



## wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 12:10 AM JST

PDB ID : 7F4V  
EMDB ID : EMD-31455  
Title : Cryo-EM structure of a primordial cyanobacterial photosystem I  
Authors : Kato, K.; Hamaguchi, T.; Nagao, R.; Kawakami, K.; Yonekura, K.; Shen, J.R.  
Deposited on : 2021-06-21  
Resolution : 2.04 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

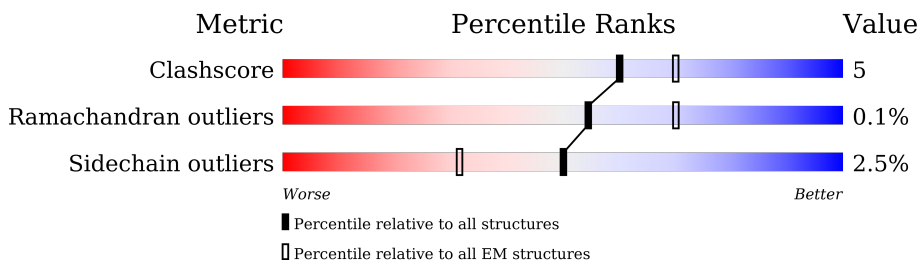
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.04 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.



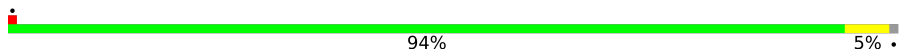


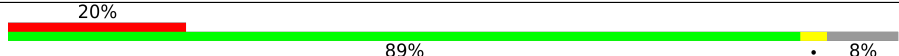
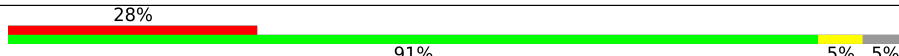
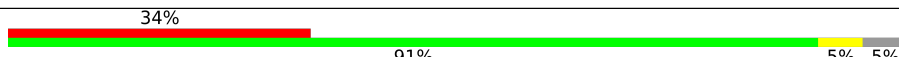
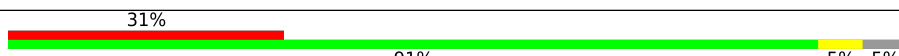
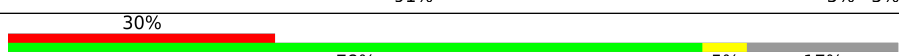
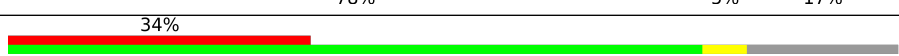

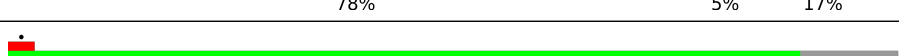
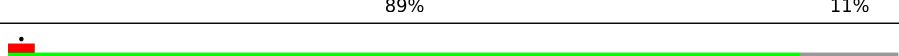
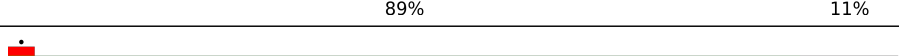
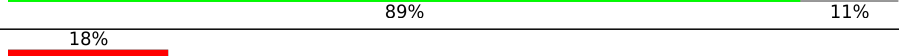
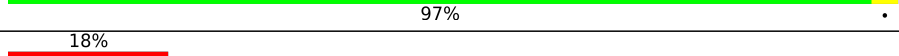
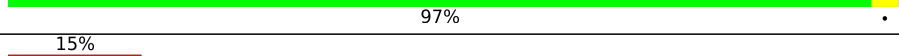
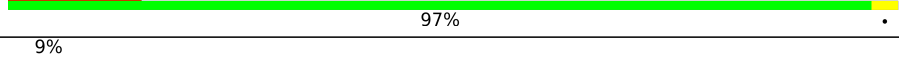


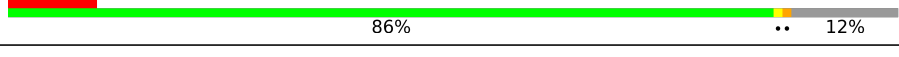

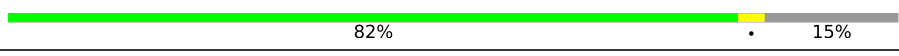
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	aA	783	
1	bA	783	
1	cA	783	
2	aB	872	
2	bB	872	
2	cB	872	
3	aC	81	
3	bC	81	

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Mol	Chain	Length	Quality of chain
3	cC	81	 94% 5%
4	aD	144	 19% 89% 8%
4	bD	144	 19% 89% 8%
4	cD	144	 20% 89% 8%
5	aE	65	 28% 91% 5% 5%
5	bE	65	 34% 91% 5% 5%
5	cE	65	 31% 91% 5% 5%
6	aF	181	 30% 78% 5% 17%
6	bF	181	 34% 78% 5% 17%
6	cF	181	 30% 78% 5% 17%
7	aI	35	 89% 11%
7	bI	35	 89% 11%
7	cI	35	 89% 11%
8	aJ	33	 18% 97%
8	bJ	33	 18% 97%
8	cJ	33	 15% 97%
9	aL	147	 9% 86% 12%
9	bL	147	 9% 86% 12%
9	cL	147	 10% 86% 12%
10	aM	34	 82% 15%
10	bM	34	 82% 15%
10	cM	34	 82% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CL0	aA	801	X	-	-	-
11	CL0	bA	801	X	-	-	-
11	CL0	cA	801	X	-	-	-
12	CLA	aA	802	X	-	-	-
12	CLA	aA	803	X	-	-	-
12	CLA	aA	804	X	-	-	-
12	CLA	aA	805	X	-	-	-
12	CLA	aA	806	X	-	-	-
12	CLA	aA	807	X	-	-	-
12	CLA	aA	808	X	-	-	-
12	CLA	aA	809	X	-	-	-
12	CLA	aA	810	X	-	-	-
12	CLA	aA	811	X	-	-	-
12	CLA	aA	812	X	-	-	-
12	CLA	aA	813	X	-	-	-
12	CLA	aA	814	X	-	-	-
12	CLA	aA	816	X	-	-	-
12	CLA	aA	818	X	-	-	-
12	CLA	aA	819	X	-	-	-
12	CLA	aA	820	X	-	-	-
12	CLA	aA	821	X	-	-	-
12	CLA	aA	823	X	-	-	-
12	CLA	aA	825	X	-	-	-
12	CLA	aA	826	X	-	-	-
12	CLA	aA	827	X	-	-	-
12	CLA	aA	828	X	-	-	-
12	CLA	aA	829	X	-	-	-
12	CLA	aA	830	X	-	-	-
12	CLA	aA	832	X	-	-	-
12	CLA	aA	833	X	-	-	-
12	CLA	aA	834	X	-	-	-
12	CLA	aA	835	X	-	-	-
12	CLA	aA	836	X	-	-	-
12	CLA	aA	837	X	-	-	-
12	CLA	aA	838	X	-	-	-
12	CLA	aA	839	X	-	-	-
12	CLA	aA	840	X	-	-	-
12	CLA	aA	841	X	-	-	-
12	CLA	aA	842	X	-	-	-
12	CLA	aA	843	X	-	-	-
12	CLA	aA	854	X	-	-	-
12	CLA	aB	901	X	-	-	-
12	CLA	aB	902	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	aB	903	X	-	-	-
12	CLA	aB	904	X	-	-	-
12	CLA	aB	905	X	-	-	-
12	CLA	aB	906	X	-	-	-
12	CLA	aB	907	X	-	-	-
12	CLA	aB	908	X	-	-	-
12	CLA	aB	909	X	-	-	-
12	CLA	aB	910	X	-	-	-
12	CLA	aB	912	X	-	-	-
12	CLA	aB	913	X	-	-	-
12	CLA	aB	914	X	-	-	-
12	CLA	aB	917	X	-	-	-
12	CLA	aB	918	X	-	-	-
12	CLA	aB	919	X	-	-	-
12	CLA	aB	922	X	-	-	-
12	CLA	aB	923	X	-	-	-
12	CLA	aB	924	X	-	-	-
12	CLA	aB	925	X	-	-	-
12	CLA	aB	926	X	-	-	-
12	CLA	aB	927	X	-	-	-
12	CLA	aB	928	X	-	-	-
12	CLA	aB	930	X	-	-	-
12	CLA	aB	931	X	-	-	-
12	CLA	aB	933	X	-	-	-
12	CLA	aB	934	X	-	-	-
12	CLA	aB	935	X	-	-	-
12	CLA	aB	936	X	-	-	-
12	CLA	aB	937	X	-	-	-
12	CLA	aB	938	X	-	-	-
12	CLA	aB	939	X	-	-	-
12	CLA	aB	949	X	-	-	-
12	CLA	aF	202	X	-	-	-
12	CLA	bA	802	X	-	-	-
12	CLA	bA	803	X	-	-	-
12	CLA	bA	804	X	-	-	-
12	CLA	bA	805	X	-	-	-
12	CLA	bA	806	X	-	-	-
12	CLA	bA	807	X	-	-	-
12	CLA	bA	808	X	-	-	-
12	CLA	bA	809	X	-	-	-
12	CLA	bA	810	X	-	-	-
12	CLA	bA	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	bA	812	X	-	-	-
12	CLA	bA	813	X	-	-	-
12	CLA	bA	814	X	-	-	-
12	CLA	bA	816	X	-	-	-
12	CLA	bA	818	X	-	-	-
12	CLA	bA	819	X	-	-	-
12	CLA	bA	820	X	-	-	-
12	CLA	bA	821	X	-	-	-
12	CLA	bA	823	X	-	-	-
12	CLA	bA	825	X	-	-	-
12	CLA	bA	826	X	-	-	-
12	CLA	bA	827	X	-	-	-
12	CLA	bA	828	X	-	-	-
12	CLA	bA	829	X	-	-	-
12	CLA	bA	830	X	-	-	-
12	CLA	bA	832	X	-	-	-
12	CLA	bA	833	X	-	-	-
12	CLA	bA	834	X	-	-	-
12	CLA	bA	835	X	-	-	-
12	CLA	bA	836	X	-	-	-
12	CLA	bA	837	X	-	-	-
12	CLA	bA	838	X	-	-	-
12	CLA	bA	839	X	-	-	-
12	CLA	bA	840	X	-	-	-
12	CLA	bA	841	X	-	-	-
12	CLA	bA	842	X	-	-	-
12	CLA	bA	843	X	-	-	-
12	CLA	bA	853	X	-	-	-
12	CLA	bB	901	X	-	-	-
12	CLA	bB	902	X	-	-	-
12	CLA	bB	903	X	-	-	-
12	CLA	bB	904	X	-	-	-
12	CLA	bB	905	X	-	-	-
12	CLA	bB	906	X	-	-	-
12	CLA	bB	907	X	-	-	-
12	CLA	bB	908	X	-	-	-
12	CLA	bB	909	X	-	-	-
12	CLA	bB	910	X	-	-	-
12	CLA	bB	912	X	-	-	-
12	CLA	bB	913	X	-	-	-
12	CLA	bB	914	X	-	-	-
12	CLA	bB	917	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	bB	918	X	-	-	-
12	CLA	bB	919	X	-	-	-
12	CLA	bB	922	X	-	-	-
12	CLA	bB	923	X	-	-	-
12	CLA	bB	924	X	-	-	-
12	CLA	bB	925	X	-	-	-
12	CLA	bB	926	X	-	-	-
12	CLA	bB	927	X	-	-	-
12	CLA	bB	928	X	-	-	-
12	CLA	bB	930	X	-	-	-
12	CLA	bB	931	X	-	-	-
12	CLA	bB	933	X	-	-	-
12	CLA	bB	934	X	-	-	-
12	CLA	bB	935	X	-	-	-
12	CLA	bB	936	X	-	-	-
12	CLA	bB	937	X	-	-	-
12	CLA	bB	938	X	-	-	-
12	CLA	bB	939	X	-	-	-
12	CLA	bB	949	X	-	-	-
12	CLA	bF	202	X	-	-	-
12	CLA	cA	802	X	-	-	-
12	CLA	cA	803	X	-	-	-
12	CLA	cA	804	X	-	-	-
12	CLA	cA	805	X	-	-	-
12	CLA	cA	806	X	-	-	-
12	CLA	cA	807	X	-	-	-
12	CLA	cA	808	X	-	-	-
12	CLA	cA	809	X	-	-	-
12	CLA	cA	810	X	-	-	-
12	CLA	cA	811	X	-	-	-
12	CLA	cA	812	X	-	-	-
12	CLA	cA	813	X	-	-	-
12	CLA	cA	814	X	-	-	-
12	CLA	cA	816	X	-	-	-
12	CLA	cA	818	X	-	-	-
12	CLA	cA	819	X	-	-	-
12	CLA	cA	820	X	-	-	-
12	CLA	cA	821	X	-	-	-
12	CLA	cA	823	X	-	-	-
12	CLA	cA	825	X	-	-	-
12	CLA	cA	826	X	-	-	-
12	CLA	cA	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	cA	828	X	-	-	-
12	CLA	cA	829	X	-	-	-
12	CLA	cA	830	X	-	-	-
12	CLA	cA	832	X	-	-	-
12	CLA	cA	833	X	-	-	-
12	CLA	cA	834	X	-	-	-
12	CLA	cA	835	X	-	-	-
12	CLA	cA	836	X	-	-	-
12	CLA	cA	837	X	-	-	-
12	CLA	cA	838	X	-	-	-
12	CLA	cA	839	X	-	-	-
12	CLA	cA	840	X	-	-	-
12	CLA	cA	841	X	-	-	-
12	CLA	cA	842	X	-	-	-
12	CLA	cA	843	X	-	-	-
12	CLA	cA	853	X	-	-	-
12	CLA	cB	901	X	-	-	-
12	CLA	cB	902	X	-	-	-
12	CLA	cB	903	X	-	-	-
12	CLA	cB	904	X	-	-	-
12	CLA	cB	905	X	-	-	-
12	CLA	cB	906	X	-	-	-
12	CLA	cB	907	X	-	-	-
12	CLA	cB	908	X	-	-	-
12	CLA	cB	909	X	-	-	-
12	CLA	cB	910	X	-	-	-
12	CLA	cB	912	X	-	-	-
12	CLA	cB	913	X	-	-	-
12	CLA	cB	914	X	-	-	-
12	CLA	cB	917	X	-	-	-
12	CLA	cB	918	X	-	-	-
12	CLA	cB	919	X	-	-	-
12	CLA	cB	922	X	-	-	-
12	CLA	cB	923	X	-	-	-
12	CLA	cB	924	X	-	-	-
12	CLA	cB	925	X	-	-	-
12	CLA	cB	926	X	-	-	-
12	CLA	cB	927	X	-	-	-
12	CLA	cB	928	X	-	-	-
12	CLA	cB	930	X	-	-	-
12	CLA	cB	931	X	-	-	-
12	CLA	cB	933	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
12	CLA	cB	934	X	-	-	-
12	CLA	cB	935	X	-	-	-
12	CLA	cB	936	X	-	-	-
12	CLA	cB	937	X	-	-	-
12	CLA	cB	938	X	-	-	-
12	CLA	cB	939	X	-	-	-
12	CLA	cB	949	X	-	-	-
12	CLA	cF	202	X	-	-	-

## 2 Entry composition i

There are 18 unique types of molecules in this entry. The entry contains 67641 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
			Total	C	N	O	S		
1	aA	772	Total 6038	C 3957	N 1031	O 1025	S 25	0	0
1	bA	772	Total 6038	C 3957	N 1031	O 1025	S 25	0	0
1	cA	772	Total 6038	C 3957	N 1031	O 1025	S 25	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	aB	725	Total 5701	C 3761	N 954	O 968	S 18	0	0
2	bB	725	Total 5701	C 3761	N 954	O 968	S 18	0	0
2	cB	725	Total 5701	C 3761	N 954	O 968	S 18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	aC	80	Total 599	C 368	N 103	O 118	S 10	0	0
3	bC	80	Total 599	C 368	N 103	O 118	S 10	0	0
3	cC	80	Total 599	C 368	N 103	O 118	S 10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	aD	133	Total 1038	C 660	N 180	O 194	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	133	Total	C	N	O	S	0	0
			1038	660	180	194	4		
4	cD	133	Total	C	N	O	S	0	0
			1038	660	180	194	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aE	62	Total	C	N	O	S	0	0
			507	321	87	99			
5	bE	62	Total	C	N	O	S	0	0
			507	321	87	99			
5	cE	62	Total	C	N	O	S	0	0
			507	321	87	99			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	151	Total	C	N	O	S	0	0
			1182	761	200	218	3		
6	bF	151	Total	C	N	O	S	0	0
			1182	761	200	218	3		
6	cF	151	Total	C	N	O	S	0	0
			1182	761	200	218	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	31	Total	C	N	O	S	0	0
			240	164	35	40	1		
7	bI	31	Total	C	N	O	S	0	0
			240	164	35	40	1		
7	cI	31	Total	C	N	O	S	0	0
			240	164	35	40	1		

- Molecule 8 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	aJ	33	Total	C	N	O	0	0
			164	98	33	33		
8	bJ	33	Total	C	N	O	0	0
			164	98	33	33		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	cJ	33	164	98	33	33	0	0

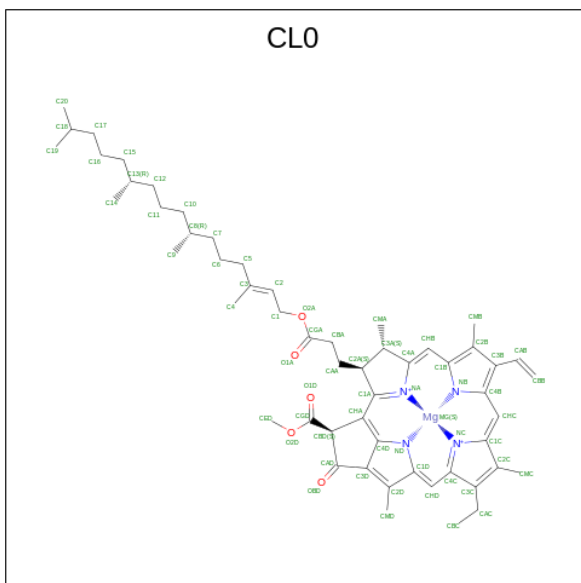
- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	aL	129	974	641	162	169	2	0	0
9	bL	129	974	641	162	169	2	0	0
9	cL	129	974	641	162	169	2	0	0

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

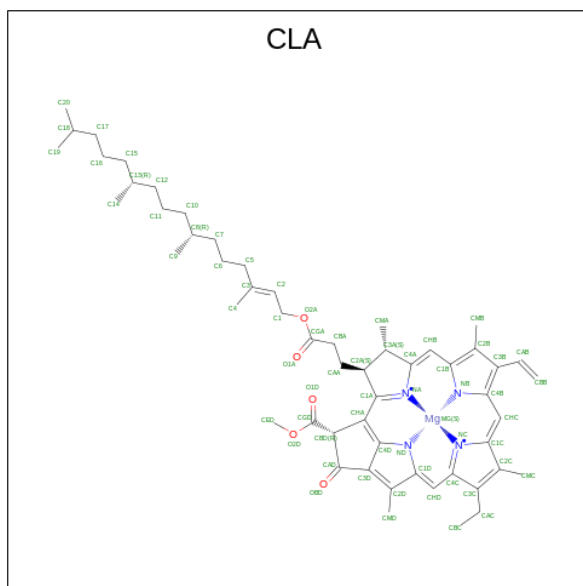
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	aM	29	190	127	30	33	0	0
10	bM	29	190	127	30	33	0	0
10	cM	29	190	127	30	33	0	0

- Molecule 11 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



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

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					AltConf
12	aA	1	Total	C	Mg	N	O	0
			2396	1956	44	176	220	
12	aA	1	Total	C	Mg	N	O	0
			2396	1956	44	176	220	
12	aA	1	Total	C	Mg	N	O	0
			2396	1956	44	176	220	
12	aA	1	Total	C	Mg	N	O	0
			2396	1956	44	176	220	
12	aA	1	Total	C	Mg	N	O	0
			2396	1956	44	176	220	
12	aA	1	Total	C	Mg	N	O	0
			2396	1956	44	176	220	
12	aA	1	Total	C	Mg	N	O	0
			2396	1956	44	176	220	
12	aA	1	Total	C	Mg	N	O	0
			2396	1956	44	176	220	
12	aA	1	Total	C	Mg	N	O	0
			2396	1956	44	176	220	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aA	1	2396	1956	44	176	220	0
12	aB	1	2144	1736	41	164	203	0
12	aB	1	2144	1736	41	164	203	0
12	aB	1	2144	1736	41	164	203	0
12	aB	1	2144	1736	41	164	203	0
12	aB	1	2144	1736	41	164	203	0
12	aB	1	2144	1736	41	164	203	0
12	aB	1	2144	1736	41	164	203	0
12	aB	1	2144	1736	41	164	203	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	aF	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	aL	1	Total 143	C 113	Mg 3	N 12	O 15	0
12	aL	1	Total 143	C 113	Mg 3	N 12	O 15	0
12	aL	1	Total 143	C 113	Mg 3	N 12	O 15	0
12	bA	1	Total 2351	C 1921	Mg 43	N 172	O 215	0
12	bA	1	Total 2351	C 1921	Mg 43	N 172	O 215	0
12	bA	1	Total 2351	C 1921	Mg 43	N 172	O 215	0
12	bA	1	Total 2351	C 1921	Mg 43	N 172	O 215	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bA	1	2351	1921	43	172	215	0
12	bB	1	2144	1736	41	164	203	0
12	bB	1	2144	1736	41	164	203	0
12	bB	1	2144	1736	41	164	203	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bB	1	Total 2144	C 1736	Mg 41	N 164	O 203	0
12	bF	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	bL	1	Total 143	C 113	Mg 3	N 12	O 15	0
12	bL	1	Total 143	C 113	Mg 3	N 12	O 15	0
12	bL	1	Total 143	C 113	Mg 3	N 12	O 15	0

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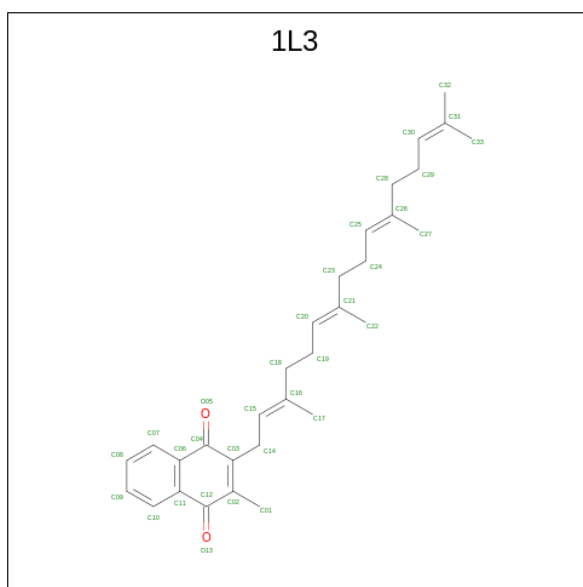
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cB	1	2099	1701	40	160	198	0
12	cF	1	45	35	1	4	5	0

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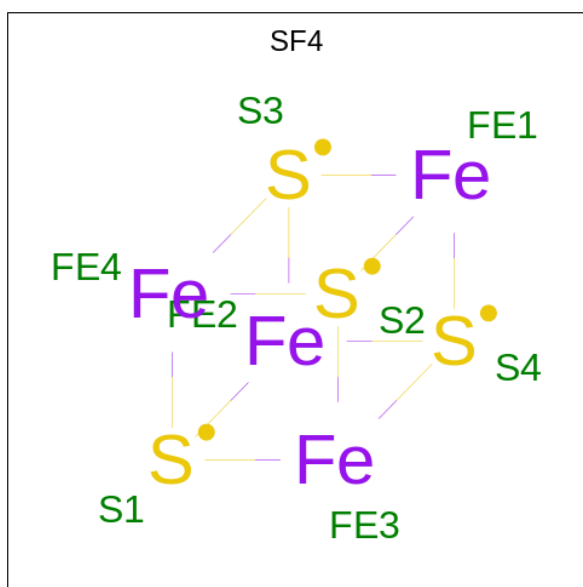
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
12	cL	1	Total 143	C 113	Mg 3	N 12	O 15	0
12	cL	1	Total 143	C 113	Mg 3	N 12	O 15	0
12	cL	1	Total 143	C 113	Mg 3	N 12	O 15	0

- Molecule 13 is Menaquinone-4 (three-letter code: 1L3) (formula:  $C_{31}H_{40}O_2$ ).



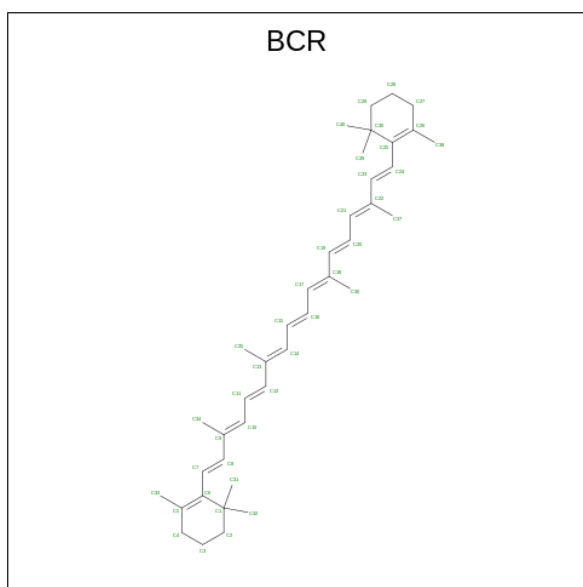
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	aA	1	Total 33	C 31	O 2	0
13	aB	1	Total 33	C 31	O 2	0
13	bA	1	Total 33	C 31	O 2	0
13	bB	1	Total 33	C 31	O 2	0
13	cA	1	Total 33	C 31	O 2	0
13	cB	1	Total 33	C 31	O 2	0

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
14	aA	1	8	4	4	0
14	aC	1	16	8	8	0
14	aC	1	16	8	8	0
14	bA	1	8	4	4	0
14	bC	1	16	8	8	0
14	bC	1	16	8	8	0
14	cA	1	8	4	4	0
14	cC	1	16	8	8	0
14	cC	1	16	8	8	0

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms	AltConf
15	aA	1	Total C 200 200	0
15	aA	1	Total C 200 200	0
15	aA	1	Total C 200 200	0
15	aA	1	Total C 200 200	0
15	aA	1	Total C 200 200	0
15	aB	1	Total C 240 240	0
15	aB	1	Total C 240 240	0
15	aB	1	Total C 240 240	0
15	aB	1	Total C 240 240	0
15	aB	1	Total C 240 240	0
15	aB	1	Total C 240 240	0
15	aB	1	Total C 240 240	0
15	aF	1	Total C 120 120	0
15	aF	1	Total C 120 120	0
15	aF	1	Total C 120 120	0

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Mol	Chain	Residues	Atoms	AltConf
15	aI	1	Total C 40 40	0
15	aJ	1	Total C 40 40	0
15	aL	1	Total C 120 120	0
15	aL	1	Total C 120 120	0
15	aL	1	Total C 120 120	0
15	aM	1	Total C 40 40	0
15	bA	1	Total C 200 200	0
15	bA	1	Total C 200 200	0
15	bA	1	Total C 200 200	0
15	bA	1	Total C 200 200	0
15	bA	1	Total C 200 200	0
15	bB	1	Total C 240 240	0
15	bB	1	Total C 240 240	0
15	bB	1	Total C 240 240	0
15	bB	1	Total C 240 240	0
15	bB	1	Total C 240 240	0
15	bB	1	Total C 240 240	0
15	bF	1	Total C 120 120	0
15	bF	1	Total C 120 120	0
15	bF	1	Total C 120 120	0
15	bI	1	Total C 40 40	0

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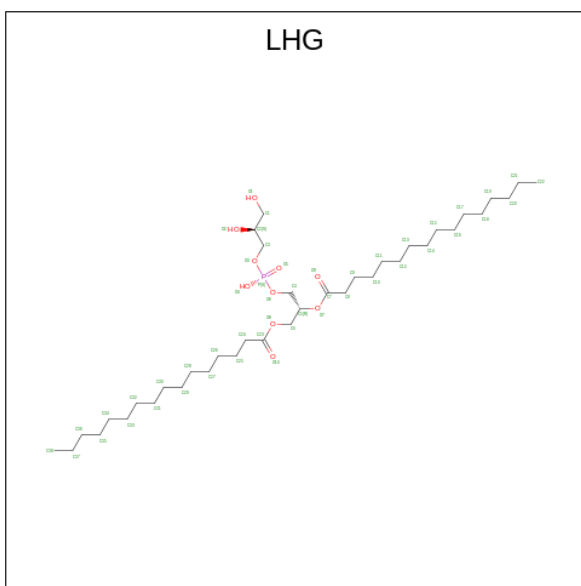
Mol	Chain	Residues	Atoms		AltConf
15	bJ	1	Total 40	C 40	0
15	bL	1	Total 120	C 120	0
15	bL	1	Total 120	C 120	0
15	bL	1	Total 120	C 120	0
15	bM	1	Total 40	C 40	0
15	cA	1	Total 200	C 200	0
15	cA	1	Total 200	C 200	0
15	cA	1	Total 200	C 200	0
15	cA	1	Total 200	C 200	0
15	cA	1	Total 200	C 200	0
15	cA	1	Total 200	C 200	0
15	cB	1	Total 240	C 240	0
15	cB	1	Total 240	C 240	0
15	cB	1	Total 240	C 240	0
15	cB	1	Total 240	C 240	0
15	cB	1	Total 240	C 240	0
15	cB	1	Total 240	C 240	0
15	cF	1	Total 120	C 120	0
15	cF	1	Total 120	C 120	0
15	cF	1	Total 120	C 120	0
15	cI	1	Total 40	C 40	0
15	cJ	1	Total 40	C 40	0

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Mol	Chain	Residues	Atoms		AltConf
15	cL	1	Total	C	0
			120	120	
15	cL	1	Total	C	0
			120	120	
15	cL	1	Total	C	0
			120	120	
15	cM	1	Total	C	0
			40	40	

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



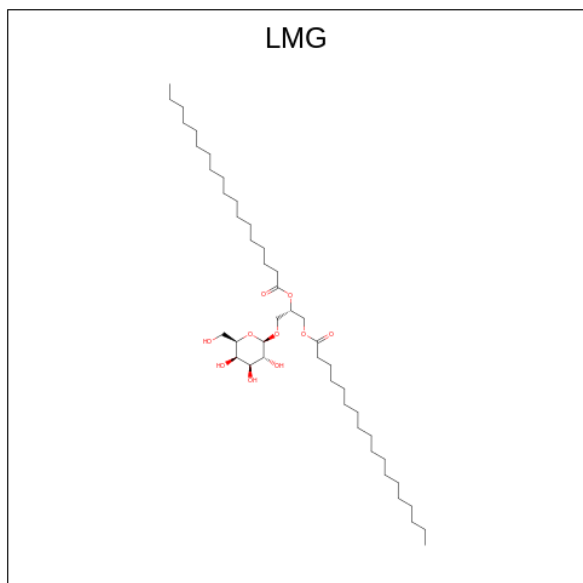
Mol	Chain	Residues	Atoms				AltConf
16	aA	1	Total	C	O	P	0
			76	54	20	2	
16	aA	1	Total	C	O	P	0
			76	54	20	2	
16	aB	1	Total	C	O	P	0
			23	12	10	1	
16	bA	1	Total	C	O	P	0
			76	54	20	2	
16	bA	1	Total	C	O	P	0
			76	54	20	2	
16	bB	1	Total	C	O	P	0
			23	12	10	1	
16	cA	1	Total	C	O	P	0
			76	54	20	2	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	cA	1	76	54	20	2	0
16	cB	1	23	12	10	1	0

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	aB	1	43	33	10	0
17	bB	1	43	33	10	0
17	cB	1	43	33	10	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
18	aA	45	45	45	0
18	aB	67	67	67	0
18	aC	14	14	14	0
18	aD	2	2	2	0

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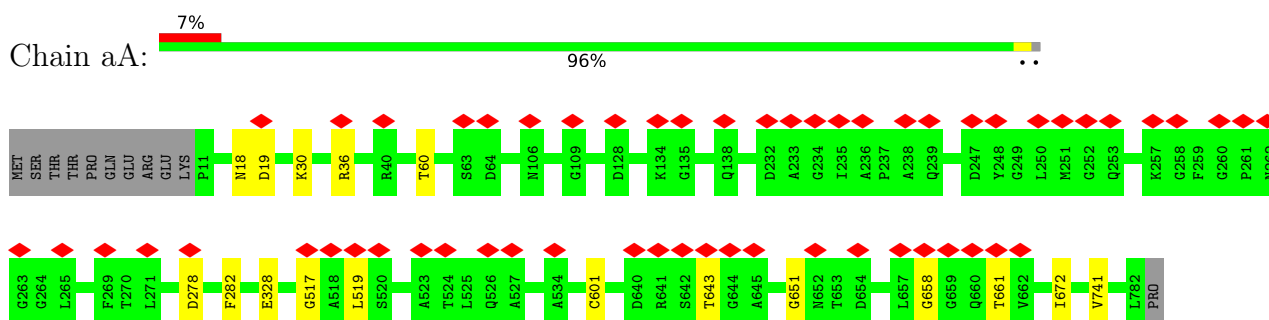
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Mol	Chain	Residues	Atoms		AltConf
18	aE	3	Total 3	O 3	0
18	aF	1	Total 1	O 1	0
18	aJ	1	Total 1	O 1	0
18	aL	1	Total 1	O 1	0
18	bA	45	Total 45	O 45	0
18	bB	67	Total 67	O 67	0
18	bC	14	Total 14	O 14	0
18	bD	2	Total 2	O 2	0
18	bE	3	Total 3	O 3	0
18	bF	1	Total 1	O 1	0
18	bJ	1	Total 1	O 1	0
18	bL	1	Total 1	O 1	0
18	cA	45	Total 45	O 45	0
18	cB	67	Total 67	O 67	0
18	cC	14	Total 14	O 14	0
18	cD	2	Total 2	O 2	0
18	cE	3	Total 3	O 3	0
18	cF	1	Total 1	O 1	0
18	cJ	1	Total 1	O 1	0
18	cL	1	Total 1	O 1	0

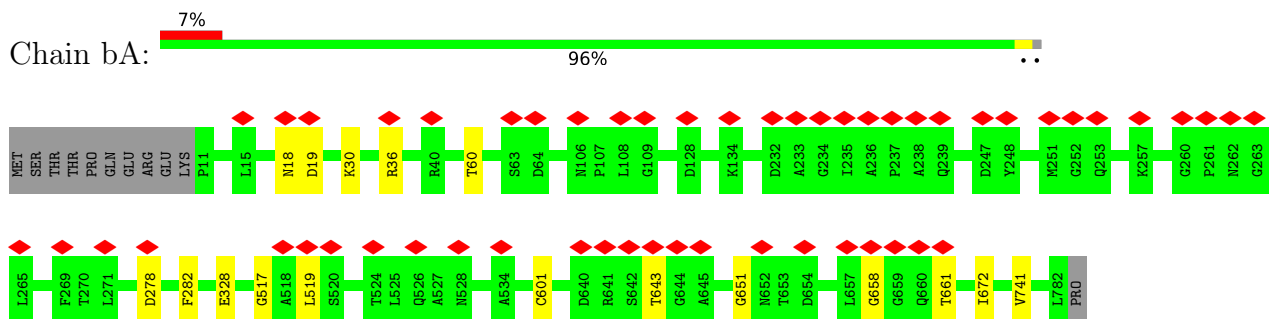
### 3 Residue-property plots

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

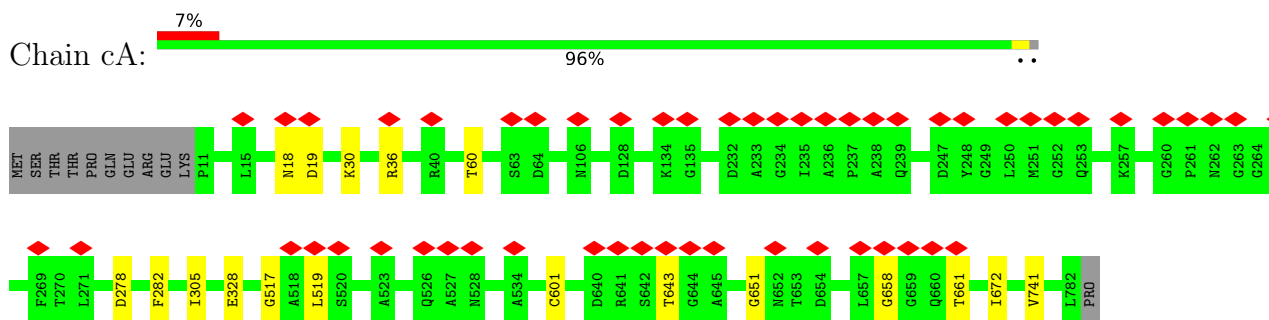
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



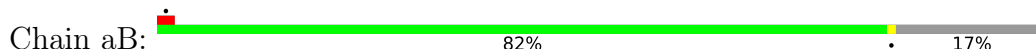
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

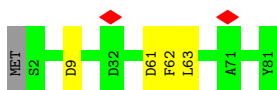


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



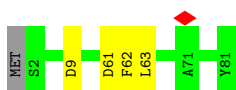


Chain bC:  94% 5%




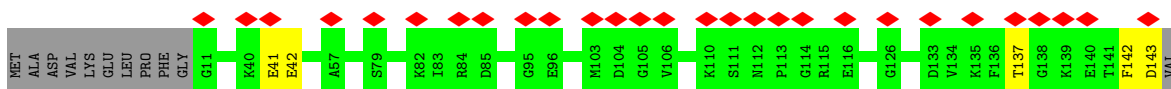
- Molecule 3: Photosystem I iron-sulfur center

Chain cC:  94% 5%

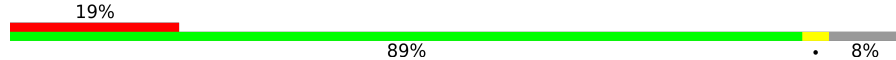


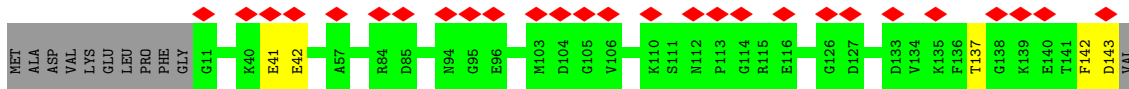
- Molecule 4: Photosystem I reaction center subunit II

Chain aD:  19% 89% 8%




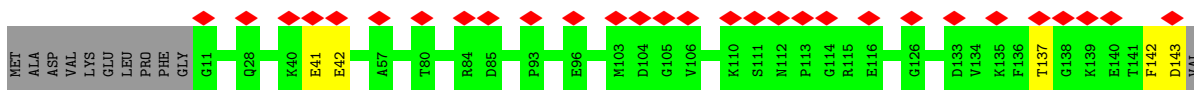
- Molecule 4: Photosystem I reaction center subunit II

Chain bD:  19% 89% 8%

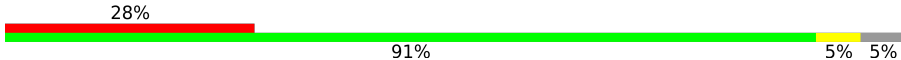


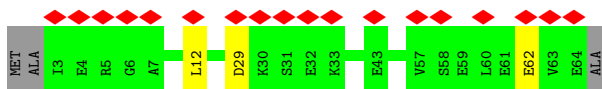
- Molecule 4: Photosystem I reaction center subunit II

Chain cD:  20% 89% 8%

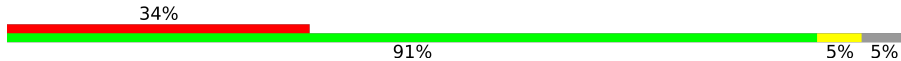


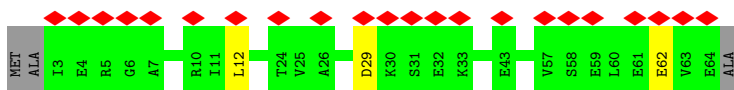
- Molecule 5: Photosystem I reaction center subunit IV

Chain aE:  28% 91% 5% 5%

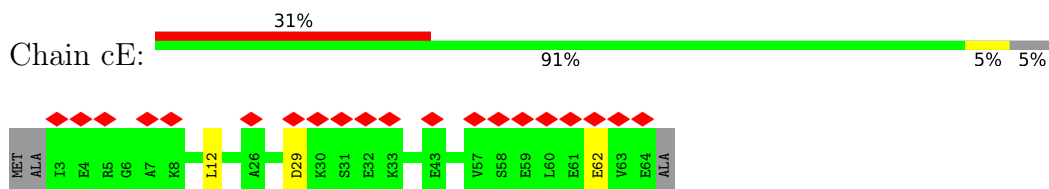


- Molecule 5: Photosystem I reaction center subunit IV

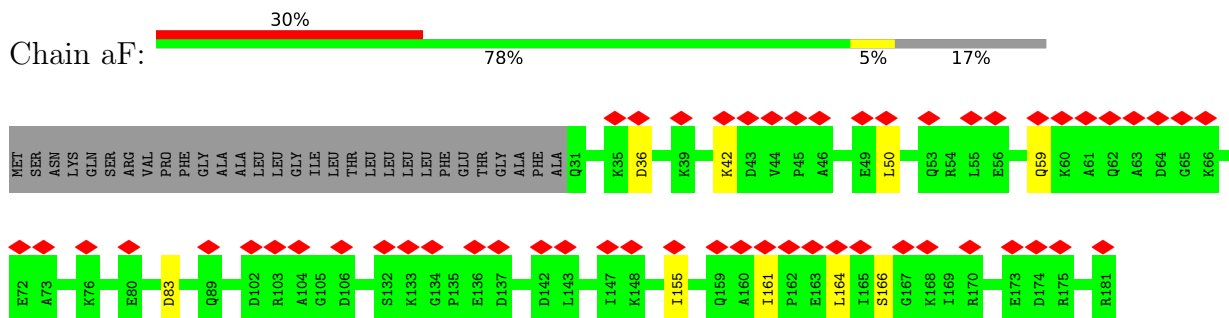
Chain bE:  34% 91% 5% 5%



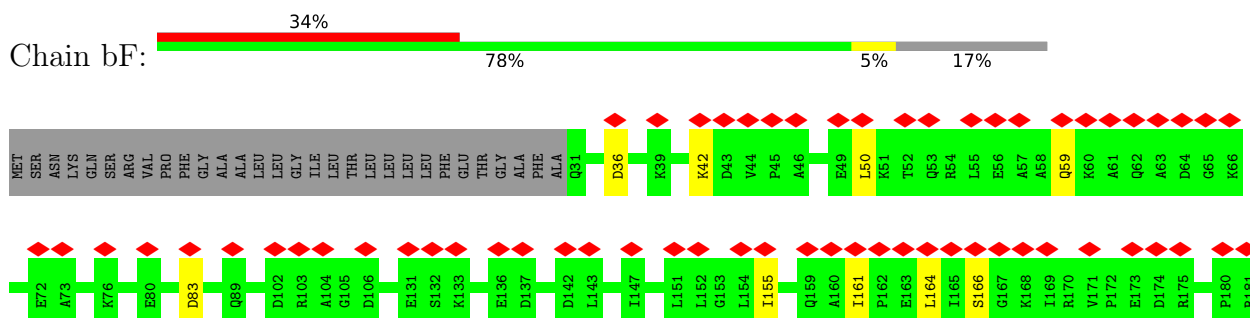
- Molecule 5: Photosystem I reaction center subunit IV



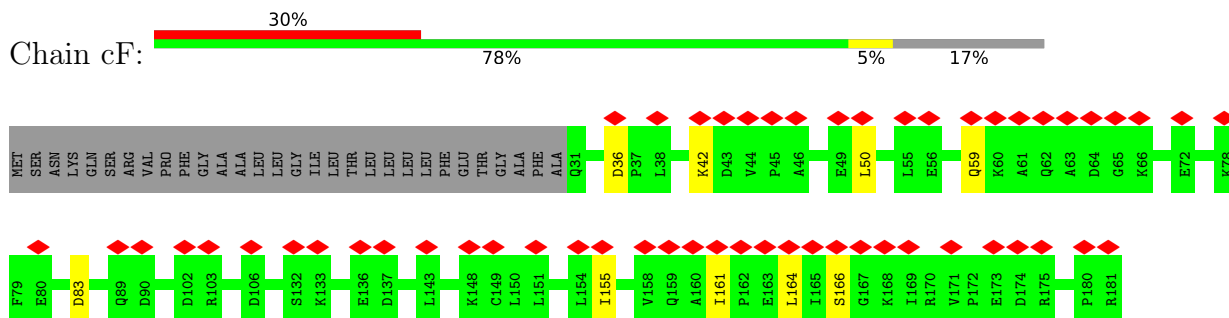
- Molecule 6: Photosystem I reaction center subunit III



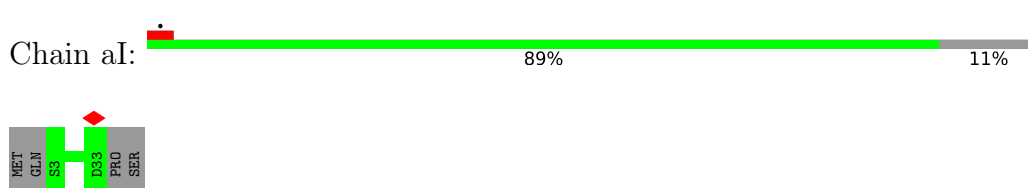
- Molecule 6: Photosystem I reaction center subunit III



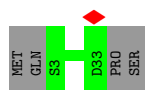
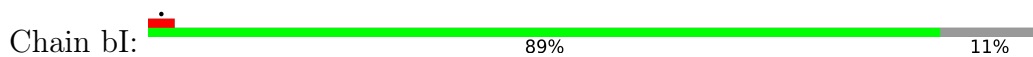
- Molecule 6: Photosystem I reaction center subunit III



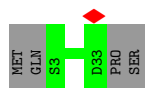
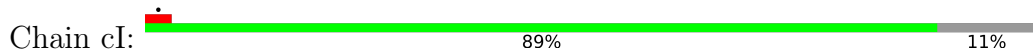
- Molecule 7: Photosystem I reaction center subunit Z



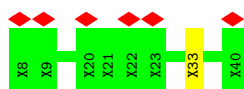
- Molecule 7: Photosystem I reaction center subunit Z



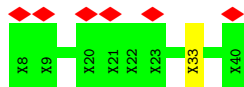
• Molecule 7: Photosystem I reaction center subunit Z



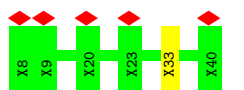
• Molecule 8: Unknown protein



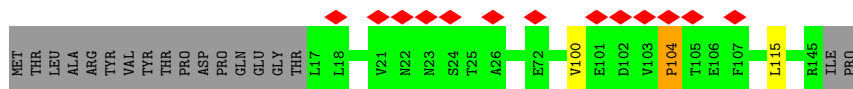
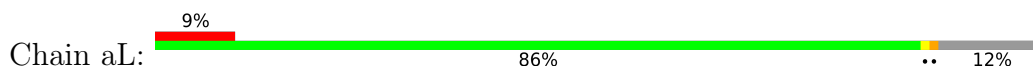
• Molecule 8: Unknown protein



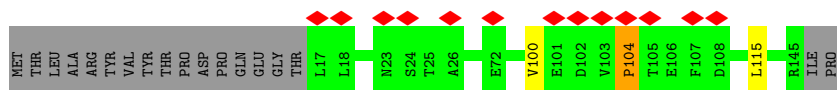
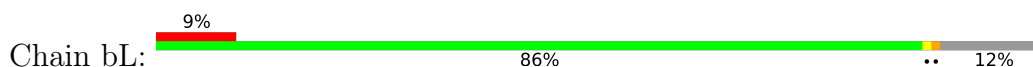
• Molecule 8: Unknown protein



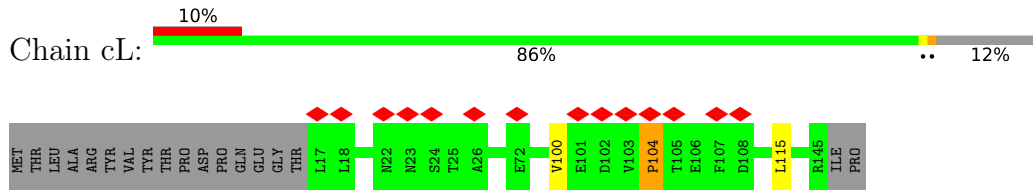
• Molecule 9: Photosystem I reaction center subunit XI



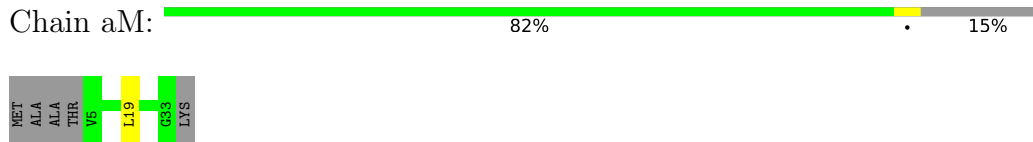
• Molecule 9: Photosystem I reaction center subunit XI



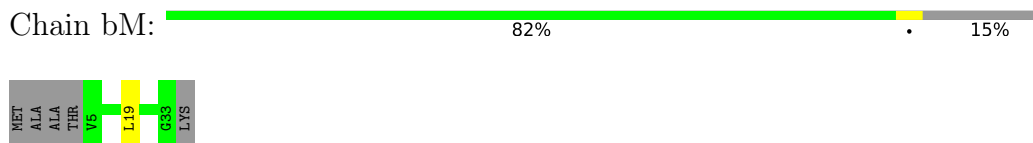
- Molecule 9: Photosystem I reaction center subunit XI



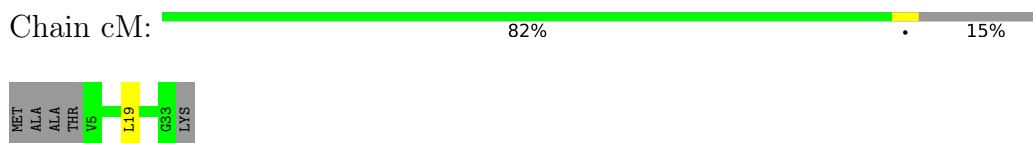
- Molecule 10: Photosystem I reaction center subunit XII



- Molecule 10: Photosystem I reaction center subunit XII



- Molecule 10: Photosystem I reaction center subunit XII



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	261743	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 ( $e^-/\text{\AA}^2$ )	70.22	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.465	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	329.2, 329.2, 329.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.823, 0.823, 0.823	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: SF4, CL0, LMG, CLA, 1L3, LHG, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	aA	0.35	0/6244	0.53	3/8520 (0.0%)
1	bA	0.35	0/6244	0.53	3/8520 (0.0%)
1	cA	0.35	0/6244	0.53	3/8520 (0.0%)
2	aB	0.36	0/5911	0.51	0/8084
2	bB	0.36	0/5911	0.51	0/8084
2	cB	0.36	0/5911	0.51	0/8084
3	aC	0.36	0/609	0.59	1/825 (0.1%)
3	bC	0.36	0/609	0.59	1/825 (0.1%)
3	cC	0.36	0/609	0.59	1/825 (0.1%)
4	aD	0.36	0/1061	0.51	0/1434
4	bD	0.36	0/1061	0.51	0/1434
4	cD	0.36	0/1061	0.51	0/1434
5	aE	0.37	0/515	0.56	0/694
5	bE	0.37	0/515	0.56	0/694
5	cE	0.37	0/515	0.56	0/694
6	aF	0.31	0/1208	0.54	0/1638
6	bF	0.31	0/1208	0.54	0/1638
6	cF	0.31	0/1208	0.54	0/1638
7	aI	0.32	0/245	0.58	0/336
7	bI	0.32	0/245	0.58	0/336
7	cI	0.32	0/245	0.58	0/336
9	aL	0.35	0/997	0.56	0/1357
9	bL	0.35	0/997	0.56	0/1357
9	cL	0.35	0/997	0.56	0/1357
10	aM	0.32	0/190	0.48	0/260
10	bM	0.32	0/190	0.48	0/260
10	cM	0.32	0/190	0.48	0/260
All	All	0.35	0/50940	0.53	12/69444 (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	aC	0	1
3	bC	0	1
3	cC	0	1
8	aJ	0	1
8	bJ	0	1
8	cJ	0	1
9	aL	0	1
9	bL	0	1
9	cL	0	1
All	All	0	9

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aA	517	GLY	C-N-CA	7.08	139.41	121.70
1	cA	517	GLY	C-N-CA	7.08	139.39	121.70
1	bA	517	GLY	C-N-CA	7.07	139.38	121.70
1	aA	658	GLY	N-CA-C	5.72	127.40	113.10
1	cA	658	GLY	N-CA-C	5.72	127.39	113.10

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	aC	61	ASP	Peptide
8	aJ	33	UNK	Peptide
9	aL	104	PRO	Peptide
3	bC	61	ASP	Peptide
8	bJ	33	UNK	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	6038	0	5897	0	0
1	bA	6038	0	5897	0	0
1	cA	6038	0	5897	0	0
2	aB	5701	0	5519	0	0
2	bB	5701	0	5519	0	0
2	cB	5701	0	5519	0	0
3	aC	599	0	579	0	0
3	bC	599	0	579	0	0
3	cC	599	0	579	0	0
4	aD	1038	0	1039	0	0
4	bD	1038	0	1039	0	0
4	cD	1038	0	1039	0	0
5	aE	507	0	504	0	0
5	bE	507	0	504	0	0
5	cE	507	0	504	0	0
6	aF	1182	0	1207	0	0
6	bF	1182	0	1207	0	0
6	cF	1182	0	1207	0	0
7	aI	240	0	255	0	0
7	bI	240	0	255	0	0
7	cI	240	0	255	0	0
8	aJ	164	0	35	0	0
8	bJ	164	0	35	0	0
8	cJ	164	0	35	0	0
9	aL	974	0	998	0	0
9	bL	974	0	998	0	0
9	cL	974	0	998	0	0
10	aM	190	0	215	0	0
10	bM	190	0	215	0	0
10	cM	190	0	215	0	0
11	aA	65	0	72	0	0
11	bA	65	0	72	0	0
11	cA	65	0	72	0	0
12	aA	2396	0	2199	0	0
12	aB	2144	0	1874	0	0
12	aF	45	0	33	0	0
12	aL	143	0	111	0	0
12	bA	2351	0	2166	0	0
12	bB	2144	0	1874	0	0
12	bF	45	0	33	0	0
12	bL	143	0	111	0	0
12	cA	2351	0	2166	0	0
12	cB	2099	0	1841	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	cF	45	0	33	0	0
12	cL	143	0	111	0	0
13	aA	33	0	0	0	0
13	aB	33	0	0	0	0
13	bA	33	0	0	0	0
13	bB	33	0	0	0	0
13	cA	33	0	0	0	0
13	cB	33	0	0	0	0
14	aA	8	0	0	0	0
14	aC	16	0	0	0	0
14	bA	8	0	0	0	0
14	bC	16	0	0	0	0
14	cA	8	0	0	0	0
14	cC	16	0	0	0	0
15	aA	200	0	280	0	0
15	aB	240	0	336	0	0
15	aF	120	0	168	0	0
15	aI	40	0	56	0	0
15	aJ	40	0	56	0	0
15	aL	120	0	168	0	0
15	aM	40	0	55	0	0
15	bA	200	0	280	0	0
15	bB	240	0	336	0	0
15	bF	120	0	168	0	0
15	bI	40	0	56	0	0
15	bJ	40	0	56	0	0
15	bL	120	0	168	0	0
15	bM	40	0	55	0	0
15	cA	200	0	280	0	0
15	cB	240	0	336	0	0
15	cF	120	0	168	0	0
15	cI	40	0	56	0	0
15	cJ	40	0	56	0	0
15	cL	120	0	168	0	0
15	cM	40	0	55	0	0
16	aA	76	0	98	0	0
16	aB	23	0	16	0	0
16	bA	76	0	98	0	0
16	bB	23	0	16	0	0
16	cA	76	0	98	0	0
16	cB	23	0	16	0	0
17	aB	43	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	bB	43	0	56	0	0
17	cB	43	0	56	0	0
18	aA	45	0	0	0	0
18	aB	67	0	0	0	0
18	aC	14	0	0	0	0
18	aD	2	0	0	0	0
18	aE	3	0	0	0	0
18	aF	1	0	0	0	0
18	aJ	1	0	0	0	0
18	aL	1	0	0	0	0
18	bA	45	0	0	0	0
18	bB	67	0	0	0	0
18	bC	14	0	0	0	0
18	bD	2	0	0	0	0
18	bE	3	0	0	0	0
18	bF	1	0	0	0	0
18	bJ	1	0	0	0	0
18	bL	1	0	0	0	0
18	cA	45	0	0	0	0
18	cB	67	0	0	0	0
18	cC	14	0	0	0	0
18	cD	2	0	0	0	0
18	cE	3	0	0	0	0
18	cF	1	0	0	0	0
18	cJ	1	0	0	0	0
18	cL	1	0	0	0	0
All	All	67641	0	65379	0	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.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	770/783 (98%)	742 (96%)	28 (4%)	0	100	100
1	bA	770/783 (98%)	742 (96%)	28 (4%)	0	100	100
1	cA	770/783 (98%)	742 (96%)	28 (4%)	0	100	100
2	aB	723/872 (83%)	708 (98%)	15 (2%)	0	100	100
2	bB	723/872 (83%)	708 (98%)	15 (2%)	0	100	100
2	cB	723/872 (83%)	708 (98%)	15 (2%)	0	100	100
3	aC	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	12	4
3	bC	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	12	4
3	cC	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	12	4
4	aD	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
4	bD	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
4	cD	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
5	aE	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
5	bE	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
5	cE	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
6	aF	149/181 (82%)	144 (97%)	5 (3%)	0	100	100
6	bF	149/181 (82%)	144 (97%)	5 (3%)	0	100	100
6	cF	149/181 (82%)	144 (97%)	5 (3%)	0	100	100
7	aI	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
7	bI	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
7	cI	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
9	aL	127/147 (86%)	122 (96%)	4 (3%)	1 (1%)	19	10
9	bL	127/147 (86%)	122 (96%)	4 (3%)	1 (1%)	19	10
9	cL	127/147 (86%)	122 (96%)	4 (3%)	1 (1%)	19	10
10	aM	27/34 (79%)	27 (100%)	0	0	100	100
10	bM	27/34 (79%)	27 (100%)	0	0	100	100
10	cM	27/34 (79%)	27 (100%)	0	0	100	100
All	All	6282/7026 (89%)	6087 (97%)	189 (3%)	6 (0%)	54	45

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	aL	104	PRO
9	bL	104	PRO
9	cL	104	PRO
3	aC	62	PHE
3	bC	62	PHE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	612/623 (98%)	598 (98%)	14 (2%)	50	44
1	bA	612/623 (98%)	598 (98%)	14 (2%)	50	44
1	cA	612/623 (98%)	597 (98%)	15 (2%)	47	40
2	aB	573/694 (83%)	566 (99%)	7 (1%)	71	70
2	bB	573/694 (83%)	566 (99%)	7 (1%)	71	70
2	cB	573/694 (83%)	566 (99%)	7 (1%)	71	70
3	aC	68/69 (99%)	67 (98%)	1 (2%)	65	62
3	bC	68/69 (99%)	67 (98%)	1 (2%)	65	62
3	cC	68/69 (99%)	67 (98%)	1 (2%)	65	62
4	aD	113/122 (93%)	108 (96%)	5 (4%)	28	21
4	bD	113/122 (93%)	108 (96%)	5 (4%)	28	21
4	cD	113/122 (93%)	108 (96%)	5 (4%)	28	21
5	aE	56/57 (98%)	53 (95%)	3 (5%)	22	13
5	bE	56/57 (98%)	53 (95%)	3 (5%)	22	13
5	cE	56/57 (98%)	53 (95%)	3 (5%)	22	13
6	aF	125/148 (84%)	116 (93%)	9 (7%)	14	7
6	bF	125/148 (84%)	116 (93%)	9 (7%)	14	7
6	cF	125/148 (84%)	116 (93%)	9 (7%)	14	7
7	aI	26/30 (87%)	26 (100%)	0	100	100
7	bI	26/30 (87%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	cI	26/30 (87%)	26 (100%)	0	100	100
9	aL	100/116 (86%)	98 (98%)	2 (2%)	55	50
9	bL	100/116 (86%)	98 (98%)	2 (2%)	55	50
9	cL	100/116 (86%)	98 (98%)	2 (2%)	55	50
10	aM	18/21 (86%)	17 (94%)	1 (6%)	21	12
10	bM	18/21 (86%)	17 (94%)	1 (6%)	21	12
10	cM	18/21 (86%)	17 (94%)	1 (6%)	21	12
All	All	5073/5640 (90%)	4946 (98%)	127 (2%)	50	40

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	bB	245	PHE
4	cD	142	PHE
5	bE	62	GLU
4	cD	137	THR
6	cF	59	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
2	bB	487	ASN
1	cA	195	GLN
4	cD	71	HIS
2	bB	655	GLN
4	bD	76	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

354 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CLA	bB	936	-	59,67,73	2.06	19 (32%)	68,105,113	2.88	29 (42%)
16	LHG	bA	852	12	26,26,48	0.94	1 (3%)	29,32,54	1.32	3 (10%)
12	CLA	aB	916	-	59,67,73	2.04	18 (30%)	68,105,113	2.91	29 (42%)
12	CLA	cB	914	-	45,53,73	2.36	17 (37%)	52,89,113	3.29	23 (44%)
16	LHG	aA	853	12	26,26,48	0.94	1 (3%)	29,32,54	1.32	3 (10%)
12	CLA	bA	831	-	50,58,73	2.21	17 (34%)	58,95,113	2.95	31 (53%)
12	CLA	cA	806	-	65,73,73	1.95	17 (26%)	76,113,113	2.76	25 (32%)
12	CLA	bA	808	-	51,59,73	2.26	17 (33%)	59,96,113	3.00	29 (49%)
12	CLA	bB	937	-	47,55,73	2.30	18 (38%)	54,91,113	3.17	25 (46%)
15	BCR	cB	944	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	7 (12%)
12	CLA	cL	202	9	53,61,73	2.21	19 (35%)	61,98,113	3.09	28 (45%)
12	CLA	aA	803	-	65,73,73	1.95	17 (26%)	76,113,113	2.72	31 (40%)
12	CLA	aA	839	-	45,53,73	2.30	17 (37%)	52,89,113	3.21	24 (46%)
12	CLA	aB	939	-	45,53,73	2.26	16 (35%)	52,89,113	3.30	23 (44%)
12	CLA	aB	928	-	50,58,73	2.28	18 (36%)	58,95,113	3.03	28 (48%)
12	CLA	cB	909	-	55,63,73	2.08	18 (32%)	64,101,113	2.78	28 (43%)
15	BCR	aA	849	-	41,41,41	1.10	3 (7%)	56,56,56	1.18	4 (7%)
12	CLA	aB	903	-	51,59,73	2.22	18 (35%)	59,96,113	3.03	29 (49%)
15	BCR	bF	201	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	6 (10%)
12	CLA	bB	925	-	55,63,73	2.08	16 (29%)	64,101,113	3.05	29 (45%)
12	CLA	bA	804	-	56,64,73	2.12	17 (30%)	65,102,113	2.91	27 (41%)
12	CLA	bA	838	-	65,73,73	1.91	17 (26%)	76,113,113	2.76	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CLA	aA	808	-	51,59,73	2.27	17 (33%)	59,96,113	2.99	29 (49%)
12	CLA	aA	805	-	53,61,73	2.19	17 (32%)	61,98,113	3.01	26 (42%)
12	CLA	aA	820	-	56,64,73	2.15	18 (32%)	65,102,113	2.89	28 (43%)
12	CLA	aB	919	-	47,55,73	2.27	15 (31%)	54,91,113	3.07	26 (48%)
12	CLA	cA	803	-	65,73,73	1.95	17 (26%)	76,113,113	2.73	31 (40%)
15	BCR	bJ	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	aB	929	-	45,53,73	2.36	17 (37%)	52,89,113	3.28	24 (46%)
12	CLA	aB	921	-	55,63,73	2.19	17 (30%)	64,101,113	2.96	26 (40%)
15	BCR	cA	849	-	41,41,41	1.18	2 (4%)	56,56,56	1.39	6 (10%)
12	CLA	aL	203	-	45,53,73	2.35	17 (37%)	52,89,113	3.22	23 (44%)
13	1L3	cA	844	-	34,34,34	2.31	9 (26%)	42,45,45	1.62	9 (21%)
12	CLA	bB	926	-	65,73,73	1.91	17 (26%)	76,113,113	2.64	30 (39%)
12	CLA	aA	840	-	65,73,73	1.98	17 (26%)	76,113,113	2.59	28 (36%)
12	CLA	aA	811	-	45,53,73	2.42	16 (35%)	52,89,113	3.14	25 (48%)
12	CLA	cA	818	-	54,62,73	2.14	17 (31%)	62,99,113	2.97	28 (45%)
12	CLA	cF	202	6	45,53,73	2.40	17 (37%)	52,89,113	3.17	26 (50%)
12	CLA	cL	204	18	45,53,73	2.40	19 (42%)	52,89,113	3.21	24 (46%)
12	CLA	aA	817	-	54,62,73	2.22	16 (29%)	62,99,113	3.04	26 (41%)
12	CLA	aB	915	-	52,60,73	2.22	16 (30%)	60,97,113	3.12	25 (41%)
12	CLA	cA	843	18	65,73,73	1.93	17 (26%)	76,113,113	2.80	30 (39%)
15	BCR	cA	846	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	7 (12%)
11	CL0	cA	801	-	65,73,73	1.91	18 (27%)	76,113,113	2.55	32 (42%)
12	CLA	bB	919	-	47,55,73	2.27	15 (31%)	54,91,113	3.07	26 (48%)
12	CLA	aA	837	-	51,59,73	2.24	17 (33%)	59,96,113	3.04	26 (44%)
12	CLA	cB	939	-	45,53,73	2.27	15 (33%)	52,89,113	3.28	23 (44%)
15	BCR	bF	204	-	41,41,41	1.04	2 (4%)	56,56,56	1.30	9 (16%)
12	CLA	bB	921	-	55,63,73	2.20	16 (29%)	64,101,113	2.97	26 (40%)
12	CLA	cB	937	-	47,55,73	2.30	17 (36%)	54,91,113	3.17	25 (46%)
12	CLA	cB	920	-	45,53,73	2.41	16 (35%)	52,89,113	3.31	23 (44%)
12	CLA	aA	825	18	65,73,73	1.94	17 (26%)	76,113,113	2.65	27 (35%)
15	BCR	aL	205	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	6 (10%)
12	CLA	cA	820	-	56,64,73	2.15	18 (32%)	65,102,113	2.87	28 (43%)
12	CLA	aB	923	18	54,62,73	2.07	17 (31%)	62,99,113	2.94	25 (40%)
12	CLA	cB	906	-	55,63,73	2.13	18 (32%)	64,101,113	2.86	28 (43%)
12	CLA	bB	927	-	65,73,73	1.99	17 (26%)	76,113,113	2.42	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	BCR	bA	846	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
15	BCR	cF	201	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	6 (10%)
12	CLA	aA	809	1	45,53,73	2.33	17 (37%)	52,89,113	3.22	27 (51%)
12	CLA	aB	902	-	61,69,73	1.97	16 (26%)	71,108,113	2.73	24 (33%)
12	CLA	bA	853	18	56,64,73	2.05	17 (30%)	65,102,113	2.98	27 (41%)
12	CLA	cA	804	-	56,64,73	2.12	18 (32%)	65,102,113	2.91	27 (41%)
15	BCR	cA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	8 (14%)
12	CLA	aB	927	-	65,73,73	1.99	17 (26%)	76,113,113	2.42	24 (31%)
15	BCR	aB	944	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	7 (12%)
15	BCR	cI	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	9 (16%)
12	CLA	bB	905	-	65,73,73	1.94	18 (27%)	76,113,113	2.67	26 (34%)
12	CLA	aA	830	-	65,73,73	1.95	17 (26%)	76,113,113	2.70	27 (35%)
12	CLA	aA	824	-	47,55,73	2.33	17 (36%)	54,91,113	2.99	27 (50%)
12	CLA	aB	949	16	41,49,73	2.51	16 (39%)	47,84,113	3.44	24 (51%)
12	CLA	cB	923	18	54,62,73	2.07	17 (31%)	62,99,113	2.95	25 (40%)
12	CLA	cA	827	-	46,54,73	2.31	18 (39%)	53,90,113	3.18	25 (47%)
12	CLA	aA	834	-	65,73,73	1.93	16 (24%)	76,113,113	2.76	27 (35%)
12	CLA	bA	806	-	65,73,73	1.95	17 (26%)	76,113,113	2.76	25 (32%)
13	1L3	bA	844	-	34,34,34	2.31	9 (26%)	42,45,45	1.61	9 (21%)
12	CLA	bB	920	-	45,53,73	2.41	16 (35%)	52,89,113	3.31	23 (44%)
12	CLA	bA	823	-	51,59,73	2.20	18 (35%)	59,96,113	3.08	27 (45%)
12	CLA	bB	918	18	46,54,73	2.33	17 (36%)	53,90,113	3.00	25 (47%)
12	CLA	aA	821	18	50,58,73	2.21	16 (32%)	58,95,113	2.92	26 (44%)
12	CLA	cB	924	18	46,54,73	2.35	17 (36%)	53,90,113	3.18	25 (47%)
12	CLA	aB	906	-	55,63,73	2.12	18 (32%)	64,101,113	2.86	28 (43%)
12	CLA	cB	927	-	65,73,73	2.00	17 (26%)	76,113,113	2.42	24 (31%)
12	CLA	bA	828	-	65,73,73	1.99	18 (27%)	76,113,113	2.70	28 (36%)
15	BCR	bA	848	-	41,41,41	1.10	3 (7%)	56,56,56	1.18	4 (7%)
12	CLA	bB	904	-	65,73,73	1.97	17 (26%)	76,113,113	2.77	30 (39%)
12	CLA	cB	919	-	47,55,73	2.27	14 (29%)	54,91,113	3.08	26 (48%)
15	BCR	bL	206	-	41,41,41	1.03	1 (2%)	56,56,56	1.19	5 (8%)
16	LHG	bA	851	-	48,48,48	0.65	1 (2%)	51,54,54	1.27	6 (11%)
12	CLA	bA	829	-	60,68,73	2.02	17 (28%)	70,107,113	2.66	28 (40%)
12	CLA	bA	839	-	45,53,73	2.31	17 (37%)	52,89,113	3.21	24 (46%)
12	CLA	aA	812	-	65,73,73	1.94	18 (27%)	76,113,113	2.72	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CLA	bB	908	2	48,56,73	2.25	18 (37%)	55,92,113	2.86	26 (47%)
12	CLA	cB	911	-	45,53,73	2.34	17 (37%)	52,89,113	3.10	26 (50%)
12	CLA	cA	834	-	65,73,73	1.93	16 (24%)	76,113,113	2.77	26 (34%)
15	BCR	aB	946	-	41,41,41	1.09	3 (7%)	56,56,56	1.23	6 (10%)
12	CLA	aB	931	-	65,73,73	1.91	17 (26%)	76,113,113	2.92	28 (36%)
12	CLA	cA	825	18	65,73,73	1.94	17 (26%)	76,113,113	2.65	27 (35%)
12	CLA	aA	819	-	60,68,73	2.03	16 (26%)	70,107,113	3.01	34 (48%)
12	CLA	aA	829	-	60,68,73	2.02	17 (28%)	70,107,113	2.66	28 (40%)
12	CLA	aB	911	-	45,53,73	2.34	17 (37%)	52,89,113	3.10	26 (50%)
12	CLA	bA	820	-	56,64,73	2.15	18 (32%)	65,102,113	2.89	28 (43%)
12	CLA	cA	811	-	45,53,73	2.42	16 (35%)	52,89,113	3.15	25 (48%)
15	BCR	aF	204	-	41,41,41	1.04	2 (4%)	56,56,56	1.29	9 (16%)
12	CLA	cB	913	-	56,64,73	2.11	18 (32%)	65,102,113	2.86	29 (44%)
12	CLA	bA	837	-	51,59,73	2.24	17 (33%)	59,96,113	3.04	27 (45%)
12	CLA	bA	827	-	46,54,73	2.31	17 (36%)	53,90,113	3.16	25 (47%)
12	CLA	bA	826	18	55,63,73	2.09	18 (32%)	64,101,113	2.98	26 (40%)
12	CLA	bA	836	1	45,53,73	2.41	17 (37%)	52,89,113	3.04	25 (48%)
12	CLA	bB	906	-	55,63,73	2.13	18 (32%)	64,101,113	2.86	28 (43%)
12	CLA	cB	910	-	45,53,73	2.39	15 (33%)	52,89,113	3.13	26 (50%)
12	CLA	bB	910	-	45,53,73	2.39	16 (35%)	52,89,113	3.14	26 (50%)
12	CLA	aB	918	18	46,54,73	2.35	17 (36%)	53,90,113	3.00	24 (45%)
12	CLA	cA	815	-	45,53,73	2.42	16 (35%)	52,89,113	3.09	24 (46%)
12	CLA	aA	806	-	65,73,73	1.95	17 (26%)	76,113,113	2.77	25 (32%)
12	CLA	bB	915	-	52,60,73	2.21	16 (30%)	60,97,113	3.12	25 (41%)
12	CLA	bB	911	-	45,53,73	2.34	17 (37%)	52,89,113	3.09	26 (50%)
15	BCR	aM	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.16	6 (10%)
12	CLA	bA	803	-	65,73,73	1.95	17 (26%)	76,113,113	2.73	31 (40%)
12	CLA	aA	832	-	55,63,73	2.17	18 (32%)	64,101,113	2.95	30 (46%)
12	CLA	aA	833	-	51,59,73	2.14	16 (31%)	59,96,113	2.96	29 (49%)
12	CLA	cA	816	-	45,53,73	2.40	18 (40%)	52,89,113	3.11	24 (46%)
15	BCR	bA	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	6 (10%)
14	SF4	cC	102	3	0,12,12	-	-	-	-	-
15	BCR	aA	848	-	41,41,41	1.13	2 (4%)	56,56,56	1.51	13 (23%)
12	CLA	bB	923	18	54,62,73	2.07	17 (31%)	62,99,113	2.94	25 (40%)
15	BCR	aA	851	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	BCR	aF	201	-	41,41,41	1.07	2 (4%)	56,56,56	1.23	7 (12%)
11	CL0	bA	801	-	65,73,73	1.92	18 (27%)	76,113,113	2.56	31 (40%)
12	CLA	bB	902	-	61,69,73	1.97	17 (27%)	71,108,113	2.72	24 (33%)
12	CLA	cB	932	-	45,53,73	2.34	16 (35%)	52,89,113	3.26	26 (50%)
12	CLA	bA	832	-	55,63,73	2.16	18 (32%)	64,101,113	2.94	30 (46%)
12	CLA	cA	822	-	49,57,73	2.33	17 (34%)	55,93,113	3.24	24 (43%)
15	BCR	cB	941	-	41,41,41	1.09	3 (7%)	56,56,56	1.27	5 (8%)
15	BCR	cL	206	-	41,41,41	1.03	2 (4%)	56,56,56	1.20	5 (8%)
12	CLA	cB	917	-	55,63,73	2.08	17 (30%)	64,101,113	2.91	28 (43%)
16	LHG	bB	948	12	22,22,48	1.06	1 (4%)	25,28,54	1.10	1 (4%)
15	BCR	bL	201	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	4 (7%)
12	CLA	cA	823	-	51,59,73	2.20	17 (33%)	59,96,113	3.07	27 (45%)
12	CLA	aB	933	18	45,53,73	2.27	17 (37%)	52,89,113	3.08	24 (46%)
12	CLA	cB	949	16	41,49,73	2.50	16 (39%)	47,84,113	3.44	24 (51%)
12	CLA	bA	819	-	60,68,73	2.02	16 (26%)	70,107,113	3.01	33 (47%)
12	CLA	cA	835	-	45,53,73	2.37	17 (37%)	52,89,113	3.00	25 (48%)
12	CLA	aB	910	-	45,53,73	2.38	16 (35%)	52,89,113	3.13	26 (50%)
12	CLA	aA	842	-	65,73,73	1.94	17 (26%)	76,113,113	2.72	27 (35%)
12	CLA	cA	853	18	56,64,73	2.05	17 (30%)	65,102,113	2.98	27 (41%)
12	CLA	cB	933	18	45,53,73	2.28	18 (40%)	52,89,113	3.08	24 (46%)
17	LMG	aB	947	-	43,43,55	0.95	1 (2%)	51,51,63	1.25	6 (11%)
15	BCR	aB	945	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	7 (12%)
16	LHG	aB	948	12	22,22,48	1.05	1 (4%)	25,28,54	1.10	1 (4%)
12	CLA	bB	950	16	45,53,73	2.41	18 (40%)	52,89,113	2.97	21 (40%)
12	CLA	cA	802	18	65,73,73	1.92	16 (24%)	76,113,113	2.76	26 (34%)
15	BCR	bB	942	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	3 (5%)
12	CLA	bA	830	-	65,73,73	1.95	16 (24%)	76,113,113	2.70	27 (35%)
12	CLA	aA	843	18	65,73,73	1.92	17 (26%)	76,113,113	2.80	30 (39%)
12	CLA	cL	203	-	45,53,73	2.35	18 (40%)	52,89,113	3.22	23 (44%)
11	CL0	aA	801	-	65,73,73	1.92	18 (27%)	76,113,113	2.56	32 (42%)
15	BCR	aL	201	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	4 (7%)
12	CLA	bB	930	-	49,57,73	2.31	17 (34%)	55,93,113	3.08	26 (47%)
12	CLA	aA	831	-	50,58,73	2.21	17 (34%)	58,95,113	2.95	31 (53%)
15	BCR	aJ	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	6 (10%)
15	BCR	bL	205	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CLA	aA	813	-	45,53,73	2.48	19 (42%)	52,89,113	3.04	23 (44%)
12	CLA	aB	926	-	65,73,73	1.92	17 (26%)	76,113,113	2.64	29 (38%)
12	CLA	cB	929	-	45,53,73	2.36	17 (37%)	52,89,113	3.28	25 (48%)
15	BCR	aF	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	bA	825	18	65,73,73	1.94	17 (26%)	76,113,113	2.65	27 (35%)
12	CLA	bA	814	-	45,53,73	2.36	17 (37%)	52,89,113	3.03	24 (46%)
15	BCR	cL	205	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	6 (10%)
12	CLA	bB	924	18	46,54,73	2.35	17 (36%)	53,90,113	3.17	25 (47%)
12	CLA	bA	805	-	53,61,73	2.19	18 (33%)	61,98,113	3.01	26 (42%)
15	BCR	cB	946	-	41,41,41	1.09	3 (7%)	56,56,56	1.23	6 (10%)
12	CLA	bA	810	1	45,53,73	2.40	17 (37%)	52,89,113	3.26	26 (50%)
12	CLA	cB	901	-	65,73,73	1.87	16 (24%)	76,113,113	2.72	28 (36%)
12	CLA	cB	903	-	51,59,73	2.22	18 (35%)	59,96,113	3.03	29 (49%)
15	BCR	aI	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.39	9 (16%)
12	CLA	aA	804	-	56,64,73	2.12	17 (30%)	65,102,113	2.91	27 (41%)
12	CLA	aA	827	-	46,54,73	2.31	16 (34%)	53,90,113	3.18	25 (47%)
12	CLA	cB	908	2	48,56,73	2.24	18 (37%)	55,92,113	2.86	26 (47%)
12	CLA	aL	204	18	45,53,73	2.40	19 (42%)	52,89,113	3.21	24 (46%)
15	BCR	aB	942	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	3 (5%)
12	CLA	bB	913	-	56,64,73	2.11	18 (32%)	65,102,113	2.86	28 (43%)
12	CLA	cA	813	-	45,53,73	2.49	19 (42%)	52,89,113	3.04	23 (44%)
15	BCR	bA	847	-	41,41,41	1.13	2 (4%)	56,56,56	1.51	13 (23%)
14	SF4	aC	101	3	0,12,12	-	-	-	-	-
14	SF4	cC	101	3	0,12,12	-	-	-	-	-
15	BCR	bB	944	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	7 (12%)
14	SF4	bC	101	3	0,12,12	-	-	-	-	-
15	BCR	cB	942	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	4 (7%)
12	CLA	aB	935	-	50,58,73	2.25	17 (34%)	58,95,113	3.13	28 (48%)
12	CLA	cB	915	-	52,60,73	2.21	16 (30%)	60,97,113	3.12	25 (41%)
12	CLA	bA	802	18	65,73,73	1.91	15 (23%)	76,113,113	2.76	26 (34%)
12	CLA	aA	836	1	45,53,73	2.40	17 (37%)	52,89,113	3.04	25 (48%)
12	CLA	bB	931	-	65,73,73	1.92	16 (24%)	76,113,113	2.91	28 (36%)
15	BCR	cL	201	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	4 (7%)
12	CLA	aB	922	-	45,53,73	2.38	17 (37%)	52,89,113	3.05	26 (50%)
15	BCR	bF	203	-	41,41,41	1.09	2 (4%)	56,56,56	1.32	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CLA	bA	815	-	45,53,73	2.43	17 (37%)	52,89,113	3.09	24 (46%)
12	CLA	aB	912	-	65,73,73	1.88	18 (27%)	76,113,113	2.58	26 (34%)
12	CLA	cB	902	-	61,69,73	1.97	16 (26%)	71,108,113	2.73	24 (33%)
12	CLA	cB	926	-	65,73,73	1.92	17 (26%)	76,113,113	2.64	30 (39%)
12	CLA	bA	841	18	51,59,73	2.22	18 (35%)	59,96,113	3.02	24 (40%)
12	CLA	cA	830	-	65,73,73	1.96	16 (24%)	76,113,113	2.70	27 (35%)
12	CLA	cB	904	-	65,73,73	1.97	17 (26%)	76,113,113	2.77	30 (39%)
12	CLA	bA	833	-	51,59,73	2.14	15 (29%)	59,96,113	2.96	29 (49%)
12	CLA	cB	918	18	46,54,73	2.34	17 (36%)	53,90,113	3.00	24 (45%)
12	CLA	bA	817	-	54,62,73	2.23	17 (31%)	62,99,113	3.04	26 (41%)
12	CLA	cA	833	-	51,59,73	2.14	16 (31%)	59,96,113	2.96	29 (49%)
12	CLA	aA	816	-	45,53,73	2.40	18 (40%)	52,89,113	3.11	24 (46%)
15	BCR	bB	943	-	41,41,41	1.07	2 (4%)	56,56,56	1.16	4 (7%)
17	LMG	bB	947	-	43,43,55	0.95	1 (2%)	51,51,63	1.25	6 (11%)
12	CLA	aA	822	-	49,57,73	2.33	17 (34%)	55,93,113	3.25	24 (43%)
15	BCR	cF	204	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	9 (16%)
12	CLA	bL	202	9	53,61,73	2.20	19 (35%)	61,98,113	3.08	28 (45%)
12	CLA	aB	938	18	51,59,73	2.21	17 (33%)	59,96,113	2.89	28 (47%)
12	CLA	cA	836	1	45,53,73	2.41	17 (37%)	52,89,113	3.05	25 (48%)
12	CLA	cB	905	-	65,73,73	1.93	18 (27%)	76,113,113	2.66	26 (34%)
15	BCR	aA	850	-	41,41,41	1.17	2 (4%)	56,56,56	1.39	6 (10%)
15	BCR	cA	847	-	41,41,41	1.13	2 (4%)	56,56,56	1.51	13 (23%)
12	CLA	bB	939	-	45,53,73	2.27	16 (35%)	52,89,113	3.29	23 (44%)
12	CLA	aB	909	-	55,63,73	2.08	18 (32%)	64,101,113	2.78	28 (43%)
12	CLA	cB	934	2	45,53,73	2.48	16 (35%)	52,89,113	3.04	22 (42%)
12	CLA	aA	823	-	51,59,73	2.19	17 (33%)	59,96,113	3.08	27 (45%)
12	CLA	bB	934	2	45,53,73	2.48	16 (35%)	52,89,113	3.04	22 (42%)
12	CLA	bB	949	16	41,49,73	2.51	17 (41%)	47,84,113	3.45	24 (51%)
12	CLA	aB	936	-	59,67,73	2.06	19 (32%)	68,105,113	2.87	29 (42%)
14	SF4	aC	102	3	0,12,12	-	-	-	-	-
12	CLA	bB	938	18	51,59,73	2.21	17 (33%)	59,96,113	2.89	28 (47%)
12	CLA	bB	916	-	59,67,73	2.04	17 (28%)	68,105,113	2.91	29 (42%)
12	CLA	cA	840	-	65,73,73	1.98	17 (26%)	76,113,113	2.59	26 (34%)
12	CLA	aA	826	18	55,63,73	2.09	18 (32%)	64,101,113	2.98	26 (40%)
12	CLA	aB	914	-	45,53,73	2.36	17 (37%)	52,89,113	3.28	23 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CLA	bB	932	-	45,53,73	2.34	16 (35%)	52,89,113	3.25	26 (50%)
12	CLA	cA	831	-	50,58,73	2.21	17 (34%)	58,95,113	2.94	31 (53%)
12	CLA	aB	907	-	52,60,73	2.14	16 (30%)	60,97,113	2.99	28 (46%)
15	BCR	aB	941	-	41,41,41	1.09	3 (7%)	56,56,56	1.28	5 (8%)
12	CLA	aA	807	-	65,73,73	1.96	16 (24%)	76,113,113	2.74	30 (39%)
12	CLA	aA	815	-	45,53,73	2.43	16 (35%)	52,89,113	3.09	24 (46%)
12	CLA	cA	826	18	55,63,73	2.09	18 (32%)	64,101,113	2.98	26 (40%)
12	CLA	cA	824	-	47,55,73	2.32	17 (36%)	54,91,113	3.00	27 (50%)
12	CLA	aA	814	-	45,53,73	2.36	17 (37%)	52,89,113	3.04	24 (46%)
12	CLA	cB	931	-	65,73,73	1.92	16 (24%)	76,113,113	2.91	28 (36%)
15	BCR	cB	945	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	7 (12%)
15	BCR	bB	945	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	7 (12%)
15	BCR	cA	848	-	41,41,41	1.10	3 (7%)	56,56,56	1.18	4 (7%)
12	CLA	bB	933	18	45,53,73	2.29	18 (40%)	52,89,113	3.10	24 (46%)
12	CLA	aA	818	-	54,62,73	2.14	17 (31%)	62,99,113	2.97	27 (43%)
12	CLA	bA	812	-	65,73,73	1.94	18 (27%)	76,113,113	2.71	30 (39%)
15	BCR	bB	941	-	41,41,41	1.10	3 (7%)	56,56,56	1.27	5 (8%)
12	CLA	bB	929	-	45,53,73	2.35	17 (37%)	52,89,113	3.28	24 (46%)
12	CLA	aB	932	-	45,53,73	2.35	16 (35%)	52,89,113	3.26	26 (50%)
16	LHG	aA	852	-	48,48,48	0.65	1 (2%)	51,54,54	1.27	6 (11%)
12	CLA	bA	818	-	54,62,73	2.14	17 (31%)	62,99,113	2.97	28 (45%)
15	BCR	bM	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	6 (10%)
15	BCR	cB	943	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	4 (7%)
17	LMG	cB	947	-	43,43,55	0.95	2 (4%)	51,51,63	1.25	6 (11%)
15	BCR	cJ	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.35	6 (10%)
14	SF4	aA	846	1,2	0,12,12	-	-	-	-	-
12	CLA	cB	938	18	51,59,73	2.20	17 (33%)	59,96,113	2.88	28 (47%)
12	CLA	cA	807	-	65,73,73	1.96	16 (24%)	76,113,113	2.75	30 (39%)
12	CLA	aA	838	-	65,73,73	1.91	17 (26%)	76,113,113	2.76	25 (32%)
12	CLA	aB	917	-	55,63,73	2.09	17 (30%)	64,101,113	2.90	28 (43%)
12	CLA	cA	805	-	53,61,73	2.19	17 (32%)	61,98,113	3.01	26 (42%)
15	BCR	bB	946	-	41,41,41	1.09	3 (7%)	56,56,56	1.23	6 (10%)
12	CLA	bA	822	-	49,57,73	2.33	17 (34%)	55,93,113	3.25	23 (41%)
12	CLA	aB	901	-	65,73,73	1.88	16 (24%)	76,113,113	2.71	28 (36%)
12	CLA	cA	842	-	65,73,73	1.94	18 (27%)	76,113,113	2.72	27 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	SF4	cA	845	1,2	0,12,12	-	-	-		
12	CLA	aB	924	18	46,54,73	2.35	17 (36%)	53,90,113	3.17	25 (47%)
12	CLA	bA	824	-	47,55,73	2.33	17 (36%)	54,91,113	3.00	26 (48%)
12	CLA	cB	928	-	50,58,73	2.28	18 (36%)	58,95,113	3.04	29 (50%)
16	LHG	cA	852	12	26,26,48	0.94	1 (3%)	29,32,54	1.32	3 (10%)
12	CLA	aA	828	-	65,73,73	1.99	18 (27%)	76,113,113	2.70	28 (36%)
16	LHG	cB	948	12	22,22,48	1.05	1 (4%)	25,28,54	1.10	1 (4%)
12	CLA	aB	937	-	47,55,73	2.29	18 (38%)	54,91,113	3.17	25 (46%)
12	CLA	bB	901	-	65,73,73	1.87	16 (24%)	76,113,113	2.71	28 (36%)
12	CLA	aB	950	16	45,53,73	2.40	18 (40%)	52,89,113	2.96	21 (40%)
12	CLA	cB	936	-	59,67,73	2.06	19 (32%)	68,105,113	2.88	29 (42%)
12	CLA	aA	841	18	51,59,73	2.22	18 (35%)	59,96,113	3.01	24 (40%)
12	CLA	bF	202	6	45,53,73	2.40	16 (35%)	52,89,113	3.17	26 (50%)
12	CLA	aB	930	-	49,57,73	2.31	17 (34%)	55,93,113	3.09	26 (47%)
13	1L3	cB	940	-	34,34,34	2.30	9 (26%)	42,45,45	1.44	7 (16%)
12	CLA	bA	835	-	45,53,73	2.37	17 (37%)	52,89,113	3.00	25 (48%)
13	1L3	bB	940	-	34,34,34	2.31	9 (26%)	42,45,45	1.43	7 (16%)
12	CLA	bB	914	-	45,53,73	2.36	17 (37%)	52,89,113	3.29	23 (44%)
12	CLA	cB	912	-	65,73,73	1.88	18 (27%)	76,113,113	2.59	26 (34%)
13	1L3	aB	940	-	34,34,34	2.31	9 (26%)	42,45,45	1.43	6 (14%)
12	CLA	cB	921	-	55,63,73	2.20	17 (30%)	64,101,113	2.96	26 (40%)
12	CLA	cB	930	-	49,57,73	2.31	17 (34%)	55,93,113	3.08	26 (47%)
12	CLA	cB	907	-	52,60,73	2.15	17 (32%)	60,97,113	3.00	28 (46%)
12	CLA	aF	202	6	45,53,73	2.40	16 (35%)	52,89,113	3.17	26 (50%)
12	CLA	bB	909	-	55,63,73	2.08	18 (32%)	64,101,113	2.78	28 (43%)
12	CLA	aB	904	-	65,73,73	1.98	17 (26%)	76,113,113	2.77	30 (39%)
12	CLA	cA	828	-	65,73,73	1.98	18 (27%)	76,113,113	2.70	28 (36%)
12	CLA	cA	814	-	45,53,73	2.35	17 (37%)	52,89,113	3.04	24 (46%)
12	CLA	cA	817	-	54,62,73	2.22	16 (29%)	62,99,113	3.05	26 (41%)
12	CLA	bL	204	18	45,53,73	2.41	19 (42%)	52,89,113	3.22	24 (46%)
12	CLA	bB	907	-	52,60,73	2.14	16 (30%)	60,97,113	2.99	28 (46%)
12	CLA	cA	837	-	51,59,73	2.23	17 (33%)	59,96,113	3.04	27 (45%)
12	CLA	cA	810	1	45,53,73	2.40	17 (37%)	52,89,113	3.26	26 (50%)
15	BCR	cF	203	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	aB	905	-	65,73,73	1.94	18 (27%)	76,113,113	2.67	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CLA	cA	841	18	51,59,73	2.22	18 (35%)	59,96,113	3.01	24 (40%)
12	CLA	bA	816	-	45,53,73	2.40	19 (42%)	52,89,113	3.11	24 (46%)
12	CLA	cA	821	18	50,58,73	2.21	15 (30%)	58,95,113	2.92	26 (44%)
12	CLA	cB	925	-	55,63,73	2.07	16 (29%)	64,101,113	3.04	29 (45%)
12	CLA	aA	835	-	45,53,73	2.36	17 (37%)	52,89,113	3.00	25 (48%)
15	BCR	cM	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	6 (10%)
12	CLA	bB	912	-	65,73,73	1.87	18 (27%)	76,113,113	2.59	26 (34%)
12	CLA	bA	813	-	45,53,73	2.49	19 (42%)	52,89,113	3.03	23 (44%)
12	CLA	aB	920	-	45,53,73	2.41	16 (35%)	52,89,113	3.31	23 (44%)
12	CLA	cA	809	1	45,53,73	2.34	17 (37%)	52,89,113	3.22	27 (51%)
15	BCR	bA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	8 (14%)
12	CLA	cB	935	-	50,58,73	2.25	17 (34%)	58,95,113	3.12	28 (48%)
14	SF4	bA	845	1,2	0,12,12	-	-	-	-	-
12	CLA	cB	916	-	59,67,73	2.03	17 (28%)	68,105,113	2.91	29 (42%)
12	CLA	bB	922	-	45,53,73	2.36	18 (40%)	52,89,113	3.05	26 (50%)
12	CLA	aB	934	2	45,53,73	2.49	16 (35%)	52,89,113	3.05	22 (42%)
12	CLA	aB	925	-	55,63,73	2.08	16 (29%)	64,101,113	3.05	29 (45%)
12	CLA	bB	935	-	50,58,73	2.25	17 (34%)	58,95,113	3.12	28 (48%)
12	CLA	bL	203	-	45,53,73	2.35	16 (35%)	52,89,113	3.21	23 (44%)
15	BCR	aB	943	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	4 (7%)
12	CLA	bB	917	-	55,63,73	2.09	17 (30%)	64,101,113	2.90	28 (43%)
12	CLA	cB	922	-	45,53,73	2.37	17 (37%)	52,89,113	3.04	27 (51%)
15	BCR	bI	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.38	9 (16%)
12	CLA	bB	903	-	51,59,73	2.22	18 (35%)	59,96,113	3.03	29 (49%)
12	CLA	aA	810	1	45,53,73	2.41	18 (40%)	52,89,113	3.26	26 (50%)
12	CLA	aA	802	18	65,73,73	1.91	16 (24%)	76,113,113	2.76	26 (34%)
15	BCR	aA	847	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
12	CLA	aB	908	2	48,56,73	2.25	18 (37%)	55,92,113	2.85	26 (47%)
12	CLA	bA	834	-	65,73,73	1.93	16 (24%)	76,113,113	2.76	28 (36%)
12	CLA	aB	913	-	56,64,73	2.11	18 (32%)	65,102,113	2.87	28 (43%)
12	CLA	aL	202	9	53,61,73	2.20	19 (35%)	61,98,113	3.08	28 (45%)
12	CLA	aA	844	16	45,53,73	2.40	18 (40%)	52,89,113	2.96	21 (40%)
12	CLA	bA	843	18	65,73,73	1.92	17 (26%)	76,113,113	2.80	30 (39%)
12	CLA	bA	807	-	65,73,73	1.96	16 (24%)	76,113,113	2.74	30 (39%)
12	CLA	cA	838	-	65,73,73	1.91	17 (26%)	76,113,113	2.76	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	BCR	aL	206	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	4 (7%)
12	CLA	cA	829	-	60,68,73	2.02	16 (26%)	70,107,113	2.66	29 (41%)
12	CLA	cA	812	-	65,73,73	1.94	17 (26%)	76,113,113	2.71	30 (39%)
12	CLA	bB	928	-	50,58,73	2.27	19 (38%)	58,95,113	3.03	29 (50%)
12	CLA	bA	821	18	50,58,73	2.20	15 (30%)	58,95,113	2.91	26 (44%)
12	CLA	cA	808	-	51,59,73	2.26	17 (33%)	59,96,113	3.00	29 (49%)
14	SF4	bC	102	3	0,12,12	-	-	-	-	-
12	CLA	cA	832	-	55,63,73	2.17	17 (30%)	64,101,113	2.95	30 (46%)
12	CLA	aA	854	18	56,64,73	2.05	17 (30%)	65,102,113	2.99	27 (41%)
12	CLA	cA	839	-	45,53,73	2.30	17 (37%)	52,89,113	3.21	24 (46%)
12	CLA	bA	809	1	45,53,73	2.34	17 (37%)	52,89,113	3.22	27 (51%)
12	CLA	cA	819	-	60,68,73	2.03	16 (26%)	70,107,113	3.01	34 (48%)
13	1L3	aA	845	-	34,34,34	2.31	9 (26%)	42,45,45	1.61	10 (23%)
12	CLA	bA	842	-	65,73,73	1.94	18 (27%)	76,113,113	2.71	27 (35%)
12	CLA	bA	840	-	65,73,73	1.99	17 (26%)	76,113,113	2.59	27 (35%)
16	LHG	cA	851	-	48,48,48	0.65	1 (2%)	51,54,54	1.27	6 (11%)
12	CLA	bA	811	-	45,53,73	2.43	16 (35%)	52,89,113	3.15	25 (48%)

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
12	CLA	bB	936	-	1/1/13/20	7/30/108/115	-
16	LHG	bA	852	12	-	11/31/31/53	-
12	CLA	aB	916	-	-	7/30/108/115	-
12	CLA	cB	914	-	1/1/11/20	6/13/91/115	-
16	LHG	aA	853	12	-	11/31/31/53	-
12	CLA	bA	831	-	-	4/19/97/115	-
12	CLA	cA	806	-	1/1/15/20	11/37/115/115	-
12	CLA	bA	808	-	1/1/12/20	7/21/99/115	-
12	CLA	bB	937	-	1/1/11/20	1/16/94/115	-
15	BCR	cB	944	-	-	16/29/63/63	0/2/2/2
12	CLA	cL	202	9	-	2/23/101/115	-
12	CLA	aA	803	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	aA	839	-	1/1/11/20	7/13/91/115	-
12	CLA	aB	939	-	1/1/11/20	3/13/91/115	-
12	CLA	aB	928	-	1/1/12/20	4/19/97/115	-
12	CLA	cB	909	-	1/1/13/20	9/25/103/115	-
15	BCR	aA	849	-	-	10/29/63/63	0/2/2/2
12	CLA	aB	903	-	1/1/12/20	5/21/99/115	-
15	BCR	bF	201	-	-	9/29/63/63	0/2/2/2
12	CLA	bB	925	-	1/1/13/20	5/25/103/115	-
12	CLA	bA	804	-	1/1/13/20	7/27/105/115	-
12	CLA	bA	838	-	1/1/15/20	8/37/115/115	-
12	CLA	aA	808	-	1/1/12/20	7/21/99/115	-
12	CLA	aA	805	-	1/1/12/20	6/23/101/115	-
12	CLA	aA	820	-	1/1/13/20	11/27/105/115	-
12	CLA	aB	919	-	1/1/11/20	5/16/94/115	-
12	CLA	cA	803	-	1/1/15/20	7/37/115/115	-
15	BCR	bJ	101	-	-	13/29/63/63	0/2/2/2
12	CLA	aB	929	-	-	5/13/91/115	-
12	CLA	aB	921	-	-	8/25/103/115	-
15	BCR	cA	849	-	-	10/29/63/63	0/2/2/2
12	CLA	aL	203	-	-	4/13/91/115	-
13	1L3	cA	844	-	-	3/23/43/43	0/2/2/2
12	CLA	bB	926	-	1/1/15/20	21/37/115/115	-
12	CLA	aA	840	-	1/1/15/20	9/37/115/115	-
12	CLA	aA	811	-	1/1/11/20	5/13/91/115	-
12	CLA	cA	818	-	1/1/12/20	12/24/102/115	-
12	CLA	cF	202	6	1/1/11/20	9/13/91/115	-
12	CLA	cL	204	18	-	0/13/91/115	-
12	CLA	cA	843	18	1/1/15/20	10/37/115/115	-
12	CLA	aA	817	-	-	7/24/102/115	-
12	CLA	aB	915	-	-	9/22/100/115	-
15	BCR	cA	846	-	-	11/29/63/63	0/2/2/2
11	CL0	cA	801	-	3/3/20/25	5/37/135/135	-
12	CLA	bB	919	-	1/1/11/20	5/16/94/115	-
12	CLA	aA	837	-	1/1/12/20	7/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	cB	939	-	1/1/11/20	3/13/91/115	-
15	BCR	bF	204	-	-	6/29/63/63	0/2/2/2
12	CLA	cB	937	-	1/1/11/20	0/16/94/115	-
12	CLA	bB	921	-	-	8/25/103/115	-
12	CLA	cB	920	-	-	3/13/91/115	-
12	CLA	aA	825	18	1/1/15/20	12/37/115/115	-
15	BCR	aL	205	-	-	10/29/63/63	0/2/2/2
12	CLA	cA	820	-	1/1/13/20	11/27/105/115	-
12	CLA	aB	923	18	1/1/12/20	10/24/102/115	-
12	CLA	cB	906	-	1/1/13/20	1/25/103/115	-
12	CLA	bB	927	-	1/1/15/20	12/37/115/115	-
15	BCR	bA	846	-	-	11/29/63/63	0/2/2/2
15	BCR	cF	201	-	-	9/29/63/63	0/2/2/2
12	CLA	aA	809	1	1/1/11/20	5/13/91/115	-
12	CLA	aB	902	-	1/1/14/20	7/33/111/115	-
12	CLA	bA	853	18	1/1/13/20	6/27/105/115	-
12	CLA	cA	804	-	1/1/13/20	7/27/105/115	-
15	BCR	cA	850	-	-	10/29/63/63	0/2/2/2
12	CLA	aB	927	-	1/1/15/20	12/37/115/115	-
15	BCR	aB	944	-	-	16/29/63/63	0/2/2/2
15	BCR	cI	101	-	-	10/29/63/63	0/2/2/2
12	CLA	bB	905	-	1/1/15/20	13/37/115/115	-
12	CLA	aA	830	-	1/1/15/20	11/37/115/115	-
12	CLA	aA	824	-	-	6/16/94/115	-
12	CLA	aB	949	16	1/1/10/20	3/8/86/115	-
12	CLA	cB	923	18	1/1/12/20	10/24/102/115	-
12	CLA	cA	827	-	1/1/11/20	6/15/93/115	-
12	CLA	aA	834	-	1/1/15/20	12/37/115/115	-
12	CLA	bA	806	-	1/1/15/20	11/37/115/115	-
13	1L3	bA	844	-	-	3/23/43/43	0/2/2/2
12	CLA	bB	920	-	-	3/13/91/115	-
12	CLA	bA	823	-	1/1/12/20	6/21/99/115	-
12	CLA	bB	918	18	1/1/11/20	1/15/93/115	-
12	CLA	aA	821	18	1/1/12/20	4/19/97/115	-
12	CLA	cB	924	18	1/1/11/20	2/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	aB	906	-	1/1/13/20	1/25/103/115	-
12	CLA	cB	927	-	1/1/15/20	12/37/115/115	-
12	CLA	bA	828	-	1/1/15/20	3/37/115/115	-
15	BCR	bA	848	-	-	10/29/63/63	0/2/2/2
12	CLA	bB	904	-	1/1/15/20	12/37/115/115	-
12	CLA	cB	919	-	1/1/11/20	5/16/94/115	-
15	BCR	bL	206	-	-	6/29/63/63	0/2/2/2
16	LHG	bA	851	-	-	23/53/53/53	-
12	CLA	bA	829	-	1/1/14/20	6/31/109/115	-
12	CLA	bA	839	-	1/1/11/20	7/13/91/115	-
12	CLA	aA	812	-	1/1/15/20	10/37/115/115	-
12	CLA	bB	908	2	1/1/11/20	8/17/95/115	-
12	CLA	cB	911	-	-	0/13/91/115	-
12	CLA	cA	834	-	1/1/15/20	12/37/115/115	-
15	BCR	aB	946	-	-	4/29/63/63	0/2/2/2
12	CLA	aB	931	-	1/1/15/20	12/37/115/115	-
12	CLA	cA	825	18	1/1/15/20	12/37/115/115	-
12	CLA	aA	819	-	1/1/14/20	4/31/109/115	-
12	CLA	aA	829	-	1/1/14/20	6/31/109/115	-
12	CLA	bA	820	-	1/1/13/20	11/27/105/115	-
12	CLA	aB	911	-	-	0/13/91/115	-
12	CLA	cA	811	-	1/1/11/20	5/13/91/115	-
15	BCR	aF	204	-	-	6/29/63/63	0/2/2/2
12	CLA	cB	913	-	1/1/13/20	6/27/105/115	-
12	CLA	bA	837	-	1/1/12/20	7/21/99/115	-
12	CLA	bA	827	-	1/1/11/20	6/15/93/115	-
12	CLA	bA	826	18	1/1/13/20	6/25/103/115	-
12	CLA	bA	836	1	1/1/11/20	3/13/91/115	-
12	CLA	bB	906	-	1/1/13/20	1/25/103/115	-
12	CLA	cB	910	-	1/1/11/20	2/13/91/115	-
12	CLA	bB	910	-	1/1/11/20	2/13/91/115	-
12	CLA	aB	918	18	1/1/11/20	1/15/93/115	-
12	CLA	cA	815	-	-	4/13/91/115	-
12	CLA	aA	806	-	1/1/15/20	11/37/115/115	-
12	CLA	bB	915	-	-	9/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	bB	911	-	-	0/13/91/115	-
15	BCR	aM	101	-	-	18/29/63/63	0/2/2/2
12	CLA	bA	803	-	1/1/15/20	7/37/115/115	-
12	CLA	aA	832	-	1/1/13/20	9/25/103/115	-
12	CLA	aA	833	-	1/1/12/20	3/21/99/115	-
12	CLA	cA	816	-	1/1/11/20	5/13/91/115	-
15	BCR	bA	849	-	-	11/29/63/63	0/2/2/2
14	SF4	cC	102	3	-	-	0/6/5/5
15	BCR	aA	848	-	-	7/29/63/63	0/2/2/2
12	CLA	bB	923	18	1/1/12/20	10/24/102/115	-
15	BCR	aA	851	-	-	10/29/63/63	0/2/2/2
15	BCR	aF	201	-	-	9/29/63/63	0/2/2/2
11	CL0	bA	801	-	3/3/20/25	5/37/135/135	-
12	CLA	bB	902	-	1/1/14/20	7/33/111/115	-
12	CLA	cB	932	-	-	2/13/91/115	-
12	CLA	bA	832	-	1/1/13/20	9/25/103/115	-
12	CLA	cA	822	-	-	8/18/96/115	-
15	BCR	cB	941	-	-	10/29/63/63	0/2/2/2
15	BCR	cL	206	-	-	6/29/63/63	0/2/2/2
12	CLA	cB	917	-	1/1/13/20	8/25/103/115	-
16	LHG	bB	948	12	-	8/26/26/53	-
15	BCR	bL	201	-	-	7/29/63/63	0/2/2/2
12	CLA	cA	823	-	1/1/12/20	6/21/99/115	-
12	CLA	aB	933	18	1/1/11/20	3/13/91/115	-
12	CLA	cB	949	16	1/1/10/20	3/8/86/115	-
12	CLA	bA	819	-	1/1/14/20	4/31/109/115	-
12	CLA	cA	835	-	1/1/11/20	0/13/91/115	-
12	CLA	aB	910	-	1/1/11/20	2/13/91/115	-
12	CLA	aA	842	-	1/1/15/20	14/37/115/115	-
12	CLA	cA	853	18	1/1/13/20	6/27/105/115	-
12	CLA	cB	933	18	1/1/11/20	3/13/91/115	-
17	LMG	aB	947	-	-	12/38/58/70	0/1/1/1
15	BCR	aB	945	-	-	9/29/63/63	0/2/2/2
16	LHG	aB	948	12	-	8/26/26/53	-
12	CLA	bB	950	16	-	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	cA	802	18	1/1/15/20	5/37/115/115	-
15	BCR	bB	942	-	-	9/29/63/63	0/2/2/2
12	CLA	bA	830	-	1/1/15/20	11/37/115/115	-
12	CLA	aA	843	18	1/1/15/20	10/37/115/115	-
12	CLA	cL	203	-	-	4/13/91/115	-
11	CL0	aA	801	-	3/3/20/25	5/37/135/135	-
15	BCR	aL	201	-	-	7/29/63/63	0/2/2/2
12	CLA	bB	930	-	1/1/11/20	4/18/96/115	-
12	CLA	aA	831	-	-	4/19/97/115	-
15	BCR	aJ	101	-	-	13/29/63/63	0/2/2/2
15	BCR	bL	205	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	813	-	1/1/11/20	3/13/91/115	-
12	CLA	aB	926	-	1/1/15/20	21/37/115/115	-
12	CLA	cB	929	-	-	5/13/91/115	-
15	BCR	aF	203	-	-	15/29/63/63	0/2/2/2
12	CLA	bA	825	18	1/1/15/20	12/37/115/115	-
12	CLA	bA	814	-	1/1/11/20	6/13/91/115	-
15	BCR	cL	205	-	-	10/29/63/63	0/2/2/2
12	CLA	bB	924	18	1/1/11/20	2/15/93/115	-
12	CLA	bA	805	-	1/1/12/20	6/23/101/115	-
15	BCR	cB	946	-	-	4/29/63/63	0/2/2/2
12	CLA	bA	810	1	1/1/11/20	5/13/91/115	-
12	CLA	cB	901	-	1/1/15/20	6/37/115/115	-
12	CLA	cB	903	-	1/1/12/20	5/21/99/115	-
15	BCR	aI	101	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	804	-	1/1/13/20	7/27/105/115	-
12	CLA	aA	827	-	1/1/11/20	6/15/93/115	-
12	CLA	cB	908	2	1/1/11/20	8/17/95/115	-
12	CLA	aL	204	18	-	0/13/91/115	-
15	BCR	aB	942	-	-	9/29/63/63	0/2/2/2
12	CLA	bB	913	-	1/1/13/20	6/27/105/115	-
12	CLA	cA	813	-	1/1/11/20	3/13/91/115	-
15	BCR	bA	847	-	-	7/29/63/63	0/2/2/2
14	SF4	aC	101	3	-	-	0/6/5/5
14	SF4	cC	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	bB	944	-	-	16/29/63/63	0/2/2/2
14	SF4	bC	101	3	-	-	0/6/5/5
15	BCR	cB	942	-	-	9/29/63/63	0/2/2/2
12	CLA	aB	935	-	1/1/12/20	7/19/97/115	-
12	CLA	cB	915	-	-	9/22/100/115	-
12	CLA	bA	802	18	1/1/15/20	5/37/115/115	-
12	CLA	aA	836	1	1/1/11/20	3/13/91/115	-
12	CLA	bB	931	-	1/1/15/20	12/37/115/115	-
15	BCR	cL	201	-	-	7/29/63/63	0/2/2/2
12	CLA	aB	922	-	1/1/11/20	7/13/91/115	-
15	BCR	bF	203	-	-	15/29/63/63	0/2/2/2
12	CLA	bA	815	-	-	4/13/91/115	-
12	CLA	aB	912	-	1/1/15/20	15/37/115/115	-
12	CLA	cB	902	-	1/1/14/20	7/33/111/115	-
12	CLA	cB	926	-	1/1/15/20	21/37/115/115	-
12	CLA	bA	841	18	1/1/12/20	5/21/99/115	-
12	CLA	cA	830	-	1/1/15/20	11/37/115/115	-
12	CLA	cB	904	-	1/1/15/20	12/37/115/115	-
12	CLA	bA	833	-	1/1/12/20	3/21/99/115	-
12	CLA	cB	918	18	1/1/11/20	1/15/93/115	-
12	CLA	bA	817	-	-	7/24/102/115	-
12	CLA	cA	833	-	1/1/12/20	3/21/99/115	-
12	CLA	aA	816	-	1/1/11/20	5/13/91/115	-
15	BCR	bB	943	-	-	9/29/63/63	0/2/2/2
17	LMG	bB	947	-	-	12/38/58/70	0/1/1/1
12	CLA	aA	822	-	-	8/18/96/115	-
15	BCR	cF	204	-	-	6/29/63/63	0/2/2/2
12	CLA	bL	202	9	-	2/23/101/115	-
12	CLA	aB	938	18	1/1/12/20	1/21/99/115	-
12	CLA	cA	836	1	1/1/11/20	3/13/91/115	-
12	CLA	cB	905	-	1/1/15/20	13/37/115/115	-
15	BCR	aA	850	-	-	10/29/63/63	0/2/2/2
15	BCR	cA	847	-	-	7/29/63/63	0/2/2/2
12	CLA	bB	939	-	1/1/11/20	3/13/91/115	-
12	CLA	aB	909	-	1/1/13/20	9/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	cB	934	2	1/1/11/20	4/13/91/115	-
12	CLA	aA	823	-	1/1/12/20	6/21/99/115	-
12	CLA	bB	934	2	1/1/11/20	3/13/91/115	-
12	CLA	bB	949	16	1/1/10/20	3/8/86/115	-
12	CLA	aB	936	-	1/1/13/20	7/30/108/115	-
14	SF4	aC	102	3	-	-	0/6/5/5
12	CLA	bB	938	18	1/1/12/20	1/21/99/115	-
12	CLA	bB	916	-	-	7/30/108/115	-
12	CLA	cA	840	-	1/1/15/20	9/37/115/115	-
12	CLA	aA	826	18	1/1/13/20	6/25/103/115	-
12	CLA	aB	914	-	1/1/11/20	6/13/91/115	-
12	CLA	bB	932	-	-	2/13/91/115	-
12	CLA	cA	831	-	-	4/19/97/115	-
12	CLA	aB	907	-	1/1/12/20	5/22/100/115	-
15	BCR	aB	941	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	807	-	1/1/15/20	13/37/115/115	-
12	CLA	aA	815	-	-	4/13/91/115	-
12	CLA	cA	826	18	1/1/13/20	6/25/103/115	-
12	CLA	cA	824	-	-	6/16/94/115	-
12	CLA	aA	814	-	1/1/11/20	6/13/91/115	-
12	CLA	cB	931	-	1/1/15/20	12/37/115/115	-
15	BCR	cB	945	-	-	9/29/63/63	0/2/2/2
15	BCR	bB	945	-	-	10/29/63/63	0/2/2/2
15	BCR	cA	848	-	-	10/29/63/63	0/2/2/2
12	CLA	bB	933	18	1/1/11/20	3/13/91/115	-
12	CLA	aA	818	-	1/1/12/20	12/24/102/115	-
12	CLA	bA	812	-	1/1/15/20	10/37/115/115	-
15	BCR	bB	941	-	-	10/29/63/63	0/2/2/2
12	CLA	bB	929	-	-	5/13/91/115	-
12	CLA	aB	932	-	-	2/13/91/115	-
16	LHG	aA	852	-	-	22/53/53/53	-
12	CLA	bA	818	-	1/1/12/20	12/24/102/115	-
15	BCR	bM	101	-	-	18/29/63/63	0/2/2/2
15	BCR	cB	943	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LMG	cB	947	-	-	12/38/58/70	0/1/1/1
15	BCR	cJ	101	-	-	13/29/63/63	0/2/2/2
14	SF4	aA	846	1,2	-	-	0/6/5/5
12	CLA	cB	938	18	1/1/12/20	1/21/99/115	-
12	CLA	cA	807	-	1/1/15/20	13/37/115/115	-
12	CLA	aA	838	-	1/1/15/20	8/37/115/115	-
15	BCR	bB	946	-	-	4/29/63/63	0/2/2/2
12	CLA	aB	917	-	1/1/13/20	8/25/103/115	-
12	CLA	cA	805	-	1/1/12/20	6/23/101/115	-
12	CLA	bA	822	-	-	8/18/96/115	-
12	CLA	aB	901	-	1/1/15/20	6/37/115/115	-
12	CLA	cA	842	-	1/1/15/20	14/37/115/115	-
14	SF4	cA	845	1,2	-	-	0/6/5/5
12	CLA	aB	924	18	1/1/11/20	2/15/93/115	-
12	CLA	bA	824	-	-	6/16/94/115	-
12	CLA	cB	928	-	1/1/12/20	4/19/97/115	-
16	LHG	cA	852	12	-	11/31/31/53	-
12	CLA	aA	828	-	1/1/15/20	3/37/115/115	-
16	LHG	cB	948	12	-	8/26/26/53	-
12	CLA	aB	937	-	1/1/11/20	1/16/94/115	-
12	CLA	bB	901	-	1/1/15/20	6/37/115/115	-
12	CLA	cB	936	-	1/1/13/20	7/30/108/115	-
12	CLA	aB	950	16	-	7/13/91/115	-
12	CLA	aA	841	18	1/1/12/20	5/21/99/115	-
12	CLA	bF	202	6	1/1/11/20	9/13/91/115	-
12	CLA	aB	930	-	1/1/11/20	4/18/96/115	-
13	1L3	cB	940	-	-	1/23/43/43	0/2/2/2
12	CLA	bA	835	-	1/1/11/20	0/13/91/115	-
13	1L3	bB	940	-	-	1/23/43/43	0/2/2/2
12	CLA	bB	914	-	1/1/11/20	6/13/91/115	-
12	CLA	cB	912	-	1/1/15/20	15/37/115/115	-
13	1L3	aB	940	-	-	1/23/43/43	0/2/2/2
12	CLA	cB	921	-	-	8/25/103/115	-
12	CLA	cB	930	-	1/1/11/20	4/18/96/115	-
12	CLA	cB	907	-	1/1/12/20	5/22/100/115	-
12	CLA	aF	202	6	1/1/11/20	9/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	bB	909	-	1/1/13/20	9/25/103/115	-
12	CLA	aB	904	-	1/1/15/20	12/37/115/115	-
12	CLA	cA	828	-	1/1/15/20	3/37/115/115	-
12	CLA	cA	814	-	1/1/11/20	6/13/91/115	-
12	CLA	cA	817	-	-	7/24/102/115	-
12	CLA	bL	204	18	-	0/13/91/115	-
12	CLA	bB	907	-	1/1/12/20	6/22/100/115	-
12	CLA	cA	837	-	1/1/12/20	7/21/99/115	-
12	CLA	cA	810	1	1/1/11/20	5/13/91/115	-
15	BCR	cF	203	-	-	15/29/63/63	0/2/2/2
12	CLA	aB	905	-	1/1/15/20	13/37/115/115	-
12	CLA	cA	841	18	1/1/12/20	5/21/99/115	-
12	CLA	bA	816	-	1/1/11/20	6/13/91/115	-
12	CLA	cA	821	18	1/1/12/20	4/19/97/115	-
12	CLA	cB	925	-	1/1/13/20	5/25/103/115	-
12	CLA	aA	835	-	1/1/11/20	0/13/91/115	-
15	BCR	cM	101	-	-	18/29/63/63	0/2/2/2
12	CLA	bB	912	-	1/1/15/20	15/37/115/115	-
12	CLA	bA	813	-	1/1/11/20	3/13/91/115	-
12	CLA	aB	920	-	-	3/13/91/115	-
12	CLA	cA	809	1	1/1/11/20	5/13/91/115	-
15	BCR	bA	850	-	-	9/29/63/63	0/2/2/2
12	CLA	cB	935	-	1/1/12/20	7/19/97/115	-
14	SF4	bA	845	1,2	-	-	0/6/5/5
12	CLA	cB	916	-	-	7/30/108/115	-
12	CLA	bB	922	-	1/1/11/20	7/13/91/115	-
12	CLA	aB	934	2	1/1/11/20	4/13/91/115	-
12	CLA	aB	925	-	1/1/13/20	5/25/103/115	-
12	CLA	bB	935	-	1/1/12/20	7/19/97/115	-
12	CLA	bL	203	-	-	4/13/91/115	-
15	BCR	aB	943	-	-	9/29/63/63	0/2/2/2
12	CLA	bB	917	-	1/1/13/20	8/25/103/115	-
12	CLA	cB	922	-	1/1/11/20	7/13/91/115	-
15	BCR	bI	101	-	-	10/29/63/63	0/2/2/2
12	CLA	bB	903	-	1/1/12/20	5/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	aA	810	1	1/1/11/20	5/13/91/115	-
12	CLA	aA	802	18	1/1/15/20	5/37/115/115	-
15	BCR	aA	847	-	-	11/29/63/63	0/2/2/2
12	CLA	aB	908	2	1/1/11/20	8/17/95/115	-
12	CLA	bA	834	-	1/1/15/20	12/37/115/115	-
12	CLA	aB	913	-	1/1/13/20	6/27/105/115	-
12	CLA	aL	202	9	-	2/23/101/115	-
12	CLA	aA	844	16	-	6/13/91/115	-
12	CLA	bA	843	18	1/1/15/20	10/37/115/115	-
12	CLA	bA	807	-	1/1/15/20	13/37/115/115	-
12	CLA	cA	838	-	1/1/15/20	8/37/115/115	-
15	BCR	aL	206	-	-	6/29/63/63	0/2/2/2
12	CLA	cA	829	-	1/1/14/20	6/31/109/115	-
12	CLA	cA	812	-	1/1/15/20	10/37/115/115	-
12	CLA	bB	928	-	1/1/12/20	4/19/97/115	-
12	CLA	bA	821	18	1/1/12/20	4/19/97/115	-
12	CLA	cA	808	-	1/1/12/20	7/21/99/115	-
14	SF4	bC	102	3	-	-	0/6/5/5
12	CLA	cA	832	-	1/1/13/20	9/25/103/115	-
12	CLA	aA	854	18	1/1/13/20	6/27/105/115	-
12	CLA	cA	839	-	1/1/11/20	7/13/91/115	-
12	CLA	bA	809	1	1/1/11/20	5/13/91/115	-
12	CLA	cA	819	-	1/1/14/20	4/31/109/115	-
13	1L3	aA	845	-	-	3/23/43/43	0/2/2/2
12	CLA	bA	842	-	1/1/15/20	14/37/115/115	-
12	CLA	bA	840	-	1/1/15/20	9/37/115/115	-
16	LHG	cA	851	-	-	22/53/53/53	-
12	CLA	bA	811	-	1/1/11/20	5/13/91/115	-

The worst 5 of 4748 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bB	940	1L3	C03-C02	7.88	1.49	1.35
13	aB	940	1L3	C03-C02	7.85	1.49	1.35
13	cB	940	1L3	C03-C02	7.83	1.49	1.35
13	bA	844	1L3	C03-C02	7.76	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	cA	844	1L3	C03-C02	7.74	1.49	1.35

The worst 5 of 7566 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	aB	931	CLA	C1D-ND-C4D	-10.64	98.77	106.33
12	cB	931	CLA	C1D-ND-C4D	-10.60	98.81	106.33
12	bB	931	CLA	C1D-ND-C4D	-10.58	98.82	106.33
12	aB	931	CLA	C2D-C1D-ND	10.15	117.58	110.10
12	cB	931	CLA	C2D-C1D-ND	10.10	117.55	110.10

5 of 225 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	aA	801	CL0	ND
11	aA	801	CL0	NC
11	aA	801	CL0	NA
11	bA	801	CL0	ND
11	bA	801	CL0	NC

5 of 2490 torsion outliers are listed below:

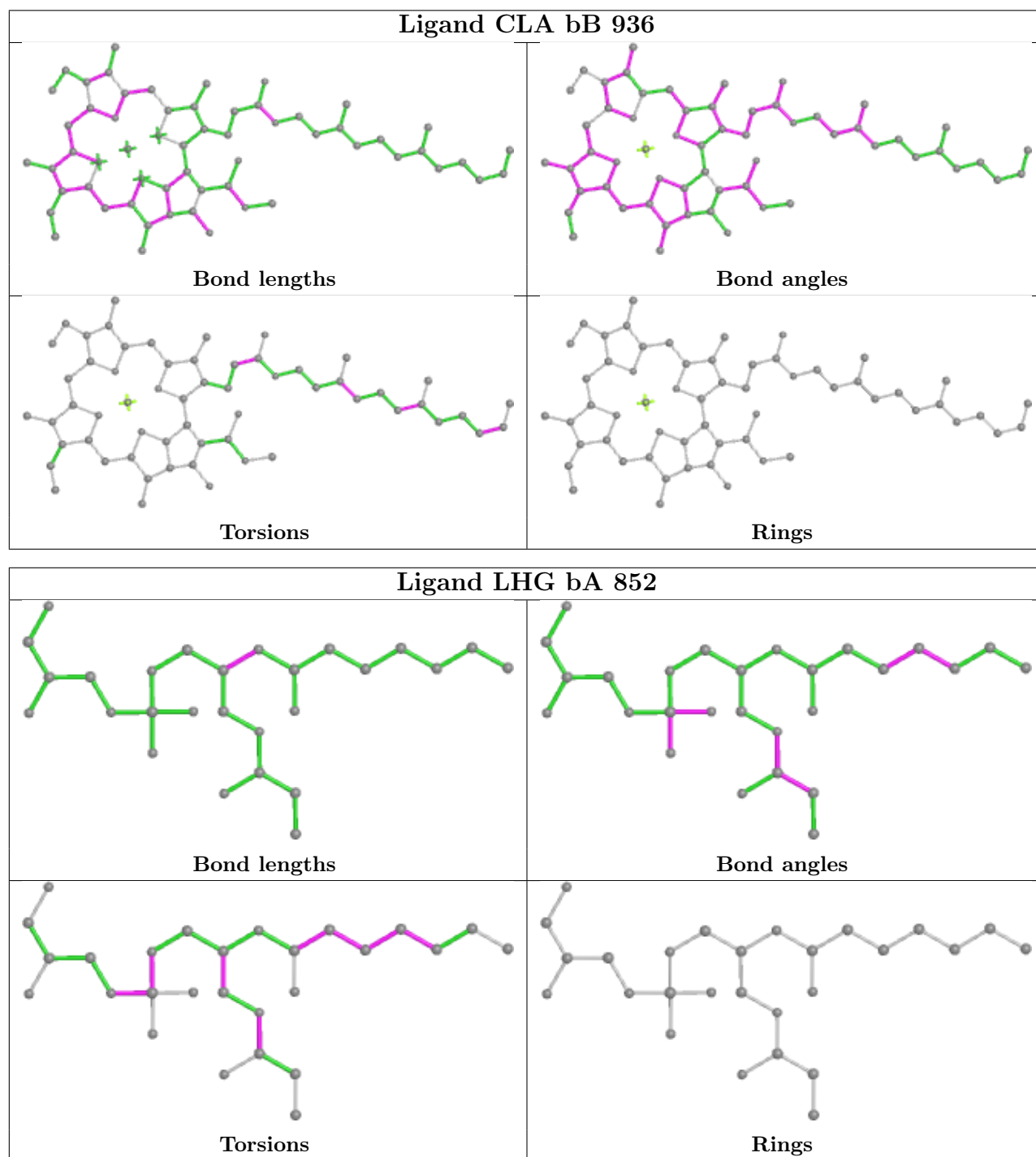
Mol	Chain	Res	Type	Atoms
12	aA	804	CLA	C1A-C2A-CAA-CBA
12	aA	804	CLA	C3A-C2A-CAA-CBA
12	aA	807	CLA	C1A-C2A-CAA-CBA
12	aA	808	CLA	C2A-CAA-CBA-CGA
12	aA	808	CLA	C2-C3-C5-C6

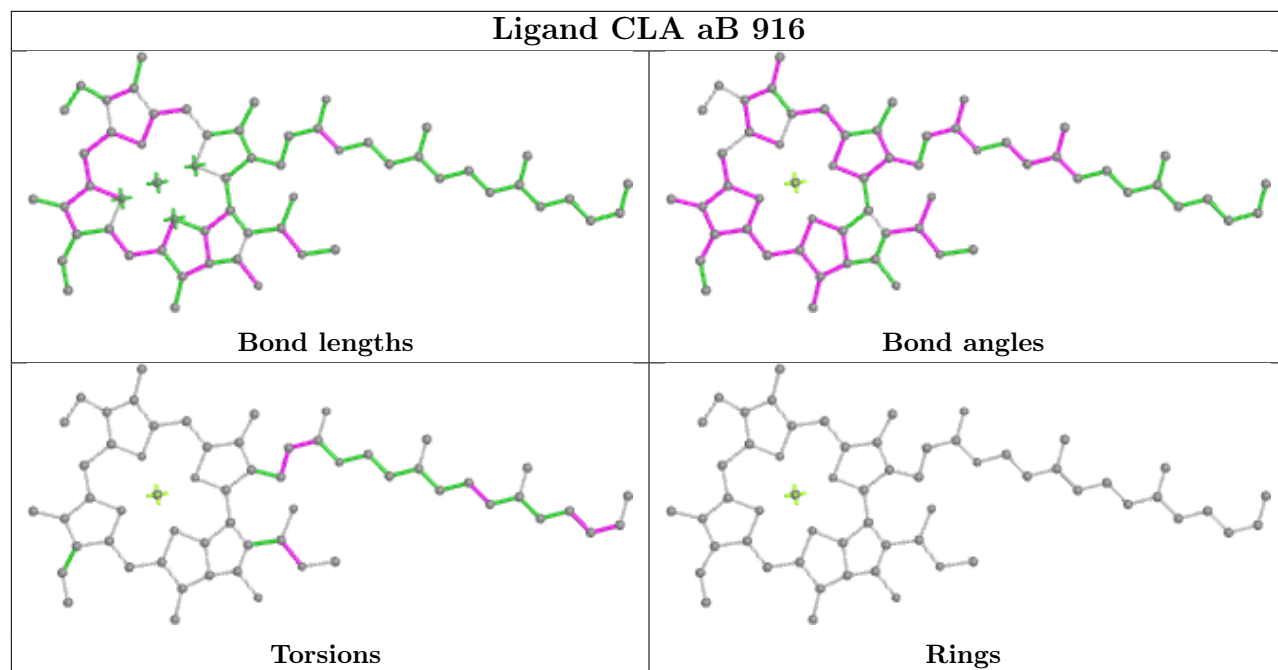
There are no ring outliers.

No monomer is involved in short contacts.

