



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 01:06 AM UTC

PDB ID : 8BCV / pdb_00008bcv
EMDB ID : EMD-15969
Title : Photosystem I assembly intermediate of Avena sativa
Authors : Naschberger, A.; Amunts, A.; Nelson, N.
Deposited on : 2022-10-17
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

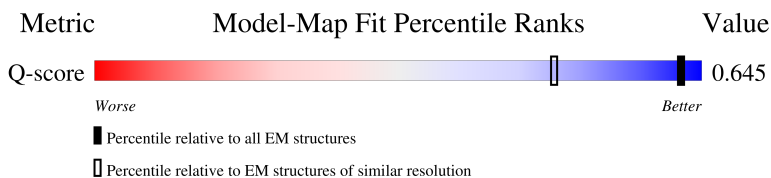
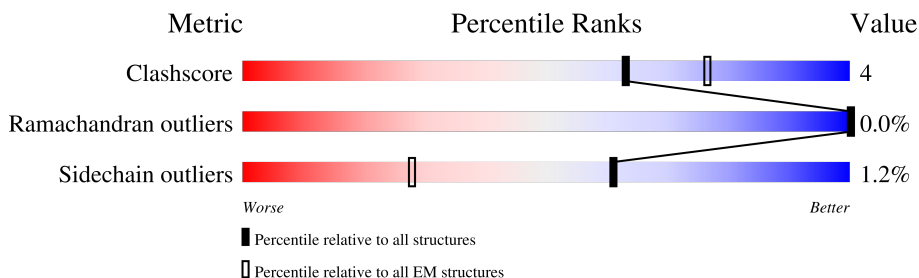
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	750	 5% 93% 6%
2	B	734	 96%
3	C	81	 99%
4	D	206	 65% 31%

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Mol	Chain	Length	Quality of chain
5	E	143	
6	H	94	
7	I	36	
8	L	213	
9	F	178	
10	G	144	
11	J	52	
12	K	130	
13	1	242	
14	2	207	
15	3	269	
16	4	256	

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
17	CL0	A	801	X	-	-	-
17	CL0	H	202	X	-	-	-
18	CLA	1	303	X	-	-	-
18	CLA	1	304	X	-	-	-
18	CLA	1	305	X	-	-	-
18	CLA	1	306	X	-	-	-
18	CLA	1	308	X	-	-	-
18	CLA	1	309	X	-	-	-
18	CLA	1	310	X	-	-	-
18	CLA	1	311	X	-	-	-
18	CLA	1	312	X	-	-	-
18	CLA	1	313	X	-	-	-
18	CLA	1	314	X	-	-	-
18	CLA	1	315	X	-	-	-
18	CLA	2	601	X	-	-	-
18	CLA	2	602	X	-	-	-
18	CLA	2	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	604	X	-	-	-
18	CLA	2	608	X	-	-	-
18	CLA	2	609	X	-	-	-
18	CLA	2	610	X	-	-	-
18	CLA	2	611	X	-	-	-
18	CLA	2	612	X	-	-	-
18	CLA	2	613	X	-	-	-
18	CLA	3	302	X	-	-	-
18	CLA	3	303	X	-	-	-
18	CLA	3	304	X	-	-	-
18	CLA	3	305	X	-	-	-
18	CLA	3	307	X	-	-	-
18	CLA	3	308	X	-	-	-
18	CLA	3	309	X	-	-	-
18	CLA	3	310	X	-	-	-
18	CLA	3	311	X	-	-	-
18	CLA	3	312	X	-	-	-
18	CLA	4	601	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	604	X	-	-	-
18	CLA	4	608	X	-	-	-
18	CLA	4	609	X	-	-	-
18	CLA	4	610	X	-	-	-
18	CLA	4	611	X	-	-	-
18	CLA	4	612	X	-	-	-
18	CLA	4	613	X	-	-	-
18	CLA	4	614	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	842	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	A	854	X	-	-	-
18	CLA	A	855	X	-	-	-
18	CLA	A	856	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	F	802	X	-	-	-
18	CLA	F	804	X	-	-	-
18	CLA	F	805	X	-	-	-
18	CLA	G	201	X	-	-	-
18	CLA	G	204	X	-	-	-
18	CLA	G	205	X	-	-	-
18	CLA	J	102	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	L	304	X	-	-	-
18	CLA	L	305	X	-	-	-
27	CHL	1	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	1	307	X	-	-	-
27	CHL	2	605	X	-	-	-
27	CHL	2	606	X	-	-	-
27	CHL	2	607	X	-	-	-
27	CHL	2	614	X	-	-	-
27	CHL	3	301	X	-	-	-
27	CHL	3	306	X	-	-	-
27	CHL	4	605	X	-	-	-
27	CHL	4	606	X	-	-	-
27	CHL	4	607	X	-	-	-
27	CHL	4	615	X	-	-	-

2 Entry composition i

There are 31 unique types of molecules in this entry. The entry contains 37485 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	742	5840	3826	992	1003	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5864	3848	996	1007	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	605	372	104	118	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1124	722	196	203	3	0	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	67	533	340	94	99	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	H	94	715	469	114	132	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	33	258	178	38	41	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	159	1192	788	189	214	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	158	1238	804	210	221	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	G	94	721	467	121	133	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	43	342	232	52	57	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	88	628	397	107	121	3	0	0

- Molecule 13 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	1	196	1519	990	254	271	4	0	0

- Molecule 14 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	2	207	1609	1050	263	292	4	0	0

