



wwPDB EM Validation Summary Report ⓘ

Sep 9, 2026 – 02:50 PM JST

PDB ID : 7WFD / pdb_00007wfd
EMDB ID : EMD-32462
Title : Left PSI in the cyclic electron transport supercomplex NDH-PSI from Arabidopsis
Authors : Pan, X.; Li, M.
Deposited on : 2021-12-26
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

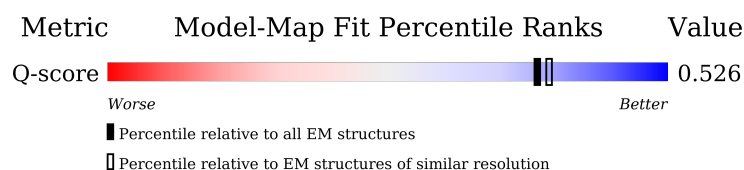
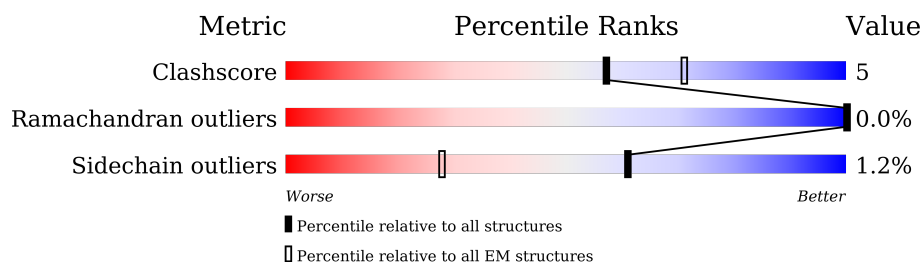
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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.



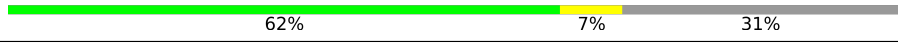
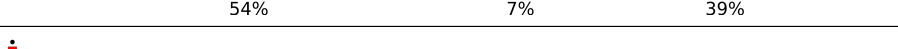
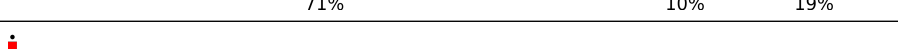
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14599 (2.75 - 3.75)

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	AA	750	
2	AB	734	
3	AC	81	
4	AD	204	

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Mol	Chain	Length	Quality of chain
5	AE	143	
6	AF	221	
7	AG	160	
8	AH	145	
9	AI	37	
10	AJ	44	
11	AK	130	
12	AL	219	
13	A1	241	
14	A3	273	
15	A4	251	
16	A6	270	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 35603 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	AA	742	Total	C	N	O	S	0	0
			5839	3826	992	1003	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	734	Total	C	N	O	S	0	0
			5862	3847	999	1001	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	80	Total	C	N	O	S	0	0
			615	381	107	116	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	141	Total	C	N	O	S	0	0
			1112	712	193	203	4		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AE	67	Total	C	N	O	0	0
			530	341	94	95		

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	153	Total	C	N	O	S	0	0
			1213	792	208	210	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AG	98	Total	C	N	O	0	0
			767	499	125	143		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AH	95	Total	C	N	O	0	0
			730	476	119	135		

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	33	Total	C	N	O	S	0	0
			257	175	41	40	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	42	Total	C	N	O	S	0	0
			338	230	51	56	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	65	Total	C	N	O	S	0	0
			451	290	74	84	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	157	Total	C	N	O	S	0	0
			1173	775	187	209	2		

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	196	Total	C	N	O	S	0	0
			1511	984	251	271	5		

- Molecule 14 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A3	219	Total	C	N	O	S	0	0
			1675	1096	272	302	5		

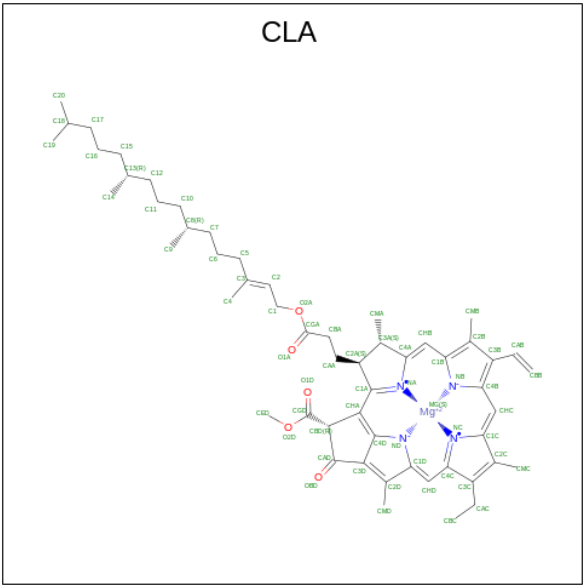
- Molecule 15 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A4	197	Total	C	N	O	S	0	0
			1562	1022	254	283	3		

- Molecule 16 is a protein called Photosystem I chlorophyll a/b-binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A6	212	Total	C	N	O	S	0	0
			1671	1088	272	299	12		

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
17	AA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	AB	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 51	C 42	Mg 1	N 4	O 4	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	AB	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	AB	1	Total 59	C 49	Mg 1	N 4	O 5	0
17	AB	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	AB	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	AB	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	AB	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	AB	1	Total 62	C 52	Mg 1	N 4	O 5	0
17	AB	1	Total 62	C 52	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 56	C 46	Mg 1	N 4	O 5	0
17	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	AB	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	AB	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AF	1	Total 57	C 47	Mg 1	N 4	O 5	0
17	AF	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	AF	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	AG	1	Total 44	C 34	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	AG	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	AG	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	AH	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	AJ	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	AK	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
17	AK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	AK	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	AL	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	AL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	AL	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	A1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	

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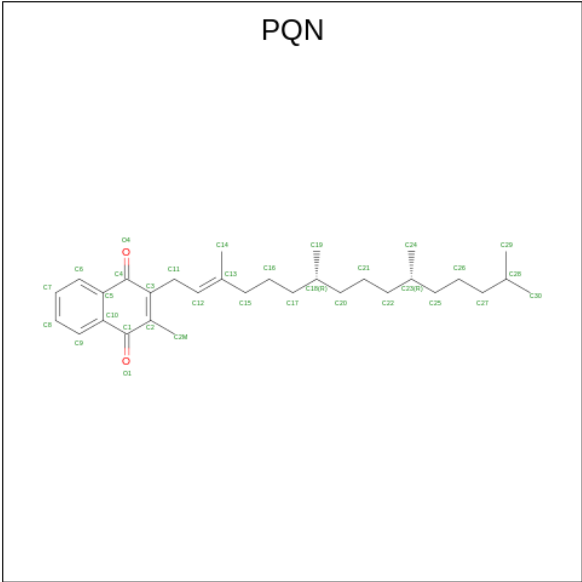
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17	A1	1	Total 43	C 33	Mg 1	N 4	O 5	0
17	A3	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A3	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A3	1	Total 42	C 32	Mg 1	N 4	O 5	0
17	A3	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	A3	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	A3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A3	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	A3	1	Total 37	C 31	Mg 1	N 4	O 1	0
17	A3	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	A3	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	A3	1	Total 40	C 32	Mg 1	N 4	O 3	0
17	A3	1	Total 36	C 30	Mg 1	N 4	O 1	0
17	A3	1	Total 40	C 32	Mg 1	N 4	O 3	0
17	A4	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A4	1	Total 44	C 34	Mg 1	N 4	O 5	0
17	A4	1	Total 43	C 33	Mg 1	N 4	O 5	0
17	A4	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A4	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	A4	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A4	1	Total 41	C 33	Mg 1	N 4	O 3	0

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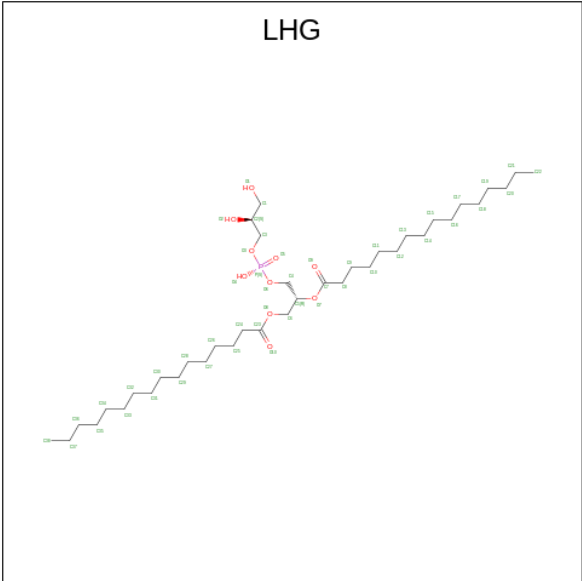
Mol	Chain	Residues	Atoms					AltConf
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			56	46	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	A6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	A6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
17	A6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	AA	1	Total	C	O	0
			33	31	2	
18	AB	1	Total	C	O	0
			33	31	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



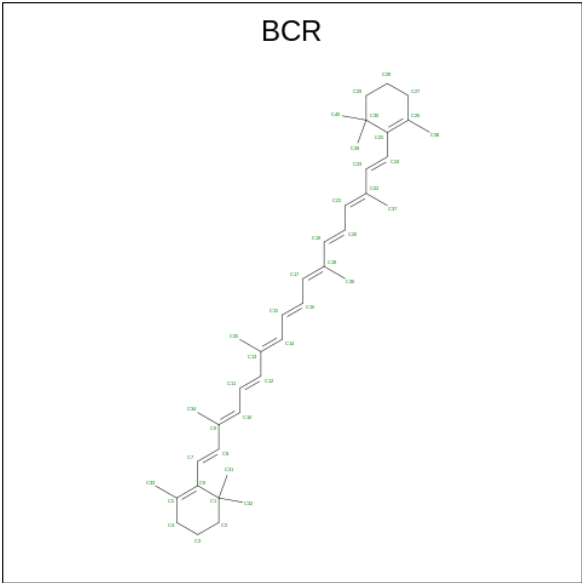
Mol	Chain	Residues	Atoms				AltConf
19	AA	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
19	AJ	1	Total	C	O	P	0
			40	29	10	1	
19	A1	1	Total	C	O	P	0
			38	27	10	1	
19	A1	1	Total	C	O	P	0
			36	25	10	1	
19	A1	1	Total	C	O	P	0
			49	38	10	1	
19	A3	1	Total	C	O	P	0
			36	25	10	1	
19	A3	1	Total	C	O	P	0
			23	12	10	1	
19	A6	1	Total	C	O	P	0
			36	25	10	1	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
20	AA	1	Total	C	0
			40	40	
20	AA	1	Total	C	0
			40	40	
20	AA	1	Total	C	0
			40	40	
20	AA	1	Total	C	0
			40	40	

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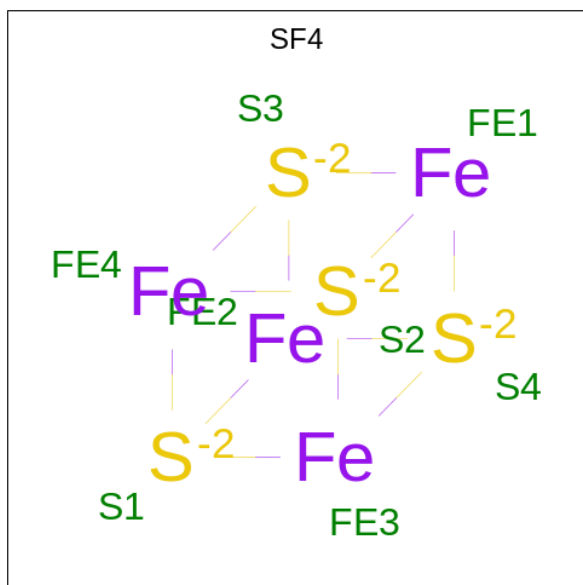
Mol	Chain	Residues	Atoms	AltConf
20	AA	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AF	1	Total C 40 40	0
20	AF	1	Total C 40 40	0
20	AG	1	Total C 40 40	0
20	AI	1	Total C 40 40	0
20	AI	1	Total C 40 40	0
20	AJ	1	Total C 40 40	0
20	AJ	1	Total C 40 40	0
20	AK	1	Total C 40 40	0
20	AK	1	Total C 40 40	0
20	AL	1	Total C 40 40	0
20	AL	1	Total C 40 40	0
20	A1	1	Total C 40 40	0
20	A3	1	Total C 40 40	0
20	A4	1	Total C 40 40	0

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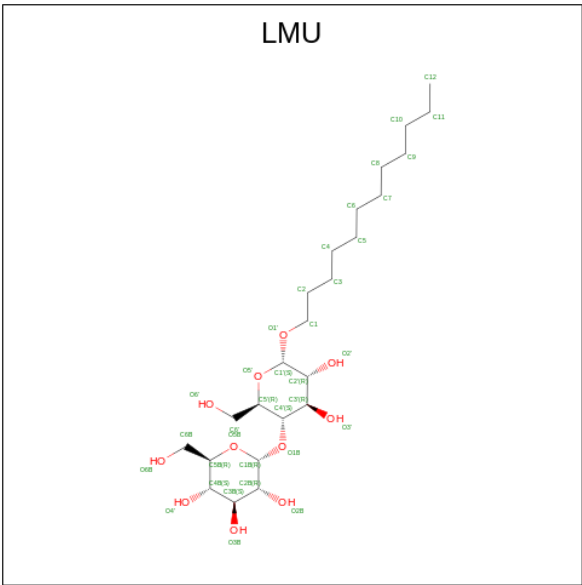
Mol	Chain	Residues	Atoms		AltConf
20	A6	1	Total	C	0
			40	40	

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



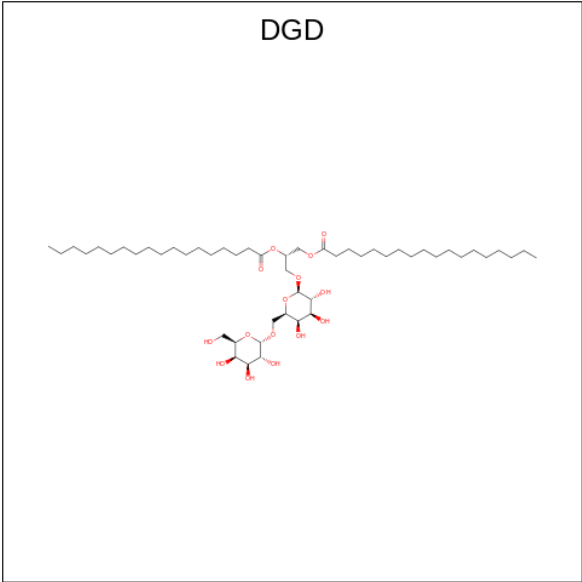
Mol	Chain	Residues	Atoms			AltConf
21	AA	1	Total	Fe	S	0
			8	4	4	
21	AC	1	Total	Fe	S	0
			8	4	4	
21	AC	1	Total	Fe	S	0
			8	4	4	

- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



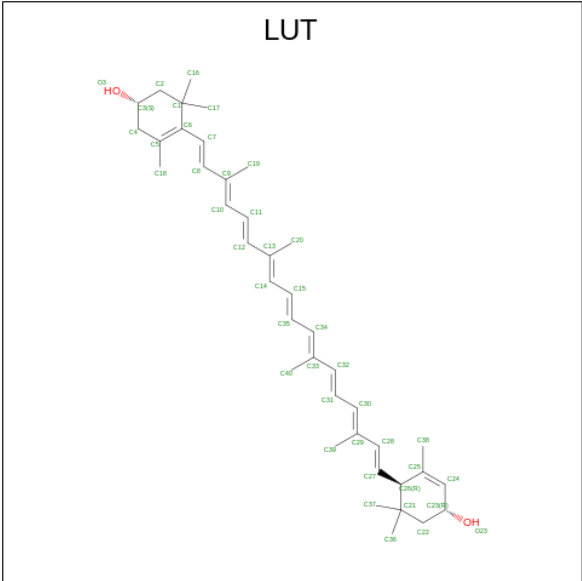
Mol	Chain	Residues	Atoms			AltConf
22	AA	1	Total	C	O	0
			35	24	11	
22	AB	1	Total	C	O	0
			35	24	11	
22	AB	1	Total	C	O	0
			35	24	11	
22	AB	1	Total	C	O	0
			35	24	11	
22	AL	1	Total	C	O	0
			34	23	11	

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
23	AB	1	Total	C	O	0
			66	51	15	

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



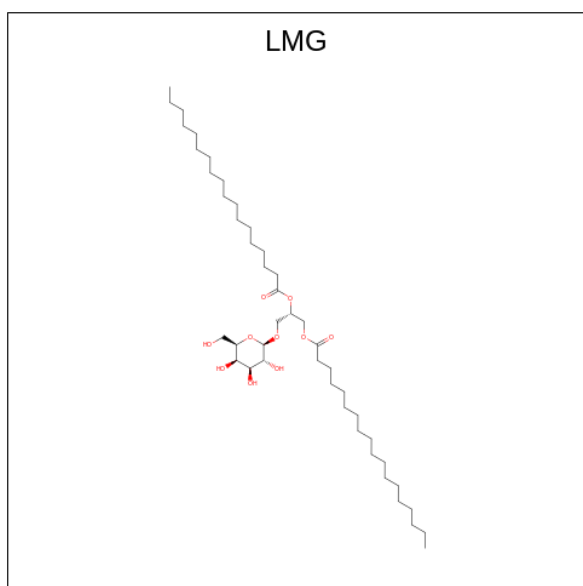
Mol	Chain	Residues	Atoms			AltConf
24	AF	1	Total	C	O	0
			42	40	2	
24	A1	1	Total	C	O	0
			42	40	2	

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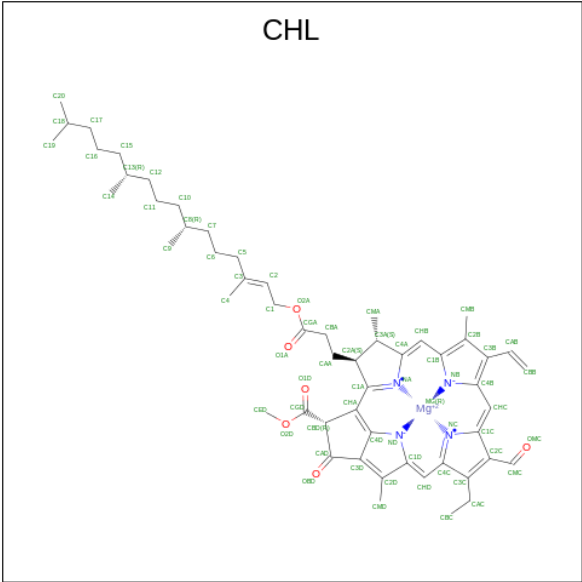
Mol	Chain	Residues	Atoms			AltConf
24	A3	1	Total	C	O	0
			42	40	2	
24	A4	1	Total	C	O	0
			42	40	2	
24	A6	1	Total	C	O	0
			42	40	2	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



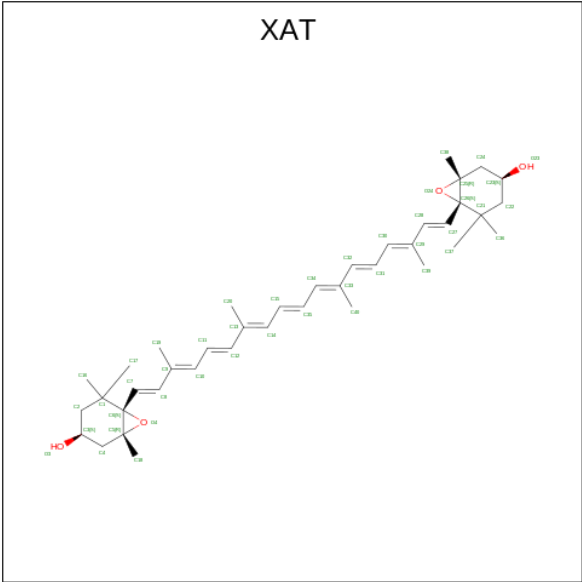
Mol	Chain	Residues	Atoms			AltConf
25	AG	1	Total	C	O	0
			38	28	10	
25	A1	1	Total	C	O	0
			44	34	10	
25	A4	1	Total	C	O	0
			39	29	10	

- Molecule 26 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
26	A1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	A1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
26	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	A3	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
26	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
26	A4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	A4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
26	A6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
26	A6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
26	A6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).

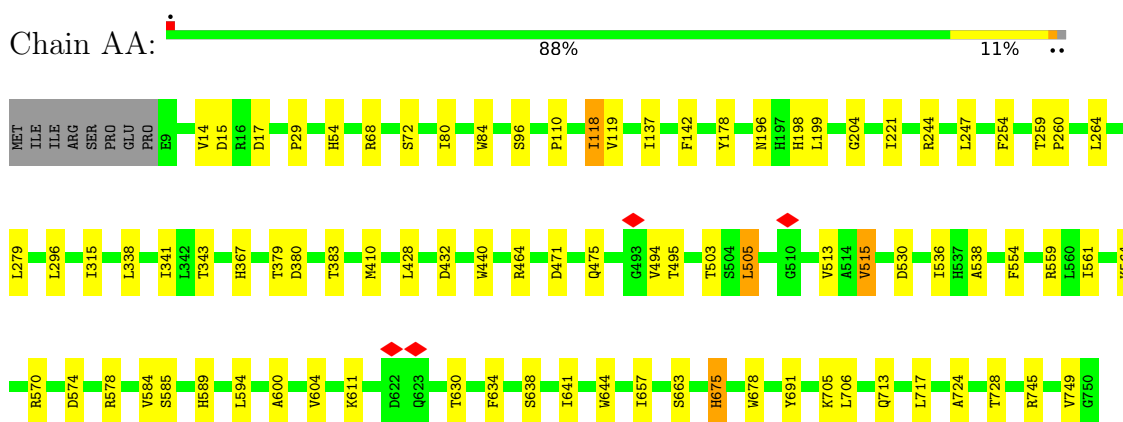


Mol	Chain	Residues	Atoms			AltConf
27	A1	1	Total	C	O	0
			44	40	4	
27	A3	1	Total	C	O	0
			44	40	4	
27	A4	1	Total	C	O	0
			44	40	4	
27	A6	1	Total	C	O	0
			44	40	4	

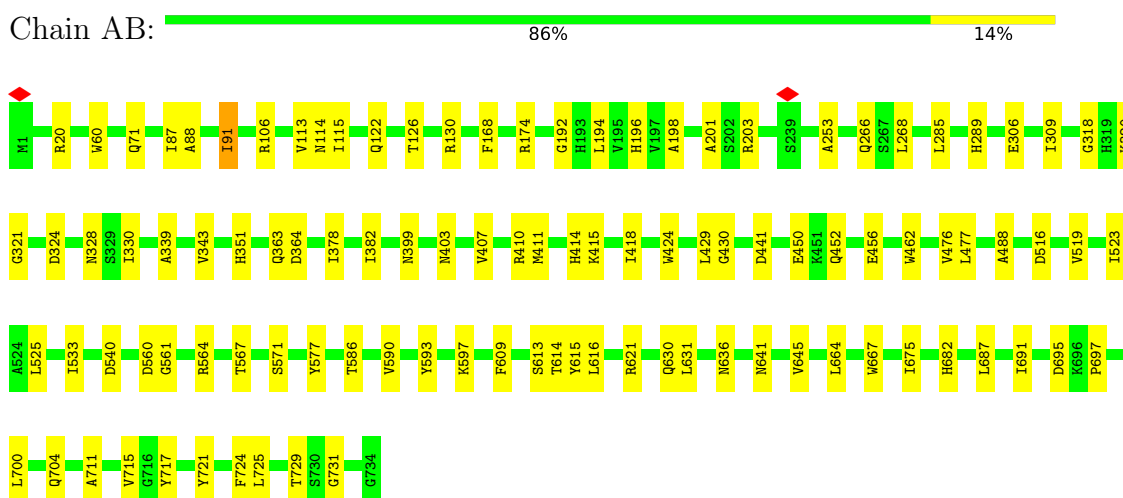
3 Residue-property plots

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

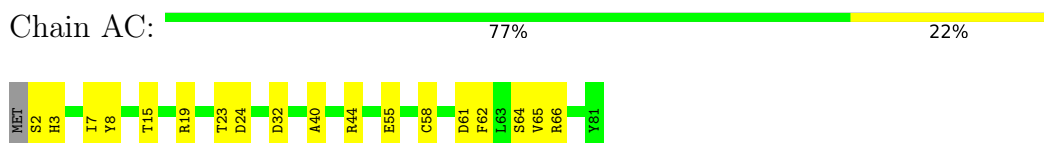
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 9: Photosystem I reaction center subunit VIII

Chain AI:  89% 11%



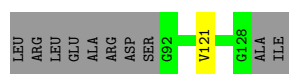
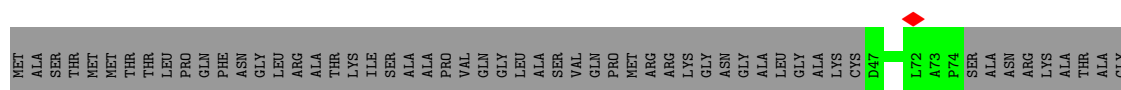
- Molecule 10: Photosystem I reaction center subunit IX

Chain AJ:  84% 11% 5%



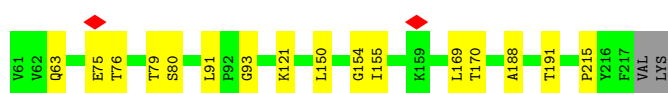
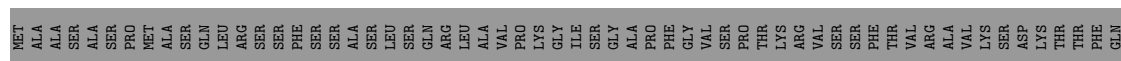
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain AK:  49% 50%



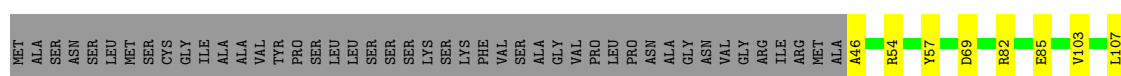
- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

Chain AL:  64% 7% 28%



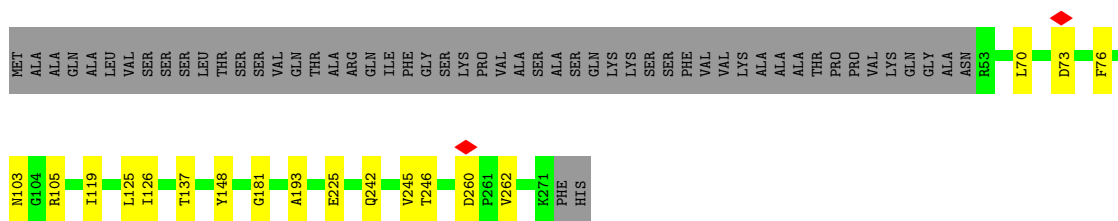
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain A1:  71% 10% 19%



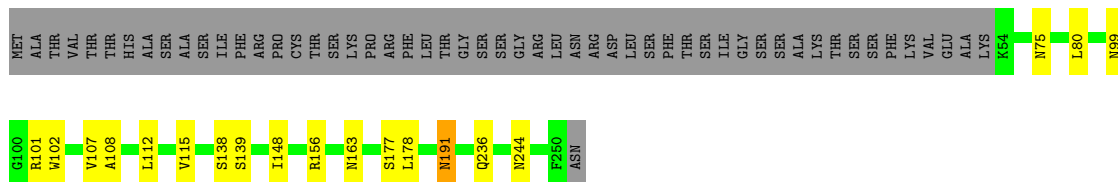
- Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

Chain A3:  74% 7% 20%



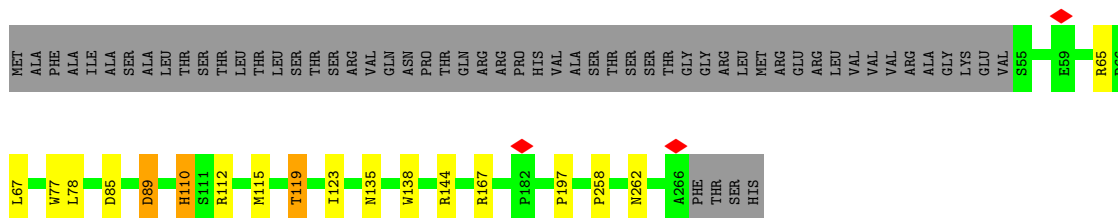
- Molecule 15: Chlorophyll a-b binding protein 4, chloroplastic

Chain A4: 71% 7% 22%



- Molecule 16: Photosystem I chlorophyll a/b-binding protein 6, chloroplastic

Chain A6: 72% 6% 21%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.422	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	AA	0.34	1/6037 (0.0%)	0.48	0/8236
2	AB	0.30	0/6073	0.44	0/8291
3	AC	0.23	0/628	0.43	0/852
4	AD	0.22	0/1140	0.45	0/1542
5	AE	0.20	0/542	0.36	0/736
6	AF	0.23	0/1243	0.44	0/1677
7	AG	0.41	1/787 (0.1%)	0.48	0/1067
8	AH	0.27	0/751	0.48	0/1018
9	AI	0.22	0/264	0.39	0/359
10	AJ	0.28	0/348	0.49	0/474
11	AK	0.22	0/456	0.40	0/617
12	AL	0.26	0/1208	0.47	1/1650 (0.1%)
13	A1	0.32	1/1562 (0.1%)	0.47	0/2131
14	A3	0.21	0/1726	0.41	0/2347
15	A4	0.27	0/1611	0.45	0/2194
16	A6	0.24	0/1732	0.46	0/2363
All	All	0.29	3/26108 (0.0%)	0.45	1/35554 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A1	103	VAL	CA-CB	8.52	1.58	1.54
7	AG	156	PRO	C-O	-6.93	1.15	1.24
1	AA	17	ASP	C-O	-5.00	1.21	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AL	215	PRO	N-CA-C	-6.45	106.29	114.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	5839	0	5683	66	0
2	AB	5862	0	5649	93	0
3	AC	615	0	592	15	0
4	AD	1112	0	1122	10	0
5	AE	530	0	536	11	0
6	AF	1213	0	1243	9	0
7	AG	767	0	746	10	0
8	AH	730	0	720	7	0
9	AI	257	0	274	0	0
10	AJ	338	0	351	5	0
11	AK	451	0	462	1	0
12	AL	1173	0	1162	16	0
13	A1	1511	0	1464	13	0
14	A3	1675	0	1647	12	0
15	A4	1562	0	1516	16	0
16	A6	1671	0	1599	15	0
17	A1	575	0	447	7	0
17	A3	575	0	420	2	0
17	A4	480	0	376	6	0
17	A6	485	0	399	4	0
17	AA	2411	0	2371	30	0
17	AB	2452	0	2461	32	0
17	AF	140	0	113	1	0
17	AG	131	0	94	4	0
17	AH	60	0	59	0	0
17	AJ	42	0	31	0	0
17	AK	126	0	88	1	0
17	AL	143	0	119	1	0
18	AA	33	0	46	3	0
18	AB	33	0	46	2	0
19	A1	123	0	162	0	0
19	A3	59	0	58	1	0
19	A6	36	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AA	49	0	74	1	0
19	AJ	40	0	53	0	0
20	A1	40	0	56	3	0
20	A3	40	0	56	2	0
20	A4	40	0	56	0	0
20	A6	40	0	56	3	0
20	AA	200	0	280	6	0
20	AB	240	0	336	9	0
20	AF	80	0	112	6	0
20	AG	40	0	56	1	0
20	AI	80	0	112	1	0
20	AJ	80	0	112	2	0
20	AK	80	0	112	2	0
20	AL	80	0	112	1	0
21	AA	8	0	0	0	0
21	AC	16	0	0	2	0
22	AA	35	0	46	0	0
22	AB	105	0	138	0	0
22	AL	34	0	41	1	0
23	AB	66	0	96	0	0
24	A1	42	0	56	1	0
24	A3	42	0	56	0	0
24	A4	42	0	56	3	0
24	A6	42	0	56	2	0
24	AF	42	0	56	2	0
25	A1	44	0	58	1	0
25	A4	39	0	48	4	0
25	AG	38	0	46	0	0
26	A1	92	0	60	2	0
26	A3	97	0	68	2	0
26	A4	169	0	100	2	0
26	A6	135	0	89	2	0
27	A1	44	0	56	1	0
27	A3	44	0	56	3	0
27	A4	44	0	56	2	0
27	A6	44	0	56	4	0
All	All	35603	0	34975	337	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 5.

The worst 5 of 337 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:87:ILE:HG23	2:AB:113:VAL:CG1	1.58	1.33
7:AG:76:LEU:HD13	17:AG:204:CLA:HMB3	1.17	1.14
2:AB:87:ILE:CG2	2:AB:113:VAL:HG11	1.78	1.14
7:AG:76:LEU:HD13	17:AG:204:CLA:CMB	1.81	1.09
2:AB:106:ARG:CZ	2:AB:115:ILE:HG12	1.83	1.08

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	AA	740/750 (99%)	688 (93%)	51 (7%)	1 (0%)	48	76
2	AB	732/734 (100%)	695 (95%)	37 (5%)	0	100	100
3	AC	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
4	AD	139/204 (68%)	126 (91%)	13 (9%)	0	100	100
5	AE	65/143 (46%)	58 (89%)	7 (11%)	0	100	100
6	AF	151/221 (68%)	144 (95%)	7 (5%)	0	100	100
7	AG	96/160 (60%)	88 (92%)	8 (8%)	0	100	100
8	AH	93/145 (64%)	90 (97%)	3 (3%)	0	100	100
9	AI	31/37 (84%)	30 (97%)	1 (3%)	0	100	100
10	AJ	40/44 (91%)	38 (95%)	2 (5%)	0	100	100
11	AK	61/130 (47%)	57 (93%)	4 (7%)	0	100	100
12	AL	155/219 (71%)	145 (94%)	10 (6%)	0	100	100
13	A1	194/241 (80%)	178 (92%)	16 (8%)	0	100	100
14	A3	217/273 (80%)	191 (88%)	26 (12%)	0	100	100
15	A4	195/251 (78%)	185 (95%)	10 (5%)	0	100	100
16	A6	210/270 (78%)	198 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3197/3903 (82%)	2983 (93%)	213 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	663	SER

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	AA	600/610 (98%)	592 (99%)	8 (1%)	61	73
2	AB	598/600 (100%)	594 (99%)	4 (1%)	76	79
3	AC	70/71 (99%)	70 (100%)	0	100	100
4	AD	120/170 (71%)	118 (98%)	2 (2%)	53	69
5	AE	56/114 (49%)	55 (98%)	1 (2%)	51	69
6	AF	125/185 (68%)	124 (99%)	1 (1%)	73	78
7	AG	83/133 (62%)	81 (98%)	2 (2%)	43	64
8	AH	77/113 (68%)	76 (99%)	1 (1%)	61	73
9	AI	29/33 (88%)	29 (100%)	0	100	100
10	AJ	37/39 (95%)	37 (100%)	0	100	100
11	AK	47/95 (50%)	47 (100%)	0	100	100
12	AL	119/174 (68%)	119 (100%)	0	100	100
13	A1	151/190 (80%)	147 (97%)	4 (3%)	40	62
14	A3	168/211 (80%)	167 (99%)	1 (1%)	78	81
15	A4	164/210 (78%)	162 (99%)	2 (1%)	63	74
16	A6	177/226 (78%)	172 (97%)	5 (3%)	38	60
All	All	2621/3174 (83%)	2590 (99%)	31 (1%)	61	74

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	AE	129	SER
16	A6	89	ASP
7	AG	109	ASP
16	A6	119	THR
15	A4	148	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
12	AL	66	ASN
13	A1	209	GLN
13	A1	208	GLN
14	A3	207	ASN
2	AB	504	ASN

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](#)

211 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
26	CHL	A4	304	-	44,49,74	2.40	21 (47%)	49,84,114	2.73	24 (48%)
17	CLA	AA	827	1	69,73,73	1.25	8 (11%)	83,113,113	1.23	6 (7%)
20	BCR	AB	847	-	41,41,41	0.87	0	56,56,56	2.02	14 (25%)
25	LMG	AG	202	-	38,38,55	1.14	3 (7%)	46,46,63	1.07	2 (4%)
17	CLA	AL	303	12	64,68,73	1.32	8 (12%)	77,107,113	1.28	9 (11%)
20	BCR	AA	848	-	41,41,41	0.77	1 (2%)	56,56,56	1.97	16 (28%)
17	CLA	AB	826	-	66,70,73	1.27	8 (12%)	79,109,113	1.21	6 (7%)
17	CLA	AA	838	1	59,63,73	1.32	9 (15%)	71,101,113	1.22	10 (14%)
20	BCR	AJ	101	-	41,41,41	0.89	1 (2%)	56,56,56	1.98	16 (28%)
17	CLA	AA	837	1	55,59,73	1.38	8 (14%)	66,96,113	1.44	9 (13%)
17	CLA	AH	201	8	64,68,73	1.30	7 (10%)	77,107,113	1.26	8 (10%)
17	CLA	AA	807	1	54,58,73	1.42	9 (16%)	65,95,113	1.27	4 (6%)
17	CLA	AB	814	2	69,73,73	1.26	11 (15%)	83,113,113	1.23	6 (7%)
17	CLA	AA	808	1	69,73,73	1.25	8 (11%)	83,113,113	1.20	6 (7%)
17	CLA	AA	814	1	49,53,73	1.48	9 (18%)	59,89,113	1.35	7 (11%)
17	CLA	AA	836	1	49,53,73	1.50	8 (16%)	59,89,113	1.36	7 (11%)
17	CLA	AG	204	7	49,53,73	1.50	8 (16%)	59,89,113	1.33	5 (8%)
17	CLA	AF	802	-	61,65,73	1.33	10 (16%)	73,103,113	1.30	7 (9%)
17	CLA	A1	306	-	53,57,73	1.41	8 (15%)	62,93,113	1.28	5 (8%)
20	BCR	AJ	103	-	41,41,41	0.74	0	56,56,56	2.38	22 (39%)
17	CLA	A1	307	-	43,48,73	1.54	8 (18%)	52,82,113	1.59	9 (17%)
17	CLA	AB	811	2	69,73,73	1.26	9 (13%)	83,113,113	1.37	8 (9%)
22	LMU	AA	851	-	36,36,36	1.16	2 (5%)	47,47,47	1.04	2 (4%)
17	CLA	AB	830	2	60,64,73	1.35	8 (13%)	72,102,113	1.24	4 (5%)
19	LHG	AA	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.89	2 (3%)
18	PQN	AA	843	-	34,34,34	3.42	10 (29%)	42,45,45	1.74	8 (19%)
17	CLA	A4	313	15	54,58,73	1.42	8 (14%)	65,95,113	1.35	7 (10%)
17	CLA	A3	308	14	49,53,73	1.48	8 (16%)	59,89,113	1.27	6 (10%)
17	CLA	A4	308	15	58,62,73	1.35	9 (15%)	69,99,113	1.17	6 (8%)
17	CLA	AB	804	-	69,73,73	1.25	11 (15%)	83,113,113	1.57	13 (15%)
17	CLA	A6	611	16	48,52,73	1.50	8 (16%)	58,88,113	1.24	4 (6%)
21	SF4	AA	850	1,2	0,12,12	-	-	-	-	-
17	CLA	AA	834	1	69,73,73	1.24	8 (11%)	83,113,113	1.38	12 (14%)
22	LMU	AB	850	-	36,36,36	1.13	2 (5%)	47,47,47	1.08	4 (8%)
17	CLA	A1	315	13	41,46,73	1.64	8 (19%)	52,81,113	1.47	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A3	313	14	43,48,73	1.55	8 (18%)	51,83,113	1.31	8 (15%)
17	CLA	AA	841	1	69,73,73	1.26	9 (13%)	83,113,113	1.26	6 (7%)
17	CLA	AA	824	1	57,62,73	1.38	8 (14%)	68,100,113	1.36	9 (13%)
26	CHL	A1	308	13	44,49,74	2.46	21 (47%)	48,84,114	2.80	23 (47%)
17	CLA	AA	812	1	58,62,73	1.37	9 (15%)	69,99,113	1.36	5 (7%)
22	LMU	AB	853	-	36,36,36	1.13	2 (5%)	47,47,47	1.05	2 (4%)
23	DGD	AB	851	-	67,67,67	0.80	2 (2%)	81,81,81	0.99	4 (4%)
27	XAT	A1	318	-	39,47,47	0.91	2 (5%)	54,74,74	2.42	24 (44%)
19	LHG	A1	320	17	48,48,48	0.93	2 (4%)	51,54,54	0.84	2 (3%)
17	CLA	AA	819	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
17	CLA	AA	830	1	69,73,73	1.28	8 (11%)	83,113,113	1.18	5 (6%)
17	CLA	A4	310	15	44,49,73	1.53	9 (20%)	52,84,113	1.33	7 (13%)
21	SF4	AC	101	3	0,12,12	-	-	-	-	-
24	LUT	A4	315	-	42,43,43	0.95	2 (4%)	51,60,60	1.84	15 (29%)
17	CLA	A1	304	13	64,68,73	1.28	8 (12%)	76,106,113	1.21	6 (7%)
17	CLA	A6	613	16	47,51,73	1.52	7 (14%)	56,86,113	1.27	4 (7%)
26	CHL	A4	306	-	50,54,74	2.30	20 (40%)	56,90,114	2.78	26 (46%)
20	BCR	AB	844	-	41,41,41	0.86	0	56,56,56	2.28	23 (41%)
17	CLA	A4	303	-	47,51,73	1.56	9 (19%)	60,87,113	1.39	8 (13%)
17	CLA	A4	309	-	46,50,73	1.46	6 (13%)	55,85,113	1.33	4 (7%)
22	LMU	AB	852	-	36,36,36	1.14	2 (5%)	47,47,47	0.94	1 (2%)
17	CLA	AA	823	1	45,49,73	1.56	8 (17%)	54,84,113	1.31	8 (14%)
20	BCR	AG	205	-	41,41,41	0.93	0	56,56,56	2.00	18 (32%)
17	CLA	AB	839	2	51,55,73	1.43	7 (13%)	61,91,113	1.42	6 (9%)
17	CLA	A6	609	16	59,63,73	1.35	9 (15%)	71,101,113	1.22	9 (12%)
17	CLA	A3	304	-	45,50,73	1.60	9 (20%)	57,86,113	1.34	7 (12%)
17	CLA	A3	315	14	43,48,73	1.53	7 (16%)	51,83,113	1.23	5 (9%)
17	CLA	AK	204	11	50,54,73	1.45	7 (14%)	60,90,113	1.34	4 (6%)
24	LUT	A1	317	-	42,43,43	0.94	1 (2%)	51,60,60	1.88	13 (25%)
17	CLA	A3	311	14	47,51,73	1.49	6 (12%)	56,86,113	1.31	4 (7%)
17	CLA	A3	302	14	64,68,73	1.30	8 (12%)	77,107,113	1.16	8 (10%)
17	CLA	AB	840	-	69,73,73	1.27	9 (13%)	83,113,113	1.14	6 (7%)
17	CLA	A4	312	15	49,53,73	1.48	8 (16%)	59,89,113	1.27	6 (10%)
25	LMG	A4	318	-	39,39,55	1.00	2 (5%)	47,47,63	1.40	7 (14%)
17	CLA	AA	835	1	47,52,73	1.51	7 (14%)	56,88,113	1.30	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	AB	812	2	58,62,73	1.41	9 (15%)	73,100,113	1.37	10 (13%)
19	LHG	A3	301	-	35,35,48	1.09	2 (5%)	38,41,54	1.01	2 (5%)
17	CLA	AA	821	-	69,73,73	1.25	10 (14%)	83,113,113	1.24	10 (12%)
20	BCR	AI	101	-	41,41,41	0.92	1 (2%)	56,56,56	2.05	20 (35%)
20	BCR	AB	845	-	41,41,41	0.85	1 (2%)	56,56,56	1.93	17 (30%)
26	CHL	A4	305	-	45,49,74	2.32	17 (37%)	57,84,114	2.85	28 (49%)
17	CLA	AB	828	2	69,73,73	1.23	9 (13%)	83,113,113	1.29	6 (7%)
17	CLA	AL	302	12	45,49,73	1.53	7 (15%)	54,84,113	1.29	7 (12%)
17	CLA	A4	307	15	49,53,73	1.50	8 (16%)	59,89,113	1.24	6 (10%)
24	LUT	A3	316	-	42,43,43	0.84	0	51,60,60	1.78	14 (27%)
27	XAT	A6	615	-	39,47,47	0.98	2 (5%)	54,74,74	2.49	21 (38%)
17	CLA	AA	820	1	49,53,73	1.47	9 (18%)	59,89,113	1.32	4 (6%)
17	CLA	AF	803	-	46,50,73	1.52	8 (17%)	55,85,113	1.41	6 (10%)
17	CLA	AB	838	2	69,73,73	1.22	10 (14%)	83,113,113	1.23	7 (8%)
24	LUT	AF	806	-	42,43,43	1.03	3 (7%)	51,60,60	1.72	12 (23%)
17	CLA	AB	802	-	68,72,73	1.35	9 (13%)	85,112,113	1.26	9 (10%)
17	CLA	AA	813	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
20	BCR	AL	306	-	41,41,41	0.94	1 (2%)	56,56,56	2.01	21 (37%)
27	XAT	A3	317	-	39,47,47	0.97	1 (2%)	54,74,74	2.31	19 (35%)
17	CLA	A3	310	19	40,45,73	1.58	7 (17%)	50,79,113	1.29	5 (10%)
17	CLA	AB	823	2	69,73,73	1.23	8 (11%)	83,113,113	1.21	7 (8%)
17	CLA	AB	832	2	69,73,73	1.24	8 (11%)	83,113,113	1.22	7 (8%)
17	CLA	AA	833	1	69,73,73	1.27	8 (11%)	83,113,113	1.31	9 (10%)
17	CLA	AK	203	-	49,53,73	1.49	8 (16%)	59,89,113	1.24	4 (6%)
26	CHL	A3	307	-	49,53,74	2.27	19 (38%)	59,89,114	2.64	27 (45%)
17	CLA	AA	839	1	56,60,73	1.38	8 (14%)	67,97,113	1.29	6 (8%)
17	CLA	AB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.23	11 (13%)
17	CLA	AB	807	2	69,73,73	1.26	11 (15%)	83,113,113	1.27	6 (7%)
17	CLA	AL	304	-	46,50,73	1.50	8 (17%)	55,85,113	1.41	6 (10%)
17	CLA	AB	803	2	69,73,73	1.24	9 (13%)	83,113,113	1.14	6 (7%)
24	LUT	A6	614	-	42,43,43	0.90	1 (2%)	51,60,60	1.59	12 (23%)
17	CLA	AB	821	2	54,58,73	1.41	9 (16%)	65,95,113	1.34	7 (10%)
25	LMG	A1	321	-	44,44,55	1.03	2 (4%)	52,52,63	1.19	5 (9%)
17	CLA	AA	818	1	63,67,73	1.31	9 (14%)	75,105,113	1.26	8 (10%)
17	CLA	AB	841	2	69,73,73	1.27	9 (13%)	83,113,113	1.15	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A3	303	14	59,63,73	1.38	9 (15%)	71,101,113	1.37	9 (12%)
17	CLA	AA	831	1	51,55,73	1.44	9 (17%)	61,91,113	1.30	5 (8%)
17	CLA	AB	831	2	47,51,73	1.49	10 (21%)	56,86,113	1.23	7 (12%)
17	CLA	AA	809	1	54,58,73	1.45	9 (16%)	65,95,113	1.35	10 (15%)
26	CHL	A1	303	13	54,59,74	2.23	19 (35%)	60,96,114	2.66	29 (48%)
20	BCR	AA	849	-	41,41,41	0.91	2 (4%)	56,56,56	2.12	20 (35%)
17	CLA	AB	820	-	59,63,73	1.39	8 (13%)	71,101,113	1.20	6 (8%)
17	CLA	A4	302	15	48,52,73	1.56	9 (18%)	61,88,113	1.46	8 (13%)
22	LMU	AL	301	-	35,35,36	1.23	2 (5%)	46,46,47	1.05	5 (10%)
17	CLA	AB	837	2	54,58,73	1.43	11 (20%)	65,95,113	1.35	7 (10%)
26	CHL	A3	320	16	55,60,74	2.18	19 (34%)	61,97,114	2.62	26 (42%)
17	CLA	AA	829	1	69,73,73	1.26	9 (13%)	83,113,113	1.41	11 (13%)
20	BCR	AF	805	-	41,41,41	0.81	0	56,56,56	1.86	14 (25%)
26	CHL	A4	314	15	44,49,74	2.32	18 (40%)	51,84,114	2.88	25 (49%)
19	LHG	AJ	104	-	39,39,48	1.06	2 (5%)	42,45,54	0.92	2 (4%)
20	BCR	A1	319	-	41,41,41	0.90	1 (2%)	56,56,56	3.13	20 (35%)
17	CLA	AA	815	1	44,49,73	1.42	6 (13%)	51,83,113	1.45	7 (13%)
17	CLA	AB	805	2	45,49,73	1.50	7 (15%)	54,84,113	1.31	6 (11%)
17	CLA	AB	824	2	47,51,73	1.47	10 (21%)	56,86,113	1.46	7 (12%)
17	CLA	A1	305	13	59,63,73	1.34	7 (11%)	71,101,113	1.50	8 (11%)
17	CLA	AA	842	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	9 (10%)
20	BCR	AA	847	-	41,41,41	1.00	2 (4%)	56,56,56	2.28	24 (42%)
20	BCR	AB	846	-	41,41,41	0.86	0	56,56,56	2.07	16 (28%)
17	CLA	A3	314	-	41,44,73	1.58	9 (21%)	49,77,113	1.25	5 (10%)
17	CLA	AA	825	-	69,73,73	1.27	9 (13%)	83,113,113	1.18	5 (6%)
17	CLA	A4	301	15	64,68,73	1.28	8 (12%)	77,107,113	1.23	8 (10%)
20	BCR	AK	202	-	41,41,41	0.94	2 (4%)	56,56,56	2.19	17 (30%)
17	CLA	A1	310	13	44,48,73	1.59	7 (15%)	56,83,113	1.46	9 (16%)
21	SF4	AC	102	3	0,12,12	-	-	-	-	-
17	CLA	AA	826	-	63,67,73	1.32	10 (15%)	75,105,113	1.16	6 (8%)
20	BCR	AA	846	-	41,41,41	0.82	0	56,56,56	2.12	21 (37%)
17	CLA	AA	804	1	56,60,73	1.37	9 (16%)	67,97,113	1.37	7 (10%)
17	CLA	AA	816	-	49,53,73	1.49	8 (16%)	59,89,113	1.39	6 (10%)
17	CLA	AB	818	2	63,67,73	1.30	8 (12%)	75,105,113	1.24	9 (12%)
19	LHG	A3	319	17	22,22,48	1.44	2 (9%)	25,28,54	1.27	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	XAT	A4	316	-	39,47,47	0.95	2 (5%)	54,74,74	2.29	16 (29%)
17	CLA	AB	809	2	69,73,73	1.24	8 (11%)	83,113,113	1.26	9 (10%)
17	CLA	AB	825	-	69,73,73	1.27	11 (15%)	83,113,113	1.24	7 (8%)
17	CLA	AA	817	1	64,68,73	1.29	7 (10%)	77,107,113	1.24	8 (10%)
17	CLA	AA	810	1	69,72,73	1.29	9 (13%)	78,111,113	1.19	5 (6%)
17	CLA	A6	608	16	49,53,73	1.48	8 (16%)	59,89,113	1.25	7 (11%)
20	BCR	AB	848	-	41,41,41	0.89	1 (2%)	56,56,56	1.97	18 (32%)
20	BCR	AB	849	-	41,41,41	0.83	0	56,56,56	2.41	24 (42%)
20	BCR	AL	305	-	41,41,41	0.86	0	56,56,56	2.54	18 (32%)
17	CLA	AB	813	2	47,51,73	1.46	8 (17%)	56,86,113	1.28	6 (10%)
17	CLA	AB	834	2	69,73,73	1.23	8 (11%)	83,113,113	1.12	6 (7%)
17	CLA	AG	201	-	47,52,73	1.52	8 (17%)	56,88,113	1.29	4 (7%)
17	CLA	A3	305	-	44,49,73	1.54	8 (18%)	52,84,113	1.30	5 (9%)
20	BCR	A3	318	-	41,41,41	0.98	1 (2%)	56,56,56	2.77	20 (35%)
17	CLA	A6	612	16	68,72,73	1.27	8 (11%)	81,111,113	1.12	5 (6%)
17	CLA	AA	805	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	9 (10%)
17	CLA	AF	804	-	45,49,73	1.52	7 (15%)	54,84,113	1.43	6 (11%)
17	CLA	AG	203	7	46,50,73	1.50	8 (17%)	55,85,113	1.29	5 (9%)
17	CLA	A1	316	13	47,51,73	1.59	8 (17%)	60,87,113	1.44	7 (11%)
17	CLA	AB	815	2	69,73,73	1.22	10 (14%)	83,113,113	1.27	10 (12%)
17	CLA	AA	811	1	69,73,73	1.24	7 (10%)	83,113,113	1.20	5 (6%)
17	CLA	AB	810	2	69,73,73	1.25	10 (14%)	83,113,113	1.25	4 (4%)
17	CLA	AB	836	-	46,50,73	1.51	7 (15%)	55,85,113	1.36	6 (10%)
17	CLA	AB	808	2	55,59,73	1.39	8 (14%)	65,95,113	1.33	7 (10%)
17	CLA	A3	312	14	57,62,73	1.37	8 (14%)	68,100,113	1.28	6 (8%)
17	CLA	AA	803	1	69,73,73	1.23	8 (11%)	83,113,113	1.27	8 (9%)
26	CHL	A6	607	-	54,58,74	2.22	19 (35%)	65,95,114	2.61	26 (40%)
17	CLA	AA	806	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
17	CLA	AB	806	2	69,73,73	1.25	8 (11%)	83,113,113	1.22	6 (7%)
17	CLA	AB	842	19	69,73,73	1.24	9 (13%)	83,113,113	1.30	9 (10%)
17	CLA	AA	828	1	69,73,73	1.25	8 (11%)	83,113,113	1.35	8 (9%)
17	CLA	AB	827	2	66,70,73	1.27	10 (15%)	79,109,113	1.37	9 (11%)
17	CLA	A6	601	15	50,54,73	1.44	10 (20%)	60,90,113	1.32	6 (10%)
26	CHL	A6	605	-	46,50,74	2.33	19 (41%)	52,85,114	2.83	25 (48%)
17	CLA	A1	309	-	47,52,73	1.52	8 (17%)	56,88,113	1.27	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A1	314	13	67,72,73	1.26	7 (10%)	80,112,113	1.17	6 (7%)
19	LHG	A1	301	17	37,37,48	1.07	2 (5%)	40,43,54	0.97	3 (7%)
20	BCR	AA	845	-	41,41,41	1.03	2 (4%)	56,56,56	1.91	13 (23%)
17	CLA	A3	306	14	45,49,73	1.57	9 (20%)	57,84,113	1.45	8 (14%)
17	CLA	A6	610	19	41,45,73	2.60	11 (26%)	47,76,113	1.41	10 (21%)
19	LHG	A6	617	17	35,35,48	1.05	2 (5%)	38,41,54	0.97	2 (5%)
17	CLA	AB	822	2	51,55,73	1.44	7 (13%)	61,91,113	1.20	4 (6%)
20	BCR	A6	616	-	41,41,41	0.99	2 (4%)	56,56,56	2.01	16 (28%)
17	CLA	AA	802	-	69,73,73	1.27	9 (13%)	83,113,113	1.25	6 (7%)
17	CLA	AA	832	1	60,64,73	1.33	6 (10%)	72,102,113	1.26	8 (11%)
17	CLA	AB	819	2	64,68,73	1.29	9 (14%)	77,107,113	1.49	12 (15%)
20	BCR	AK	205	-	41,41,41	1.02	3 (7%)	56,56,56	2.06	14 (25%)
17	CLA	AK	201	11	39,43,73	1.72	8 (20%)	50,75,113	1.45	9 (18%)
17	CLA	AB	835	2	64,68,73	1.28	7 (10%)	77,107,113	1.24	7 (9%)
17	CLA	A1	313	13	49,53,73	1.48	9 (18%)	59,89,113	1.39	5 (8%)
20	BCR	AF	801	-	41,41,41	0.86	1 (2%)	56,56,56	1.56	10 (17%)
17	CLA	A1	311	13	63,67,73	1.32	8 (12%)	76,106,113	1.12	5 (6%)
17	CLA	A3	309	14	45,49,73	1.53	8 (17%)	54,84,113	1.33	9 (16%)
26	CHL	A6	606	-	47,51,74	2.32	19 (40%)	52,86,114	2.78	24 (46%)
19	LHG	A1	302	-	35,35,48	1.10	2 (5%)	38,41,54	1.04	2 (5%)
17	CLA	AB	817	2	59,63,73	1.35	7 (11%)	71,101,113	1.21	5 (7%)
17	CLA	AA	840	1	69,73,73	1.25	9 (13%)	83,113,113	1.25	9 (10%)
17	CLA	AJ	102	10	46,50,73	1.49	6 (13%)	55,85,113	1.30	4 (7%)
17	CLA	AB	833	2	69,73,73	1.24	7 (10%)	83,113,113	1.18	8 (9%)
17	CLA	AB	816	2	47,51,73	1.47	8 (17%)	56,86,113	1.21	3 (5%)
17	CLA	A1	312	19	41,46,73	1.65	9 (21%)	52,81,113	1.30	9 (17%)
17	CLA	A6	603	16	45,50,73	1.55	8 (17%)	53,85,113	1.44	5 (9%)
20	BCR	A4	317	-	41,41,41	0.82	0	56,56,56	2.37	23 (41%)
17	CLA	AA	822	1	46,50,73	1.50	7 (15%)	55,85,113	1.31	5 (9%)
20	BCR	AI	102	-	41,41,41	0.78	0	56,56,56	2.22	22 (39%)
17	CLA	A4	311	15	59,64,73	1.35	7 (11%)	70,102,113	1.20	6 (8%)
18	PQN	AB	843	-	34,34,34	3.39	11 (32%)	42,45,45	1.83	6 (14%)
17	CLA	A6	604	-	47,51,73	1.49	8 (17%)	55,86,113	1.23	4 (7%)
17	CLA	AA	801	1	69,73,73	1.24	7 (10%)	83,113,113	1.20	6 (7%)
17	CLA	A6	602	16	69,73,73	1.25	9 (13%)	83,113,113	1.20	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	AB	801	2	69,73,73	1.24	8 (11%)	83,113,113	1.49	12 (14%)

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
26	CHL	A4	304	-	-	1/10/86/117	-
17	CLA	AA	827	1	-	18/39/115/115	-
20	BCR	AB	847	-	-	0/29/63/63	0/2/2/2
25	LMG	AG	202	-	-	5/33/53/70	0/1/1/1
17	CLA	AL	303	12	-	9/33/109/115	-
20	BCR	AA	848	-	-	4/29/63/63	0/2/2/2
17	CLA	AB	826	-	-	6/36/112/115	-
17	CLA	AA	838	1	-	8/27/103/115	-
20	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
17	CLA	AA	837	1	-	6/23/99/115	-
17	CLA	AH	201	8	-	12/33/109/115	-
17	CLA	AA	807	1	-	4/21/97/115	-
17	CLA	AB	814	2	-	16/39/115/115	-
17	CLA	AA	808	1	-	10/39/115/115	-
17	CLA	AA	814	1	-	5/15/91/115	-
17	CLA	AA	836	1	-	9/15/91/115	-
17	CLA	AG	204	7	-	6/15/91/115	-
17	CLA	AF	802	-	-	10/30/106/115	-
17	CLA	A1	306	-	-	9/20/96/115	-
20	BCR	AJ	103	-	-	5/29/63/63	0/2/2/2
17	CLA	A1	307	-	-	6/10/82/115	-
17	CLA	AB	811	2	-	15/39/115/115	-
22	LMU	AA	851	-	-	10/21/61/61	0/2/2/2
17	CLA	AB	830	2	-	10/29/105/115	-
19	LHG	AA	844	-	-	18/53/53/53	-
18	PQN	AA	843	-	-	6/23/43/43	0/2/2/2
17	CLA	A4	313	15	-	11/21/97/115	-
17	CLA	A3	308	14	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A4	308	15	-	6/26/102/115	-
17	CLA	AB	804	-	-	16/39/115/115	-
17	CLA	A6	611	16	-	8/13/89/115	-
21	SF4	AA	850	1,2	-	-	0/6/5/5
17	CLA	AA	834	1	-	17/39/115/115	-
22	LMU	AB	850	-	-	9/21/61/61	0/2/2/2
17	CLA	A1	315	13	-	0/4/80/115	-
17	CLA	A3	313	14	-	3/8/84/115	-
17	CLA	AA	841	1	-	12/39/115/115	-
17	CLA	AA	824	1	-	9/25/101/115	-
26	CHL	A1	308	13	-	2/10/86/117	-
17	CLA	AA	812	1	-	9/26/102/115	-
22	LMU	AB	853	-	-	13/21/61/61	0/2/2/2
23	DGD	AB	851	-	-	21/55/95/95	0/2/2/2
27	XAT	A1	318	-	-	0/31/93/93	0/4/4/4
19	LHG	A1	320	17	-	16/53/53/53	-
17	CLA	AA	819	1	-	14/39/115/115	-
17	CLA	AA	830	1	-	14/39/115/115	-
17	CLA	A4	310	15	-	7/10/86/115	-
21	SF4	AC	101	3	-	-	0/6/5/5
24	LUT	A4	315	-	-	1/29/67/67	0/2/2/2
17	CLA	A1	304	13	-	11/33/109/115	-
17	CLA	A6	613	16	-	4/13/89/115	-
26	CHL	A4	306	-	-	2/17/93/117	-
20	BCR	AB	844	-	-	5/29/63/63	0/2/2/2
17	CLA	A4	303	-	-	4/11/87/115	-
17	CLA	A4	309	-	-	5/12/88/115	-
22	LMU	AB	852	-	-	9/21/61/61	0/2/2/2
17	CLA	AA	823	1	-	6/10/86/115	-
20	BCR	AG	205	-	-	2/29/63/63	0/2/2/2
17	CLA	AB	839	2	-	3/18/94/115	-
17	CLA	A6	609	16	-	6/27/103/115	-
17	CLA	A3	304	-	-	0/9/85/115	-
17	CLA	A3	315	14	-	0/8/84/115	-
17	CLA	AK	204	11	-	9/17/93/115	-
24	LUT	A1	317	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A3	311	14	-	1/13/89/115	-
17	CLA	A3	302	14	-	8/33/109/115	-
17	CLA	AB	840	-	-	7/39/115/115	-
17	CLA	A4	312	15	-	6/15/91/115	-
25	LMG	A4	318	-	-	15/34/54/70	0/1/1/1
17	CLA	AA	835	1	-	2/13/89/115	-
17	CLA	AB	812	2	-	8/25/101/115	-
19	LHG	A3	301	-	-	11/40/40/53	-
17	CLA	AA	821	-	-	15/39/115/115	-
20	BCR	AI	101	-	-	7/29/63/63	0/2/2/2
20	BCR	AB	845	-	-	6/29/63/63	0/2/2/2
26	CHL	A4	305	-	-	0/10/86/117	-
17	CLA	AB	828	2	-	13/39/115/115	-
17	CLA	AL	302	12	-	7/10/86/115	-
17	CLA	A4	307	15	-	3/15/91/115	-
24	LUT	A3	316	-	-	0/29/67/67	0/2/2/2
27	XAT	A6	615	-	-	0/31/93/93	0/4/4/4
17	CLA	AA	820	1	-	5/15/91/115	-
17	CLA	AF	803	-	-	3/12/88/115	-
17	CLA	AB	838	2	-	7/39/115/115	-
24	LUT	AF	806	-	-	0/29/67/67	0/2/2/2
17	CLA	AB	802	-	-	16/37/113/115	-
17	CLA	AA	813	1	-	19/39/115/115	-
20	BCR	AL	306	-	-	5/29/63/63	0/2/2/2
27	XAT	A3	317	-	-	0/31/93/93	0/4/4/4
17	CLA	A3	310	19	-	2/2/78/115	-
17	CLA	AB	823	2	-	19/39/115/115	-
17	CLA	AB	832	2	-	9/39/115/115	-
17	CLA	AA	833	1	-	21/39/115/115	-
17	CLA	AK	203	-	-	7/15/91/115	-
26	CHL	A3	307	-	-	4/15/91/117	-
17	CLA	AA	839	1	-	6/24/100/115	-
17	CLA	AB	829	2	-	15/39/115/115	-
17	CLA	AB	807	2	-	11/39/115/115	-
17	CLA	AL	304	-	-	5/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AB	803	2	-	19/39/115/115	-
24	LUT	A6	614	-	-	0/29/67/67	0/2/2/2
17	CLA	AB	821	2	-	9/21/97/115	-
25	LMG	A1	321	-	-	17/39/59/70	0/1/1/1
17	CLA	AA	818	1	-	9/32/108/115	-
17	CLA	AB	841	2	-	9/39/115/115	-
17	CLA	A3	303	14	-	10/27/103/115	-
17	CLA	AA	831	1	-	9/18/94/115	-
17	CLA	AB	831	2	-	5/13/89/115	-
17	CLA	AA	809	1	-	7/21/97/115	-
26	CHL	A1	303	13	-	4/23/99/117	-
20	BCR	AA	849	-	-	8/29/63/63	0/2/2/2
17	CLA	AB	820	-	-	10/27/103/115	-
17	CLA	A4	302	15	-	5/13/89/115	-
22	LMU	AL	301	-	-	11/20/60/61	0/2/2/2
17	CLA	AB	837	2	-	7/21/97/115	-
26	CHL	A3	320	16	-	8/24/100/117	-
17	CLA	AA	829	1	-	18/39/115/115	-
20	BCR	AF	805	-	-	6/29/63/63	0/2/2/2
26	CHL	A4	314	15	-	0/10/86/117	-
19	LHG	AJ	104	-	-	16/44/44/53	-
20	BCR	A1	319	-	-	4/29/63/63	0/2/2/2
17	CLA	AA	815	1	-	3/12/88/115	-
17	CLA	AB	805	2	-	2/10/86/115	-
17	CLA	AB	824	2	-	5/13/89/115	-
17	CLA	A1	305	13	-	8/27/103/115	-
17	CLA	AA	842	-	-	20/39/115/115	-
20	BCR	AA	847	-	-	13/29/63/63	0/2/2/2
20	BCR	AB	846	-	-	6/29/63/63	0/2/2/2
17	CLA	A3	314	-	-	2/2/74/115	-
17	CLA	AA	825	-	-	10/39/115/115	-
17	CLA	A4	301	15	-	10/33/109/115	-
20	BCR	AK	202	-	-	5/29/63/63	0/2/2/2
17	CLA	A1	310	13	-	2/8/84/115	-
21	SF4	AC	102	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AA	826	-	-	12/32/108/115	-
20	BCR	AA	846	-	-	6/29/63/63	0/2/2/2
17	CLA	AA	804	1	-	7/24/100/115	-
17	CLA	AA	816	-	-	8/15/91/115	-
17	CLA	AB	818	2	-	12/32/108/115	-
19	LHG	A3	319	17	-	14/26/26/53	-
27	XAT	A4	316	-	-	0/31/93/93	0/4/4/4
17	CLA	AB	809	2	-	16/39/115/115	-
17	CLA	AB	825	-	-	14/39/115/115	-
17	CLA	AA	817	1	-	6/33/109/115	-
17	CLA	AA	810	1	-	10/39/111/115	-
17	CLA	A6	608	16	-	3/15/91/115	-
20	BCR	AB	848	-	-	2/29/63/63	0/2/2/2
20	BCR	AB	849	-	-	5/29/63/63	0/2/2/2
20	BCR	AL	305	-	-	3/29/63/63	0/2/2/2
17	CLA	AB	813	2	-	5/13/89/115	-
17	CLA	AB	834	2	-	18/39/115/115	-
17	CLA	AG	201	-	-	5/13/89/115	-
17	CLA	A3	305	-	-	6/10/86/115	-
20	BCR	A3	318	-	-	4/29/63/63	0/2/2/2
17	CLA	A6	612	16	-	7/37/113/115	-
17	CLA	AA	805	1	-	17/39/115/115	-
17	CLA	AF	804	-	-	4/10/86/115	-
17	CLA	AG	203	7	-	4/12/88/115	-
17	CLA	A1	316	13	-	9/11/87/115	-
17	CLA	AB	815	2	-	17/39/115/115	-
17	CLA	AA	811	1	-	13/39/115/115	-
17	CLA	AB	810	2	-	17/39/115/115	-
17	CLA	AB	836	-	-	3/12/88/115	-
17	CLA	AB	808	2	-	6/22/98/115	-
17	CLA	A3	312	14	-	13/25/101/115	-
17	CLA	AA	803	1	-	15/39/115/115	-
26	CHL	A6	607	-	-	8/21/97/117	-
17	CLA	AA	806	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AB	806	2	-	15/39/115/115	-
17	CLA	AB	842	19	-	20/39/115/115	-
17	CLA	AA	828	1	-	15/39/115/115	-
17	CLA	AB	827	2	-	14/36/112/115	-
17	CLA	A6	601	15	-	2/17/93/115	-
26	CHL	A6	605	-	-	2/12/88/117	-
17	CLA	A1	309	-	-	7/13/89/115	-
17	CLA	A1	314	13	-	14/37/113/115	-
19	LHG	A1	301	17	-	11/42/42/53	-
20	BCR	AA	845	-	-	2/29/63/63	0/2/2/2
17	CLA	A3	306	14	-	0/10/86/115	-
17	CLA	A6	610	19	-	5/10/70/115	-
19	LHG	A6	617	17	-	17/40/40/53	-
17	CLA	AB	822	2	-	7/18/94/115	-
20	BCR	A6	616	-	-	2/29/63/63	0/2/2/2
17	CLA	AA	802	-	-	8/39/115/115	-
17	CLA	AA	832	1	-	7/29/105/115	-
17	CLA	AB	819	2	-	14/33/109/115	-
20	BCR	AK	205	-	-	6/29/63/63	0/2/2/2
17	CLA	AK	201	11	-	0/2/74/115	-
17	CLA	AB	835	2	-	7/33/109/115	-
17	CLA	A1	313	13	-	4/15/91/115	-
20	BCR	AF	801	-	-	2/29/63/63	0/2/2/2
17	CLA	A1	311	13	-	3/31/107/115	-
17	CLA	A3	309	14	-	5/10/86/115	-
26	CHL	A6	606	-	-	2/14/90/117	-
19	LHG	A1	302	-	-	15/40/40/53	-
17	CLA	AB	817	2	-	8/27/103/115	-
17	CLA	AA	840	1	-	16/39/115/115	-
17	CLA	AJ	102	10	-	5/12/88/115	-
17	CLA	AB	833	2	-	10/39/115/115	-
17	CLA	AB	816	2	-	4/13/89/115	-
17	CLA	A1	312	19	-	0/4/80/115	-
17	CLA	A6	603	16	-	2/11/87/115	-
20	BCR	A4	317	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AA	822	1	-	5/12/88/115	-
20	BCR	AI	102	-	-	5/29/63/63	0/2/2/2
17	CLA	A4	311	15	-	8/28/104/115	-
18	PQN	AB	843	-	-	8/23/43/43	0/2/2/2
17	CLA	A6	604	-	-	3/11/88/115	-
17	CLA	AA	801	1	-	13/39/115/115	-
17	CLA	A6	602	16	-	11/39/115/115	-
17	CLA	AB	801	2	-	17/39/115/115	-

The worst 5 of 1493 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A6	610	CLA	C1A-NA	12.69	1.40	1.29
18	AA	843	PQN	C12-C13	9.56	1.55	1.33
18	AB	843	PQN	C12-C13	9.36	1.55	1.33
18	AB	843	PQN	O4-C4	7.78	1.39	1.23
18	AA	843	PQN	O4-C4	7.78	1.39	1.23

The worst 5 of 1954 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A1	319	BCR	C40-C30-C25	-13.95	87.67	110.30
20	A3	318	BCR	C40-C30-C25	-10.15	93.83	110.30
20	AL	305	BCR	C7-C8-C9	-9.80	111.42	126.23
20	A1	319	BCR	C39-C30-C25	9.45	125.63	110.30
27	A4	316	XAT	O4-C5-C4	9.12	120.24	113.38

There are no chirality outliers.

