



wwPDB EM Validation Summary Report ⓘ

Nov 18, 2024 – 07:04 PM JST

PDB ID : 8XLS
EMDB ID : EMD-38457
Title : PSI-FCPI of the diatom *Thalassiosira pseudonana* CCMP1335
Authors : Kato, K.; Nakajima, Y.; Shen, J.R.; Nagao, R.
Deposited on : 2023-12-26
Resolution : 2.30 Å (reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

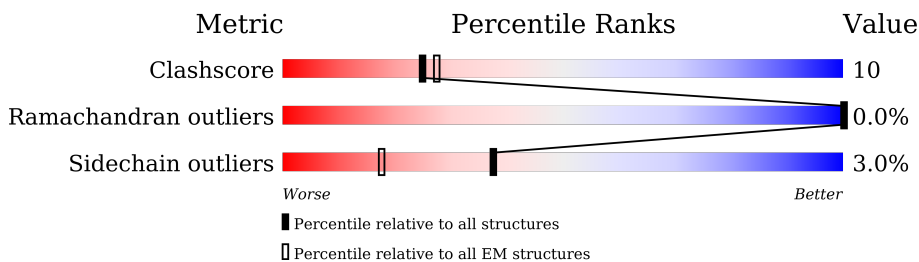
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	752	
2	B	733	
3	C	81	
4	D	139	
5	E	65	
6	F	185	
7	I	36	
8	J	41	

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Mol	Chain	Length	Quality of chain
9	L	148	
10	M	30	
11	W	188	
12	u	84	
13	1	221	
14	2	198	
15	3	196	
16	4	201	
17	5	194	

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
18	CL0	A	801	X	-	-	-
19	CLA	1	301	X	-	-	-
19	CLA	1	303	X	-	-	-
19	CLA	1	304	X	-	-	-
19	CLA	1	306	X	-	-	-
19	CLA	1	307	X	-	-	-
19	CLA	1	308	X	-	-	-
19	CLA	1	309	X	-	-	-
19	CLA	1	310	X	-	-	-
19	CLA	2	205	X	-	-	-
19	CLA	2	206	X	-	-	-
19	CLA	2	207	X	-	-	-
19	CLA	2	208	X	-	-	-
19	CLA	2	209	X	-	-	-
19	CLA	2	210	X	-	-	-
19	CLA	2	212	X	-	-	-
19	CLA	2	213	X	-	-	-
19	CLA	2	214	X	-	-	-
19	CLA	2	215	X	-	-	-
19	CLA	3	202	X	-	-	-
19	CLA	3	203	X	-	-	-
19	CLA	3	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	3	206	X	-	-	-
19	CLA	3	207	X	-	-	-
19	CLA	3	209	X	-	-	-
19	CLA	3	210	X	-	-	-
19	CLA	4	301	X	-	-	-
19	CLA	4	303	X	-	-	-
19	CLA	4	304	X	-	-	-
19	CLA	4	305	X	-	-	-
19	CLA	4	306	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	5	207	X	-	-	-
19	CLA	5	208	X	-	-	-
19	CLA	5	209	X	-	-	-
19	CLA	5	210	X	-	-	-
19	CLA	5	211	X	-	-	-
19	CLA	5	212	X	-	-	-
19	CLA	5	213	X	-	-	-
19	CLA	5	214	X	-	-	-
19	CLA	A	802	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	843	X	-	-	-
19	CLA	A	844	X	-	-	-
19	CLA	A	878	X	-	-	-
19	CLA	A	880	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	B	846	X	-	-	-
19	CLA	F	203	X	-	-	-
19	CLA	F	204	X	-	-	-
19	CLA	J	103	X	-	-	-
19	CLA	L	204	X	-	-	-
19	CLA	L	206	X	-	-	-
19	CLA	u	201	X	-	-	-
19	CLA	u	202	X	-	-	-
27	5X6	J	105	-	X	-	-

2 Entry composition i

There are 32 unique types of molecules in this entry. The entry contains 37637 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	A	741	5858	3828	994	1007	29	2	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	B	731	5835	3833	985	998	19	2	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	607	373	105	119	10	1	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	D	132	1050	671	181	195	3	1	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	61	494	312	88	94	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	161	1253	801	215	234	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	36	276	191	37	46	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	41	342	233	49	57	3	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	L	146	1106	728	182	194	2	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	30	228	152	35	39	2	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit Psa29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	W	122	912	576	144	188	4	0	0

- Molecule 12 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	u	76	380	228	76	76	0	0

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c-binding protein RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	1	185	1413	902	235	262	14	0	0

- Molecule 14 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	2	167	1288	825	213	240	10	0	0

- Molecule 15 is a protein called Pt17531-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	3	164	1273	821	208	234	10	0	0

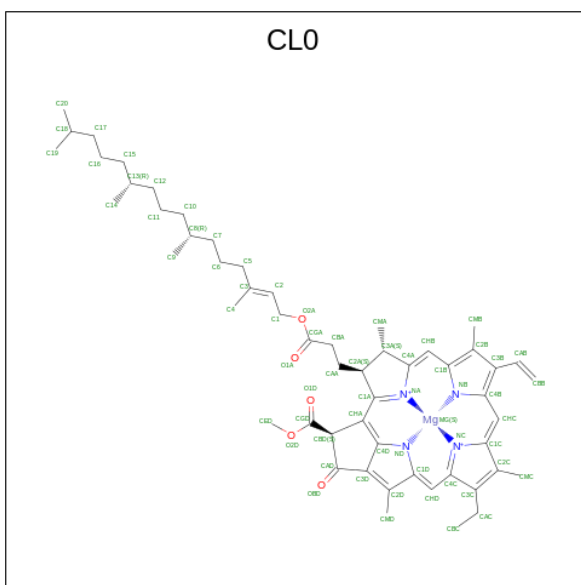
- Molecule 16 is a protein called Fucoxanthin chl a/c light-harvesting protein, major type.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	4	167	1289	834	210	237	8	0	0

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

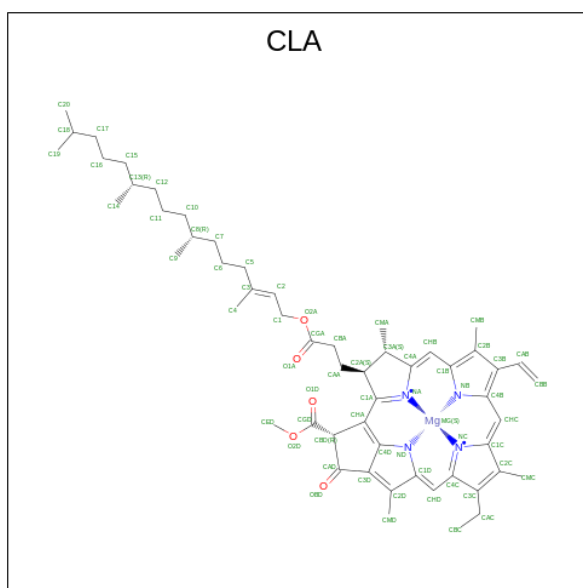
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	5	165	1285	833	204	240	8	0	0

- Molecule 18 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms				AltConf	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	A	1	50	40	1	4	5	0
19	A	1	50	40	1	4	5	0
19	A	1	49	39	1	4	5	0
19	A	1	54	44	1	4	5	0
19	A	1	54	44	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	54	44	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	49	39	1	4	5	0
19	A	1	51	41	1	4	5	0
19	A	1	59	49	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	60	50	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	A	1	54	44	1	4	5	0
19	A	1	45	35	1	4	5	0
19	A	1	51	41	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	47	37	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	45	35	1	4	5	0
19	B	1	55	45	1	4	5	0
19	B	1	59	49	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	45	35	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	54	44	1	4	5	0
19	B	1	56	46	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	45	35	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	58	48	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	1	1	Total 55	C 45	Mg 1	N 4	O 5	0

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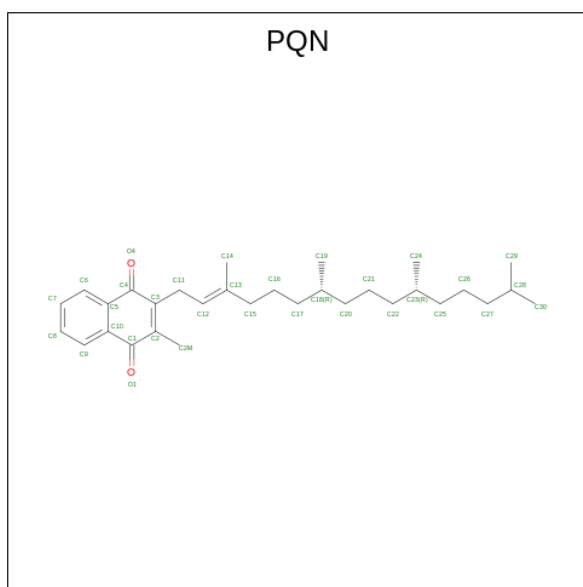
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	1	1	45	35	1	4	5	0
19	1	1	65	55	1	4	5	0
19	1	1	65	55	1	4	5	0
19	2	1	65	55	1	4	5	0
19	2	1	65	55	1	4	5	0
19	2	1	65	55	1	4	5	0
19	2	1	52	42	1	4	5	0
19	2	1	58	48	1	4	5	0
19	2	1	60	50	1	4	5	0
19	2	1	45	35	1	4	5	0
19	2	1	45	35	1	4	5	0
19	2	1	45	35	1	4	5	0
19	2	1	42	34	1	4	3	0
19	3	1	65	55	1	4	5	0
19	3	1	55	45	1	4	5	0
19	3	1	61	51	1	4	5	0
19	3	1	65	55	1	4	5	0
19	3	1	65	55	1	4	5	0
19	3	1	51	41	1	4	5	0
19	3	1	45	35	1	4	5	0
19	4	1	65	55	1	4	5	0

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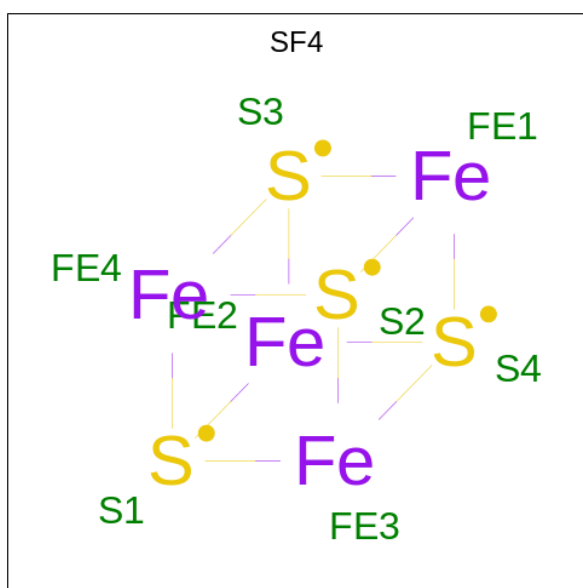
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	4	1	55	45	1	4	5	0
19	4	1	50	40	1	4	5	0
19	4	1	65	55	1	4	5	0
19	4	1	58	48	1	4	5	0
19	4	1	45	35	1	4	5	0
19	4	1	45	35	1	4	5	0
19	4	1	45	35	1	4	5	0
19	4	1	50	40	1	4	5	0
19	4	1	52	42	1	4	5	0
19	4	1	55	45	1	4	5	0
19	5	1	60	50	1	4	5	0
19	5	1	60	50	1	4	5	0
19	5	1	65	55	1	4	5	0
19	5	1	65	55	1	4	5	0
19	5	1	58	48	1	4	5	0
19	5	1	56	46	1	4	5	0
19	5	1	45	35	1	4	5	0
19	5	1	45	35	1	4	5	0
19	5	1	45	35	1	4	5	0
19	5	1	42	34	1	4	3	0

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



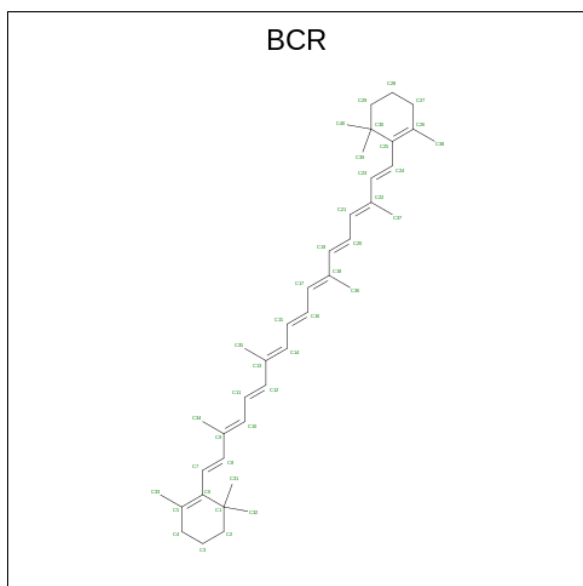
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



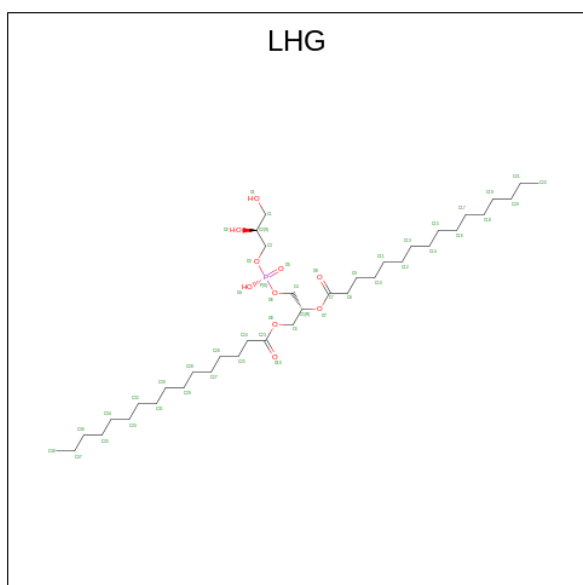
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
22	F	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	M	1	Total C 40 40	0
22	1	1	Total C 40 40	0
22	1	1	Total C 40 40	0

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



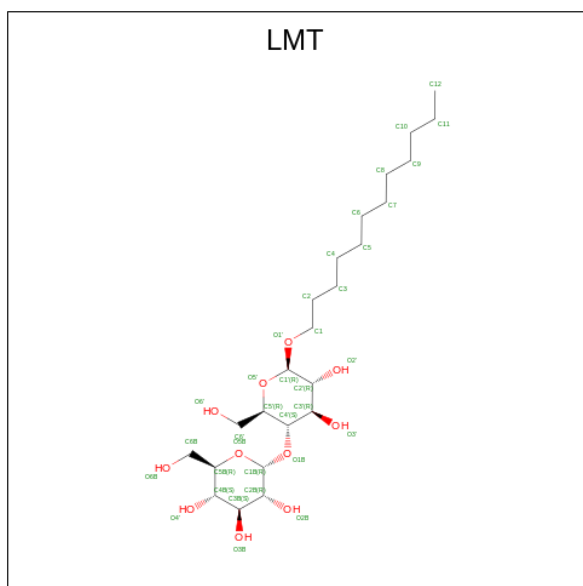
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O P 47 36 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
23	A	1	Total 49	C 38	O 10	P 1	0
23	B	1	Total 35	C 24	O 10	P 1	0
23	M	1	Total 41	C 30	O 10	P 1	0
23	1	1	Total 41	C 30	O 10	P 1	0
23	3	1	Total 34	C 23	O 10	P 1	0
23	4	1	Total 49	C 38	O 10	P 1	0

- Molecule 24 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

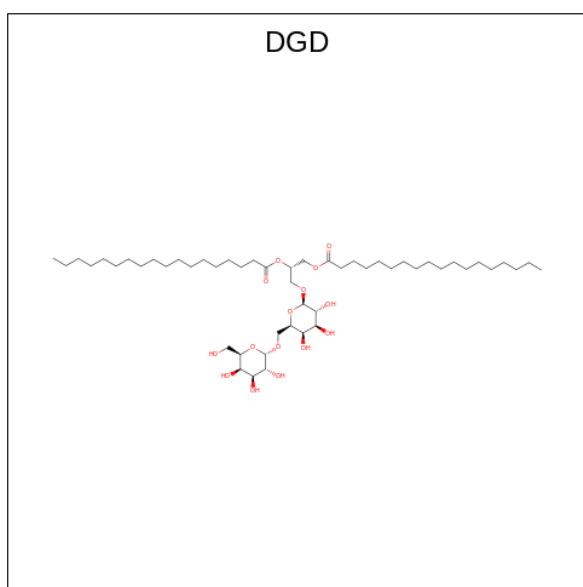


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	A	1	Total 35	C 24	O 11	0
24	1	1	Total 35	C 24	O 11	0
24	2	1	Total 35	C 24	O 11	0
24	3	1	Total 35	C 24	O 11	0

- Molecule 25 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

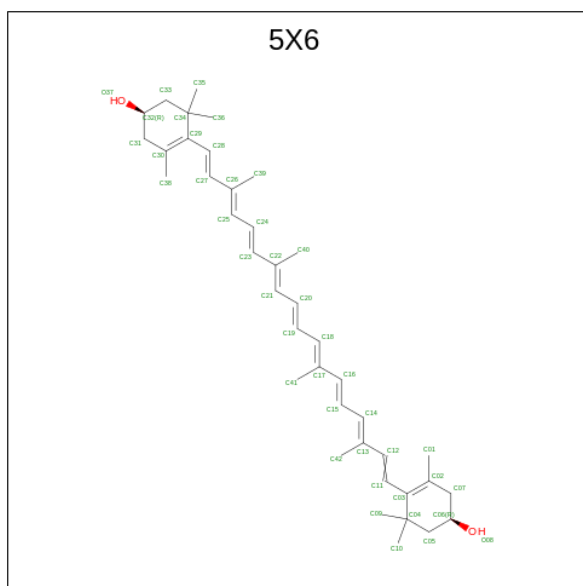
Mol	Chain	Residues	Atoms	AltConf
25	A	25	Total C 230 230	0
25	B	8	Total C 73 73	0
25	F	3	Total C 38 38	0
25	J	4	Total C 39 39	0
25	L	5	Total C 72 72	0
25	M	3	Total C 28 28	0
25	1	4	Total C 38 38	0
25	2	12	Total C 86 86	0
25	3	12	Total C 124 124	0
25	4	3	Total C 21 21	0
25	5	10	Total C 111 111	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



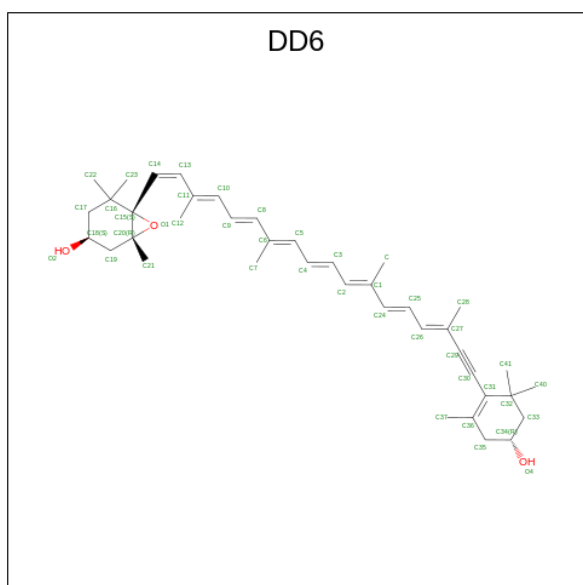
Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	C	O	0
			66	51	15	

- Molecule 27 is Zeaxanthin (three-letter code: 5X6) (formula: $C_{40}H_{56}O_2$).



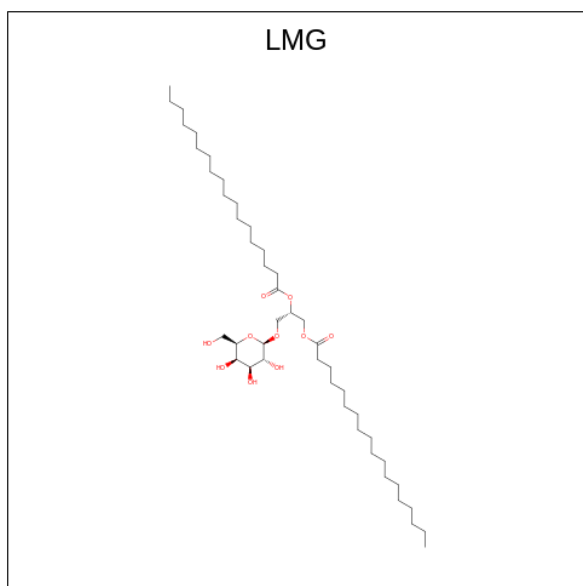
Mol	Chain	Residues	Atoms			AltConf
27	J	1	Total	C	O	0
			42	40	2	

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (three-letter code: DD6) (formula: $C_{40}H_{54}O_3$).



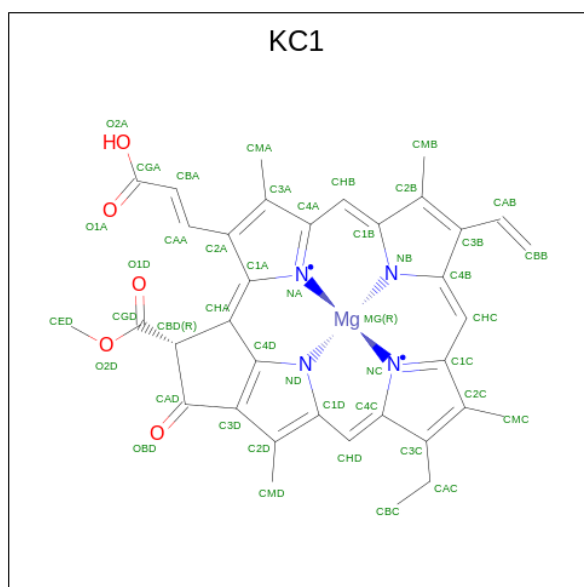
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	L	1	43	40	3	0
28	1	1	43	40	3	0
28	1	1	43	40	3	0
28	1	1	43	40	3	0
28	2	1	43	40	3	0
28	3	1	43	40	3	0
28	5	1	43	40	3	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



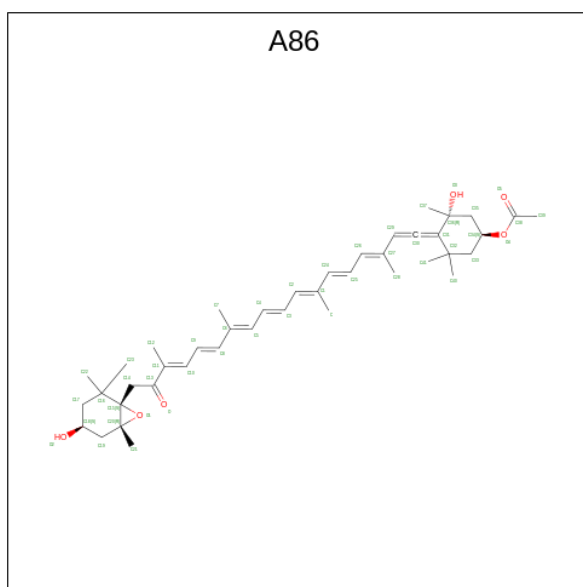
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	1	1	49	39	10	0

- Molecule 30 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
30	1	1	45	35	1	4	5	0
30	2	1	45	35	1	4	5	0
30	3	1	45	35	1	4	5	0
30	3	1	45	35	1	4	5	0
30	3	1	45	35	1	4	5	0
30	4	1	45	35	1	4	5	0
30	4	1	45	35	1	4	5	0

- Molecule 31 is (3*S*,3'*S*,5*R*,5'*R*,6*S*,6'*R*,8'*R*)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (three-letter code: A86) (formula: C₄₂H₅₈O₆).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			48	42	6	
31	1	1	Total	C	O	0
			48	42	6	
31	2	1	Total	C	O	0
			48	42	6	
31	2	1	Total	C	O	0
			48	42	6	
31	2	1	Total	C	O	0
			48	42	6	
31	3	1	Total	C	O	0
			48	42	6	
31	3	1	Total	C	O	0
			48	42	6	
31	3	1	Total	C	O	0
			48	42	6	
31	4	1	Total	C	O	0
			48	42	6	
31	4	1	Total	C	O	0
			48	42	6	
31	4	1	Total	C	O	0
			48	42	6	
31	5	1	Total	C	O	0
			48	42	6	
31	5	1	Total	C	O	0
			48	42	6	
31	5	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	5	1	48	42	6	0

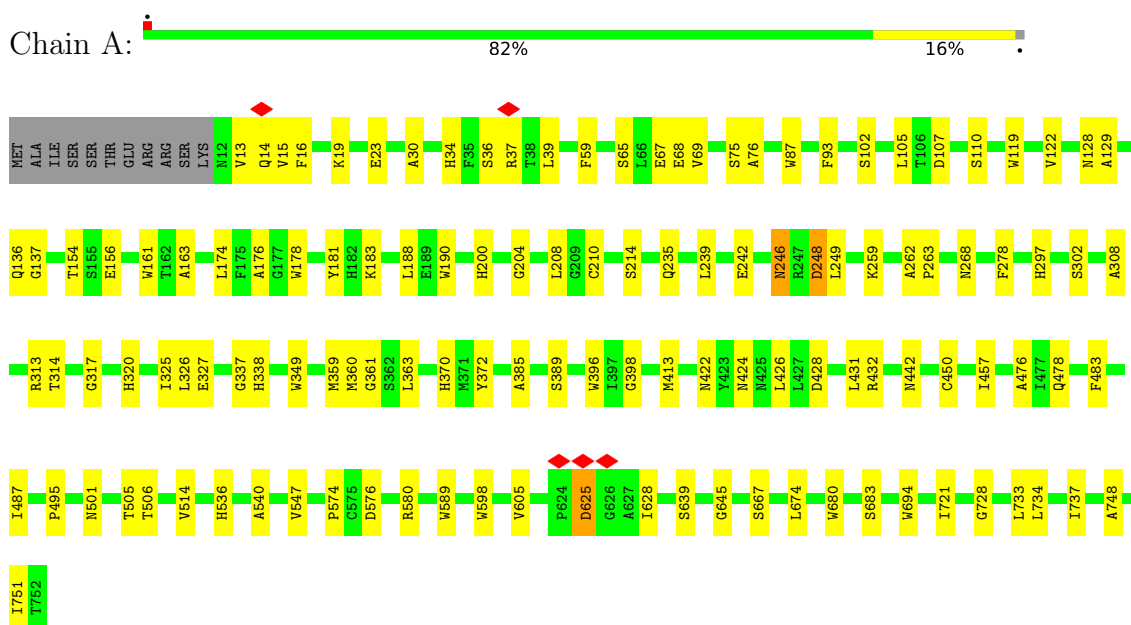
- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
32	A	240	240	240	0
32	B	300	300	300	0
32	C	50	50	50	0
32	D	56	56	56	0
32	E	24	24	24	0
32	F	46	46	46	0
32	I	6	6	6	0
32	J	7	7	7	0
32	L	30	30	30	0
32	M	7	7	7	0
32	W	20	20	20	0
32	u	3	3	3	0
32	1	49	49	49	0
32	2	22	22	22	0
32	3	34	34	34	0
32	4	11	11	11	0
32	5	17	17	17	0

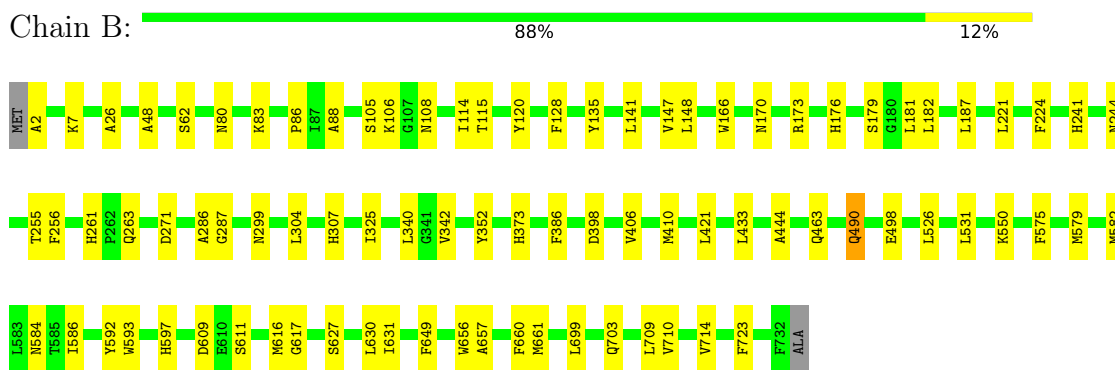
3 Residue-property plots i

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center

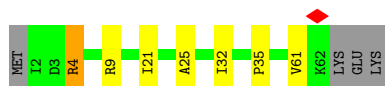
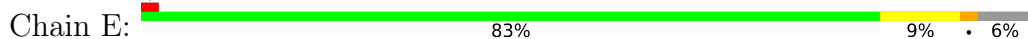




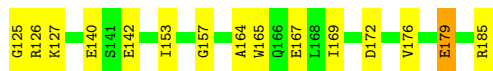
• Molecule 4: Photosystem I reaction center subunit II



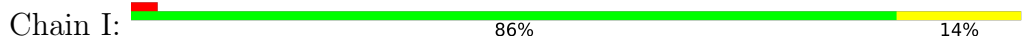
• Molecule 5: Photosystem I reaction center subunit IV



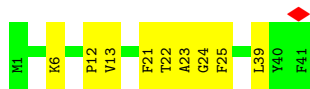
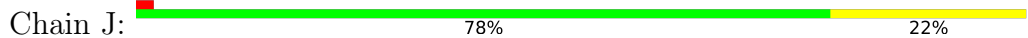
• Molecule 6: Photosystem I reaction center subunit III



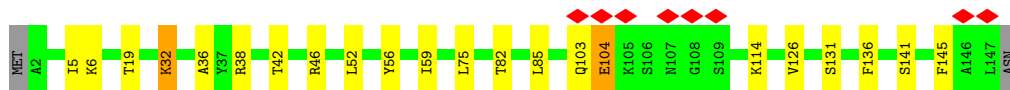
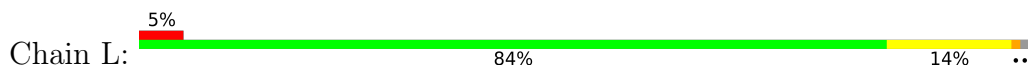
• Molecule 7: Photosystem I reaction center subunit VIII



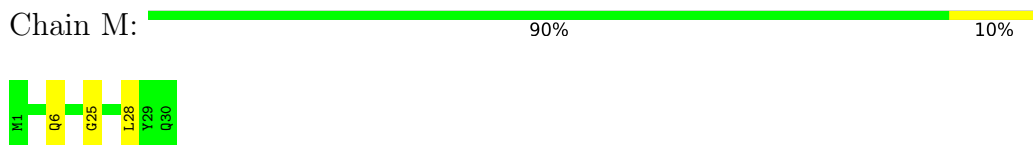
• Molecule 8: Photosystem I reaction center subunit IX



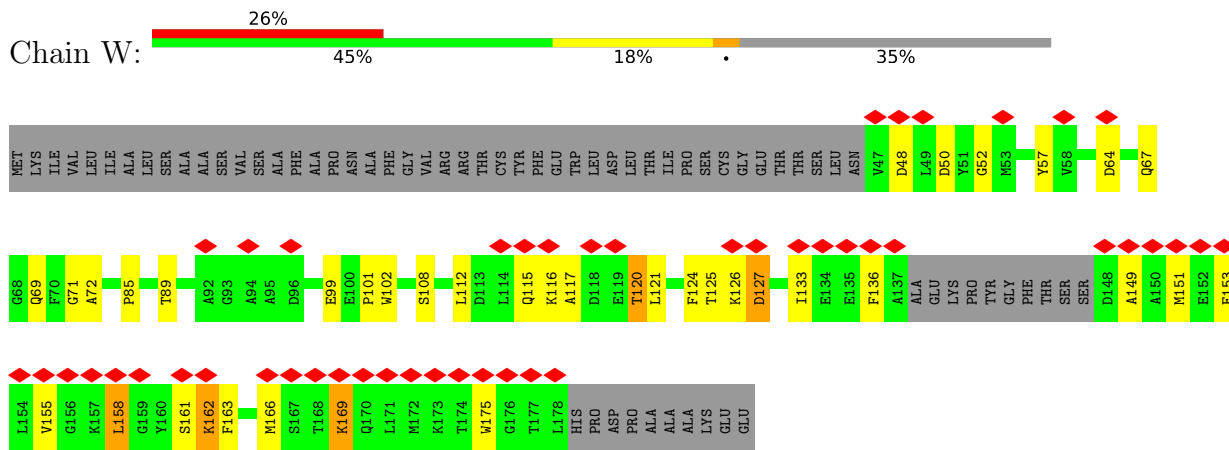
• Molecule 9: Photosystem I reaction center subunit XI



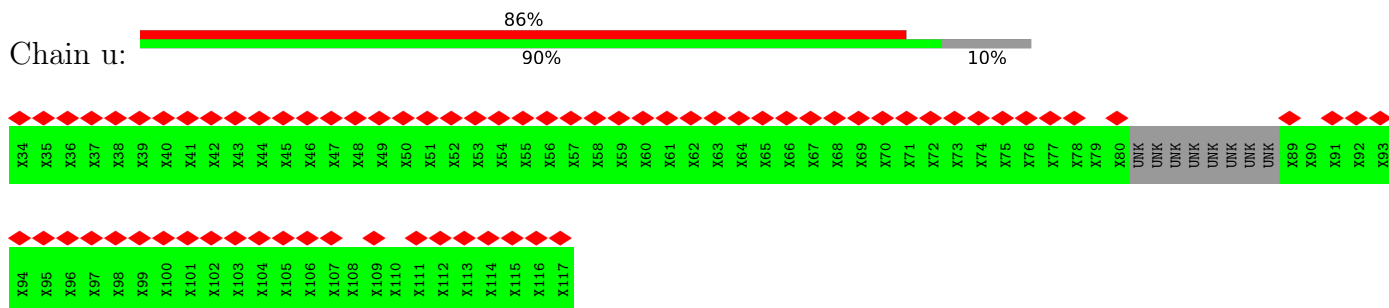
• Molecule 10: Photosystem I reaction center subunit XII



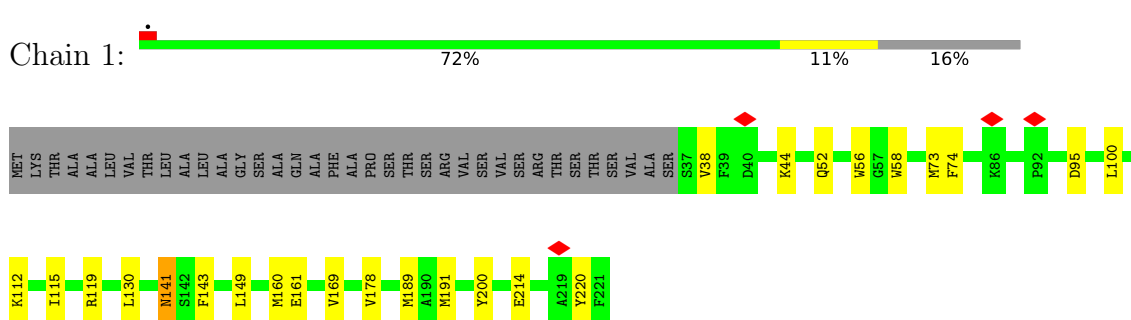
• Molecule 11: Photosystem I reaction center subunit Psa29



• Molecule 12: Unknown protein

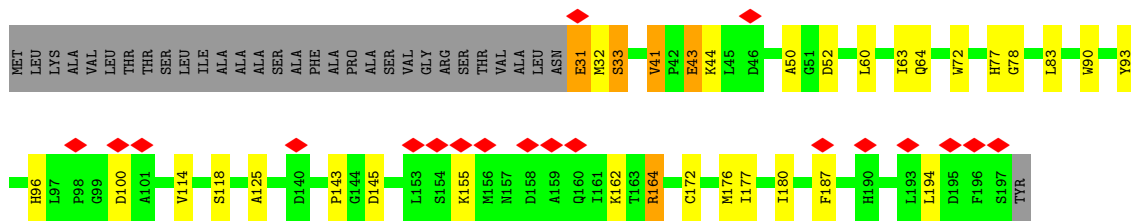


• Molecule 13: Fucoxanthin chlorophyll a/c-binding protein RedCAP

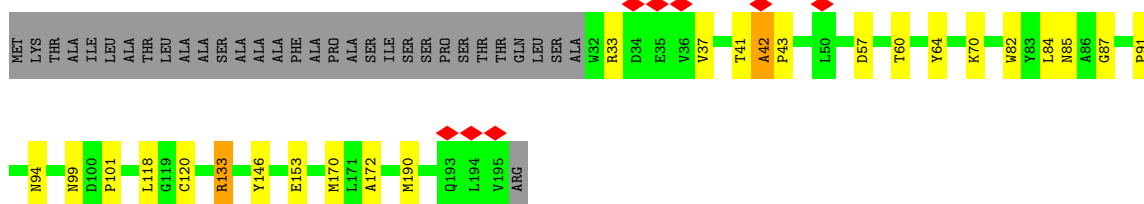


• Molecule 14: Fucoxanthin chl a/c light-harvesting protein

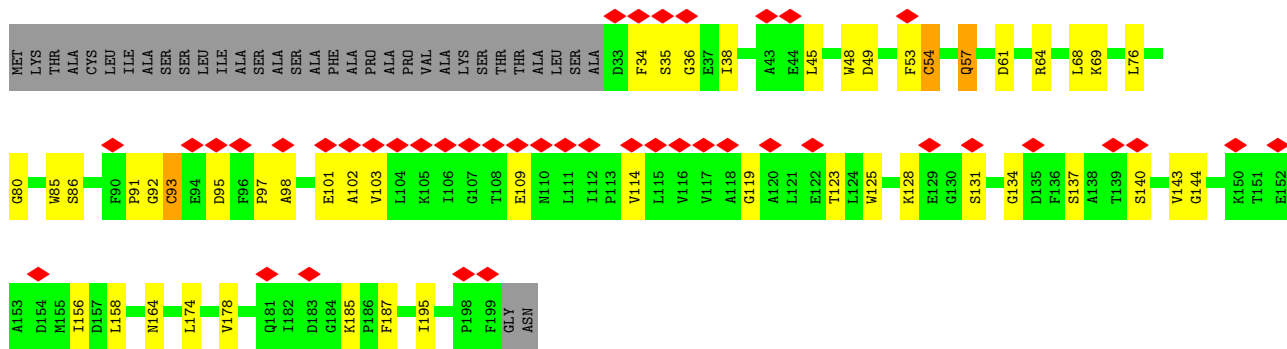




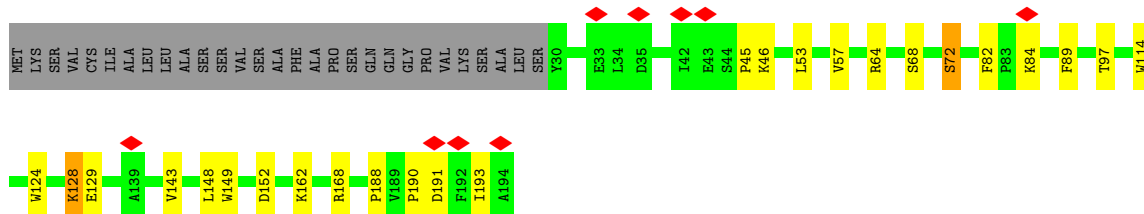
• Molecule 15: Pt17531-like protein



• Molecule 16: Fucoxanthin chl a/c light-harvesting protein, major type



• Molecule 17: Fucoxanthin chlorophyll a/c-binding protein Lhcq8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75667	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	191.008, 191.008, 191.008	wwPDB
Map dimensions	254, 254, 254	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DD6, BCR, LMG, A86, PQN, LHG, CL0, 5X6, LMT, CLA, DGD, SF4, KC1, UNL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/6056	0.49	0/8245
2	B	0.30	0/6045	0.49	0/8252
3	C	0.29	0/617	0.54	0/838
4	D	0.30	0/1077	0.56	0/1455
5	E	0.31	0/502	0.57	0/680
6	F	0.29	0/1282	0.50	0/1741
7	I	0.30	0/284	0.45	0/388
8	J	0.32	0/353	0.50	0/479
9	L	0.30	0/1134	0.51	0/1537
10	M	0.27	0/230	0.47	0/312
11	W	0.28	0/930	0.46	0/1255
13	1	0.28	0/1450	0.45	1/1974 (0.1%)
14	2	0.28	0/1321	0.47	0/1791
15	3	0.31	0/1306	0.50	0/1774
16	4	0.30	0/1326	0.48	0/1795
17	5	0.29	0/1324	0.47	0/1804
All	All	0.30	0/25237	0.49	1/34320 (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
15	3	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	169	VAL	C-N-CA	-5.01	109.17	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	3	42	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5858	0	5684	89	0
2	B	5835	0	5649	76	0
3	C	607	0	586	7	0
4	D	1050	0	1039	18	0
5	E	494	0	488	4	0
6	F	1253	0	1252	21	0
7	I	276	0	287	6	0
8	J	342	0	340	8	0
9	L	1106	0	1128	17	0
10	M	228	0	249	3	0
11	W	912	0	863	24	0
12	u	380	0	81	0	0
13	1	1413	0	1365	14	0
14	2	1288	0	1253	25	0
15	3	1273	0	1231	20	0
16	4	1289	0	1235	37	0
17	5	1285	0	1239	17	0
18	A	65	0	72	5	0
19	1	476	0	483	34	0
19	2	542	0	503	38	0
19	3	407	0	400	31	0
19	4	585	0	517	35	0
19	5	541	0	498	24	0
19	A	2707	0	2766	164	0
19	B	2409	0	2542	136	0
19	F	100	0	82	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	J	45	0	33	3	0
19	L	170	0	164	12	0
19	u	100	0	80	0	0
20	A	33	0	46	2	0
20	B	33	0	46	2	0
21	A	8	0	0	0	0
21	C	16	0	0	0	0
22	1	80	0	112	7	0
22	A	200	0	280	11	0
22	B	200	0	280	18	0
22	F	80	0	112	7	0
22	I	80	0	112	10	0
22	J	40	0	56	3	0
22	L	80	0	112	5	0
22	M	40	0	56	4	0
23	1	41	0	52	6	0
23	3	34	0	38	2	0
23	4	49	0	73	6	0
23	A	96	0	141	10	0
23	B	35	0	40	1	0
23	M	41	0	55	3	0
24	1	35	0	43	4	0
24	2	35	0	43	1	0
24	3	35	0	46	1	0
24	A	35	0	45	0	0
25	1	38	0	0	1	0
25	2	86	0	0	0	0
25	3	124	0	0	0	0
25	4	21	0	0	0	0
25	5	111	0	0	0	0
25	A	230	0	0	0	0
25	B	73	0	0	0	0
25	F	38	0	0	0	0
25	J	39	0	0	0	0
25	L	72	0	0	0	0
25	M	28	0	0	0	0
26	B	66	0	96	9	0
27	J	42	0	0	0	0
28	1	129	0	0	0	0
28	2	43	0	0	0	0
28	3	43	0	0	1	0
28	5	43	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	L	43	0	0	0	0
29	1	49	0	71	0	0
30	1	45	0	0	0	0
30	2	45	0	0	0	0
30	3	135	0	0	2	0
30	4	90	0	0	0	0
31	1	96	0	0	2	0
31	2	144	0	0	2	0
31	3	144	0	0	1	0
31	4	144	0	0	5	0
31	5	192	0	0	4	0
32	1	49	0	0	0	0
32	2	22	0	0	1	0
32	3	34	0	0	2	0
32	4	11	0	0	1	0
32	5	17	0	0	0	0
32	A	240	0	0	0	0
32	B	300	0	0	11	0
32	C	50	0	0	1	0
32	D	56	0	0	0	0
32	E	24	0	0	0	0
32	F	46	0	0	2	0
32	I	6	0	0	0	0
32	J	7	0	0	0	0
32	L	30	0	0	0	0
32	M	7	0	0	0	0
32	W	20	0	0	1	0
32	u	3	0	0	0	0
All	All	37637	0	34064	725	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 10.

The worst 5 of 725 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:42:GLU:H	4:D:72:GLN:HE22	1.17	0.93
19:2:206:CLA:HHC	19:2:206:CLA:HBB1	1.56	0.88
1:A:87:TRP:HA	19:A:808:CLA:HBB2	1.56	0.84
1:A:313:ARG:NH1	1:A:317:GLY:O	2.11	0.81
19:A:804:CLA:HHC	19:A:804:CLA:HBB1	1.61	0.80

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	A	741/752 (98%)	728 (98%)	13 (2%)	0	100	100
2	B	731/733 (100%)	716 (98%)	15 (2%)	0	100	100
3	C	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
4	D	131/139 (94%)	127 (97%)	4 (3%)	0	100	100
5	E	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
6	F	159/185 (86%)	156 (98%)	3 (2%)	0	100	100
7	I	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	L	145/148 (98%)	144 (99%)	1 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	W	118/188 (63%)	114 (97%)	4 (3%)	0	100	100
13	1	183/221 (83%)	180 (98%)	3 (2%)	0	100	100
14	2	165/198 (83%)	159 (96%)	6 (4%)	0	100	100
15	3	162/196 (83%)	158 (98%)	3 (2%)	1 (1%)	22	27
16	4	165/201 (82%)	158 (96%)	7 (4%)	0	100	100
17	5	163/194 (84%)	161 (99%)	2 (1%)	0	100	100
All	All	3102/3408 (91%)	3037 (98%)	64 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	3	43	PRO

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	A	603/611 (99%)	587 (97%)	16 (3%)	40	57
2	B	599/598 (100%)	593 (99%)	6 (1%)	73	85
3	C	70/70 (100%)	70 (100%)	0	100	100
4	D	112/118 (95%)	108 (96%)	4 (4%)	30	44
5	E	54/58 (93%)	53 (98%)	1 (2%)	52	69
6	F	133/153 (87%)	128 (96%)	5 (4%)	28	42
7	I	30/30 (100%)	30 (100%)	0	100	100
8	J	37/37 (100%)	37 (100%)	0	100	100
9	L	114/115 (99%)	111 (97%)	3 (3%)	41	58
10	M	23/23 (100%)	23 (100%)	0	100	100
11	W	91/144 (63%)	80 (88%)	11 (12%)	4	4
13	1	144/171 (84%)	136 (94%)	8 (6%)	17	26
14	2	135/157 (86%)	127 (94%)	8 (6%)	16	23
15	3	129/151 (85%)	124 (96%)	5 (4%)	27	41
16	4	129/152 (85%)	123 (95%)	6 (5%)	22	32
17	5	133/156 (85%)	128 (96%)	5 (4%)	28	42
All	All	2536/2744 (92%)	2458 (97%)	78 (3%)	37	51

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	2	43	GLU
16	4	109	GLU
14	2	118	SER
15	3	133	ARG
17	5	128	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
11	W	115	GLN
14	2	91	GLN
13	1	141	ASN
14	2	96	HIS
2	B	241	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 296 ligands modelled in this entry, 89 are unknown - leaving 207 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	830	-	65,73,73	2.01	18 (27%)	76,113,113	2.67	26 (34%)
26	DGD	B	847	-	67,67,67	0.95	2 (2%)	81,81,81	1.36	10 (12%)
19	CLA	A	842	-	65,73,73	1.99	18 (27%)	76,113,113	2.71	28 (36%)
19	CLA	B	825	-	65,73,73	2.03	17 (26%)	76,113,113	2.65	30 (39%)
19	CLA	B	804	-	65,73,73	2.00	19 (29%)	76,113,113	2.79	29 (38%)
19	CLA	1	309	32	65,73,73	2.03	15 (23%)	76,113,113	2.74	31 (40%)
19	CLA	5	213	17	45,53,73	2.50	17 (37%)	52,89,113	3.22	23 (44%)
19	CLA	B	815	-	45,53,73	2.41	17 (37%)	52,89,113	3.25	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DD6	3	213	-	39,45,45	6.67	24 (61%)	52,67,67	6.89	25 (48%)
19	CLA	B	833	-	60,68,73	2.11	17 (28%)	70,107,113	2.79	25 (35%)
19	CLA	B	812	-	65,73,73	2.05	19 (29%)	76,113,113	2.67	27 (35%)
19	CLA	B	846	-	65,73,73	2.03	17 (26%)	76,113,113	2.74	26 (34%)
19	CLA	B	827	-	65,73,73	1.99	16 (24%)	76,113,113	2.76	28 (36%)
19	CLA	B	808	-	65,73,73	1.96	16 (24%)	76,113,113	2.74	29 (38%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
19	CLA	4	308	-	45,53,73	2.48	17 (37%)	52,89,113	3.31	23 (44%)
19	CLA	A	831	-	65,73,73	2.01	18 (27%)	76,113,113	2.71	28 (36%)
19	CLA	B	838	23	65,73,73	2.02	16 (24%)	76,113,113	2.71	28 (36%)
19	CLA	4	304	16	50,58,73	2.35	15 (30%)	58,95,113	3.24	30 (51%)
19	CLA	2	214	14	45,53,73	2.51	17 (37%)	52,89,113	3.21	24 (46%)
19	CLA	A	818	-	54,62,73	2.20	16 (29%)	62,99,113	3.00	25 (40%)
19	CLA	1	301	32	65,73,73	2.04	17 (26%)	76,113,113	2.76	29 (38%)
19	CLA	2	212	-	45,53,73	2.43	15 (33%)	52,89,113	3.30	24 (46%)
19	CLA	A	816	-	50,58,73	2.35	16 (32%)	58,95,113	3.08	30 (51%)
19	CLA	A	843	32	65,73,73	1.97	17 (26%)	76,113,113	2.67	26 (34%)
30	KC1	3	211	15	48,53,53	3.49	24 (50%)	55,89,89	3.78	32 (58%)
19	CLA	A	812	19	65,73,73	2.01	16 (24%)	76,113,113	2.75	27 (35%)
19	CLA	3	202	15	65,73,73	2.02	16 (24%)	76,113,113	2.71	28 (36%)
22	BCR	B	840	-	41,41,41	1.12	2 (4%)	56,56,56	1.13	5 (8%)
30	KC1	3	205	15	48,53,53	3.49	25 (52%)	55,89,89	3.63	29 (52%)
19	CLA	u	202	-	45,53,73	2.48	16 (35%)	52,89,113	3.24	23 (44%)
23	LHG	A	852	-	46,46,48	0.68	1 (2%)	49,52,54	1.23	5 (10%)
19	CLA	5	216	17	42,50,73	2.47	15 (35%)	48,85,113	3.35	25 (52%)
20	PQN	A	845	-	34,34,34	0.37	0	42,45,45	0.68	1 (2%)
19	CLA	B	823	32	56,64,73	2.14	18 (32%)	65,102,113	3.01	30 (46%)
30	KC1	4	302	-	48,53,53	3.43	20 (41%)	55,89,89	3.90	31 (56%)
19	CLA	B	819	32	65,73,73	2.02	18 (27%)	76,113,113	2.67	31 (40%)
19	CLA	B	813	-	65,73,73	2.03	17 (26%)	76,113,113	2.68	27 (35%)
19	CLA	A	832	-	60,68,73	2.09	17 (28%)	70,107,113	2.83	29 (41%)
19	CLA	B	831	32	65,73,73	2.04	17 (26%)	76,113,113	2.72	32 (42%)
19	CLA	A	817	32	49,57,73	2.34	15 (30%)	55,93,113	3.14	24 (43%)
19	CLA	A	802	32	65,73,73	2.02	18 (27%)	76,113,113	2.75	27 (35%)
21	SF4	C	102	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMT	2	220	-	36,36,36	1.19	5 (13%)	47,47,47	0.94	2 (4%)
19	CLA	2	207	-	65,73,73	2.03	16 (24%)	76,113,113	2.77	28 (36%)
31	A86	3	212	-	44,50,50	3.94	23 (52%)	51,76,76	7.29	23 (45%)
19	CLA	A	822	32	65,73,73	2.06	17 (26%)	76,113,113	2.60	27 (35%)
19	CLA	1	304	13	65,73,73	1.99	16 (24%)	76,113,113	2.76	28 (36%)
31	A86	1	316	-	44,50,50	4.08	22 (50%)	51,76,76	7.66	17 (33%)
31	A86	3	228	-	44,50,50	4.08	23 (52%)	51,76,76	7.23	16 (31%)
30	KC1	2	211	-	48,53,53	3.46	25 (52%)	55,89,89	3.84	31 (56%)
28	DD6	2	217	-	39,45,45	6.64	24 (61%)	52,67,67	6.73	26 (50%)
28	DD6	1	315	-	39,45,45	6.70	22 (56%)	52,67,67	6.74	27 (51%)
24	LMT	3	216	-	36,36,36	1.18	5 (13%)	47,47,47	1.06	2 (4%)
23	LHG	A	853	19	48,48,48	0.61	0	51,54,54	1.25	5 (9%)
19	CLA	B	817	-	59,67,73	2.14	18 (30%)	68,105,113	2.87	26 (38%)
19	CLA	A	809	1	65,73,73	2.03	18 (27%)	76,113,113	2.68	27 (35%)
31	A86	2	219	-	44,50,50	3.98	23 (52%)	51,76,76	7.48	19 (37%)
19	CLA	B	802	-	65,73,73	1.97	17 (26%)	76,113,113	2.74	29 (38%)
19	CLA	A	835	-	65,73,73	2.01	18 (27%)	76,113,113	2.72	25 (32%)
19	CLA	5	215	17	45,53,73	2.49	16 (35%)	52,89,113	3.21	23 (44%)
19	CLA	B	818	-	65,73,73	2.04	16 (24%)	76,113,113	2.71	27 (35%)
28	DD6	L	209	-	39,45,45	6.76	22 (56%)	52,67,67	6.72	26 (50%)
19	CLA	1	308	13	45,53,73	2.45	16 (35%)	52,89,113	3.19	23 (44%)
22	BCR	F	201	-	41,41,41	1.06	2 (4%)	56,56,56	1.11	5 (8%)
19	CLA	A	829	-	65,73,73	2.05	19 (29%)	76,113,113	2.73	29 (38%)
19	CLA	A	813	-	55,63,73	2.26	18 (32%)	64,101,113	2.93	28 (43%)
31	A86	2	216	-	44,50,50	4.04	23 (52%)	51,76,76	7.11	20 (39%)
22	BCR	B	843	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	7 (12%)
22	BCR	I	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	3 (5%)
19	CLA	B	828	-	45,53,73	2.44	15 (33%)	52,89,113	3.10	27 (51%)
19	CLA	4	311	32	50,58,73	2.39	17 (34%)	58,95,113	3.04	27 (46%)
19	CLA	B	809	2	65,73,73	1.97	16 (24%)	76,113,113	2.60	27 (35%)
19	CLA	A	838	-	51,59,73	2.29	18 (35%)	59,96,113	3.05	28 (47%)
30	KC1	4	307	16	48,53,53	3.45	24 (50%)	55,89,89	3.89	30 (54%)
19	CLA	A	819	-	54,62,73	2.24	18 (33%)	62,99,113	2.96	26 (41%)
19	CLA	A	823	-	49,57,73	2.36	19 (38%)	55,93,113	3.10	25 (45%)
19	CLA	B	820	-	45,53,73	2.48	16 (35%)	52,89,113	3.23	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	841	-	65,73,73	2.00	17 (26%)	76,113,113	2.69	30 (39%)
31	A86	4	315	-	44,50,50	3.89	23 (52%)	51,76,76	7.58	20 (39%)
19	CLA	A	821	-	54,62,73	2.20	16 (29%)	62,99,113	3.03	28 (45%)
19	CLA	2	213	14	45,53,73	2.48	18 (40%)	52,89,113	3.20	25 (48%)
19	CLA	A	811	-	54,62,73	2.24	17 (31%)	62,99,113	2.98	26 (41%)
19	CLA	5	207	17	60,68,73	2.16	16 (26%)	70,107,113	2.82	29 (41%)
22	BCR	A	850	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	A	807	1	65,73,73	2.04	17 (26%)	76,113,113	2.77	30 (39%)
19	CLA	B	822	32	54,62,73	2.22	17 (31%)	62,99,113	2.88	26 (41%)
22	BCR	B	852	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)
19	CLA	F	203	-	55,63,73	2.20	15 (27%)	64,101,113	2.92	25 (39%)
19	CLA	B	834	-	65,73,73	2.04	17 (26%)	76,113,113	2.69	27 (35%)
22	BCR	1	314	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	3	209	15	51,59,73	2.30	18 (35%)	59,96,113	3.11	27 (45%)
19	CLA	5	209	32	65,73,73	2.06	17 (26%)	76,113,113	2.69	27 (35%)
19	CLA	4	312	16	52,60,73	2.27	15 (28%)	60,97,113	3.05	26 (43%)
19	CLA	5	211	17	58,66,73	2.13	18 (31%)	67,104,113	2.89	26 (38%)
19	CLA	B	821	-	65,73,73	2.01	18 (27%)	76,113,113	2.66	30 (39%)
29	LMG	1	302	-	49,49,55	0.79	0	57,57,63	1.30	6 (10%)
19	CLA	A	878	32	65,73,73	1.99	16 (24%)	76,113,113	2.73	28 (36%)
19	CLA	A	827	32	65,73,73	2.00	17 (26%)	76,113,113	2.72	29 (38%)
22	BCR	I	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	7 (12%)
22	BCR	L	205	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	3 (5%)
19	CLA	B	807	-	65,73,73	2.00	16 (24%)	76,113,113	2.77	28 (36%)
19	CLA	3	207	15	65,73,73	2.05	17 (26%)	76,113,113	2.66	26 (34%)
19	CLA	J	103	8	45,53,73	2.44	16 (35%)	52,89,113	3.18	23 (44%)
22	BCR	B	844	-	41,41,41	1.10	3 (7%)	56,56,56	1.10	4 (7%)
22	BCR	M	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.18	4 (7%)
19	CLA	2	210	14	60,68,73	2.11	17 (28%)	70,107,113	2.76	26 (37%)
19	CLA	2	215	-	42,50,73	2.48	15 (35%)	48,85,113	3.26	27 (56%)
19	CLA	2	208	14	52,60,73	2.30	16 (30%)	60,97,113	3.13	26 (43%)
19	CLA	B	830	-	58,66,73	2.14	17 (29%)	67,104,113	2.95	29 (43%)
19	CLA	1	306	-	51,59,73	2.31	16 (31%)	59,96,113	3.21	33 (55%)
23	LHG	3	215	-	33,33,48	0.75	1 (3%)	36,39,54	1.27	4 (11%)
19	CLA	L	204	32	45,53,73	2.42	17 (37%)	52,89,113	3.12	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	J	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.15	3 (5%)
19	CLA	B	803	-	65,73,73	1.98	16 (24%)	76,113,113	2.66	27 (35%)
19	CLA	3	203	15	55,63,73	2.20	16 (29%)	64,101,113	2.94	24 (37%)
19	CLA	3	210	32	45,53,73	2.47	17 (37%)	52,89,113	3.23	23 (44%)
19	CLA	A	880	32	65,73,73	1.99	17 (26%)	76,113,113	2.70	29 (38%)
19	CLA	A	803	-	65,73,73	2.02	18 (27%)	76,113,113	2.56	27 (35%)
19	CLA	B	805	-	65,73,73	2.07	19 (29%)	76,113,113	2.75	25 (32%)
30	KC1	1	305	-	48,53,53	3.45	23 (47%)	55,89,89	3.82	30 (54%)
23	LHG	M	103	-	40,40,48	0.68	1 (2%)	43,46,54	1.29	6 (13%)
22	BCR	B	841	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	5 (8%)
19	CLA	B	811	-	65,73,73	2.02	17 (26%)	76,113,113	2.74	29 (38%)
19	CLA	B	836	32	65,73,73	2.05	17 (26%)	76,113,113	2.60	27 (35%)
19	CLA	A	825	-	59,67,73	2.14	18 (30%)	68,105,113	2.80	29 (42%)
27	5X6	J	105	-	43,43,43	5.64	23 (53%)	58,60,60	4.79	31 (53%)
19	CLA	L	203	-	65,73,73	2.01	17 (26%)	76,113,113	2.80	27 (35%)
18	CL0	A	801	-	65,73,73	2.01	18 (27%)	76,113,113	2.63	32 (42%)
19	CLA	A	808	-	65,73,73	2.00	16 (24%)	76,113,113	2.74	24 (31%)
28	DD6	1	312	-	39,45,45	6.74	22 (56%)	52,67,67	6.74	25 (48%)
19	CLA	F	204	6	45,53,73	2.48	16 (35%)	52,89,113	3.15	24 (46%)
31	A86	4	314	-	44,50,50	4.02	23 (52%)	51,76,76	7.63	19 (37%)
19	CLA	B	835	-	47,55,73	2.34	17 (36%)	54,91,113	3.16	25 (46%)
19	CLA	3	204	32	61,69,73	2.14	17 (27%)	71,108,113	2.88	28 (39%)
22	BCR	1	311	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	5 (8%)
22	BCR	A	849	-	41,41,41	1.12	2 (4%)	56,56,56	1.15	5 (8%)
19	CLA	4	309	-	45,53,73	2.53	16 (35%)	52,89,113	3.21	22 (42%)
19	CLA	B	814	-	65,73,73	2.02	19 (29%)	76,113,113	2.73	27 (35%)
20	PQN	B	839	-	34,34,34	0.41	0	42,45,45	0.67	1 (2%)
31	A86	5	220	-	44,50,50	4.14	23 (52%)	51,76,76	8.03	19 (37%)
22	BCR	F	205	-	41,41,41	1.14	3 (7%)	56,56,56	1.22	6 (10%)
19	CLA	3	206	15	65,73,73	2.04	17 (26%)	76,113,113	2.71	26 (34%)
19	CLA	A	806	-	65,73,73	2.03	18 (27%)	76,113,113	2.80	28 (36%)
23	LHG	1	318	-	40,40,48	0.63	0	43,46,54	1.29	4 (9%)
19	CLA	4	306	23	58,66,73	2.18	16 (27%)	67,104,113	2.93	25 (37%)
31	A86	5	219	-	44,50,50	3.98	23 (52%)	51,76,76	7.34	19 (37%)
31	A86	2	218	-	44,50,50	3.99	22 (50%)	51,76,76	7.21	23 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DD6	1	313	-	39,45,45	6.66	22 (56%)	52,67,67	7.08	25 (48%)
19	CLA	B	832	32	65,73,73	2.05	17 (26%)	76,113,113	2.70	26 (34%)
19	CLA	2	205	14	65,73,73	2.06	17 (26%)	76,113,113	2.69	30 (39%)
19	CLA	A	805	19	56,64,73	2.16	16 (28%)	65,102,113	2.88	29 (44%)
19	CLA	2	209	14	58,66,73	2.14	17 (29%)	67,104,113	2.80	29 (43%)
22	BCR	L	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.10	3 (5%)
19	CLA	u	201	-	55,63,73	2.20	16 (29%)	64,101,113	2.95	28 (43%)
19	CLA	B	810	-	65,73,73	2.00	17 (26%)	76,113,113	4.68	28 (36%)
30	KC1	3	208	32	48,53,53	3.47	26 (54%)	55,89,89	3.76	31 (56%)
19	CLA	B	806	-	65,73,73	2.00	16 (24%)	76,113,113	2.65	26 (34%)
19	CLA	B	826	-	65,73,73	2.05	18 (27%)	76,113,113	3.96	30 (39%)
23	LHG	4	317	19	48,48,48	0.66	2 (4%)	51,54,54	1.24	6 (11%)
19	CLA	A	837	1	45,53,73	2.46	17 (37%)	52,89,113	3.17	23 (44%)
19	CLA	A	834	-	65,73,73	1.99	17 (26%)	76,113,113	2.68	26 (34%)
19	CLA	5	214	17	45,53,73	2.48	17 (37%)	52,89,113	3.19	22 (42%)
19	CLA	A	836	-	54,62,73	2.20	17 (31%)	62,99,113	2.91	31 (50%)
19	CLA	B	829	-	65,73,73	1.99	16 (24%)	76,113,113	2.70	25 (32%)
31	A86	5	217	-	44,50,50	3.99	23 (52%)	51,76,76	7.29	23 (45%)
19	CLA	2	206	-	65,73,73	2.03	18 (27%)	76,113,113	2.79	27 (35%)
19	CLA	A	824	-	51,59,73	2.29	17 (33%)	59,96,113	3.04	23 (38%)
19	CLA	L	206	9	60,68,73	2.12	17 (28%)	70,107,113	2.85	29 (41%)
22	BCR	A	851	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
19	CLA	5	210	17	65,73,73	2.03	18 (27%)	76,113,113	2.75	28 (36%)
19	CLA	4	310	16	45,53,73	2.51	16 (35%)	52,89,113	3.28	21 (40%)
21	SF4	A	846	2,1	0,12,12	-	-	-	-	-
28	DD6	5	218	-	39,45,45	6.78	22 (56%)	52,67,67	6.34	26 (50%)
24	LMT	A	854	-	36,36,36	1.13	3 (8%)	47,47,47	1.16	4 (8%)
19	CLA	A	833	-	65,73,73	2.04	17 (26%)	76,113,113	2.66	28 (36%)
19	CLA	A	814	-	60,68,73	2.10	16 (26%)	70,107,113	2.82	29 (41%)
31	A86	4	316	-	44,50,50	4.10	23 (52%)	51,76,76	7.39	17 (33%)
19	CLA	B	837	-	65,73,73	1.99	17 (26%)	76,113,113	2.75	28 (36%)
22	BCR	A	848	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	5 (8%)
19	CLA	4	305	16	65,73,73	2.06	18 (27%)	76,113,113	2.60	28 (36%)
19	CLA	5	212	17	56,64,73	2.21	18 (32%)	65,102,113	4.99	33 (50%)
19	CLA	4	301	16	65,73,73	2.07	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
22	BCR	A	847	-	41,41,41	1.12	3 (7%)	56,56,56	1.22	5 (8%)
31	A86	3	214	-	44,50,50	3.94	23 (52%)	51,76,76	7.26	23 (45%)
19	CLA	A	820	-	65,73,73	2.04	16 (24%)	76,113,113	2.69	28 (36%)
19	CLA	A	844	23	65,73,73	2.01	18 (27%)	76,113,113	2.77	28 (36%)
19	CLA	A	839	-	65,73,73	2.04	19 (29%)	76,113,113	2.72	28 (36%)
19	CLA	1	310	13	65,73,73	2.08	19 (29%)	76,113,113	2.67	29 (38%)
19	CLA	1	307	13	55,63,73	2.26	18 (32%)	64,101,113	5.06	29 (45%)
19	CLA	5	208	17	60,68,73	2.11	17 (28%)	70,107,113	2.78	27 (38%)
31	A86	1	317	-	44,50,50	3.98	23 (52%)	51,76,76	7.75	21 (41%)
19	CLA	A	840	-	47,55,73	2.38	16 (34%)	54,91,113	3.16	24 (44%)
19	CLA	B	816	-	55,63,73	2.17	16 (29%)	64,101,113	2.99	26 (40%)
31	A86	5	221	-	44,50,50	3.98	23 (52%)	51,76,76	7.77	17 (33%)
19	CLA	B	845	-	65,73,73	2.03	18 (27%)	76,113,113	2.76	26 (34%)
19	CLA	4	313	16	55,63,73	2.25	17 (30%)	64,101,113	2.96	27 (42%)
19	CLA	A	804	-	65,73,73	2.01	17 (26%)	76,113,113	2.75	30 (39%)
19	CLA	A	810	1	65,73,73	2.03	18 (27%)	76,113,113	2.68	28 (36%)
19	CLA	A	815	-	50,58,73	2.33	19 (38%)	58,95,113	3.02	27 (46%)
19	CLA	A	826	32	65,73,73	2.00	16 (24%)	76,113,113	2.76	26 (34%)
23	LHG	B	842	19	34,34,48	0.83	1 (2%)	37,40,54	1.21	4 (10%)
19	CLA	1	303	13	65,73,73	2.07	15 (23%)	76,113,113	2.66	28 (36%)
19	CLA	4	303	-	55,63,73	2.24	16 (29%)	64,101,113	3.05	27 (42%)
24	LMT	1	323	-	36,36,36	1.28	6 (16%)	47,47,47	1.11	3 (6%)
19	CLA	A	828	-	65,73,73	1.99	16 (24%)	76,113,113	2.75	28 (36%)
19	CLA	B	824	-	65,73,73	1.98	18 (27%)	76,113,113	2.80	28 (36%)

