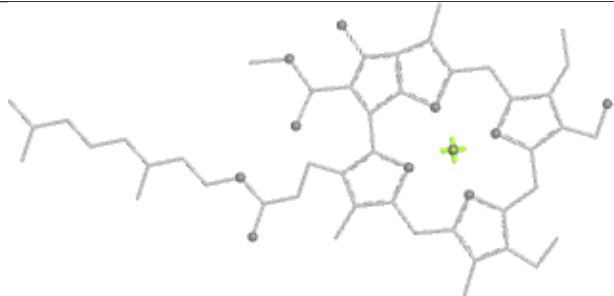


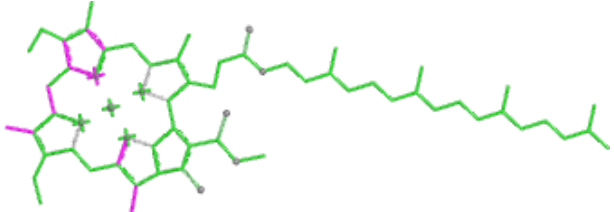
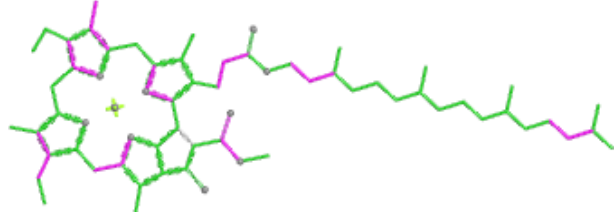
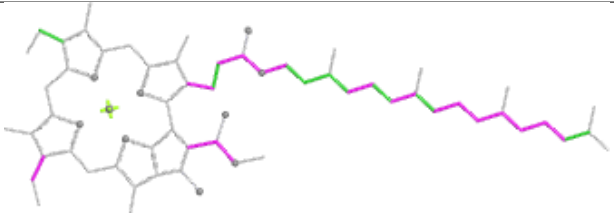
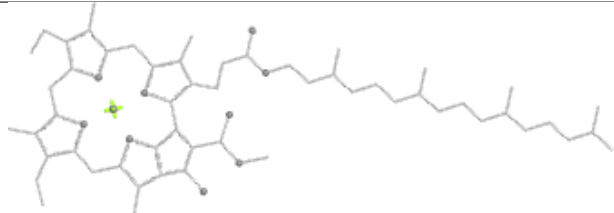
Ligand CLA K 201

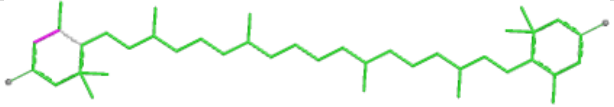
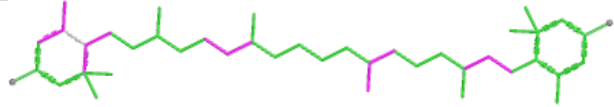
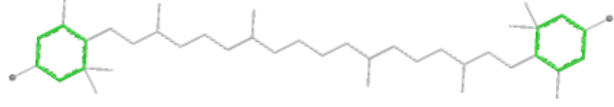


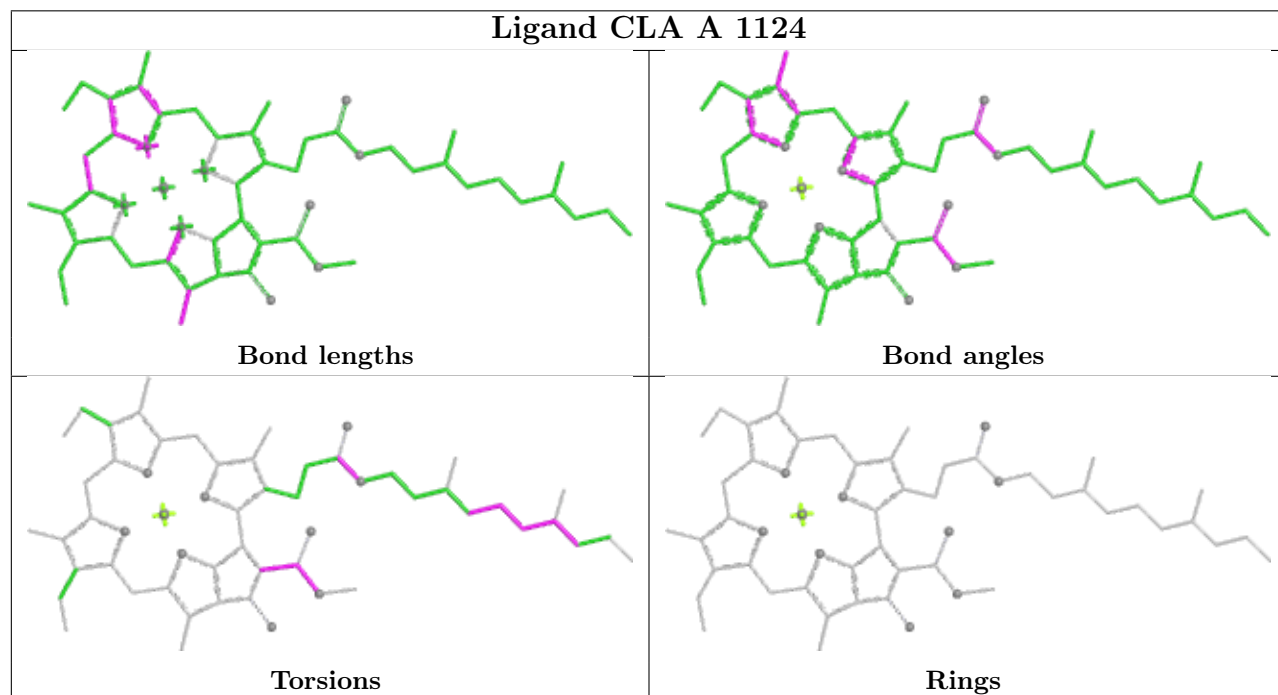
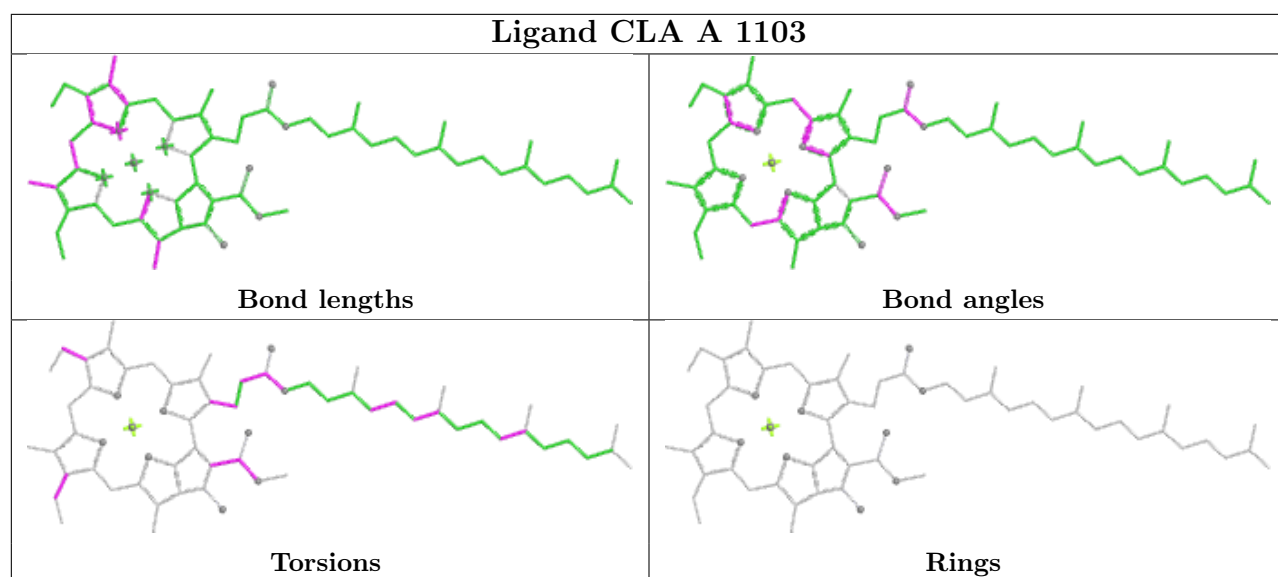
Ligand CLA 3 604



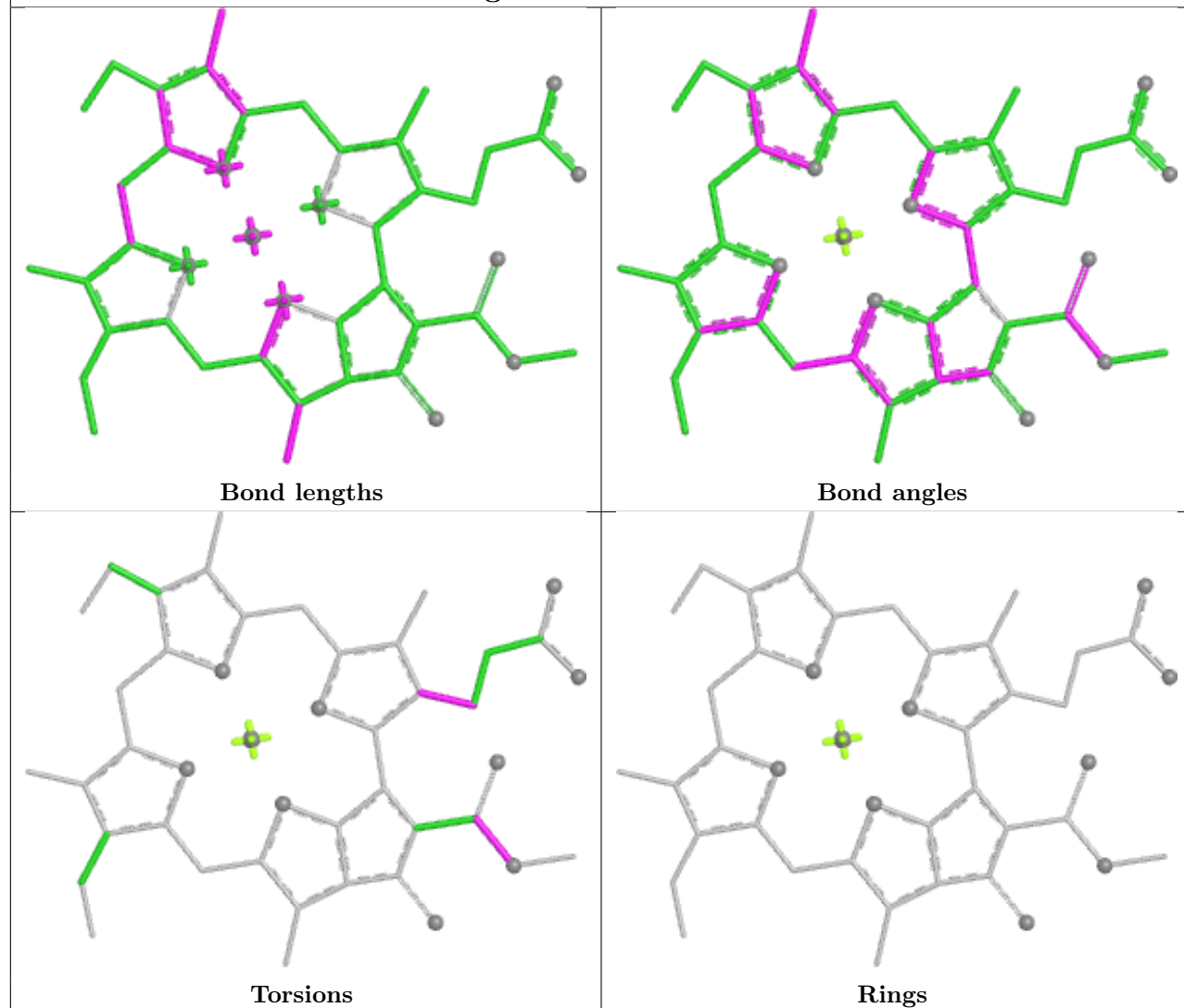
Ligand CHL 2 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1210	
	
Bond lengths	Bond angles
	
Torsions	Rings

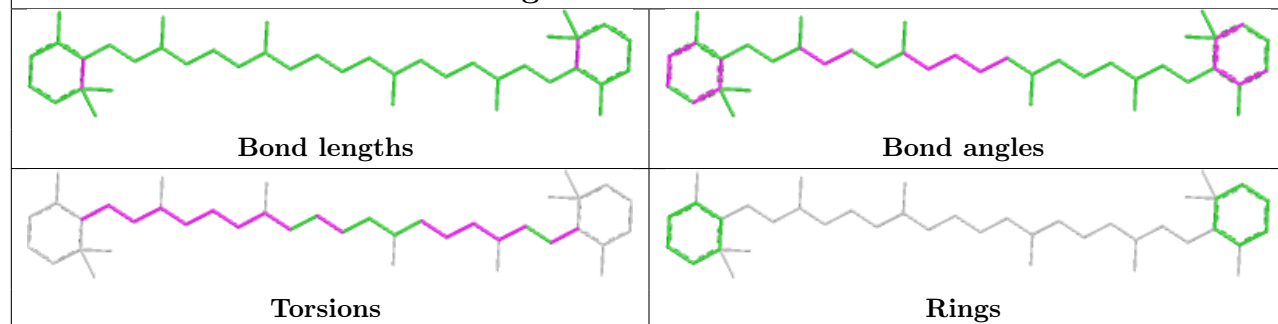
Ligand LUT 3 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