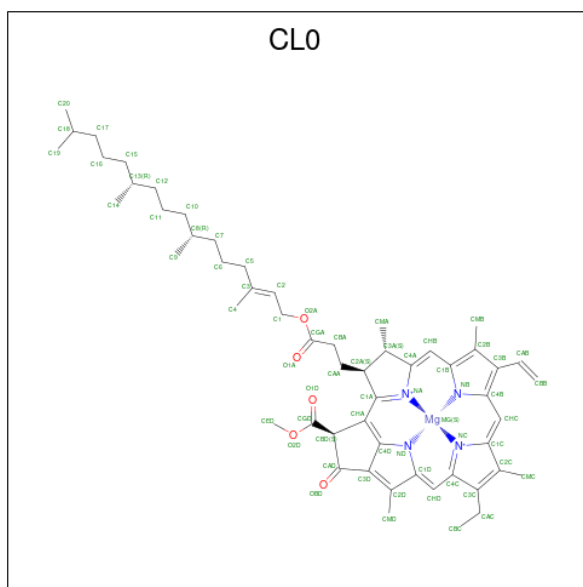
- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

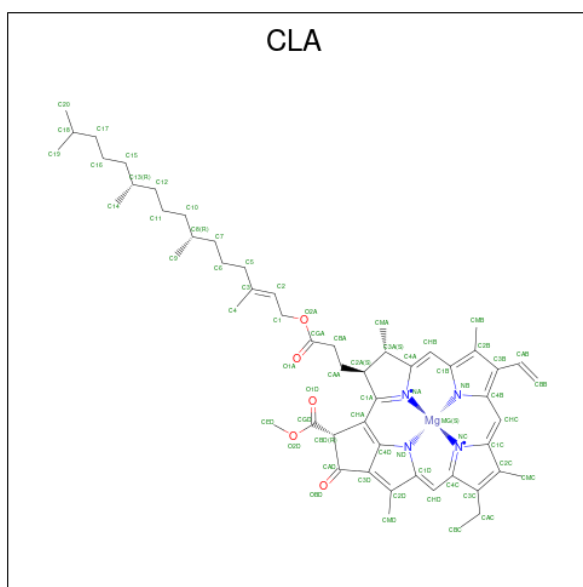
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	3	222	1725	1130	278	309	8	0	0

- Molecule 16 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	4	199	1555	1012	257	282	4	0	0

- Molecule 17 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	60	50	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	60	50	1	4	5	0
18	A	1	56	46	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	52	42	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	60	50	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	55	45	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	55	45	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	45	35	1	4	5	0
18	A	1	51	41	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	55	45	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	45	35	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	45	35	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	60	50	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	56	46	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	B	1	52	42	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	45	35	1	4	5	0
18	B	1	60	50	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	55	45	1	4	5	0
18	B	1	60	50	1	4	5	0
18	B	1	58	48	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	45	35	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	45	35	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	B	1	45	35	1	4	5	0
18	B	1	61	51	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	50	40	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	L	1	45	35	1	4	5	0
18	L	1	60	50	1	4	5	0
18	L	1	45	35	1	4	5	0
18	F	1	65	55	1	4	5	0
18	F	1	65	55	1	4	5	0
18	F	1	50	40	1	4	5	0
18	G	1	57	47	1	4	5	0
18	G	1	45	35	1	4	5	0
18	G	1	46	36	1	4	5	0
18	J	1	45	35	1	4	5	0
18	K	1	45	35	1	4	5	0
18	K	1	60	50	1	4	5	0
18	K	1	45	35	1	4	5	0
18	1	1	65	55	1	4	5	0

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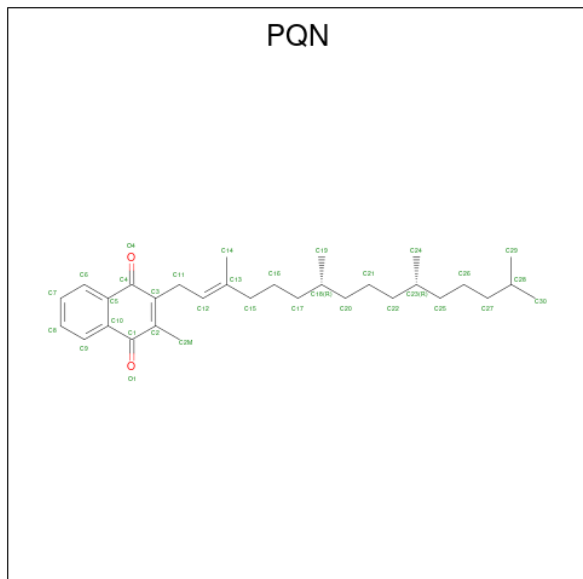
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	1	1	60	50	1	4	5	0
18	1	1	50	40	1	4	5	0
18	1	1	45	35	1	4	5	0
18	1	1	45	35	1	4	5	0
18	1	1	65	55	1	4	5	0
18	1	1	55	45	1	4	5	0
18	1	1	45	35	1	4	5	0
18	1	1	45	35	1	4	5	0
18	1	1	65	55	1	4	5	0
18	1	1	45	35	1	4	5	0
18	1	1	45	35	1	4	5	0
18	2	1	65	55	1	4	5	0
18	2	1	65	55	1	4	5	0
18	2	1	65	55	1	4	5	0
18	2	1	45	35	1	4	5	0
18	2	1	45	35	1	4	5	0
18	2	1	60	50	1	4	5	0
18	2	1	60	50	1	4	5	0
18	2	1	45	35	1	4	5	0
18	2	1	65	55	1	4	5	0
18	2	1	50	40	1	4	5	0