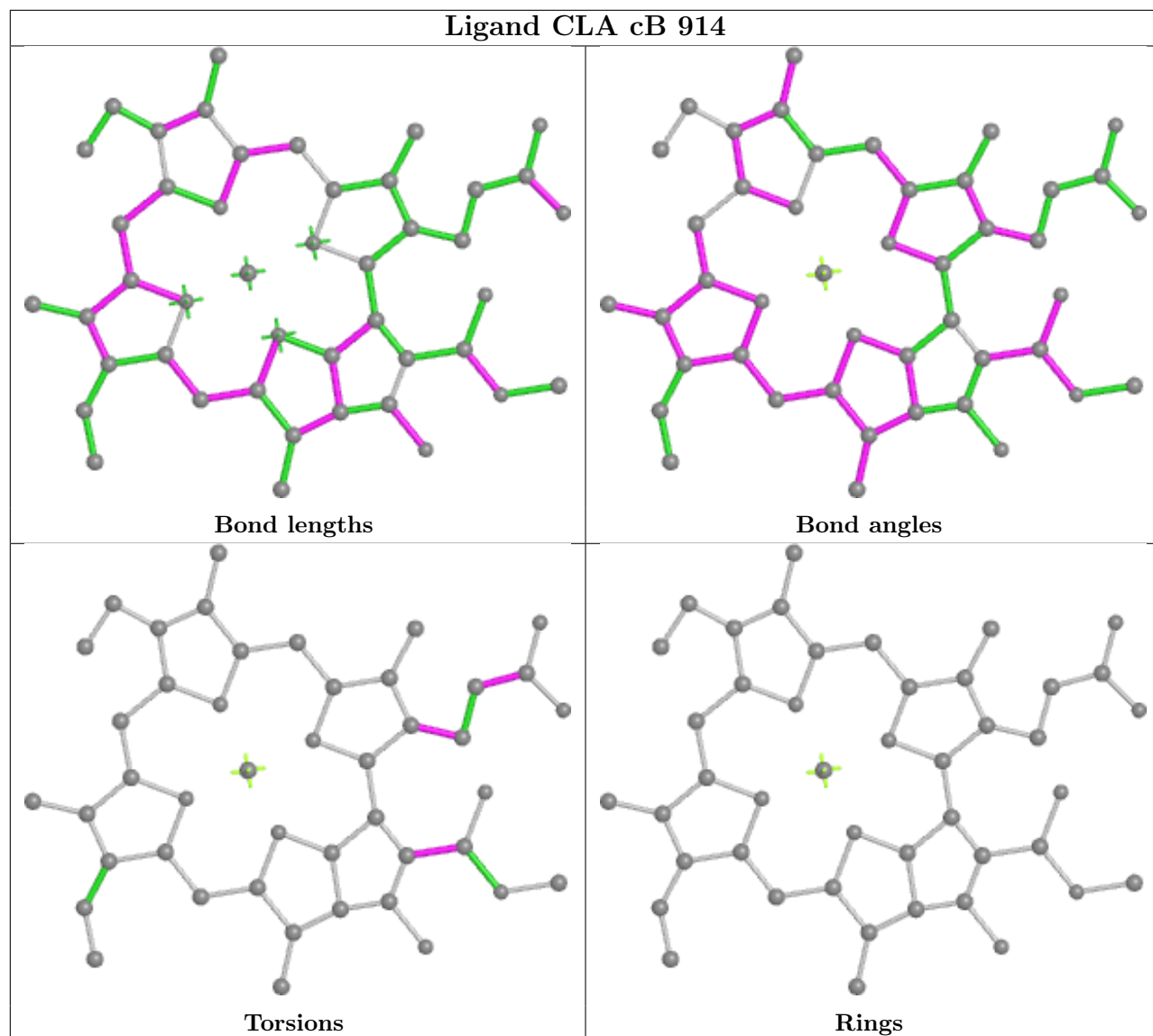
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

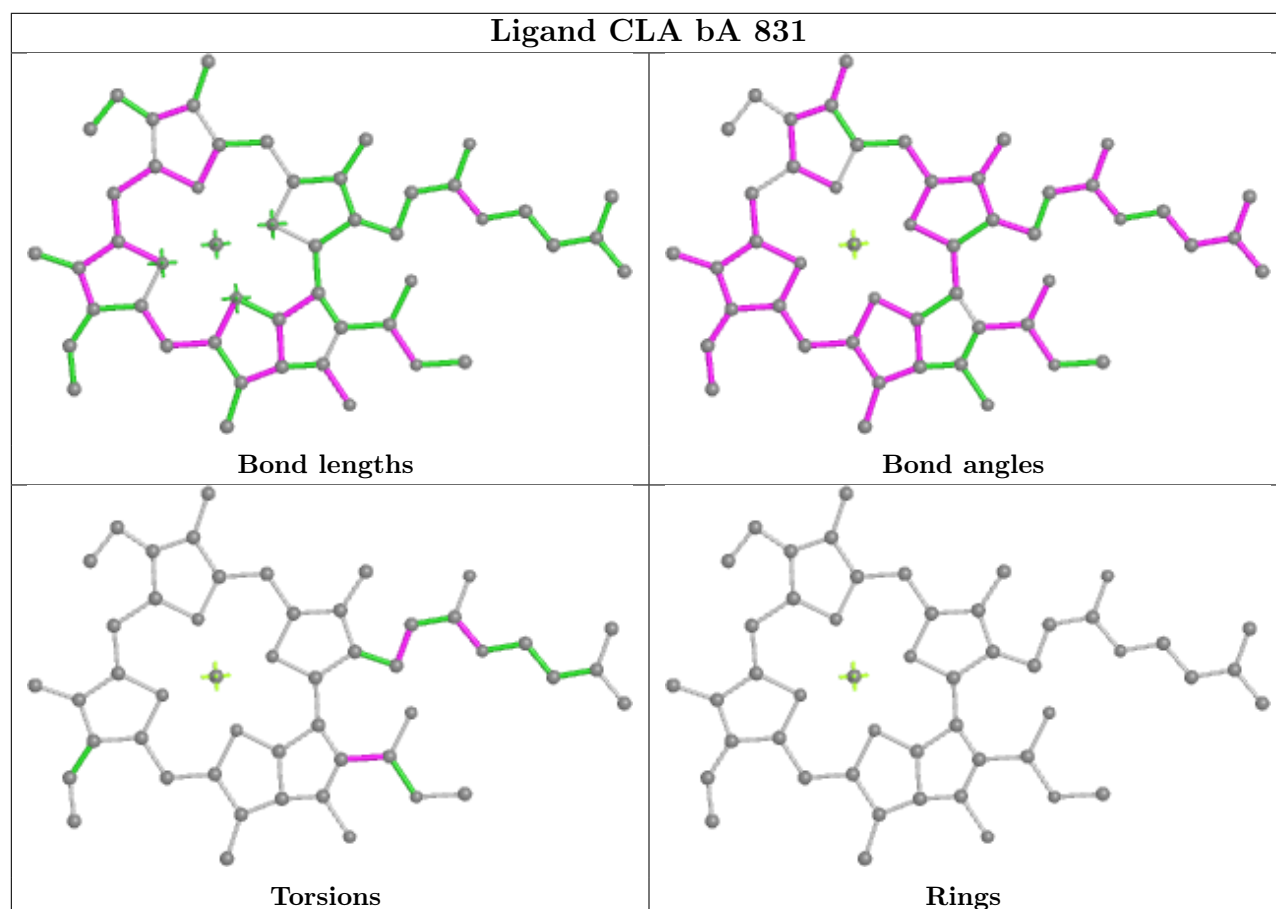
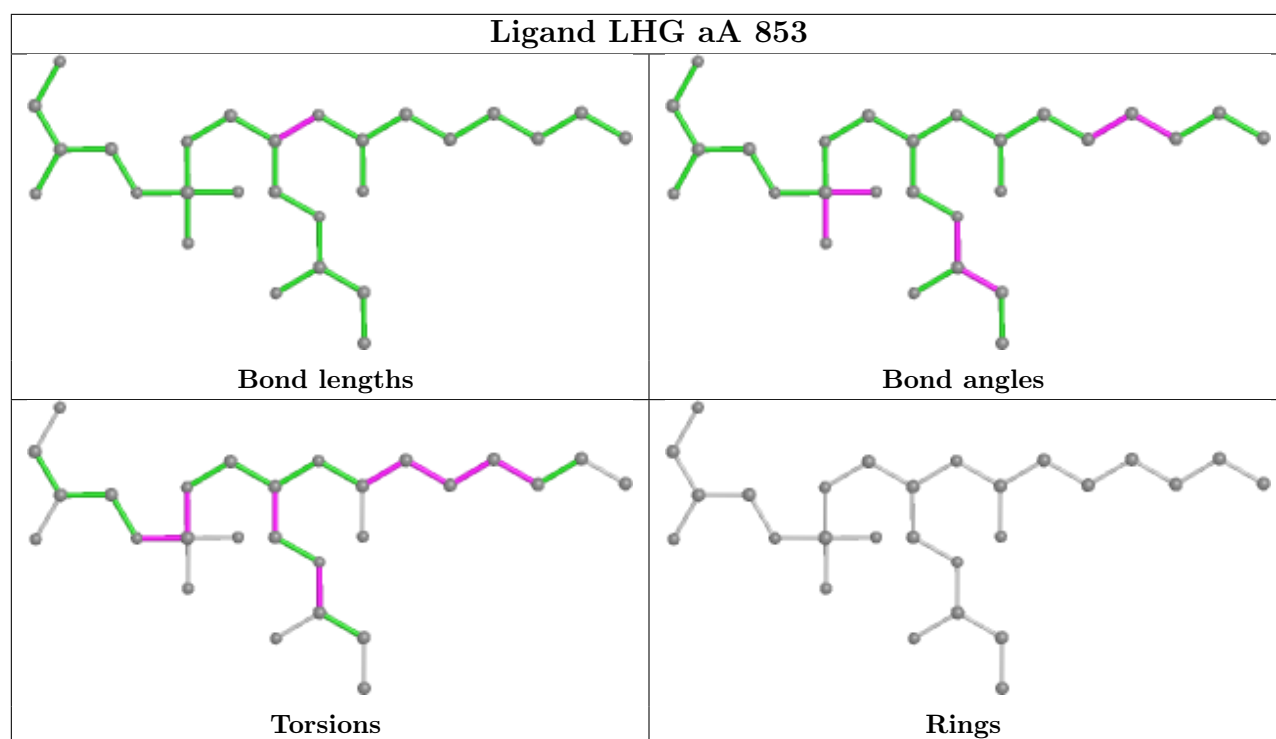
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

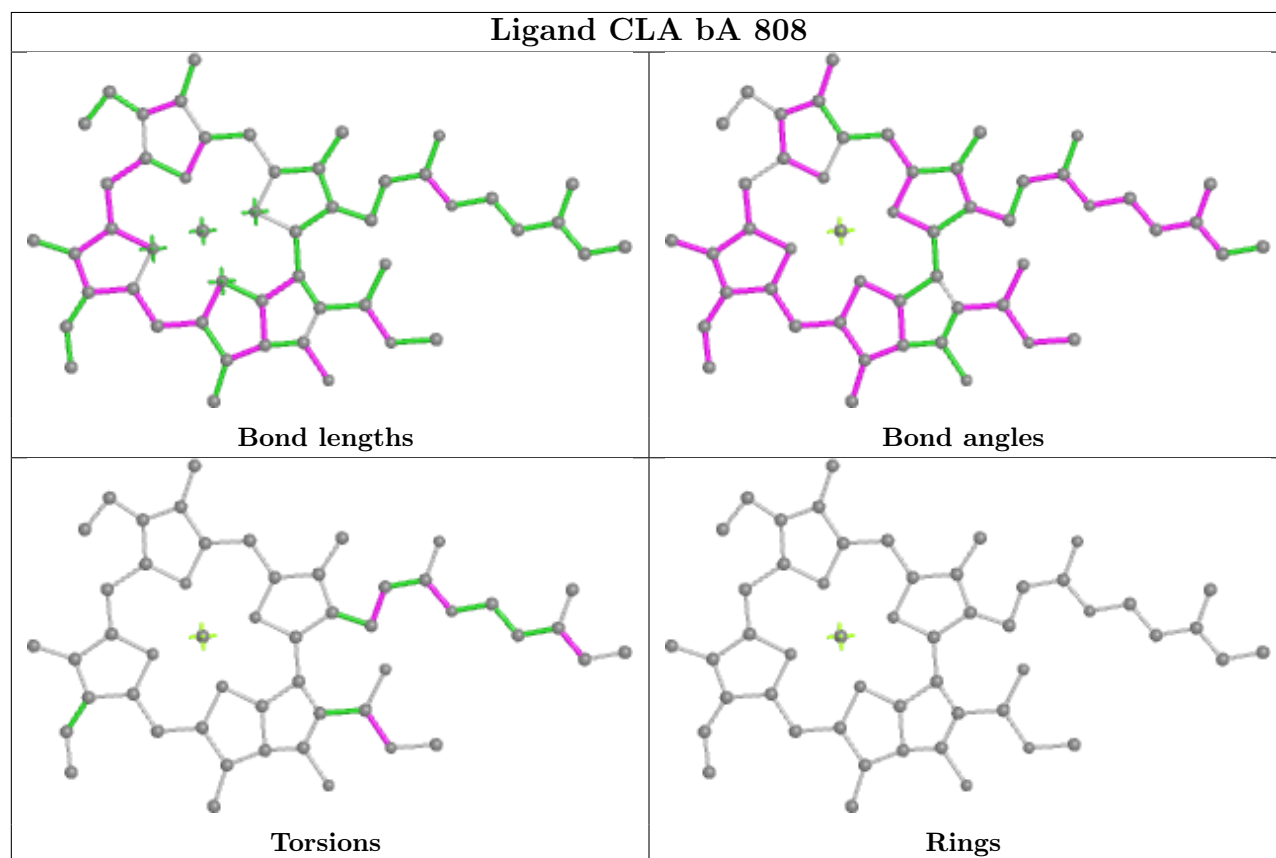
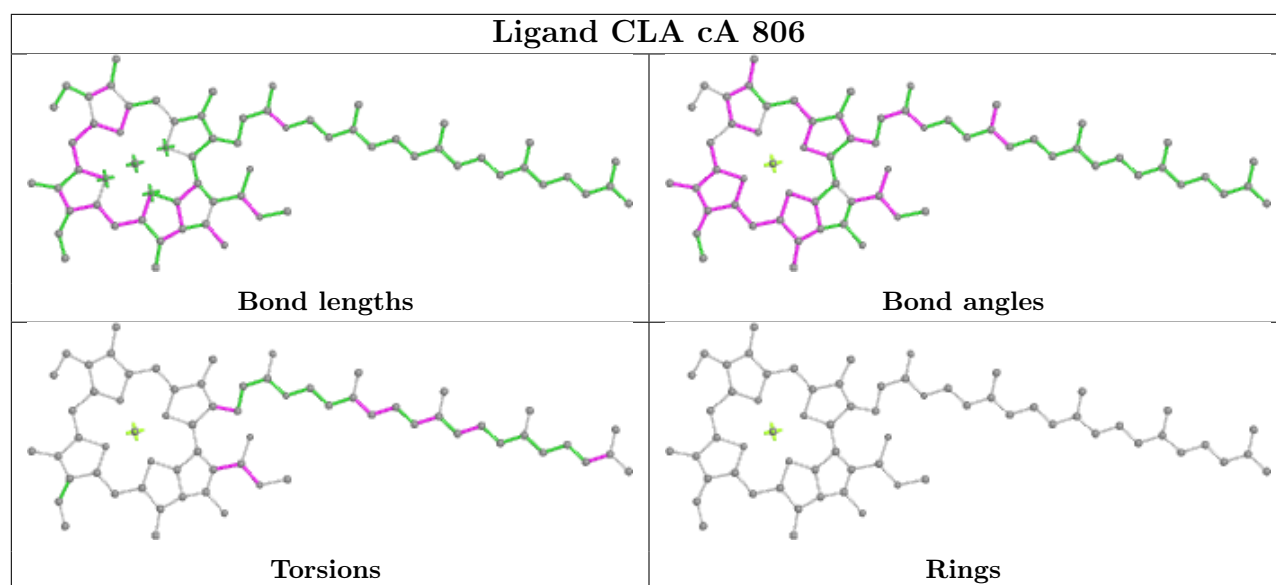


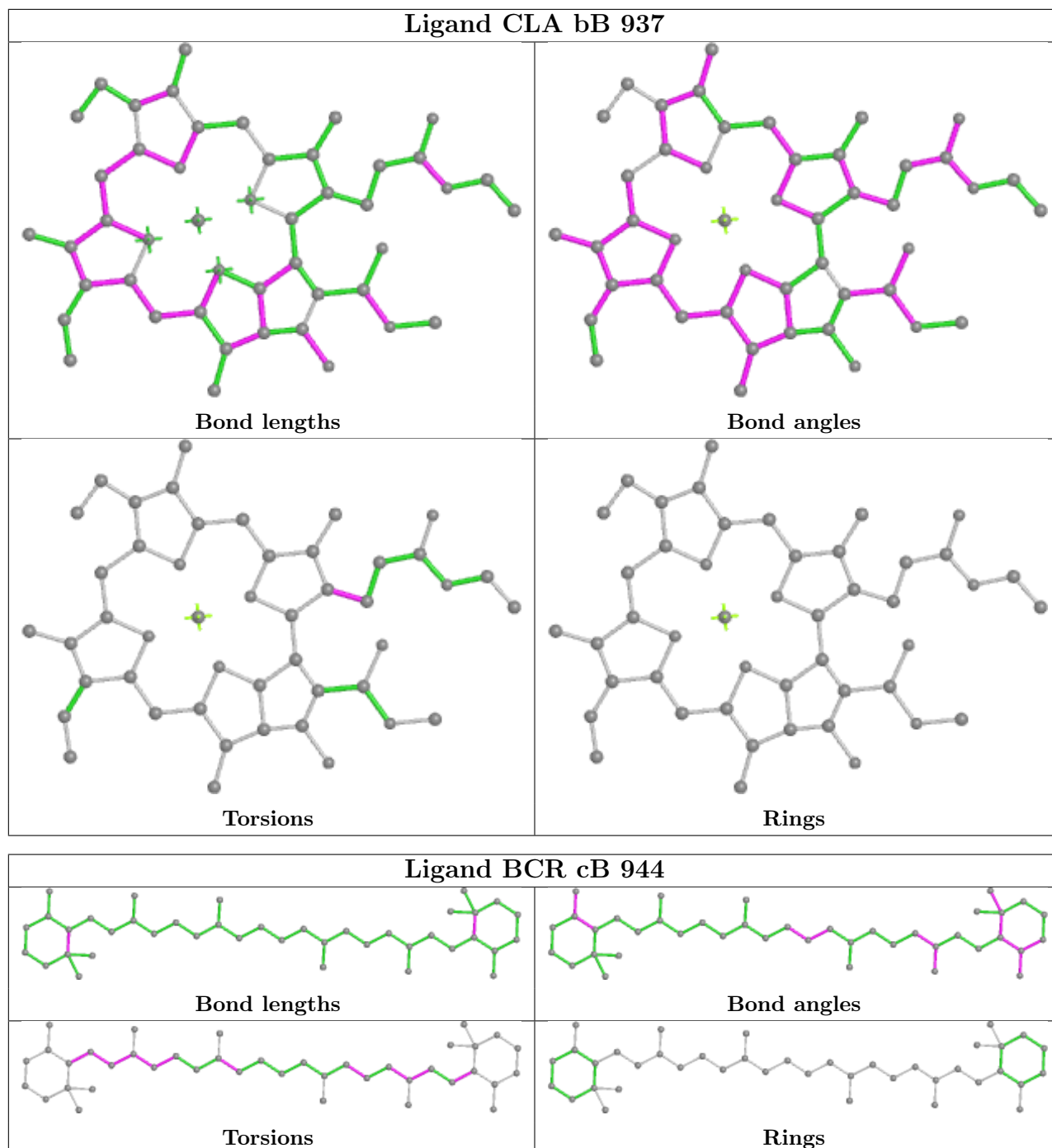


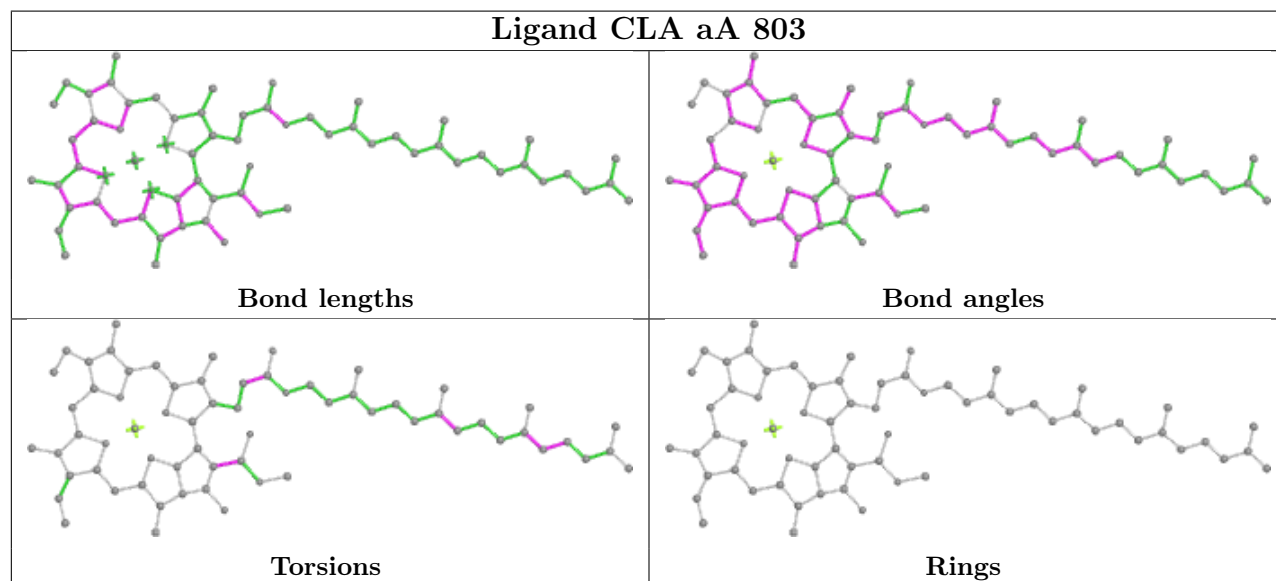
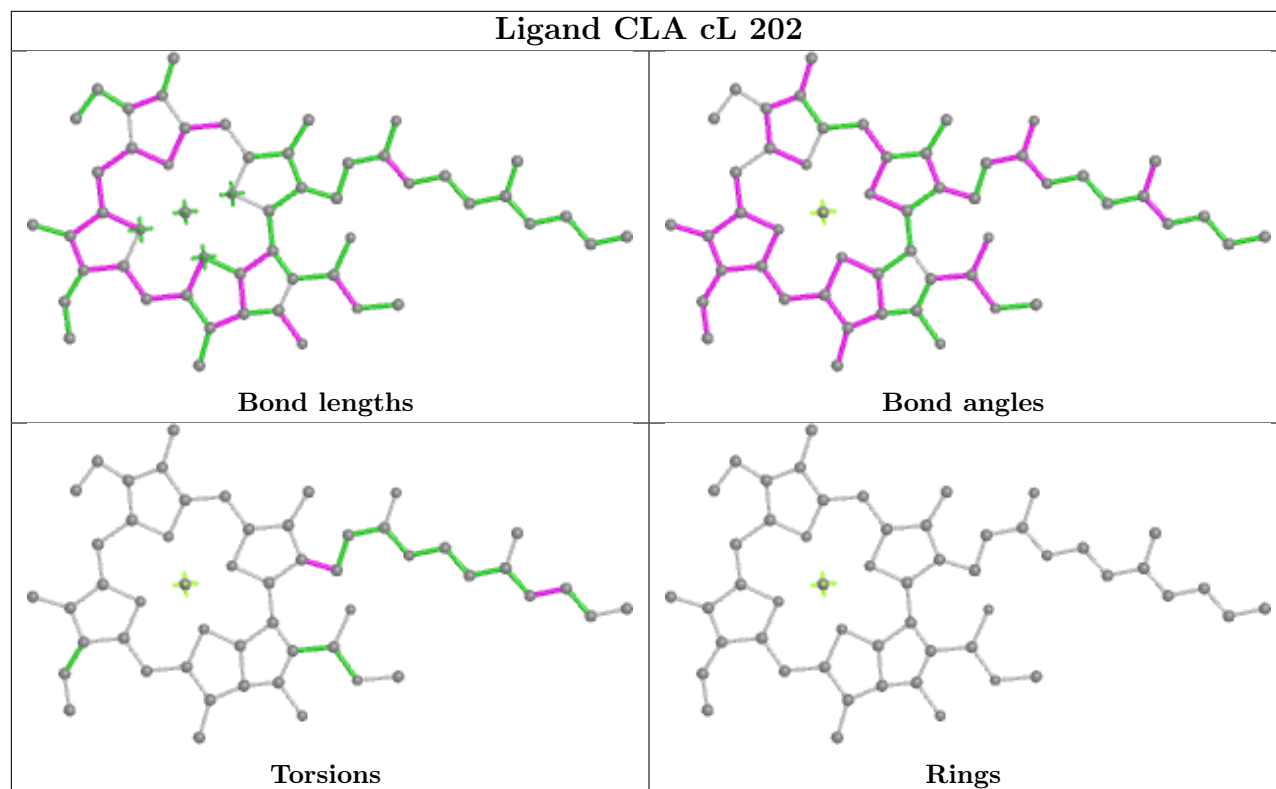


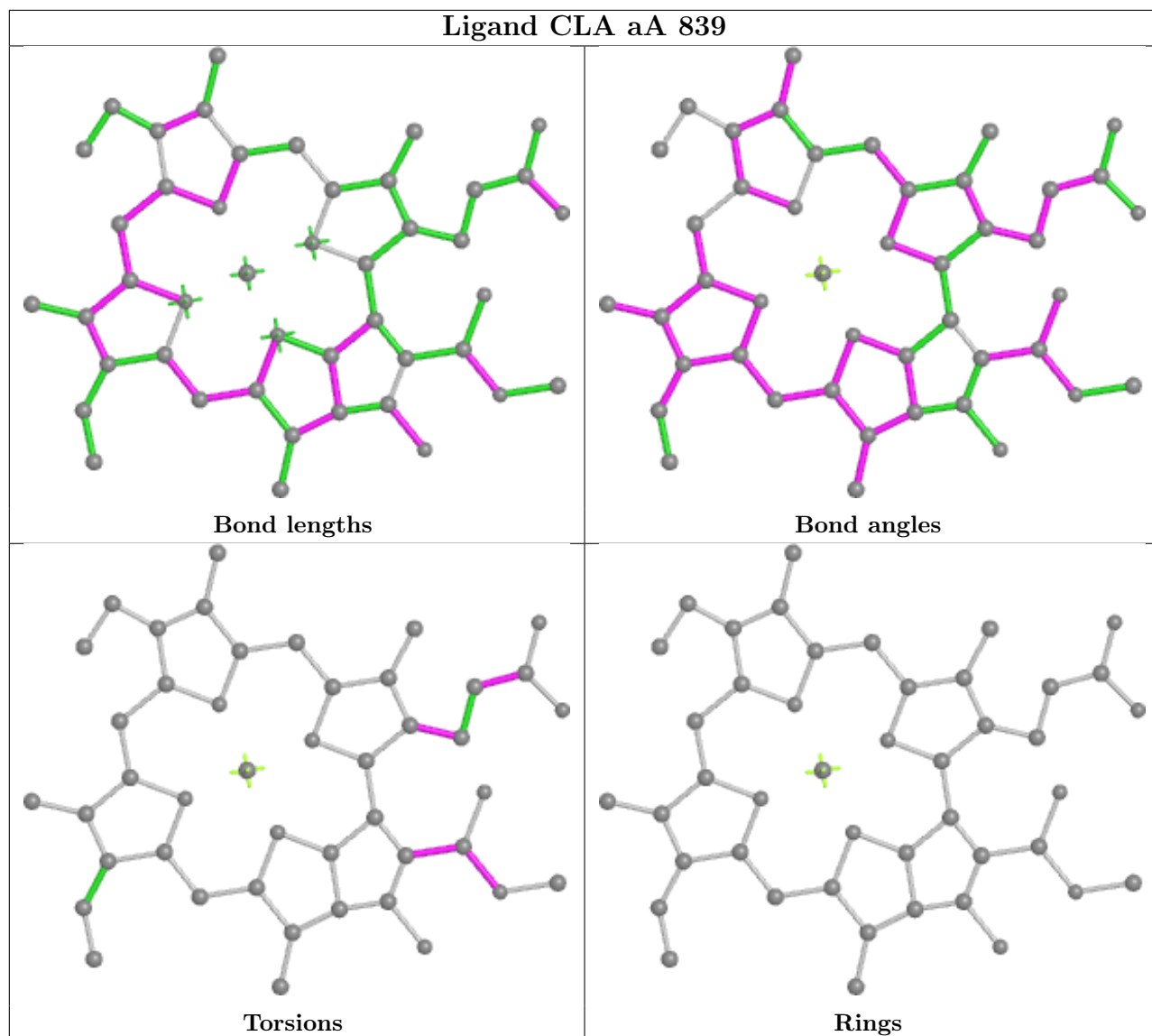


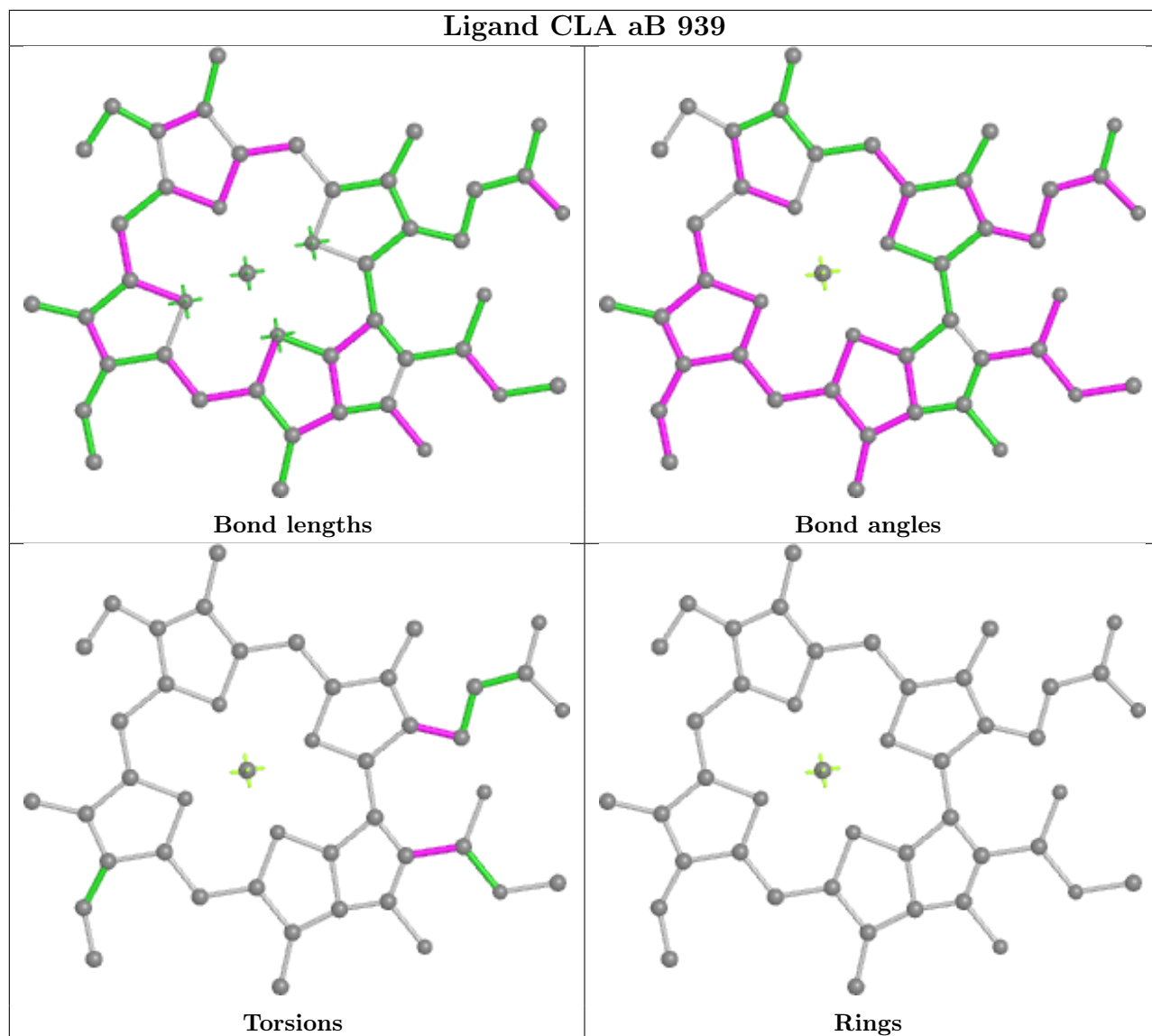


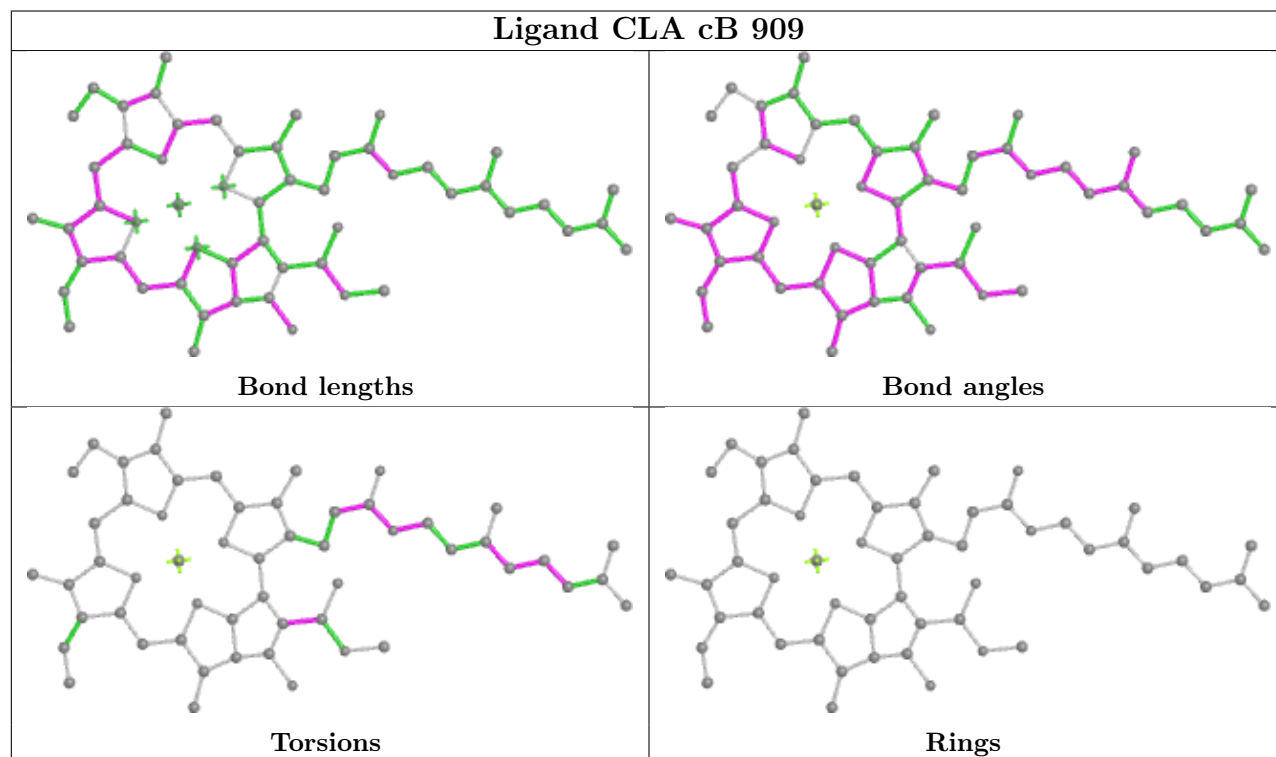
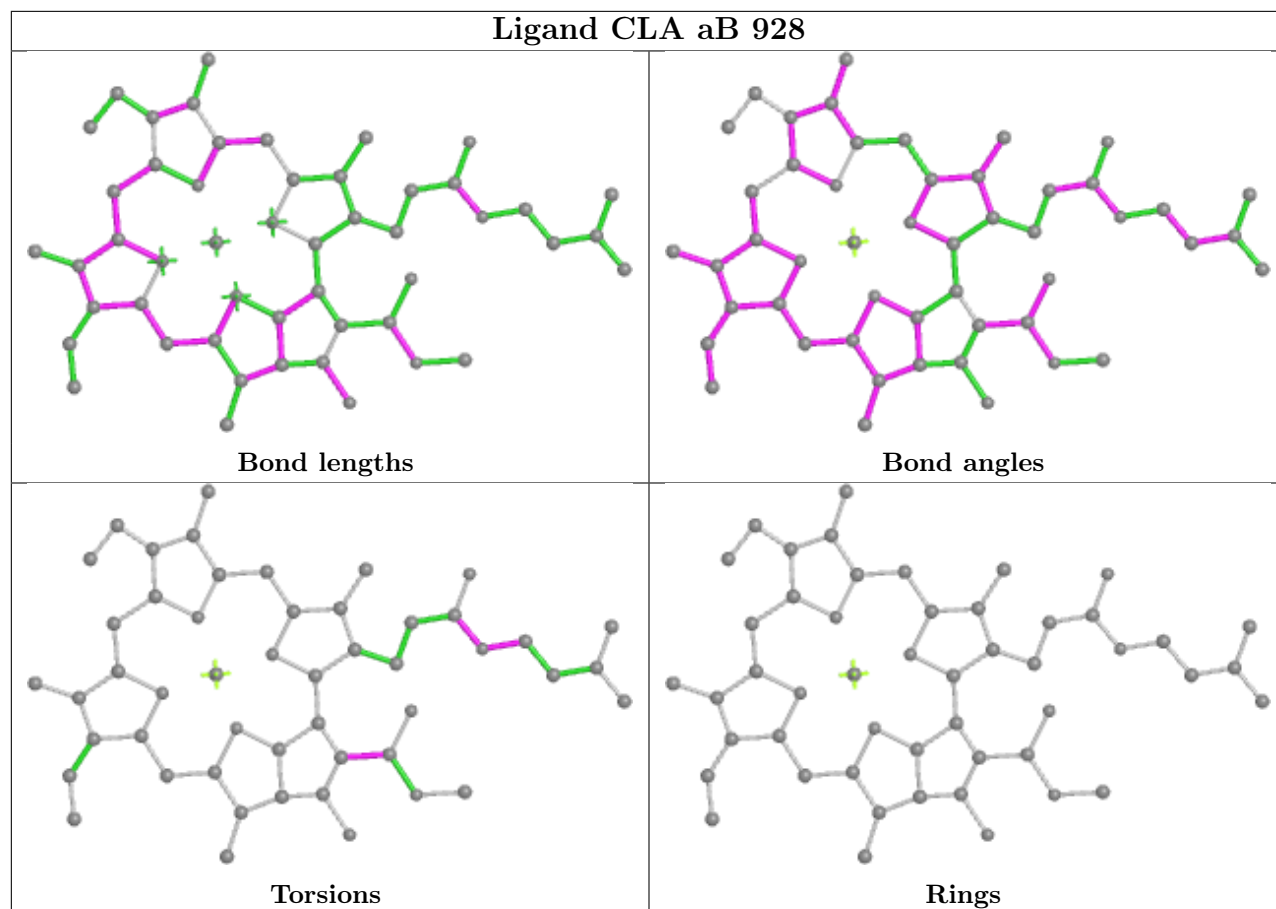




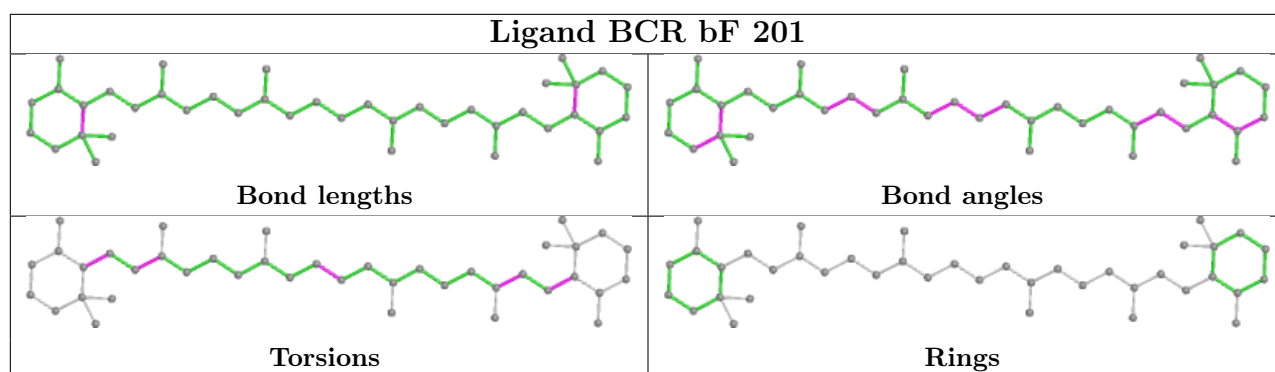
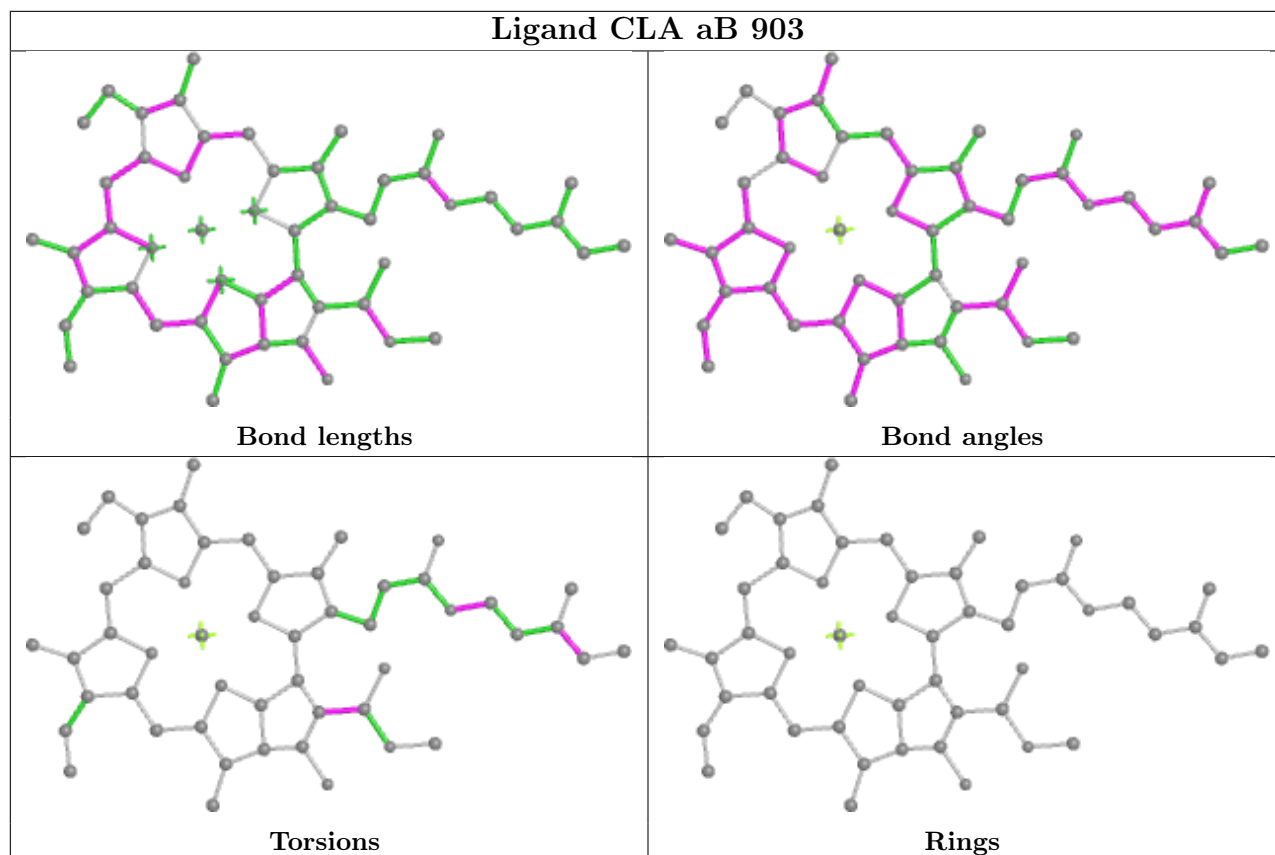
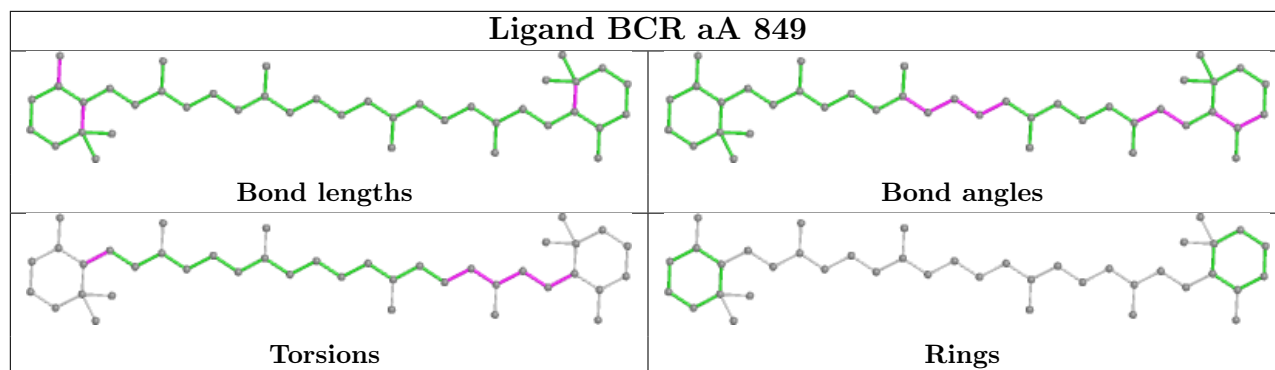


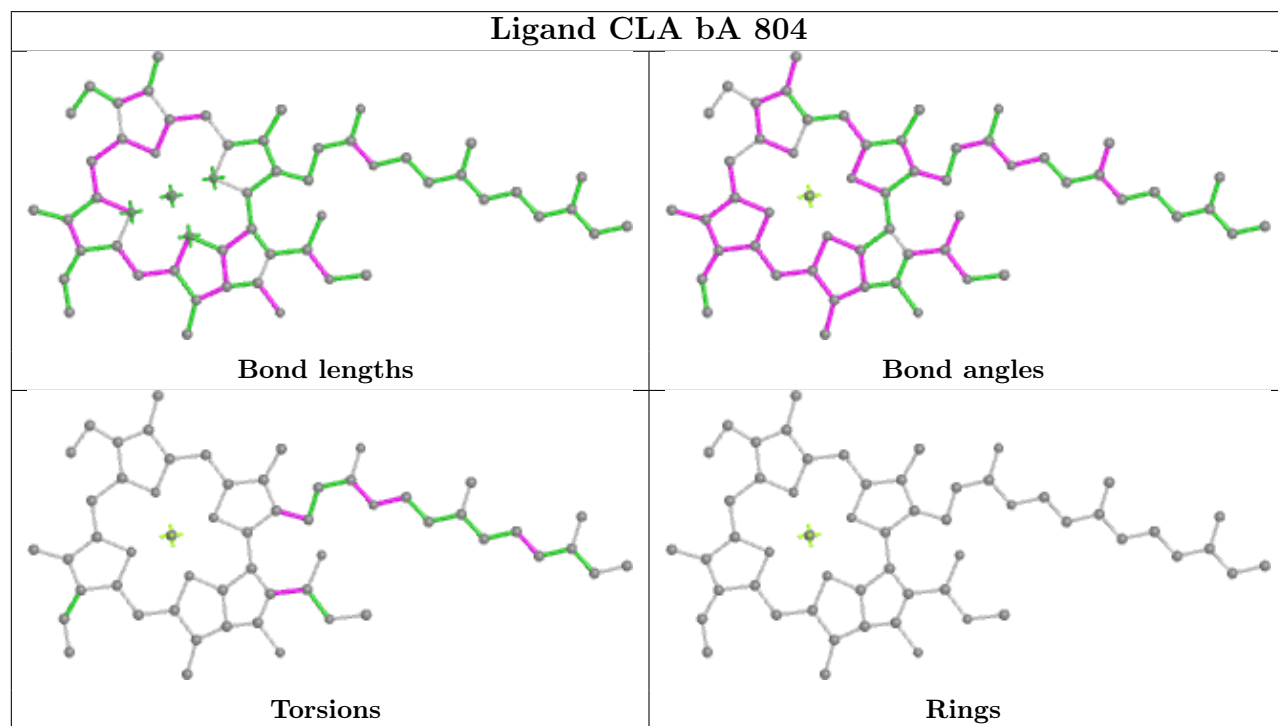
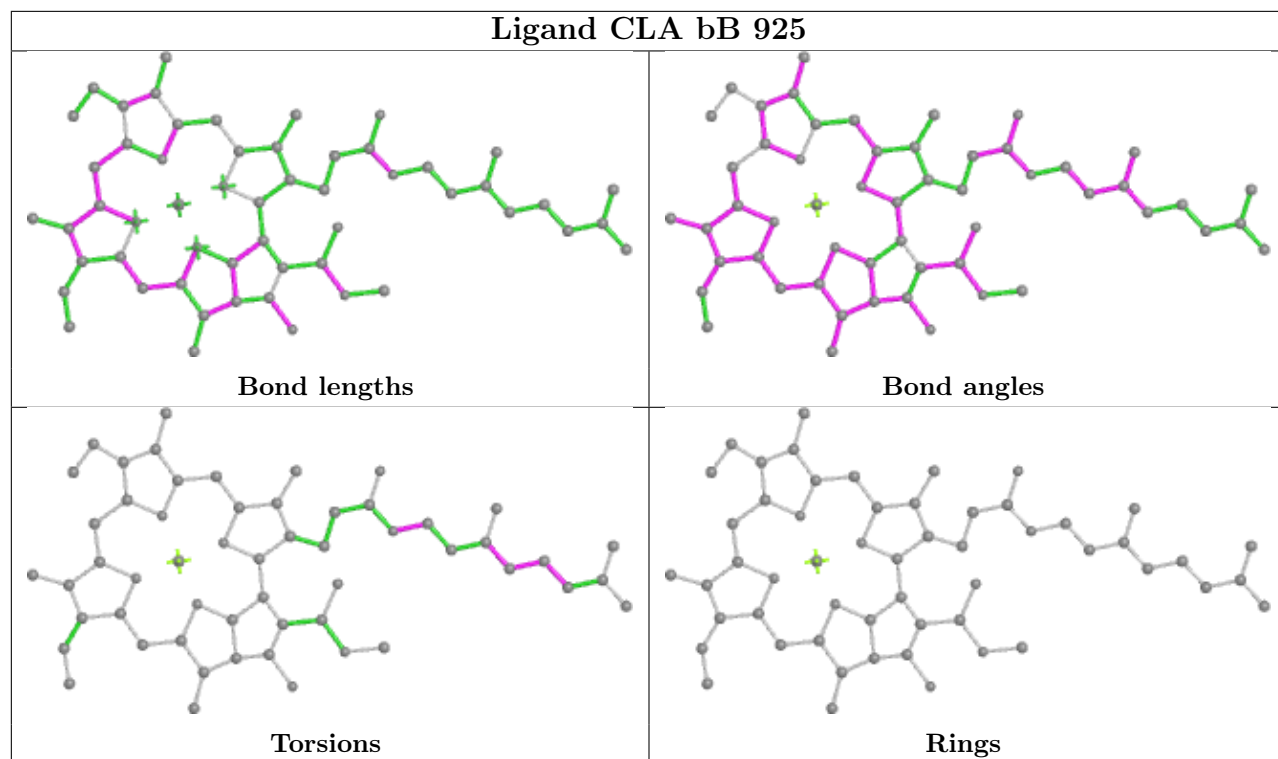


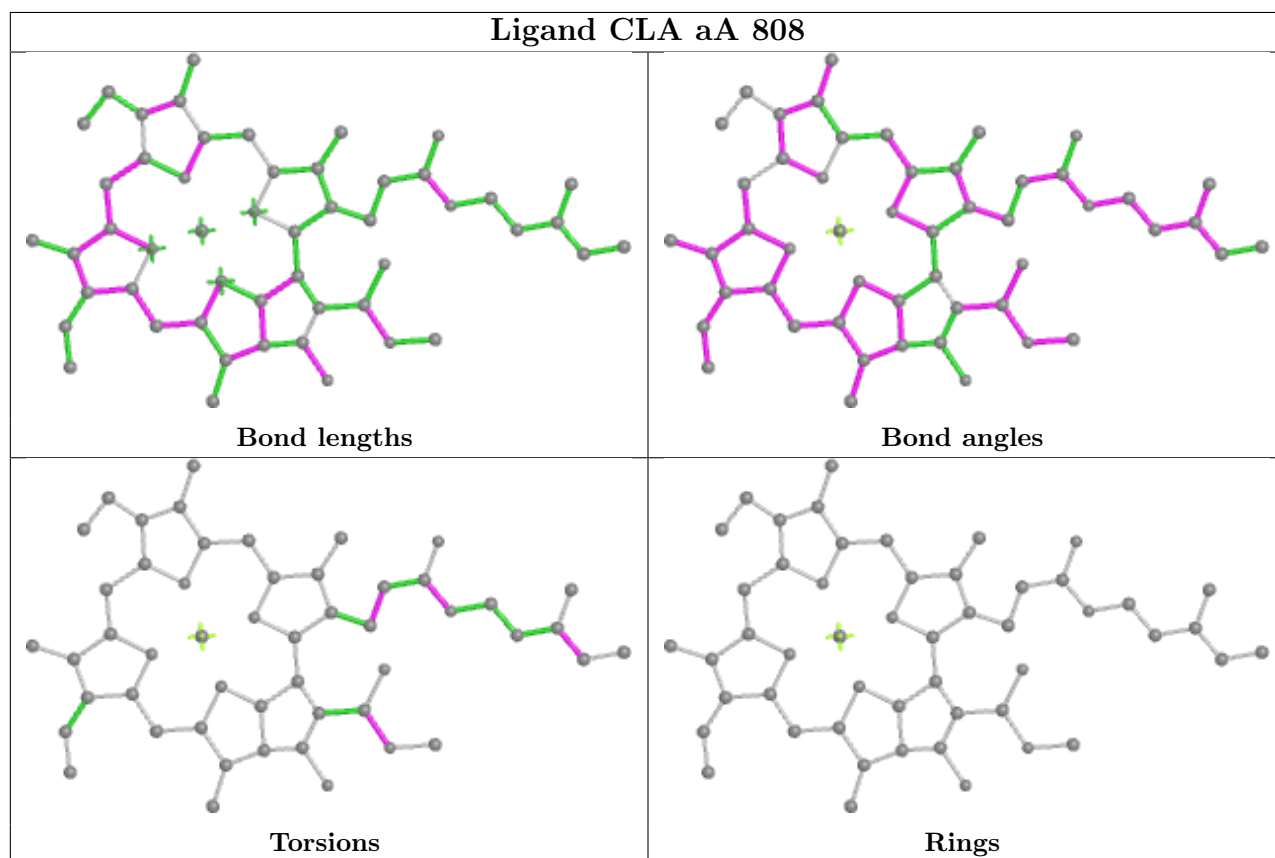
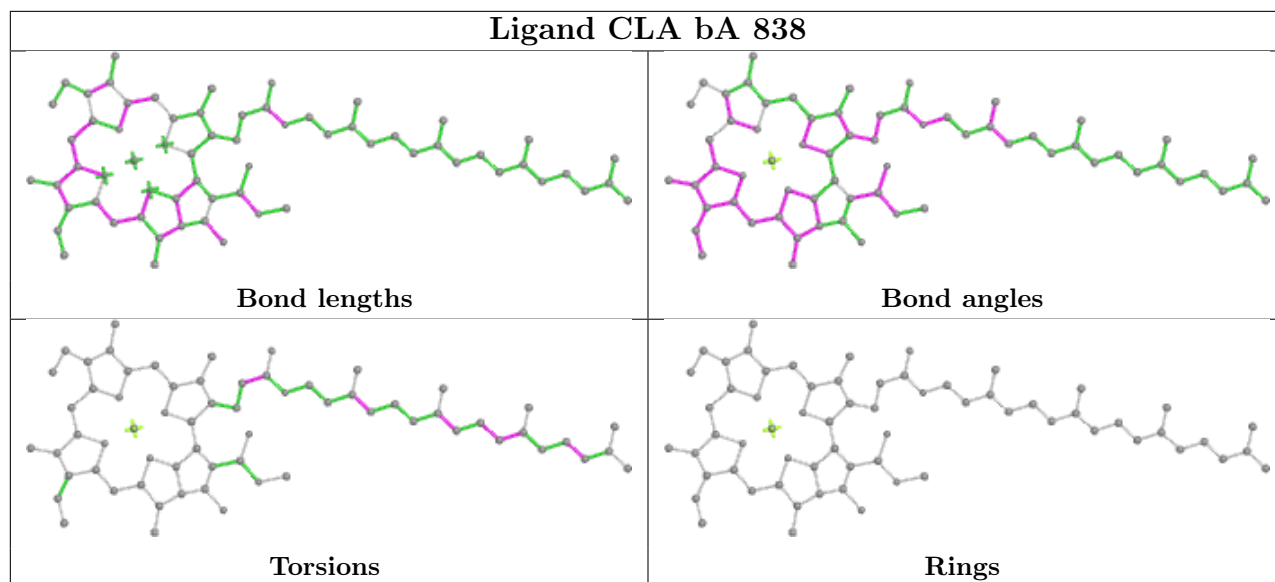


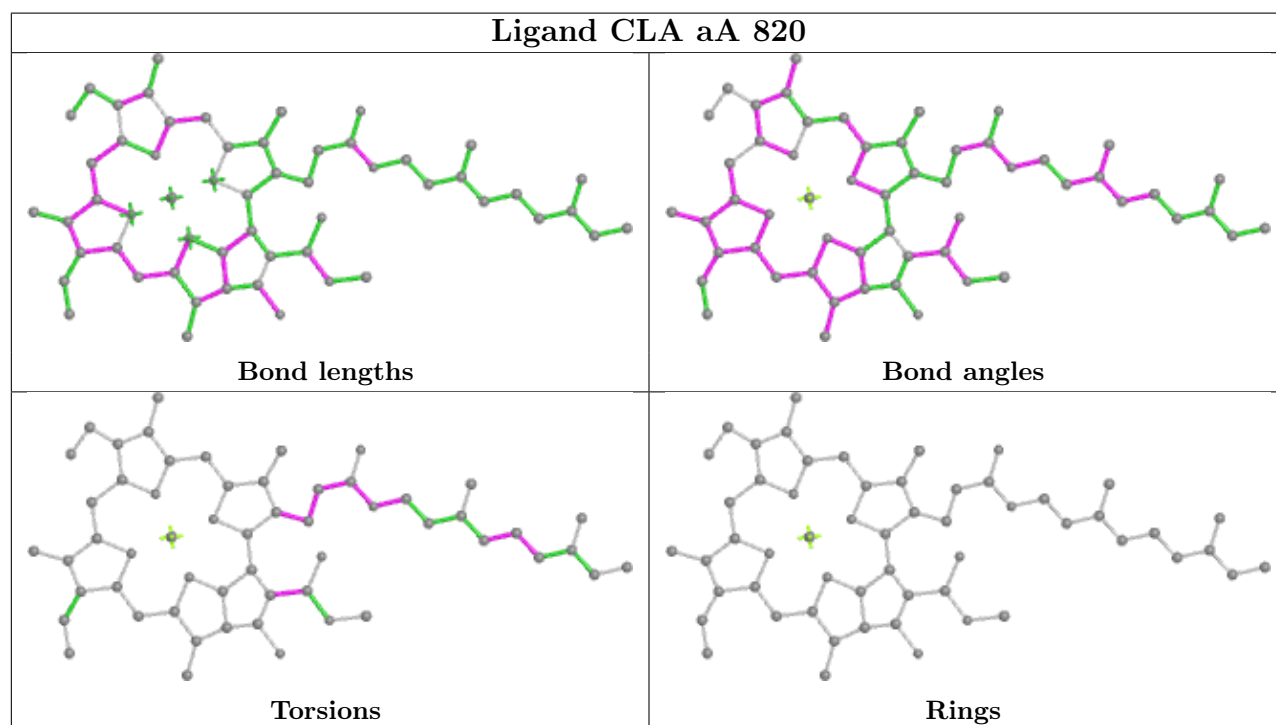
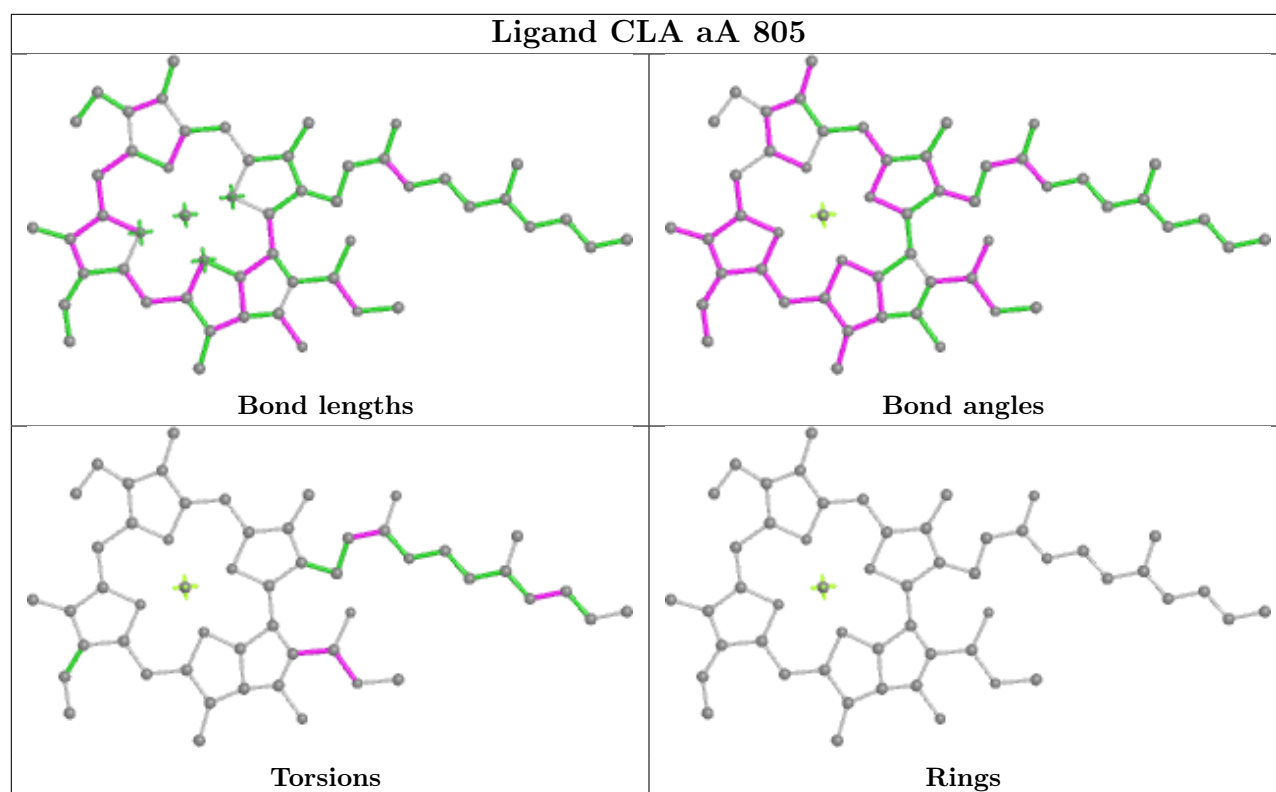


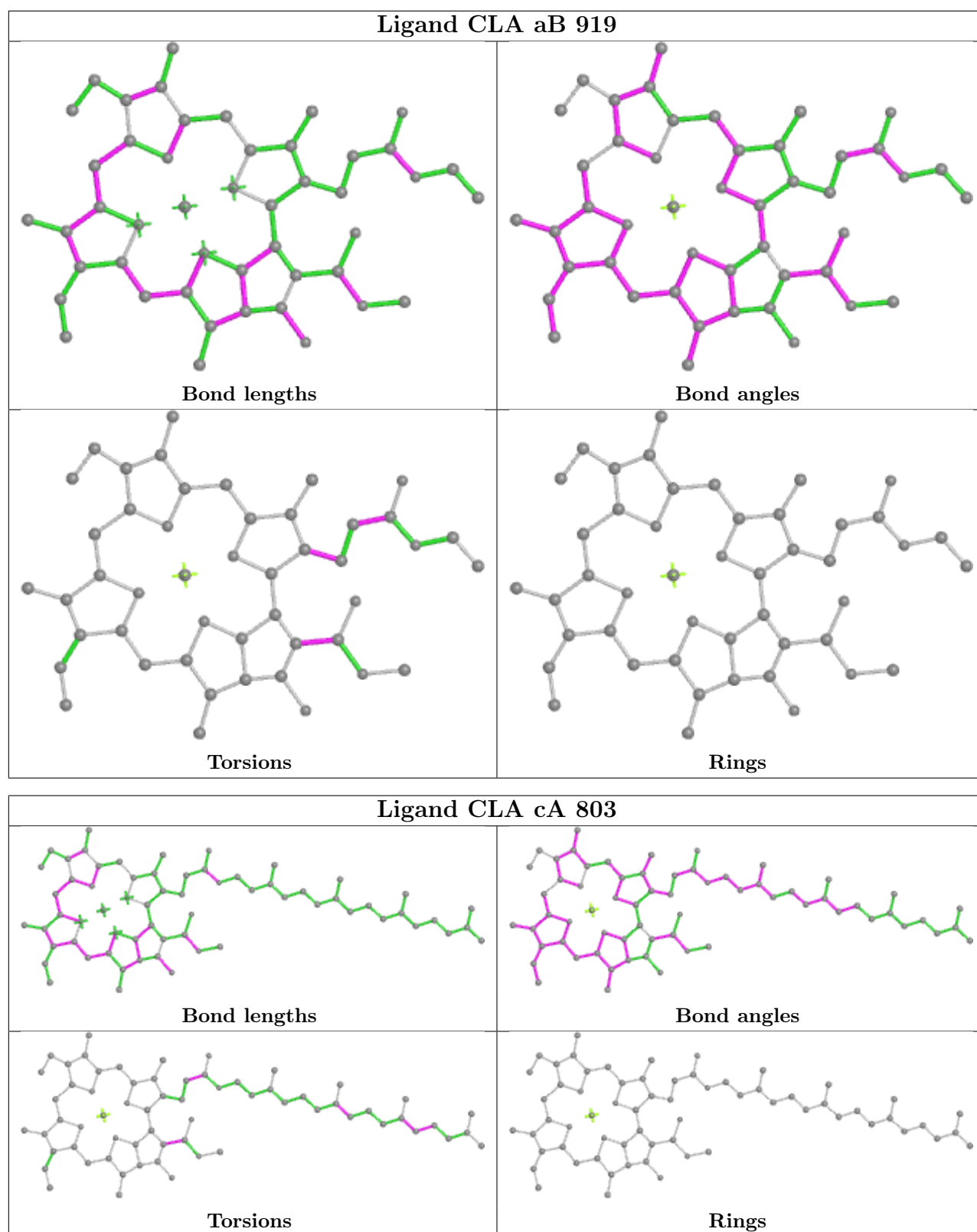


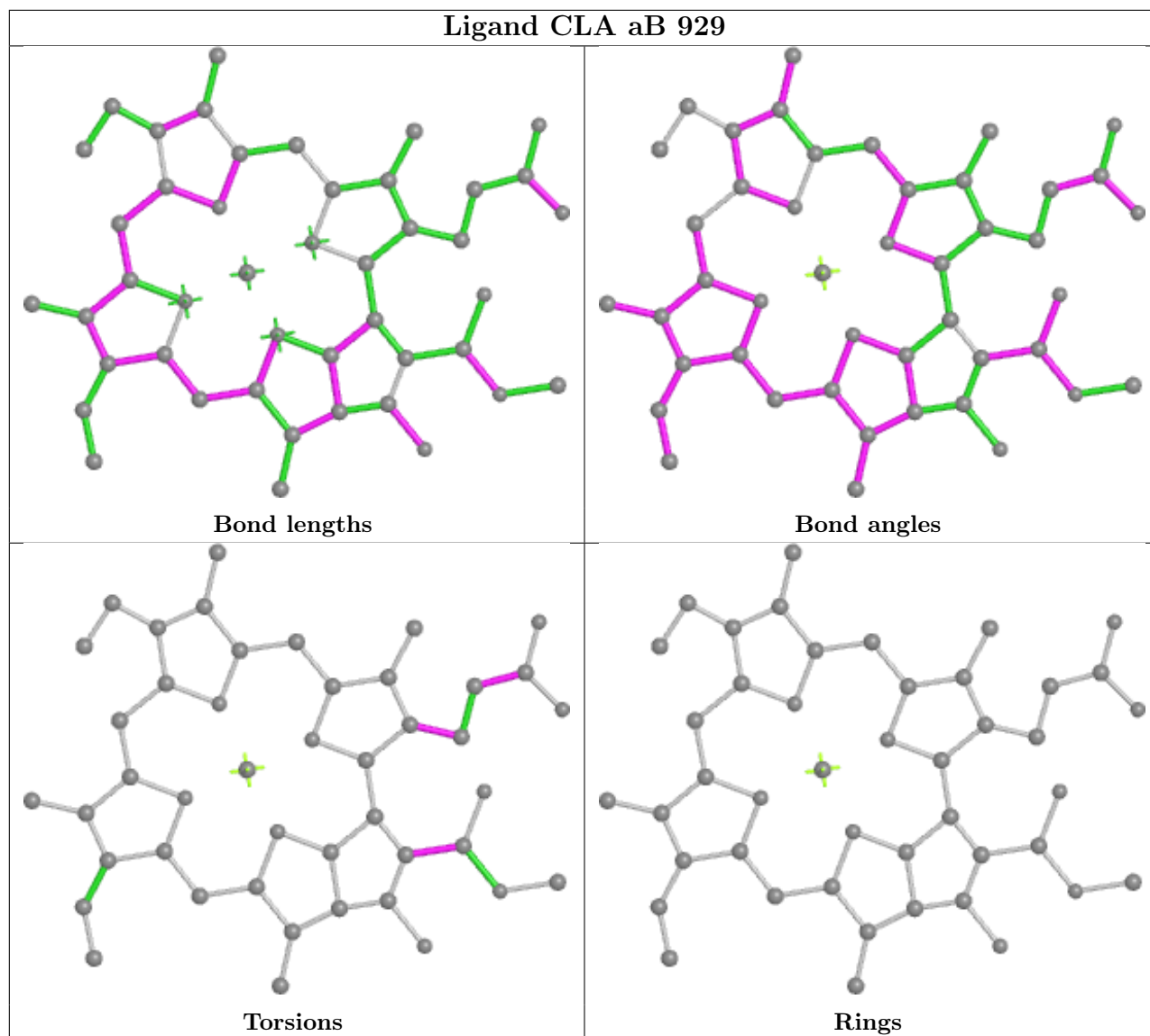
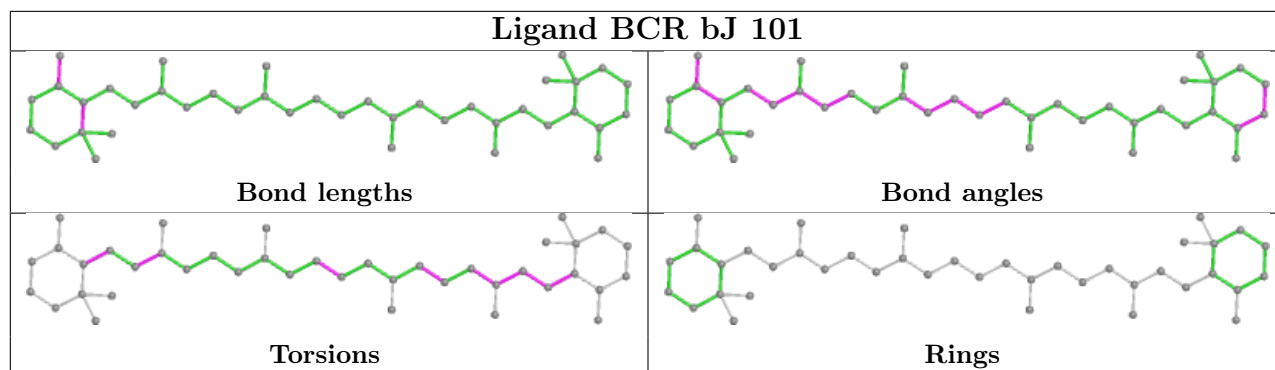


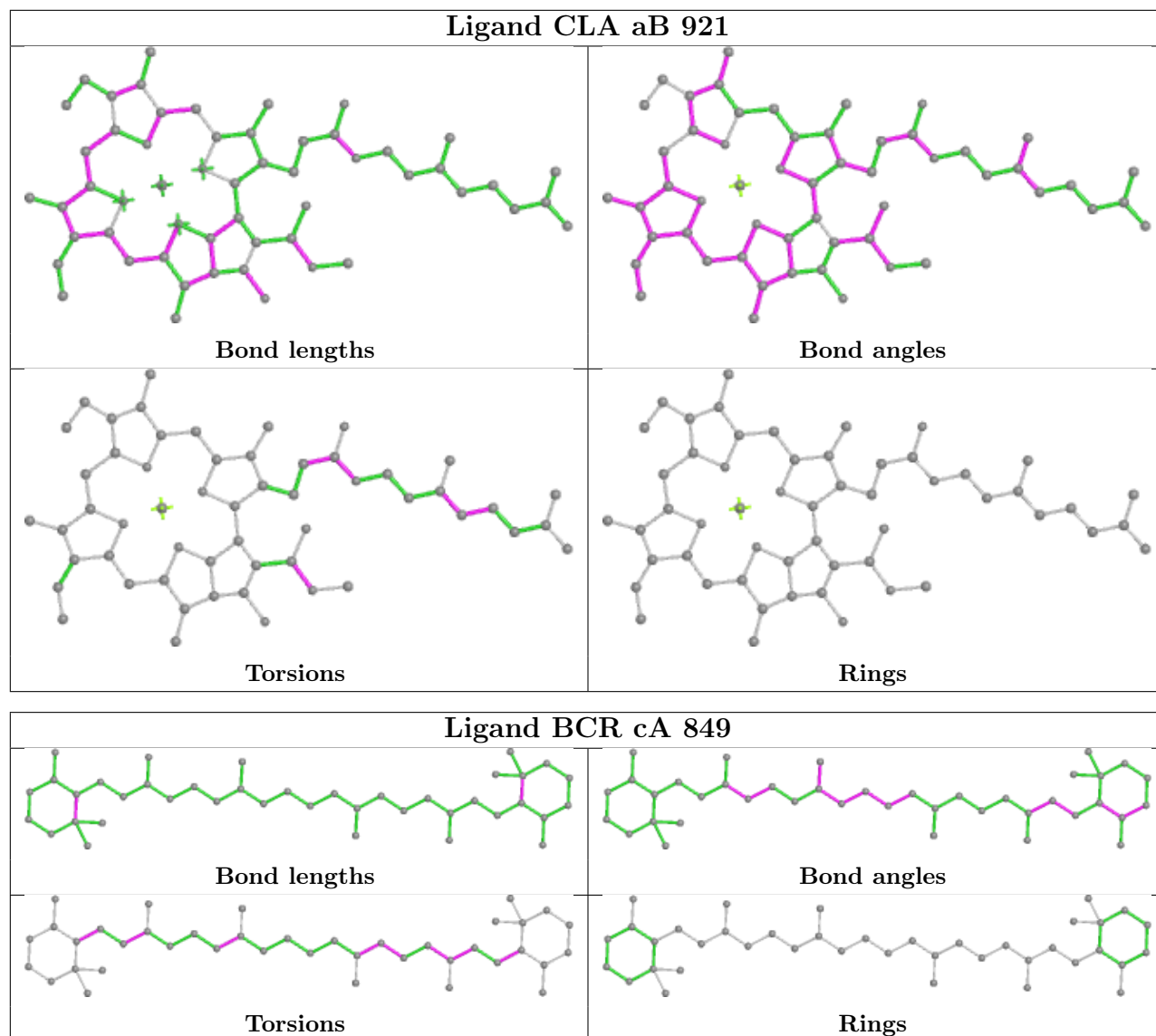


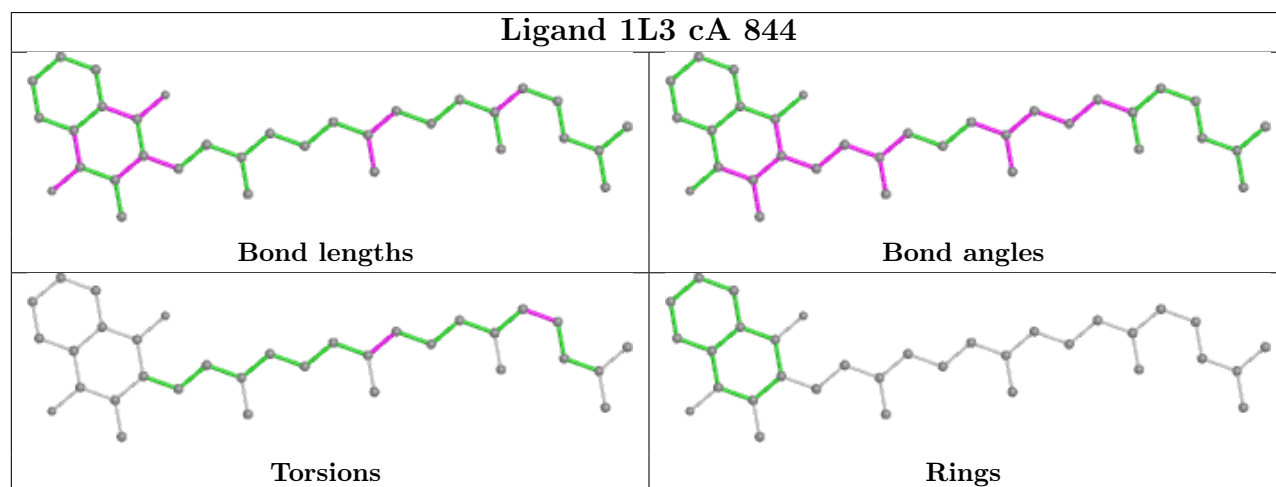
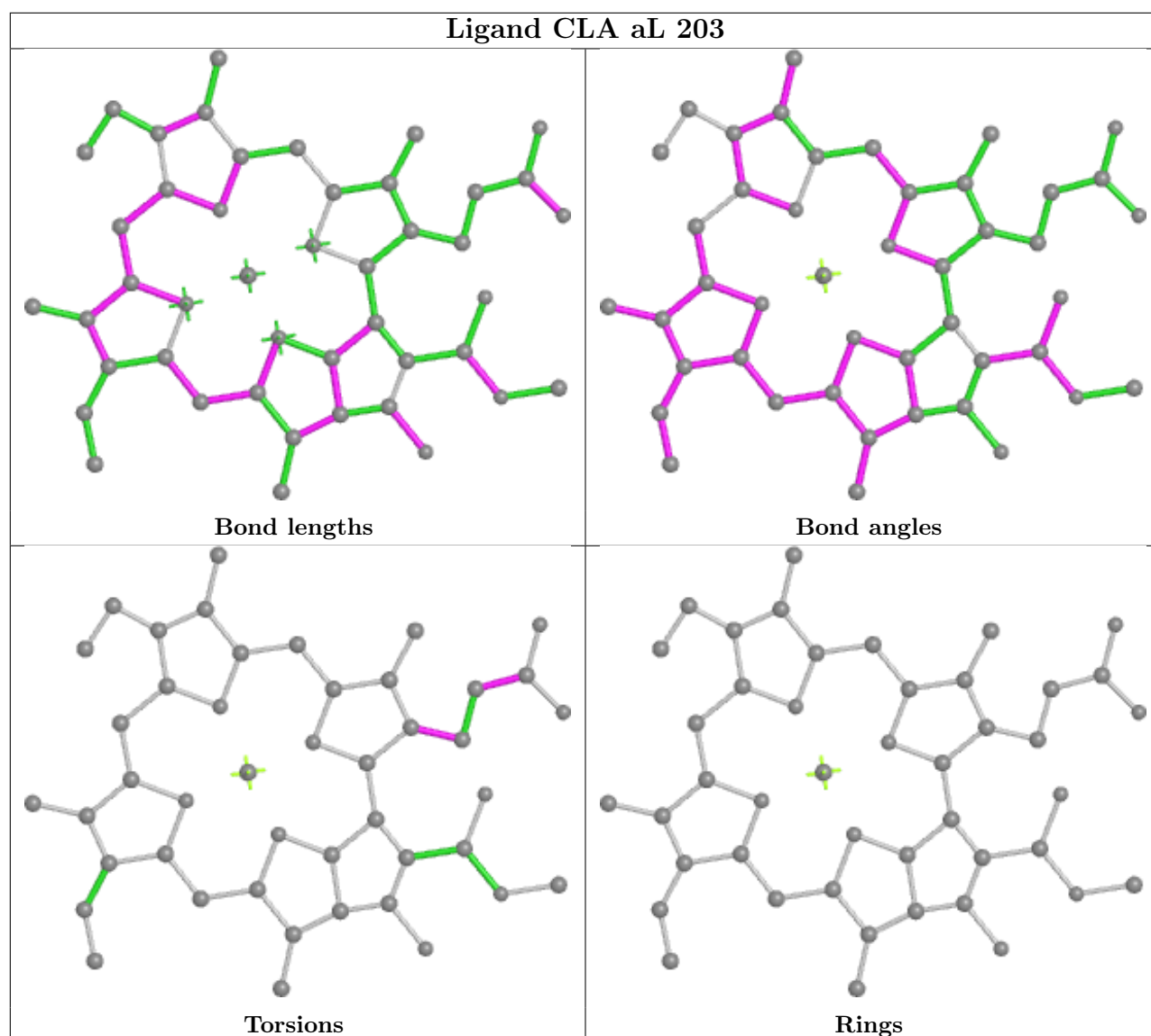




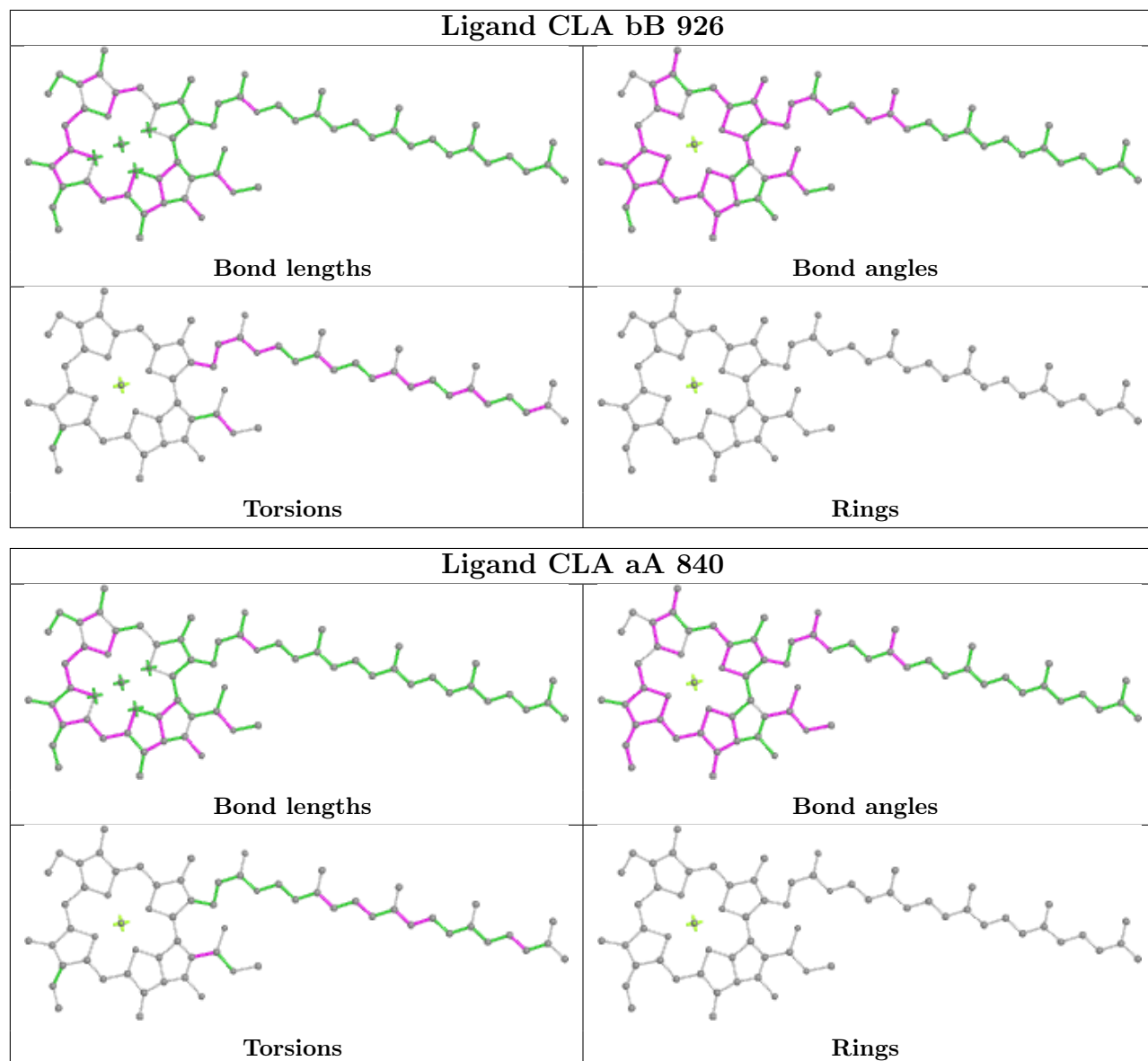


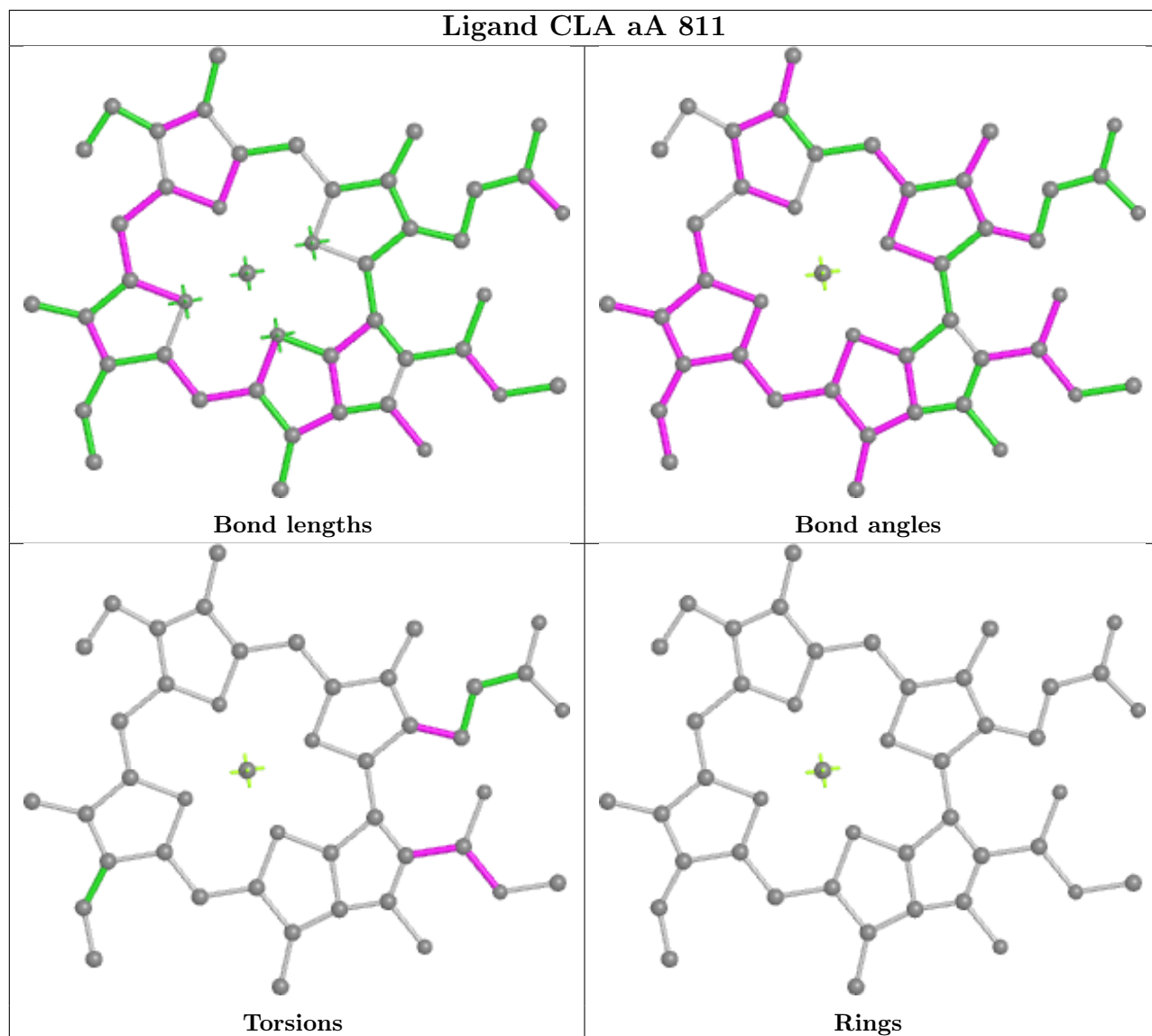


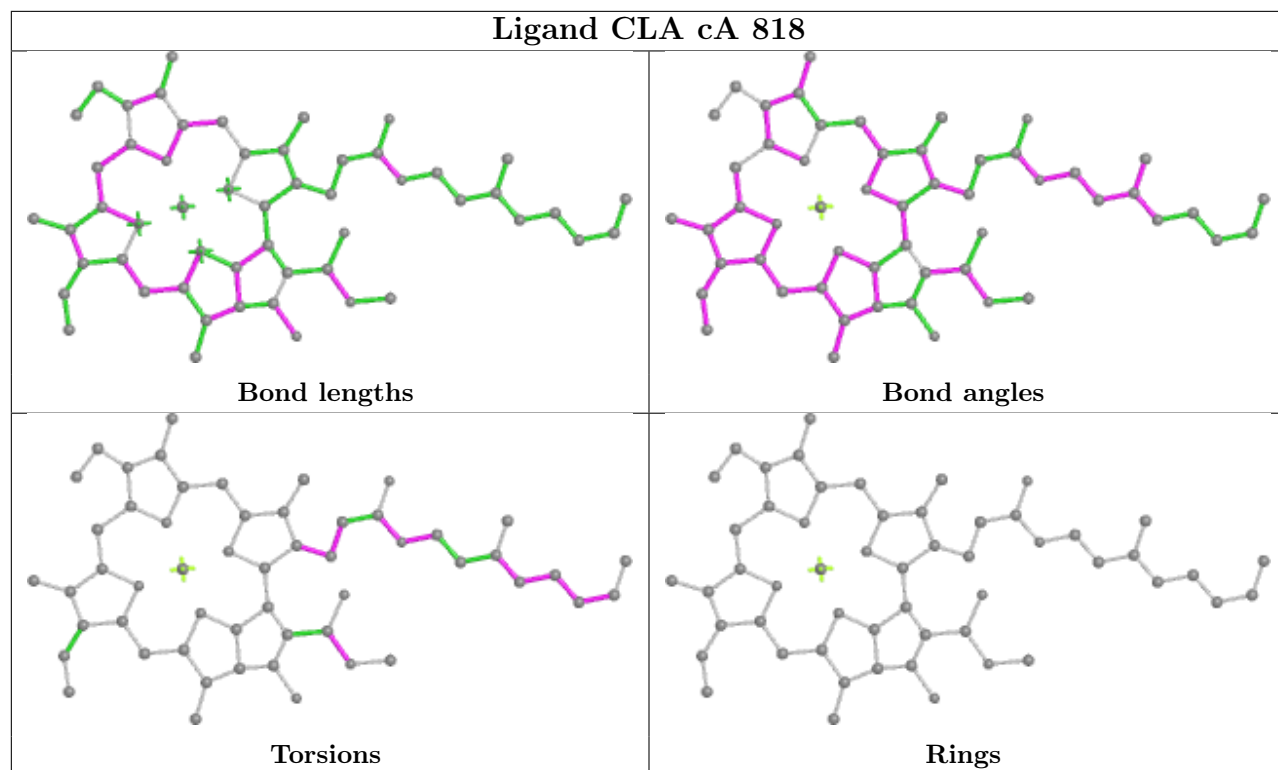


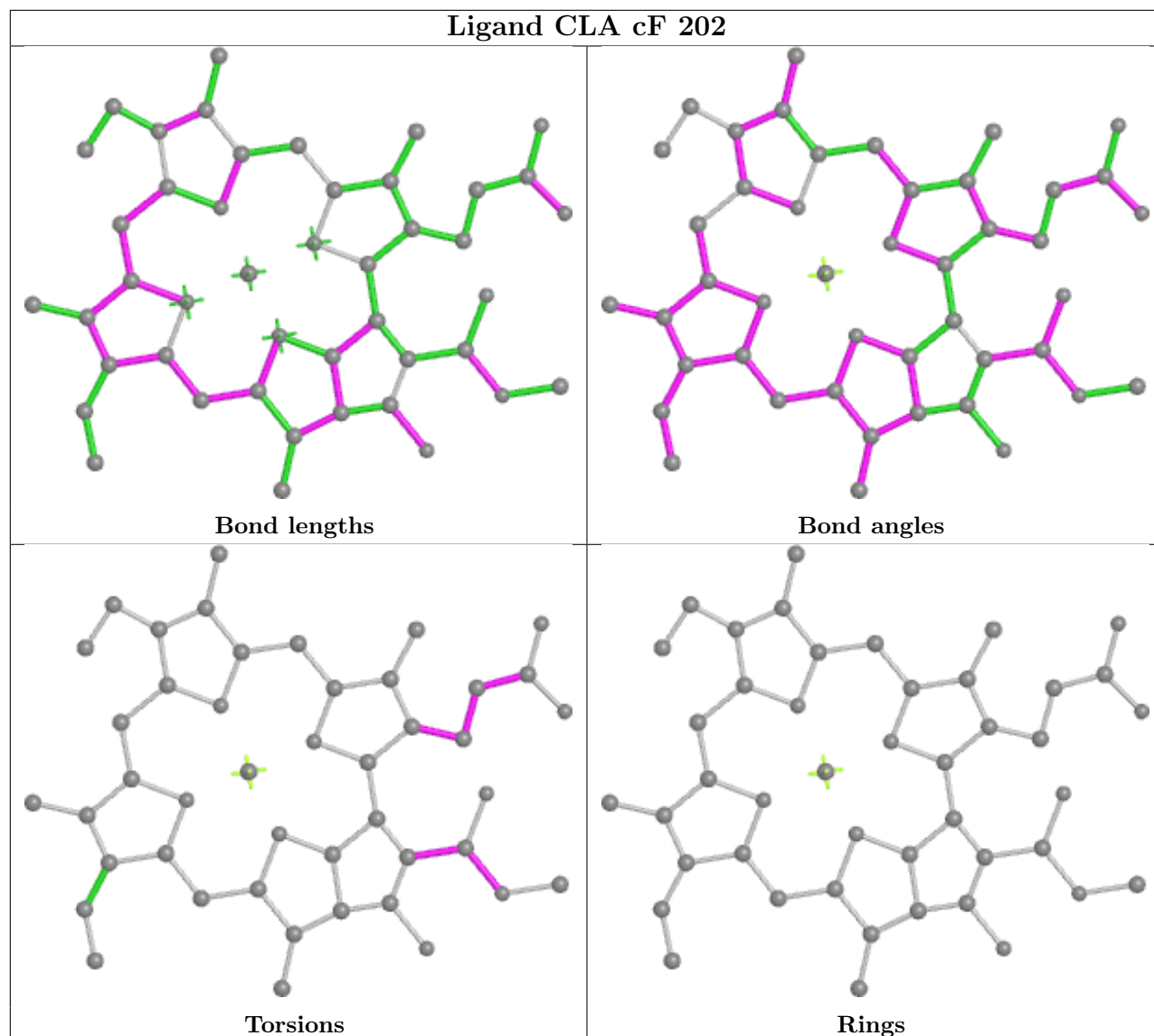


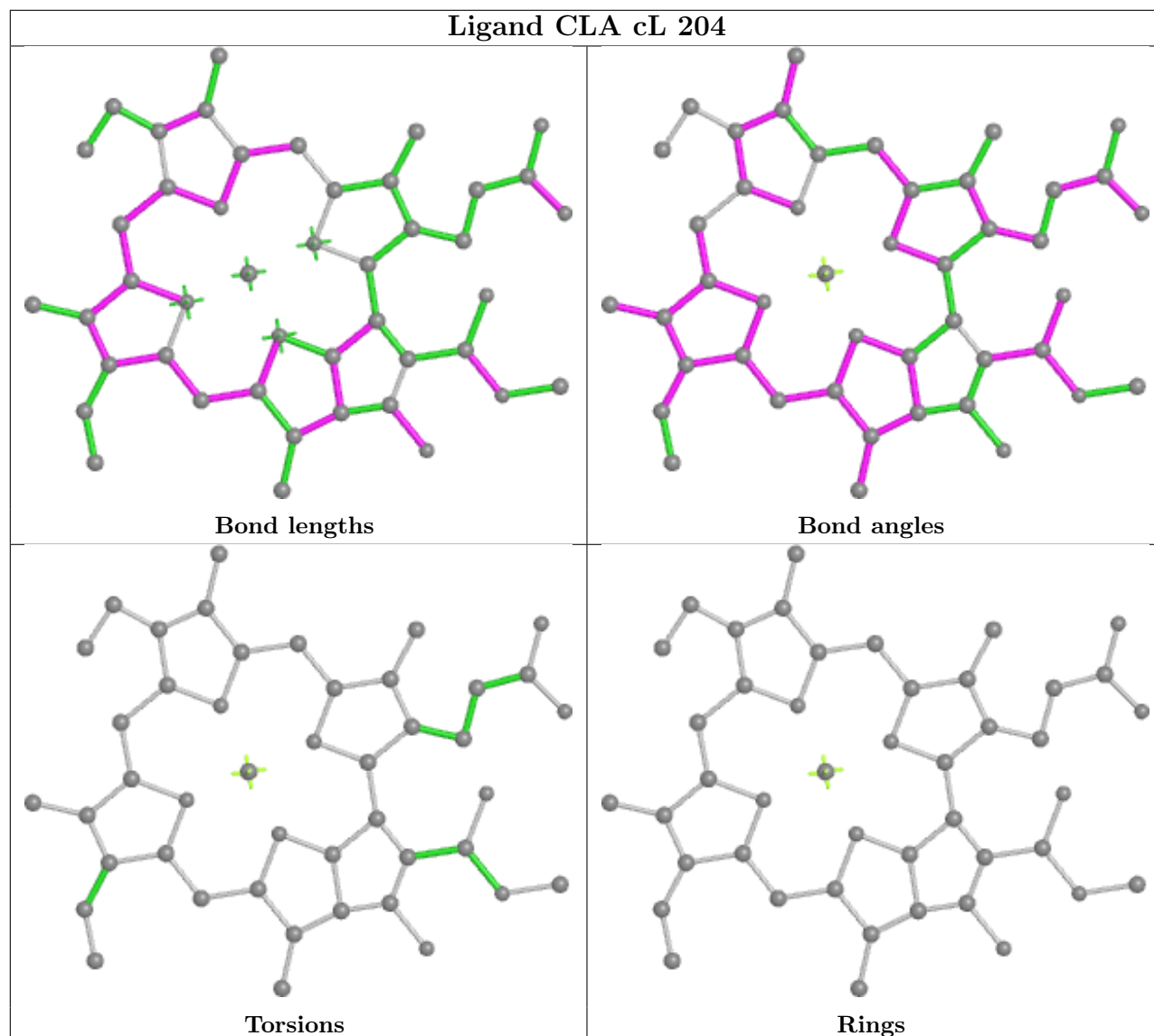


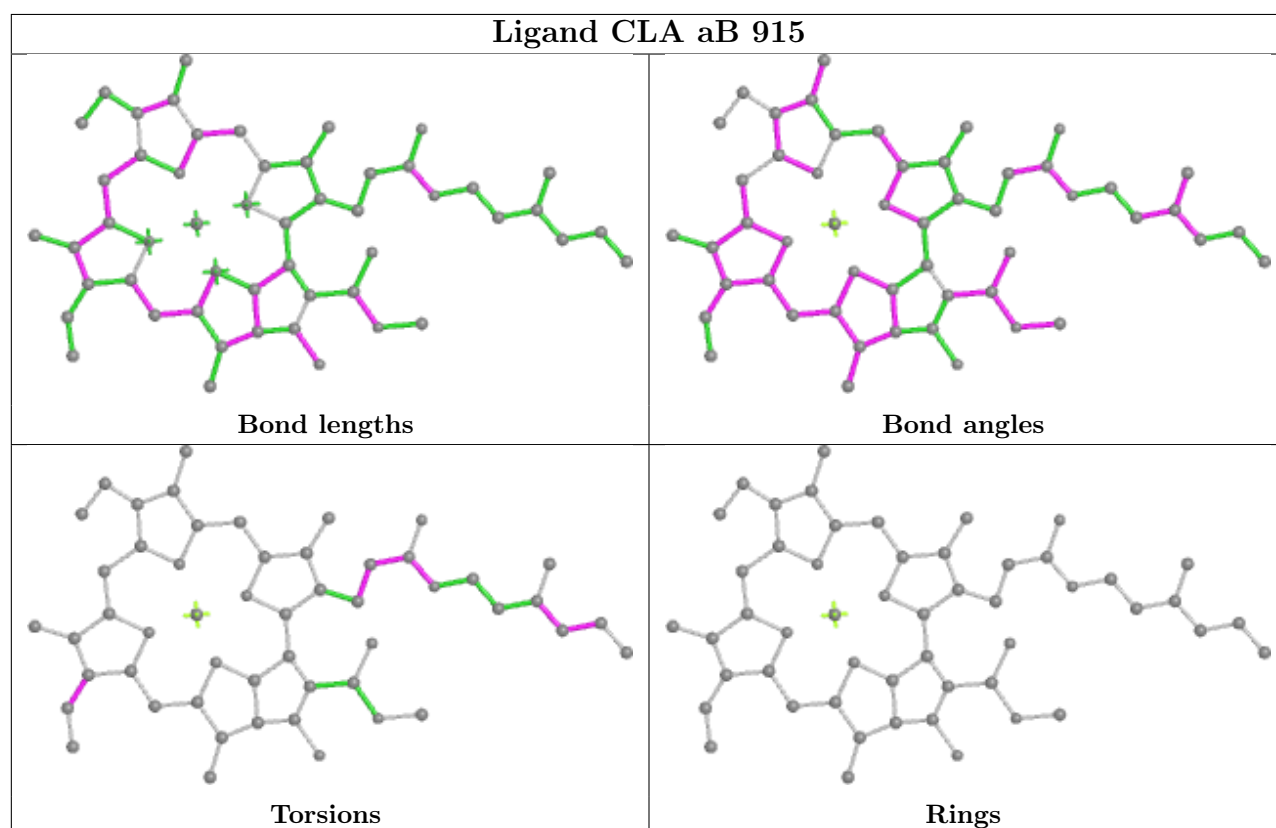
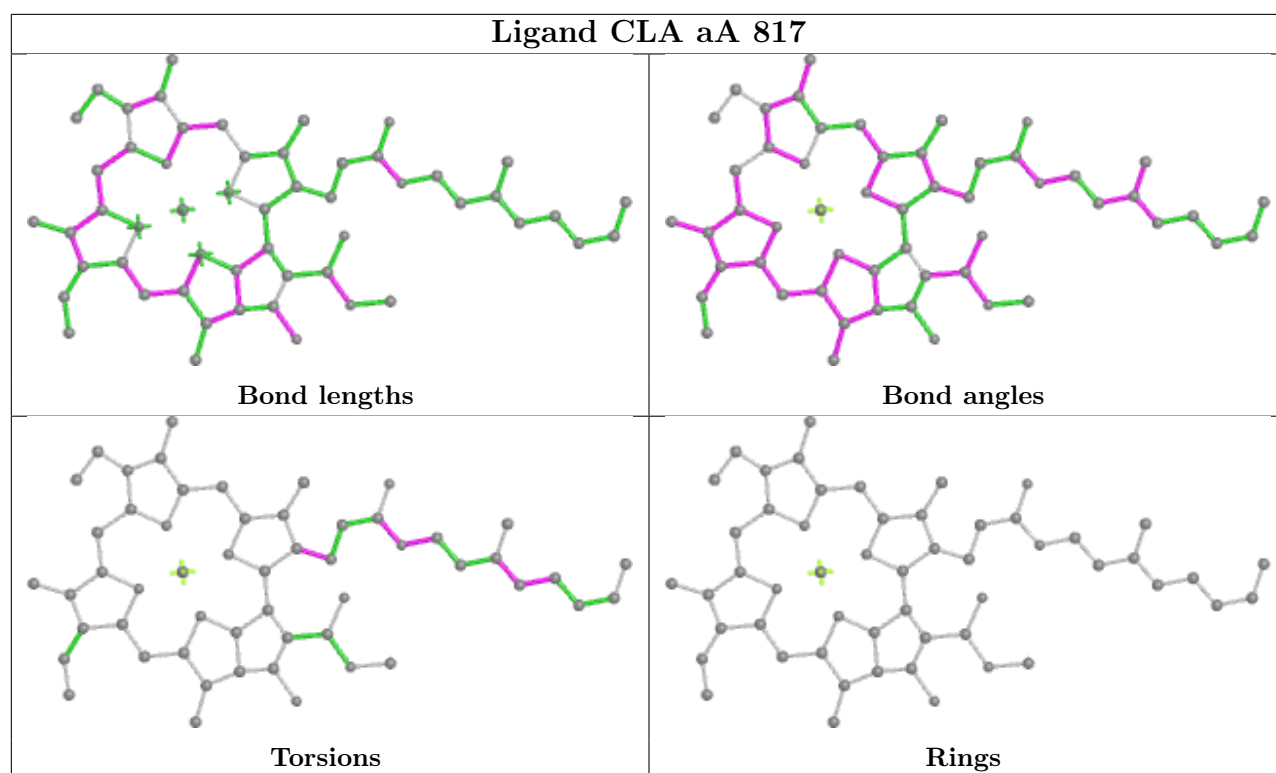


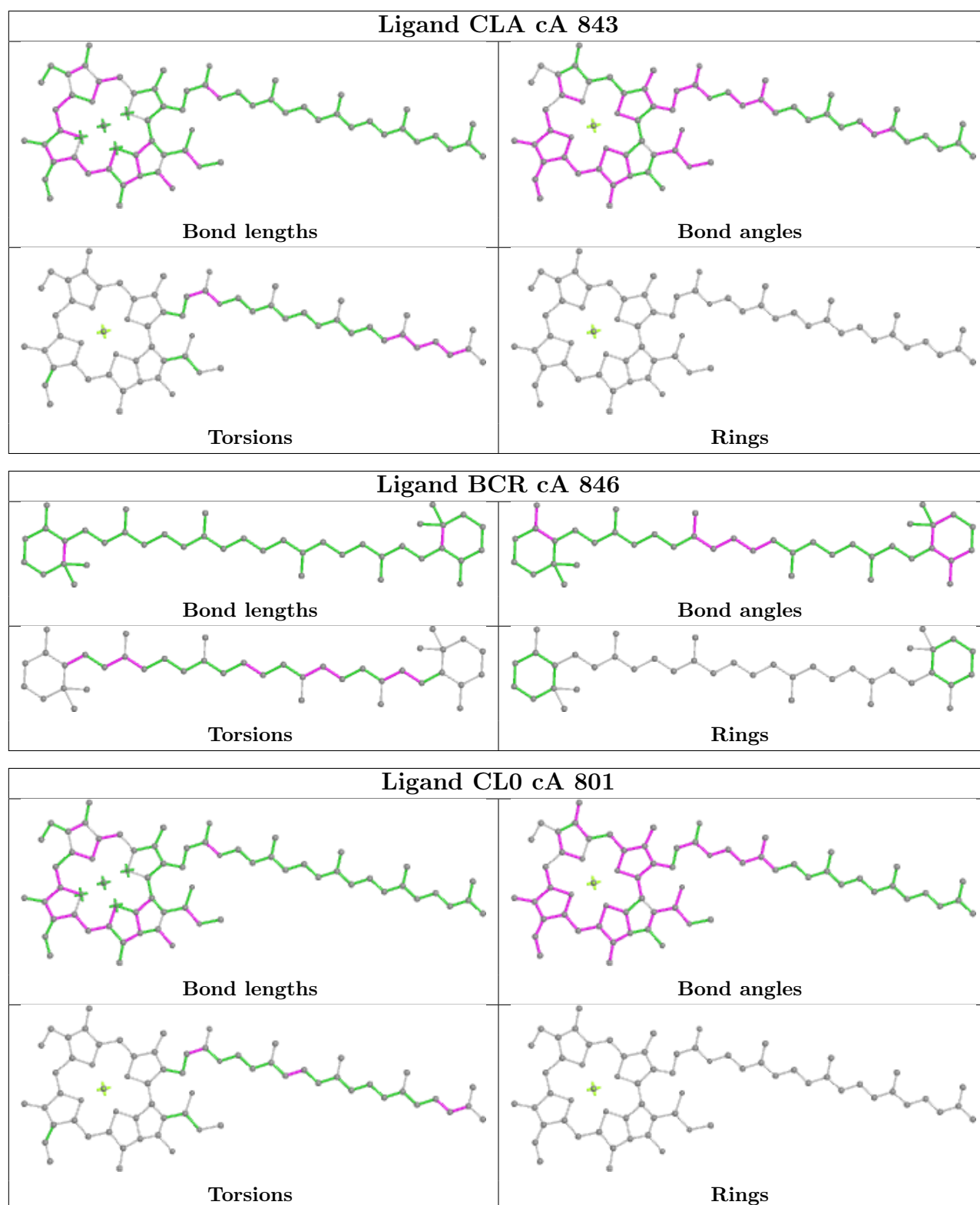


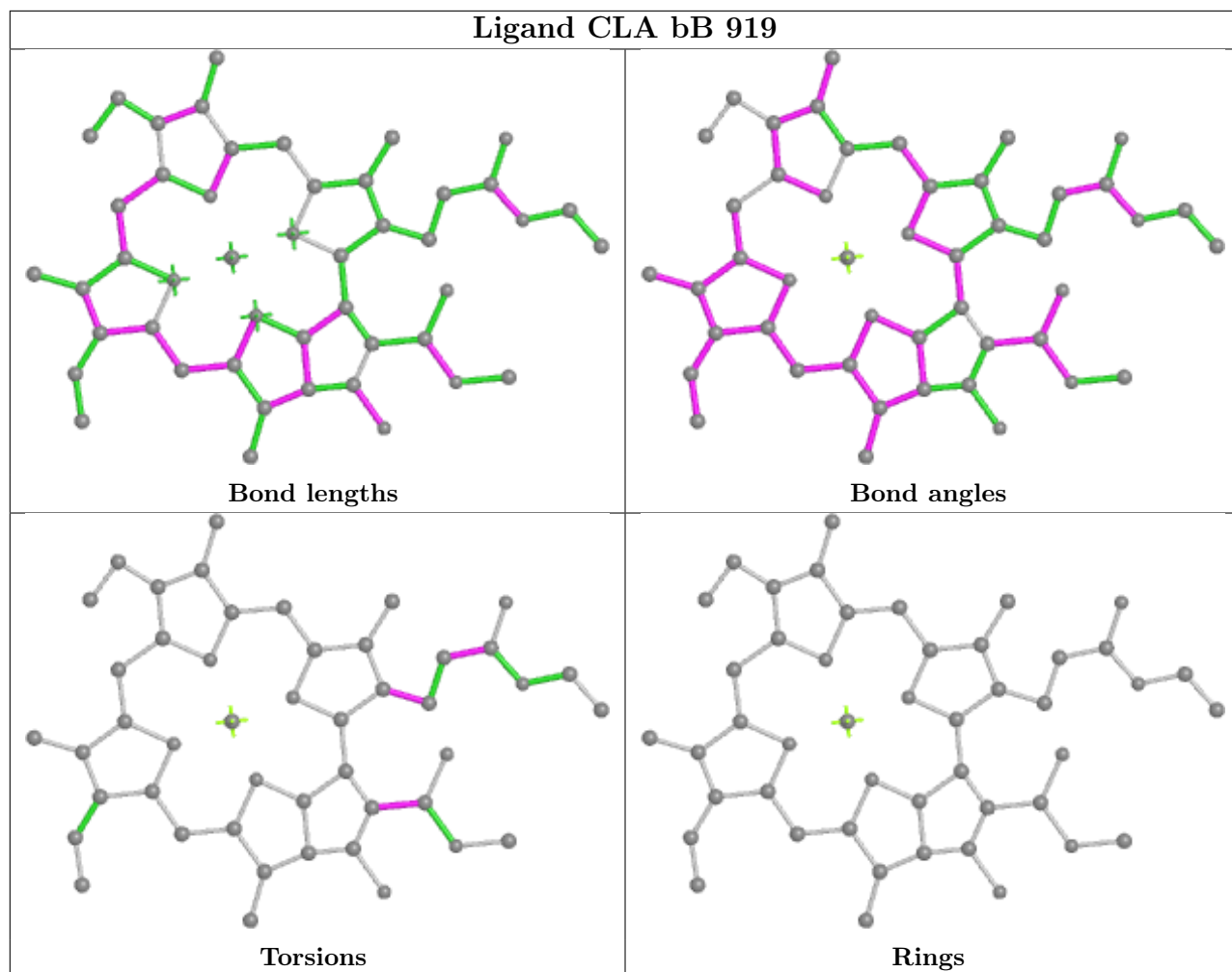




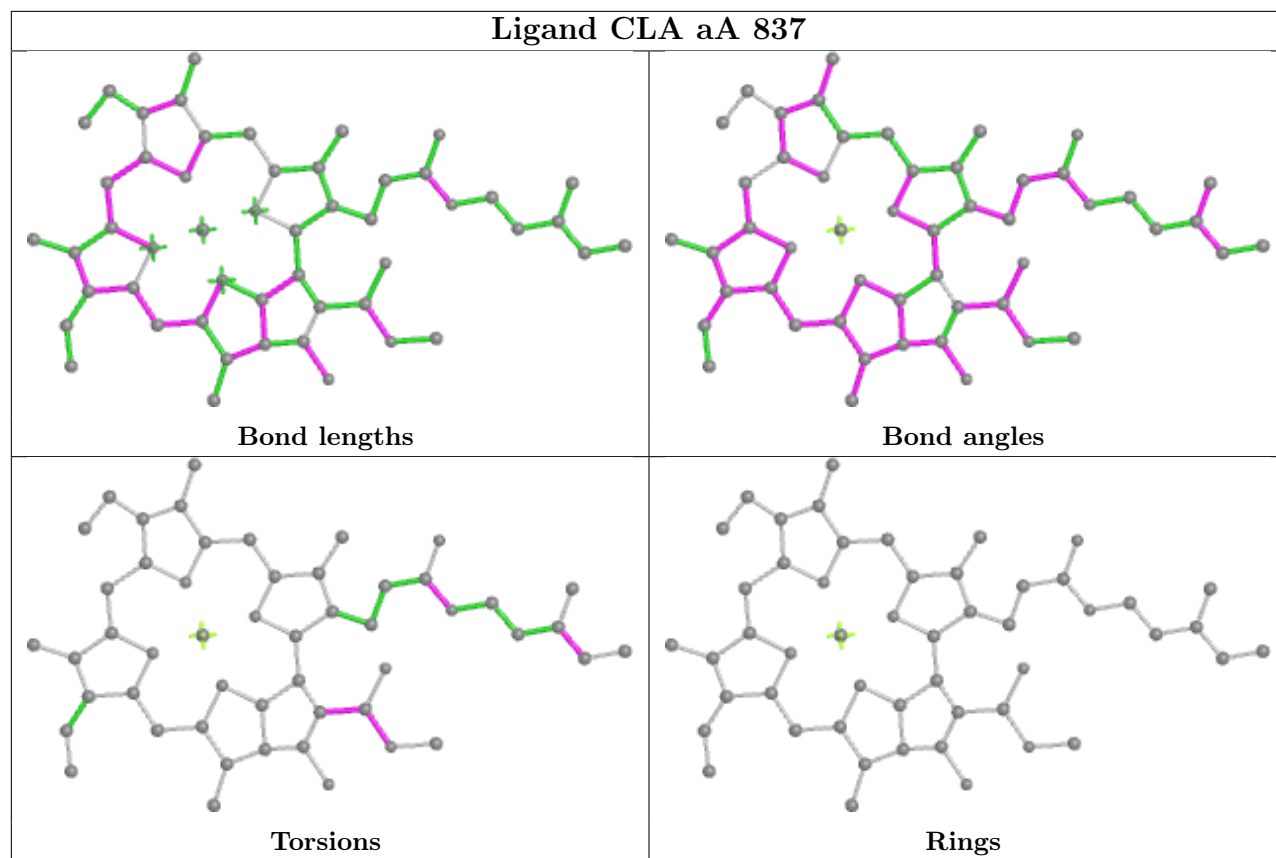


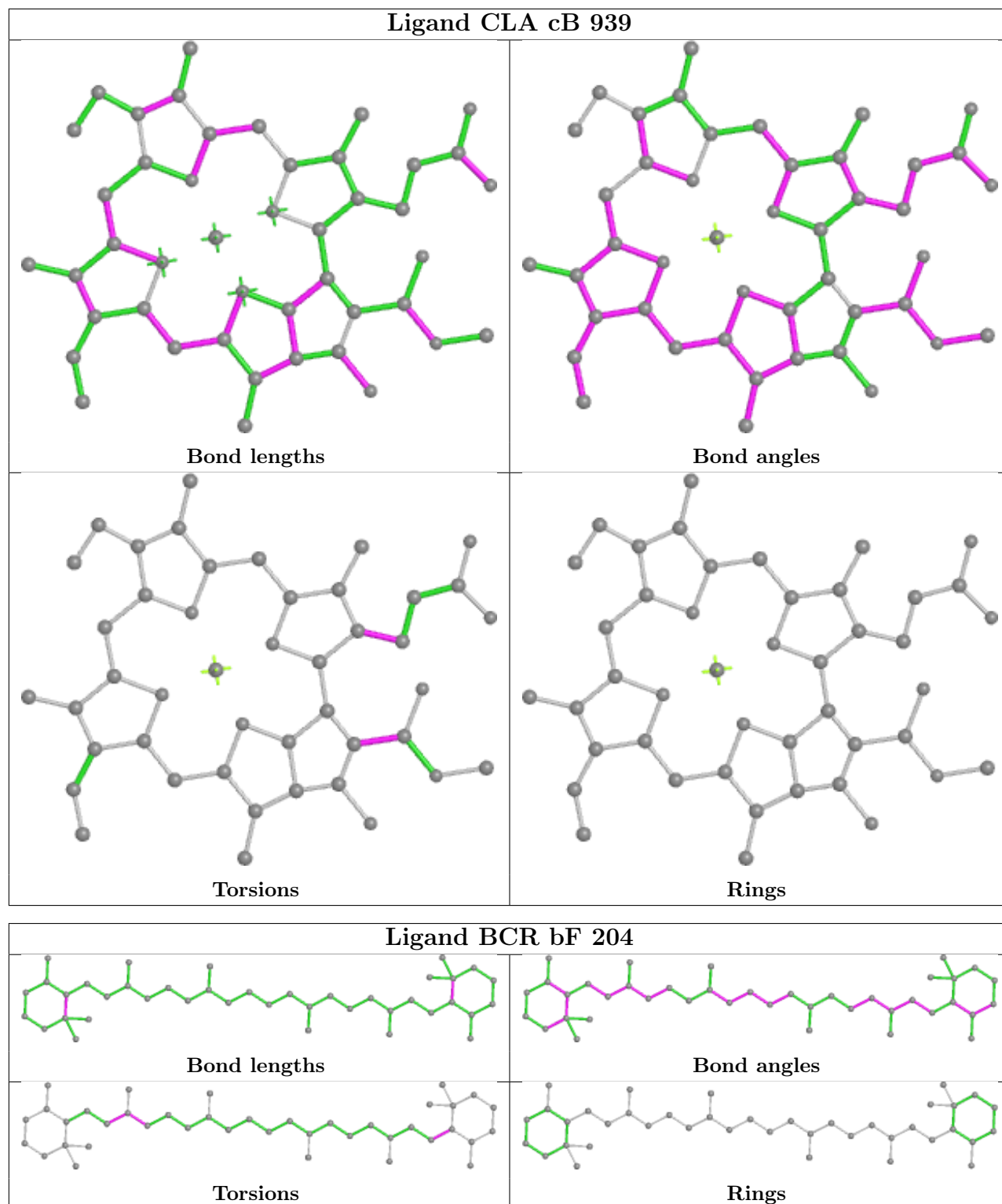


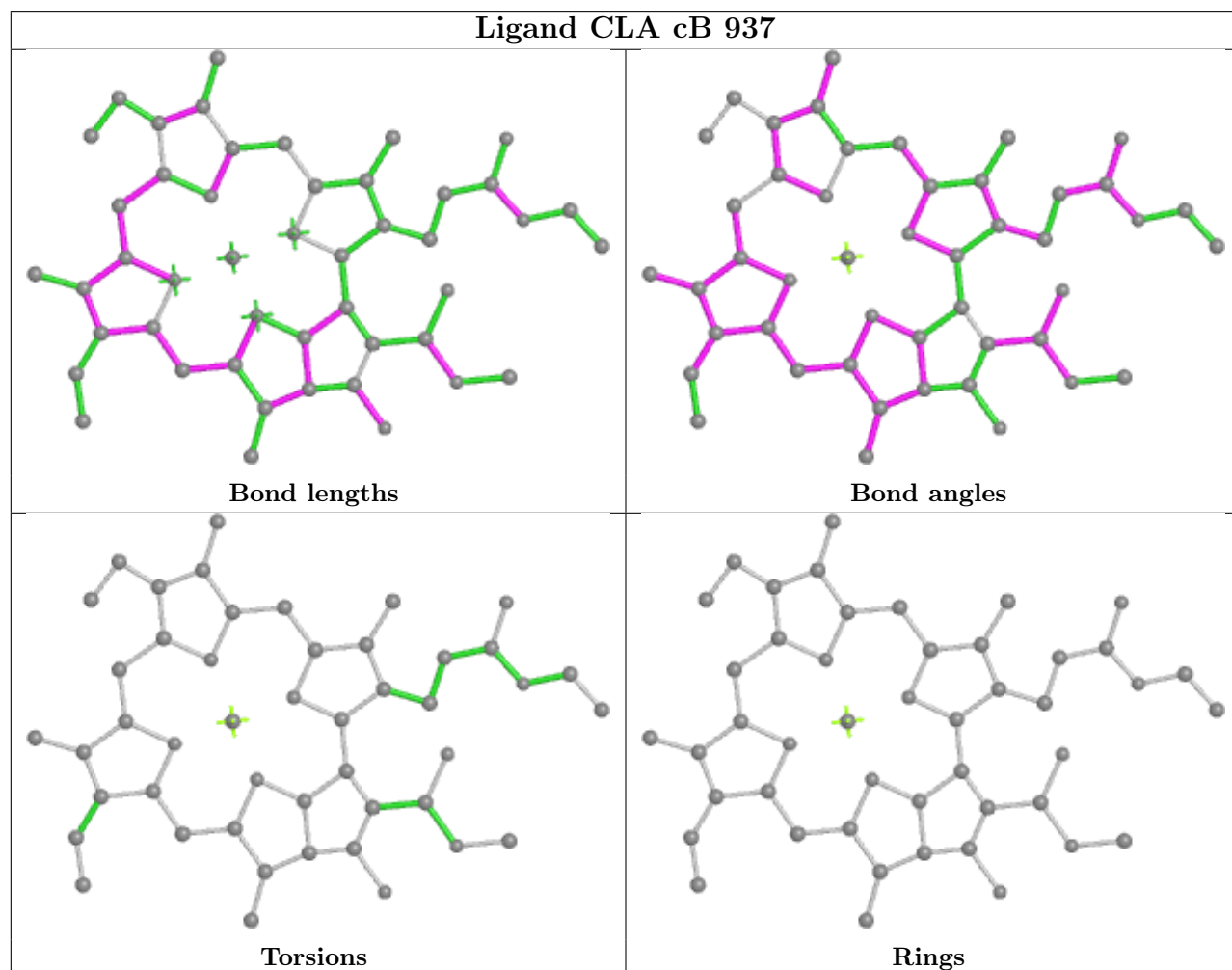
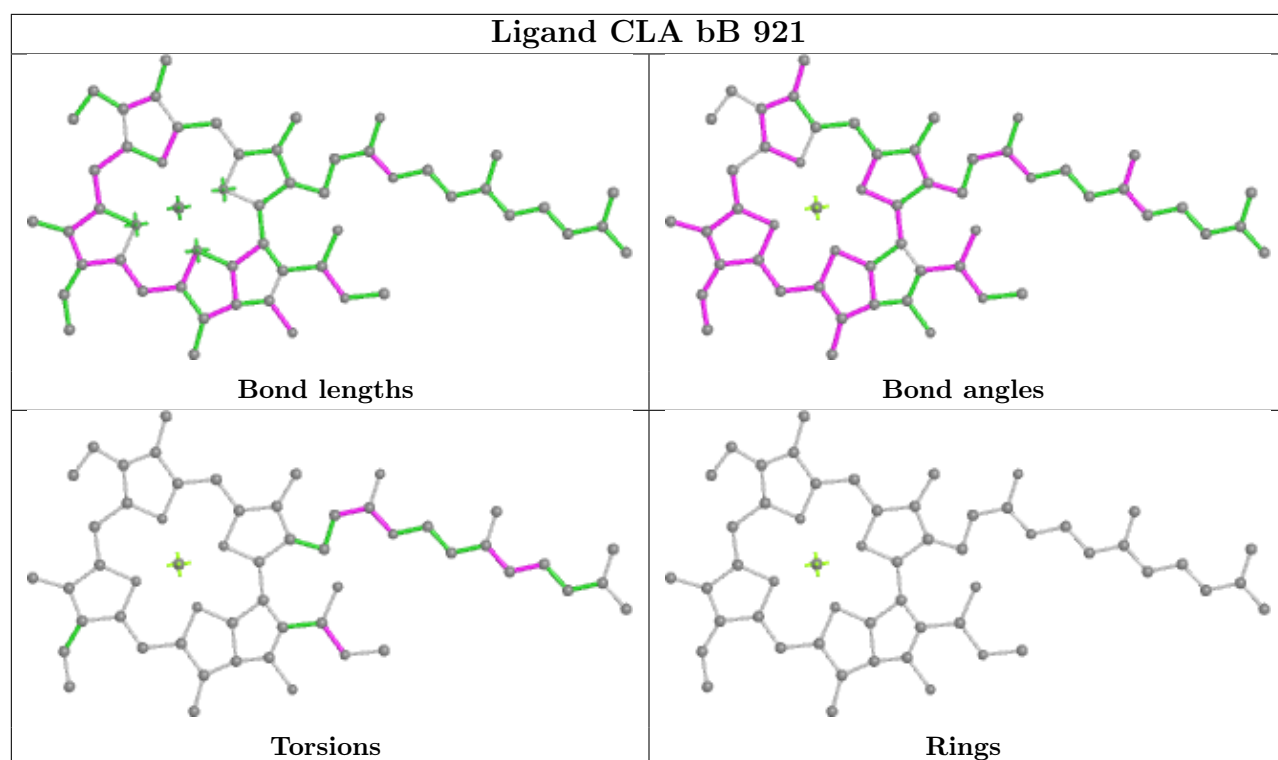