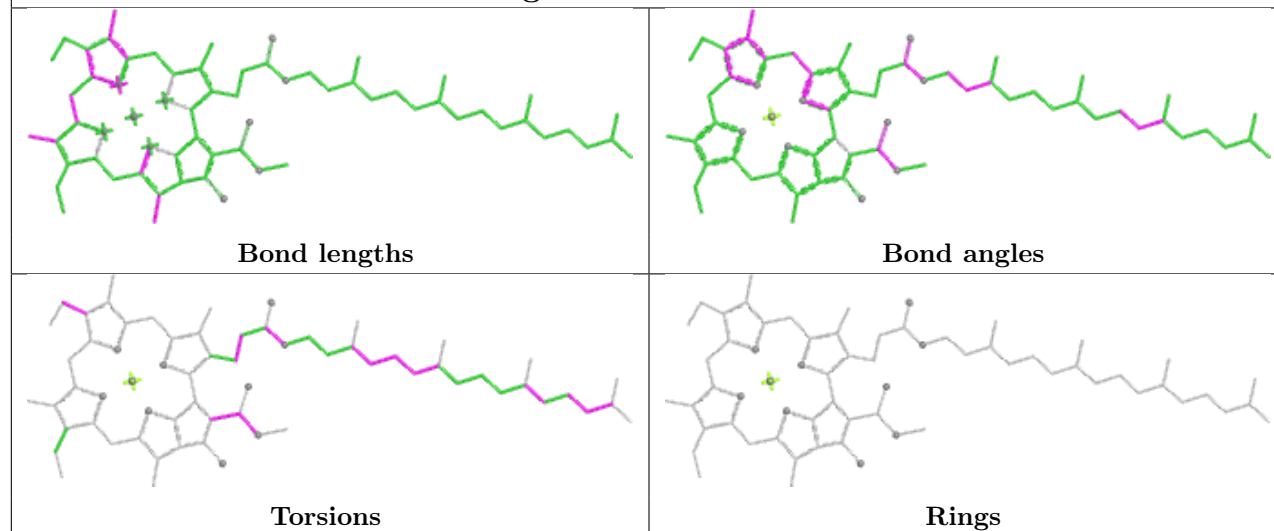
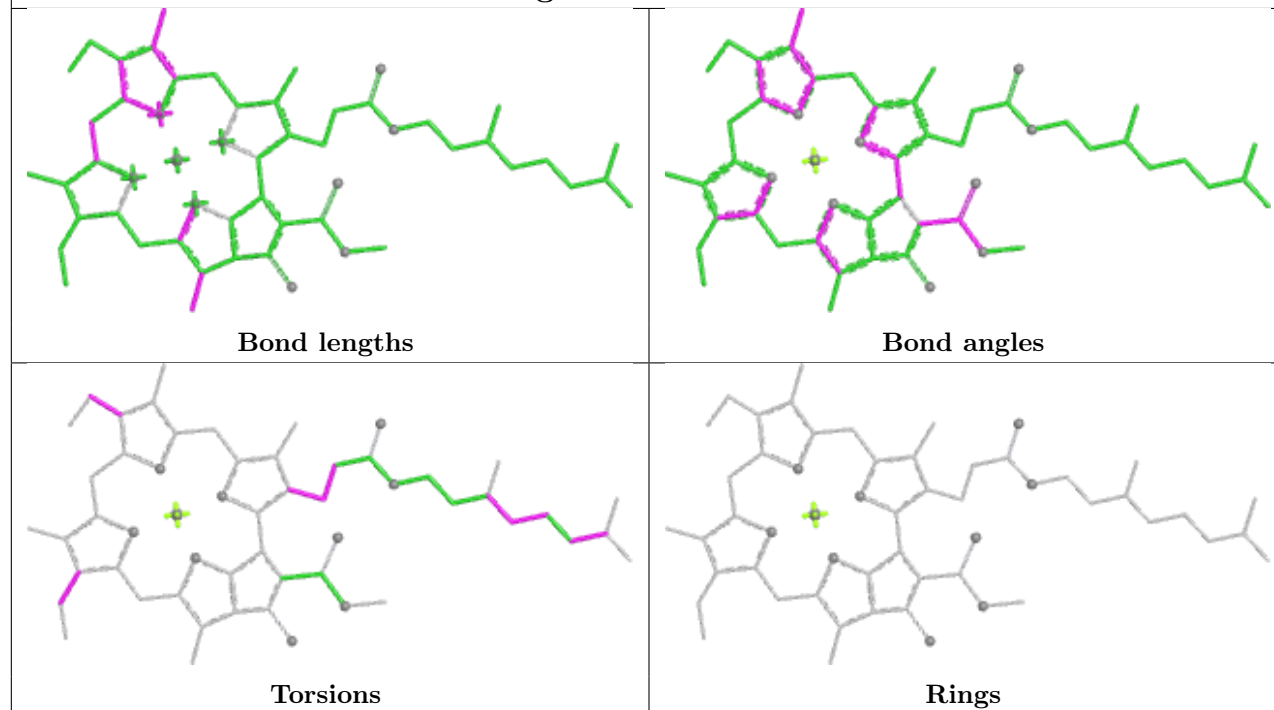


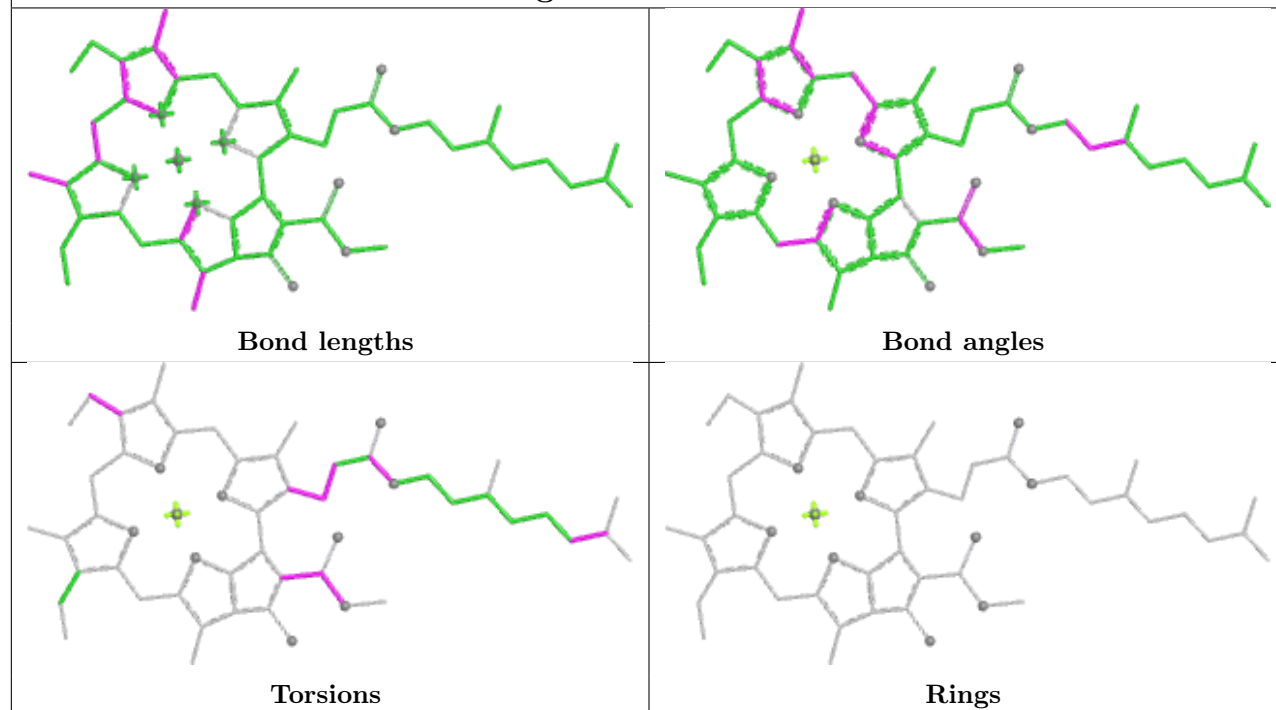
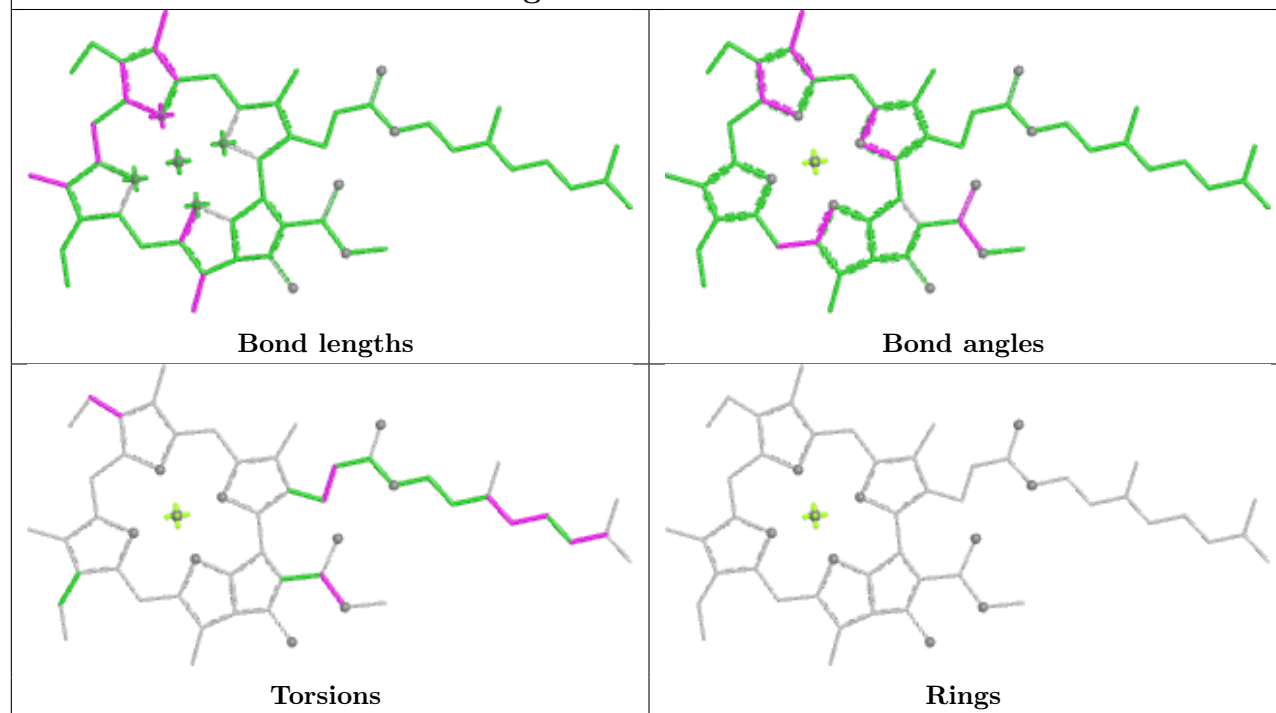
Ligand CLA B 1219

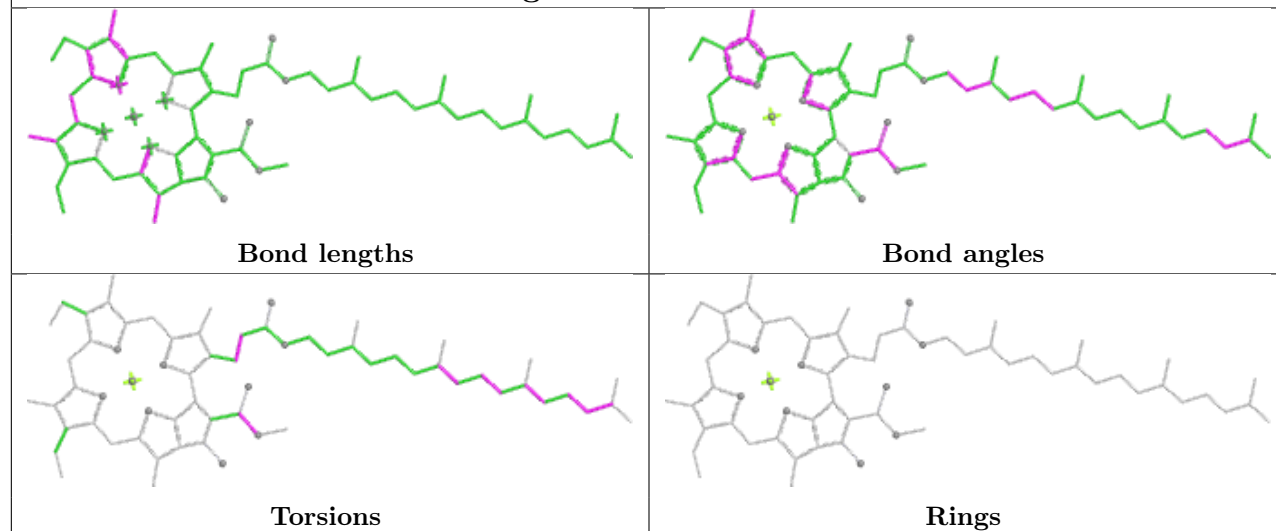
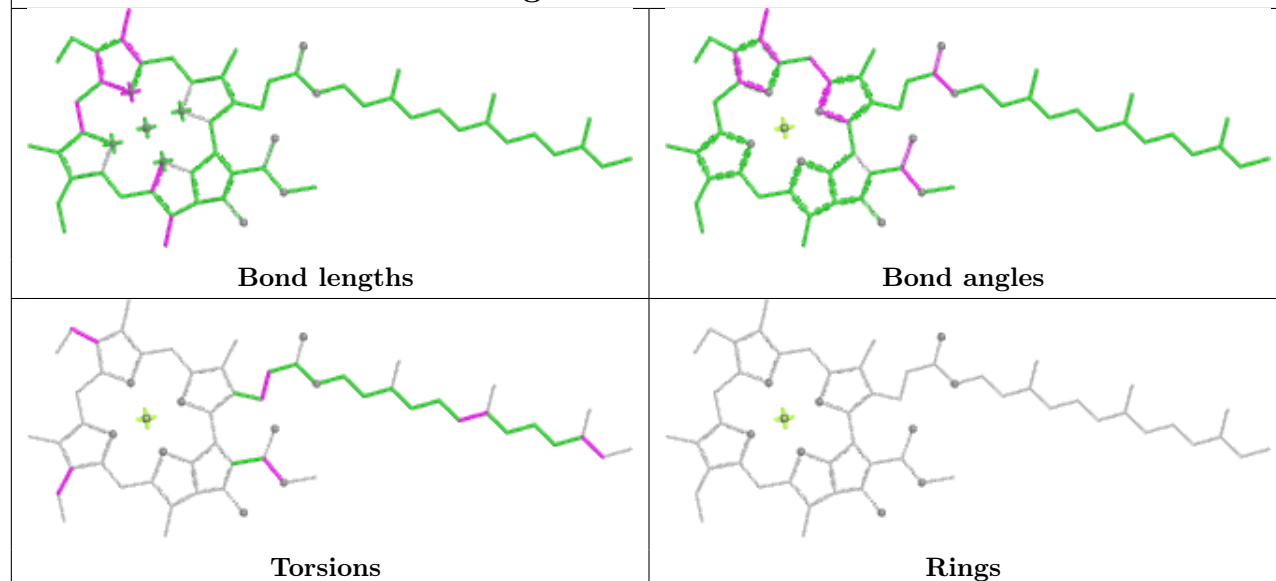