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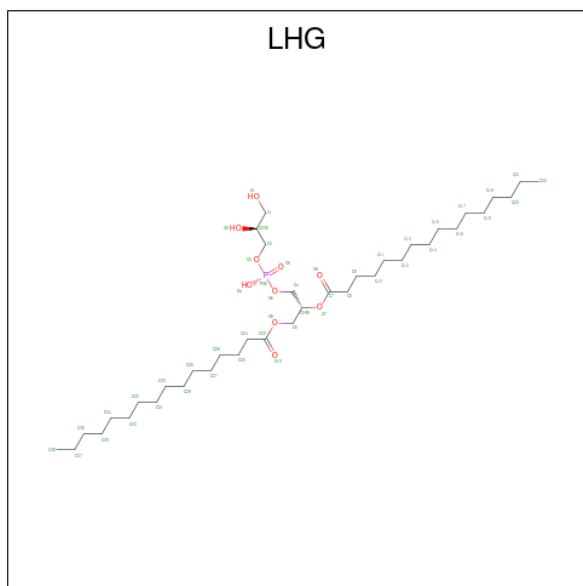
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	3	1	55	45	1	4	5	0
18	3	1	45	35	1	4	5	0
18	3	1	45	35	1	4	5	0
18	3	1	61	51	1	4	5	0
18	3	1	60	50	1	4	5	0
18	3	1	55	45	1	4	5	0
18	3	1	45	35	1	4	5	0
18	3	1	55	45	1	4	5	0
18	3	1	45	35	1	4	5	0
18	3	1	45	35	1	4	5	0
18	4	1	50	40	1	4	5	0
18	4	1	60	50	1	4	5	0
18	4	1	65	55	1	4	5	0
18	4	1	45	35	1	4	5	0
18	4	1	65	55	1	4	5	0
18	4	1	60	50	1	4	5	0
18	4	1	45	35	1	4	5	0
18	4	1	47	37	1	4	5	0
18	4	1	65	55	1	4	5	0
18	4	1	46	36	1	4	5	0
18	4	1	50	40	1	4	5	0

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



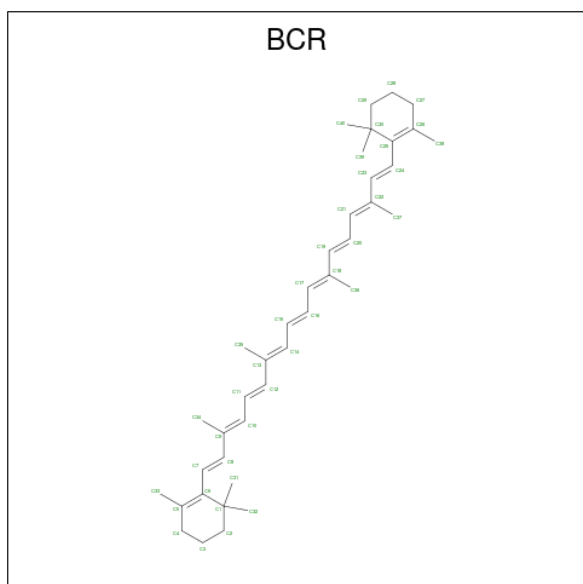
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			33	31	2	
19	B	1	Total	C	O	0
			33	31	2	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms			AltConf	
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	A	1	Total	C	O	P	0
			31	20	10	1	
20	B	1	Total	C	O	P	0
			39	28	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



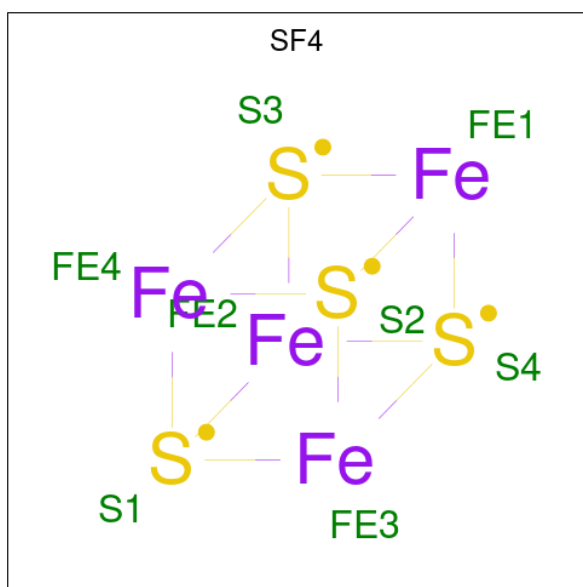
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	

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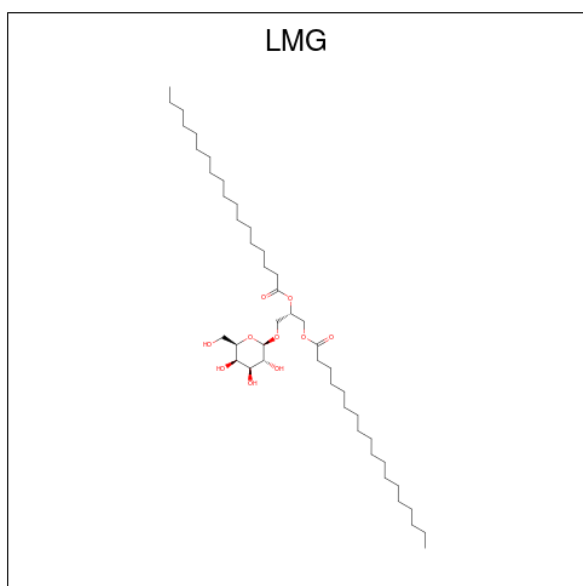
Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	4	1	Total C 40 40	0