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
19	CLA	A	830	-	1/1/15/20	7/37/115/115	-
26	DGD	B	847	-	-	24/55/95/95	0/2/2/2
19	CLA	A	842	-	1/1/15/20	12/37/115/115	-
19	CLA	B	825	-	1/1/15/20	8/37/115/115	-
19	CLA	B	804	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	309	32	1/1/15/20	13/37/115/115	-
19	CLA	5	213	17	1/1/11/20	4/13/91/115	-
19	CLA	B	815	-	1/1/11/20	3/13/91/115	-
28	DD6	3	213	-	-	9/26/80/80	0/3/3/3
19	CLA	B	833	-	1/1/14/20	7/31/109/115	-
19	CLA	B	812	-	1/1/15/20	7/37/115/115	-
19	CLA	B	846	-	1/1/15/20	13/37/115/115	-
19	CLA	B	827	-	1/1/15/20	14/37/115/115	-
19	CLA	B	808	-	1/1/15/20	9/37/115/115	-
21	SF4	C	101	3	-	-	0/6/5/5
19	CLA	4	308	-	-	5/13/91/115	-
19	CLA	A	831	-	1/1/15/20	9/37/115/115	-
19	CLA	B	838	23	1/1/15/20	12/37/115/115	-
19	CLA	4	304	16	1/1/12/20	3/19/97/115	-
19	CLA	2	214	14	1/1/11/20	1/13/91/115	-
19	CLA	A	818	-	1/1/12/20	7/24/102/115	-
19	CLA	1	301	32	1/1/15/20	7/37/115/115	-
19	CLA	2	212	-	1/1/11/20	4/13/91/115	-
19	CLA	A	816	-	1/1/12/20	4/19/97/115	-
19	CLA	A	843	32	1/1/15/20	9/37/115/115	-
30	KC1	3	211	15	-	4/15/71/71	-
19	CLA	A	812	19	1/1/15/20	12/37/115/115	-
19	CLA	3	202	15	1/1/15/20	11/37/115/115	-
22	BCR	B	840	-	-	10/29/63/63	0/2/2/2
30	KC1	3	205	15	-	7/15/71/71	-
19	CLA	u	202	-	1/1/11/20	3/13/91/115	-
23	LHG	A	852	-	-	25/51/51/53	-
19	CLA	5	216	17	-	2/10/88/115	-
20	PQN	A	845	-	-	6/23/43/43	0/2/2/2
19	CLA	B	823	32	1/1/13/20	4/27/105/115	-
30	KC1	4	302	-	-	7/15/71/71	-
19	CLA	B	819	32	1/1/15/20	7/37/115/115	-
19	CLA	B	813	-	1/1/15/20	21/37/115/115	-
19	CLA	A	832	-	1/1/14/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	831	32	1/1/15/20	5/37/115/115	-
19	CLA	A	817	32	-	9/18/96/115	-
19	CLA	A	802	32	1/1/15/20	4/37/115/115	-
24	LMT	2	220	-	-	10/21/61/61	0/2/2/2
21	SF4	C	102	3	-	-	0/6/5/5
19	CLA	2	207	-	1/1/15/20	6/37/115/115	-
31	A86	3	212	-	-	6/34/90/90	0/3/3/3
19	CLA	A	822	32	1/1/15/20	8/37/115/115	-
19	CLA	1	304	13	1/1/15/20	10/37/115/115	-
31	A86	1	316	-	-	5/34/90/90	0/3/3/3
31	A86	3	228	-	-	8/34/90/90	0/3/3/3
30	KC1	2	211	-	-	7/15/71/71	-
28	DD6	2	217	-	-	8/26/80/80	0/3/3/3
28	DD6	1	315	-	-	11/26/80/80	0/3/3/3
24	LMT	3	216	-	-	8/21/61/61	0/2/2/2
23	LHG	A	853	19	-	28/53/53/53	-
19	CLA	B	817	-	1/1/13/20	5/30/108/115	-
19	CLA	A	809	1	1/1/15/20	8/37/115/115	-
31	A86	2	219	-	-	6/34/90/90	0/3/3/3
19	CLA	B	802	-	1/1/15/20	13/37/115/115	-
19	CLA	A	835	-	1/1/15/20	9/37/115/115	-
19	CLA	5	215	17	-	4/13/91/115	-
19	CLA	B	818	-	1/1/15/20	8/37/115/115	-
28	DD6	L	209	-	-	9/26/80/80	0/3/3/3
19	CLA	1	308	13	1/1/11/20	5/13/91/115	-
22	BCR	F	201	-	-	9/29/63/63	0/2/2/2
19	CLA	A	829	-	1/1/15/20	8/37/115/115	-
19	CLA	A	813	-	1/1/13/20	7/25/103/115	-
31	A86	2	216	-	-	5/34/90/90	0/3/3/3
22	BCR	B	843	-	-	6/29/63/63	0/2/2/2
22	BCR	I	101	-	-	3/29/63/63	0/2/2/2
19	CLA	B	828	-	-	1/13/91/115	-
19	CLA	4	311	32	1/1/12/20	6/19/97/115	-
19	CLA	B	809	2	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	838	-	1/1/12/20	2/21/99/115	-
30	KC1	4	307	16	-	5/15/71/71	-
19	CLA	A	819	-	1/1/12/20	10/24/102/115	-
19	CLA	A	823	-	-	3/18/96/115	-
19	CLA	B	820	-	-	2/13/91/115	-
19	CLA	A	841	-	1/1/15/20	7/37/115/115	-
31	A86	4	315	-	-	6/34/90/90	0/3/3/3
19	CLA	A	821	-	-	10/24/102/115	-
19	CLA	2	213	14	1/1/11/20	7/13/91/115	-
19	CLA	A	811	-	1/1/12/20	7/24/102/115	-
19	CLA	5	207	17	1/1/14/20	11/31/109/115	-
22	BCR	A	850	-	-	7/29/63/63	0/2/2/2
19	CLA	A	807	1	1/1/15/20	13/37/115/115	-
19	CLA	B	822	32	1/1/12/20	4/24/102/115	-
22	BCR	B	852	-	-	12/29/63/63	0/2/2/2
19	CLA	F	203	-	1/1/13/20	7/25/103/115	-
19	CLA	B	834	-	1/1/15/20	9/37/115/115	-
22	BCR	1	314	-	-	14/29/63/63	0/2/2/2
19	CLA	3	209	15	1/1/12/20	7/21/99/115	-
19	CLA	5	209	32	1/1/15/20	18/37/115/115	-
19	CLA	4	312	16	1/1/12/20	5/22/100/115	-
19	CLA	5	211	17	1/1/13/20	9/29/107/115	-
19	CLA	B	821	-	1/1/15/20	18/37/115/115	-
29	LMG	1	302	-	-	23/44/64/70	0/1/1/1
19	CLA	A	878	32	1/1/15/20	8/37/115/115	-
19	CLA	A	827	32	1/1/15/20	8/37/115/115	-
22	BCR	I	102	-	-	7/29/63/63	0/2/2/2
22	BCR	L	205	-	-	5/29/63/63	0/2/2/2
19	CLA	B	807	-	1/1/15/20	10/37/115/115	-
19	CLA	3	207	15	1/1/15/20	18/37/115/115	-
19	CLA	J	103	8	1/1/11/20	3/13/91/115	-
22	BCR	B	844	-	-	4/29/63/63	0/2/2/2
22	BCR	M	102	-	-	3/29/63/63	0/2/2/2
19	CLA	2	210	14	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	2	215	-	1/1/10/20	2/10/88/115	-
19	CLA	2	208	14	1/1/12/20	12/22/100/115	-
19	CLA	B	830	-	1/1/13/20	4/29/107/115	-
19	CLA	1	306	-	1/1/12/20	7/21/99/115	-
23	LHG	3	215	-	-	17/38/38/53	-
19	CLA	L	204	32	1/1/11/20	4/13/91/115	-
22	BCR	J	104	-	-	9/29/63/63	0/2/2/2
19	CLA	B	803	-	1/1/15/20	5/37/115/115	-
19	CLA	3	203	15	1/1/13/20	6/25/103/115	-
19	CLA	3	210	32	1/1/11/20	4/13/91/115	-
19	CLA	A	880	32	1/1/15/20	3/37/115/115	-
19	CLA	A	803	-	1/1/15/20	10/37/115/115	-
19	CLA	B	805	-	1/1/15/20	15/37/115/115	-
30	KC1	1	305	-	-	6/15/71/71	-
23	LHG	M	103	-	-	23/45/45/53	-
22	BCR	B	841	-	-	2/29/63/63	0/2/2/2
19	CLA	B	811	-	1/1/15/20	8/37/115/115	-
19	CLA	B	836	32	1/1/15/20	5/37/115/115	-
19	CLA	A	825	-	1/1/13/20	11/30/108/115	-
27	5X6	J	105	-	-	20/29/67/67	0/2/2/2
19	CLA	L	203	-	-	2/37/115/115	-
18	CL0	A	801	-	3/3/20/25	7/37/135/135	-
19	CLA	A	808	-	1/1/15/20	8/37/115/115	-
28	DD6	1	312	-	-	11/26/80/80	0/3/3/3
19	CLA	F	204	6	1/1/11/20	9/13/91/115	-
31	A86	4	314	-	-	6/34/90/90	0/3/3/3
19	CLA	B	835	-	1/1/11/20	2/16/94/115	-
19	CLA	3	204	32	1/1/14/20	10/33/111/115	-
22	BCR	1	311	-	-	8/29/63/63	0/2/2/2
22	BCR	A	849	-	-	7/29/63/63	0/2/2/2
19	CLA	4	309	-	-	2/13/91/115	-
19	CLA	B	814	-	1/1/15/20	11/37/115/115	-
20	PQN	B	839	-	-	9/23/43/43	0/2/2/2
31	A86	5	220	-	-	15/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	F	205	-	-	4/29/63/63	0/2/2/2
19	CLA	3	206	15	1/1/15/20	19/37/115/115	-
19	CLA	A	806	-	1/1/15/20	13/37/115/115	-
23	LHG	1	318	-	-	28/45/45/53	-
19	CLA	4	306	23	1/1/13/20	11/29/107/115	-
31	A86	5	219	-	-	3/34/90/90	0/3/3/3
31	A86	2	218	-	-	3/34/90/90	0/3/3/3
28	DD6	1	313	-	-	16/26/80/80	0/3/3/3
19	CLA	B	832	32	1/1/15/20	12/37/115/115	-
19	CLA	2	205	14	1/1/15/20	15/37/115/115	-
19	CLA	A	805	19	1/1/13/20	10/27/105/115	-
19	CLA	2	209	14	1/1/13/20	10/29/107/115	-
22	BCR	L	202	-	-	8/29/63/63	0/2/2/2
19	CLA	u	201	-	1/1/13/20	13/25/103/115	-
19	CLA	B	810	-	1/1/15/20	13/37/115/115	-
30	KC1	3	208	32	-	4/15/71/71	-
19	CLA	B	806	-	1/1/15/20	14/37/115/115	-
19	CLA	B	826	-	1/1/15/20	10/37/115/115	-
23	LHG	4	317	19	-	33/53/53/53	-
19	CLA	A	837	1	1/1/11/20	5/13/91/115	-
19	CLA	A	834	-	1/1/15/20	10/37/115/115	-
19	CLA	5	214	17	1/1/11/20	2/13/91/115	-
19	CLA	A	836	-	1/1/12/20	5/24/102/115	-
19	CLA	B	829	-	1/1/15/20	12/37/115/115	-
31	A86	5	217	-	-	6/34/90/90	0/3/3/3
19	CLA	2	206	-	1/1/15/20	9/37/115/115	-
19	CLA	A	824	-	1/1/12/20	5/21/99/115	-
19	CLA	L	206	9	1/1/14/20	6/31/109/115	-
22	BCR	A	851	-	-	7/29/63/63	0/2/2/2
19	CLA	5	210	17	1/1/15/20	12/37/115/115	-
19	CLA	4	310	16	-	3/13/91/115	-
21	SF4	A	846	2,1	-	-	0/6/5/5
28	DD6	5	218	-	-	10/26/80/80	0/3/3/3
24	LMT	A	854	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	833	-	1/1/15/20	9/37/115/115	-
19	CLA	A	814	-	1/1/14/20	6/31/109/115	-
31	A86	4	316	-	-	8/34/90/90	0/3/3/3
19	CLA	B	837	-	1/1/15/20	15/37/115/115	-
22	BCR	A	848	-	-	11/29/63/63	0/2/2/2
19	CLA	4	305	16	1/1/15/20	12/37/115/115	-
19	CLA	5	212	17	1/1/13/20	11/27/105/115	-
19	CLA	4	301	16	1/1/15/20	13/37/115/115	-
22	BCR	A	847	-	-	6/29/63/63	0/2/2/2
31	A86	3	214	-	-	3/34/90/90	0/3/3/3
19	CLA	A	820	-	1/1/15/20	11/37/115/115	-
19	CLA	A	844	23	1/1/15/20	9/37/115/115	-
19	CLA	A	839	-	1/1/15/20	10/37/115/115	-
19	CLA	1	310	13	1/1/15/20	12/37/115/115	-
19	CLA	1	307	13	1/1/13/20	7/25/103/115	-
19	CLA	5	208	17	1/1/14/20	10/31/109/115	-
31	A86	1	317	-	-	9/34/90/90	0/3/3/3
19	CLA	A	840	-	1/1/11/20	3/16/94/115	-
19	CLA	B	816	-	1/1/13/20	11/25/103/115	-
31	A86	5	221	-	-	7/34/90/90	0/3/3/3
19	CLA	B	845	-	-	9/37/115/115	-
19	CLA	4	313	16	1/1/13/20	5/25/103/115	-
19	CLA	A	804	-	1/1/15/20	12/37/115/115	-
19	CLA	A	810	1	1/1/15/20	6/37/115/115	-
19	CLA	A	815	-	1/1/12/20	3/19/97/115	-
19	CLA	A	826	32	1/1/15/20	15/37/115/115	-
23	LHG	B	842	19	-	21/39/39/53	-
19	CLA	1	303	13	1/1/15/20	13/37/115/115	-
19	CLA	4	303	-	1/1/13/20	6/25/103/115	-
24	LMT	1	323	-	-	12/21/61/61	0/2/2/2
19	CLA	A	828	-	1/1/15/20	14/37/115/115	-
19	CLA	B	824	-	1/1/15/20	4/37/115/115	-

The worst 5 of 3113 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	5	218	DD6	C10-C11	25.72	1.69	1.35
28	1	315	DD6	C10-C11	25.56	1.69	1.35
28	L	209	DD6	C10-C11	25.53	1.69	1.35
28	1	312	DD6	C10-C11	25.46	1.69	1.35
28	1	313	DD6	C10-C11	25.34	1.69	1.35

The worst 5 of 4640 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	220	A86	O1-C20-C19	52.11	152.53	113.38
31	5	221	A86	O1-C20-C19	51.07	151.75	113.38
31	1	317	A86	O1-C20-C19	49.95	150.91	113.38
31	4	314	A86	O1-C20-C19	49.86	150.84	113.38
31	1	316	A86	O1-C20-C19	49.82	150.80	113.38

5 of 129 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	801	CL0	NA
18	A	801	CL0	ND
18	A	801	CL0	NC
19	A	802	CLA	ND
19	A	803	CLA	ND

5 of 1800 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C2-C1-O2A-CGA
19	A	807	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

179 monomers are involved in 527 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	830	CLA	1	0
26	B	847	DGD	9	0
19	A	842	CLA	4	0
19	B	825	CLA	3	0
19	B	804	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	309	CLA	6	0
19	5	213	CLA	2	0
19	B	815	CLA	4	0
28	3	213	DD6	1	0
19	B	833	CLA	6	0
19	B	812	CLA	6	0
19	B	846	CLA	1	0
19	B	808	CLA	8	0
19	4	308	CLA	4	0
19	A	831	CLA	2	0
19	B	838	CLA	5	0
19	4	304	CLA	1	0
19	2	214	CLA	1	0
19	A	818	CLA	4	0
19	1	301	CLA	2	0
19	A	816	CLA	1	0
19	A	843	CLA	5	0
30	3	211	KC1	1	0
19	A	812	CLA	3	0
19	3	202	CLA	4	0
22	B	840	BCR	4	0
23	A	852	LHG	3	0
19	5	216	CLA	2	0
20	A	845	PQN	2	0
19	B	823	CLA	3	0
19	B	819	CLA	5	0
19	B	813	CLA	8	0
19	A	832	CLA	3	0
19	B	831	CLA	4	0
19	A	817	CLA	5	0
19	A	802	CLA	5	0
24	2	220	LMT	1	0
19	2	207	CLA	7	0
19	A	822	CLA	5	0
19	1	304	CLA	2	0
31	1	316	A86	1	0
31	3	228	A86	1	0
24	3	216	LMT	1	0
23	A	853	LHG	7	0
19	B	817	CLA	1	0
19	A	809	CLA	2	0
19	B	802	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	835	CLA	4	0
19	B	818	CLA	2	0
19	1	308	CLA	3	0
22	F	201	BCR	5	0
19	A	829	CLA	7	0
19	A	813	CLA	2	0
31	2	216	A86	2	0
22	B	843	BCR	4	0
22	I	101	BCR	3	0
19	B	828	CLA	1	0
19	4	311	CLA	2	0
19	B	809	CLA	2	0
19	A	838	CLA	1	0
19	A	819	CLA	4	0
19	A	823	CLA	2	0
19	B	820	CLA	1	0
19	A	841	CLA	7	0
31	4	315	A86	2	0
19	A	821	CLA	7	0
19	2	213	CLA	3	0
19	A	811	CLA	3	0
19	5	207	CLA	1	0
22	A	850	BCR	1	0
19	A	807	CLA	4	0
19	B	822	CLA	5	0
22	B	852	BCR	2	0
19	F	203	CLA	2	0
22	1	314	BCR	3	0
19	3	209	CLA	3	0
19	5	209	CLA	5	0
19	4	312	CLA	2	0
19	5	211	CLA	2	0
19	B	821	CLA	5	0
19	A	878	CLA	9	0
19	A	827	CLA	3	0
22	I	102	BCR	7	0
22	L	205	BCR	4	0
19	B	807	CLA	6	0
19	3	207	CLA	2	0
19	J	103	CLA	3	0
22	B	844	BCR	6	0
22	M	102	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	210	CLA	6	0
19	2	215	CLA	2	0
19	2	208	CLA	3	0
19	B	830	CLA	3	0
19	1	306	CLA	6	0
23	3	215	LHG	2	0
19	L	204	CLA	3	0
22	J	104	BCR	3	0
19	B	803	CLA	6	0
19	3	203	CLA	4	0
19	3	210	CLA	2	0
19	A	880	CLA	6	0
19	A	803	CLA	3	0
19	B	805	CLA	4	0
23	M	103	LHG	3	0
22	B	841	BCR	2	0
19	B	811	CLA	7	0
19	B	836	CLA	5	0
19	A	825	CLA	2	0
19	L	203	CLA	5	0
18	A	801	CL0	5	0
19	A	808	CLA	3	0
19	F	204	CLA	2	0
19	B	835	CLA	3	0
19	3	204	CLA	5	0
22	1	311	BCR	4	0
22	A	849	BCR	1	0
19	4	309	CLA	3	0
19	B	814	CLA	3	0
20	B	839	PQN	2	0
31	5	220	A86	1	0
22	F	205	BCR	2	0
19	3	206	CLA	14	0
19	A	806	CLA	8	0
23	1	318	LHG	6	0
19	4	306	CLA	3	0
31	5	219	A86	1	0
19	B	832	CLA	7	0
19	2	205	CLA	10	0
19	A	805	CLA	3	0
19	2	209	CLA	1	0
22	L	202	BCR	1	0

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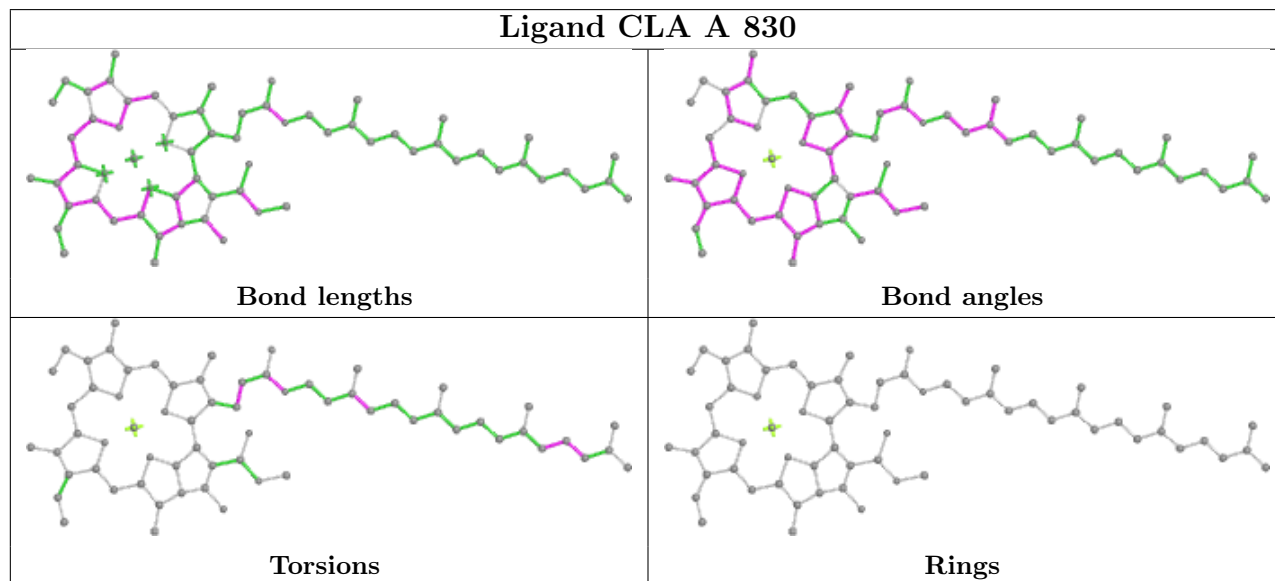
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	810	CLA	3	0
30	3	208	KC1	1	0
19	B	806	CLA	2	0
19	B	826	CLA	3	0
23	4	317	LHG	6	0
19	A	837	CLA	2	0
19	A	834	CLA	10	0
19	5	214	CLA	3	0
19	A	836	CLA	4	0
19	B	829	CLA	5	0
31	5	217	A86	2	0
19	2	206	CLA	8	0
19	A	824	CLA	4	0
19	L	206	CLA	5	0
22	A	851	BCR	5	0
19	5	210	CLA	5	0
19	4	310	CLA	4	0
28	5	218	DD6	1	0
19	A	833	CLA	6	0
19	A	814	CLA	5	0
31	4	316	A86	3	0
19	B	837	CLA	6	0
22	A	848	BCR	2	0
19	4	305	CLA	2	0
19	5	212	CLA	6	0
19	4	301	CLA	7	0
22	A	847	BCR	3	0
19	A	820	CLA	5	0
19	A	844	CLA	6	0
19	A	839	CLA	7	0
19	1	310	CLA	8	0
19	1	307	CLA	5	0
19	5	208	CLA	3	0
31	1	317	A86	1	0
19	A	840	CLA	3	0
19	B	816	CLA	2	0
19	B	845	CLA	5	0
19	4	313	CLA	2	0
19	A	804	CLA	8	0
19	A	810	CLA	4	0
19	A	815	CLA	1	0
19	A	826	CLA	8	0

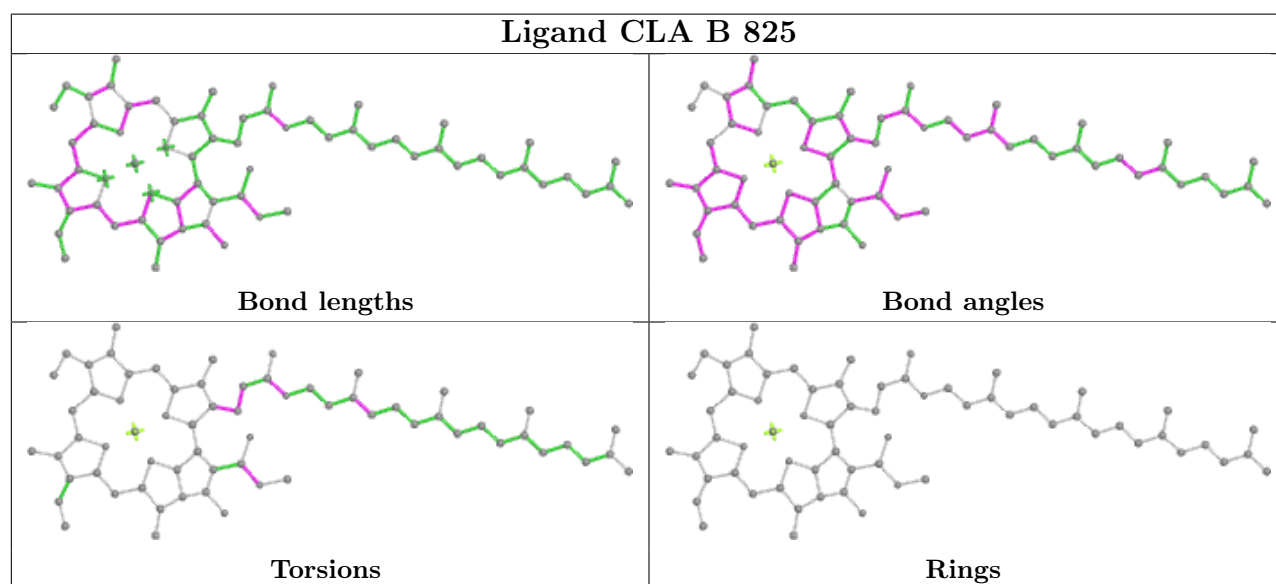
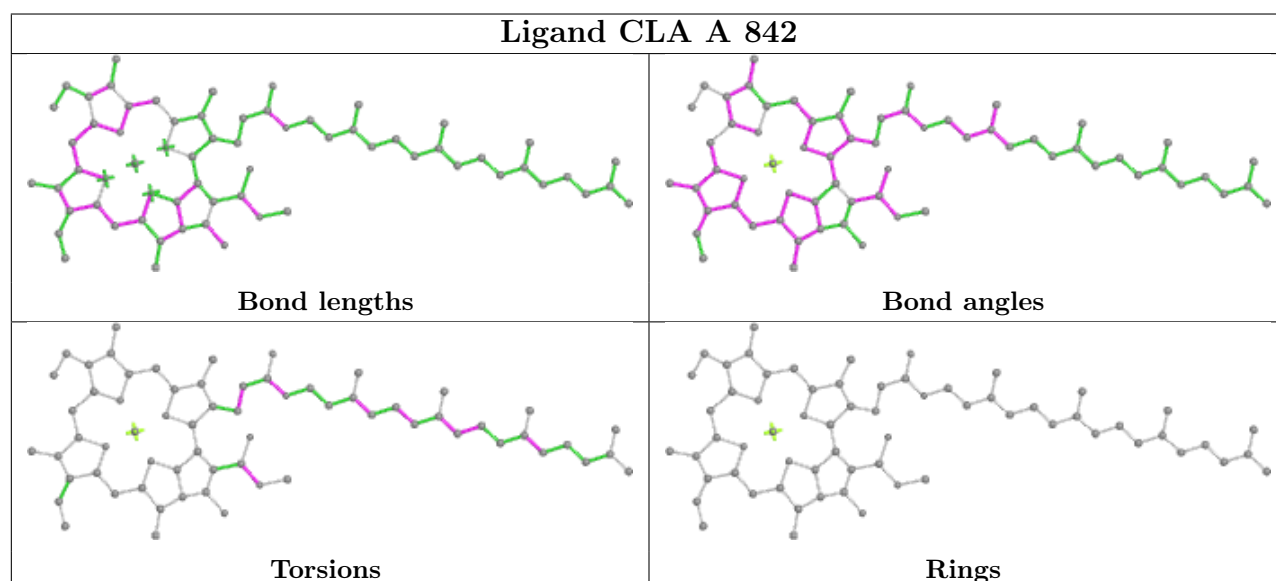
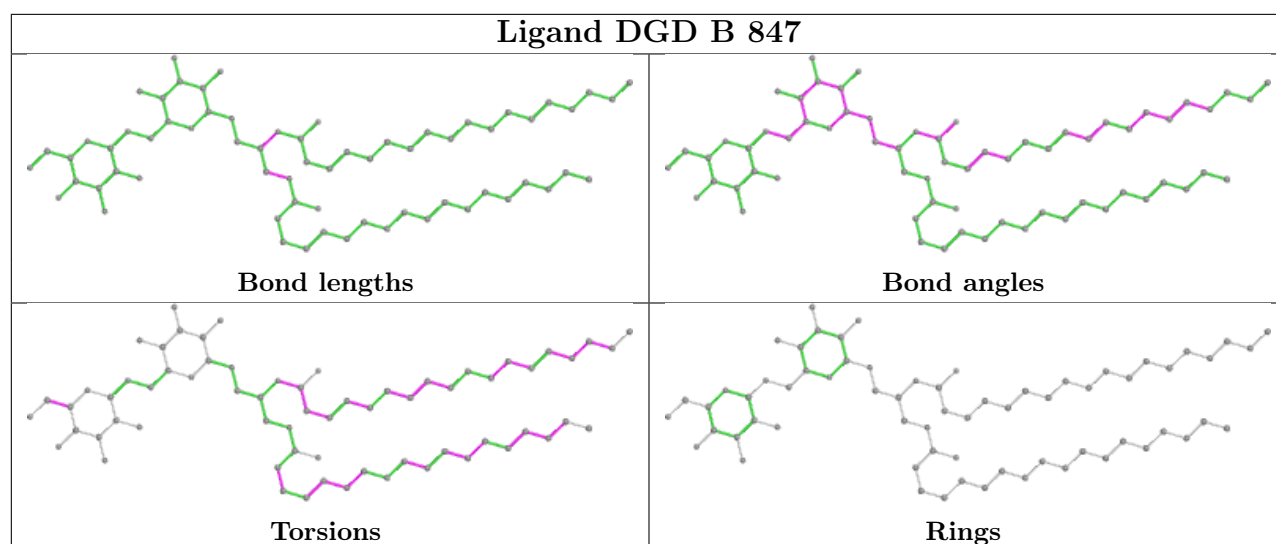
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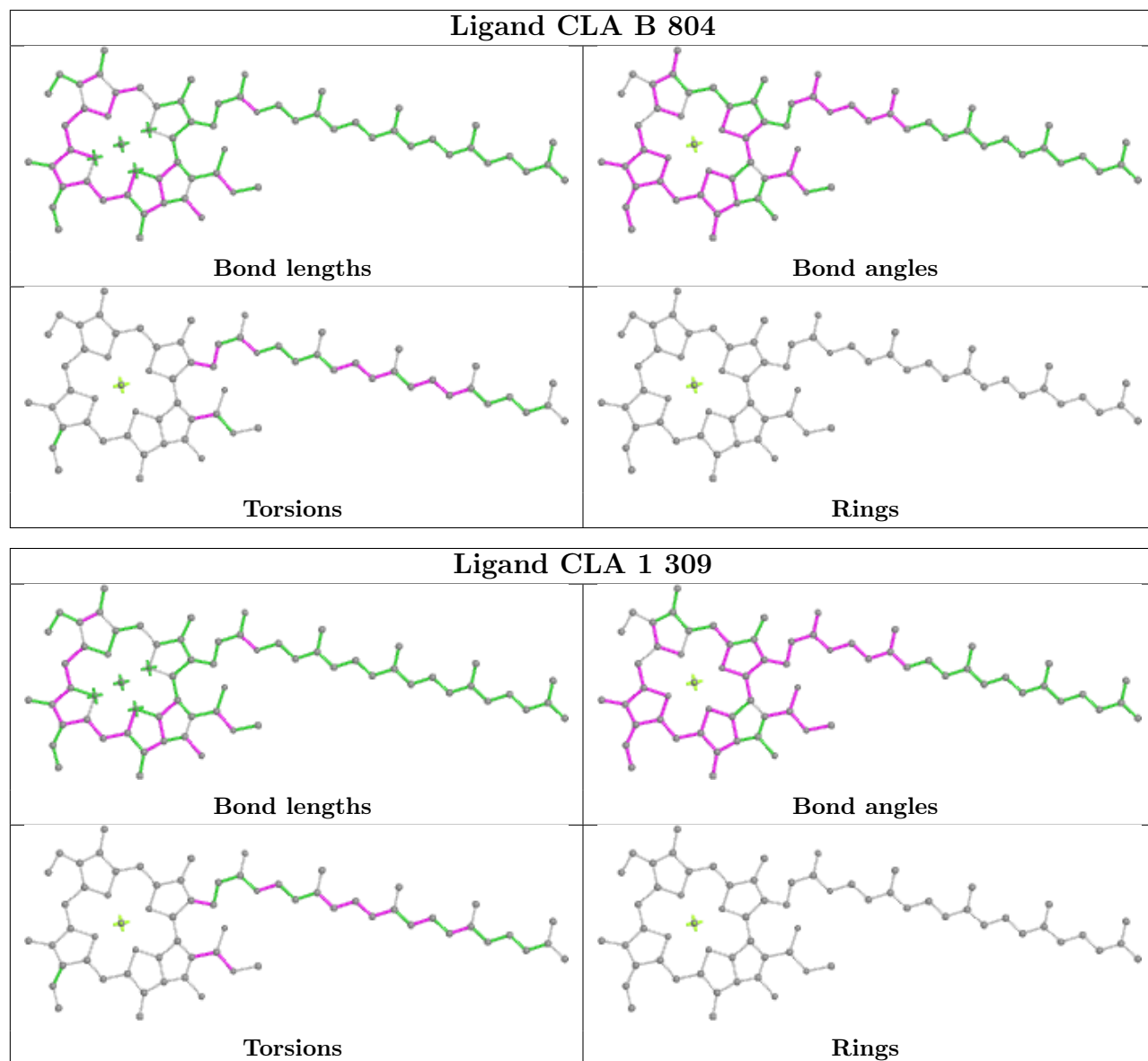
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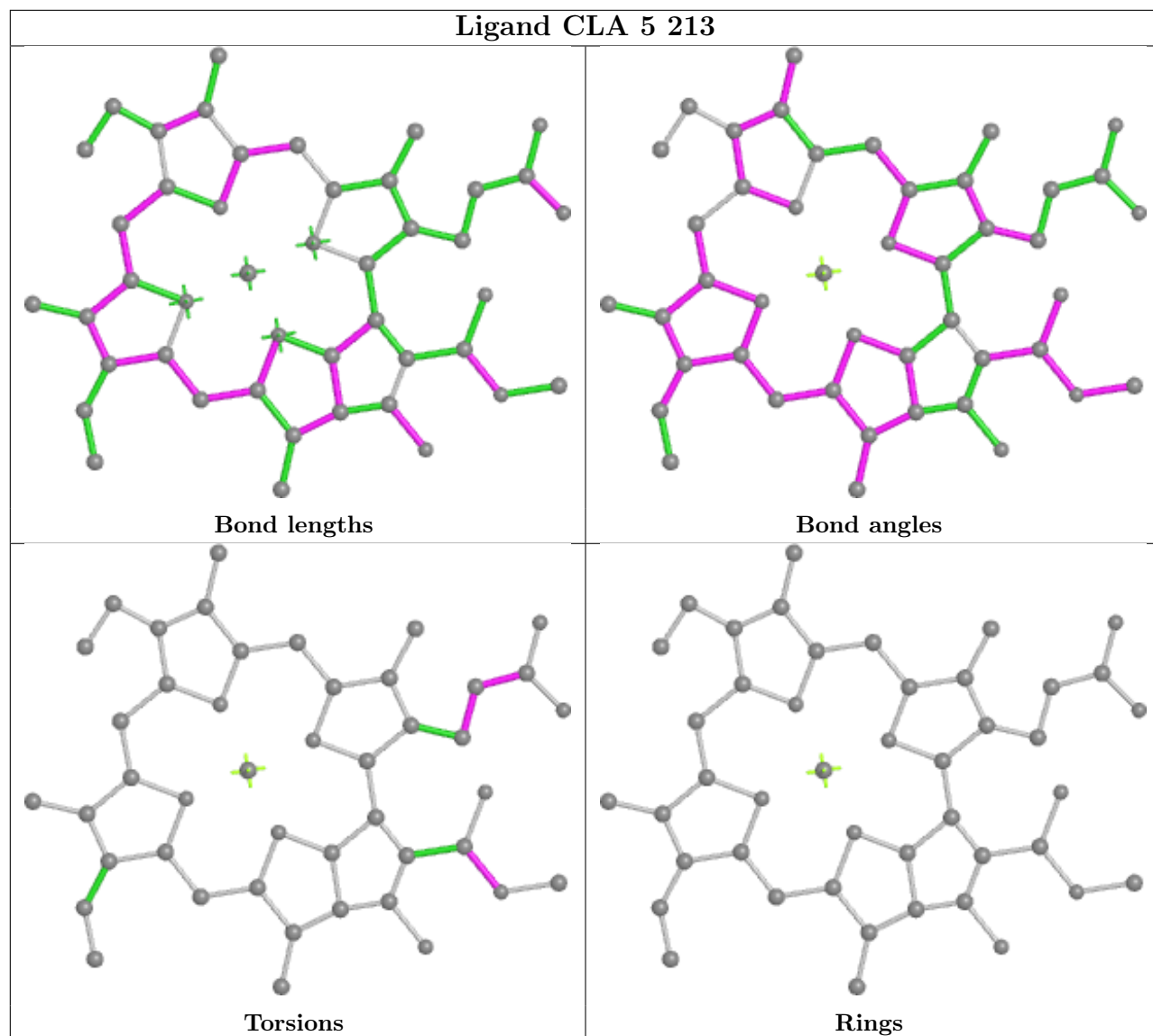
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	842	LHG	1	0
19	1	303	CLA	6	0
19	4	303	CLA	5	0
24	1	323	LMT	4	0
19	A	828	CLA	3	0
19	B	824	CLA	1	0

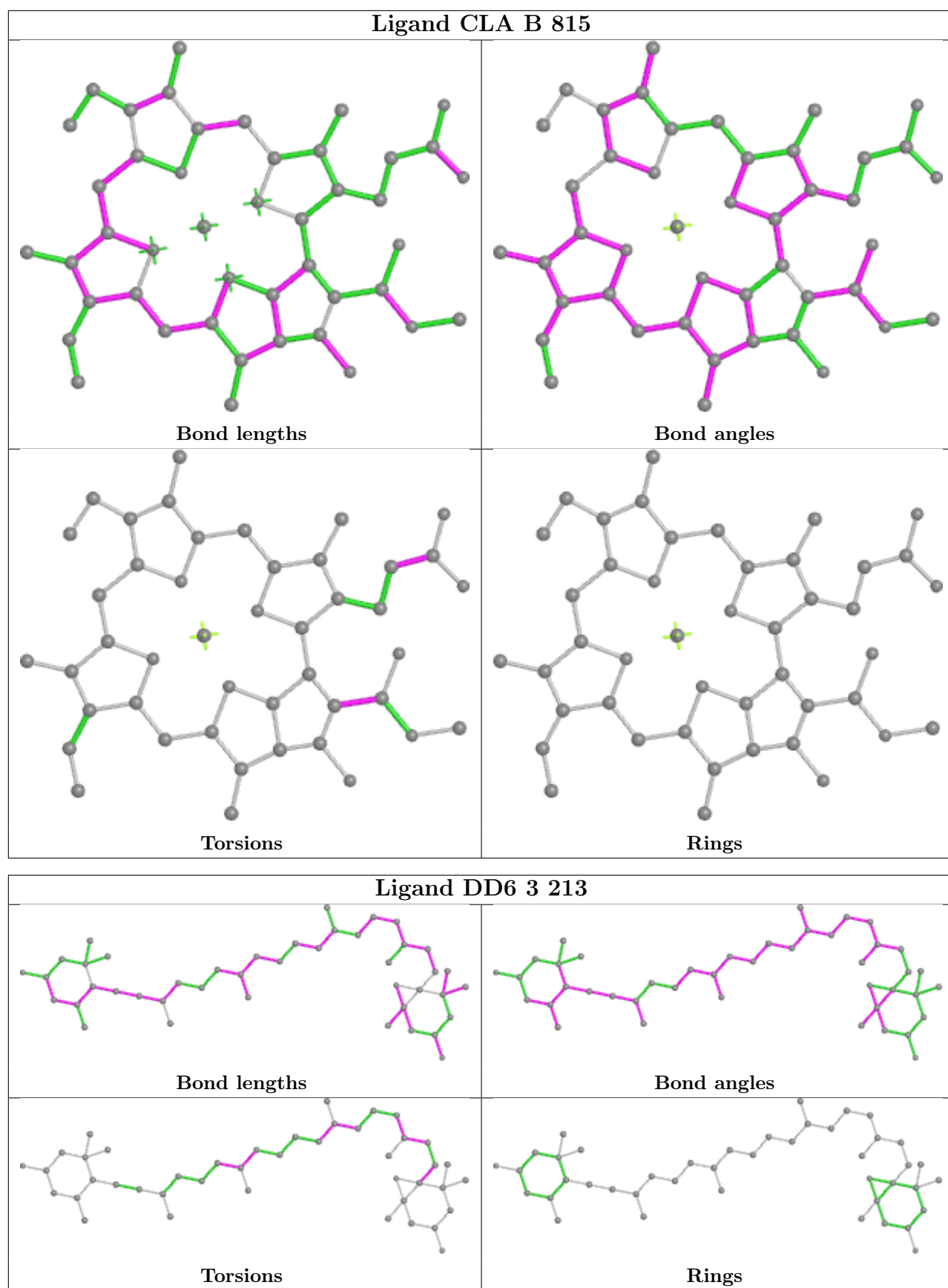
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

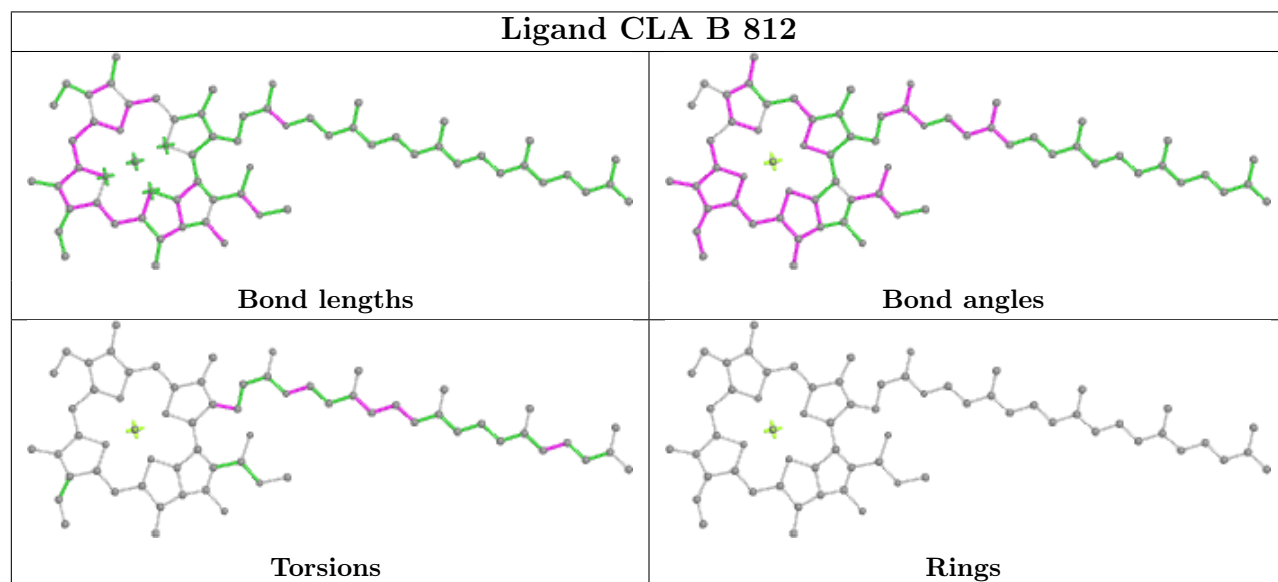
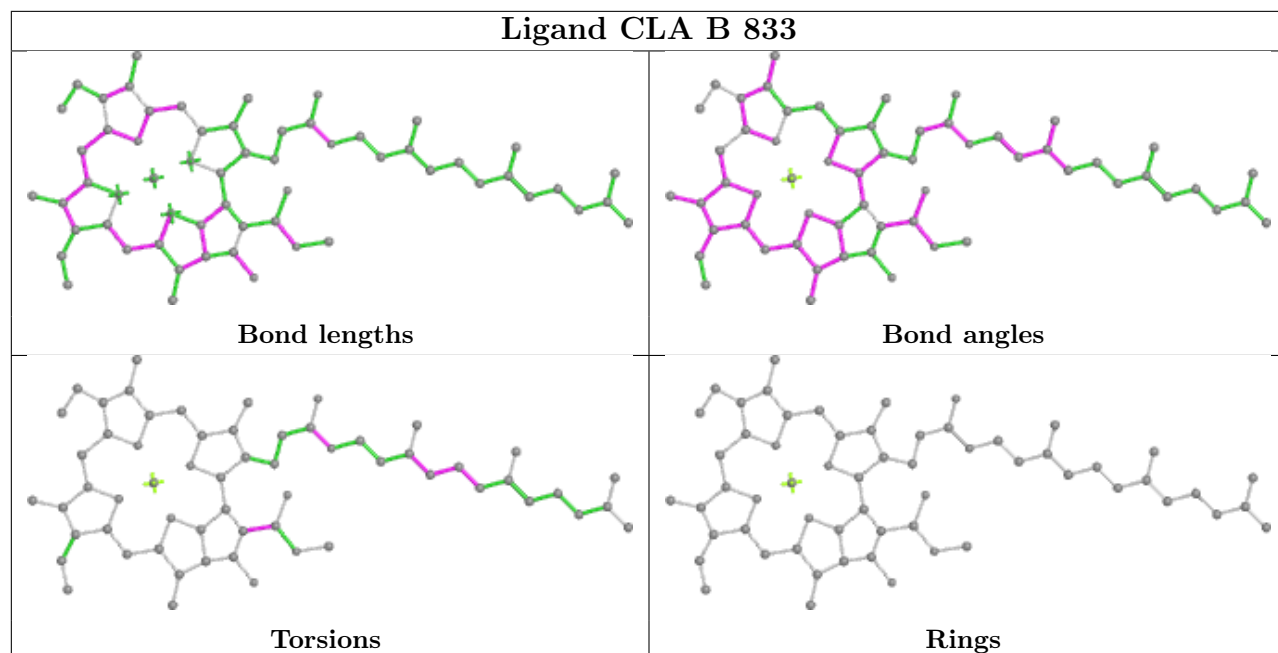


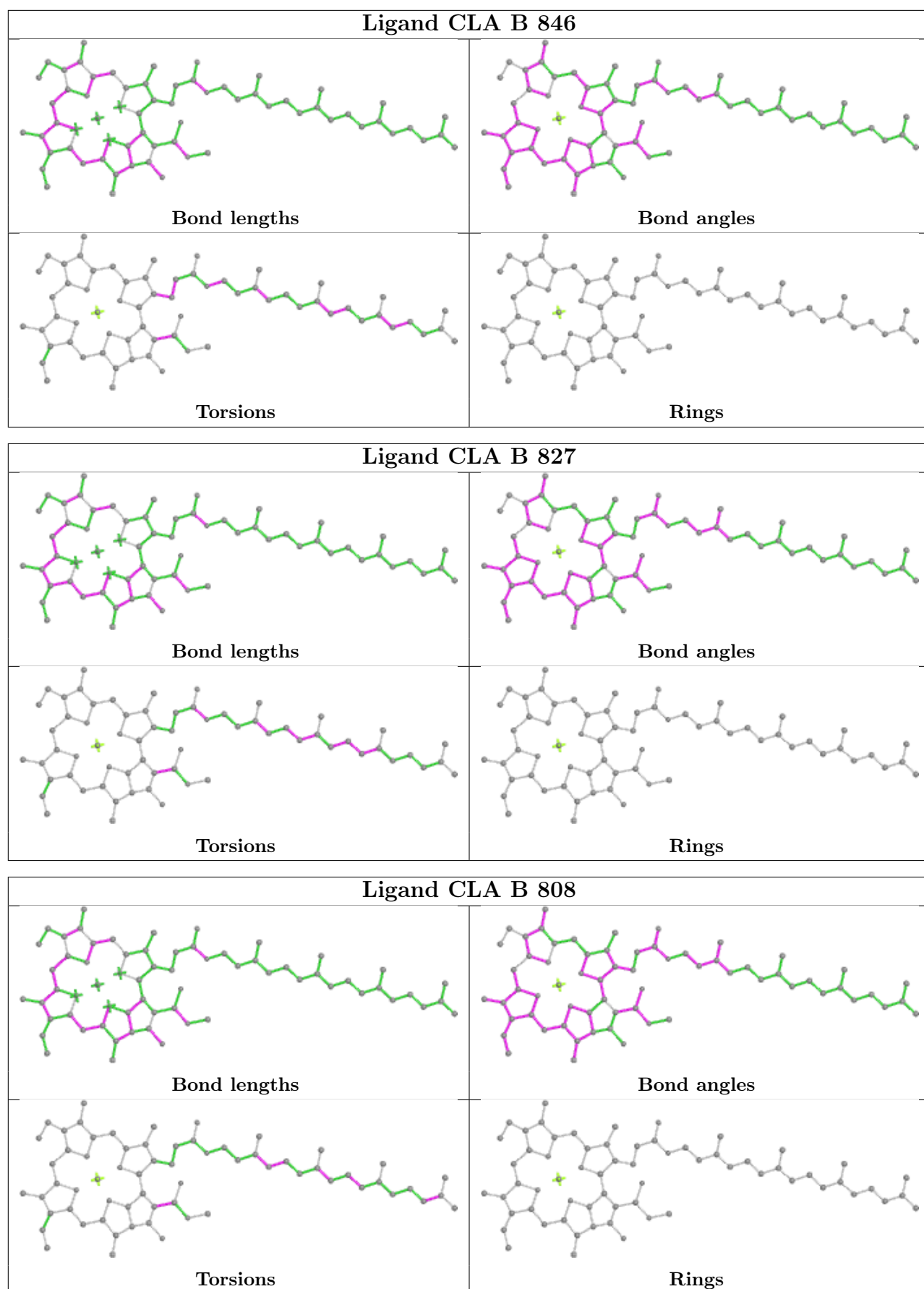


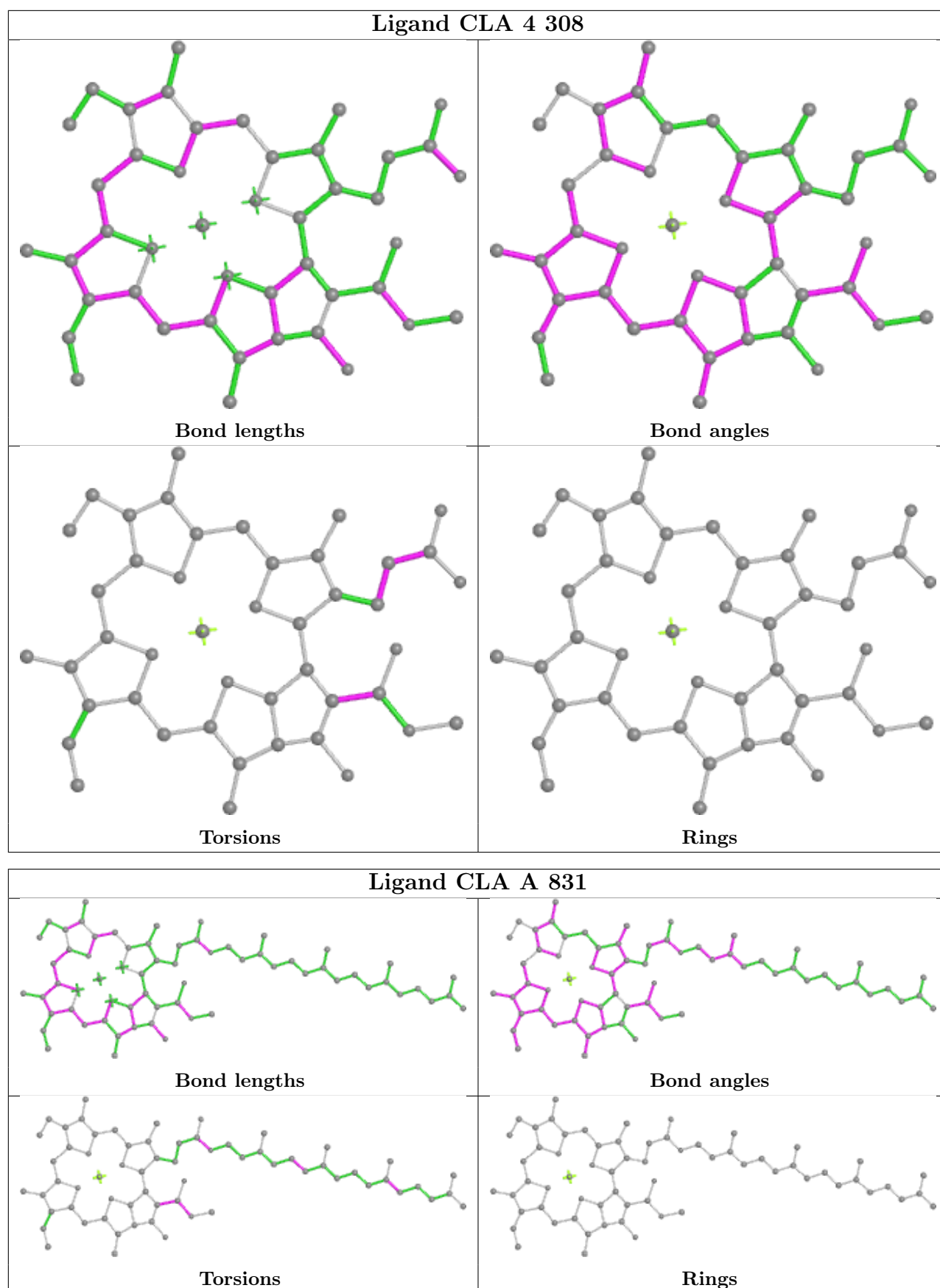


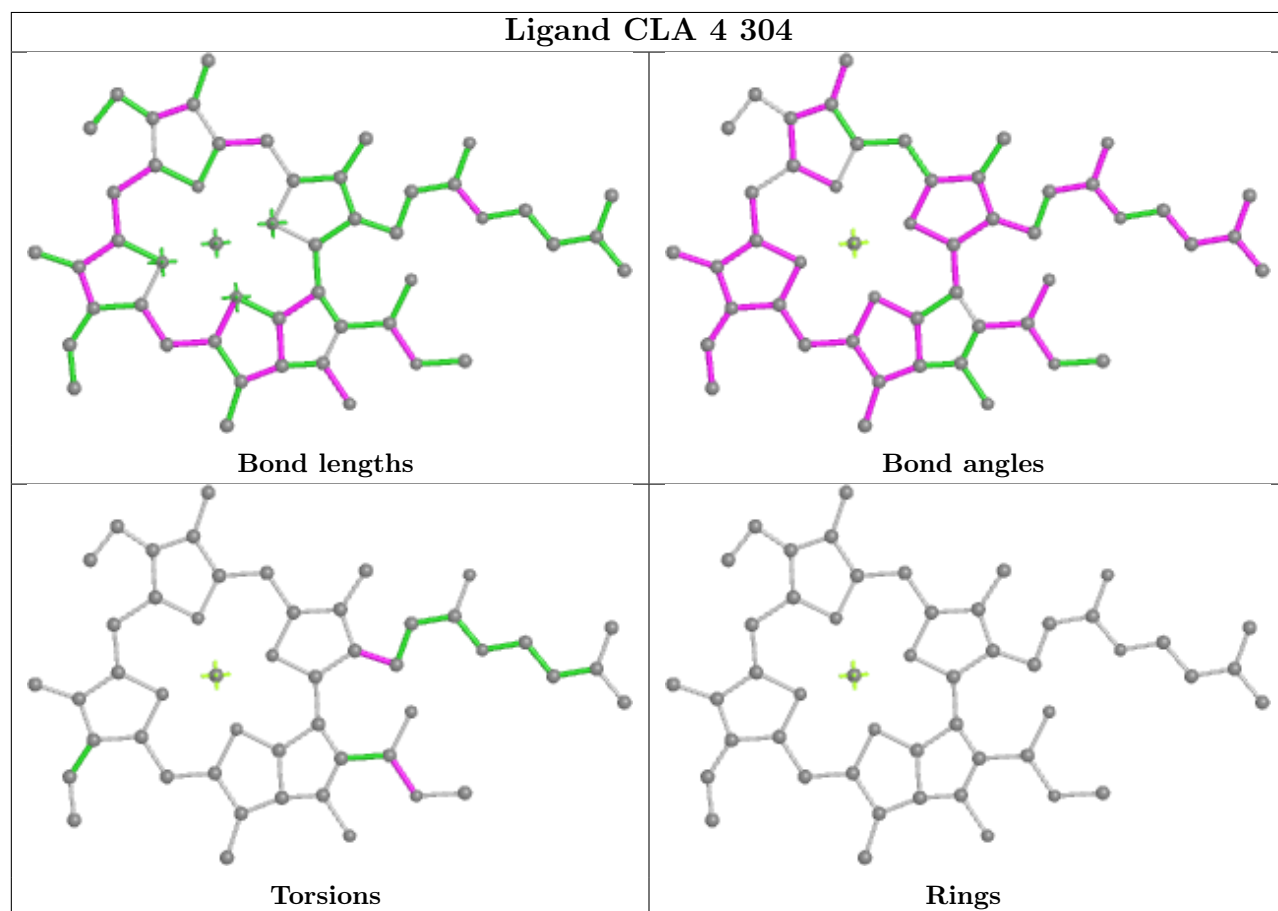
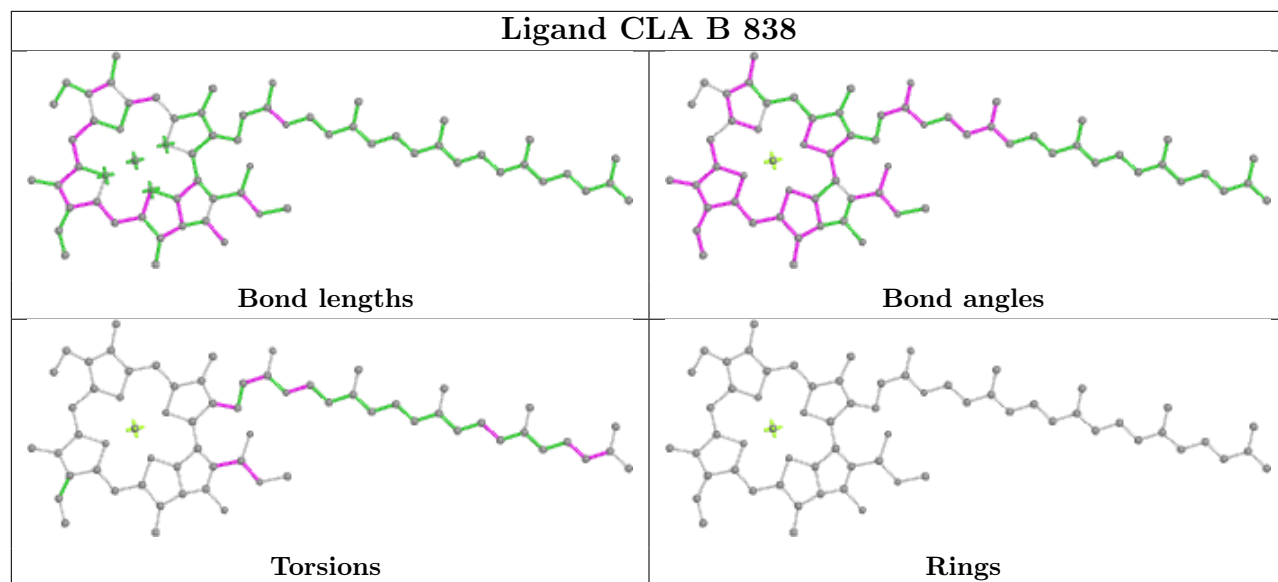


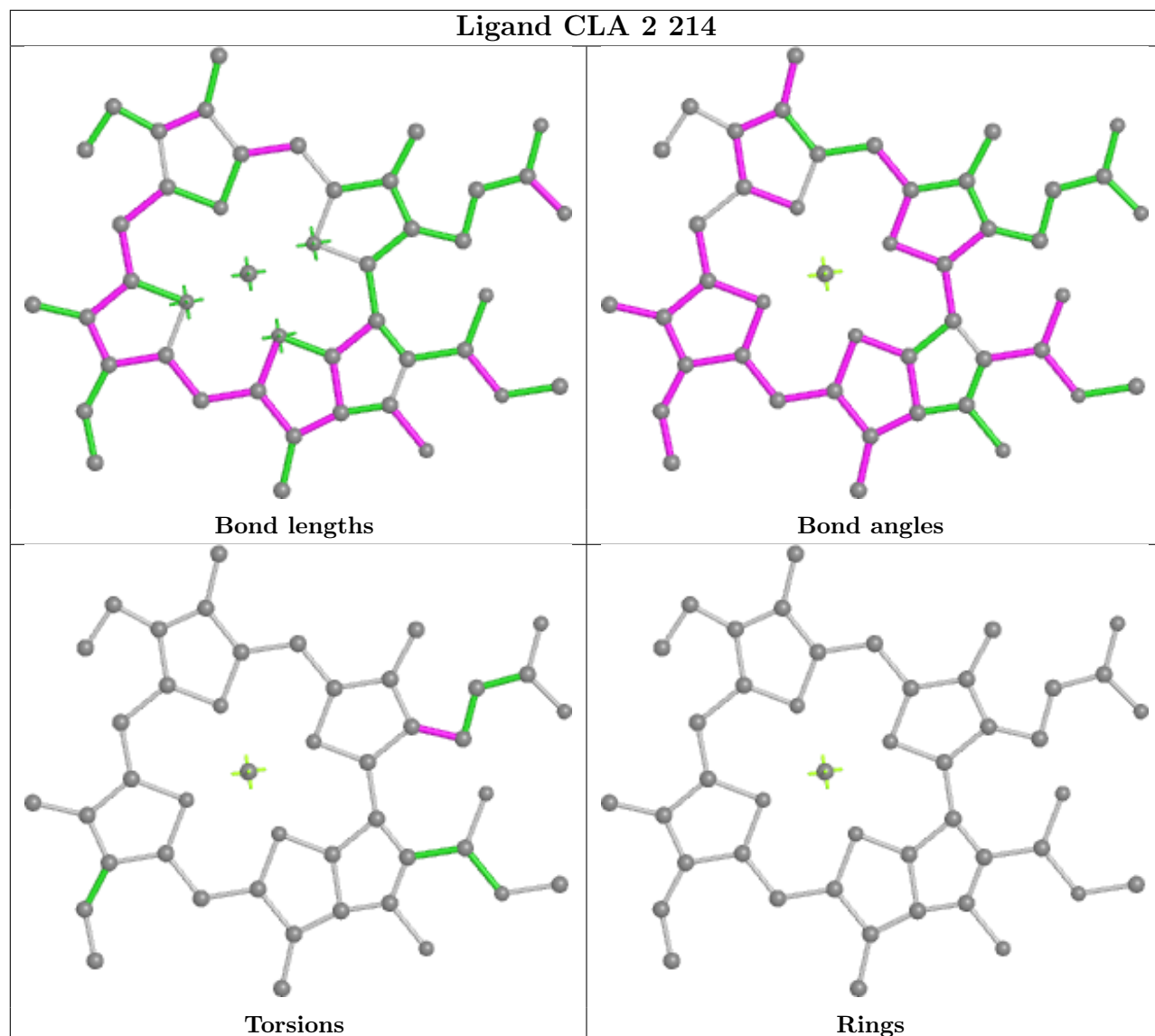


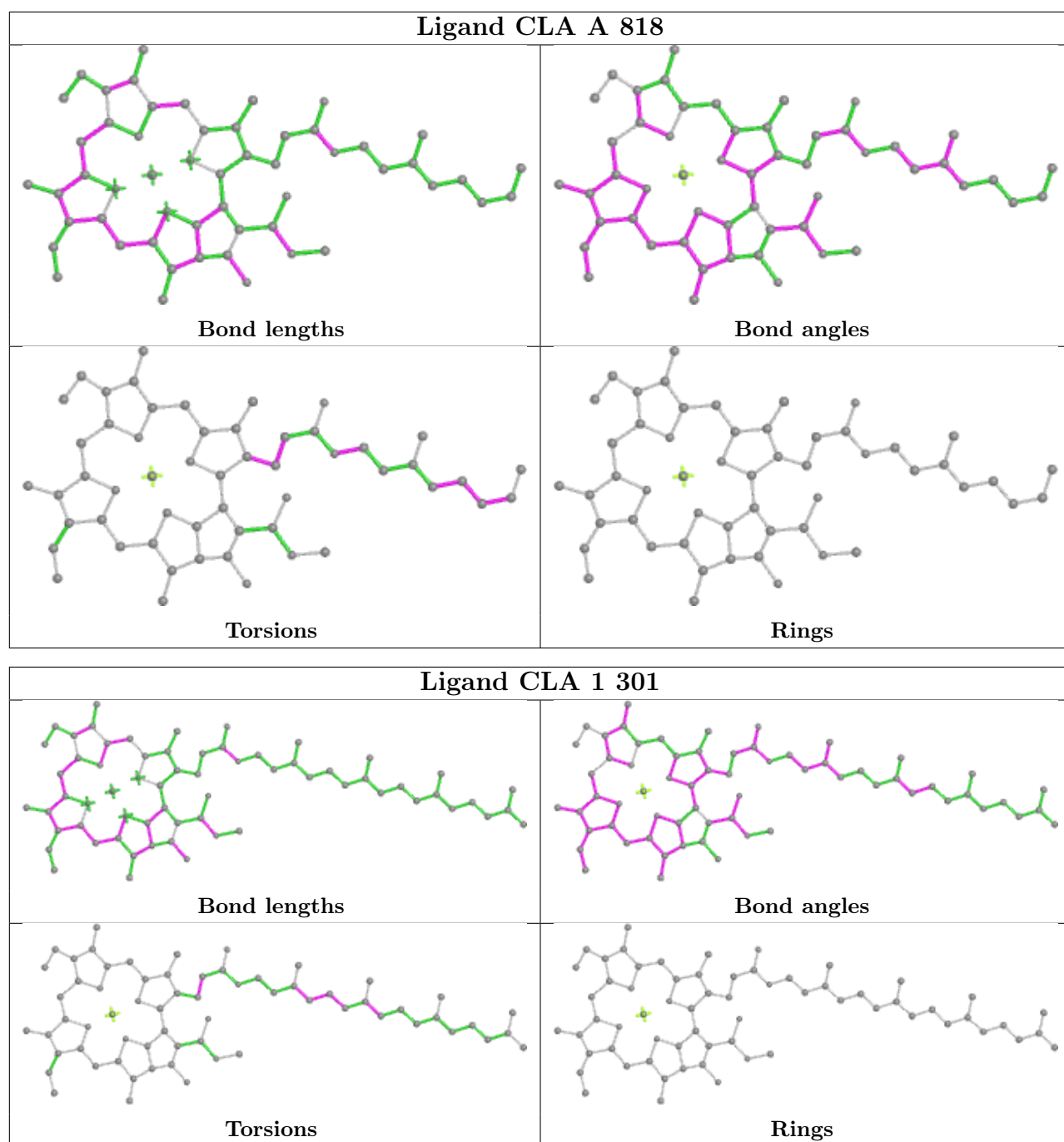


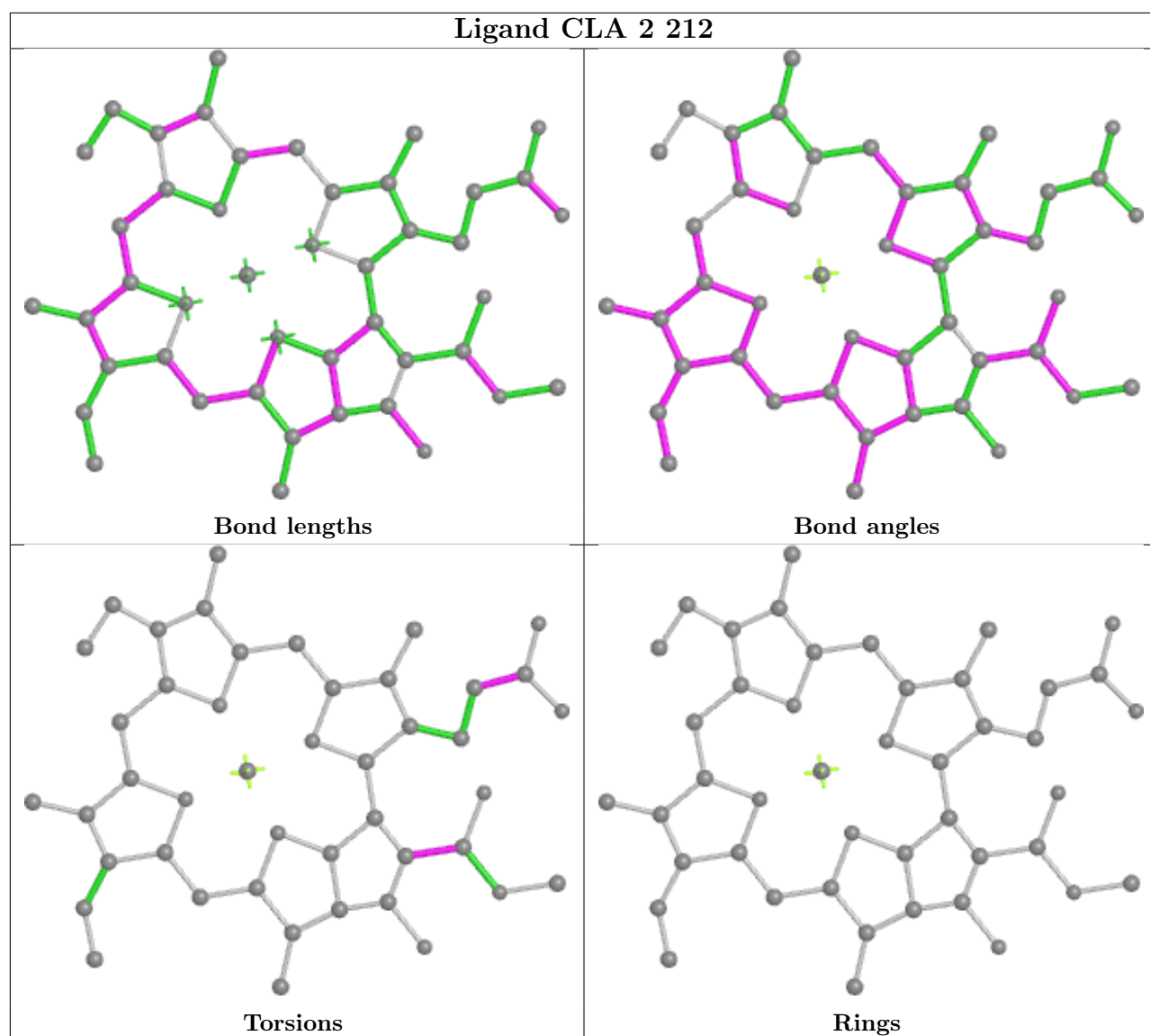


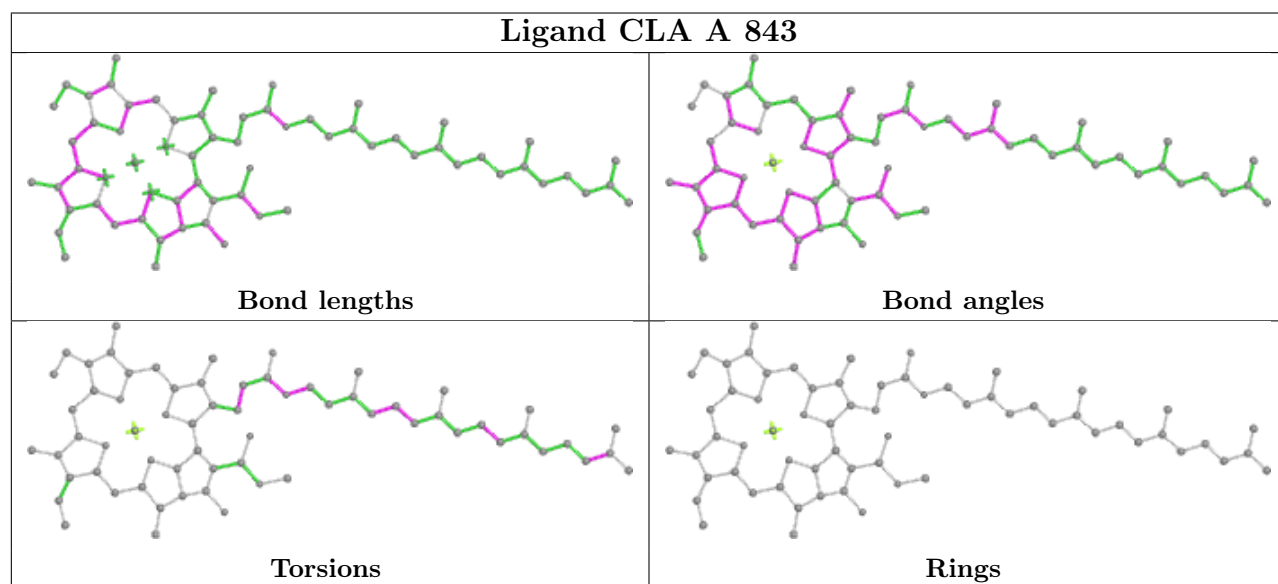
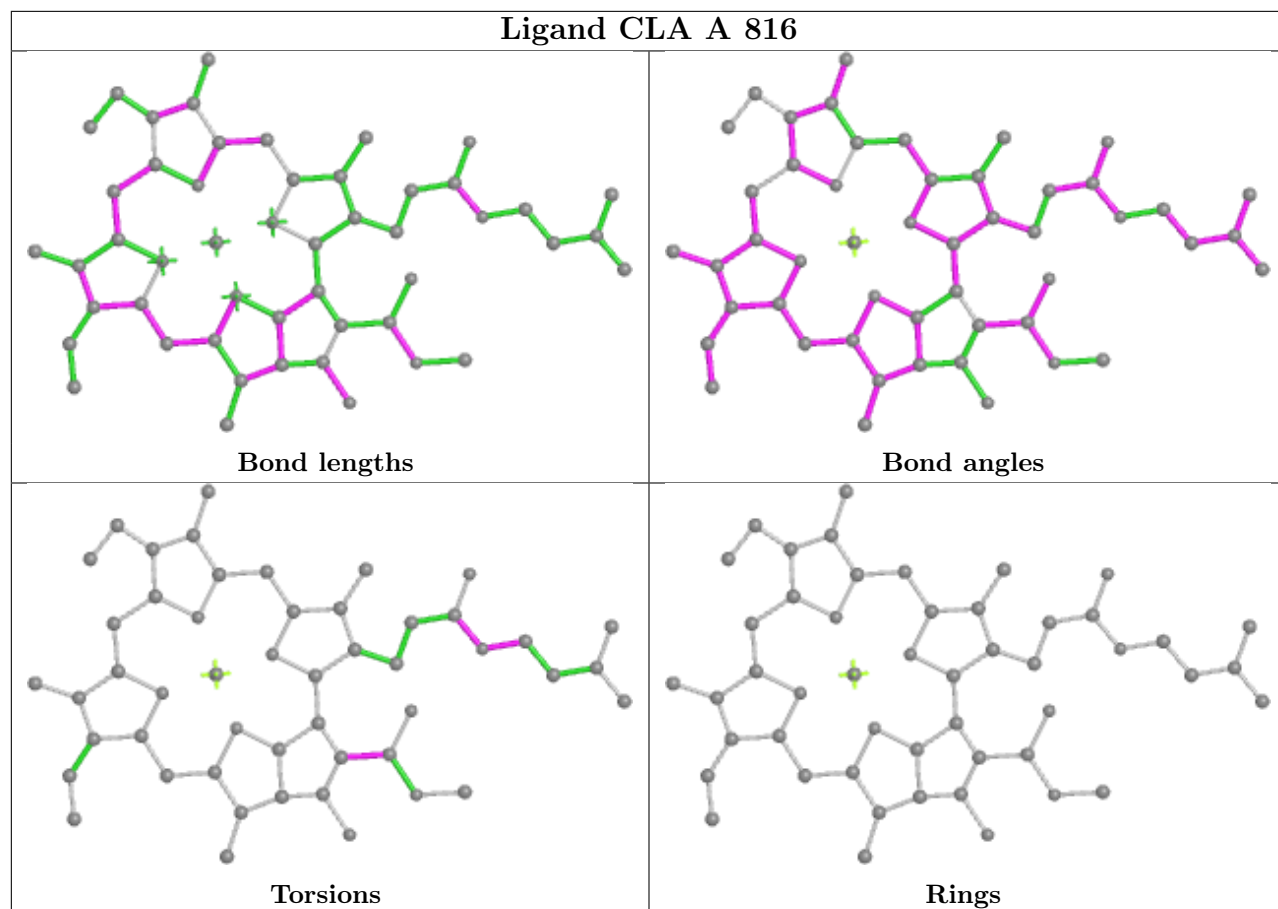


