



wwPDB EM Validation Summary Report ⓘ

Jul 8, 2026 – 12:37 PM JST

PDB ID : 9L0A / pdb_00009l0a
EMDB ID : EMD-62693
Title : PSI trimer of Arthrospira platensis NIES-39
Authors : Kato, K.; Nakajima, Y.; Shen, J.R.; Nagao, R.
Deposited on : 2024-12-12
Resolution : 2.17 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

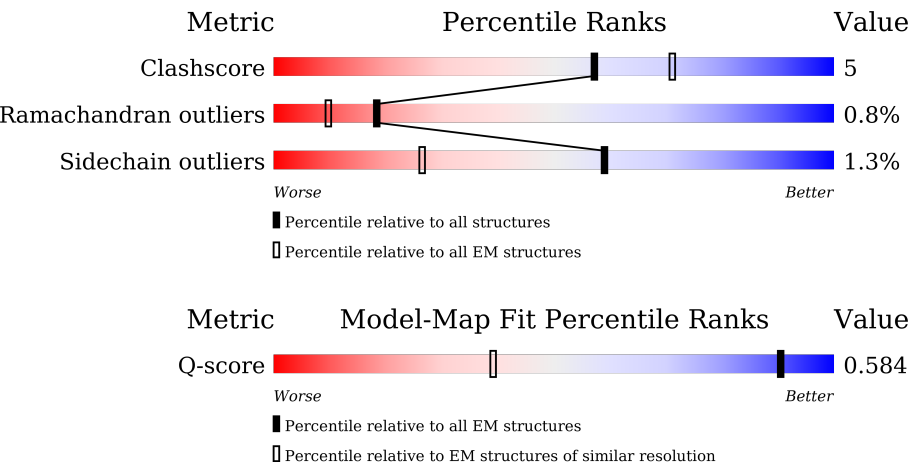
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.17 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	2651 (1.67 - 2.67)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	
1	bA	751	
1	cA	751	
2	B	741	

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Mol	Chain	Length	Quality of chain
2	bB	741	18% 91% 8% ..
2	cB	741	17% 91% 8% ..
3	C	81	93% 5% ..
3	bC	81	93% 5% ..
3	cC	81	95% ...
4	D	142	11% 94% . .
4	bD	142	13% 94% . .
4	cD	142	13% 94% . .
5	E	77	36% 84% . 12%
5	bE	77	35% 83% 5% 12%
5	cE	77	36% 84% . 12%
6	F	162	69% 76% 5% . 19%
6	bF	162	72% 76% 5% . 19%
6	cF	162	72% 76% 5% . 19%
7	I	38	89% 11%
7	bI	38	89% 11%
7	cI	38	89% 11%
8	J	41	78% 95% 5%
8	bJ	41	83% 93% 7%
8	cJ	41	83% 95% 5%
9	K	82	50% 52% 48%
9	bK	82	46% 52% 48%
9	cK	82	50% 52% 48%
10	L	161	6% 88% 9% ..
10	bL	161	6% 88% 9% ..

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Mol	Chain	Length	Quality of chain
10	cL	161	6% 88% 10%
11	M	31	13% 90% 6%
11	bM	31	13% 90% 6%
11	cM	31	13% 90% 6%
12	X	36	56% 56% 42%
12	bX	36	56% 56% 42%
12	cX	36	53% 56% 42%

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 70131 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	731	Total	C	N	O	S	0	0
			5742	3755	981	979	27		
1	bA	731	Total	C	N	O	S	0	0
			5742	3755	981	979	27		
1	cA	731	Total	C	N	O	S	0	0
			5742	3755	981	979	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	736	Total	C	N	O	S	0	0
			5886	3873	989	1004	20		
2	bB	736	Total	C	N	O	S	0	0
			5886	3873	989	1004	20		
2	cB	736	Total	C	N	O	S	0	0
			5886	3873	989	1004	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			599	368	103	117	11		
3	bC	80	Total	C	N	O	S	0	0
			599	368	103	117	11		
3	cC	80	Total	C	N	O	S	0	0
			599	368	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1084	692	183	205	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	138	Total	C	N	O	S	0	0
			1084	692	183	205	4		
4	cD	138	Total	C	N	O	S	0	0
			1084	692	183	205	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	68	Total	C	N	O	S	0	0
			544	344	95	104	1		
5	bE	68	Total	C	N	O	S	0	0
			544	344	95	104	1		
5	cE	68	Total	C	N	O	S	0	0
			544	344	95	104	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	132	Total	C	N	O	S	0	0
			1023	656	169	193	5		
6	bF	132	Total	C	N	O	S	0	0
			1023	656	169	193	5		
6	cF	132	Total	C	N	O	S	0	0
			1023	656	169	193	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			297	202	42	49	4		
7	bI	38	Total	C	N	O	S	0	0
			297	202	42	49	4		
7	cI	38	Total	C	N	O	S	0	0
			297	202	42	49	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			339	234	51	53	1		
8	bJ	41	Total	C	N	O	S	0	0
			339	234	51	53	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	cJ	41	Total	C	N	O	S	0	0
			339	234	51	53	1		

- Molecule 9 is a protein called Unknown.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	43	Total	C	N	O		0	0
			208	122	43	43			
9	bK	43	Total	C	N	O		0	0
			208	122	43	43			
9	cK	43	Total	C	N	O		0	0
			208	122	43	43			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	158	Total	C	N	O	S	0	0
			1178	765	194	214	5		
10	bL	158	Total	C	N	O	S	0	0
			1178	765	194	214	5		
10	cL	158	Total	C	N	O	S	0	0
			1178	765	194	214	5		

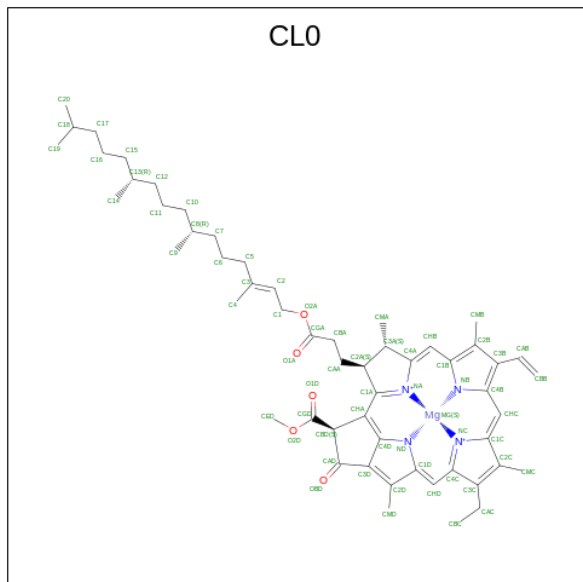
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	bM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	cM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit psaX.

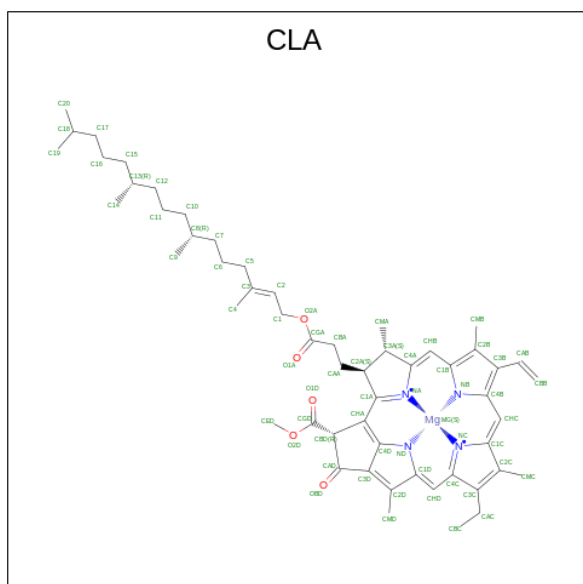
Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	21	Total	C	N	O		0	0
			171	120	26	25			
12	bX	21	Total	C	N	O		0	0
			171	120	26	25			
12	cX	21	Total	C	N	O		0	0
			171	120	26	25			

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bB	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 48	C 38	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bB	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	bB	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	bB	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 42	C 34	Mg 1	N 4	O 3	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bF	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	bJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bL	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bX	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 53	C 43	Mg 1	N 4	O 5	0
14	cA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cB	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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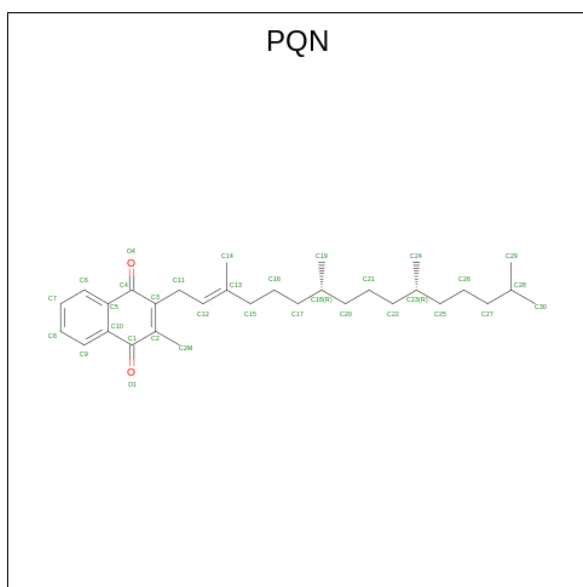
Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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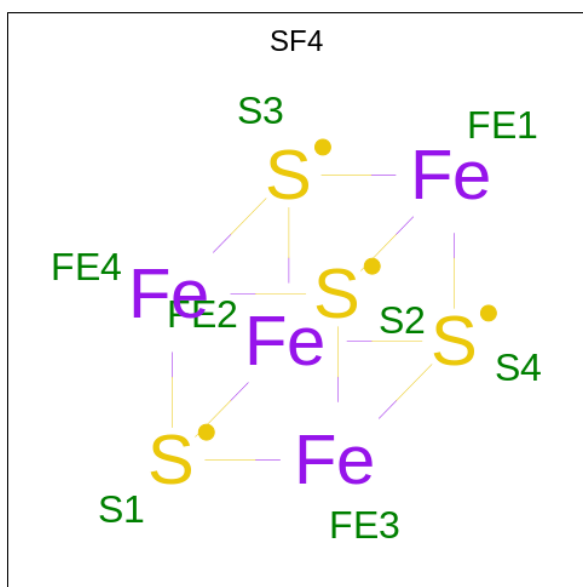
Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	cJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



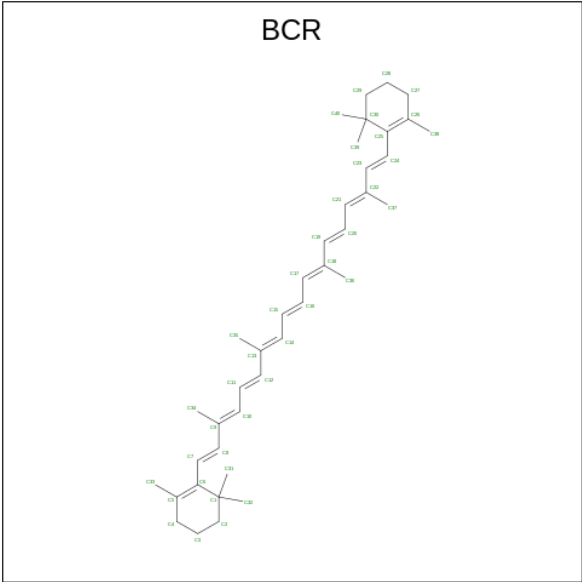
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	
15	bA	1	Total	C	O	0
			33	31	2	
15	bB	1	Total	C	O	0
			33	31	2	
15	cA	1	Total	C	O	0
			33	31	2	
15	cB	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	Fe	S	0
			8	4	4	
16	C	1	Total	Fe	S	0
			8	4	4	
16	C	1	Total	Fe	S	0
			8	4	4	
16	bA	1	Total	Fe	S	0
			8	4	4	
16	bC	1	Total	Fe	S	0
			8	4	4	
16	bC	1	Total	Fe	S	0
			8	4	4	
16	cA	1	Total	Fe	S	0
			8	4	4	
16	cC	1	Total	Fe	S	0
			8	4	4	
16	cC	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms	AltConf
17	I	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bI	1	Total C 40 40	0

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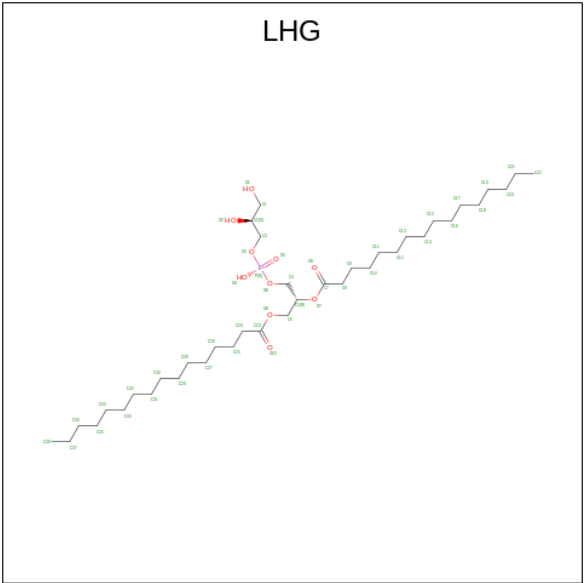
Mol	Chain	Residues	Atoms	AltConf
17	bI	1	Total C 40 40	0
17	bJ	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bM	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cI	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
17	cJ	1	Total	C	0
			40	40	
17	cL	1	Total	C	0
			40	40	
17	cL	1	Total	C	0
			40	40	
17	cM	1	Total	C	0
			40	40	

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).

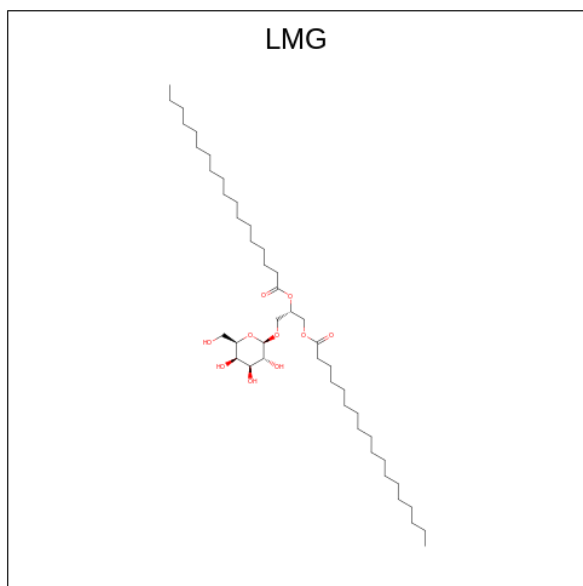


Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			49	38	10	1	
18	A	1	Total	C	O	P	0
			27	16	10	1	
18	bA	1	Total	C	O	P	0
			49	38	10	1	
18	bA	1	Total	C	O	P	0
			27	16	10	1	
18	cA	1	Total	C	O	P	0
			49	38	10	1	
18	cA	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 19 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	C	0
			12	12	
19	I	2	Total	C	0
			22	22	
19	L	2	Total	C	0
			29	29	
19	bA	1	Total	C	0
			12	12	
19	bI	2	Total	C	0
			22	22	
19	bL	2	Total	C	0
			29	29	
19	cA	1	Total	C	0
			12	12	
19	cI	2	Total	C	0
			22	22	
19	cL	2	Total	C	0
			29	29	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	C	O	0
			43	33	10	
20	bB	1	Total	C	O	0
			43	33	10	

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Mol	Chain	Residues	Atoms			AltConf
20	cB	1	Total	C	O	0
			43	33	10	

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	L	1	Total	Ca	0
			1	1	
21	bL	1	Total	Ca	0
			1	1	
21	cL	1	Total	Ca	0
			1	1	

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	A	39	Total	O	0
			39	39	
22	B	30	Total	O	0
			30	30	
22	C	14	Total	O	0
			14	14	
22	D	10	Total	O	0
			10	10	
22	E	3	Total	O	0
			3	3	
22	I	2	Total	O	0
			2	2	
22	L	19	Total	O	0
			19	19	
22	bA	39	Total	O	0
			39	39	
22	bB	30	Total	O	0
			30	30	
22	bC	14	Total	O	0
			14	14	
22	bD	10	Total	O	0
			10	10	
22	bE	3	Total	O	0
			3	3	
22	bI	2	Total	O	0
			2	2	

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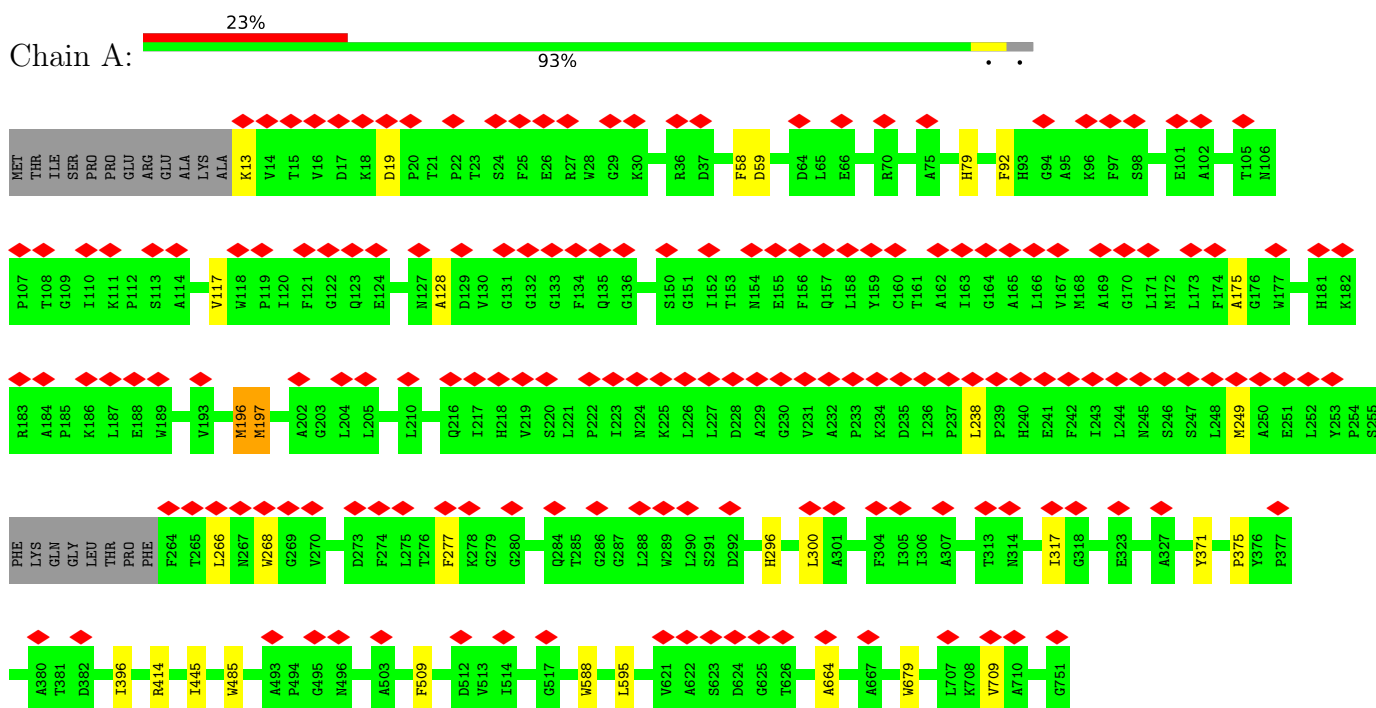
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Mol	Chain	Residues	Atoms		AltConf
22	bL	19	Total 19	O 19	0
22	cA	39	Total 39	O 39	0
22	cB	30	Total 30	O 30	0
22	cC	14	Total 14	O 14	0
22	cD	10	Total 10	O 10	0
22	cE	3	Total 3	O 3	0
22	cI	2	Total 2	O 2	0
22	cL	19	Total 19	O 19	0

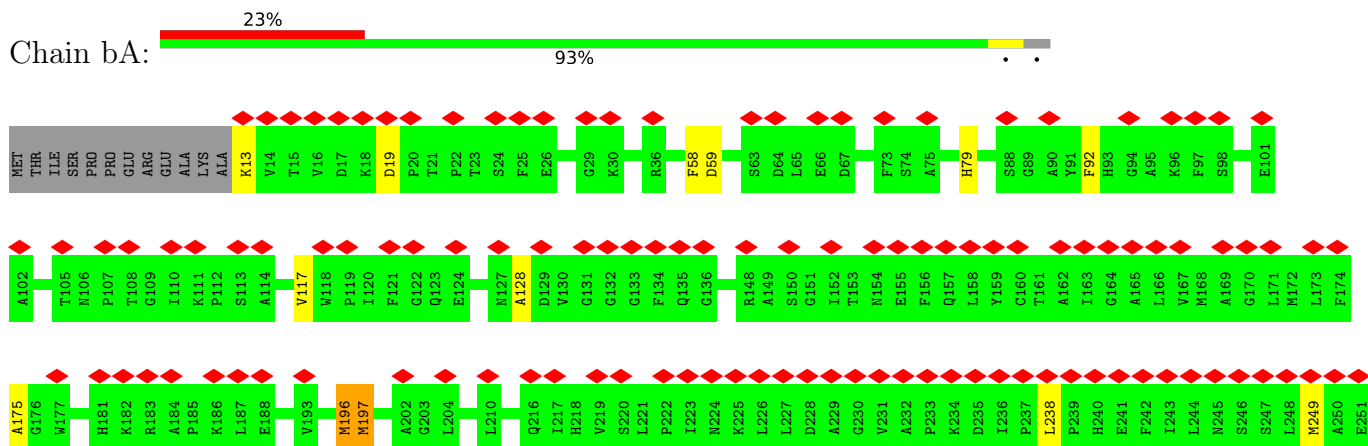
3 Residue-property plots

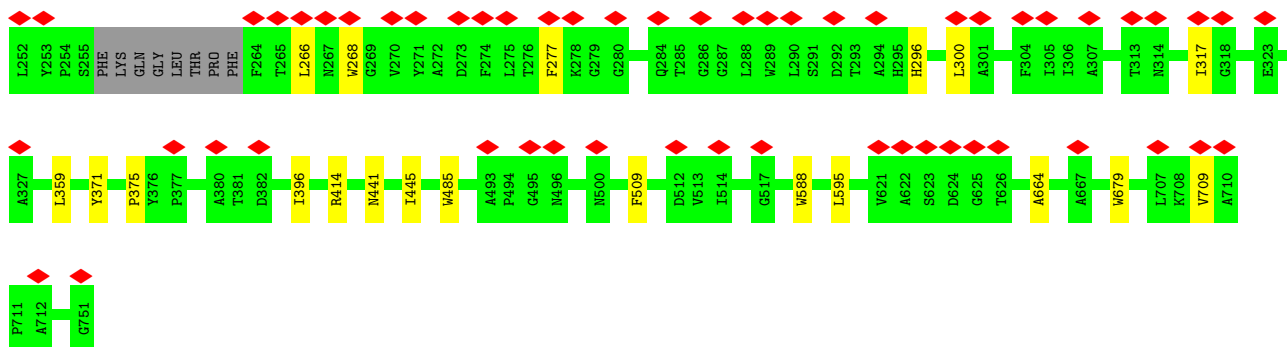
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

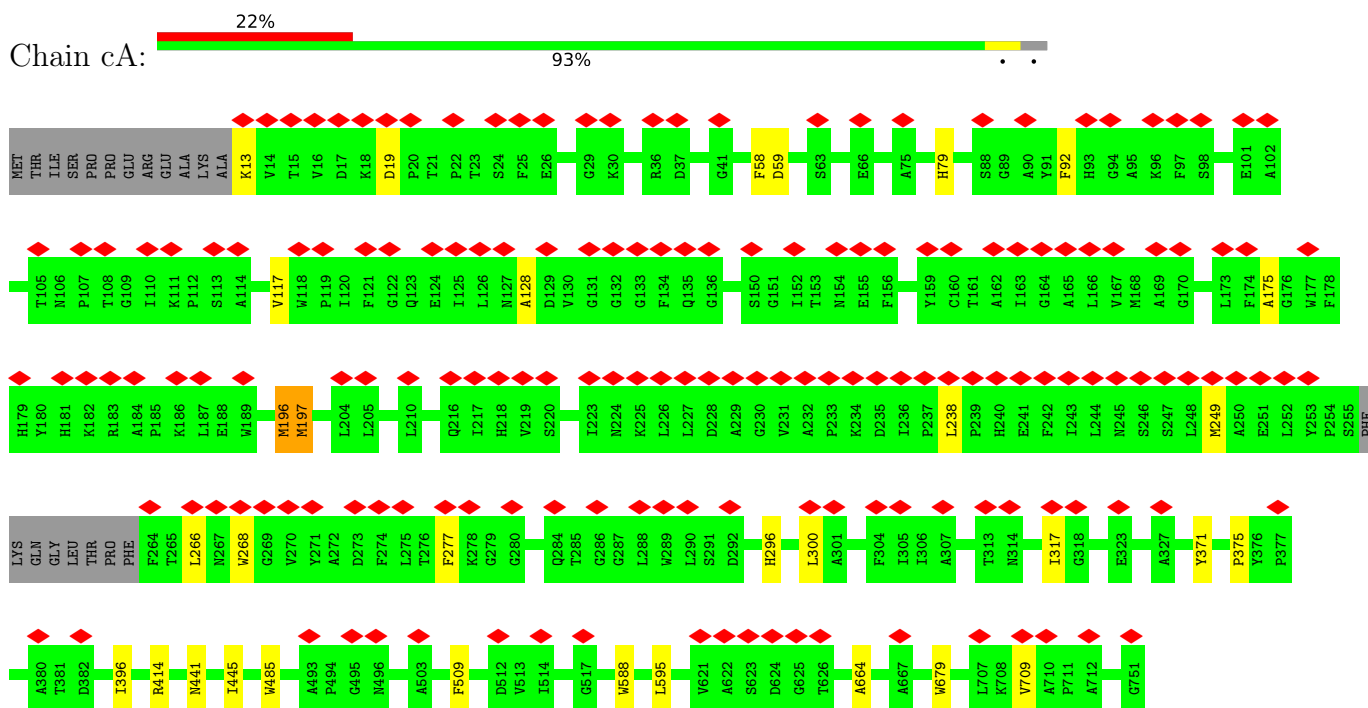


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

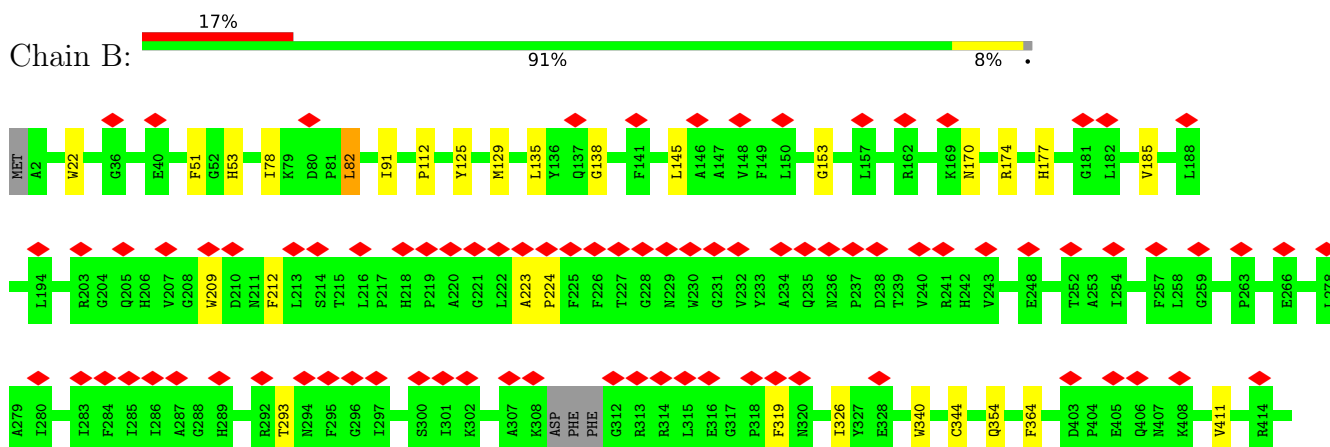


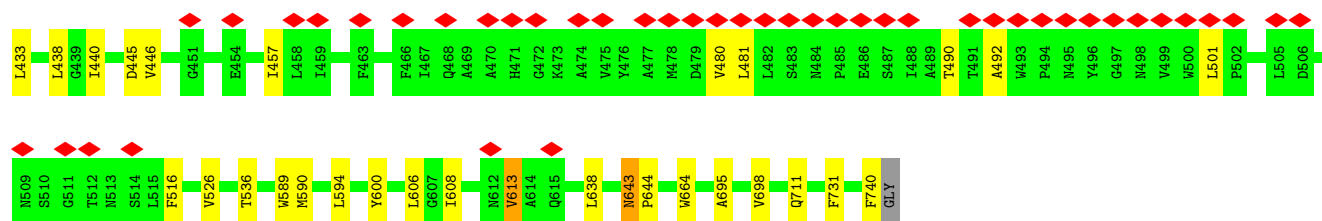


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

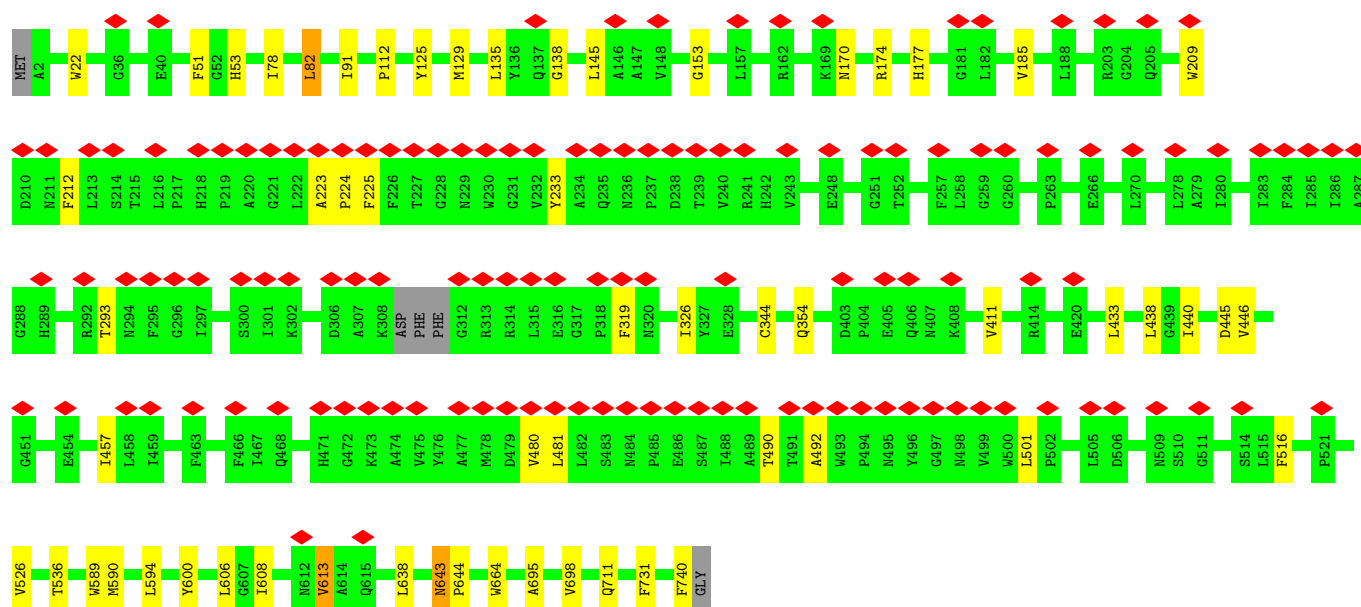
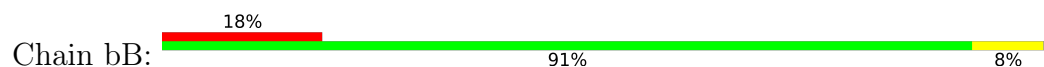


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

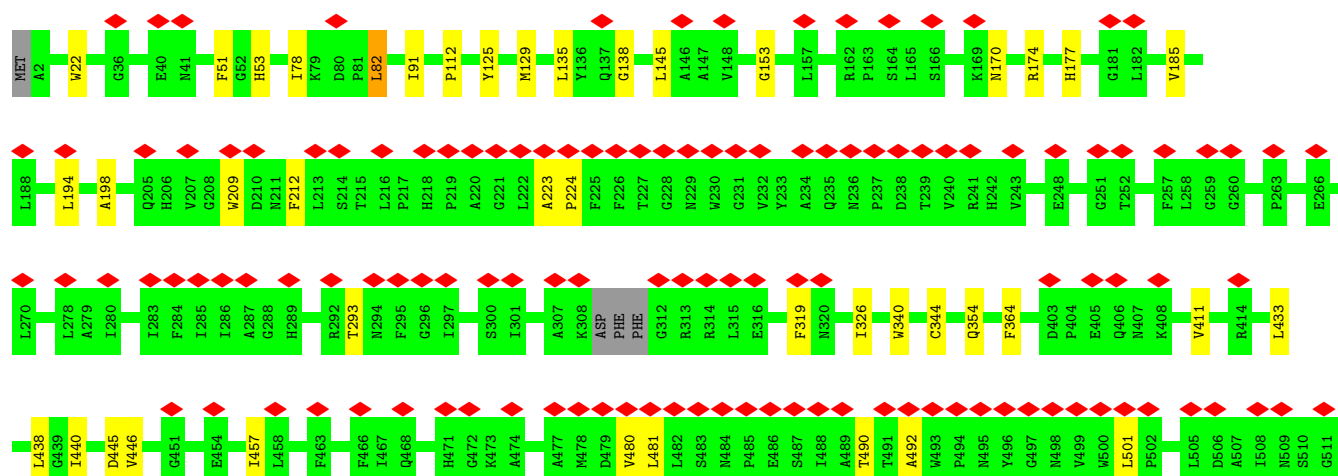


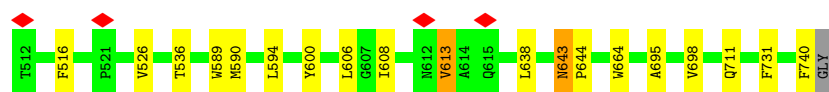


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

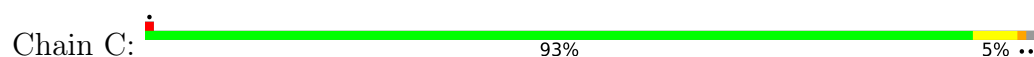


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





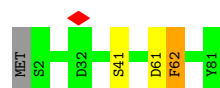
- Molecule 3: Photosystem I iron-sulfur center



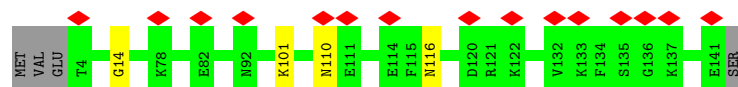
- Molecule 3: Photosystem I iron-sulfur center



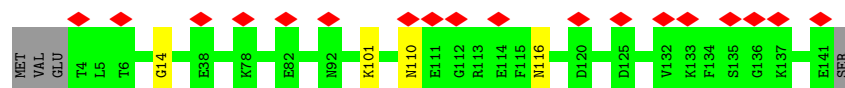
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II



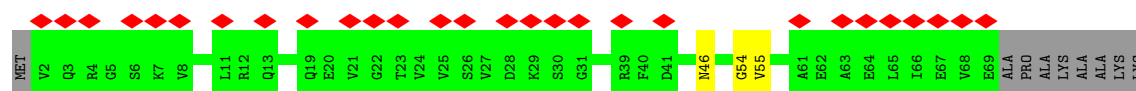
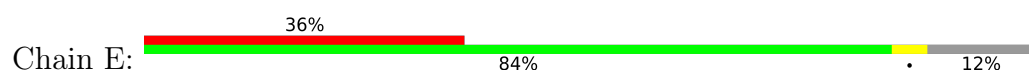
- Molecule 4: Photosystem I reaction center subunit II



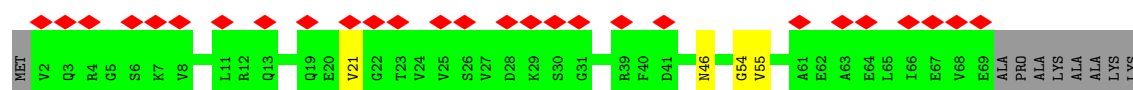
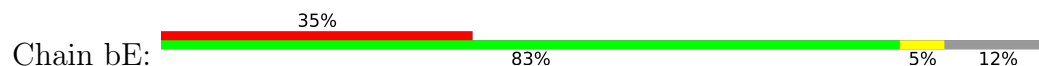
- Molecule 4: Photosystem I reaction center subunit II



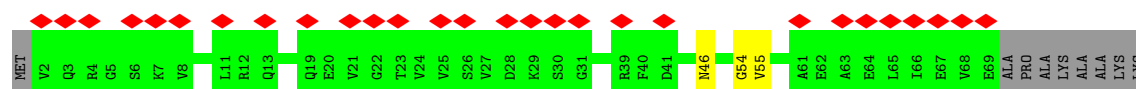
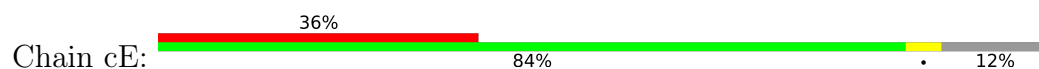
- Molecule 5: Photosystem I reaction center subunit IV



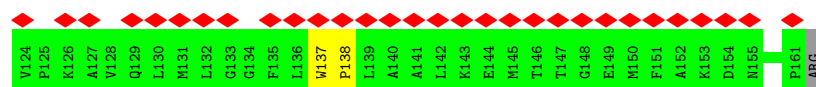
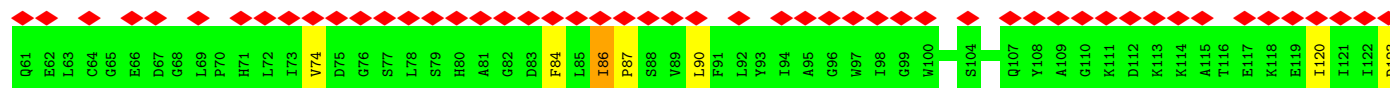
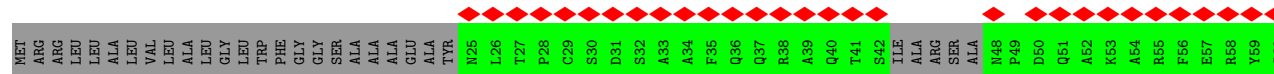
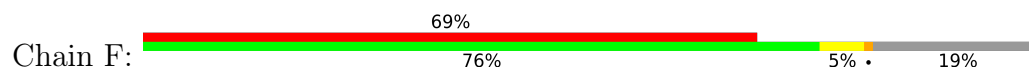
• Molecule 5: Photosystem I reaction center subunit IV



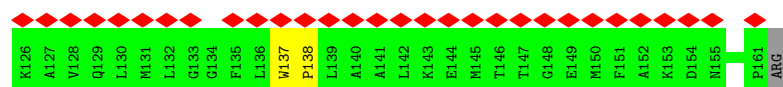
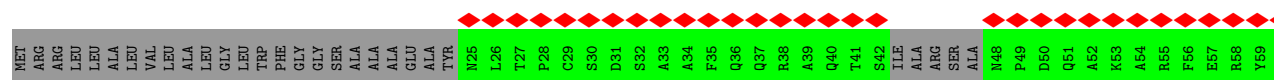
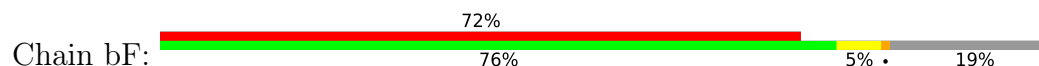
• Molecule 5: Photosystem I reaction center subunit IV



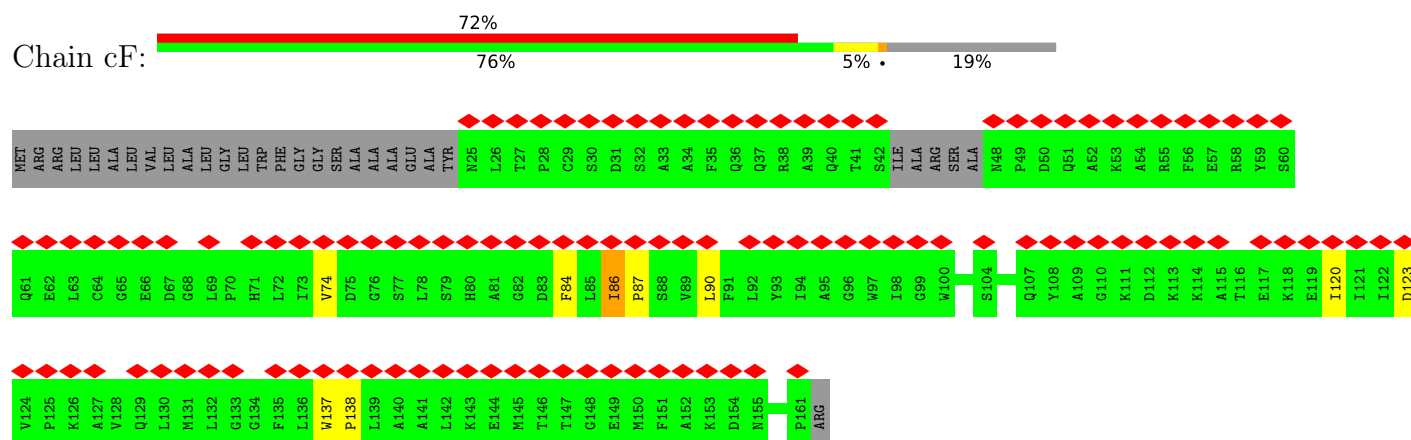
• Molecule 6: Photosystem I reaction center subunit III



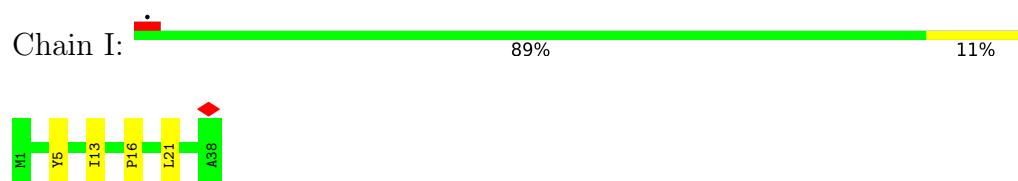
• Molecule 6: Photosystem I reaction center subunit III



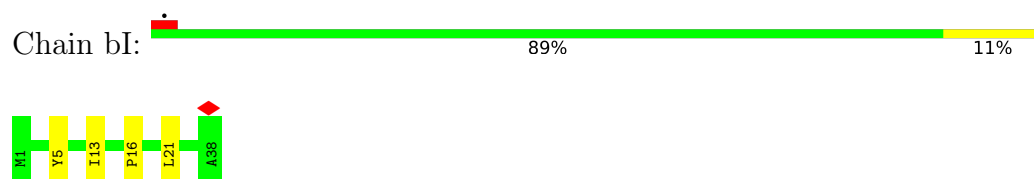
- Molecule 6: Photosystem I reaction center subunit III



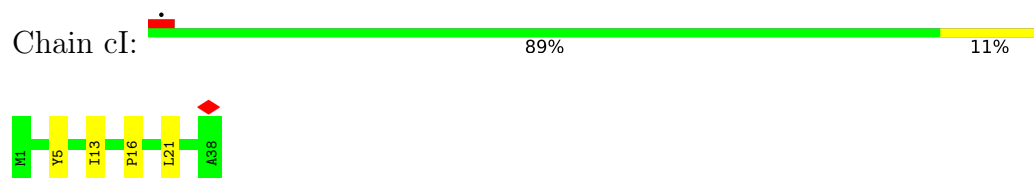
- Molecule 7: Photosystem I reaction center subunit VIII



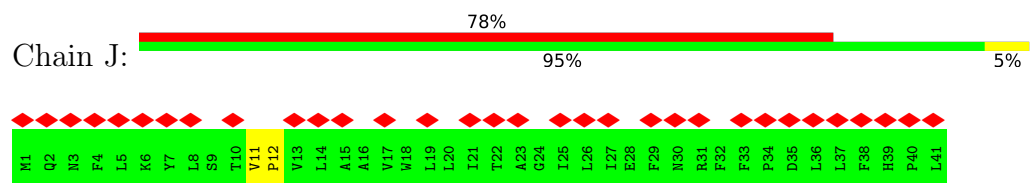
- Molecule 7: Photosystem I reaction center subunit VIII



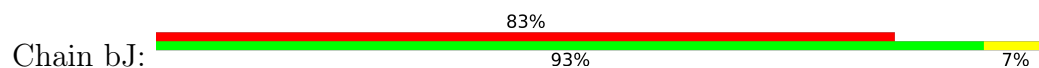
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX

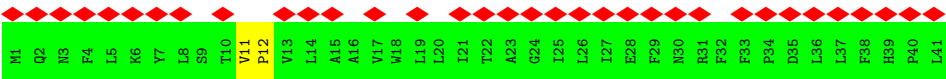
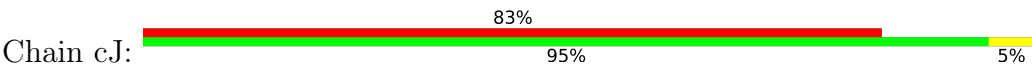


- Molecule 8: Photosystem I reaction center subunit IX

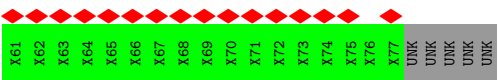
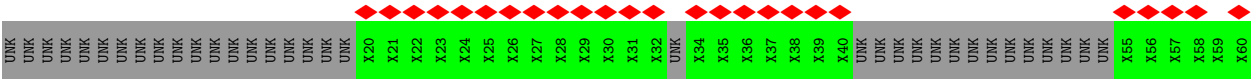




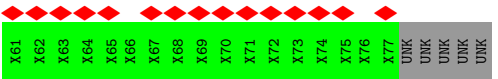
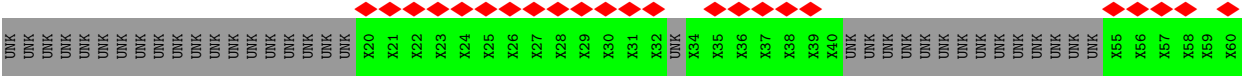
• Molecule 8: Photosystem I reaction center subunit IX



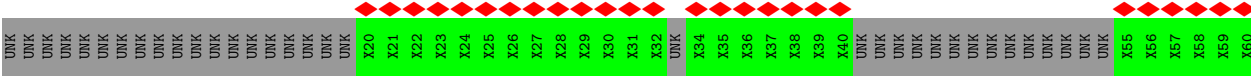
• Molecule 9: Unknown



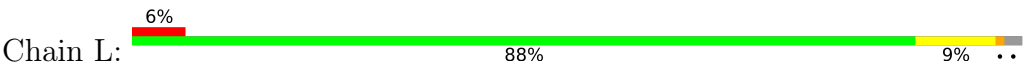
• Molecule 9: Unknown



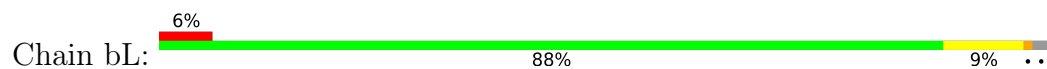
• Molecule 9: Unknown



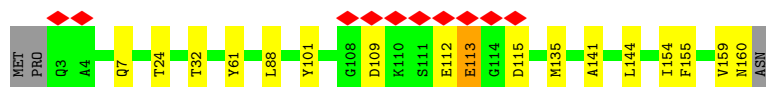
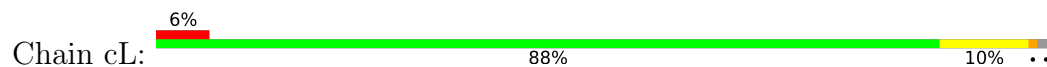
• Molecule 10: Photosystem I reaction center subunit XI



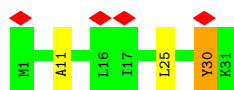
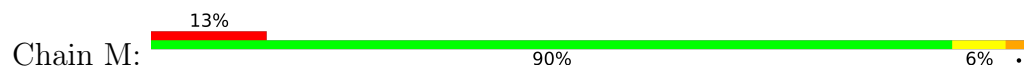
- Molecule 10: Photosystem I reaction center subunit XI



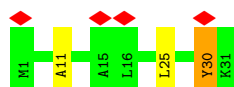
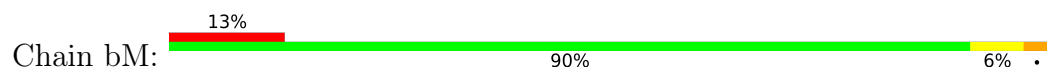
- Molecule 10: Photosystem I reaction center subunit XI



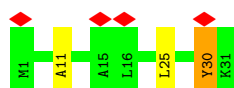
- Molecule 11: Photosystem I reaction center subunit XII



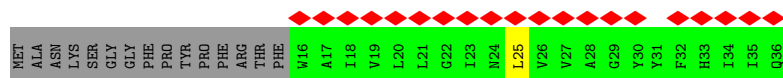
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII

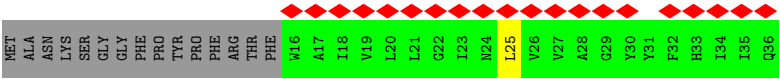


- Molecule 12: Photosystem I reaction center subunit psaX

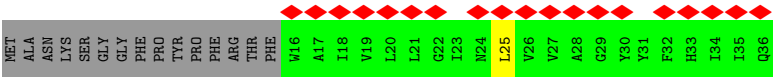


- Molecule 12: Photosystem I reaction center subunit psaX





● Molecule 12: Photosystem I reaction center subunit psaX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	121244	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	222.592, 222.592, 222.592	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	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: CLA, UNL, PQN, SF4, LMG, LHG, CL0, BCR, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.03	0/5935	1.58	0/8086
1	bA	1.03	0/5935	1.58	0/8086
1	cA	1.03	0/5935	1.58	0/8086
2	B	1.02	0/6103	1.58	5/8339 (0.1%)
2	bB	1.02	0/6103	1.58	5/8339 (0.1%)
2	cB	1.02	0/6103	1.58	5/8339 (0.1%)
3	C	1.05	0/609	1.43	0/824
3	bC	1.05	0/609	1.43	0/824
3	cC	1.05	0/609	1.43	0/824
4	D	1.05	0/1107	1.39	1/1487 (0.1%)
4	bD	1.05	0/1107	1.39	1/1487 (0.1%)
4	cD	1.05	0/1107	1.39	1/1487 (0.1%)
5	E	1.08	0/553	1.37	0/748
5	bE	1.08	0/553	1.37	2/748 (0.3%)
5	cE	1.08	0/553	1.37	0/748
6	F	1.06	0/1046	1.64	2/1416 (0.1%)
6	bF	1.06	0/1046	1.64	2/1416 (0.1%)
6	cF	1.06	0/1046	1.64	2/1416 (0.1%)
7	I	1.07	0/307	1.52	0/420
7	bI	1.07	0/307	1.52	0/420
7	cI	1.07	0/307	1.52	0/420
8	J	0.99	0/350	1.54	0/477
8	bJ	0.99	0/350	1.54	0/477
8	cJ	0.99	0/350	1.54	0/477
10	L	1.23	2/1208 (0.2%)	1.65	2/1637 (0.1%)
10	bL	1.23	2/1208 (0.2%)	1.65	2/1637 (0.1%)
10	cL	1.23	3/1208 (0.2%)	1.65	2/1637 (0.1%)
11	M	1.06	0/244	1.62	0/330
11	bM	1.05	0/244	1.61	0/330
11	cM	1.05	0/244	1.61	0/330
12	X	1.04	0/176	1.71	0/241
12	bX	1.03	0/176	1.71	0/241

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	cX	1.03	0/176	1.71	0/241
All	All	1.05	7/52914 (0.0%)	1.57	32/72015 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	bC	0	1
3	cC	0	1
All	All	0	3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cL	113	GLU	CD-OE2	20.57	1.64	1.25
10	bL	113	GLU	CD-OE2	20.57	1.64	1.25
10	L	113	GLU	CD-OE2	20.56	1.64	1.25
10	bL	113	GLU	CD-OE1	12.51	1.49	1.25
10	cL	113	GLU	CD-OE1	12.50	1.49	1.25

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	14	GLY	CA-C-O	-6.59	117.94	122.22
4	bD	14	GLY	CA-C-O	-6.57	117.95	122.22
4	cD	14	GLY	CA-C-O	-6.56	117.95	122.22
6	F	123	ASP	CA-C-N	6.28	125.35	120.33
6	F	123	ASP	C-N-CA	6.28	125.35	120.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	62	PHE	Peptide
3	bC	62	PHE	Peptide
3	cC	62	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5742	0	5606	20	0
1	bA	5742	0	5606	22	0
1	cA	5742	0	5606	21	0
2	B	5886	0	5653	37	0
2	bB	5886	0	5653	37	0
2	cB	5886	0	5653	37	0
3	C	599	0	579	2	0
3	bC	599	0	579	2	0
3	cC	599	0	579	1	0
4	D	1084	0	1087	1	0
4	bD	1084	0	1087	1	0
4	cD	1084	0	1087	1	0
5	E	544	0	531	0	0
5	bE	544	0	531	0	0
5	cE	544	0	531	0	0
6	F	1023	0	1007	3	0
6	bF	1023	0	1007	3	0
6	cF	1023	0	1007	3	0
7	I	297	0	303	9	0
7	bI	297	0	303	9	0
7	cI	297	0	303	9	0
8	J	339	0	355	1	0
8	bJ	339	0	355	2	0
8	cJ	339	0	355	1	0
9	K	208	0	45	0	0
9	bK	208	0	45	0	0
9	cK	208	0	45	0	0
10	L	1178	0	1145	18	0
10	bL	1178	0	1145	18	0
10	cL	1178	0	1145	18	0
11	M	241	0	264	2	0
11	bM	241	0	264	2	0
11	cM	241	0	264	2	0
12	X	171	0	177	2	0
12	bX	171	0	177	2	0
12	cX	171	0	177	2	0
13	A	65	0	72	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	bA	65	0	72	5	0
13	cA	65	0	72	5	0
14	A	2204	0	1960	68	0
14	B	2166	0	1946	62	0
14	F	51	0	41	1	0
14	J	90	0	66	3	0
14	L	254	0	274	14	0
14	X	45	0	33	3	0
14	bA	2204	0	1960	71	0
14	bB	2166	0	1946	62	0
14	bF	51	0	41	1	0
14	bJ	90	0	66	3	0
14	bL	254	0	274	15	0
14	bX	45	0	33	3	0
14	cA	2204	0	1960	69	0
14	cB	2166	0	1946	65	0
14	cF	51	0	41	1	0
14	cJ	90	0	66	3	0
14	cL	254	0	274	13	0
14	cX	45	0	33	3	0
15	A	33	0	46	0	0
15	B	33	0	46	1	0
15	bA	33	0	46	0	0
15	bB	33	0	46	1	0
15	cA	33	0	46	0	0
15	cB	33	0	46	1	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
16	bA	8	0	0	0	0
16	bC	16	0	0	0	0
16	cA	8	0	0	0	0
16	cC	16	0	0	0	0
17	A	200	0	280	5	0
17	B	320	0	448	12	0
17	F	40	0	56	0	0
17	I	80	0	112	2	0
17	J	40	0	56	6	0
17	L	80	0	112	6	0
17	M	40	0	56	2	0
17	bA	200	0	280	5	0
17	bB	320	0	448	13	0
17	bF	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	bI	80	0	112	2	0
17	bJ	40	0	56	6	0
17	bL	80	0	112	6	0
17	bM	40	0	56	2	0
17	cA	200	0	280	5	0
17	cB	320	0	448	13	0
17	cF	40	0	56	0	0
17	cI	80	0	112	2	0
17	cJ	40	0	56	6	0
17	cL	80	0	112	7	0
17	cM	40	0	56	2	0
18	A	76	0	98	0	0
18	bA	76	0	98	0	0
18	cA	76	0	98	0	0
19	A	12	0	0	0	0
19	I	22	0	0	0	0
19	L	29	0	0	0	0
19	bA	12	0	0	0	0
19	bI	22	0	0	0	0
19	bL	29	0	0	0	0
19	cA	12	0	0	0	0
19	cI	22	0	0	0	0
19	cL	29	0	0	0	0
20	B	43	0	56	0	0
20	bB	43	0	56	0	0
20	cB	43	0	56	0	0
21	L	1	0	0	0	0
21	bL	1	0	0	0	0
21	cL	1	0	0	0	0
22	A	39	0	0	0	0
22	B	30	0	0	0	0
22	C	14	0	0	0	0
22	D	10	0	0	0	0
22	E	3	0	0	0	0
22	I	2	0	0	0	0
22	L	19	0	0	1	0
22	bA	39	0	0	0	0
22	bB	30	0	0	0	0
22	bC	14	0	0	0	0
22	bD	10	0	0	0	0
22	bE	3	0	0	0	0
22	bI	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	bL	19	0	0	0	0
22	cA	39	0	0	0	0
22	cB	30	0	0	0	0
22	cC	14	0	0	0	0
22	cD	10	0	0	0	0
22	cE	3	0	0	0	0
22	cI	2	0	0	0	0
22	cL	19	0	0	0	0
All	All	70131	0	67530	652	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 652 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)
10:cL:113:GLU:CD	10:cL:113:GLU:OE2	1.64	1.41
10:bL:113:GLU:CD	10:bL:113:GLU:OE2	1.64	1.39
10:L:113:GLU:CD	10:L:113:GLU:OE2	1.64	1.38
14:bA:829:CLA:H191	14:bB:801:CLA:H191	1.70	0.73
14:cA:829:CLA:H191	14:cB:802:CLA:H191	1.70	0.73

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	727/751 (97%)	676 (93%)	47 (6%)	4 (1%)	21	20
1	bA	727/751 (97%)	677 (93%)	46 (6%)	4 (1%)	21	20
1	cA	727/751 (97%)	676 (93%)	47 (6%)	4 (1%)	21	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	732/741 (99%)	681 (93%)	47 (6%)	4 (0%)	24	25
2	bB	732/741 (99%)	681 (93%)	47 (6%)	4 (0%)	24	25
2	cB	732/741 (99%)	681 (93%)	47 (6%)	4 (0%)	24	25
3	C	78/81 (96%)	74 (95%)	2 (3%)	2 (3%)	4	2
3	bC	78/81 (96%)	74 (95%)	2 (3%)	2 (3%)	4	2
3	cC	78/81 (96%)	74 (95%)	2 (3%)	2 (3%)	4	2
4	D	136/142 (96%)	131 (96%)	5 (4%)	0	100	100
4	bD	136/142 (96%)	131 (96%)	5 (4%)	0	100	100
4	cD	136/142 (96%)	131 (96%)	5 (4%)	0	100	100
5	E	66/77 (86%)	60 (91%)	3 (4%)	3 (4%)	2	0
5	bE	66/77 (86%)	60 (91%)	3 (4%)	3 (4%)	2	0
5	cE	66/77 (86%)	60 (91%)	3 (4%)	3 (4%)	2	0
6	F	128/162 (79%)	116 (91%)	12 (9%)	0	100	100
6	bF	128/162 (79%)	116 (91%)	12 (9%)	0	100	100
6	cF	128/162 (79%)	116 (91%)	12 (9%)	0	100	100
7	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	1
7	bI	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	1
7	cI	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	1
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	bJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	cJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
10	L	156/161 (97%)	149 (96%)	5 (3%)	2 (1%)	9	7
10	bL	156/161 (97%)	149 (96%)	5 (3%)	2 (1%)	9	7
10	cL	156/161 (97%)	149 (96%)	5 (3%)	2 (1%)	9	7
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	3	1
11	bM	29/31 (94%)	28 (97%)	0	1 (3%)	3	1
11	cM	29/31 (94%)	28 (97%)	0	1 (3%)	3	1
12	X	19/36 (53%)	18 (95%)	1 (5%)	0	100	100
12	bX	19/36 (53%)	18 (95%)	1 (5%)	0	100	100
12	cX	19/36 (53%)	18 (95%)	1 (5%)	0	100	100
All	All	6438/6783 (95%)	6013 (93%)	374 (6%)	51 (1%)	18	14

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	ILE
1	bA	317	ILE
1	cA	317	ILE
1	A	268	TRP
2	B	492	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	592/609 (97%)	584 (99%)	8 (1%)	59	72
1	bA	592/609 (97%)	584 (99%)	8 (1%)	59	72
1	cA	592/609 (97%)	584 (99%)	8 (1%)	59	72
2	B	600/604 (99%)	592 (99%)	8 (1%)	61	74
2	bB	600/604 (99%)	592 (99%)	8 (1%)	61	74
2	cB	600/604 (99%)	592 (99%)	8 (1%)	61	74
3	C	68/69 (99%)	68 (100%)	0	100	100
3	bC	68/69 (99%)	68 (100%)	0	100	100
3	cC	68/69 (99%)	68 (100%)	0	100	100
4	D	114/118 (97%)	112 (98%)	2 (2%)	51	65
4	bD	114/118 (97%)	112 (98%)	2 (2%)	51	65
4	cD	114/118 (97%)	112 (98%)	2 (2%)	51	65
5	E	59/64 (92%)	59 (100%)	0	100	100
5	bE	59/64 (92%)	59 (100%)	0	100	100
5	cE	59/64 (92%)	59 (100%)	0	100	100
6	F	108/127 (85%)	105 (97%)	3 (3%)	38	49
6	bF	108/127 (85%)	105 (97%)	3 (3%)	38	49
6	cF	108/127 (85%)	105 (97%)	3 (3%)	38	49
7	I	32/32 (100%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	bI	32/32 (100%)	32 (100%)	0	100	100
7	cI	32/32 (100%)	32 (100%)	0	100	100
8	J	37/37 (100%)	37 (100%)	0	100	100
8	bJ	37/37 (100%)	37 (100%)	0	100	100
8	cJ	37/37 (100%)	37 (100%)	0	100	100
10	L	116/119 (98%)	115 (99%)	1 (1%)	70	81
10	bL	116/119 (98%)	115 (99%)	1 (1%)	70	81
10	cL	116/119 (98%)	115 (99%)	1 (1%)	70	81
11	M	27/27 (100%)	26 (96%)	1 (4%)	30	38
11	bM	27/27 (100%)	26 (96%)	1 (4%)	30	38
11	cM	27/27 (100%)	26 (96%)	1 (4%)	30	38
12	X	17/29 (59%)	17 (100%)	0	100	100
12	bX	17/29 (59%)	17 (100%)	0	100	100
12	cX	17/29 (59%)	17 (100%)	0	100	100
All	All	5310/5505 (96%)	5241 (99%)	69 (1%)	59	74

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	cB	354	GLN
2	cB	606	LEU
6	cF	90	LEU
1	bA	117	VAL
1	bA	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
4	bD	116	ASN
10	cL	38	ASN
10	bL	73	GLN
10	cL	3	GLN
2	cB	617	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 378 ligands modelled in this entry, 15 are unknown and 3 are monoatomic - leaving 360 for Mogul analysis.

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
14	CLA	bA	829	1	69,73,73	2.05	20 (28%)	83,113,113	2.69	29 (34%)
14	CLA	cB	839	-	69,73,73	1.95	20 (28%)	83,113,113	2.63	27 (32%)
14	CLA	bB	812	2	69,73,73	2.10	20 (28%)	83,113,113	2.88	29 (34%)
14	CLA	cA	813	1	49,53,73	2.47	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	B	806	2	69,73,73	2.07	20 (28%)	83,113,113	2.75	31 (37%)
17	BCR	bB	842	-	41,41,41	1.79	7 (17%)	56,56,56	1.60	12 (21%)
14	CLA	A	810	-	49,53,73	2.49	21 (42%)	59,89,113	3.16	25 (42%)
14	CLA	A	829	1	69,73,73	2.05	20 (28%)	83,113,113	2.69	29 (34%)
14	CLA	bF	201	22	55,59,73	2.29	19 (34%)	66,96,113	3.04	31 (46%)
14	CLA	cB	806	2	69,73,73	2.08	21 (30%)	83,113,113	2.83	30 (36%)
14	CLA	B	825	2	59,63,73	2.26	20 (33%)	71,101,113	2.99	32 (45%)
17	BCR	cL	207	-	41,41,41	1.74	8 (19%)	56,56,56	1.39	8 (14%)
14	CLA	A	807	1	49,53,73	2.50	21 (42%)	59,89,113	3.19	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	bB	814	-	49,53,73	2.50	21 (42%)	59,89,113	3.24	27 (45%)
14	CLA	bA	840	1	69,73,73	2.11	20 (28%)	83,113,113	2.69	26 (31%)
14	CLA	J	102	8	49,53,73	2.50	21 (42%)	59,89,113	3.20	26 (44%)
17	BCR	B	841	-	41,41,41	1.75	7 (17%)	56,56,56	1.37	9 (16%)
14	CLA	A	833	1	69,73,73	2.00	21 (30%)	83,113,113	2.71	30 (36%)
14	CLA	bB	807	2	69,73,73	2.06	20 (28%)	83,113,113	2.75	27 (32%)
14	CLA	bX	201	-	49,53,73	2.50	21 (42%)	59,89,113	3.22	28 (47%)
16	SF4	bC	101	3	0,12,12	-	-	-	-	-
14	CLA	A	840	1	69,73,73	2.11	20 (28%)	83,113,113	2.69	26 (31%)
14	CLA	cA	804	1	57,61,73	2.32	21 (36%)	68,98,113	3.10	29 (42%)
17	BCR	bF	202	-	41,41,41	1.80	6 (14%)	56,56,56	1.49	8 (14%)
14	CLA	bB	849	-	49,53,73	2.50	20 (40%)	59,89,113	3.18	27 (45%)
14	CLA	bL	202	10	69,73,73	2.10	21 (30%)	83,113,113	3.98	30 (36%)
14	CLA	cB	819	-	50,54,73	2.45	20 (40%)	60,90,113	3.13	26 (43%)
14	CLA	A	821	-	49,53,73	2.52	20 (40%)	59,89,113	3.23	26 (44%)
17	BCR	M	101	-	41,41,41	1.75	8 (19%)	56,56,56	1.50	12 (21%)
14	CLA	cA	852	-	69,73,73	1.86	18 (26%)	83,113,113	2.50	28 (33%)
14	CLA	cA	803	1	49,53,73	2.49	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	bB	819	-	51,55,73	2.45	20 (39%)	61,91,113	3.21	32 (52%)
17	BCR	cI	101	-	41,41,41	1.68	8 (19%)	56,56,56	1.39	10 (17%)
14	CLA	bA	805	1	59,63,73	2.24	21 (35%)	71,101,113	3.04	29 (40%)
14	CLA	B	831	2	69,73,73	2.10	20 (28%)	83,113,113	2.84	29 (34%)
14	CLA	bA	815	-	49,53,73	2.51	21 (42%)	59,89,113	3.22	27 (45%)
14	CLA	bJ	102	8	49,53,73	2.50	21 (42%)	59,89,113	3.20	26 (44%)
14	CLA	bA	812	1	49,53,73	2.51	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	cA	832	1	69,73,73	1.98	20 (28%)	83,113,113	2.74	31 (37%)
14	CLA	bL	203	10	63,67,73	2.11	21 (33%)	75,105,113	2.96	30 (40%)
14	CLA	bA	839	1	69,73,73	2.07	20 (28%)	83,113,113	2.72	28 (33%)
14	CLA	cB	822	-	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	B	814	-	49,53,73	2.50	21 (42%)	59,89,113	3.24	28 (47%)
17	BCR	bB	843	-	41,41,41	1.86	7 (17%)	56,56,56	1.57	11 (19%)
14	CLA	bB	816	2	49,53,73	2.52	21 (42%)	59,89,113	3.25	30 (50%)
17	BCR	bA	848	-	41,41,41	1.68	8 (19%)	56,56,56	1.51	13 (23%)
14	CLA	cA	826	1	50,54,73	2.43	20 (40%)	60,90,113	3.24	27 (45%)
14	CLA	bB	837	2	51,55,73	2.41	20 (39%)	61,91,113	3.20	25 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	bA	846	-	41,41,41	1.77	7 (17%)	56,56,56	1.77	14 (25%)
18	LHG	bA	850	-	48,48,48	0.27	0	51,54,54	0.31	0
14	CLA	cA	809	1	49,53,73	2.47	20 (40%)	59,89,113	3.19	26 (44%)
14	CLA	A	822	1	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	cA	808	1	49,53,73	2.45	20 (40%)	59,89,113	3.23	30 (50%)
14	CLA	X	201	-	49,53,73	2.50	21 (42%)	59,89,113	3.23	28 (47%)
14	CLA	cB	813	2	69,73,73	2.10	21 (30%)	83,113,113	2.88	29 (34%)
14	CLA	cB	801	-	49,53,73	2.51	20 (40%)	59,89,113	3.23	26 (44%)
17	BCR	bB	847	-	41,41,41	1.73	8 (19%)	56,56,56	1.48	13 (23%)
14	CLA	cB	823	2	49,53,73	2.48	20 (40%)	59,89,113	3.25	26 (44%)
17	BCR	B	850	-	41,41,41	1.76	8 (19%)	56,56,56	1.38	8 (14%)
14	CLA	A	834	1	49,53,73	2.50	20 (40%)	59,89,113	3.17	27 (45%)
14	CLA	cA	835	1	49,53,73	2.49	20 (40%)	59,89,113	3.15	28 (47%)
17	BCR	cA	848	-	41,41,41	1.68	8 (19%)	56,56,56	1.52	13 (23%)
14	CLA	bB	820	2	49,53,73	2.52	20 (40%)	59,89,113	3.23	27 (45%)
14	CLA	bB	803	-	59,63,73	2.17	20 (33%)	71,101,113	2.96	30 (42%)
14	CLA	bA	819	1	49,53,73	2.51	20 (40%)	59,89,113	3.19	29 (49%)
17	BCR	cB	851	-	41,41,41	1.76	8 (19%)	56,56,56	1.38	8 (14%)
16	SF4	A	844	1,2	0,12,12	-	-	-	-	-
14	CLA	cA	833	1	69,73,73	2.00	21 (30%)	83,113,113	2.71	30 (36%)
16	SF4	C	102	3	0,12,12	-	-	-	-	-
17	BCR	cA	846	-	41,41,41	1.76	6 (14%)	56,56,56	1.76	14 (25%)
14	CLA	cA	807	1	49,53,73	2.50	21 (42%)	59,89,113	3.18	27 (45%)
14	CLA	B	828	2	69,73,73	2.01	19 (27%)	83,113,113	2.81	29 (34%)
14	CLA	cJ	102	8	49,53,73	2.50	21 (42%)	59,89,113	3.20	26 (44%)
14	CLA	bB	822	2	49,53,73	2.48	20 (40%)	59,89,113	3.26	26 (44%)
14	CLA	cL	203	10	69,73,73	2.10	21 (30%)	83,113,113	3.99	30 (36%)
14	CLA	cB	832	2	69,73,73	2.10	20 (28%)	83,113,113	2.84	27 (32%)
18	LHG	bA	851	14	26,26,48	0.33	0	29,32,54	0.39	0
17	BCR	A	845	-	41,41,41	1.79	7 (17%)	56,56,56	1.48	11 (19%)
14	CLA	cA	841	-	69,73,73	1.97	19 (27%)	83,113,113	2.65	31 (37%)
14	CLA	bA	820	22	49,53,73	2.51	21 (42%)	59,89,113	3.17	28 (47%)
13	CL0	bA	801	1	63,73,73	3.18	18 (28%)	61,113,113	2.43	17 (27%)
14	CLA	A	818	1	64,68,73	2.18	21 (32%)	77,107,113	2.94	31 (40%)
14	CLA	A	831	1	59,63,73	2.23	20 (33%)	71,101,113	2.99	31 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	809	1	49,53,73	2.47	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	cA	825	-	54,58,73	2.31	20 (37%)	65,95,113	3.19	30 (46%)
14	CLA	B	807	2	69,73,73	2.06	20 (28%)	83,113,113	2.75	27 (32%)
14	CLA	bA	832	1	69,73,73	1.98	20 (28%)	83,113,113	2.75	31 (37%)
14	CLA	bB	830	2	46,50,73	2.51	20 (43%)	55,85,113	3.30	25 (45%)
17	BCR	L	205	-	41,41,41	1.70	8 (19%)	56,56,56	1.40	9 (16%)
17	BCR	cB	842	-	41,41,41	1.75	7 (17%)	56,56,56	1.37	9 (16%)
14	CLA	A	816	1	49,53,73	2.48	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	B	824	-	50,54,73	2.48	20 (40%)	60,90,113	3.20	26 (43%)
14	CLA	cB	817	2	49,53,73	2.52	21 (42%)	59,89,113	3.24	29 (49%)
14	CLA	bA	822	1	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	cA	839	1	69,73,73	2.07	20 (28%)	83,113,113	2.72	28 (33%)
14	CLA	B	808	2	56,60,73	2.23	20 (35%)	67,97,113	3.08	30 (44%)
14	CLA	cB	805	2	55,59,73	2.33	20 (36%)	66,96,113	3.12	30 (45%)
17	BCR	cB	847	-	41,41,41	1.71	7 (17%)	56,56,56	1.41	10 (17%)
14	CLA	B	826	2	69,73,73	2.02	21 (30%)	83,113,113	2.82	32 (38%)
14	CLA	cB	850	-	49,53,73	2.50	21 (42%)	59,89,113	3.18	27 (45%)
16	SF4	cA	844	1,2	0,12,12	-	-	-	-	-
14	CLA	cA	840	1	69,73,73	2.11	20 (28%)	83,113,113	2.69	26 (31%)
17	BCR	bA	849	-	41,41,41	1.72	7 (17%)	56,56,56	1.48	10 (17%)
14	CLA	B	801	-	69,73,73	2.02	19 (27%)	83,113,113	2.71	28 (33%)
14	CLA	cA	830	1	54,58,73	2.24	18 (33%)	65,95,113	3.07	29 (44%)
15	PQN	cB	841	-	34,34,34	0.45	1 (2%)	42,45,45	0.35	0
16	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	cB	836	2	49,53,73	2.49	20 (40%)	59,89,113	3.22	26 (44%)
17	BCR	cJ	103	-	41,41,41	1.84	7 (17%)	56,56,56	1.61	11 (19%)
17	BCR	A	848	-	41,41,41	1.68	8 (19%)	56,56,56	1.51	13 (23%)
17	BCR	cB	848	-	41,41,41	1.73	8 (19%)	56,56,56	1.48	13 (23%)
14	CLA	B	835	2	49,53,73	2.48	20 (40%)	59,89,113	3.22	26 (44%)
14	CLA	cB	812	2	49,53,73	2.49	20 (40%)	59,89,113	3.15	26 (44%)
20	LMG	bB	848	-	43,43,55	0.21	0	51,51,63	0.30	0
14	CLA	bA	823	1	49,53,73	2.48	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	A	826	1	50,54,73	2.43	20 (40%)	60,90,113	3.24	27 (45%)
15	PQN	B	840	-	34,34,34	0.45	1 (2%)	42,45,45	0.35	0
14	CLA	cB	833	2	49,53,73	2.44	19 (38%)	59,89,113	3.21	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	842	18	49,53,73	2.44	20 (40%)	59,89,113	3.19	26 (44%)
14	CLA	cB	803	2	69,73,73	2.01	20 (28%)	83,113,113	2.75	32 (38%)
14	CLA	A	803	1	49,53,73	2.49	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	bB	836	2	49,53,73	2.47	20 (40%)	59,89,113	3.20	26 (44%)
14	CLA	cB	834	-	49,53,73	2.51	20 (40%)	59,89,113	3.17	28 (47%)
14	CLA	bB	829	2	49,53,73	2.49	20 (40%)	59,89,113	3.17	26 (44%)
14	CLA	cB	816	2	56,60,73	2.33	21 (37%)	67,97,113	3.09	31 (46%)
14	CLA	A	835	1	49,53,73	2.49	20 (40%)	59,89,113	3.15	28 (47%)
14	CLA	B	802	2	69,73,73	2.02	20 (28%)	83,113,113	2.75	32 (38%)
14	CLA	cA	819	1	49,53,73	2.51	20 (40%)	59,89,113	3.19	29 (49%)
14	CLA	A	841	-	69,73,73	1.97	19 (27%)	83,113,113	2.66	31 (37%)
14	CLA	cA	802	-	69,73,73	1.94	21 (30%)	83,113,113	2.85	31 (37%)
14	CLA	A	827	1	65,69,73	2.16	20 (30%)	78,108,113	2.87	29 (37%)
14	CLA	A	838	1	49,53,73	2.32	19 (38%)	59,89,113	3.30	27 (45%)
14	CLA	bJ	101	8	49,53,73	2.51	21 (42%)	59,89,113	3.21	27 (45%)
17	BCR	bL	205	-	41,41,41	1.69	8 (19%)	56,56,56	1.40	9 (16%)
17	BCR	cF	202	-	41,41,41	1.79	6 (14%)	56,56,56	1.49	8 (14%)
15	PQN	bA	843	-	34,34,34	0.47	1 (2%)	42,45,45	0.34	0
14	CLA	cL	204	10	63,67,73	2.11	21 (33%)	75,105,113	2.96	30 (40%)
14	CLA	bB	827	2	69,73,73	2.10	20 (28%)	83,113,113	2.71	28 (33%)
14	CLA	bB	838	-	69,73,73	1.95	20 (28%)	83,113,113	2.64	27 (32%)
14	CLA	cL	205	-	69,73,73	2.09	20 (28%)	83,113,113	2.72	27 (32%)
17	BCR	L	206	-	41,41,41	1.74	8 (19%)	56,56,56	1.39	8 (14%)
17	BCR	cB	845	-	41,41,41	1.72	8 (19%)	56,56,56	1.42	10 (17%)
14	CLA	A	839	1	69,73,73	2.07	20 (28%)	83,113,113	2.73	28 (33%)
14	CLA	bA	817	1	58,62,73	2.30	20 (34%)	69,99,113	2.95	26 (37%)
15	PQN	A	843	-	34,34,34	0.47	1 (2%)	42,45,45	0.34	0
14	CLA	A	823	1	49,53,73	2.48	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	cA	814	-	49,53,73	2.52	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	B	827	2	69,73,73	2.10	20 (28%)	83,113,113	2.71	28 (33%)
14	CLA	cA	815	-	49,53,73	2.51	21 (42%)	59,89,113	3.22	27 (45%)
14	CLA	cA	812	1	49,53,73	2.51	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	B	811	2	49,53,73	2.50	20 (40%)	59,89,113	3.15	27 (45%)
14	CLA	J	101	8	49,53,73	2.51	21 (42%)	59,89,113	3.21	27 (45%)
17	BCR	B	846	-	41,41,41	1.71	7 (17%)	56,56,56	1.41	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	cA	849	-	41,41,41	1.72	7 (17%)	56,56,56	1.48	10 (17%)
18	LHG	cA	850	-	48,48,48	0.27	0	51,54,54	0.31	0
17	BCR	B	843	-	41,41,41	1.85	8 (19%)	56,56,56	1.57	11 (19%)
14	CLA	bA	821	-	49,53,73	2.52	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	B	816	2	49,53,73	2.52	21 (42%)	59,89,113	3.24	29 (49%)
14	CLA	bB	828	2	69,73,73	2.01	19 (27%)	83,113,113	2.82	29 (34%)
14	CLA	cB	807	2	69,73,73	2.07	20 (28%)	83,113,113	2.74	31 (37%)
14	CLA	bB	821	-	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	B	834	-	49,53,73	2.47	21 (42%)	59,89,113	3.14	27 (45%)
14	CLA	bB	851	-	49,53,73	2.51	20 (40%)	59,89,113	3.23	26 (44%)
17	BCR	B	842	-	41,41,41	1.80	7 (17%)	56,56,56	1.60	12 (21%)
13	CL0	cA	801	1	63,73,73	3.18	18 (28%)	61,113,113	2.43	17 (27%)
14	CLA	bA	813	1	49,53,73	2.47	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	A	802	22	69,73,73	1.94	21 (30%)	83,113,113	2.85	31 (37%)
14	CLA	bA	816	1	49,53,73	2.48	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	cB	837	2	49,53,73	2.47	20 (40%)	59,89,113	3.20	26 (44%)
17	BCR	bB	845	-	41,41,41	1.79	7 (17%)	56,56,56	1.46	12 (21%)
14	CLA	bA	837	1	69,73,73	2.00	20 (28%)	83,113,113	2.73	28 (33%)
17	BCR	bA	847	-	41,41,41	1.77	7 (17%)	56,56,56	1.37	8 (14%)
17	BCR	I	101	-	41,41,41	1.69	8 (19%)	56,56,56	1.39	10 (17%)
17	BCR	B	844	-	41,41,41	1.72	8 (19%)	56,56,56	1.43	10 (17%)
17	BCR	bL	206	-	41,41,41	1.74	8 (19%)	56,56,56	1.39	8 (14%)
14	CLA	B	813	-	52,56,73	2.42	20 (38%)	62,92,113	3.13	30 (48%)
14	CLA	bA	836	1	55,59,73	2.26	19 (34%)	66,96,113	3.10	31 (46%)
18	LHG	cA	851	14	26,26,48	0.33	0	29,32,54	0.39	0
17	BCR	bI	102	-	41,41,41	1.67	8 (19%)	56,56,56	1.46	9 (16%)
16	SF4	cC	102	3	0,12,12	-	-	-	-	-
14	CLA	bB	835	2	49,53,73	2.48	20 (40%)	59,89,113	3.22	26 (44%)
14	CLA	cJ	101	8	49,53,73	2.51	21 (42%)	59,89,113	3.21	27 (45%)
14	CLA	bA	831	1	59,63,73	2.23	20 (33%)	71,101,113	2.99	32 (45%)
14	CLA	A	814	-	49,53,73	2.52	20 (40%)	59,89,113	3.19	26 (44%)
17	BCR	A	849	-	41,41,41	1.72	7 (17%)	56,56,56	1.48	10 (17%)
14	CLA	B	819	-	51,55,73	2.45	20 (39%)	61,91,113	3.21	32 (52%)
14	CLA	B	849	-	49,53,73	2.50	21 (42%)	59,89,113	3.18	27 (45%)
14	CLA	bB	810	2	49,53,73	2.50	21 (42%)	59,89,113	3.18	25 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	bB	818	-	50,54,73	2.45	20 (40%)	60,90,113	3.13	26 (43%)
14	CLA	bA	803	1	49,53,73	2.49	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	cA	806	1	69,73,73	2.06	20 (28%)	83,113,113	2.74	28 (33%)
17	BCR	bM	101	-	41,41,41	1.75	8 (19%)	56,56,56	1.50	12 (21%)
14	CLA	cA	817	1	58,62,73	2.30	20 (34%)	69,99,113	2.95	26 (37%)
14	CLA	bA	834	1	49,53,73	2.50	20 (40%)	59,89,113	3.17	27 (45%)
17	BCR	I	102	-	41,41,41	1.67	8 (19%)	56,56,56	1.46	9 (16%)
17	BCR	cA	847	-	41,41,41	1.77	7 (17%)	56,56,56	1.37	8 (14%)
14	CLA	B	830	2	46,50,73	2.51	20 (43%)	55,85,113	3.30	25 (45%)
14	CLA	bA	828	1	64,68,73	2.13	20 (31%)	77,107,113	2.80	25 (32%)
14	CLA	cA	836	1	55,59,73	2.27	19 (34%)	66,96,113	3.10	31 (46%)
14	CLA	B	832	2	49,53,73	2.44	19 (38%)	59,89,113	3.22	27 (45%)
14	CLA	bA	807	1	49,53,73	2.50	20 (40%)	59,89,113	3.19	26 (44%)
16	SF4	bA	844	1,2	0,12,12	-	-	-	-	-
14	CLA	cB	838	2	51,55,73	2.41	20 (39%)	61,91,113	3.20	25 (40%)
14	CLA	cA	816	1	49,53,73	2.48	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	bA	833	1	69,73,73	2.00	21 (30%)	83,113,113	2.71	30 (36%)
14	CLA	B	809	2	69,73,73	1.94	19 (27%)	83,113,113	2.70	30 (36%)
14	CLA	cB	811	2	49,53,73	2.50	21 (42%)	59,89,113	3.18	25 (42%)
17	BCR	bB	841	-	41,41,41	1.75	6 (14%)	56,56,56	1.37	9 (16%)
17	BCR	bA	845	-	41,41,41	1.80	7 (17%)	56,56,56	1.49	11 (19%)
14	CLA	bB	831	2	69,73,73	2.10	20 (28%)	83,113,113	2.85	29 (34%)
14	CLA	B	836	2	49,53,73	2.47	20 (40%)	59,89,113	3.21	26 (44%)
14	CLA	cL	202	2	69,73,73	1.95	21 (30%)	83,113,113	2.87	31 (37%)
18	LHG	A	851	14	26,26,48	0.33	0	29,32,54	0.39	0
14	CLA	cA	810	-	49,53,73	2.49	21 (42%)	59,89,113	3.16	25 (42%)
14	CLA	bA	841	22	69,73,73	1.97	19 (27%)	83,113,113	2.66	31 (37%)
17	BCR	F	202	-	41,41,41	1.80	6 (14%)	56,56,56	1.49	8 (14%)
14	CLA	B	804	2	55,59,73	2.33	20 (36%)	66,96,113	3.12	30 (45%)
14	CLA	cB	821	2	49,53,73	2.52	20 (40%)	59,89,113	3.23	27 (45%)
14	CLA	bB	811	2	49,53,73	2.49	20 (40%)	59,89,113	3.15	26 (44%)
14	CLA	bA	818	1	64,68,73	2.18	21 (32%)	77,107,113	2.94	31 (40%)
15	PQN	bB	840	-	34,34,34	0.45	1 (2%)	42,45,45	0.35	0
14	CLA	F	201	22	55,59,73	2.29	19 (34%)	66,96,113	3.05	31 (46%)
14	CLA	cX	201	-	49,53,73	2.50	21 (42%)	59,89,113	3.23	28 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	cB	844	-	41,41,41	1.85	7 (17%)	56,56,56	1.57	11 (19%)
14	CLA	cB	831	2	46,50,73	2.51	20 (43%)	55,85,113	3.30	25 (45%)
14	CLA	L	203	10	63,67,73	2.11	21 (33%)	75,105,113	2.96	30 (40%)
14	CLA	bA	842	18	49,53,73	2.44	20 (40%)	59,89,113	3.19	26 (44%)
14	CLA	cA	834	1	49,53,73	2.50	20 (40%)	59,89,113	3.18	27 (45%)
14	CLA	bB	813	-	52,56,73	2.42	20 (38%)	62,92,113	3.12	30 (48%)
14	CLA	bB	826	2	69,73,73	2.02	21 (30%)	83,113,113	2.81	32 (38%)
14	CLA	bA	809	1	49,53,73	2.47	20 (40%)	59,89,113	3.20	26 (44%)
14	CLA	bB	802	2	69,73,73	2.02	20 (28%)	83,113,113	2.75	32 (38%)
14	CLA	bA	835	1	49,53,73	2.49	20 (40%)	59,89,113	3.16	28 (47%)
14	CLA	cA	821	-	49,53,73	2.52	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	bB	805	2	69,73,73	2.07	21 (30%)	83,113,113	2.83	30 (36%)
17	BCR	bB	844	-	41,41,41	1.71	8 (19%)	56,56,56	1.43	10 (17%)
14	CLA	A	837	1	69,73,73	1.99	20 (28%)	83,113,113	2.72	28 (33%)
14	CLA	cA	824	-	63,67,73	2.17	20 (31%)	75,105,113	2.83	30 (40%)
20	LMG	cB	849	-	43,43,55	0.21	0	51,51,63	0.30	0
14	CLA	bA	838	1	49,53,73	2.32	19 (38%)	59,89,113	3.30	27 (45%)
14	CLA	B	833	-	49,53,73	2.51	21 (42%)	59,89,113	3.17	28 (47%)
14	CLA	bA	811	1	49,53,73	2.47	21 (42%)	59,89,113	3.21	28 (47%)
14	CLA	B	817	2	59,63,73	2.26	22 (37%)	71,101,113	3.04	30 (42%)
14	CLA	A	824	22	63,67,73	2.17	20 (31%)	75,105,113	2.83	30 (40%)
14	CLA	cB	810	2	69,73,73	1.94	19 (27%)	83,113,113	2.71	30 (36%)
14	CLA	L	201	2	69,73,73	1.95	21 (30%)	83,113,113	2.87	31 (37%)
17	BCR	cA	845	-	41,41,41	1.80	7 (17%)	56,56,56	1.49	11 (19%)
14	CLA	B	821	-	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	bA	827	1	65,69,73	2.17	20 (30%)	78,108,113	2.88	29 (37%)
14	CLA	bA	802	22	69,73,73	1.94	21 (30%)	83,113,113	2.85	31 (37%)
14	CLA	B	810	2	49,53,73	2.50	21 (42%)	59,89,113	3.18	25 (42%)
14	CLA	cA	829	1	69,73,73	2.05	20 (28%)	83,113,113	2.69	29 (34%)
14	CLA	cB	814	-	52,56,73	2.42	20 (38%)	62,92,113	3.13	30 (48%)
14	CLA	cA	805	1	59,63,73	2.24	21 (35%)	71,101,113	3.03	29 (40%)
14	CLA	cF	201	22	55,59,73	2.29	19 (34%)	66,96,113	3.04	31 (46%)
17	BCR	bJ	103	-	41,41,41	1.84	7 (17%)	56,56,56	1.61	11 (19%)
17	BCR	B	845	-	41,41,41	1.78	7 (17%)	56,56,56	1.46	12 (21%)
14	CLA	cB	828	2	69,73,73	2.10	20 (28%)	83,113,113	2.71	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	bA	852	-	69,73,73	1.86	18 (26%)	83,113,113	2.50	28 (33%)
16	SF4	bC	102	3	0,12,12	-	-	-		
14	CLA	bB	823	2	54,58,73	2.38	20 (37%)	65,95,113	3.13	28 (43%)
14	CLA	B	829	2	49,53,73	2.49	20 (40%)	59,89,113	3.17	26 (44%)
14	CLA	B	803	-	59,63,73	2.17	20 (33%)	71,101,113	2.96	30 (42%)
14	CLA	cA	831	1	59,63,73	2.23	20 (33%)	71,101,113	2.99	32 (45%)
14	CLA	cB	827	2	69,73,73	2.02	21 (30%)	83,113,113	2.82	32 (38%)
14	CLA	A	811	1	49,53,73	2.47	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	B	837	2	51,55,73	2.41	20 (39%)	61,91,113	3.21	25 (40%)
14	CLA	B	805	2	69,73,73	2.08	21 (30%)	83,113,113	2.83	30 (36%)
14	CLA	cB	818	2	59,63,73	2.26	22 (37%)	71,101,113	3.03	30 (42%)
14	CLA	A	825	-	54,58,73	2.31	20 (37%)	65,95,113	3.19	30 (46%)
14	CLA	cB	802	-	69,73,73	2.02	19 (27%)	83,113,113	2.70	28 (33%)
14	CLA	cB	824	2	54,58,73	2.38	20 (37%)	65,95,113	3.13	28 (43%)
14	CLA	cA	828	1	64,68,73	2.13	20 (31%)	77,107,113	2.80	25 (32%)
14	CLA	bL	201	2	69,73,73	1.95	21 (30%)	83,113,113	2.88	31 (37%)
14	CLA	A	813	1	49,53,73	2.47	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	bA	806	1	69,73,73	2.06	20 (28%)	83,113,113	2.75	28 (33%)
17	BCR	cM	101	-	41,41,41	1.75	8 (19%)	56,56,56	1.50	12 (21%)
17	BCR	cI	102	-	41,41,41	1.66	8 (19%)	56,56,56	1.46	9 (16%)
14	CLA	bB	806	2	69,73,73	2.07	20 (28%)	83,113,113	2.75	31 (37%)
14	CLA	B	815	2	56,60,73	2.33	21 (37%)	67,97,113	3.09	31 (46%)
14	CLA	bB	832	2	49,53,73	2.44	19 (38%)	59,89,113	3.22	27 (45%)
14	CLA	B	812	2	69,73,73	2.10	21 (30%)	83,113,113	2.88	29 (34%)
14	CLA	A	805	1	59,63,73	2.23	21 (35%)	71,101,113	3.03	29 (40%)
14	CLA	bB	809	2	69,73,73	1.94	19 (27%)	83,113,113	2.71	30 (36%)
14	CLA	A	815	-	49,53,73	2.51	21 (42%)	59,89,113	3.22	27 (45%)
14	CLA	A	812	1	49,53,73	2.50	21 (42%)	59,89,113	3.22	26 (44%)
14	CLA	B	851	-	49,53,73	2.50	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	cB	804	-	59,63,73	2.17	20 (33%)	71,101,113	2.96	30 (42%)
14	CLA	bB	815	2	56,60,73	2.33	21 (37%)	67,97,113	3.10	31 (46%)
14	CLA	cA	837	1	69,73,73	2.00	20 (28%)	83,113,113	2.73	28 (33%)
14	CLA	bA	814	-	49,53,73	2.52	20 (40%)	59,89,113	3.19	26 (44%)
14	CLA	bA	830	1	54,58,73	2.25	19 (35%)	65,95,113	3.07	29 (44%)
14	CLA	bB	804	2	55,59,73	2.33	20 (36%)	66,96,113	3.12	30 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	cB	826	2	59,63,73	2.26	20 (33%)	71,101,113	2.99	32 (45%)
18	LHG	A	850	-	48,48,48	0.27	0	51,54,54	0.31	0
16	SF4	cC	101	3	0,12,12	-	-	-		
14	CLA	B	839	2	69,73,73	2.04	21 (30%)	83,113,113	2.78	28 (33%)
14	CLA	cB	808	2	69,73,73	2.06	20 (28%)	83,113,113	2.75	27 (32%)
14	CLA	cB	835	-	49,53,73	2.47	21 (42%)	59,89,113	3.13	27 (45%)
17	BCR	A	846	-	41,41,41	1.76	6 (14%)	56,56,56	1.76	14 (25%)
14	CLA	A	820	22	49,53,73	2.51	21 (42%)	59,89,113	3.17	28 (47%)
14	CLA	bB	824	-	50,54,73	2.48	20 (40%)	60,90,113	3.20	26 (43%)
14	CLA	cB	840	2	69,73,73	2.04	21 (30%)	83,113,113	2.78	28 (33%)
17	BCR	bB	846	-	41,41,41	1.71	7 (17%)	56,56,56	1.41	10 (17%)
14	CLA	bA	810	-	49,53,73	2.49	21 (42%)	59,89,113	3.16	25 (42%)
14	CLA	A	817	1	58,62,73	2.30	20 (34%)	69,99,113	2.95	26 (37%)
14	CLA	cB	830	2	49,53,73	2.49	20 (40%)	59,89,113	3.17	26 (44%)
13	CL0	A	801	1	63,73,73	3.17	18 (28%)	61,113,113	2.43	18 (29%)
14	CLA	A	819	1	49,53,73	2.51	20 (40%)	59,89,113	3.19	29 (49%)
14	CLA	cB	825	-	50,54,73	2.48	20 (40%)	60,90,113	3.20	26 (43%)
14	CLA	bB	808	2	56,60,73	2.24	20 (35%)	67,97,113	3.08	30 (44%)
14	CLA	bB	834	-	49,53,73	2.48	21 (42%)	59,89,113	3.14	27 (45%)
17	BCR	bI	101	-	41,41,41	1.68	8 (19%)	56,56,56	1.39	10 (17%)
14	CLA	cB	829	2	69,73,73	2.01	19 (27%)	83,113,113	2.81	29 (34%)
14	CLA	bB	801	-	69,73,73	2.02	19 (27%)	83,113,113	2.70	28 (33%)
17	BCR	J	103	-	41,41,41	1.84	7 (17%)	56,56,56	1.61	11 (19%)
14	CLA	cA	842	18	49,53,73	2.44	20 (40%)	59,89,113	3.18	26 (44%)
17	BCR	cB	846	-	41,41,41	1.79	7 (17%)	56,56,56	1.46	12 (21%)
14	CLA	bL	204	-	69,73,73	2.09	20 (28%)	83,113,113	2.72	27 (32%)
14	CLA	bB	839	2	69,73,73	2.04	21 (30%)	83,113,113	2.78	28 (33%)
14	CLA	cB	809	2	56,60,73	2.24	20 (35%)	67,97,113	3.07	30 (44%)
17	BCR	cB	843	-	41,41,41	1.80	7 (17%)	56,56,56	1.60	12 (21%)
15	PQN	cA	843	-	34,34,34	0.47	1 (2%)	42,45,45	0.34	0
14	CLA	bB	825	2	59,63,73	2.26	20 (33%)	71,101,113	2.99	32 (45%)
14	CLA	A	830	1	54,58,73	2.24	18 (33%)	65,95,113	3.07	29 (44%)
14	CLA	B	818	-	50,54,73	2.44	20 (40%)	60,90,113	3.12	26 (43%)
14	CLA	A	806	1	69,73,73	2.06	20 (28%)	83,113,113	2.75	28 (33%)
14	CLA	A	832	1	69,73,73	1.98	20 (28%)	83,113,113	2.74	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	bB	833	-	49,53,73	2.51	21 (42%)	59,89,113	3.17	28 (47%)
14	CLA	cA	838	1	49,53,73	2.32	19 (38%)	59,89,113	3.30	27 (45%)
14	CLA	A	828	1	64,68,73	2.13	20 (31%)	77,107,113	2.80	25 (32%)
14	CLA	A	852	-	69,73,73	1.86	18 (26%)	83,113,113	2.50	28 (33%)
14	CLA	bA	804	1	57,61,73	2.32	21 (36%)	68,98,113	3.11	29 (42%)
17	BCR	A	847	-	41,41,41	1.77	7 (17%)	56,56,56	1.37	8 (14%)
14	CLA	bA	824	22	63,67,73	2.17	20 (31%)	75,105,113	2.83	30 (40%)
14	CLA	L	204	-	69,73,73	2.09	20 (28%)	83,113,113	2.72	27 (32%)
17	BCR	bB	850	-	41,41,41	1.76	8 (19%)	56,56,56	1.38	8 (14%)
14	CLA	bA	826	1	50,54,73	2.43	20 (40%)	60,90,113	3.24	27 (45%)
14	CLA	cA	820	-	49,53,73	2.51	21 (42%)	59,89,113	3.17	28 (47%)
14	CLA	cA	822	1	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	bB	817	2	59,63,73	2.26	22 (37%)	71,101,113	3.03	30 (42%)
20	LMG	B	848	-	43,43,55	0.21	0	51,51,63	0.30	0
14	CLA	A	804	1	57,61,73	2.32	21 (36%)	68,98,113	3.10	29 (42%)
14	CLA	bA	808	1	49,53,73	2.45	20 (40%)	59,89,113	3.23	30 (50%)
14	CLA	cA	823	1	49,53,73	2.48	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	cA	811	1	49,53,73	2.47	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	A	836	1	55,59,73	2.26	19 (34%)	66,96,113	3.10	31 (46%)
14	CLA	B	822	2	49,53,73	2.48	20 (40%)	59,89,113	3.25	26 (44%)
17	BCR	cL	206	-	41,41,41	1.70	8 (19%)	56,56,56	1.40	9 (16%)
17	BCR	B	847	-	41,41,41	1.73	8 (19%)	56,56,56	1.47	13 (23%)
14	CLA	cB	820	-	51,55,73	2.45	20 (39%)	61,91,113	3.22	32 (52%)
14	CLA	B	838	-	69,73,73	1.95	20 (28%)	83,113,113	2.63	27 (32%)
14	CLA	cA	827	1	65,69,73	2.17	20 (30%)	78,108,113	2.88	28 (35%)
14	CLA	B	823	2	54,58,73	2.38	20 (37%)	65,95,113	3.13	28 (43%)
14	CLA	B	820	2	49,53,73	2.51	20 (40%)	59,89,113	3.23	27 (45%)
14	CLA	L	202	10	69,73,73	2.10	21 (30%)	83,113,113	3.98	30 (36%)
14	CLA	bA	825	22	54,58,73	2.31	20 (37%)	65,95,113	3.19	30 (46%)
14	CLA	cB	815	-	49,53,73	2.50	21 (42%)	59,89,113	3.24	27 (45%)
14	CLA	cA	818	1	64,68,73	2.18	21 (32%)	77,107,113	2.94	31 (40%)
14	CLA	A	808	1	49,53,73	2.45	20 (40%)	59,89,113	3.24	30 (50%)

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
14	CLA	bA	829	1	-	12/39/115/115	-
14	CLA	cB	839	-	-	5/39/115/115	-
14	CLA	bB	812	2	-	9/39/115/115	-
14	CLA	cA	813	1	-	5/15/91/115	-
14	CLA	B	806	2	-	10/39/115/115	-
17	BCR	bB	842	-	-	9/29/63/63	0/2/2/2
14	CLA	A	810	-	-	5/15/91/115	-
14	CLA	A	829	1	-	12/39/115/115	-
14	CLA	bF	201	22	-	5/23/99/115	-
14	CLA	cB	806	2	-	15/39/115/115	-
14	CLA	B	825	2	-	5/27/103/115	-
17	BCR	cL	207	-	-	3/29/63/63	0/2/2/2
14	CLA	A	807	1	-	8/15/91/115	-
14	CLA	bB	814	-	-	7/15/91/115	-
14	CLA	bA	840	1	-	13/39/115/115	-
14	CLA	J	102	8	-	2/15/91/115	-
17	BCR	B	841	-	-	7/29/63/63	0/2/2/2
14	CLA	A	833	1	-	8/39/115/115	-
14	CLA	bB	807	2	-	12/39/115/115	-
14	CLA	bX	201	-	-	5/15/91/115	-
16	SF4	bC	101	3	-	-	0/6/5/5
14	CLA	A	840	1	-	13/39/115/115	-
14	CLA	cA	804	1	-	8/25/101/115	-
17	BCR	bF	202	-	-	6/29/63/63	0/2/2/2
14	CLA	bB	849	-	-	4/15/91/115	-
14	CLA	bL	202	10	-	15/39/115/115	-
14	CLA	cB	819	-	-	5/17/93/115	-
14	CLA	A	821	-	-	4/15/91/115	-
17	BCR	M	101	-	-	6/29/63/63	0/2/2/2
14	CLA	cA	852	-	-	7/39/115/115	-
14	CLA	cA	803	1	-	8/15/91/115	-
14	CLA	bB	819	-	-	11/18/94/115	-
17	BCR	cI	101	-	-	1/29/63/63	0/2/2/2
14	CLA	bA	805	1	-	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	831	2	-	16/39/115/115	-
14	CLA	bA	815	-	-	7/15/91/115	-
14	CLA	bJ	102	8	-	3/15/91/115	-
14	CLA	bA	812	1	-	5/15/91/115	-
14	CLA	cA	832	1	-	8/39/115/115	-
14	CLA	bL	203	10	-	9/32/108/115	-
14	CLA	bA	839	1	-	9/39/115/115	-
14	CLA	cB	822	-	-	8/15/91/115	-
14	CLA	B	814	-	-	7/15/91/115	-
17	BCR	bB	843	-	-	10/29/63/63	0/2/2/2
14	CLA	bB	816	2	-	6/15/91/115	-
17	BCR	bA	848	-	-	3/29/63/63	0/2/2/2
14	CLA	cA	826	1	-	6/17/93/115	-
14	CLA	bB	837	2	-	6/18/94/115	-
17	BCR	bA	846	-	-	15/29/63/63	0/2/2/2
18	LHG	bA	850	-	-	15/53/53/53	-
14	CLA	cA	809	1	-	6/15/91/115	-
14	CLA	A	822	1	-	3/15/91/115	-
14	CLA	cA	808	1	-	7/15/91/115	-
14	CLA	X	201	-	-	5/15/91/115	-
14	CLA	cB	813	2	-	9/39/115/115	-
14	CLA	cB	801	-	-	6/15/91/115	-
17	BCR	bB	847	-	-	2/29/63/63	0/2/2/2
14	CLA	cB	823	2	-	6/15/91/115	-
17	BCR	B	850	-	-	12/29/63/63	0/2/2/2
14	CLA	A	834	1	-	3/15/91/115	-
14	CLA	cA	835	1	-	5/15/91/115	-
17	BCR	cA	848	-	-	3/29/63/63	0/2/2/2
14	CLA	bB	820	2	-	10/15/91/115	-
14	CLA	bB	803	-	-	8/27/103/115	-
14	CLA	bA	819	1	-	6/15/91/115	-
17	BCR	cB	851	-	-	12/29/63/63	0/2/2/2
16	SF4	A	844	1,2	-	-	0/6/5/5
14	CLA	cA	833	1	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SF4	C	102	3	-	-	0/6/5/5
17	BCR	cA	846	-	-	15/29/63/63	0/2/2/2
14	CLA	cA	807	1	-	8/15/91/115	-
14	CLA	B	828	2	-	13/39/115/115	-
14	CLA	cJ	102	8	-	3/15/91/115	-
14	CLA	bB	822	2	-	6/15/91/115	-
14	CLA	cL	203	10	-	15/39/115/115	-
14	CLA	cB	832	2	-	16/39/115/115	-
18	LHG	bA	851	14	-	13/31/31/53	-
17	BCR	A	845	-	-	10/29/63/63	0/2/2/2
14	CLA	cA	841	-	-	11/39/115/115	-
14	CLA	bA	820	22	-	5/15/91/115	-
13	CL0	bA	801	1	-	6/37/135/135	-
14	CLA	A	818	1	-	10/33/109/115	-
14	CLA	A	831	1	-	13/27/103/115	-
14	CLA	A	809	1	-	6/15/91/115	-
14	CLA	cA	825	-	-	2/21/97/115	-
14	CLA	B	807	2	-	12/39/115/115	-
14	CLA	bA	832	1	-	8/39/115/115	-
14	CLA	bB	830	2	-	4/12/88/115	-
17	BCR	L	205	-	-	4/29/63/63	0/2/2/2
17	BCR	cB	842	-	-	7/29/63/63	0/2/2/2
14	CLA	A	816	1	-	7/15/91/115	-
14	CLA	B	824	-	-	6/17/93/115	-
14	CLA	cB	817	2	-	6/15/91/115	-
14	CLA	bA	822	1	-	3/15/91/115	-
14	CLA	cA	839	1	-	9/39/115/115	-
14	CLA	B	808	2	-	3/24/100/115	-
14	CLA	cB	805	2	-	8/23/99/115	-
17	BCR	cB	847	-	-	10/29/63/63	0/2/2/2
14	CLA	B	826	2	-	6/39/115/115	-
14	CLA	cB	850	-	-	4/15/91/115	-
16	SF4	cA	844	1,2	-	-	0/6/5/5
14	CLA	cA	840	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	bA	849	-	-	8/29/63/63	0/2/2/2
14	CLA	B	801	-	-	9/39/115/115	-
14	CLA	cA	830	1	-	4/21/97/115	-
15	PQN	cB	841	-	-	4/23/43/43	0/2/2/2
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	cB	836	2	-	3/15/91/115	-
17	BCR	cJ	103	-	-	17/29/63/63	0/2/2/2
17	BCR	A	848	-	-	3/29/63/63	0/2/2/2
17	BCR	cB	848	-	-	2/29/63/63	0/2/2/2
14	CLA	B	835	2	-	3/15/91/115	-
14	CLA	cB	812	2	-	3/15/91/115	-
20	LMG	bB	848	-	-	9/38/58/70	0/1/1/1
14	CLA	bA	823	1	-	6/15/91/115	-
14	CLA	A	826	1	-	6/17/93/115	-
15	PQN	B	840	-	-	4/23/43/43	0/2/2/2
14	CLA	cB	833	2	-	4/15/91/115	-
14	CLA	A	842	18	-	8/15/91/115	-
14	CLA	cB	803	2	-	11/39/115/115	-
14	CLA	A	803	1	-	8/15/91/115	-
14	CLA	bB	836	2	-	7/15/91/115	-
14	CLA	cB	834	-	-	2/15/91/115	-
14	CLA	bB	829	2	-	7/15/91/115	-
14	CLA	cB	816	2	-	11/24/100/115	-
14	CLA	A	835	1	-	5/15/91/115	-
14	CLA	B	802	2	-	11/39/115/115	-
14	CLA	cA	819	1	-	6/15/91/115	-
14	CLA	A	841	-	-	11/39/115/115	-
14	CLA	cA	802	-	-	3/39/115/115	-
14	CLA	A	827	1	-	3/35/111/115	-
14	CLA	A	838	1	-	5/15/91/115	-
14	CLA	bJ	101	8	-	4/15/91/115	-
17	BCR	bL	205	-	-	4/29/63/63	0/2/2/2
17	BCR	cF	202	-	-	6/29/63/63	0/2/2/2
15	PQN	bA	843	-	-	4/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cL	204	10	-	9/32/108/115	-
14	CLA	bB	827	2	-	5/39/115/115	-
14	CLA	bB	838	-	-	5/39/115/115	-
14	CLA	cL	205	-	-	17/39/115/115	-
17	BCR	L	206	-	-	3/29/63/63	0/2/2/2
17	BCR	cB	845	-	-	15/29/63/63	0/2/2/2
14	CLA	A	839	1	-	9/39/115/115	-
14	CLA	bA	817	1	-	8/26/102/115	-
15	PQN	A	843	-	-	4/23/43/43	0/2/2/2
14	CLA	A	823	1	-	6/15/91/115	-
14	CLA	cA	814	-	-	1/15/91/115	-
14	CLA	B	827	2	-	5/39/115/115	-
14	CLA	cA	815	-	-	7/15/91/115	-
14	CLA	cA	812	1	-	5/15/91/115	-
14	CLA	B	811	2	-	3/15/91/115	-
14	CLA	J	101	8	-	4/15/91/115	-
17	BCR	B	846	-	-	10/29/63/63	0/2/2/2
17	BCR	cA	849	-	-	8/29/63/63	0/2/2/2
18	LHG	cA	850	-	-	15/53/53/53	-
17	BCR	B	843	-	-	10/29/63/63	0/2/2/2
14	CLA	bA	821	-	-	4/15/91/115	-
14	CLA	B	816	2	-	5/15/91/115	-
14	CLA	bB	828	2	-	13/39/115/115	-
14	CLA	cB	807	2	-	10/39/115/115	-
14	CLA	bB	821	-	-	8/15/91/115	-
14	CLA	B	834	-	-	3/15/91/115	-
14	CLA	bB	851	-	-	5/15/91/115	-
17	BCR	B	842	-	-	9/29/63/63	0/2/2/2
13	CL0	cA	801	1	-	6/37/135/135	-
14	CLA	bA	813	1	-	5/15/91/115	-
14	CLA	A	802	22	-	3/39/115/115	-
14	CLA	bA	816	1	-	7/15/91/115	-
14	CLA	cB	837	2	-	7/15/91/115	-
17	BCR	bB	845	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bA	837	1	-	9/39/115/115	-
17	BCR	bA	847	-	-	6/29/63/63	0/2/2/2
17	BCR	I	101	-	-	1/29/63/63	0/2/2/2
17	BCR	B	844	-	-	15/29/63/63	0/2/2/2
17	BCR	bL	206	-	-	3/29/63/63	0/2/2/2
14	CLA	B	813	-	-	5/19/95/115	-
14	CLA	bA	836	1	-	6/23/99/115	-
18	LHG	cA	851	14	-	14/31/31/53	-
17	BCR	bI	102	-	-	3/29/63/63	0/2/2/2
16	SF4	cC	102	3	-	-	0/6/5/5
14	CLA	bB	835	2	-	3/15/91/115	-
14	CLA	cJ	101	8	-	4/15/91/115	-
14	CLA	bA	831	1	-	13/27/103/115	-
14	CLA	A	814	-	-	1/15/91/115	-
17	BCR	A	849	-	-	8/29/63/63	0/2/2/2
14	CLA	B	819	-	-	11/18/94/115	-
14	CLA	B	849	-	-	4/15/91/115	-
14	CLA	bB	810	2	-	5/15/91/115	-
14	CLA	bB	818	-	-	5/17/93/115	-
14	CLA	bA	803	1	-	8/15/91/115	-
14	CLA	cA	806	1	-	11/39/115/115	-
17	BCR	bM	101	-	-	5/29/63/63	0/2/2/2
14	CLA	cA	817	1	-	8/26/102/115	-
14	CLA	bA	834	1	-	3/15/91/115	-
17	BCR	I	102	-	-	3/29/63/63	0/2/2/2
17	BCR	cA	847	-	-	6/29/63/63	0/2/2/2
14	CLA	B	830	2	-	4/12/88/115	-
14	CLA	bA	828	1	-	7/33/109/115	-
14	CLA	cA	836	1	-	6/23/99/115	-
14	CLA	B	832	2	-	4/15/91/115	-
14	CLA	bA	807	1	-	8/15/91/115	-
16	SF4	bA	844	1,2	-	-	0/6/5/5
14	CLA	cB	838	2	-	6/18/94/115	-
14	CLA	cA	816	1	-	7/15/91/115	-
14	CLA	bA	833	1	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	809	2	-	11/39/115/115	-
14	CLA	cB	811	2	-	5/15/91/115	-
17	BCR	bB	841	-	-	7/29/63/63	0/2/2/2
17	BCR	bA	845	-	-	10/29/63/63	0/2/2/2
14	CLA	bB	831	2	-	16/39/115/115	-
14	CLA	B	836	2	-	7/15/91/115	-
14	CLA	cL	202	2	-	10/39/115/115	-
18	LHG	A	851	14	-	14/31/31/53	-
14	CLA	cA	810	-	-	5/15/91/115	-
14	CLA	bA	841	22	-	10/39/115/115	-
17	BCR	F	202	-	-	6/29/63/63	0/2/2/2
14	CLA	B	804	2	-	7/23/99/115	-
14	CLA	cB	821	2	-	10/15/91/115	-
14	CLA	bB	811	2	-	3/15/91/115	-
14	CLA	bA	818	1	-	10/33/109/115	-
15	PQN	bB	840	-	-	4/23/43/43	0/2/2/2
14	CLA	F	201	22	-	5/23/99/115	-
14	CLA	cX	201	-	-	5/15/91/115	-
17	BCR	cB	844	-	-	10/29/63/63	0/2/2/2
14	CLA	cB	831	2	-	4/12/88/115	-
14	CLA	L	203	10	-	9/32/108/115	-
14	CLA	bA	842	18	-	8/15/91/115	-
14	CLA	cA	834	1	-	3/15/91/115	-
14	CLA	bB	813	-	-	5/19/95/115	-
14	CLA	bB	826	2	-	6/39/115/115	-
14	CLA	bA	809	1	-	6/15/91/115	-
14	CLA	bB	802	2	-	11/39/115/115	-
14	CLA	bA	835	1	-	5/15/91/115	-
14	CLA	cA	821	-	-	4/15/91/115	-
14	CLA	bB	805	2	-	15/39/115/115	-
17	BCR	bB	844	-	-	15/29/63/63	0/2/2/2
14	CLA	A	837	1	-	9/39/115/115	-
14	CLA	cA	824	-	-	7/32/108/115	-
20	LMG	cB	849	-	-	9/38/58/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bA	838	1	-	5/15/91/115	-
14	CLA	B	833	-	-	2/15/91/115	-
14	CLA	bA	811	1	-	5/15/91/115	-
14	CLA	B	817	2	-	6/27/103/115	-
14	CLA	A	824	22	-	7/32/108/115	-
14	CLA	cB	810	2	-	11/39/115/115	-
14	CLA	L	201	2	-	10/39/115/115	-
17	BCR	cA	845	-	-	10/29/63/63	0/2/2/2
14	CLA	B	821	-	-	8/15/91/115	-
14	CLA	bA	827	1	-	3/35/111/115	-
14	CLA	bA	802	22	-	3/39/115/115	-
14	CLA	B	810	2	-	5/15/91/115	-
14	CLA	cA	829	1	-	12/39/115/115	-
14	CLA	cB	814	-	-	5/19/95/115	-
14	CLA	cA	805	1	-	6/27/103/115	-
14	CLA	cF	201	22	-	5/23/99/115	-
17	BCR	bJ	103	-	-	17/29/63/63	0/2/2/2
17	BCR	B	845	-	-	3/29/63/63	0/2/2/2
14	CLA	cB	828	2	-	5/39/115/115	-
14	CLA	bA	852	-	-	7/39/115/115	-
16	SF4	bC	102	3	-	-	0/6/5/5
14	CLA	bB	823	2	-	6/21/97/115	-
14	CLA	B	829	2	-	7/15/91/115	-
14	CLA	B	803	-	-	8/27/103/115	-
14	CLA	cA	831	1	-	13/27/103/115	-
14	CLA	cB	827	2	-	6/39/115/115	-
14	CLA	A	811	1	-	5/15/91/115	-
14	CLA	B	837	2	-	6/18/94/115	-
14	CLA	B	805	2	-	15/39/115/115	-
14	CLA	cB	818	2	-	6/27/103/115	-
14	CLA	A	825	-	-	2/21/97/115	-
14	CLA	cB	802	-	-	9/39/115/115	-
14	CLA	cB	824	2	-	6/21/97/115	-
14	CLA	cA	828	1	-	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bL	201	2	-	10/39/115/115	-
14	CLA	A	813	1	-	4/15/91/115	-
14	CLA	bA	806	1	-	11/39/115/115	-
17	BCR	cM	101	-	-	6/29/63/63	0/2/2/2
17	BCR	cI	102	-	-	3/29/63/63	0/2/2/2
14	CLA	bB	806	2	-	10/39/115/115	-
14	CLA	B	815	2	-	11/24/100/115	-
14	CLA	bB	832	2	-	4/15/91/115	-
14	CLA	B	812	2	-	9/39/115/115	-
14	CLA	A	805	1	-	6/27/103/115	-
14	CLA	bB	809	2	-	11/39/115/115	-
14	CLA	A	815	-	-	7/15/91/115	-
14	CLA	A	812	1	-	5/15/91/115	-
14	CLA	B	851	-	-	5/15/91/115	-
14	CLA	cB	804	-	-	8/27/103/115	-
14	CLA	bB	815	2	-	11/24/100/115	-
14	CLA	cA	837	1	-	9/39/115/115	-
14	CLA	bA	814	-	-	1/15/91/115	-
14	CLA	bA	830	1	-	4/21/97/115	-
14	CLA	bB	804	2	-	6/23/99/115	-
14	CLA	cB	826	2	-	4/27/103/115	-
18	LHG	A	850	-	-	15/53/53/53	-
16	SF4	cC	101	3	-	-	0/6/5/5
14	CLA	B	839	2	-	13/39/115/115	-
14	CLA	cB	808	2	-	12/39/115/115	-
14	CLA	cB	835	-	-	3/15/91/115	-
17	BCR	A	846	-	-	15/29/63/63	0/2/2/2
14	CLA	A	820	22	-	5/15/91/115	-
14	CLA	bB	824	-	-	6/17/93/115	-
14	CLA	cB	840	2	-	13/39/115/115	-
17	BCR	bB	846	-	-	10/29/63/63	0/2/2/2
14	CLA	bA	810	-	-	5/15/91/115	-
14	CLA	A	817	1	-	8/26/102/115	-
14	CLA	cB	830	2	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL0	A	801	1	-	6/37/135/135	-
14	CLA	A	819	1	-	6/15/91/115	-
14	CLA	cB	825	-	-	6/17/93/115	-
14	CLA	bB	808	2	-	3/24/100/115	-
14	CLA	bB	834	-	-	3/15/91/115	-
17	BCR	bI	101	-	-	1/29/63/63	0/2/2/2
14	CLA	cB	829	2	-	13/39/115/115	-
14	CLA	bB	801	-	-	9/39/115/115	-
17	BCR	J	103	-	-	17/29/63/63	0/2/2/2
14	CLA	cA	842	18	-	8/15/91/115	-
17	BCR	cB	846	-	-	3/29/63/63	0/2/2/2
14	CLA	bL	204	-	-	17/39/115/115	-
14	CLA	bB	839	2	-	13/39/115/115	-
14	CLA	cB	809	2	-	3/24/100/115	-
17	BCR	cB	843	-	-	9/29/63/63	0/2/2/2
15	PQN	cA	843	-	-	4/23/43/43	0/2/2/2
14	CLA	bB	825	2	-	4/27/103/115	-
14	CLA	A	830	1	-	4/21/97/115	-
14	CLA	B	818	-	-	5/17/93/115	-
14	CLA	A	806	1	-	11/39/115/115	-
14	CLA	A	832	1	-	8/39/115/115	-
14	CLA	bB	833	-	-	2/15/91/115	-
14	CLA	cA	838	1	-	5/15/91/115	-
14	CLA	A	828	1	-	7/33/109/115	-
14	CLA	A	852	-	-	7/39/115/115	-
14	CLA	bA	804	1	-	8/25/101/115	-
17	BCR	A	847	-	-	6/29/63/63	0/2/2/2
14	CLA	bA	824	22	-	7/32/108/115	-
14	CLA	L	204	-	-	17/39/115/115	-
17	BCR	bB	850	-	-	12/29/63/63	0/2/2/2
14	CLA	bA	826	1	-	6/17/93/115	-
14	CLA	cA	820	-	-	5/15/91/115	-
14	CLA	cA	822	1	-	3/15/91/115	-
14	CLA	bB	817	2	-	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMG	B	848	-	-	9/38/58/70	0/1/1/1
14	CLA	A	804	1	-	8/25/101/115	-
14	CLA	bA	808	1	-	7/15/91/115	-
14	CLA	cA	823	1	-	6/15/91/115	-
14	CLA	cA	811	1	-	5/15/91/115	-
14	CLA	A	836	1	-	6/23/99/115	-
14	CLA	B	822	2	-	6/15/91/115	-
17	BCR	cL	206	-	-	4/29/63/63	0/2/2/2
17	BCR	B	847	-	-	2/29/63/63	0/2/2/2
14	CLA	cB	820	-	-	11/18/94/115	-
14	CLA	B	838	-	-	5/39/115/115	-
14	CLA	cA	827	1	-	3/35/111/115	-
14	CLA	B	823	2	-	6/21/97/115	-
14	CLA	B	820	2	-	10/15/91/115	-
14	CLA	L	202	10	-	15/39/115/115	-
14	CLA	bA	825	22	-	2/21/97/115	-
14	CLA	cB	815	-	-	7/15/91/115	-
14	CLA	cA	818	1	-	10/33/109/115	-
14	CLA	A	808	1	-	7/15/91/115	-

The worst 5 of 6015 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bA	801	CL0	C3B-C4B	11.22	1.50	1.41
13	A	801	CL0	C3B-C4B	11.14	1.50	1.41
13	cA	801	CL0	C3B-C4B	11.14	1.50	1.41
13	cA	801	CL0	C1A-CHA	8.90	1.50	1.40
13	A	801	CL0	C1A-CHA	8.87	1.50	1.40

The worst 5 of 8360 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	cL	203	CLA	O2A-CGA-O1A	-18.70	76.39	123.59
14	bL	202	CLA	O2A-CGA-O1A	-18.70	76.40	123.59
14	L	202	CLA	O2A-CGA-O1A	-18.70	76.40	123.59
14	cL	203	CLA	O2A-CGA-CBA	15.63	160.95	111.91
14	L	202	CLA	O2A-CGA-CBA	15.62	160.94	111.91

There are no chirality outliers.