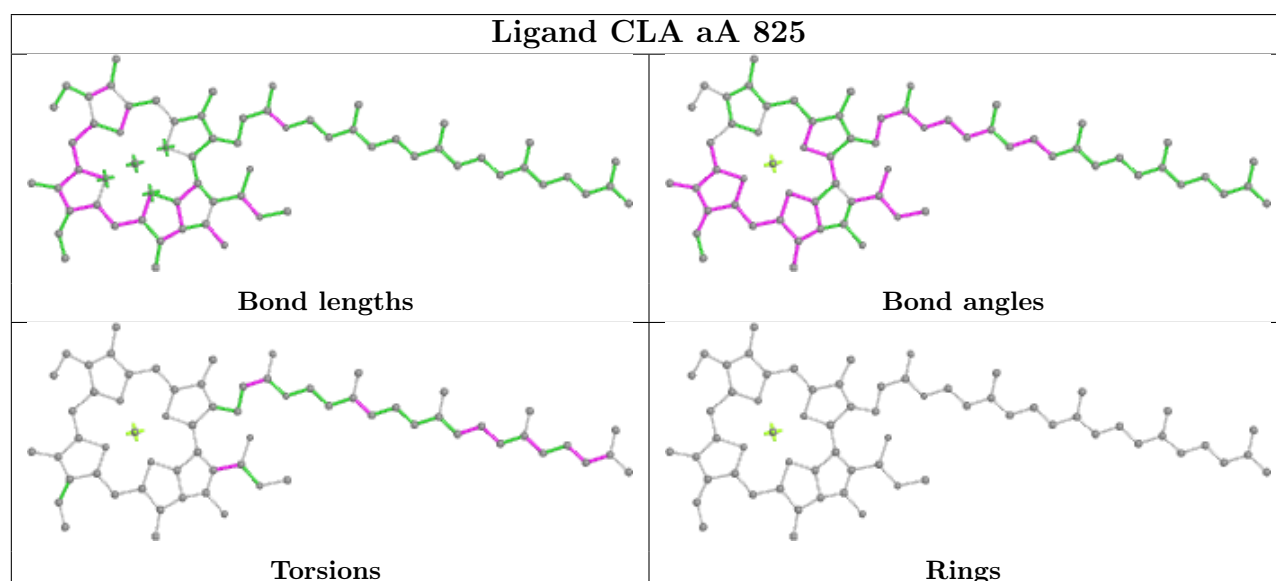
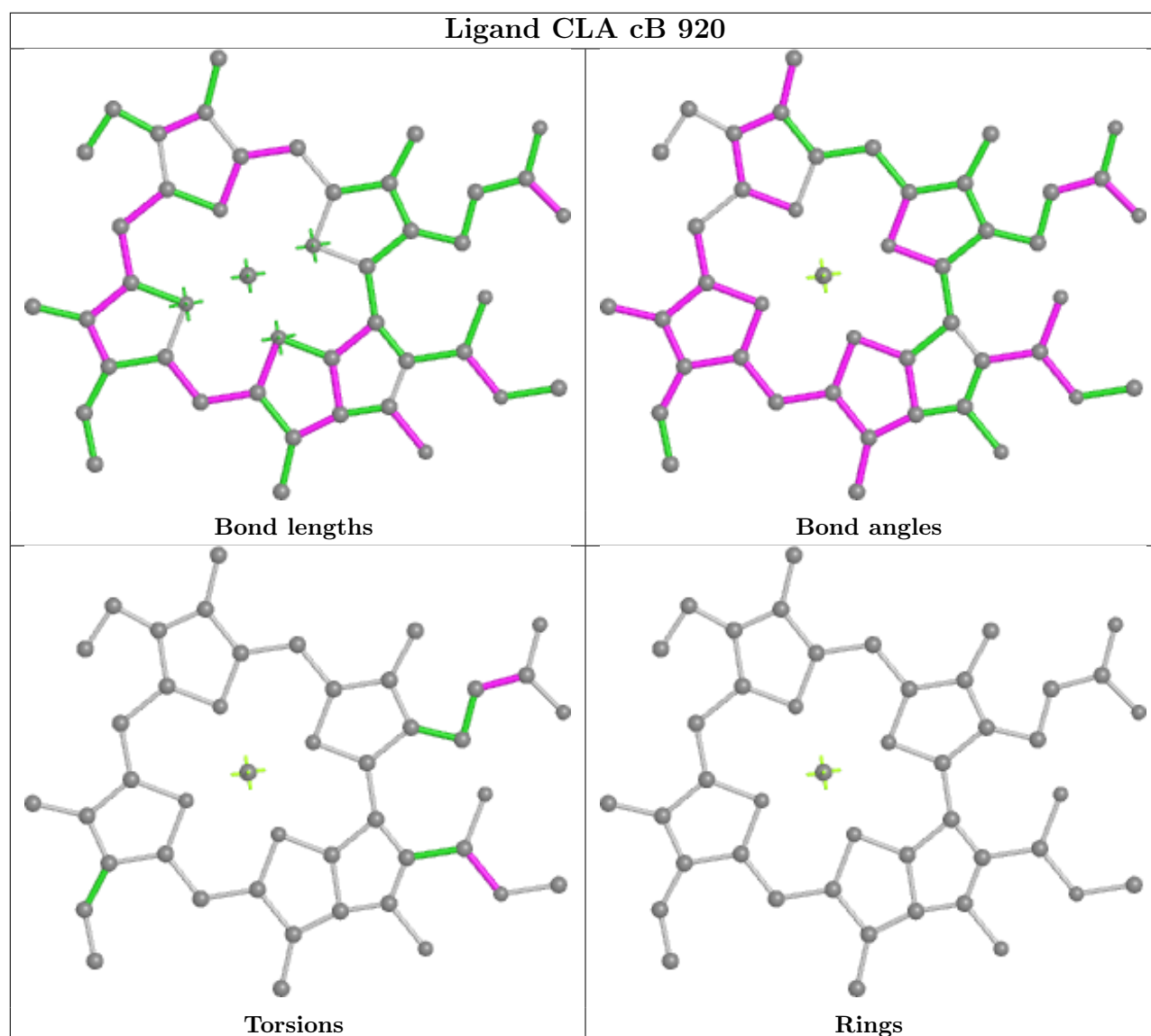


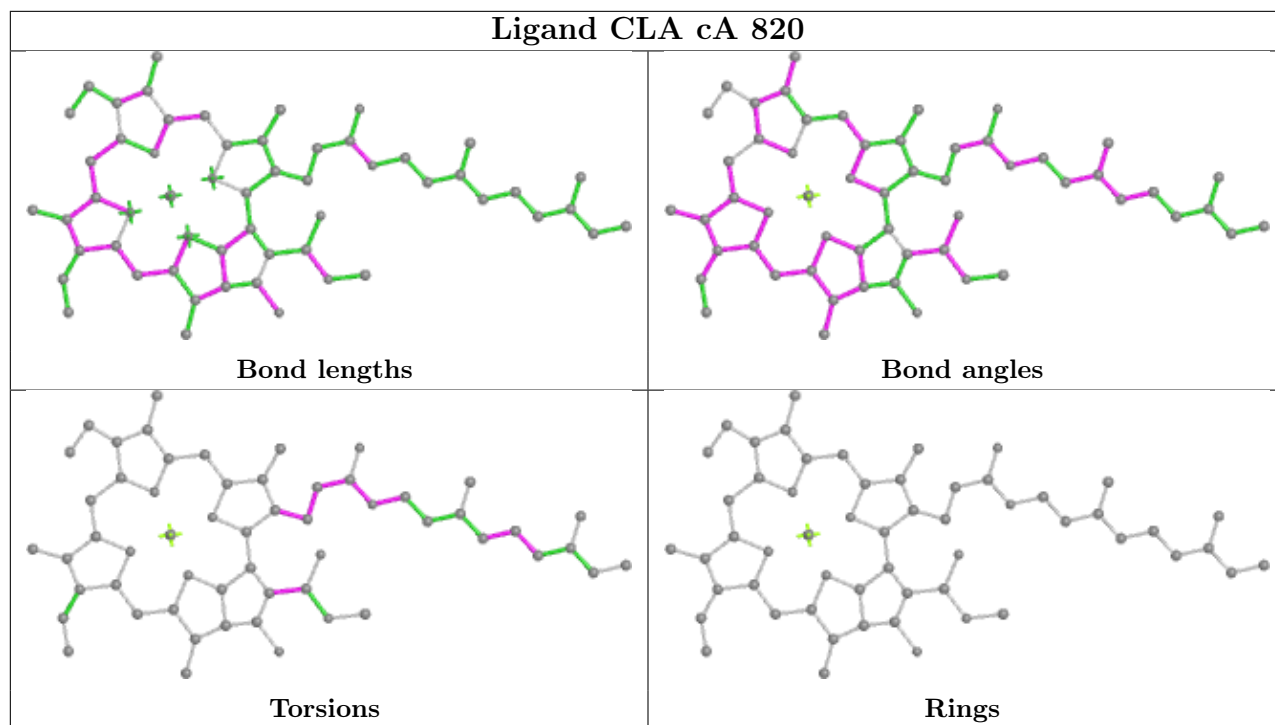
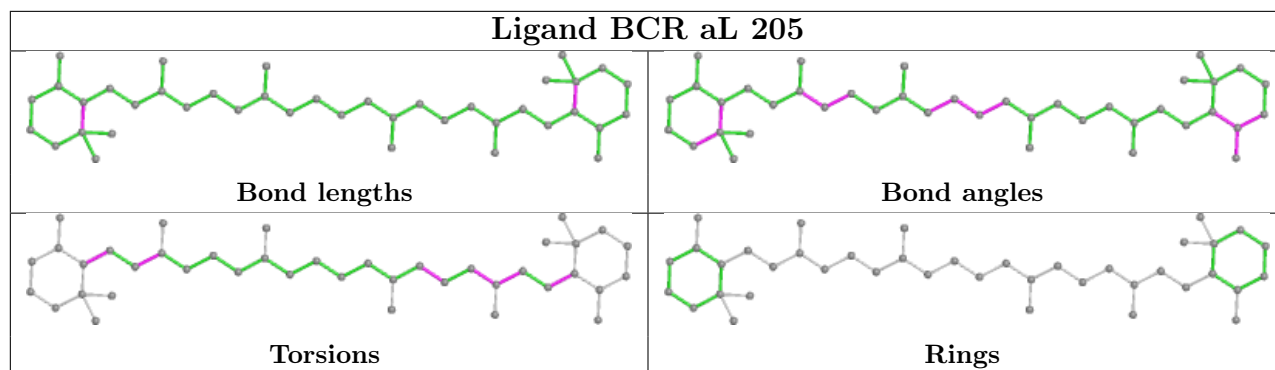


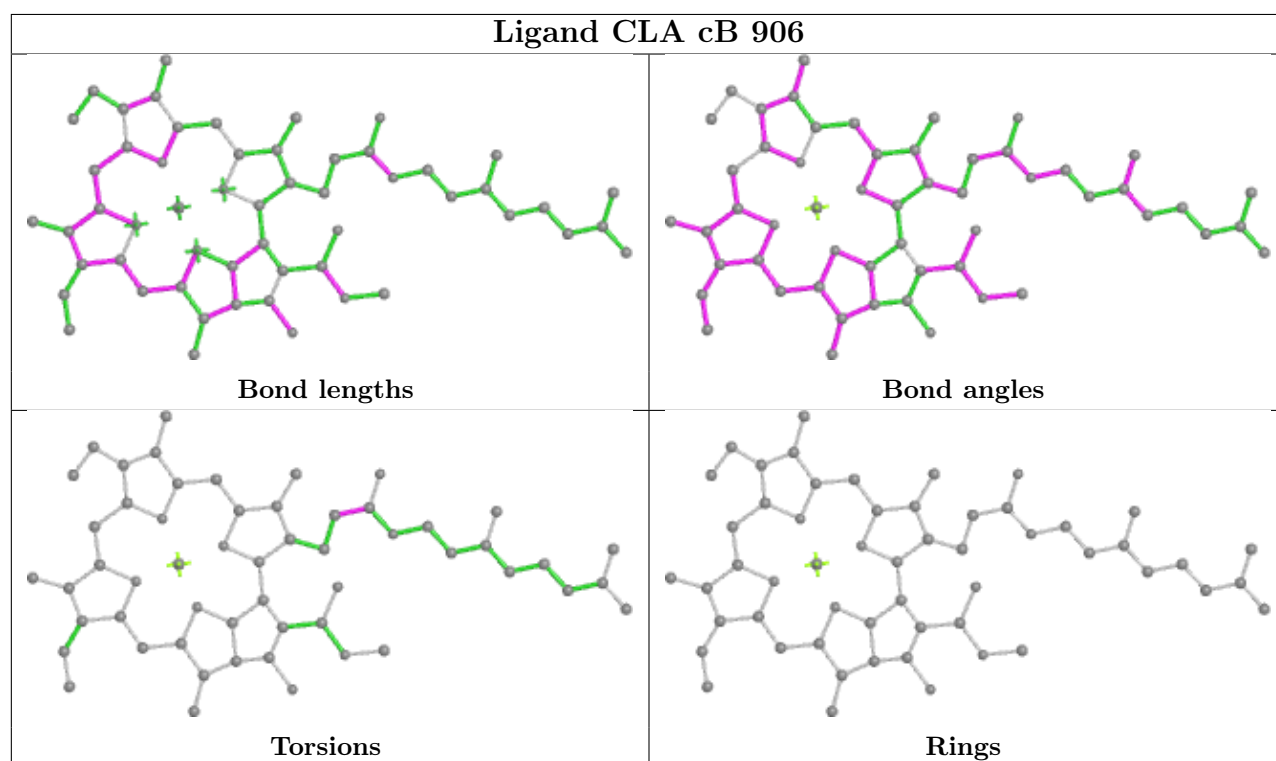
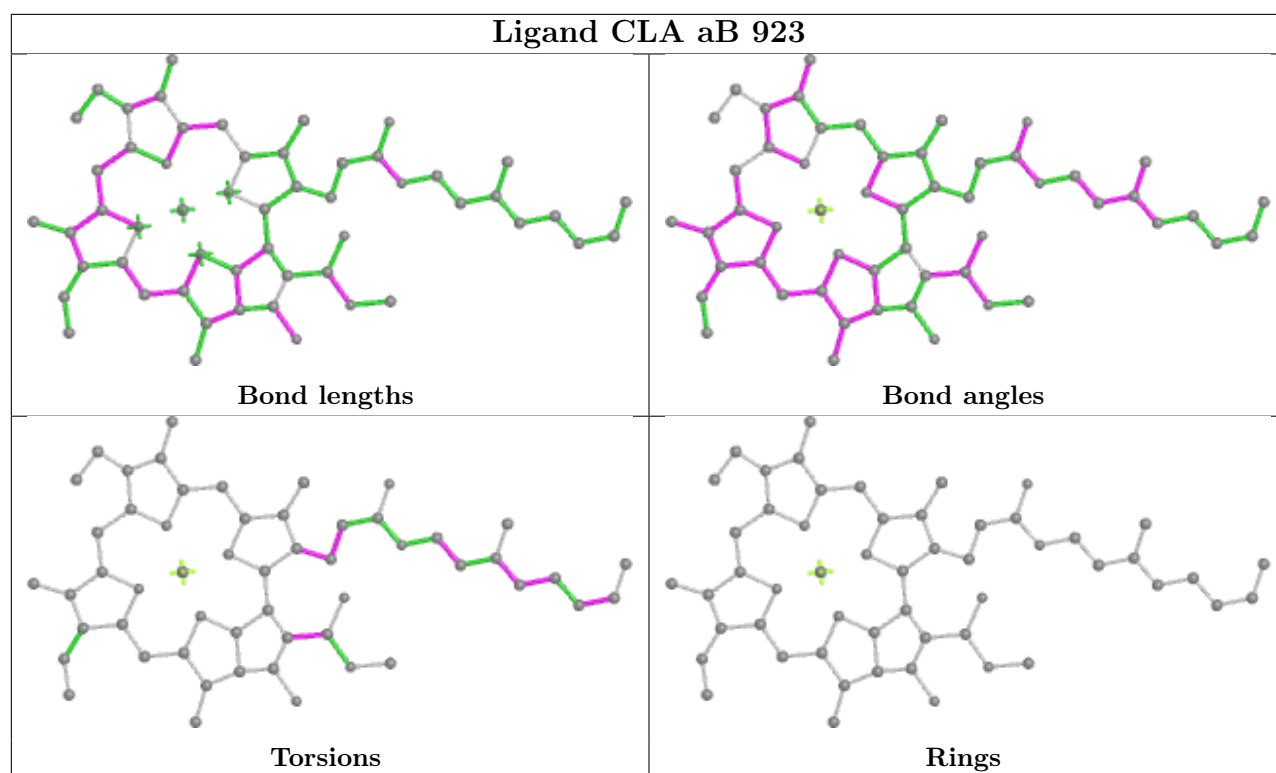


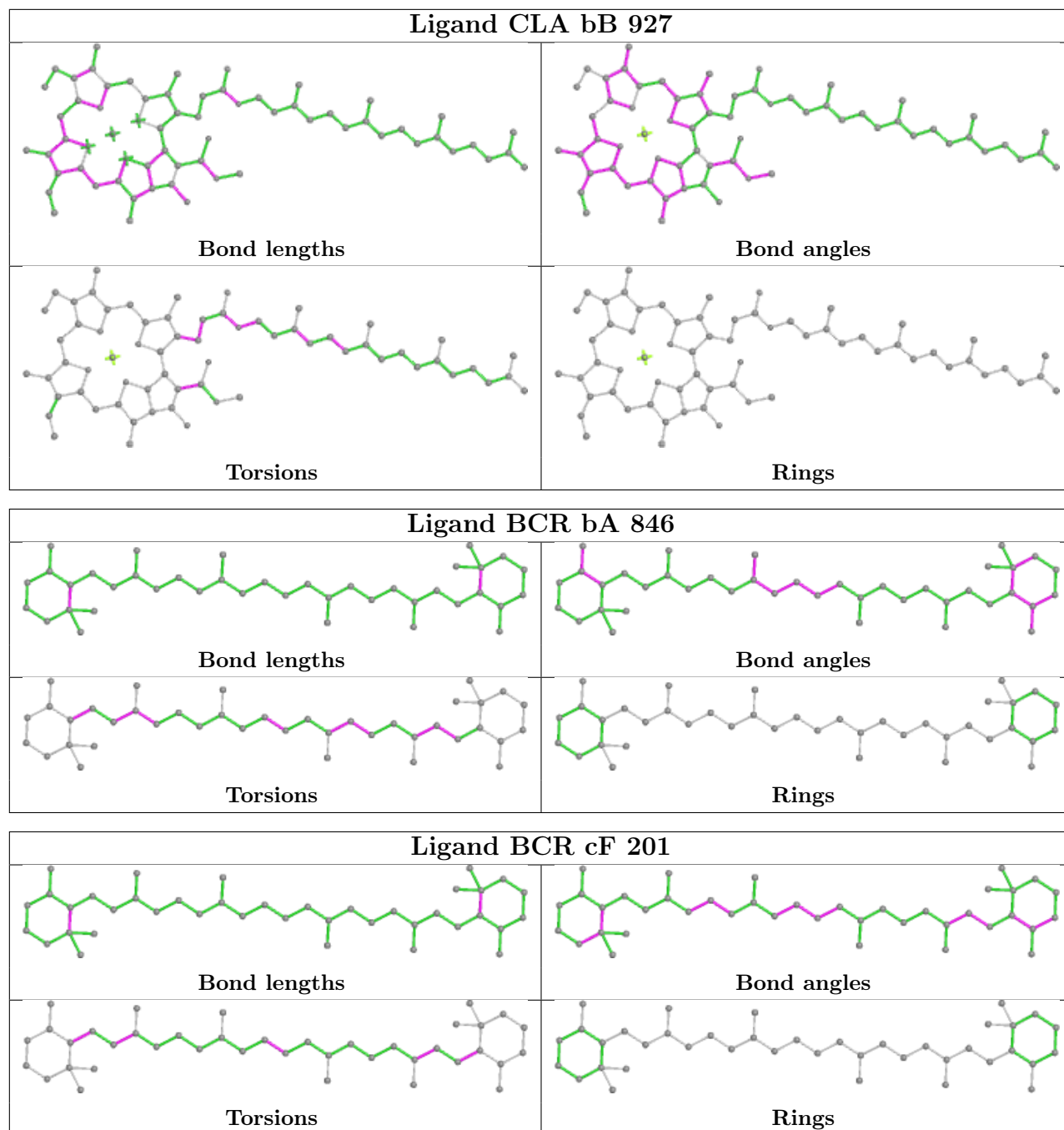


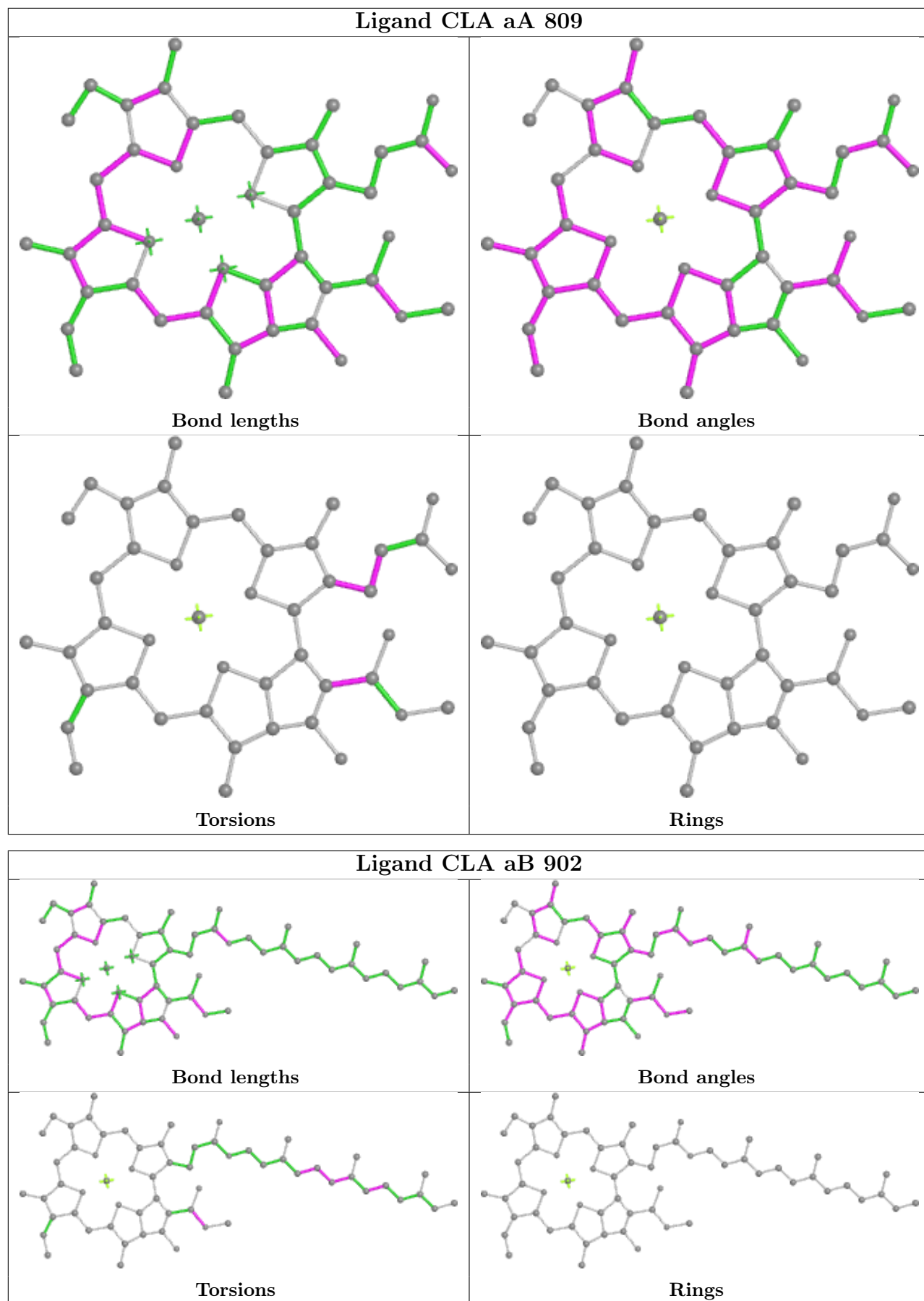




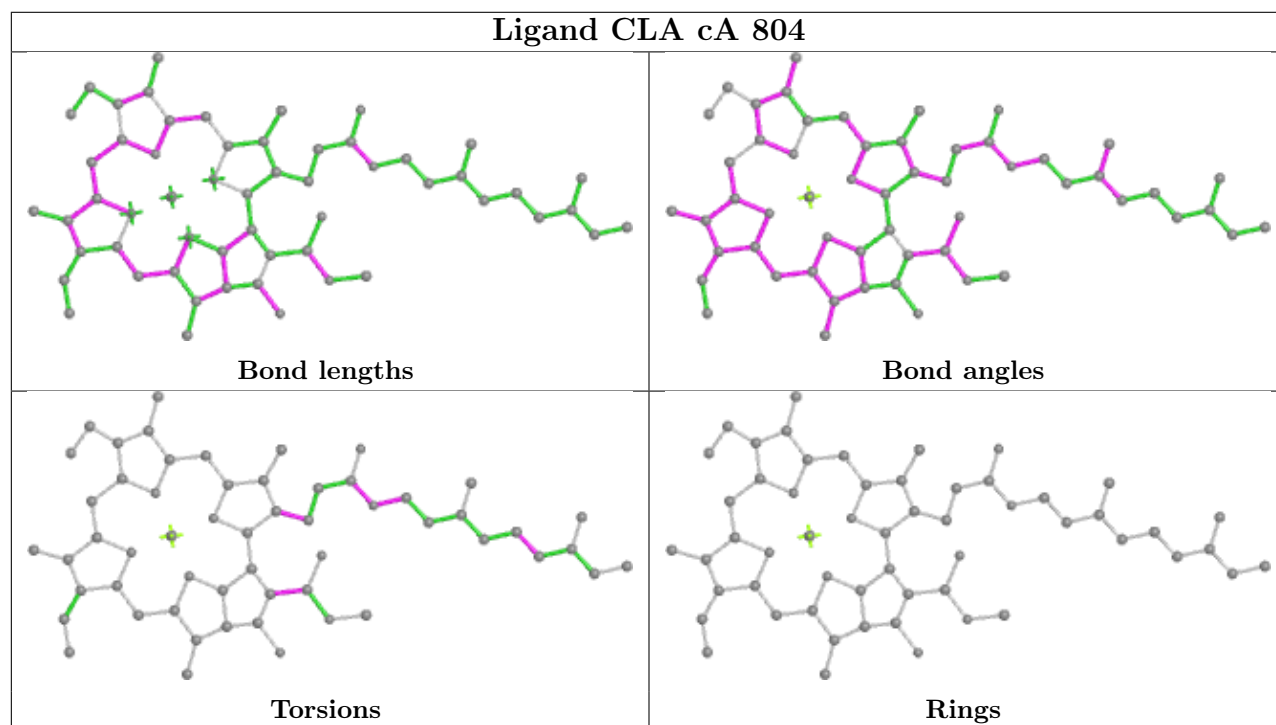
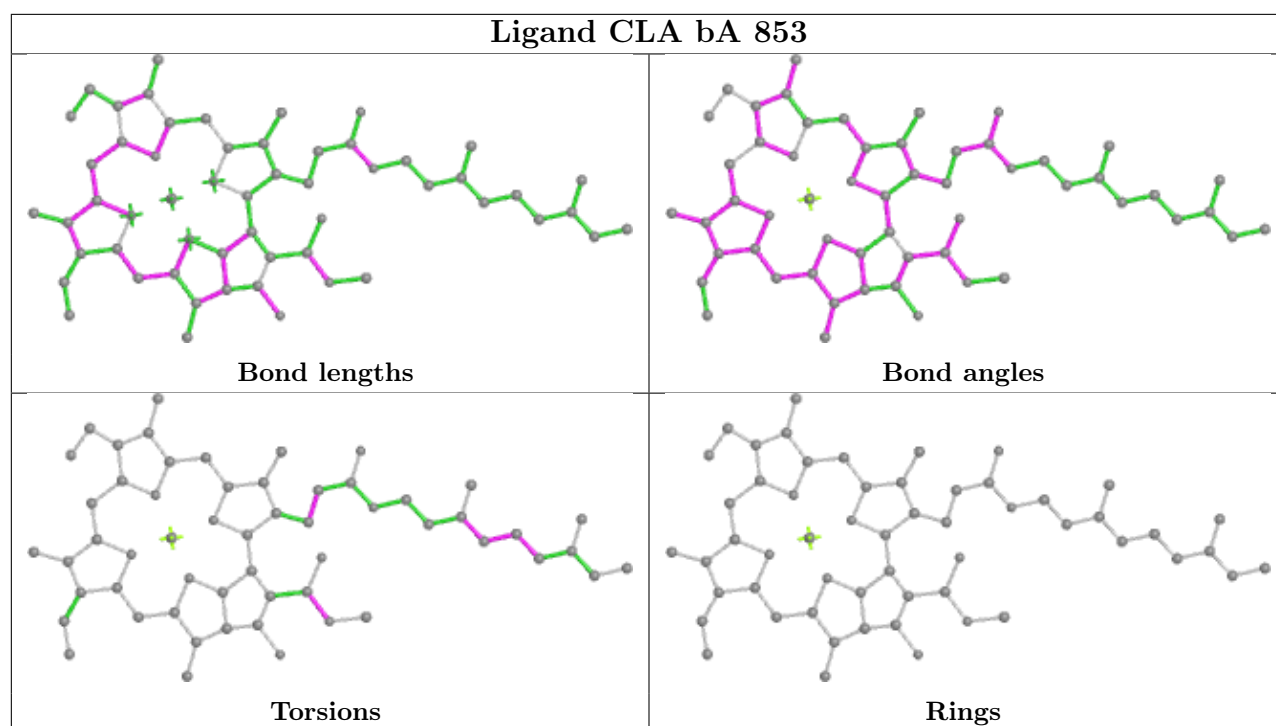


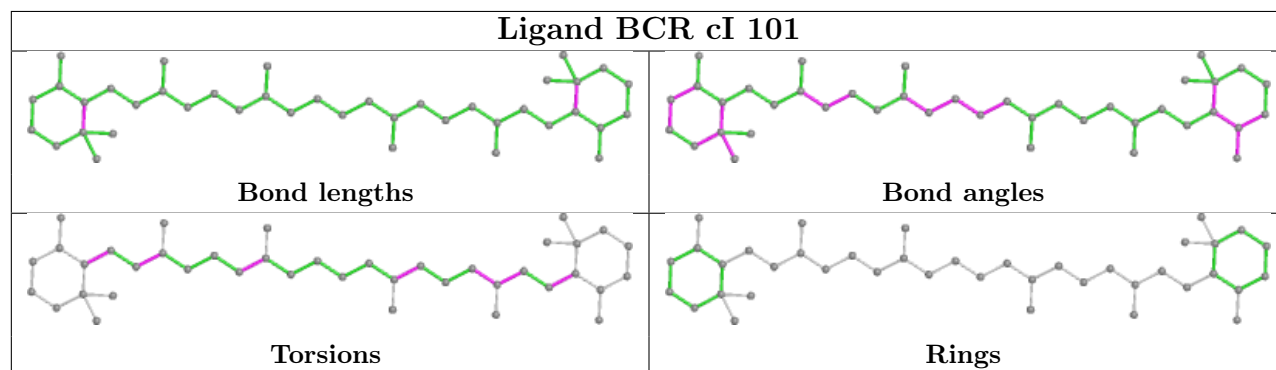
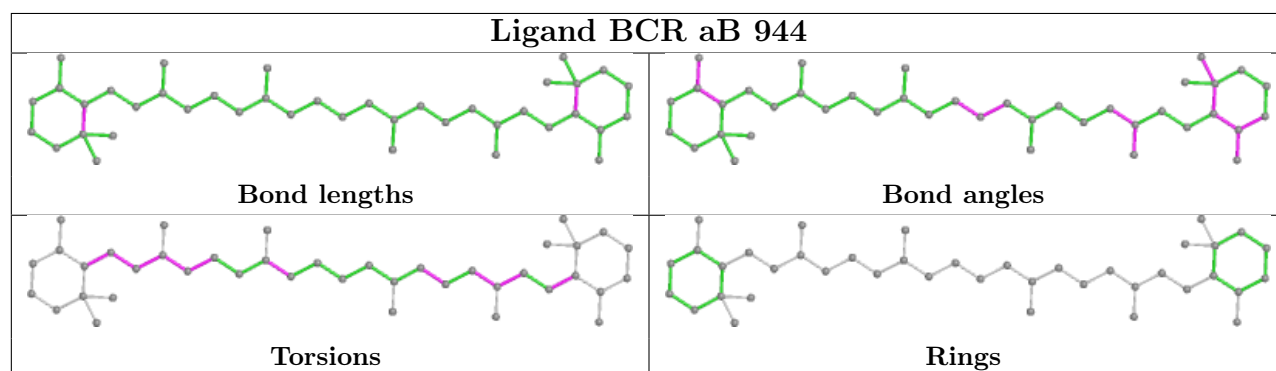
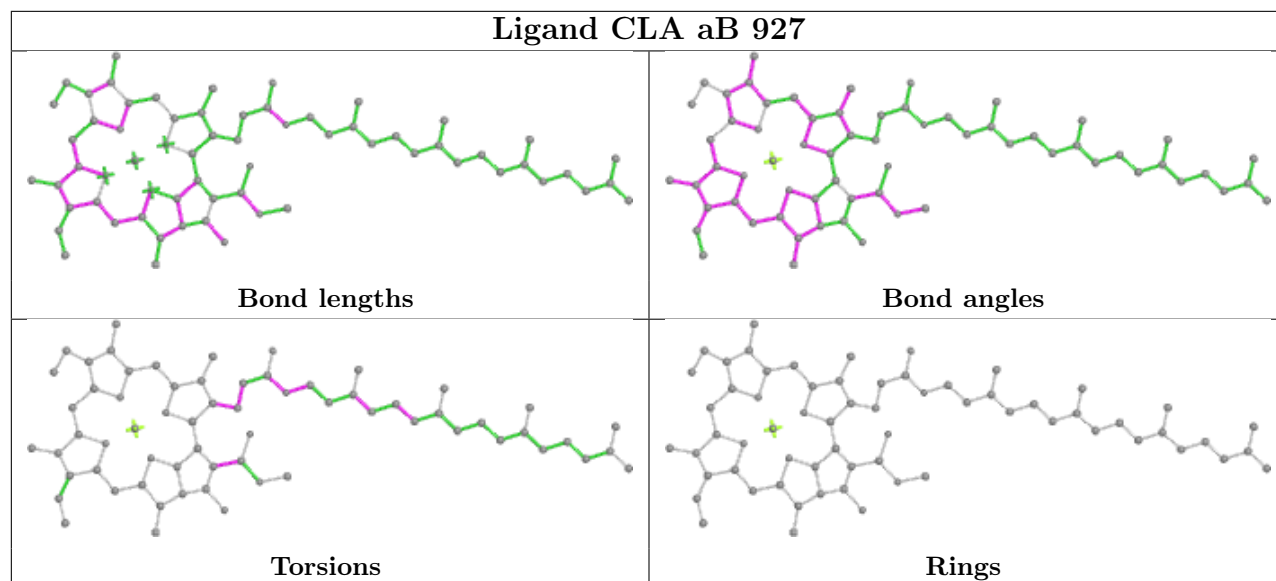
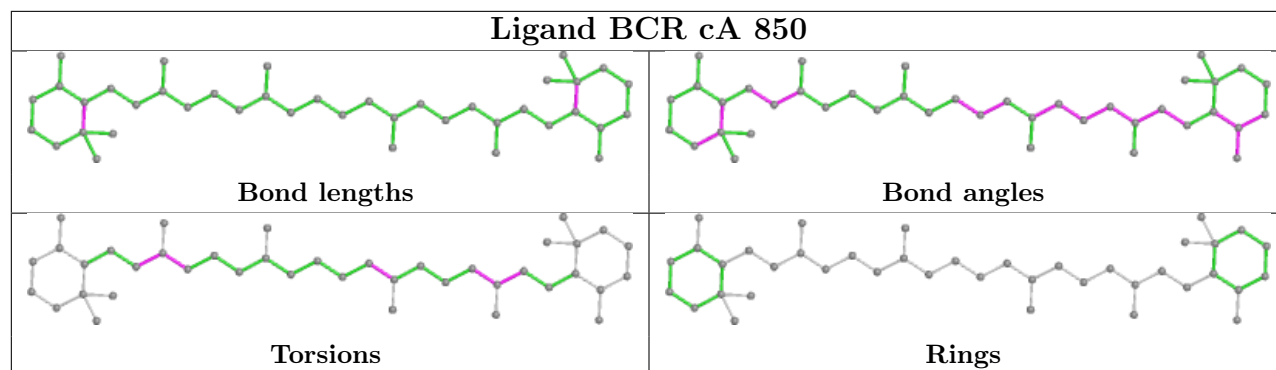


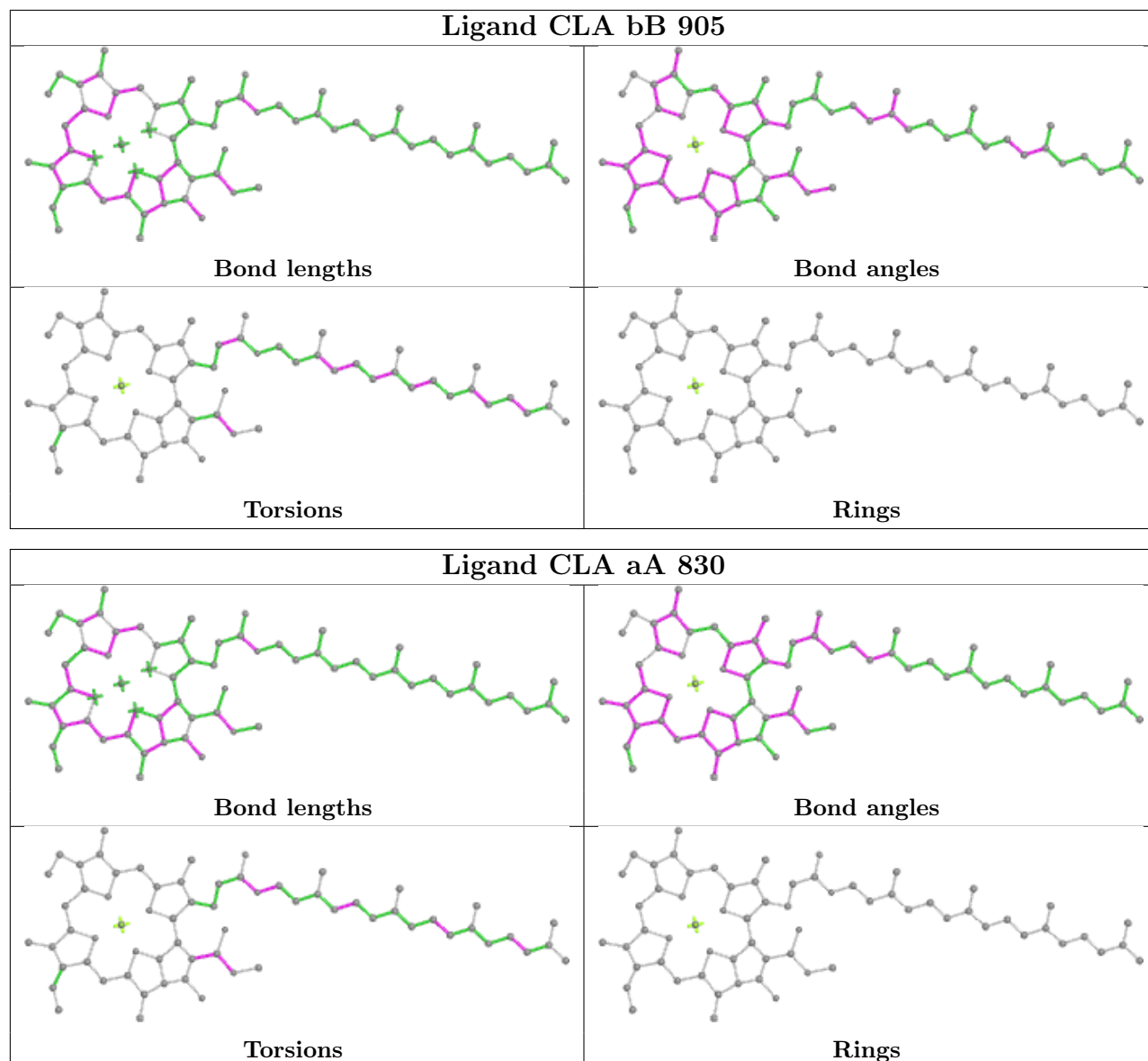


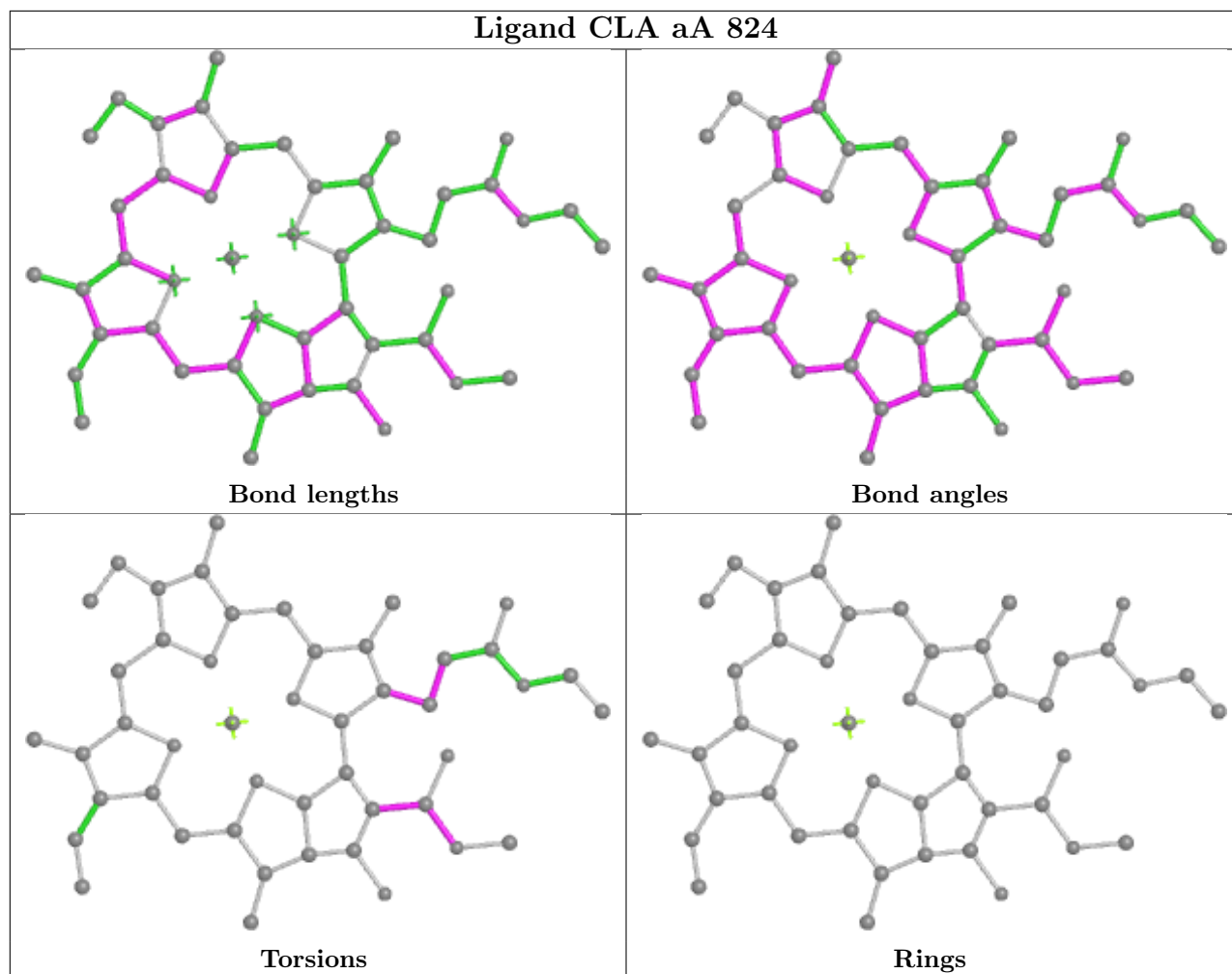


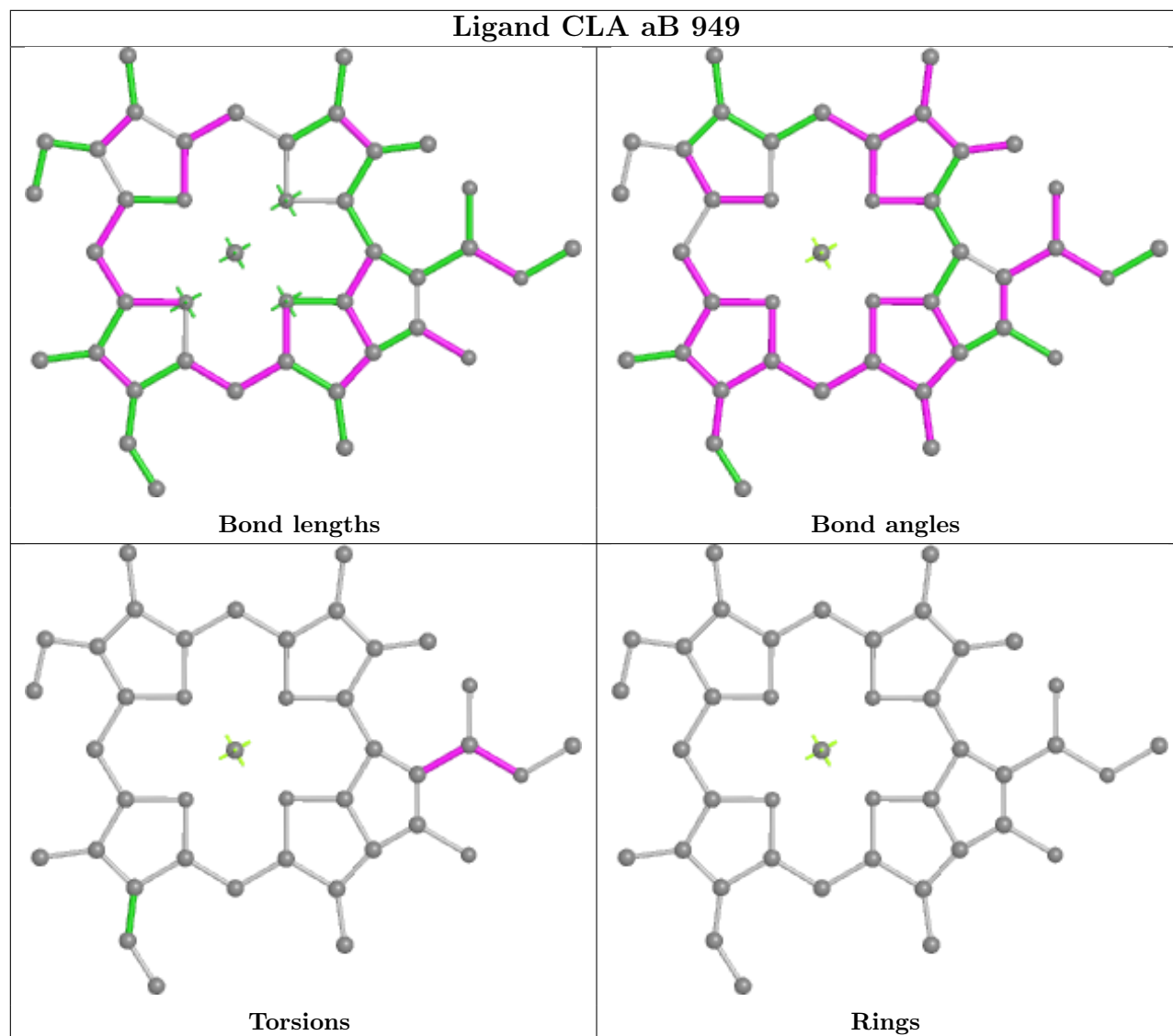


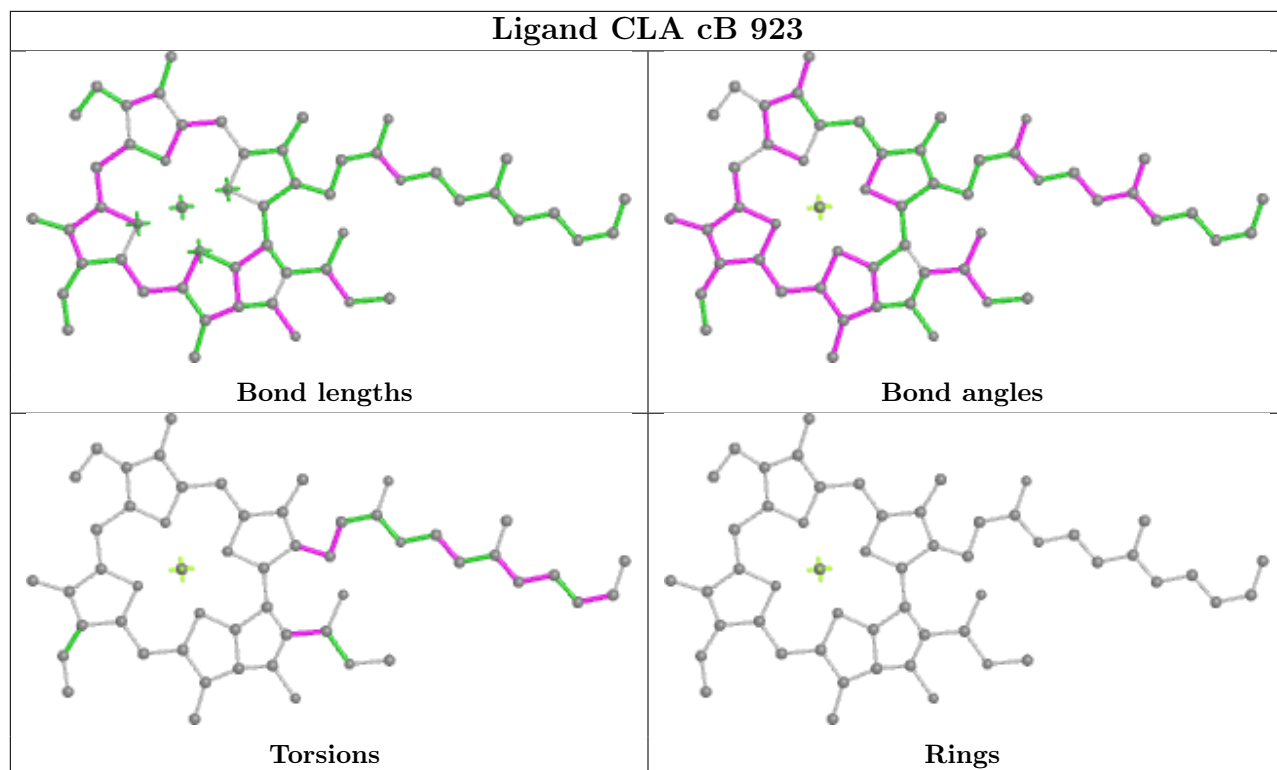


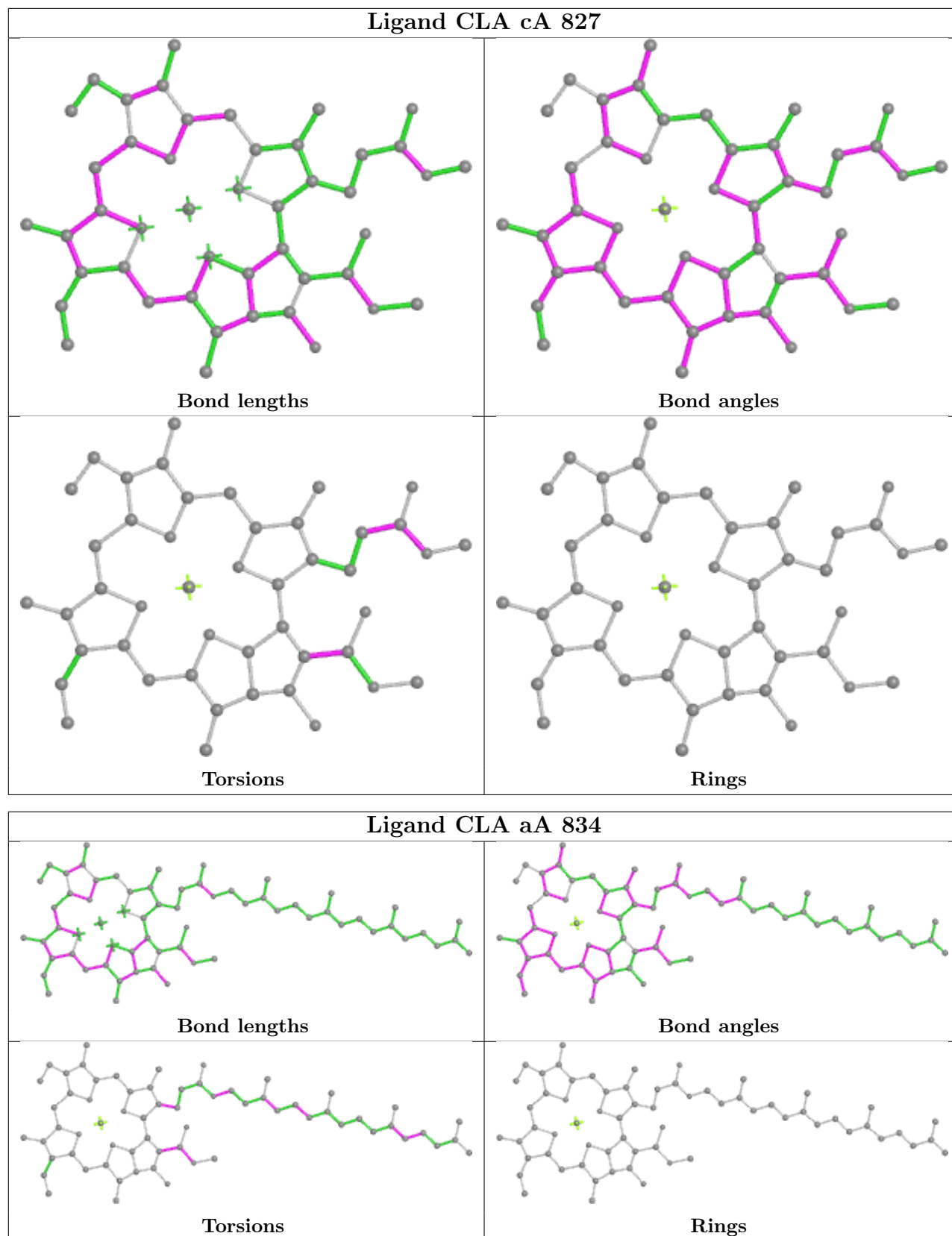


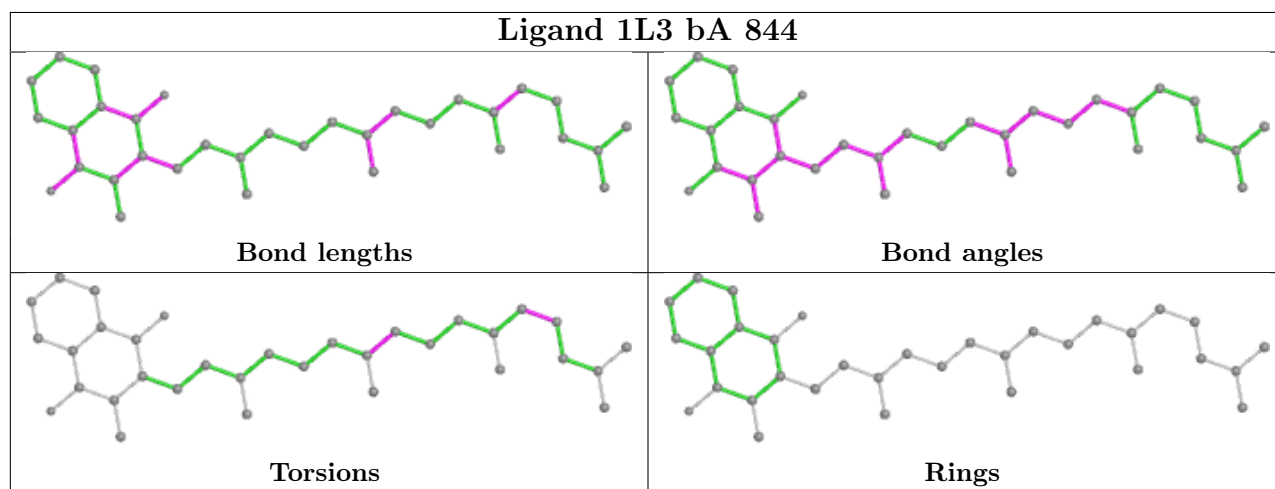
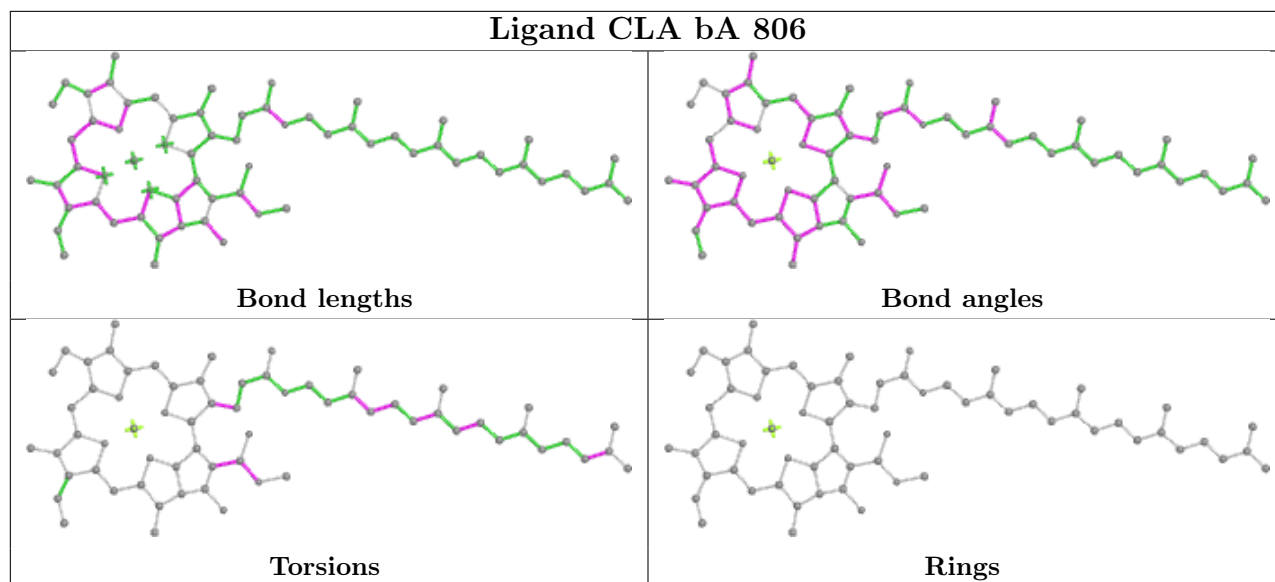




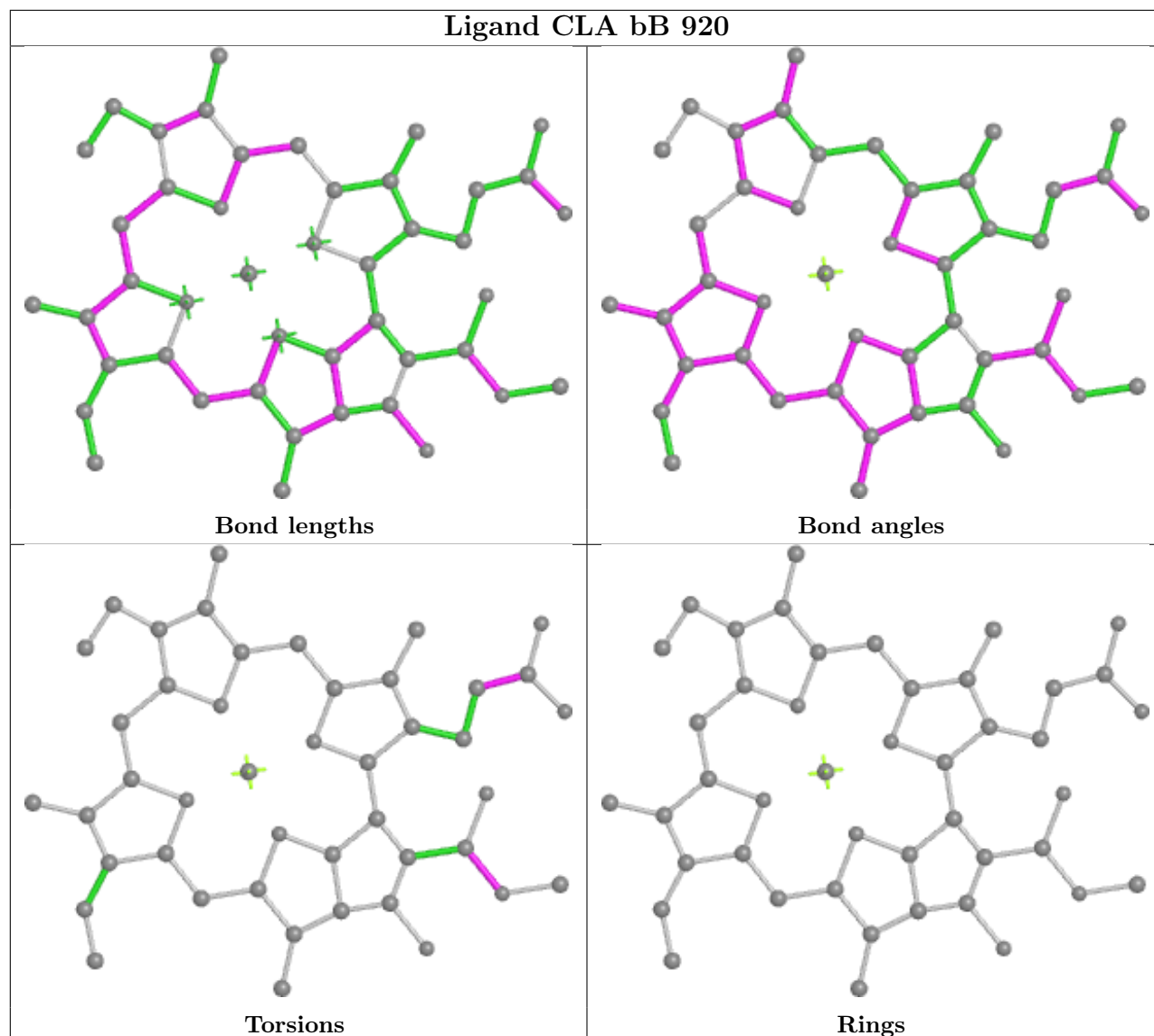


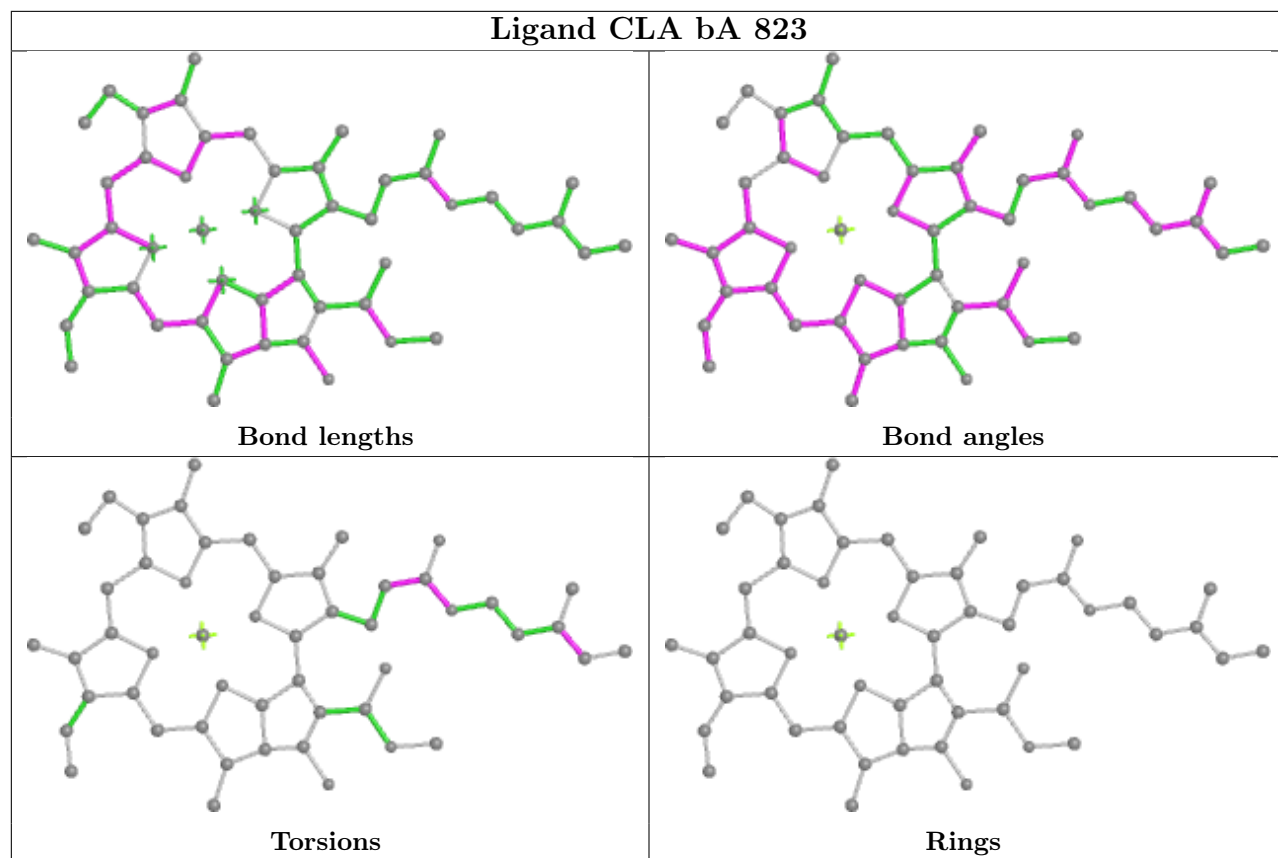


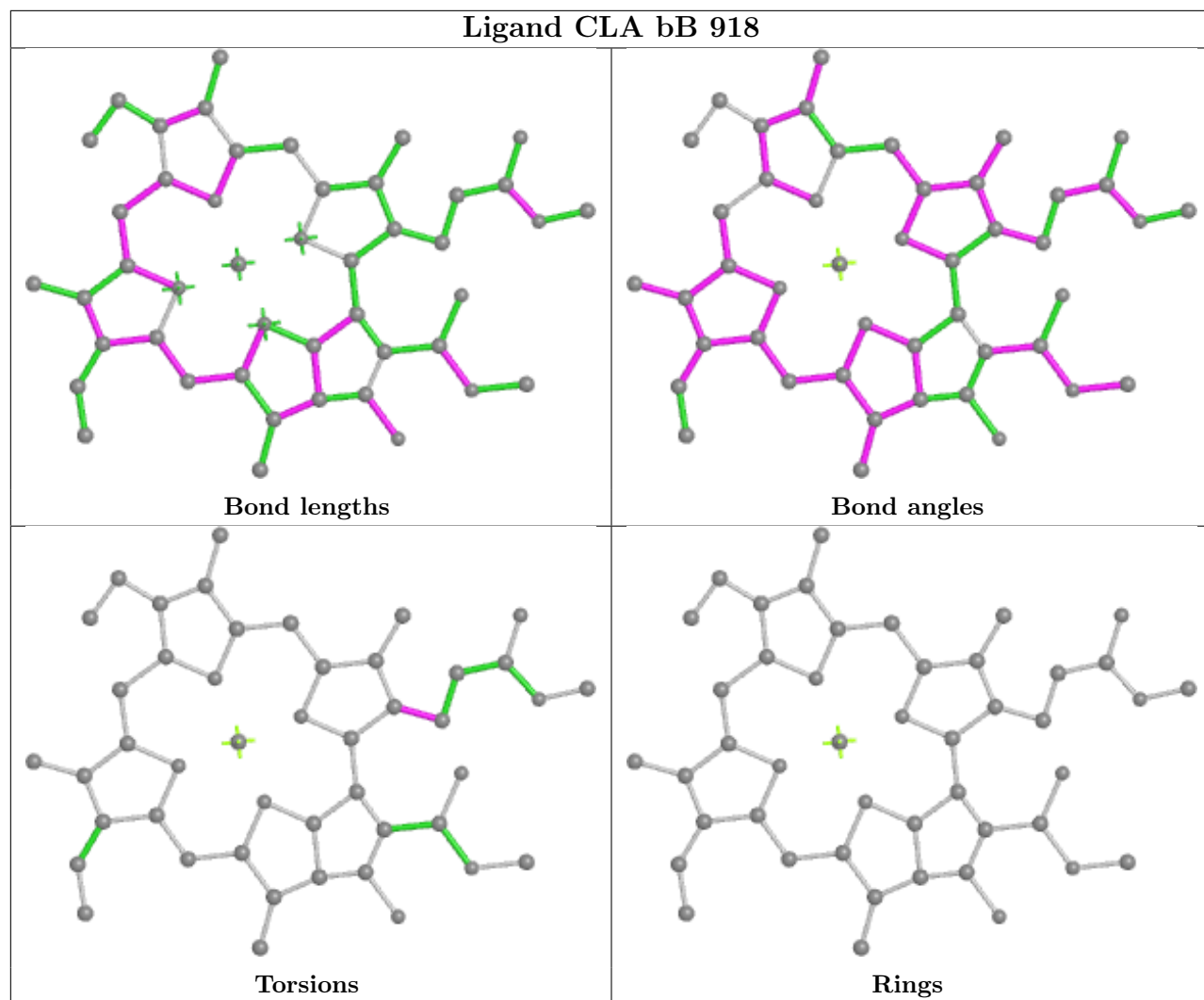


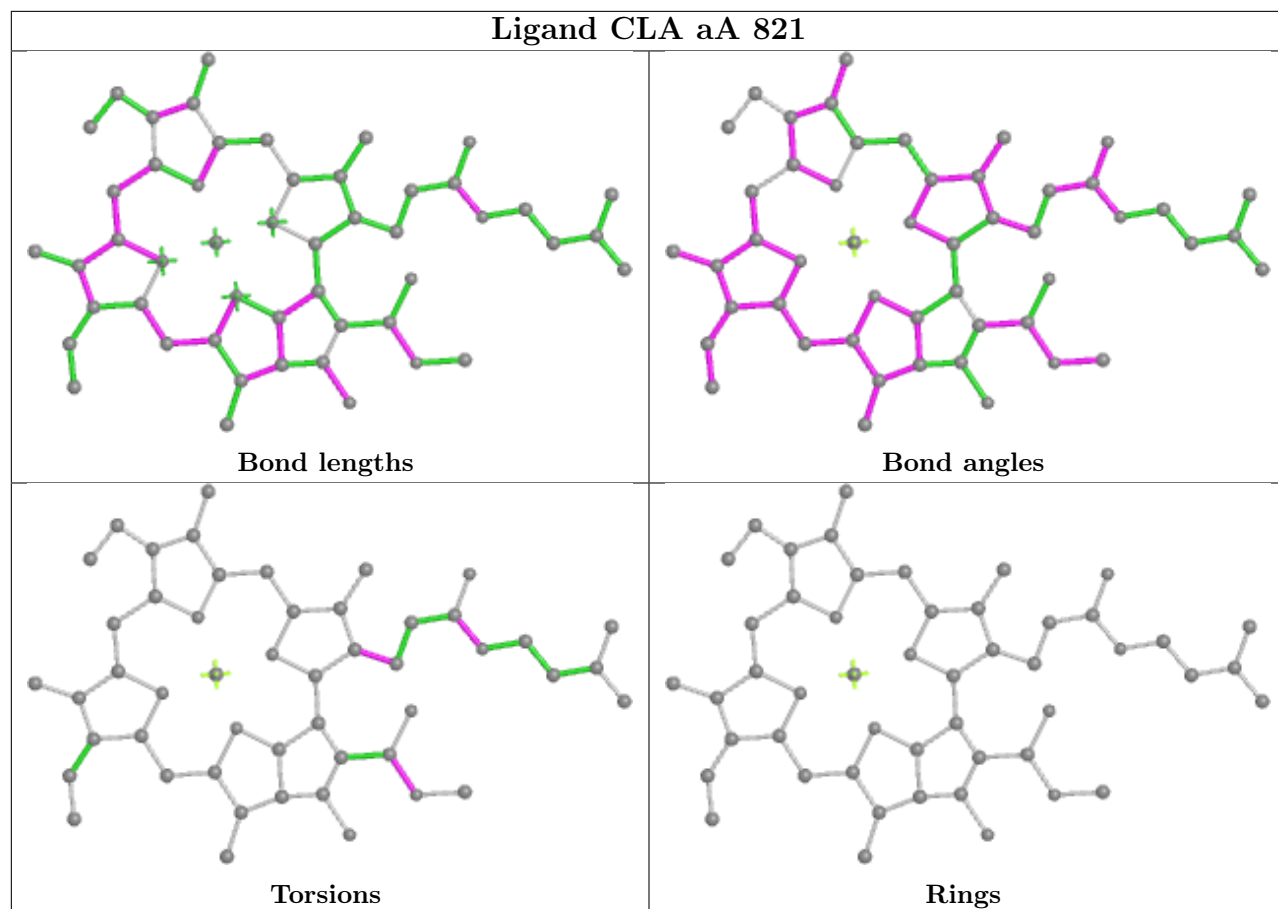


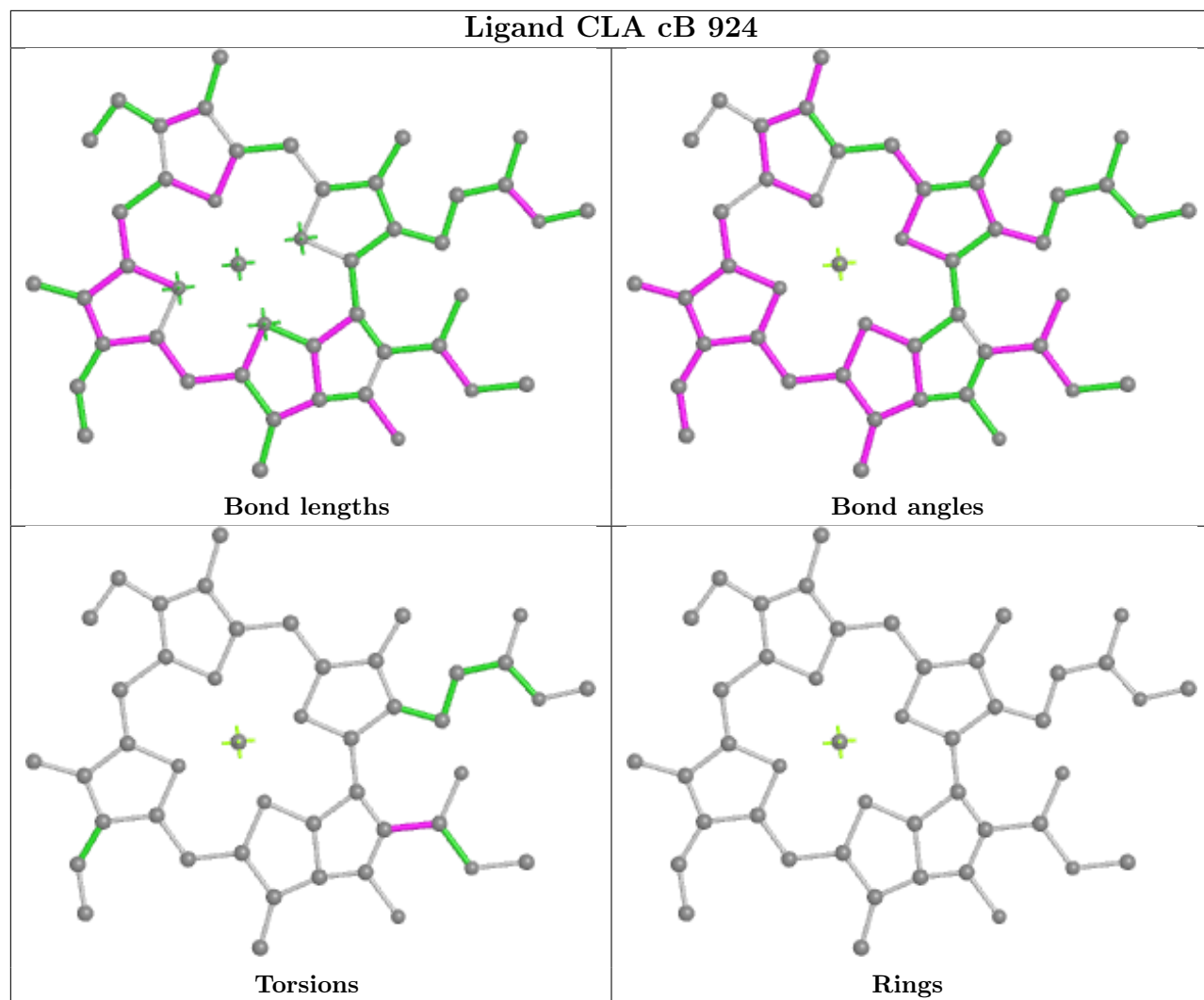


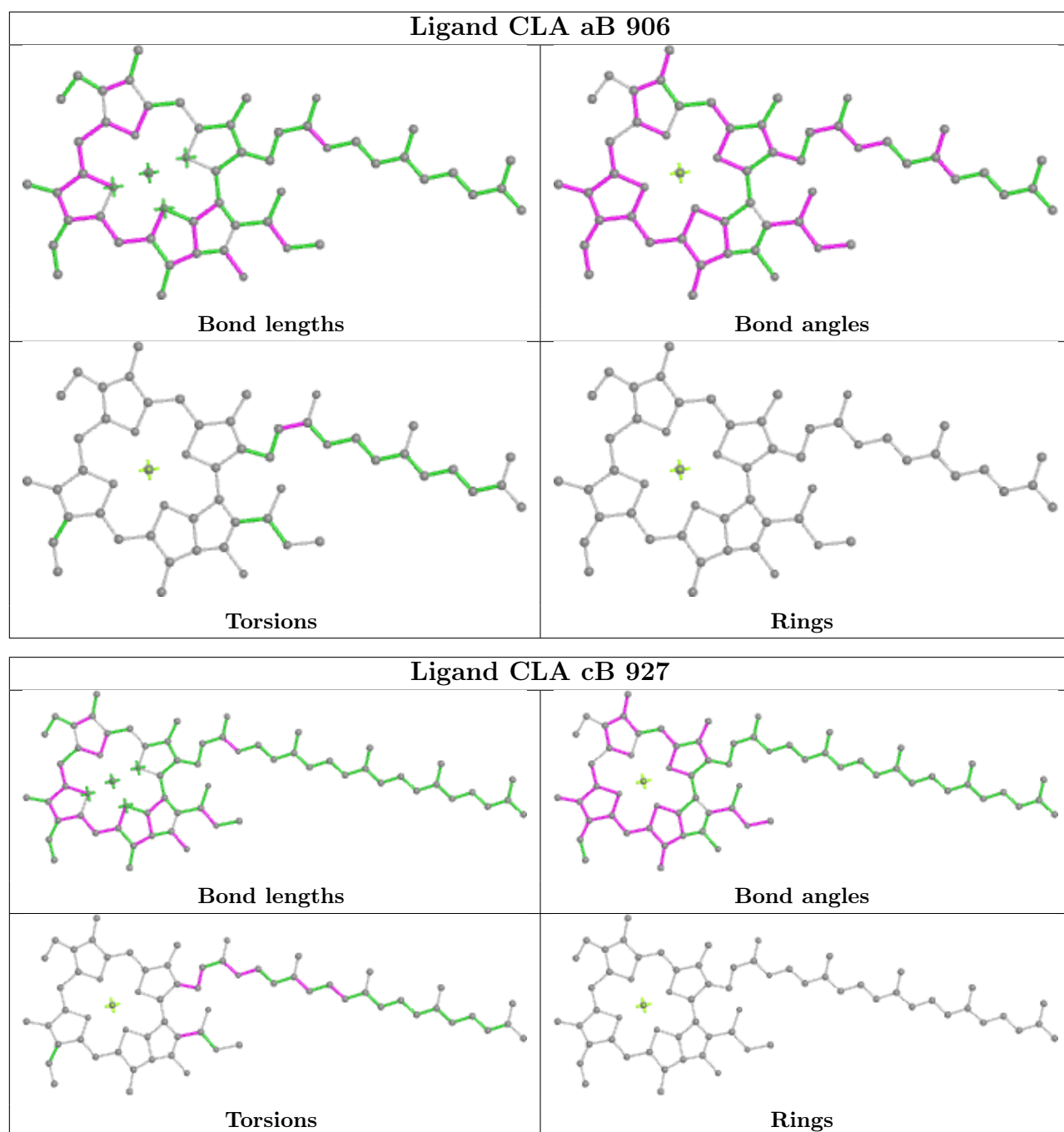


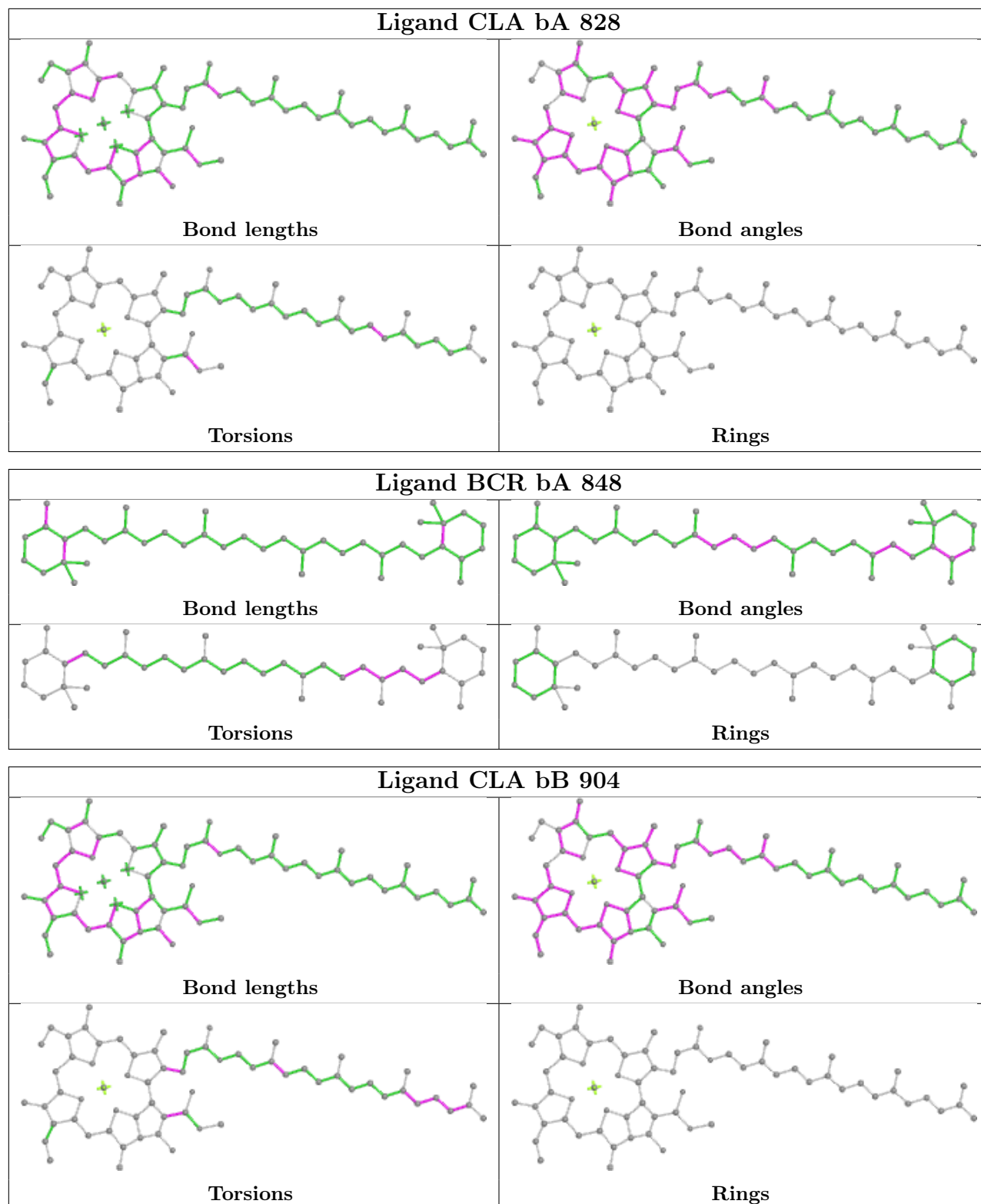


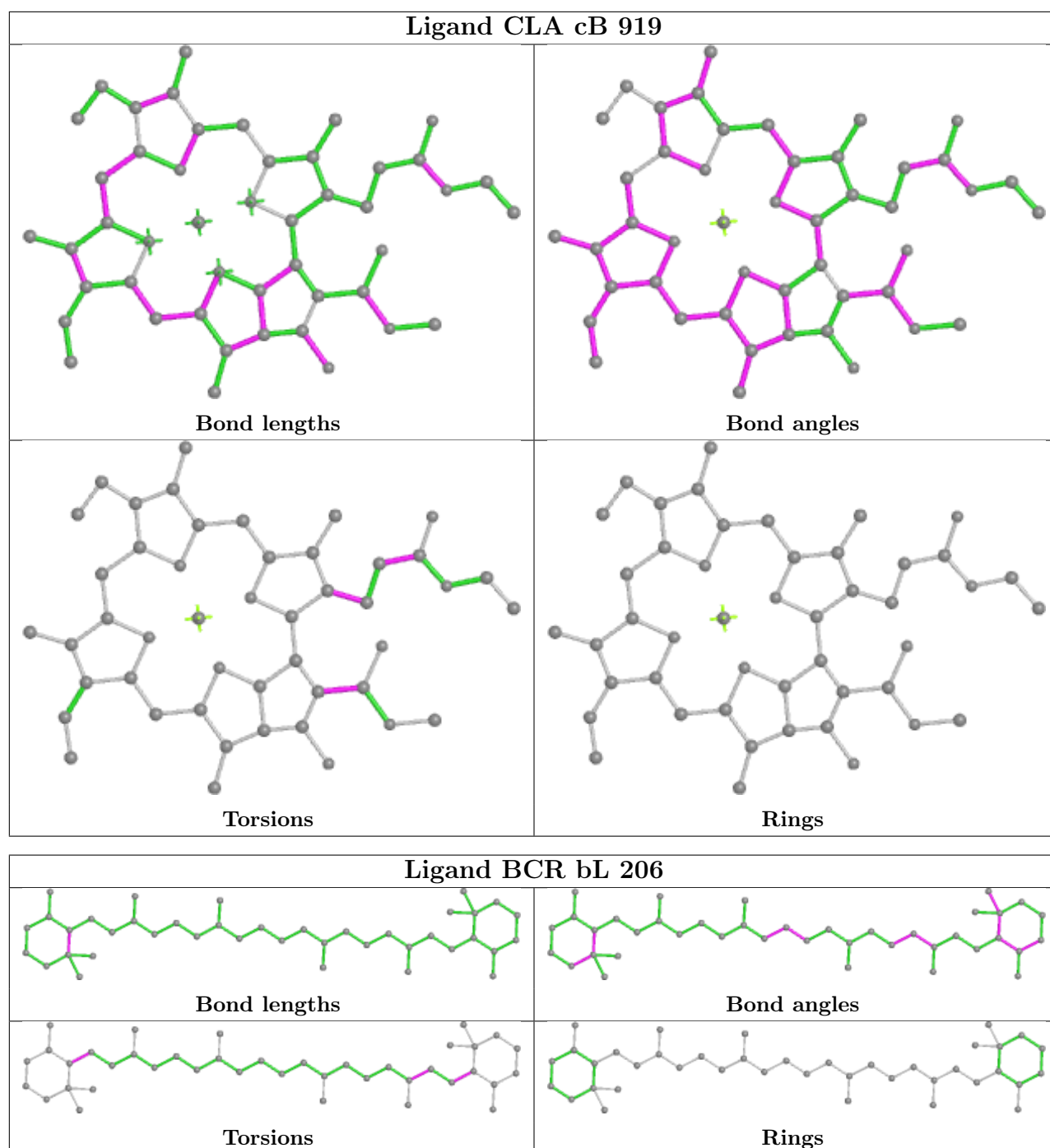




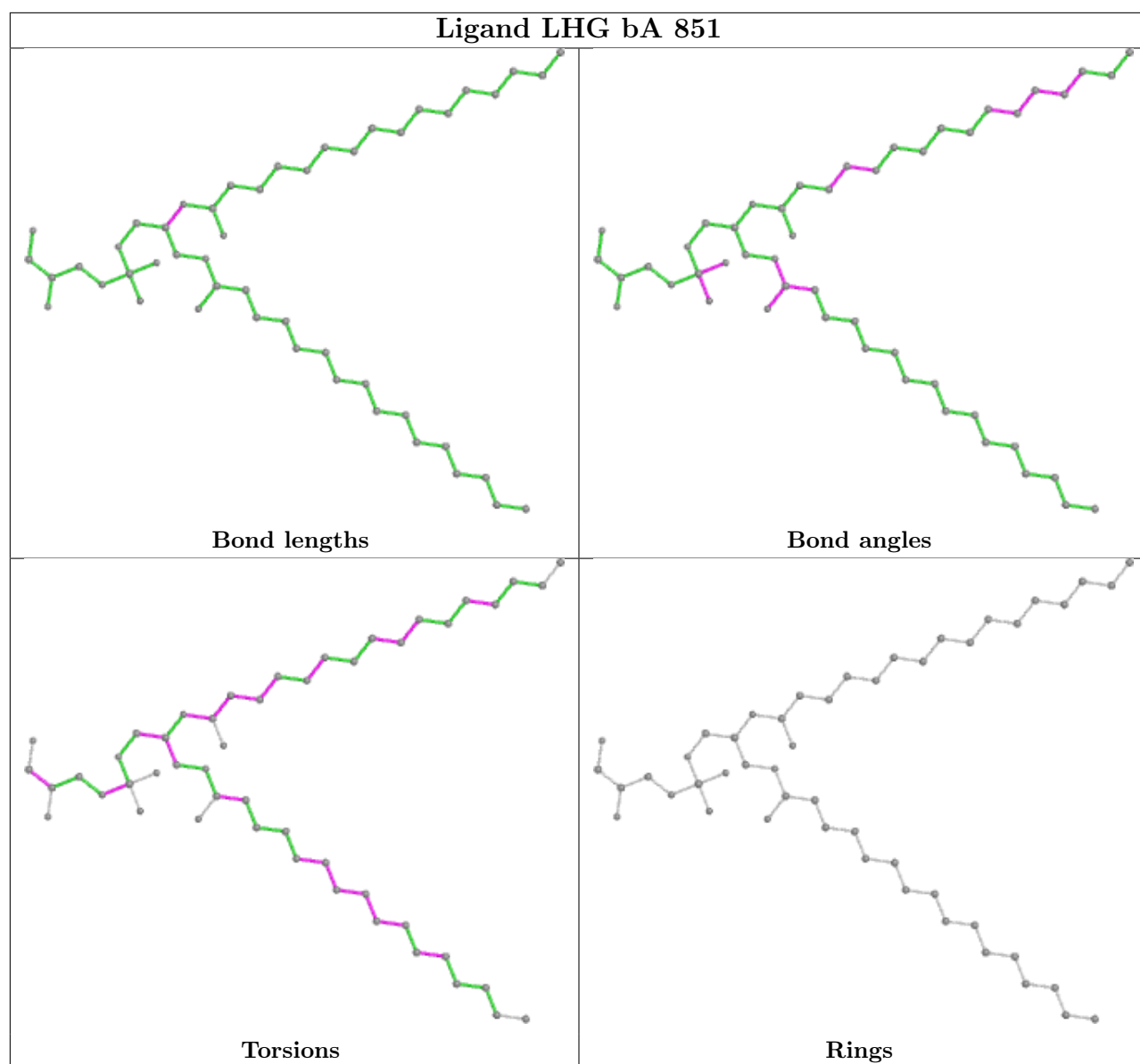


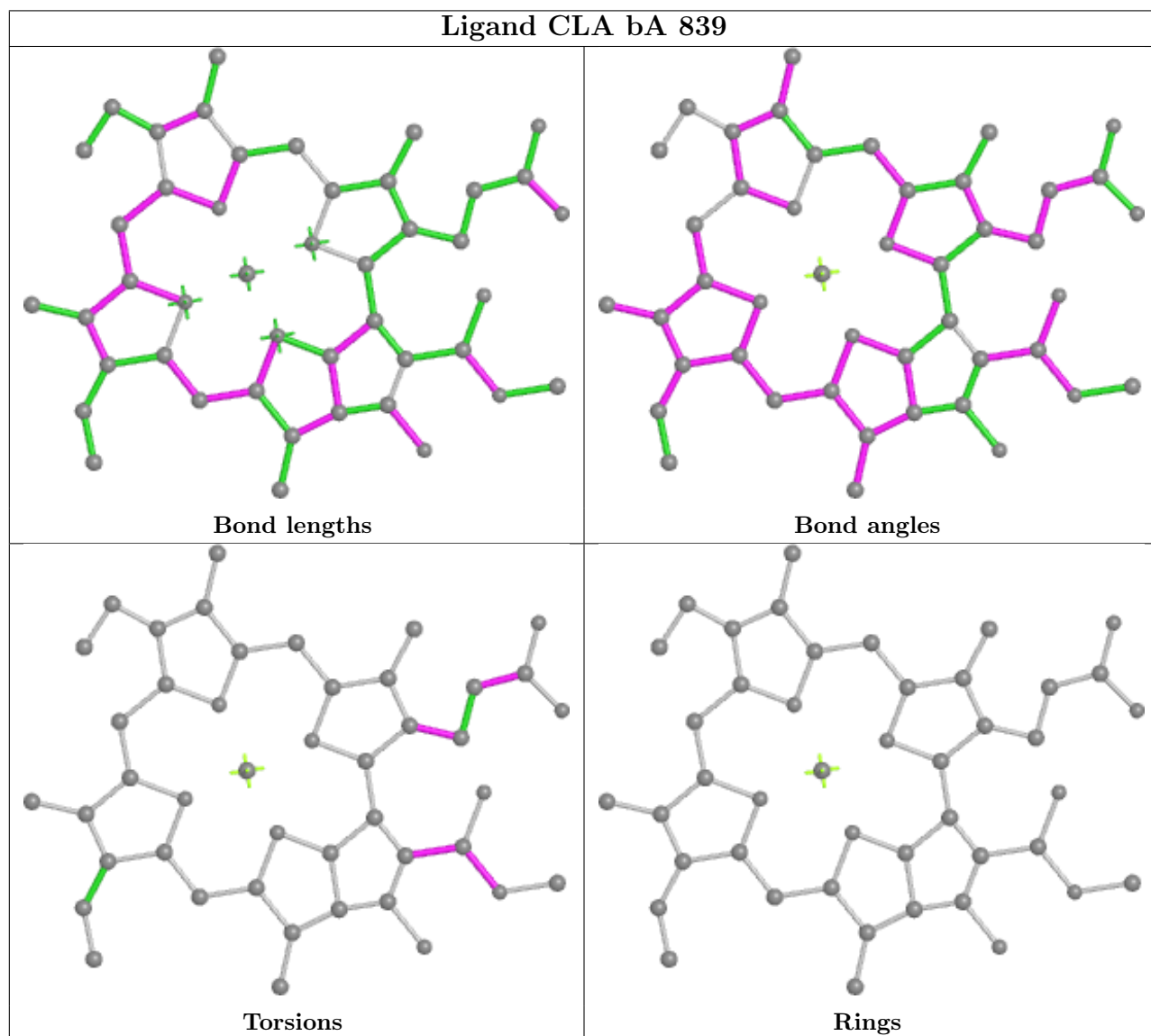
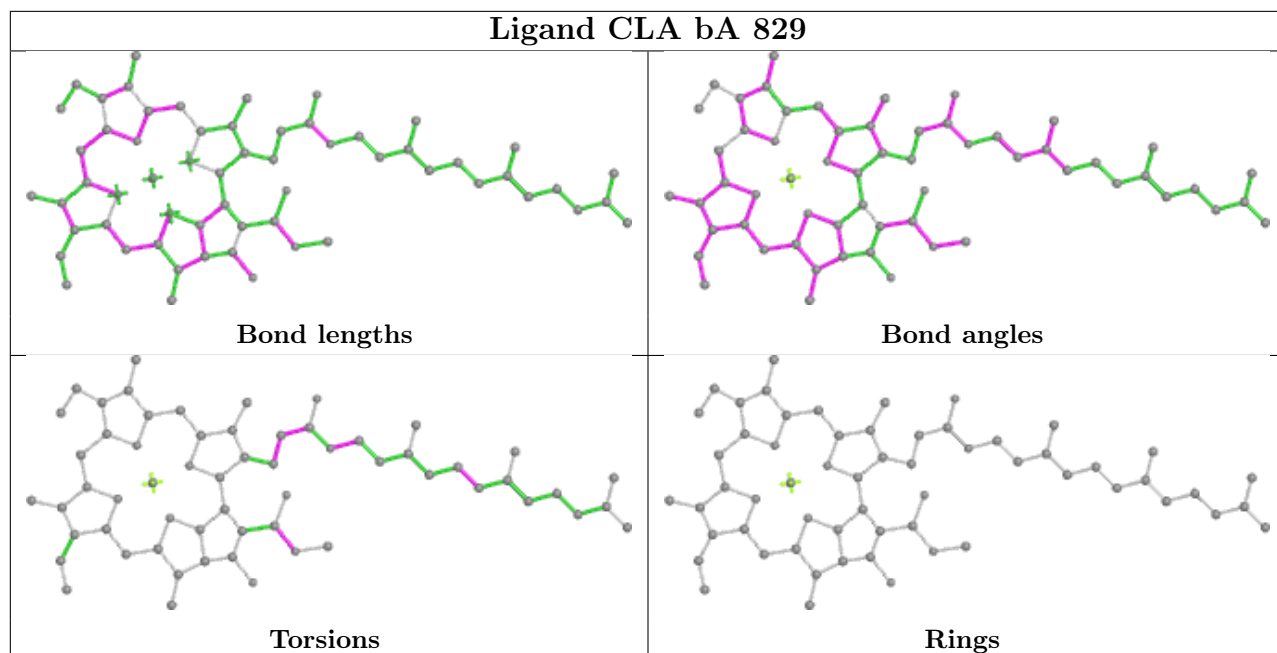


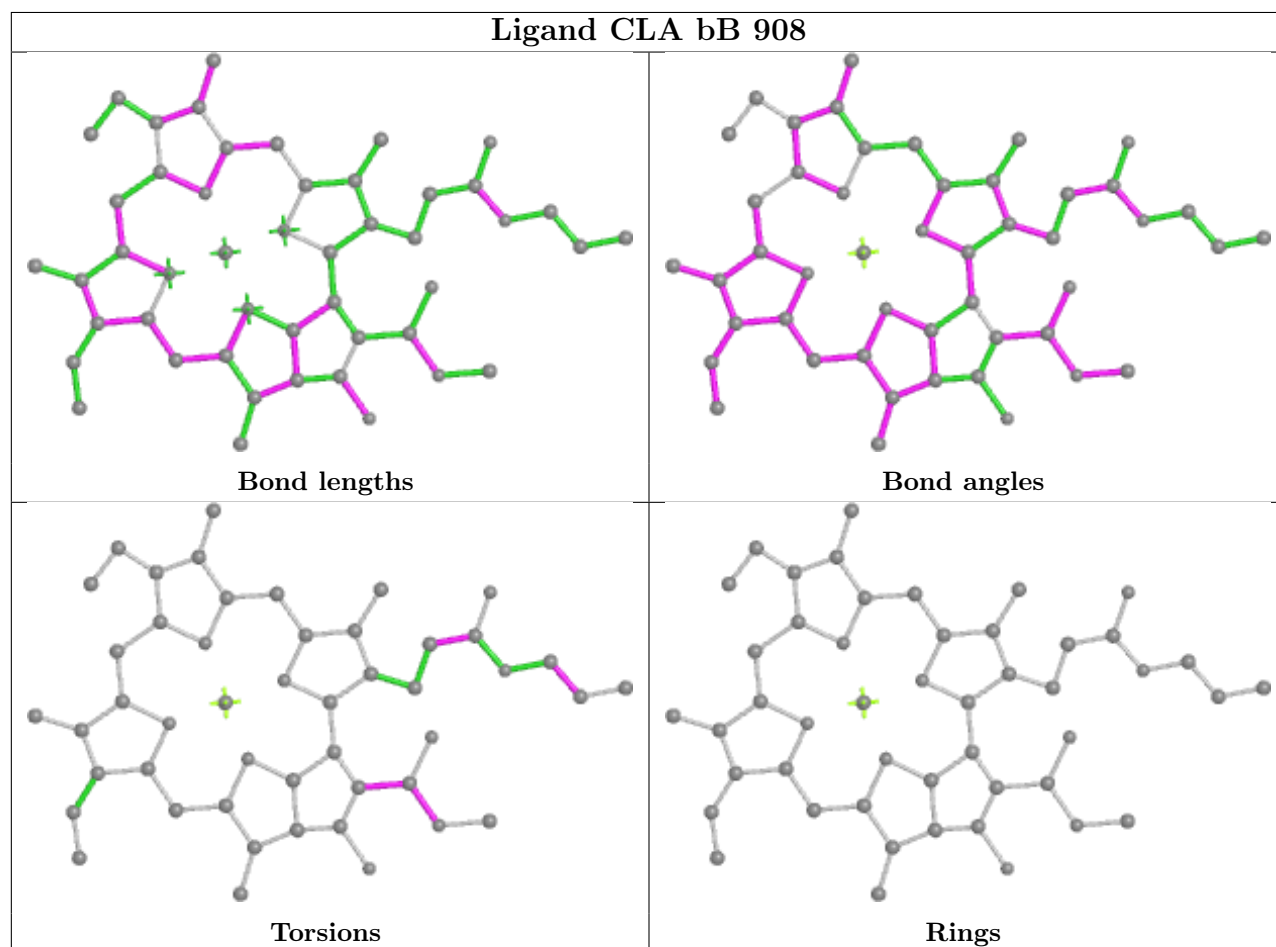
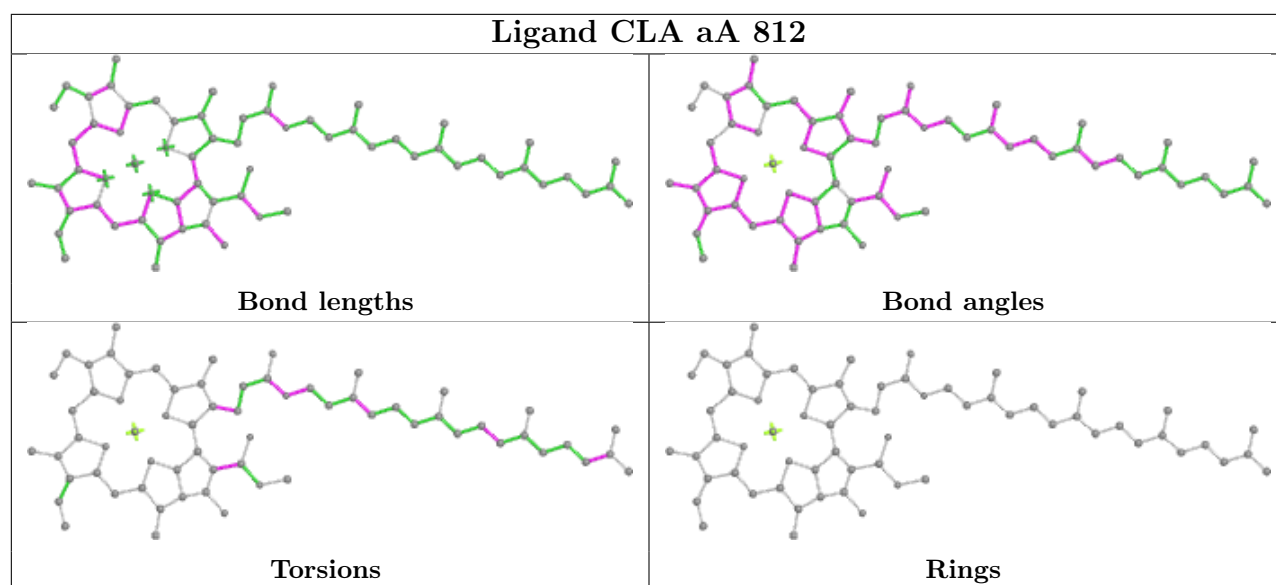


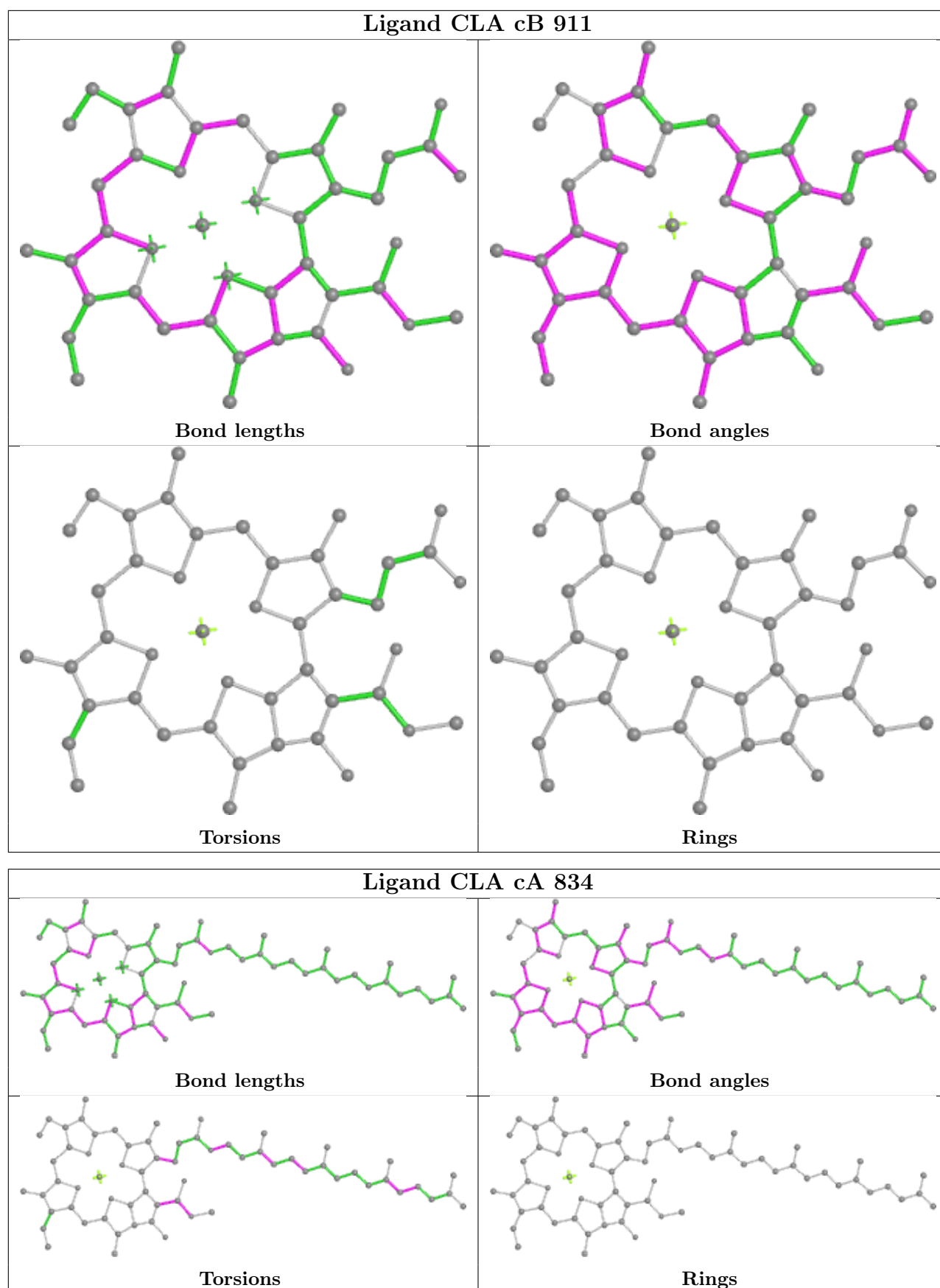


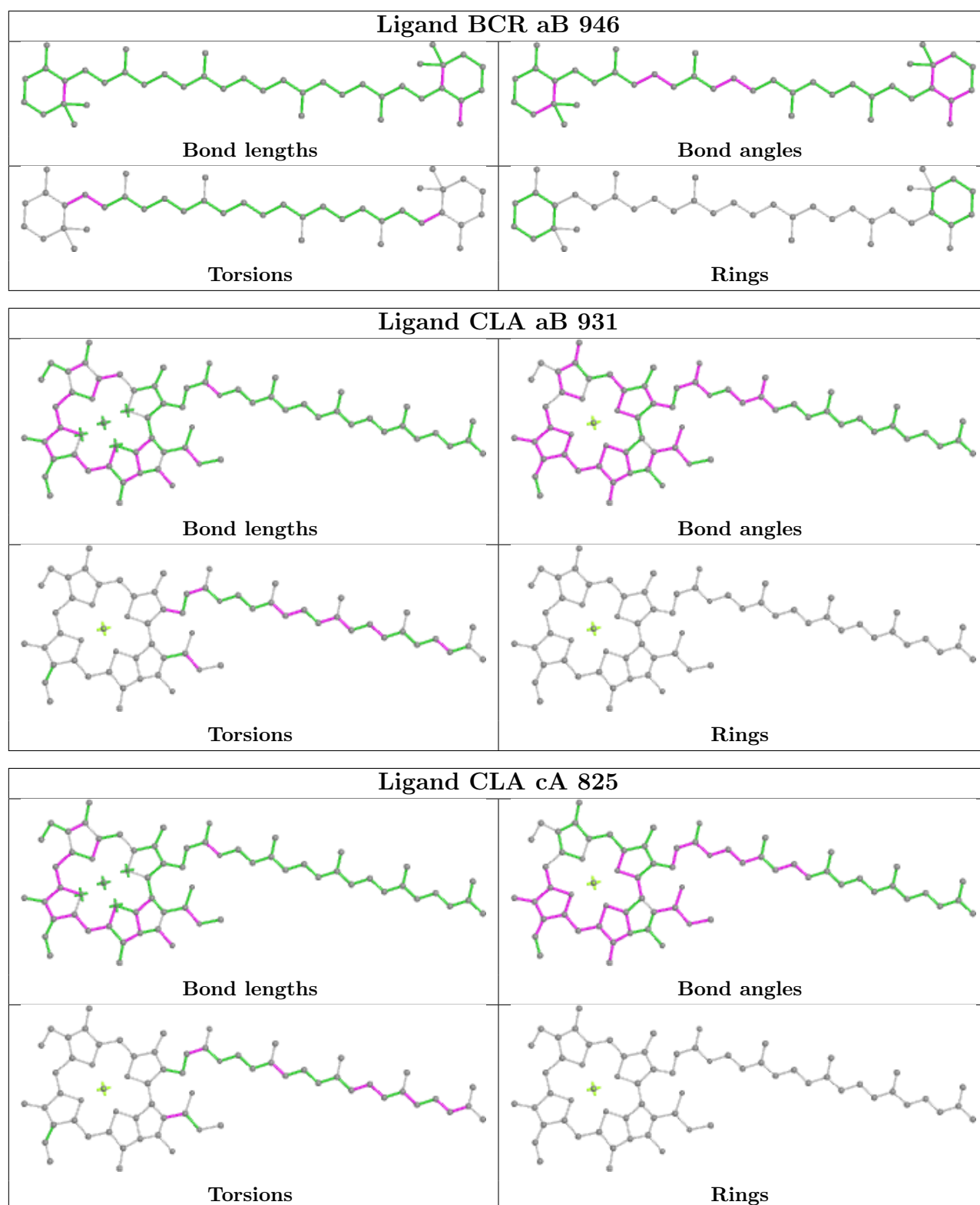


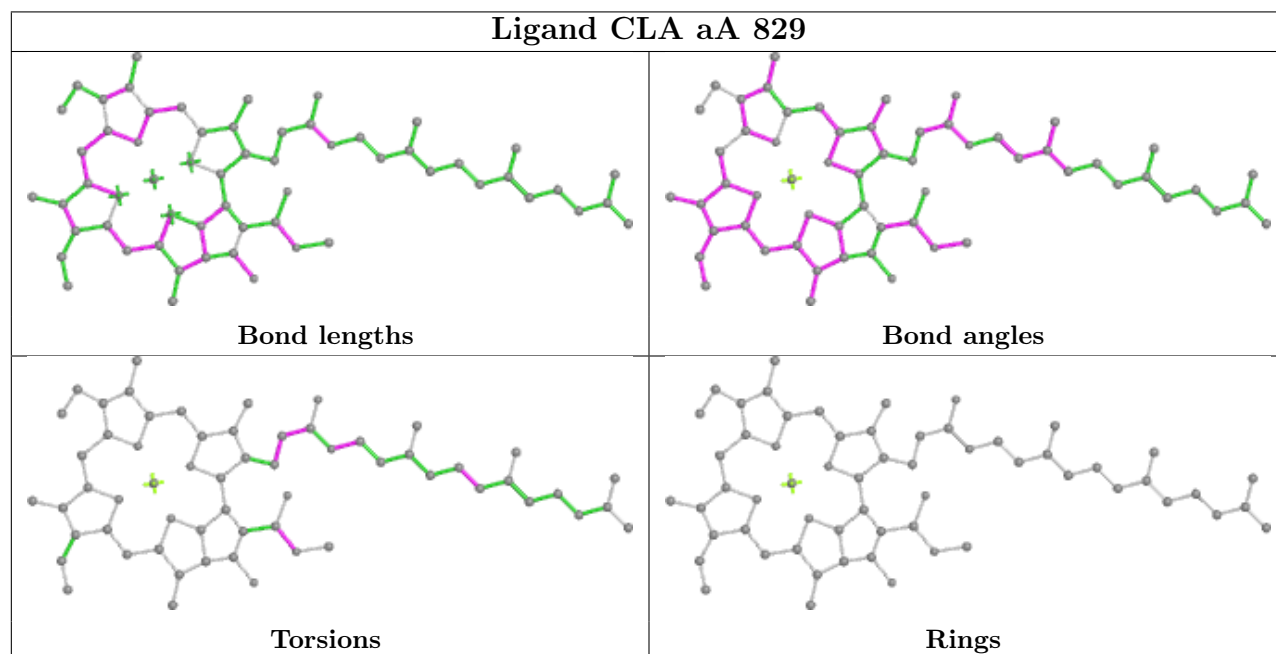
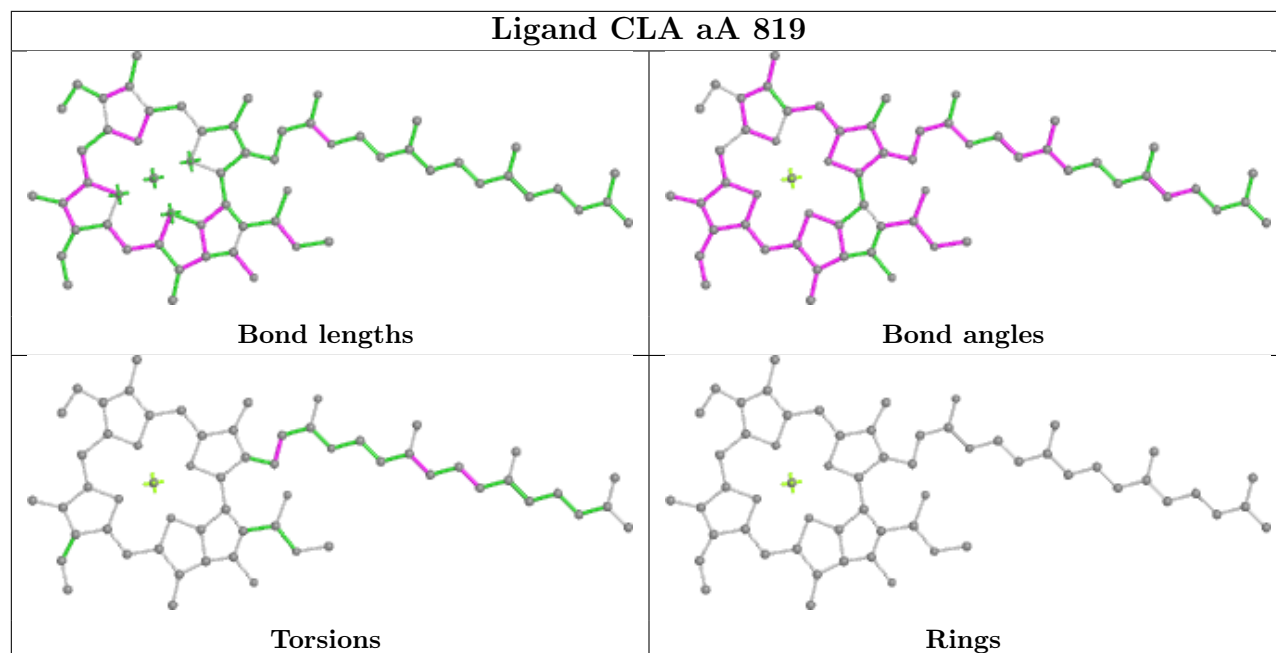


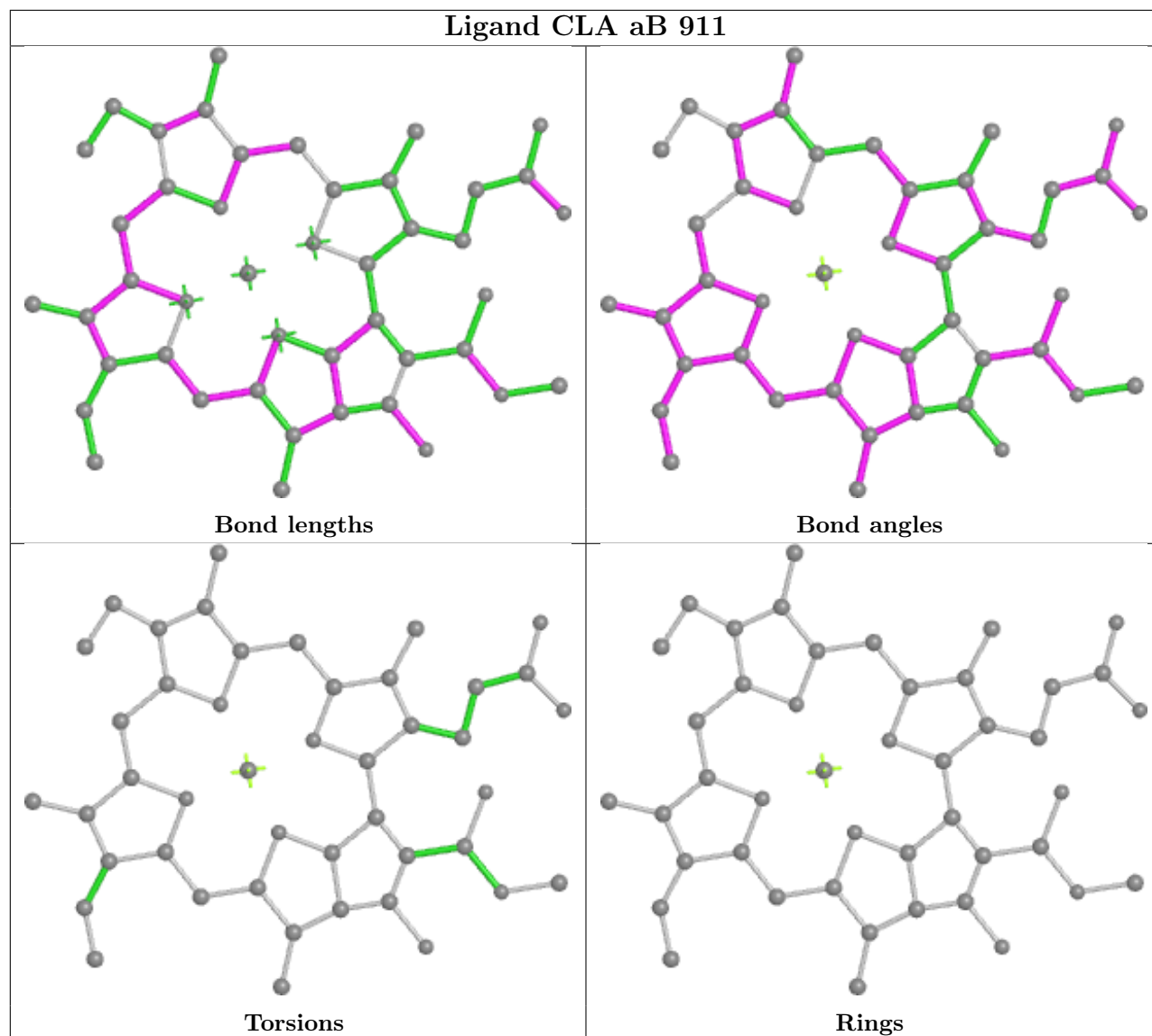


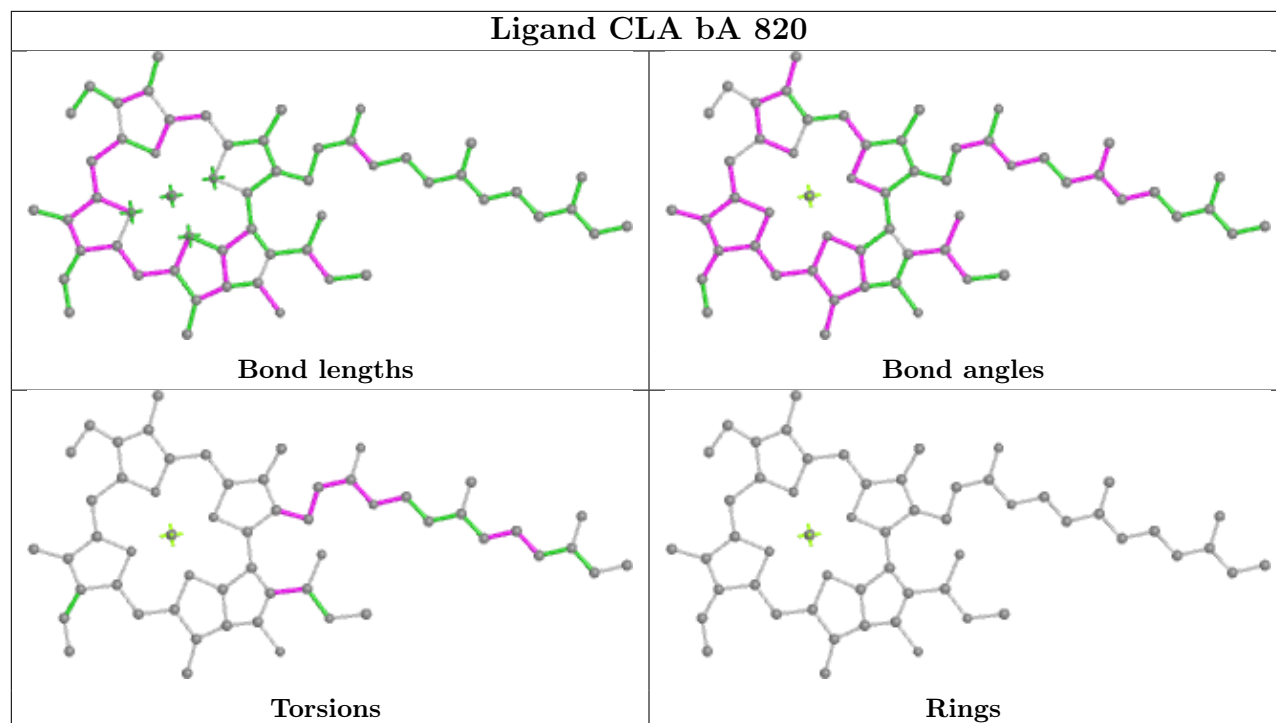




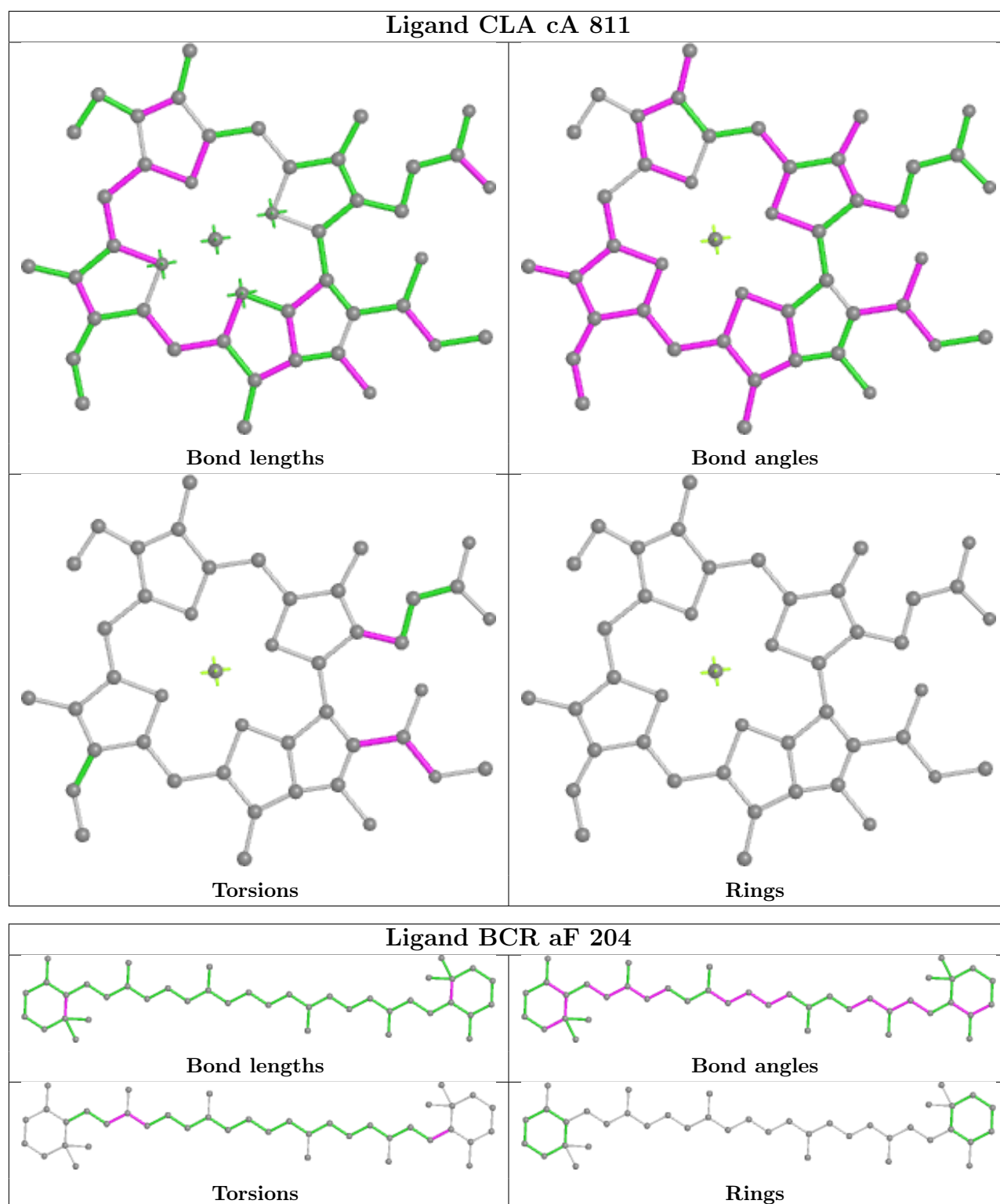


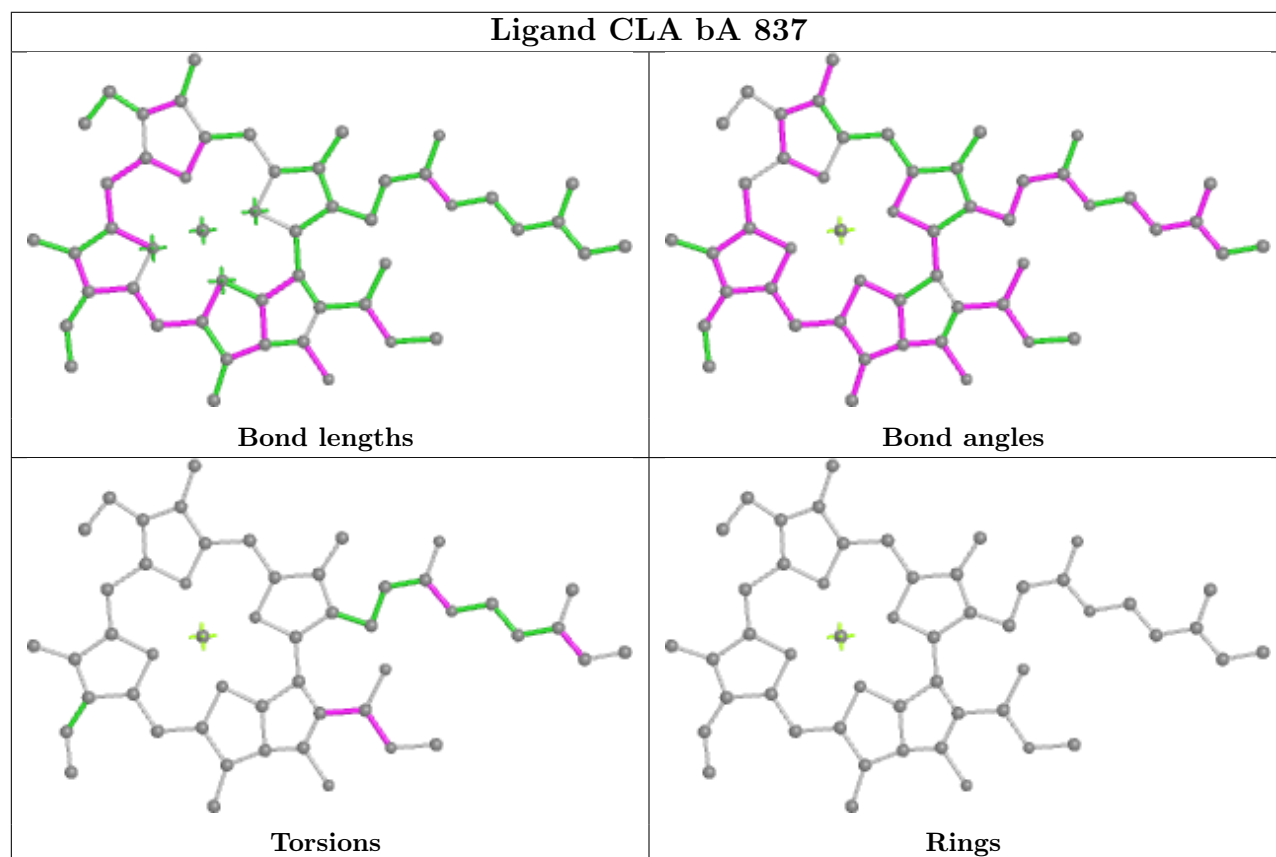
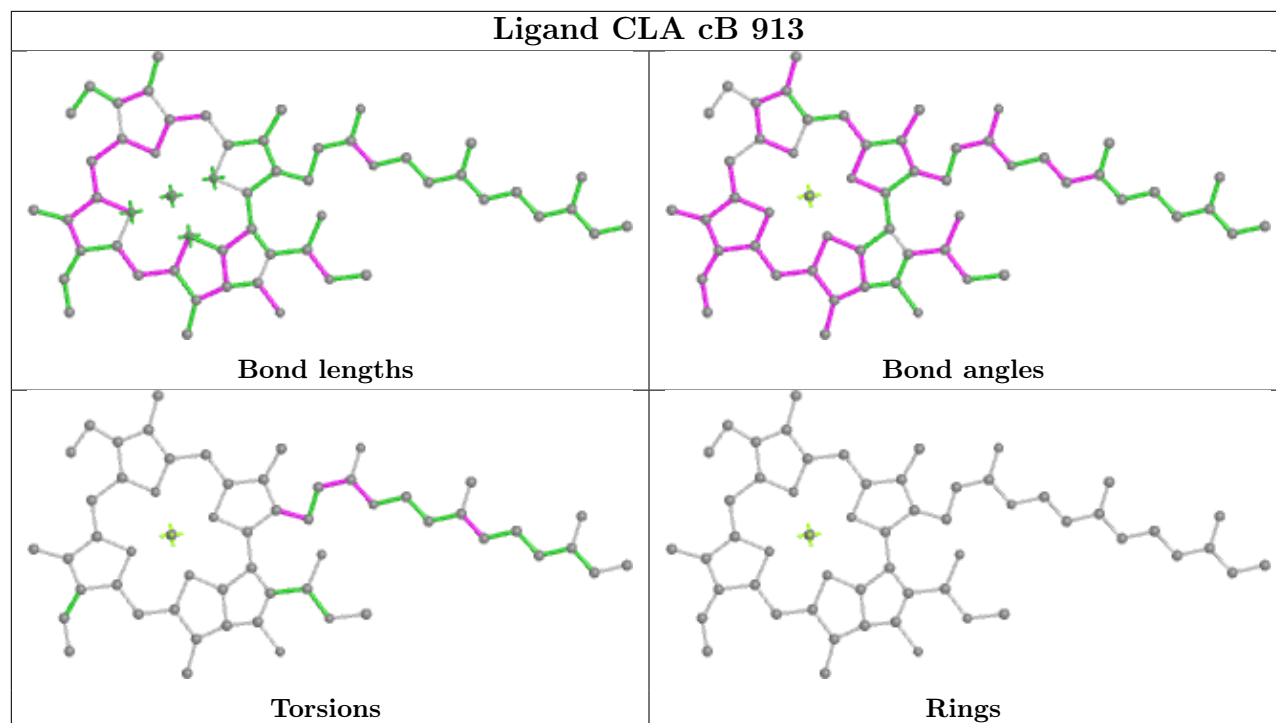