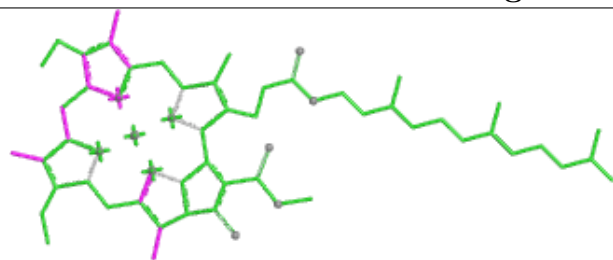
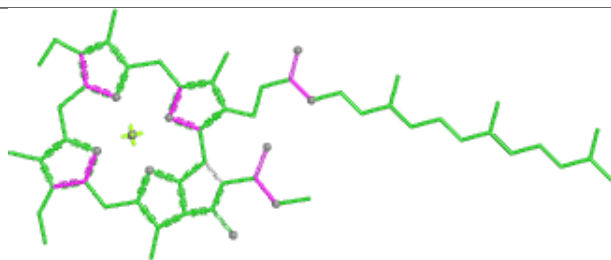
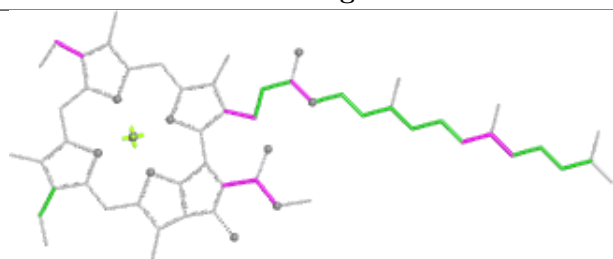
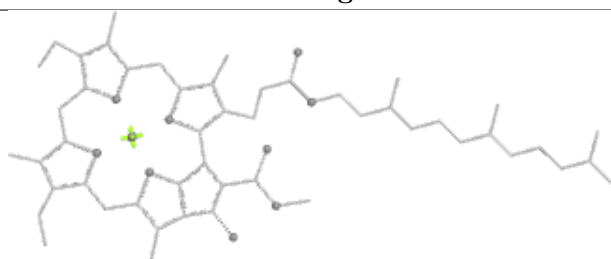
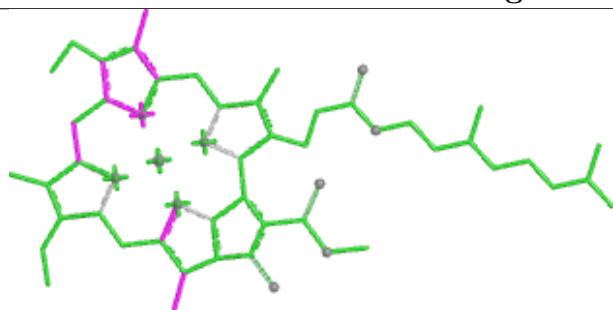
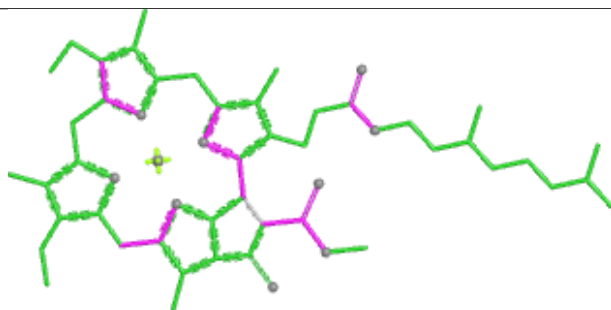
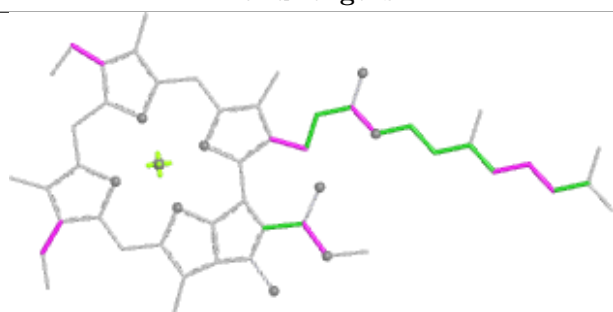
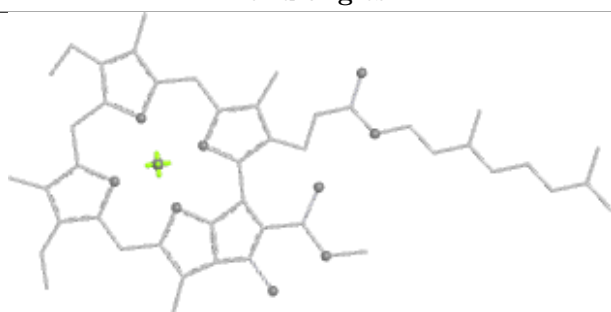
Ligand BCR B 4014

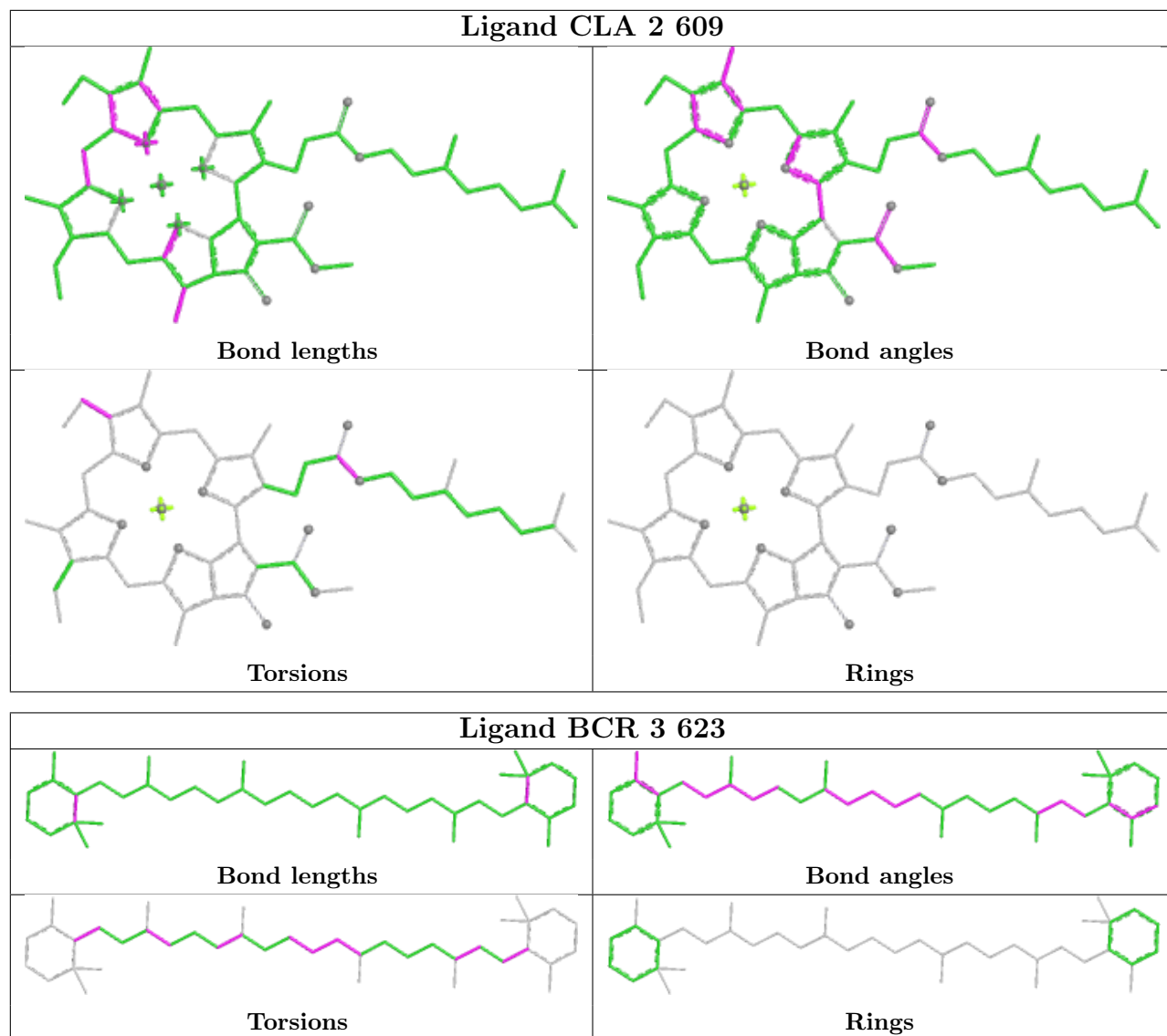


Ligand CLA A 1104**Ligand CLA 4 609**

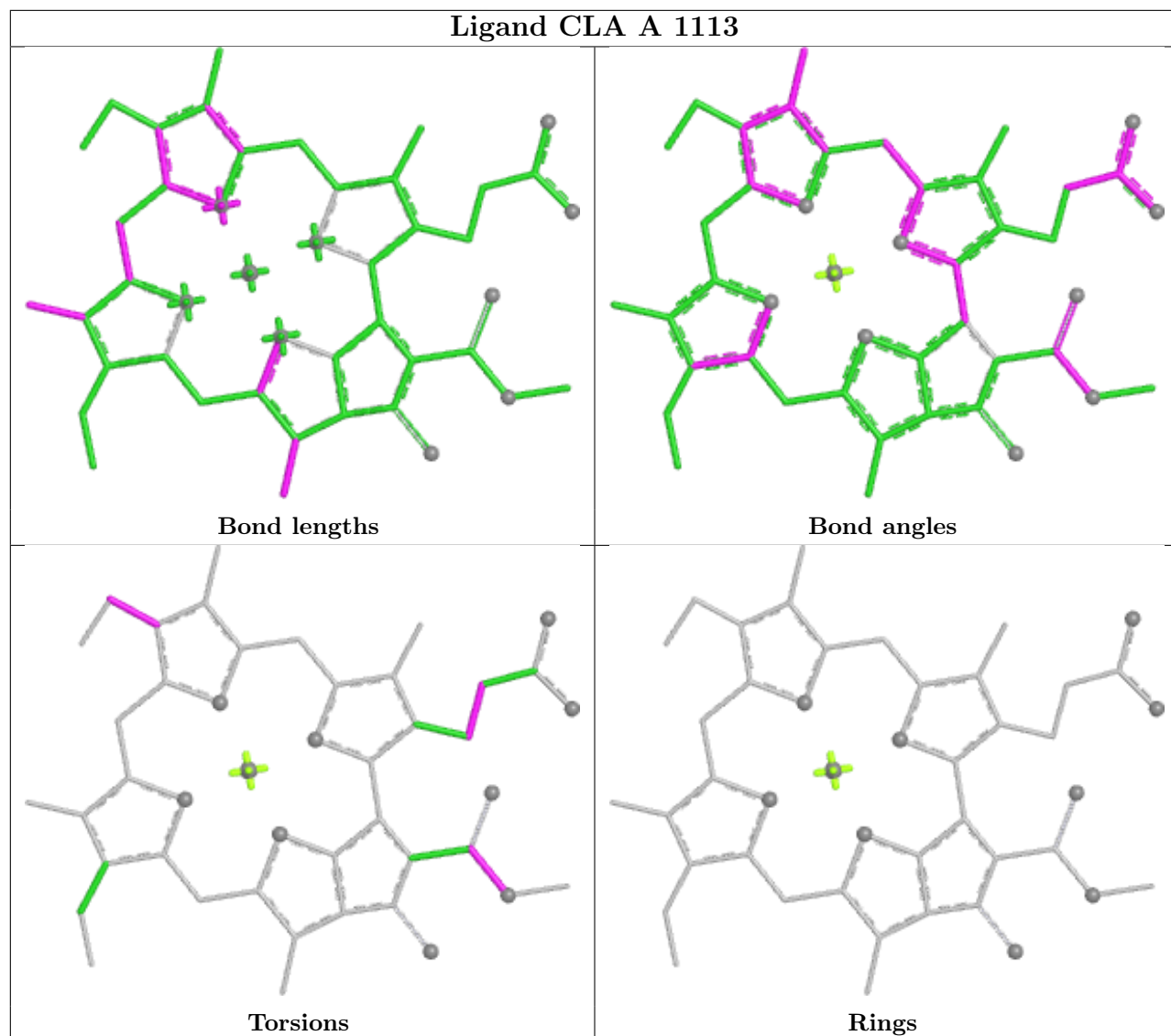
Ligand CLA 4 603**Ligand CLA B 1235**

Ligand CLA A 1117**Ligand CLA B 1204**

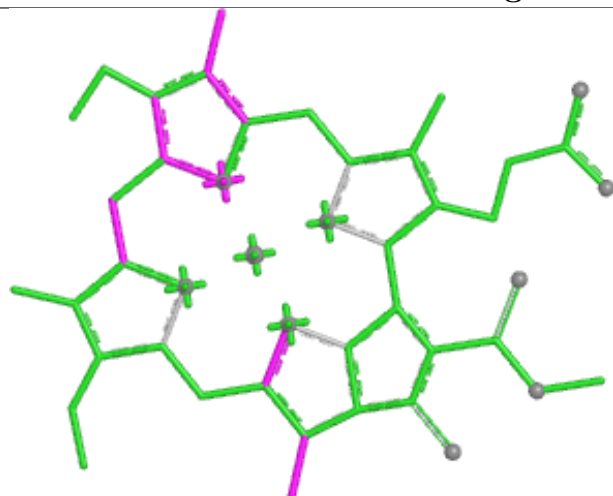
Ligand CLA A 1122**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 1229****Bond lengths****Bond angles****Torsions****Rings**