5 of 2537 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CL0	CHA-CBD-CGD-O1D
13	bA	801	CL0	CHA-CBD-CGD-O1D
13	cA	801	CL0	CHA-CBD-CGD-O1D
14	A	803	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

316 monomers are involved in 542 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bA	829	CLA	4	0
14	cB	839	CLA	2	0
14	bB	812	CLA	3	0
14	cA	813	CLA	3	0
14	B	806	CLA	2	0
17	bB	842	BCR	2	0
14	A	810	CLA	2	0
14	A	829	CLA	4	0
14	bF	201	CLA	1	0
14	cB	806	CLA	1	0
14	B	825	CLA	3	0
17	cL	207	BCR	5	0
14	A	807	CLA	2	0
14	bB	814	CLA	2	0
14	bA	840	CLA	2	0
14	J	102	CLA	1	0
14	bB	807	CLA	1	0
14	bX	201	CLA	3	0
14	A	840	CLA	1	0
14	cA	804	CLA	1	0
14	bB	849	CLA	1	0
14	bL	202	CLA	1	0
14	cB	819	CLA	1	0
14	A	821	CLA	1	0
17	M	101	BCR	2	0
14	cA	852	CLA	5	0
14	cA	803	CLA	1	0
14	bB	819	CLA	2	0
14	bA	805	CLA	3	0
14	B	831	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bA	815	CLA	2	0
14	bJ	102	CLA	1	0
14	bA	812	CLA	1	0
14	cA	832	CLA	2	0
14	bL	203	CLA	2	0
14	bA	839	CLA	1	0
14	cB	822	CLA	1	0
14	B	814	CLA	2	0
17	bB	843	BCR	2	0
14	bB	816	CLA	1	0
14	cA	826	CLA	2	0
14	bB	837	CLA	2	0
14	cA	809	CLA	2	0
14	A	822	CLA	1	0
14	cA	808	CLA	1	0
14	X	201	CLA	3	0
14	cB	813	CLA	3	0
14	cB	801	CLA	1	0
17	bB	847	BCR	1	0
14	cB	823	CLA	2	0
17	B	850	BCR	2	0
14	A	834	CLA	1	0
14	cA	835	CLA	2	0
14	bB	820	CLA	1	0
14	bB	803	CLA	2	0
14	bA	819	CLA	1	0
17	cB	851	BCR	2	0
14	cA	807	CLA	2	0
14	B	828	CLA	3	0
14	cJ	102	CLA	1	0
14	bB	822	CLA	2	0
14	cL	203	CLA	1	0
14	cB	832	CLA	4	0
17	A	845	BCR	2	0
14	cA	841	CLA	3	0
14	bA	820	CLA	2	0
13	bA	801	CL0	5	0
14	A	818	CLA	1	0
14	A	831	CLA	5	0
14	A	809	CLA	2	0
14	cA	825	CLA	1	0
14	B	807	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bA	832	CLA	2	0
14	bB	830	CLA	1	0
17	L	205	BCR	1	0
14	A	816	CLA	1	0
14	B	824	CLA	1	0
14	cB	817	CLA	1	0
14	bA	822	CLA	1	0
14	cA	839	CLA	1	0
14	B	808	CLA	1	0
14	cB	805	CLA	1	0
17	cB	847	BCR	3	0
14	B	826	CLA	3	0
14	cB	850	CLA	1	0
14	cA	840	CLA	1	0
17	bA	849	BCR	2	0
14	B	801	CLA	2	0
14	cA	830	CLA	2	0
15	cB	841	PQN	1	0
14	cB	836	CLA	3	0
17	cJ	103	BCR	6	0
17	cB	848	BCR	1	0
14	B	835	CLA	3	0
14	cB	812	CLA	1	0
14	bA	823	CLA	1	0
14	A	826	CLA	2	0
15	B	840	PQN	1	0
14	cB	833	CLA	1	0
14	A	842	CLA	1	0
14	cB	803	CLA	5	0
14	A	803	CLA	1	0
14	bB	836	CLA	1	0
14	cB	834	CLA	1	0
14	cB	816	CLA	1	0
14	A	835	CLA	2	0
14	B	802	CLA	4	0
14	cA	819	CLA	1	0
14	A	841	CLA	3	0
14	cA	802	CLA	5	0
14	A	827	CLA	4	0
14	A	838	CLA	3	0
14	bJ	101	CLA	2	0
17	bL	205	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	cL	204	CLA	1	0
14	bB	827	CLA	3	0
14	bB	838	CLA	2	0
14	cL	205	CLA	8	0
17	L	206	BCR	5	0
17	cB	845	BCR	2	0
14	A	839	CLA	1	0
14	bA	817	CLA	1	0
14	A	823	CLA	1	0
14	cA	814	CLA	1	0
14	B	827	CLA	3	0
14	cA	815	CLA	2	0
14	cA	812	CLA	1	0
14	B	811	CLA	1	0
14	J	101	CLA	2	0
17	B	846	BCR	2	0
17	cA	849	BCR	2	0
17	B	843	BCR	2	0
14	bA	821	CLA	1	0
14	B	816	CLA	1	0
14	bB	828	CLA	3	0
14	cB	807	CLA	2	0
14	bB	821	CLA	1	0
14	B	834	CLA	1	0
14	bB	851	CLA	1	0
17	B	842	BCR	2	0
13	cA	801	CL0	5	0
14	bA	813	CLA	3	0
14	A	802	CLA	5	0
14	bA	816	CLA	1	0
14	cB	837	CLA	1	0
17	bB	845	BCR	2	0
14	bA	837	CLA	1	0
17	bA	847	BCR	1	0
17	B	844	BCR	2	0
17	bL	206	BCR	5	0
14	B	813	CLA	3	0
14	bA	836	CLA	1	0
17	bI	102	BCR	2	0
14	bB	835	CLA	3	0
14	cJ	101	CLA	2	0
14	bA	831	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	814	CLA	1	0
17	A	849	BCR	2	0
14	B	819	CLA	2	0
14	B	849	CLA	1	0
14	bB	810	CLA	1	0
14	bB	818	CLA	1	0
14	bA	803	CLA	1	0
14	cA	806	CLA	2	0
17	bM	101	BCR	2	0
14	cA	817	CLA	1	0
14	bA	834	CLA	1	0
17	I	102	BCR	2	0
17	cA	847	BCR	1	0
14	B	830	CLA	1	0
14	bA	828	CLA	1	0
14	cA	836	CLA	1	0
14	B	832	CLA	1	0
14	bA	807	CLA	2	0
14	cB	838	CLA	2	0
14	cA	816	CLA	1	0
14	cB	811	CLA	1	0
17	bA	845	BCR	2	0
14	bB	831	CLA	4	0
14	B	836	CLA	1	0
14	cL	202	CLA	3	0
14	cA	810	CLA	2	0
14	bA	841	CLA	3	0
14	B	804	CLA	1	0
14	cB	821	CLA	1	0
14	bB	811	CLA	1	0
14	bA	818	CLA	1	0
15	bB	840	PQN	1	0
14	F	201	CLA	1	0
14	cX	201	CLA	3	0
17	cB	844	BCR	2	0
14	cB	831	CLA	1	0
14	L	203	CLA	1	0
14	bA	842	CLA	1	0
14	cA	834	CLA	1	0
14	bB	813	CLA	3	0
14	bB	826	CLA	3	0
14	bA	809	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bB	802	CLA	4	0
14	bA	835	CLA	2	0
14	cA	821	CLA	1	0
14	bB	805	CLA	1	0
17	bB	844	BCR	2	0
14	A	837	CLA	1	0
14	cA	824	CLA	1	0
14	bA	838	CLA	3	0
14	B	833	CLA	1	0
14	bA	811	CLA	1	0
14	B	817	CLA	1	0
14	A	824	CLA	1	0
14	L	201	CLA	4	0
17	cA	845	BCR	2	0
14	B	821	CLA	1	0
14	bA	827	CLA	4	0
14	bA	802	CLA	5	0
14	B	810	CLA	1	0
14	cA	829	CLA	4	0
14	cB	814	CLA	3	0
14	cA	805	CLA	2	0
14	cF	201	CLA	1	0
17	bJ	103	BCR	6	0
17	B	845	BCR	2	0
14	cB	828	CLA	3	0
14	bA	852	CLA	5	0
14	bB	823	CLA	1	0
14	B	803	CLA	3	0
14	cA	831	CLA	5	0
14	cB	827	CLA	3	0
14	A	811	CLA	1	0
14	B	837	CLA	2	0
14	B	805	CLA	1	0
14	cB	818	CLA	1	0
14	A	825	CLA	1	0
14	cB	802	CLA	2	0
14	cB	824	CLA	1	0
14	cA	828	CLA	1	0
14	bL	201	CLA	4	0
14	A	813	CLA	3	0
14	bA	806	CLA	2	0
17	cM	101	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	cI	102	BCR	2	0
14	bB	806	CLA	2	0
14	B	815	CLA	1	0
14	bB	832	CLA	1	0
14	B	812	CLA	3	0
14	A	805	CLA	2	0
14	A	815	CLA	2	0
14	A	812	CLA	1	0
14	B	851	CLA	1	0
14	cB	804	CLA	3	0
14	bB	815	CLA	1	0
14	cA	837	CLA	1	0
14	bA	814	CLA	1	0
14	bA	830	CLA	2	0
14	bB	804	CLA	1	0
14	cB	826	CLA	3	0
14	B	839	CLA	2	0
14	cB	808	CLA	1	0
14	cB	835	CLA	1	0
14	A	820	CLA	2	0
14	bB	824	CLA	1	0
14	cB	840	CLA	2	0
17	bB	846	BCR	3	0
14	bA	810	CLA	2	0
14	A	817	CLA	1	0
14	cB	830	CLA	1	0
13	A	801	CL0	5	0
14	A	819	CLA	1	0
14	cB	825	CLA	1	0
14	bB	808	CLA	1	0
14	bB	834	CLA	1	0
14	cB	829	CLA	3	0
14	bB	801	CLA	2	0
17	J	103	BCR	6	0
14	cA	842	CLA	1	0
17	cB	846	BCR	2	0
14	bL	204	CLA	8	0
14	bB	839	CLA	2	0
14	cB	809	CLA	1	0
17	cB	843	BCR	2	0
14	bB	825	CLA	2	0
14	A	830	CLA	2	0

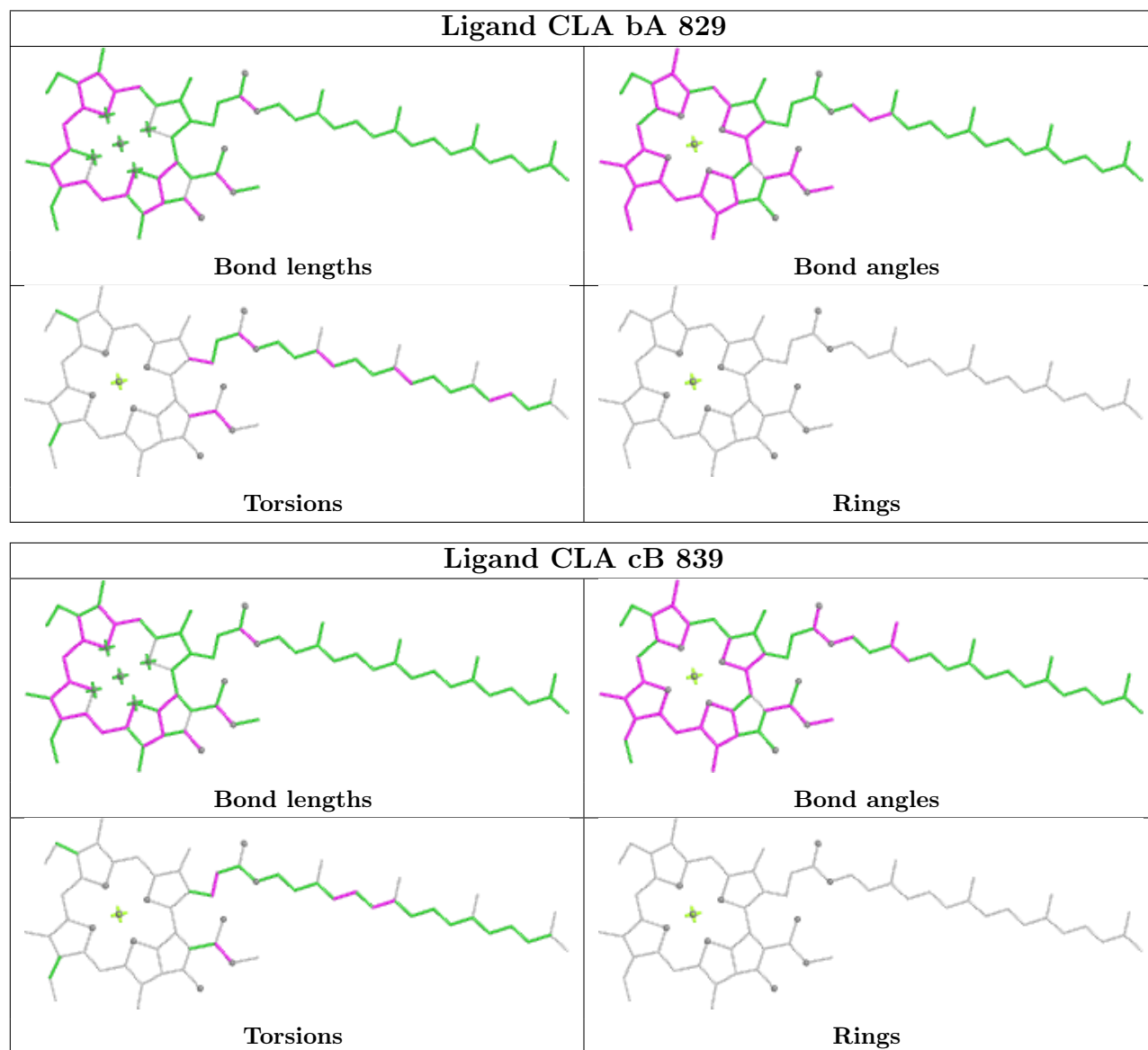
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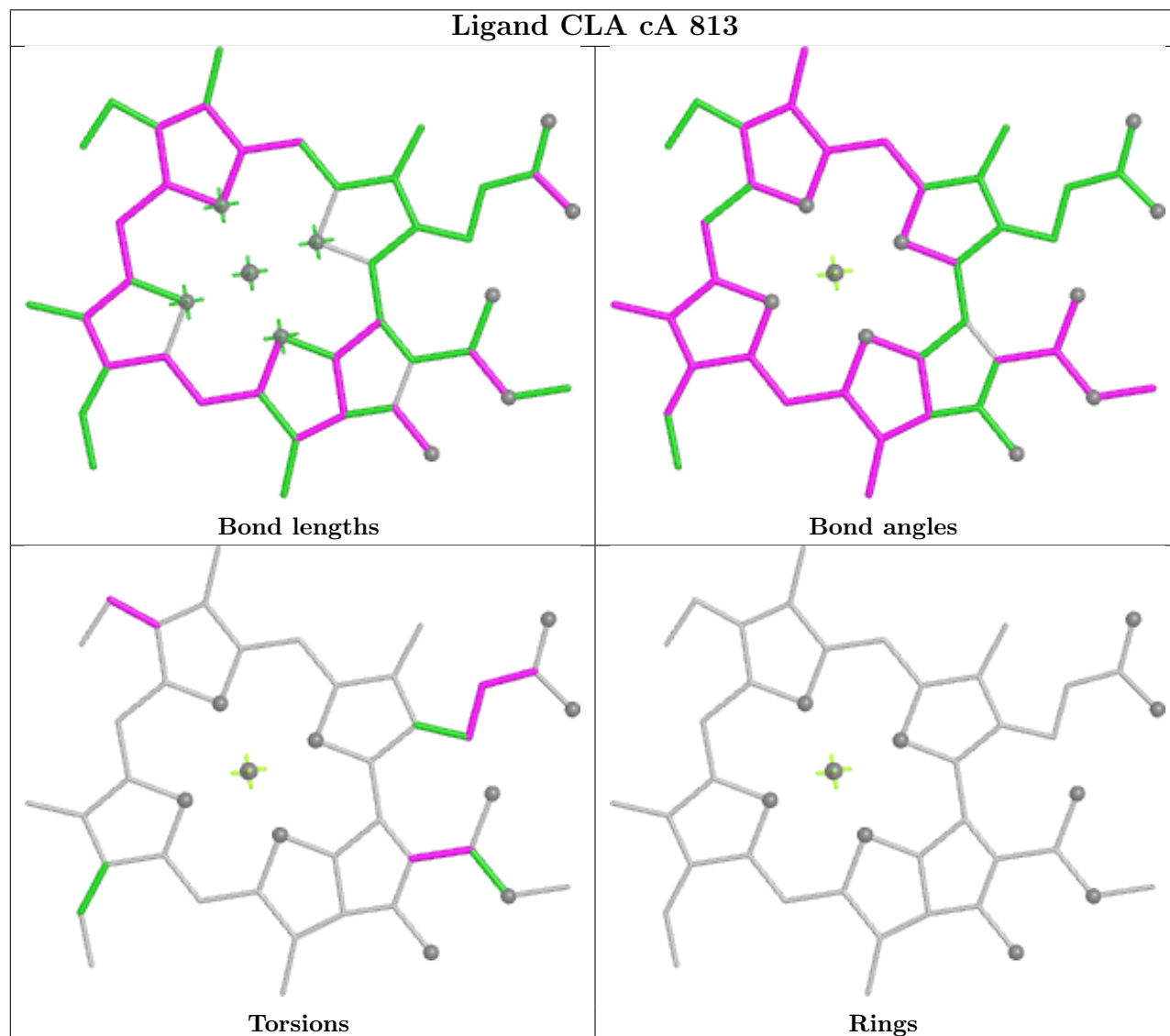
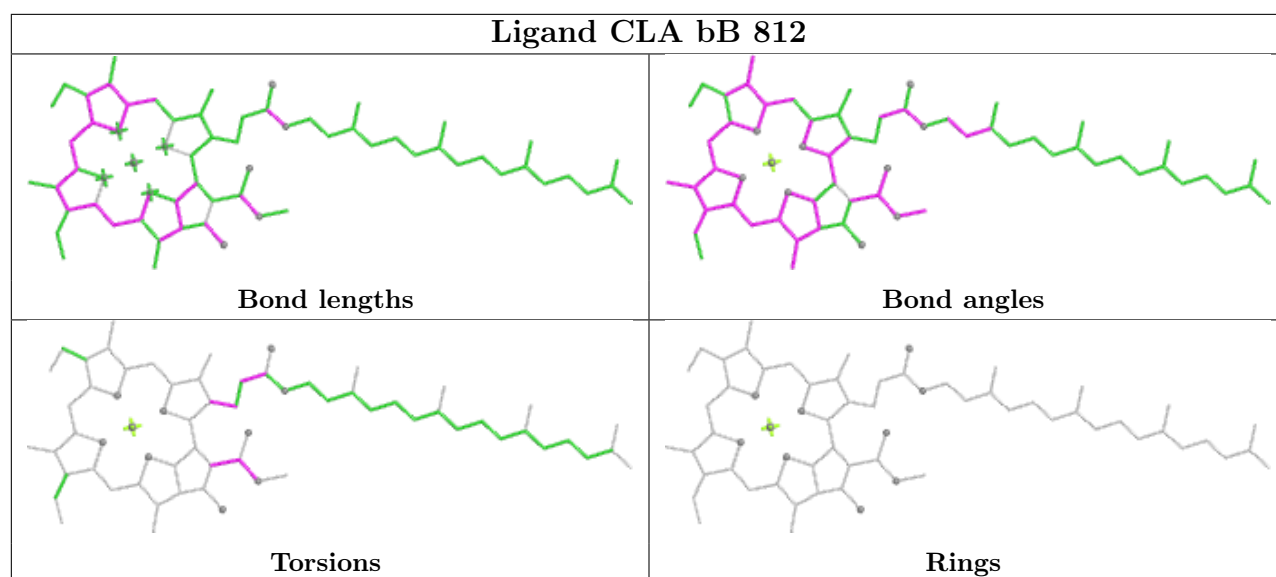
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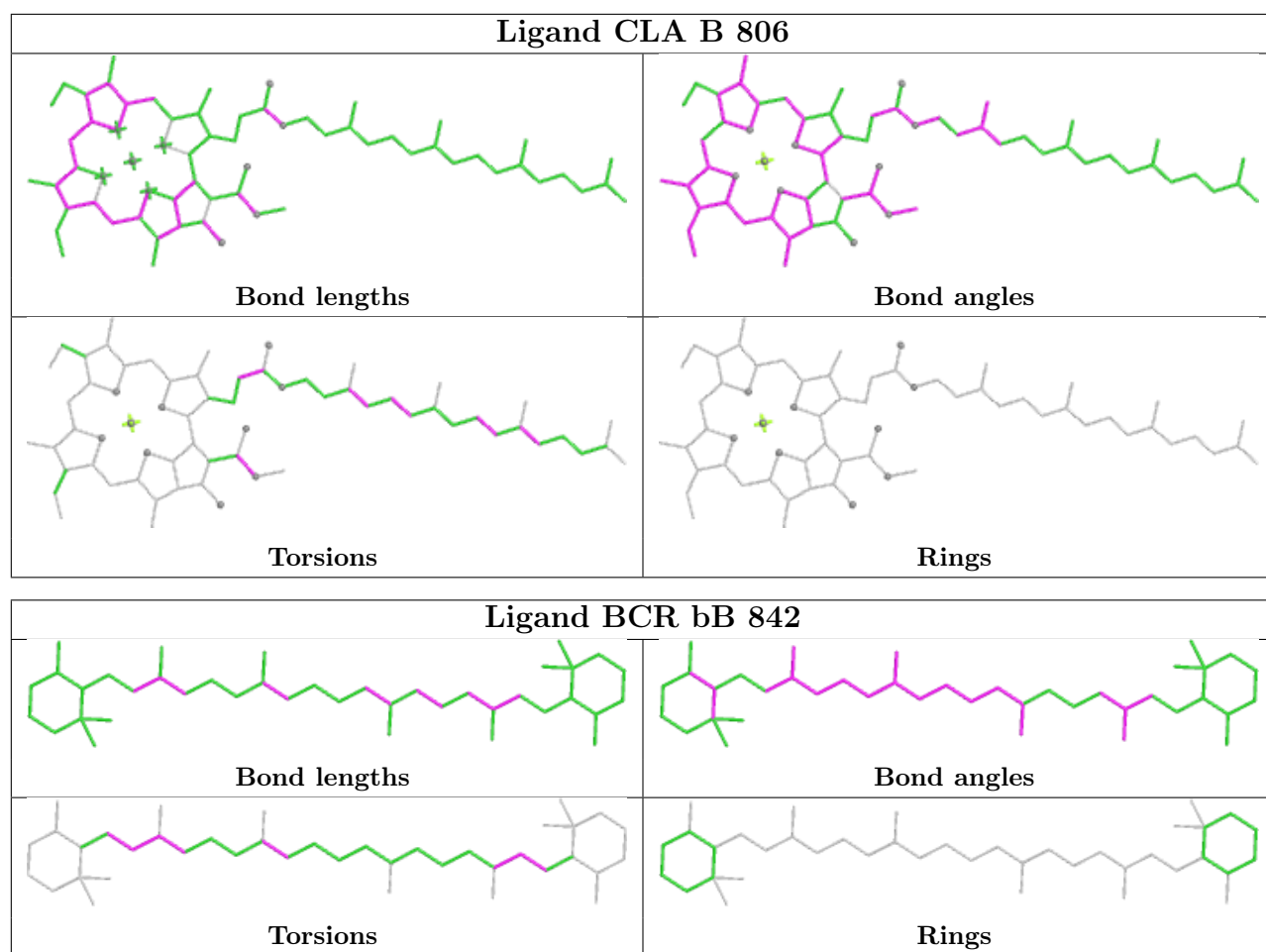
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	818	CLA	1	0
14	A	806	CLA	2	0
14	A	832	CLA	2	0
14	bB	833	CLA	1	0
14	cA	838	CLA	3	0
14	A	828	CLA	1	0
14	A	852	CLA	4	0
14	bA	804	CLA	1	0
17	A	847	BCR	1	0
14	bA	824	CLA	1	0
14	L	204	CLA	8	0
17	bB	850	BCR	2	0
14	bA	826	CLA	2	0
14	cA	820	CLA	2	0
14	cA	822	CLA	1	0
14	bB	817	CLA	1	0
14	A	804	CLA	1	0
14	bA	808	CLA	1	0
14	cA	823	CLA	1	0
14	cA	811	CLA	1	0
14	A	836	CLA	1	0
14	B	822	CLA	2	0
17	cL	206	BCR	2	0
17	B	847	BCR	1	0
14	cB	820	CLA	2	0
14	B	838	CLA	2	0
14	cA	827	CLA	4	0
14	B	823	CLA	1	0
14	B	820	CLA	1	0
14	L	202	CLA	1	0
14	bA	825	CLA	1	0
14	cB	815	CLA	2	0
14	cA	818	CLA	1	0
14	A	808	CLA	1	0

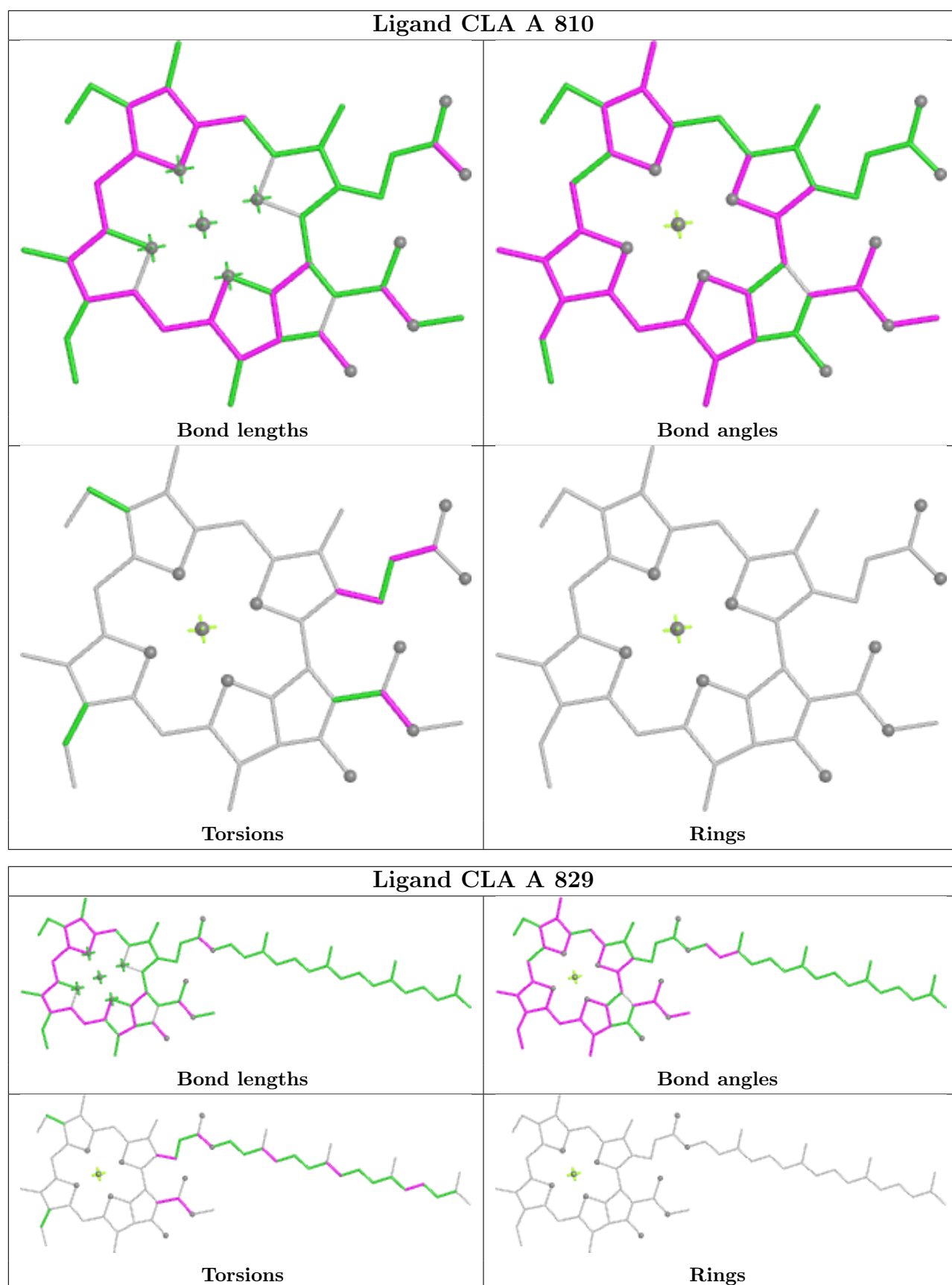
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

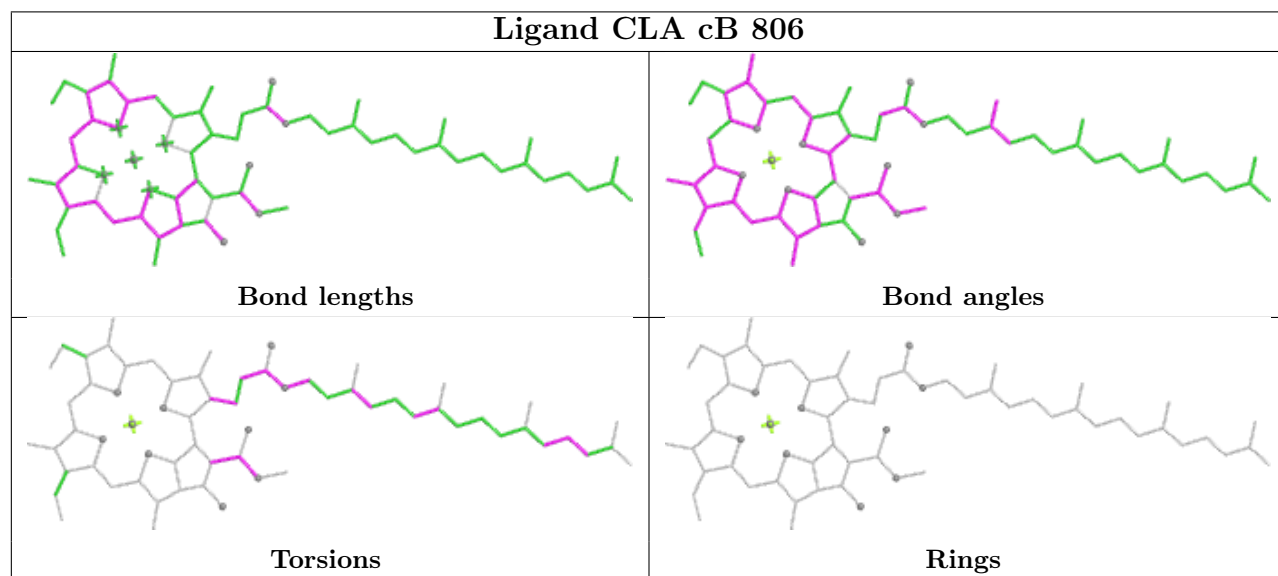
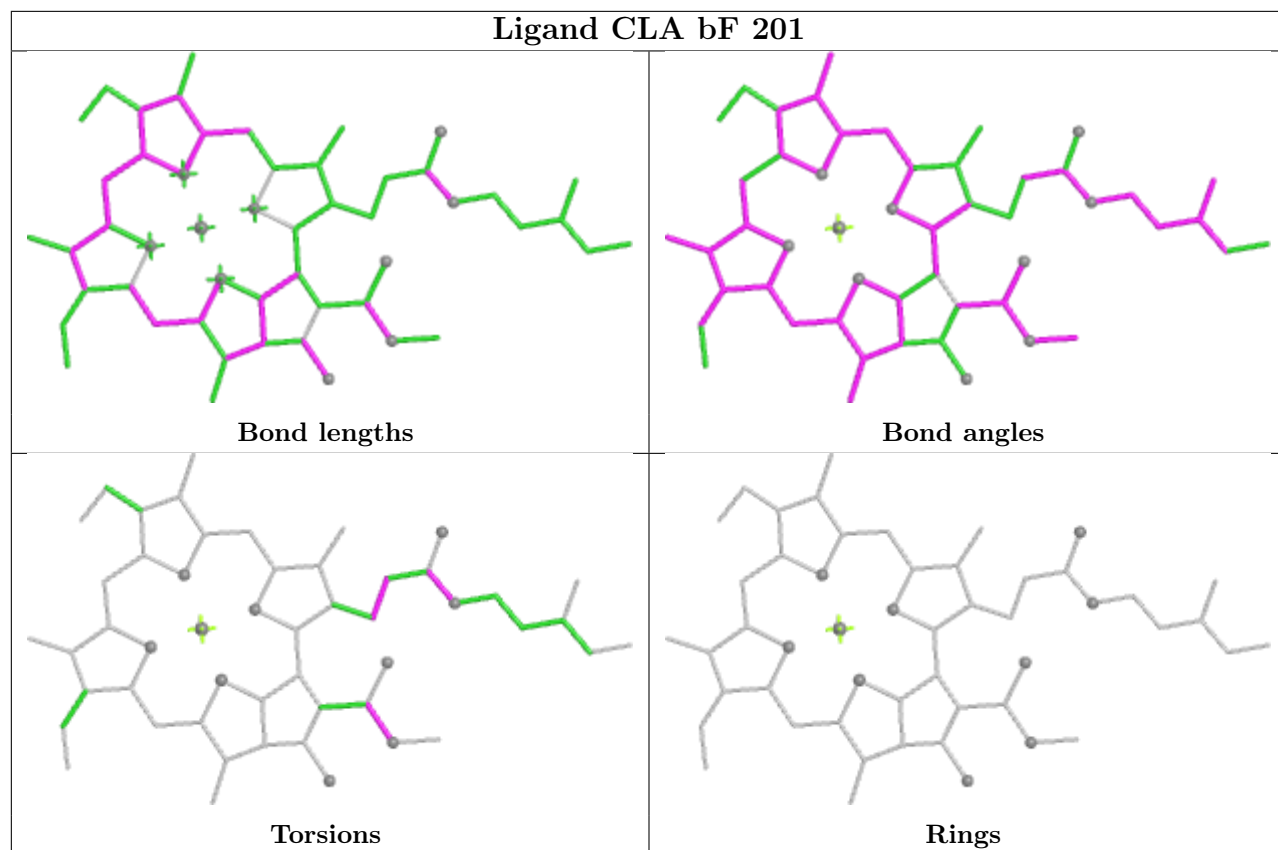
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

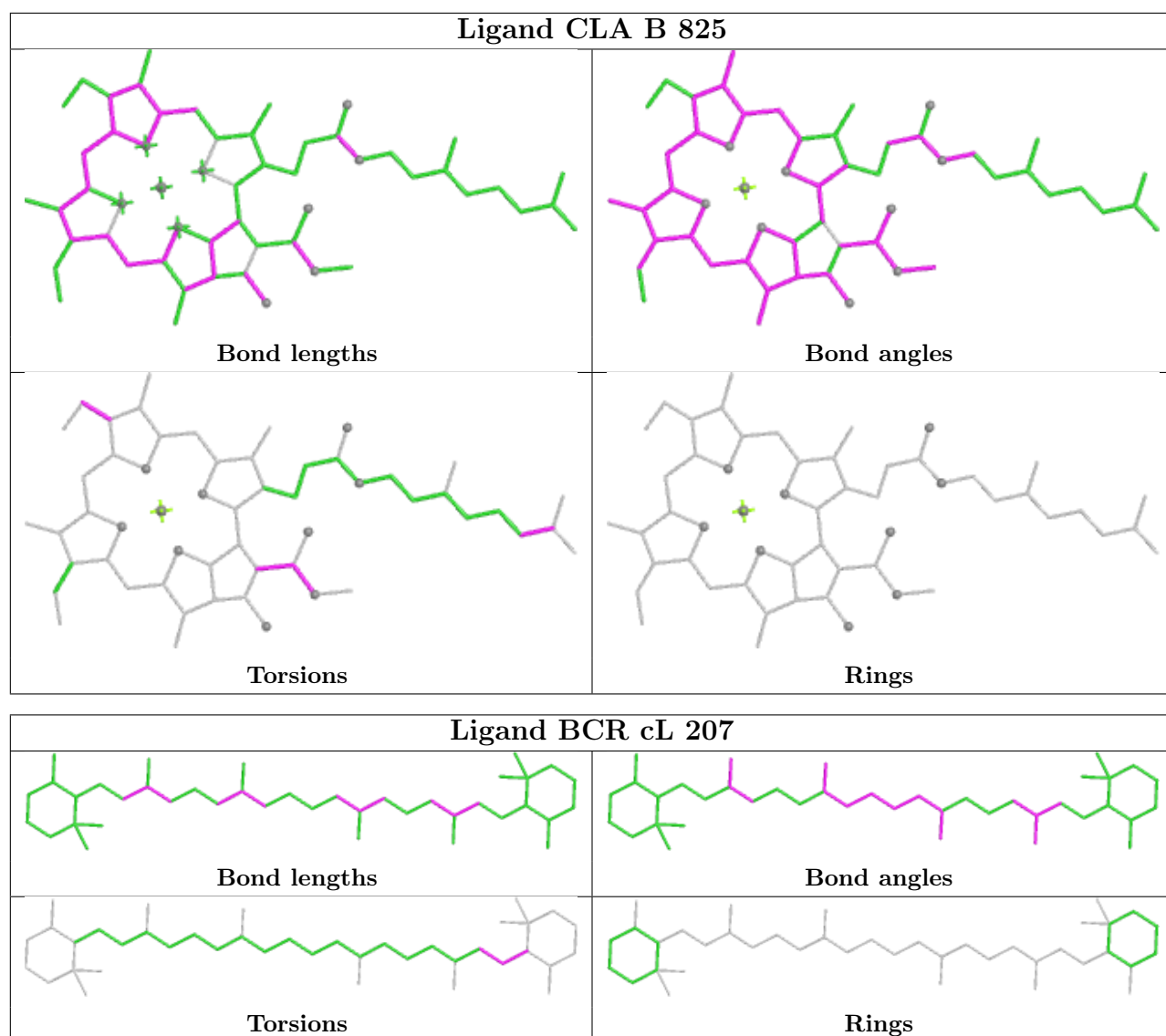


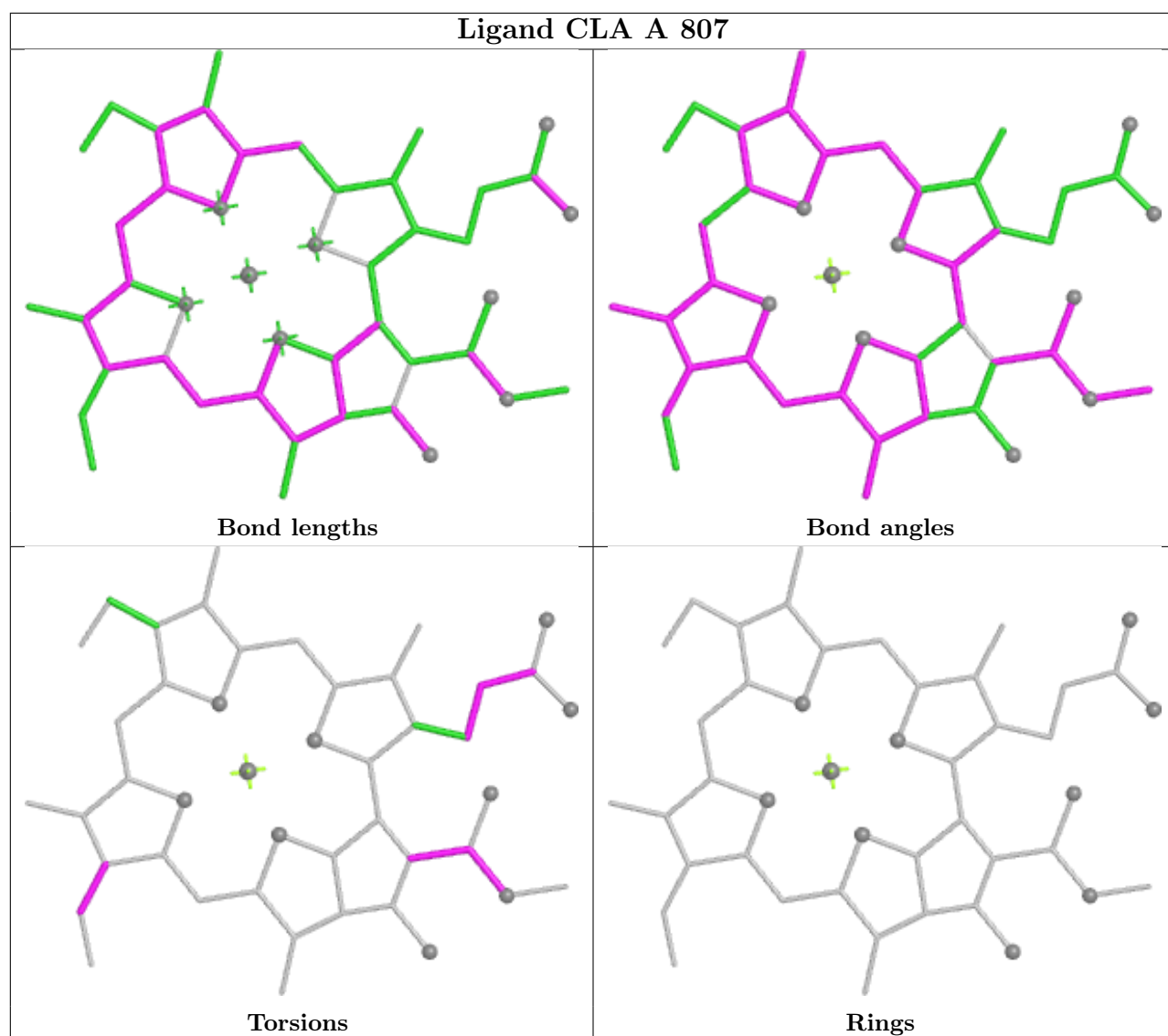


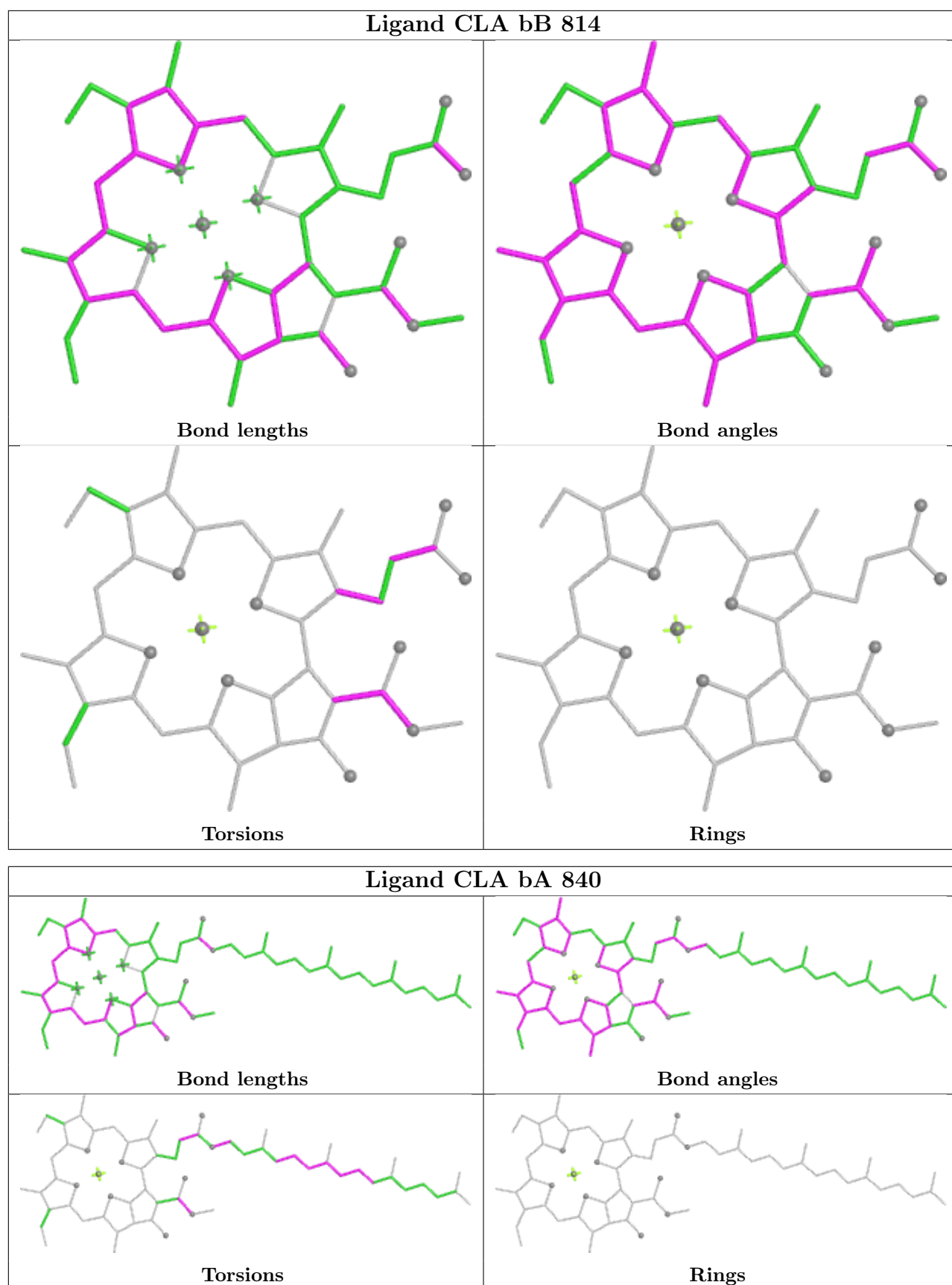




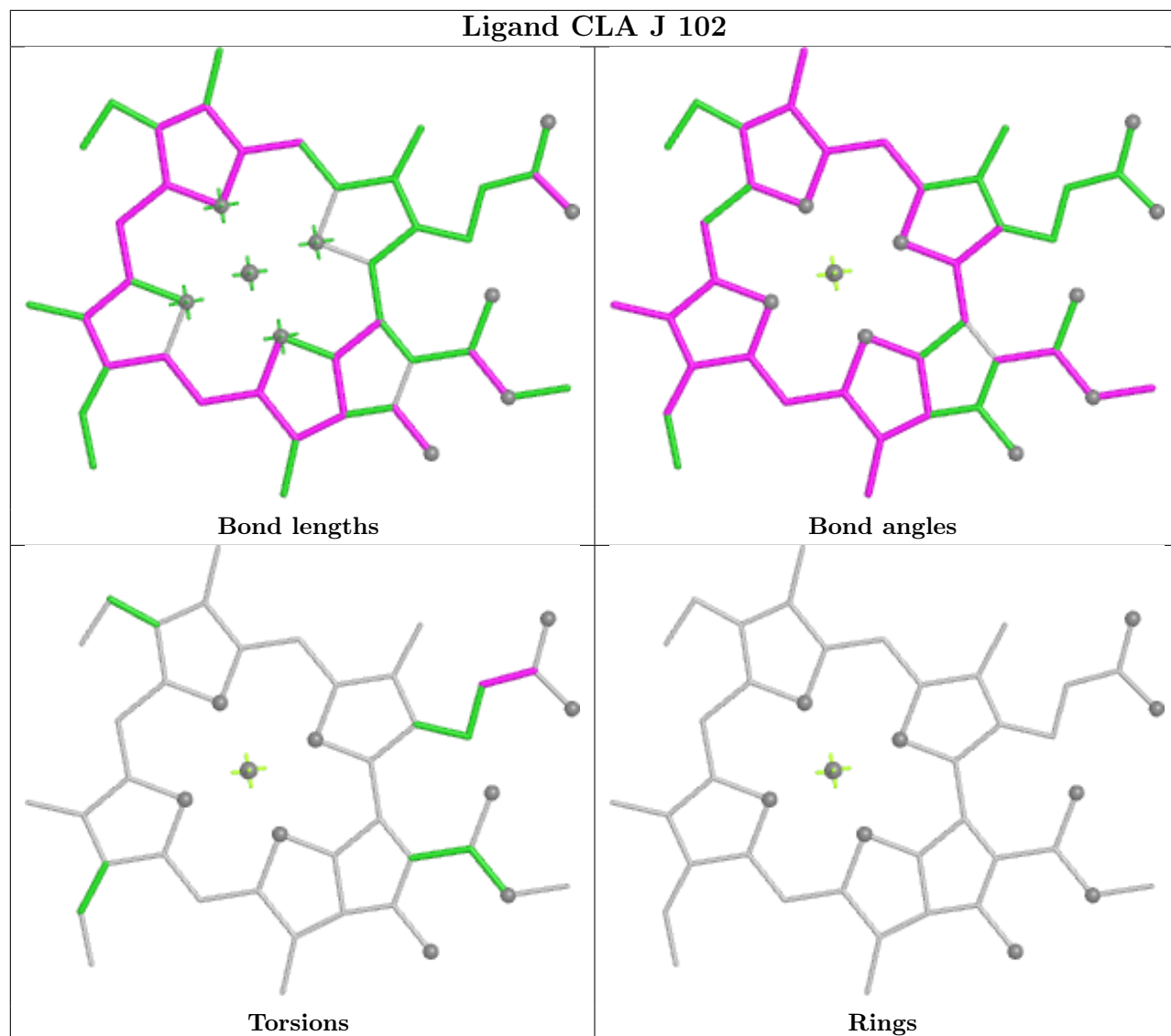




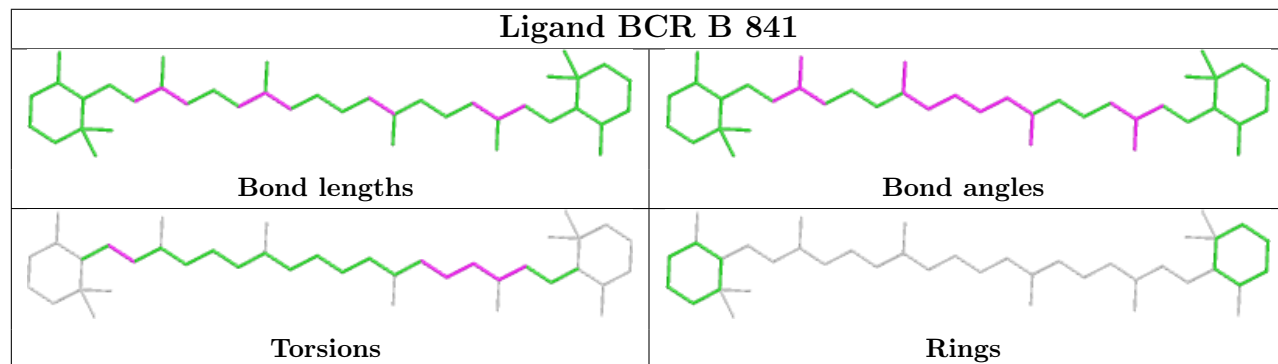


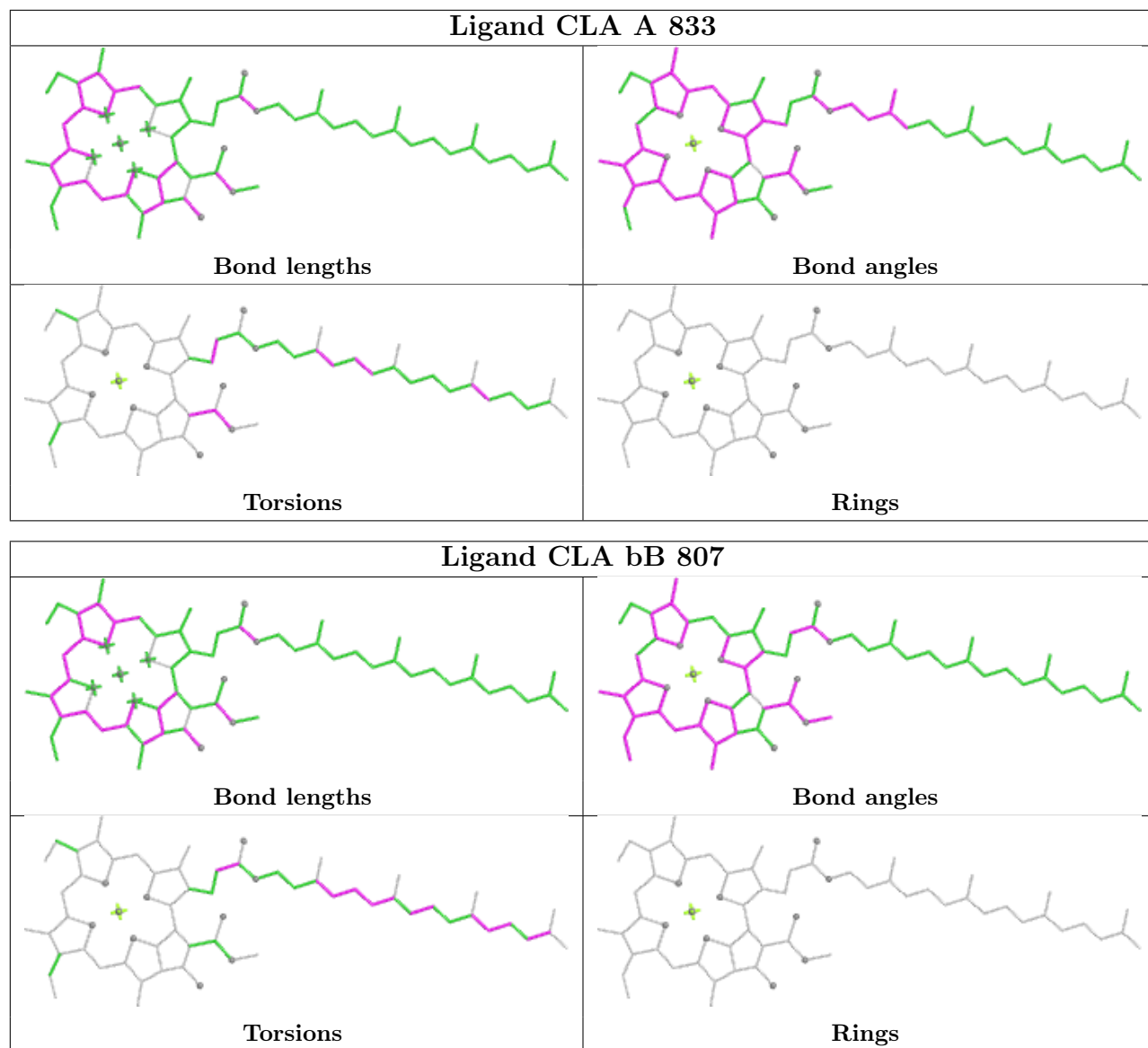


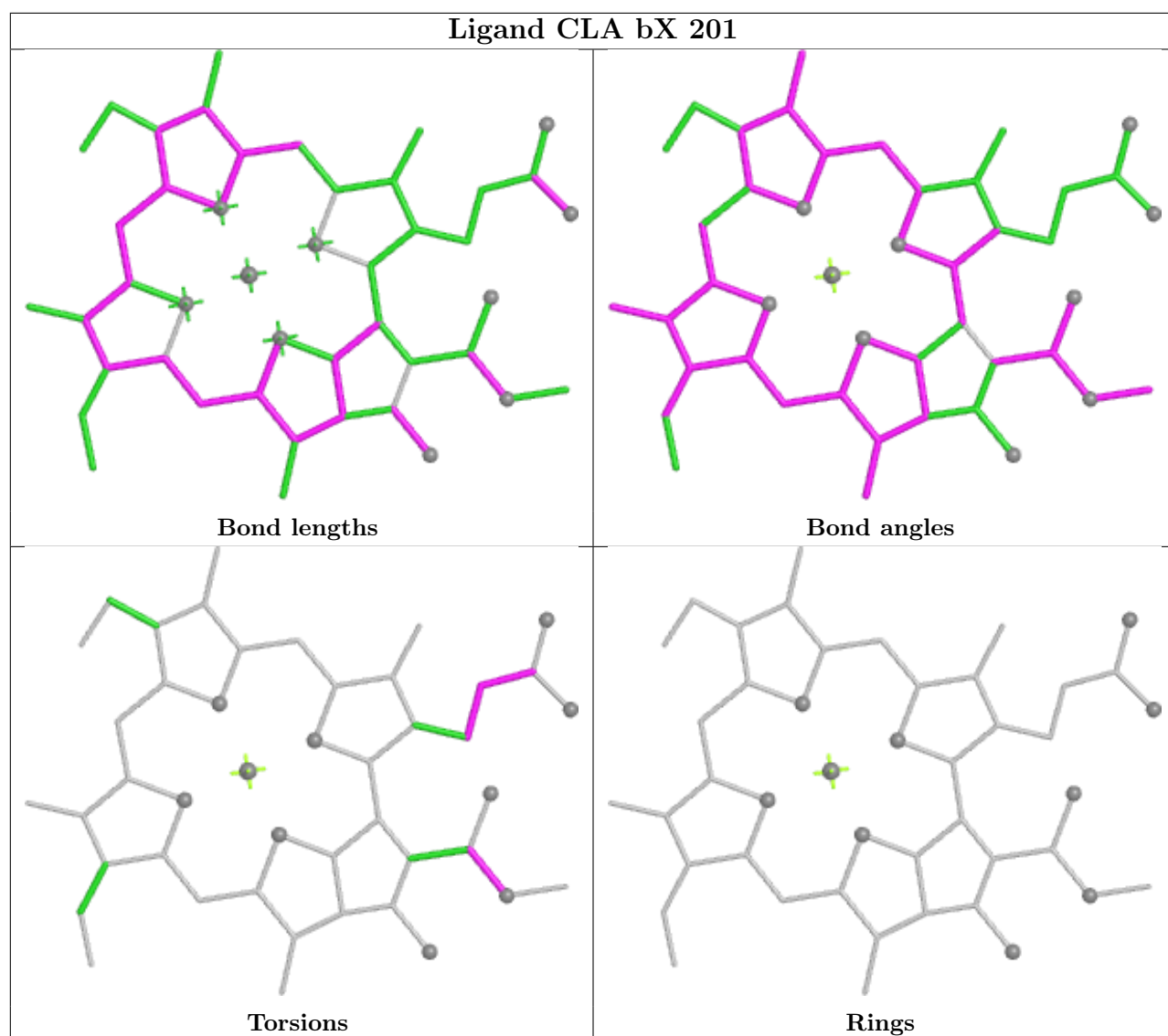
Ligand CLA J 102

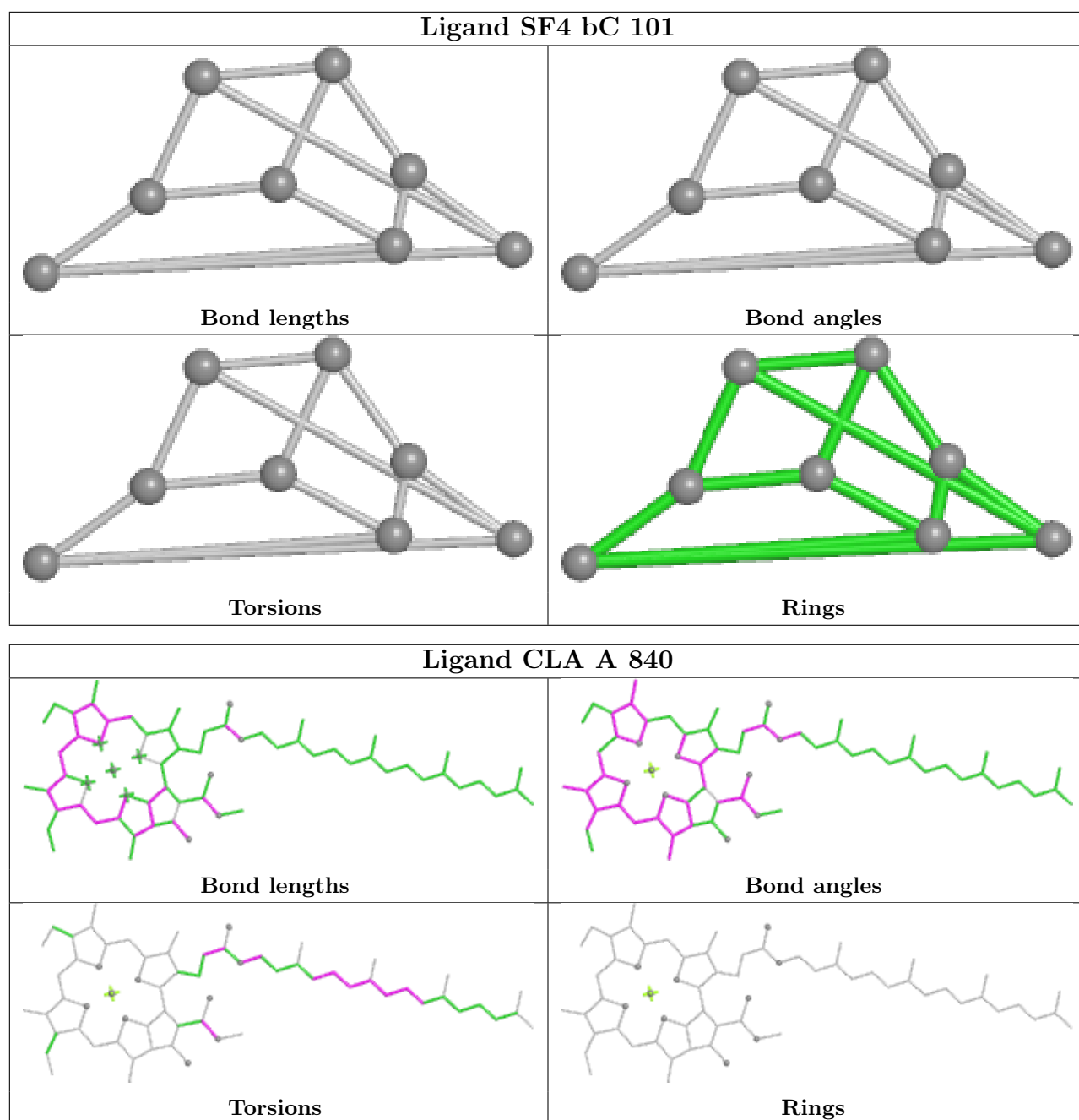


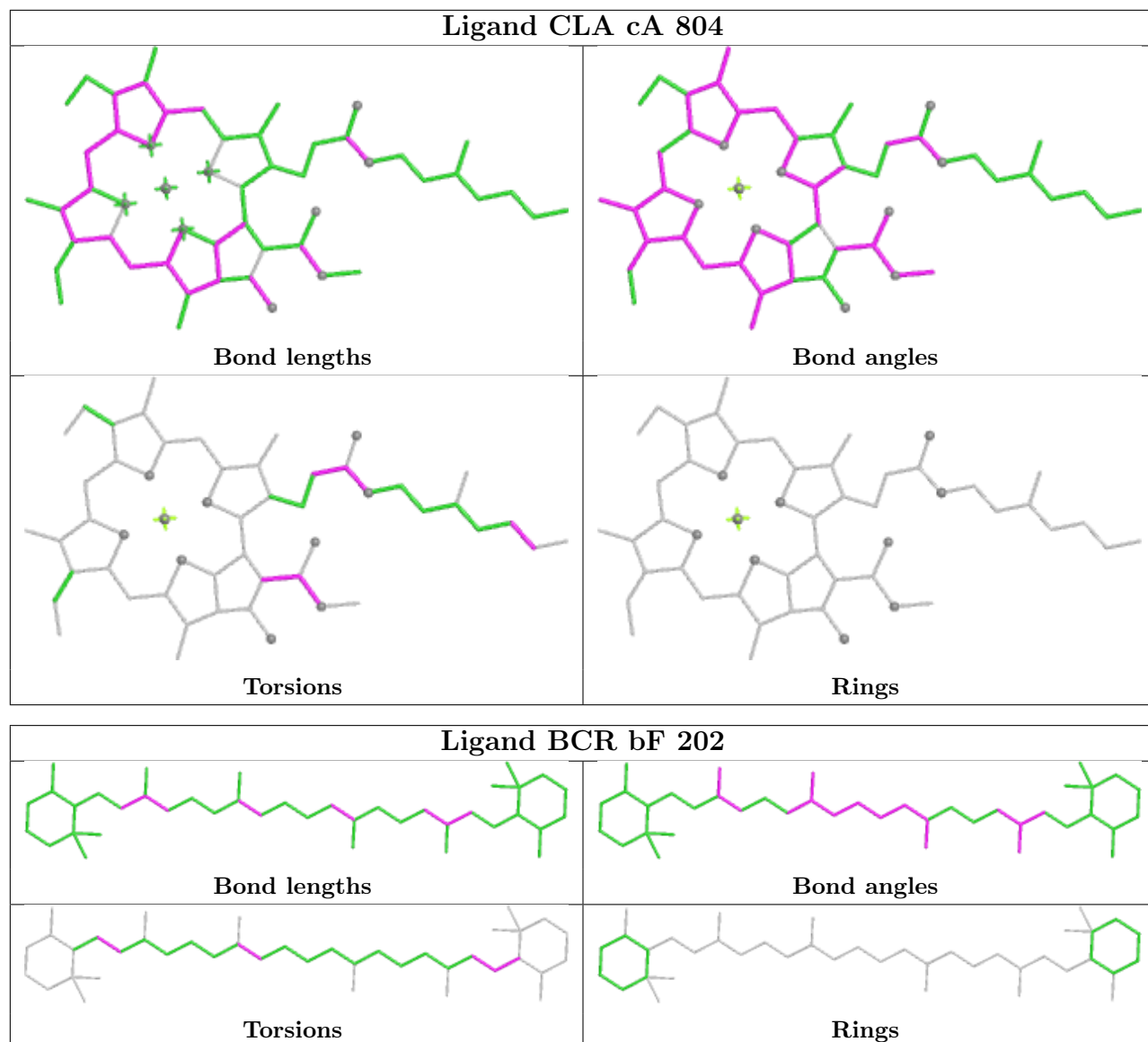
Ligand BCR B 841

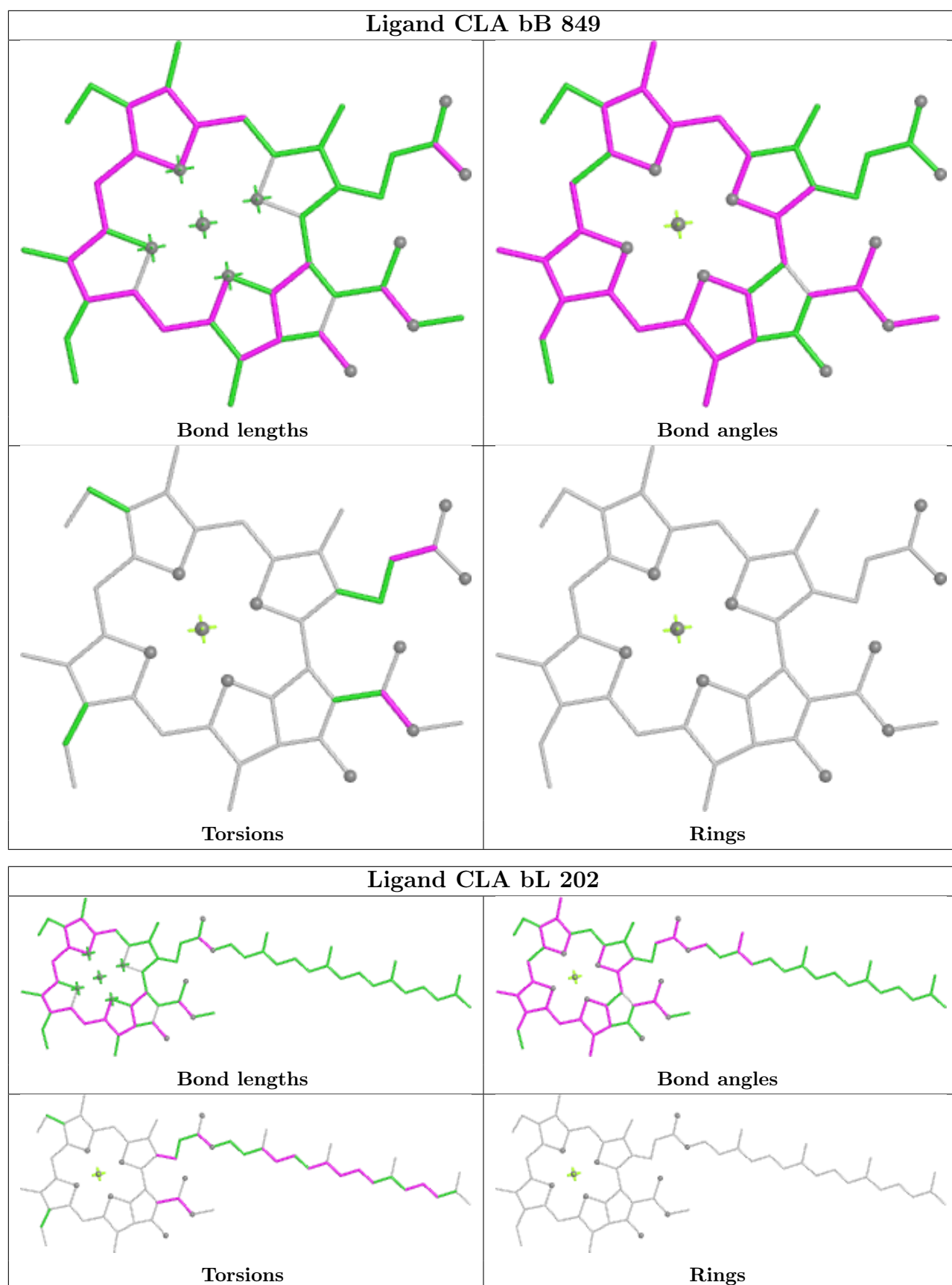


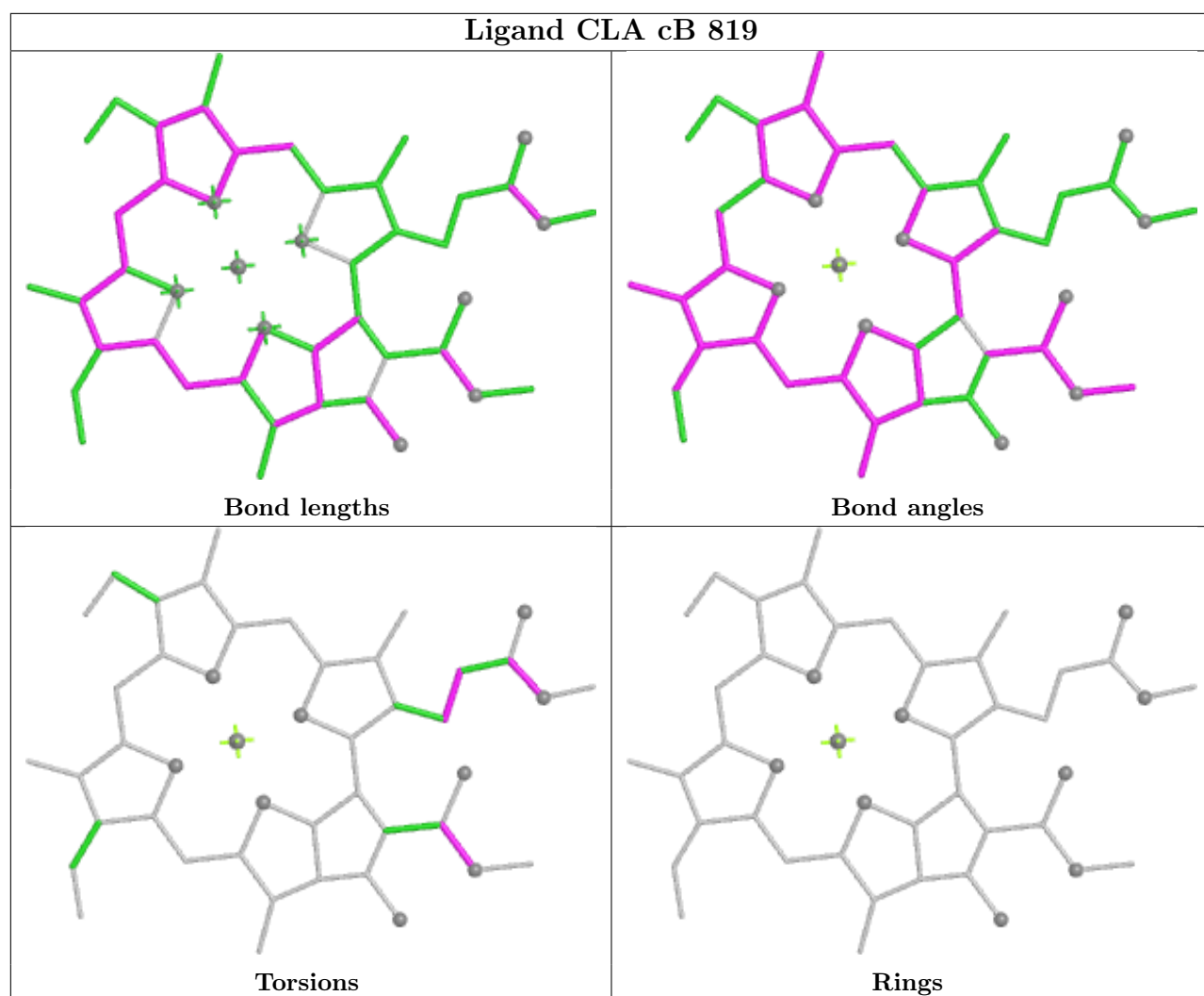


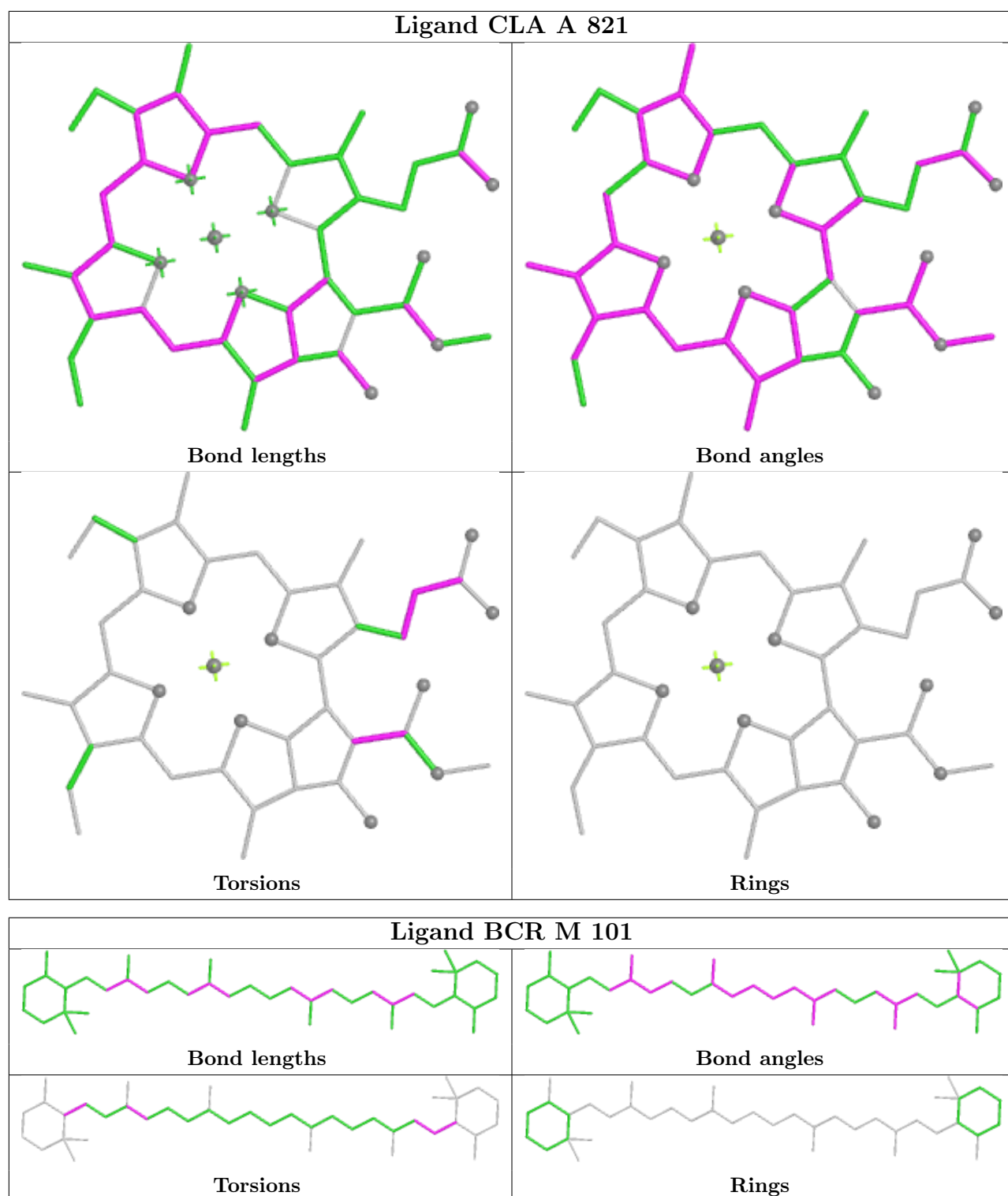


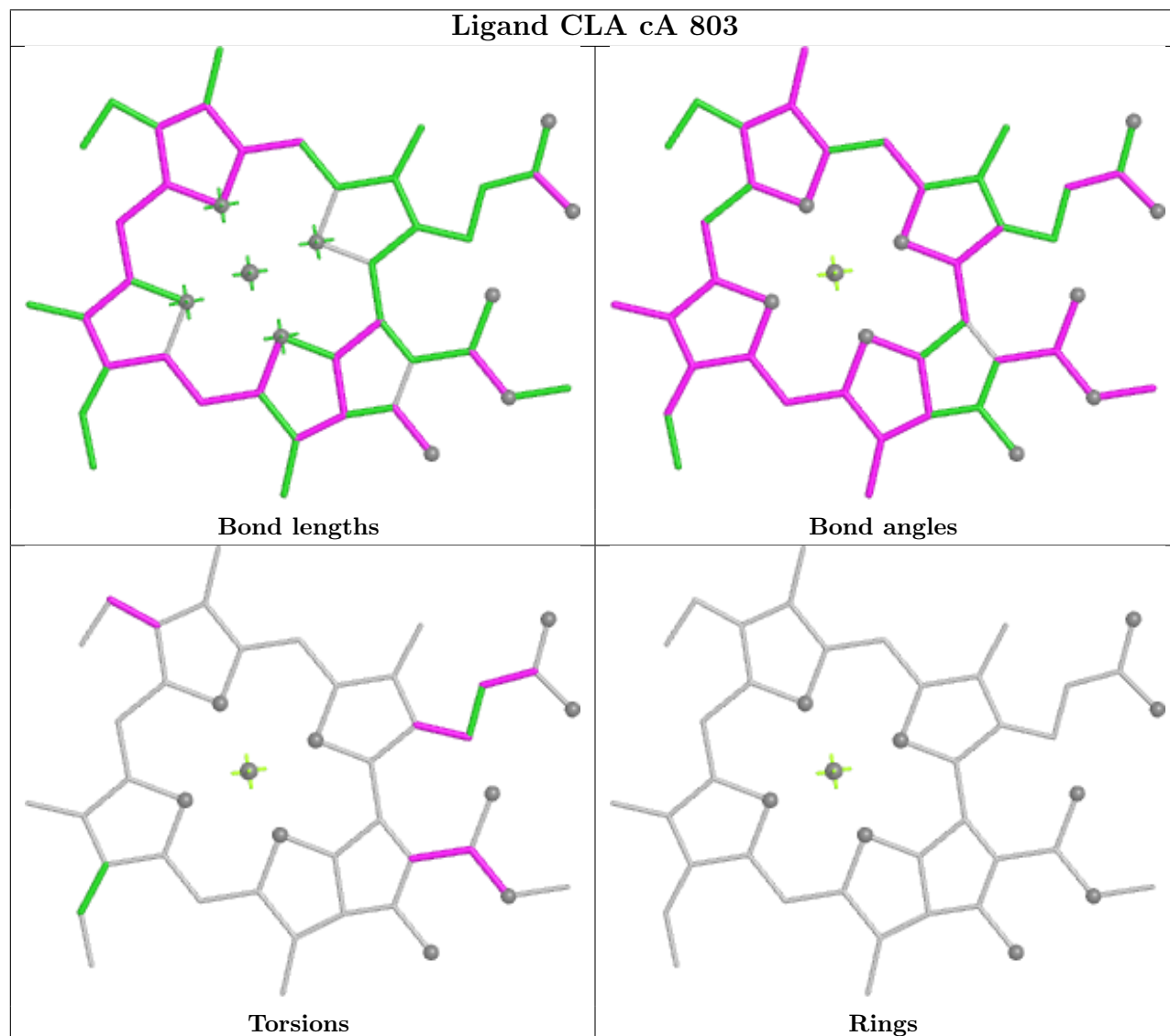
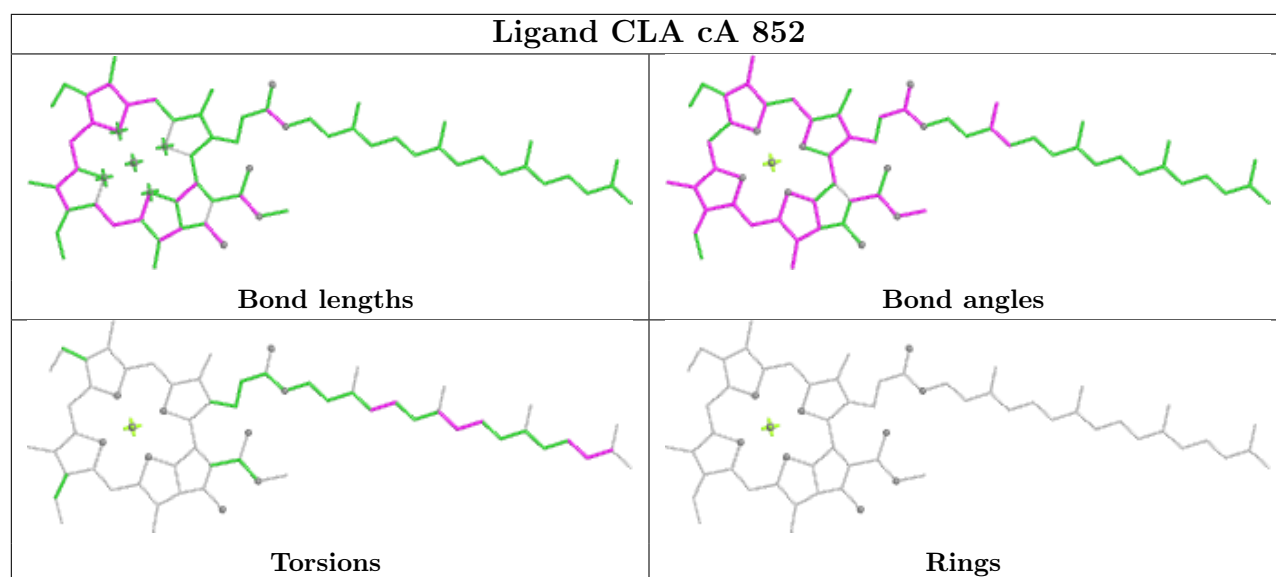