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



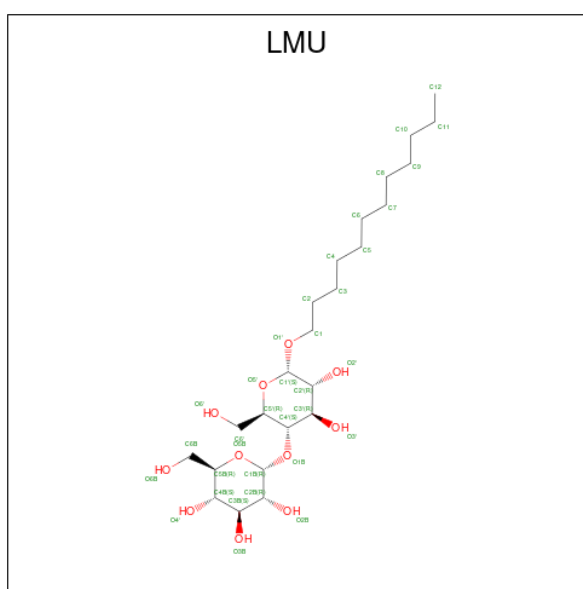
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
22	A	1	8	4	4	0
22	C	1	8	4	4	0
22	C	1	8	4	4	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			43	33	10	
23	F	1	Total	C	O	0
			30	20	10	
23	4	1	Total	C	O	0
			46	36	10	
23	4	1	Total	C	O	0
			45	35	10	

- Molecule 24 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



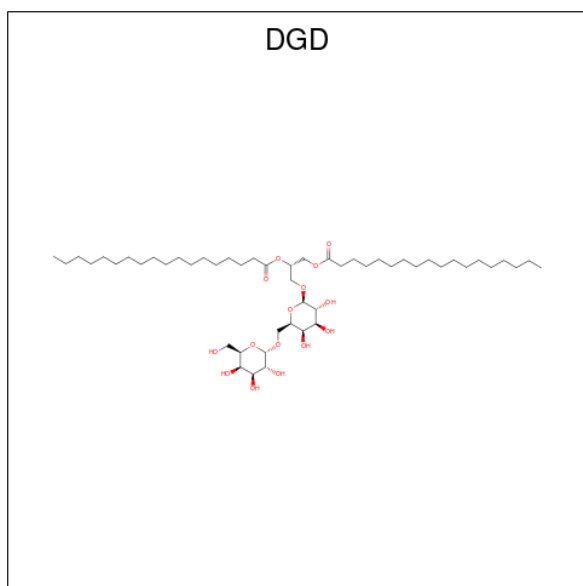
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			24	18	6	
24	A	1	Total	C	O	0
			35	24	11	
24	B	1	Total	C	O	0
			24	18	6	
24	H	1	Total	C	O	0
			24	18	6	
24	L	1	Total	C	O	0
			20	14	6	
24	F	1	Total	C	O	0
			35	24	11	
24	F	1	Total	C	O	0
			35	24	11	

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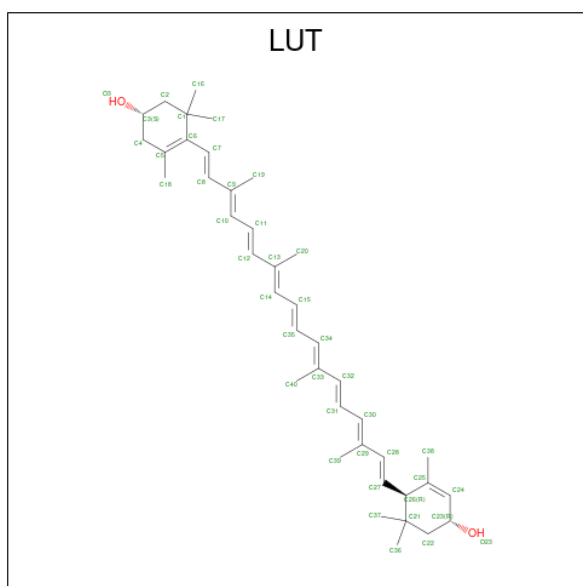
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	F	1	Total 35	C 24	O 11	0
24	F	1	Total 35	C 24	O 11	0
24	G	1	Total 35	C 24	O 11	0
24	G	1	Total 35	C 24	O 11	0
24	1	1	Total 35	C 24	O 11	0
24	1	1	Total 35	C 24	O 11	0
24	1	1	Total 24	C 18	O 6	0
24	2	1	Total 35	C 24	O 11	0
24	4	1	Total 23	C 17	O 6	0
24	4	1	Total 35	C 24	O 11	0
24	4	1	Total 24	C 18	O 6	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			61	46	15	
25	J	1	Total	C	O	0
			58	43	15	
25	4	1	Total	C	O	0
			49	34	15	