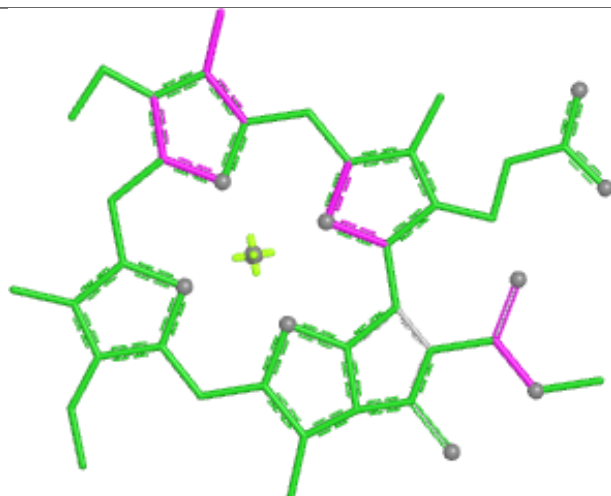
Ligand CLA A 1113



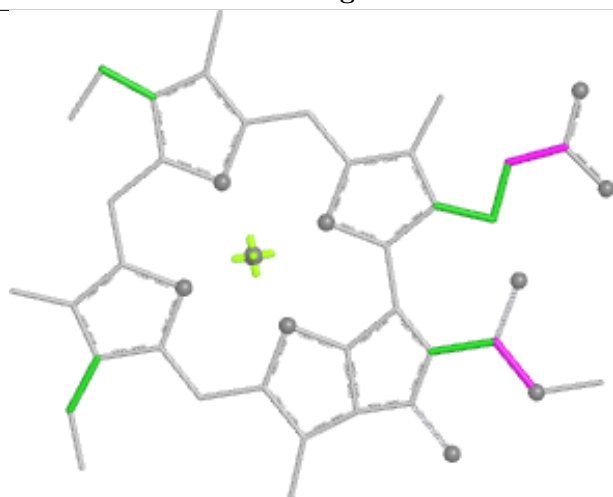
Ligand CLA A 1120



Bond lengths



Bond angles

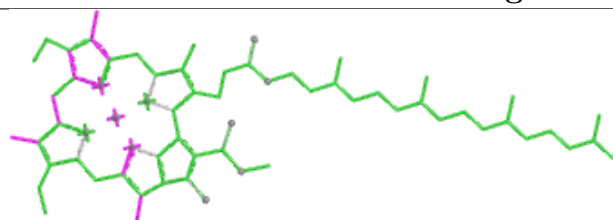


Torsions

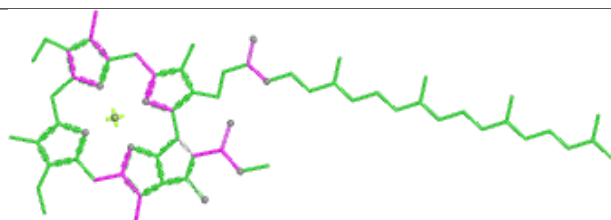


Rings

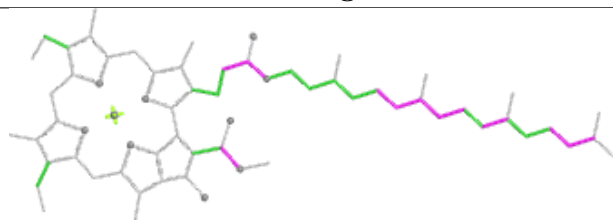
Ligand CLA B 1021



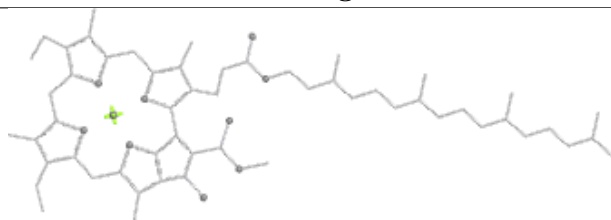
Bond lengths



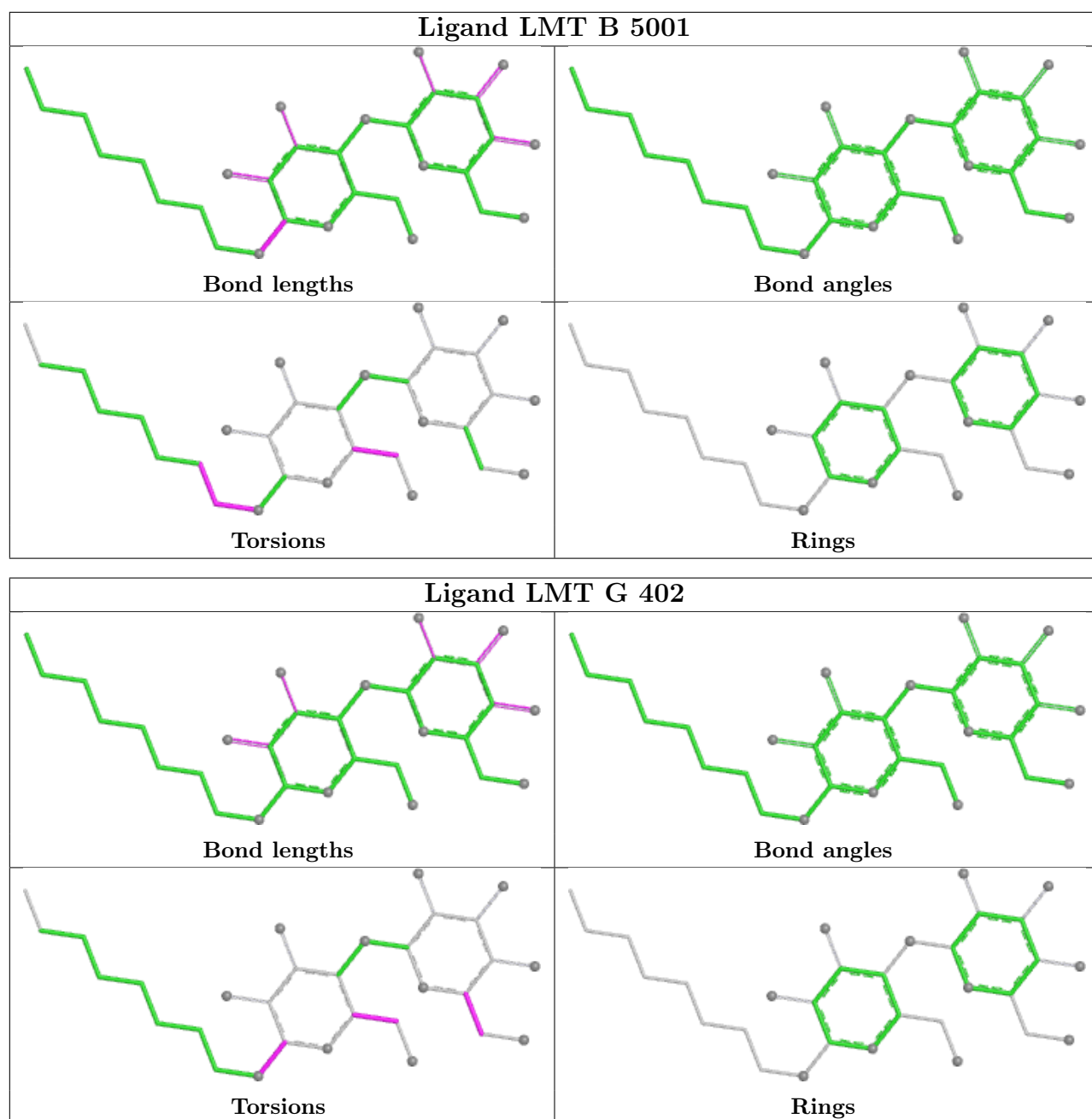
Bond angles



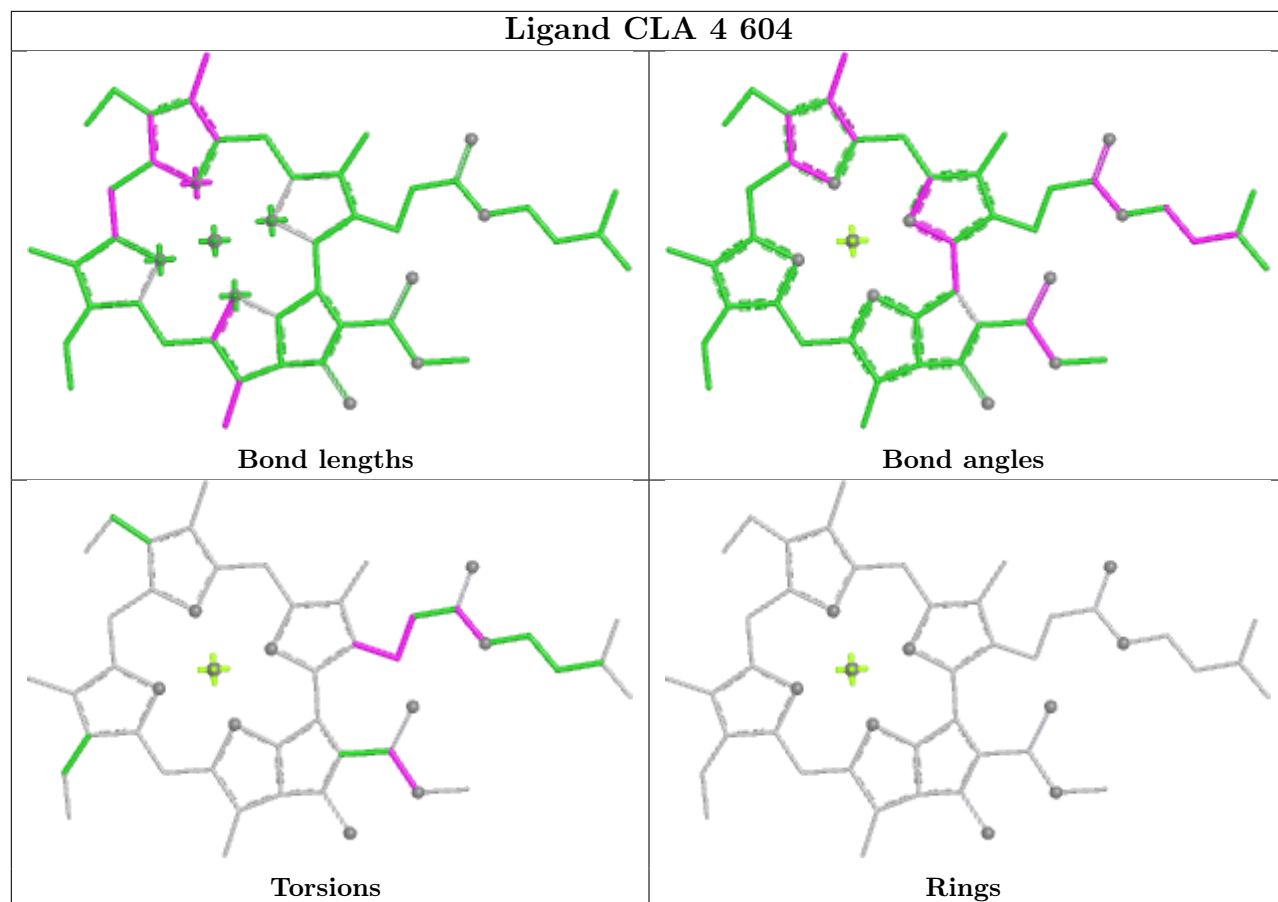
Torsions



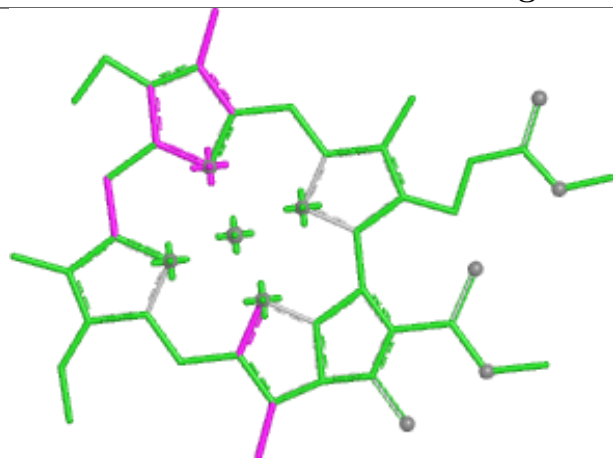
Rings



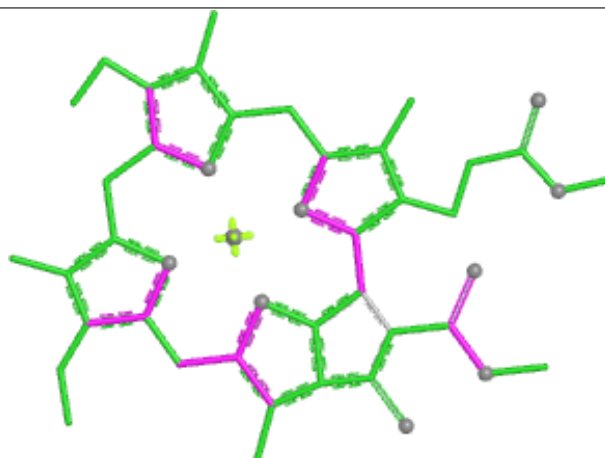
Ligand CLA 4 604



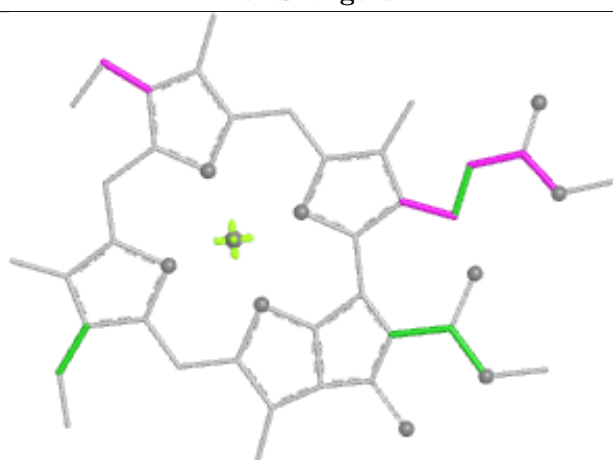
Ligand CLA 1 614



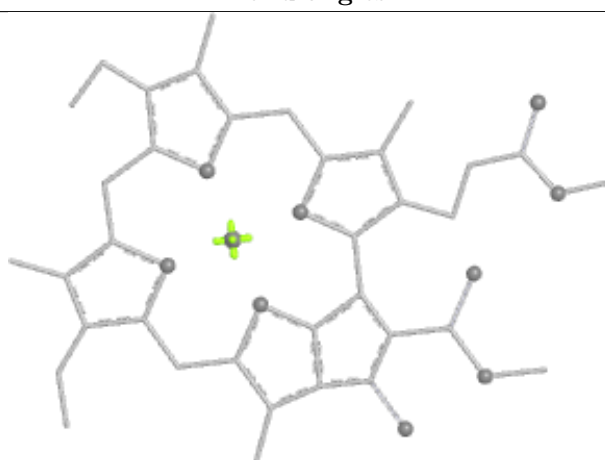
Bond lengths



Bond angles

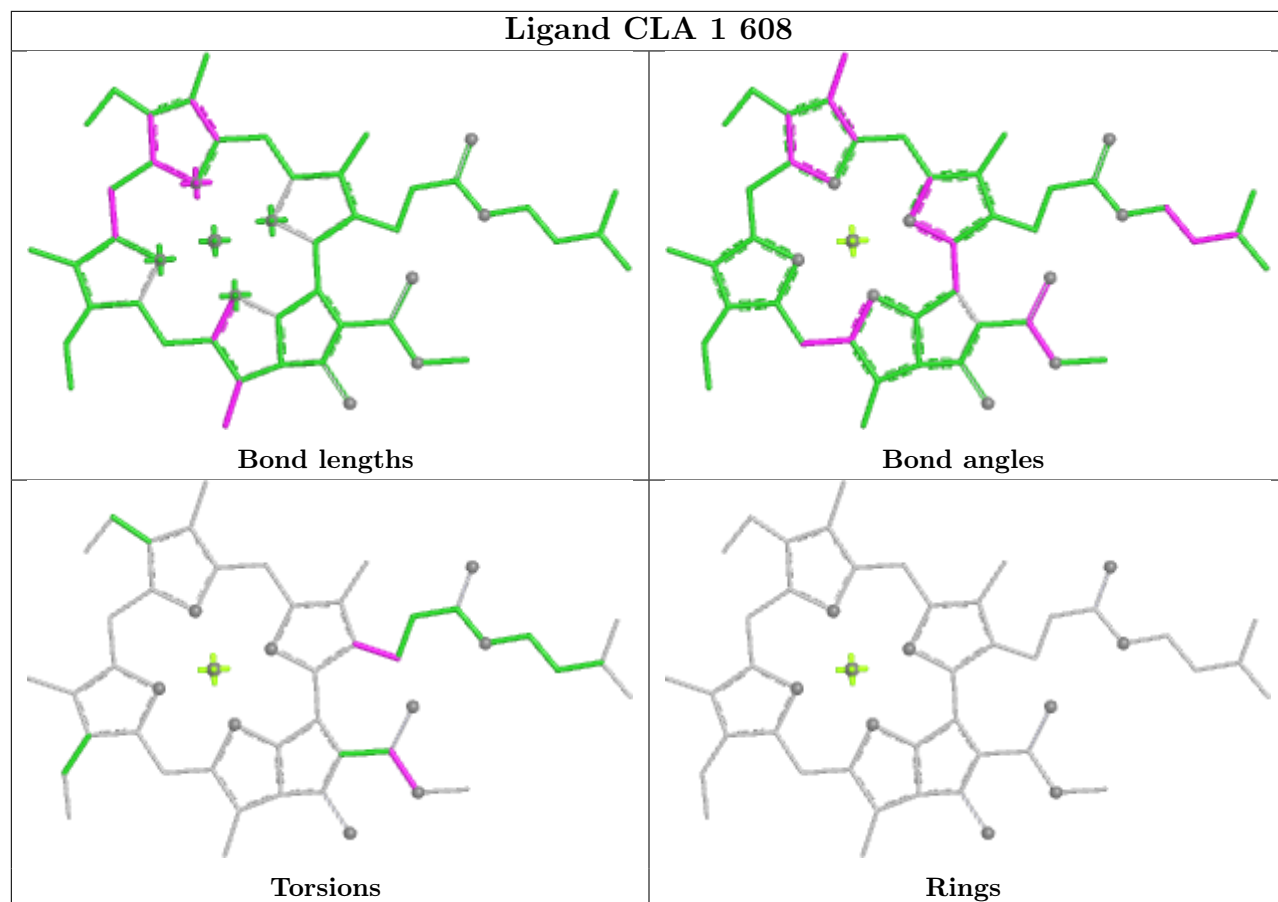


Torsions

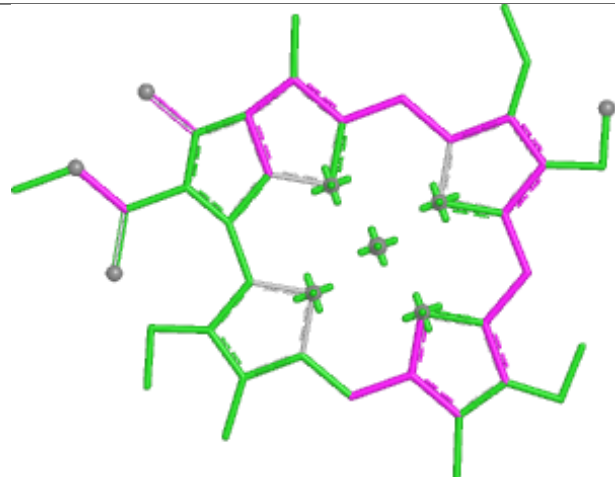


Rings

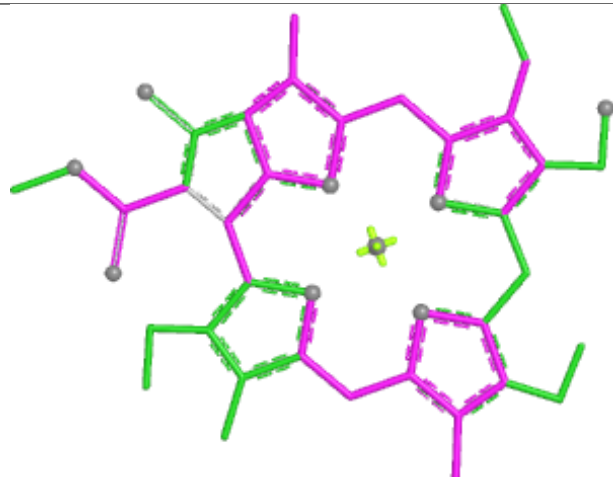
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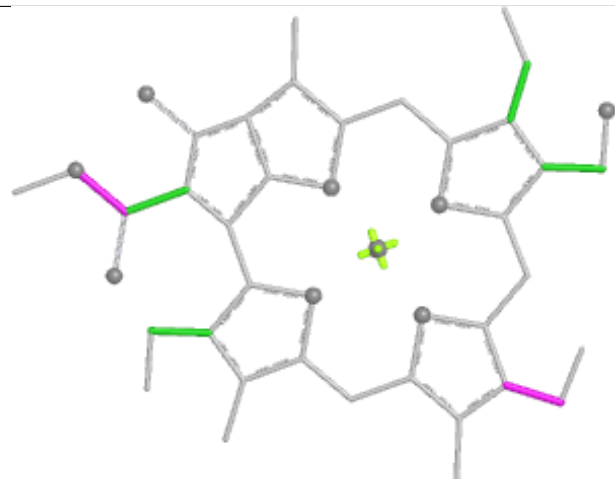
Ligand CHL 4 615