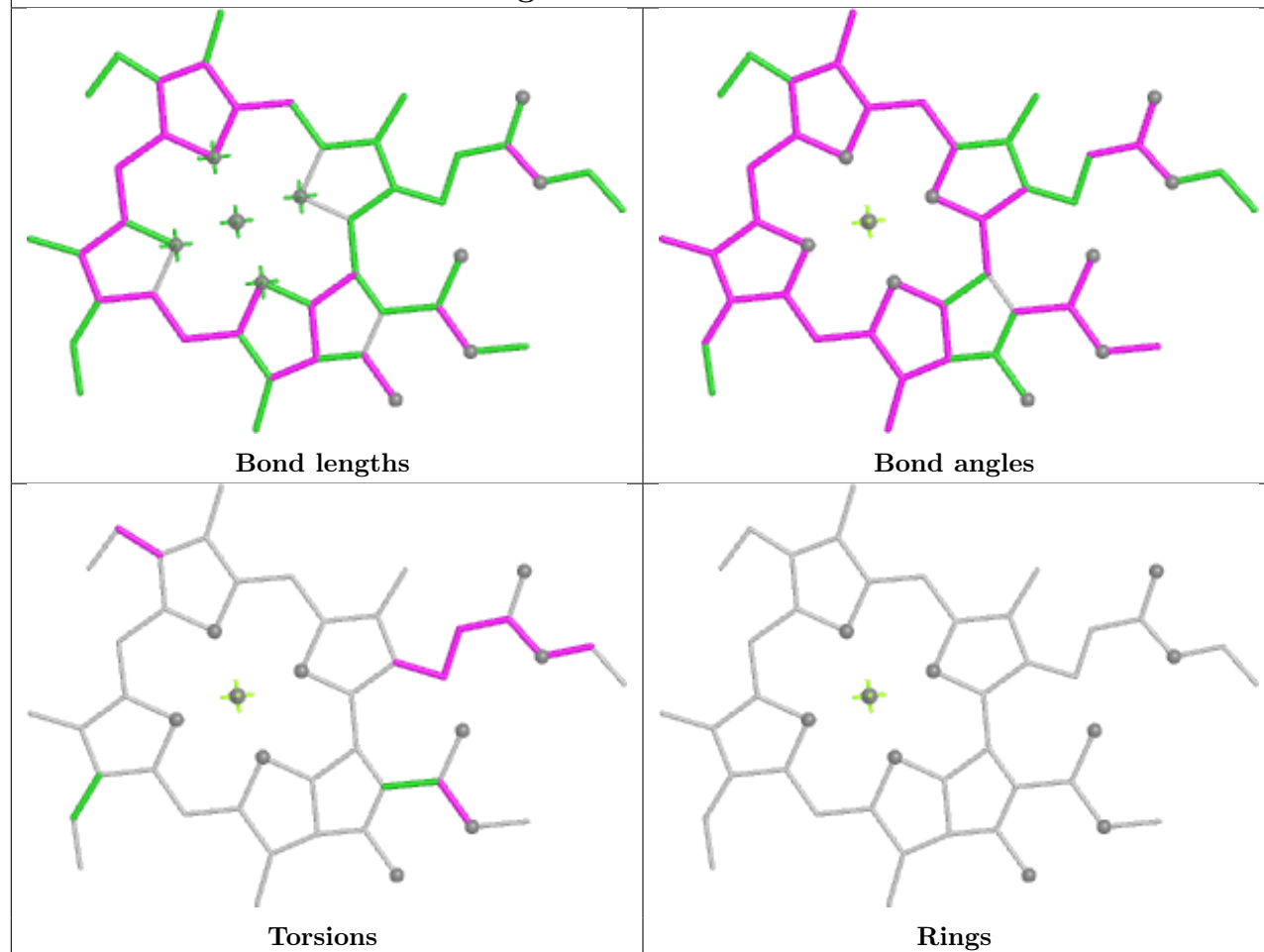




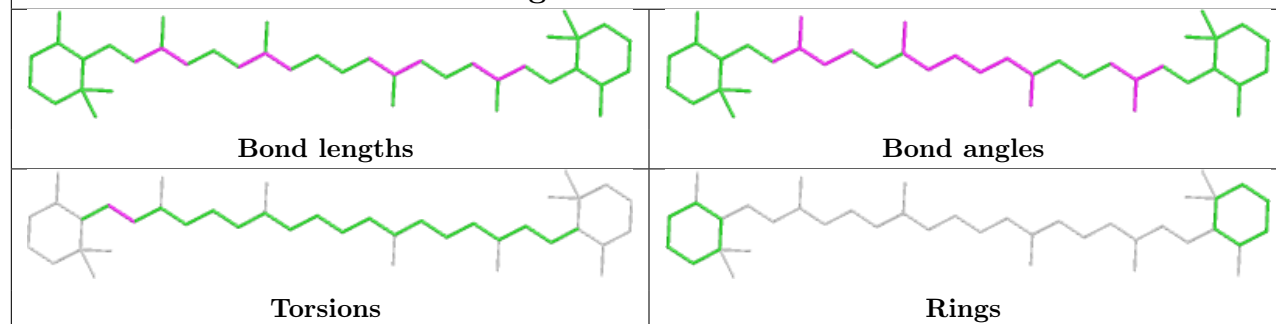




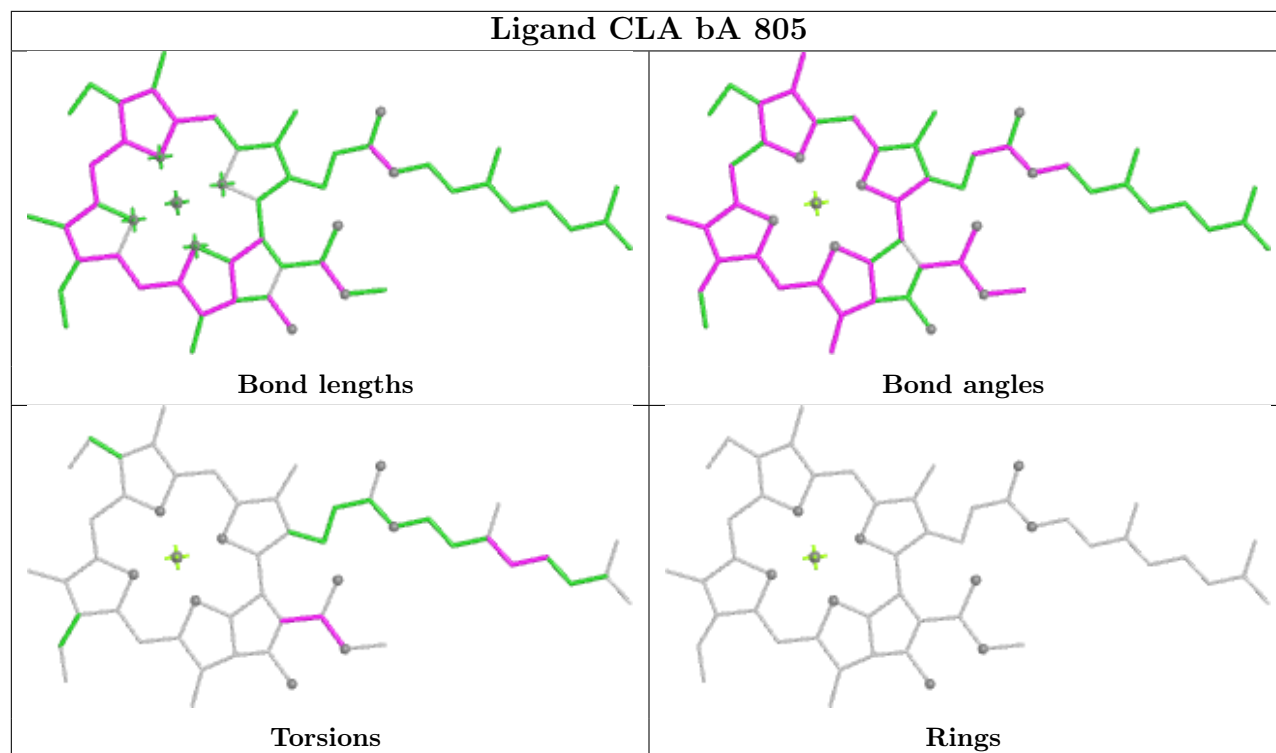
Ligand CLA bB 819



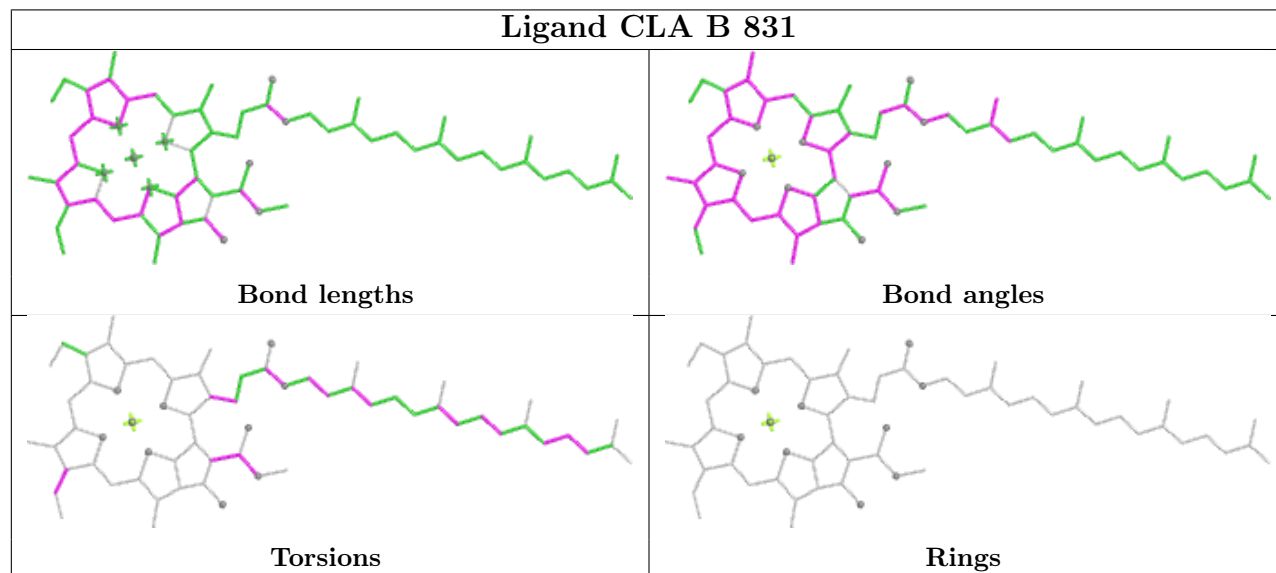
Ligand BCR cI 101

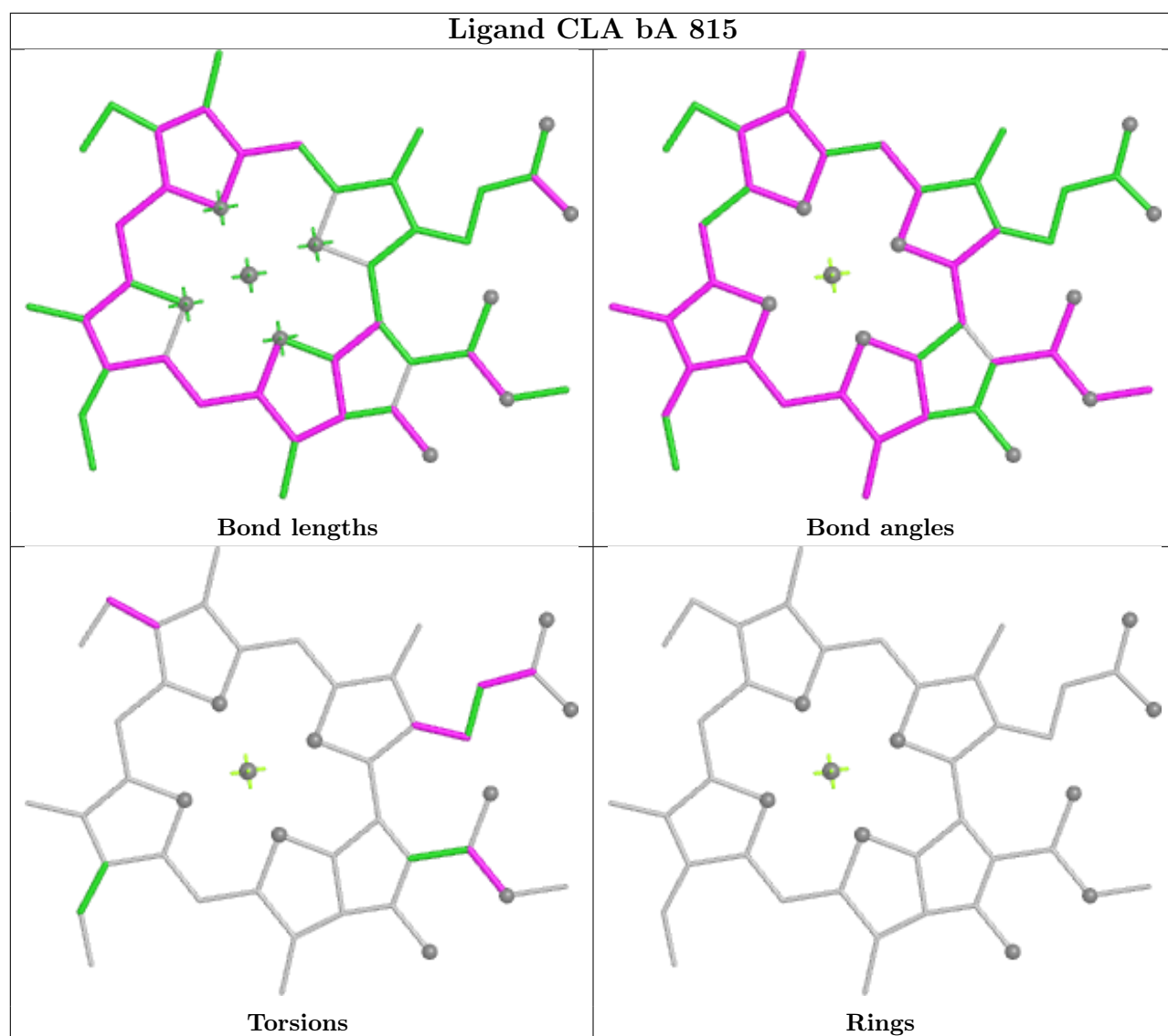


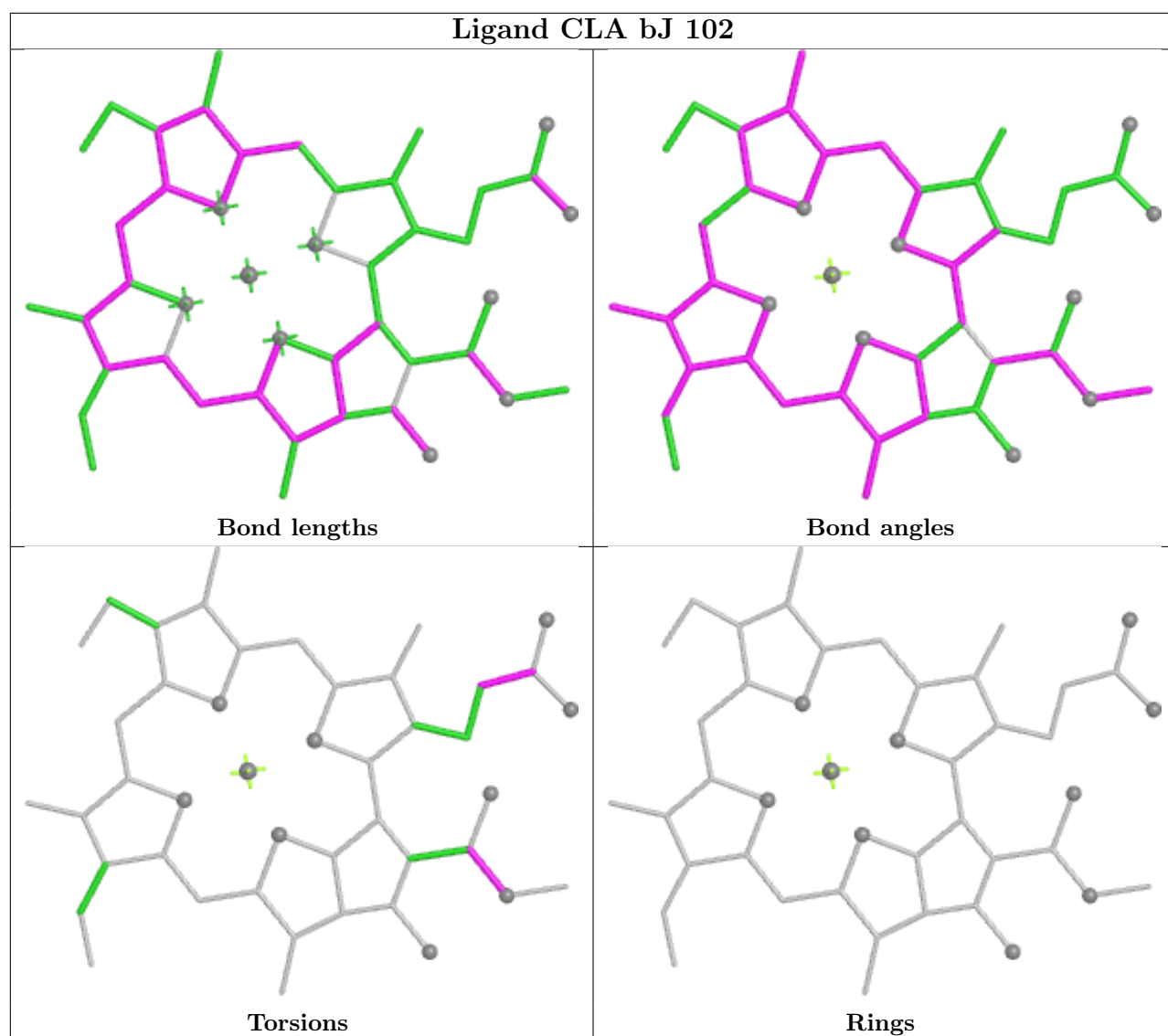
Ligand CLA bA 805

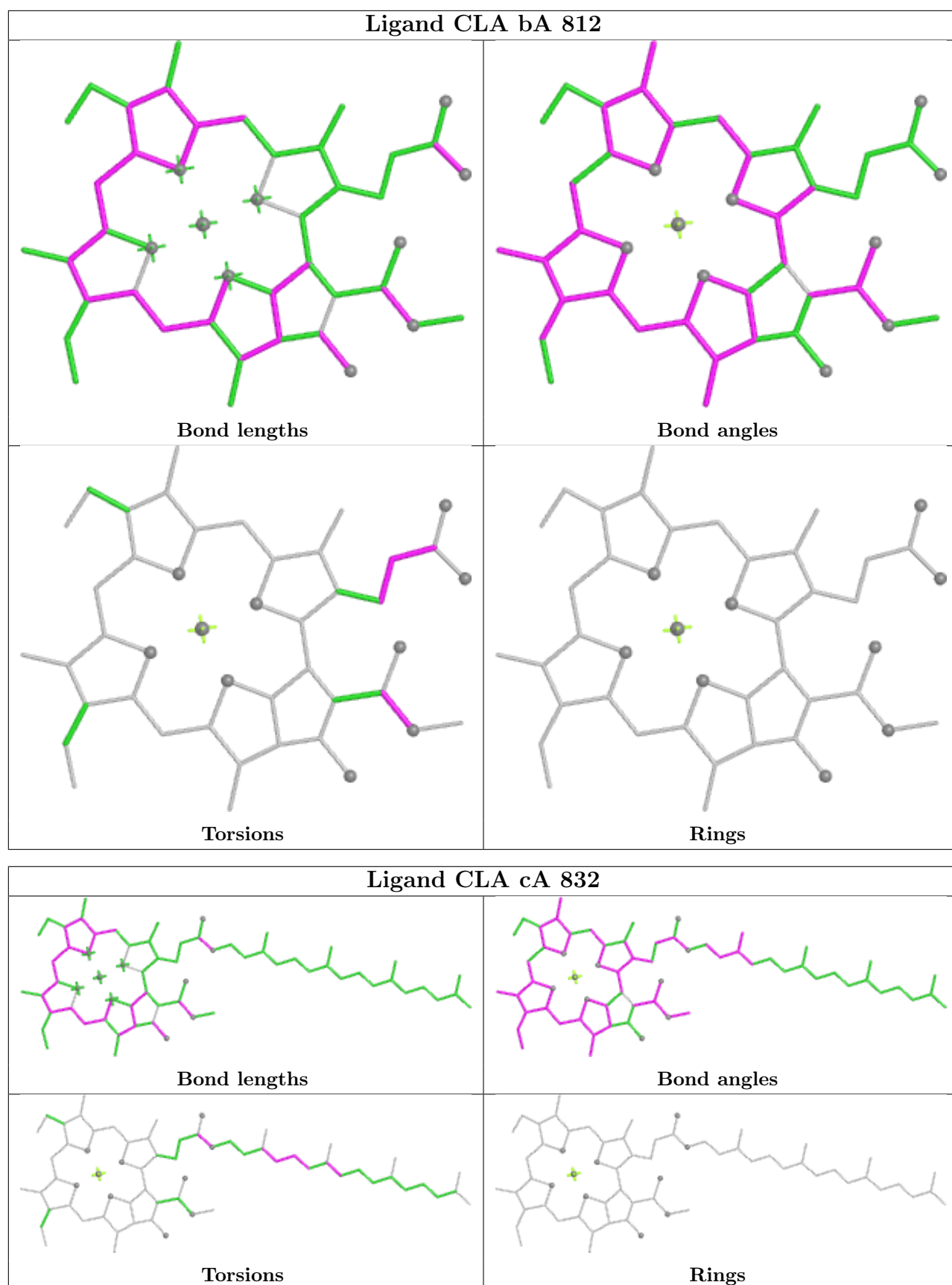


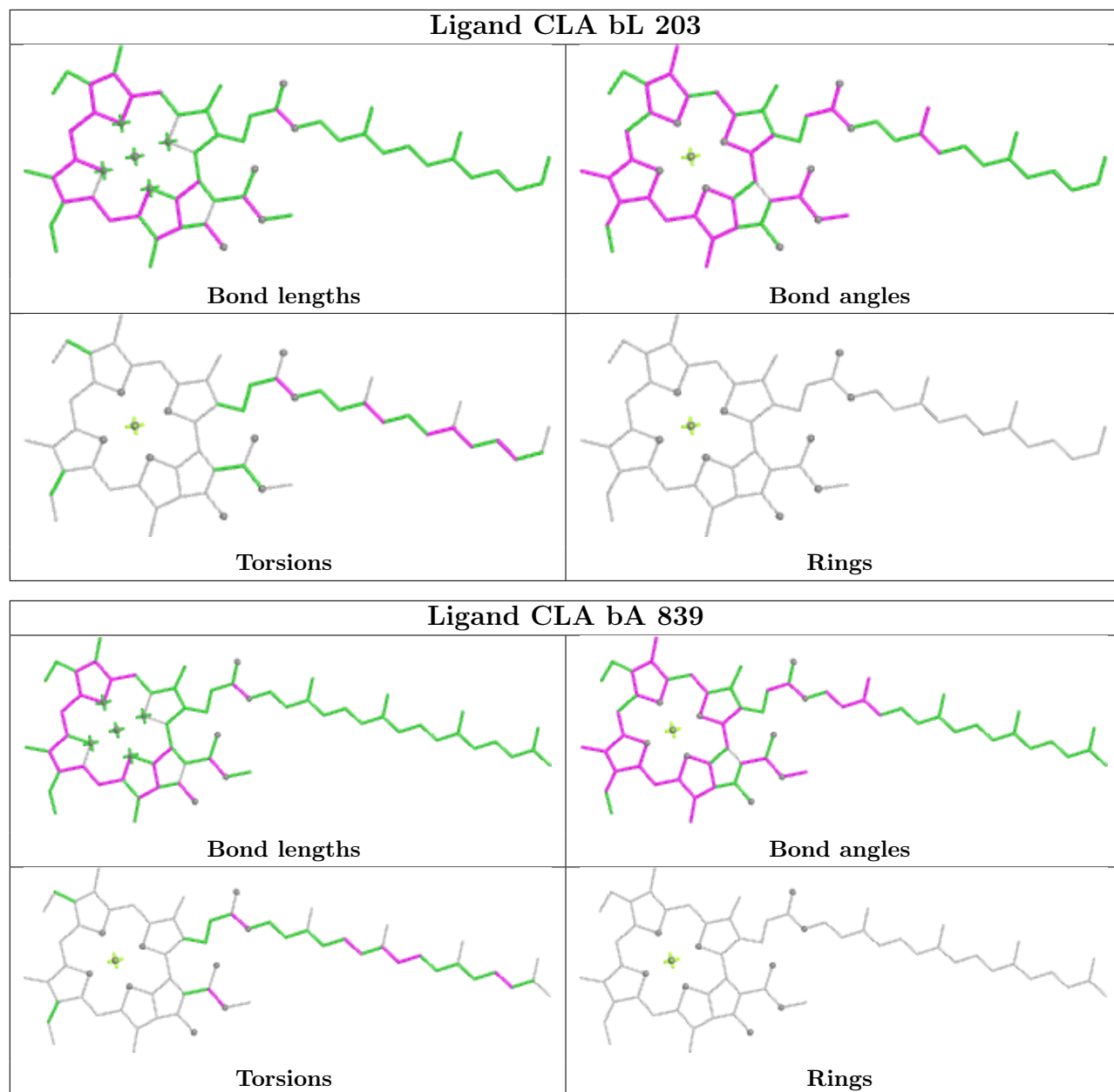
Ligand CLA B 831

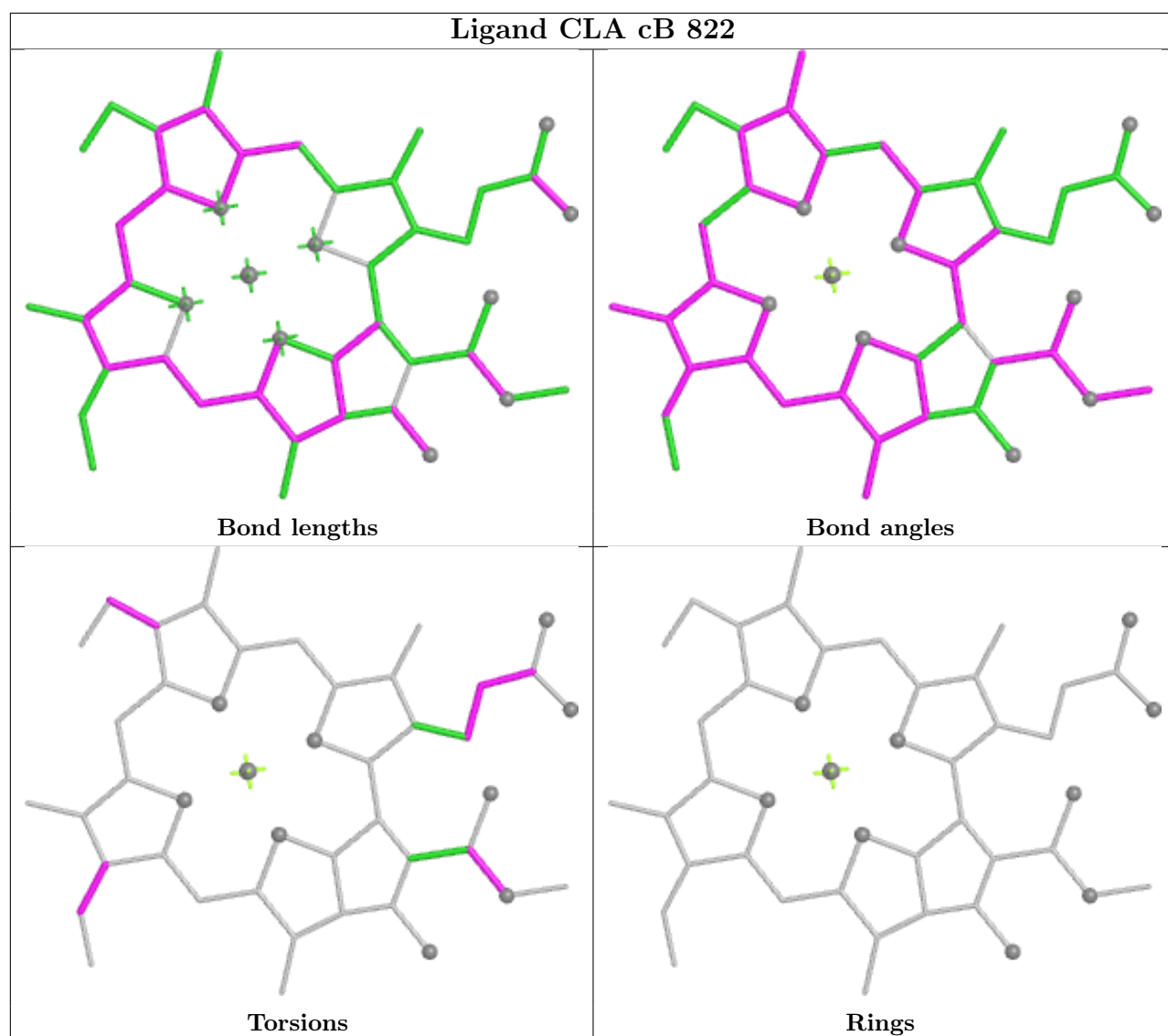


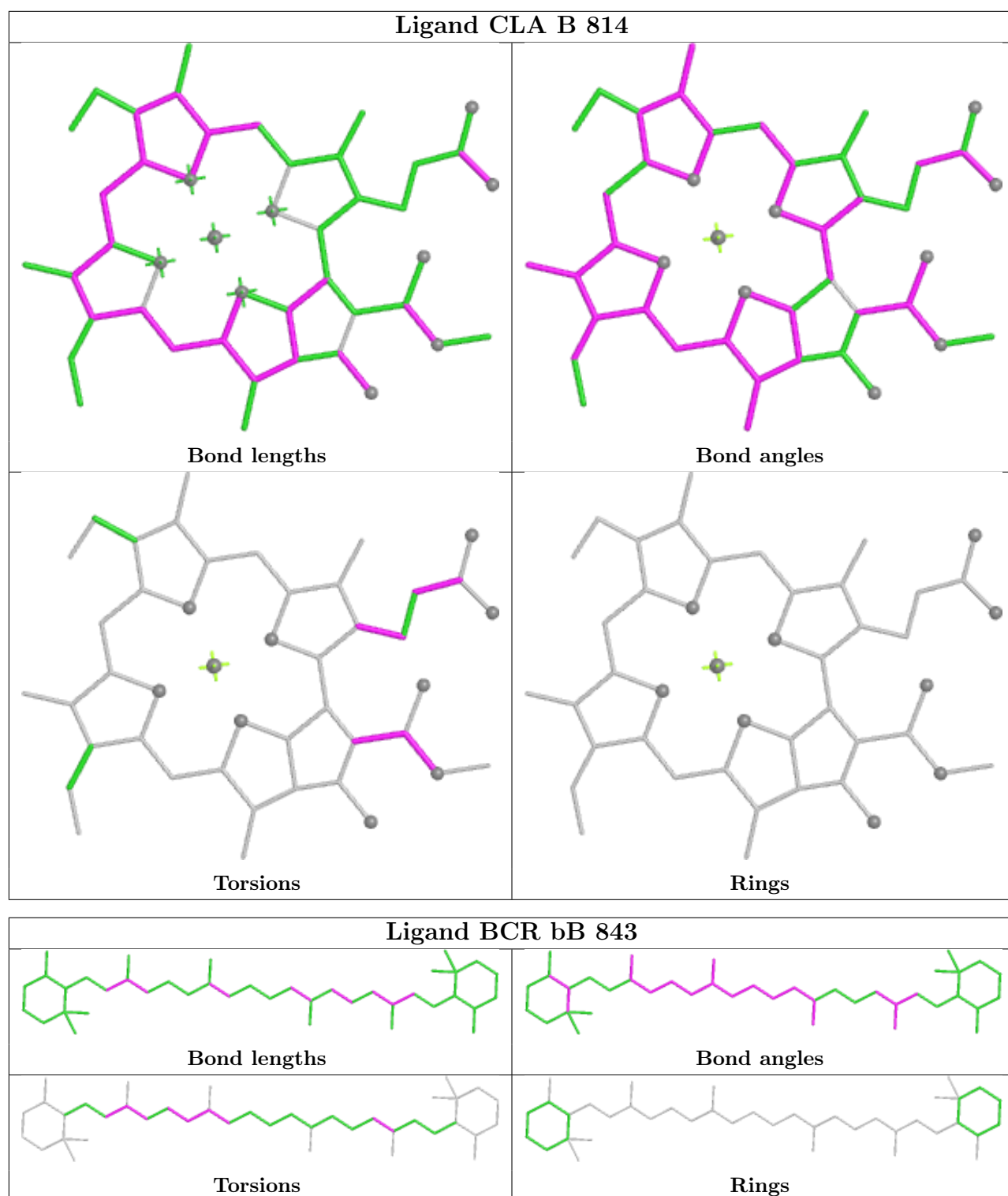


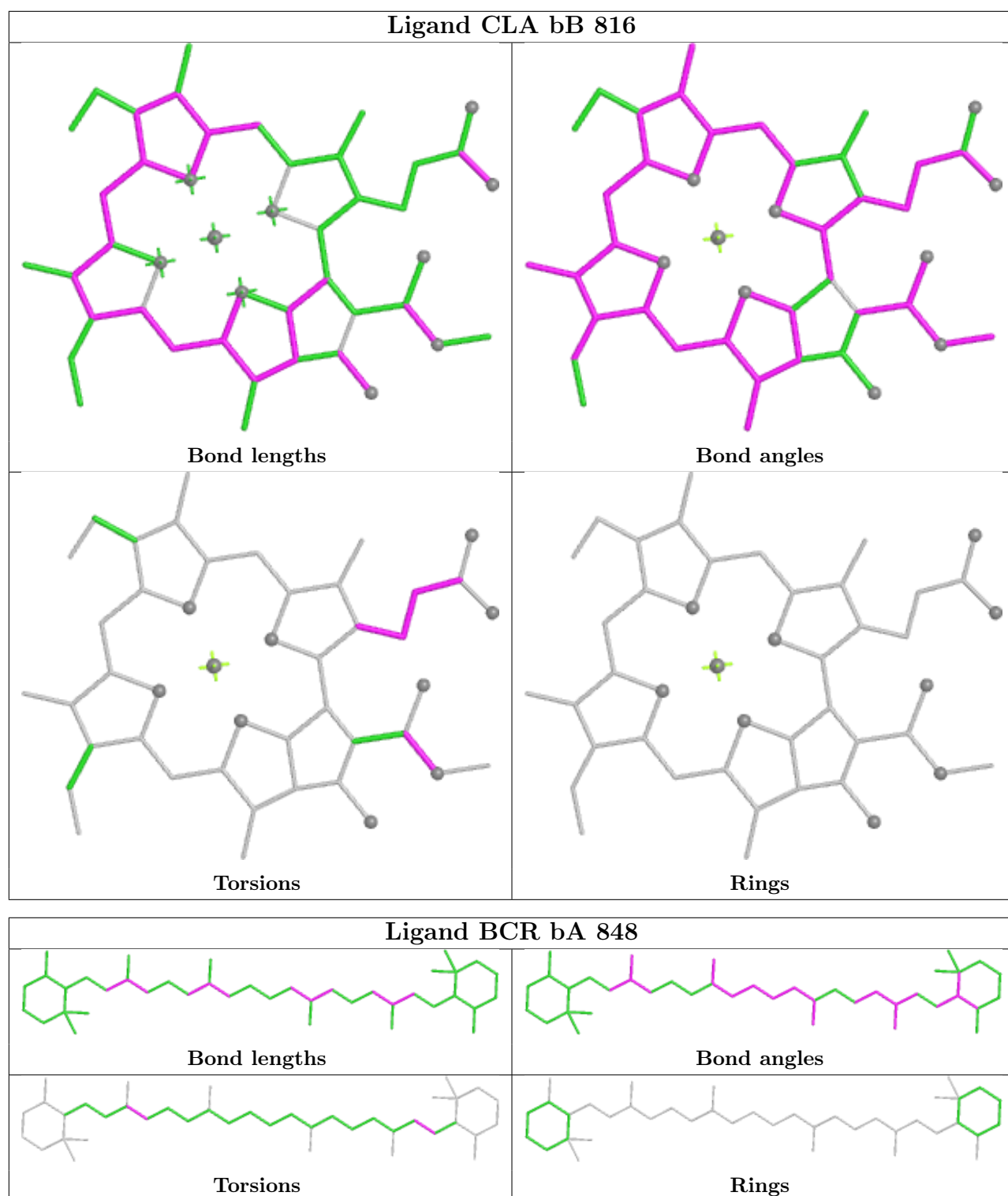


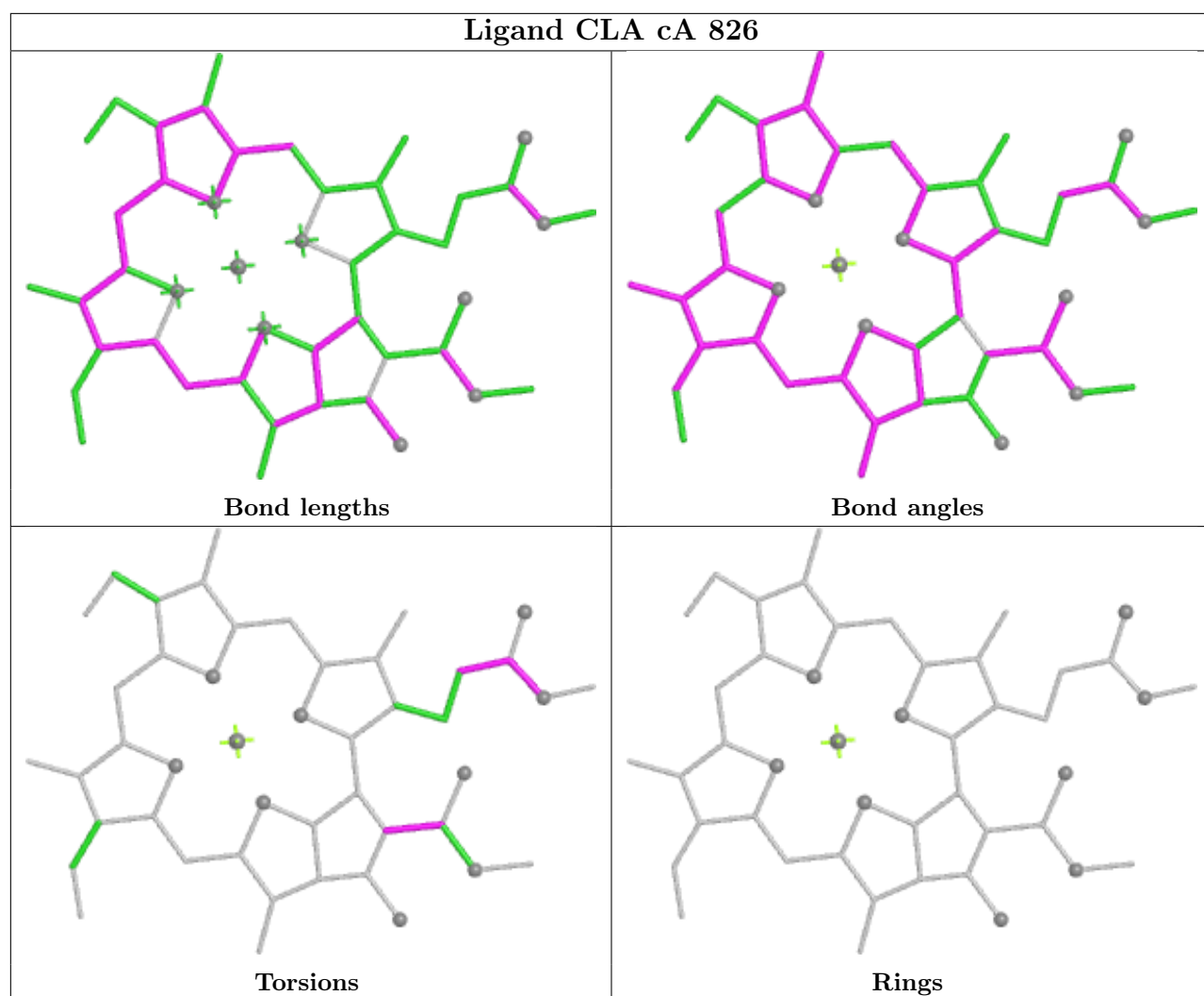




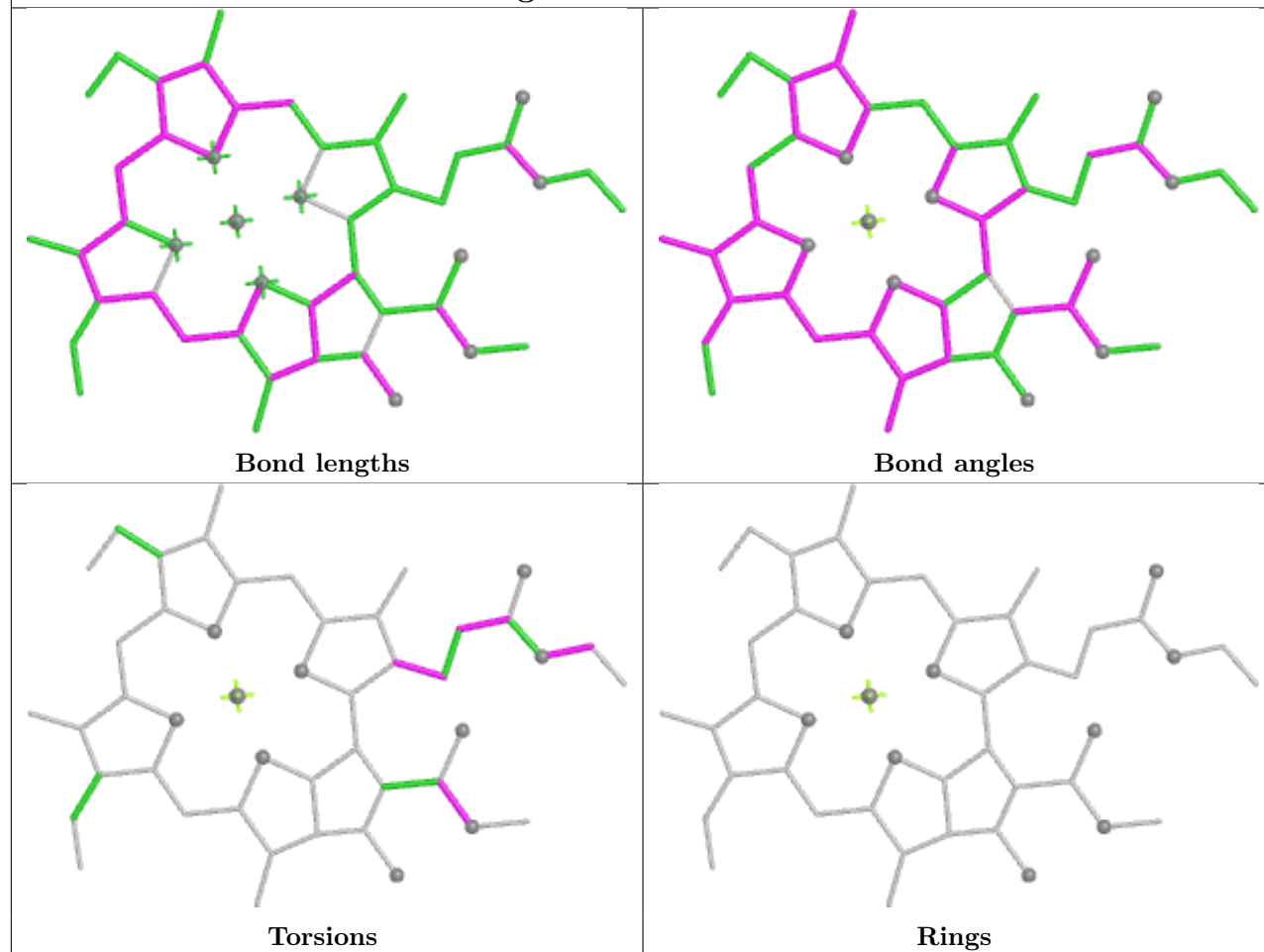




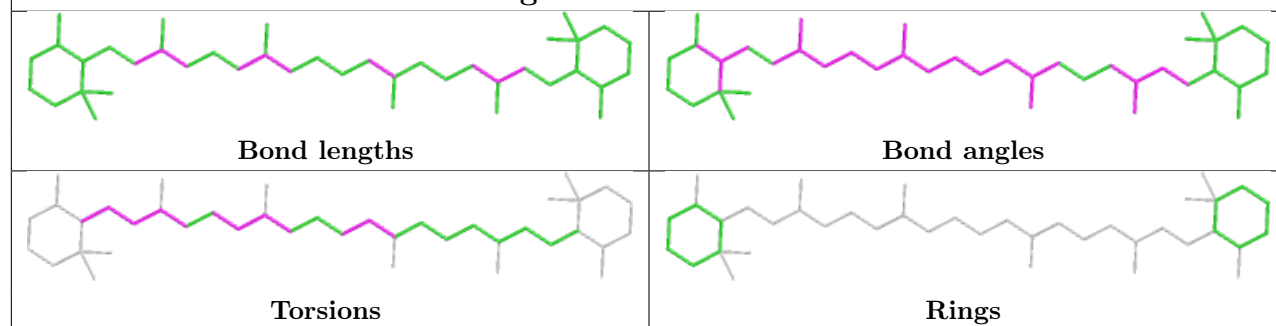


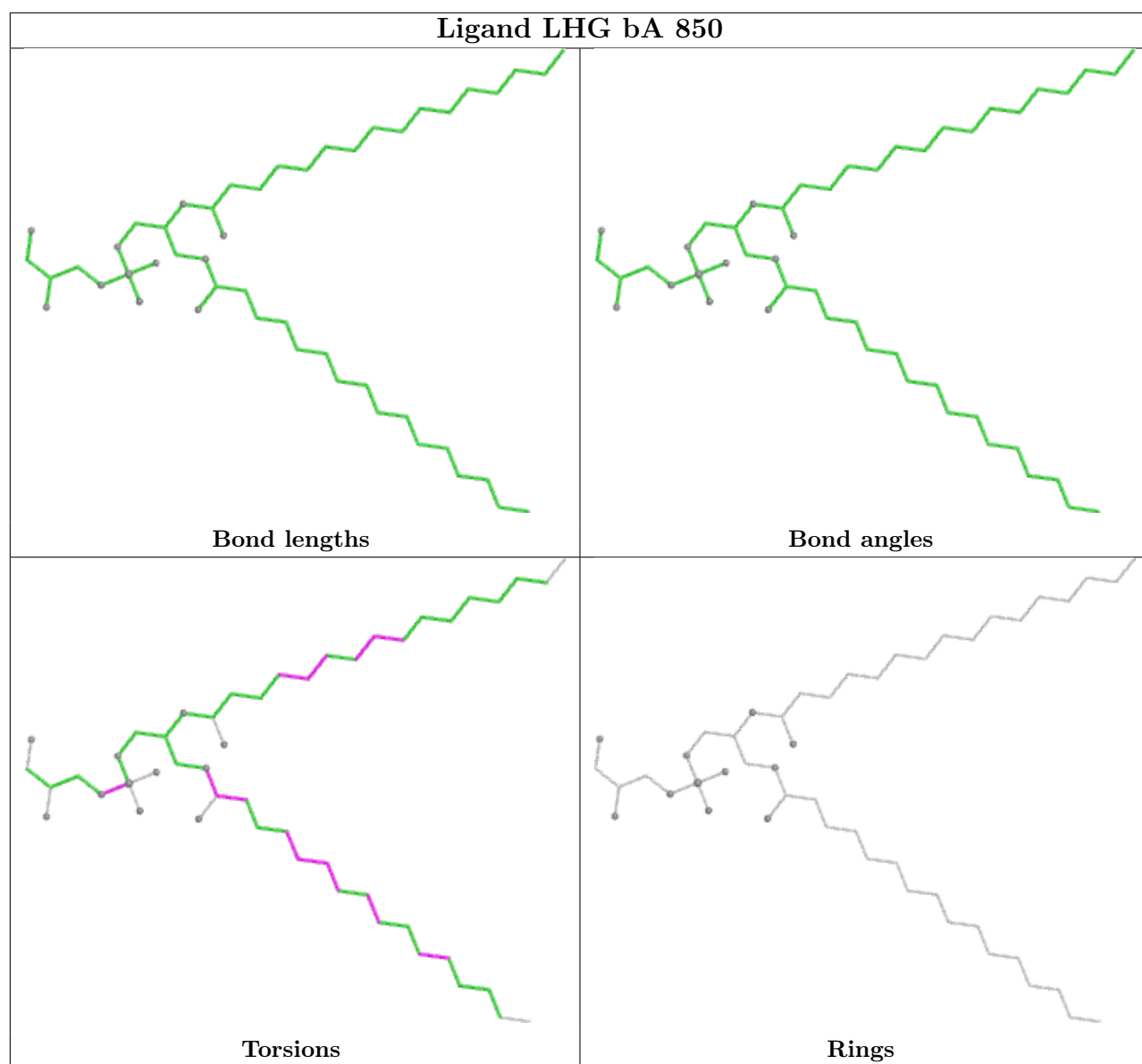


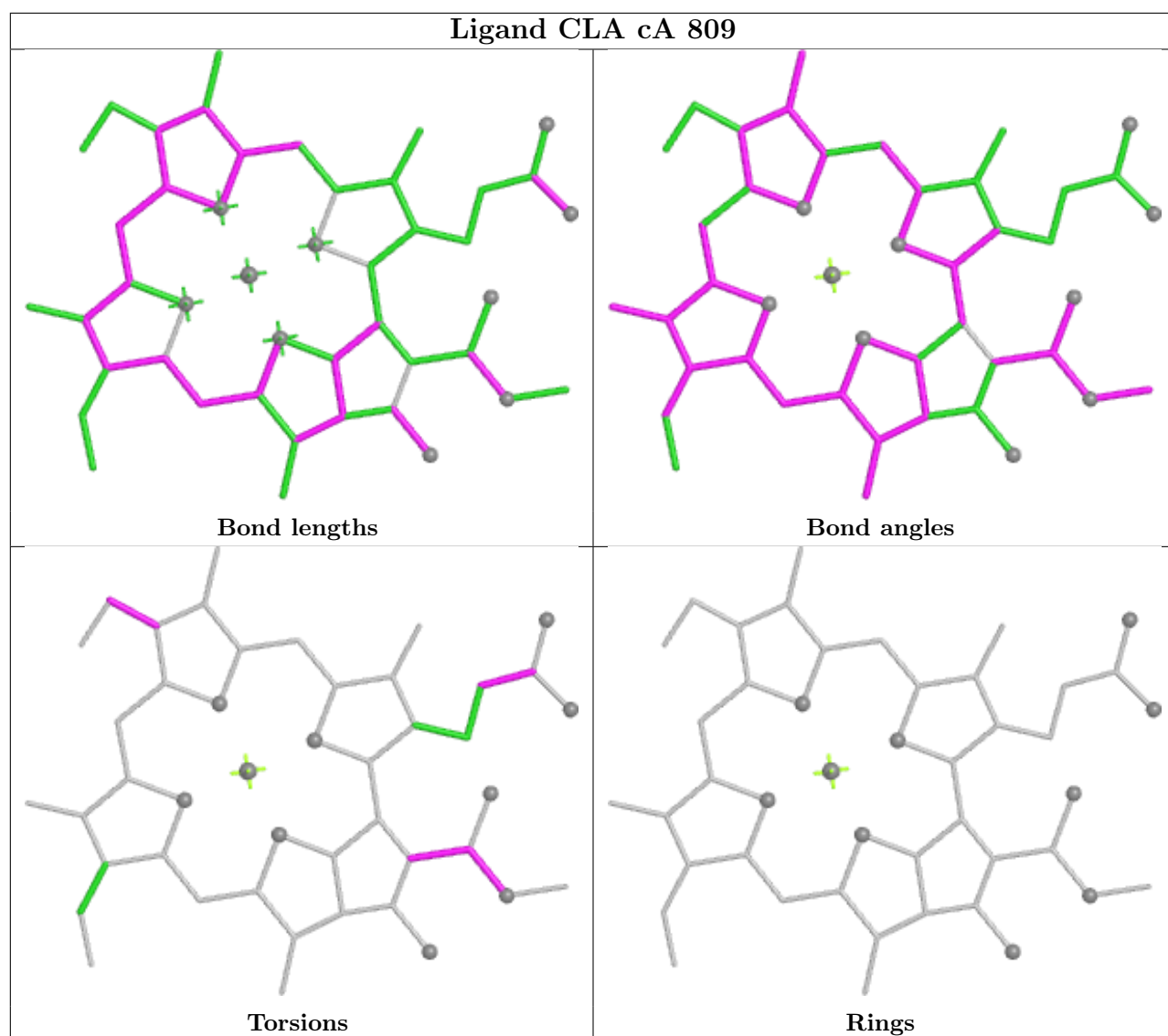
Ligand CLA bB 837

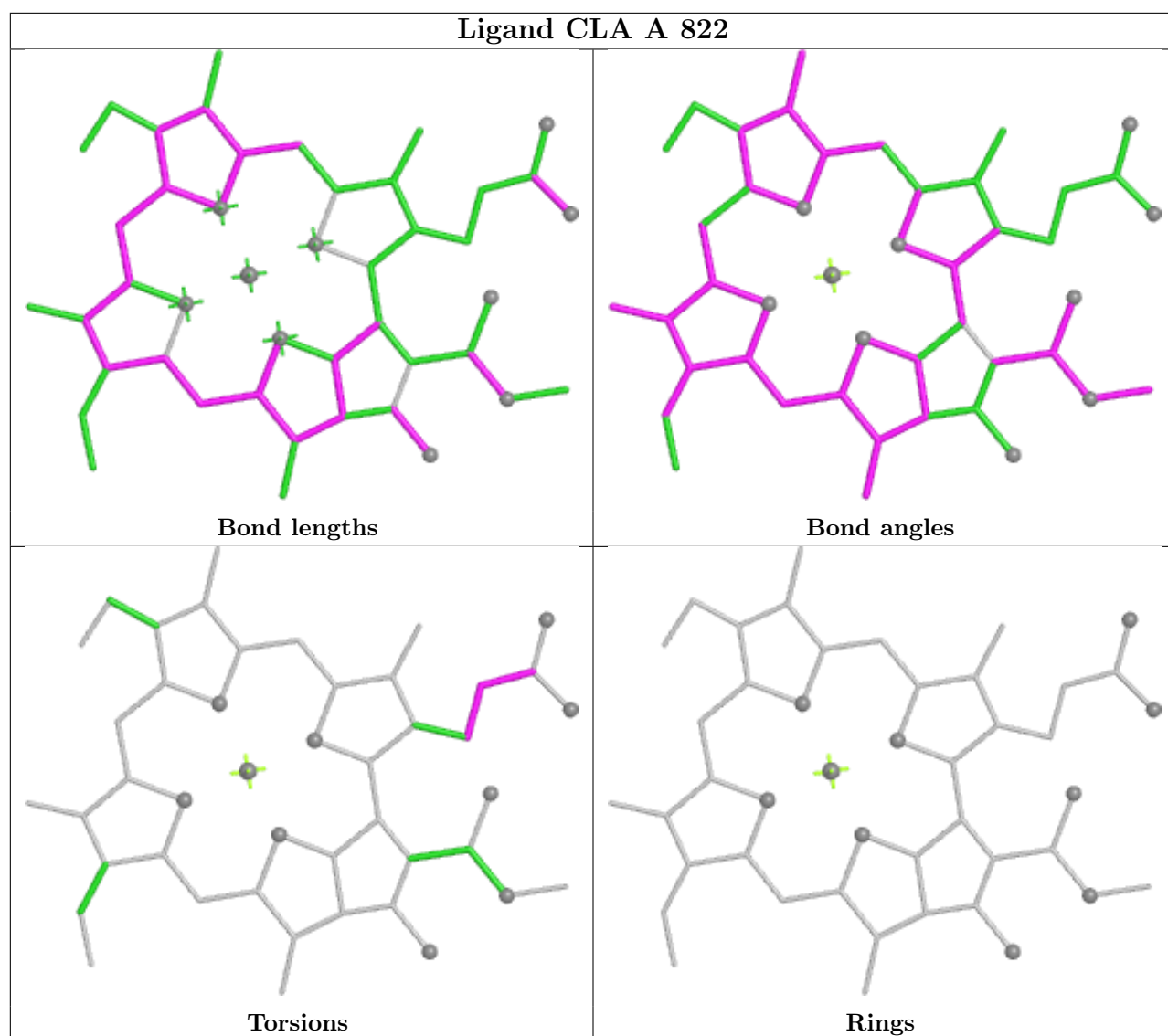


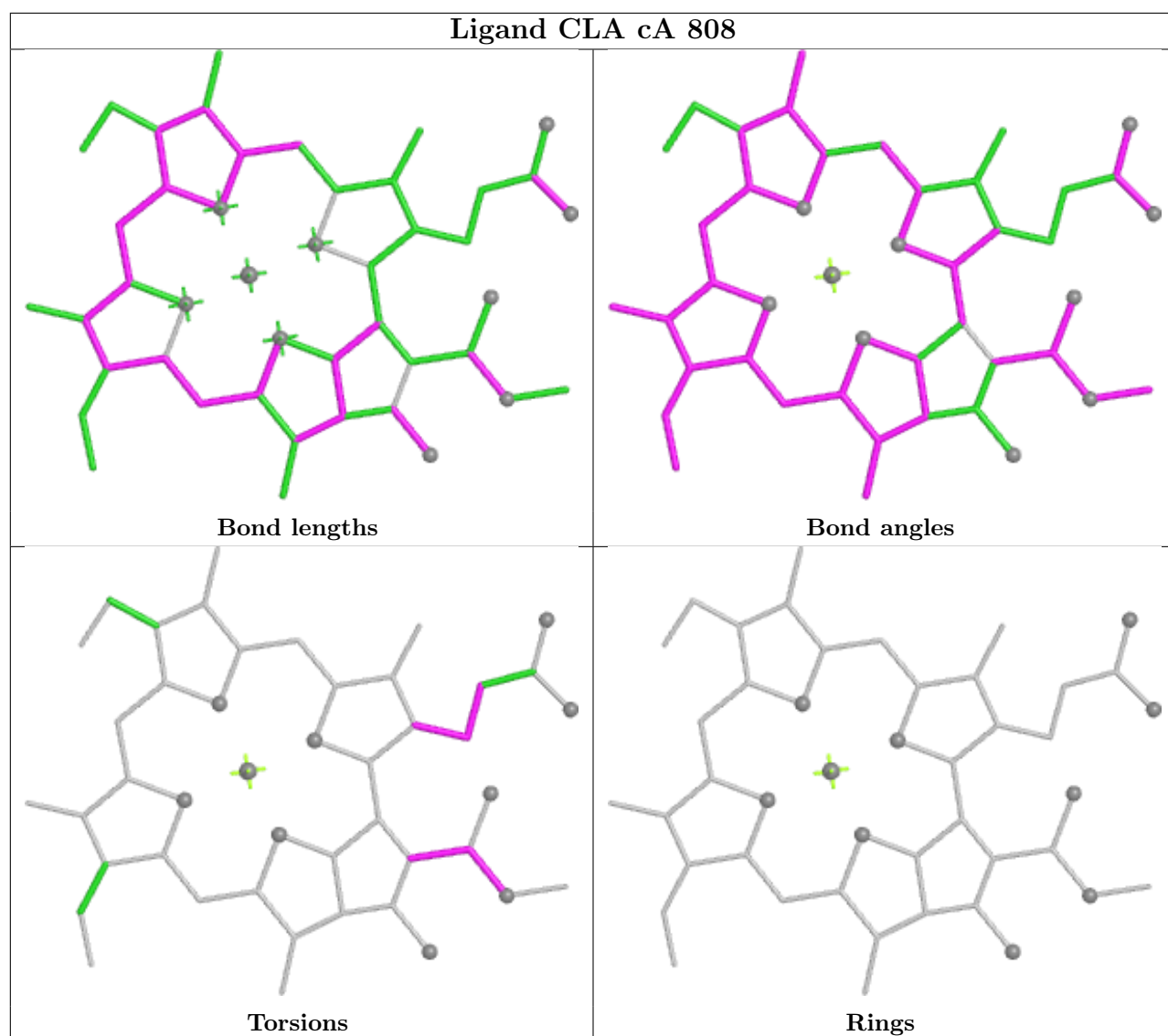
Ligand BCR bA 846

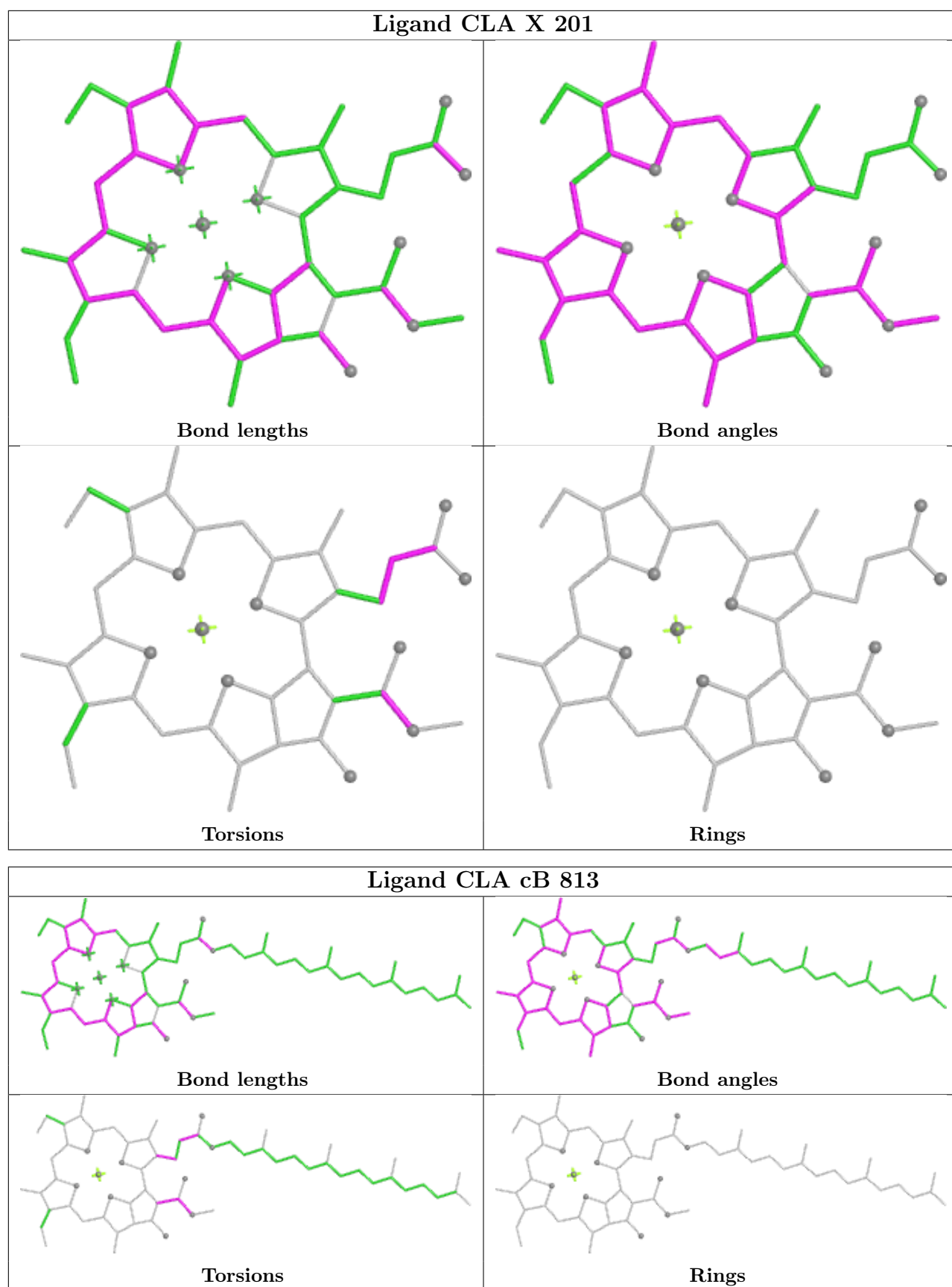


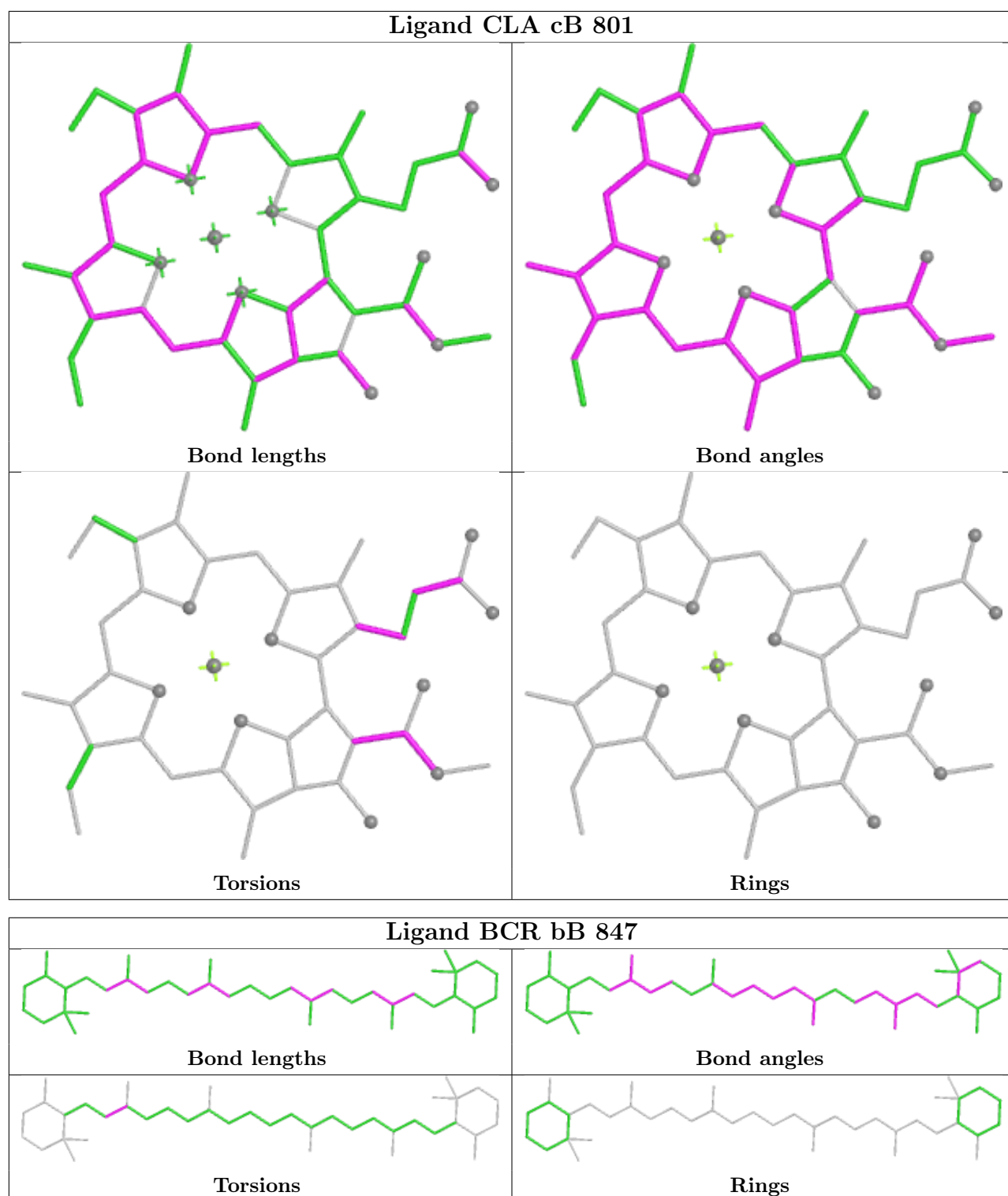


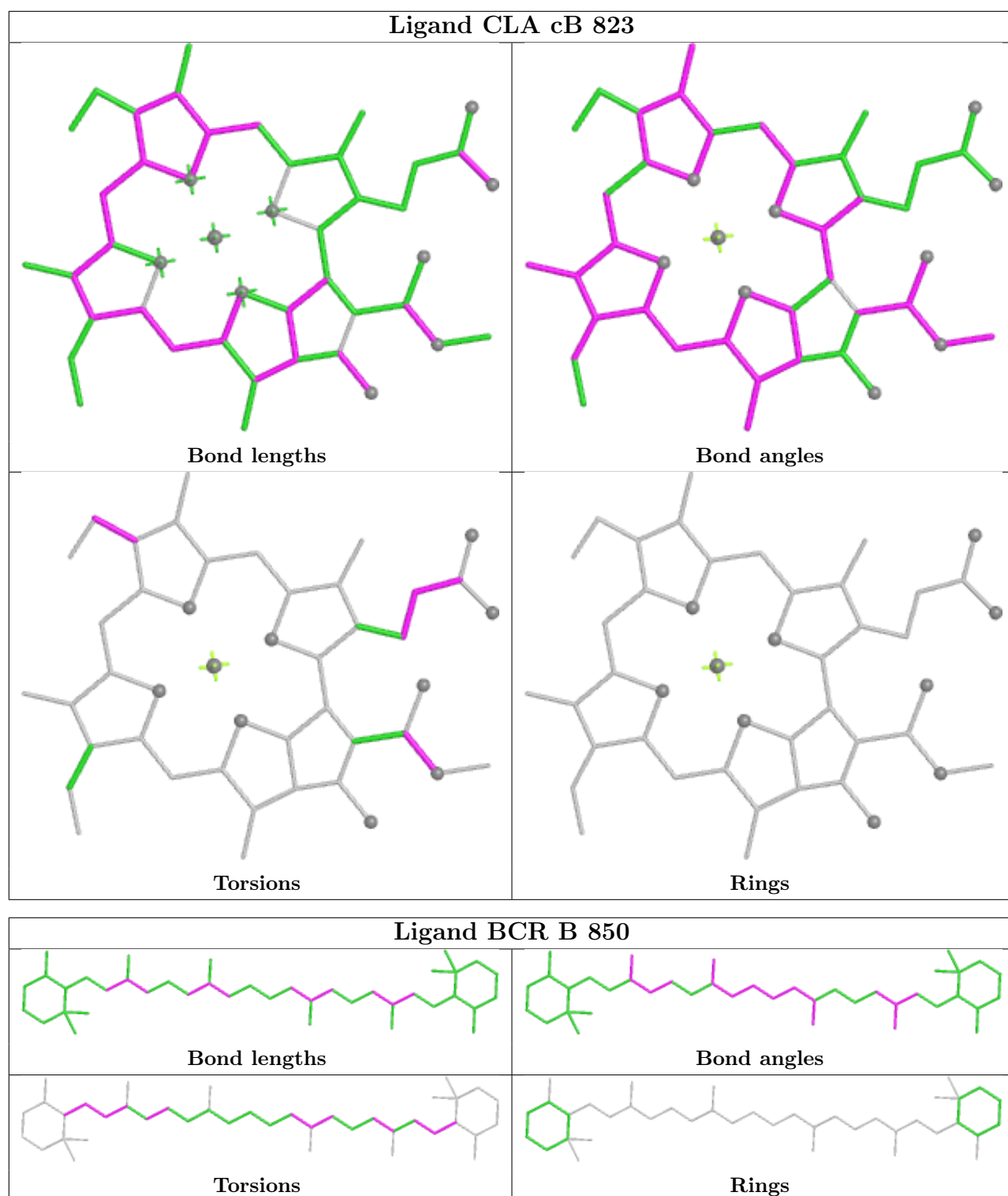




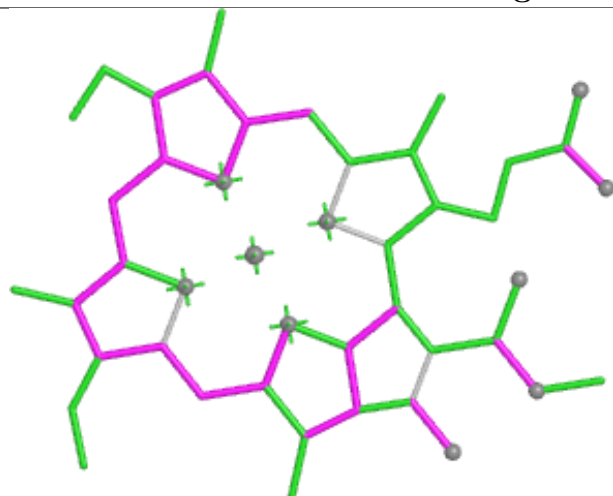




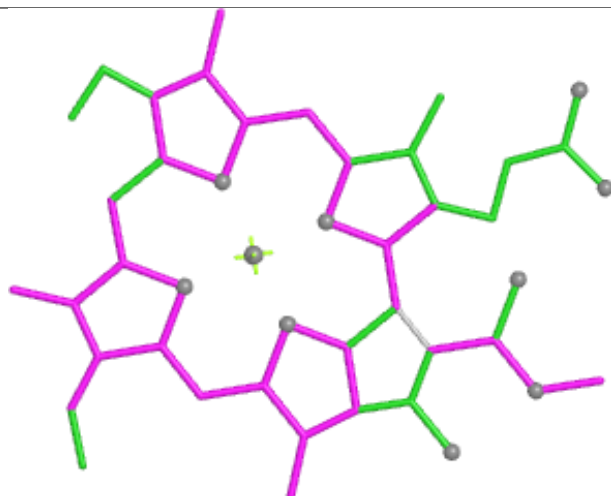




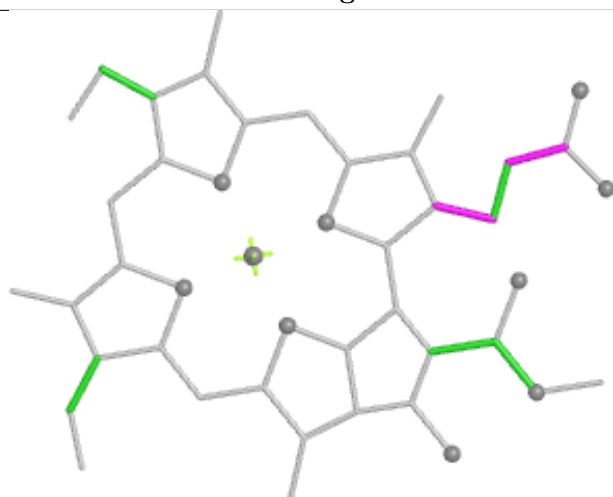
Ligand CLA A 834



Bond lengths



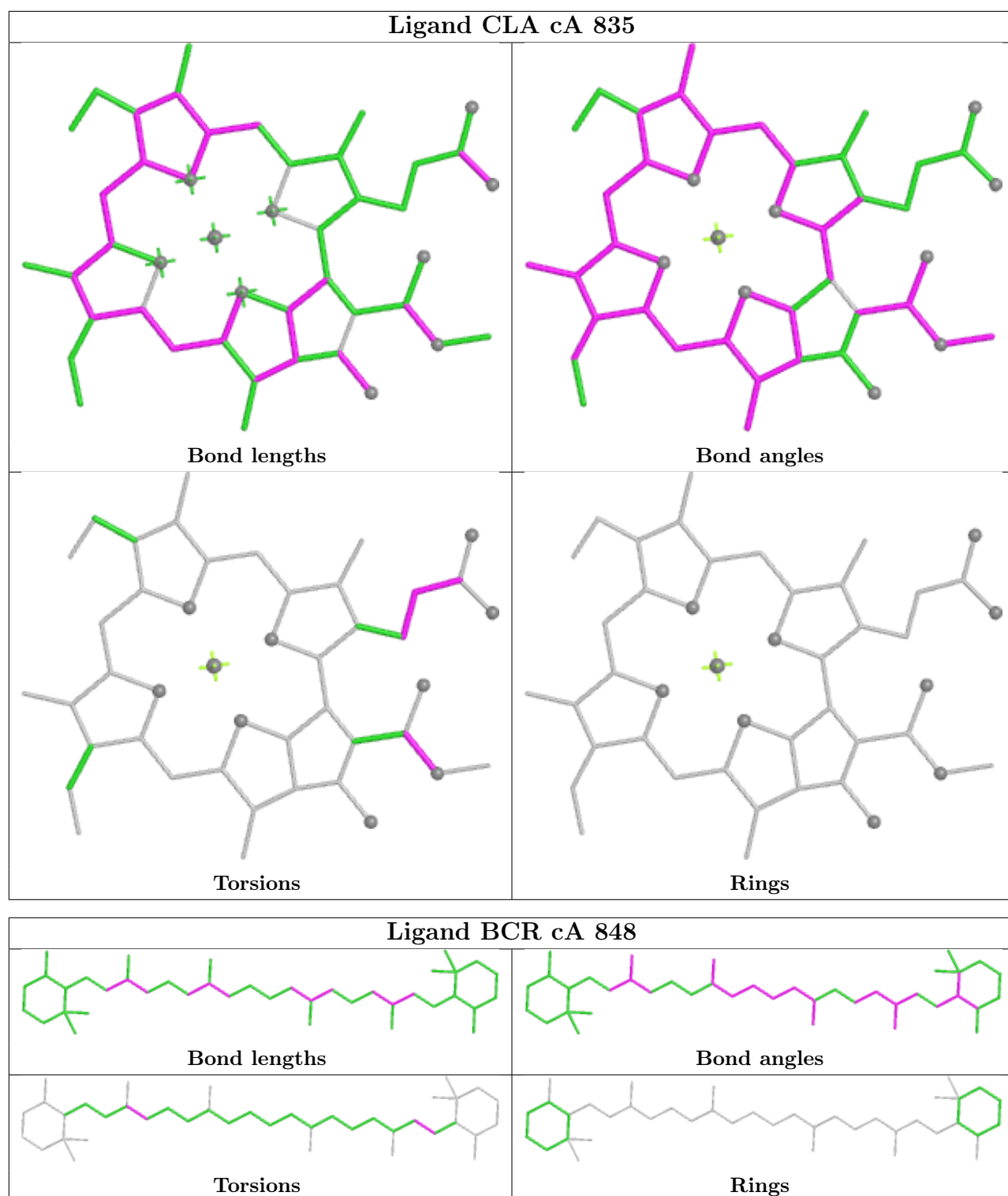
Bond angles

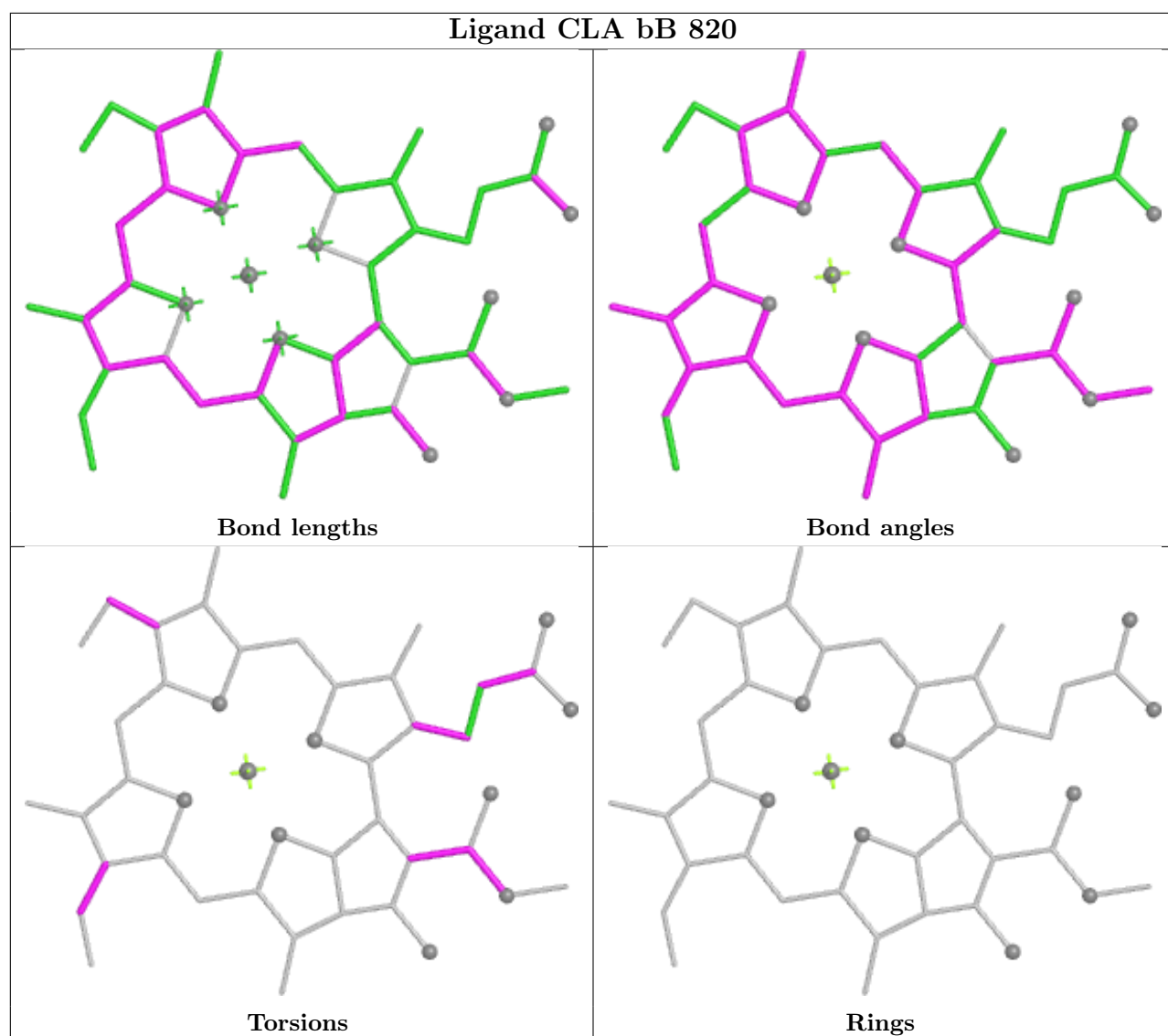


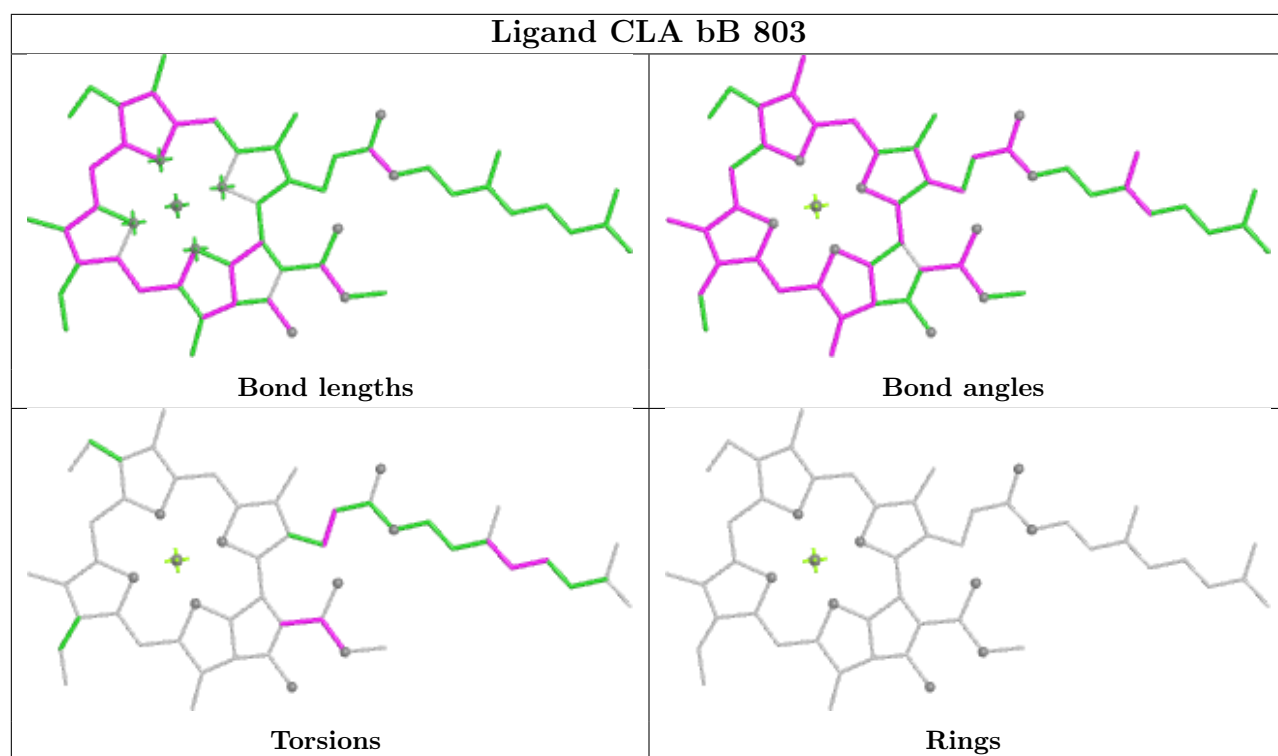
Torsions

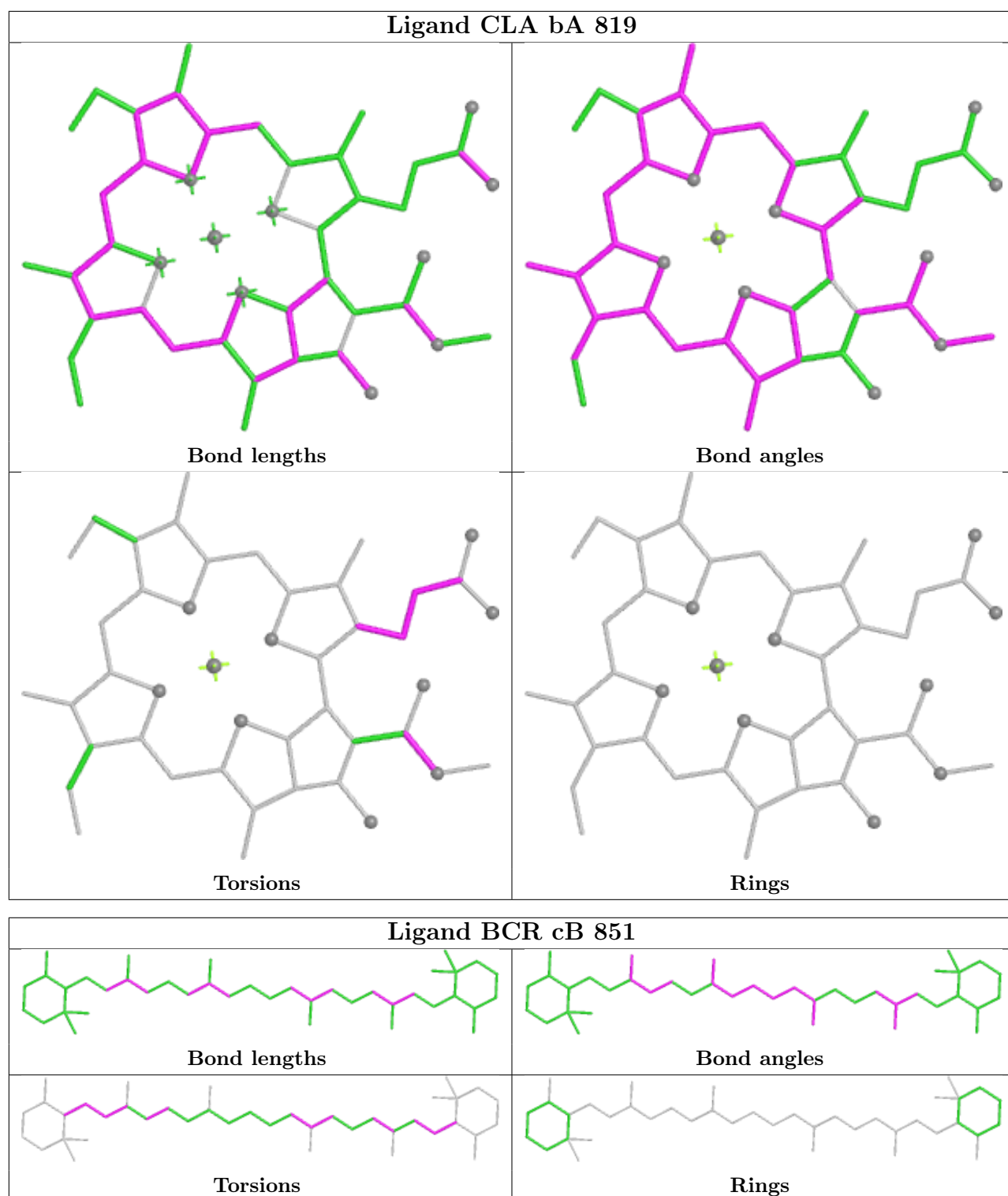


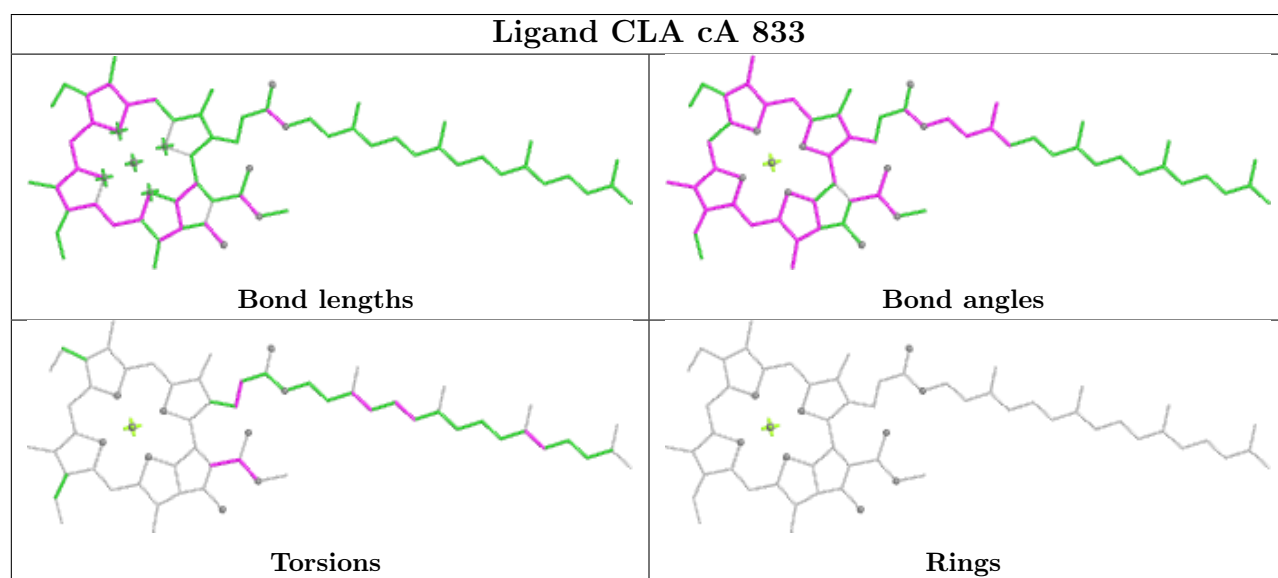
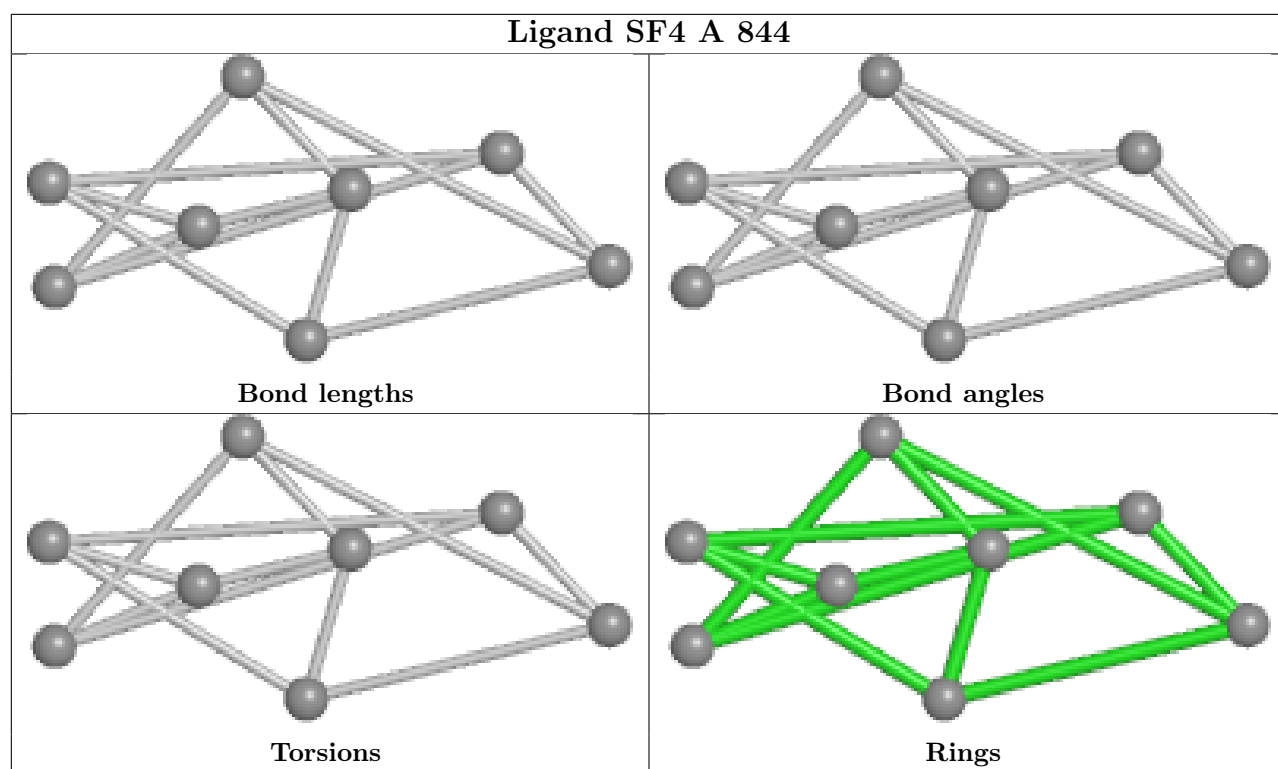
Rings

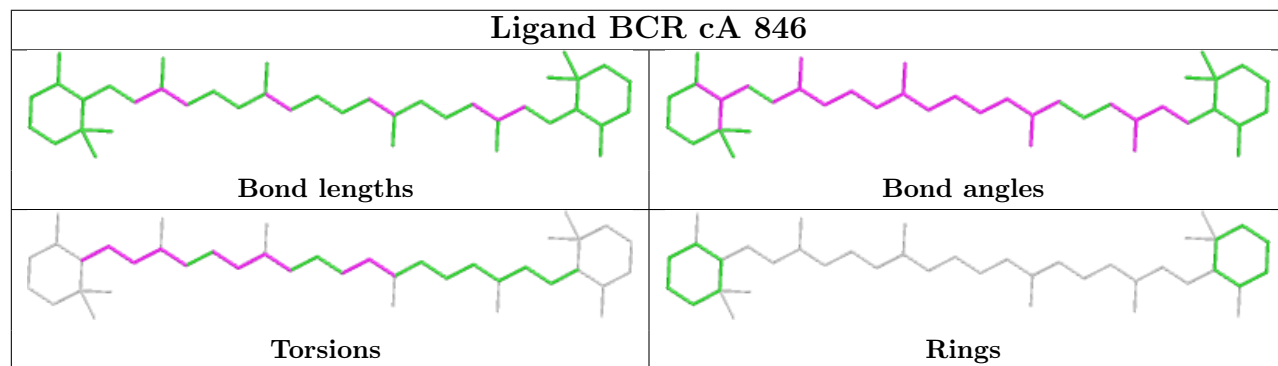
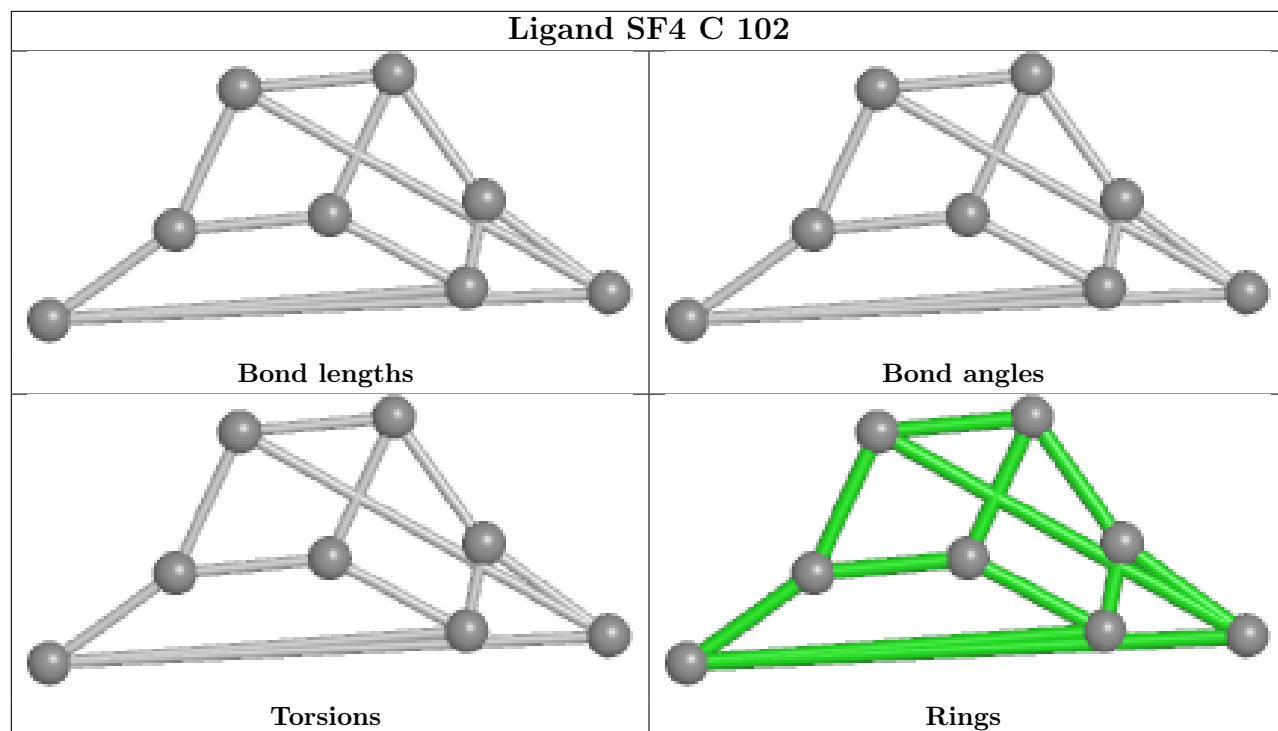


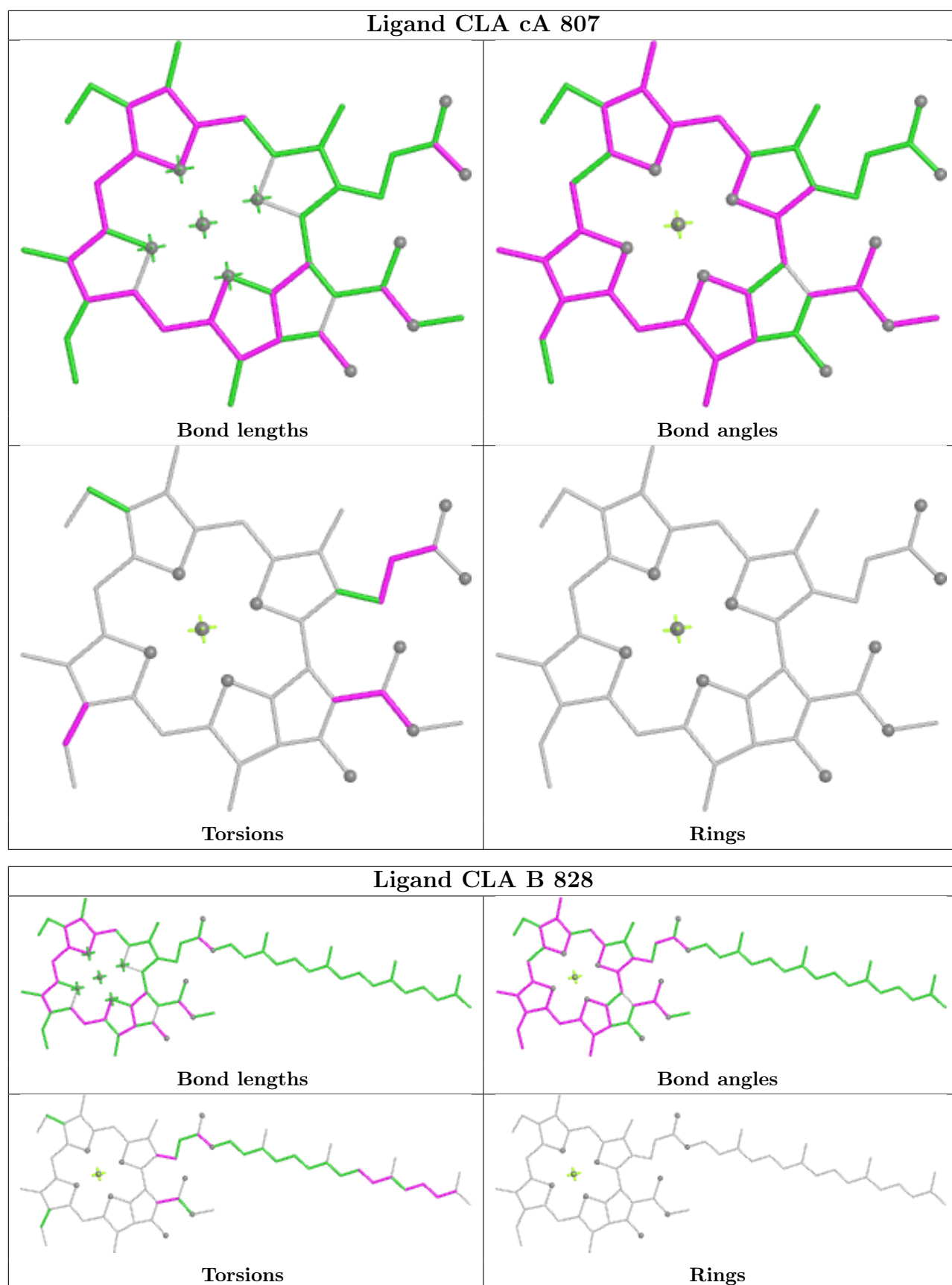


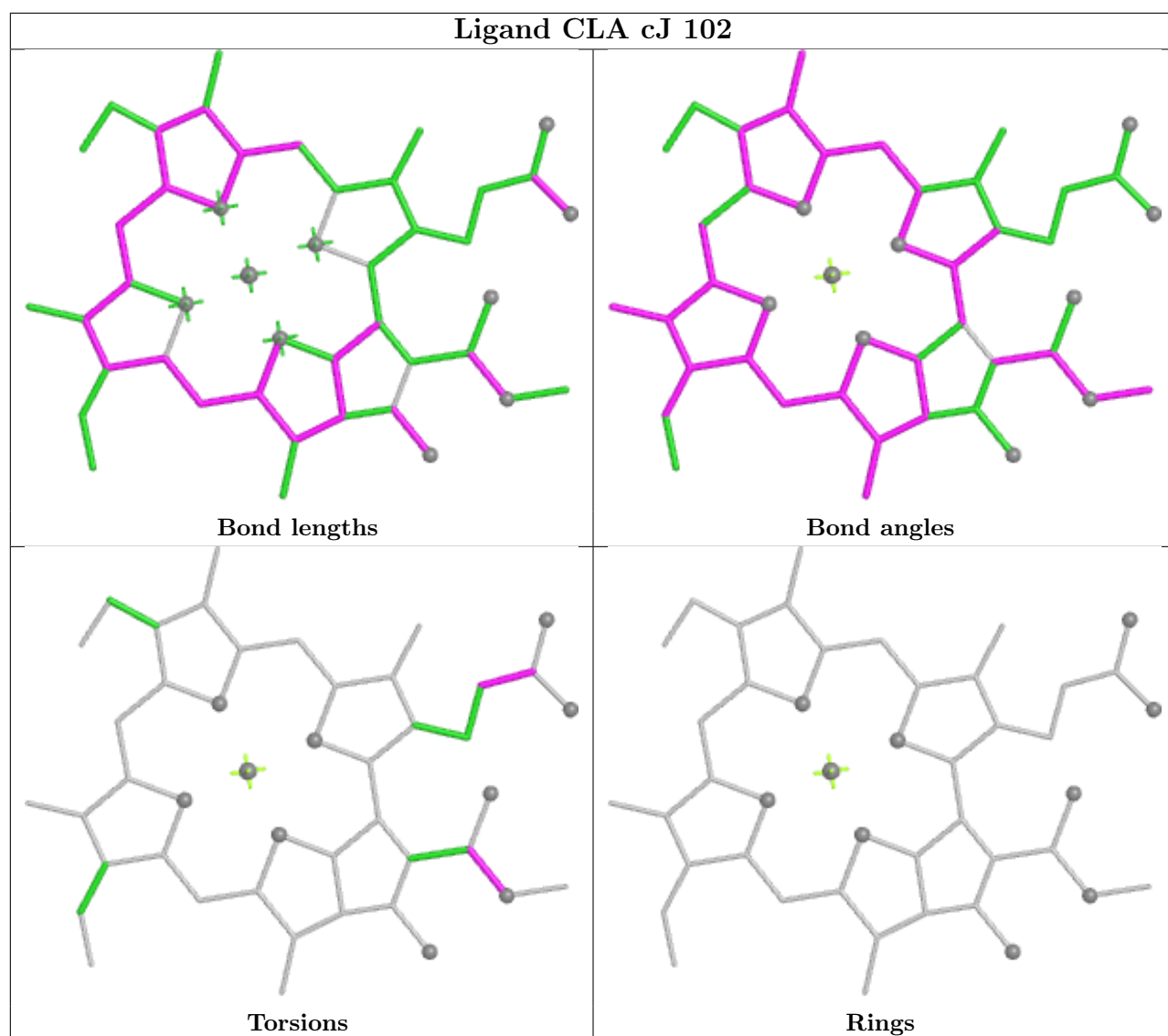


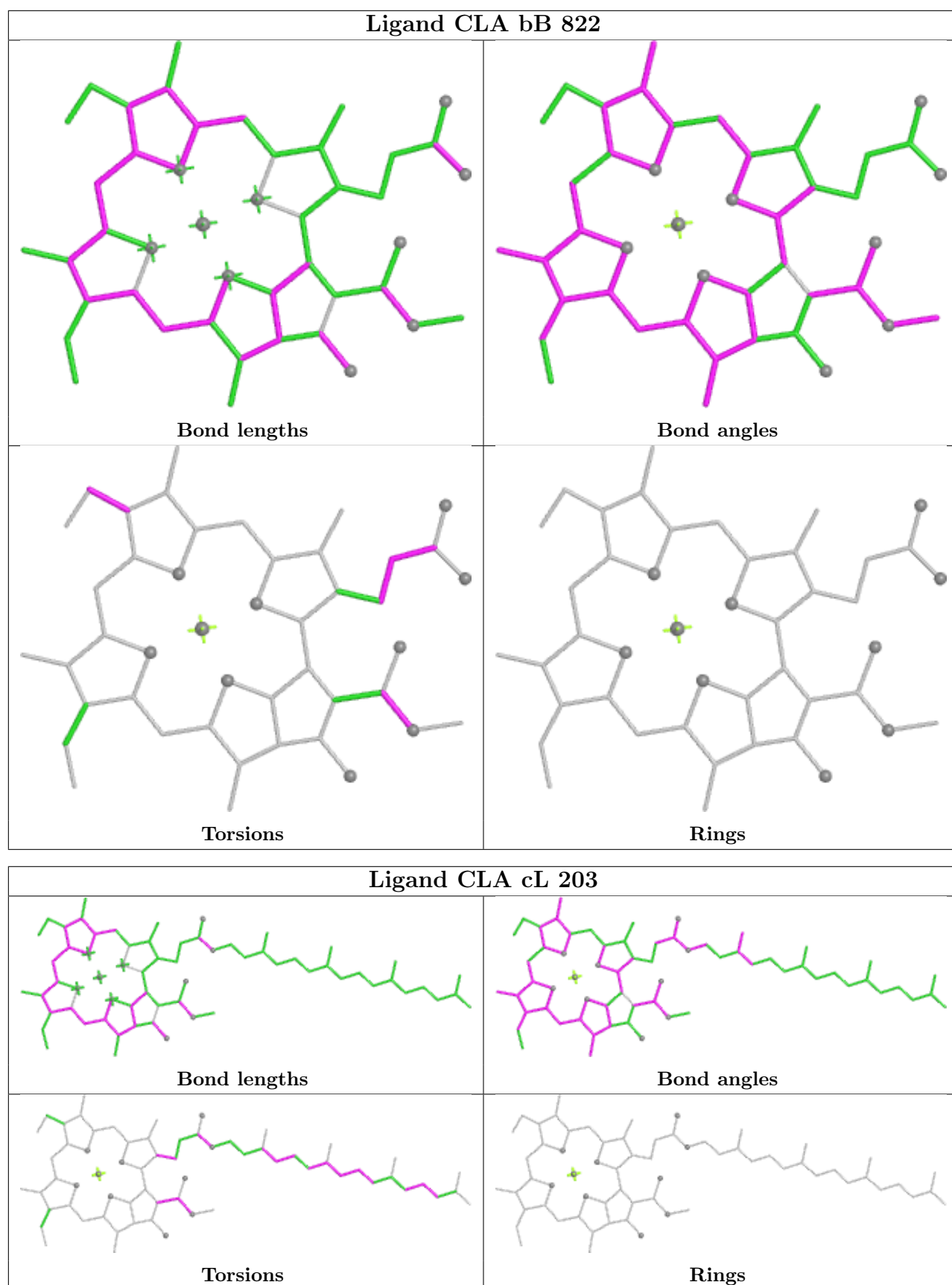


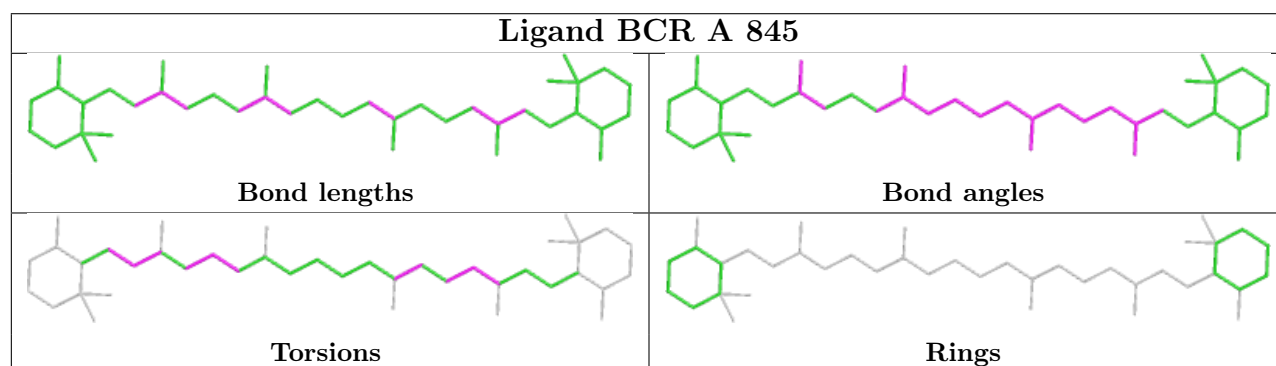
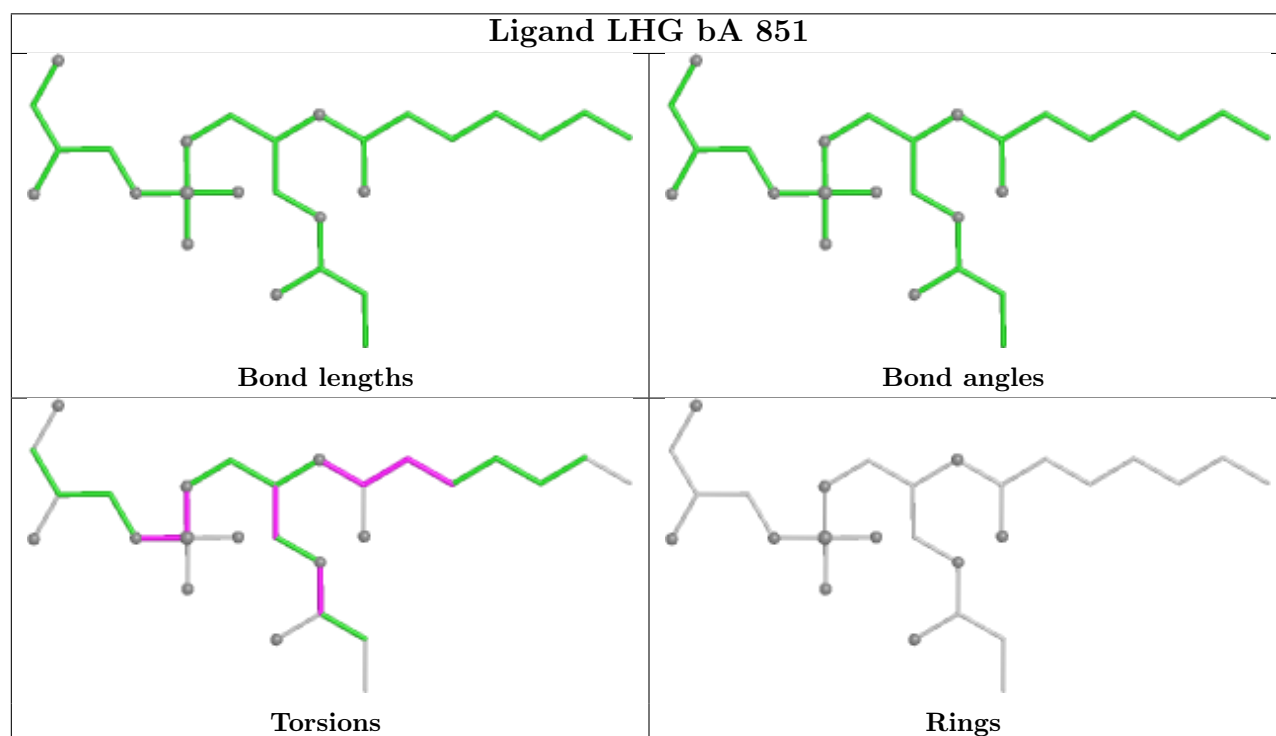
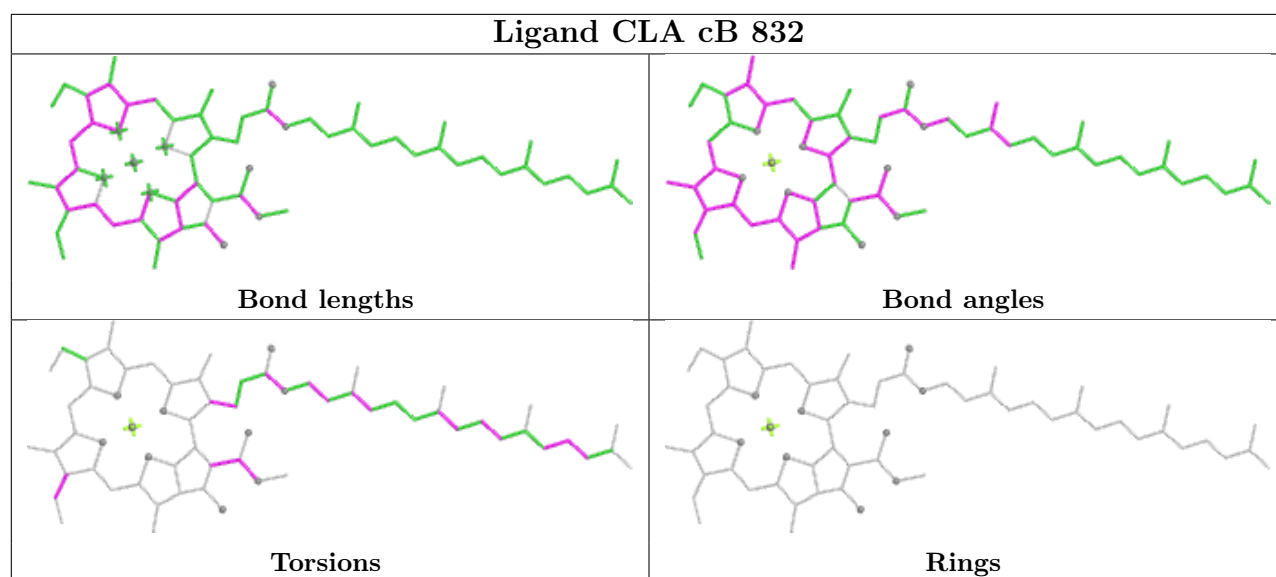


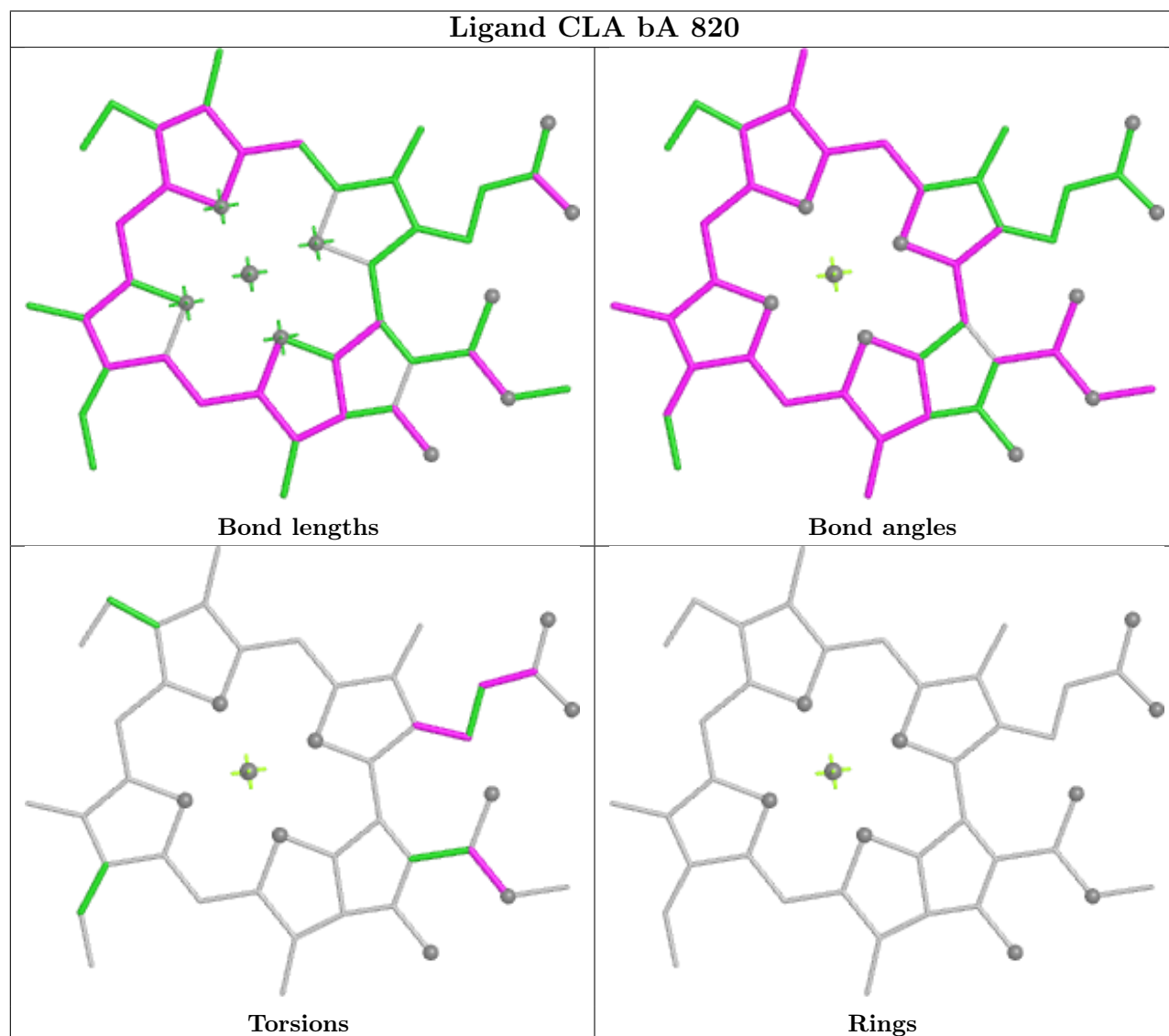
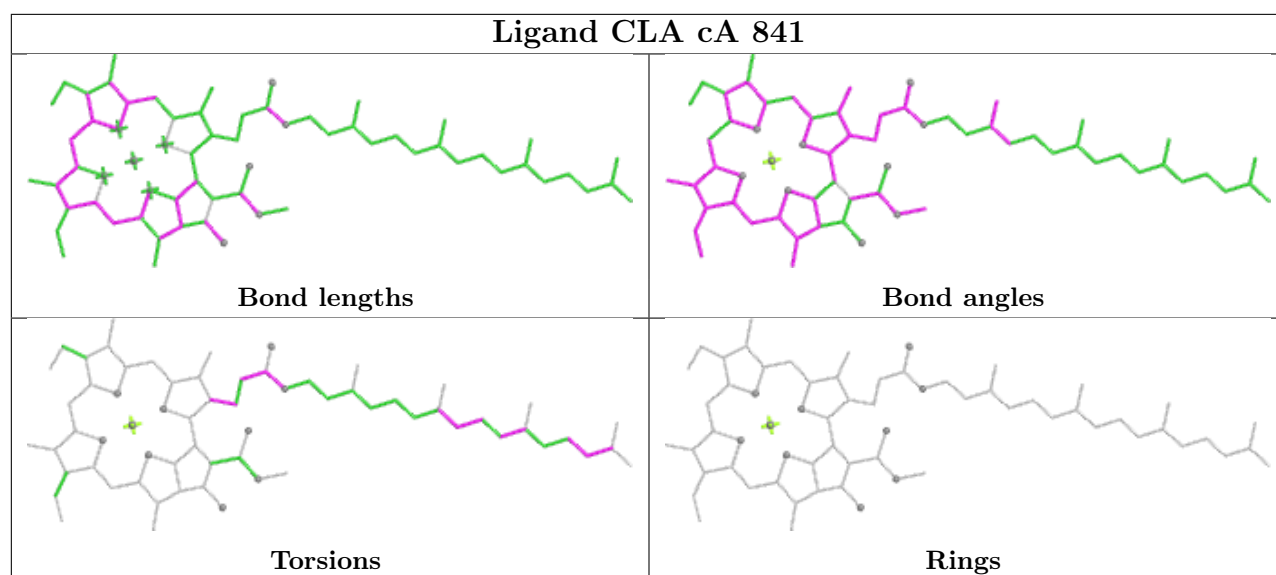


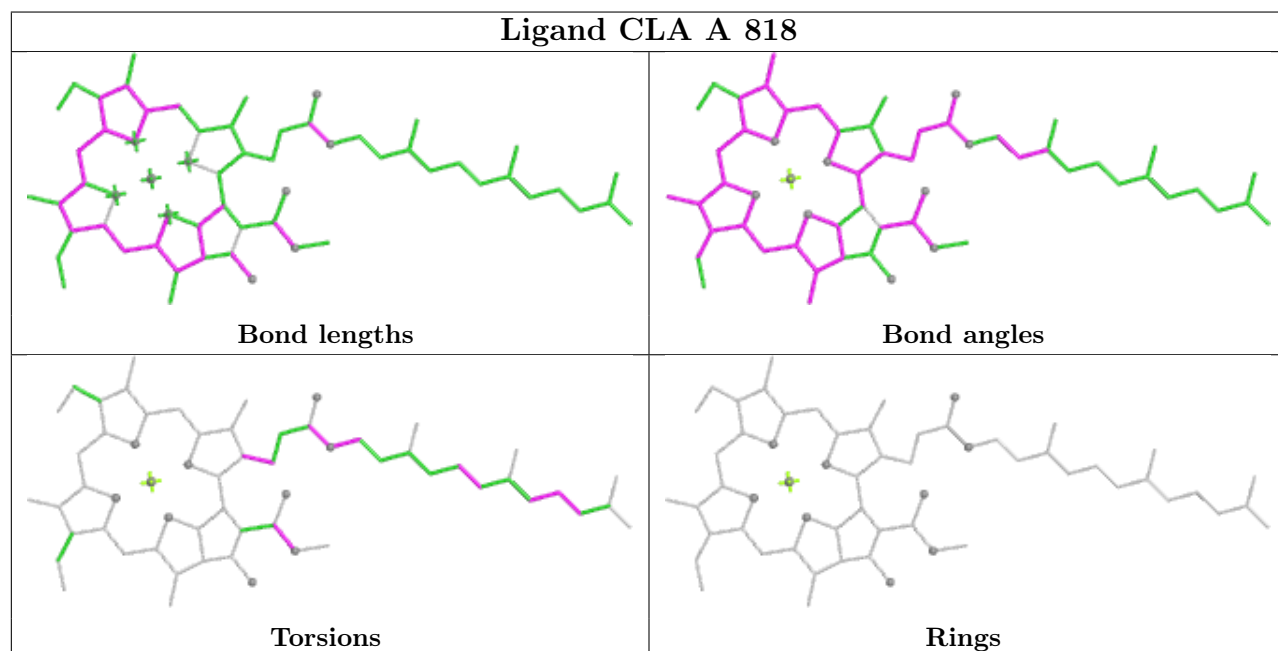
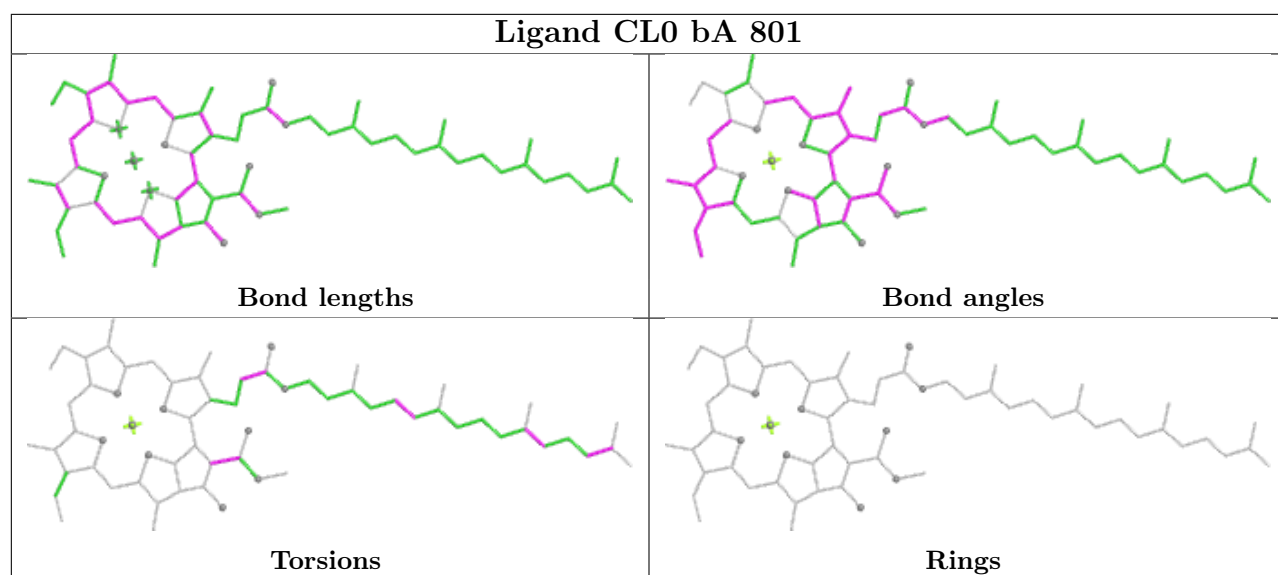


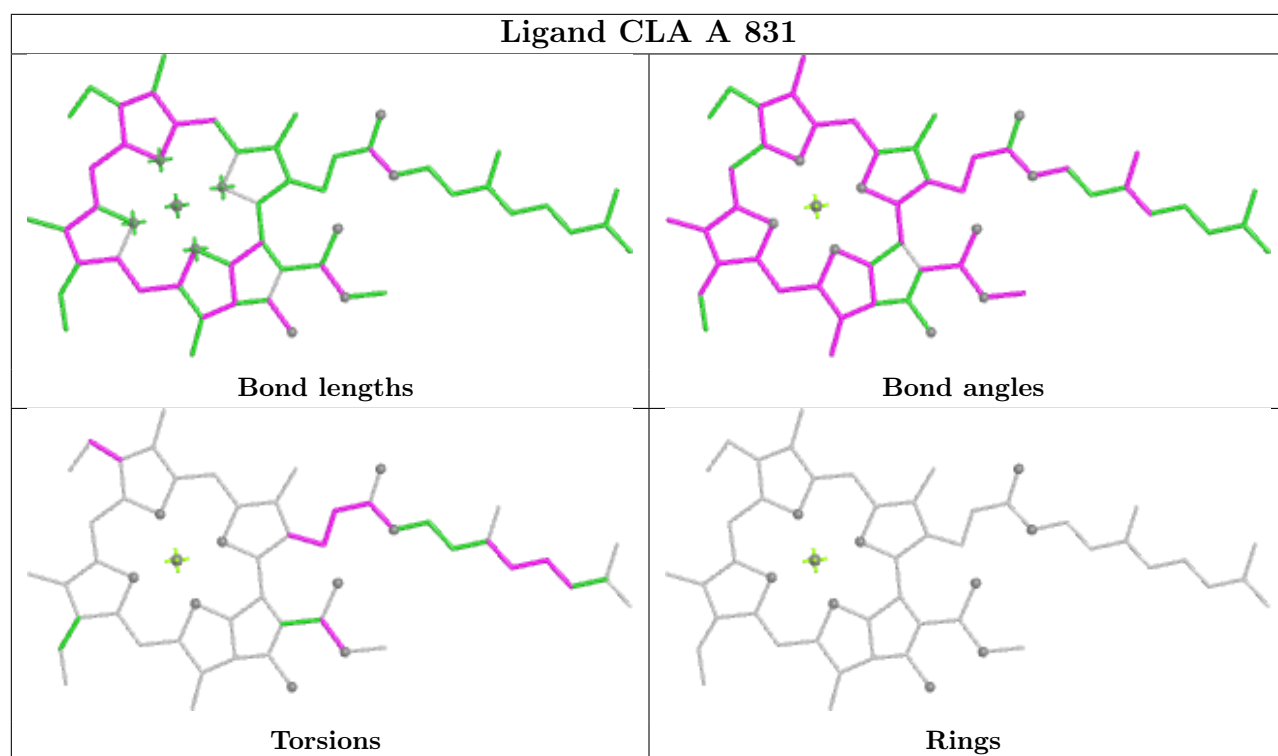




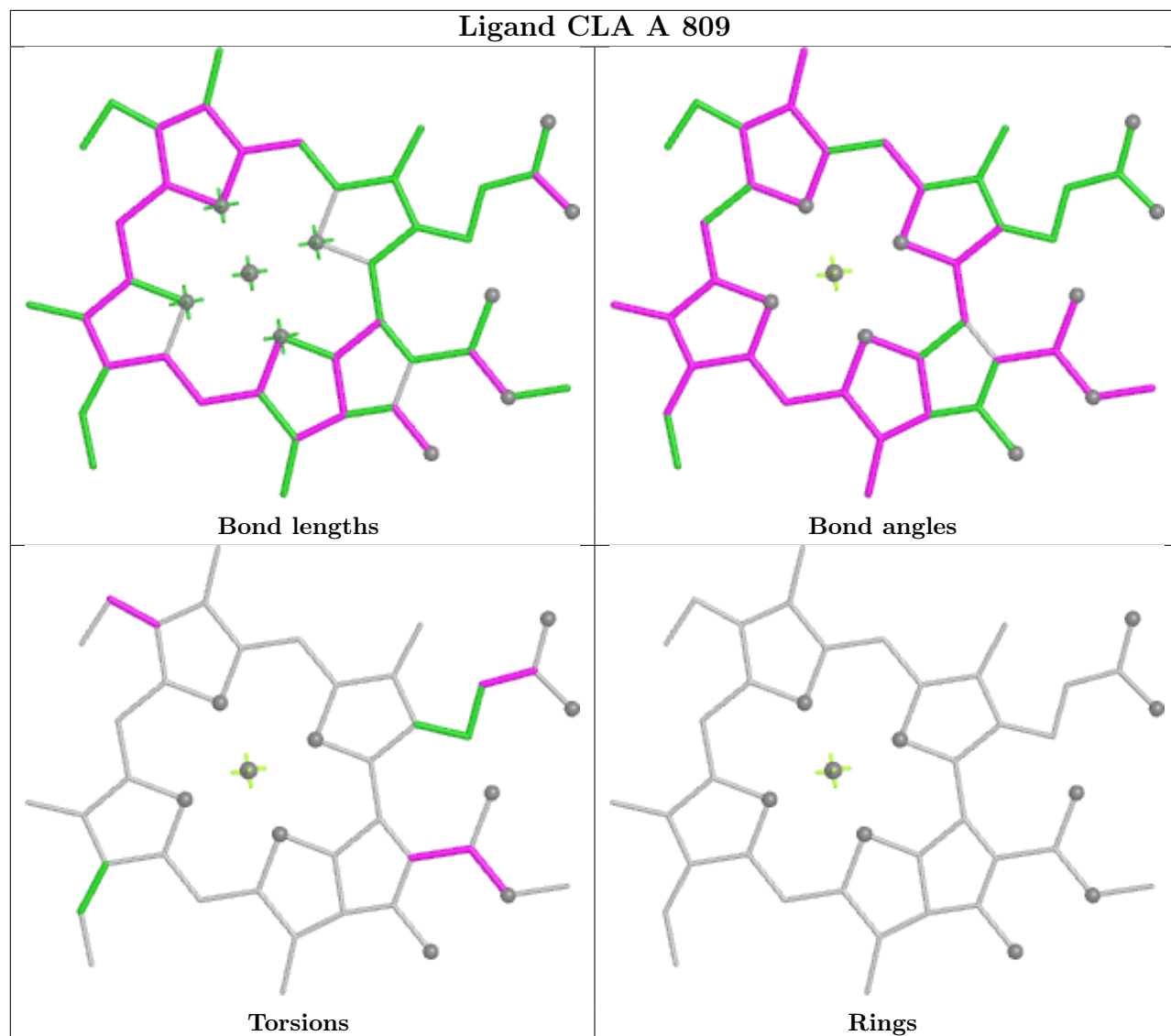




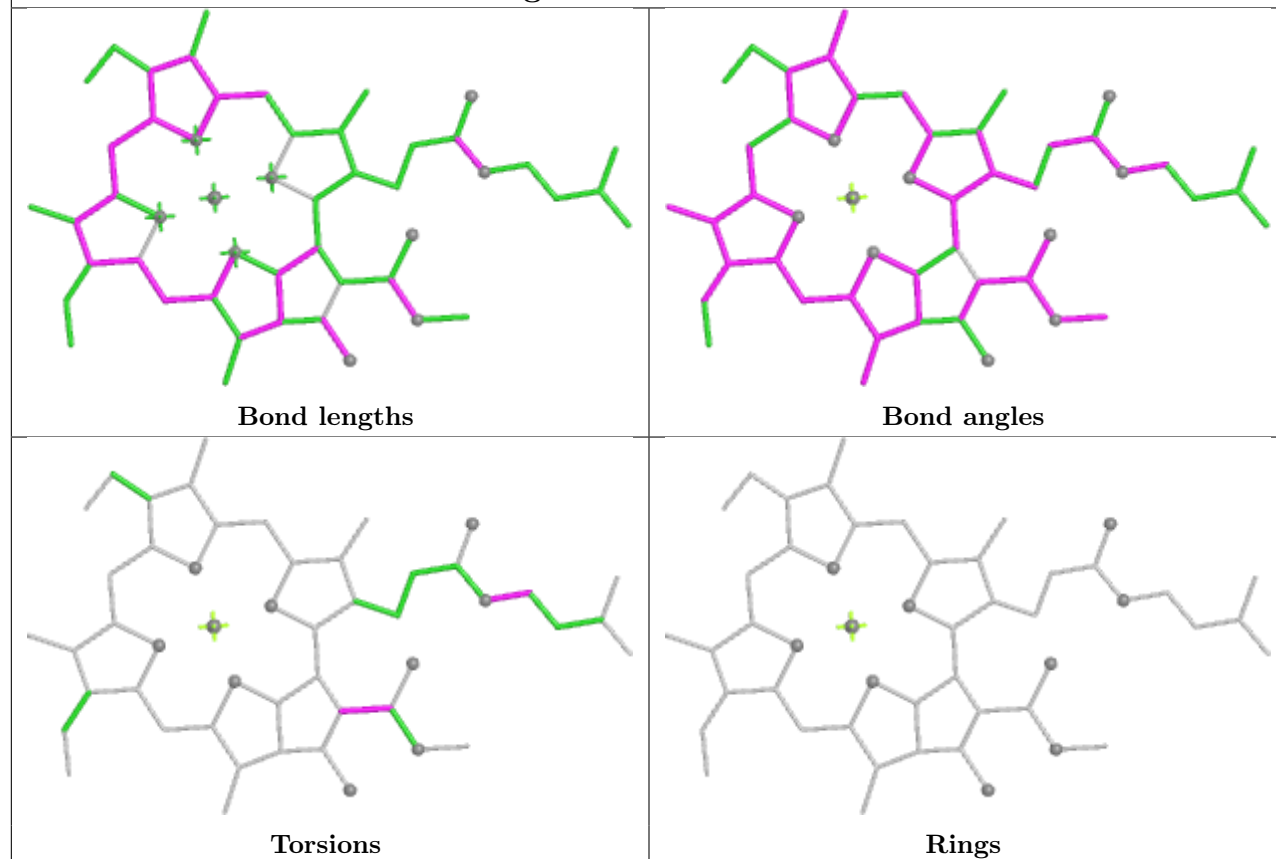




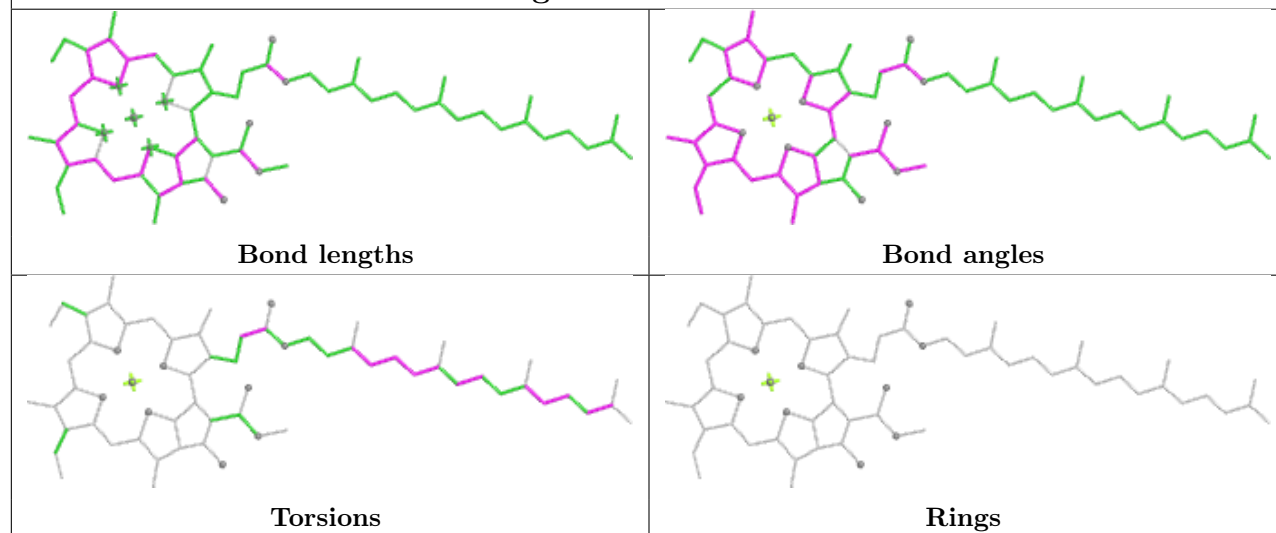
Ligand CLA A 809

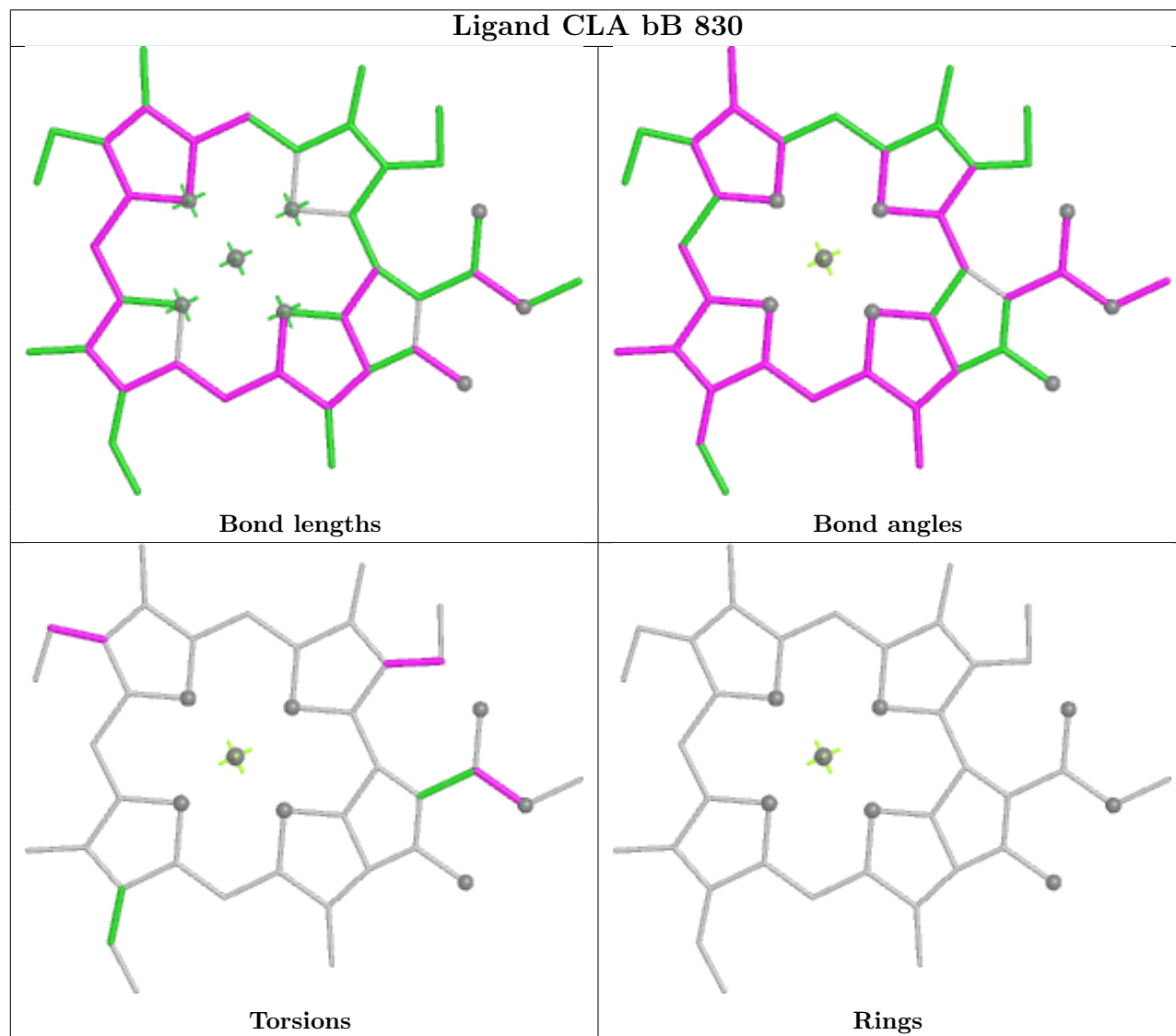
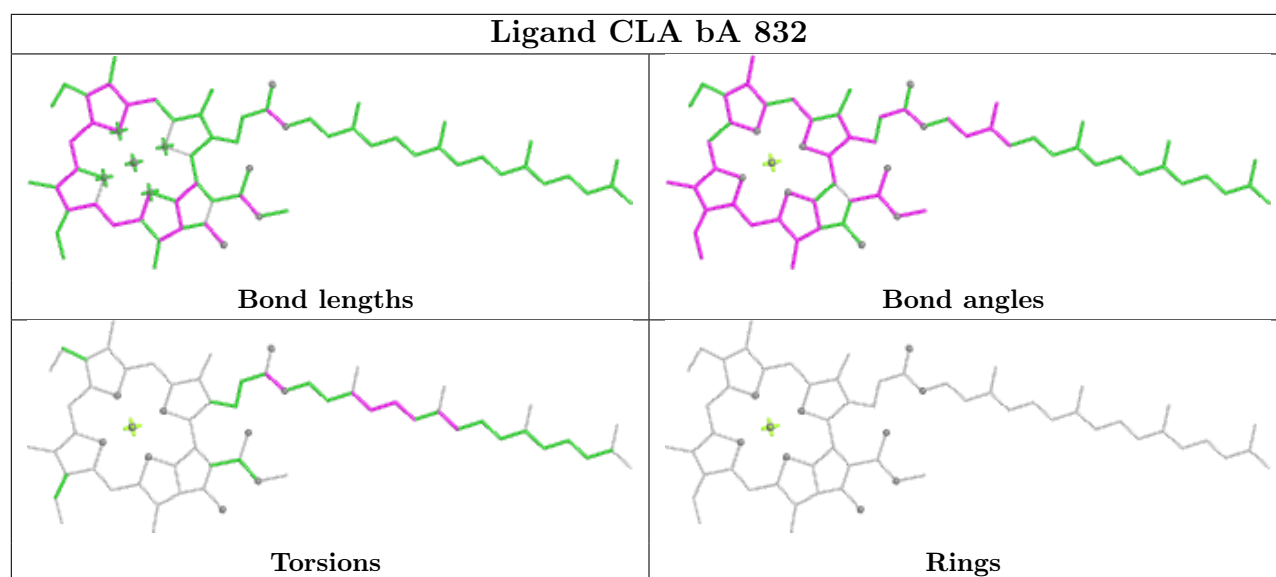


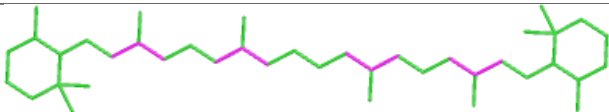
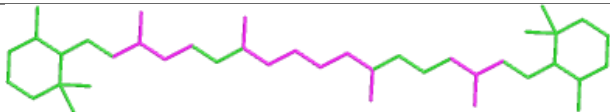
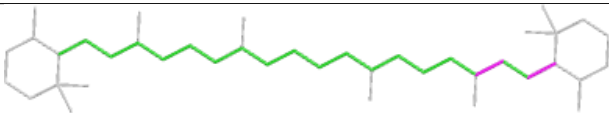
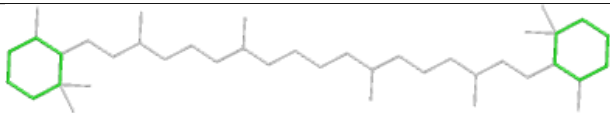
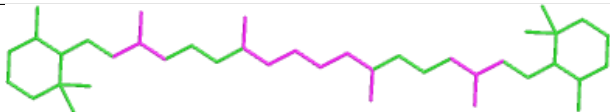
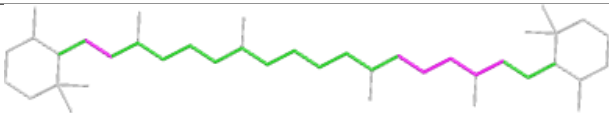
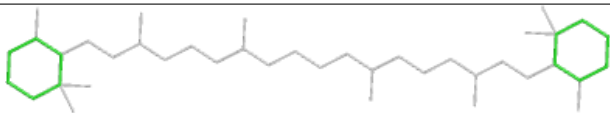
Ligand CLA cA 825



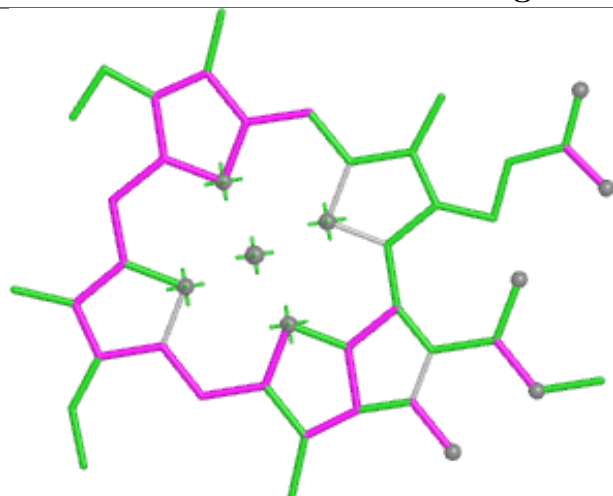
Ligand CLA B 807



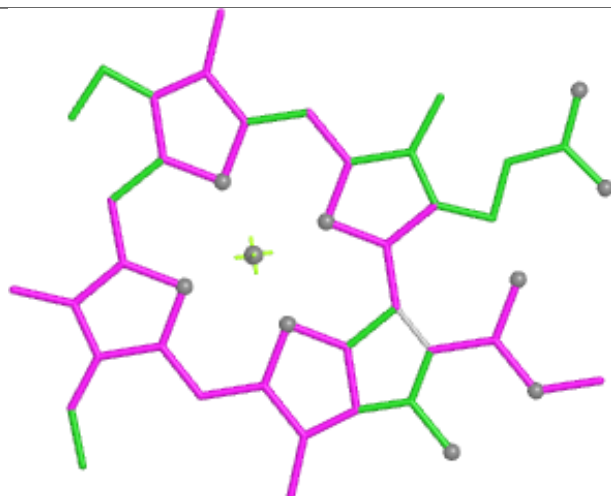


Ligand BCR L 205					
	Bond lengths				
	Torsions				
Rings					
Ligand BCR cB 842					
	Bond lengths				
	Torsions				
Rings					

Ligand CLA A 816



Bond lengths



Bond angles

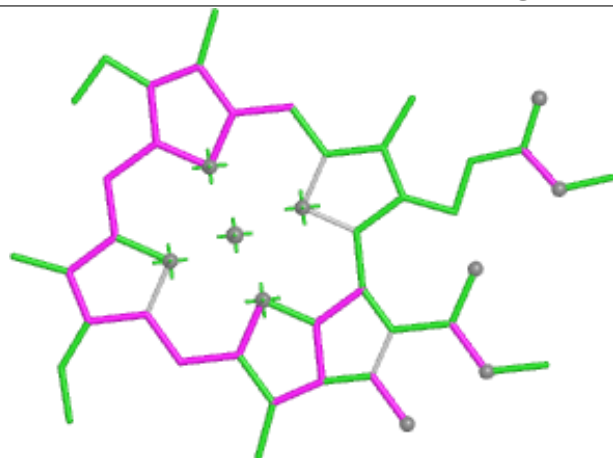


Torsions

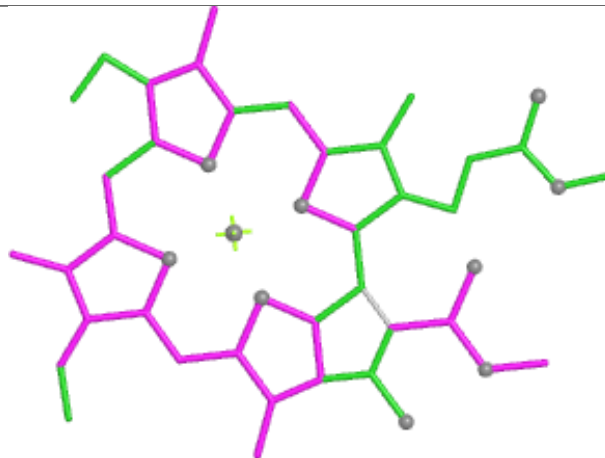


Rings

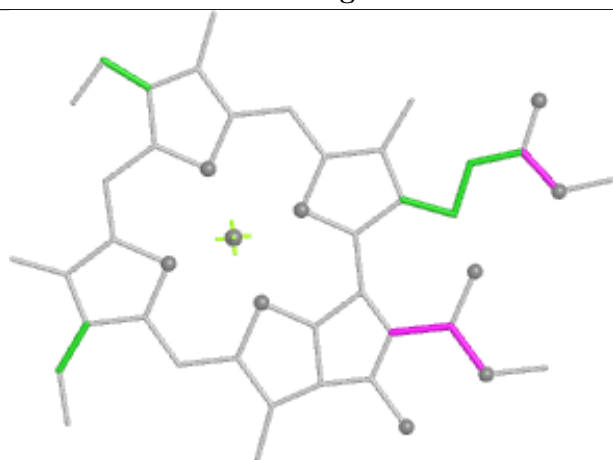
Ligand CLA B 824



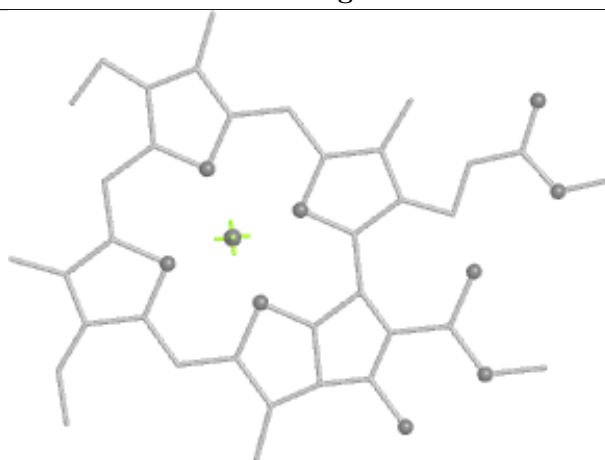
Bond lengths



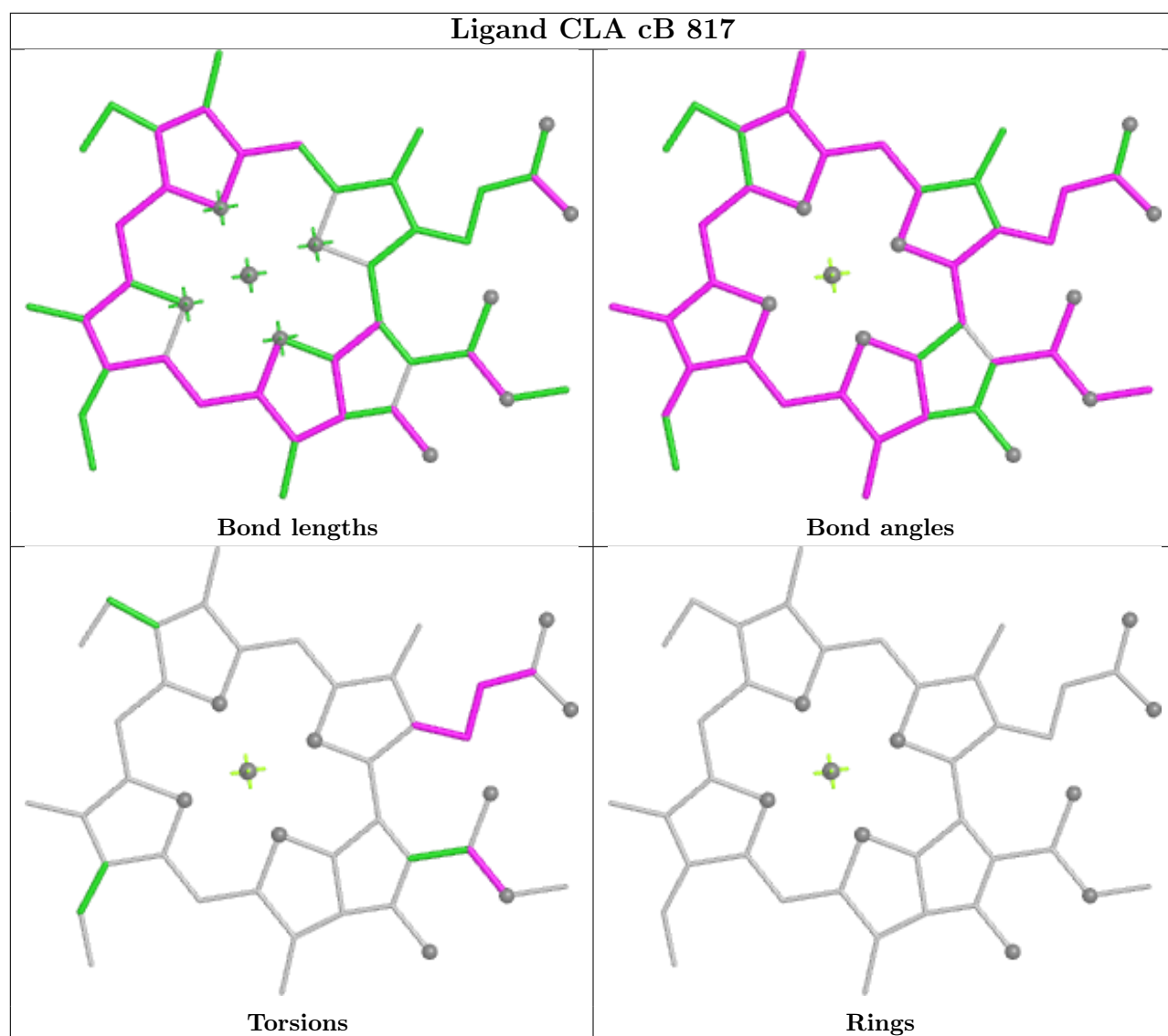
Bond angles

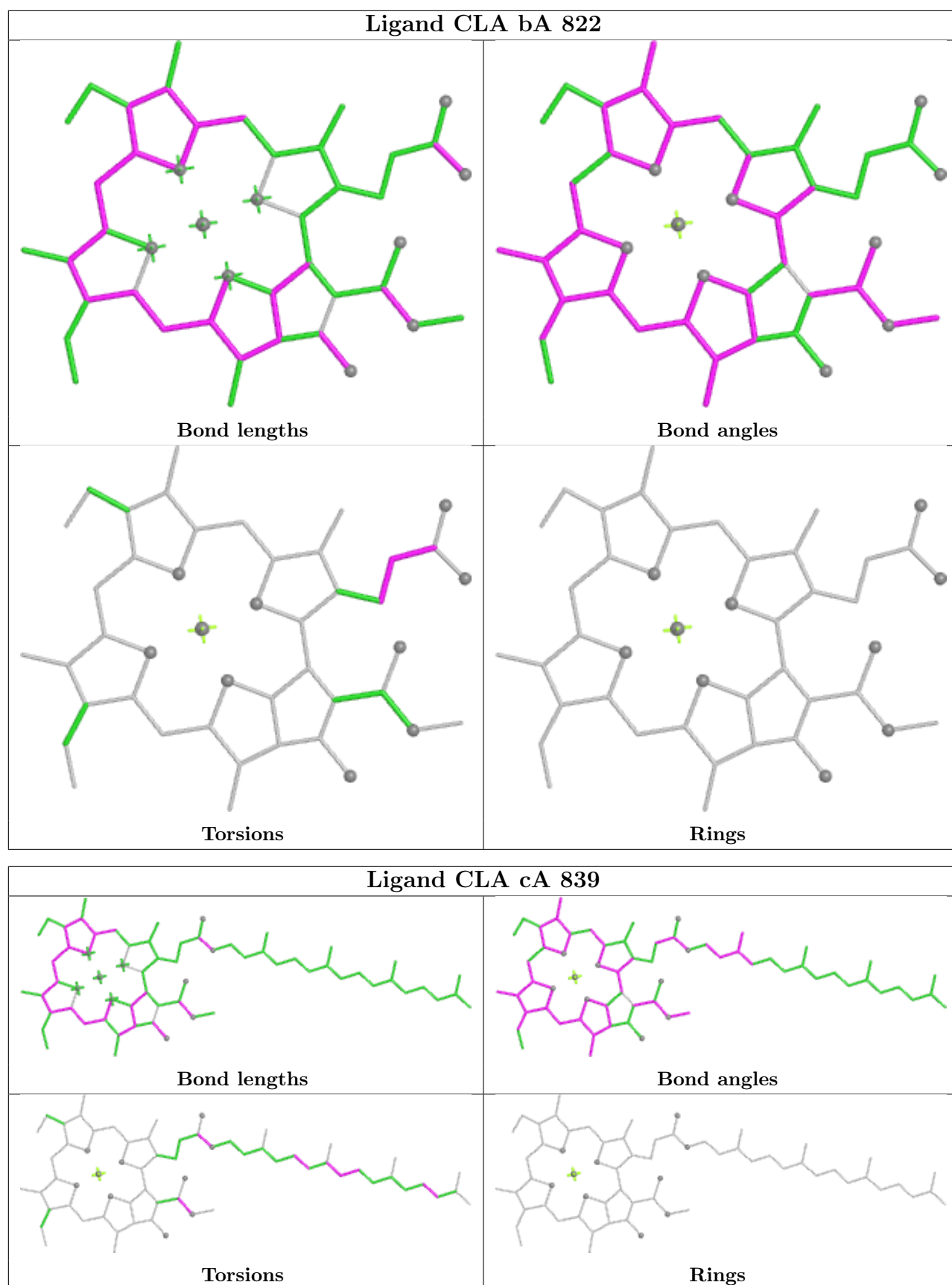


Torsions

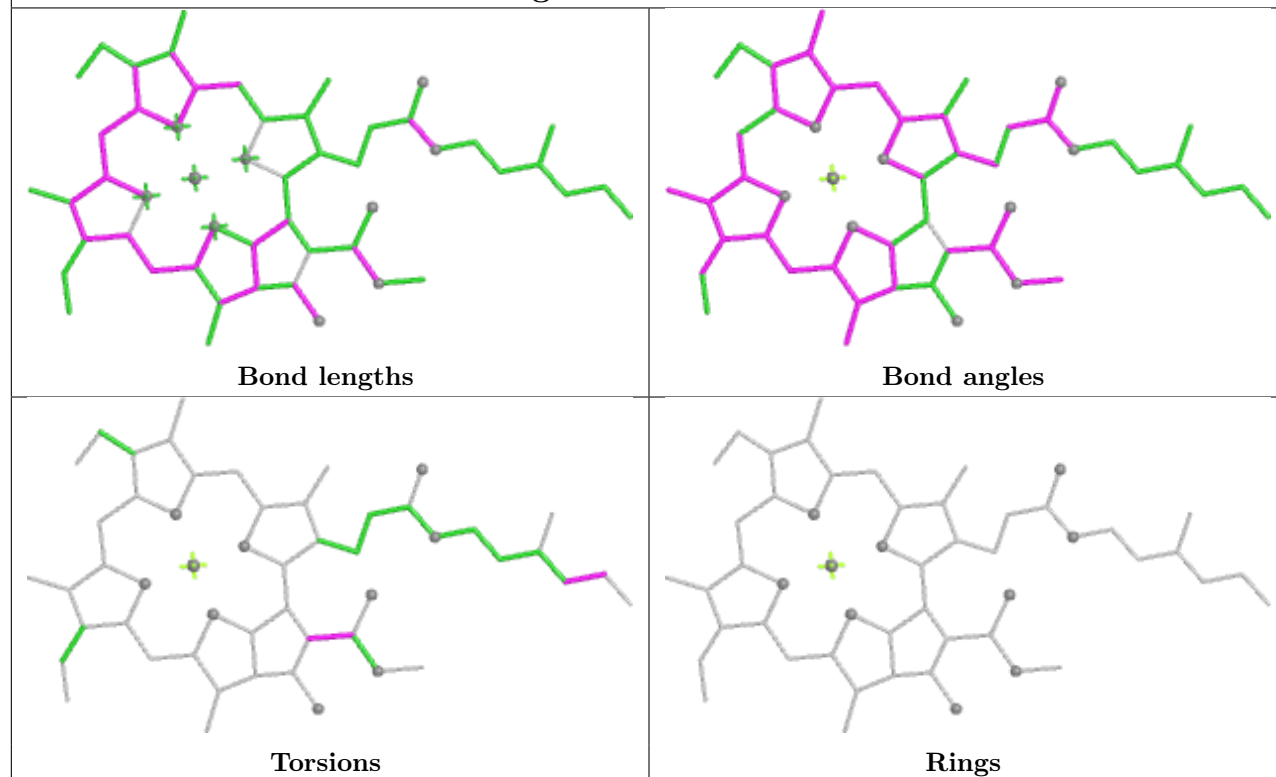


Rings

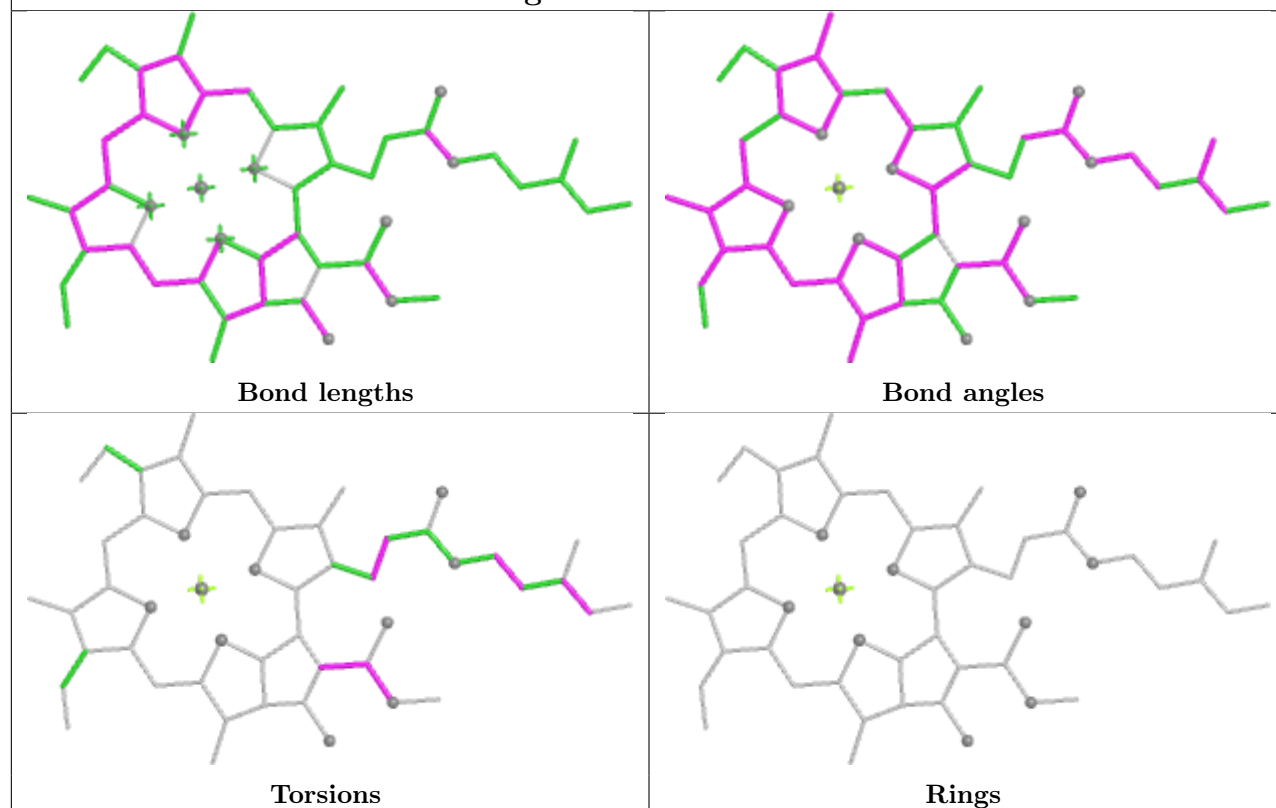


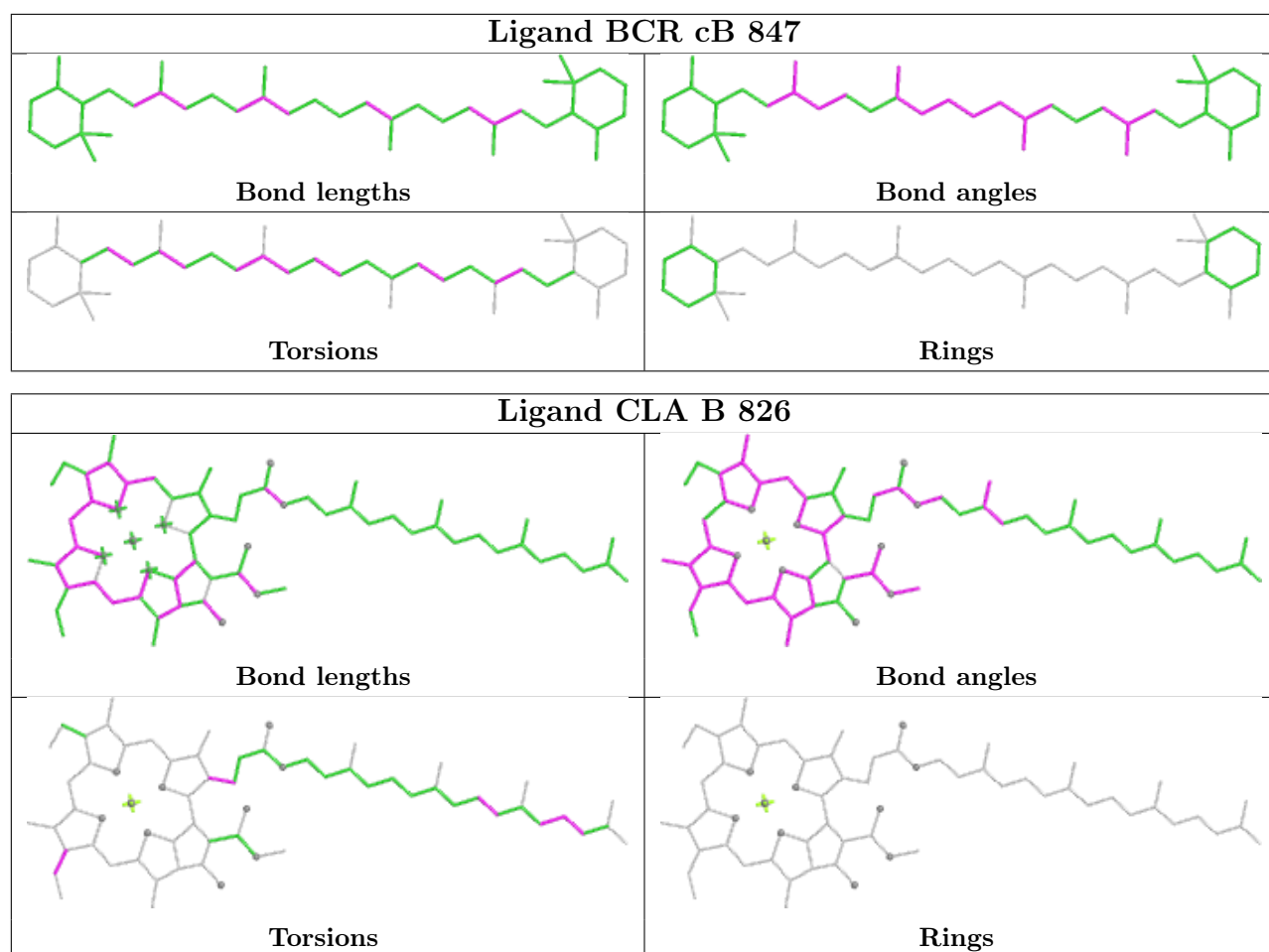


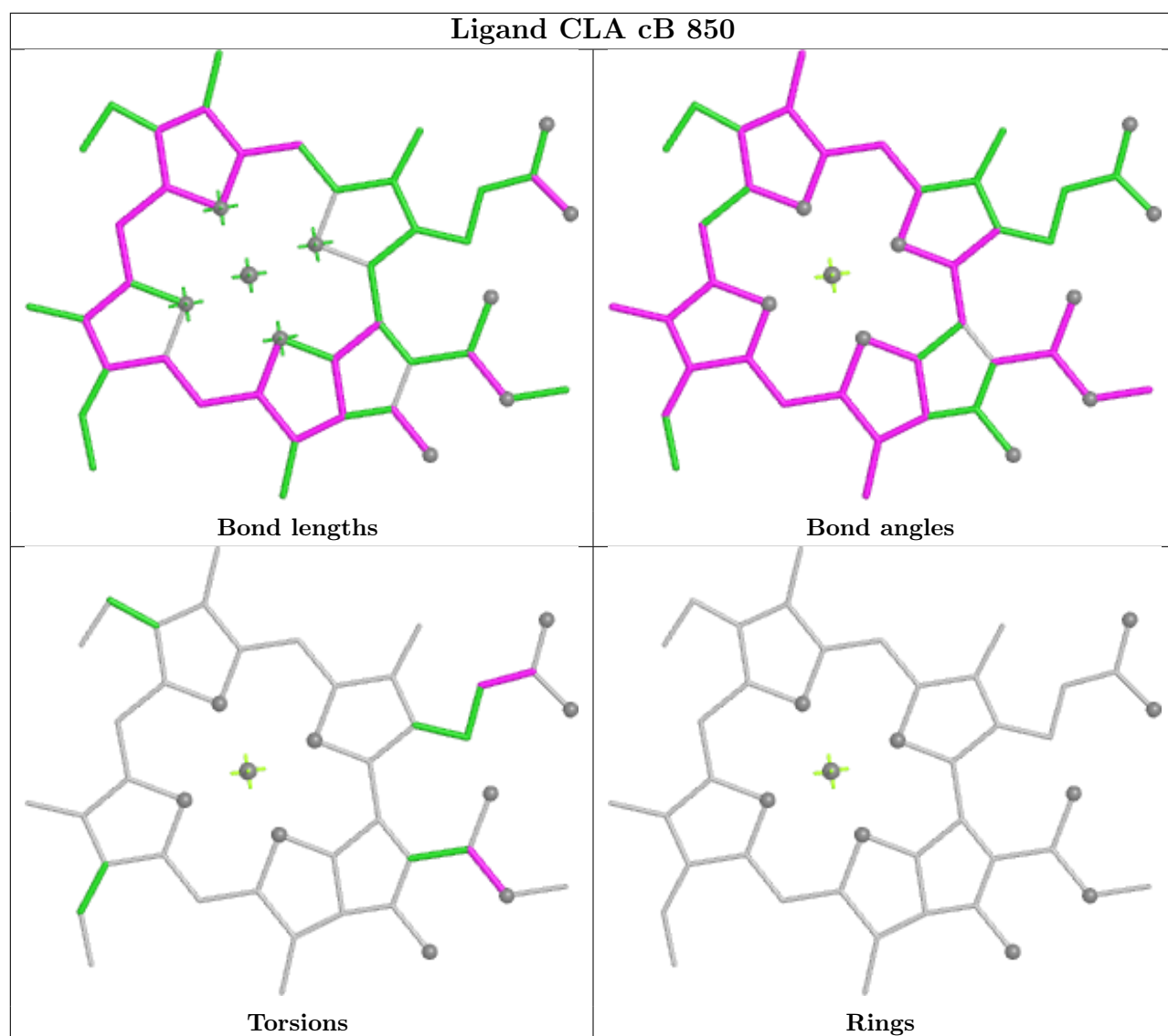
Ligand CLA B 808

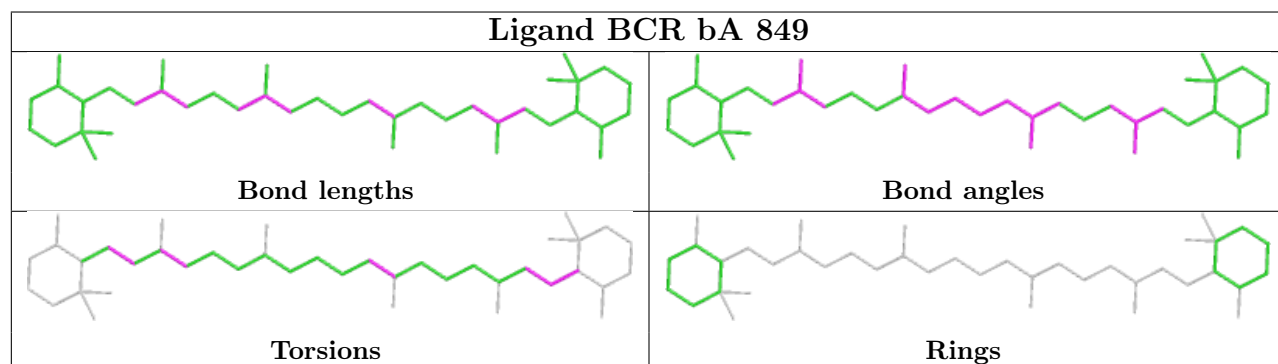
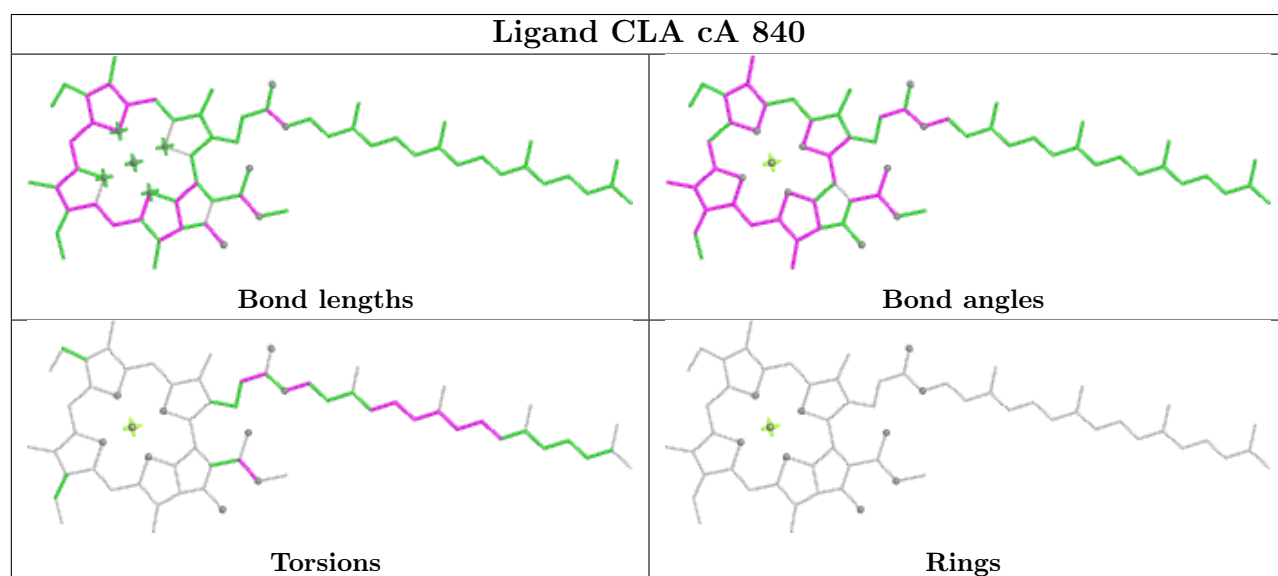
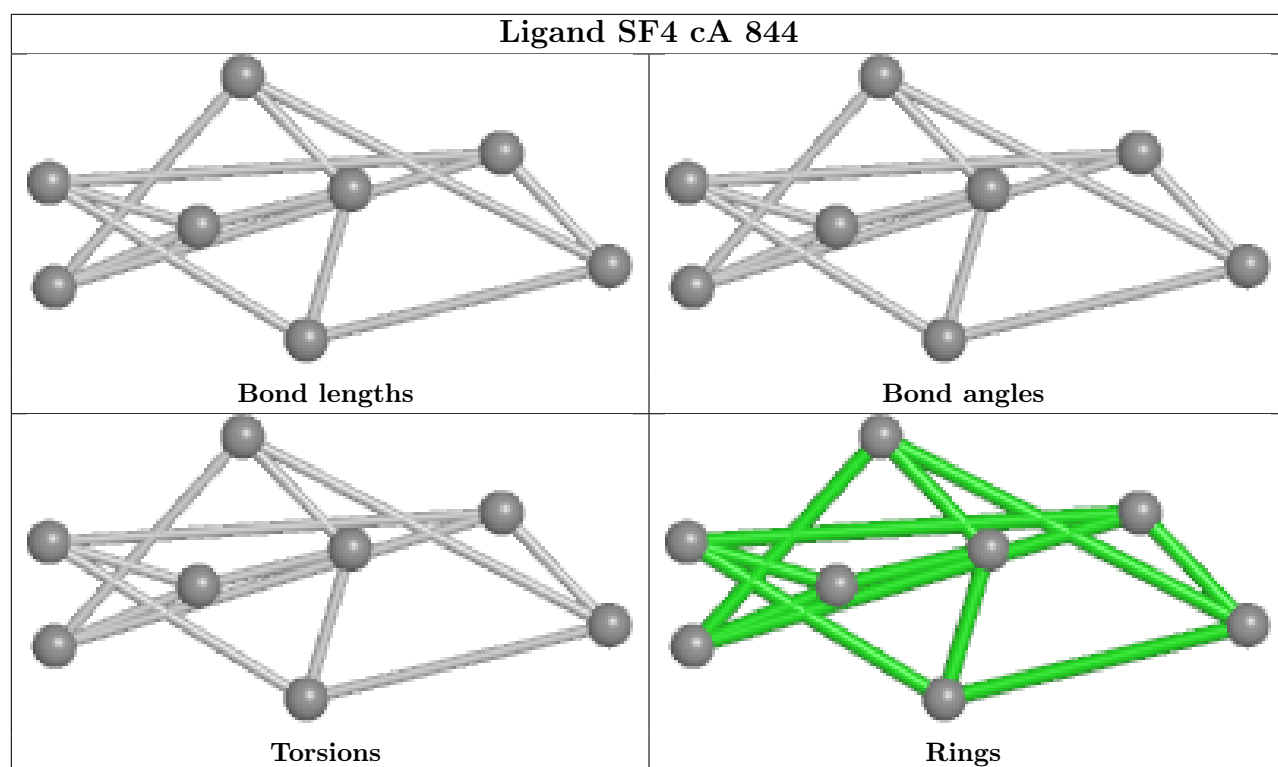


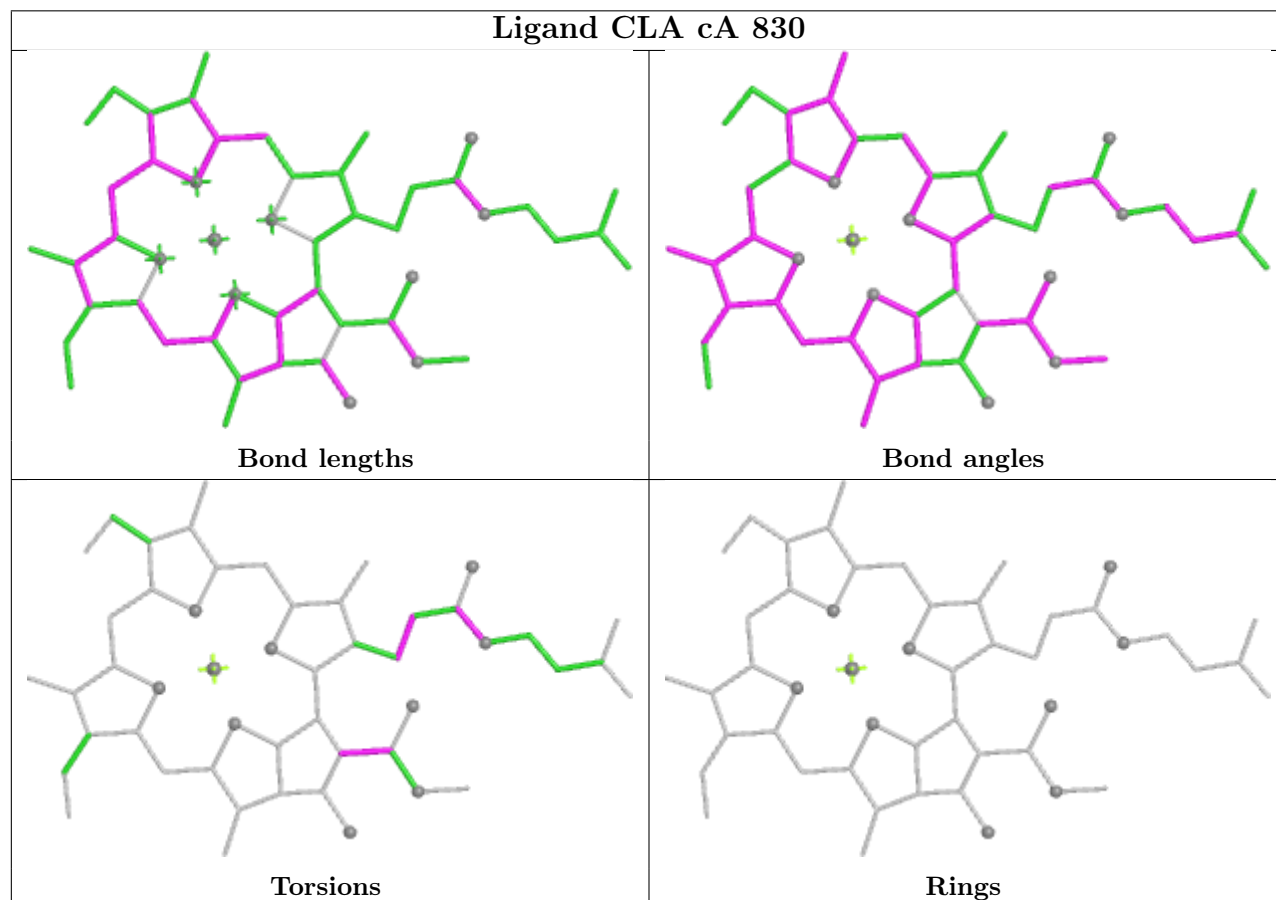
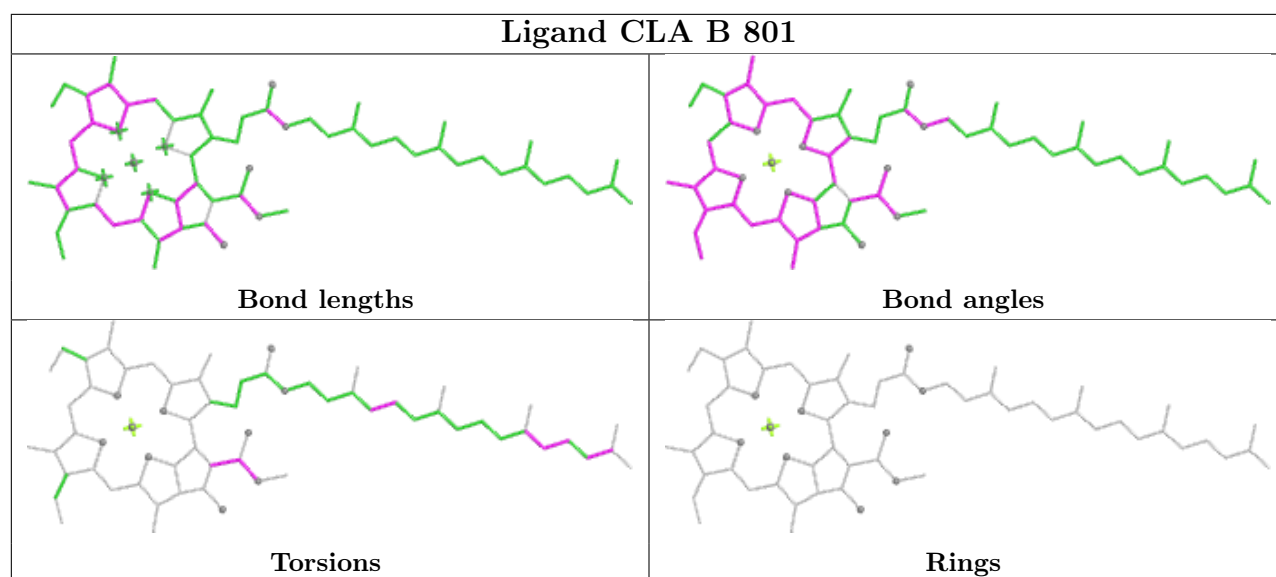
Ligand CLA cB 805

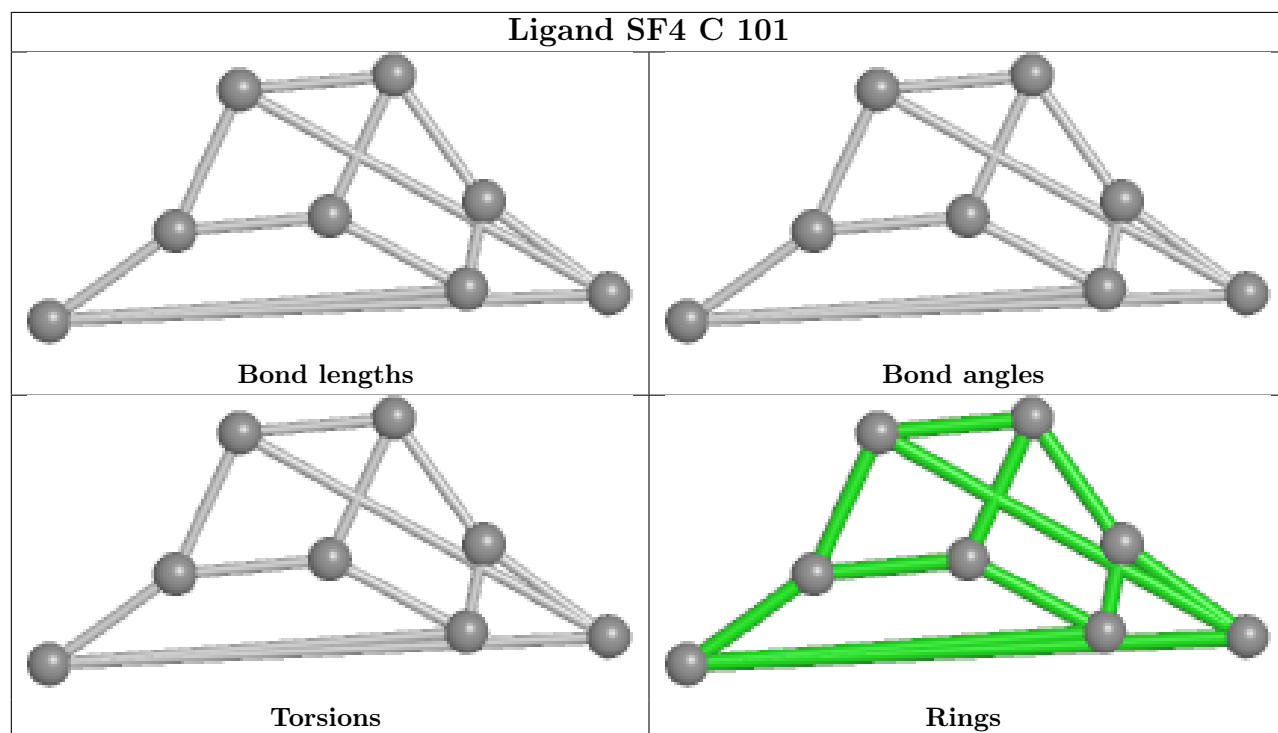
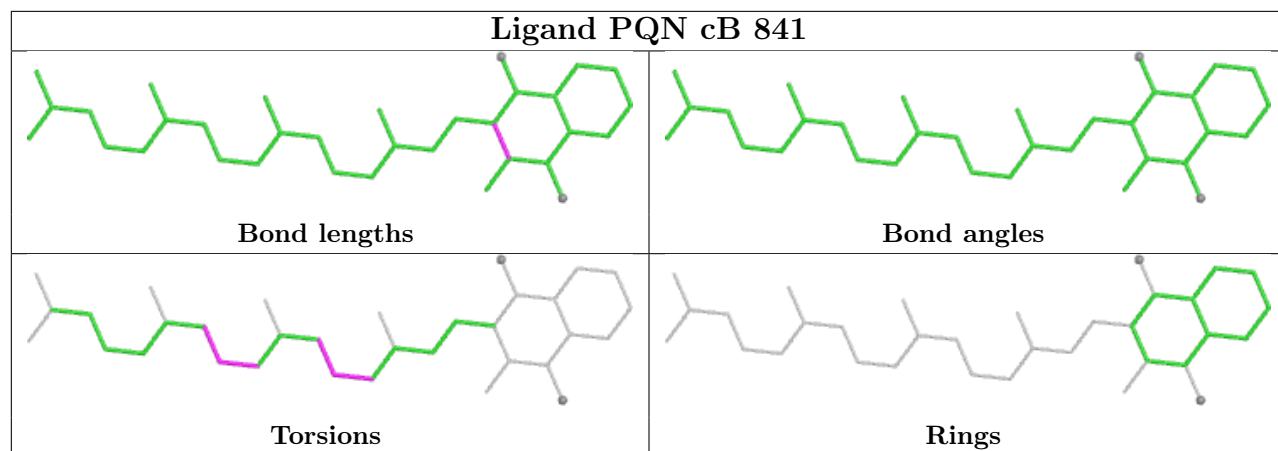


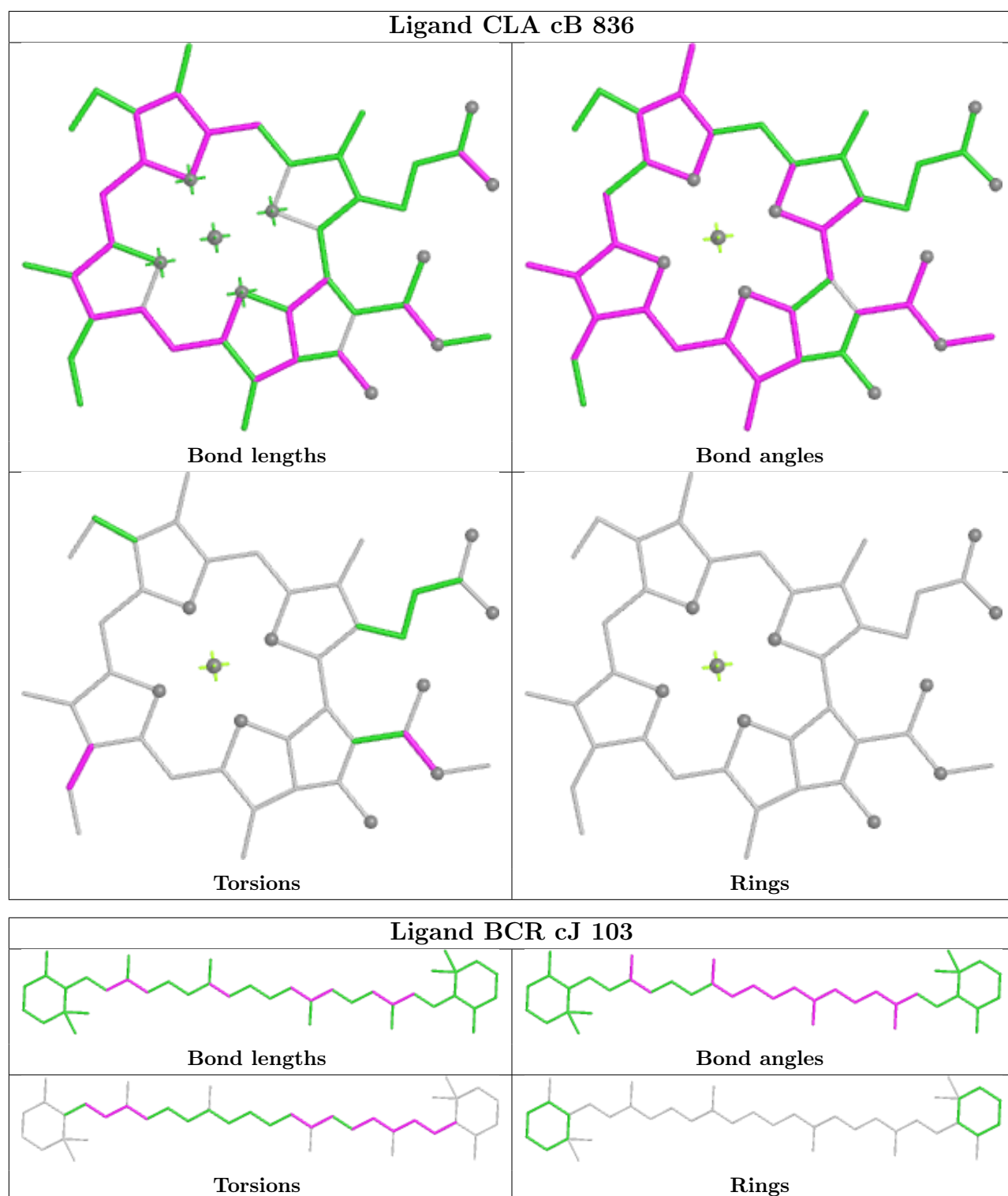


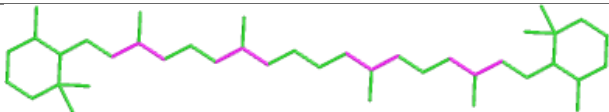
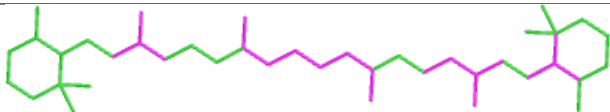
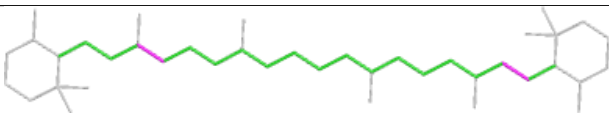
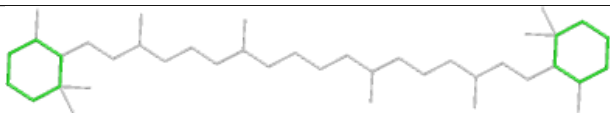


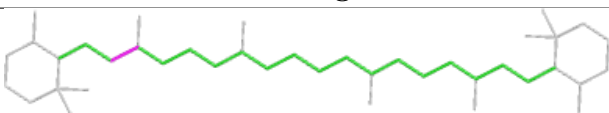
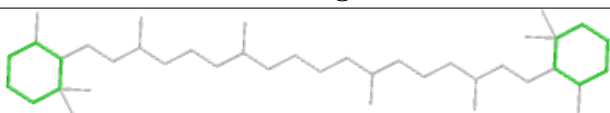




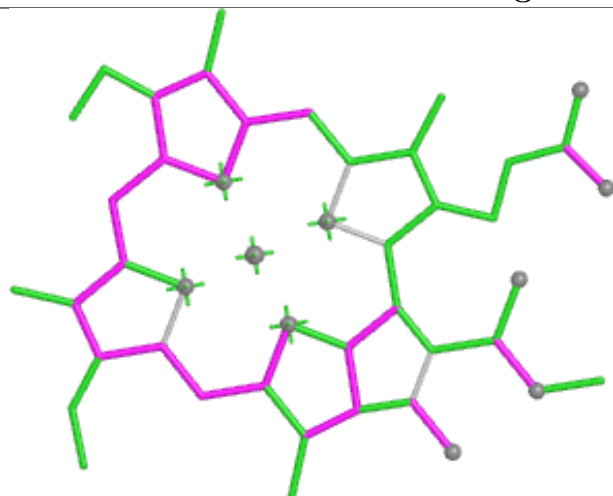




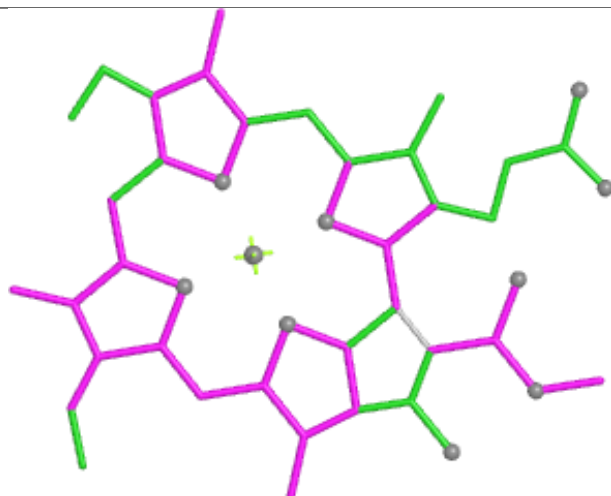
Ligand BCR A 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR cB 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