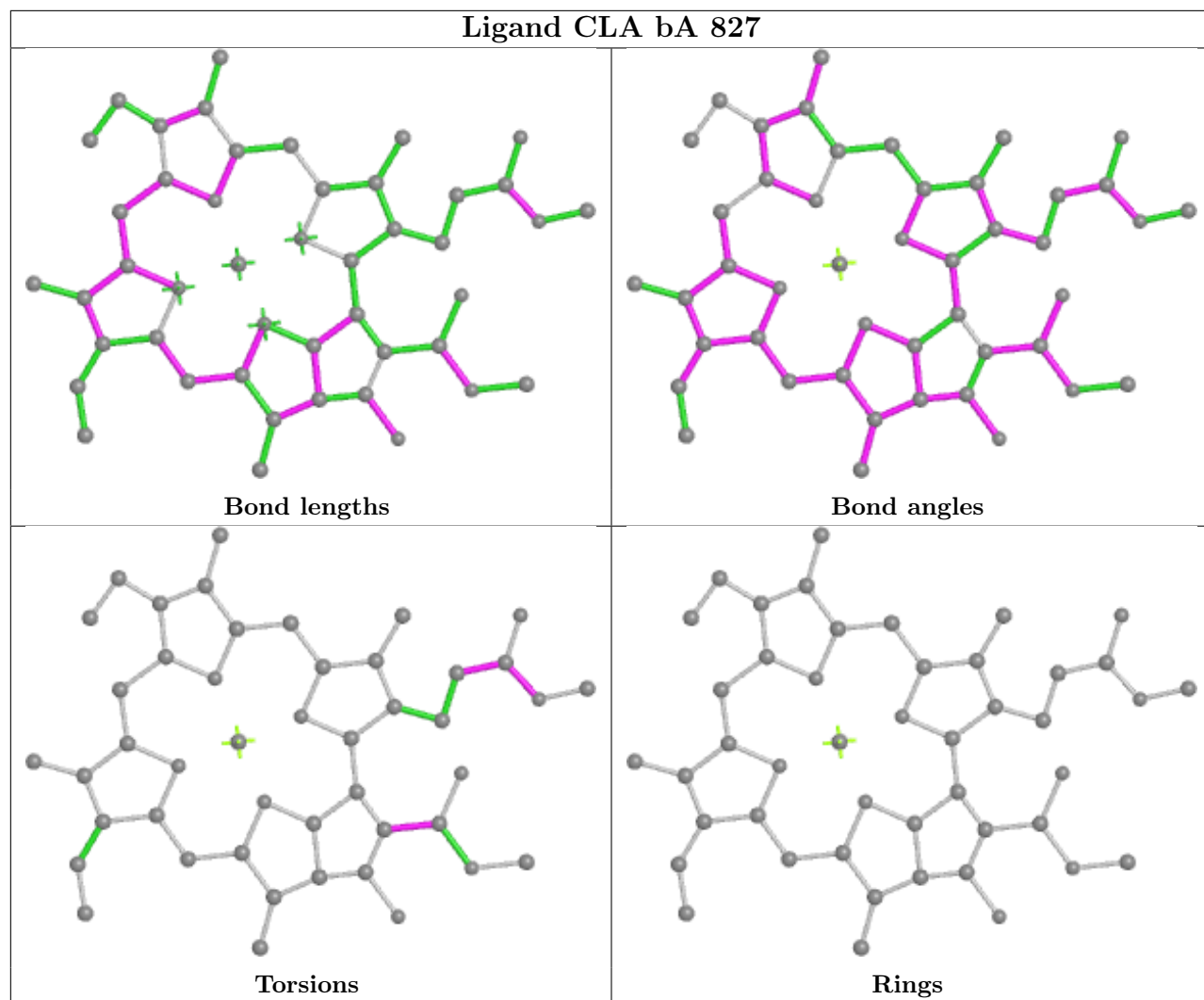


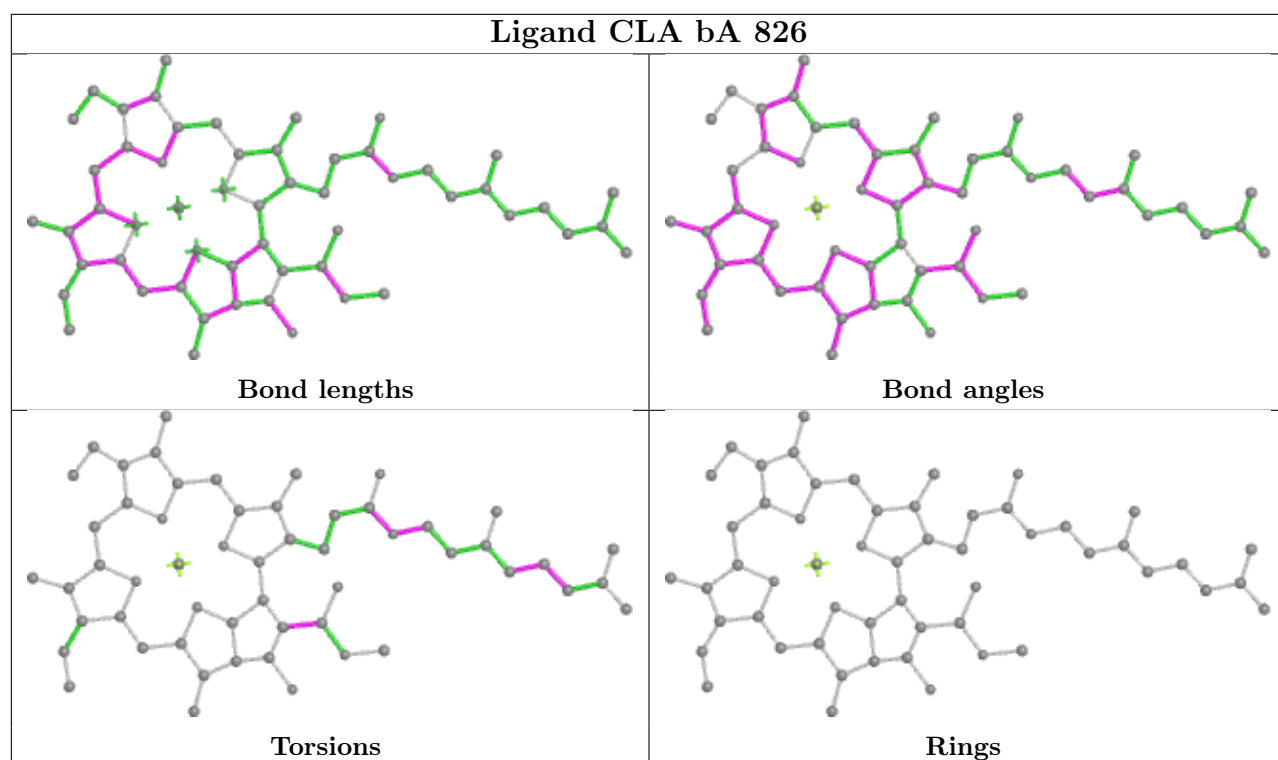


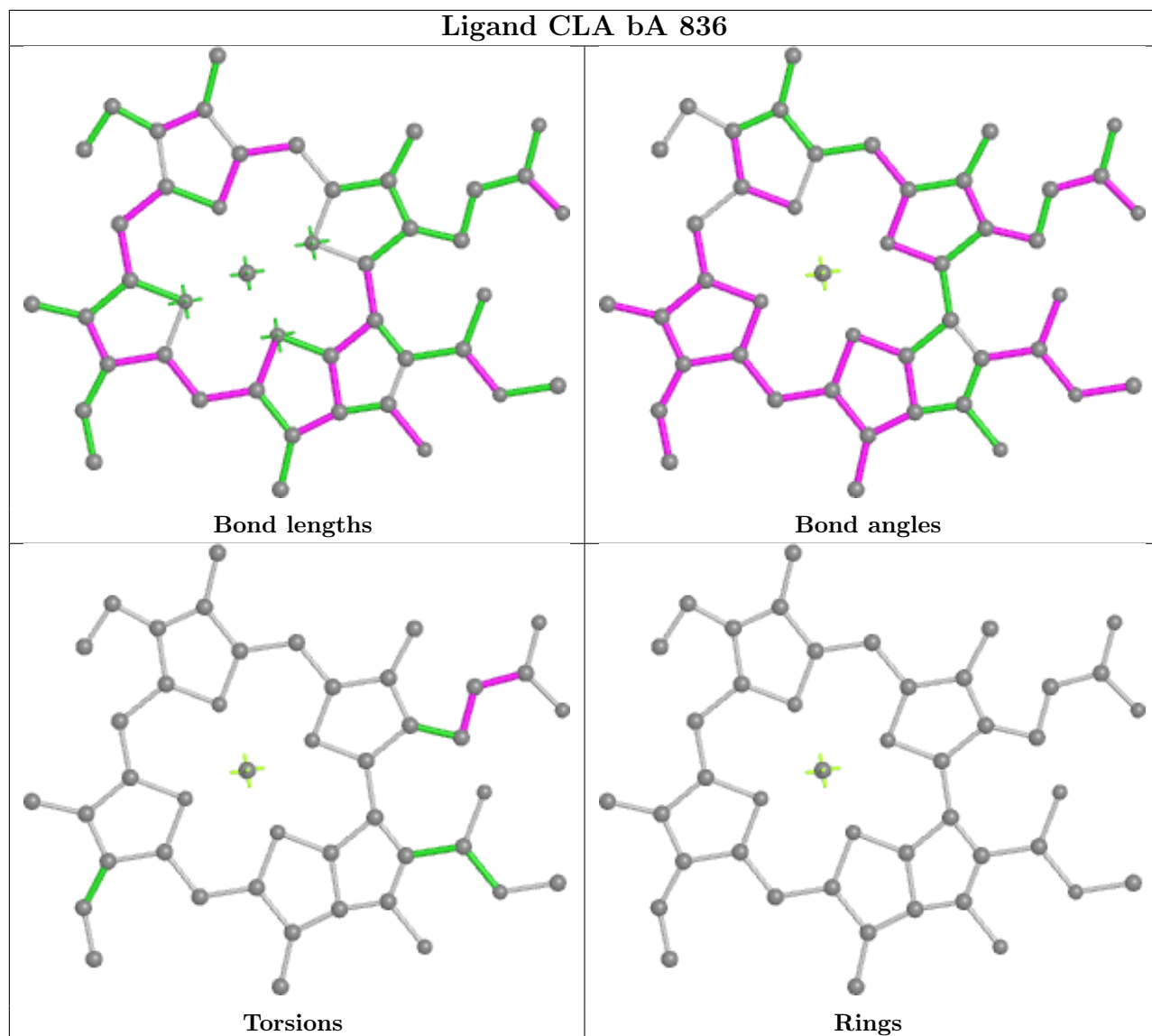


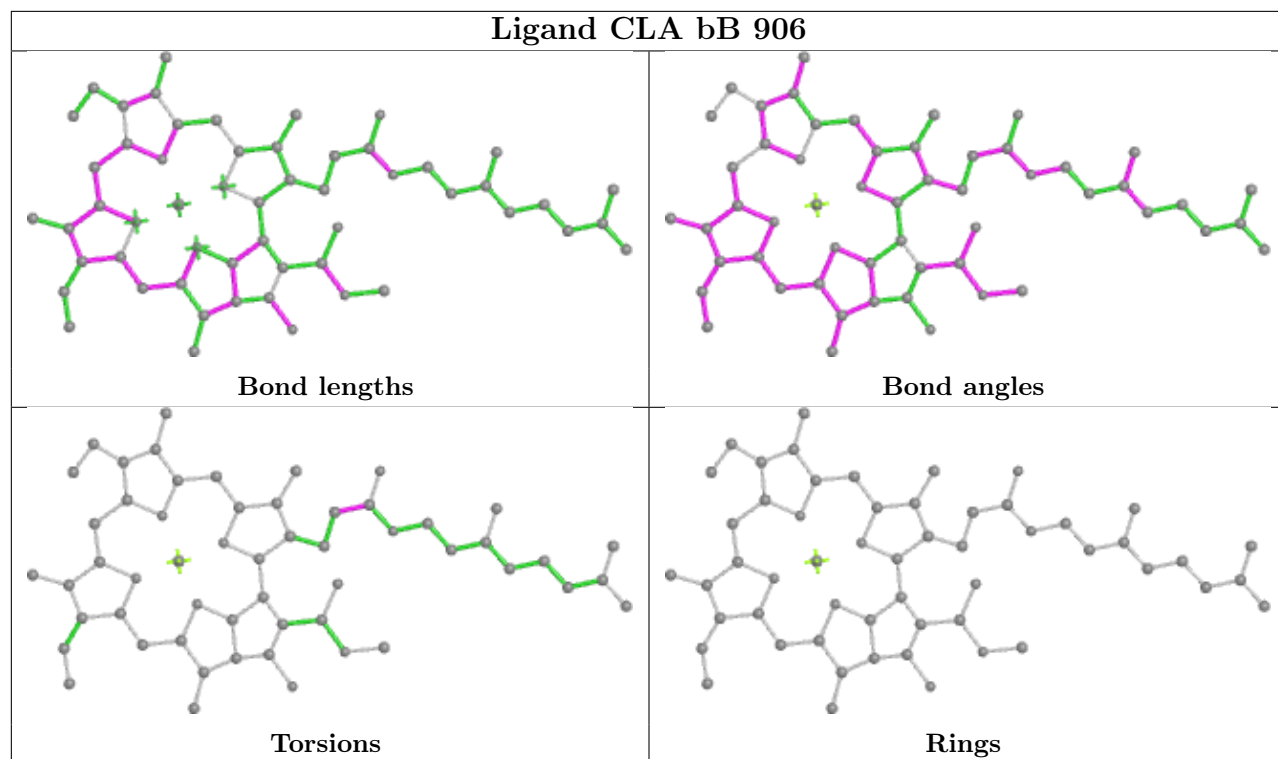


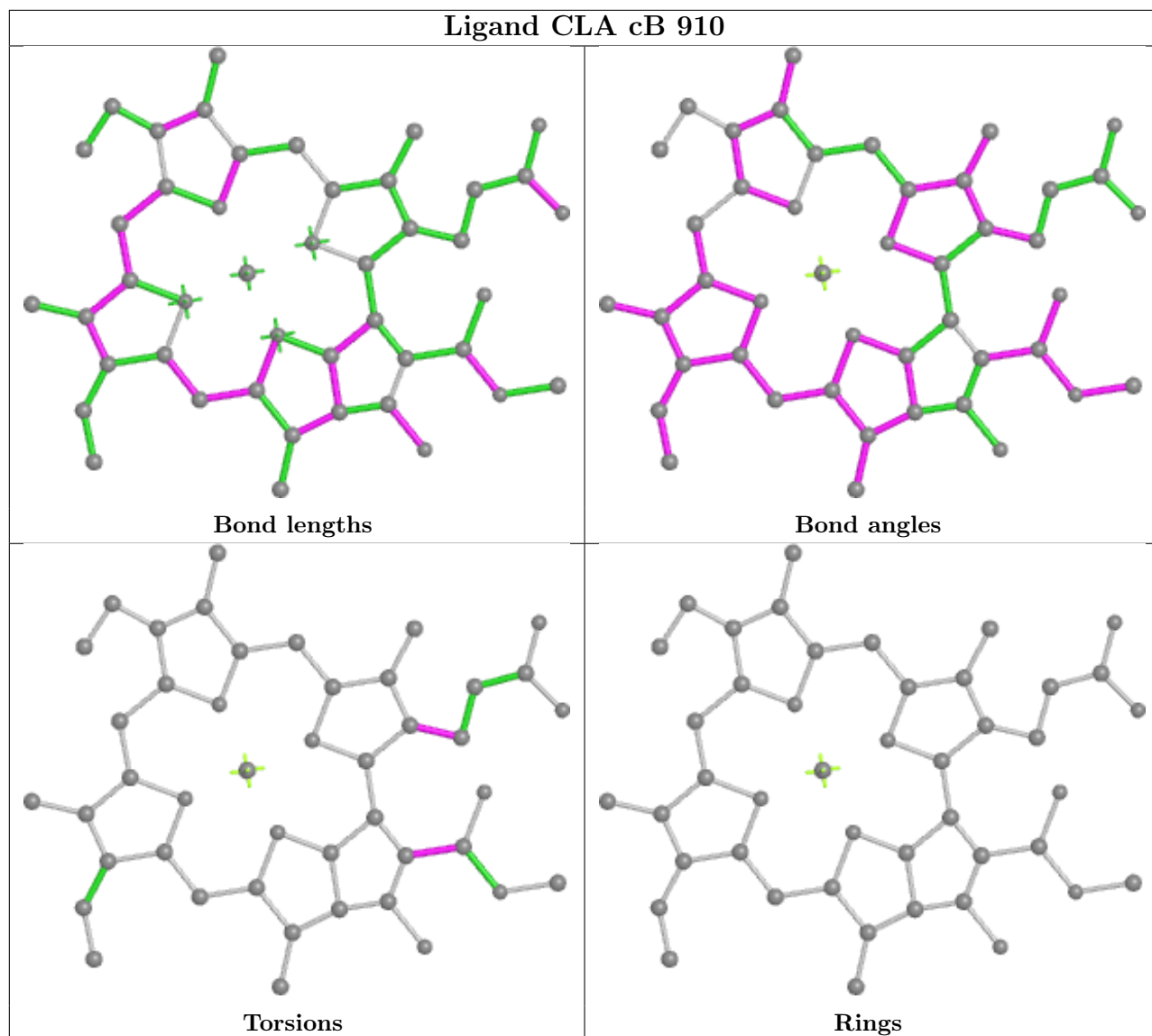


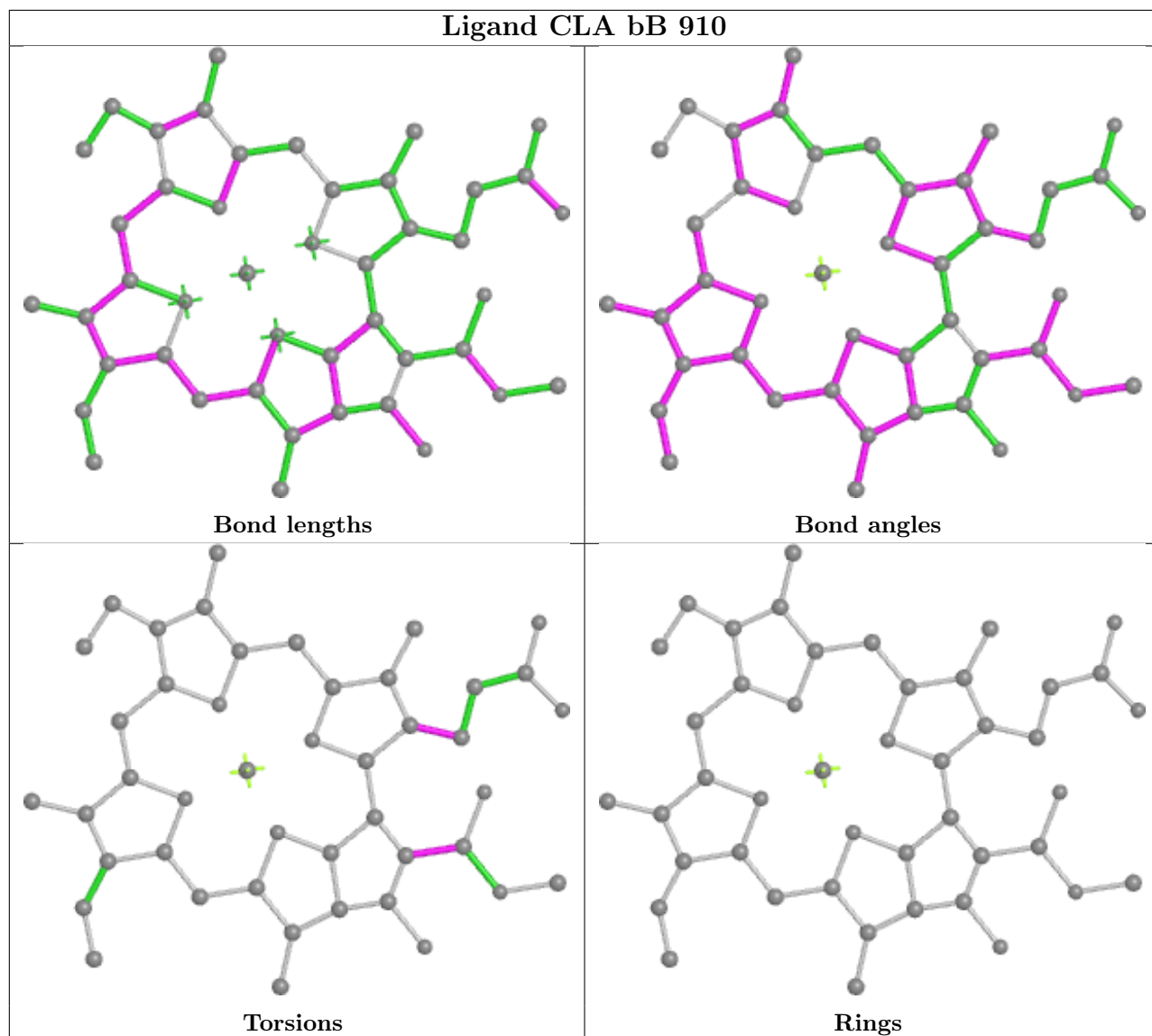




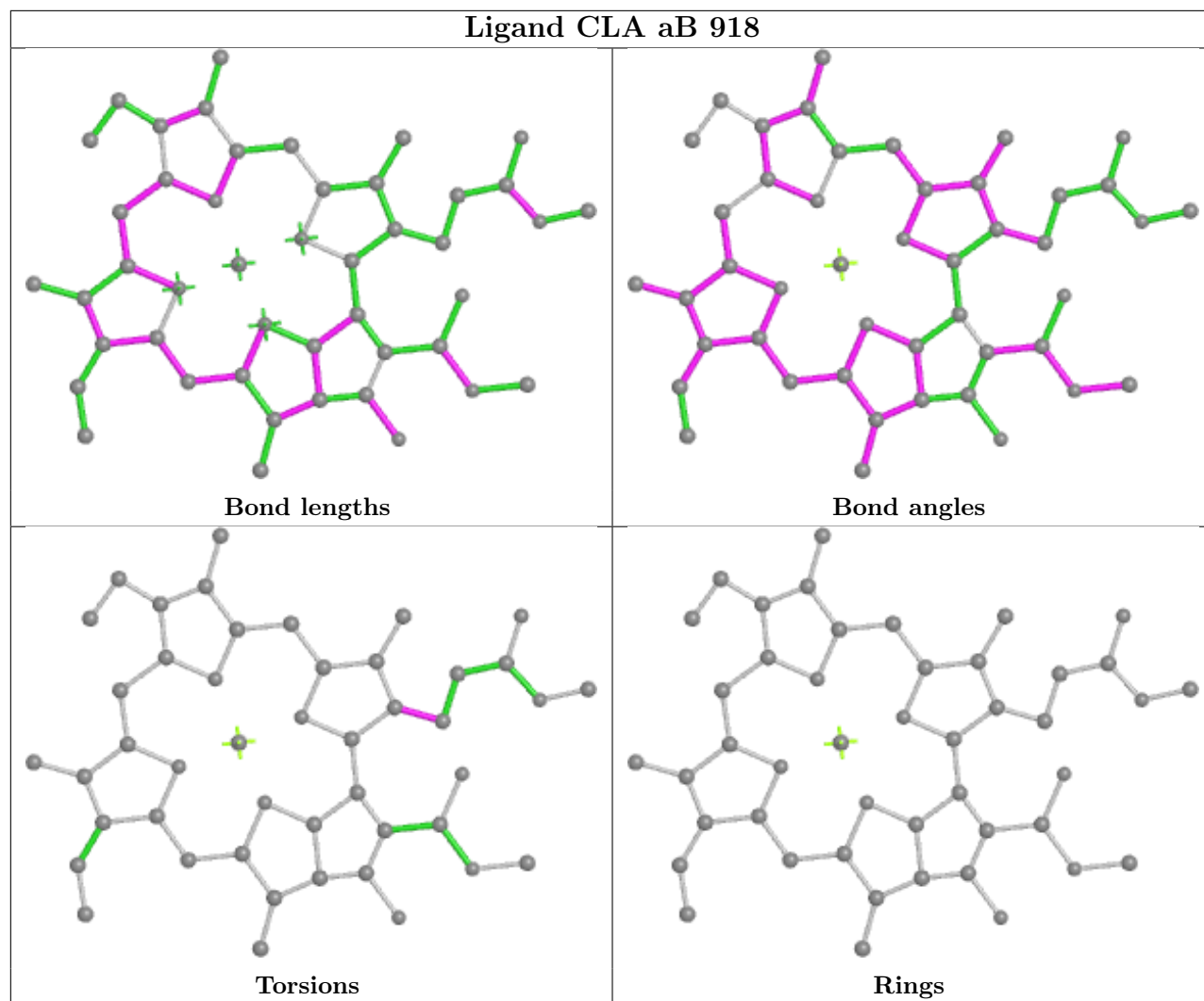


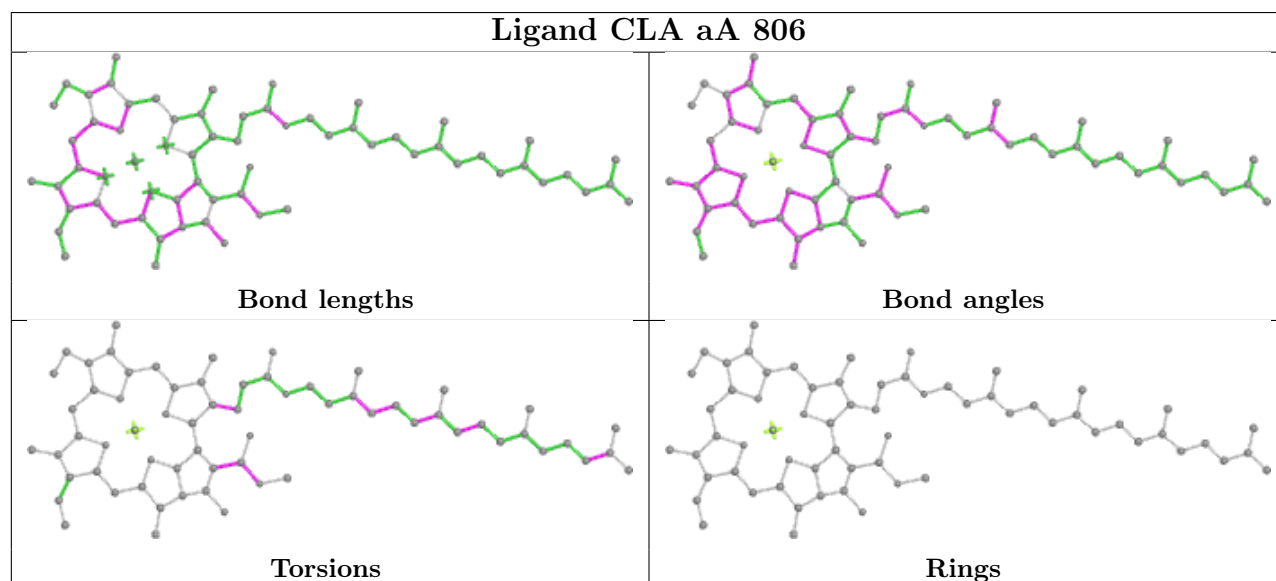
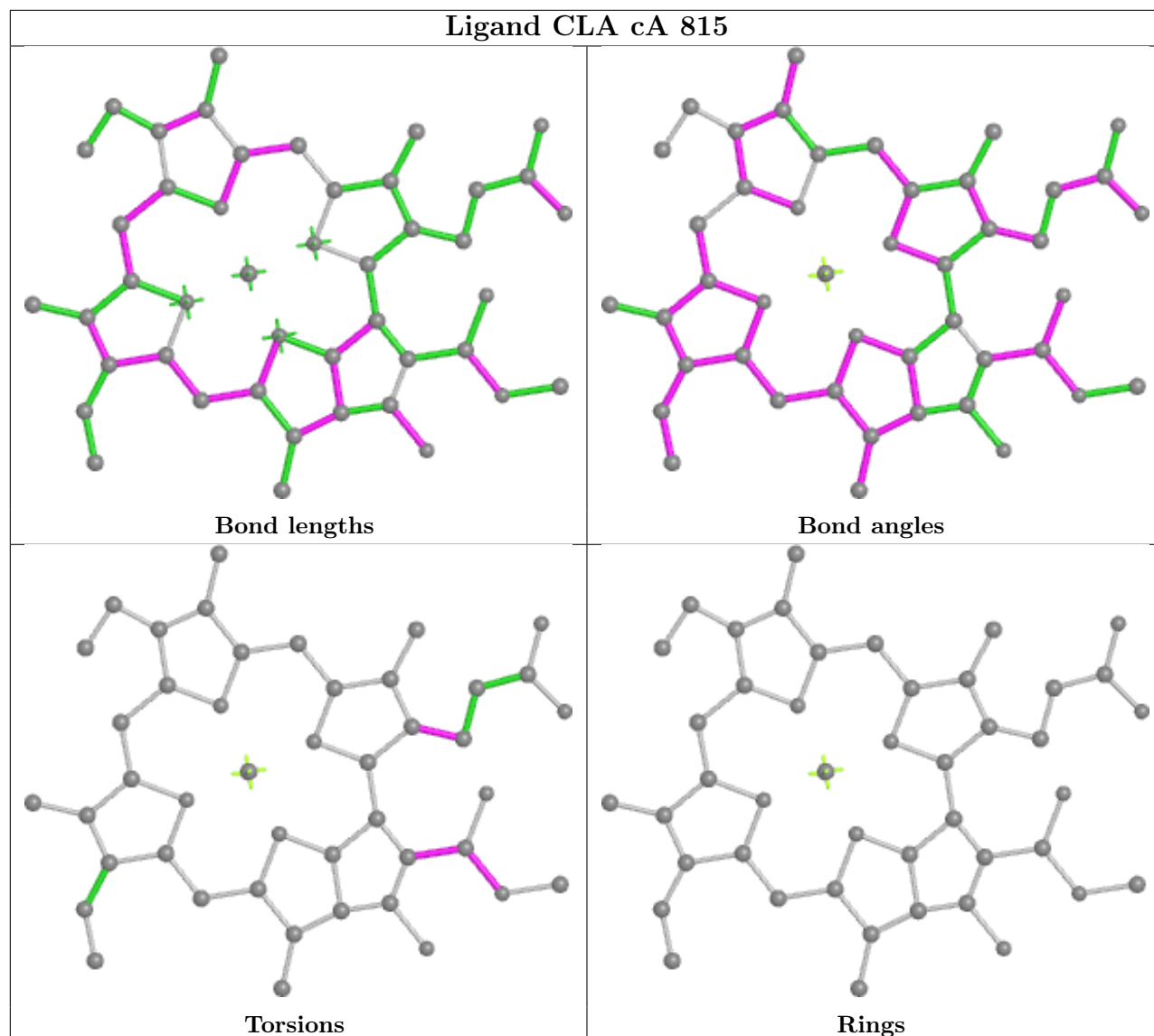


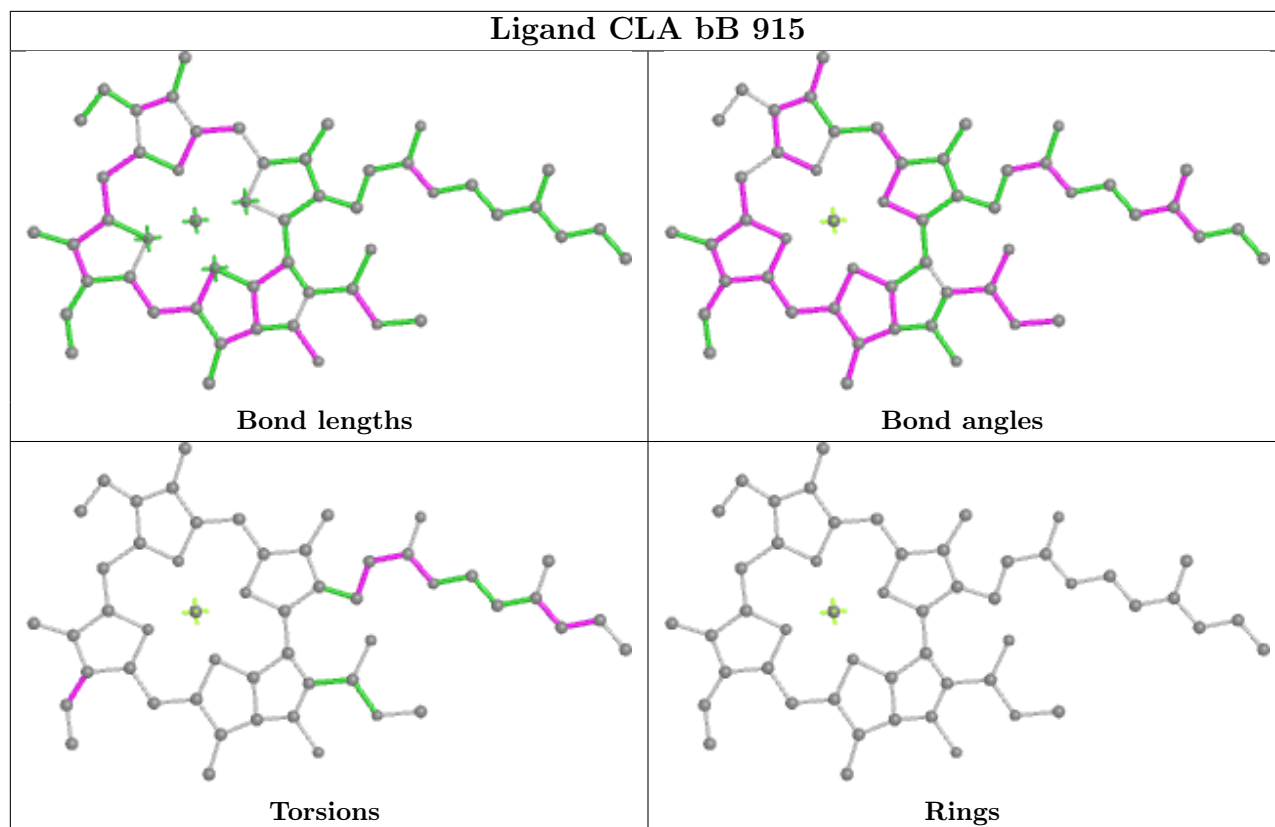


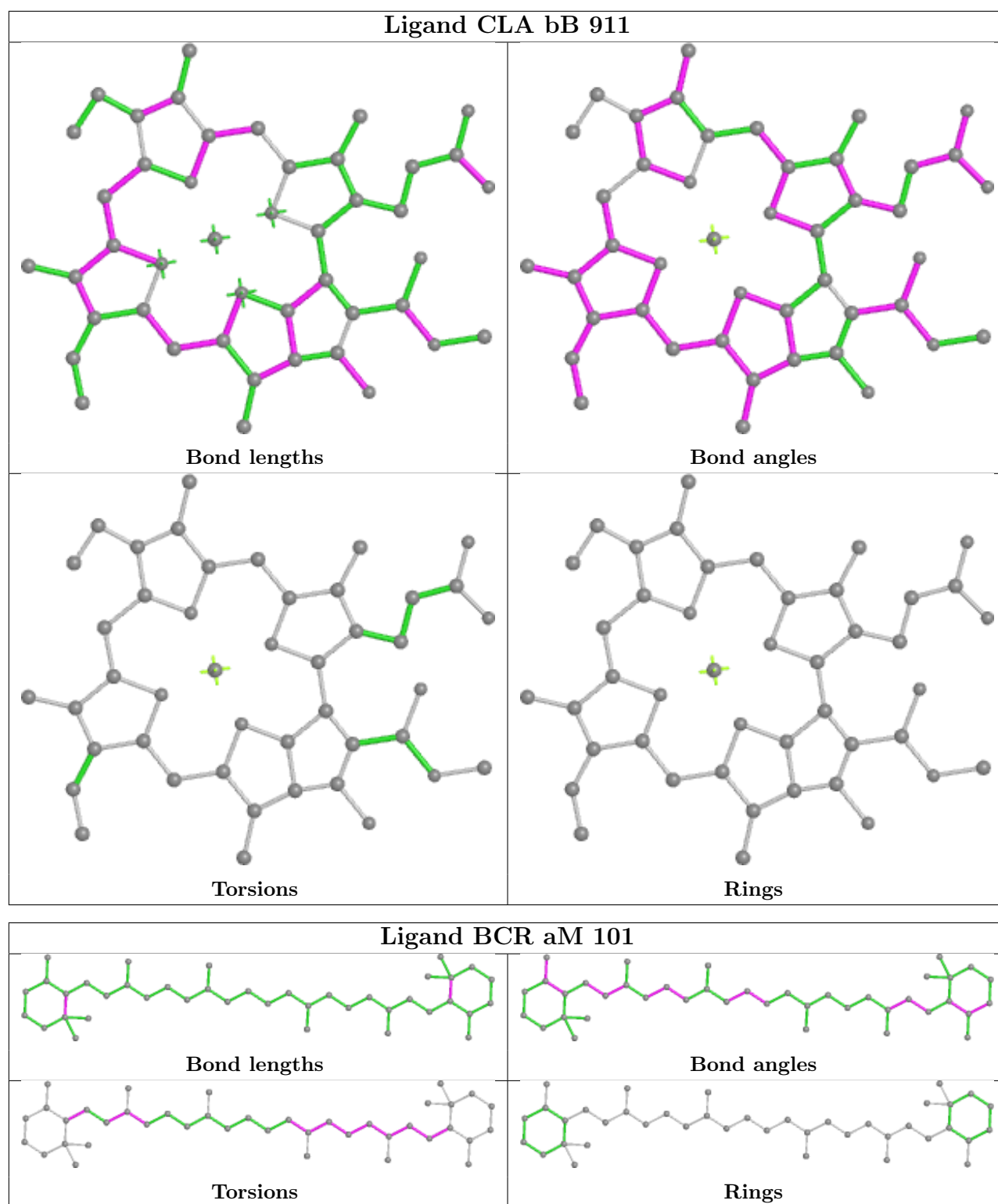


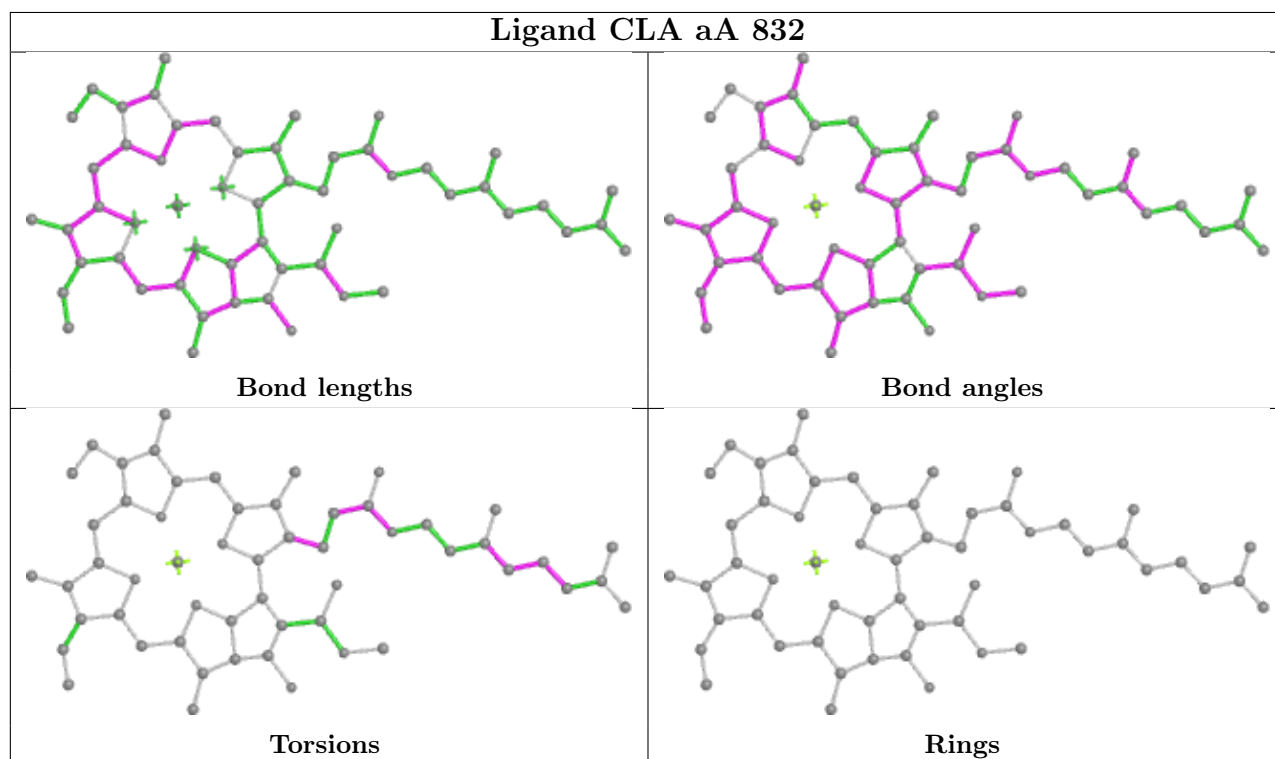
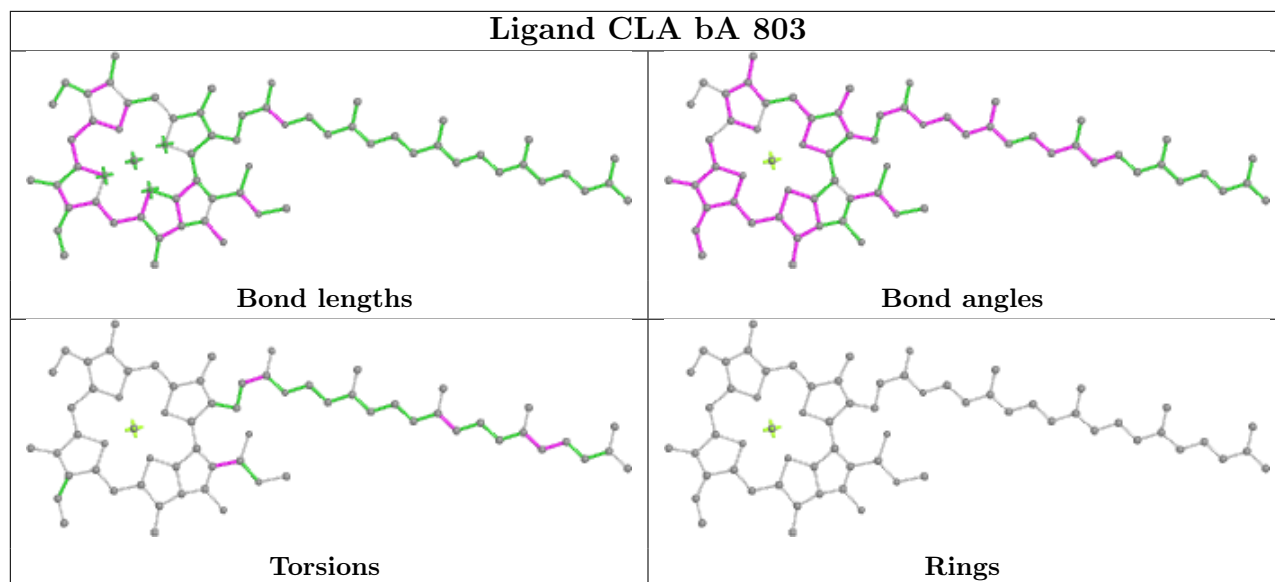


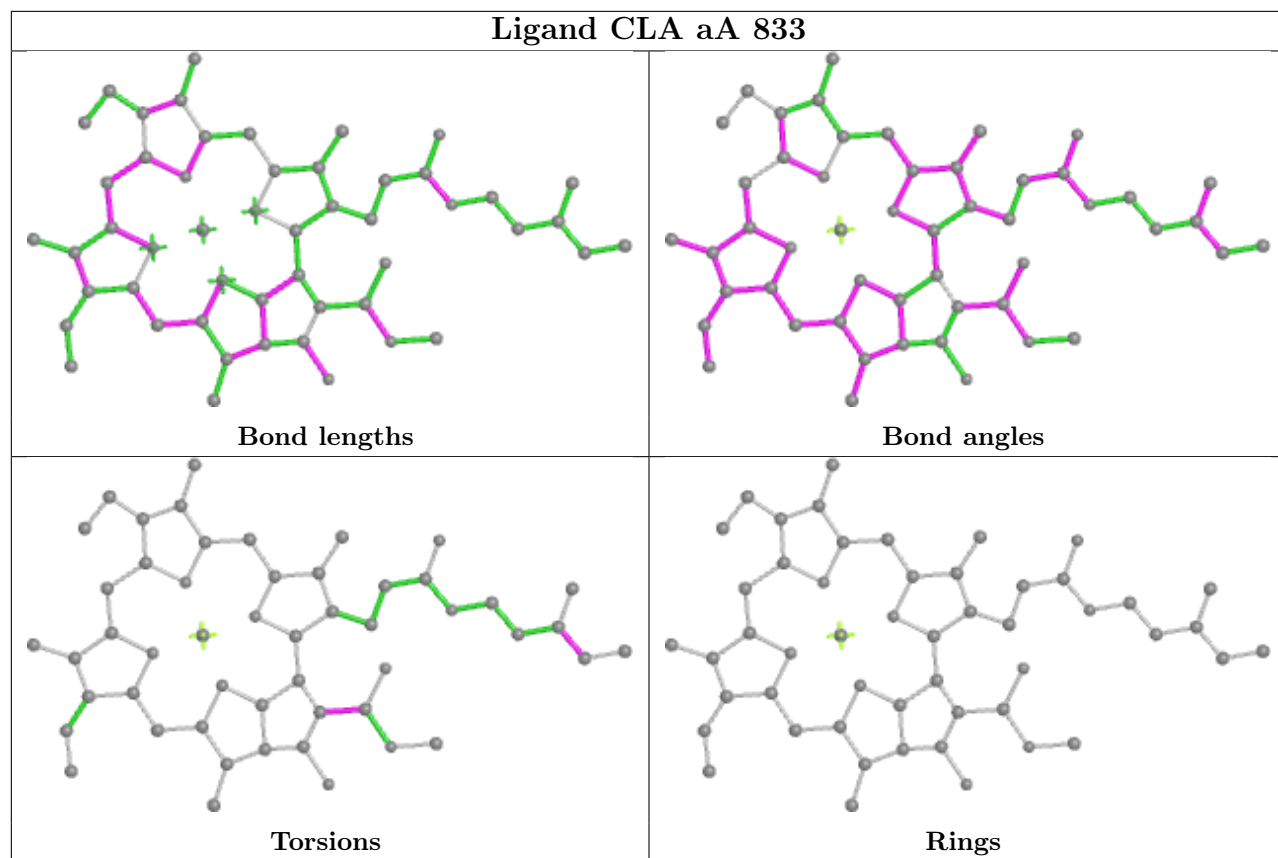


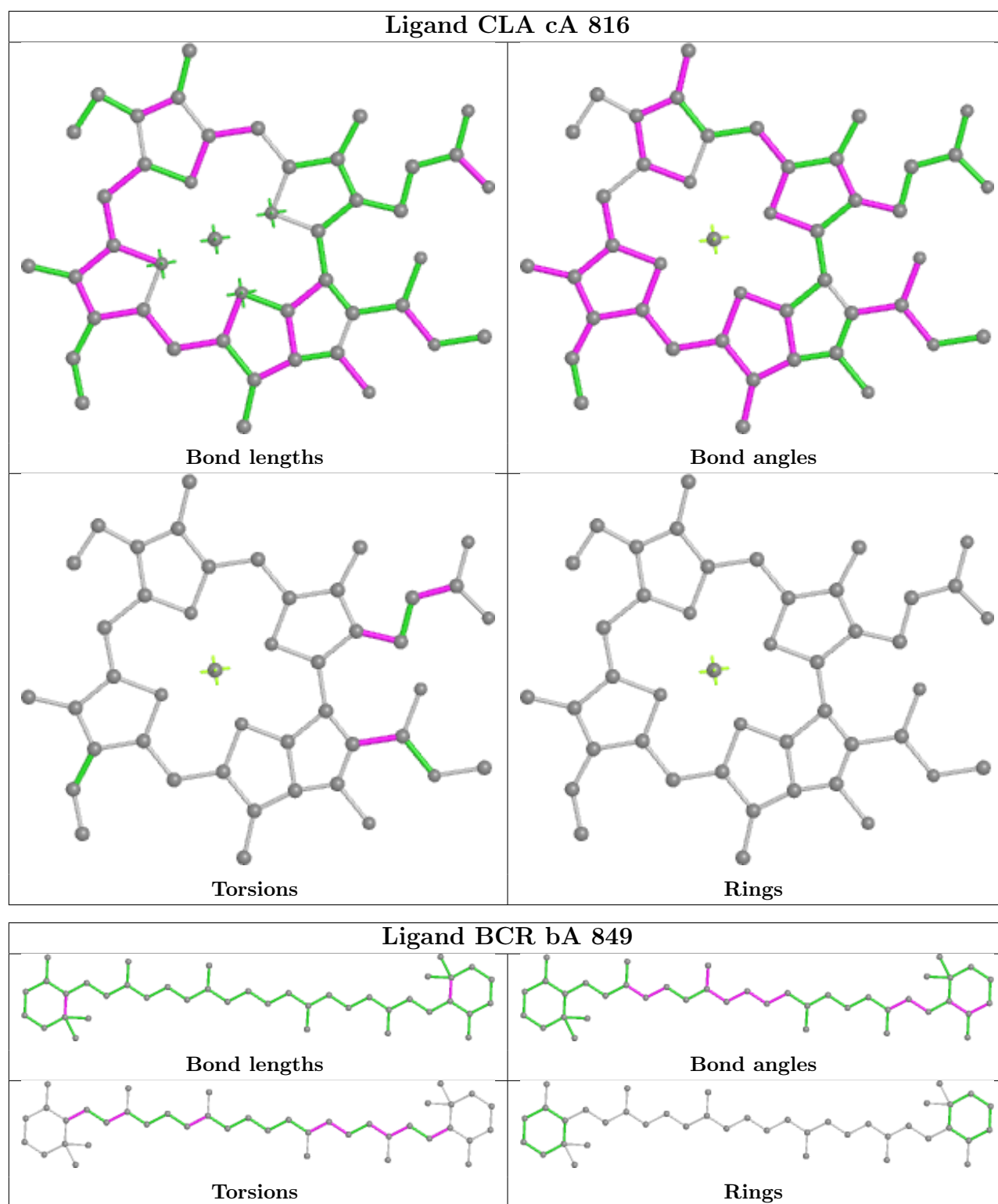


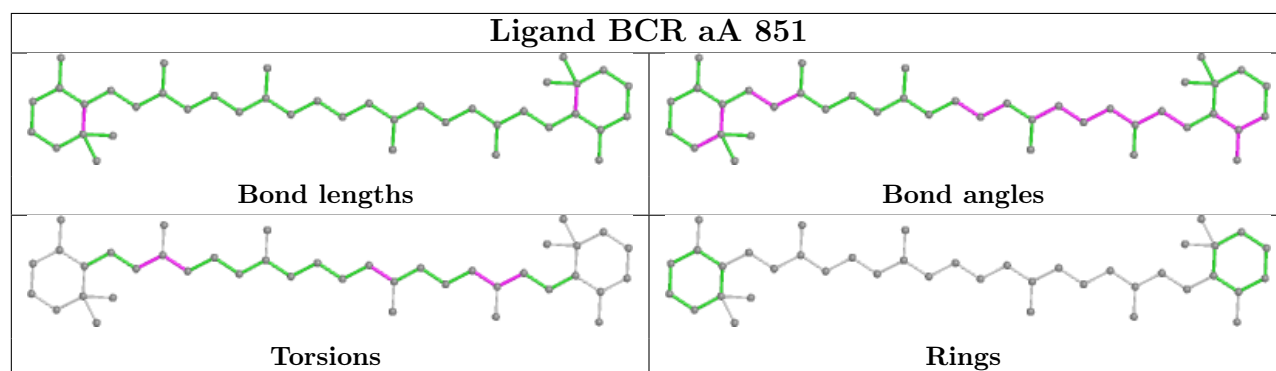
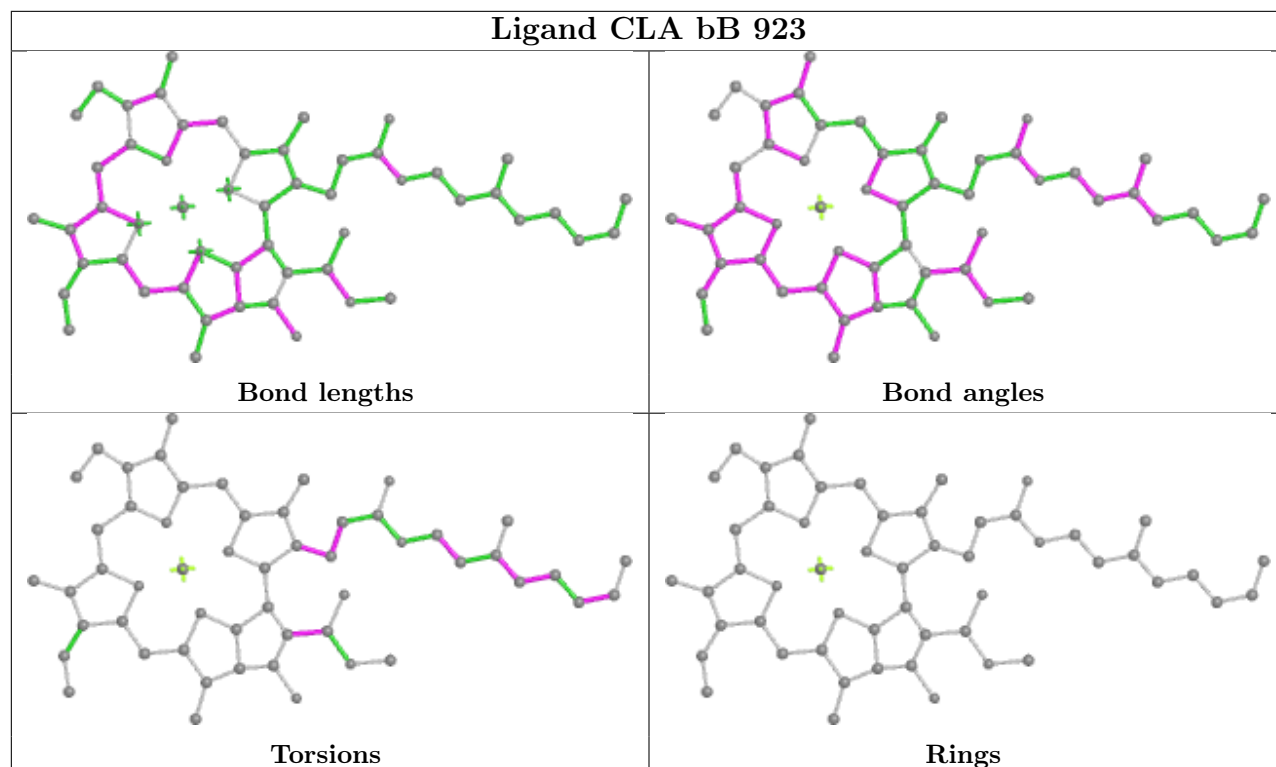
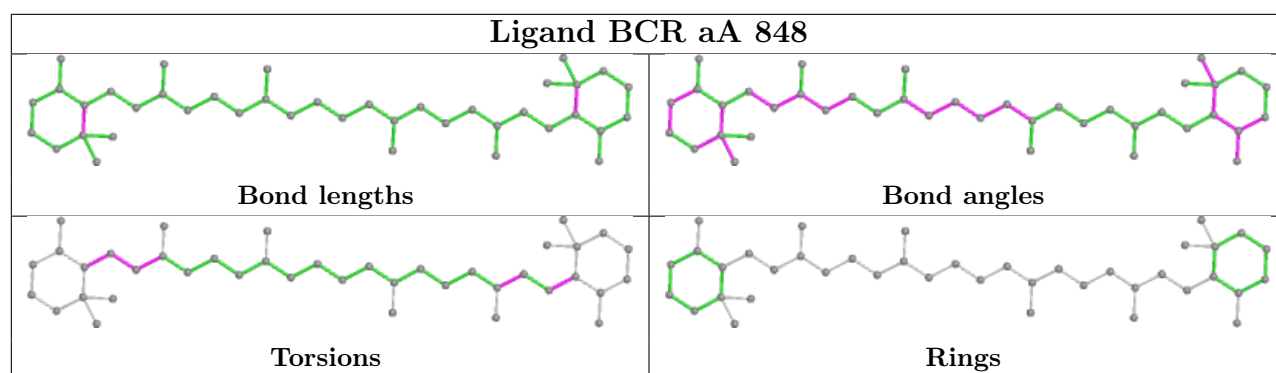




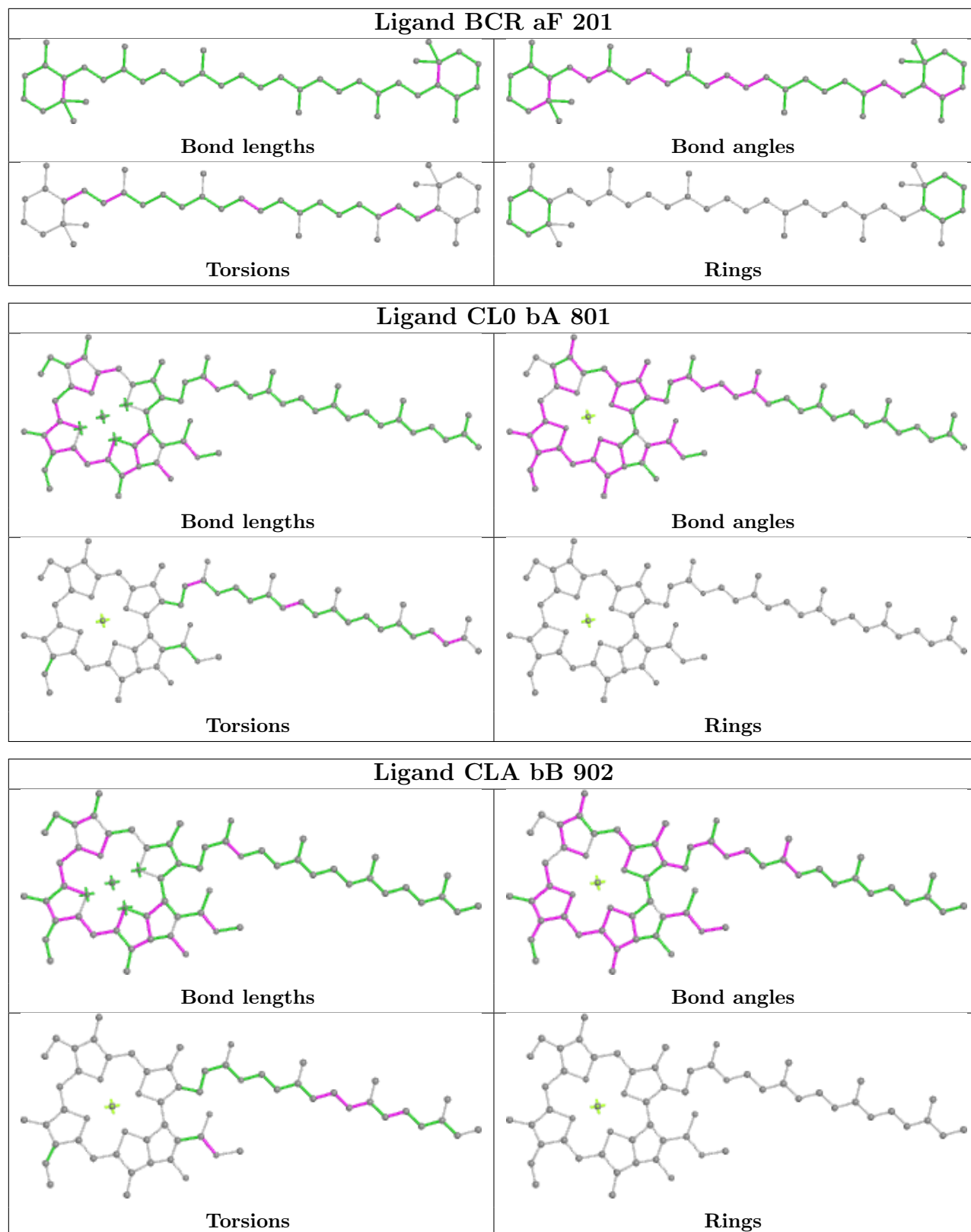


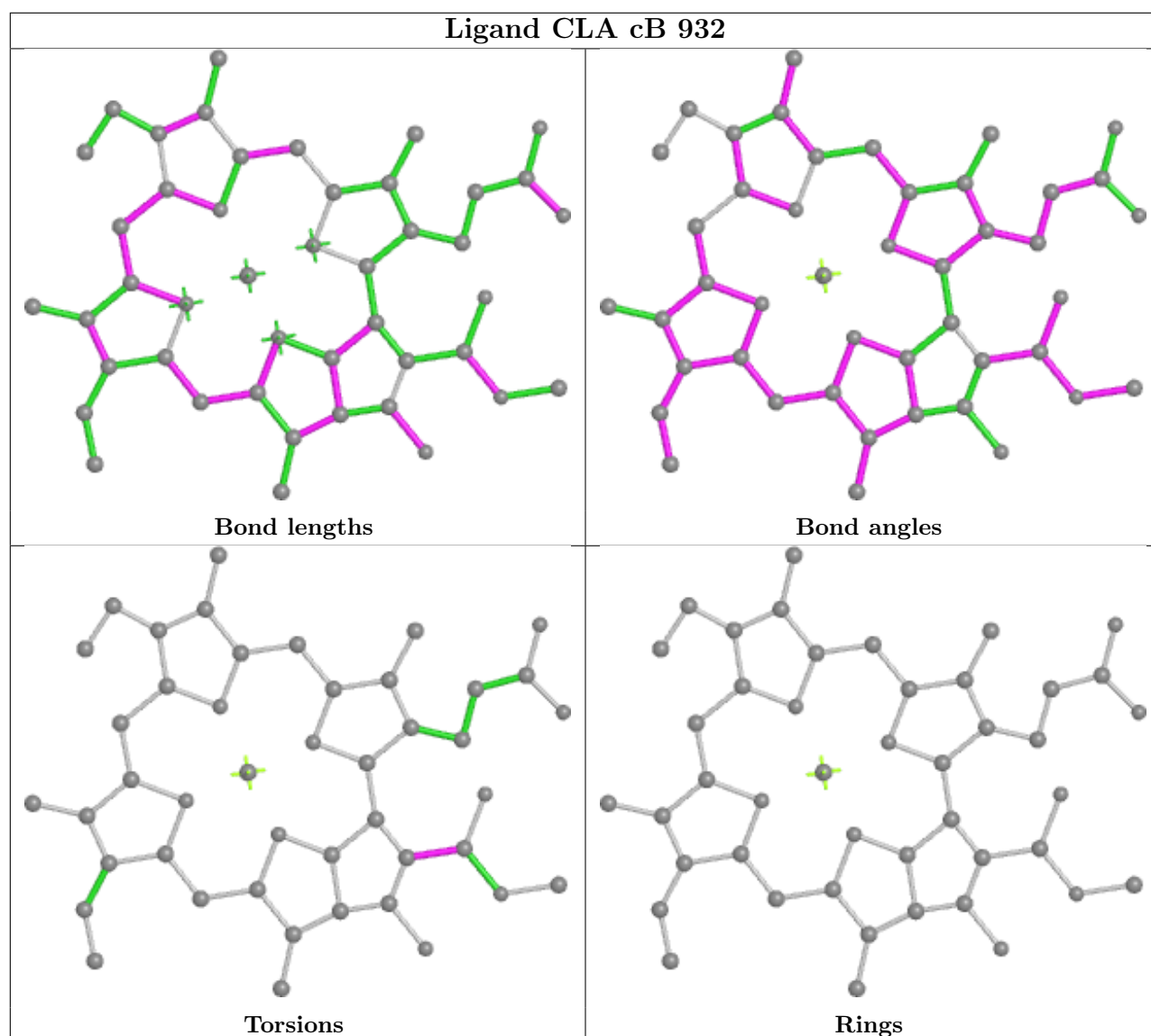


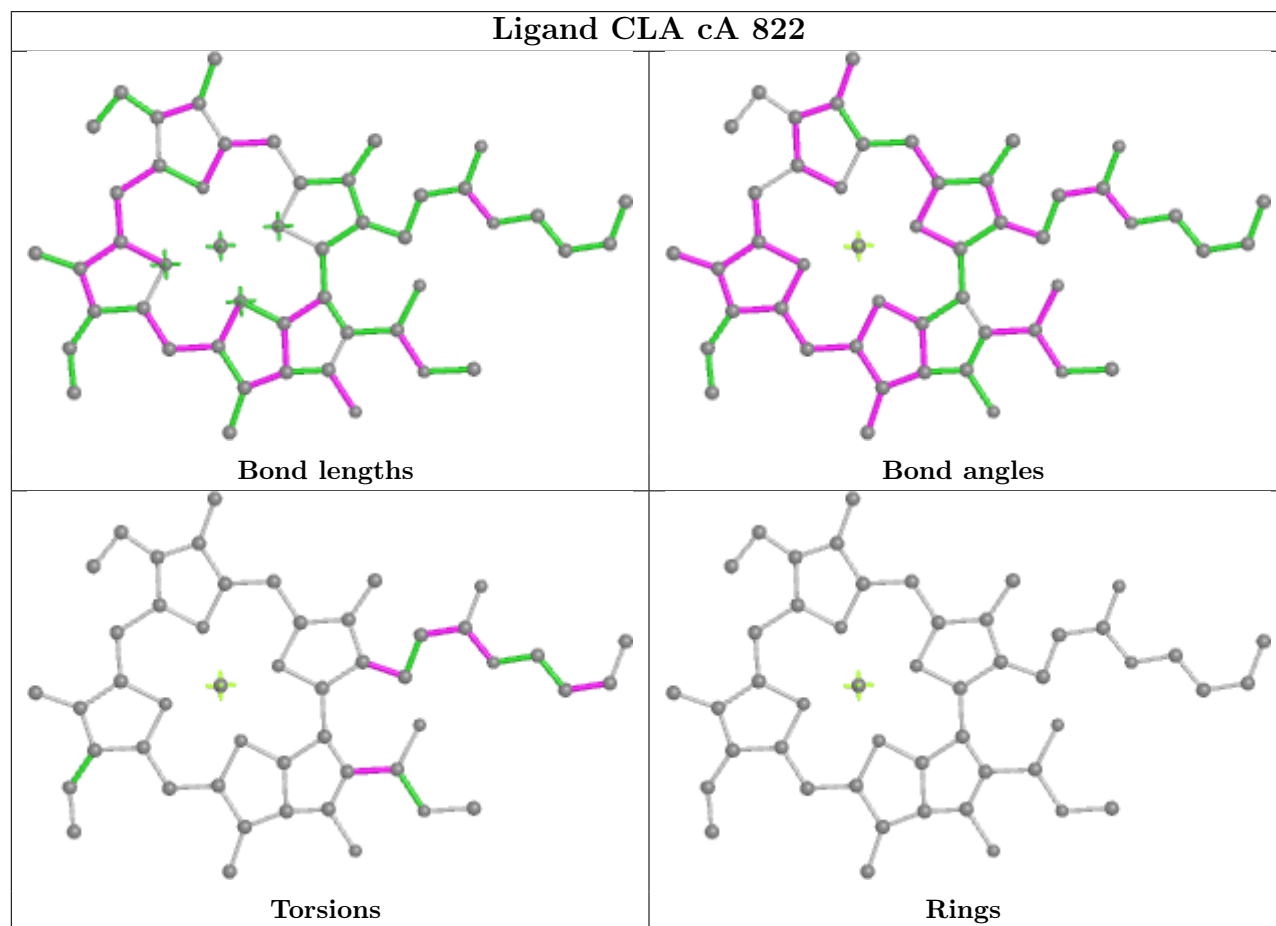
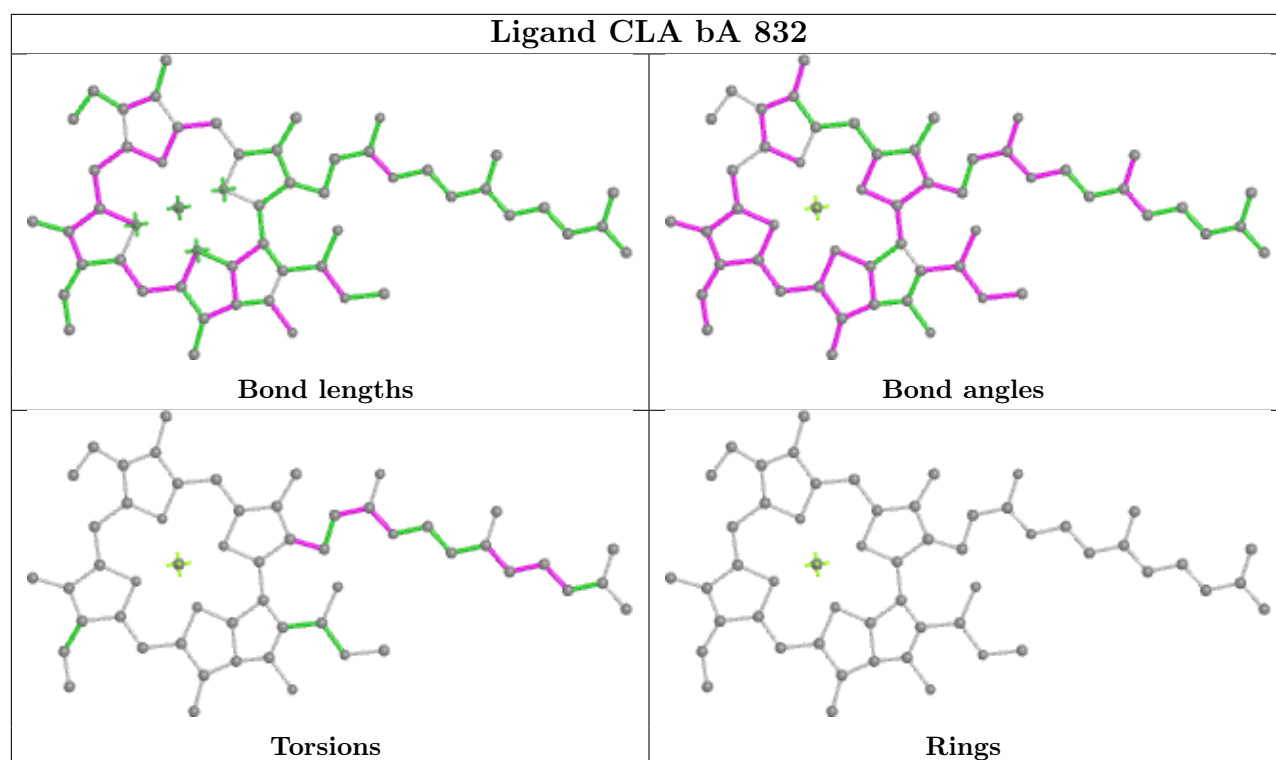


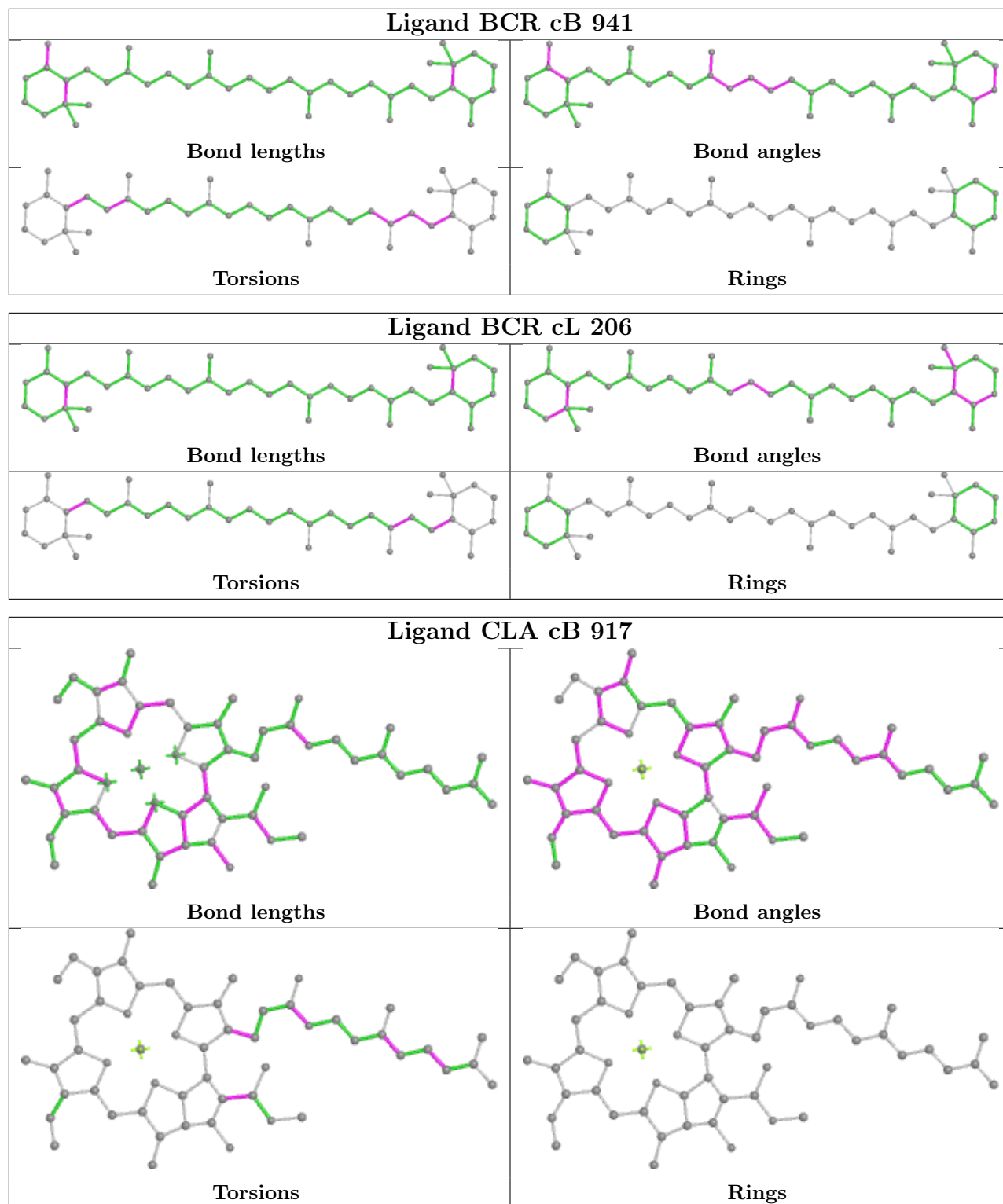


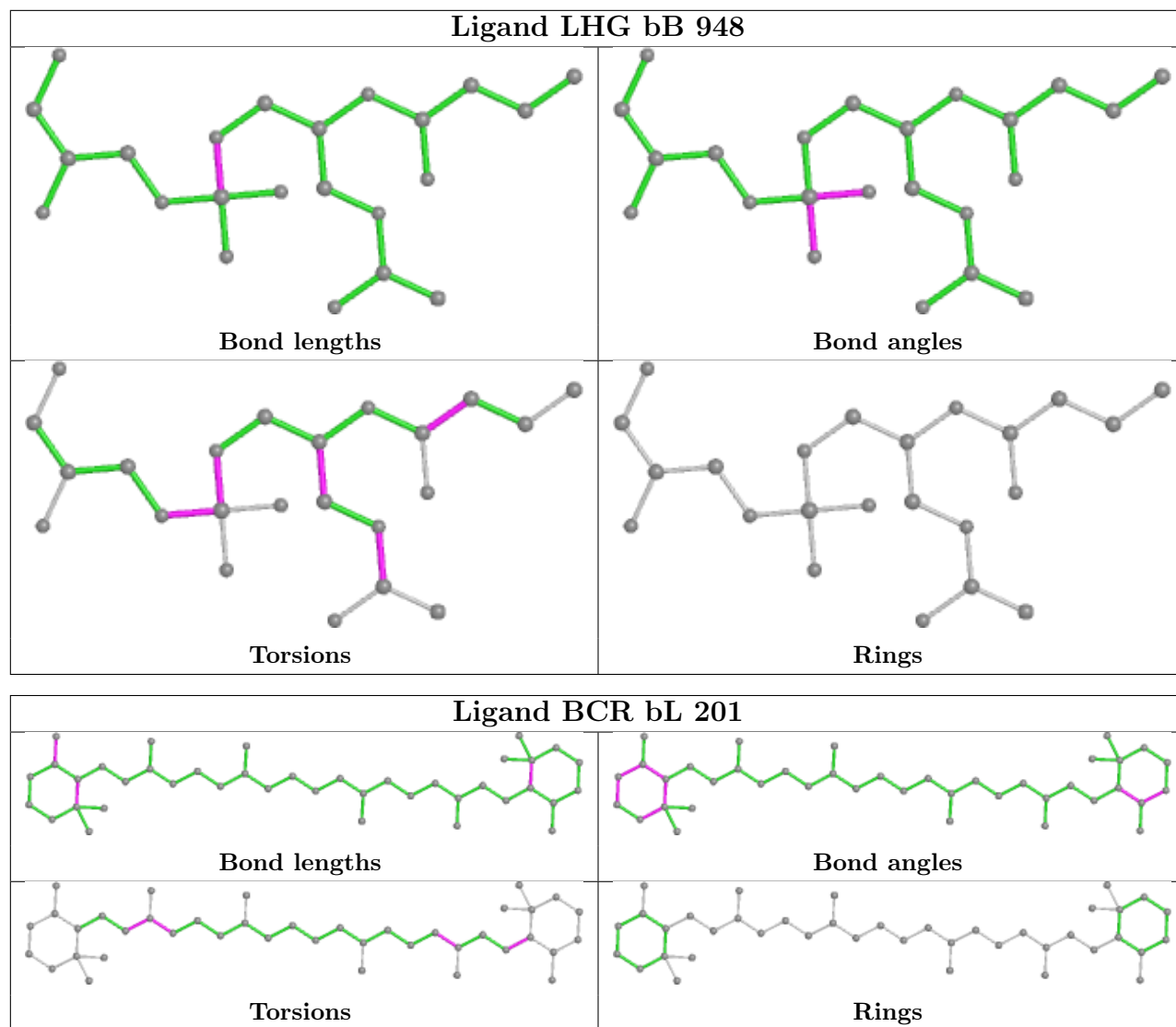


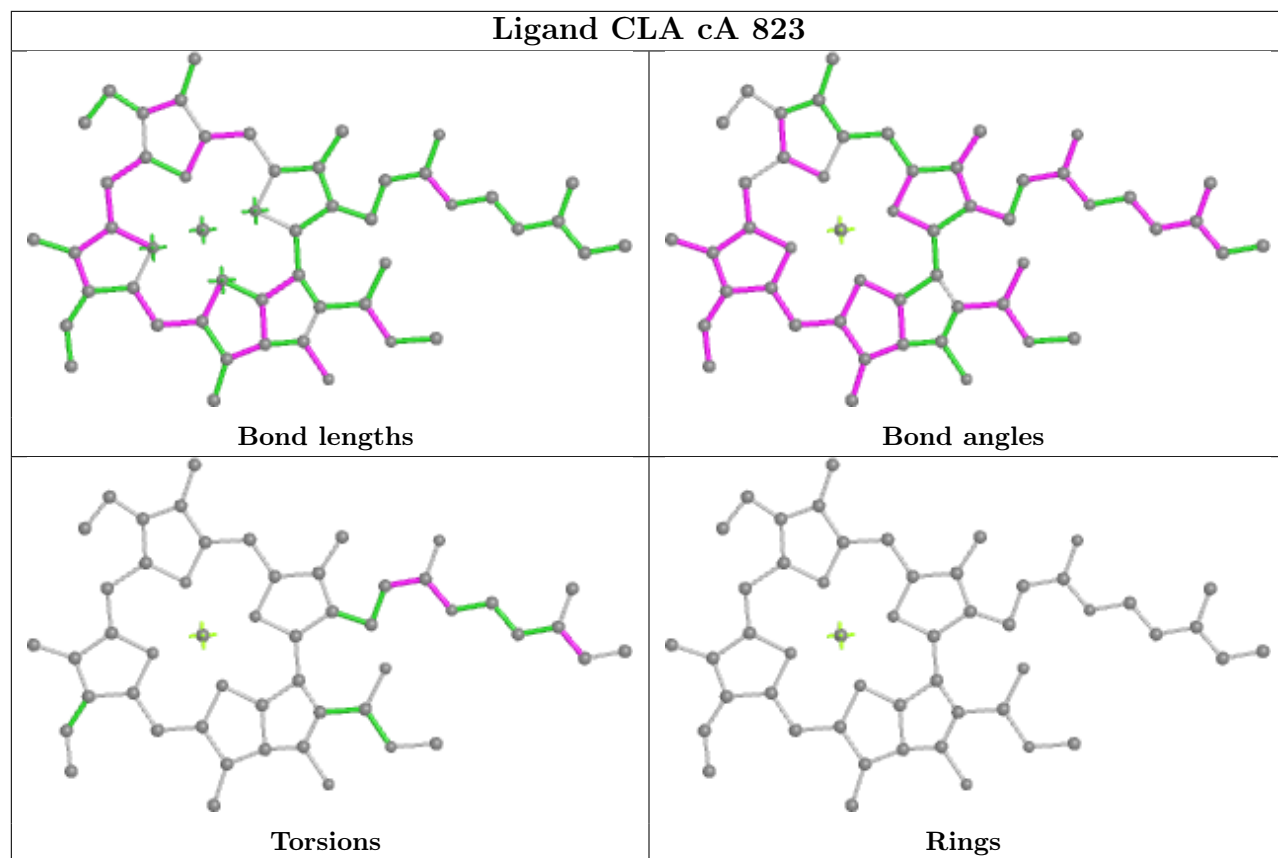


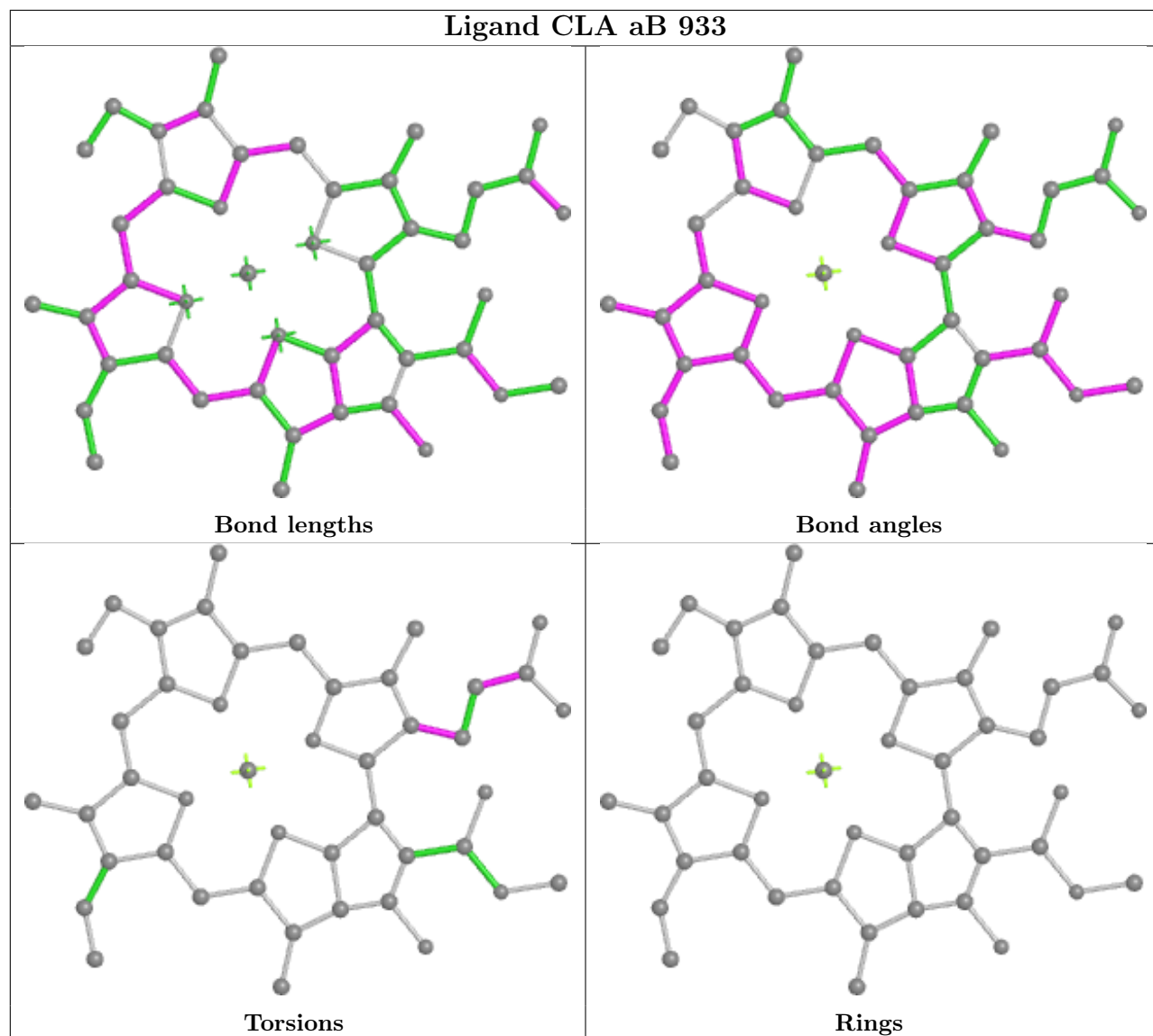


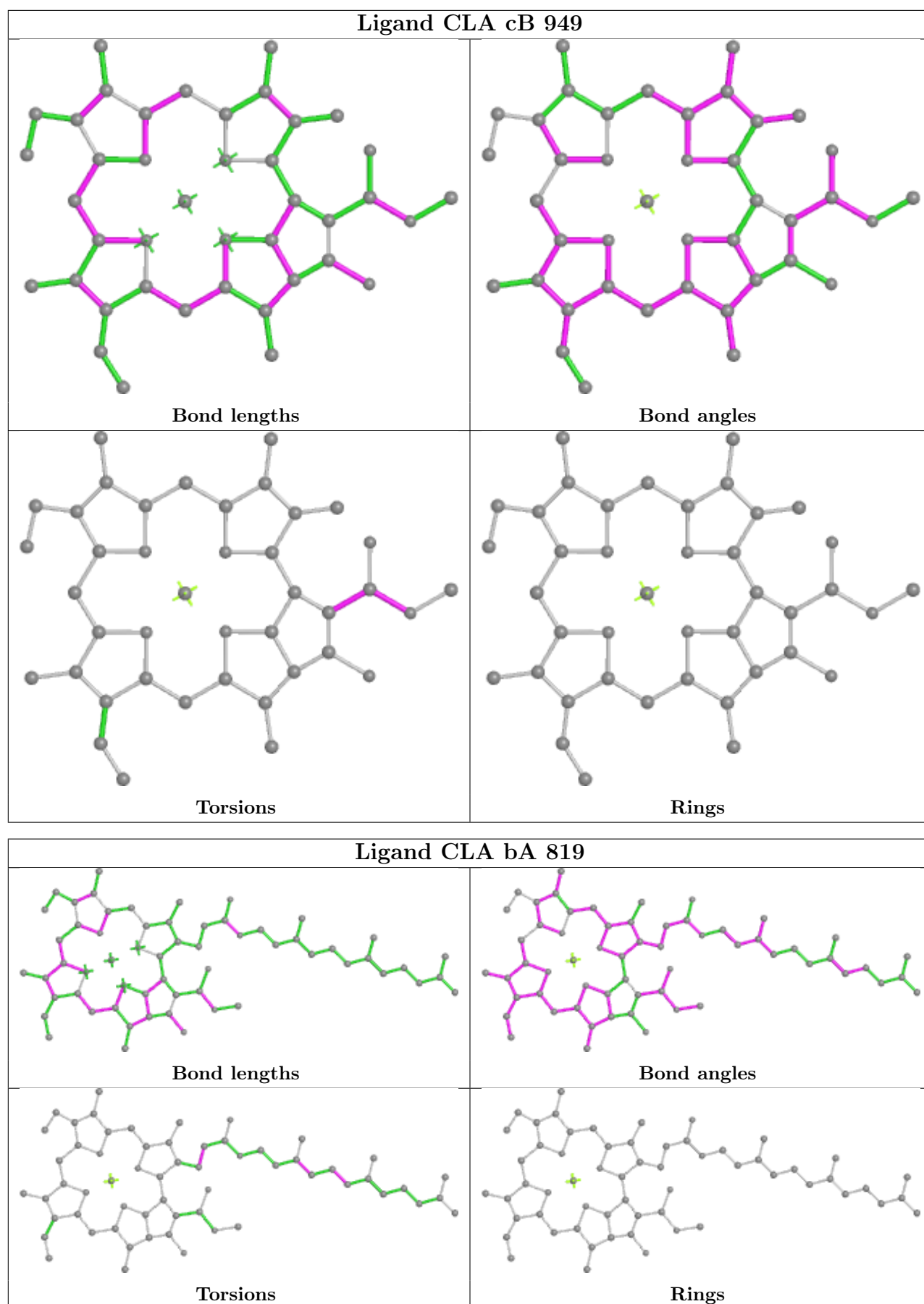




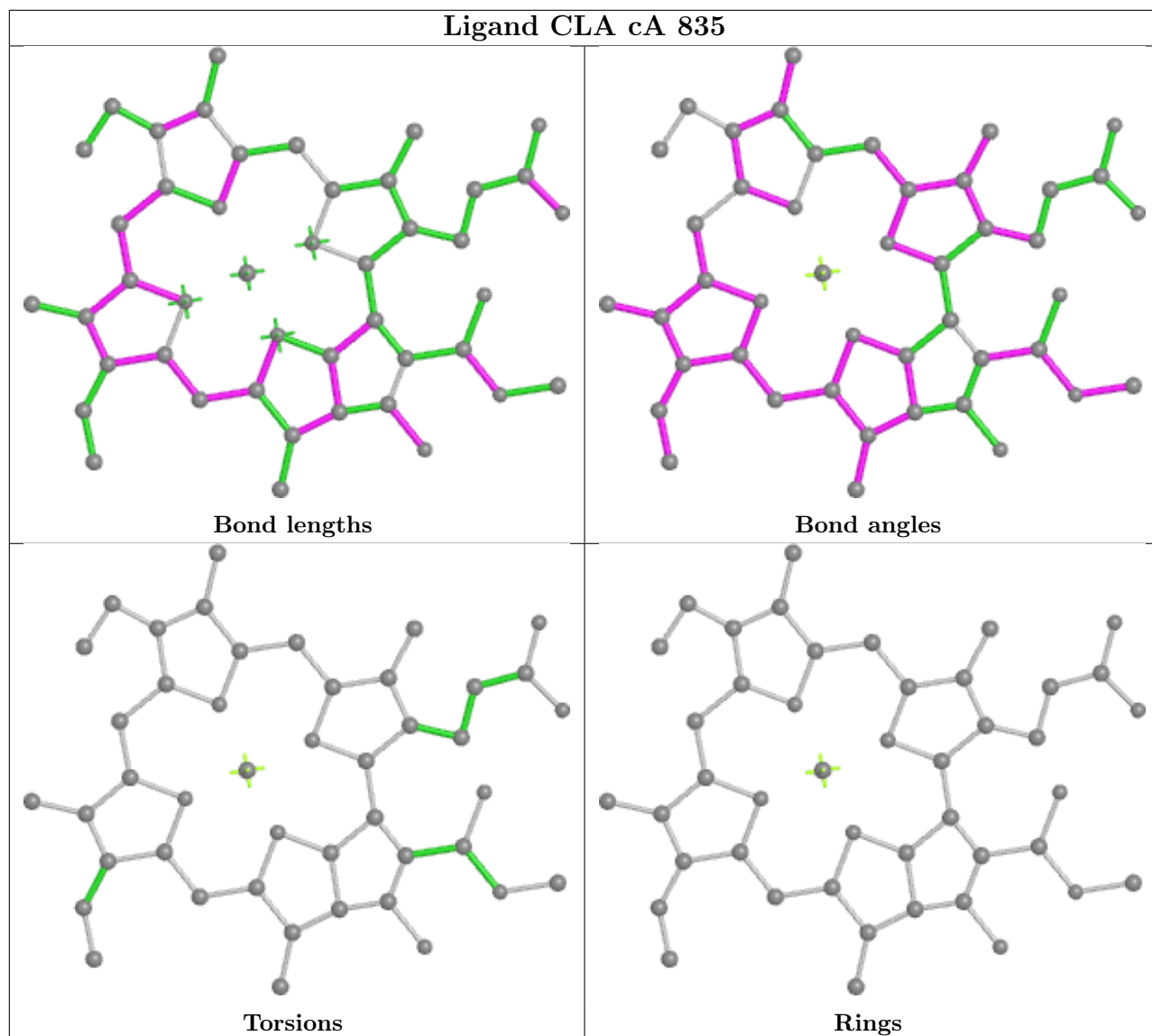


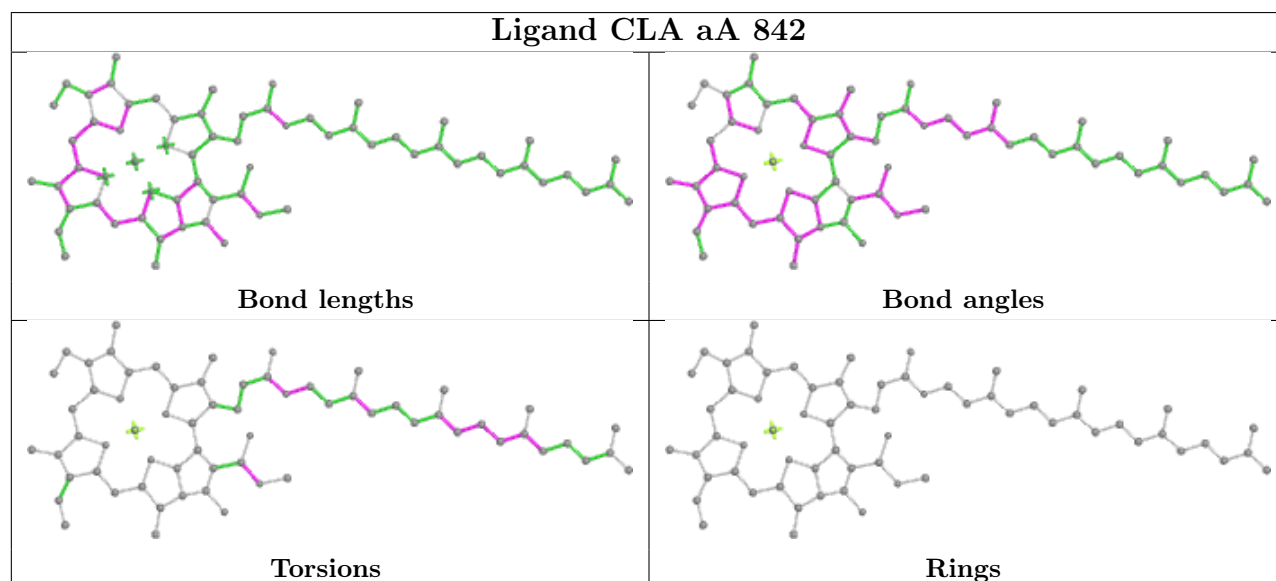
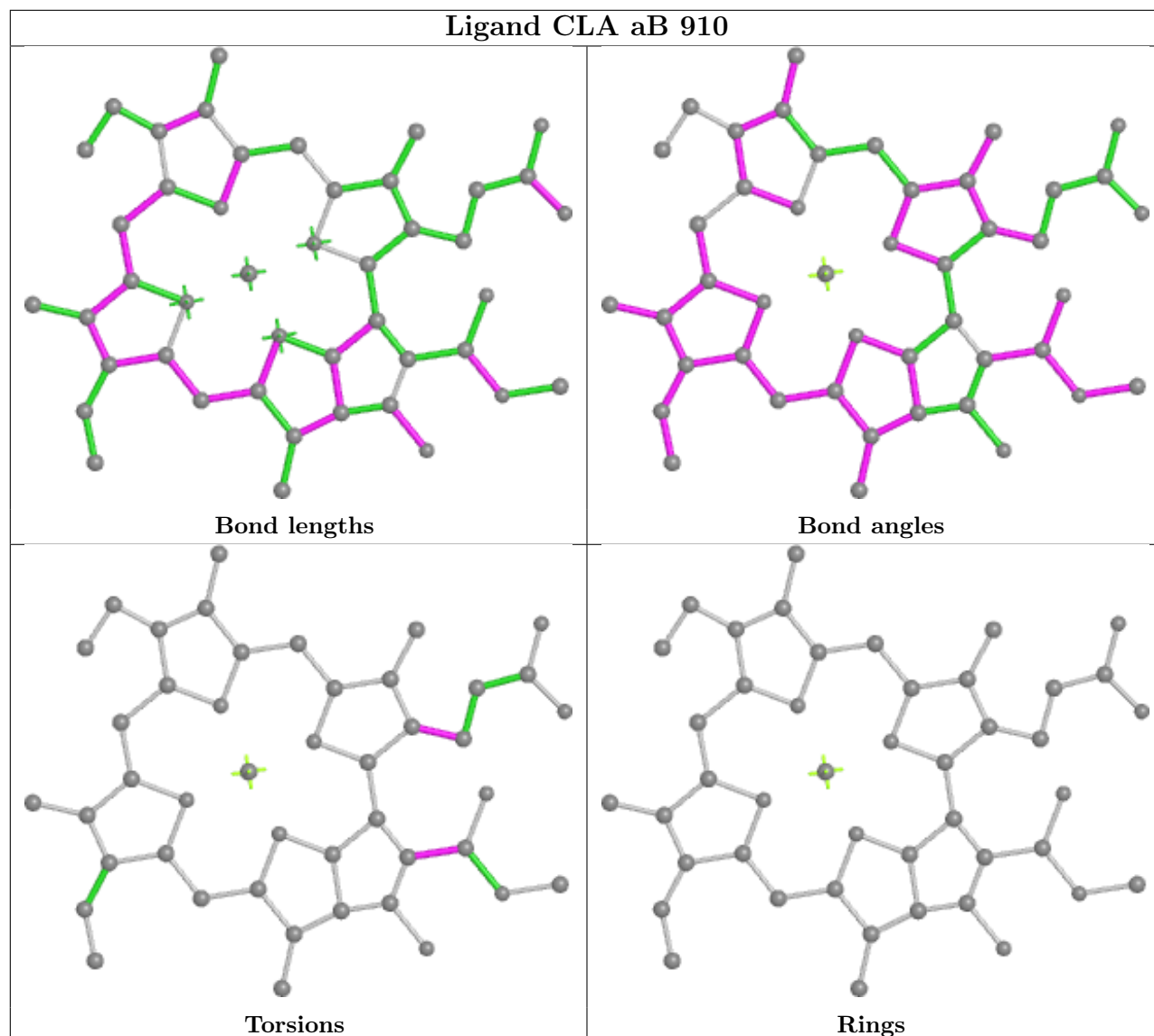


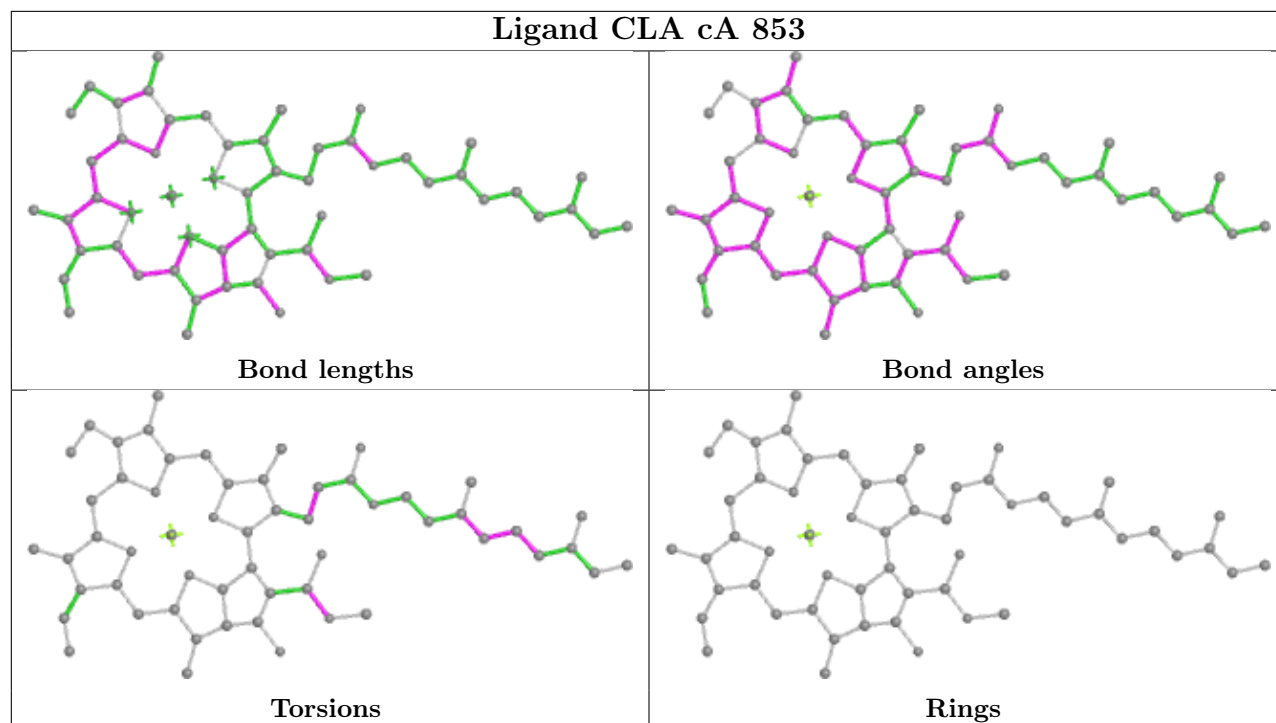


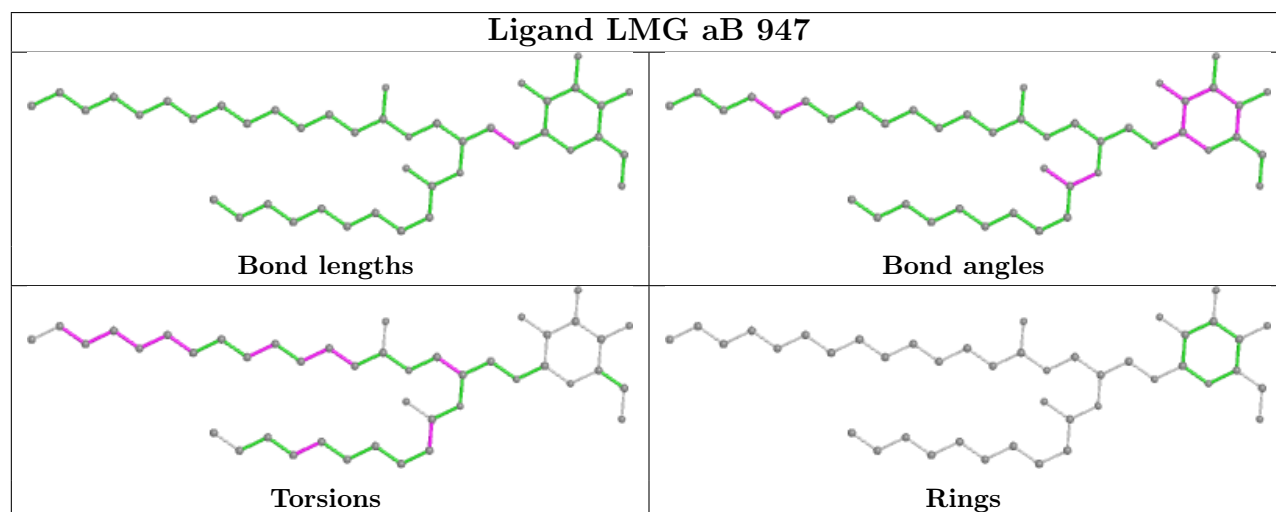
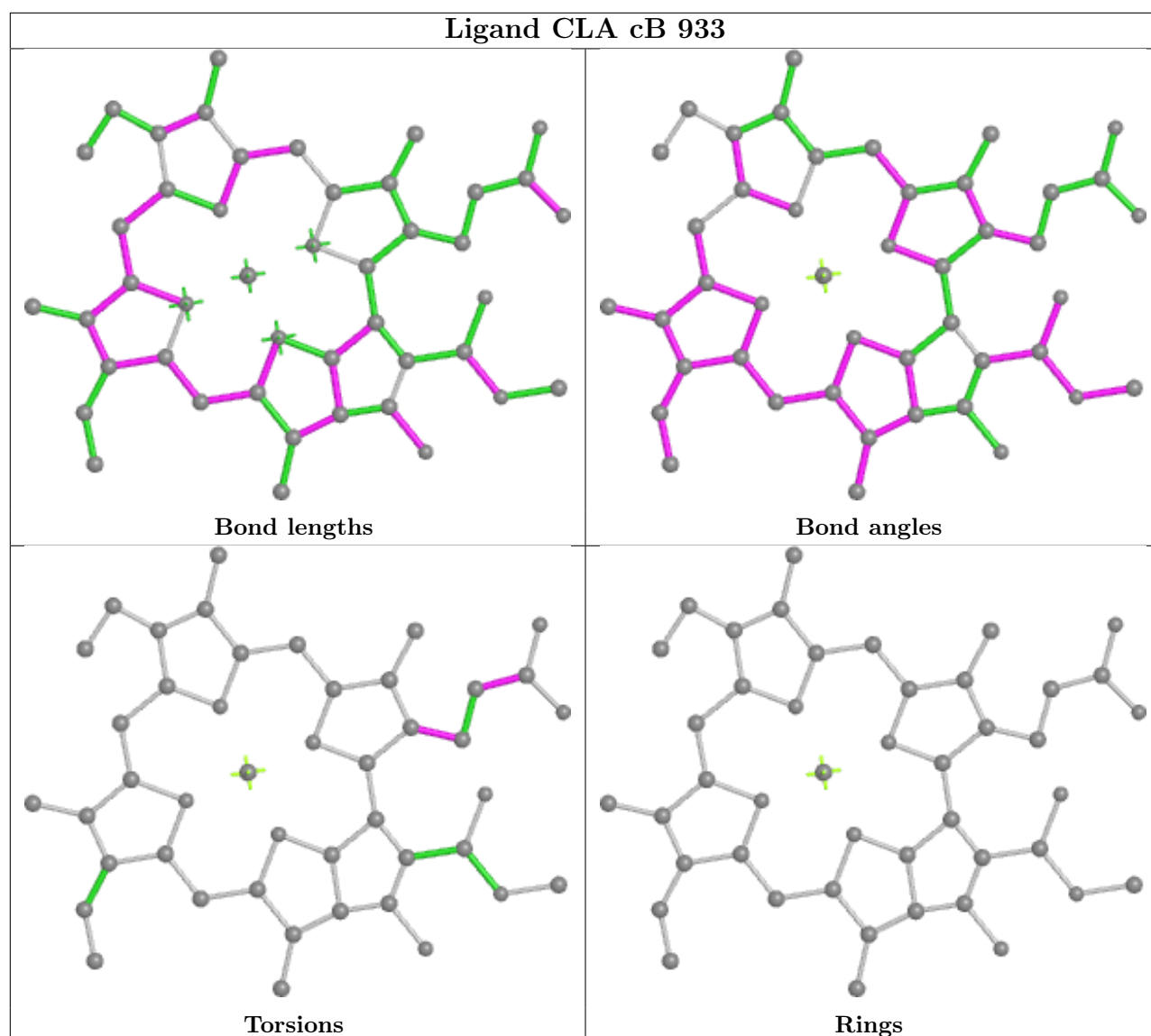


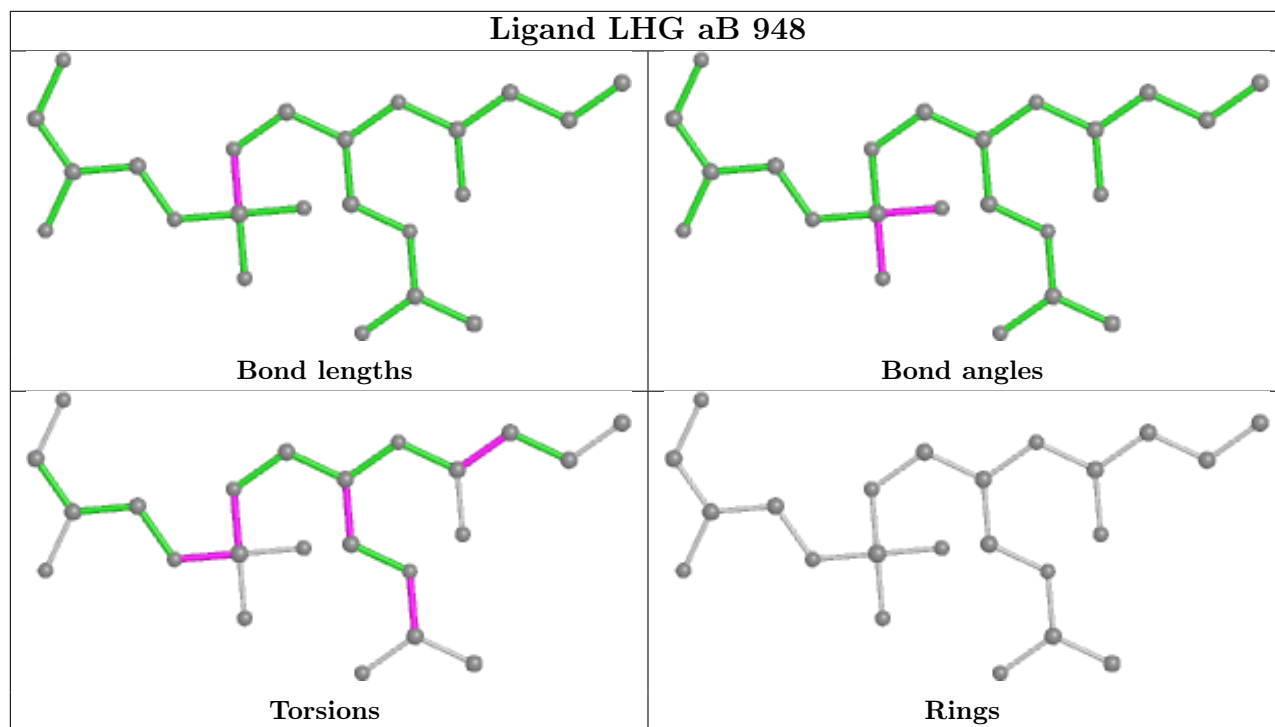
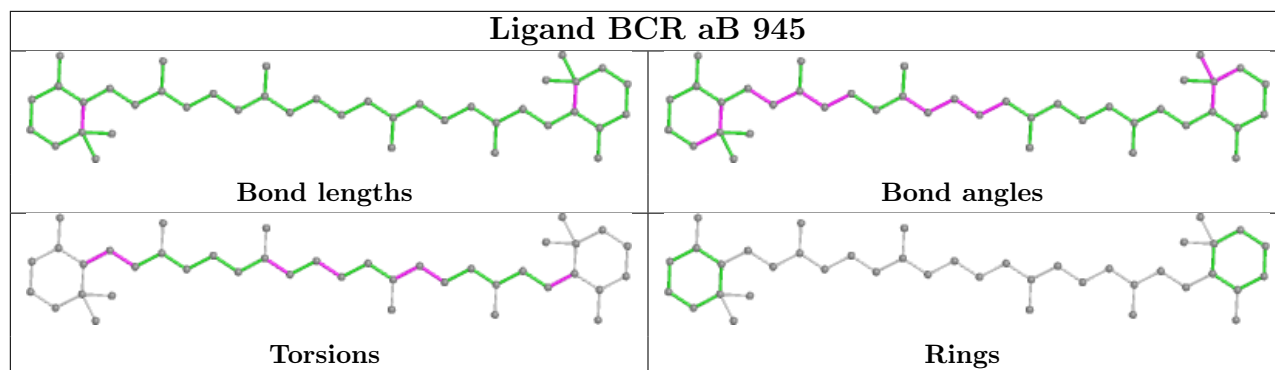


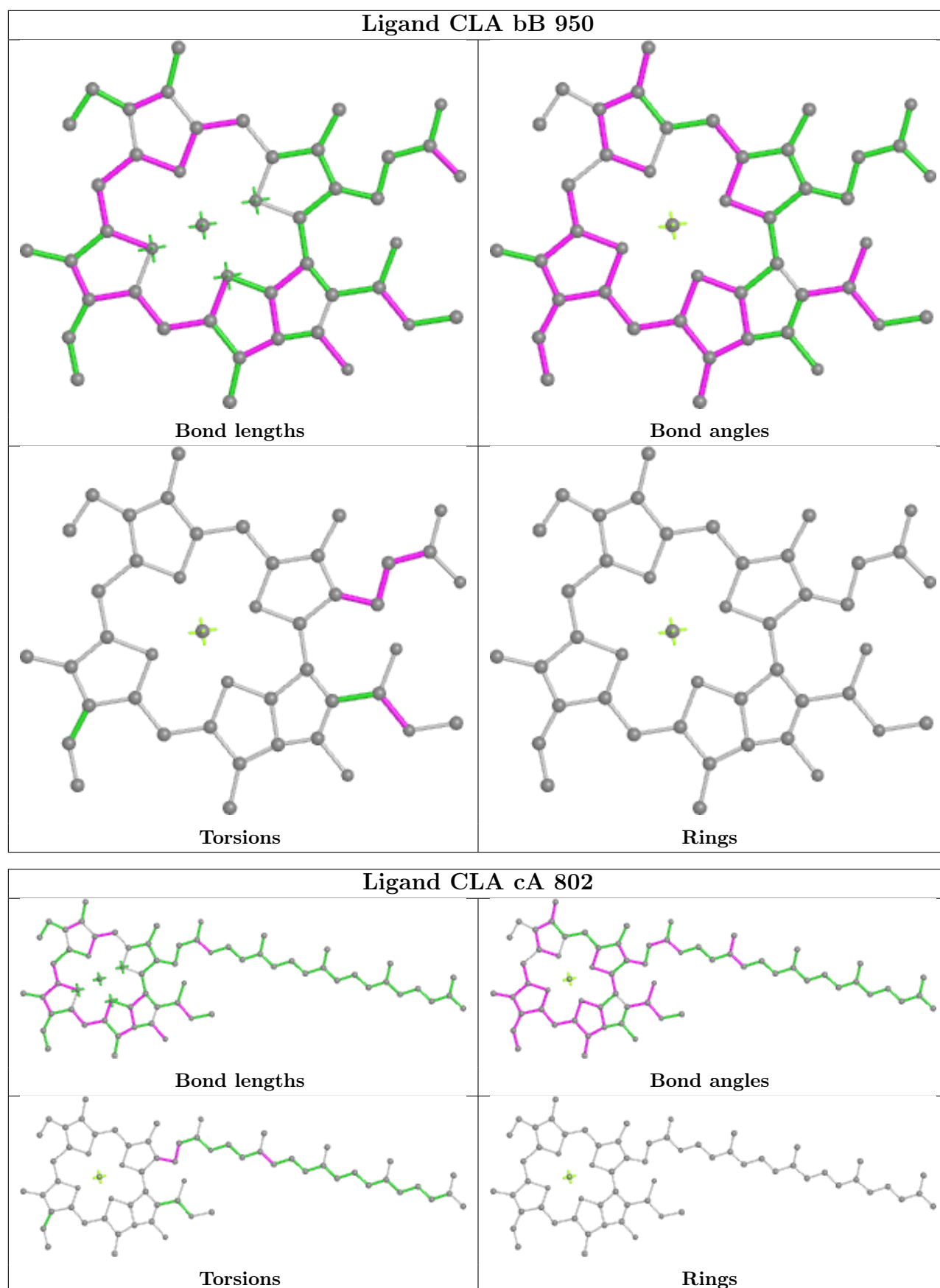


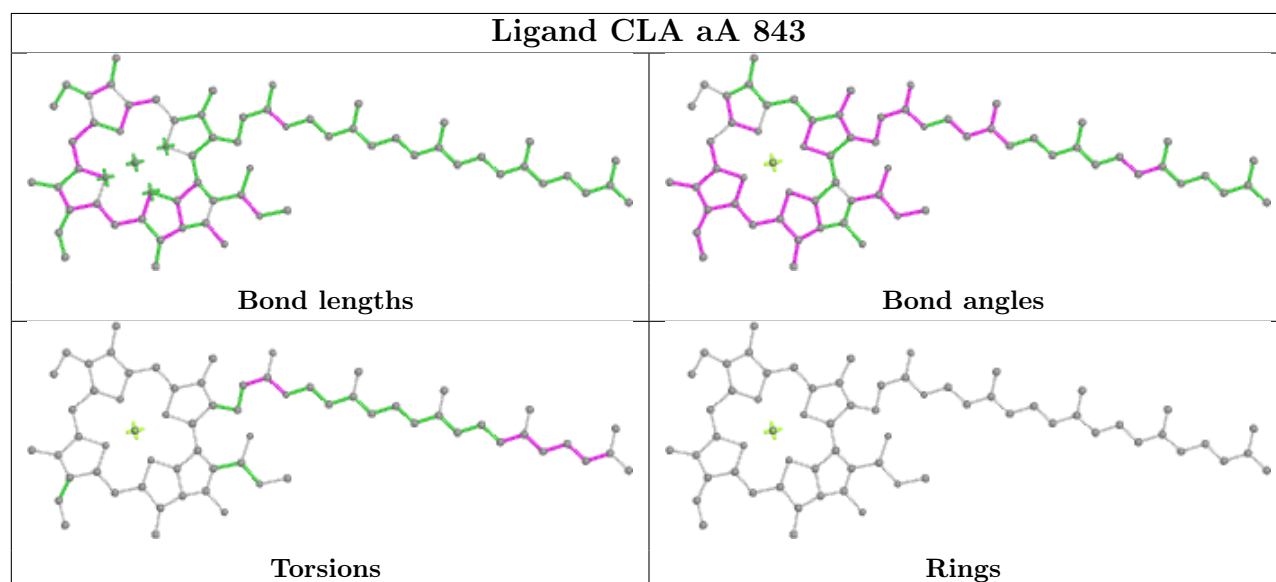
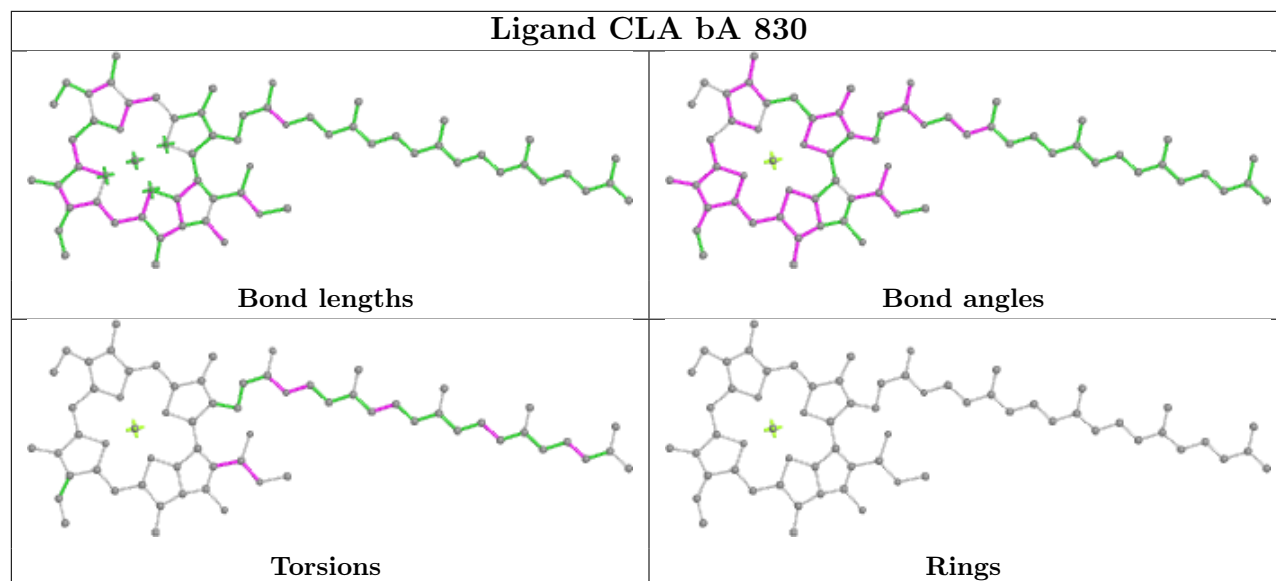
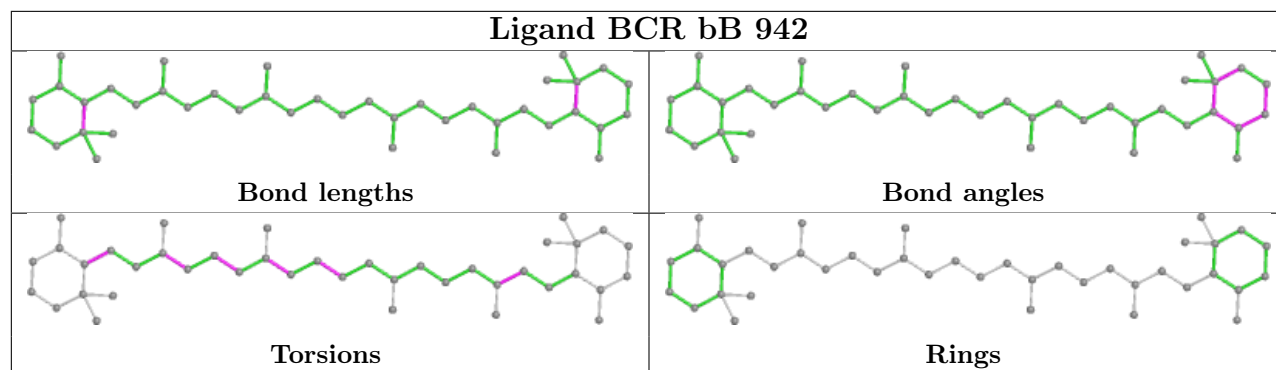


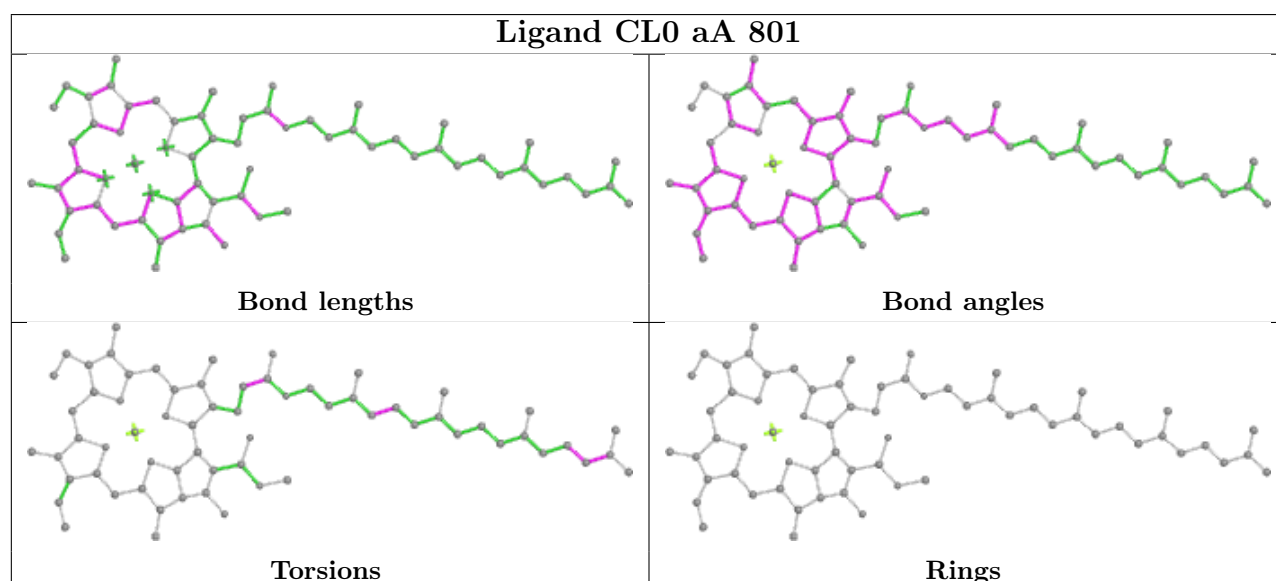
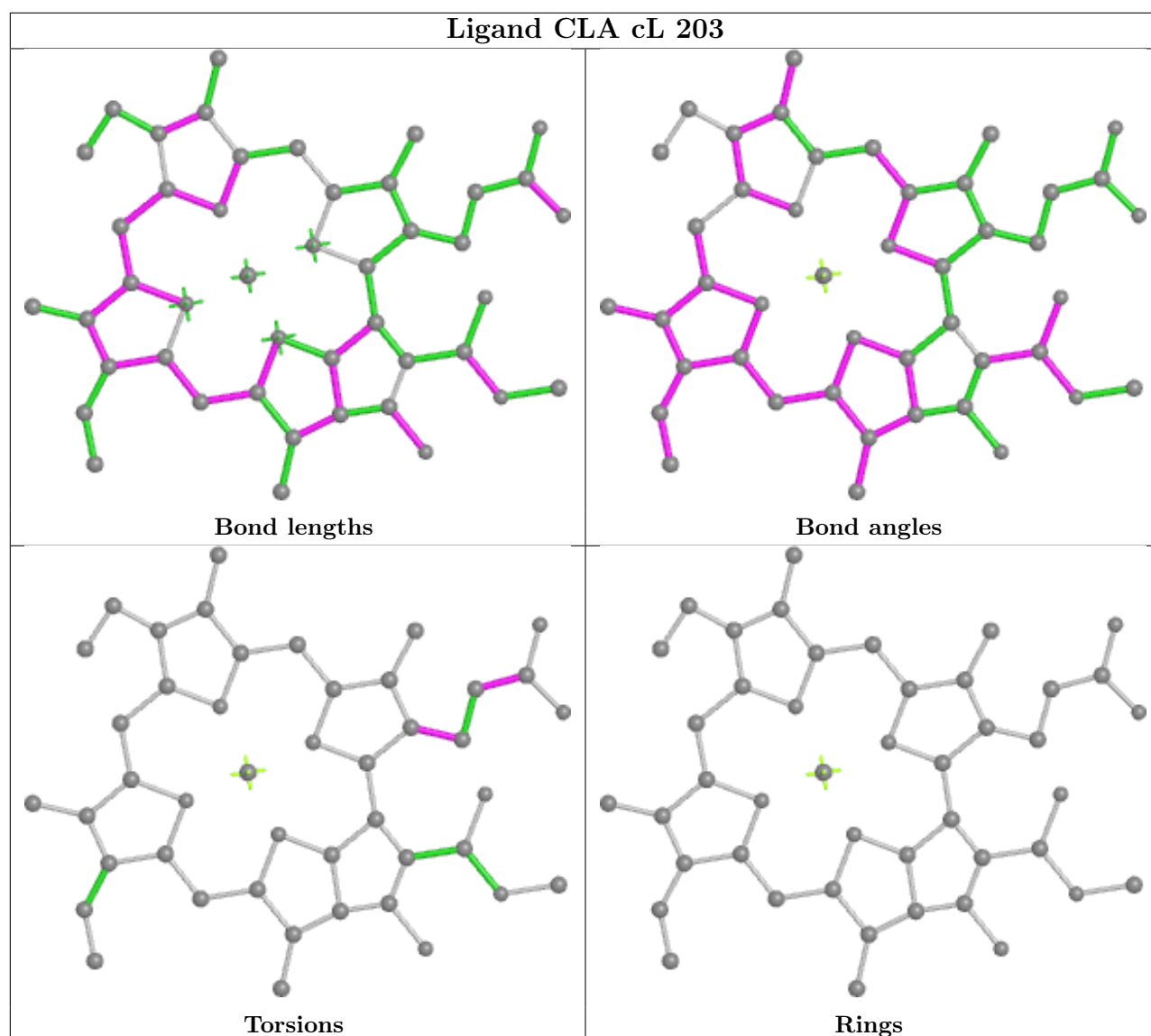