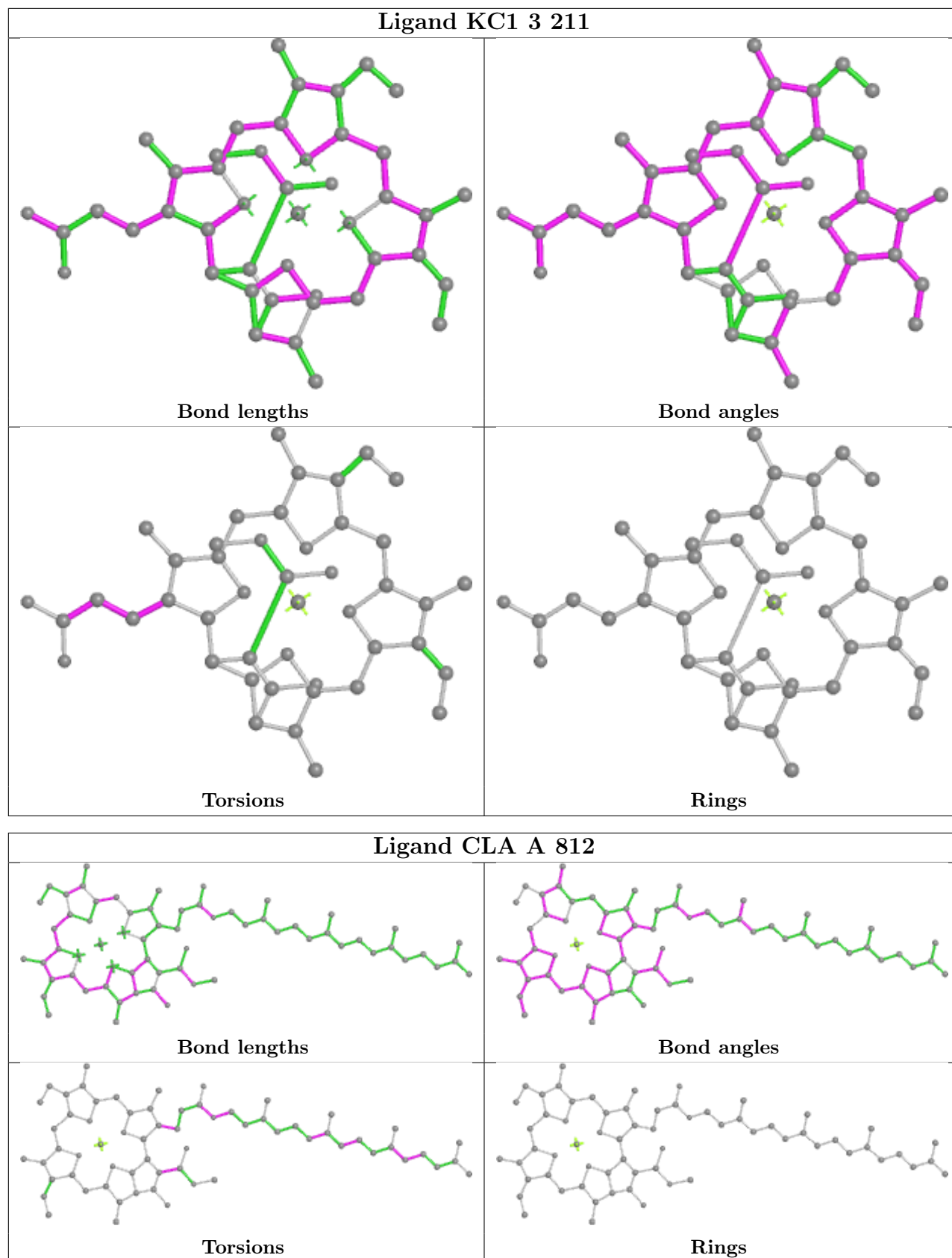


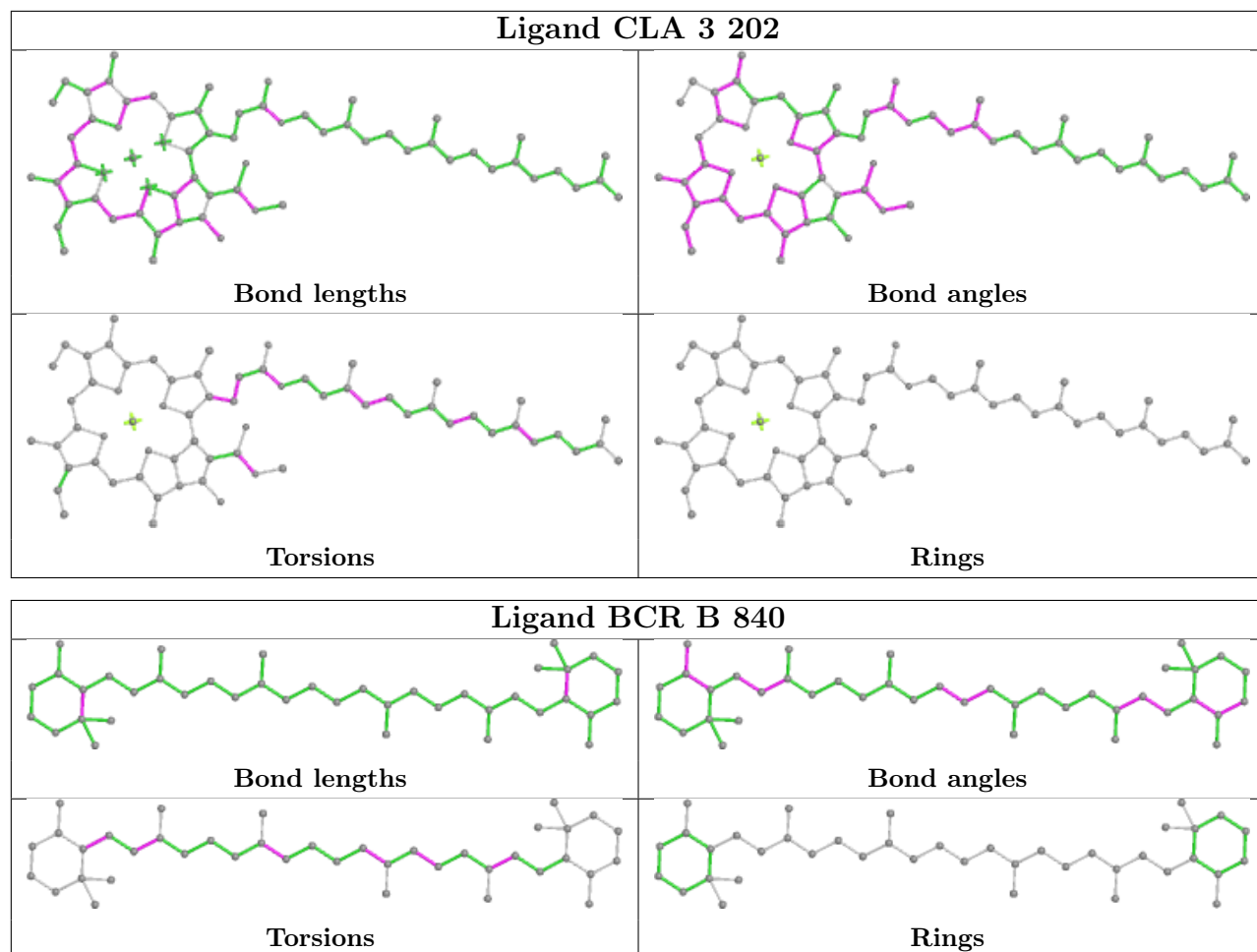


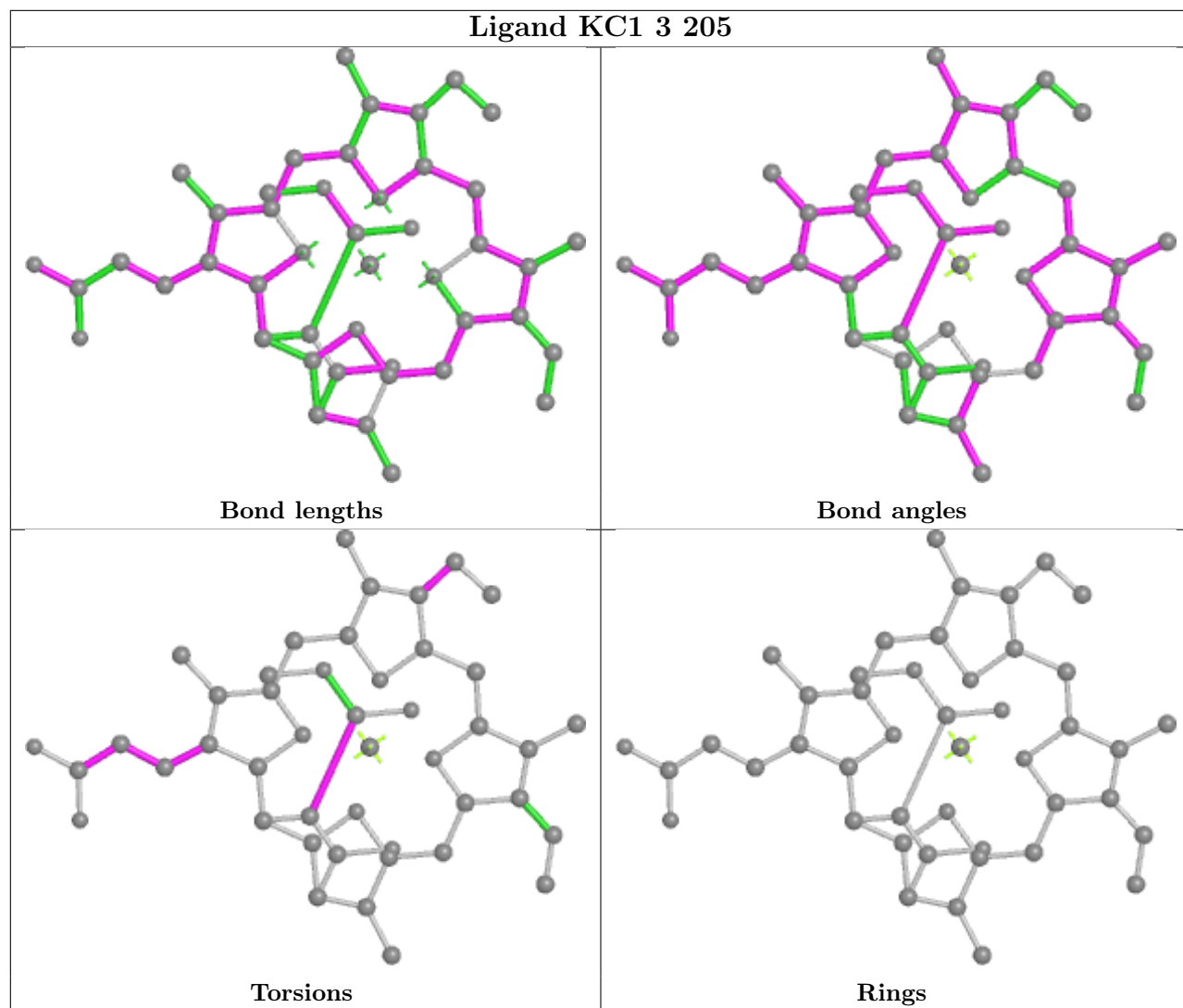


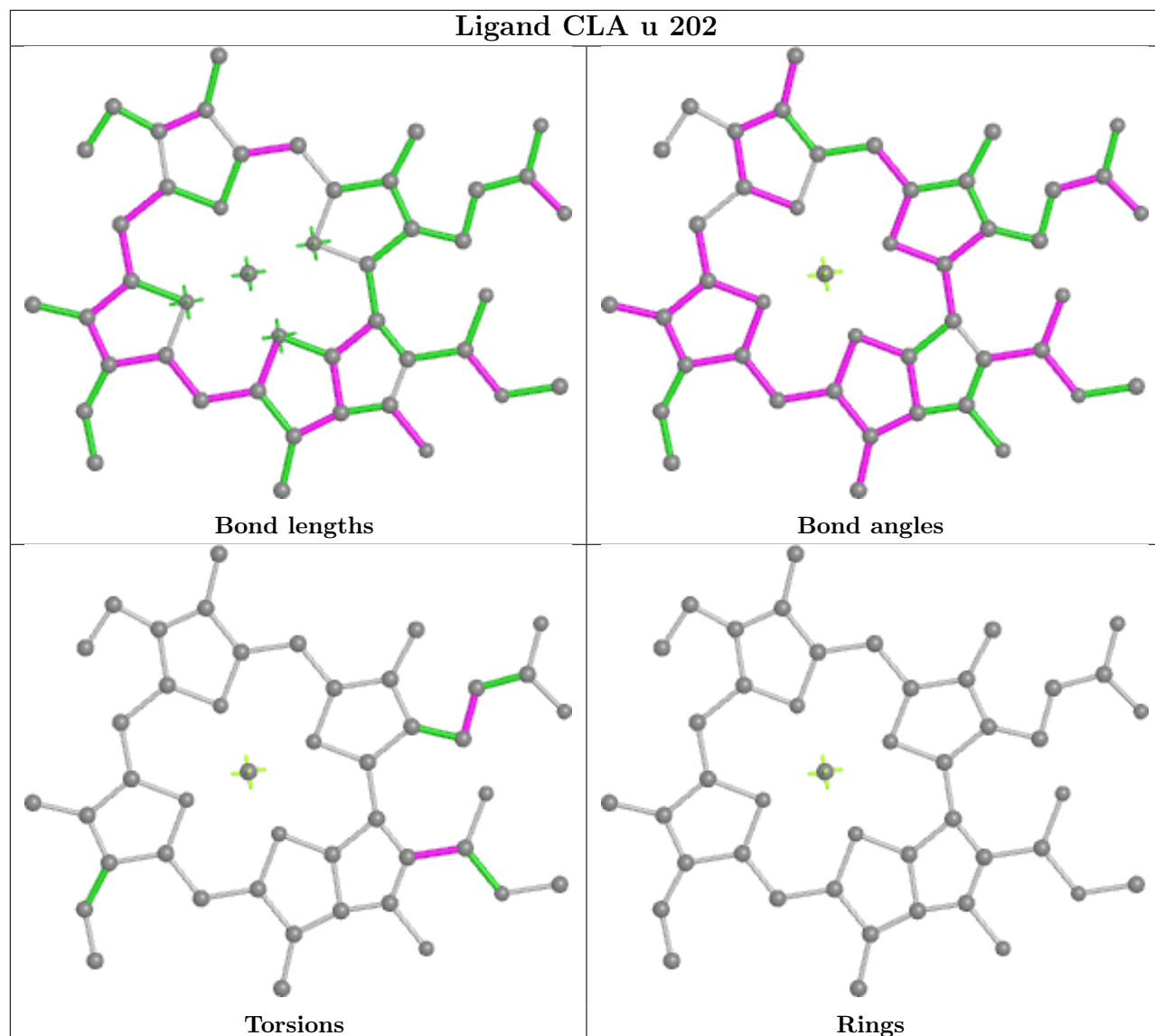


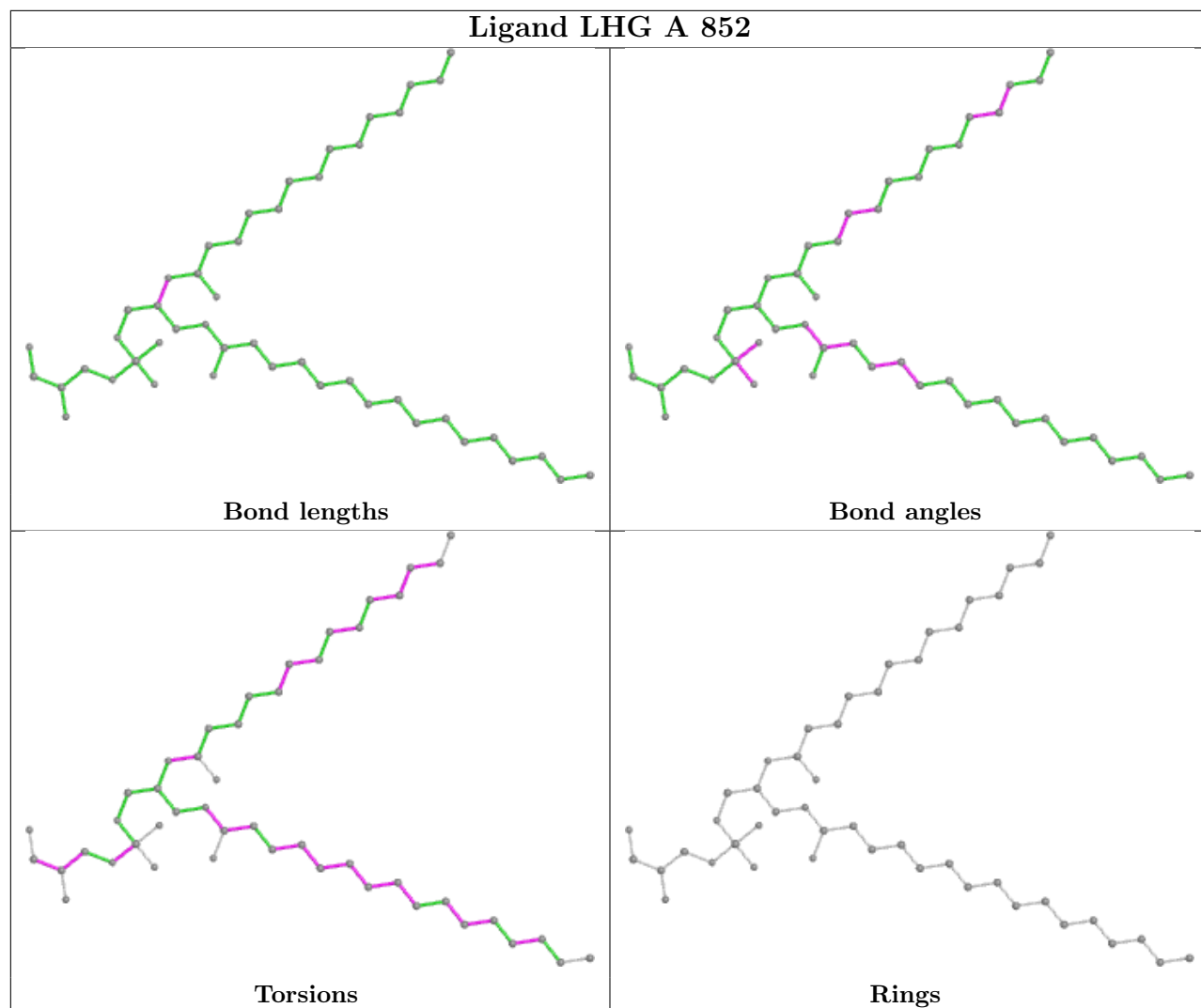


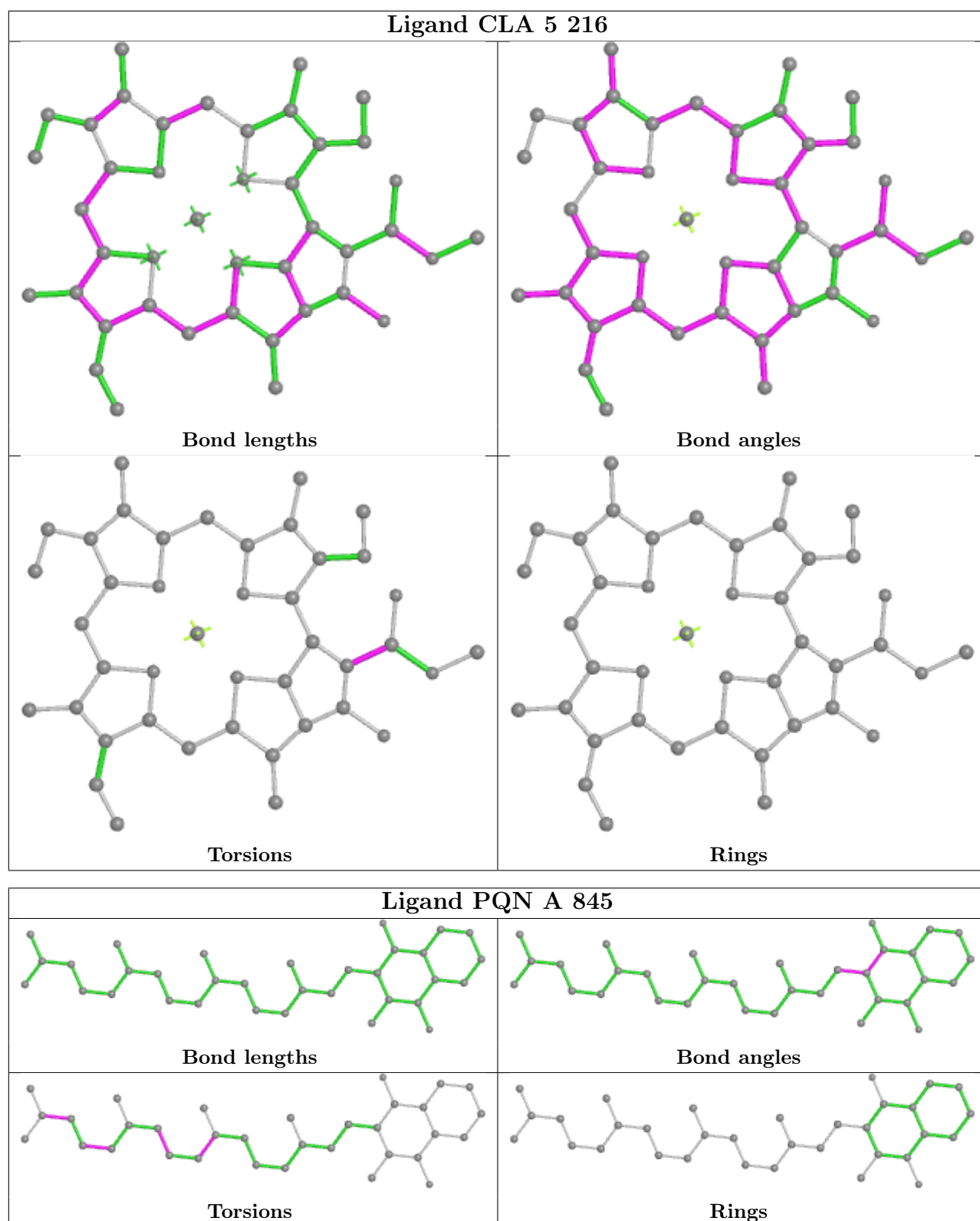


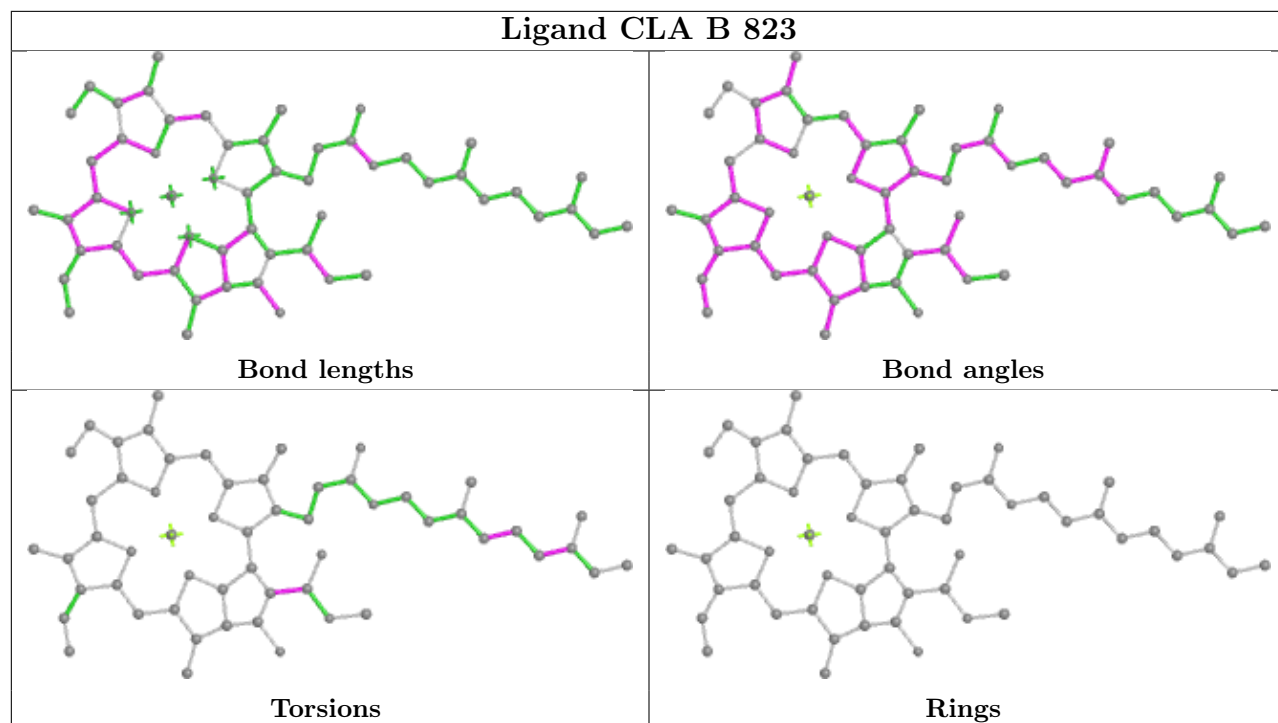


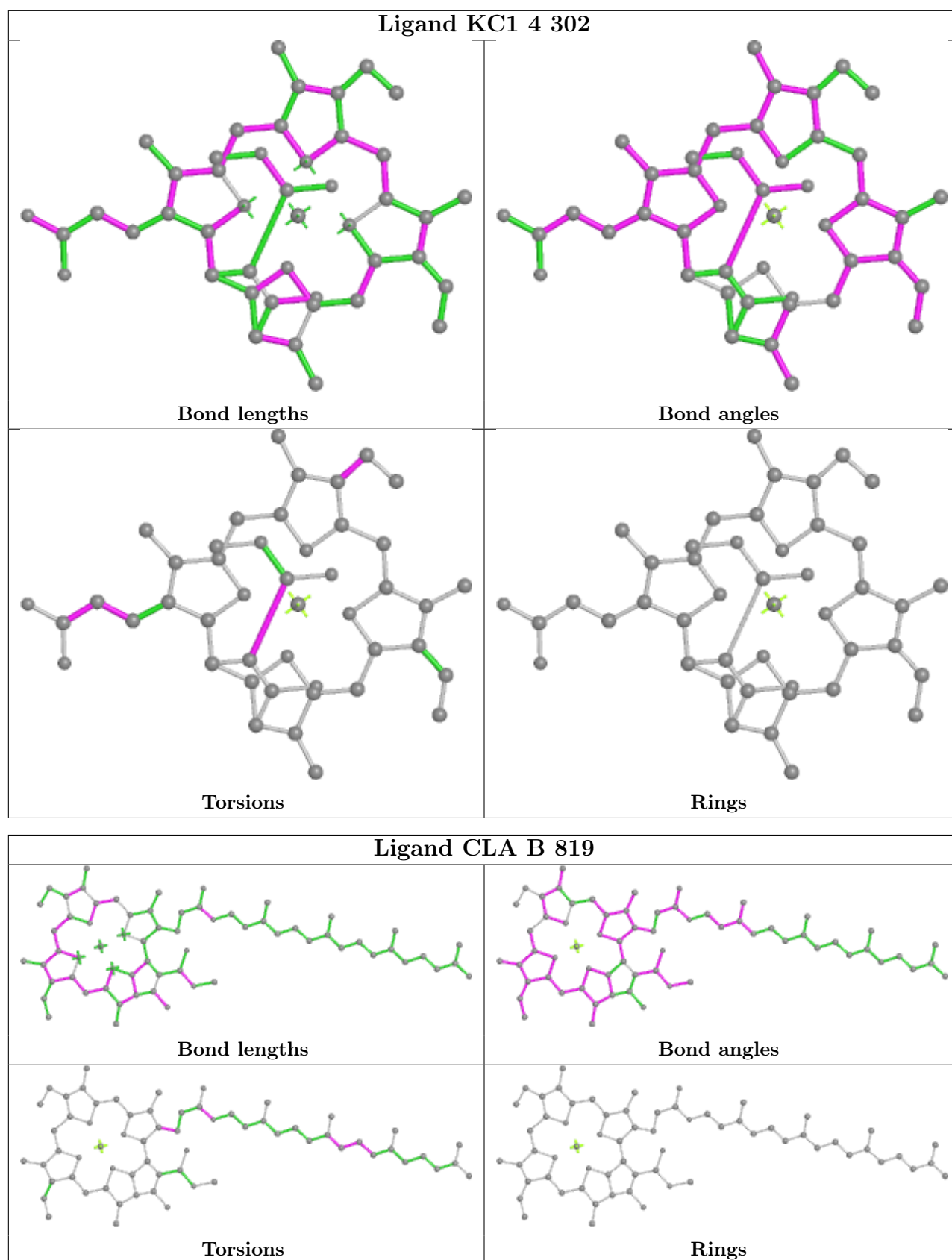


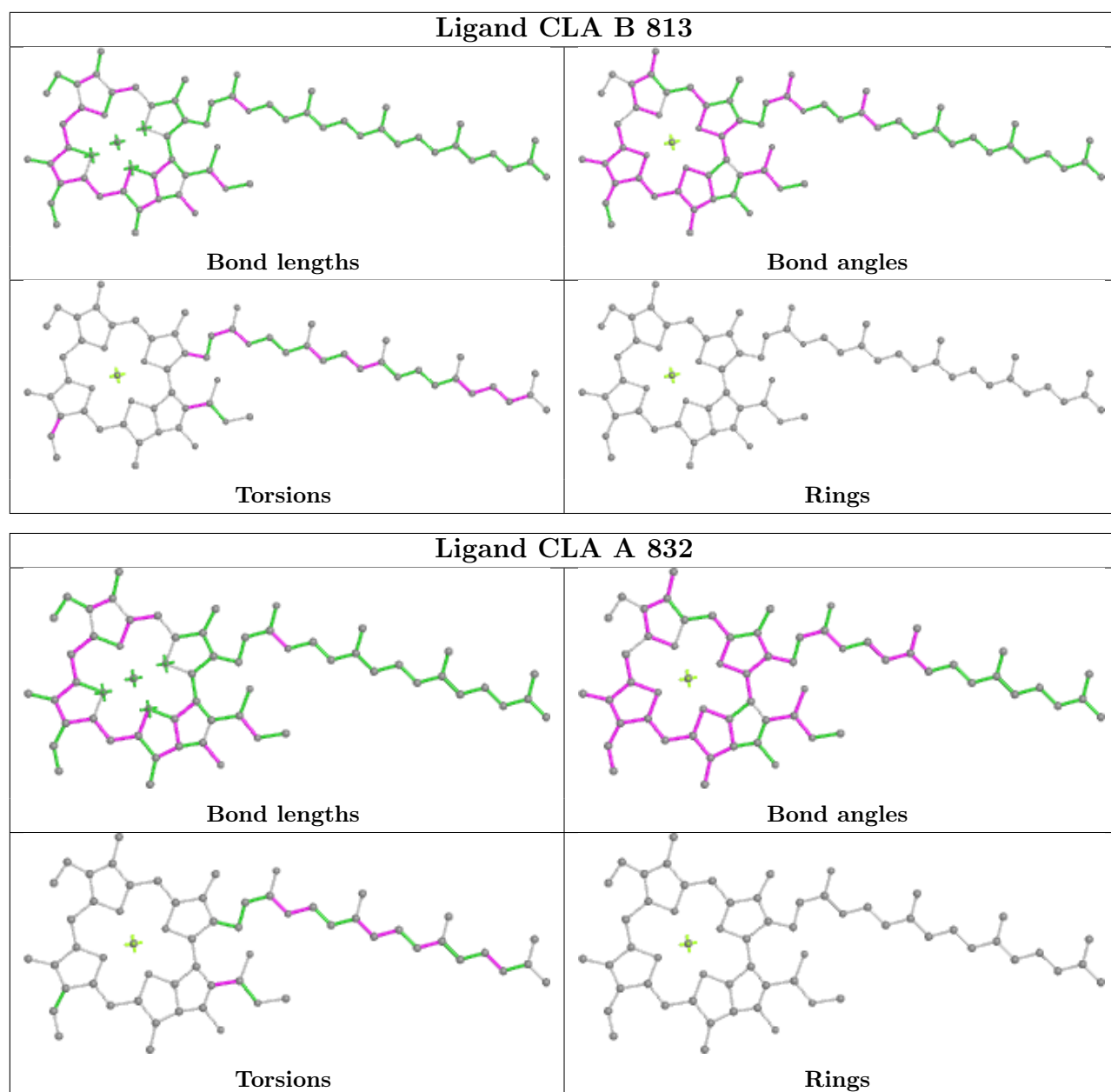


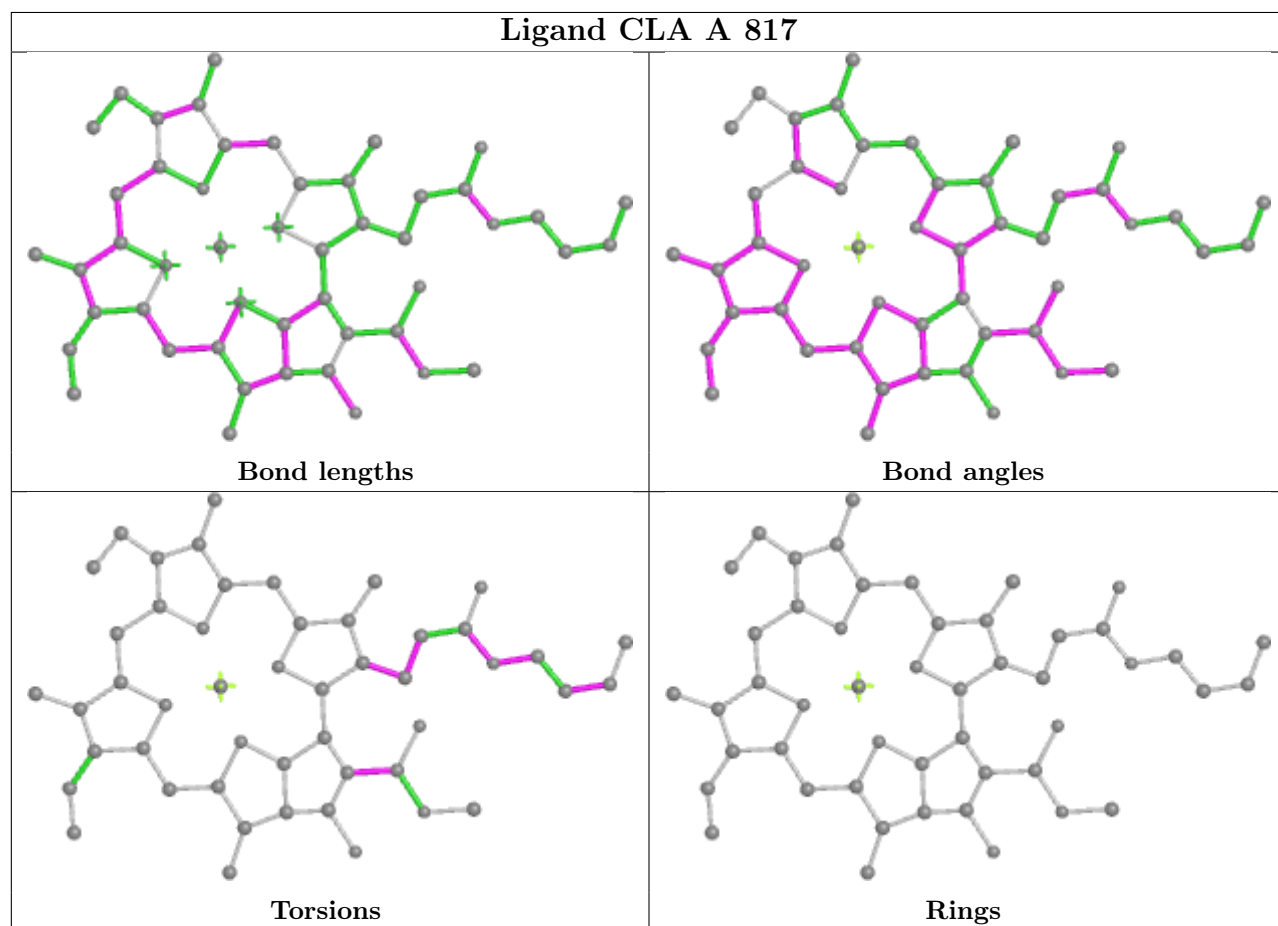
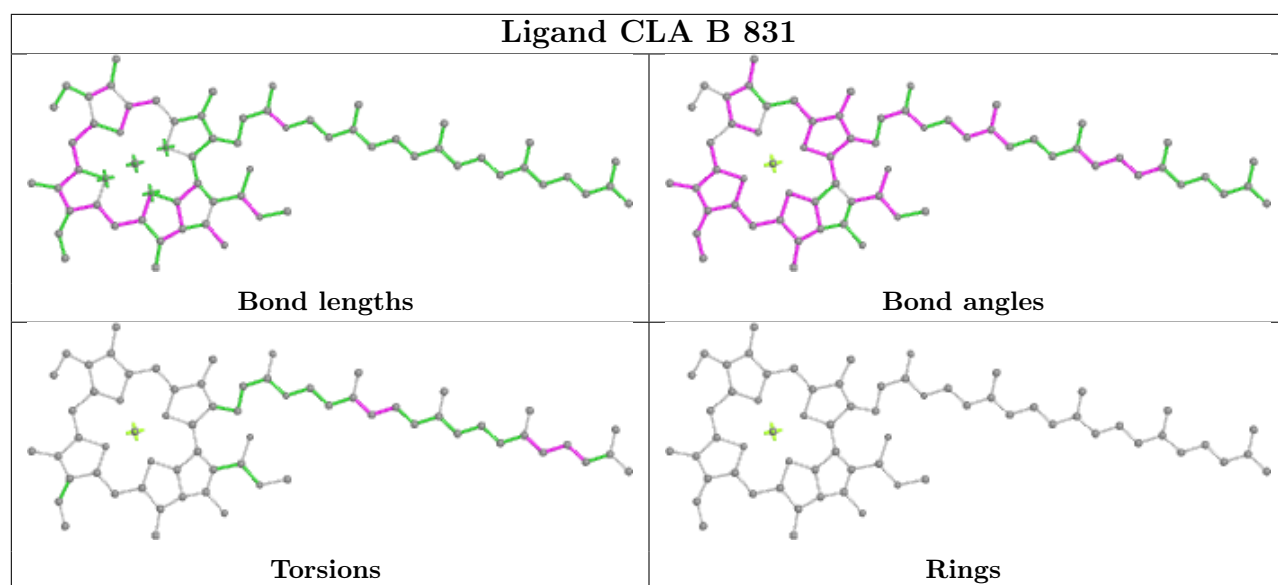


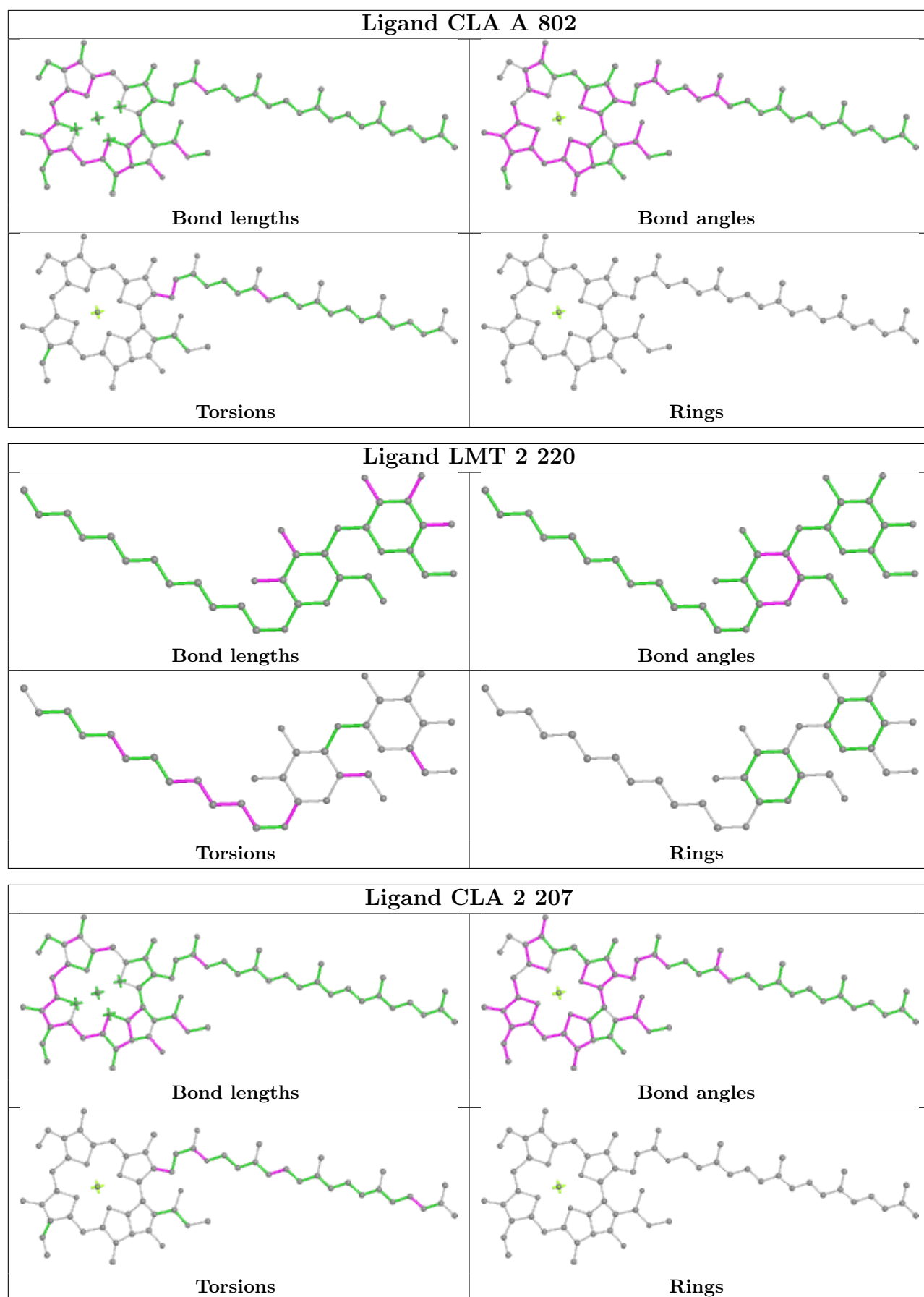


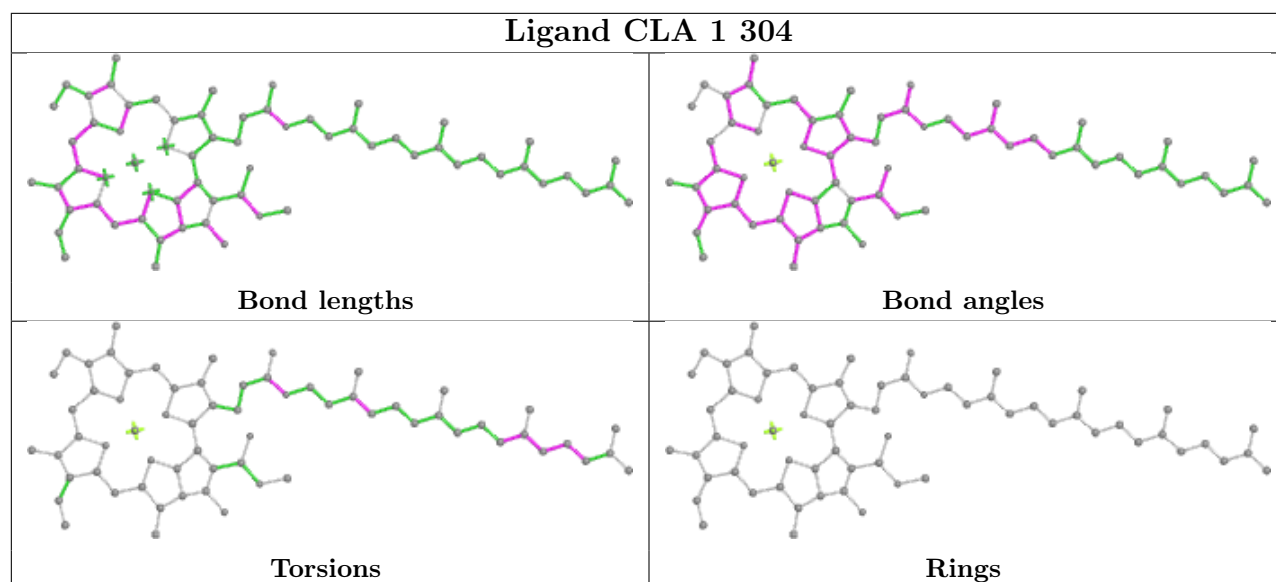
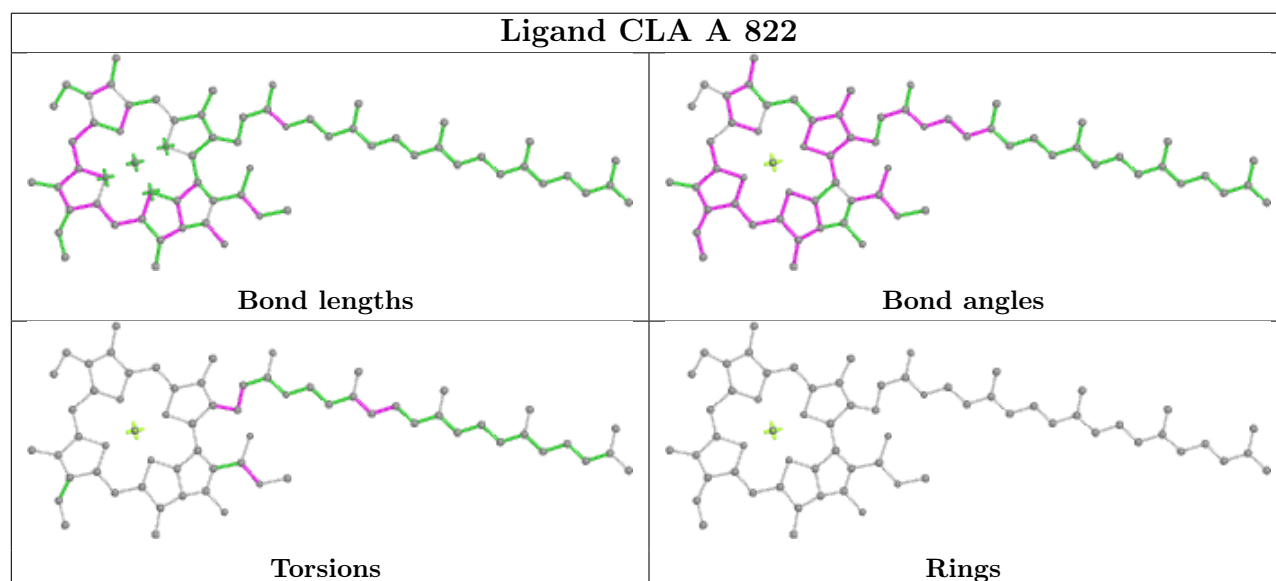
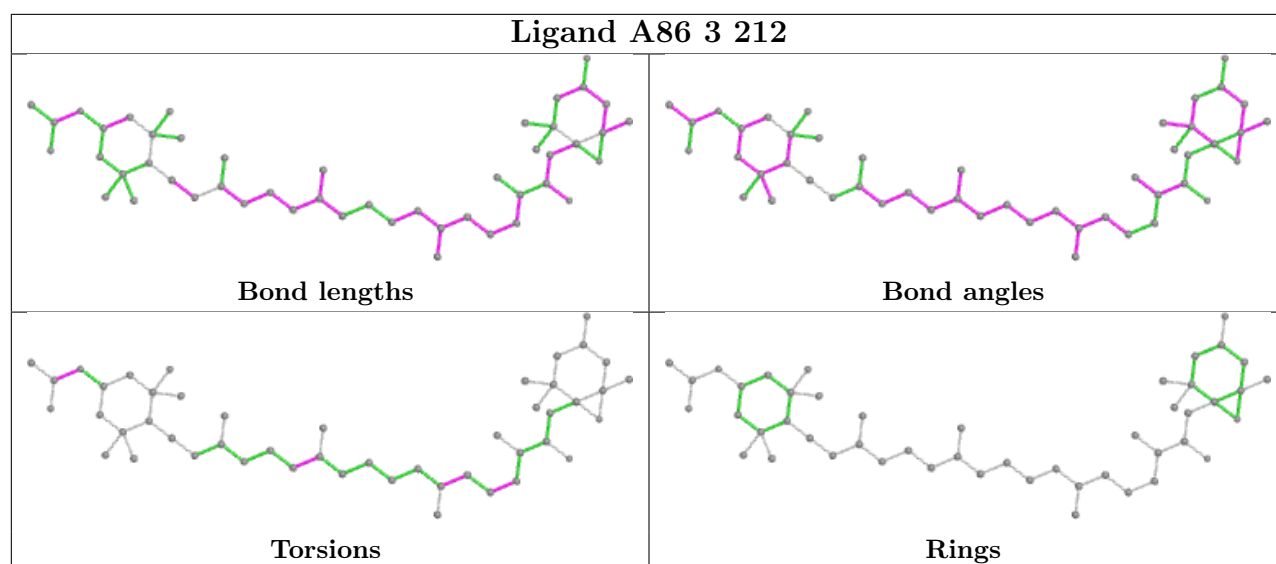


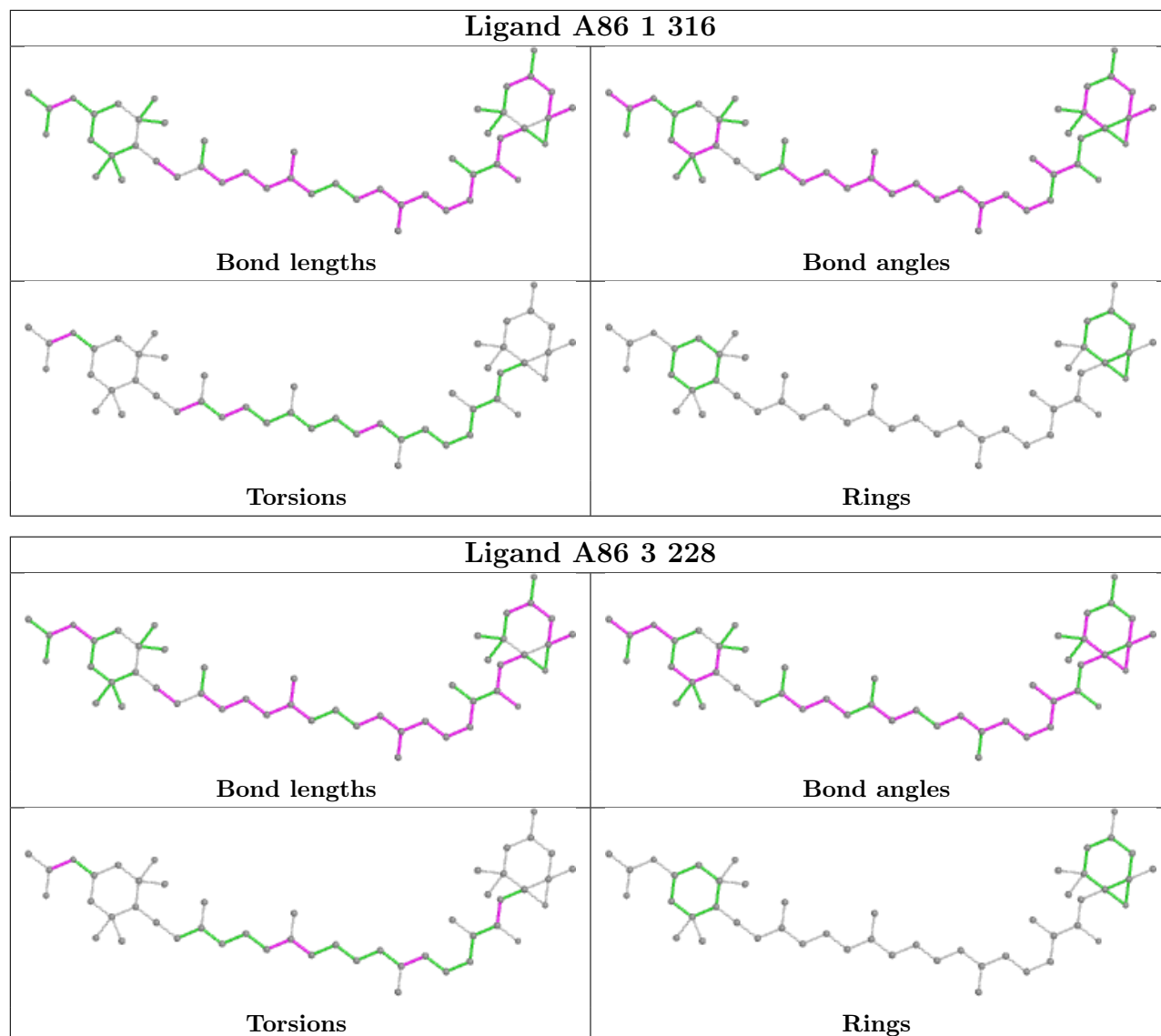


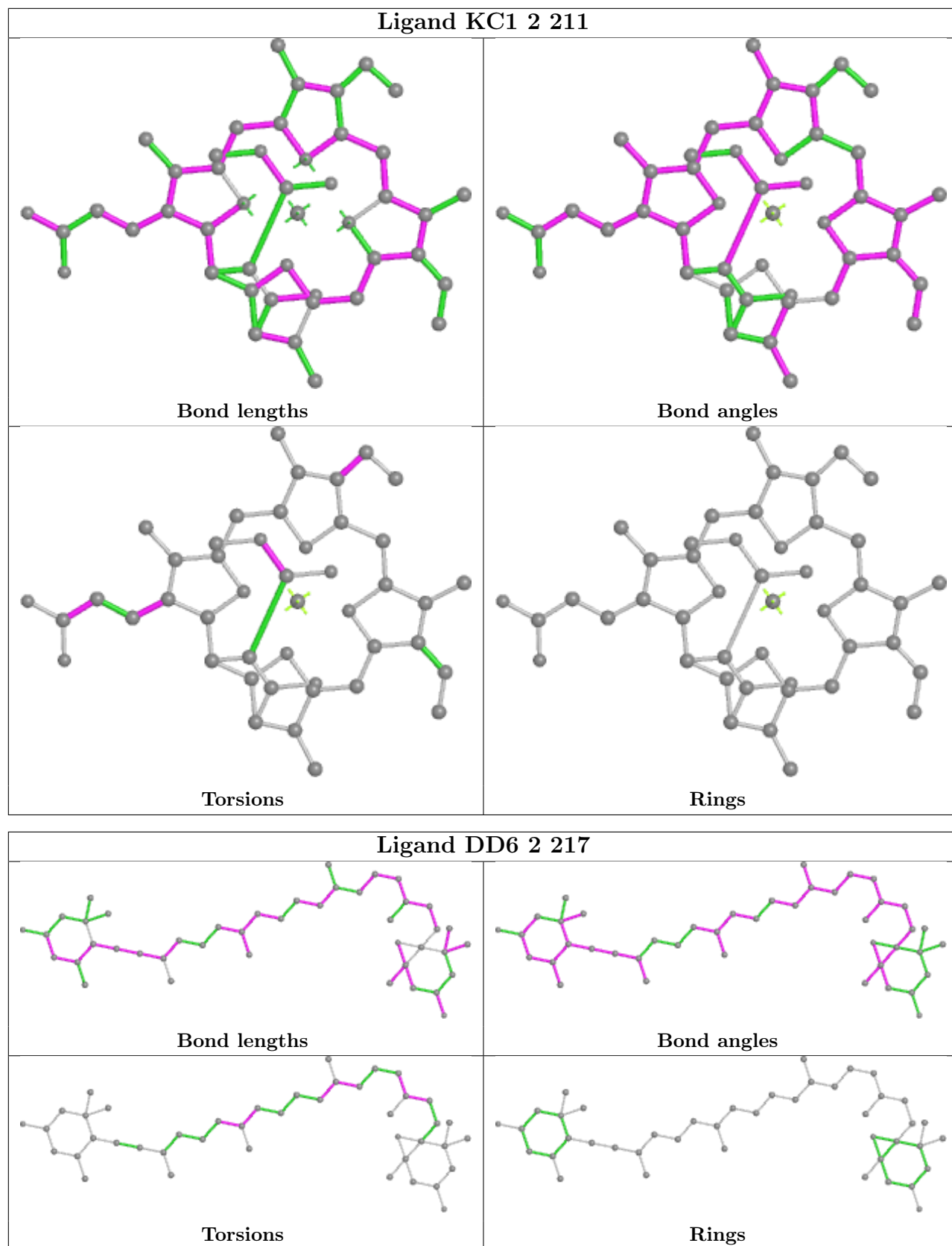


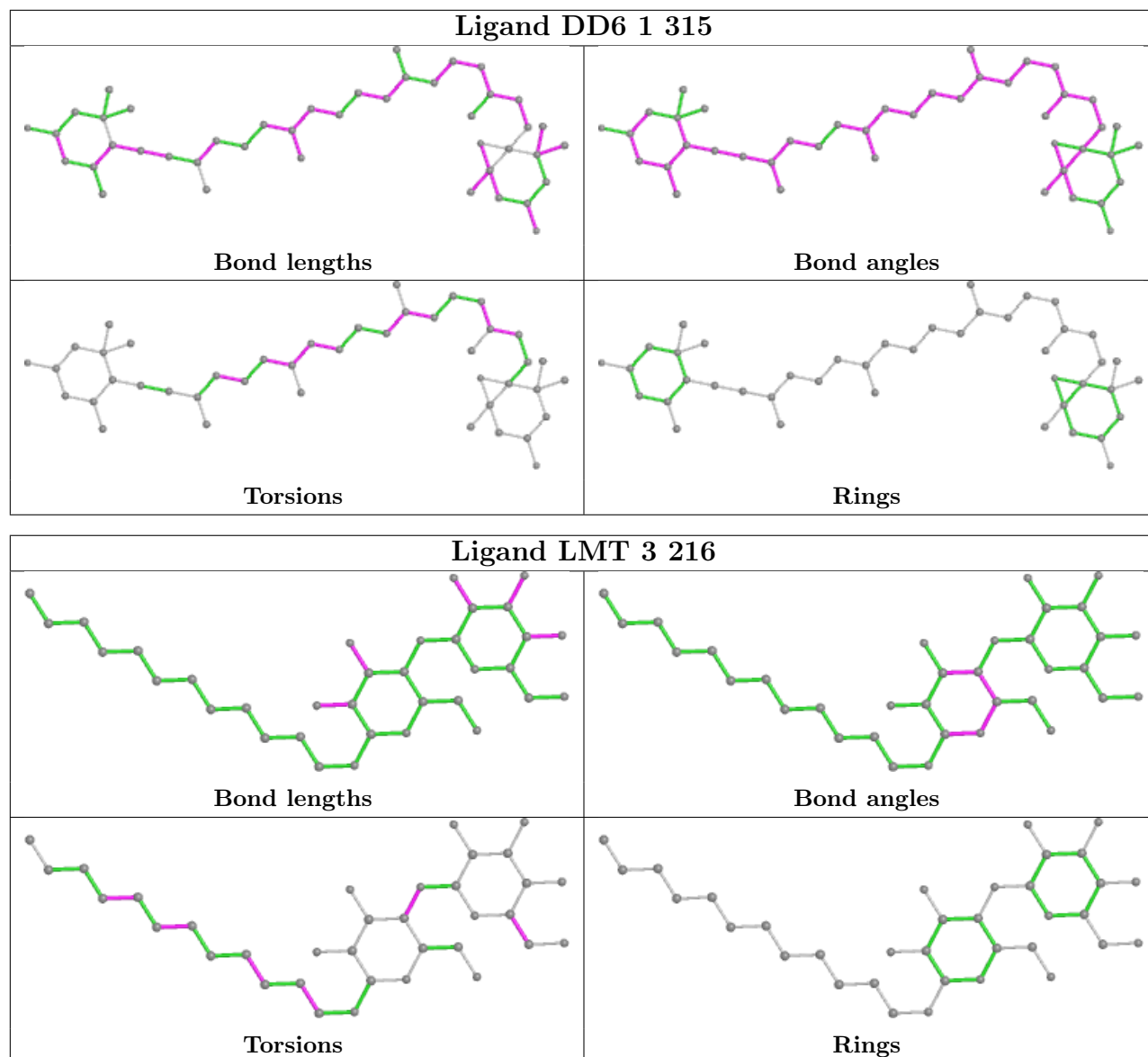


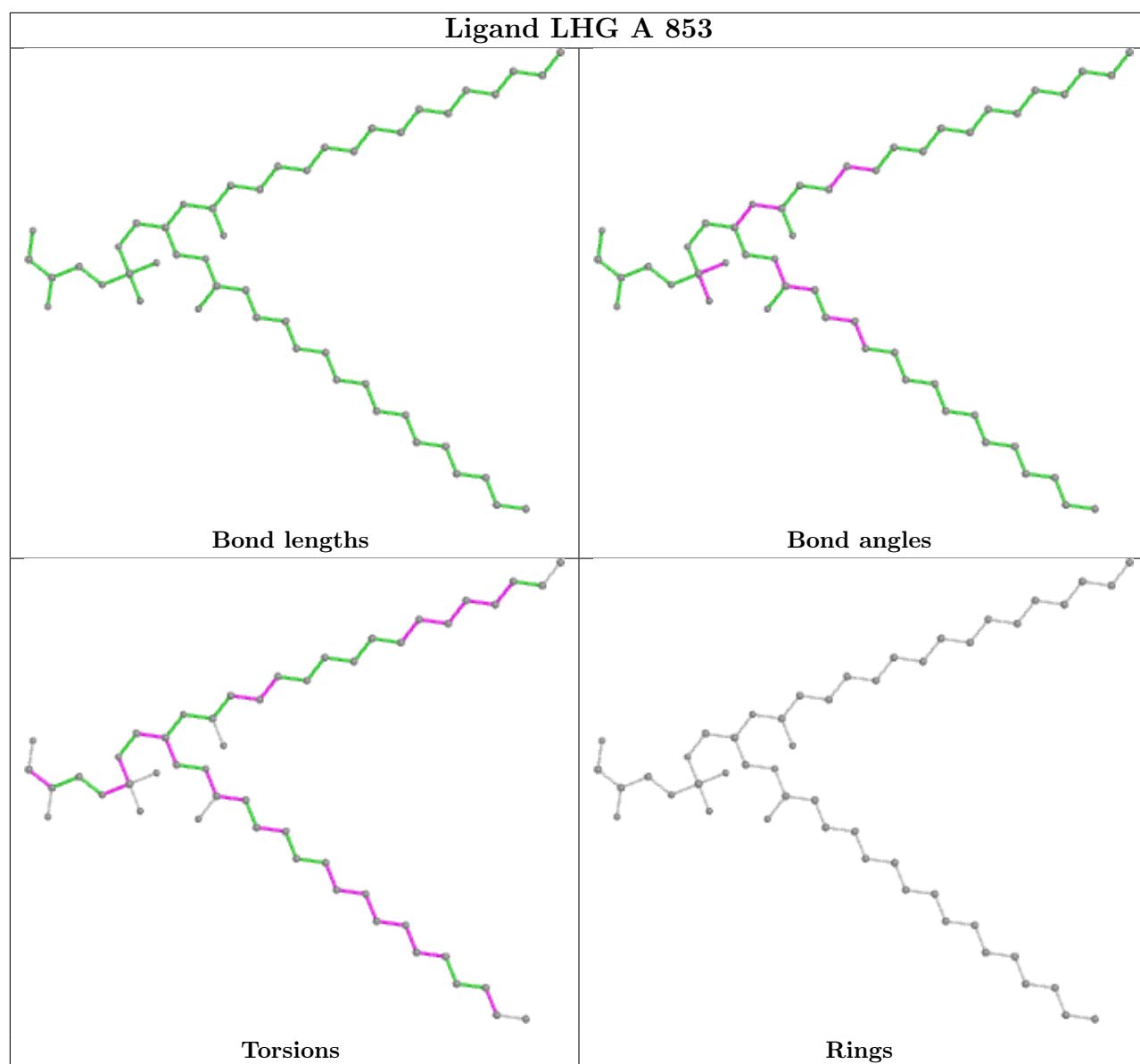


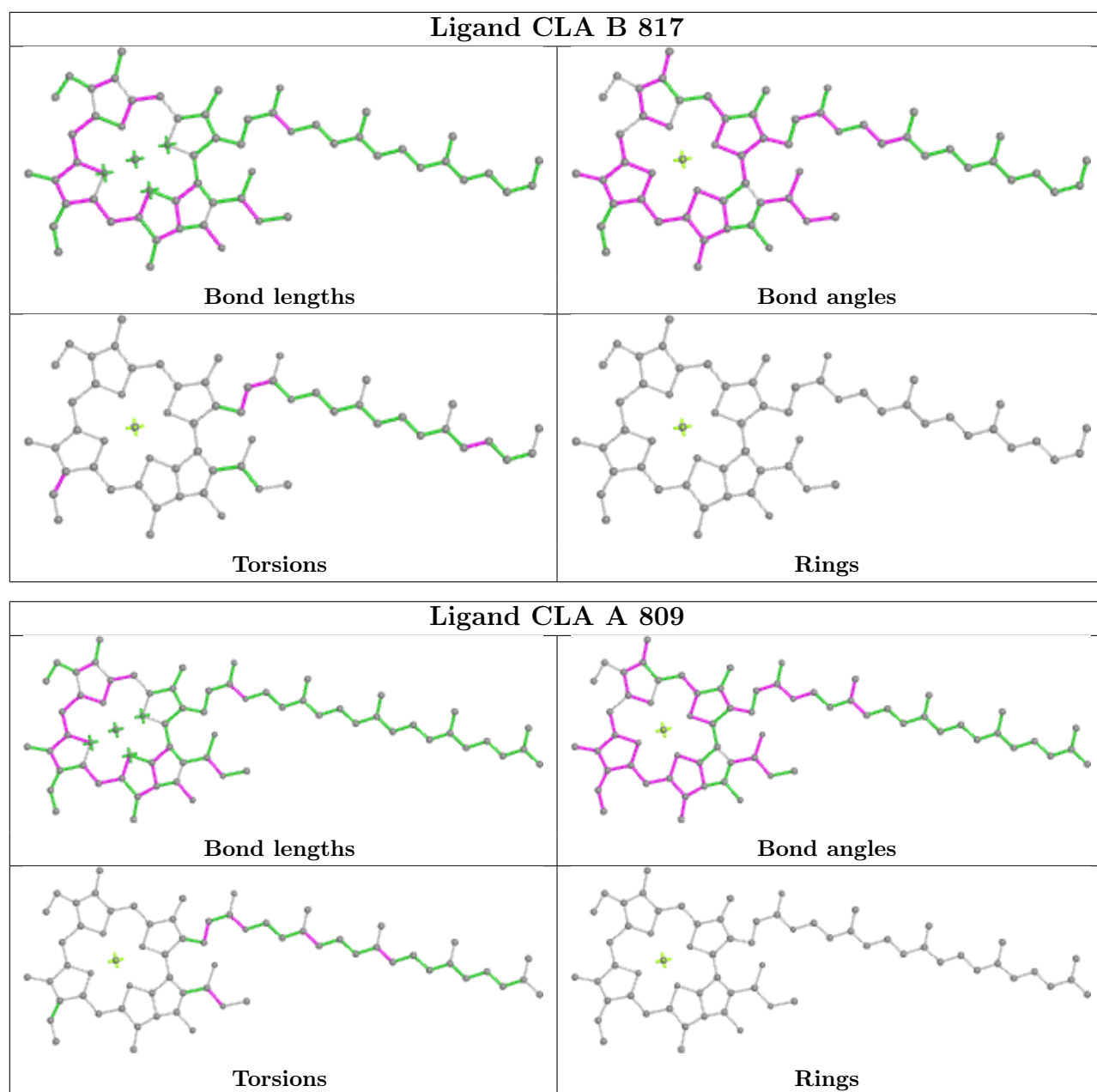


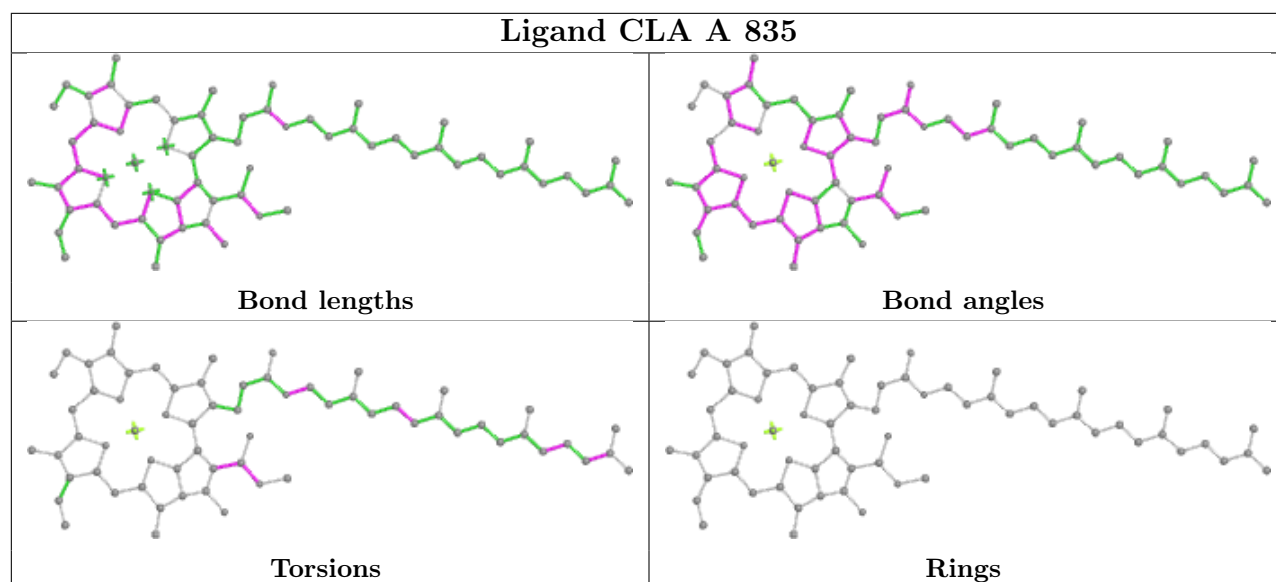
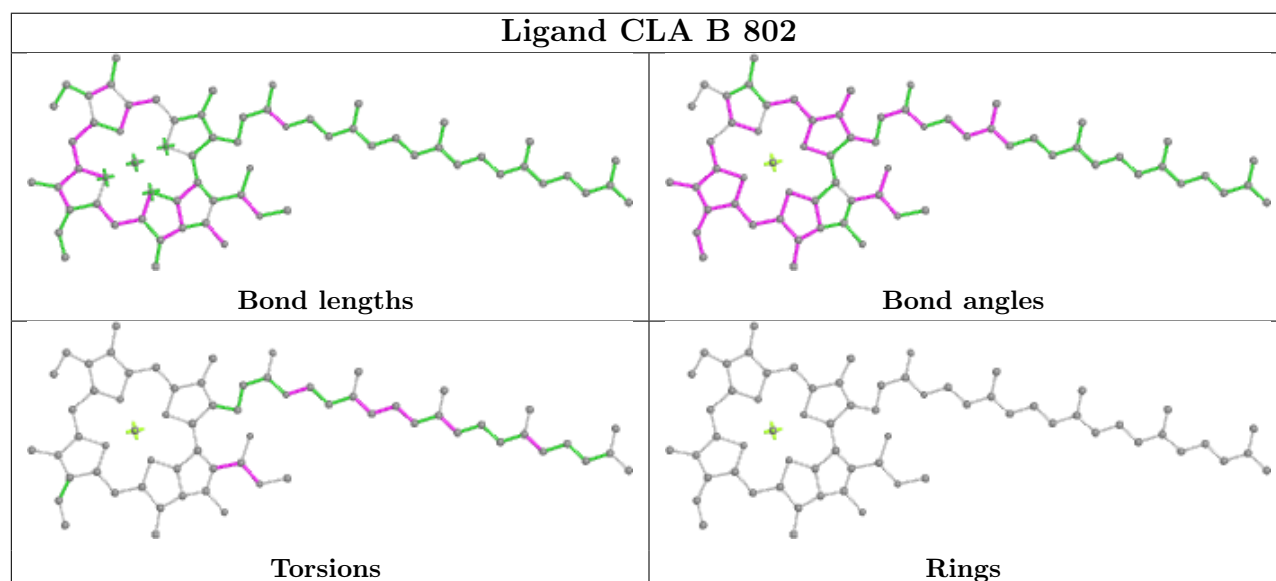
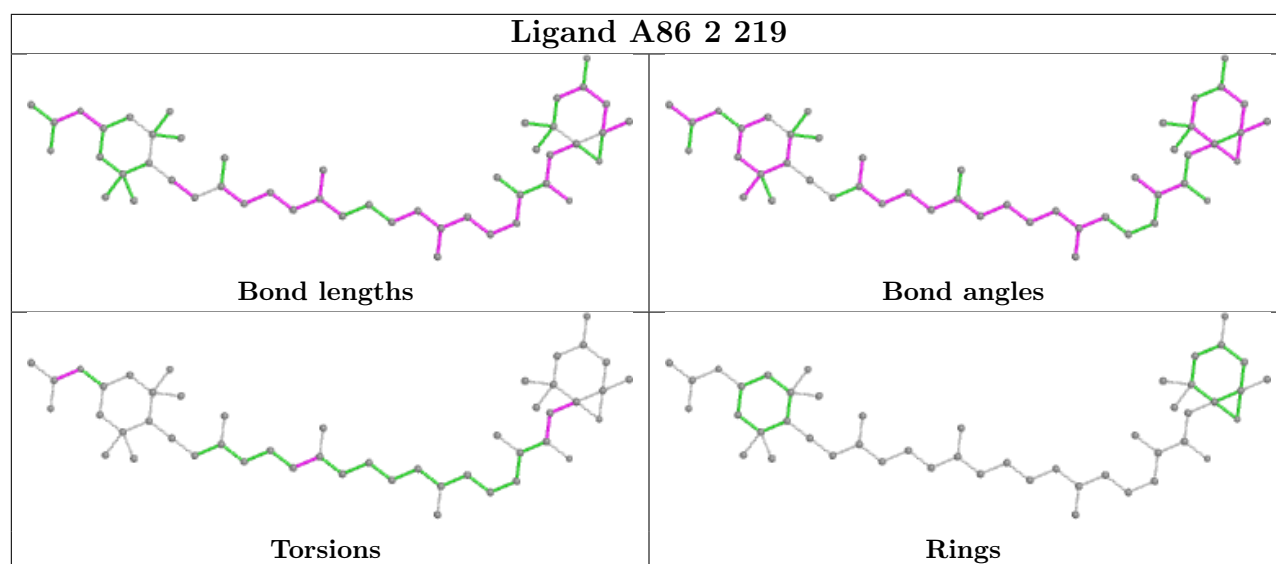