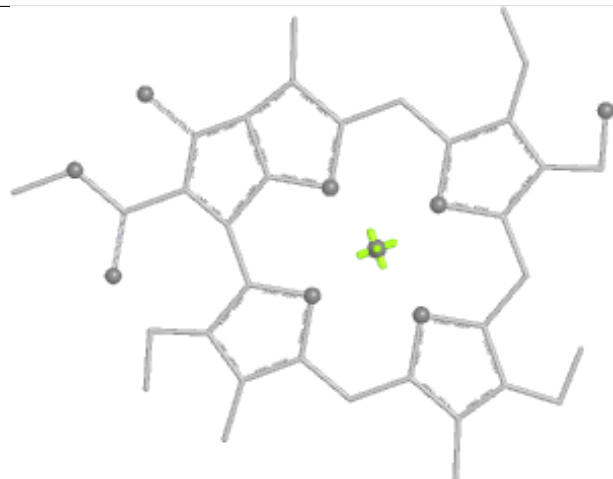
Bond lengths



Bond angles

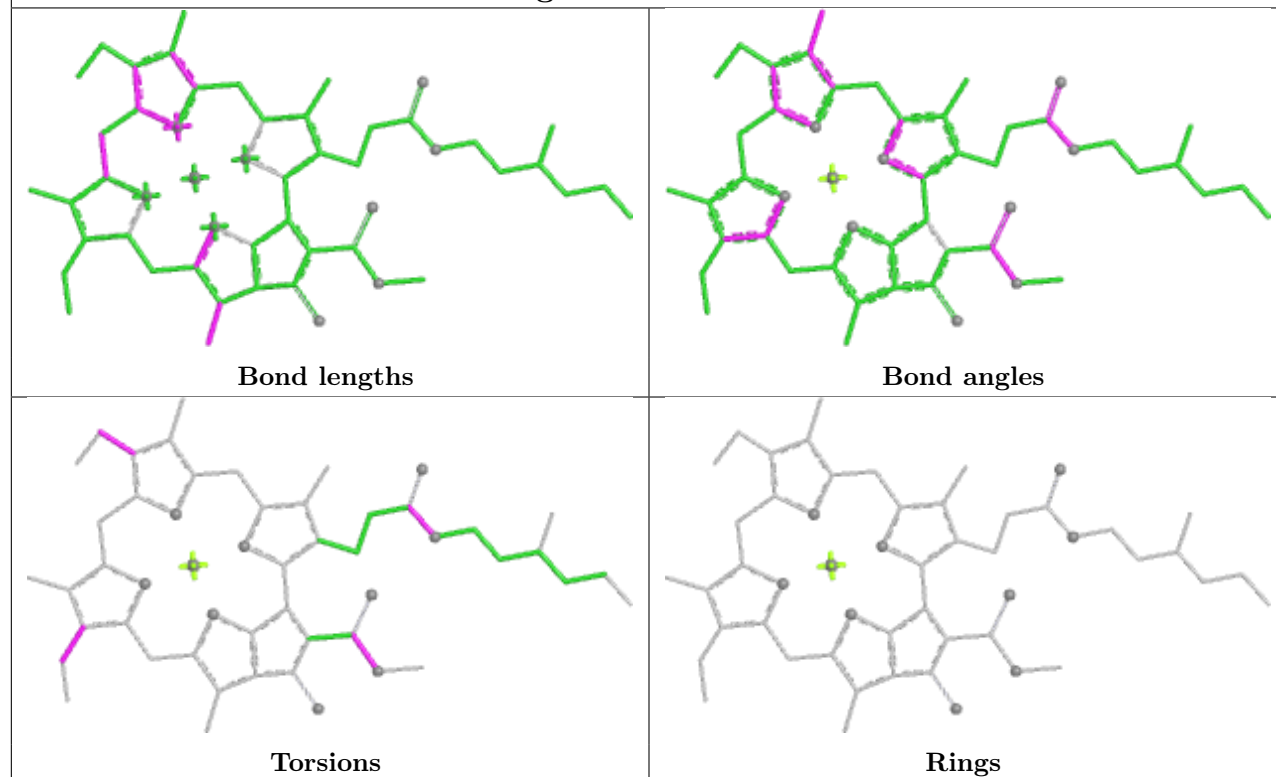


Torsions

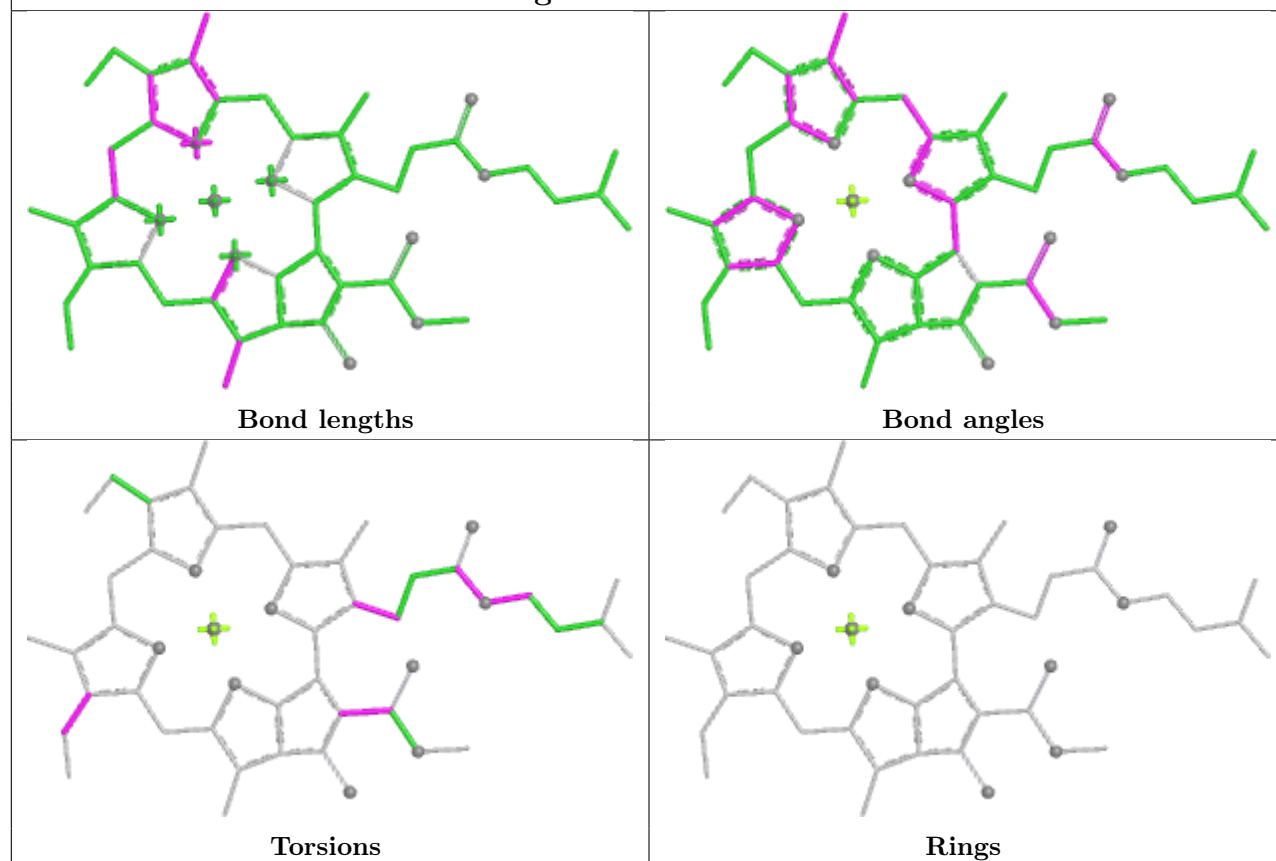


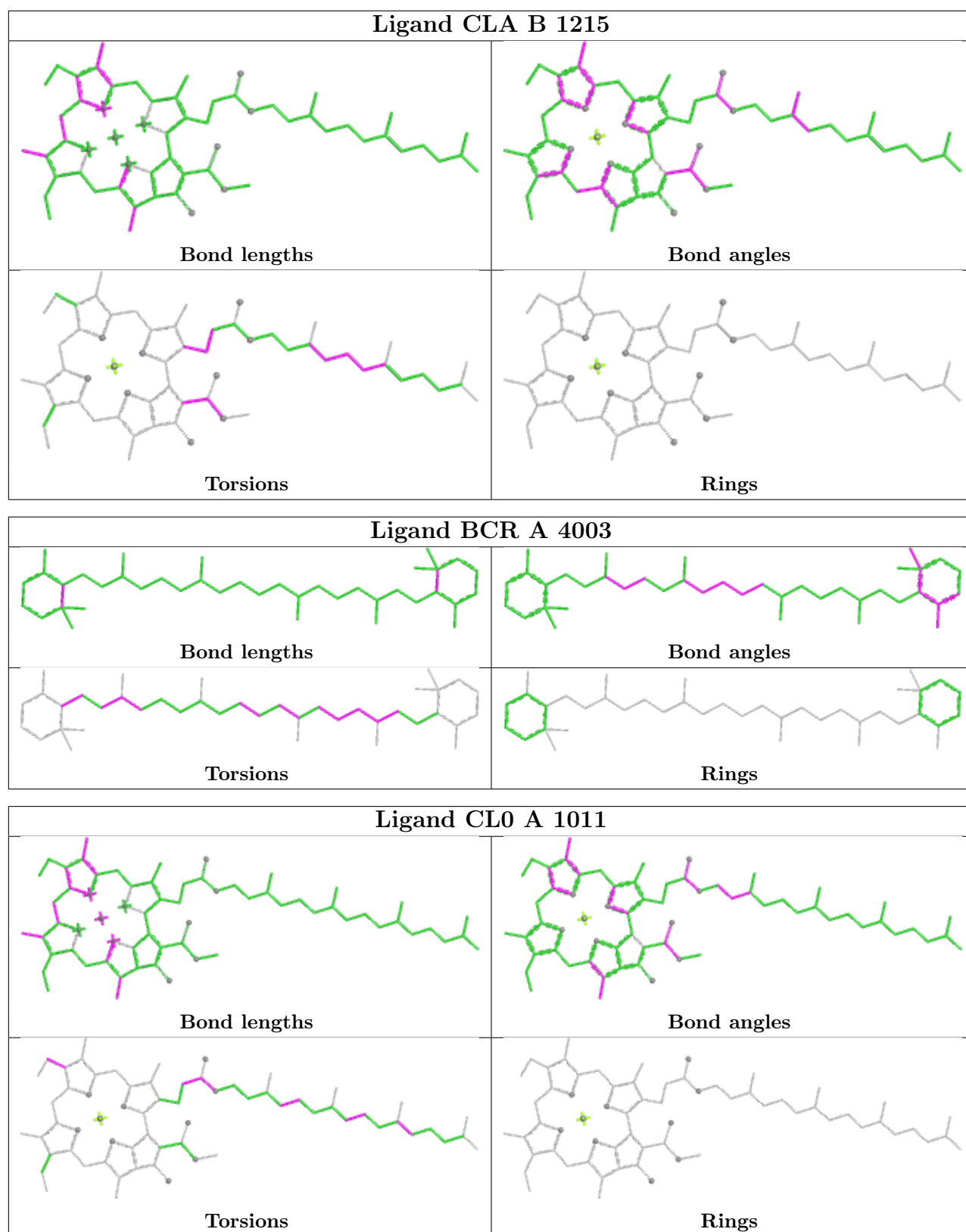
Rings

Ligand CLA 2 612

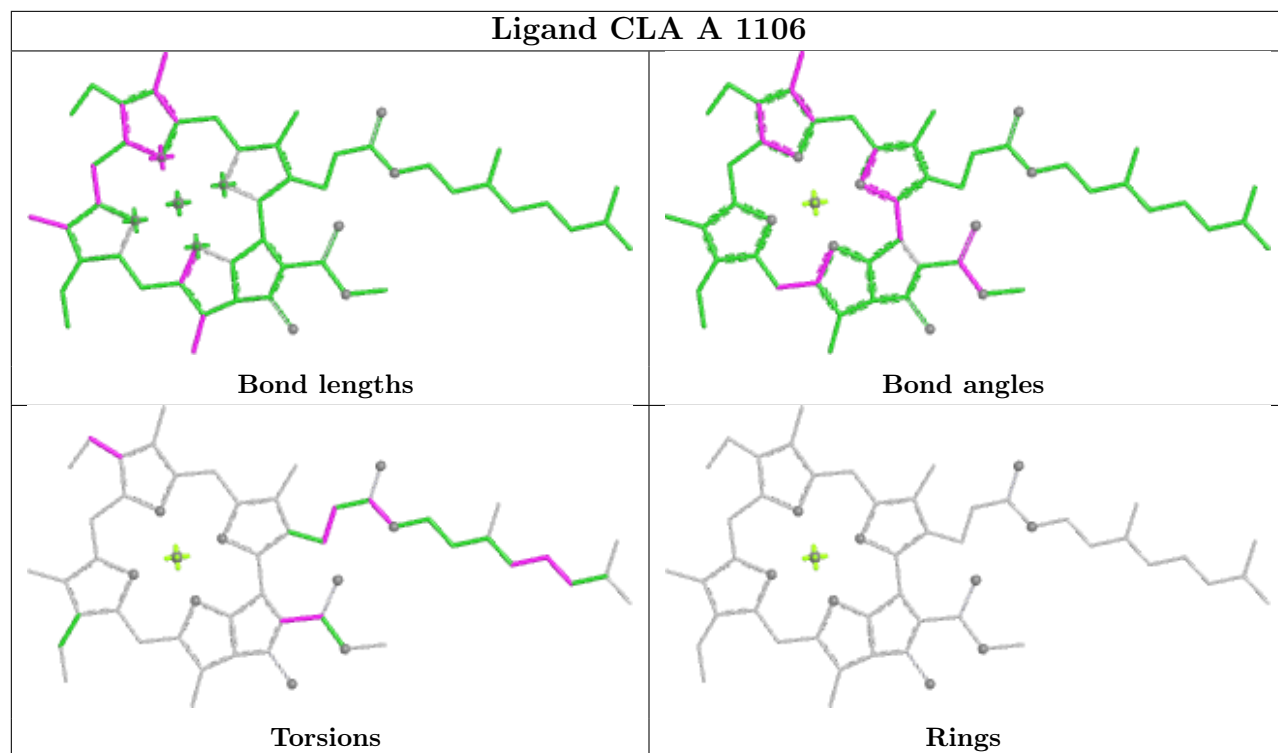


Ligand CLA L 301

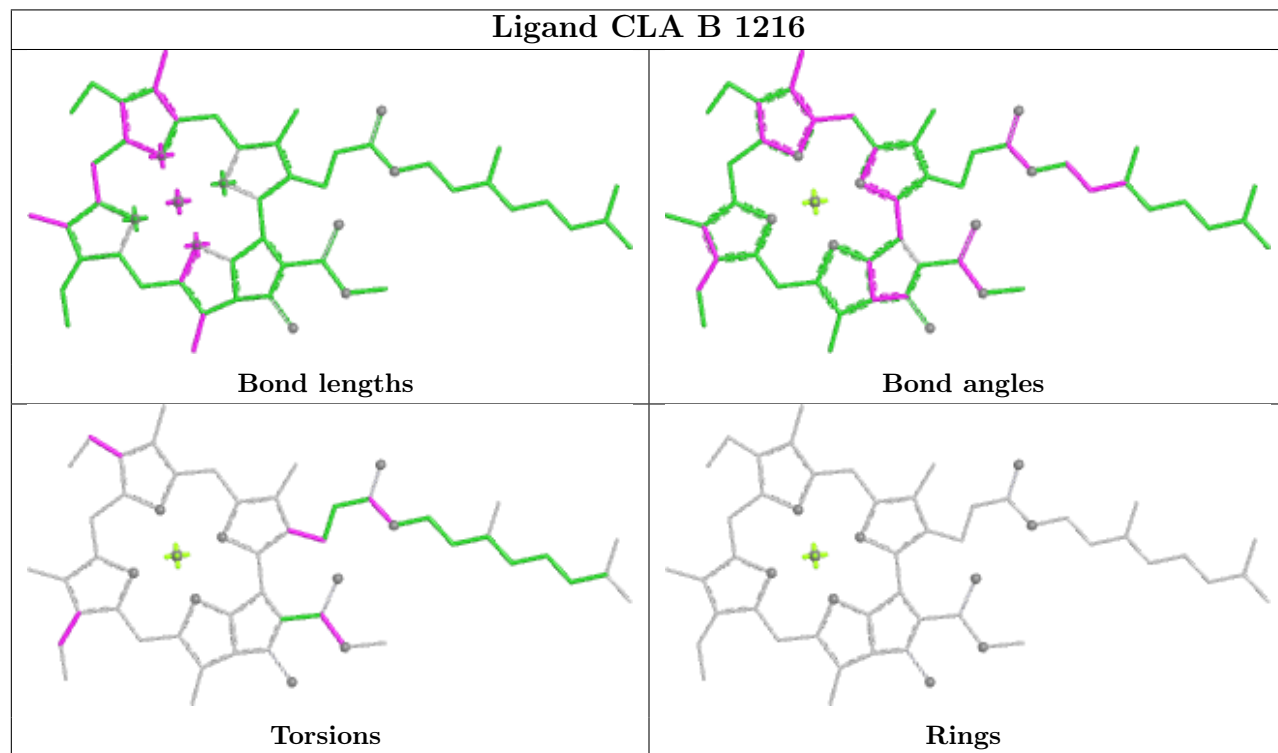




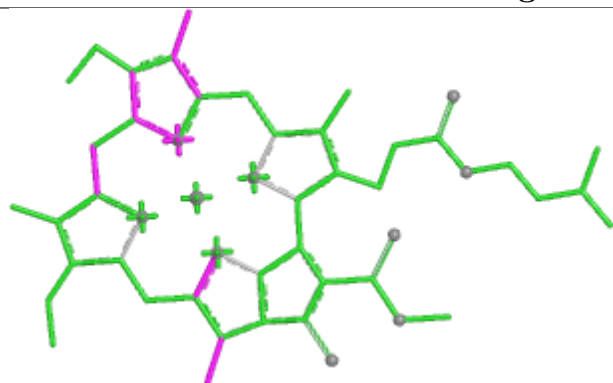
Ligand CLA A 1106



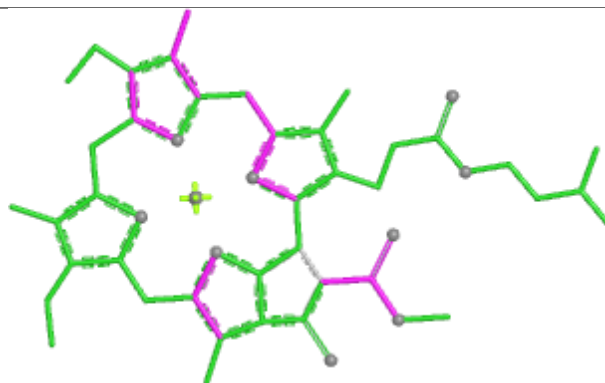
Ligand CLA B 1216