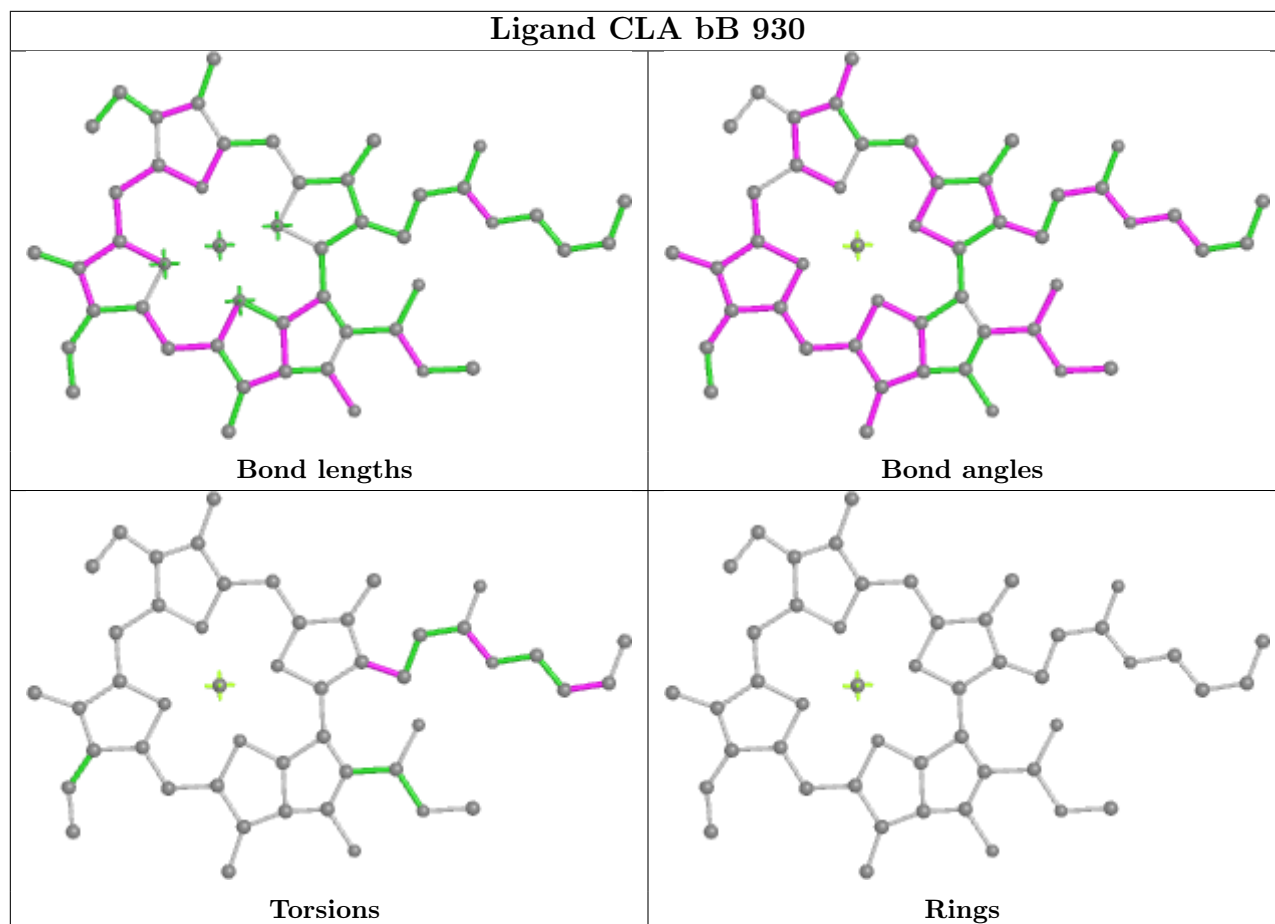
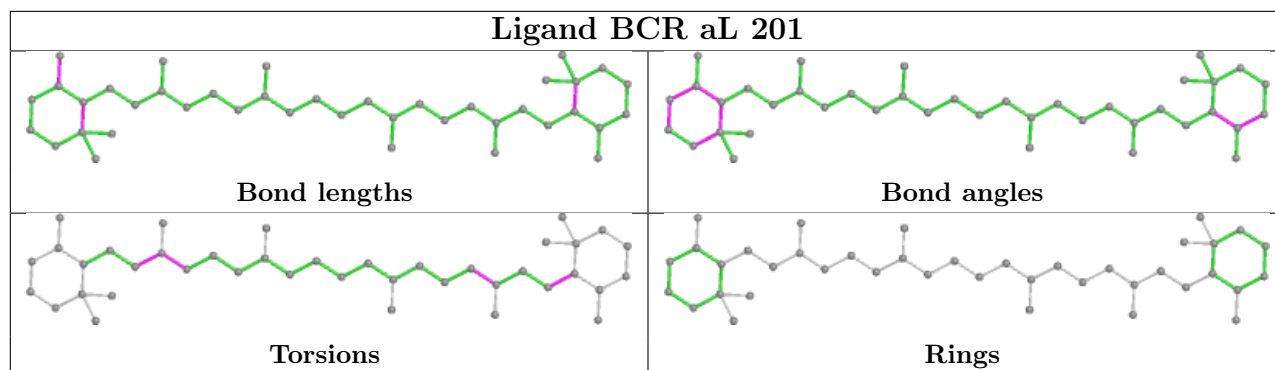


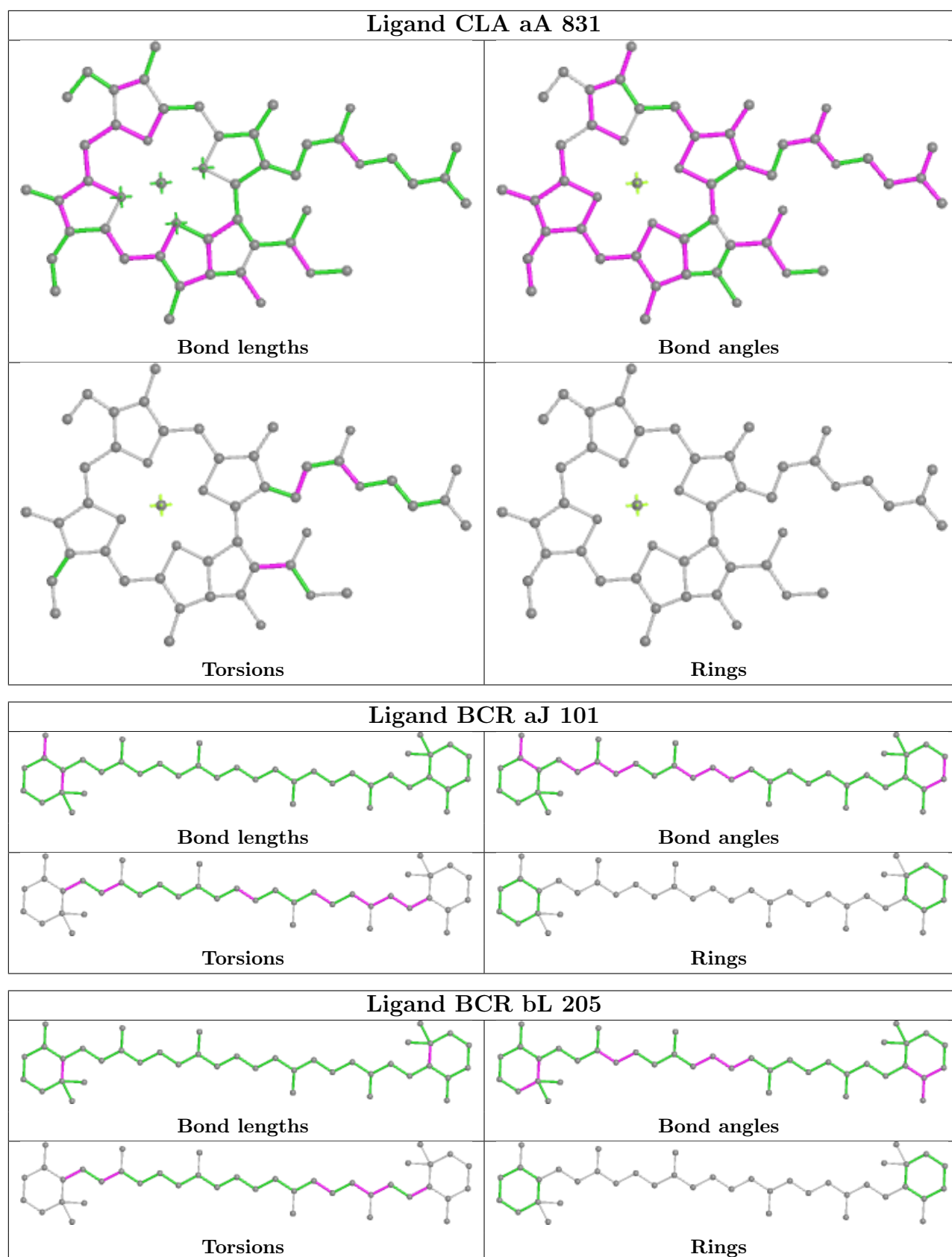


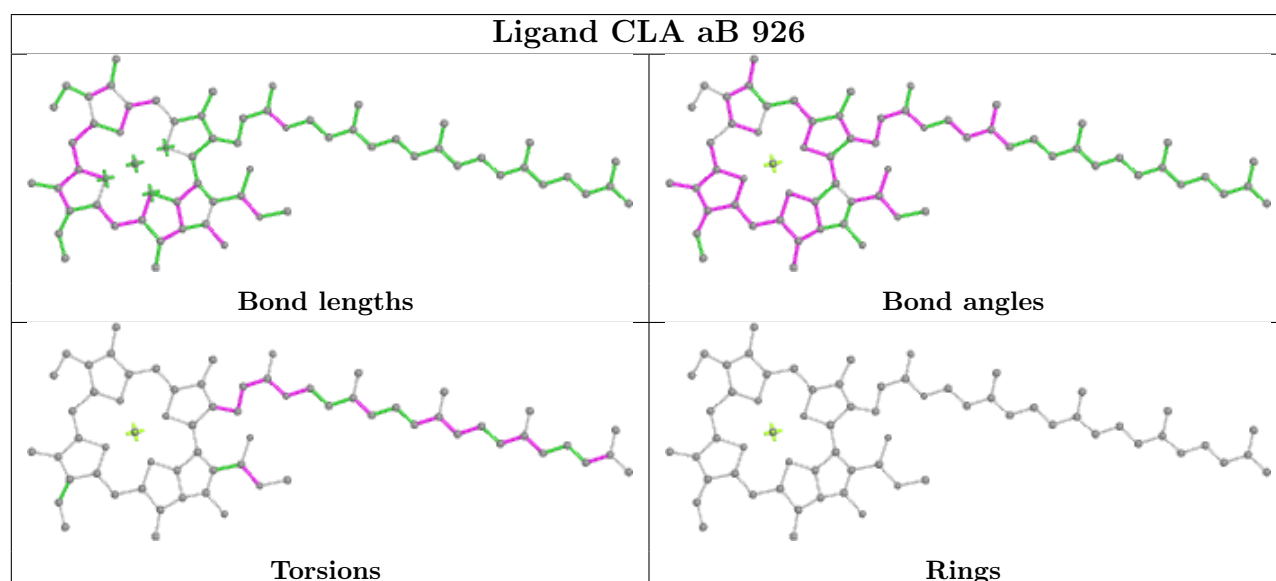
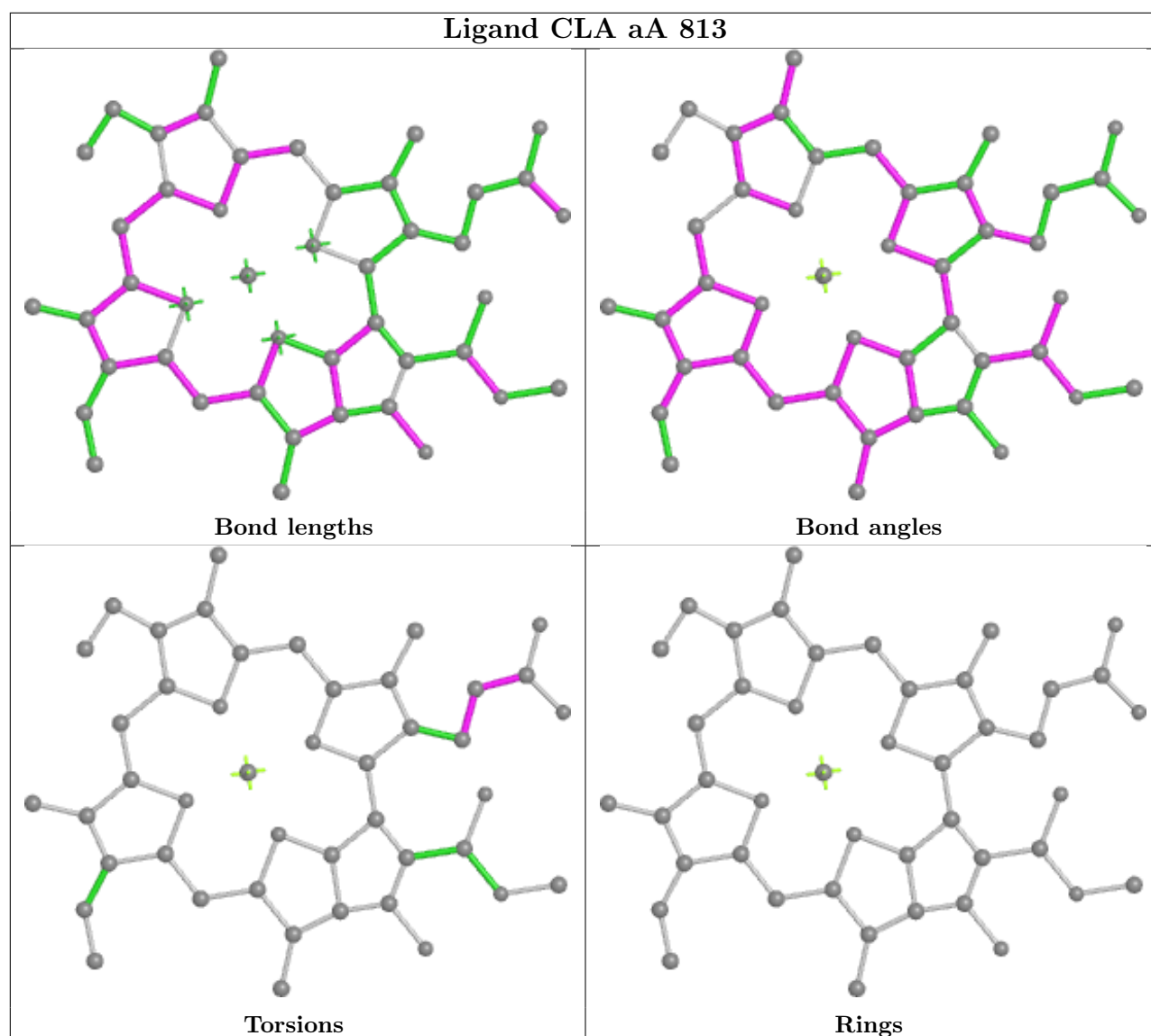


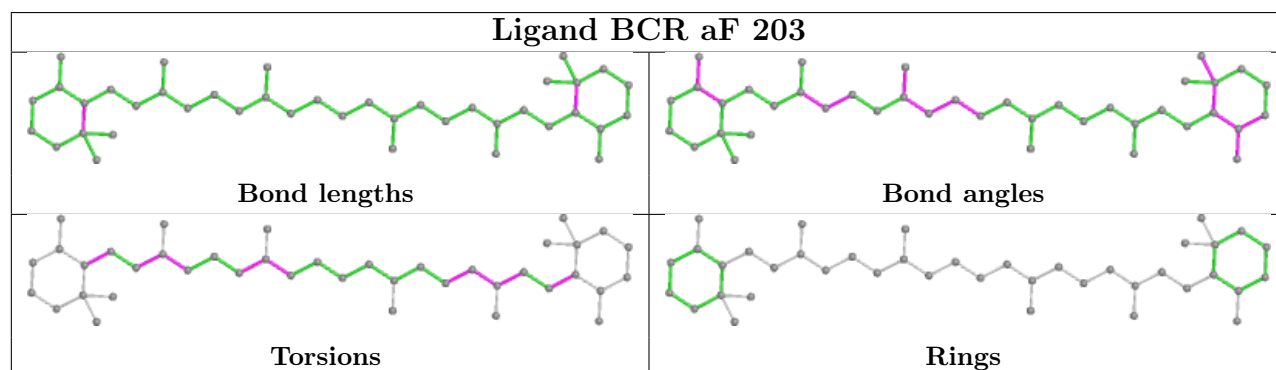
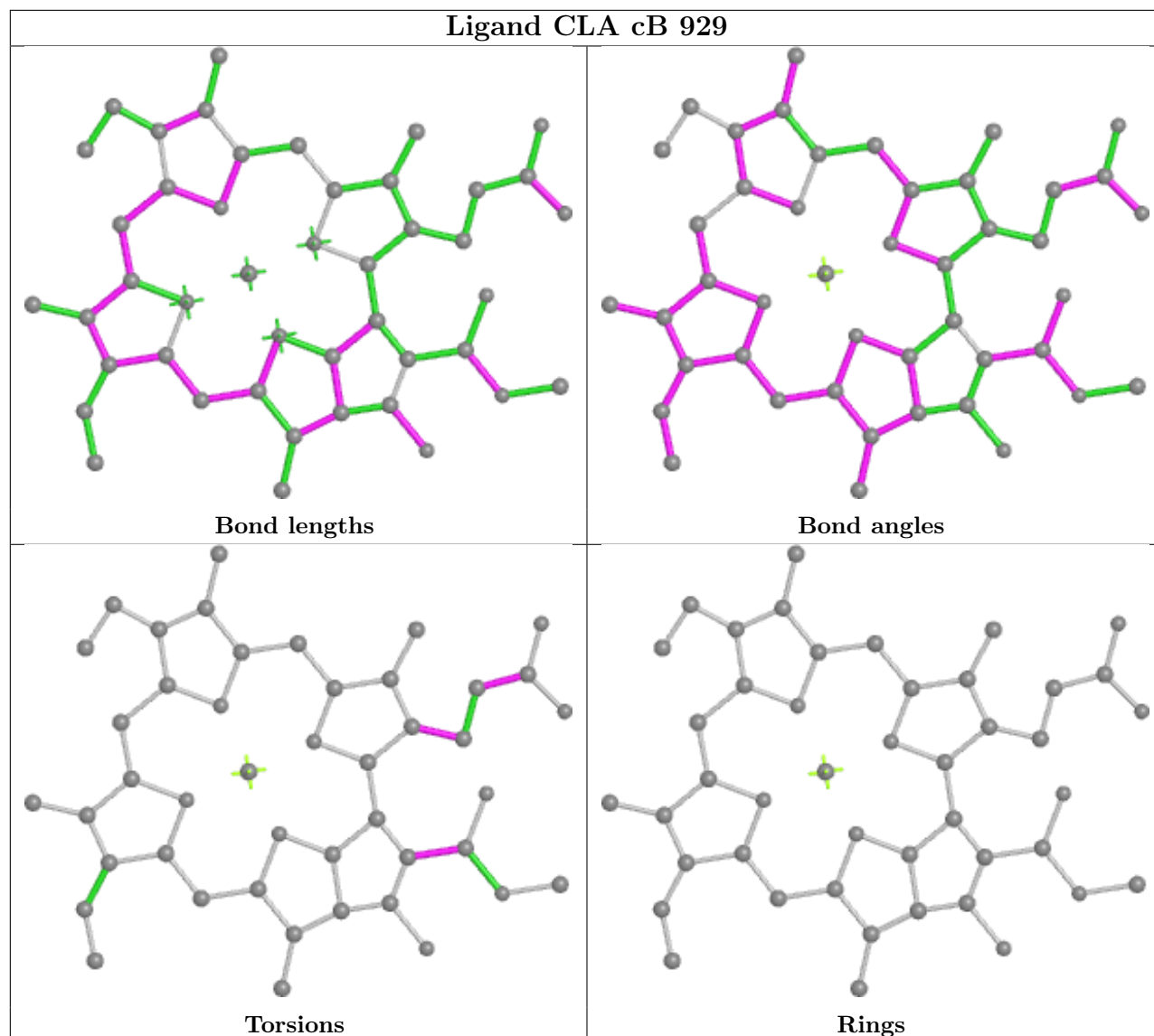


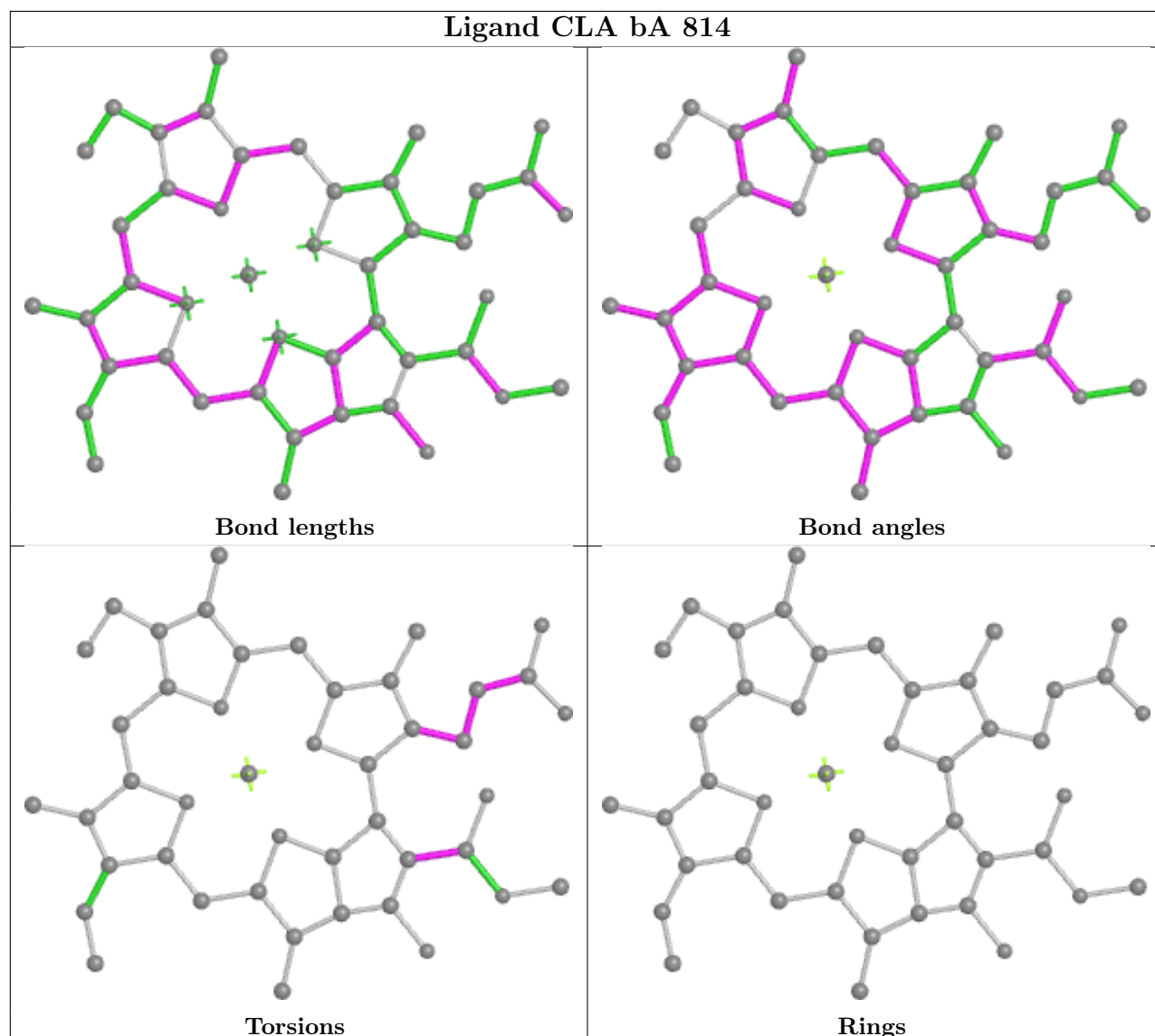
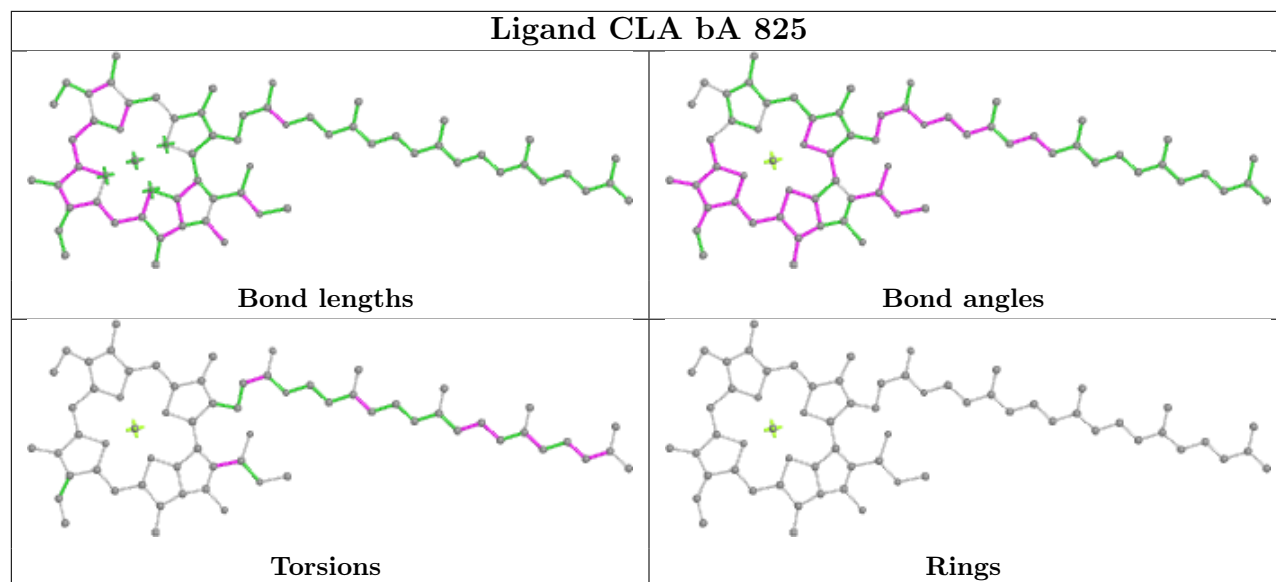


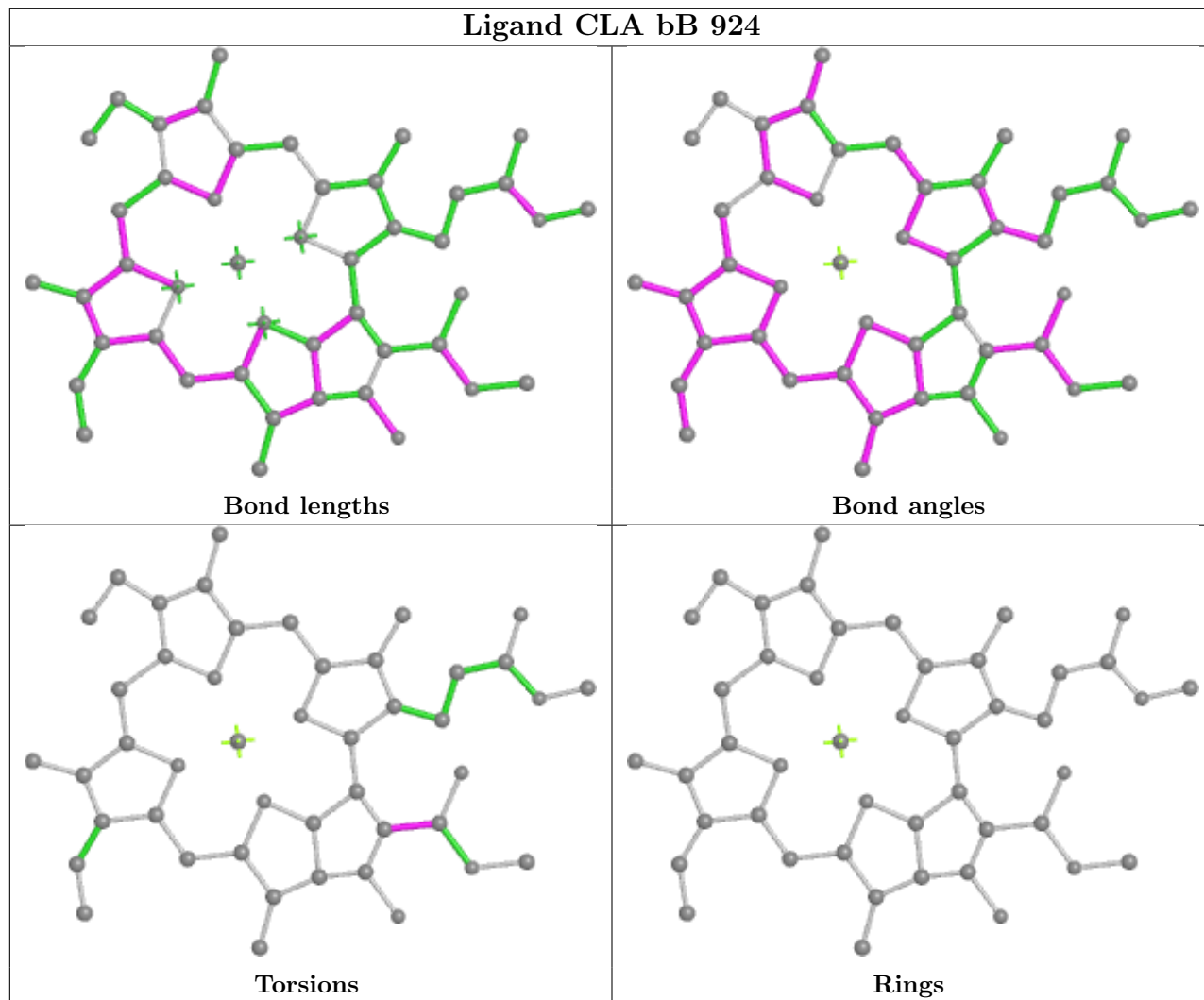
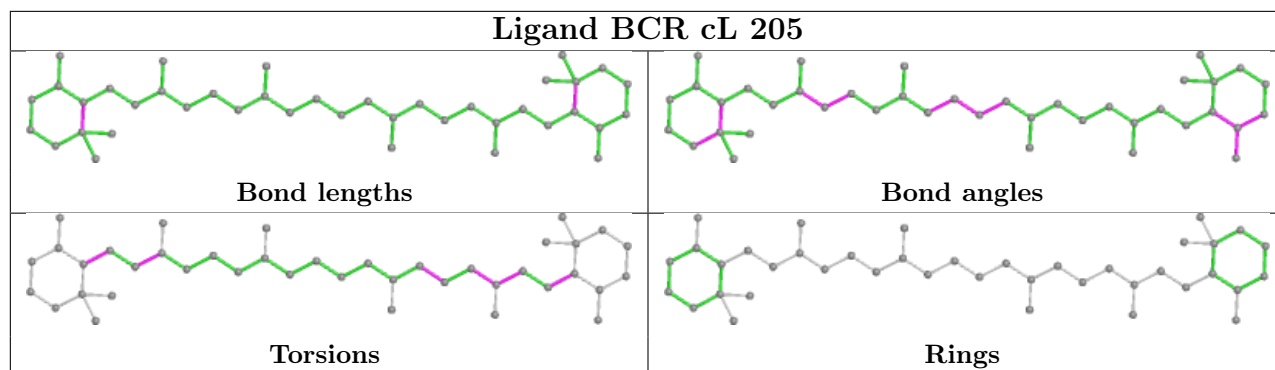


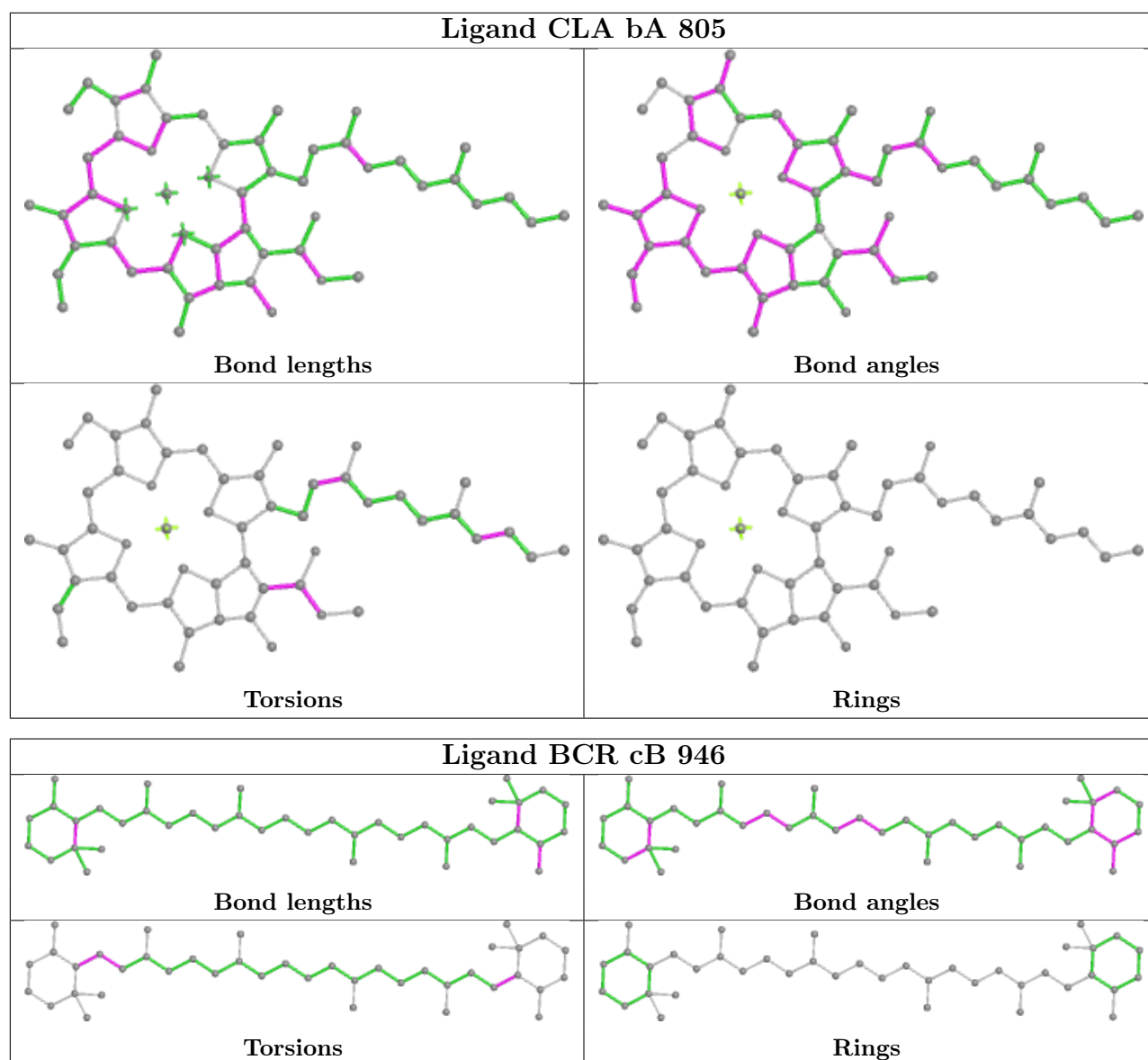


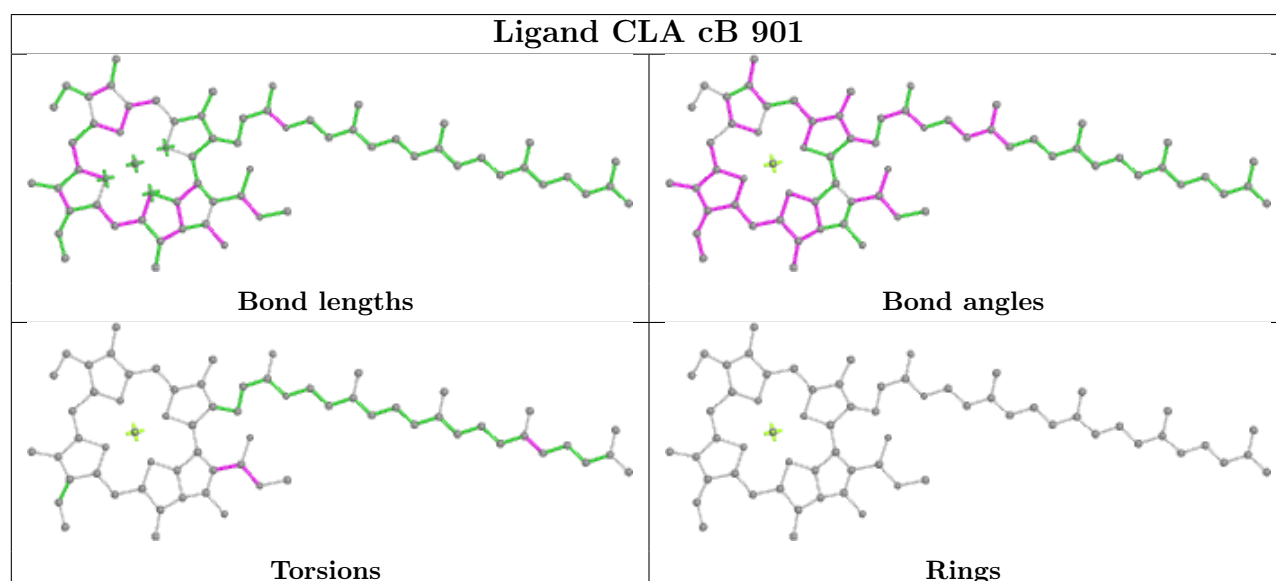
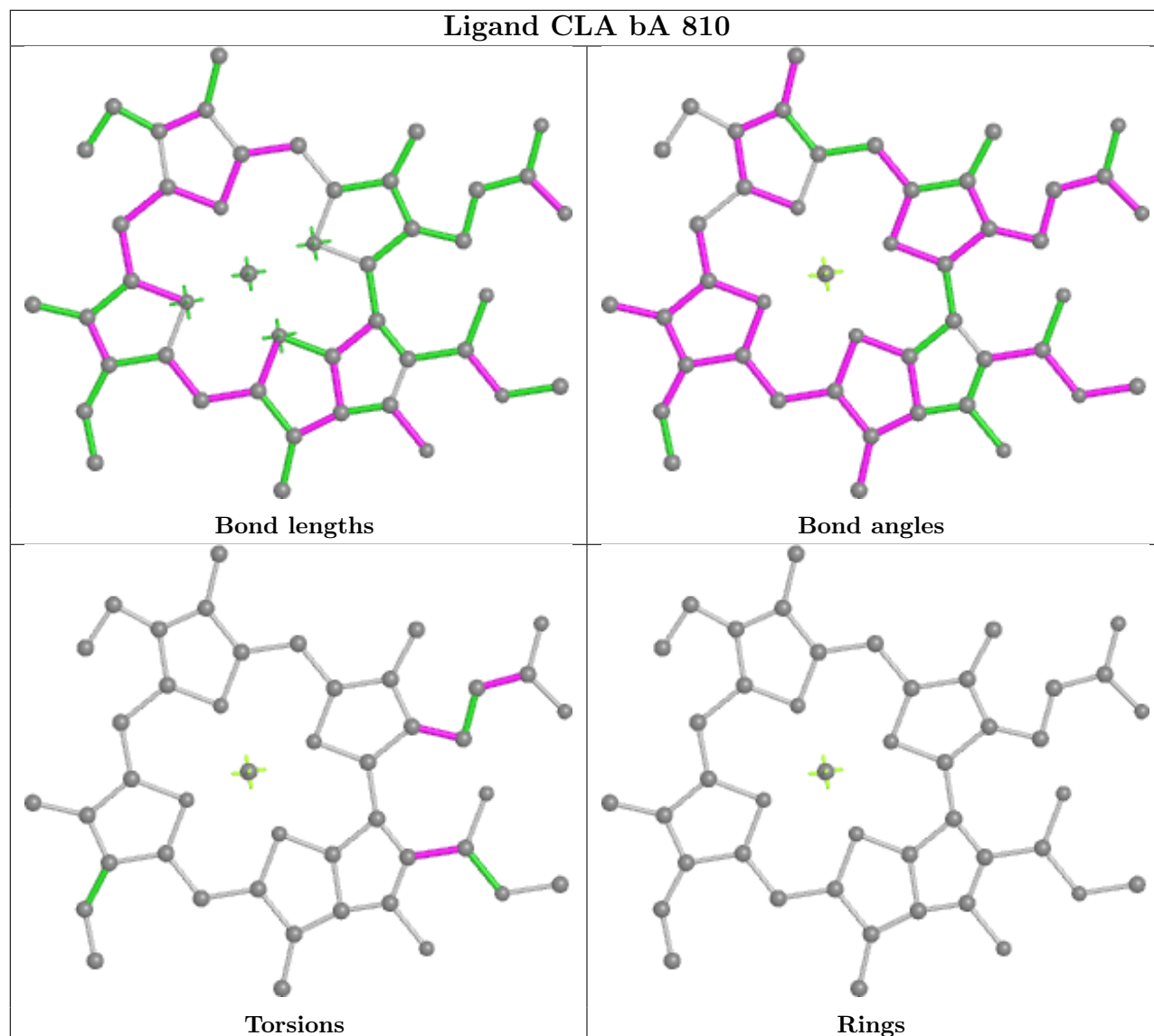




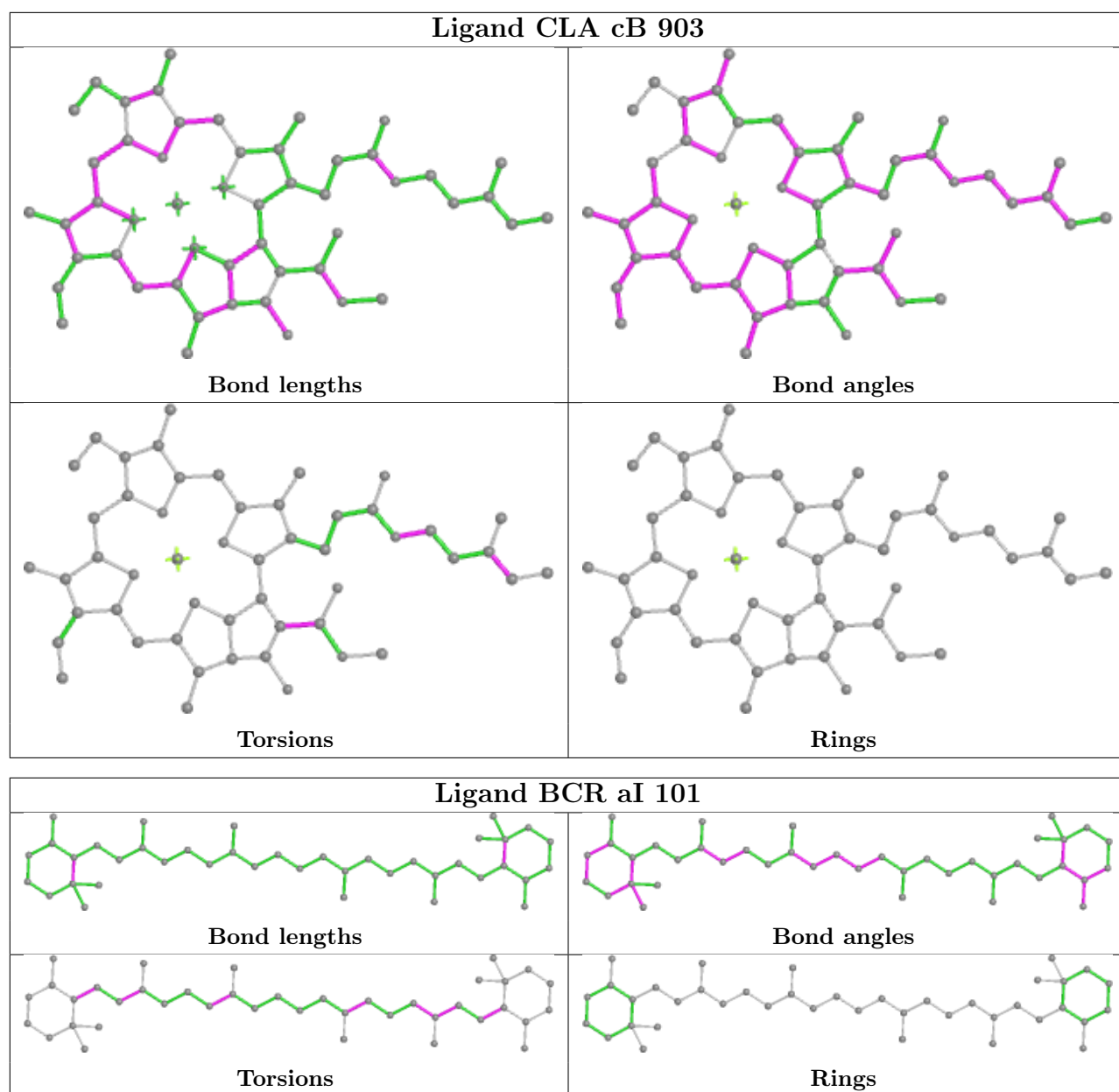


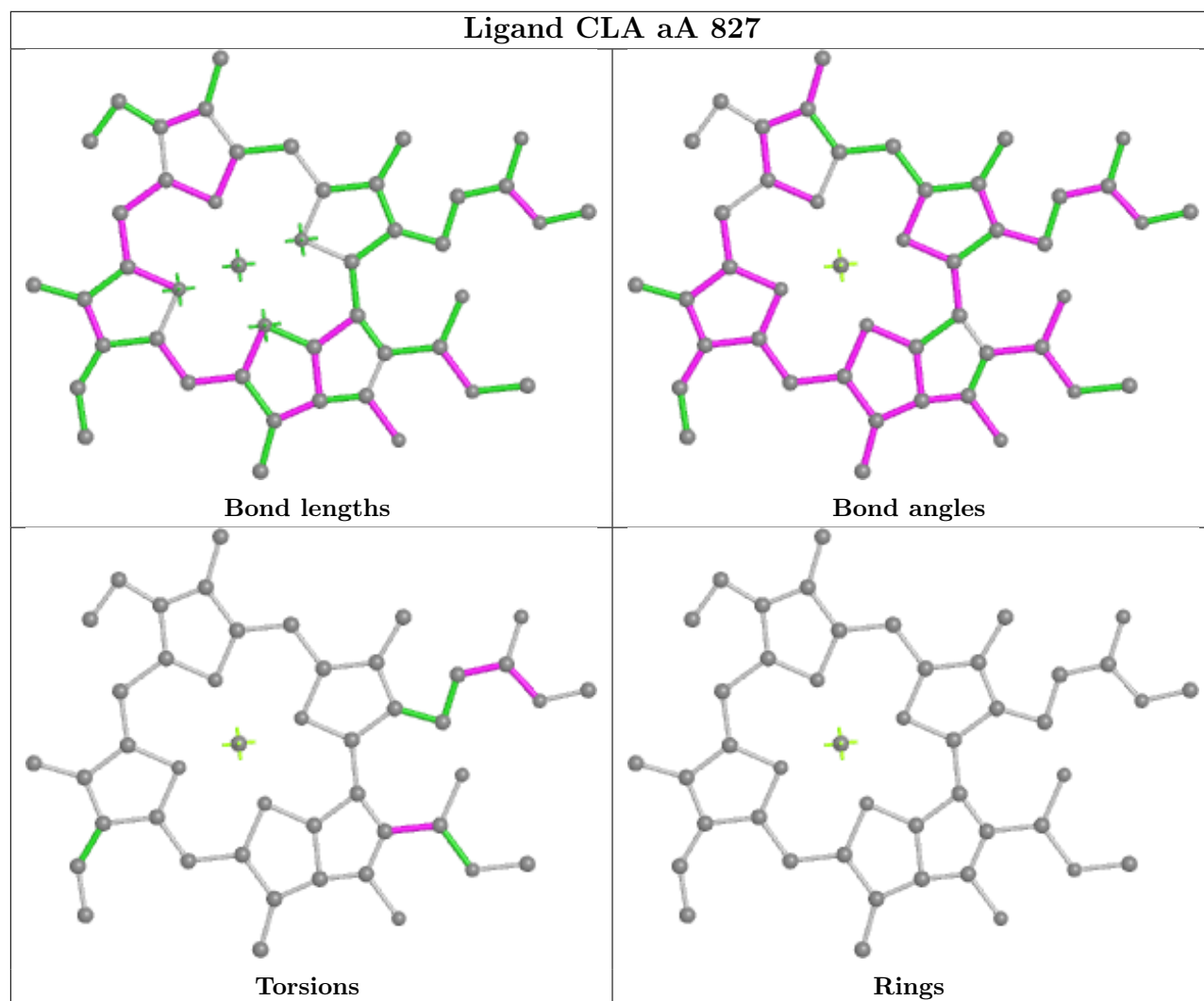
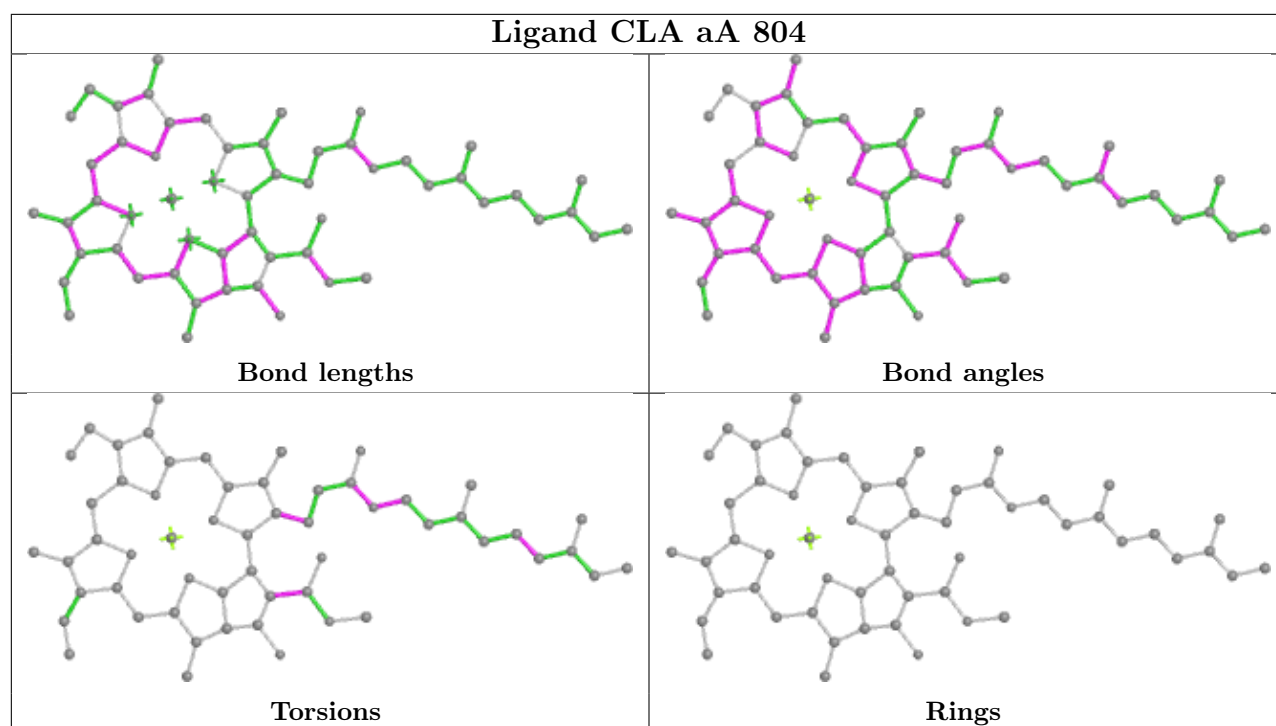


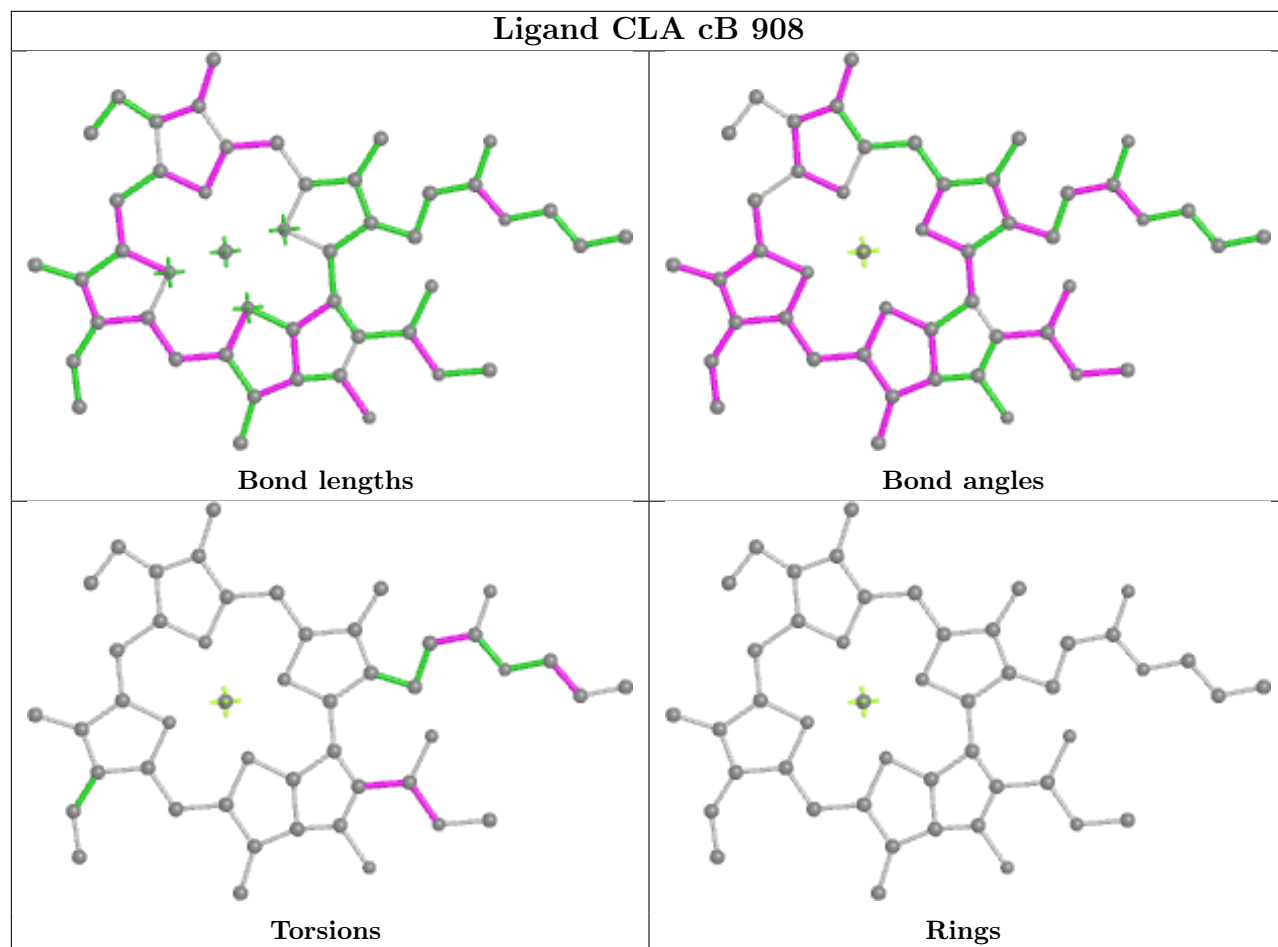


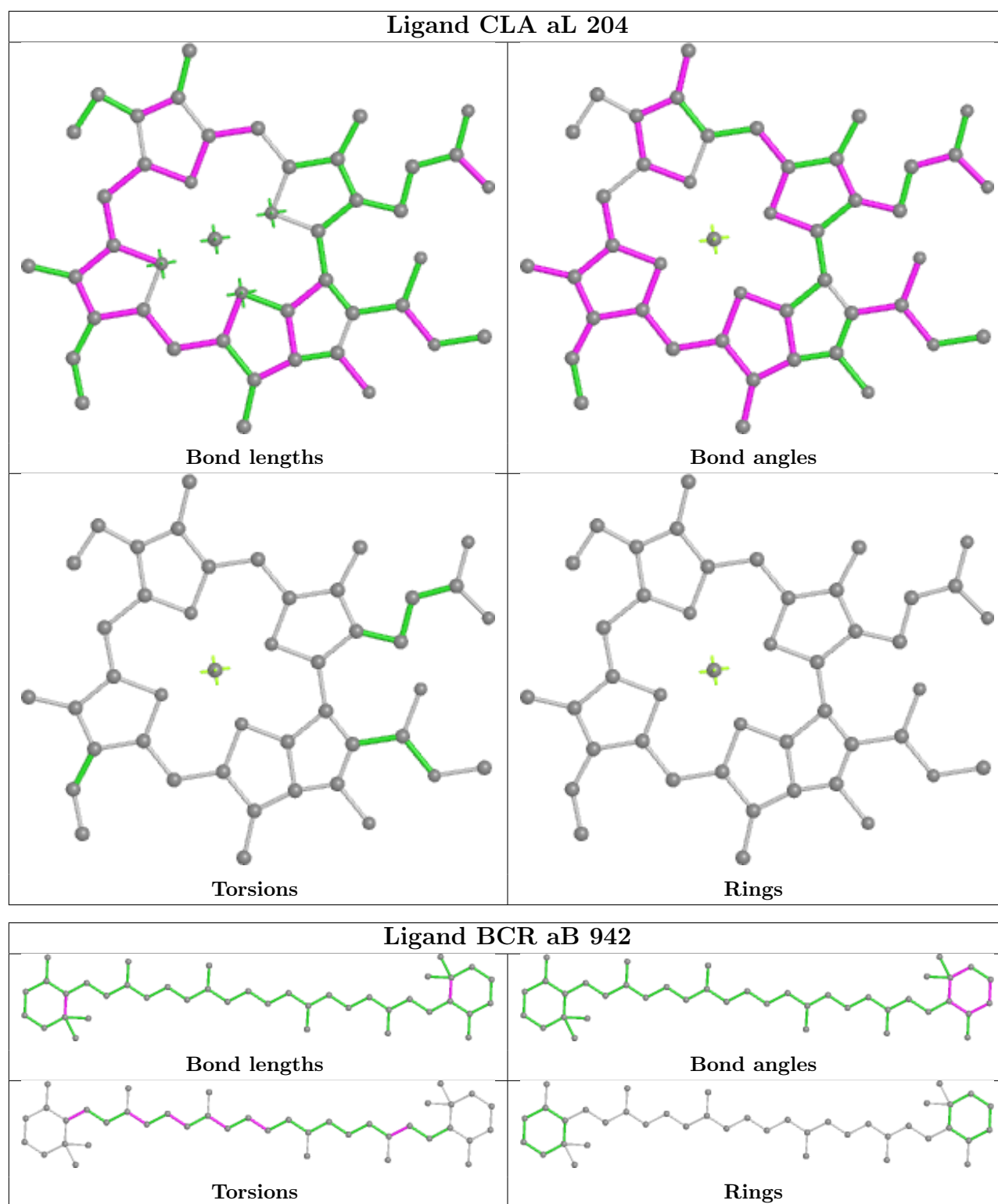


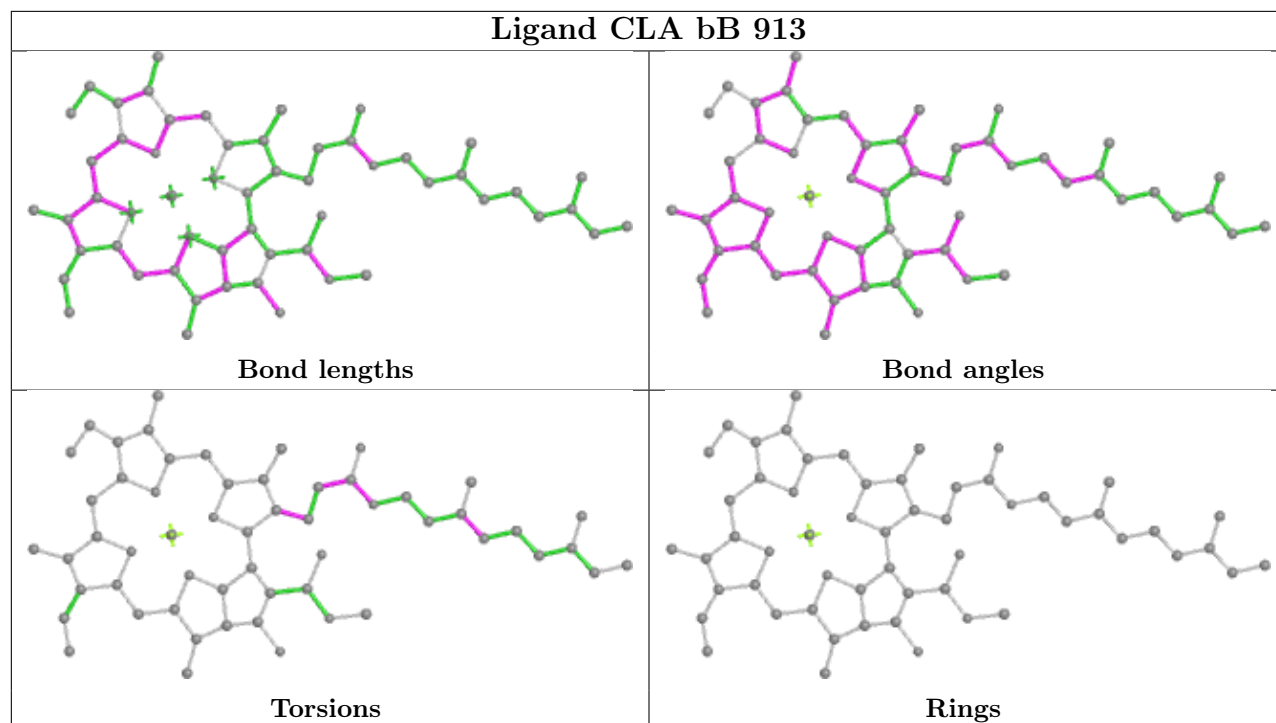


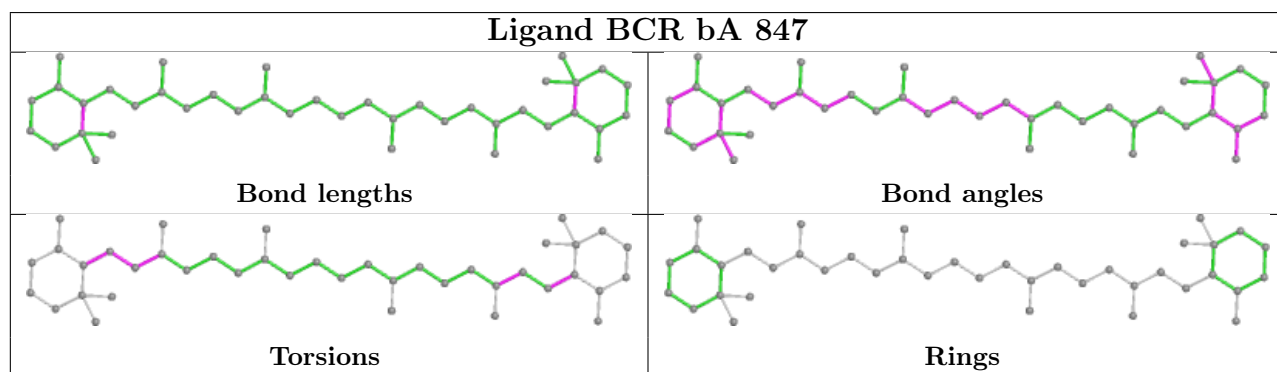
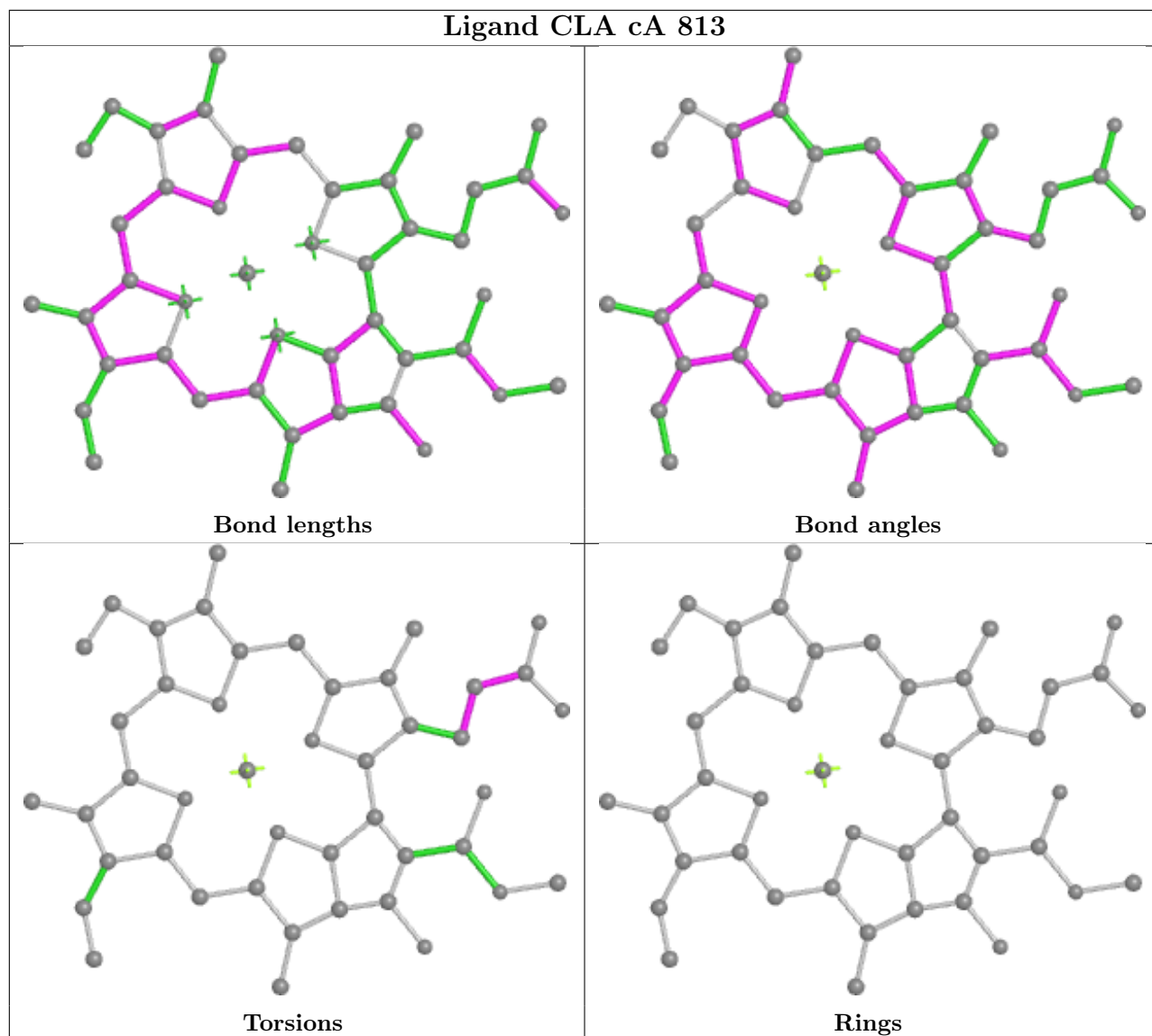


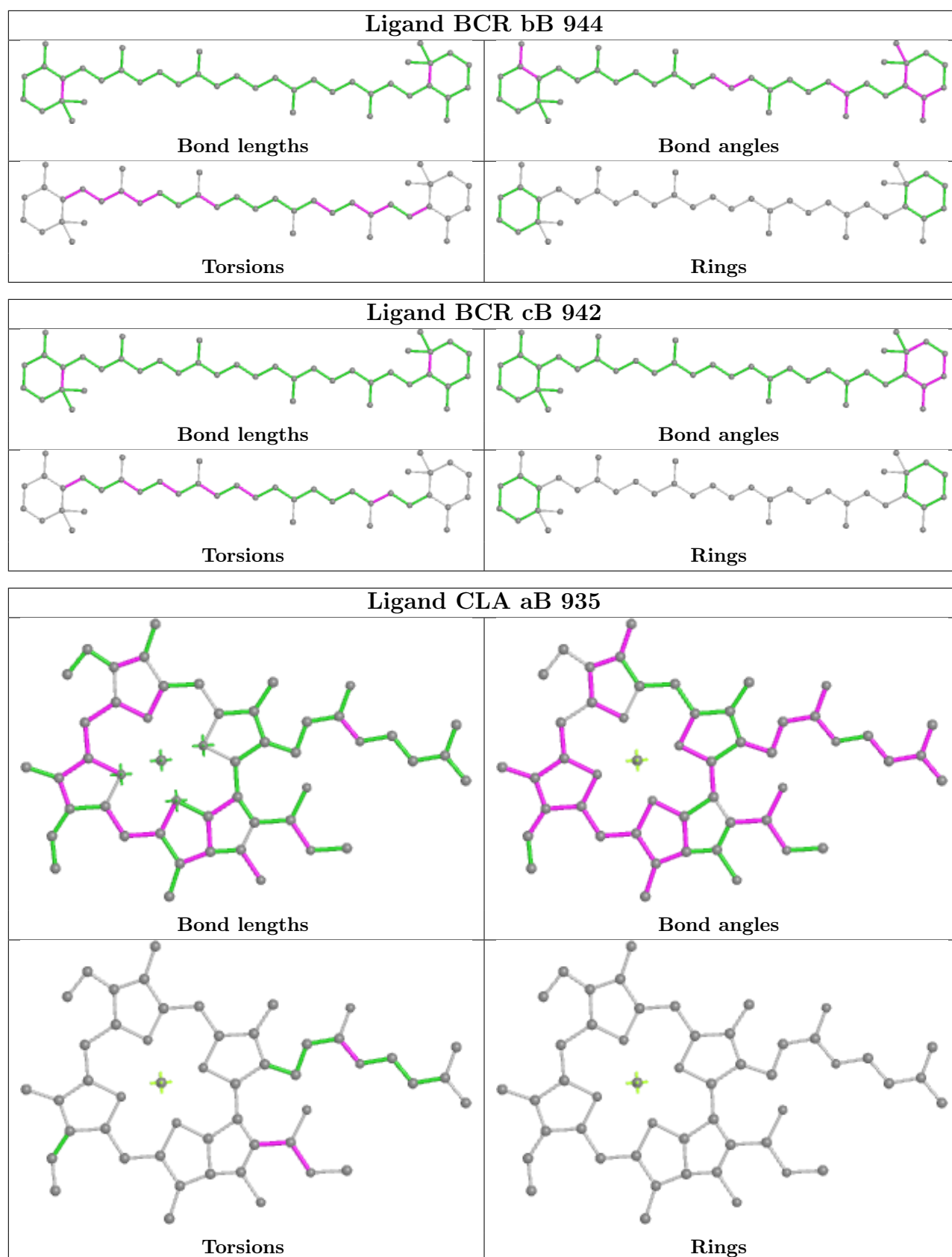


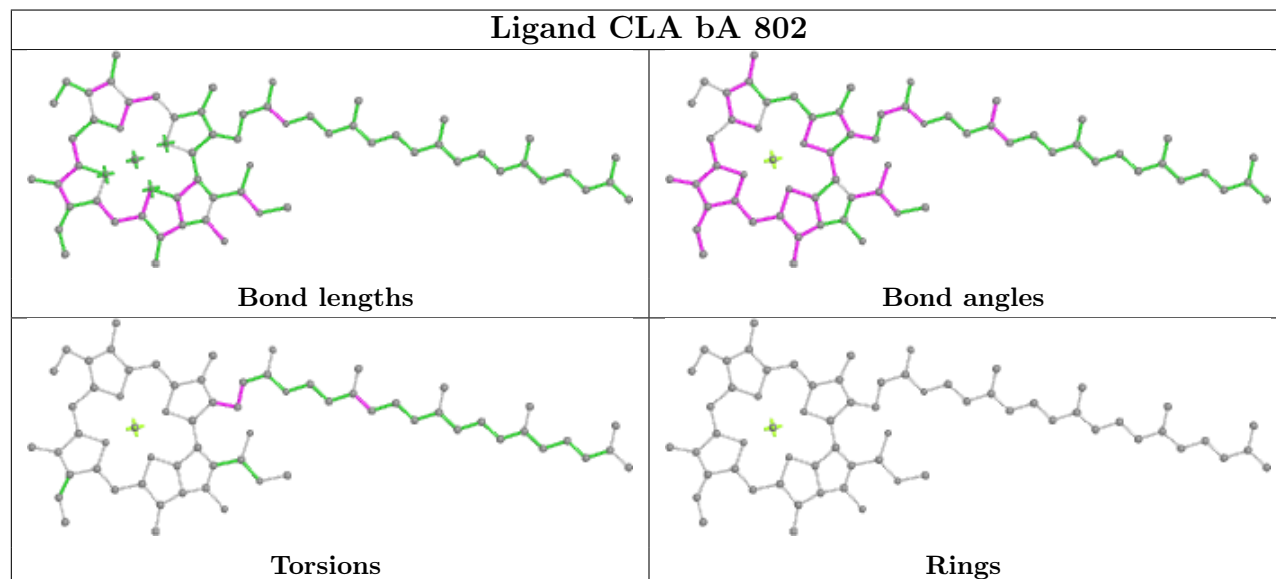
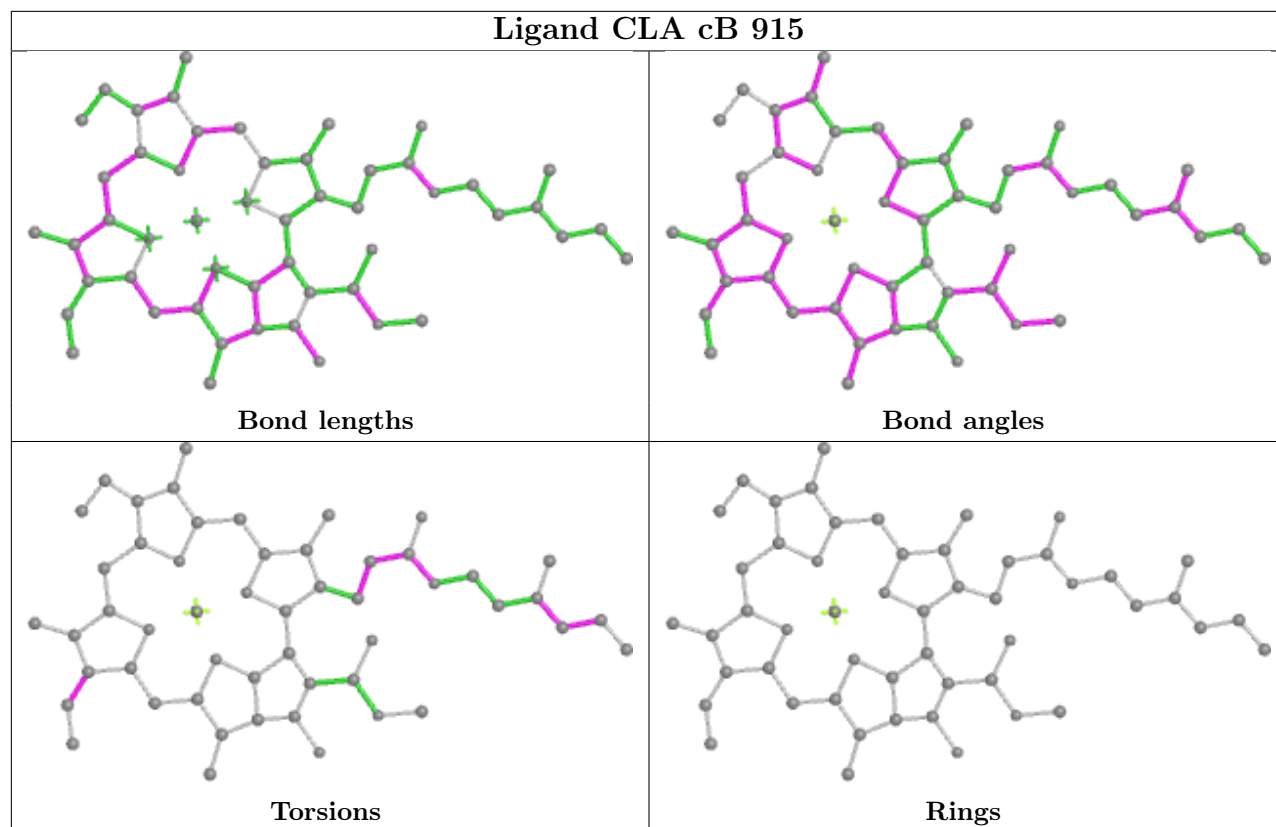




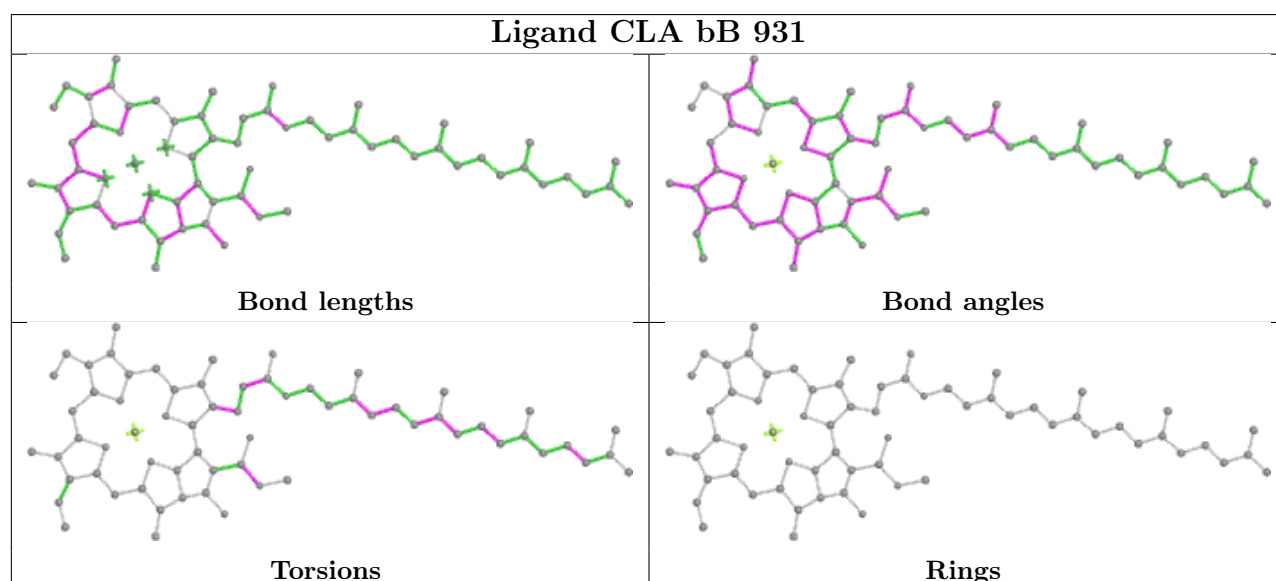
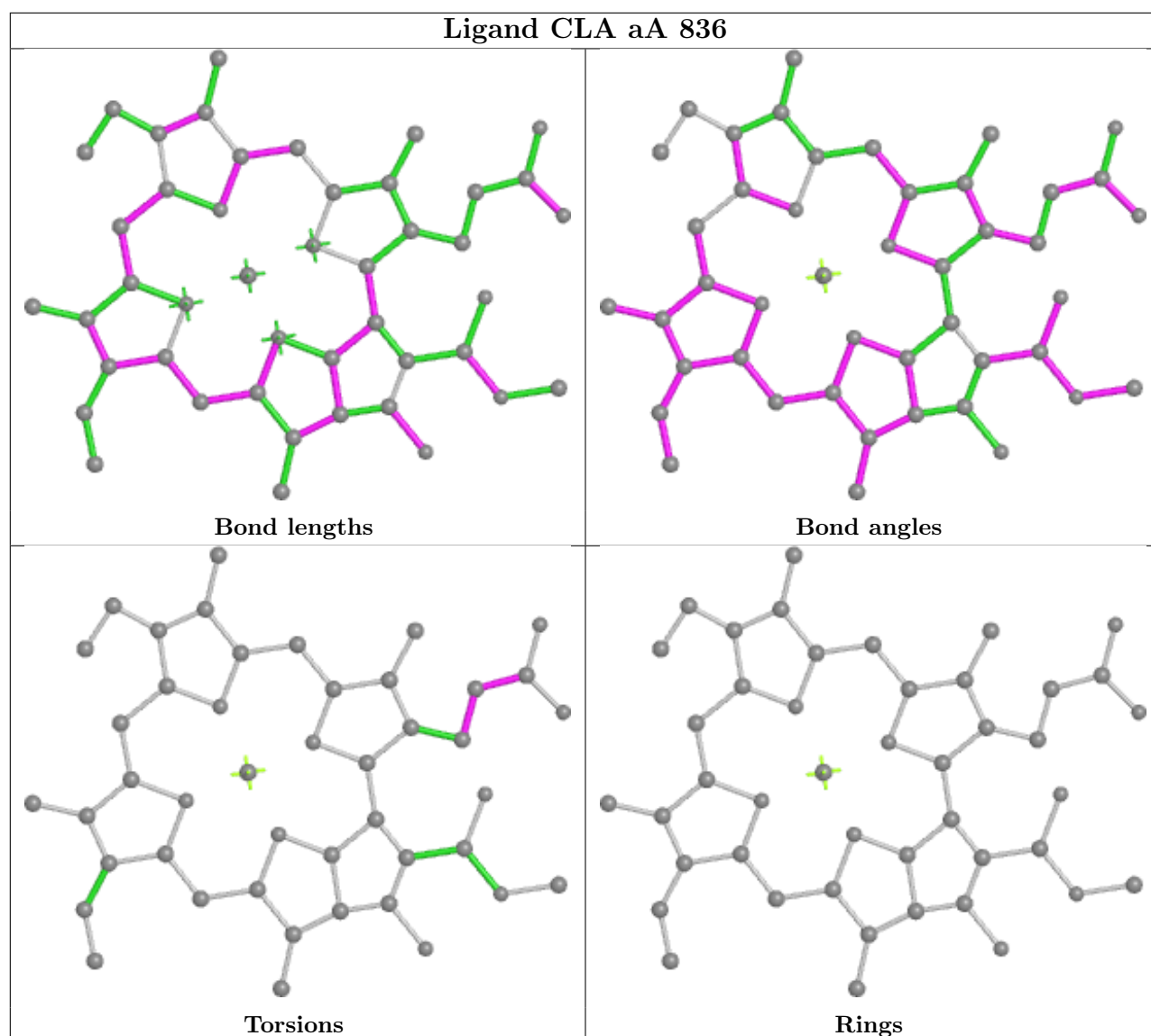


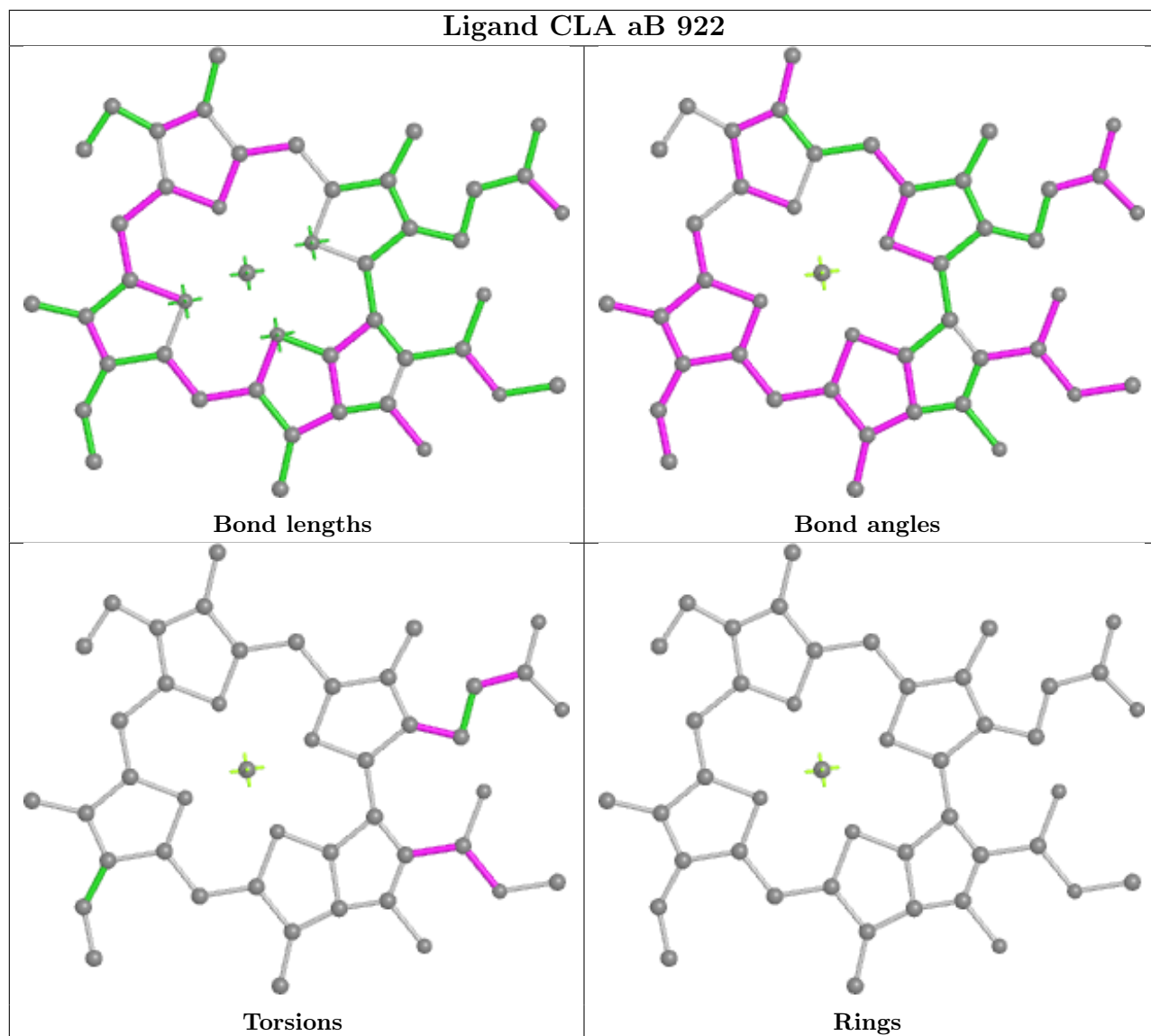
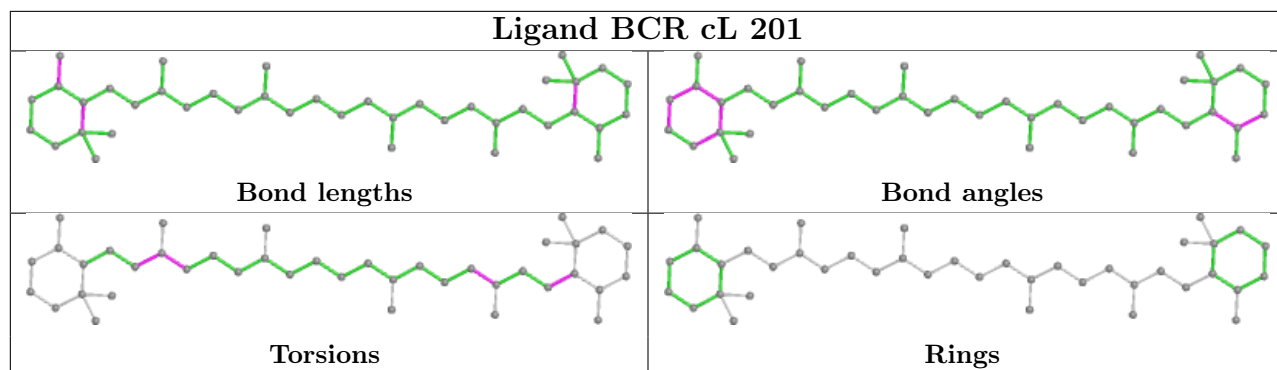


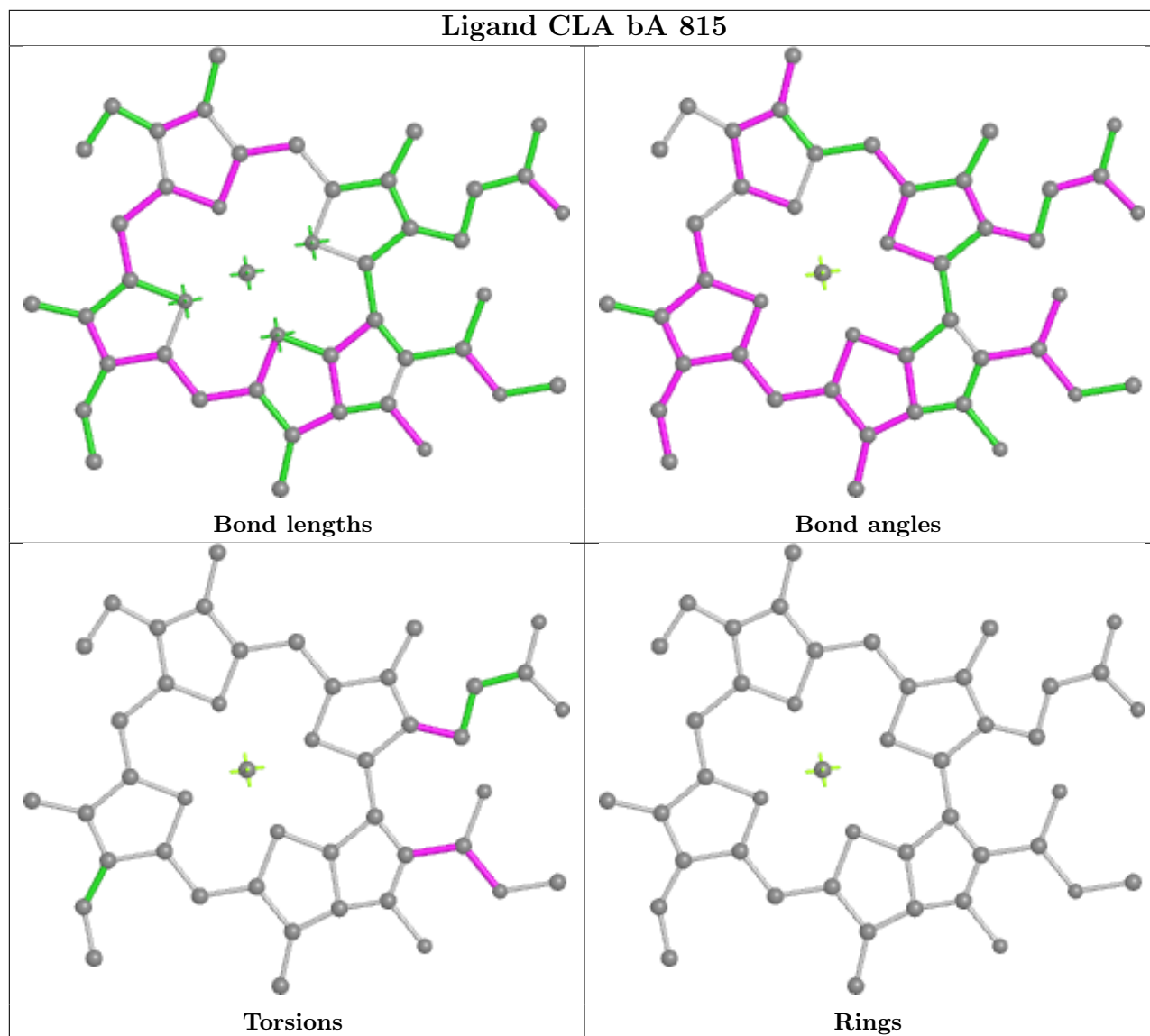
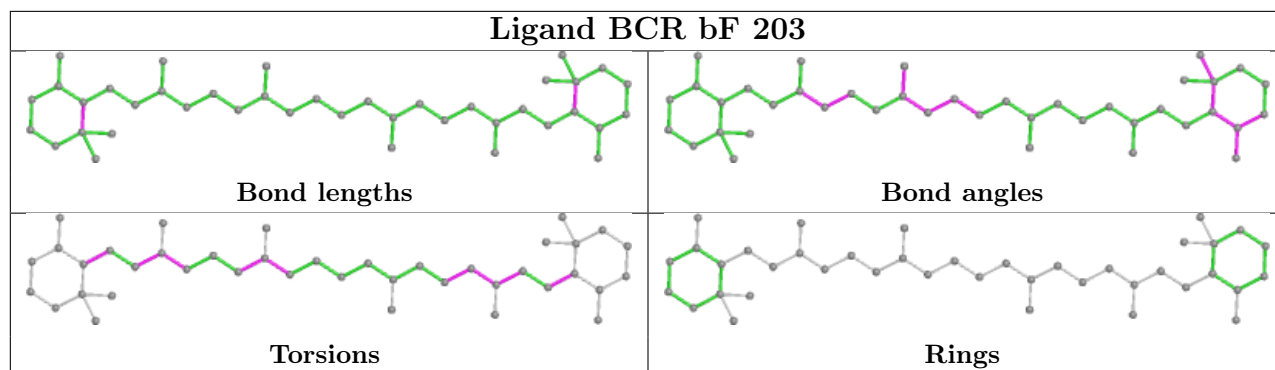


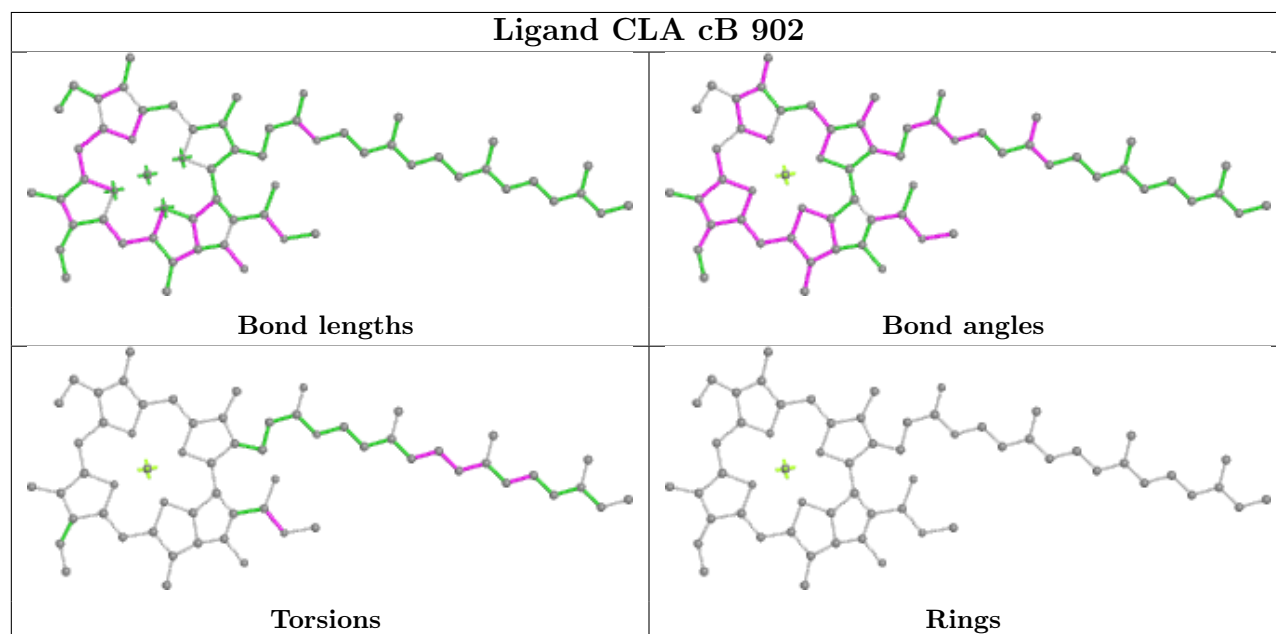
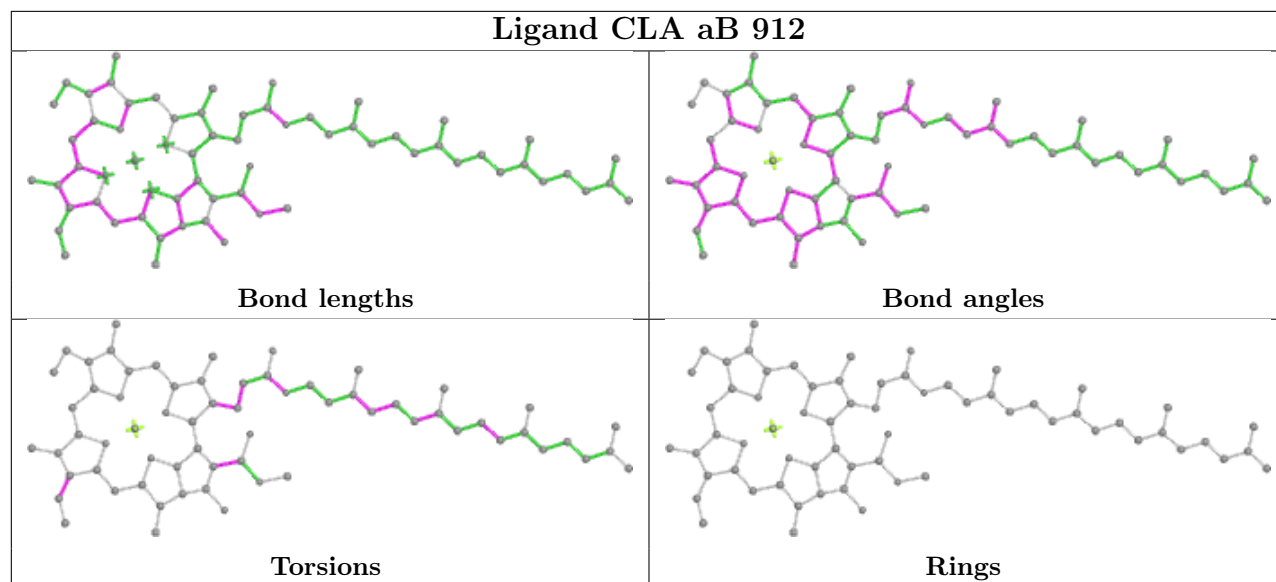


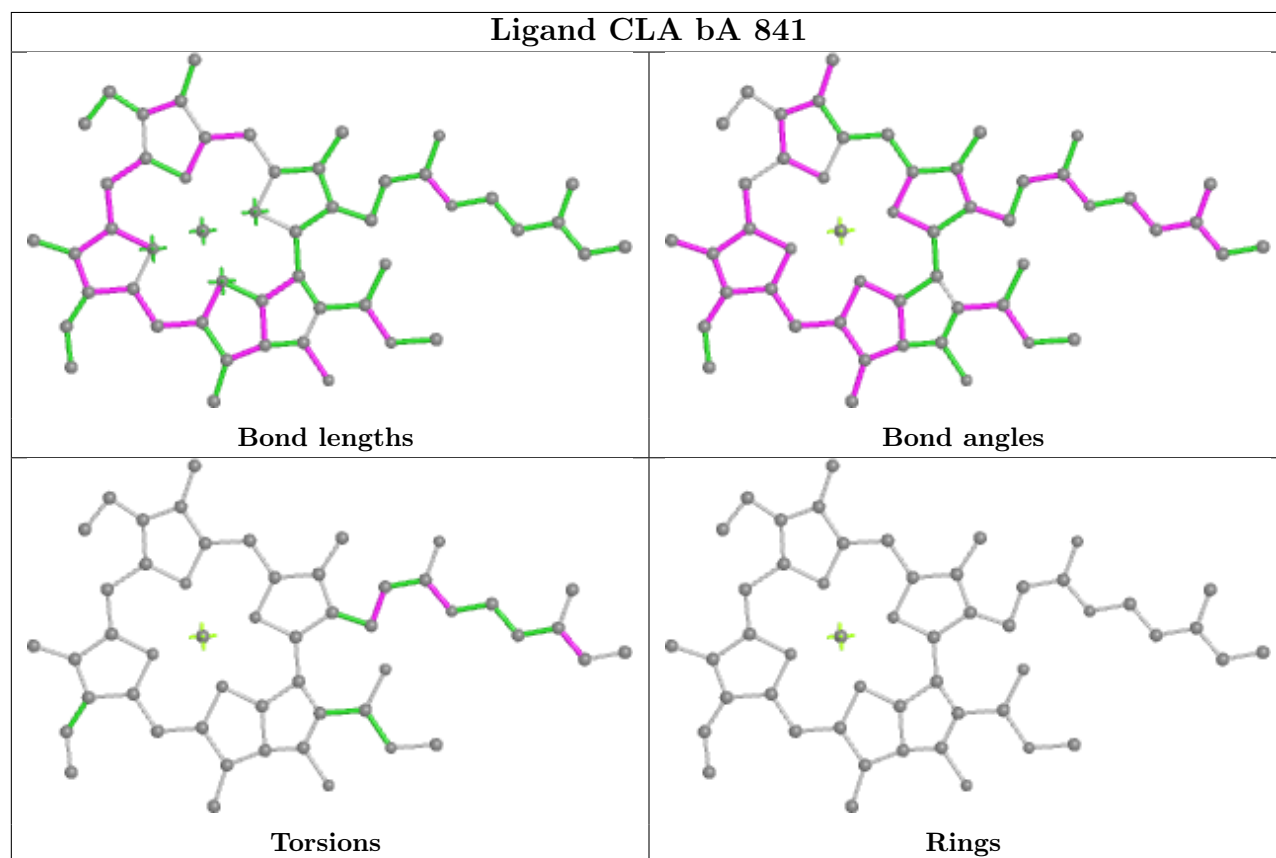
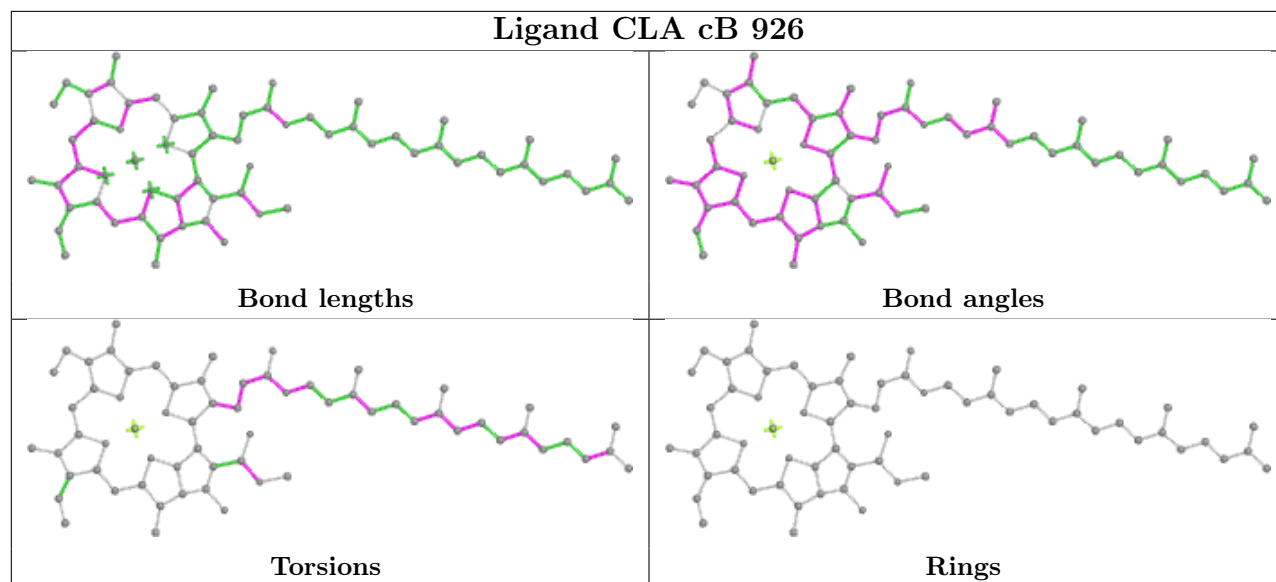


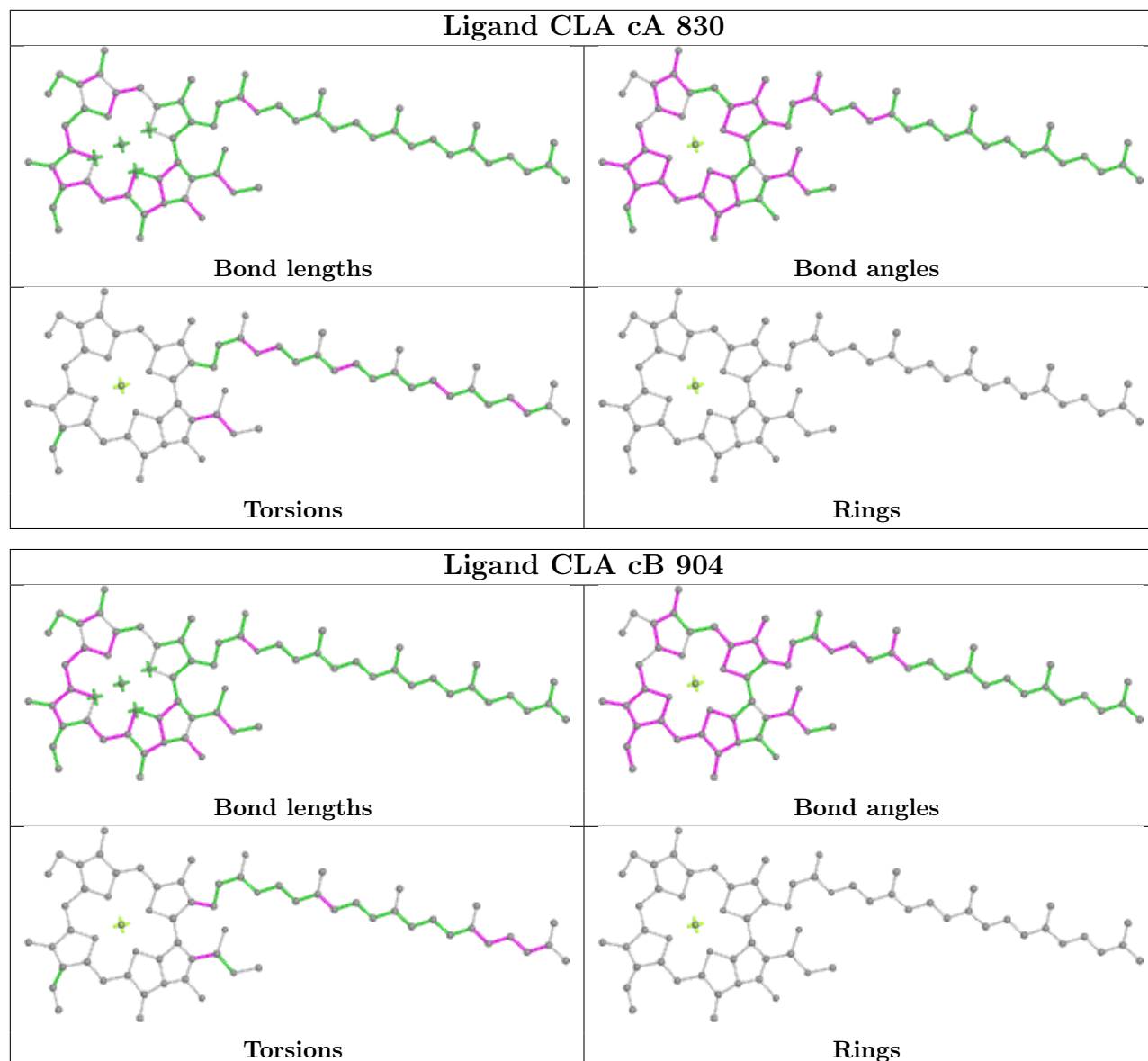


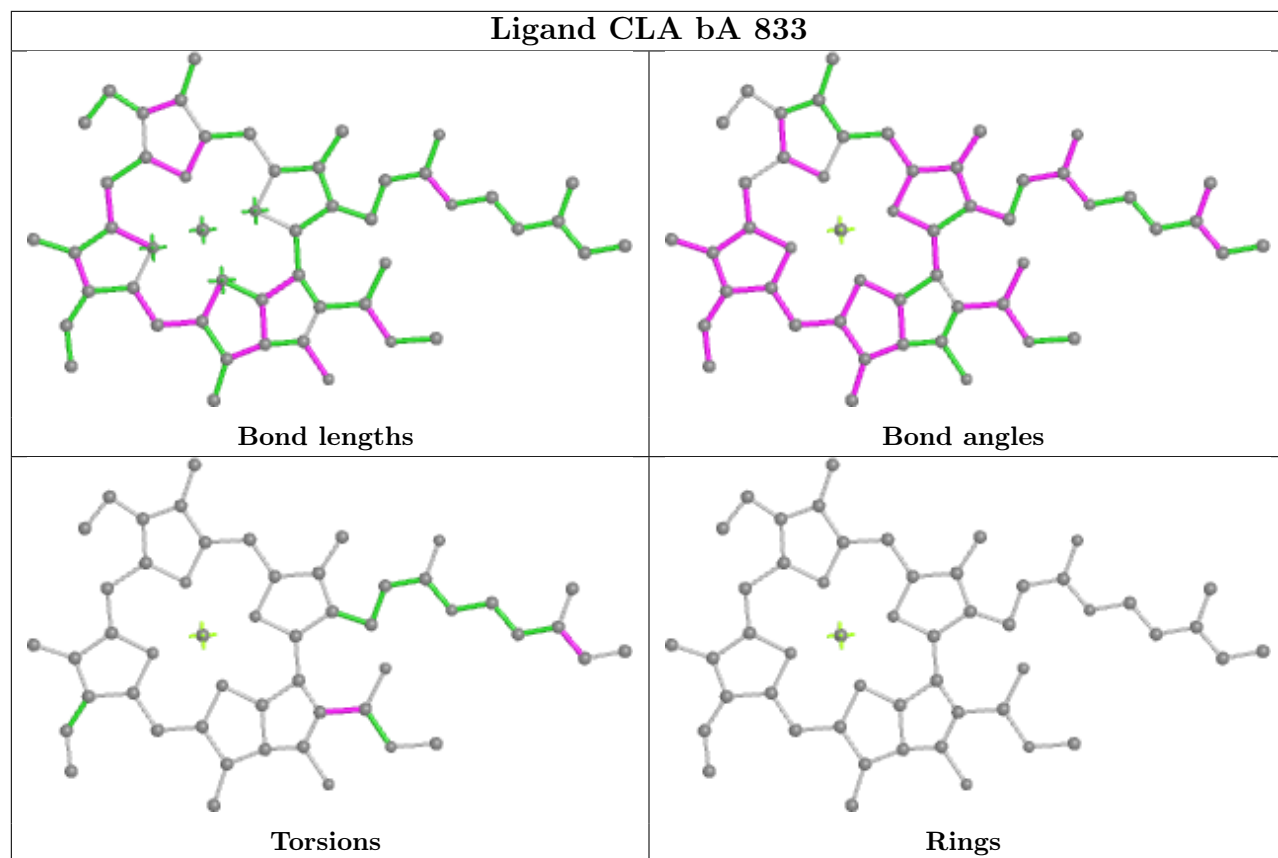


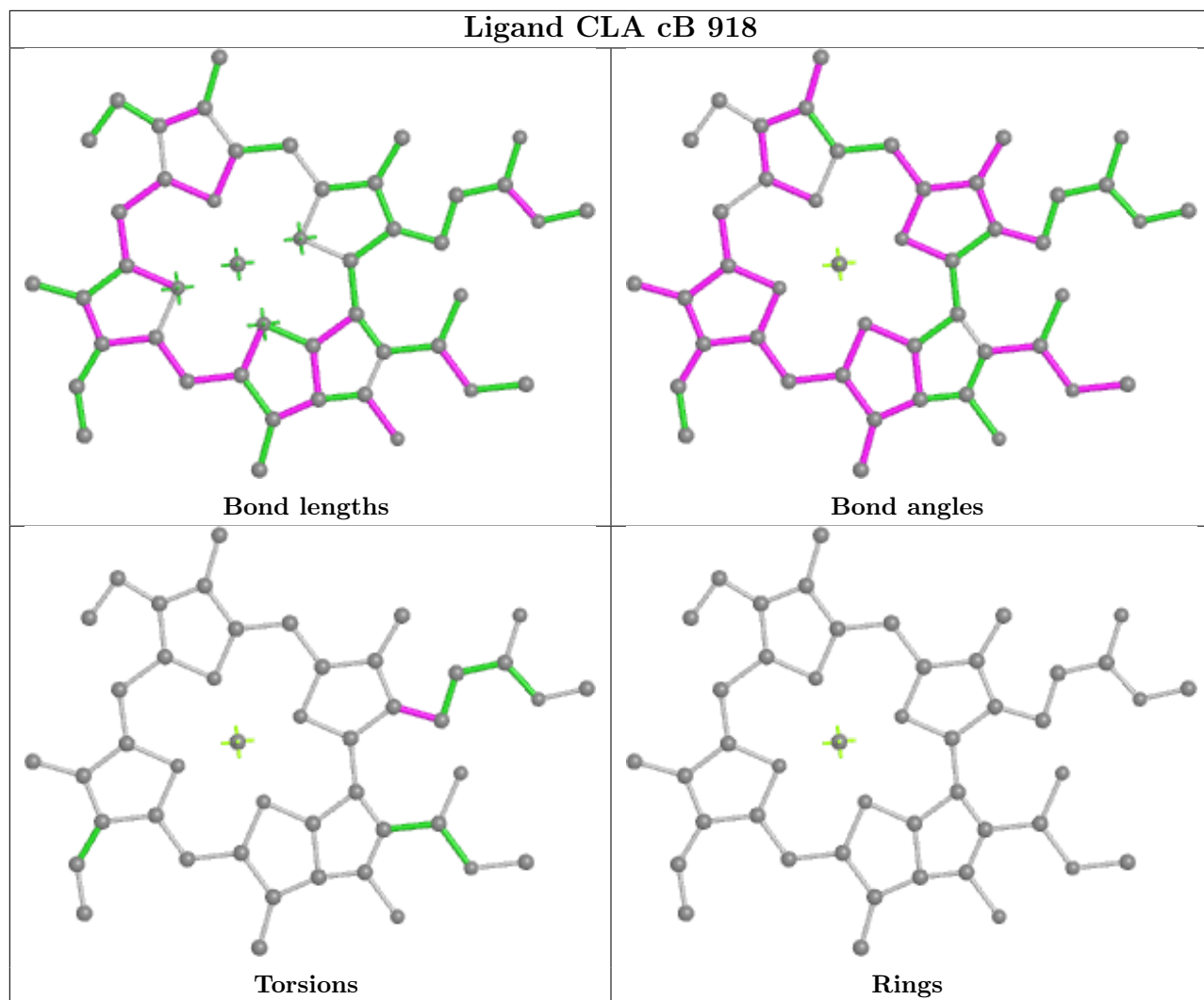




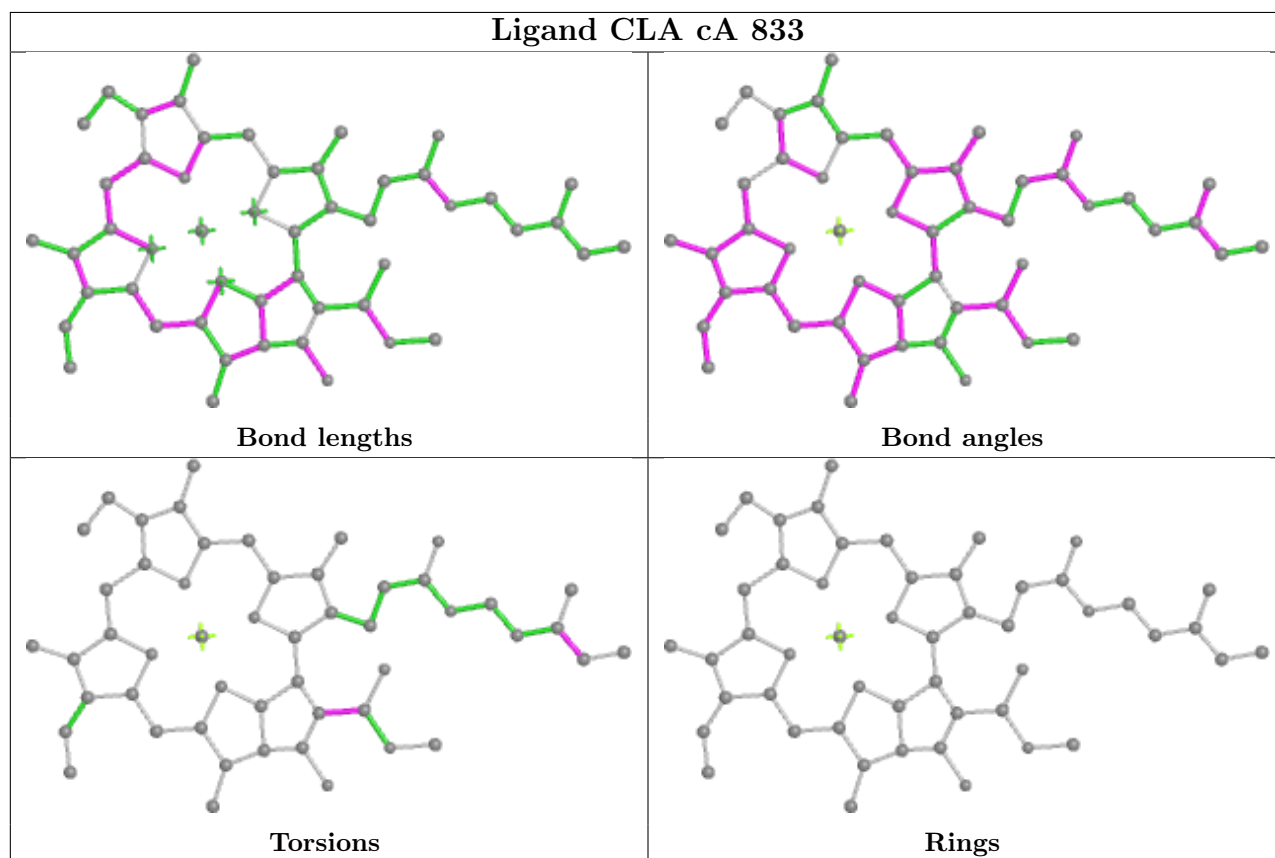
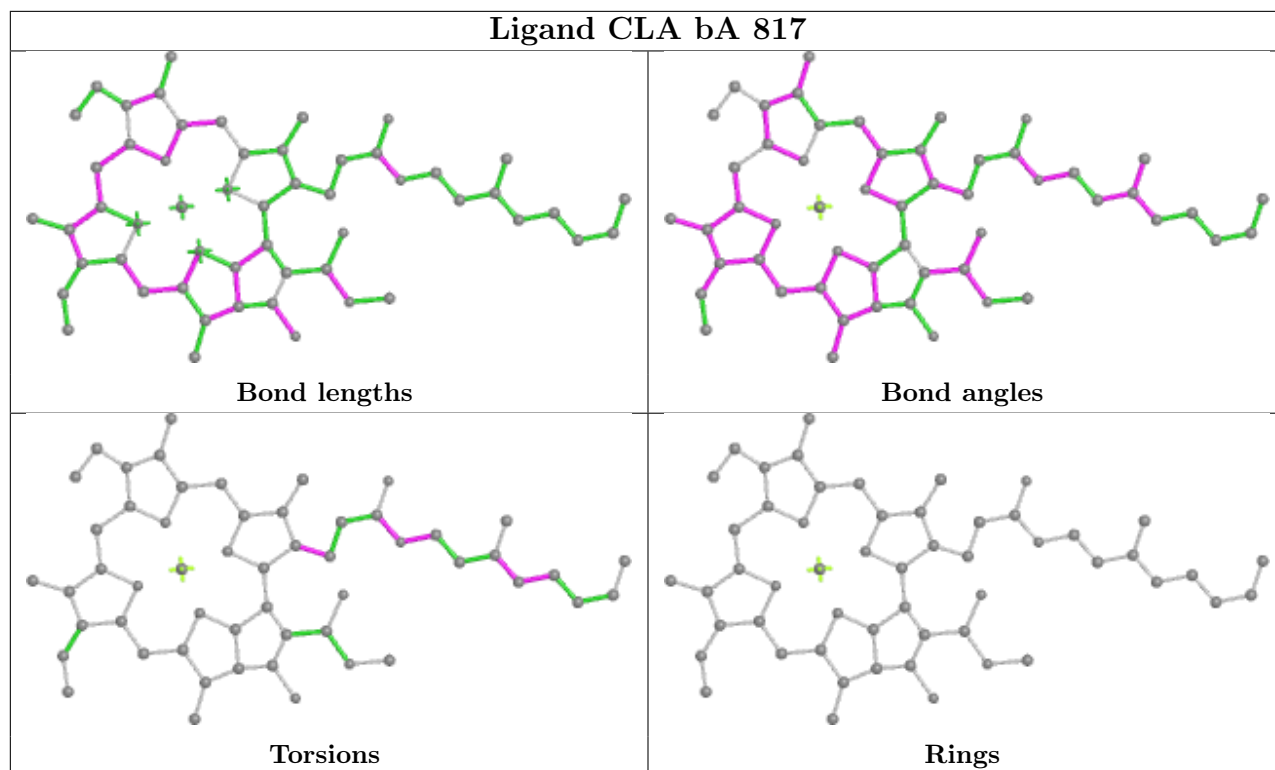


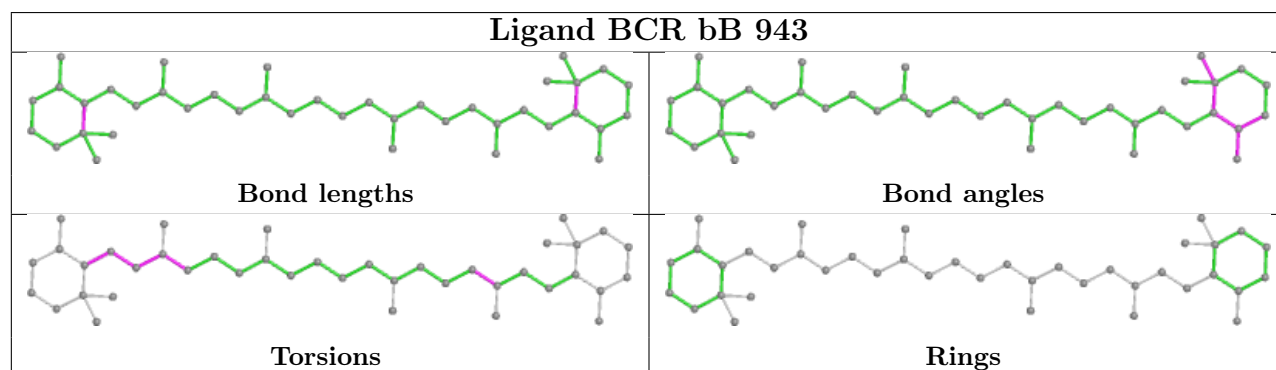
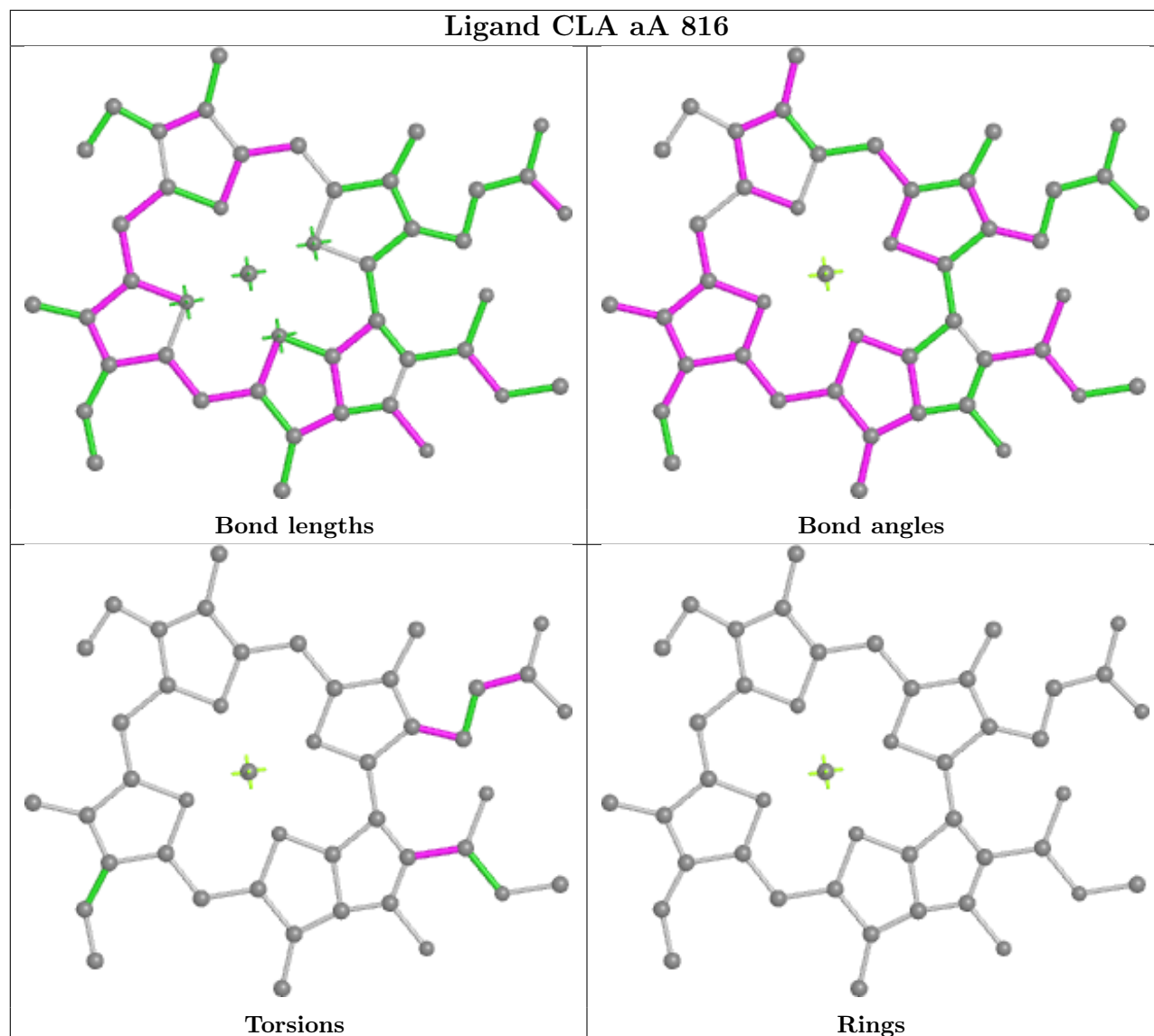


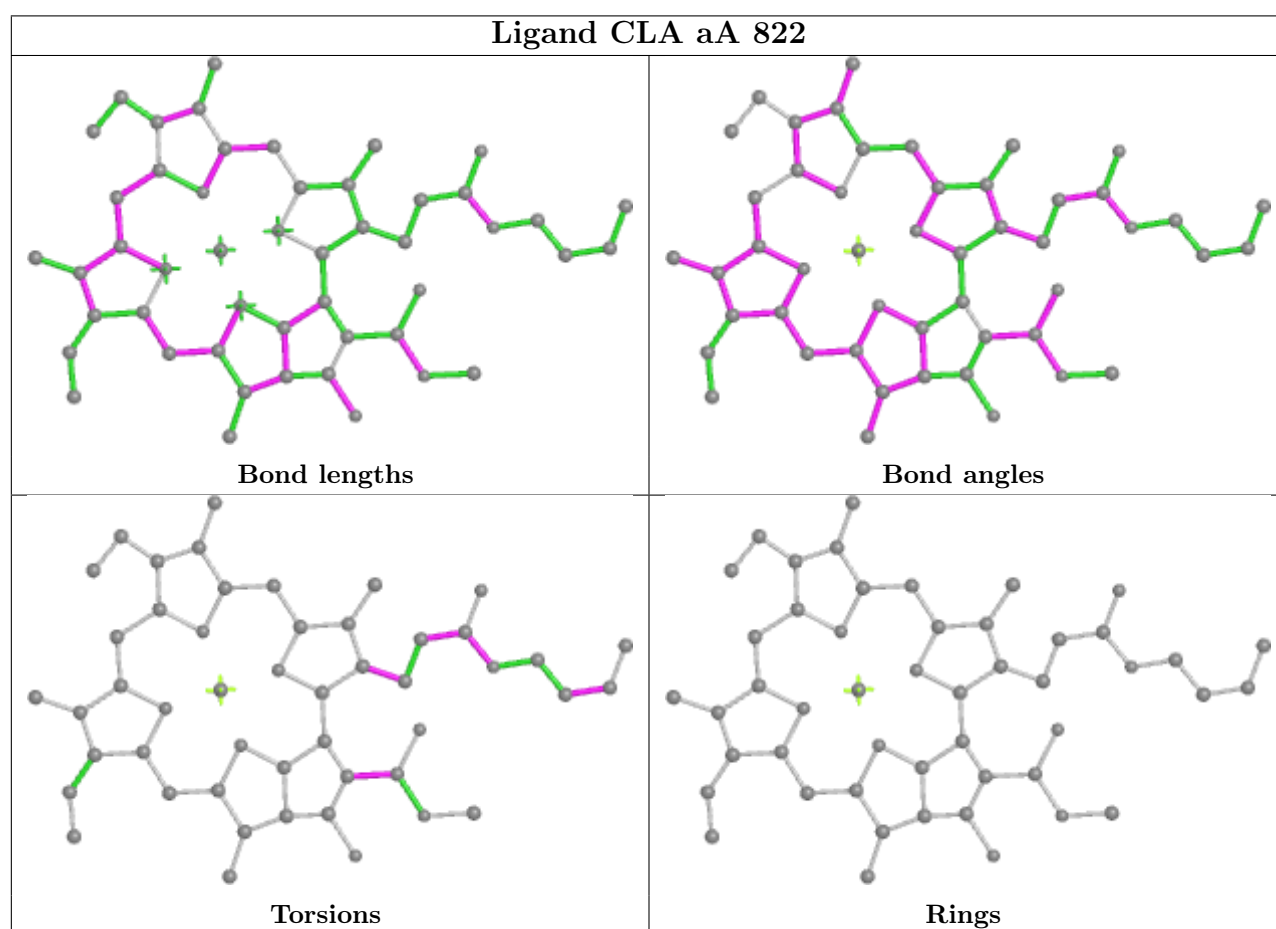
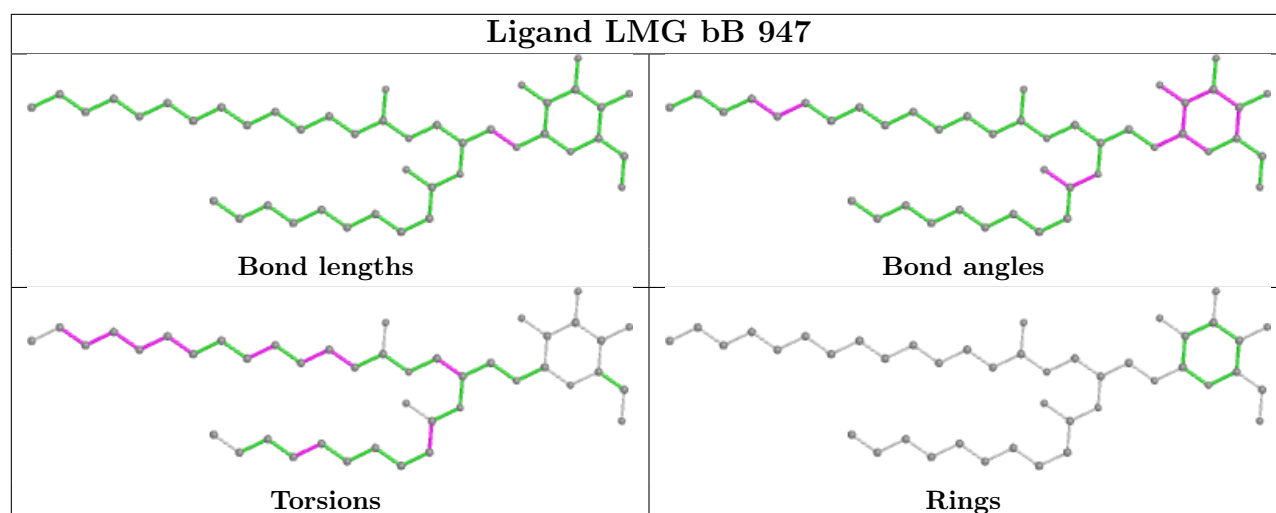