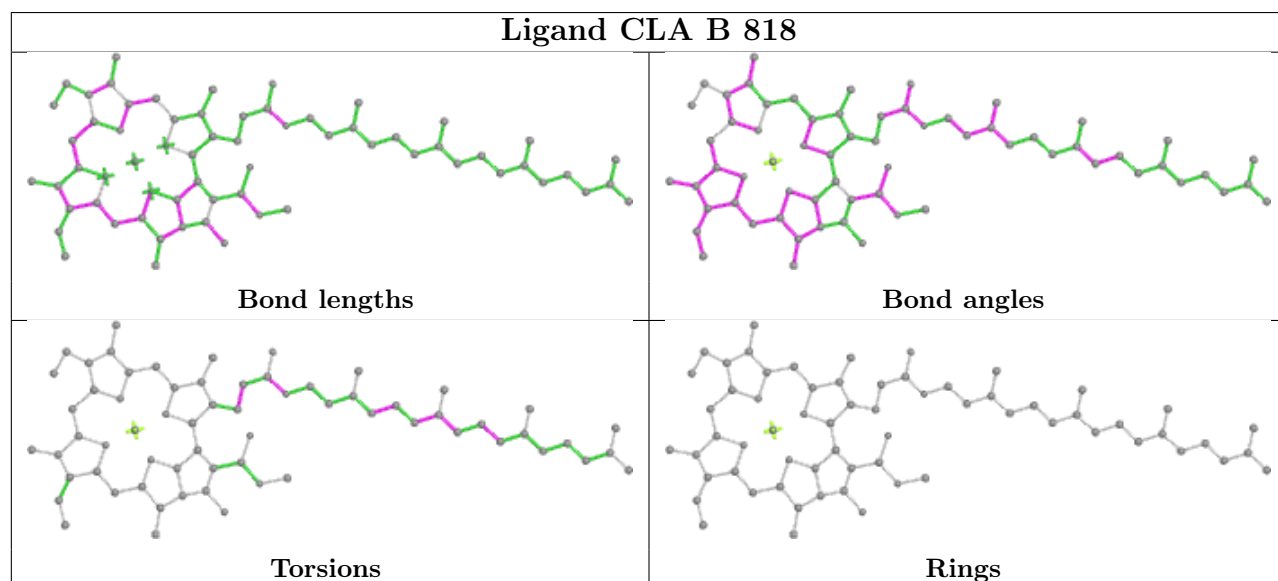
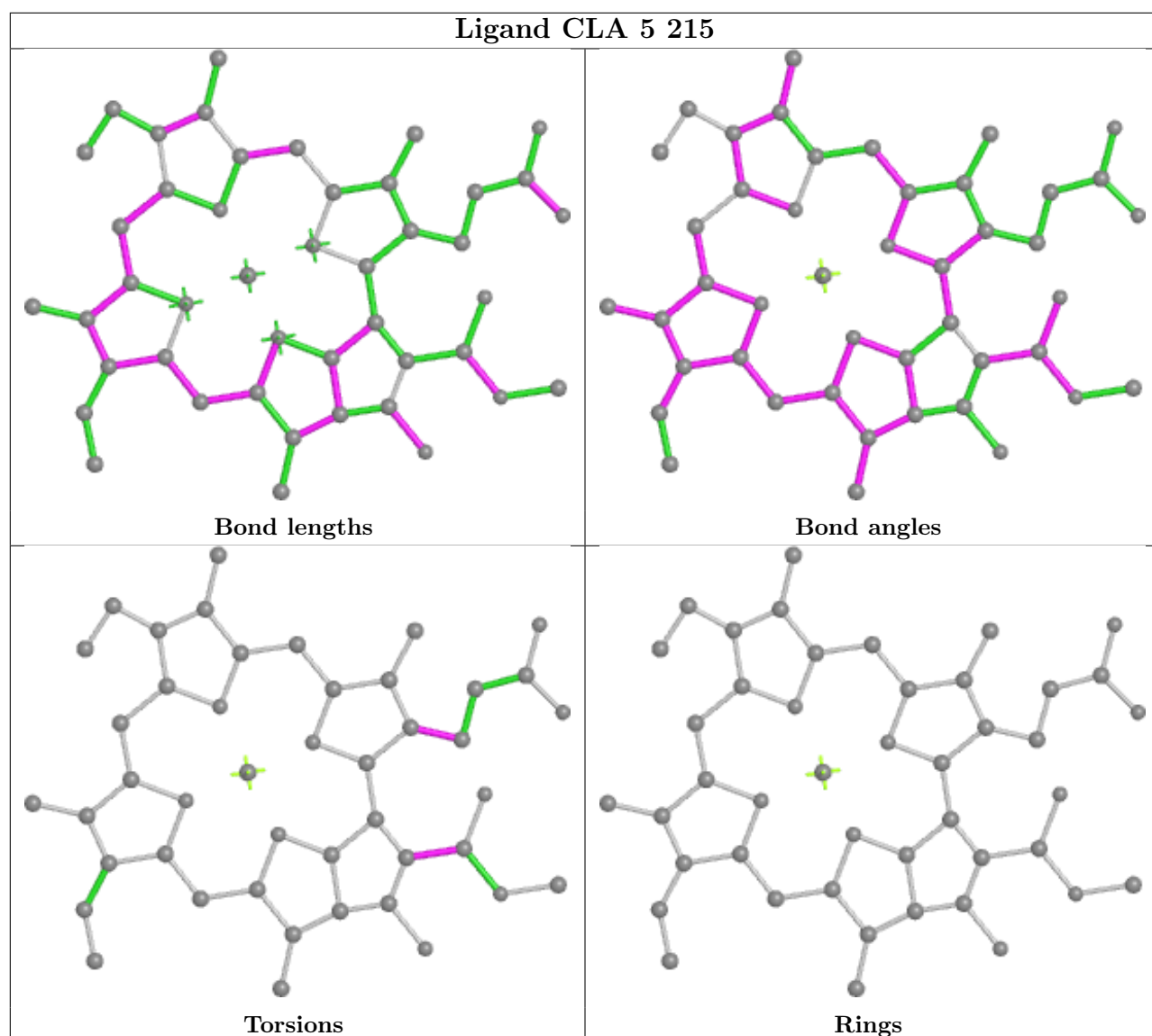


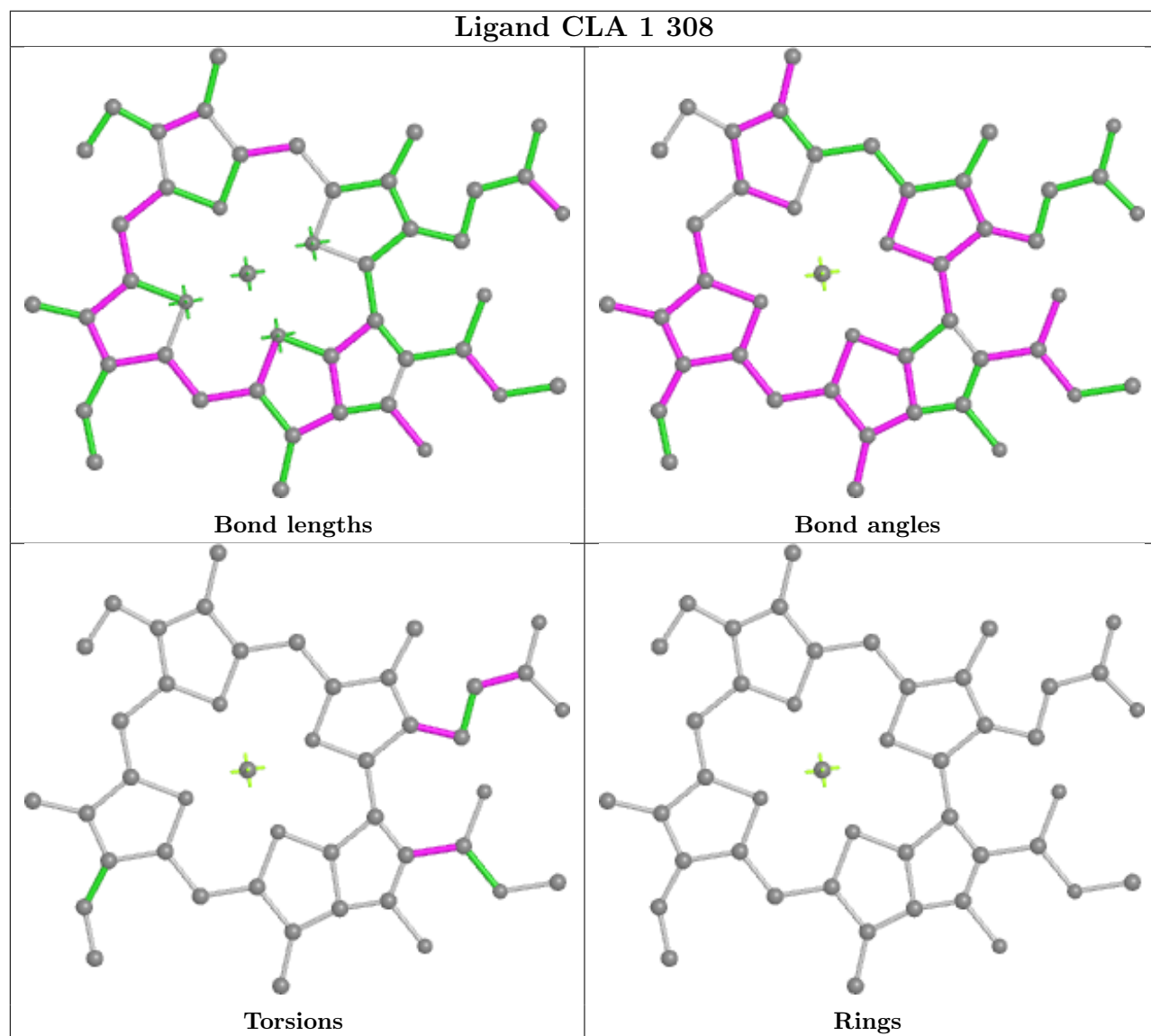
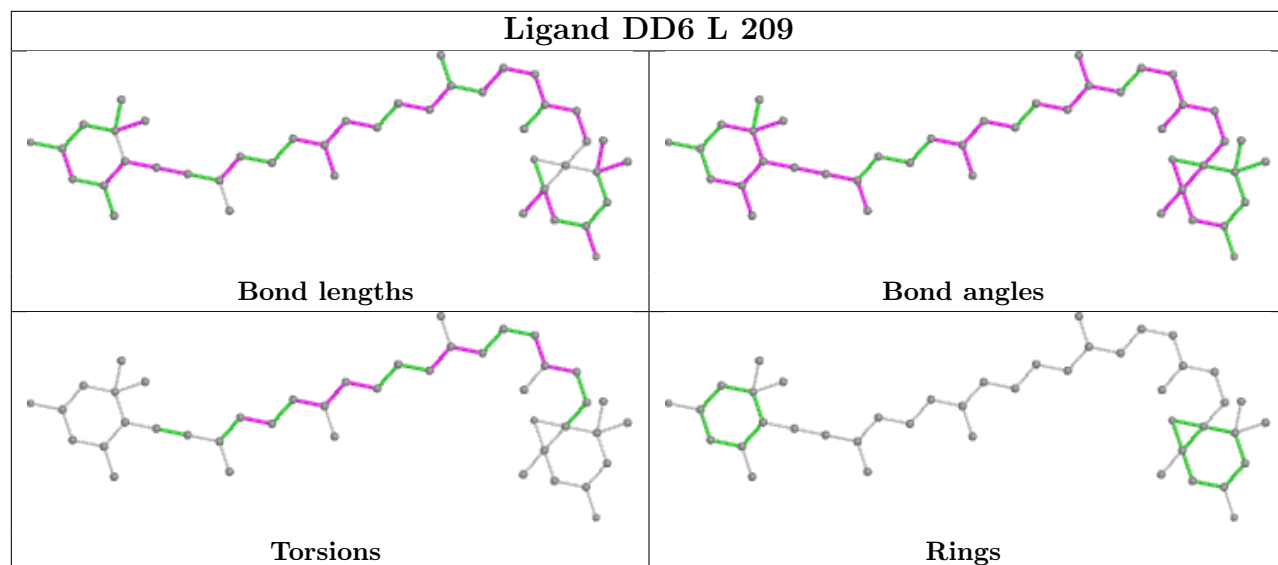


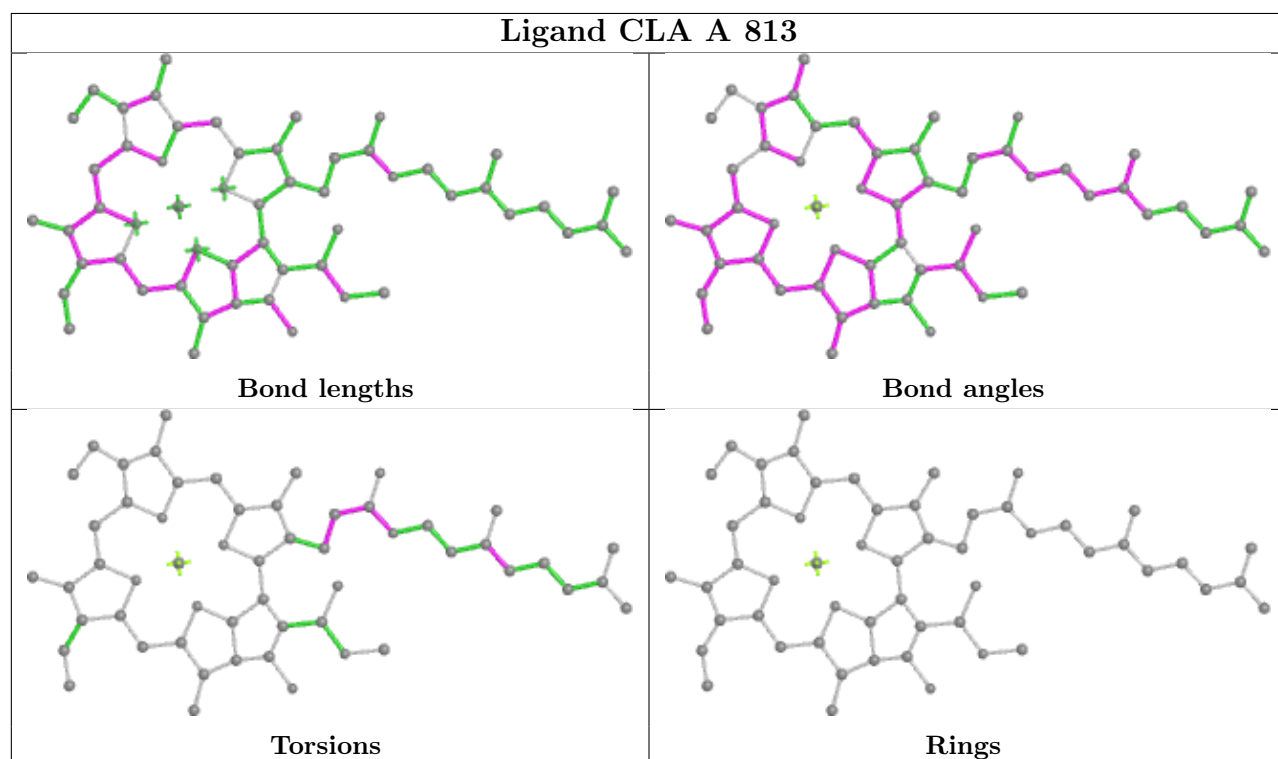
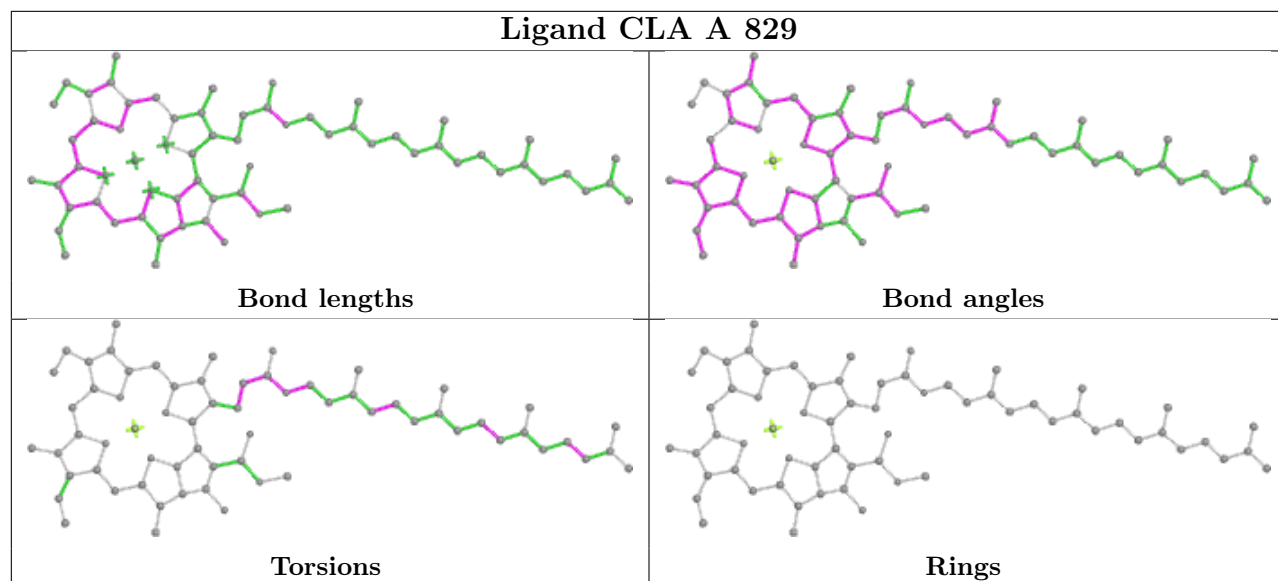
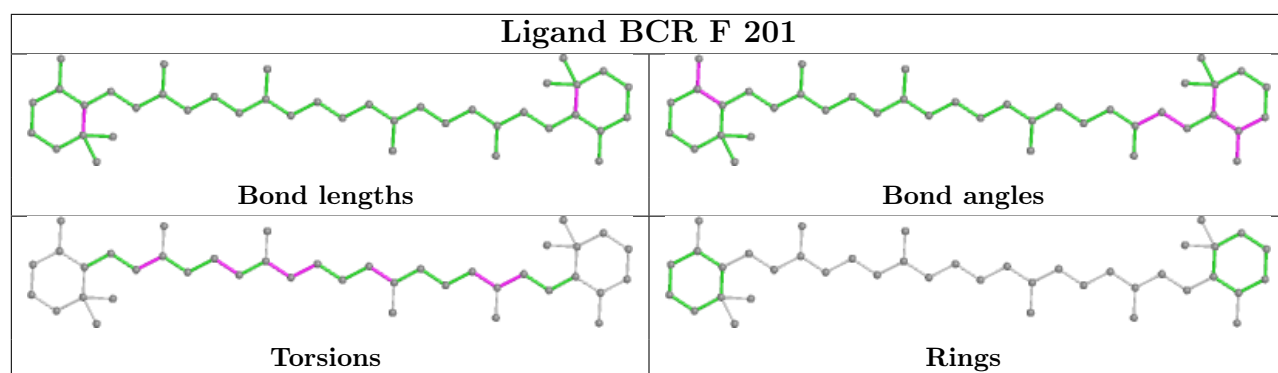


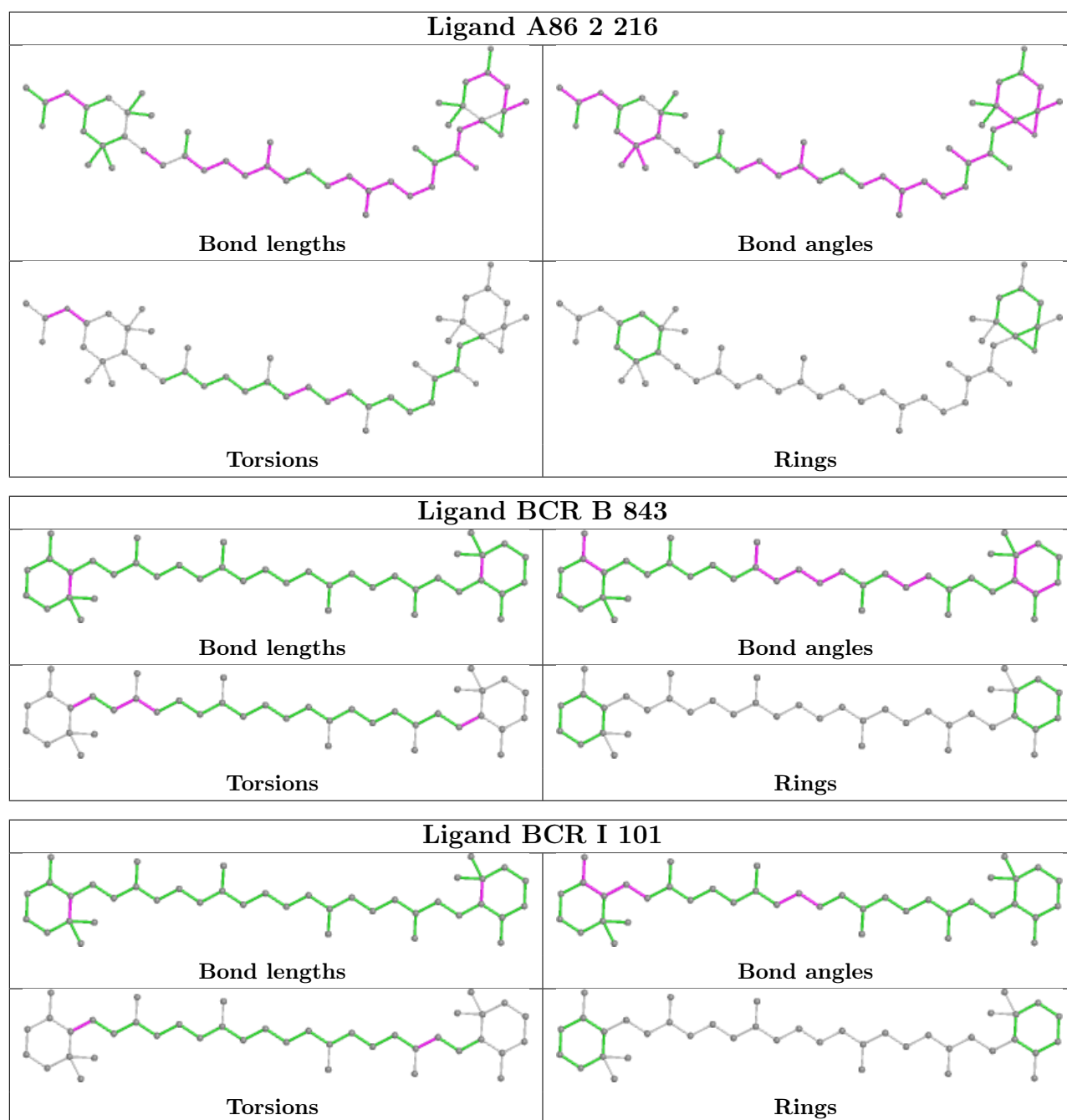


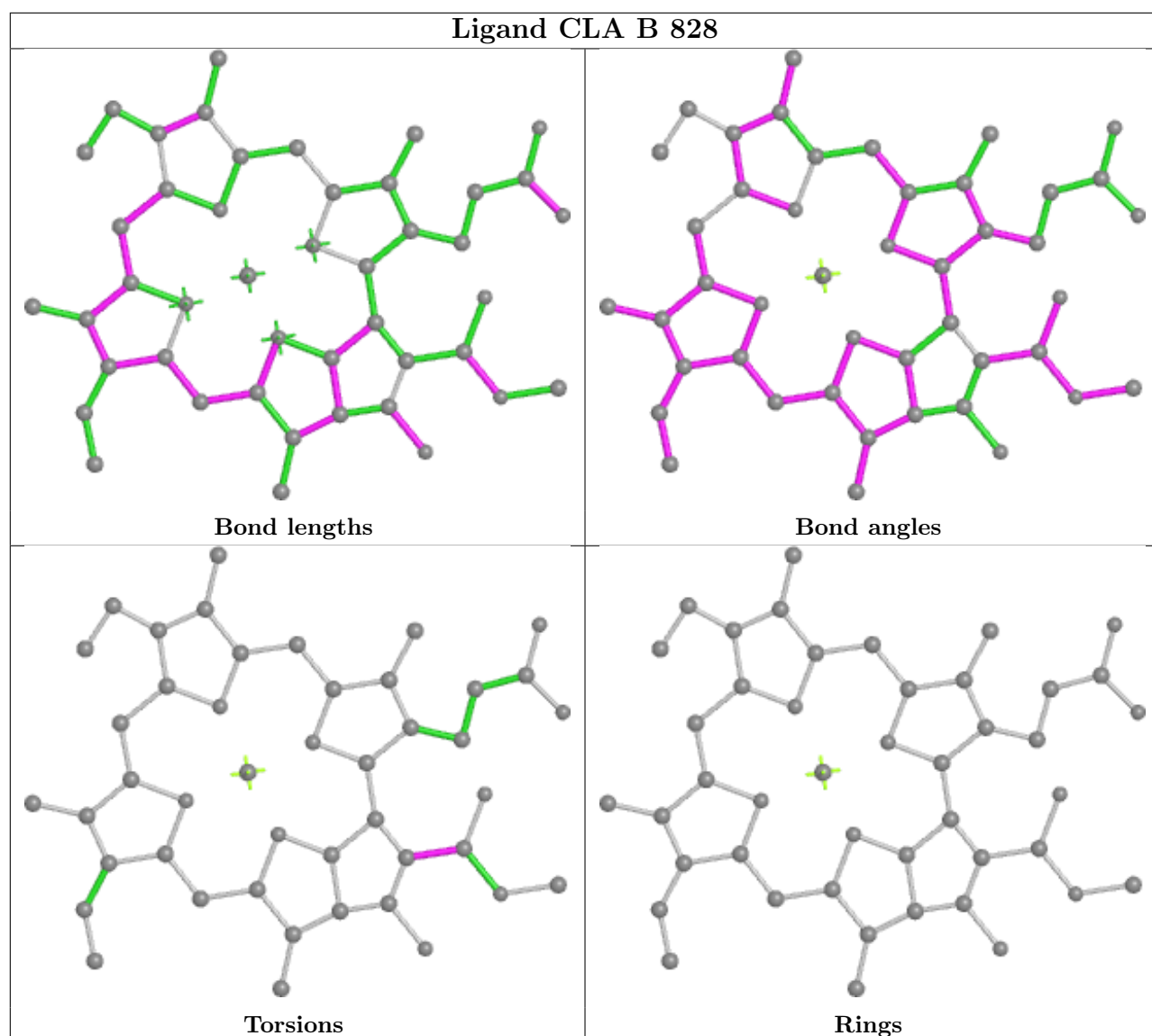


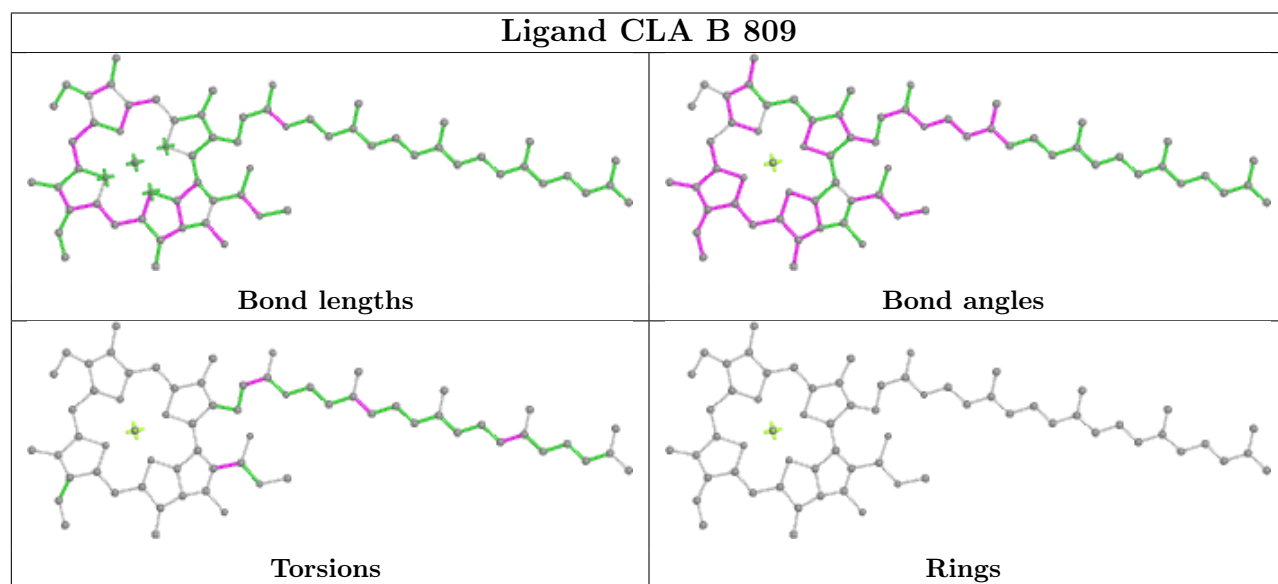
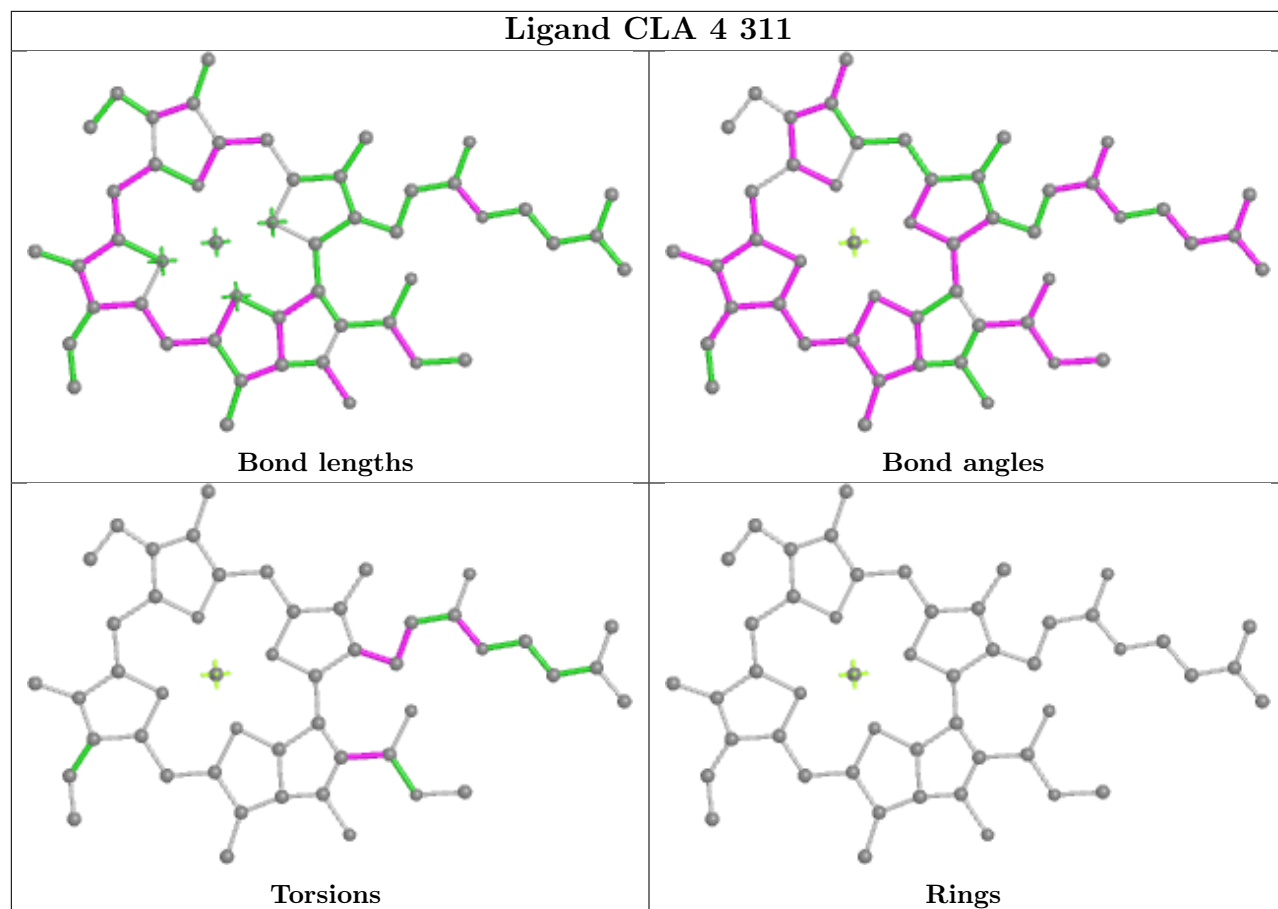


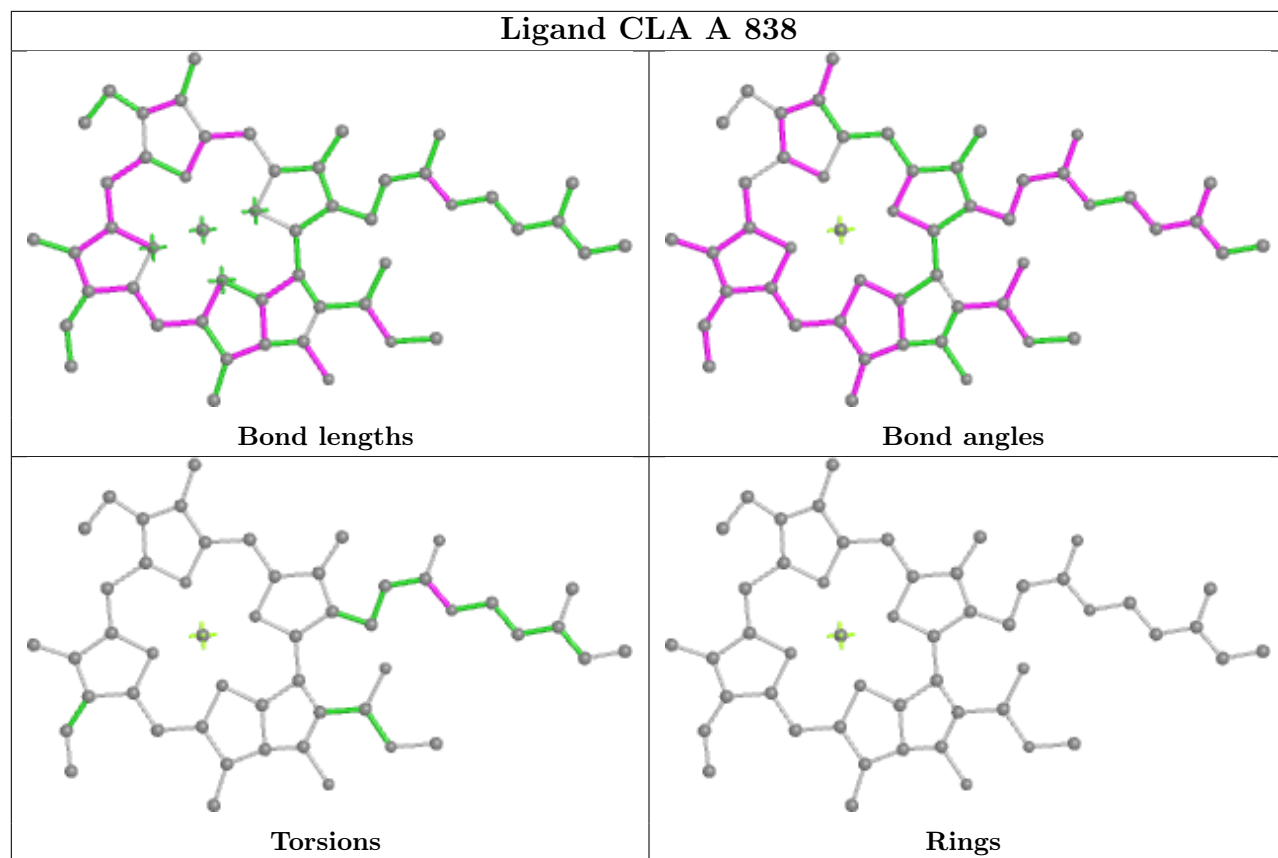


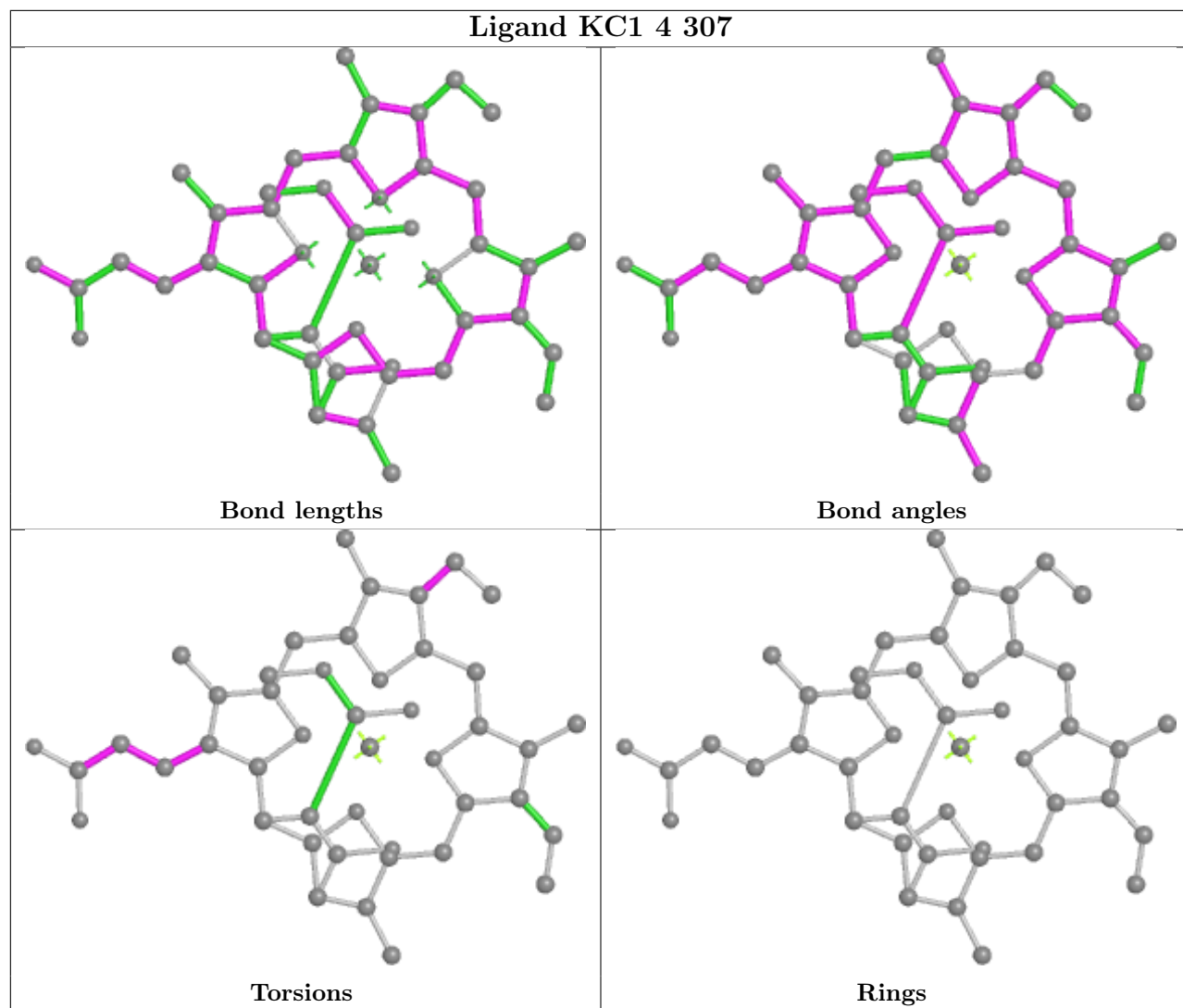


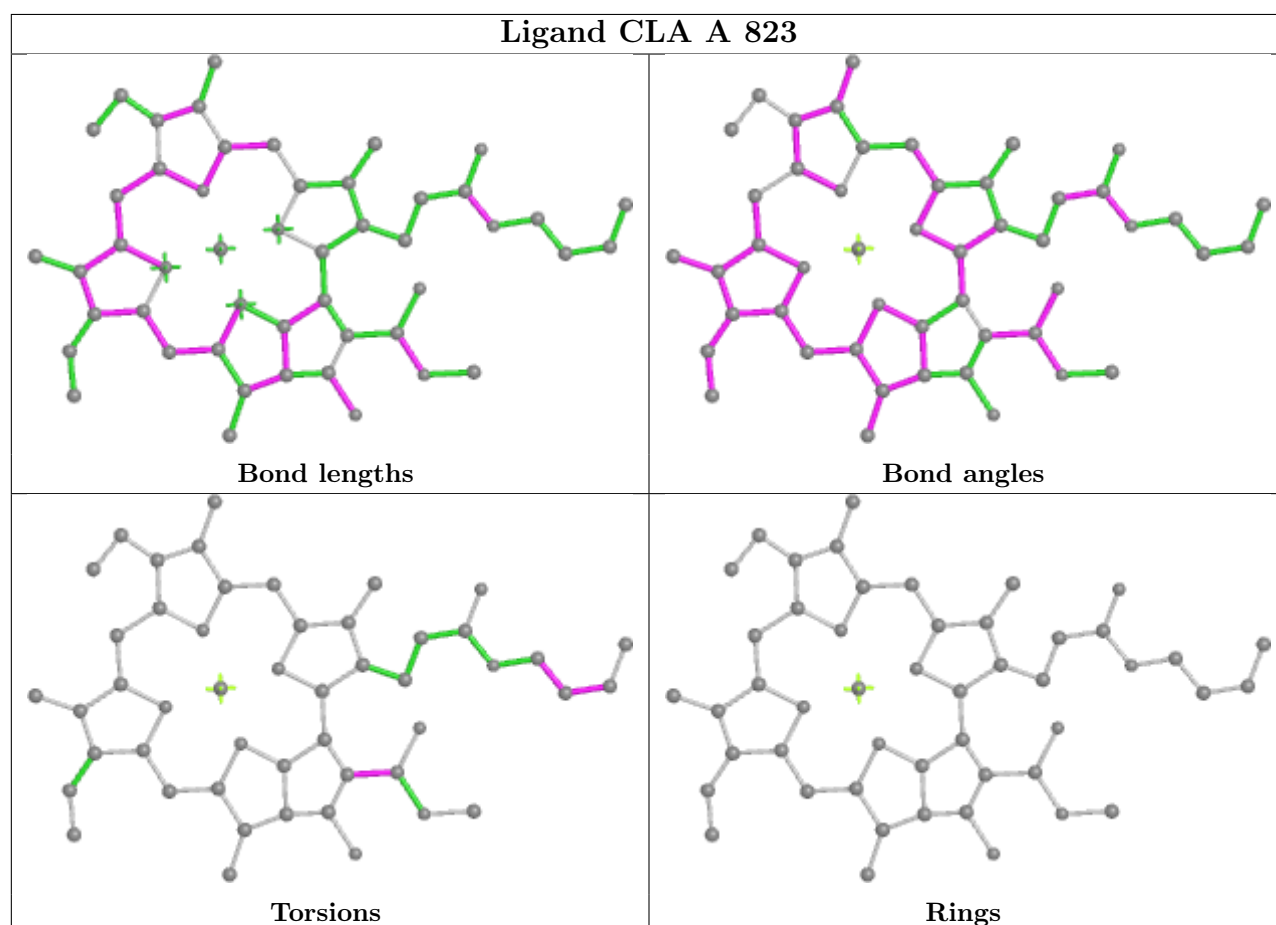
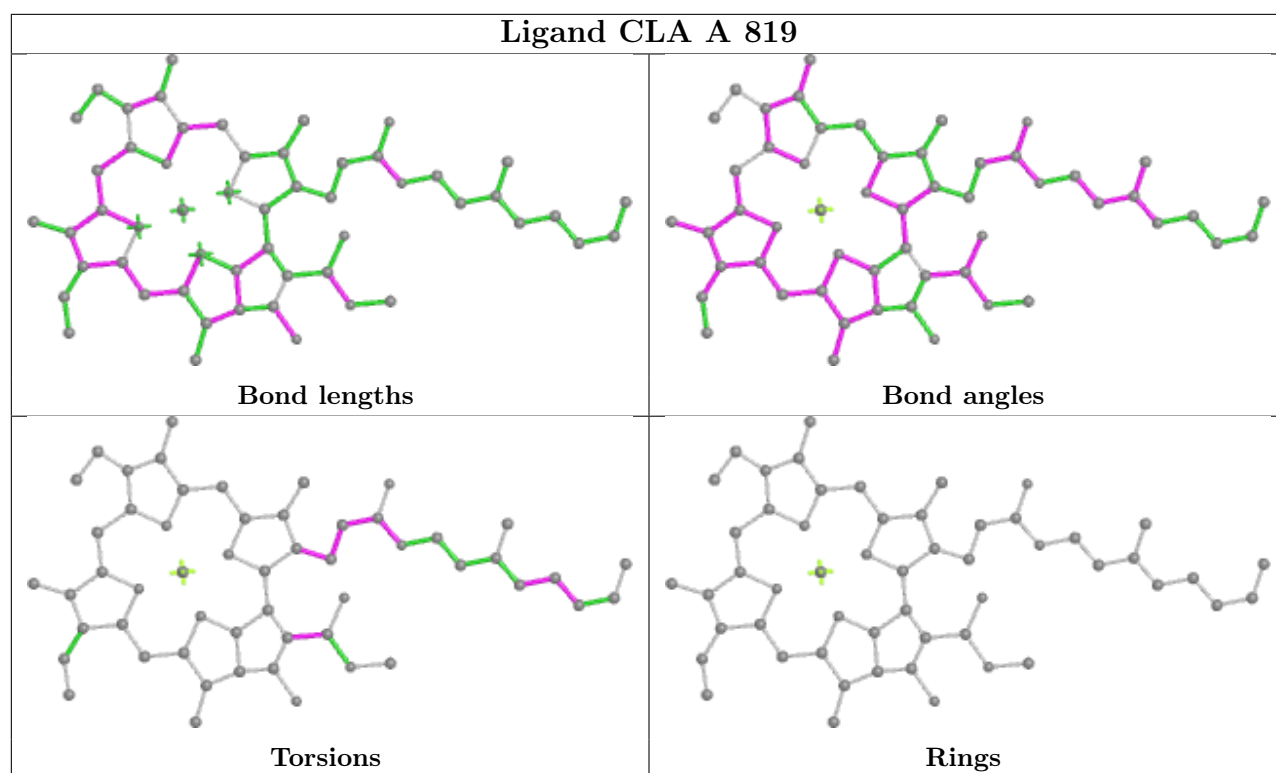


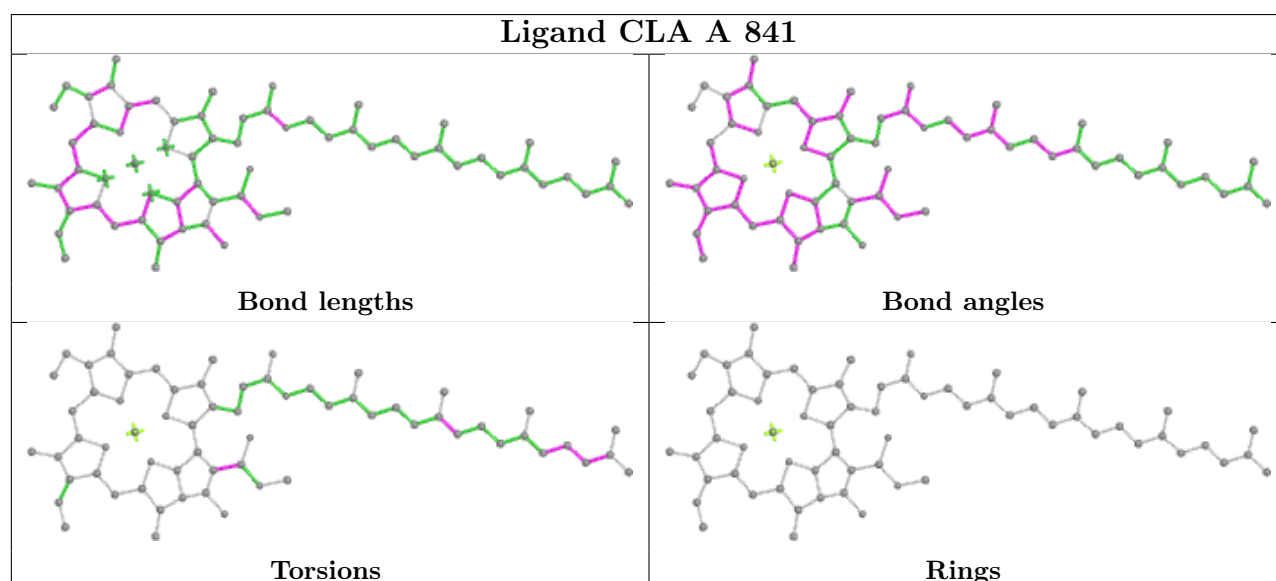
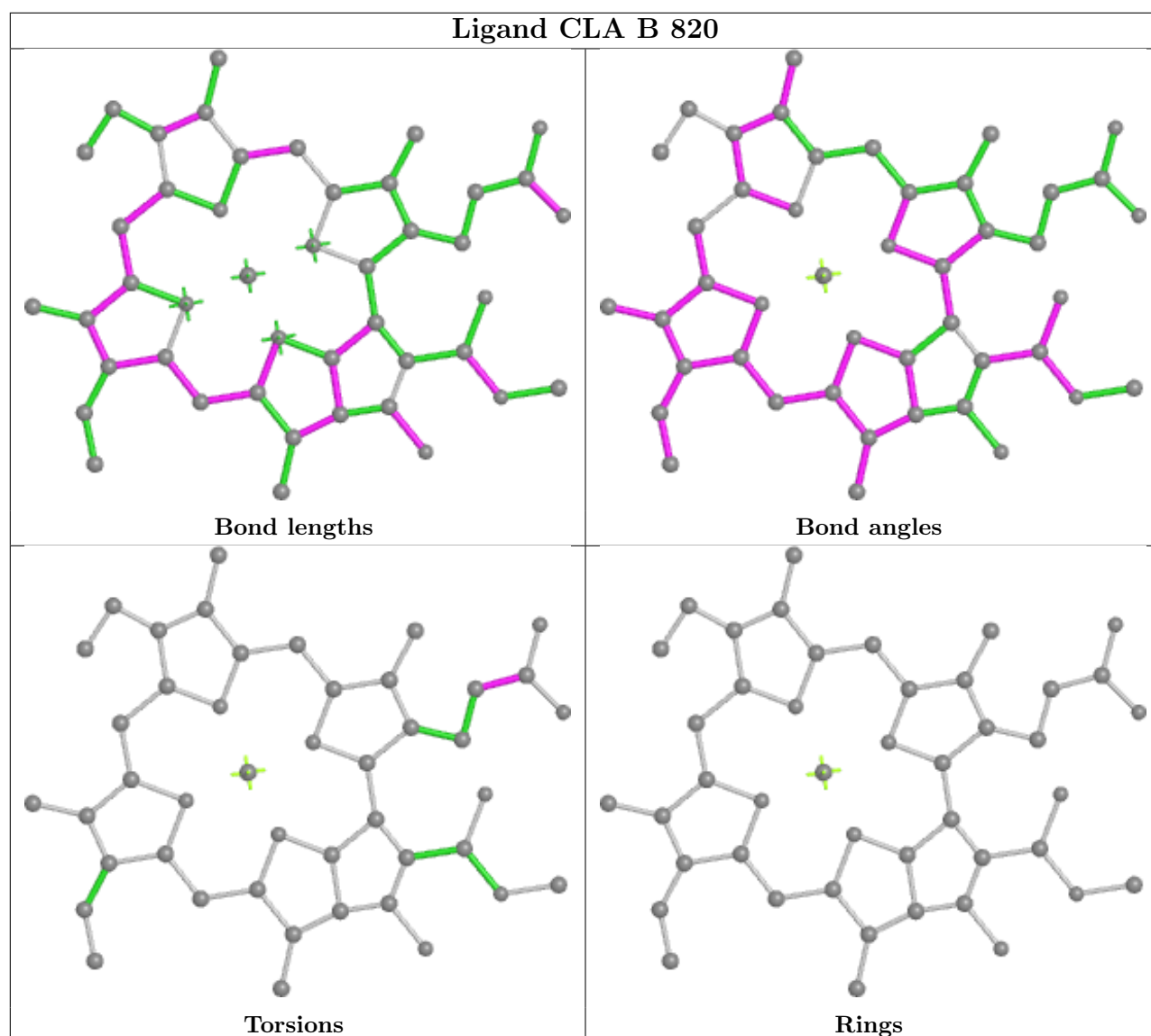


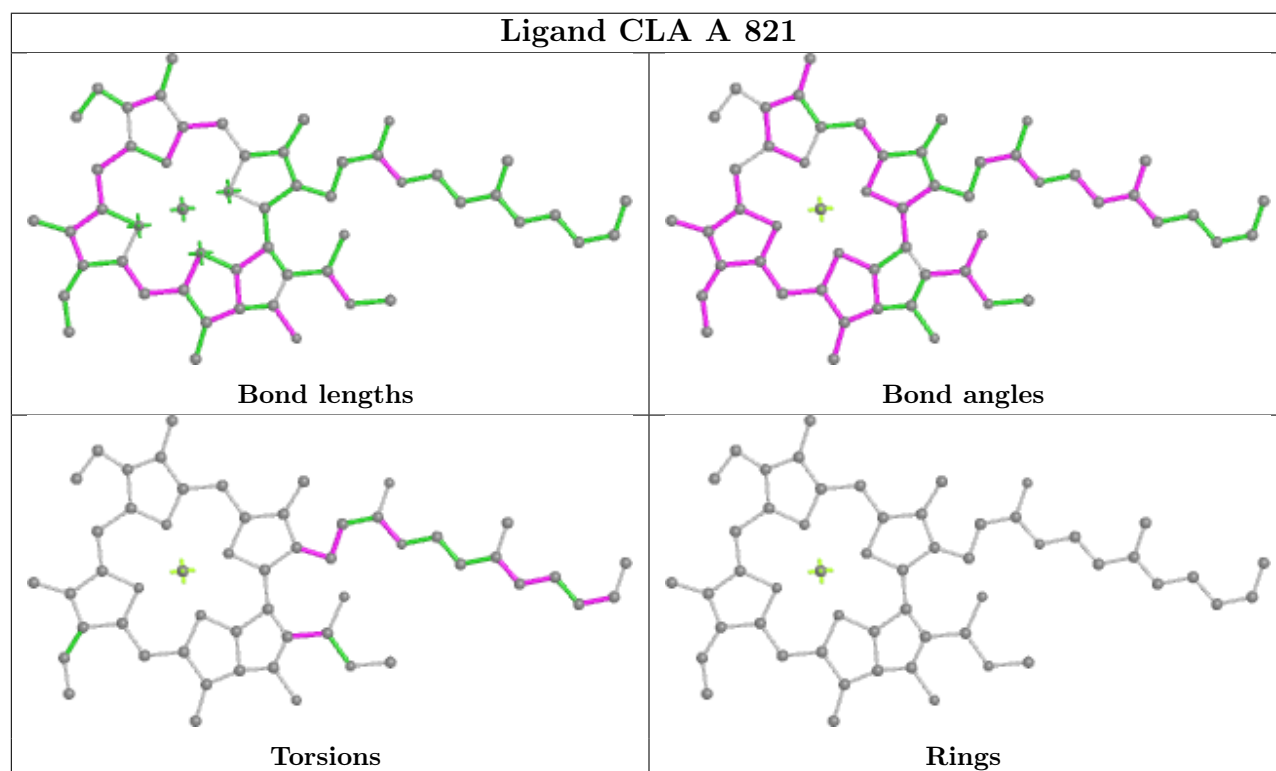
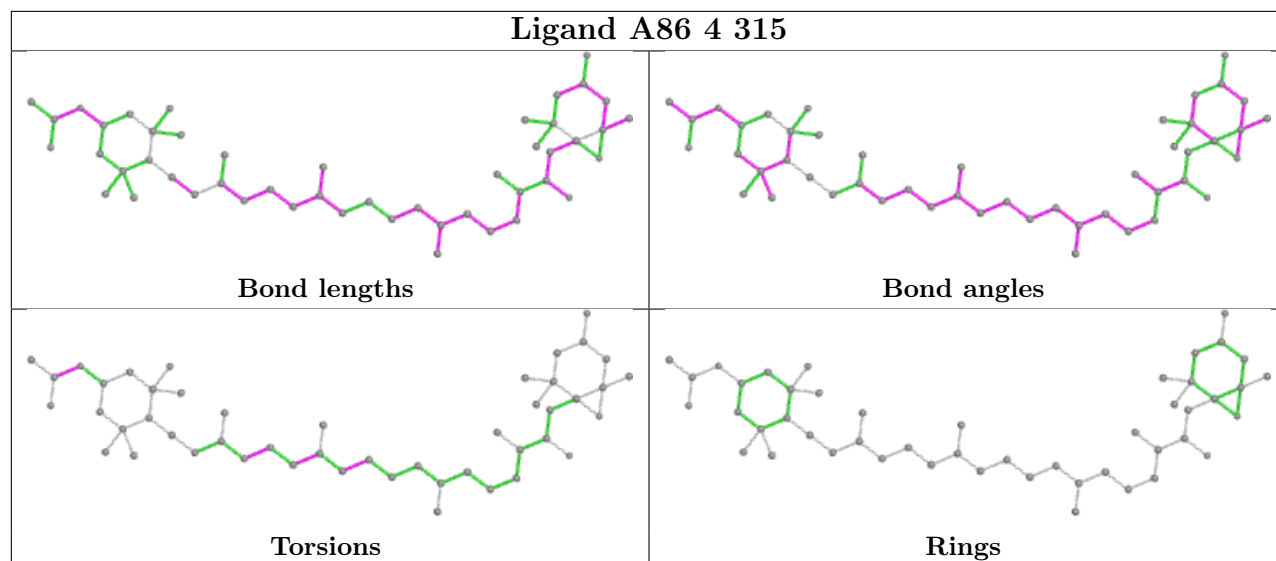


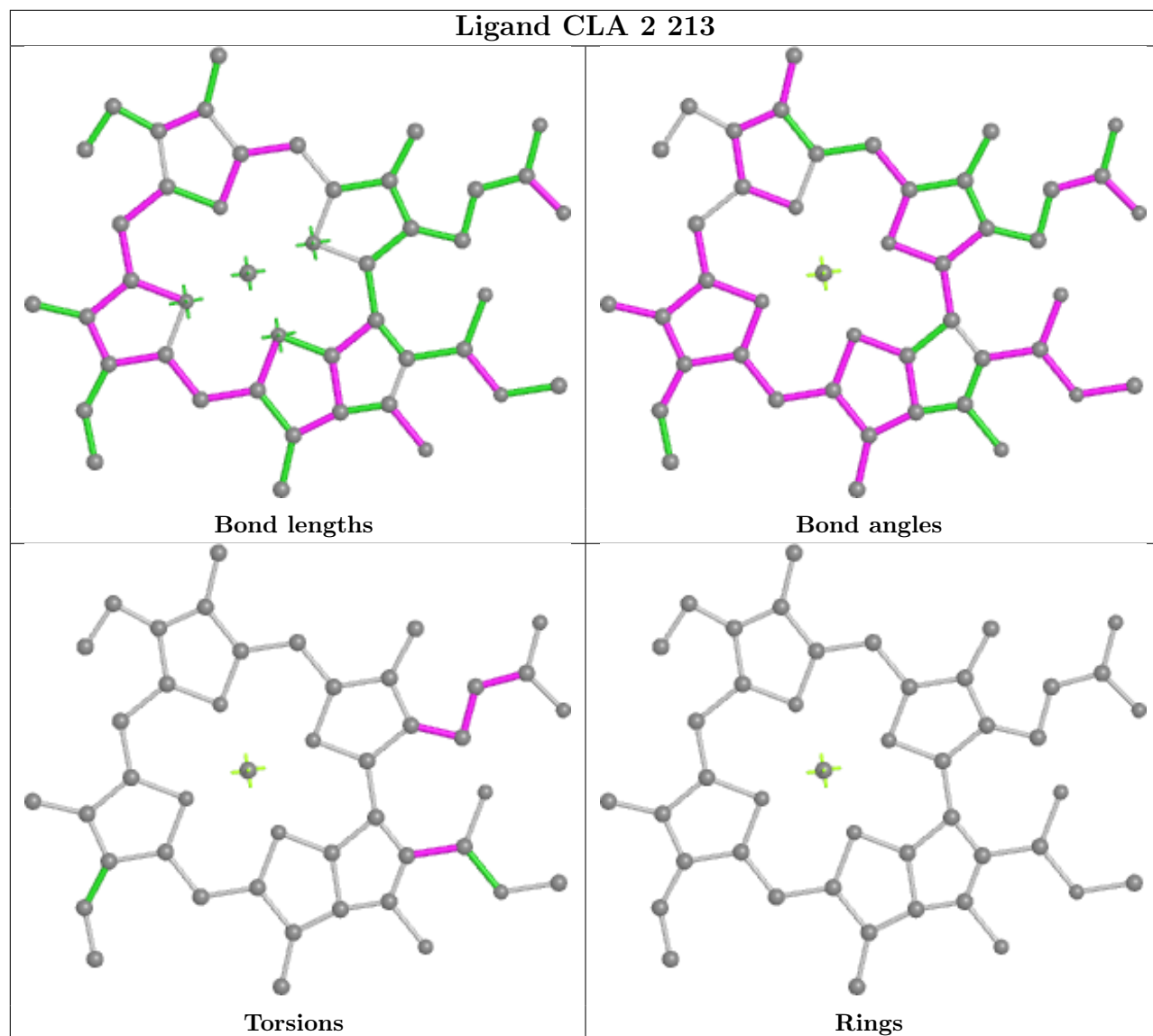


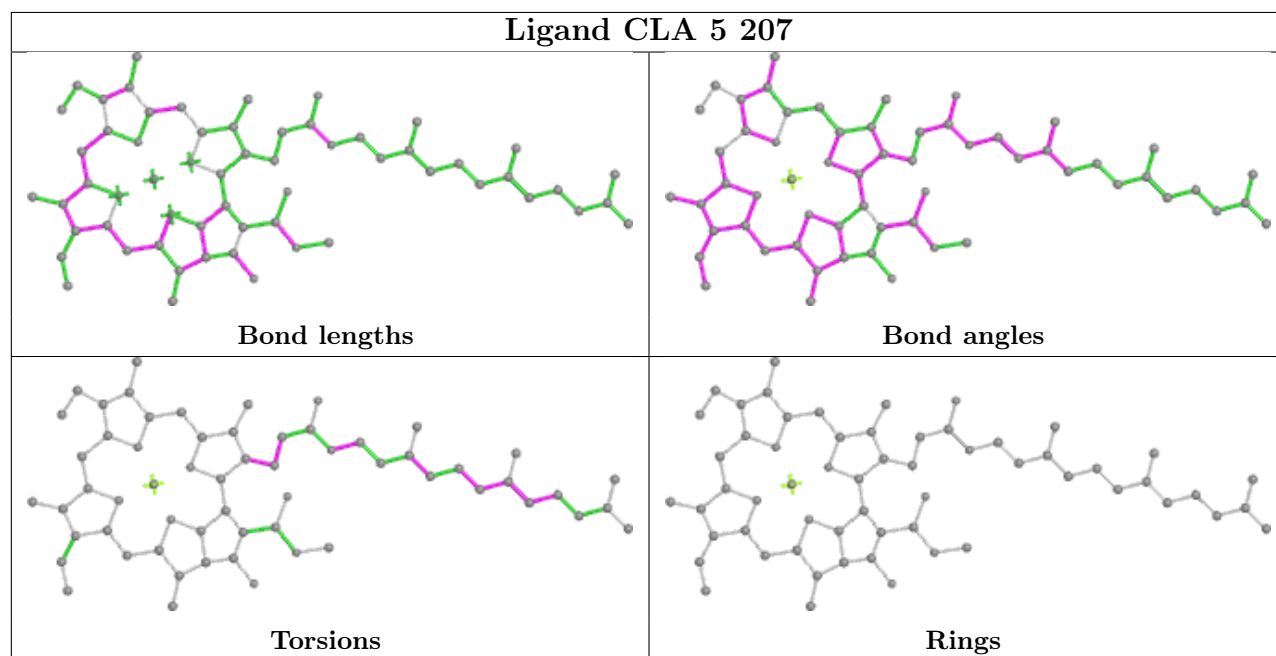
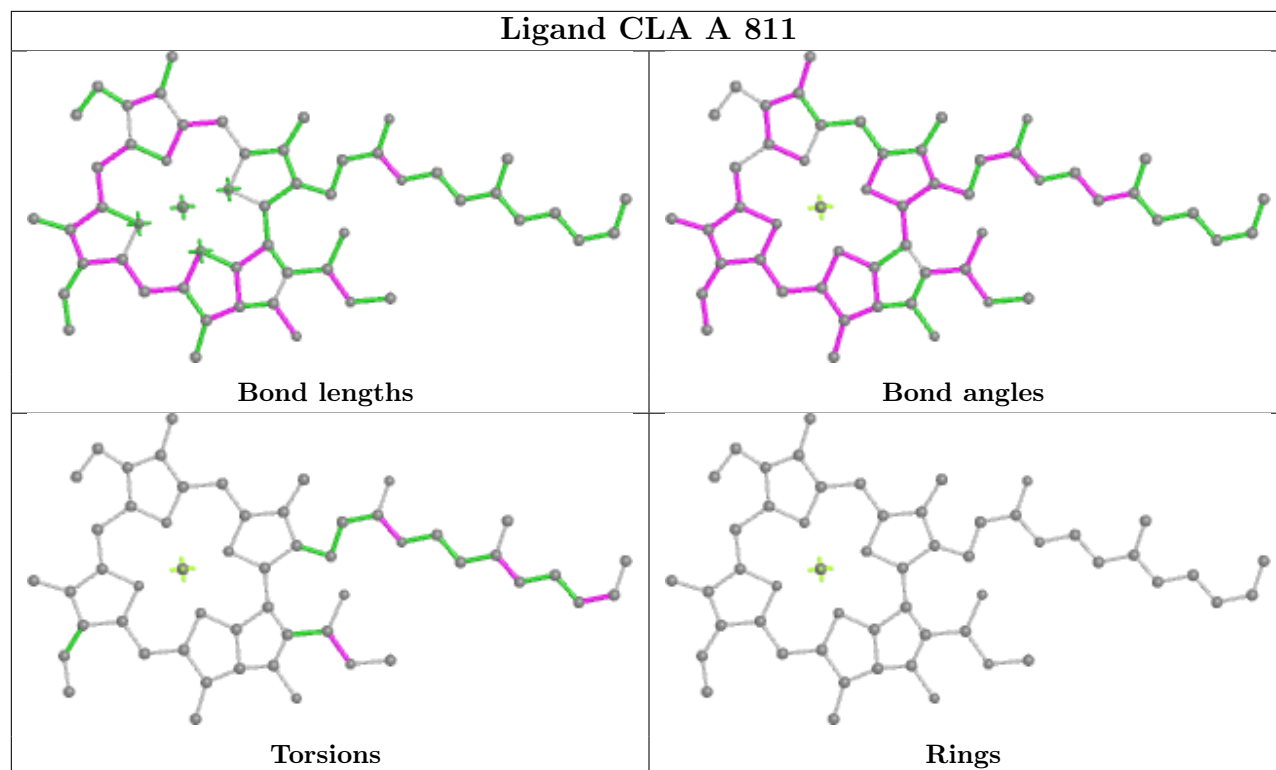


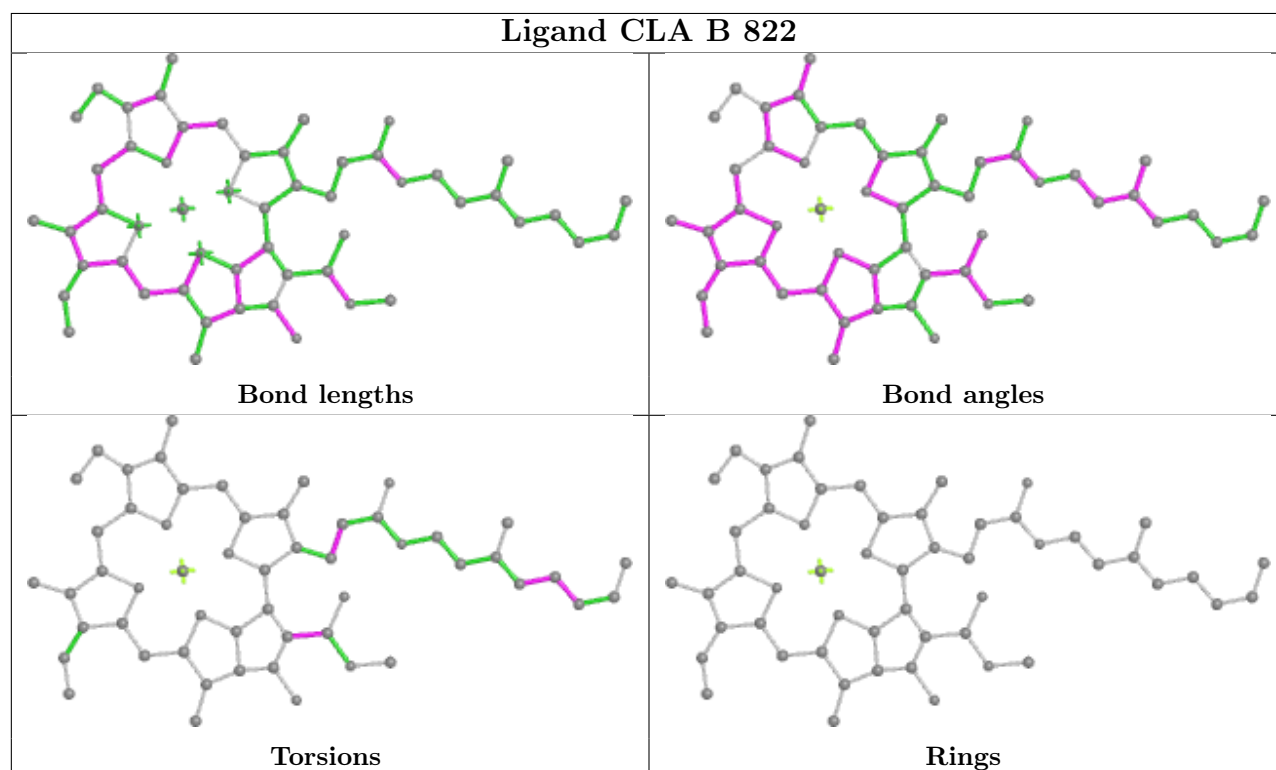
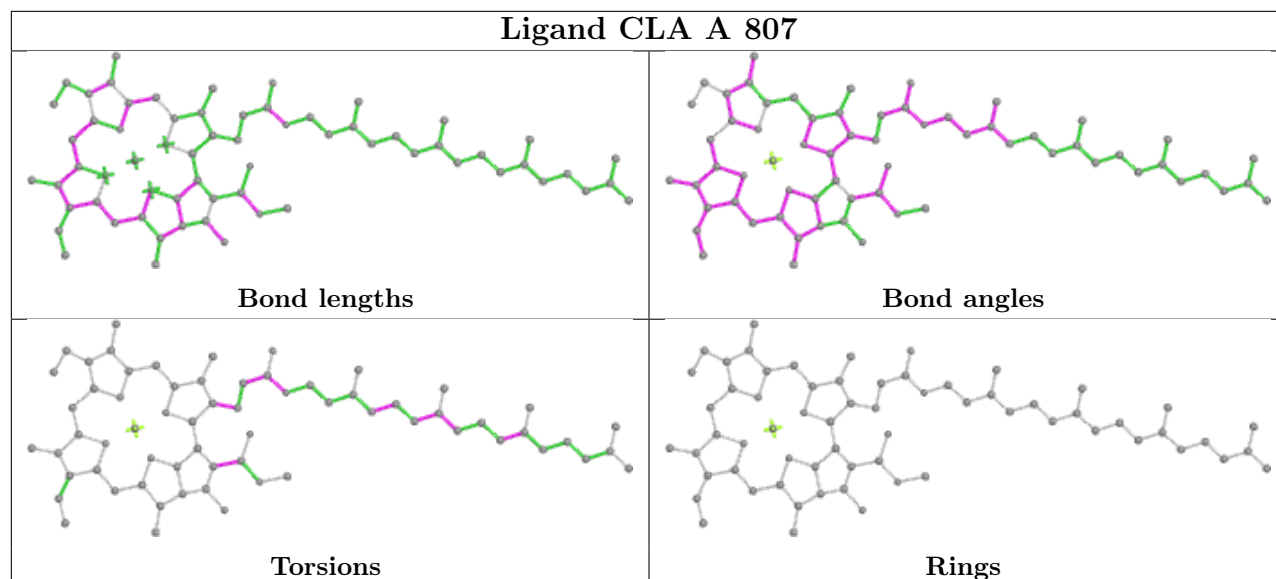
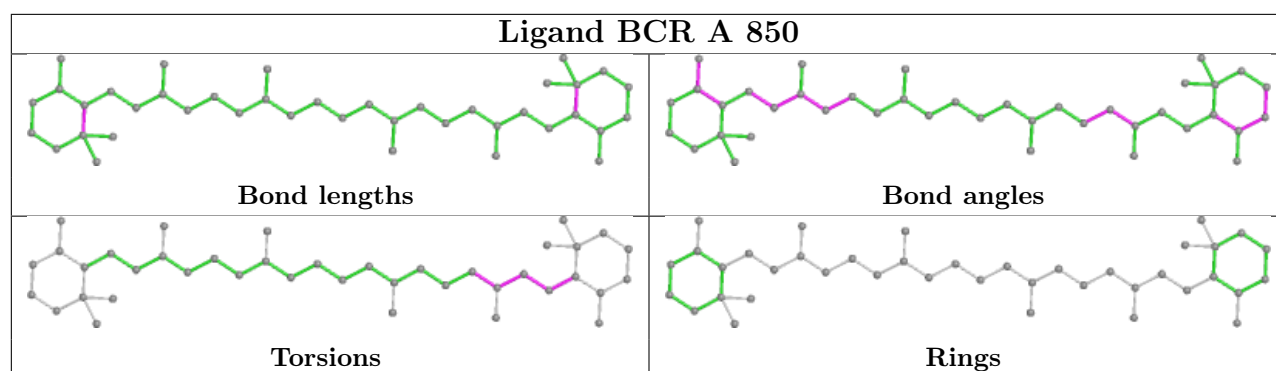