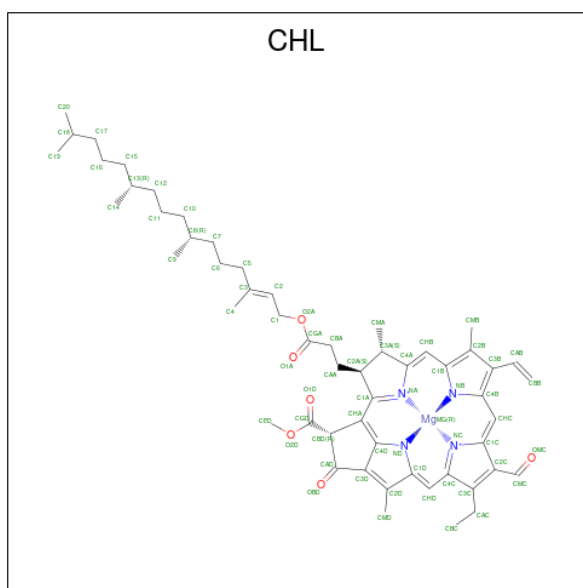
- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	J	1	Total	C	O	0
			42	40	2	
26	1	1	Total	C	O	0
			42	40	2	
26	1	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	

- Molecule 27 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as

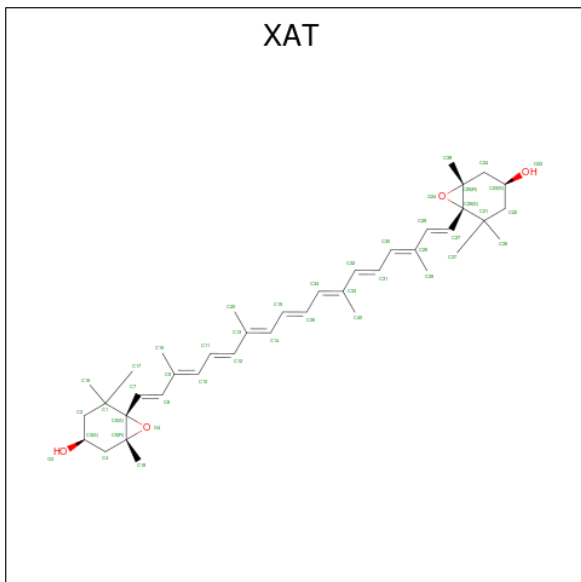
"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
27	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
27	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
27	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
27	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
27	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

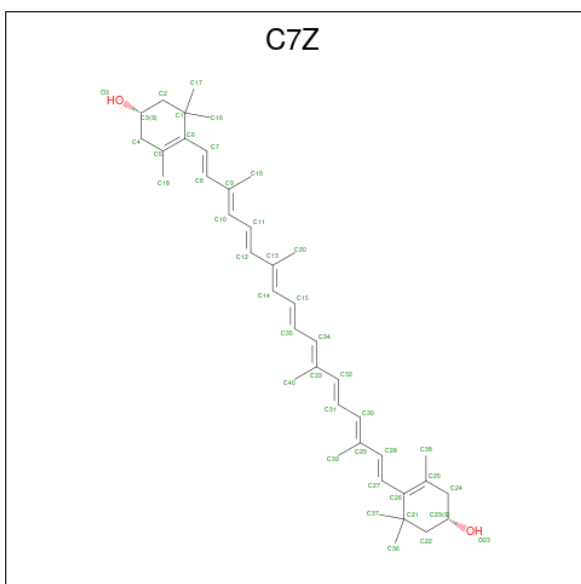
- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA

,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



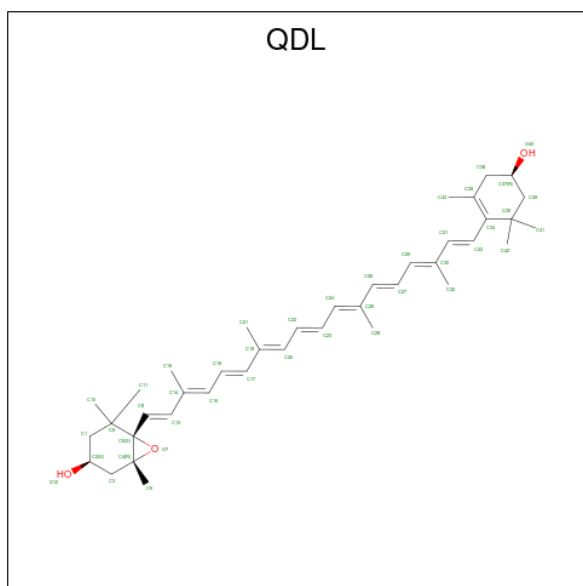
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	

- Molecule 29 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 is Antheraxanthin (CCD ID: QDL) (formula: $C_{40}H_{56}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	4	1	Total	C	O	0
			43	40	3	

- Molecule 31 is water.