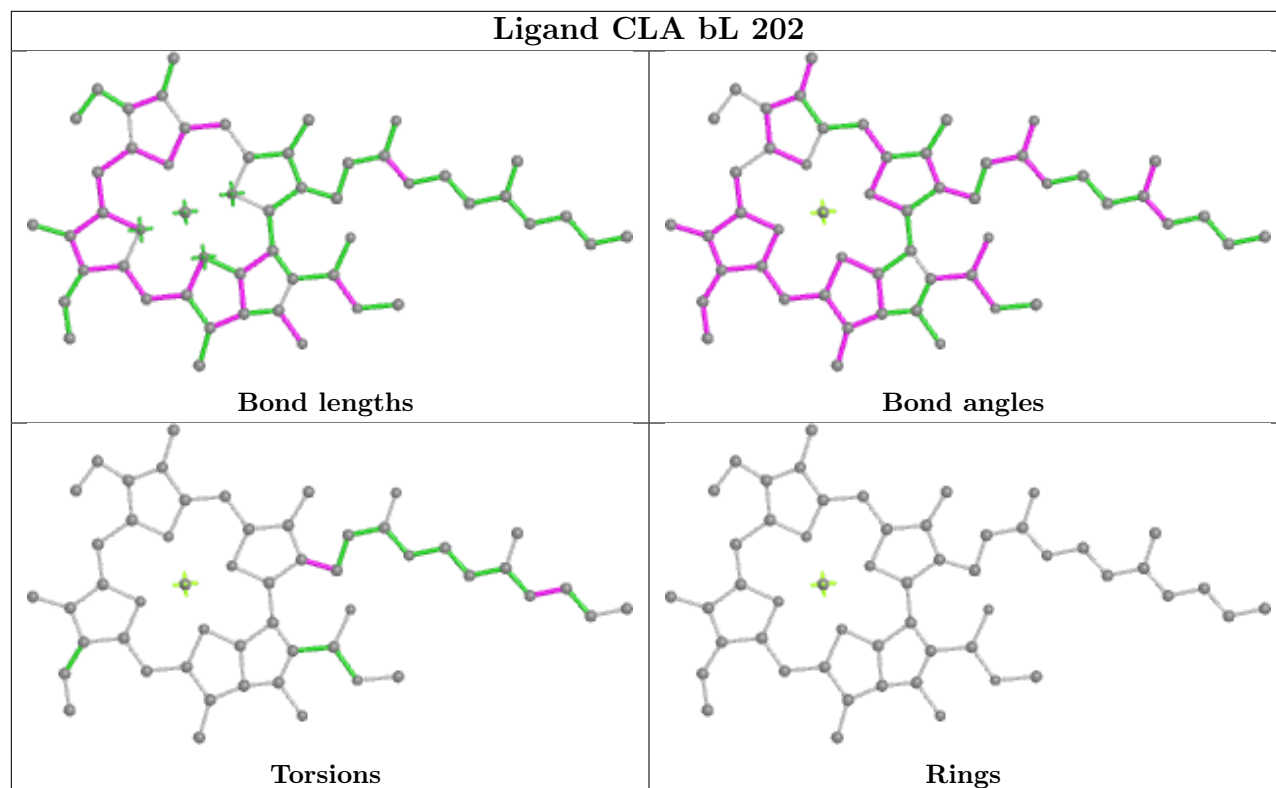
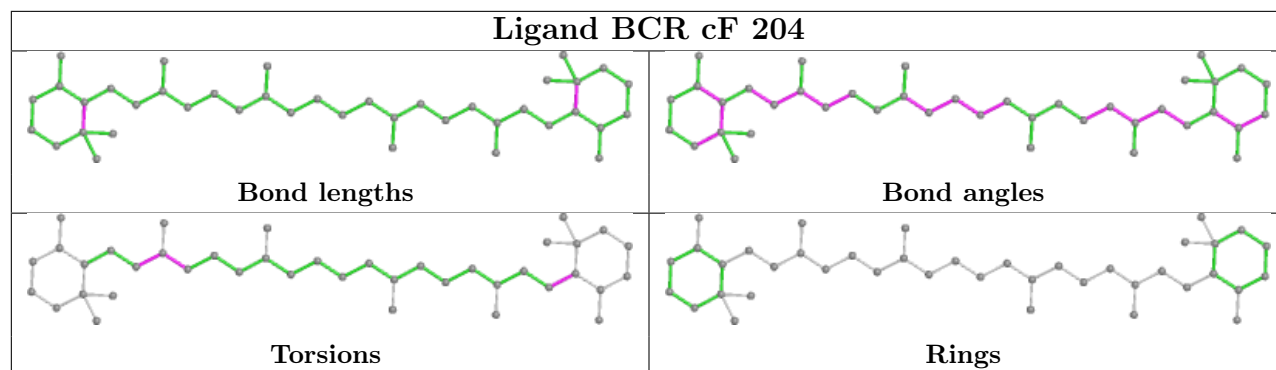


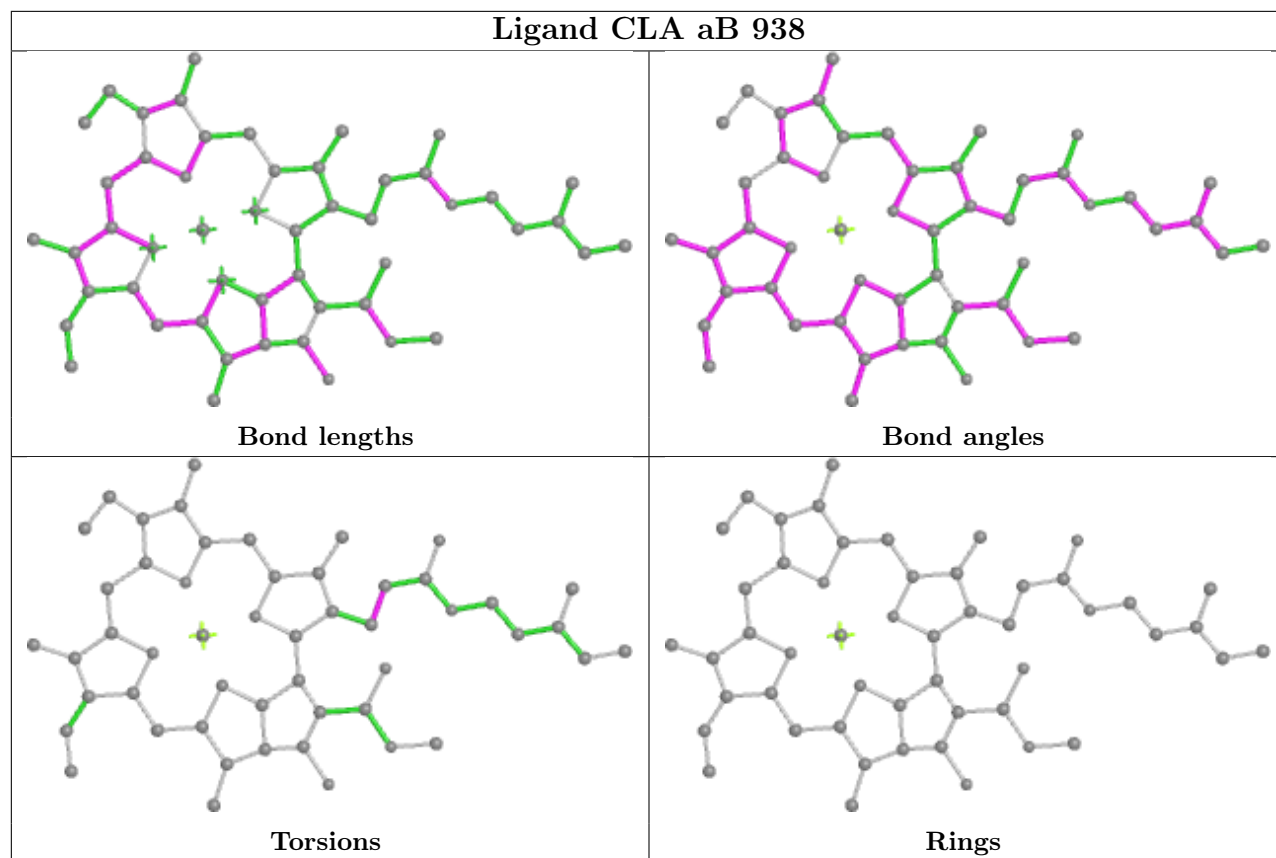


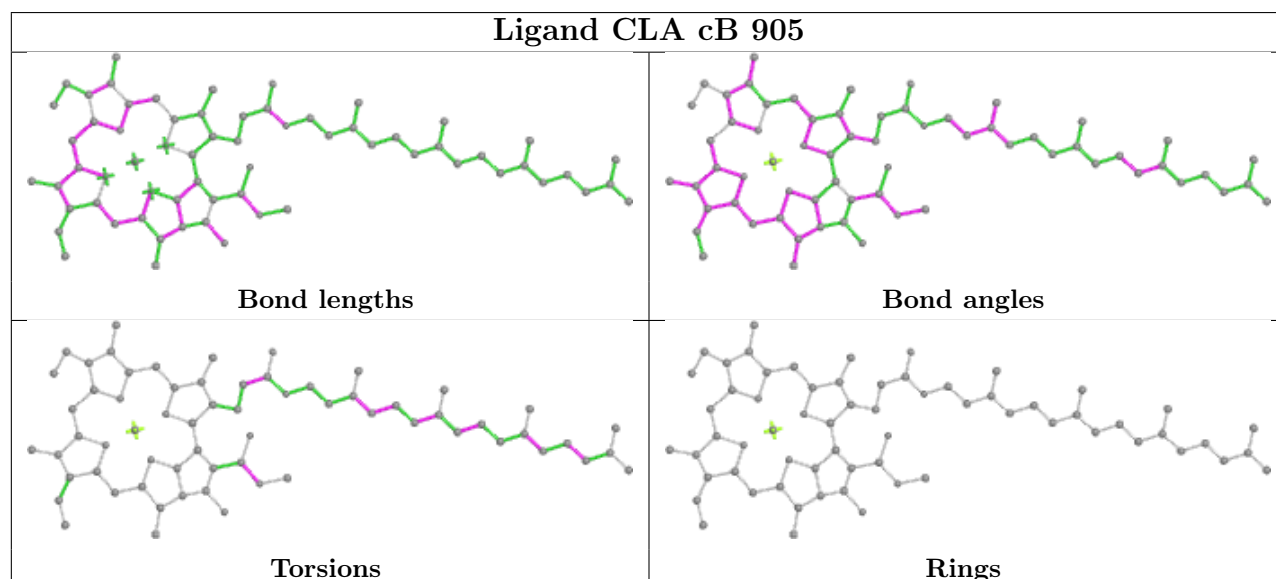
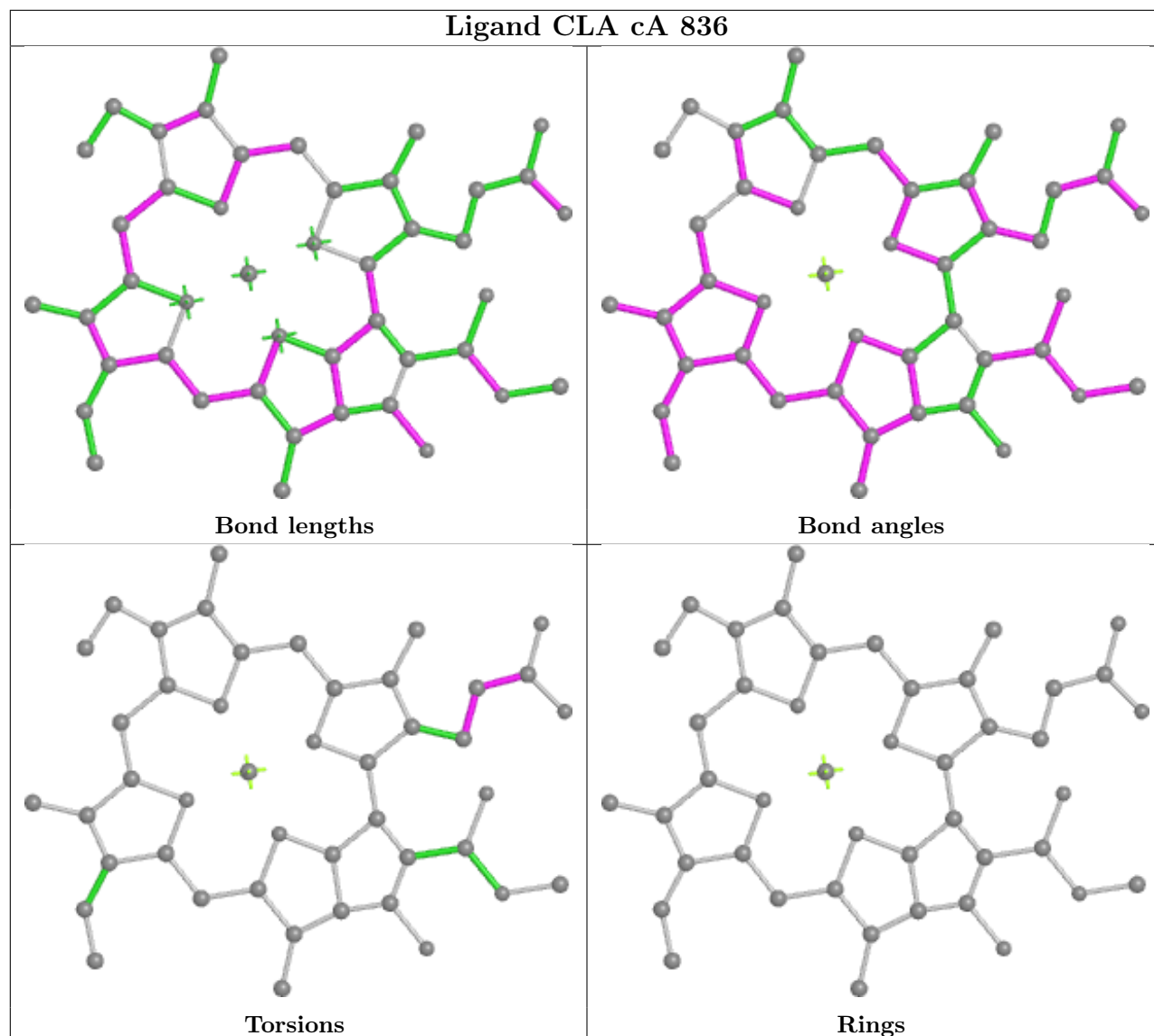


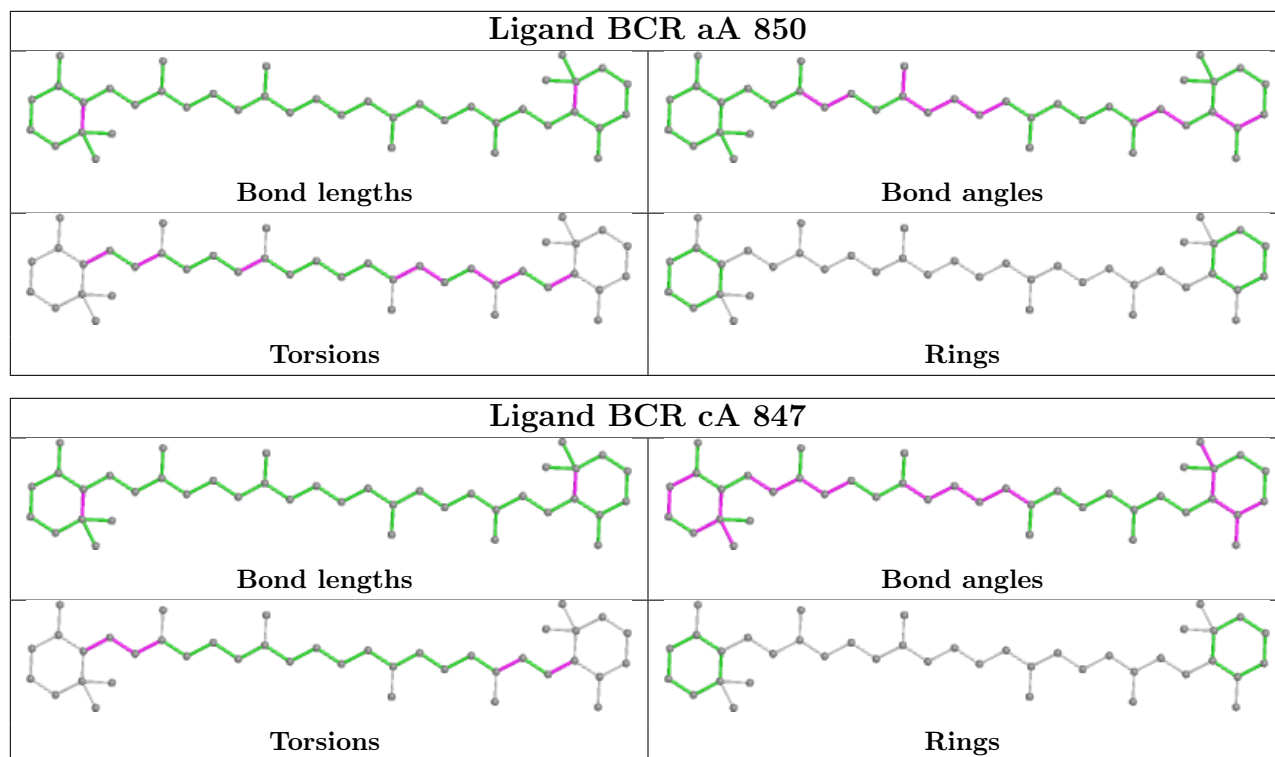


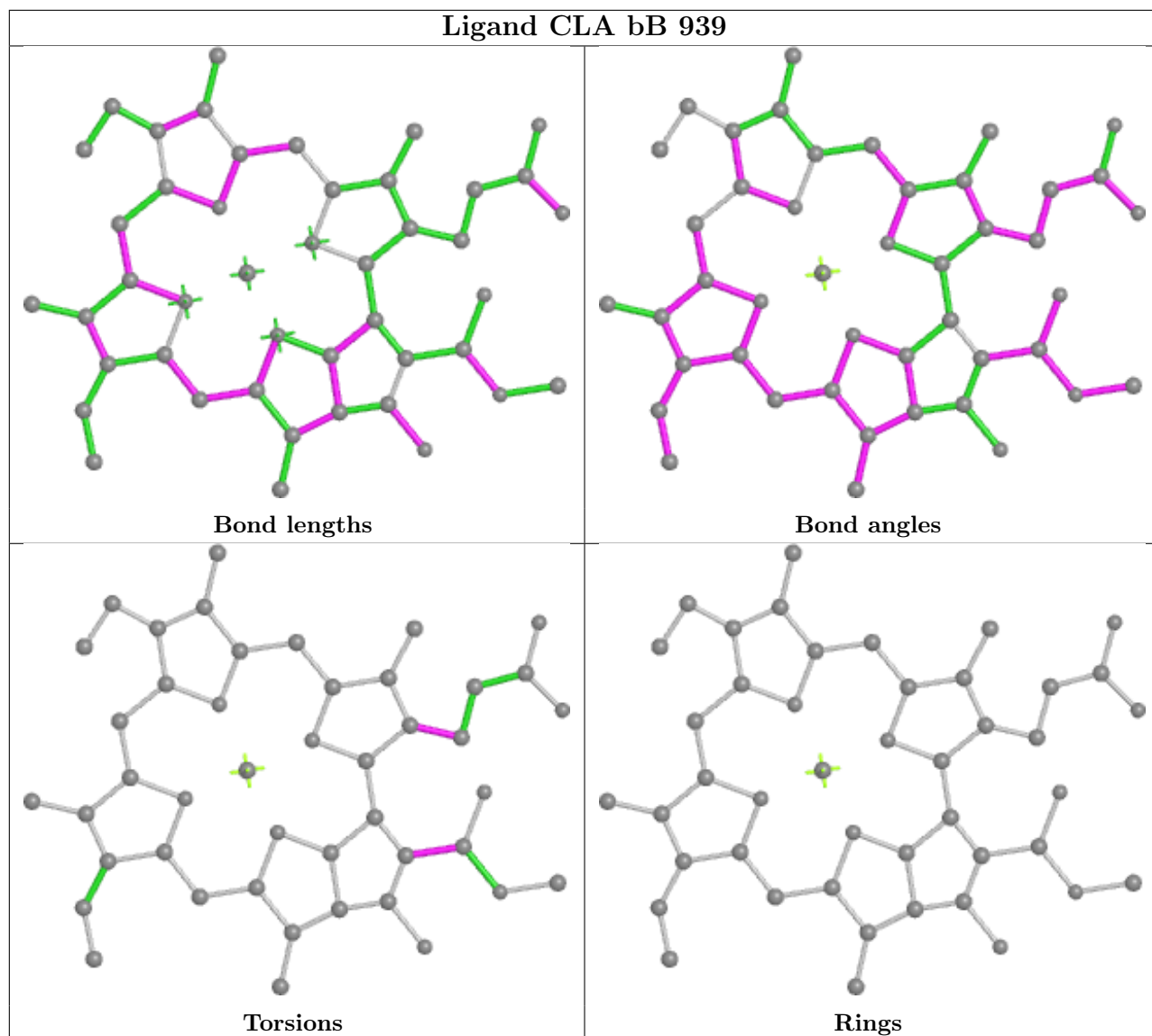




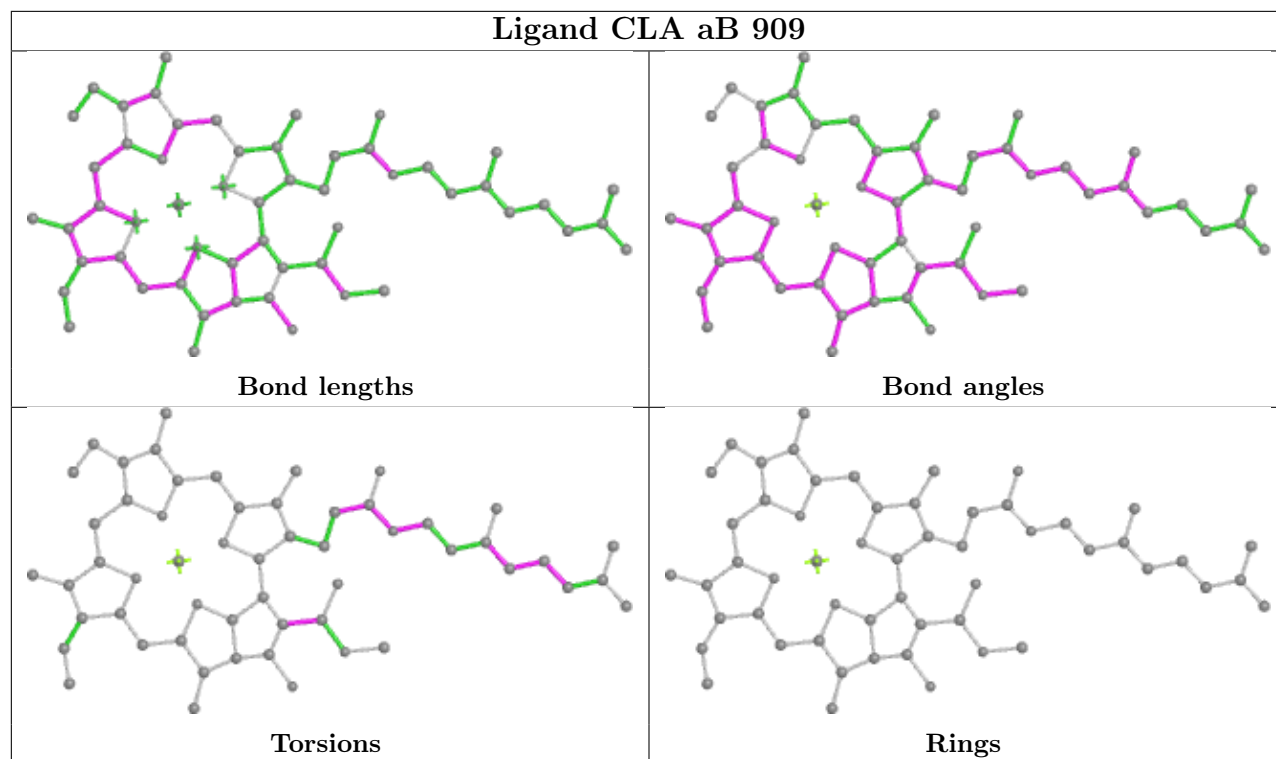


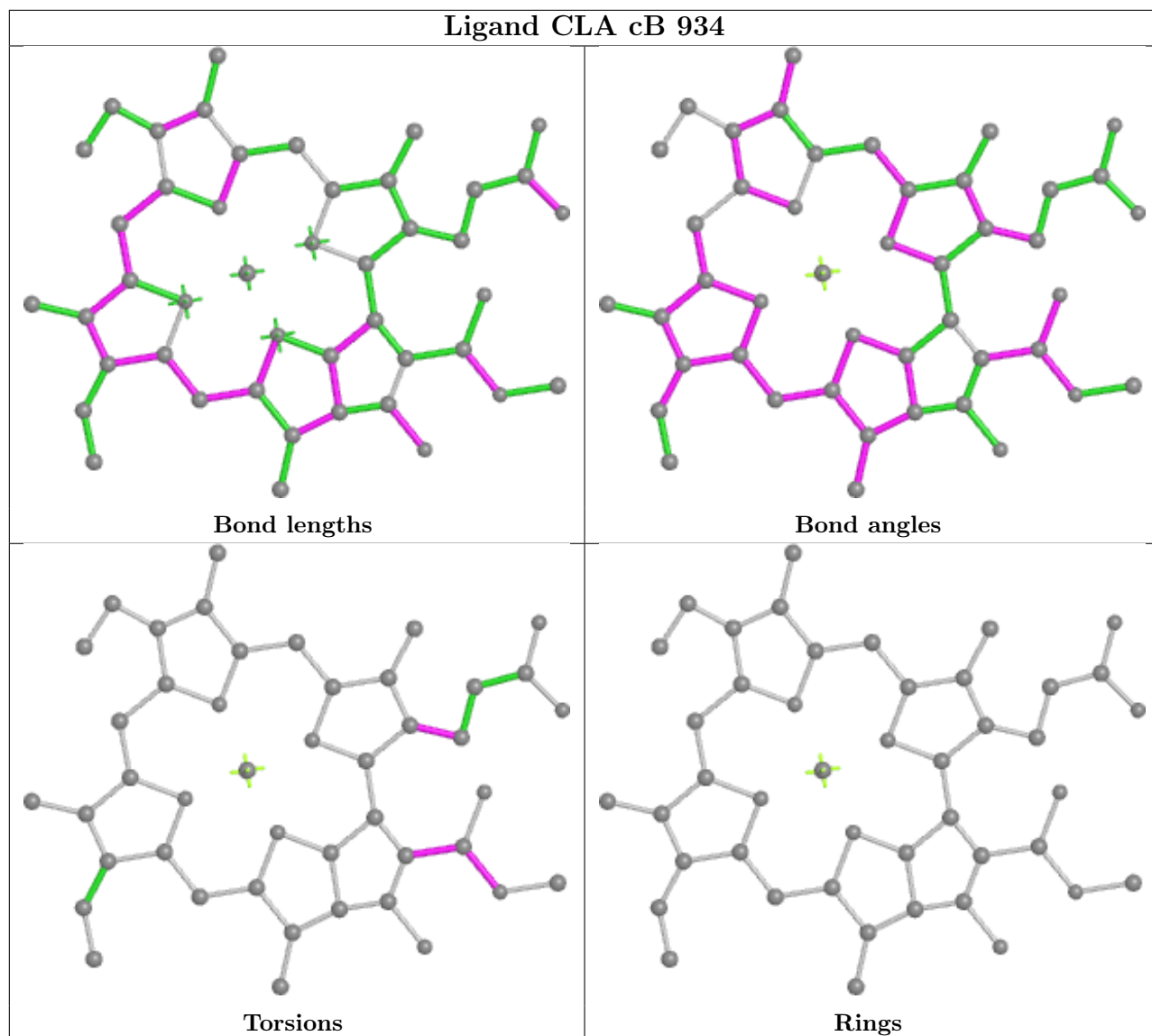


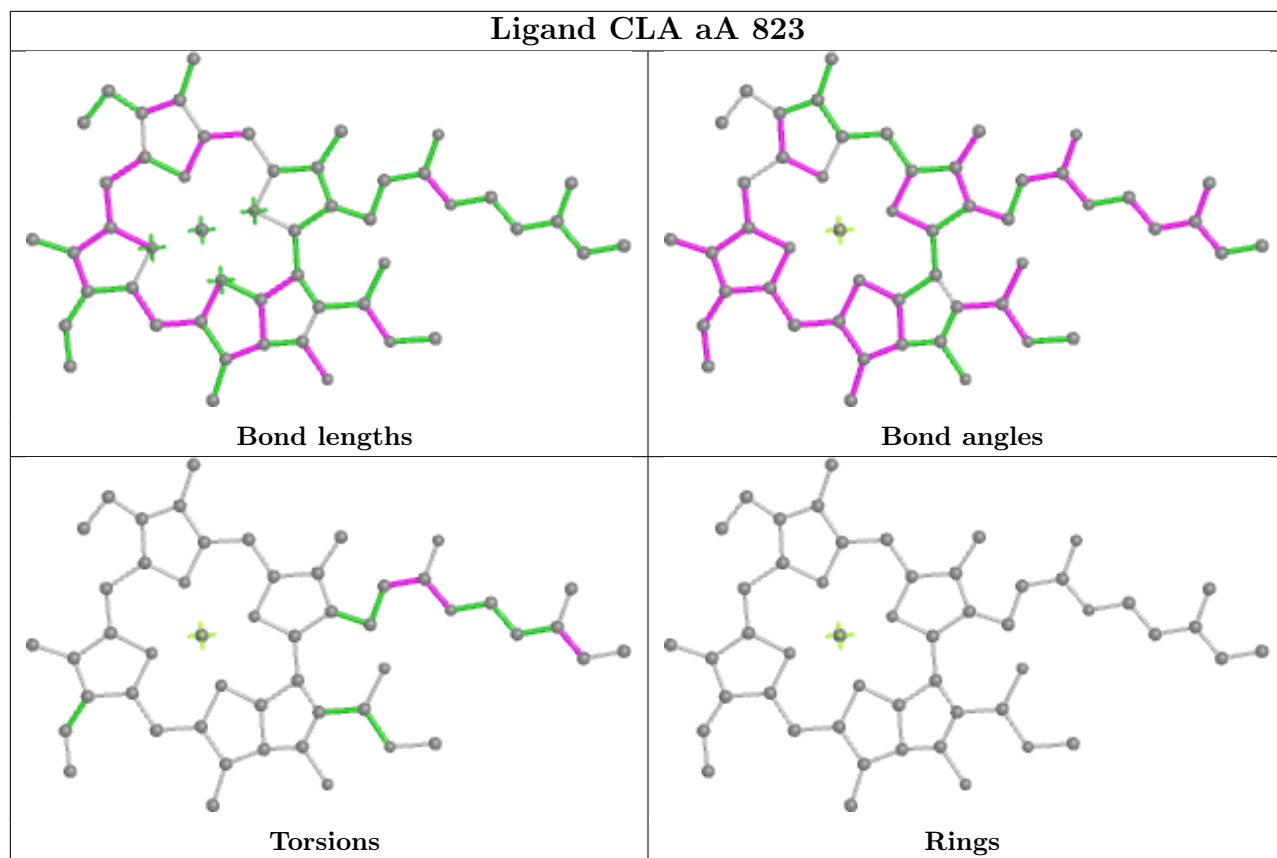


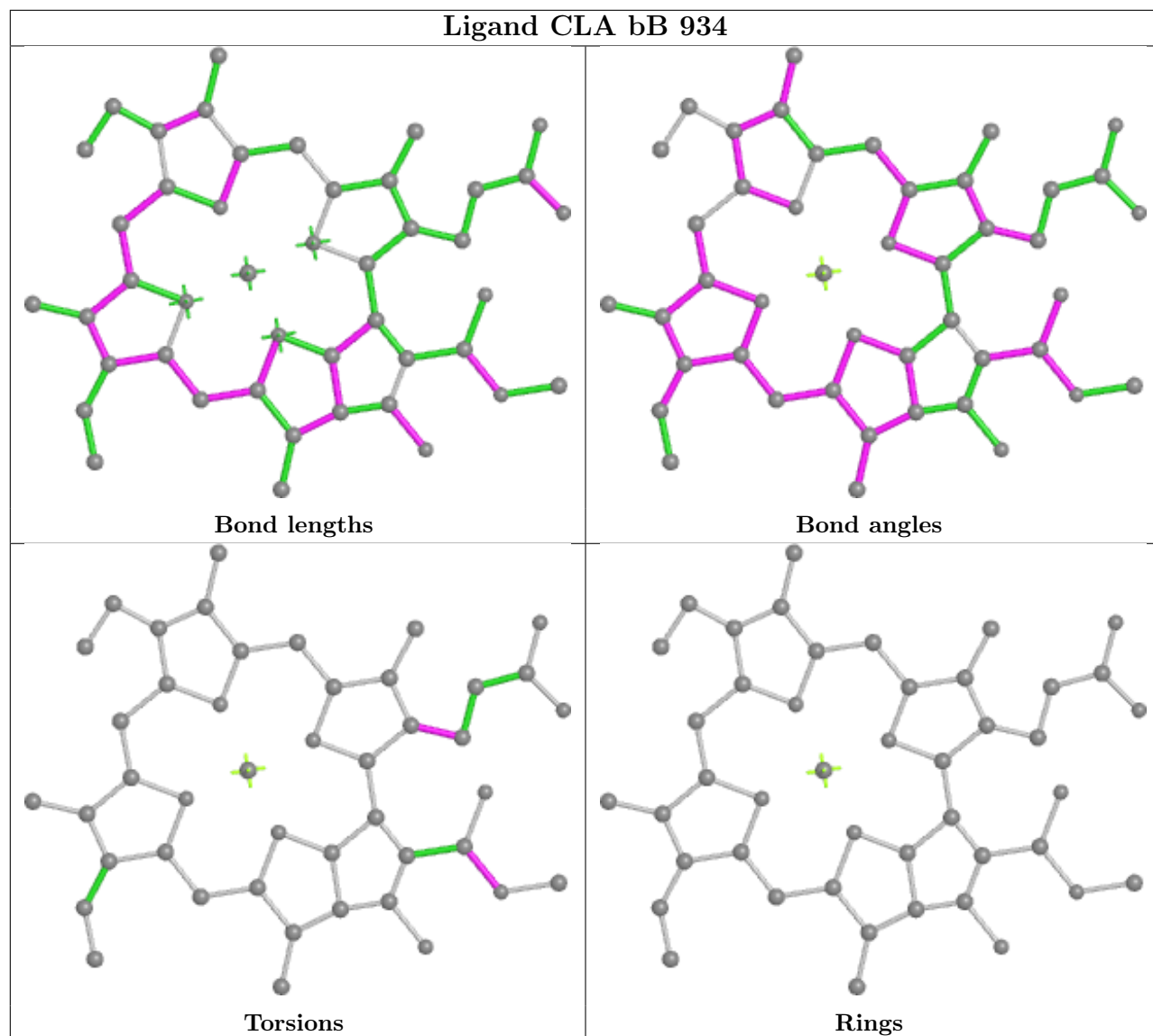


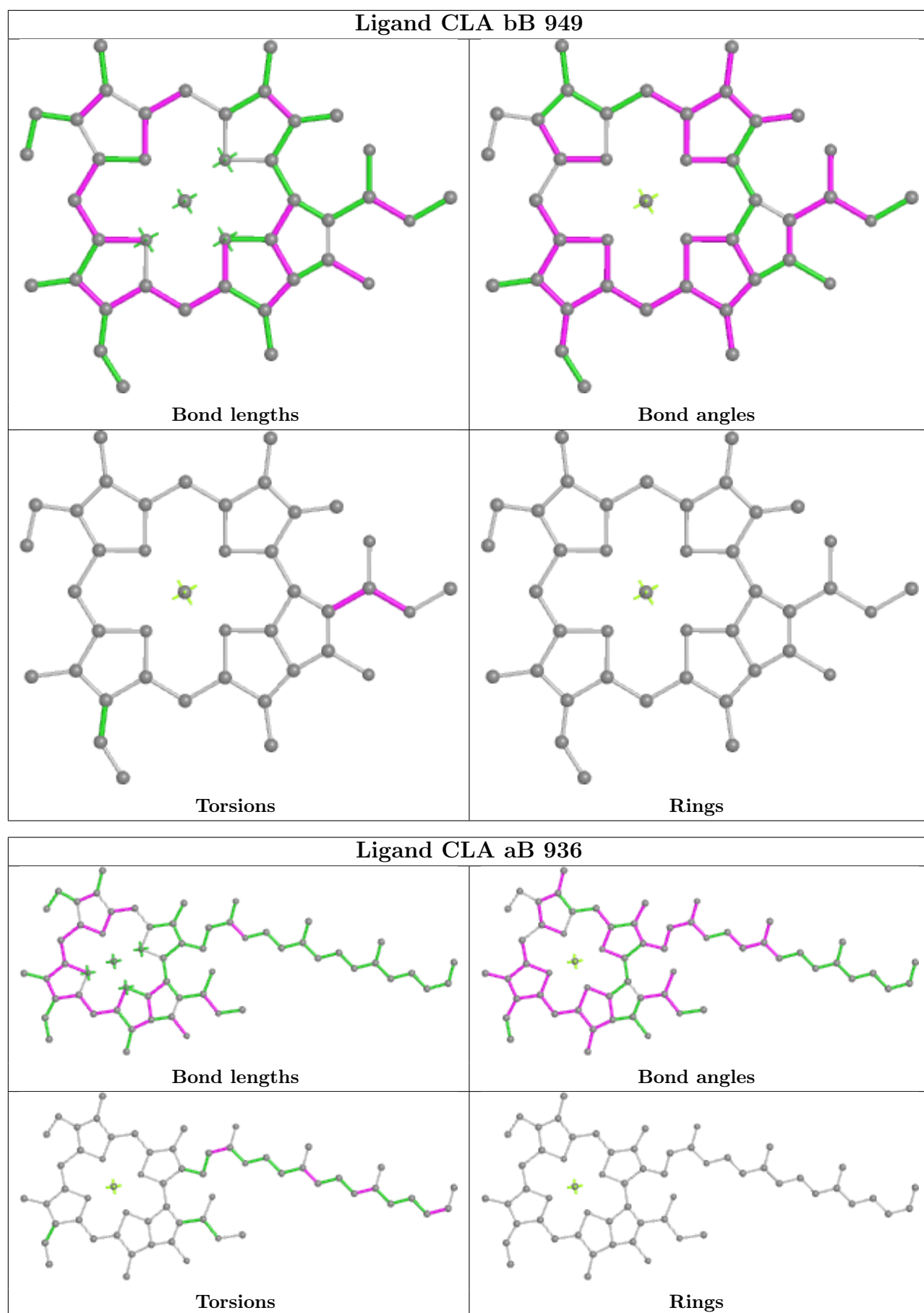


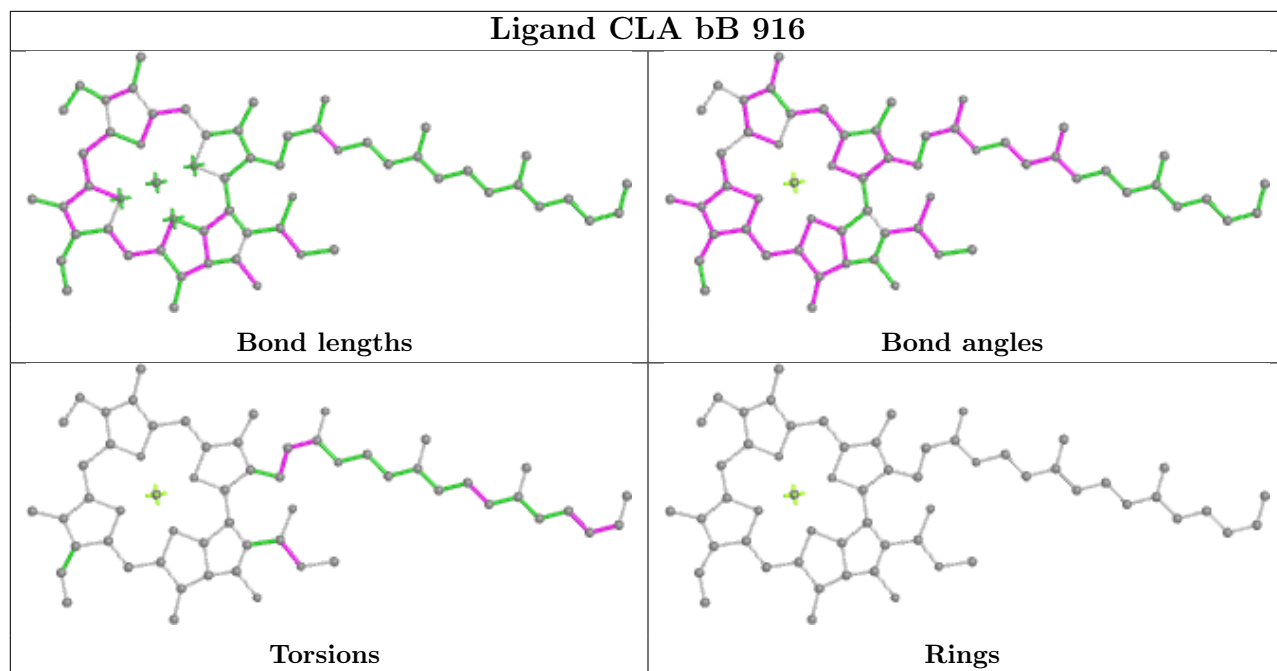
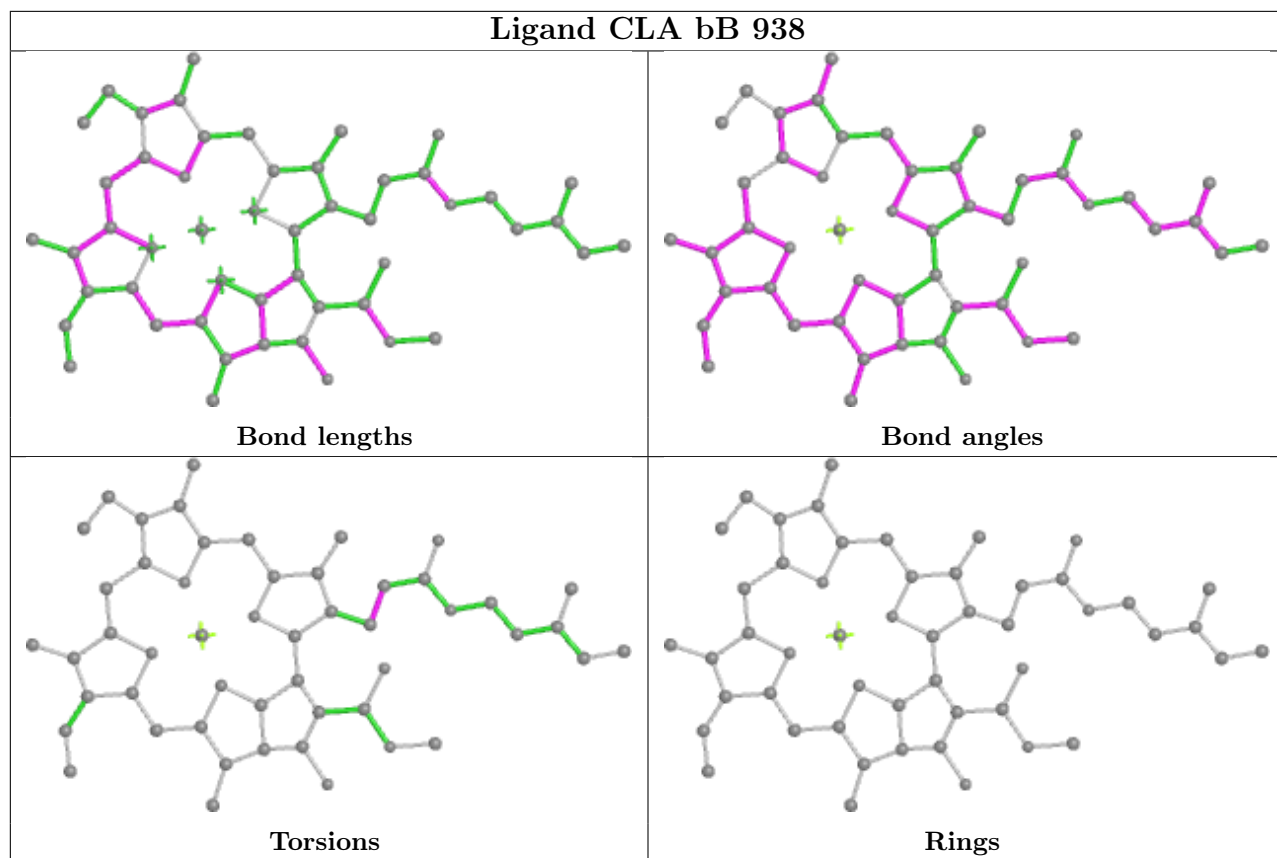


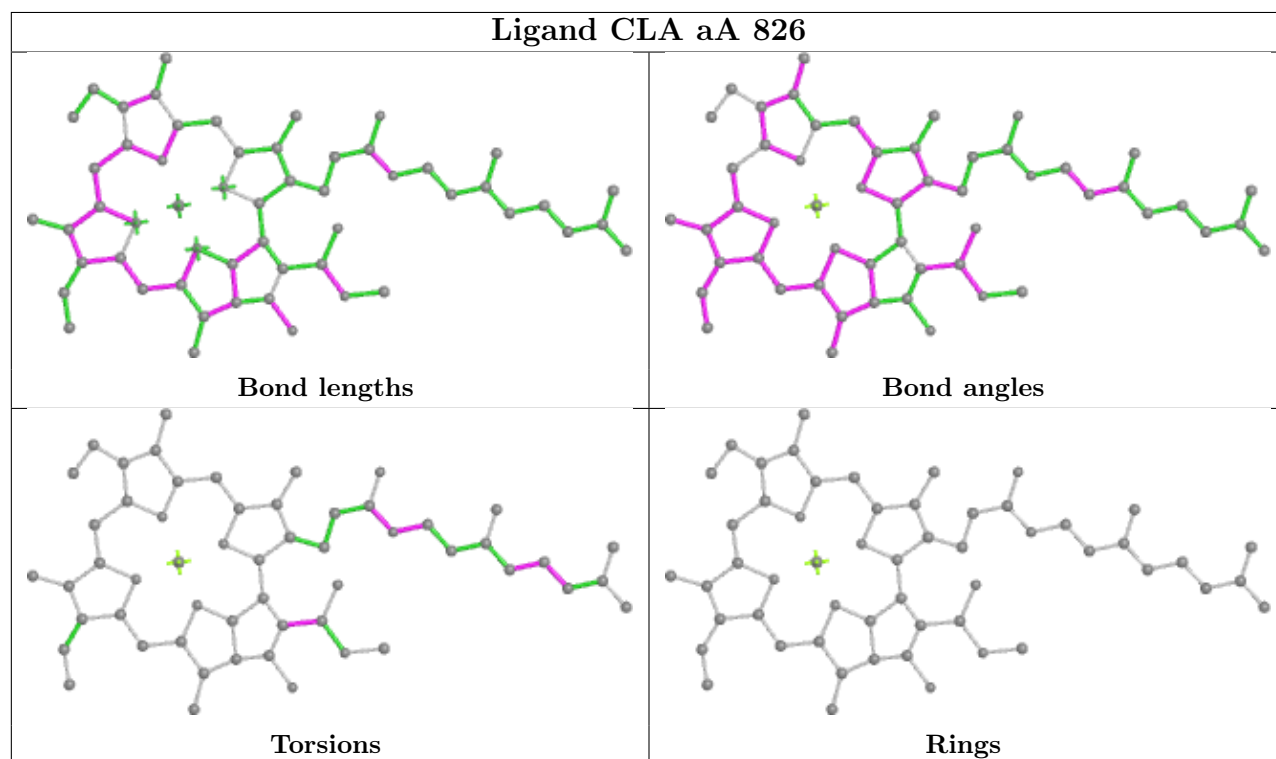
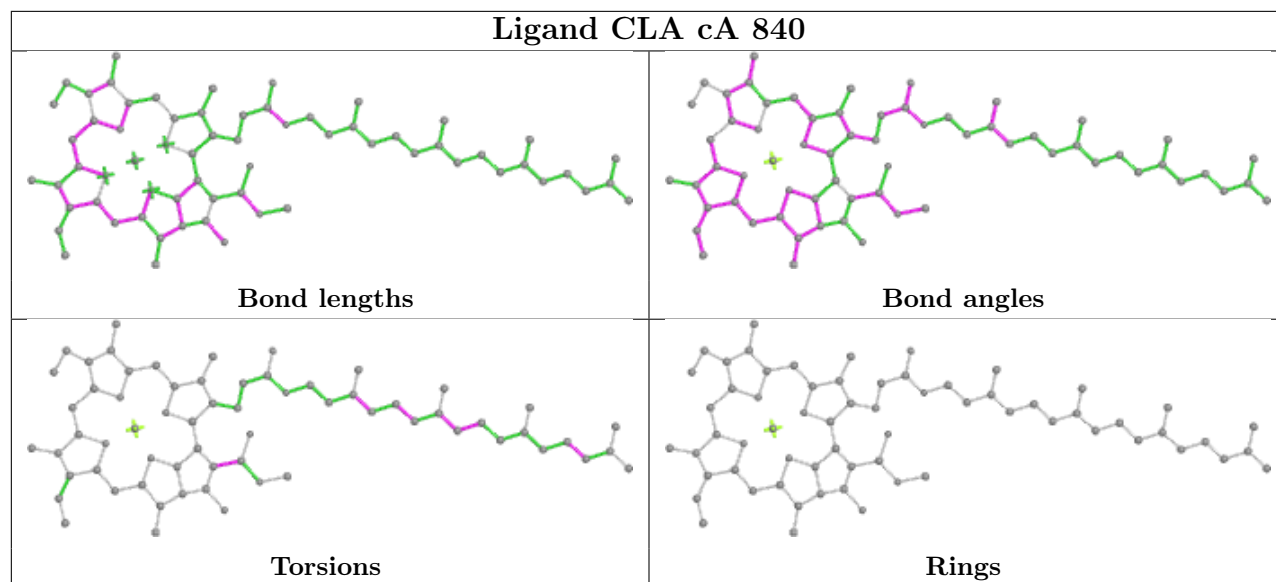


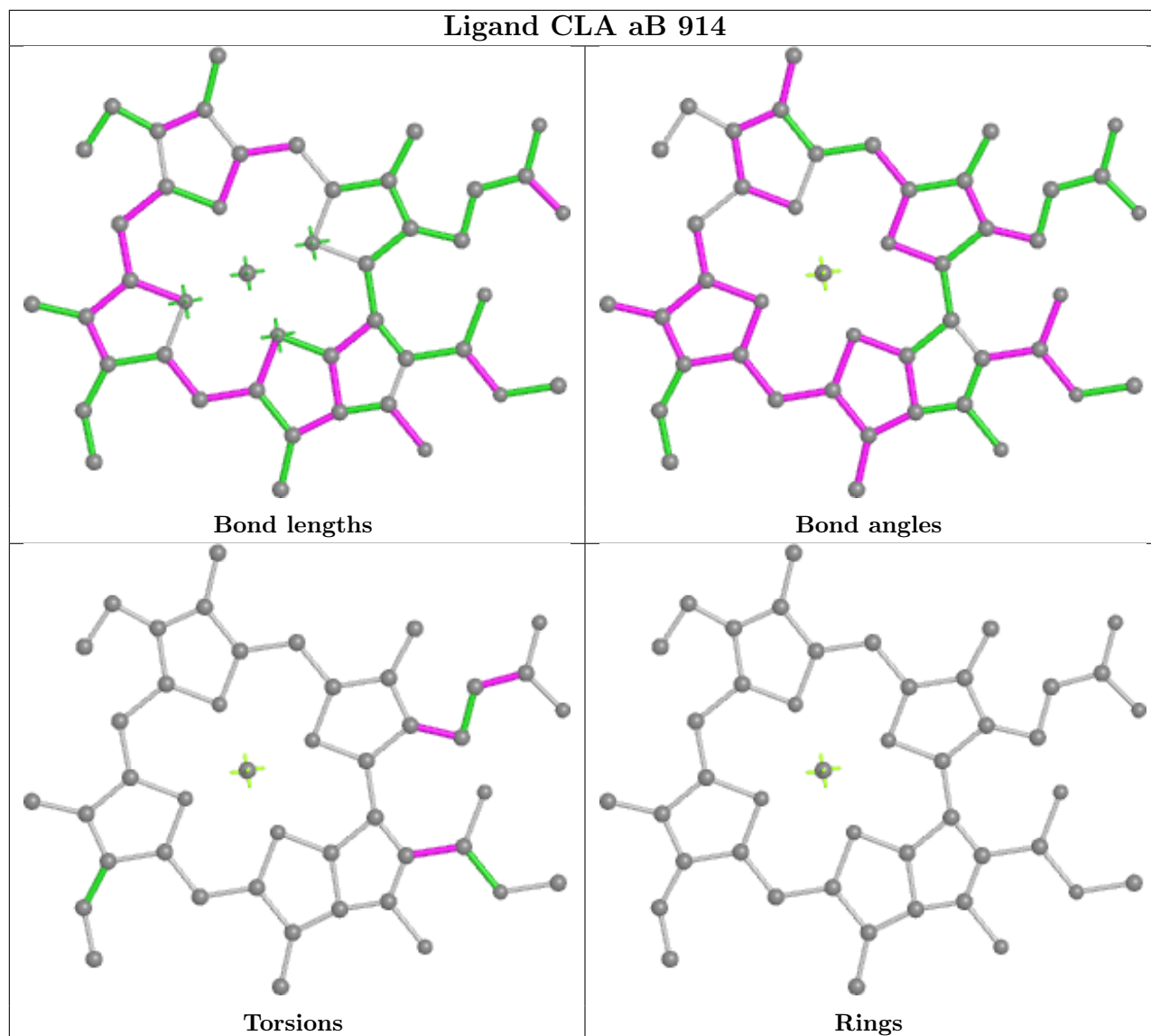




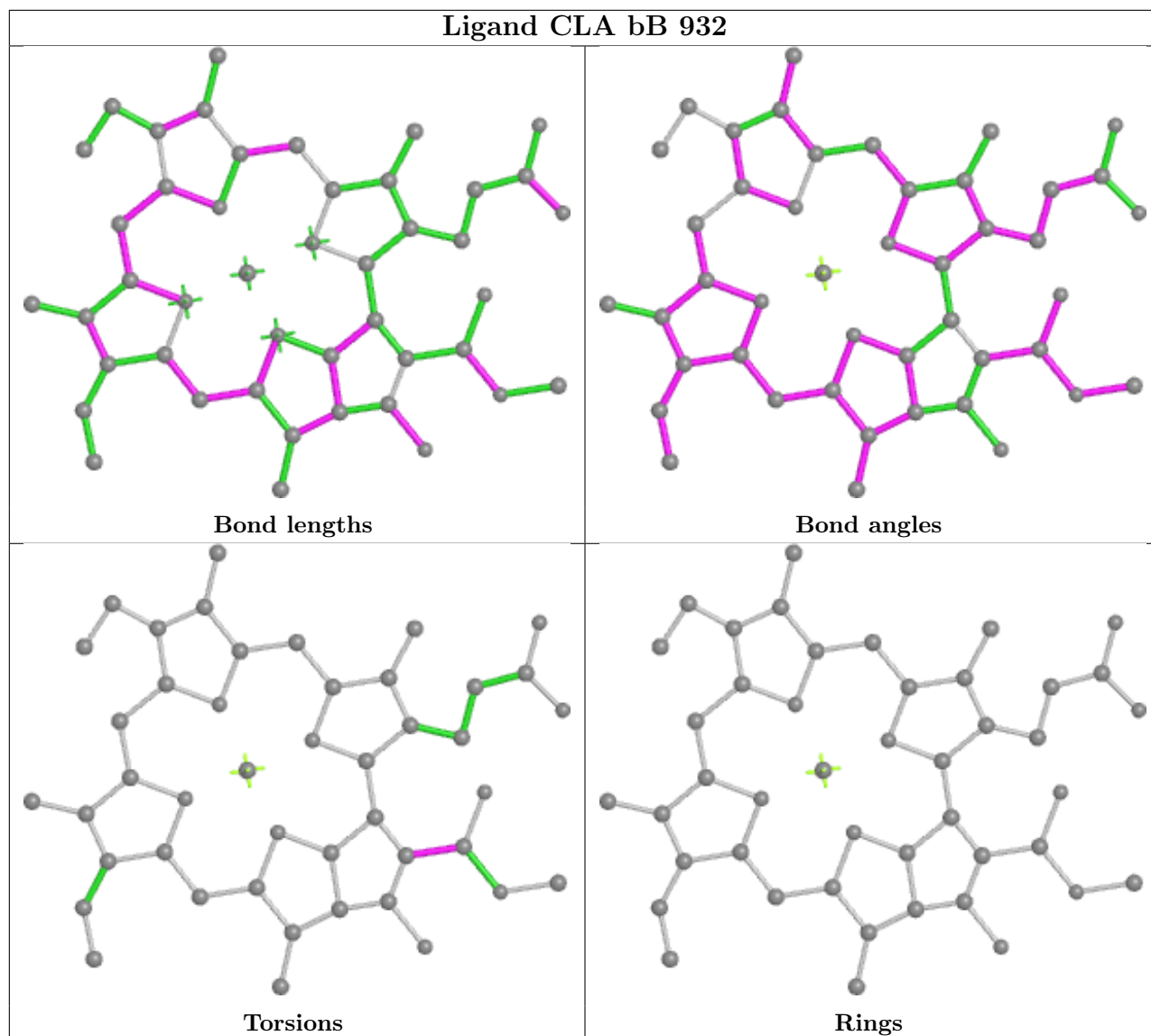


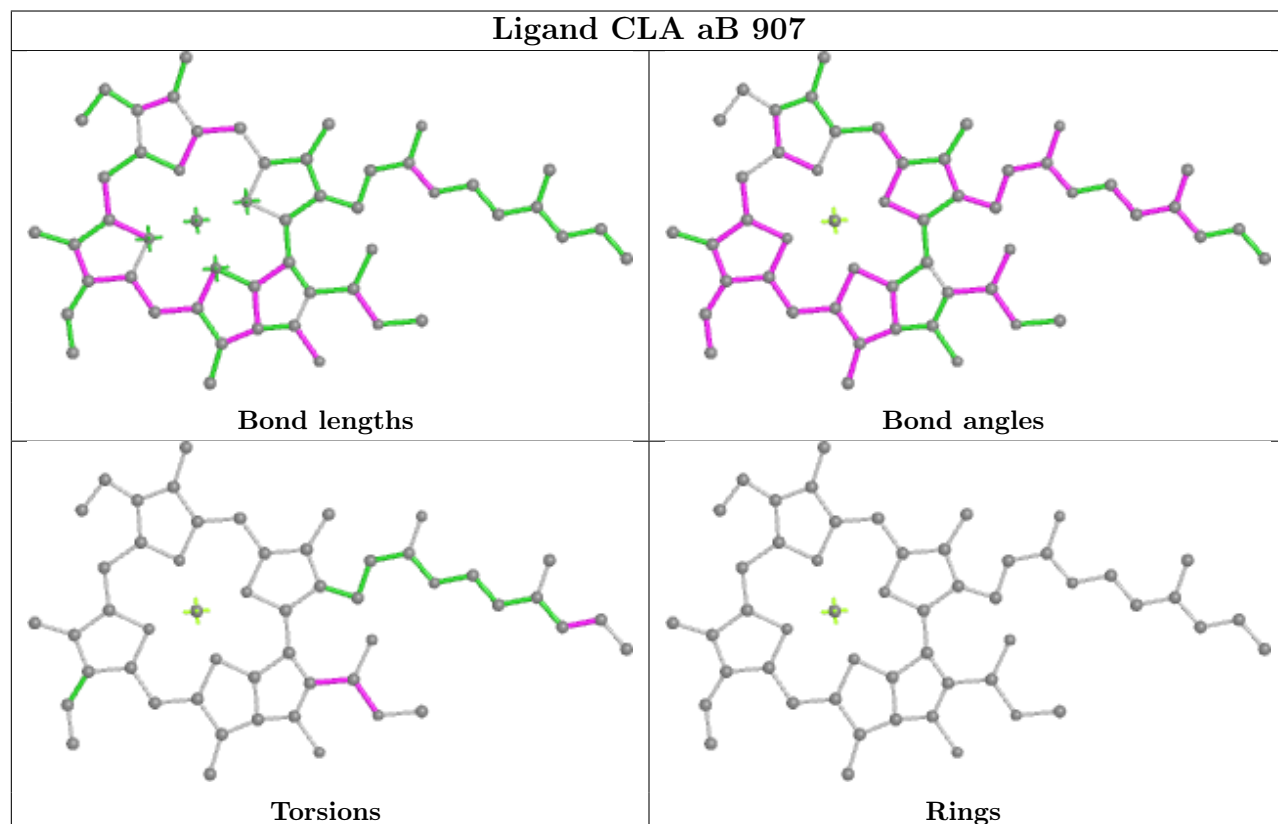
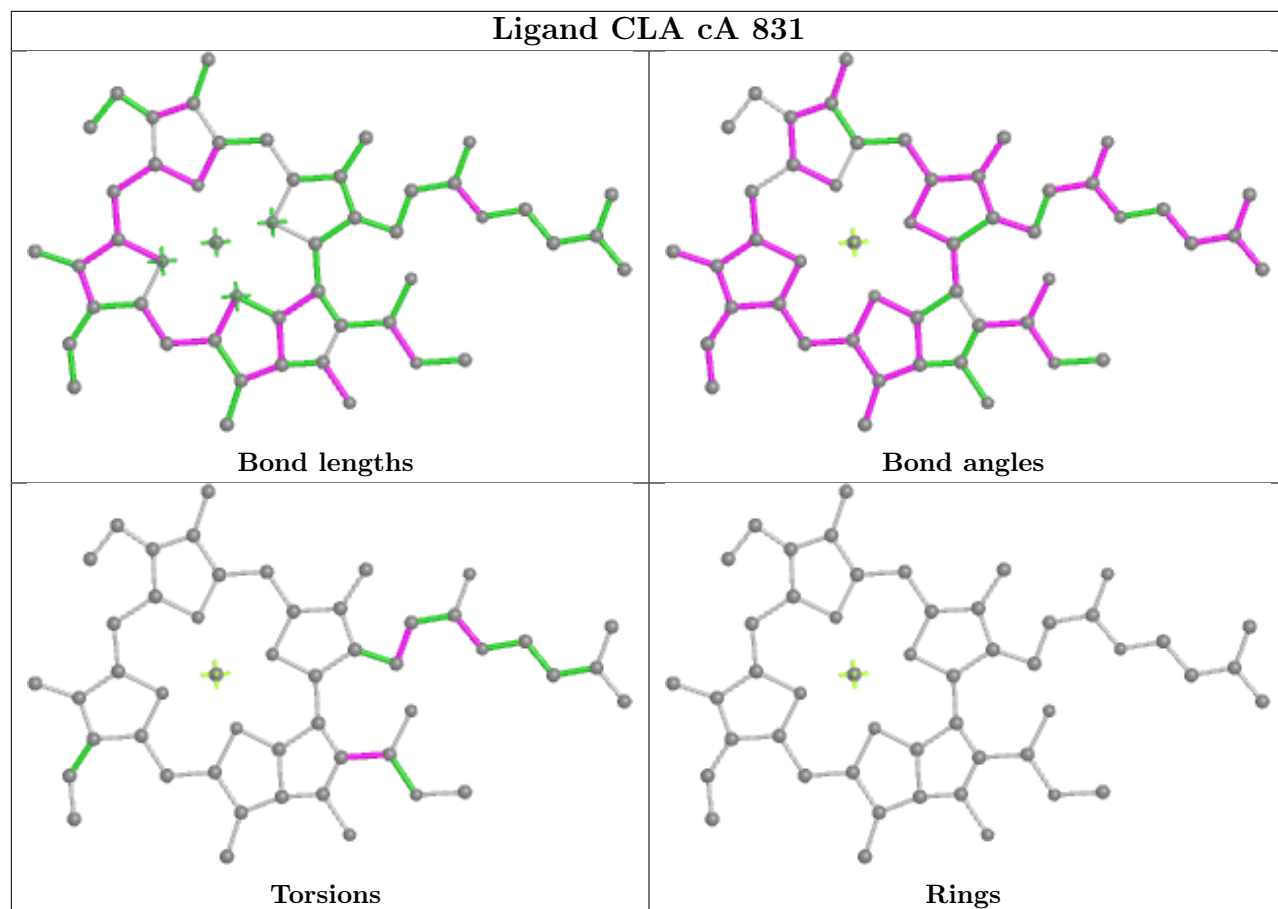


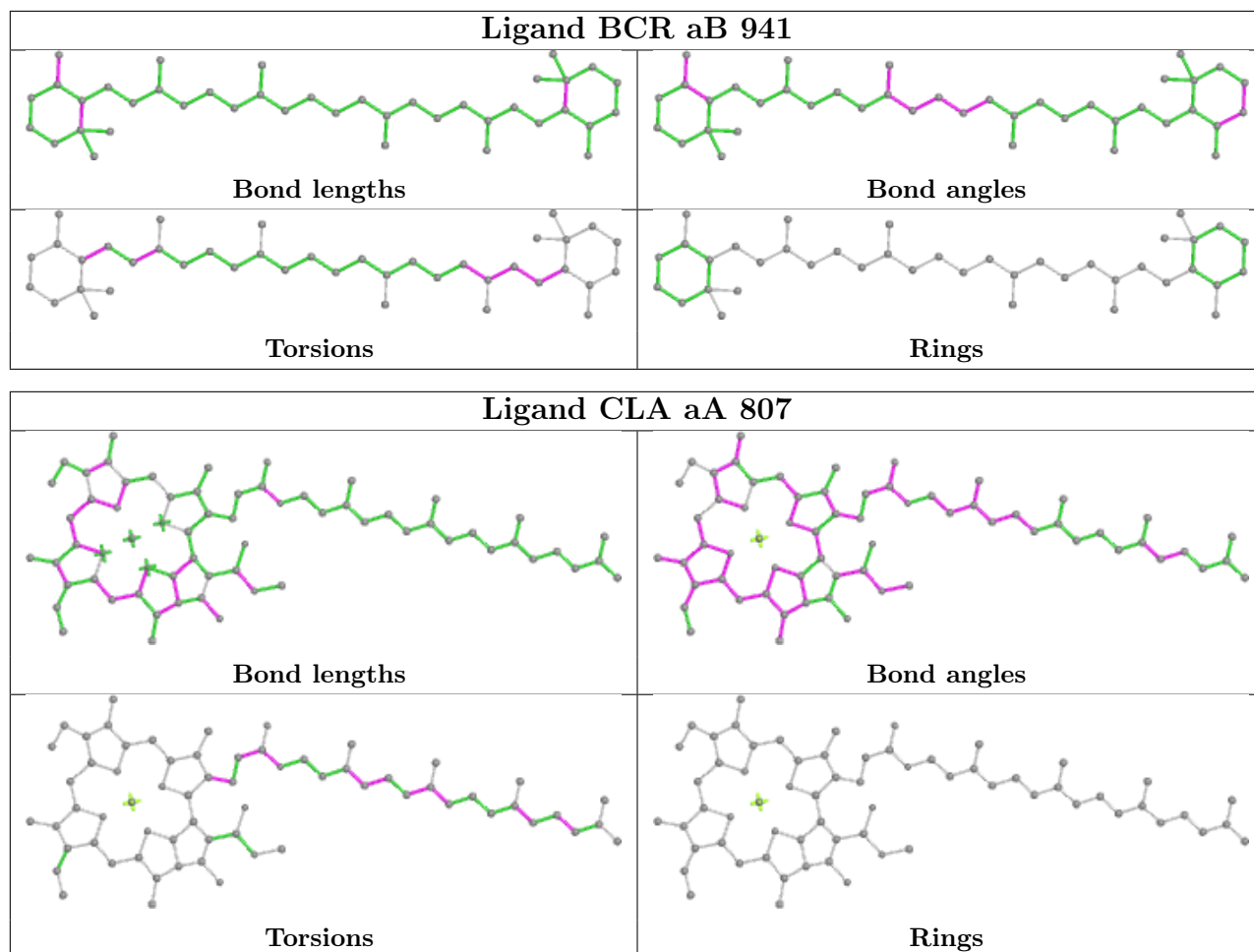


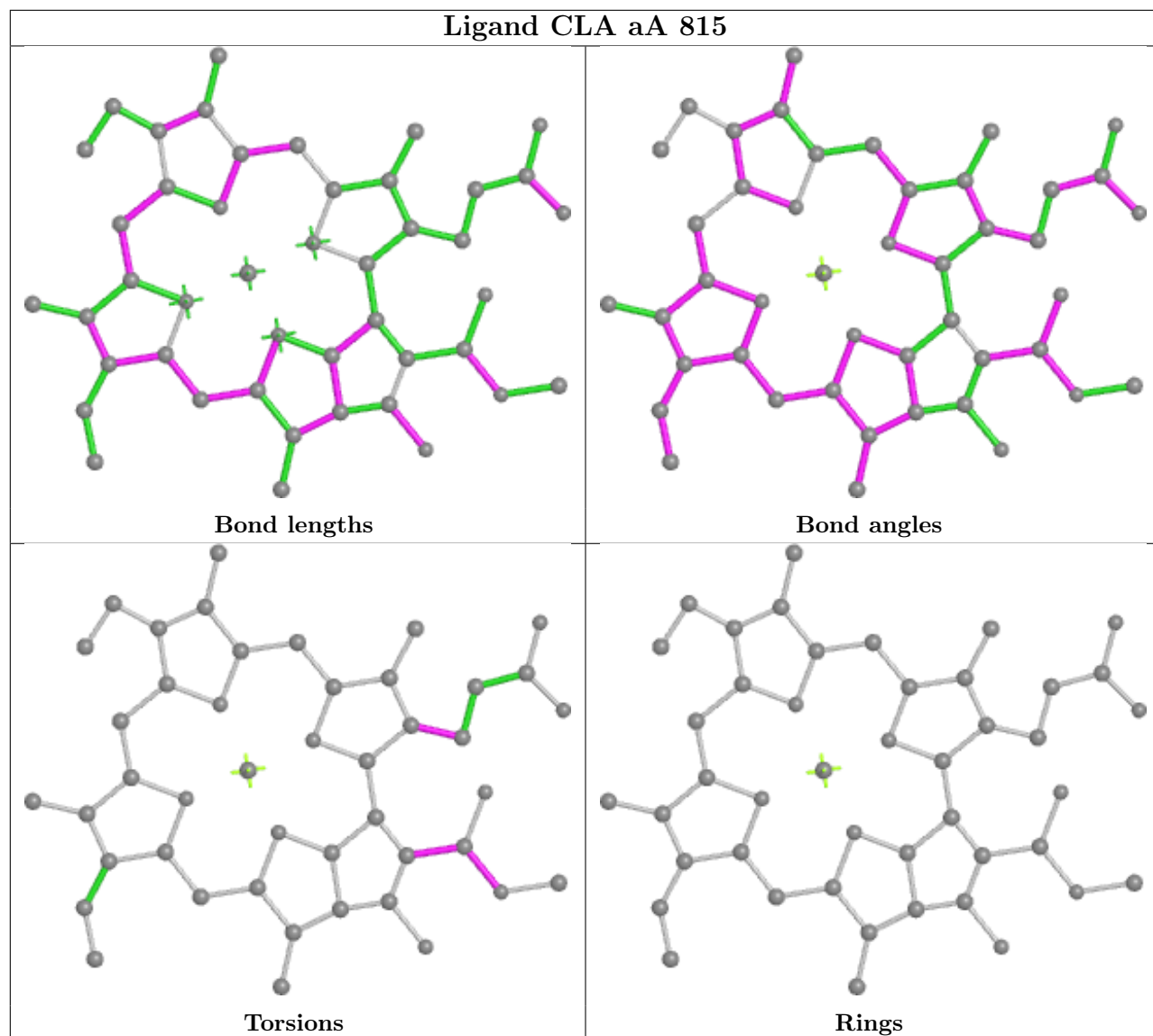


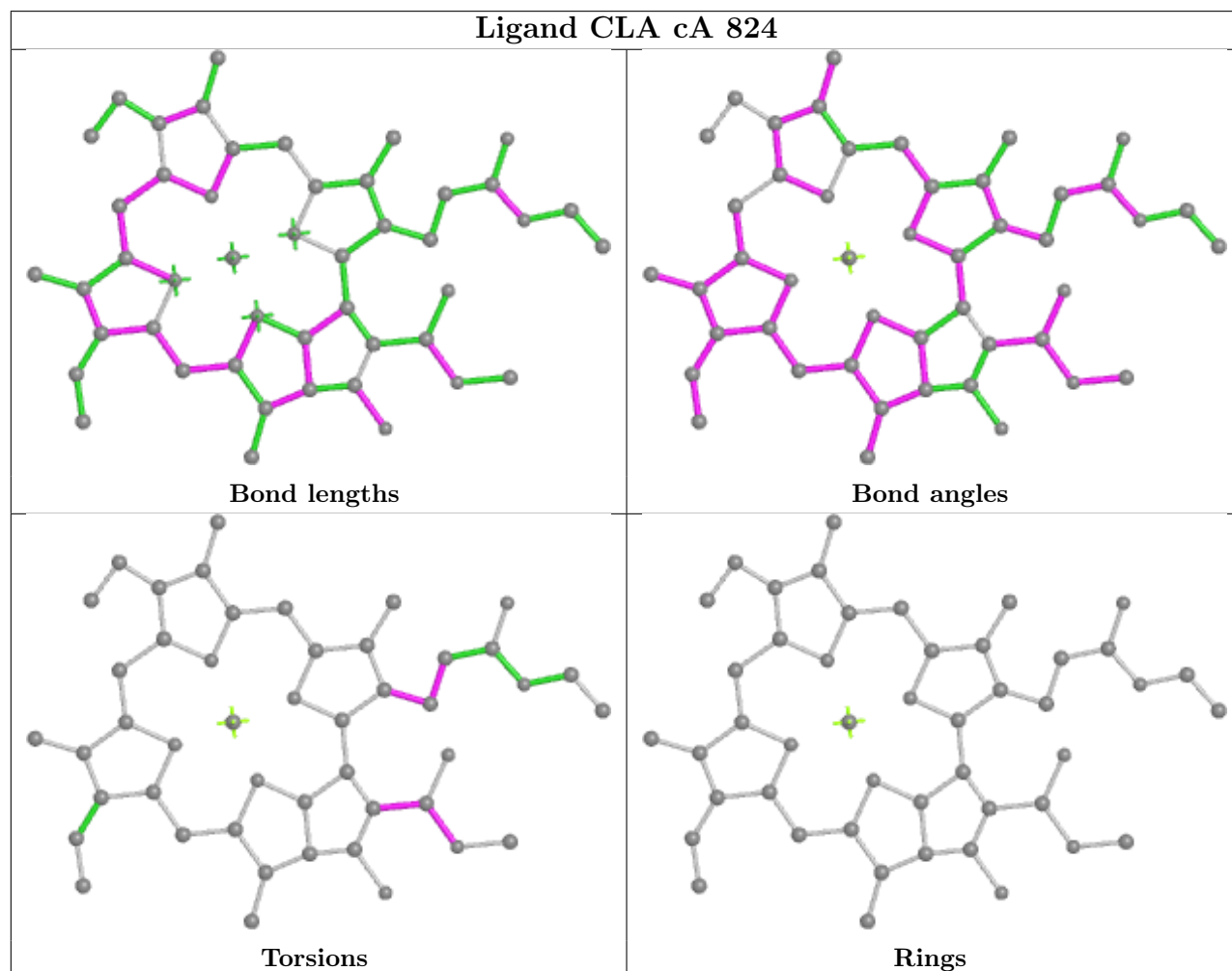
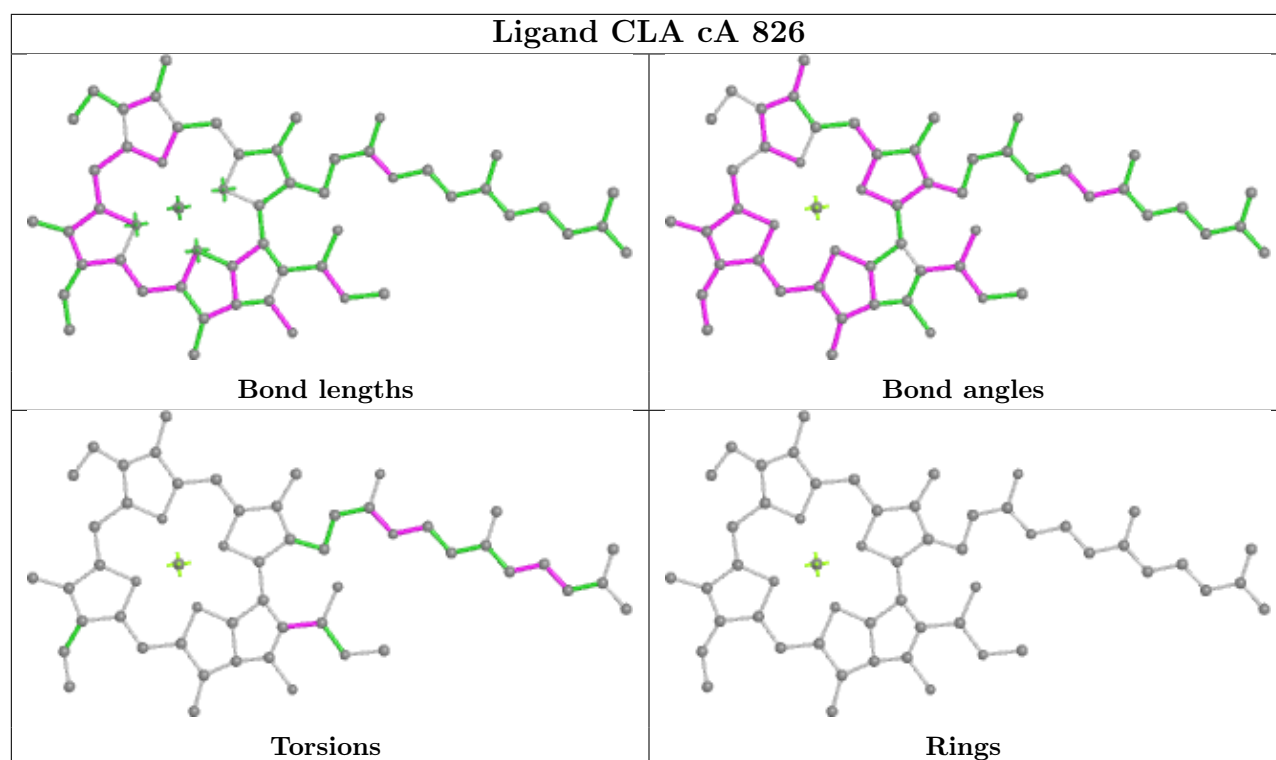


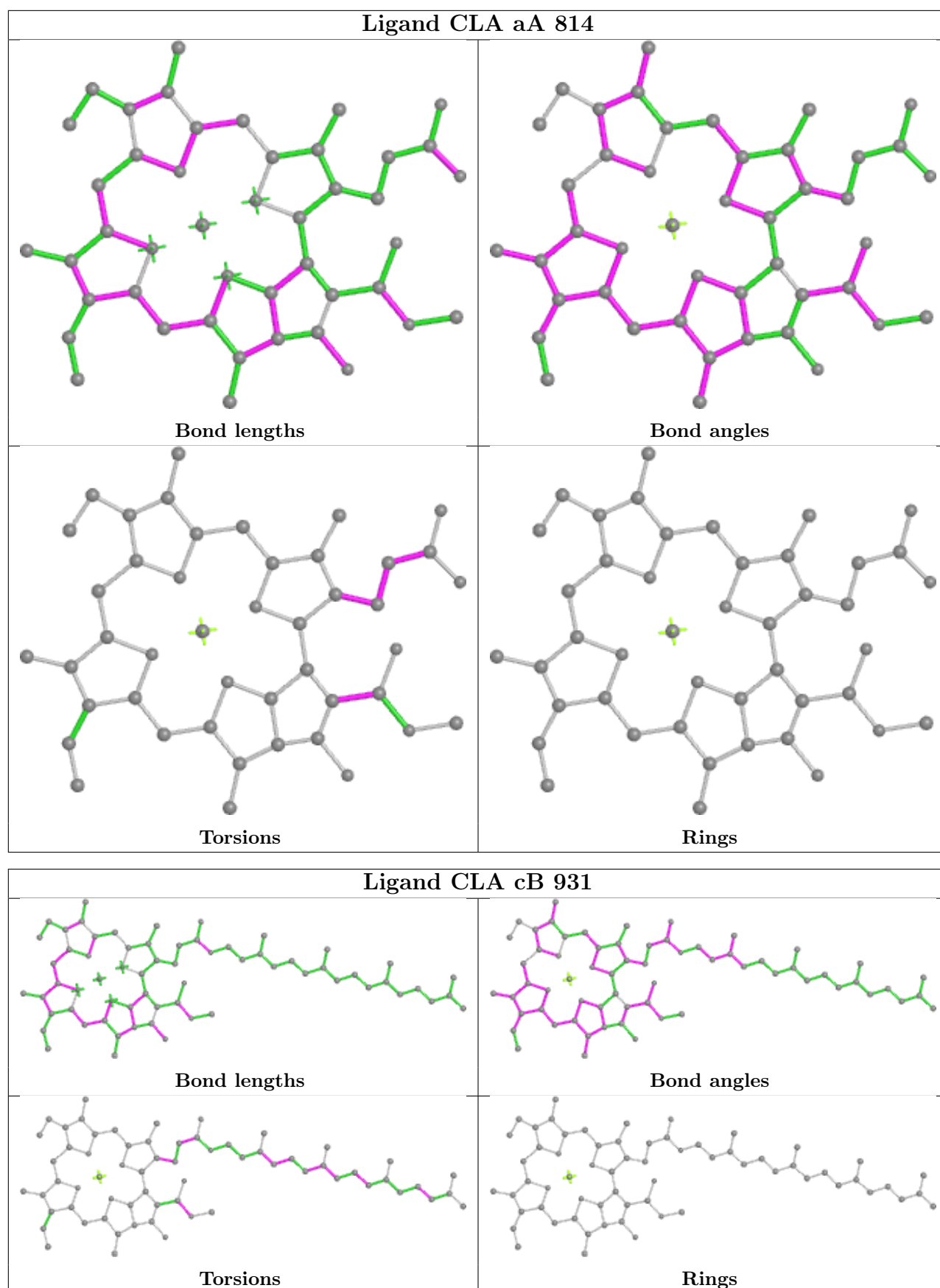


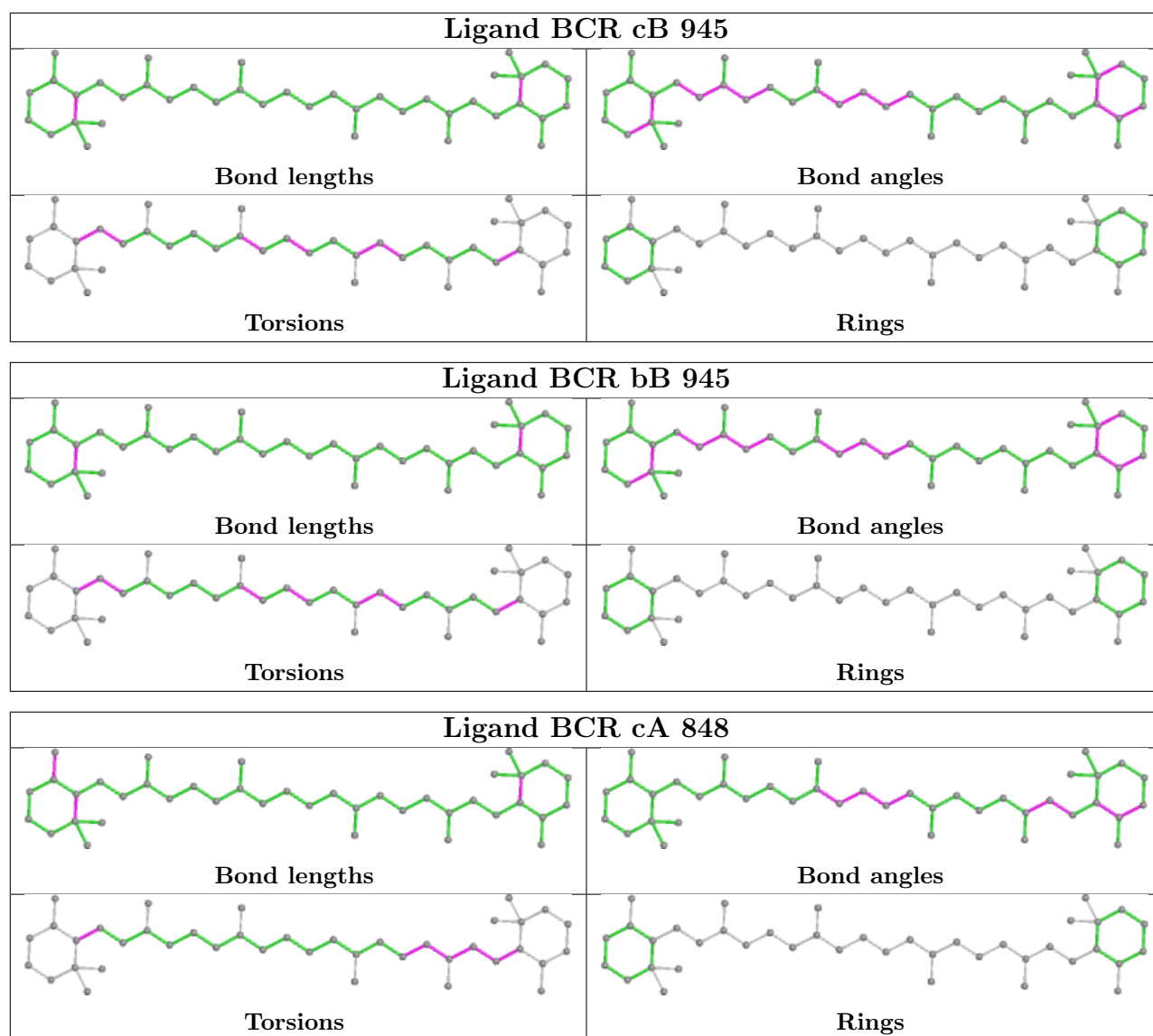


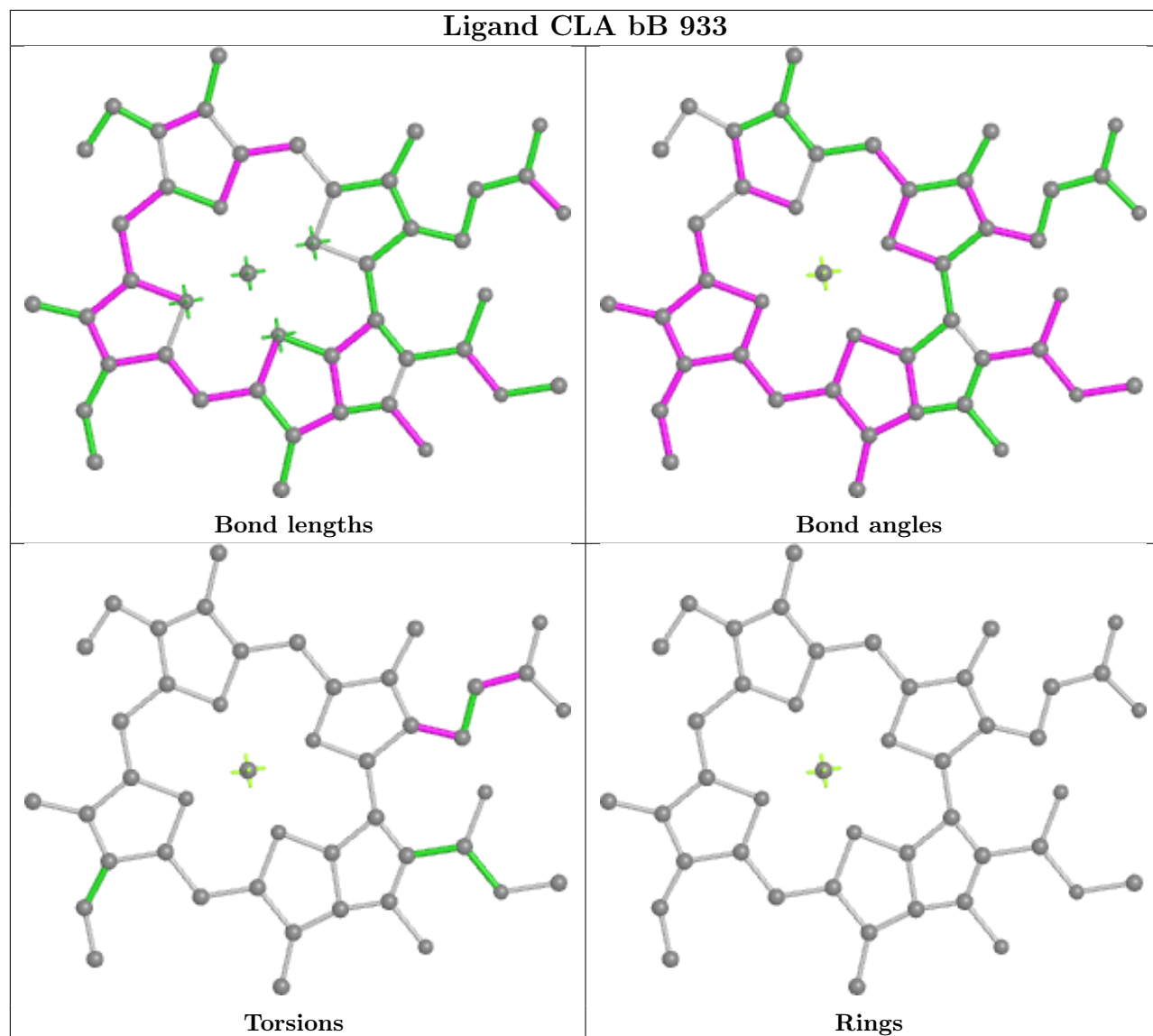




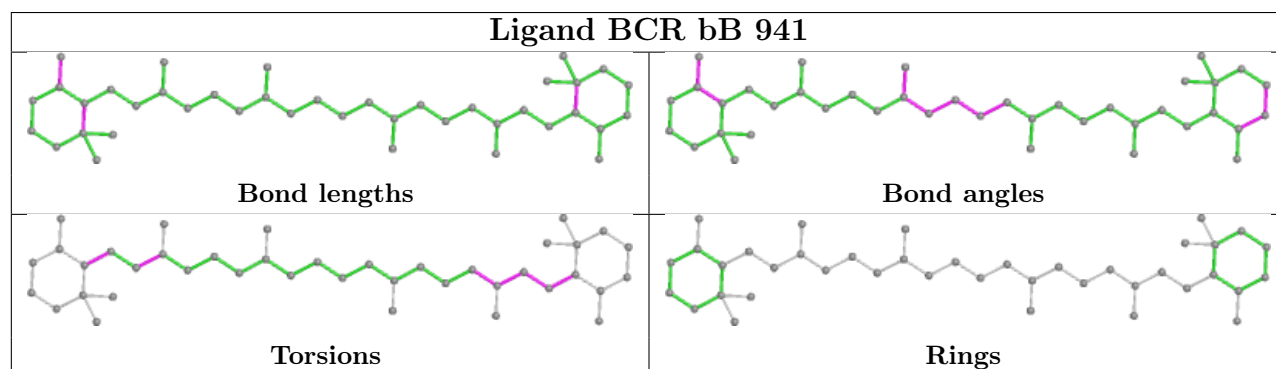
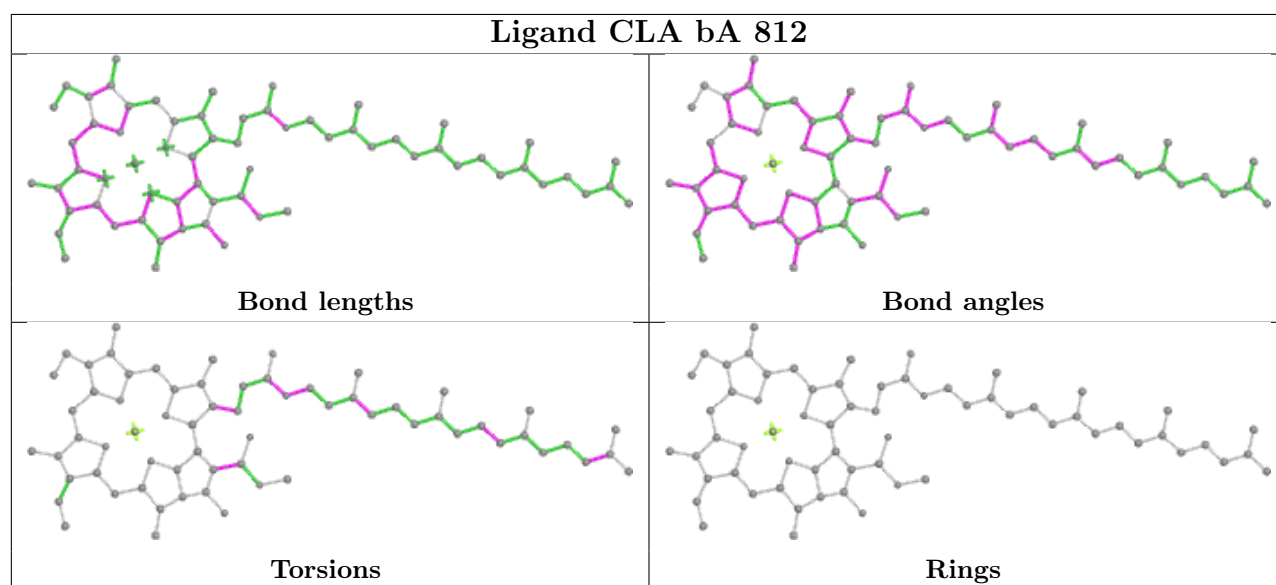
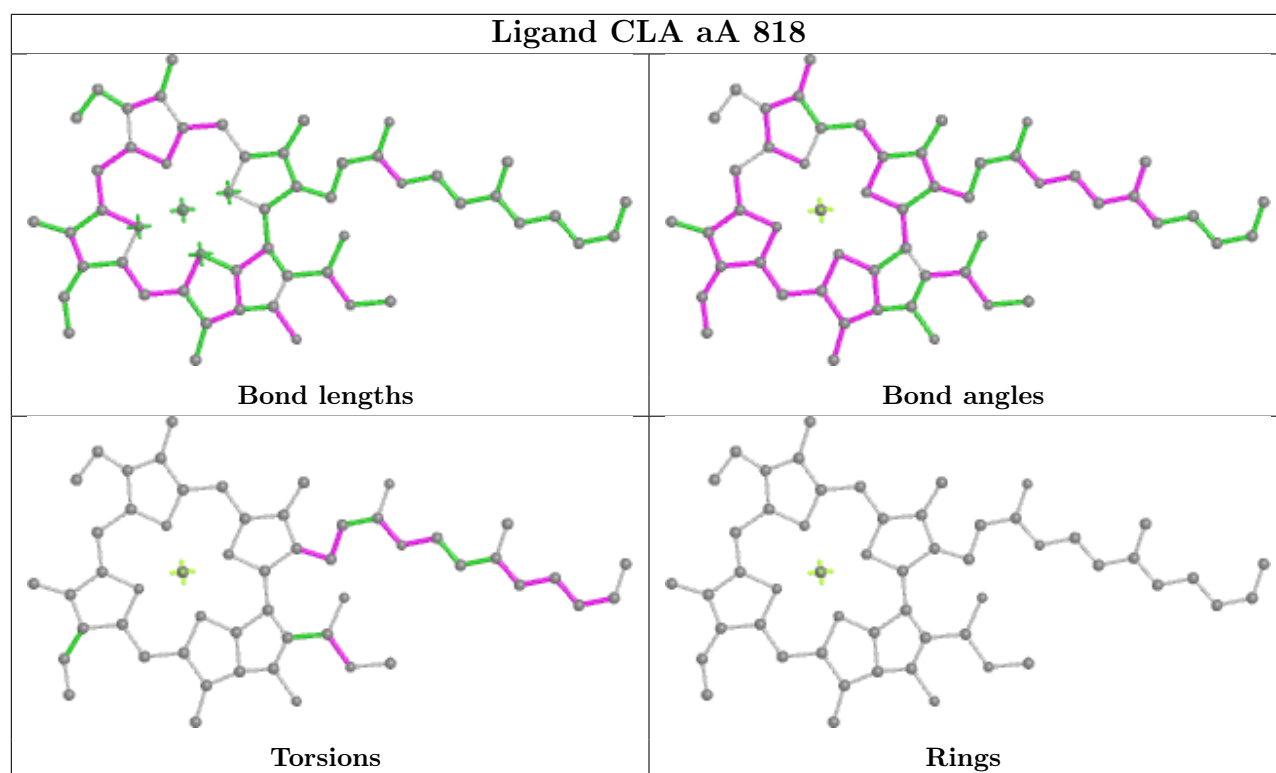


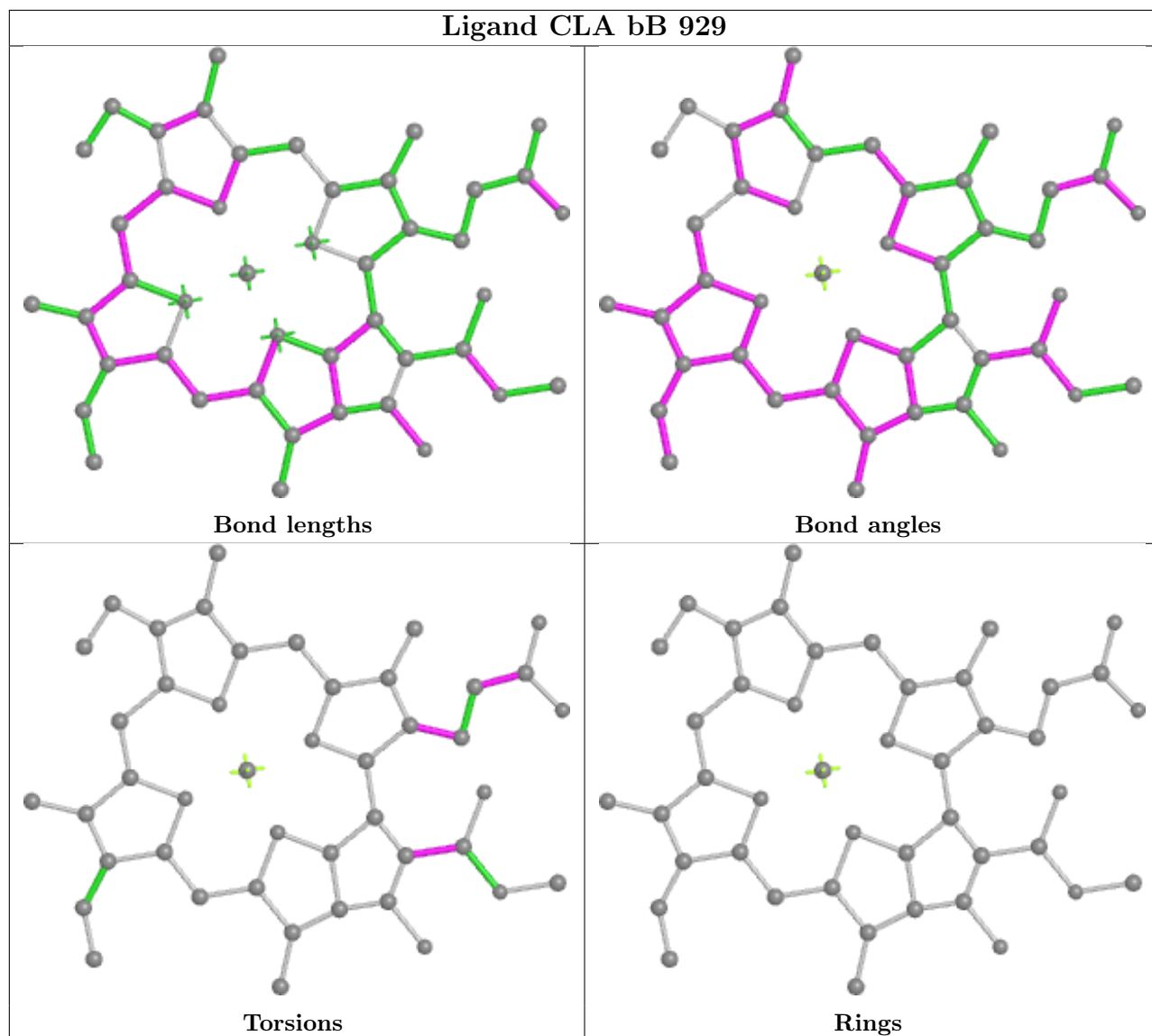


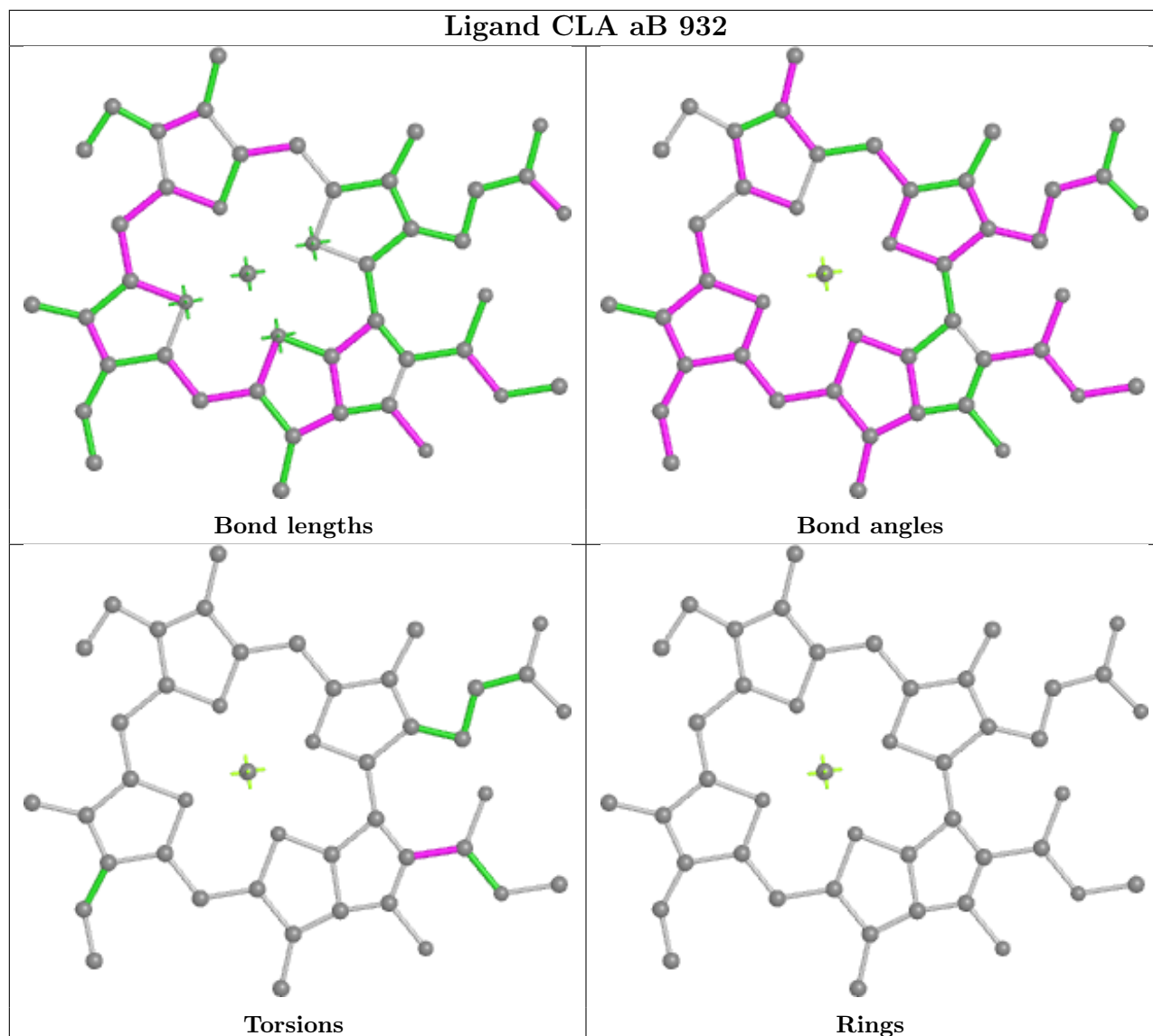


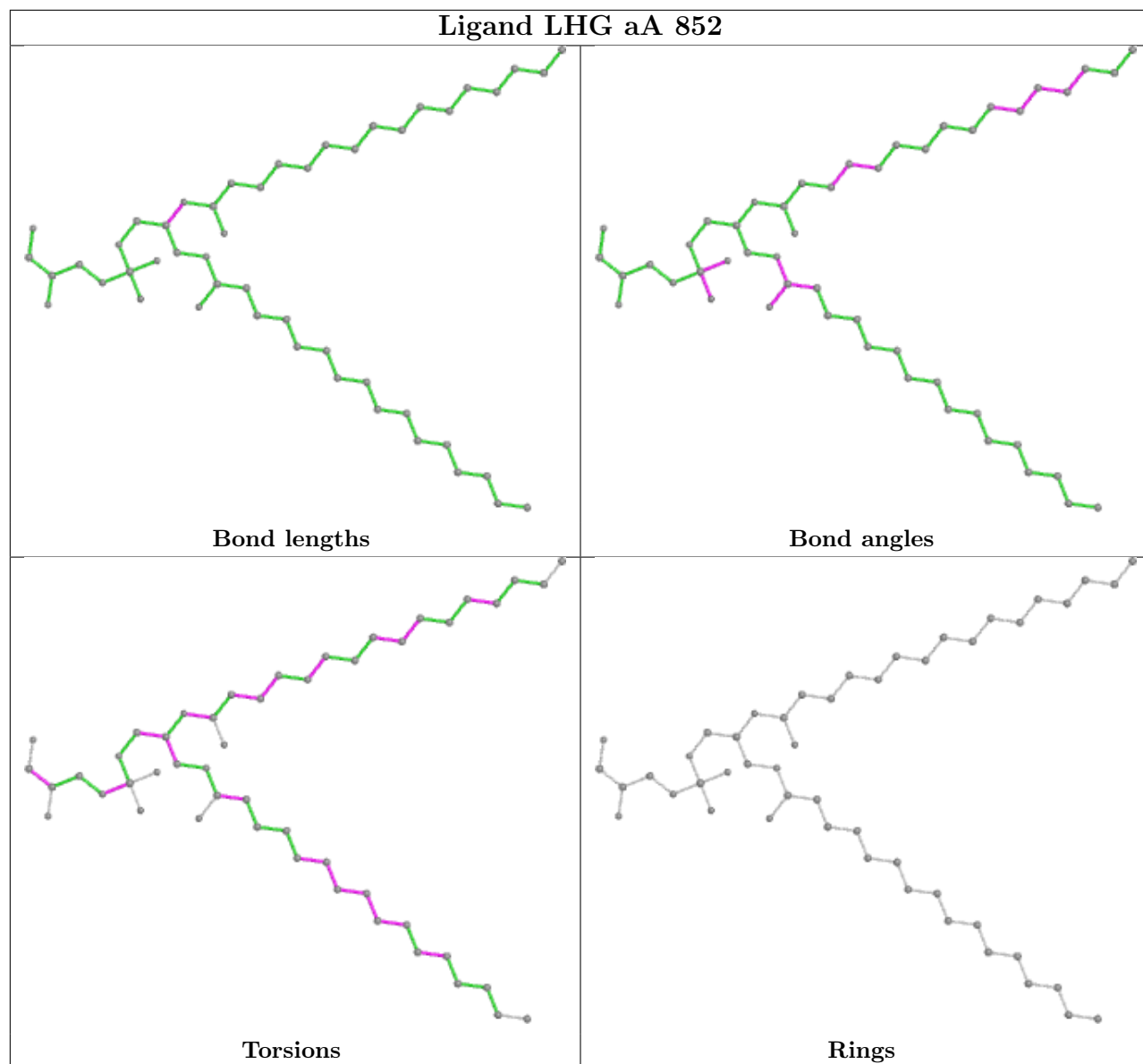


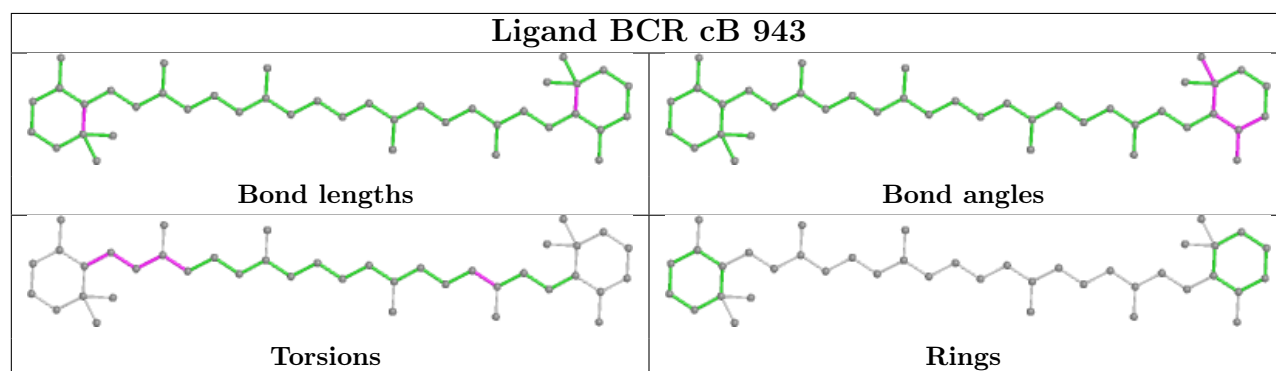
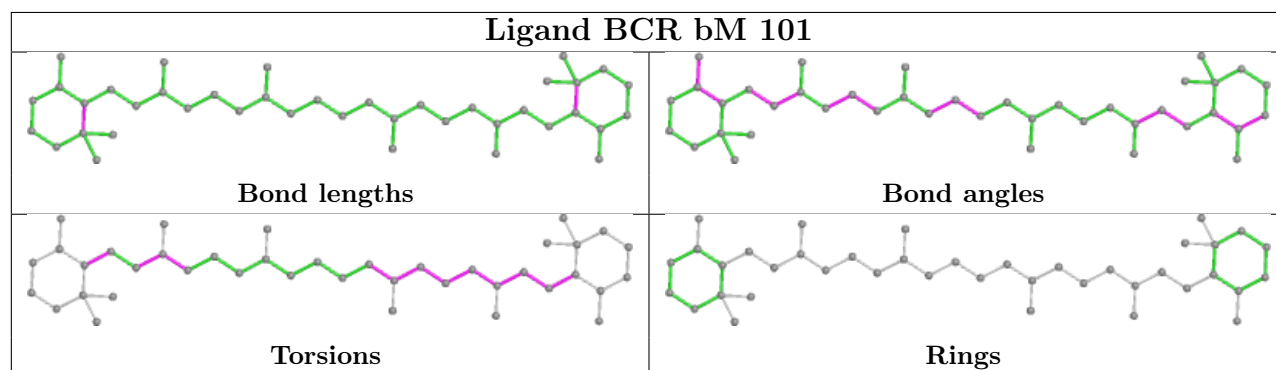
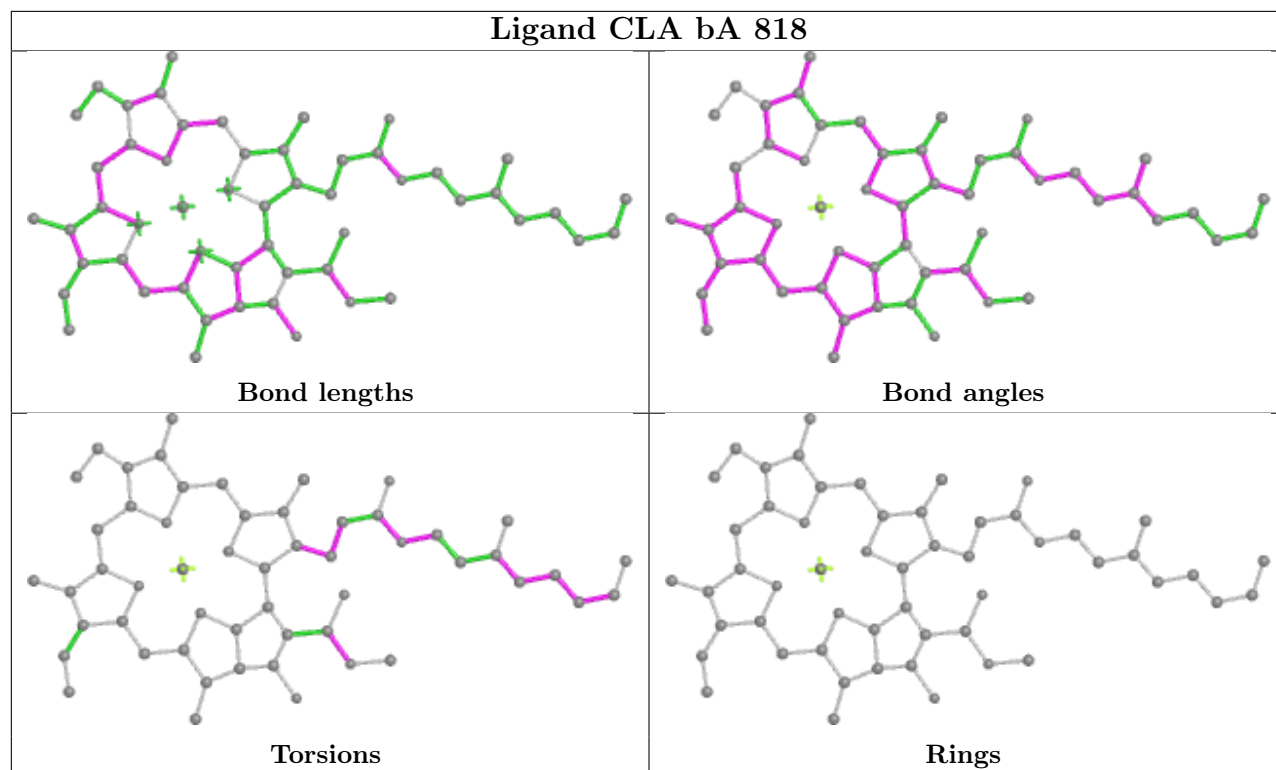


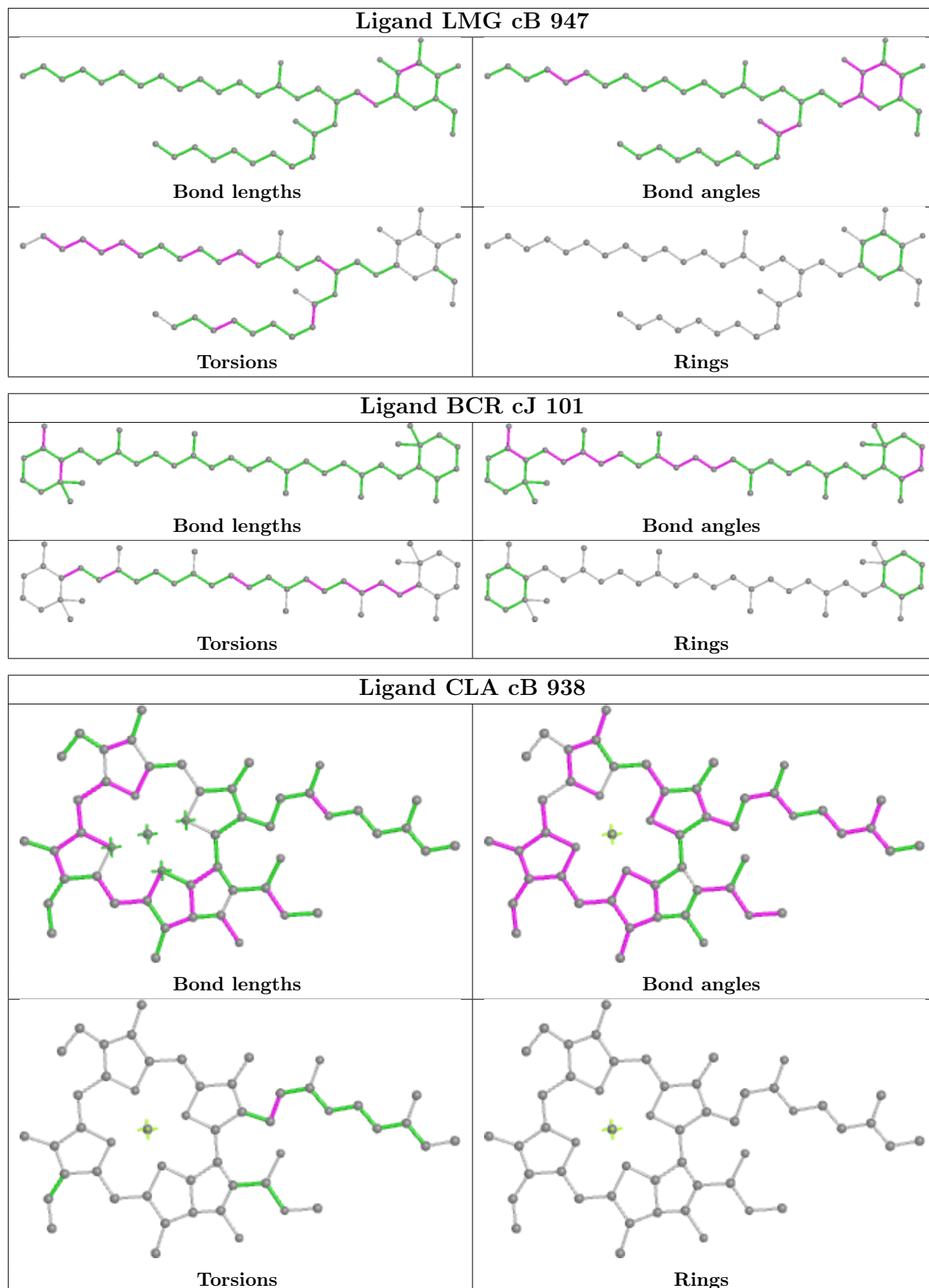


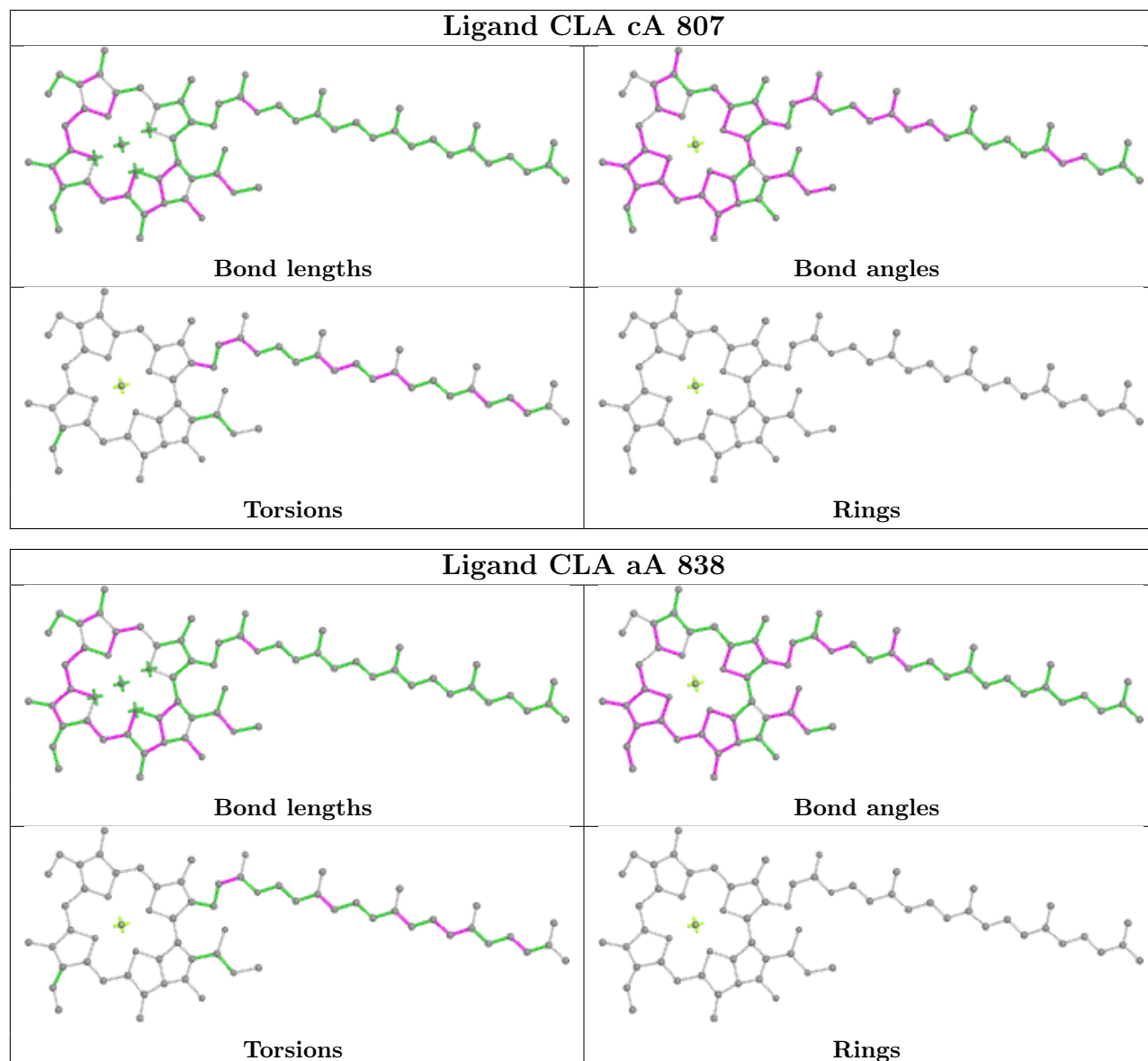


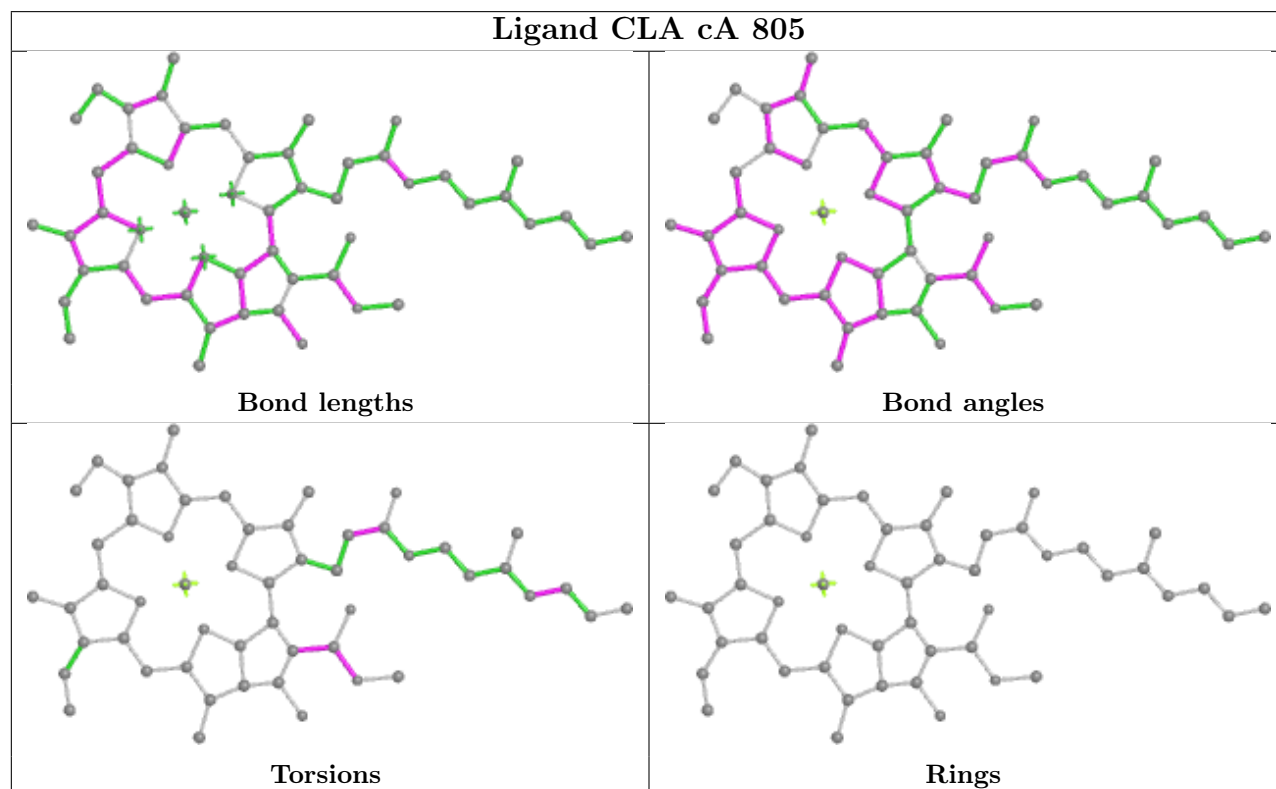
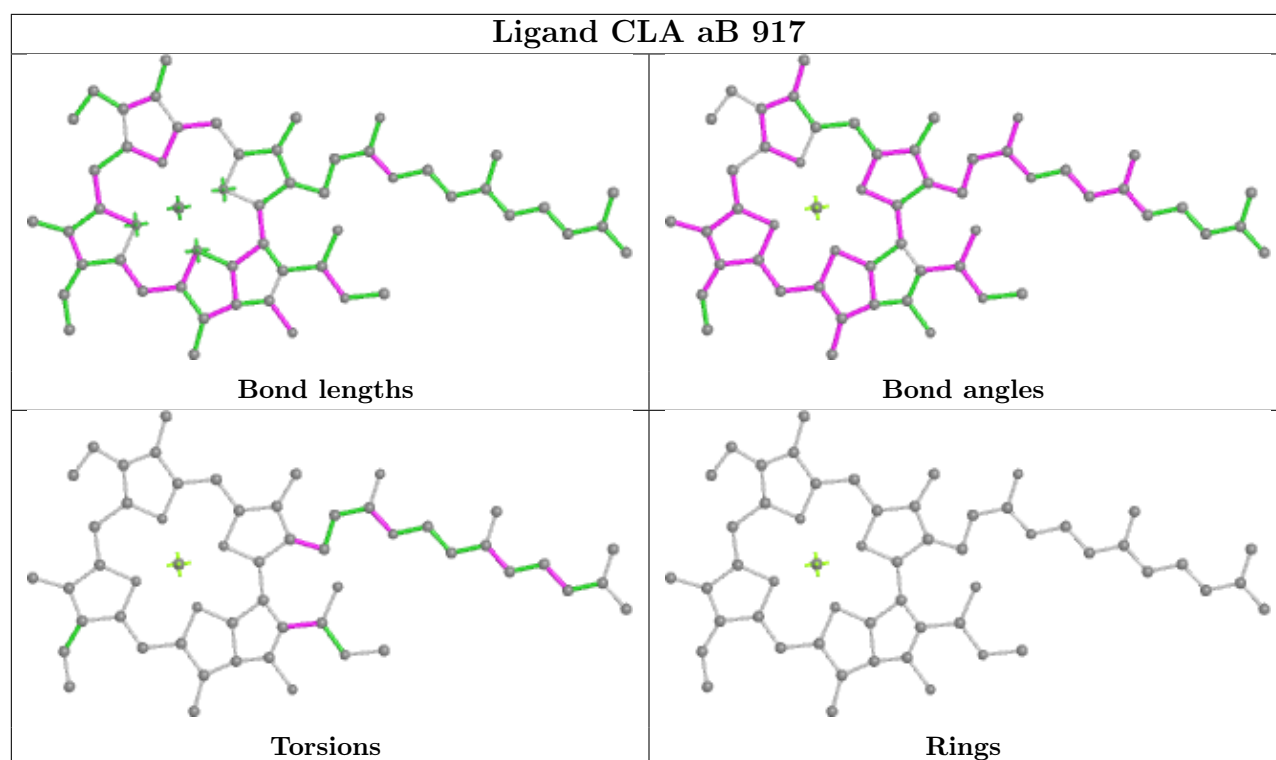