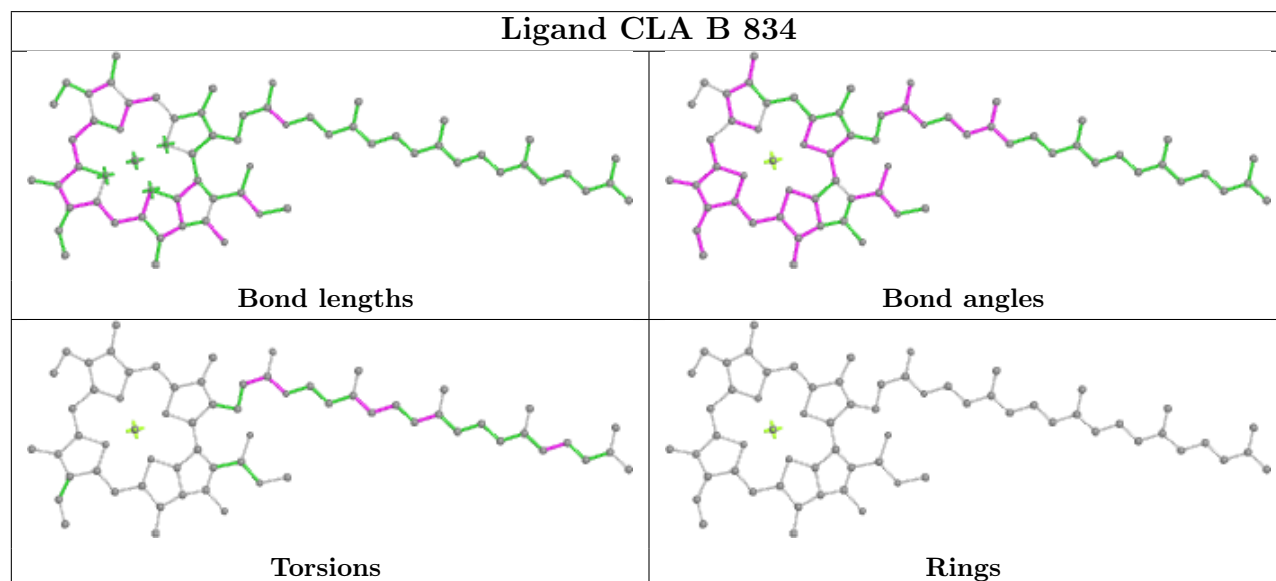
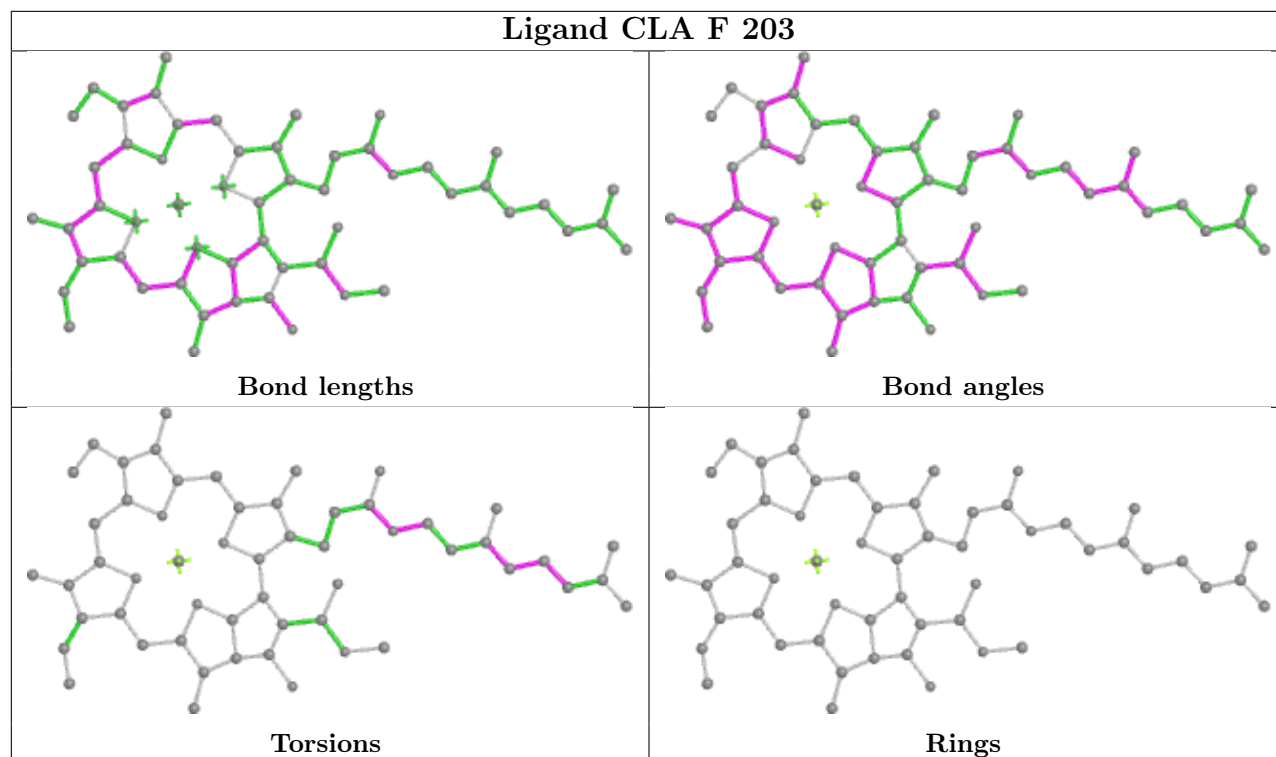
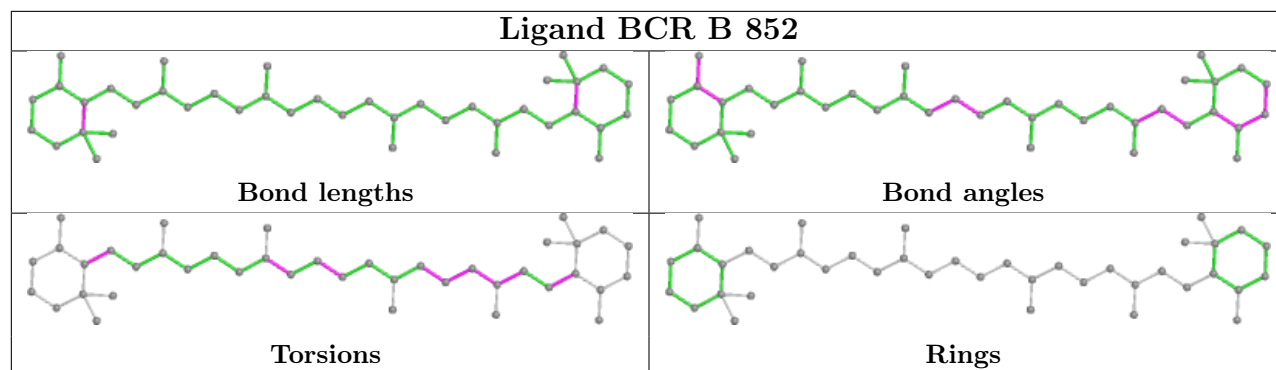


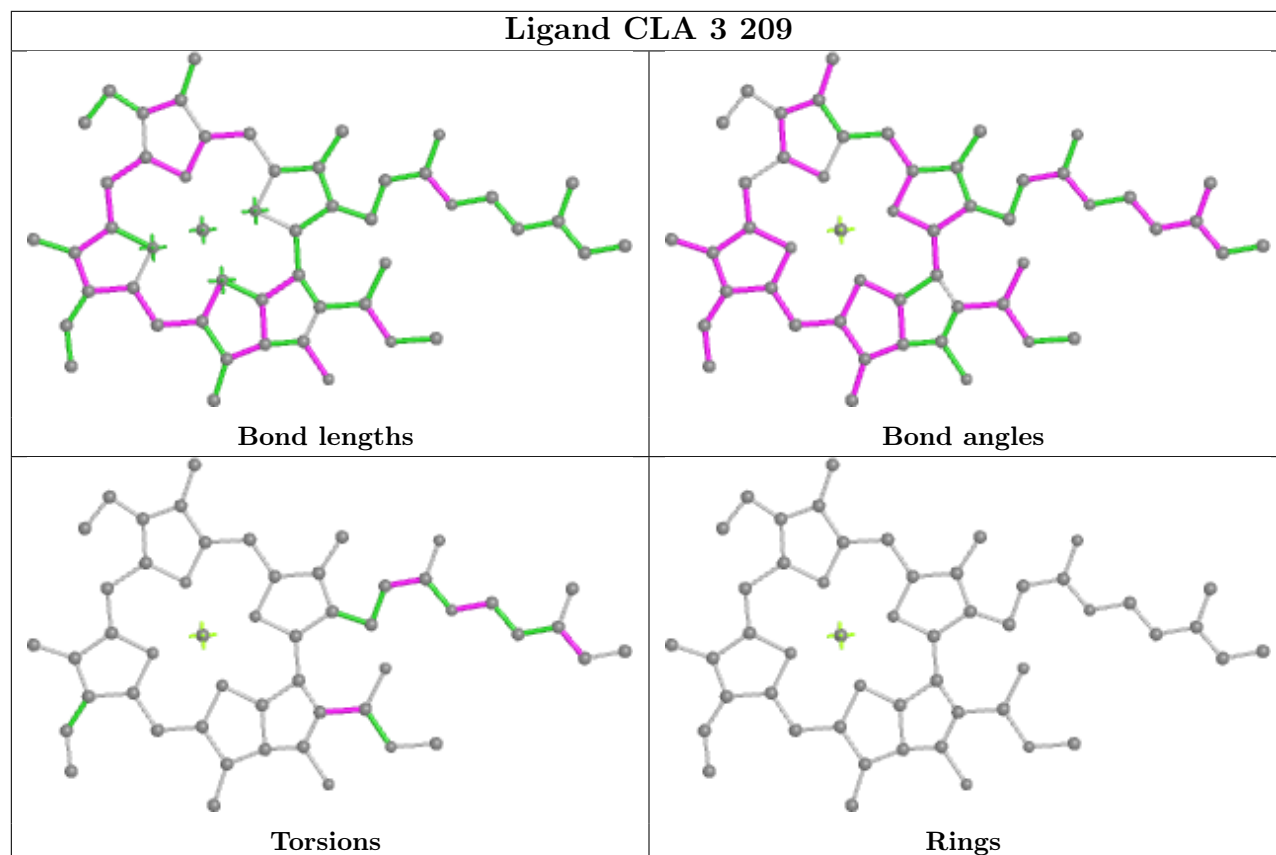
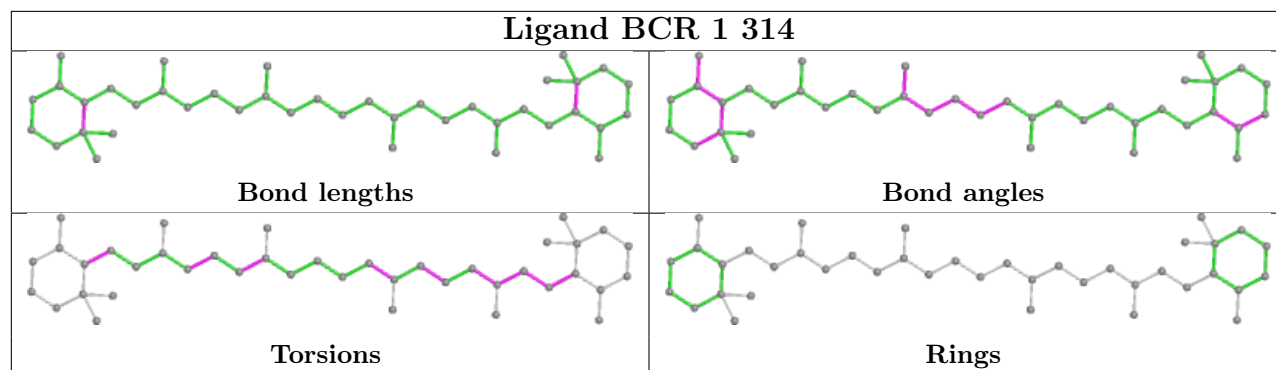


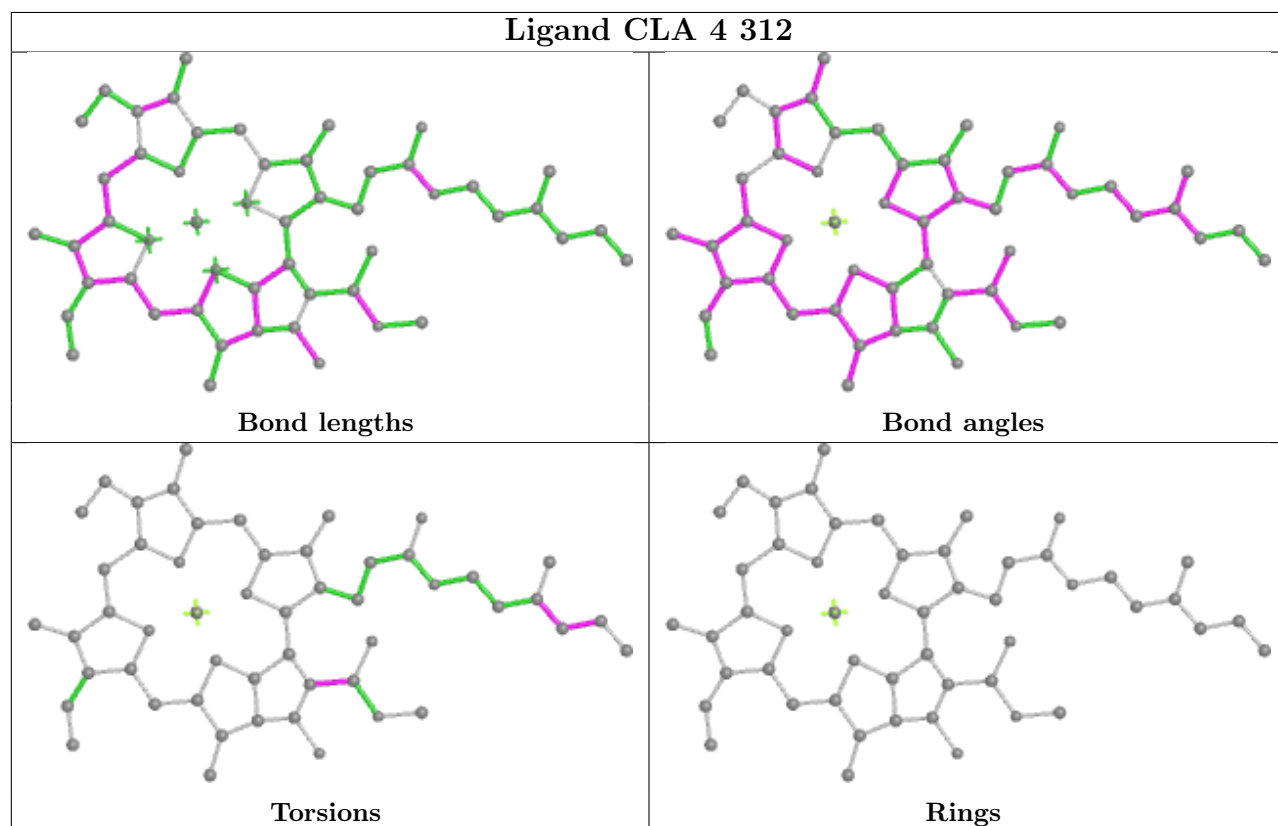
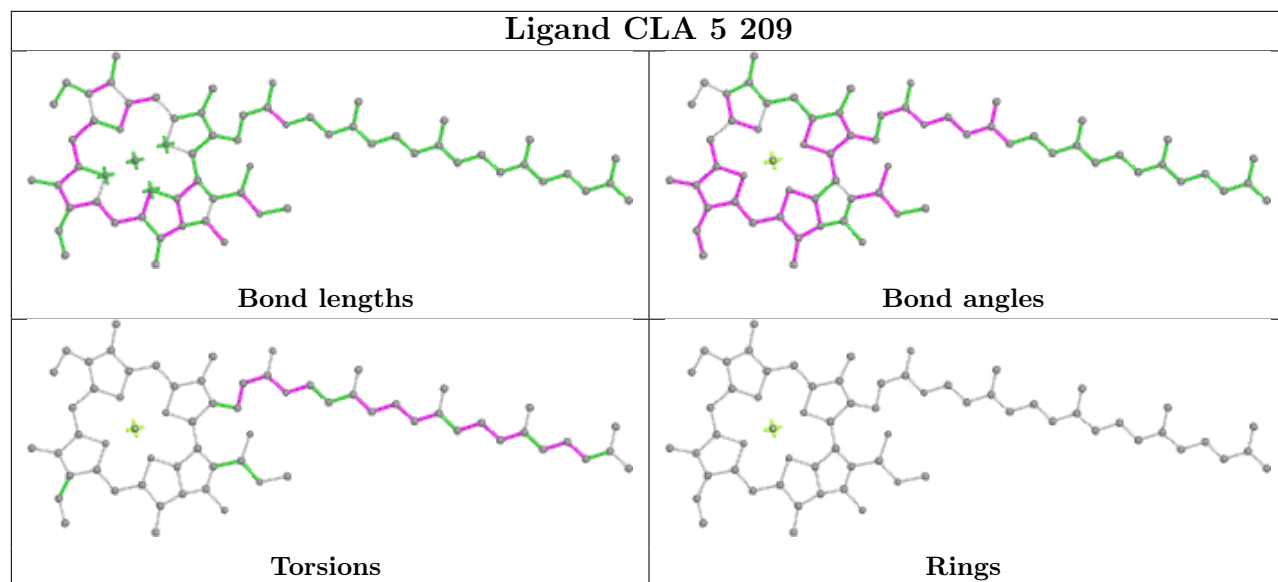


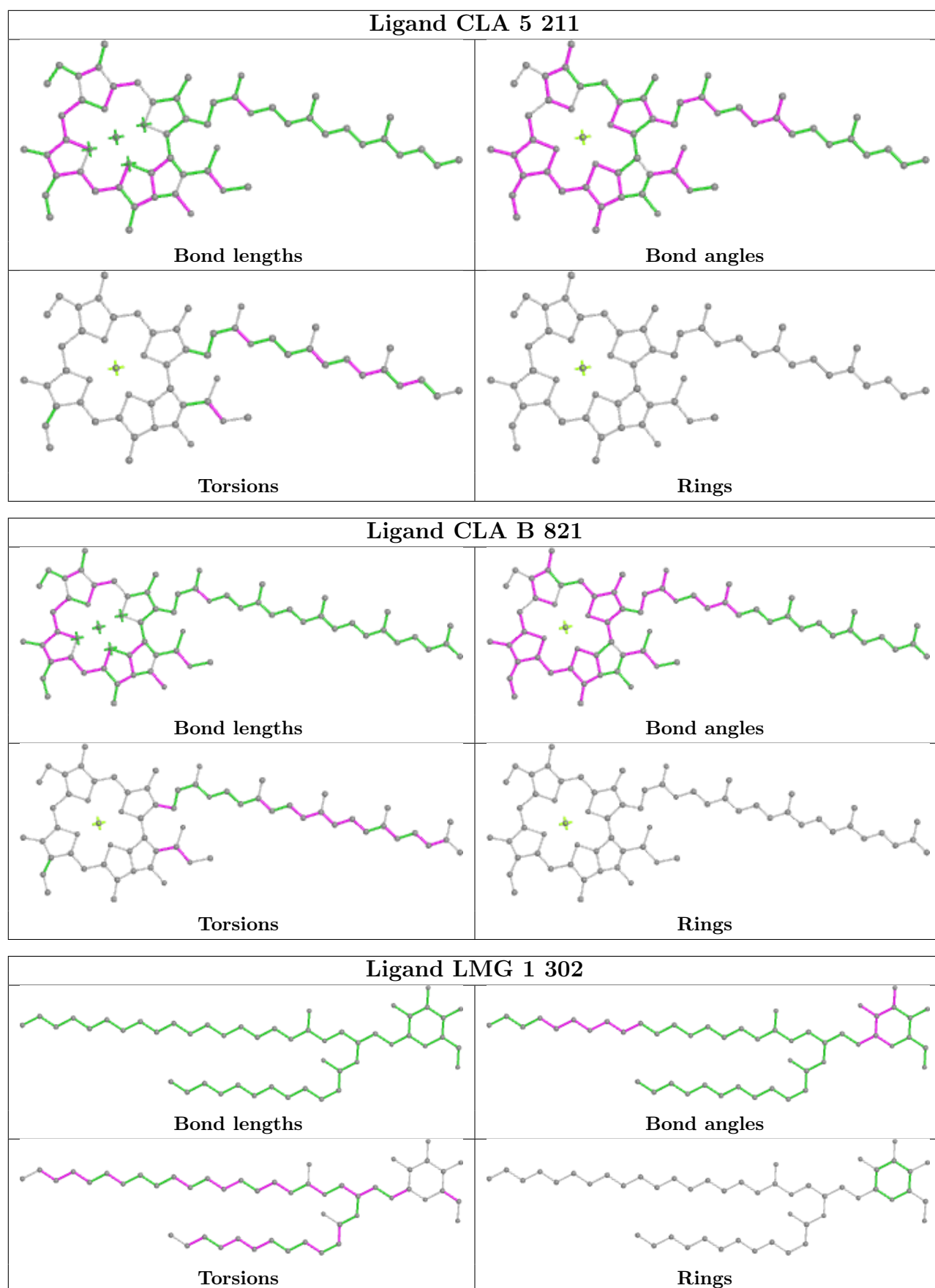


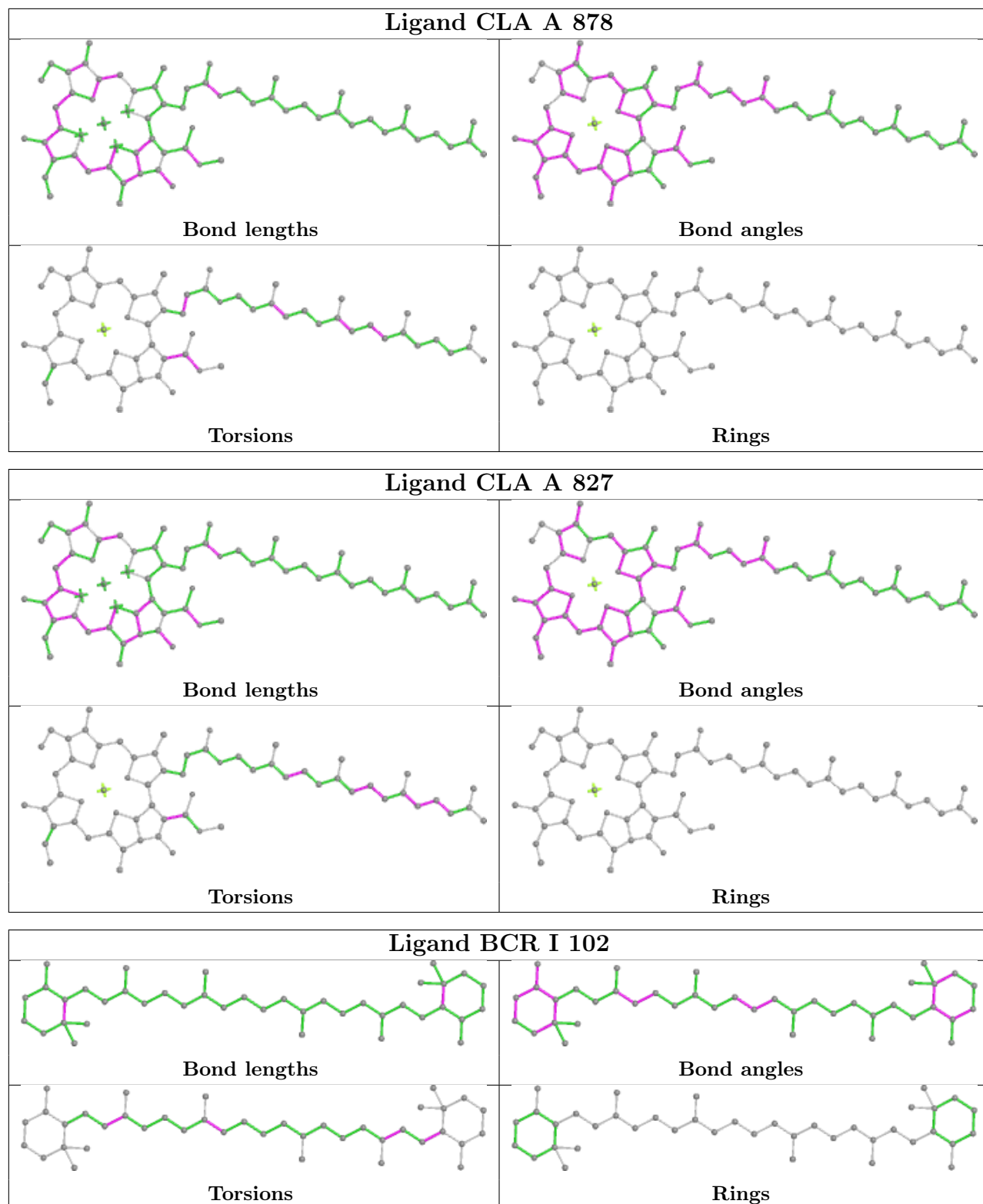


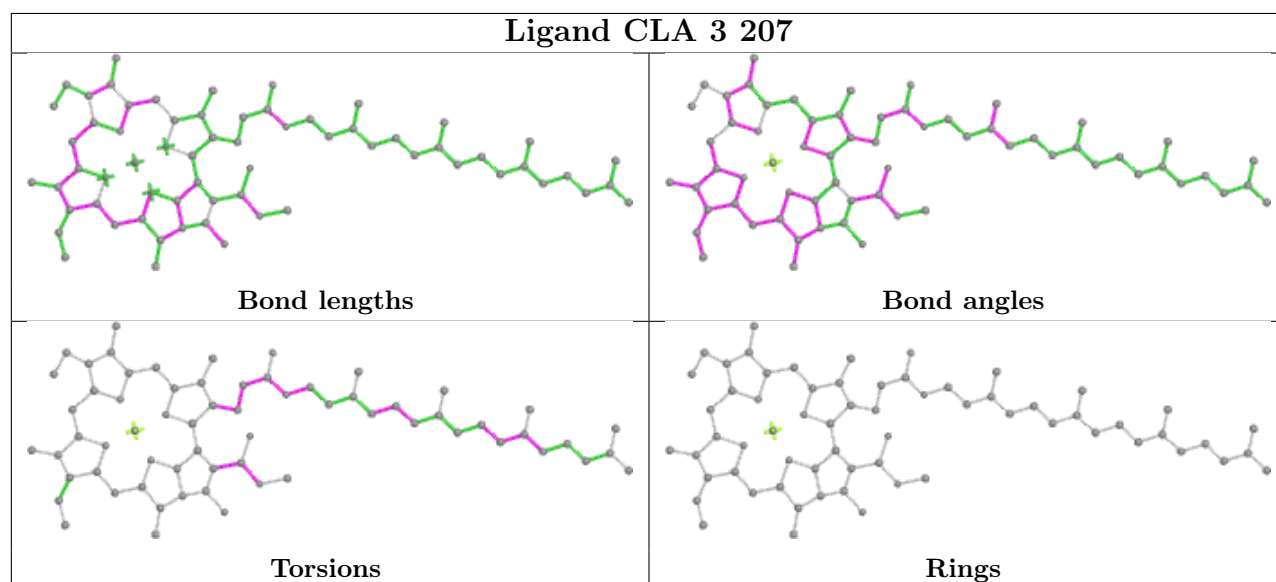
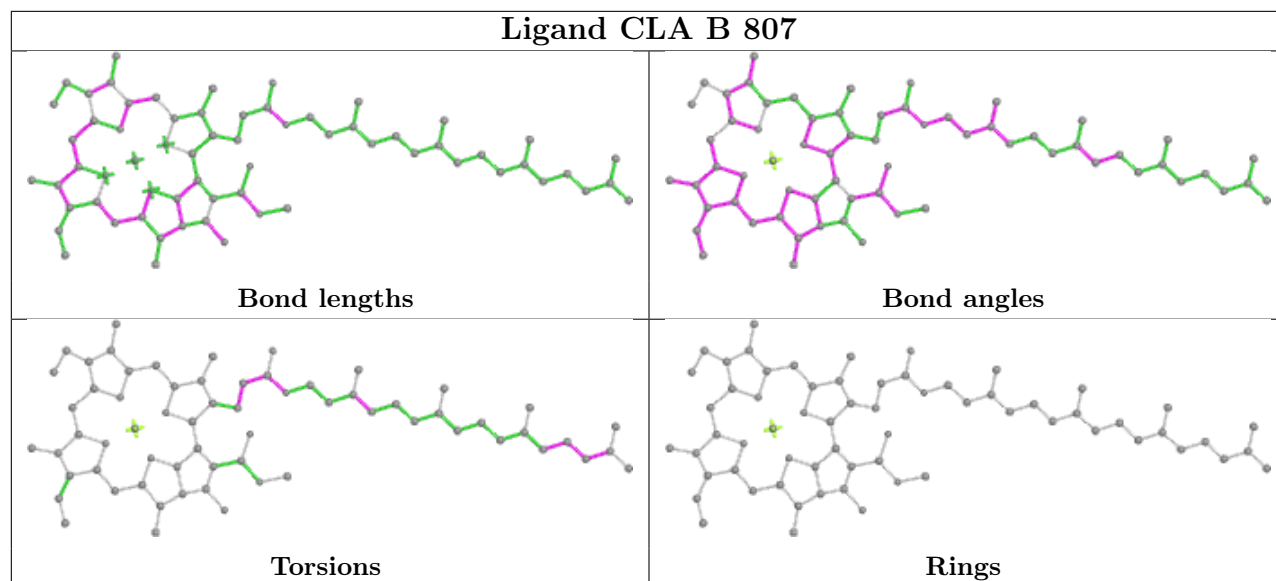
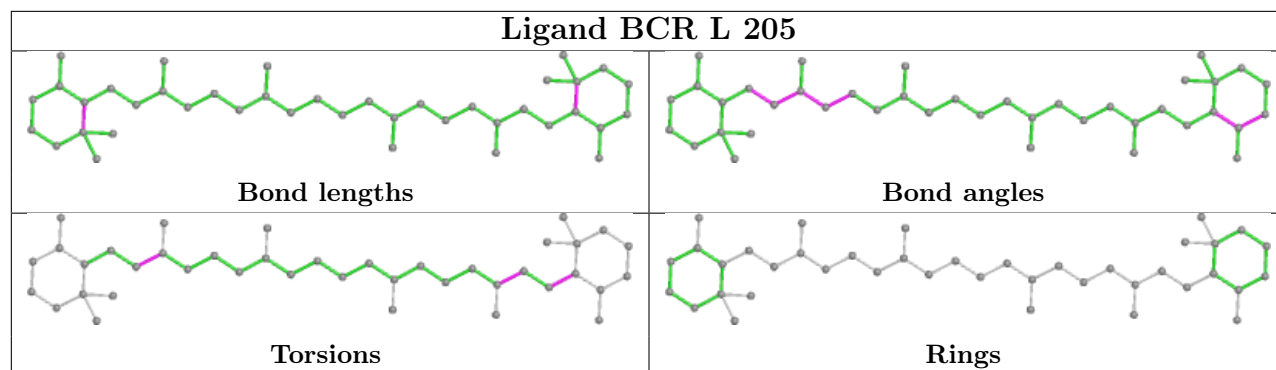


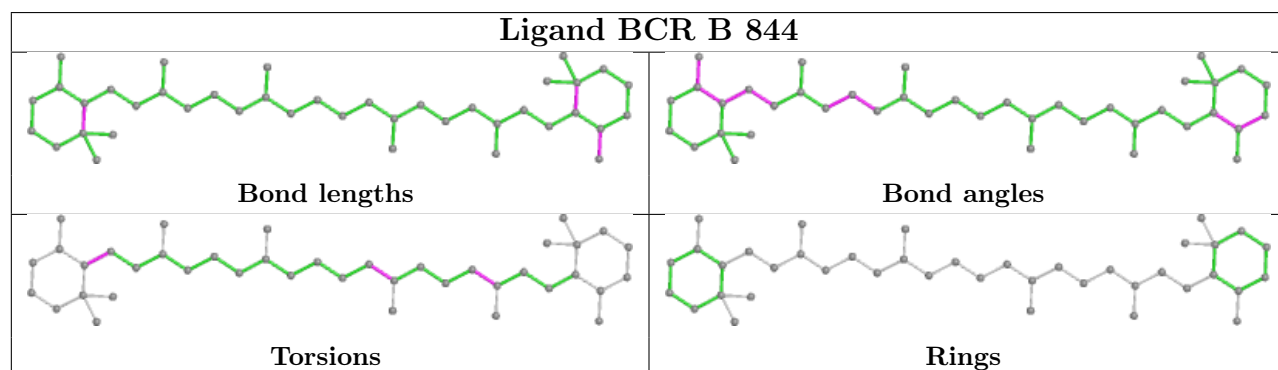
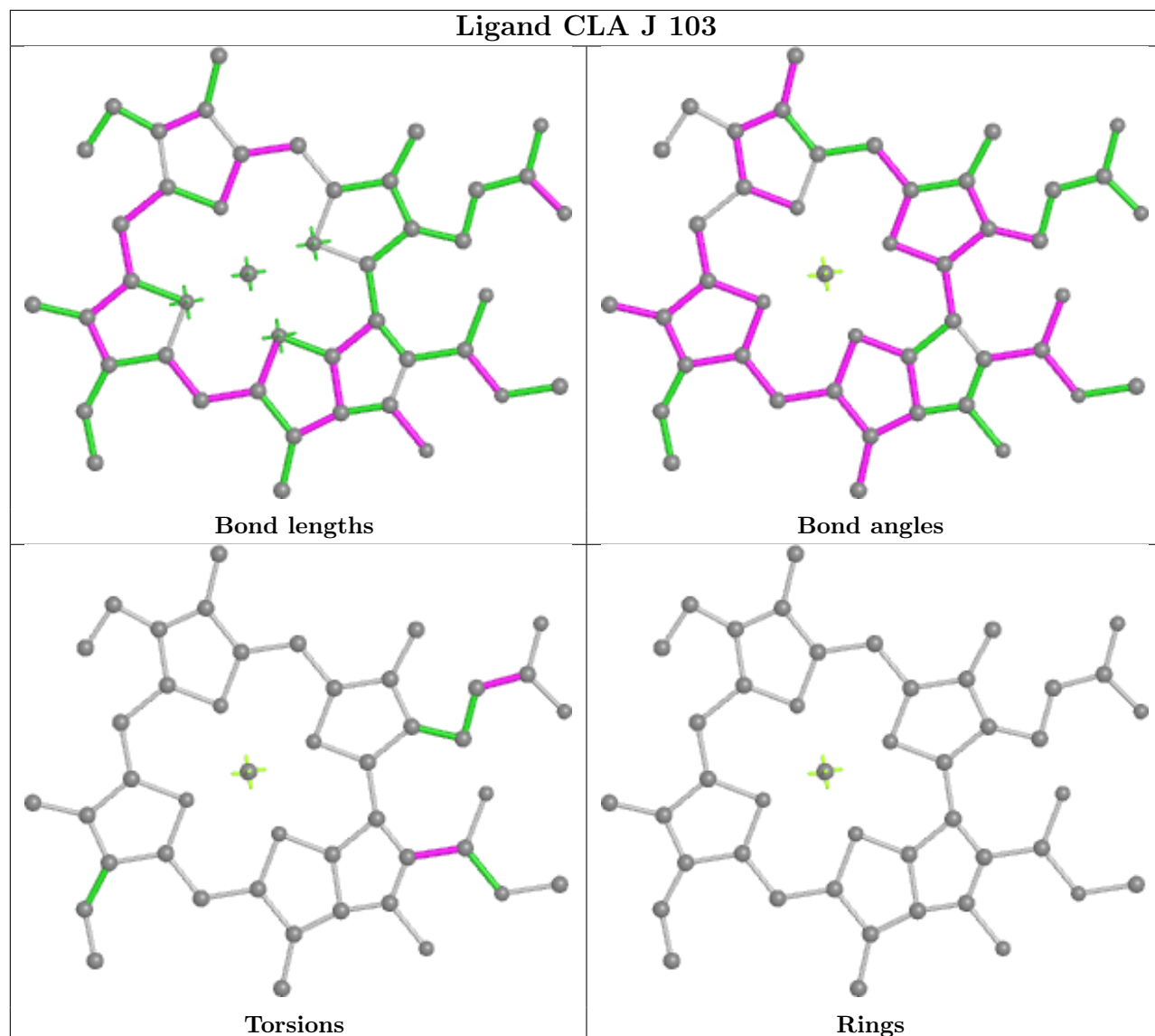


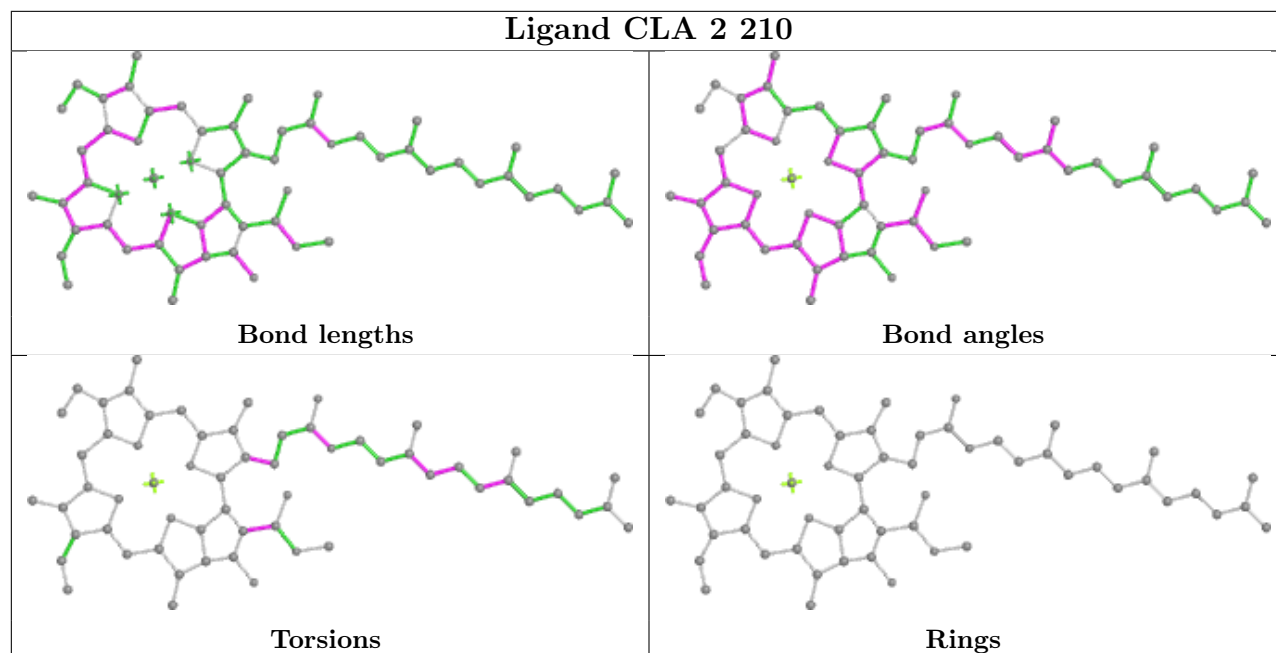
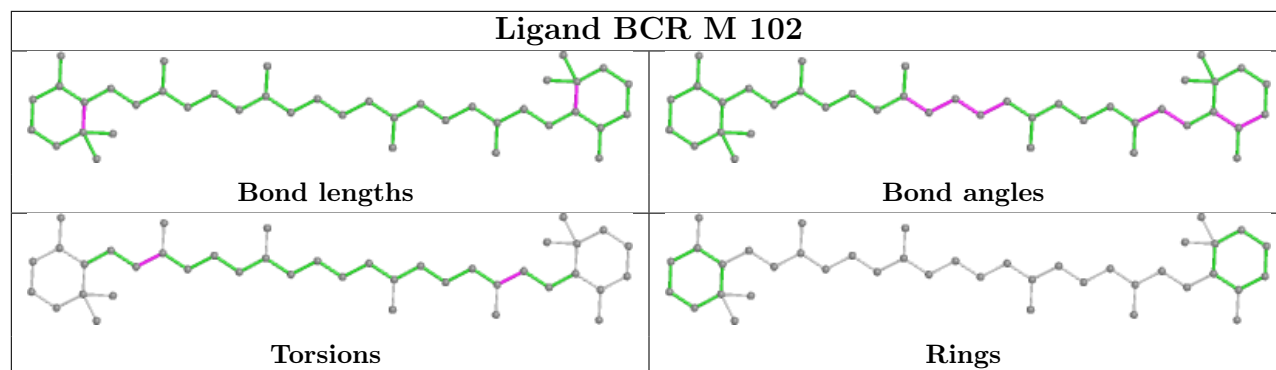


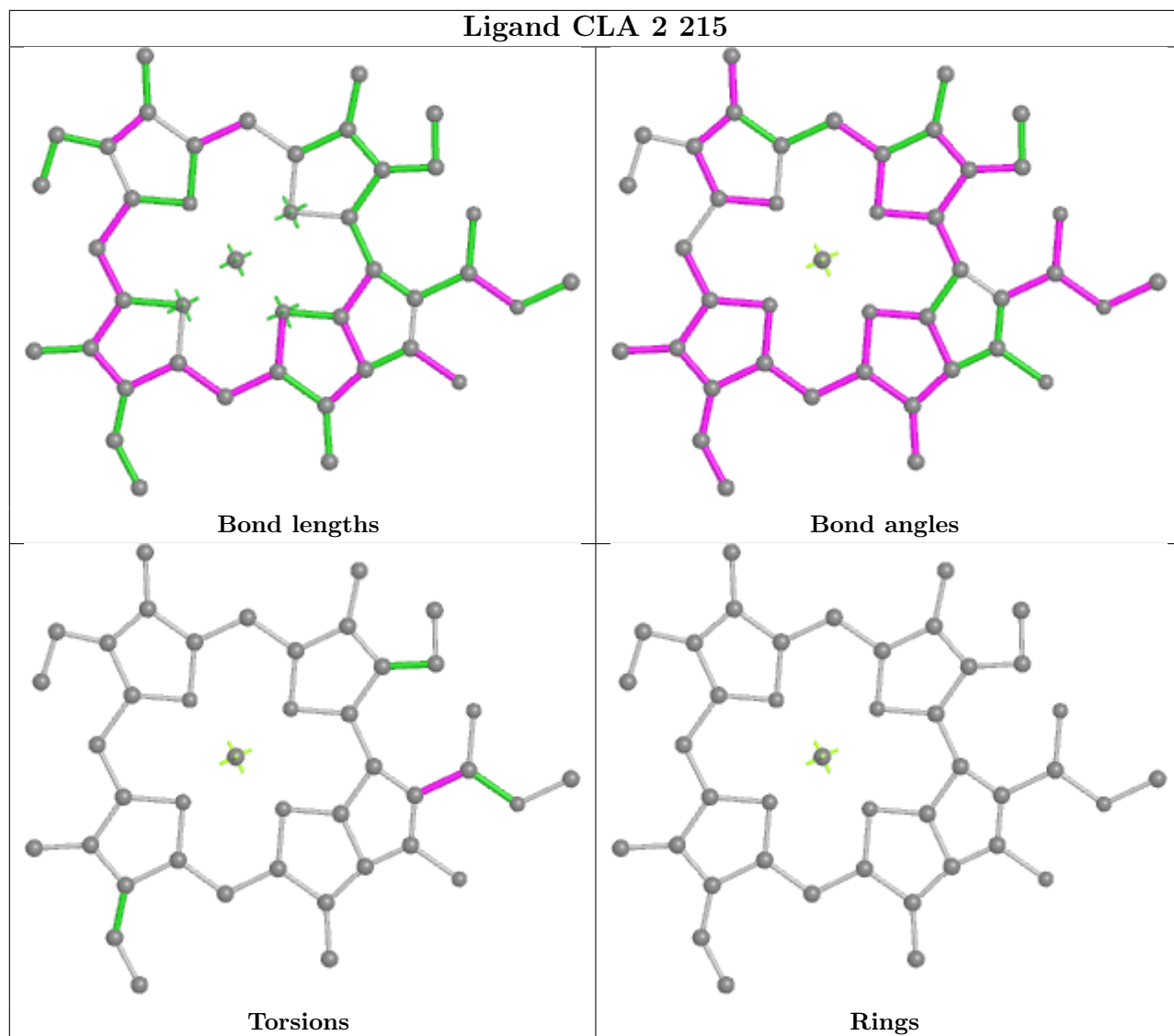


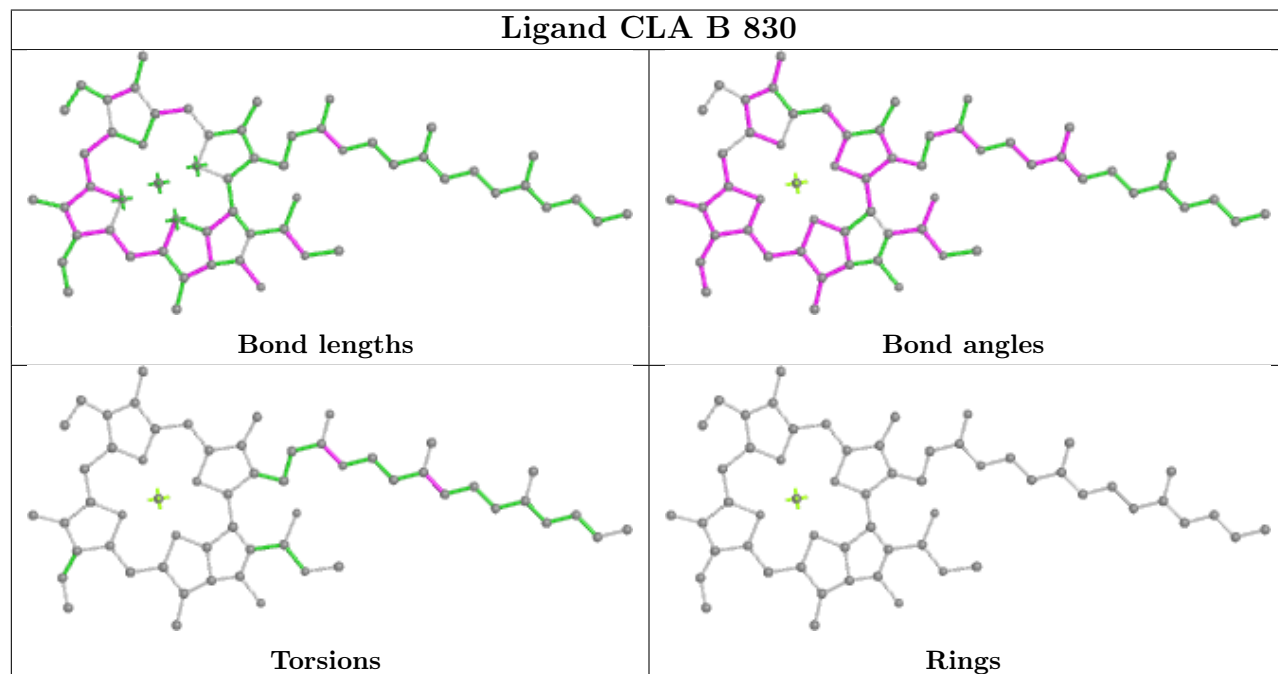
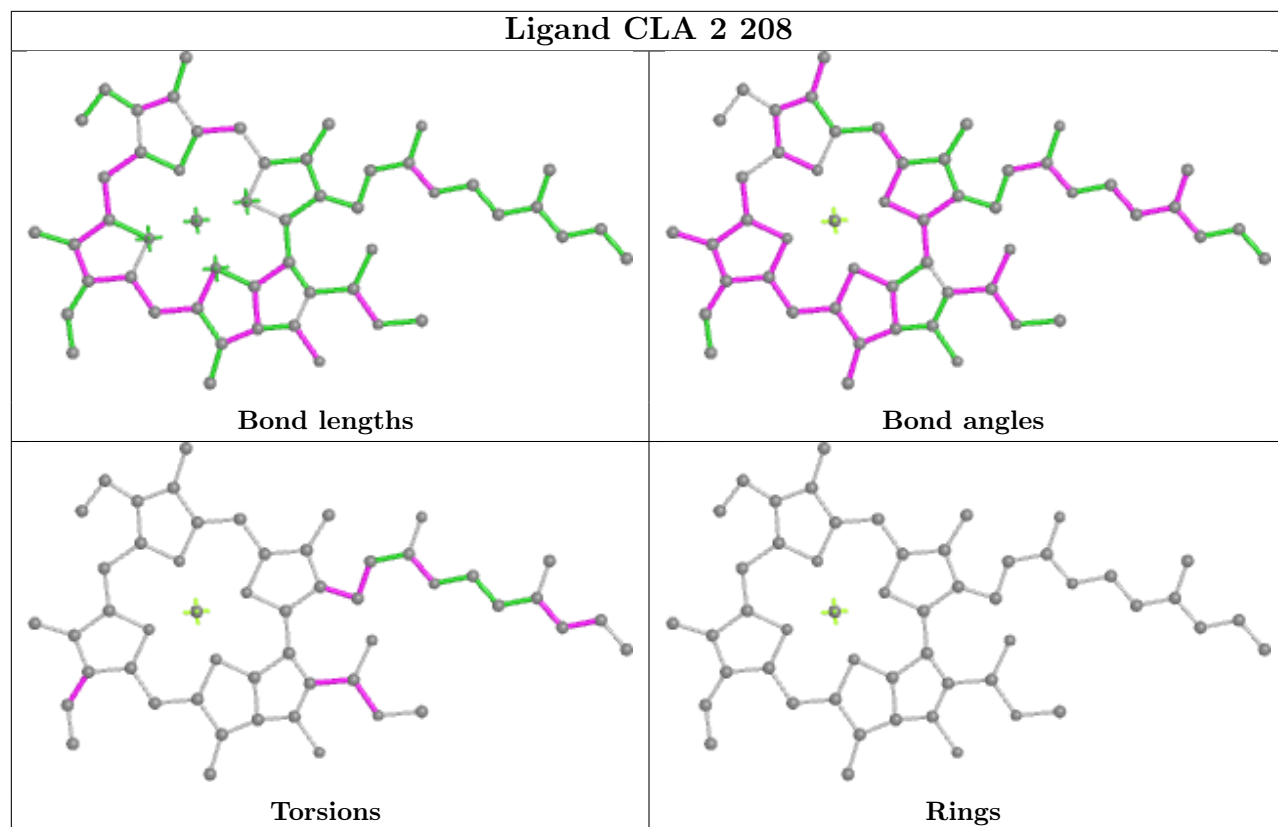


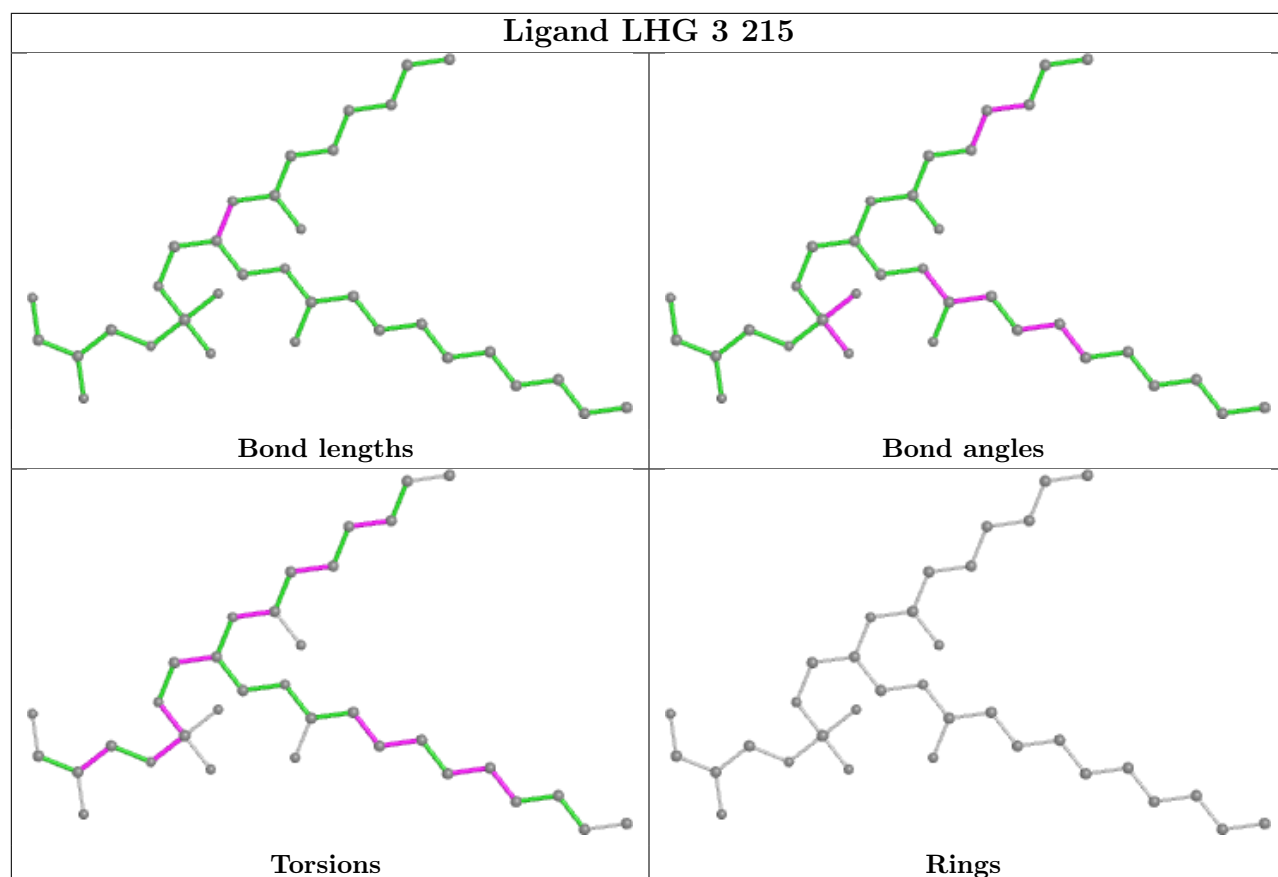
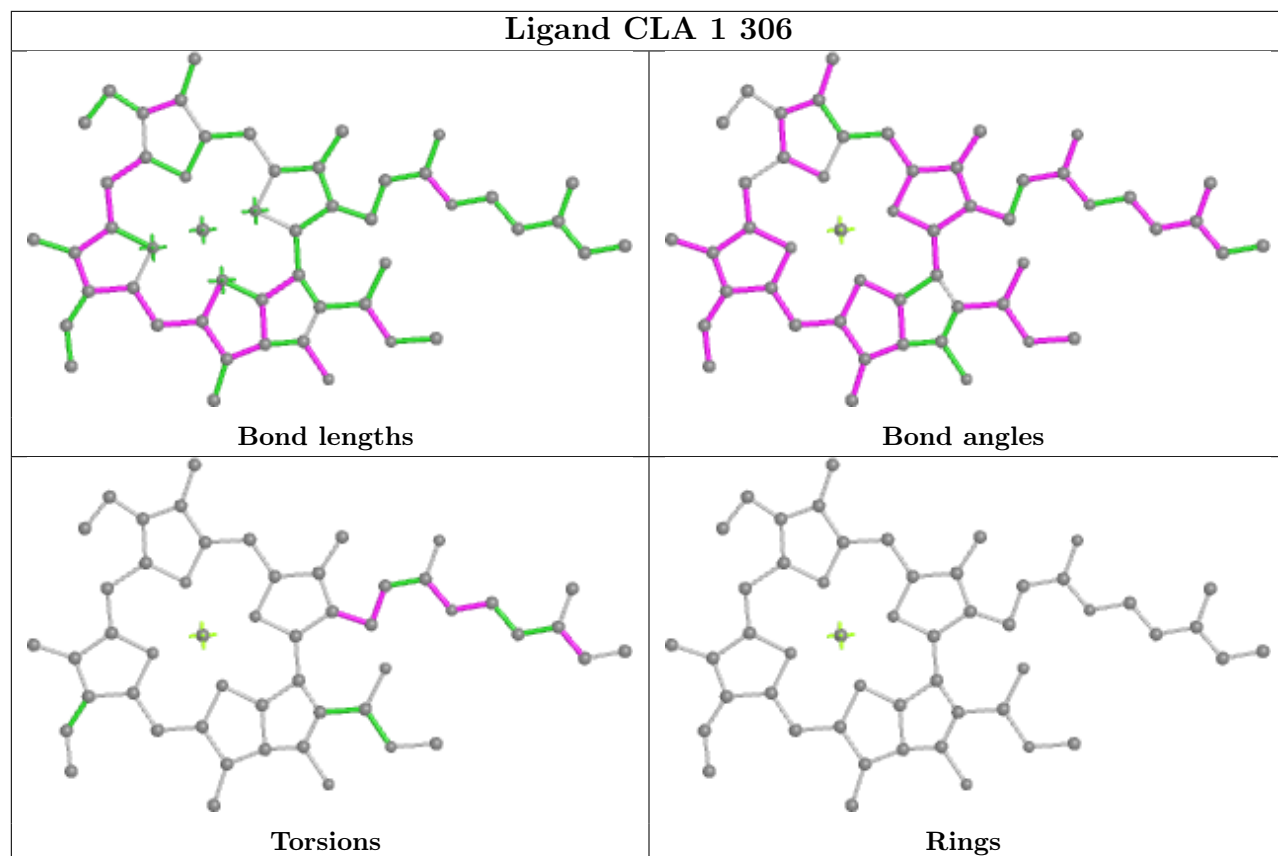


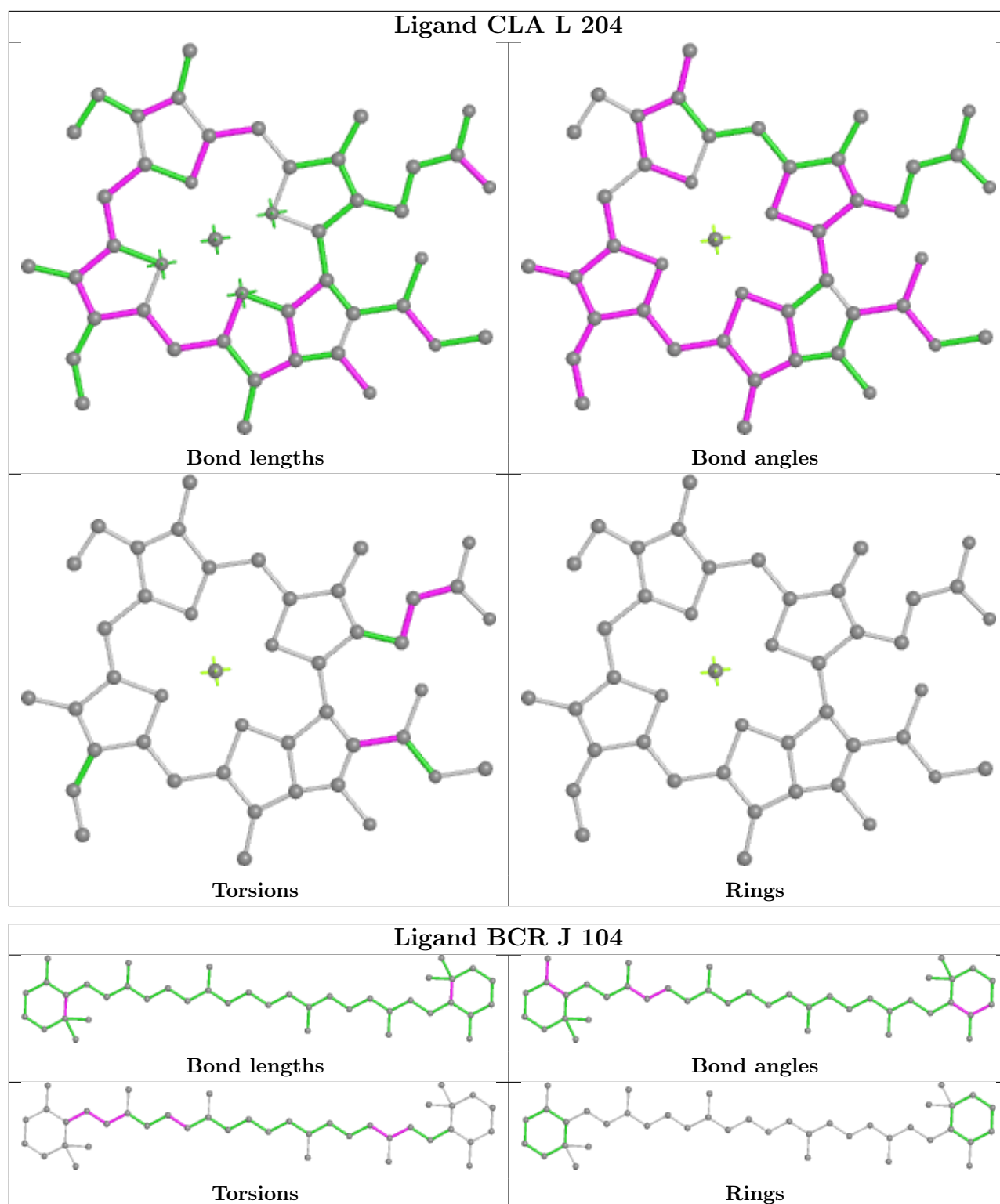


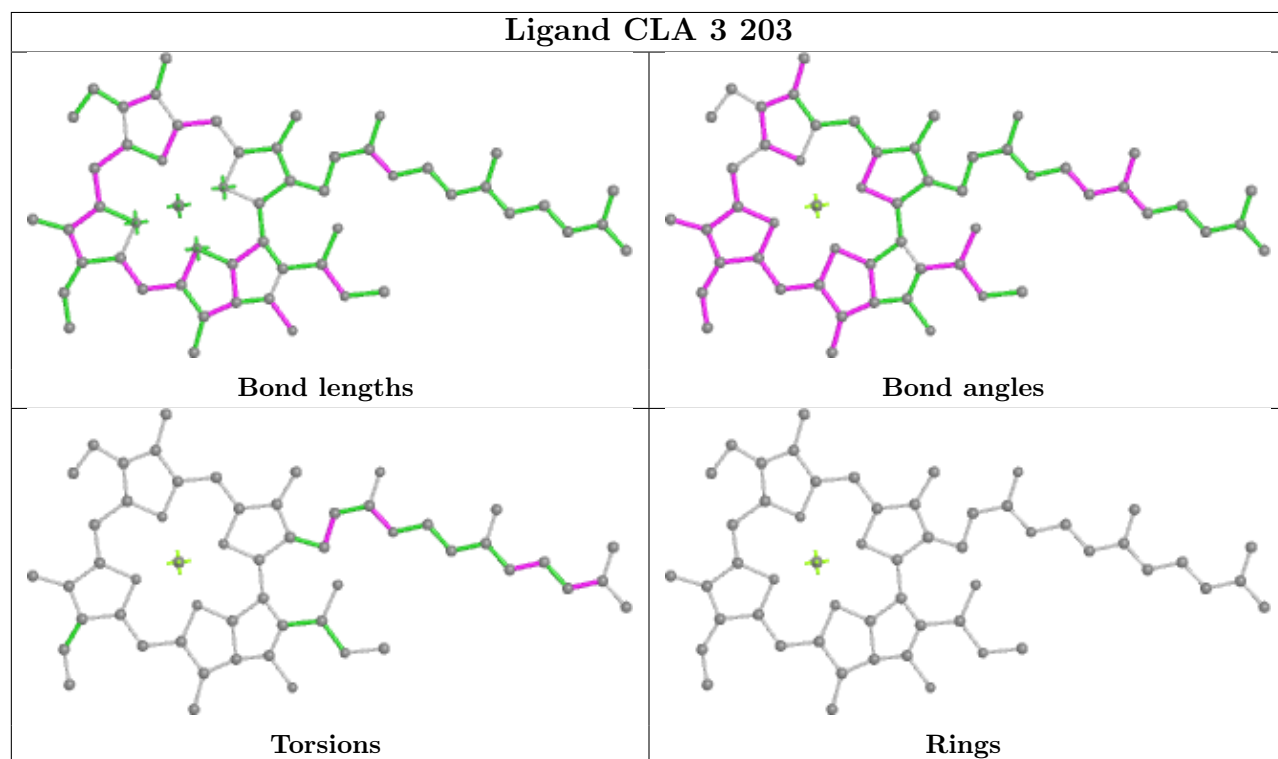
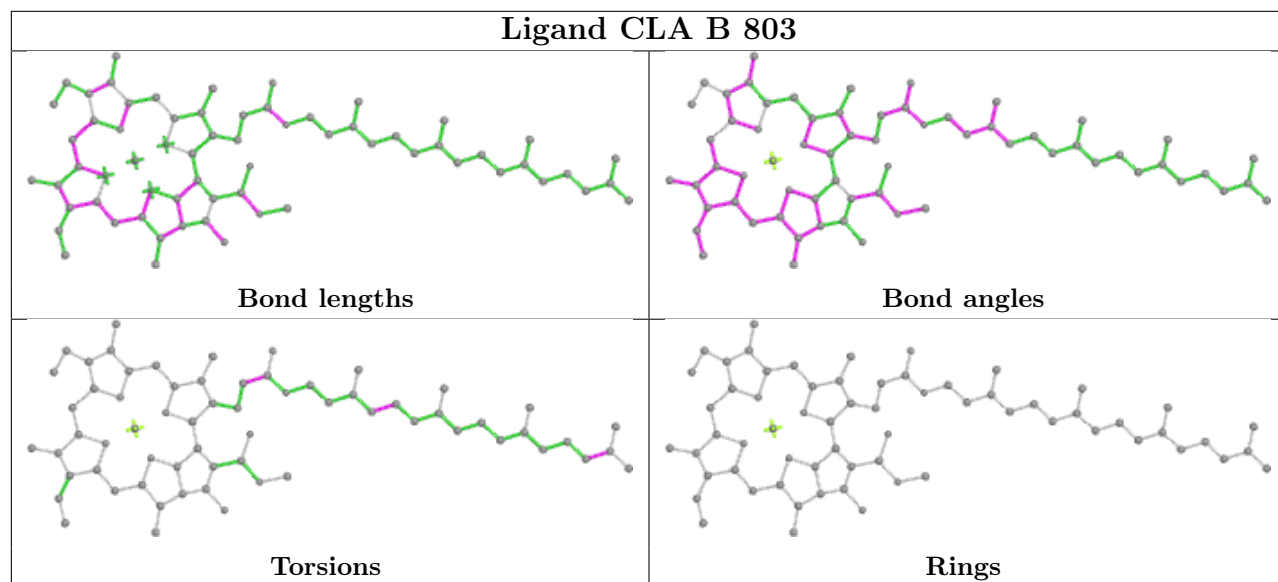