5 of 1635 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	AA	801	CLA	CBD-CGD-O2D-CED
17	AA	802	CLA	CBD-CGD-O2D-CED
17	AA	804	CLA	C1A-C2A-CAA-CBA
17	AA	804	CLA	C3A-C2A-CAA-CBA
17	AA	805	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

101 monomers are involved in 142 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	AB	847	BCR	3	0
17	AL	303	CLA	1	0
20	AA	848	BCR	2	0
17	AA	838	CLA	1	0
20	AJ	101	BCR	1	0
17	AB	814	CLA	1	0
17	AG	204	CLA	4	0
17	A1	306	CLA	2	0
20	AJ	103	BCR	1	0
19	AA	844	LHG	1	0
18	AA	843	PQN	3	0
17	A4	313	CLA	1	0
17	A3	308	CLA	1	0
17	A4	308	CLA	1	0
17	AA	834	CLA	1	0
17	AA	841	CLA	1	0
27	A1	318	XAT	1	0
17	AA	830	CLA	1	0
21	AC	101	SF4	1	0
24	A4	315	LUT	3	0
26	A4	306	CHL	2	0
20	AB	844	BCR	2	0
17	A4	309	CLA	1	0
20	AG	205	BCR	1	0
17	AB	839	CLA	2	0
17	A3	304	CLA	1	0
17	AK	204	CLA	1	0
24	A1	317	LUT	1	0
17	AB	840	CLA	1	0
25	A4	318	LMG	4	0
17	AA	835	CLA	1	0
19	A3	301	LHG	1	0
20	AB	845	BCR	1	0
17	AB	828	CLA	1	0
17	A4	307	CLA	1	0
27	A6	615	XAT	4	0
17	AA	820	CLA	1	0
17	AF	803	CLA	1	0
17	AB	838	CLA	1	0
24	AF	806	LUT	2	0
17	AB	802	CLA	4	0
27	A3	317	XAT	3	0
17	AA	833	CLA	1	0

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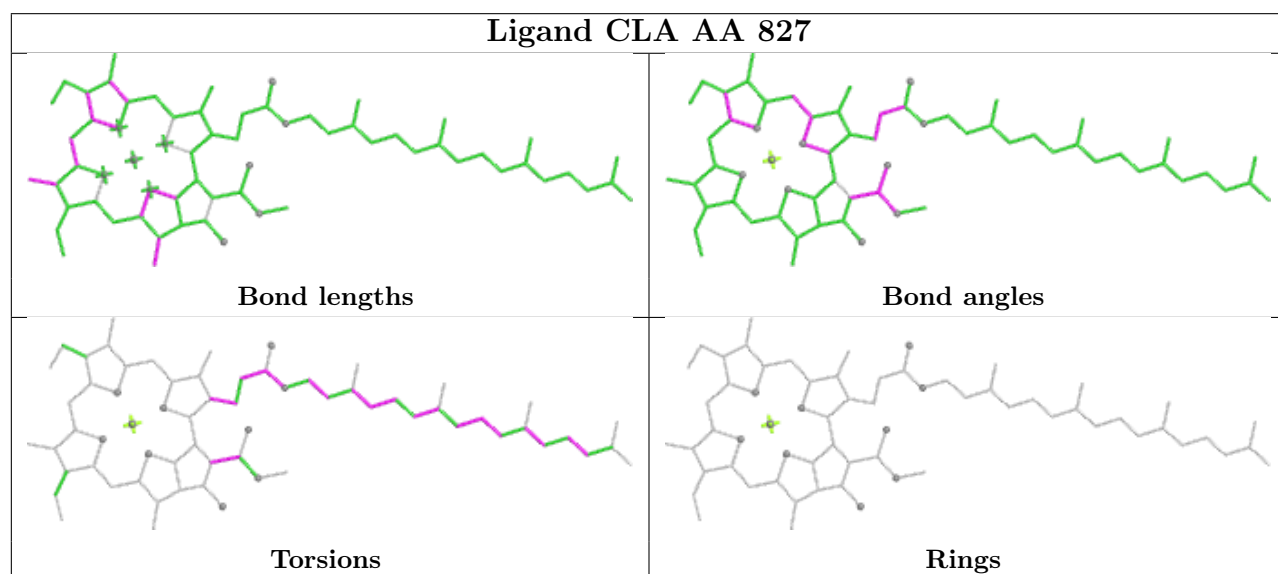
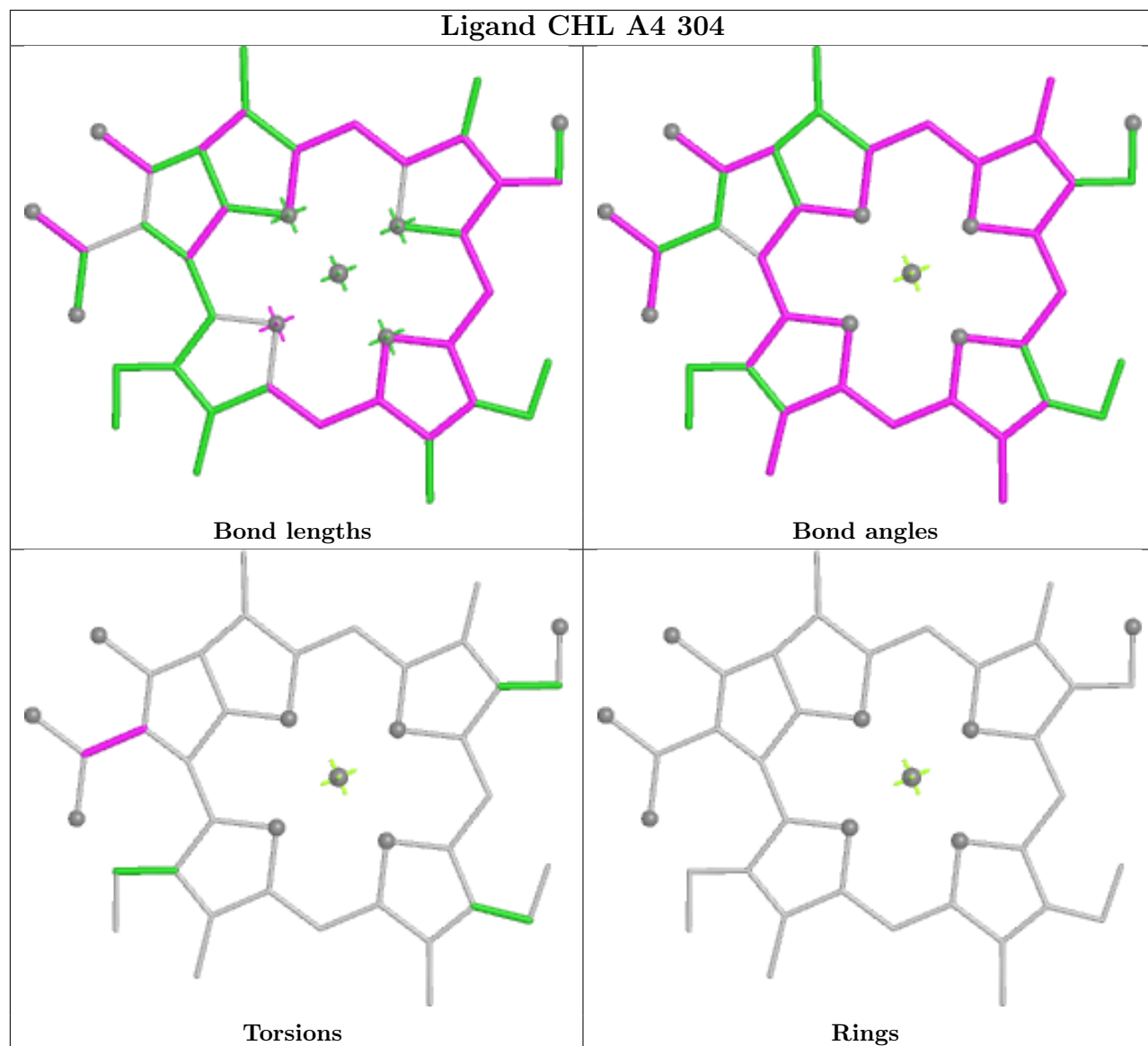
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A3	307	CHL	1	0
17	AB	803	CLA	3	0
24	A6	614	LUT	2	0
25	A1	321	LMG	1	0
17	AA	818	CLA	1	0
17	AB	831	CLA	1	0
26	A1	303	CHL	2	0
20	AA	849	BCR	2	0
22	AL	301	LMU	1	0
26	A3	320	CHL	1	0
20	AF	805	BCR	2	0
20	A1	319	BCR	3	0
17	AA	815	CLA	1	0
17	AB	824	CLA	1	0
17	A1	305	CLA	1	0
20	AA	847	BCR	1	0
20	AB	846	BCR	1	0
17	AA	825	CLA	2	0
17	A4	301	CLA	1	0
21	AC	102	SF4	1	0
20	AA	846	BCR	1	0
17	AB	818	CLA	2	0
27	A4	316	XAT	2	0
17	AB	809	CLA	2	0
17	AB	825	CLA	1	0
17	AA	817	CLA	1	0
17	AA	810	CLA	1	0
20	AB	848	BCR	2	0
20	AL	305	BCR	1	0
17	AB	834	CLA	3	0
20	A3	318	BCR	2	0
17	A6	612	CLA	1	0
17	A1	316	CLA	1	0
17	AA	811	CLA	3	0
17	AB	810	CLA	1	0
17	AB	808	CLA	1	0
17	AA	803	CLA	1	0
26	A6	607	CHL	2	0
17	AA	806	CLA	1	0
17	AB	842	CLA	1	0
17	AA	828	CLA	1	0
17	AB	827	CLA	4	0

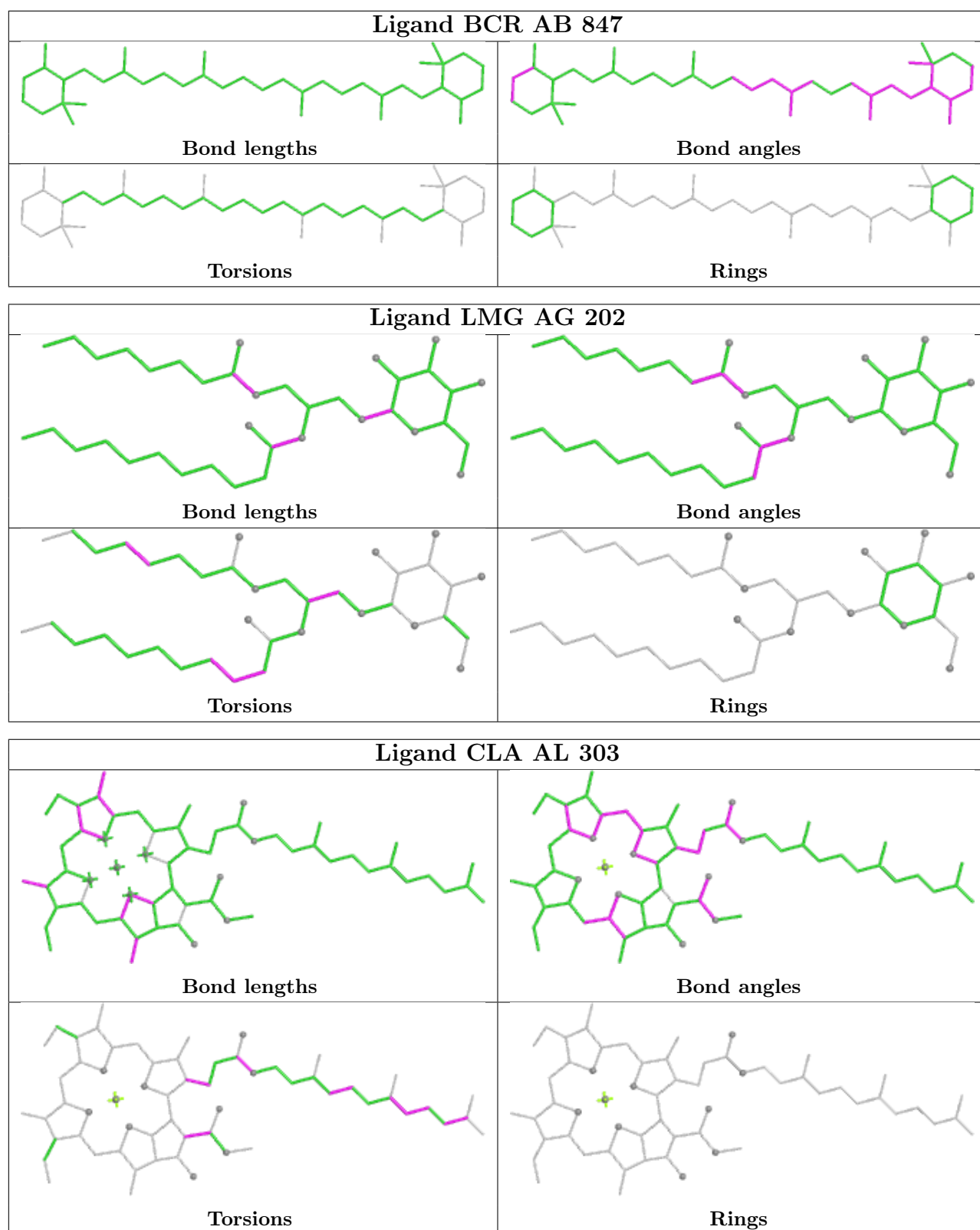
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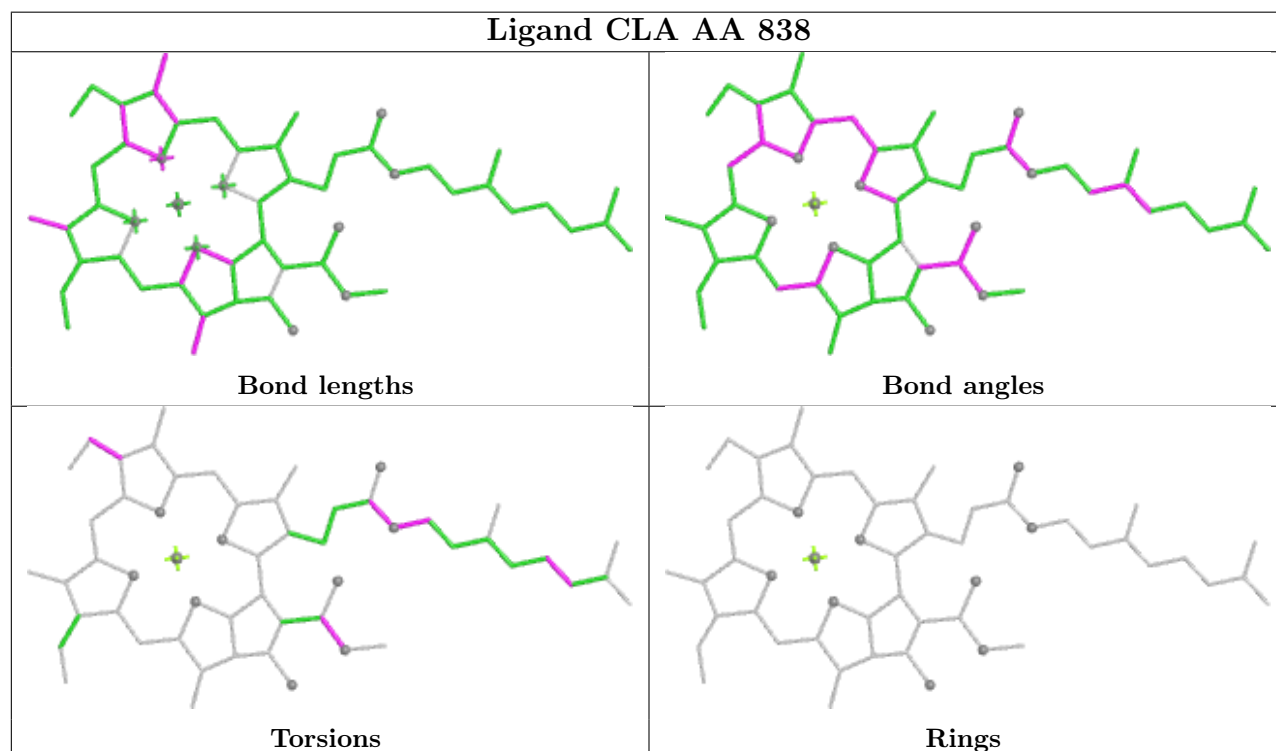
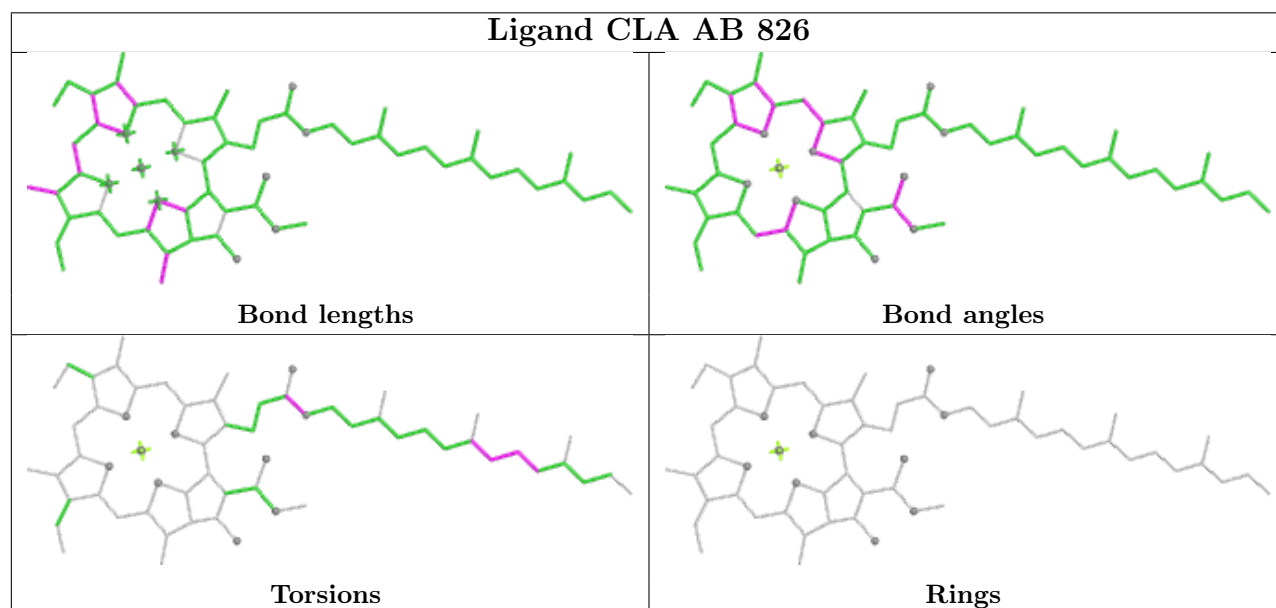
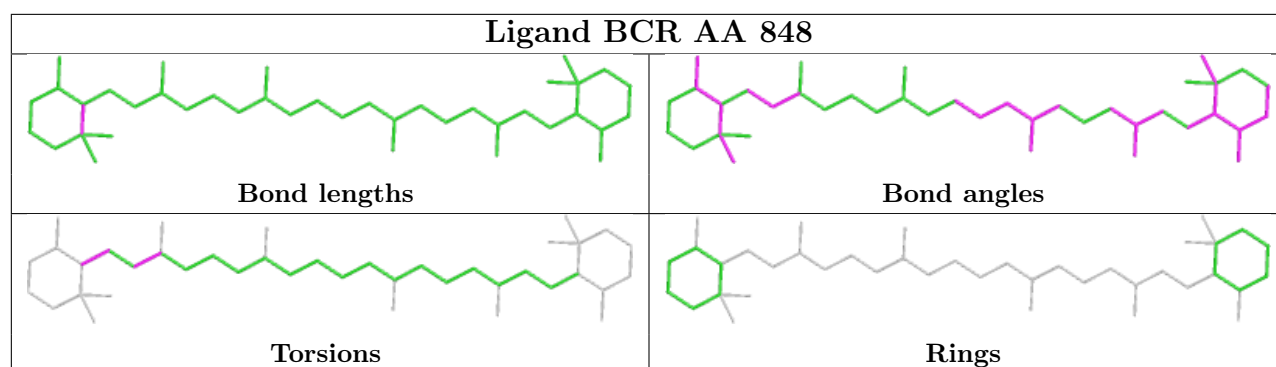
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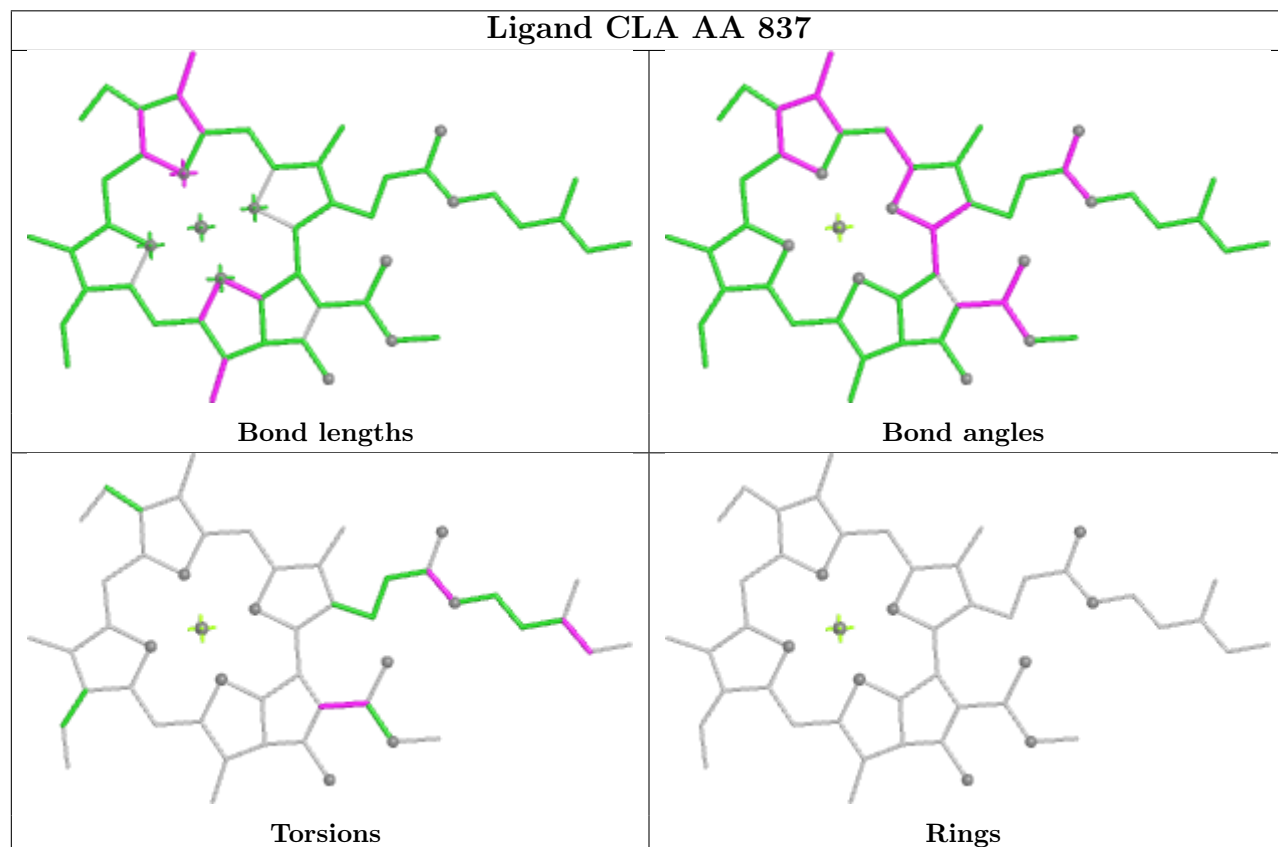
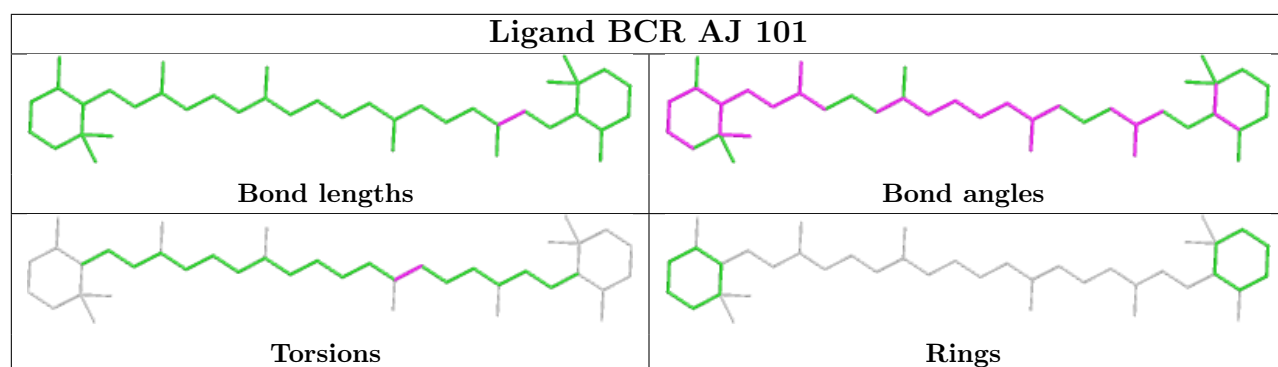
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A6	601	CLA	1	0
17	A1	314	CLA	1	0
19	A6	617	LHG	1	0
17	AB	822	CLA	1	0
20	A6	616	BCR	3	0
17	AA	802	CLA	1	0
20	AK	205	BCR	2	0
20	AF	801	BCR	4	0
17	A1	311	CLA	2	0
17	AB	833	CLA	2	0
17	A6	603	CLA	2	0
20	AI	102	BCR	1	0
17	A4	311	CLA	1	0
18	AB	843	PQN	2	0
17	AA	801	CLA	11	0
17	AB	801	CLA	1	0

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

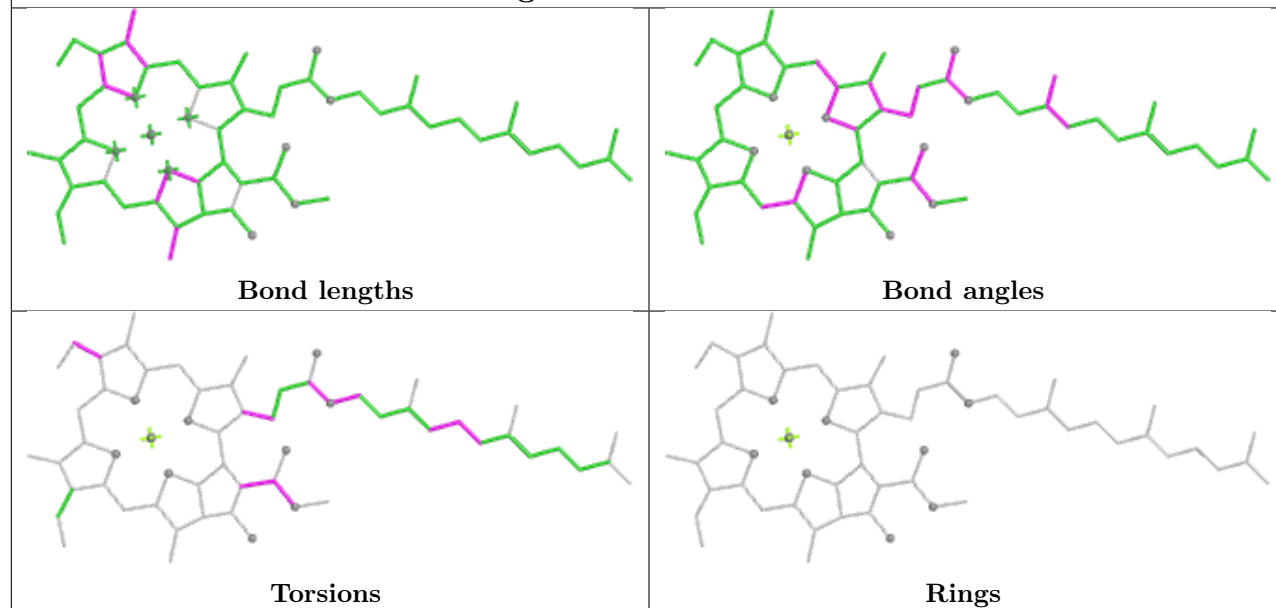




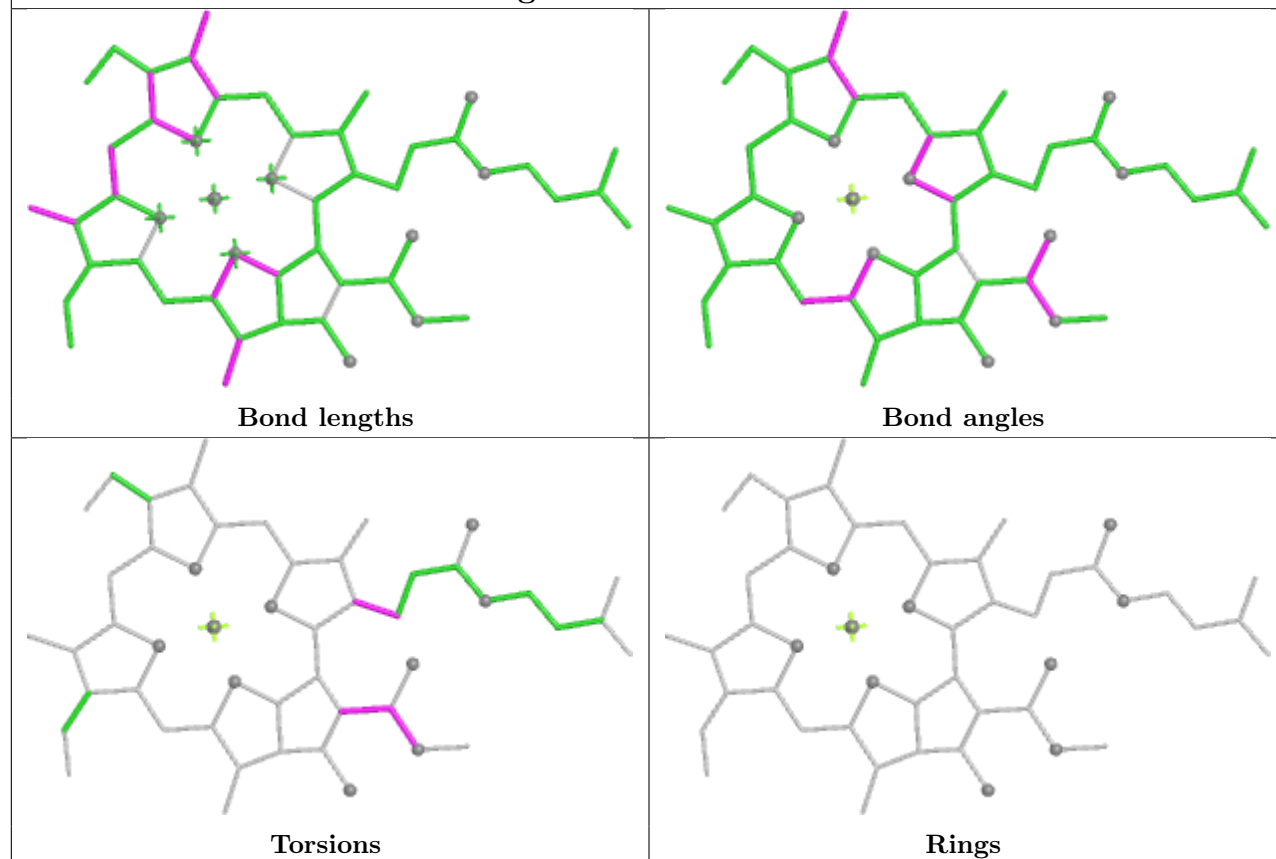




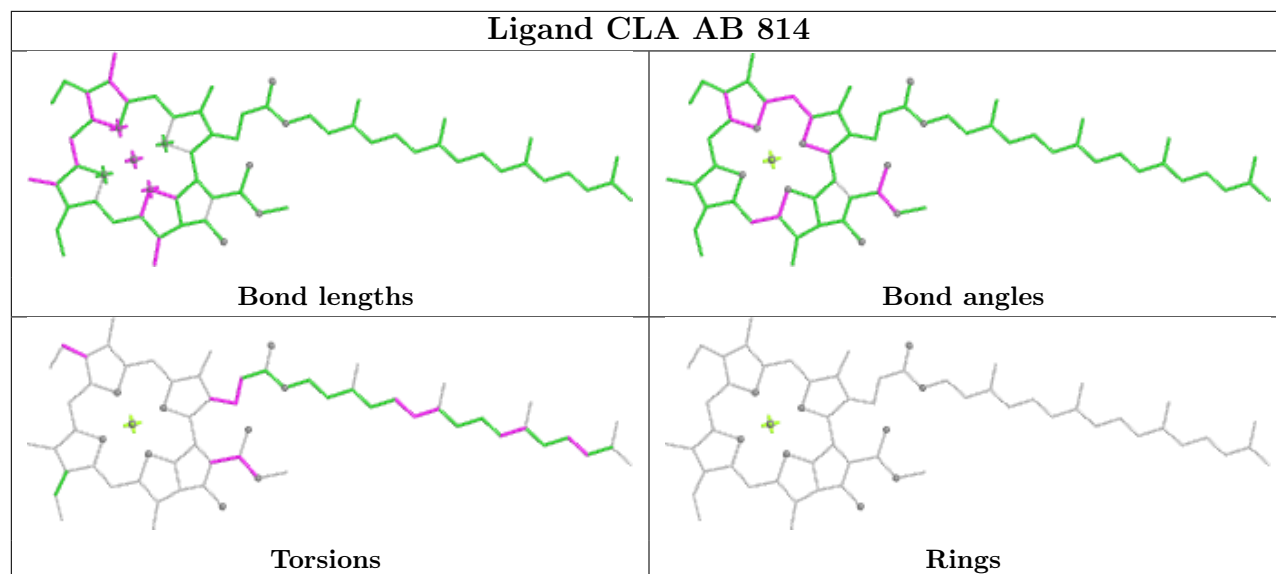
Ligand CLA AH 201



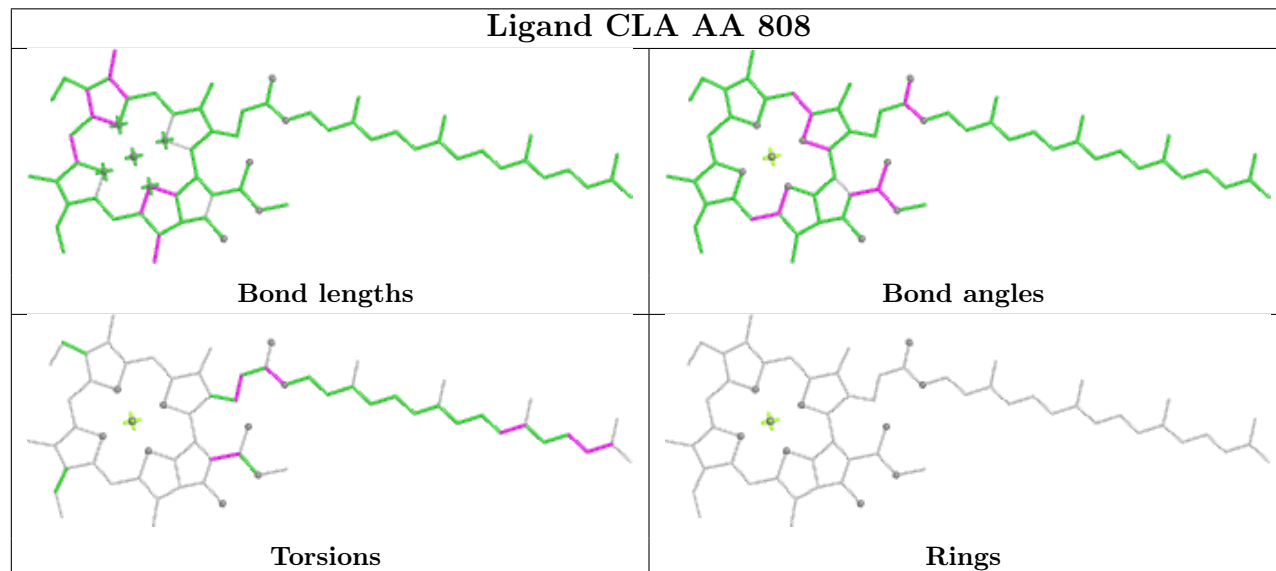
Ligand CLA AA 807



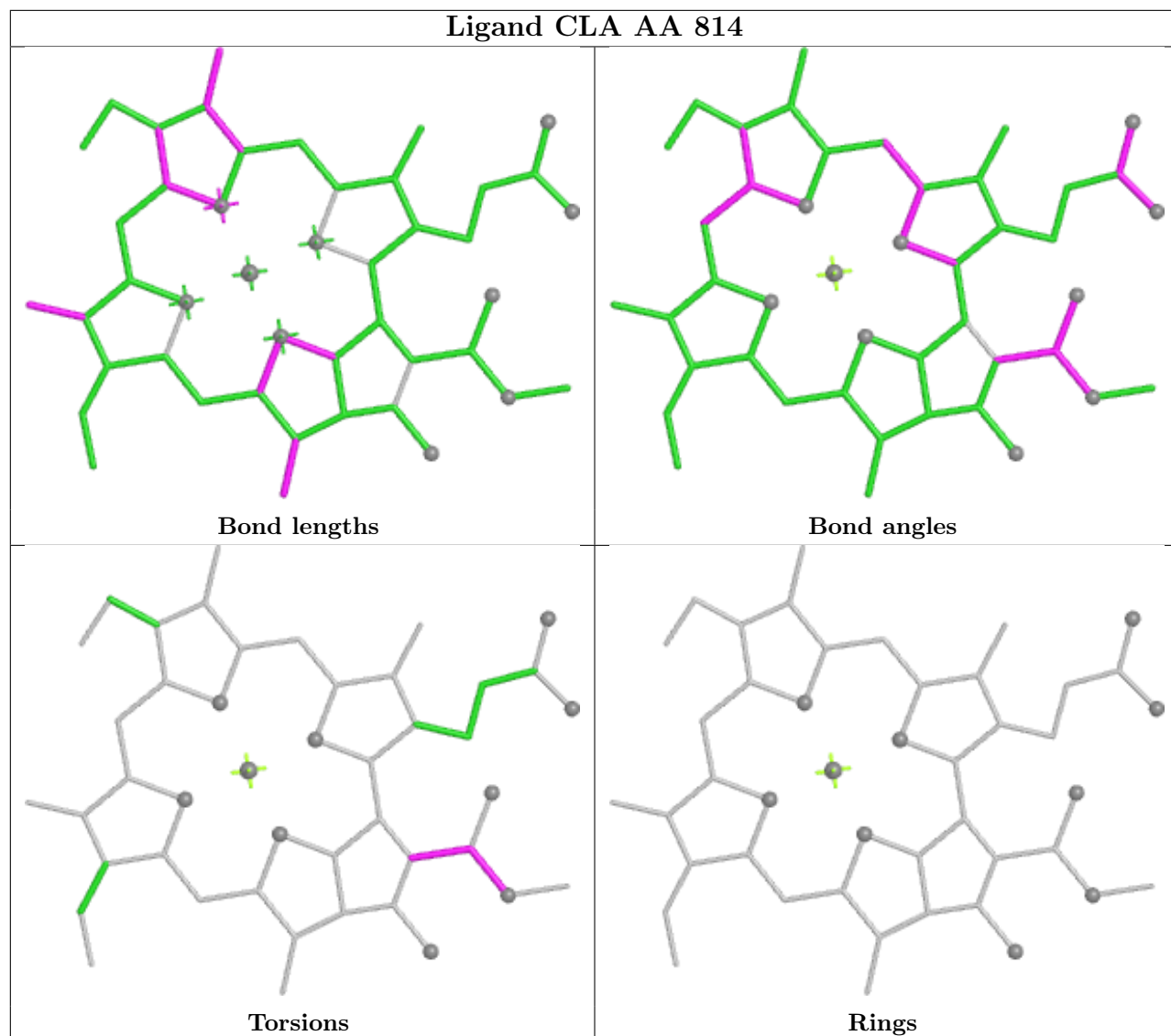
Ligand CLA AB 814



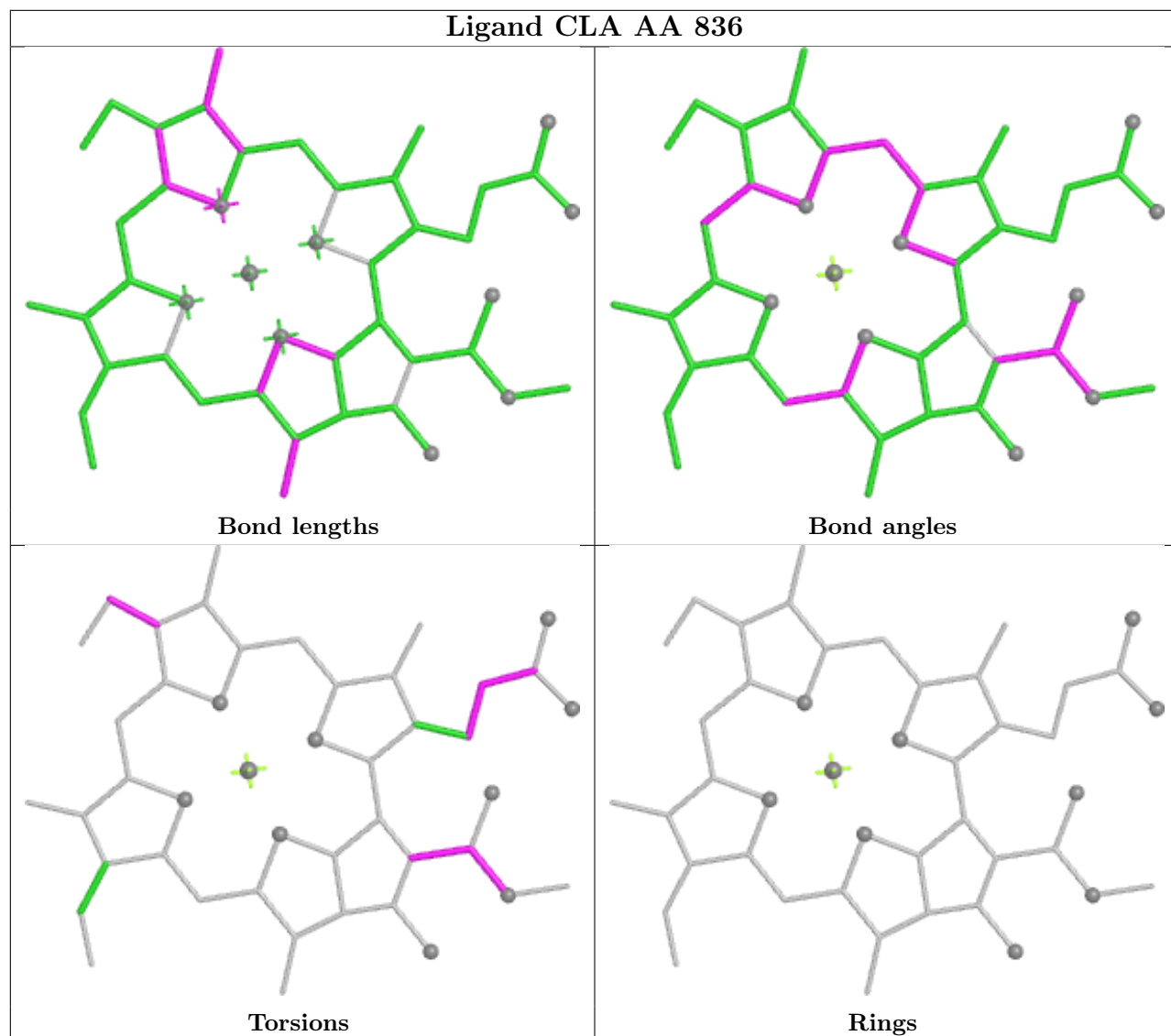
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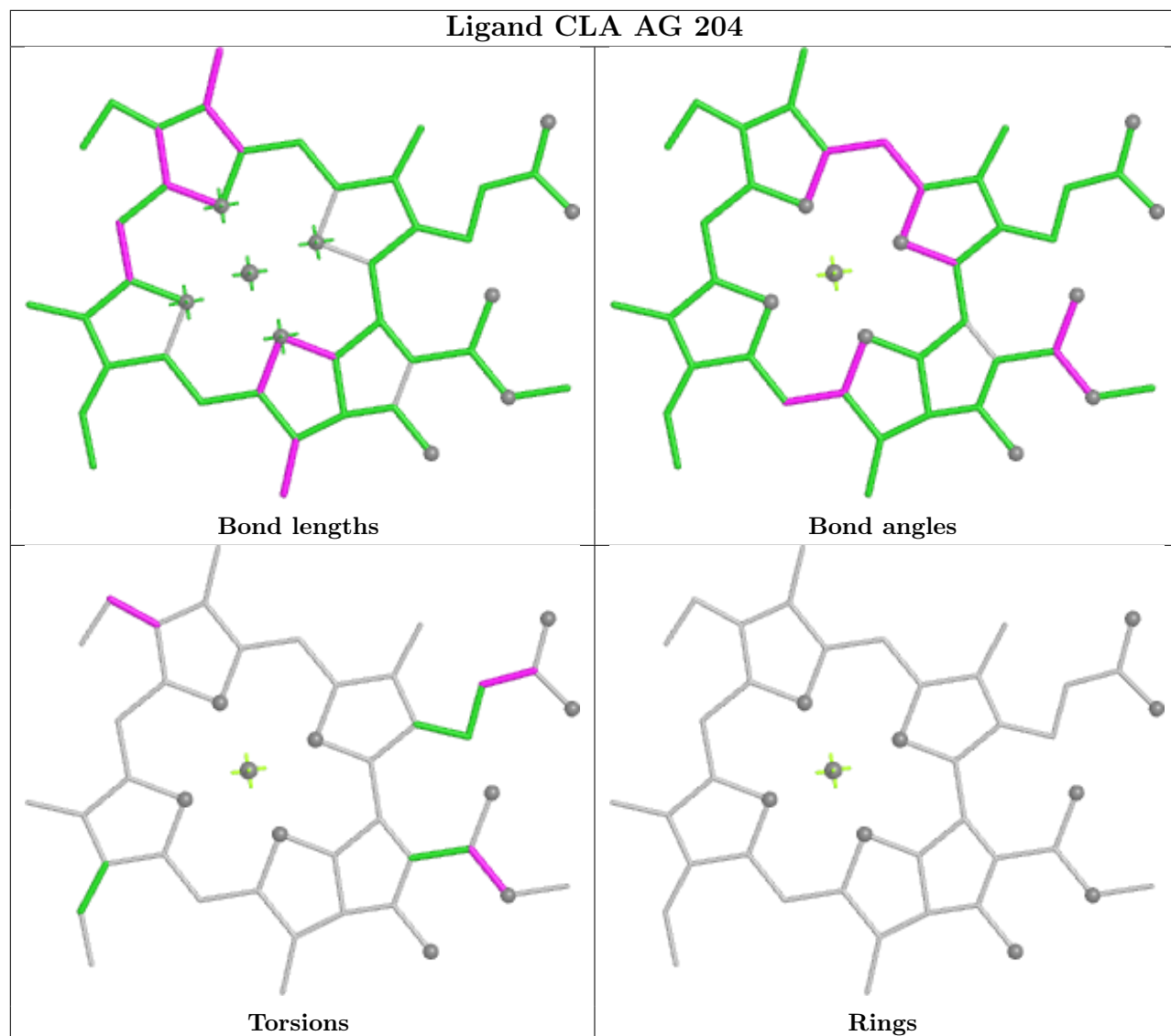
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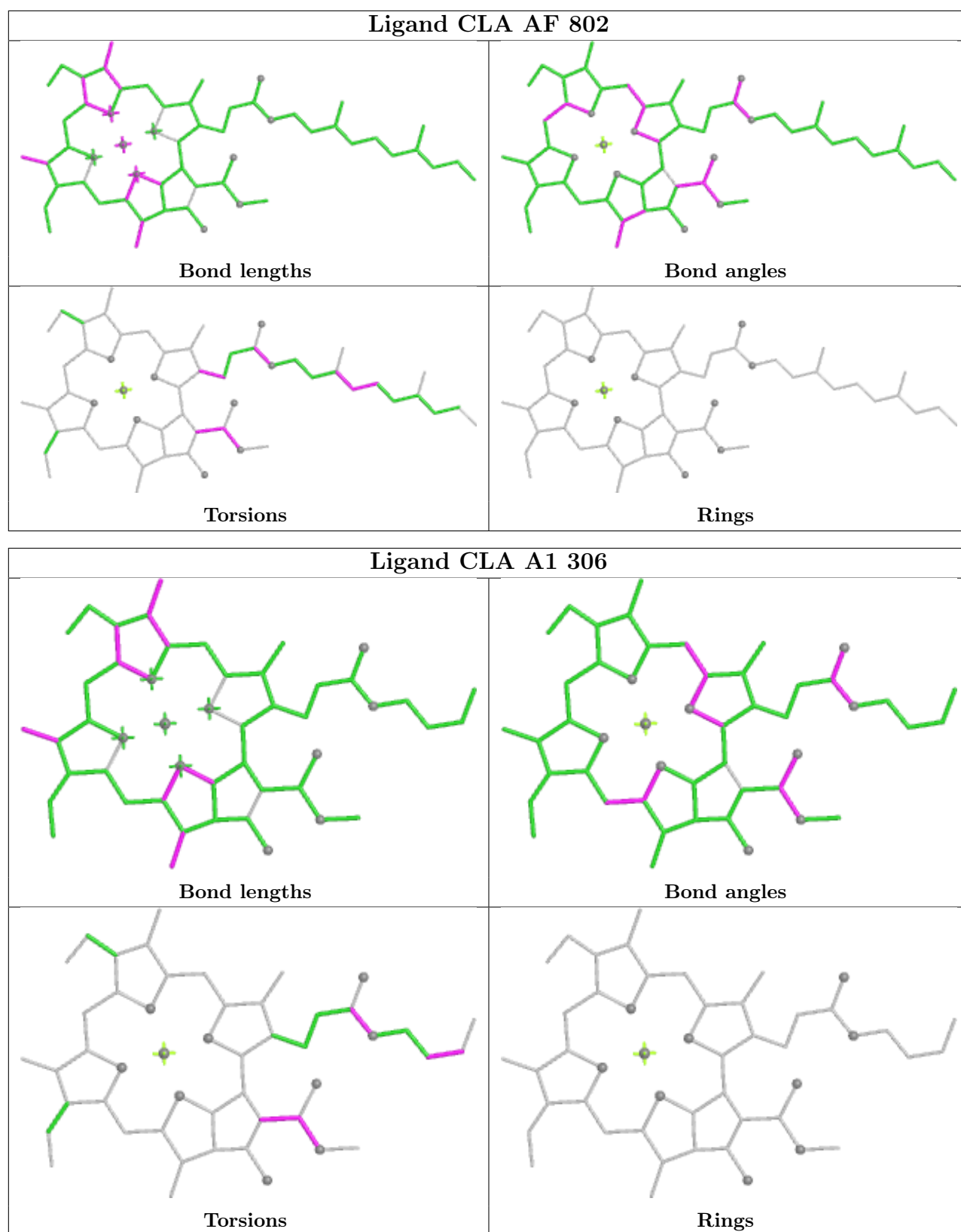


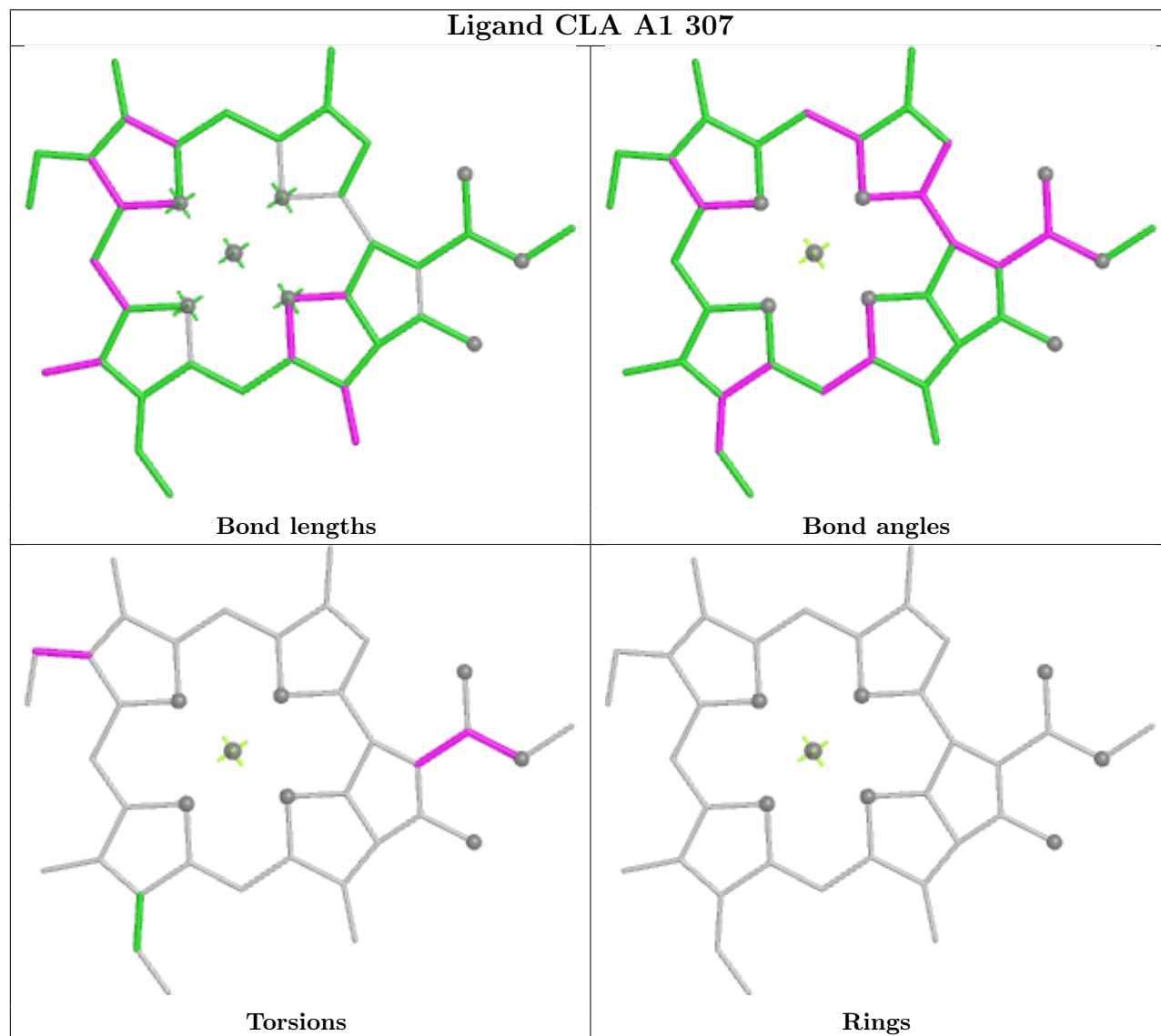
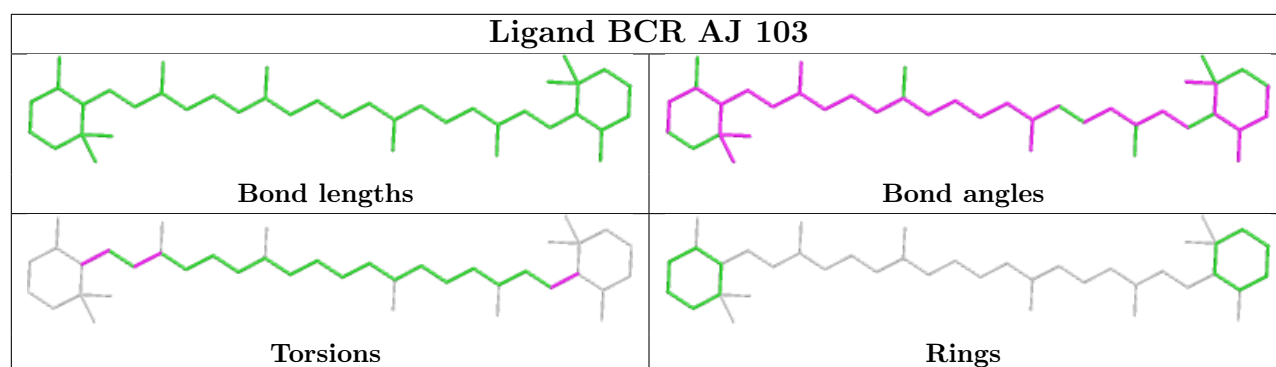
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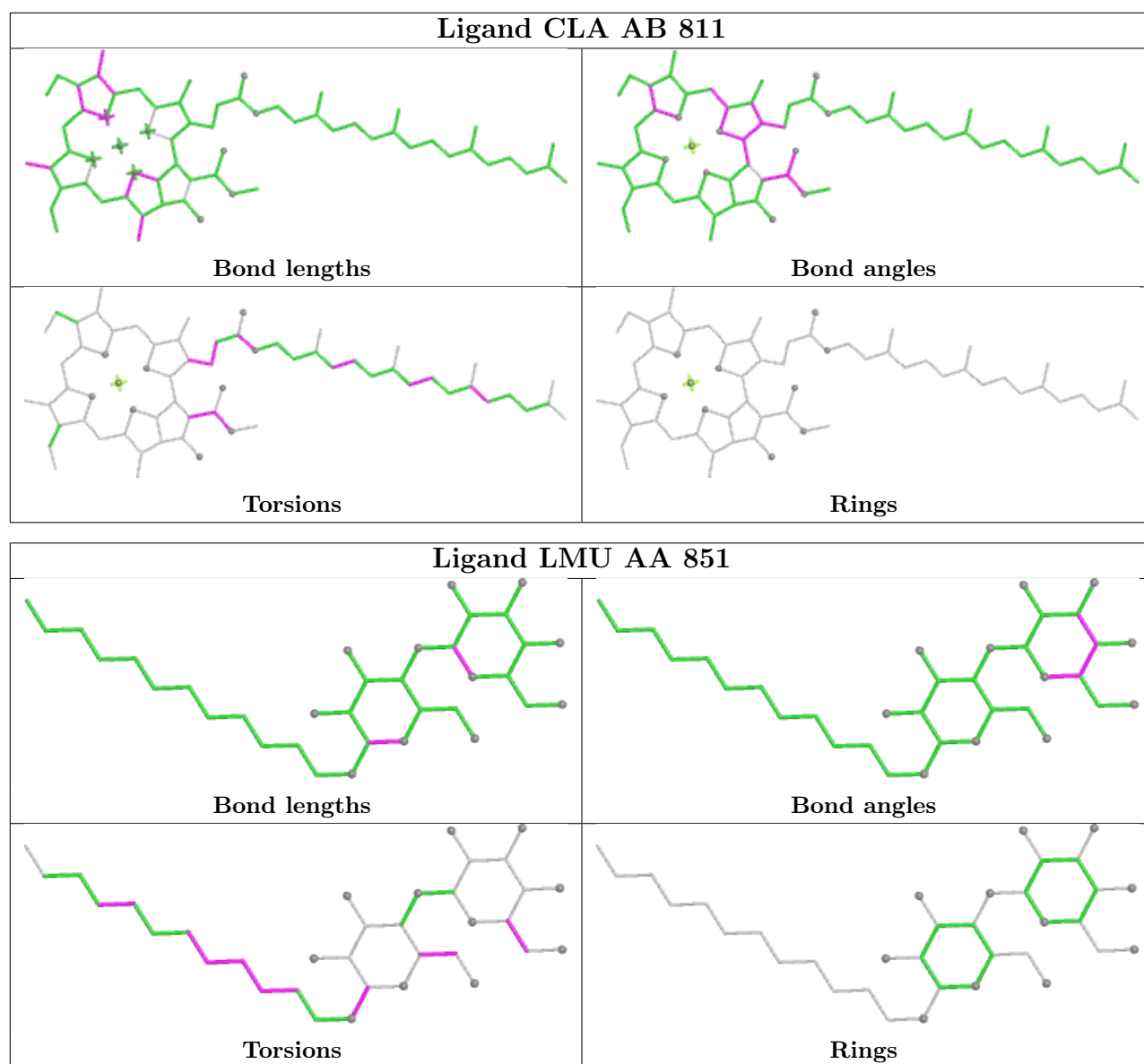


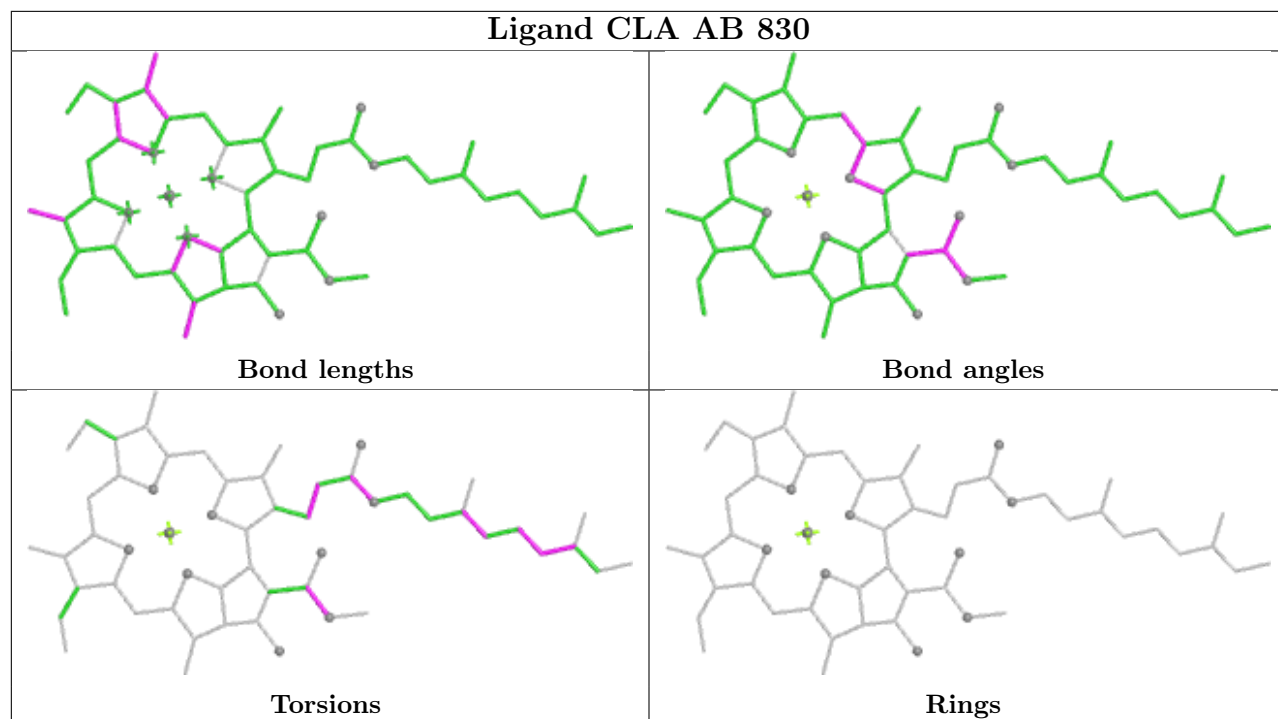
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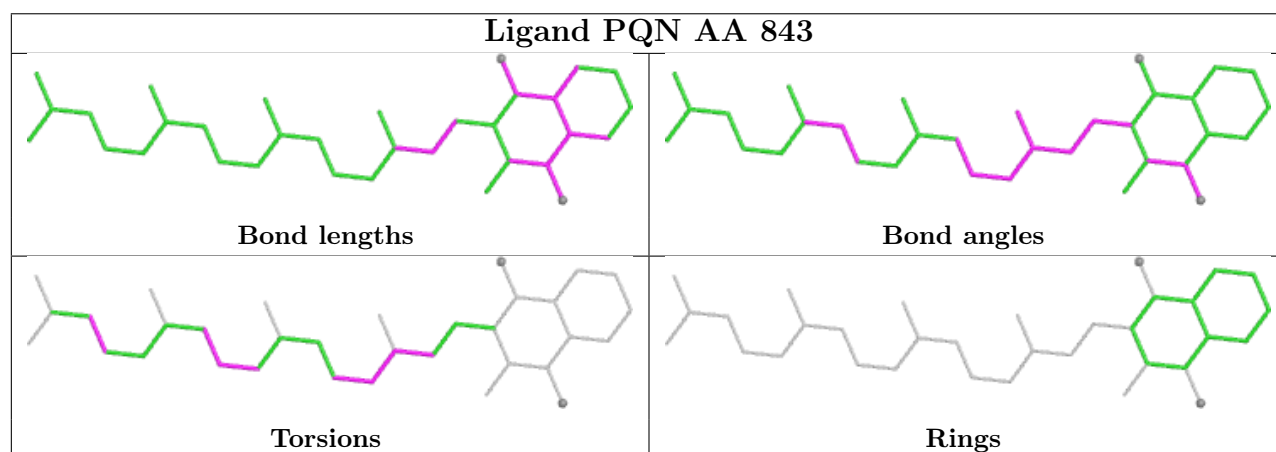
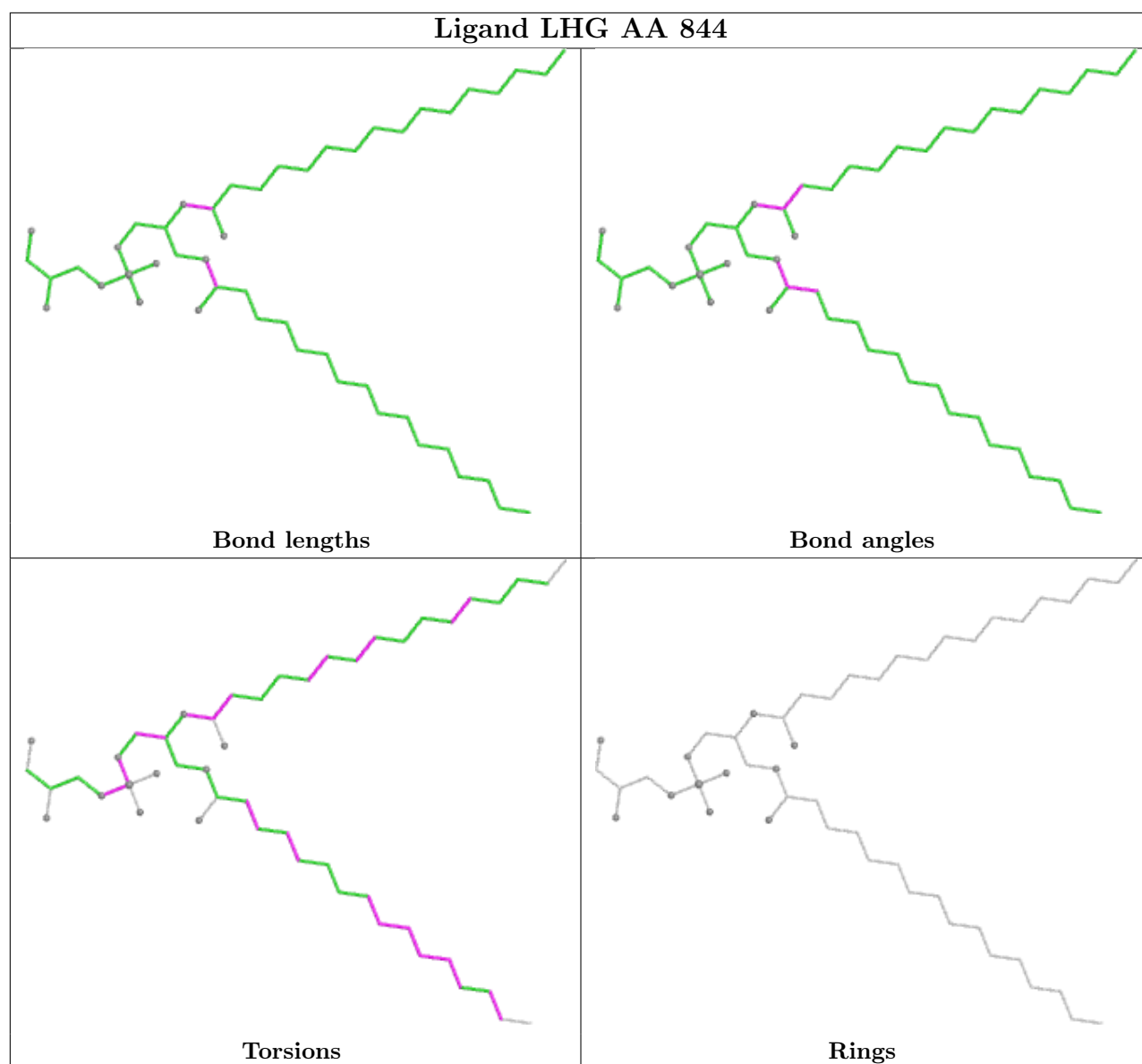


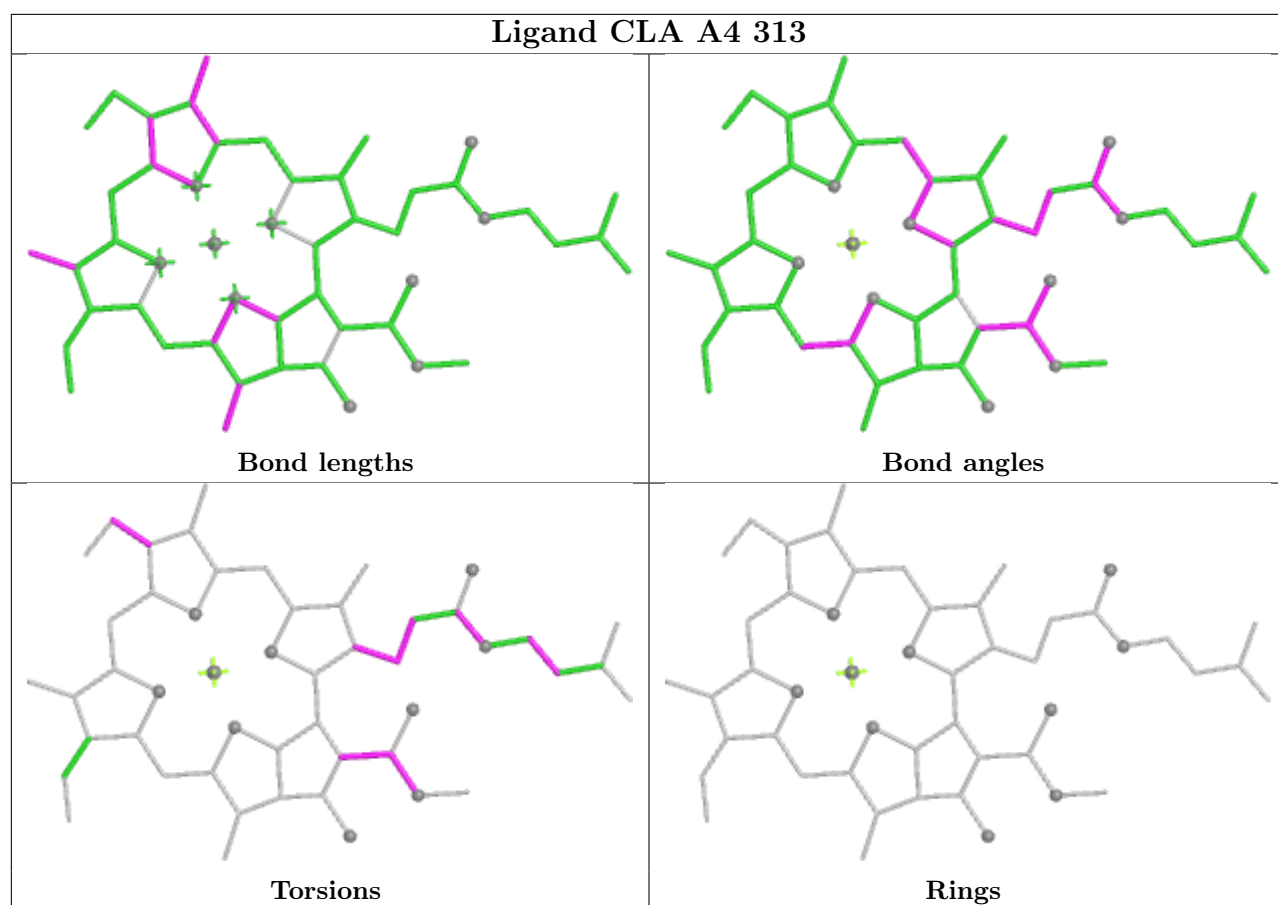




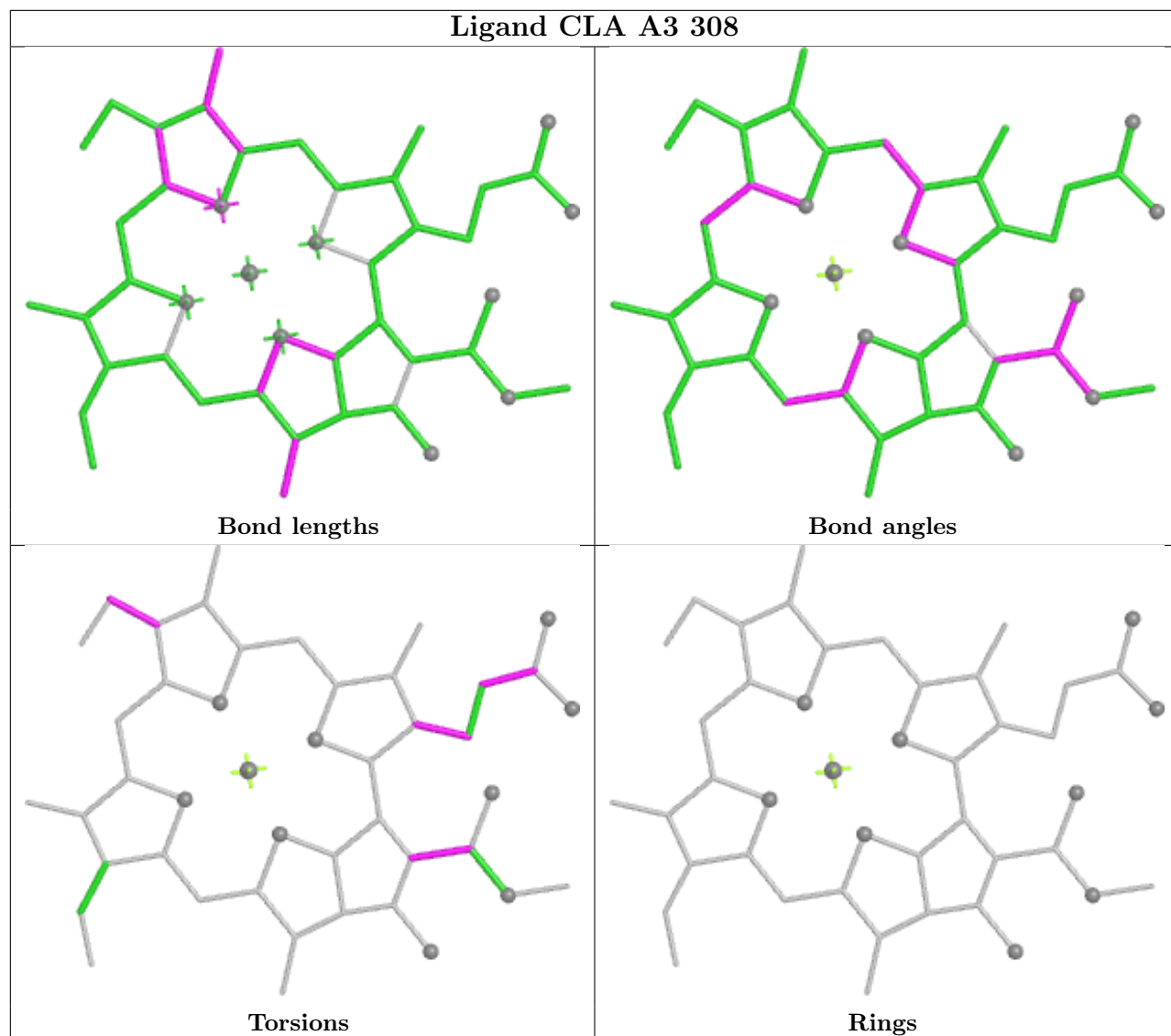




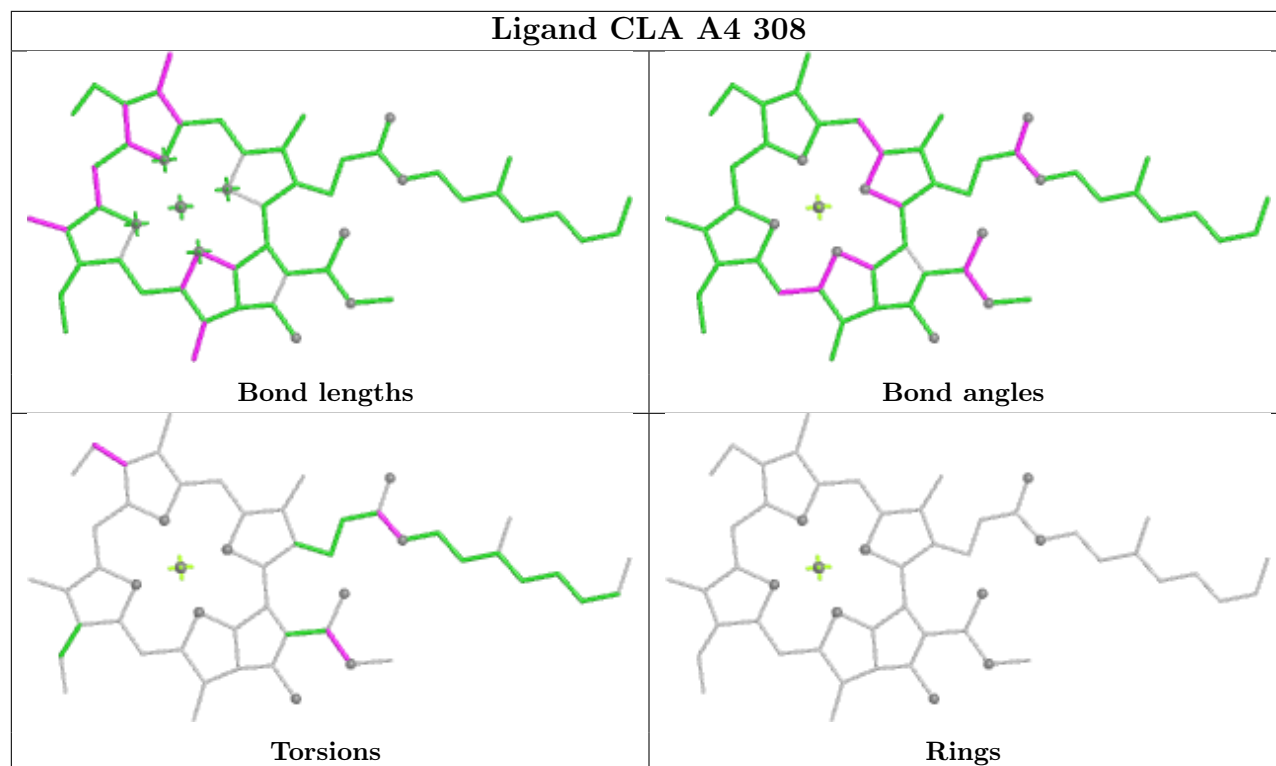




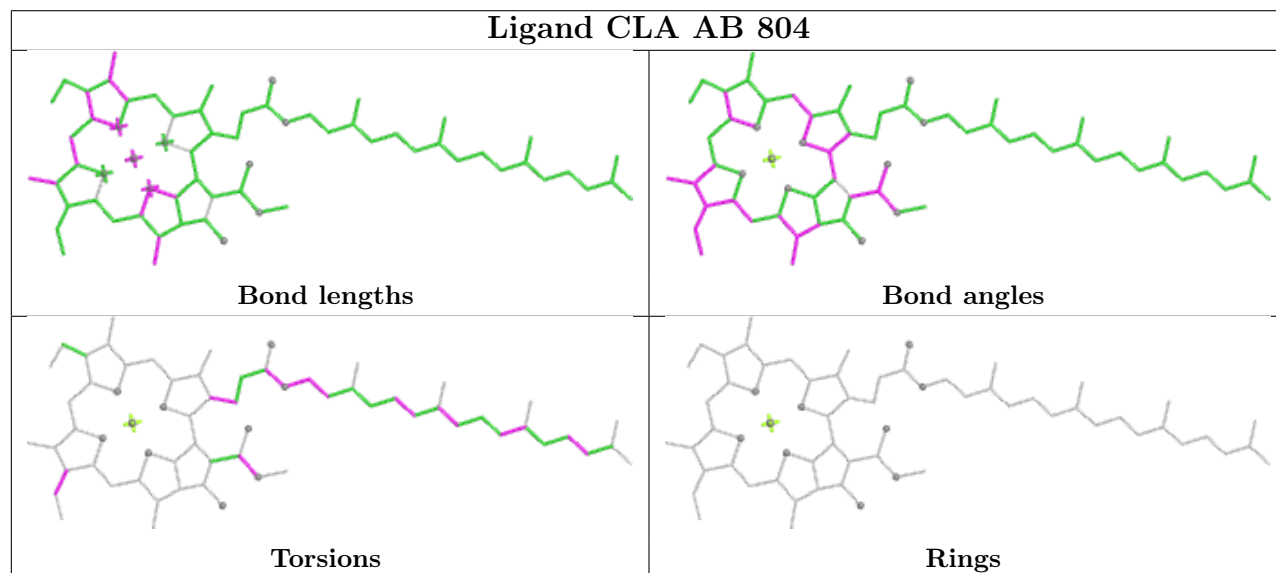
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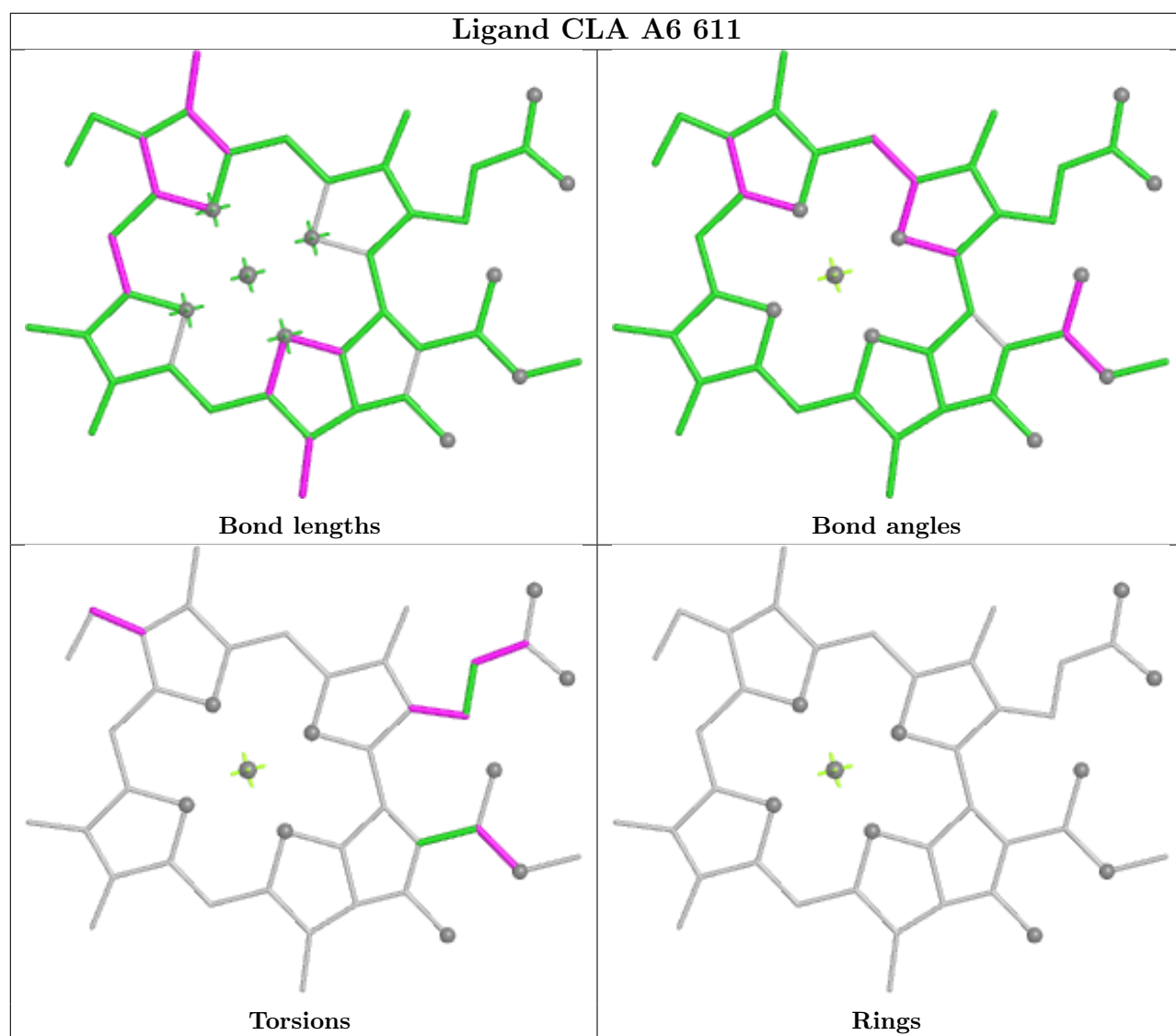


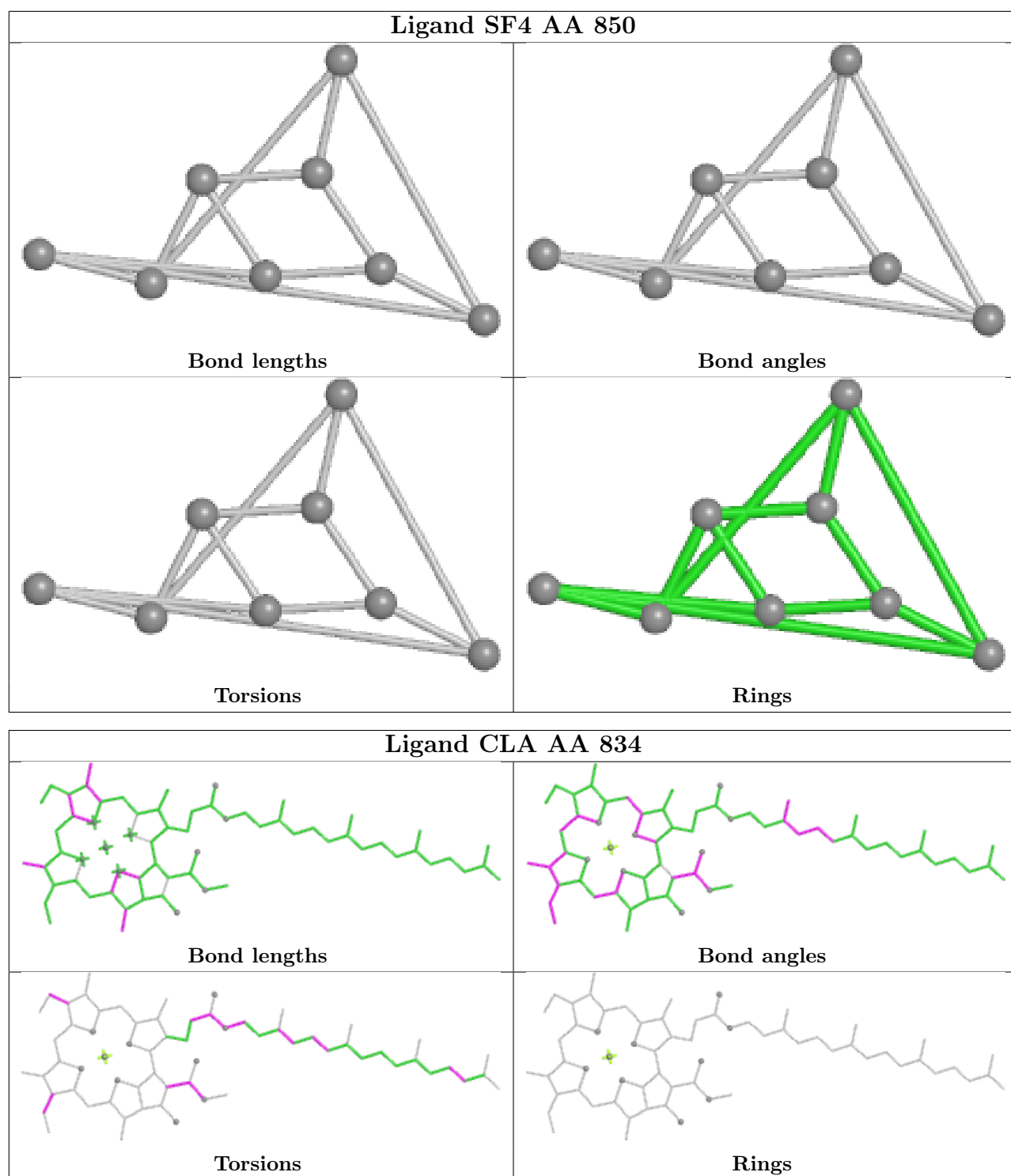
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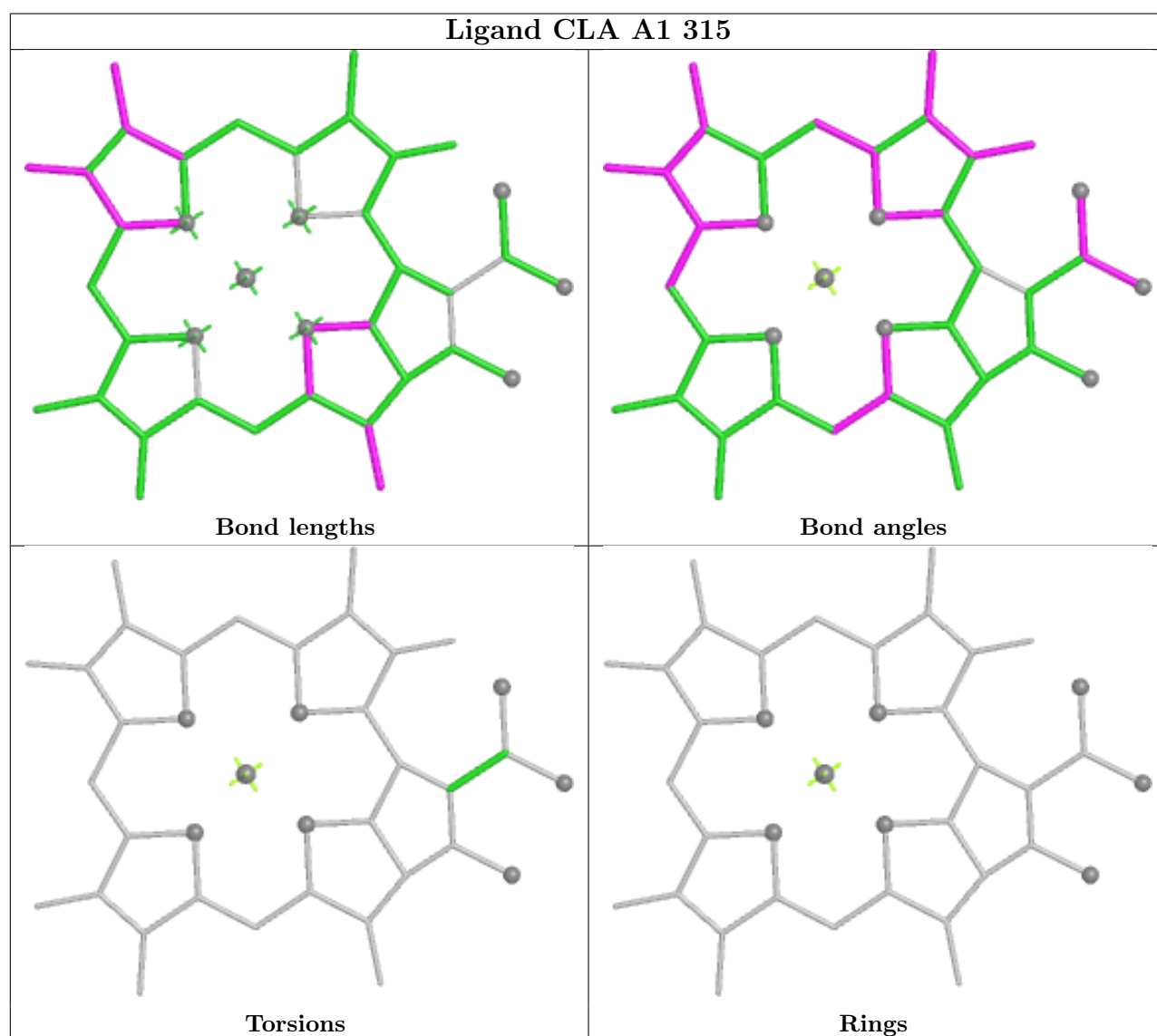
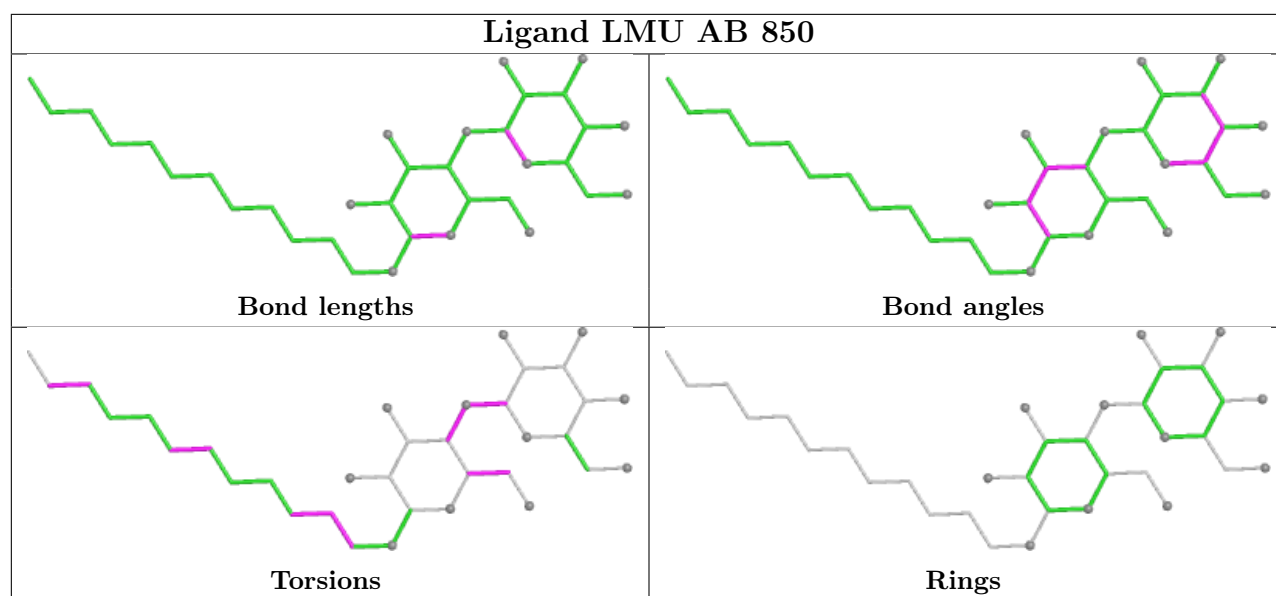