Mol	Chain	Residues	Atoms		AltConf
31	A	199	Total	O	0
			199	199	
31	B	267	Total	O	0
			267	267	
31	C	75	Total	O	0
			75	75	
31	D	58	Total	O	0
			58	58	
31	E	22	Total	O	0
			22	22	
31	H	7	Total	O	0
			7	7	
31	I	5	Total	O	0
			5	5	

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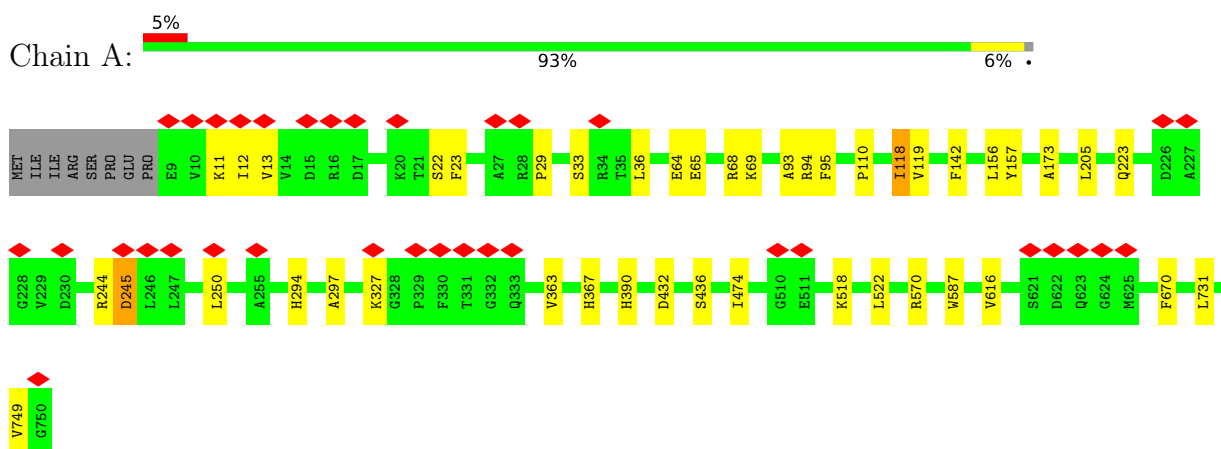
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Mol	Chain	Residues	Atoms		AltConf
31	L	12	Total 12	O 12	0
31	F	32	Total 32	O 32	0
31	G	2	Total 2	O 2	0
31	J	8	Total 8	O 8	0
31	K	2	Total 2	O 2	0
31	1	4	Total 4	O 4	0
31	2	4	Total 4	O 4	0
31	3	2	Total 2	O 2	0
31	4	4	Total 4	O 4	0

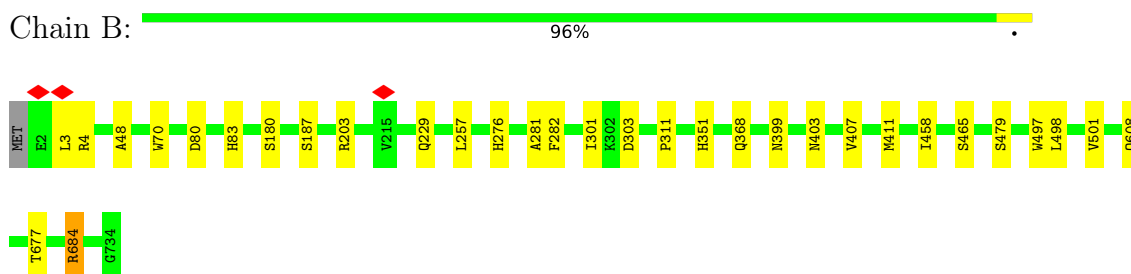
3 Residue-property plots [i](#)

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.

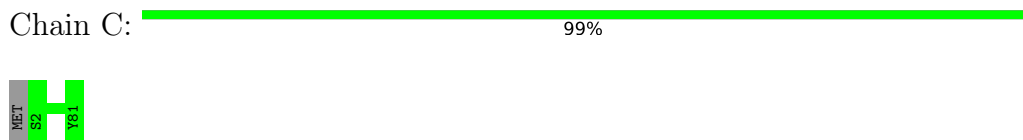
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2




- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II

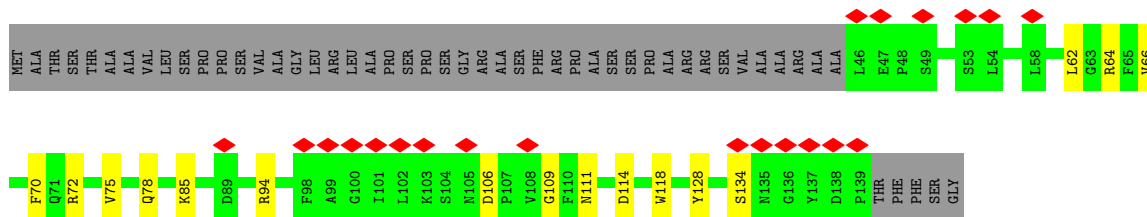


Chain F: 




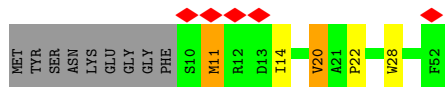
• Molecule 10: Photosystem I reaction center subunit V

Chain G: 



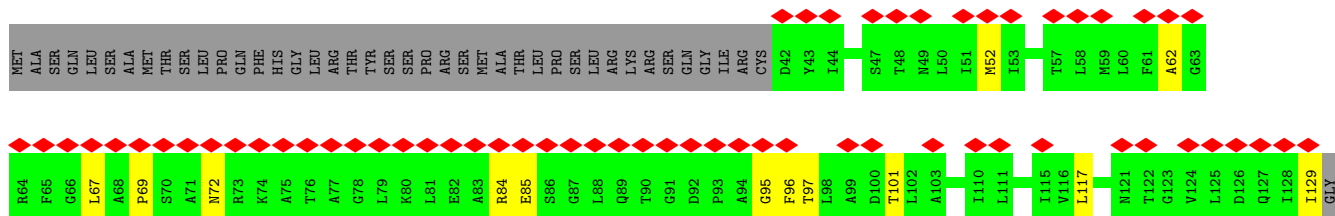
• Molecule 11: Photosystem I reaction center subunit IX