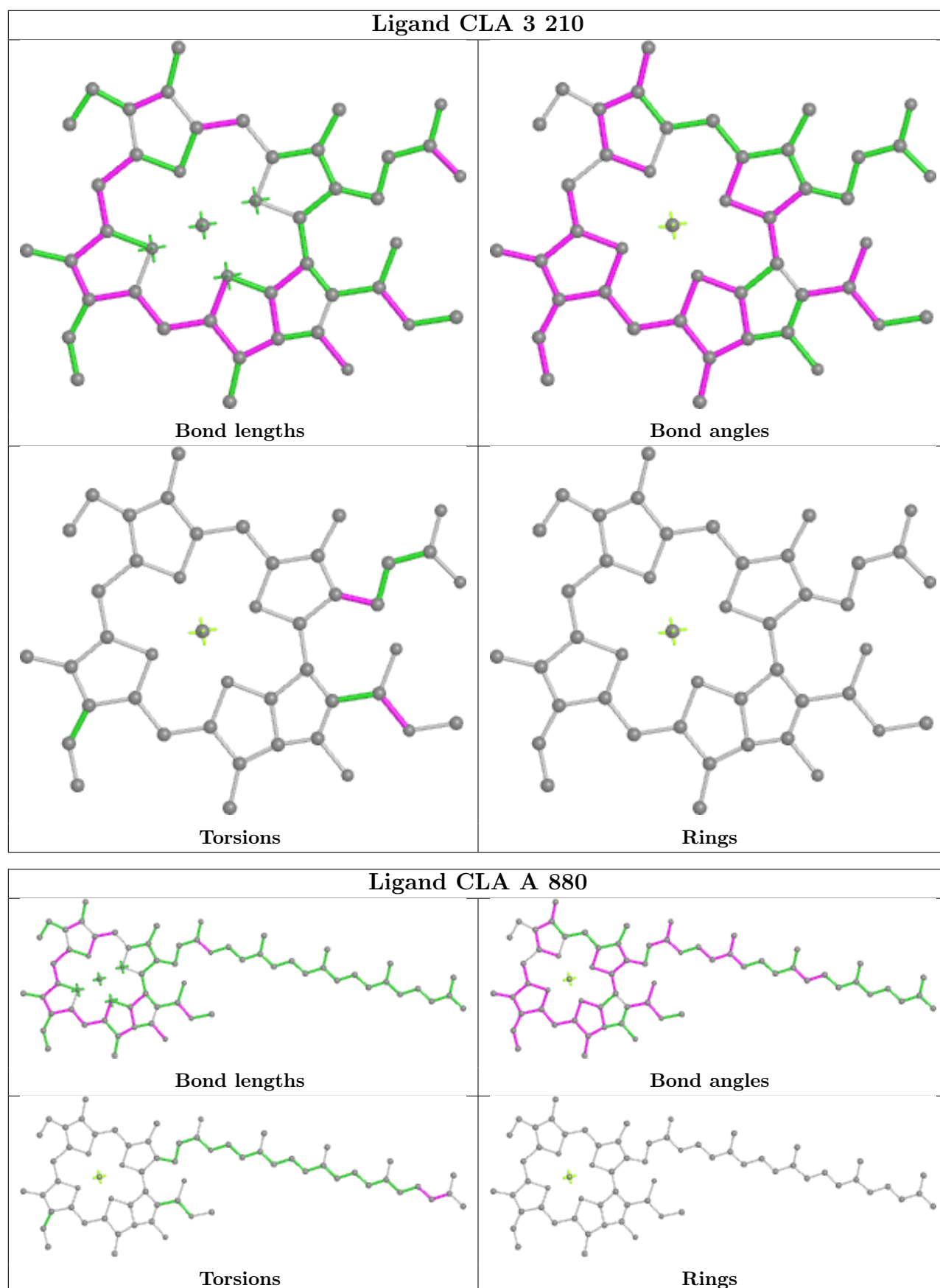


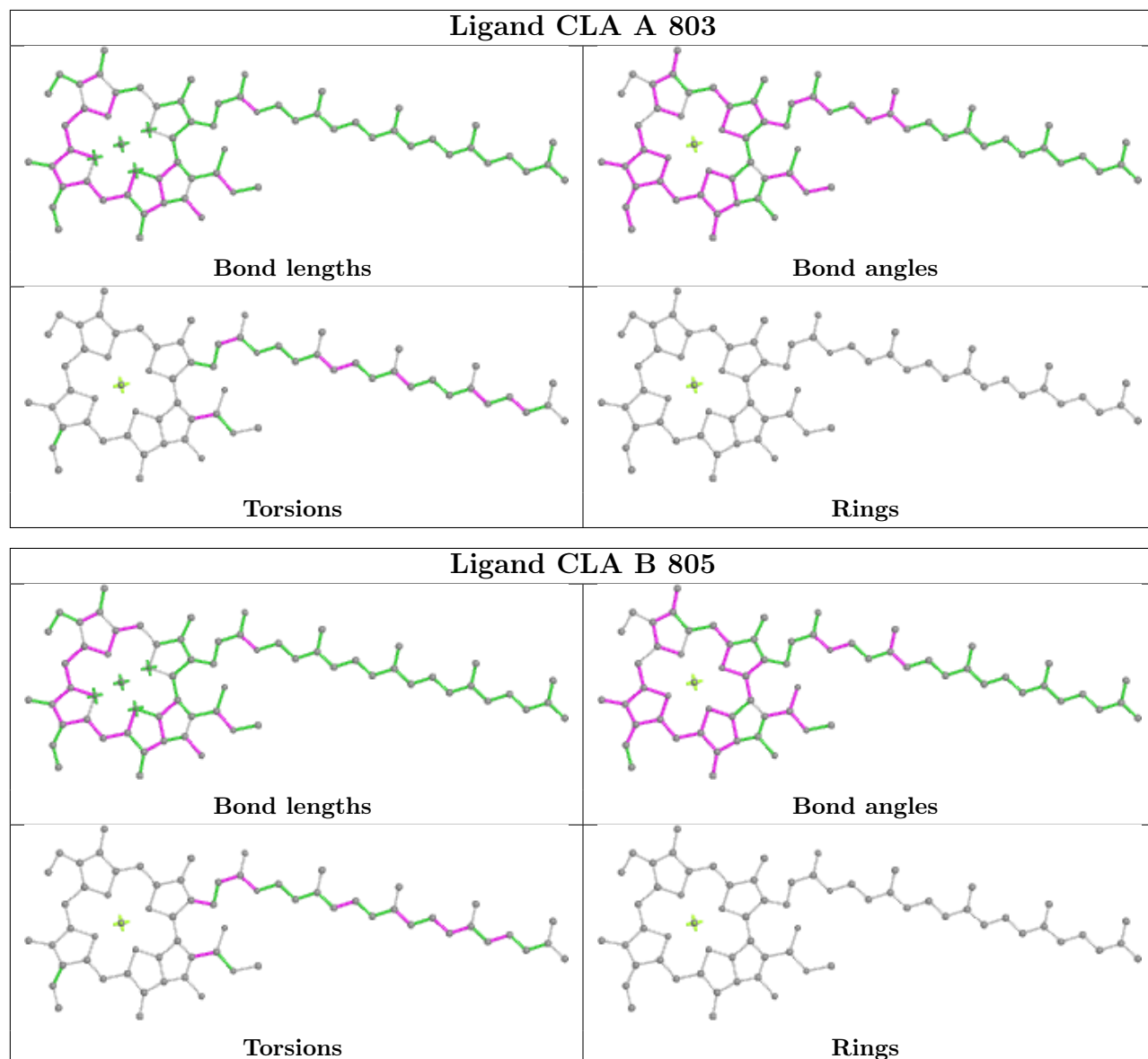


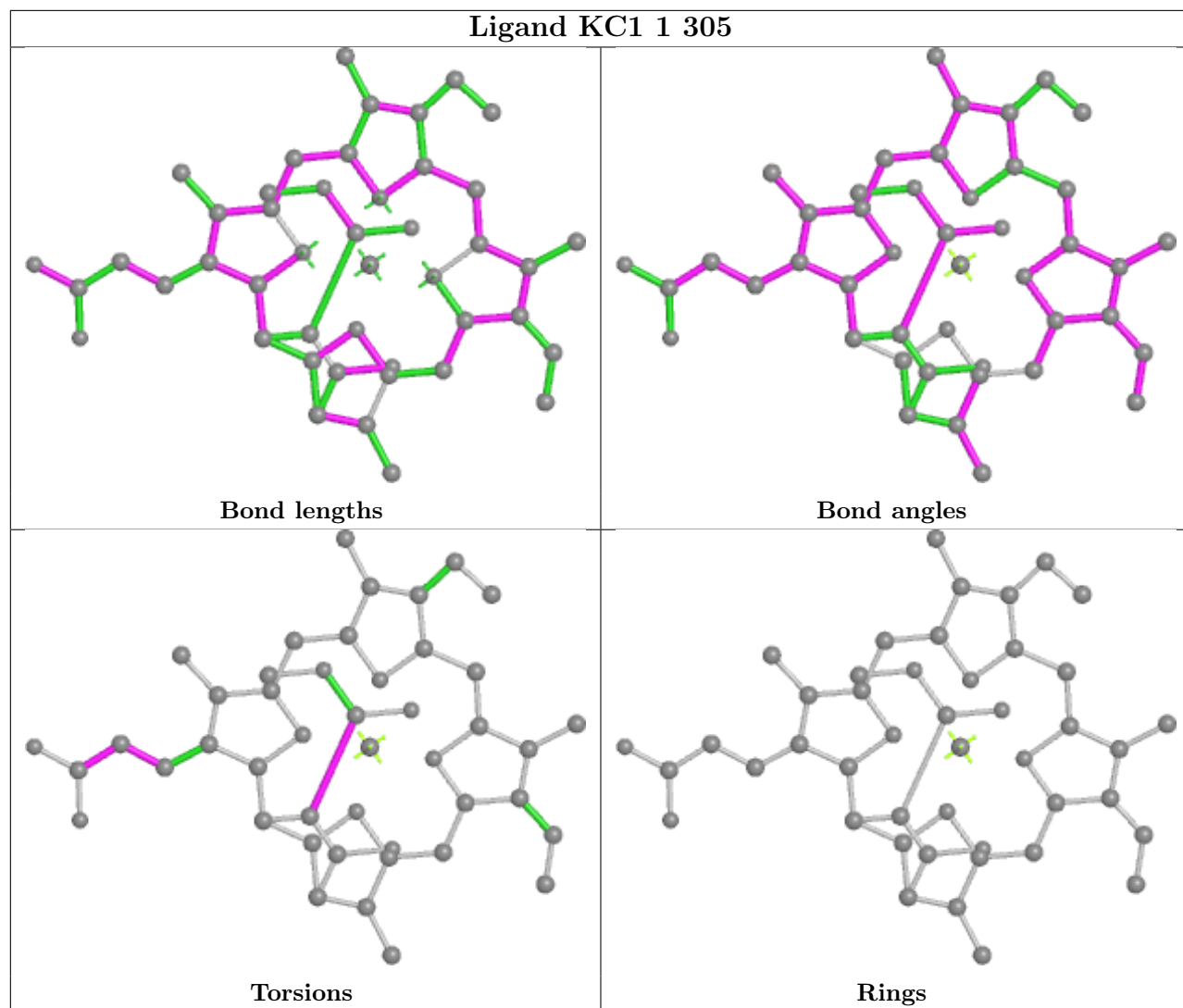


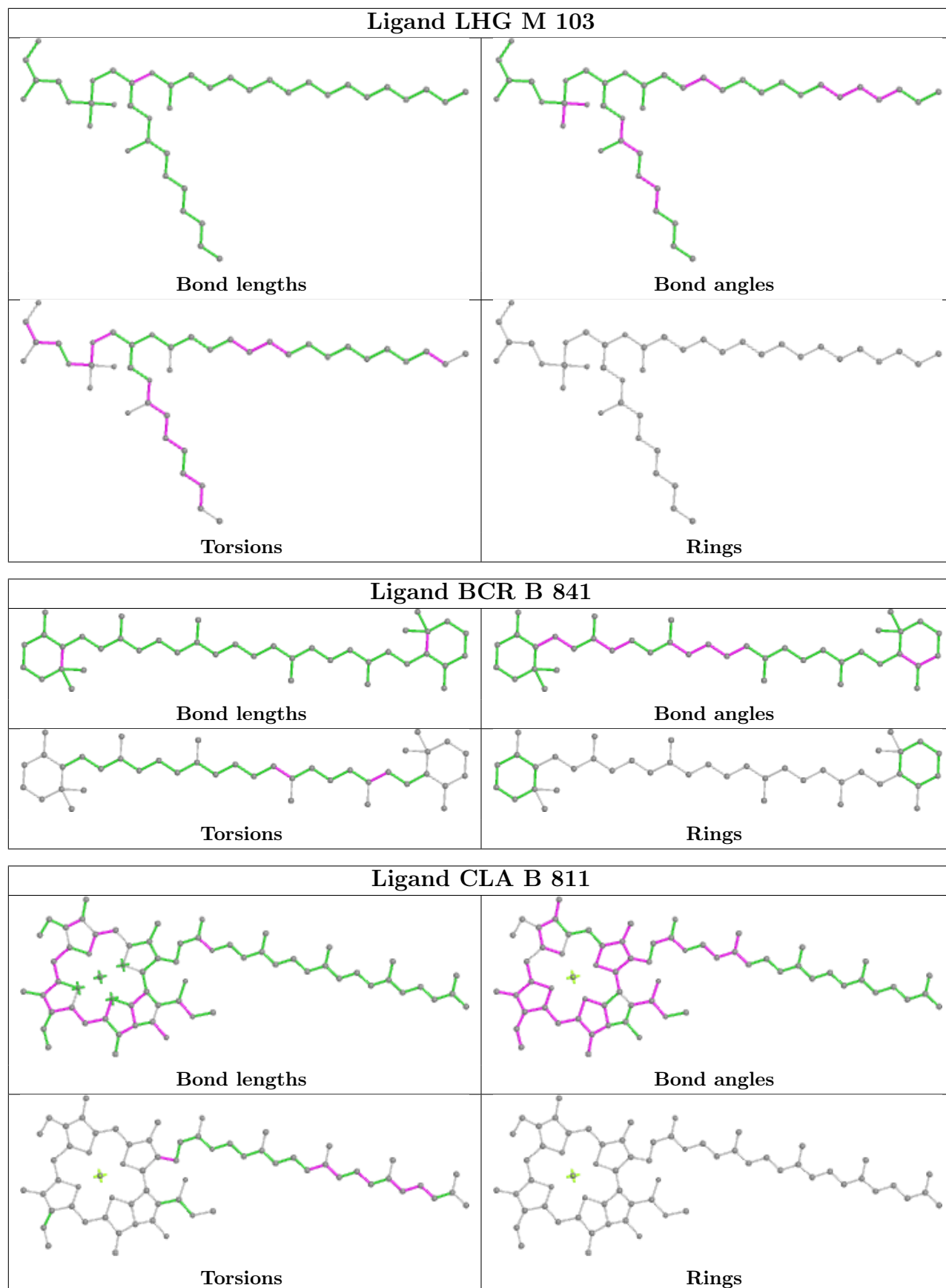


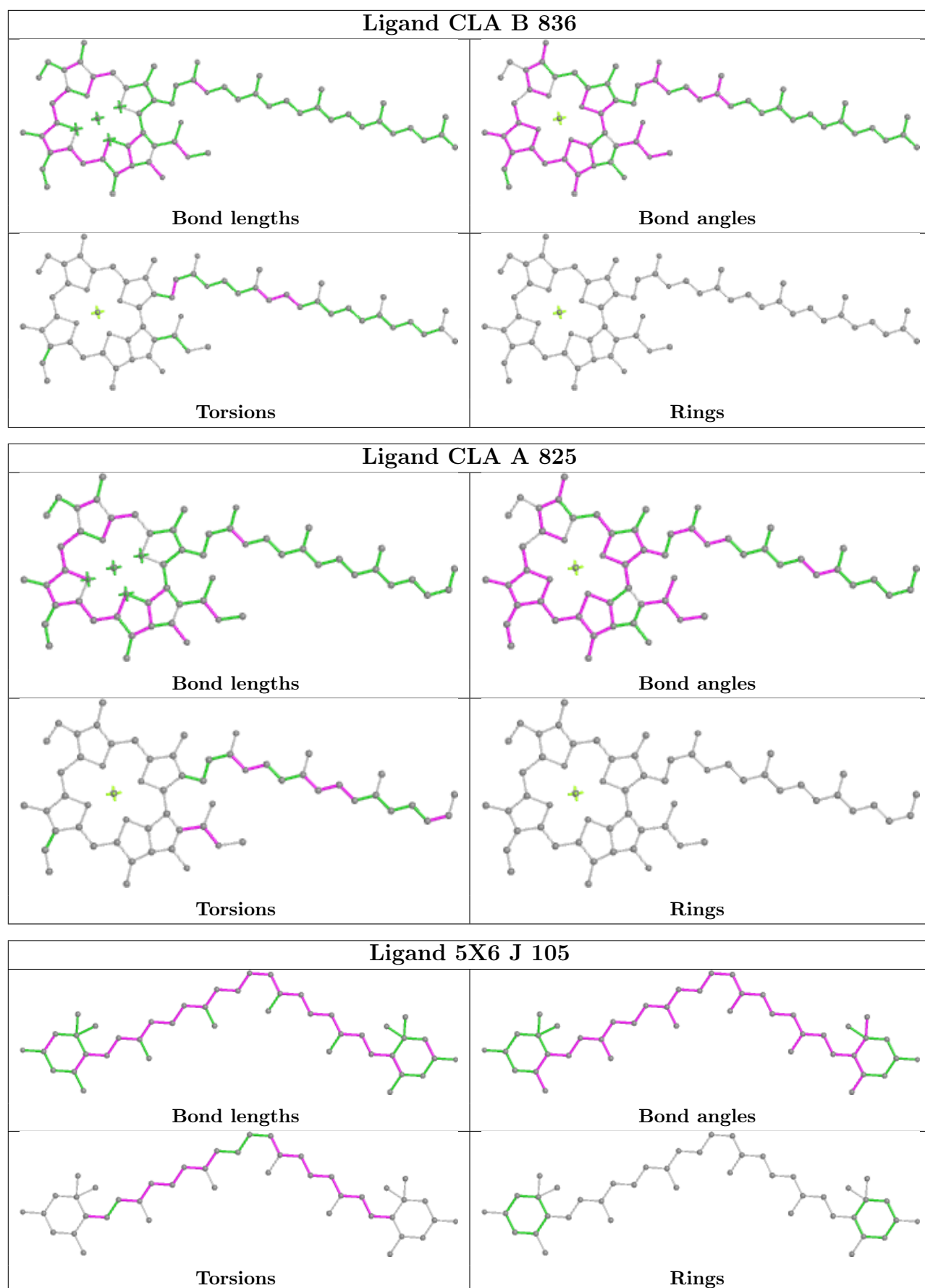


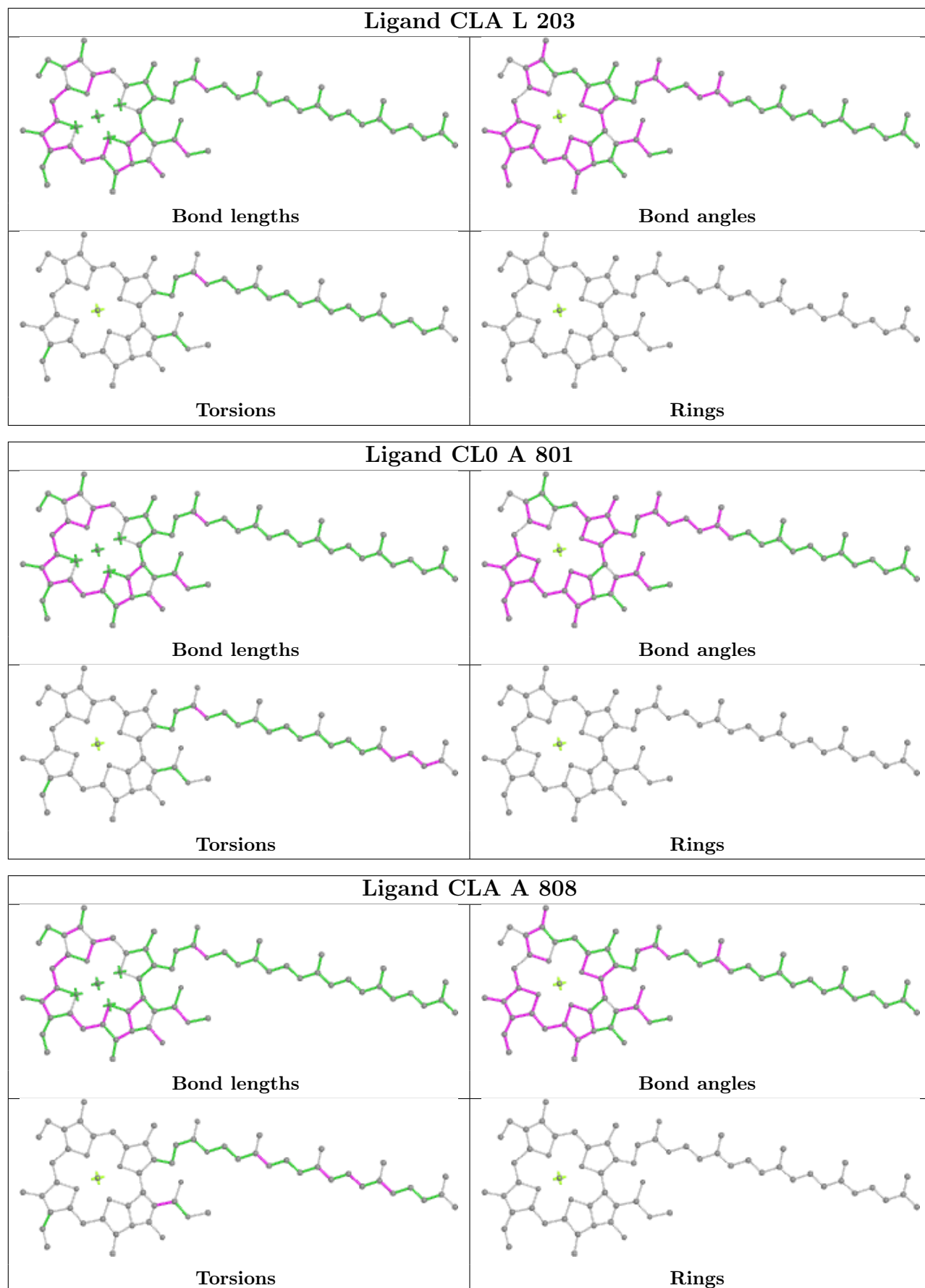


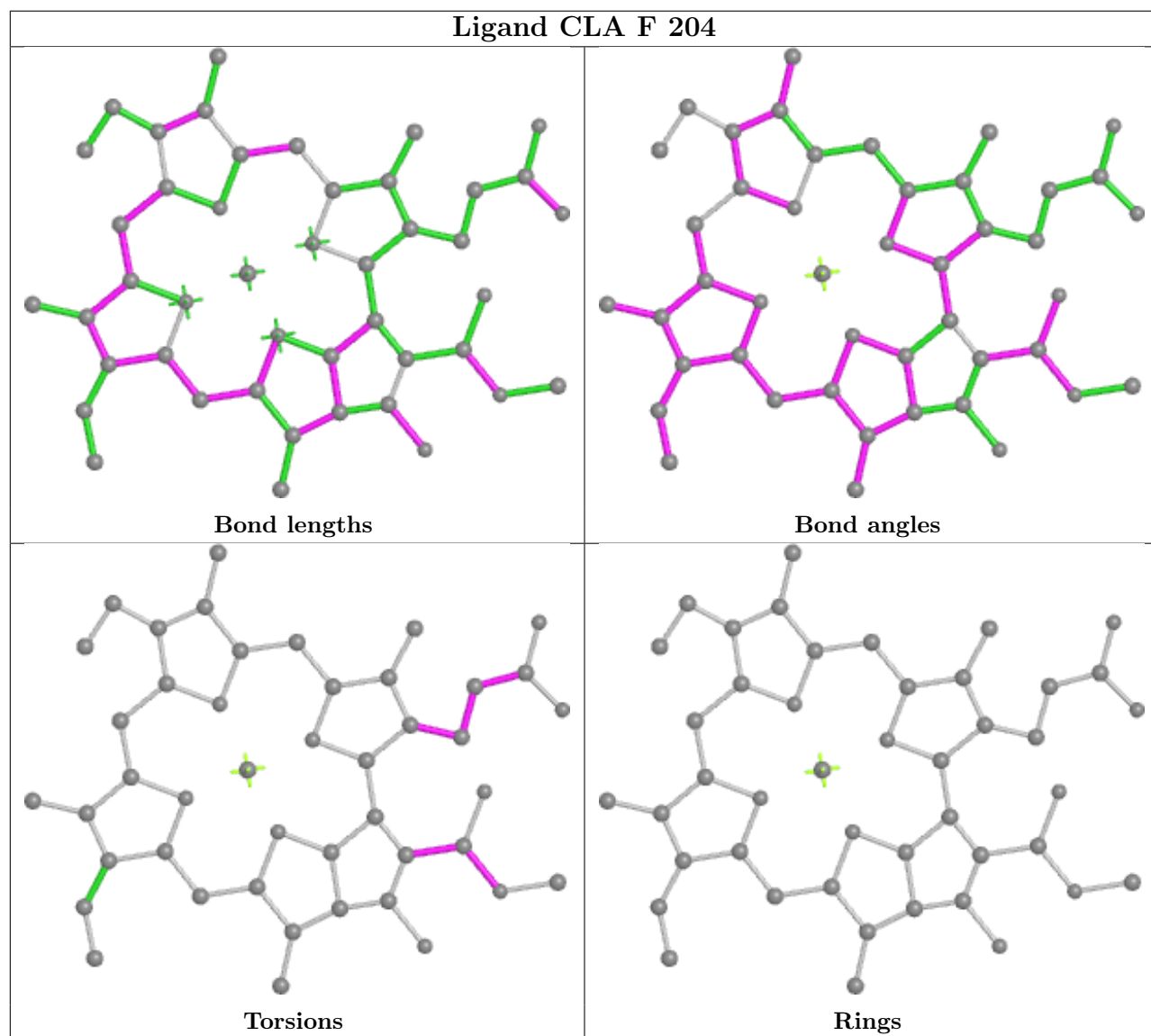
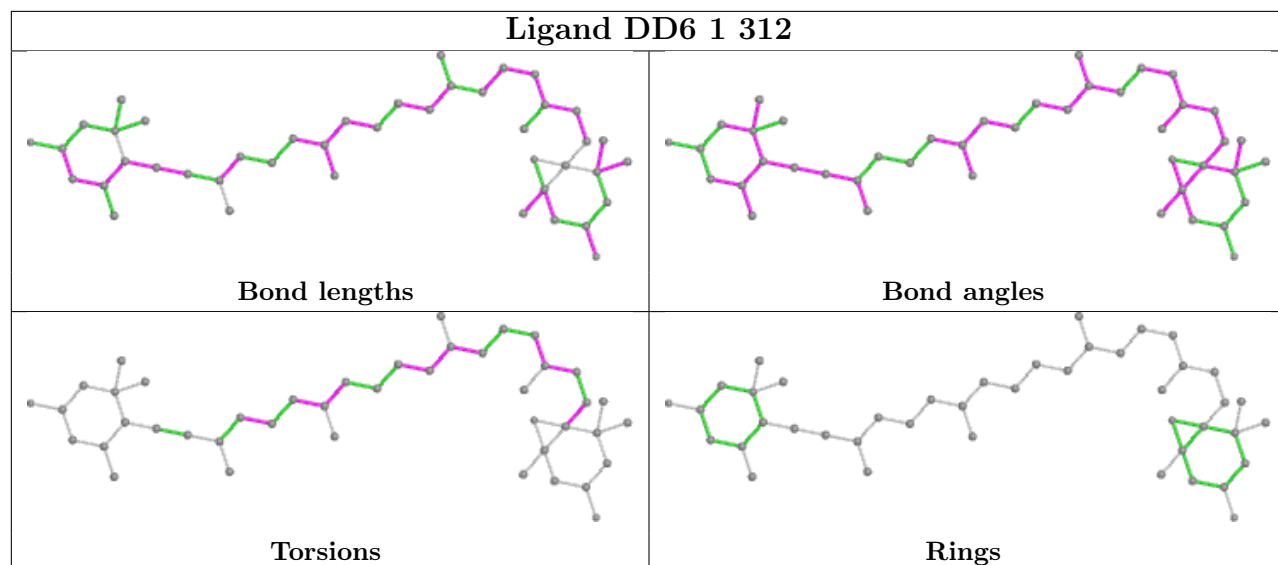


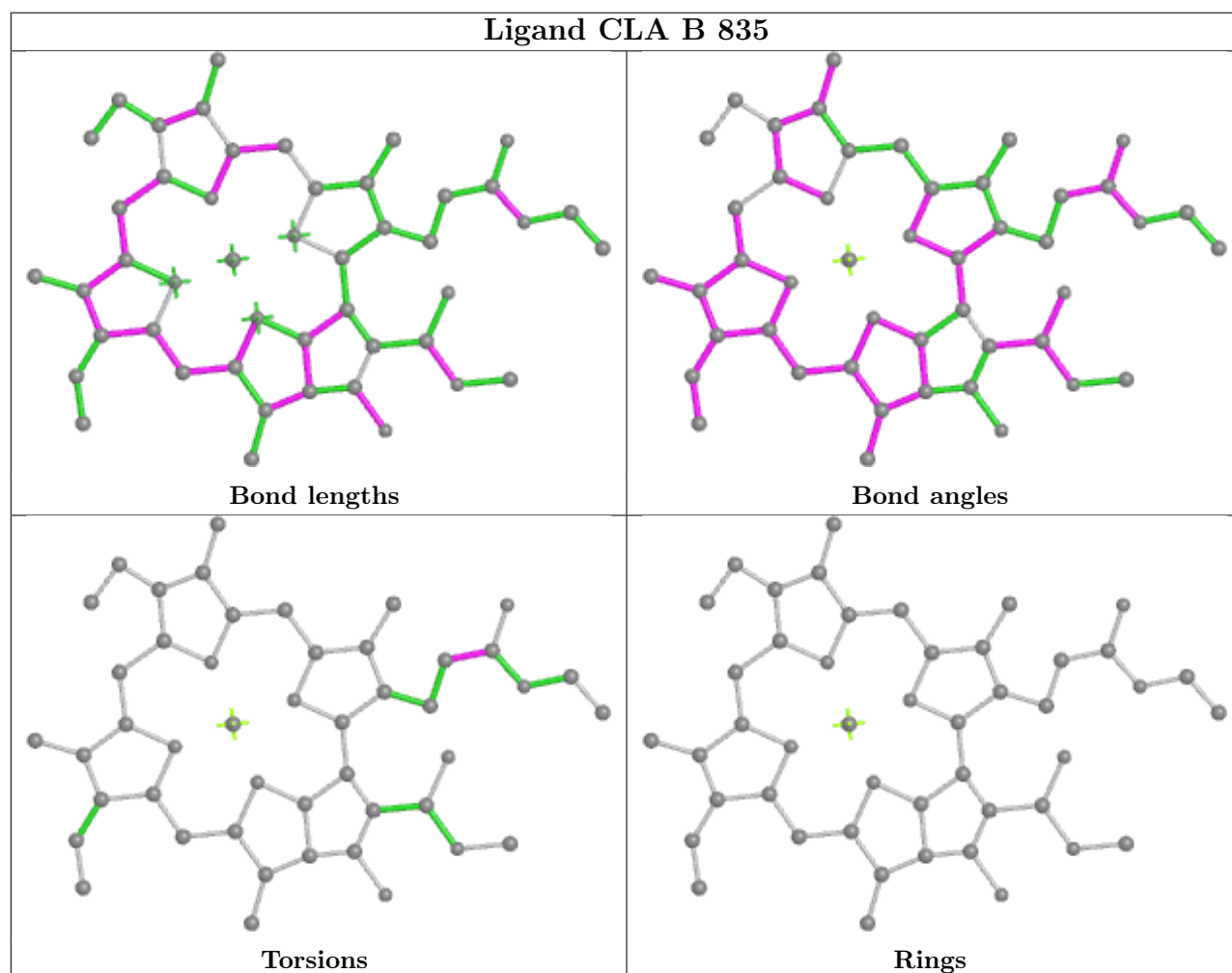
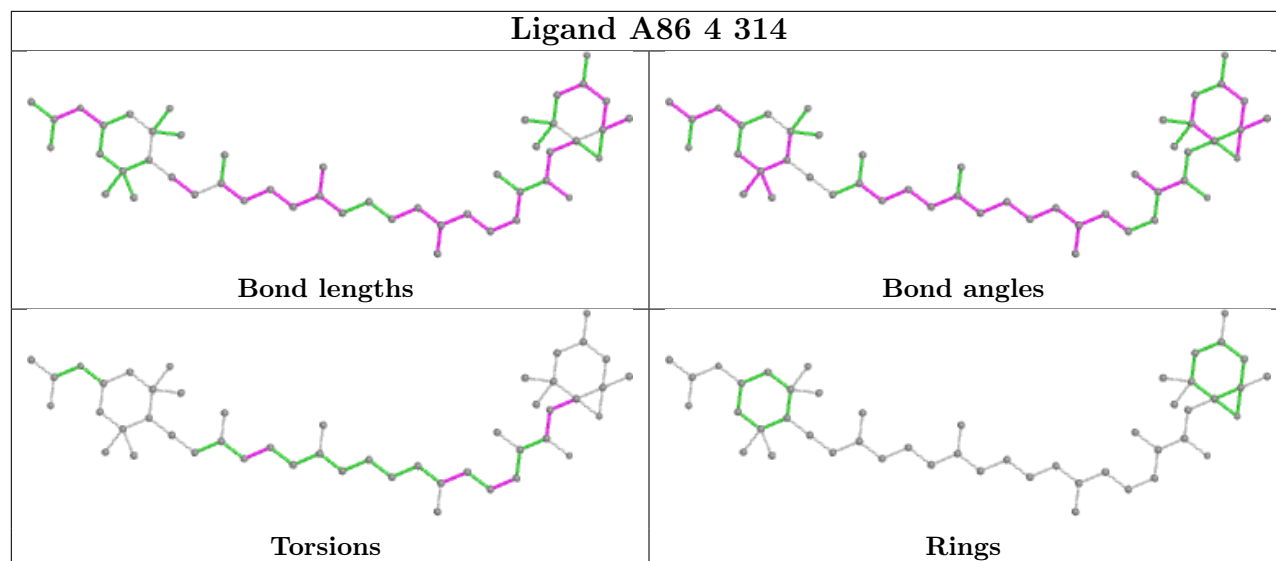


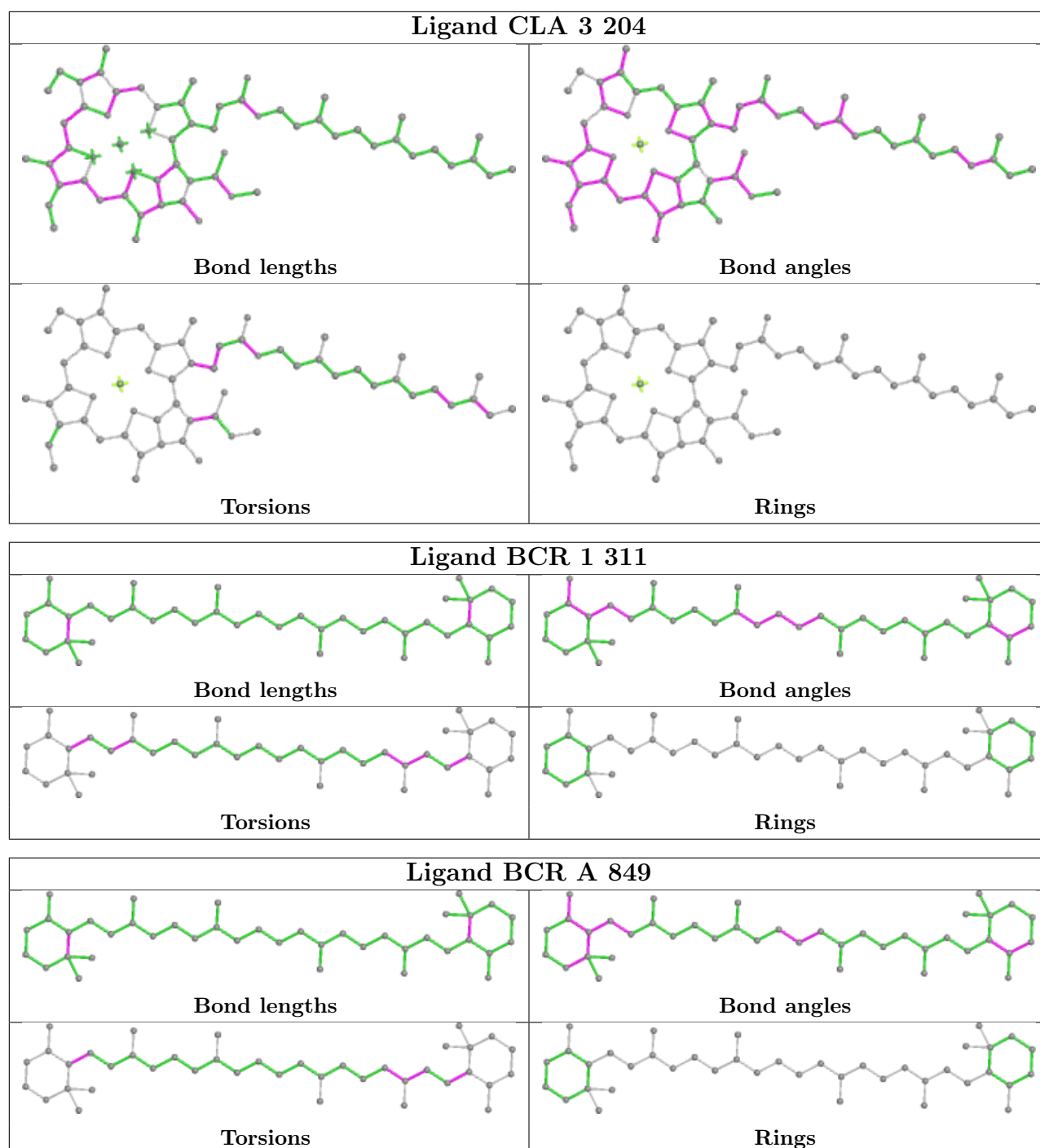


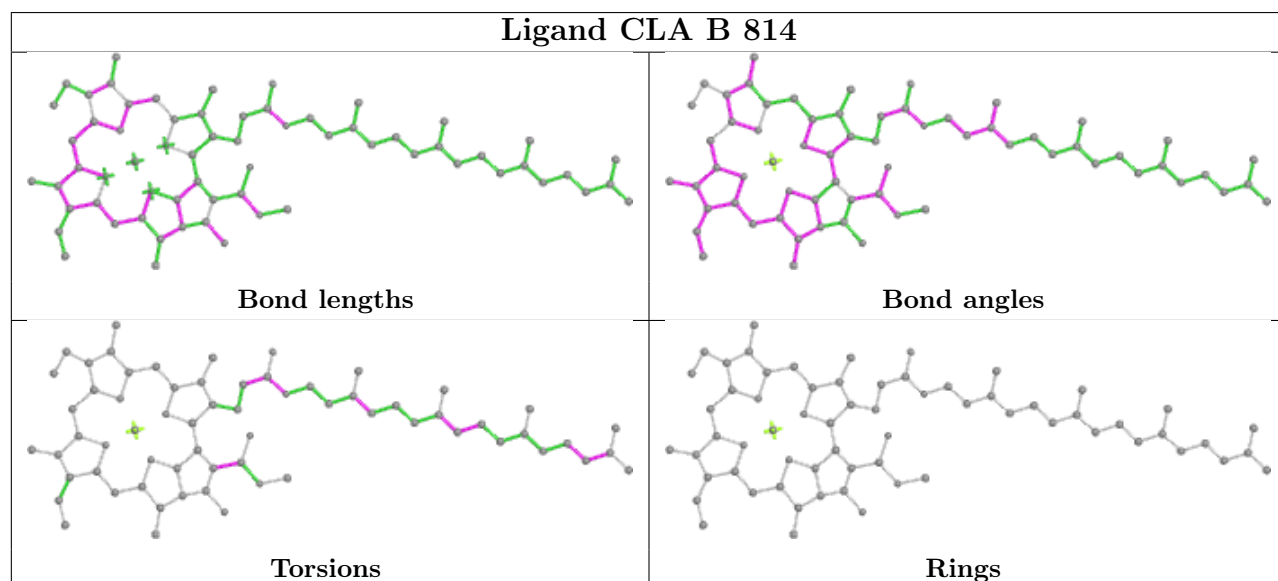
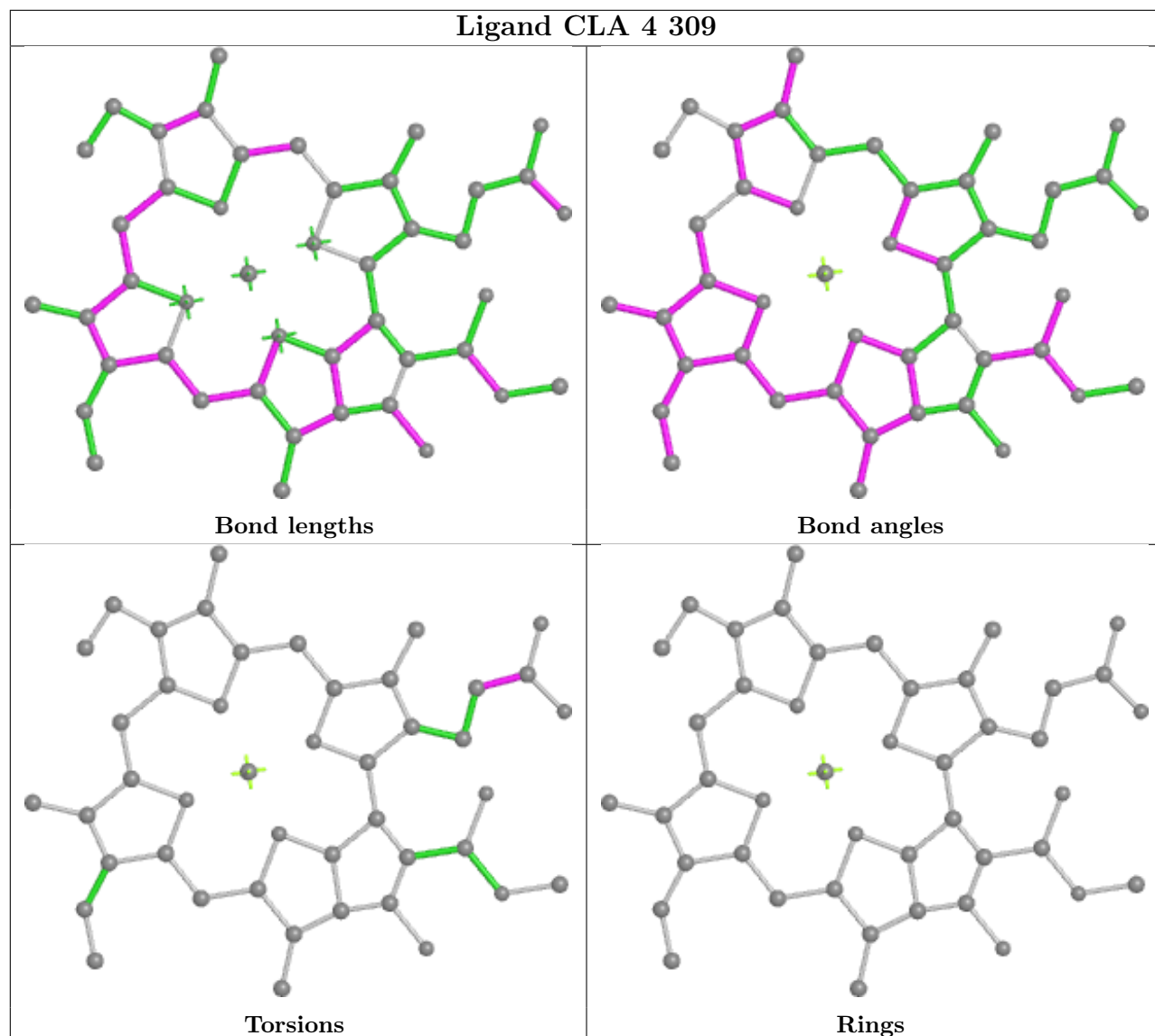


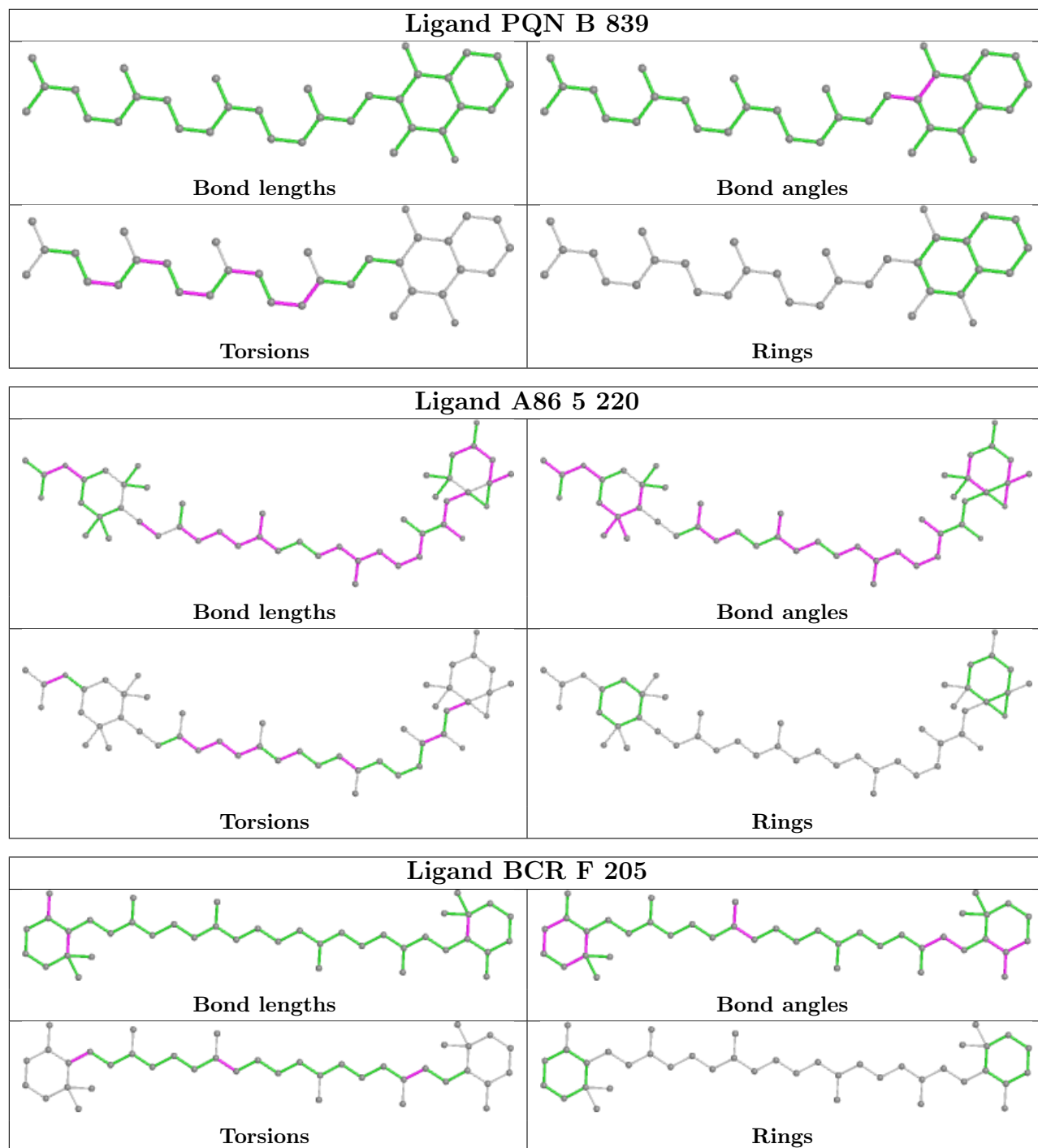


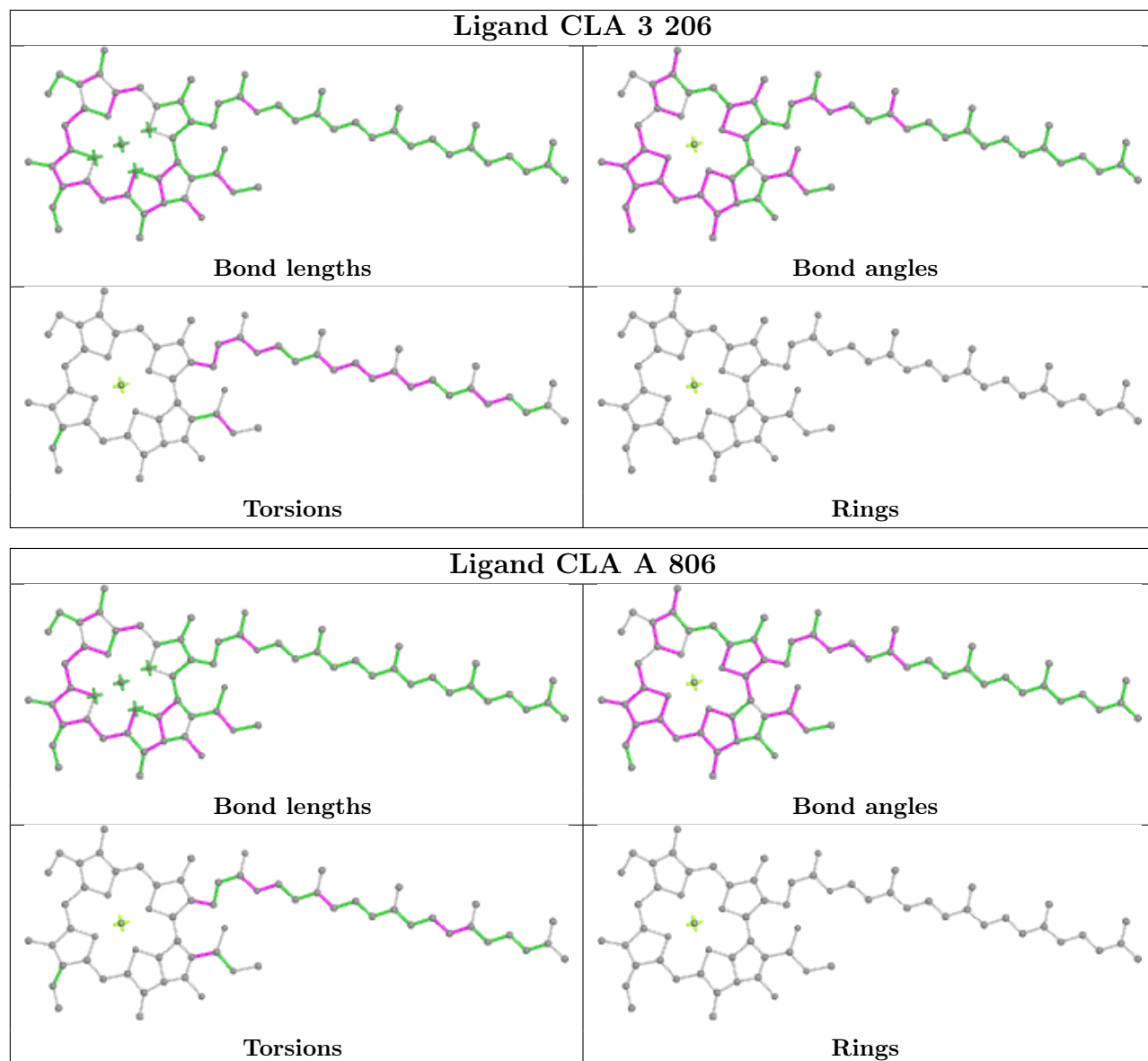


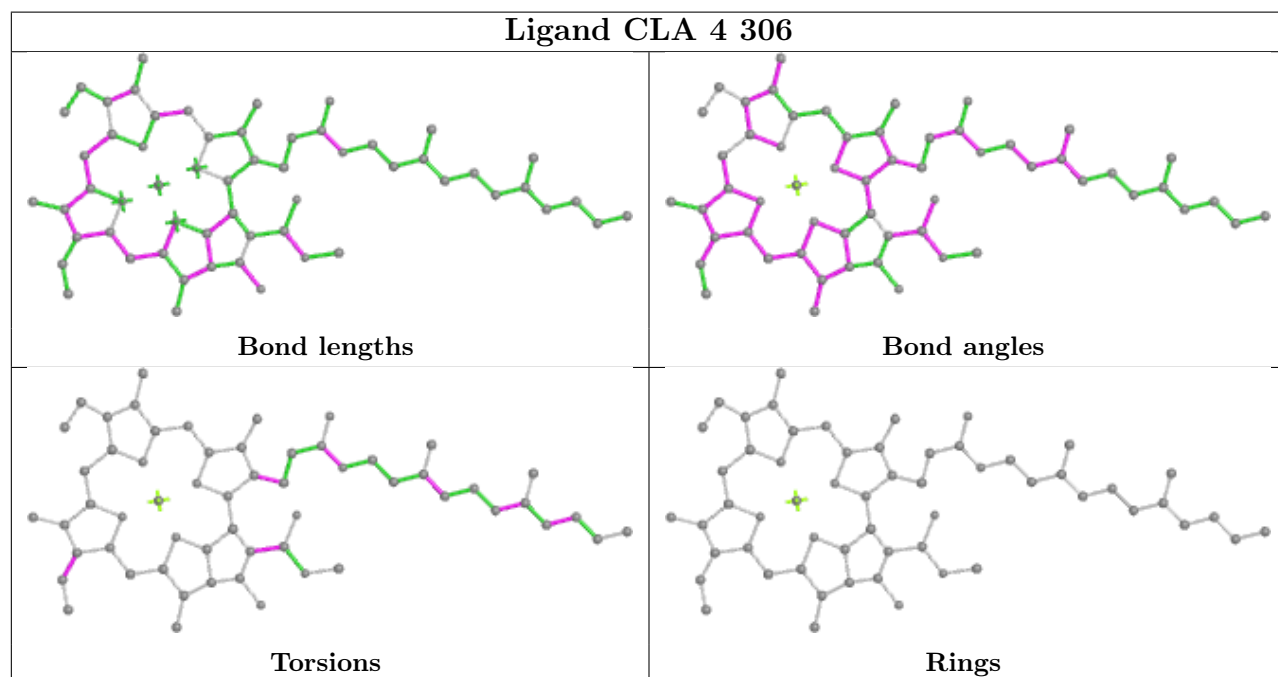
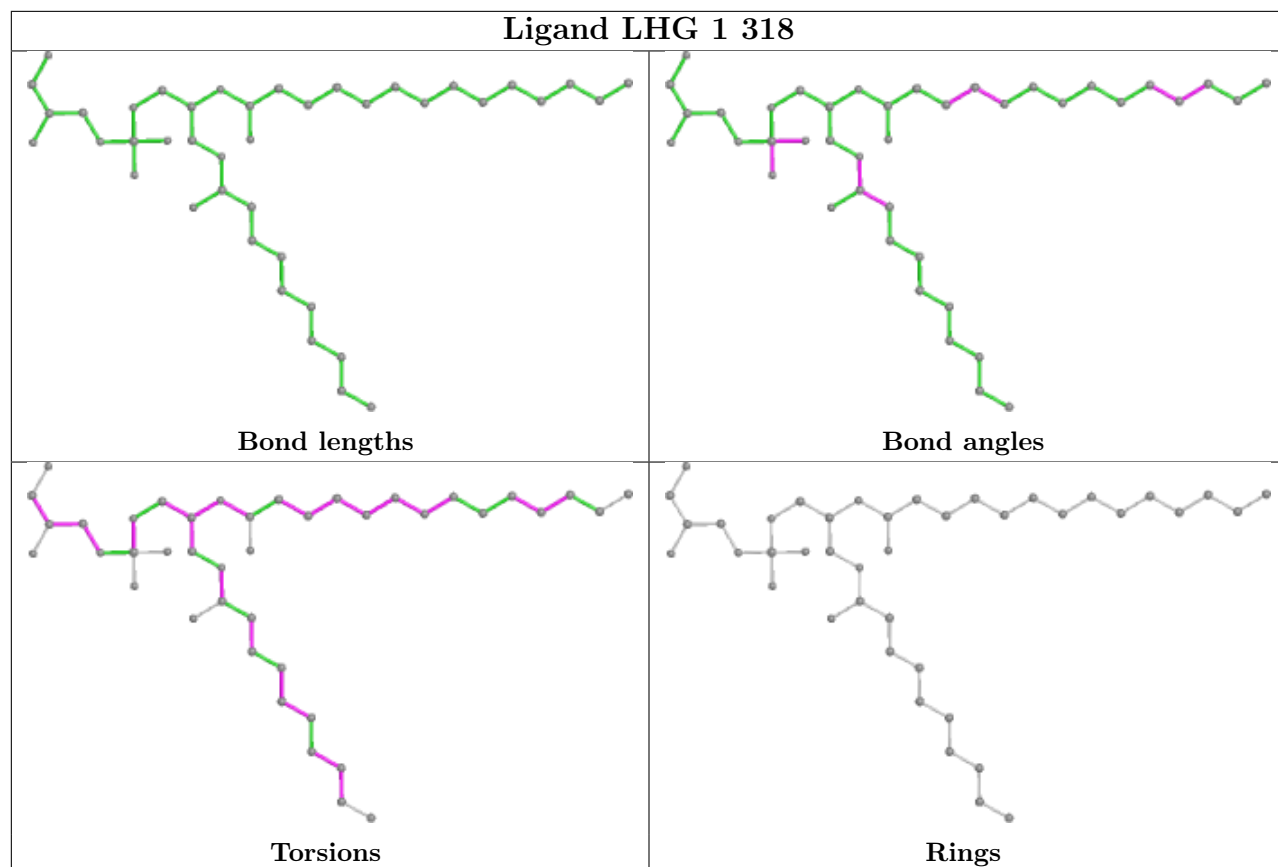


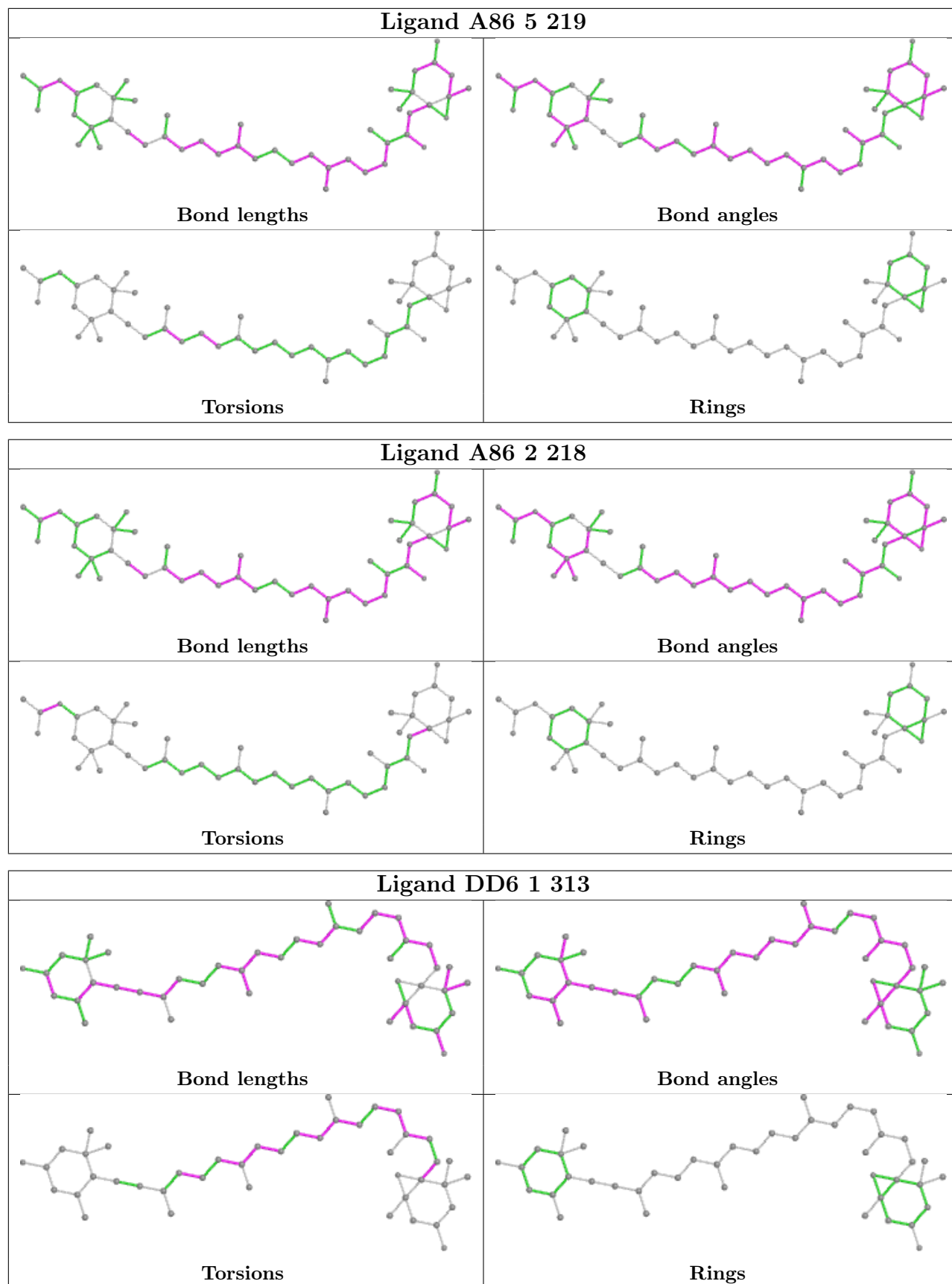


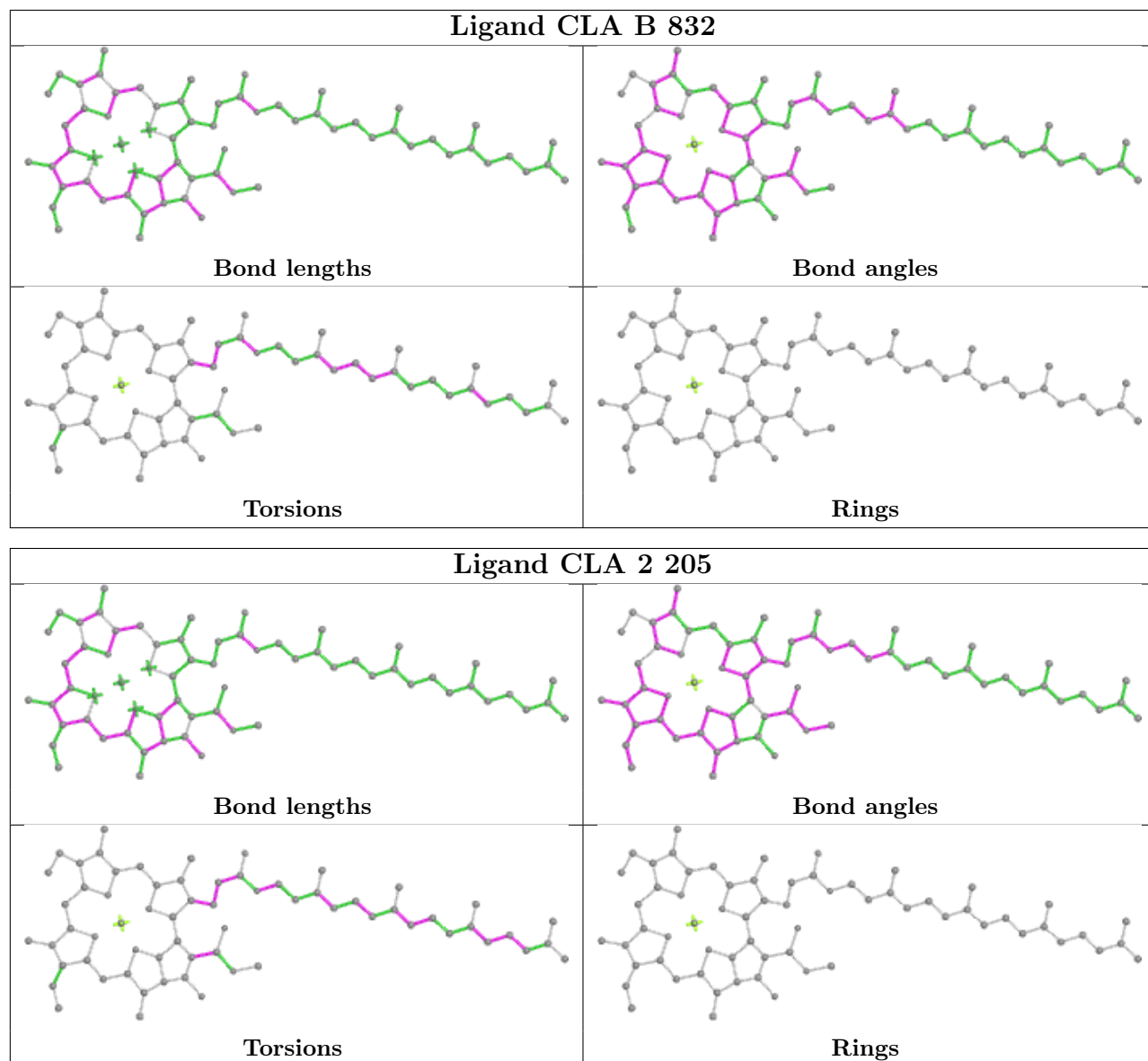


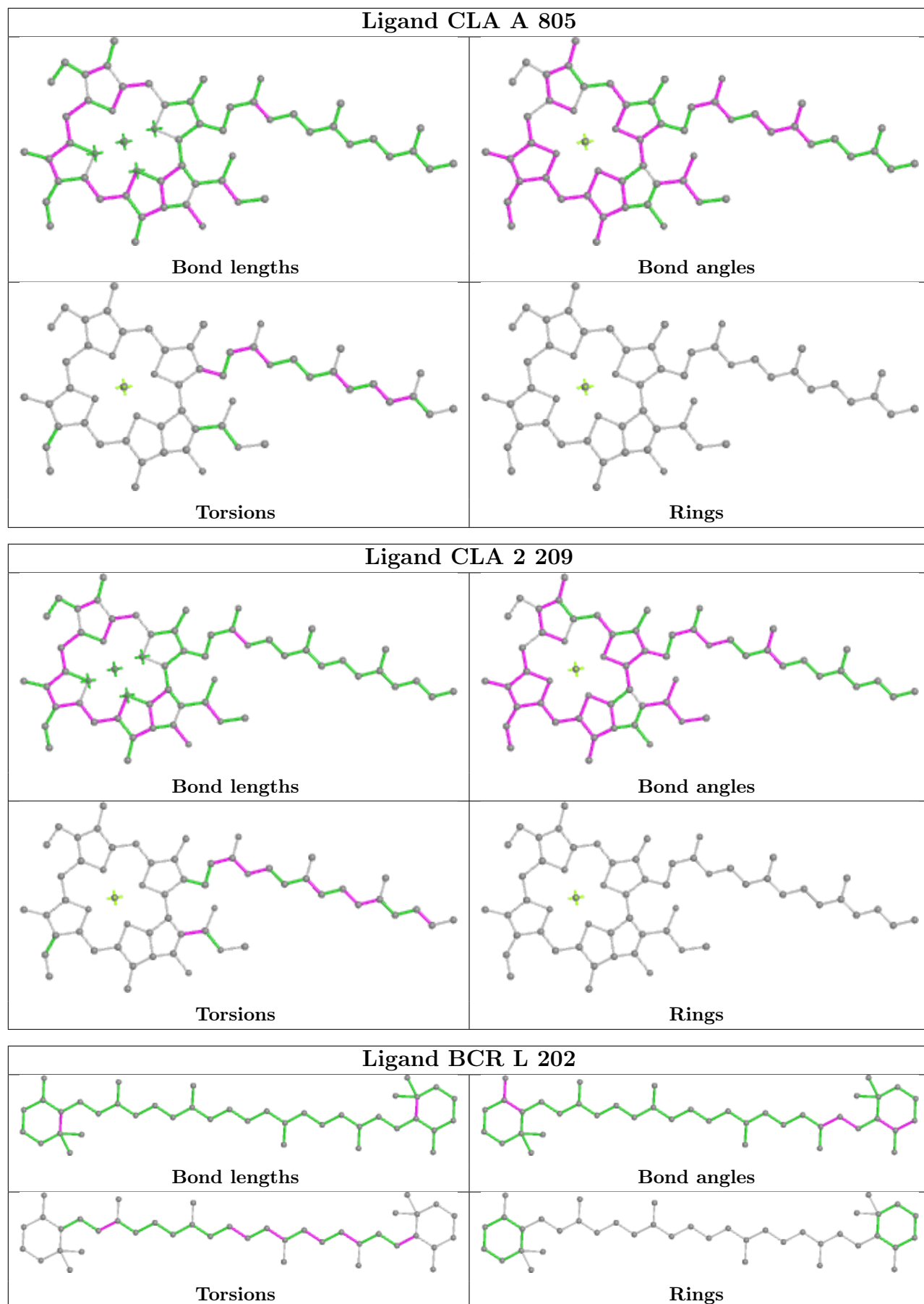


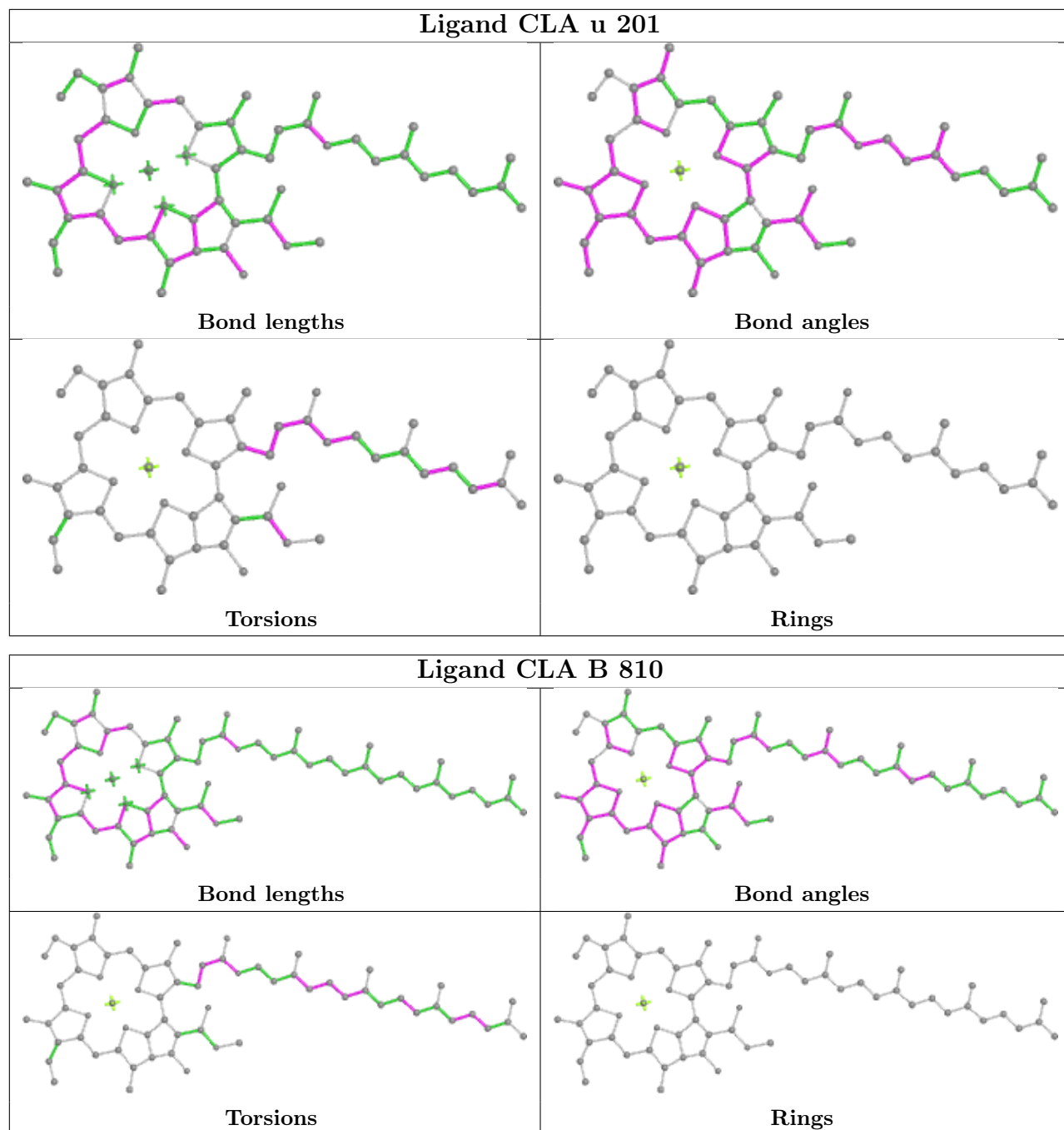


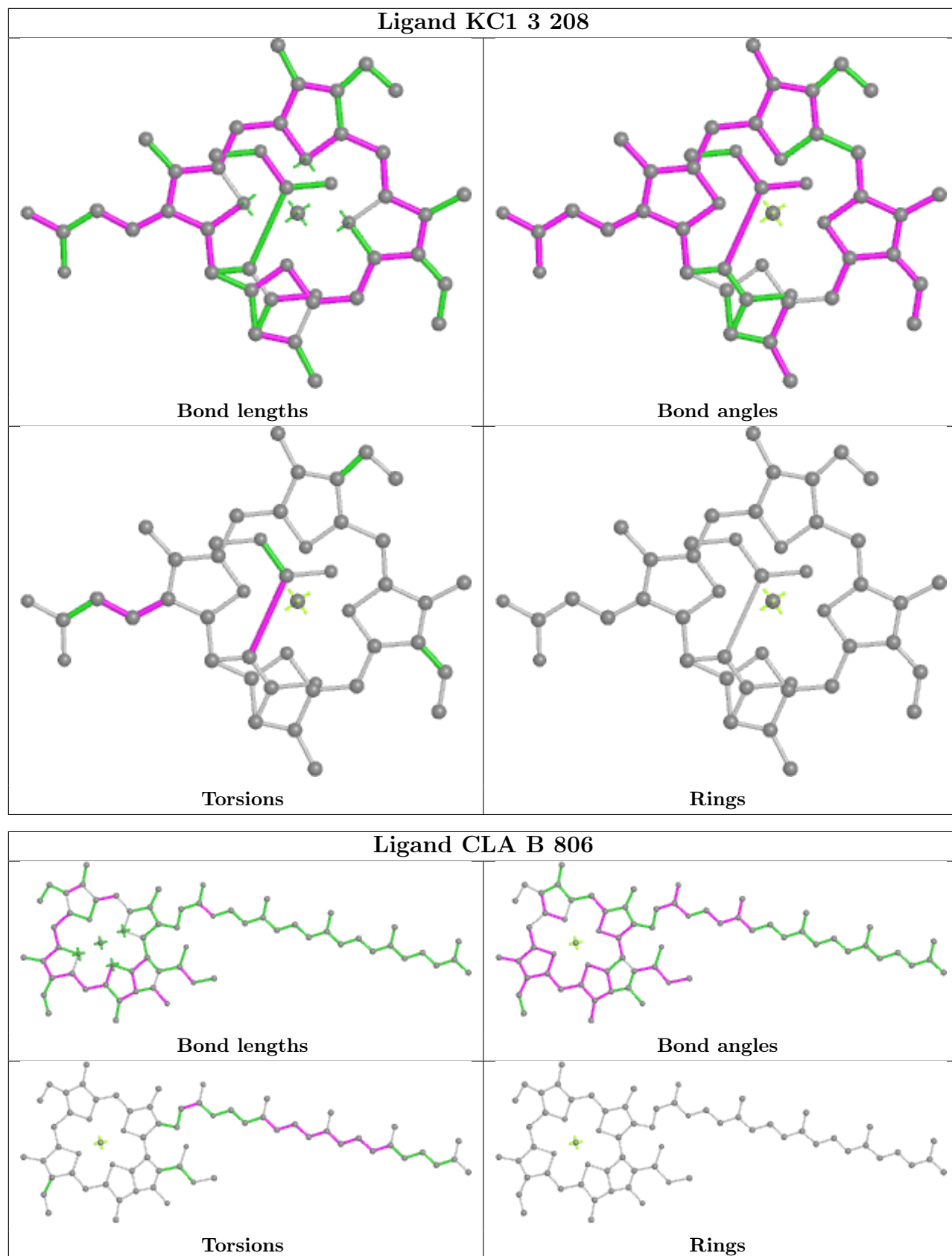


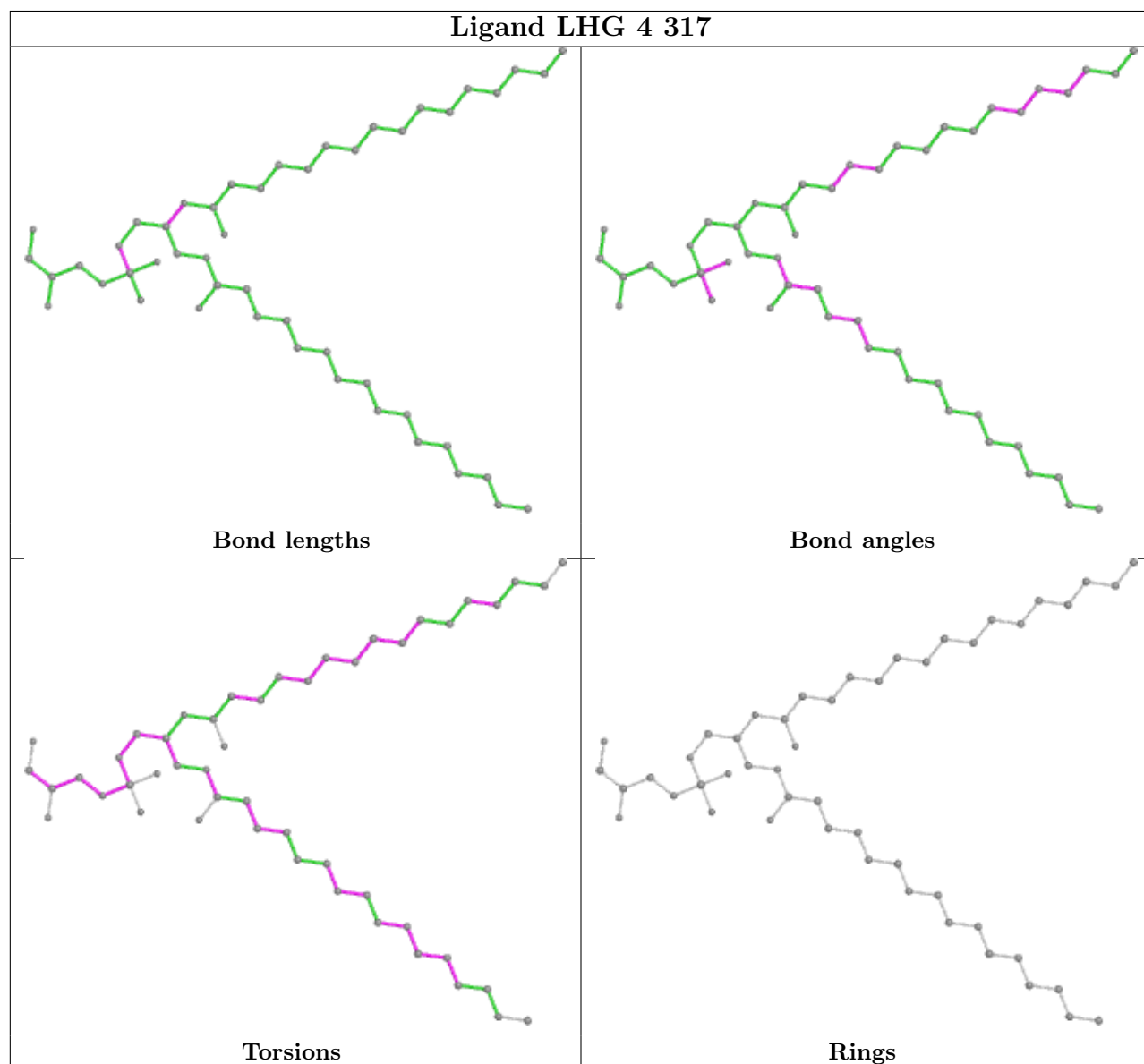
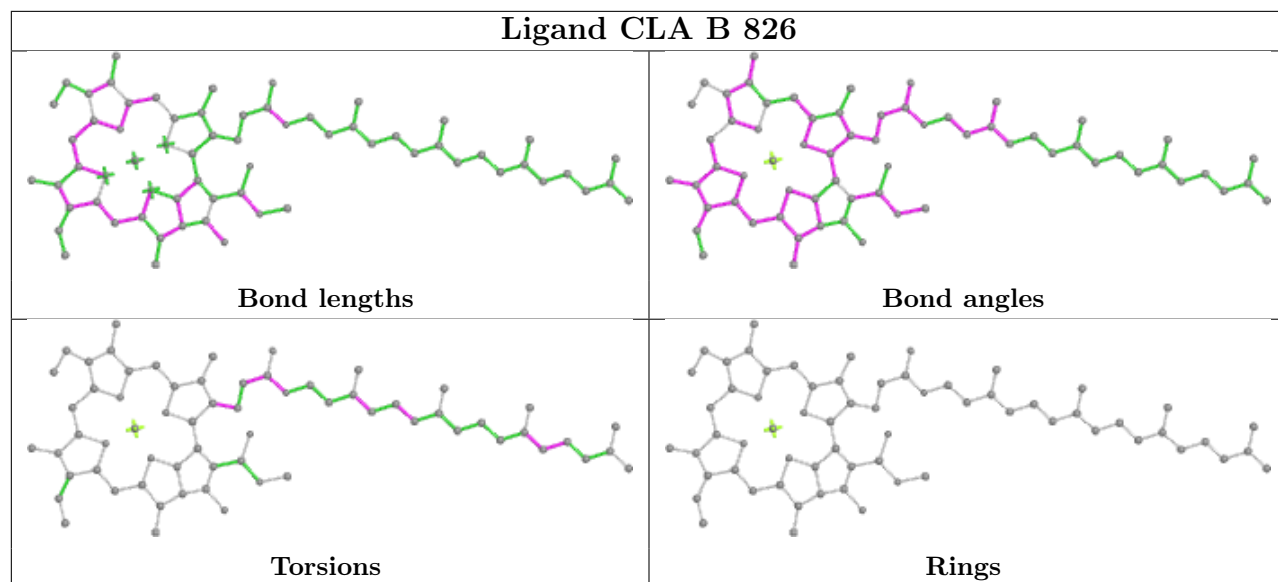