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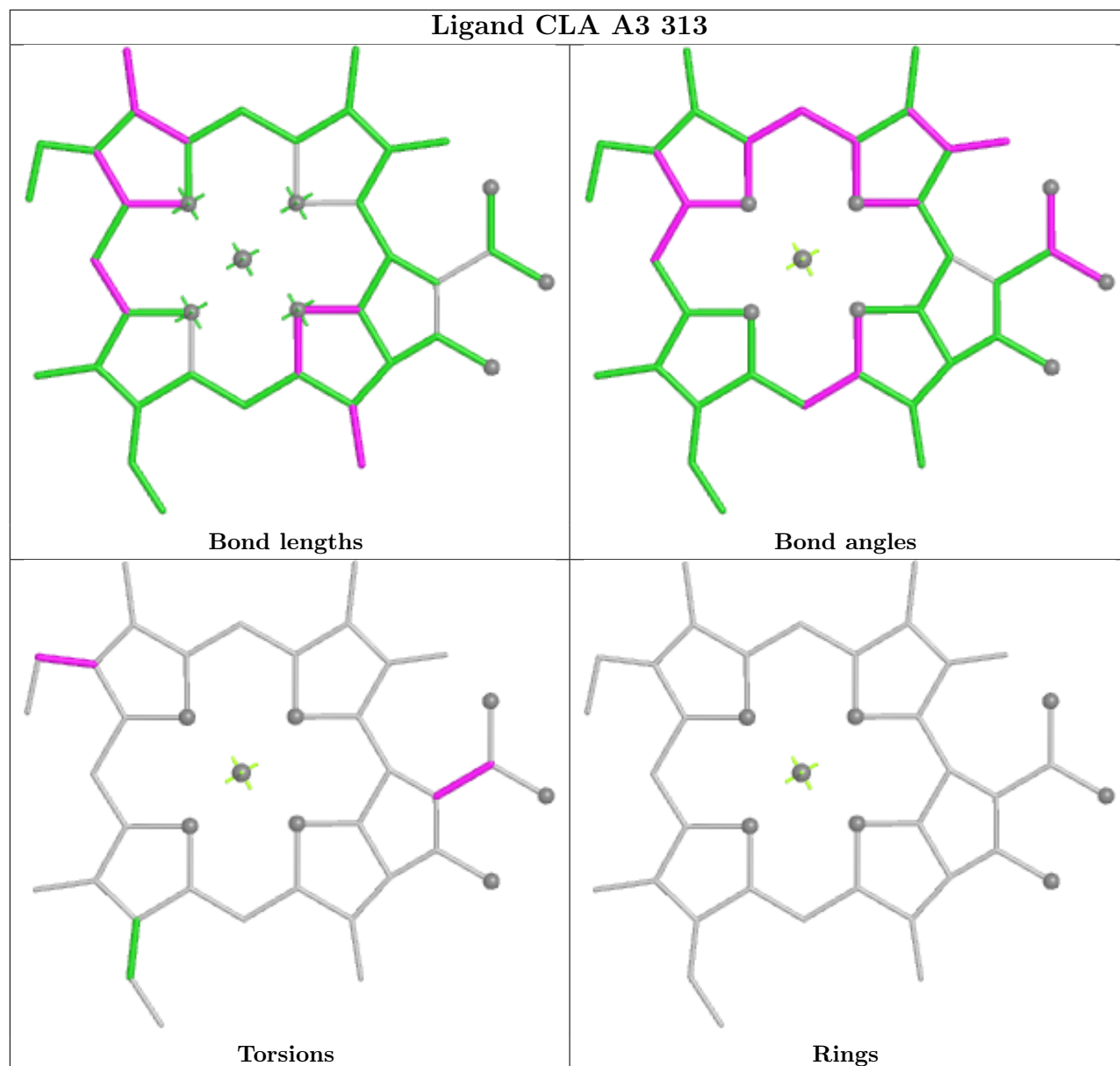




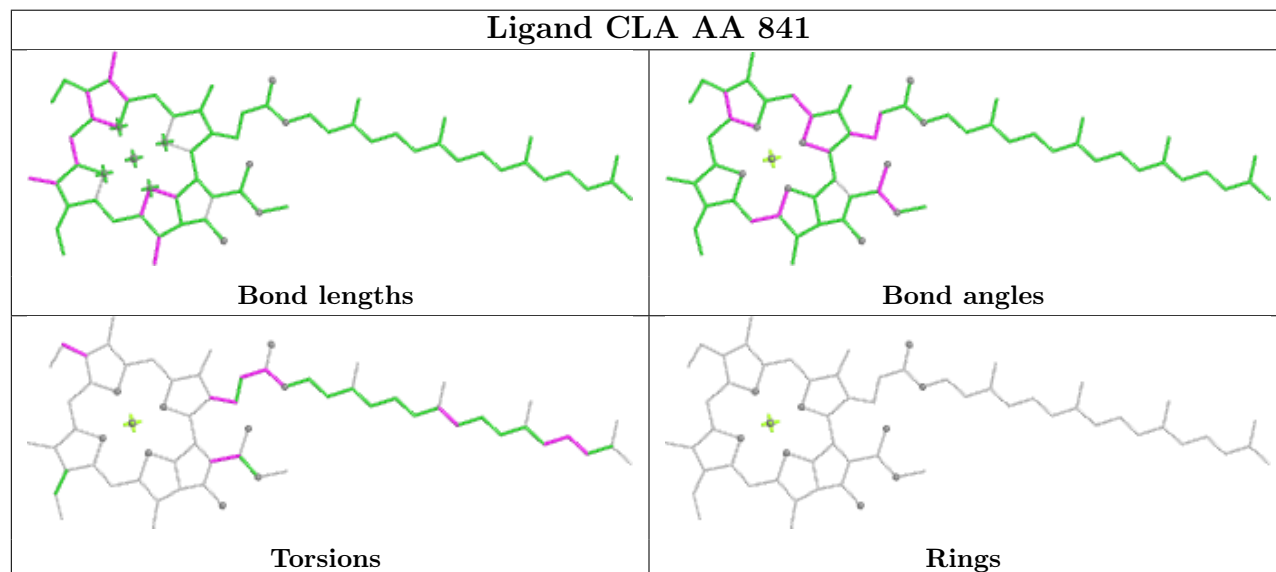


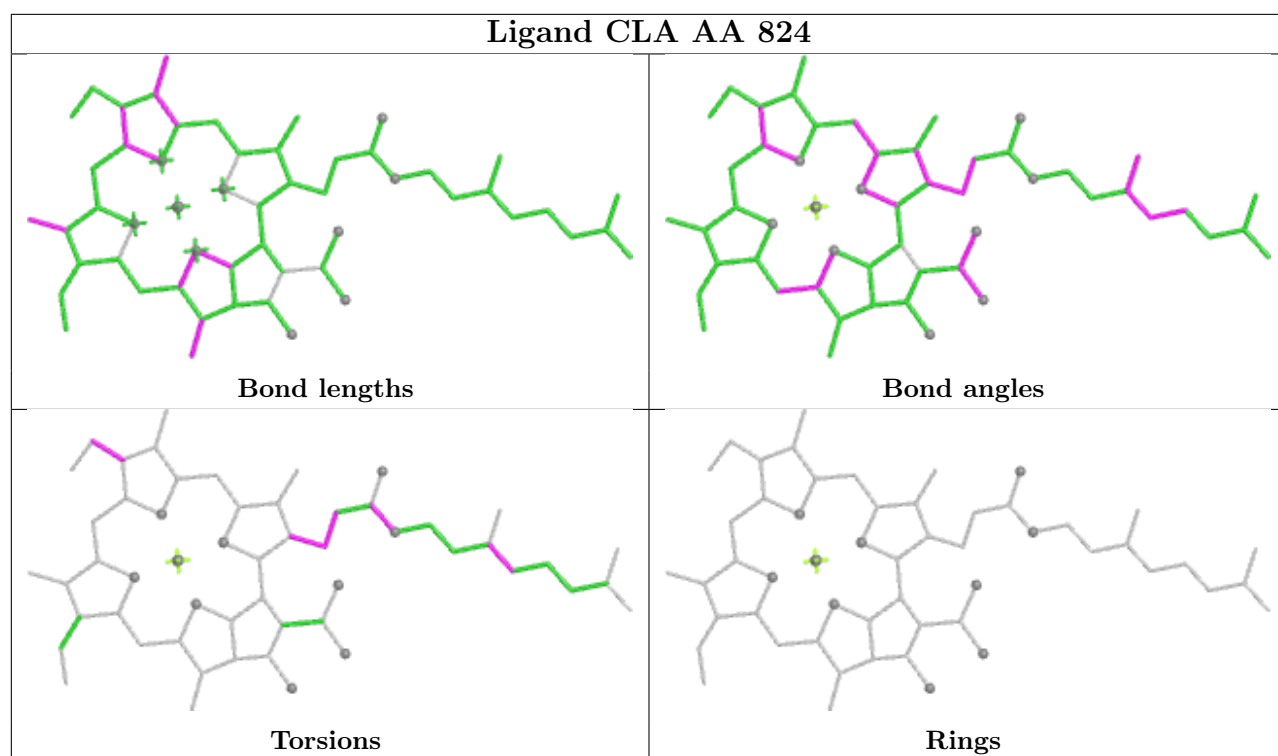


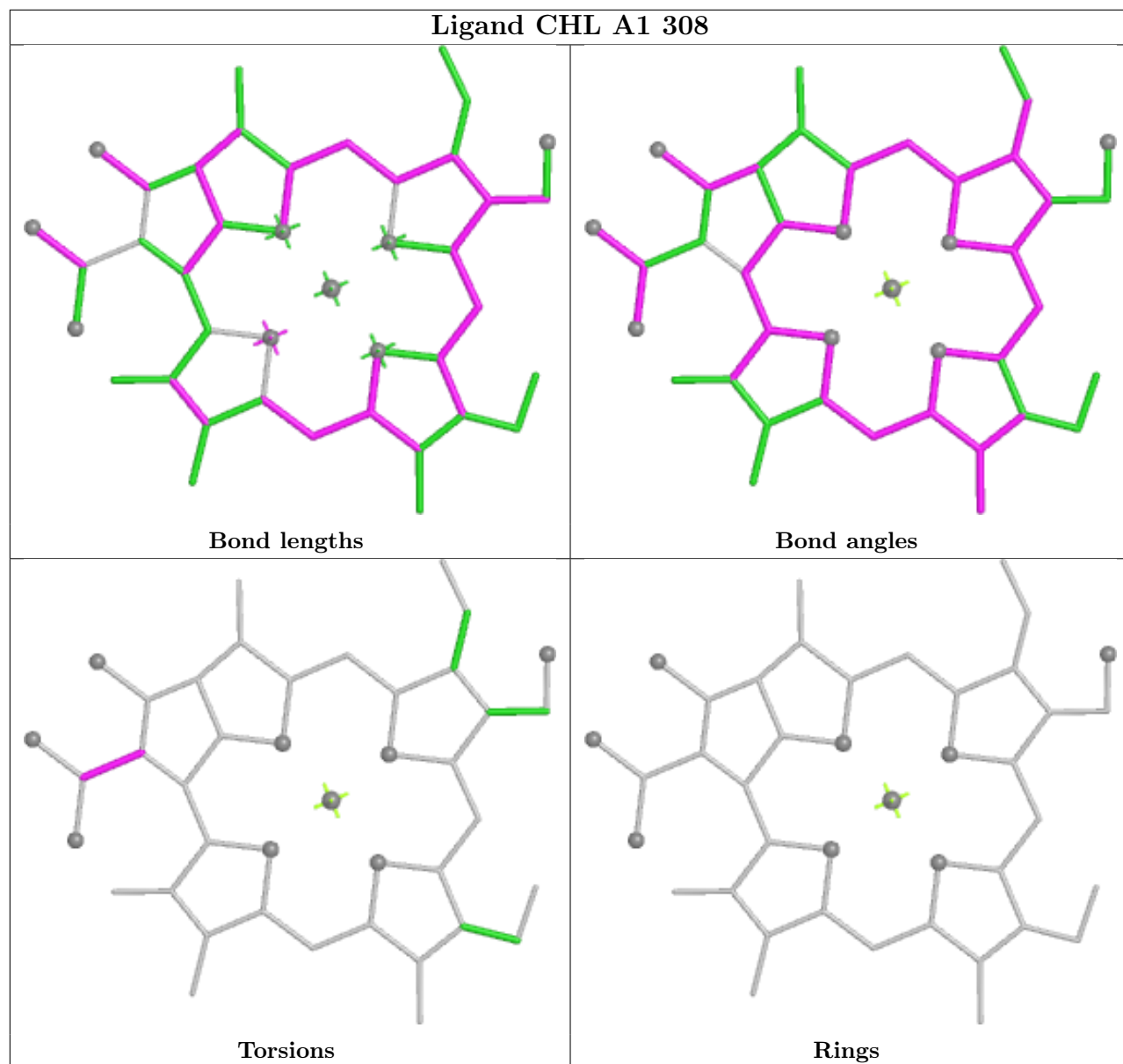
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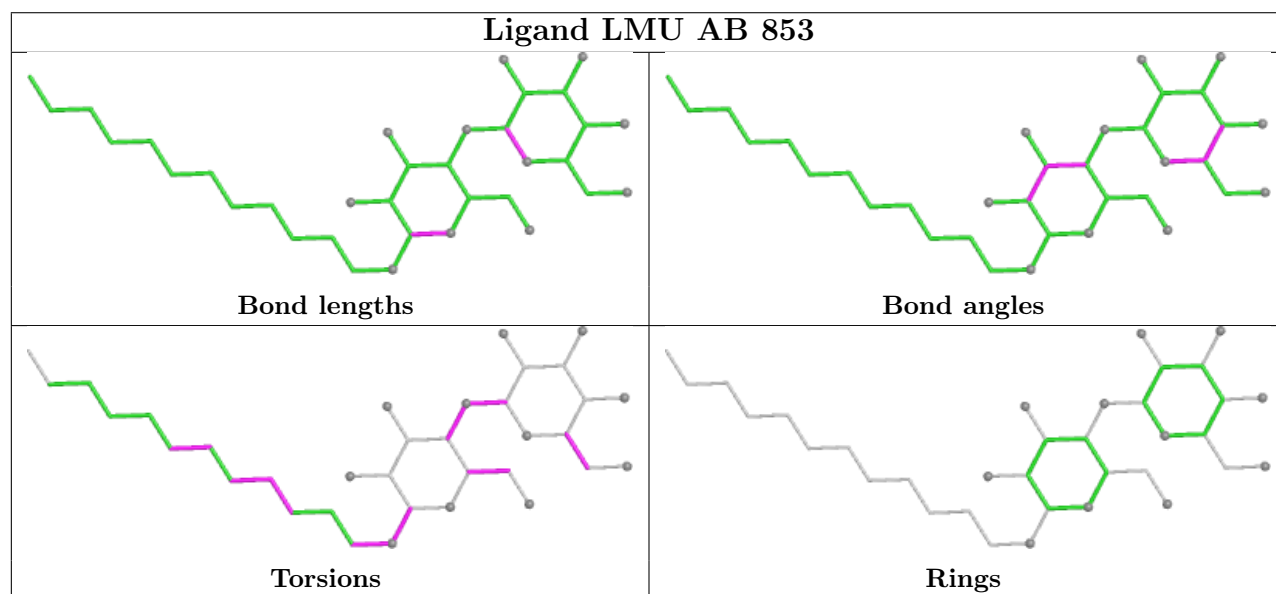
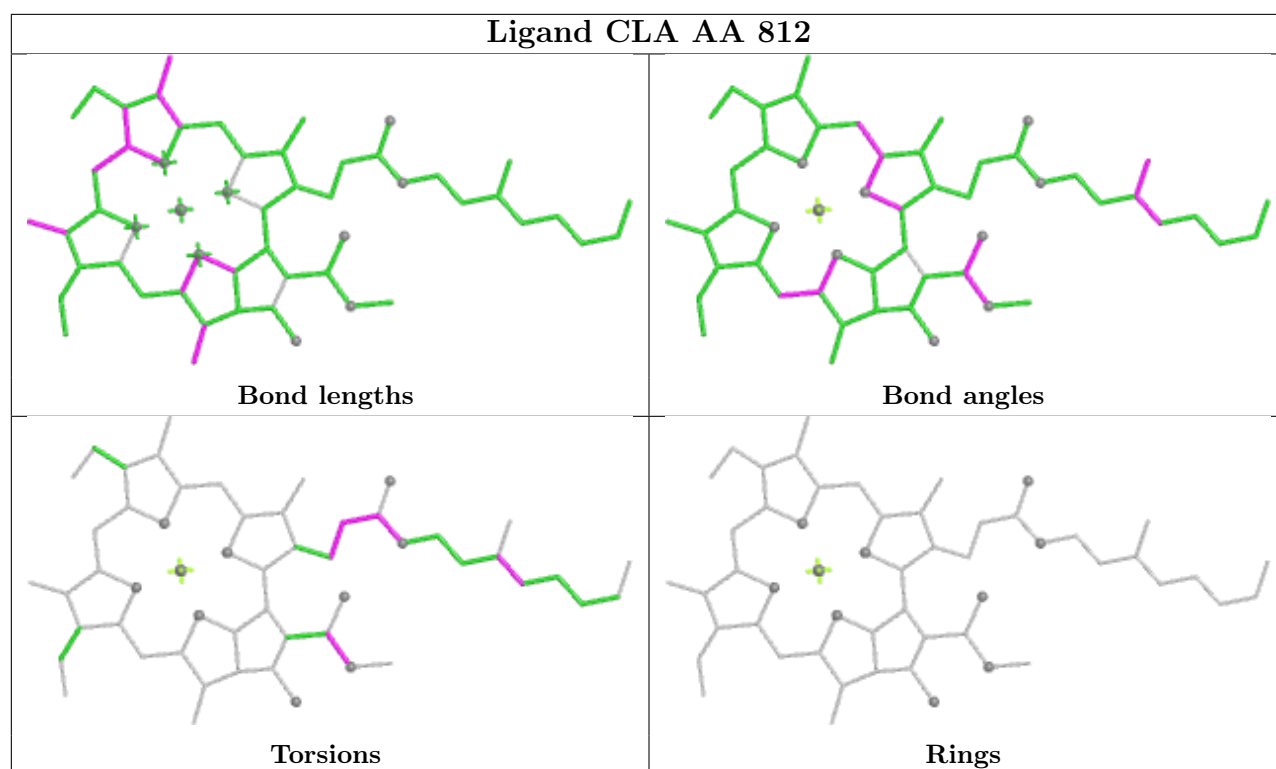


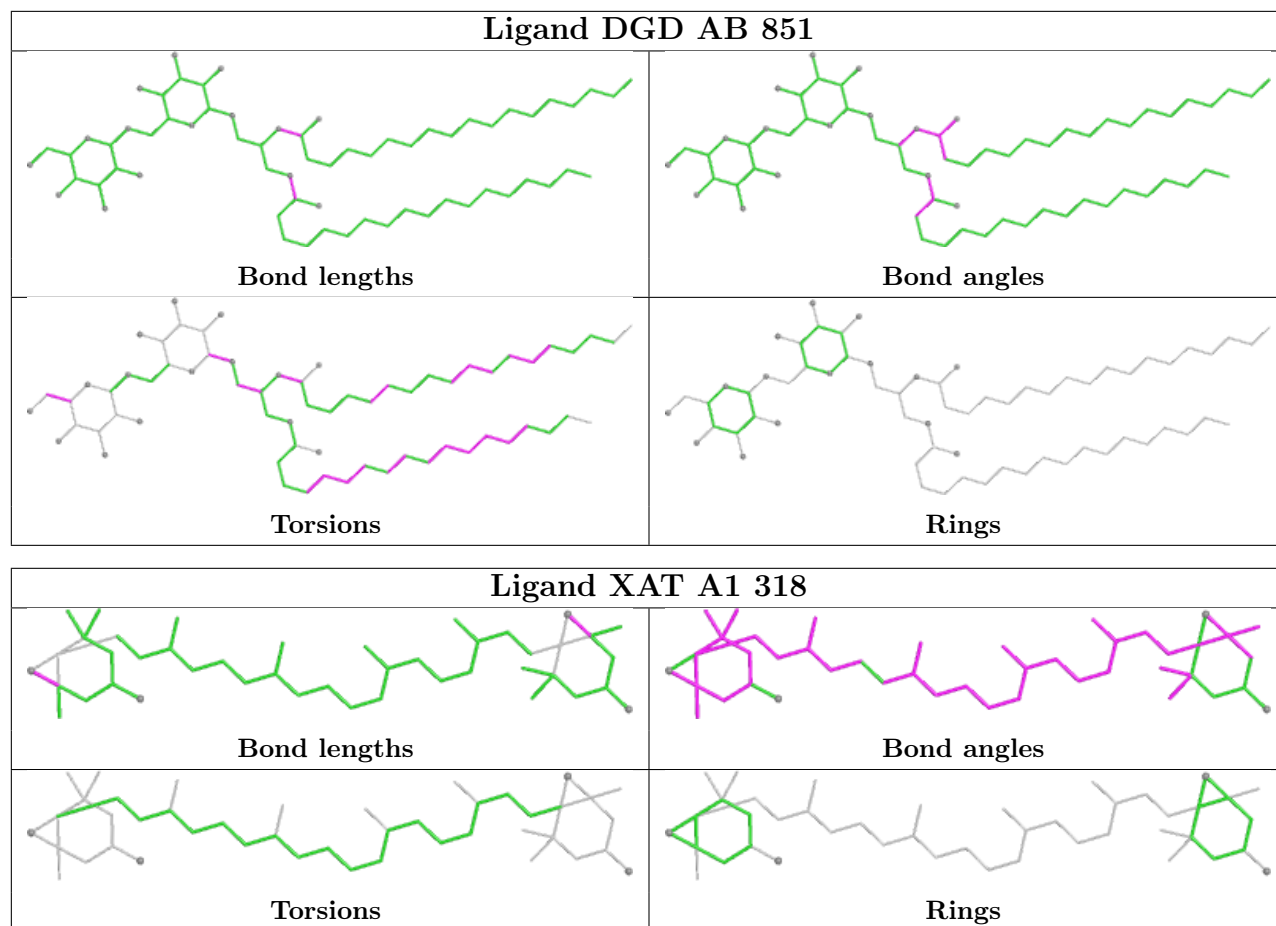
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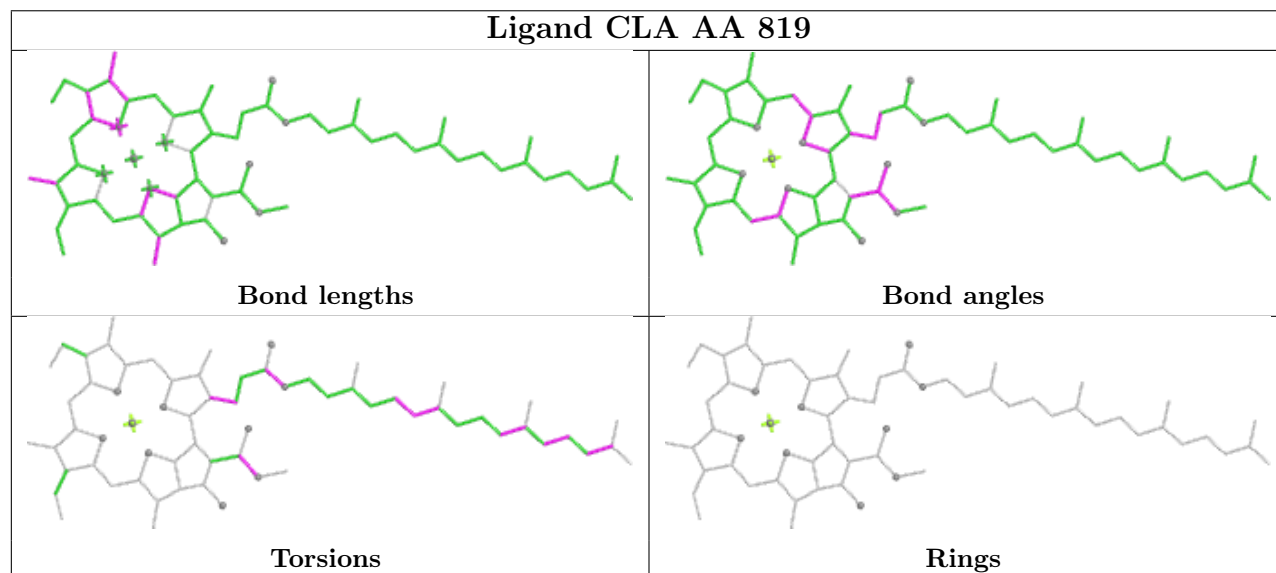
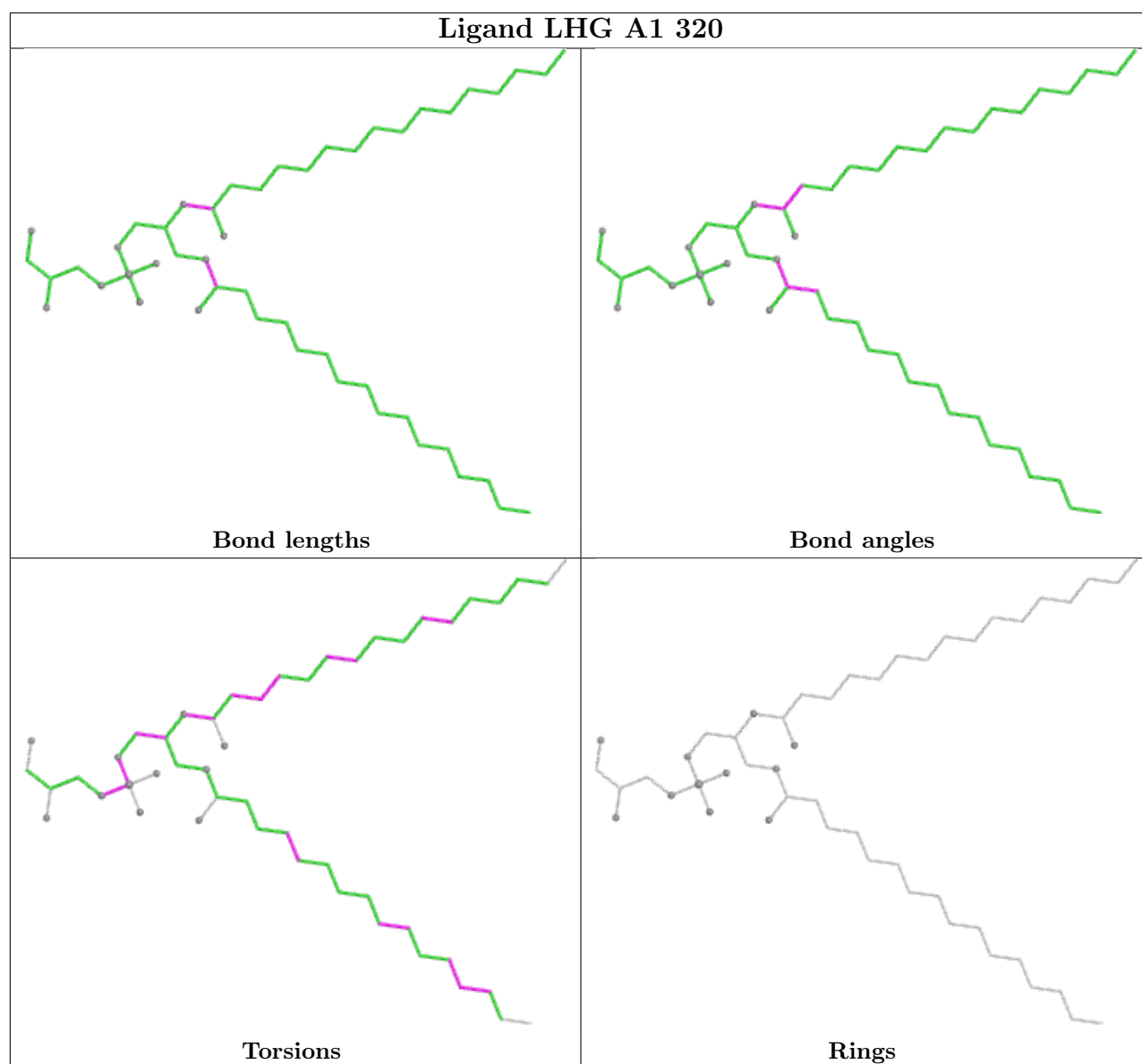




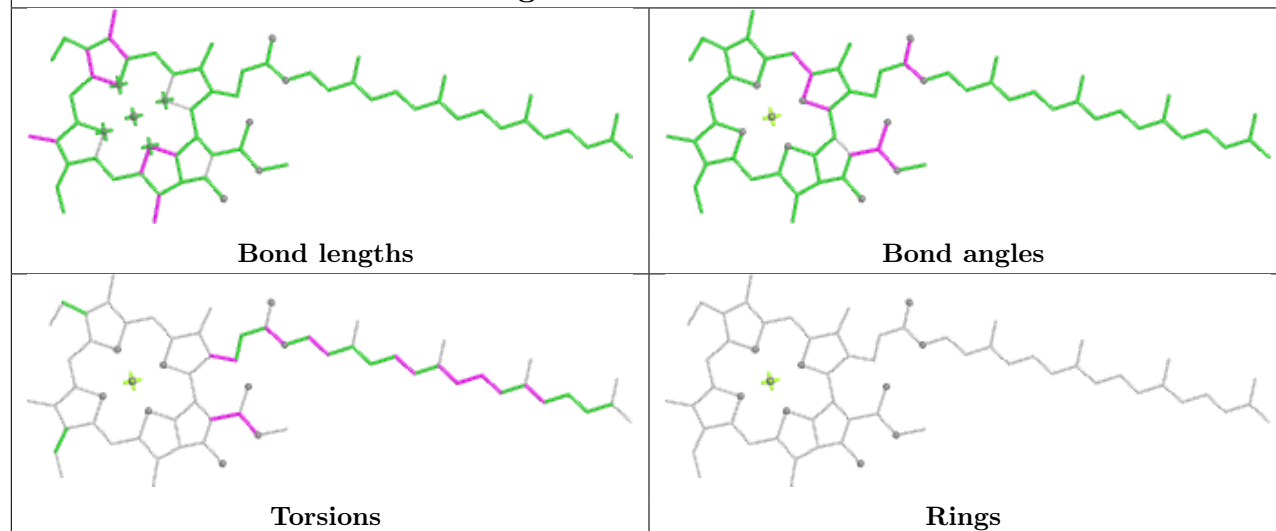




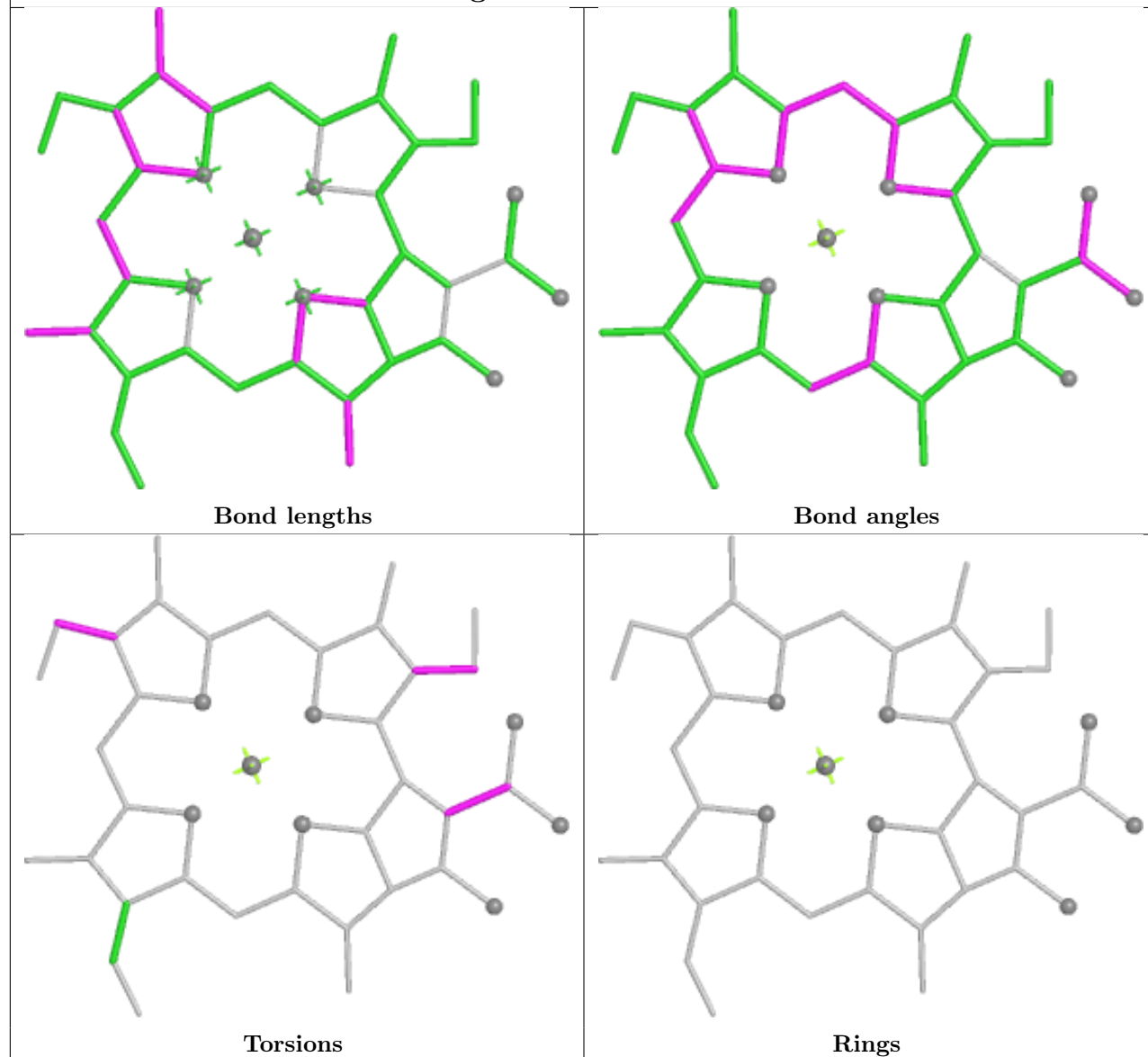


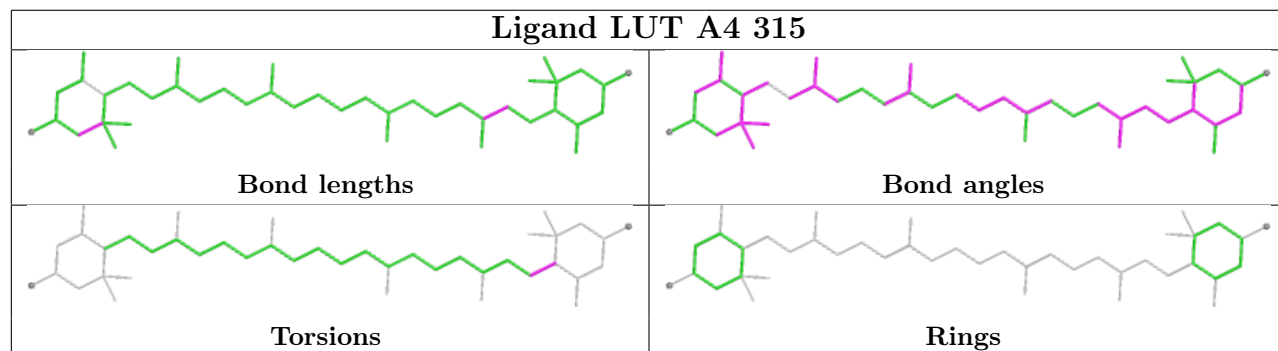
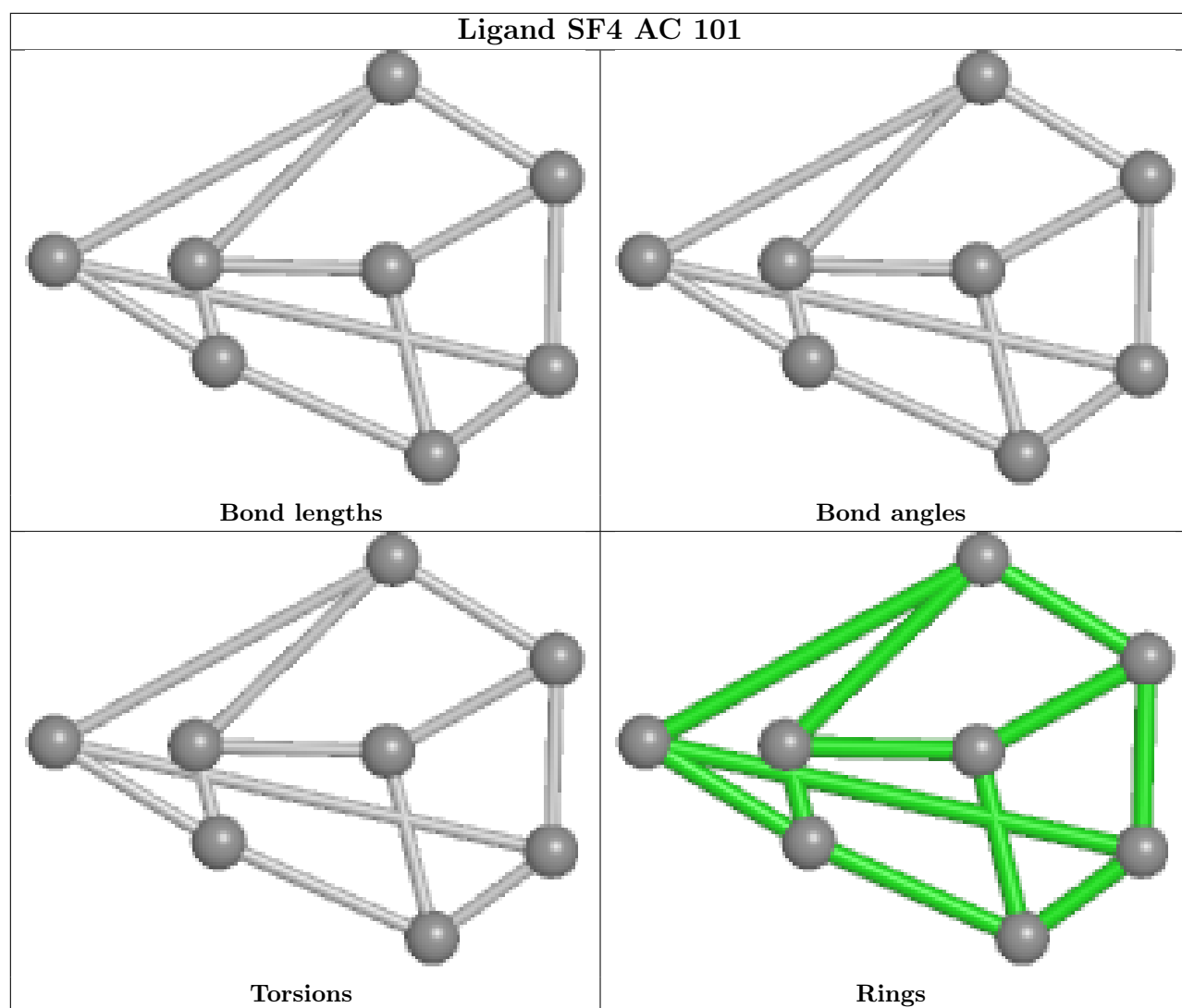


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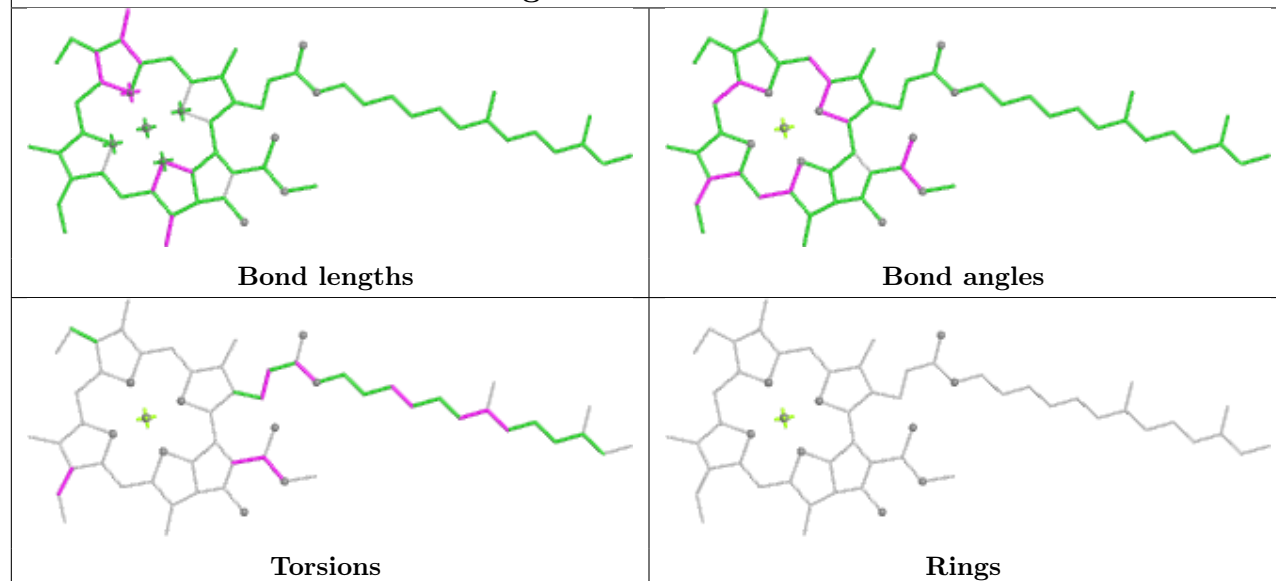


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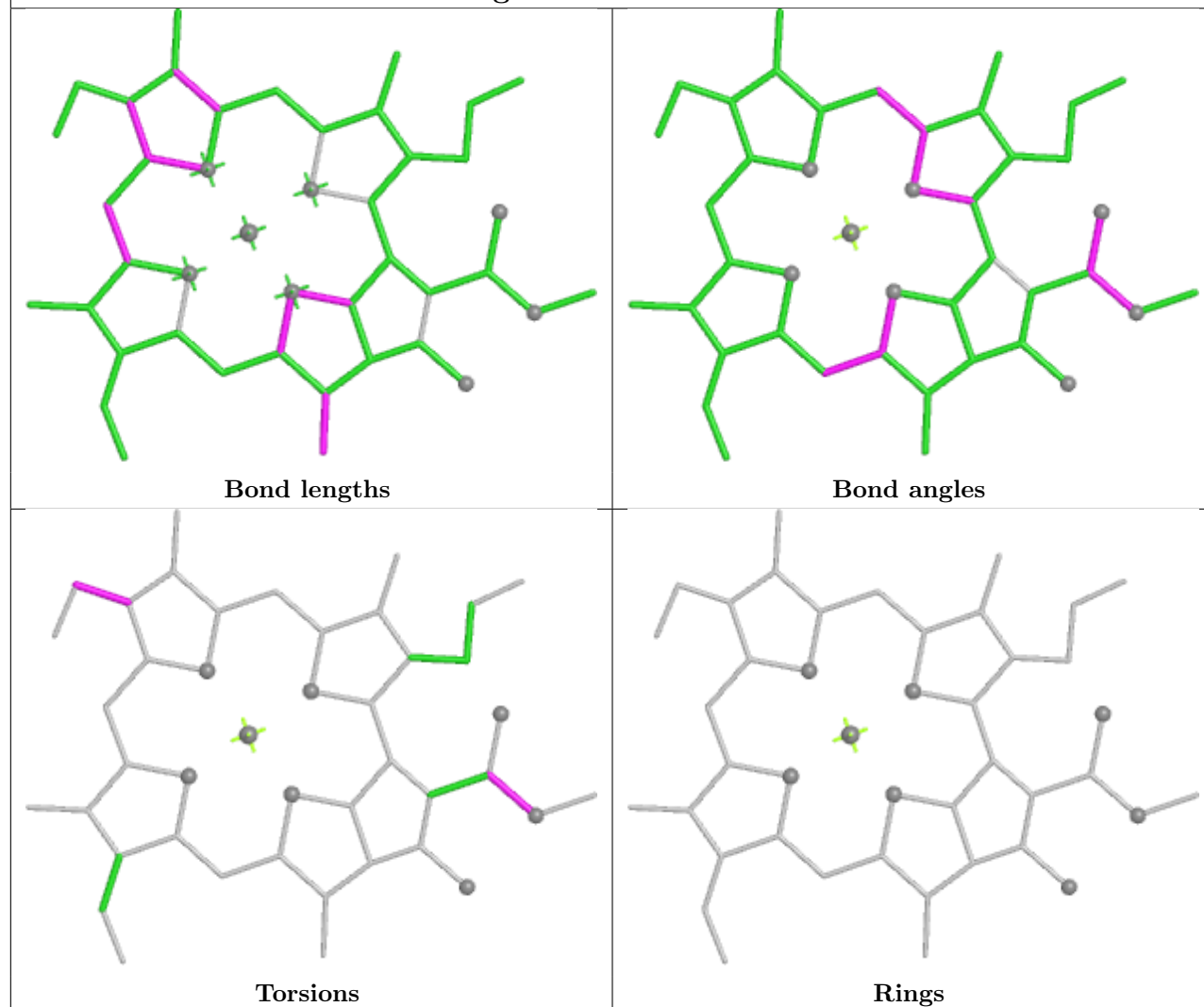




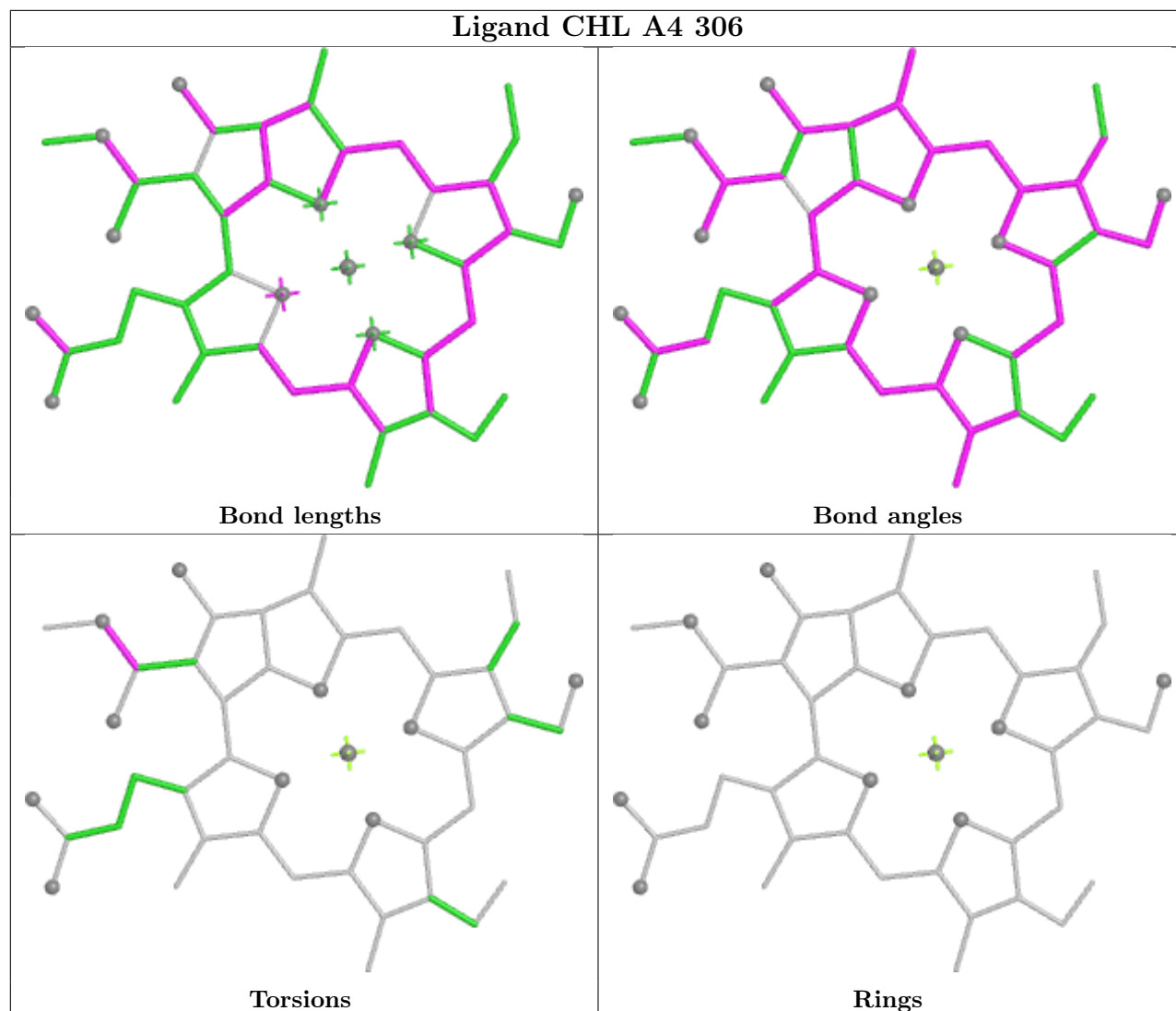
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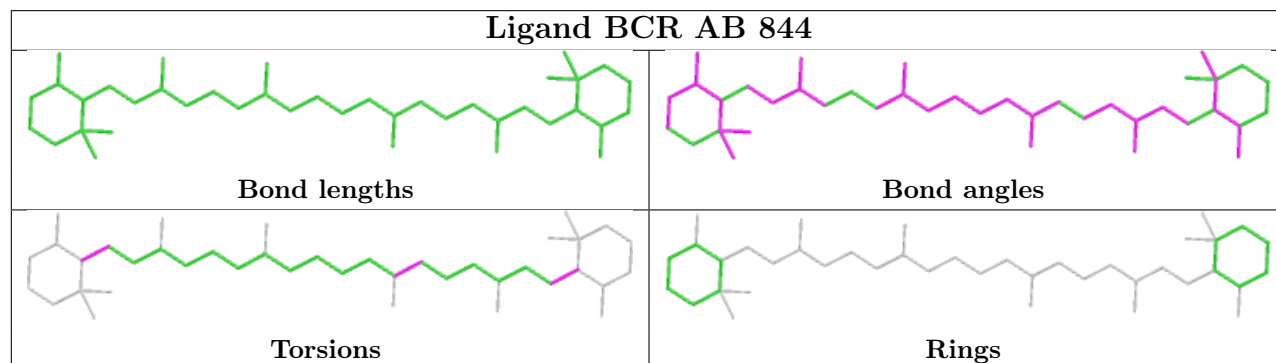
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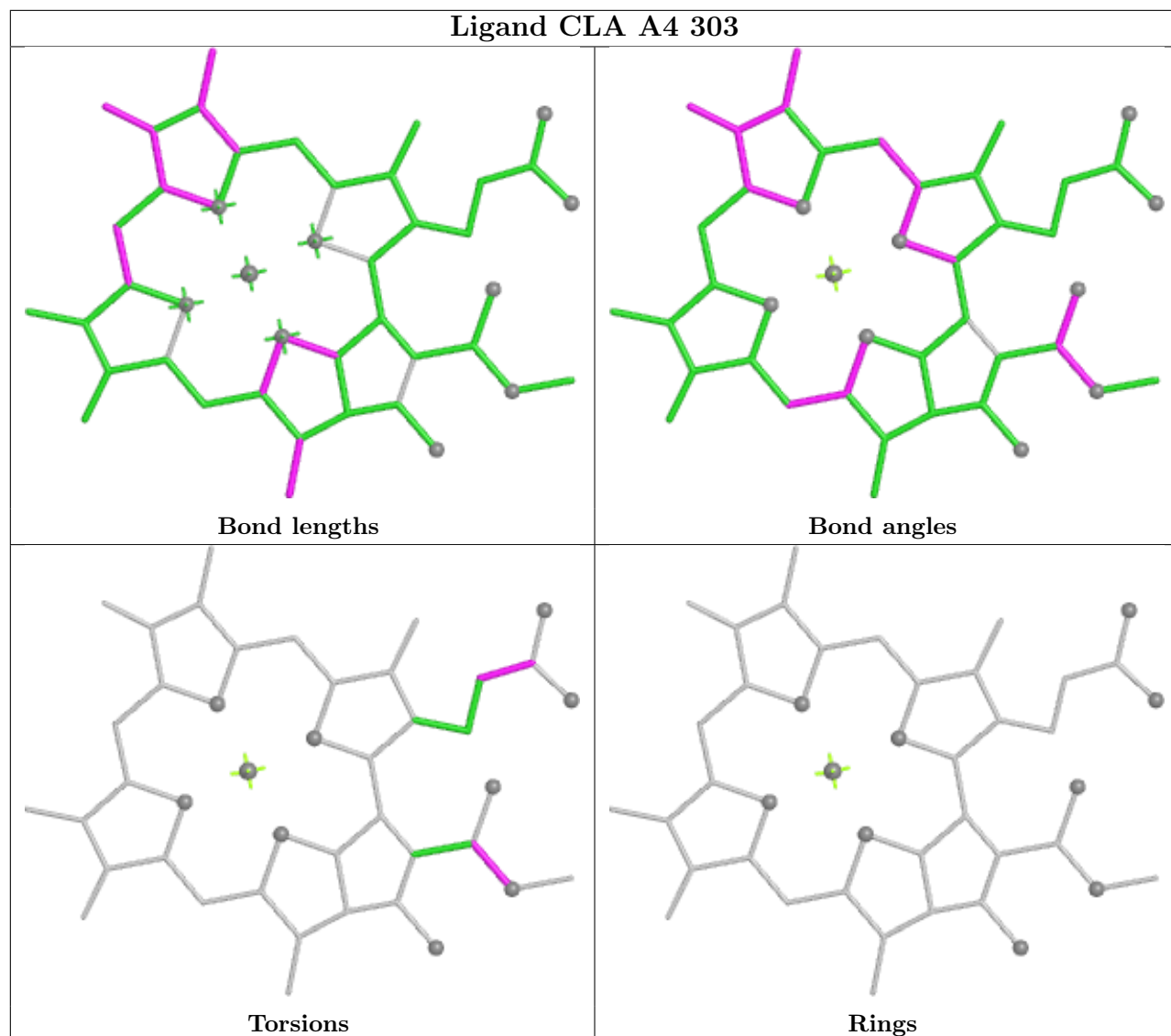
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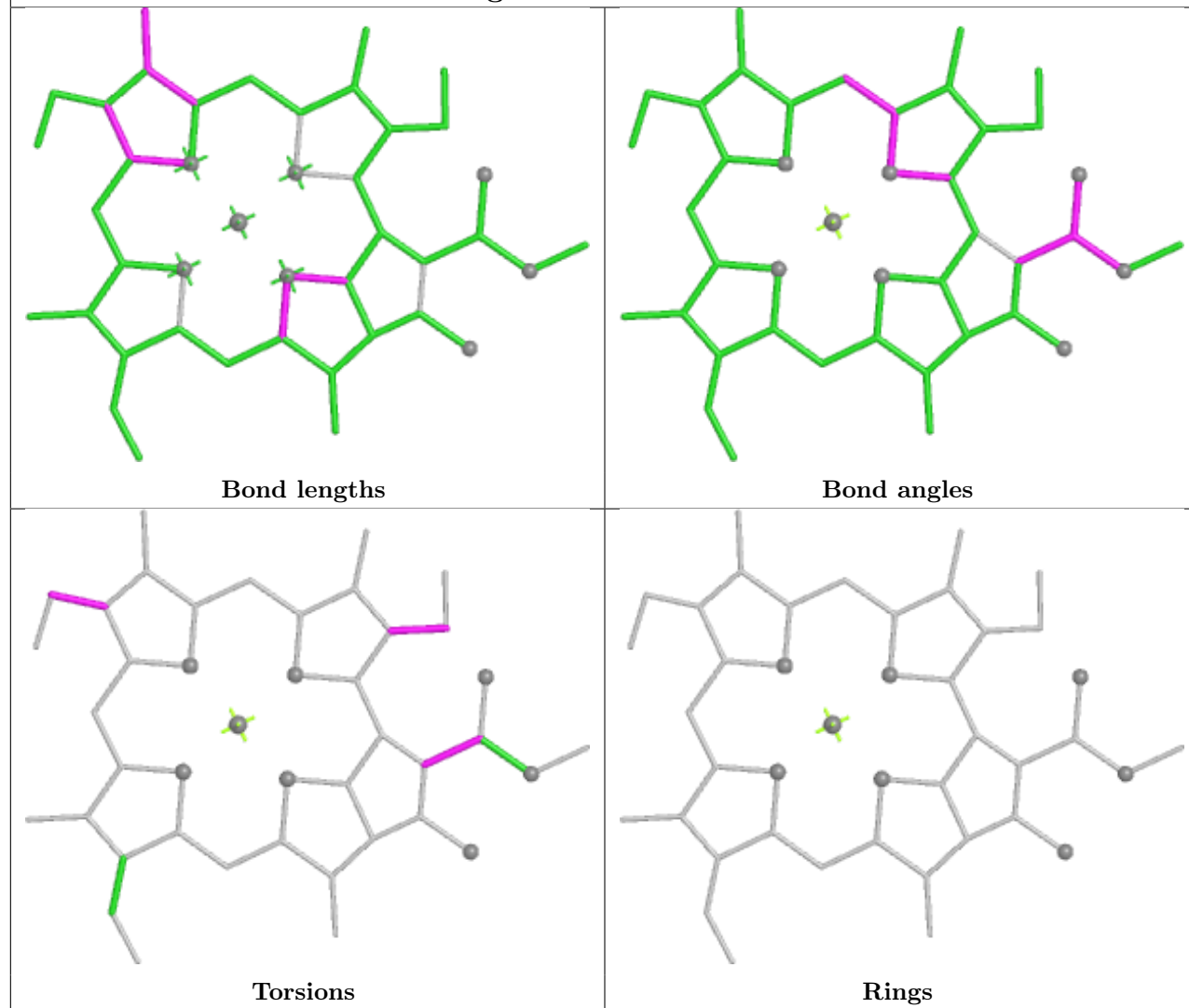
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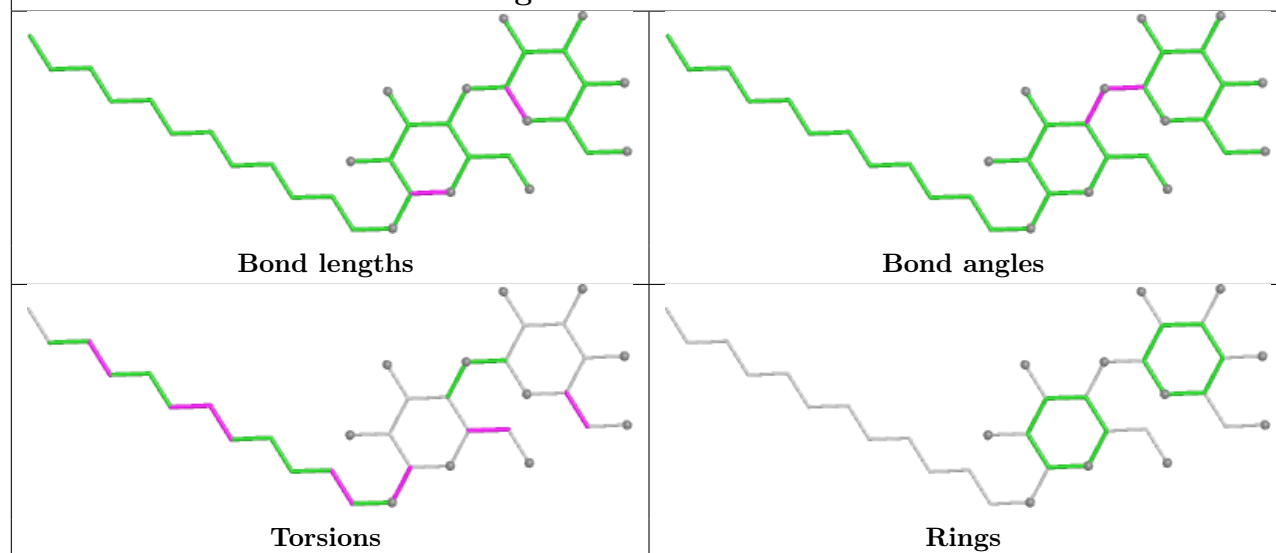
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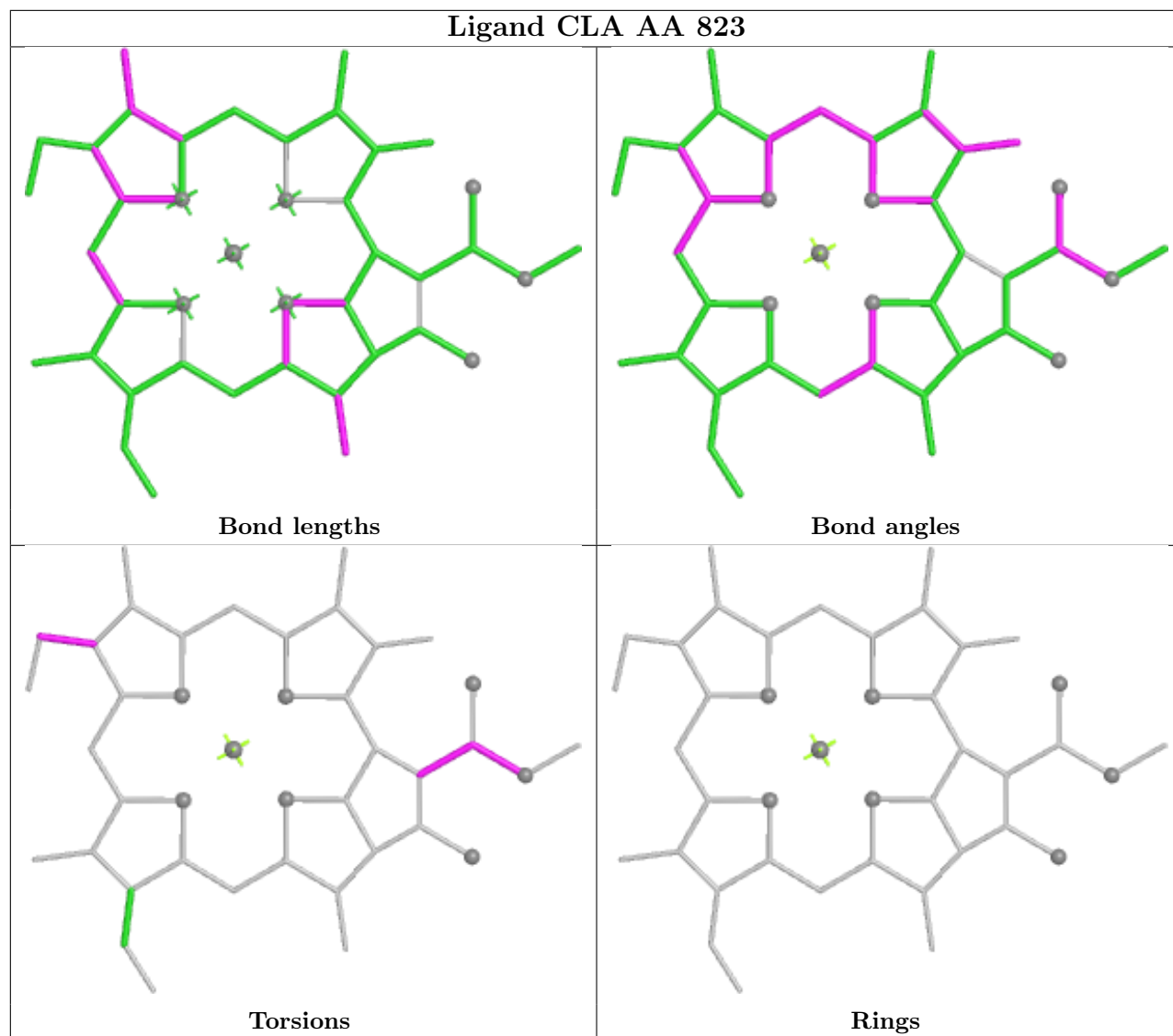
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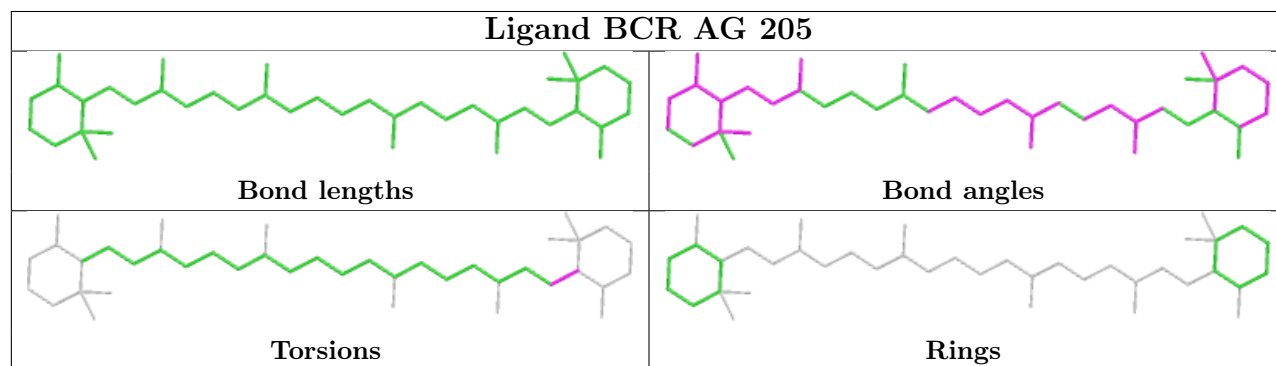
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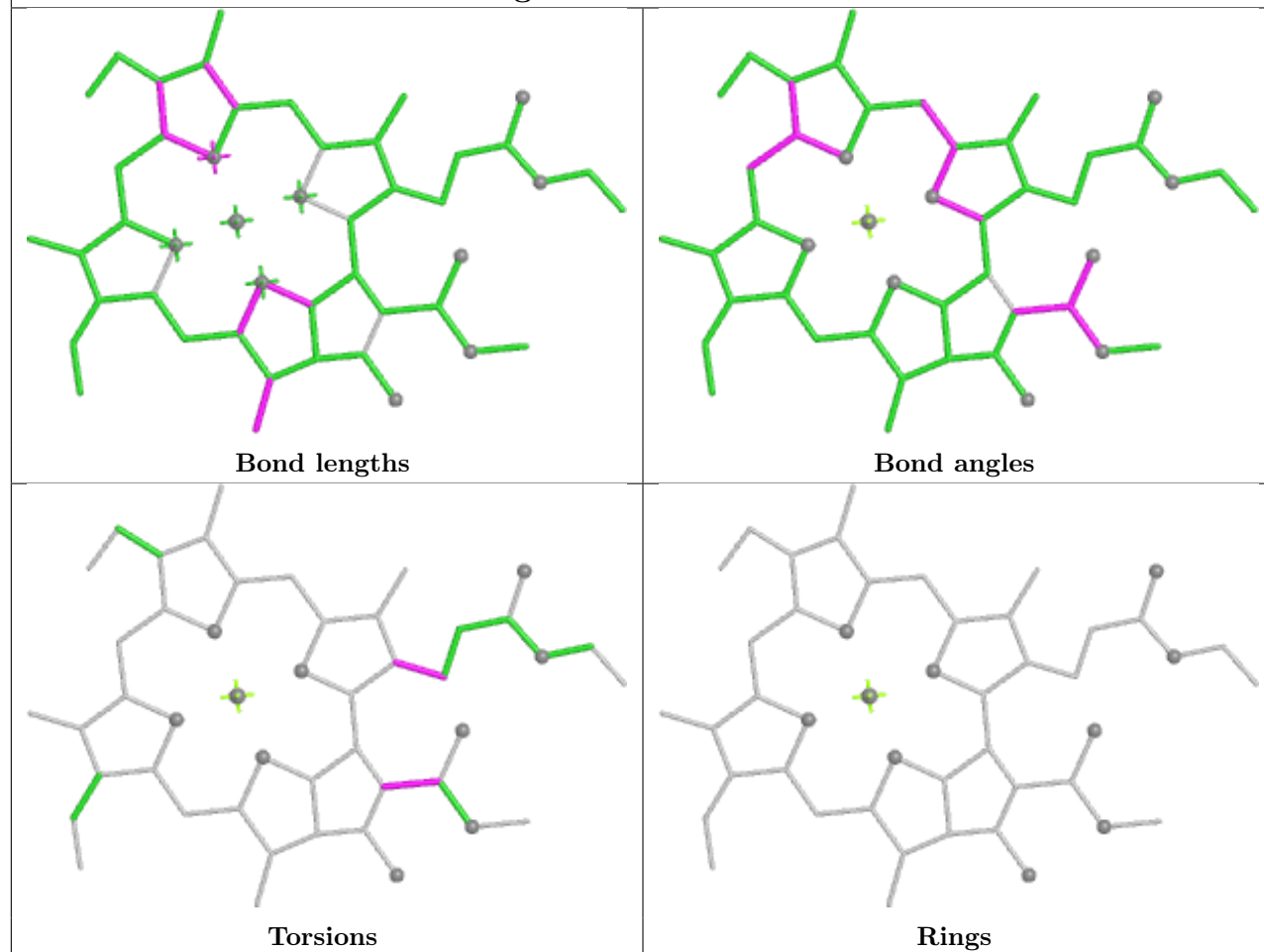
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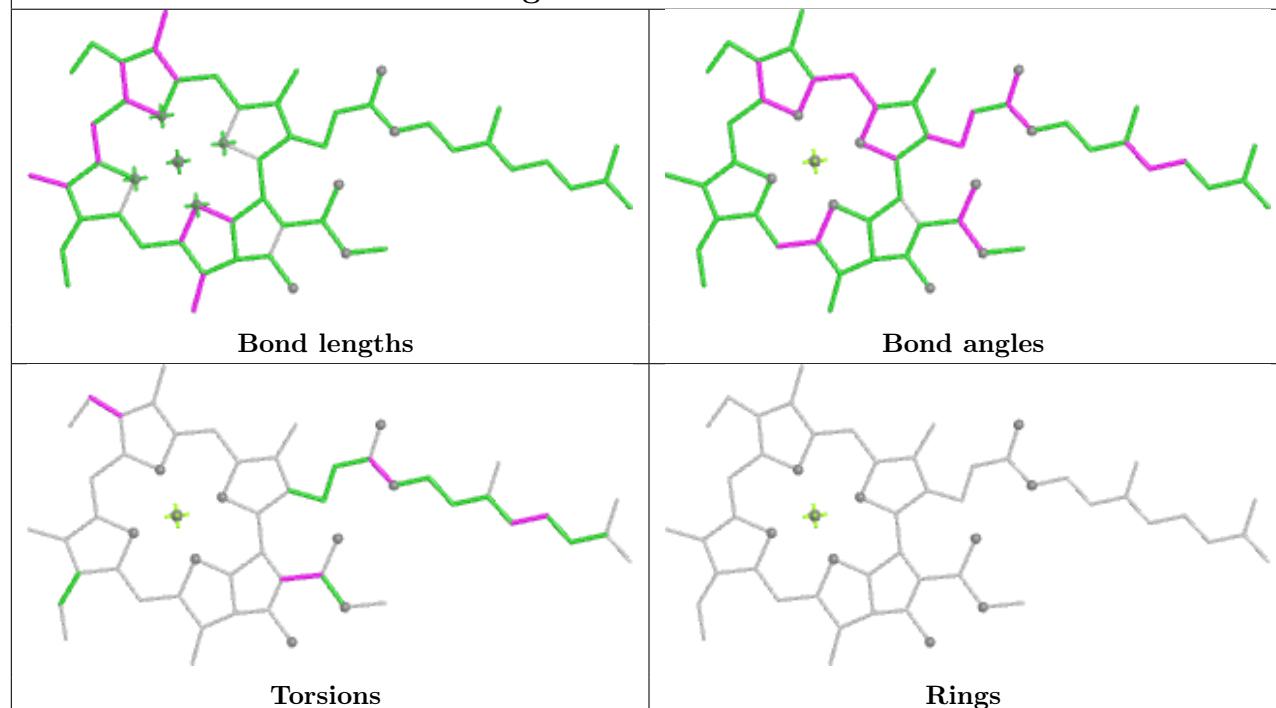
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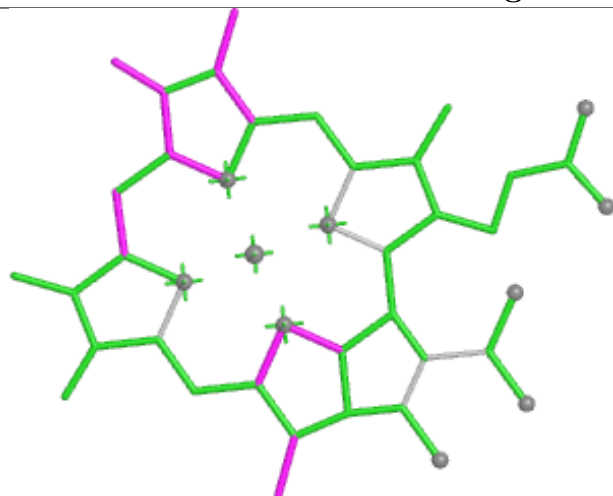
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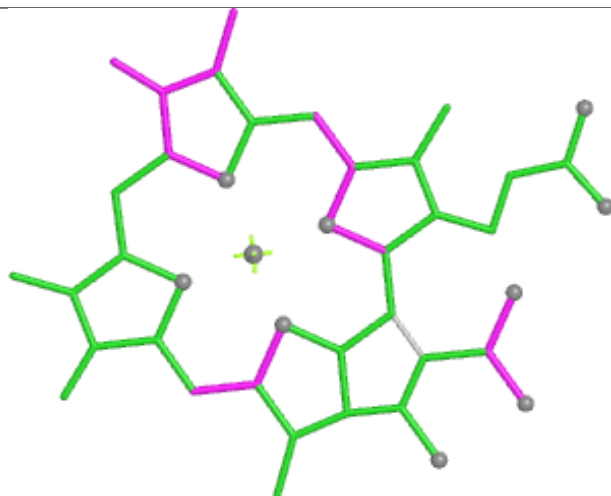
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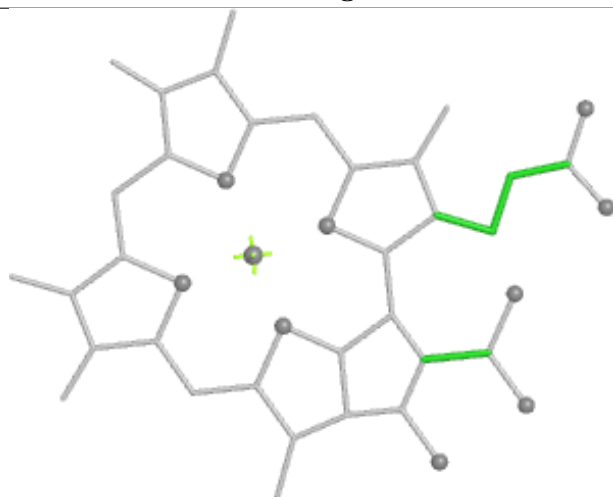
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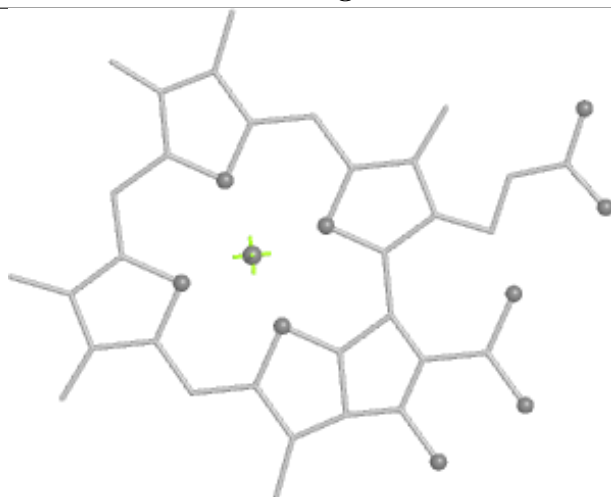
Bond lengths