Chain J: 



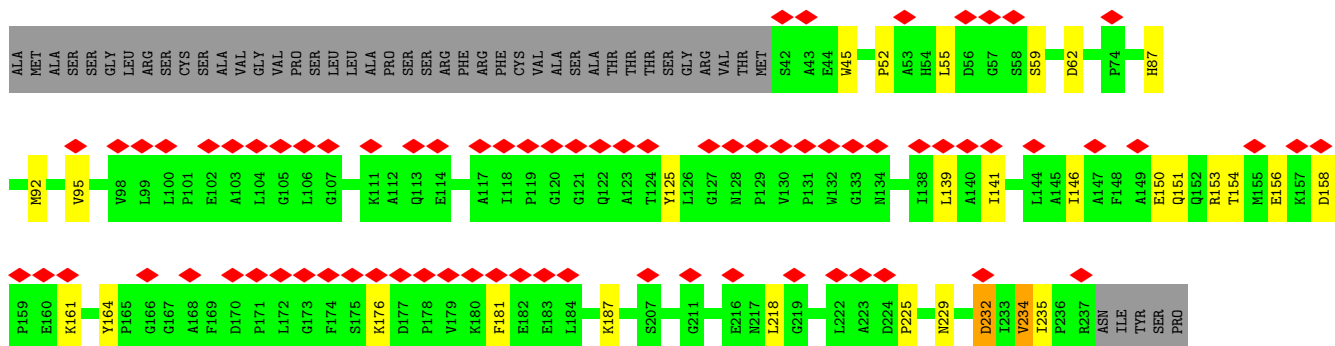
• Molecule 12: Photosystem I reaction center subunit X

Chain K: 

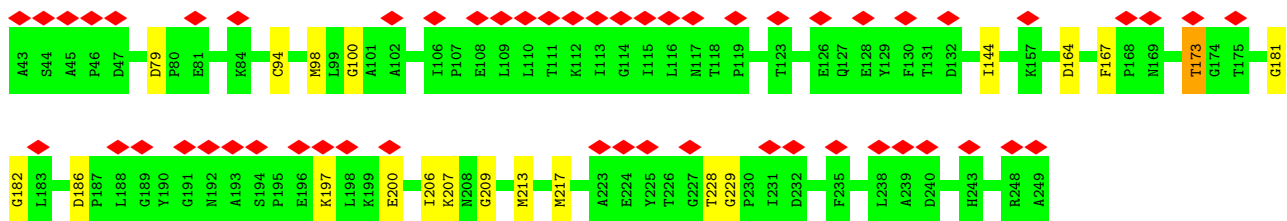
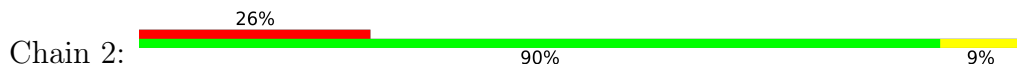


• Molecule 13: Chlorophyll a-b binding protein 1, chloroplastic

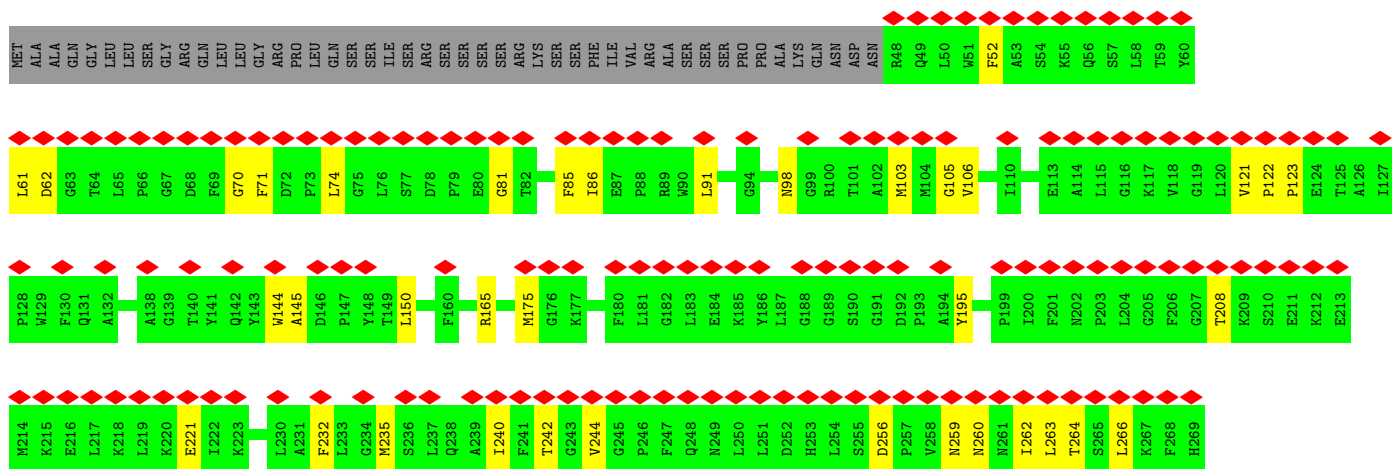
Chain 1: 