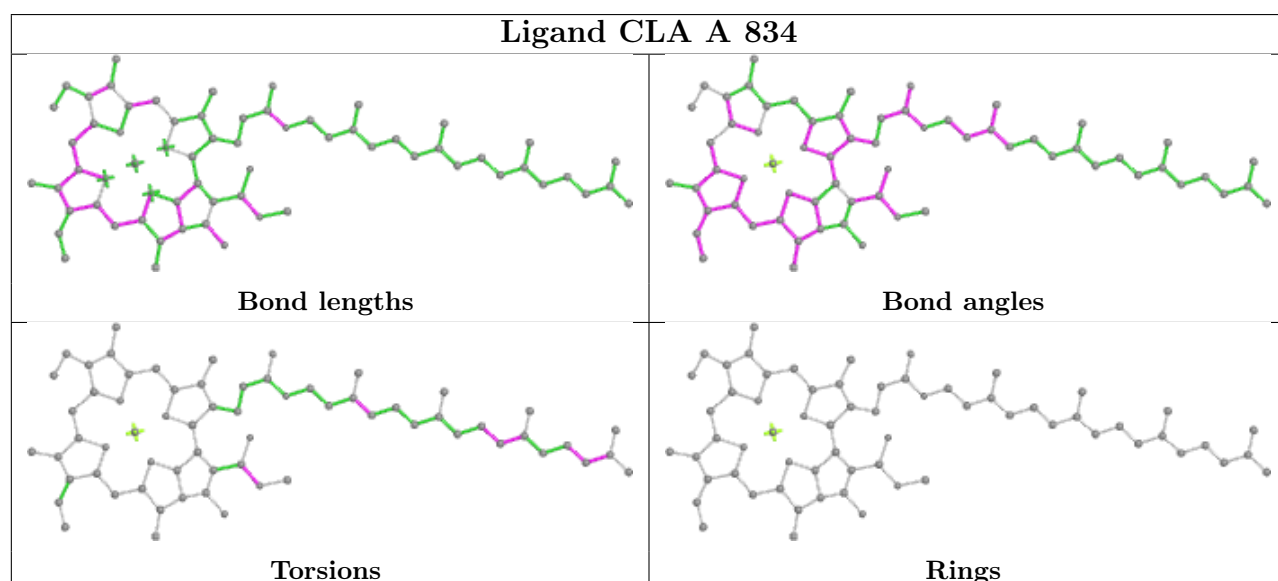
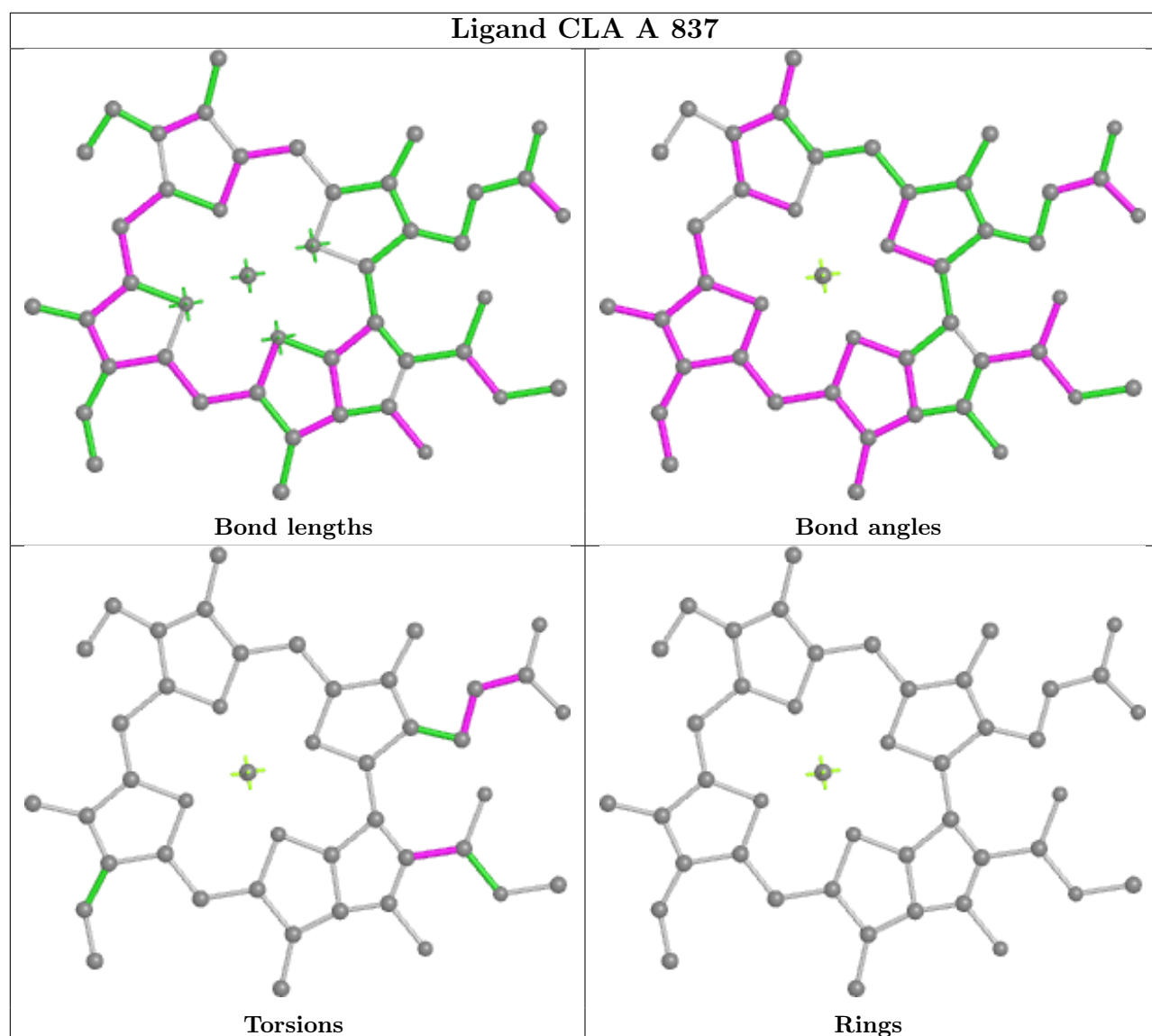


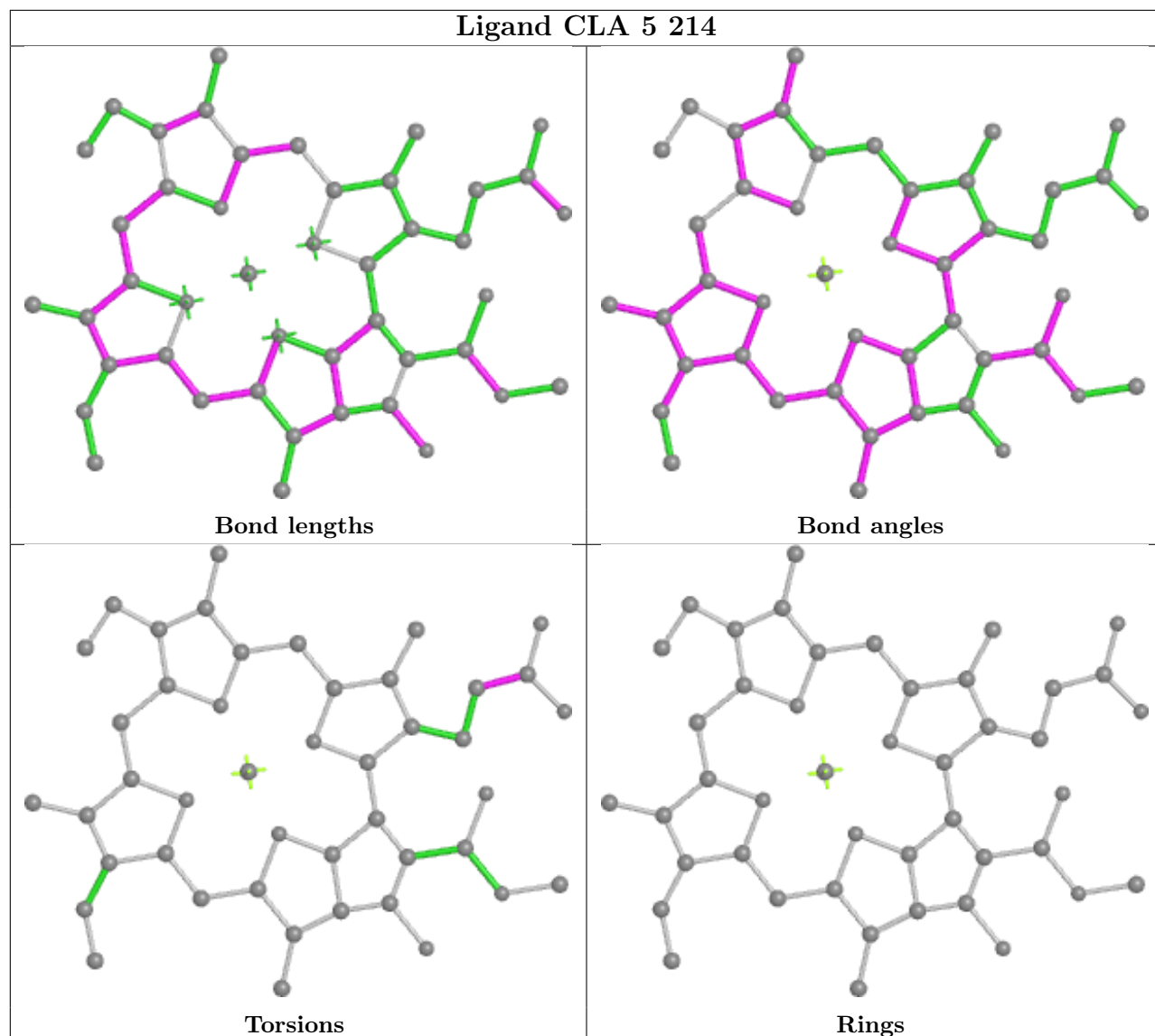


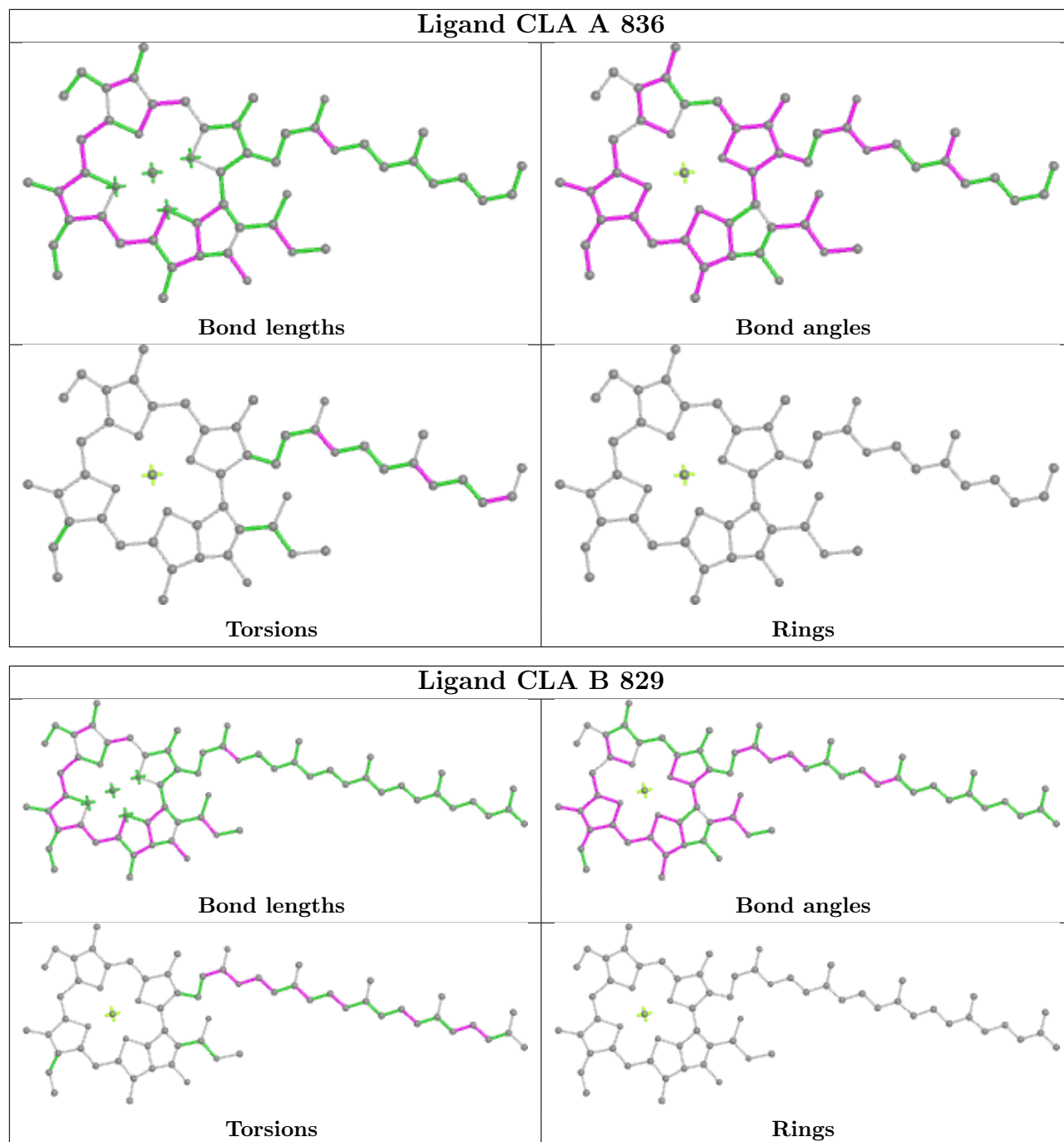


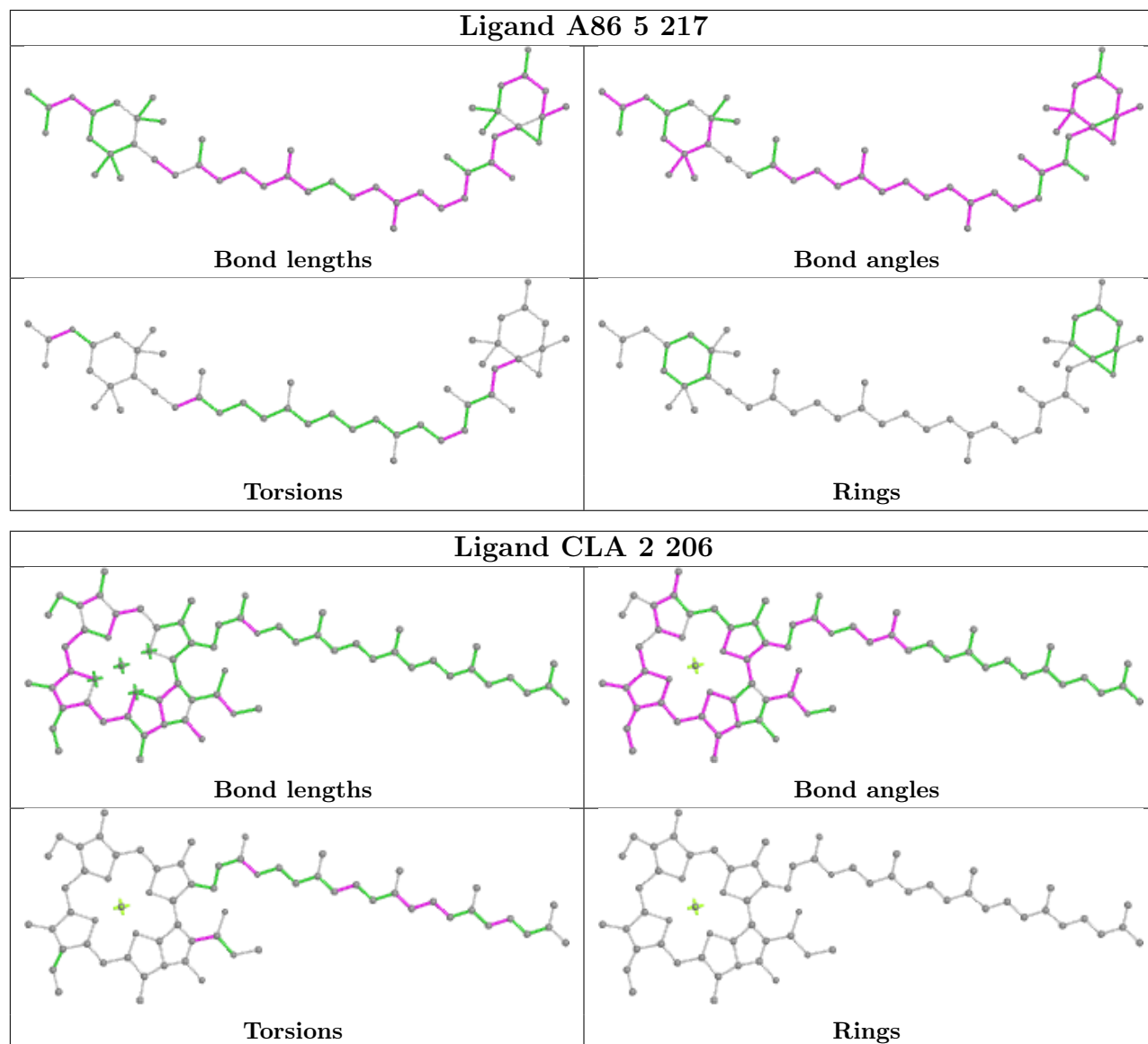


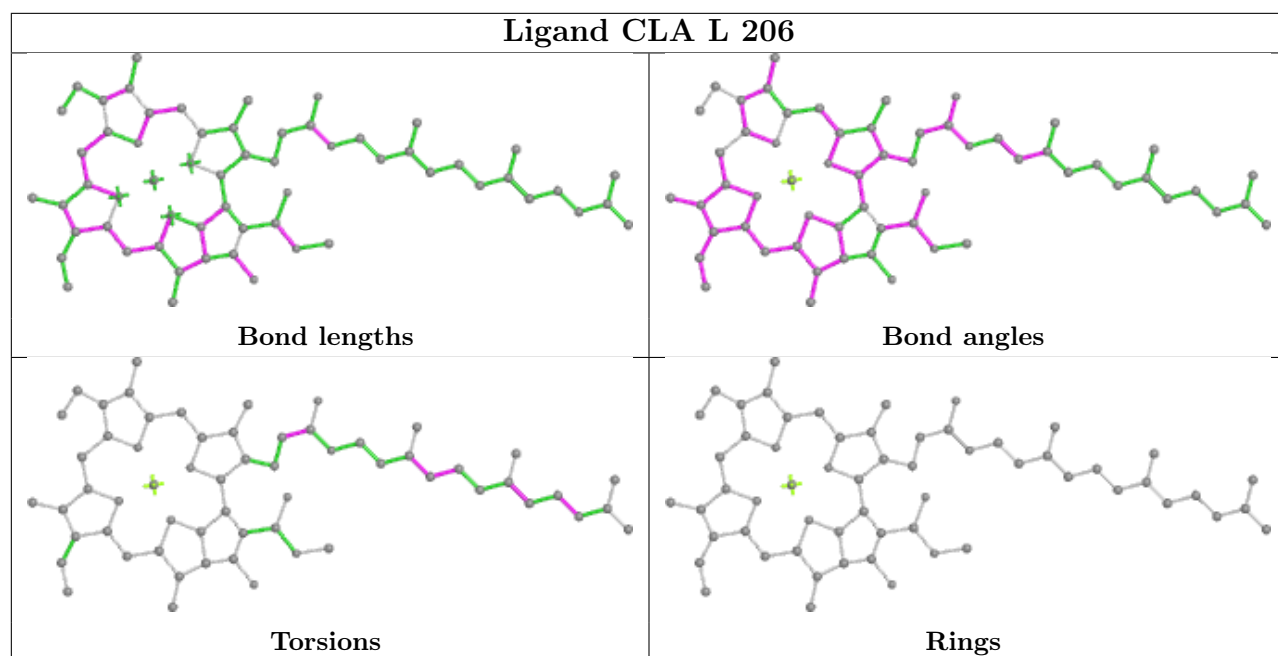
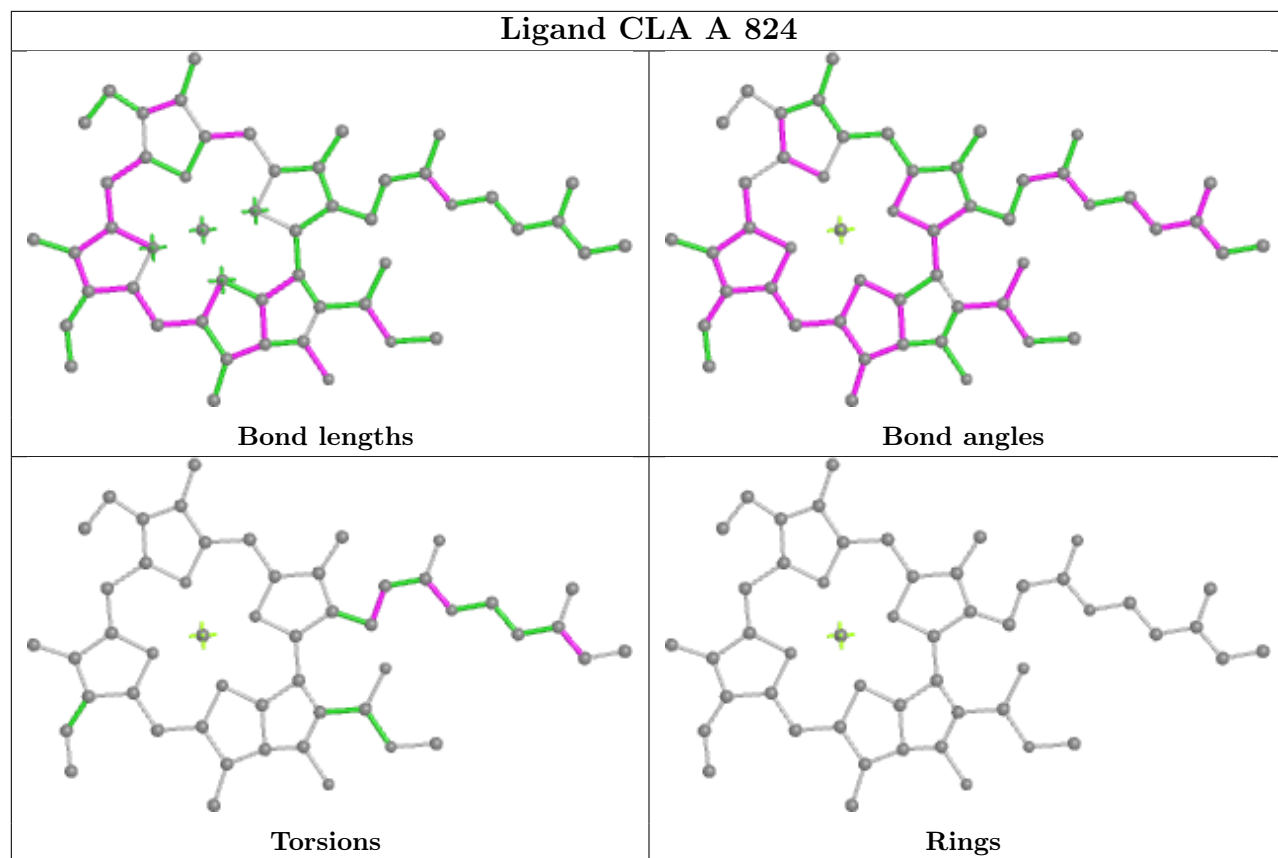


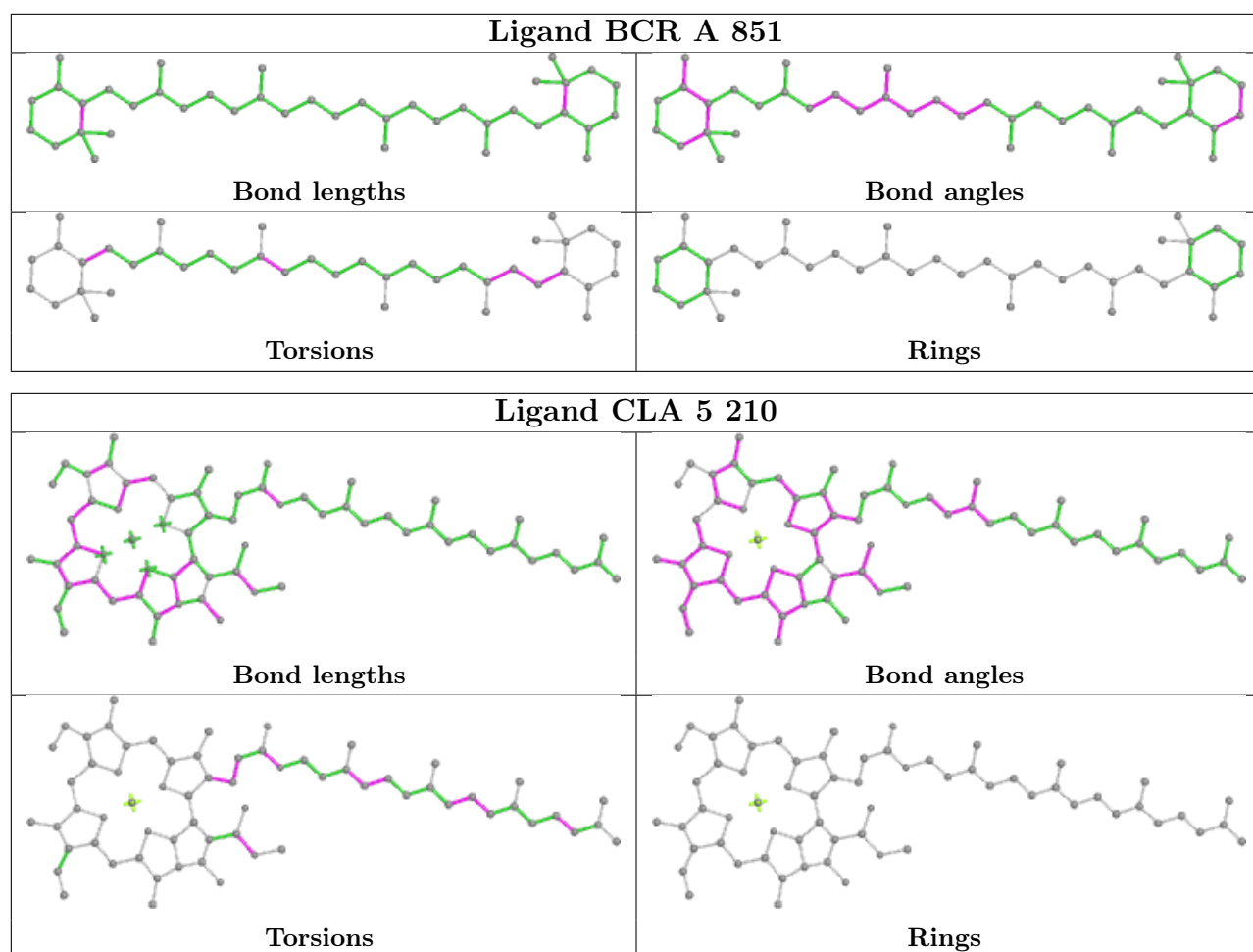


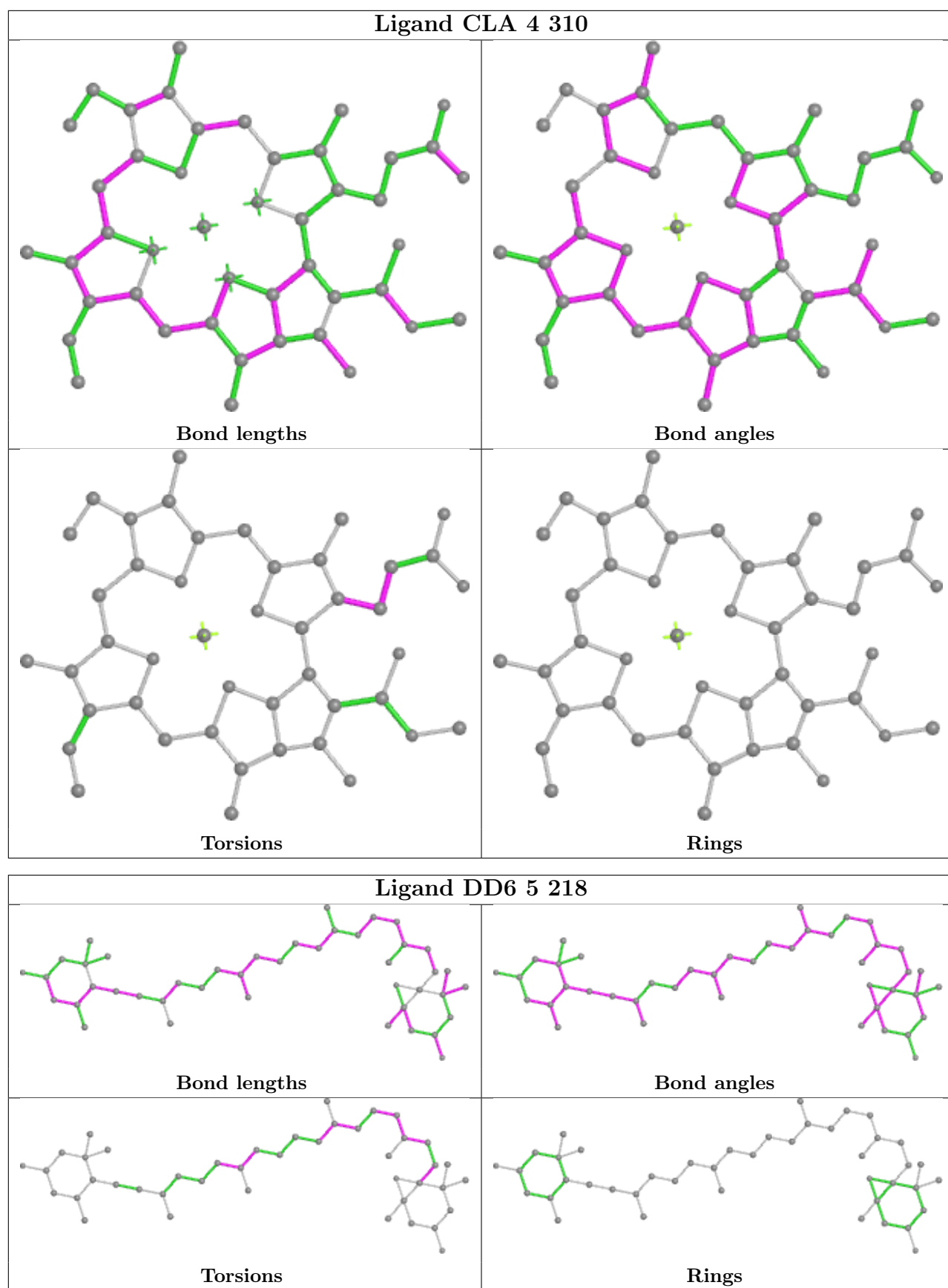


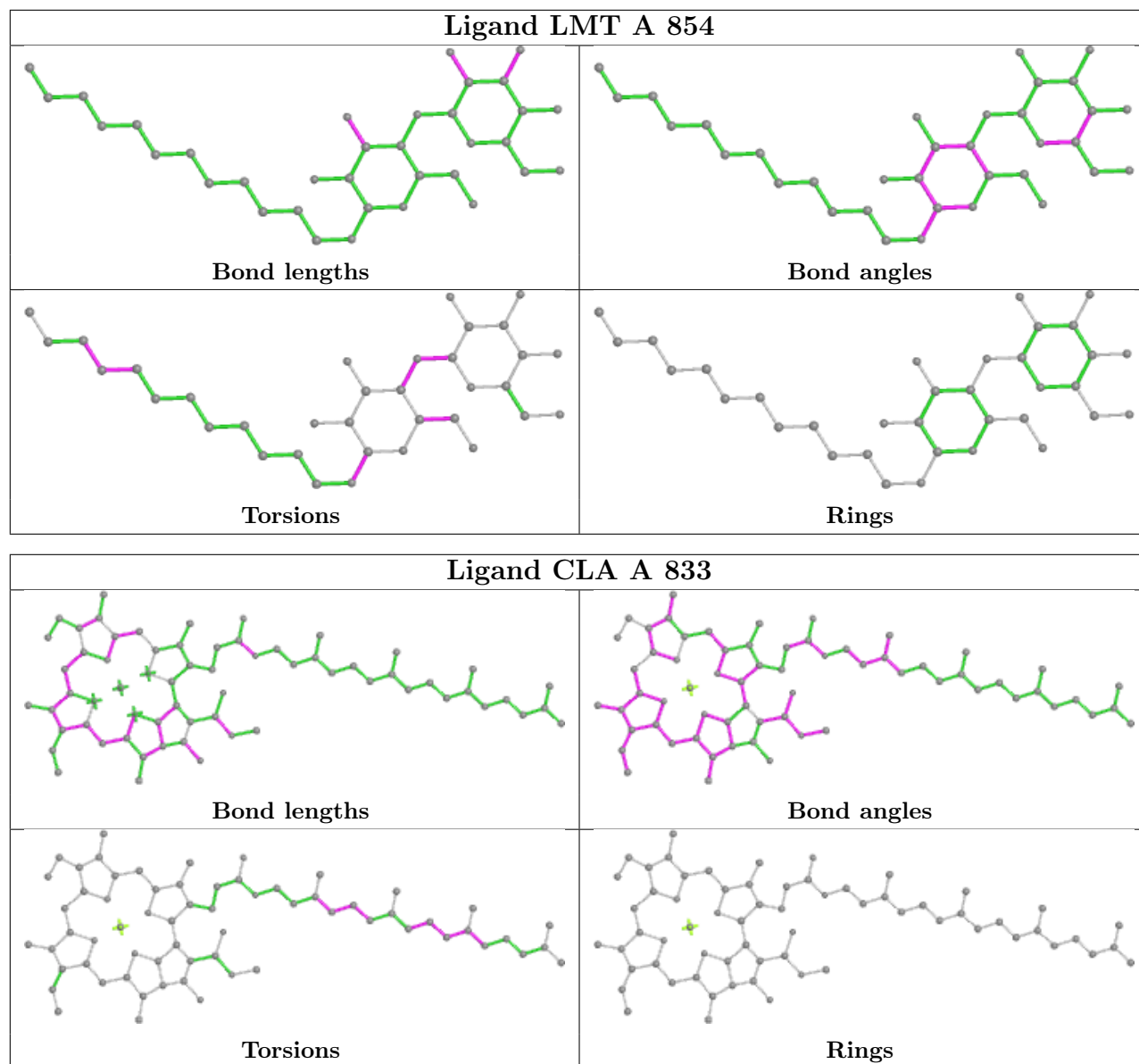


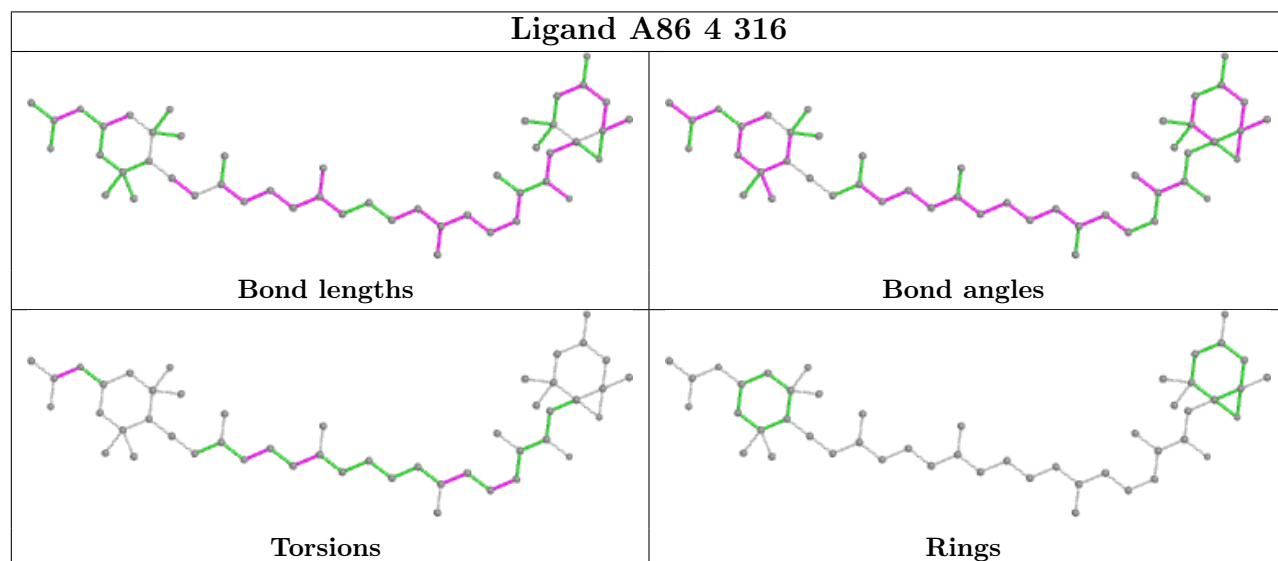
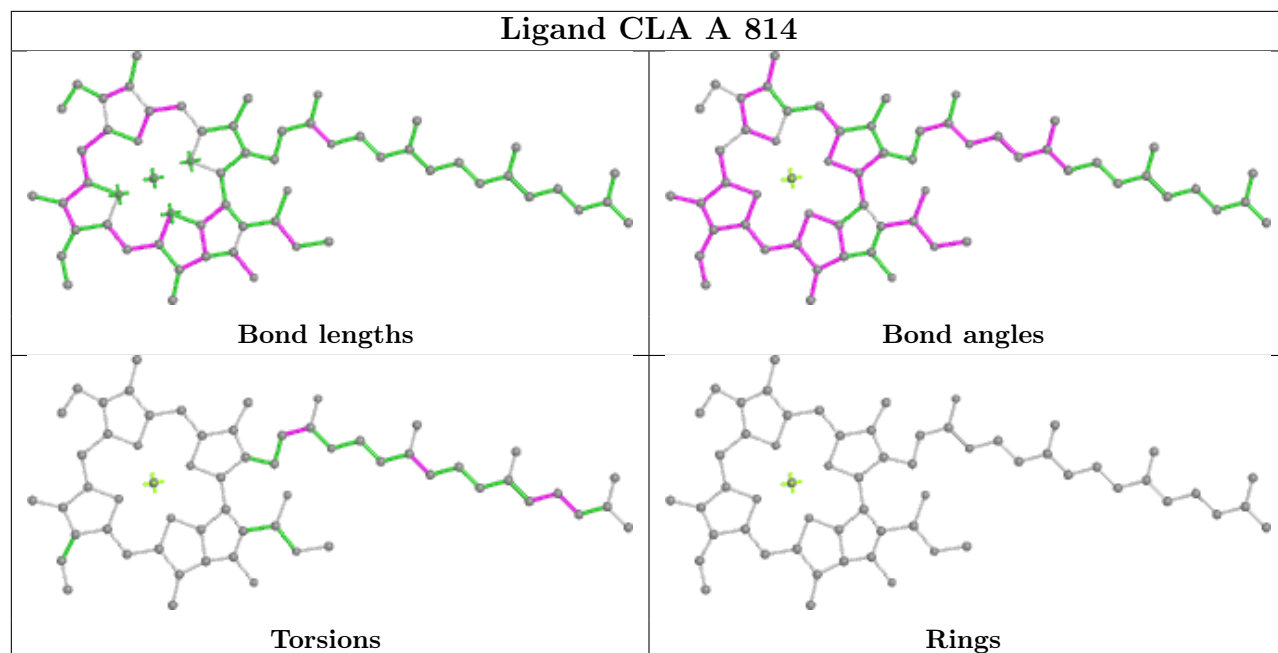


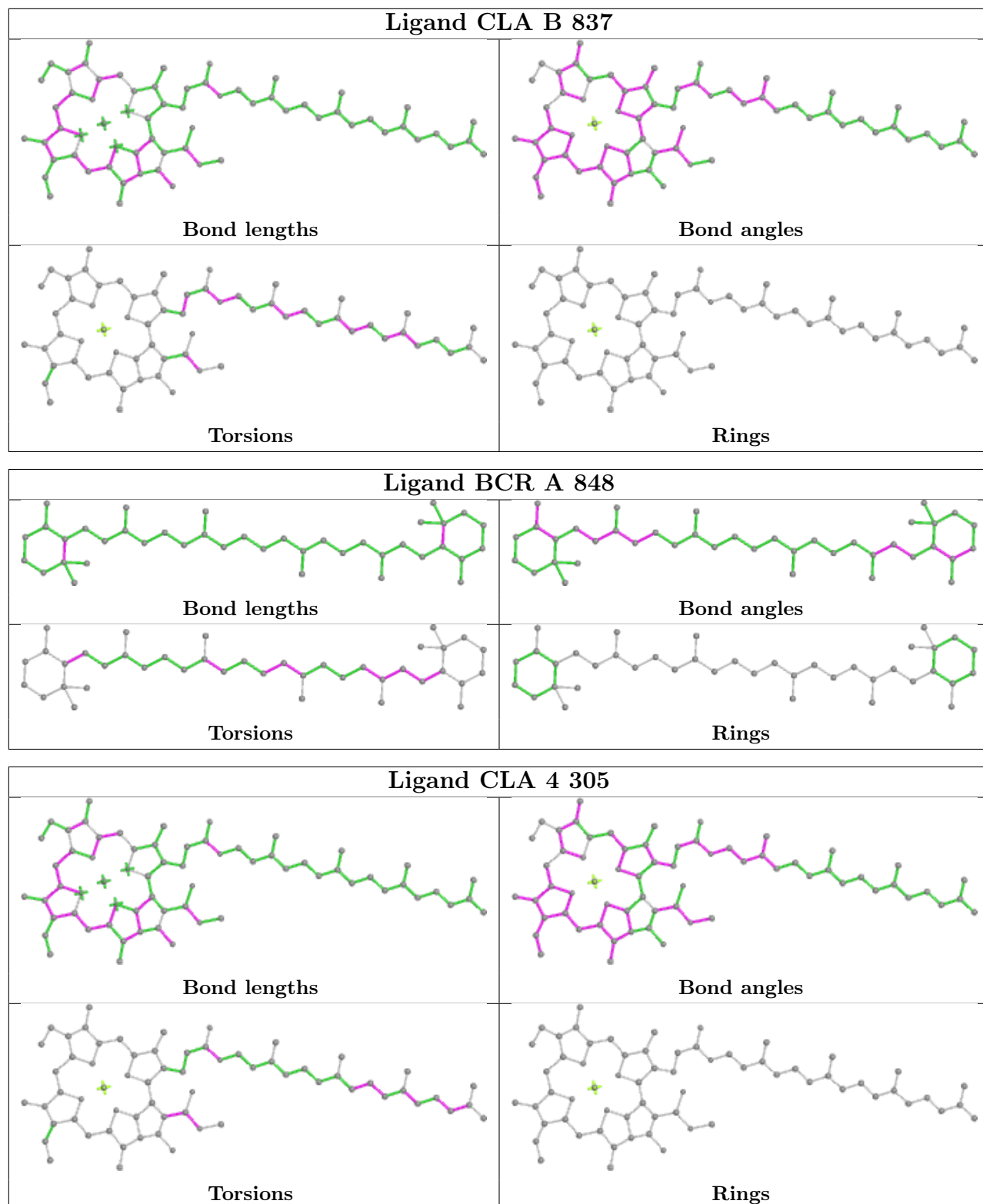


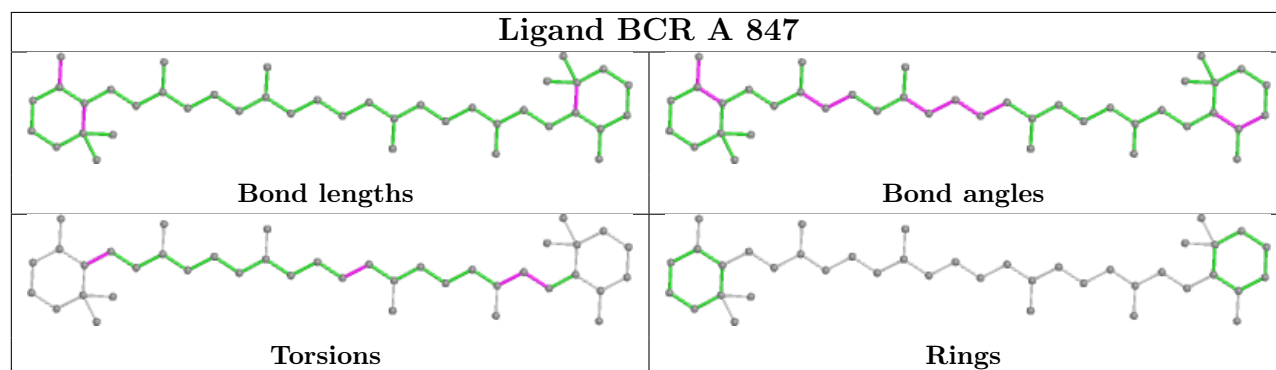
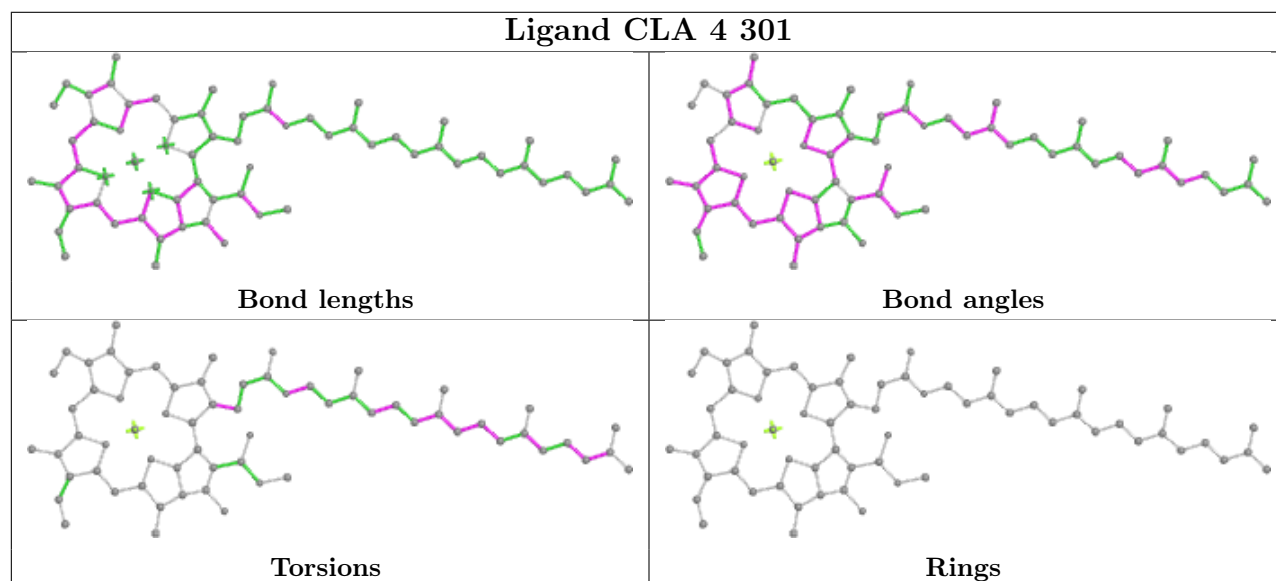
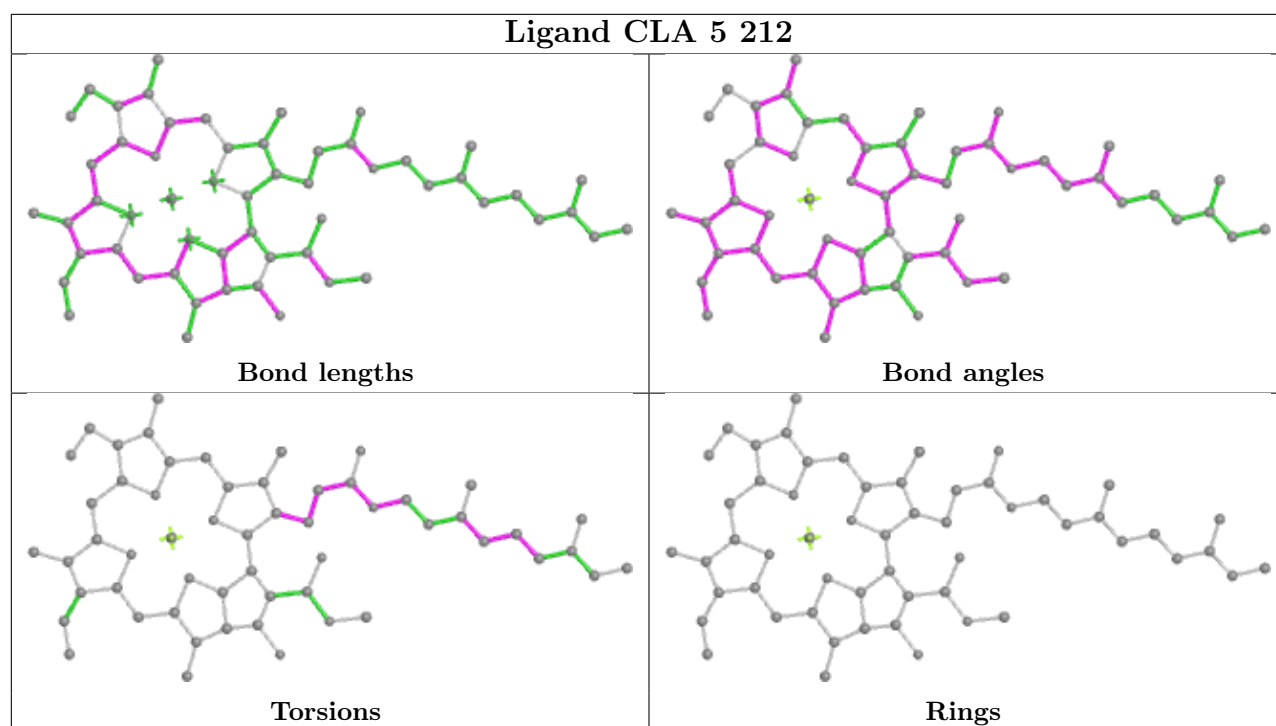


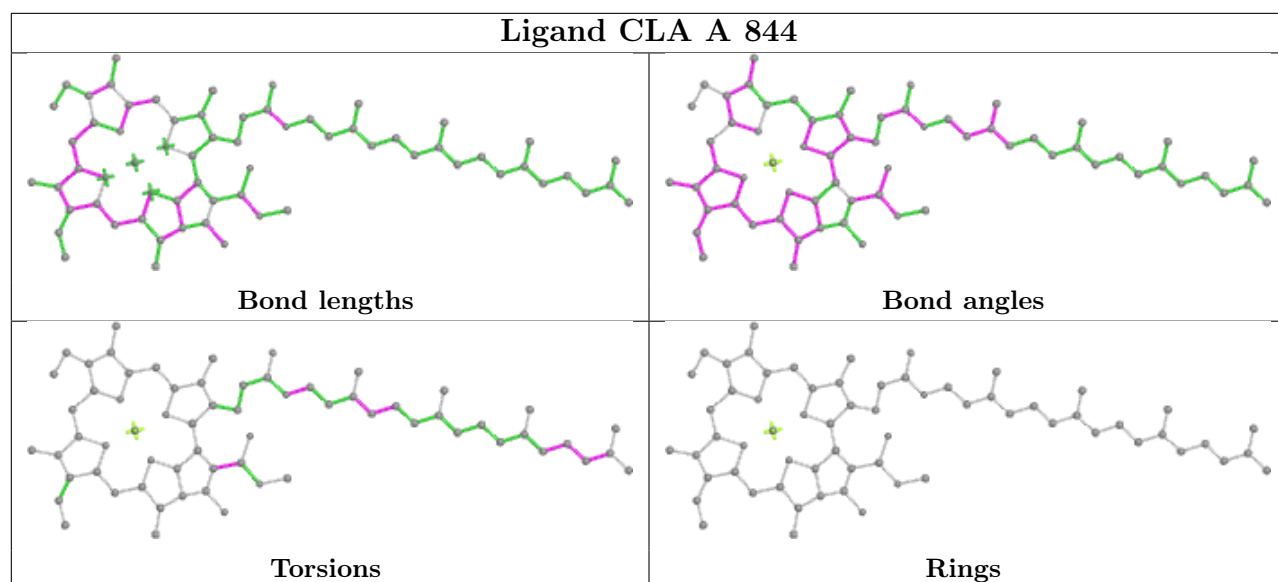
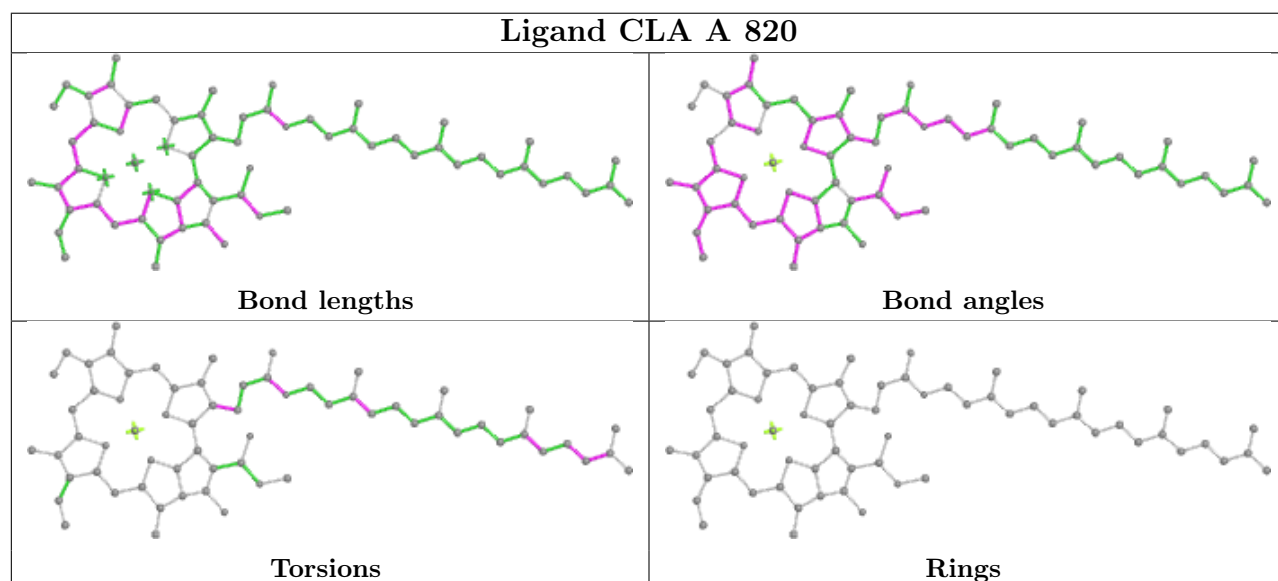
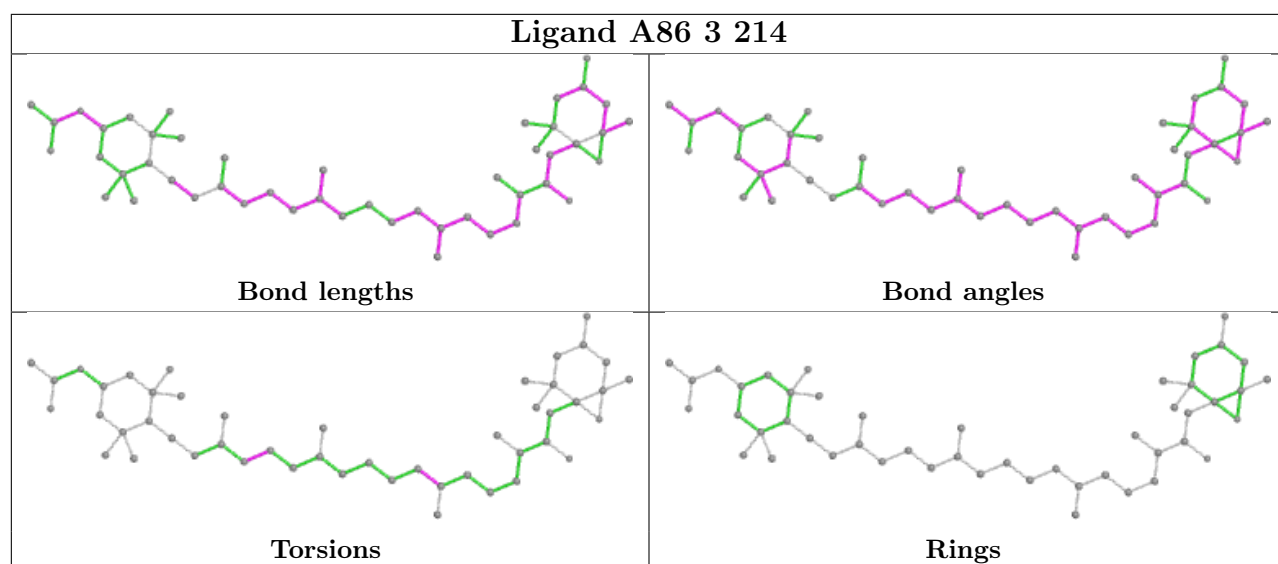


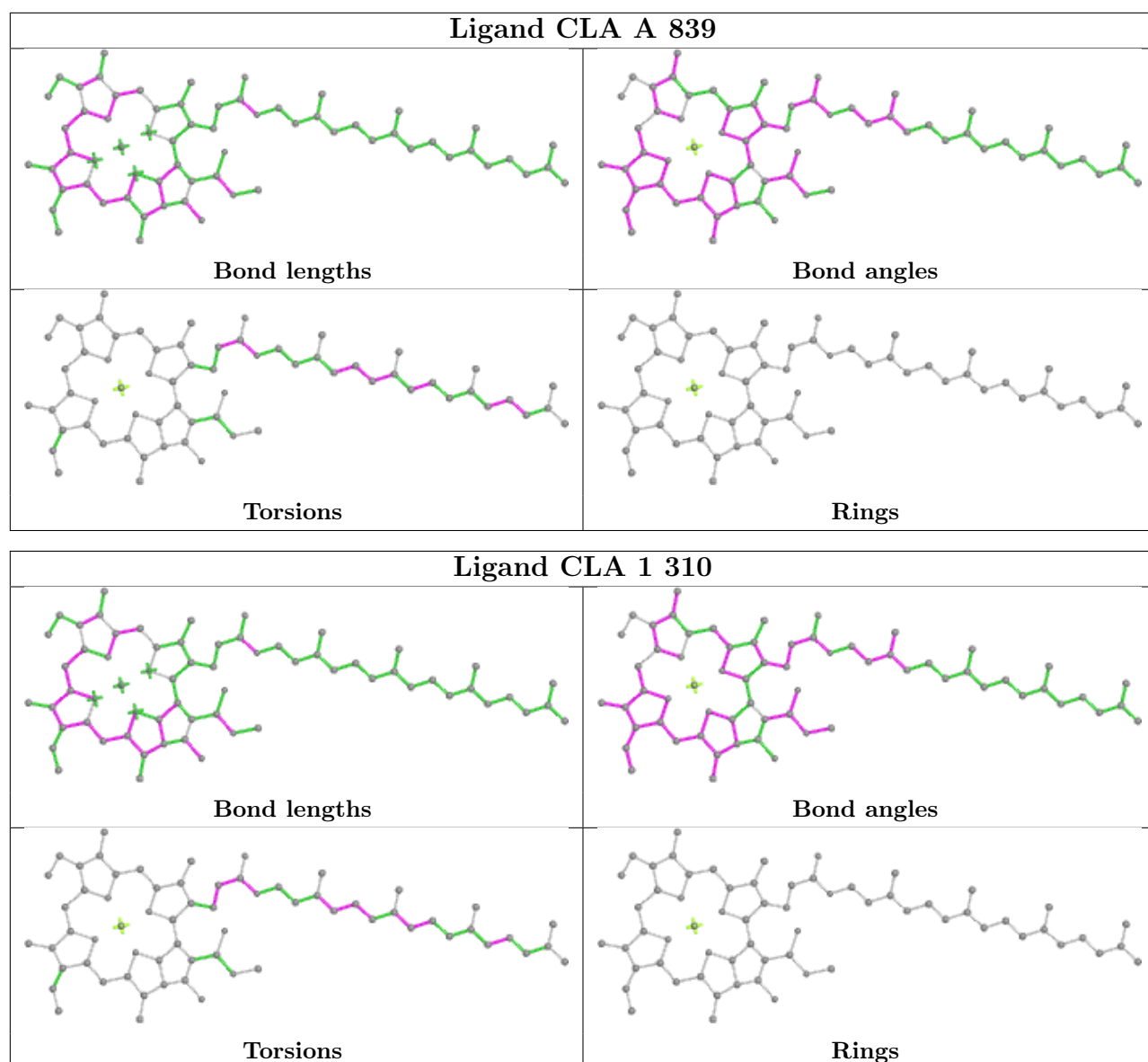


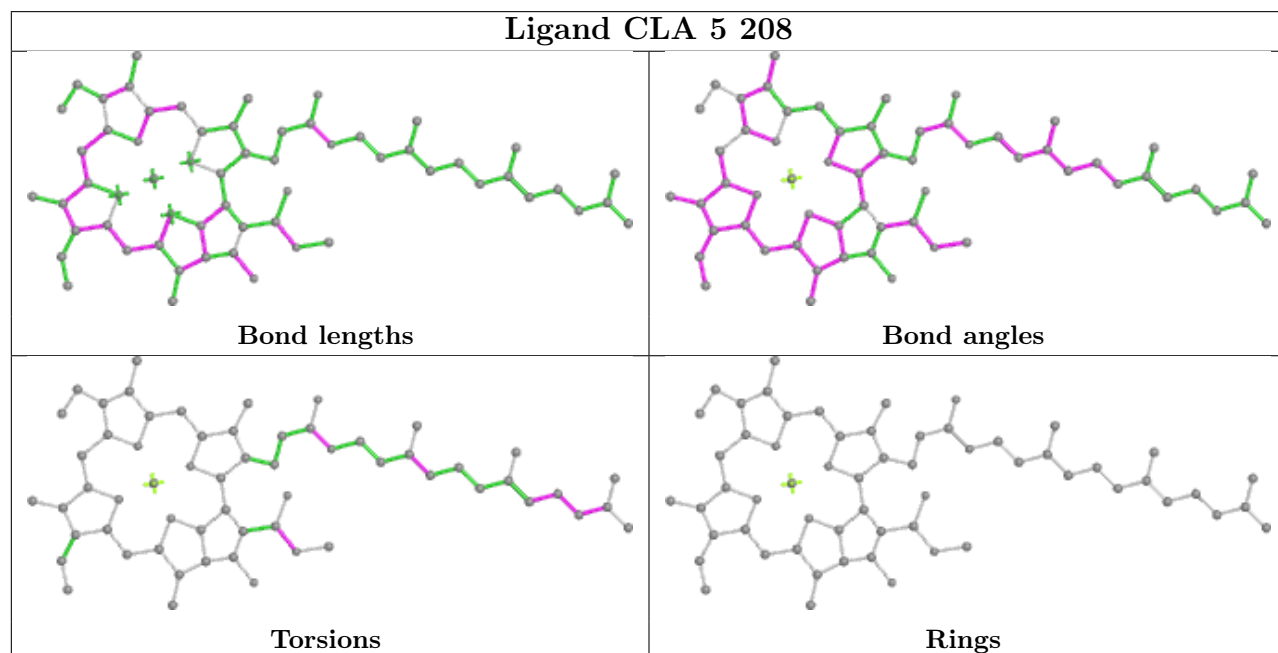
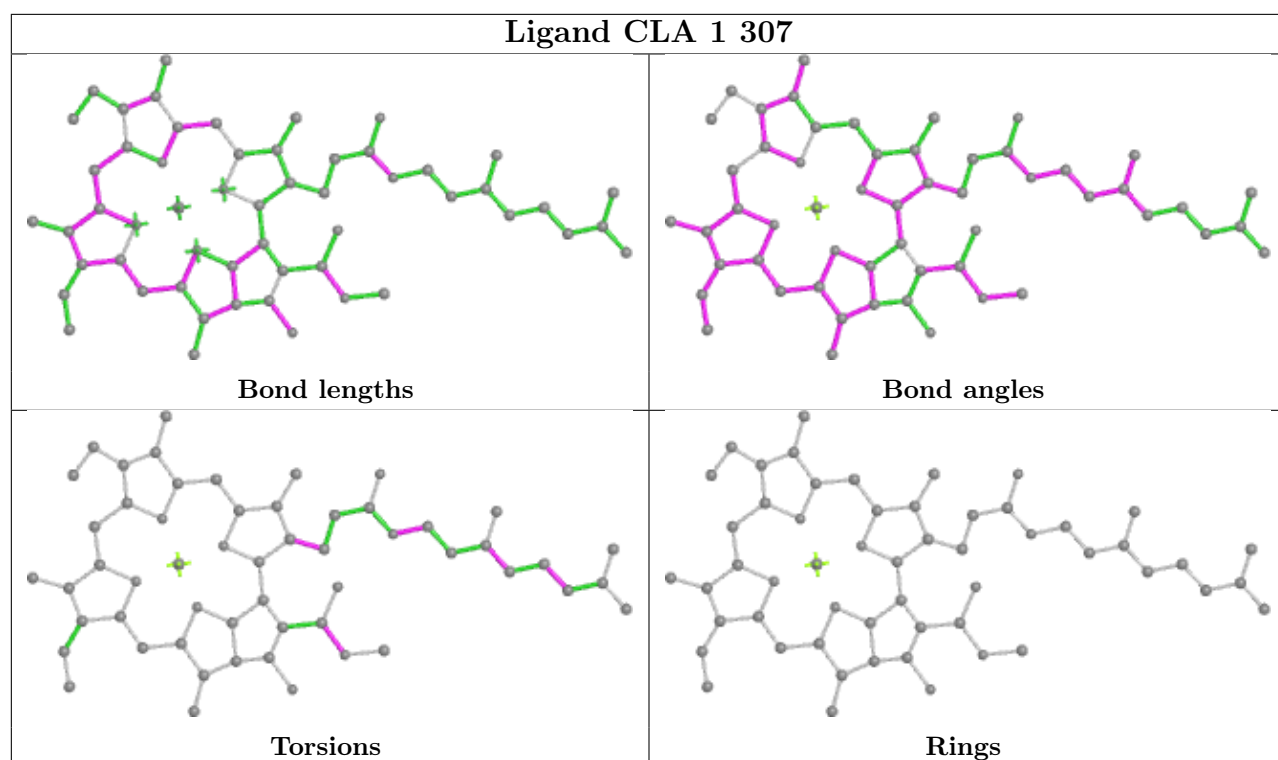


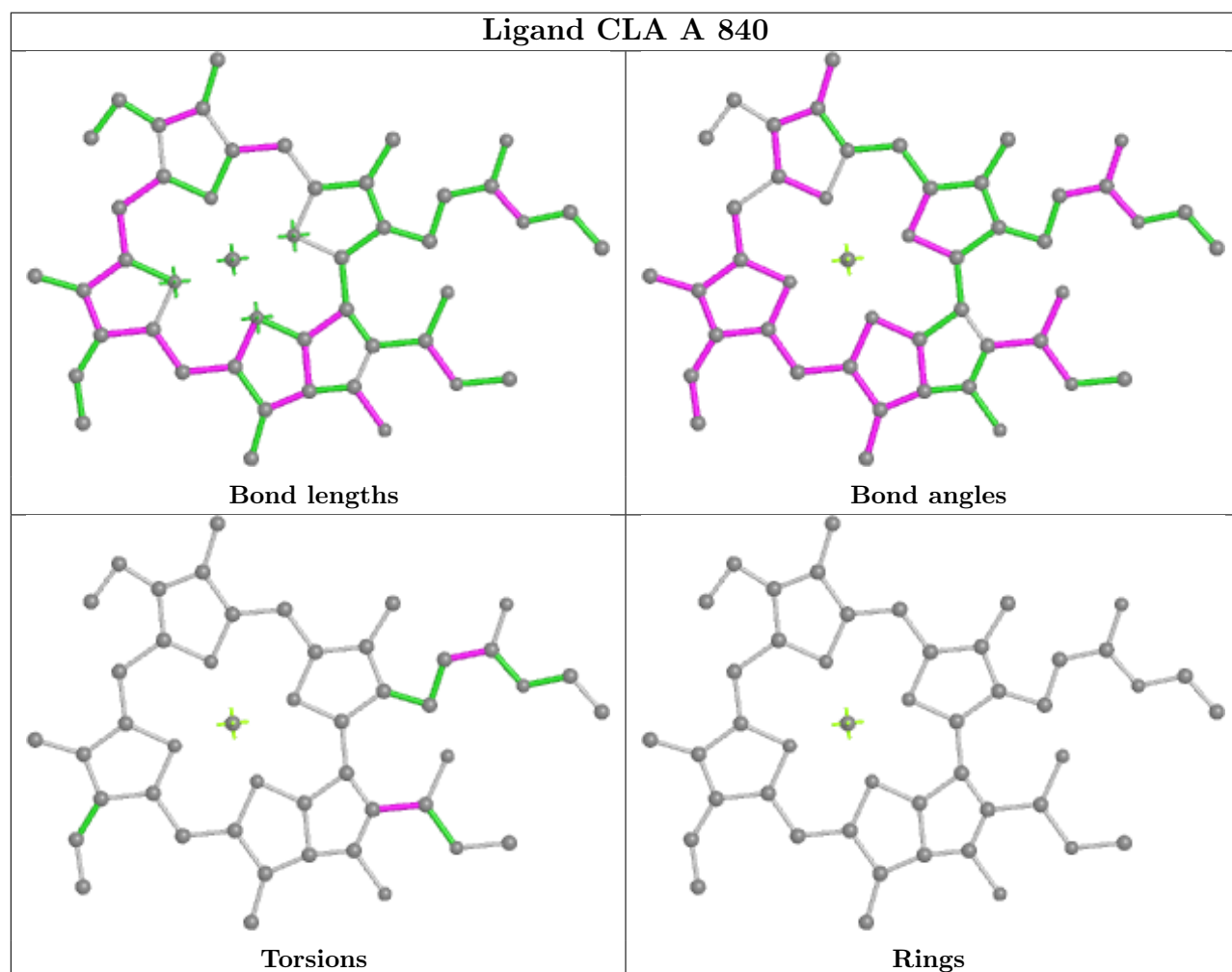
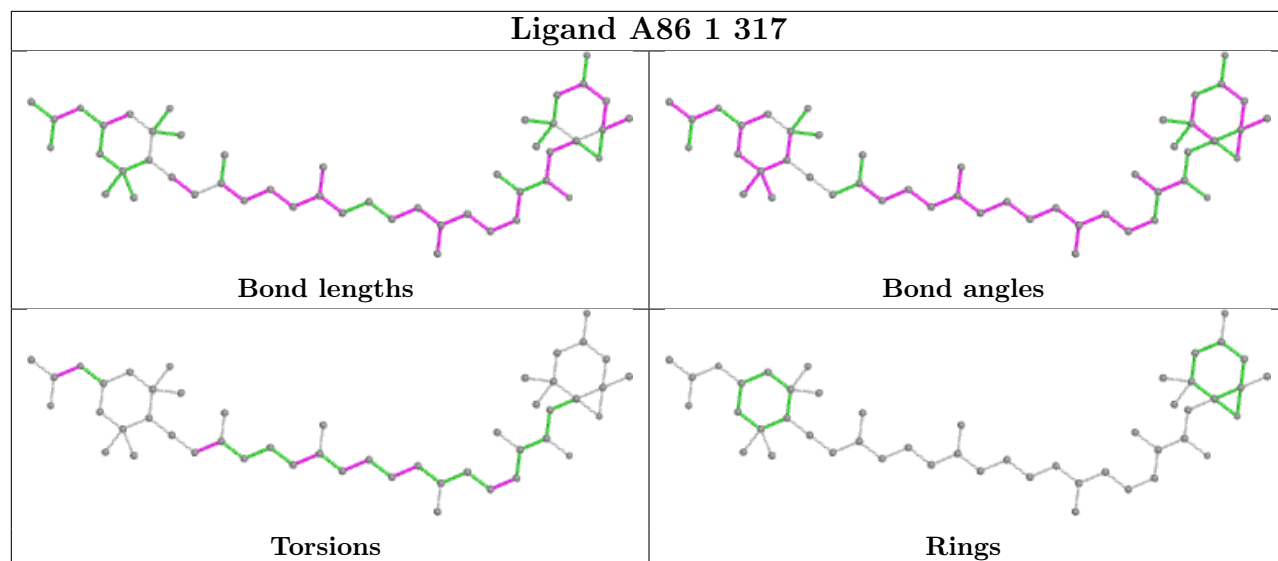