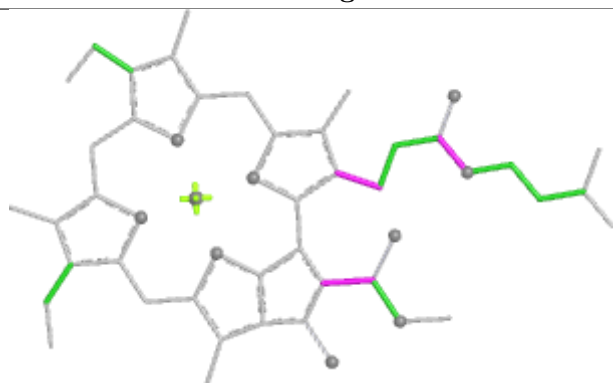
Ligand CLA 2 614



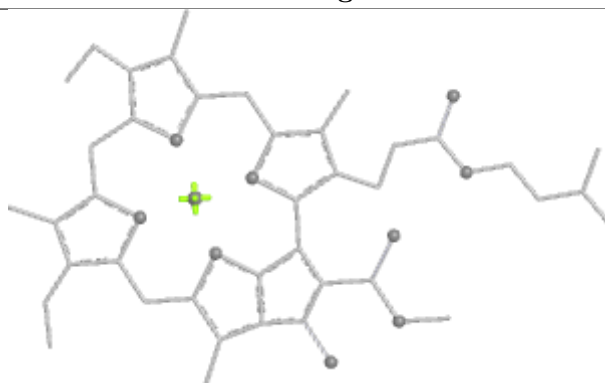
Bond lengths



Bond angles

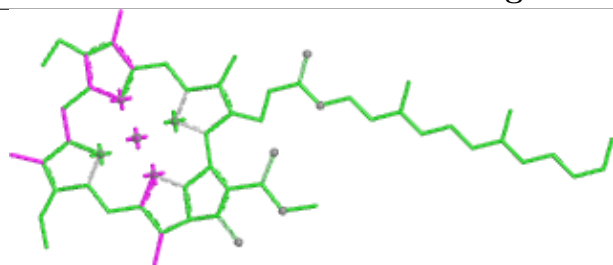


Torsions

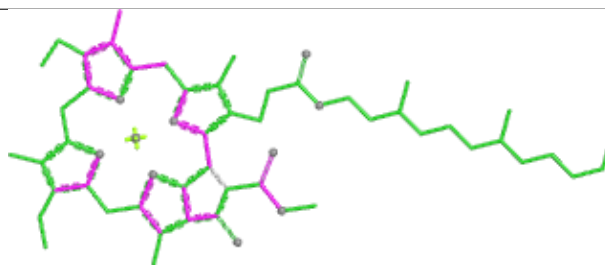


Rings

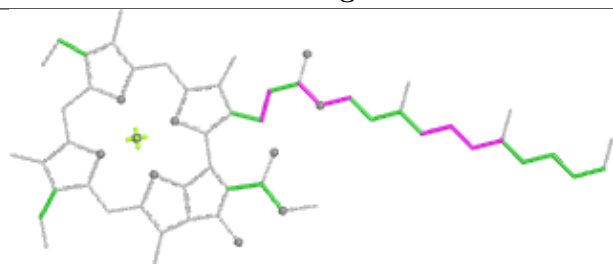
Ligand CLA B 1214



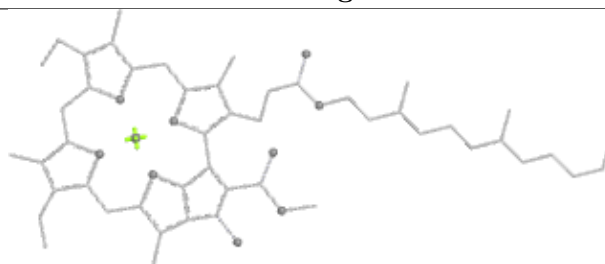
Bond lengths



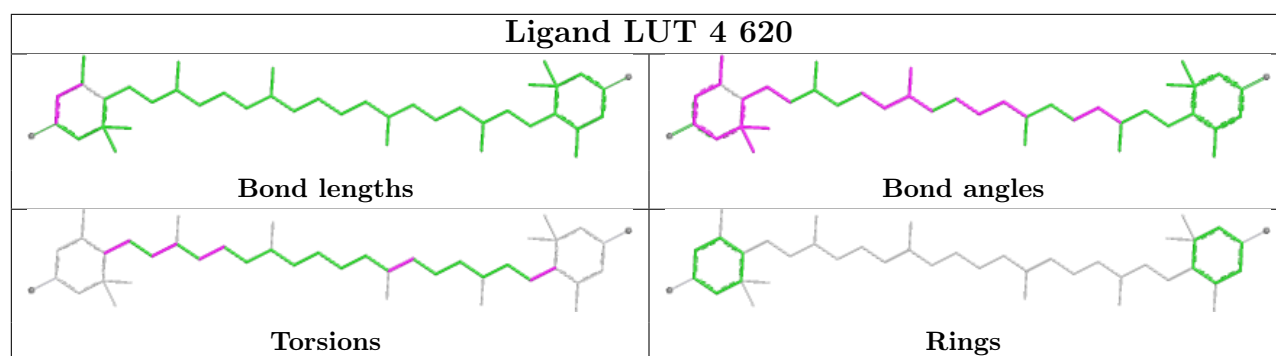
Bond angles



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.