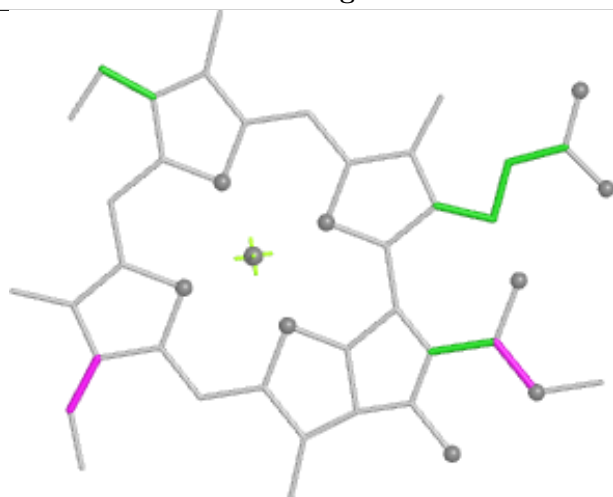
Ligand CLA B 835



Bond lengths



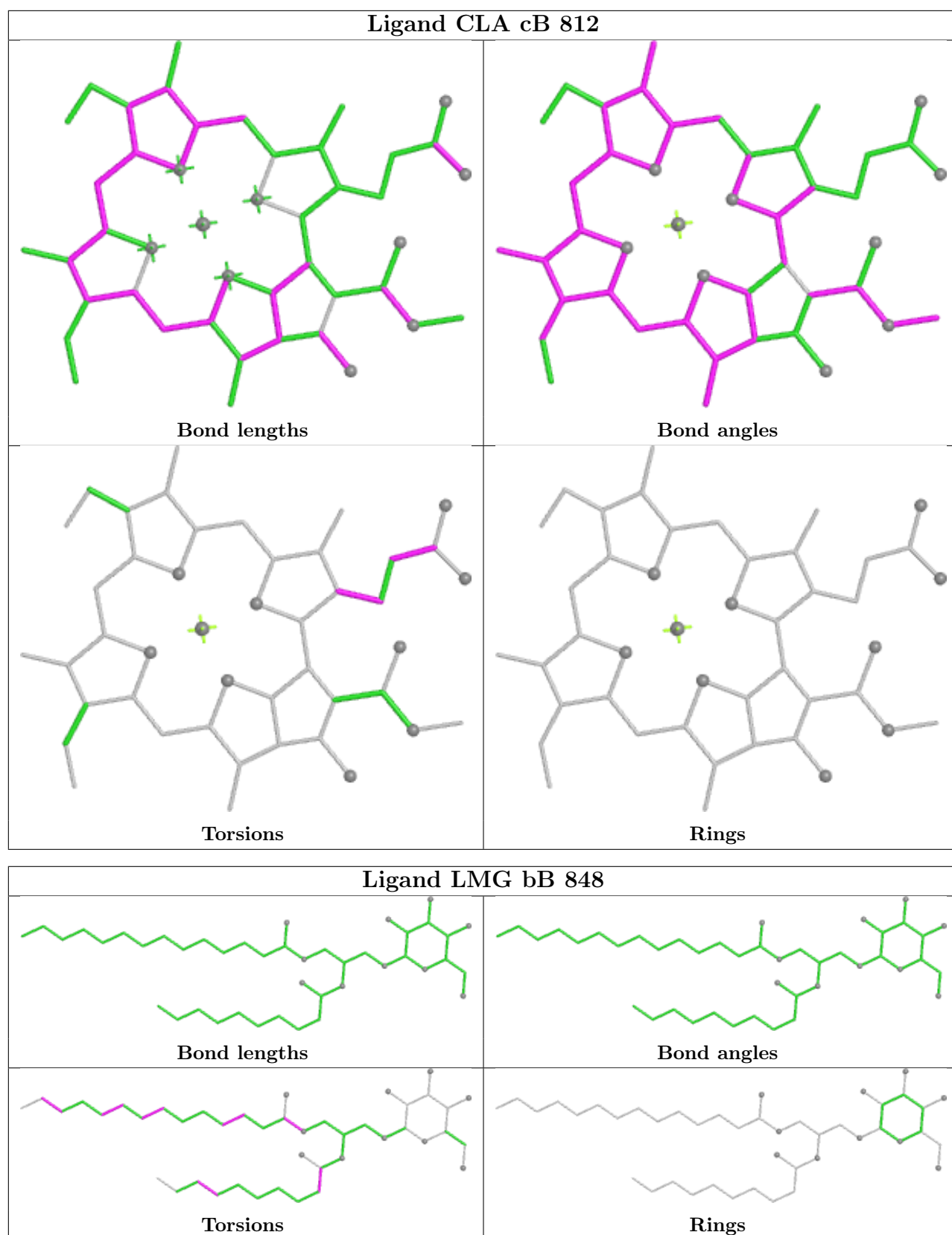
Bond angles

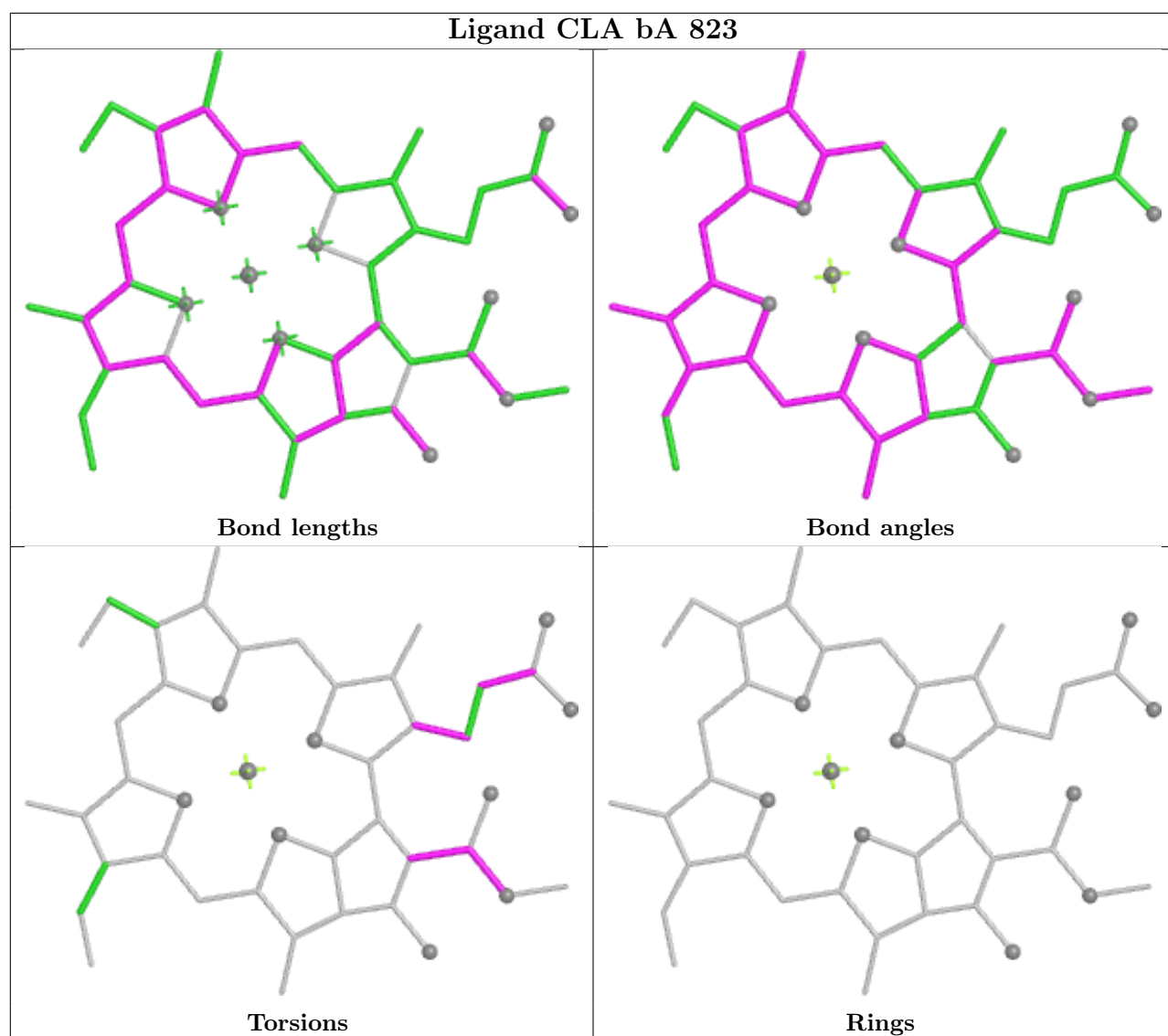


Torsions

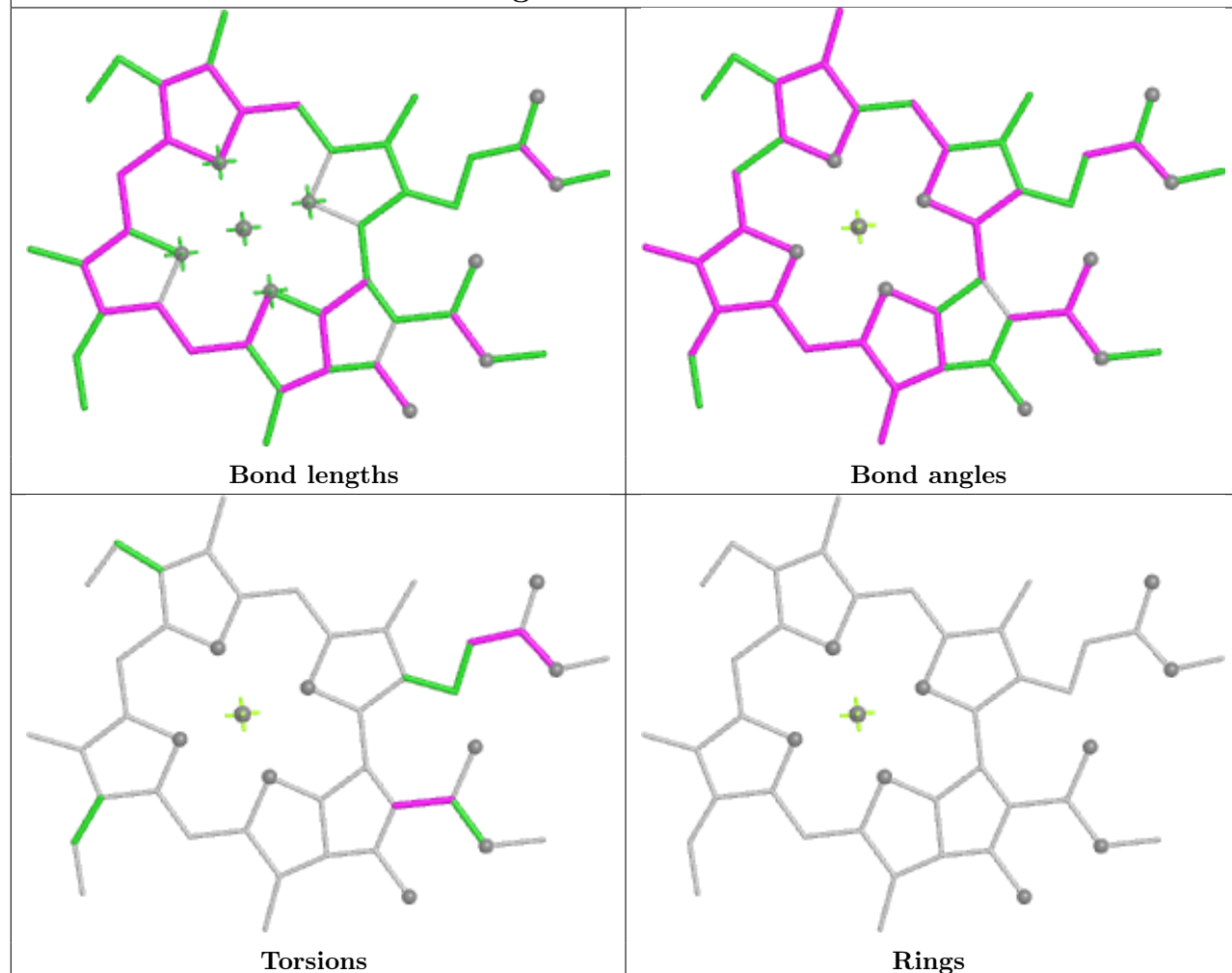


Rings

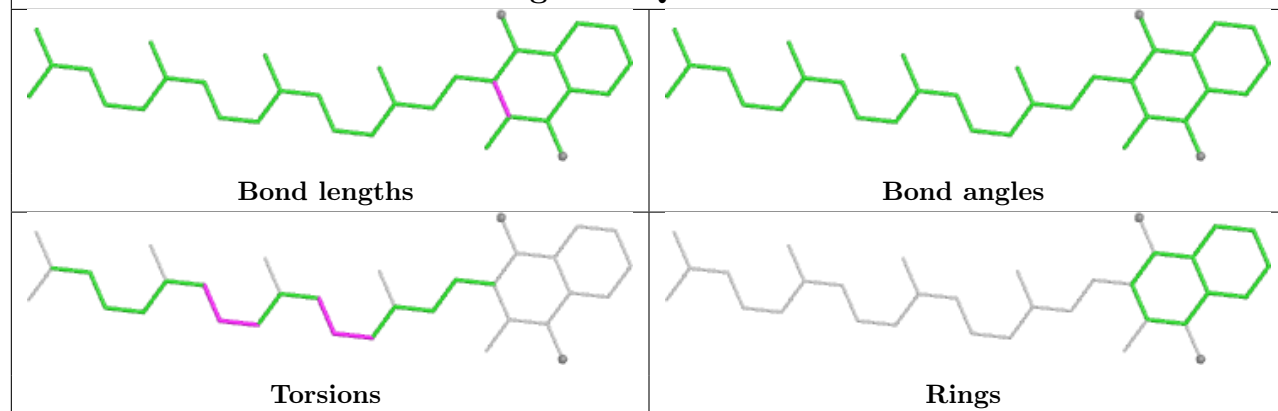


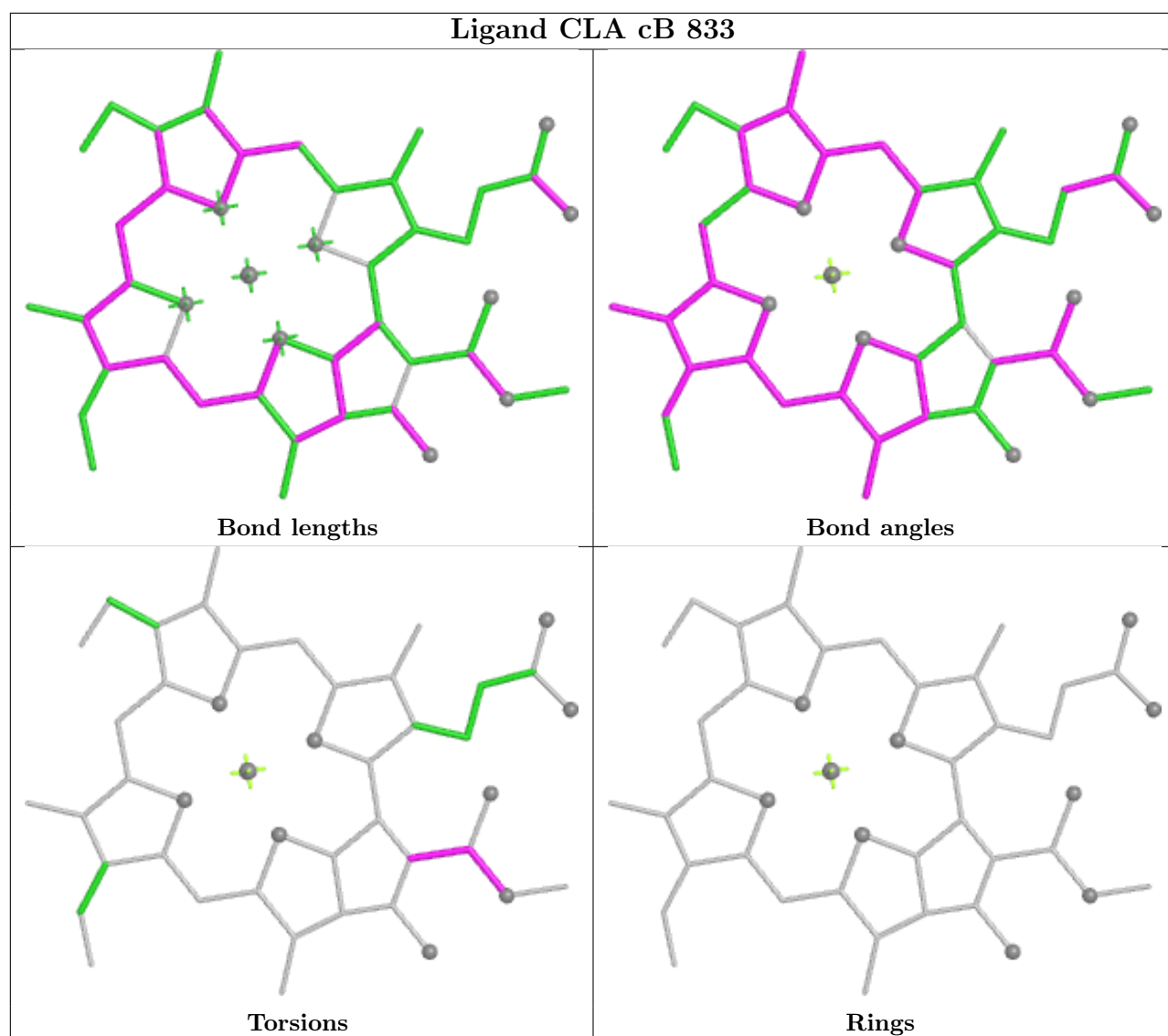


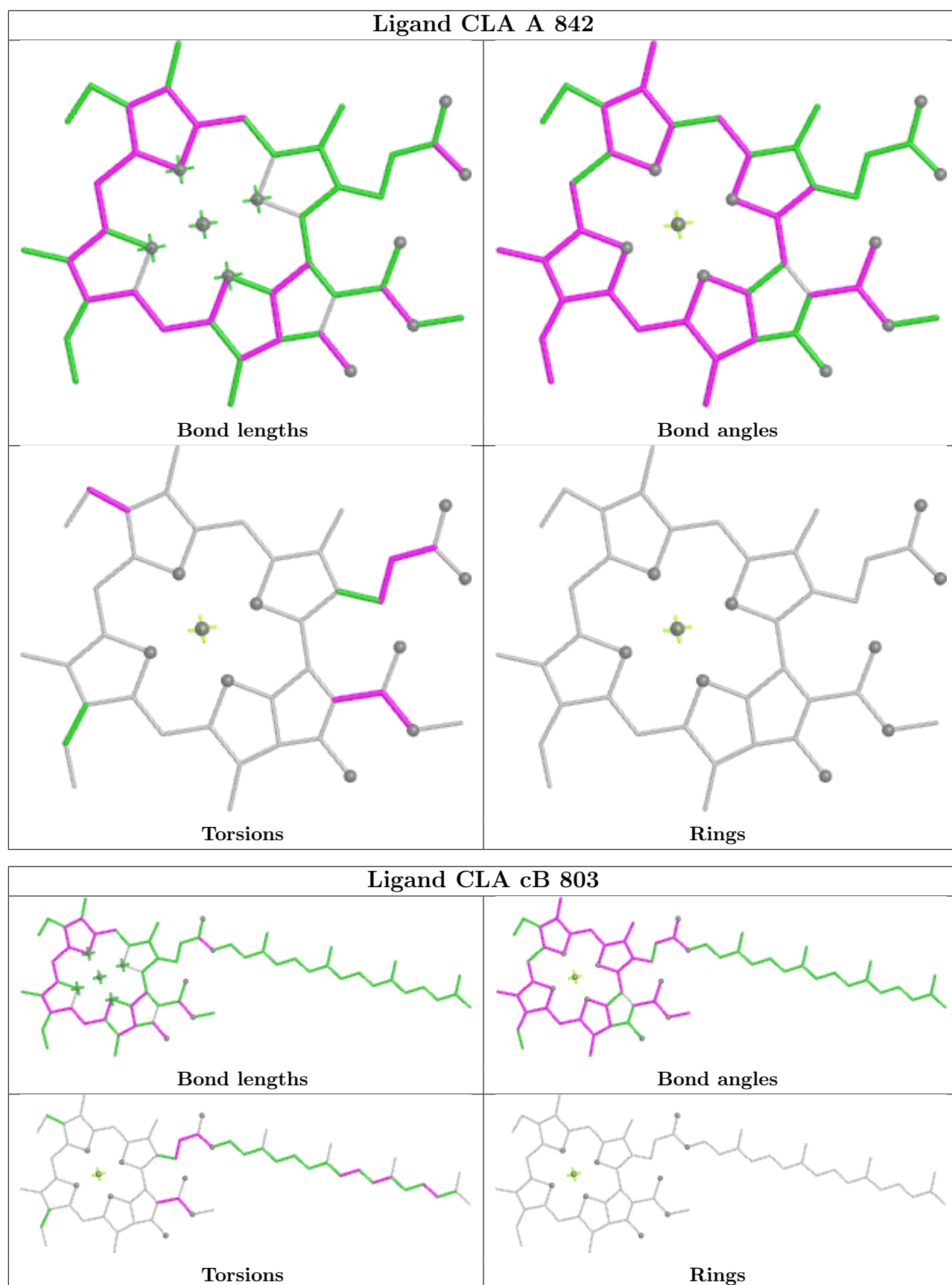
Ligand CLA A 826

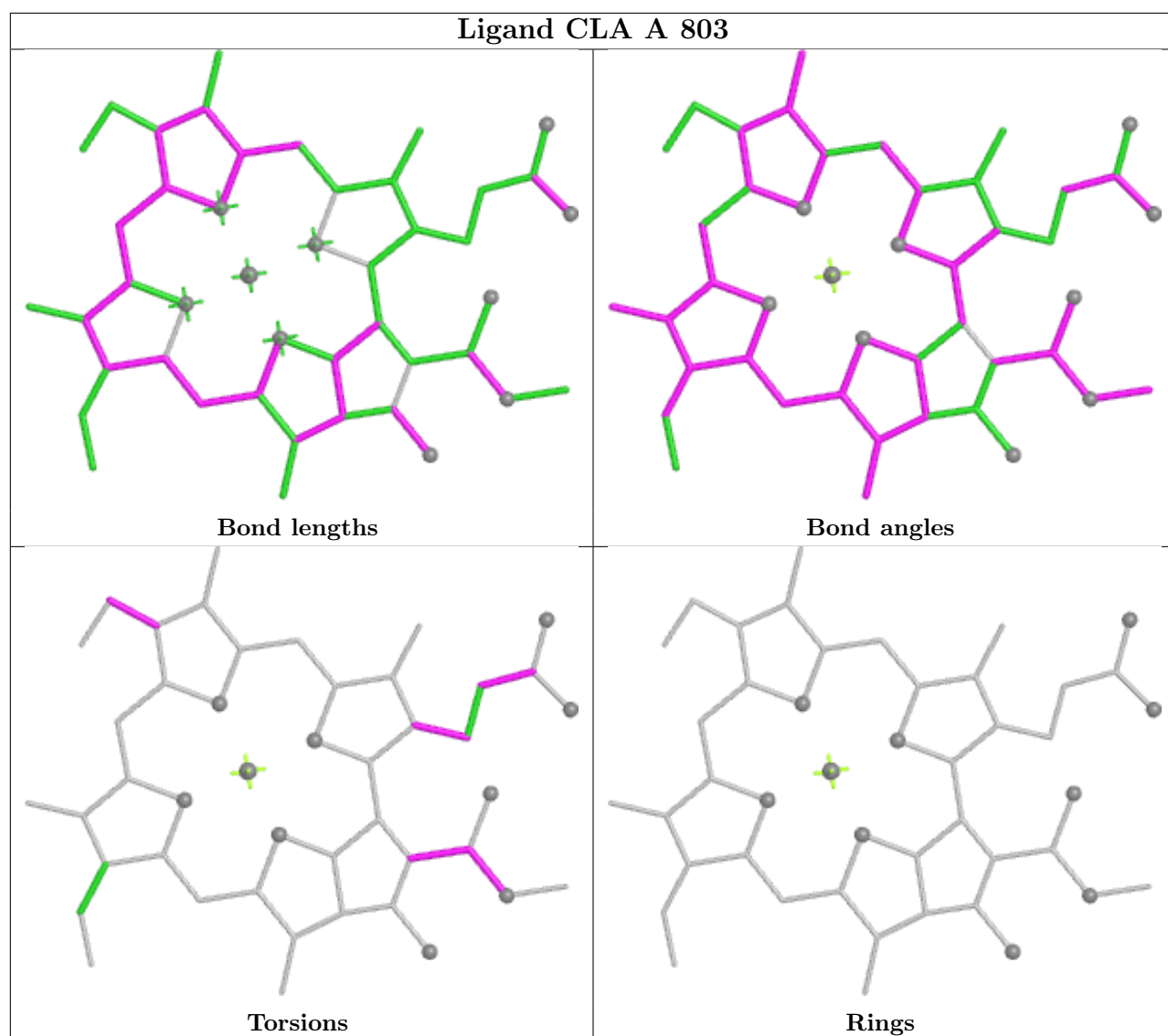


Ligand PQN B 840

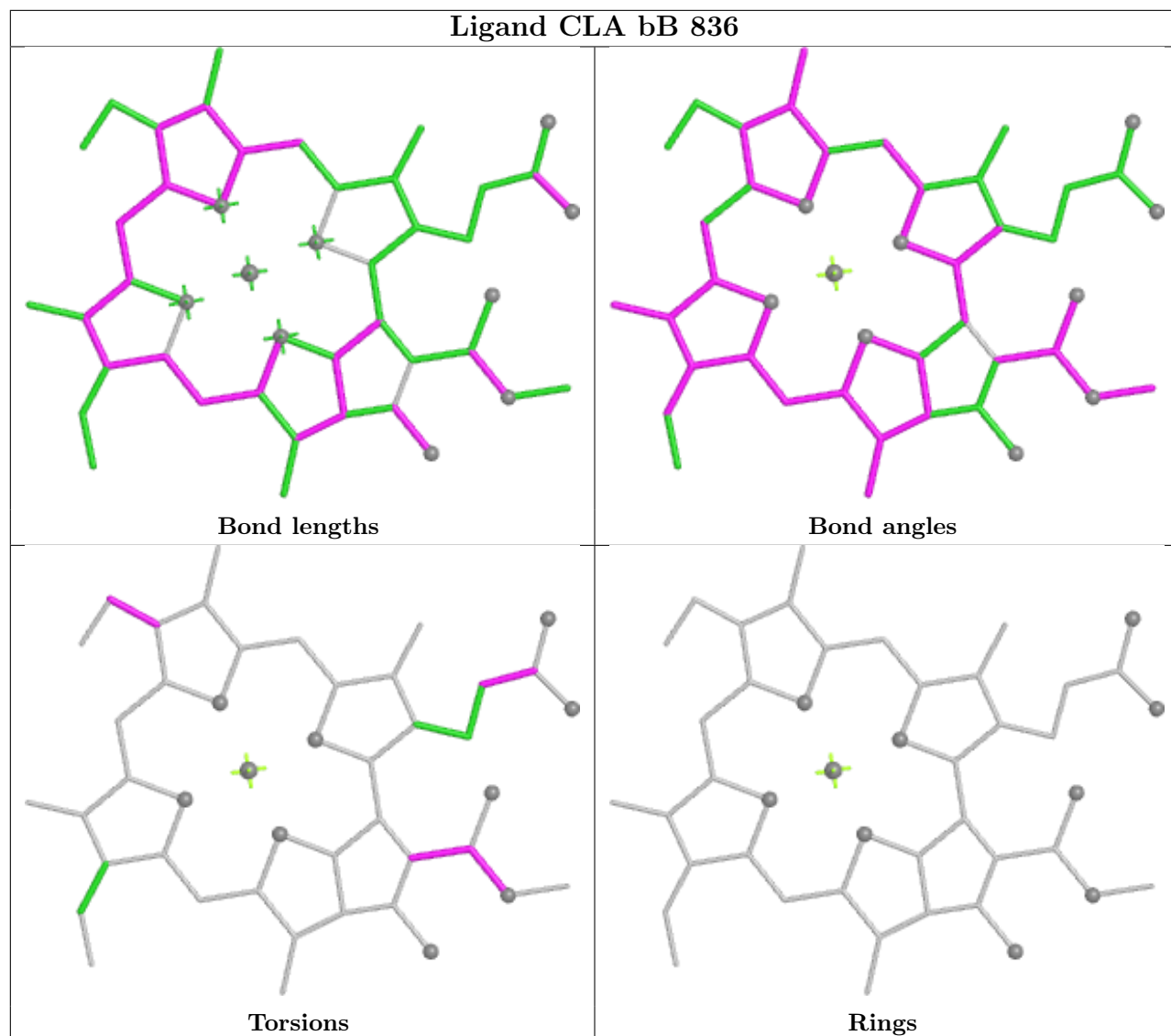


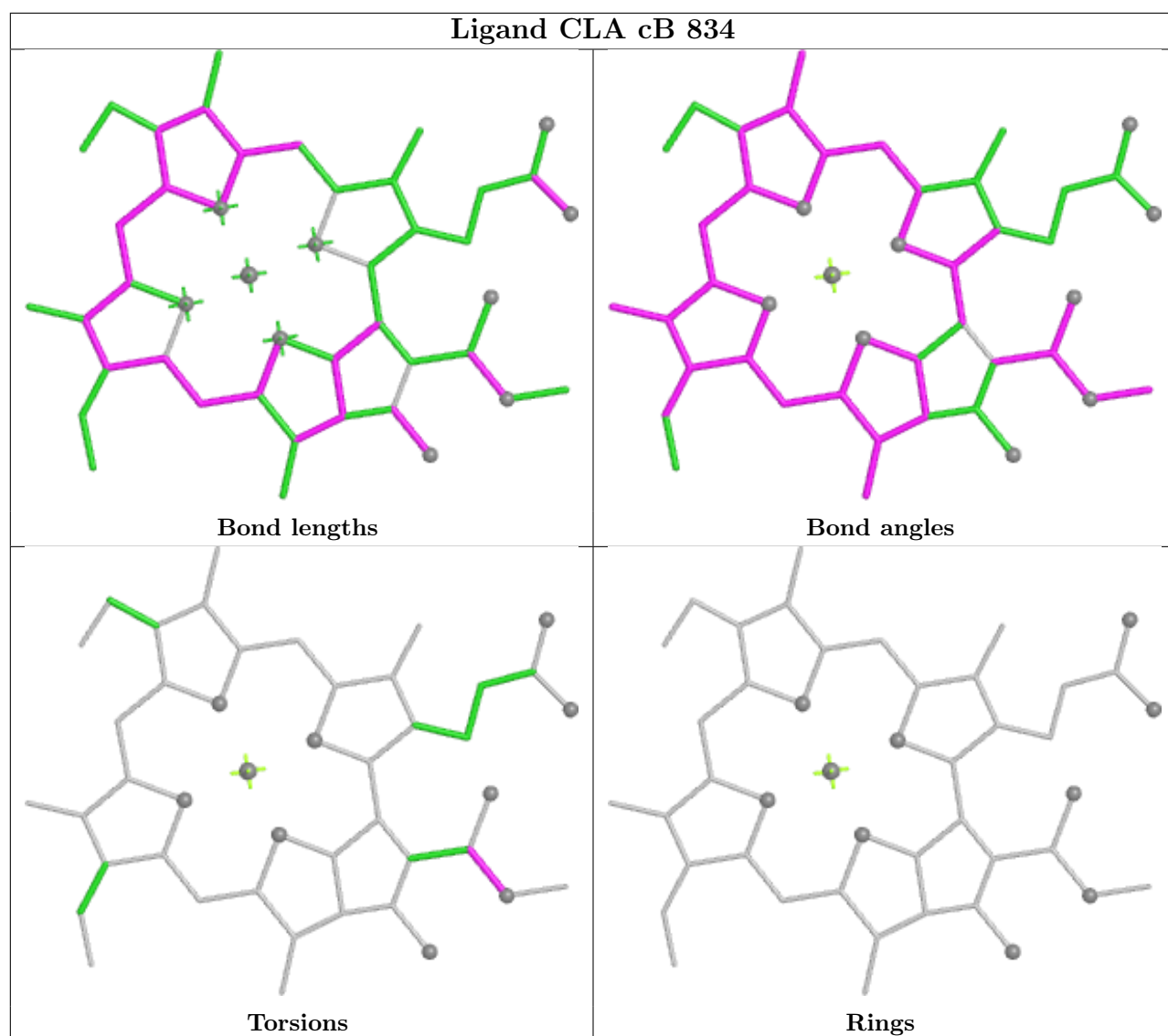


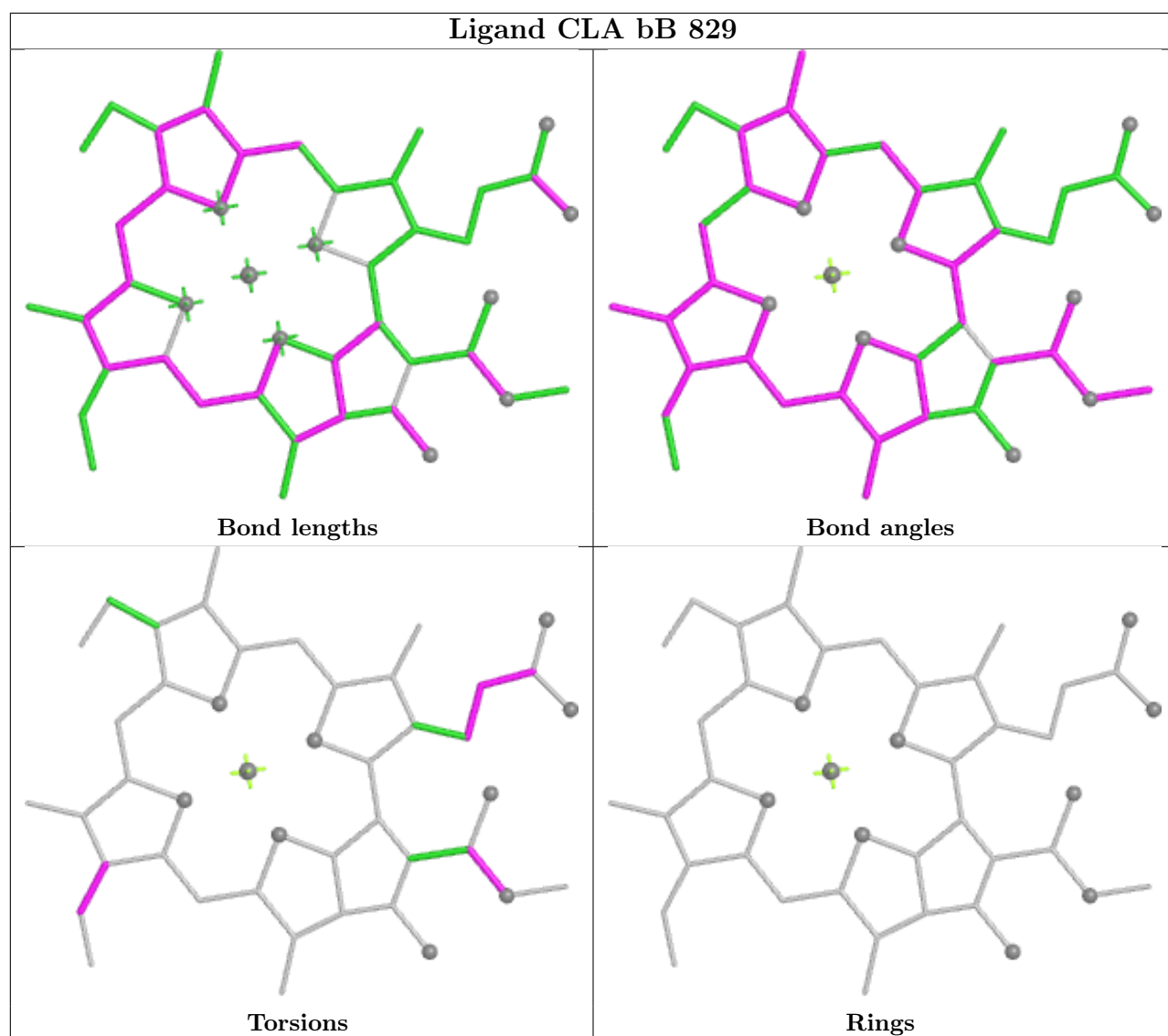


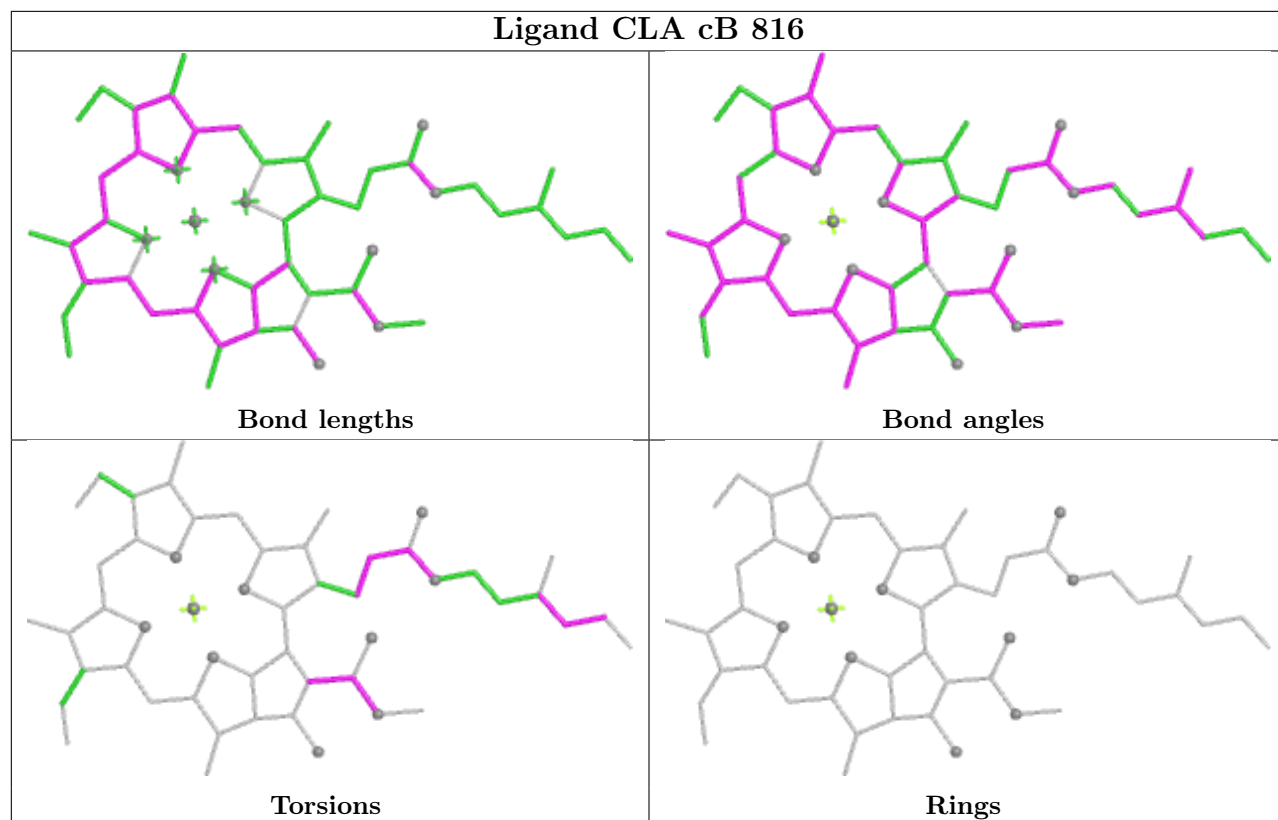


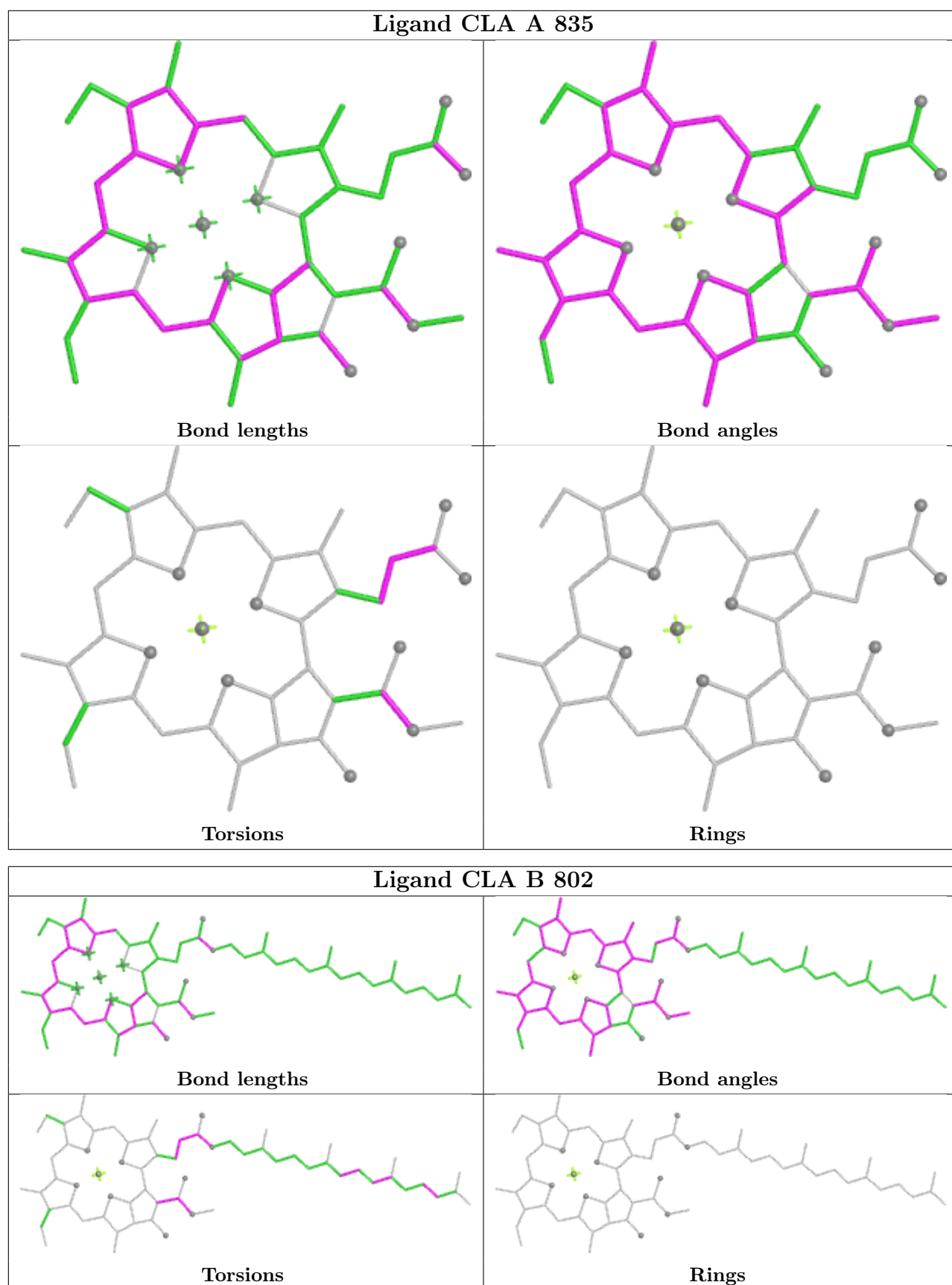
Ligand CLA bB 836

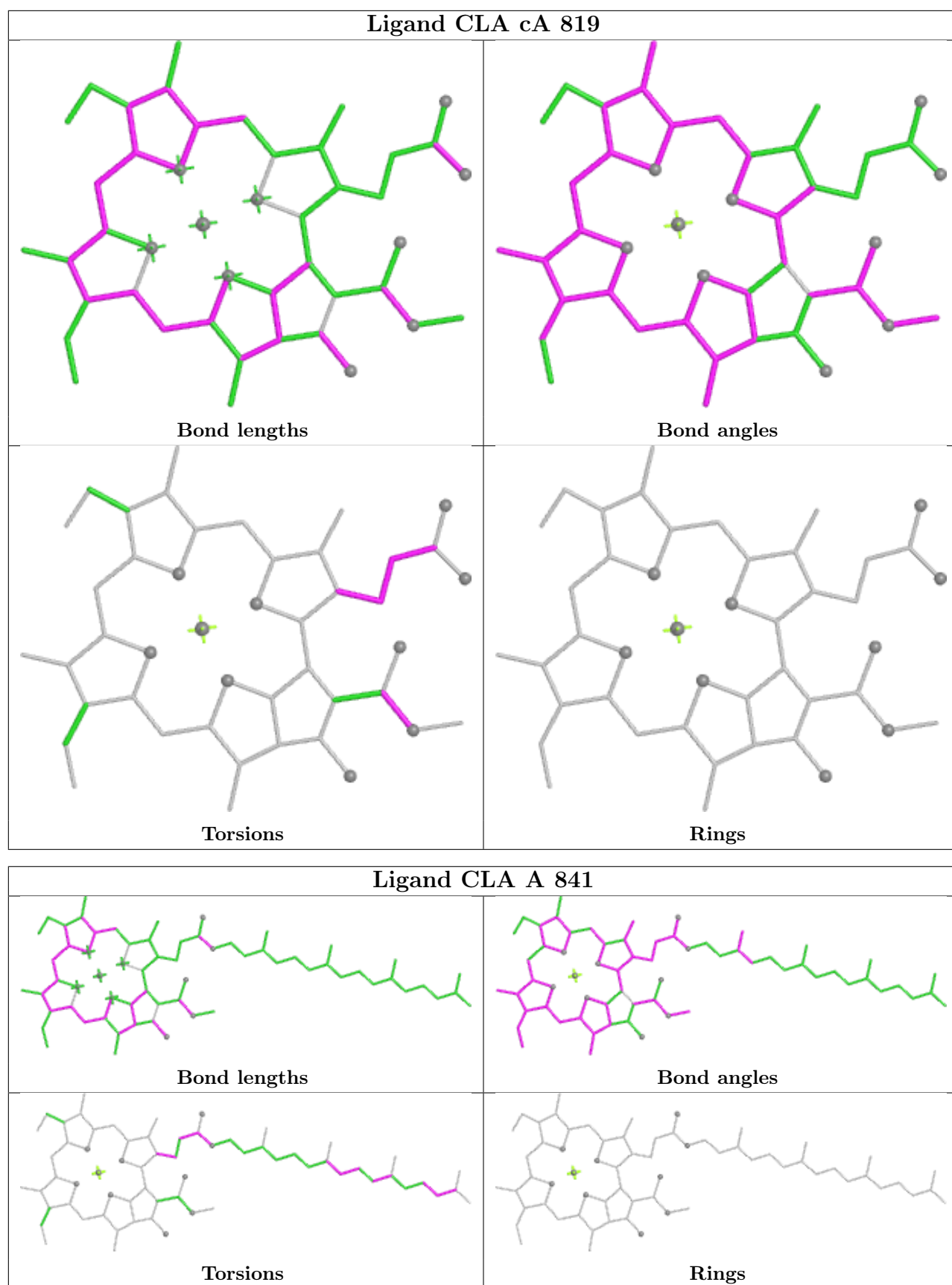


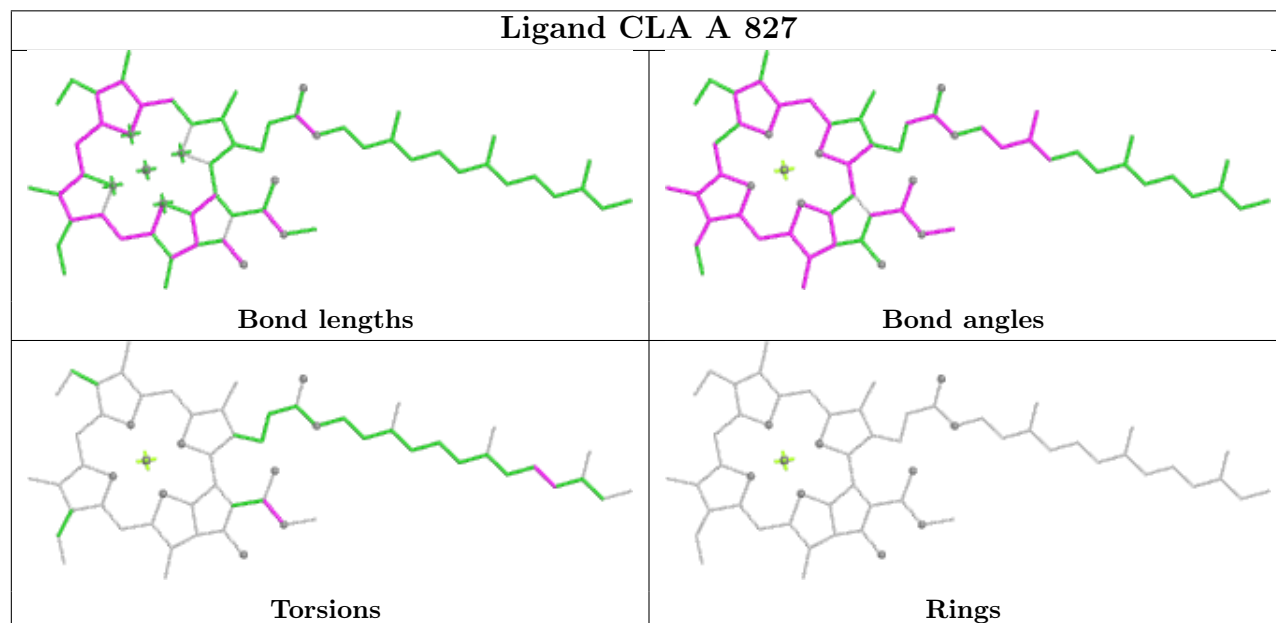
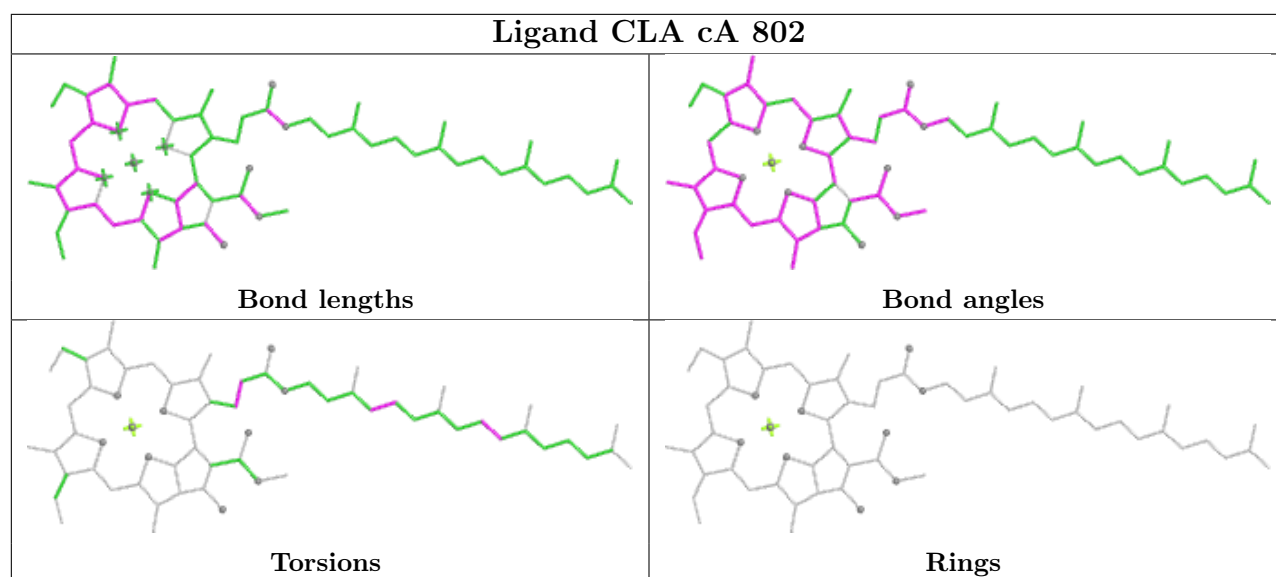




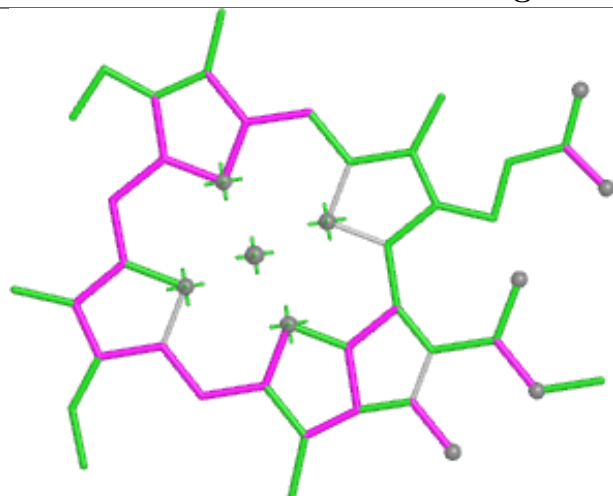




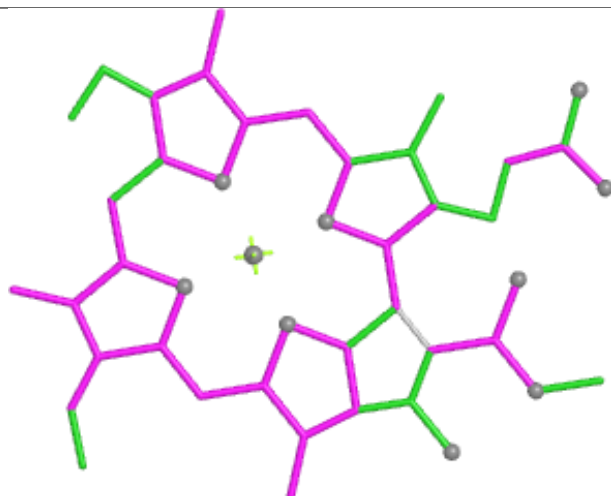




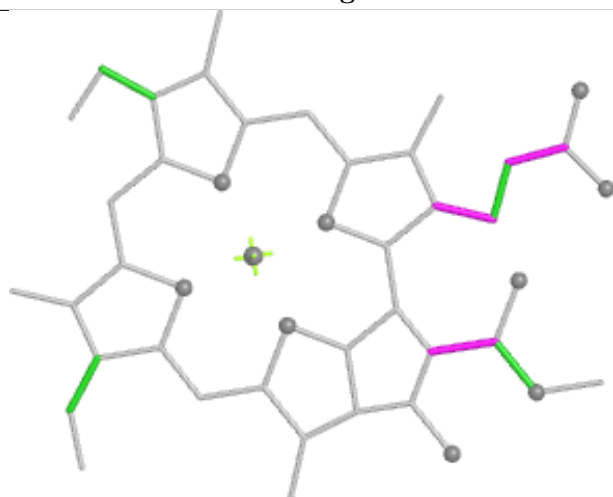
Ligand CLA A 838



Bond lengths



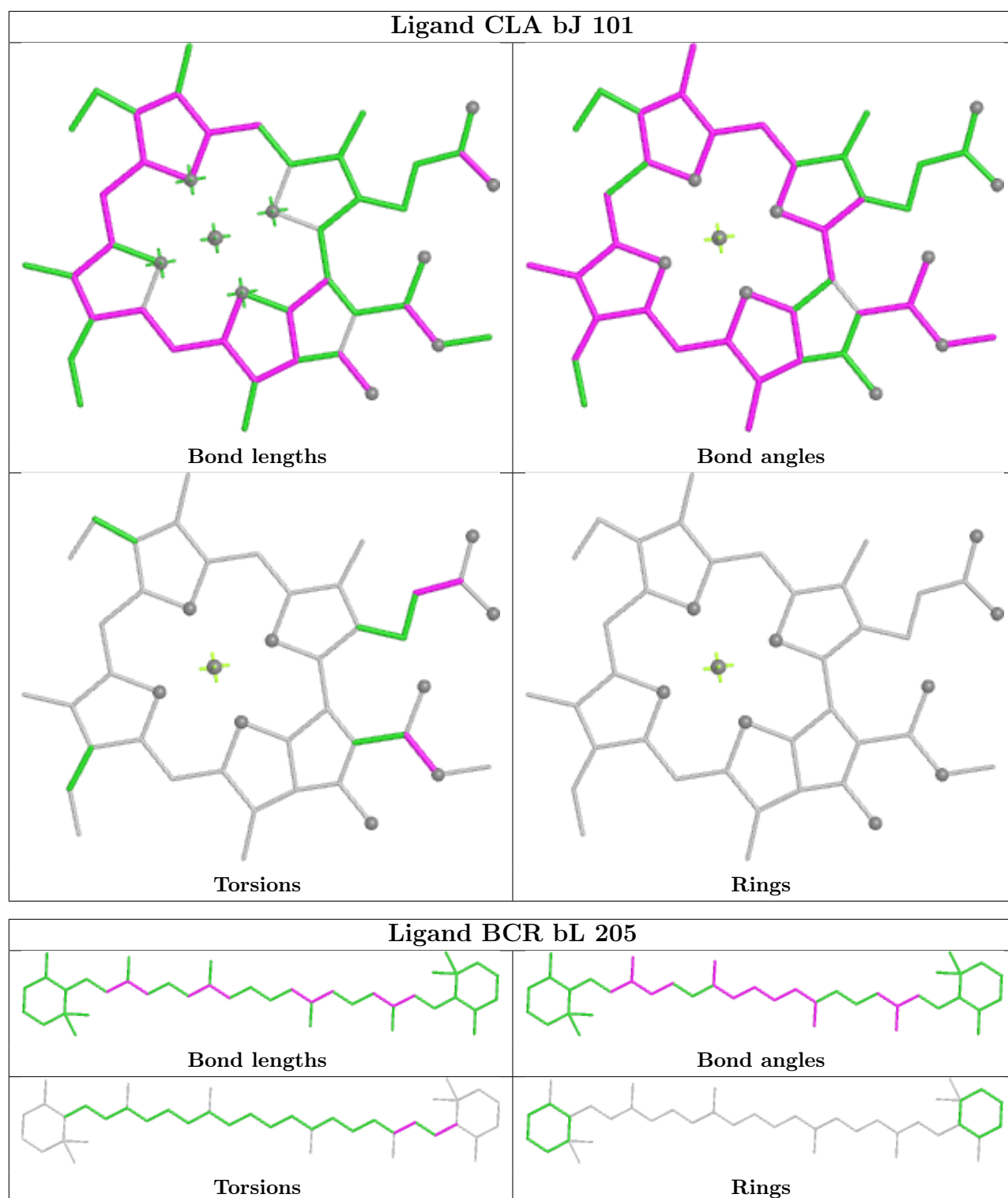
Bond angles

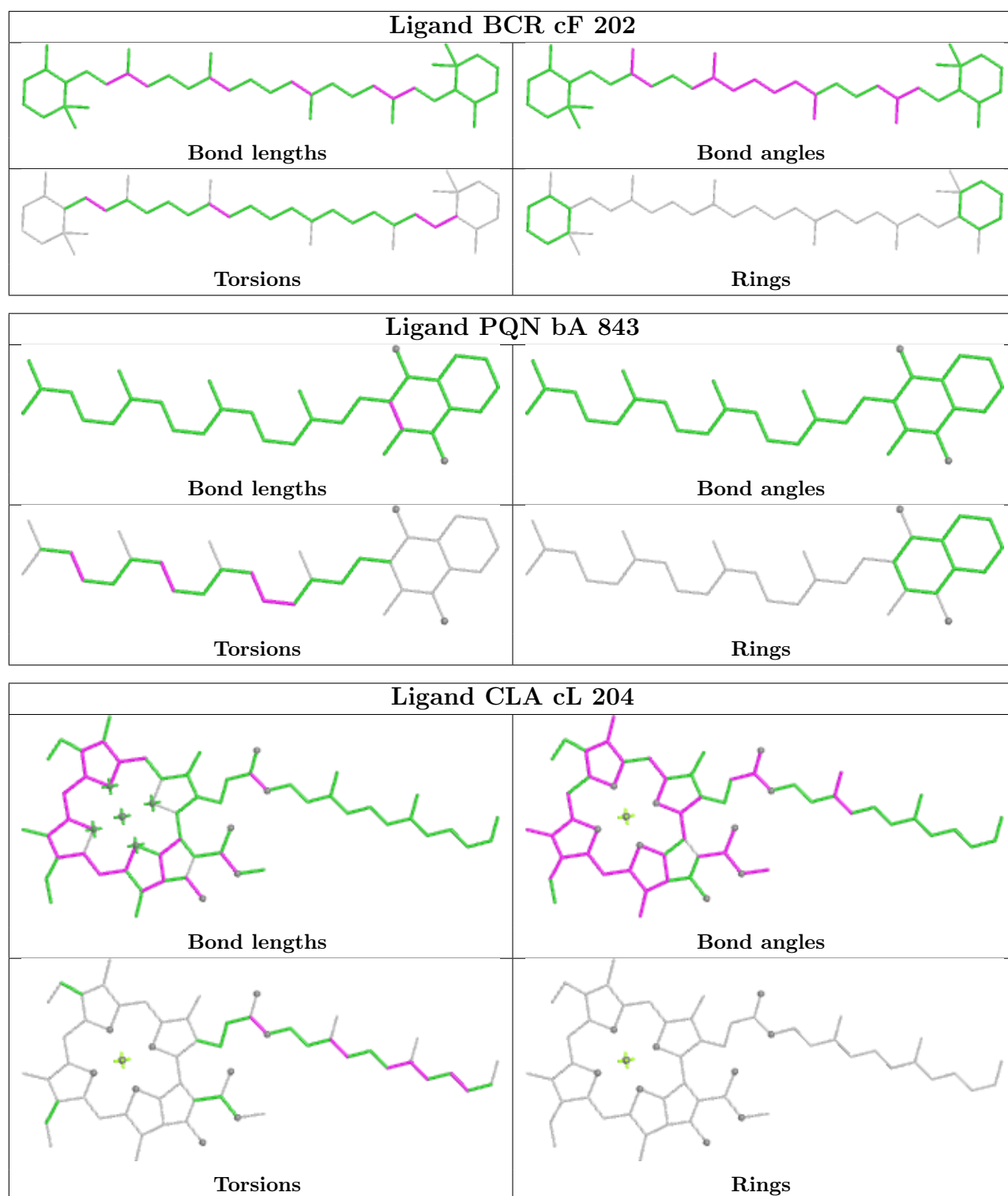


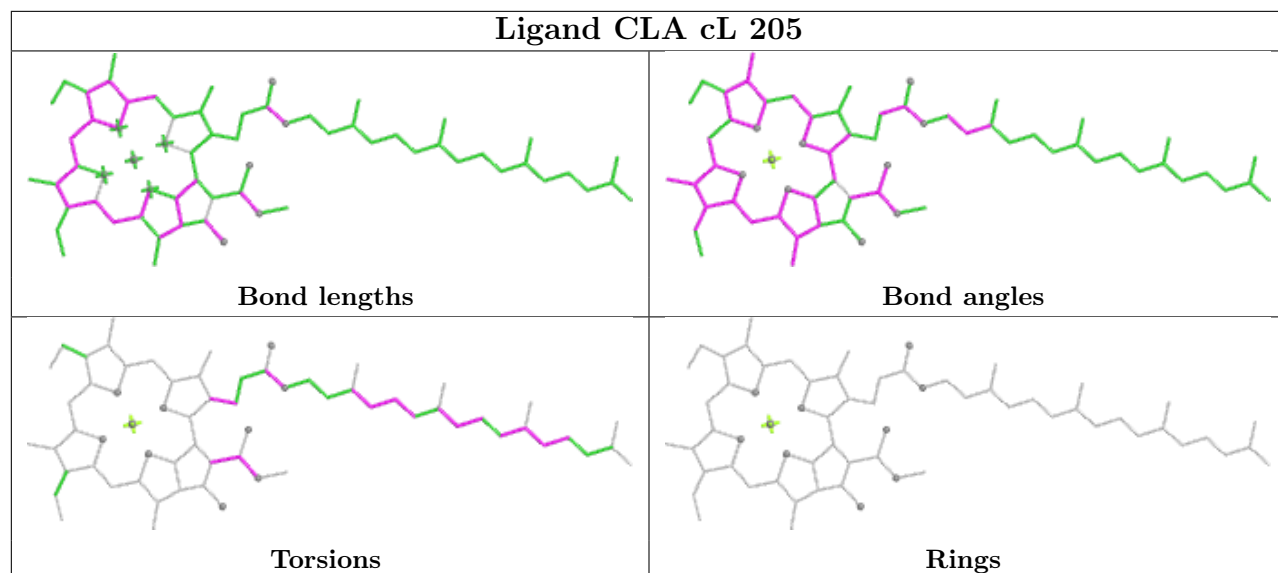
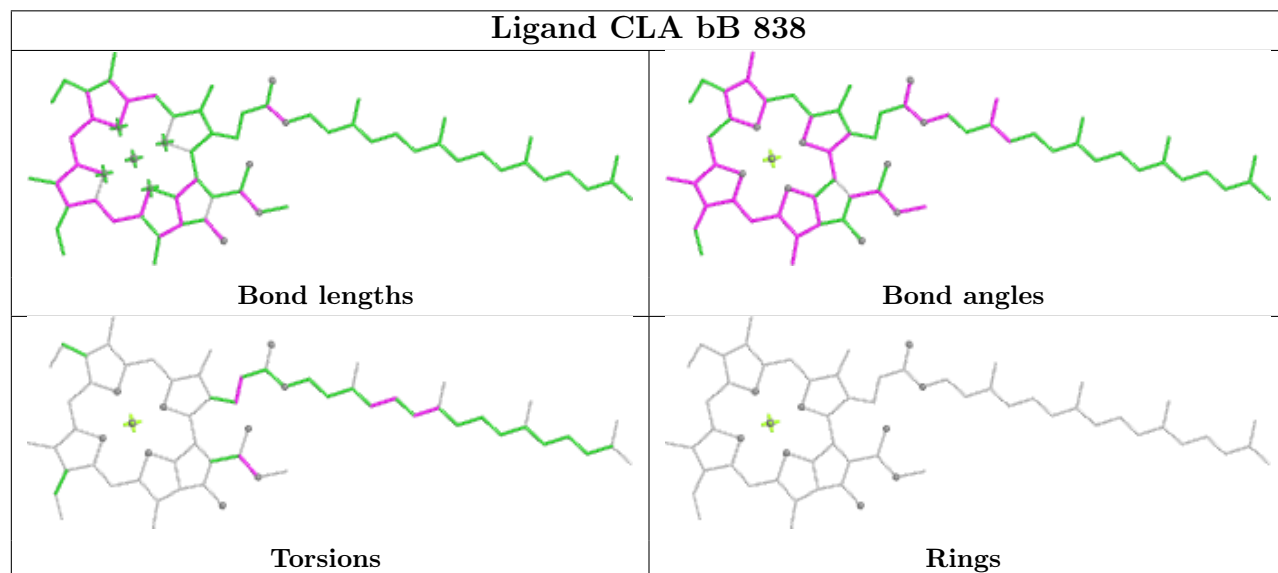
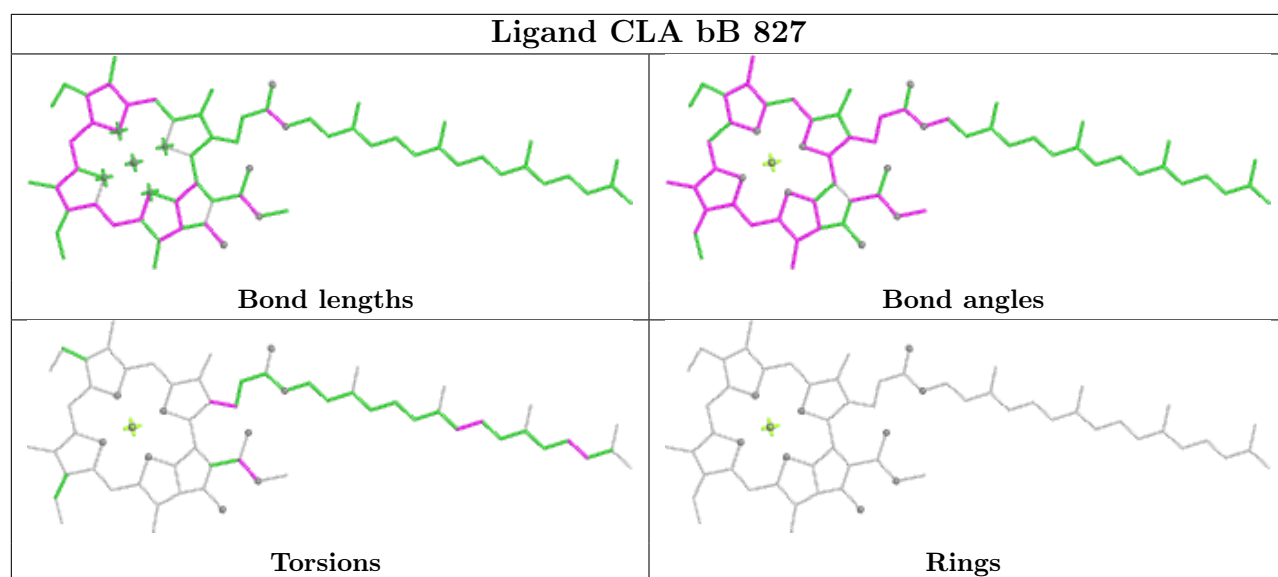
Torsions

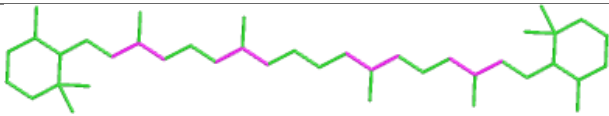
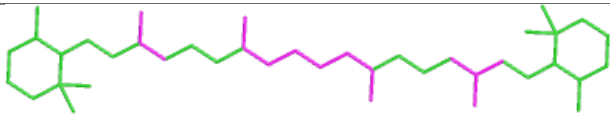
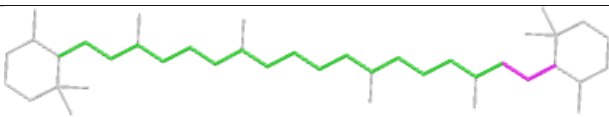
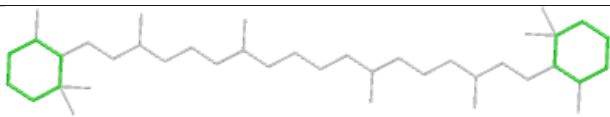


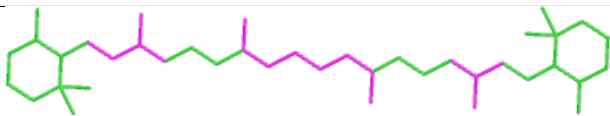
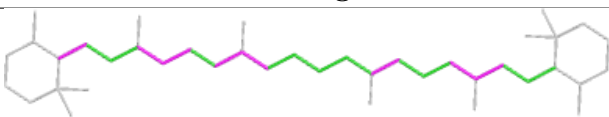
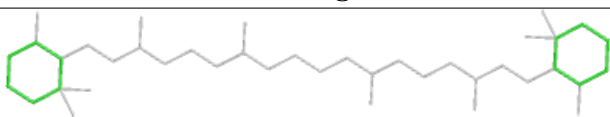
Rings

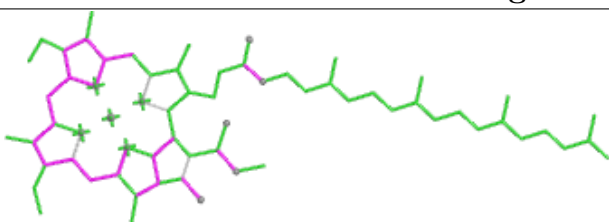
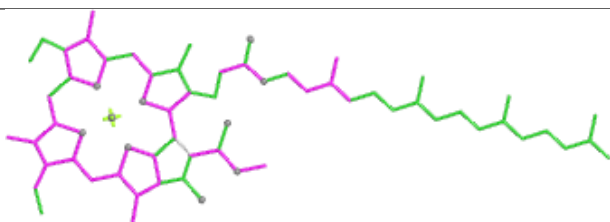
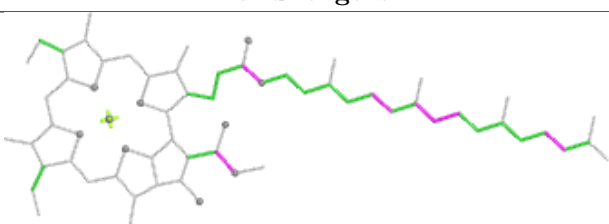
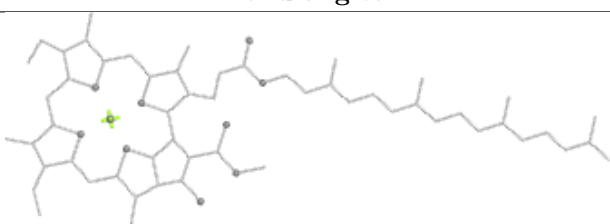


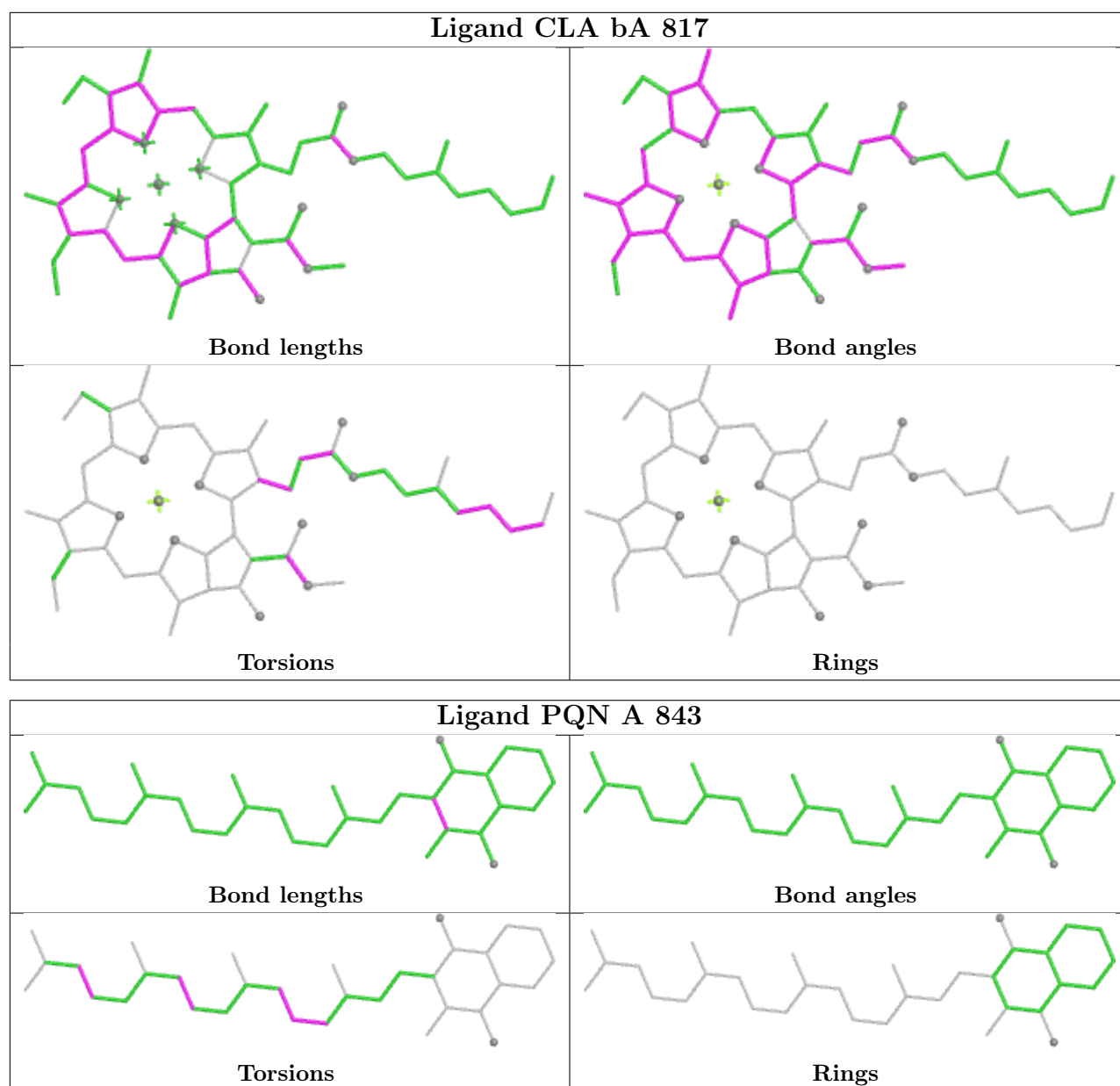




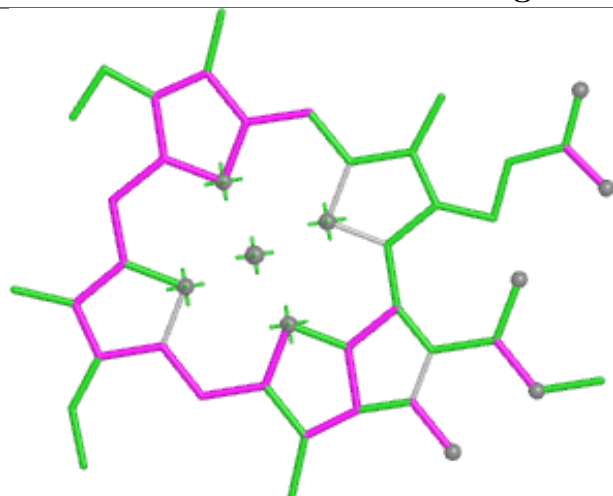
Ligand BCR L 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR cB 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

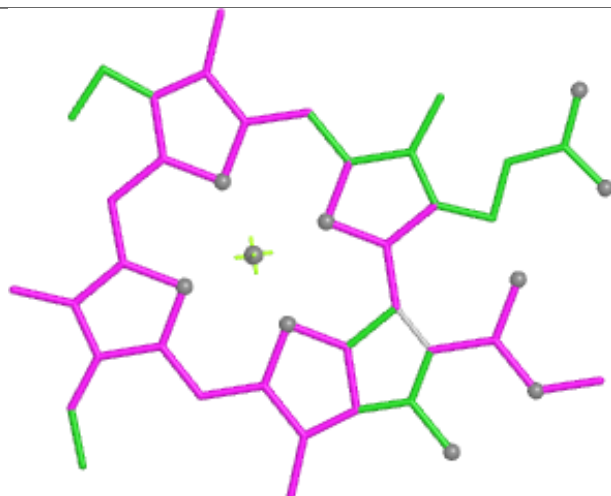
Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings



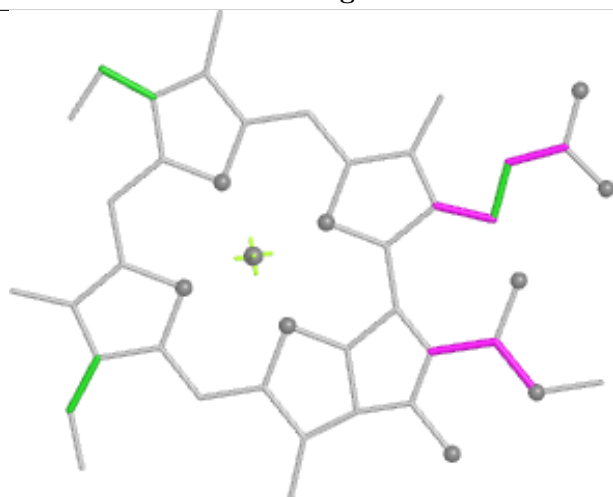
Ligand CLA A 823



Bond lengths



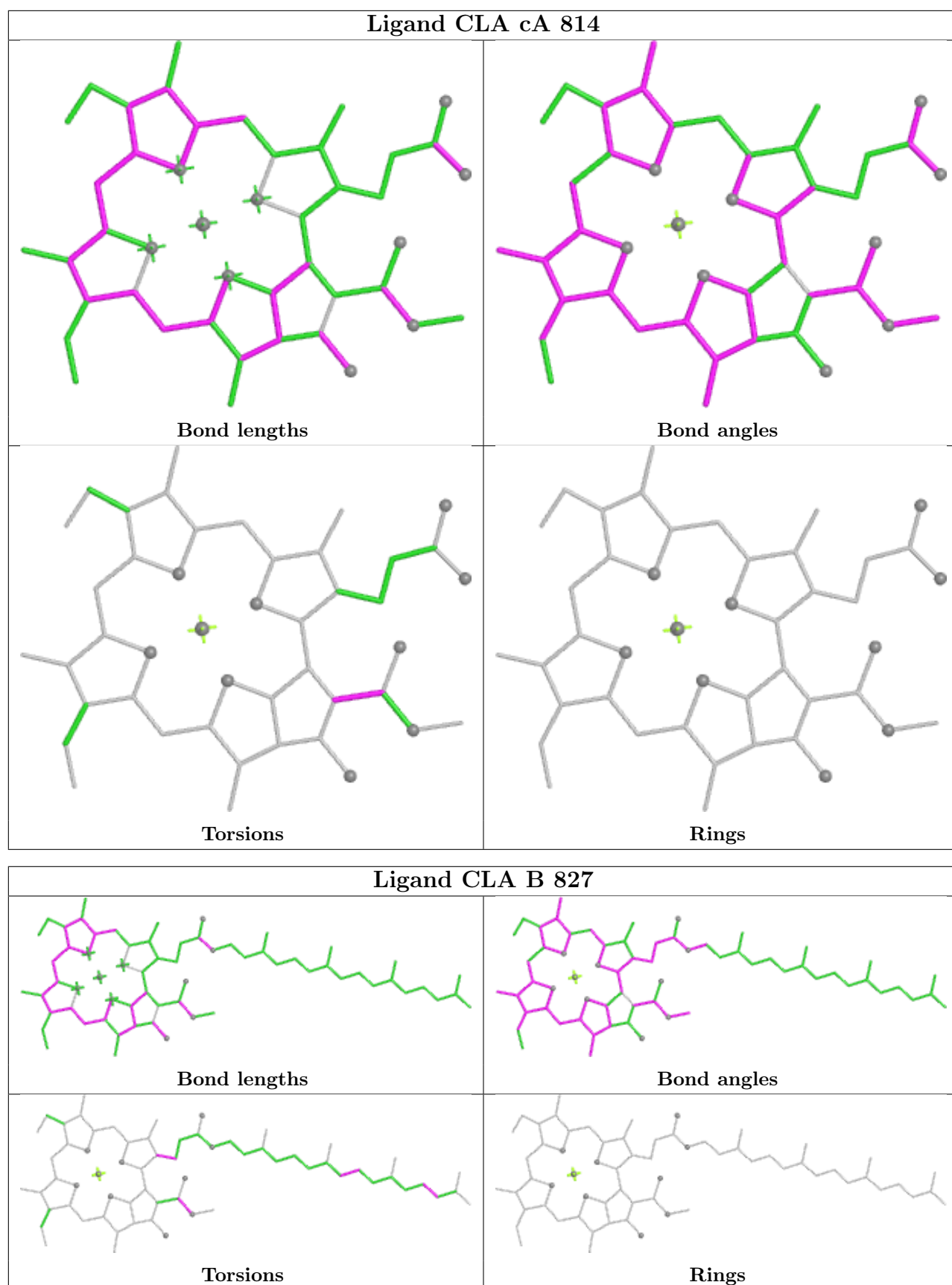
Bond angles

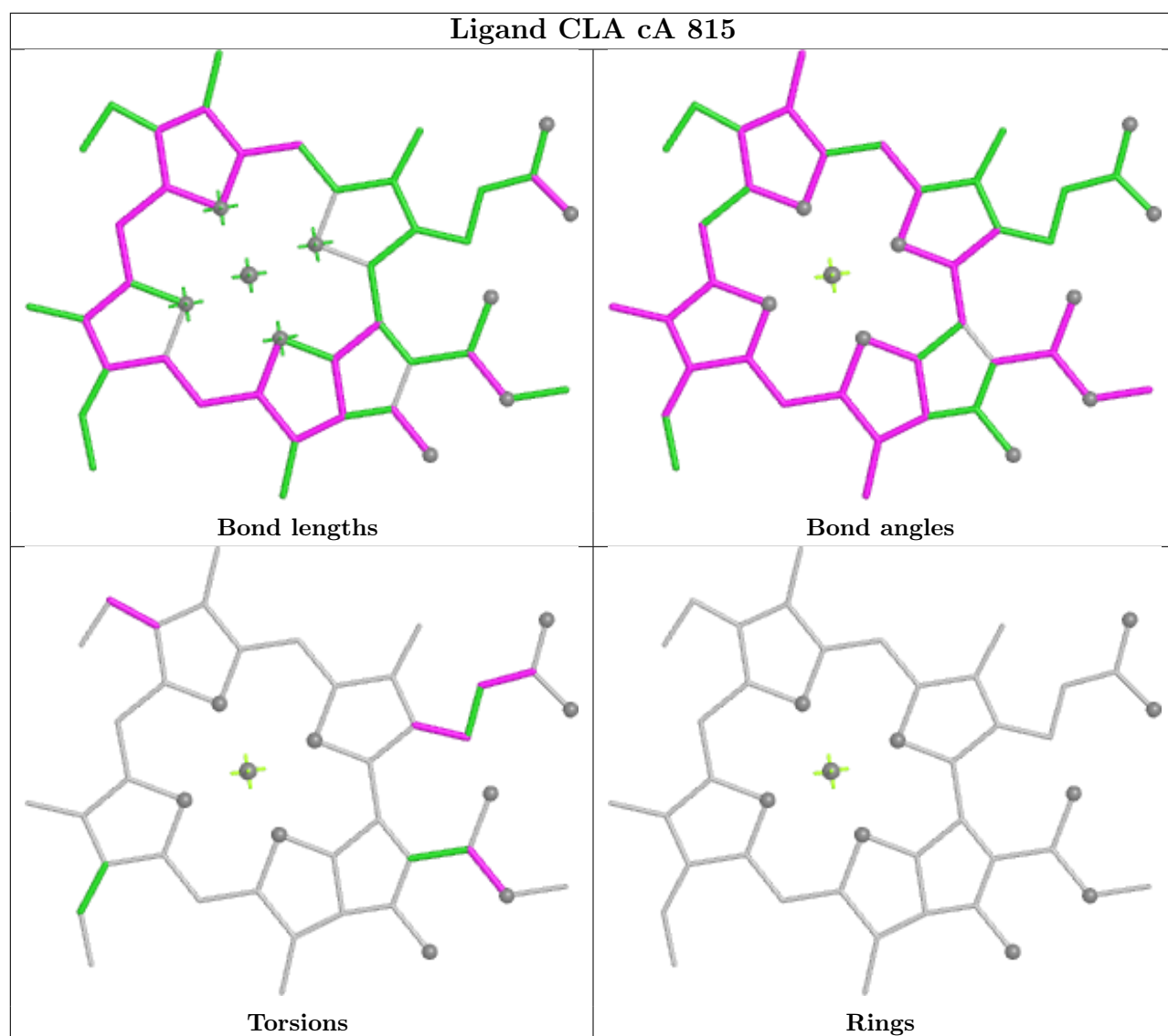


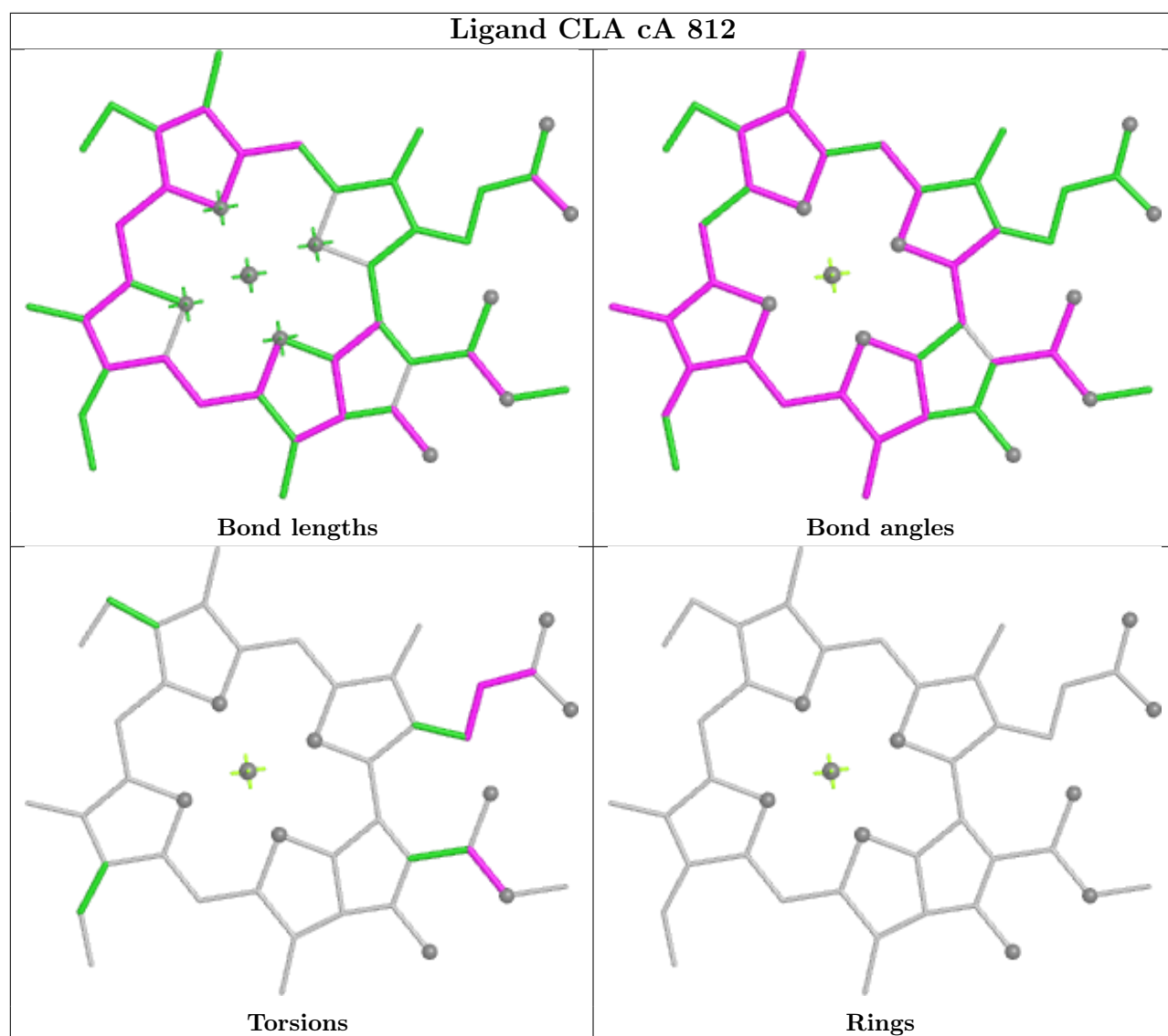
Torsions



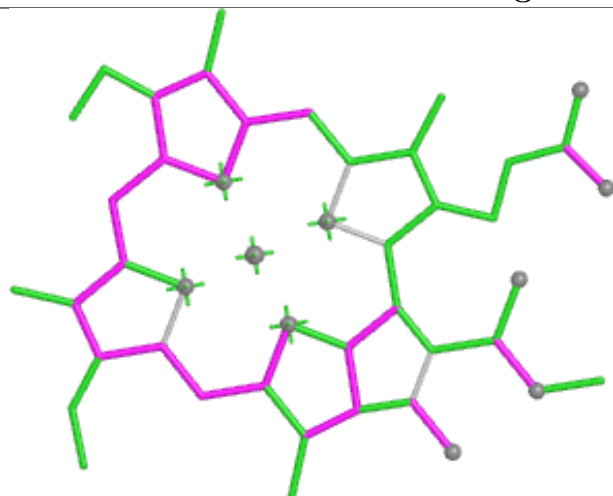
Rings



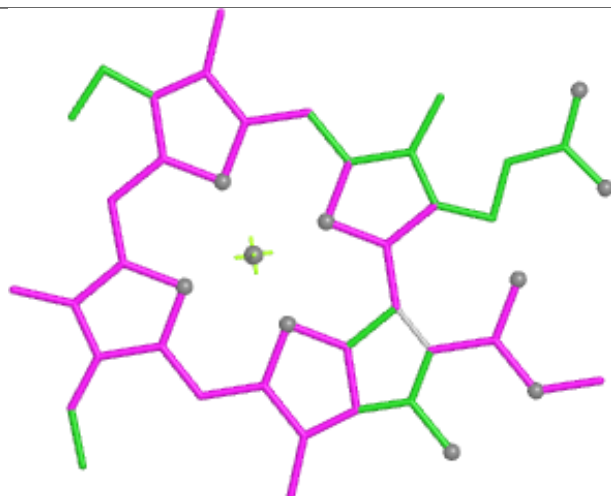




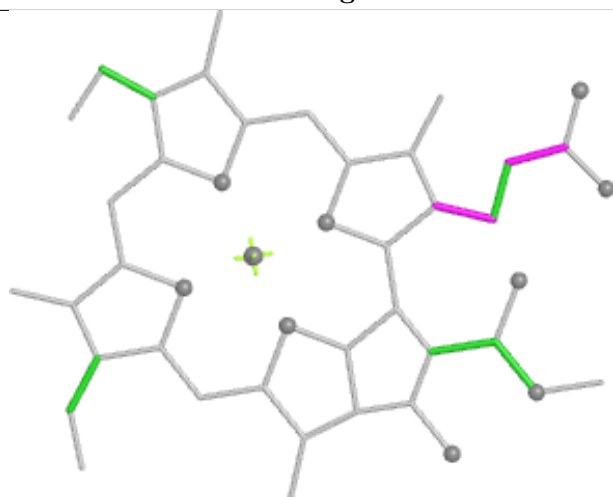
Ligand CLA B 811



Bond lengths



Bond angles

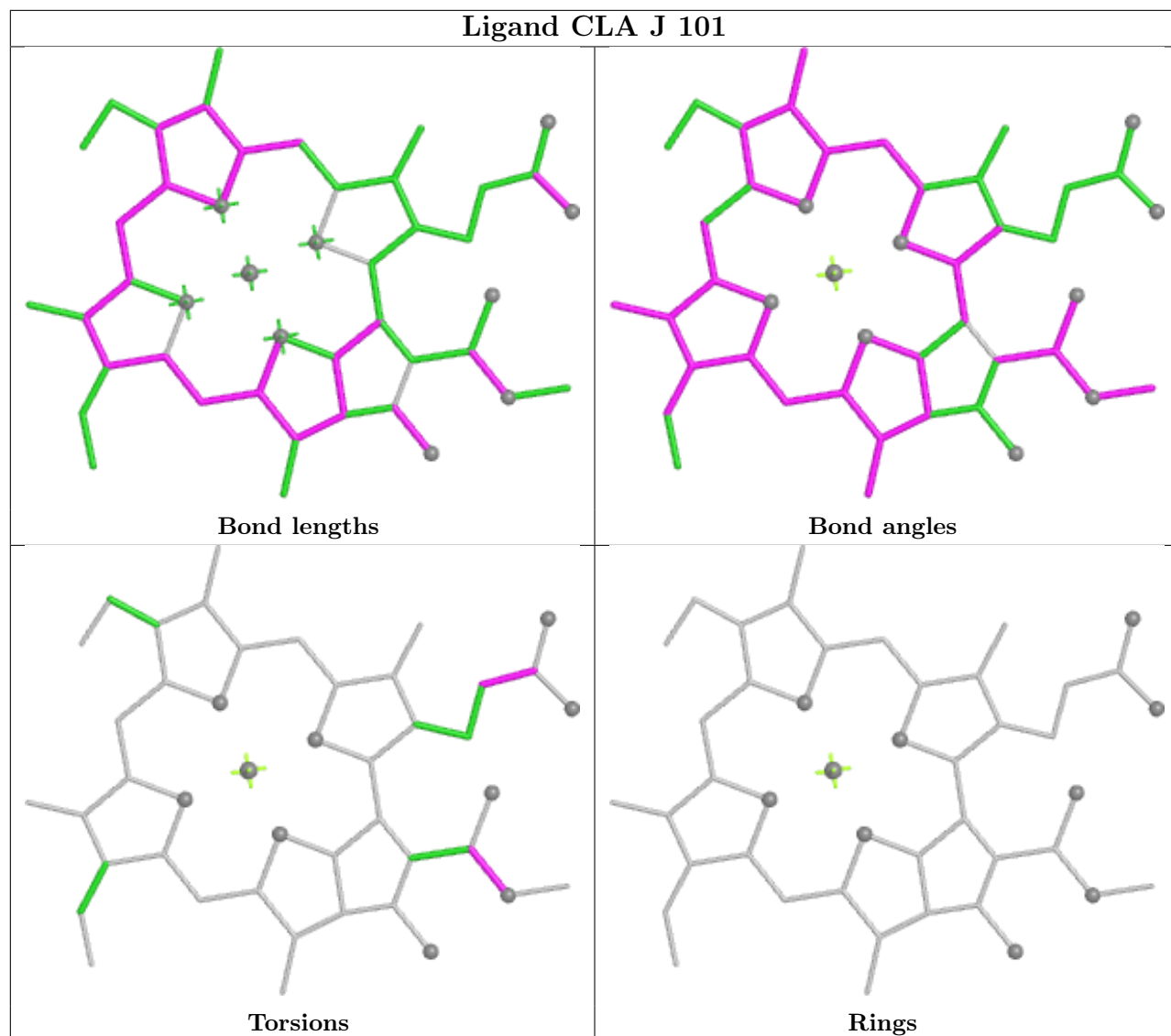


Torsions

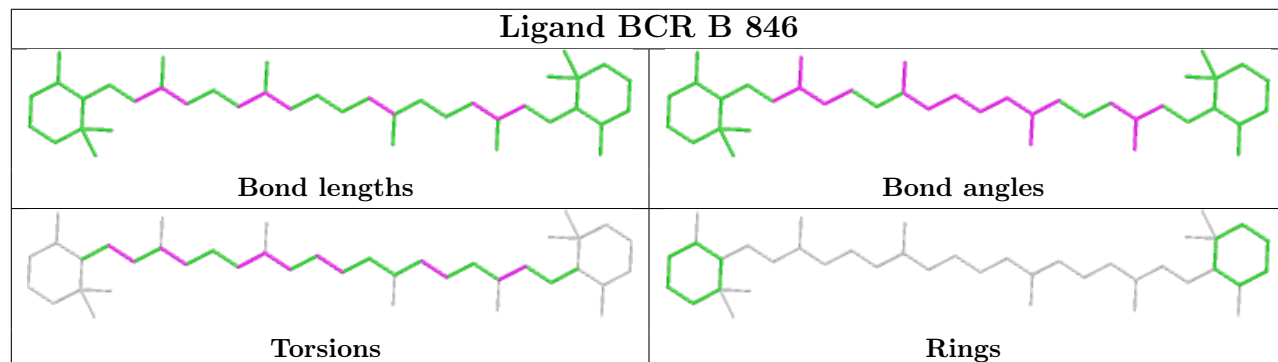


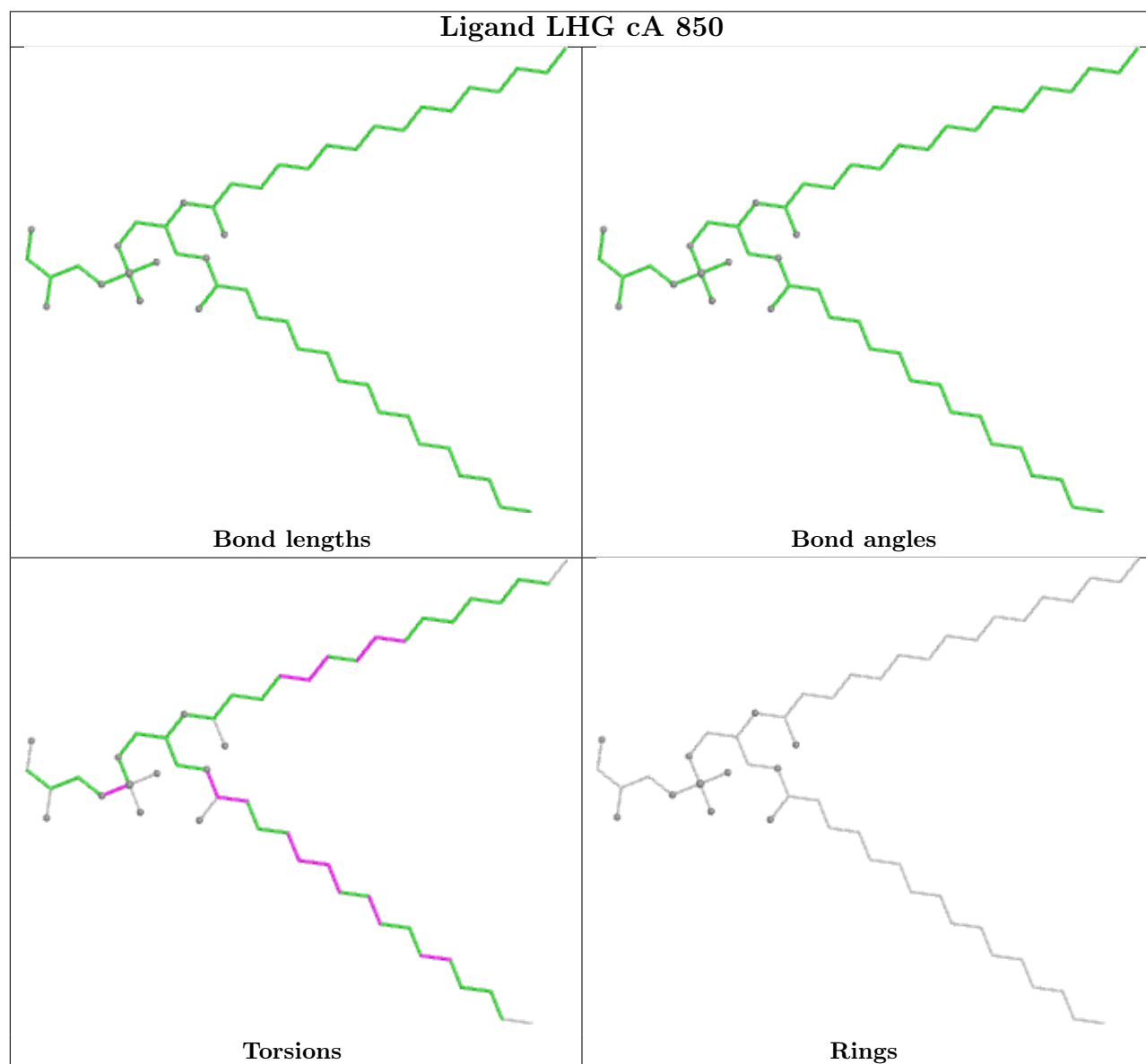
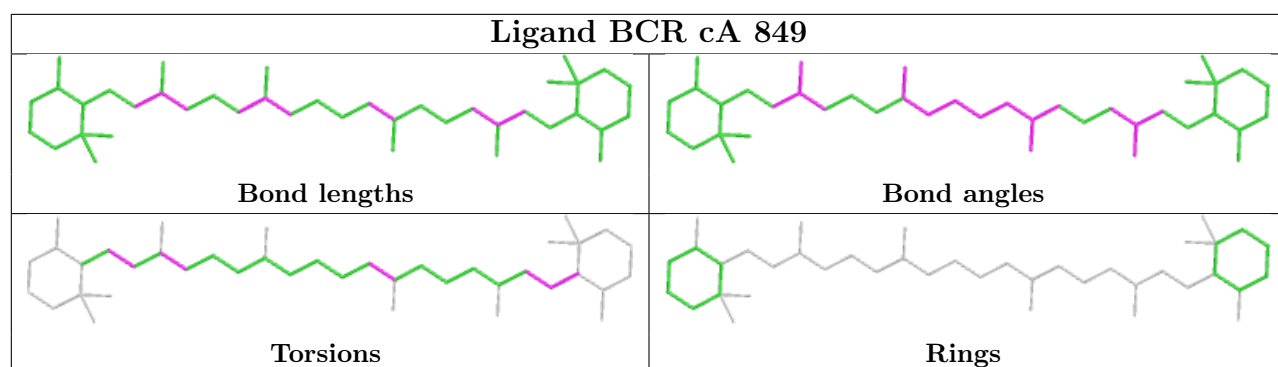
Rings

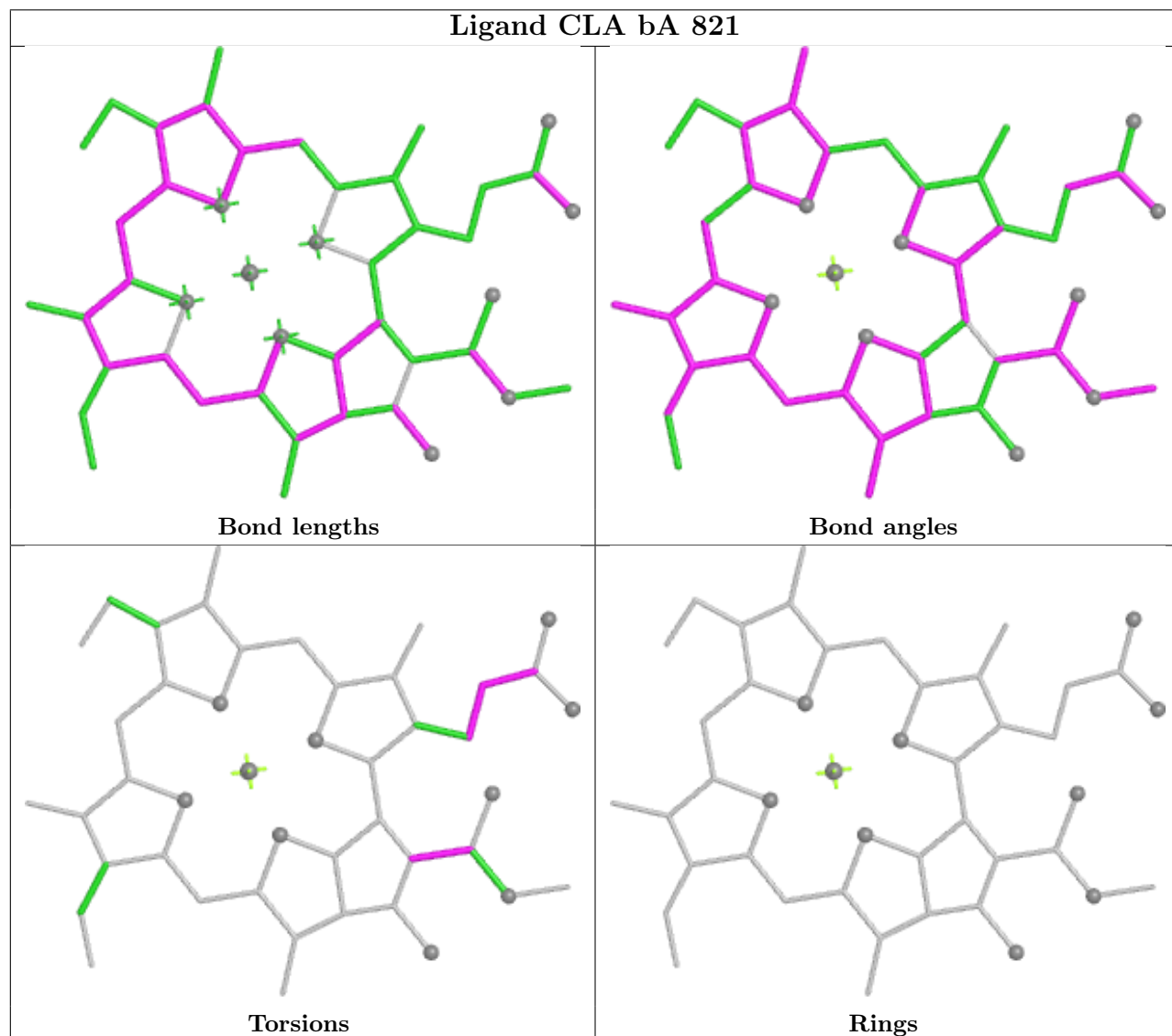
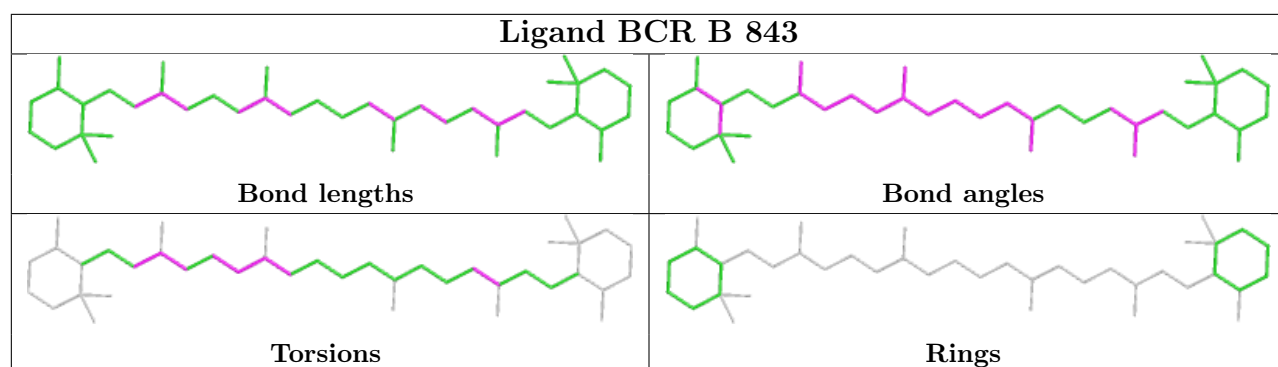
Ligand CLA J 101



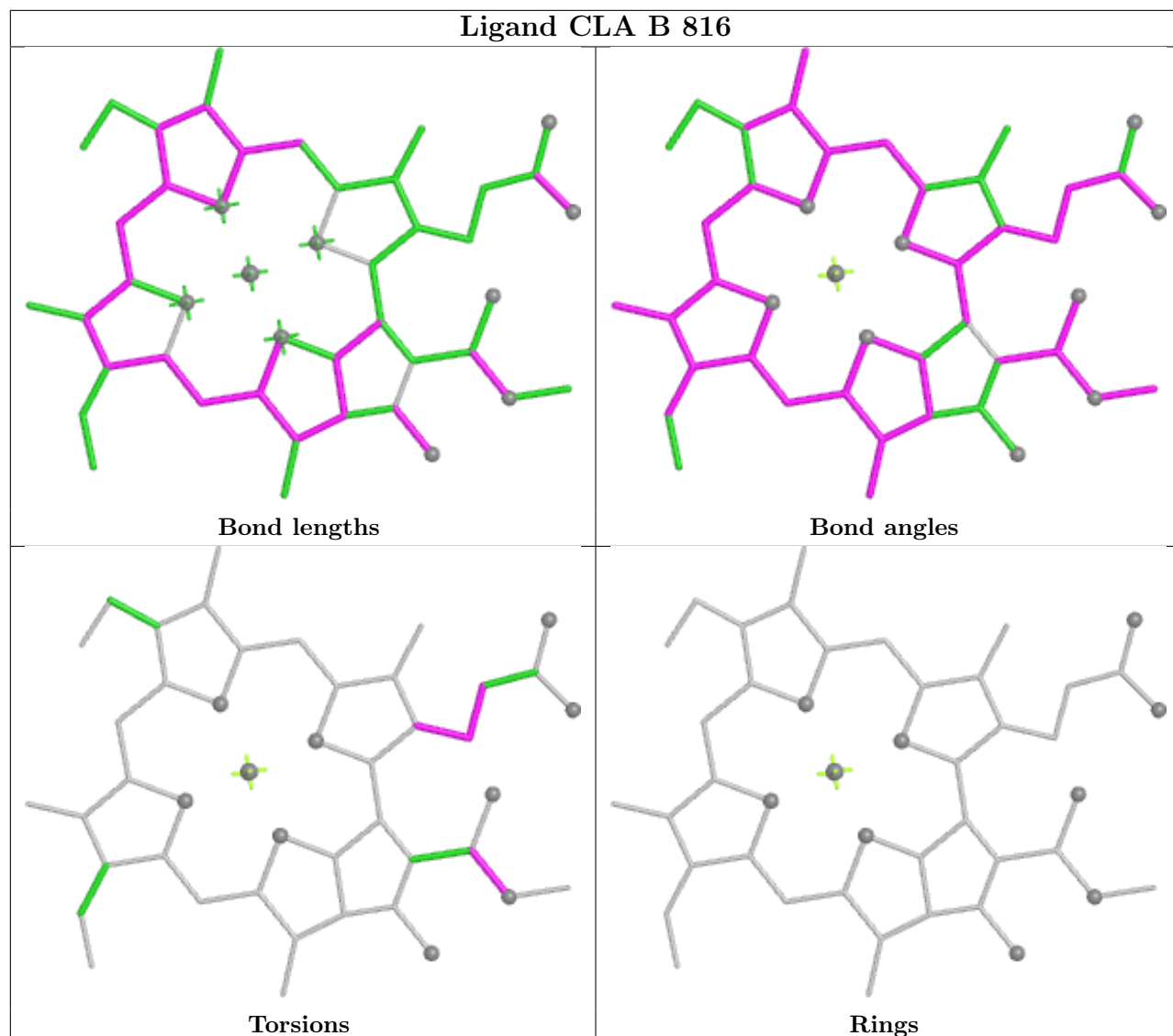
Ligand BCR B 846



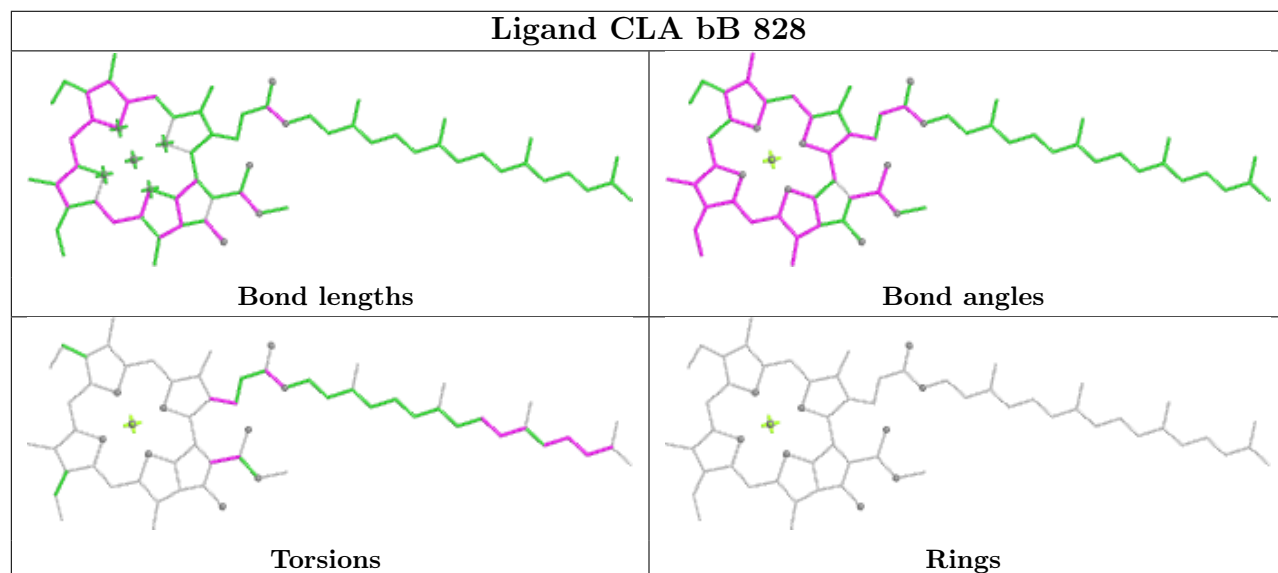


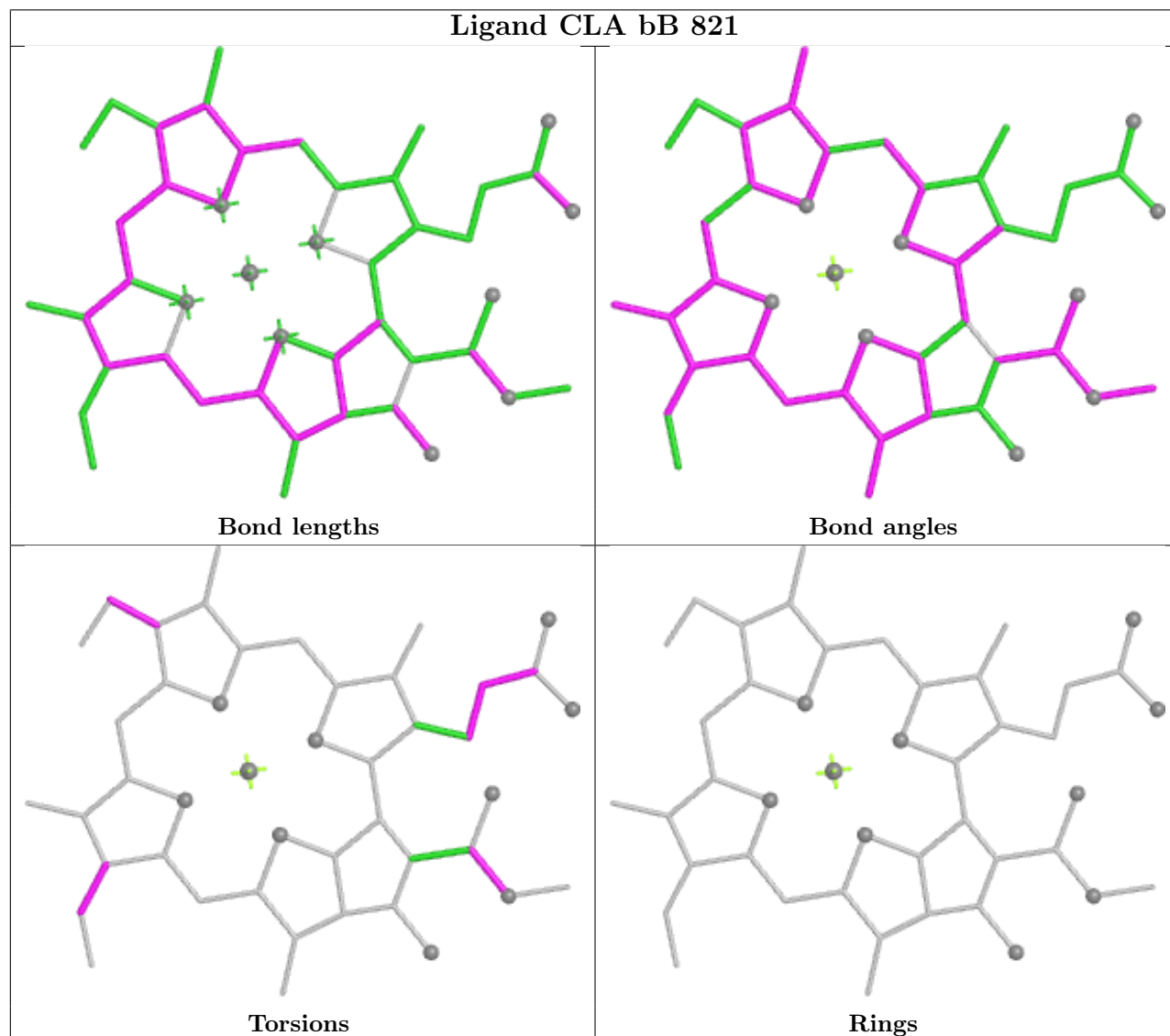
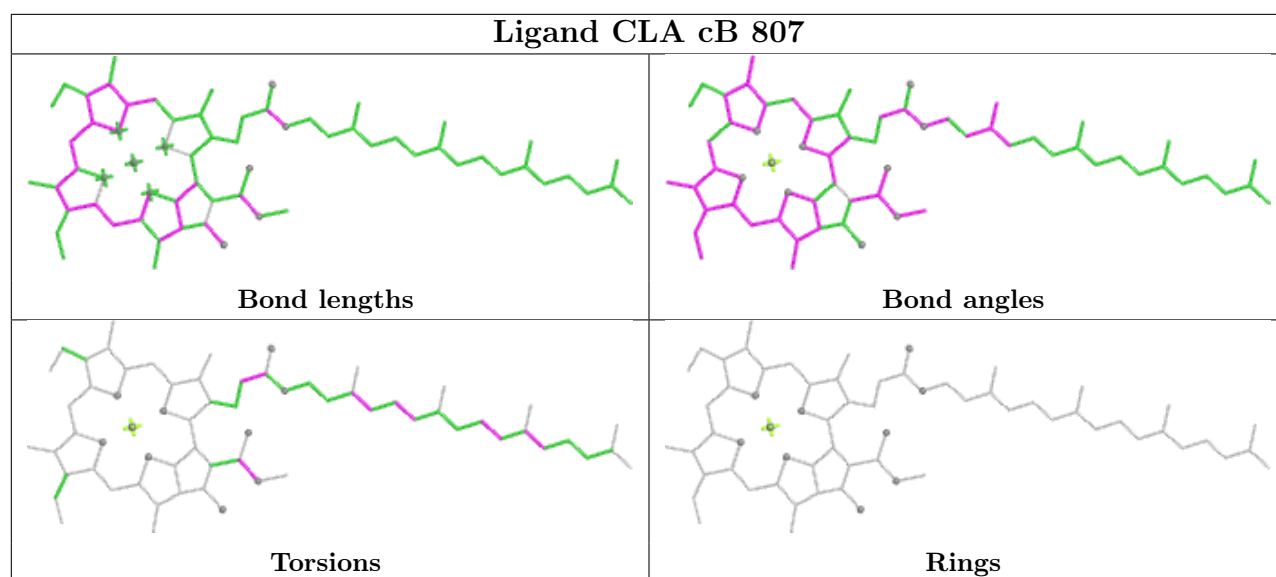


Ligand CLA B 816

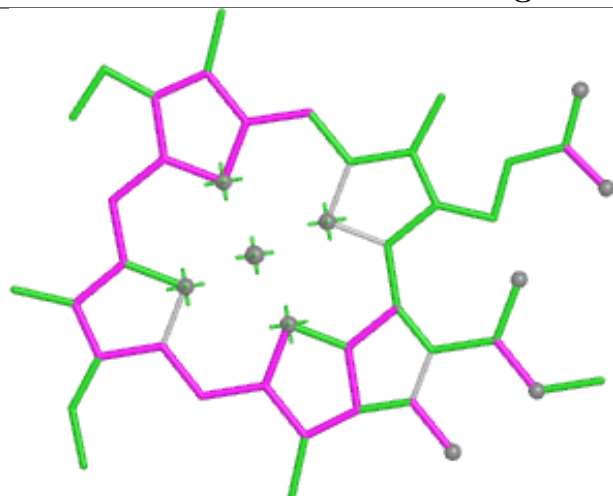


Ligand CLA bB 828

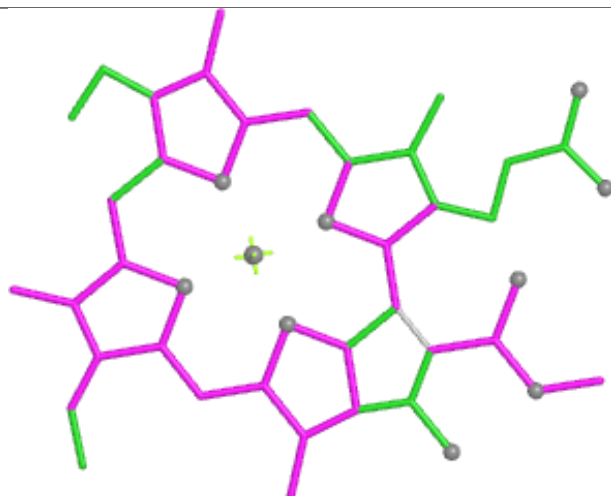




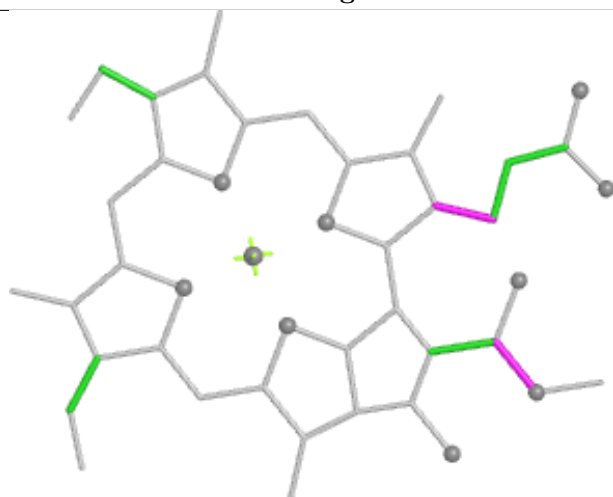
Ligand CLA B 834



Bond lengths



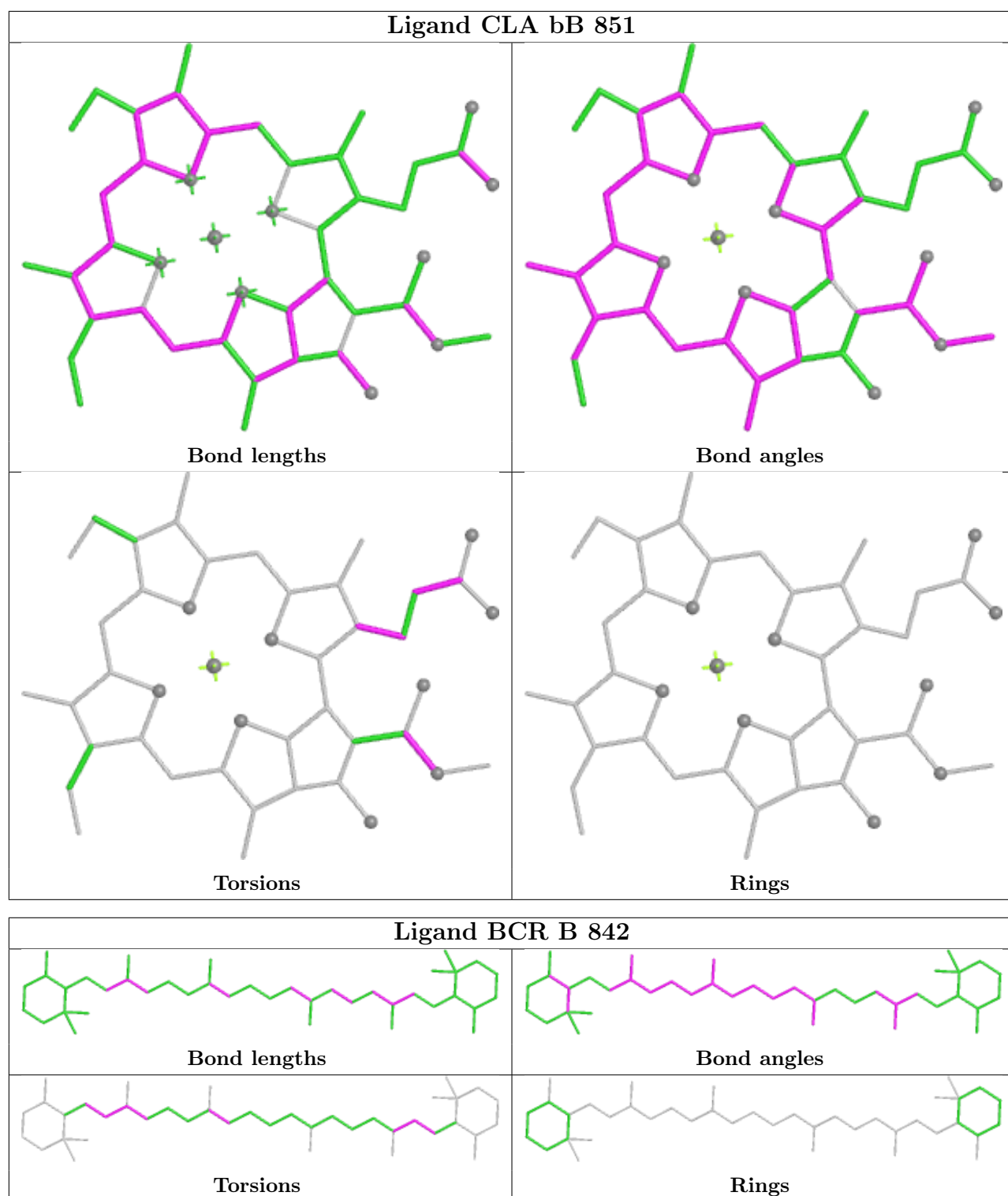
Bond angles

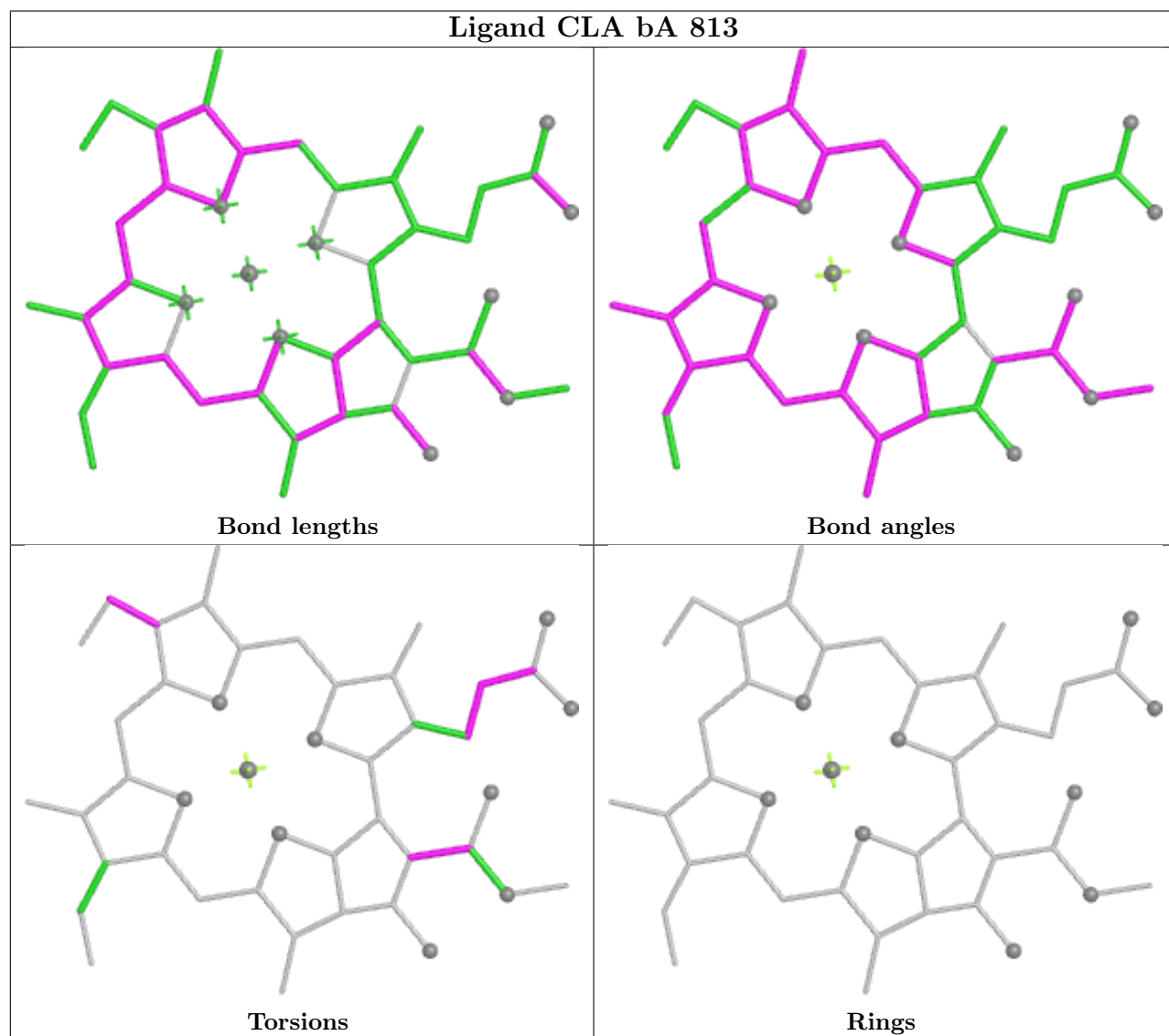
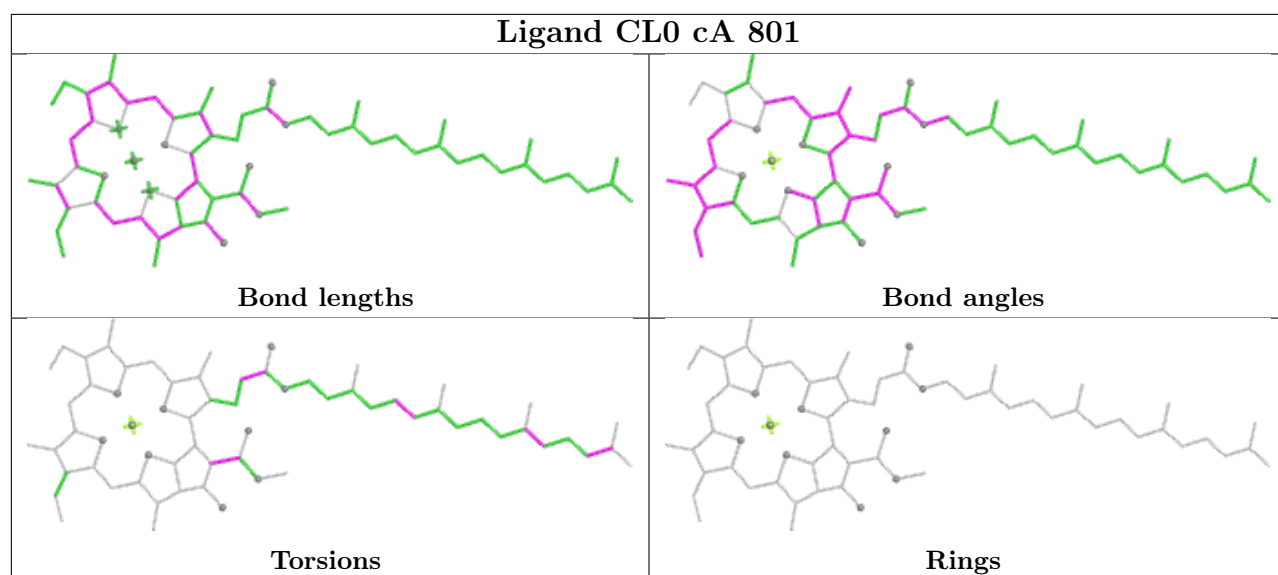


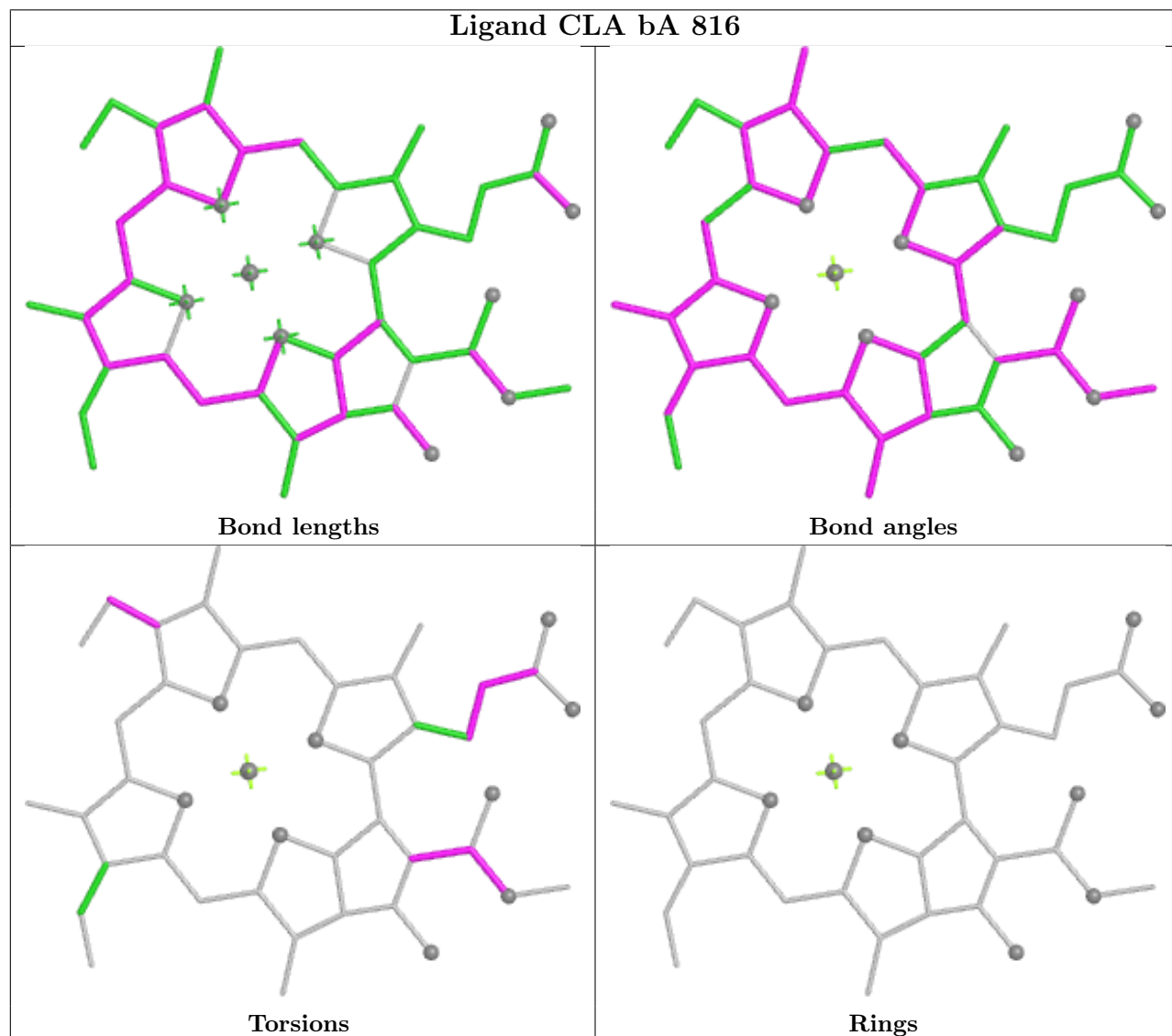
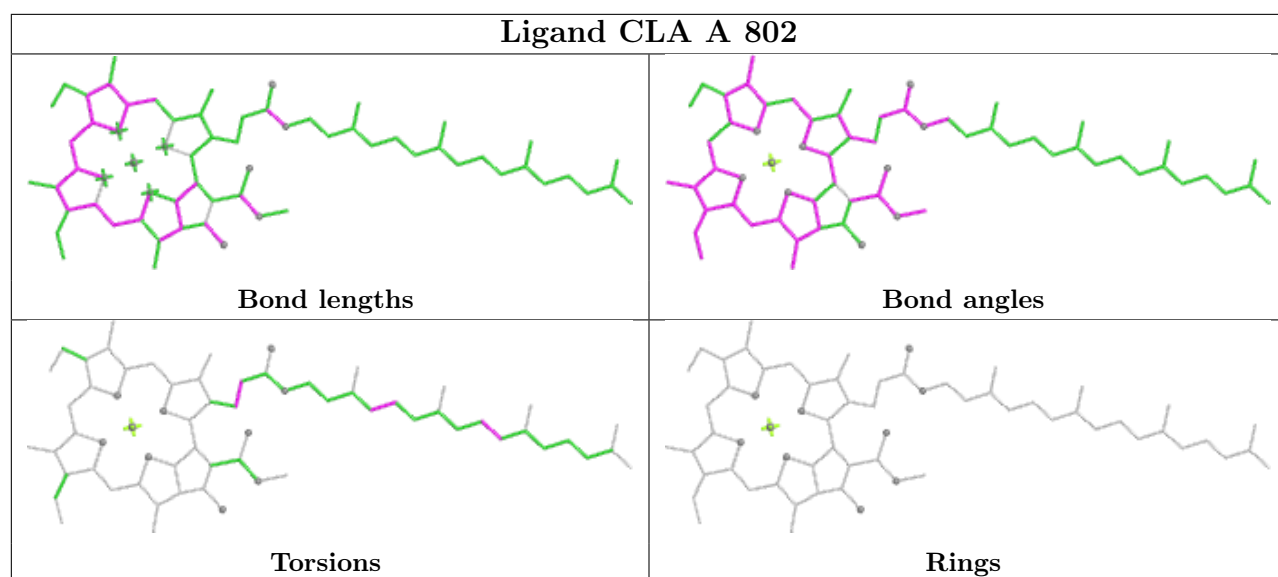
Torsions