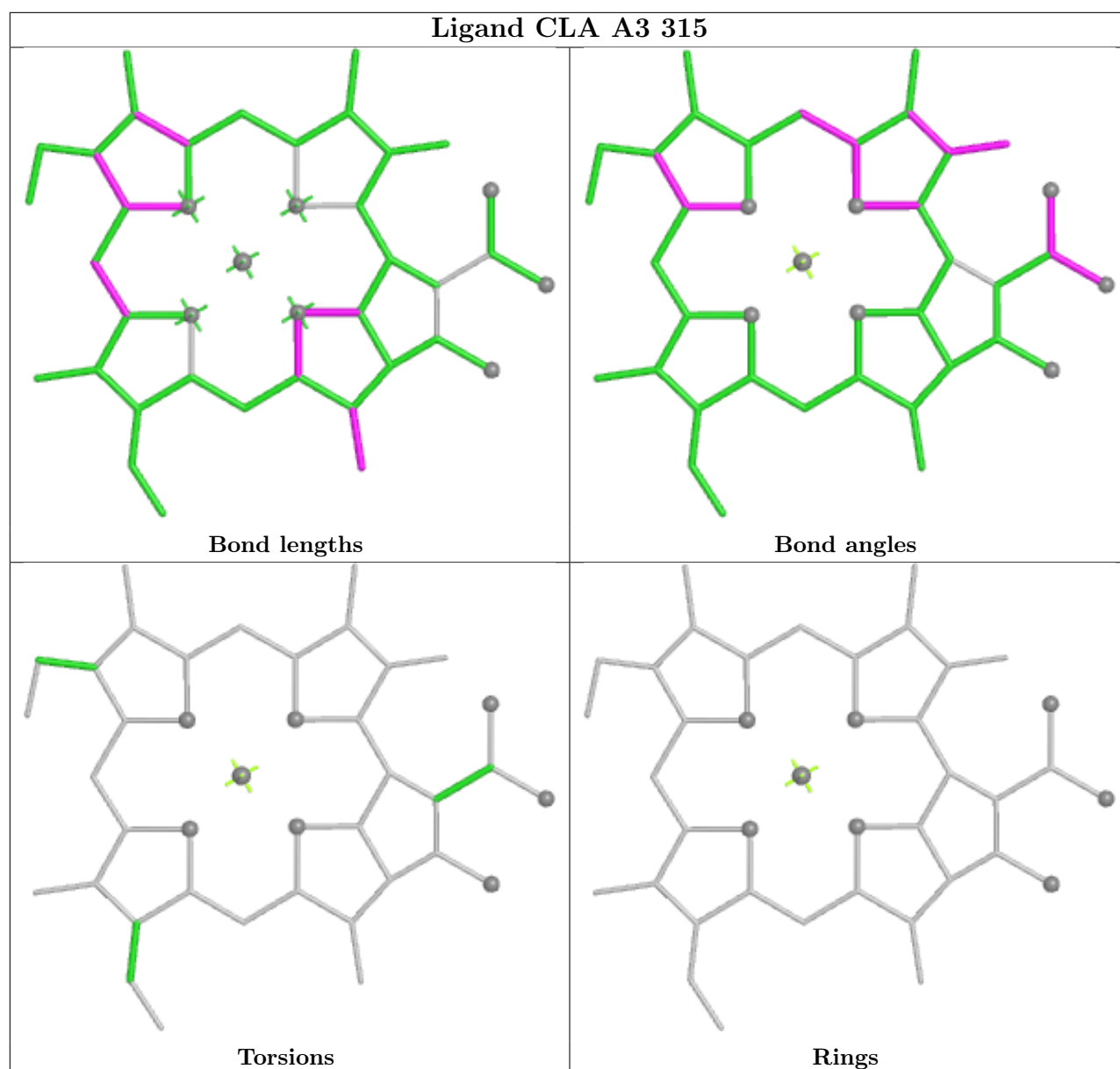
Bond angles



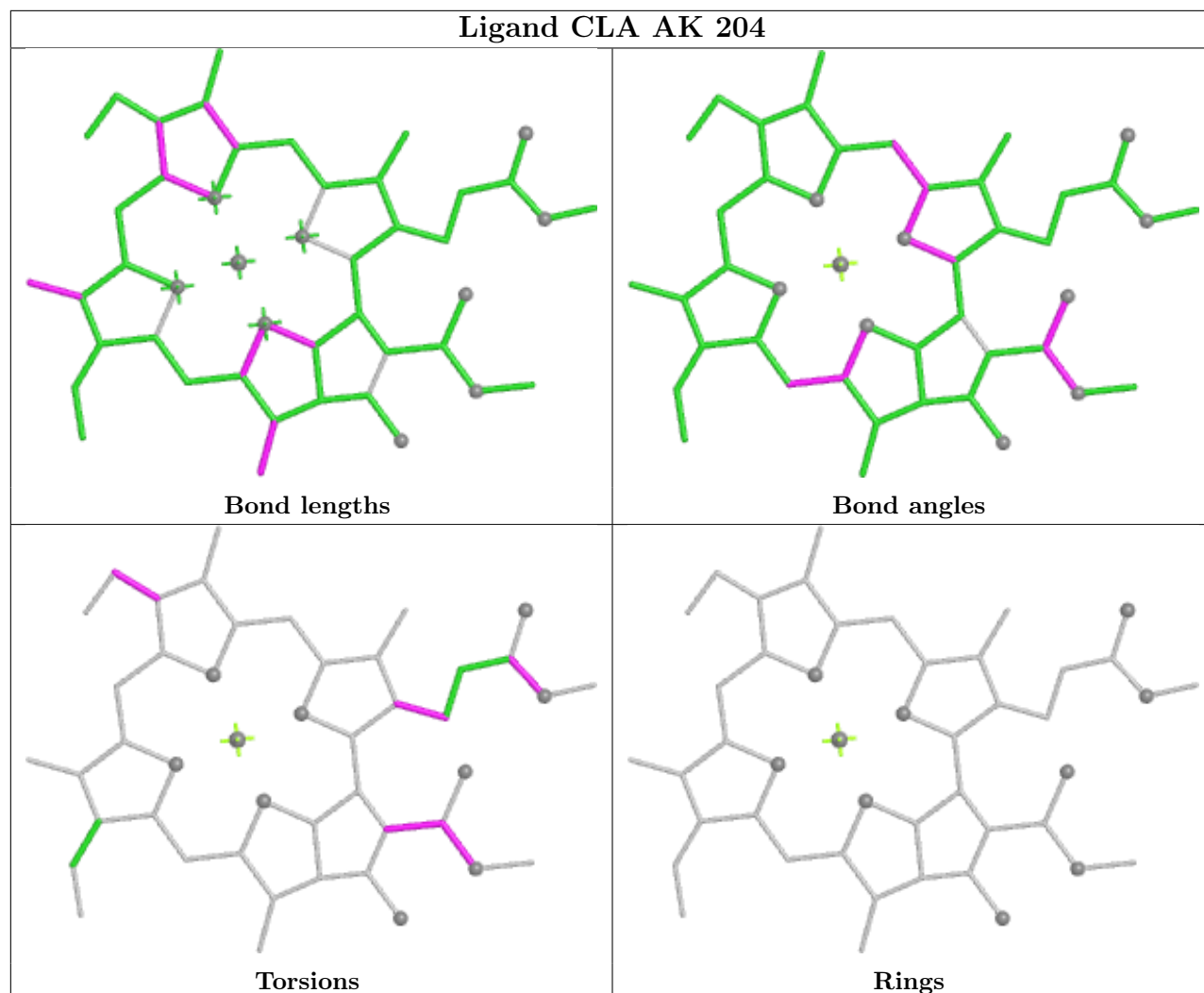
Torsions



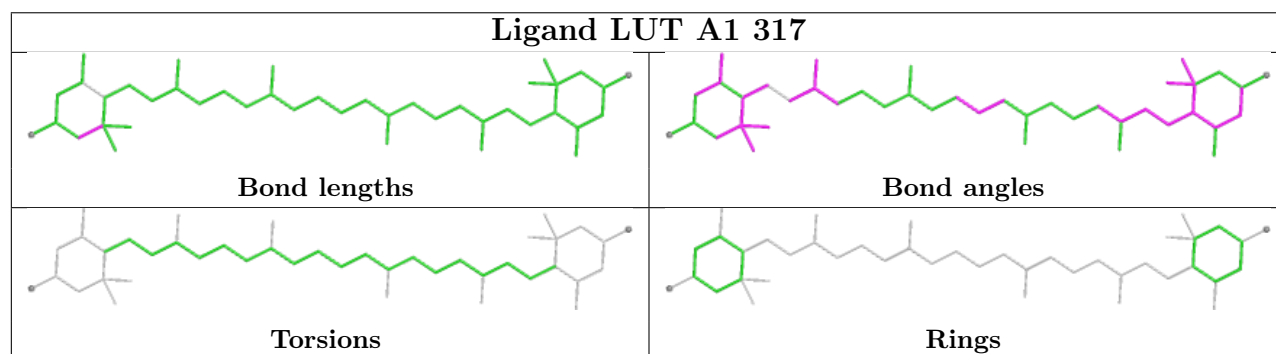
Rings



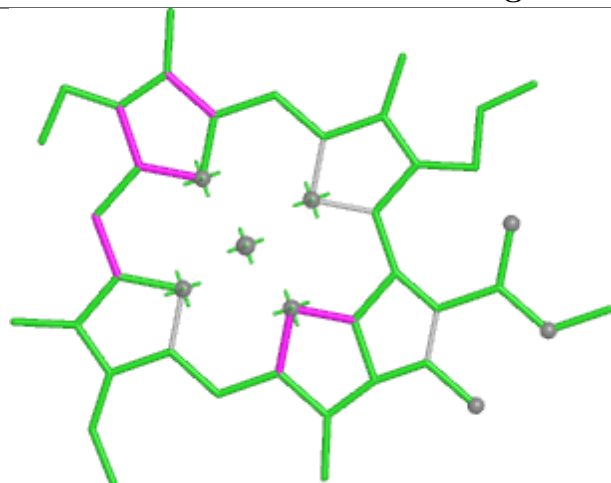
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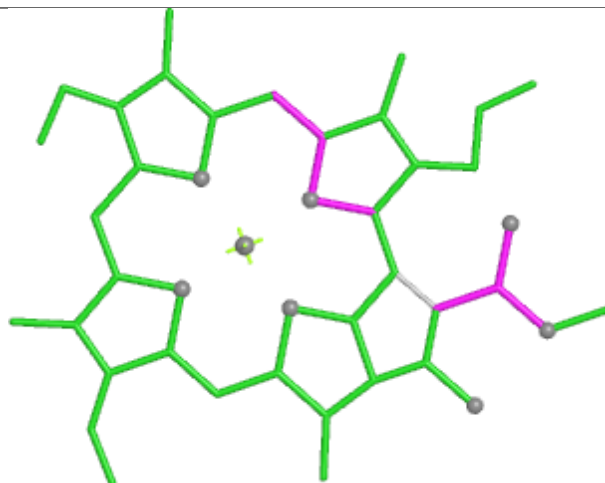
Ligand LUT A1 317



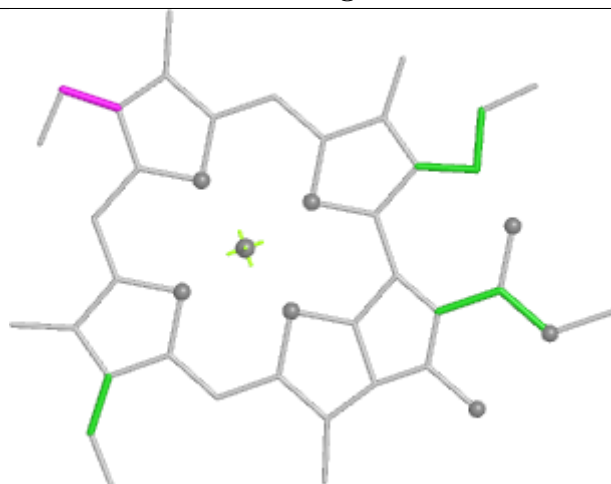
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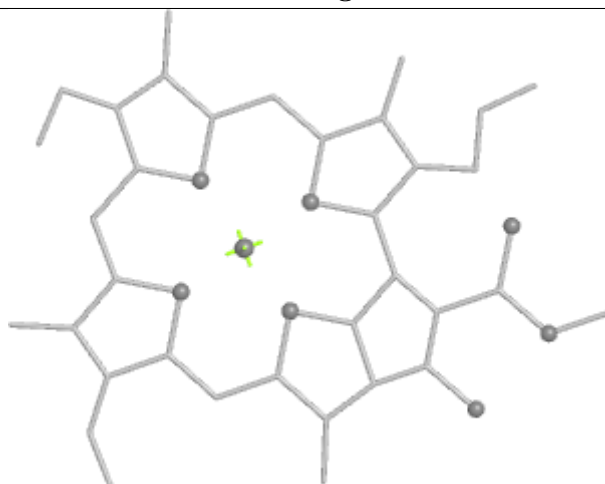
Bond lengths



Bond angles

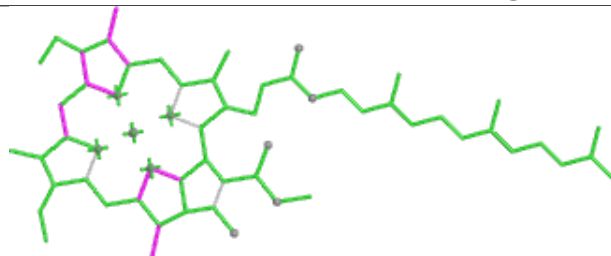


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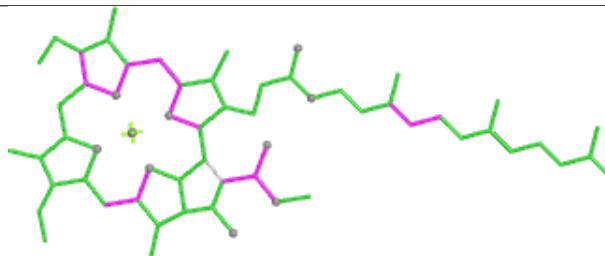


Rings

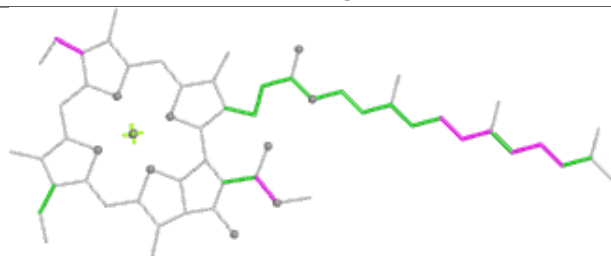
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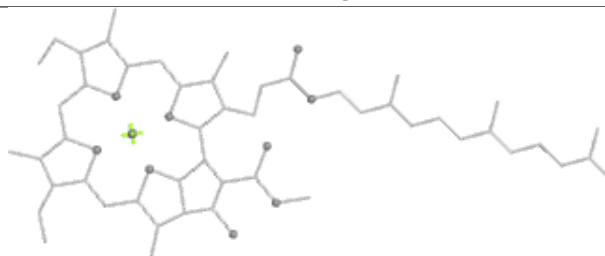
Bond lengths



Bond angles

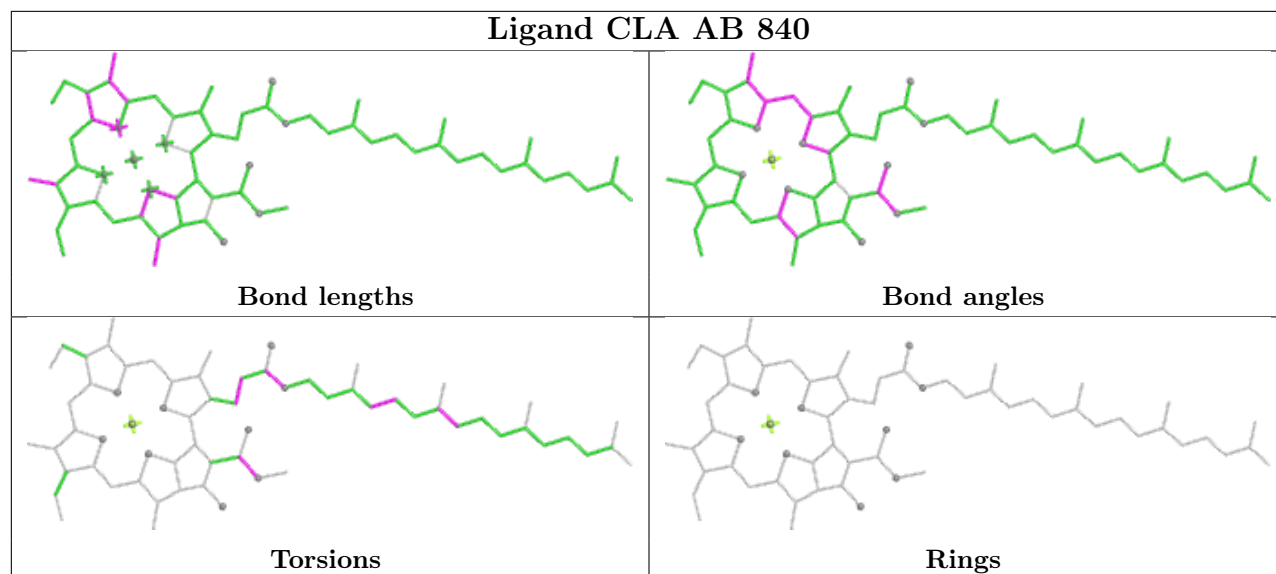


Torsions

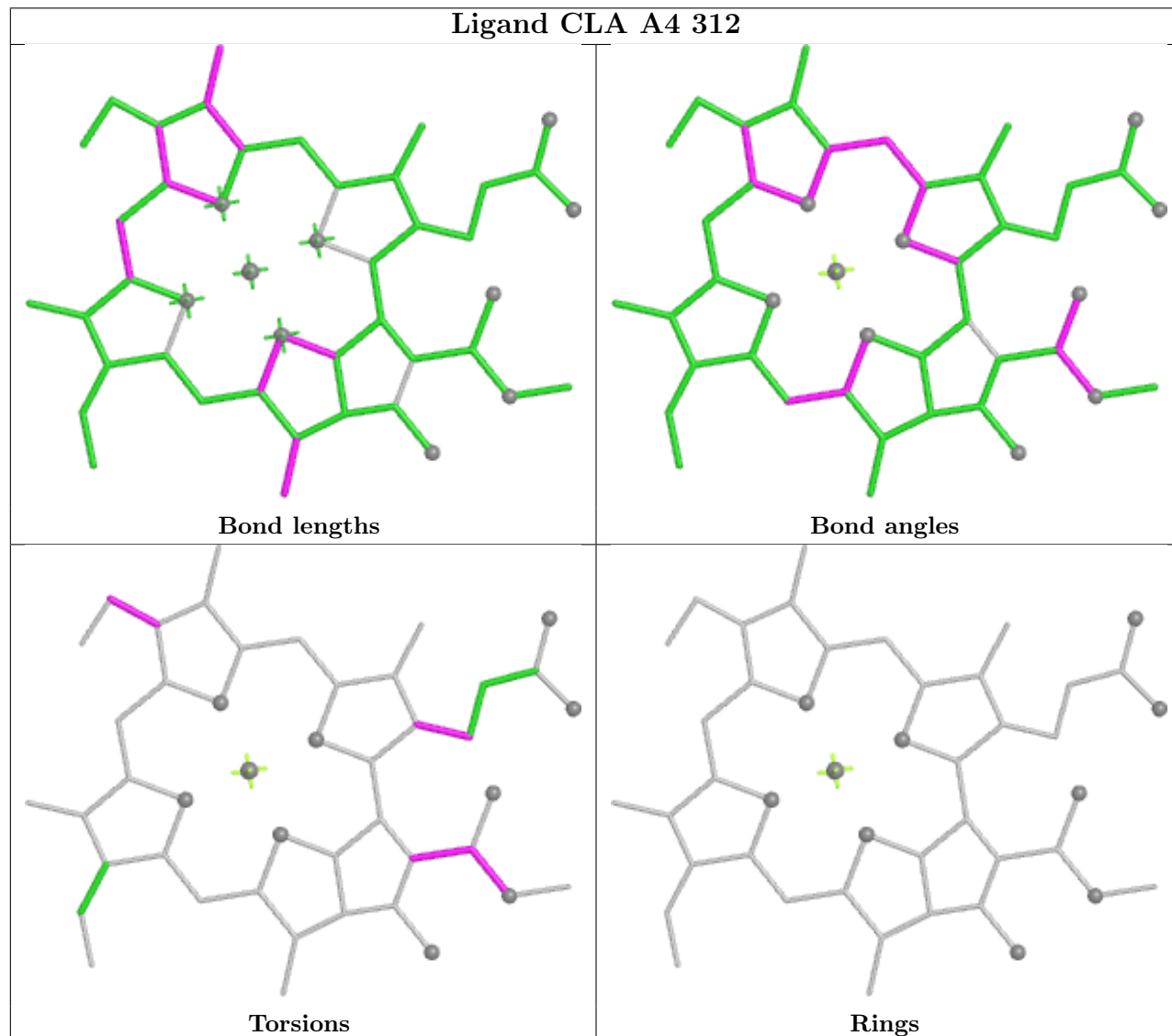


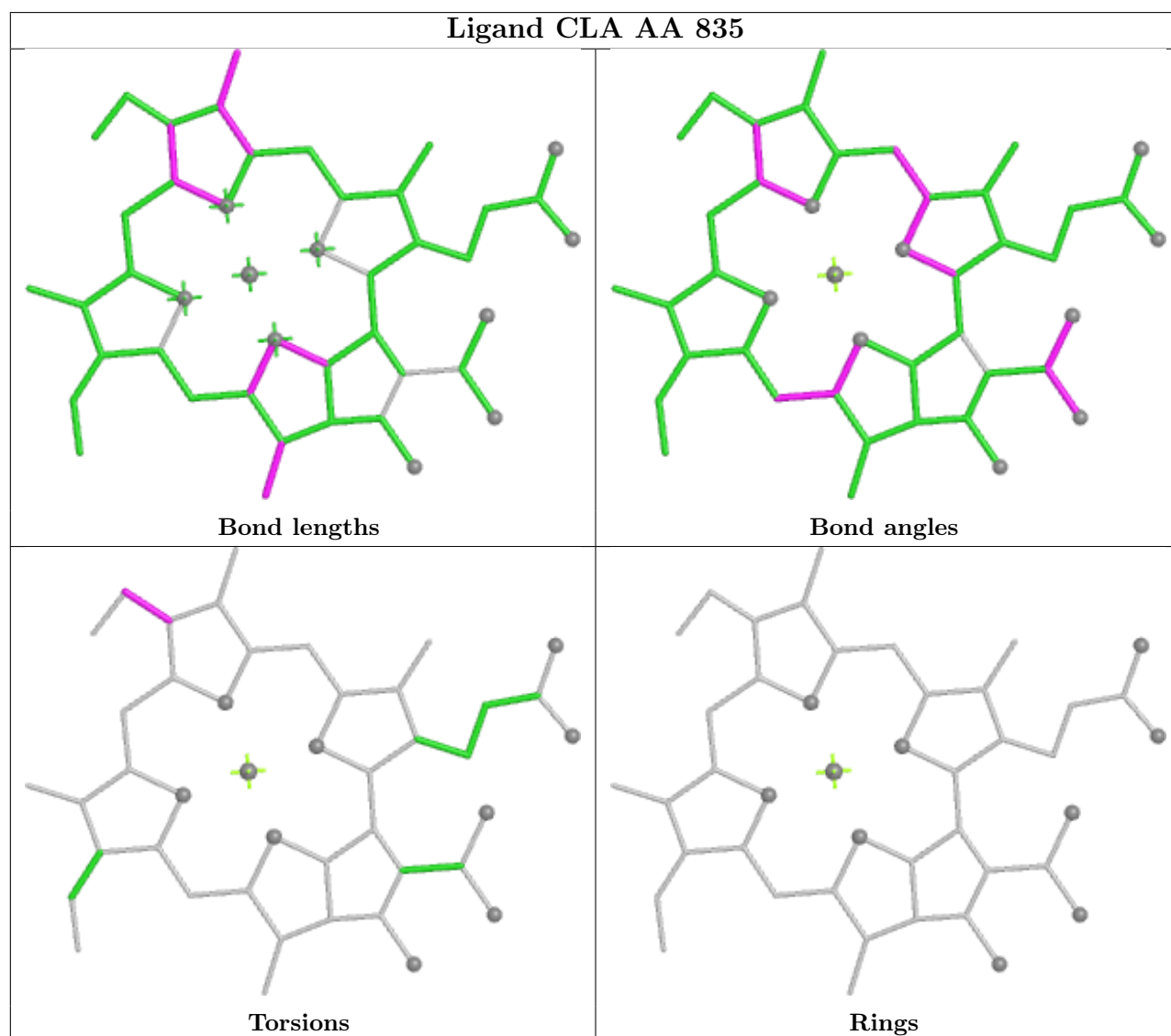
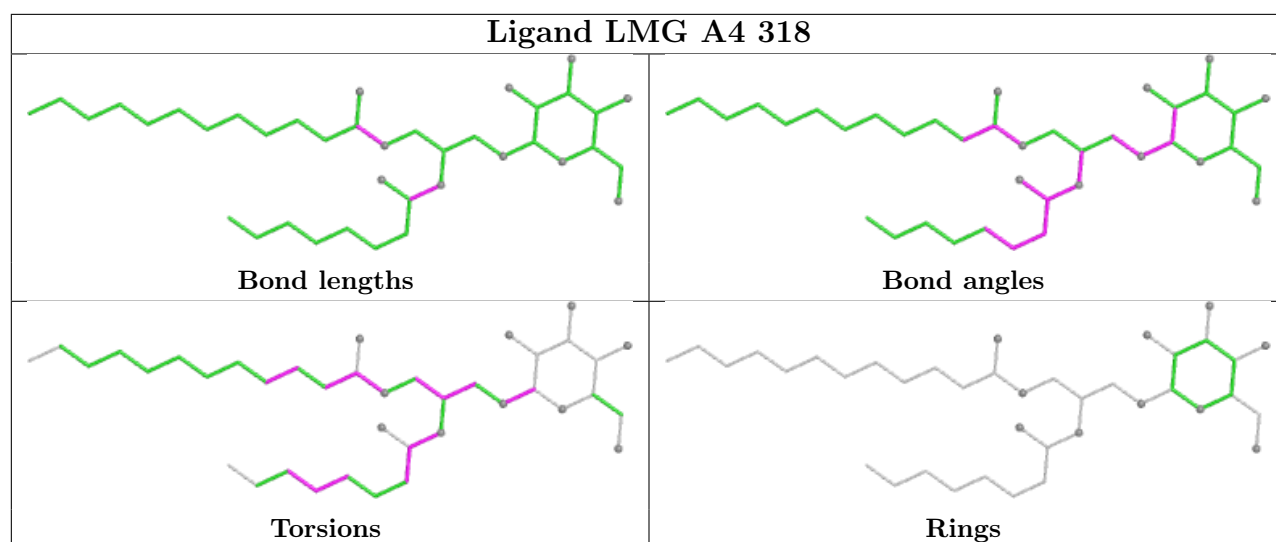
Rings

Ligand CLA AB 840

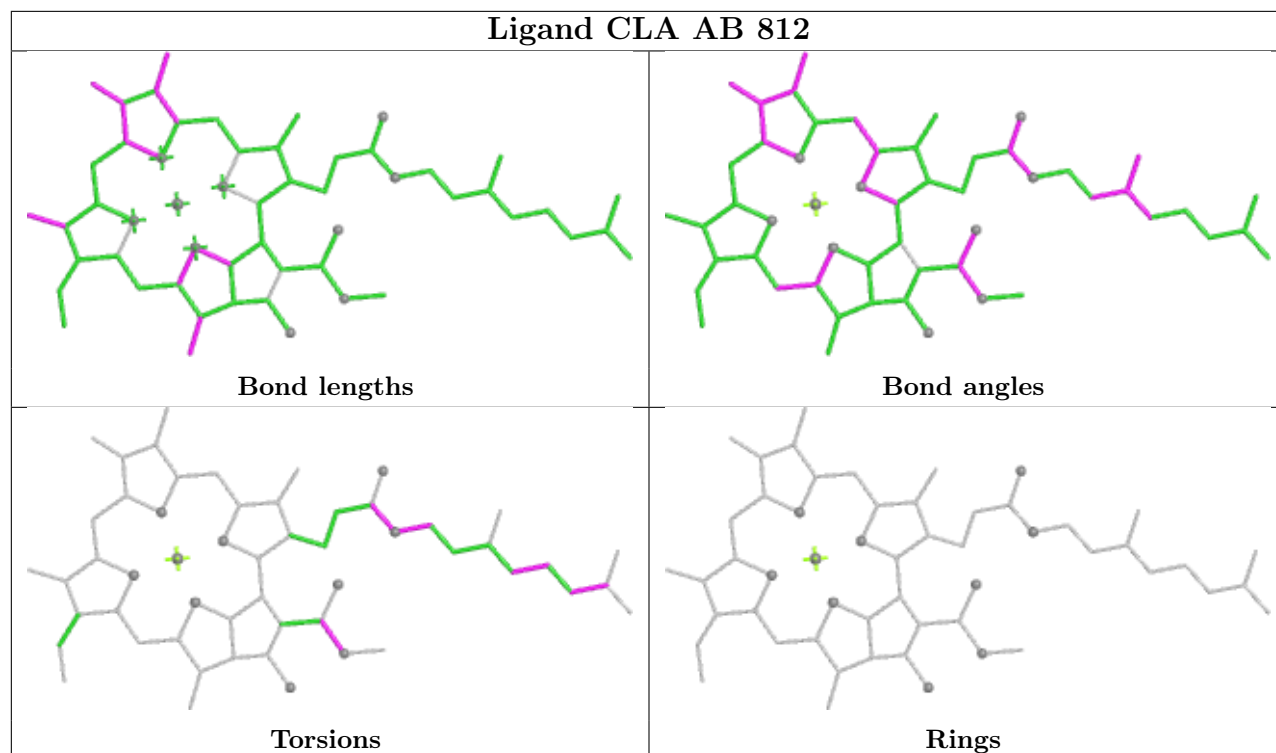


Ligand CLA A4 312

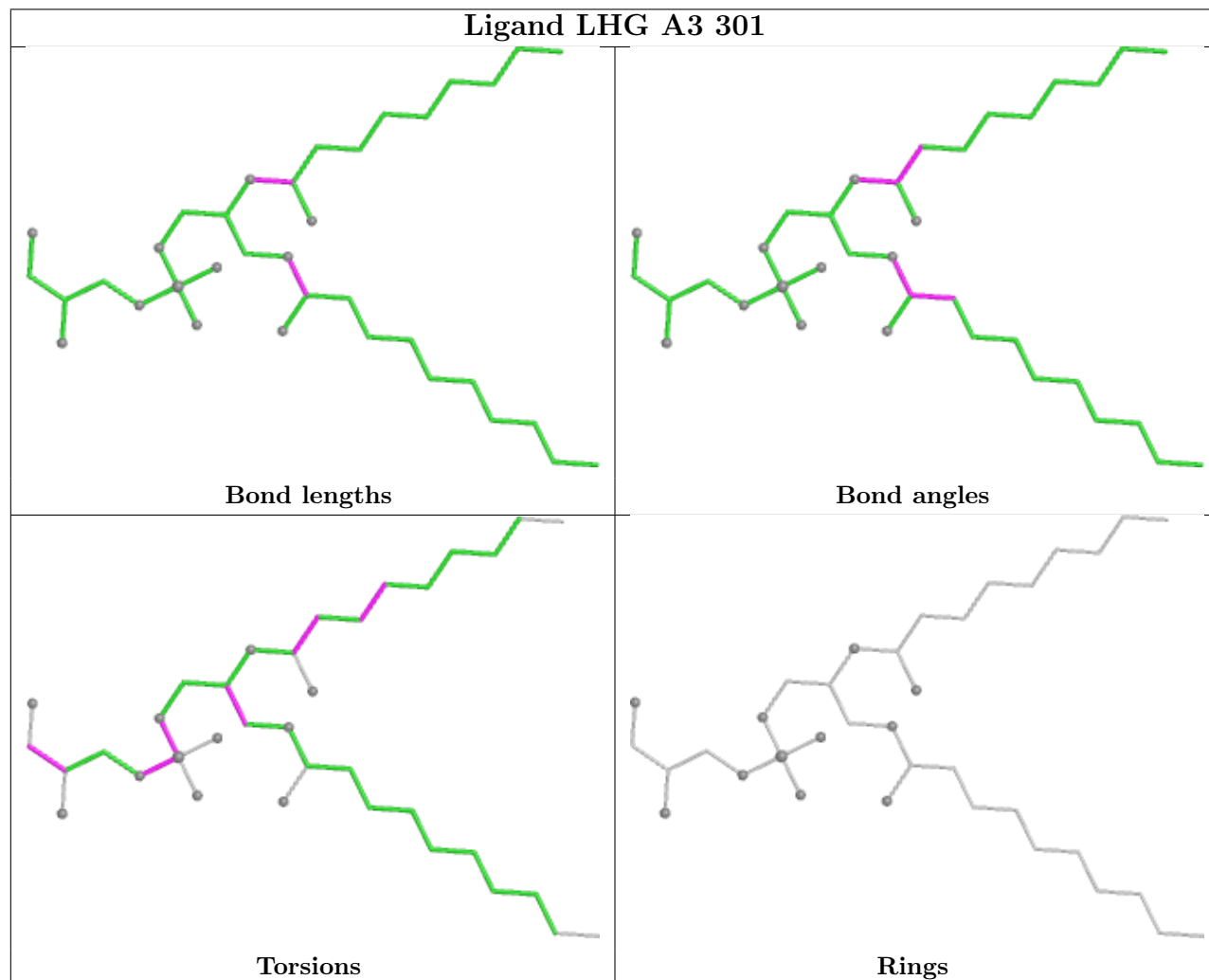


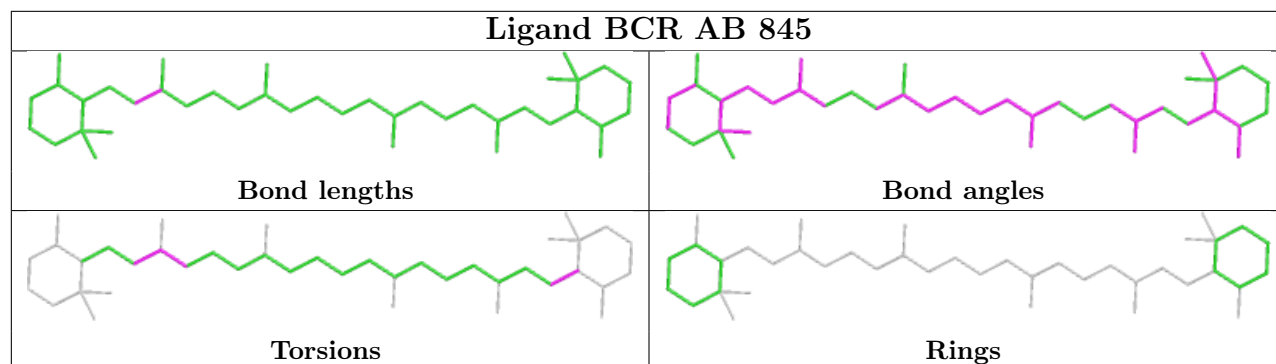
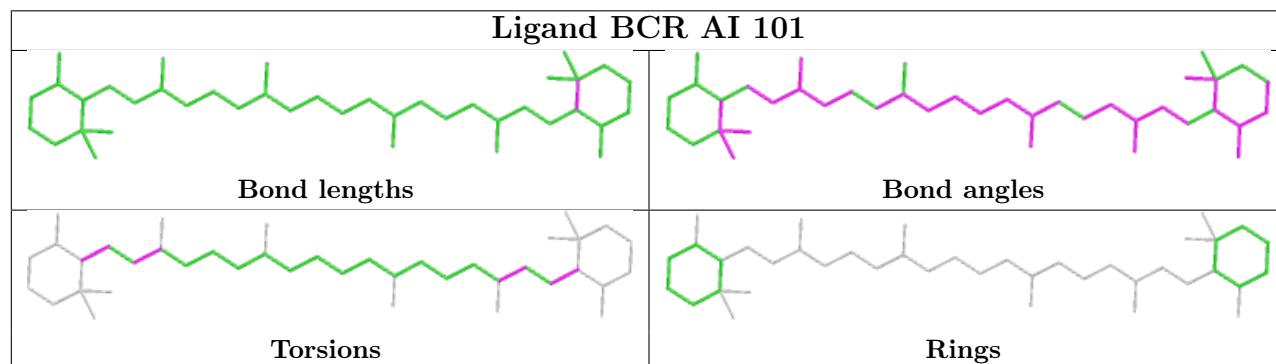
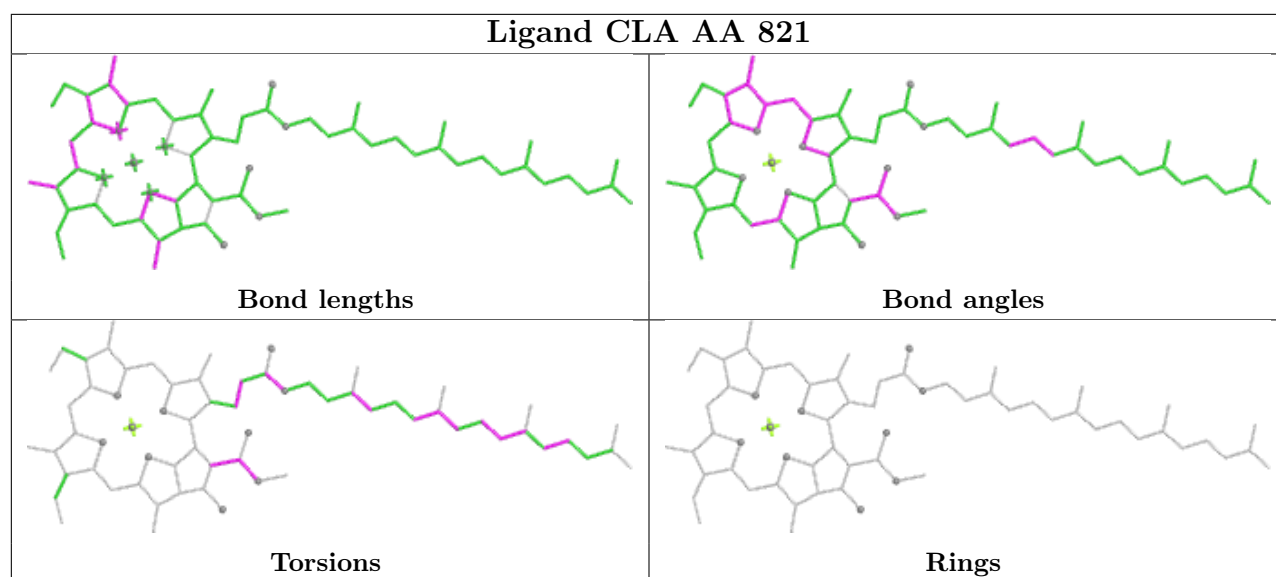


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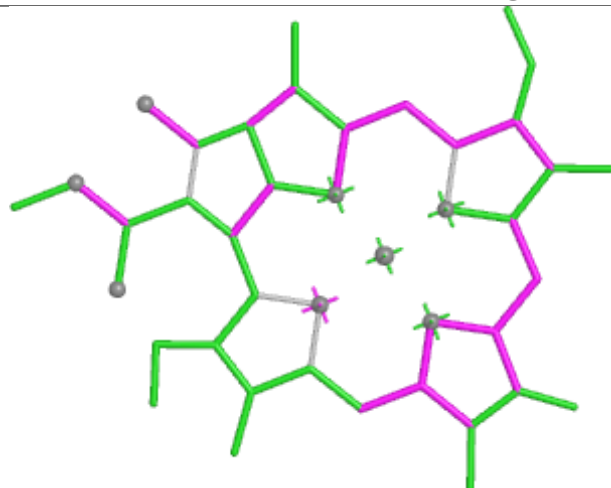


Ligand LHG A3 301

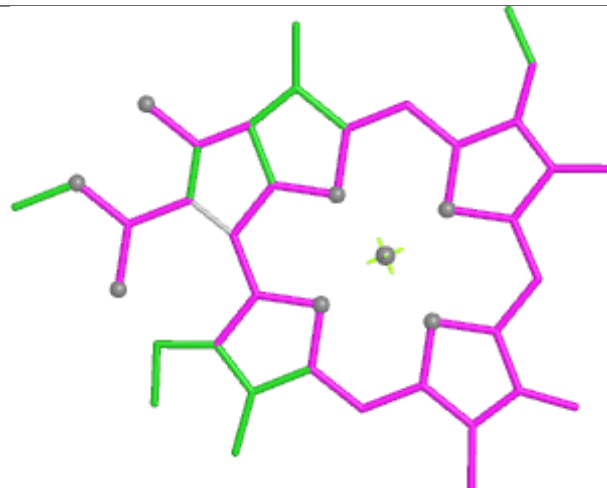




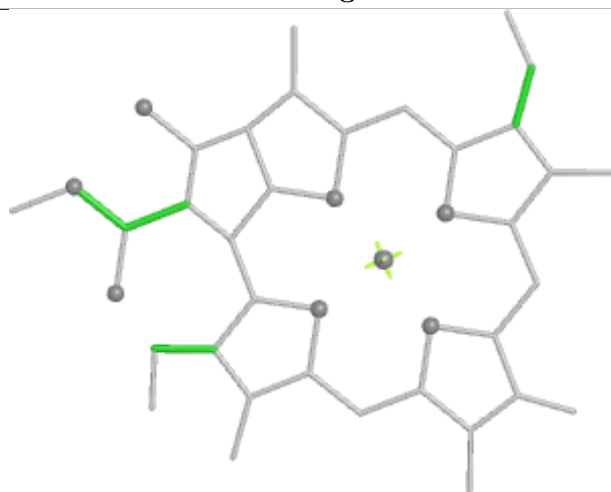
Ligand CHL A4 305



Bond lengths



Bond angles

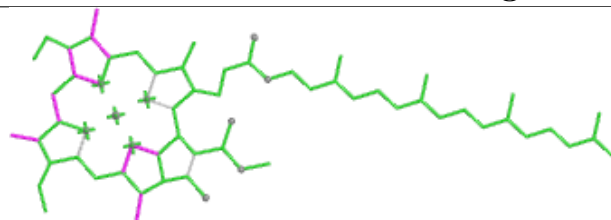


Torsions

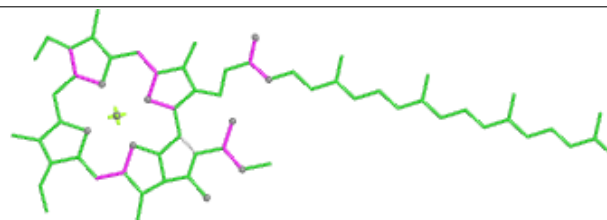


Rings

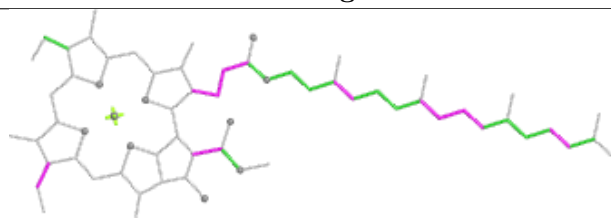
Ligand CLA AB 828



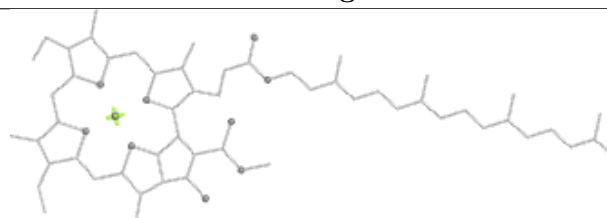
Bond lengths



Bond angles

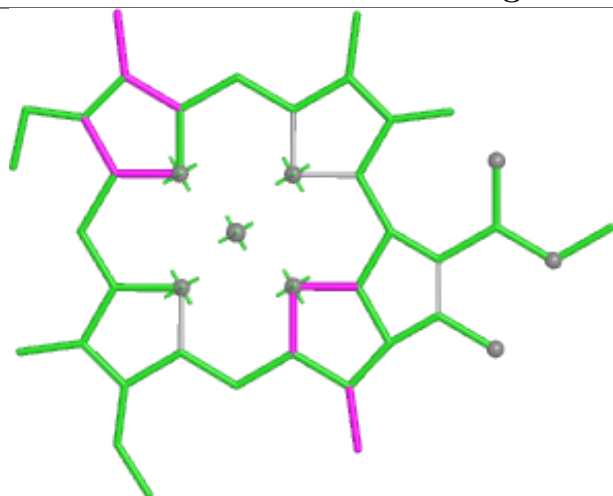


Torsions



Rings

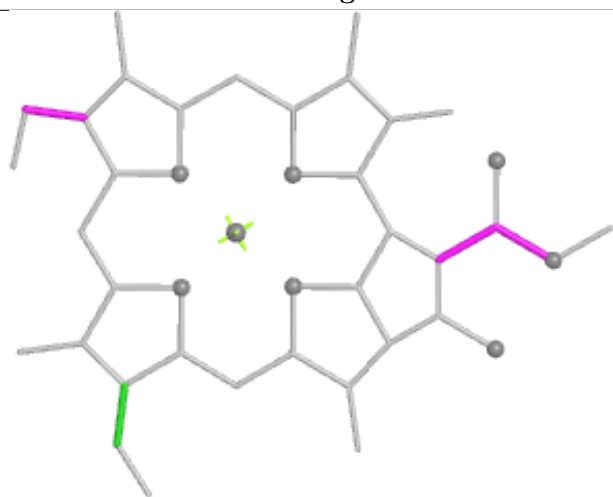
Ligand CLA AL 302



Bond lengths



Bond angles

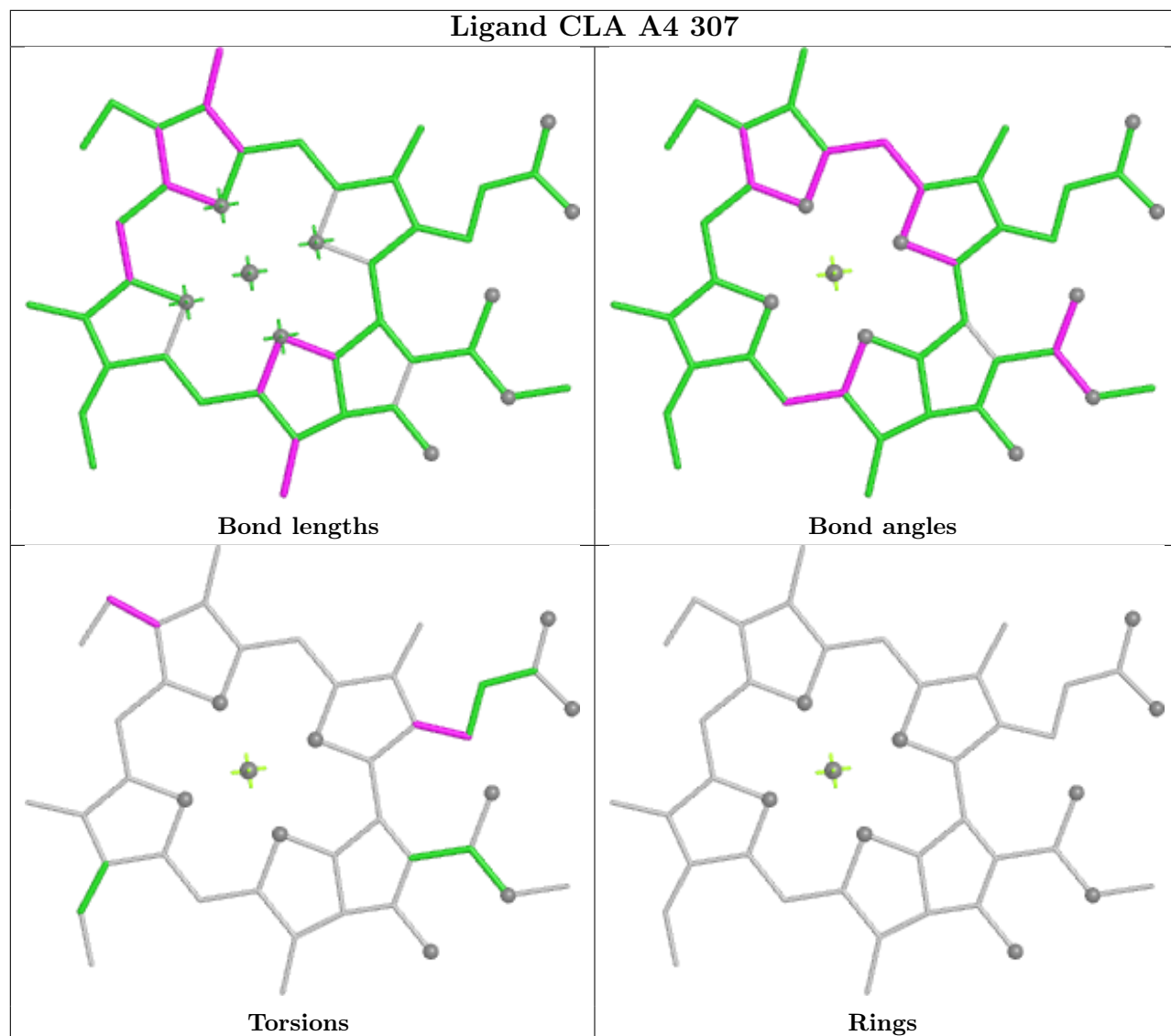


Torsions

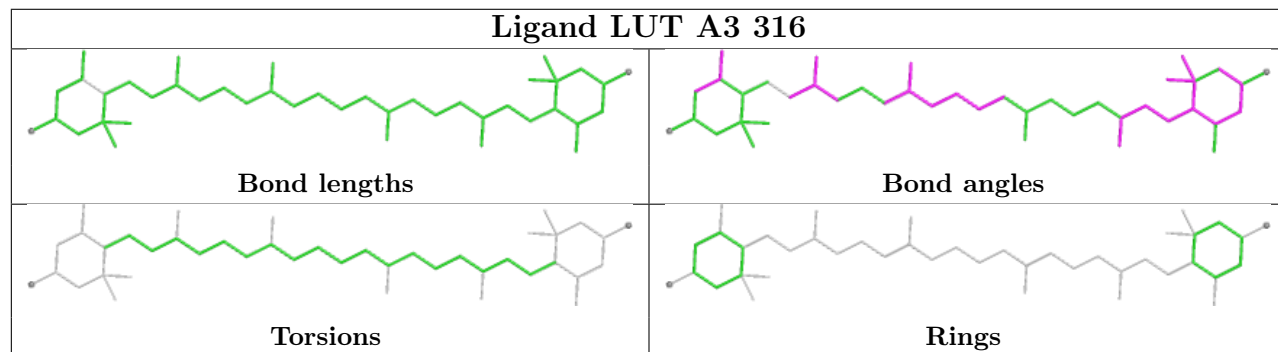


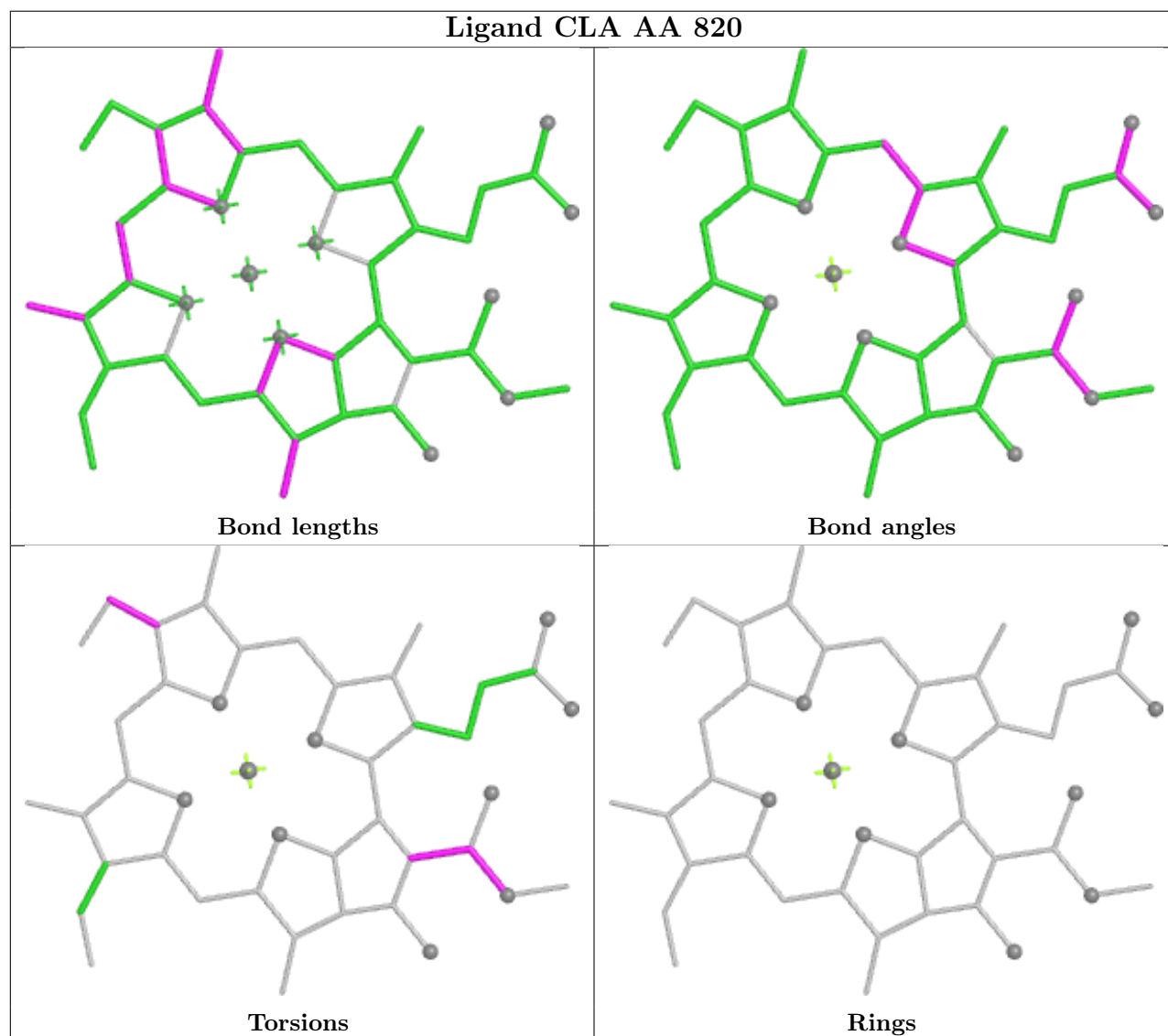
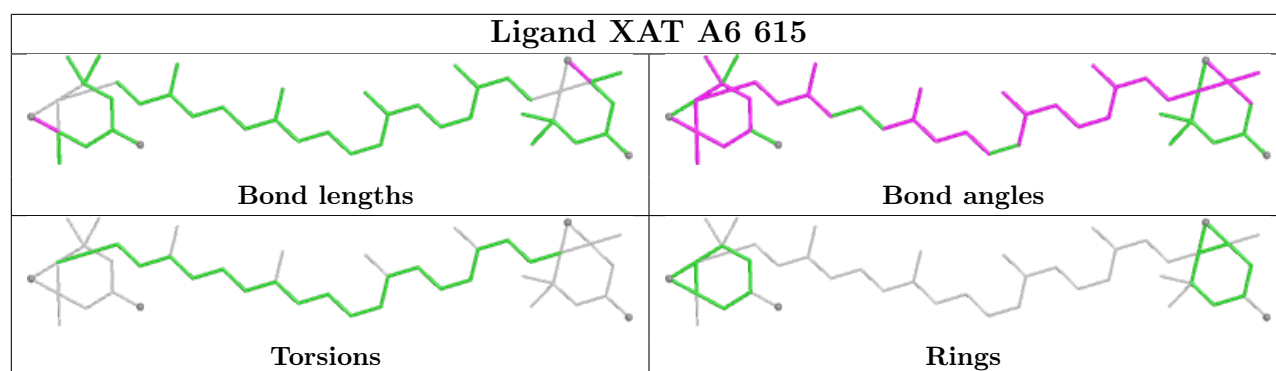
Rings

Ligand CLA A4 307

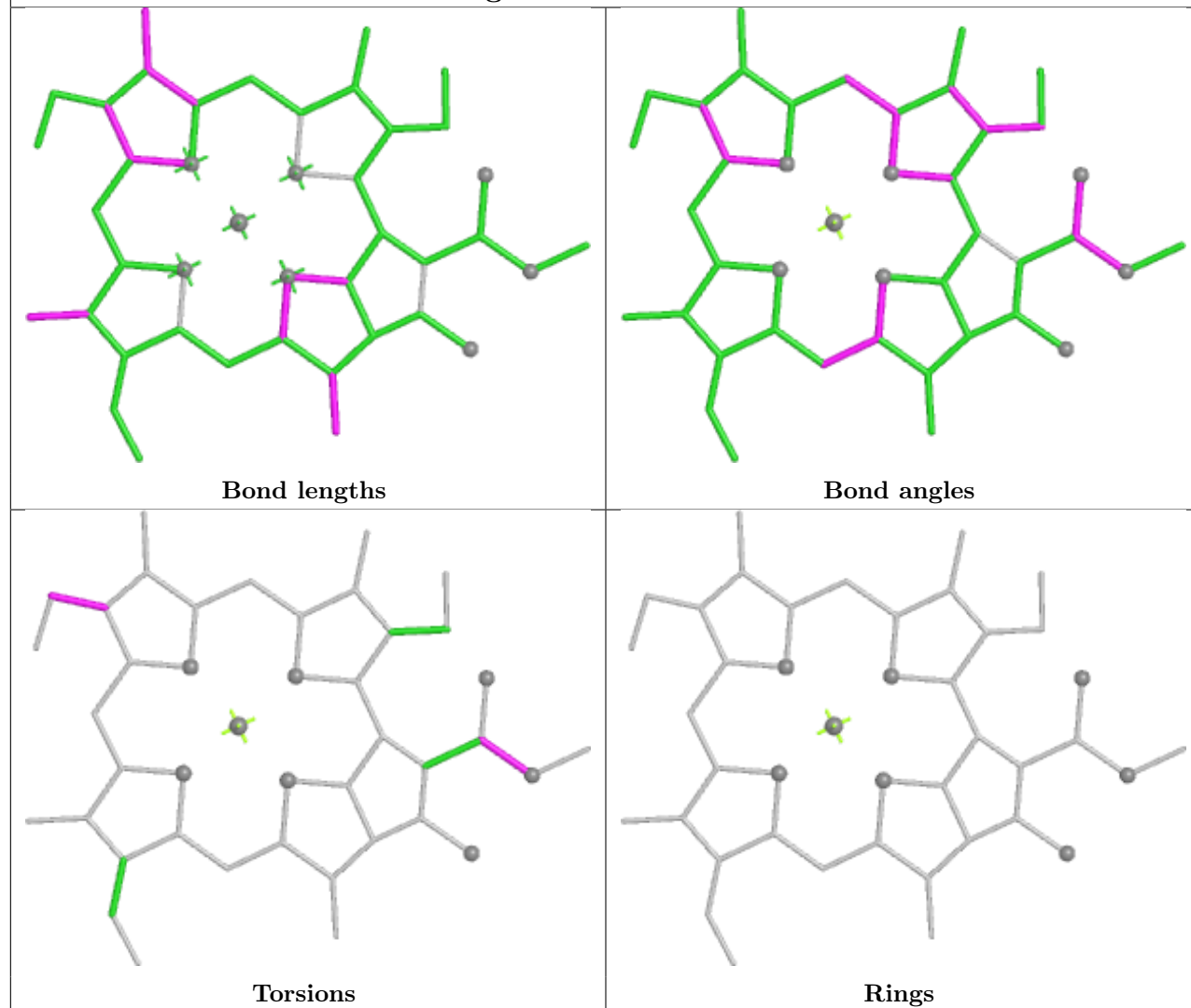


Ligand LUT A3 316

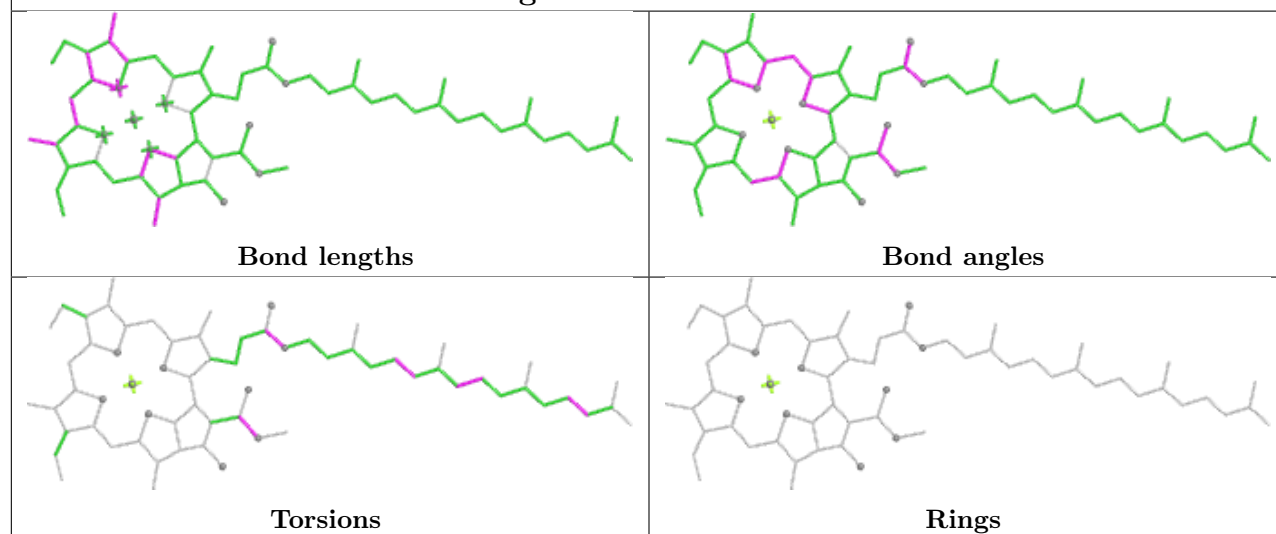


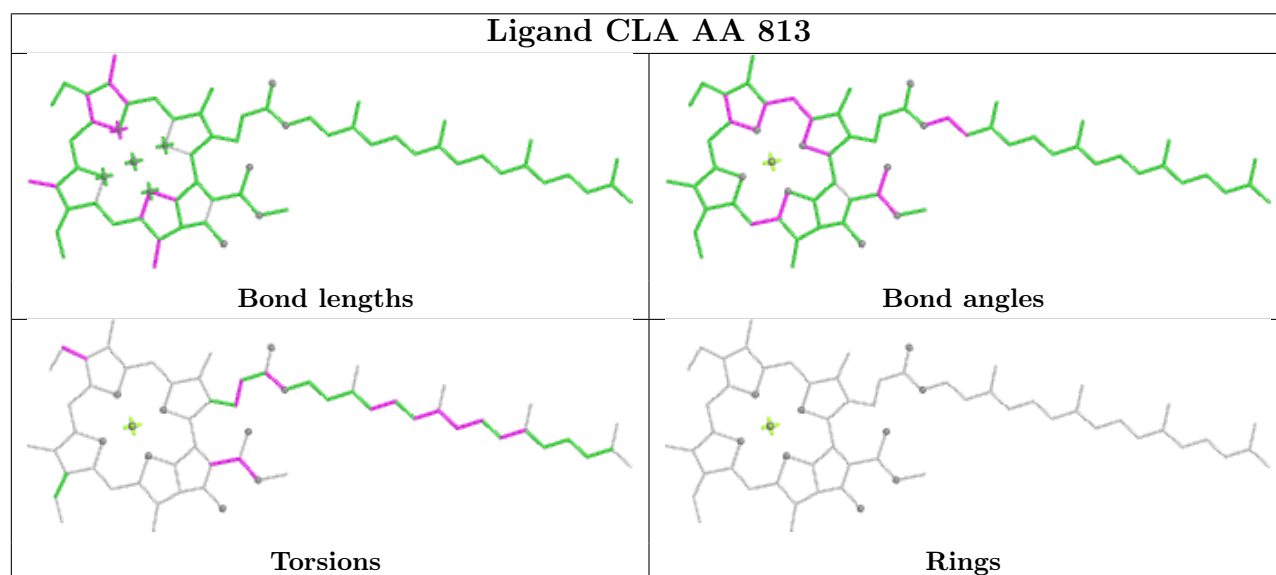
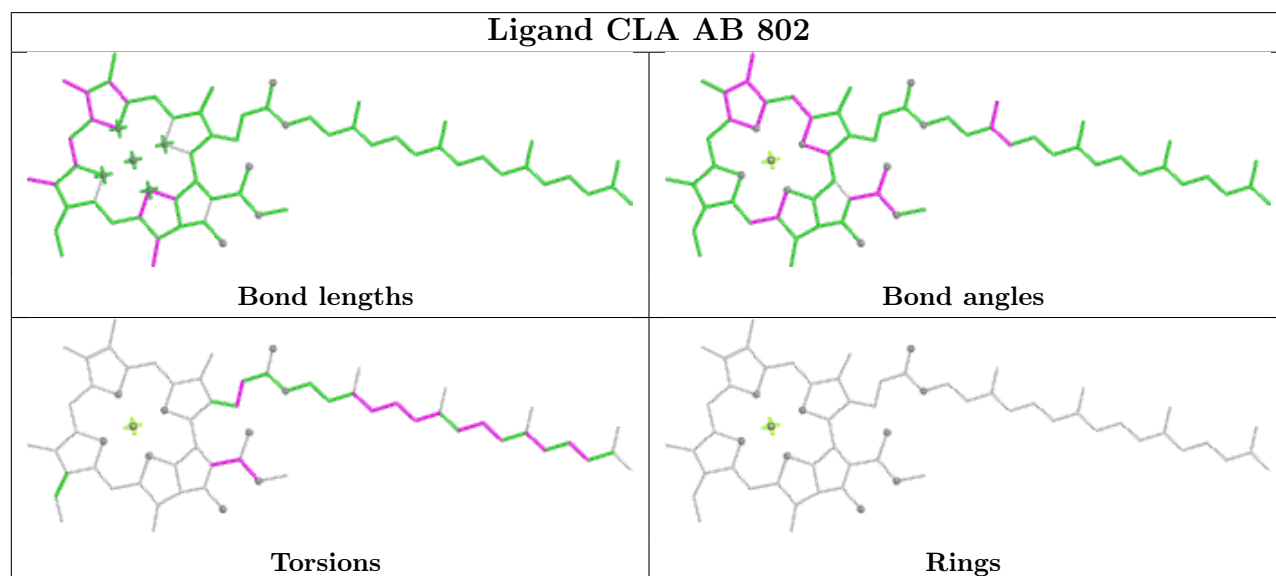
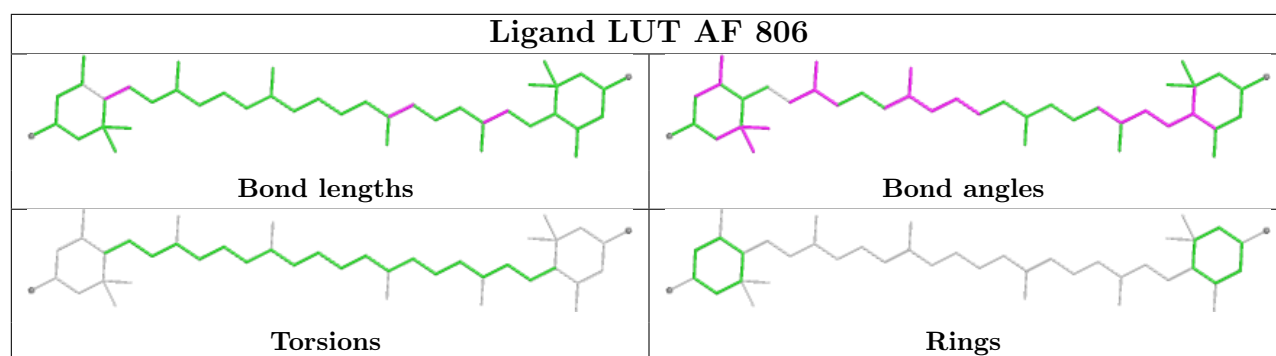


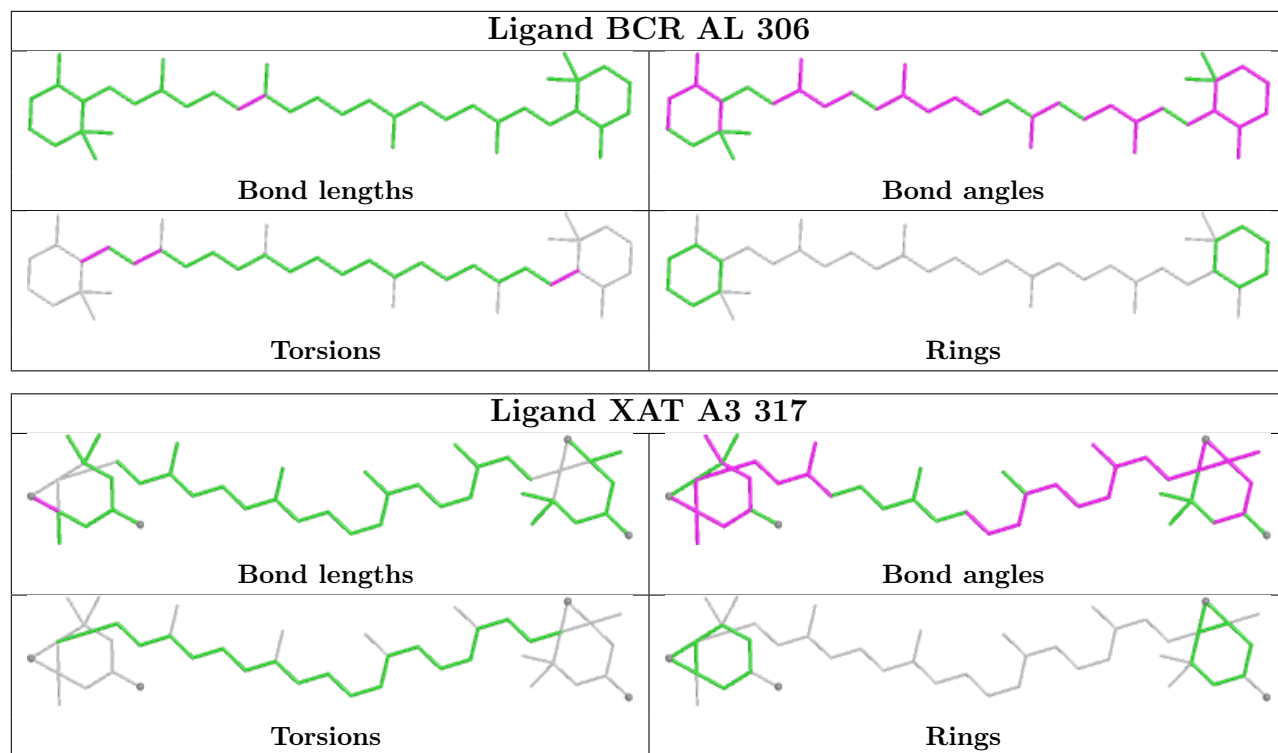
Ligand CLA AF 803



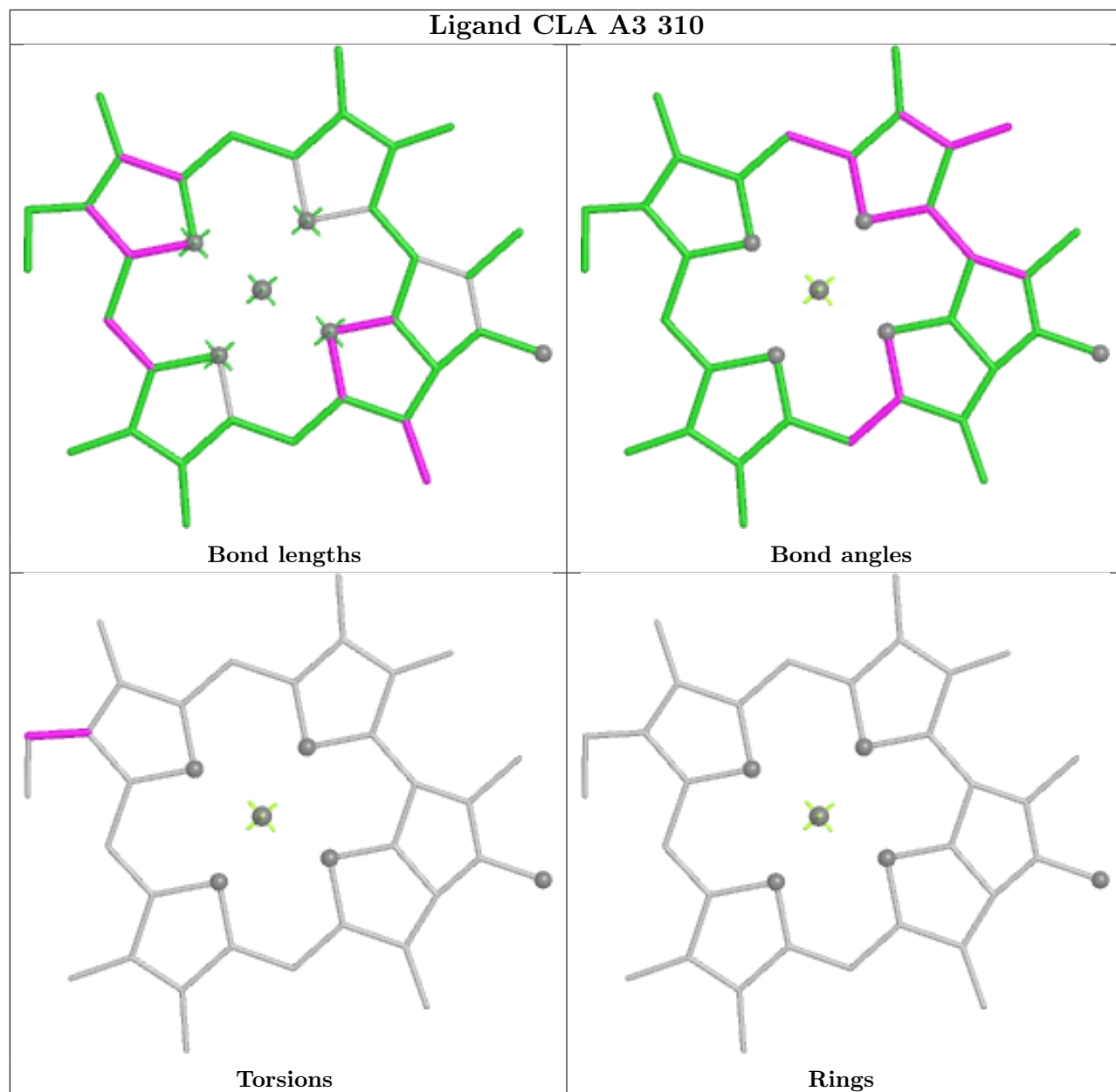
Ligand CLA AB 838

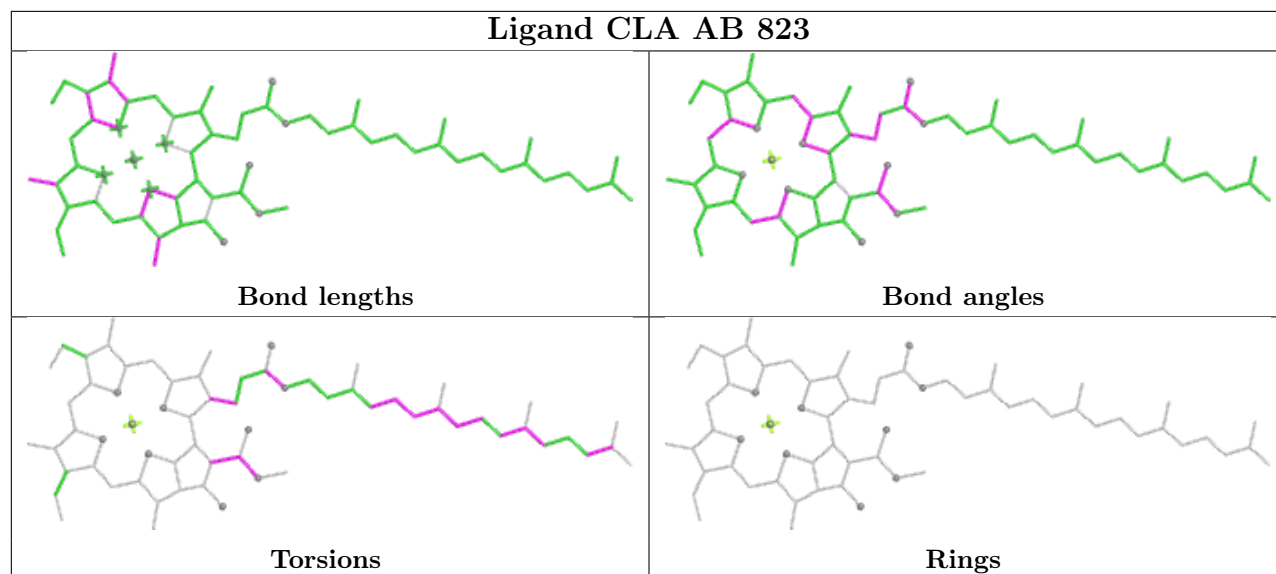
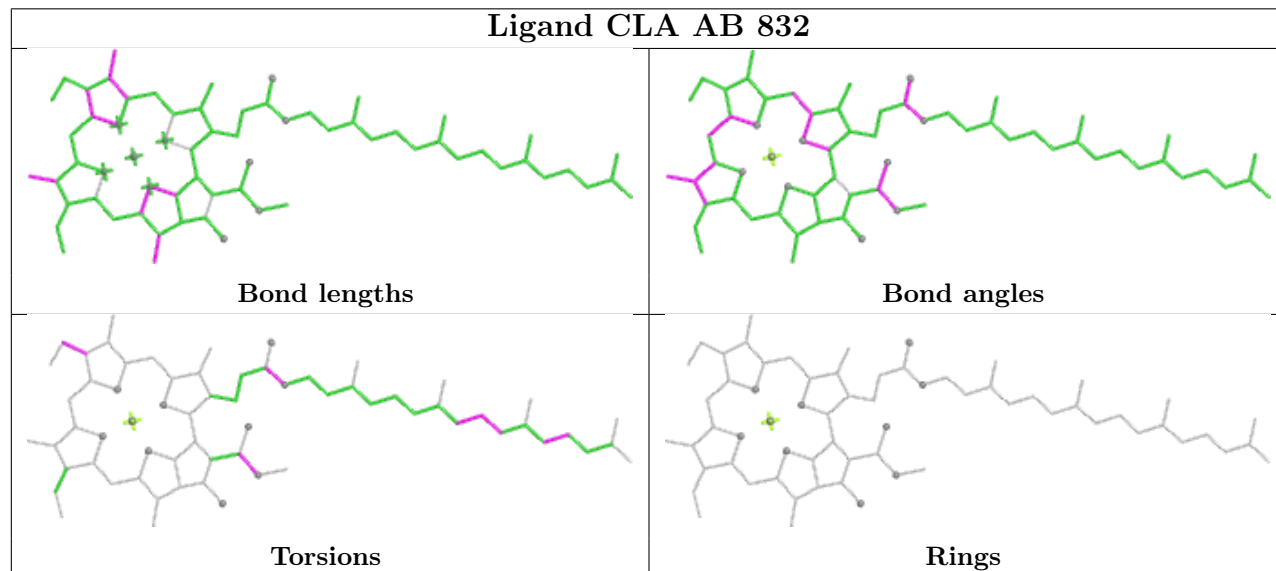
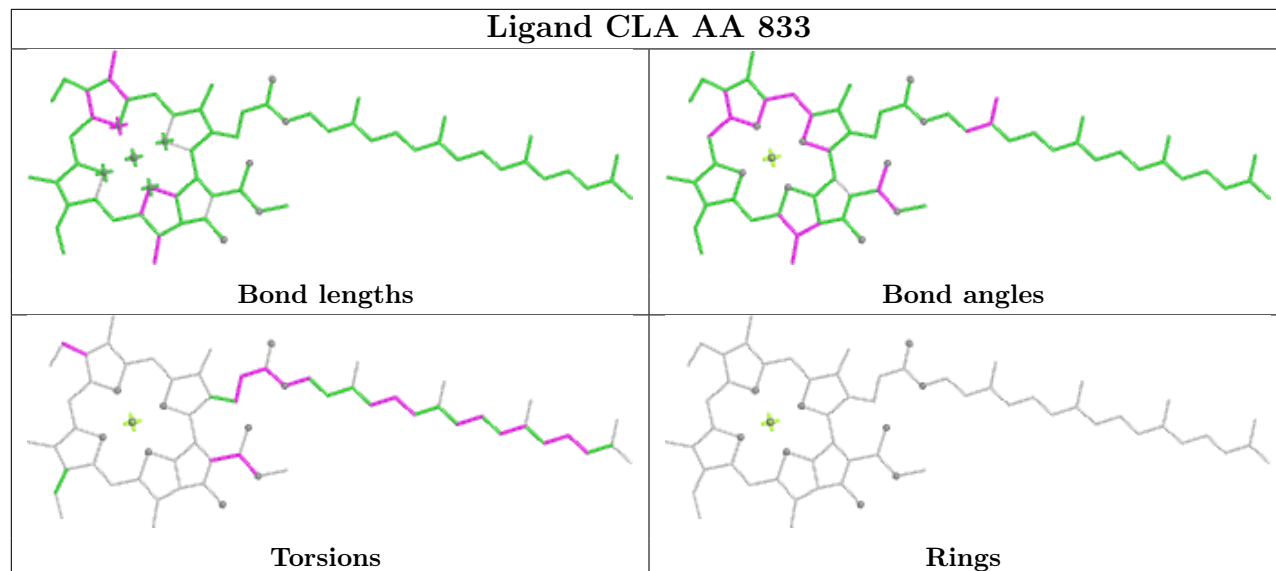