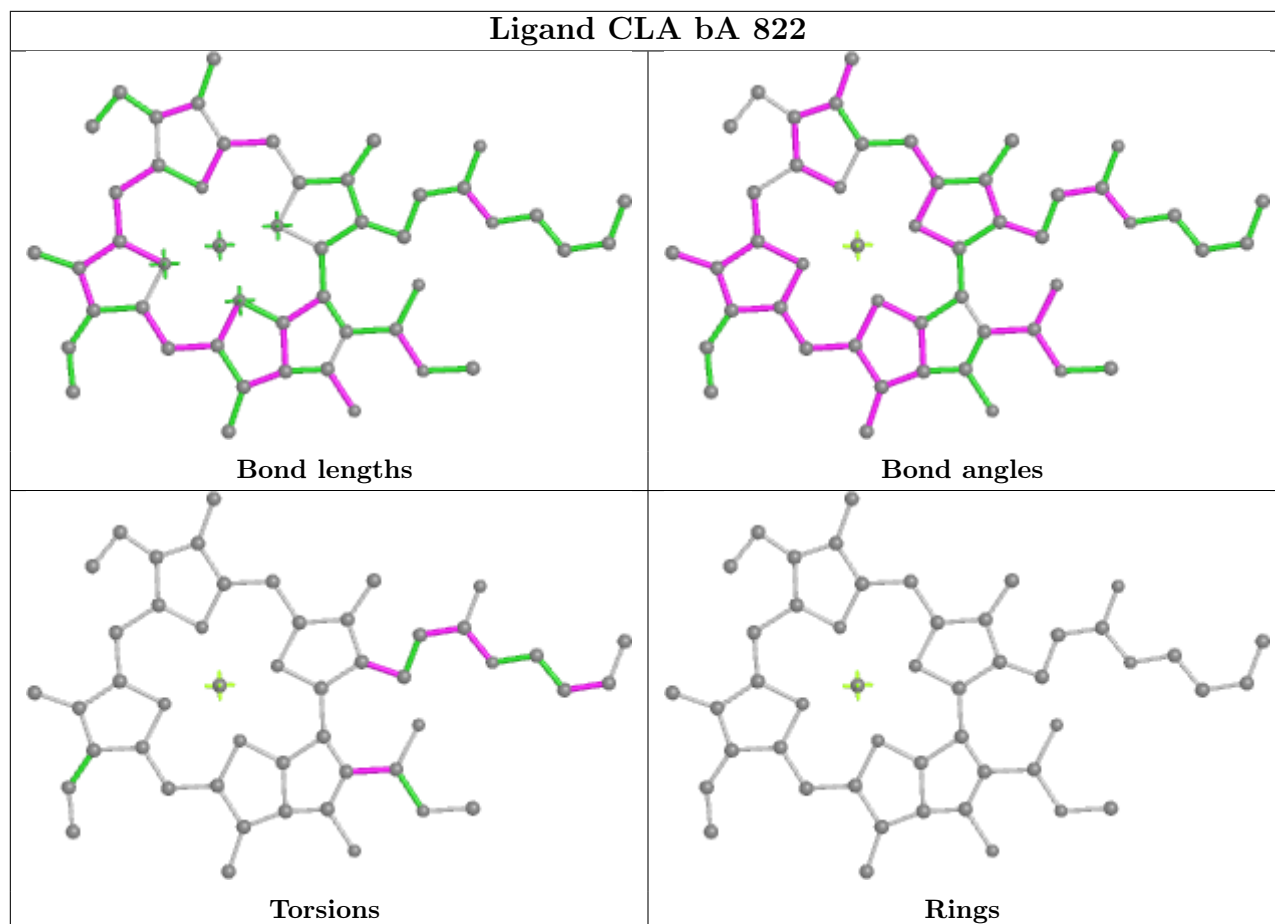
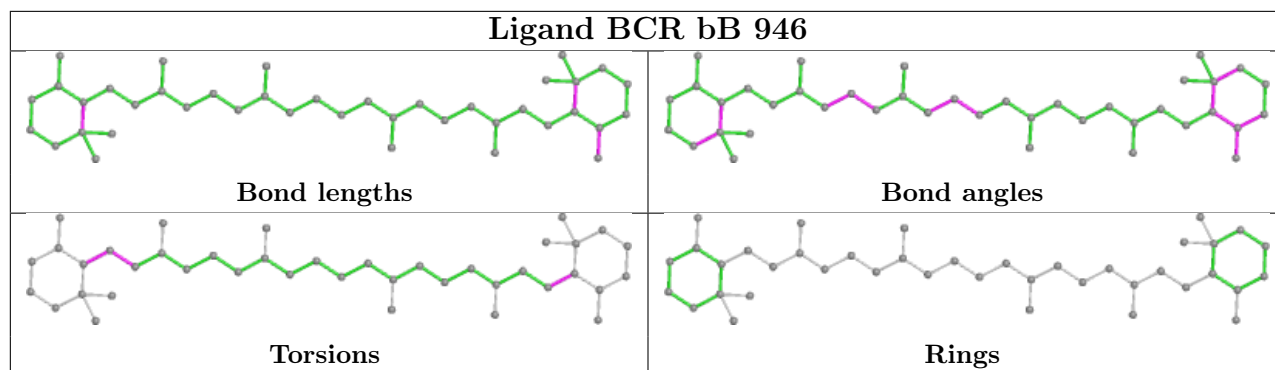


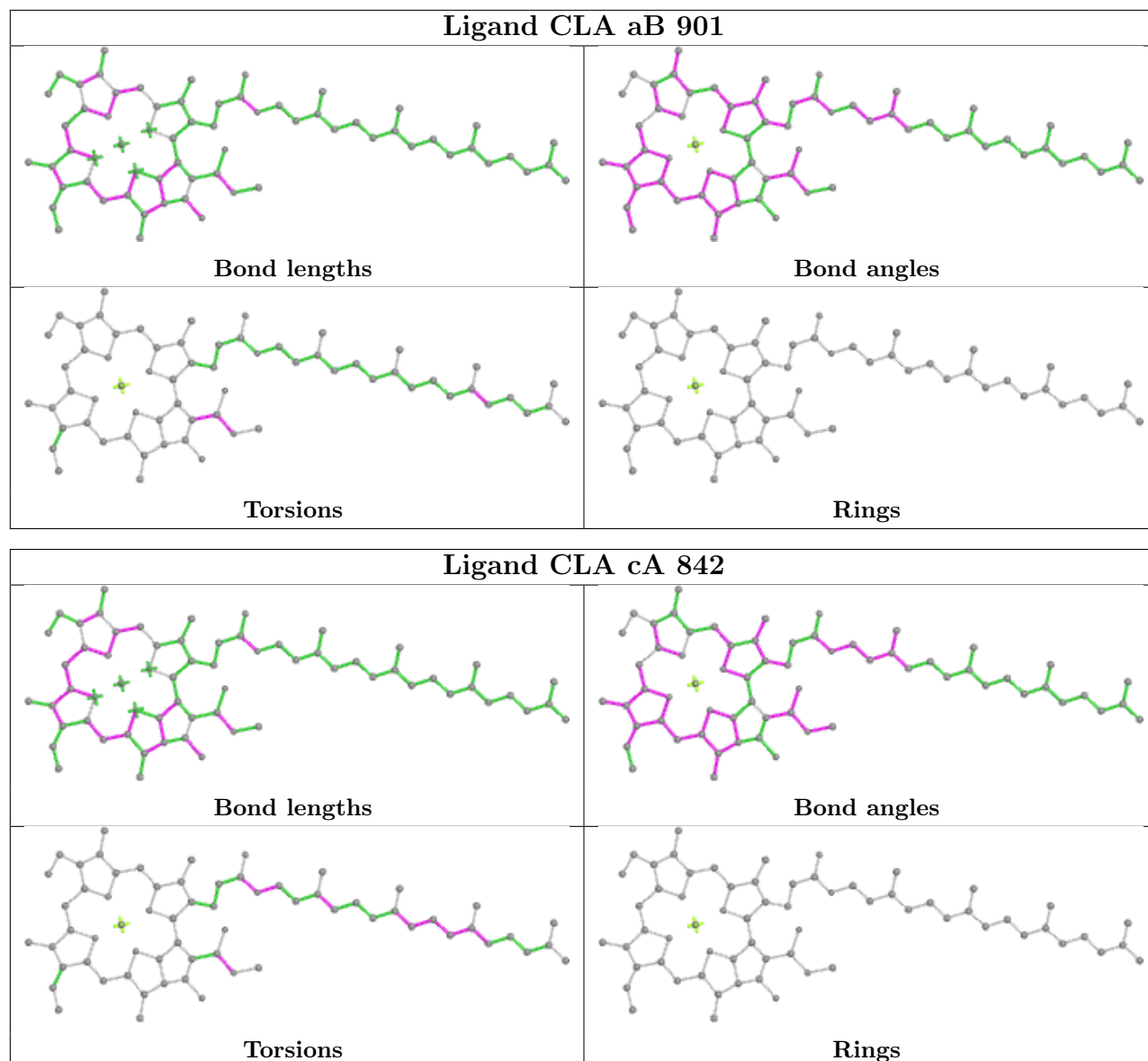


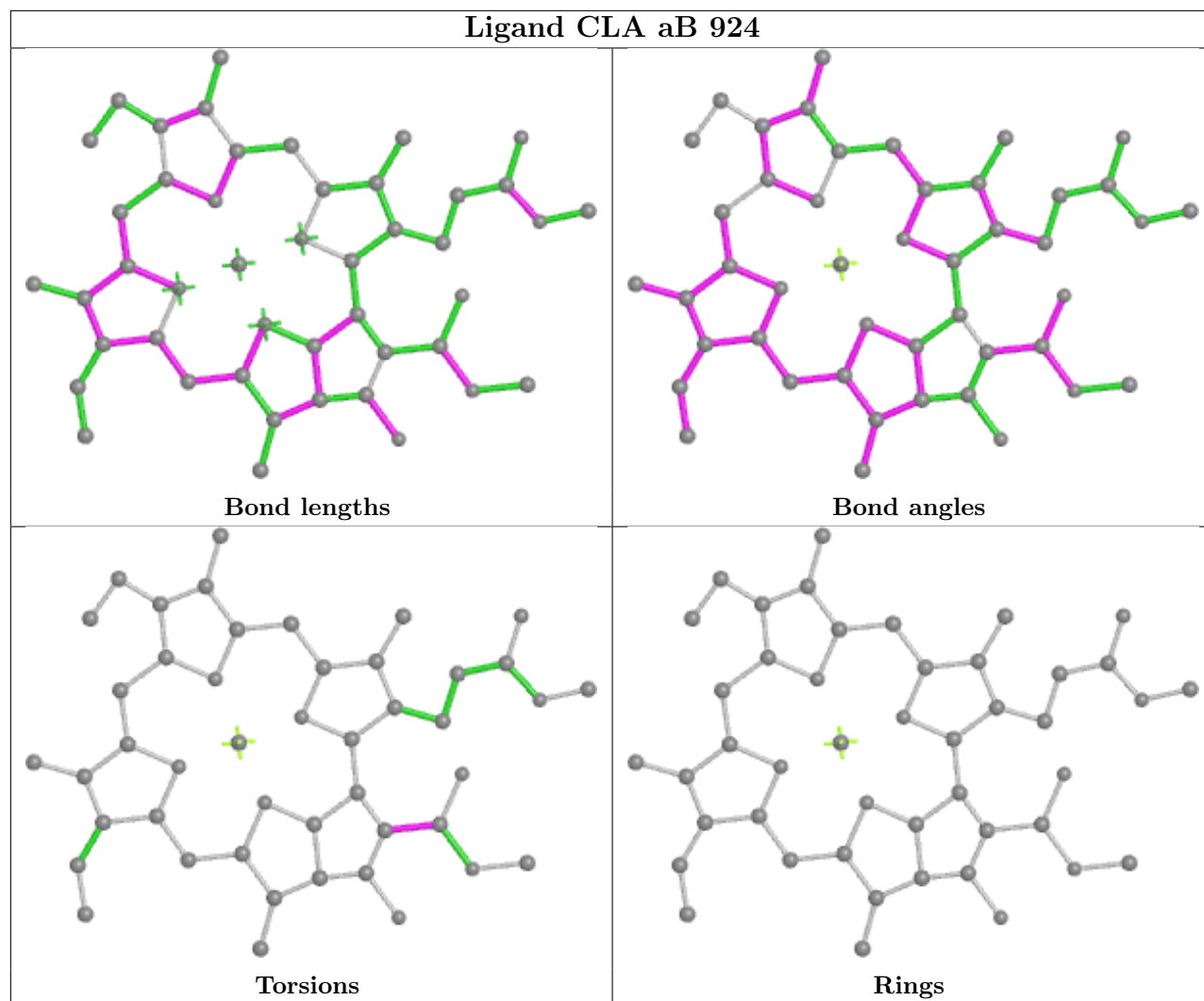


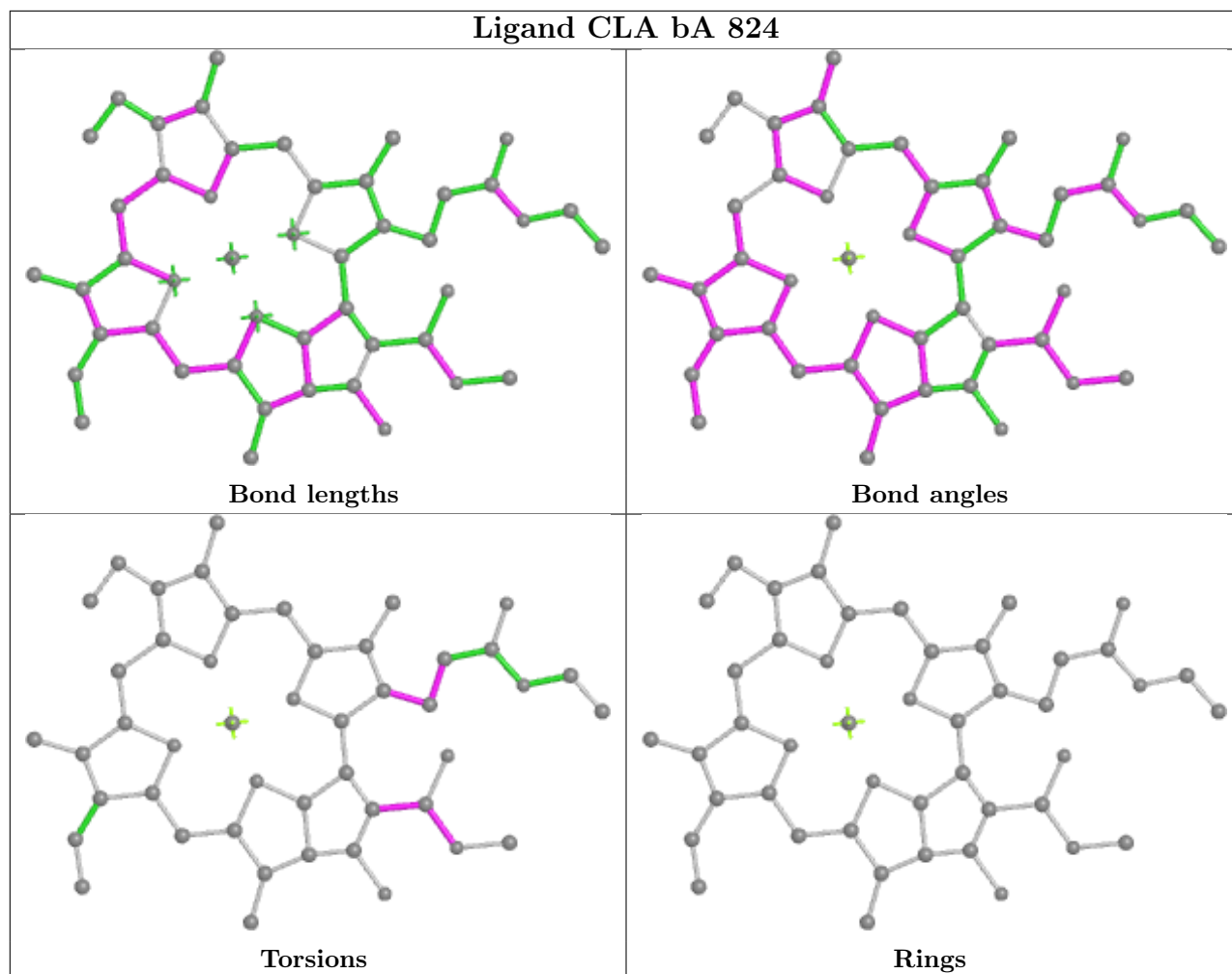


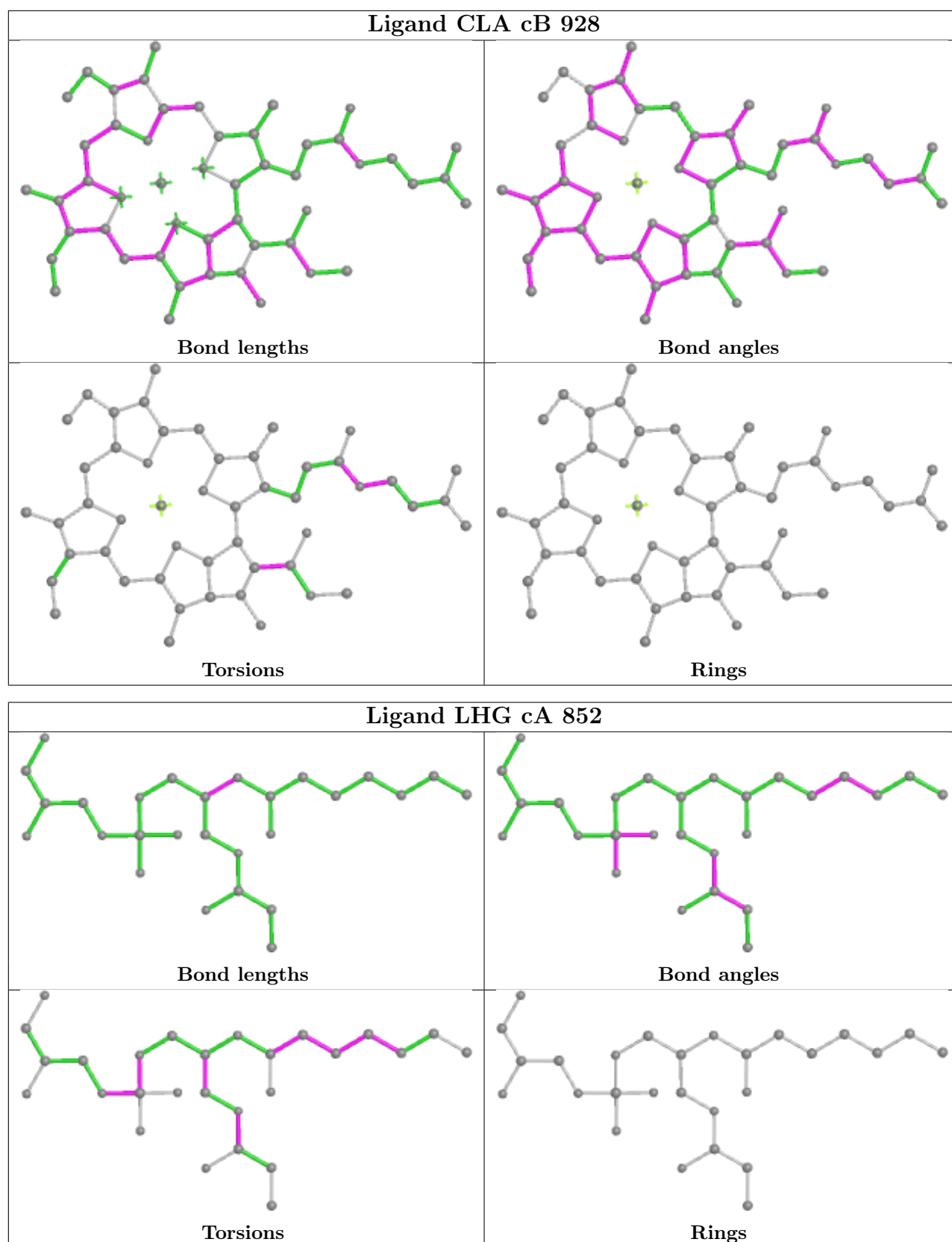


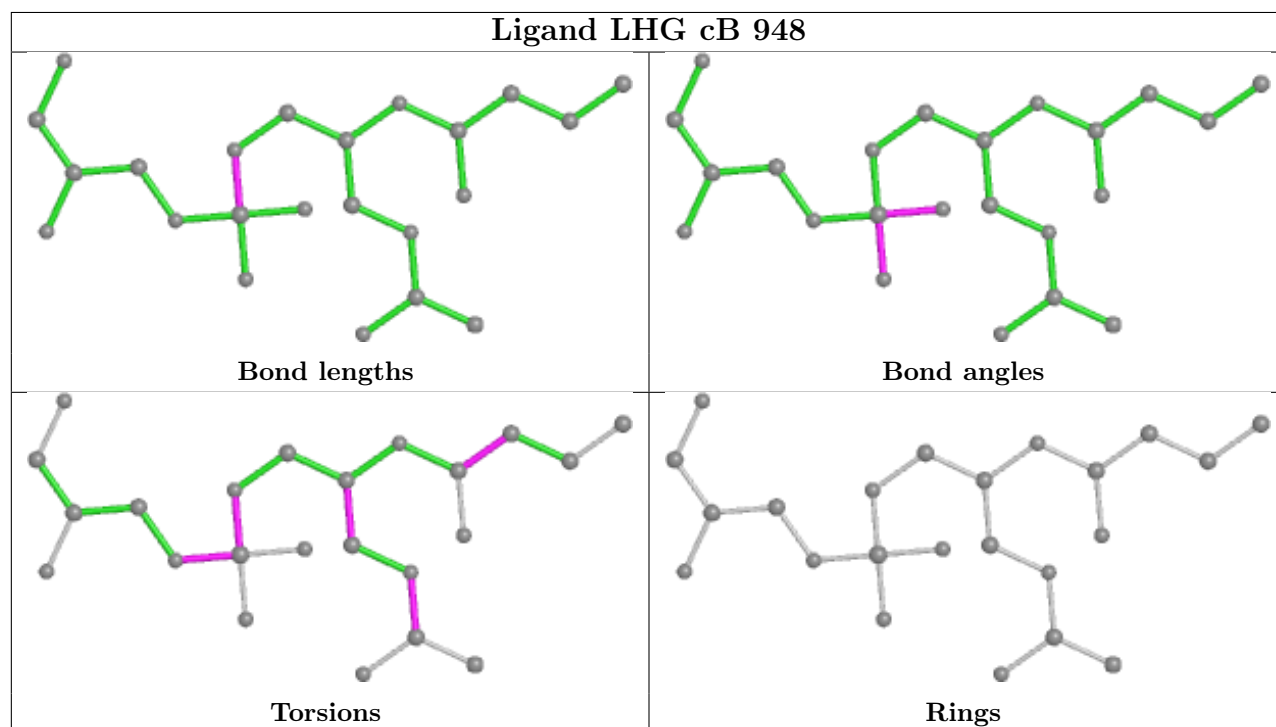
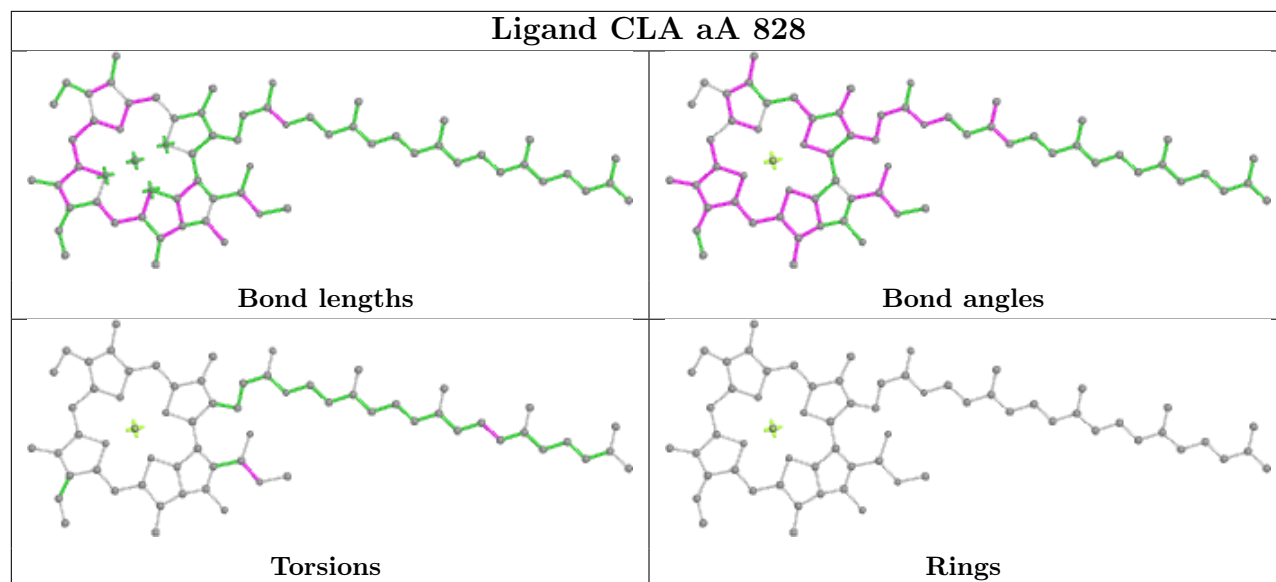


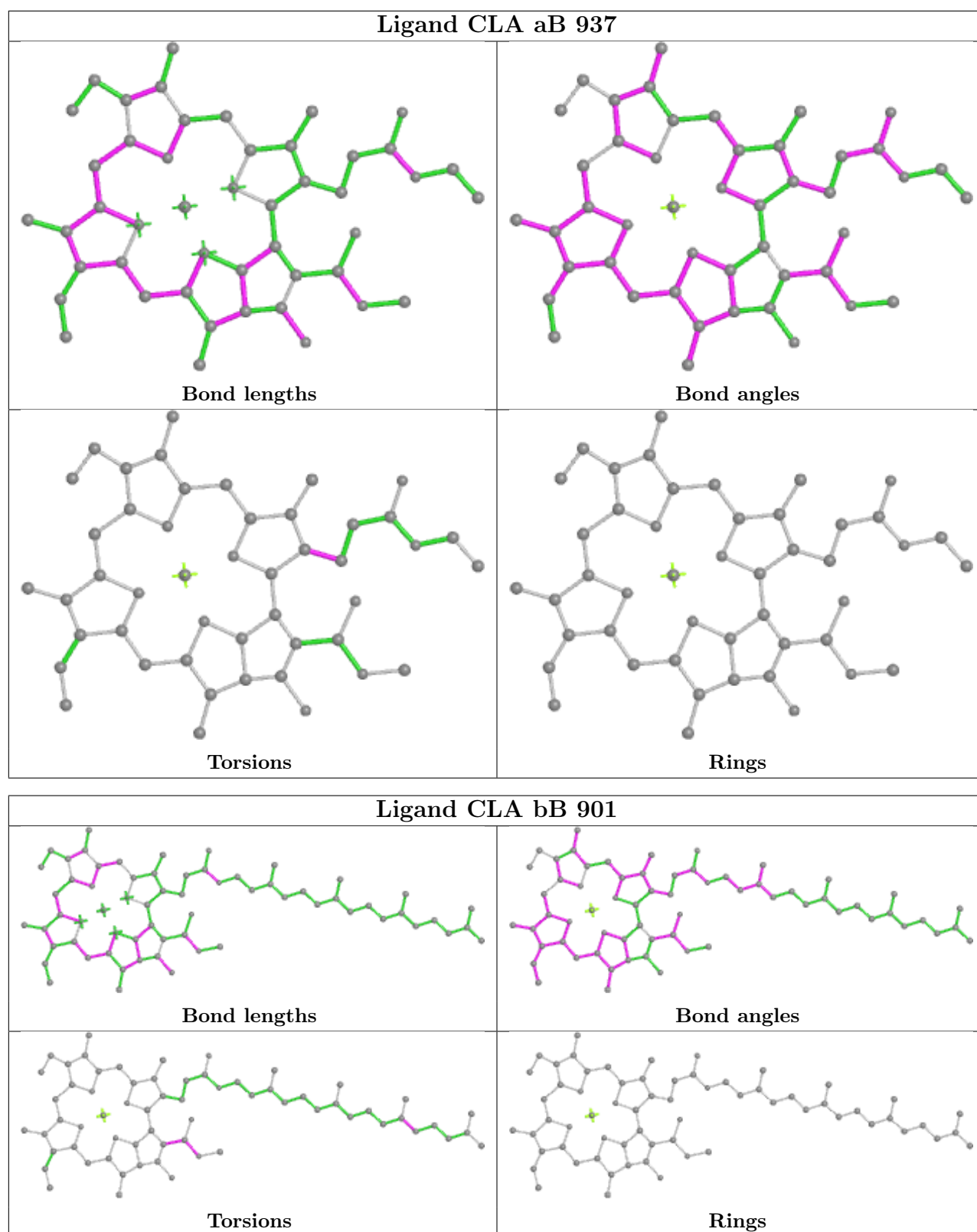


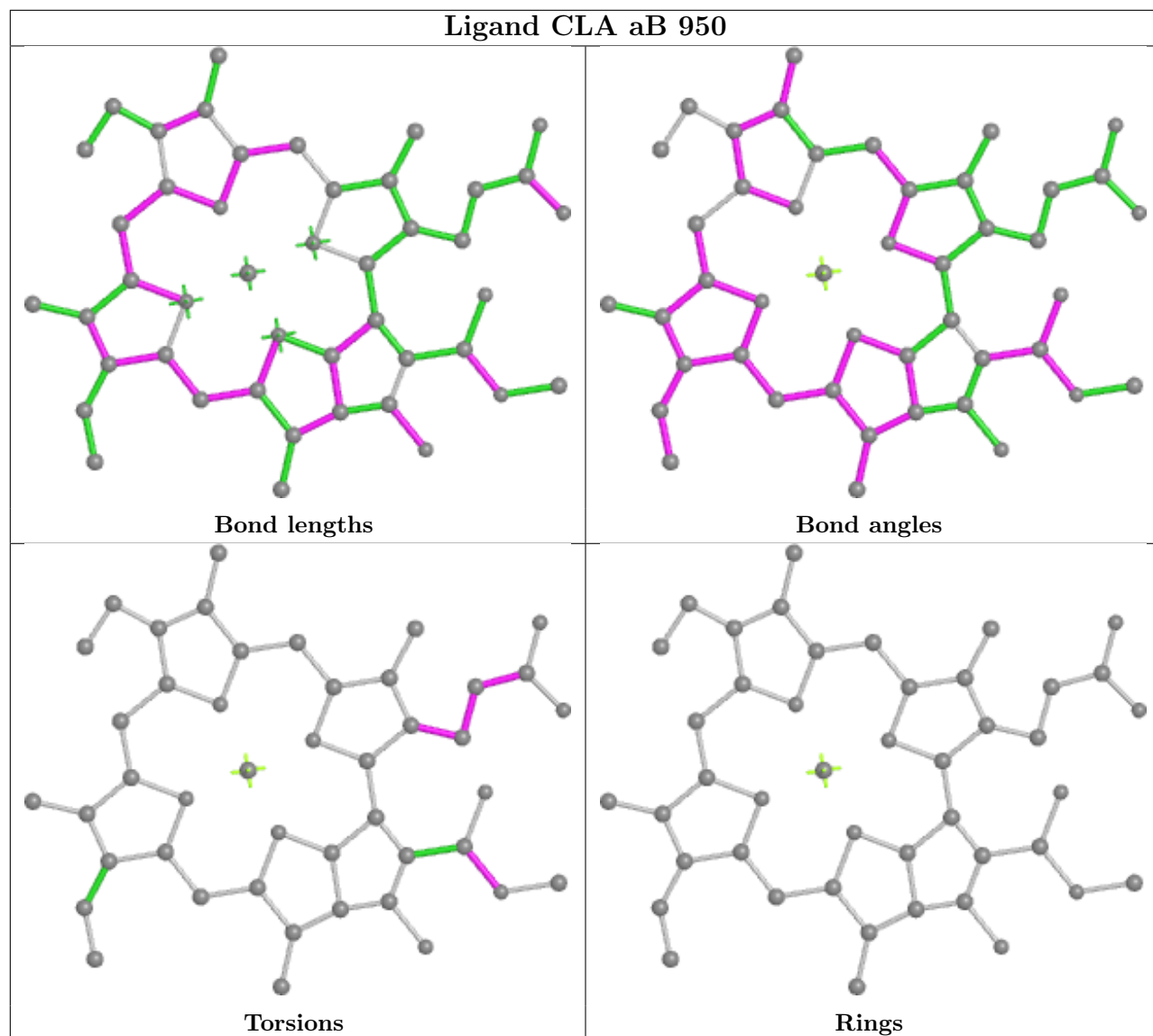




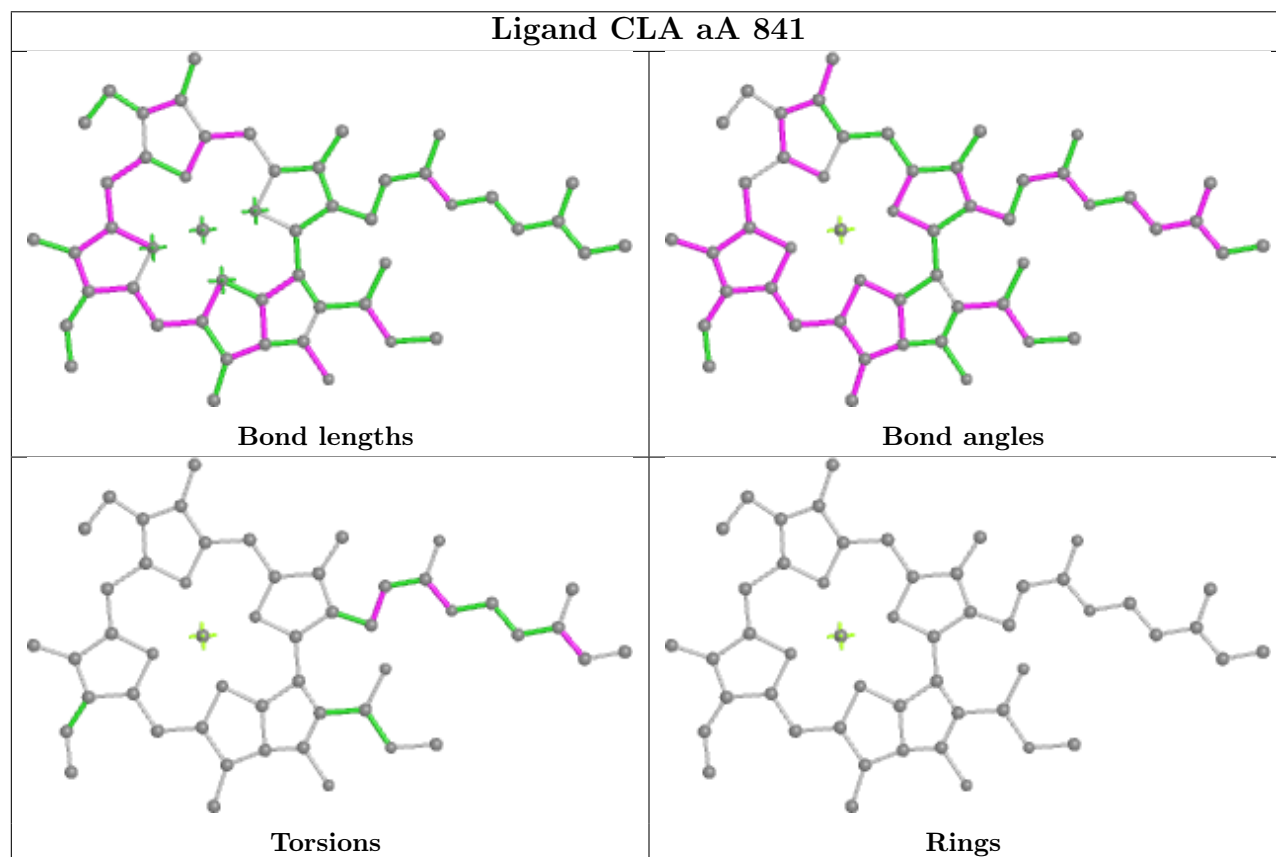
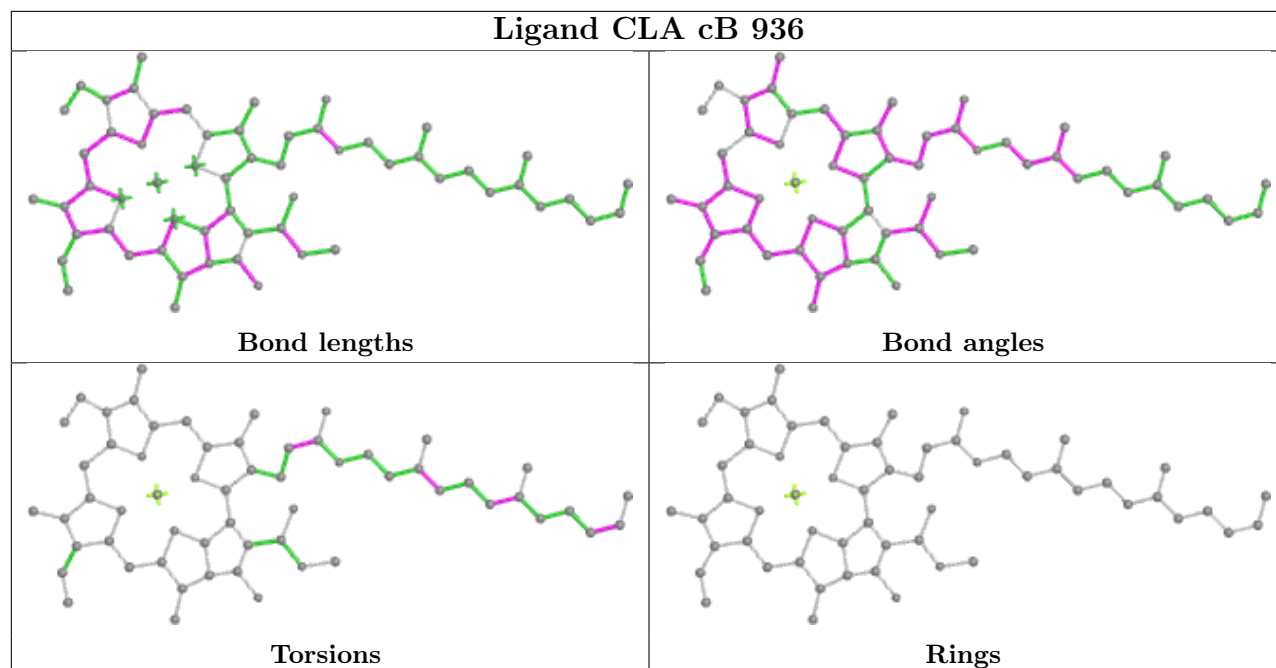


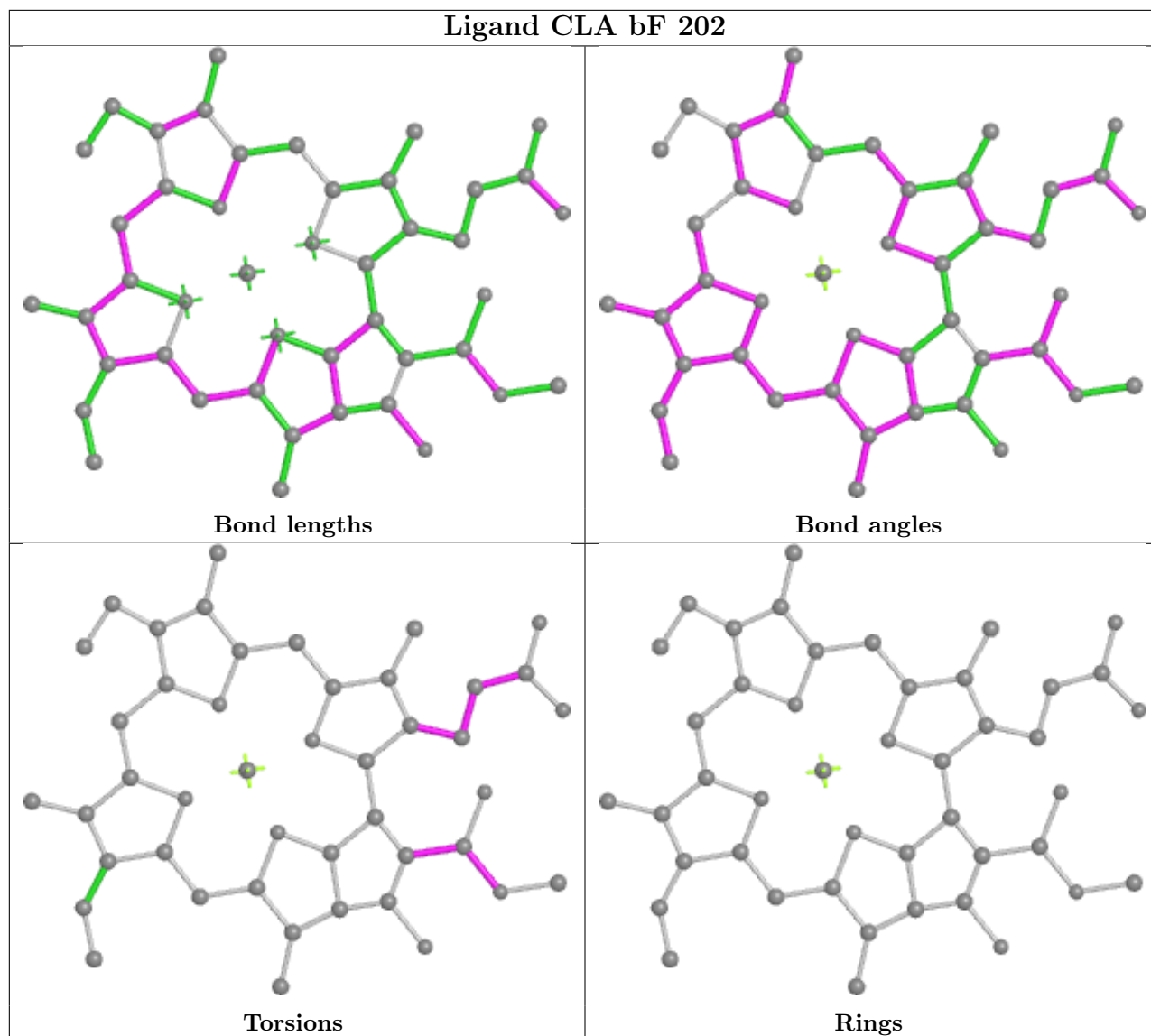


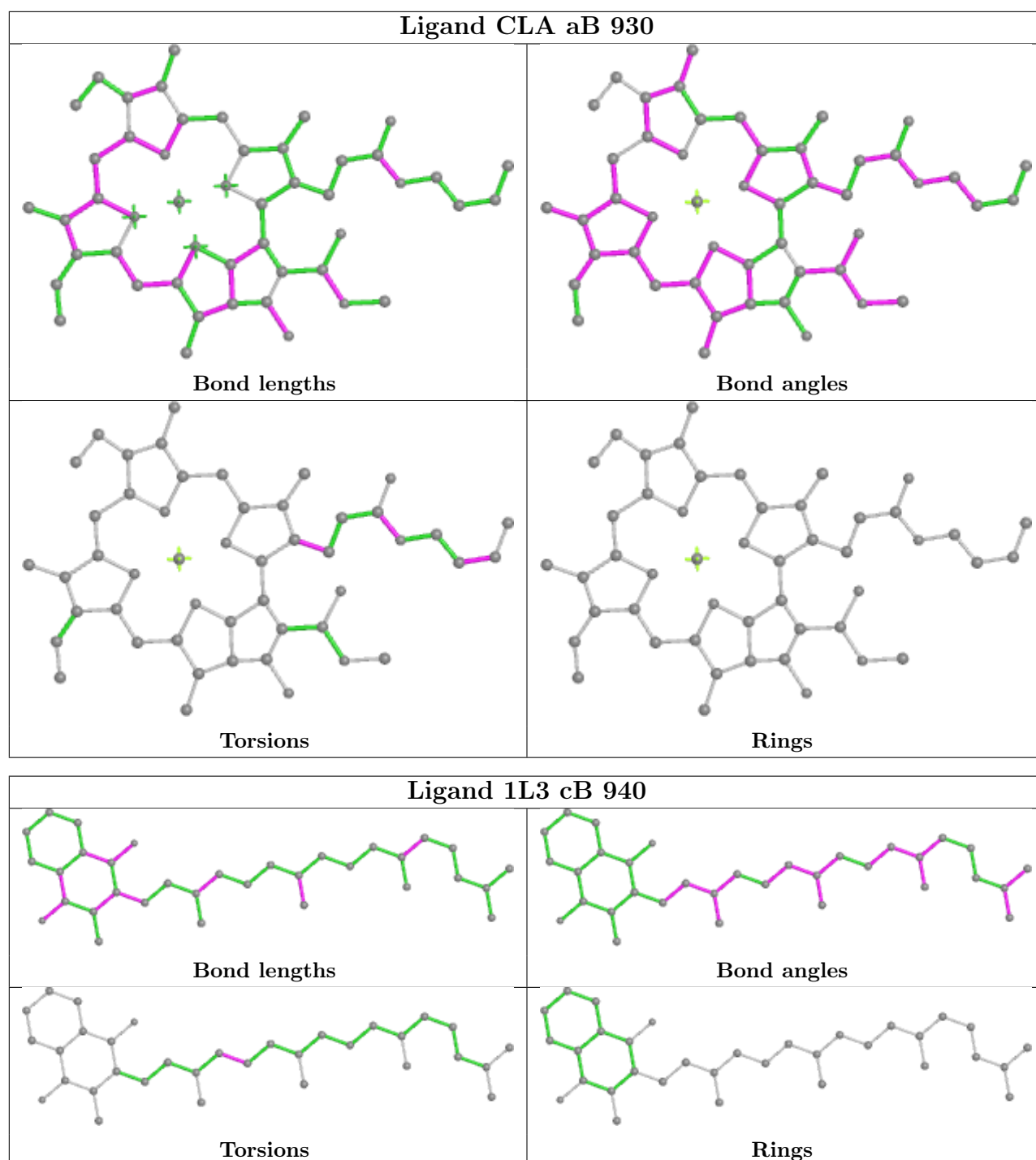


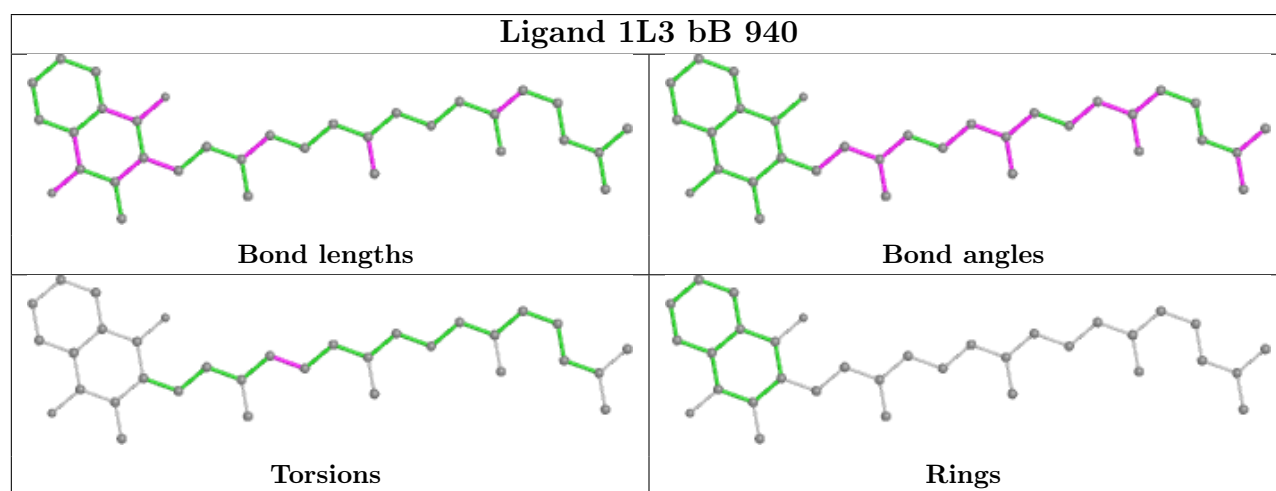
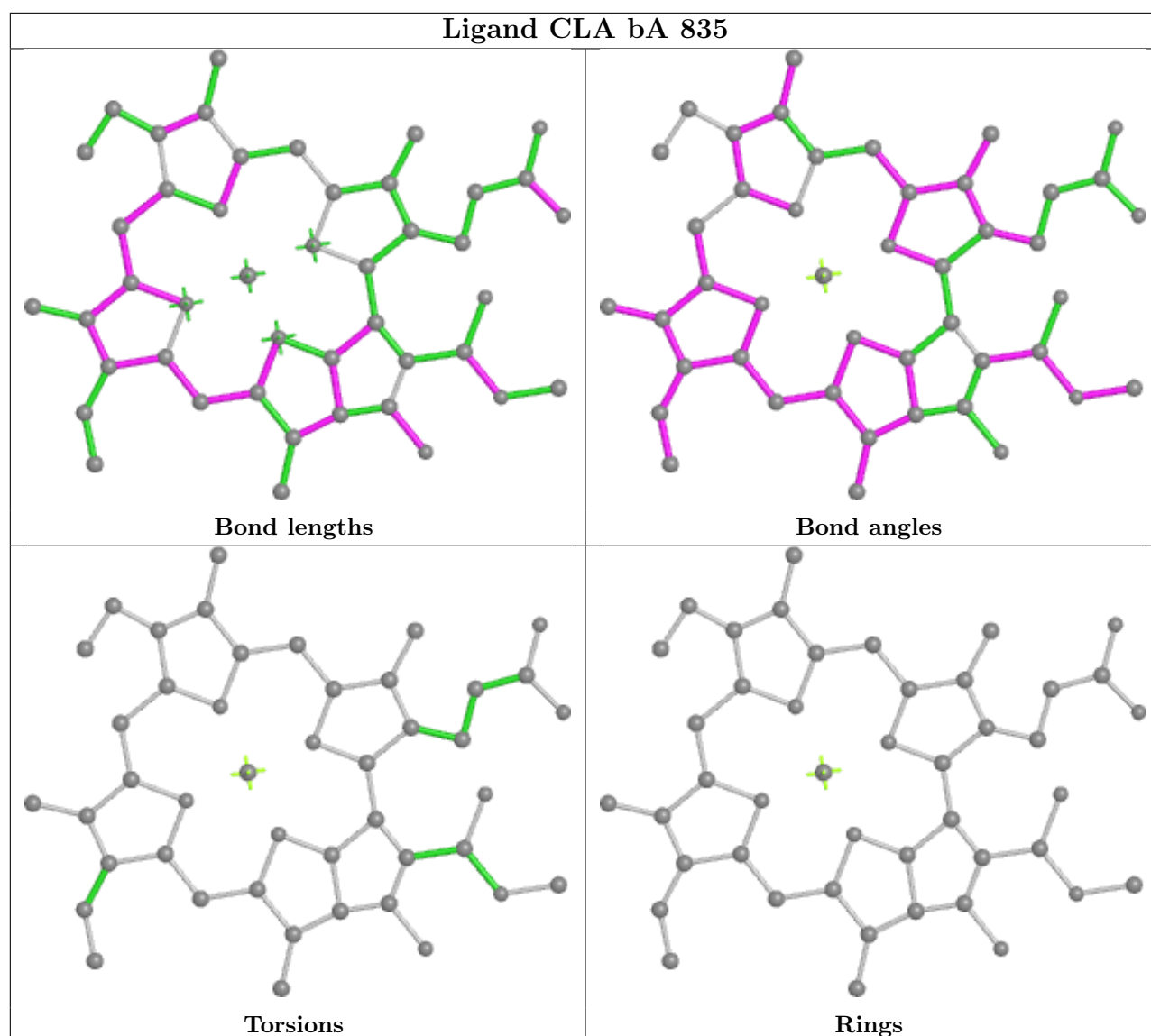


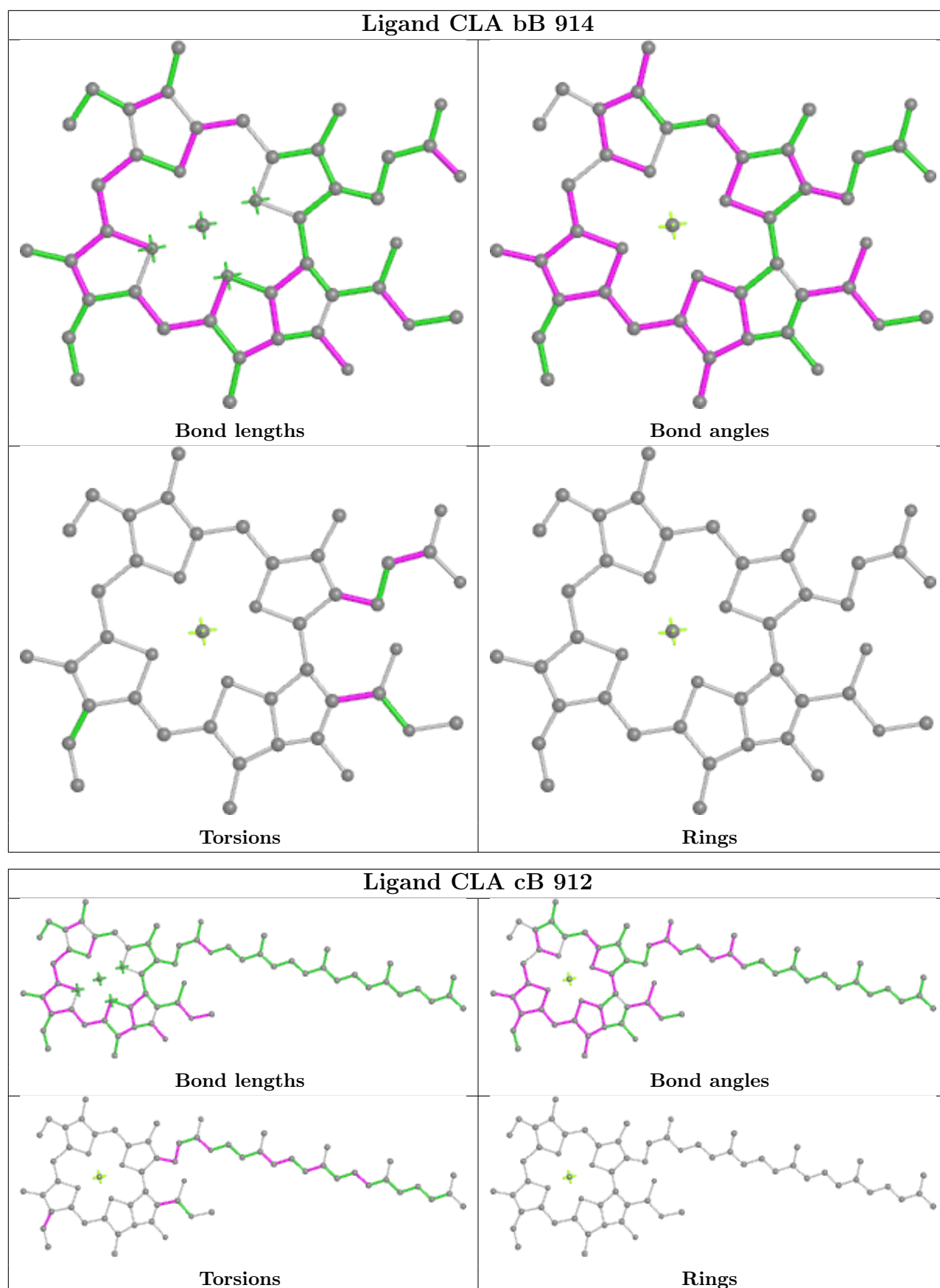


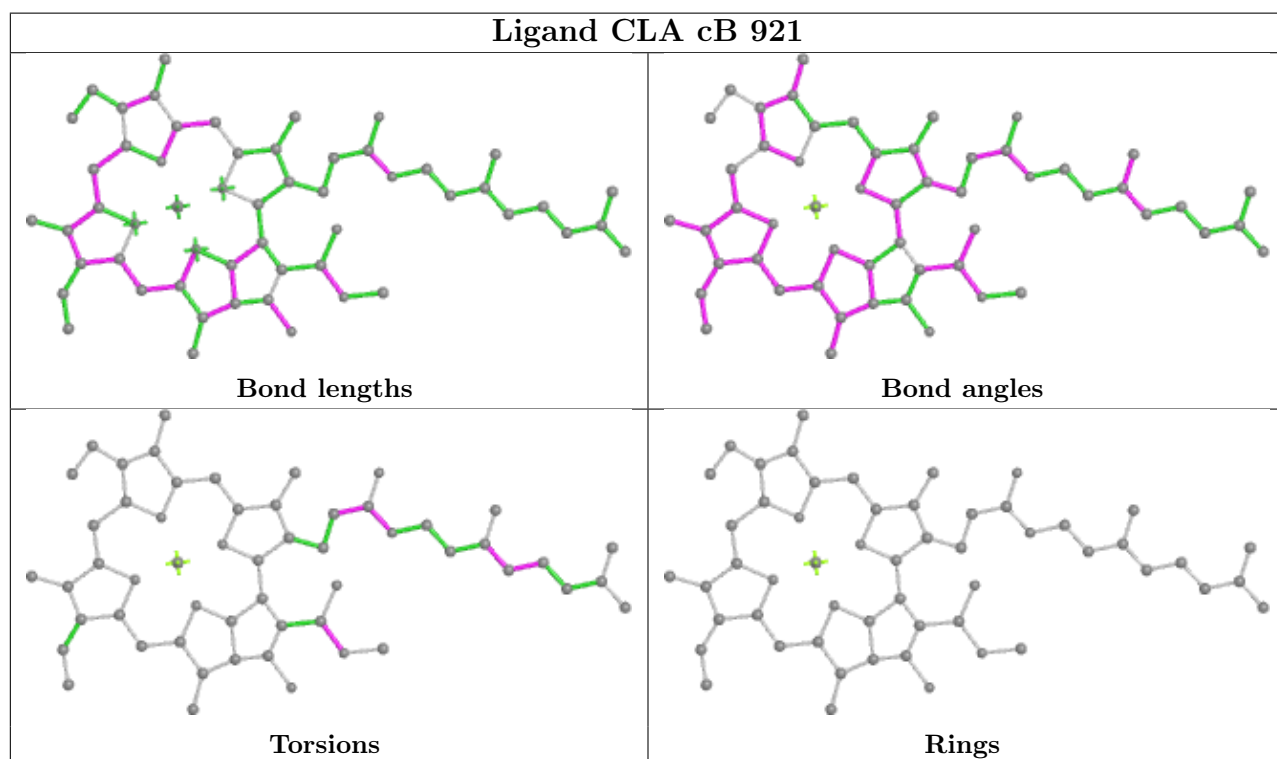
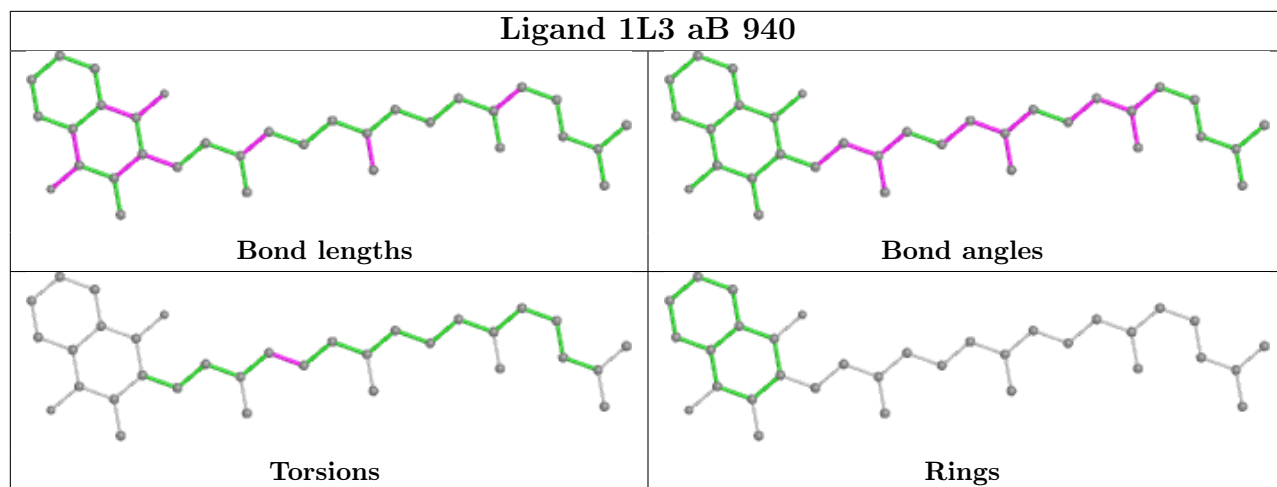


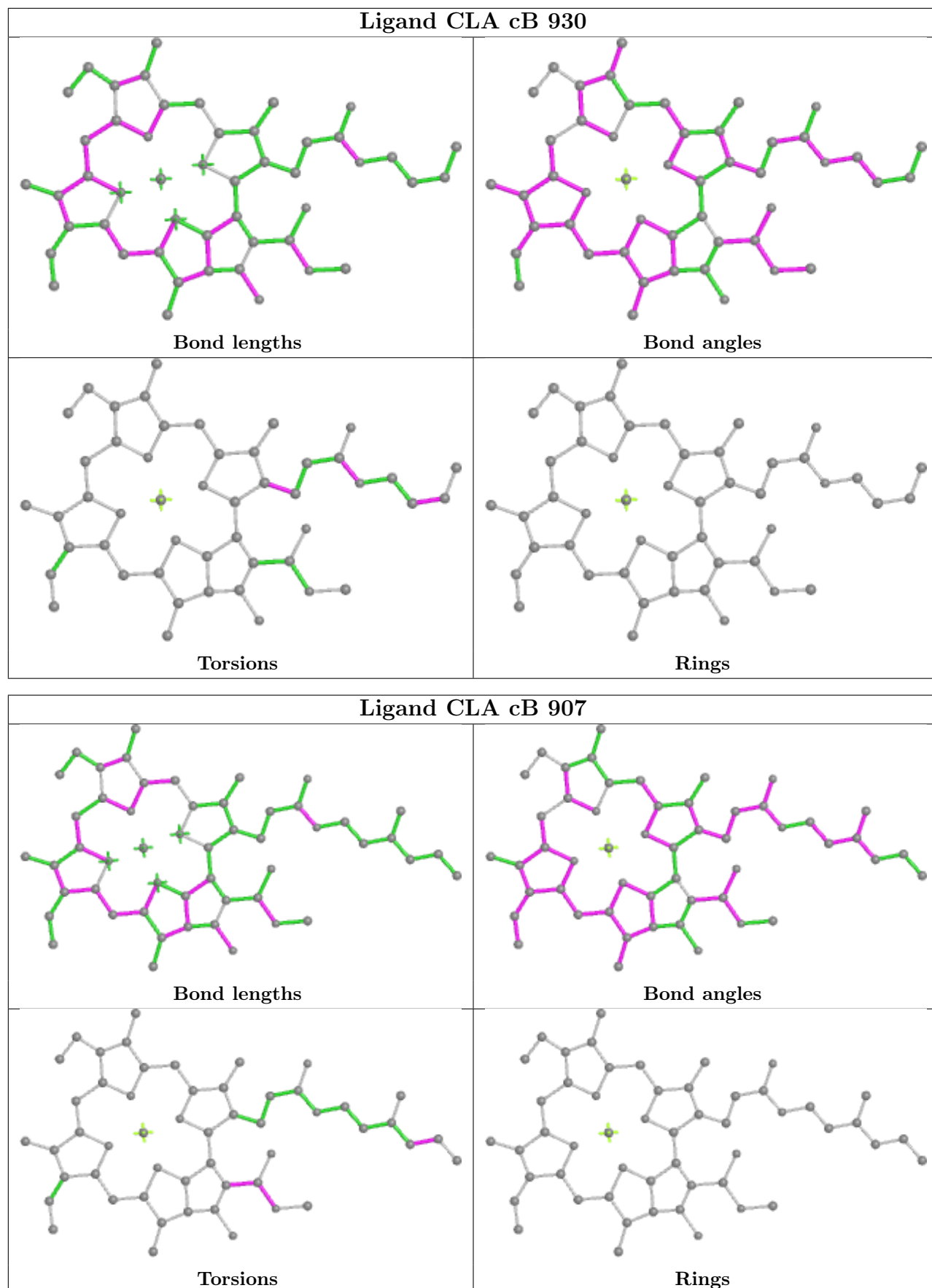


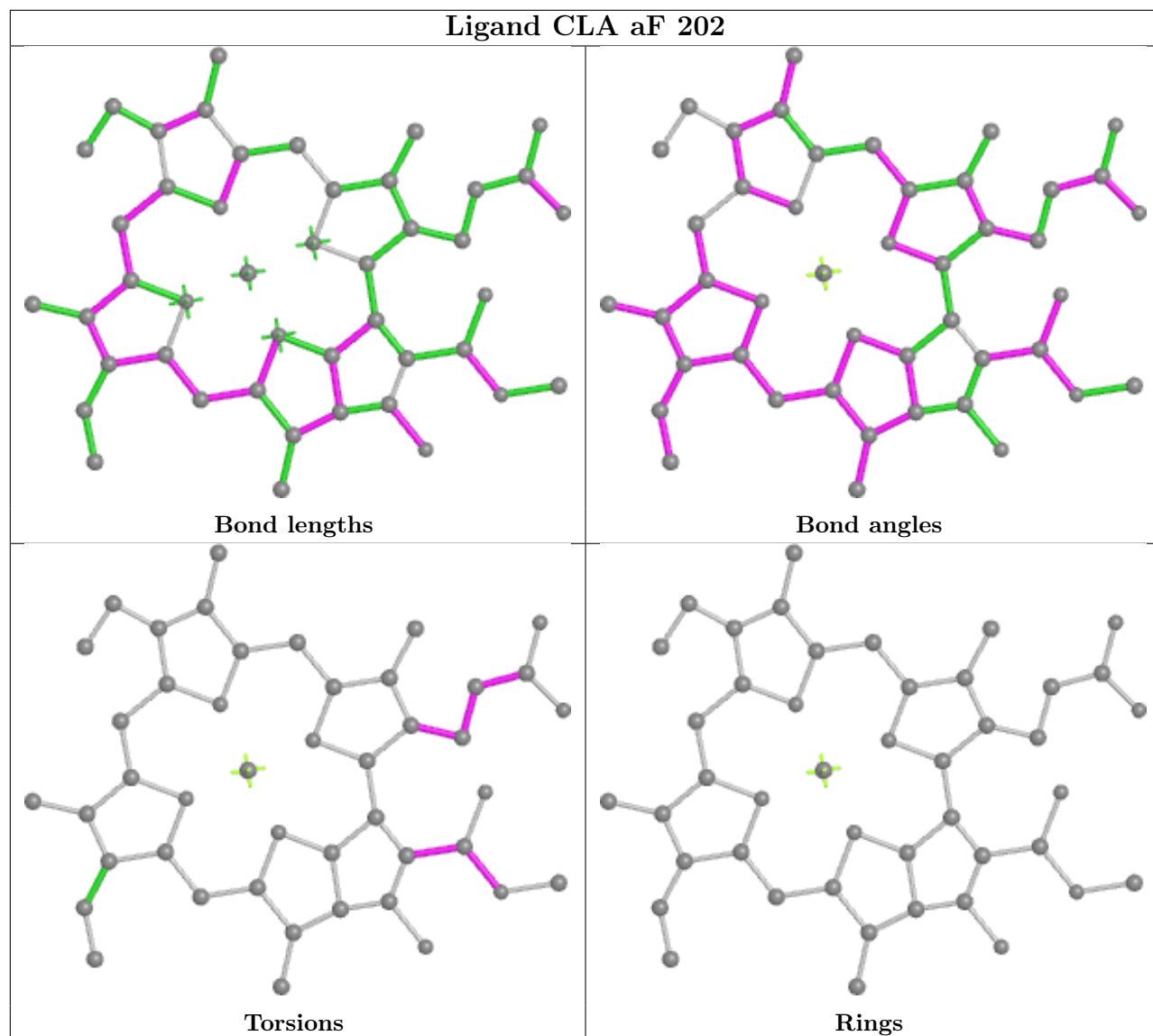




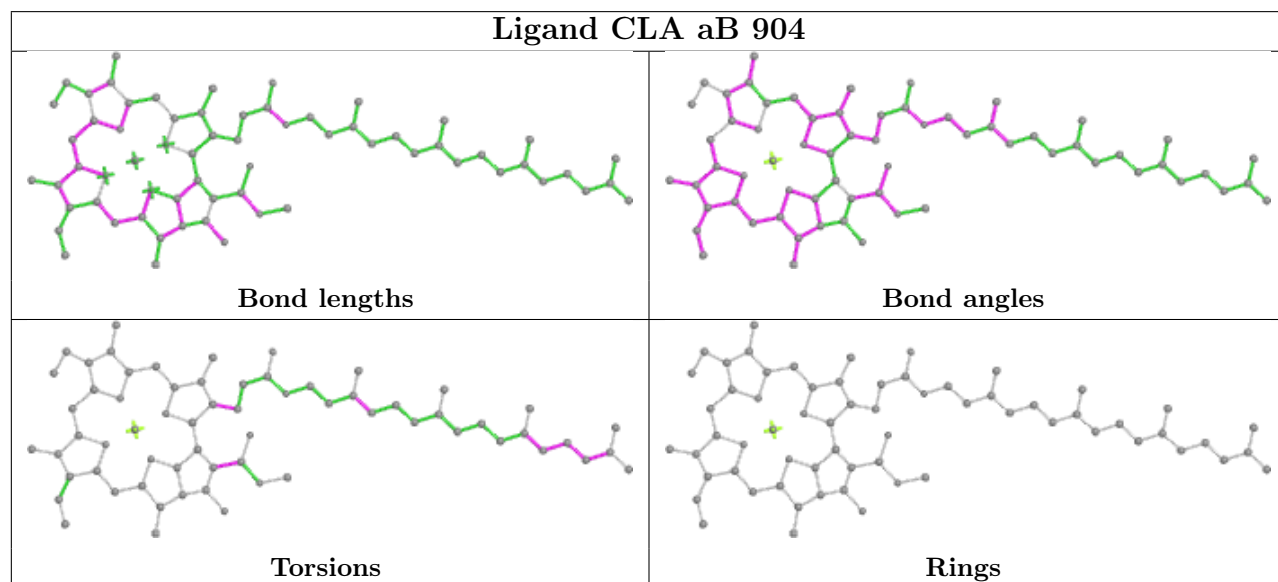
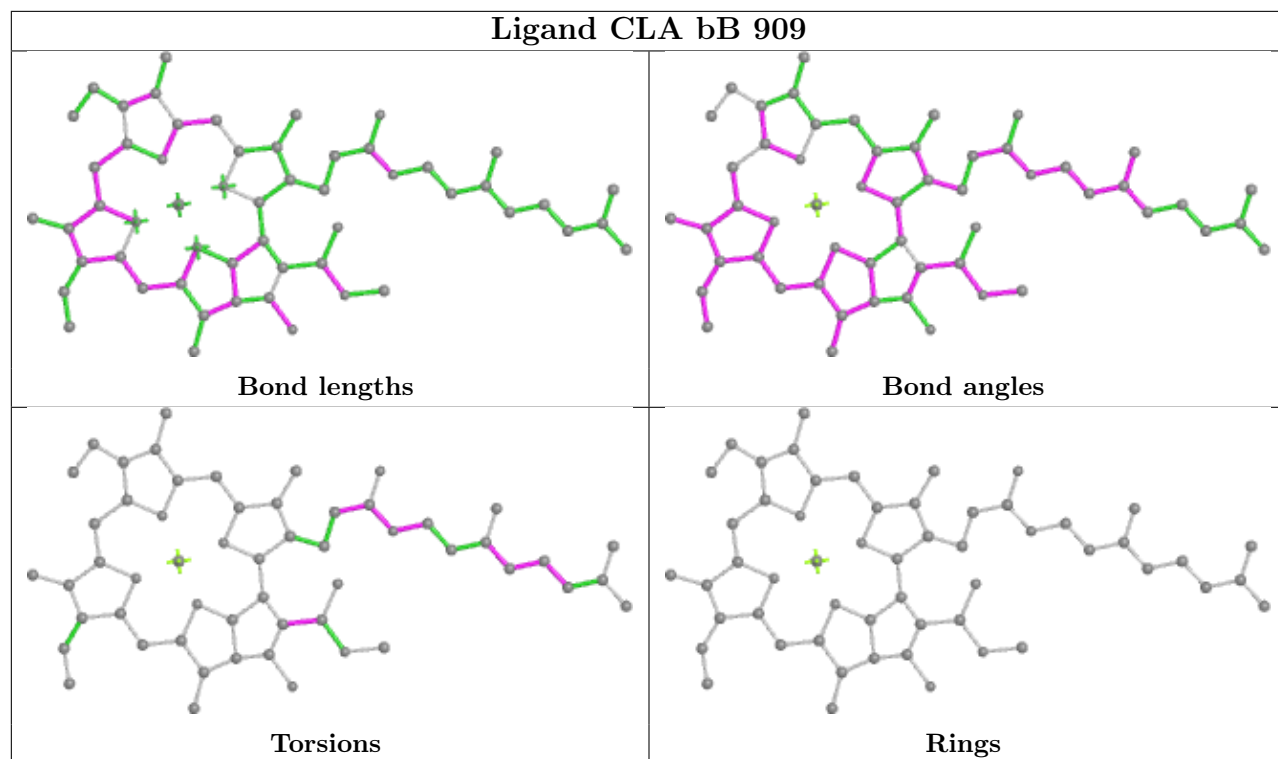


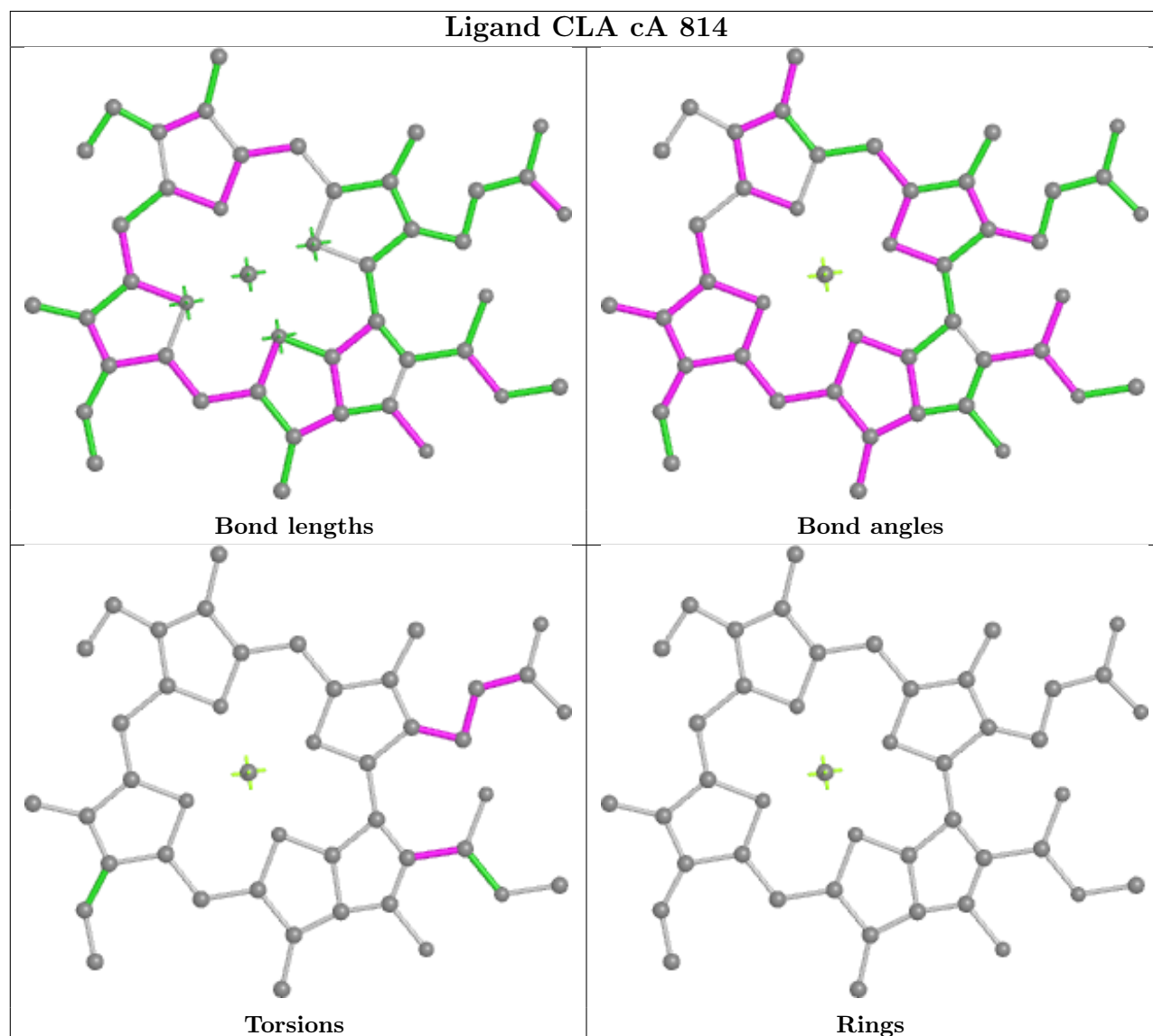
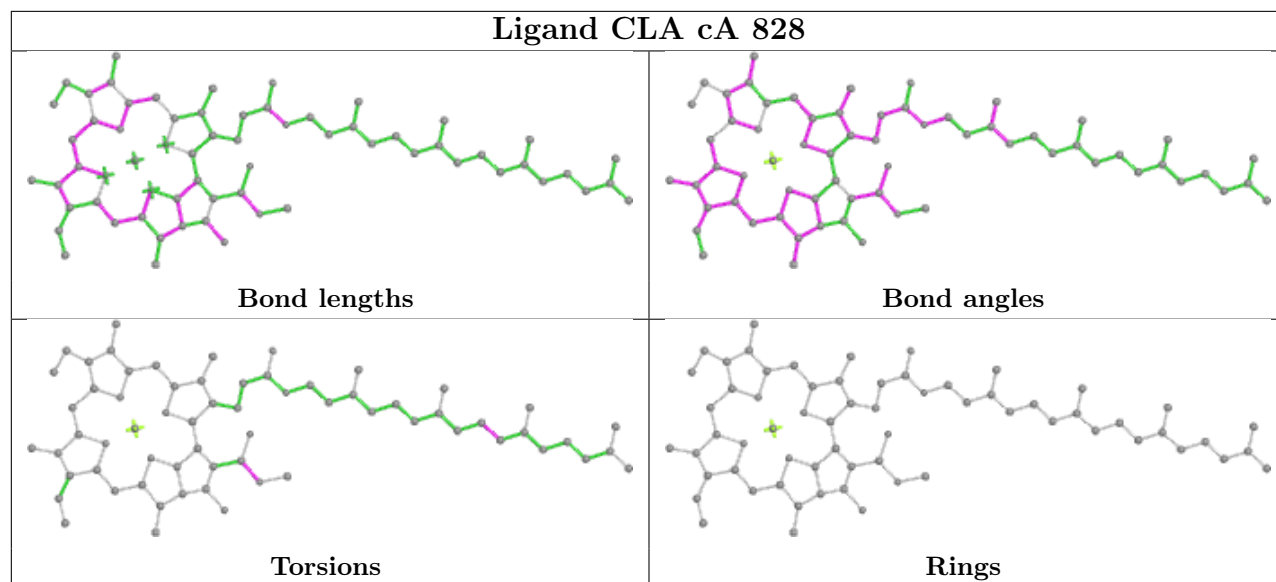


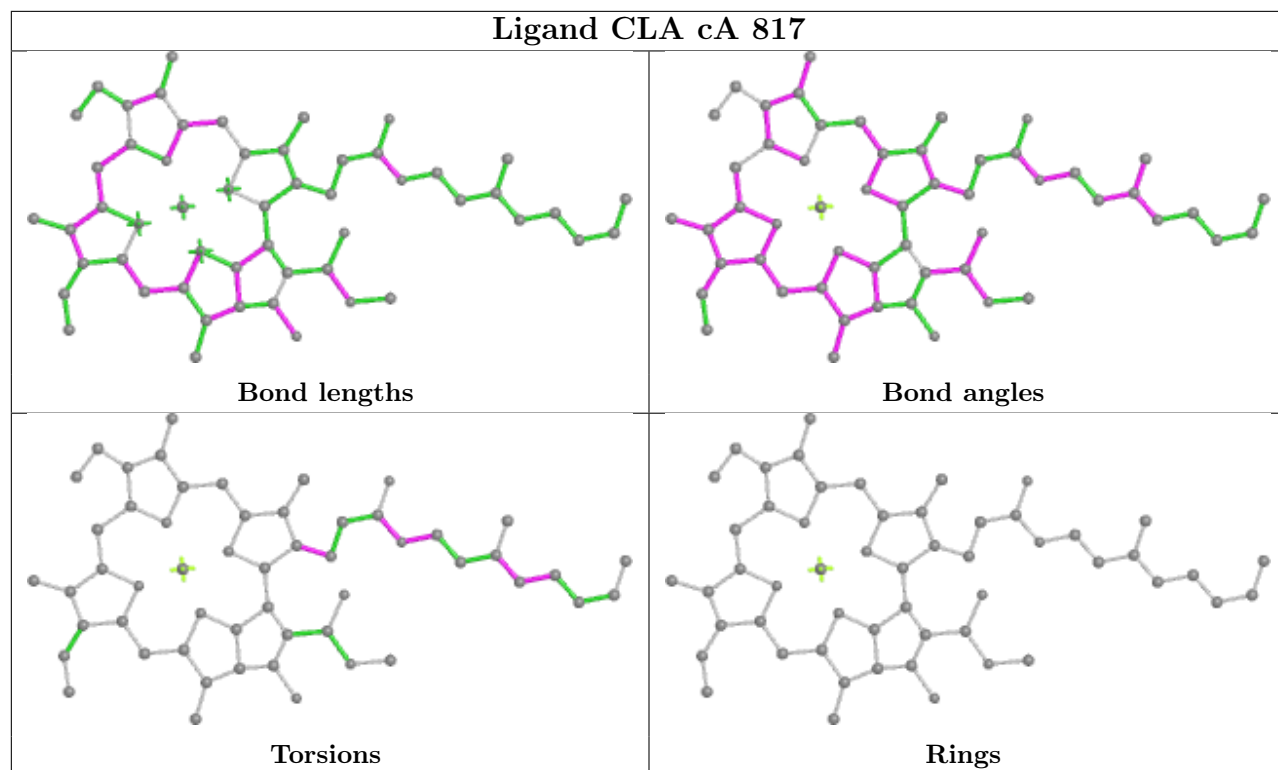


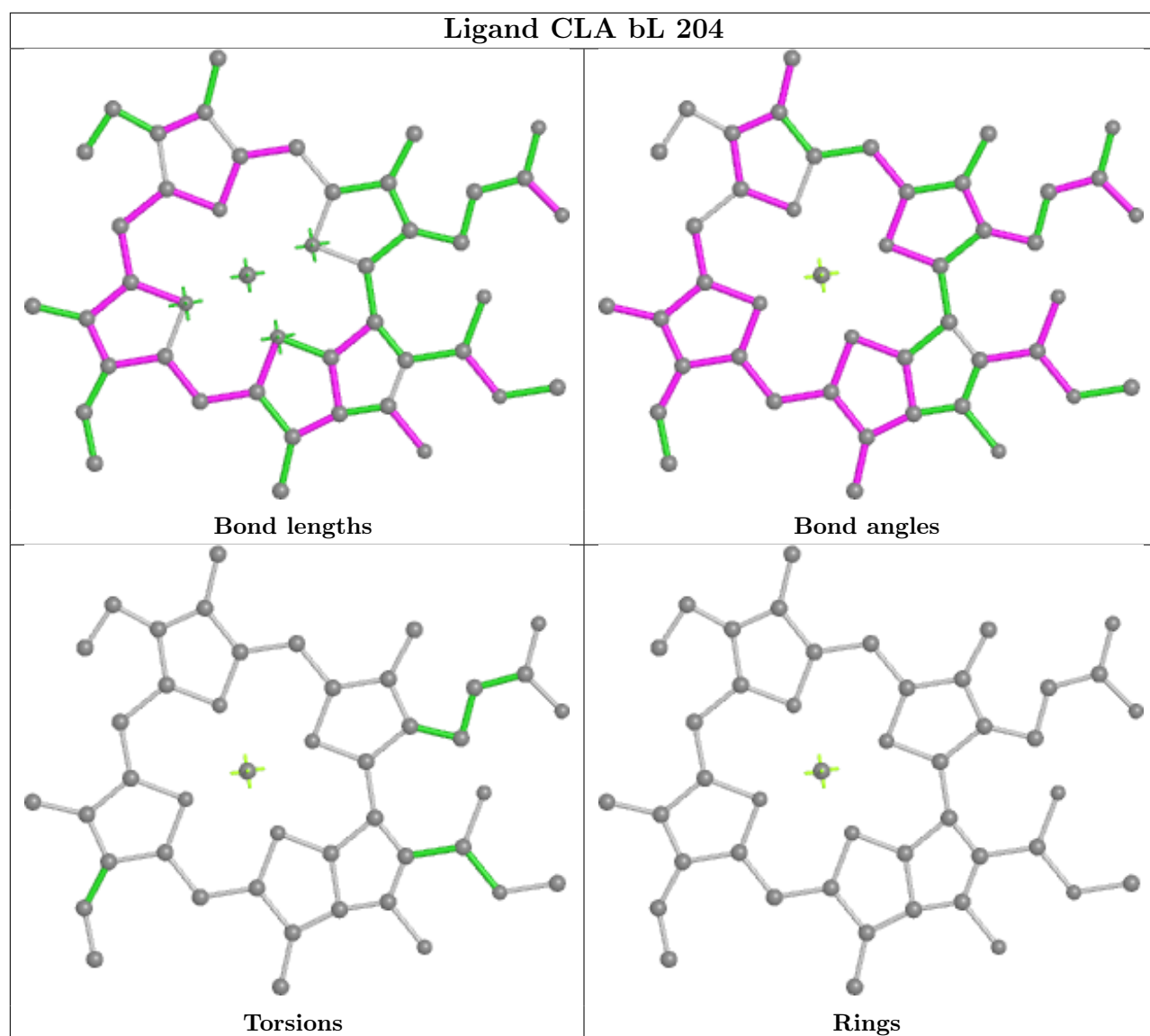


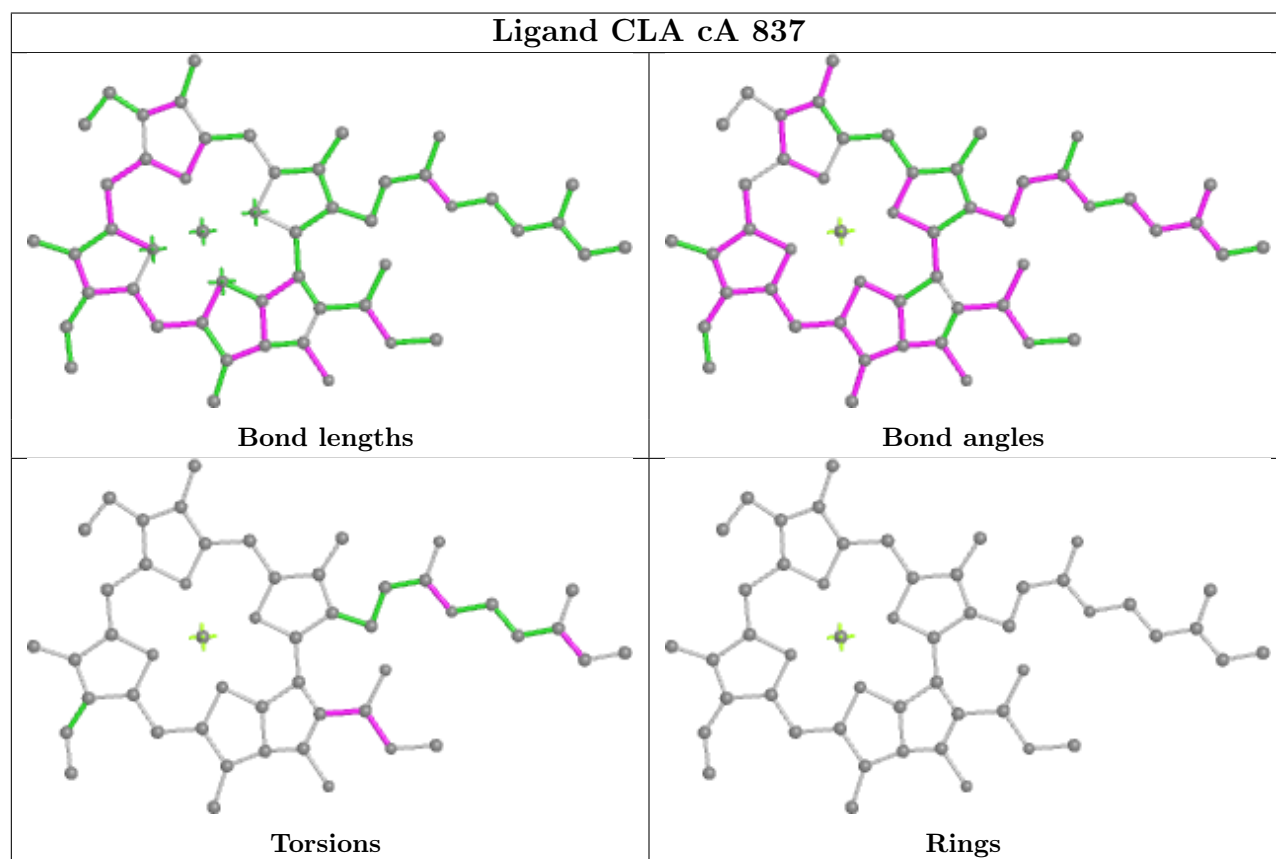
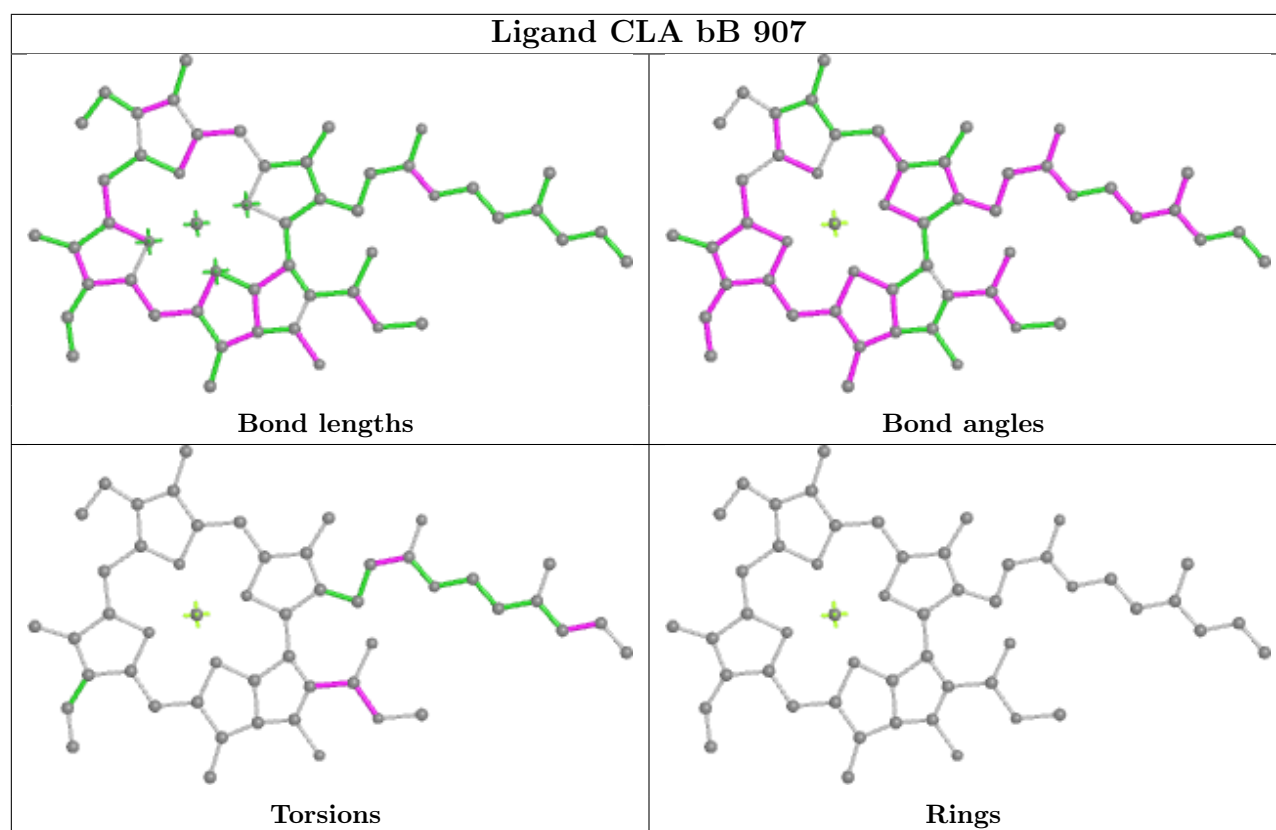


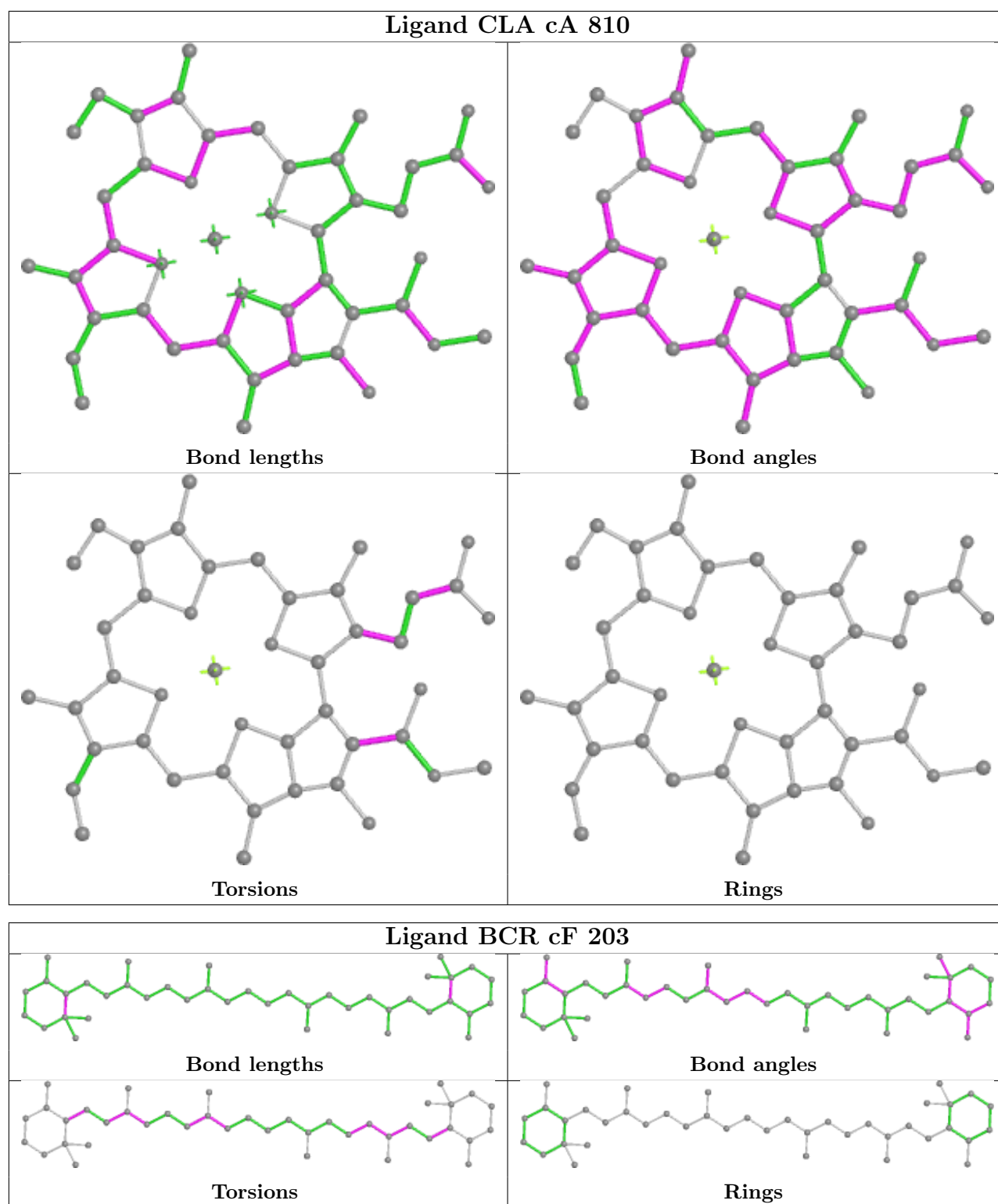


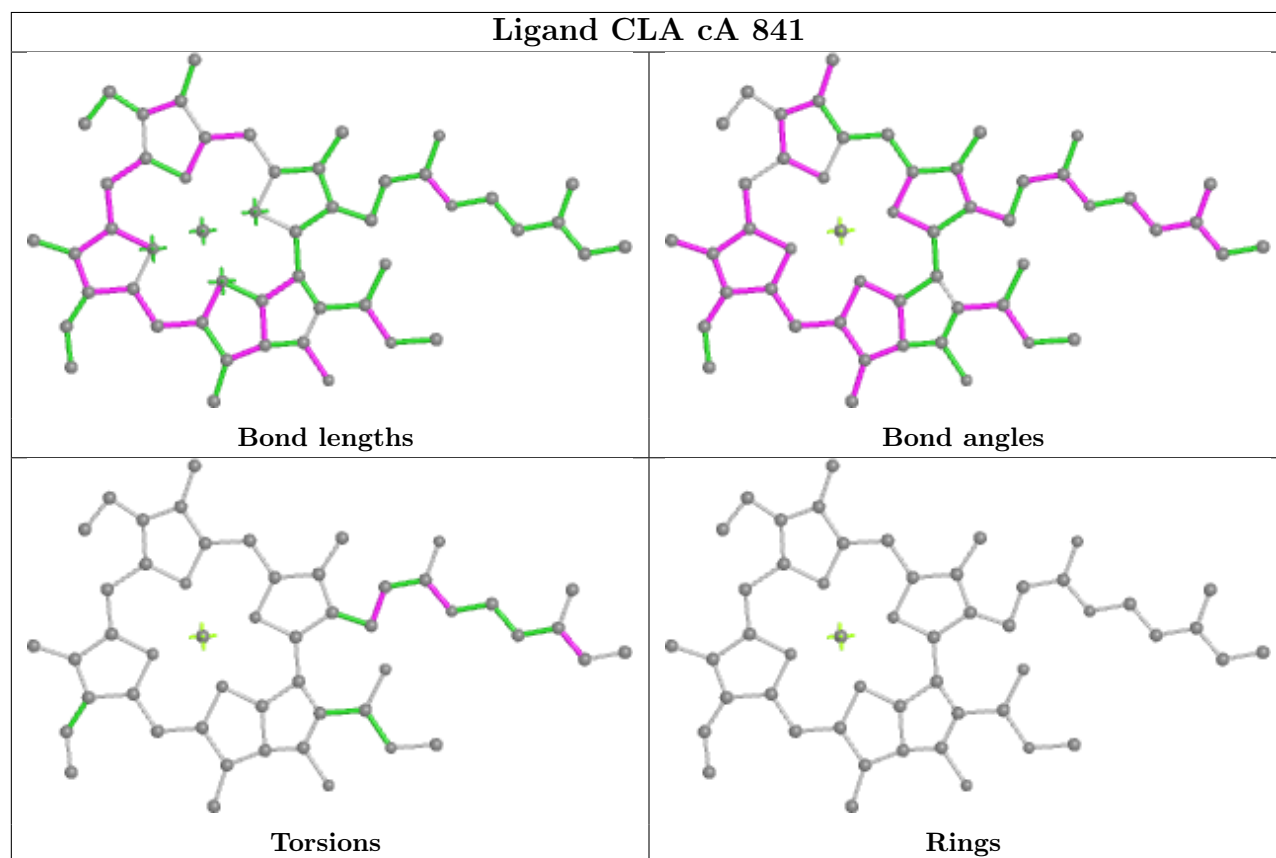
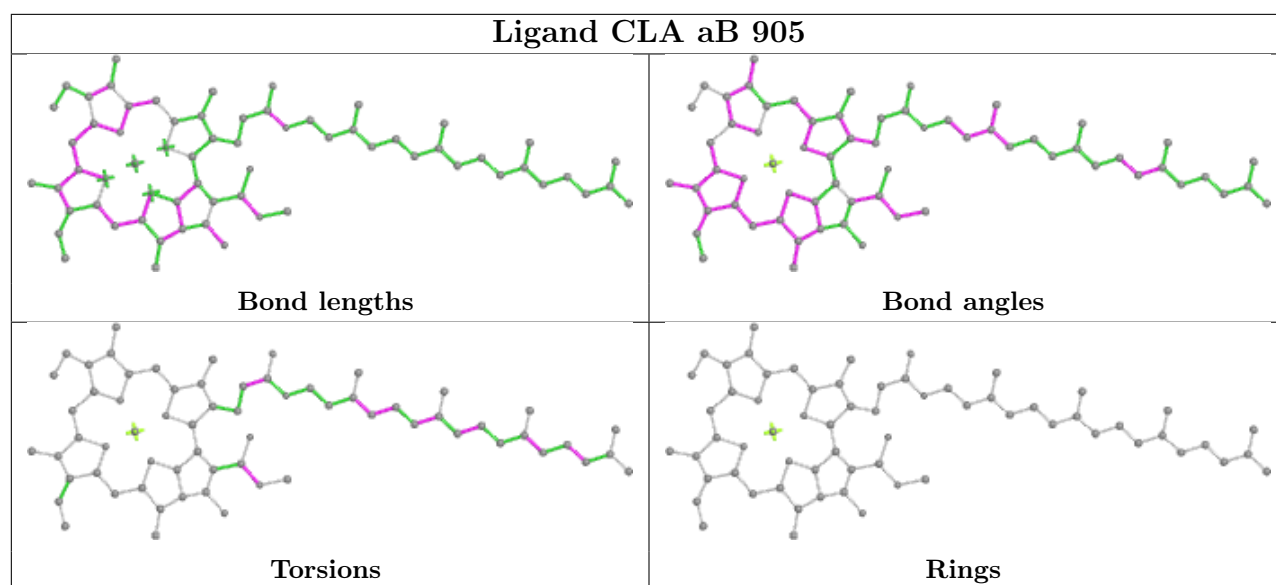


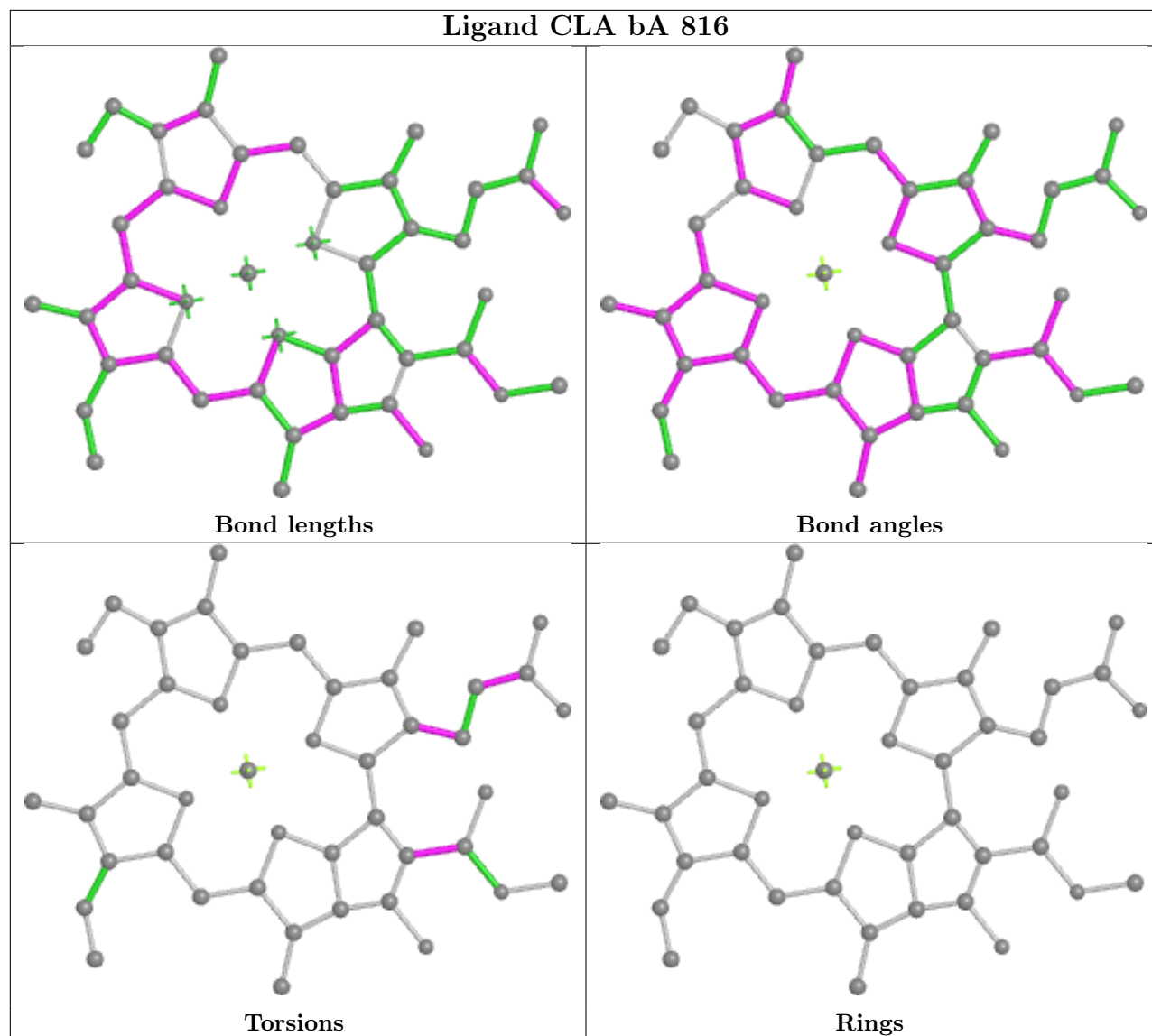




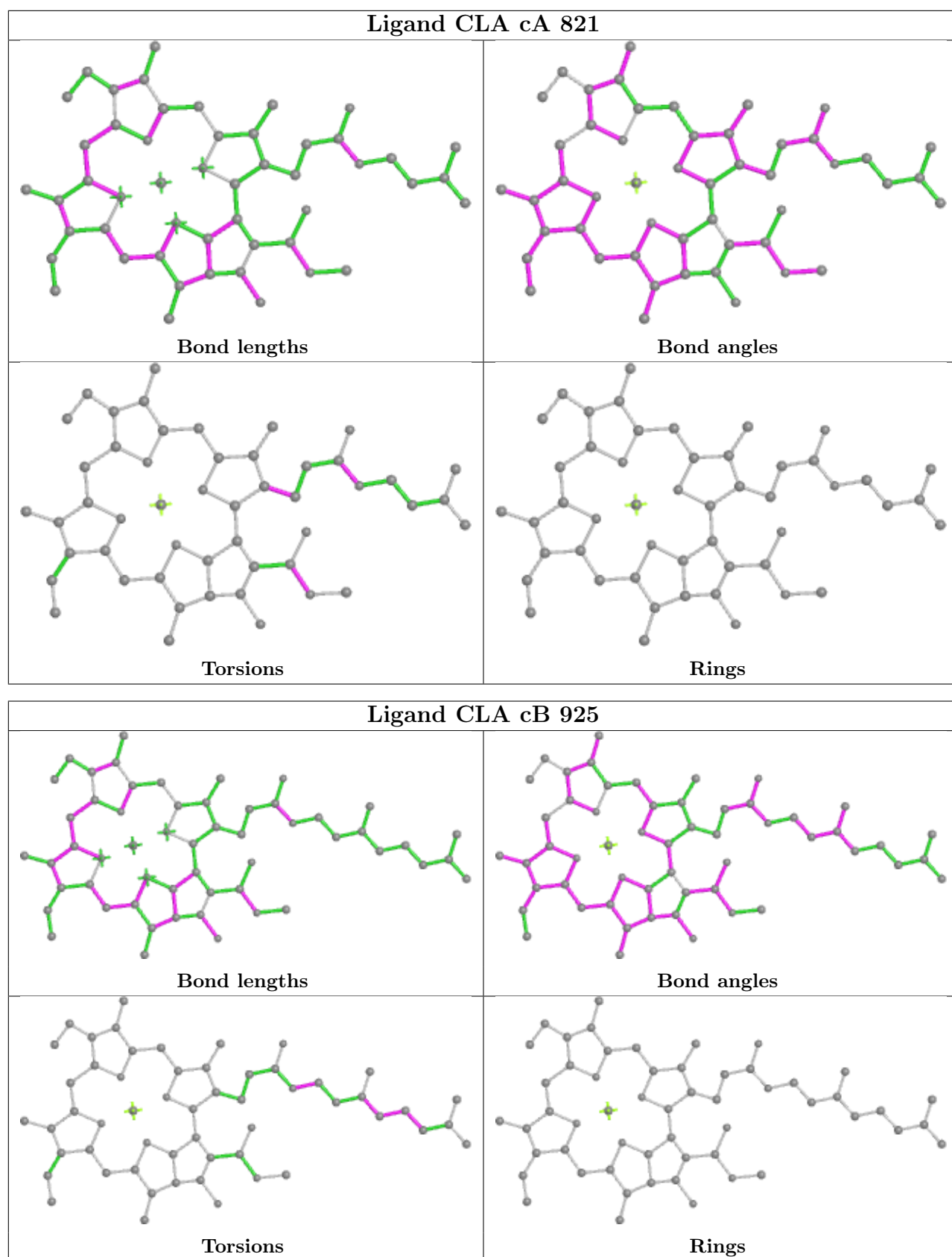


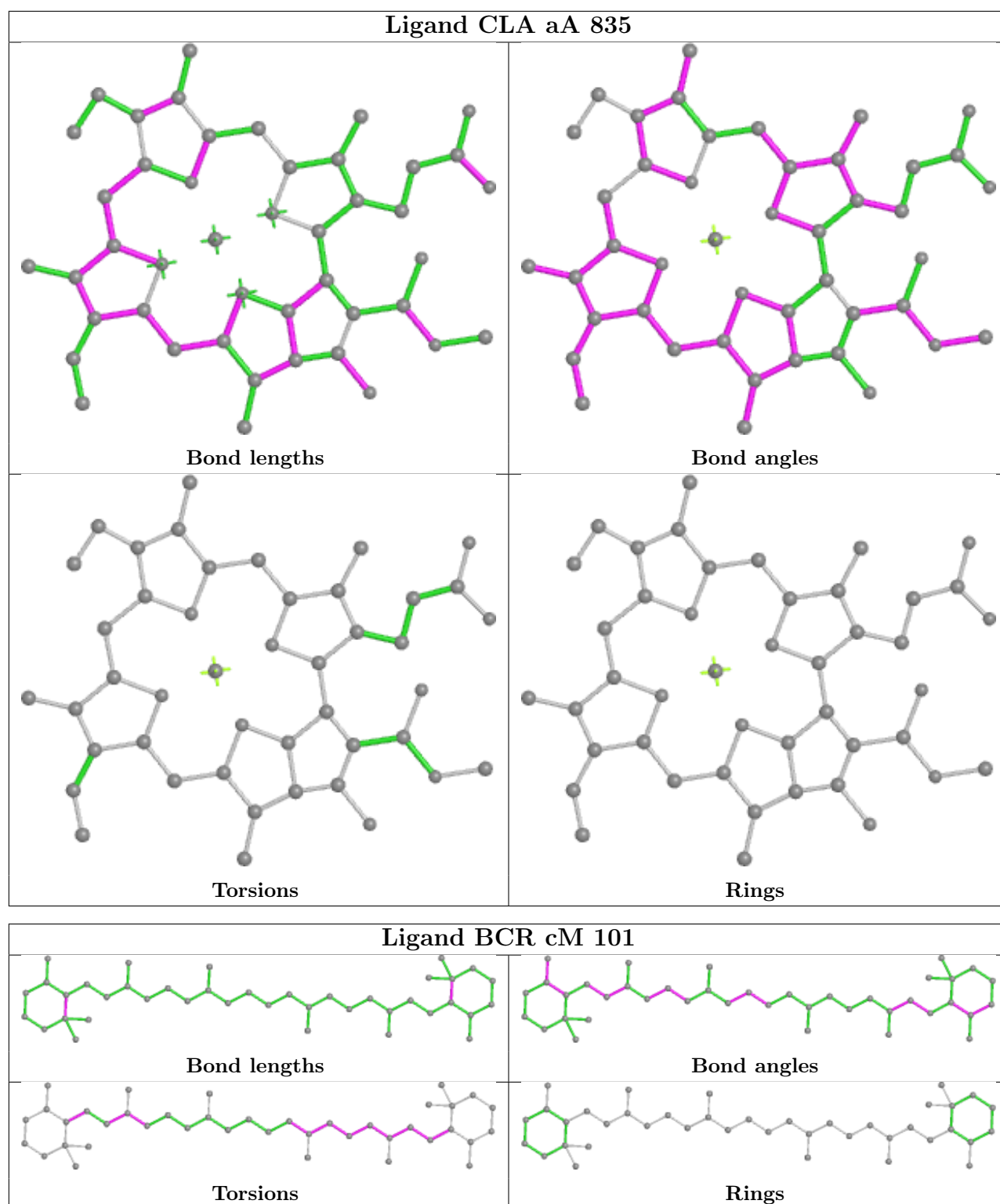


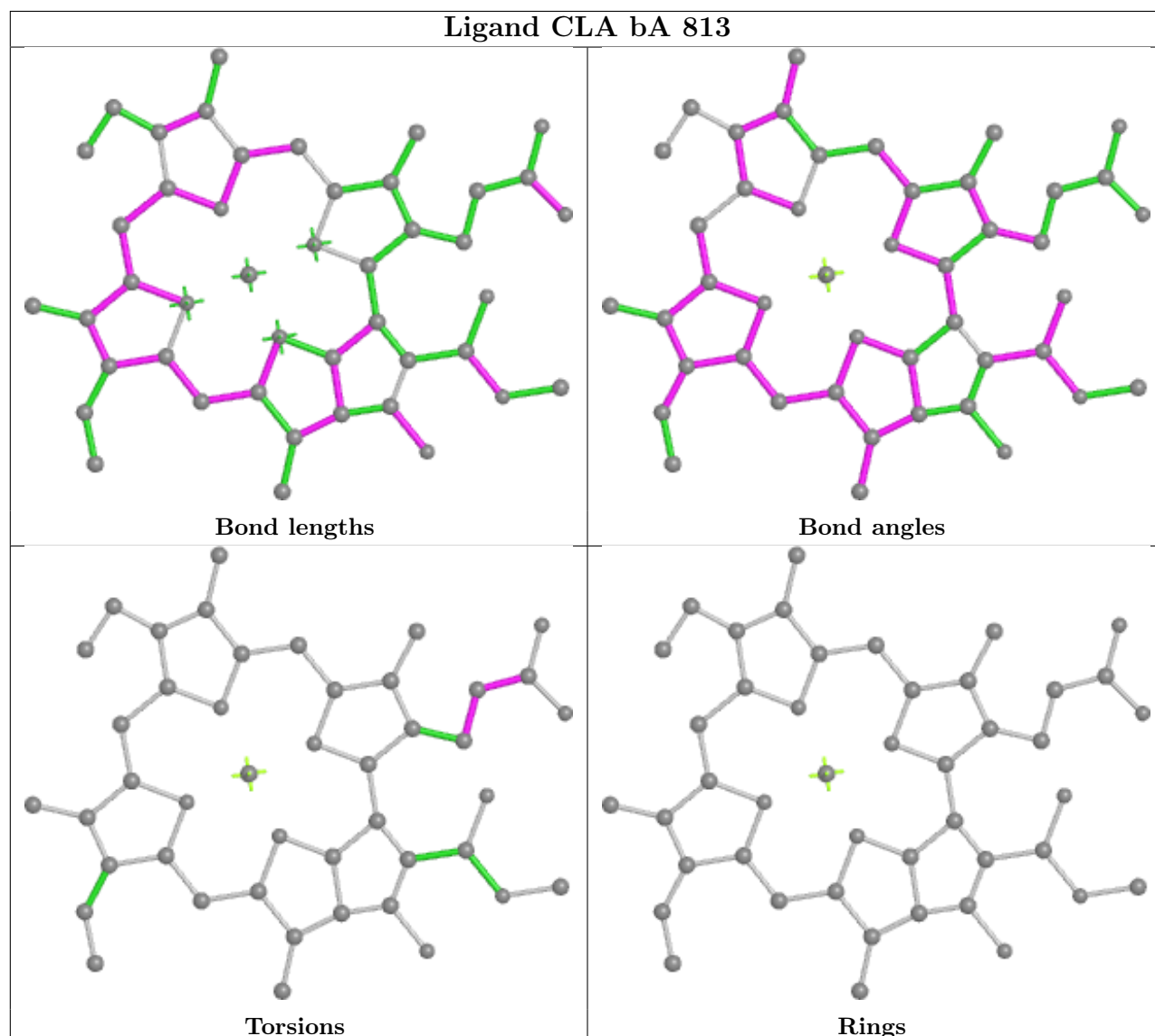
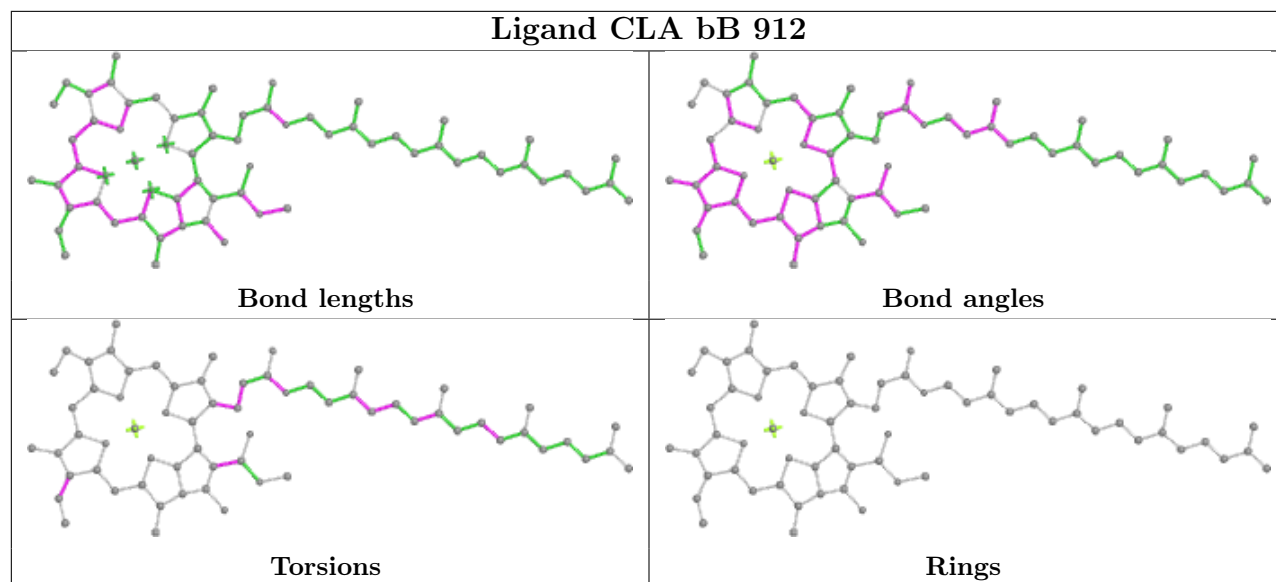


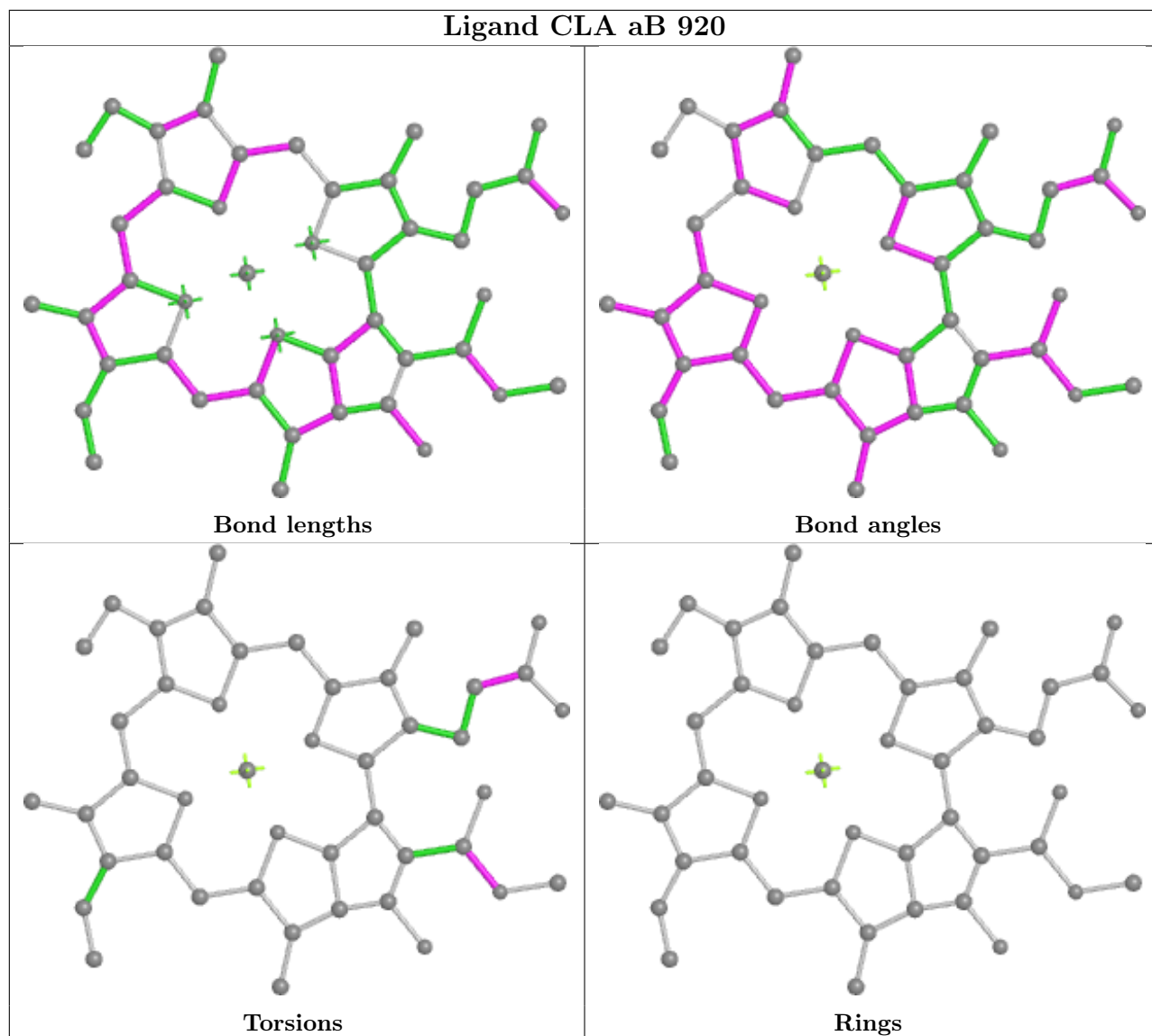


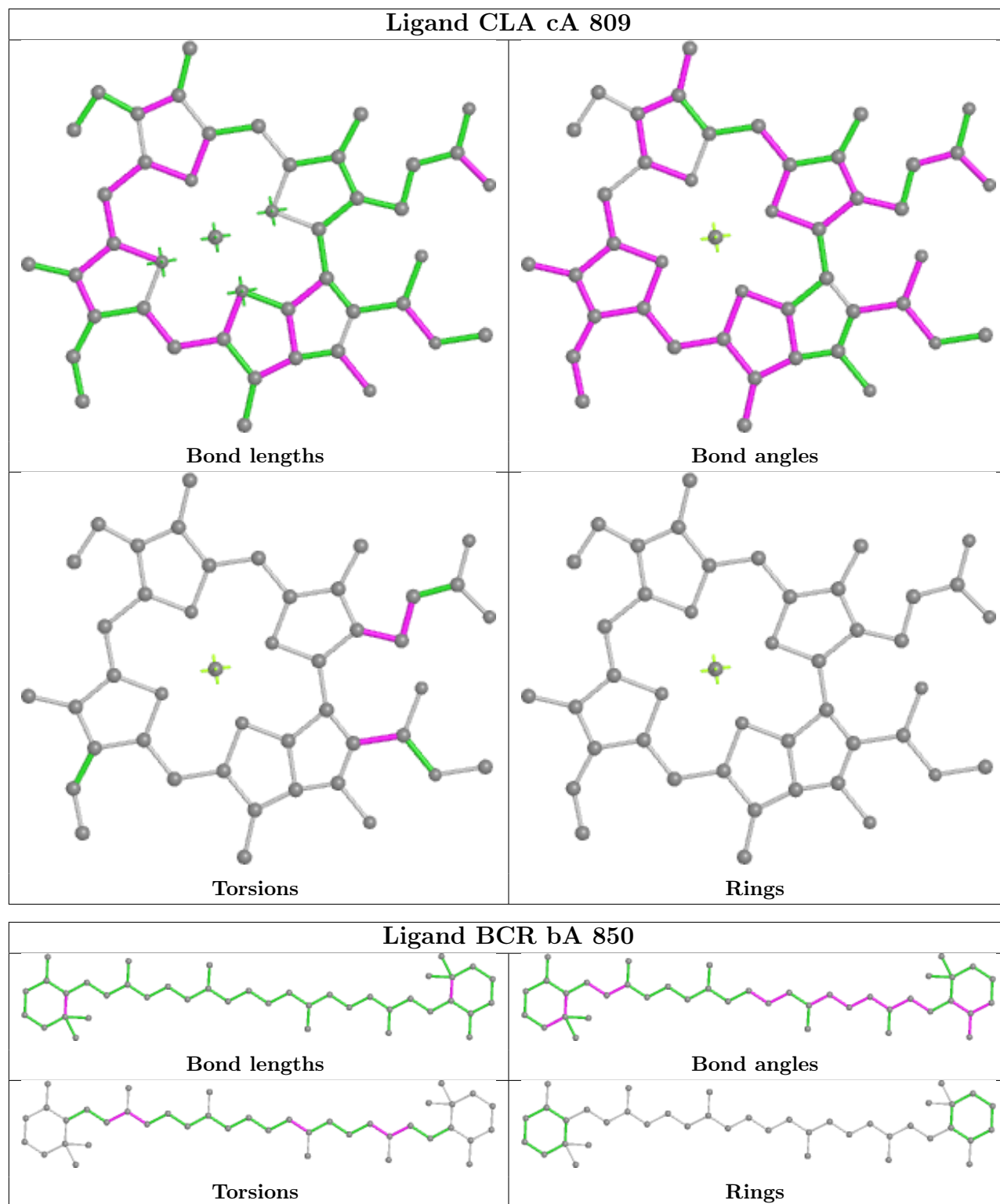


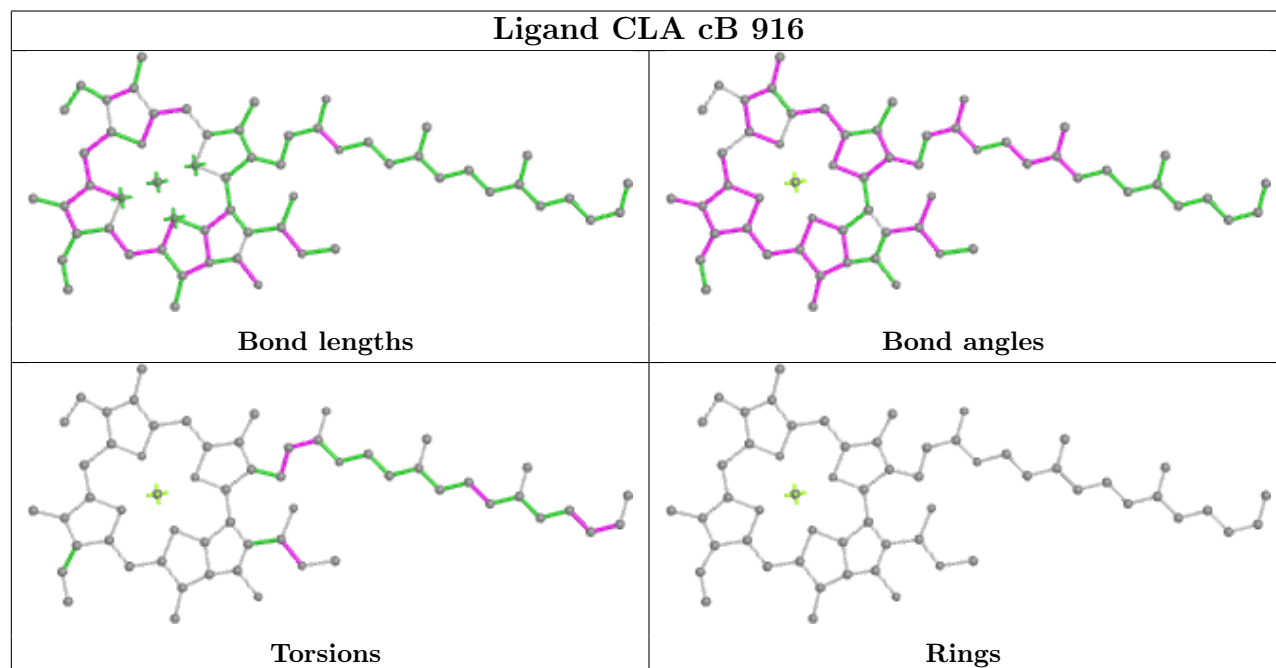
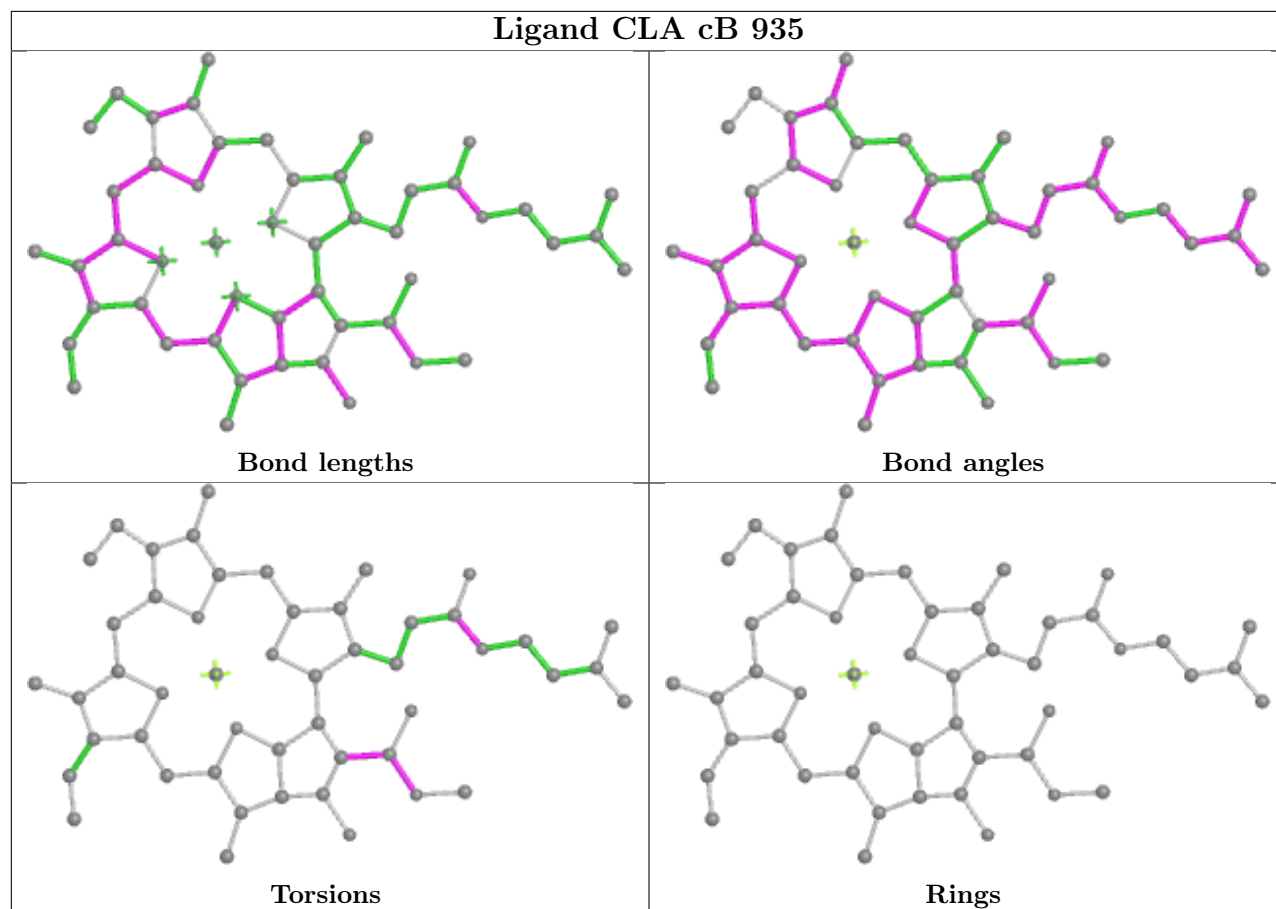