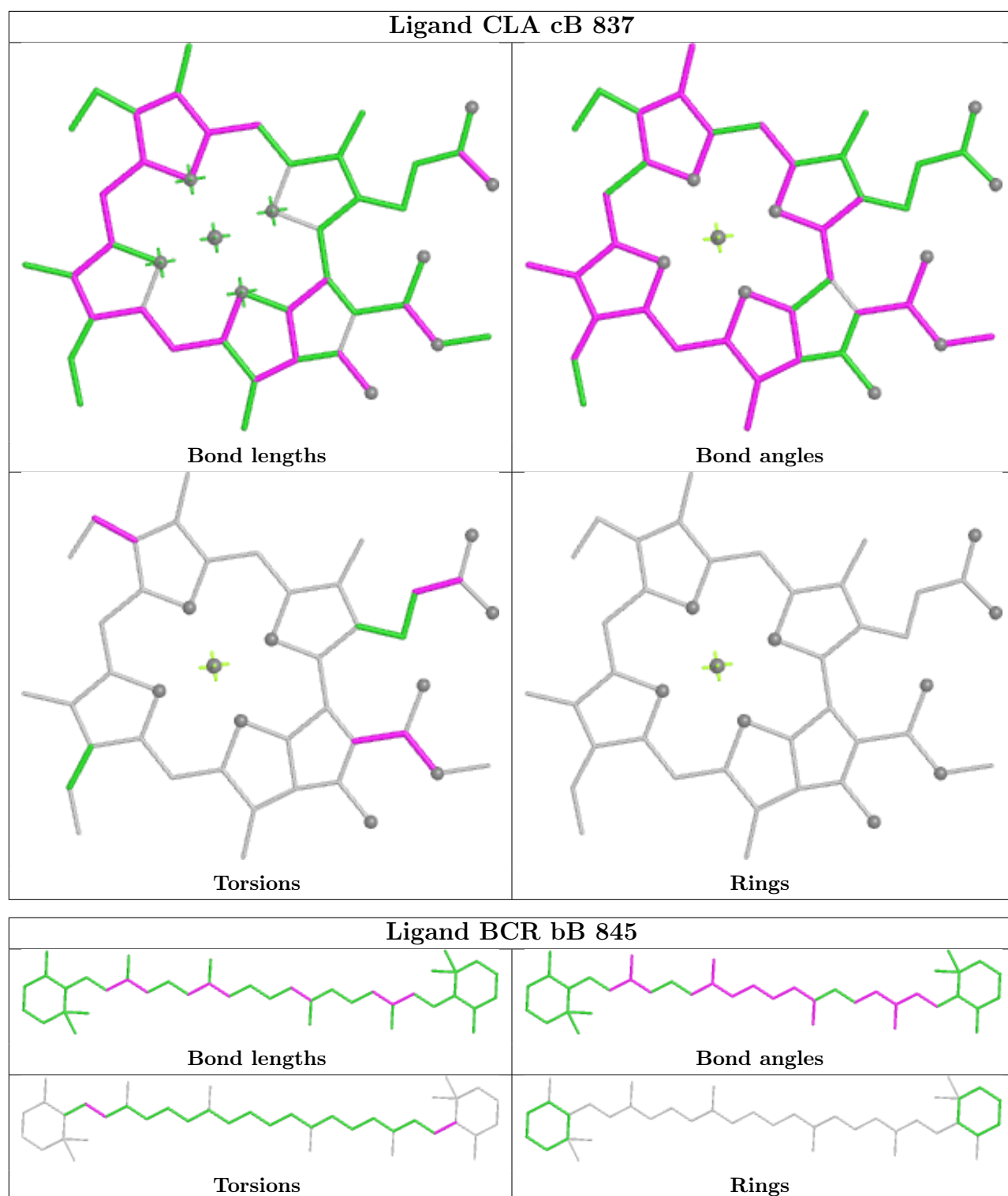


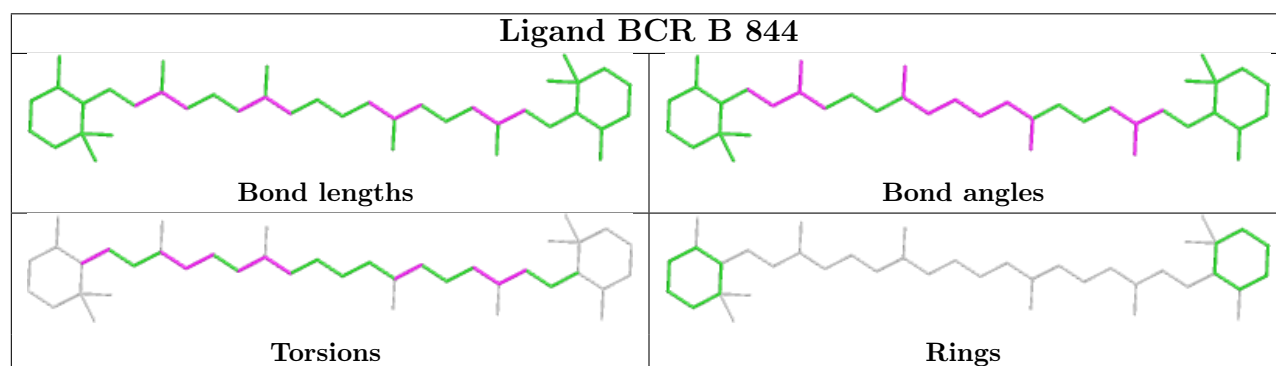
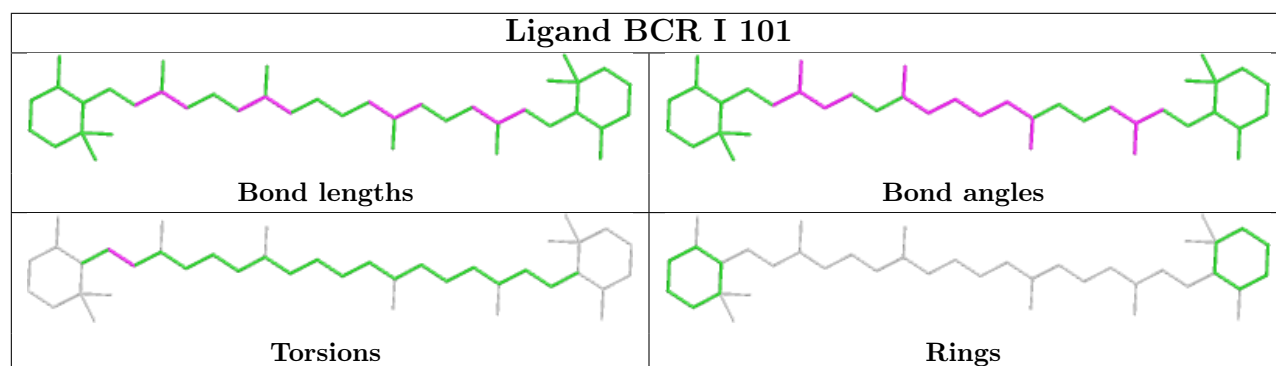
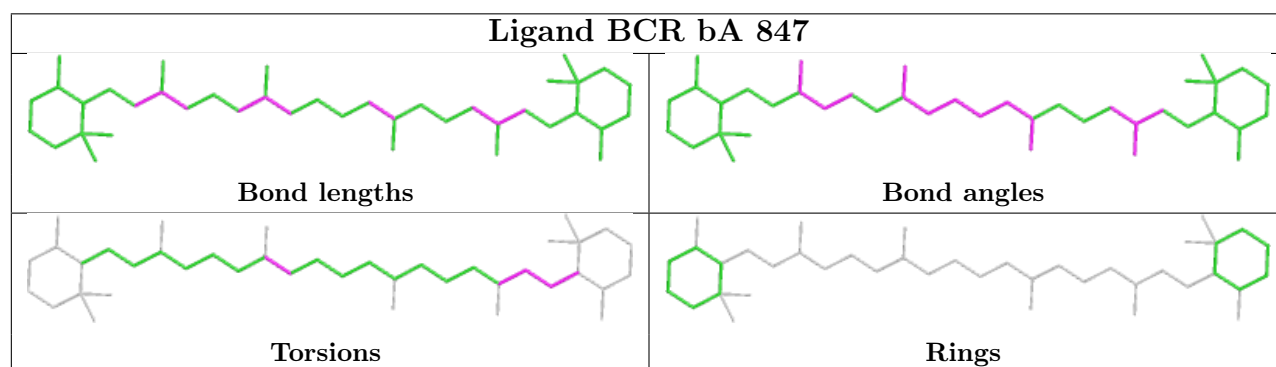
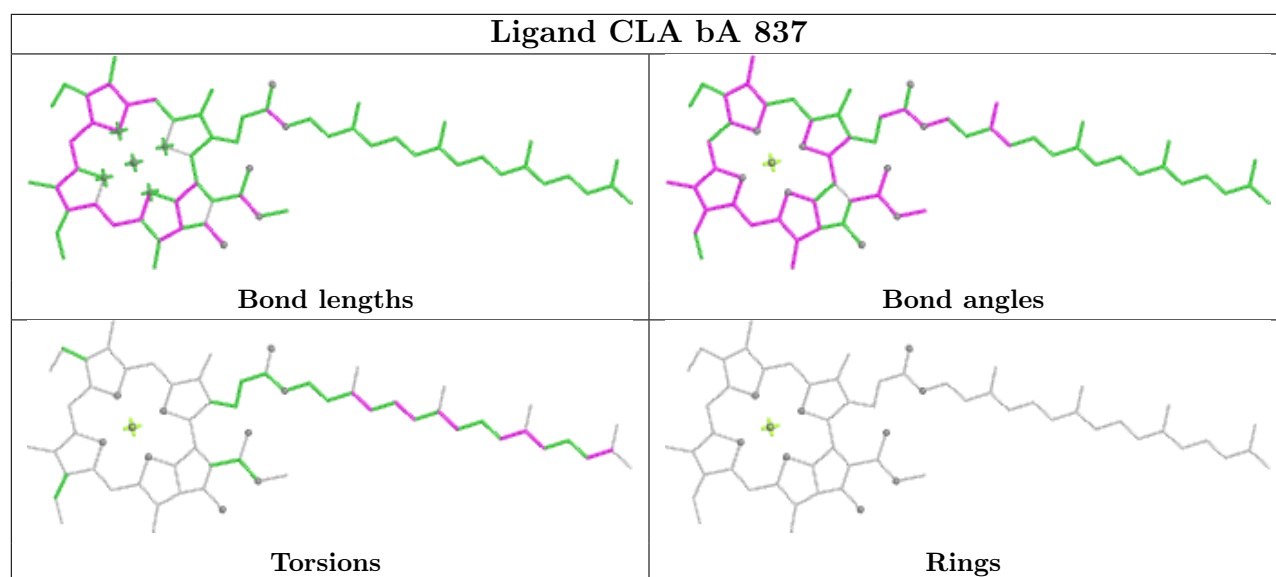
Rings

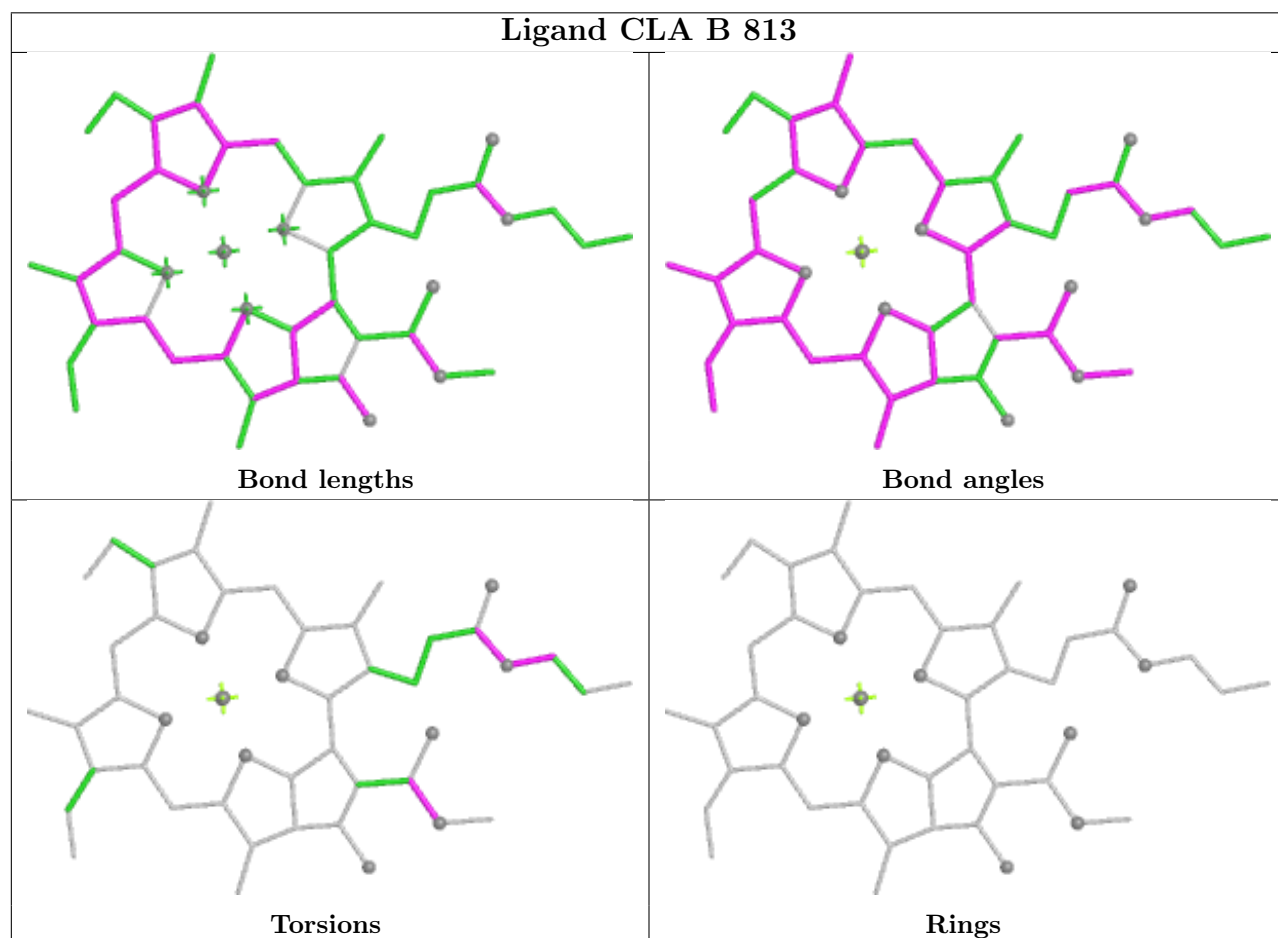
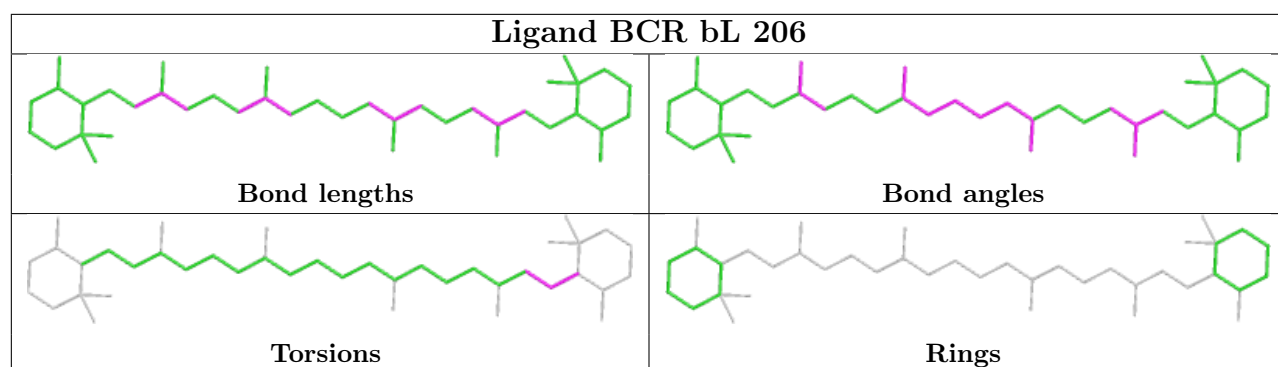




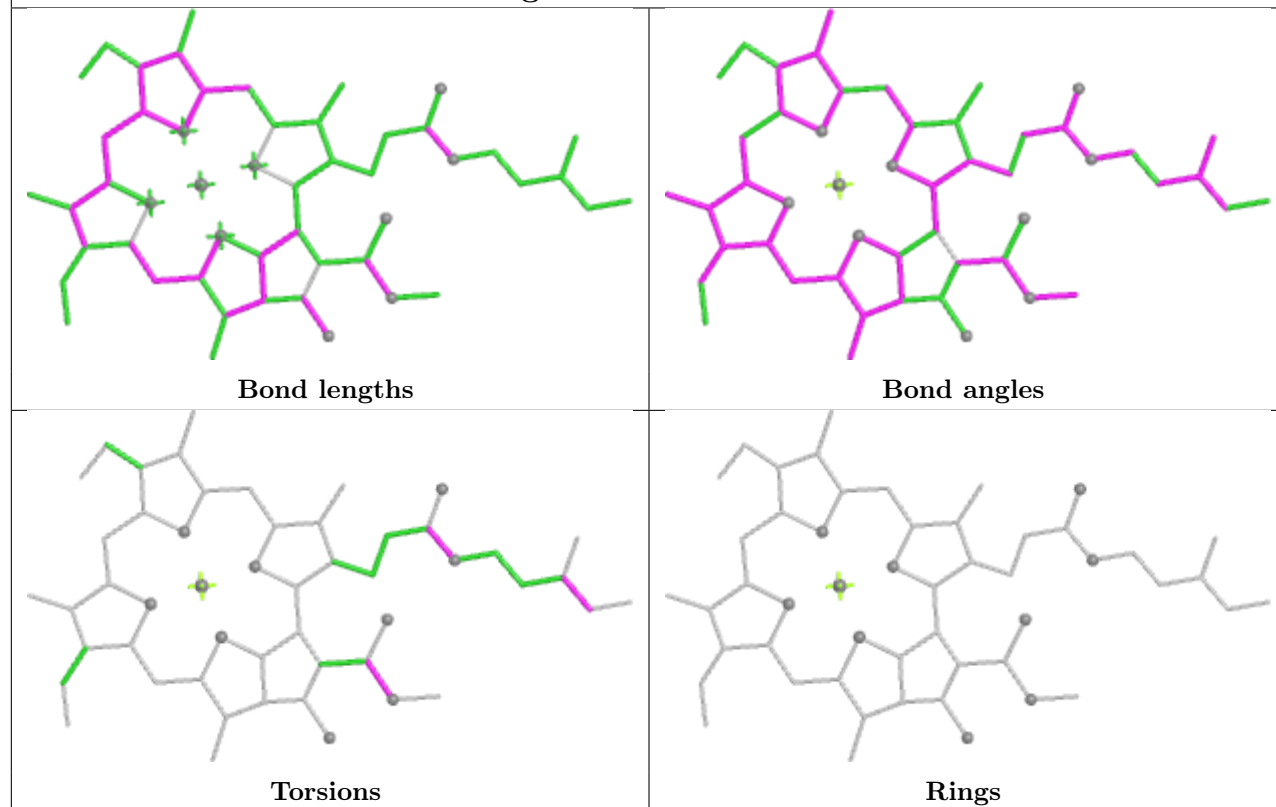




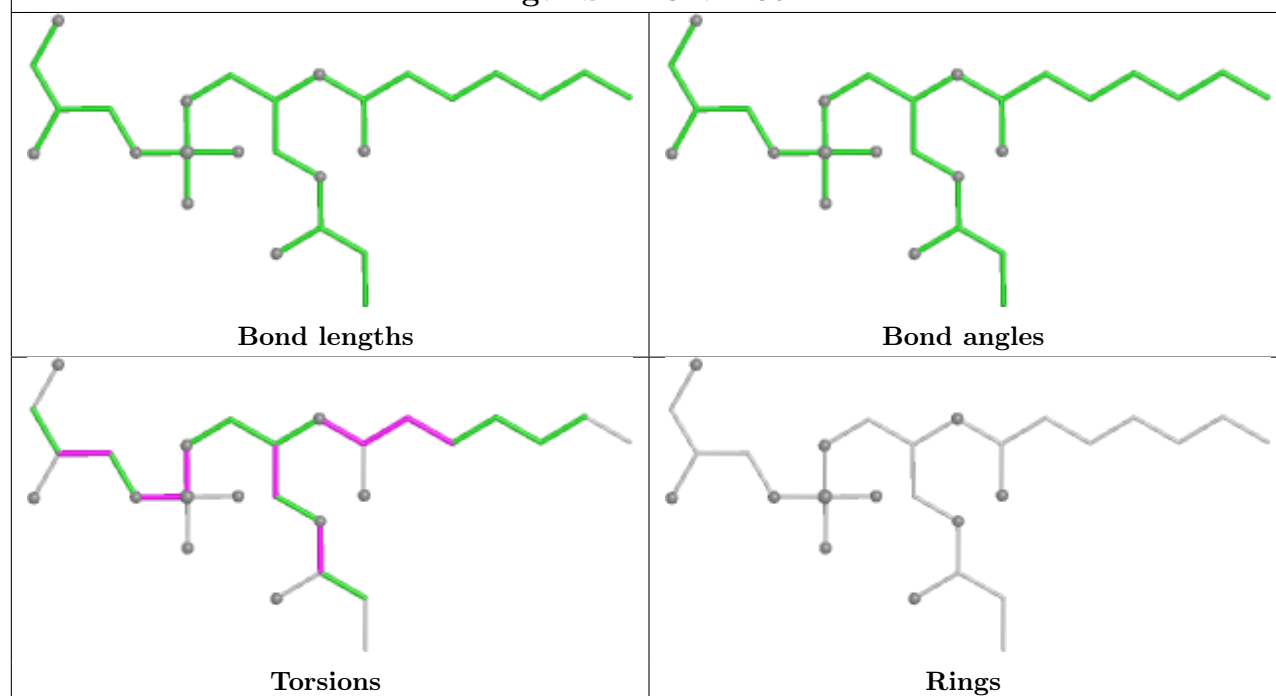


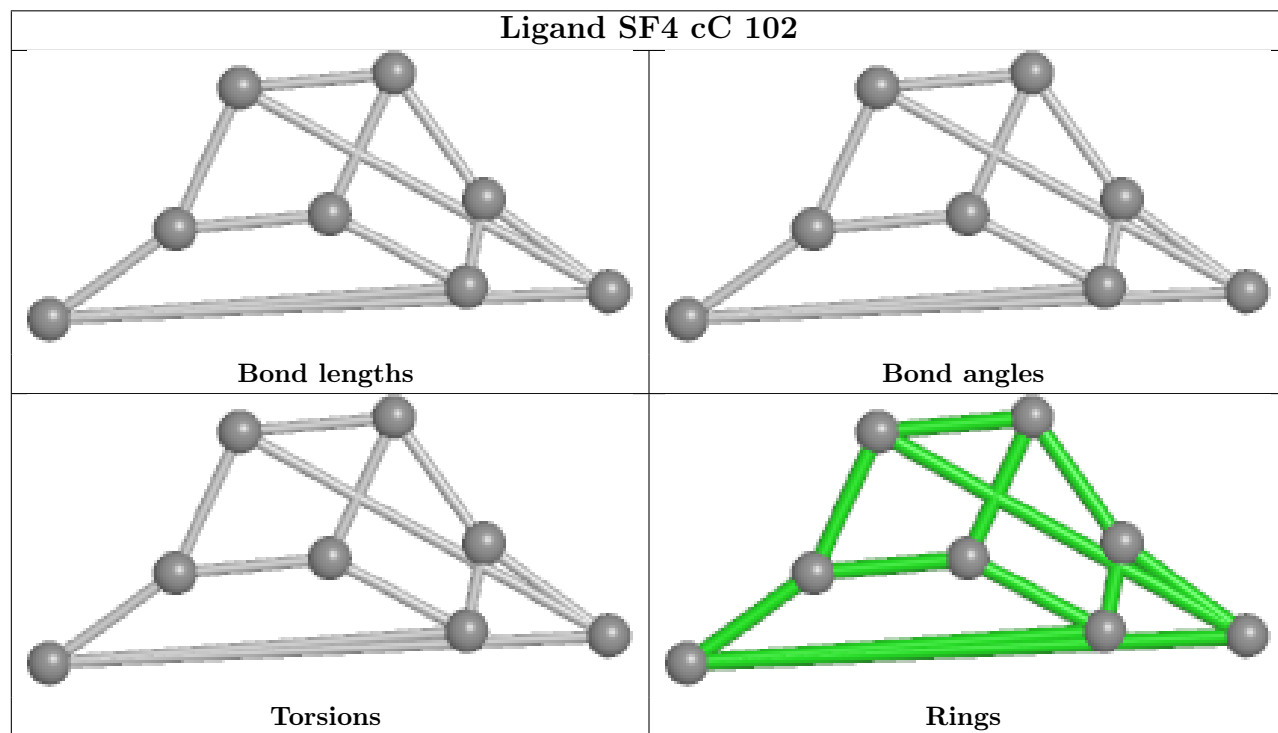
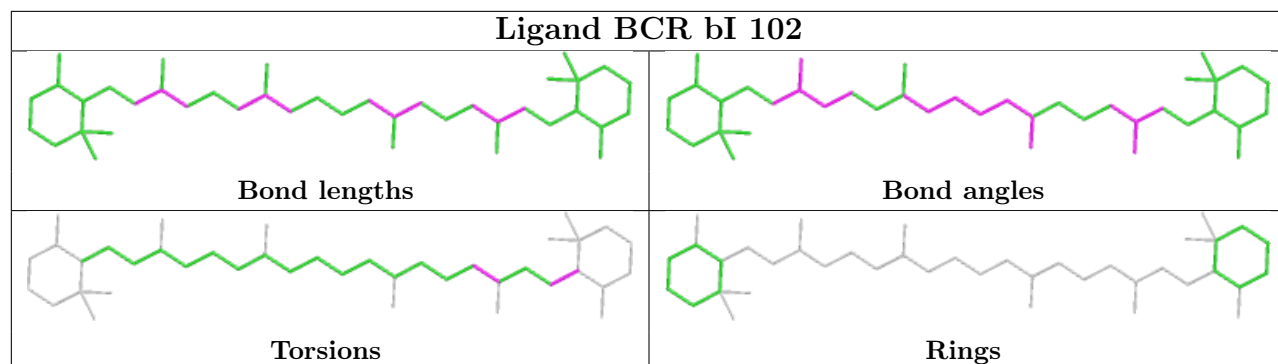


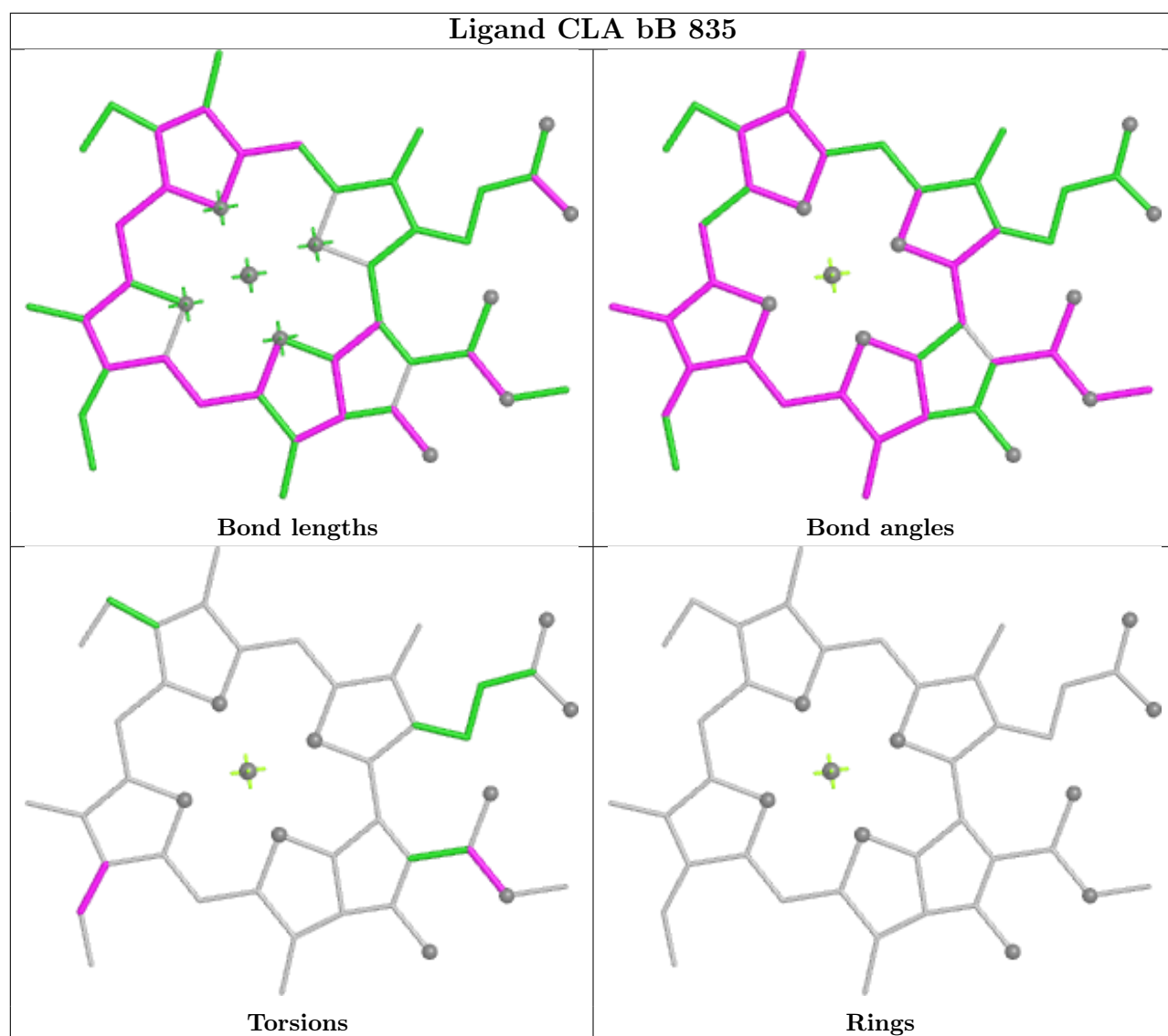
Ligand CLA bA 836

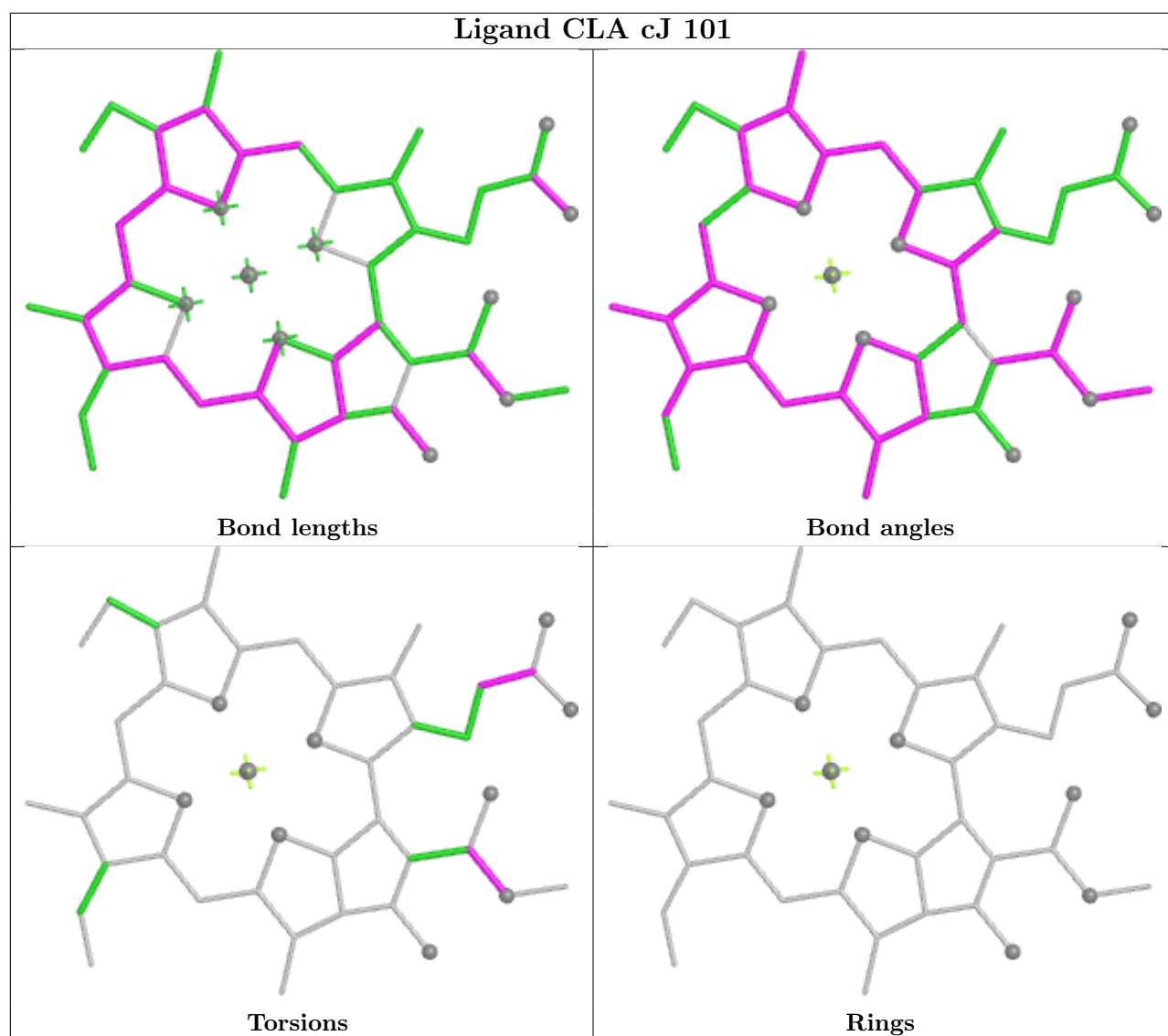


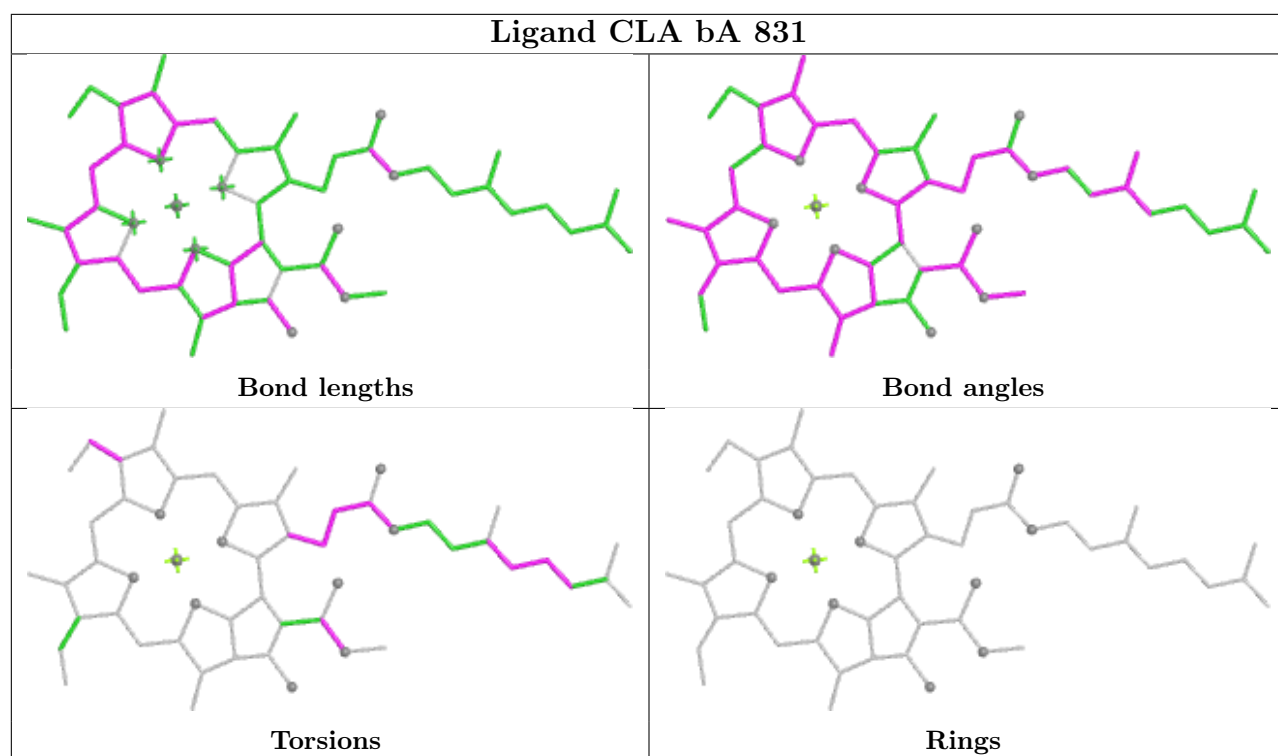
Ligand LHG cA 851

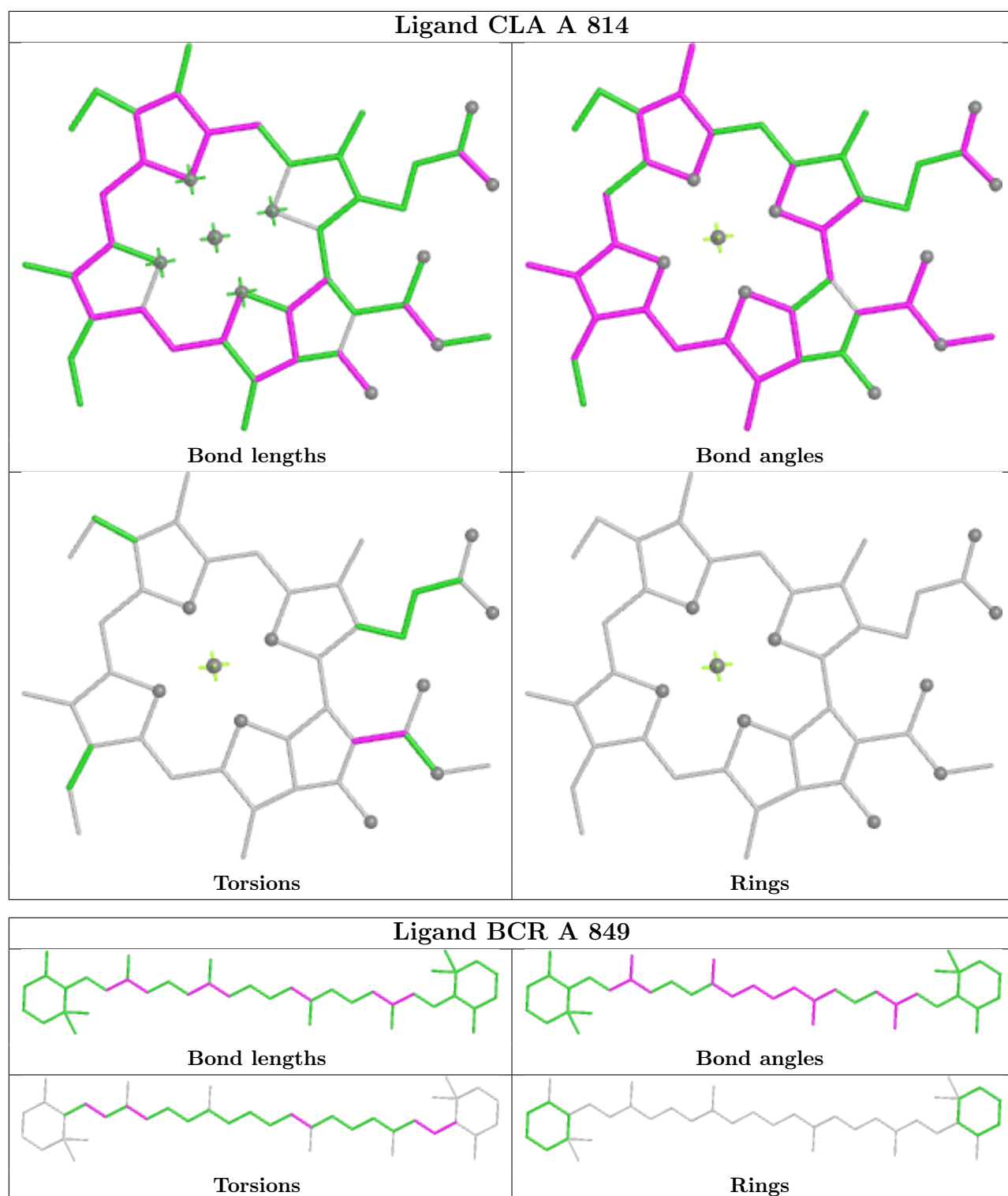




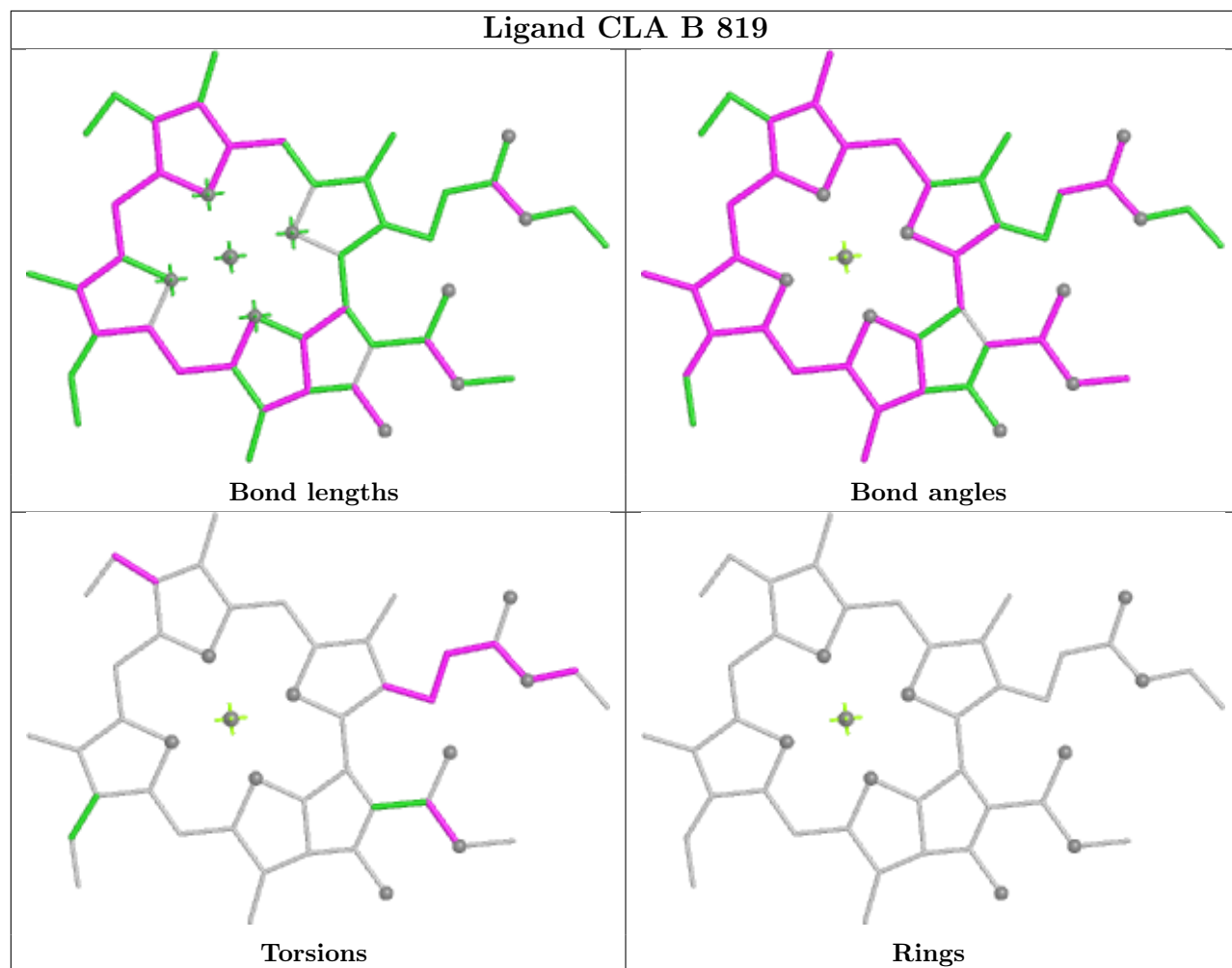


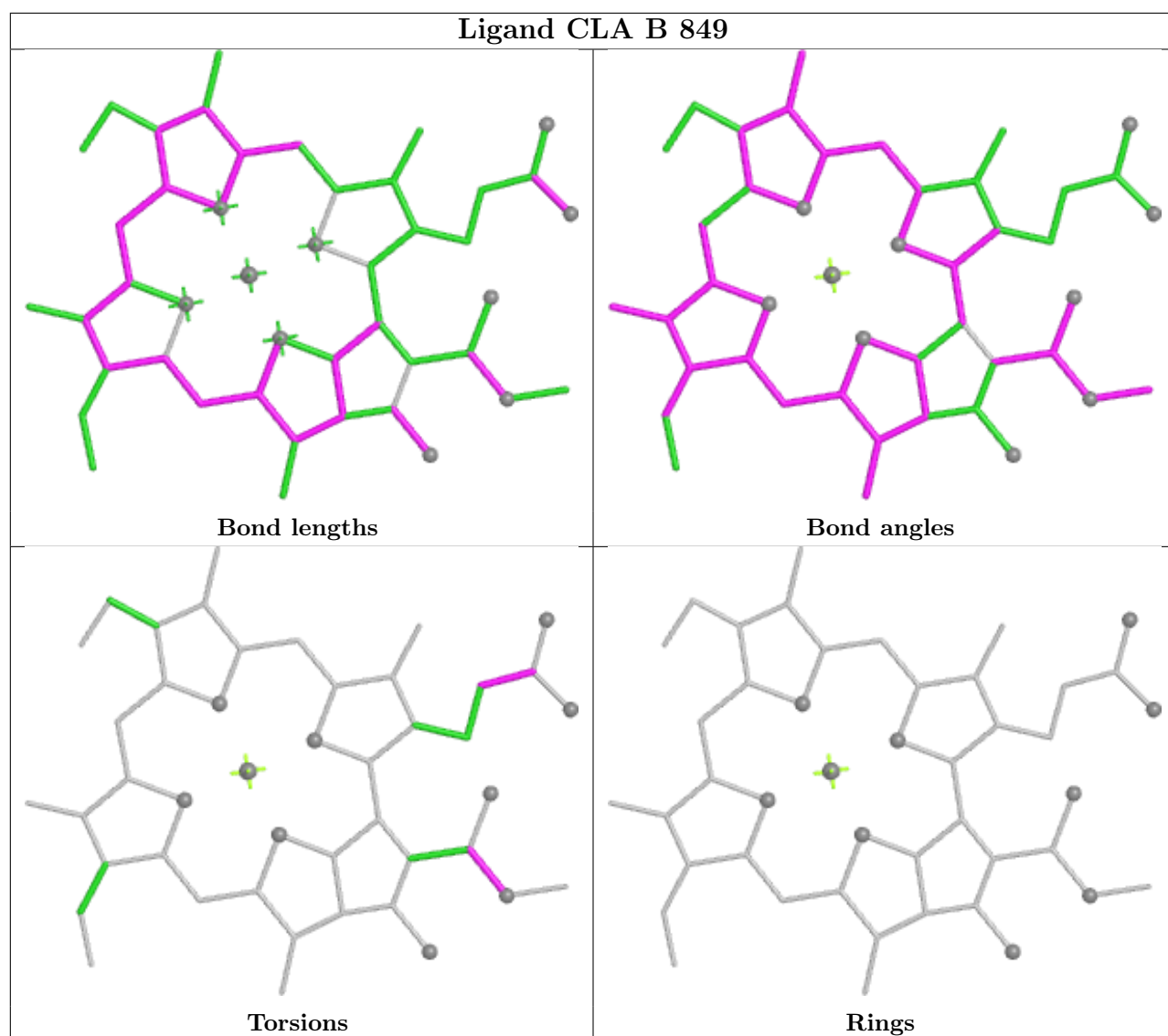


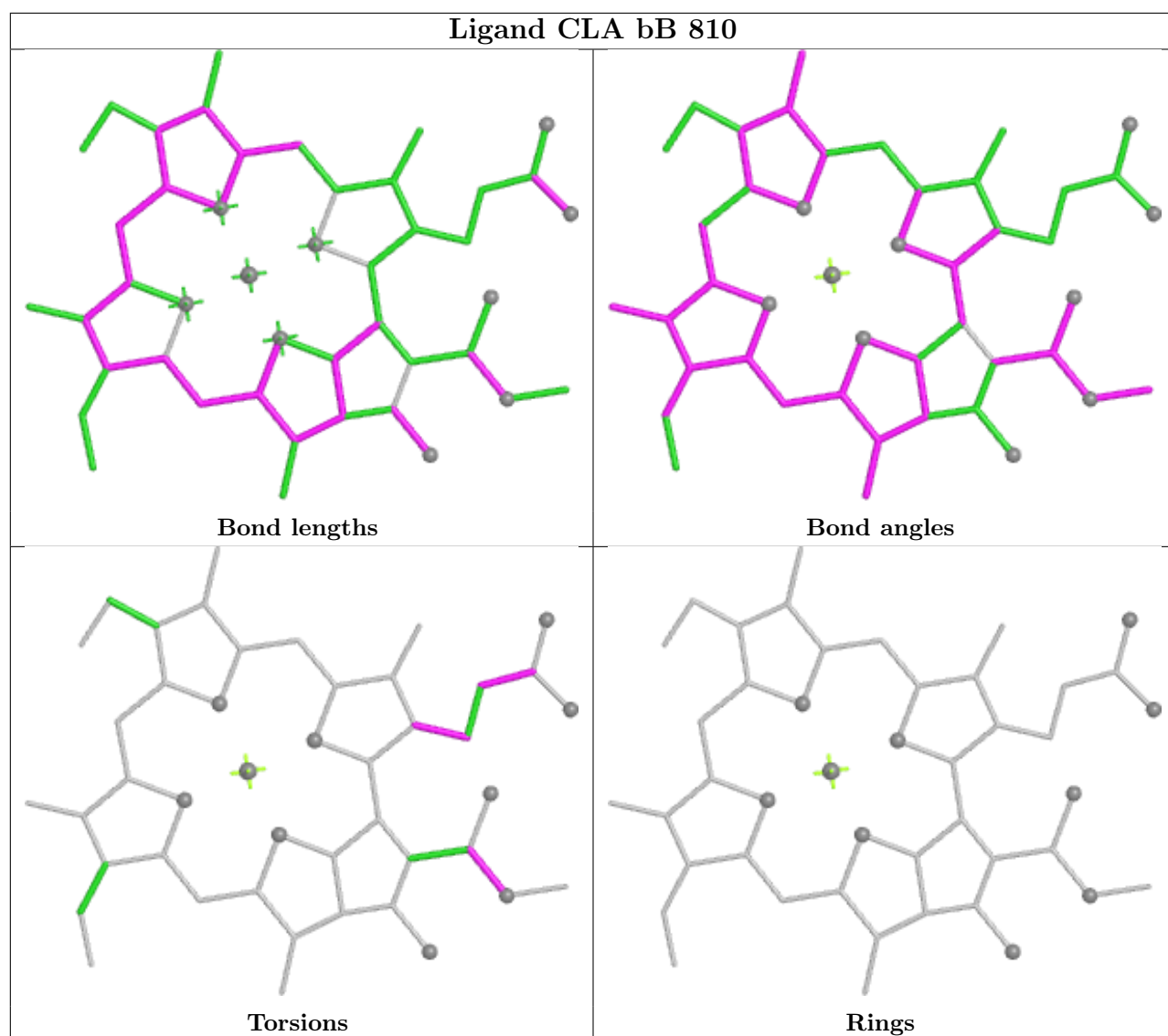


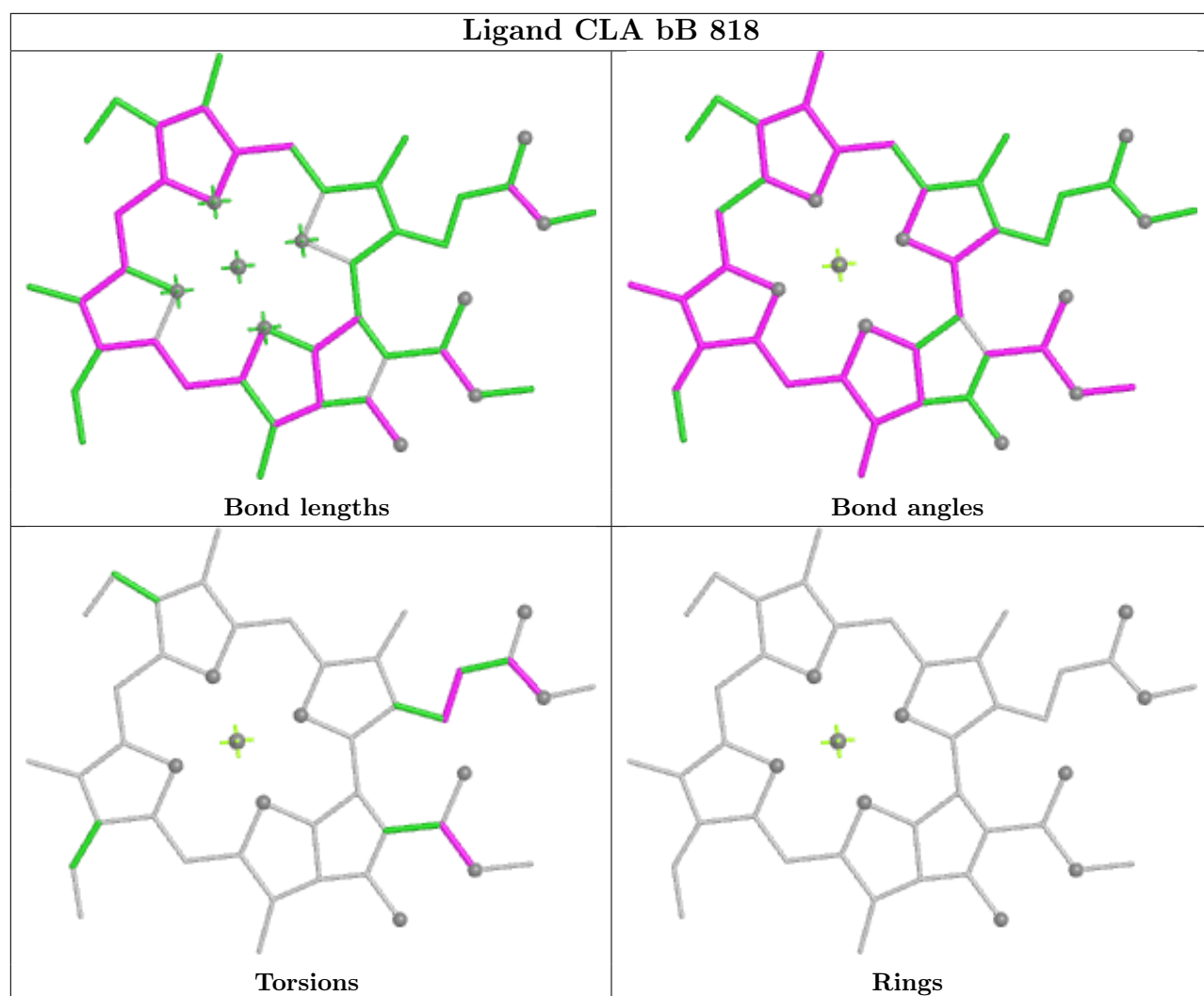


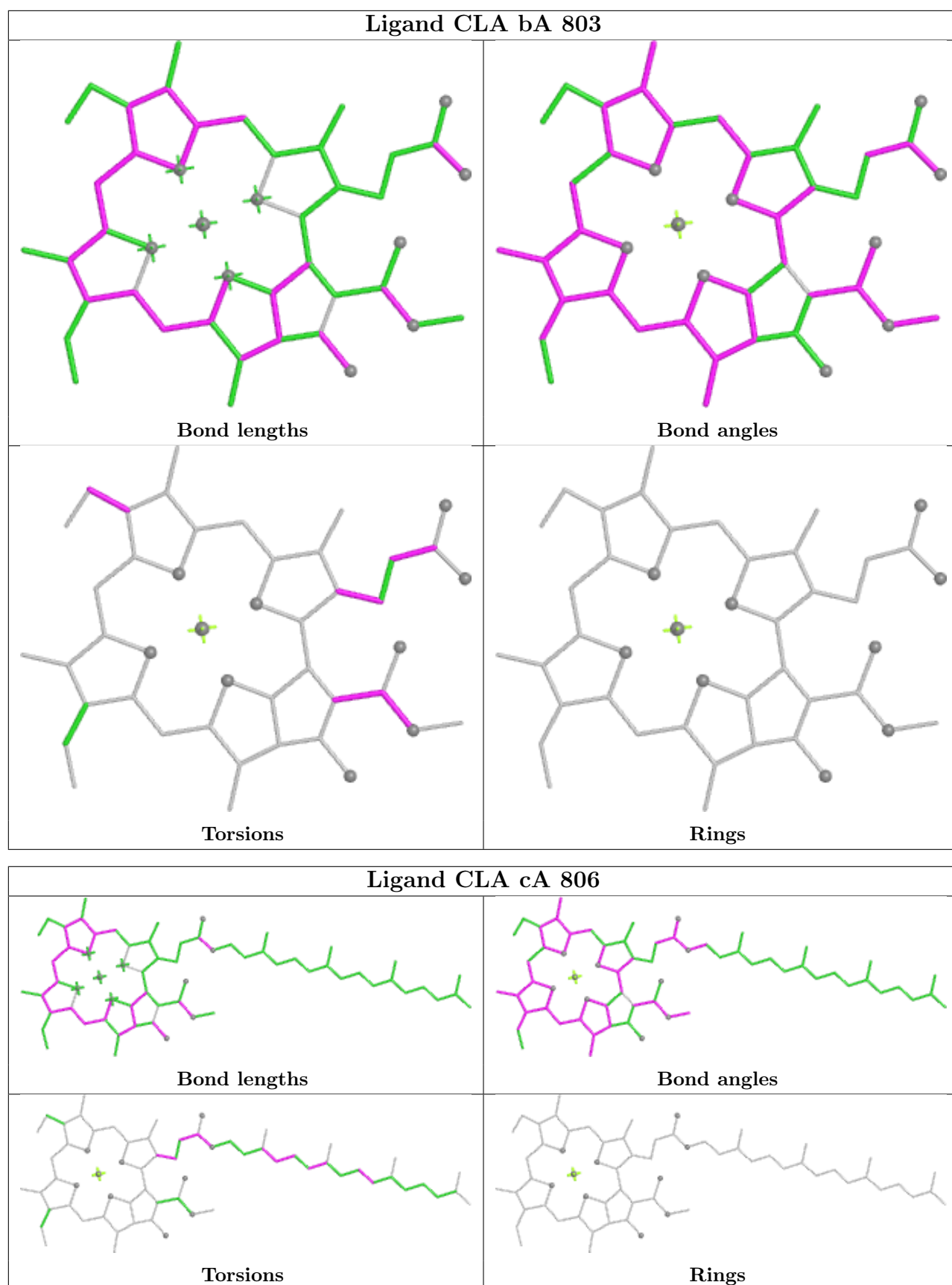
Ligand CLA B 819

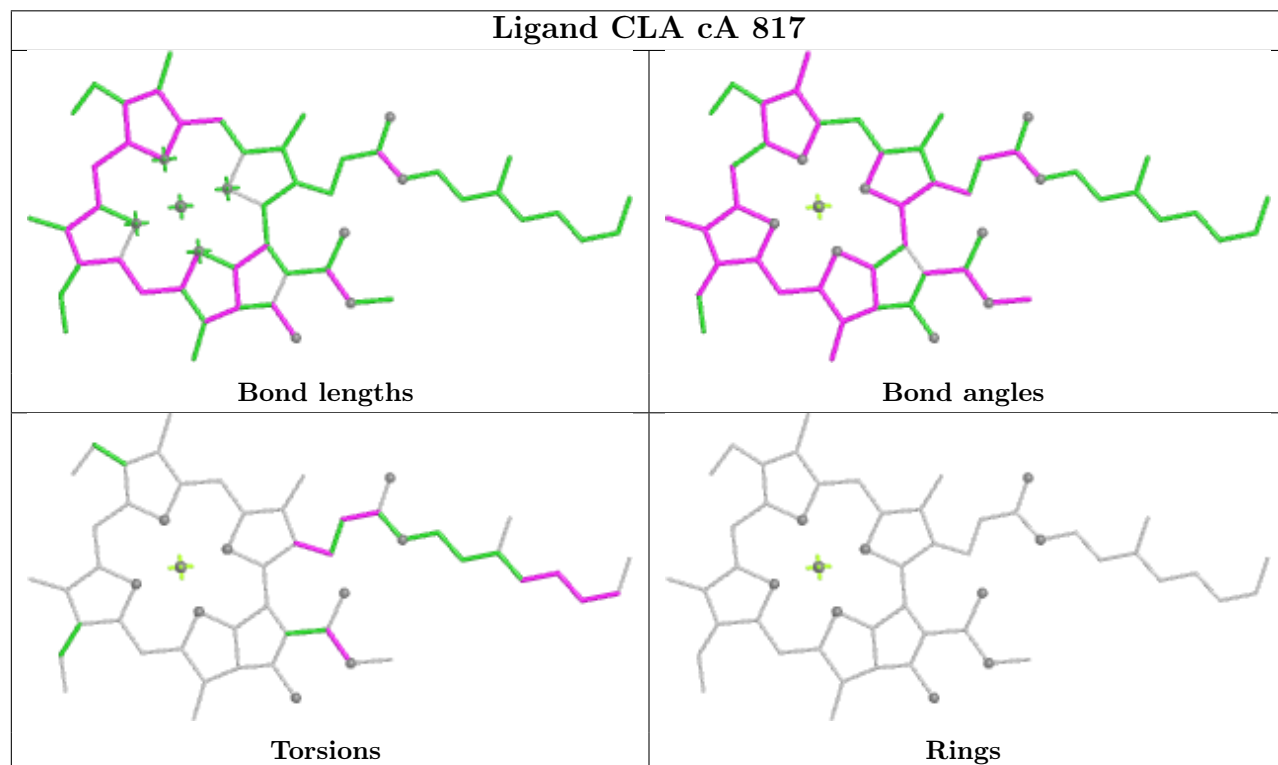
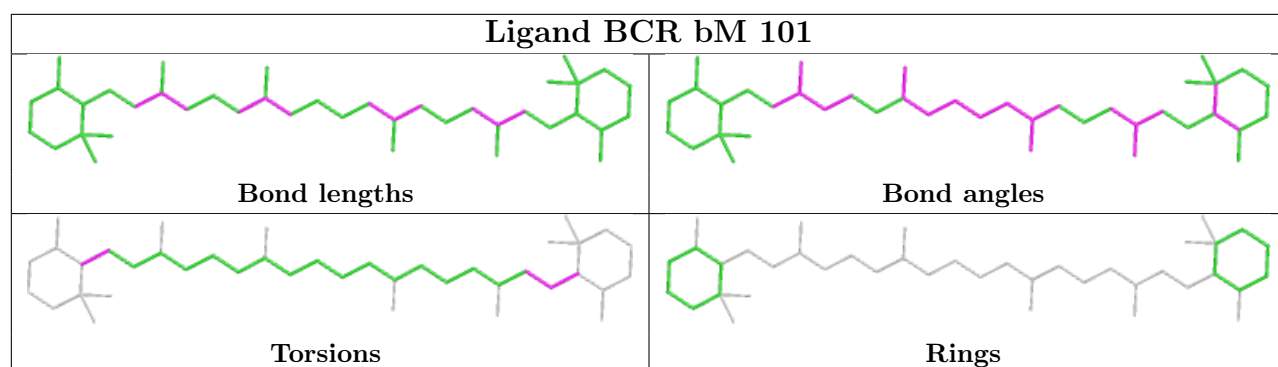




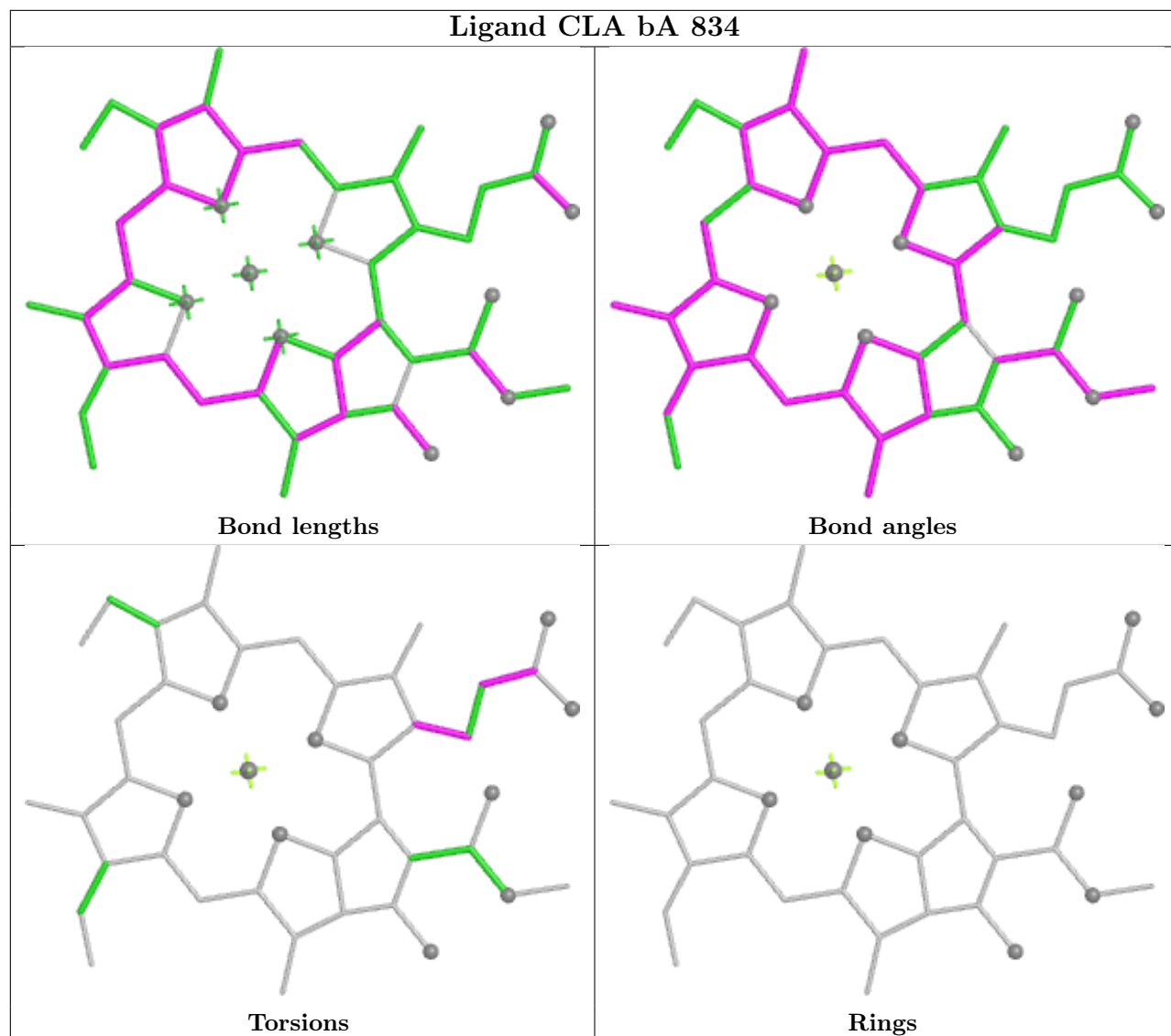




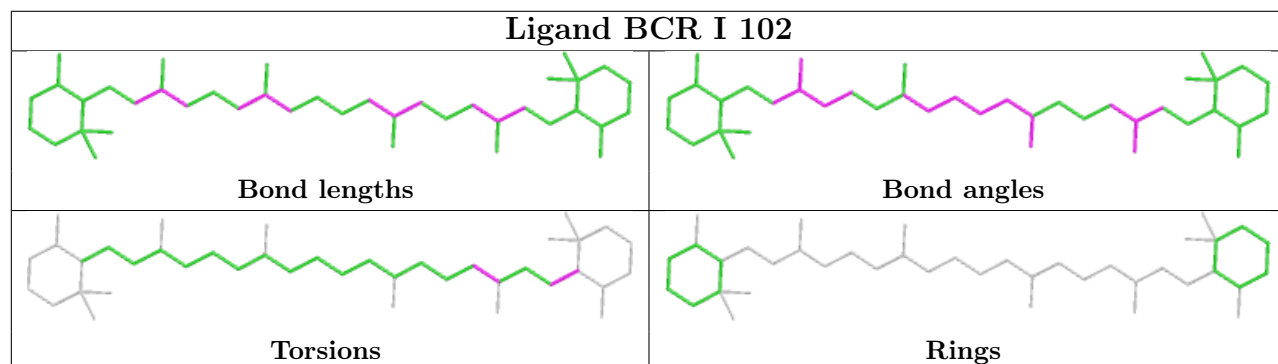


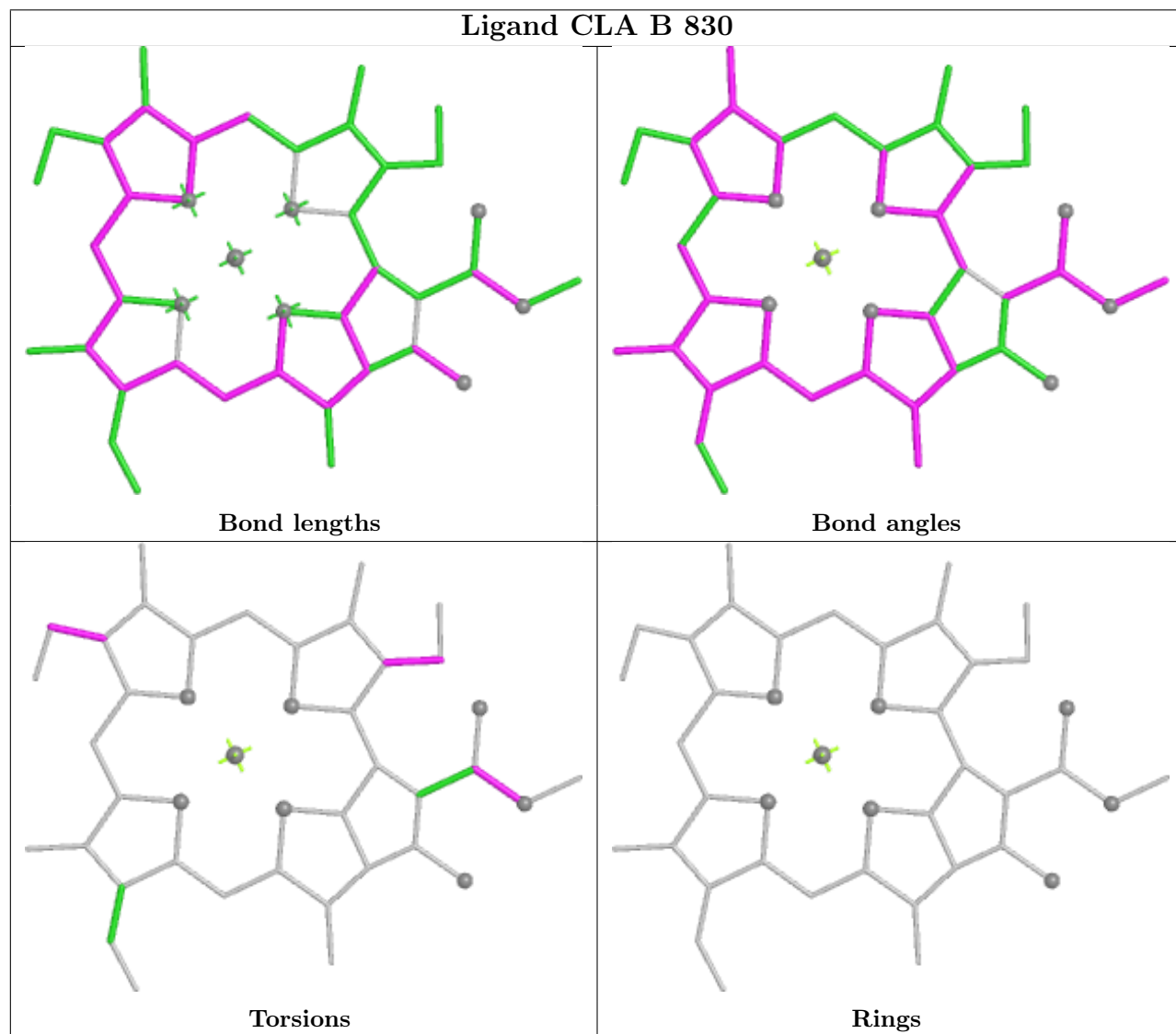
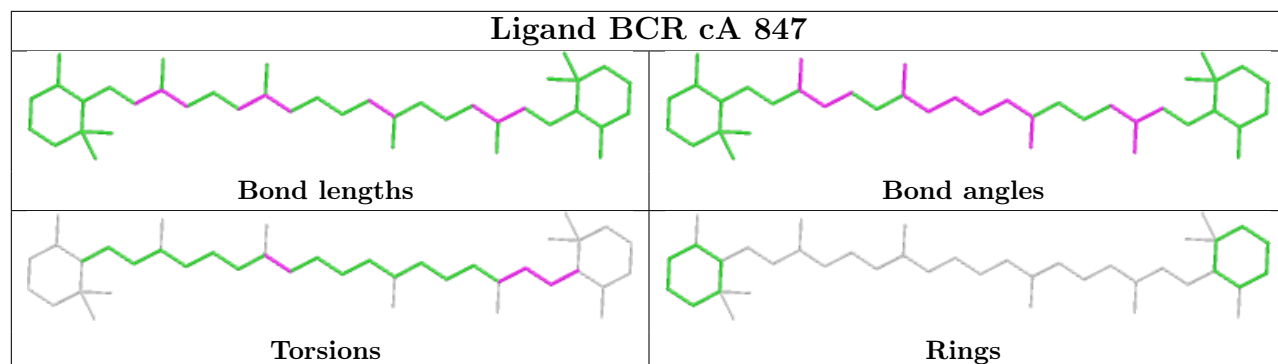


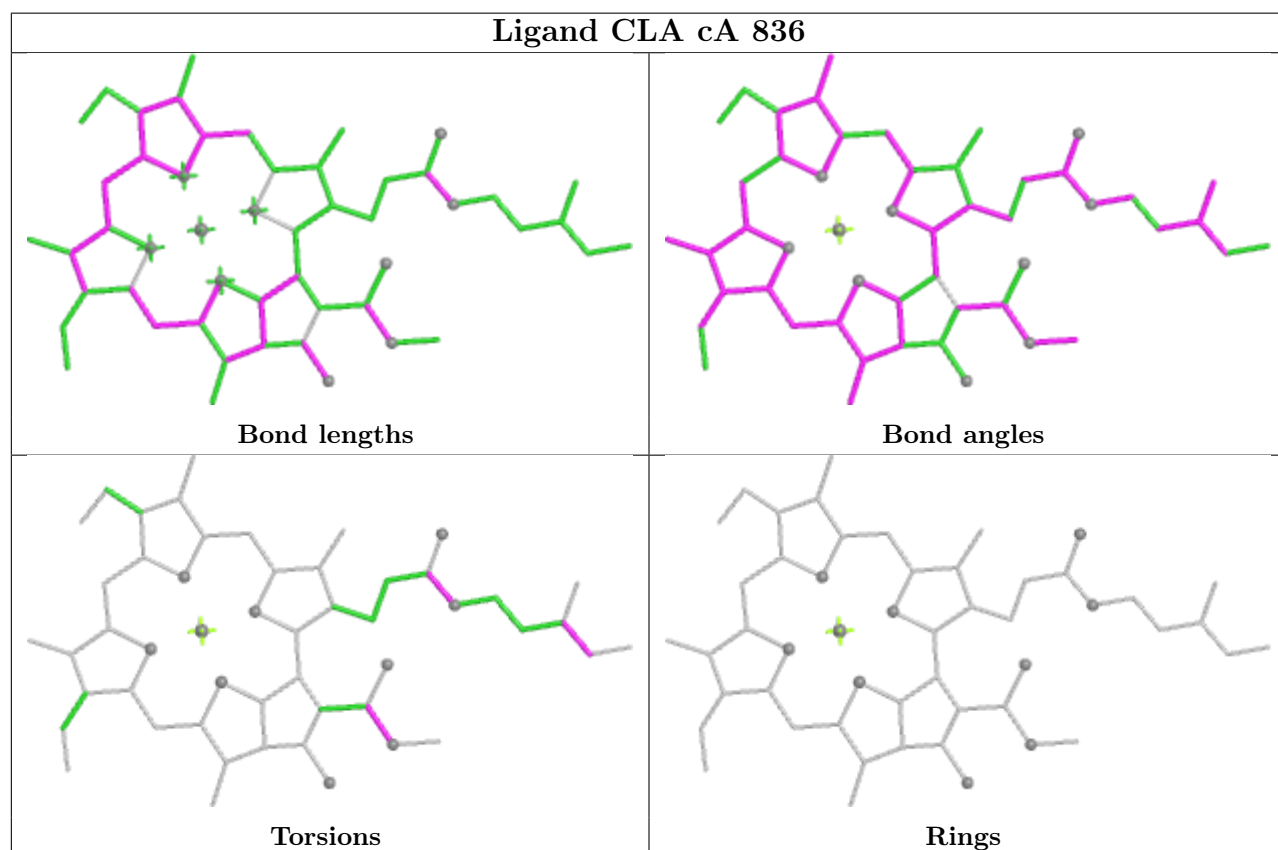
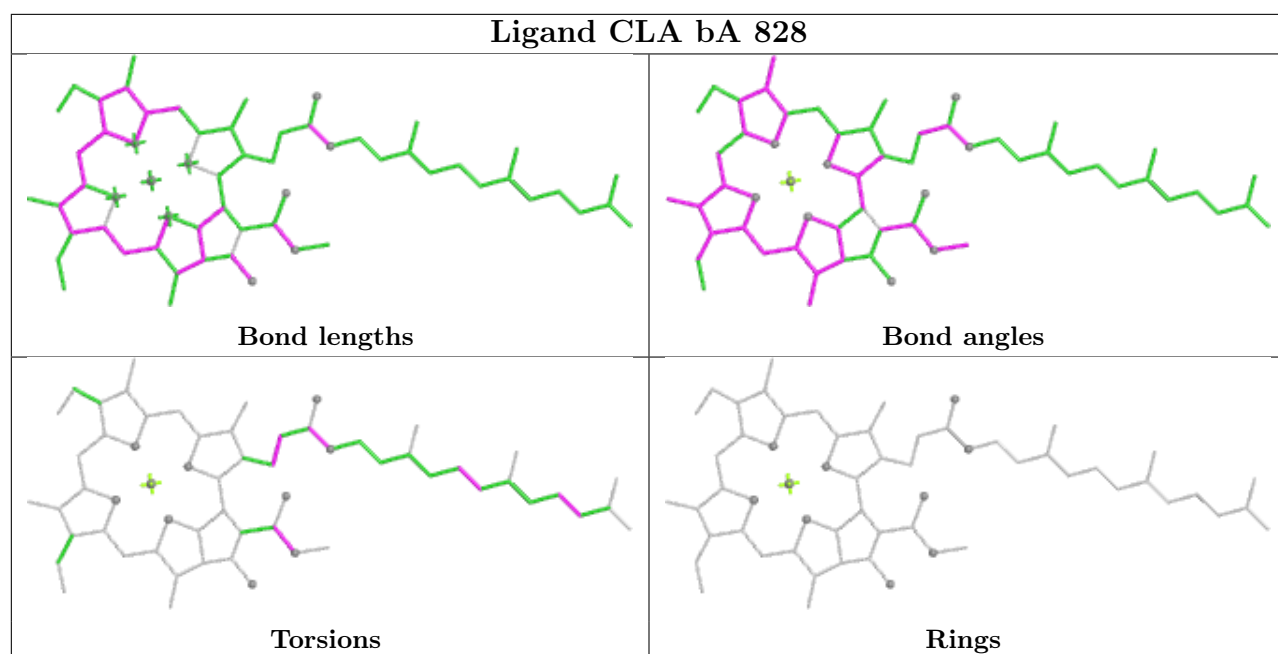
Ligand CLA bA 834



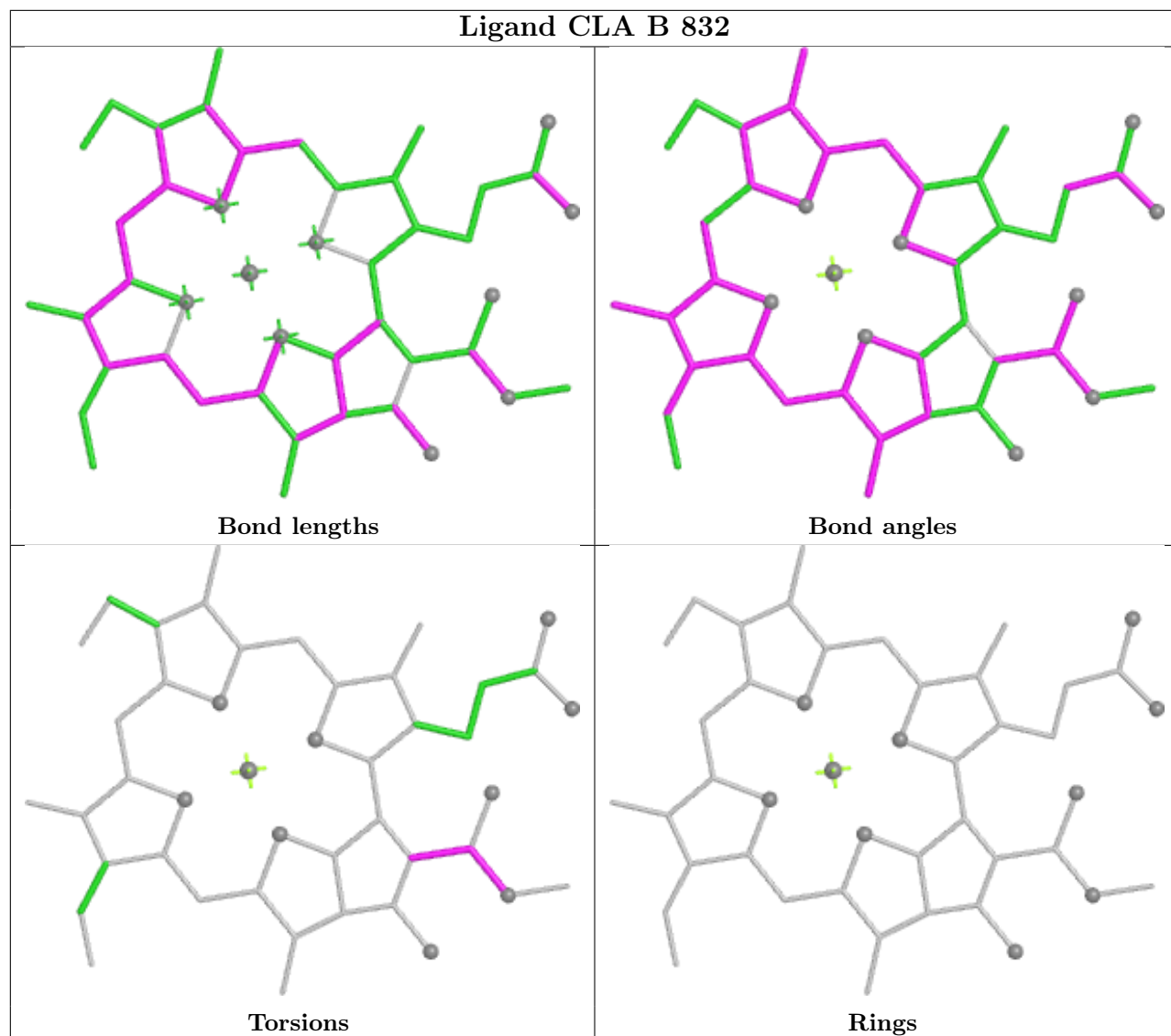
Ligand BCR I 102



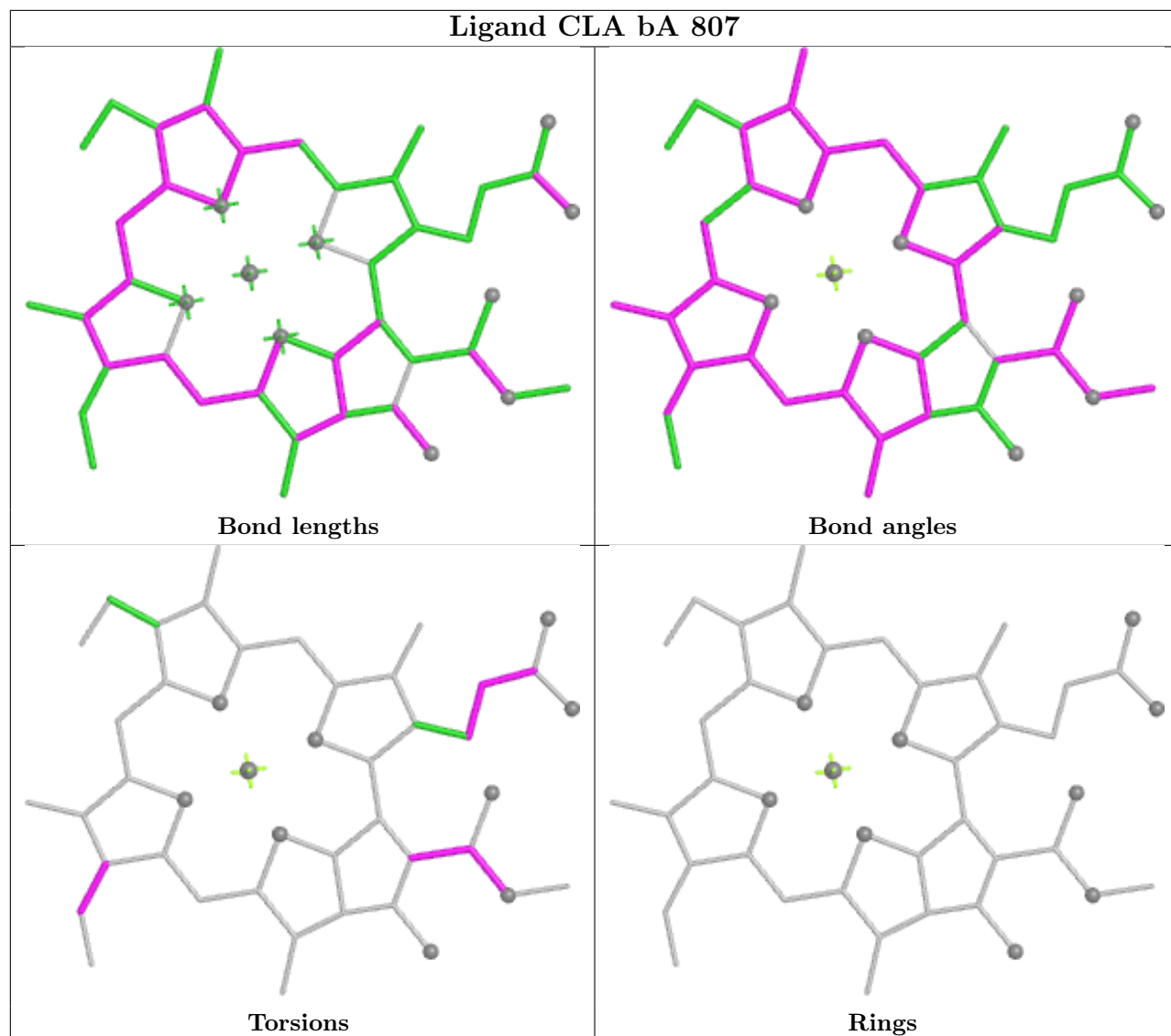


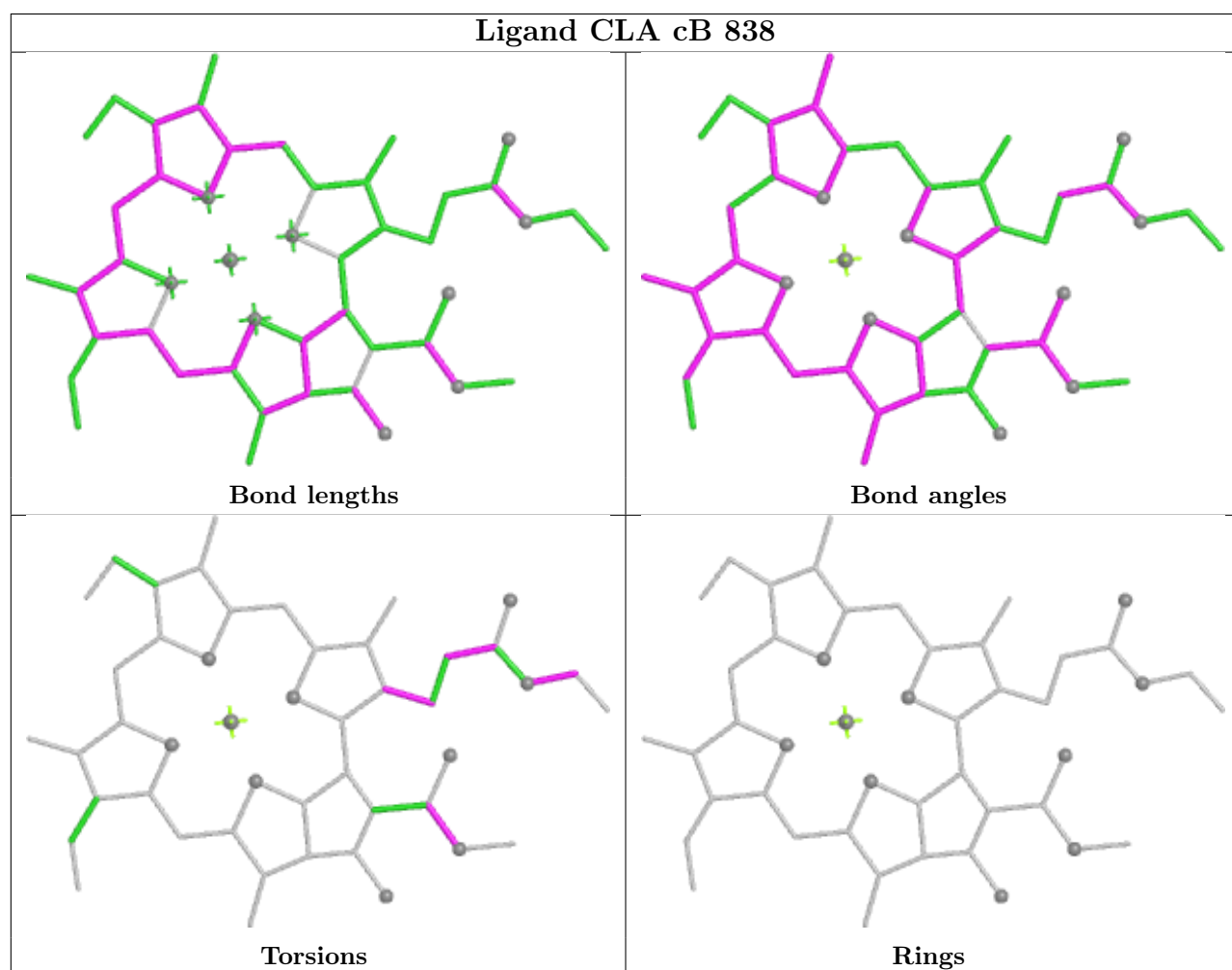
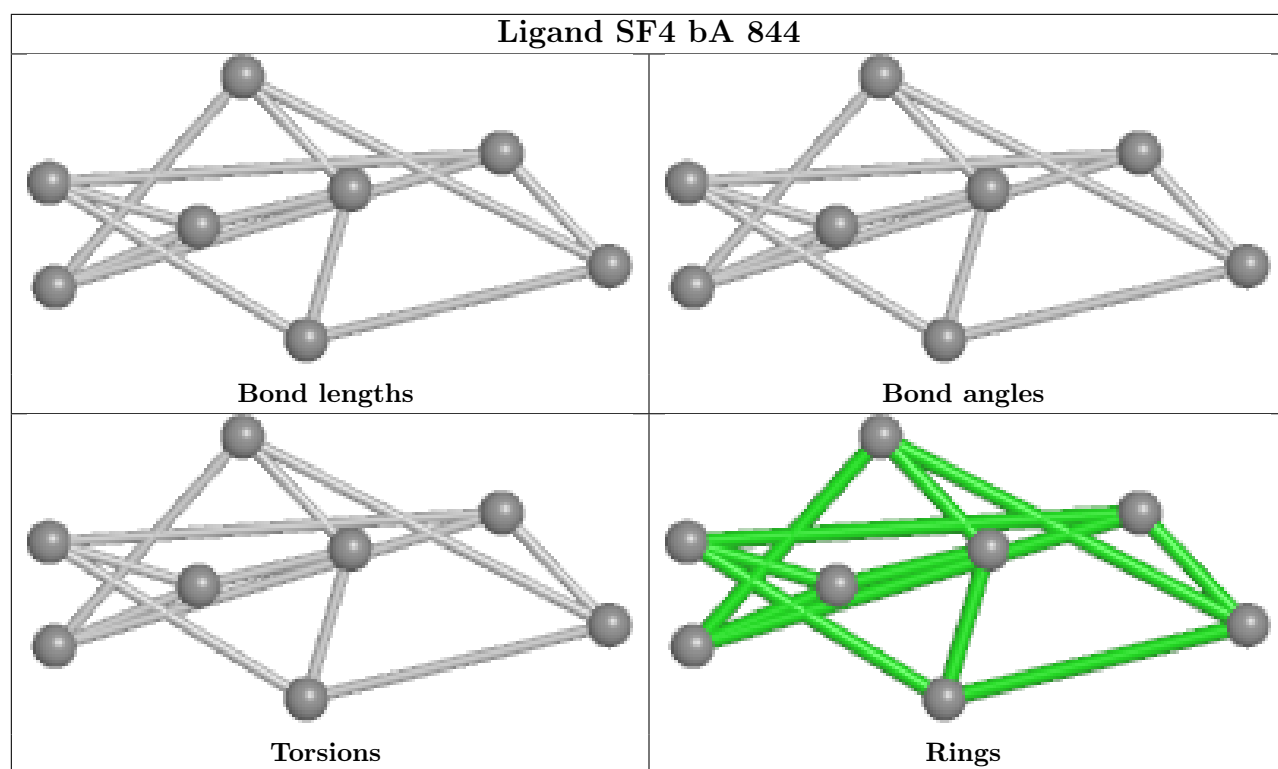


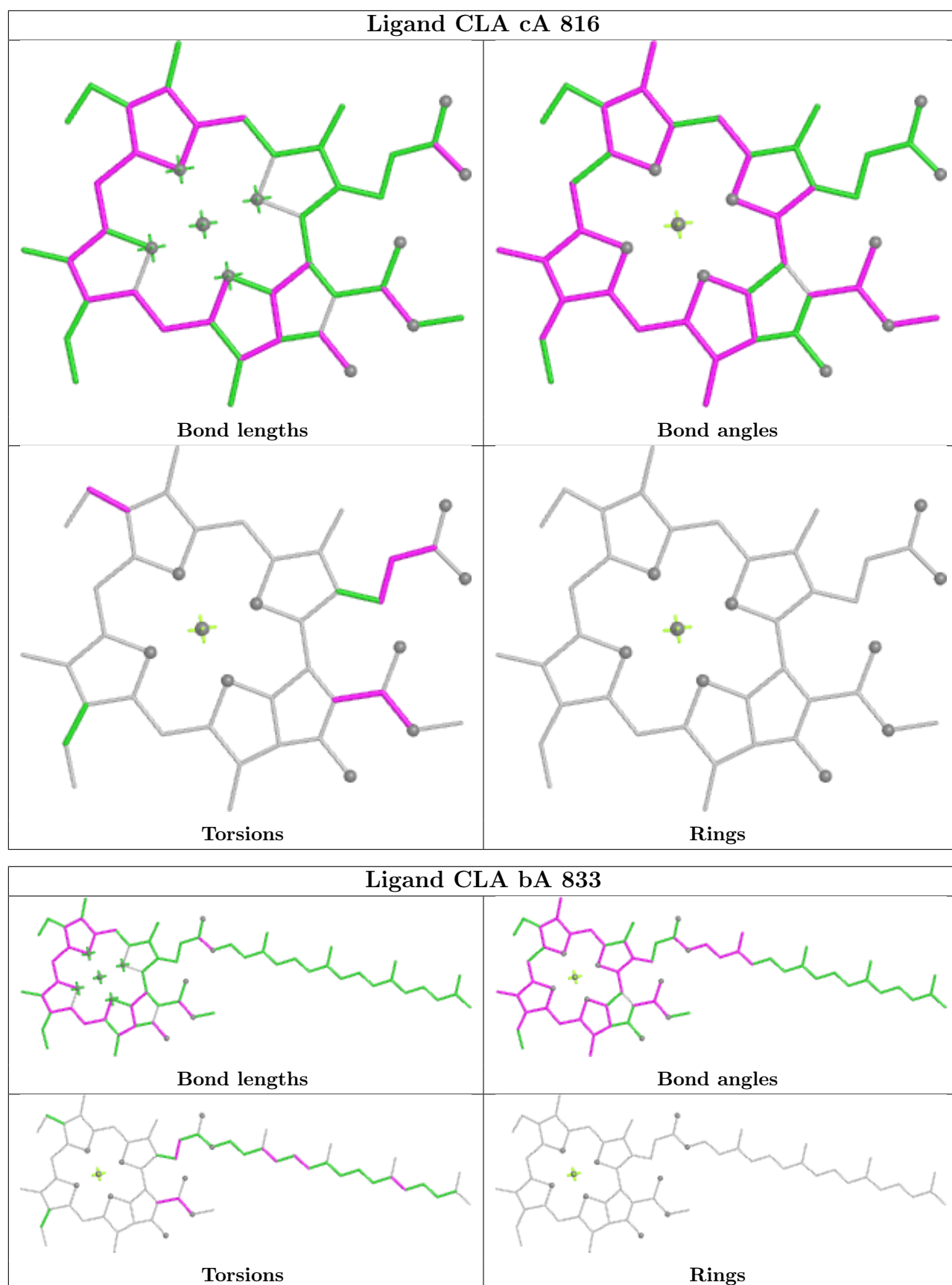
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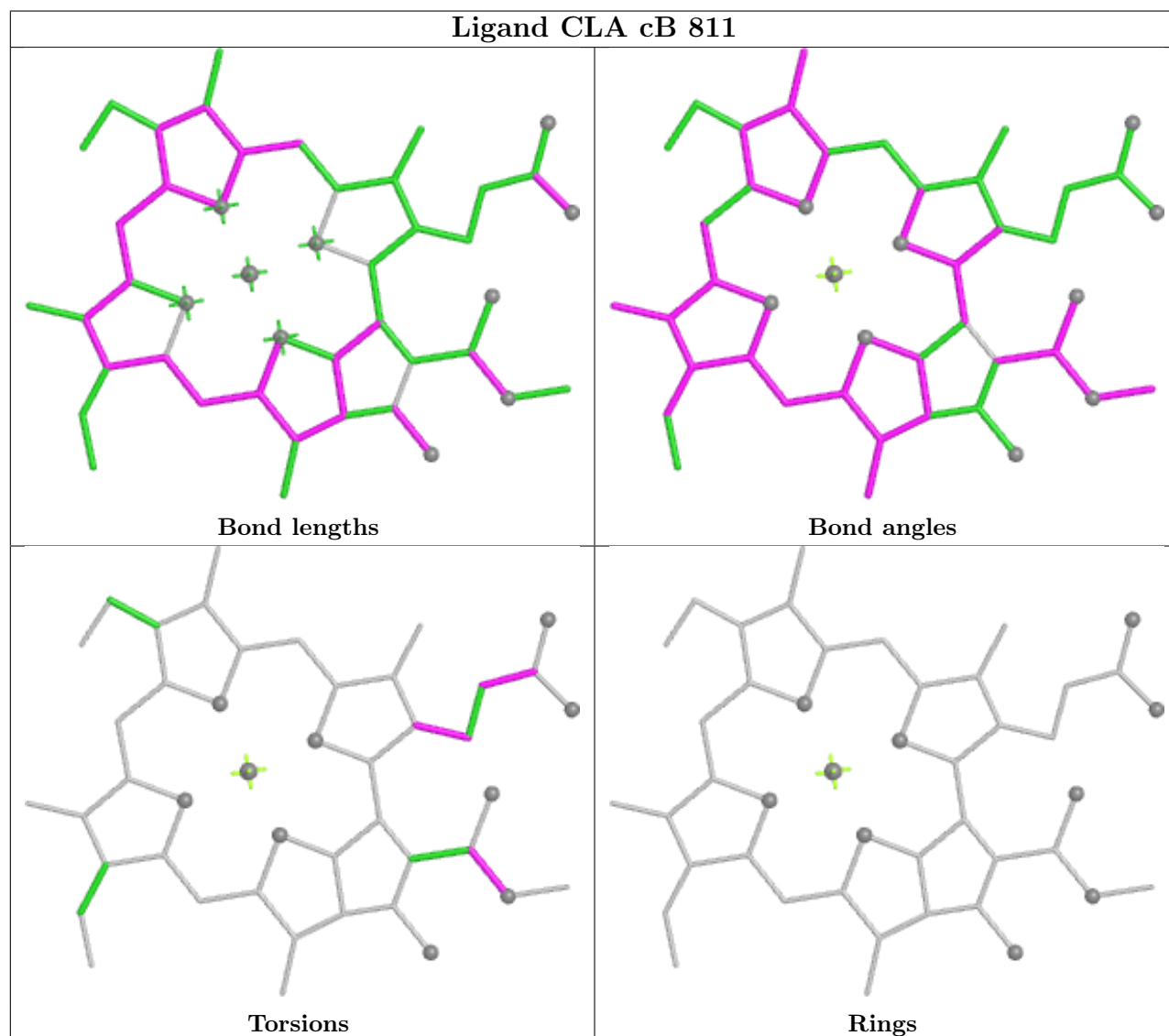
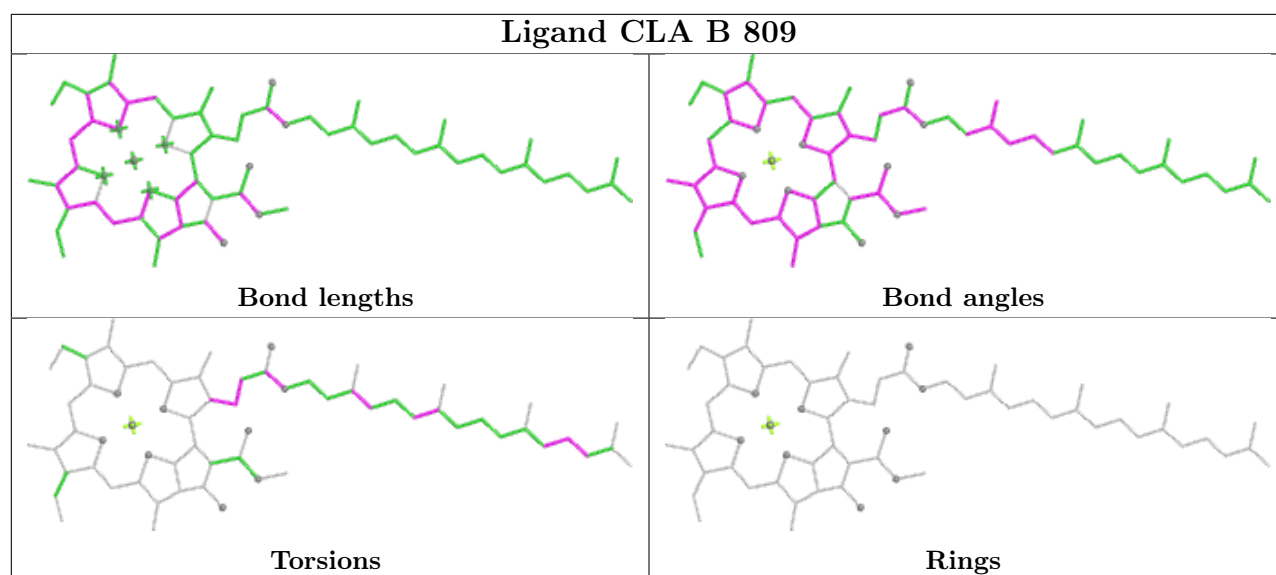


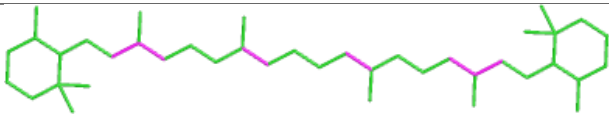
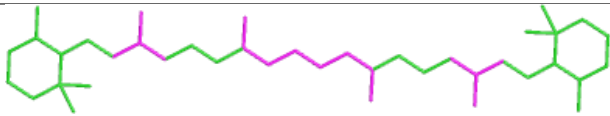
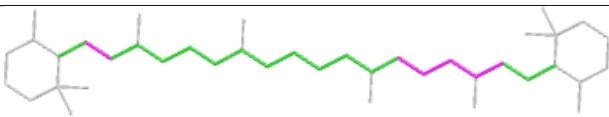
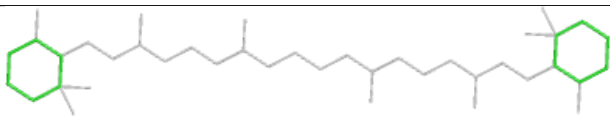
Ligand CLA bA 807

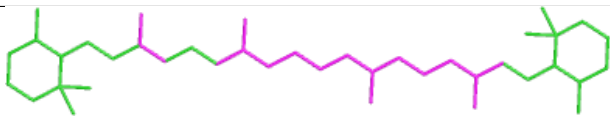
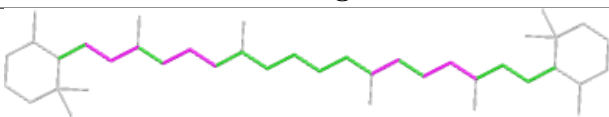
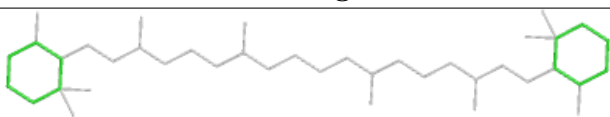


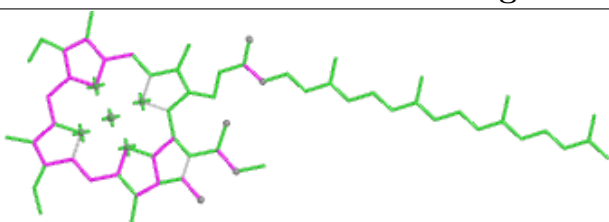
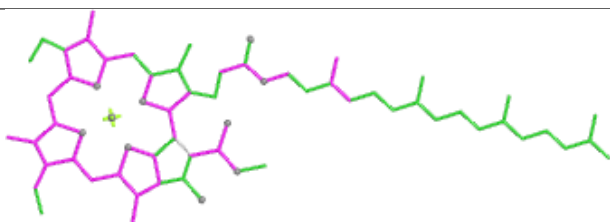
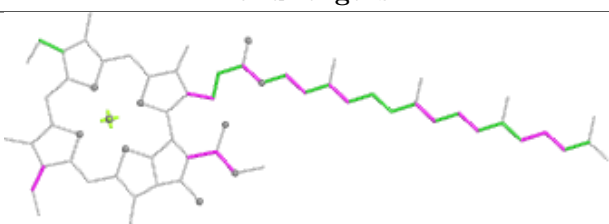
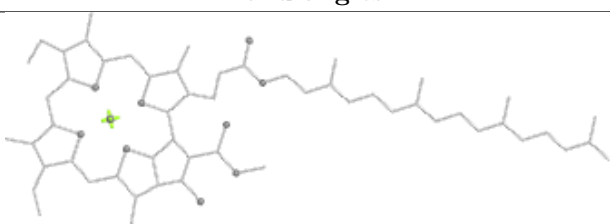




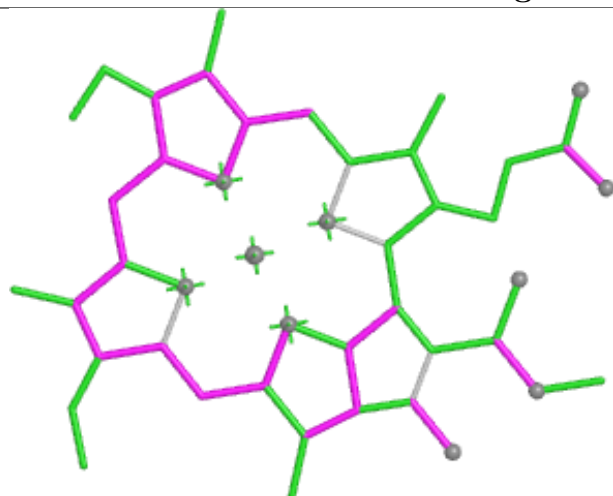


Ligand BCR bB 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

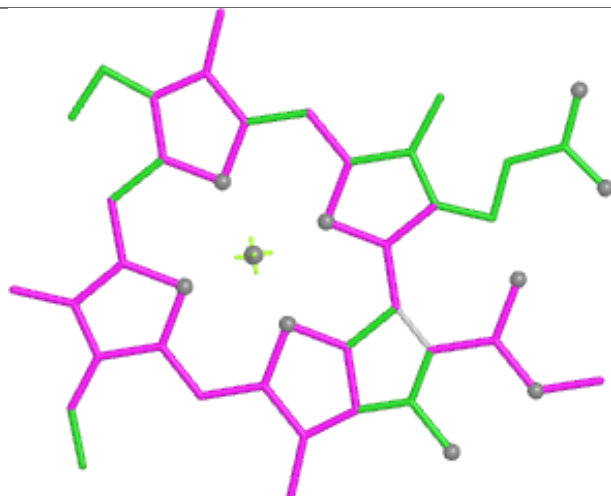
Ligand BCR bA 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bB 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

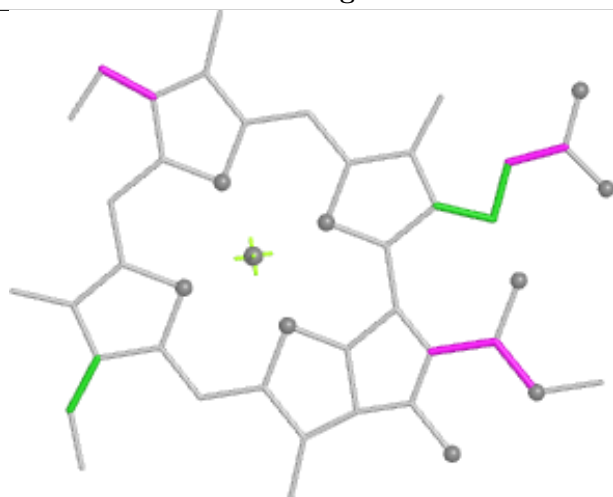
Ligand CLA B 836



Bond lengths



Bond angles

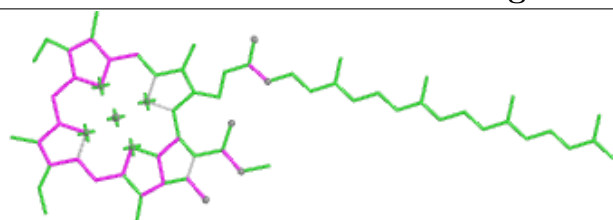


Torsions

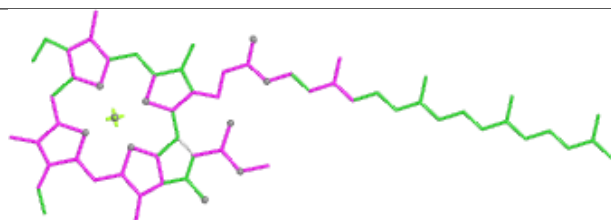


Rings

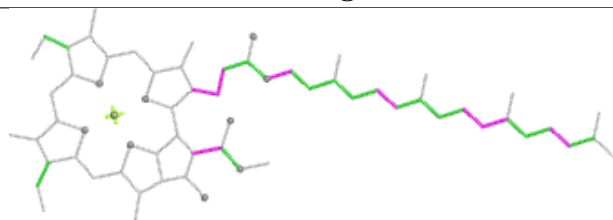
Ligand CLA cL 202



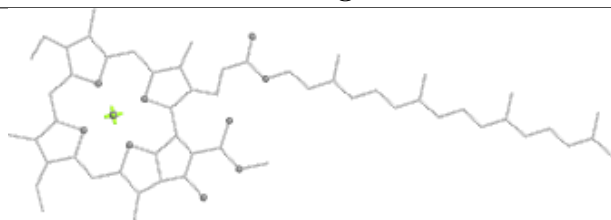
Bond lengths



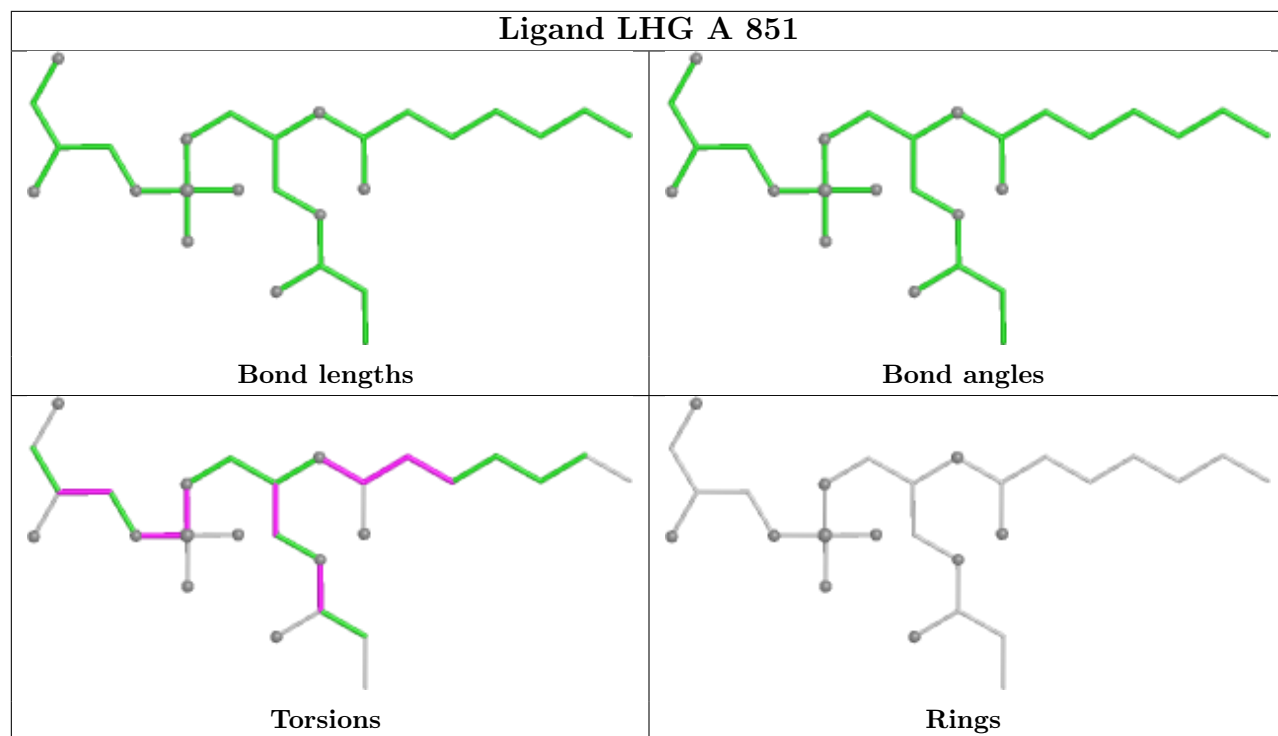
Bond angles

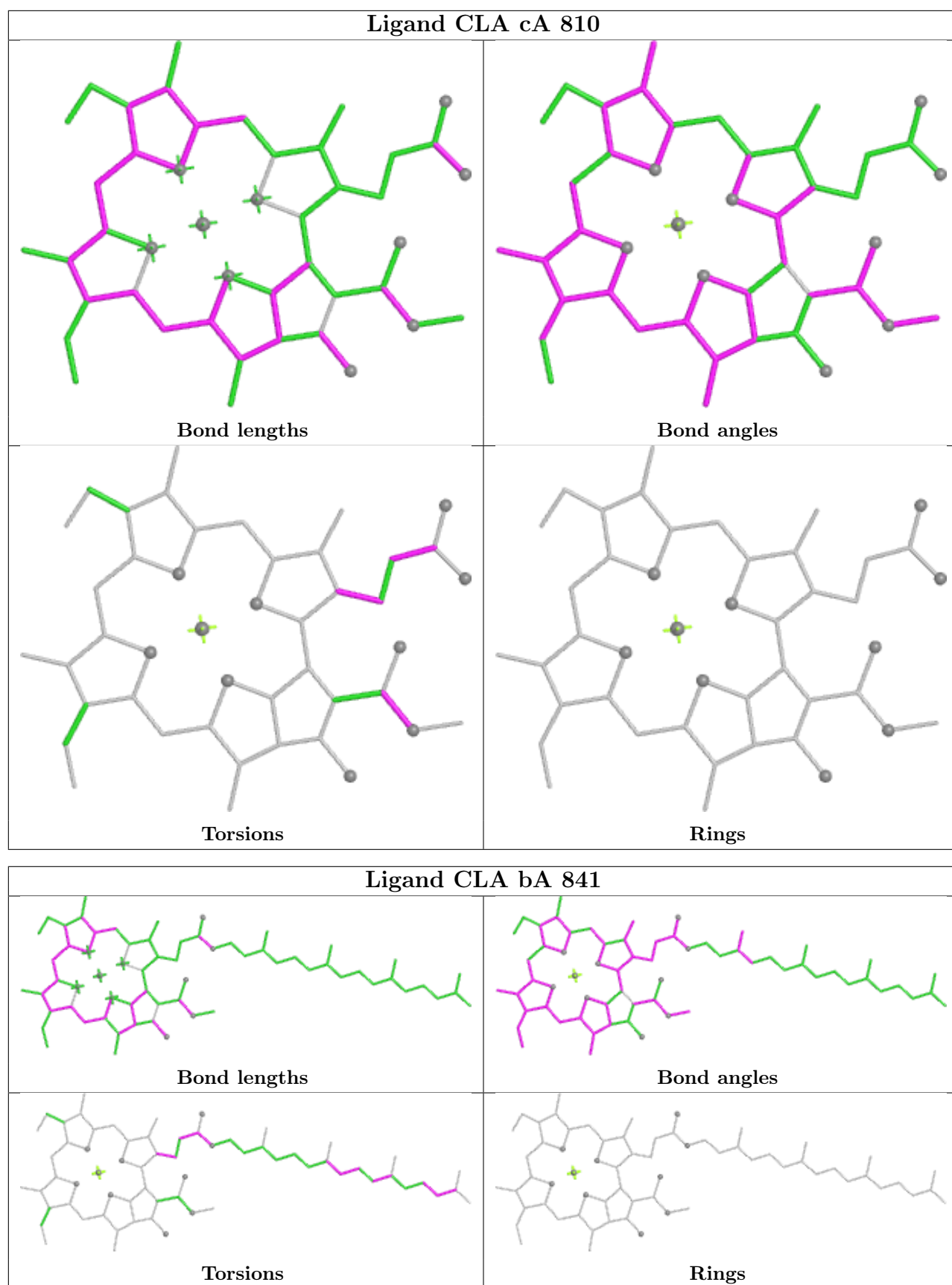


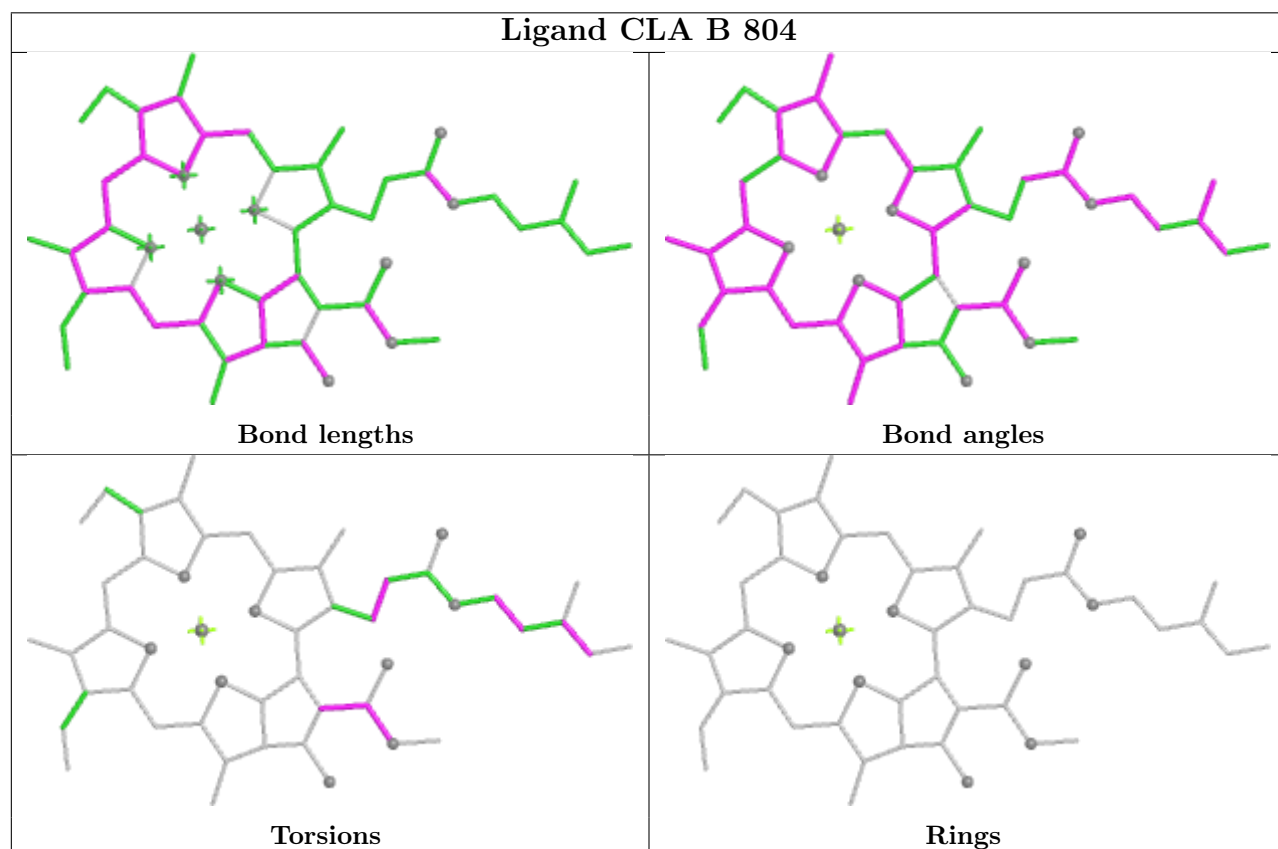
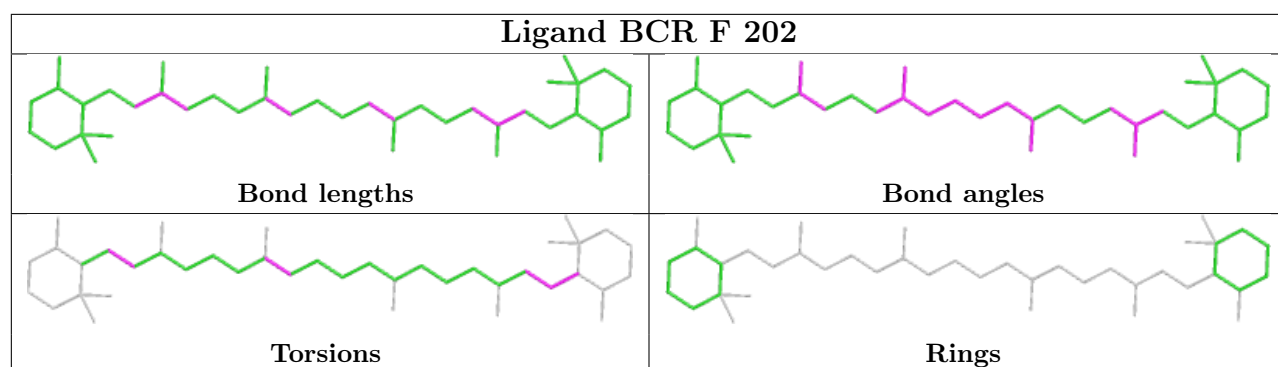
Torsions

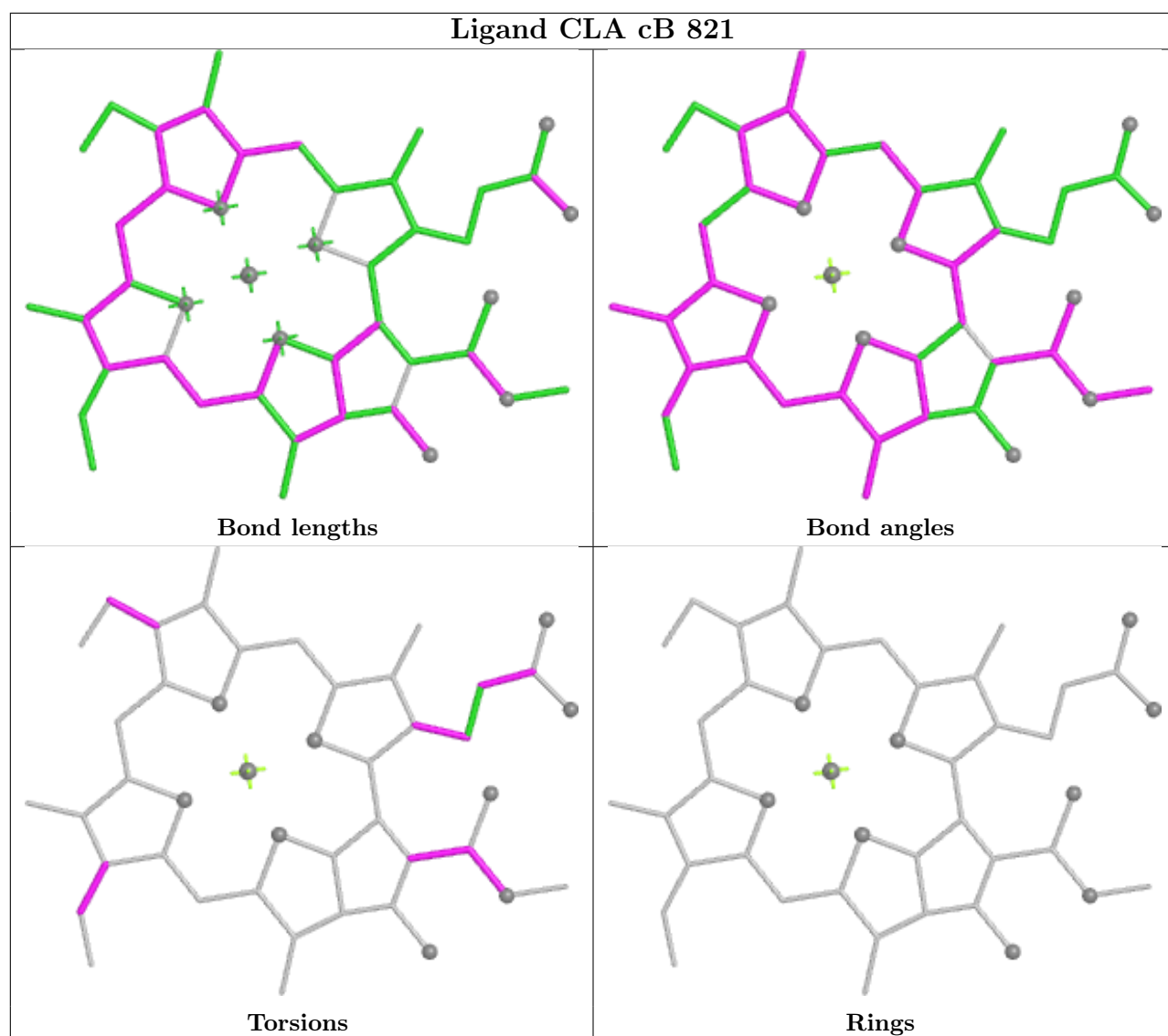


Rings

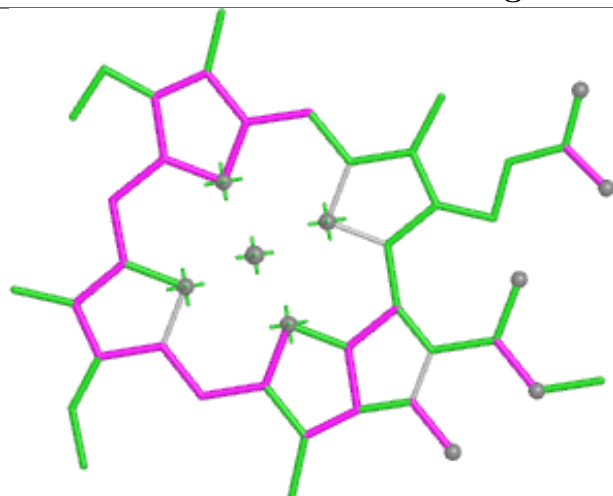




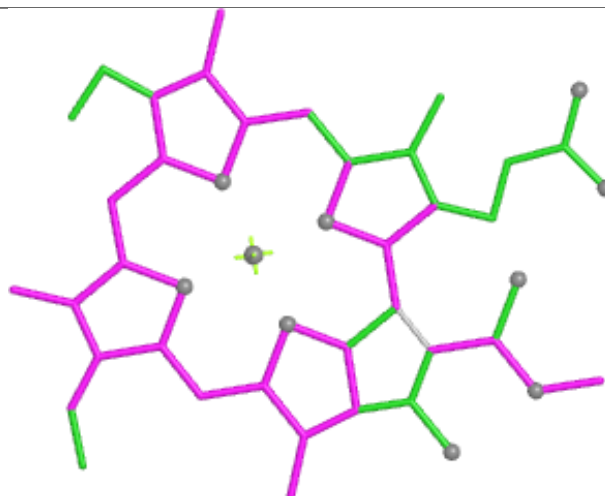




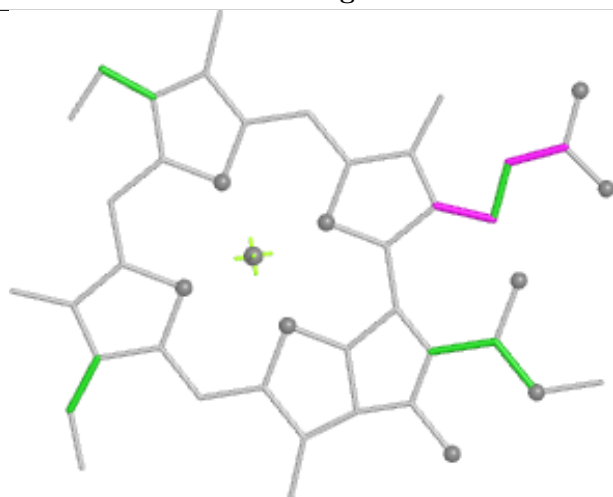
Ligand CLA bB 811



Bond lengths



Bond angles

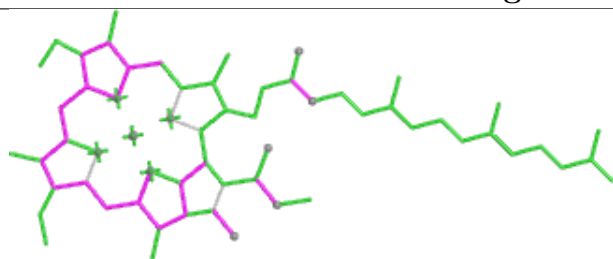


Torsions

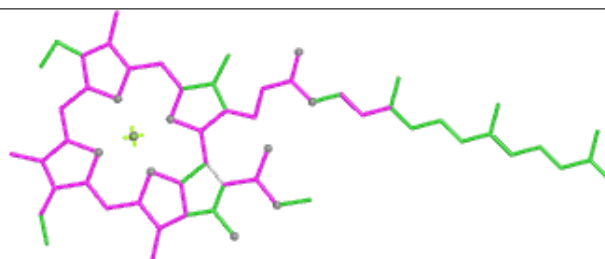


Rings

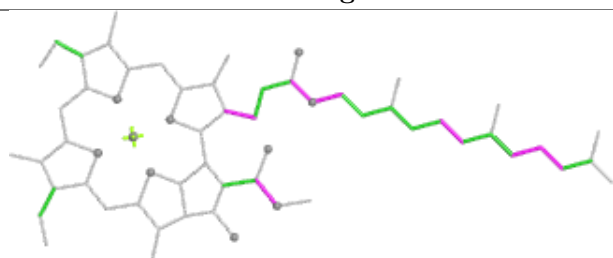
Ligand CLA bA 818



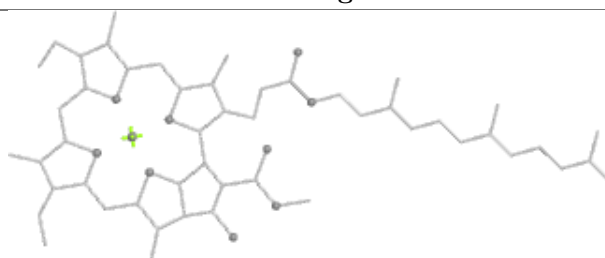
Bond lengths



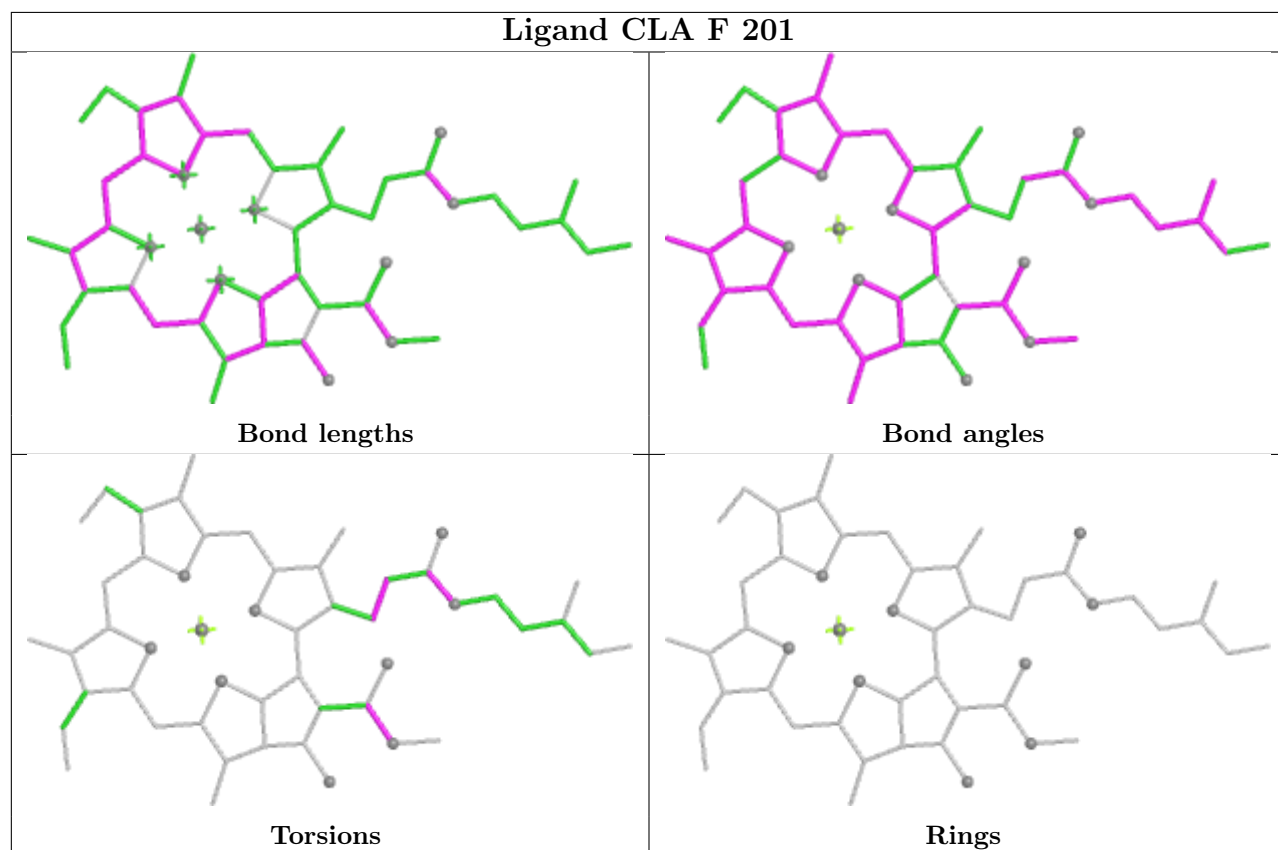
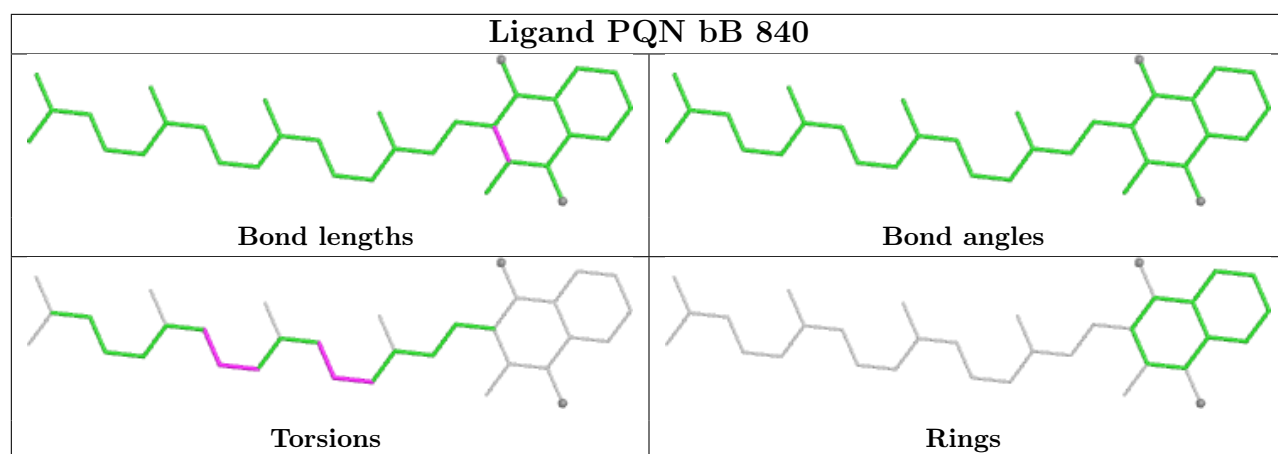
Bond angles