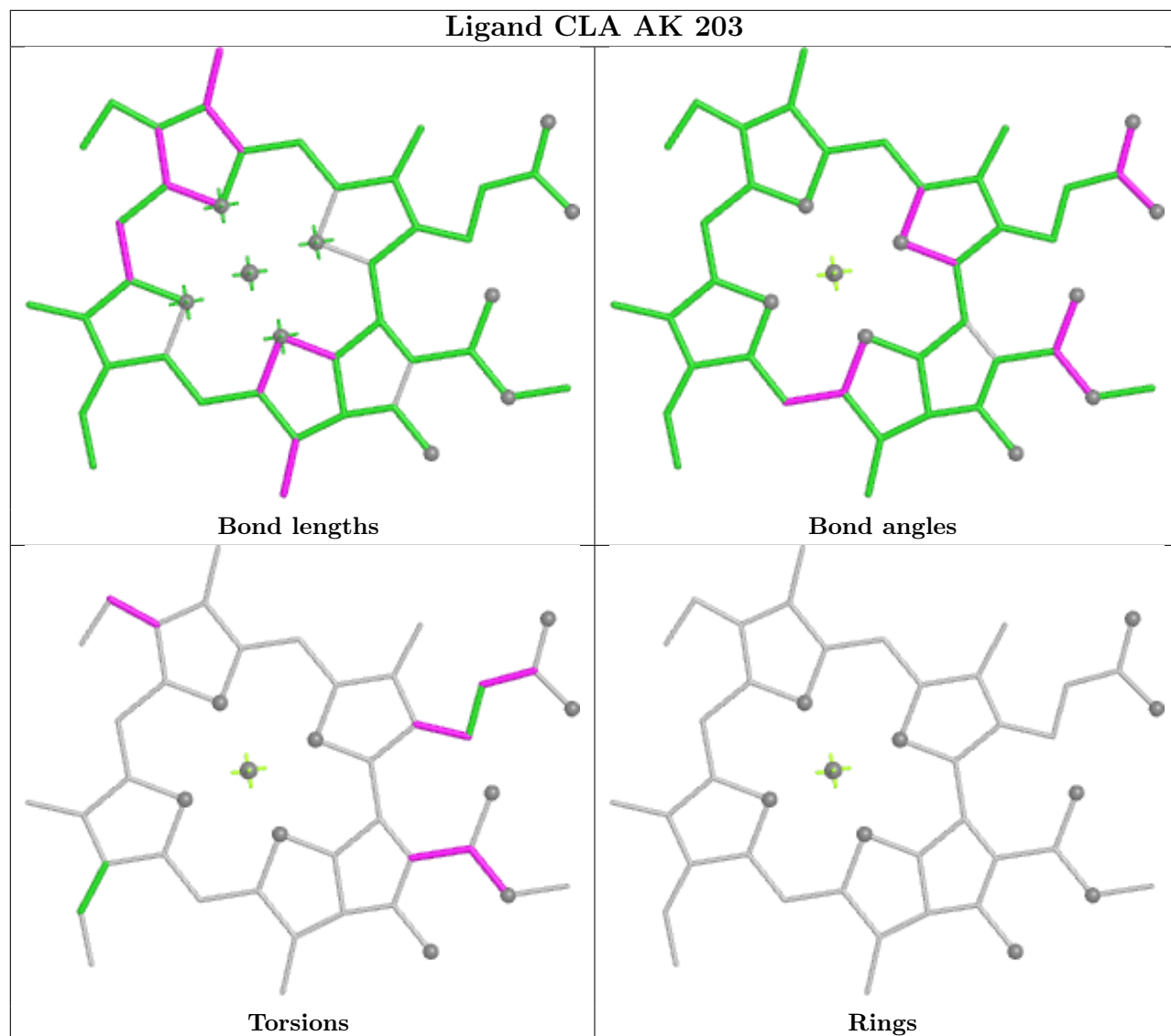


Ligand CLA A3 310

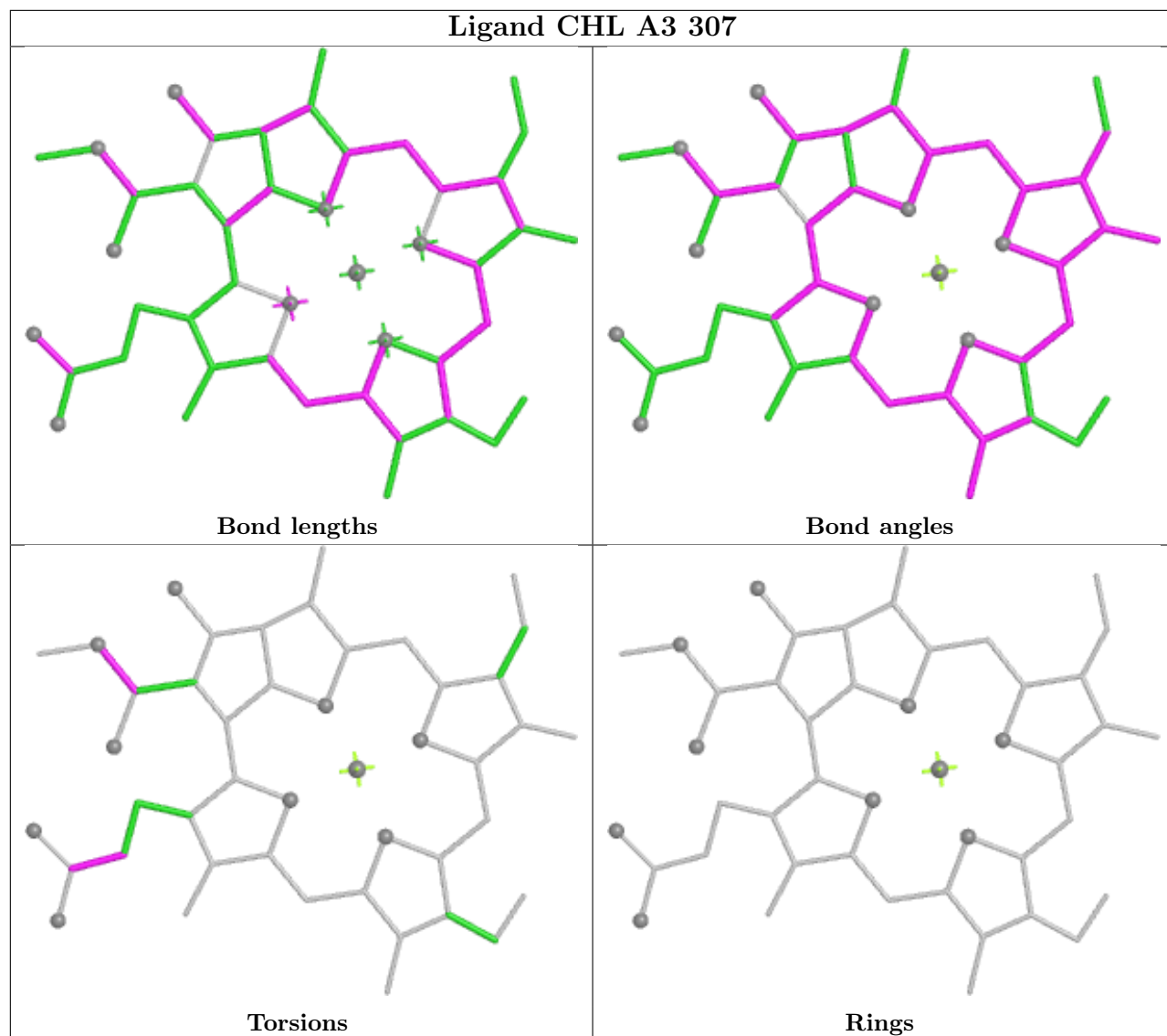


Ligand CLA AB 823**Ligand CLA AB 832****Ligand CLA AA 833**

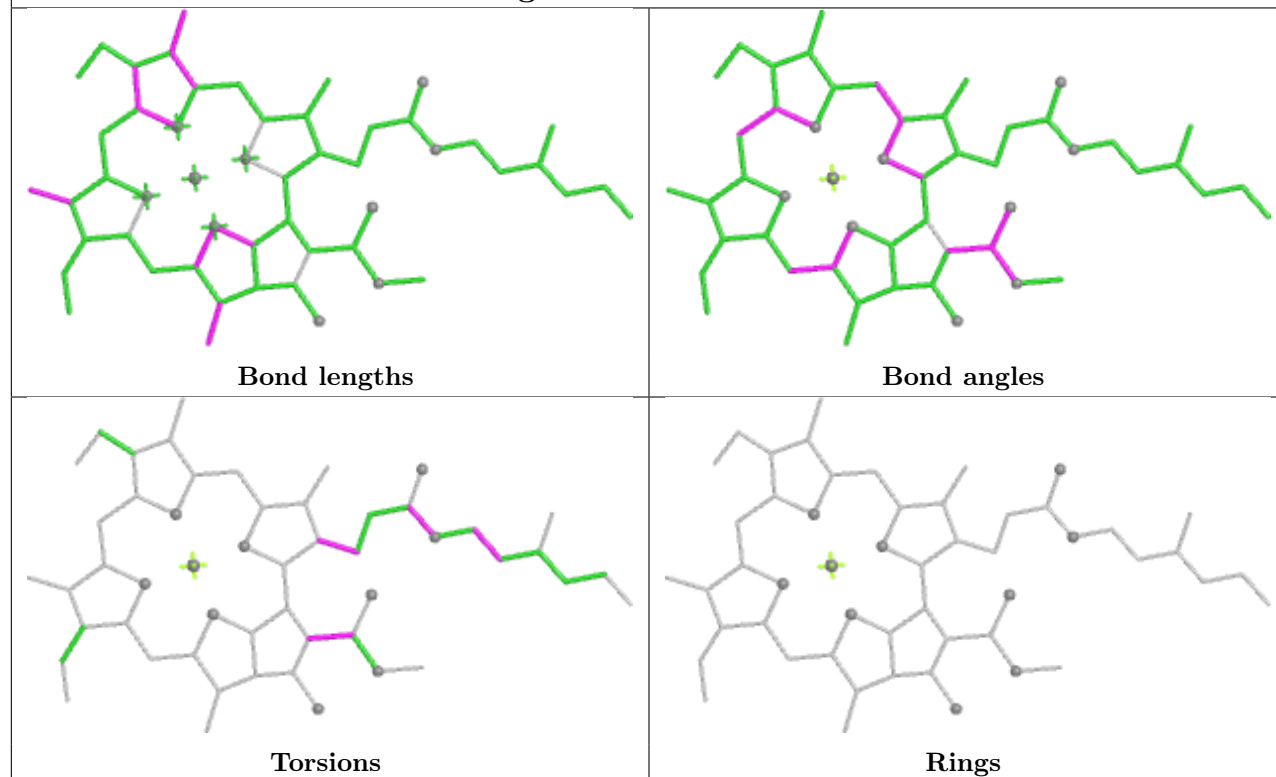
Ligand CLA AK 203



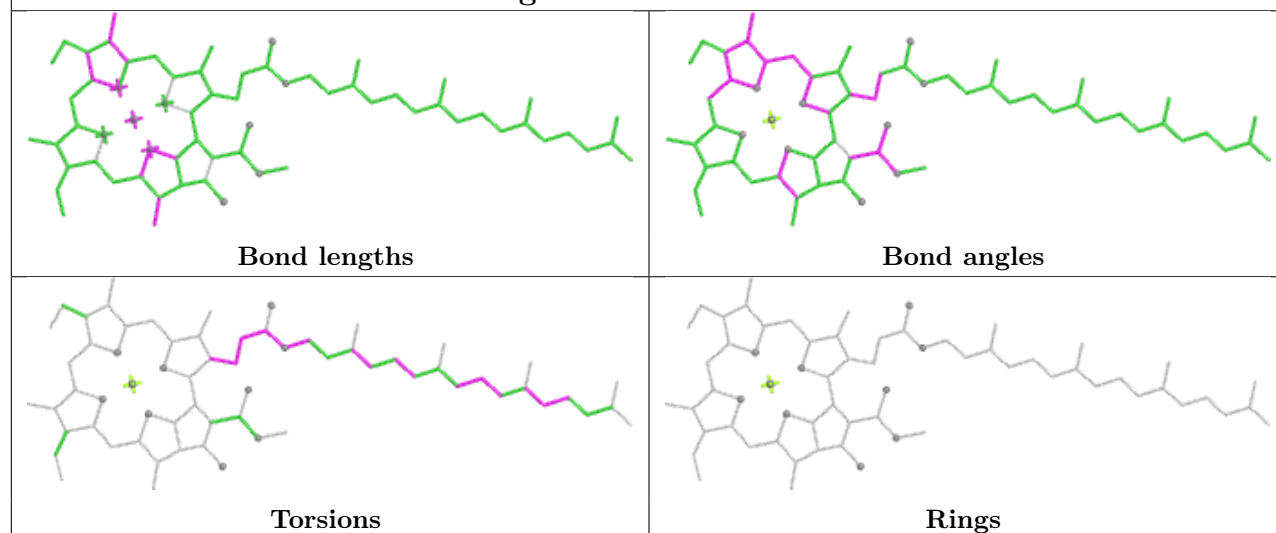
Ligand CHL A3 307



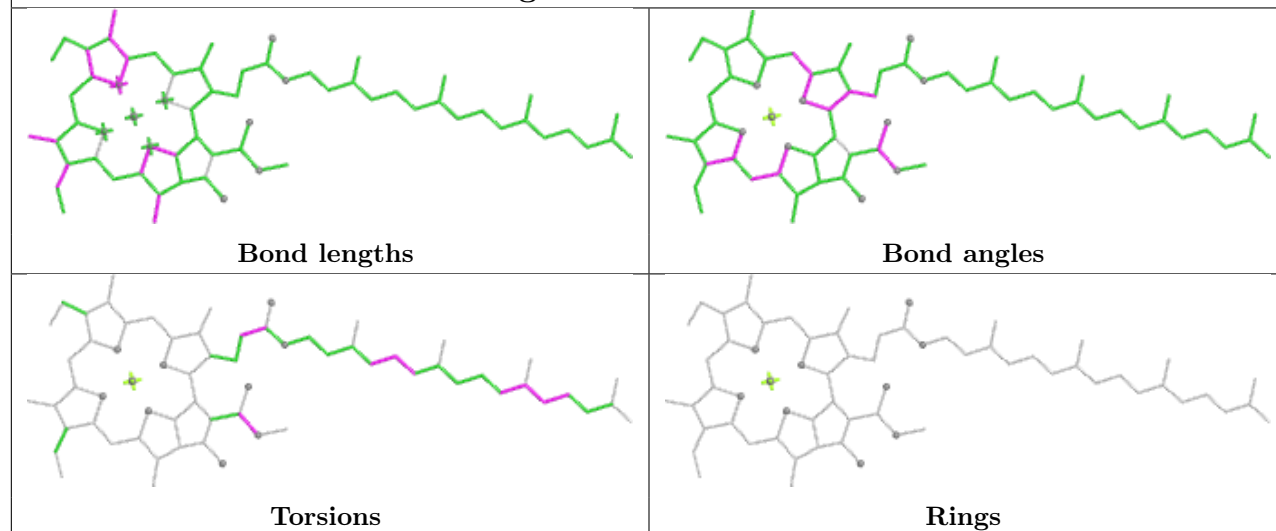
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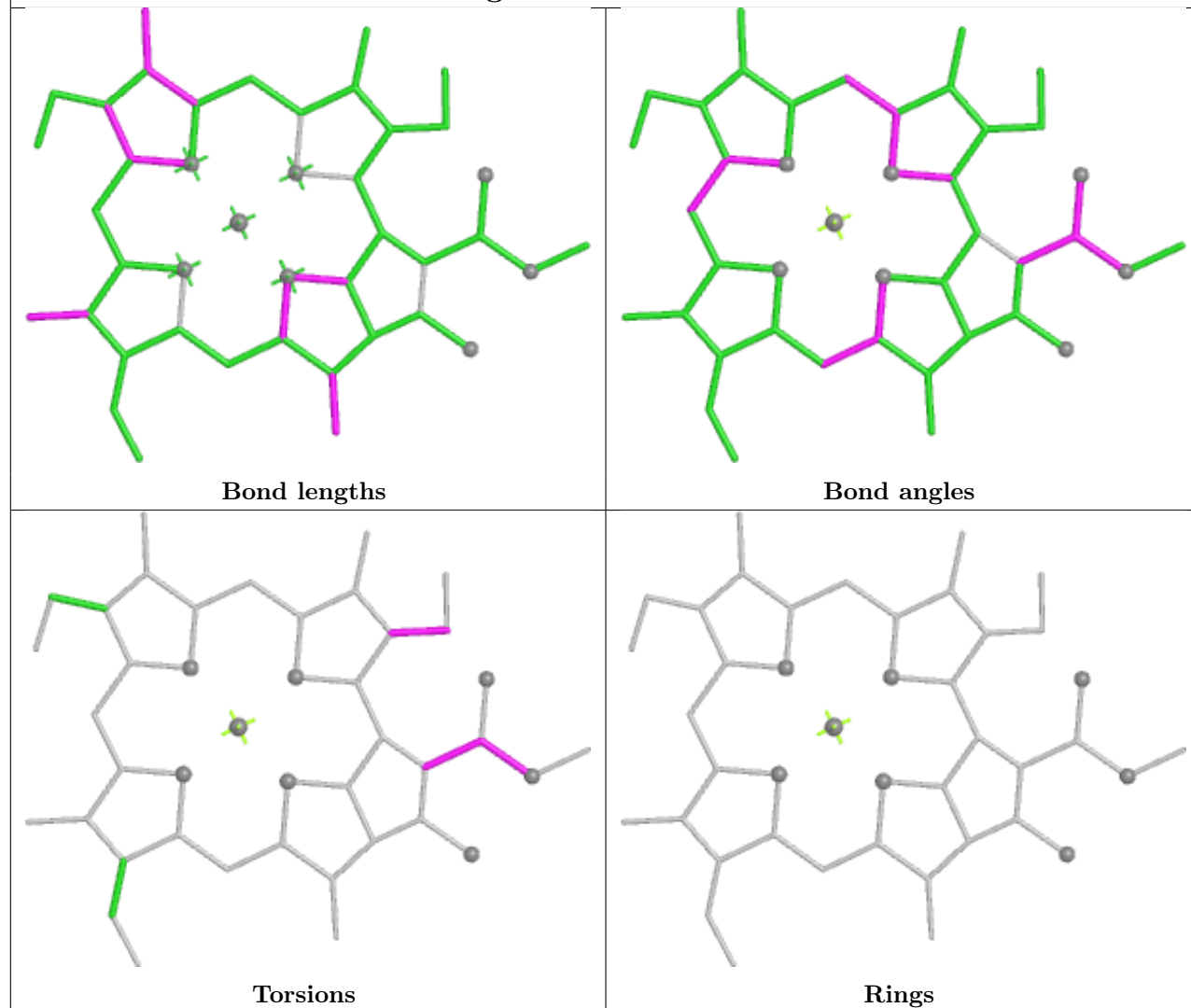
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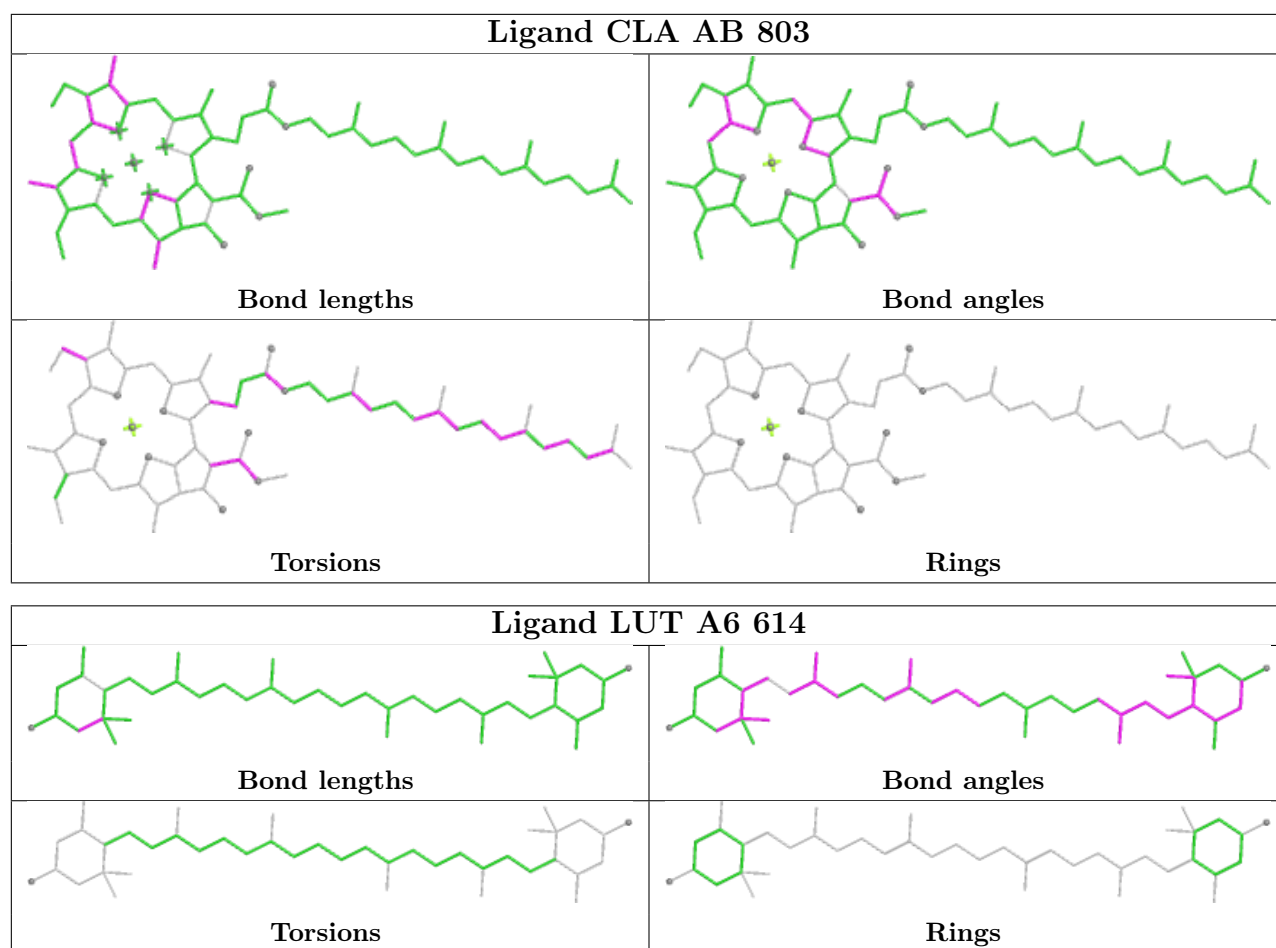


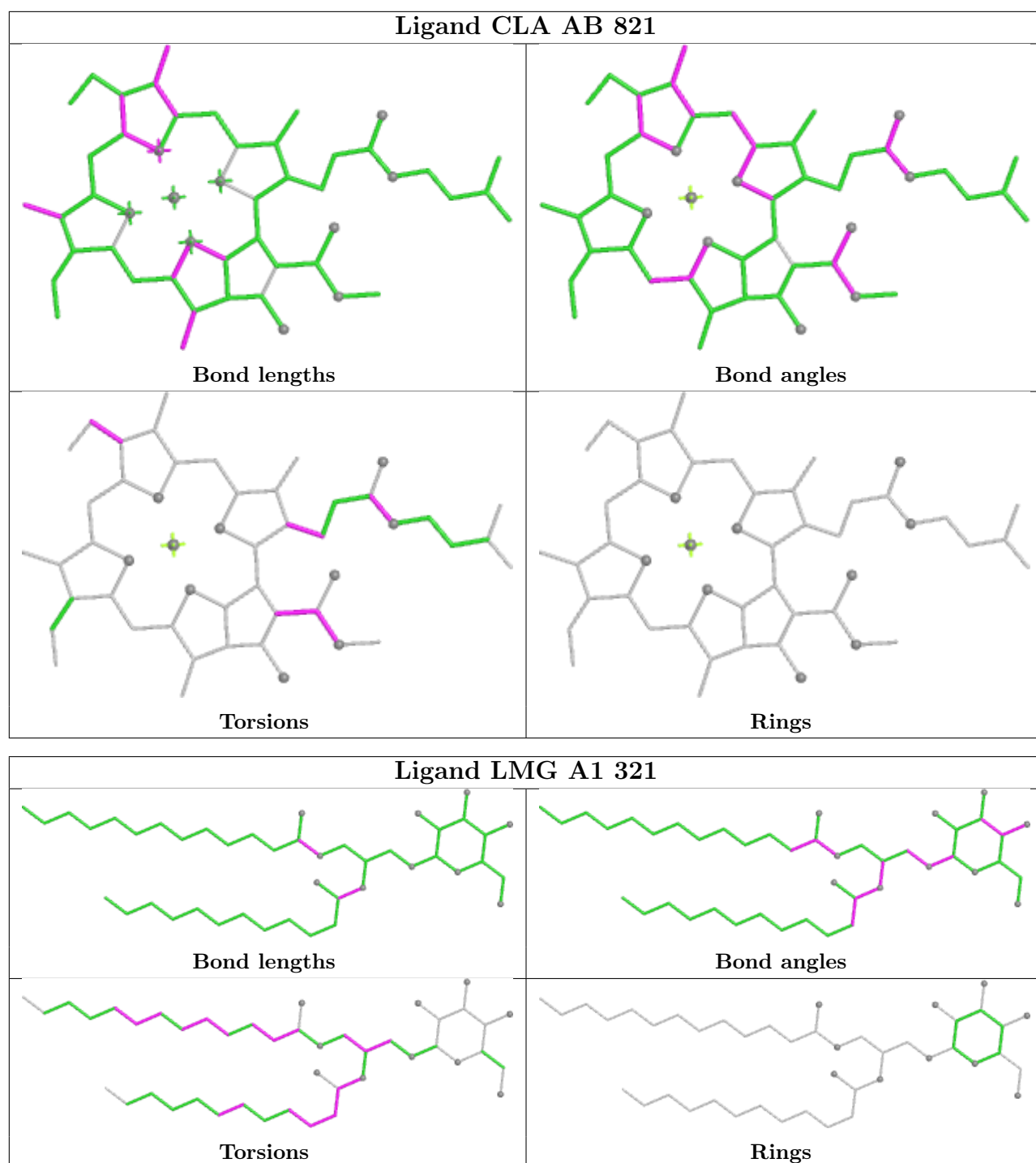
Ligand CLA AB 807



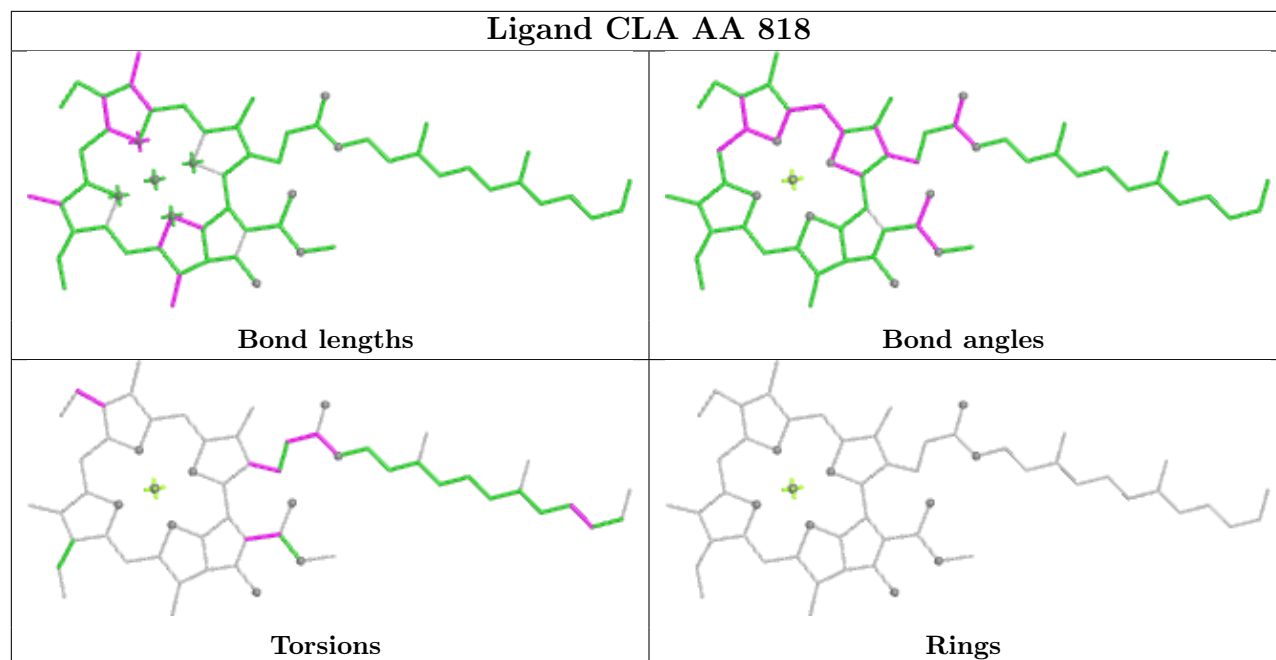
Ligand CLA AL 304



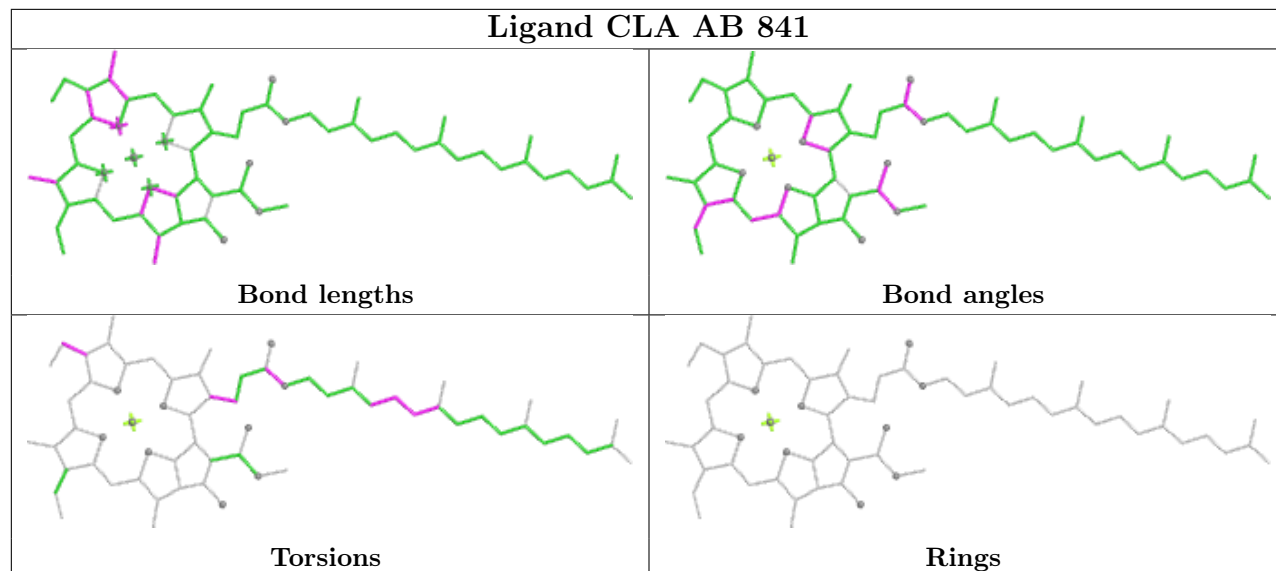




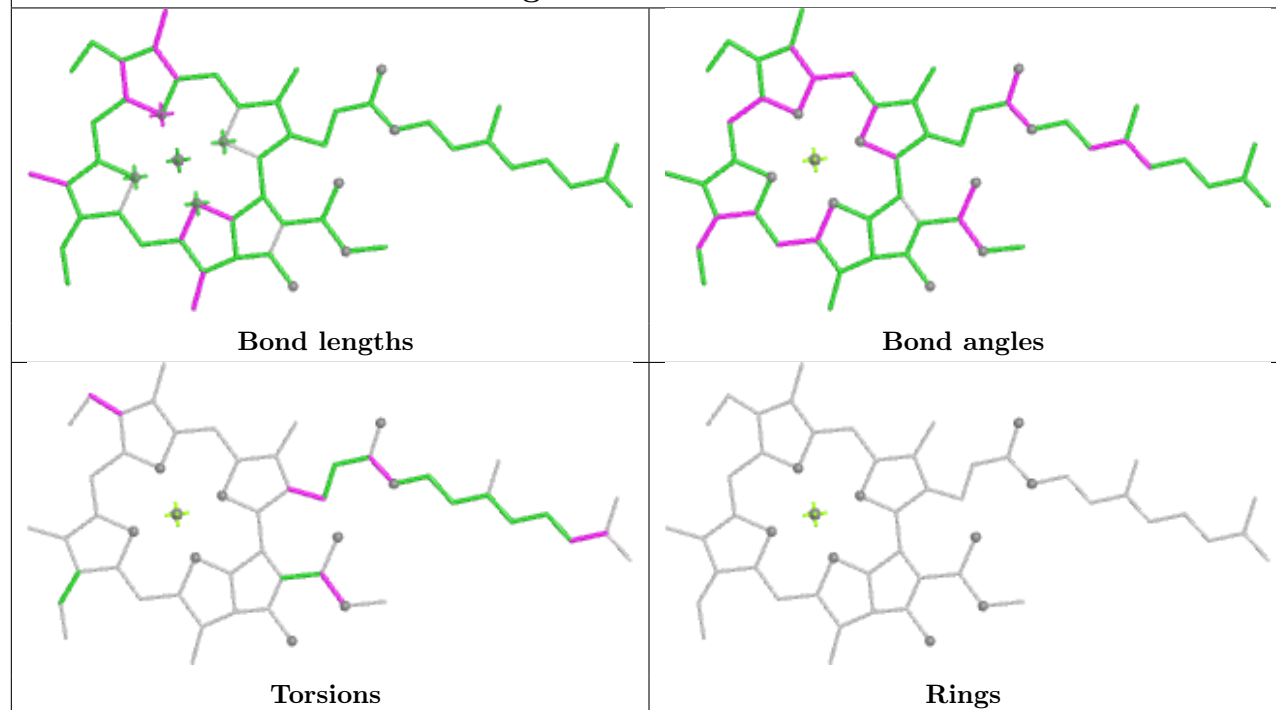
Ligand CLA AA 818



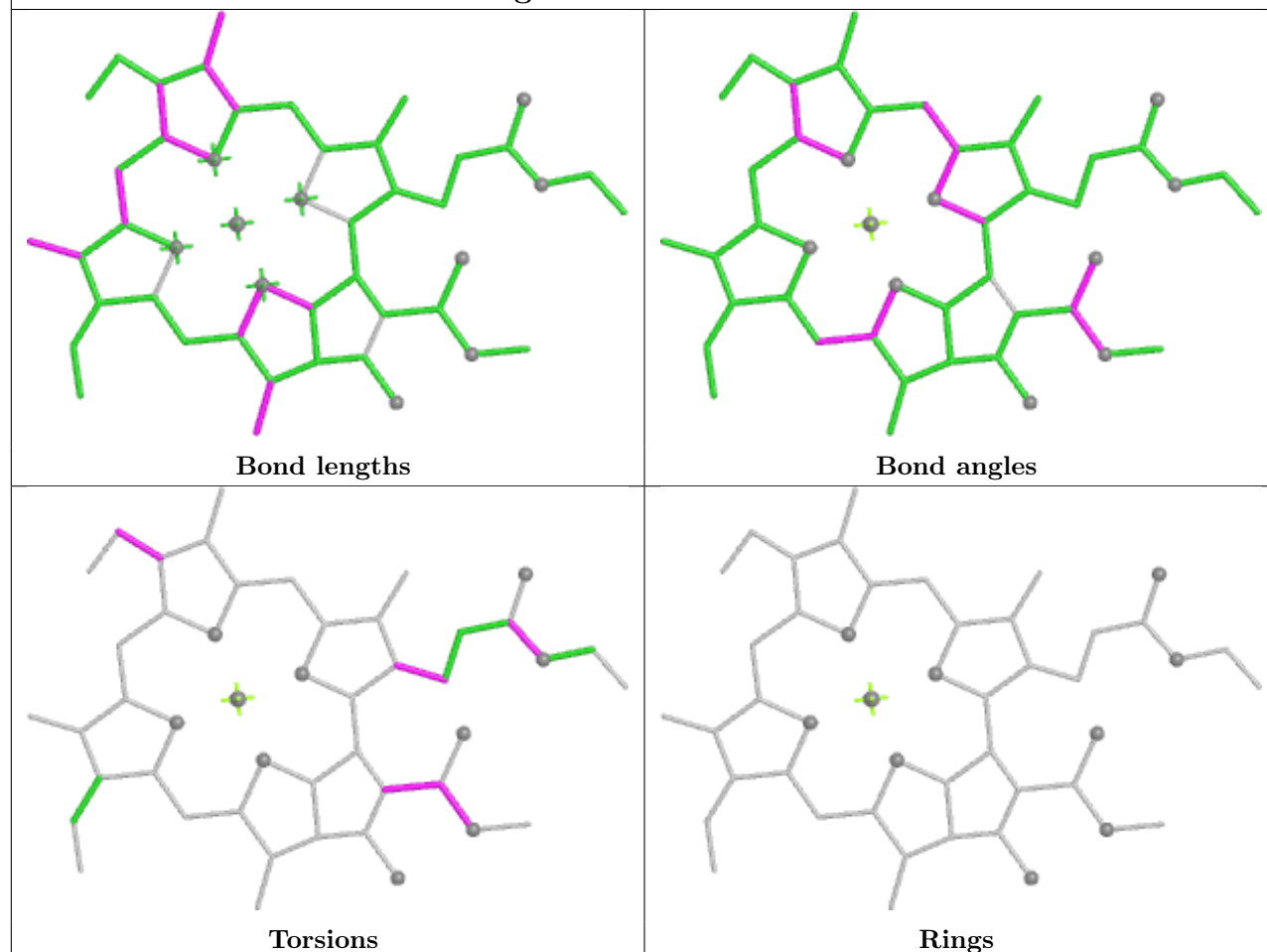
Ligand CLA AB 841



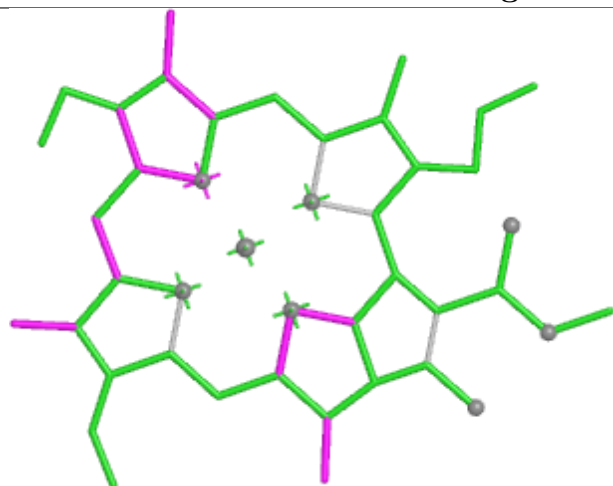
Ligand CLA A3 303



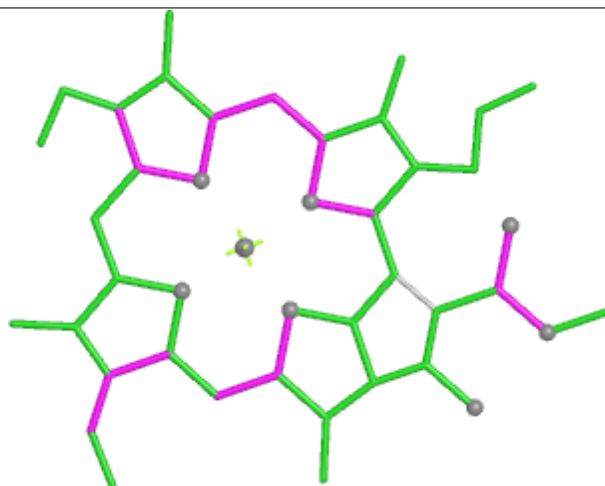
Ligand CLA AA 831



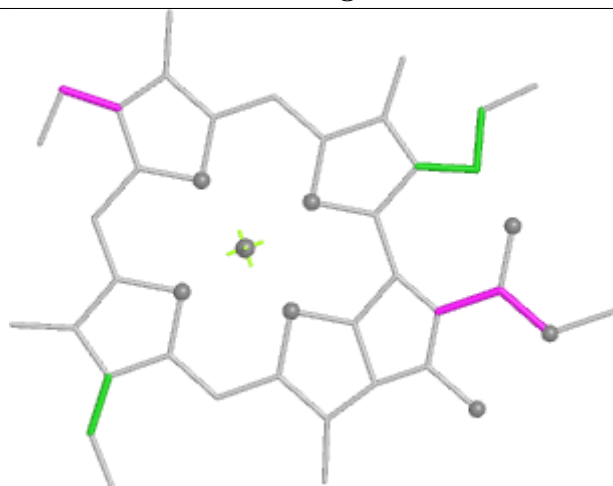
Ligand CLA AB 831



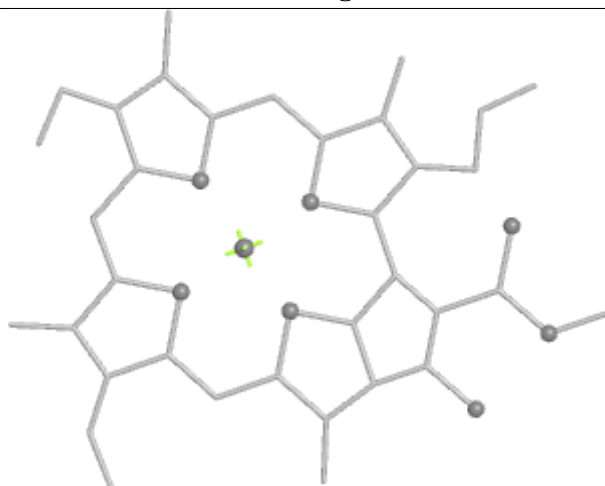
Bond lengths



Bond angles

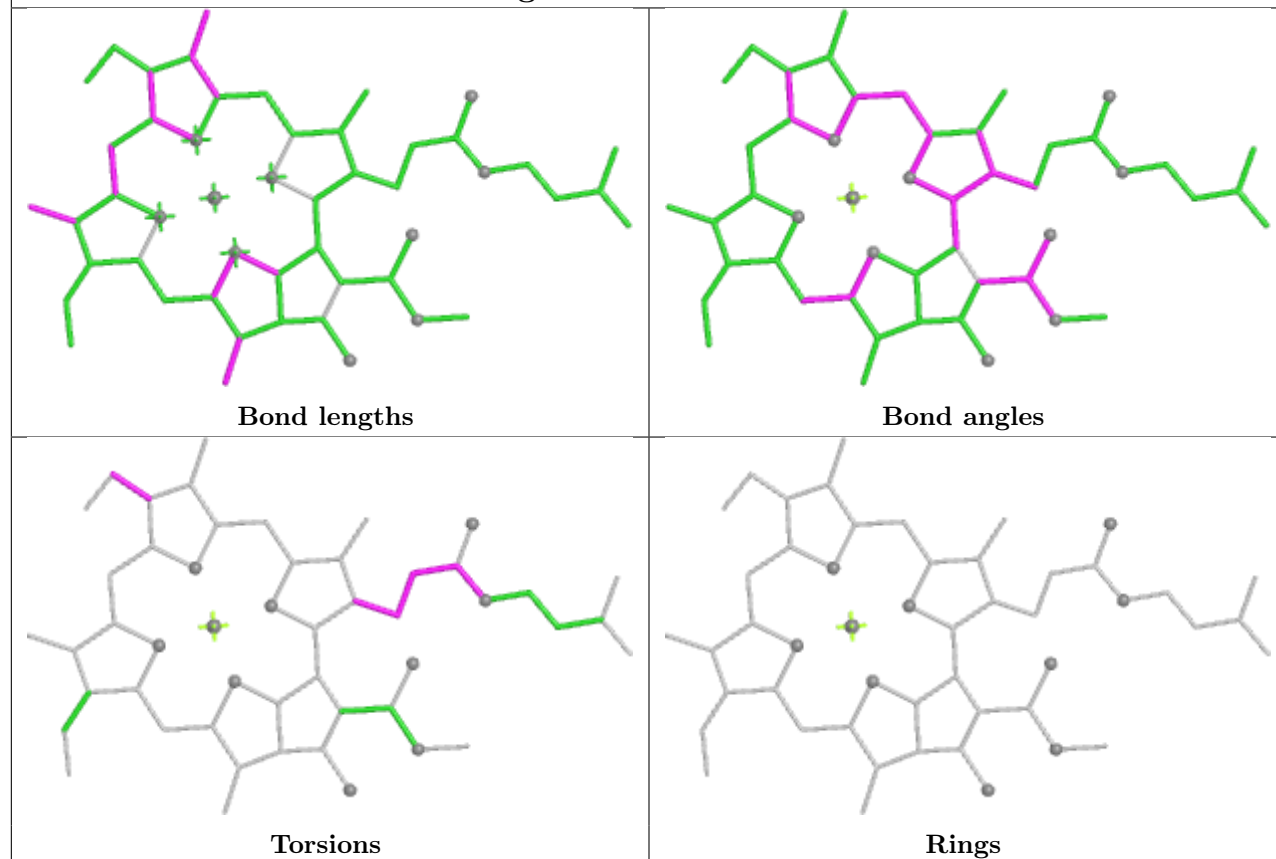


Torsions

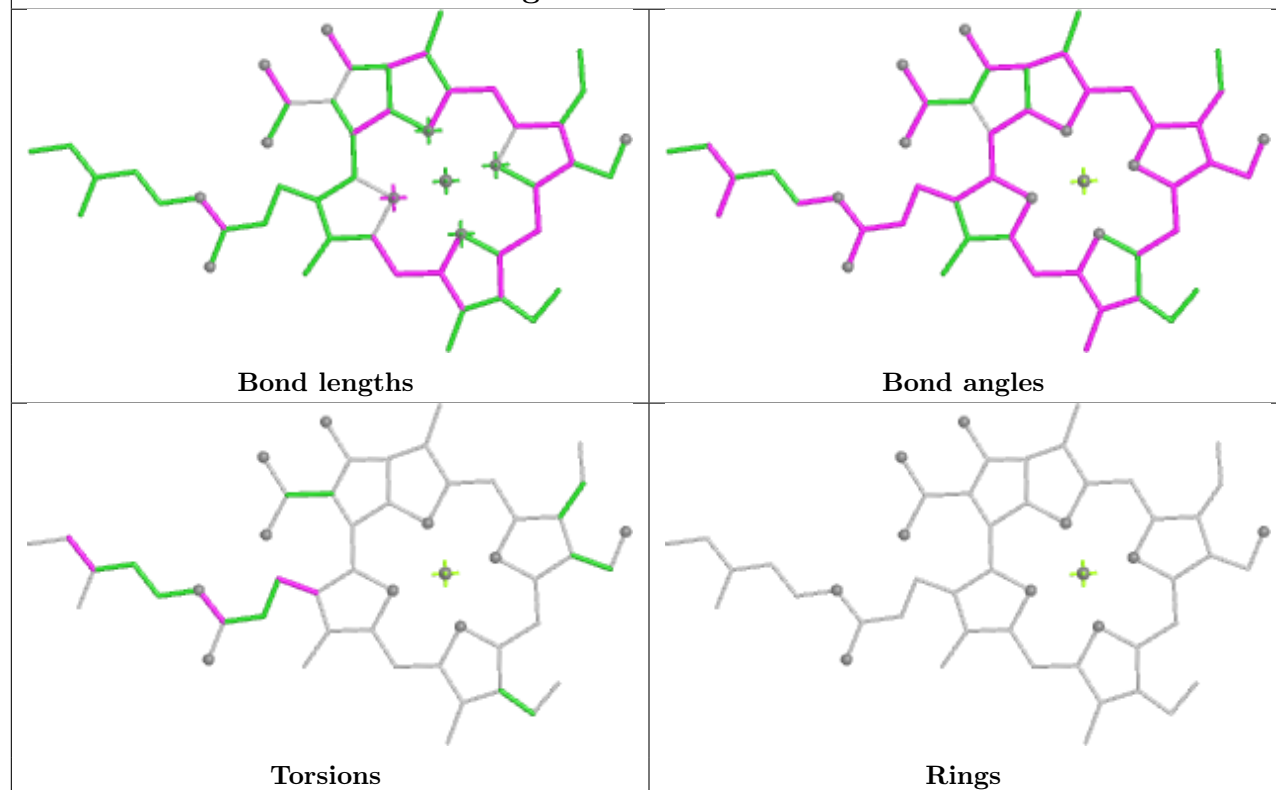


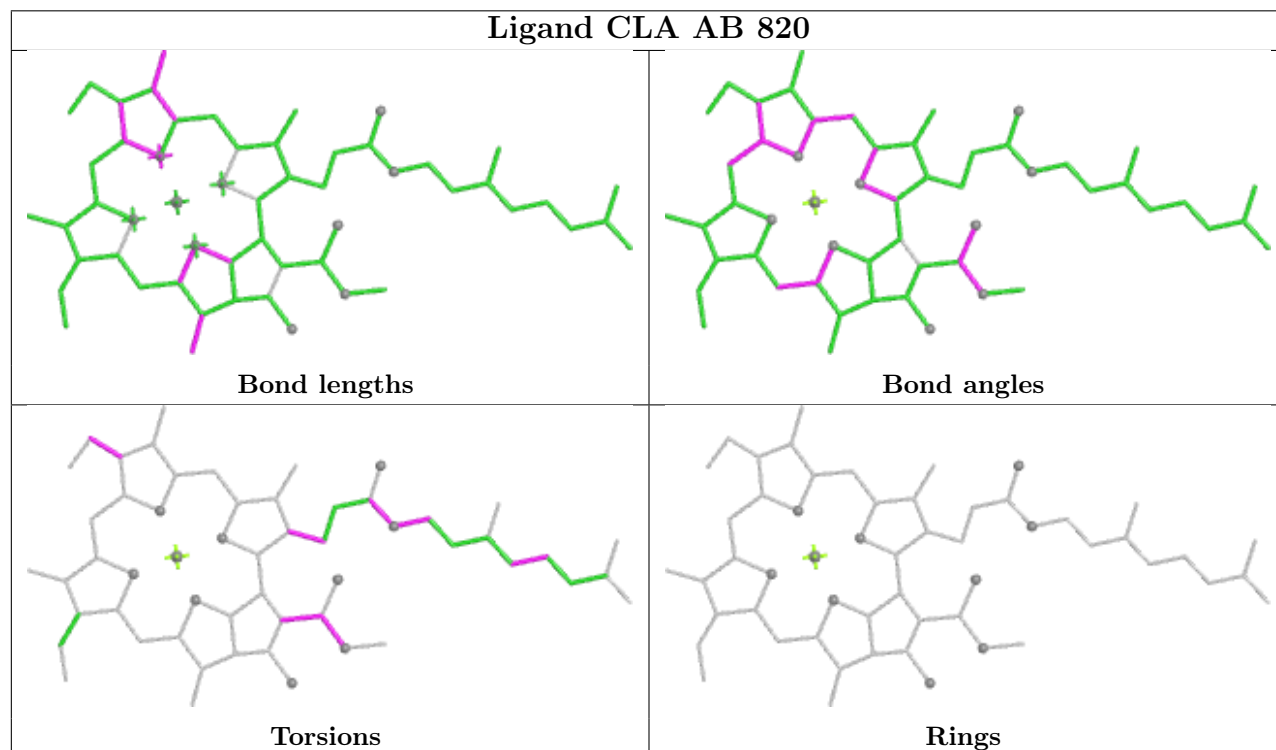
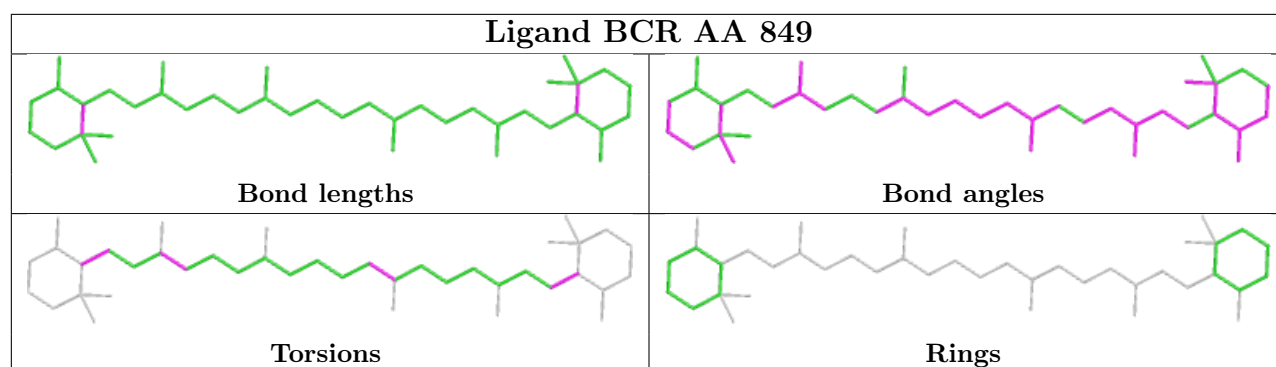
Rings

Ligand CLA AA 809

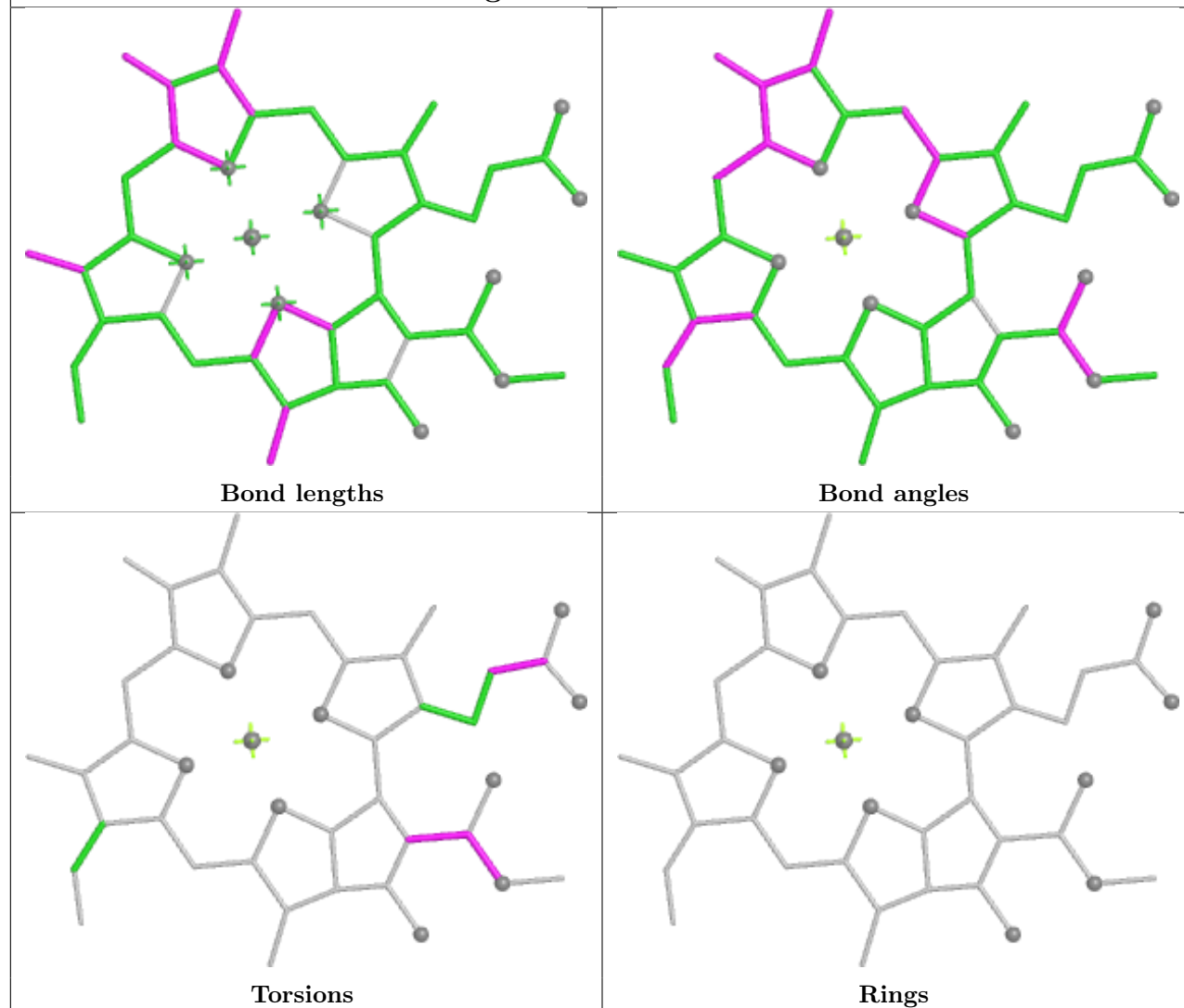


Ligand CHL A1 303

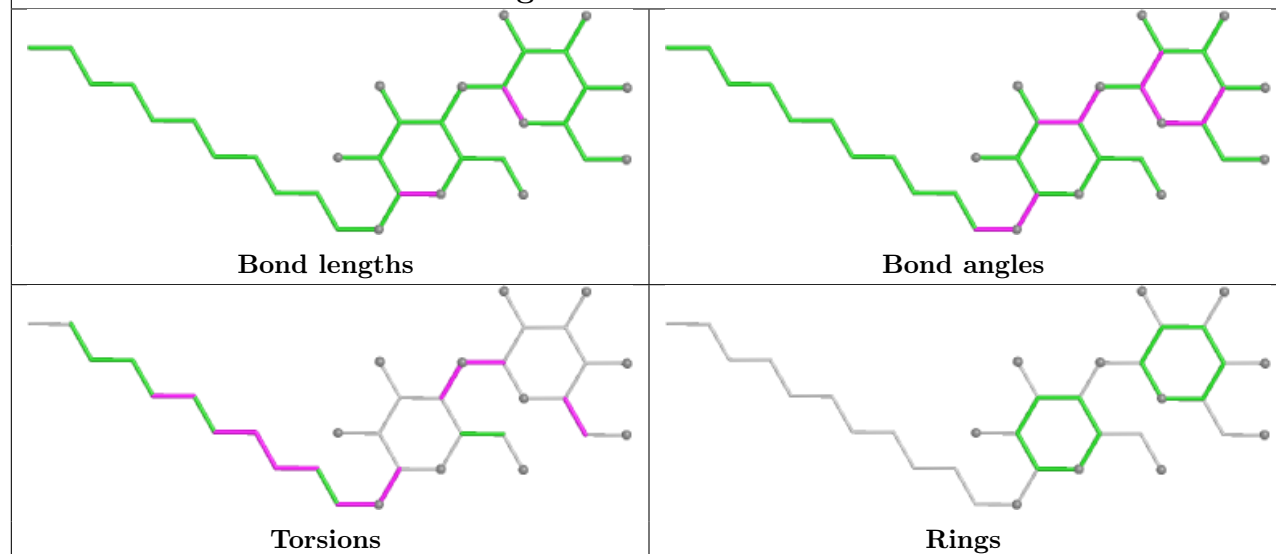




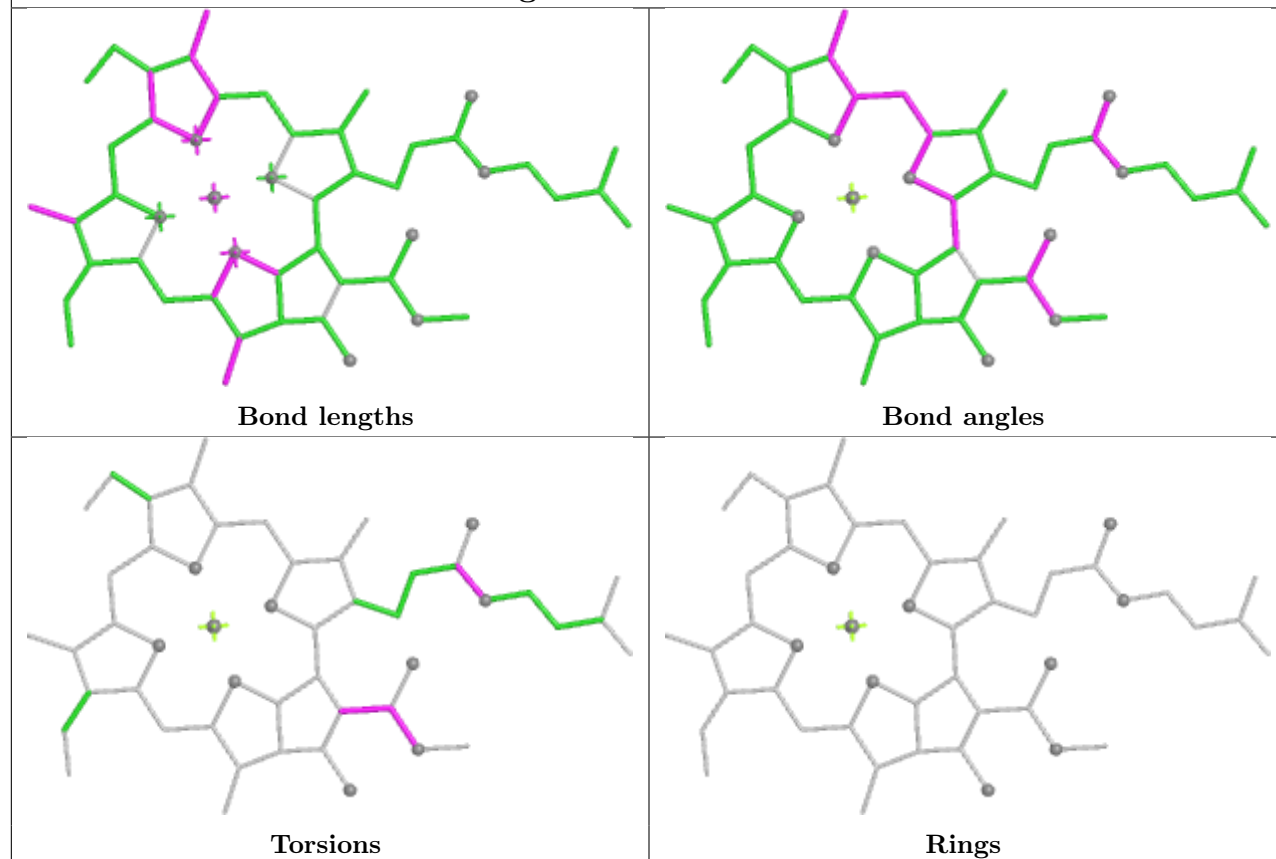
Ligand CLA A4 302



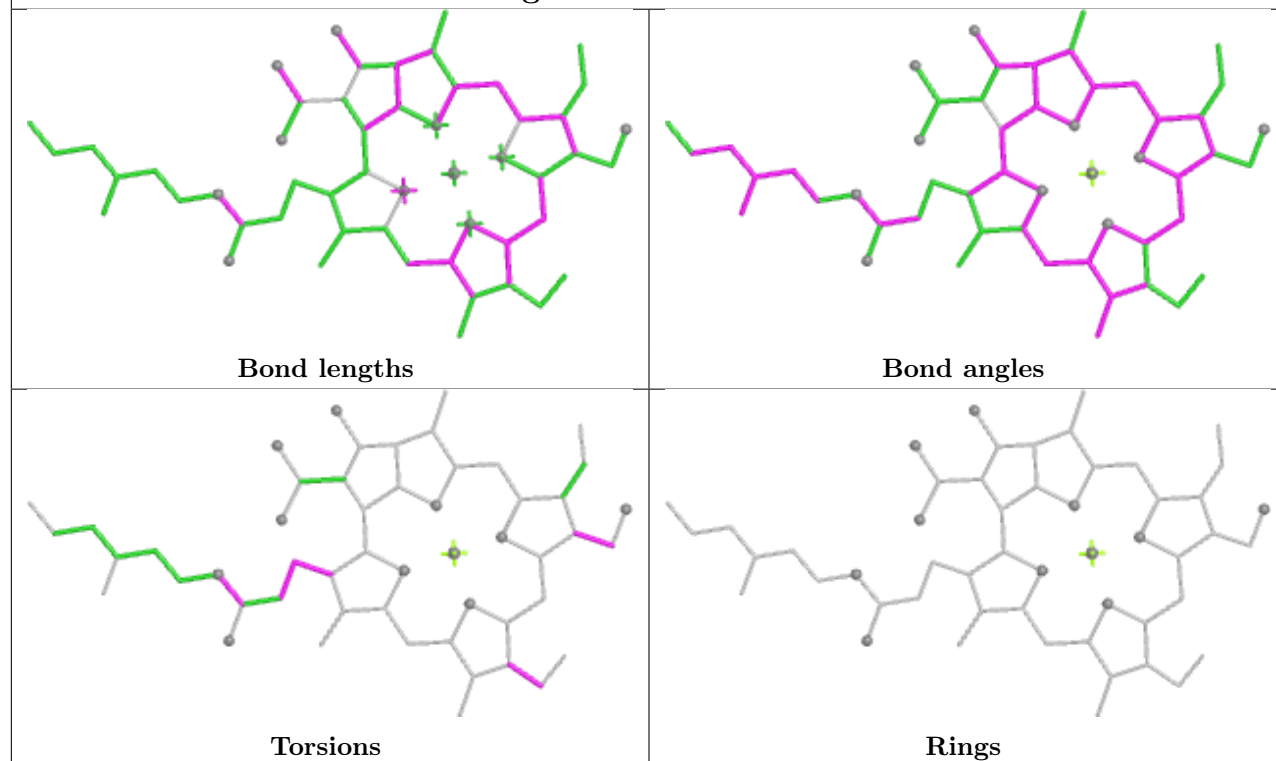
Ligand LMU AL 301

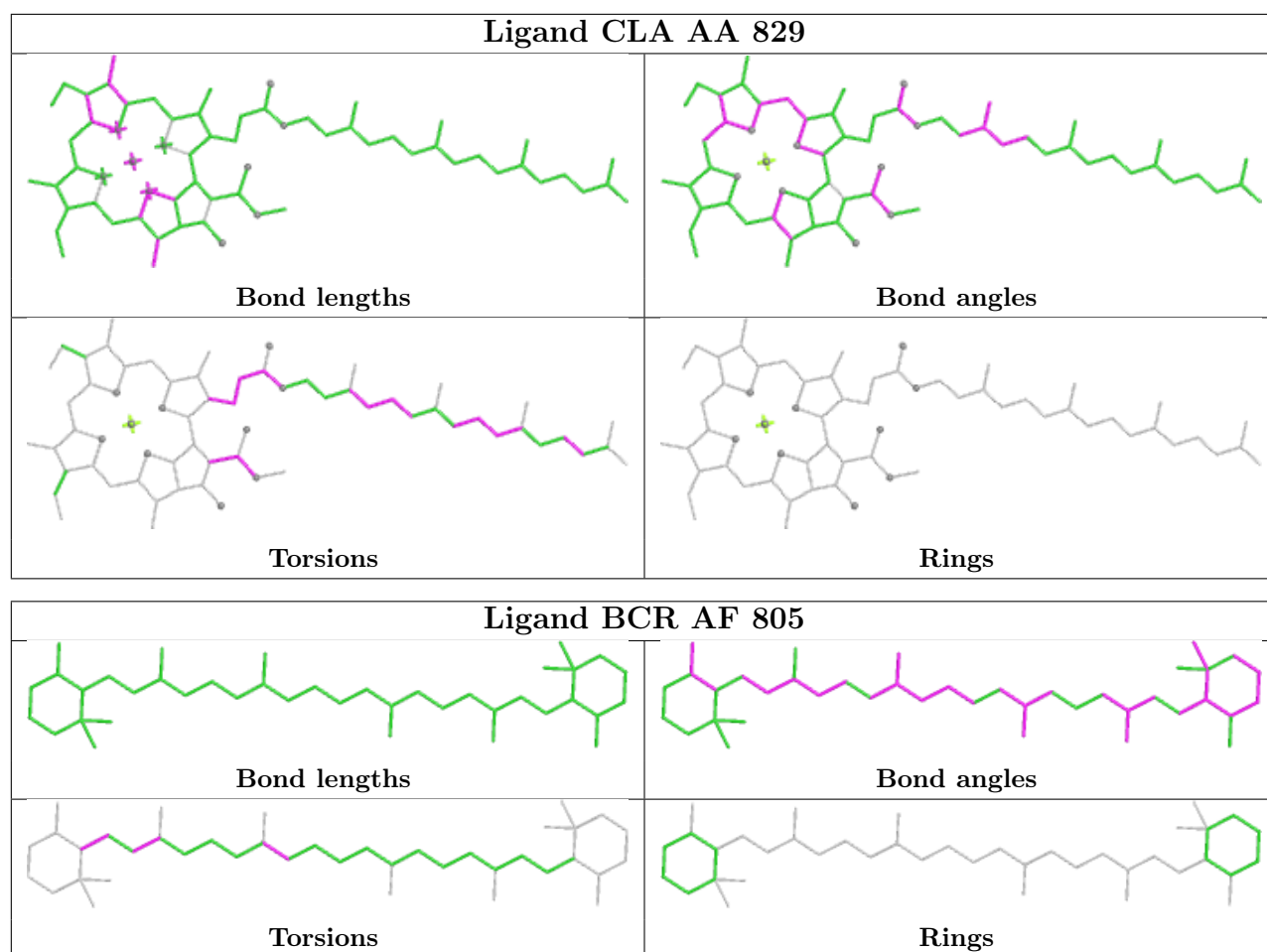


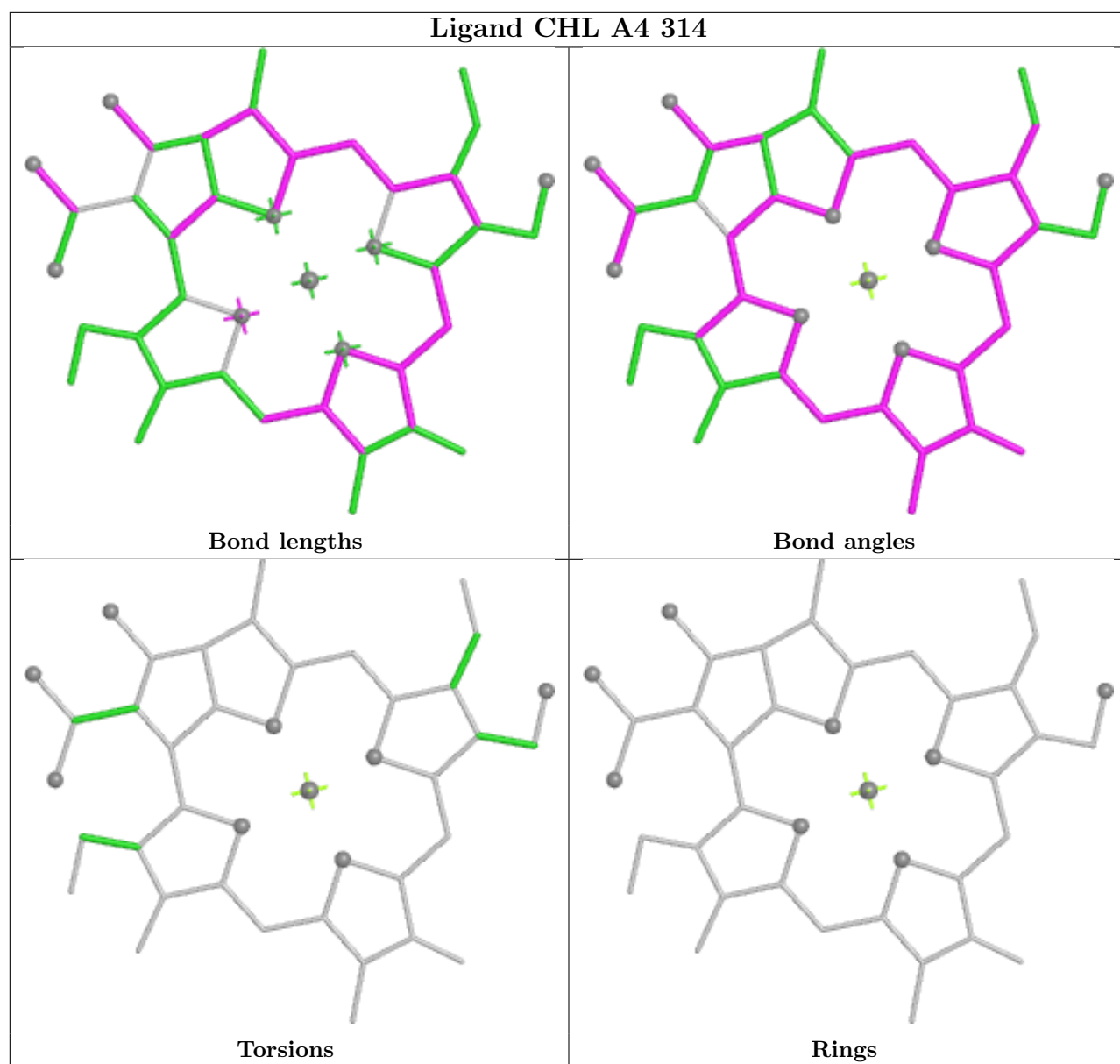
Ligand CLA AB 837

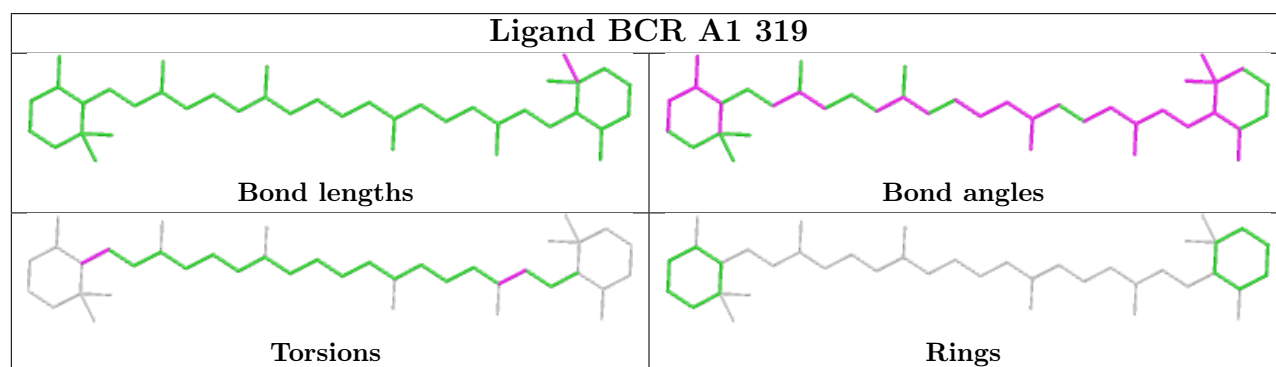
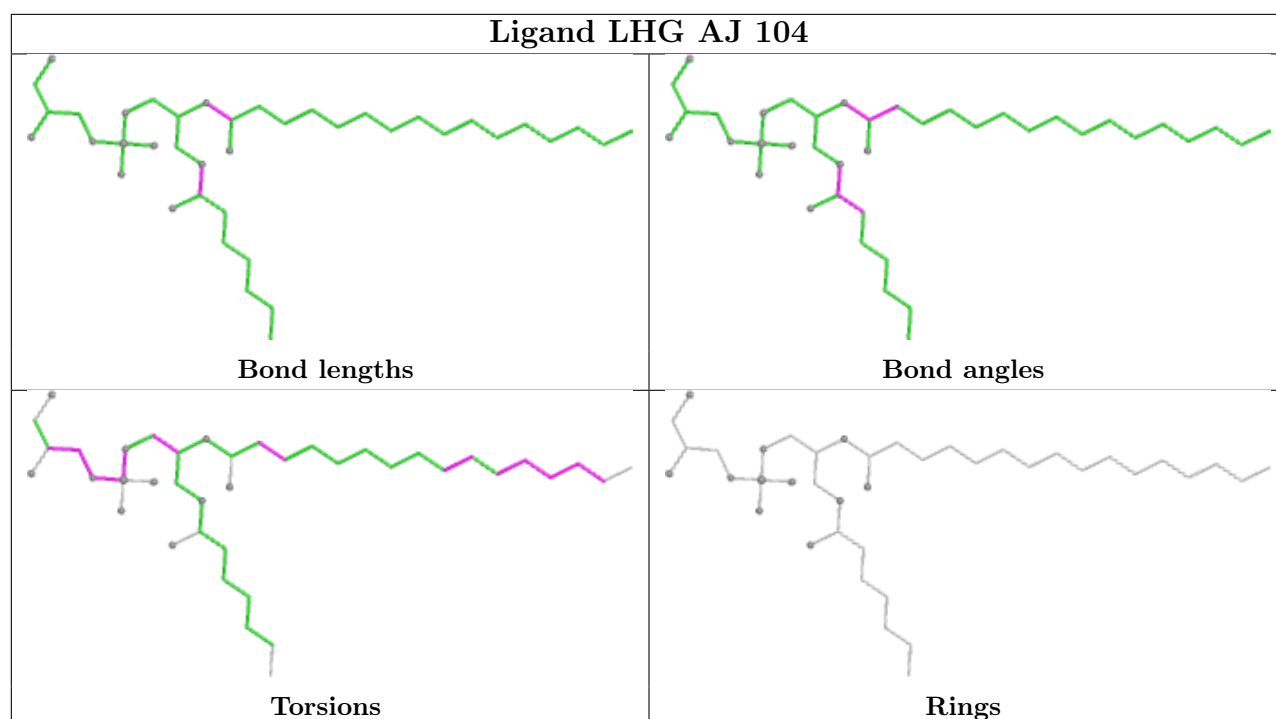


Ligand CHL A3 320

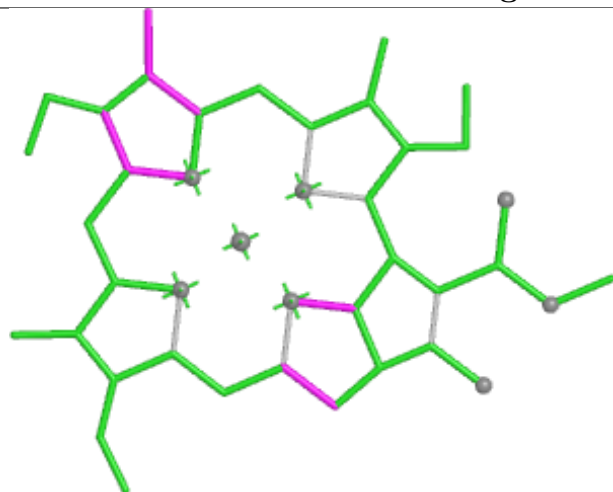








Ligand CLA AA 815



Bond lengths



Bond angles

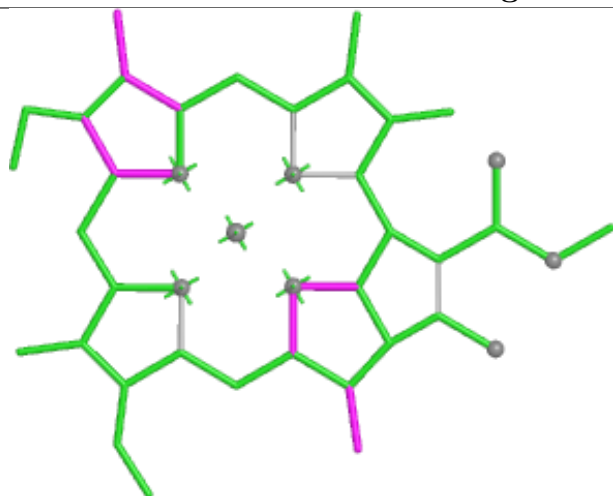


Torsions



Rings

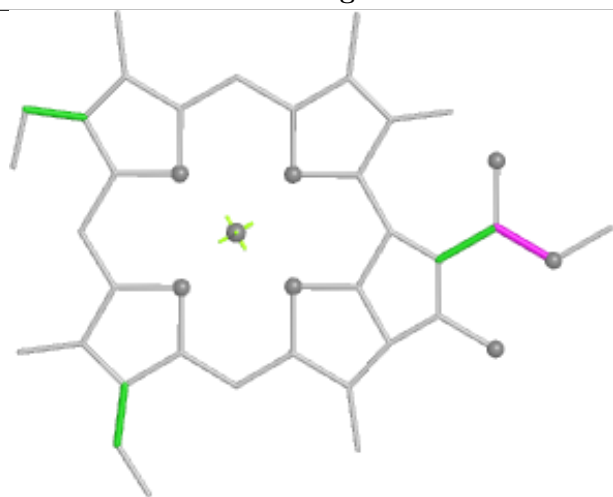
Ligand CLA AB 805



Bond lengths



Bond angles

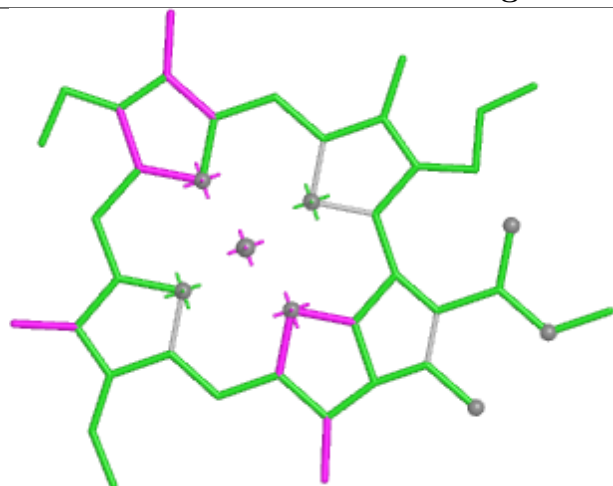


Torsions

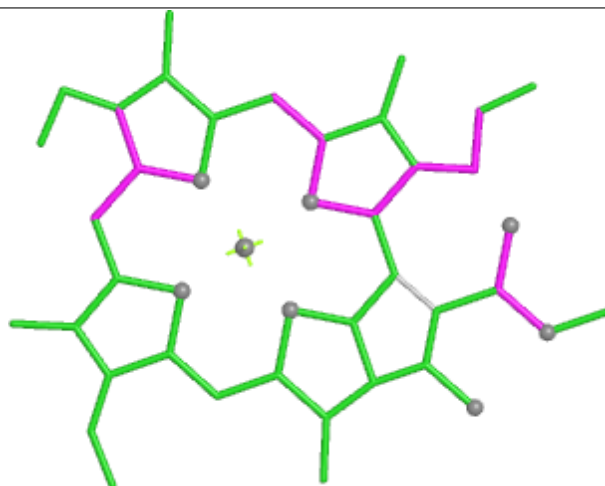


Rings

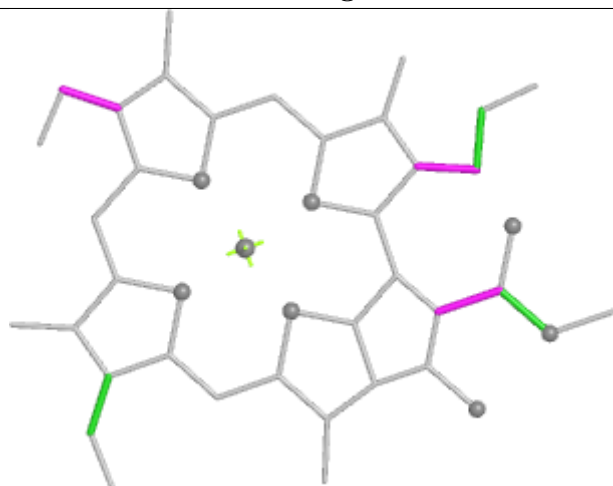
Ligand CLA AB 824



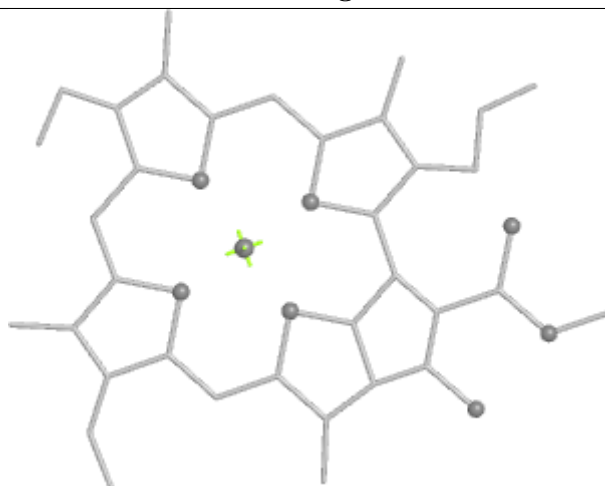
Bond lengths



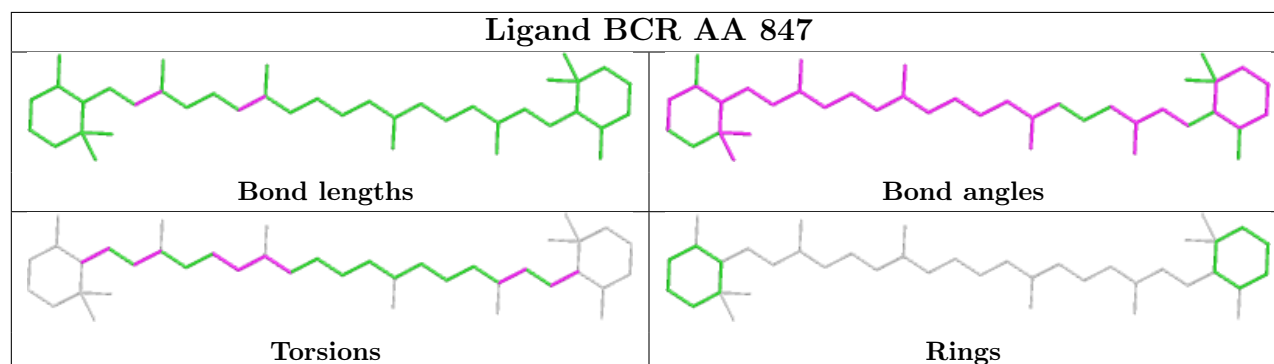
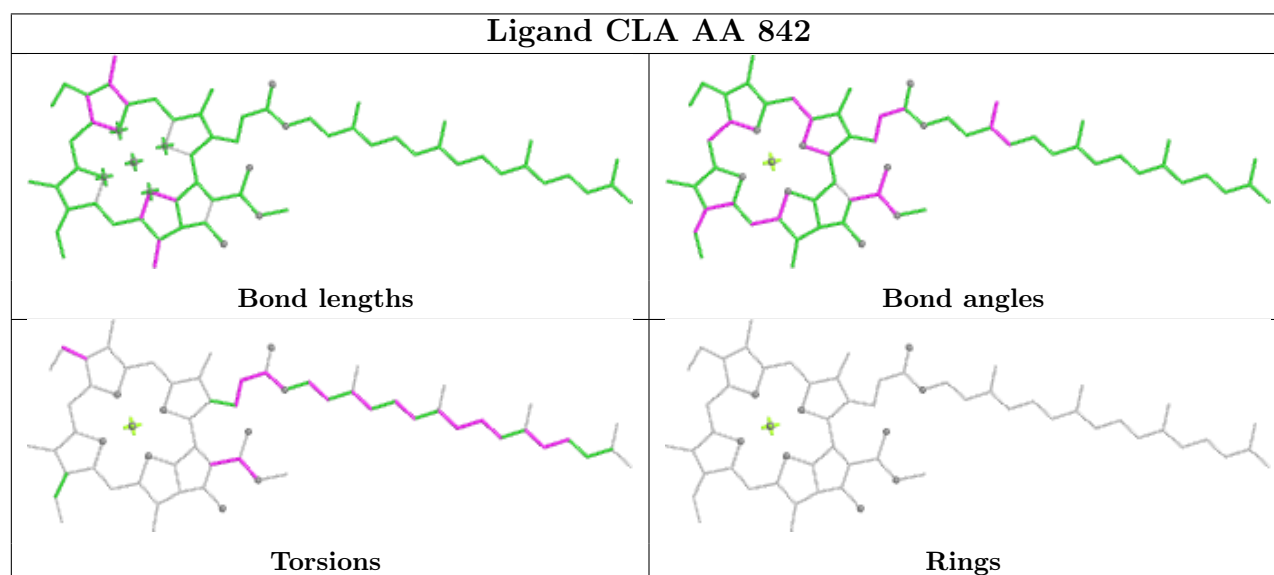
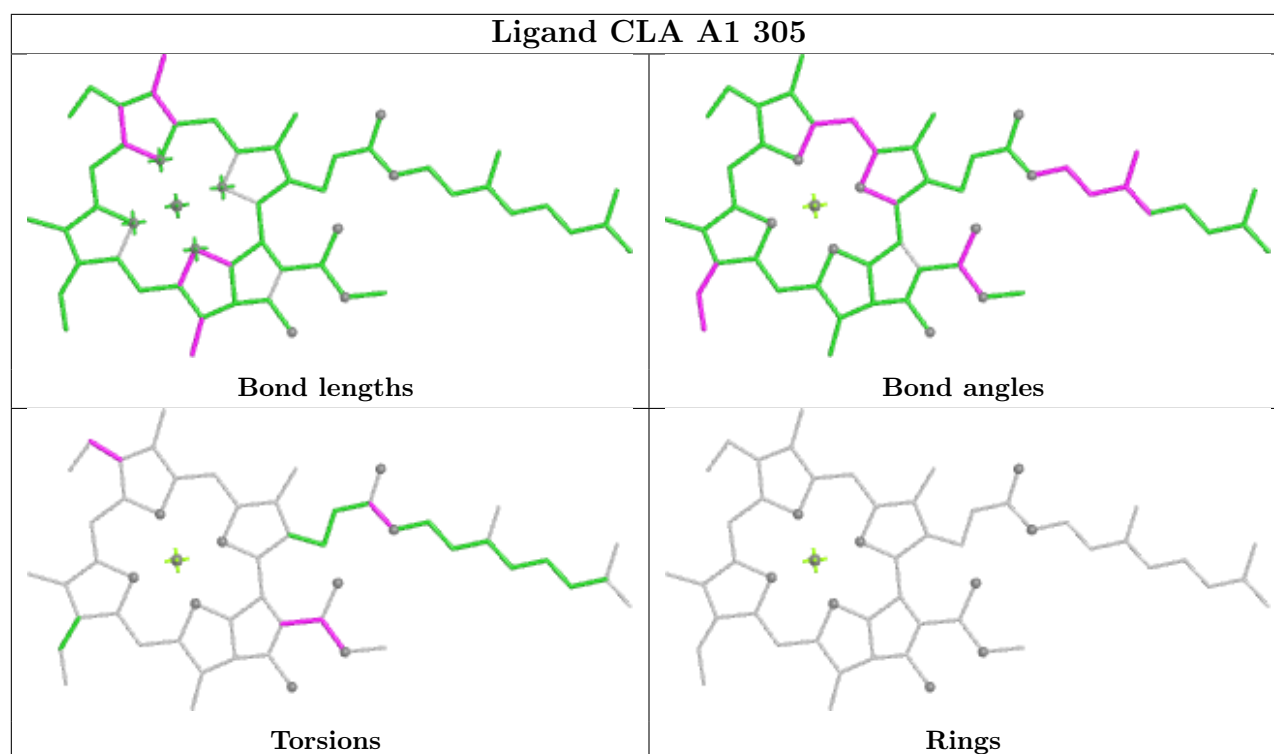
Bond angles