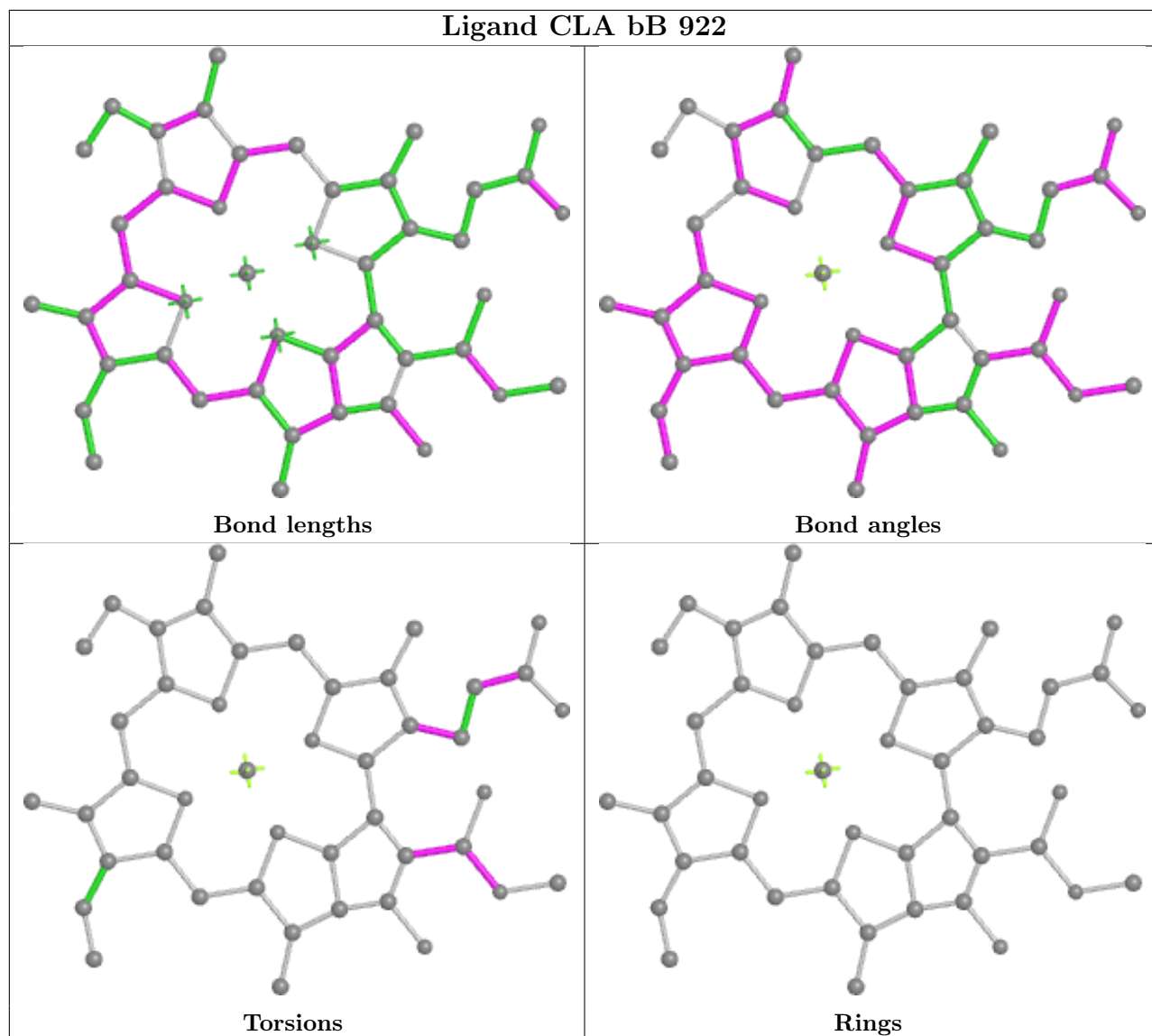


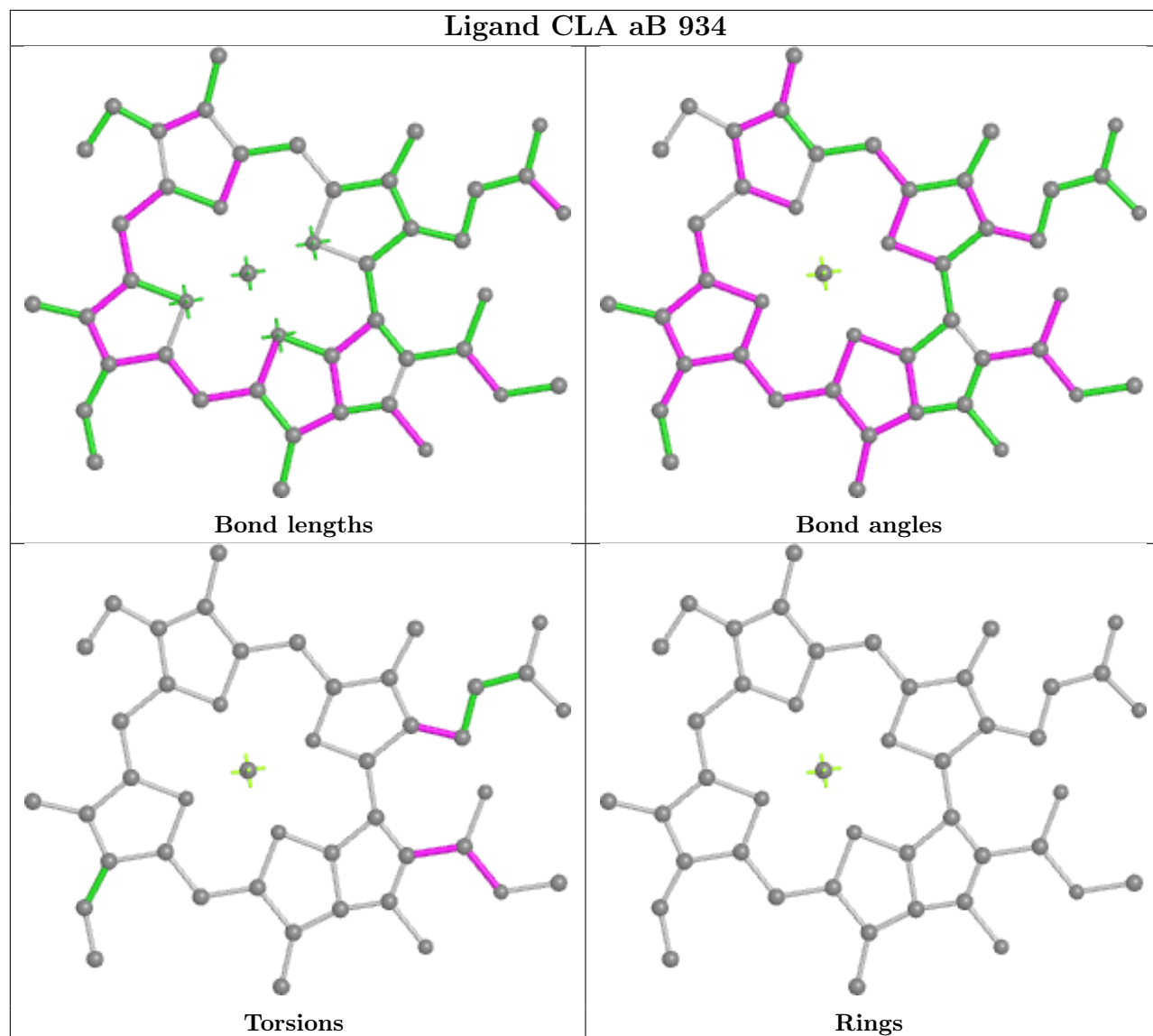




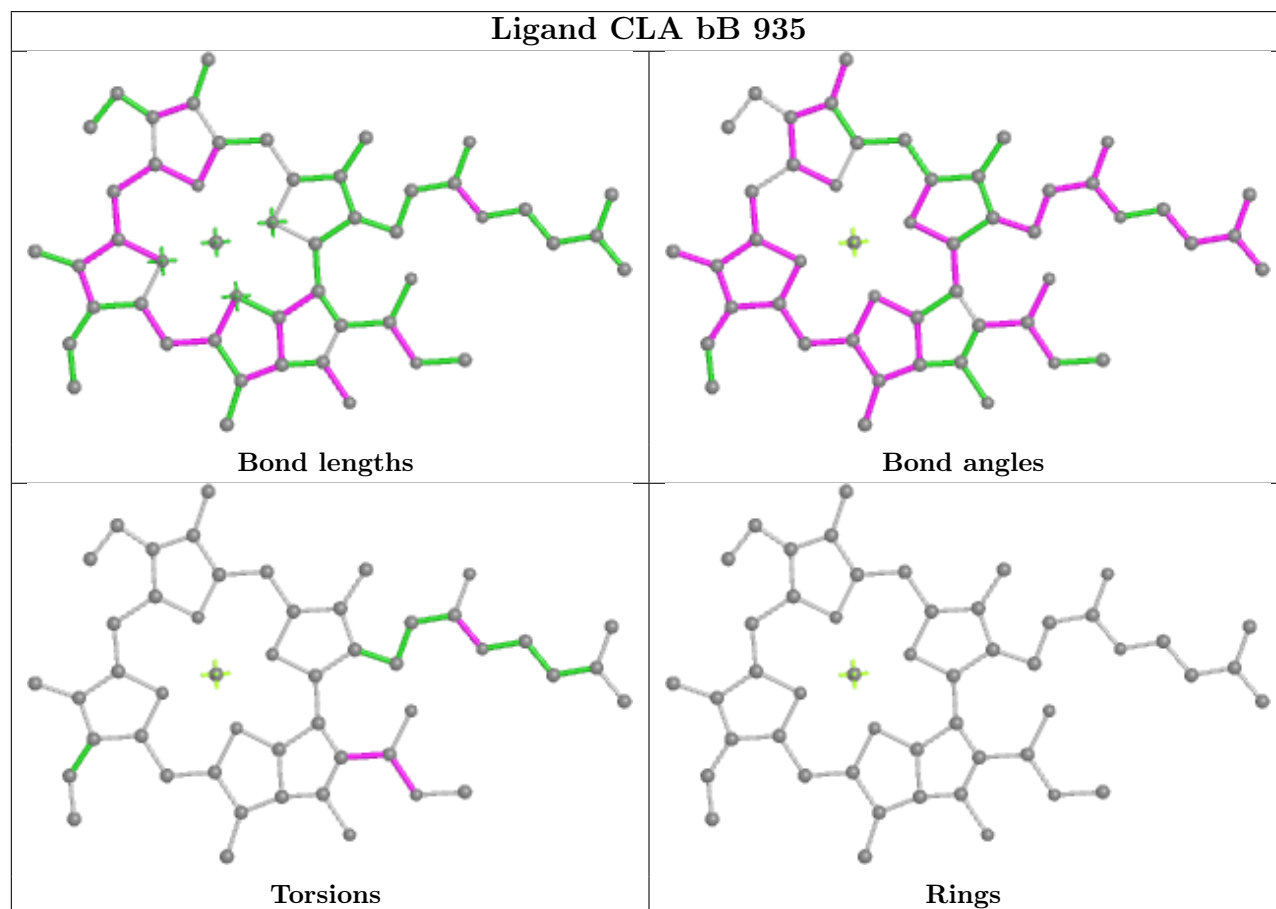
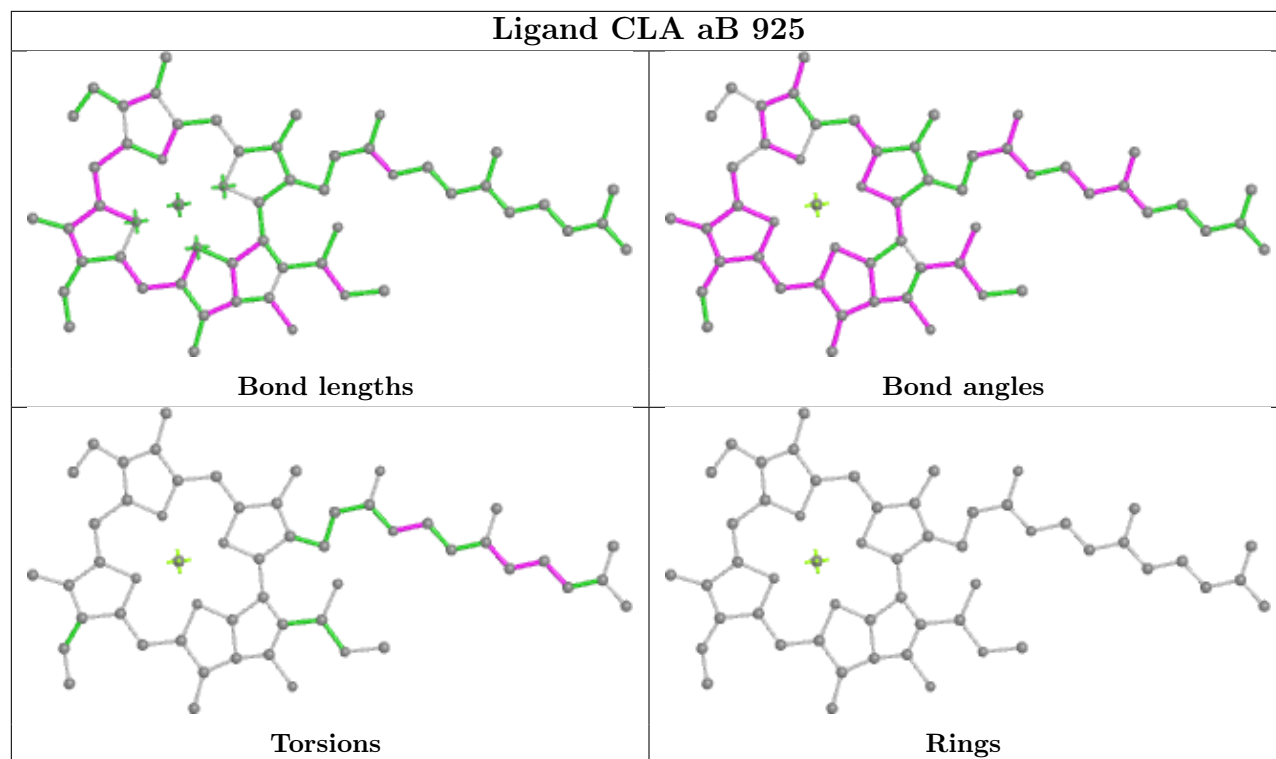


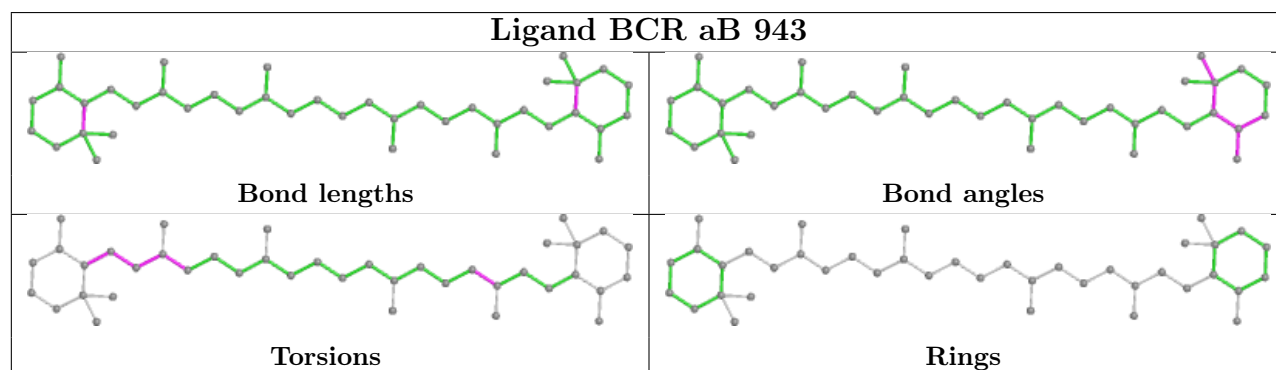
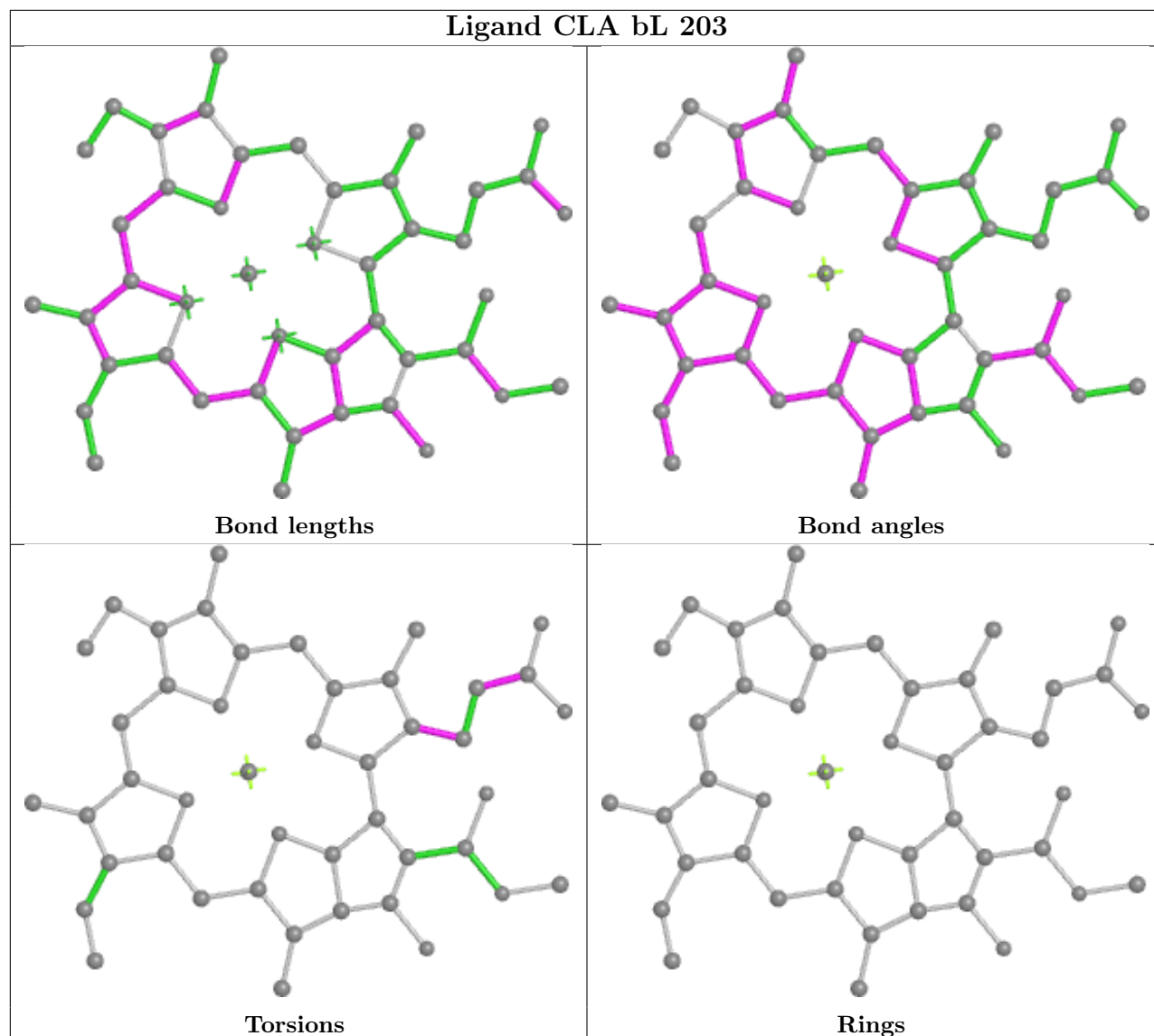


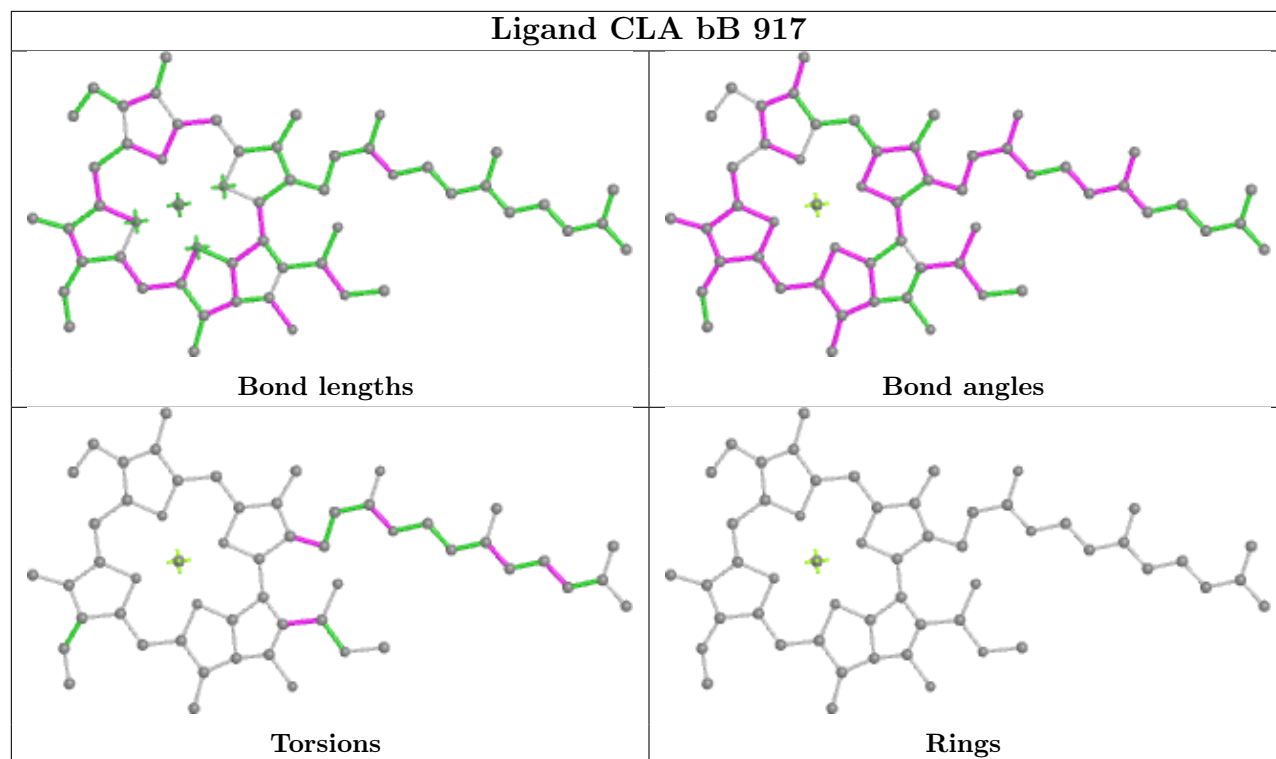


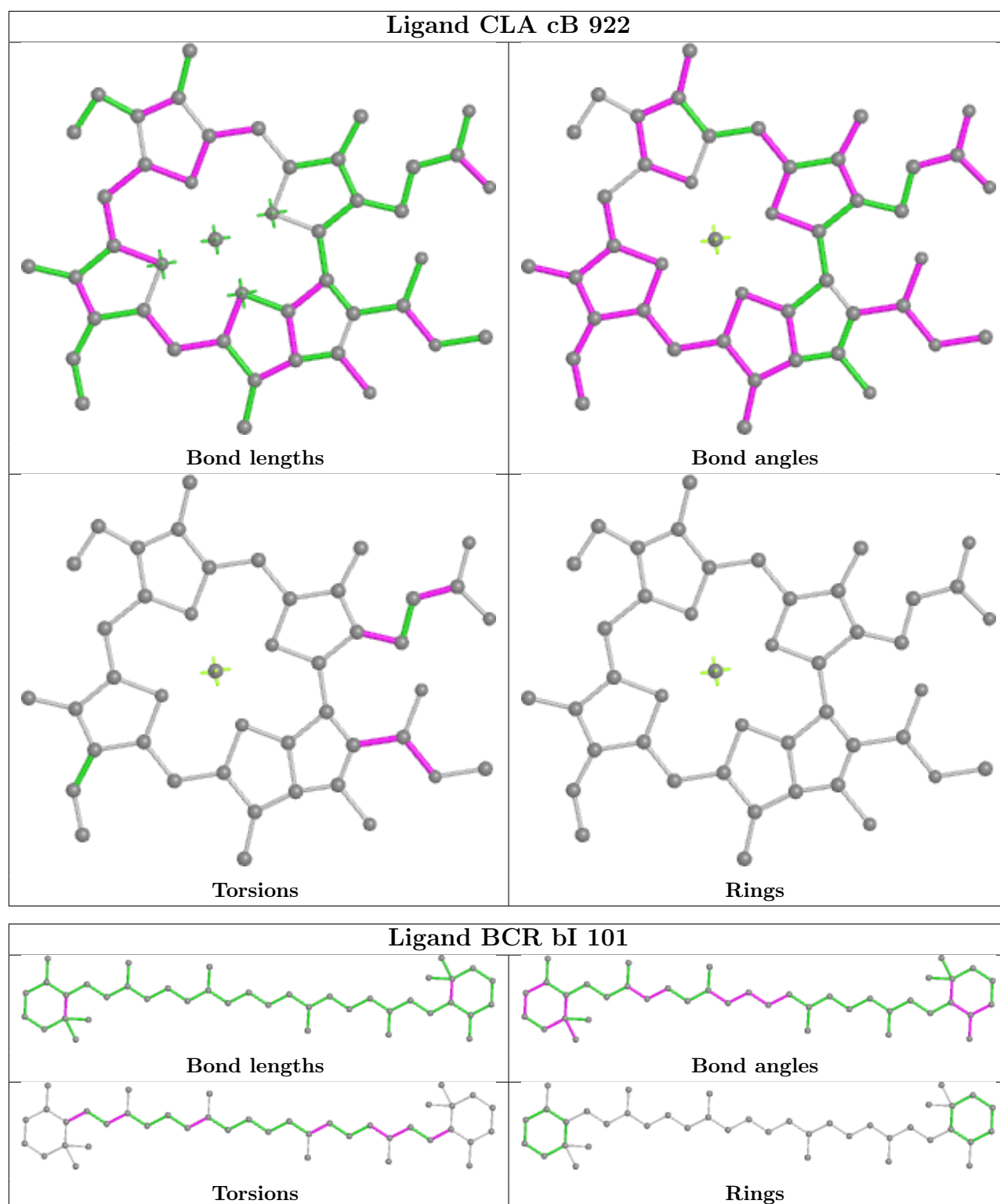


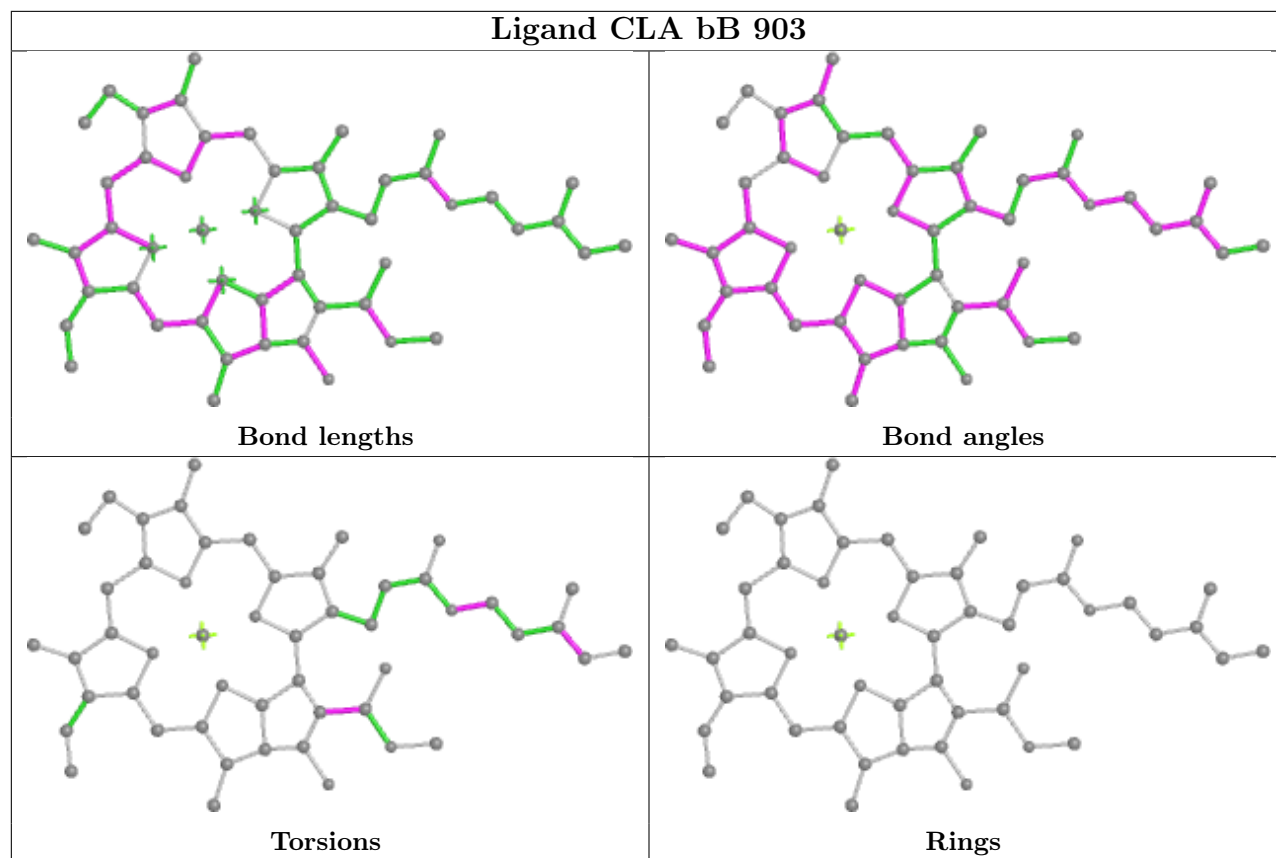


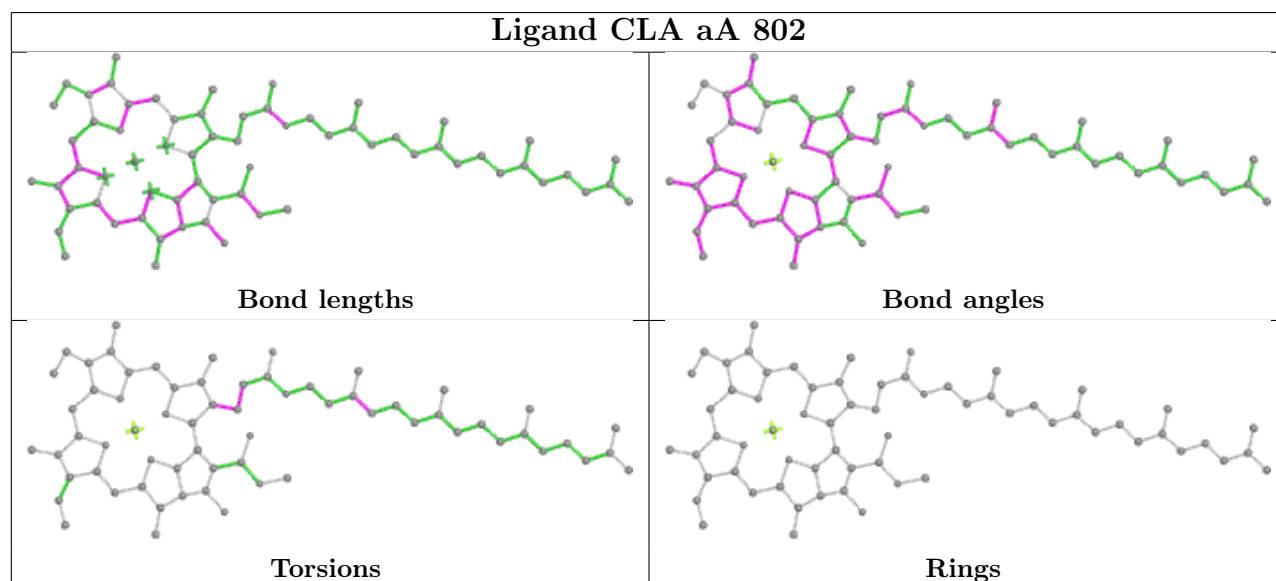
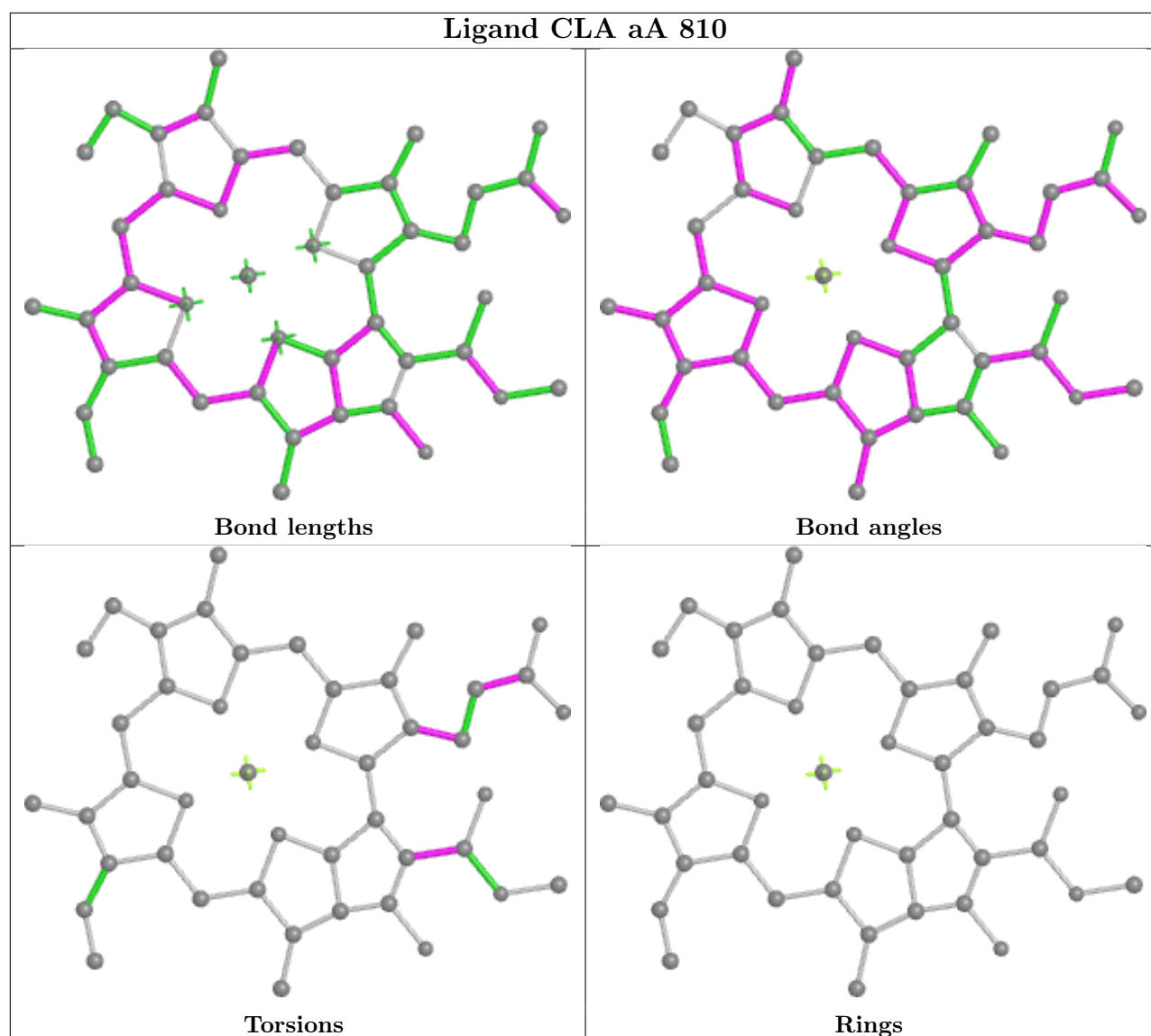


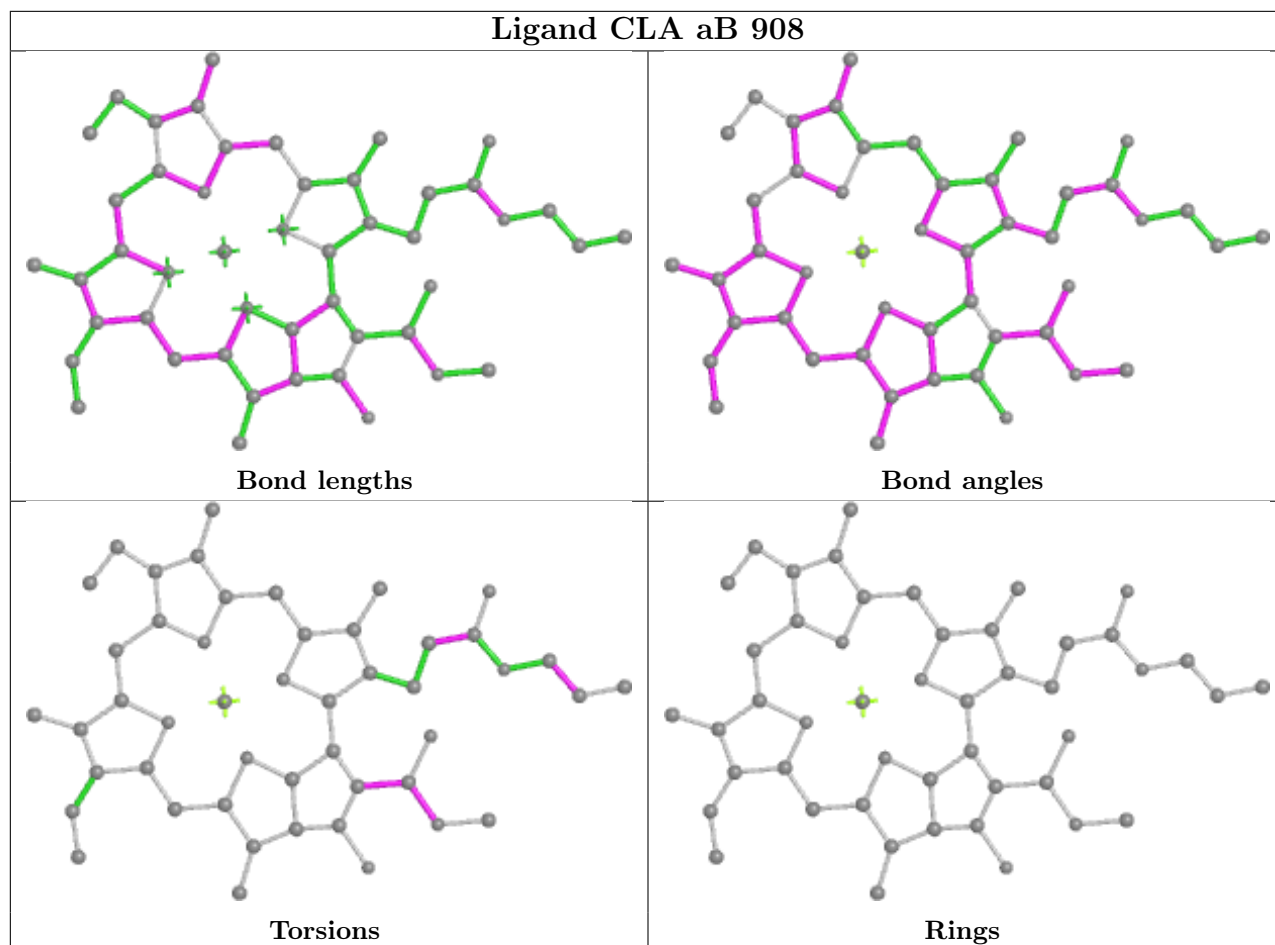
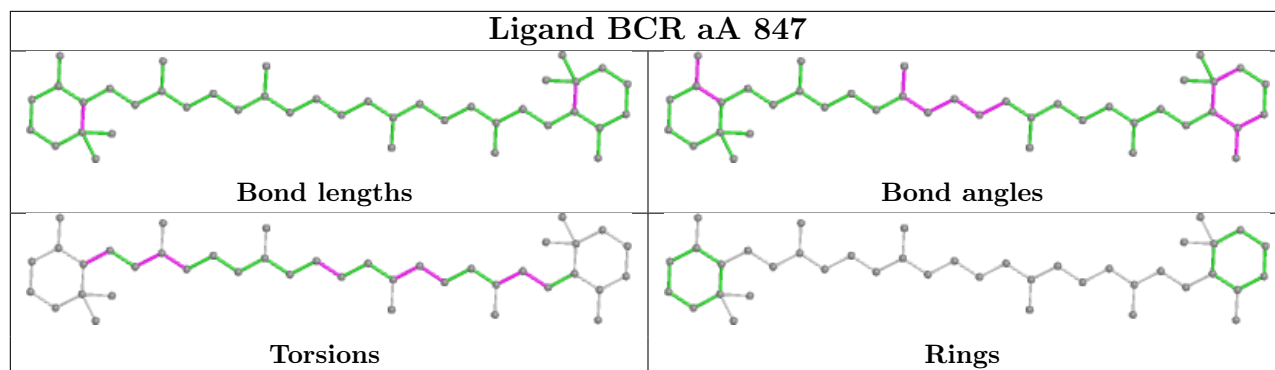


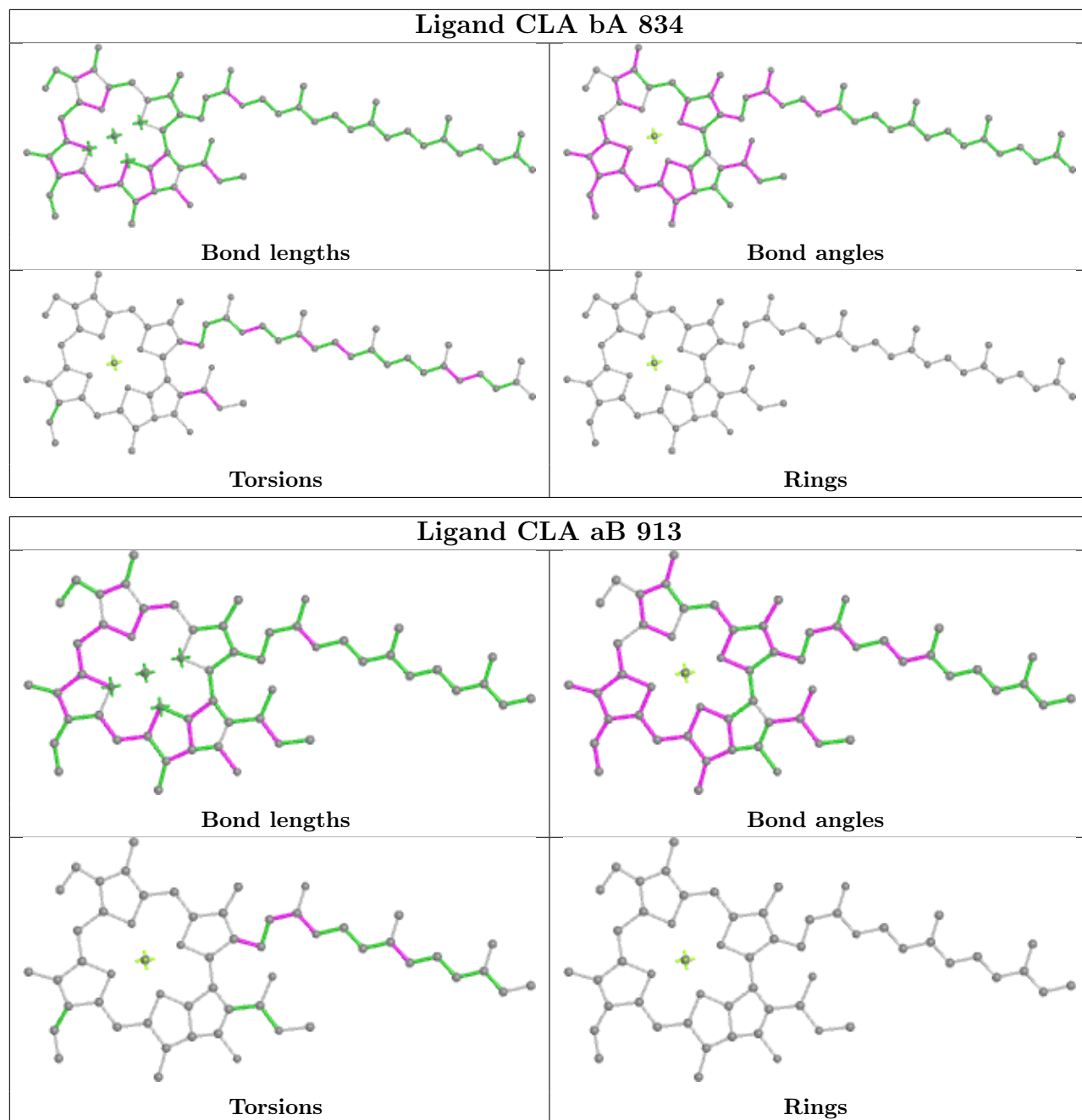




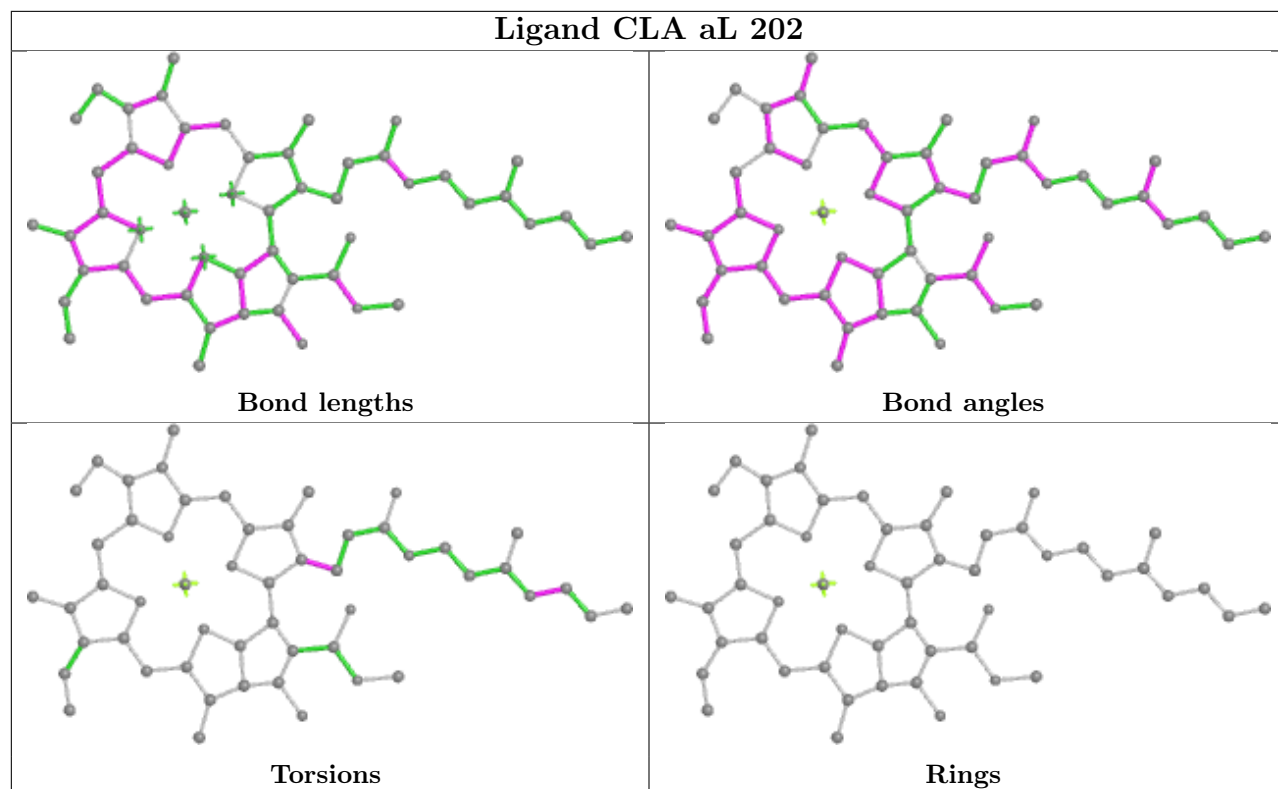


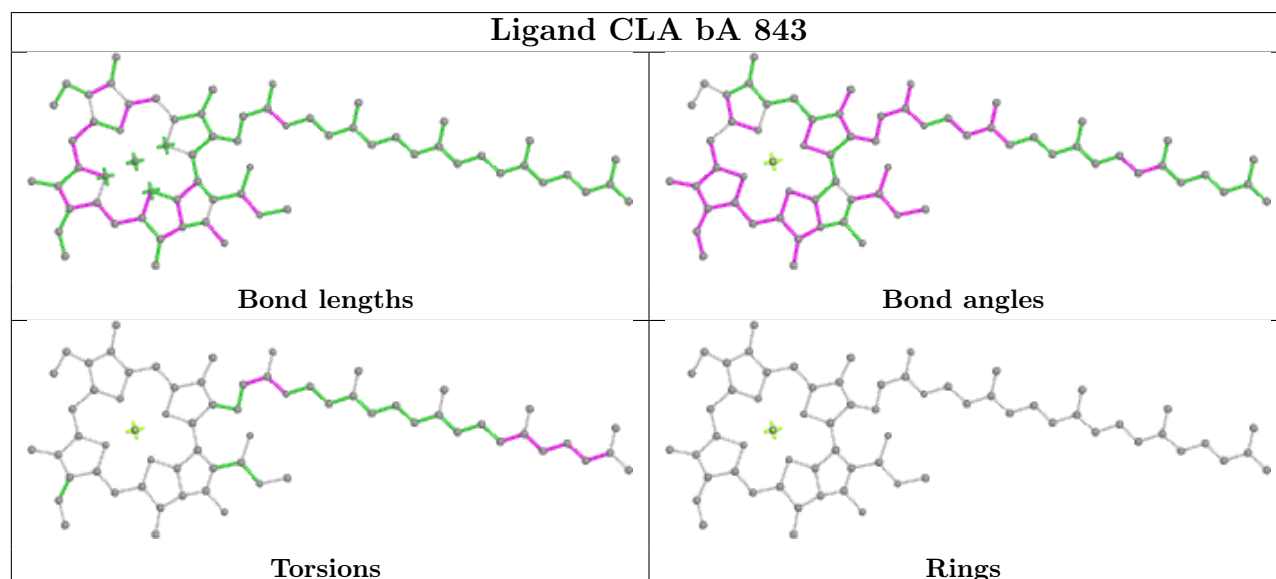
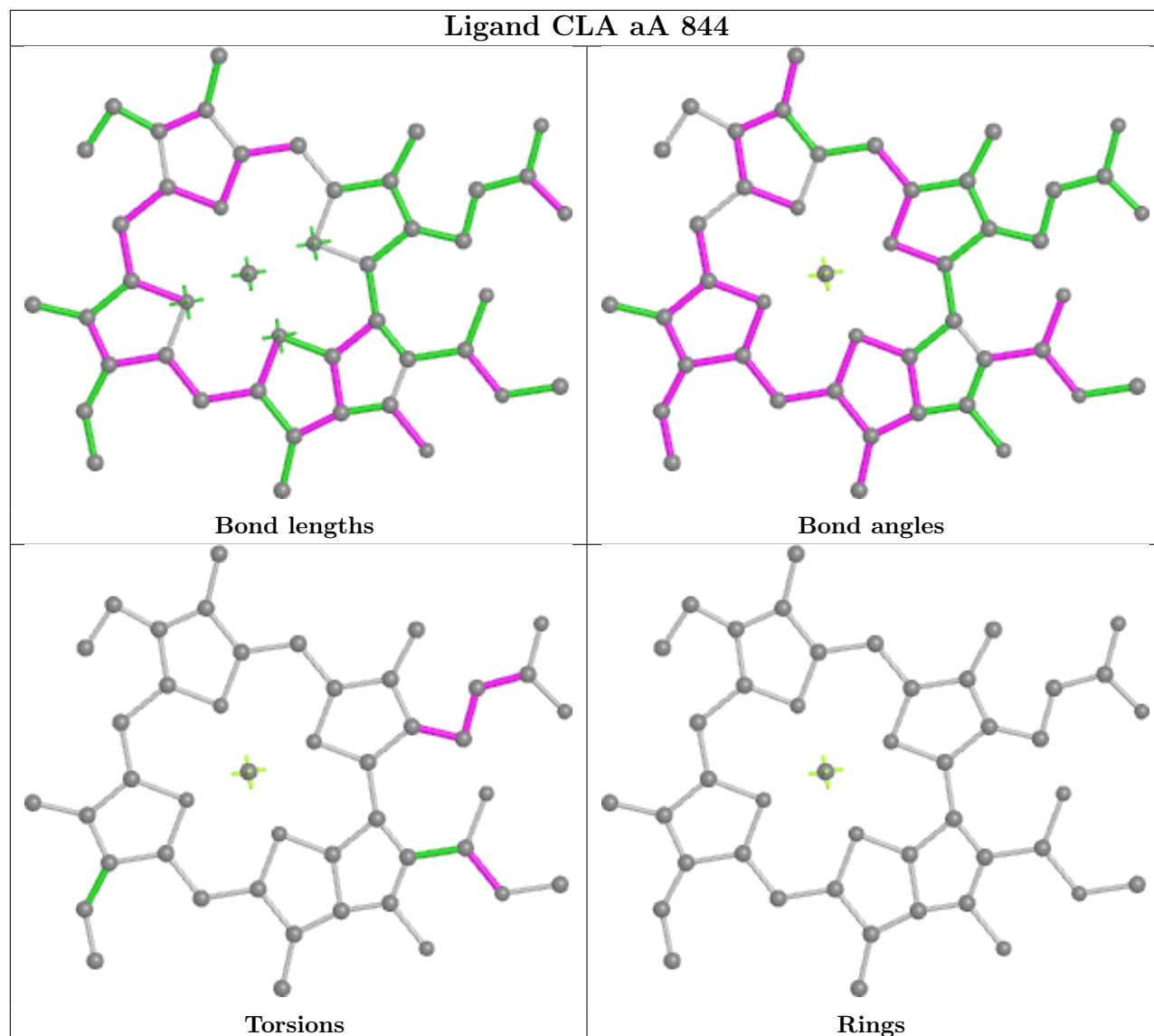


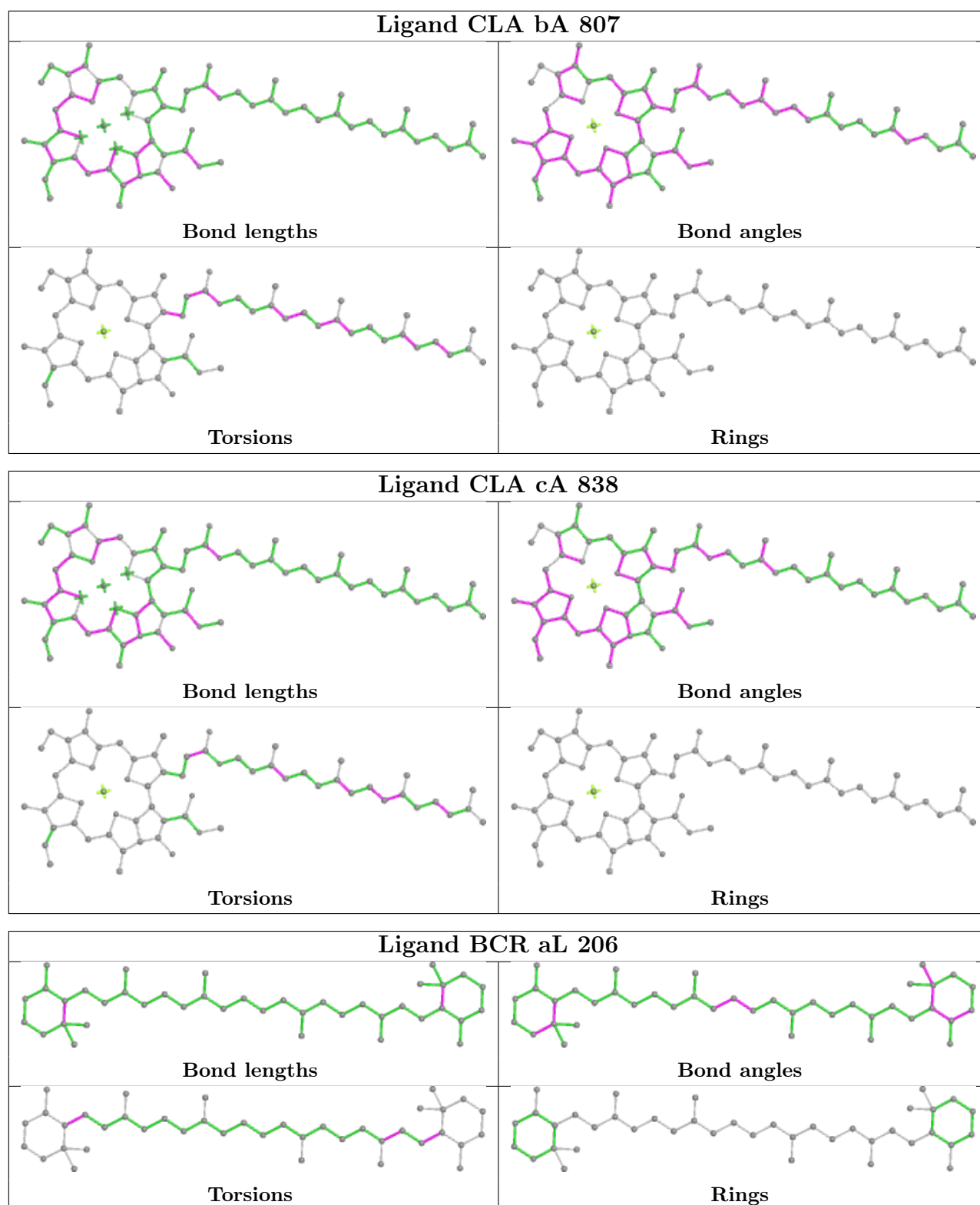


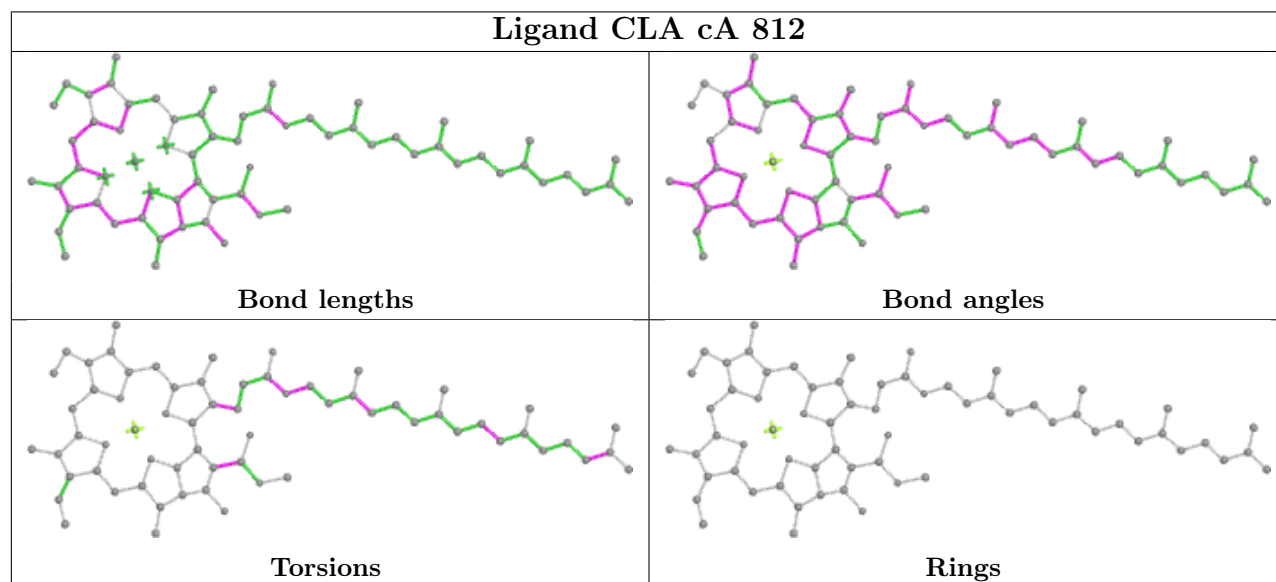
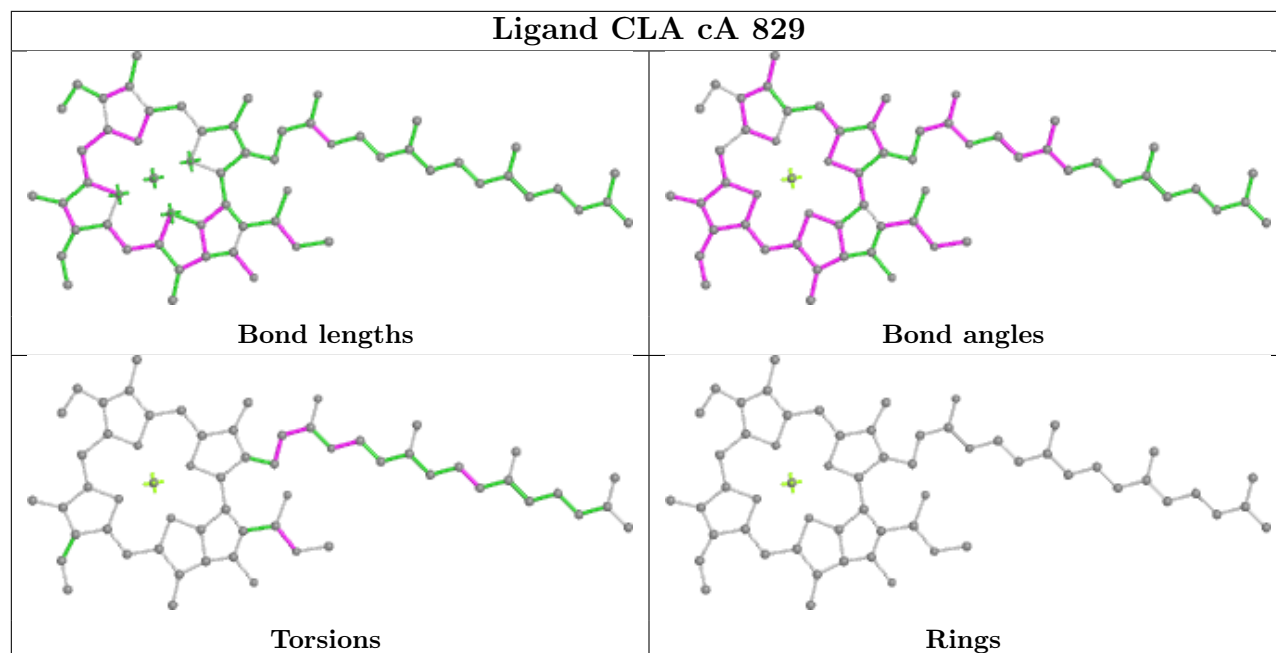


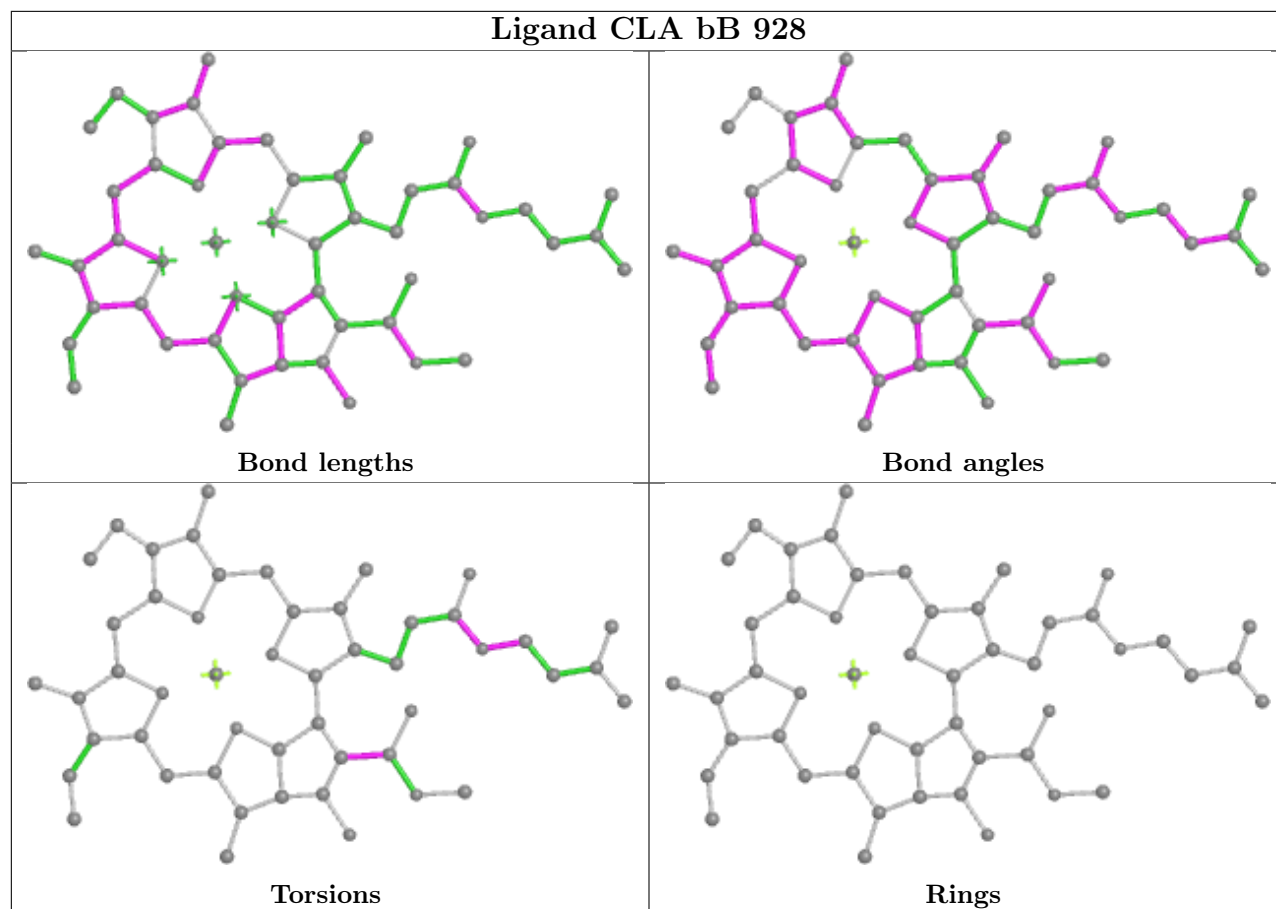


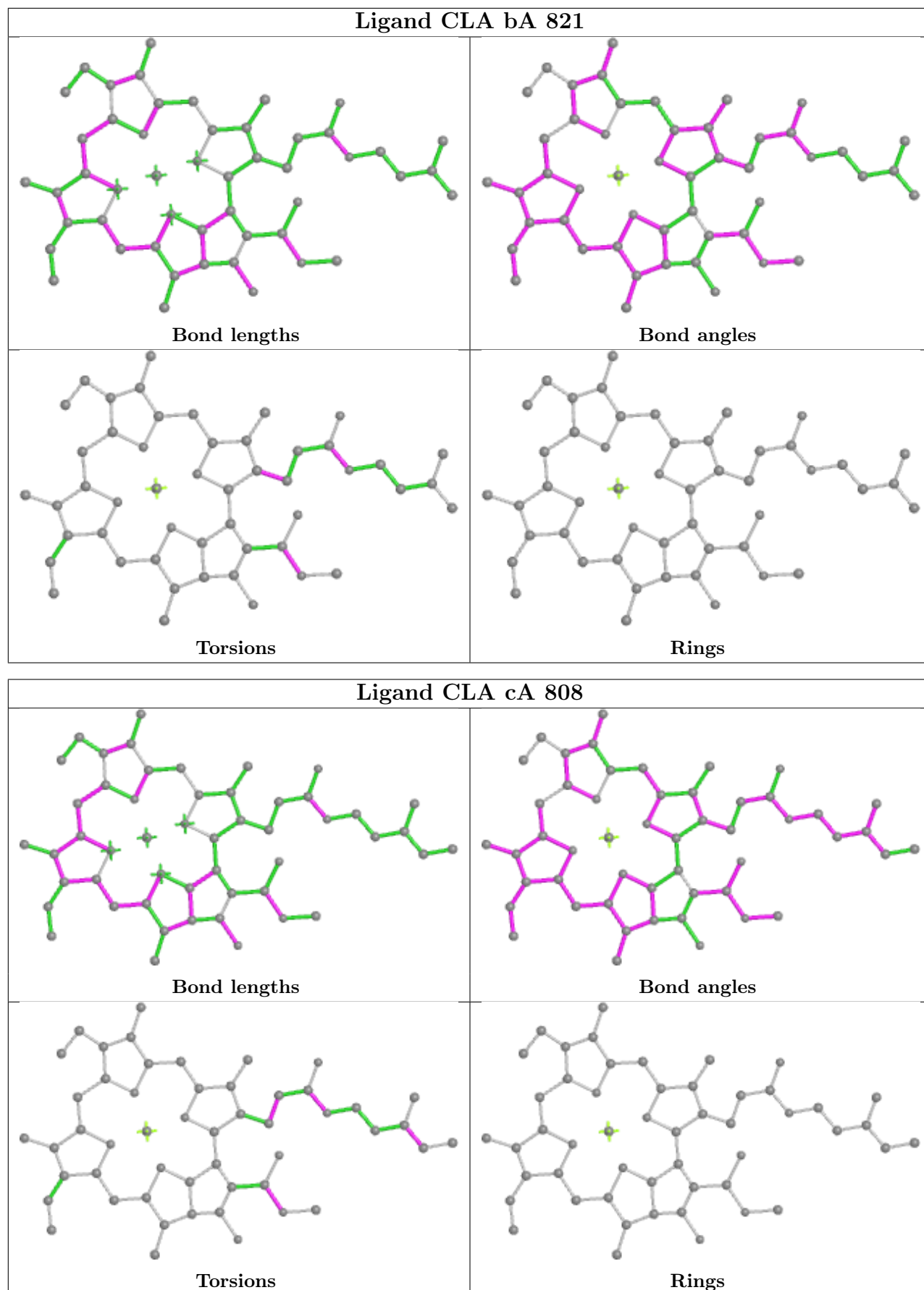


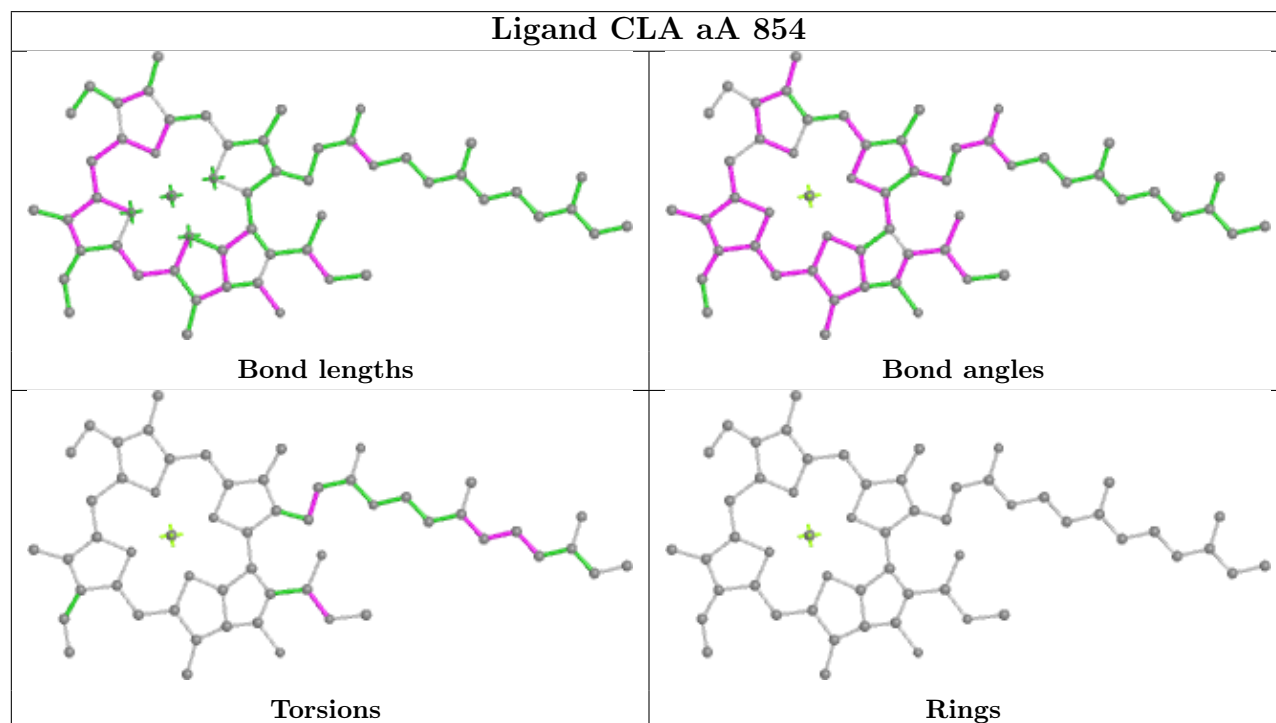
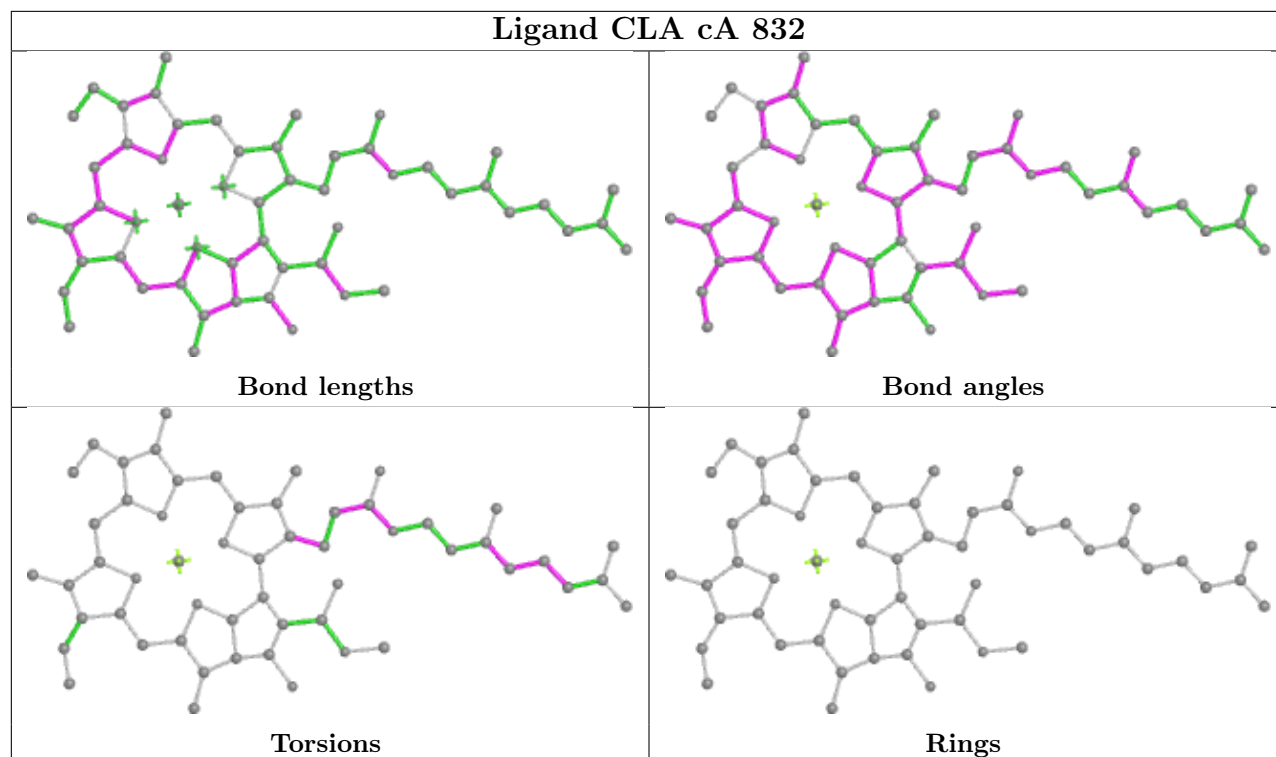


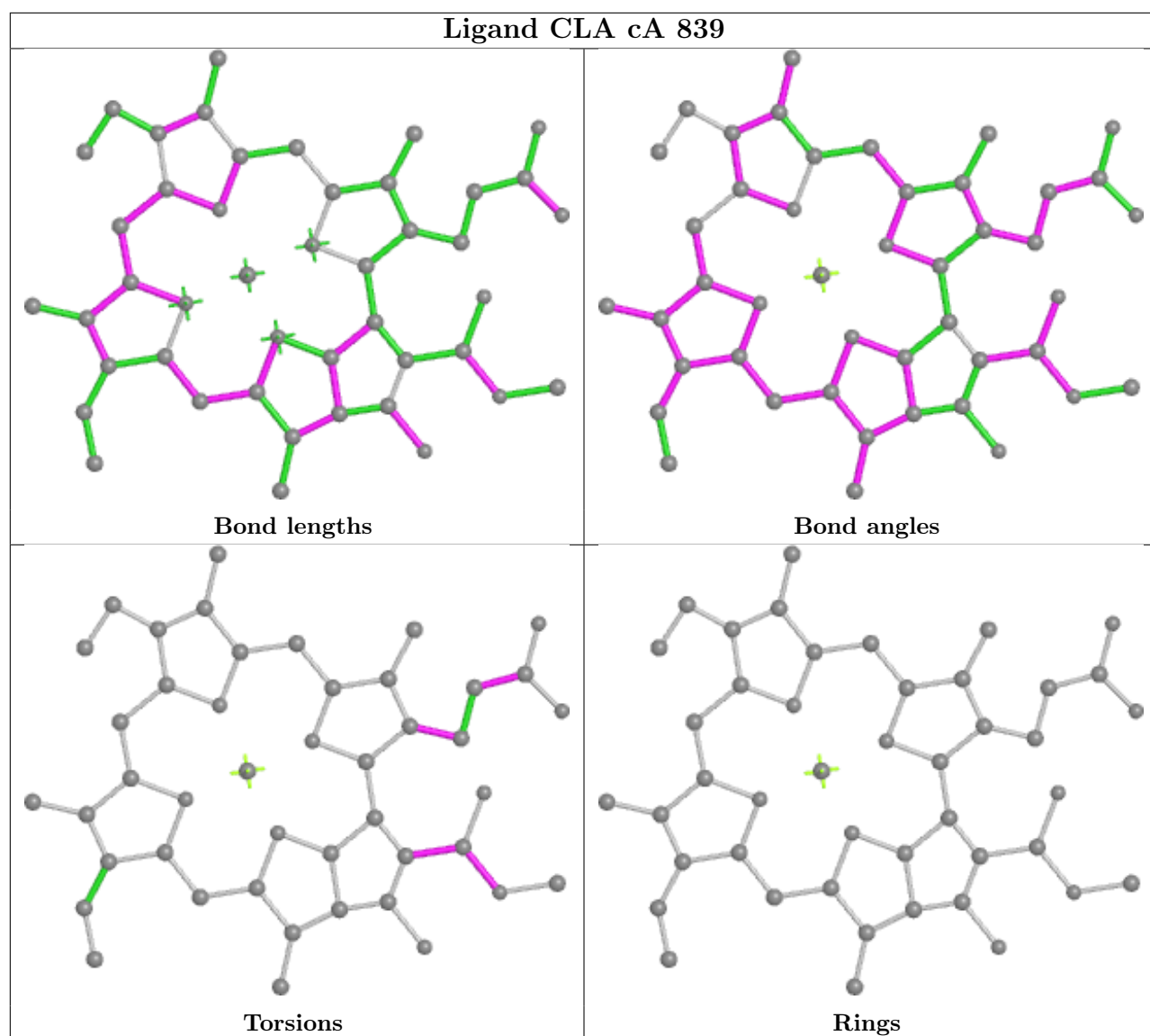




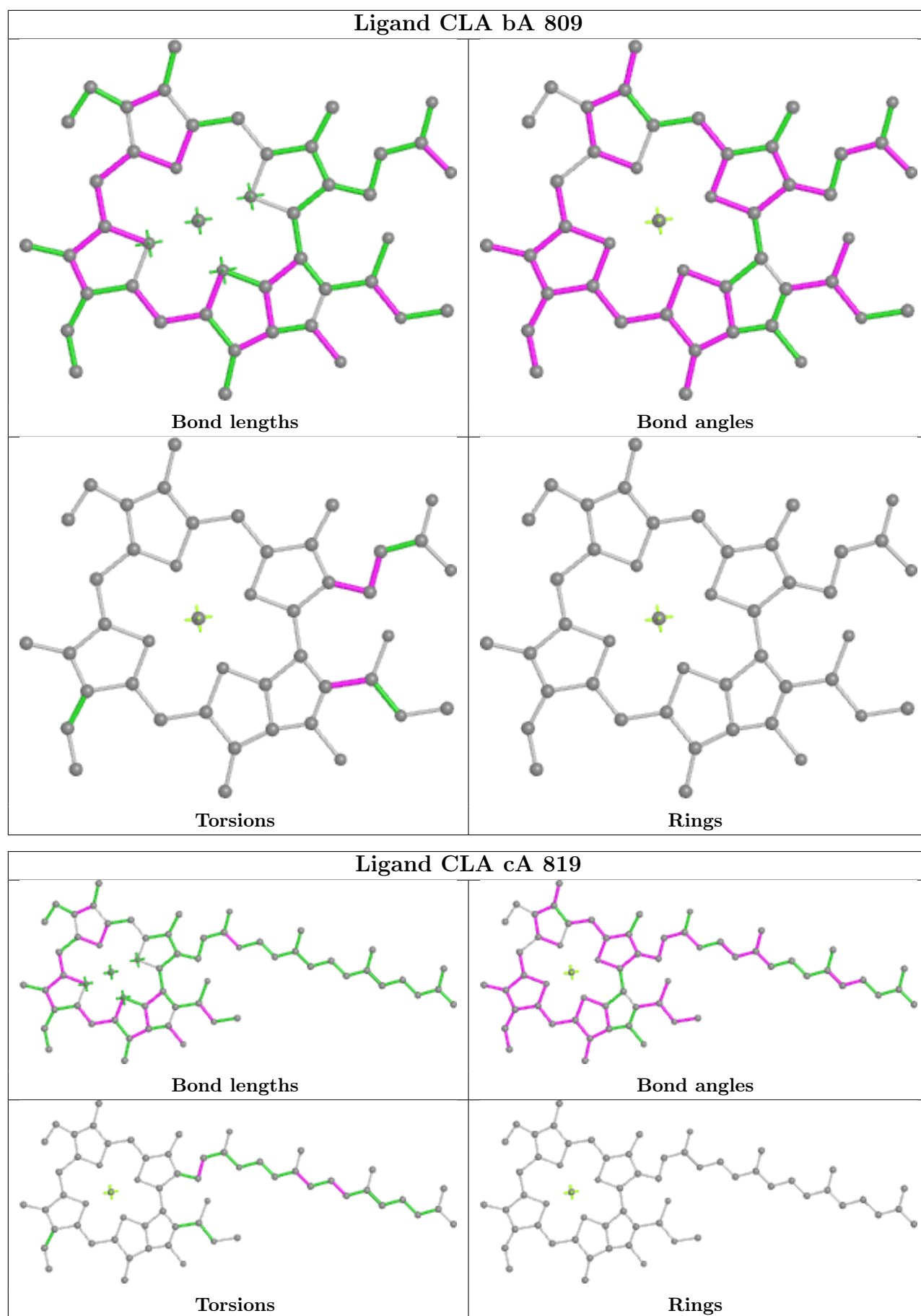


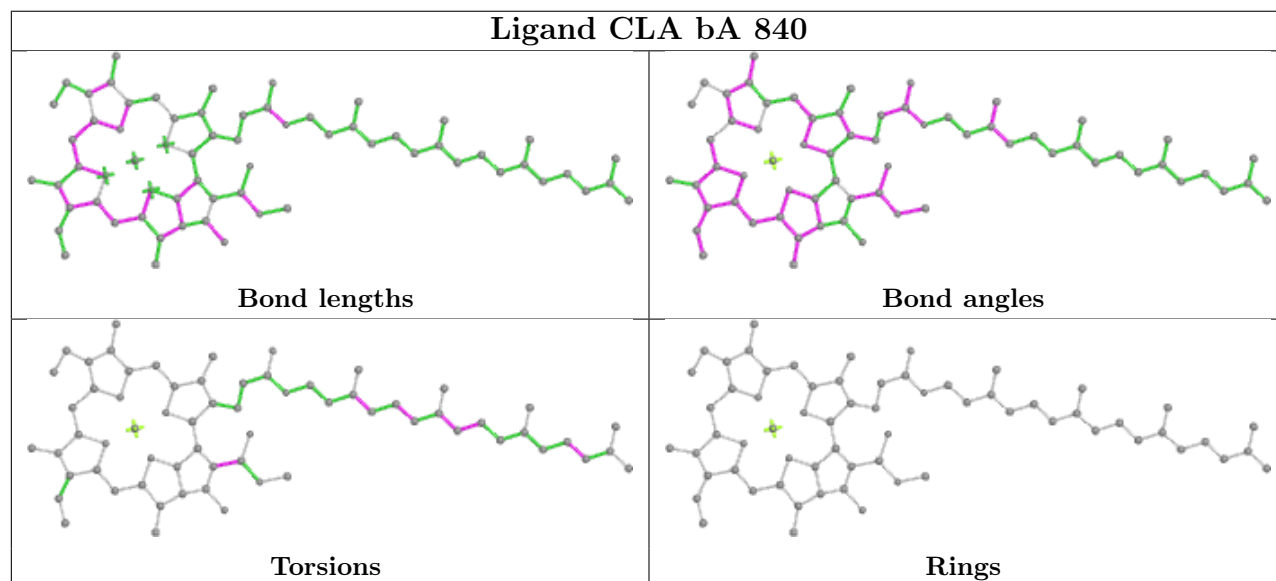
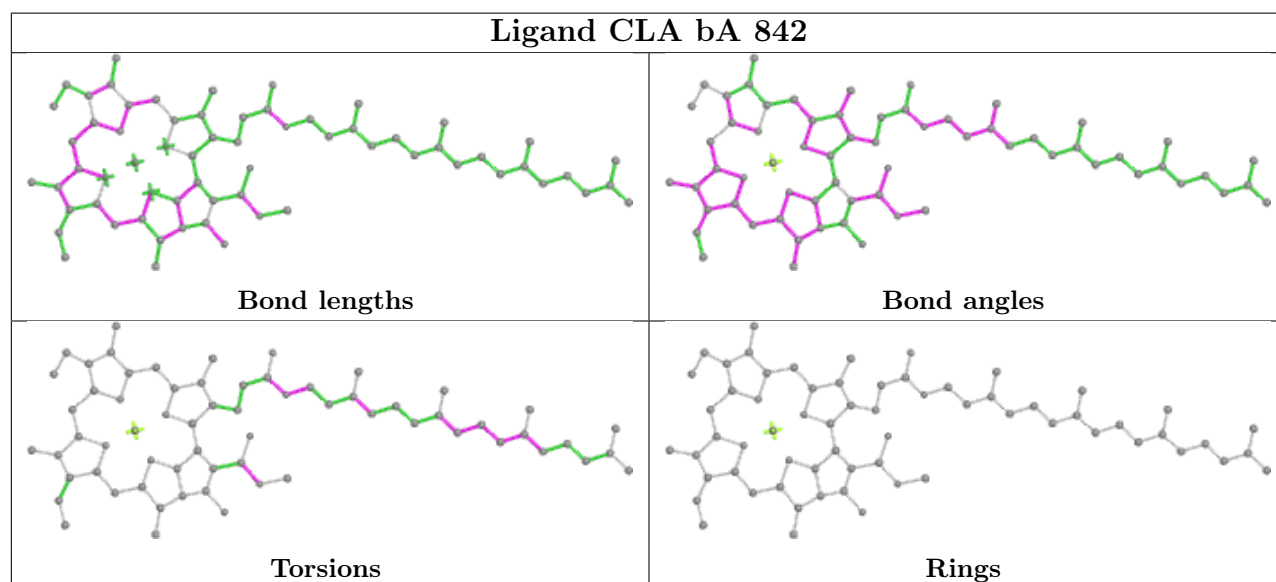
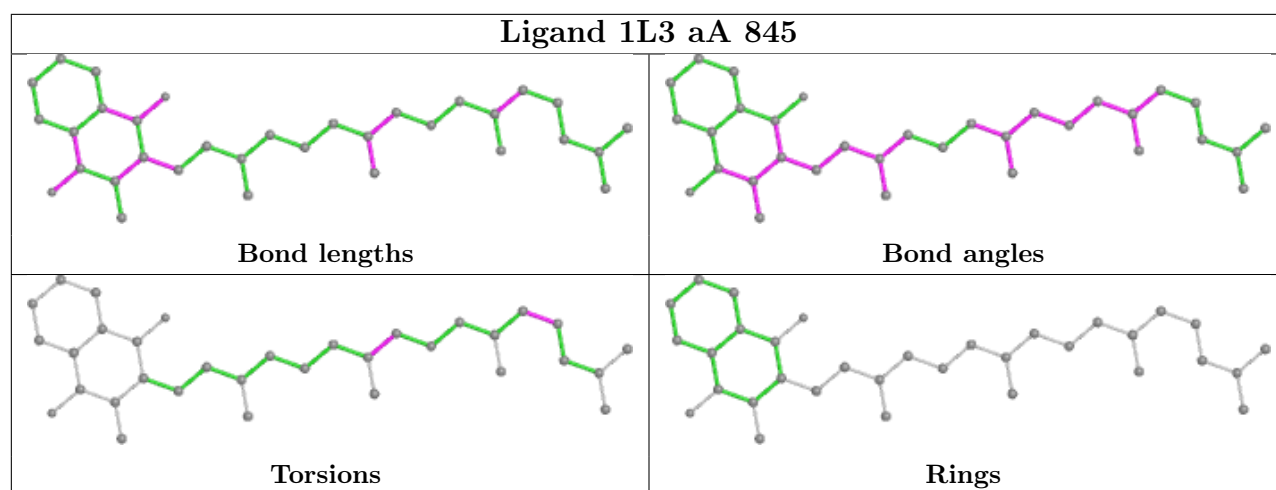


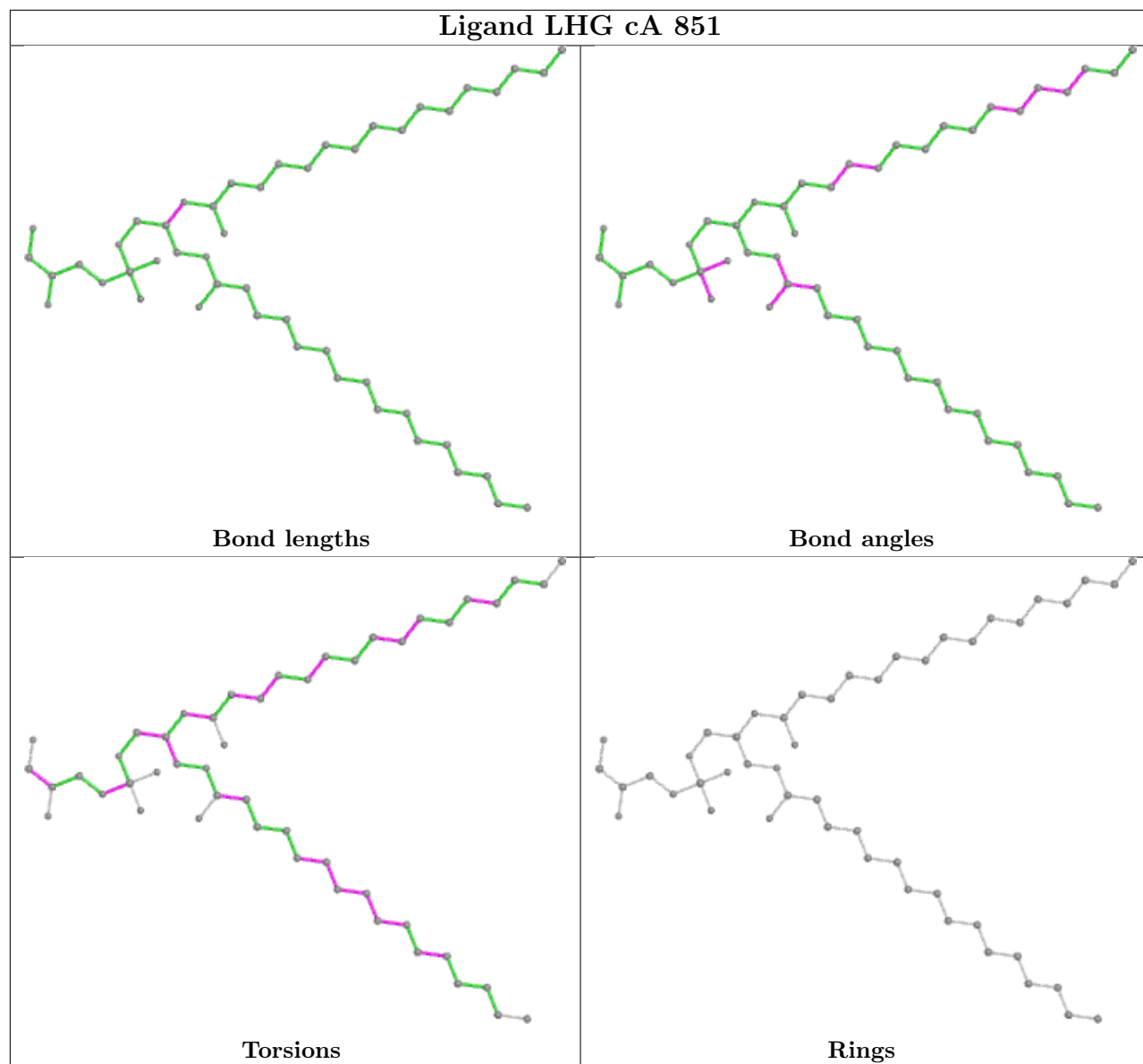


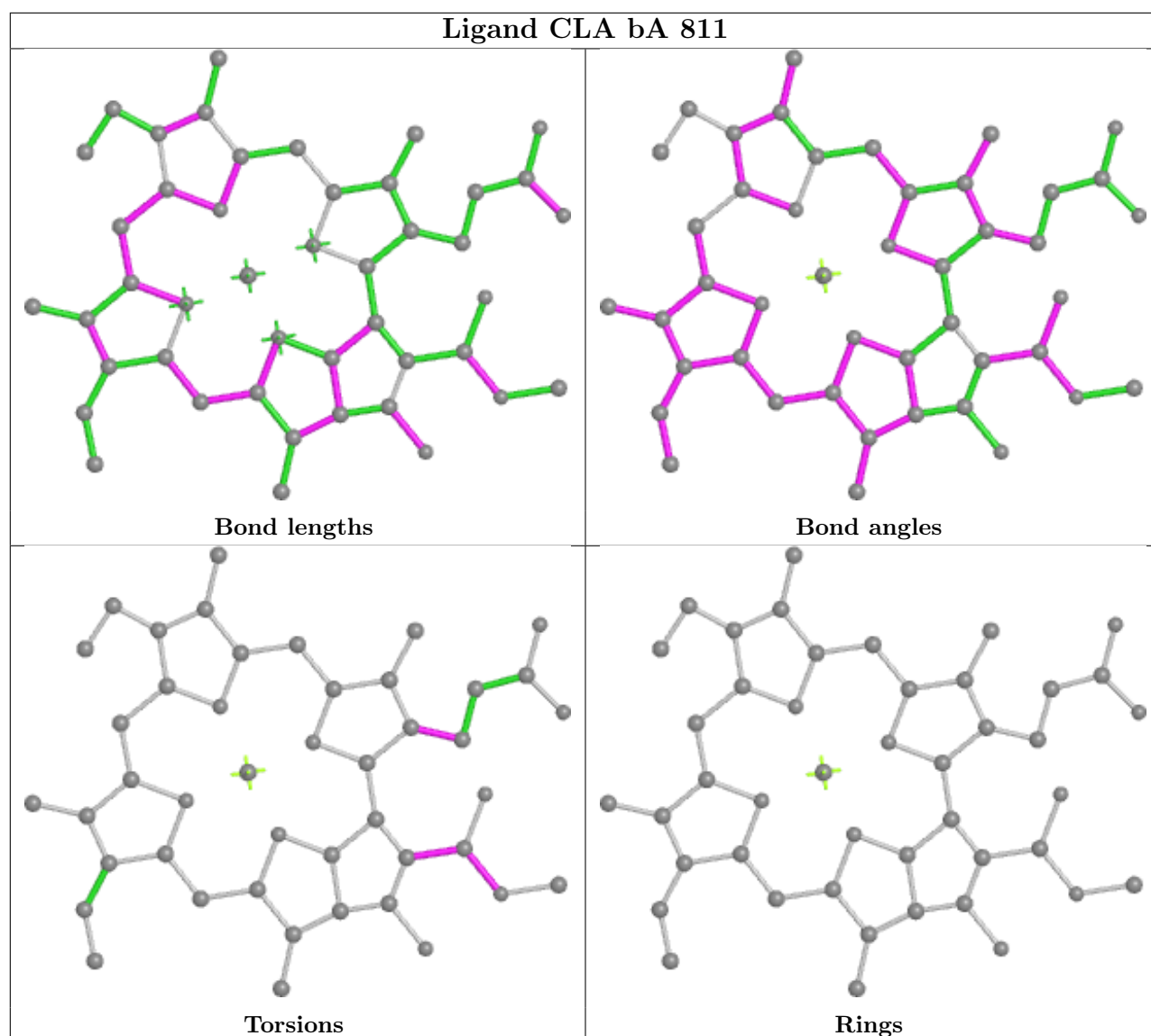












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

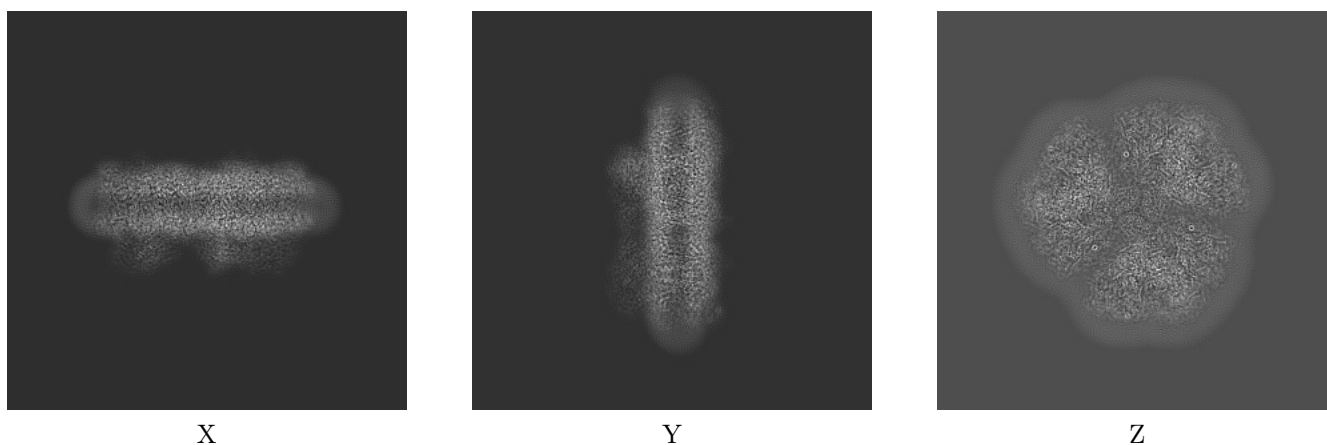
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31455. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

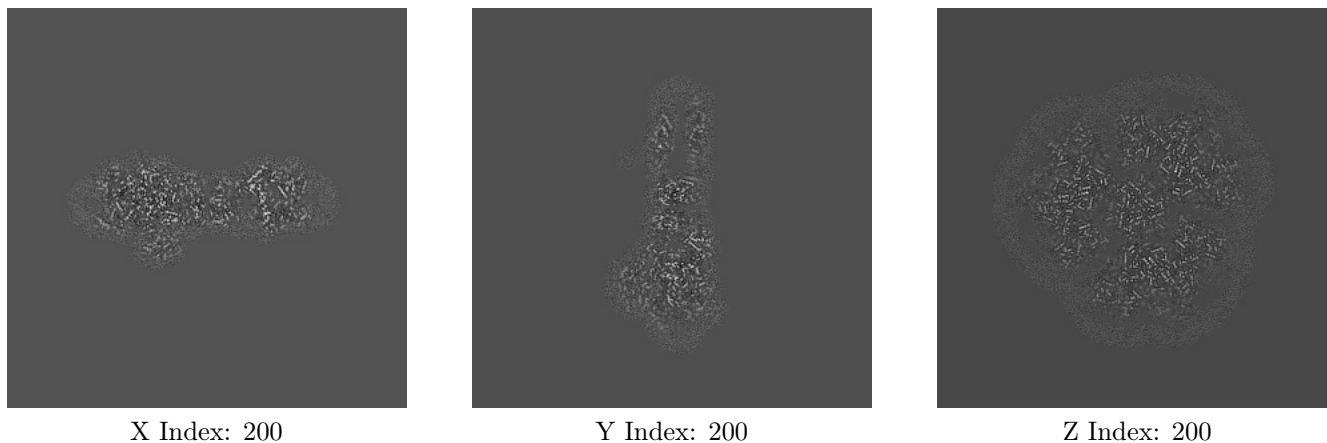
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

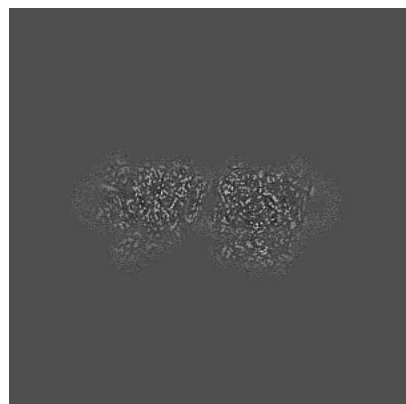
#### 6.2.1 Primary map



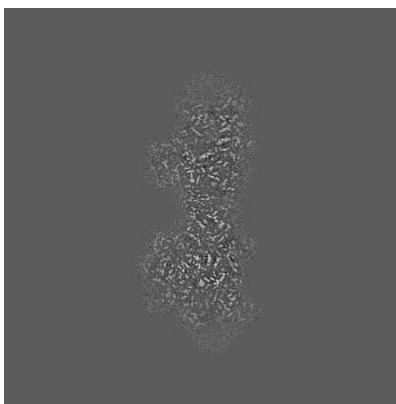
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

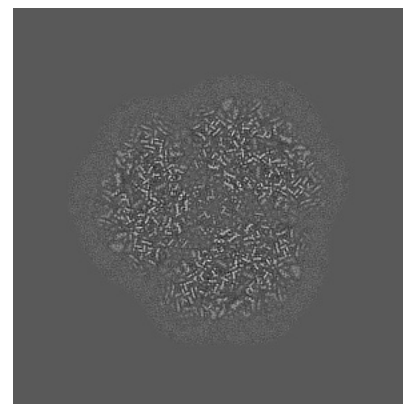
### 6.3.1 Primary map



X Index: 245



Y Index: 216

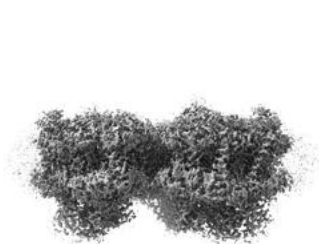


Z Index: 219

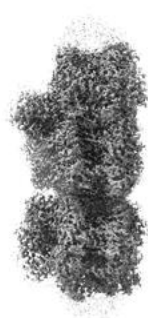
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

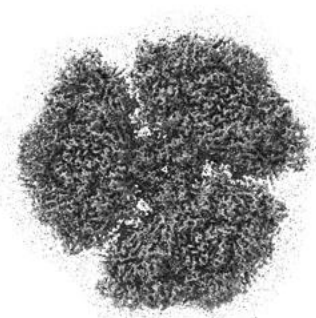
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

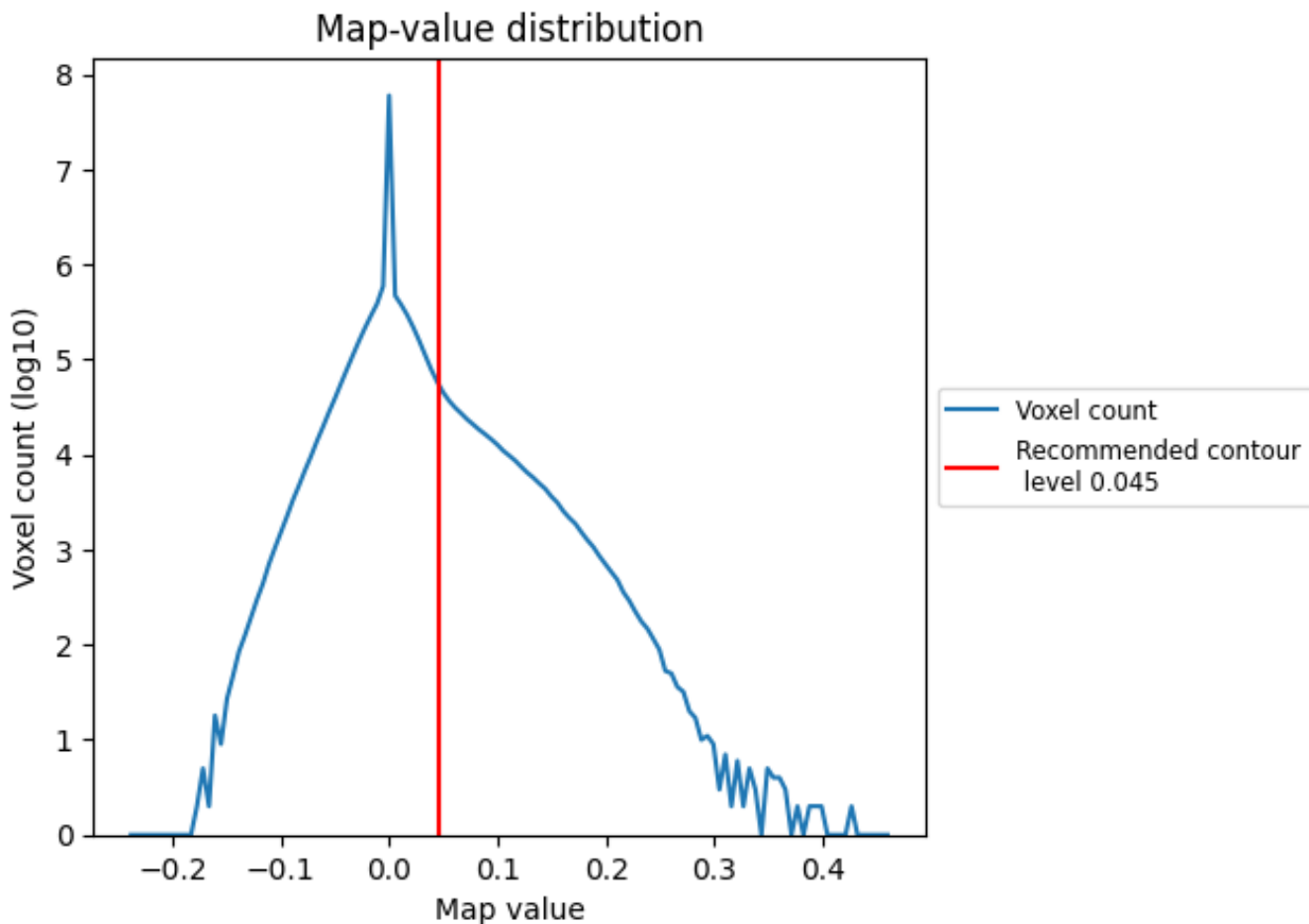
## 6.5 Mask visualisation

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.

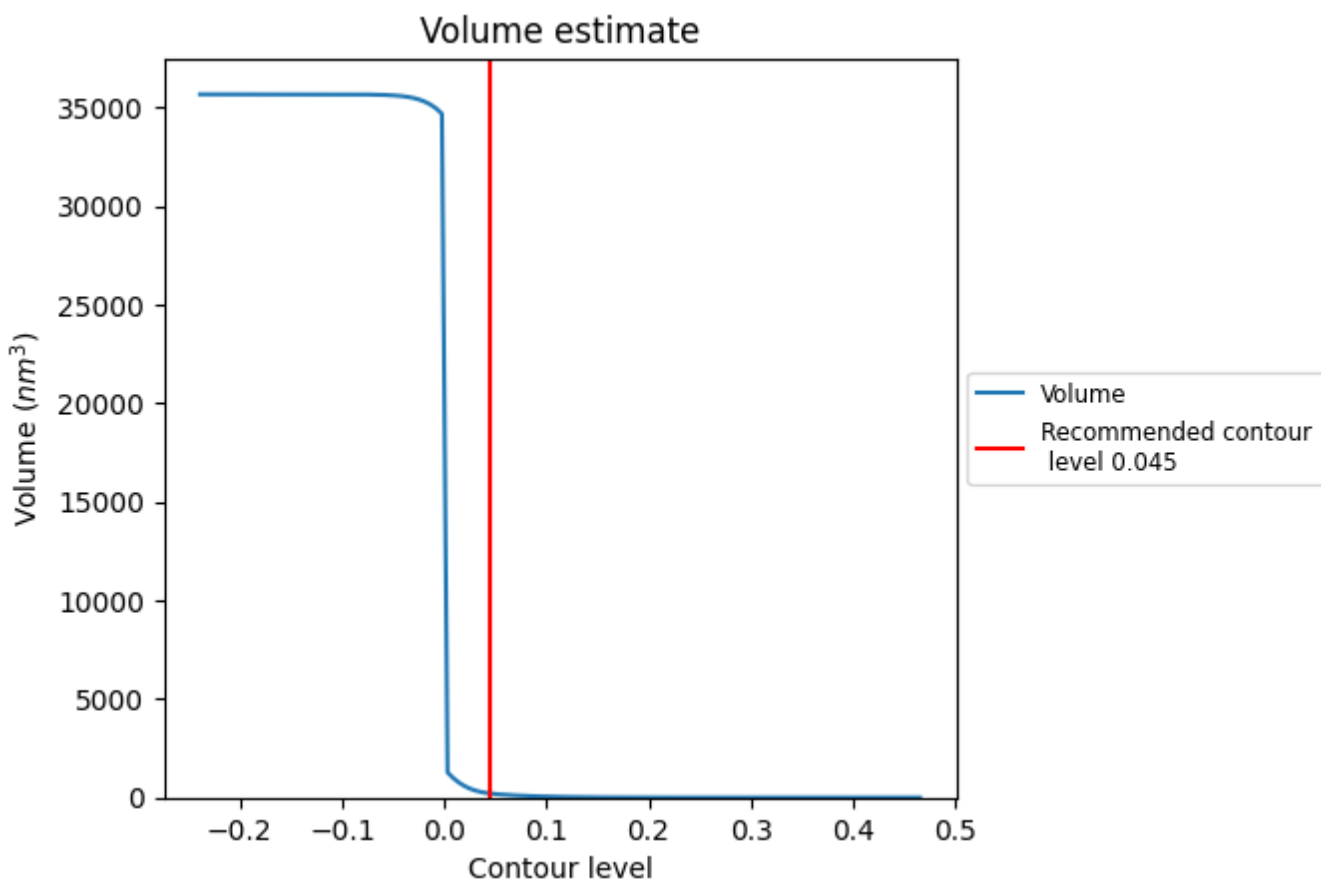
### 7.1 Map-value distribution [i](#)



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.



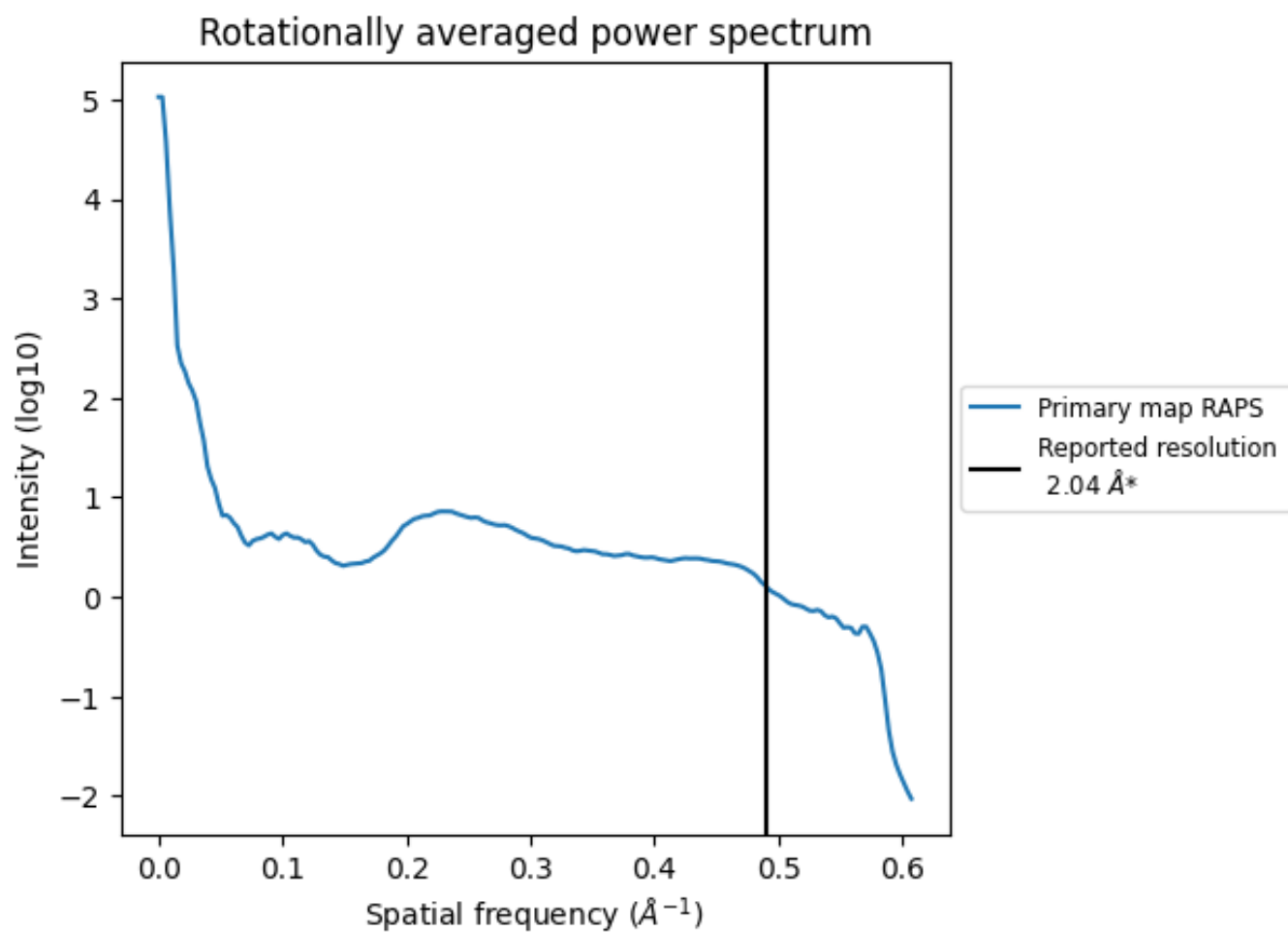
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 209 nm<sup>3</sup>; this corresponds to an approximate mass of 189 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 i

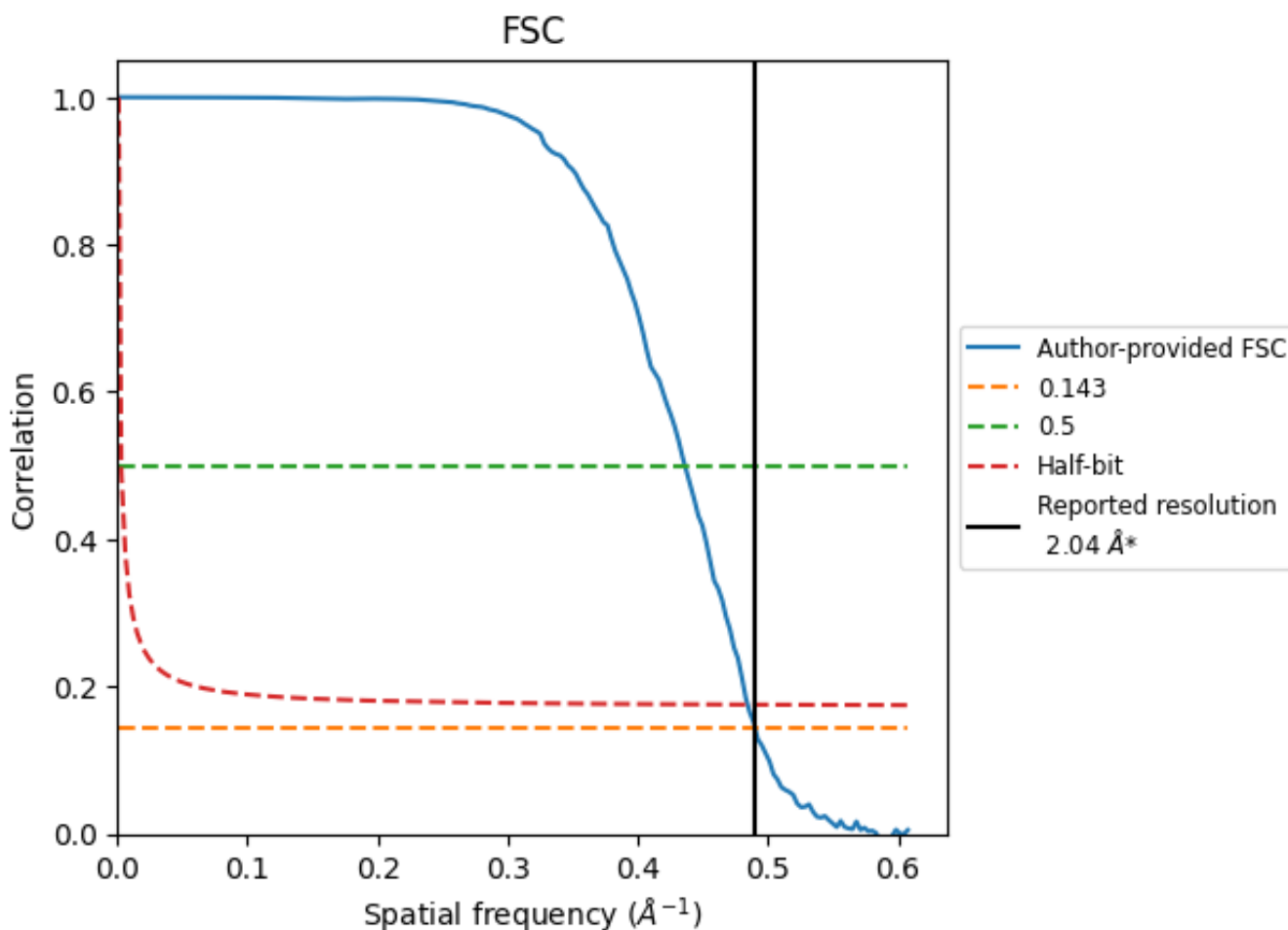


\*Reported resolution corresponds to spatial frequency of 0.490 Å<sup>-1</sup>

## 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 0.490 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

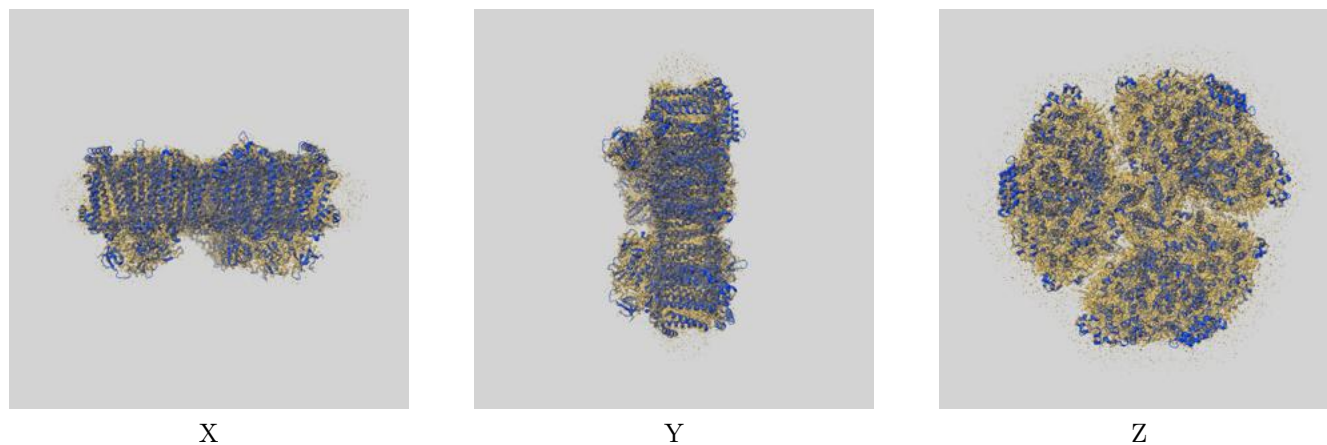
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.04	-	-
Author-provided FSC curve	2.04	2.29	2.06
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

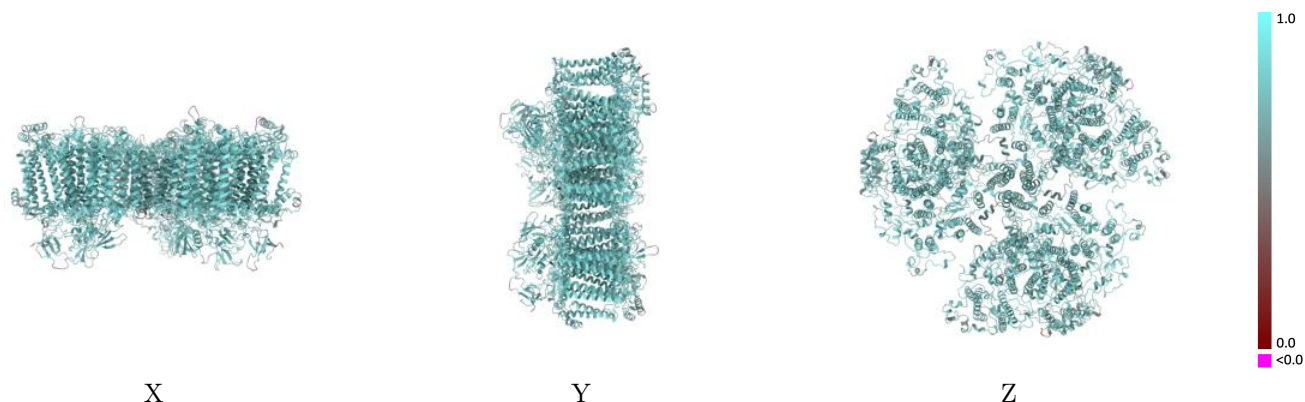
This section contains information regarding the fit between EMDB map EMD-31455 and PDB model 7F4V. Per-residue inclusion information can be found in section [3](#) on page [34](#).

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



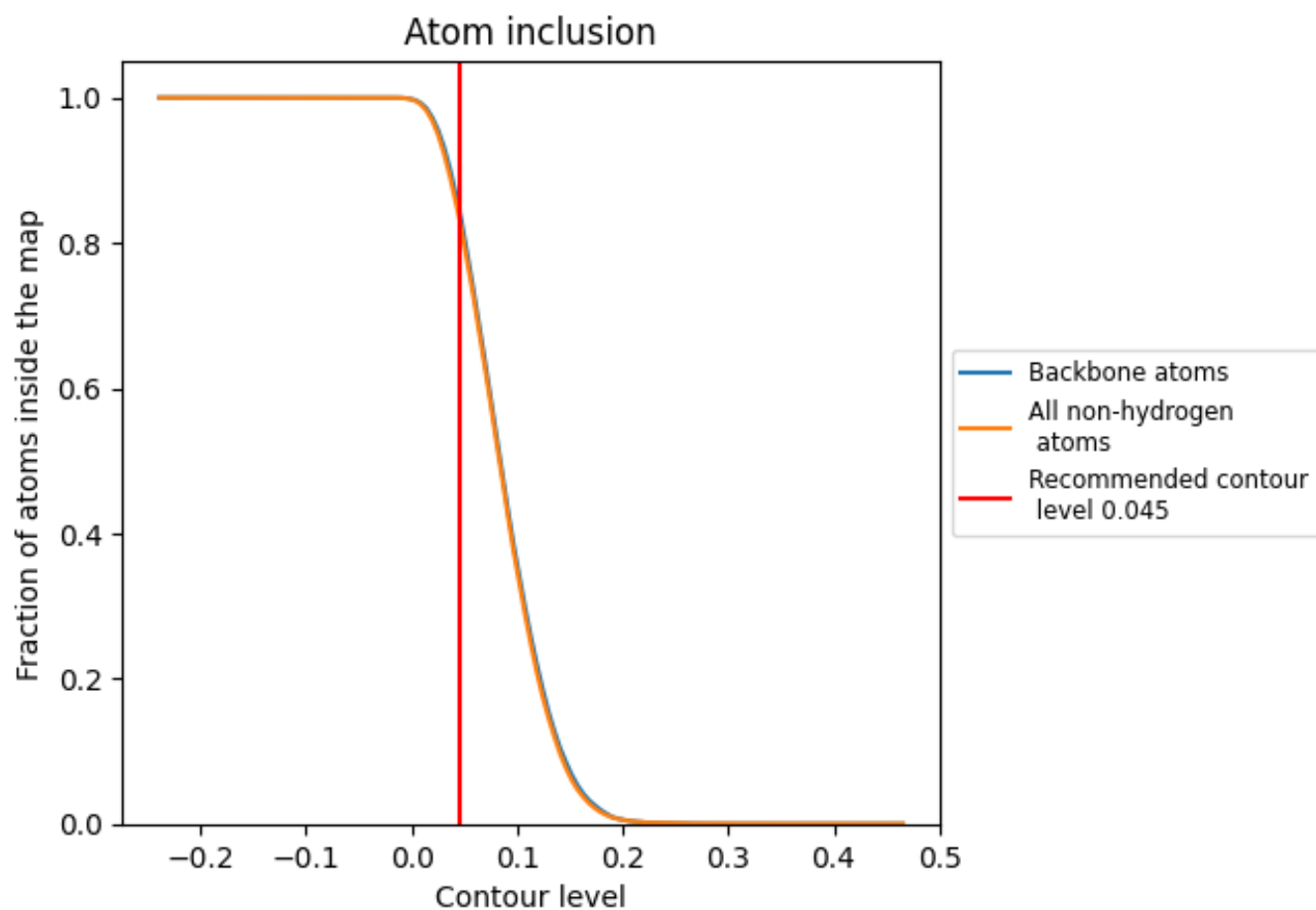
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8363	 0.7520
aA	 0.8580	 0.7580
aB	 0.8963	 0.7710
aC	 0.9168	 0.7710
aD	 0.6994	 0.7180
aE	 0.6138	 0.6720
aF	 0.5443	 0.6770
aI	 0.8339	 0.7470
aJ	 0.7451	 0.7110
aL	 0.8458	 0.7570
aM	 0.8478	 0.7480
bA	 0.8530	 0.7560
bB	 0.8941	 0.7690
bC	 0.9185	 0.7680
bD	 0.6925	 0.7150
bE	 0.5955	 0.6670
bF	 0.5276	 0.6720
bI	 0.8339	 0.7450
bJ	 0.7500	 0.7120
bL	 0.8400	 0.7540
bM	 0.8391	 0.7460
cA	 0.8501	 0.7550
cB	 0.8923	 0.7690
cC	 0.9318	 0.7690
cD	 0.6876	 0.7150
cE	 0.6016	 0.6650
cF	 0.5299	 0.6720
cI	 0.8303	 0.7480
cJ	 0.7451	 0.7060
cL	 0.8375	 0.7500
cM	 0.8478	 0.7470