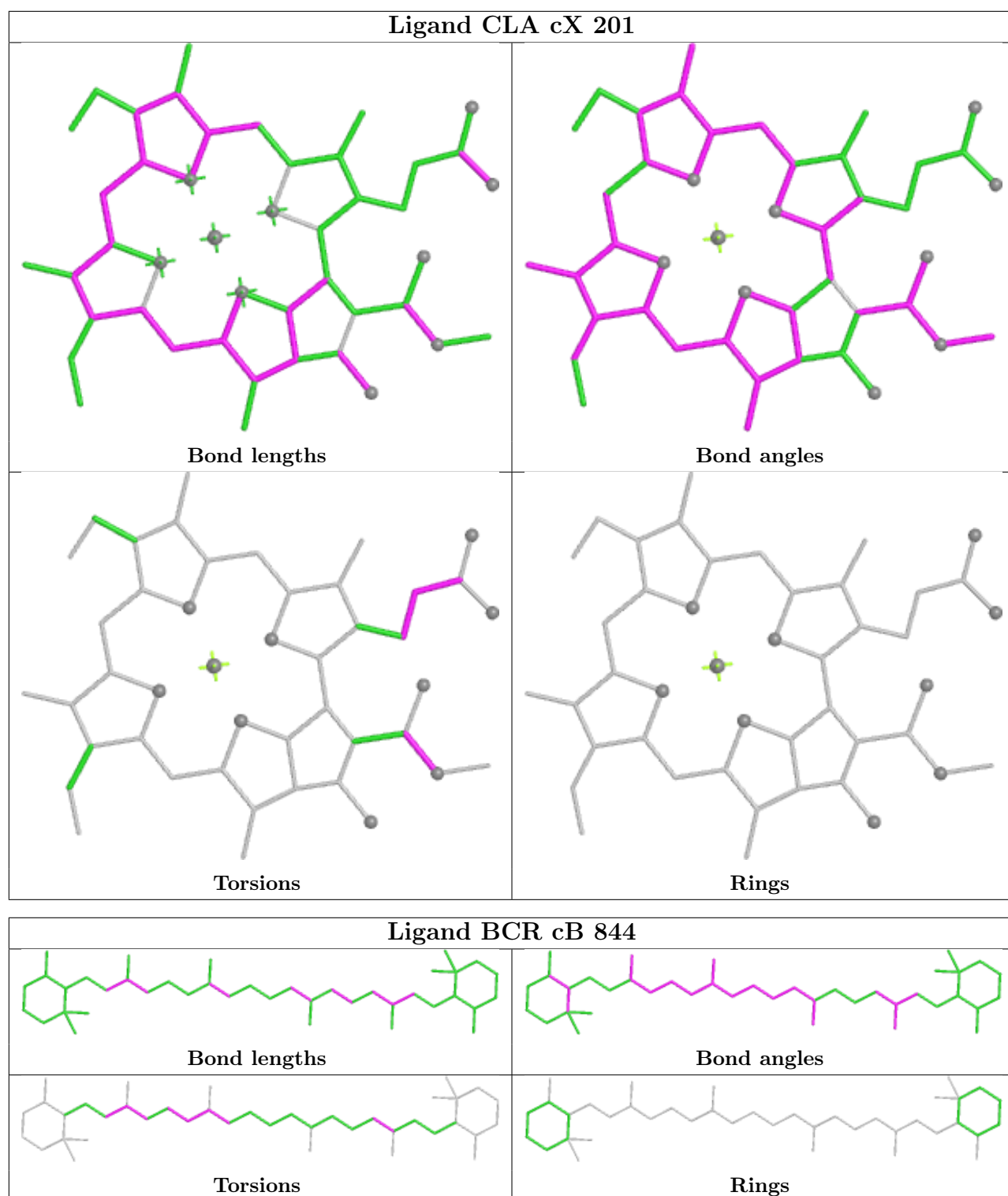


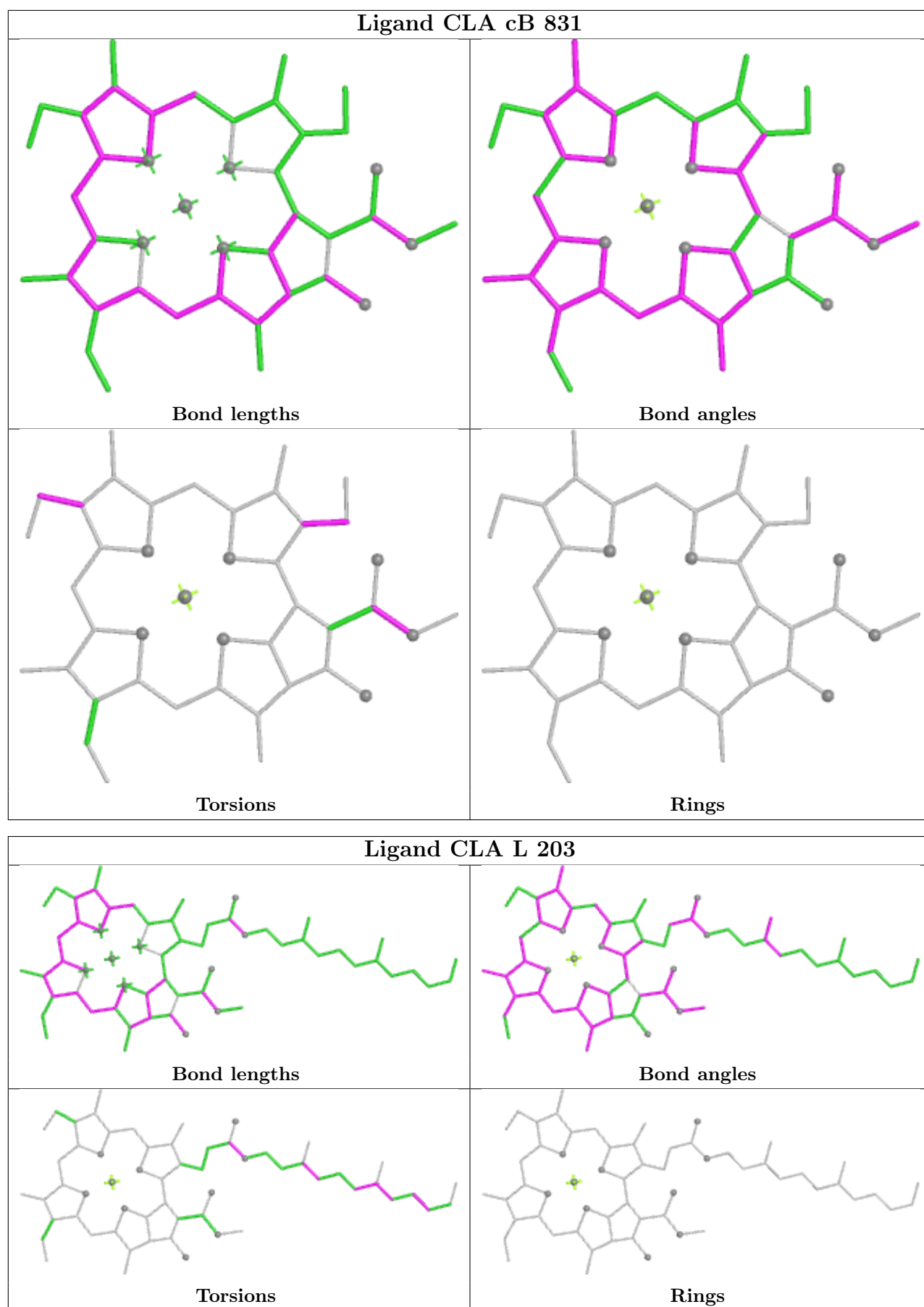
Torsions



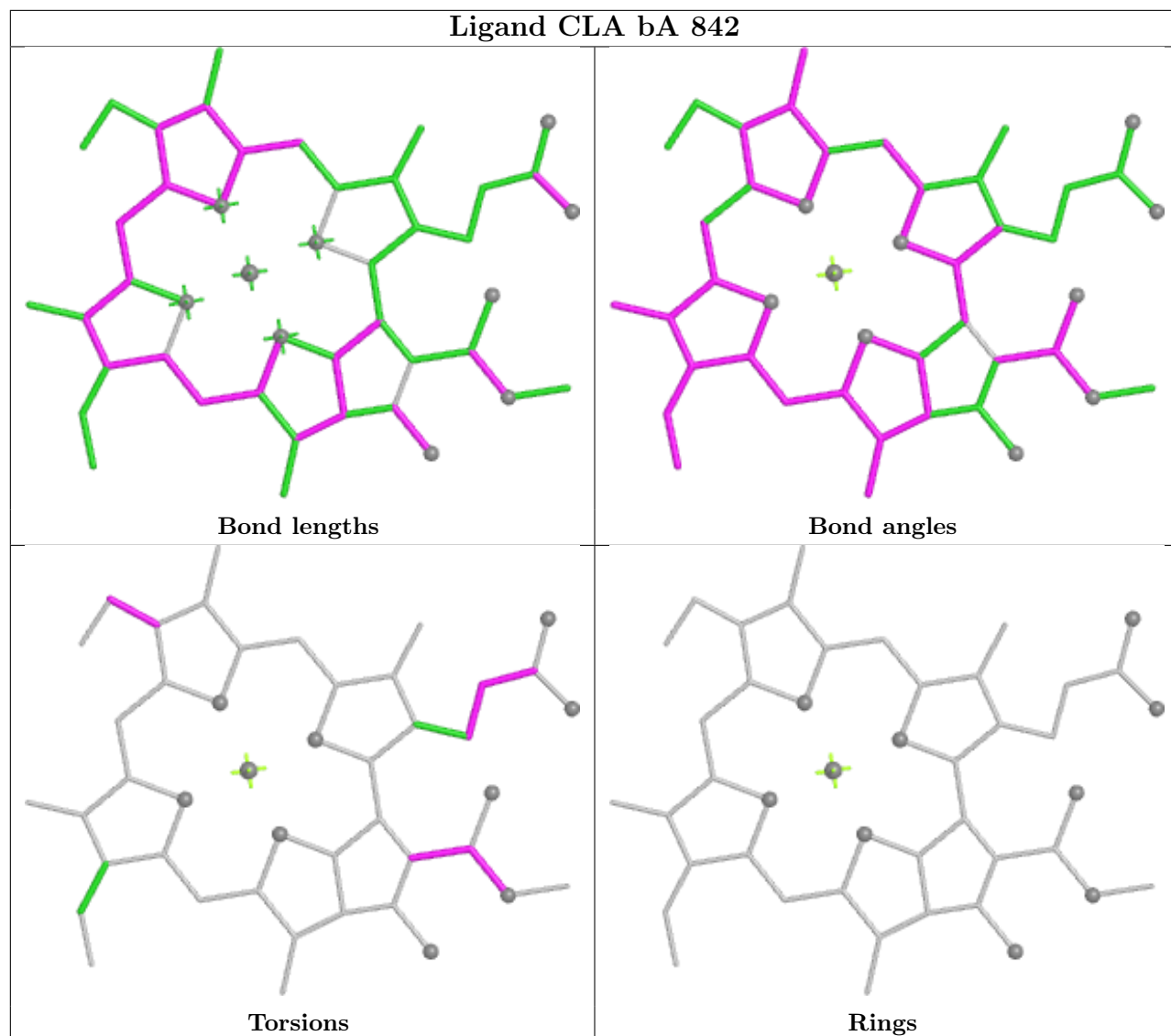
Rings

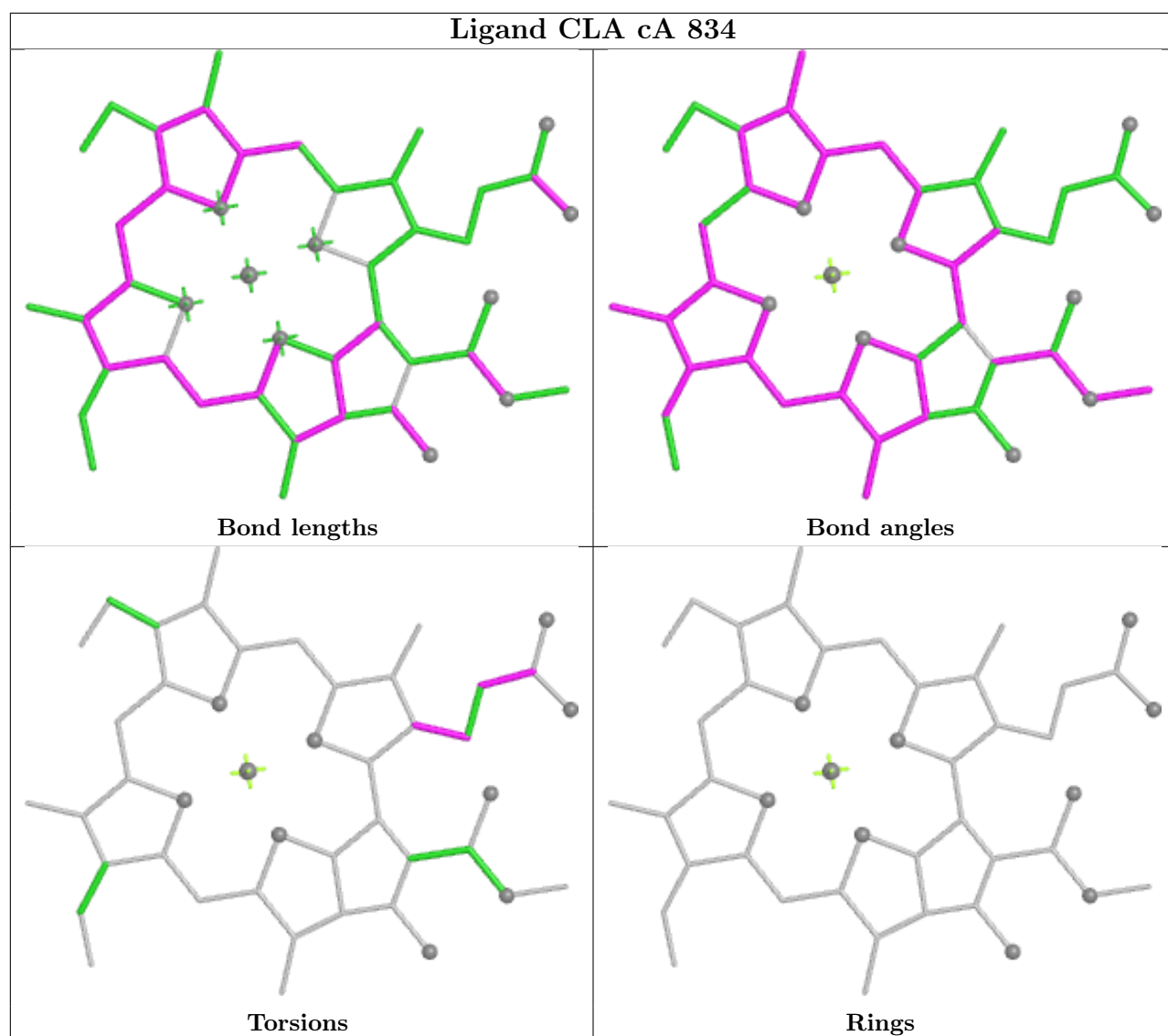




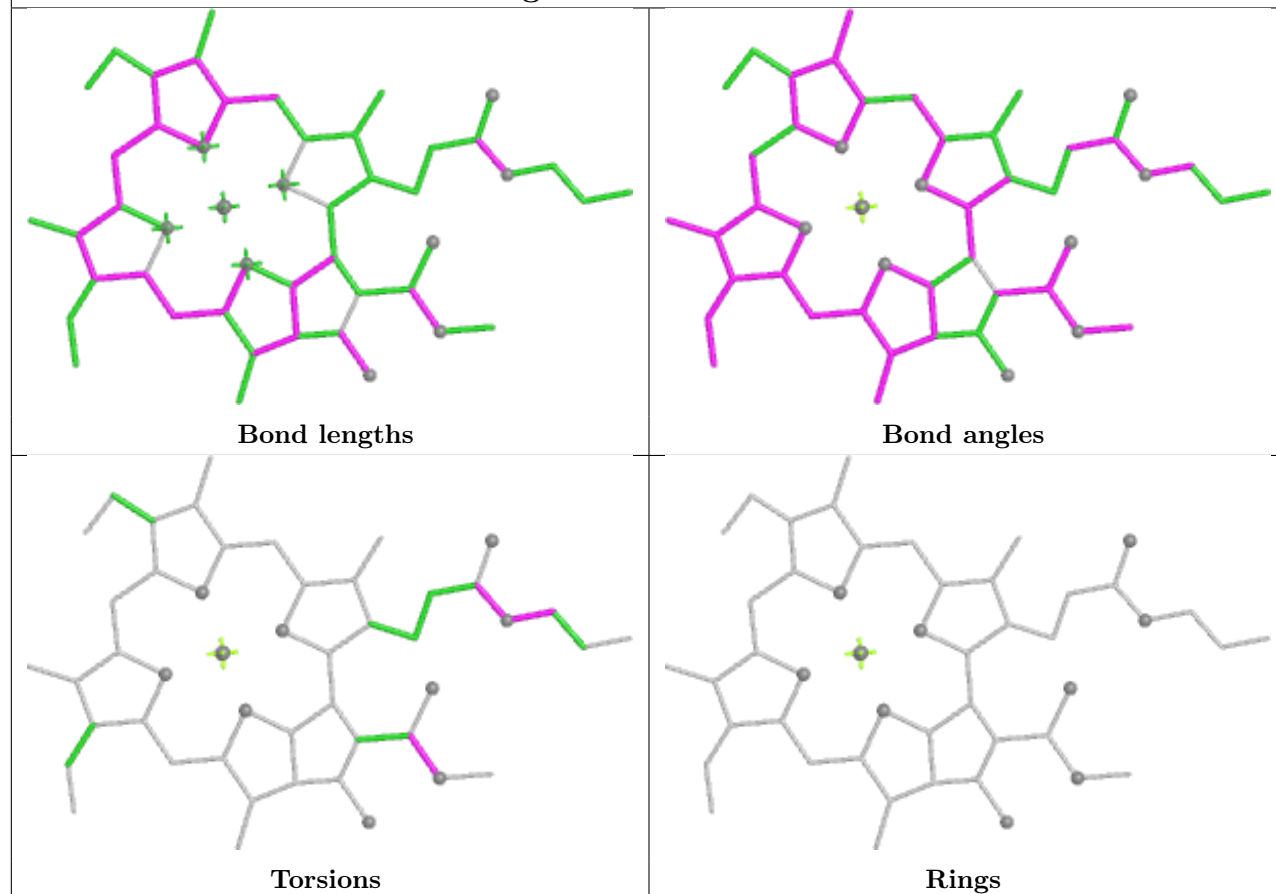


Ligand CLA bA 842

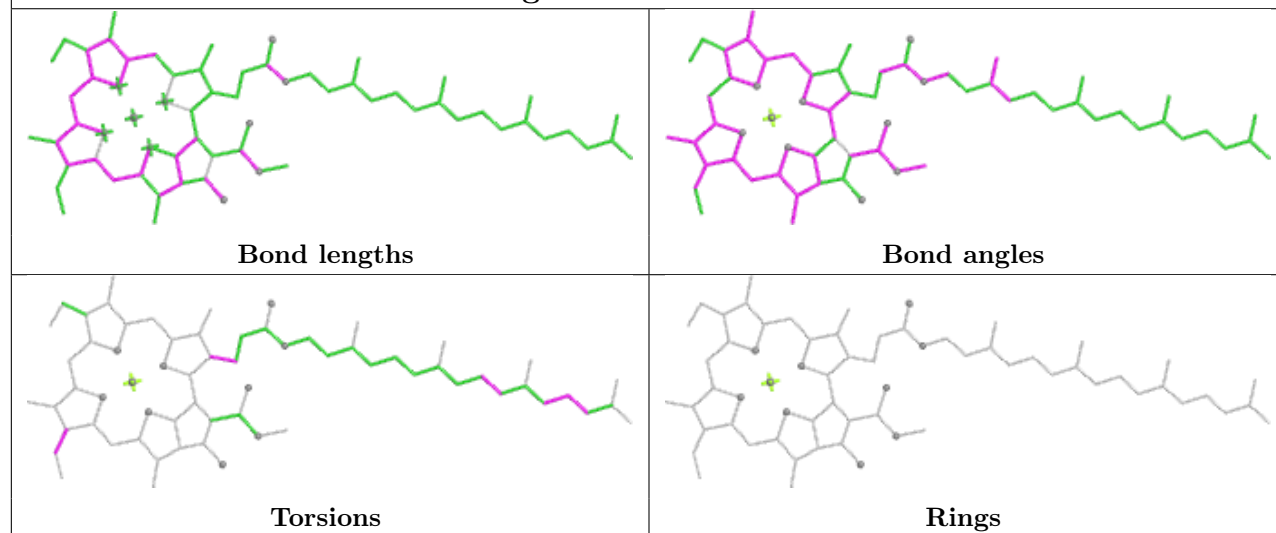




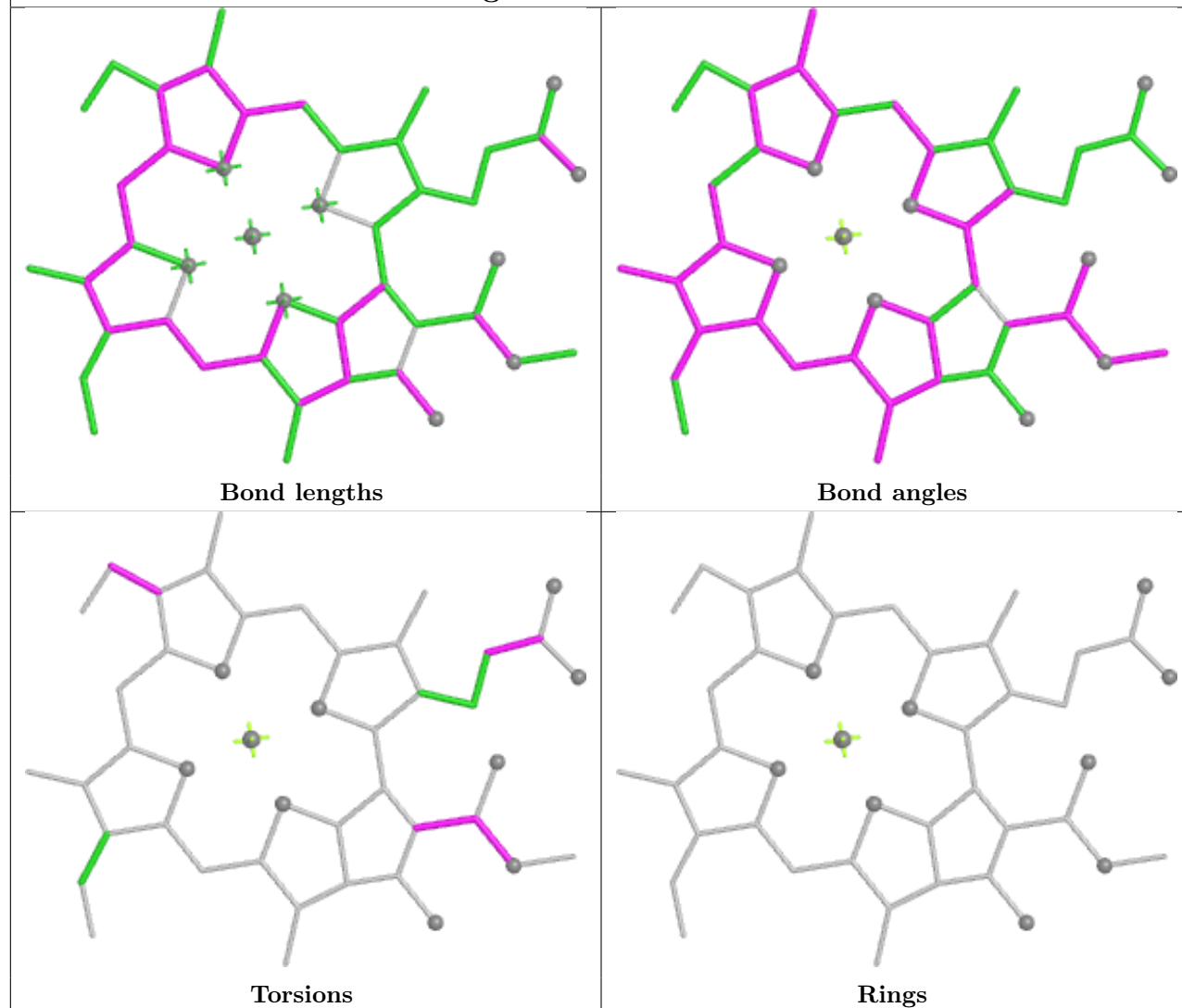
Ligand CLA bB 813



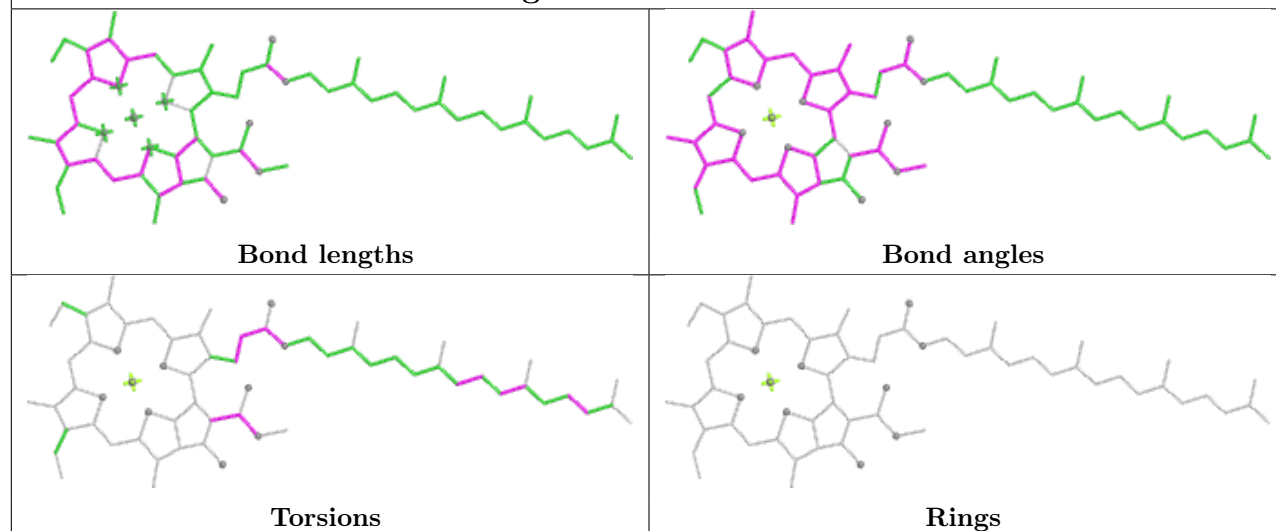
Ligand CLA bB 826

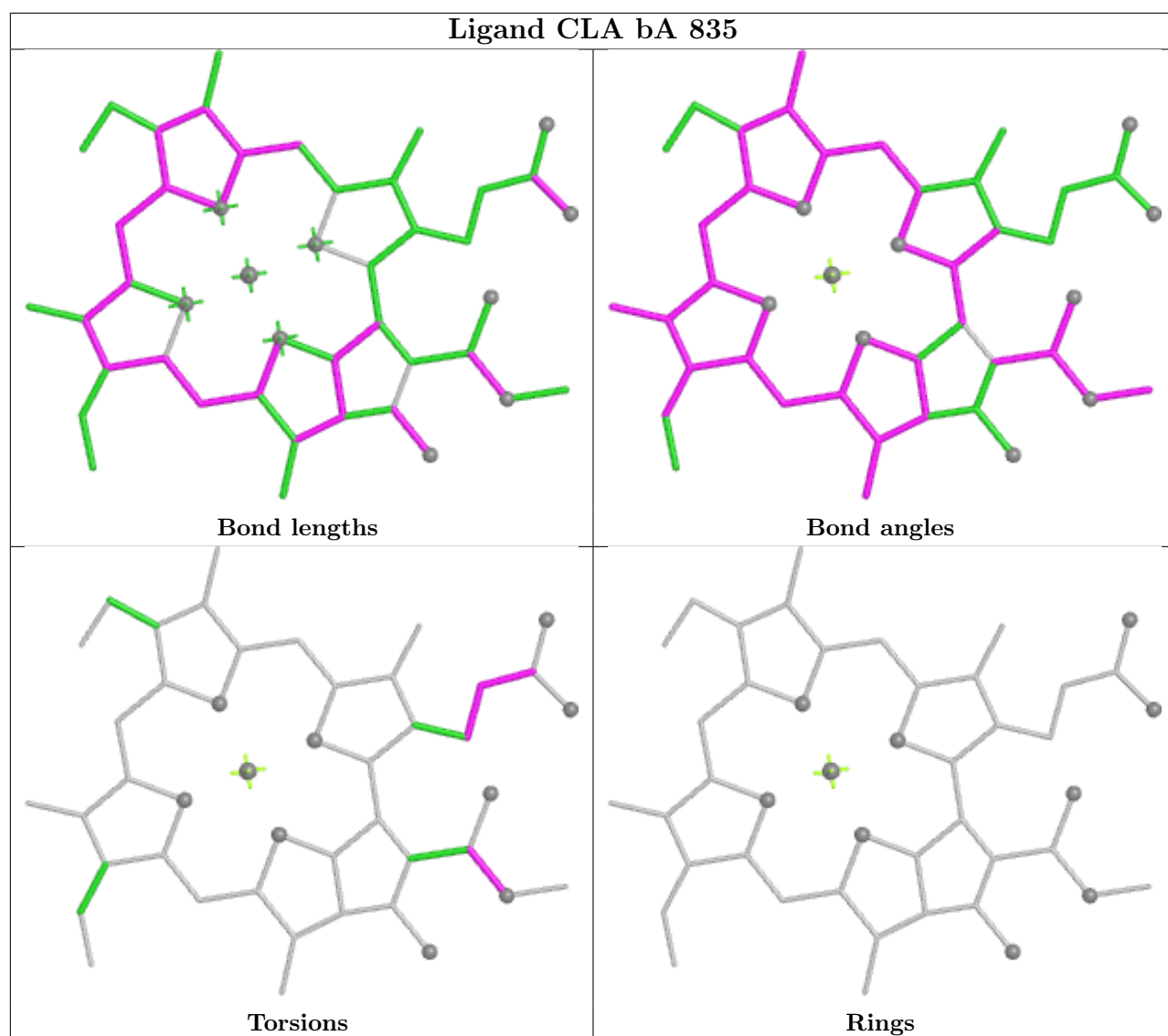


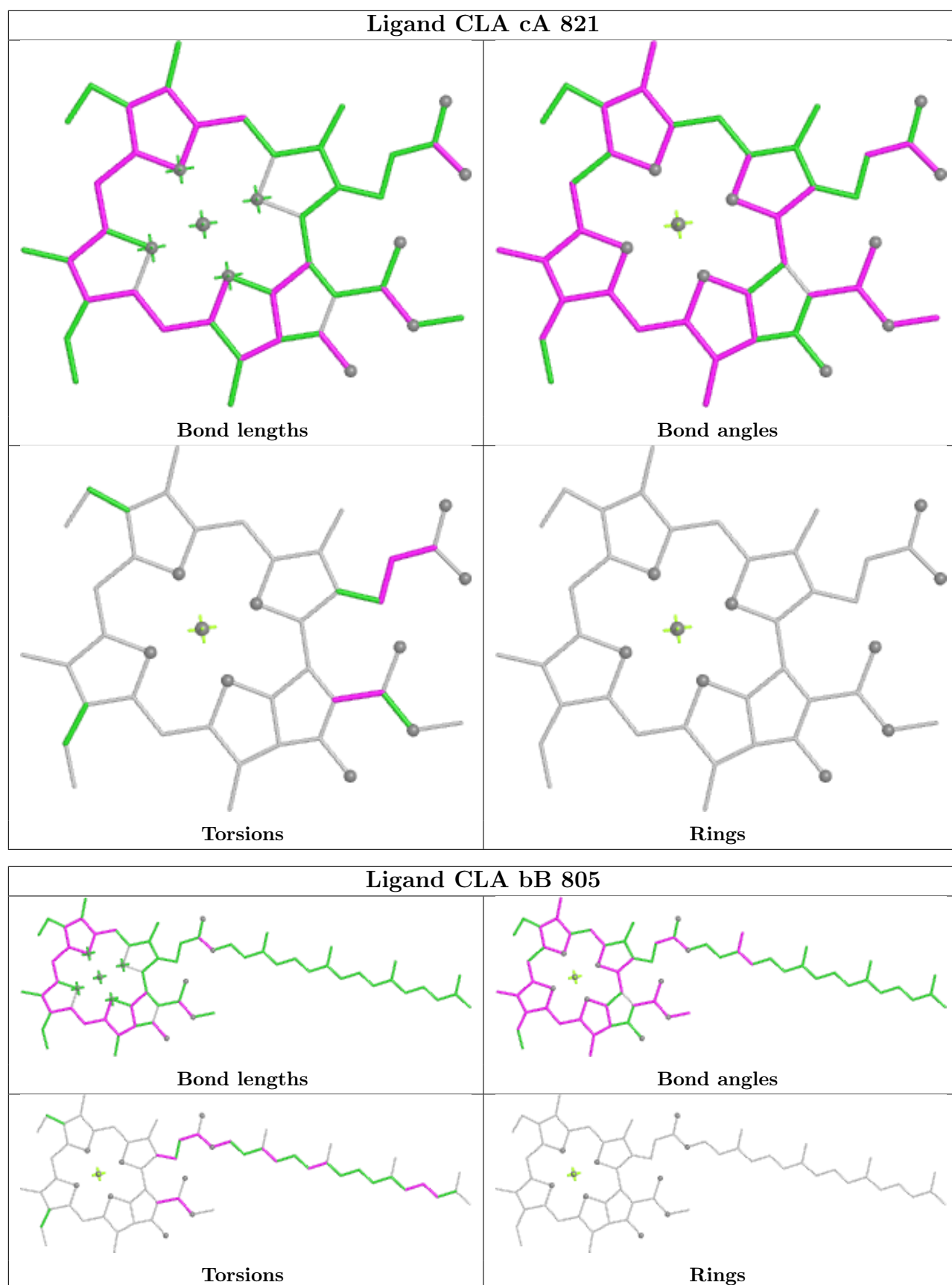
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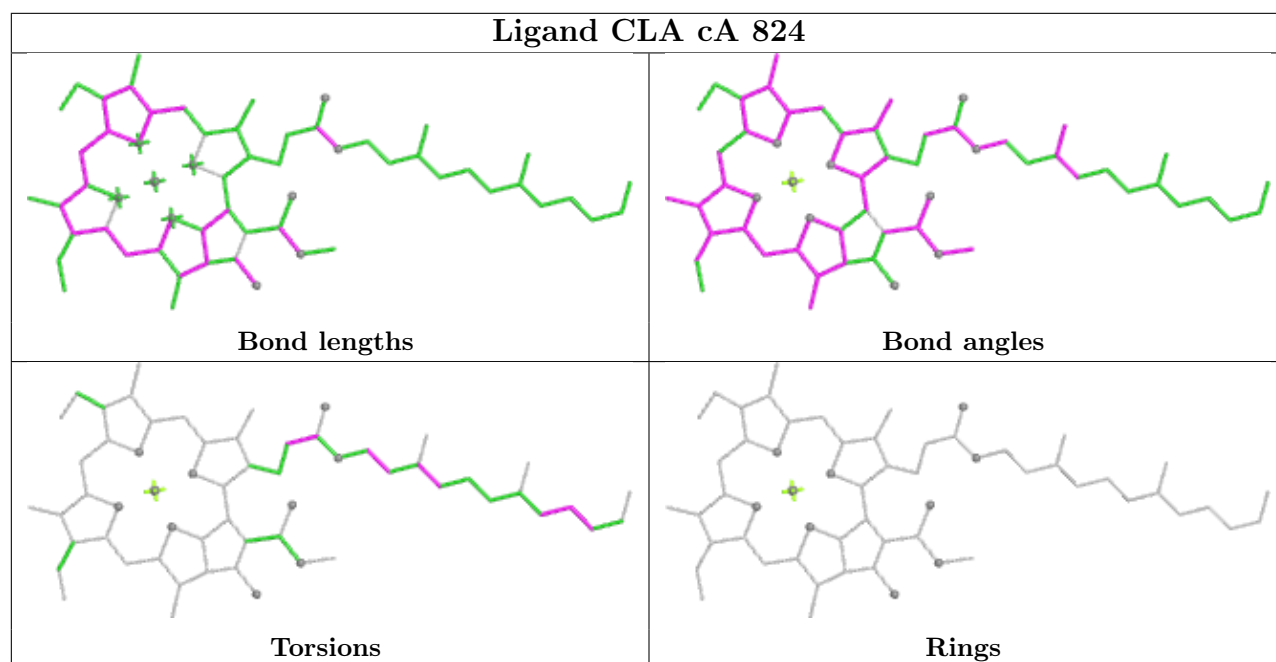
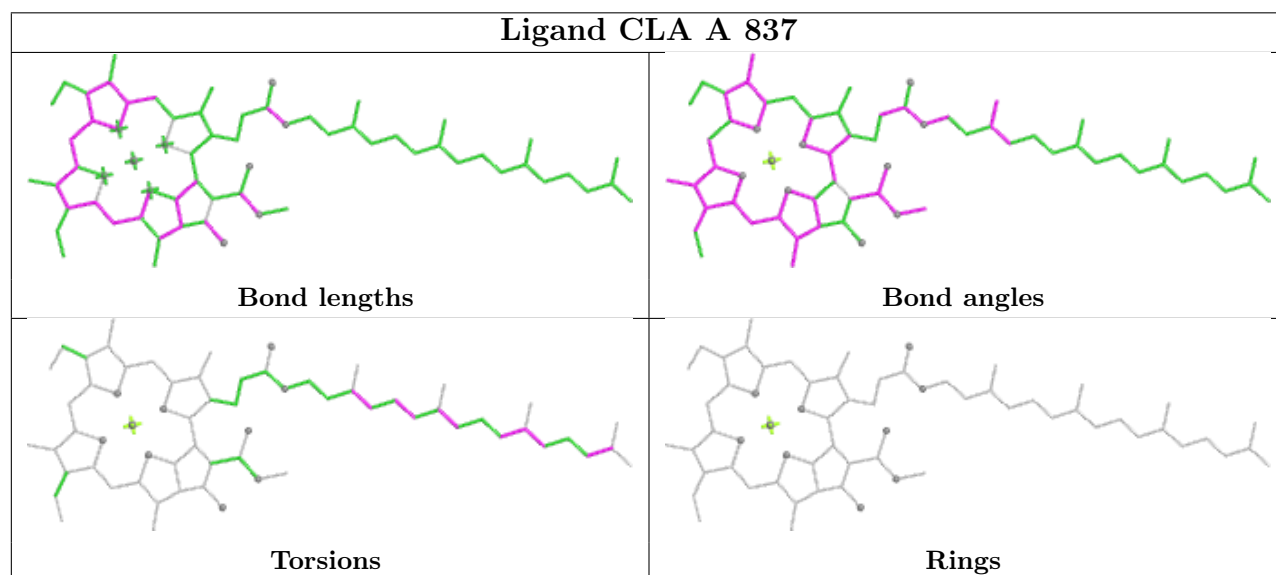
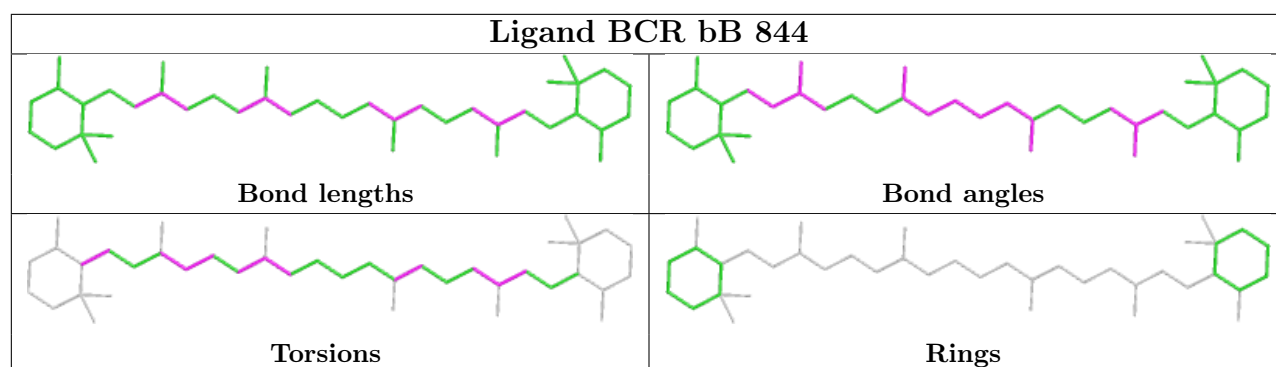


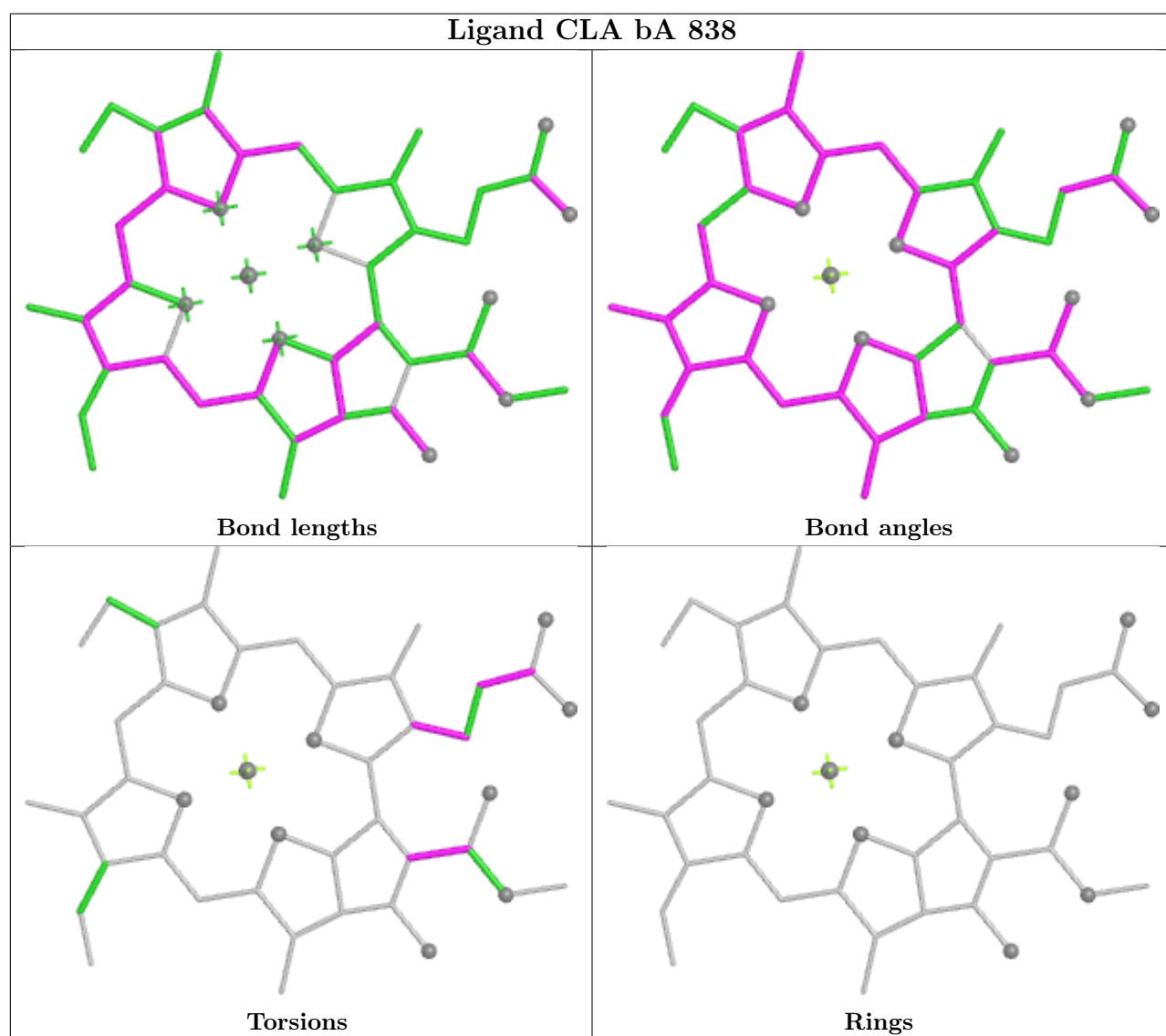
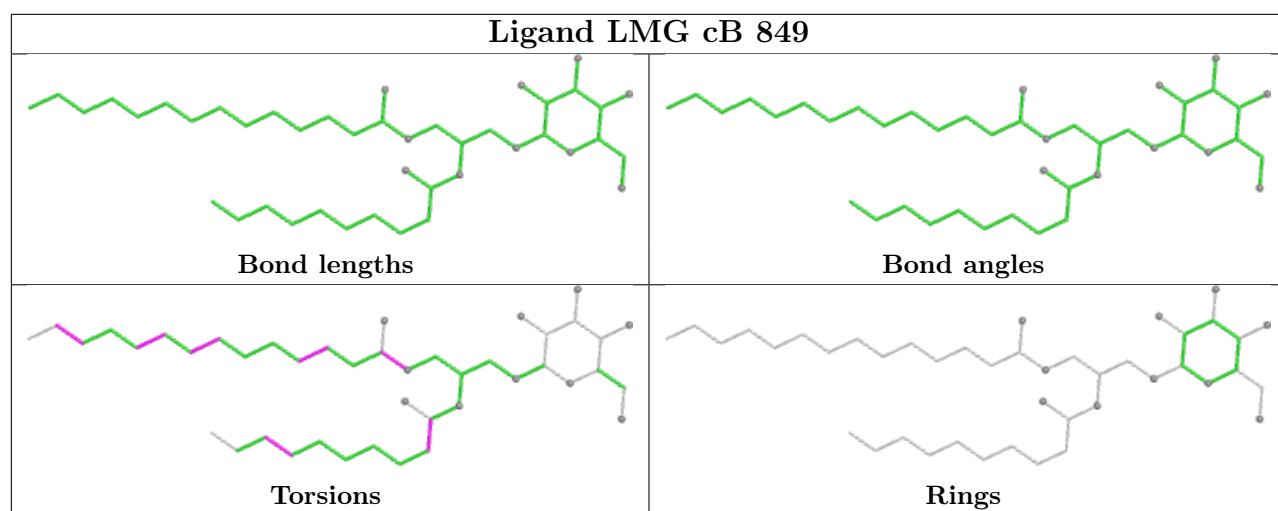
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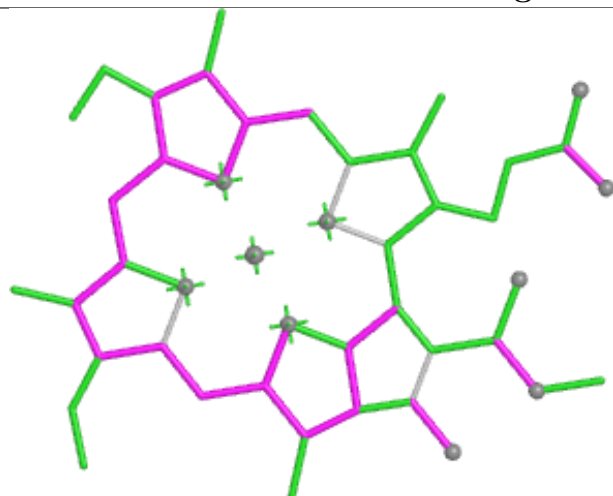




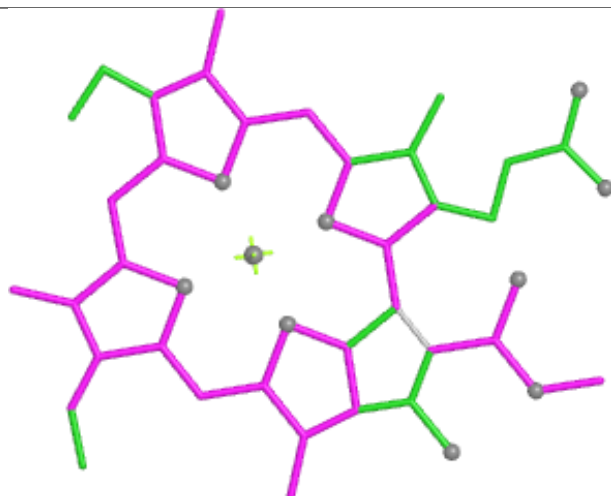




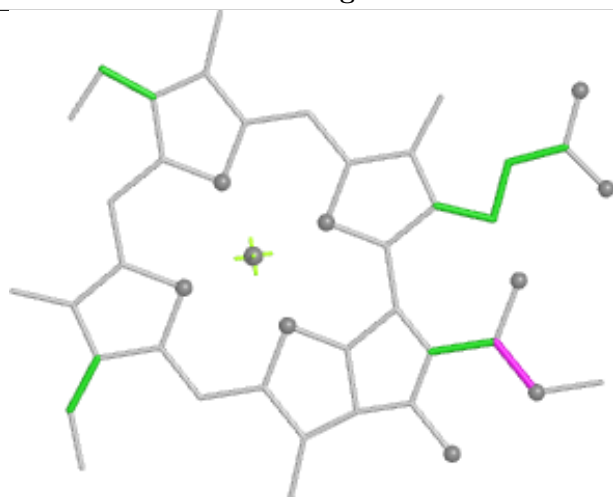
Ligand CLA B 833



Bond lengths



Bond angles

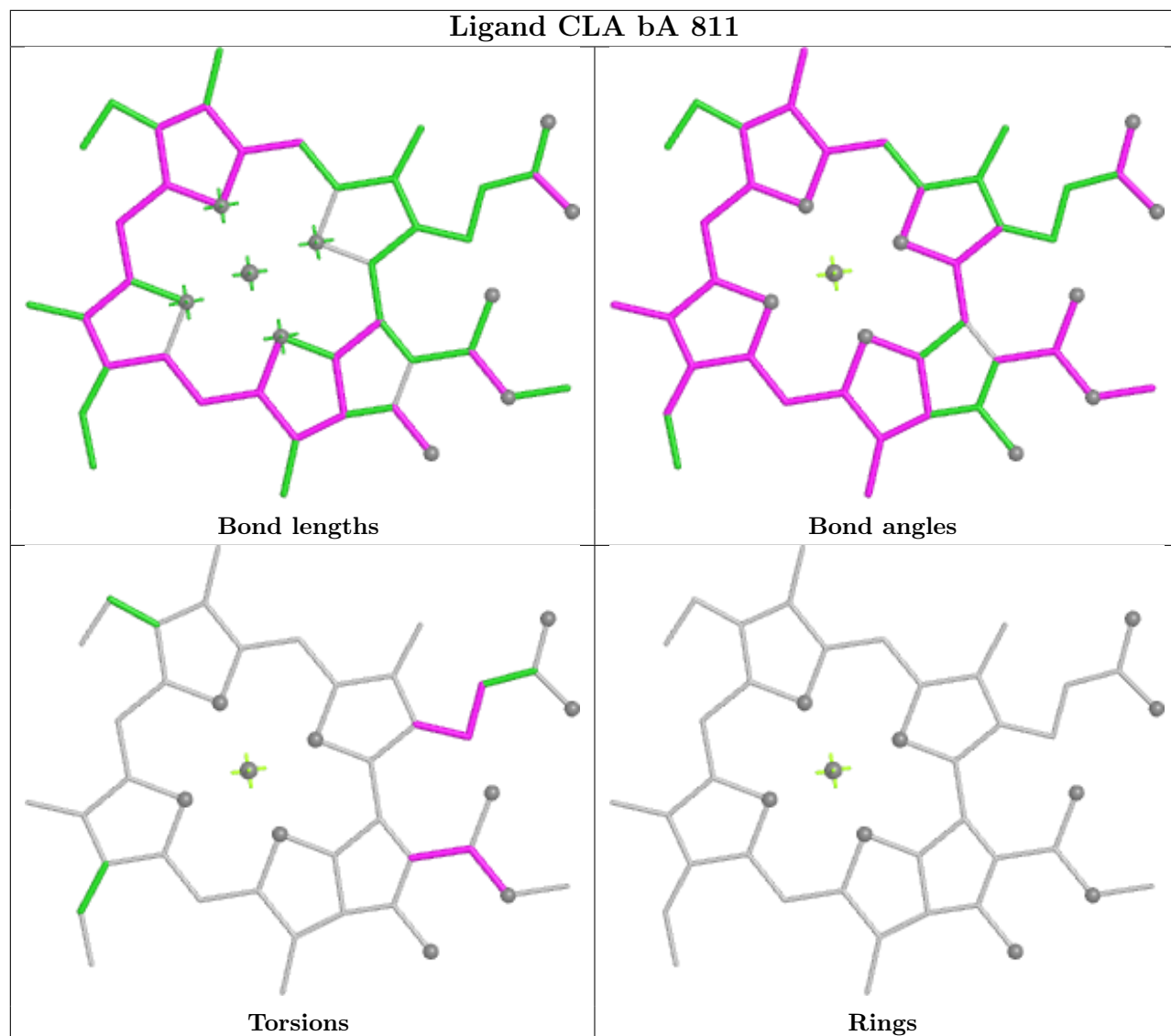


Torsions

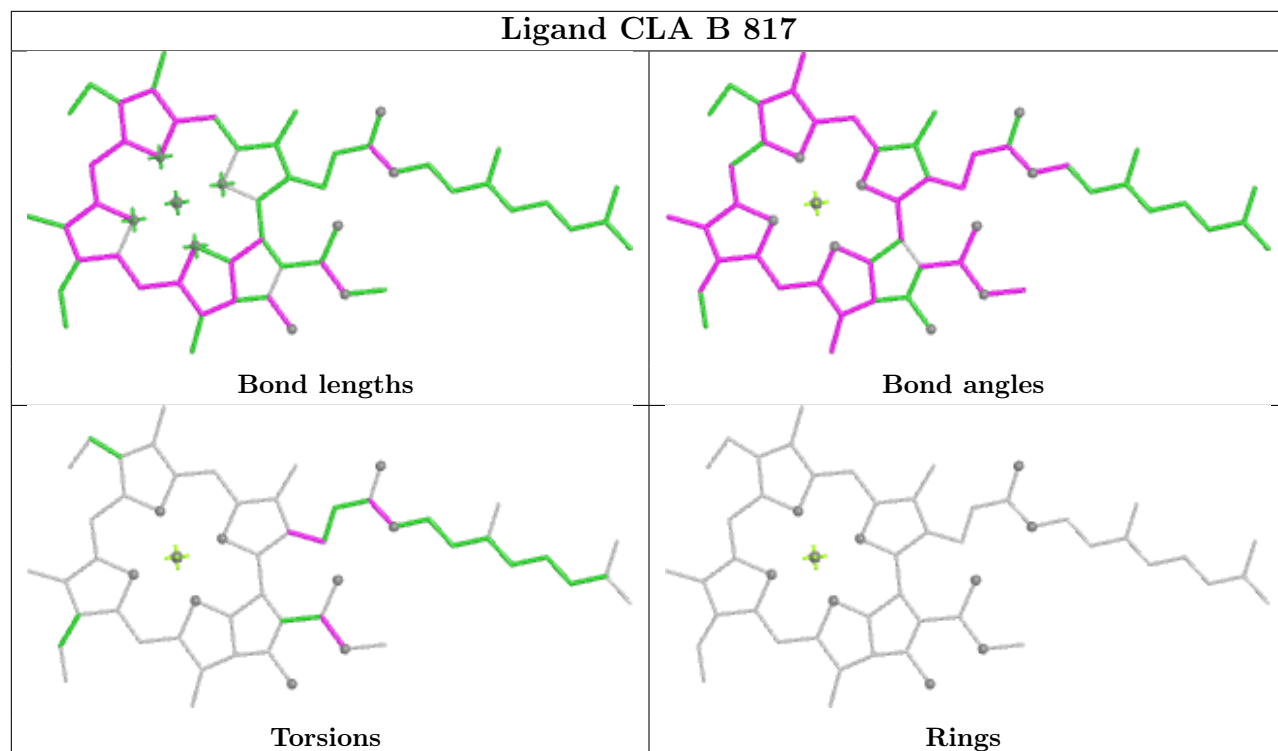


Rings

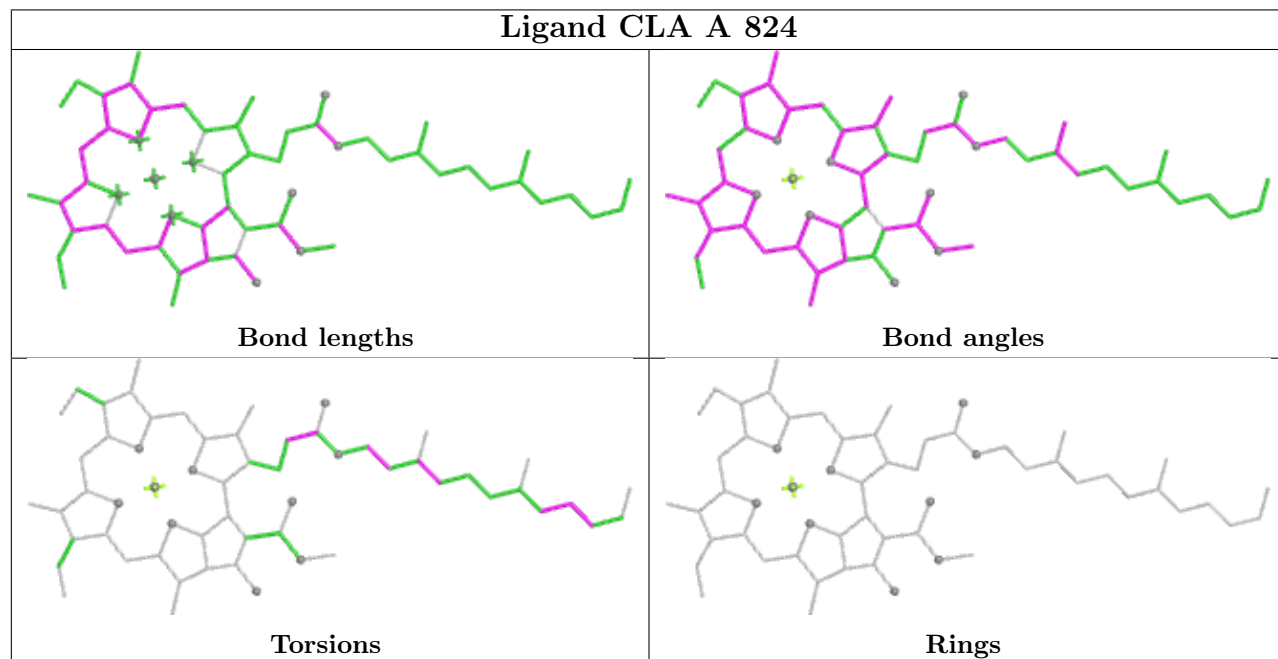
Ligand CLA bA 811

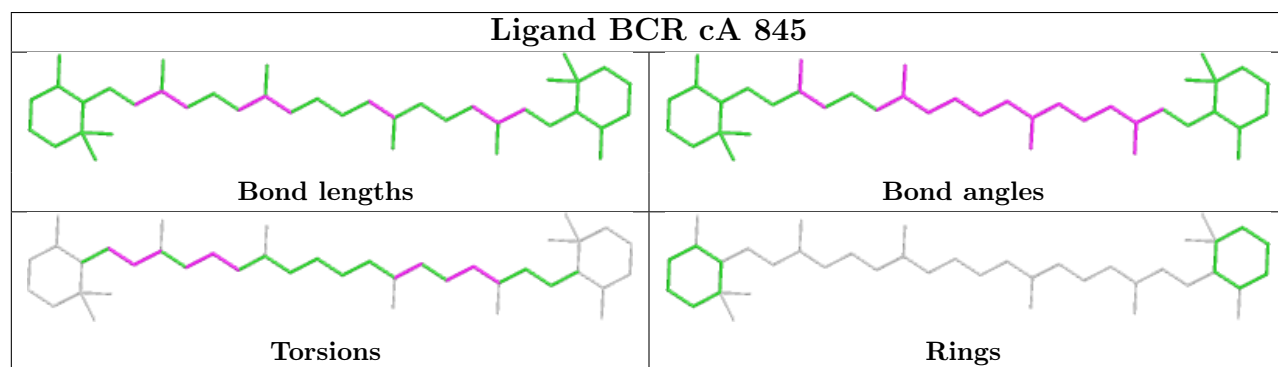
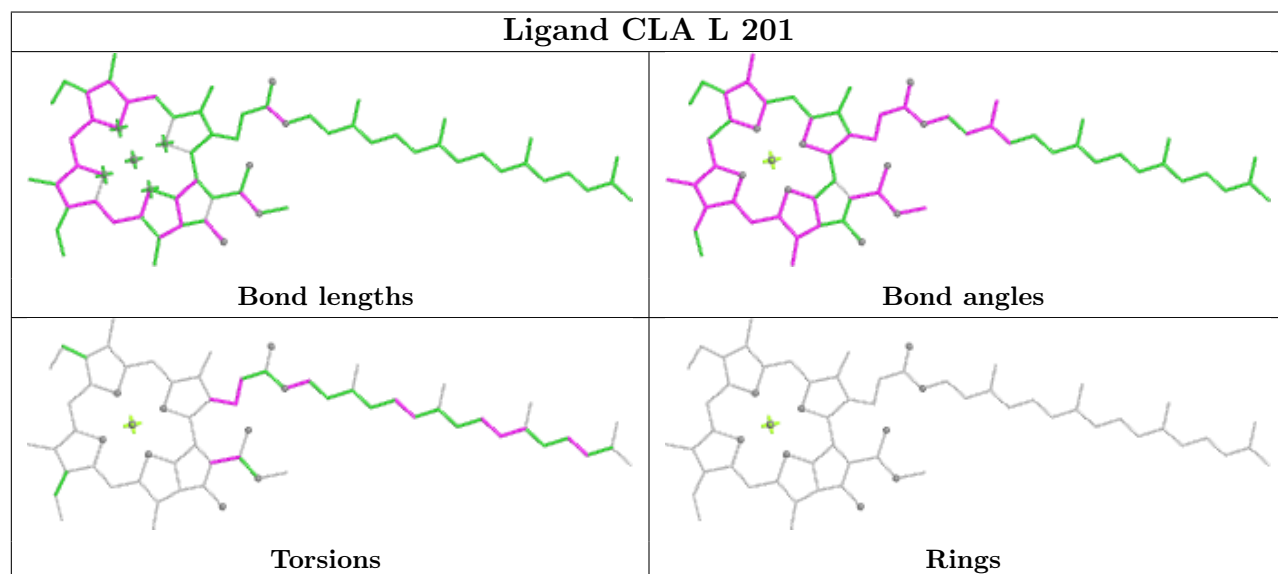
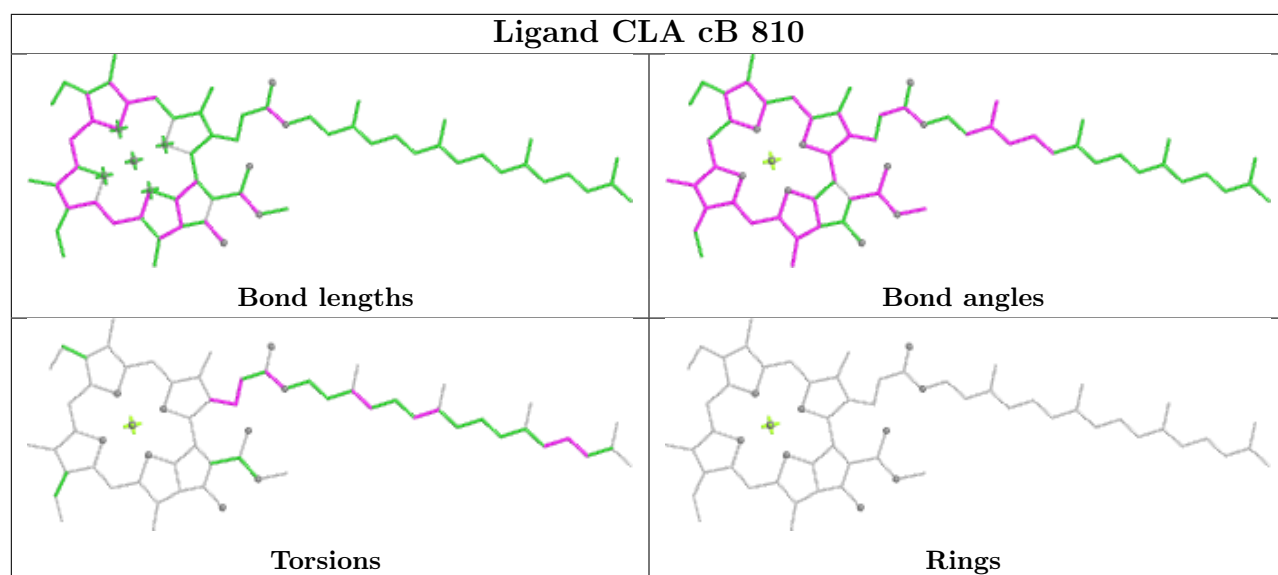


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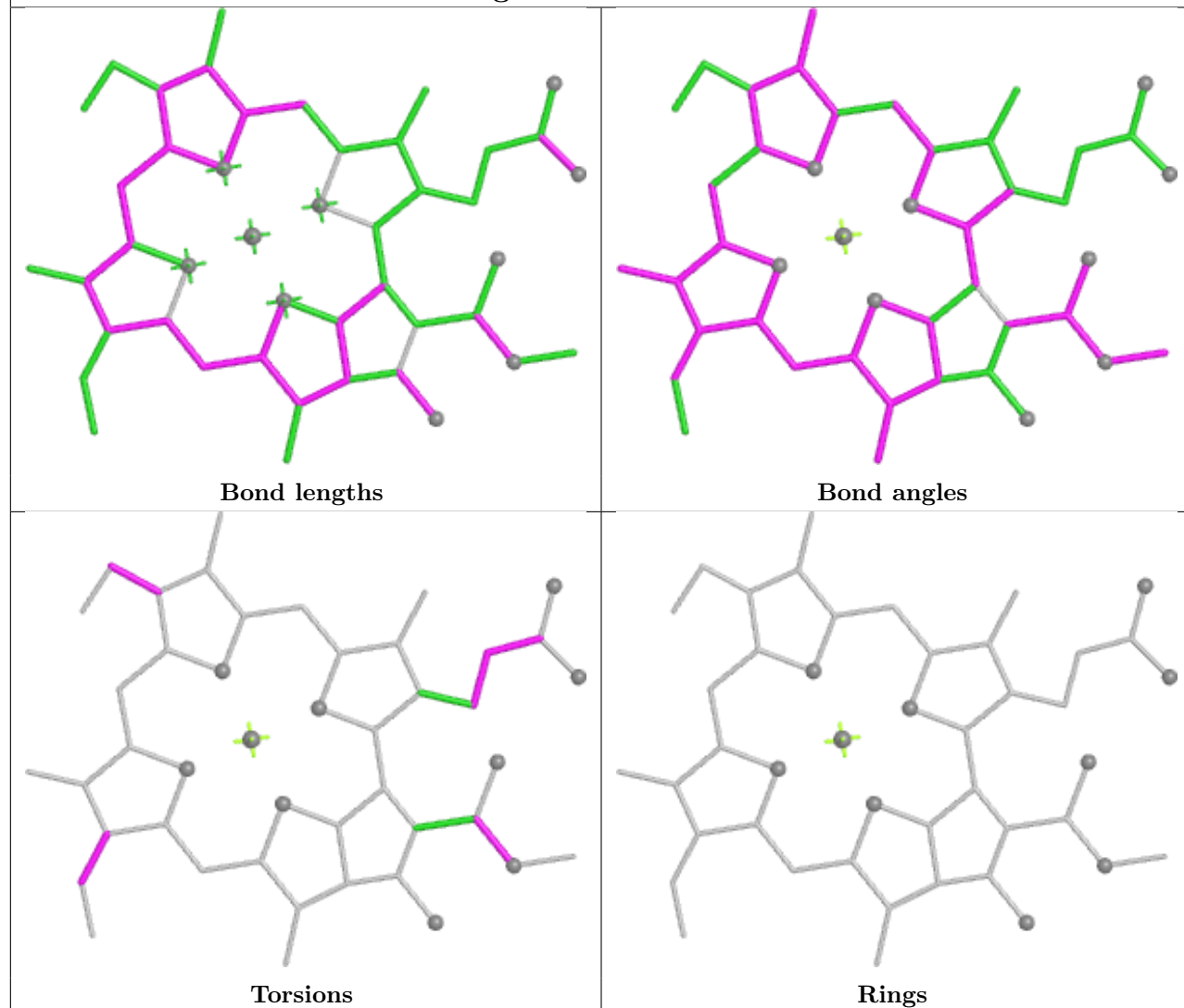


Ligand CLA A 824

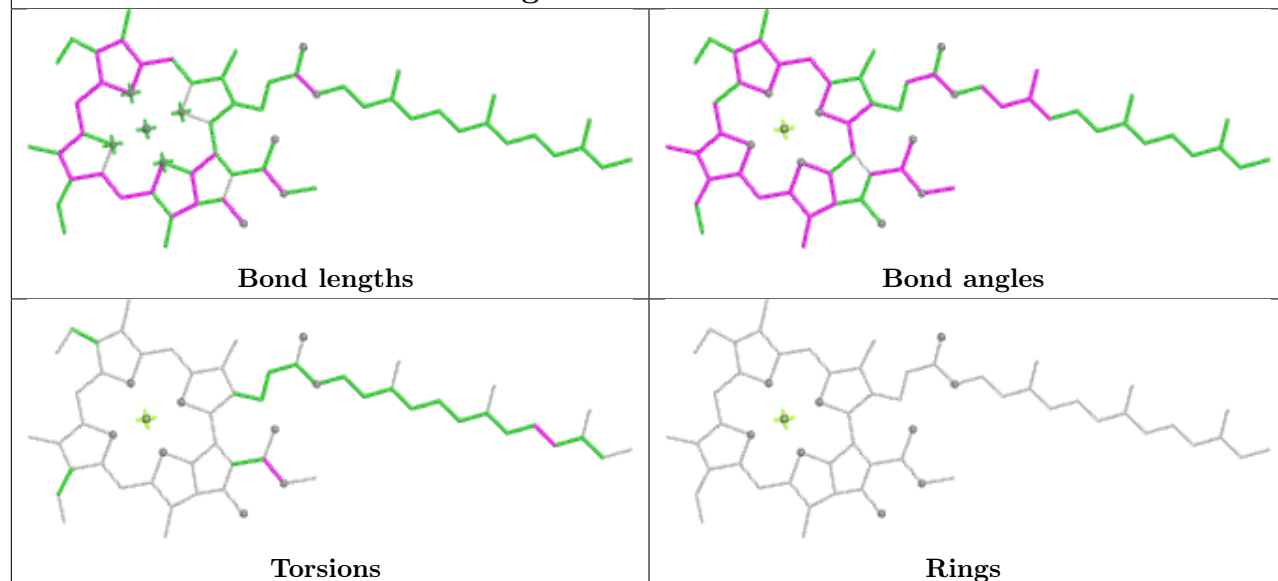




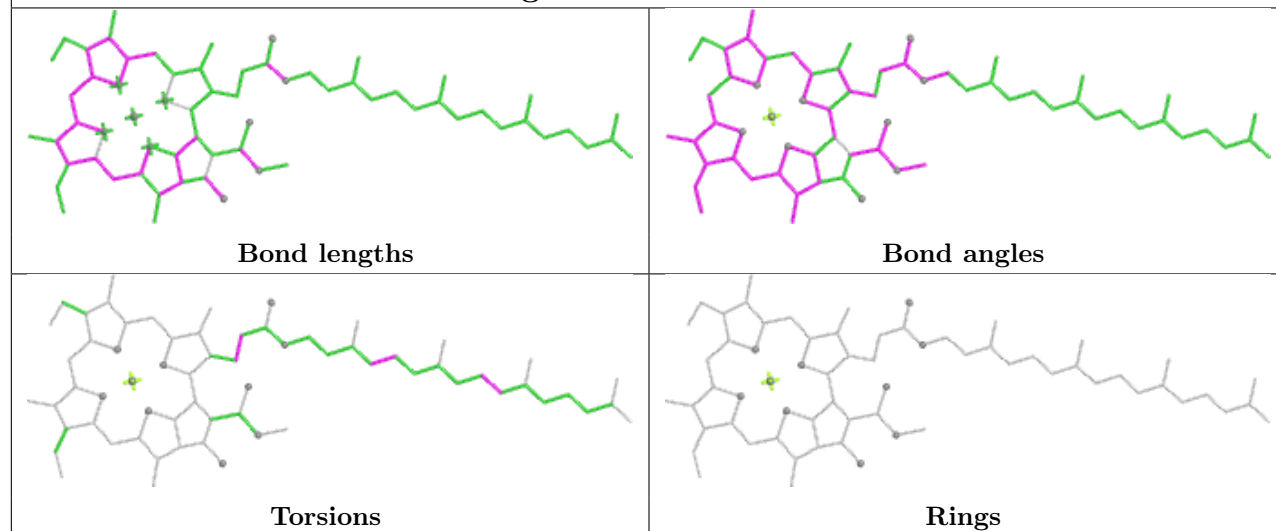
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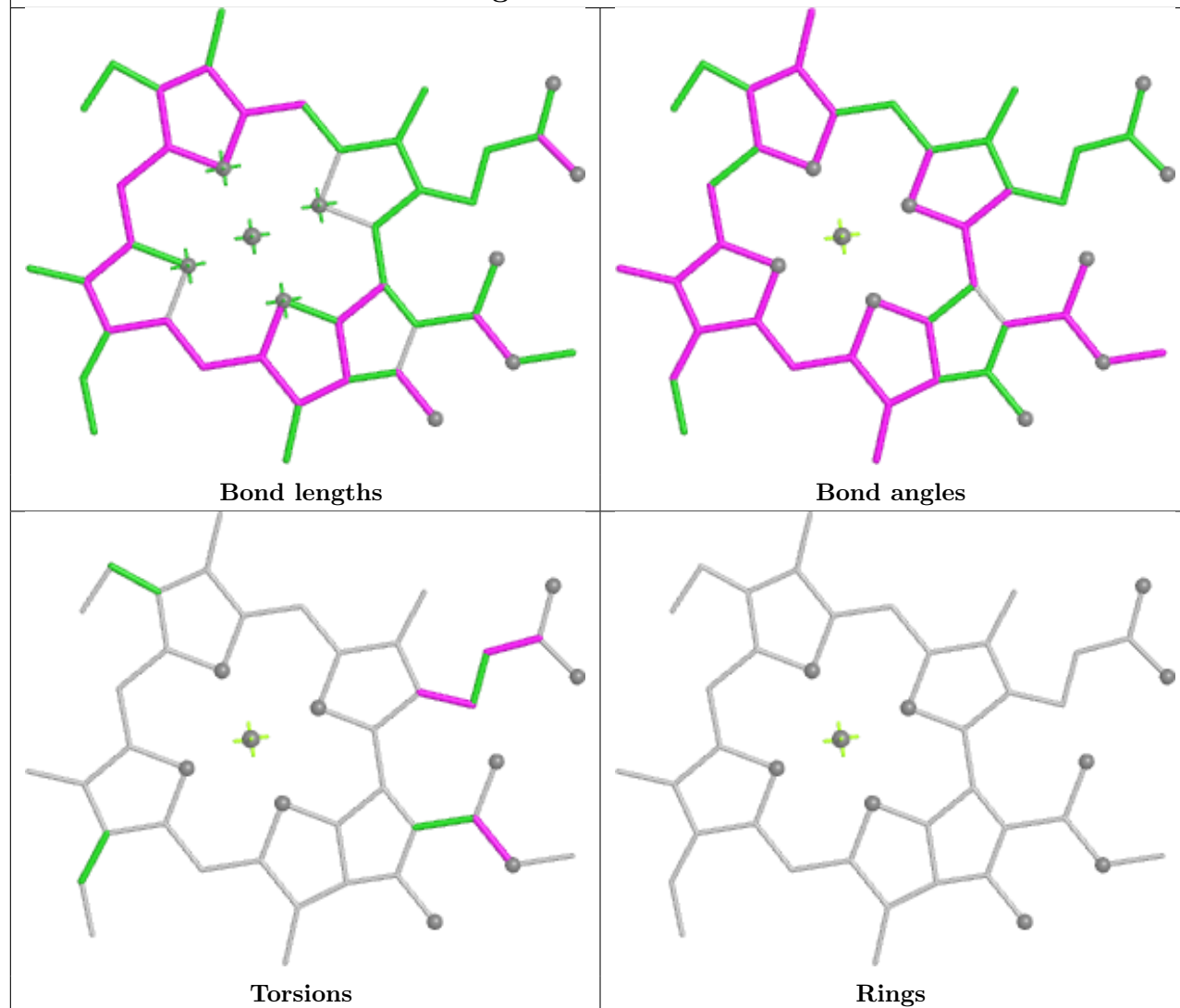
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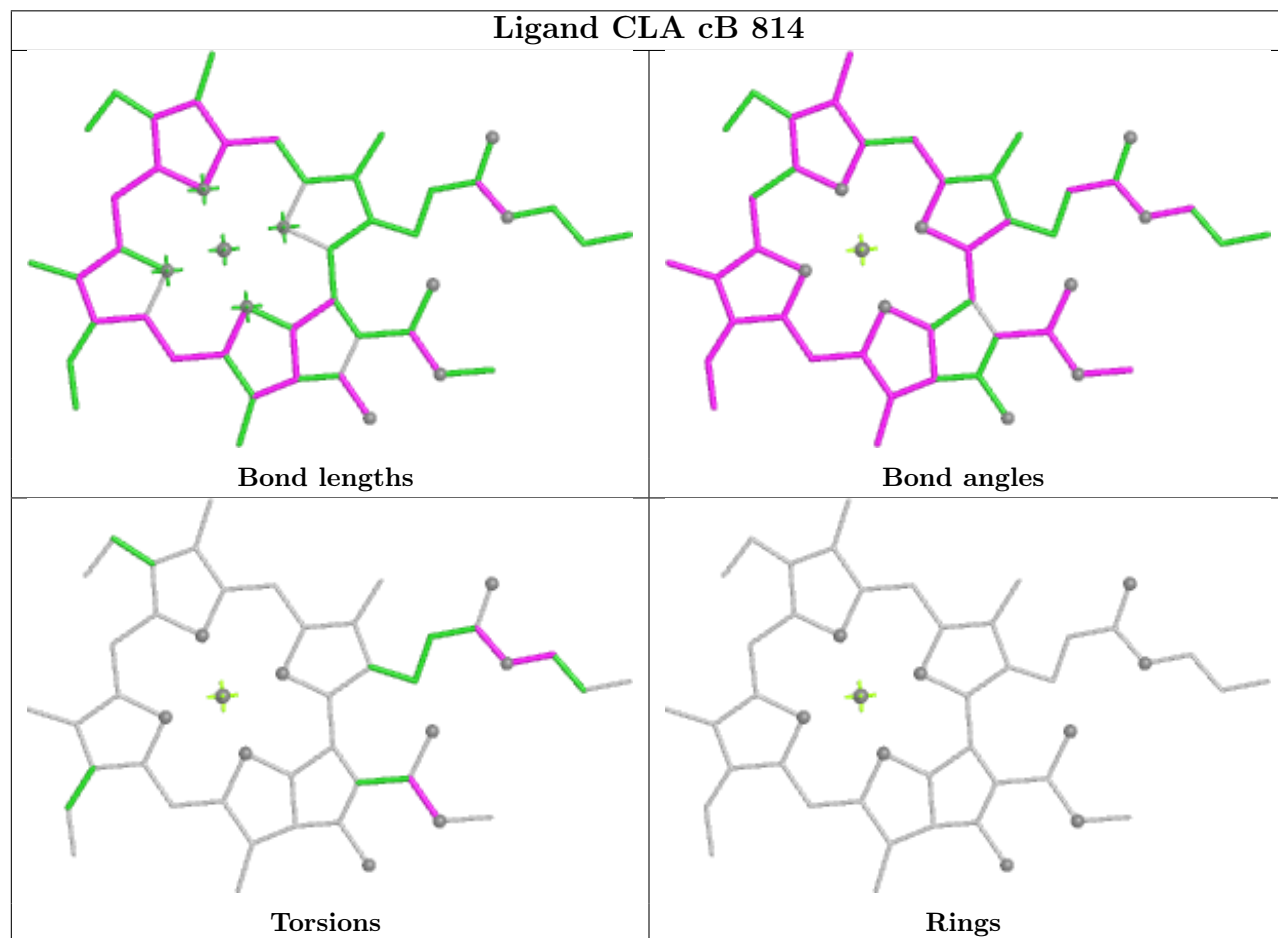
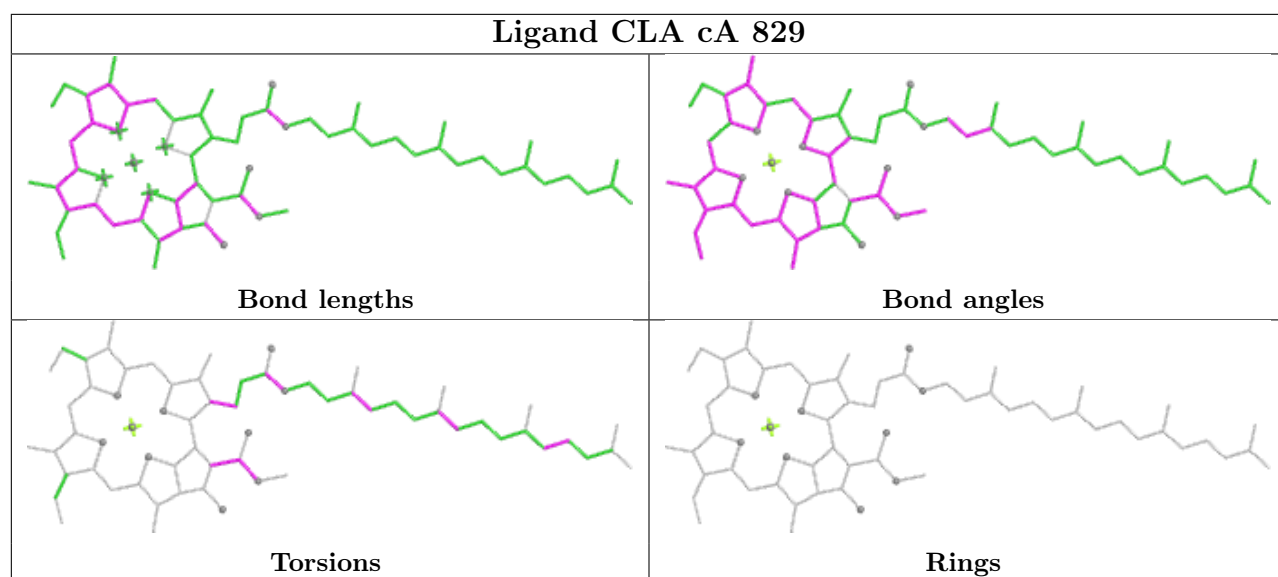


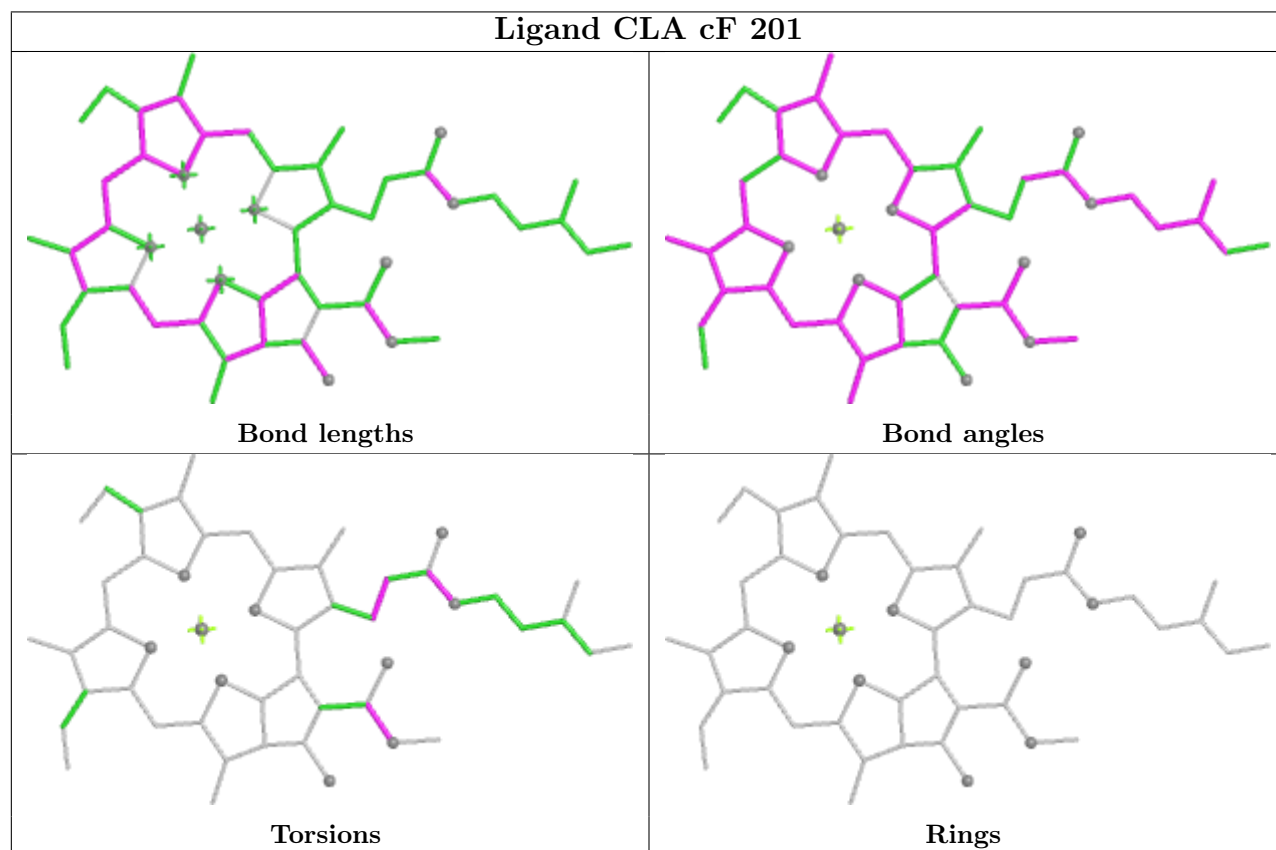
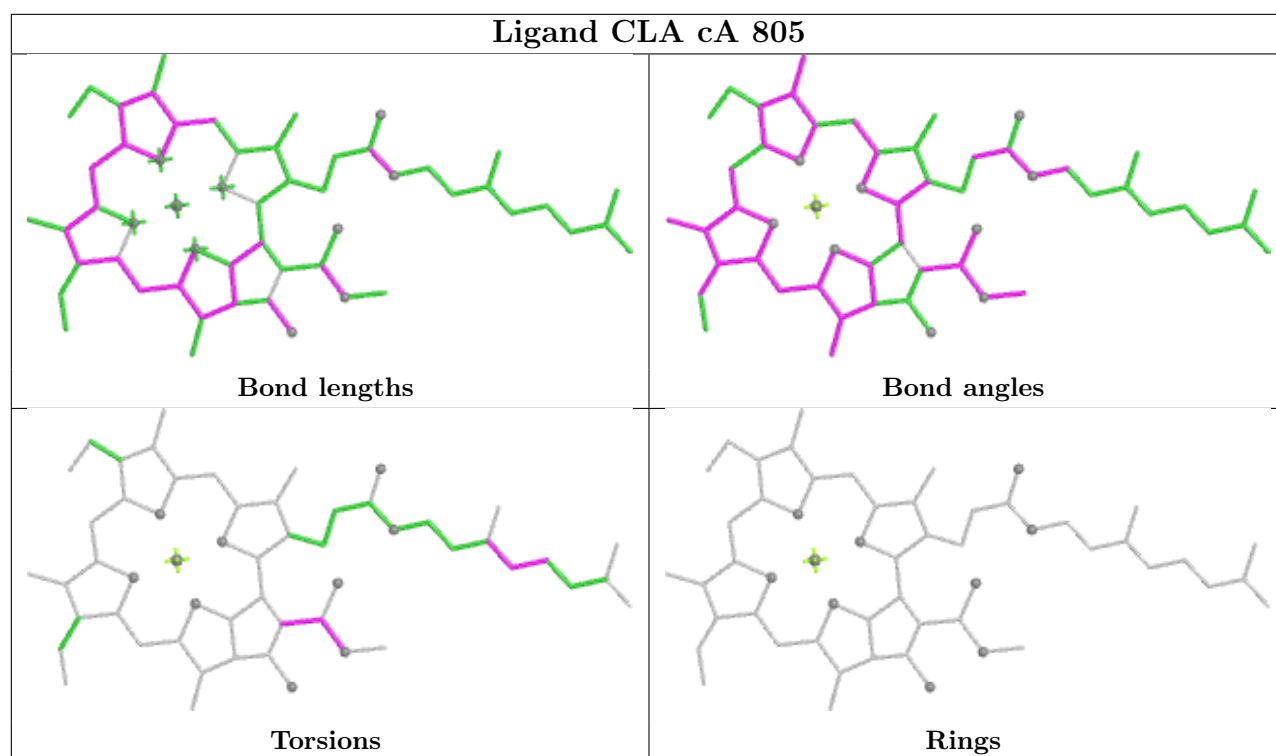
Ligand CLA bA 802

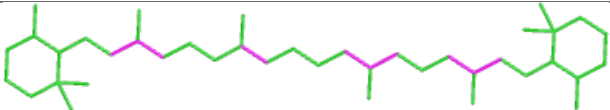
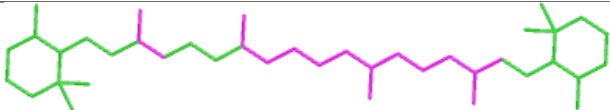
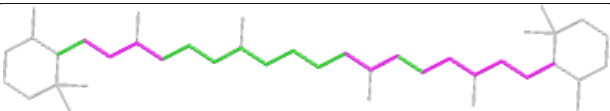
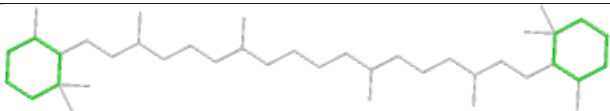
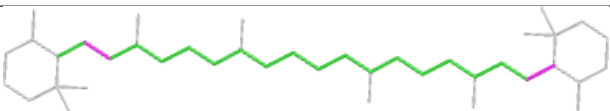
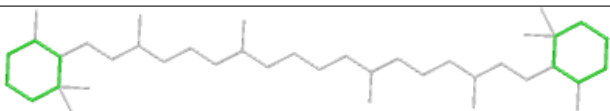
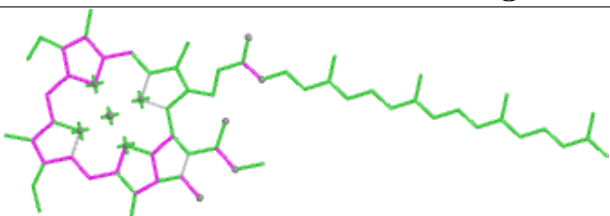
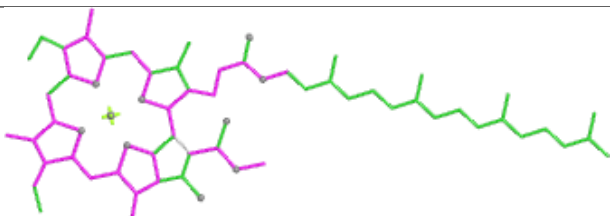
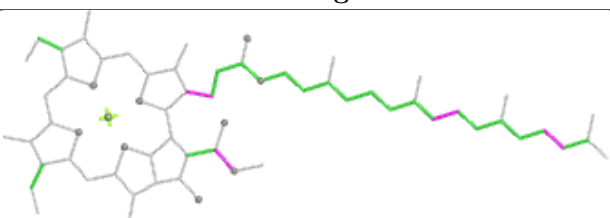
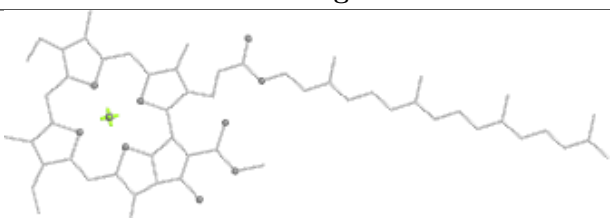


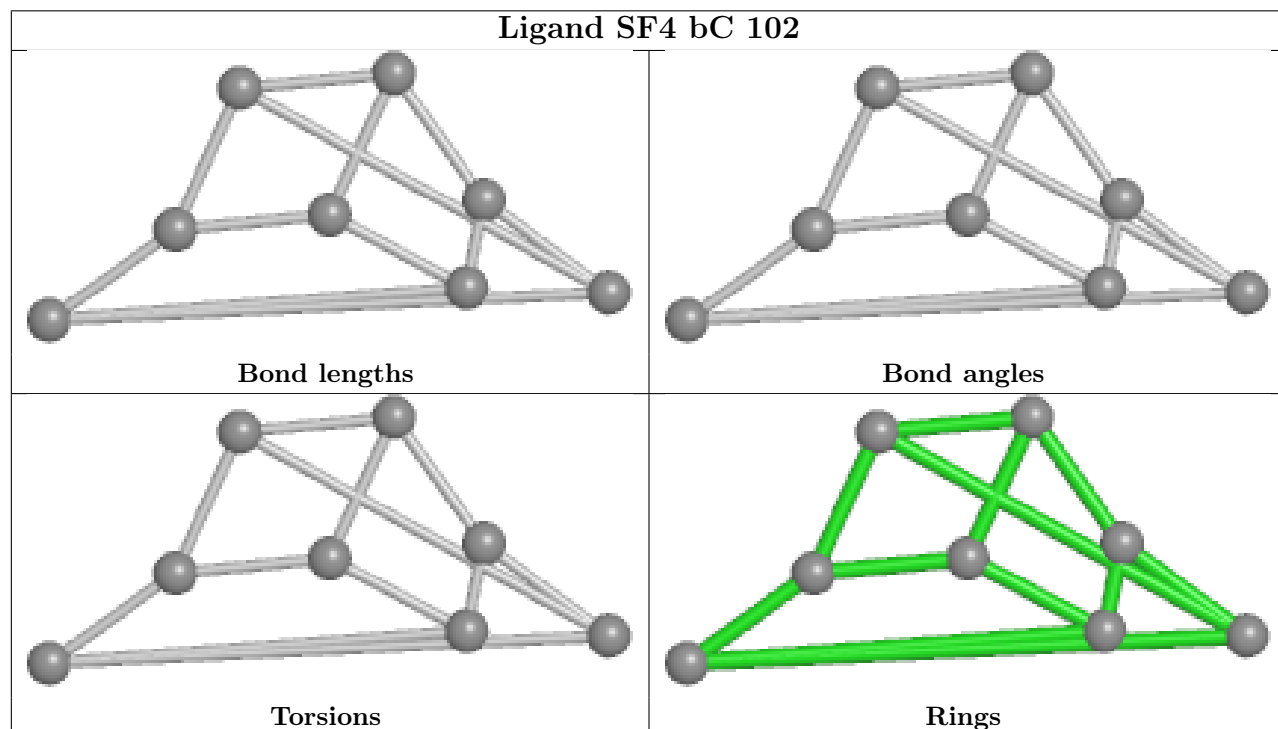
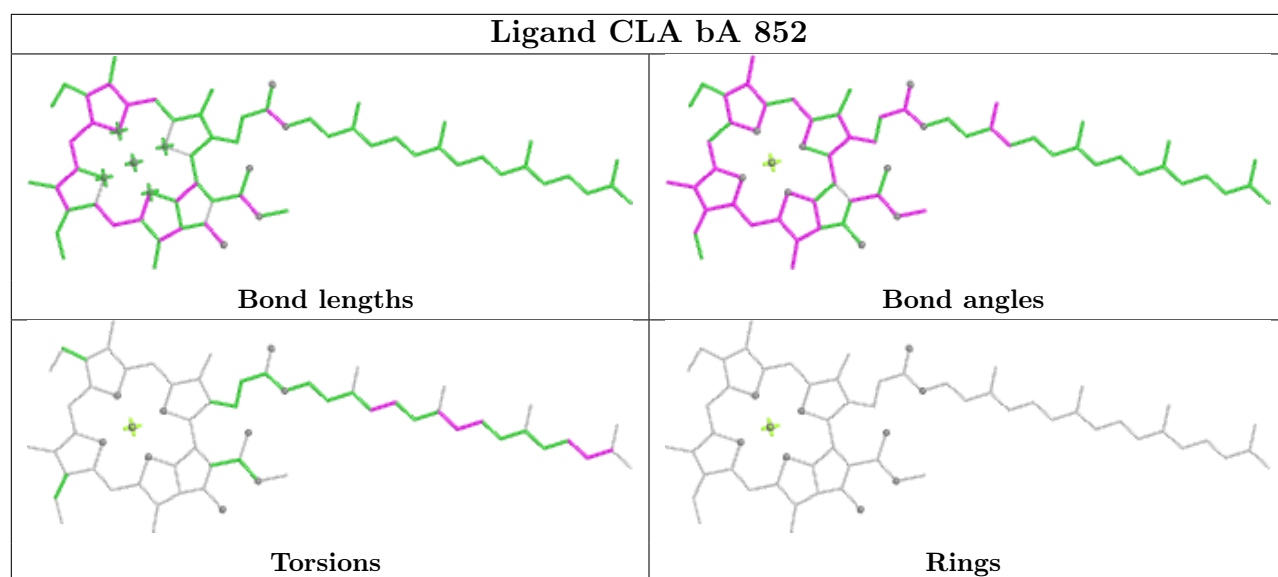
Ligand CLA B 810

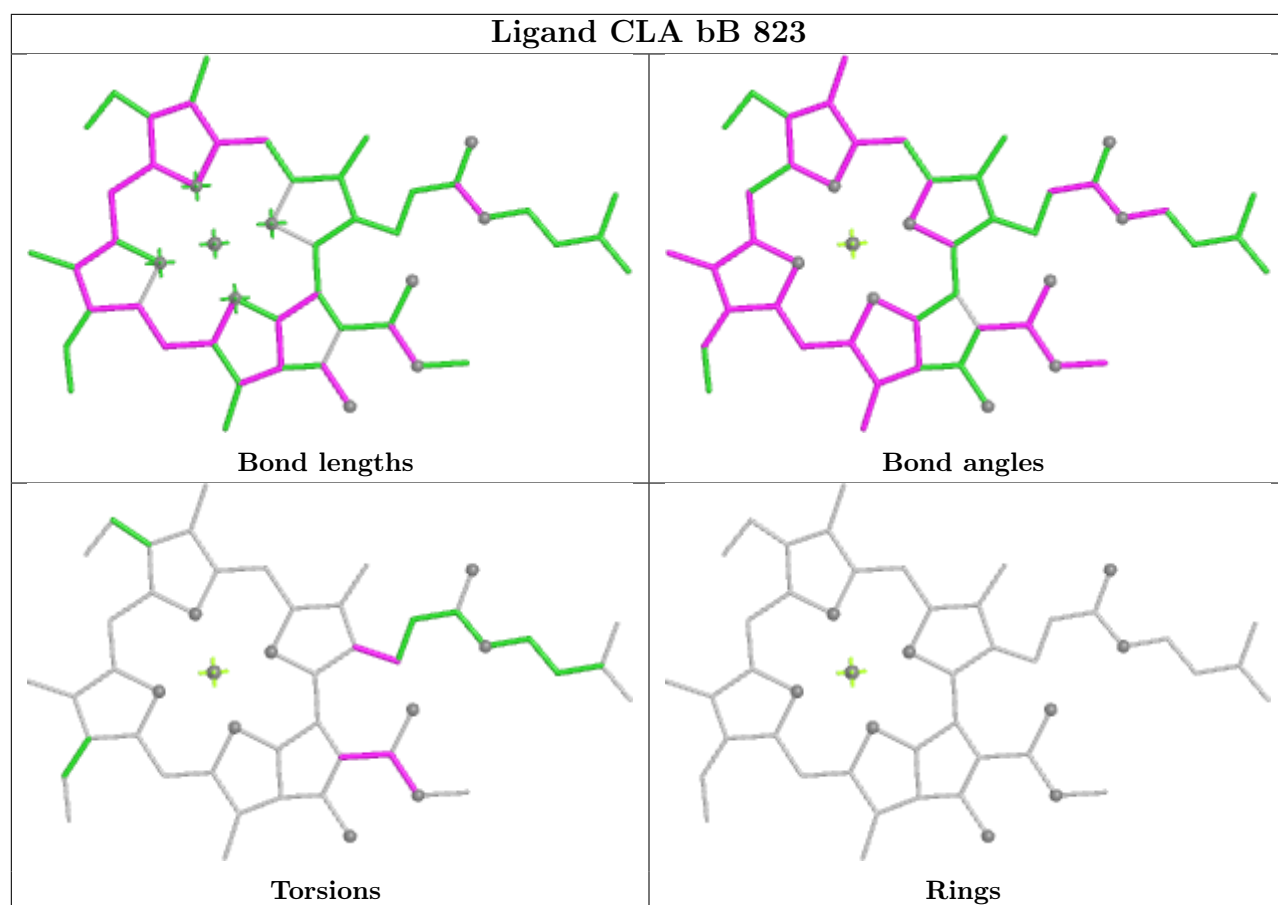




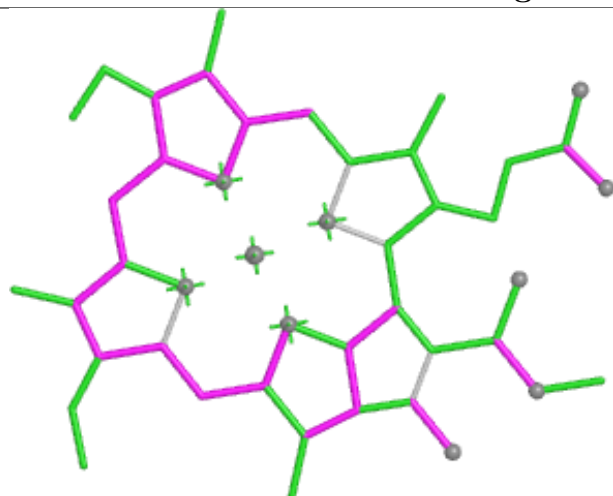


Ligand BCR bJ 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 845	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA cB 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

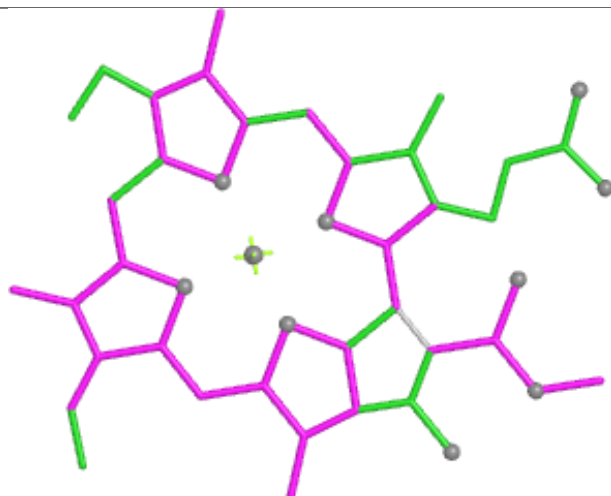




Ligand CLA B 829



Bond lengths



Bond angles

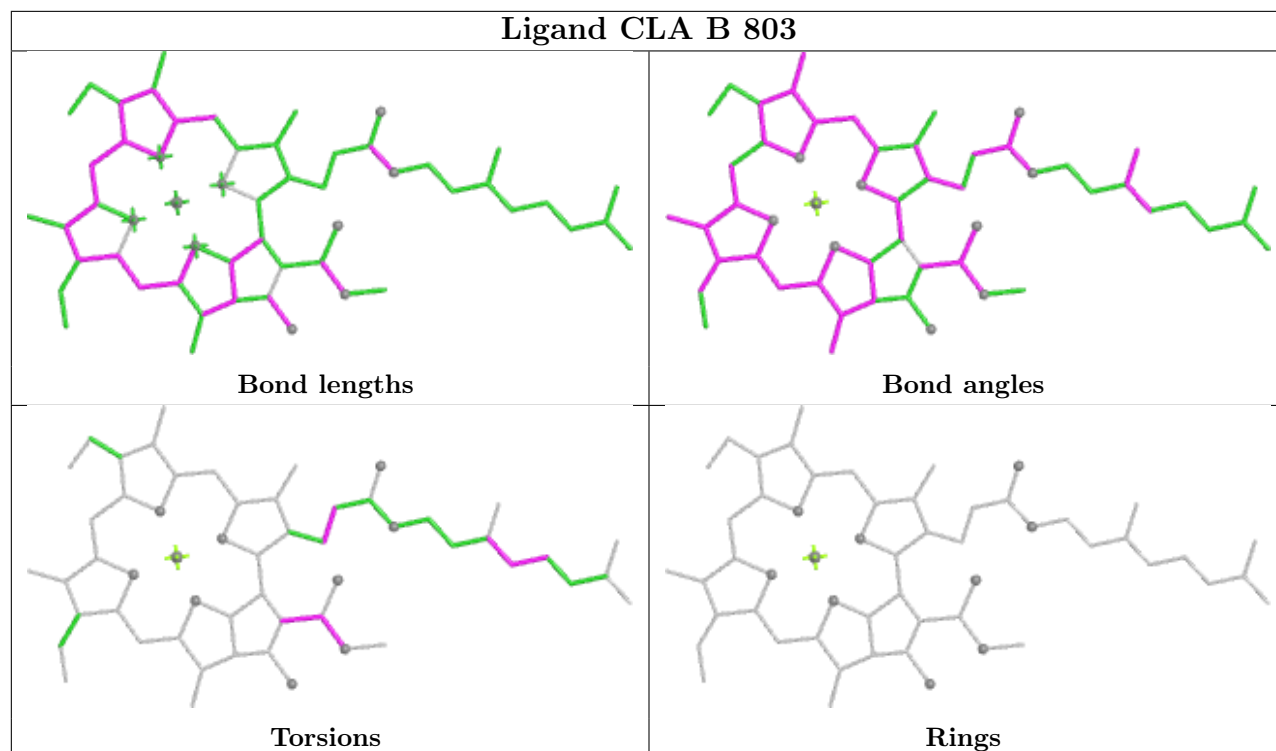


Torsions

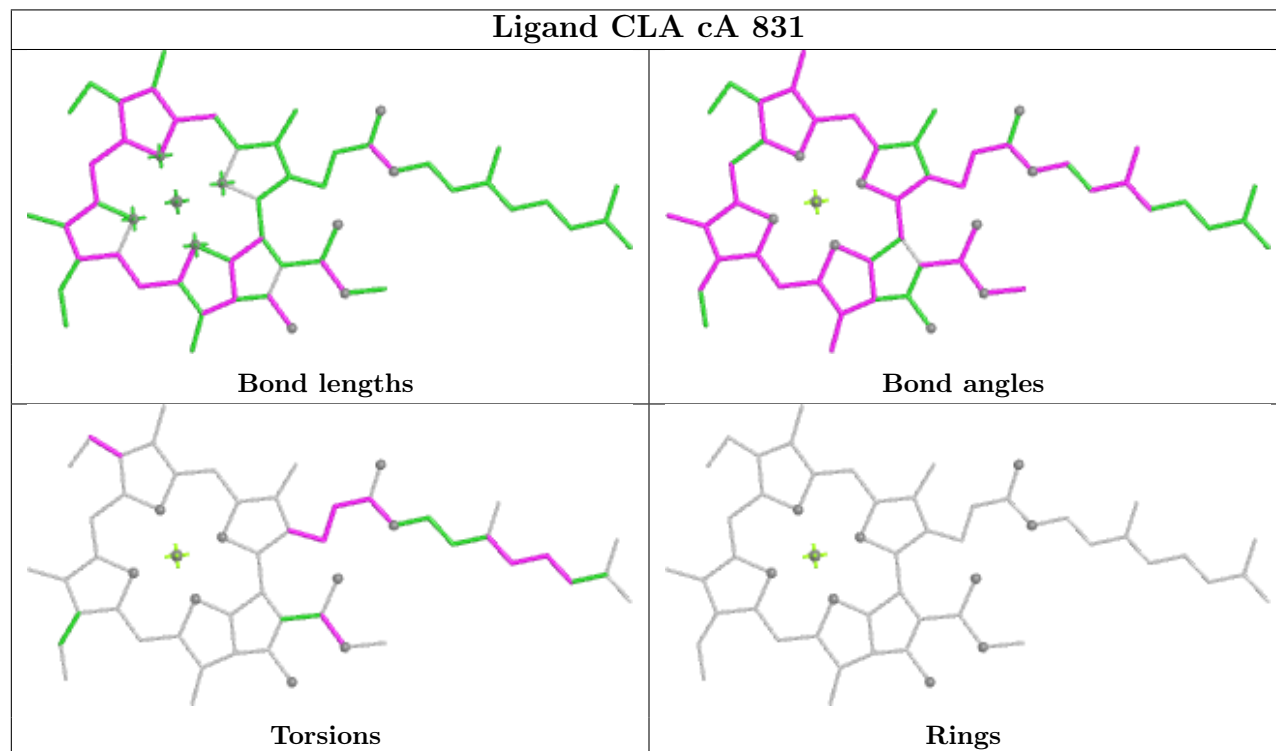


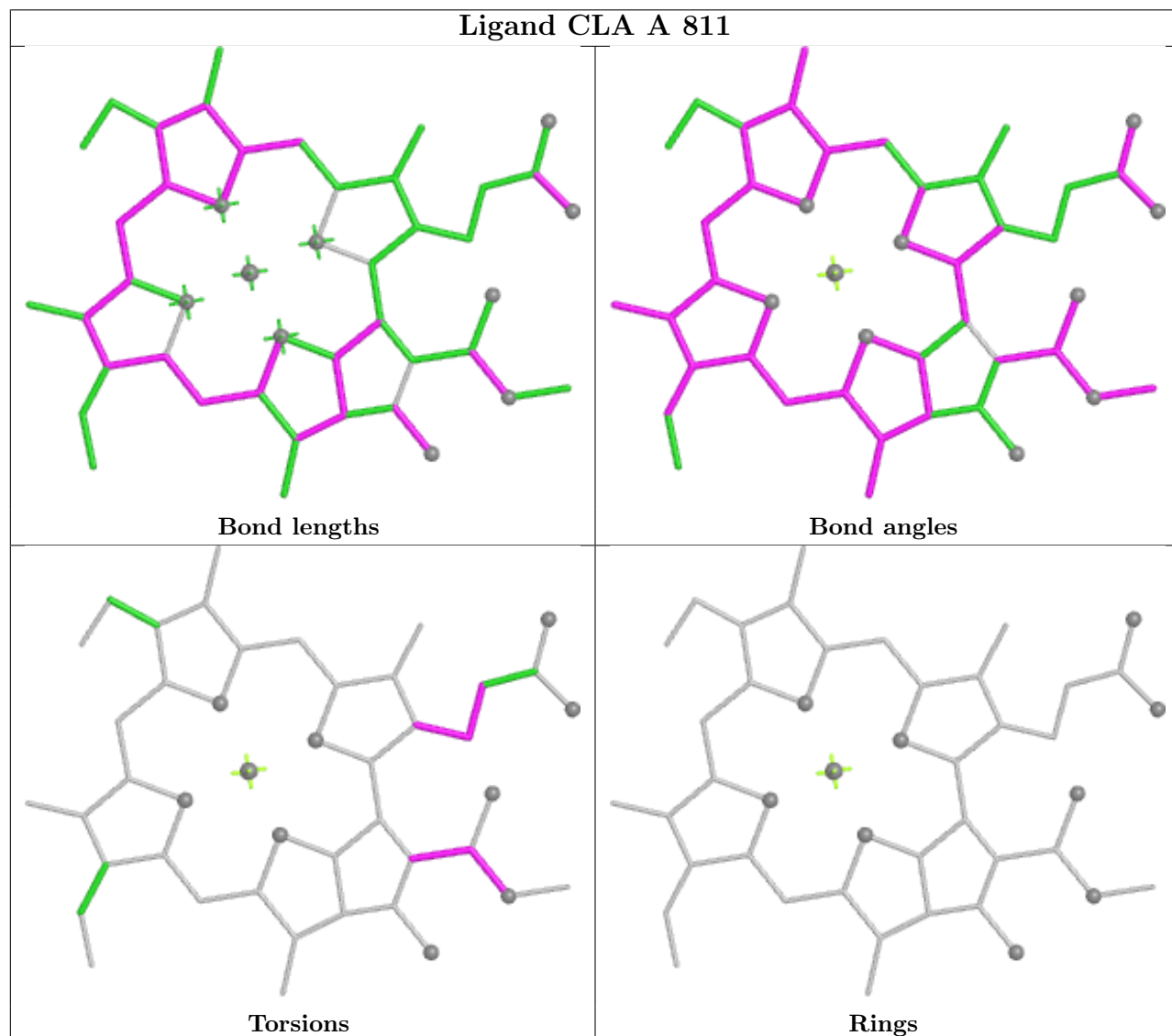
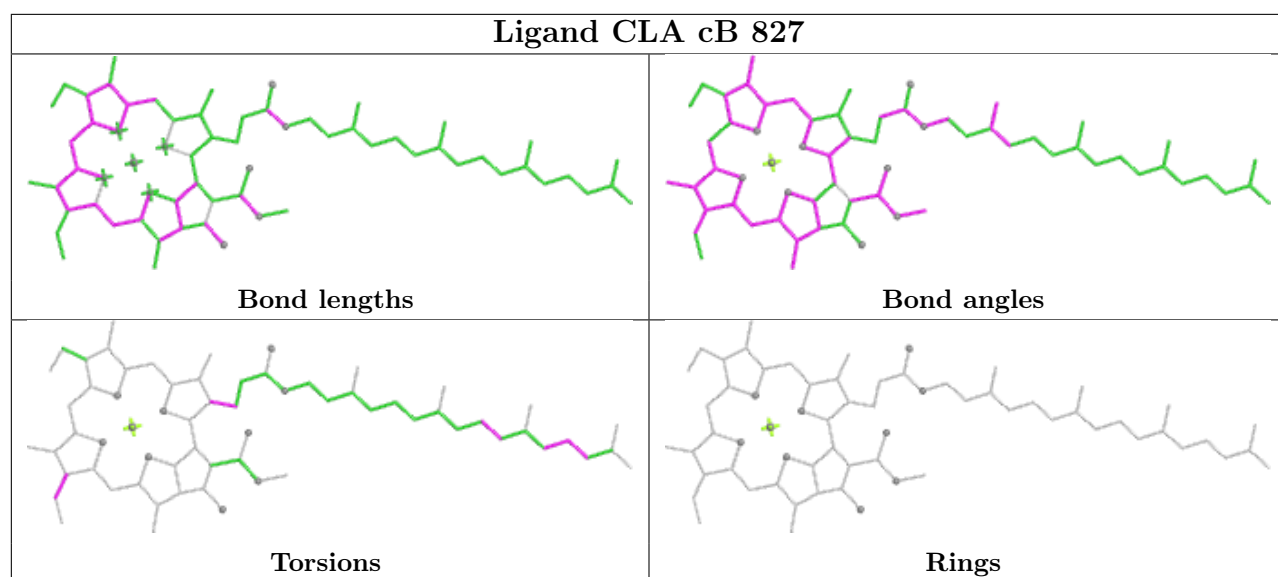
Rings

Ligand CLA B 803

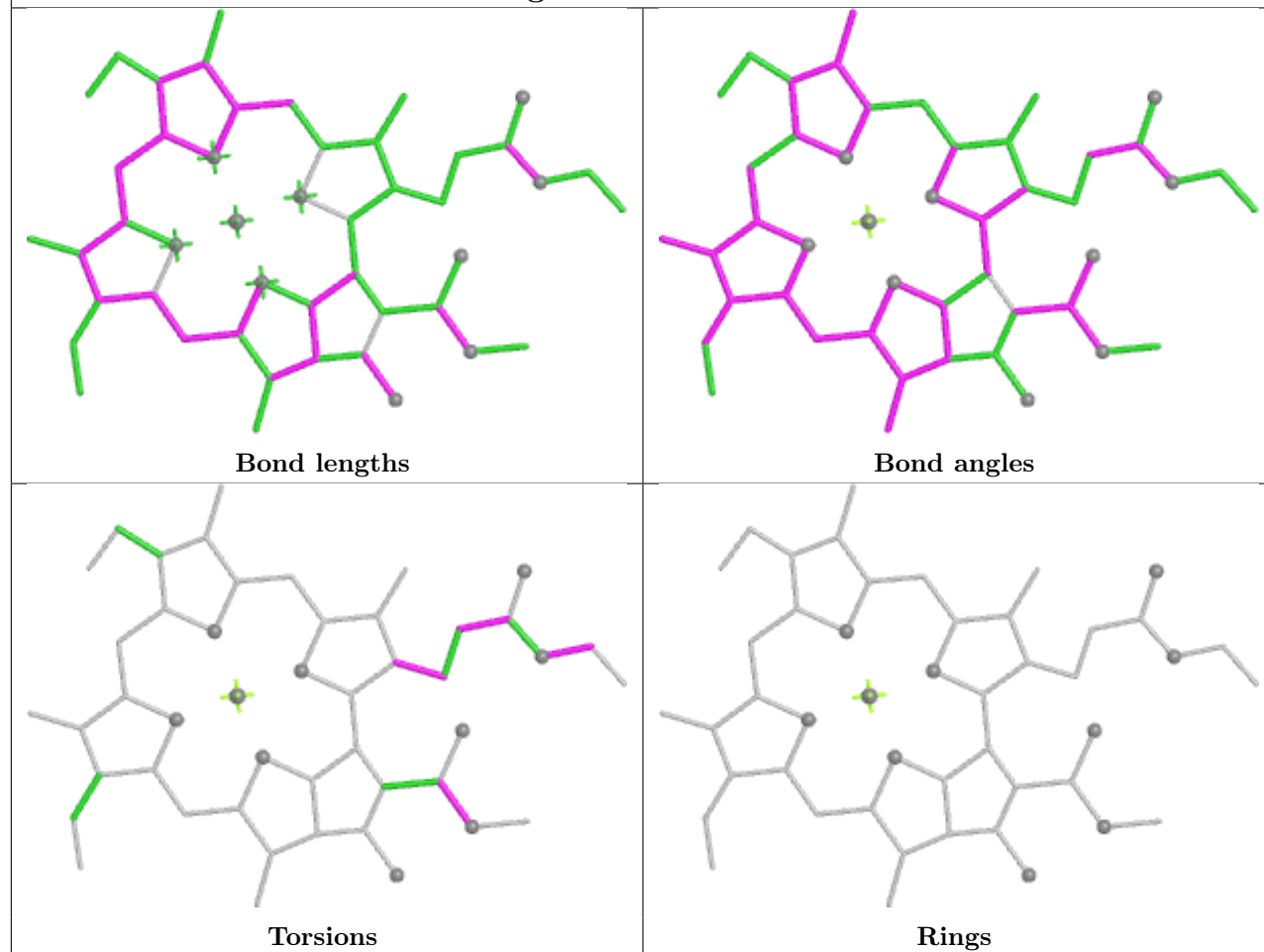


Ligand CLA cA 831

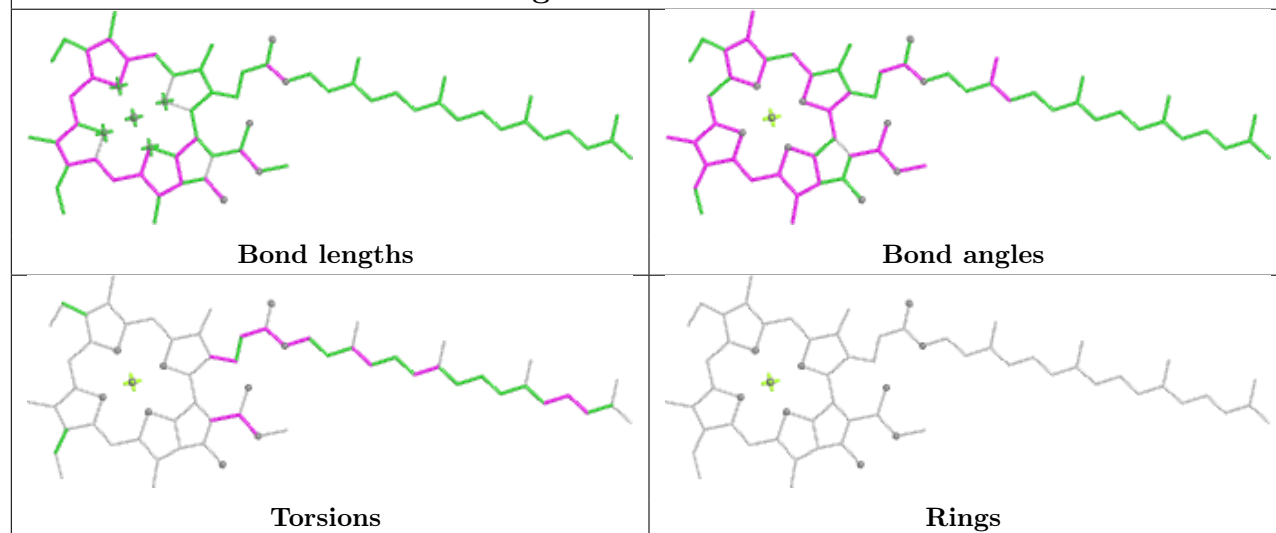


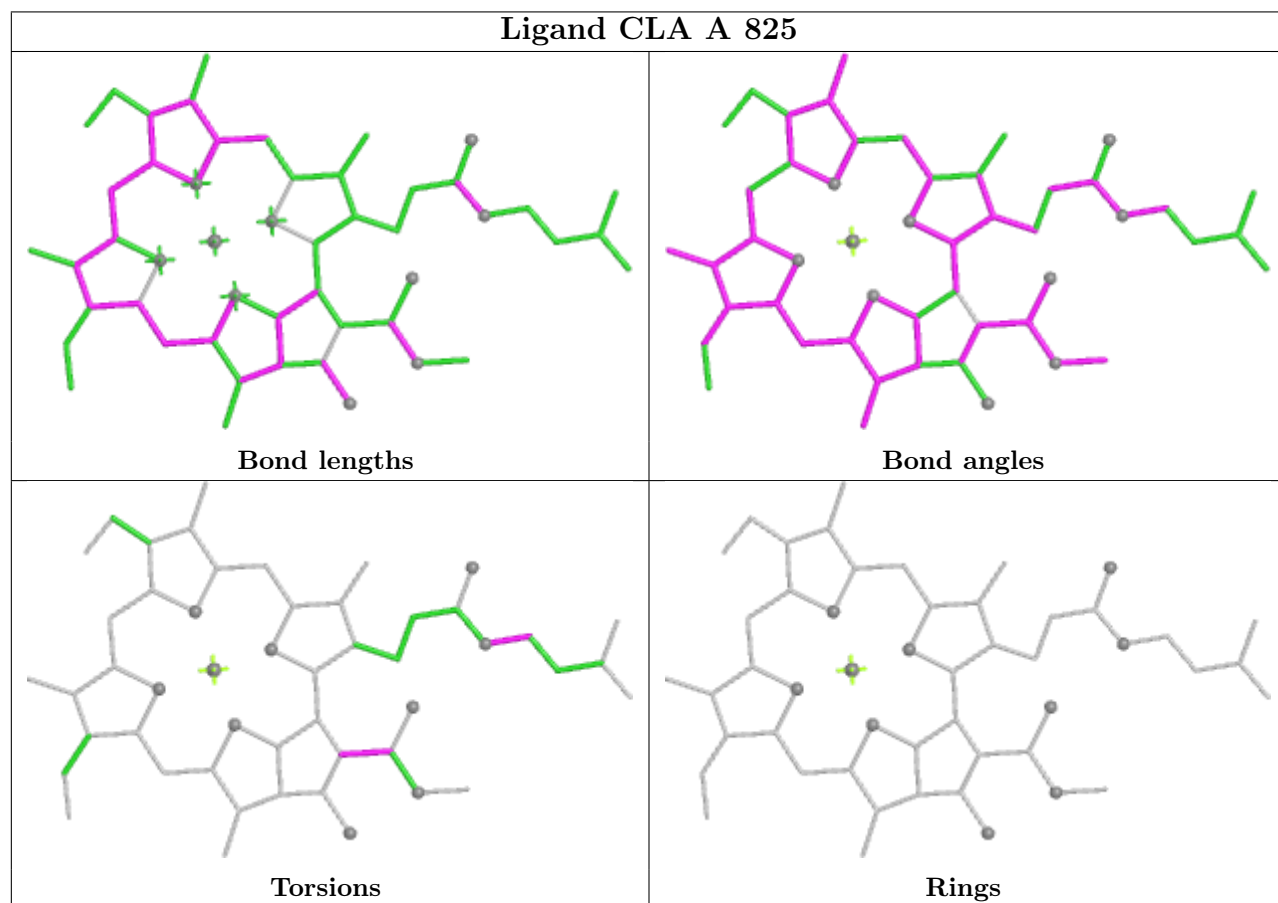
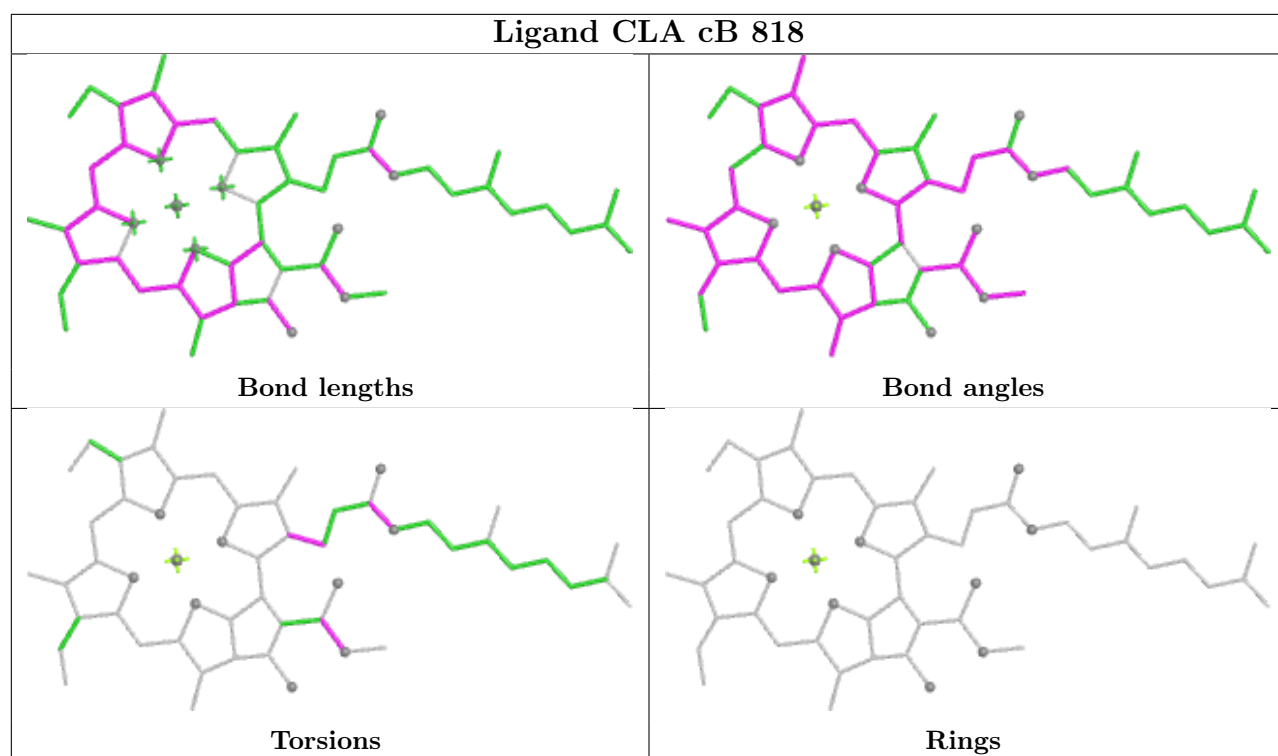


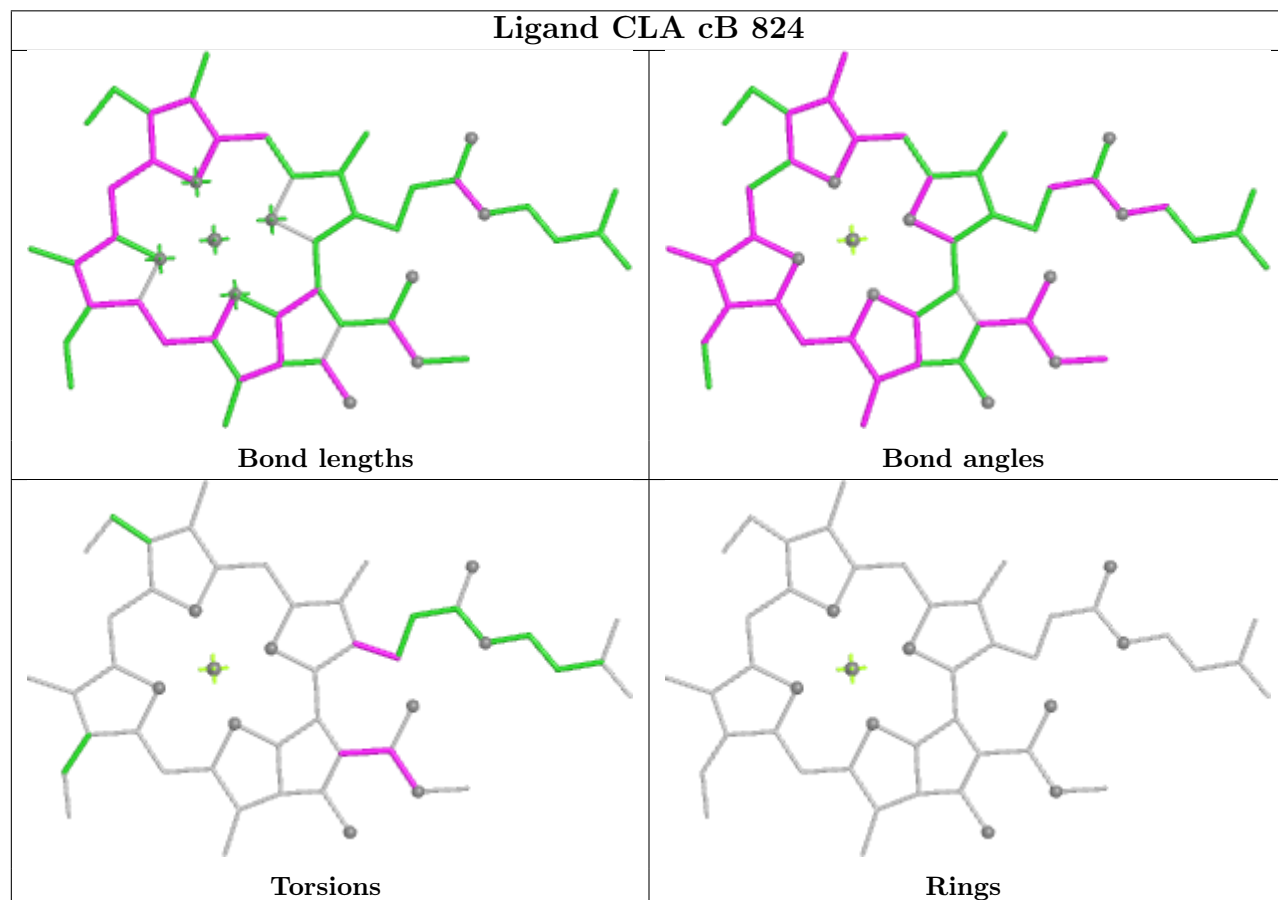
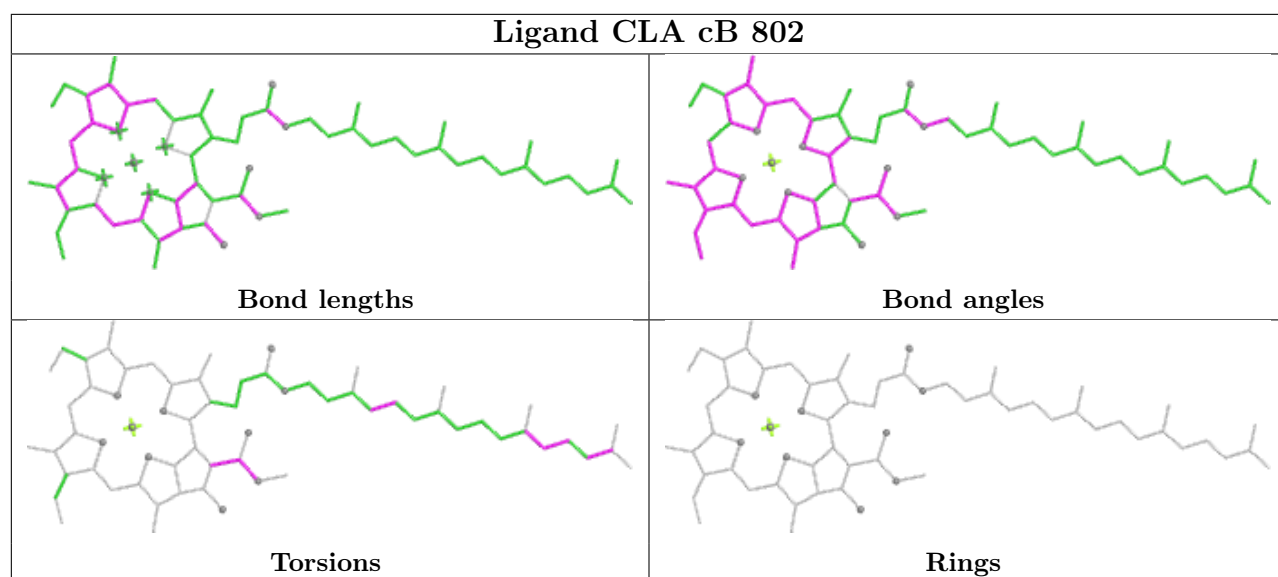
Ligand CLA B 837