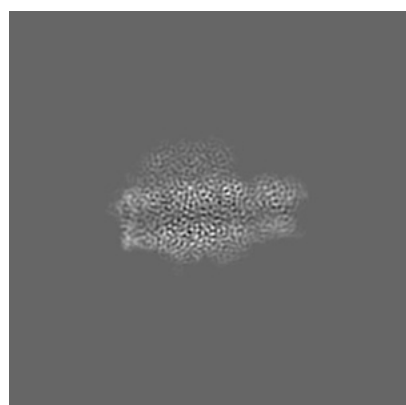
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23023. 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](#)

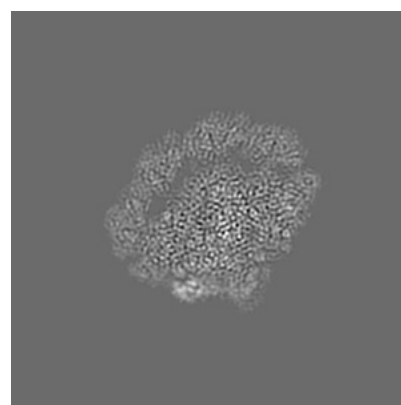
6.1.1 Primary map



X



Y

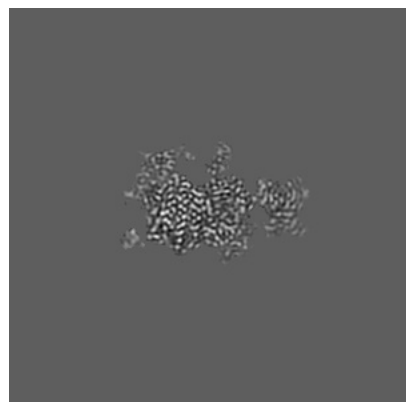


Z

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

6.2 Central slices [i](#)

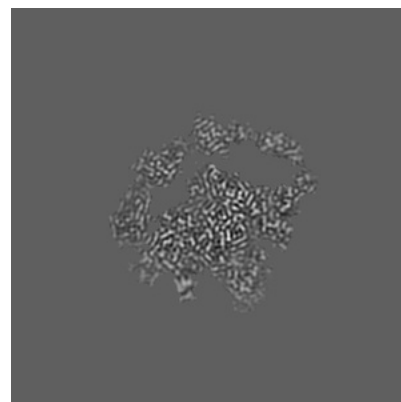
6.2.1 Primary map



X Index: 140



Y Index: 140



Z Index: 140

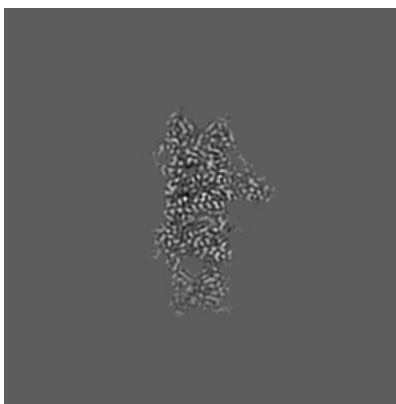
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

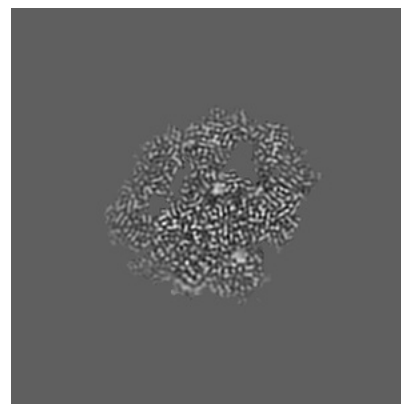
6.3.1 Primary map



X Index: 150



Y Index: 133

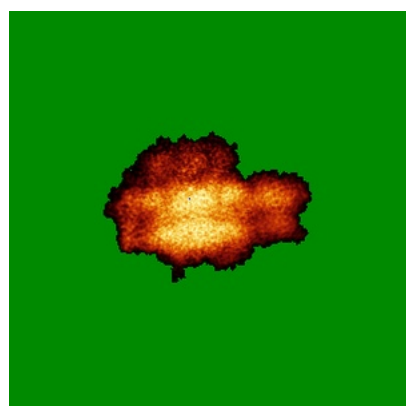


Z Index: 148

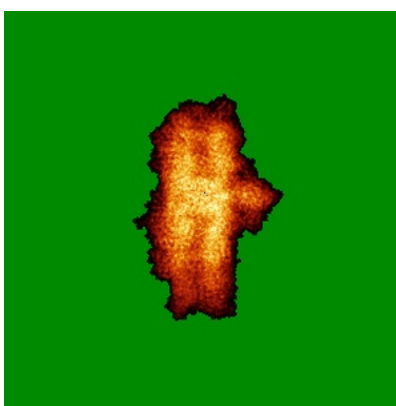
The images above show the largest variance slices of the map in three orthogonal directions.

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

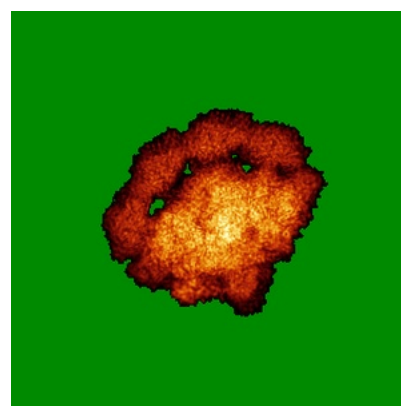
6.4.1 Primary map



X



Y

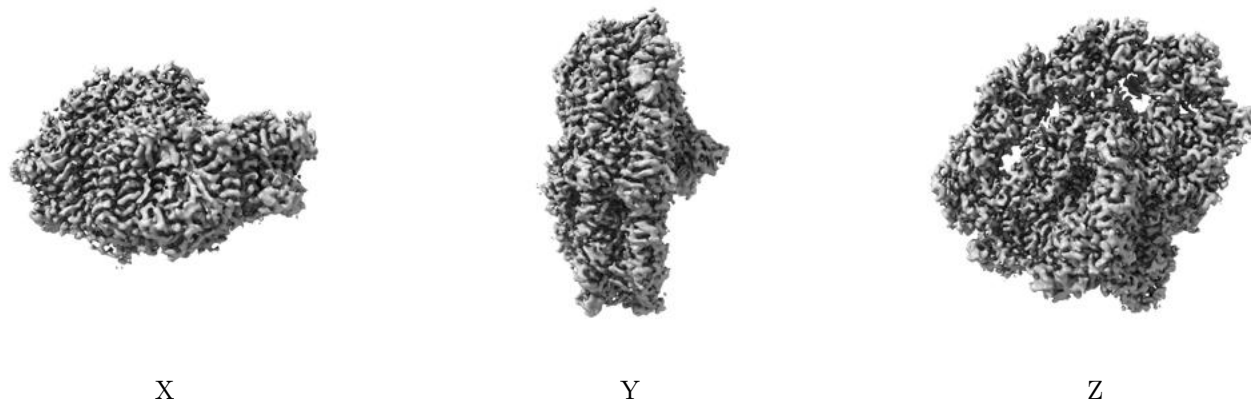


Z

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 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

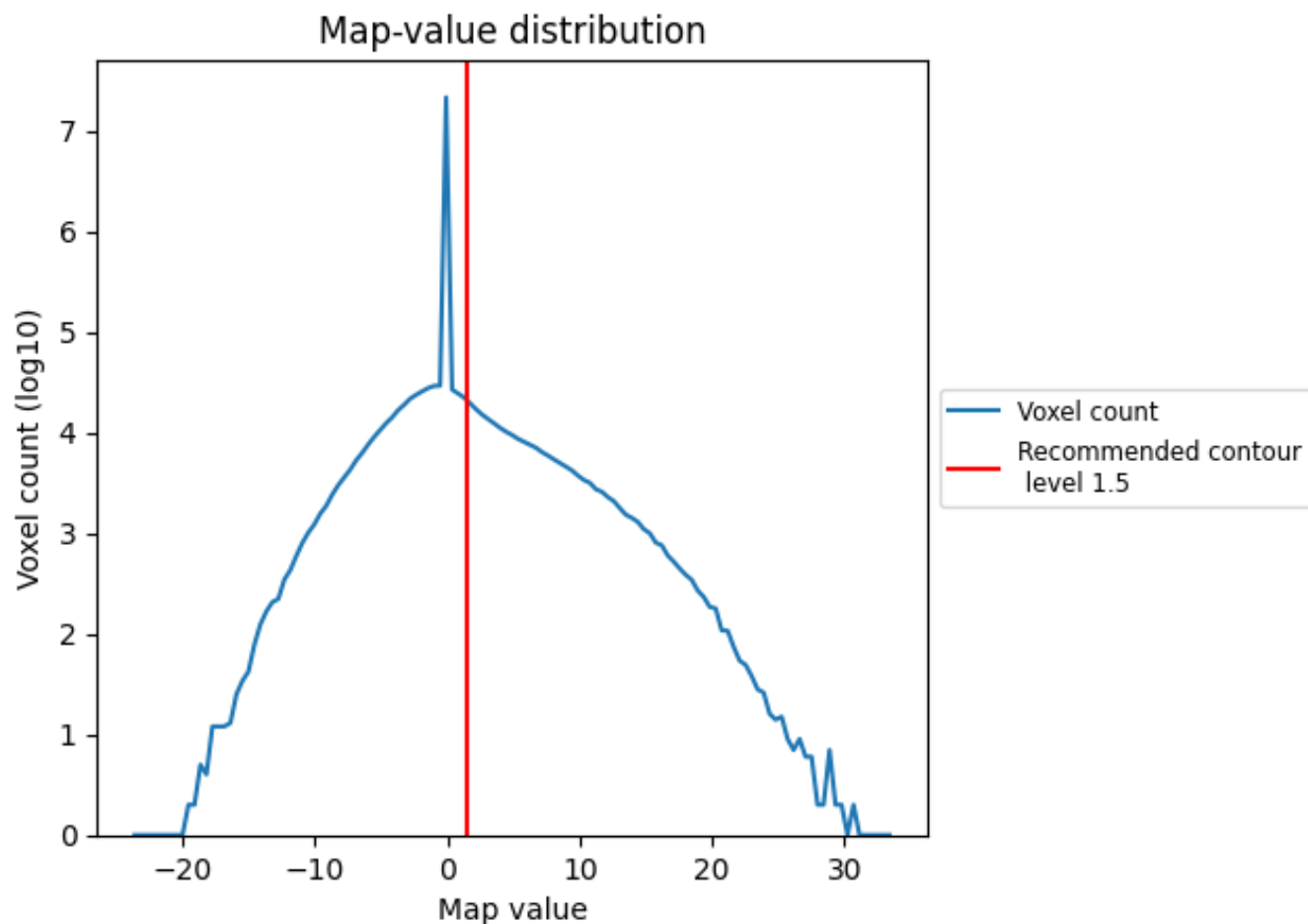
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

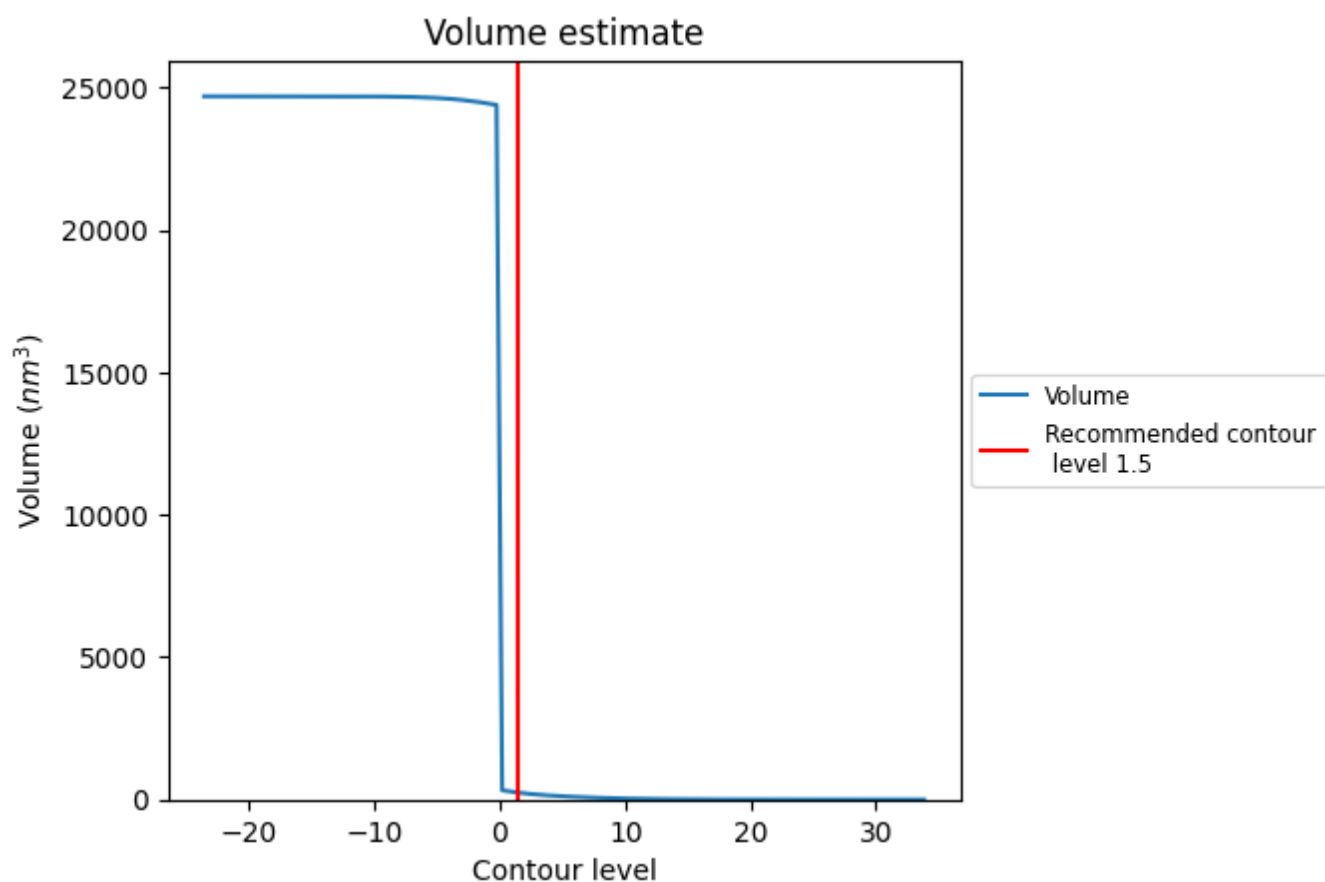
This section contains the results of statistical analysis of the map.