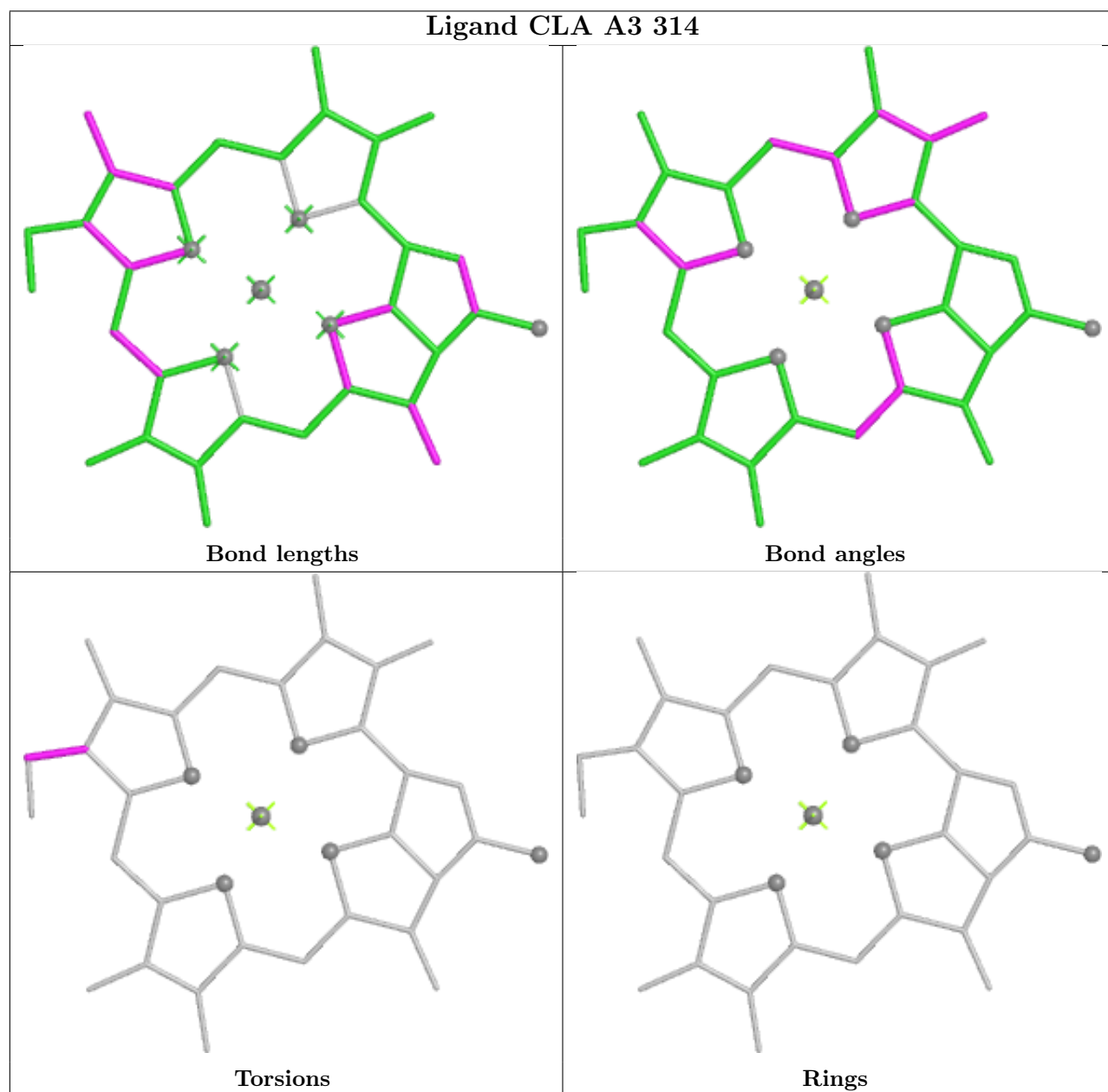
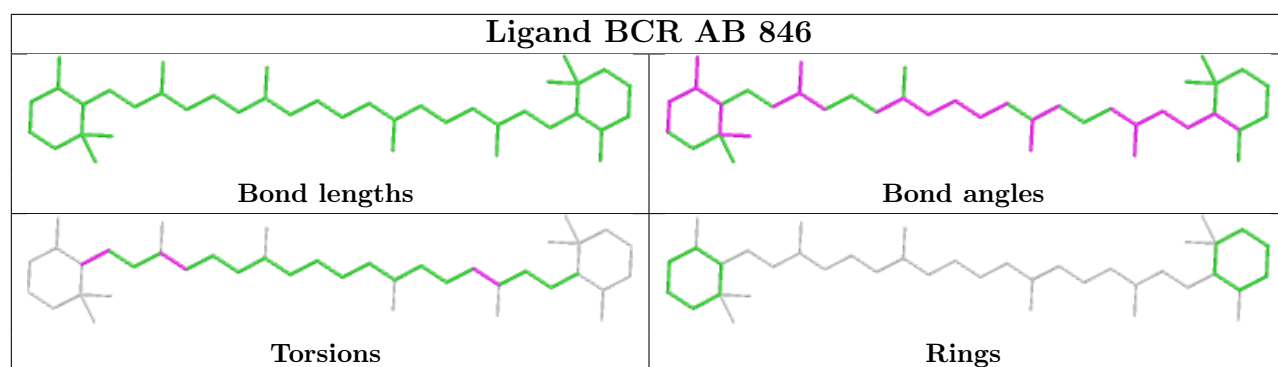


Torsions

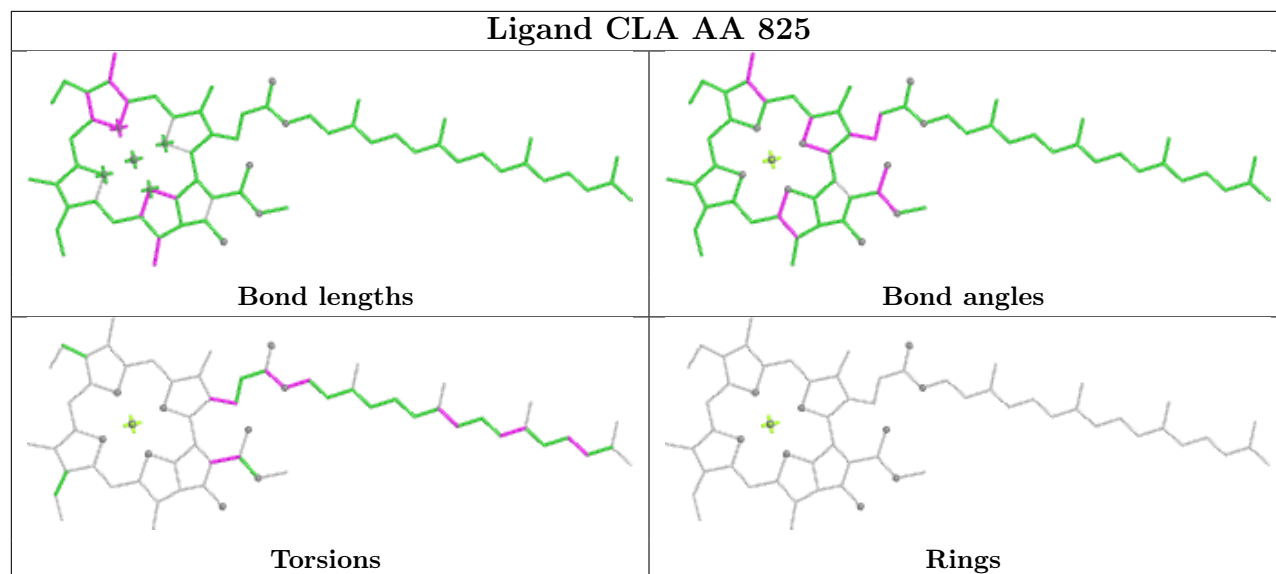


Rings

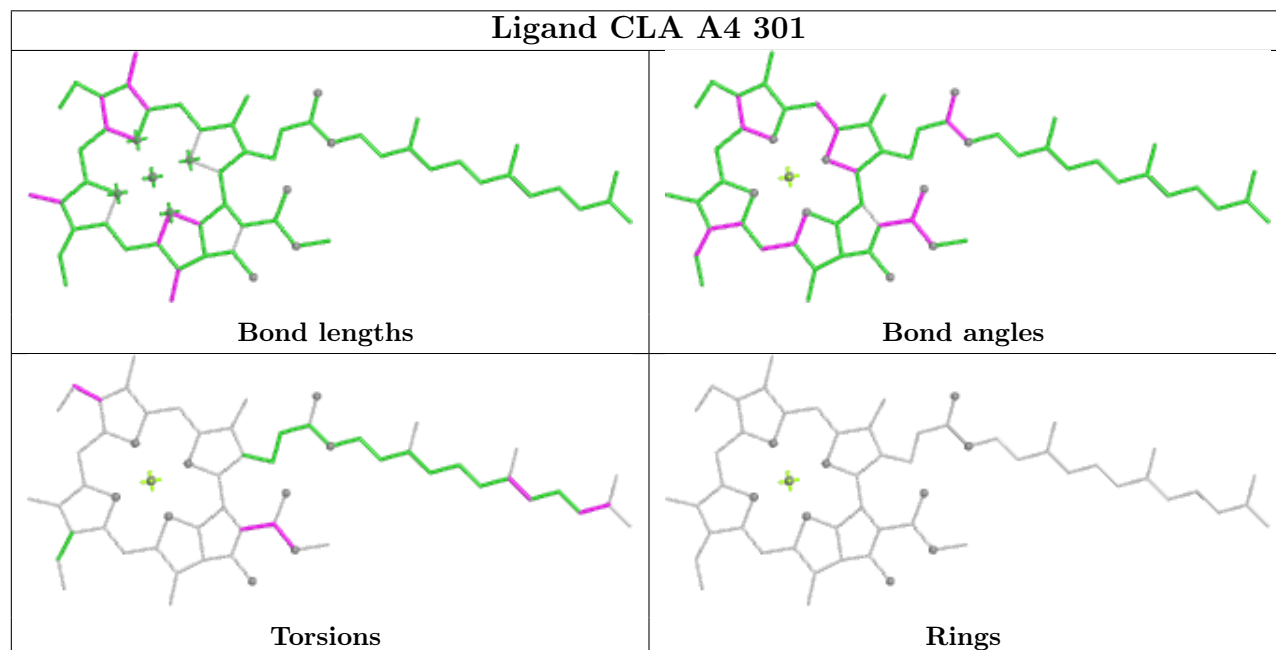




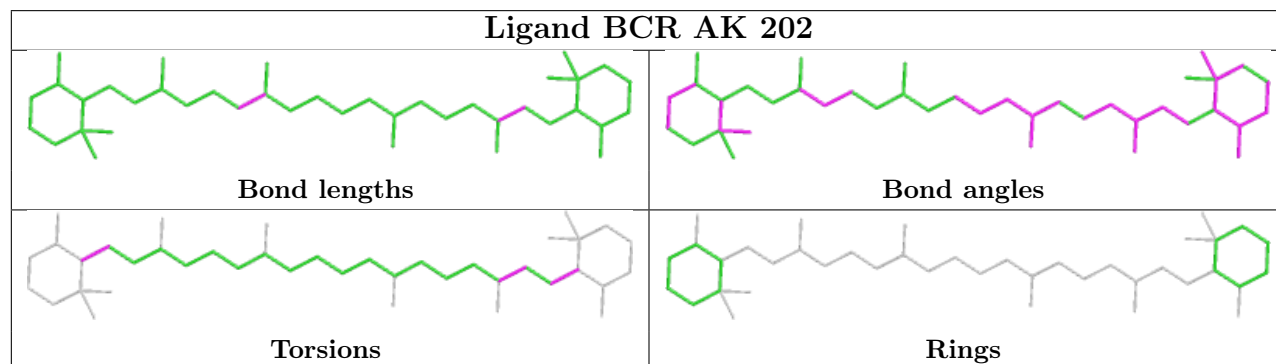
Ligand CLA AA 825



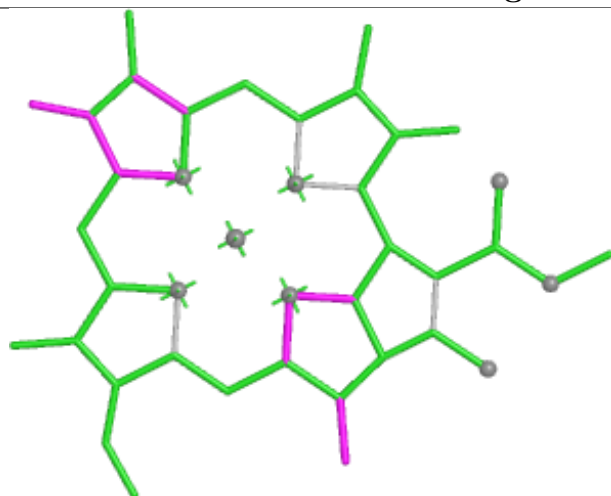
Ligand CLA A4 301



Ligand BCR AK 202



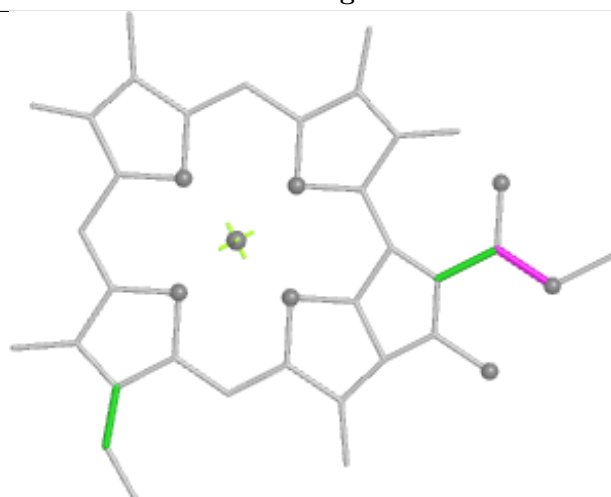
Ligand CLA A1 310



Bond lengths



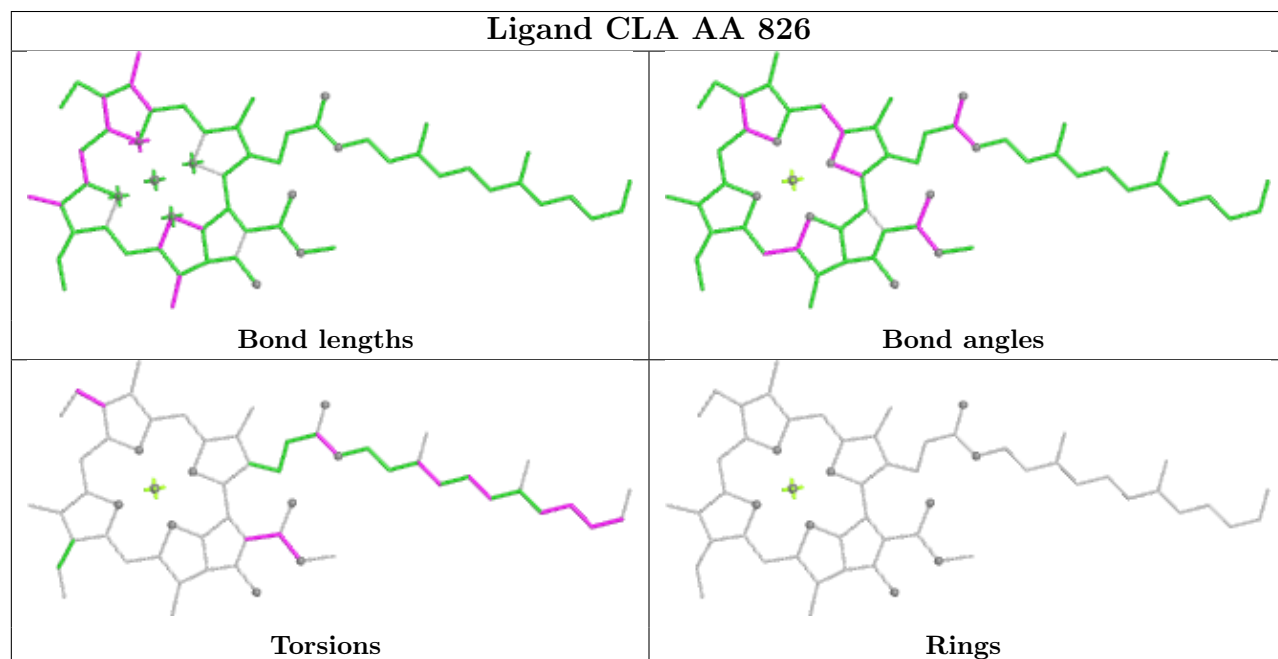
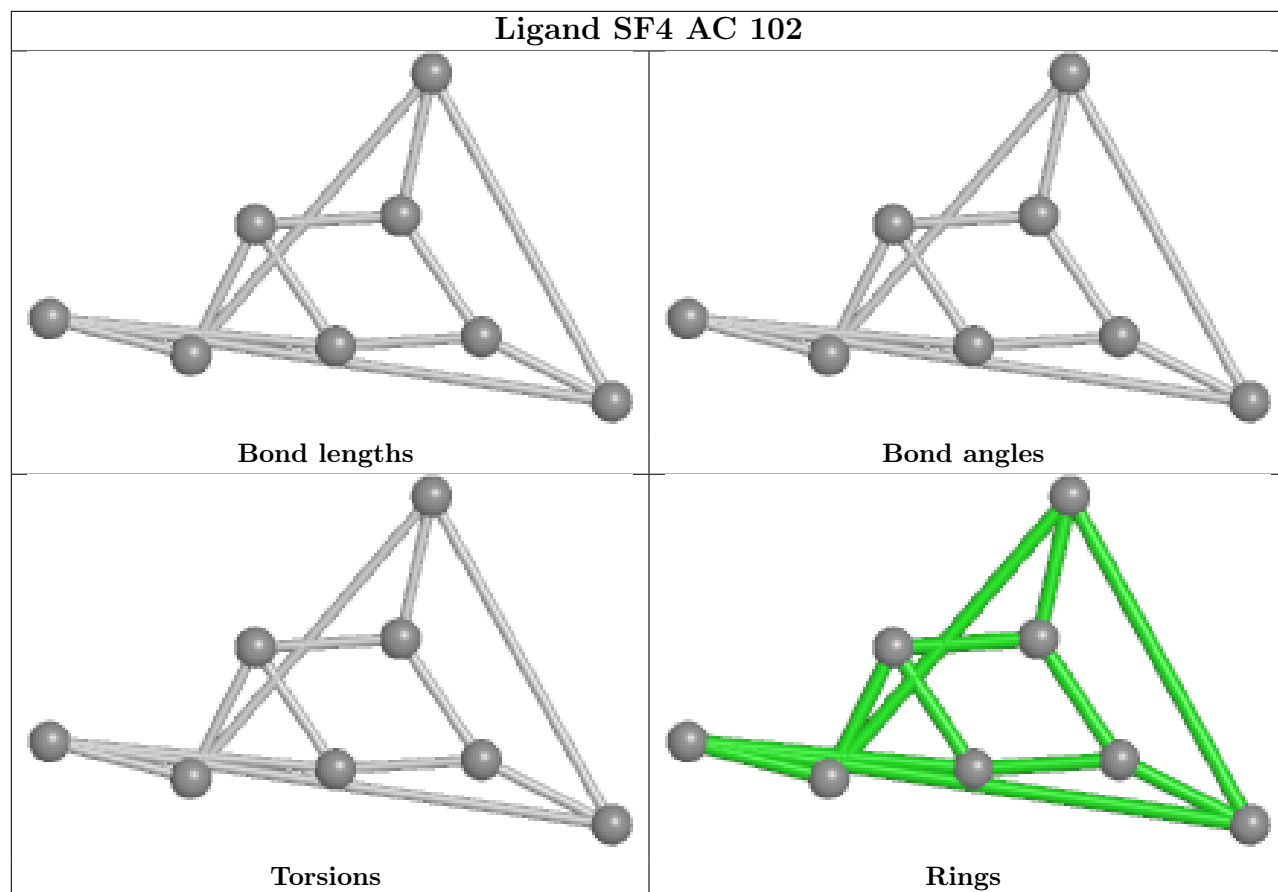
Bond angles

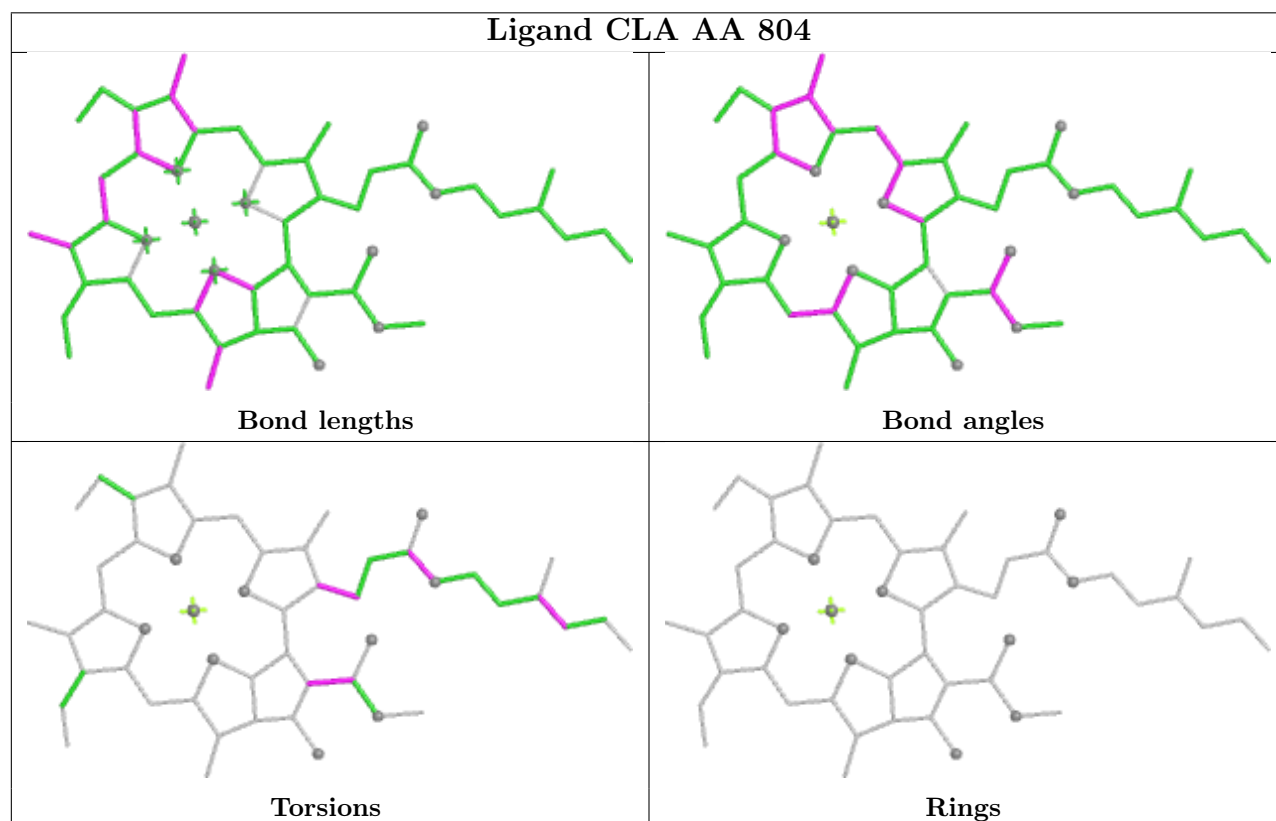
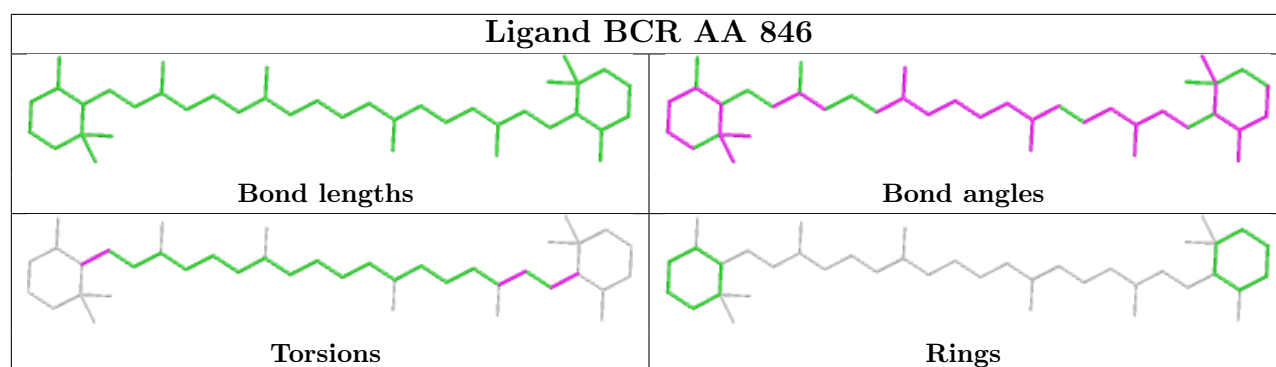


Torsions

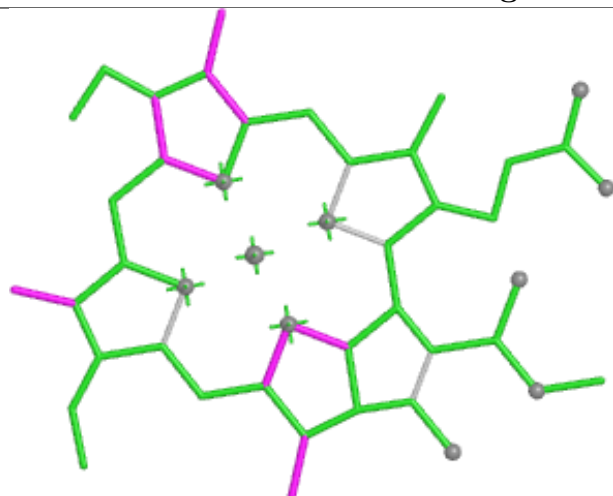


Rings

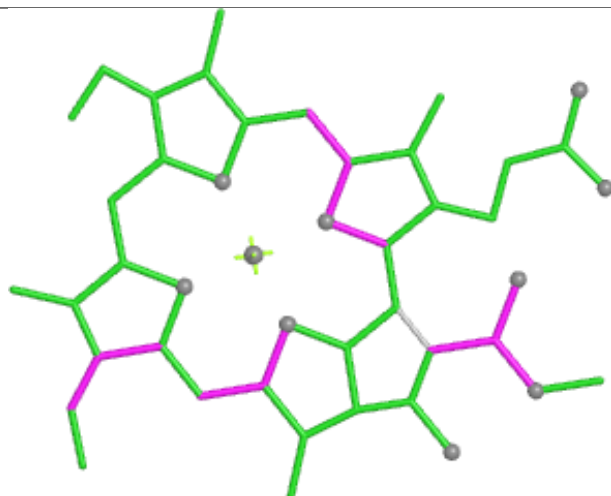




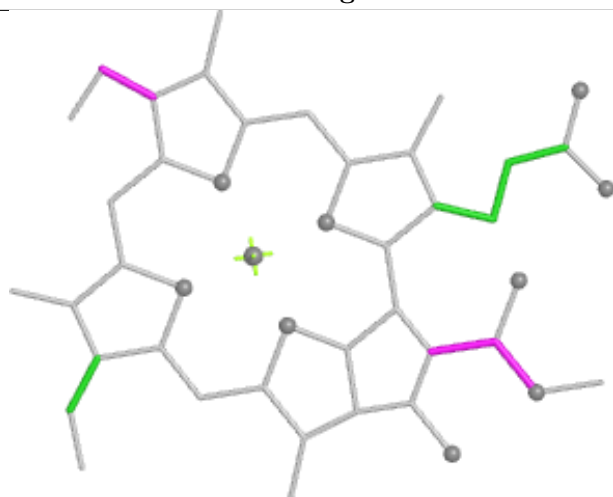
Ligand CLA AA 816



Bond lengths



Bond angles

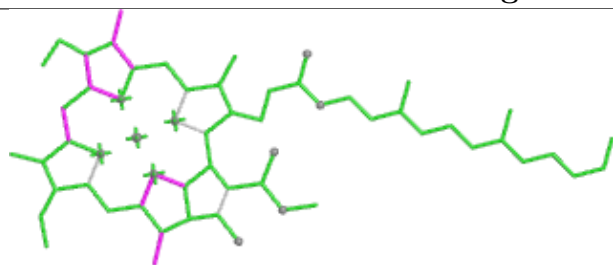


Torsions

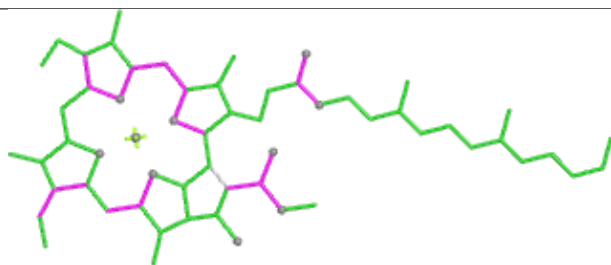


Rings

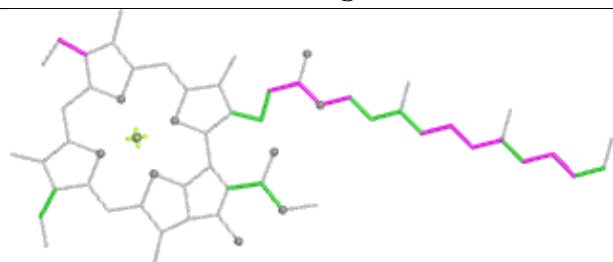
Ligand CLA AB 818



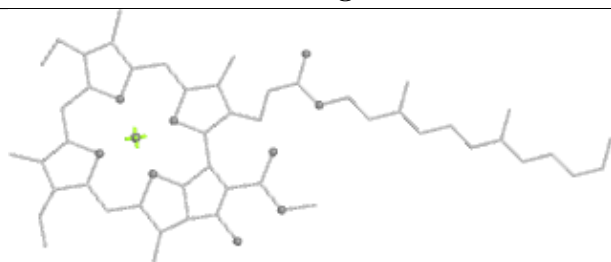
Bond lengths



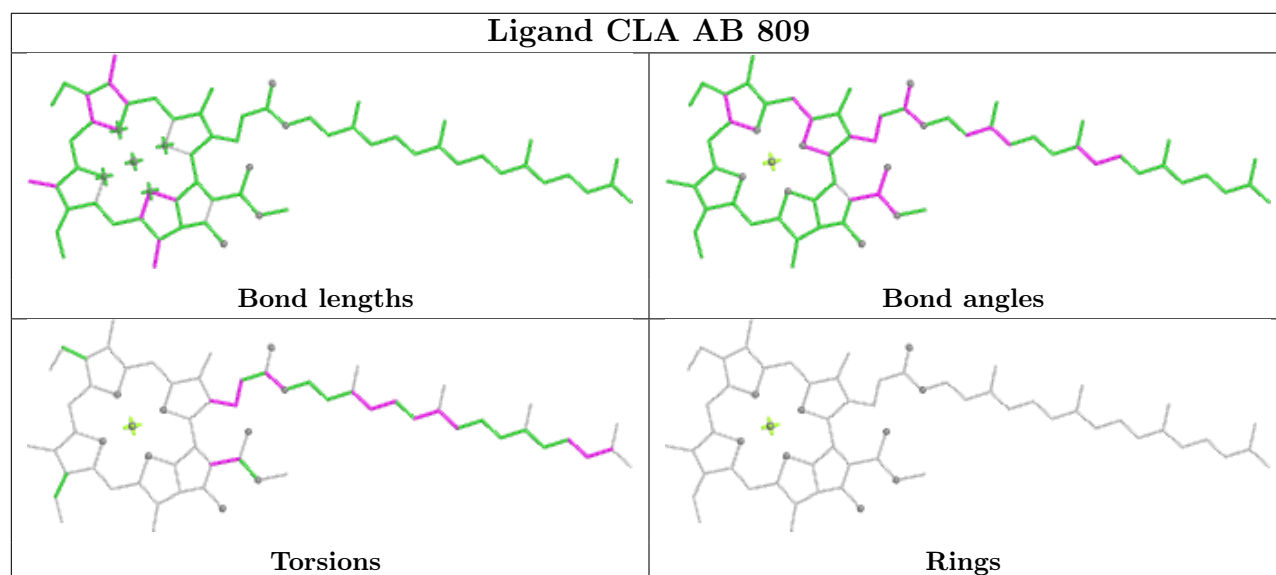
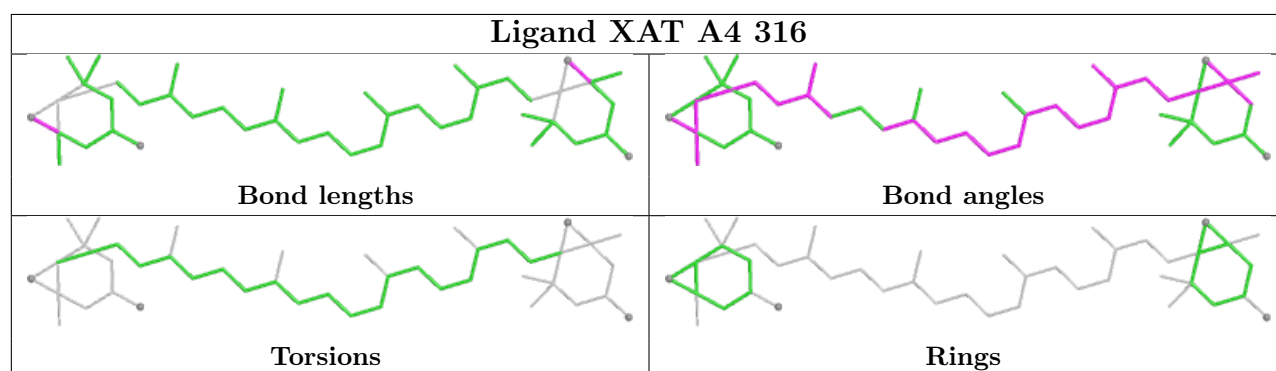
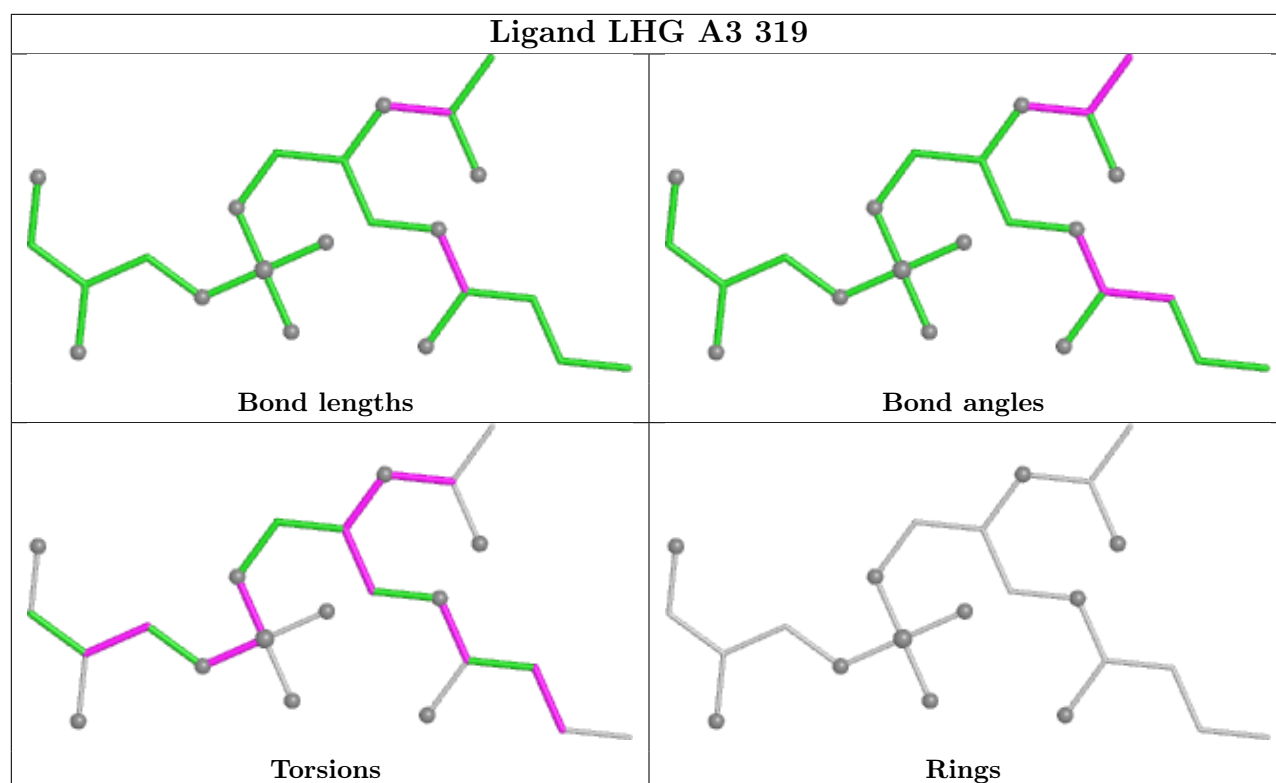
Bond angles

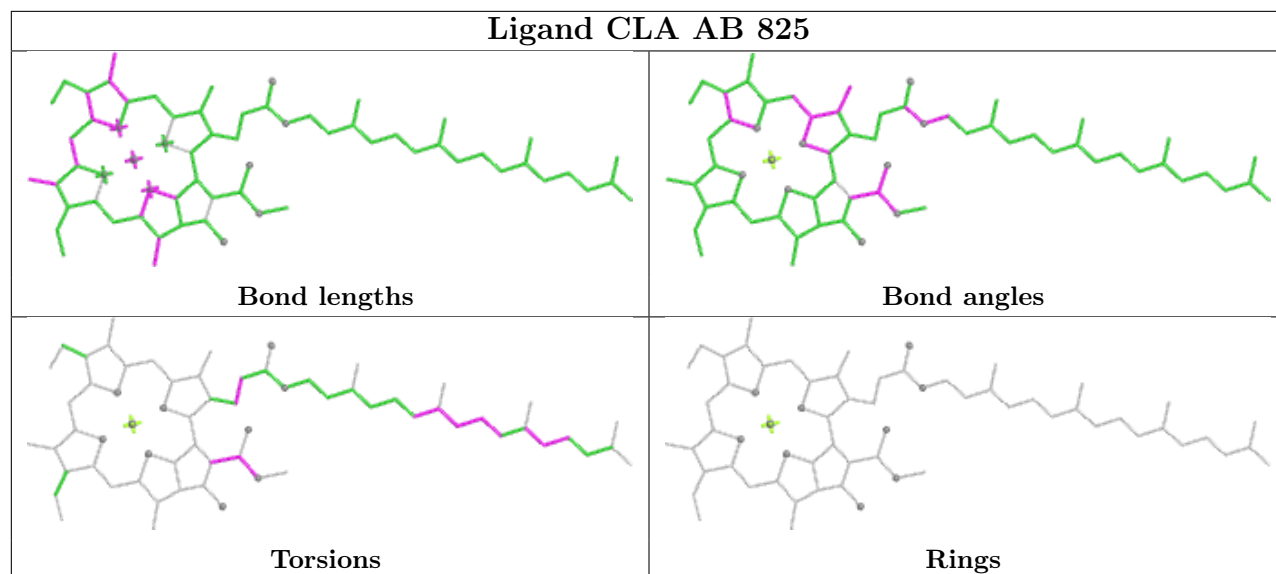
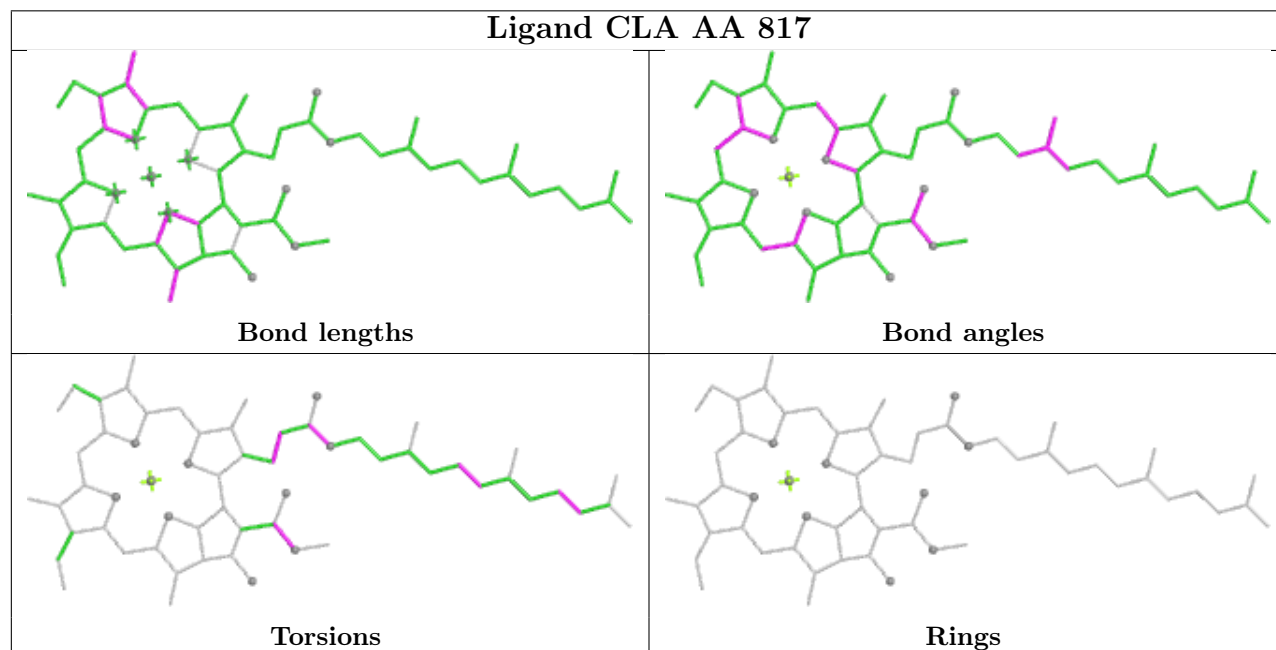


Torsions

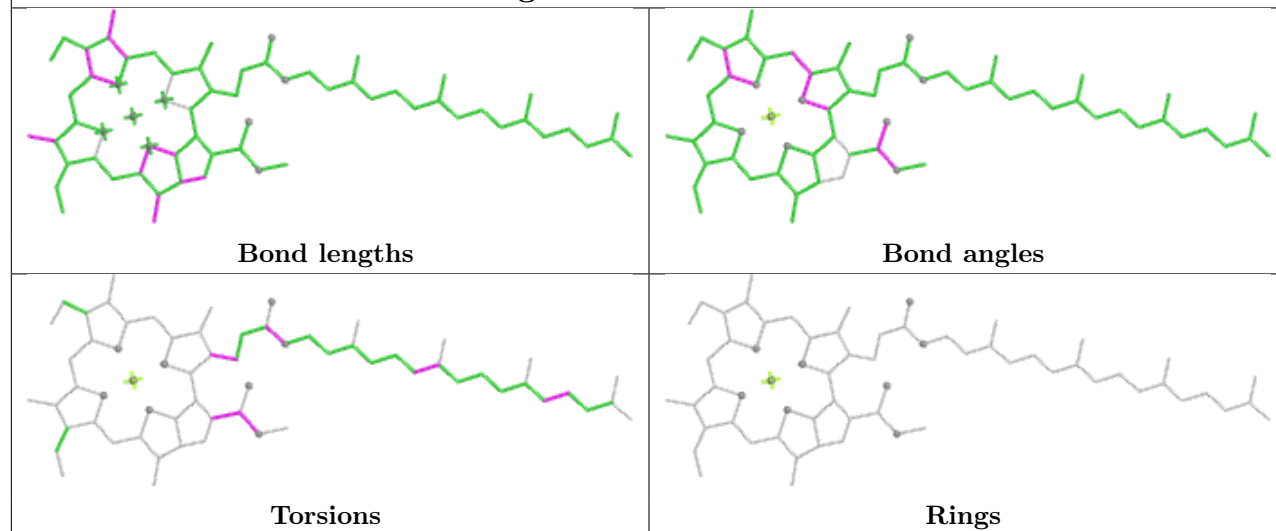


Rings

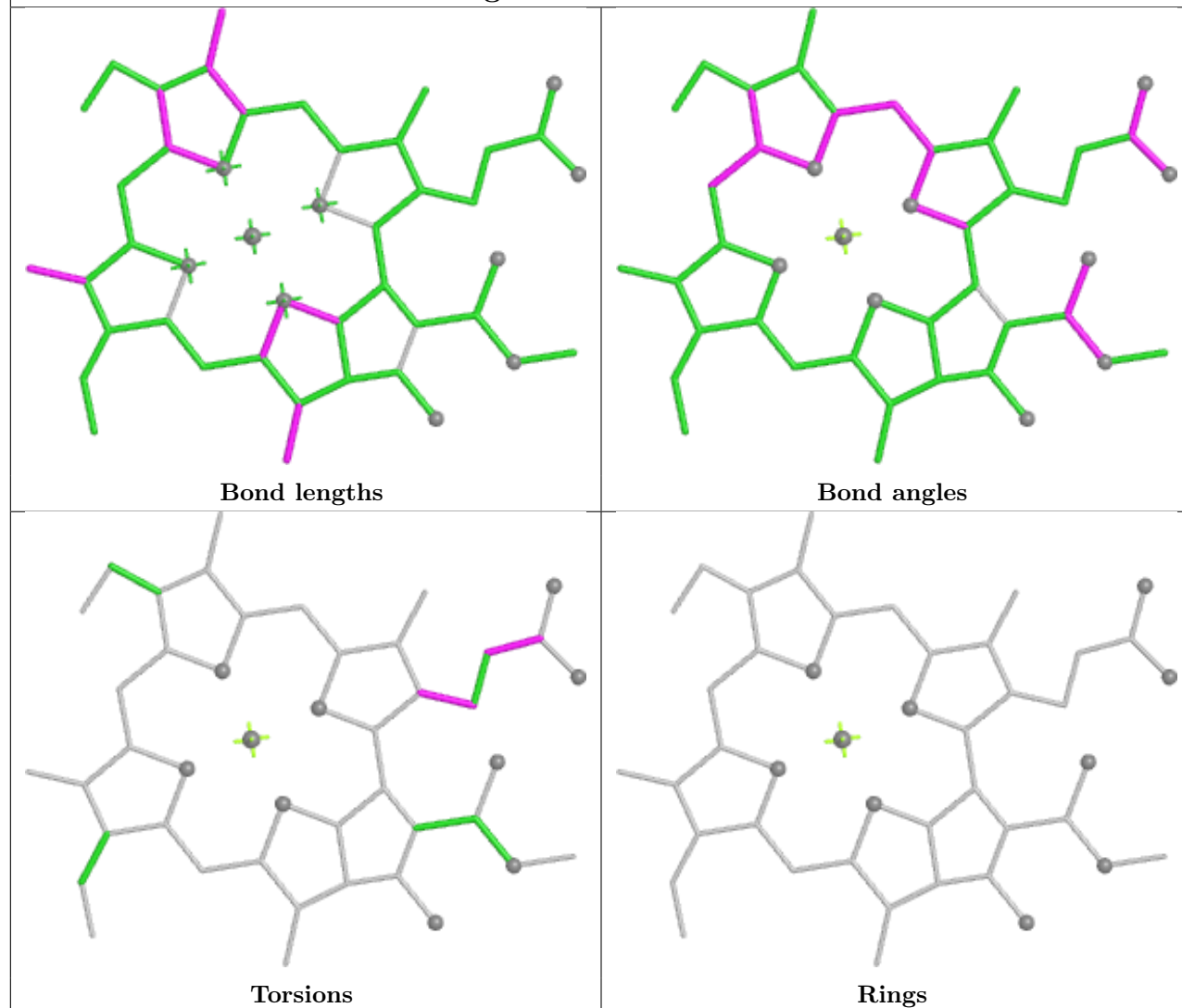


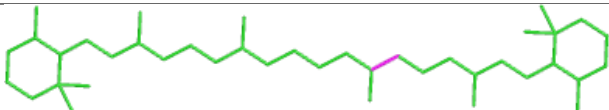
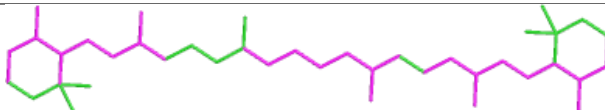
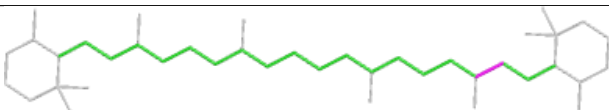
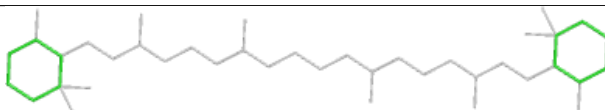
Ligand CLA AB 825**Ligand CLA AA 817**

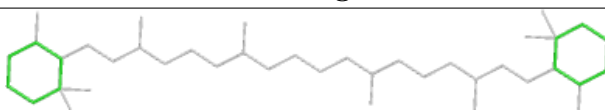
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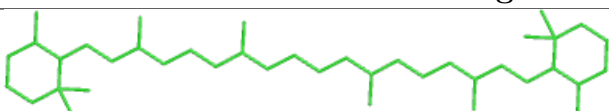
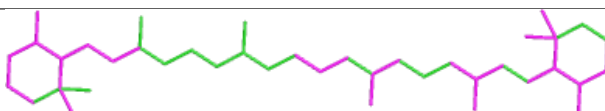
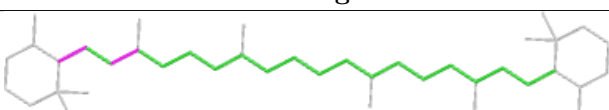
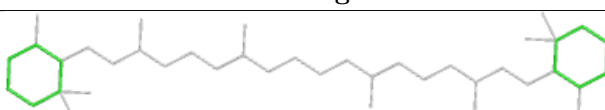


Ligand CLA A6 608

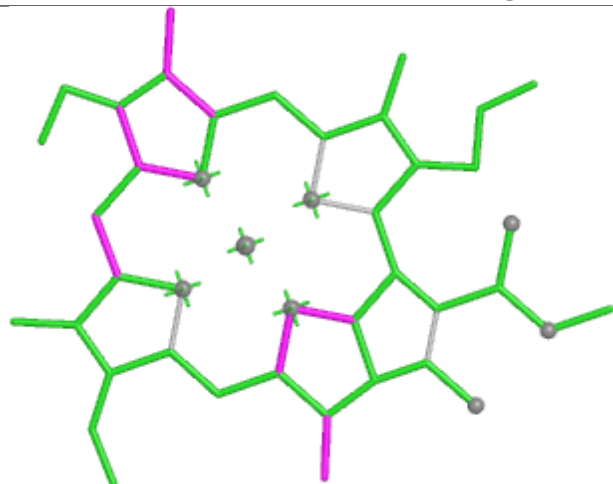


Ligand BCR AB 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

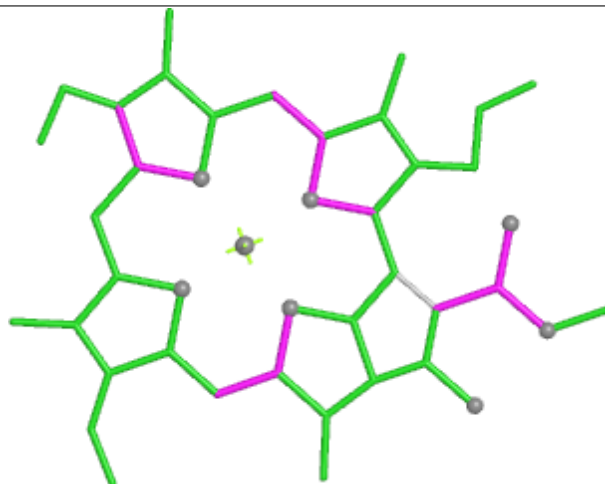
Ligand BCR AB 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR AL 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

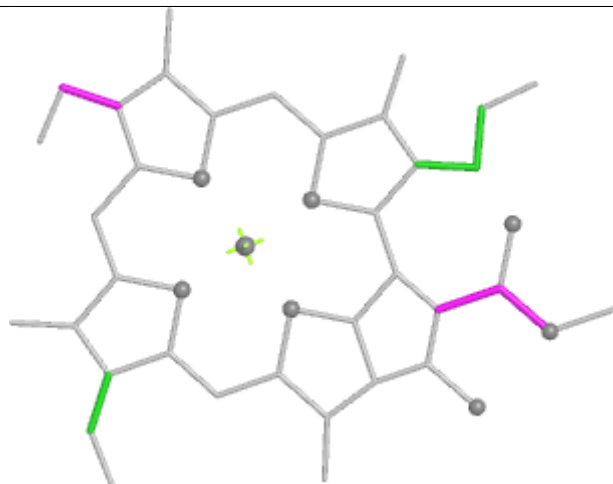
Ligand CLA AB 813



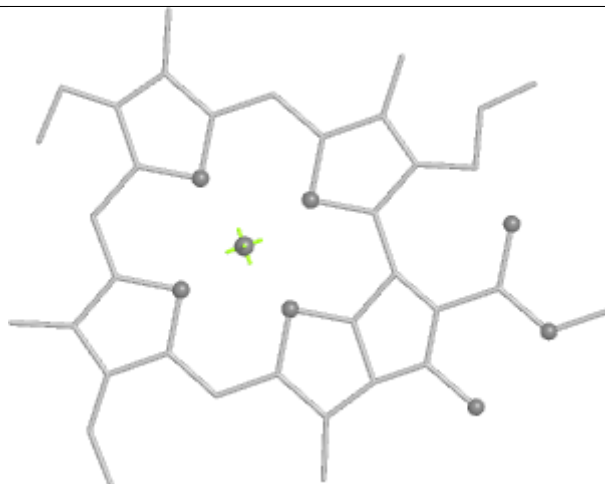
Bond lengths



Bond angles

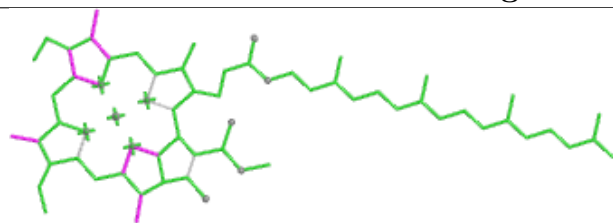


Torsions

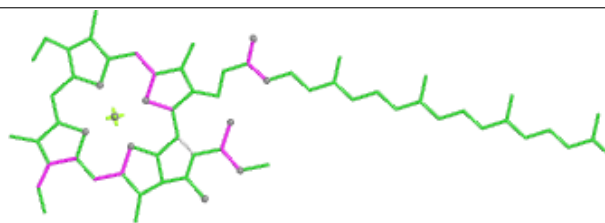


Rings

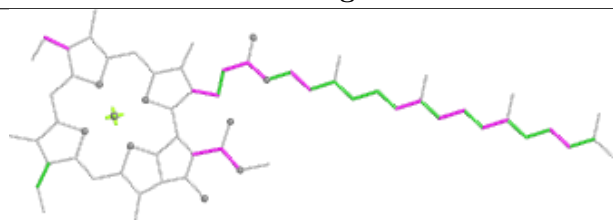
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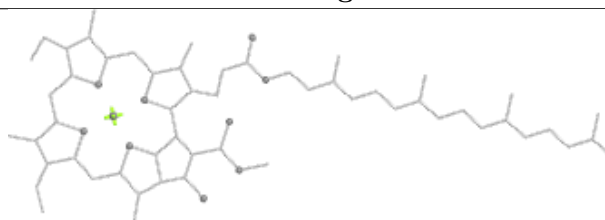
Bond lengths



Bond angles

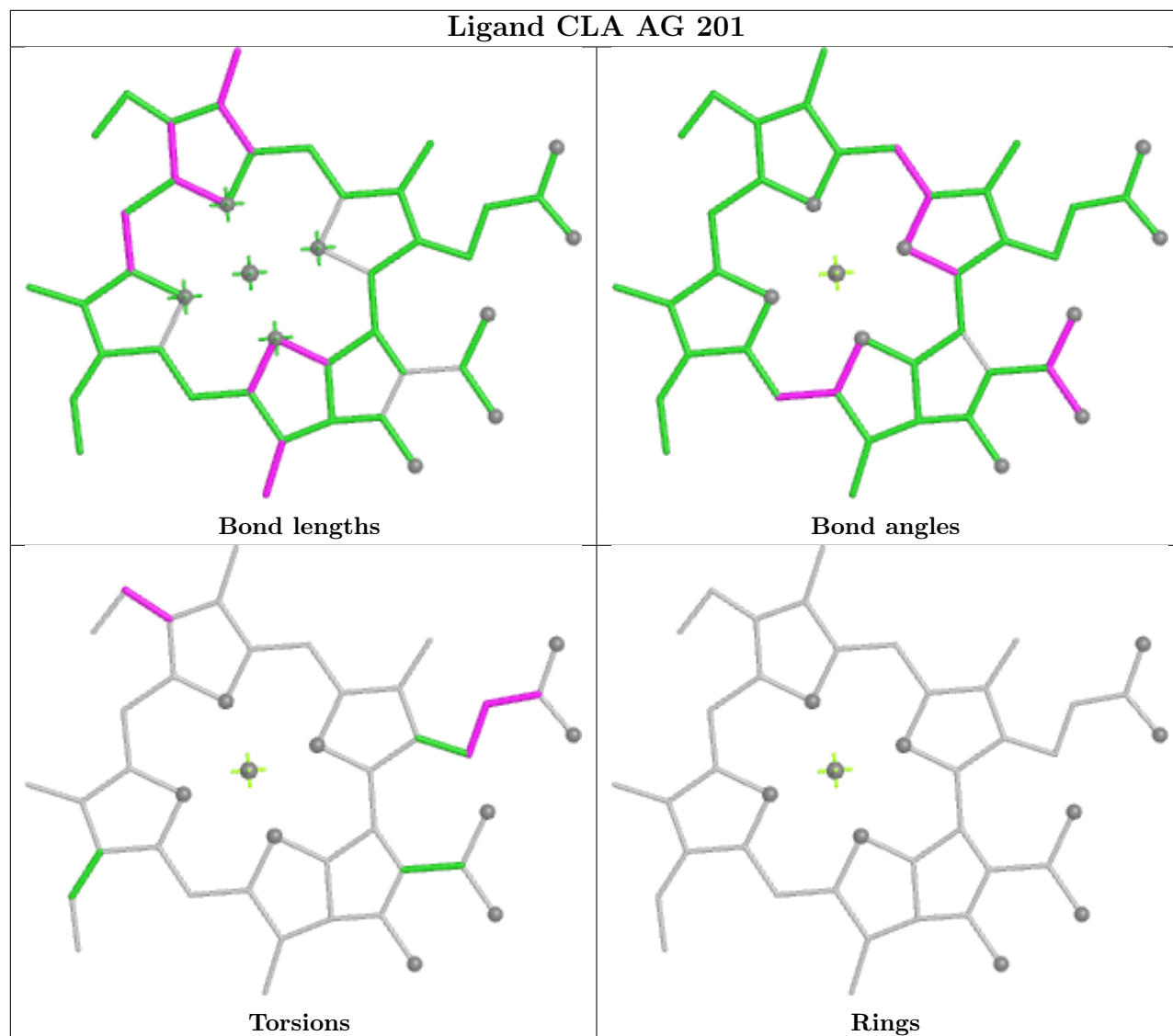


Torsions

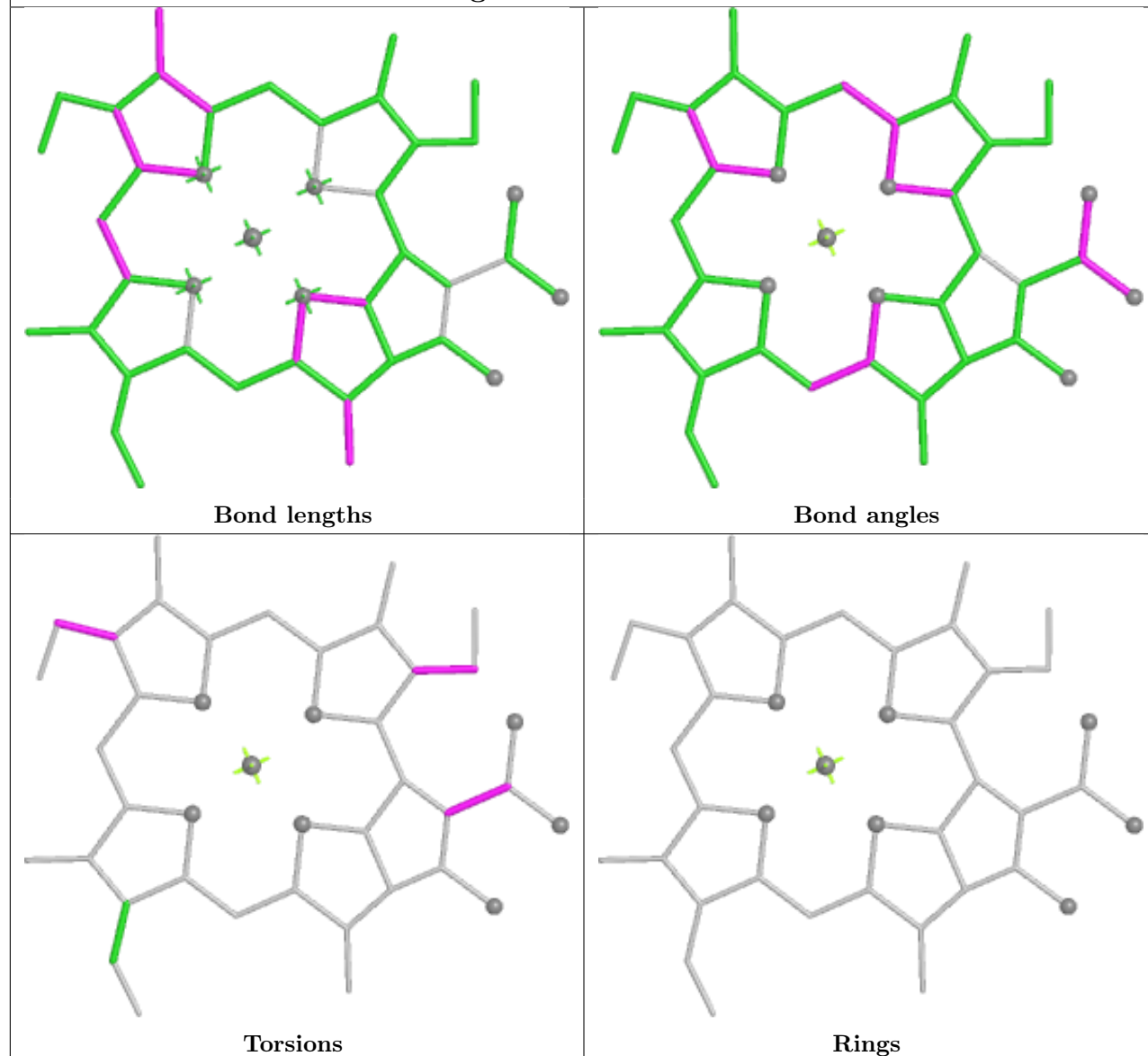


Rings

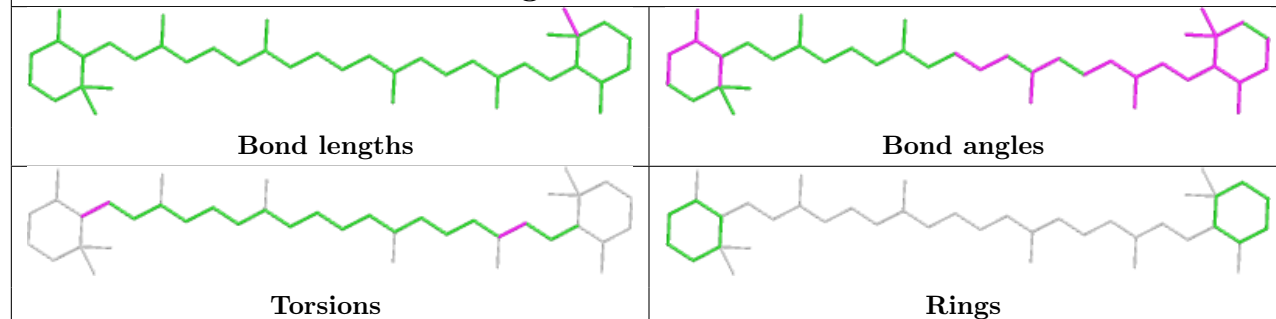
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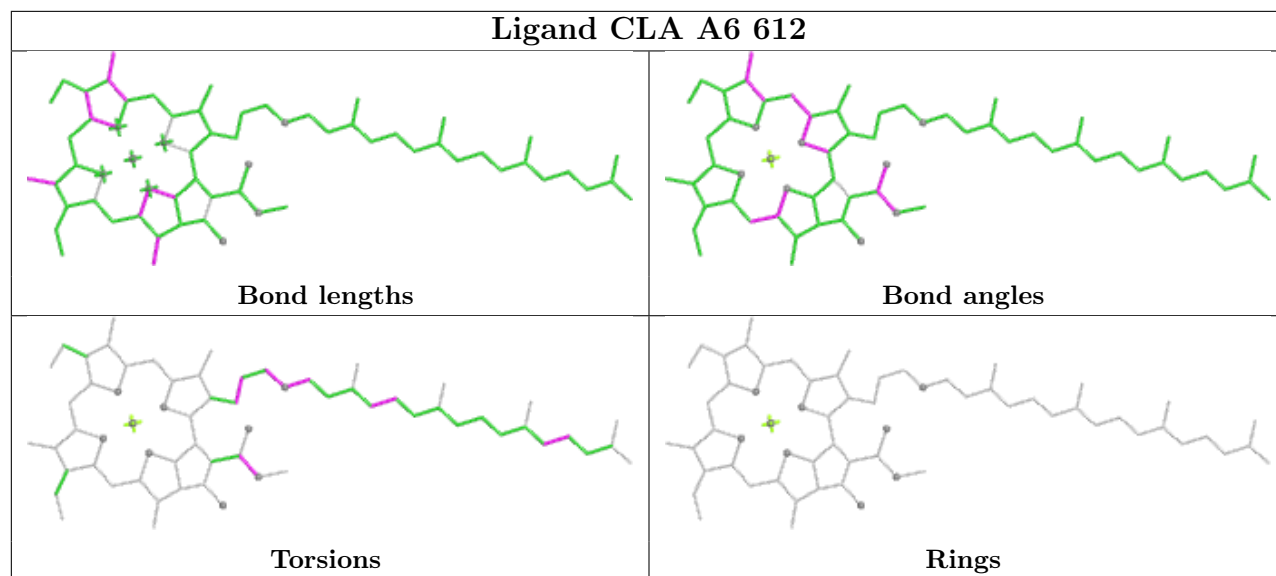
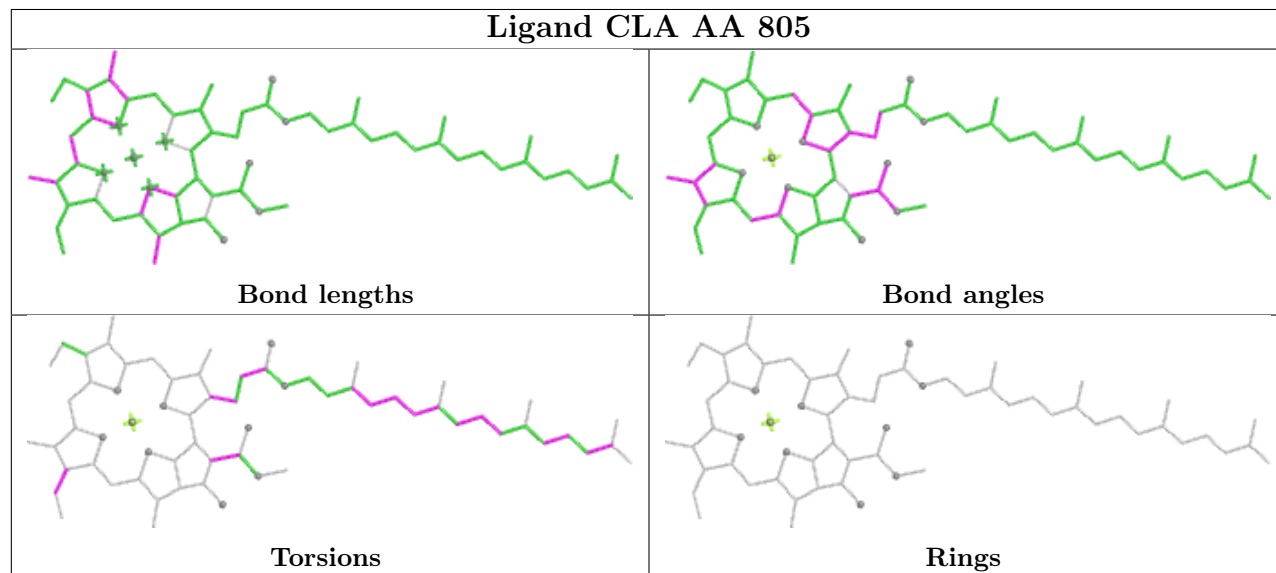


Ligand CLA A3 305

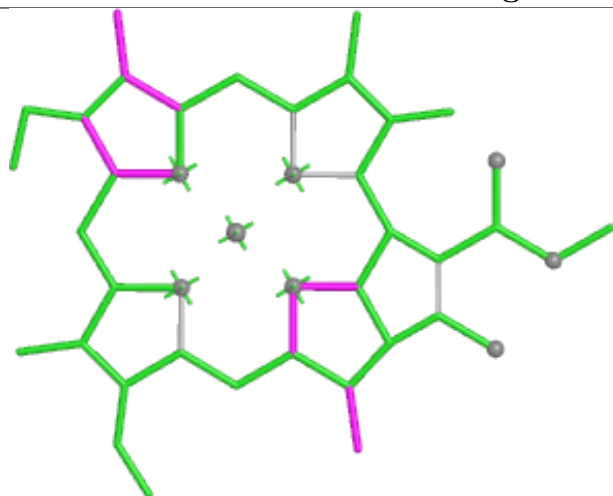


Ligand BCR A3 318



Ligand CLA A6 612**Ligand CLA AA 805**

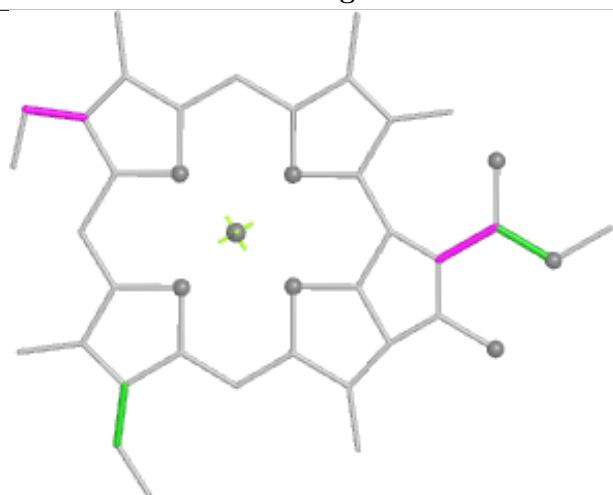
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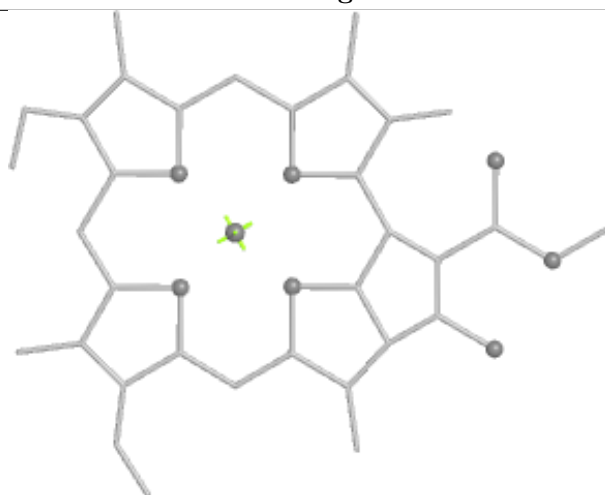
Bond lengths



Bond angles

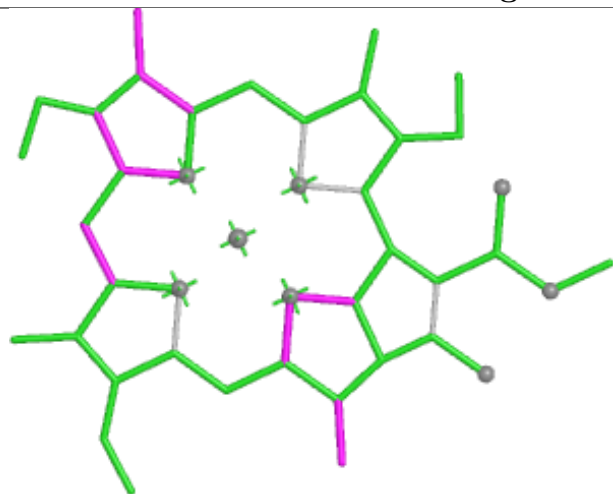


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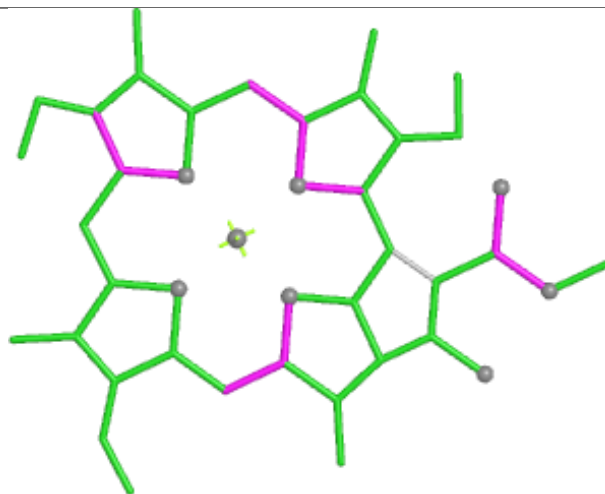


Rings

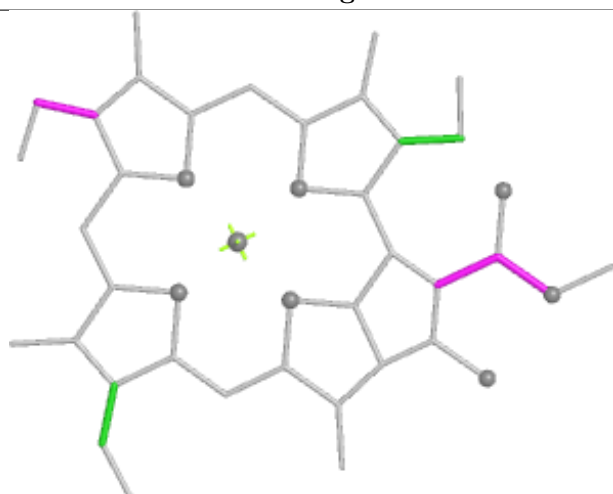
Ligand CLA AG 203



Bond lengths



Bond angles

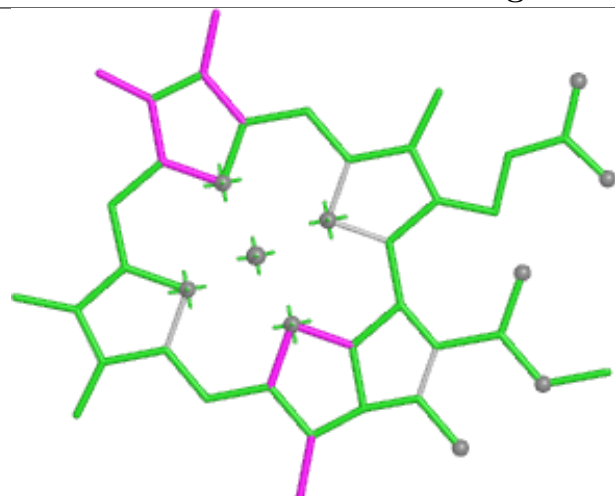


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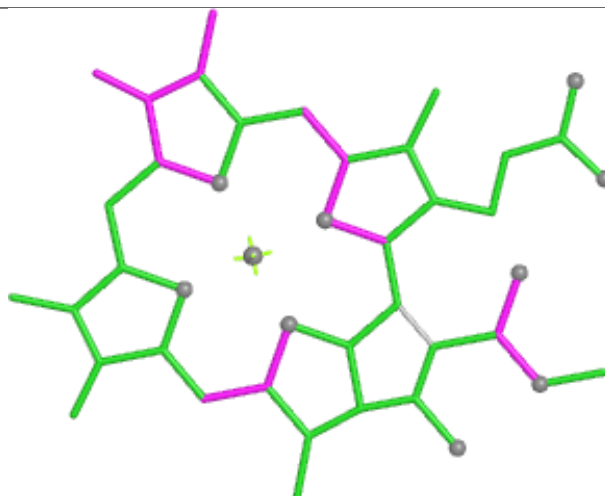


Rings

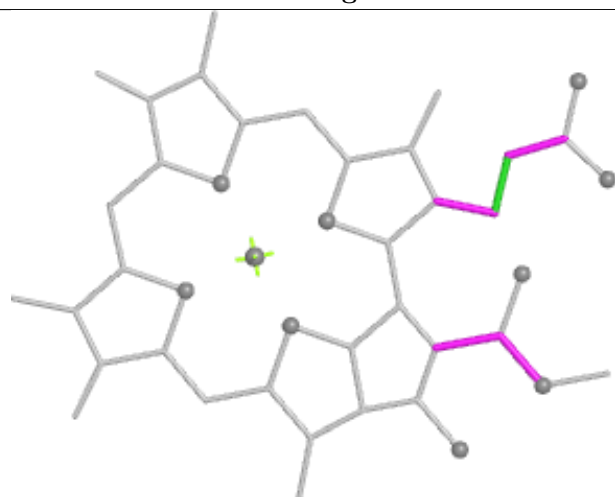
Ligand CLA A1 316



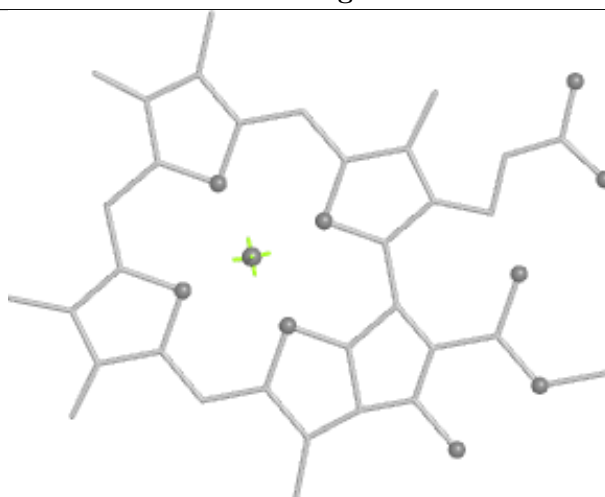
Bond lengths



Bond angles

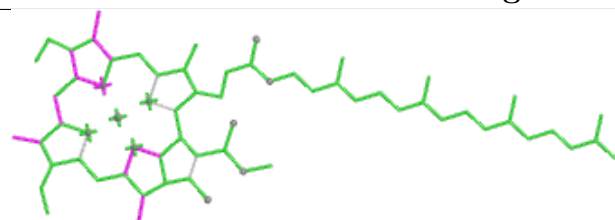


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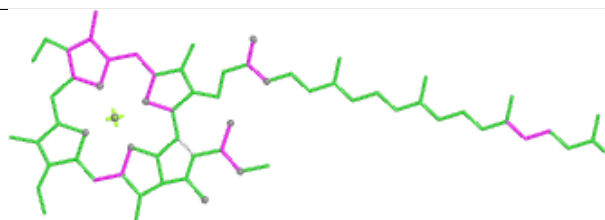