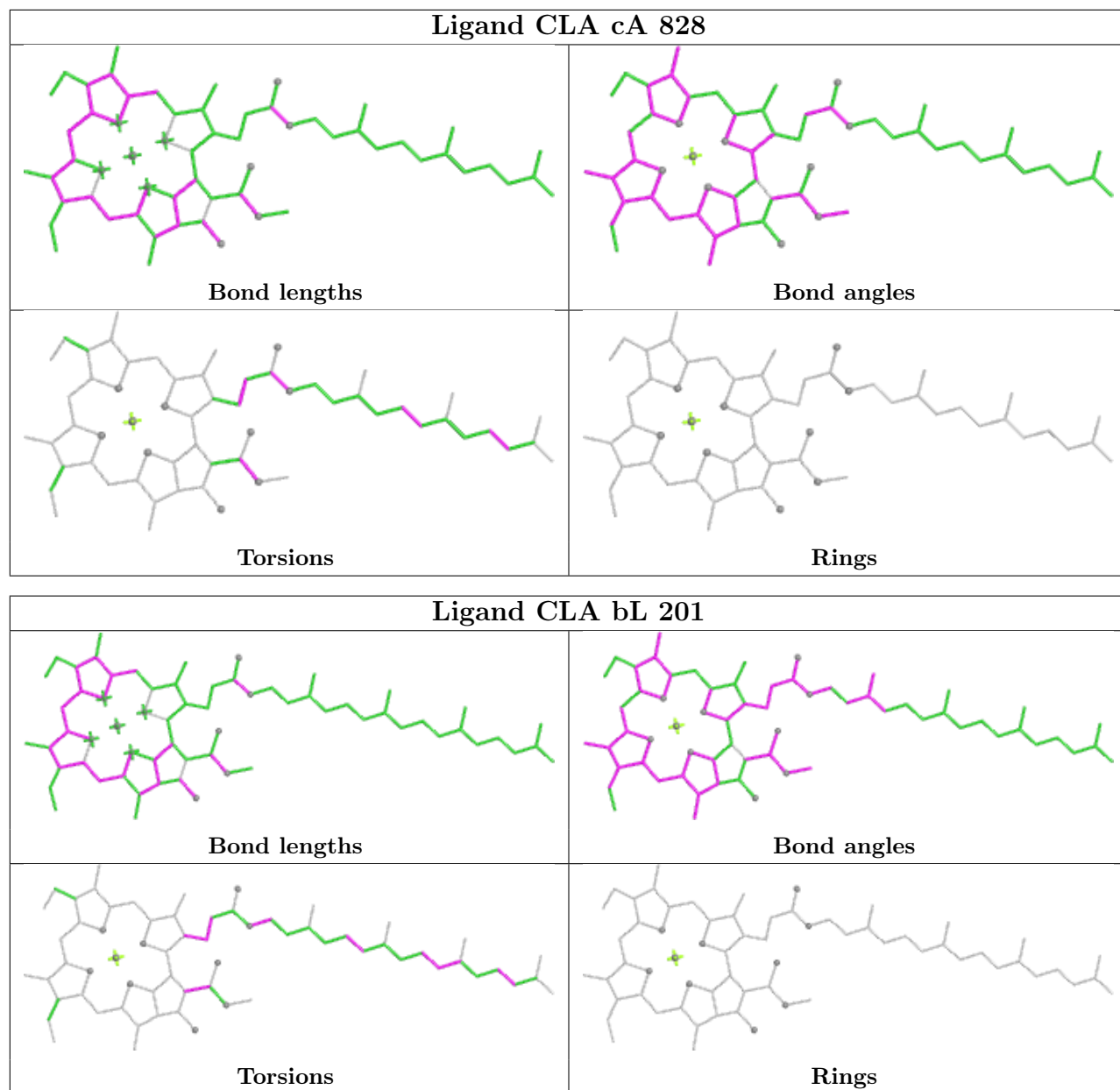


Ligand CLA B 805

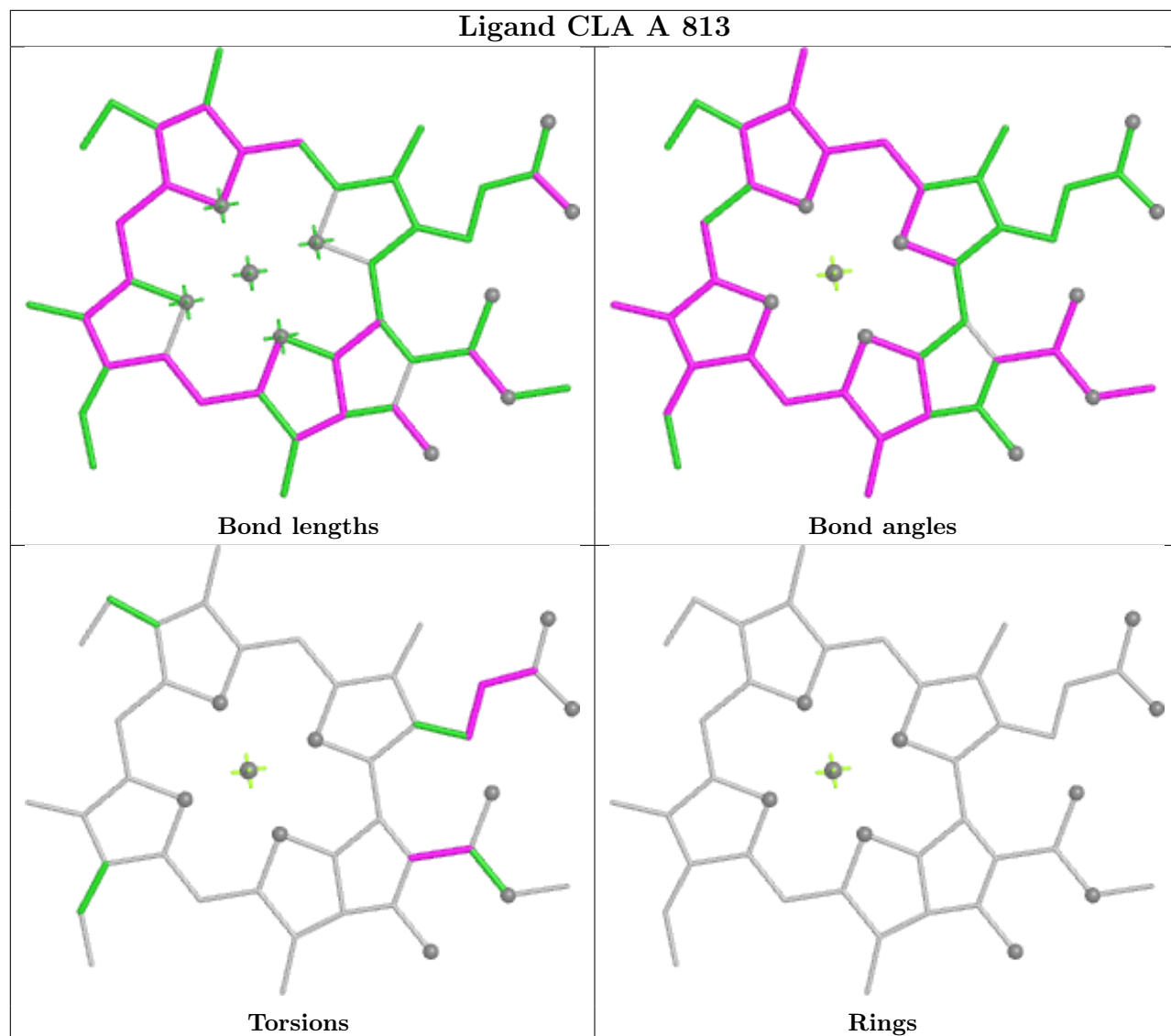




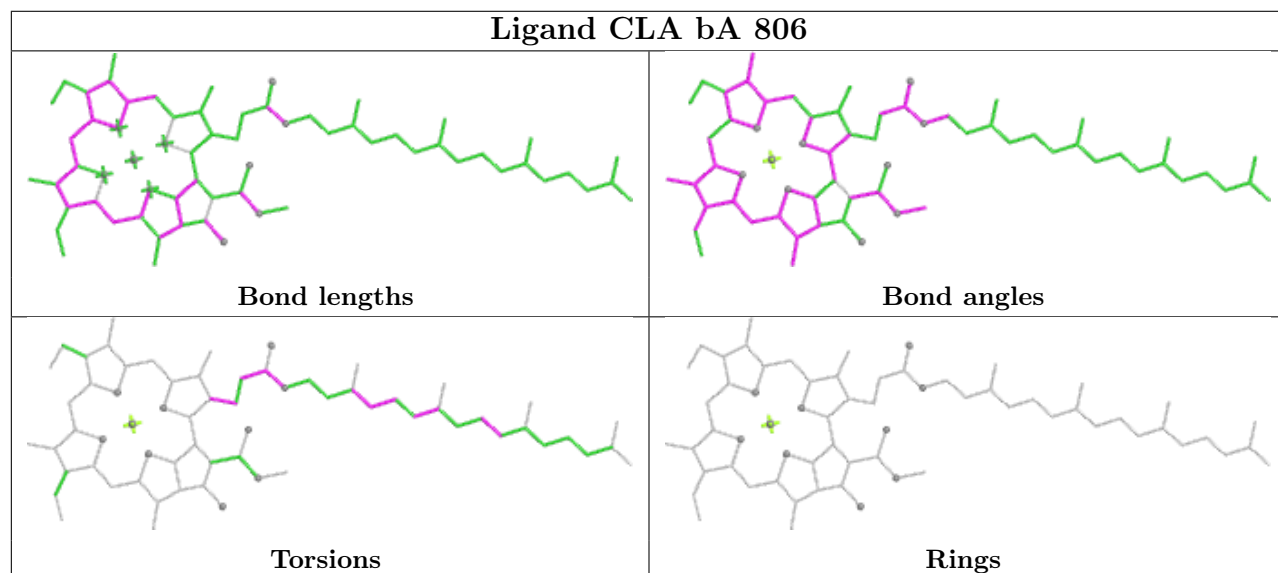


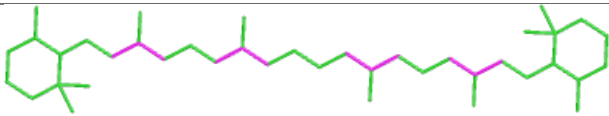
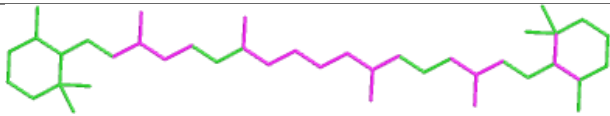
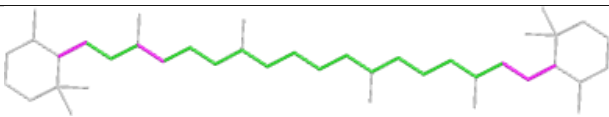
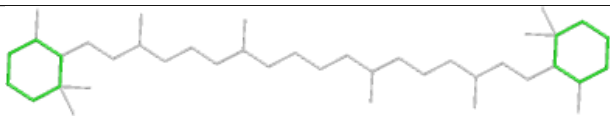


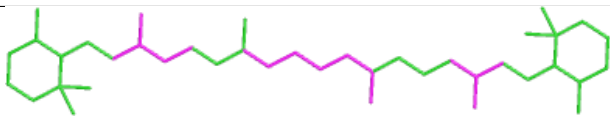
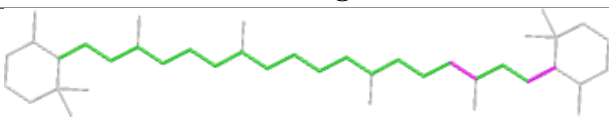
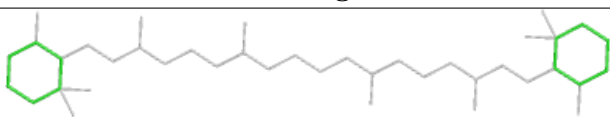
Ligand CLA A 813

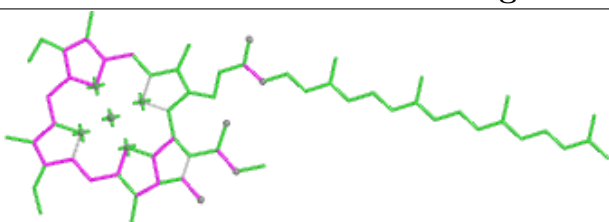
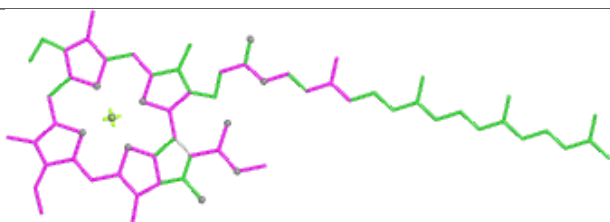
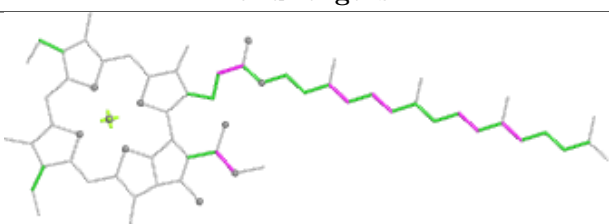
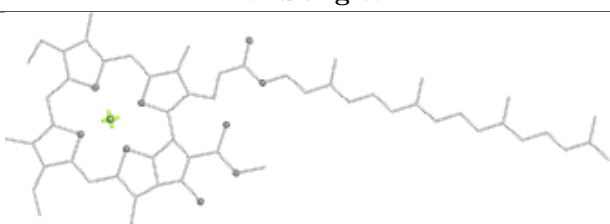


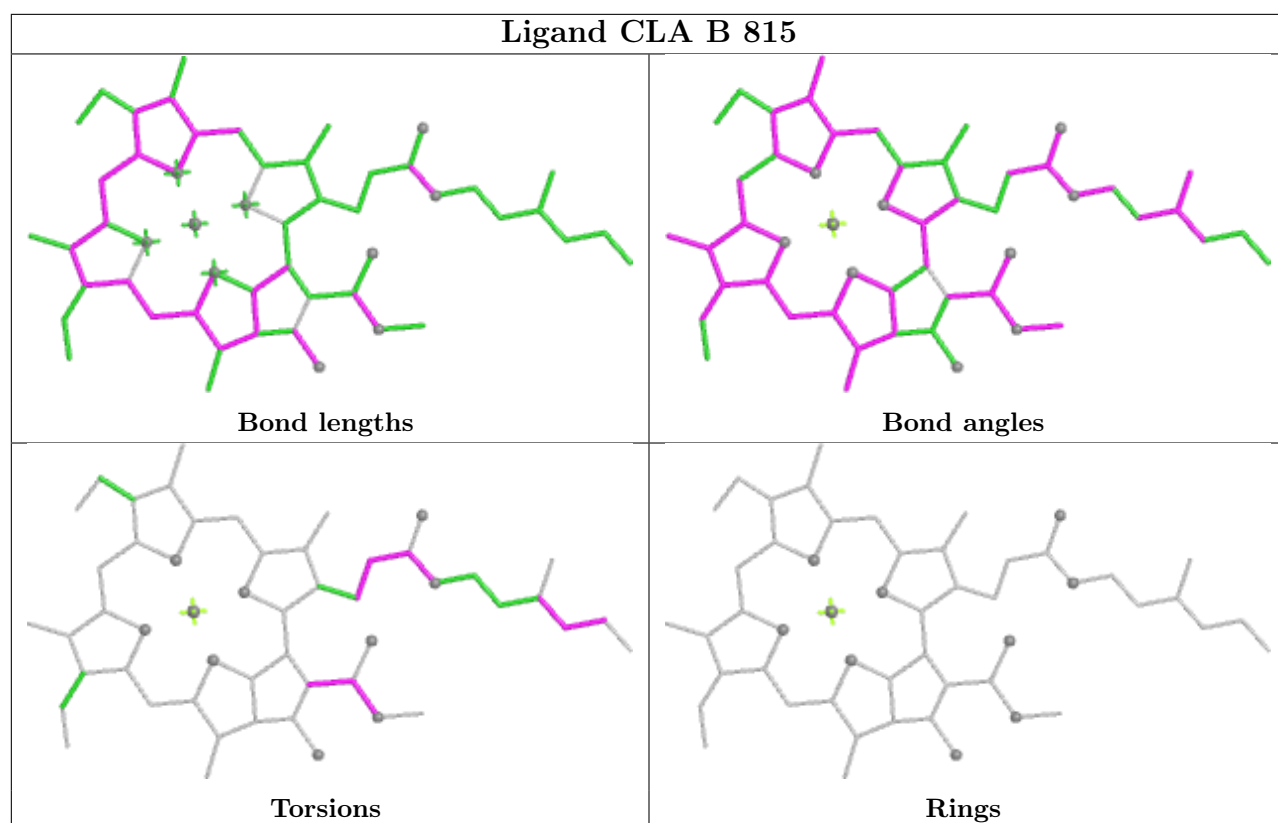
Ligand CLA bA 806



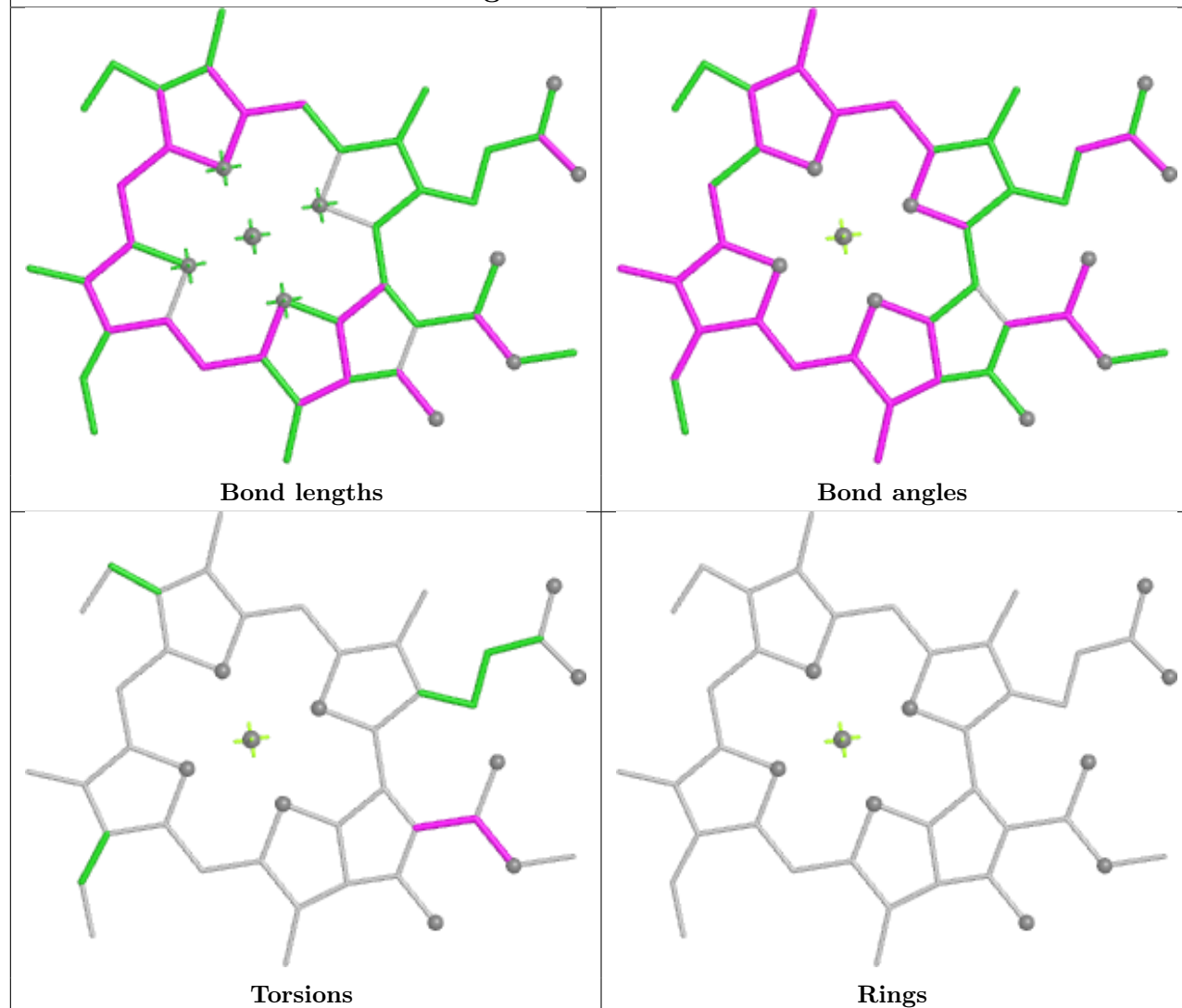
Ligand BCR cM 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR cI 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

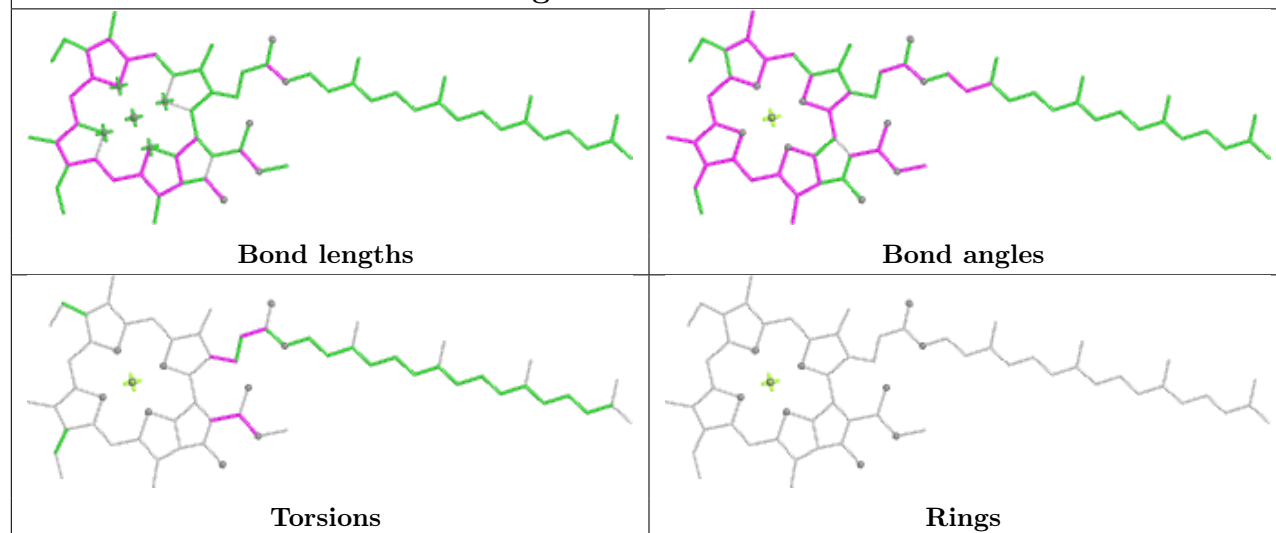
Ligand CLA bB 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

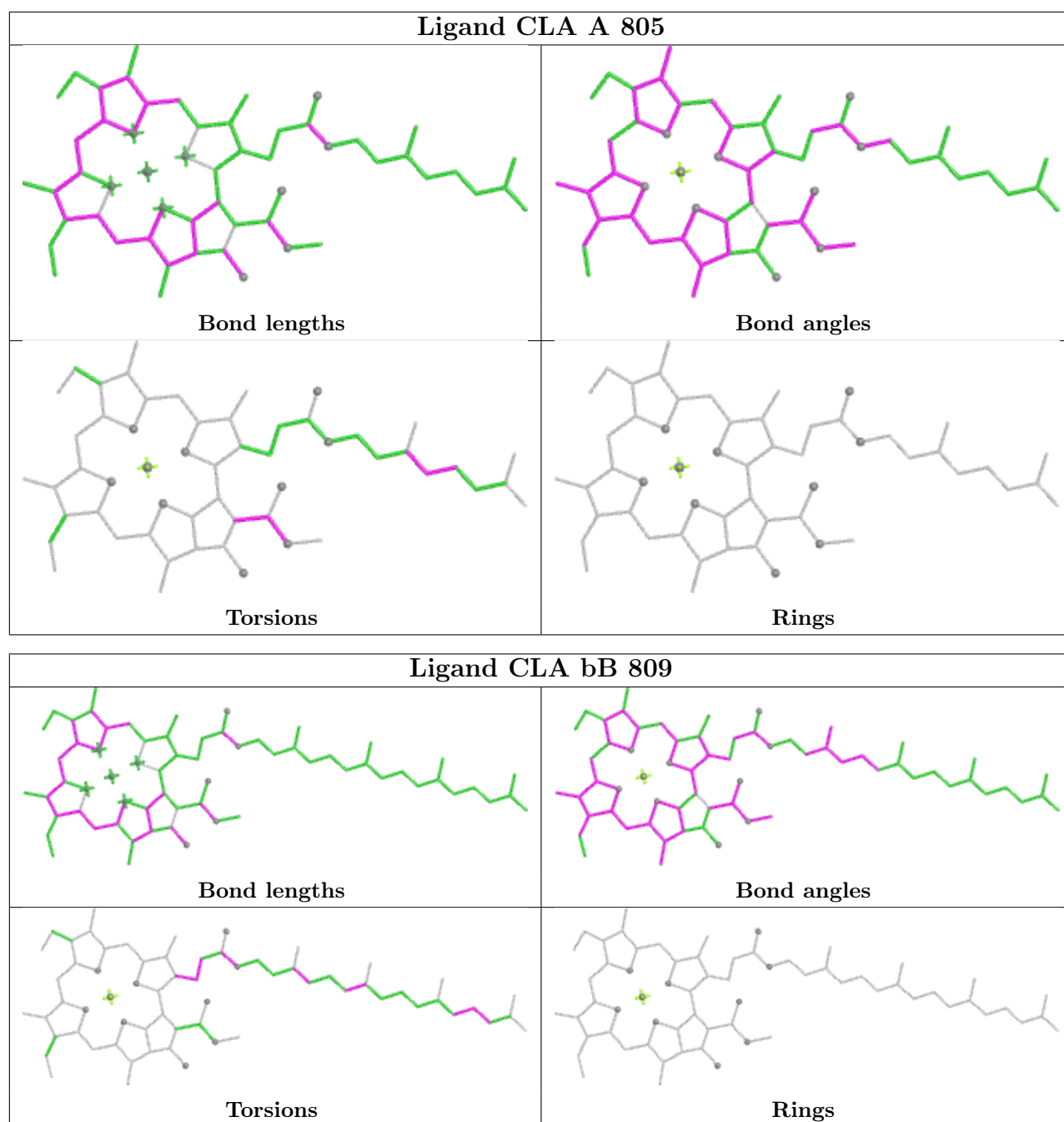


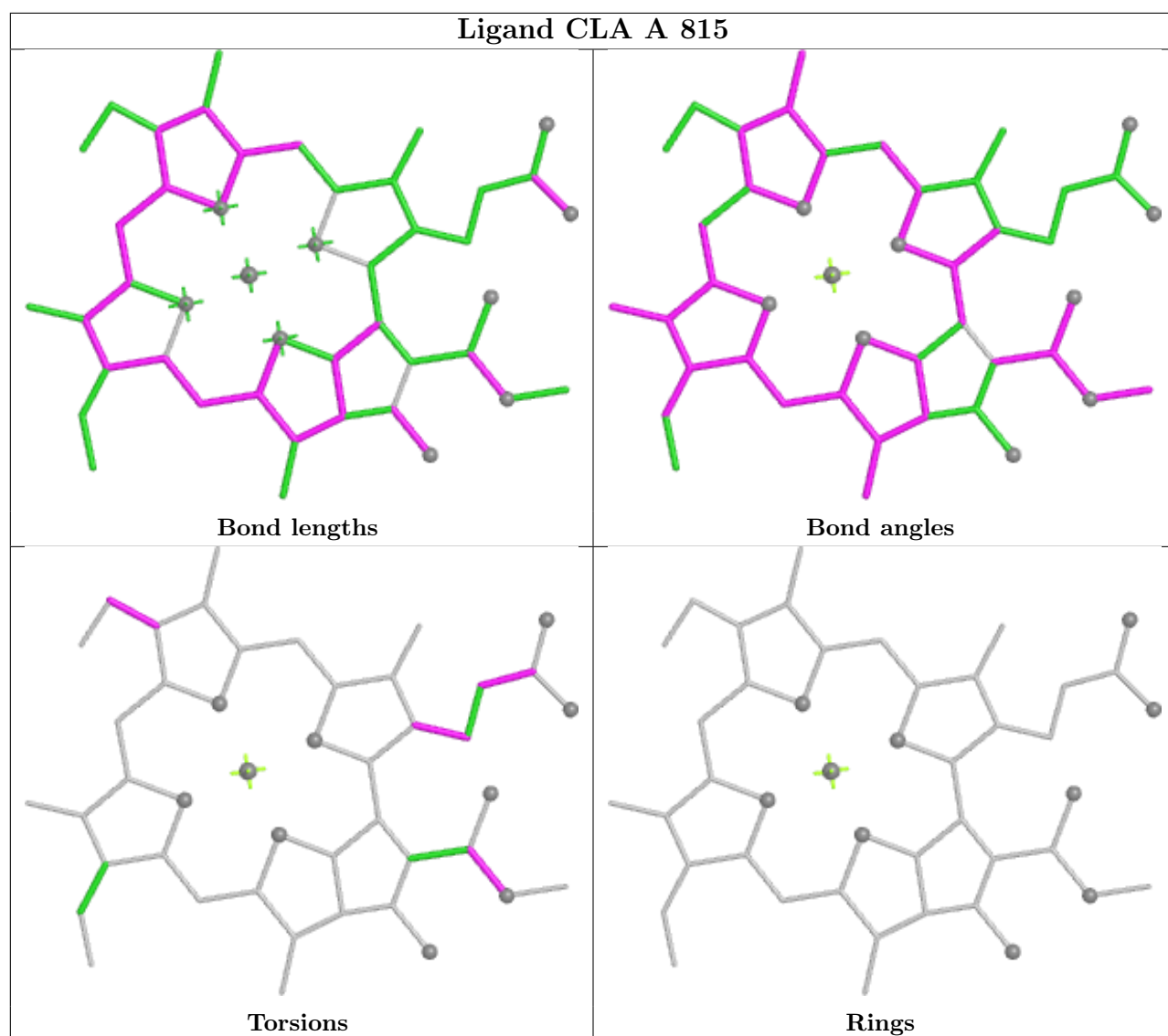
Ligand CLA bB 832



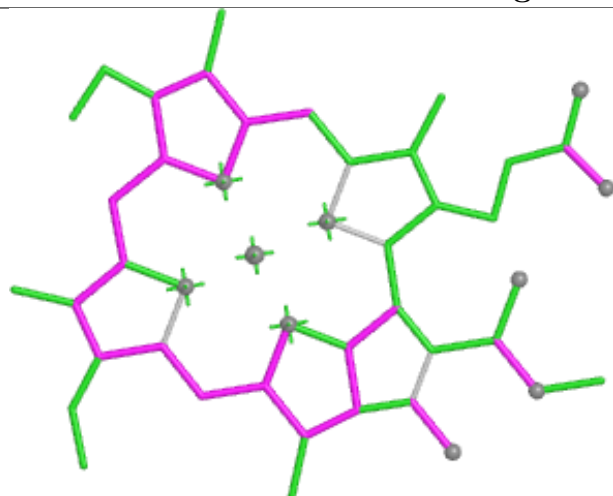
Ligand CLA B 812



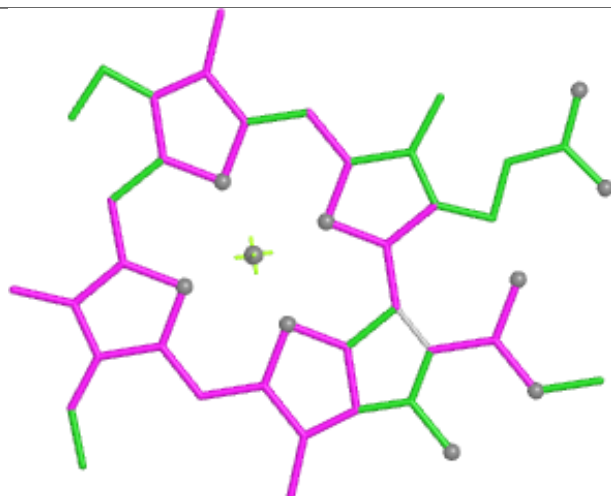




Ligand CLA A 812



Bond lengths



Bond angles

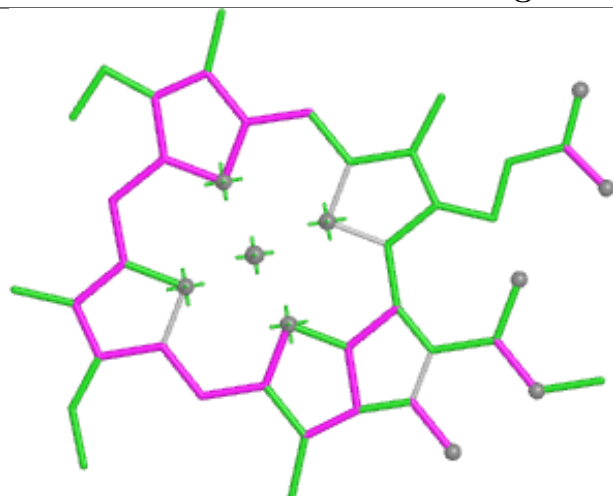


Torsions

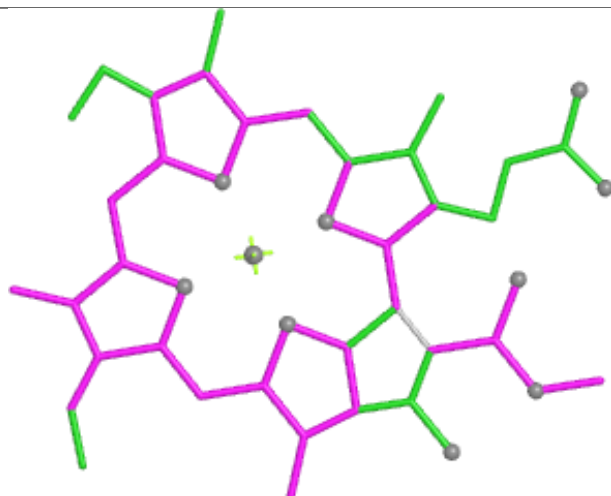


Rings

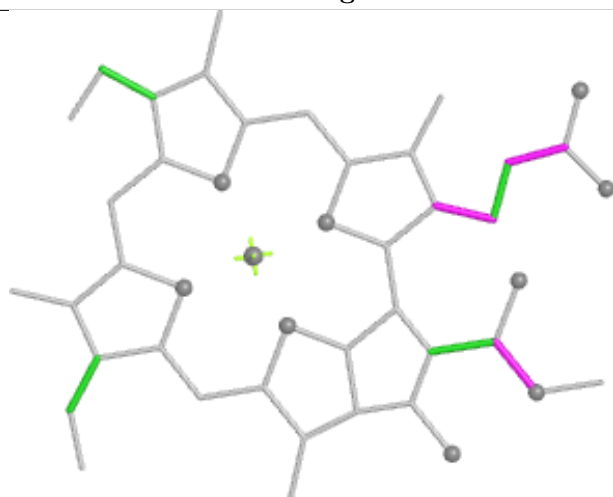
Ligand CLA B 851



Bond lengths



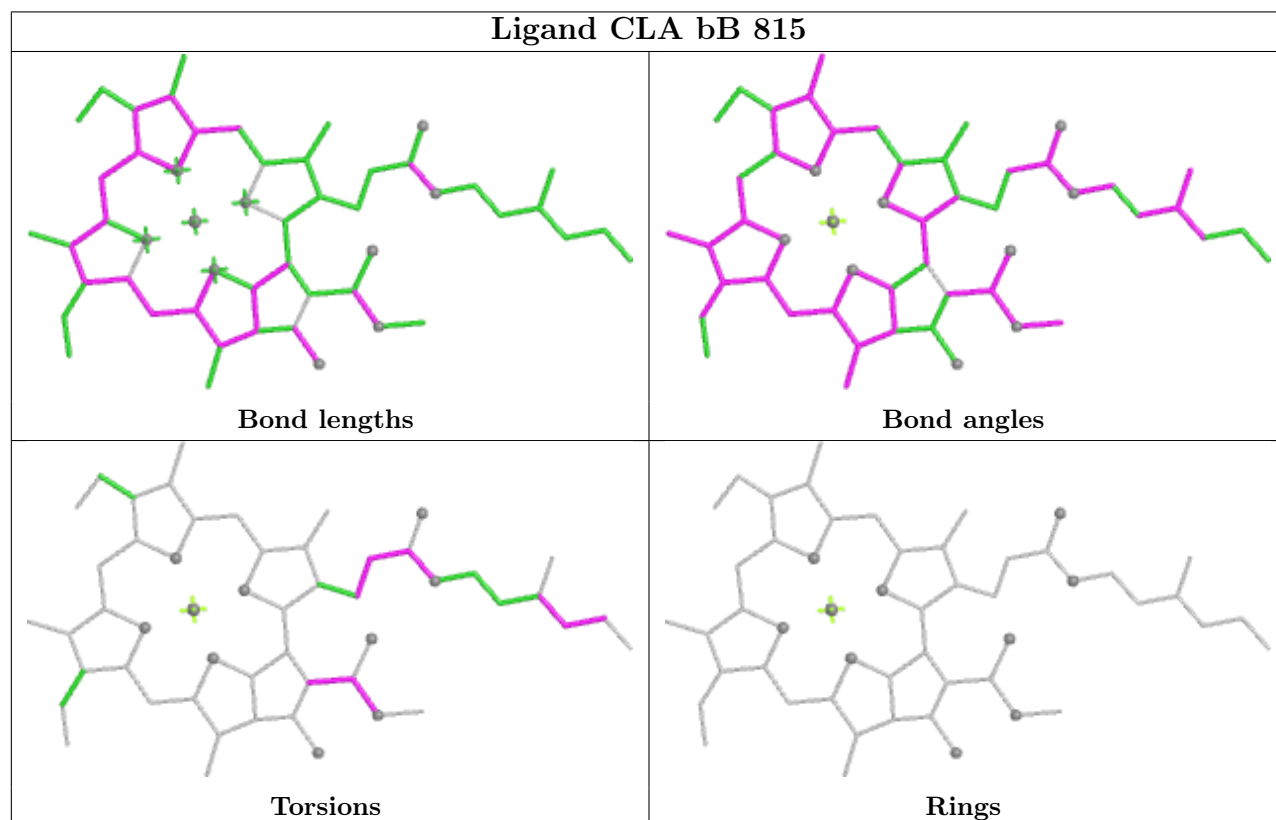
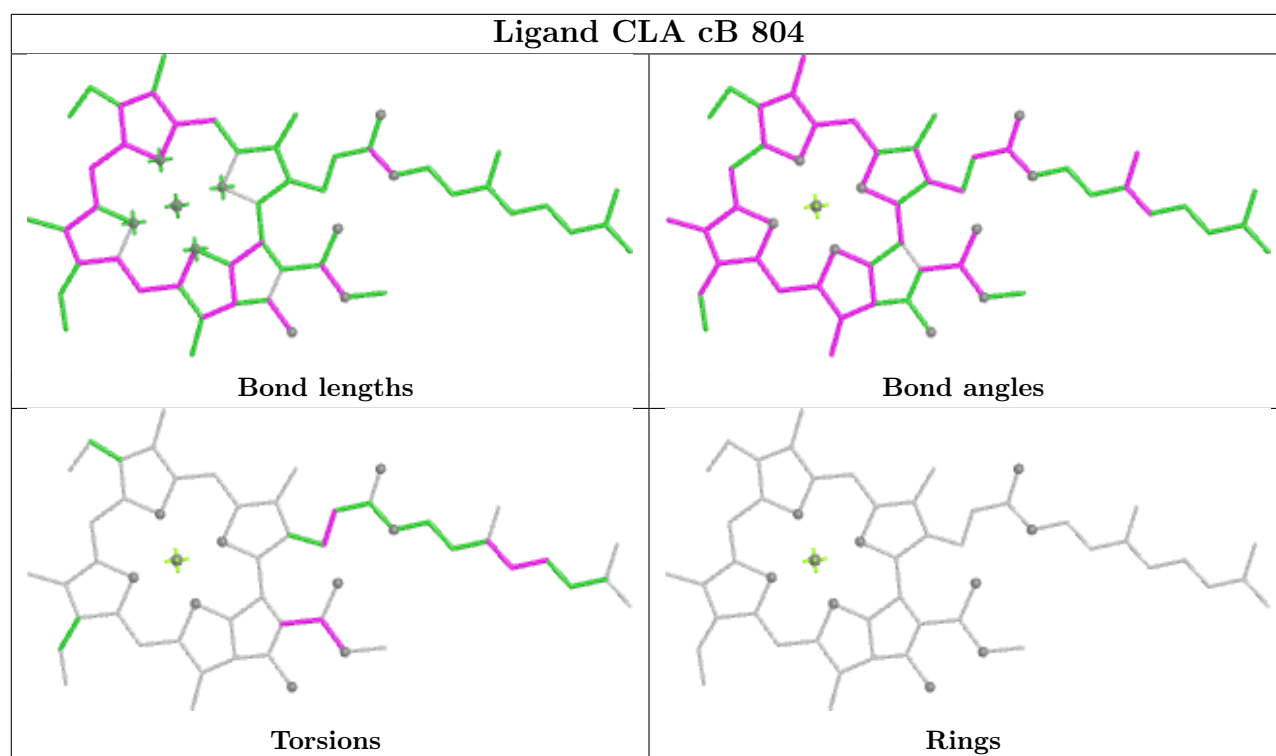
Bond angles

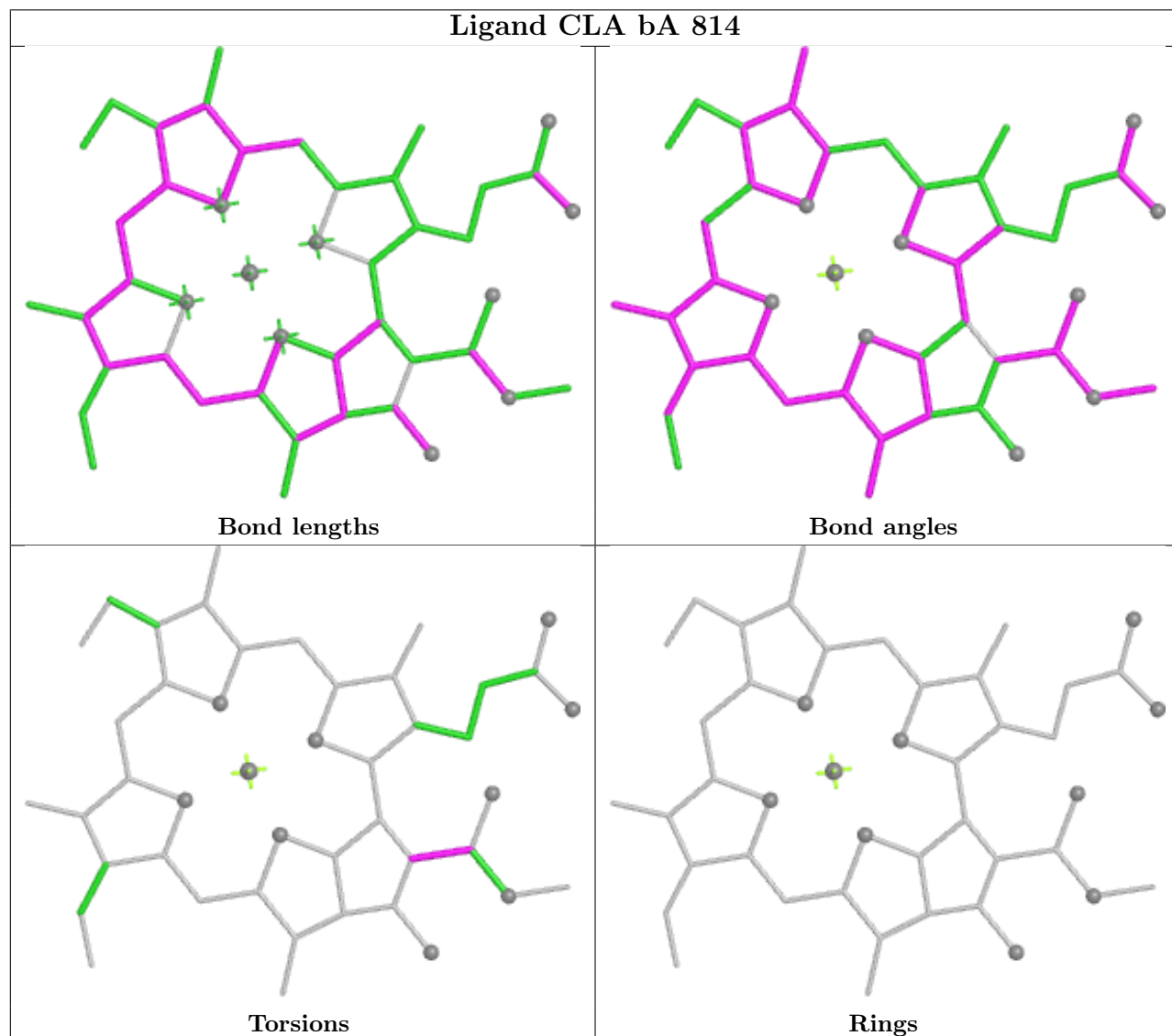
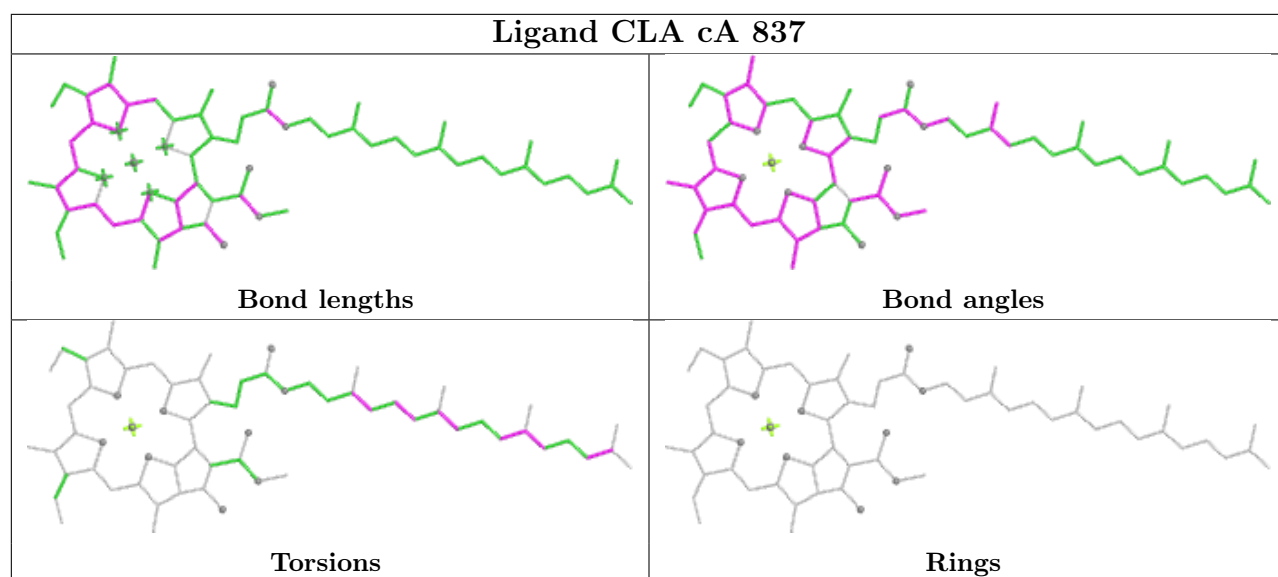


Torsions

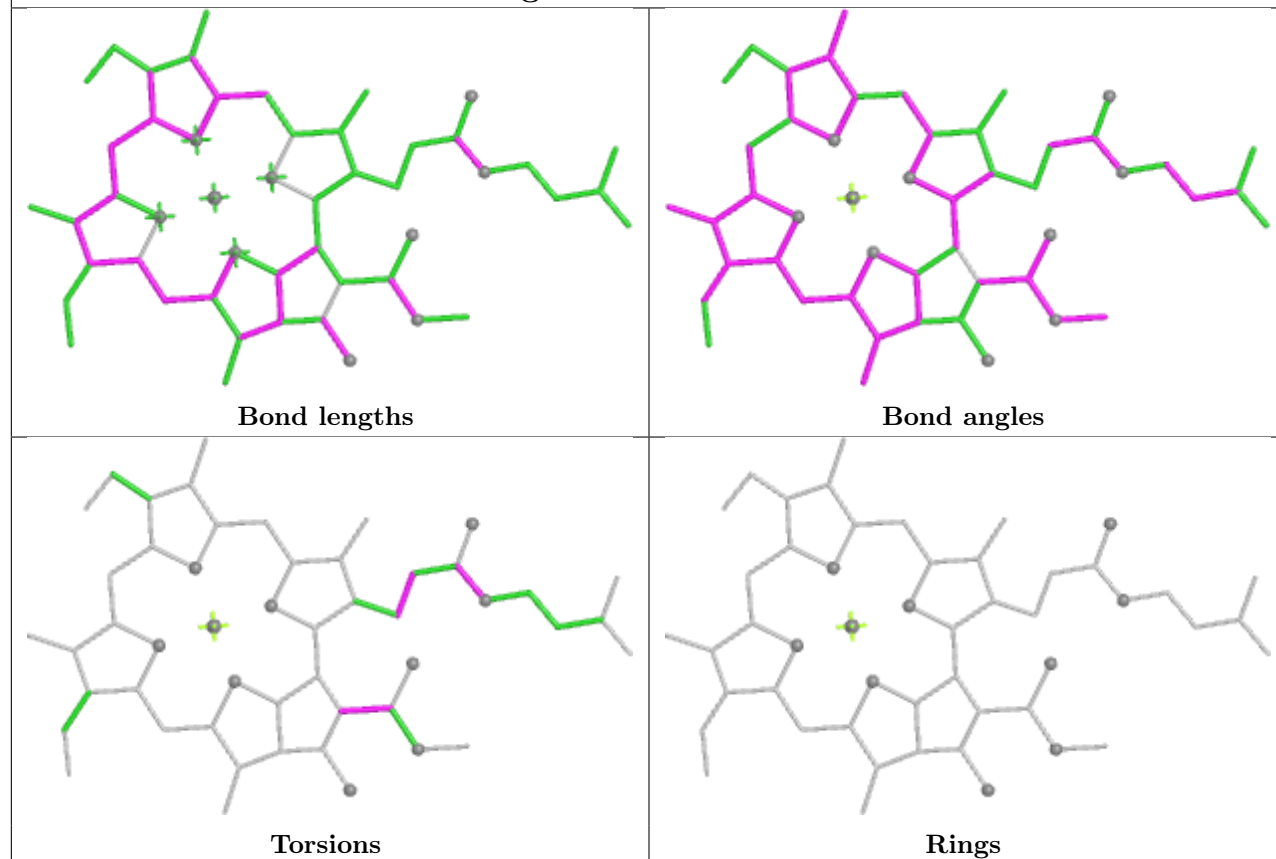


Rings

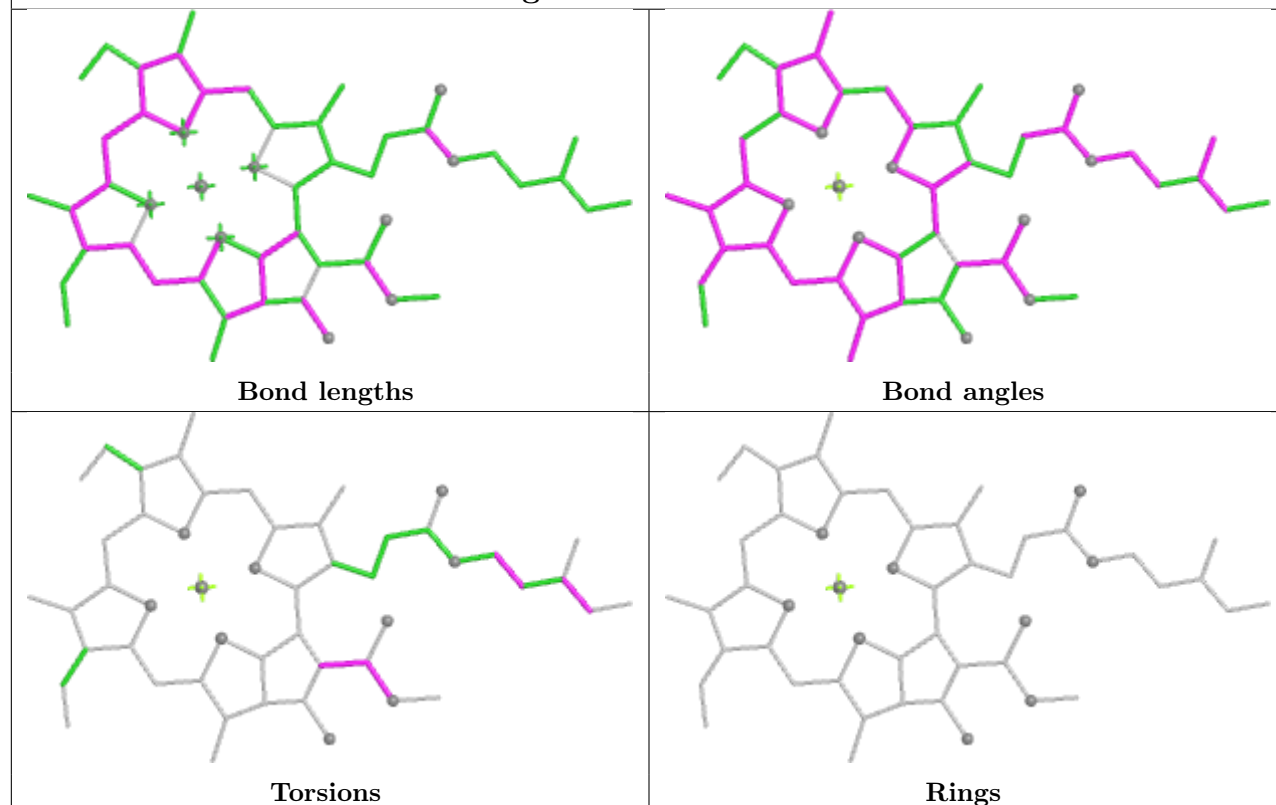


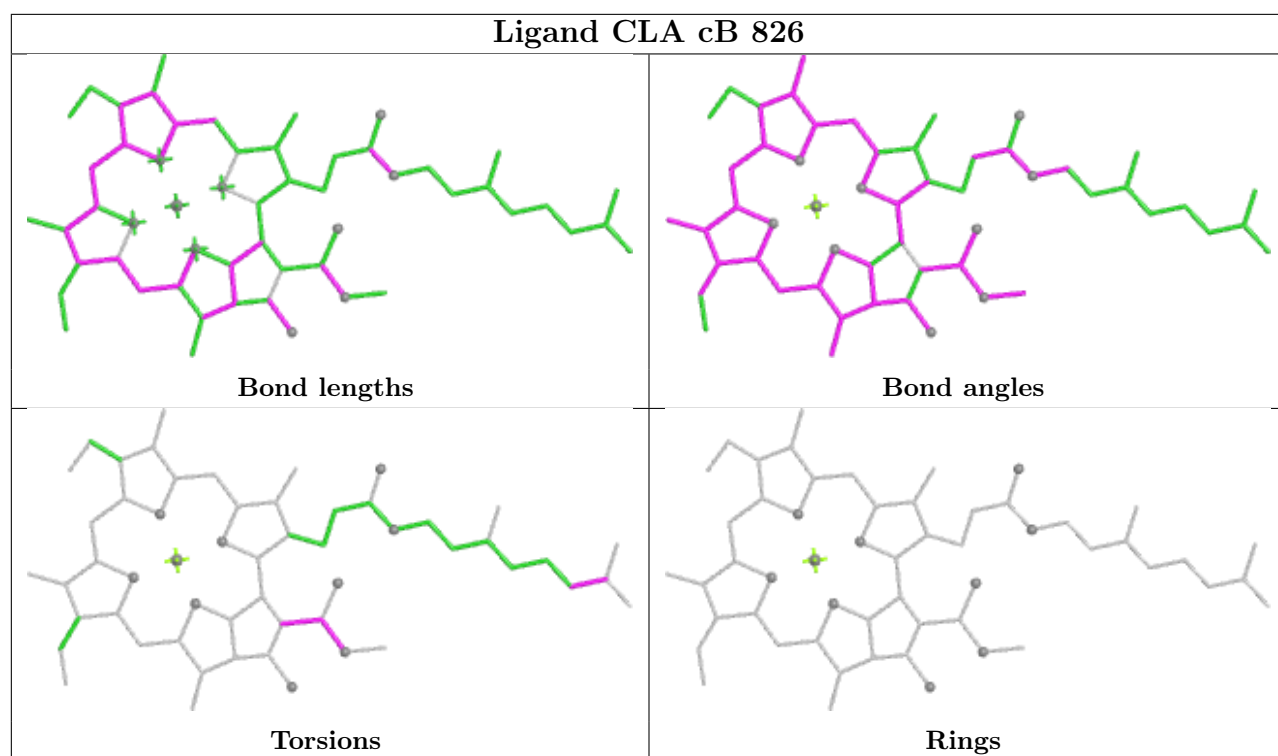


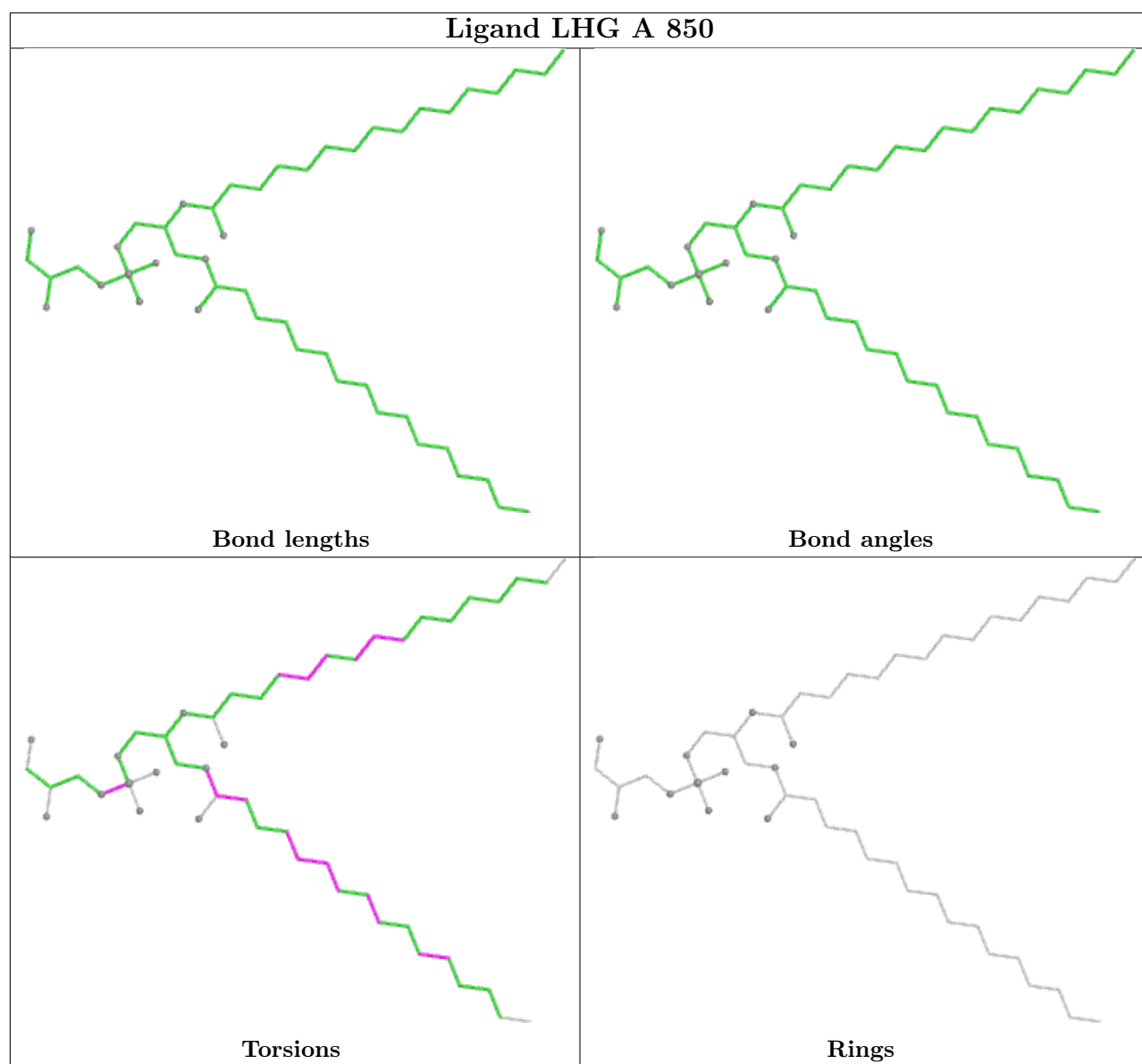
Ligand CLA bA 830

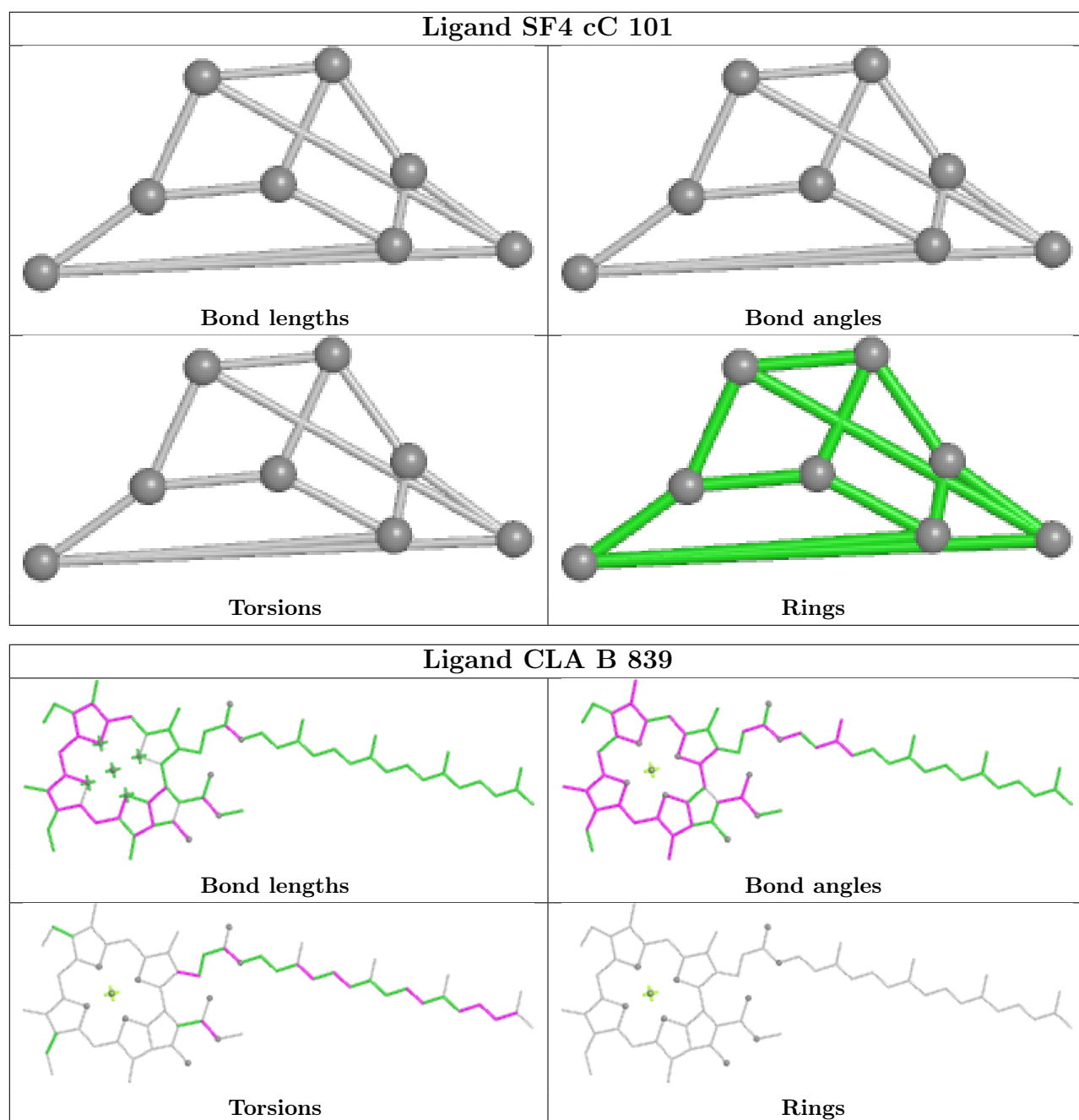


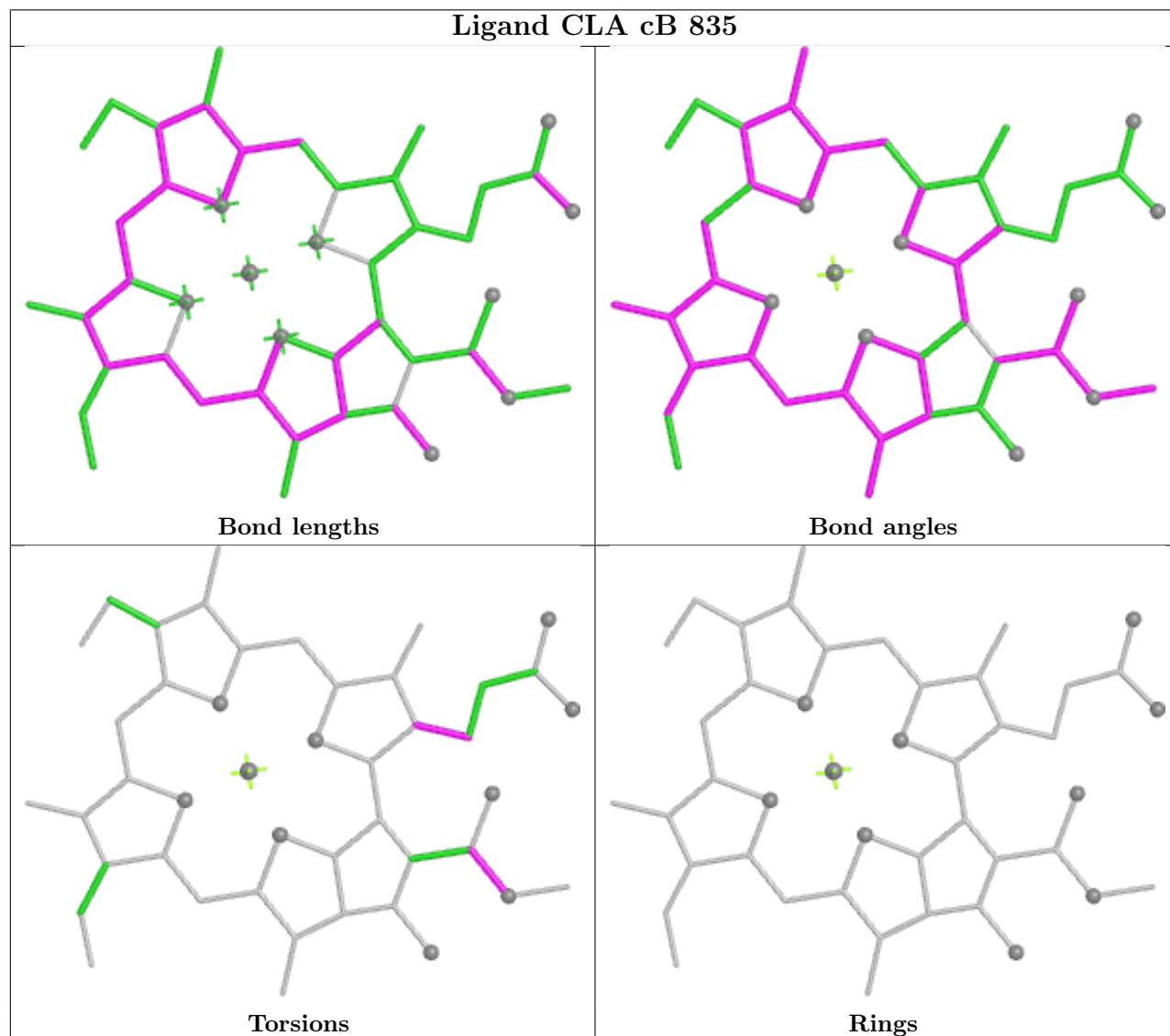
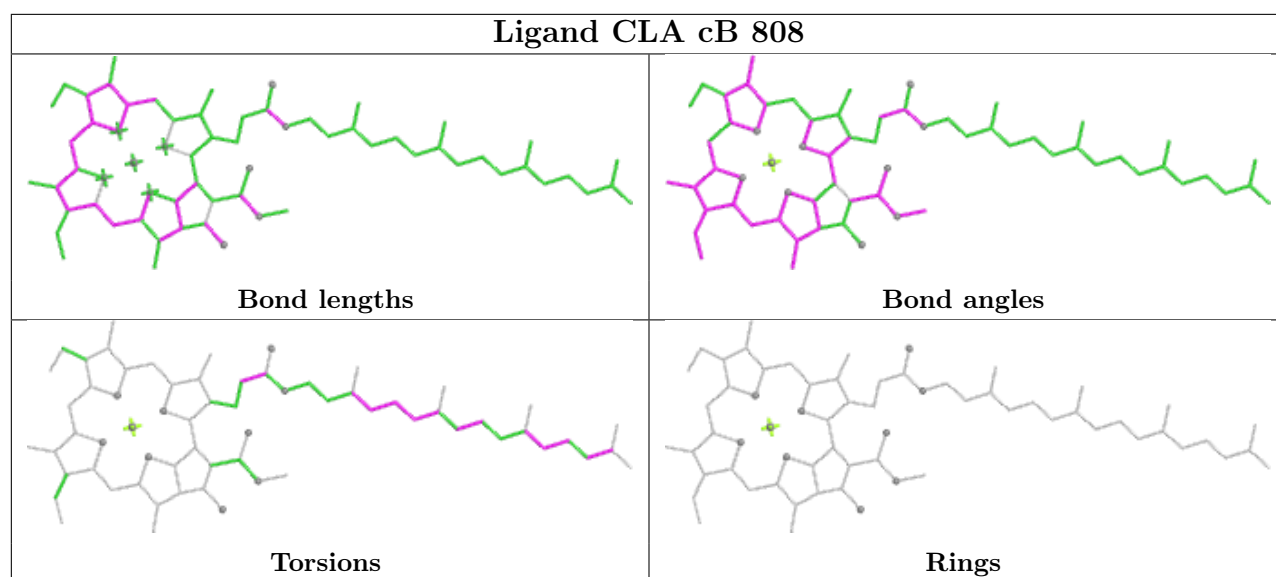
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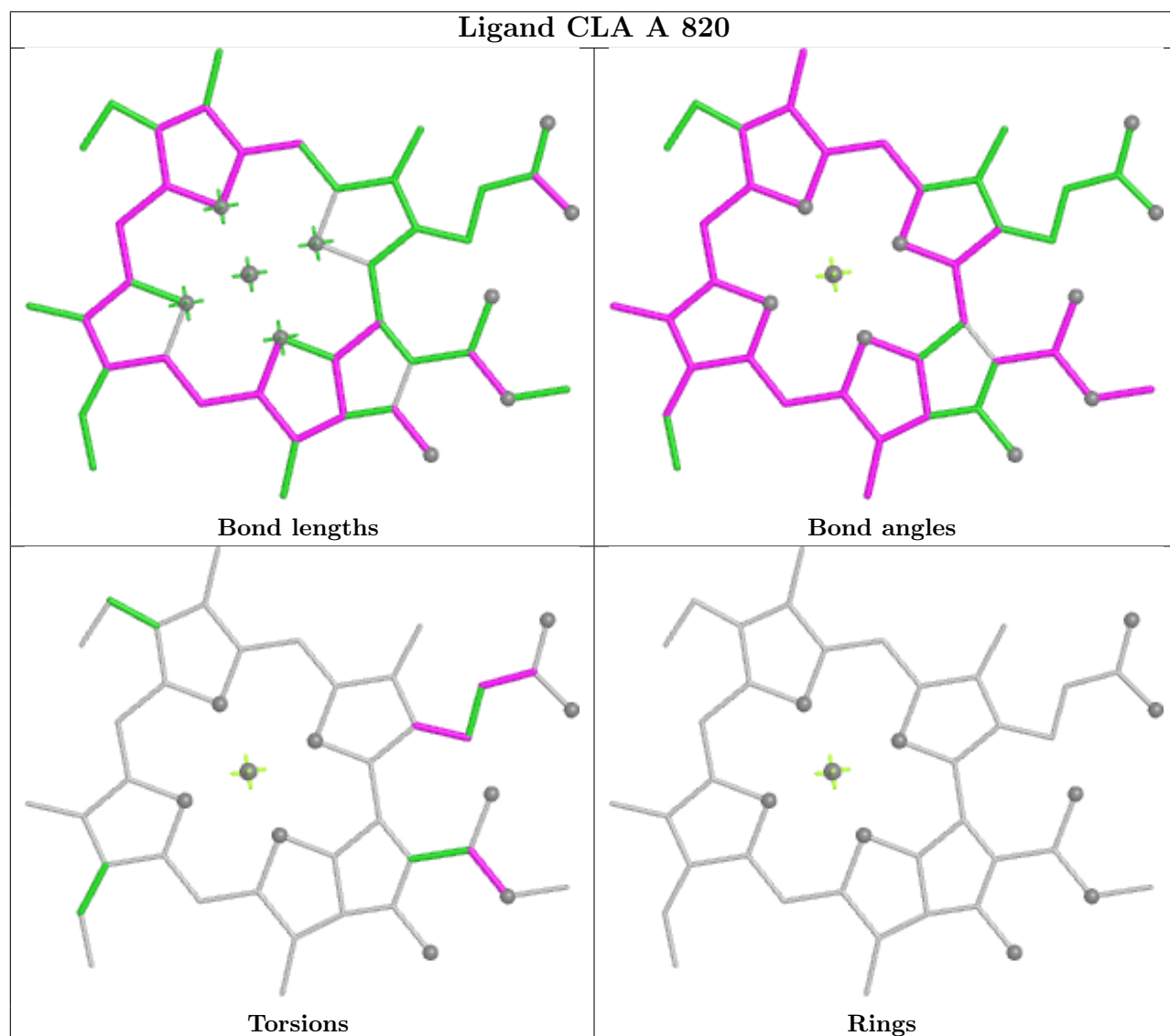
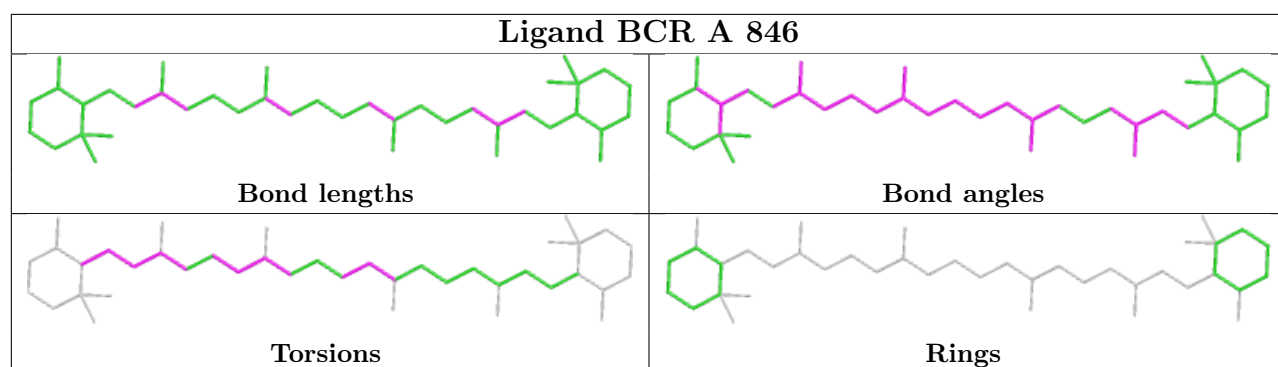




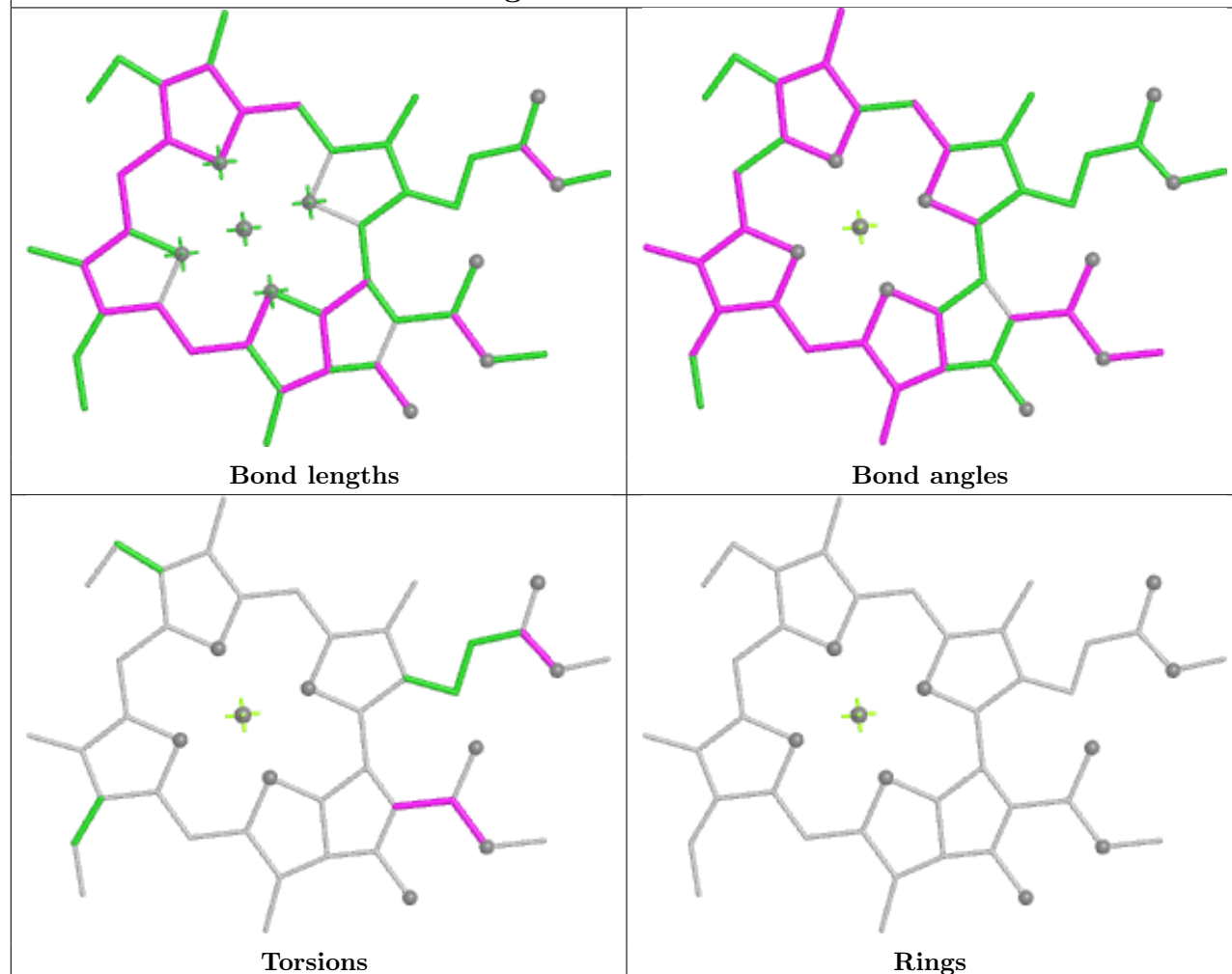




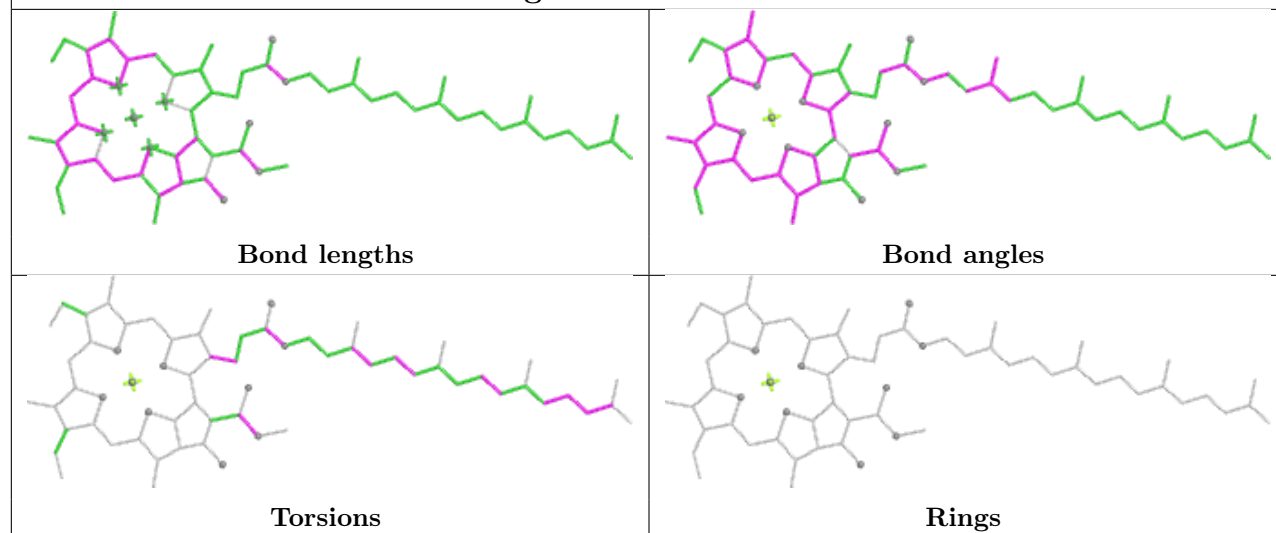


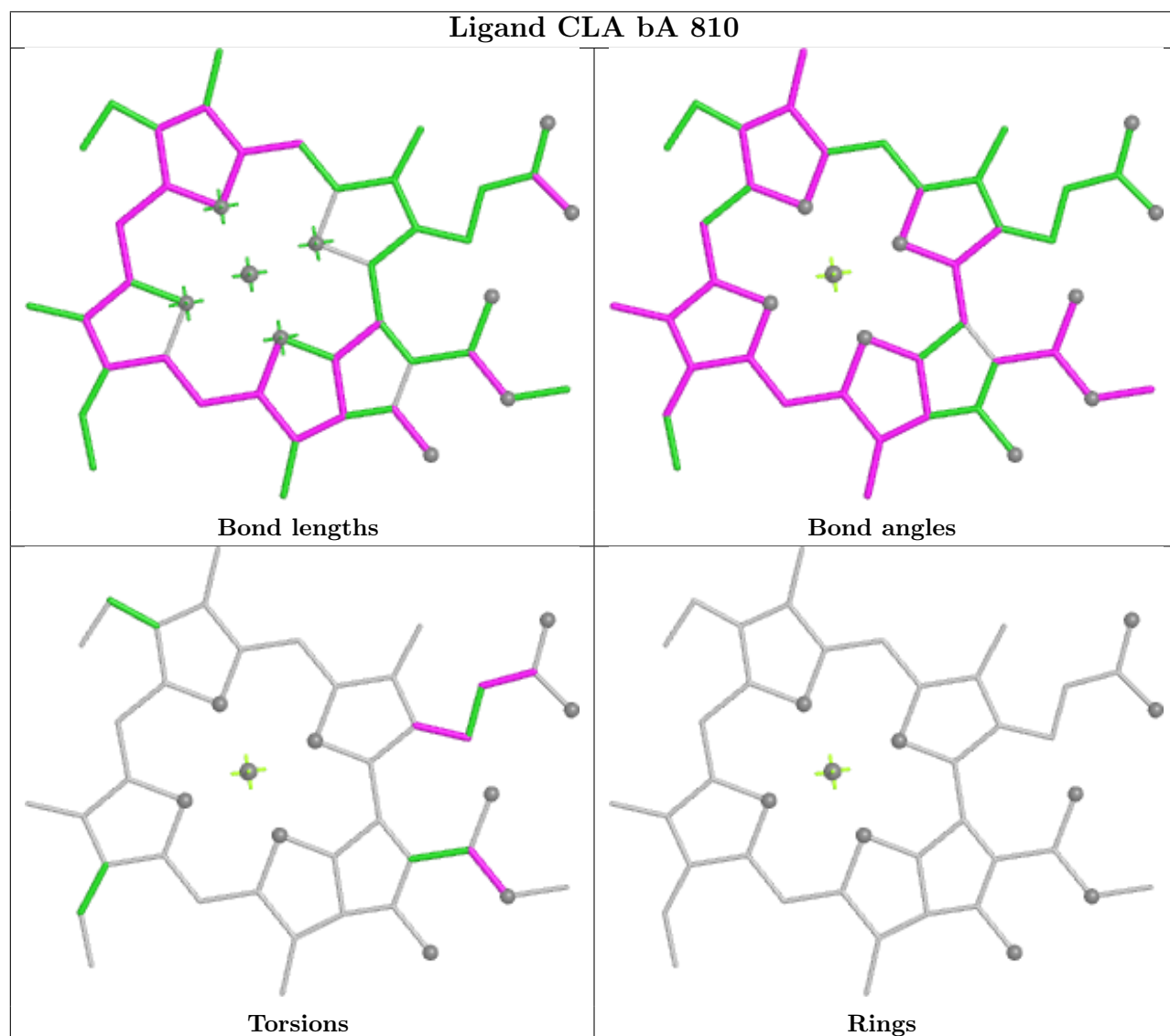
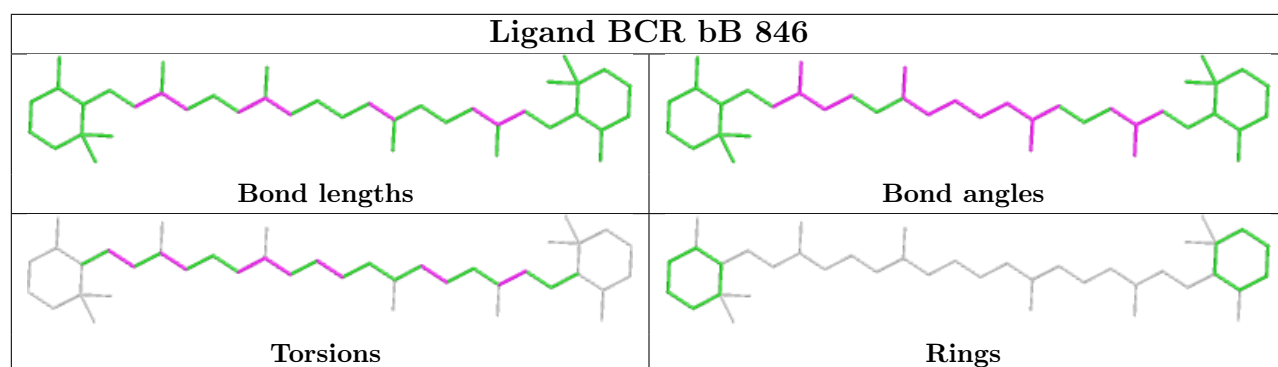


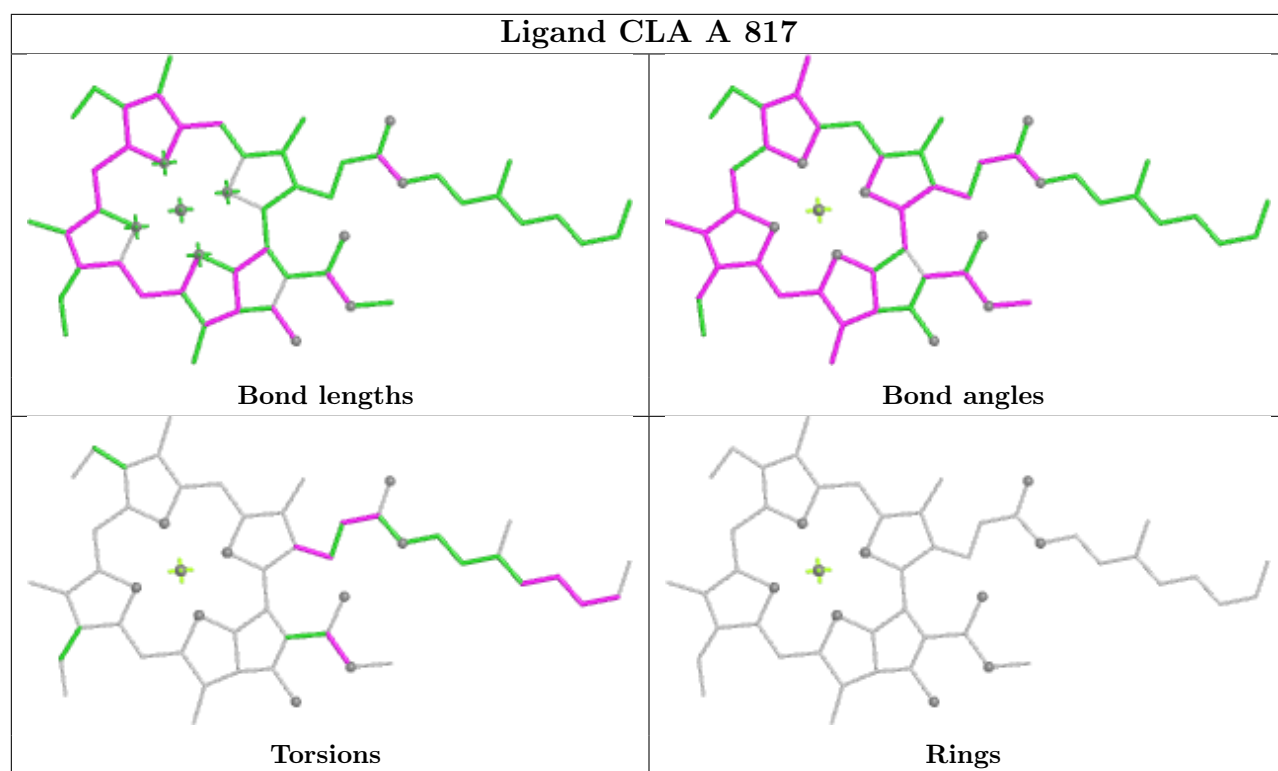
Ligand CLA bB 824

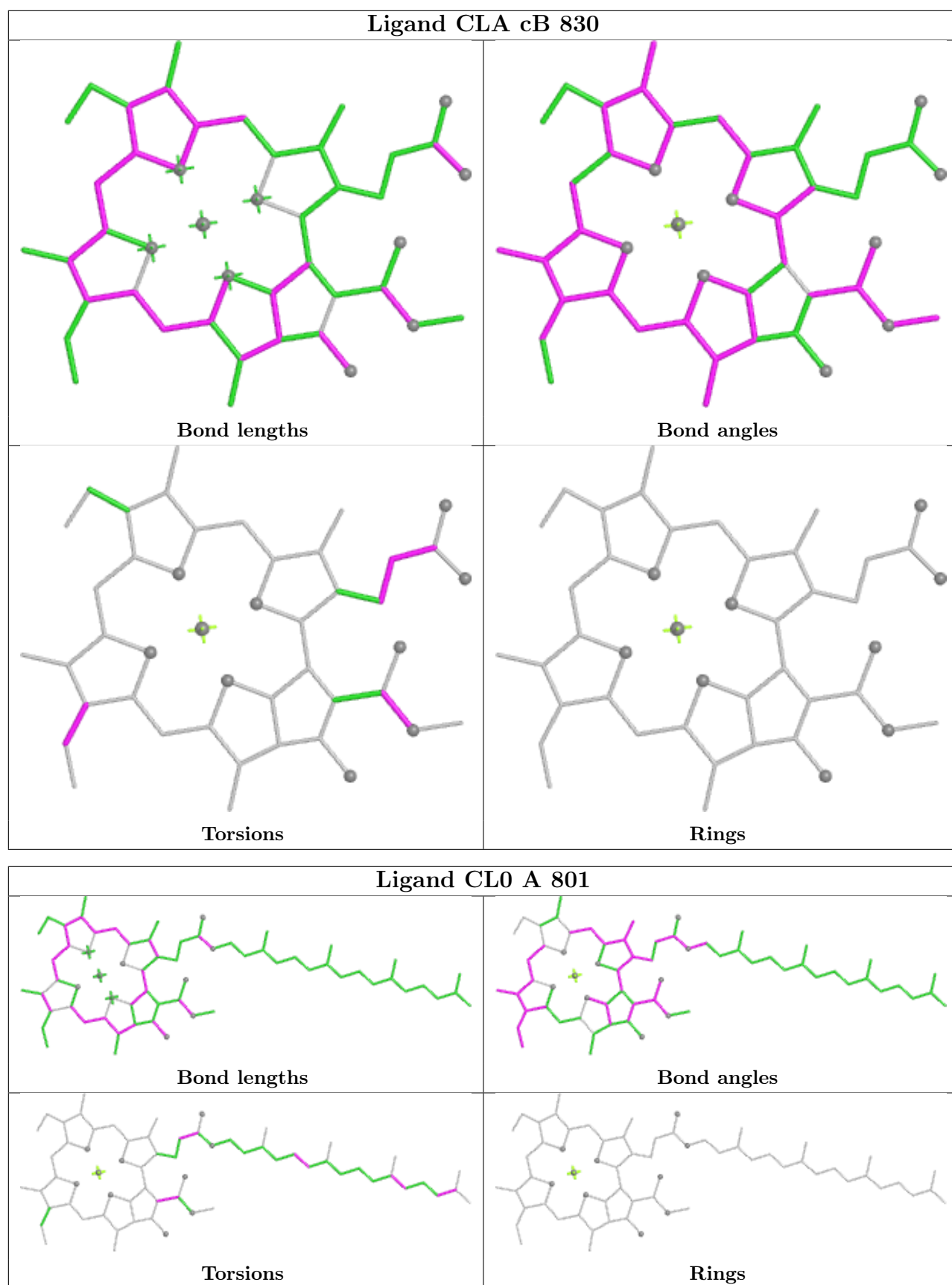


Ligand CLA cB 840

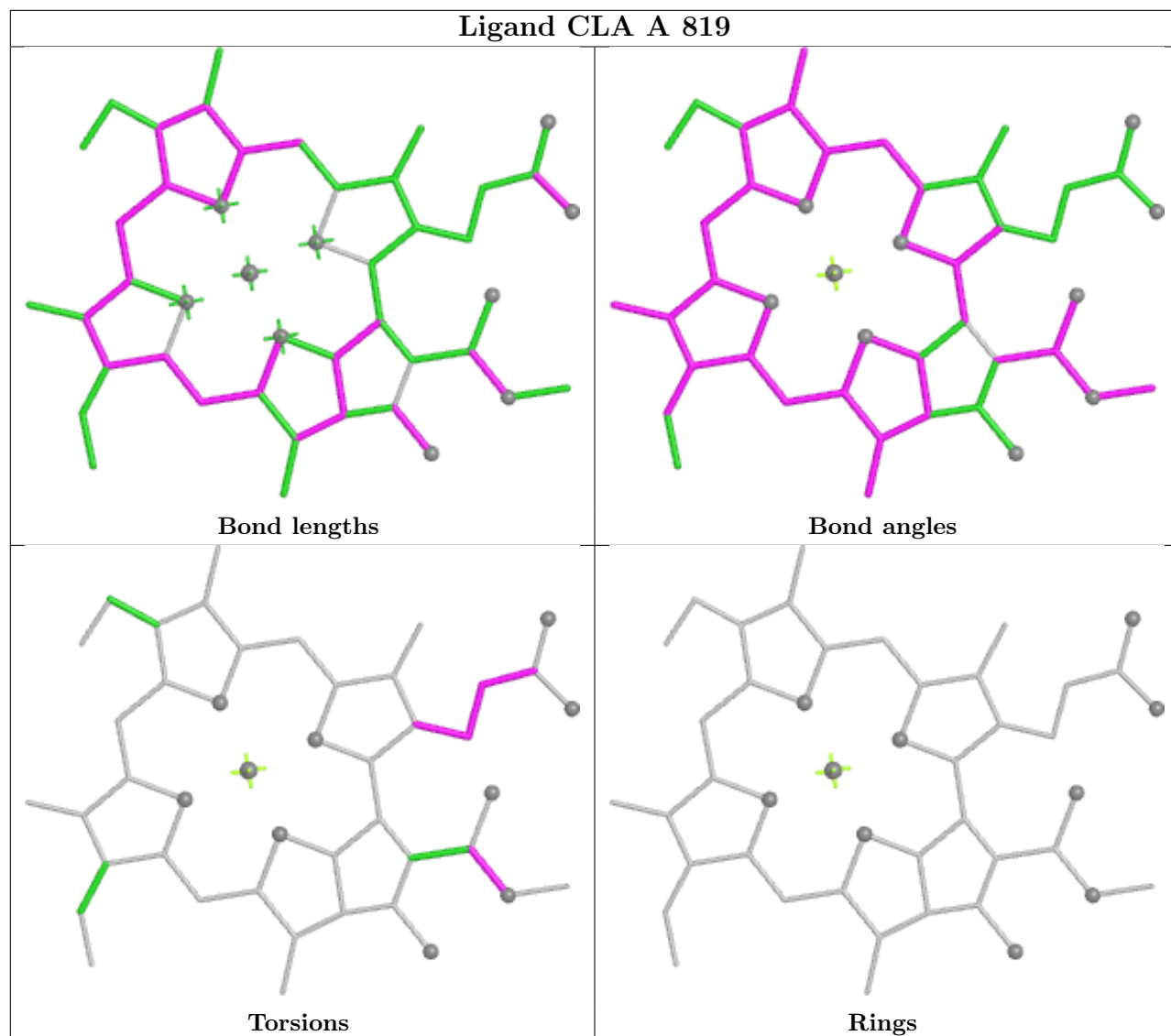


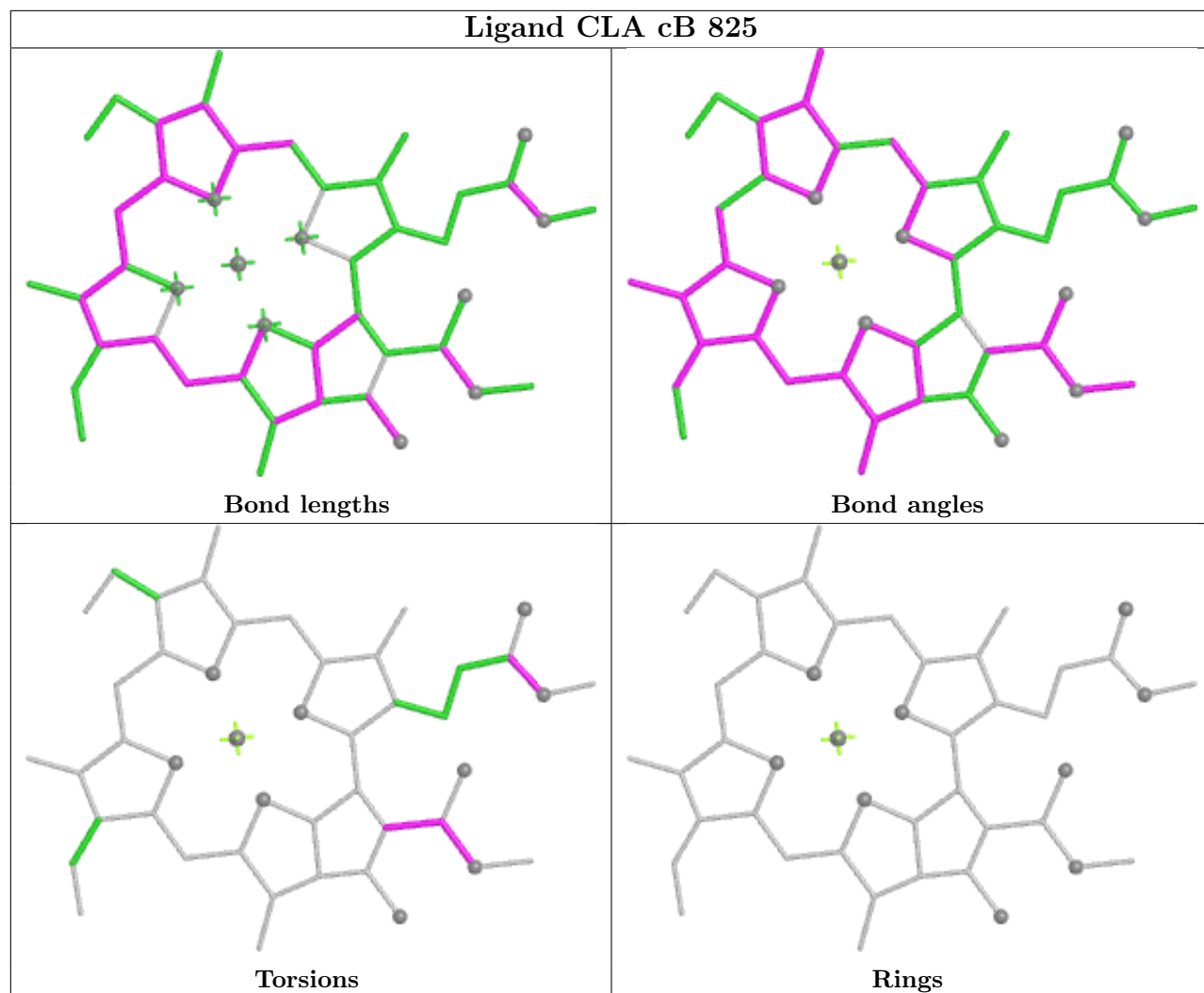


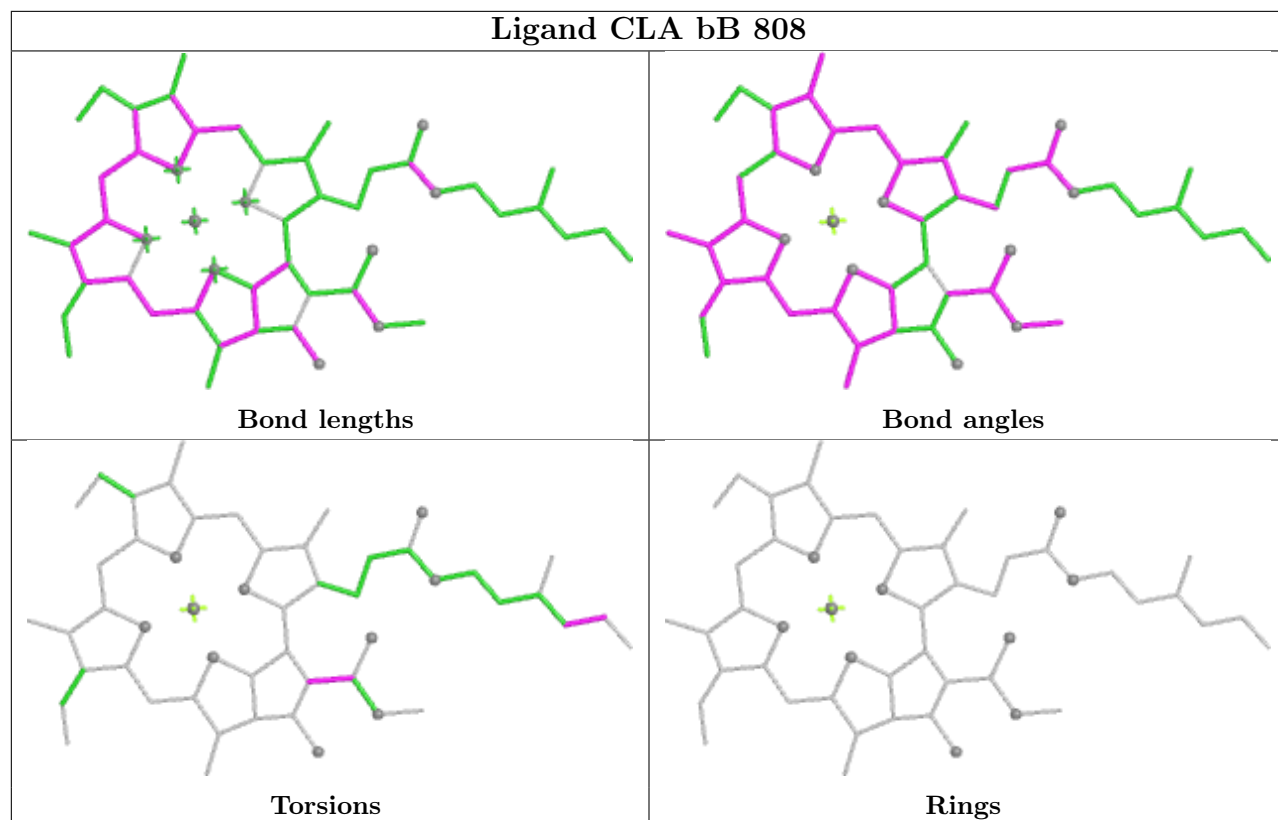


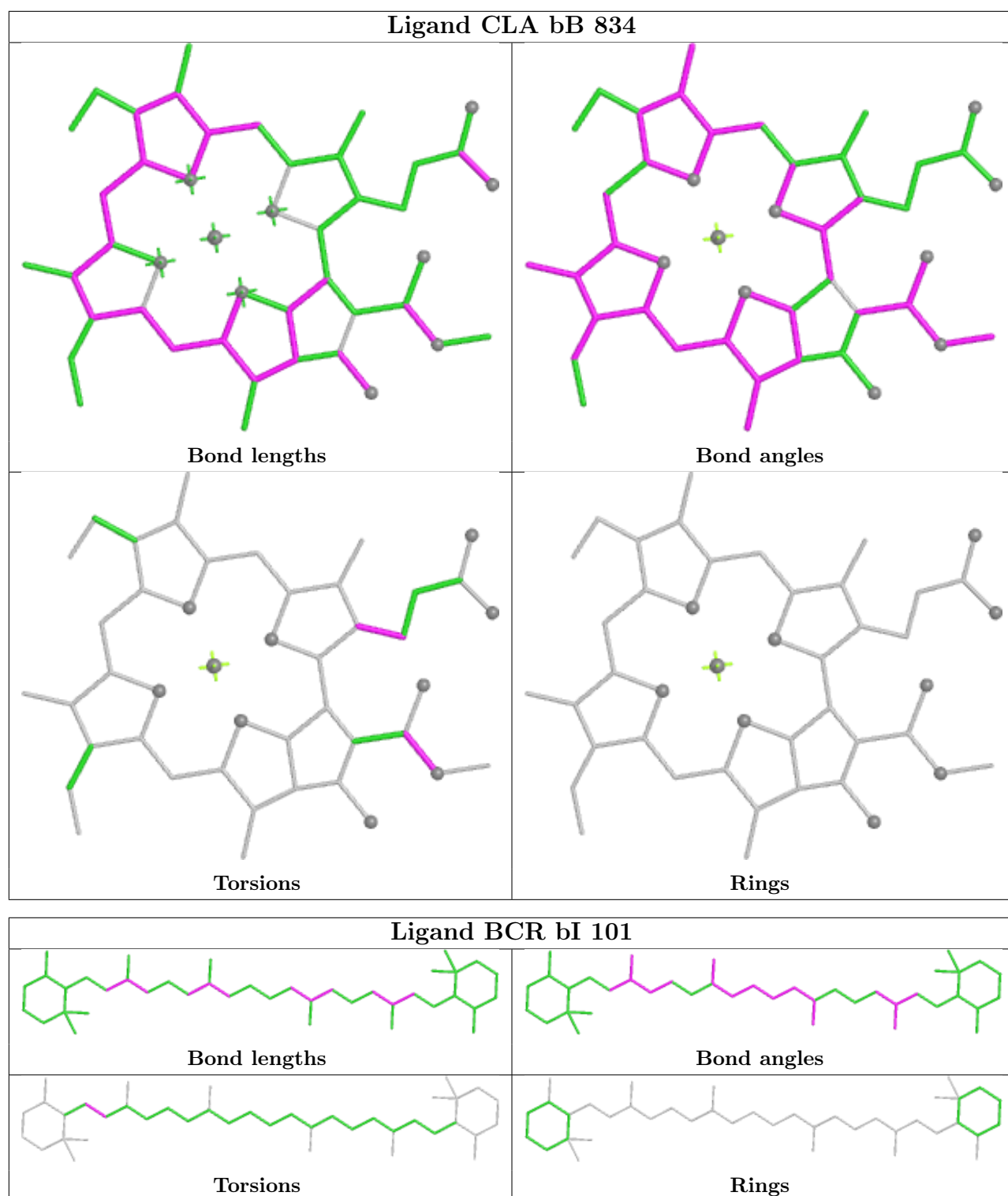


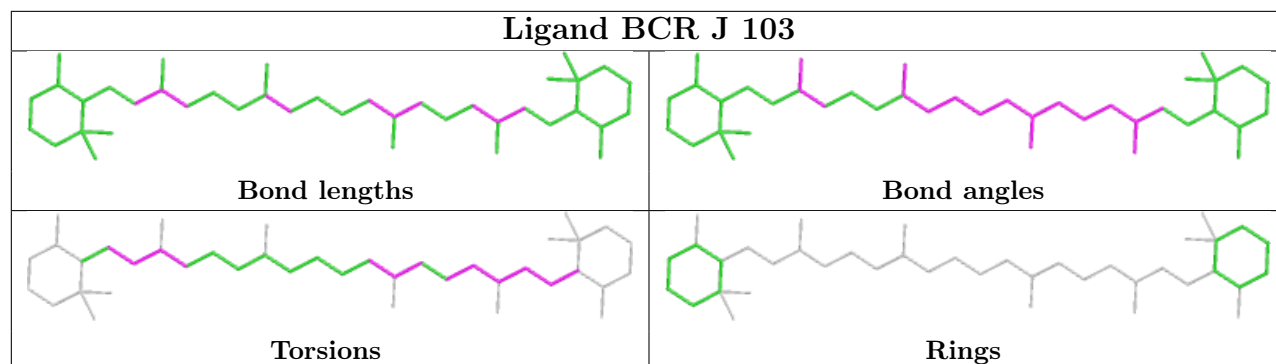
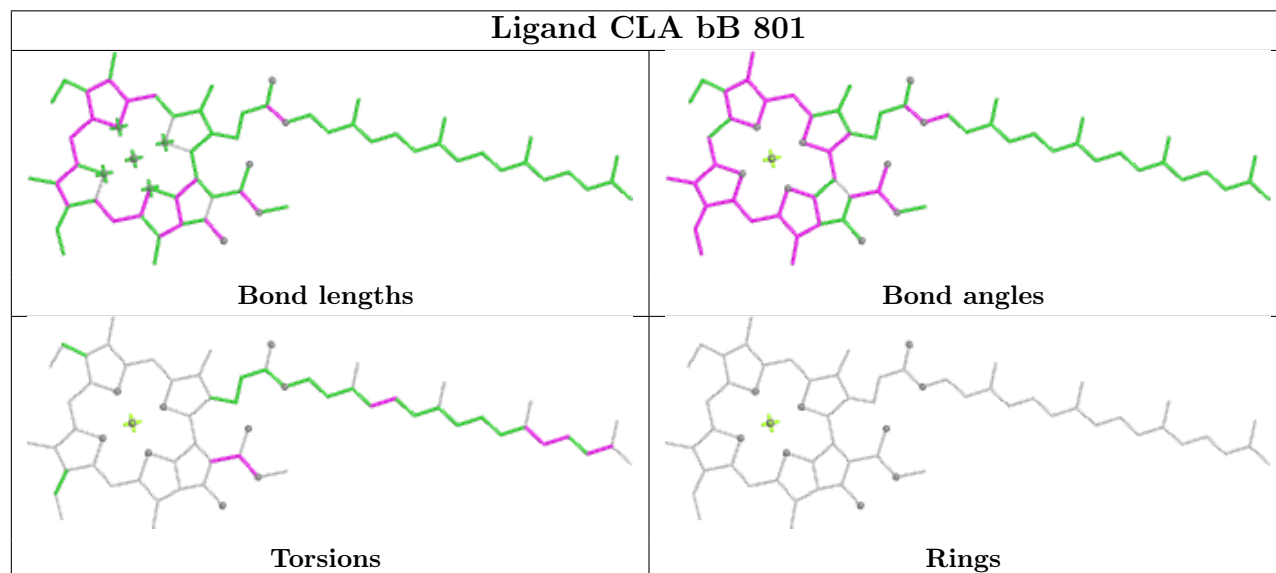
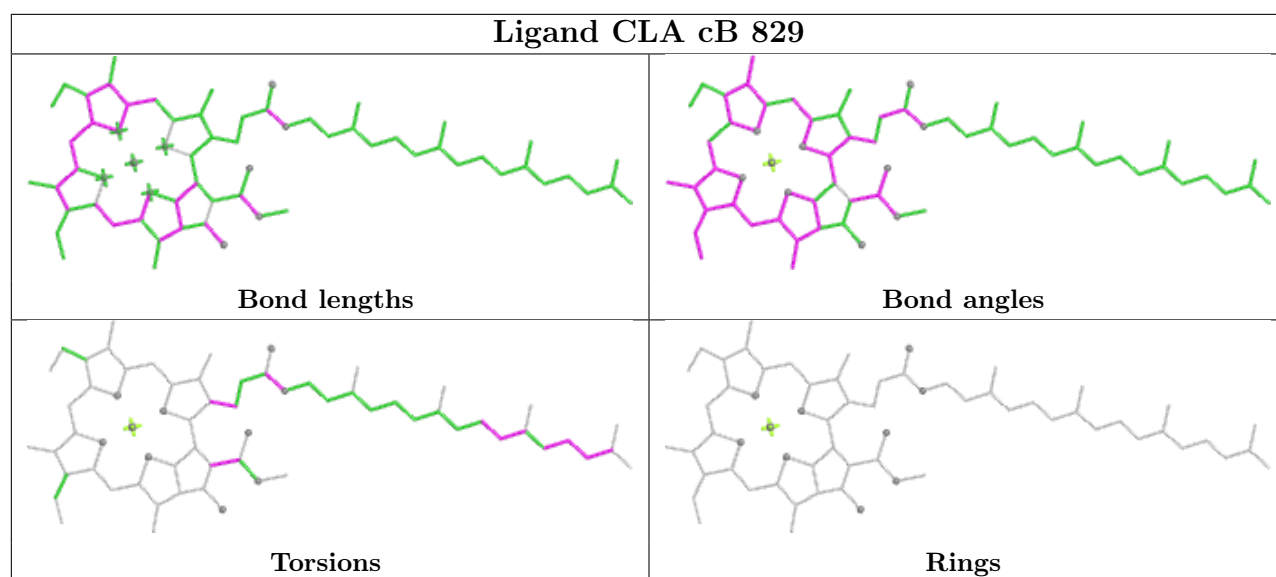
Ligand CLA A 819

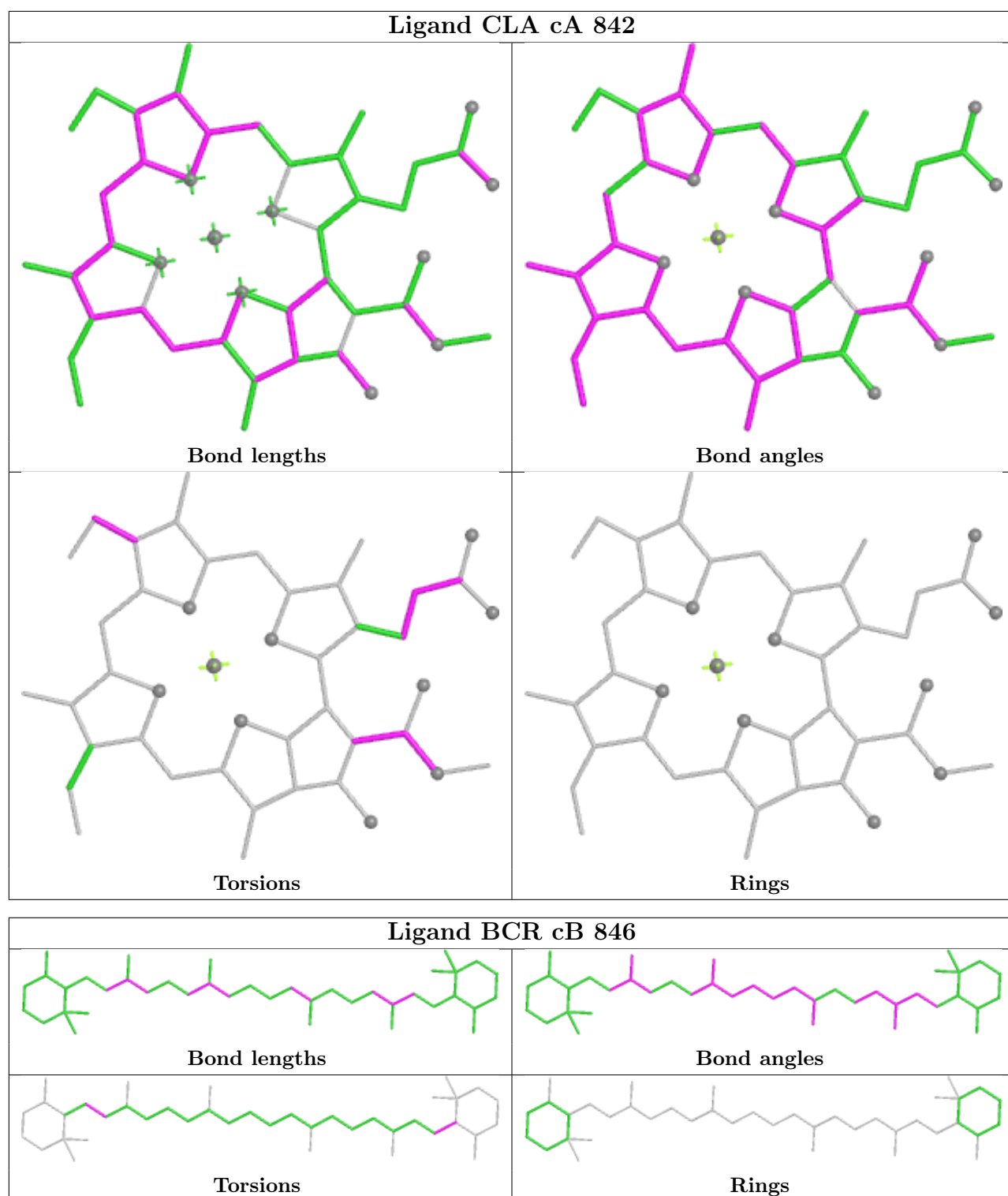


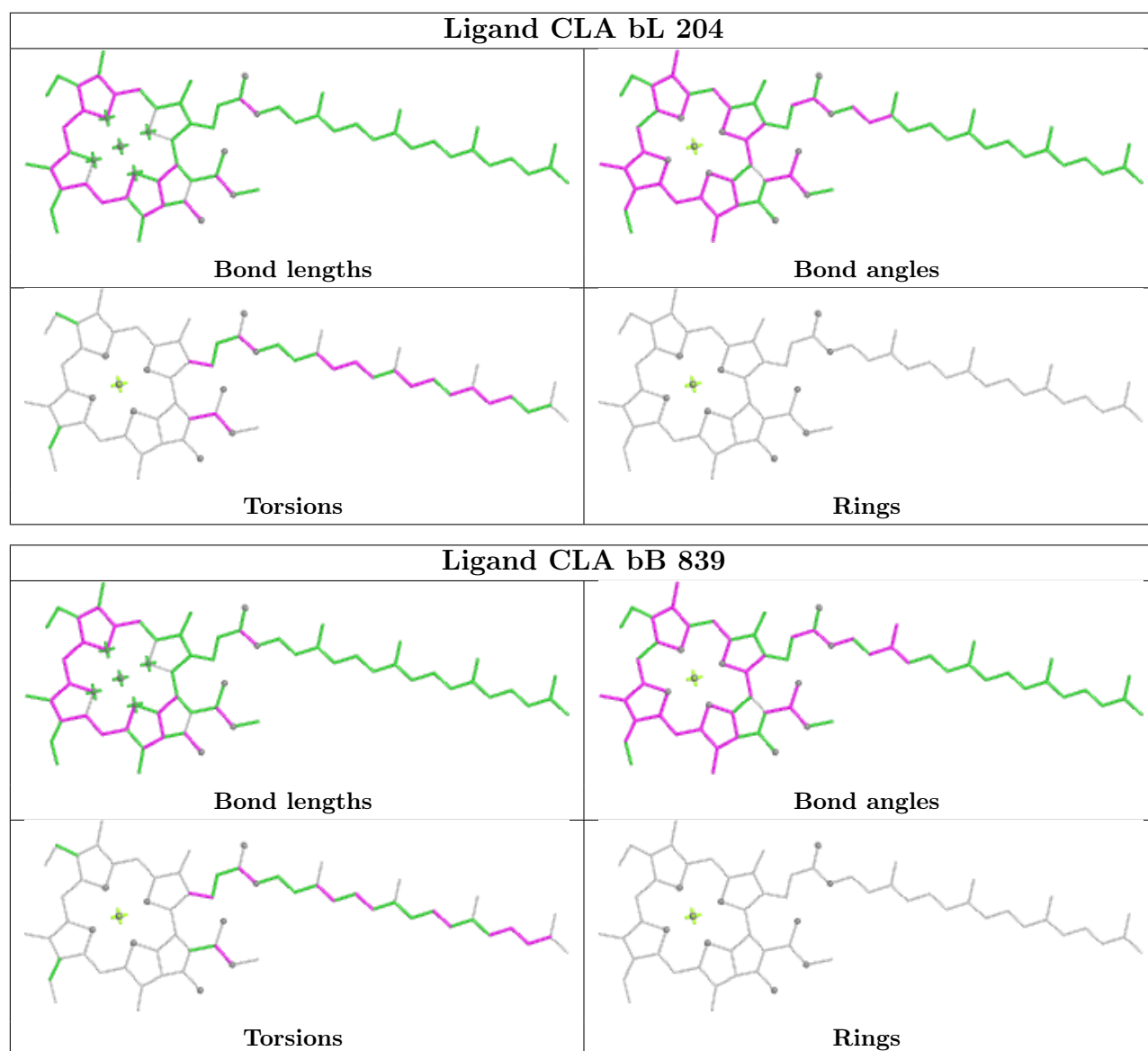


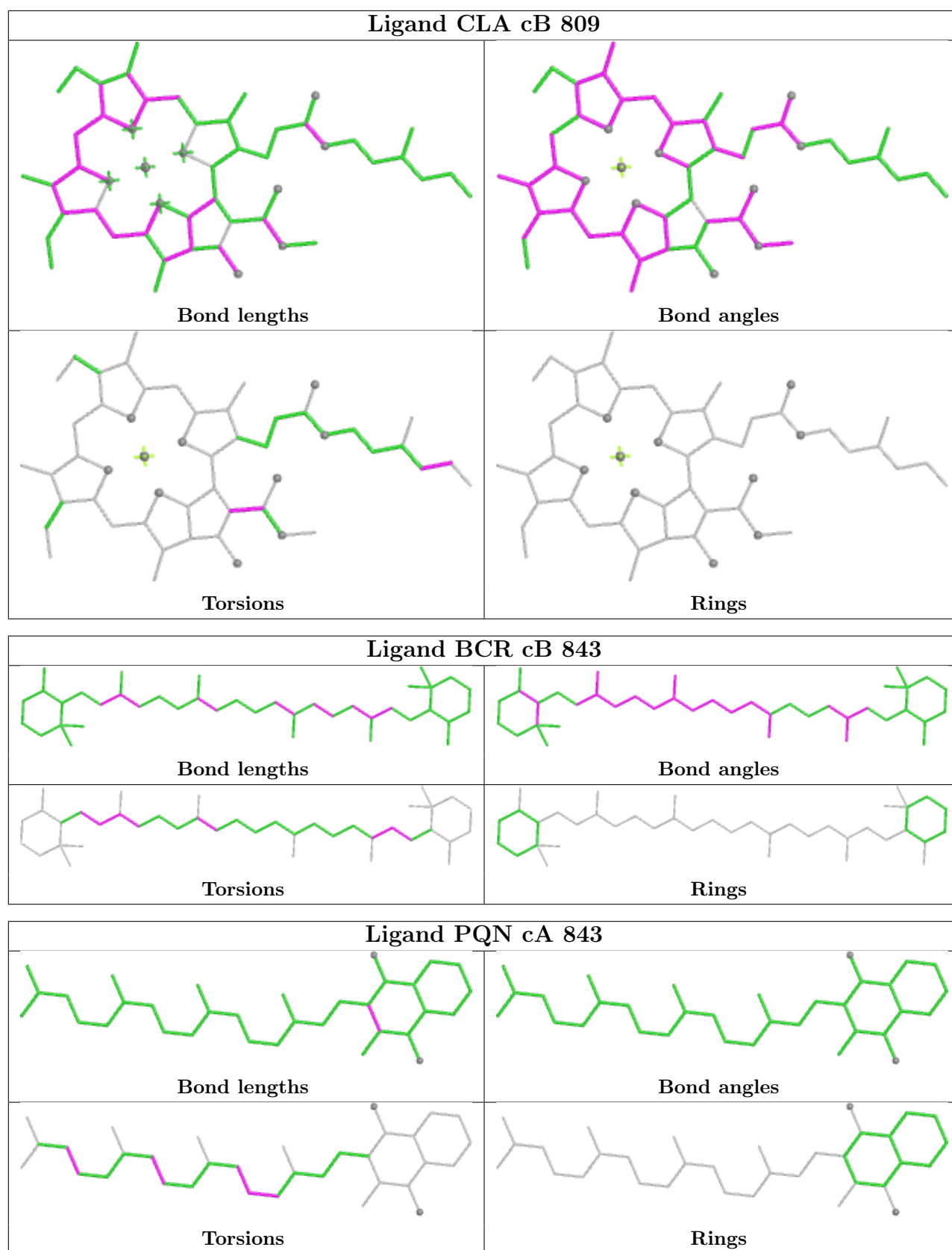


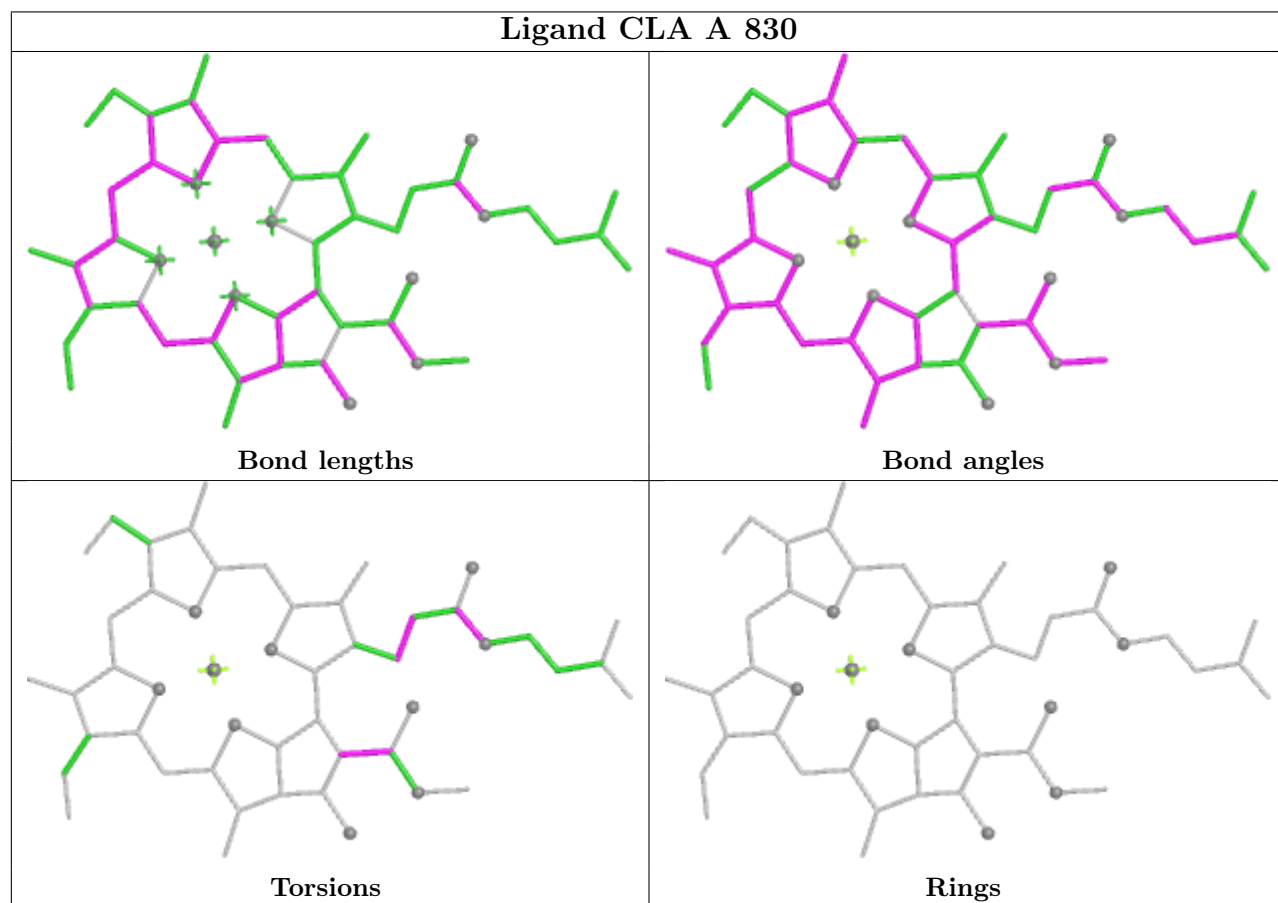
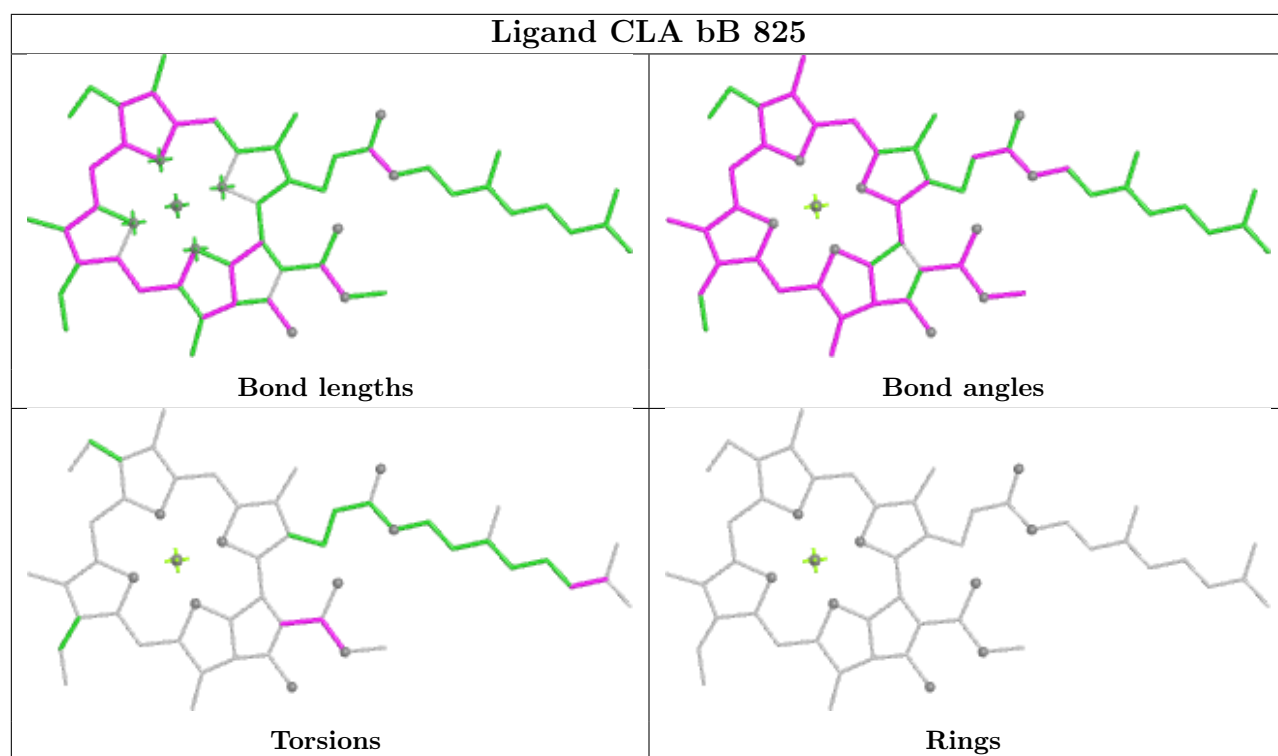