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.

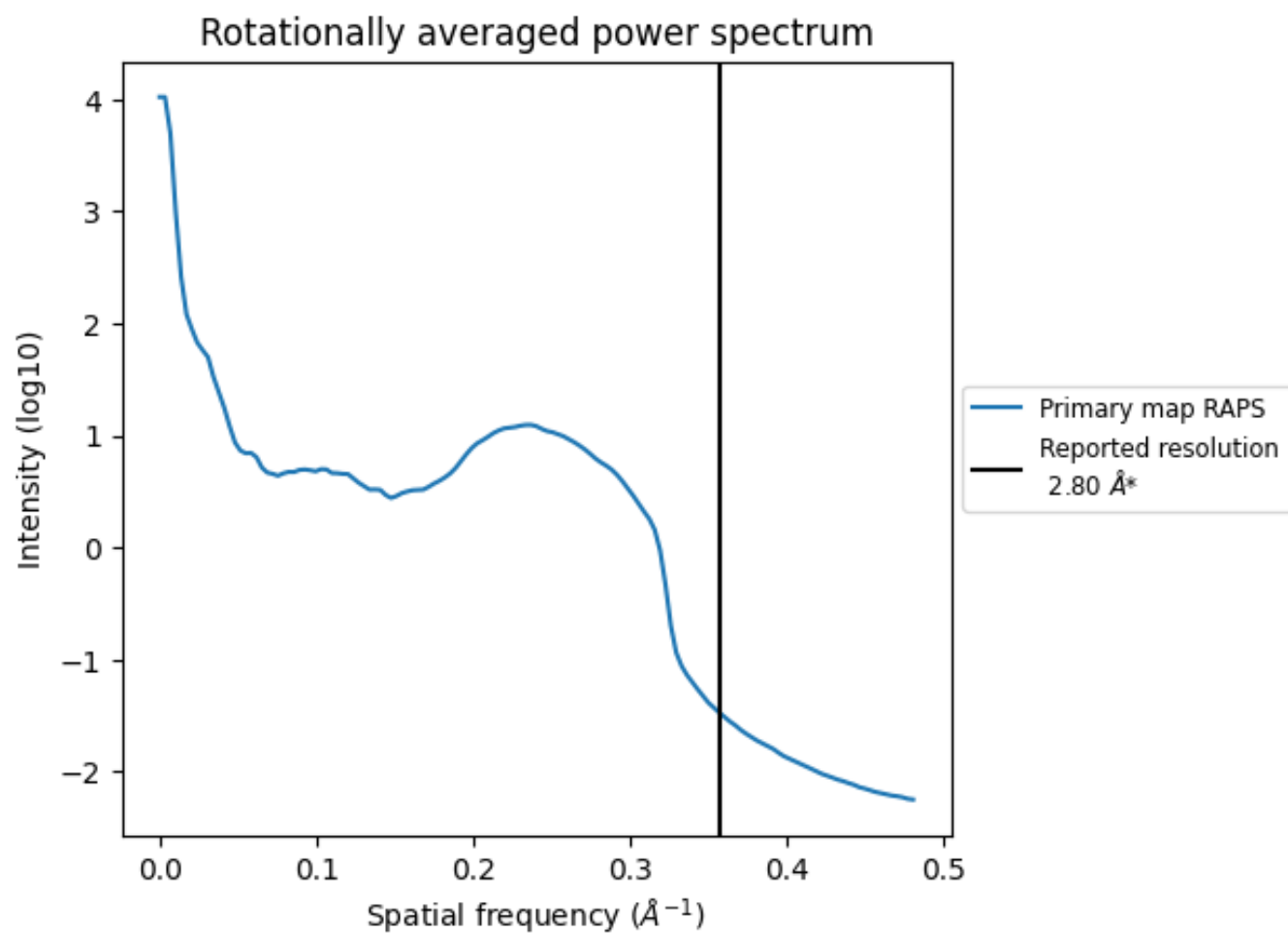
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm^3 ; this corresponds to an approximate mass of 219 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



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

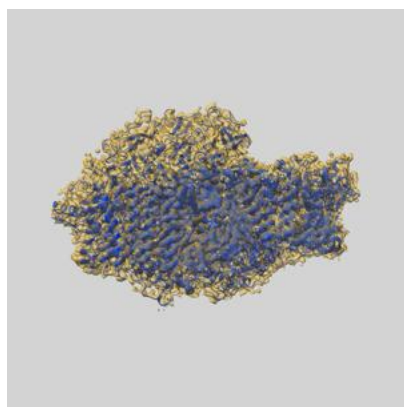
8 Fourier-Shell correlation

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

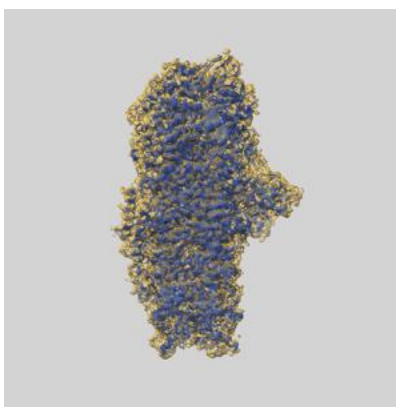
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23023 and PDB model 7KSQ. Per-residue inclusion information can be found in section 3 on page 24.

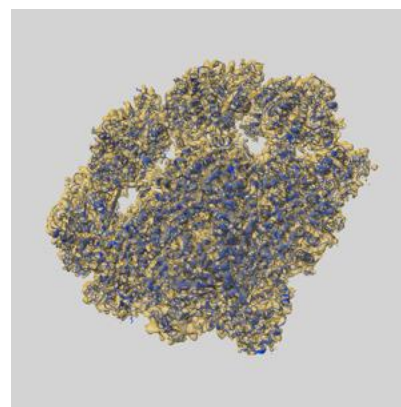
9.1 Map-model overlay [i](#)



X



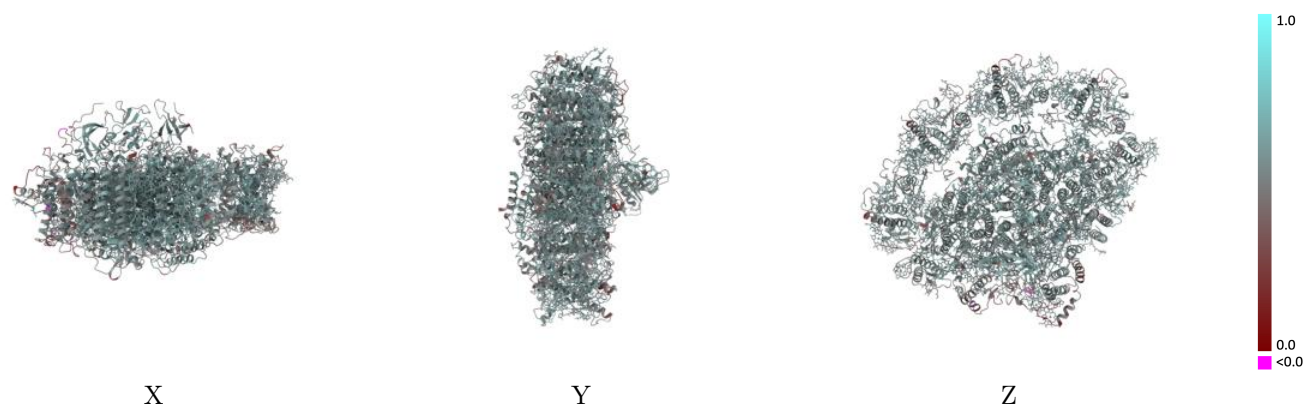
Y



Z

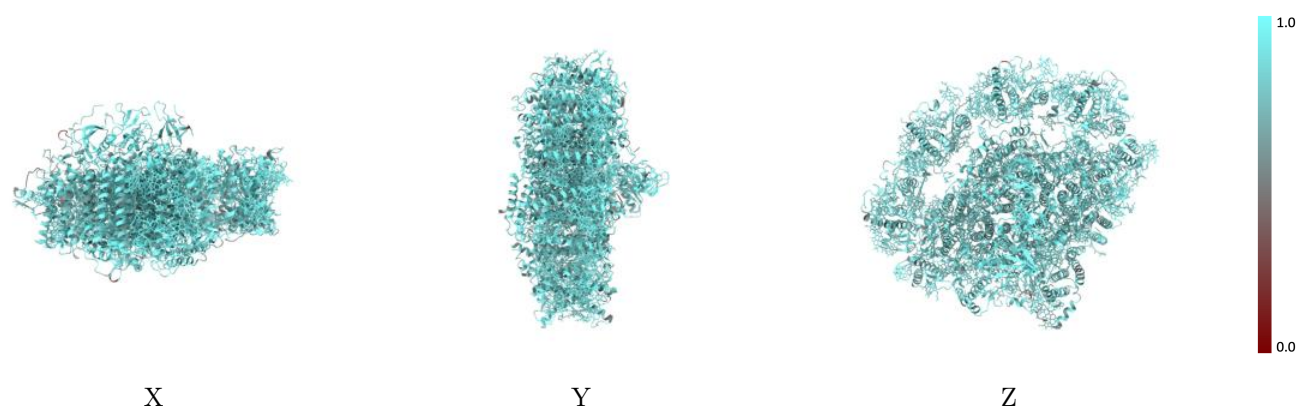
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



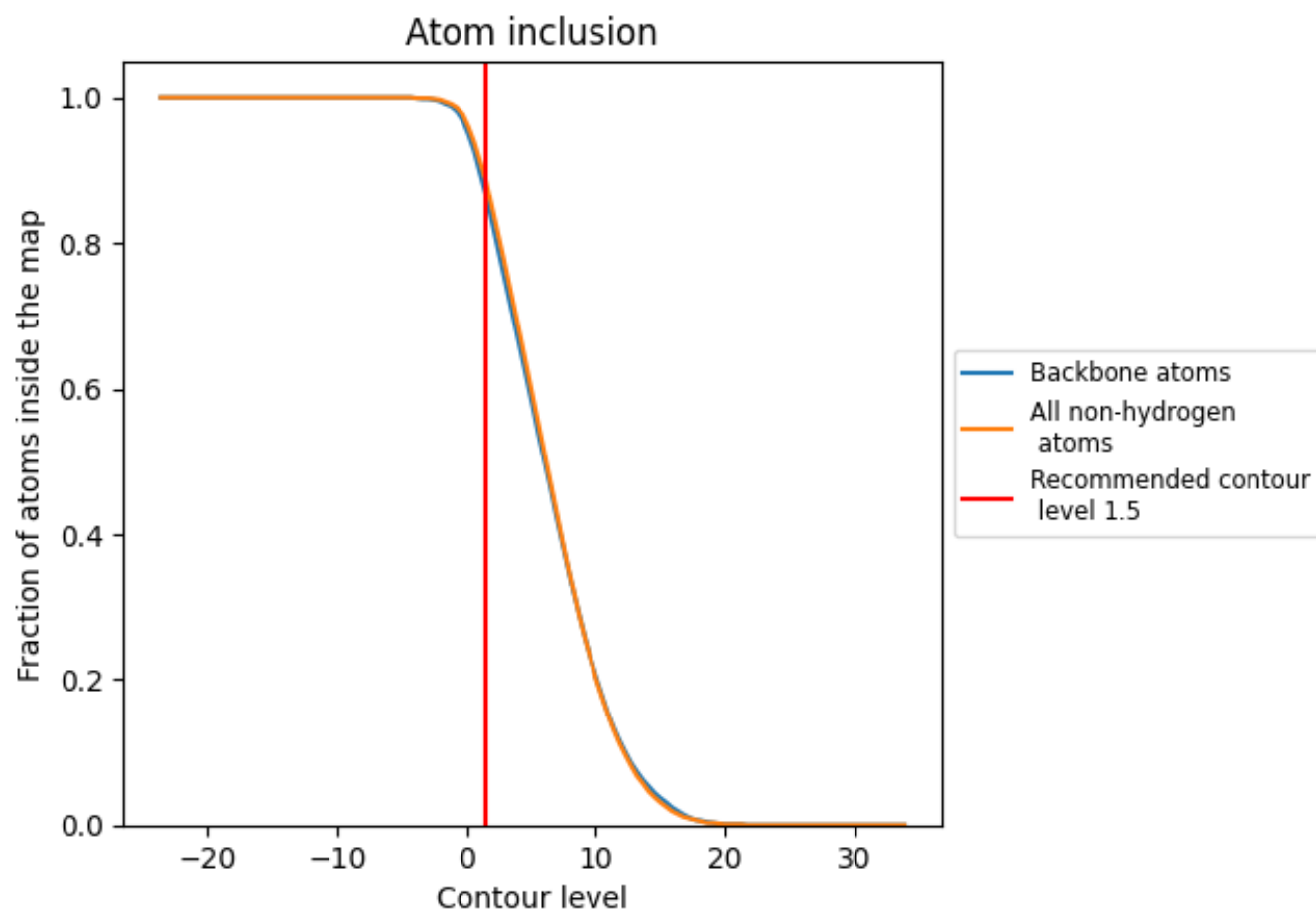
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 89% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.5440
1	 0.8670	 0.5280
2	 0.8610	 0.5260
3	 0.8620	 0.5330
4	 0.8650	 0.5220
A	 0.9090	 0.5680
B	 0.9180	 0.5730
C	 0.9350	 0.5700
D	 0.8770	 0.5340
E	 0.8740	 0.5380
F	 0.8720	 0.5480
G	 0.8720	 0.5400
H	 0.7220	 0.4090
I	 0.8740	 0.5450
J	 0.8940	 0.5590
K	 0.8310	 0.5070
L	 0.8480	 0.5110
M	 0.8540	 0.5140
O	 0.8950	 0.3850