Rings

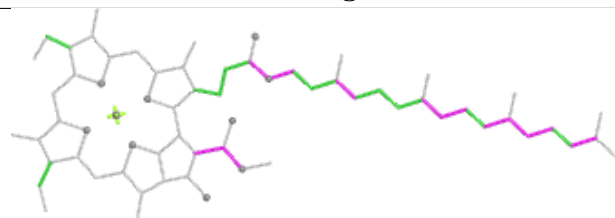
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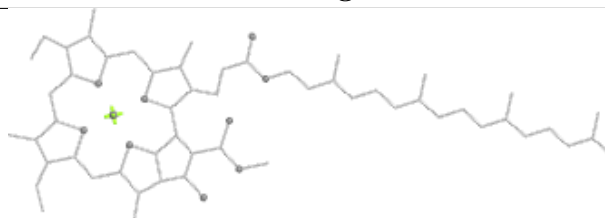
Bond lengths



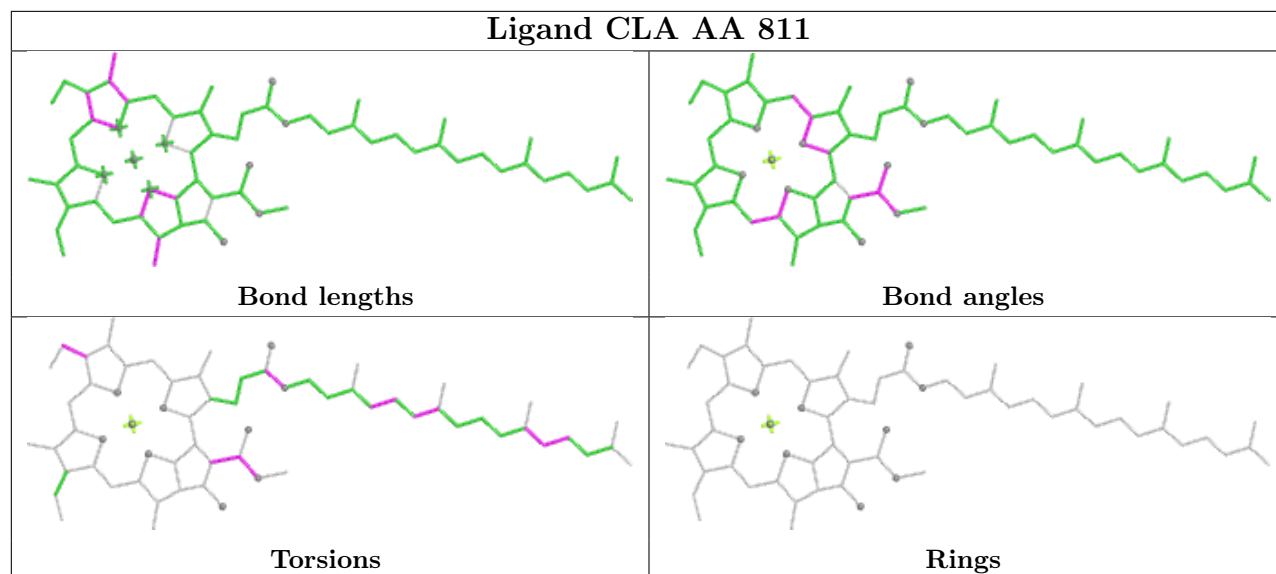
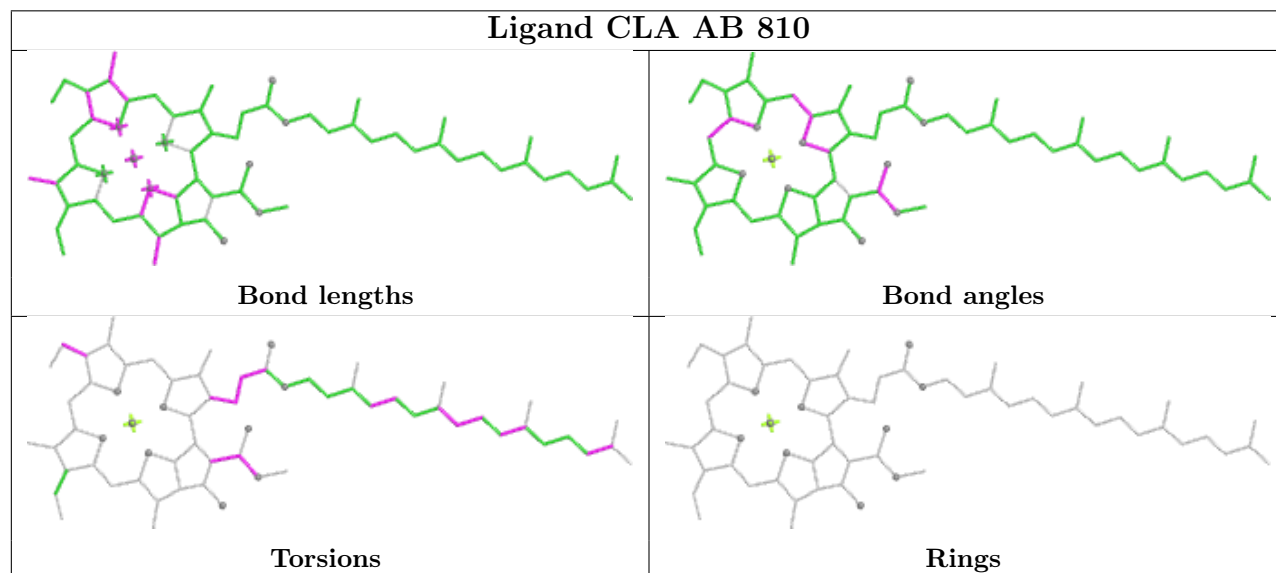
Bond angles



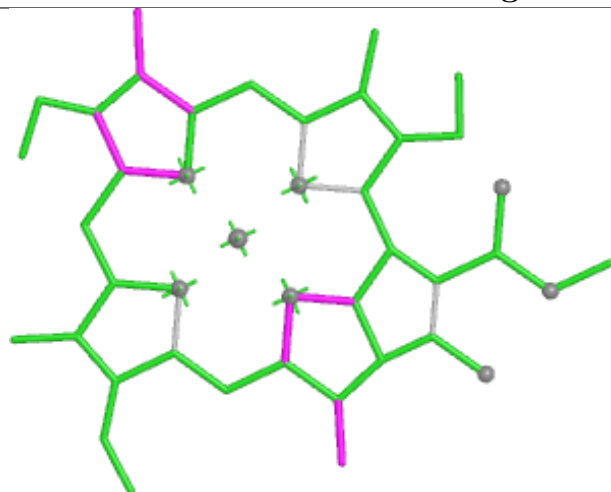
Torsions



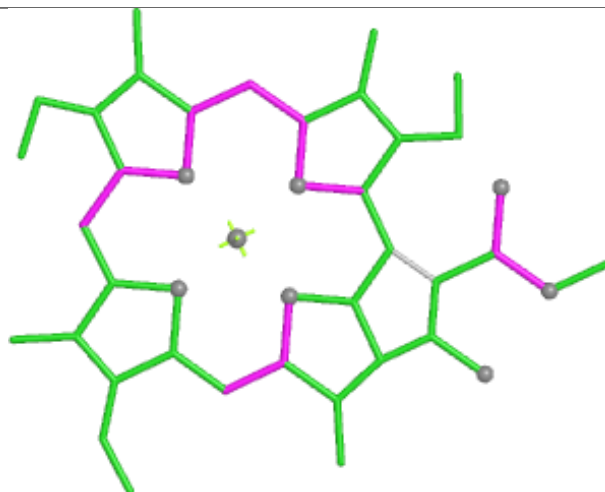
Rings

Ligand CLA AA 811**Ligand CLA AB 810**

Ligand CLA AB 836



Bond lengths



Bond angles

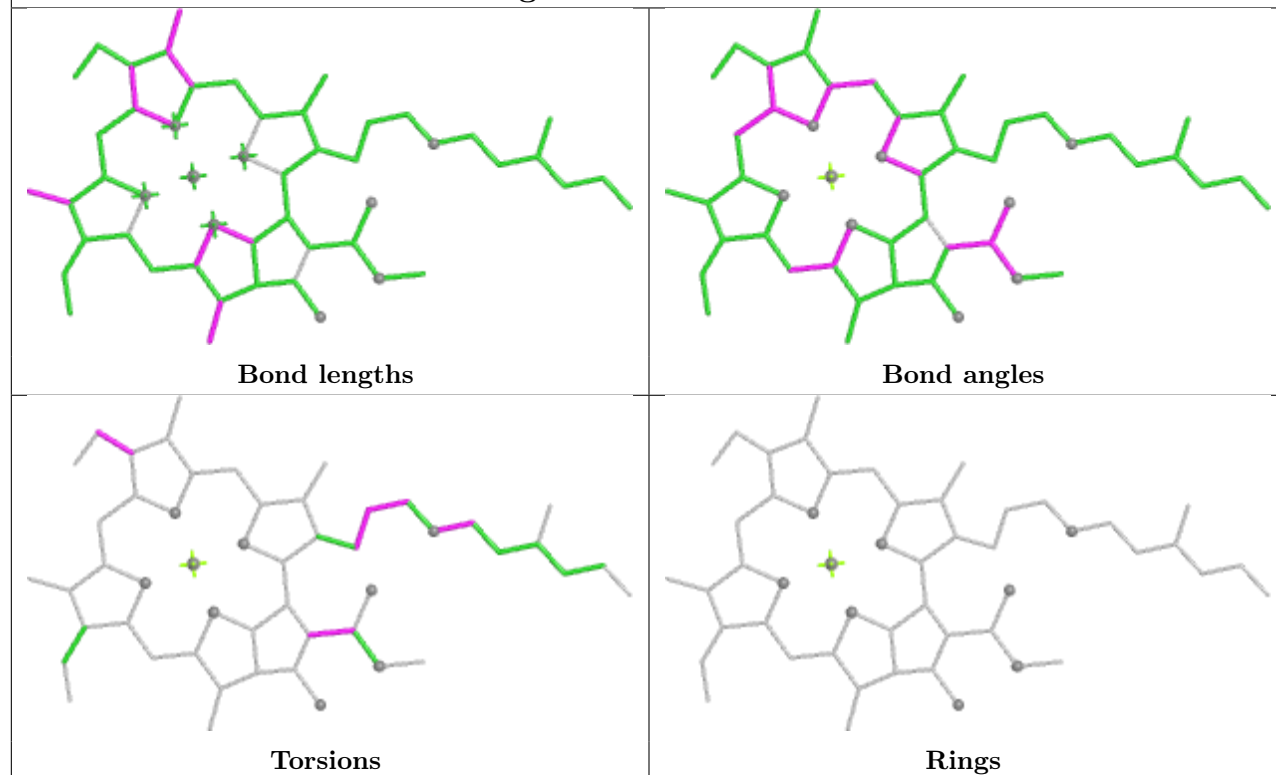


Torsions

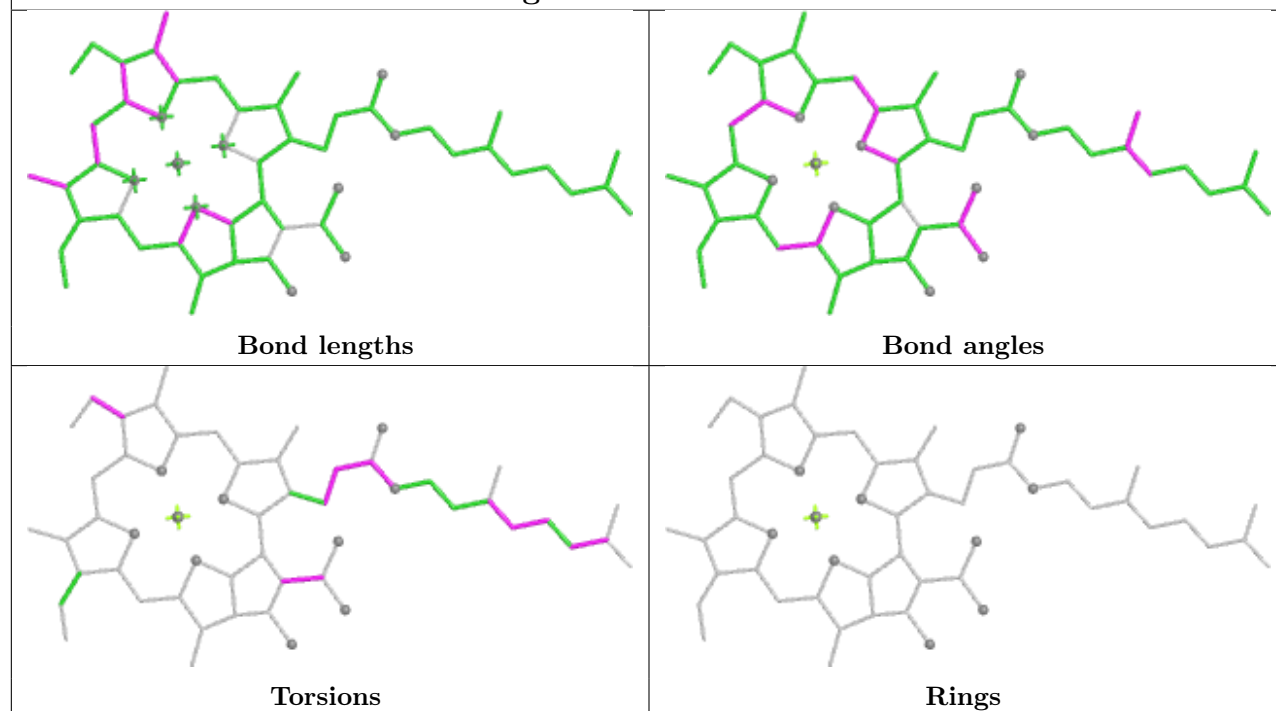


Rings

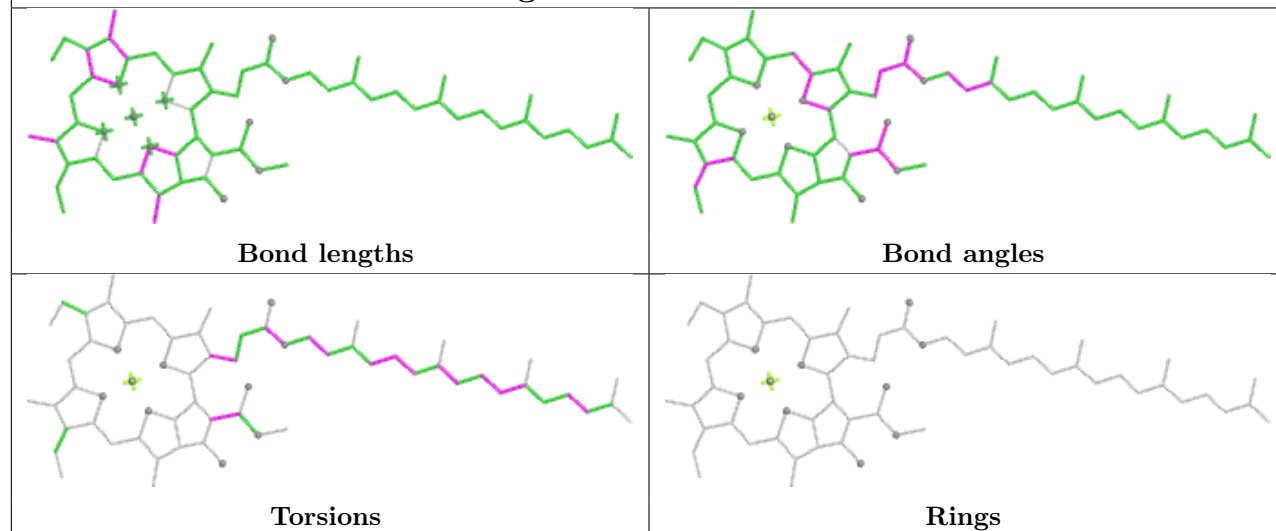
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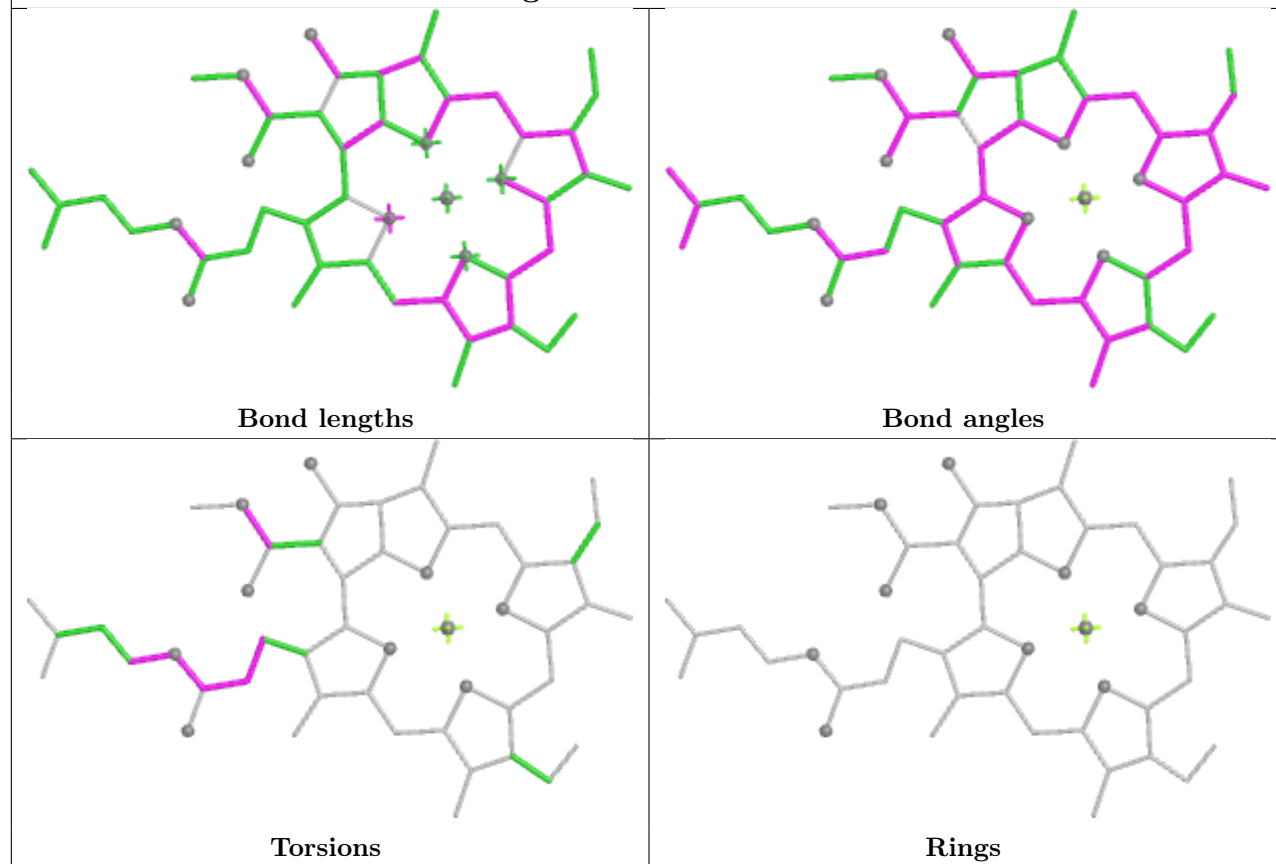
Ligand CLA A3 312



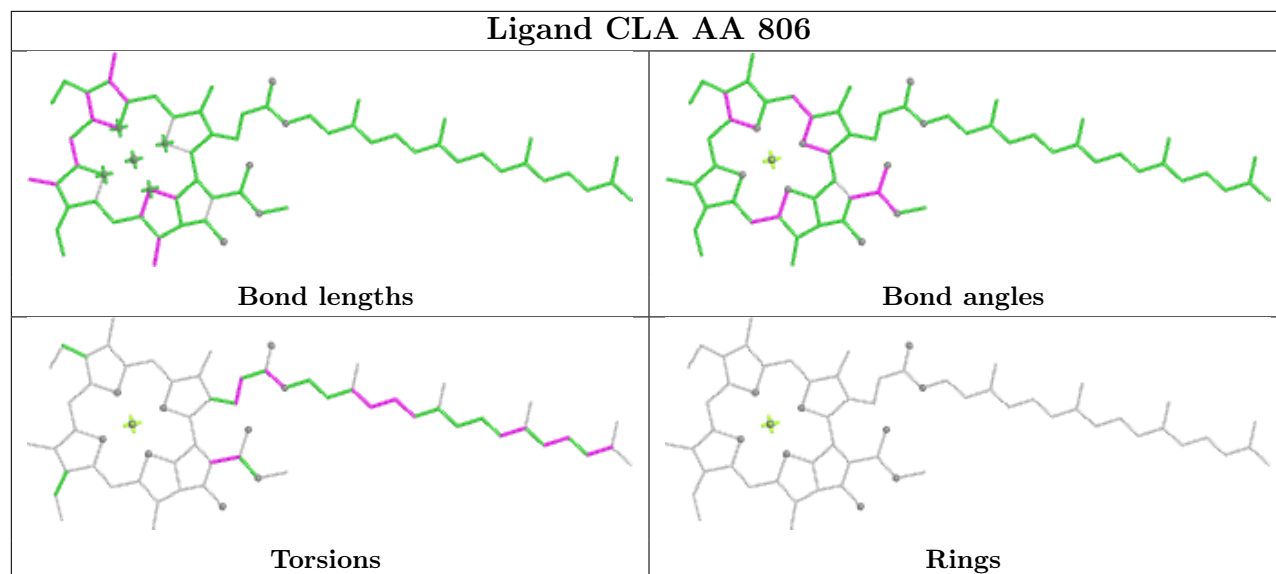
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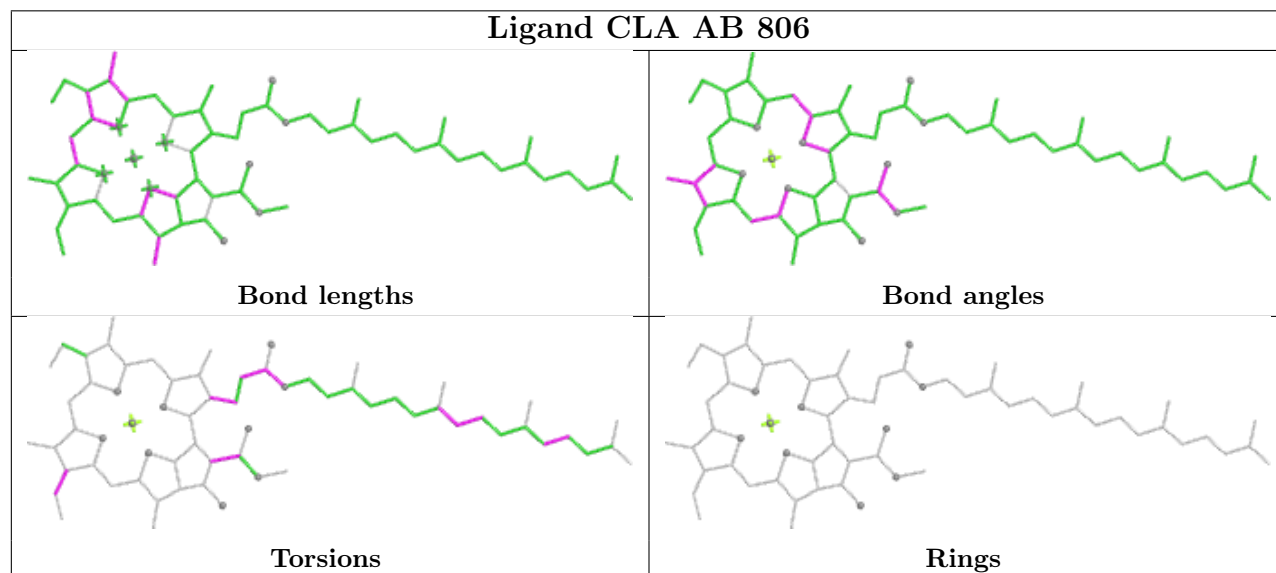
Ligand CHL A6 607



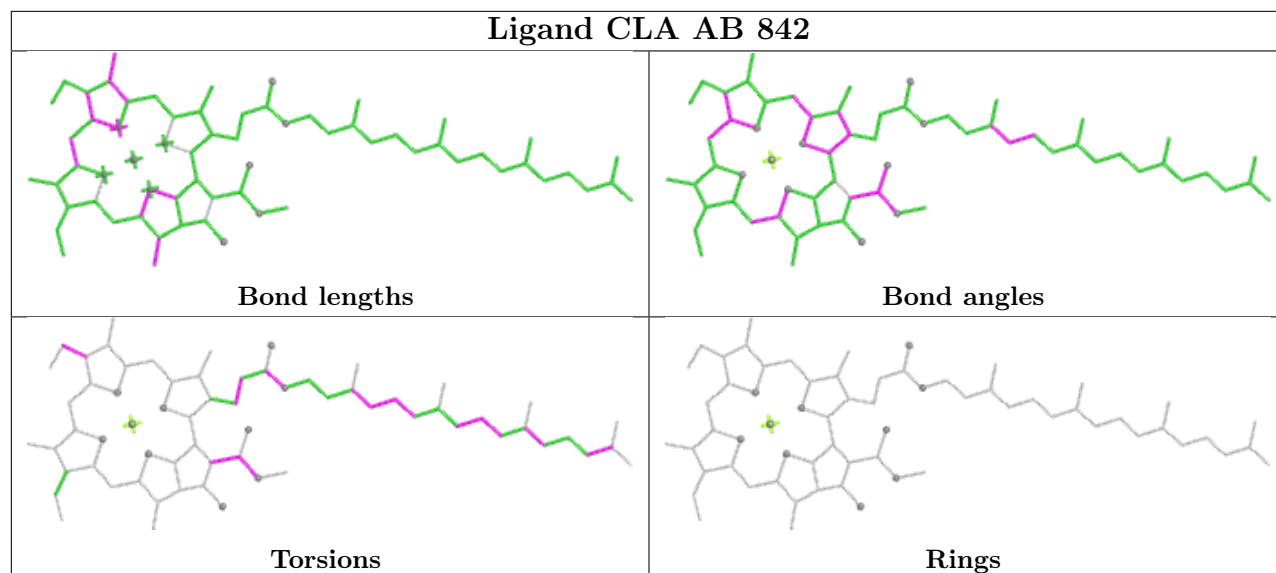
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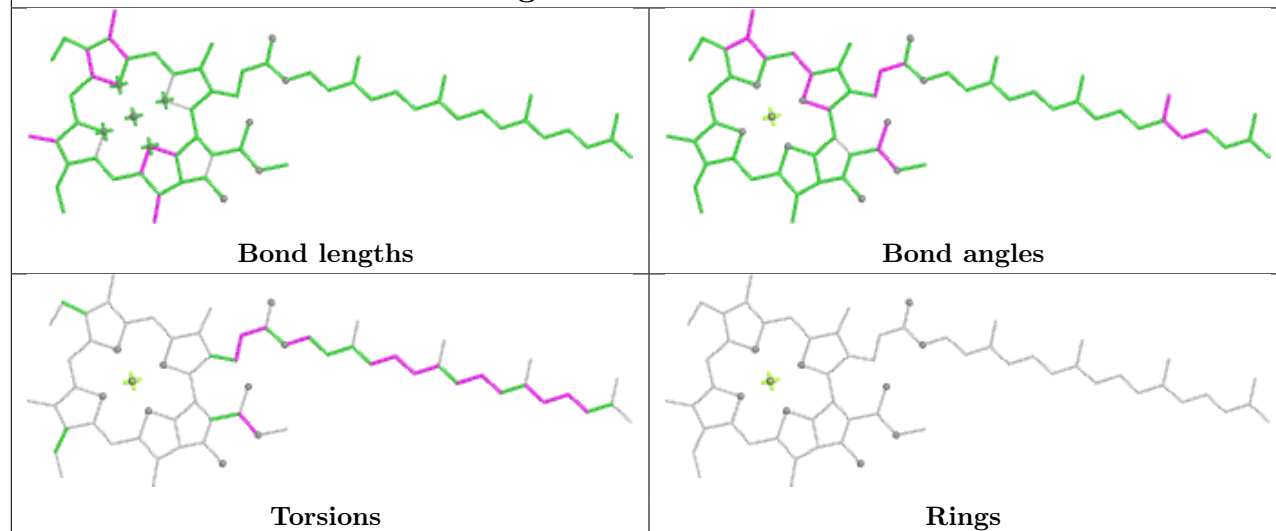
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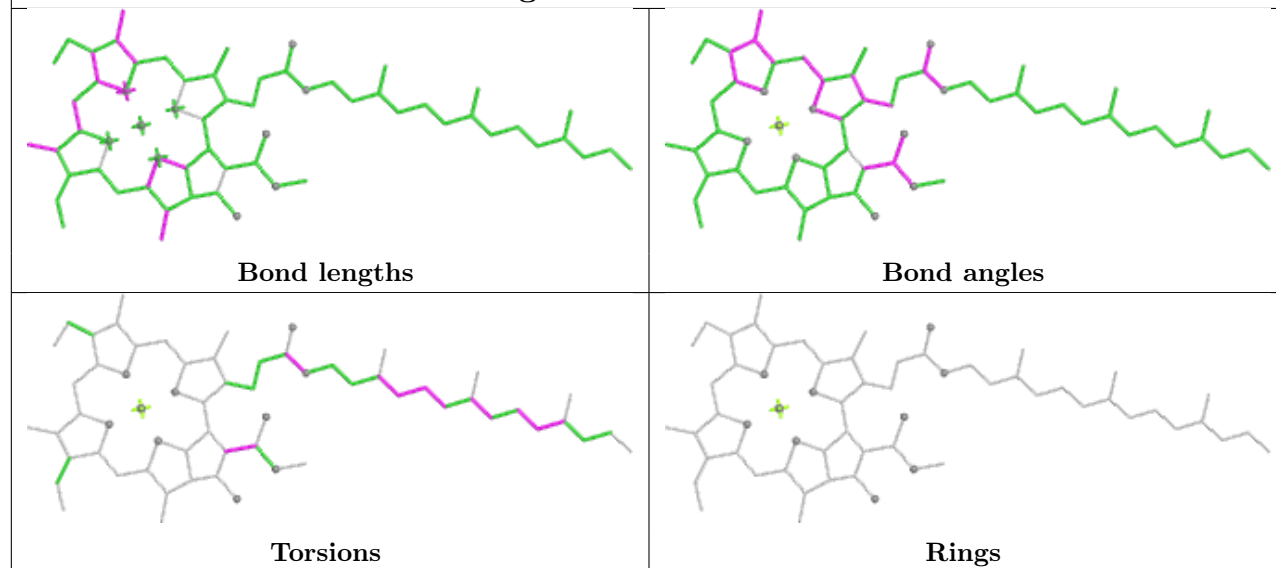
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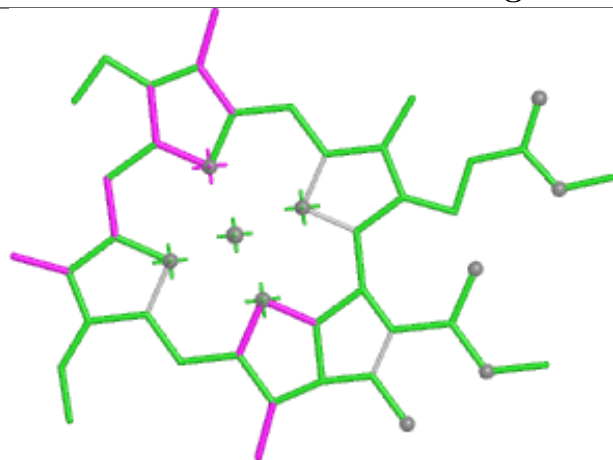
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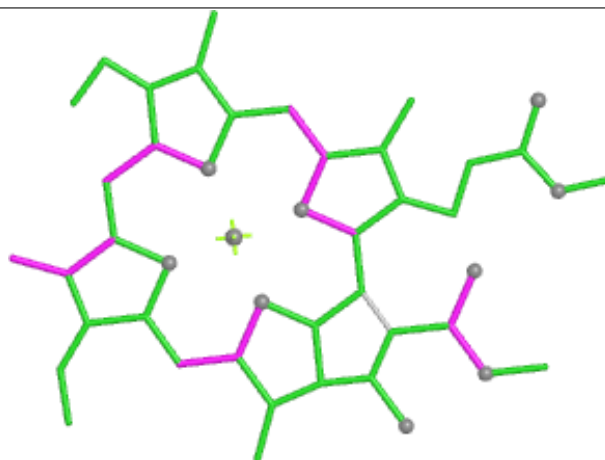
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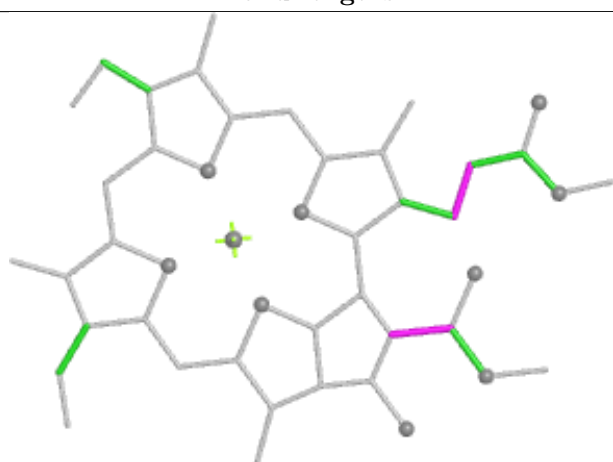
Ligand CLA A6 601



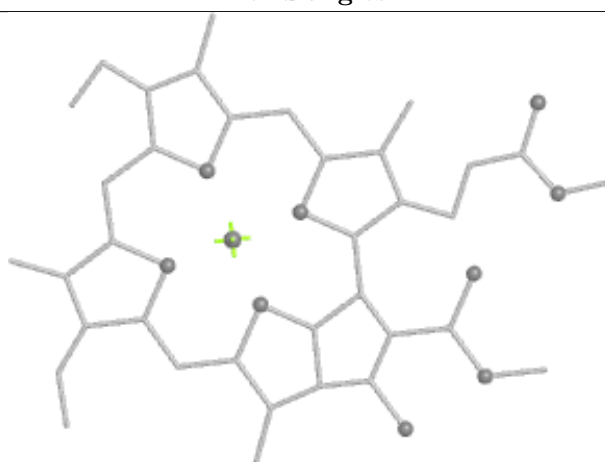
Bond lengths



Bond angles

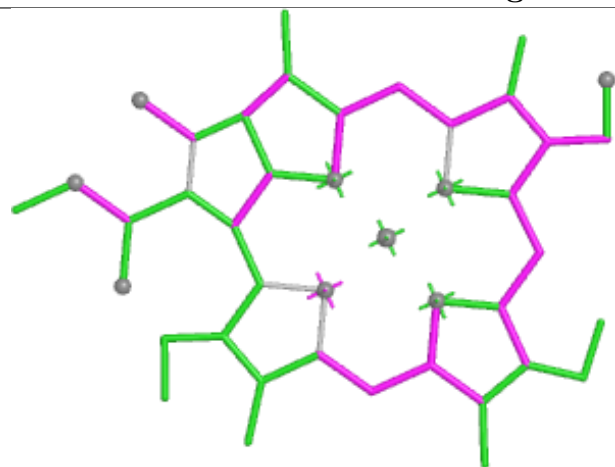


Torsions

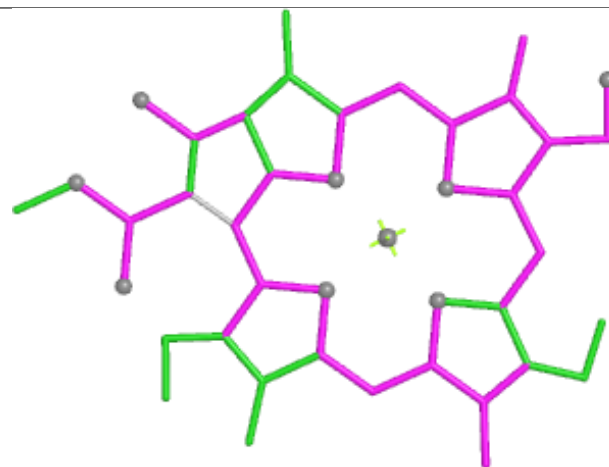


Rings

Ligand CHL A6 605



Bond lengths



Bond angles

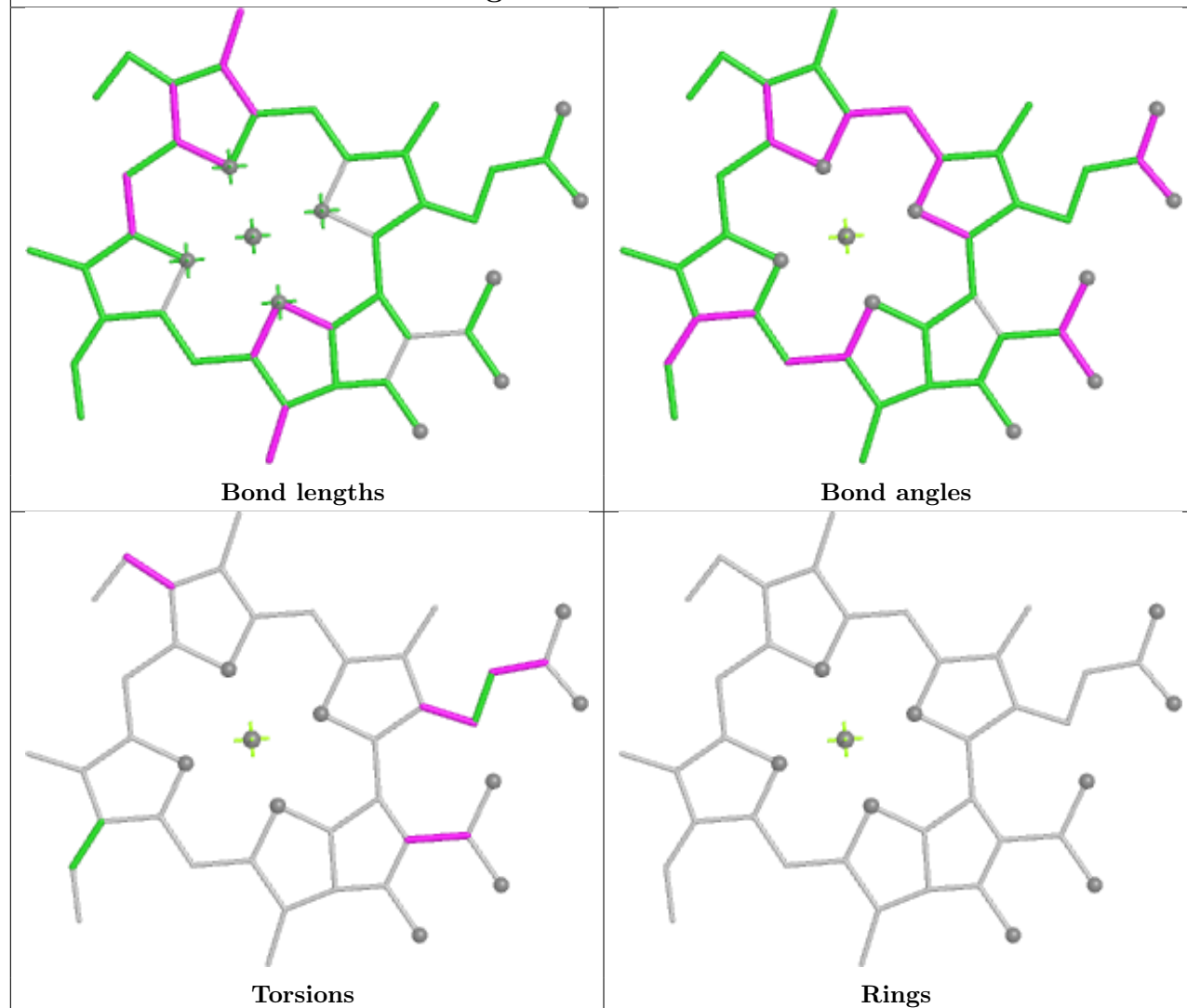


Torsions

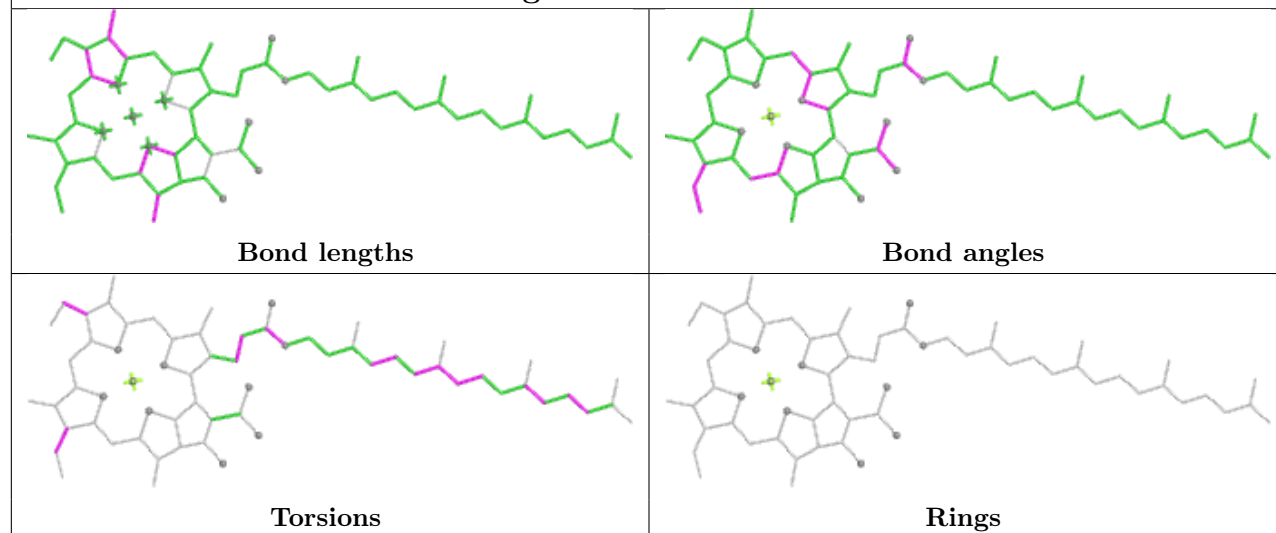


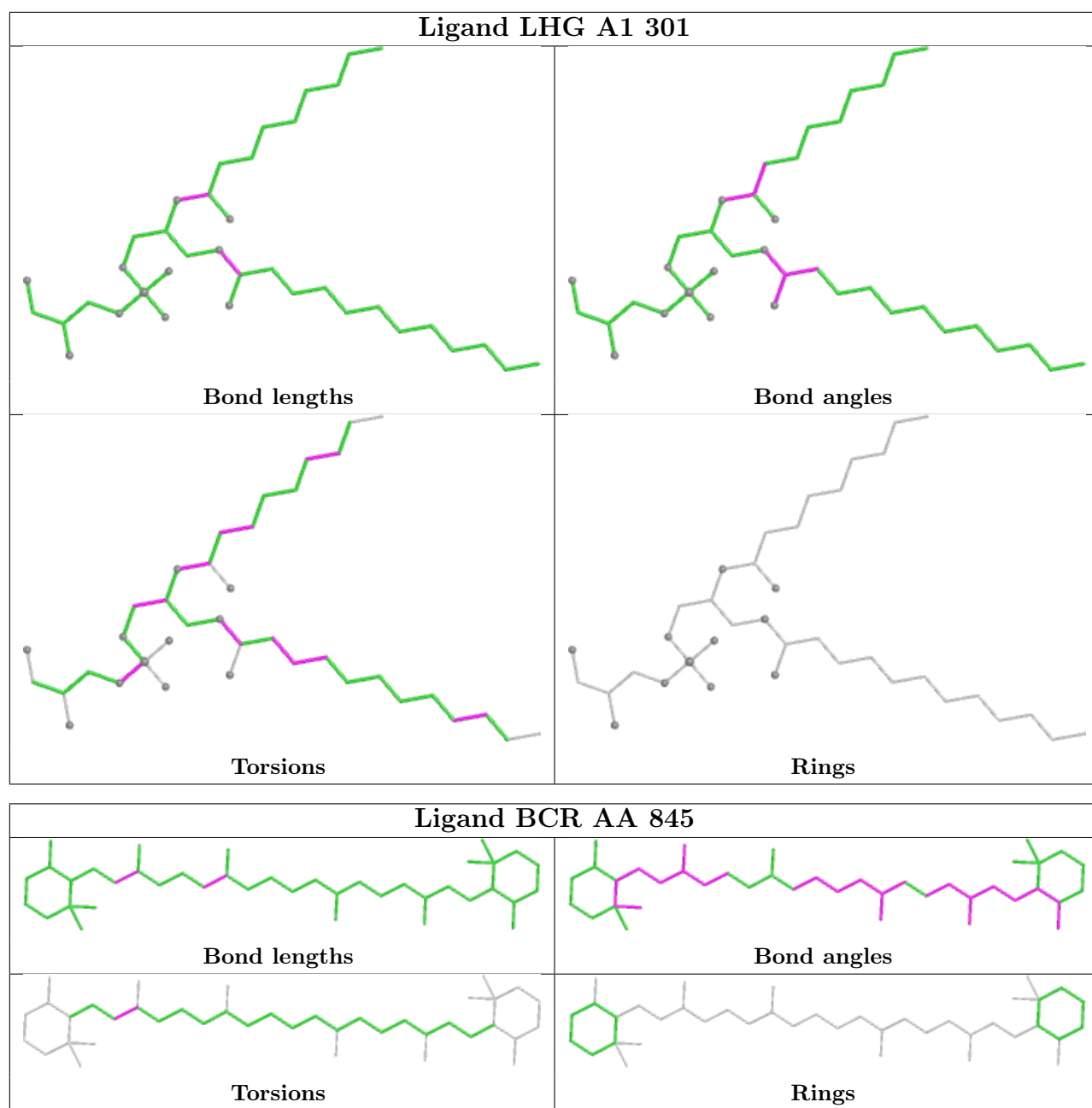
Rings

Ligand CLA A1 309

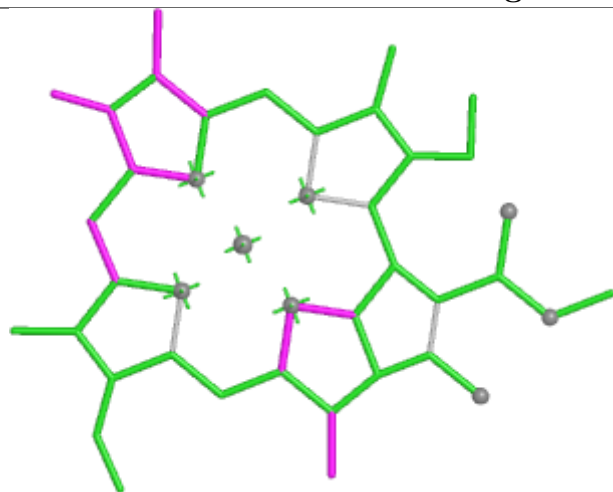


Ligand CLA A1 314

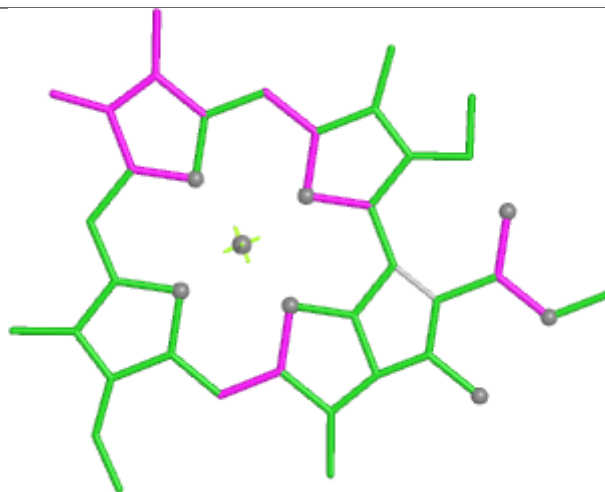




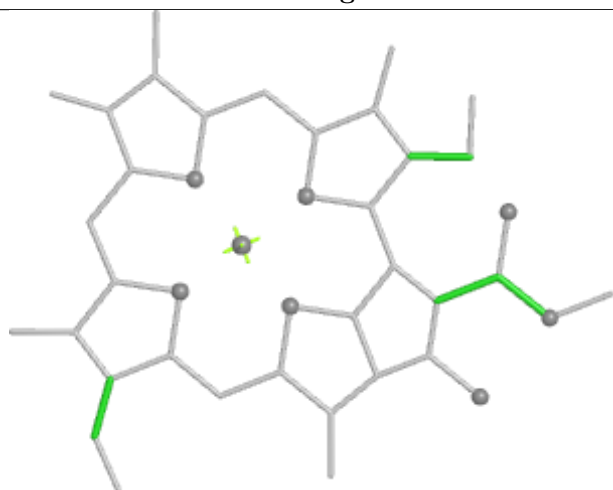
Ligand CLA A3 306



Bond lengths



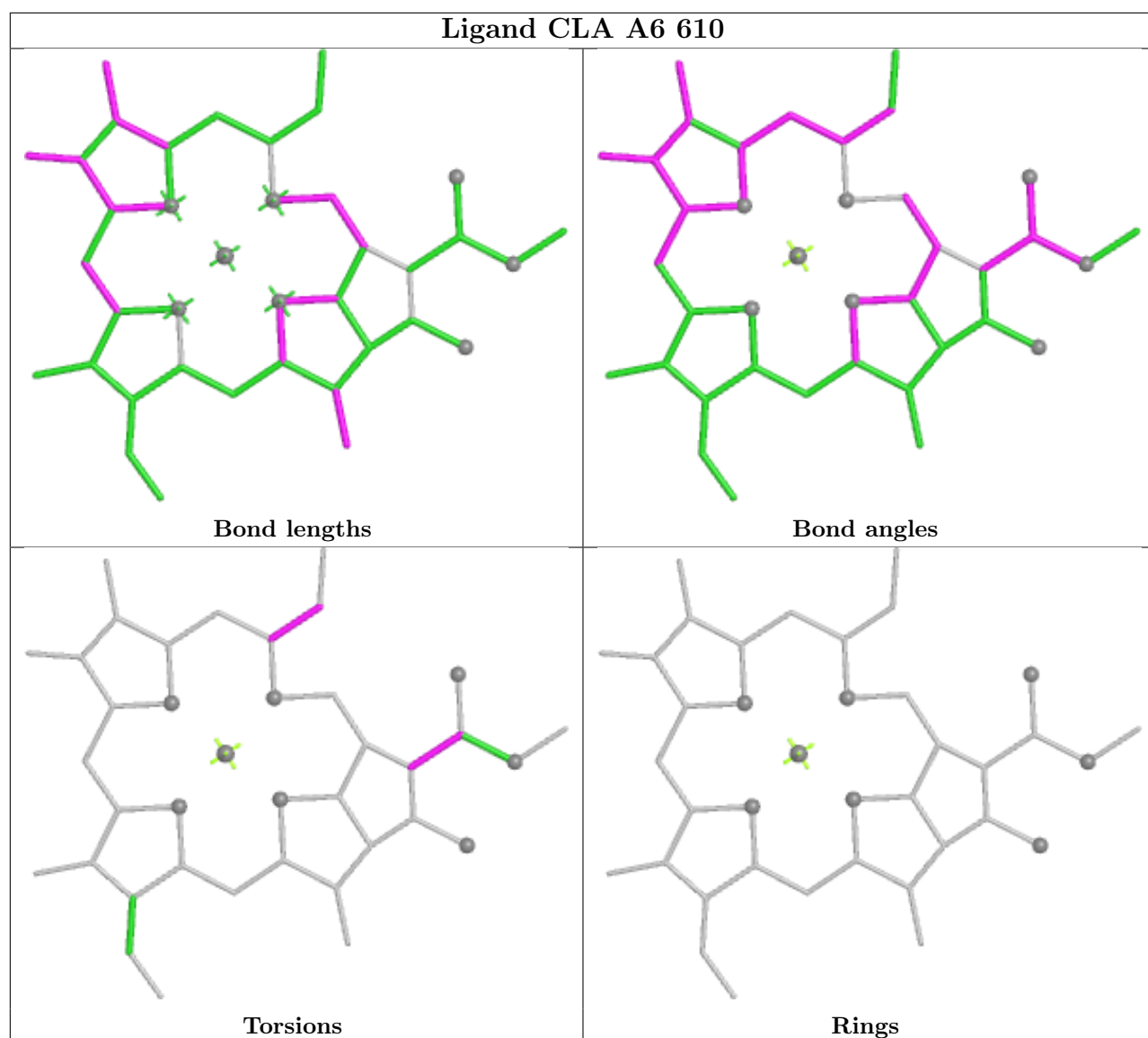
Bond angles

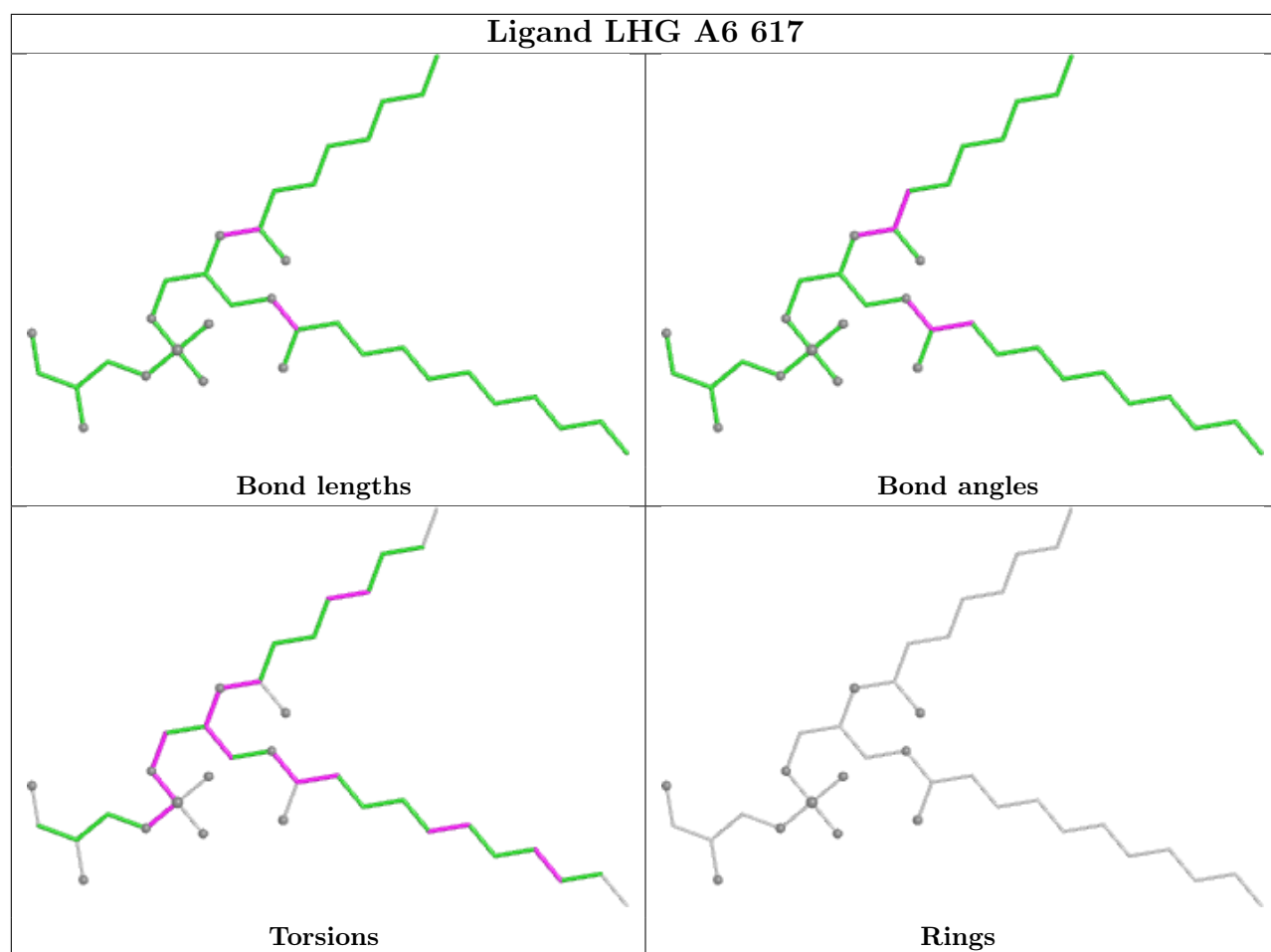


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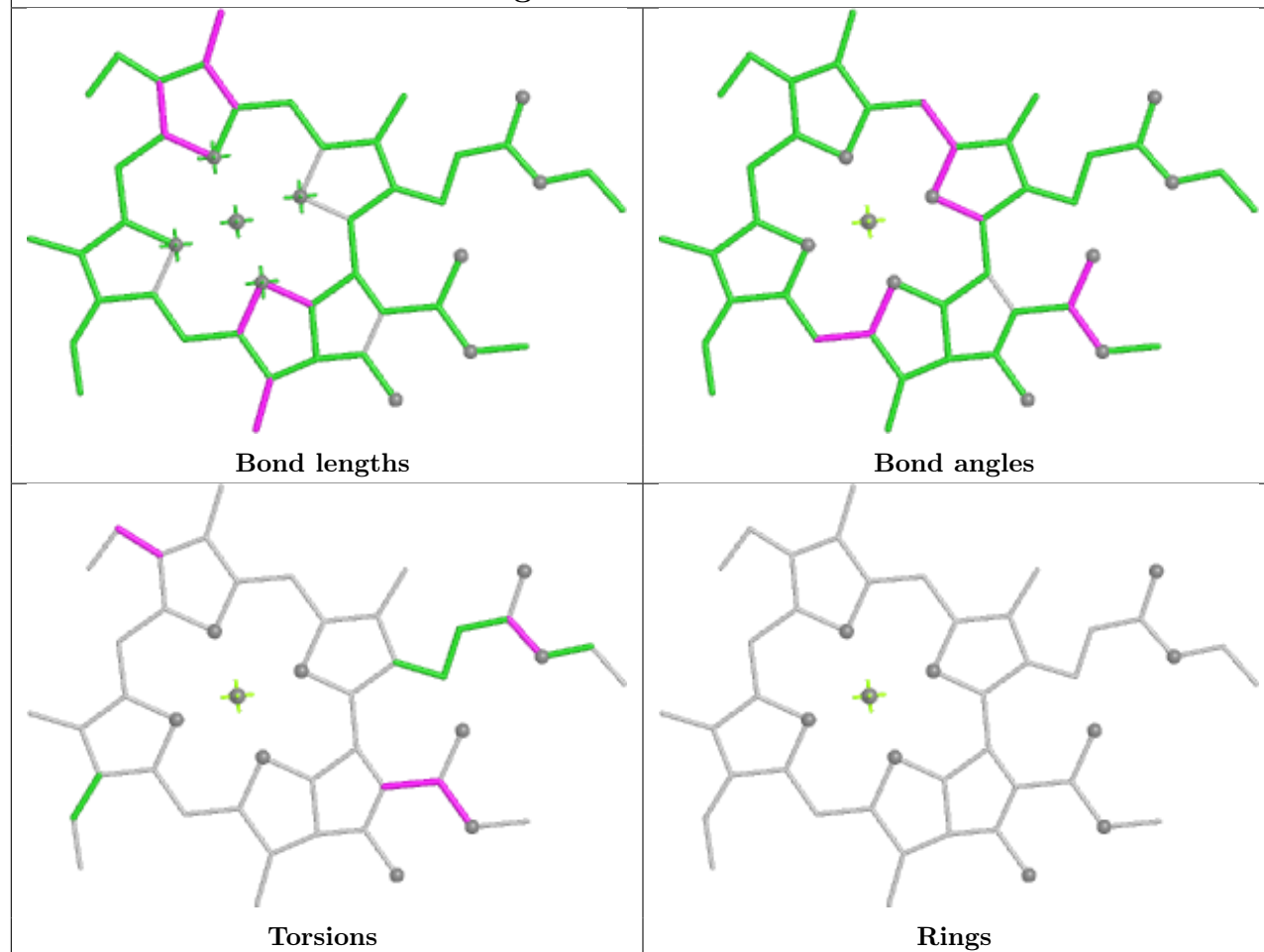


Rings

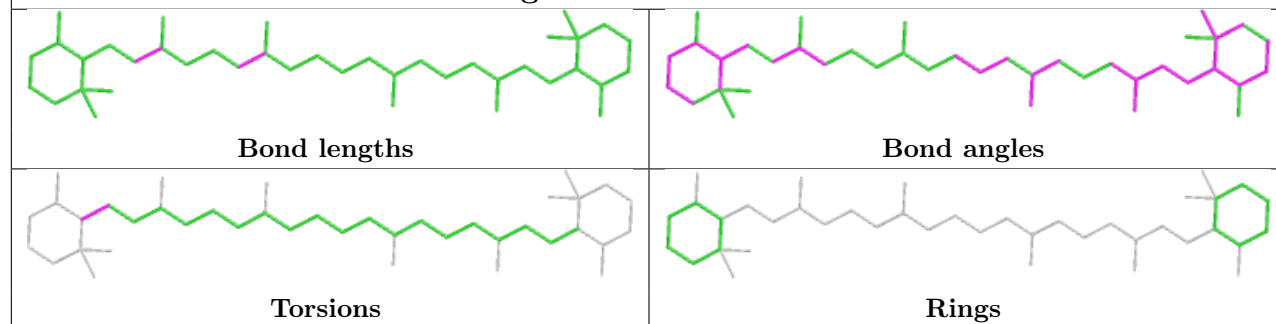


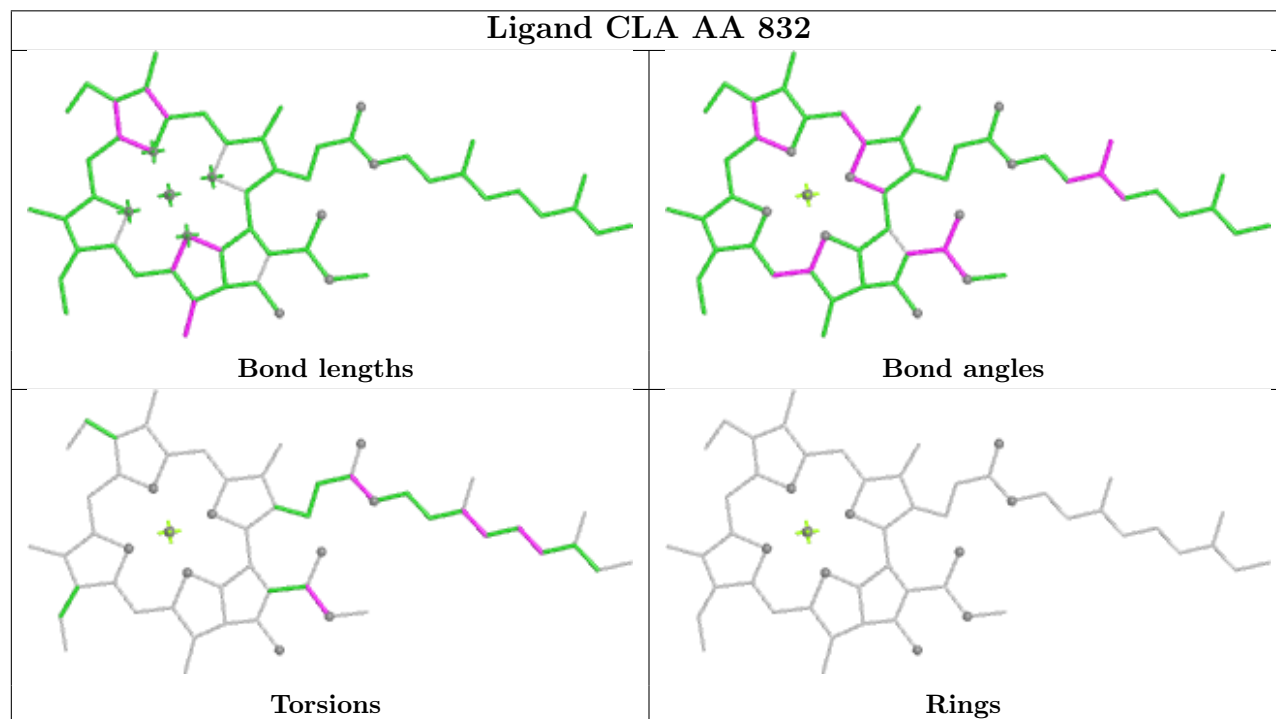
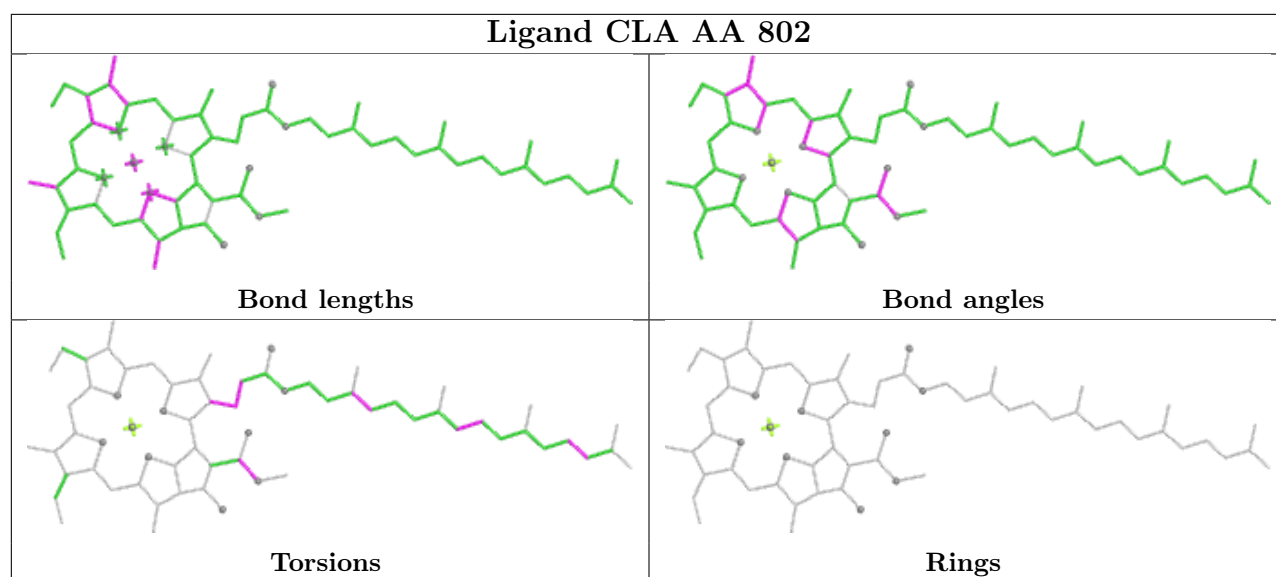