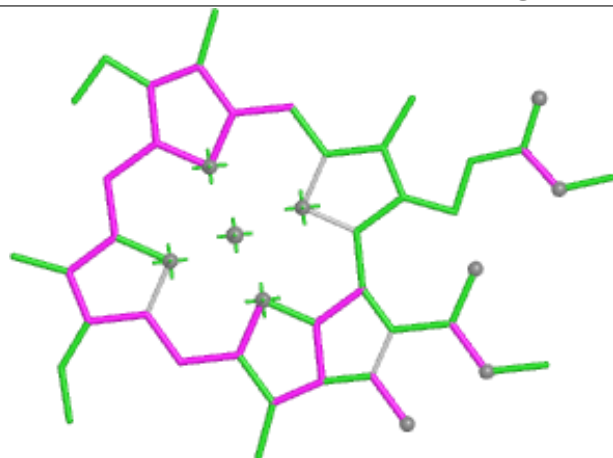




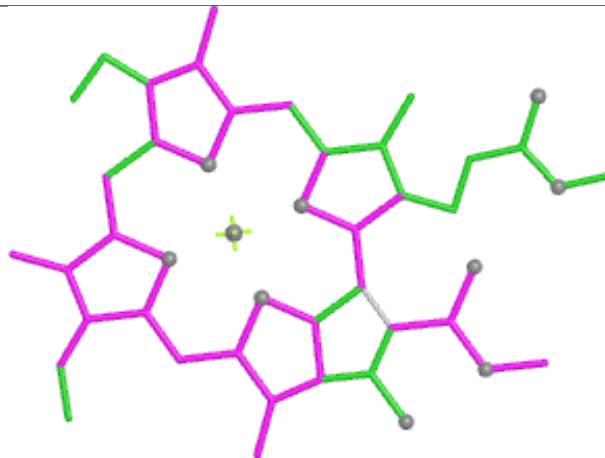




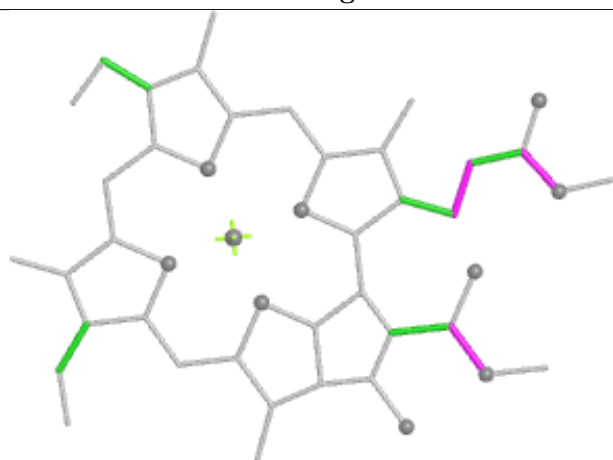
Ligand CLA B 818



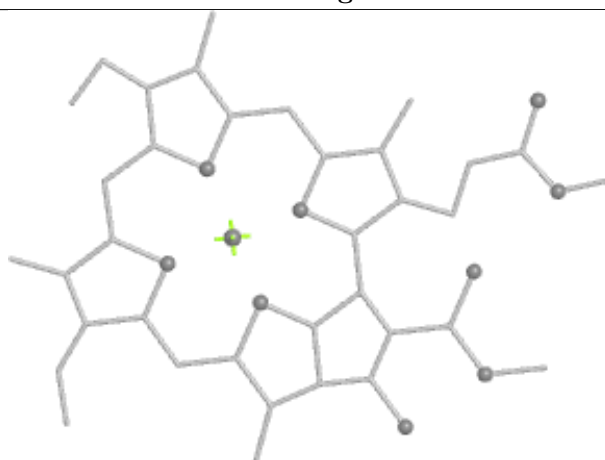
Bond lengths



Bond angles

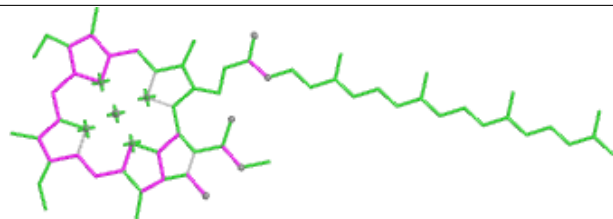


Torsions

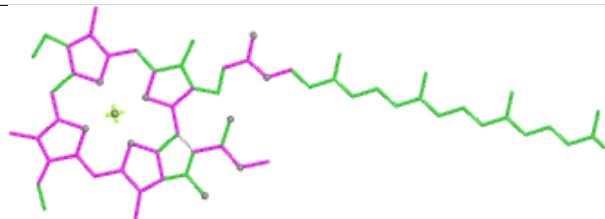


Rings

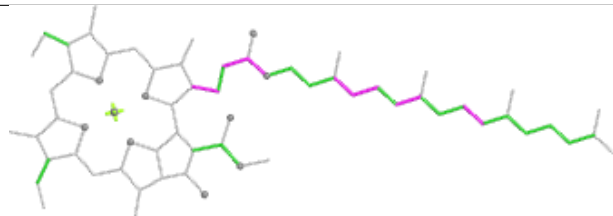
Ligand CLA A 806



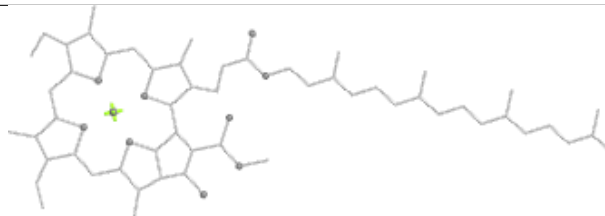
Bond lengths



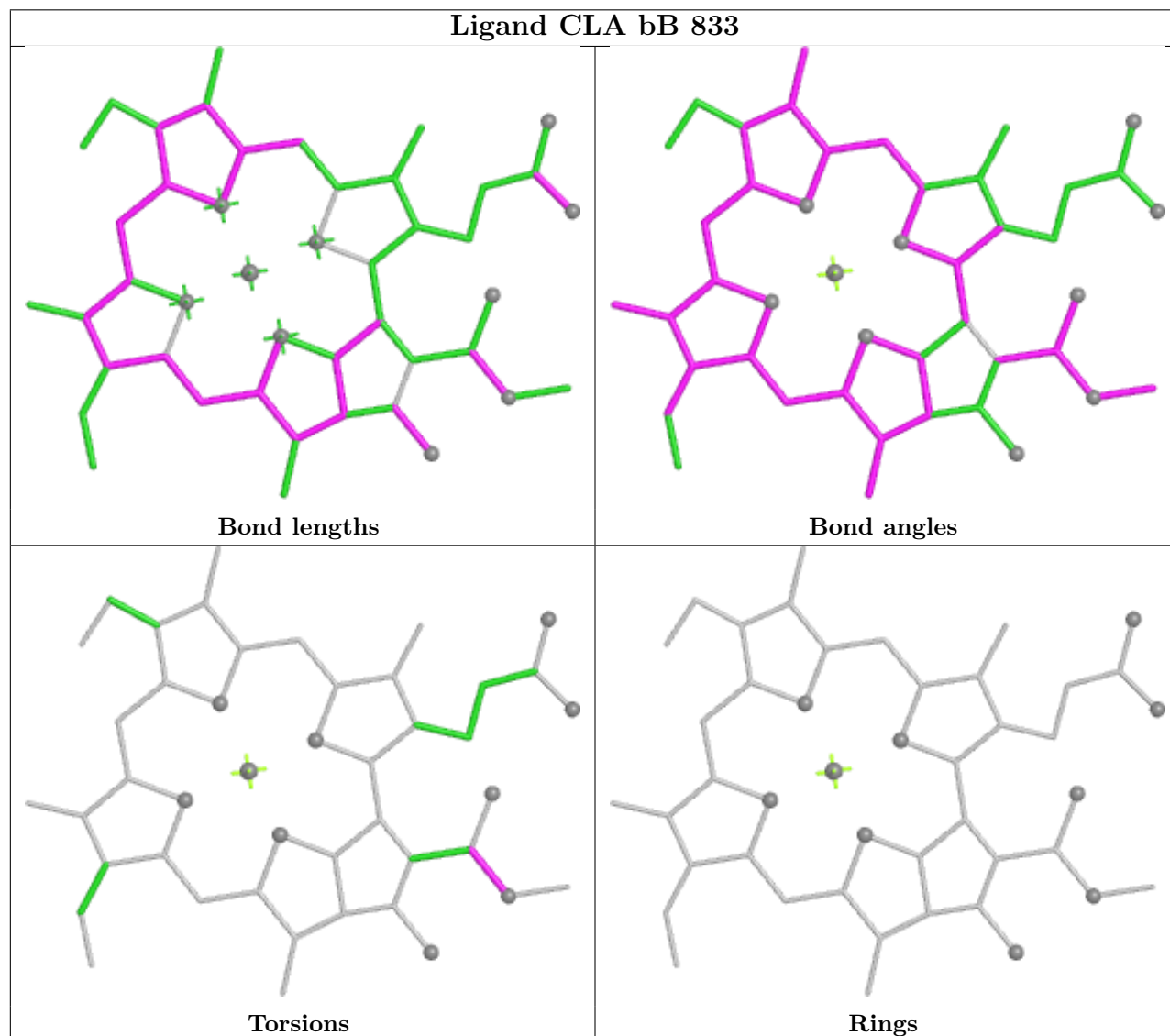
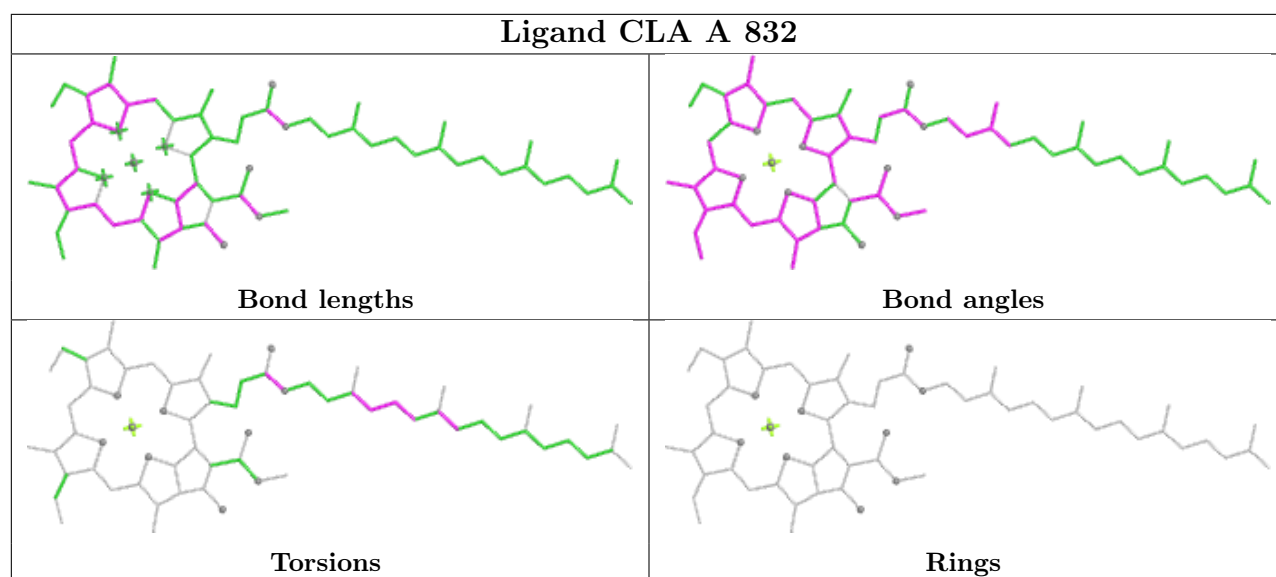
Bond angles



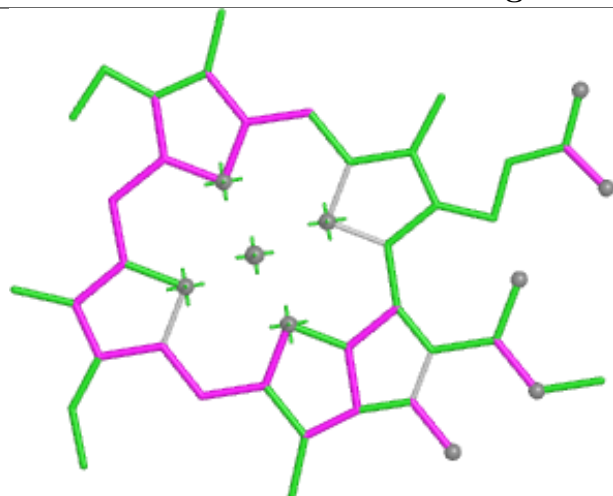
Torsions



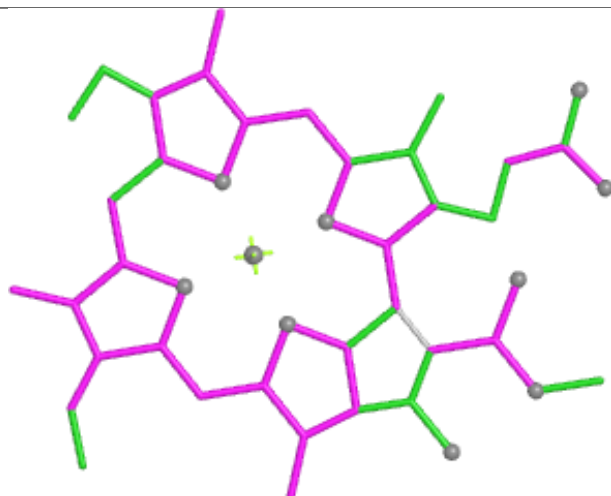
Rings



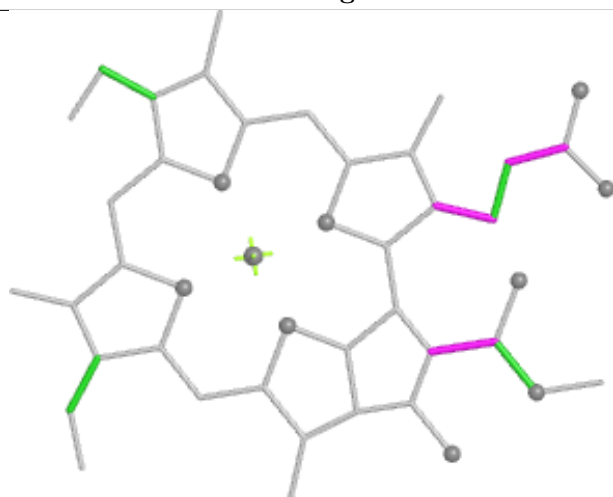
Ligand CLA cA 838



Bond lengths



Bond angles

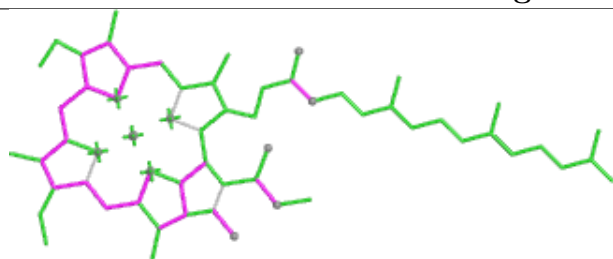


Torsions

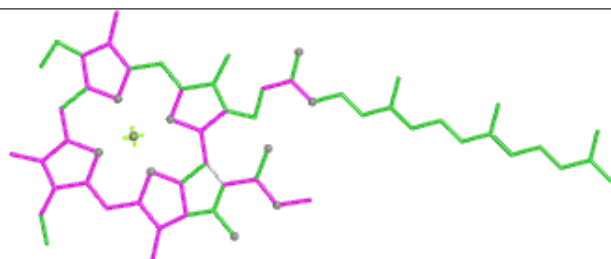


Rings

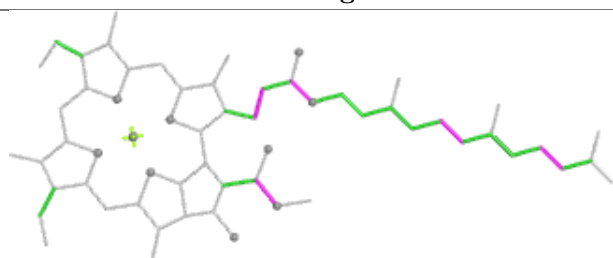
Ligand CLA A 828



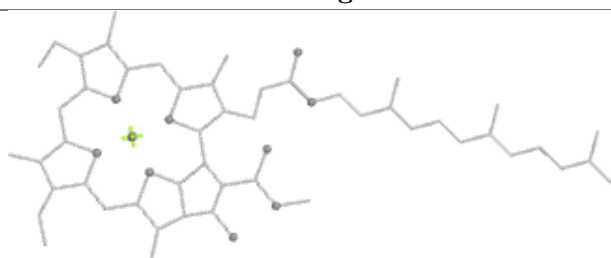
Bond lengths



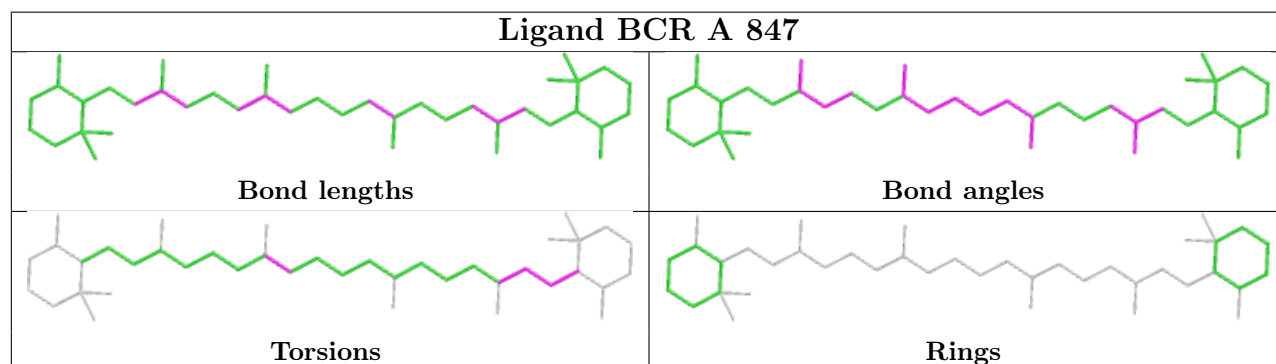
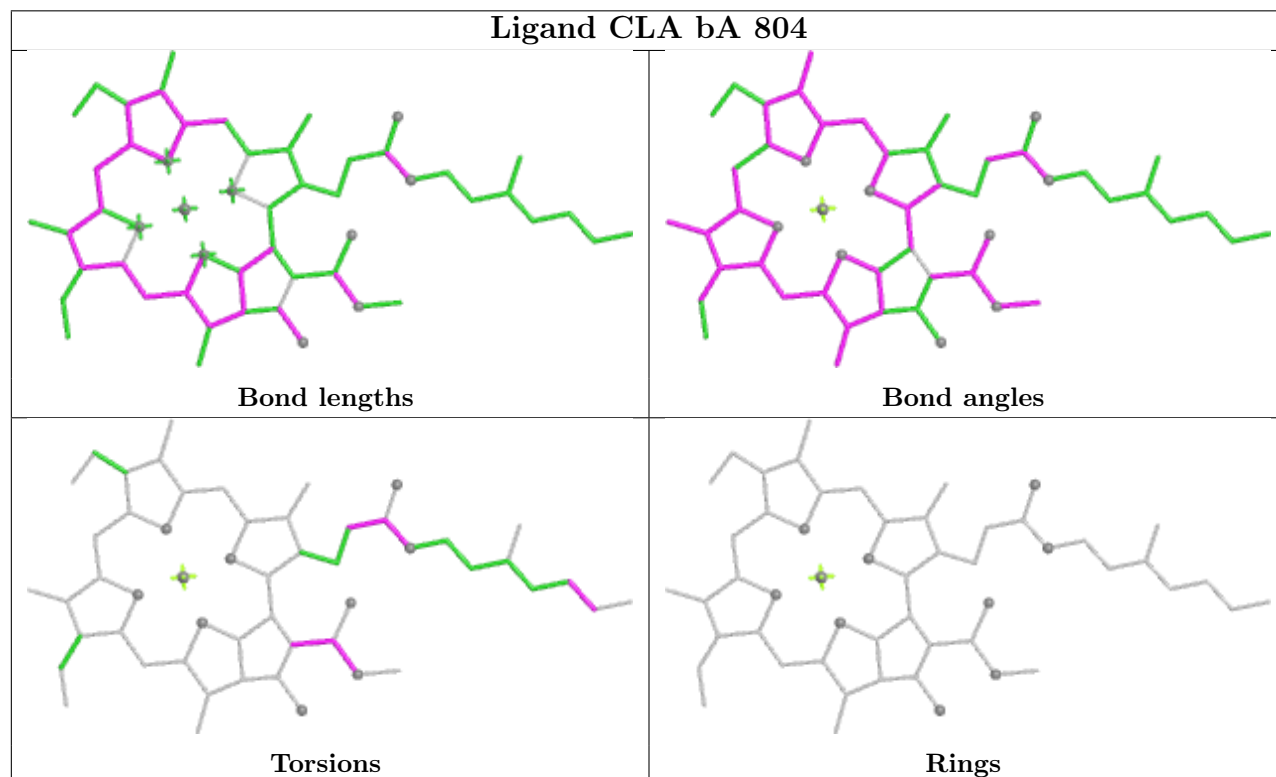
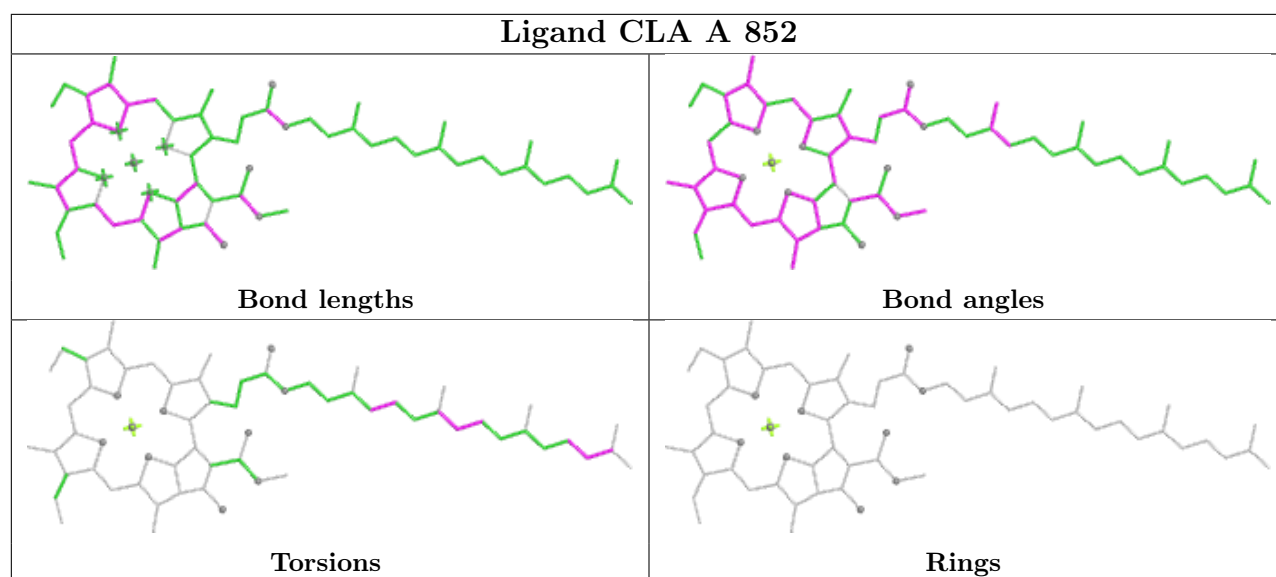
Bond angles

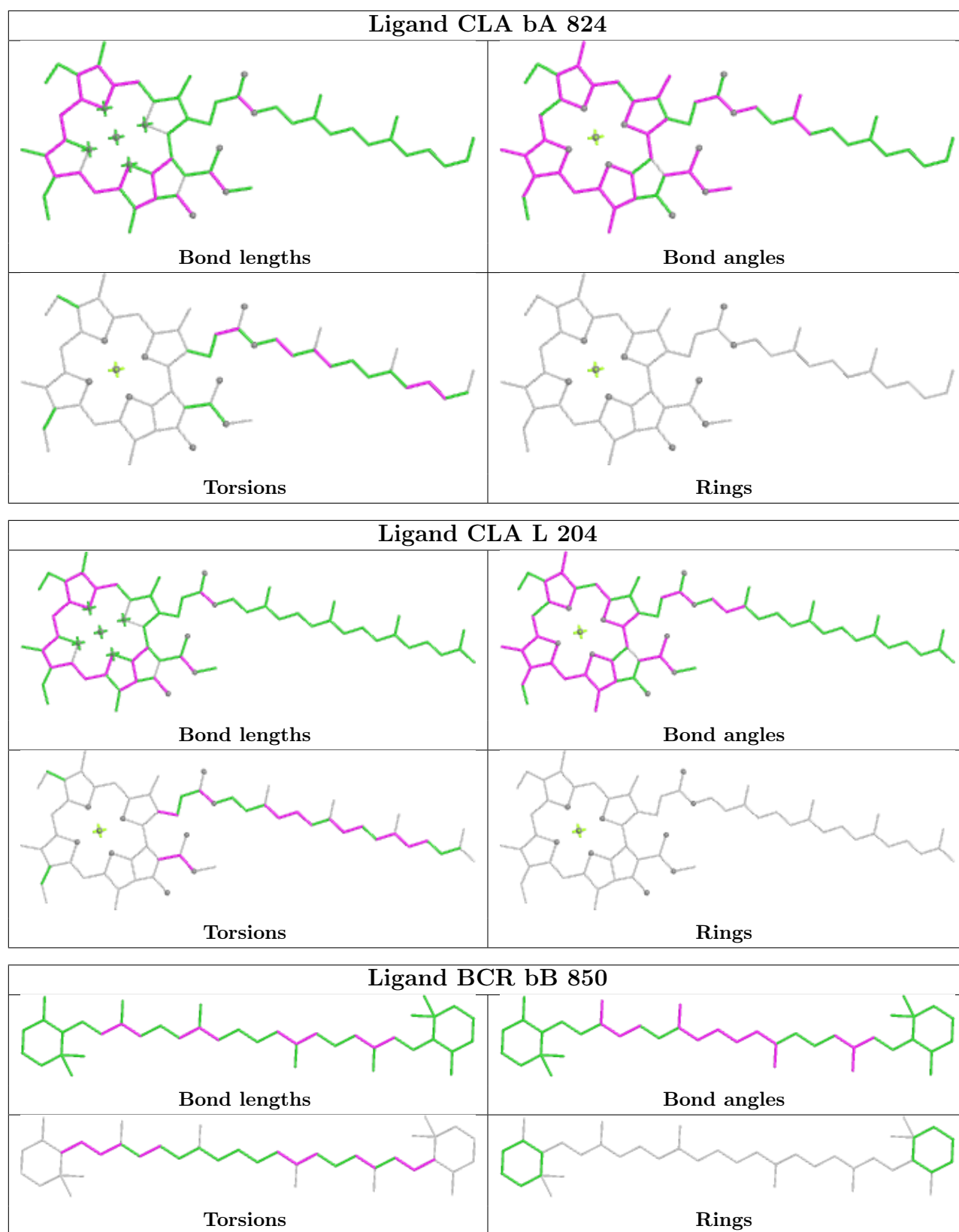


Torsions

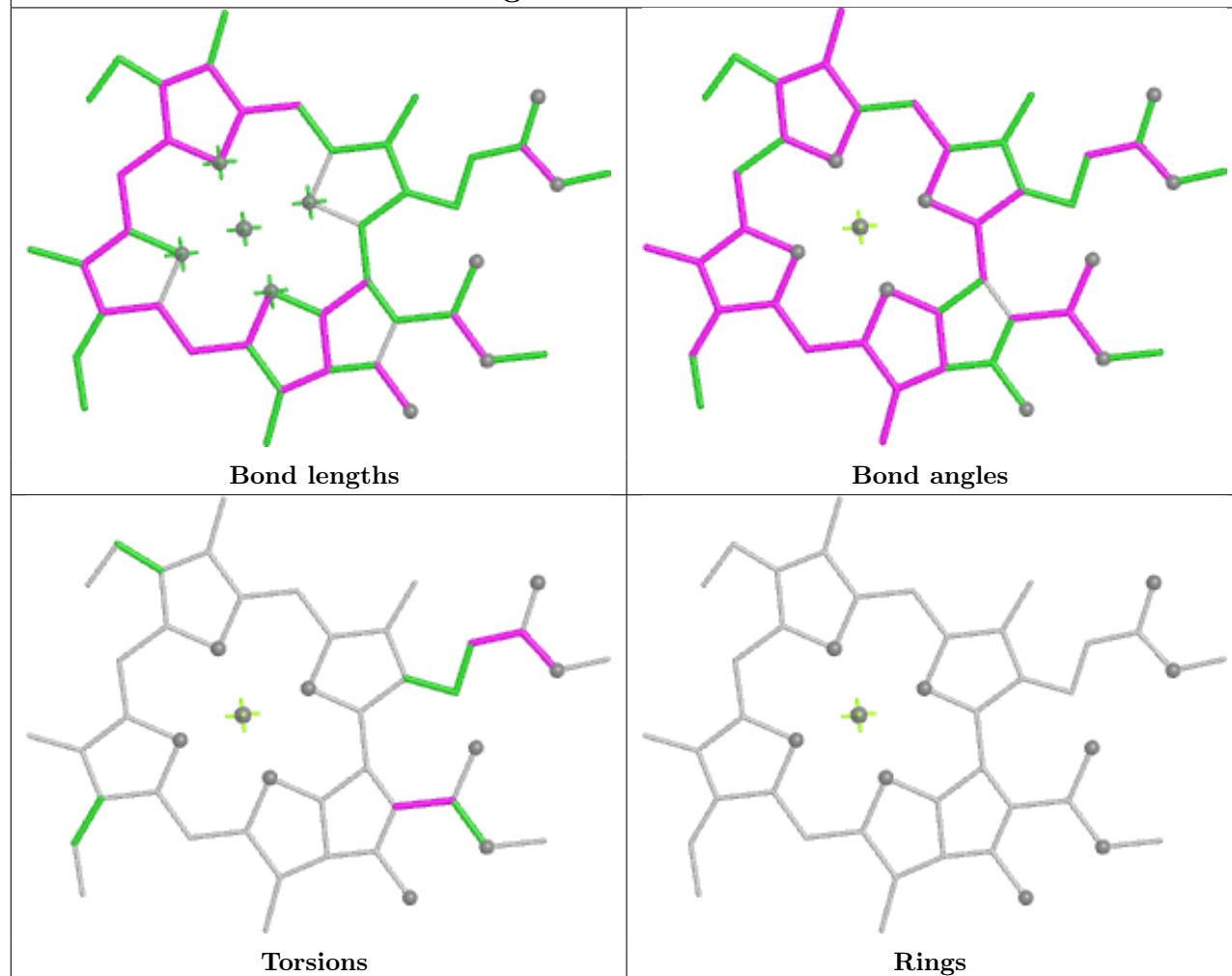


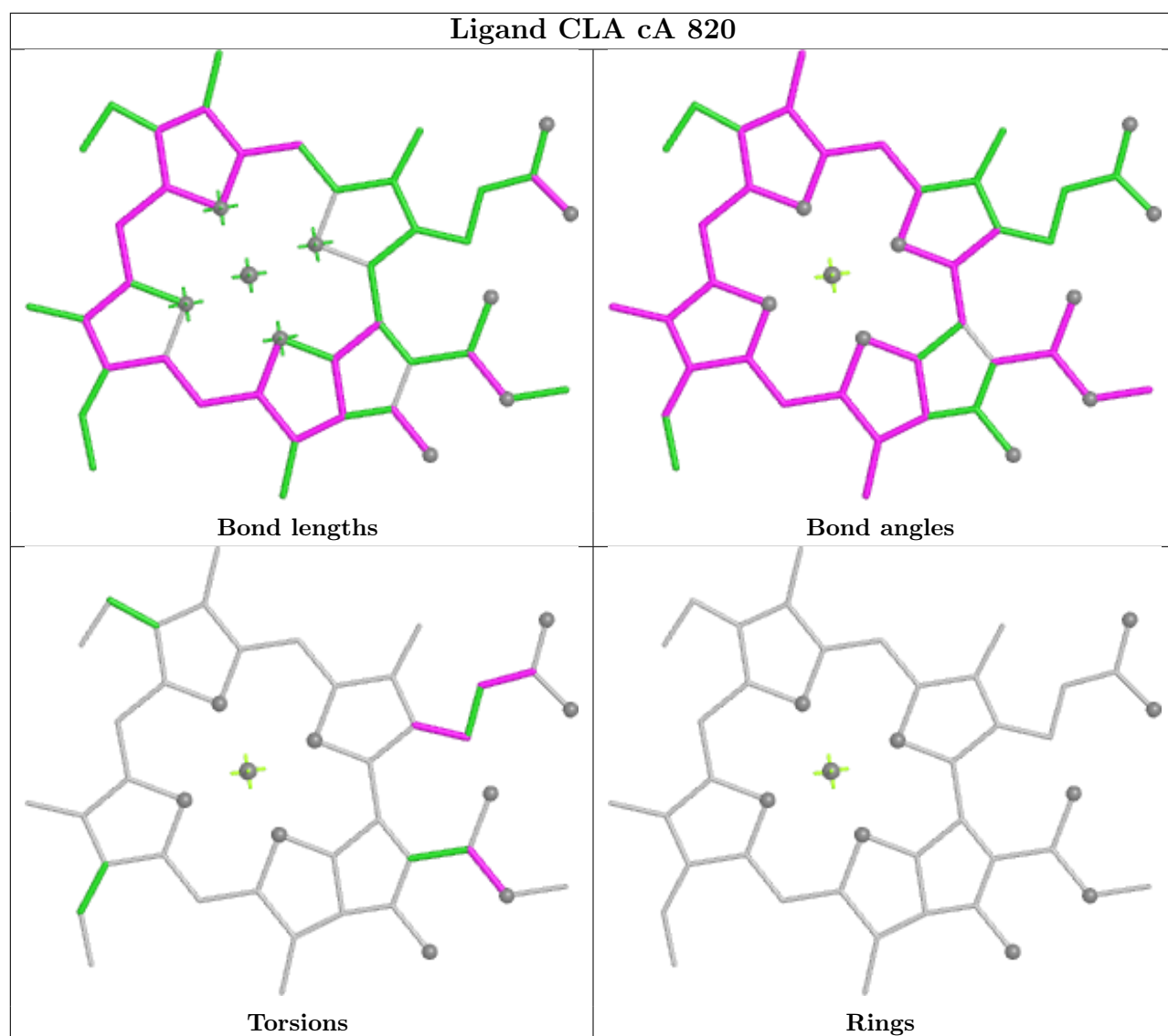
Rings

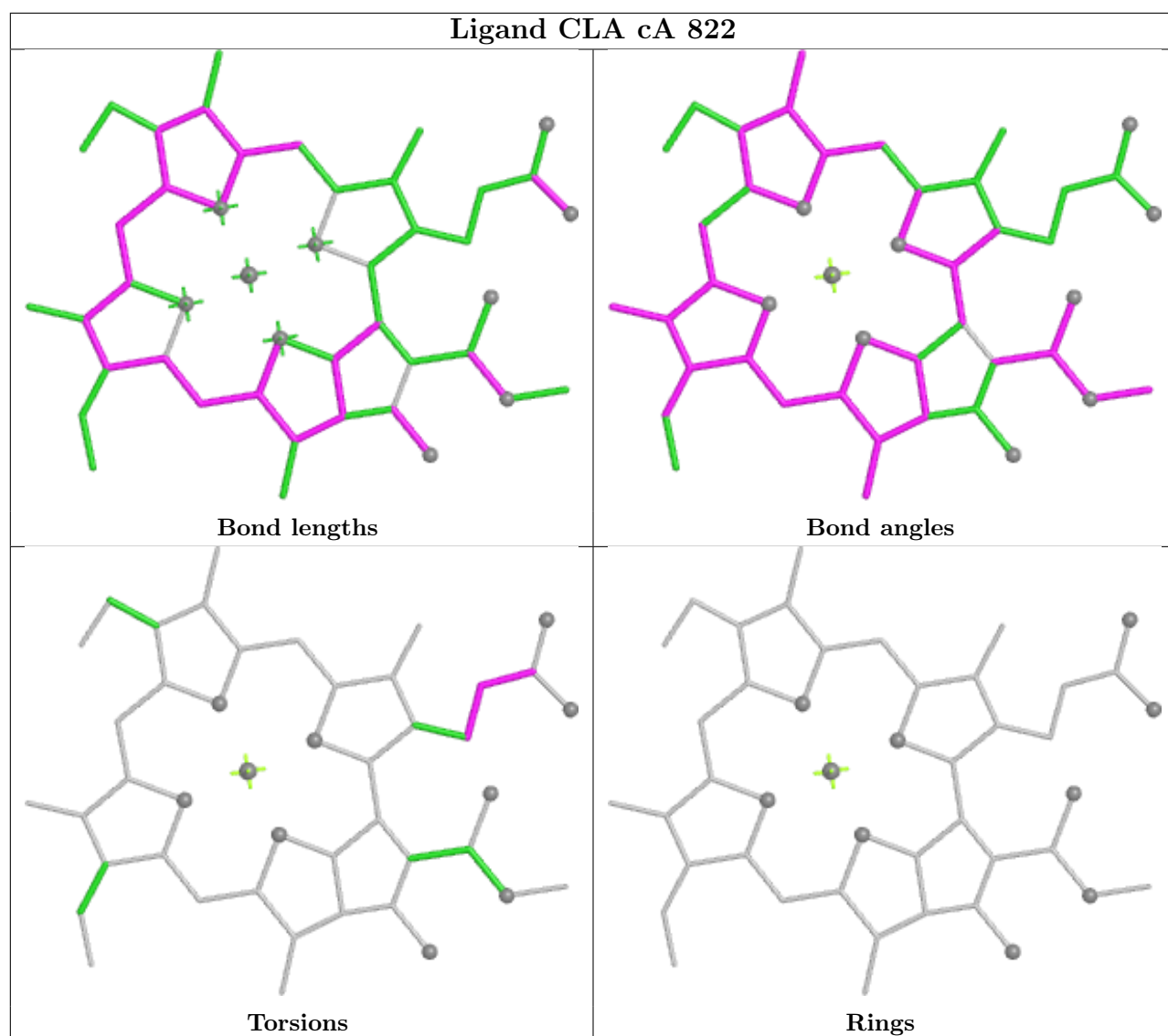


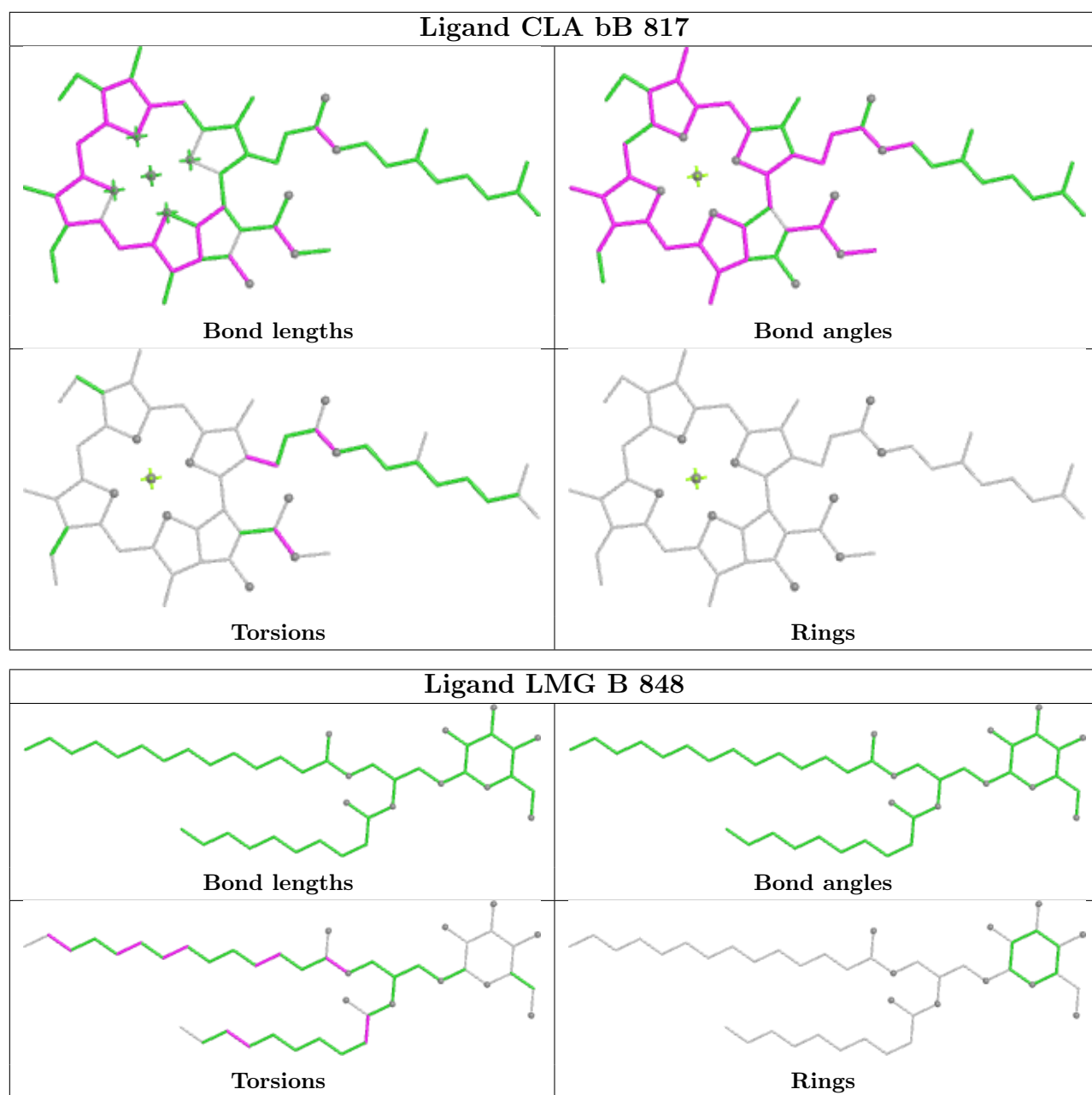


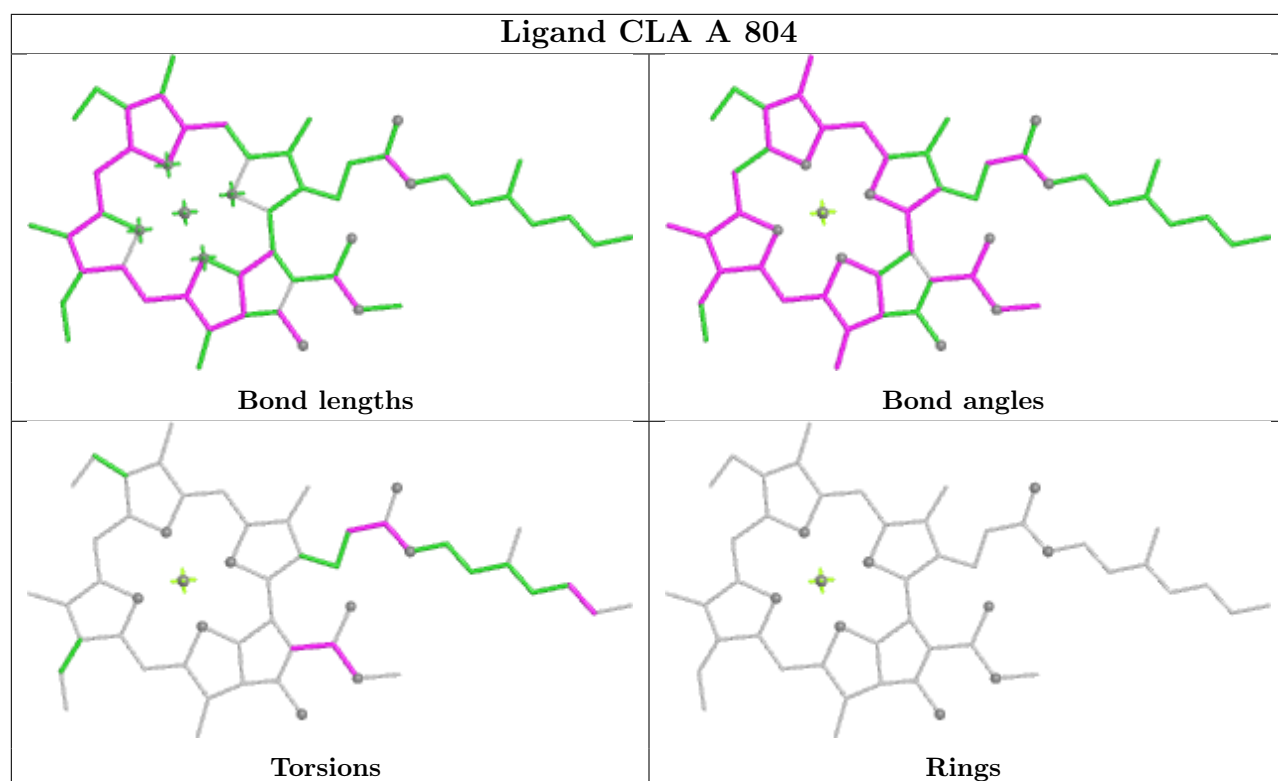
Ligand CLA bA 826

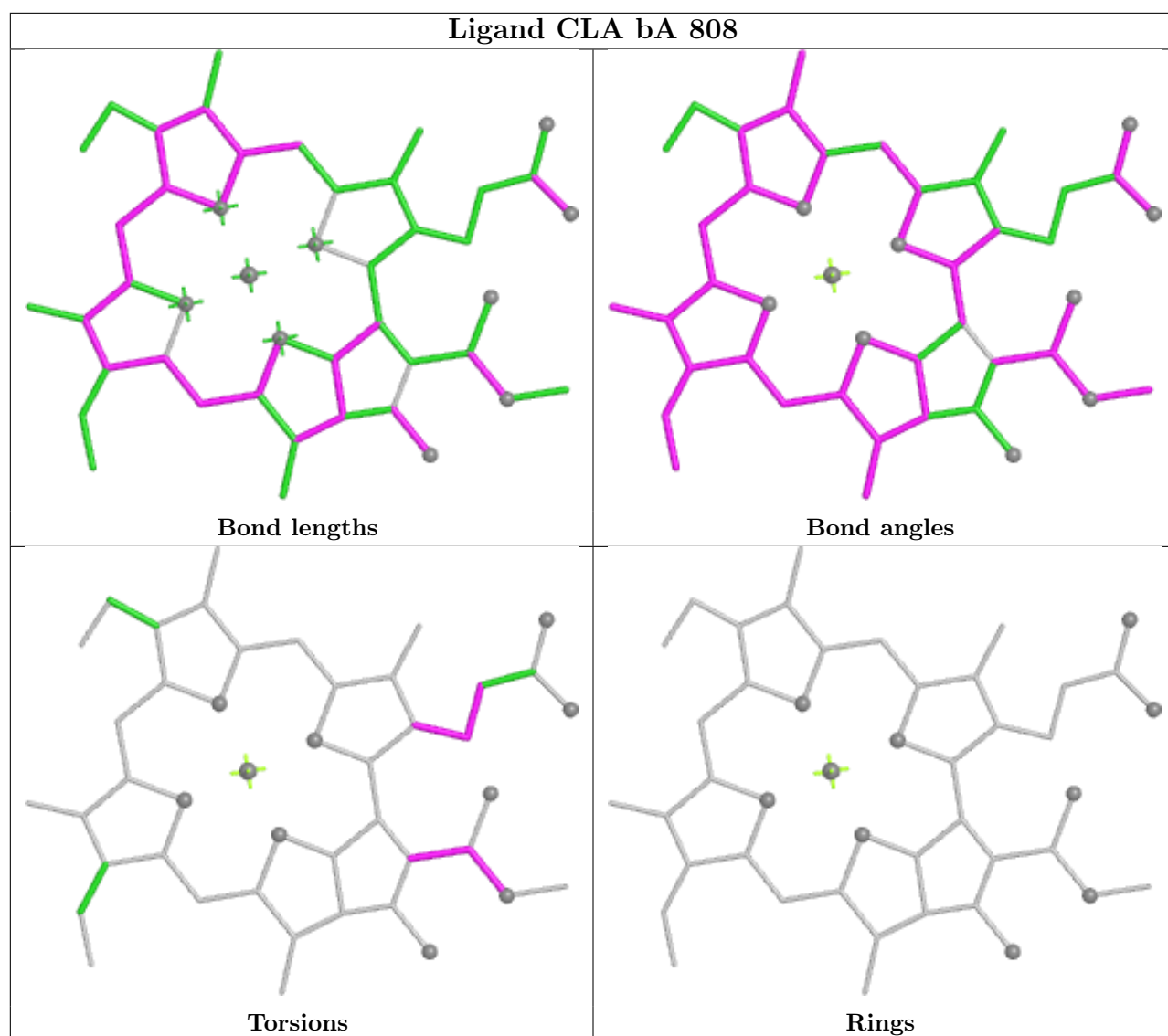


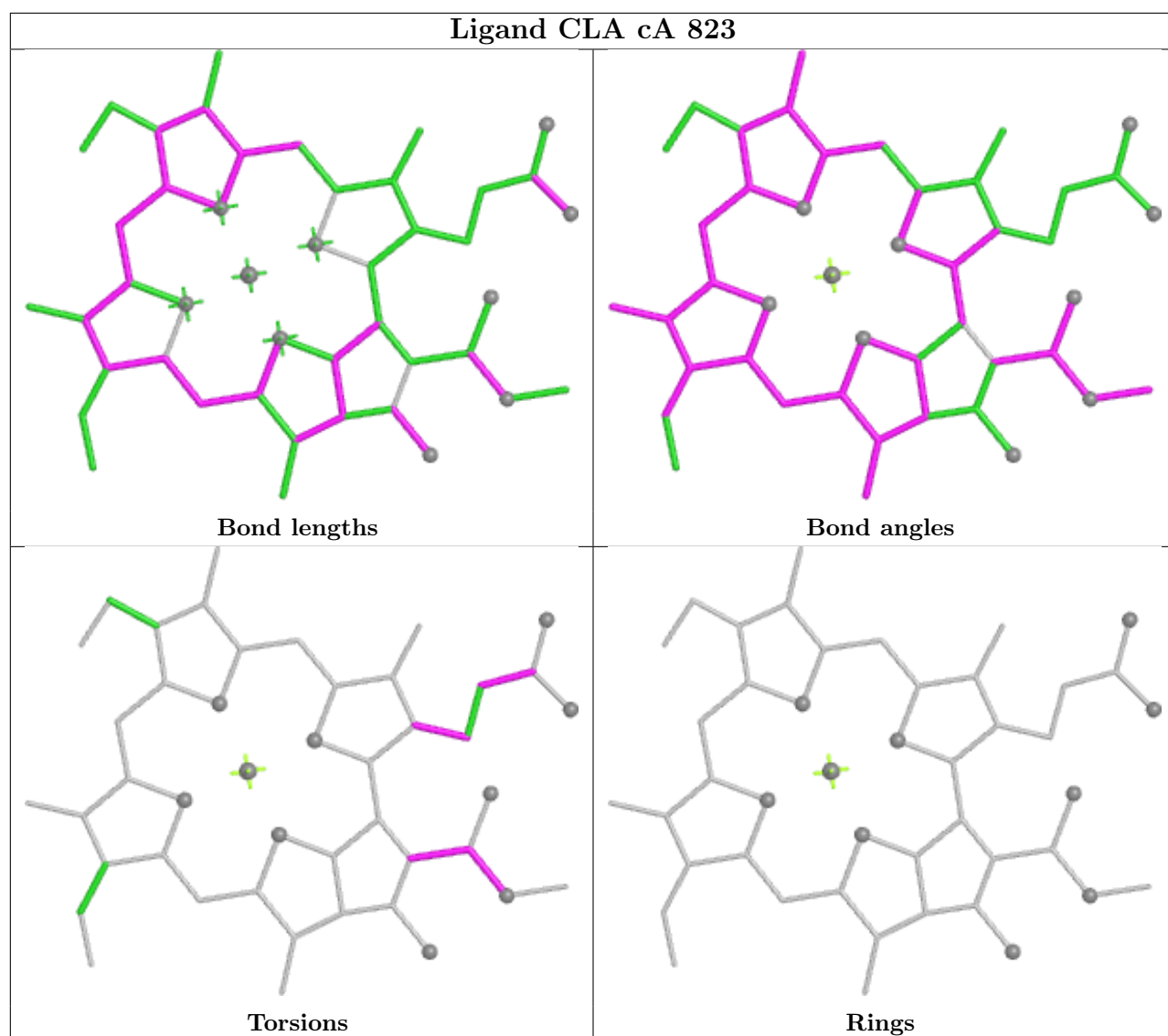


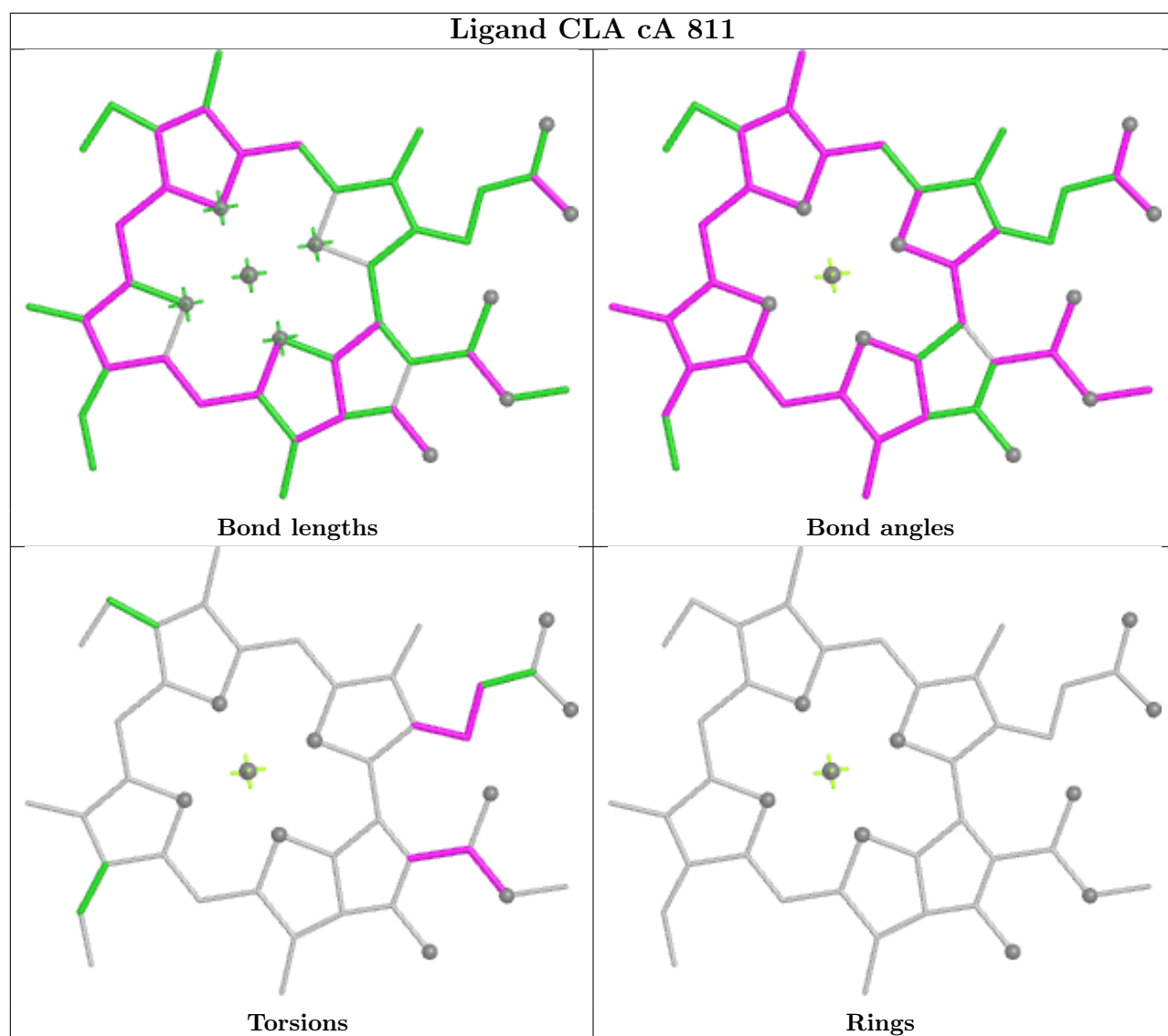


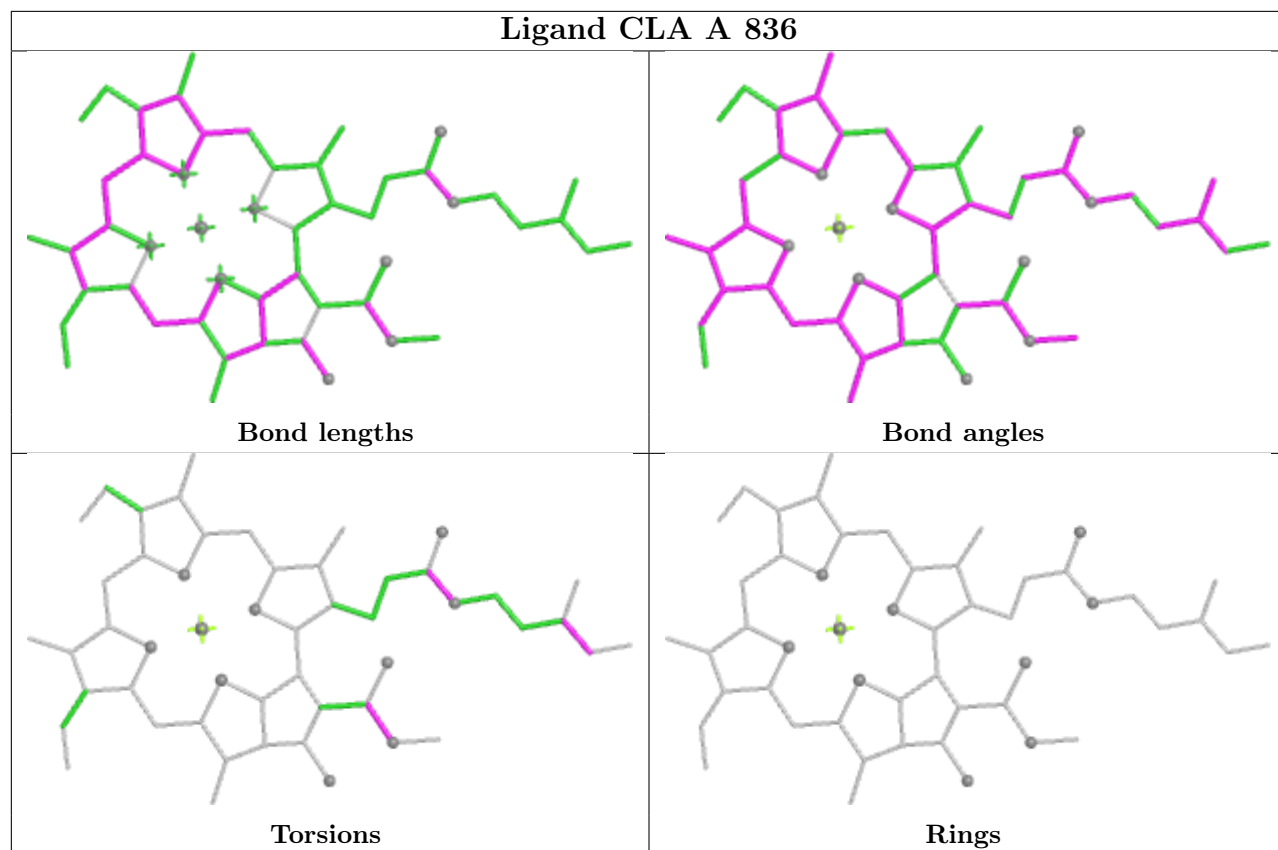


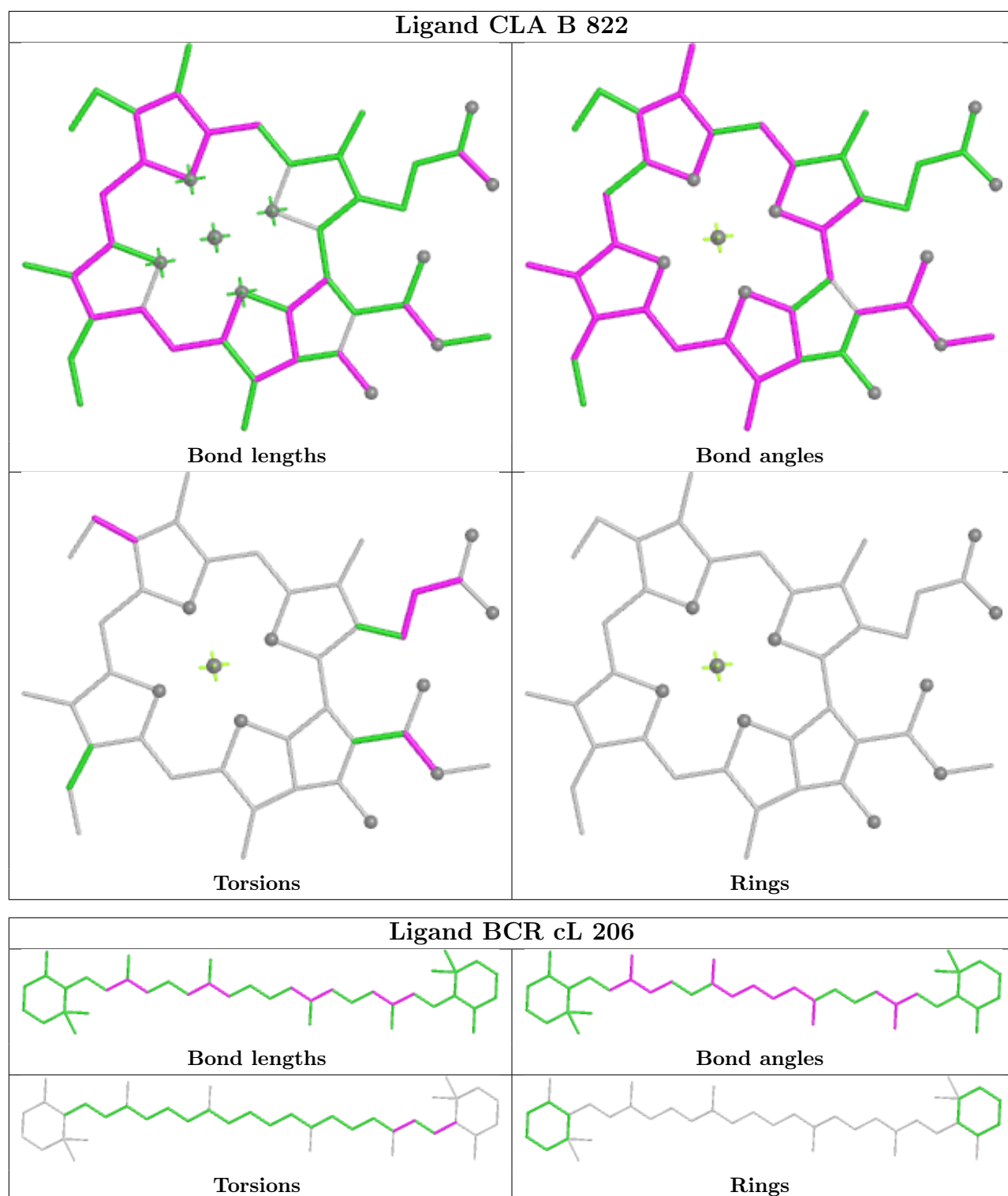


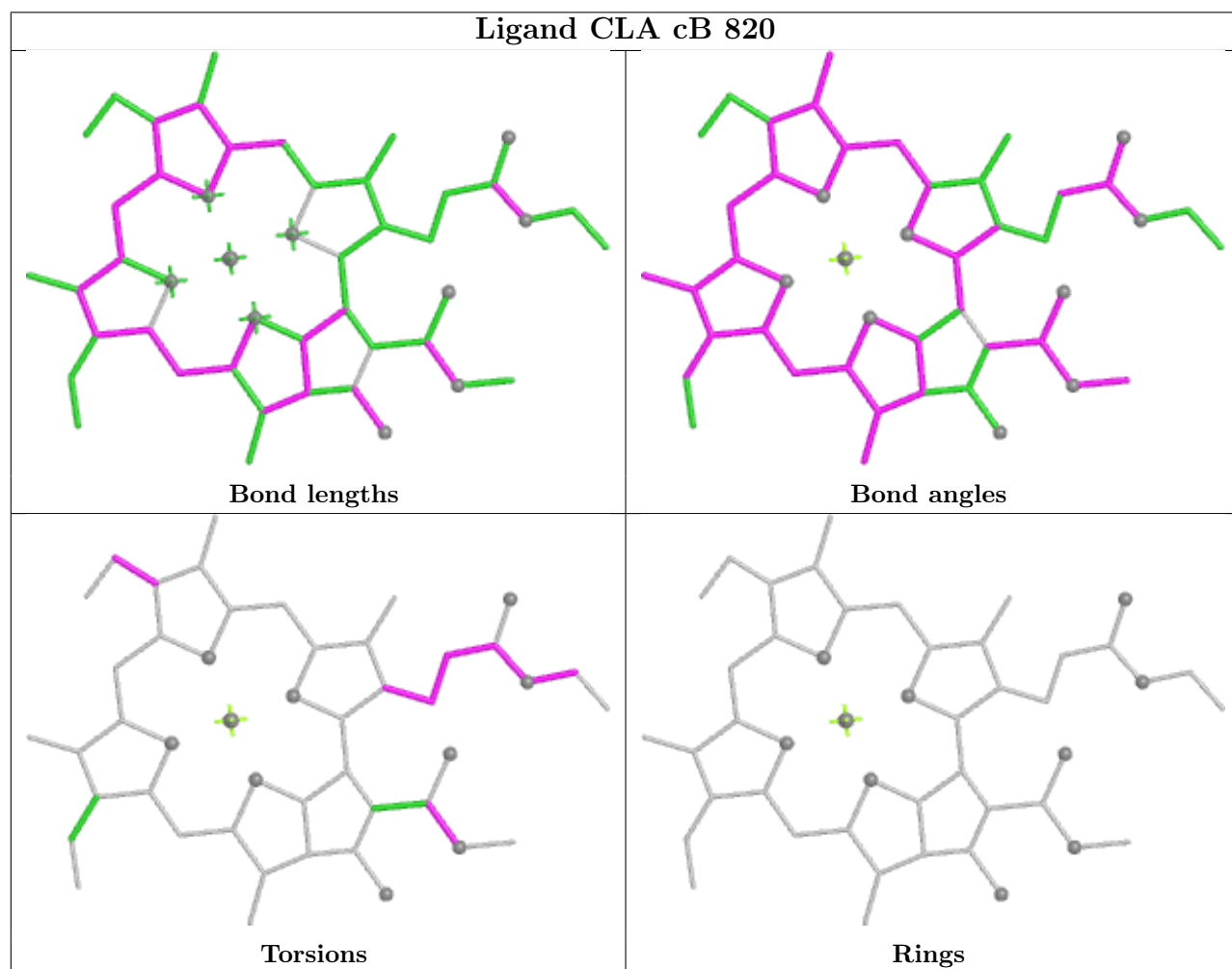
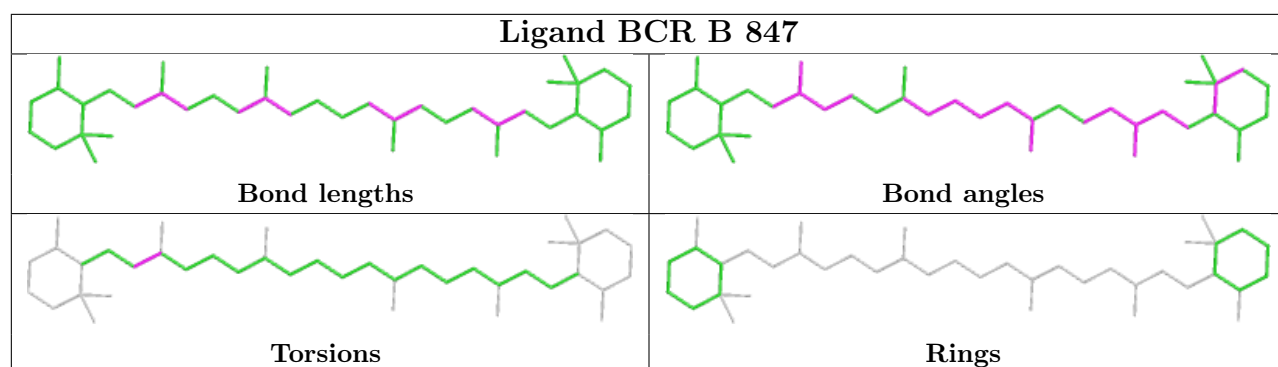


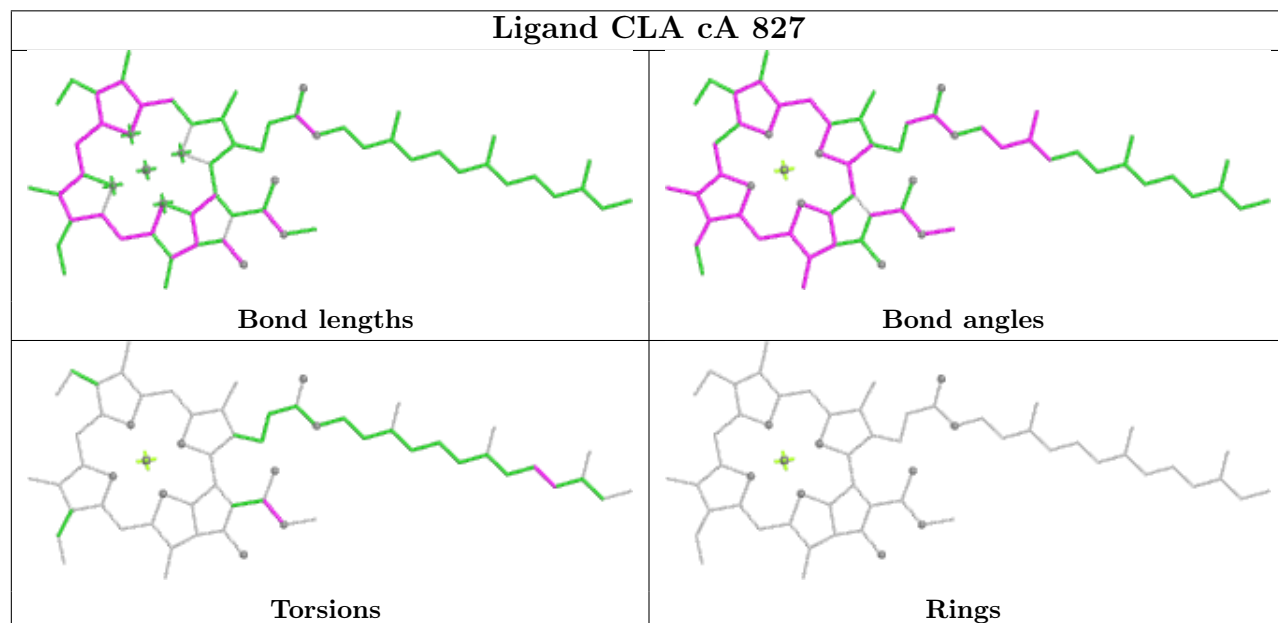
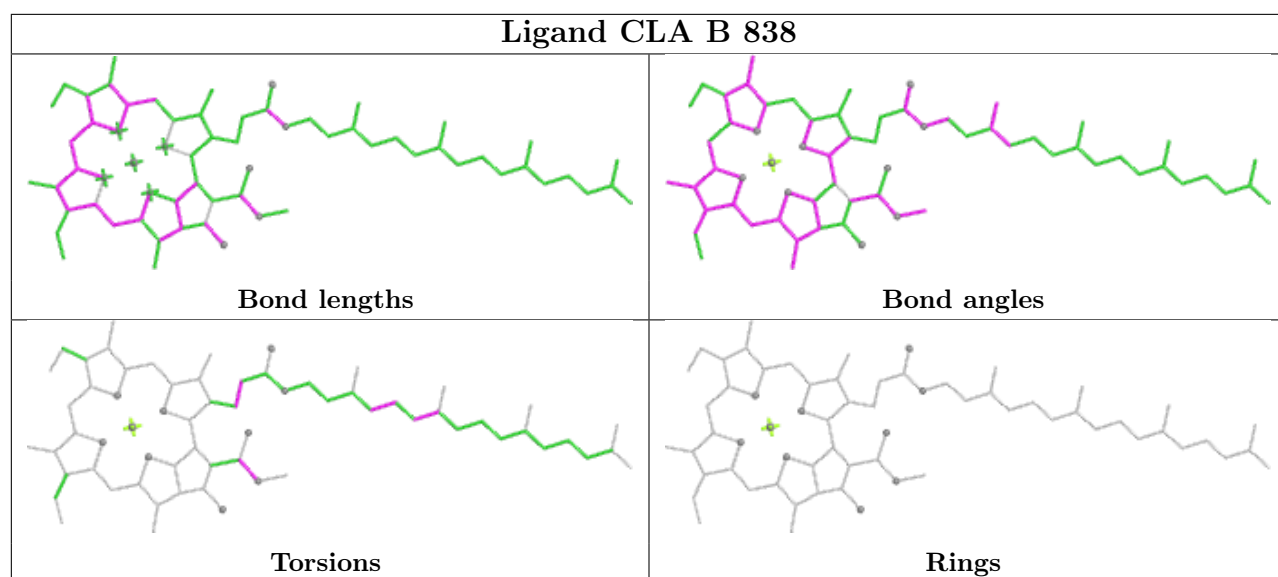


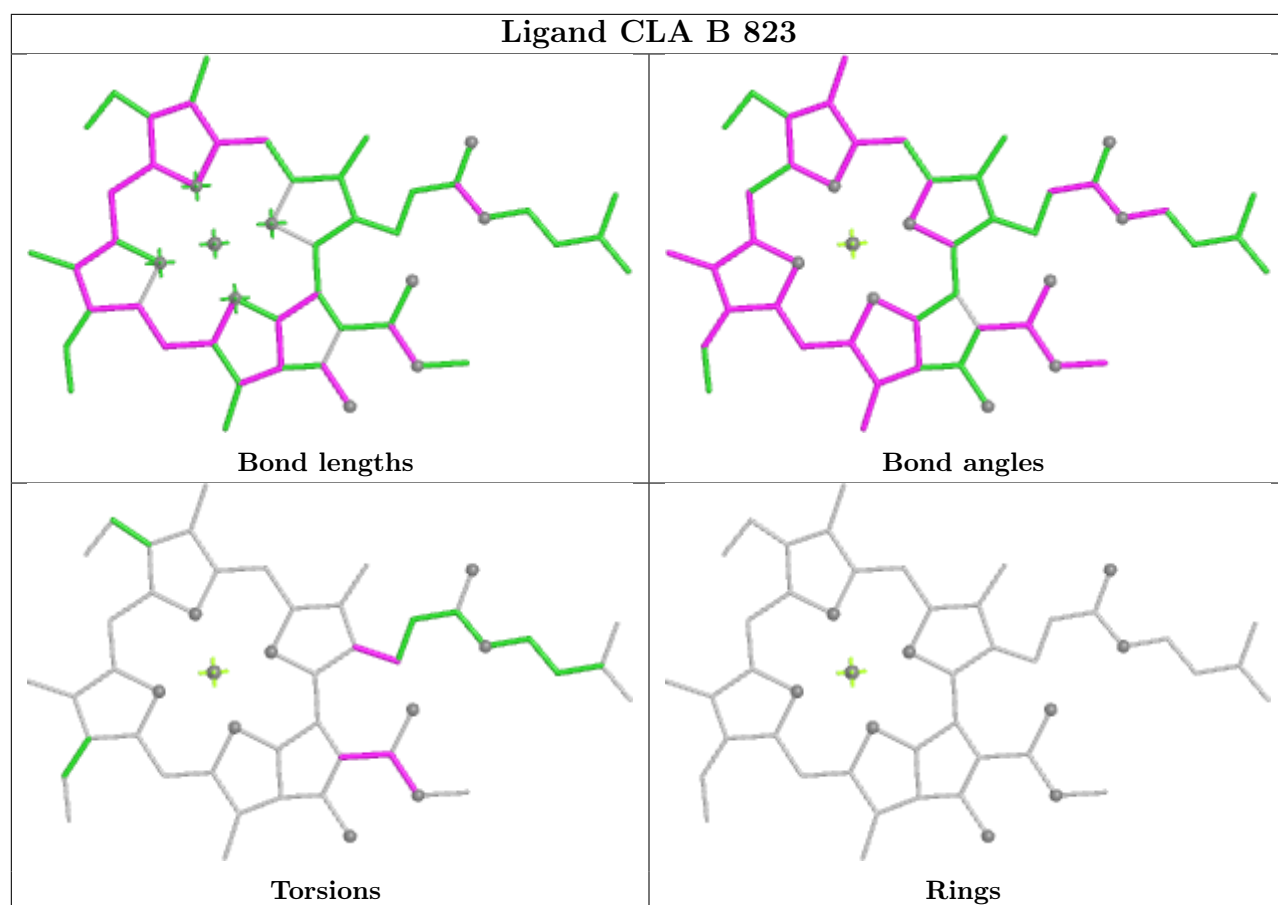




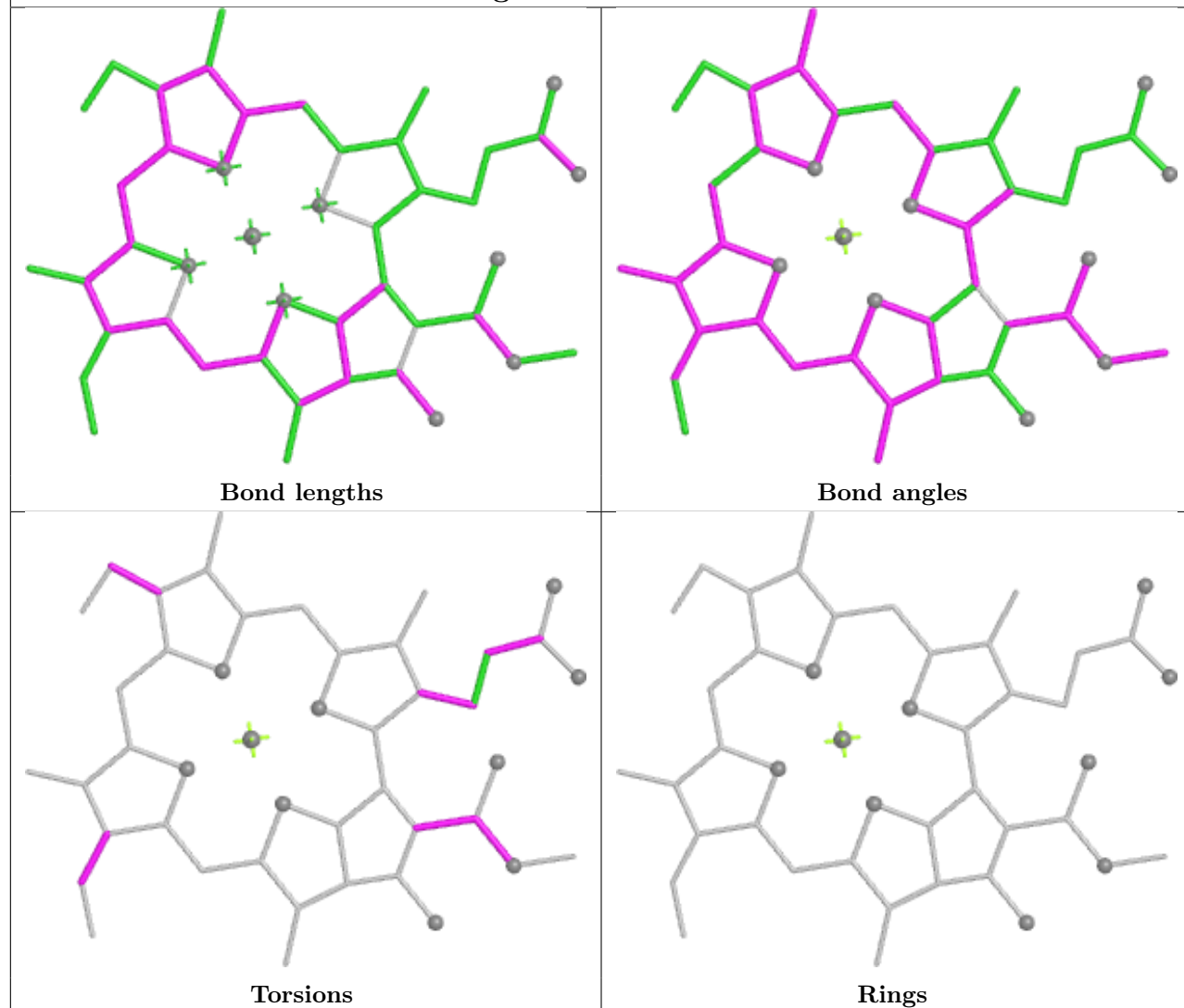




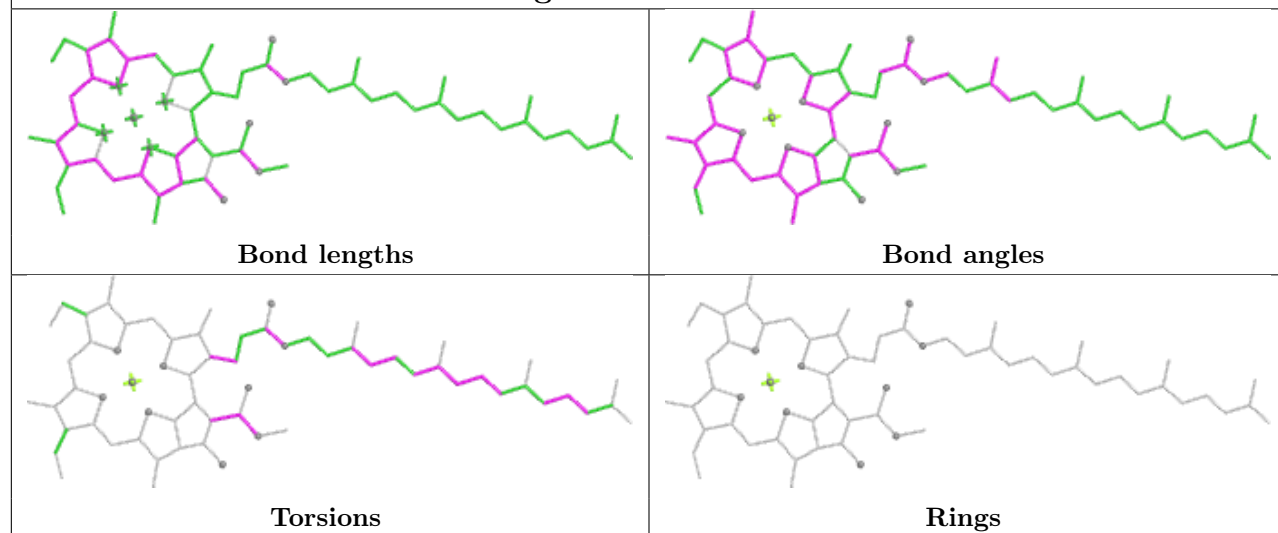


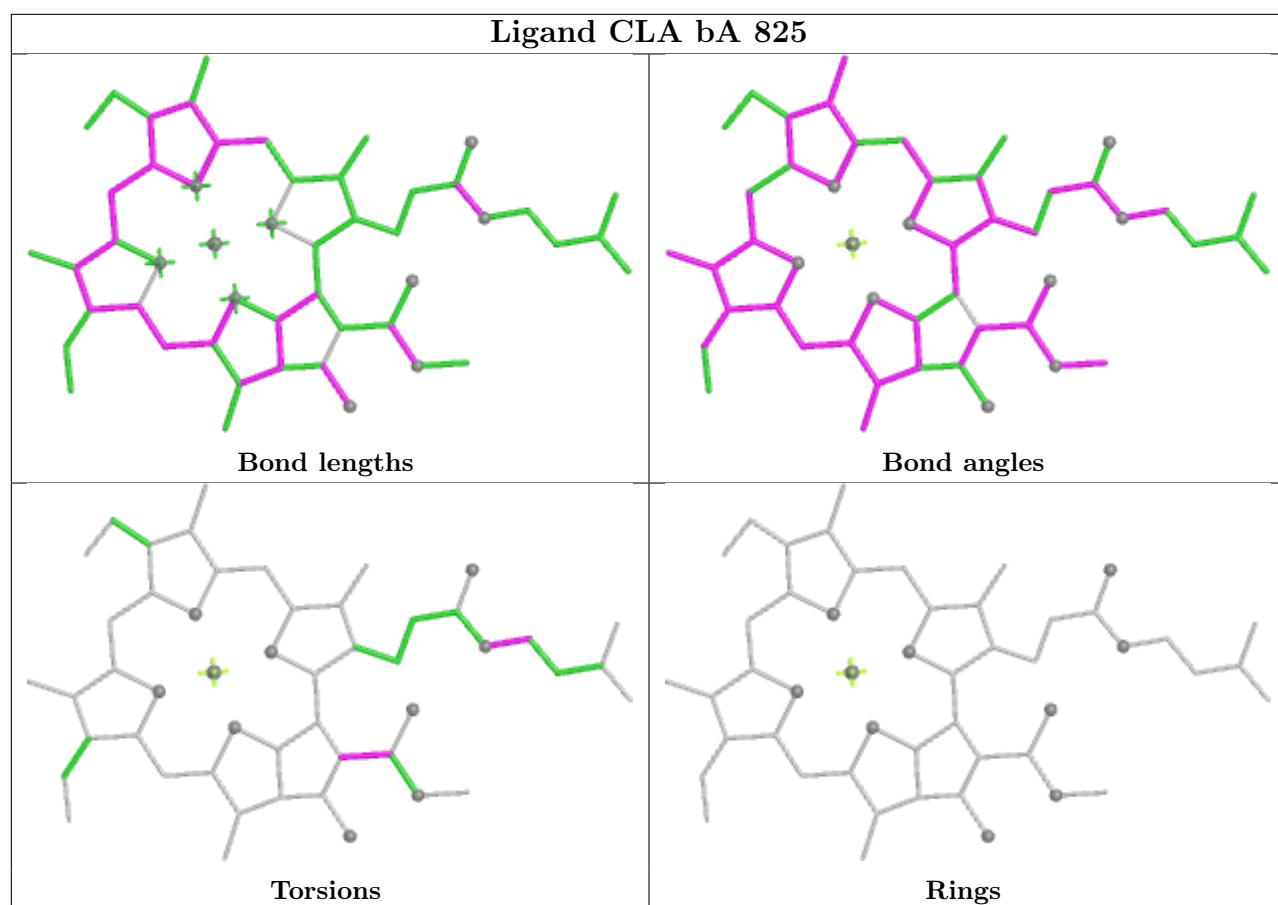


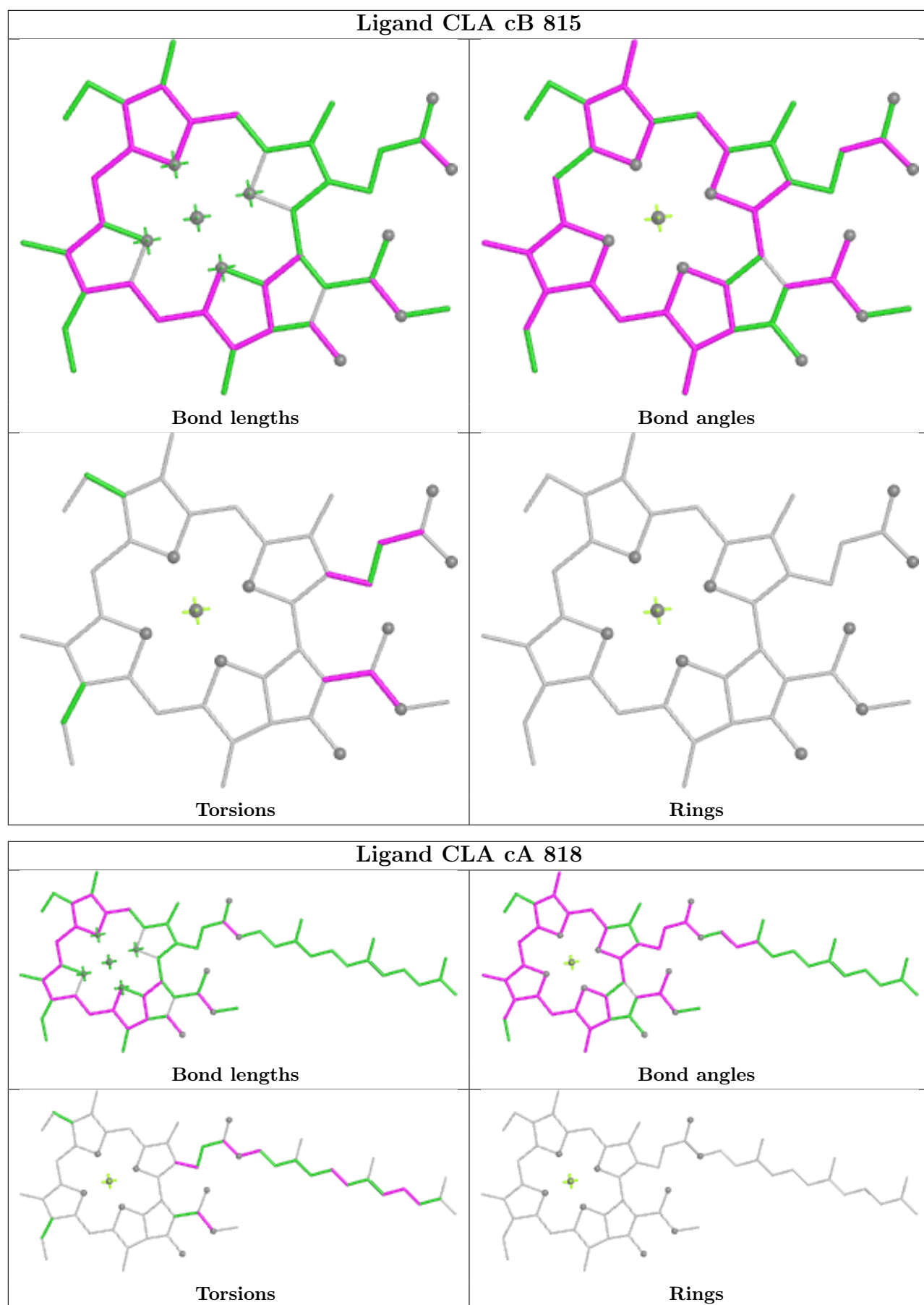
Ligand CLA B 820

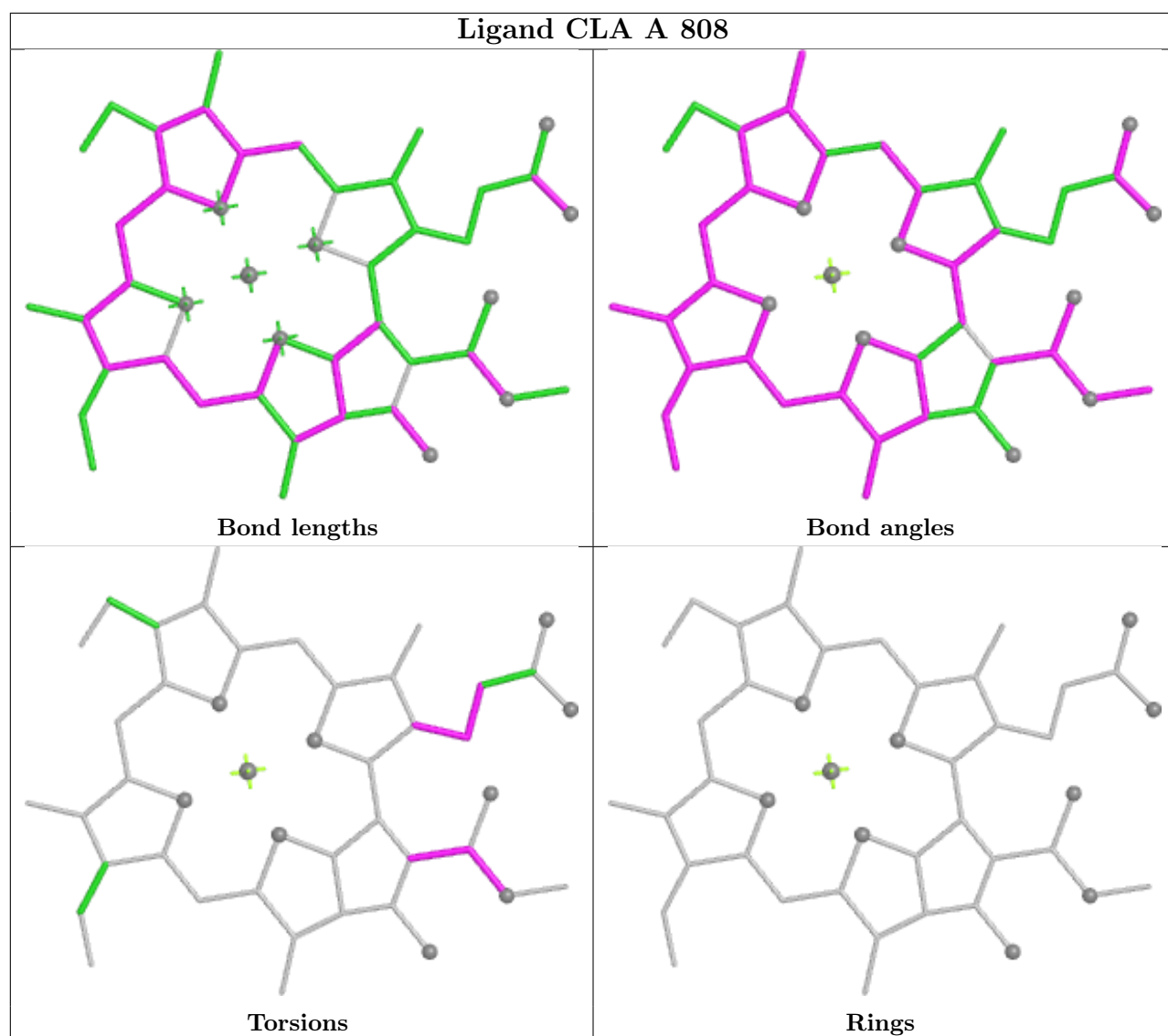


Ligand CLA L 202









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.

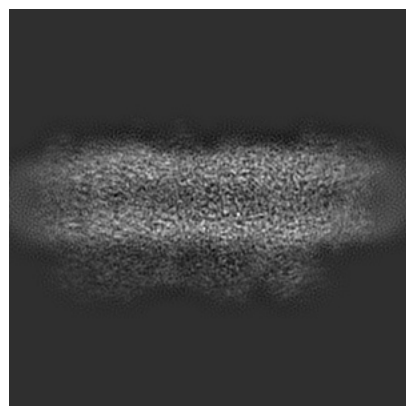
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62693. These allow visual inspection of the internal detail of the map and identification of artifacts.

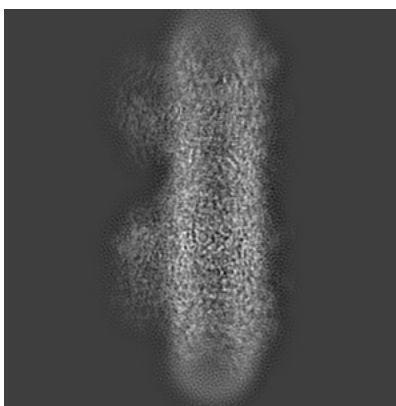
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

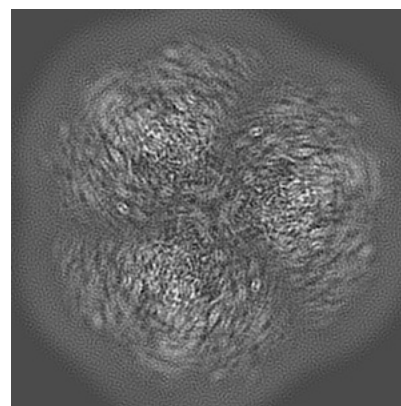
6.1.1 Primary map



X

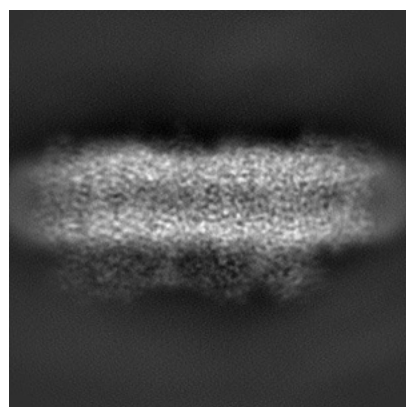


Y

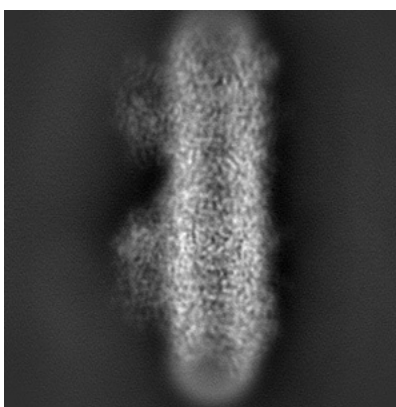


Z

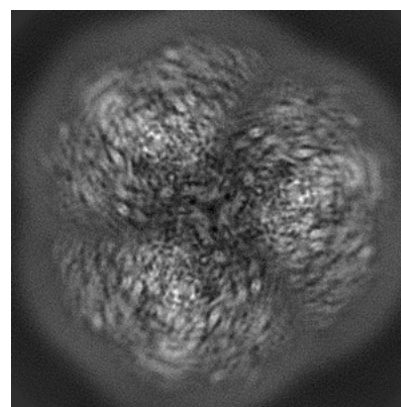
6.1.2 Raw map



X



Y

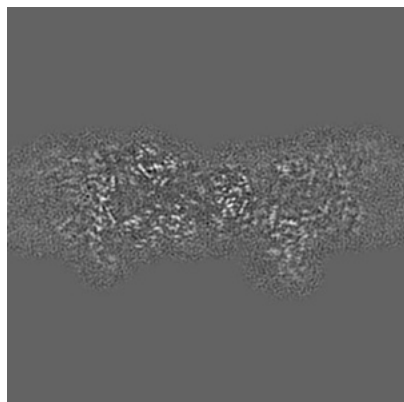


Z

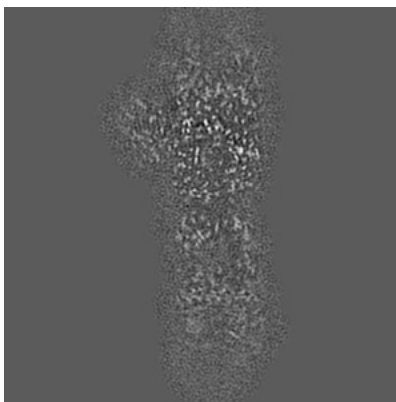
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

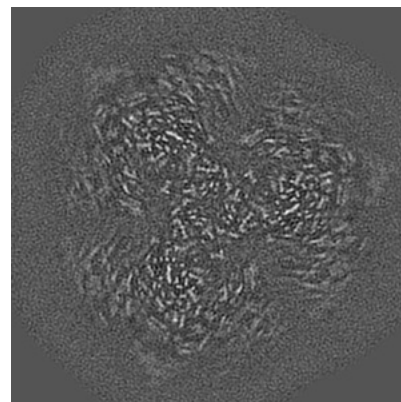
6.2.1 Primary map



X Index: 148

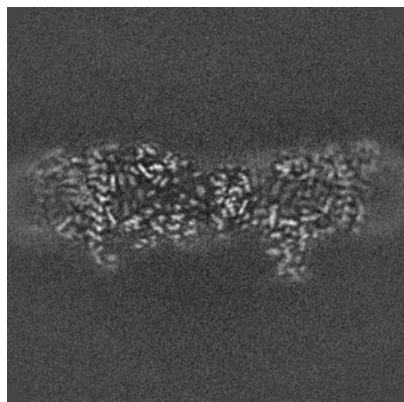


Y Index: 148

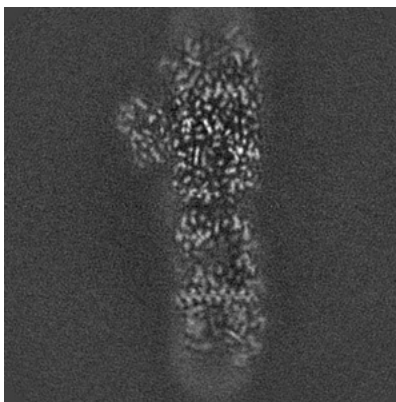


Z Index: 148

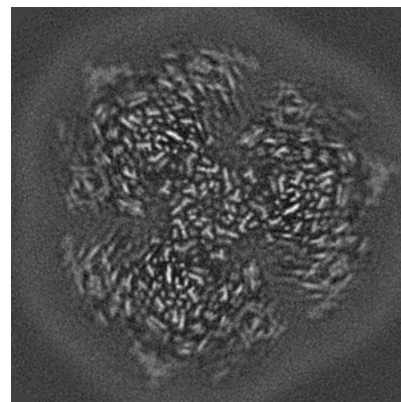
6.2.2 Raw map



X Index: 148



Y Index: 148

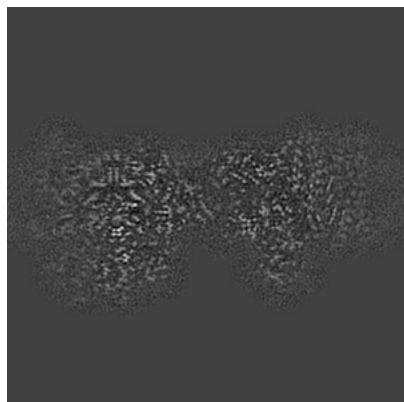


Z Index: 148

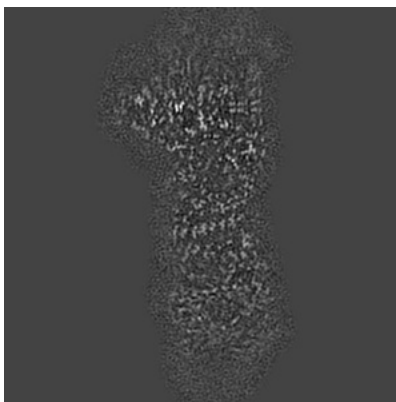
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

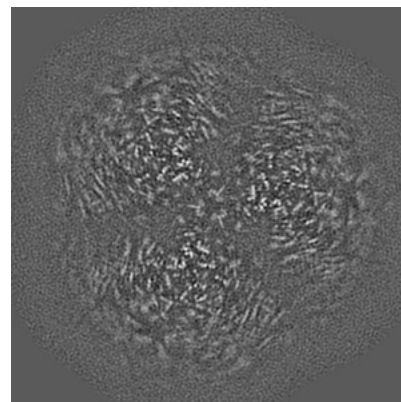
6.3.1 Primary map



X Index: 122

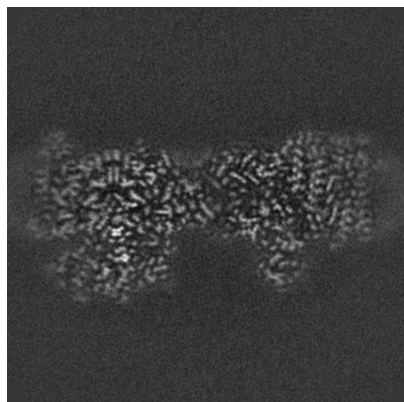


Y Index: 160

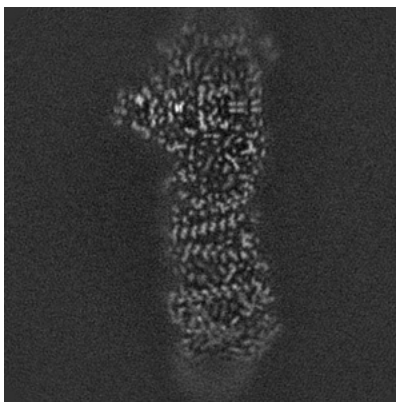


Z Index: 171

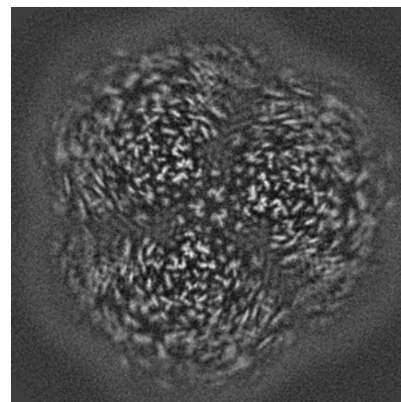
6.3.2 Raw map



X Index: 122



Y Index: 160

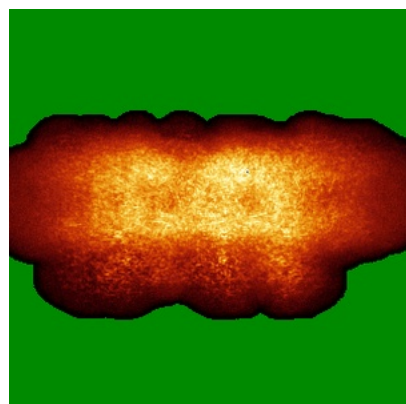


Z Index: 171

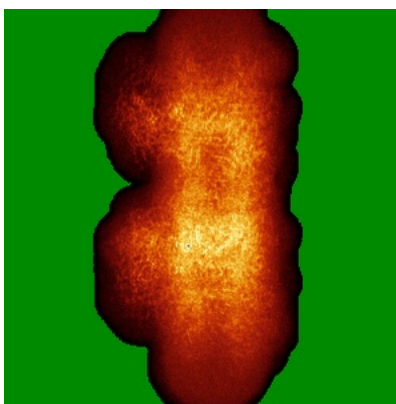
The images above show the largest variance slices of the map in three orthogonal directions.

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

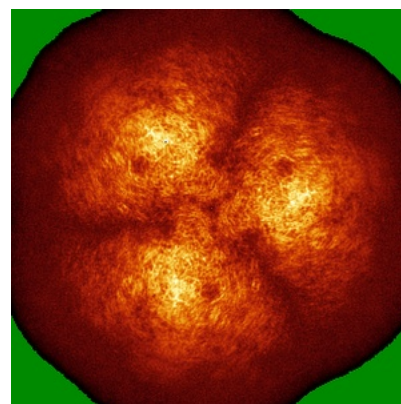
6.4.1 Primary map



X

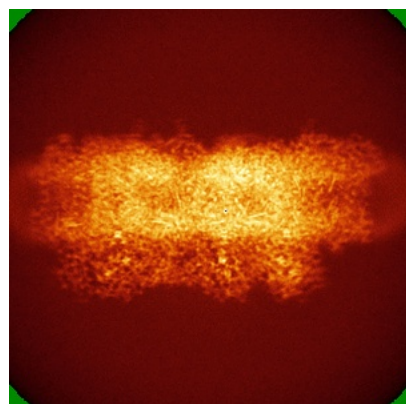


Y

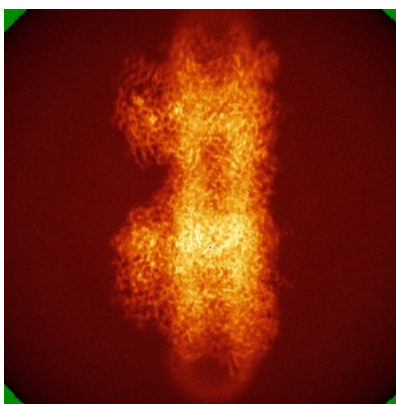


Z

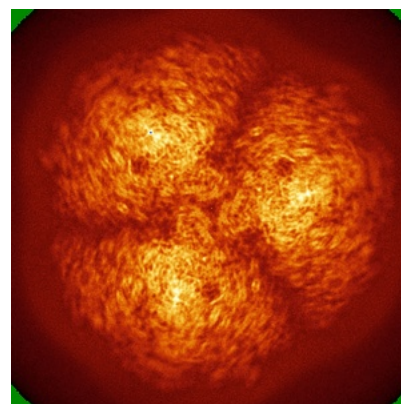
6.4.2 Raw map



X



Y

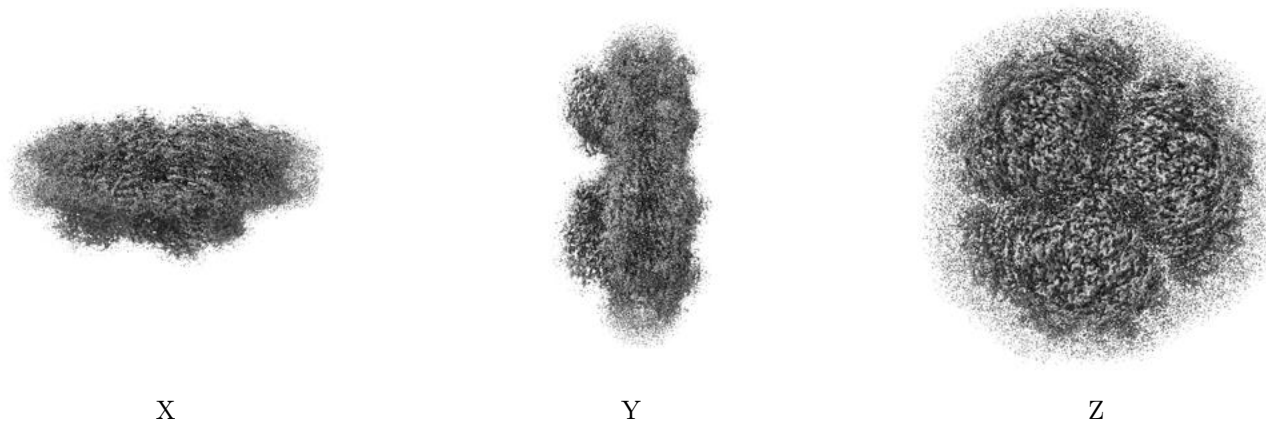


Z

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

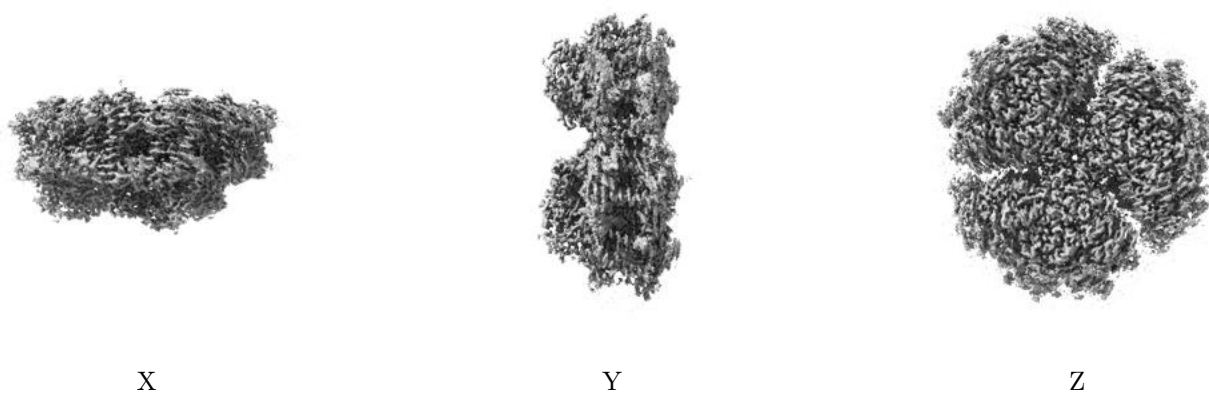
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

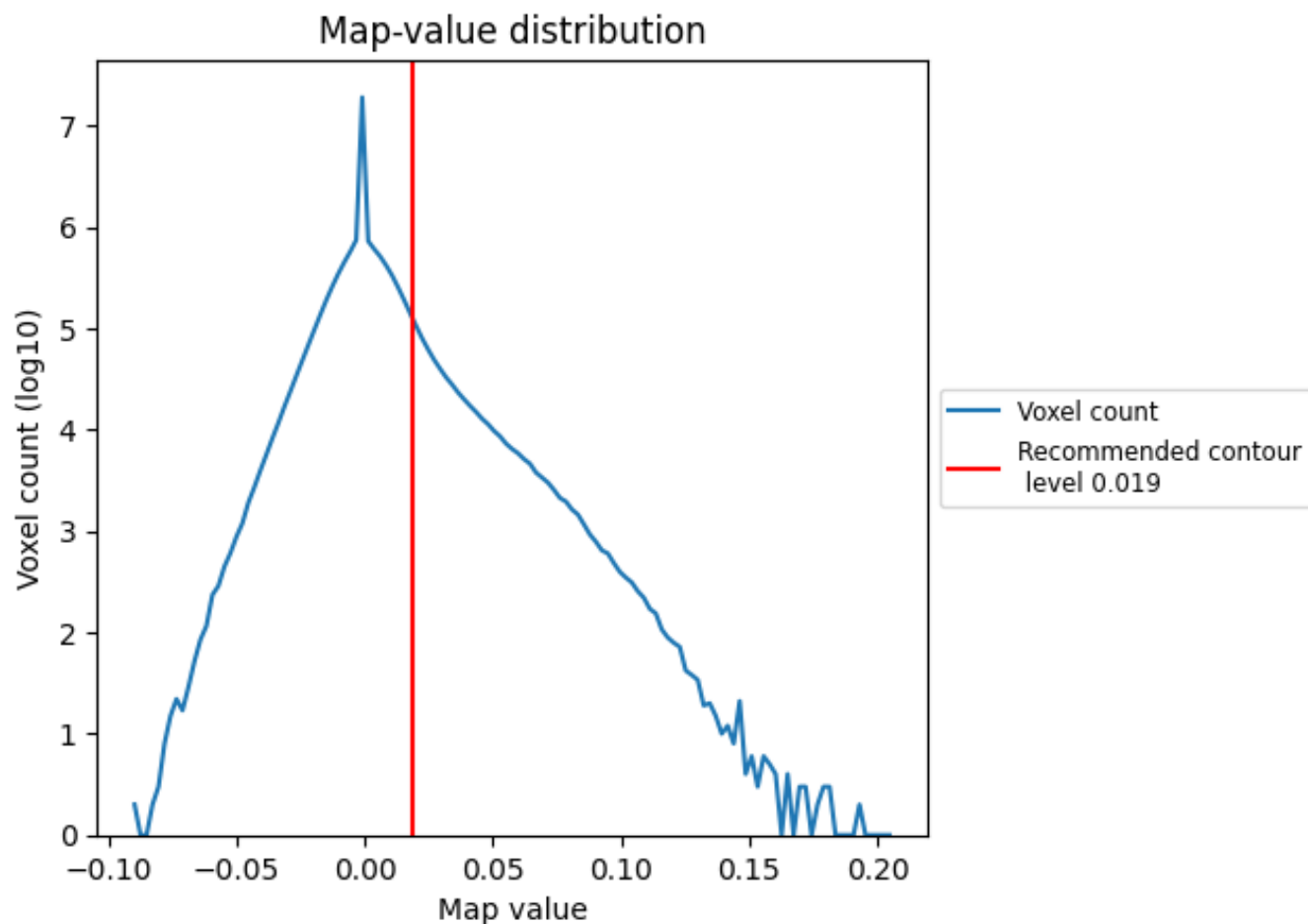
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

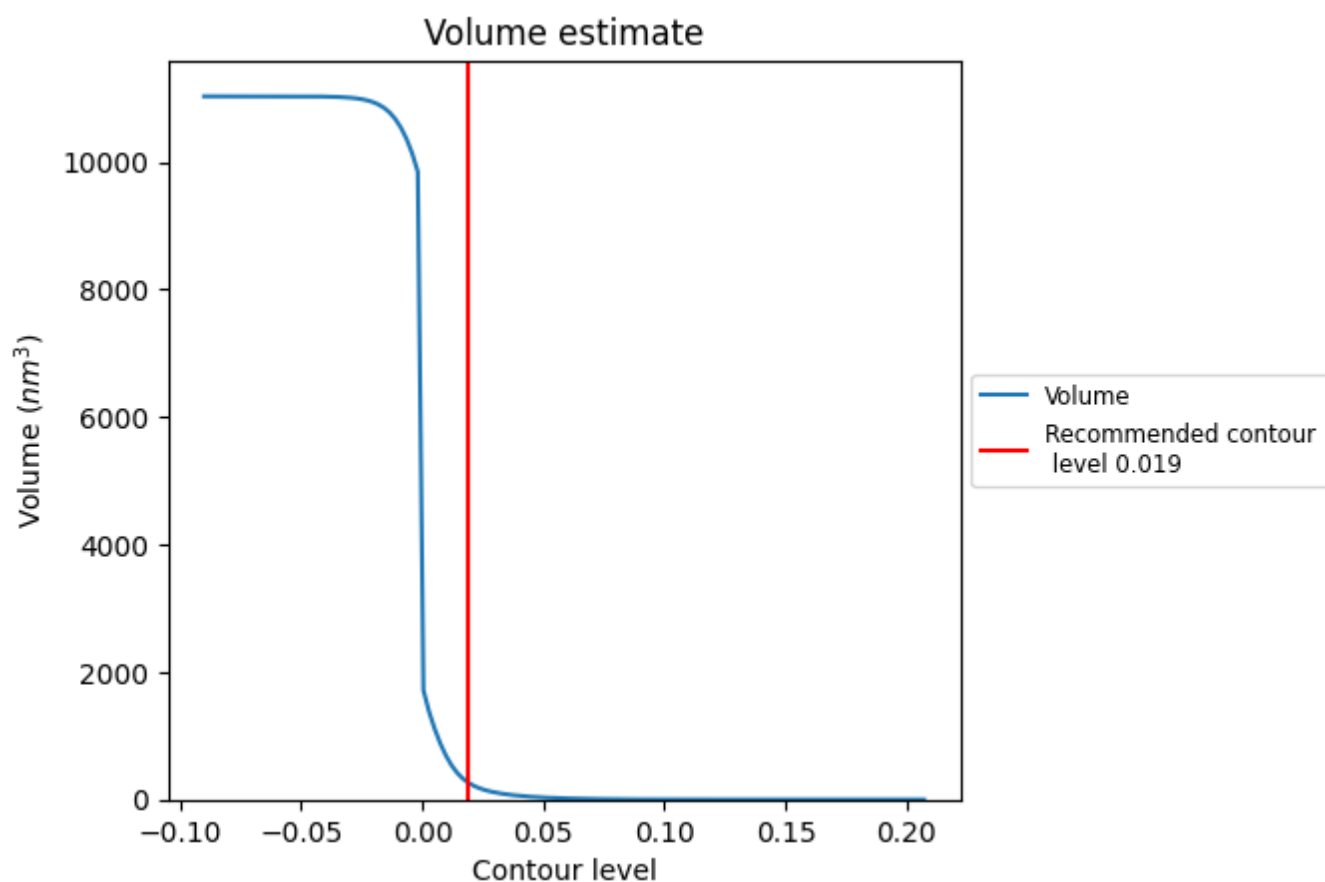
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

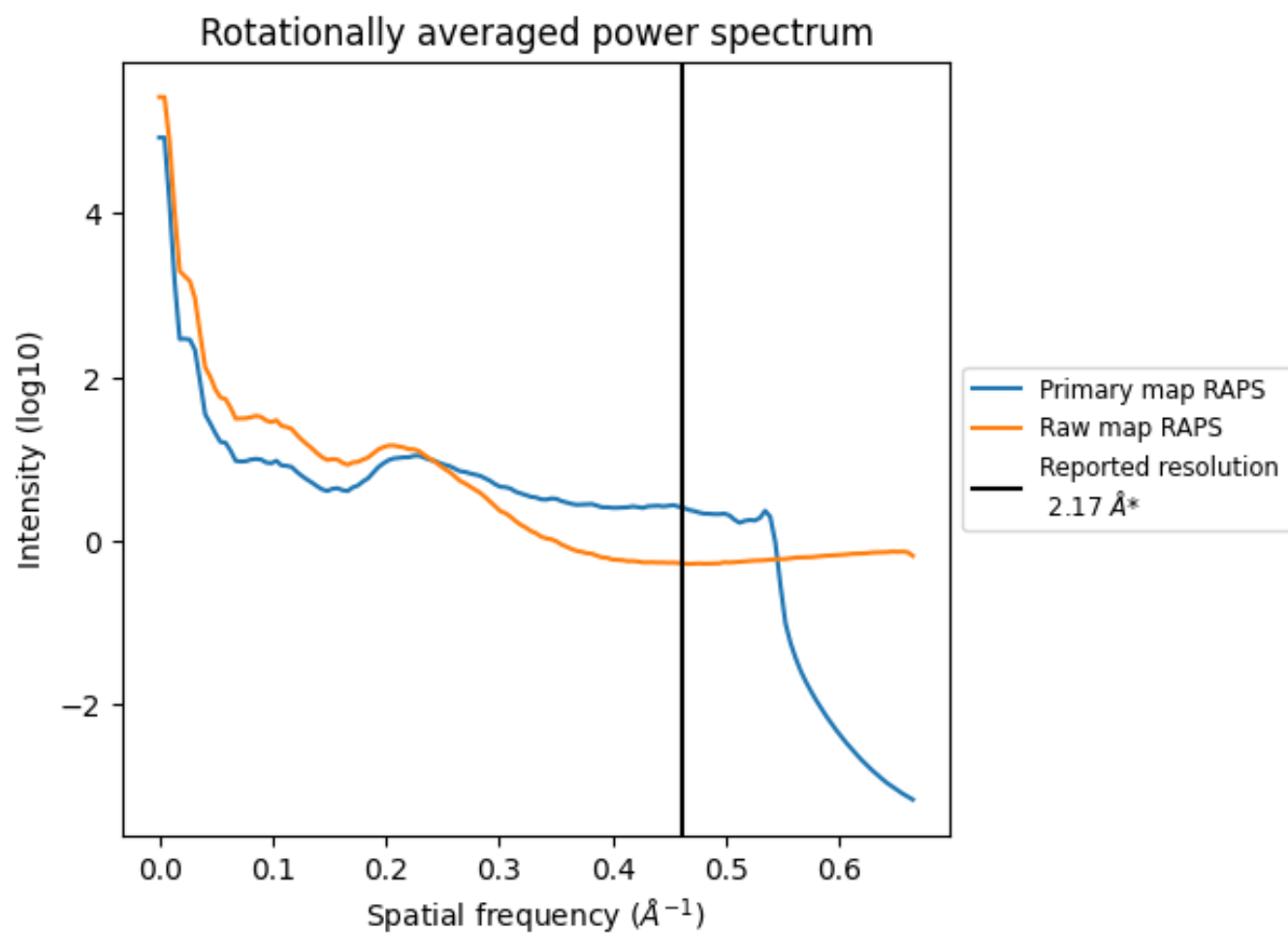
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 268 nm^3 ; this corresponds to an approximate mass of 242 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 ⓘ

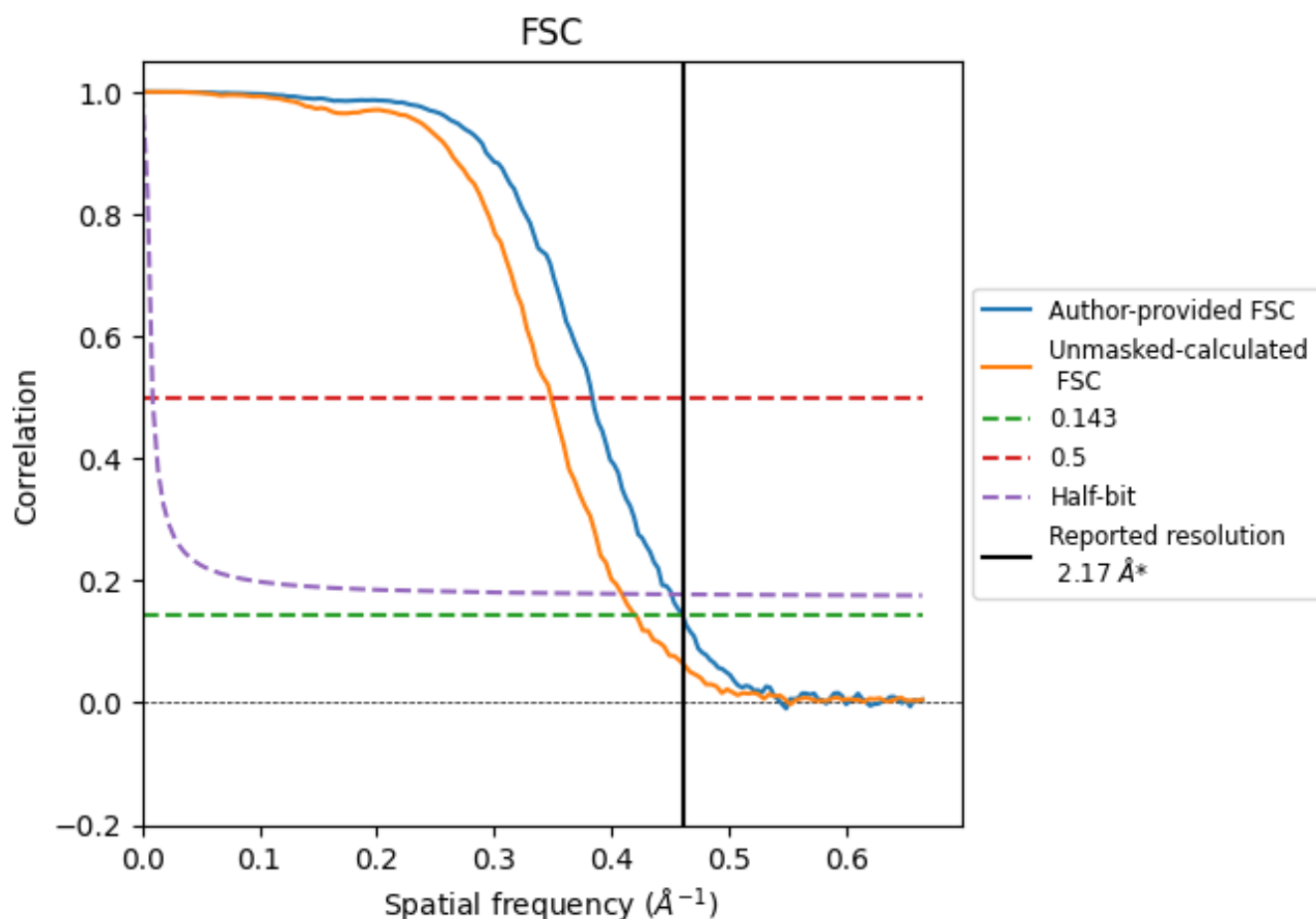


*Reported resolution corresponds to spatial frequency of 0.461 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.461 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

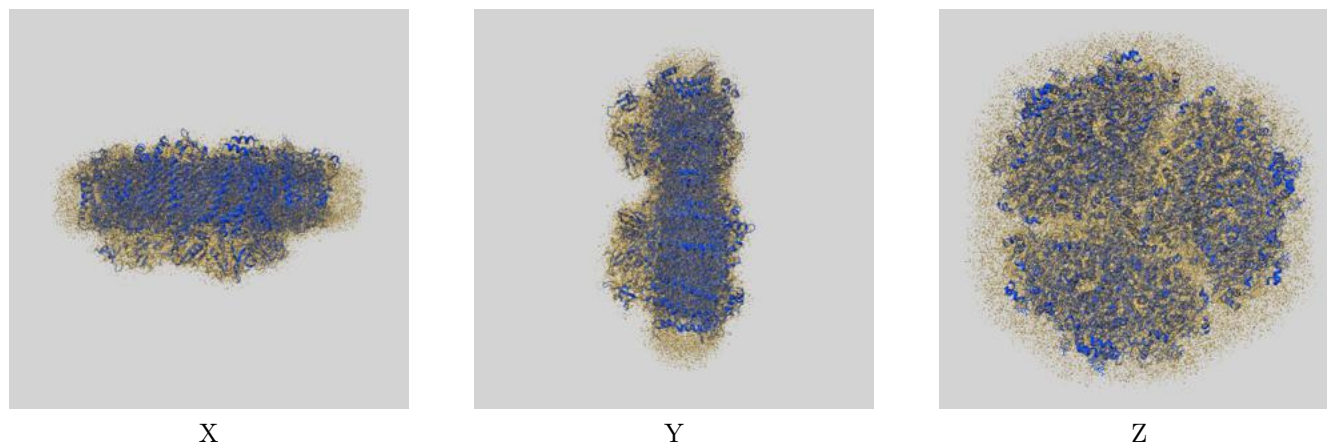
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.17	-	-
Author-provided FSC curve	2.17	2.61	2.22
Unmasked-calculated*	2.38	2.87	2.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

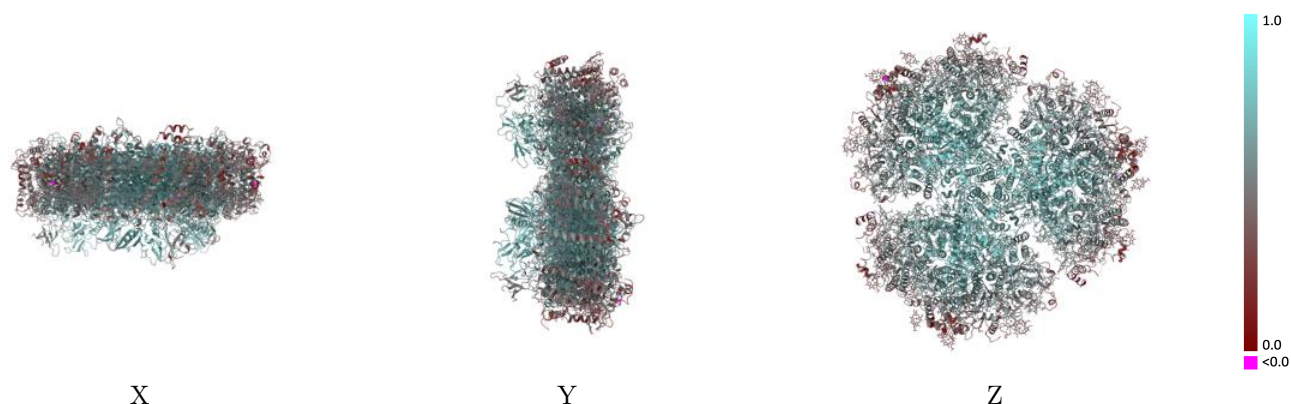
This section contains information regarding the fit between EMDB map EMD-62693 and PDB model 9L0A. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



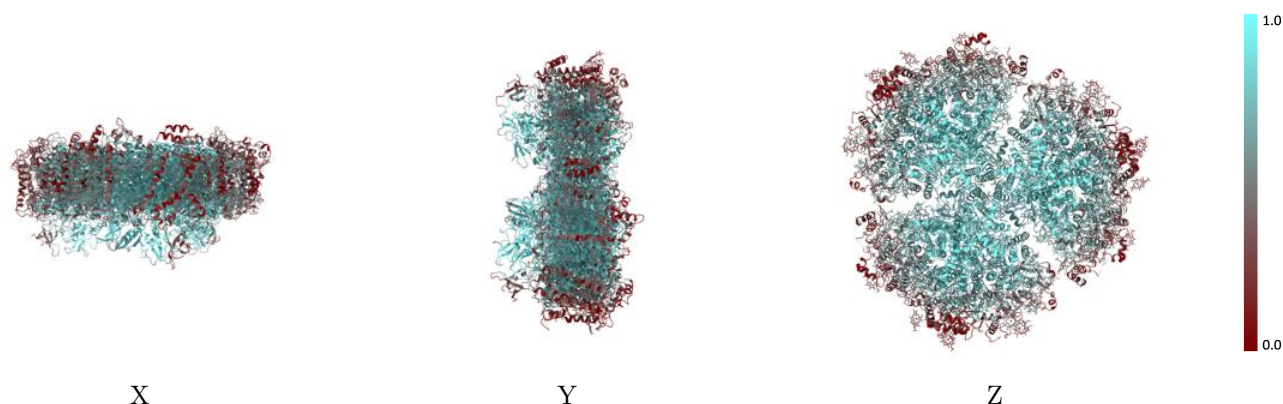
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



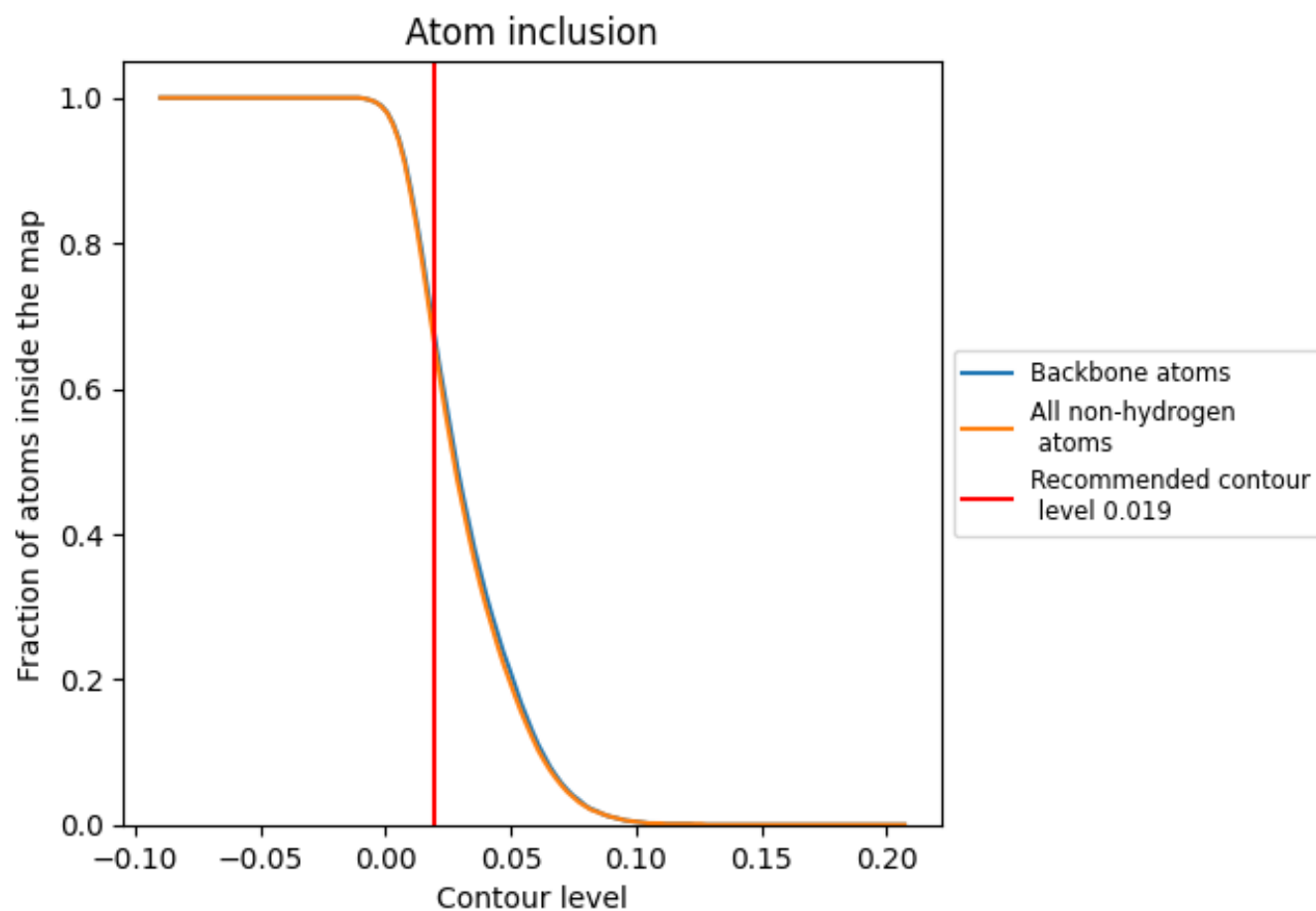
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 67% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6710	 0.5840
A	 0.6890	 0.5940
B	 0.6950	 0.5840
C	 0.9380	 0.7320
D	 0.7640	 0.6450
E	 0.5290	 0.5390
F	 0.2250	 0.3800
I	 0.9190	 0.7320
J	 0.2450	 0.3840
K	 0.1490	 0.3020
L	 0.8660	 0.7020
M	 0.6010	 0.5210
X	 0.1430	 0.3040
bA	 0.6870	 0.5940
bB	 0.6970	 0.5870
bC	 0.9320	 0.7320
bD	 0.7610	 0.6440
bE	 0.5290	 0.5400
bF	 0.2240	 0.3840
bI	 0.9070	 0.7310
bJ	 0.2280	 0.3770
bK	 0.1680	 0.2930
bL	 0.8660	 0.7030
bM	 0.6120	 0.5180
bX	 0.1430	 0.3090
cA	 0.6890	 0.5940
cB	 0.6930	 0.5830
cC	 0.9350	 0.7290
cD	 0.7600	 0.6450
cE	 0.5350	 0.5410
cF	 0.2230	 0.3790
cI	 0.9090	 0.7320
cJ	 0.2300	 0.3770
cK	 0.1730	 0.2970
cL	 0.8650	 0.7020



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Chain	Atom inclusion	Q-score
cM	 0.6150	 0.5240
cX	 0.1430	 0.3130