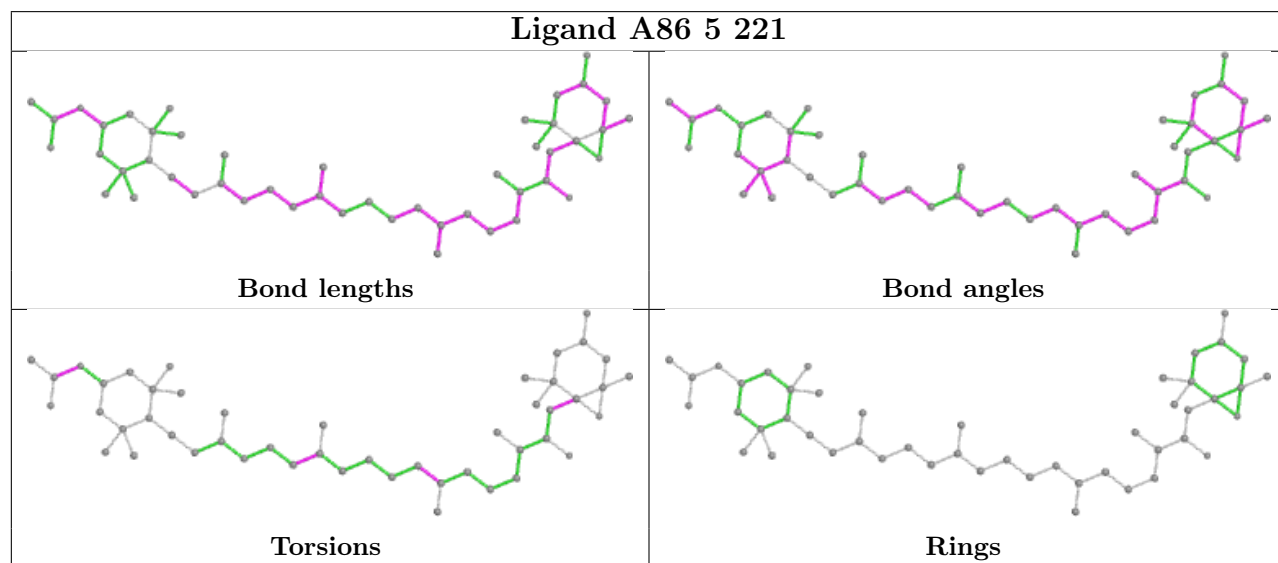
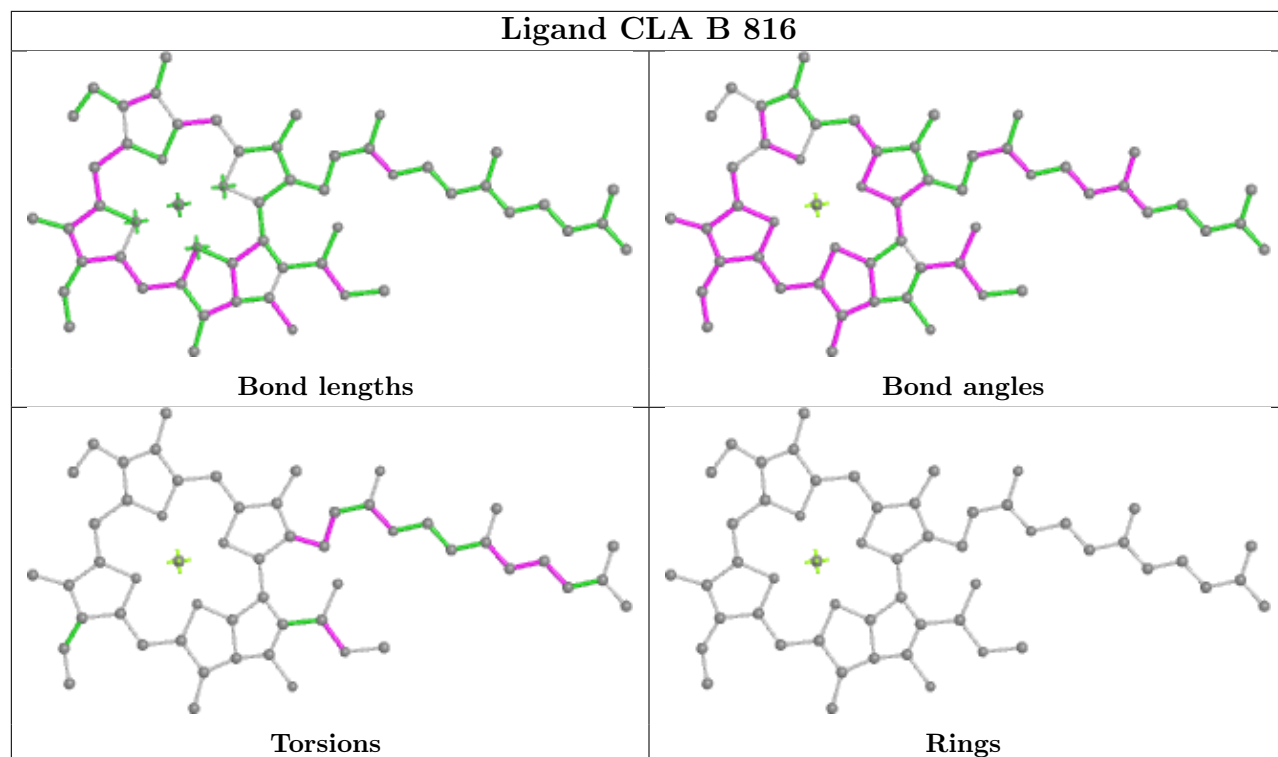


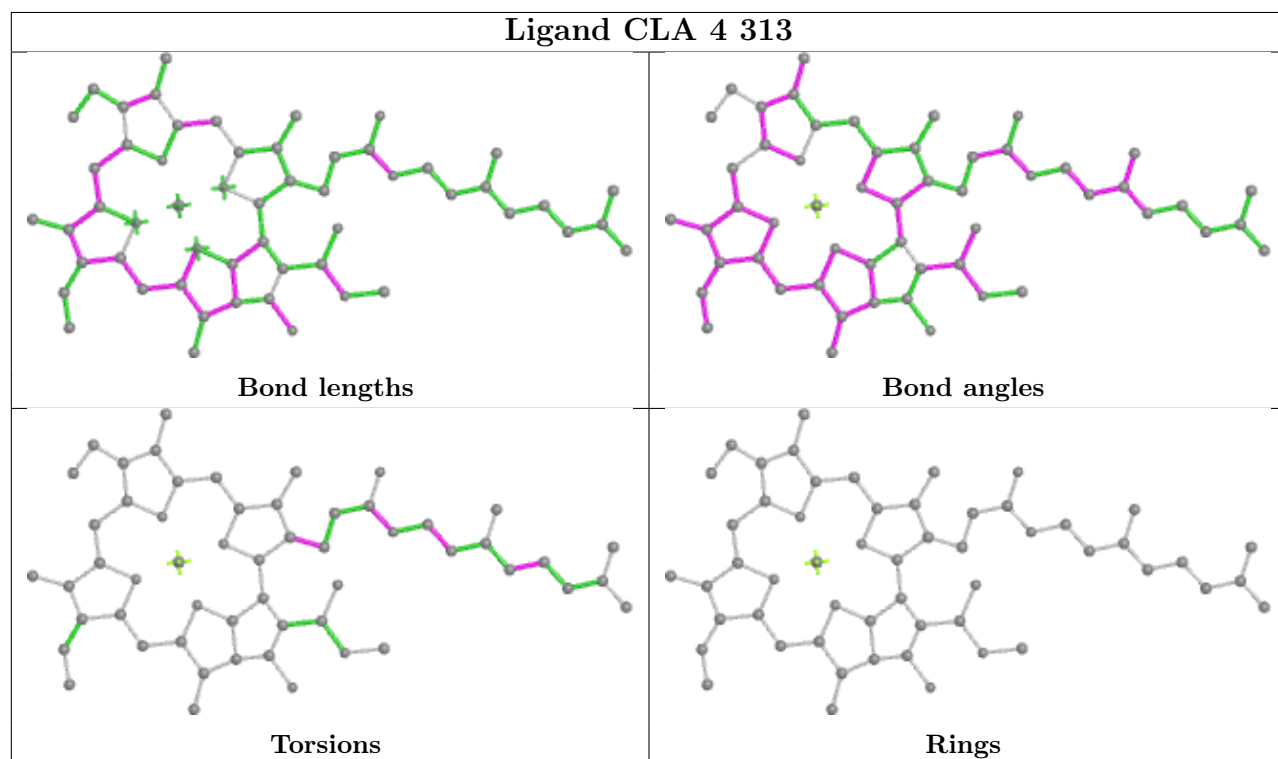
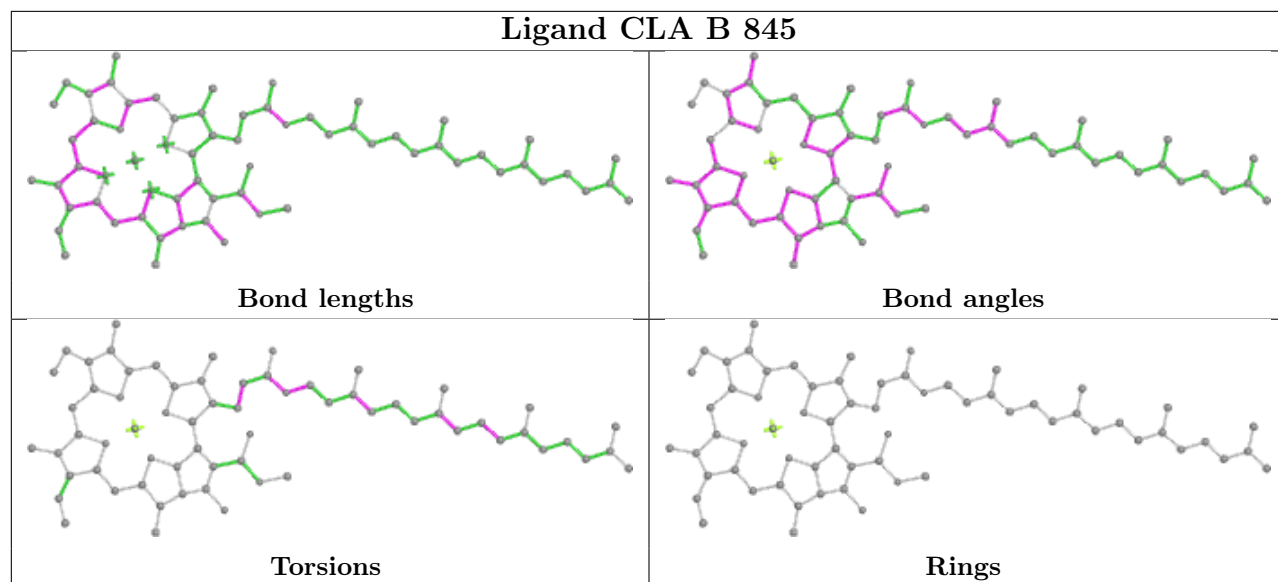


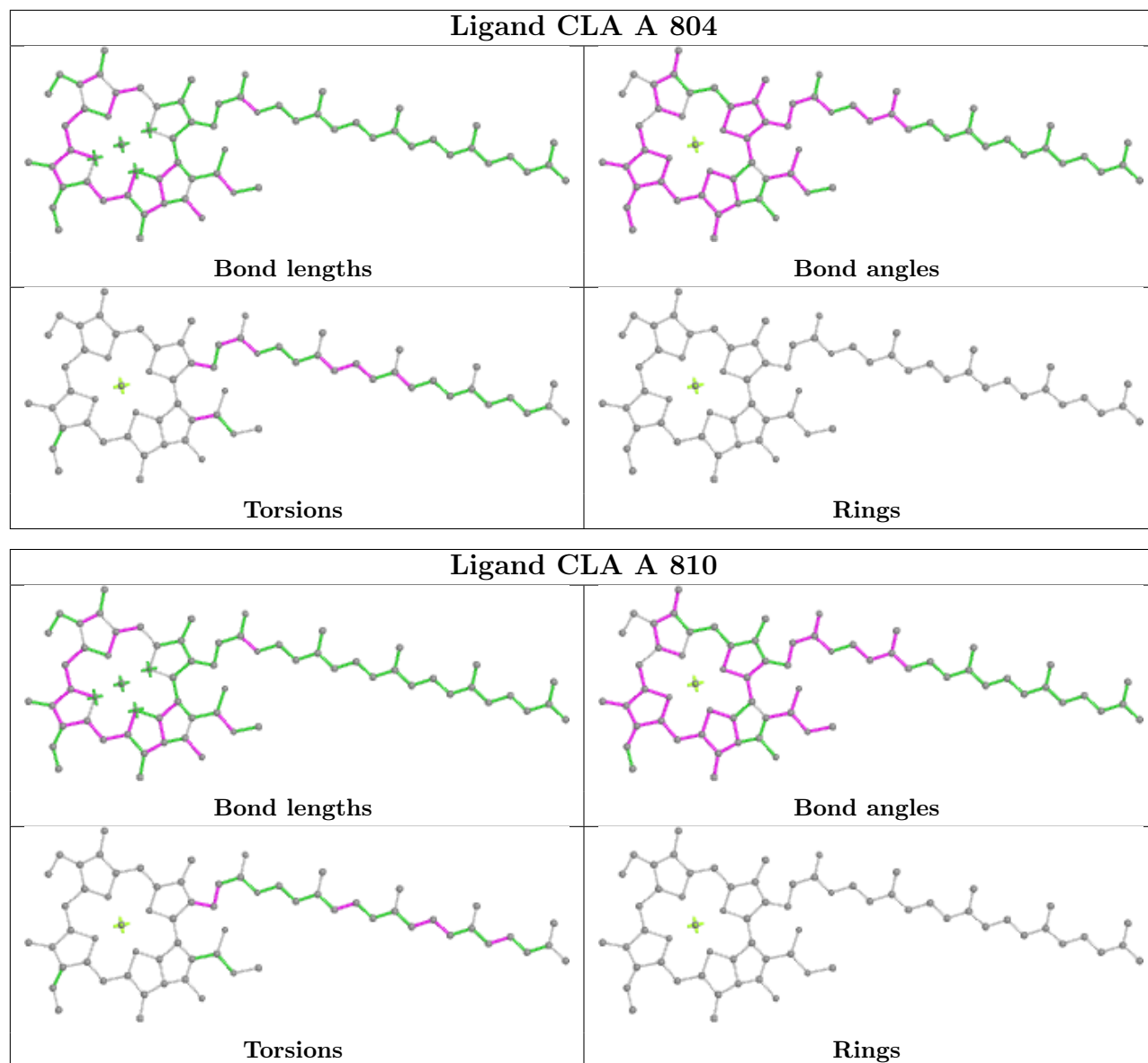


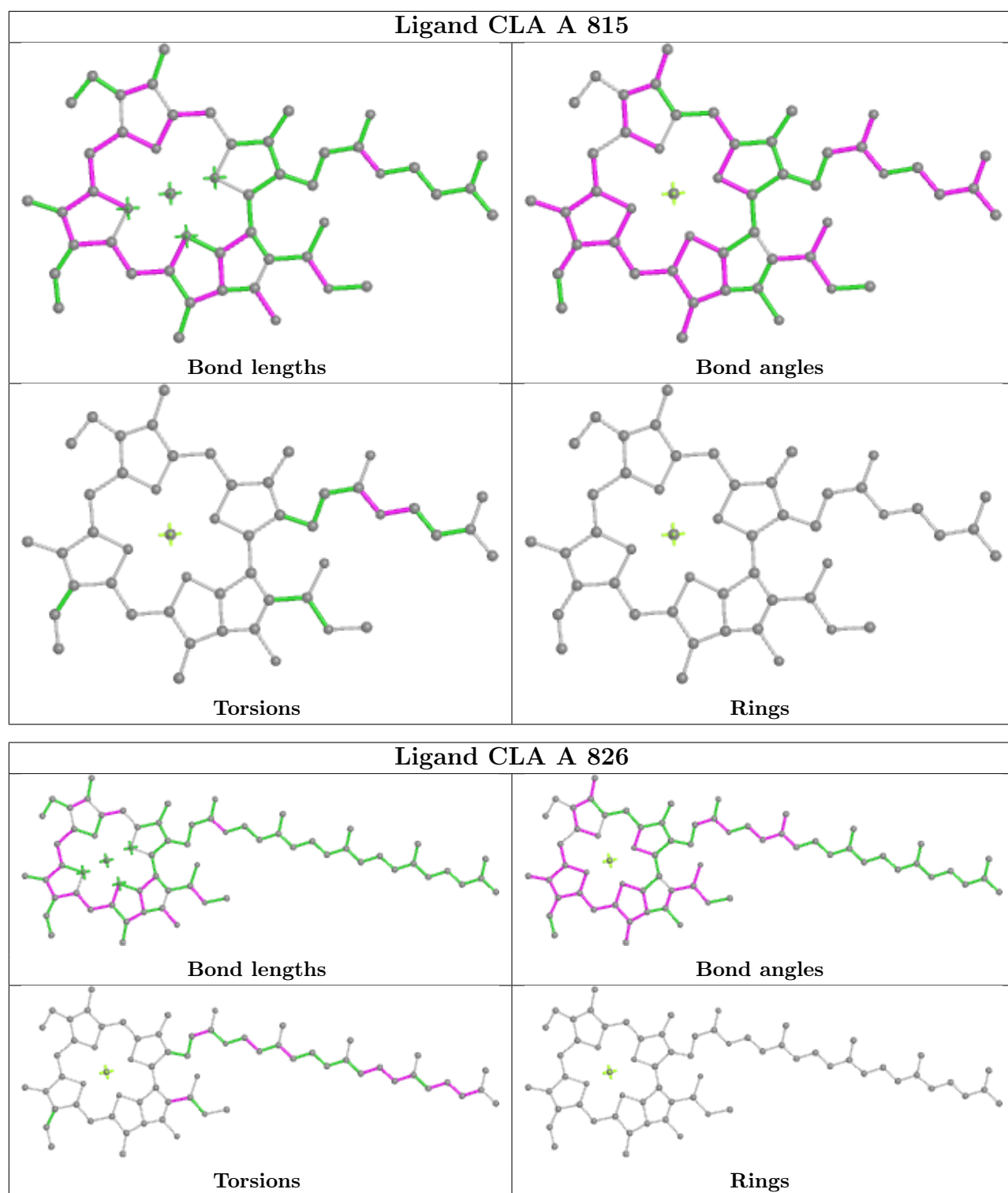


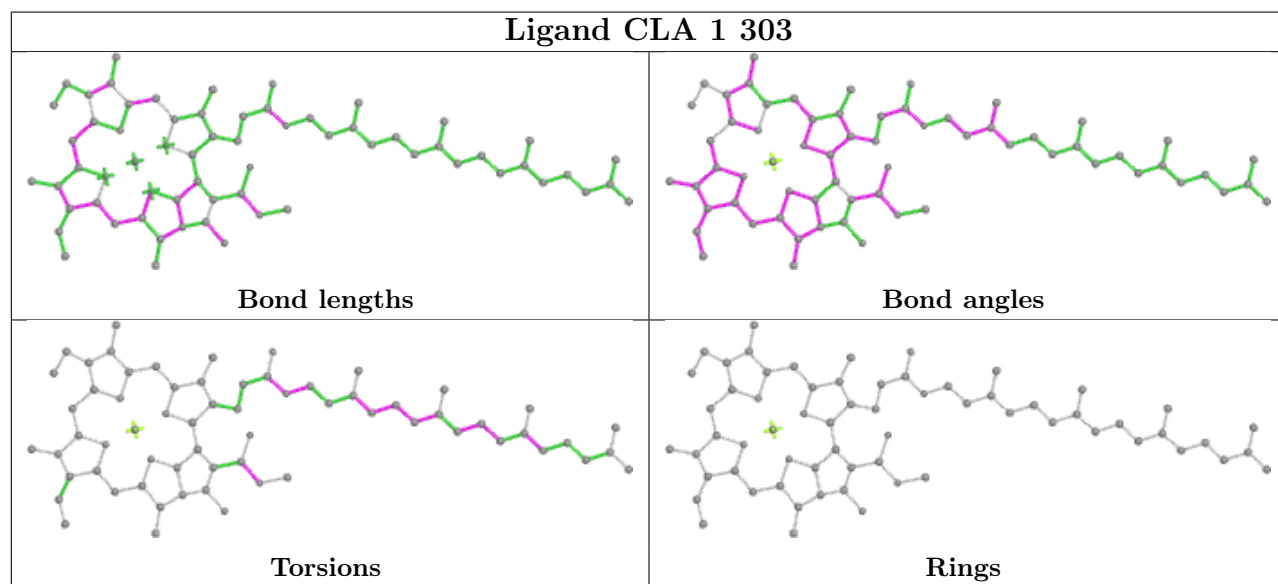
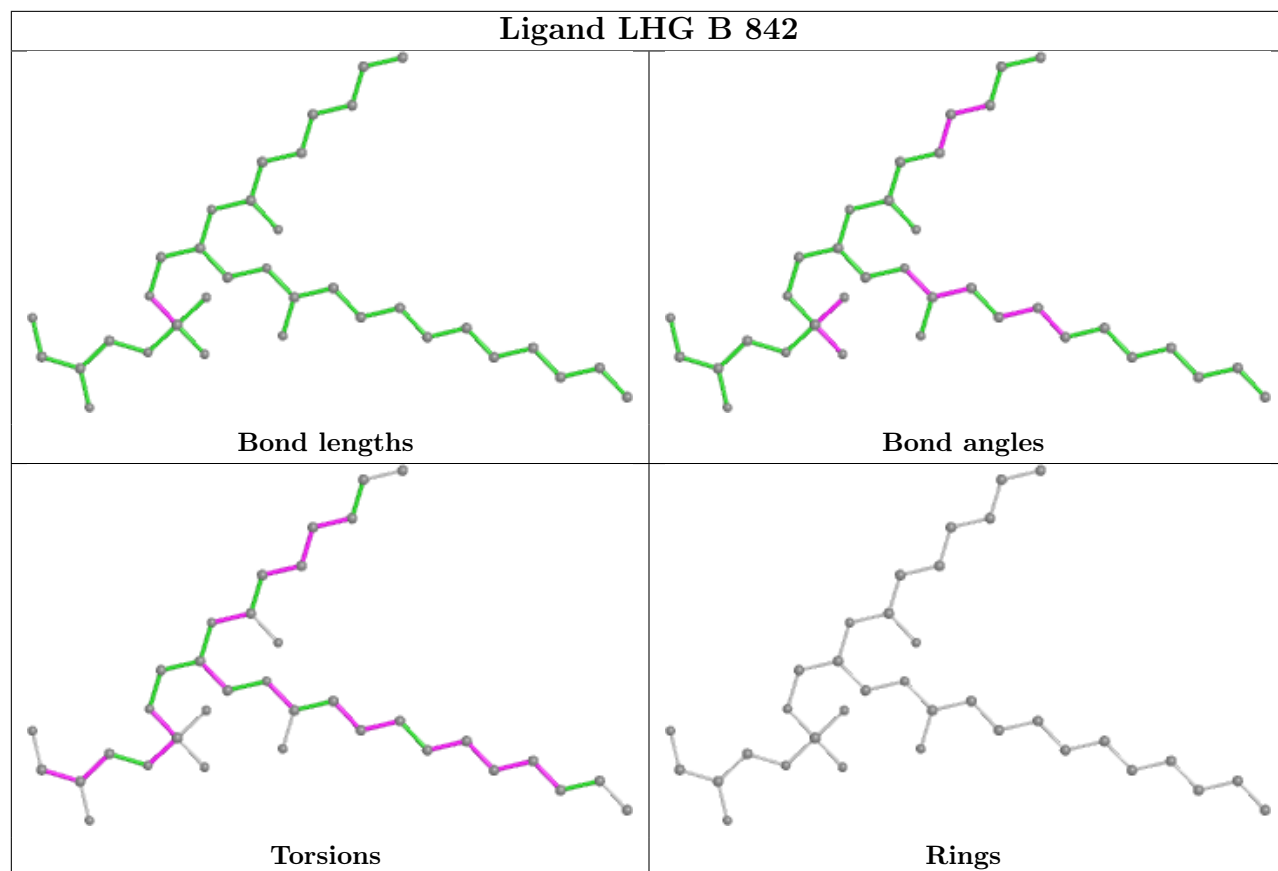


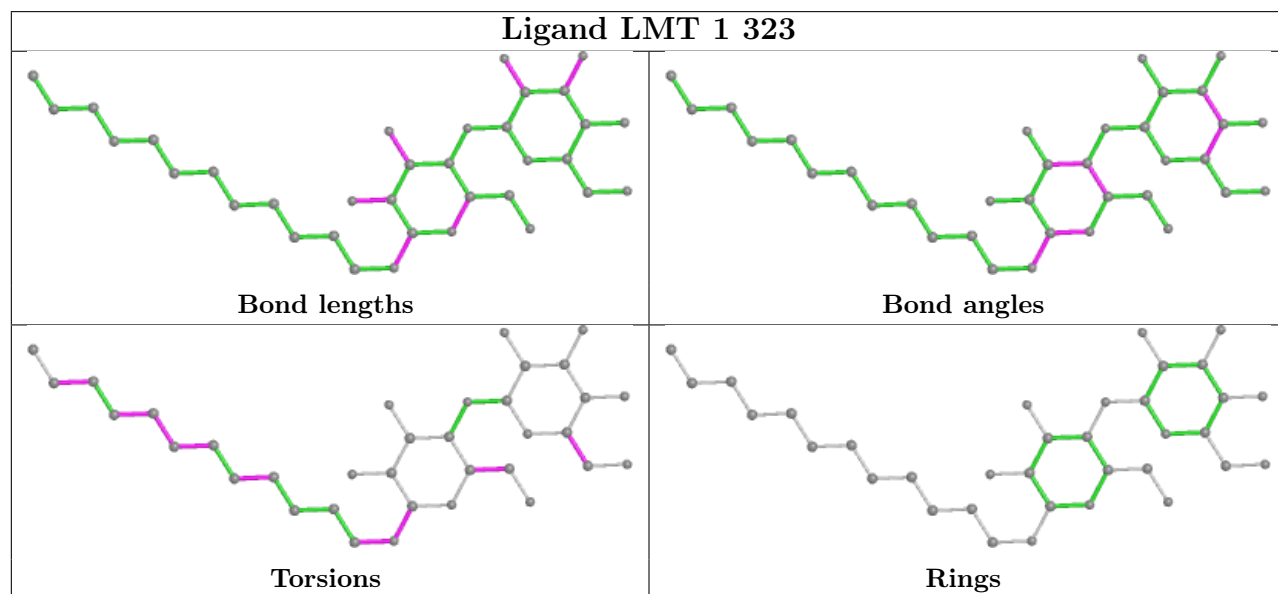
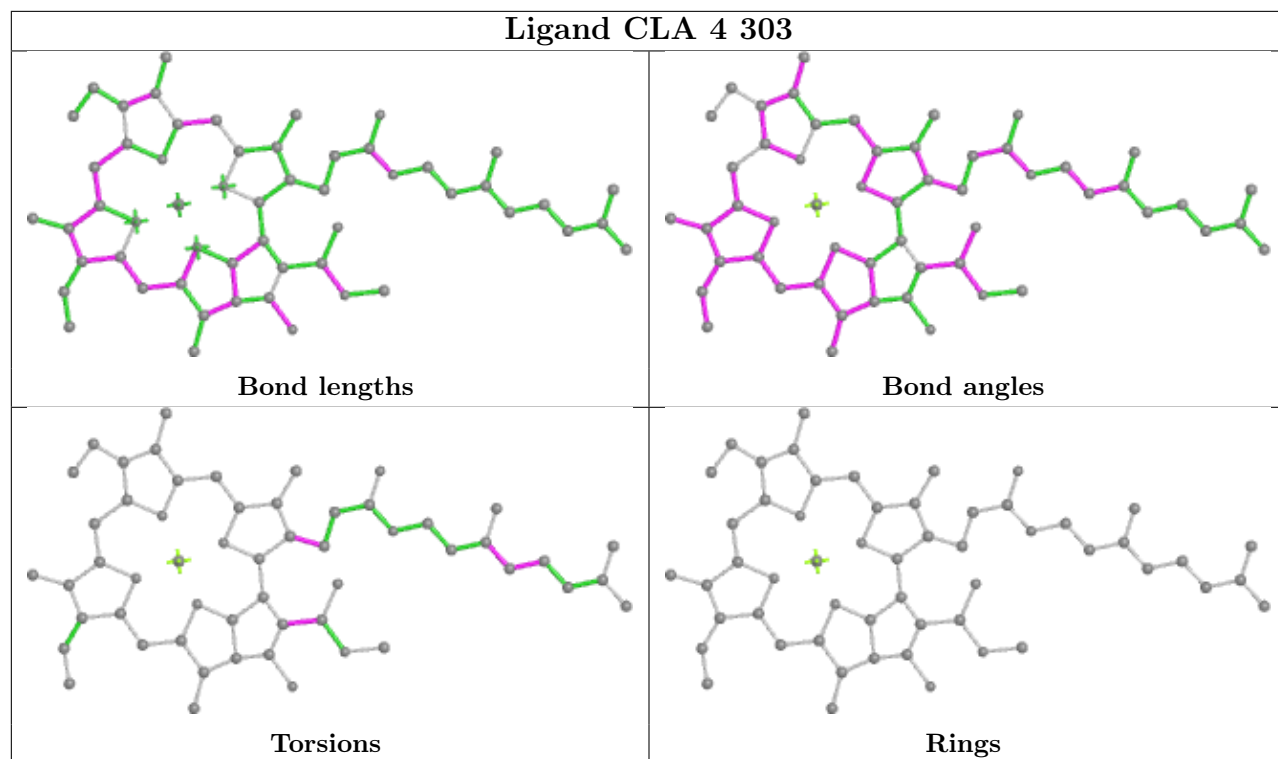


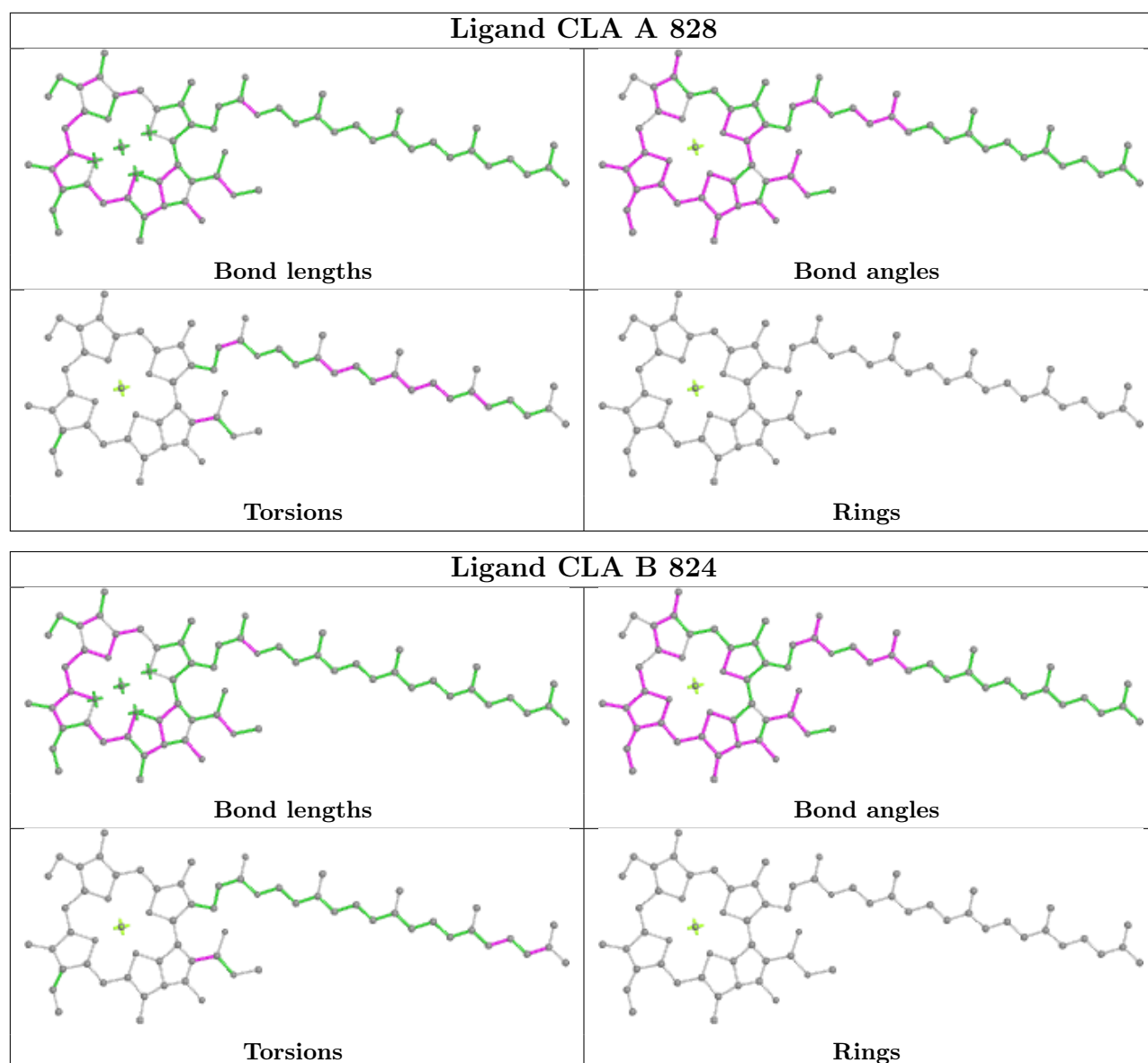












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

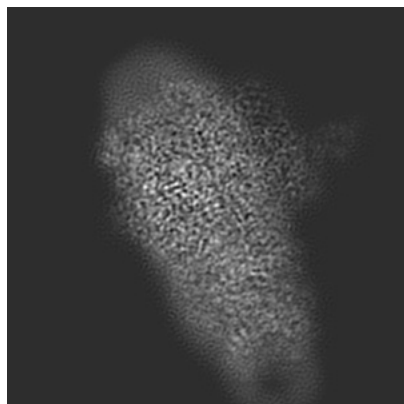
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38457. These allow visual inspection of the internal detail of the map and identification of artifacts.

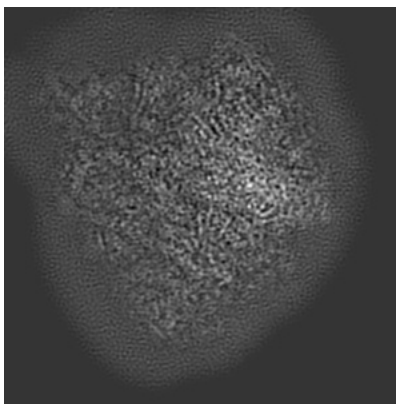
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

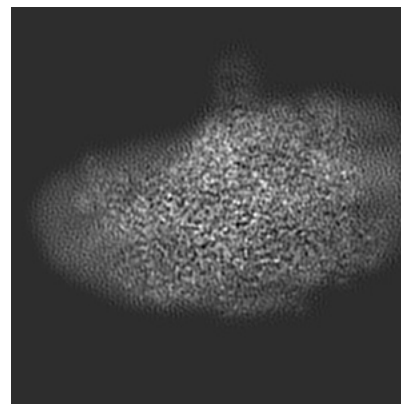
6.1.1 Primary map



X

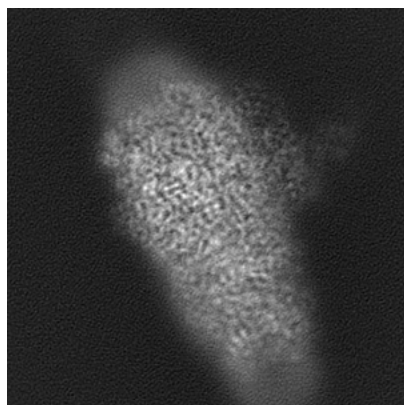


Y

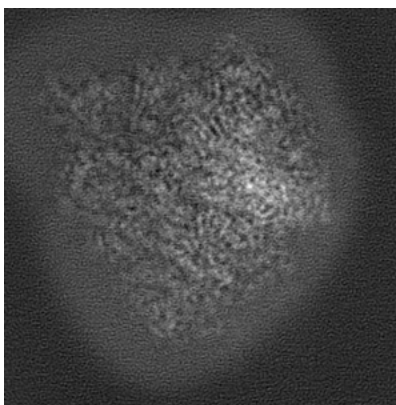


Z

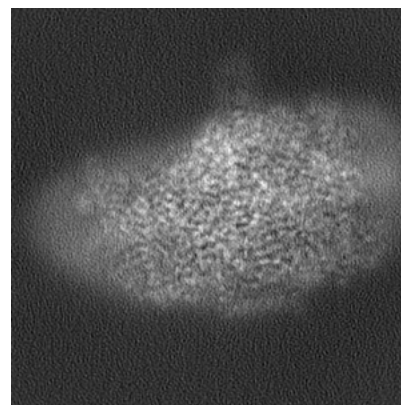
6.1.2 Raw map



X



Y

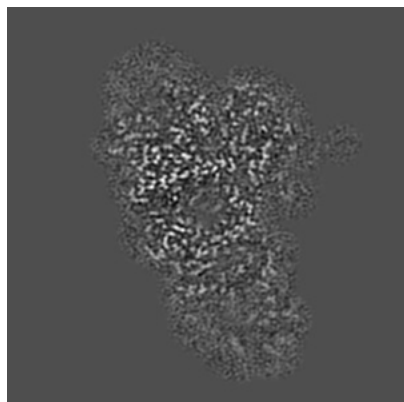


Z

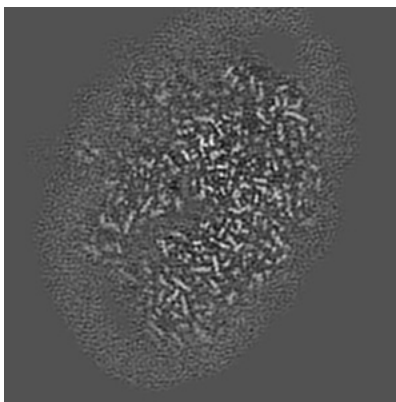
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

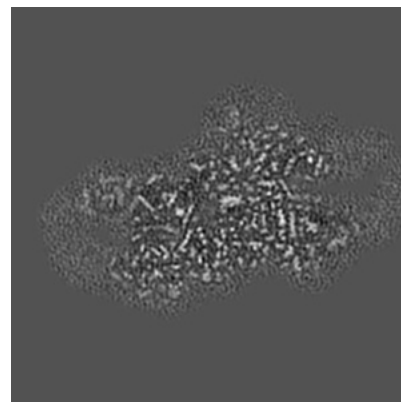
6.2.1 Primary map



X Index: 127

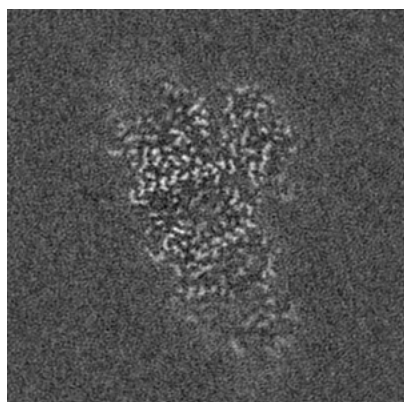


Y Index: 127

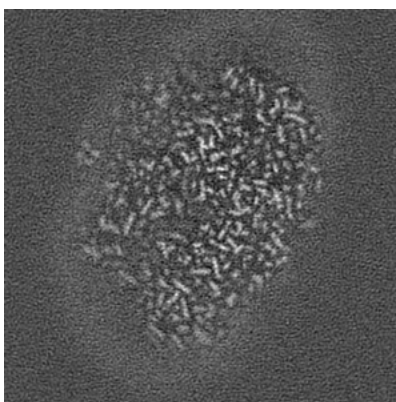


Z Index: 127

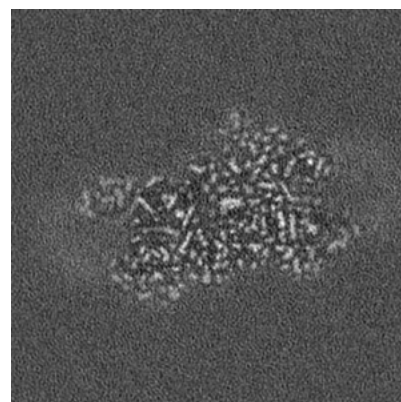
6.2.2 Raw map



X Index: 127



Y Index: 127

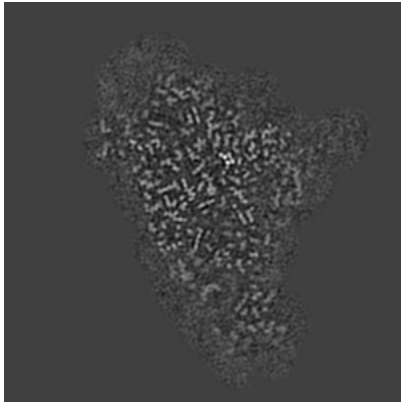


Z Index: 127

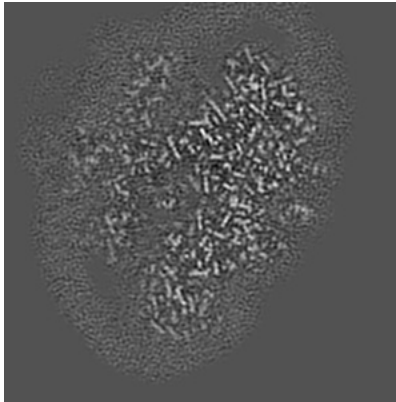
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

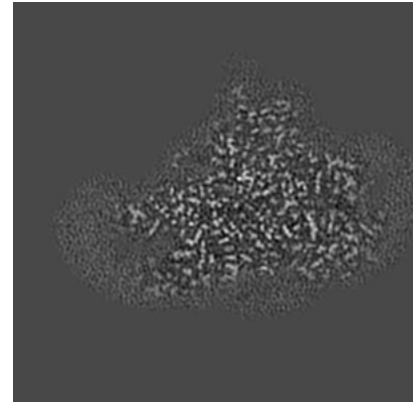
6.3.1 Primary map



X Index: 142

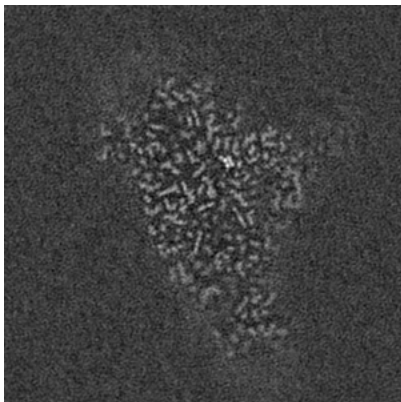


Y Index: 133

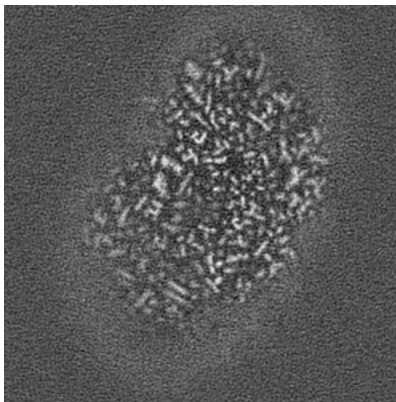


Z Index: 149

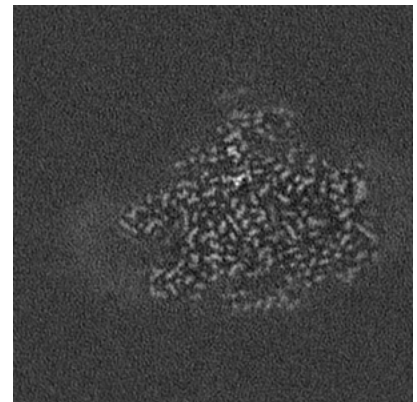
6.3.2 Raw map



X Index: 142



Y Index: 121

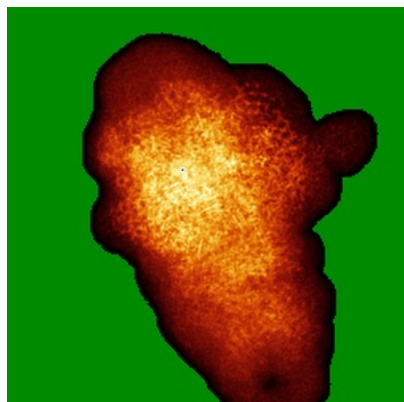


Z Index: 155

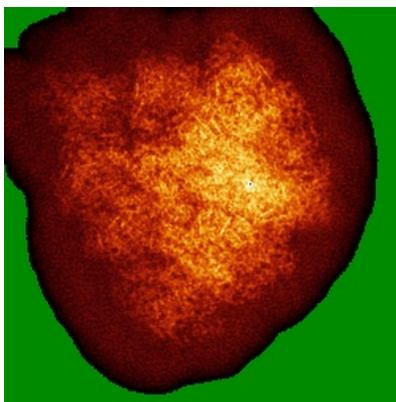
The images above show the largest variance slices of the map in three orthogonal directions.

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

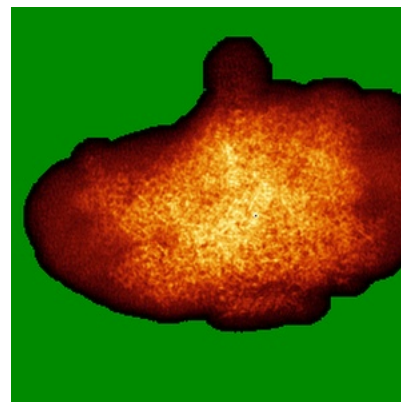
6.4.1 Primary map



X

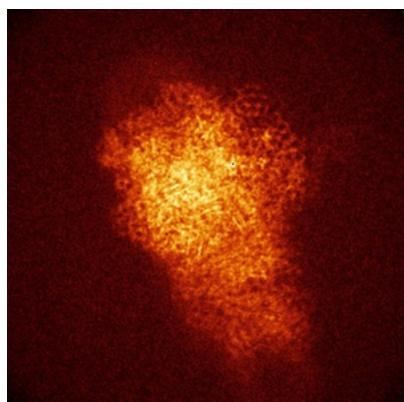


Y

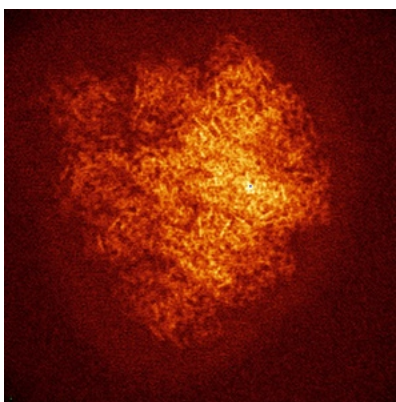


Z

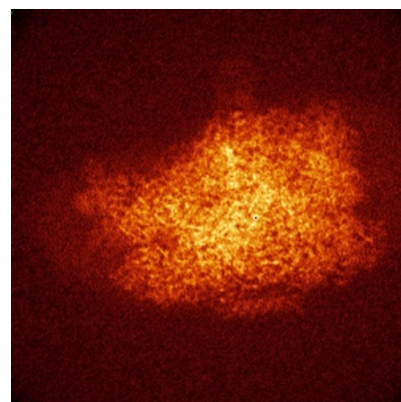
6.4.2 Raw map



X



Y

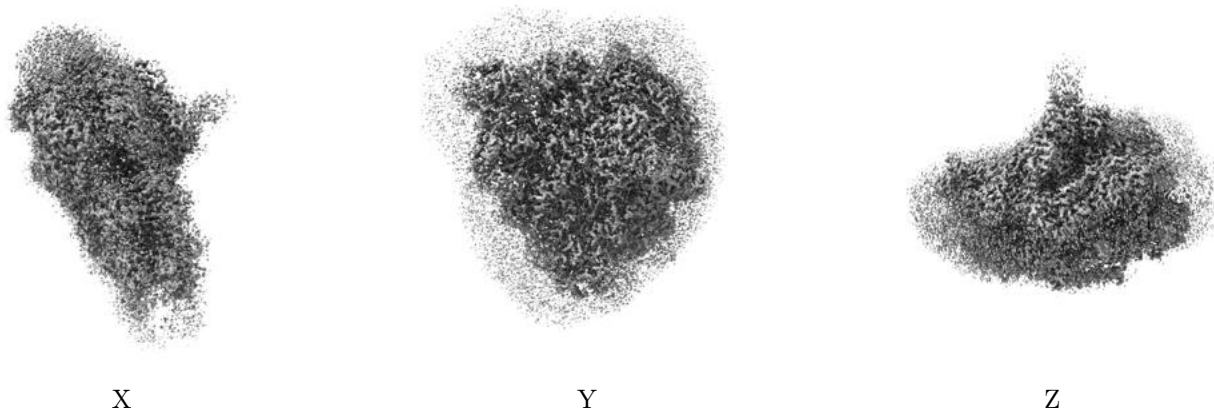


Z

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

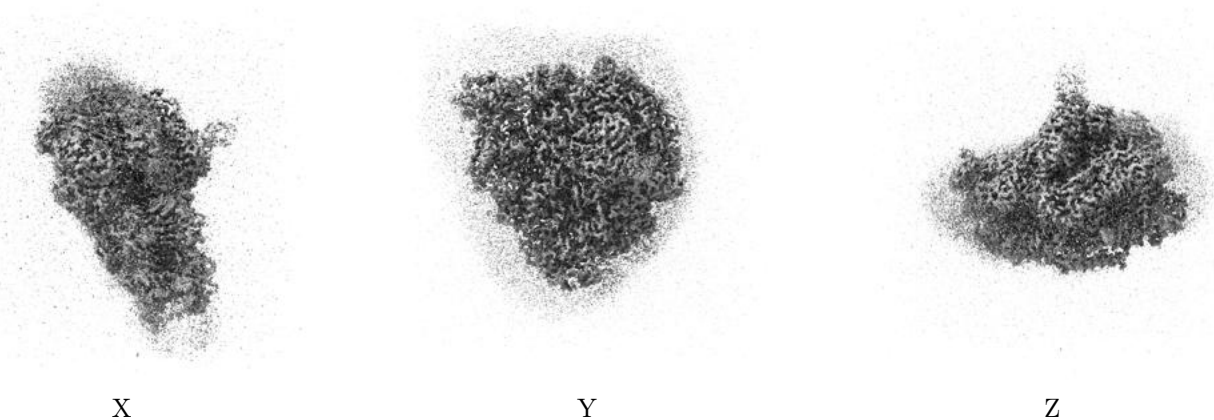
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

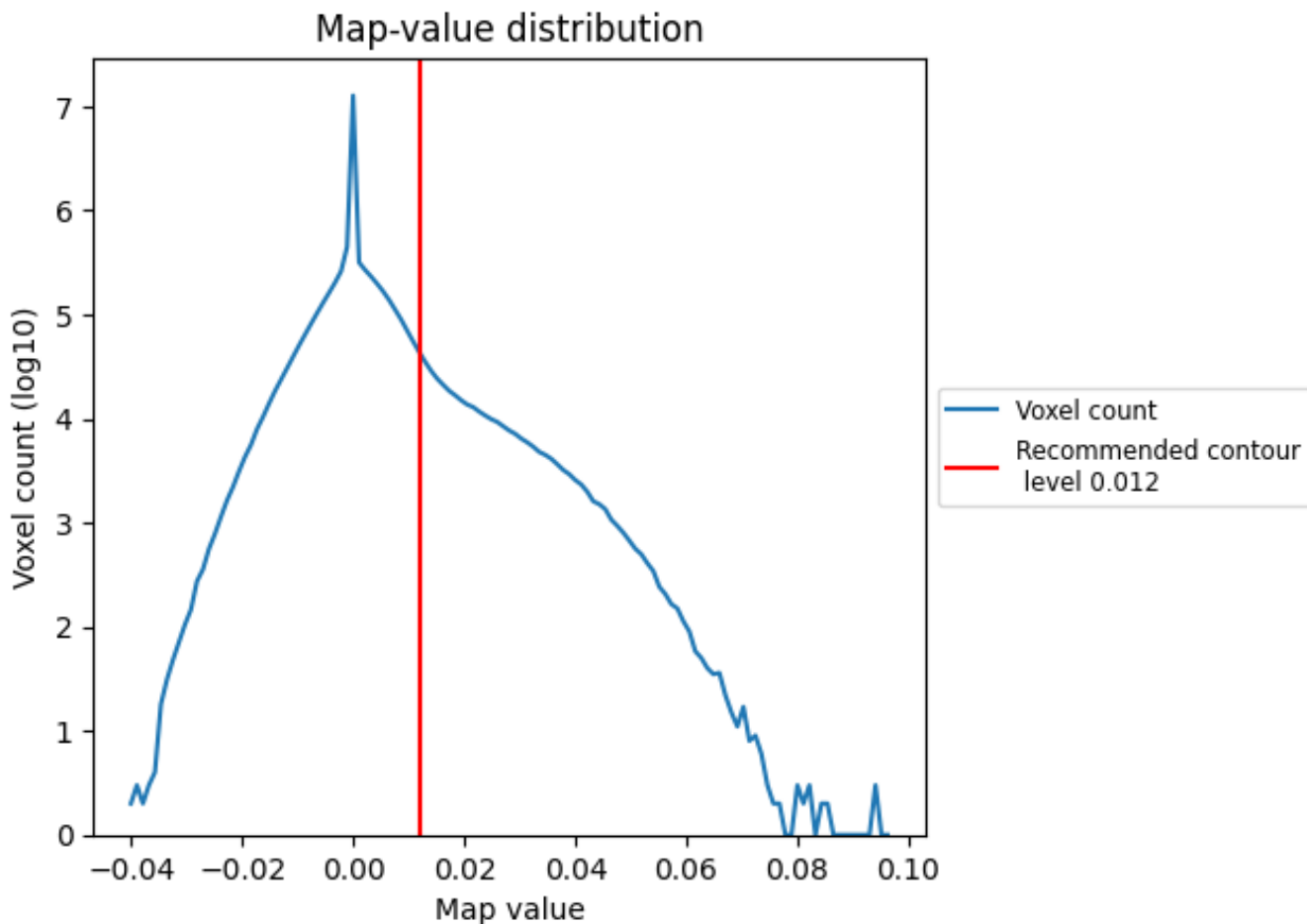
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

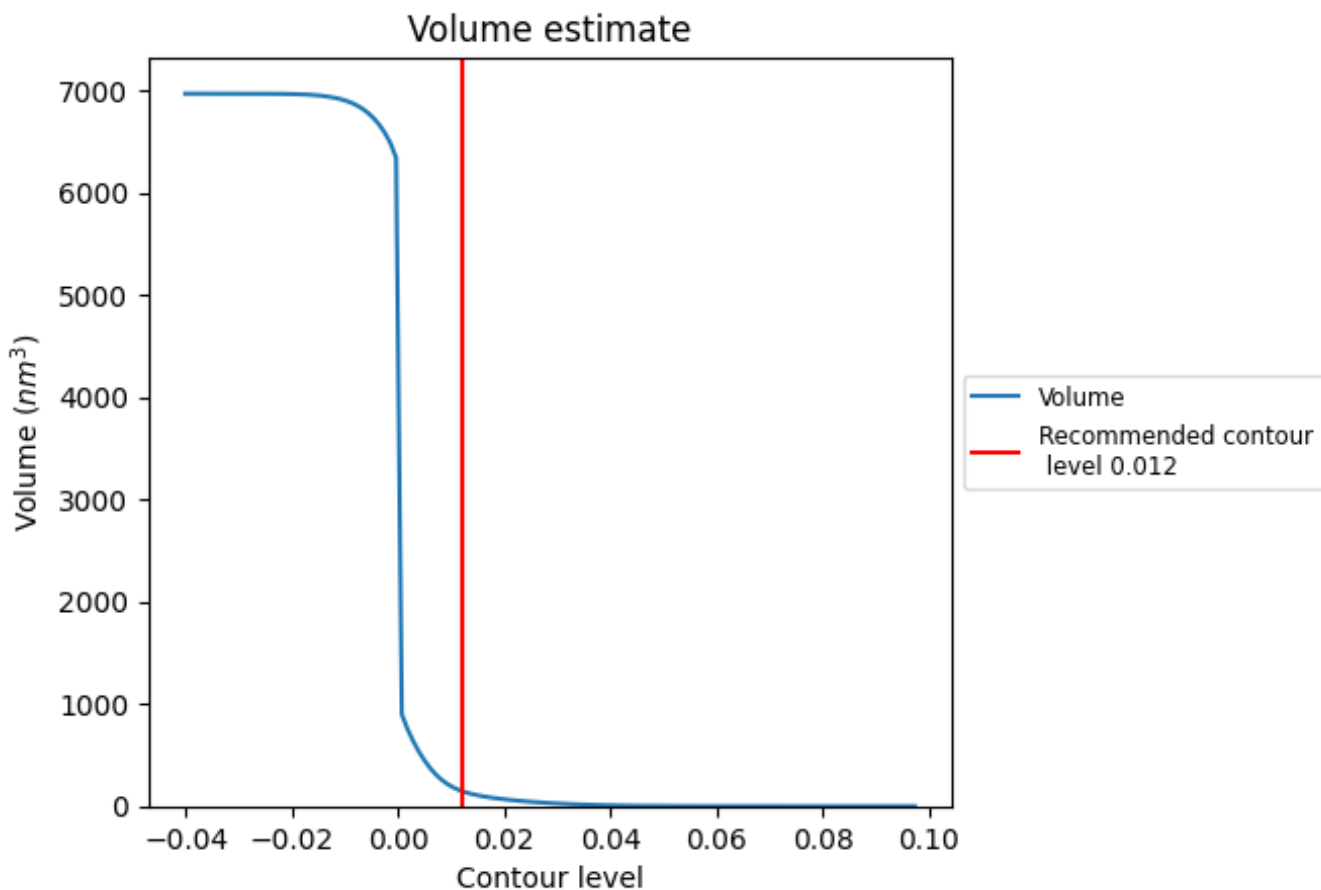
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

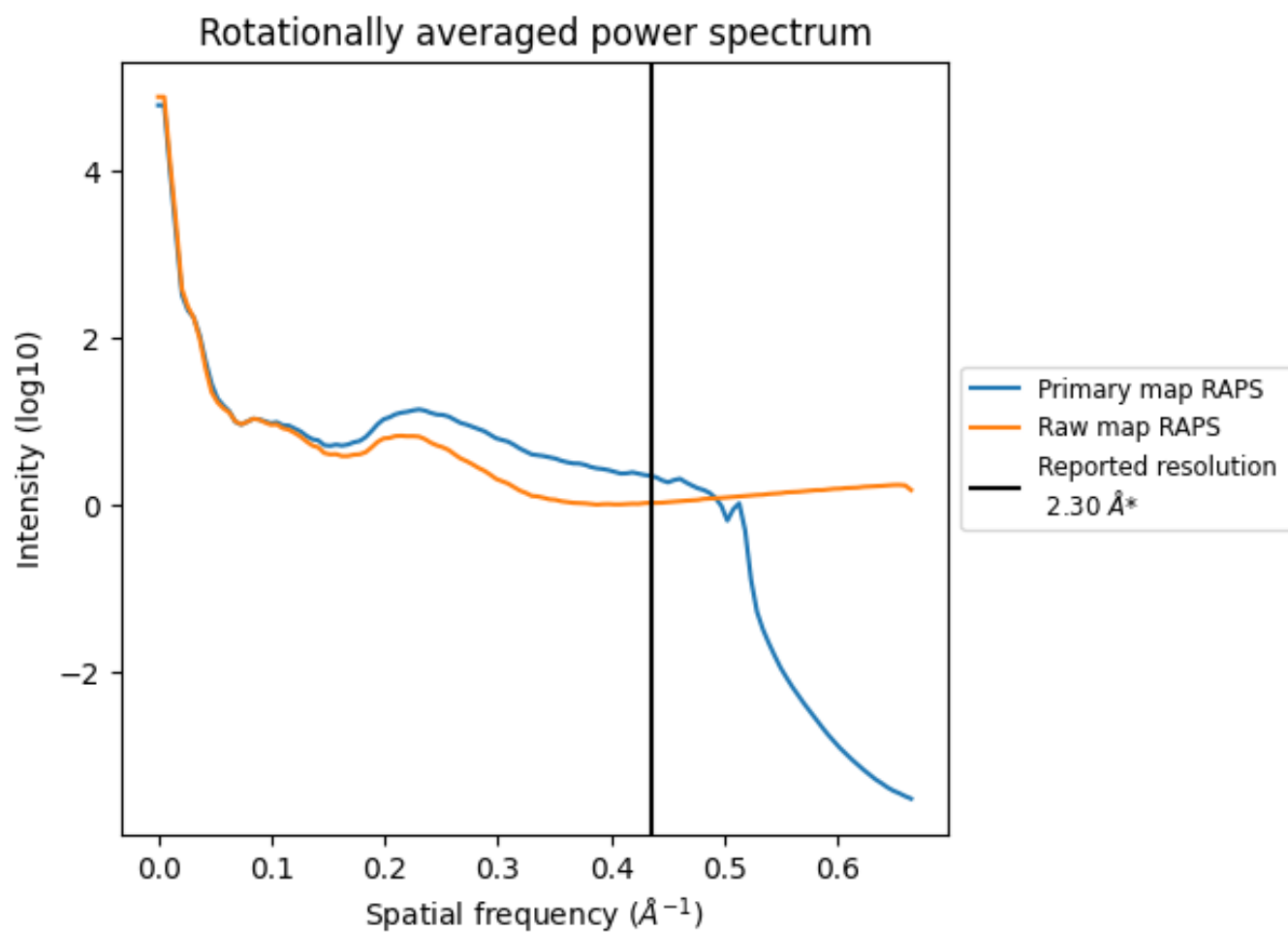
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm^3 ; this corresponds to an approximate mass of 134 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

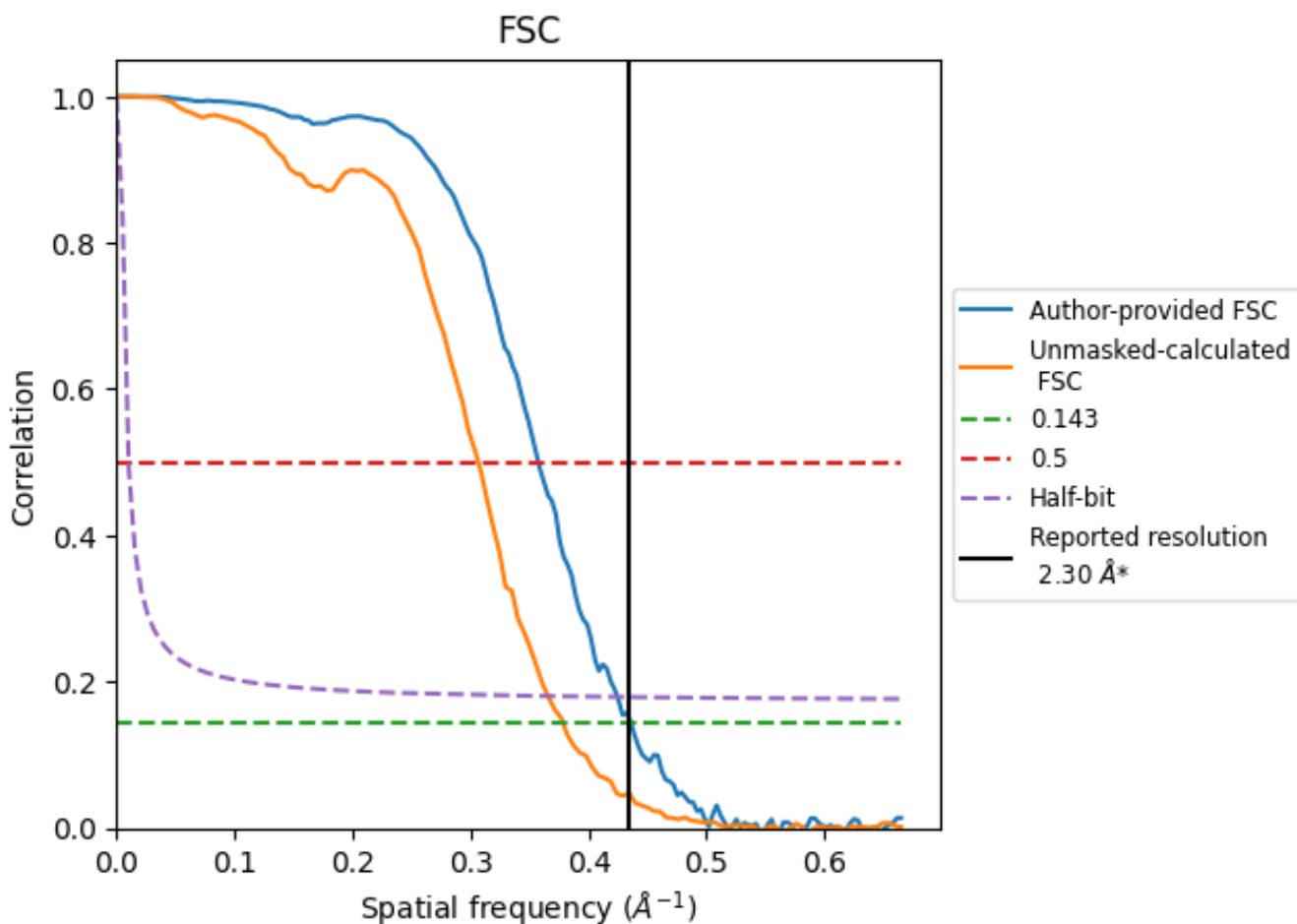


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

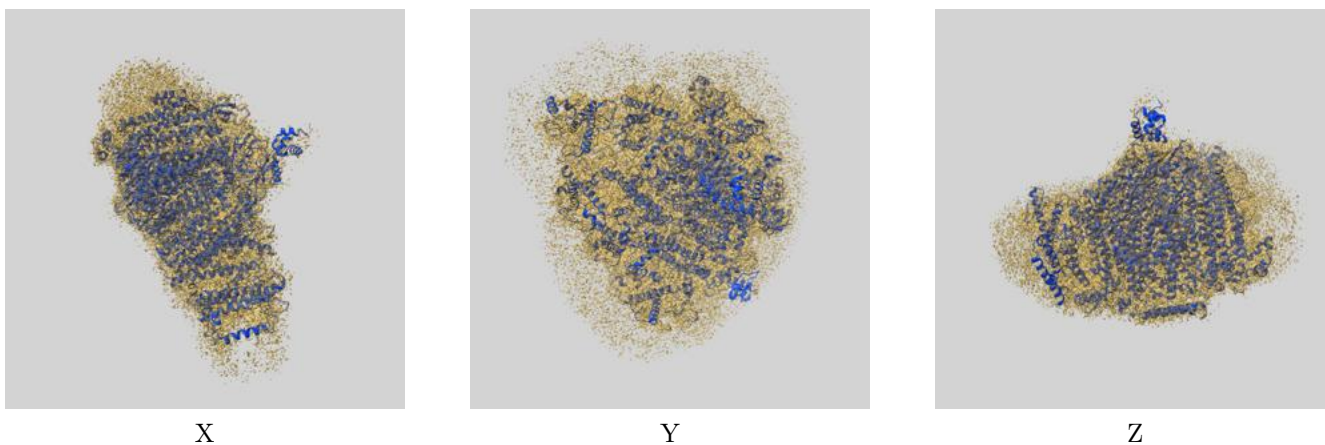
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.29	2.80	2.35
Unmasked-calculated*	2.64	3.26	2.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.64 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

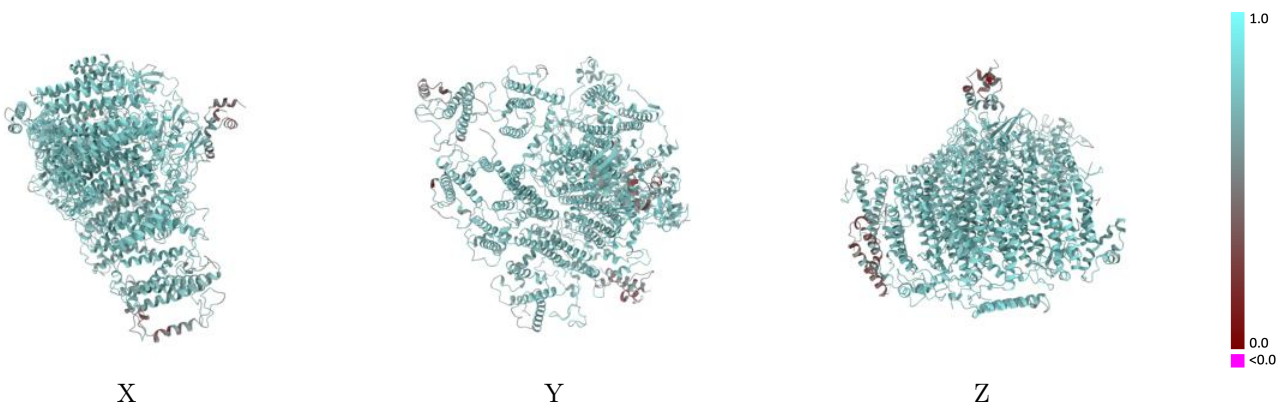
This section contains information regarding the fit between EMDB map EMD-38457 and PDB model 8XLS. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



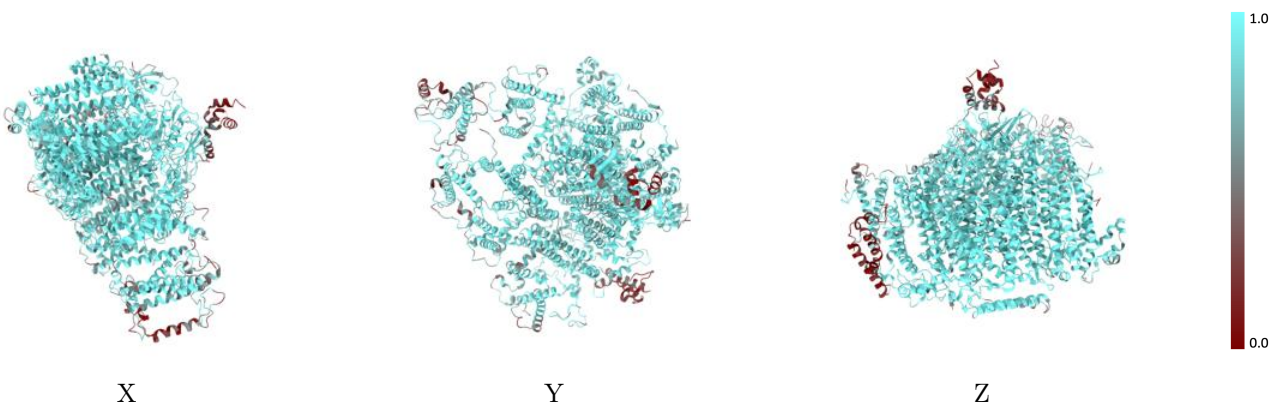
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



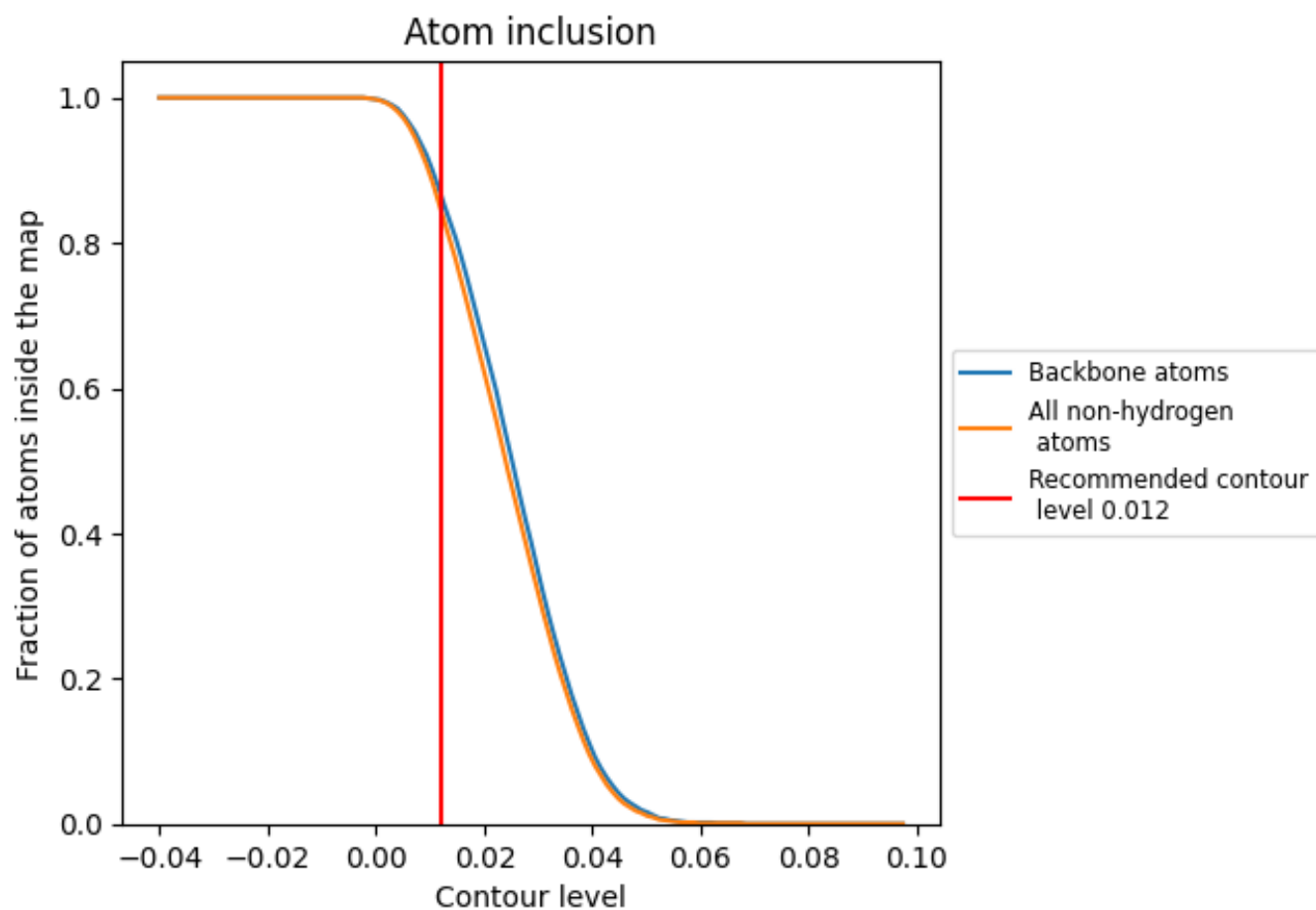
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.7000
1	 0.7930	 0.6780
2	 0.7590	 0.6490
3	 0.7860	 0.6700
4	 0.5900	 0.5890
5	 0.7560	 0.6470
A	 0.9140	 0.7340
B	 0.9300	 0.7390
C	 0.9780	 0.7600
D	 0.9360	 0.7310
E	 0.8460	 0.7050
F	 0.8780	 0.7060
I	 0.9350	 0.7340
J	 0.9060	 0.7140
L	 0.9040	 0.7280
M	 0.8620	 0.7220
W	 0.5100	 0.5830
u	 0.2160	 0.4540