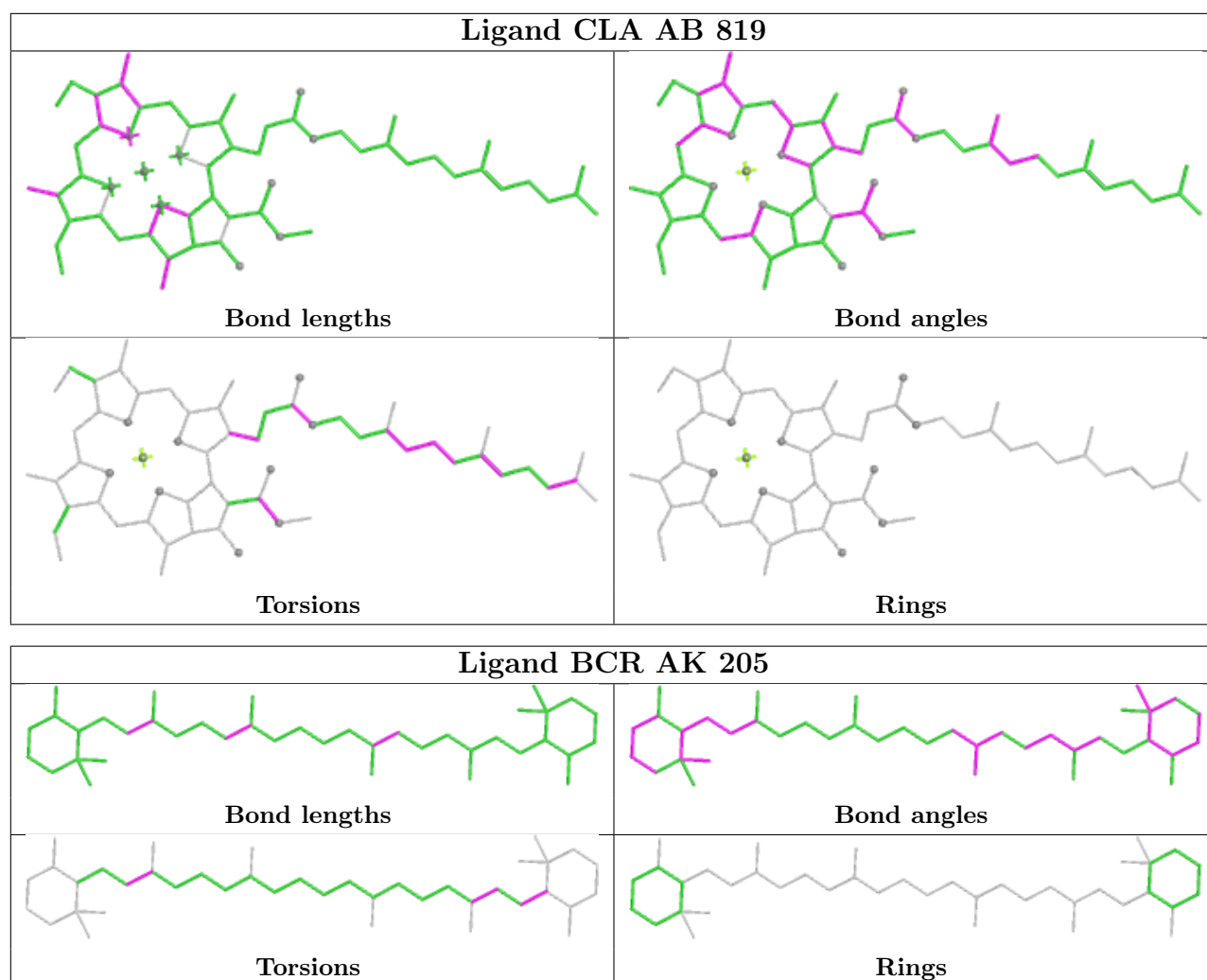
Ligand CLA AB 822



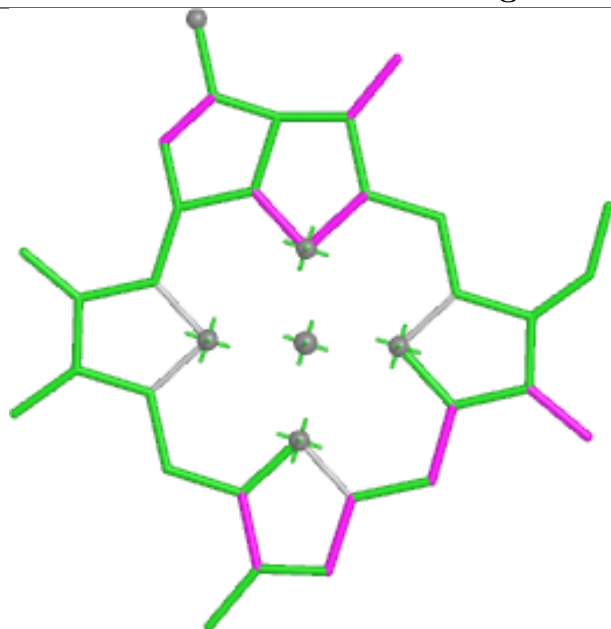
Ligand BCR A6 616



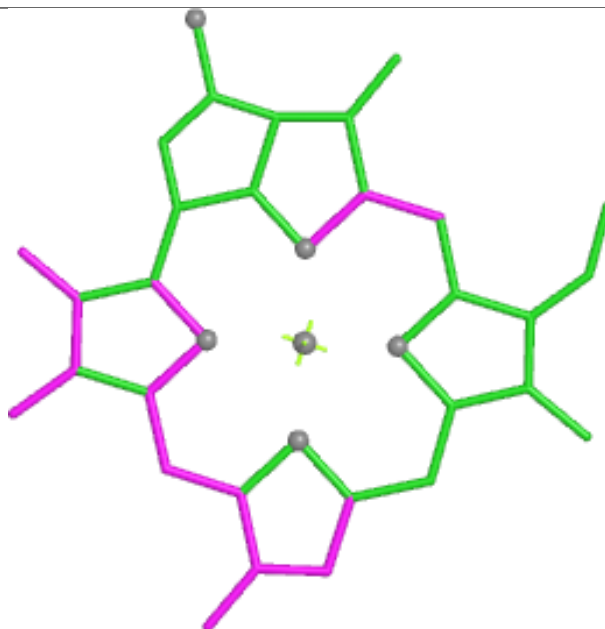




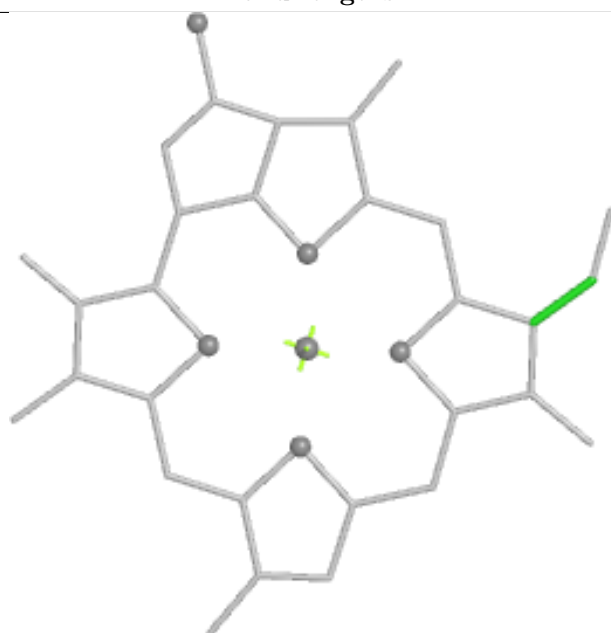
Ligand CLA AK 201



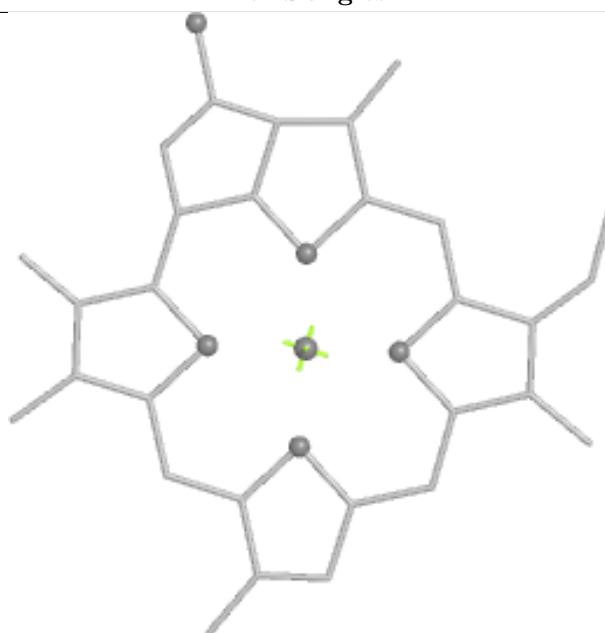
Bond lengths



Bond angles

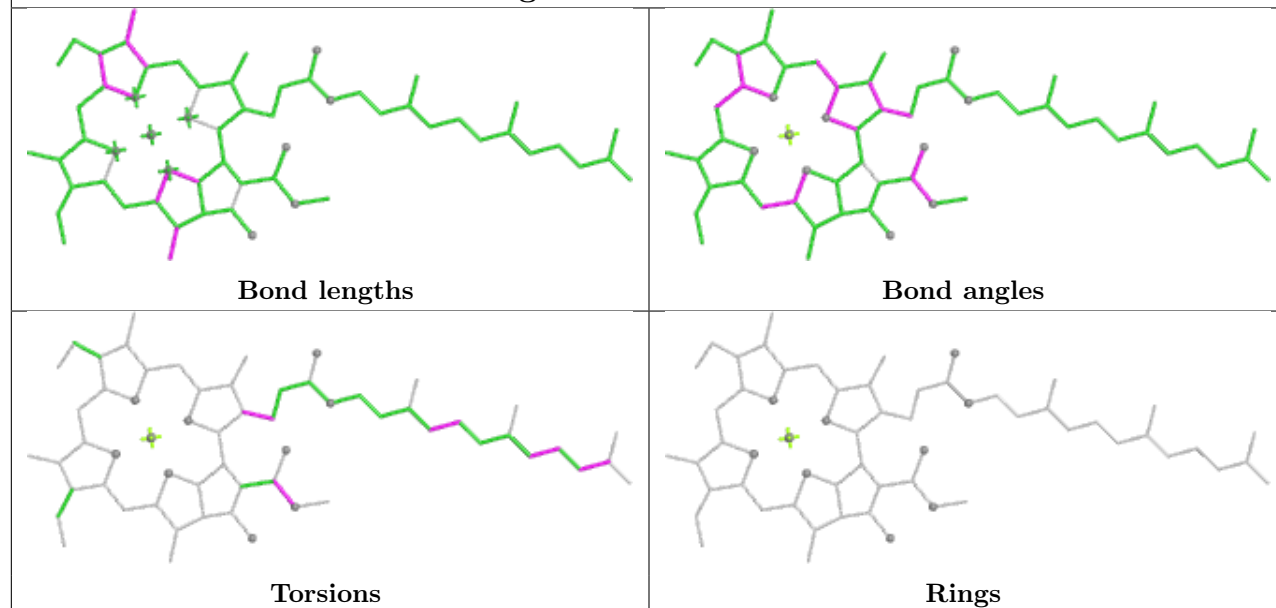


Torsions

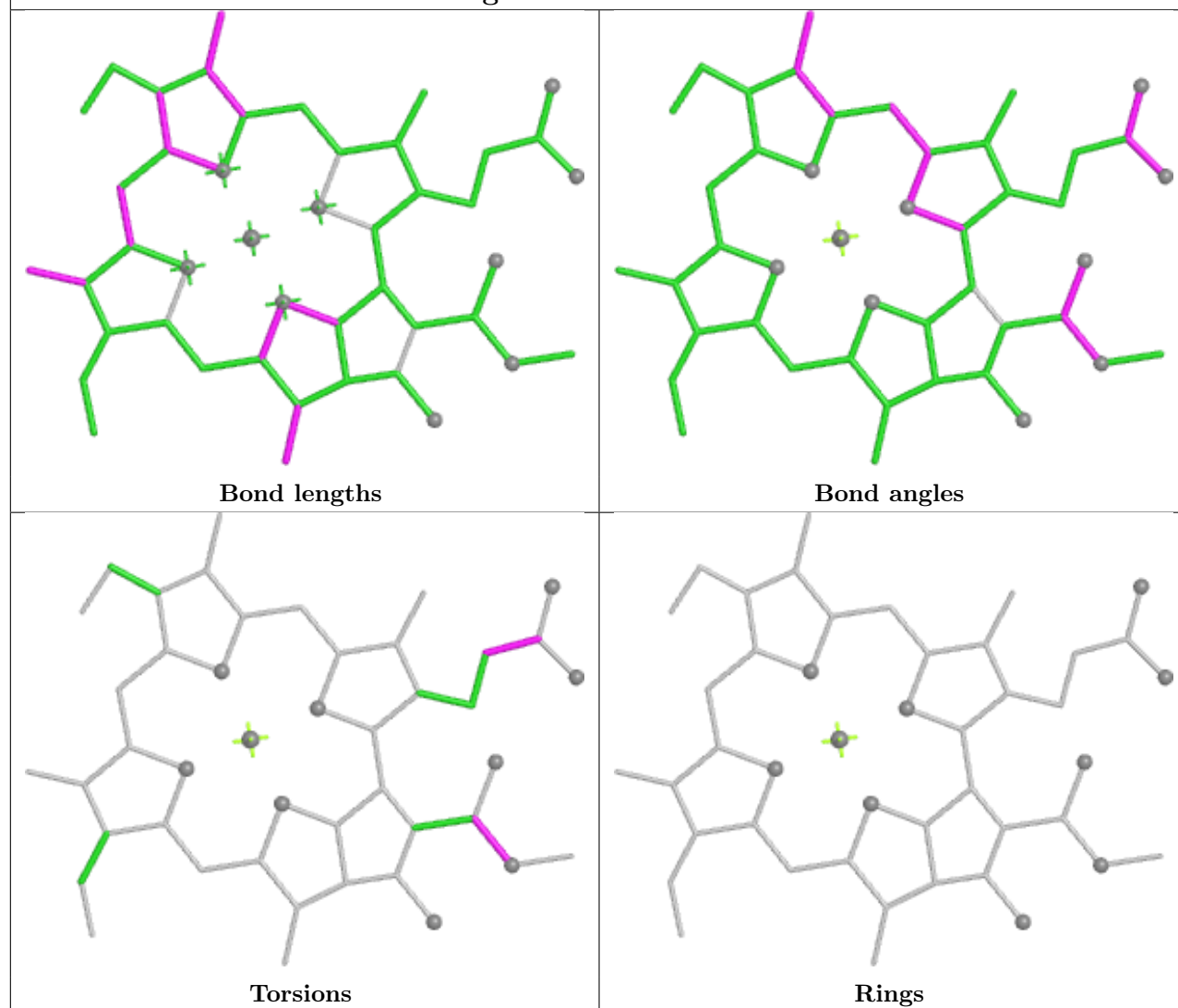


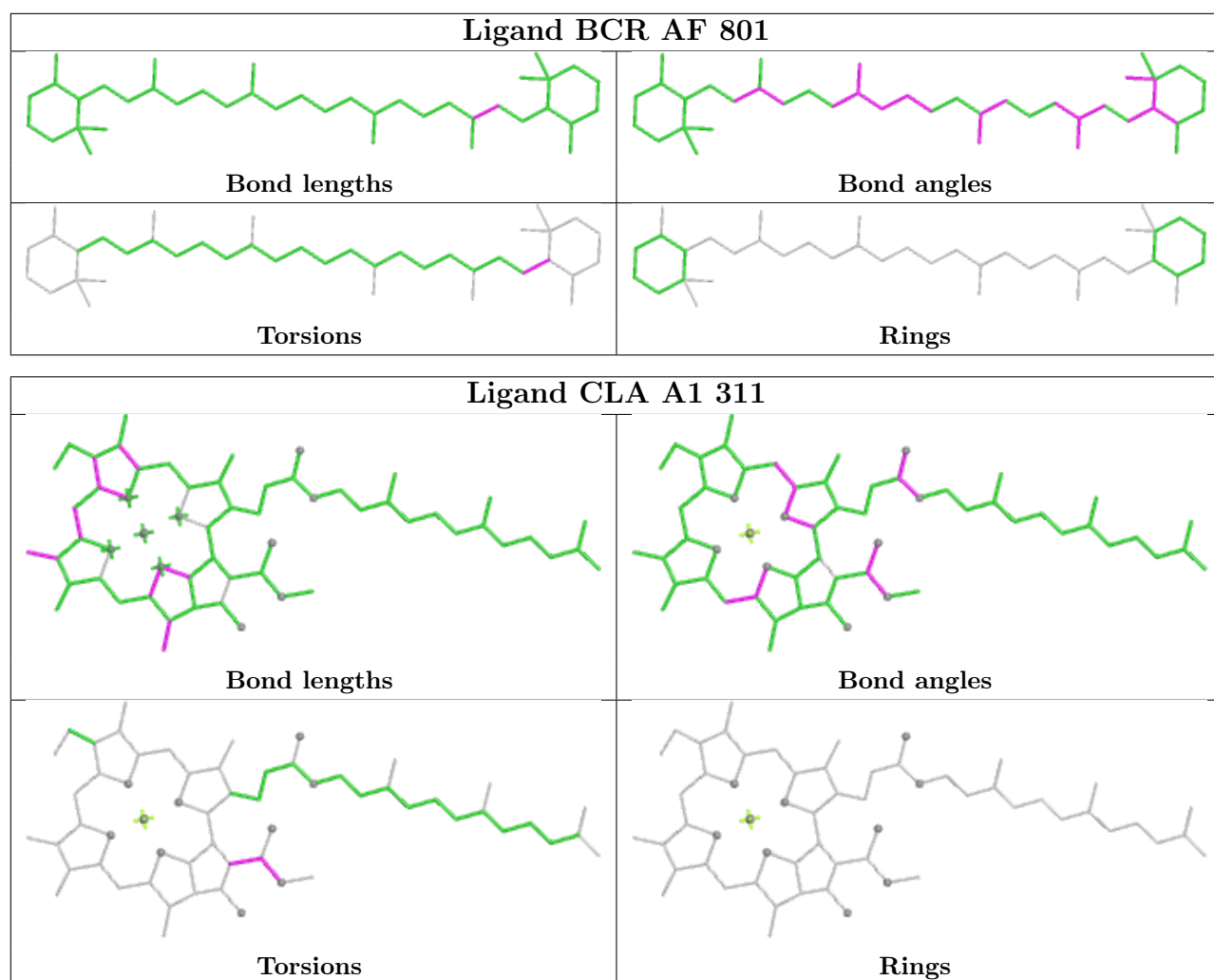
Rings

Ligand CLA AB 835

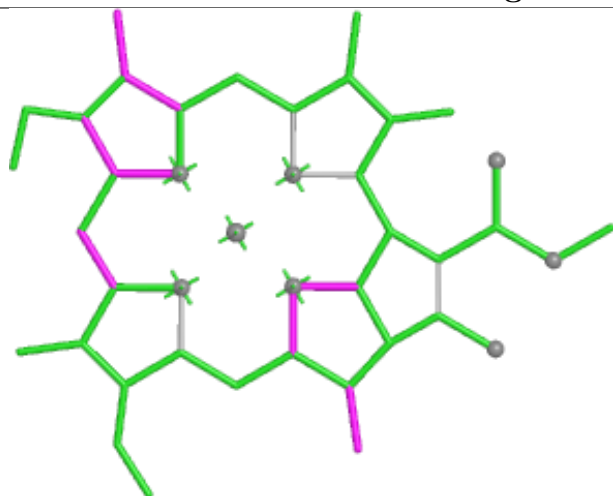


Ligand CLA A1 313





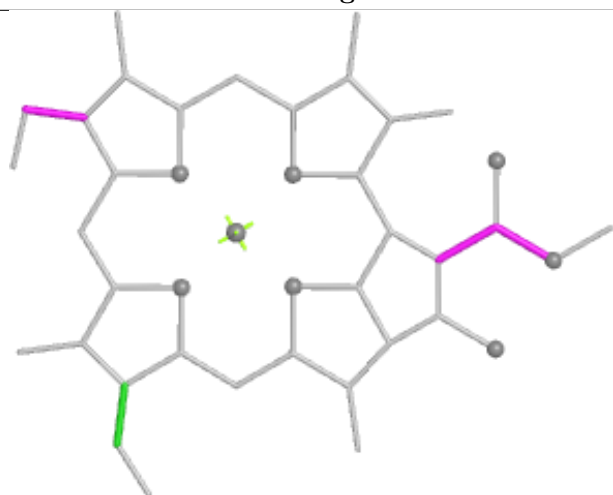
Ligand CLA A3 309



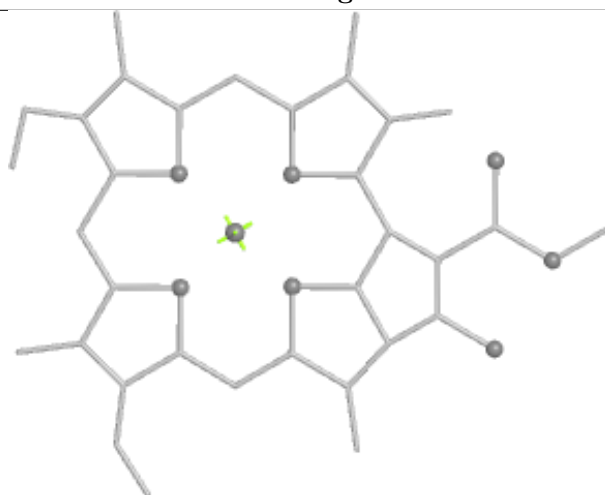
Bond lengths



Bond angles

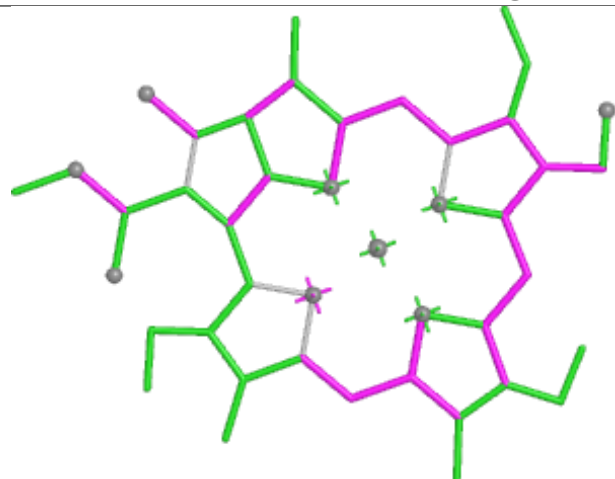


Torsions

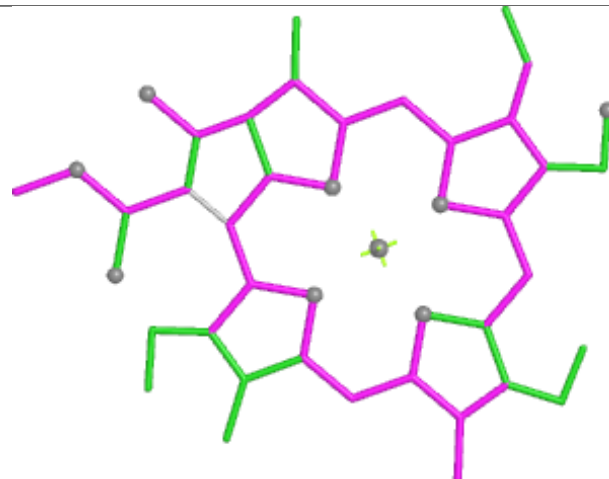


Rings

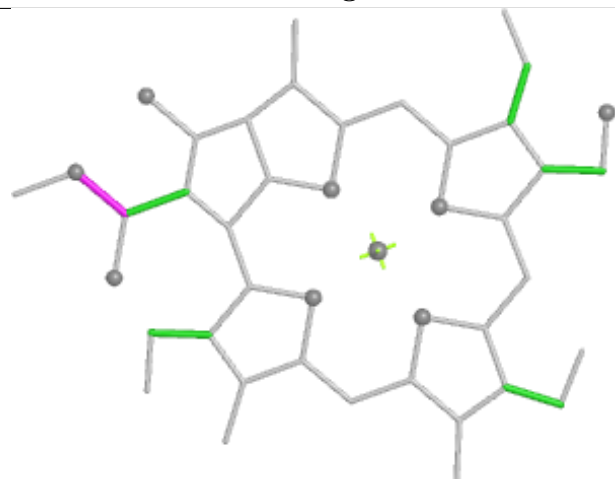
Ligand CHL A6 606



Bond lengths



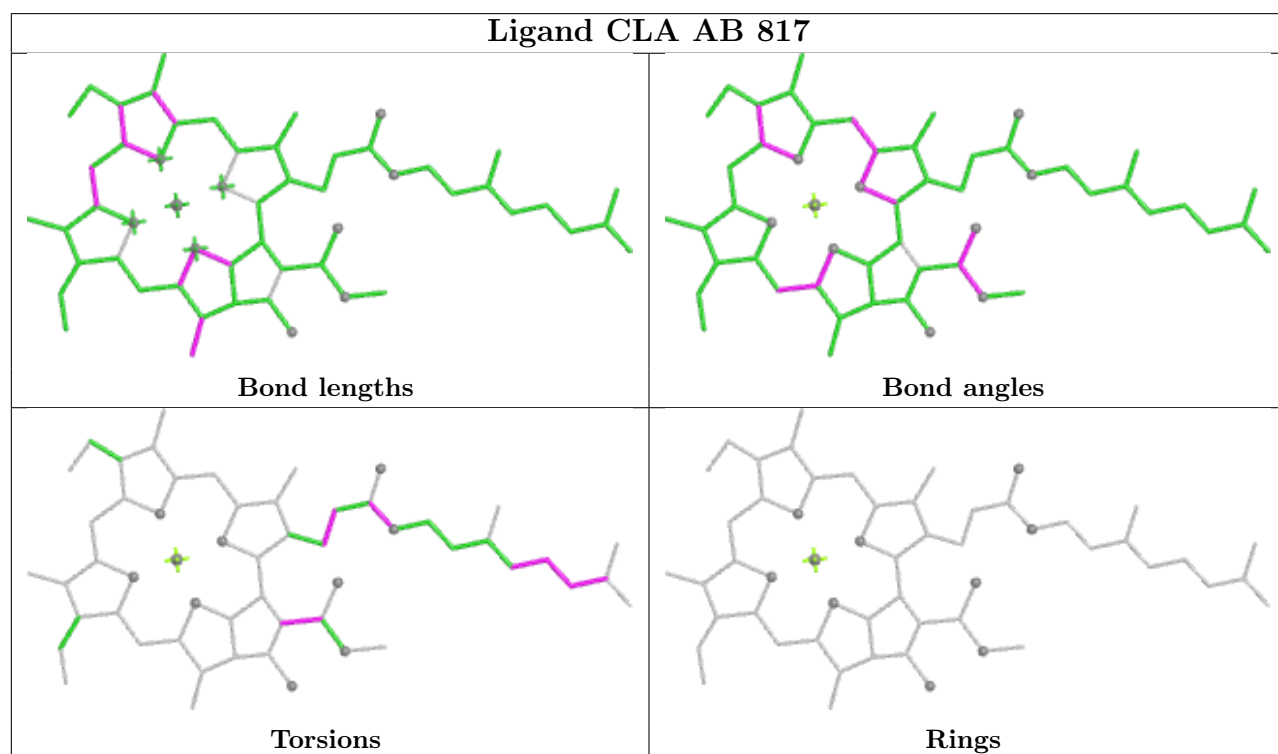
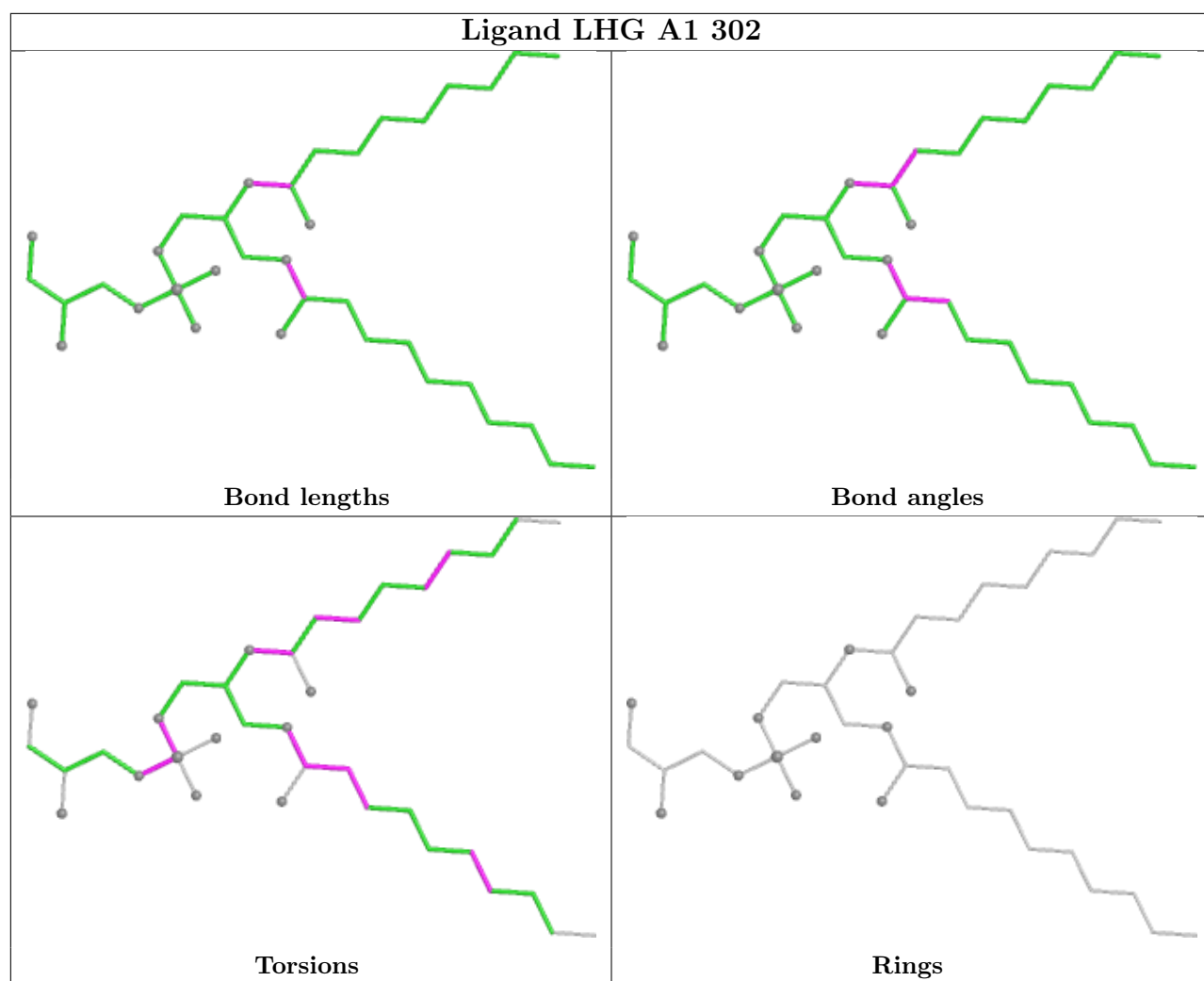
Bond angles



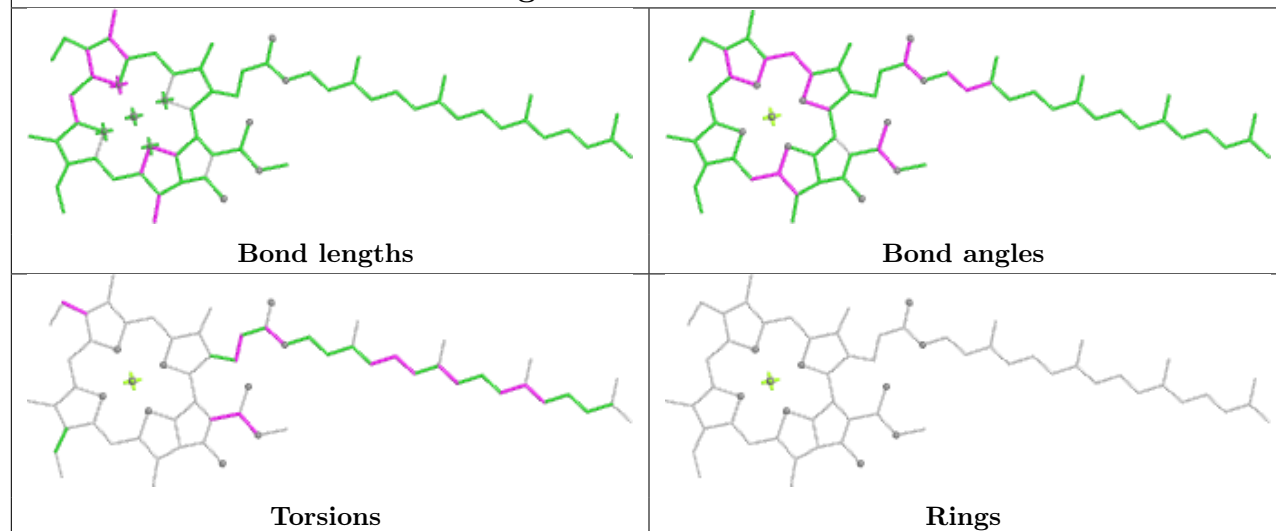
Torsions



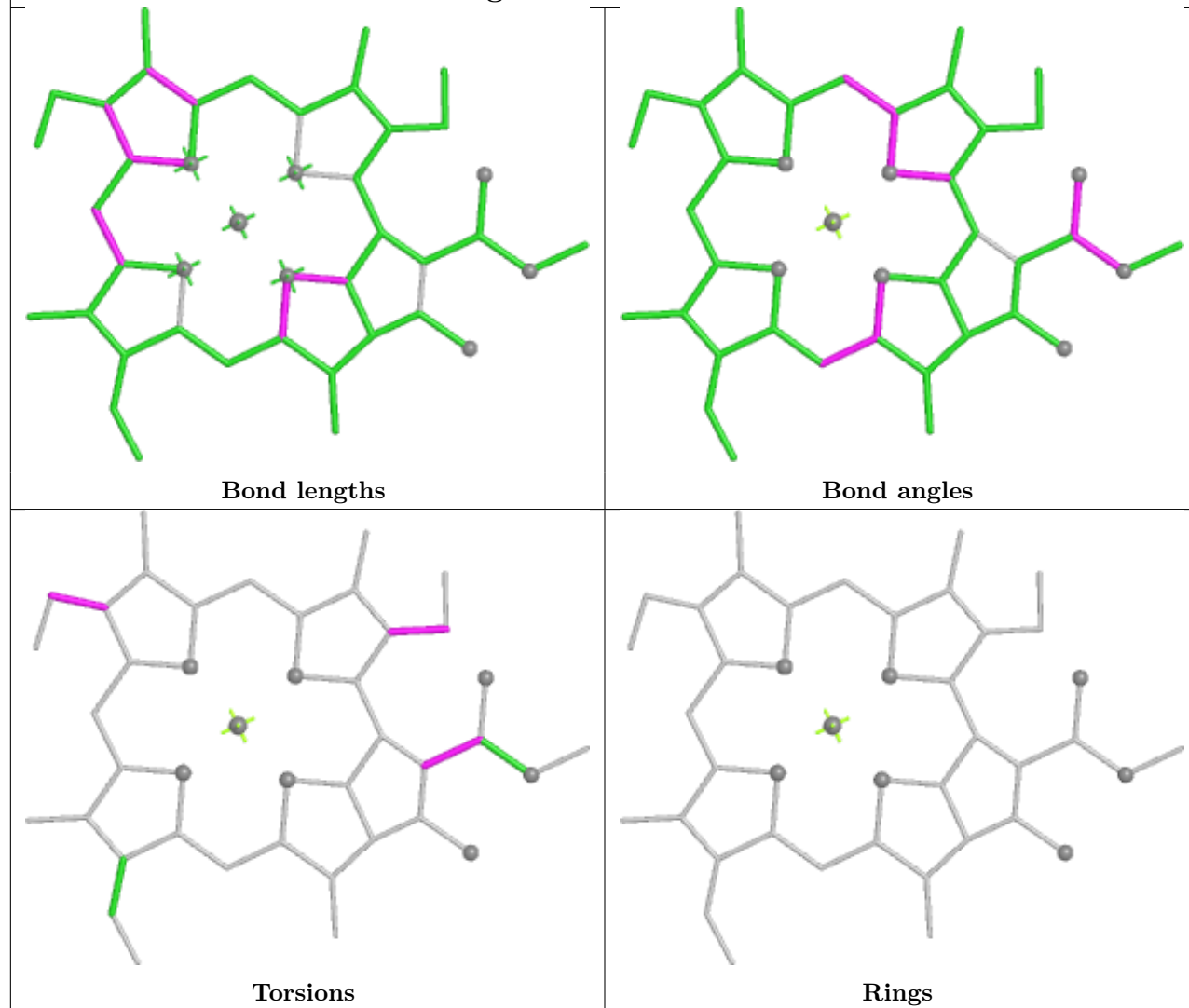
Rings

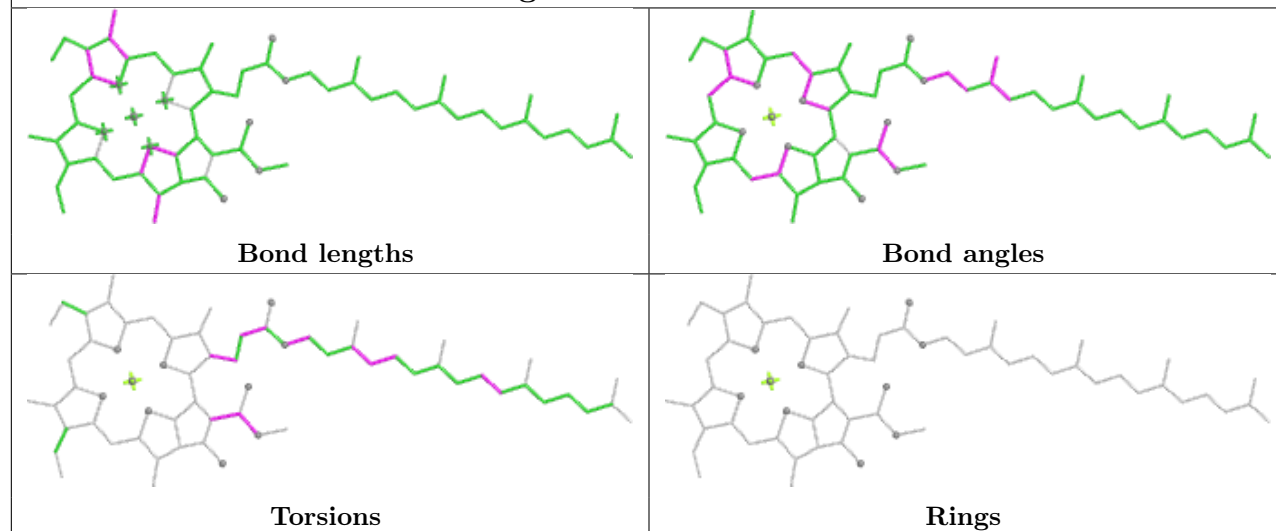
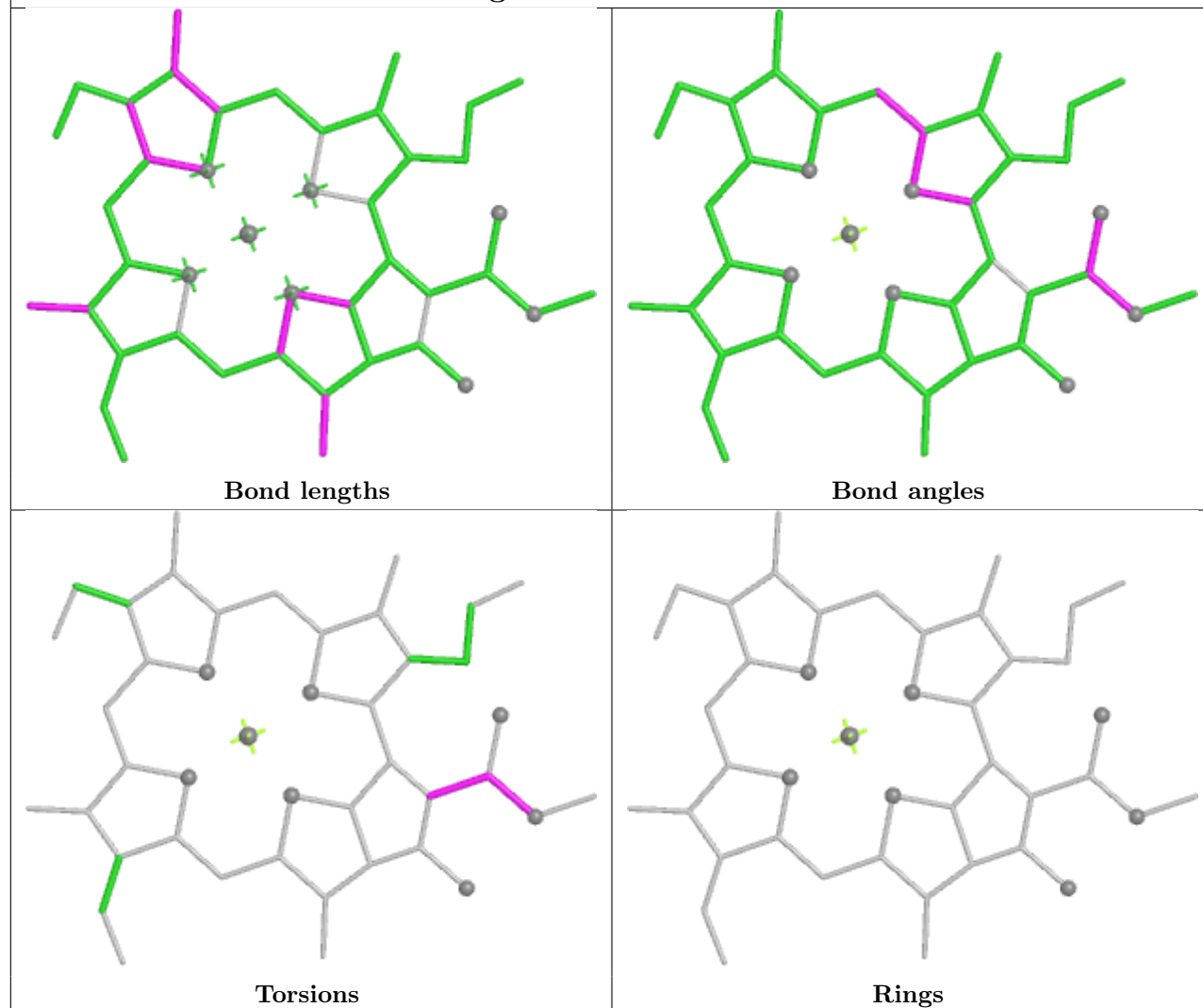


Ligand CLA AA 840

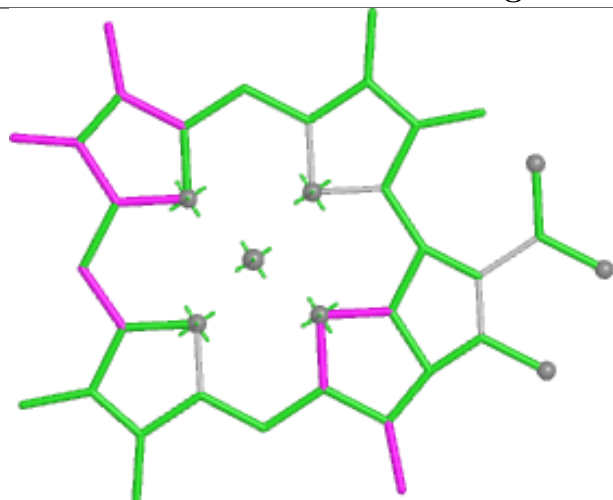


Ligand CLA AJ 102

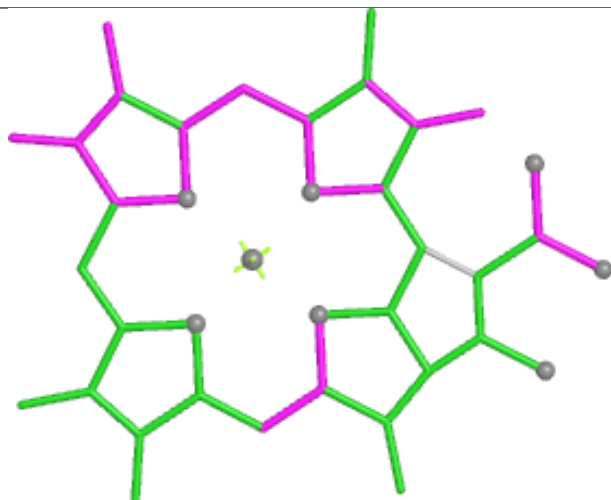


Ligand CLA AB 833**Ligand CLA AB 816**

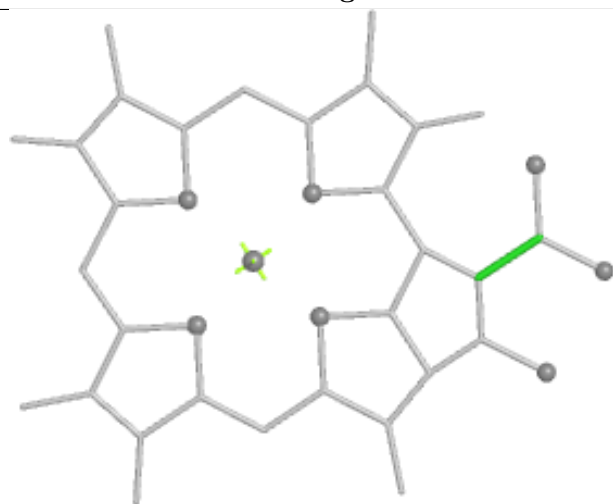
Ligand CLA A1 312



Bond lengths



Bond angles

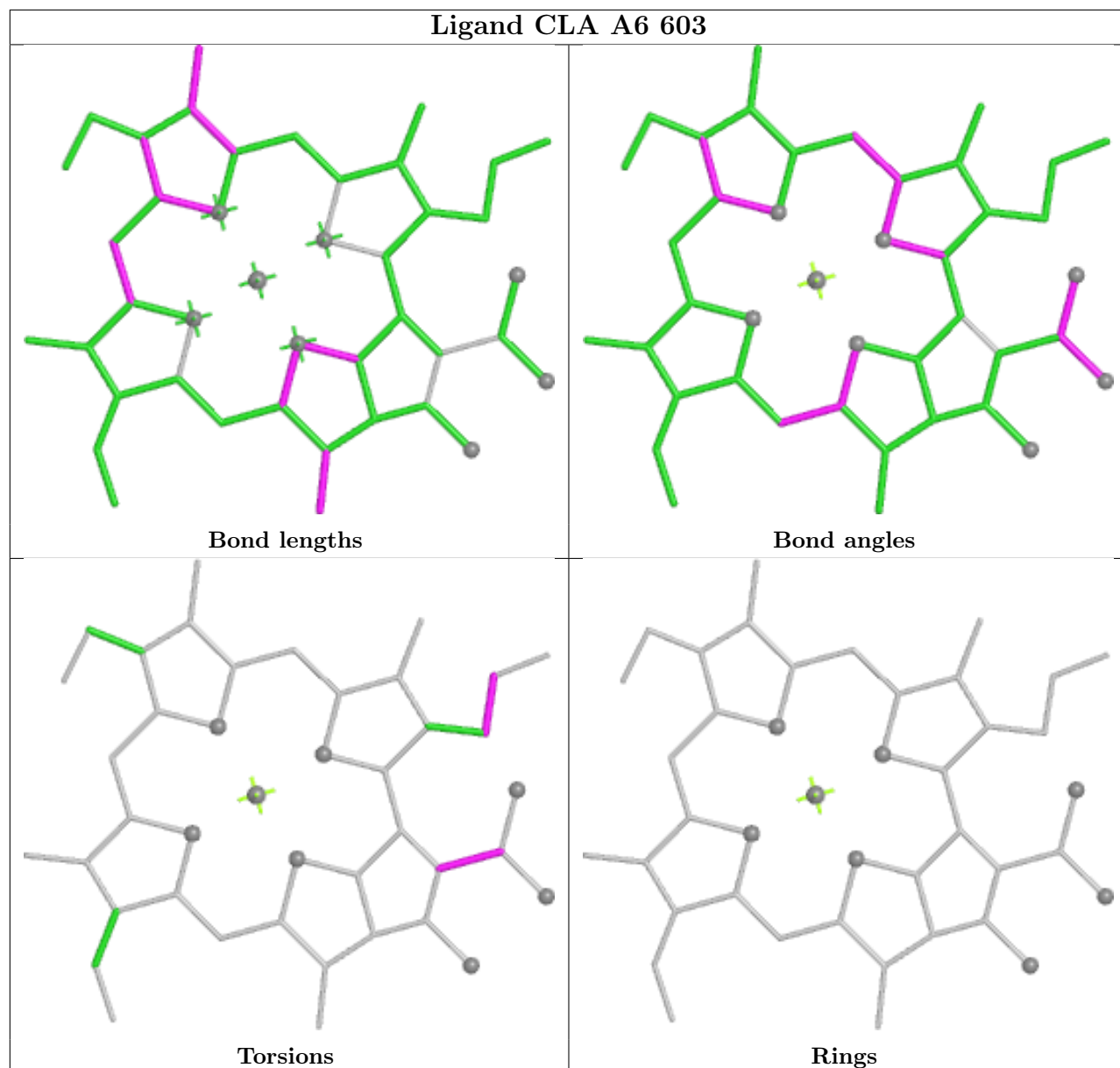


Torsions

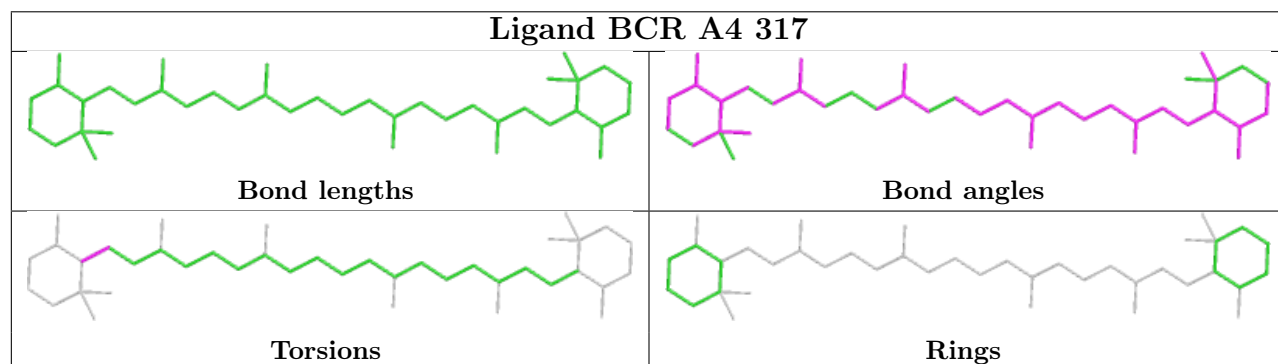


Rings

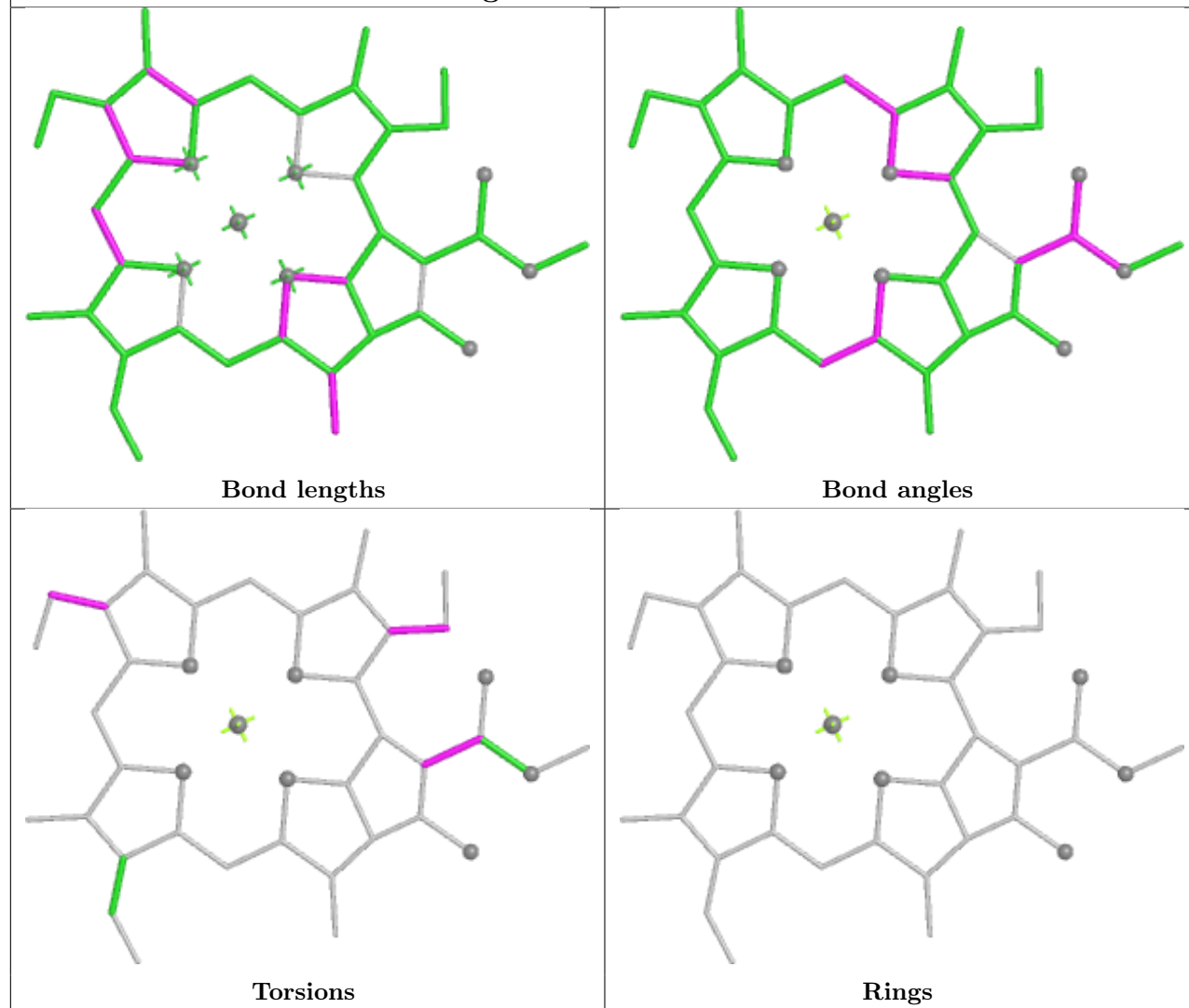
Ligand CLA A6 603



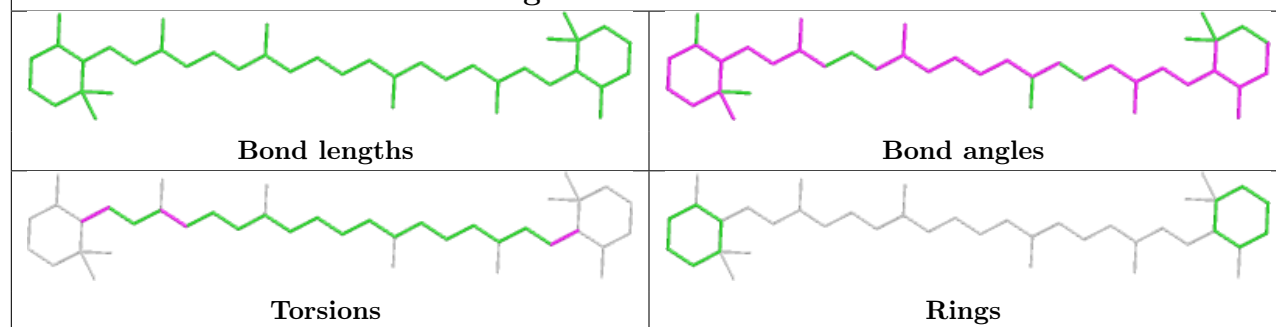
Ligand BCR A4 317

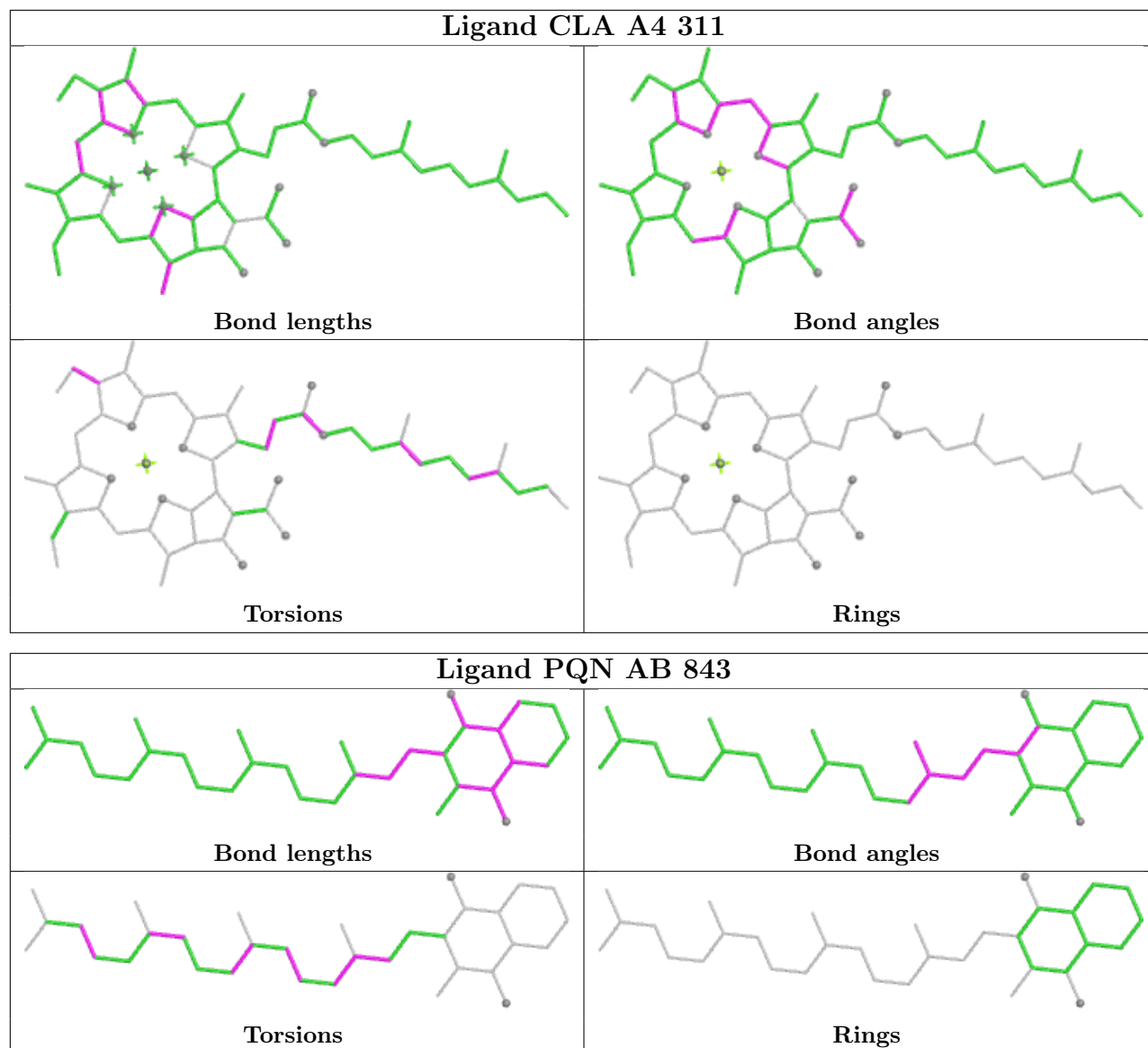


Ligand CLA AA 822

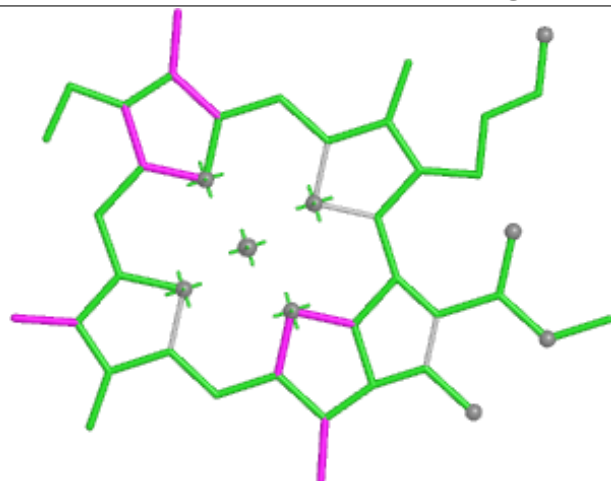


Ligand BCR AI 102

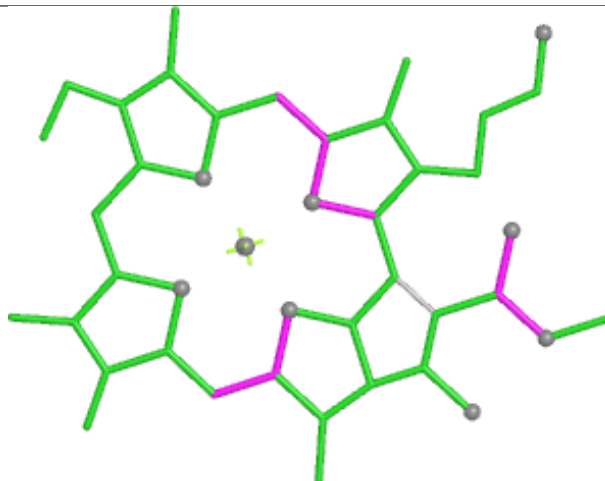




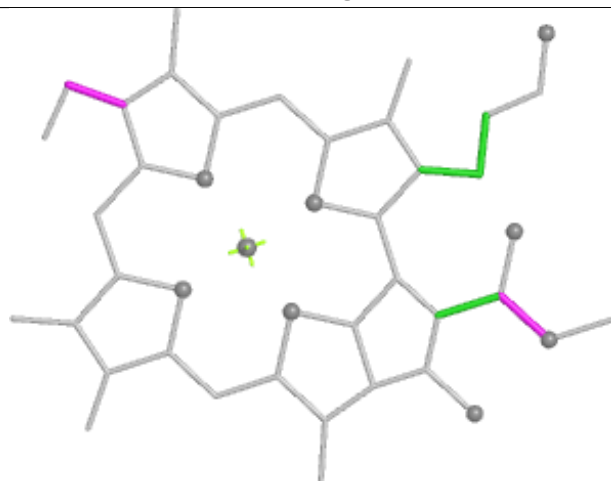
Ligand CLA A6 604



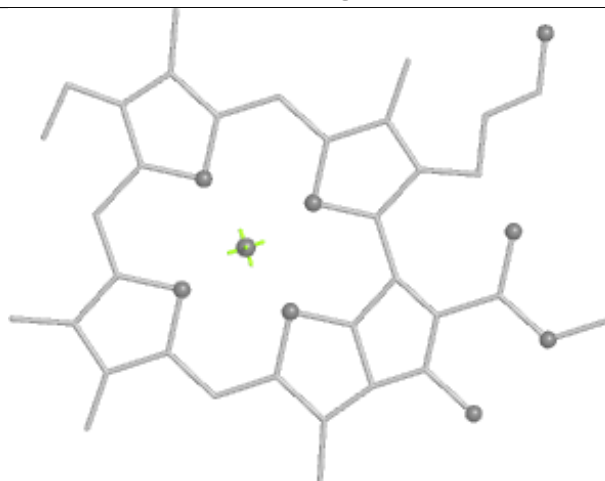
Bond lengths



Bond angles

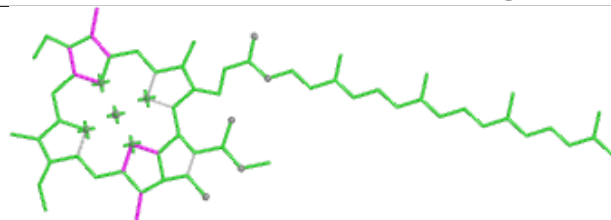


Torsions

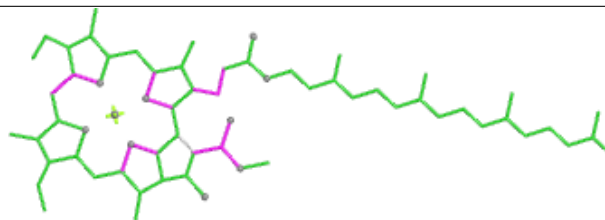


Rings

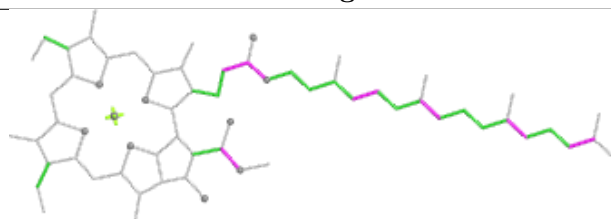
Ligand CLA AA 801



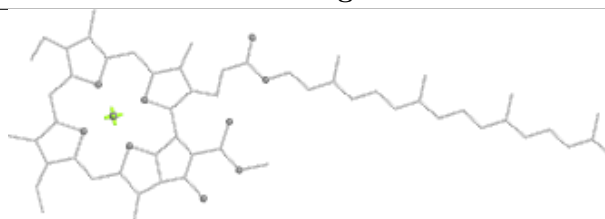
Bond lengths



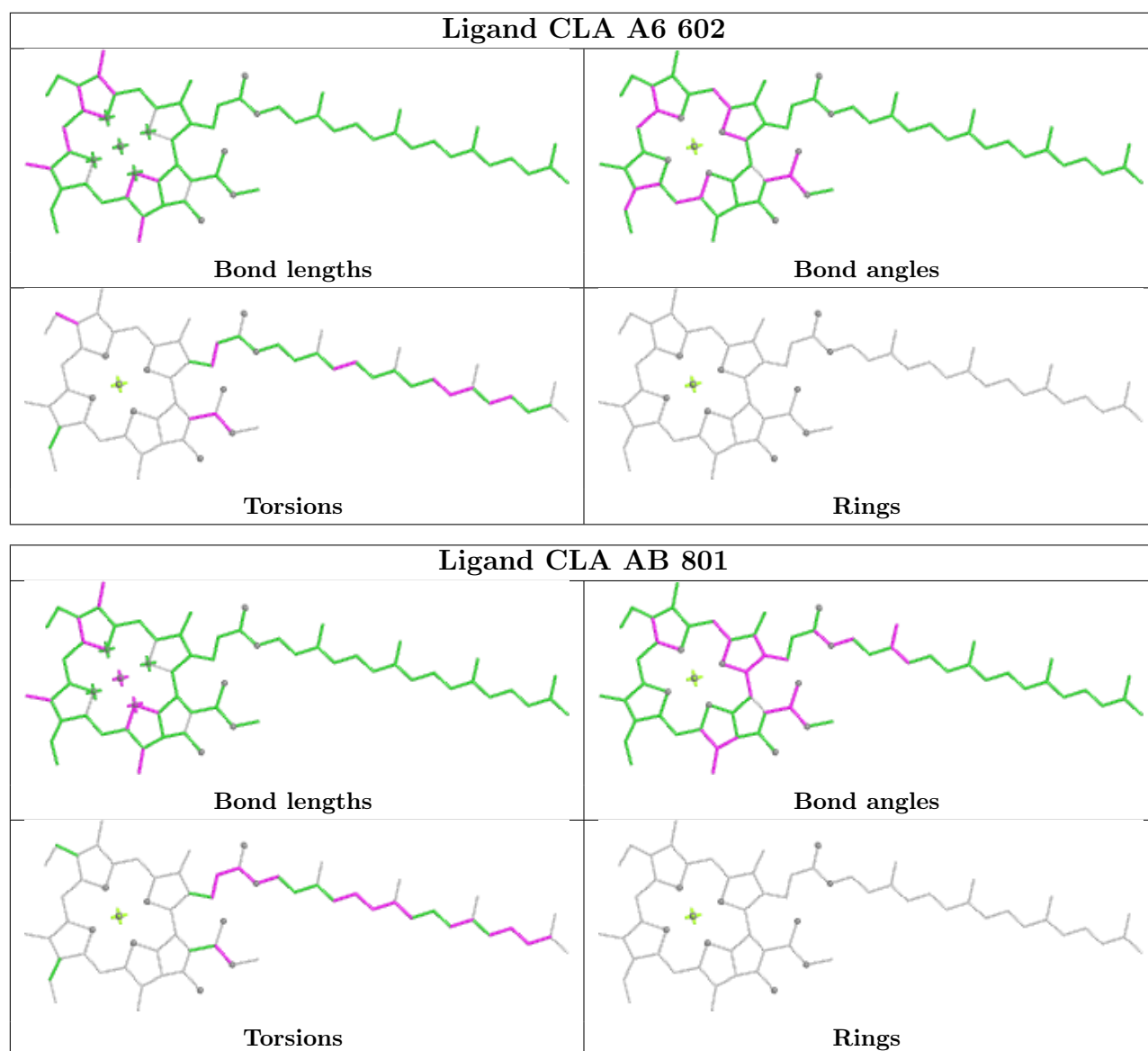
Bond angles



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.

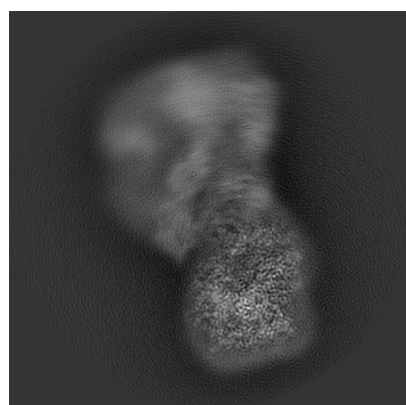
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32462. These allow visual inspection of the internal detail of the map and identification of artifacts.

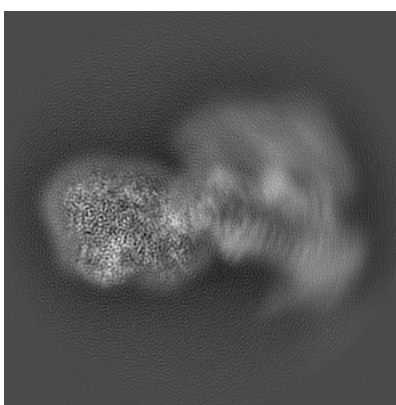
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

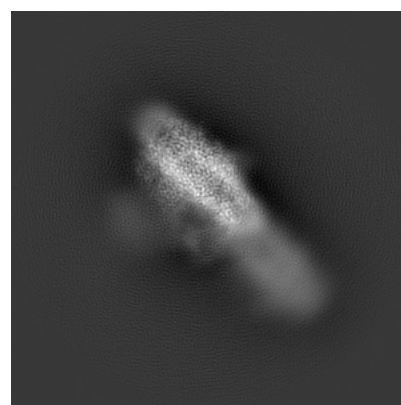
6.1.1 Primary map



X



Y

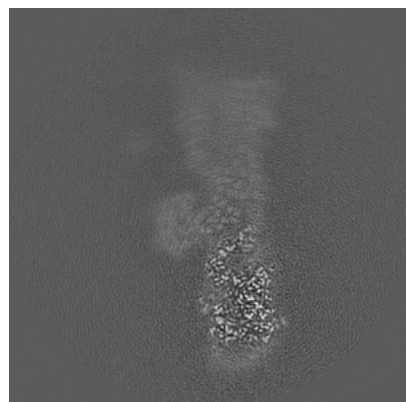


Z

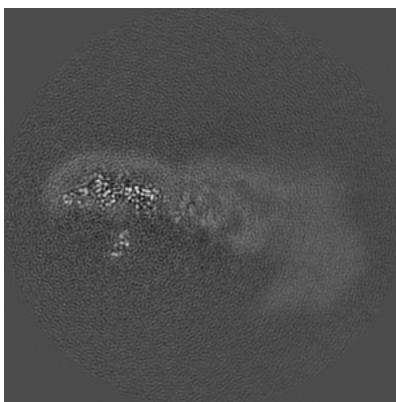
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

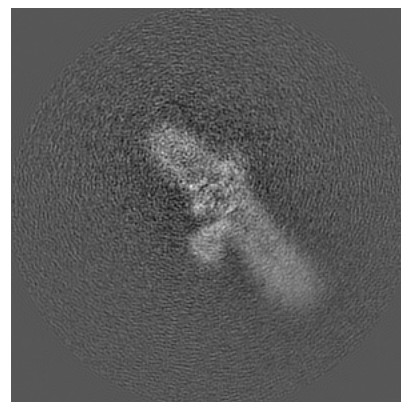
6.2.1 Primary map



X Index: 200



Y Index: 200

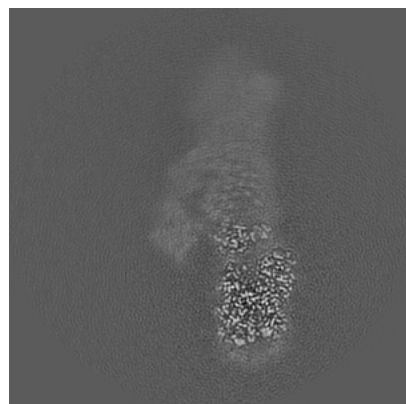


Z Index: 200

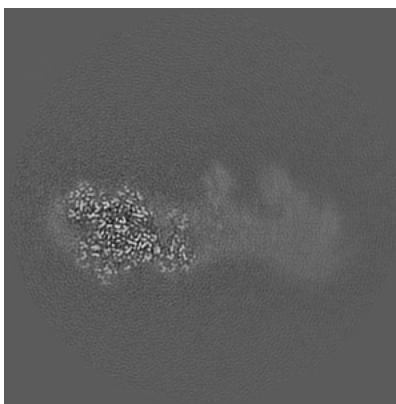
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

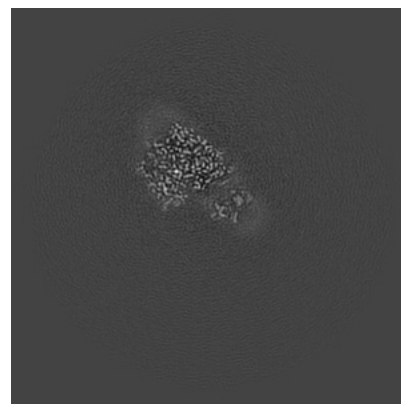
6.3.1 Primary map



X Index: 185



Y Index: 251

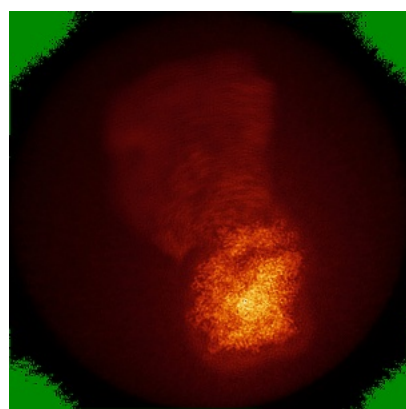


Z Index: 109

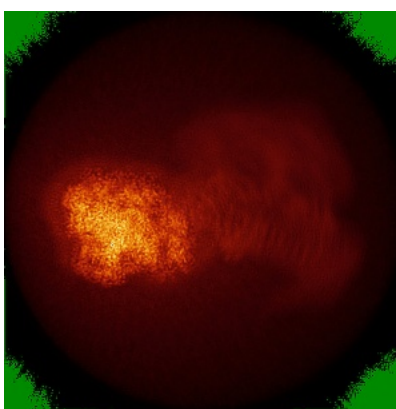
The images above show the largest variance slices of the map in three orthogonal directions.

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

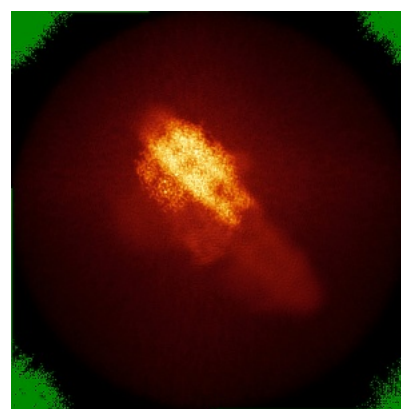
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

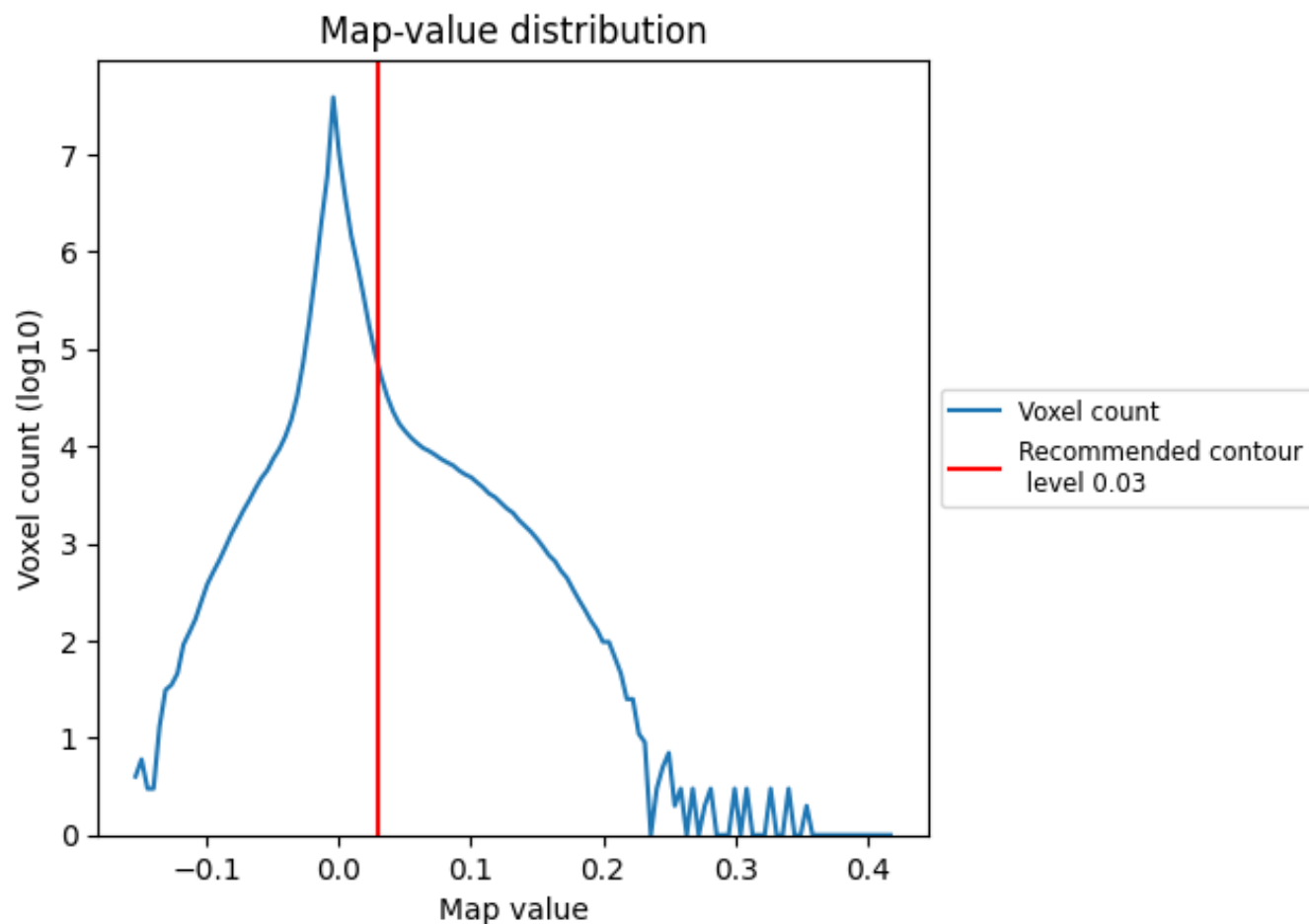
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

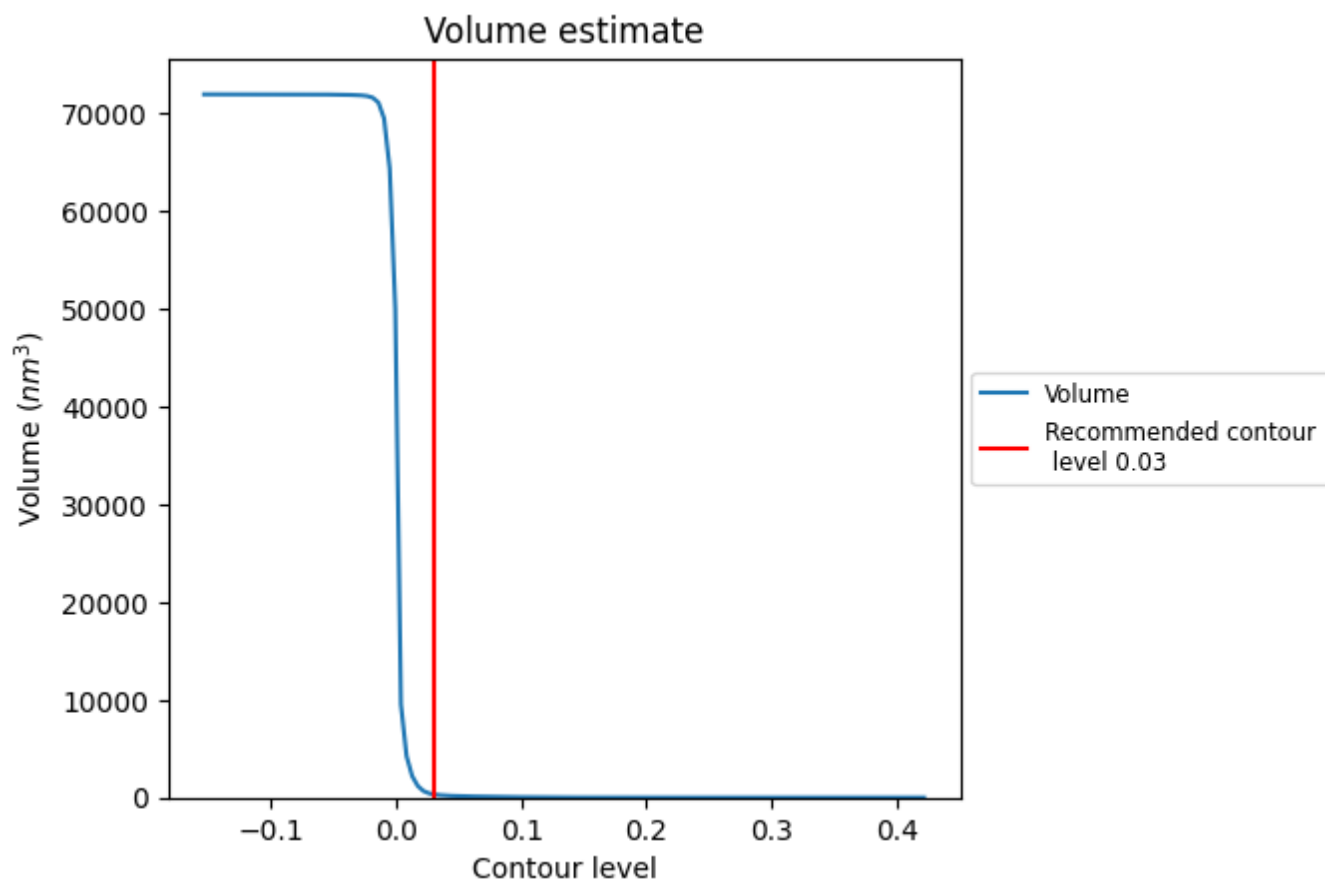
This section contains the results of statistical analysis of the map.

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.

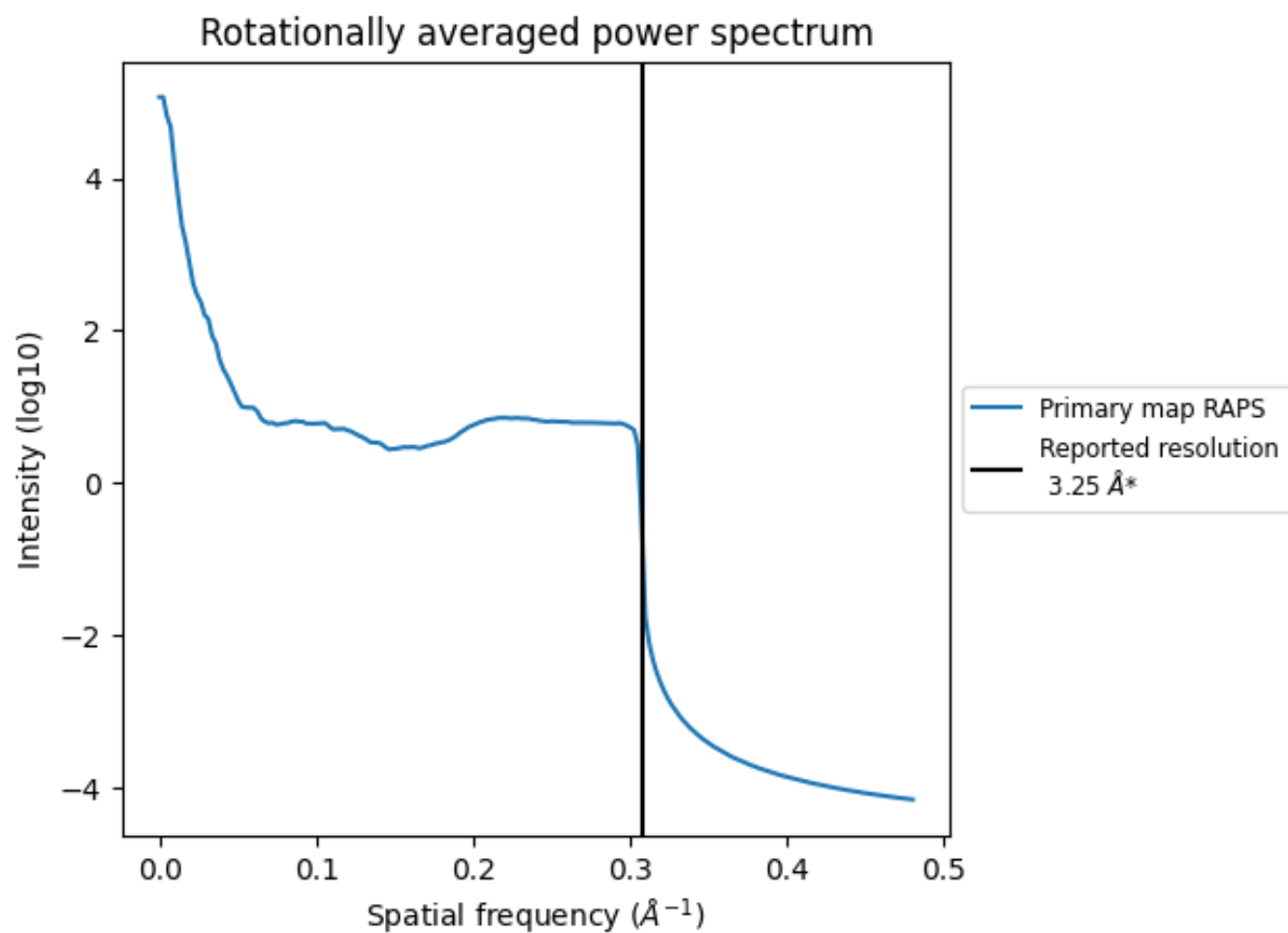
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm^3 ; this corresponds to an approximate mass of 305 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 0.308 Å⁻¹

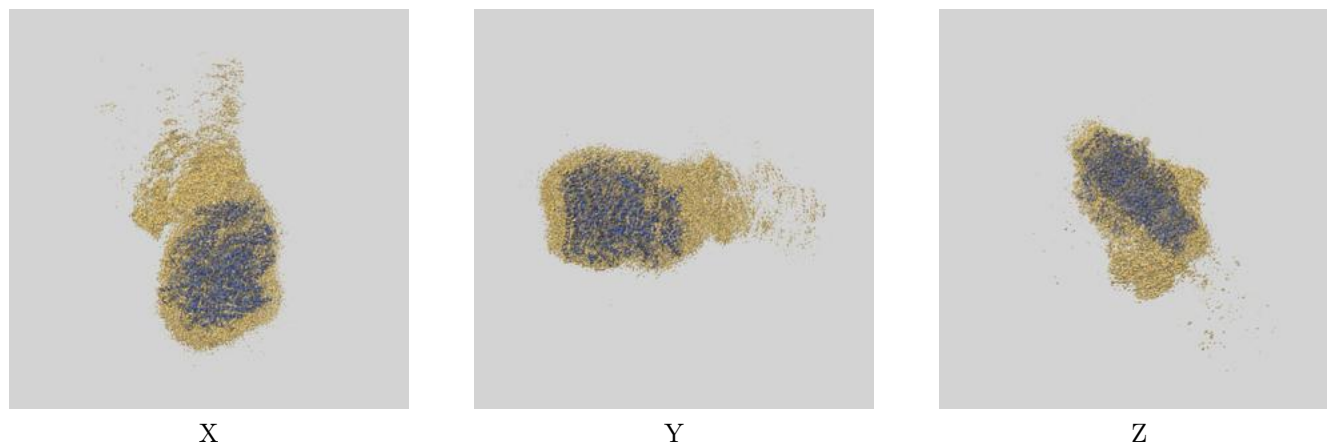
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

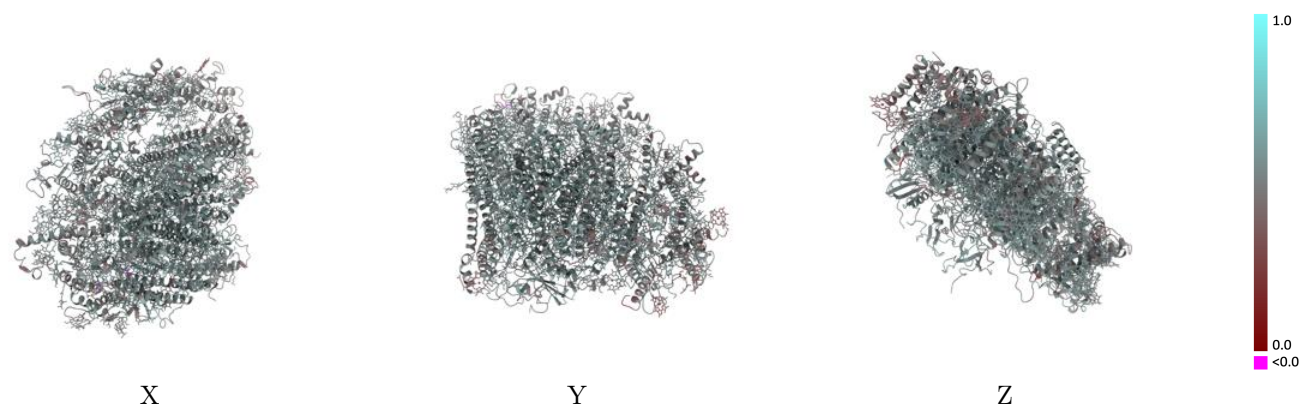
This section contains information regarding the fit between EMDB map EMD-32462 and PDB model 7WFD. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



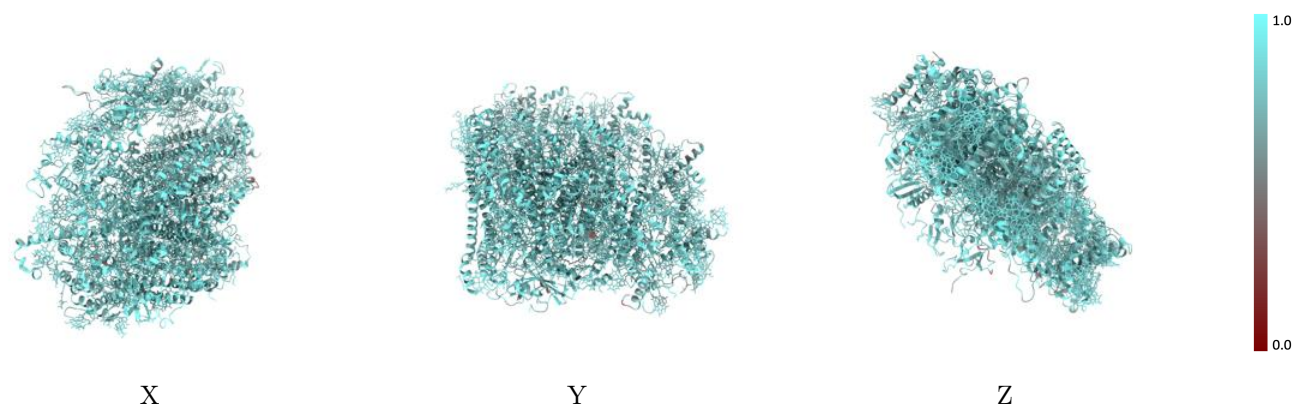
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



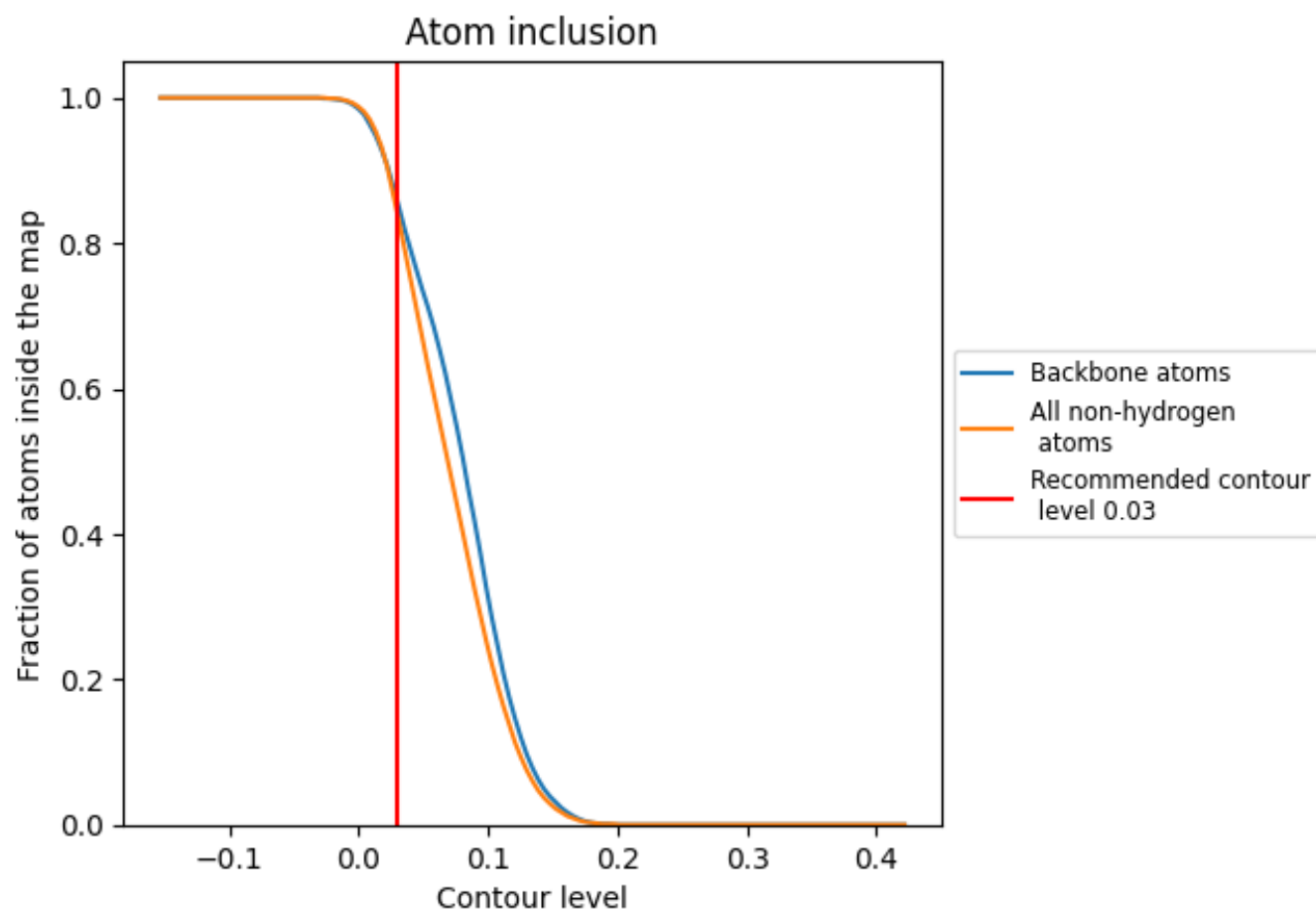
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8400	 0.5260
A1	 0.8080	 0.4950
A3	 0.8200	 0.4920
A4	 0.8260	 0.5120
A6	 0.7940	 0.5080
AA	 0.8520	 0.5410
AB	 0.8730	 0.5510
AC	 0.9040	 0.5380
AD	 0.8780	 0.5350
AE	 0.8330	 0.5360
AF	 0.8530	 0.5450
AG	 0.8030	 0.4910
AH	 0.8220	 0.4920
AI	 0.8040	 0.5050
AJ	 0.7780	 0.5130
AK	 0.7230	 0.4550
AL	 0.8090	 0.5000