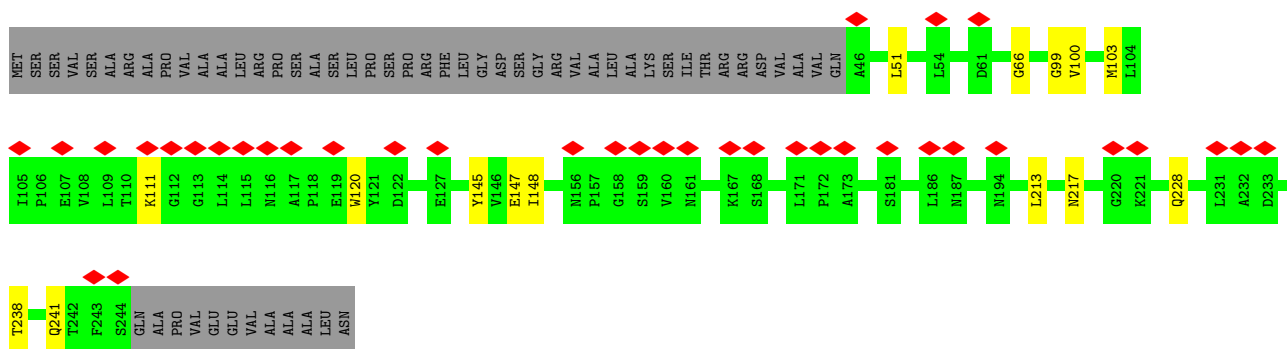
• Molecule 14: Chlorophyll a-b binding protein 2, chloroplastic



• Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



• Molecule 16: Chlorophyll a-b binding protein 4, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.346	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.434	Depositor
Minimum map value	-0.157	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	425.0, 425.0, 425.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, DGD, XAT, C7Z, CLA, LUT, QDL, LMU, SF4, CL0, LMG, BCR, CHL, LHG

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	0.20	0/6038	0.36	0/8237
2	B	0.20	0/6075	0.36	0/8297
3	C	0.16	0/616	0.41	0/834
4	D	0.14	0/1153	0.35	0/1557
5	E	0.11	0/546	0.29	0/743
6	H	0.12	0/737	0.31	0/1002
7	I	0.14	0/264	0.33	0/359
8	L	0.13	0/1227	0.32	0/1678
9	F	0.16	0/1269	0.30	0/1716
10	G	0.12	0/738	0.31	0/1004
11	J	0.14	0/352	0.35	0/479
12	K	0.10	0/633	0.24	0/855
13	1	0.14	0/1569	0.32	0/2137
14	2	0.12	0/1666	0.27	0/2282
15	3	0.13	0/1780	0.33	0/2414
16	4	0.16	0/1604	0.34	0/2187
All	All	0.17	0/26267	0.34	0/35781

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5840	0	5691	37	0
2	B	5864	0	5642	25	0
3	C	605	0	587	0	0
4	D	1124	0	1128	5	0
5	E	533	0	538	0	0
6	H	715	0	715	5	0
7	I	258	0	285	3	0
8	L	1192	0	1196	11	0
9	F	1238	0	1257	8	0
10	G	721	0	713	13	0
11	J	342	0	351	3	0
12	K	628	0	653	6	0
13	1	1519	0	1485	24	0
14	2	1609	0	1554	11	0
15	3	1725	0	1689	28	0
16	4	1555	0	1502	12	0
17	A	65	0	72	0	0
17	H	55	0	49	2	0
18	1	630	0	561	24	0
18	2	565	0	544	6	0
18	3	511	0	432	16	0
18	4	598	0	546	11	0
18	A	2670	0	2645	46	0
18	B	2297	0	2368	30	0
18	F	180	0	183	6	0
18	G	148	0	119	6	0
18	J	45	0	33	0	0
18	K	150	0	125	0	0
18	L	150	0	125	3	0
19	A	33	0	46	0	0
19	B	33	0	46	0	0
20	1	49	0	74	5	0
20	2	43	0	56	2	0
20	A	80	0	106	4	0
20	B	88	0	125	2	0
21	3	40	0	56	4	0
21	4	40	0	56	3	0
21	A	200	0	280	11	0
21	B	200	0	280	4	0
21	F	80	0	111	2	0
21	G	80	0	112	4	0
21	I	40	0	56	0	0
21	J	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	K	80	0	112	2	0
21	L	120	0	168	3	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	4	91	0	128	5	0
23	A	43	0	59	3	0
23	F	30	0	30	2	0
24	1	94	0	127	4	0
24	2	35	0	46	1	0
24	4	82	0	111	2	0
24	A	59	0	81	1	0
24	B	24	0	35	1	0
24	F	140	0	184	6	0
24	G	70	0	92	4	0
24	H	24	0	35	1	0
24	L	20	0	24	2	0
25	4	49	0	56	1	0
25	B	61	0	83	0	0
25	J	58	0	77	3	0
26	1	84	0	112	5	0
26	2	42	0	56	1	0
26	3	84	0	112	4	0
26	4	42	0	56	4	0
26	J	42	0	56	3	0
27	1	112	0	101	5	0
27	2	195	0	136	1	0
27	3	117	0	107	5	0
27	4	209	0	169	2	0
28	1	44	0	56	2	0
28	2	44	0	56	1	0
29	1	42	0	0	0	0
30	4	43	0	0	0	0
31	1	4	0	0	0	0
31	2	4	0	0	0	0
31	3	2	0	0	0	0
31	4	4	0	0	0	0
31	A	199	0	0	2	0
31	B	267	0	0	3	0
31	C	75	0	0	0	0
31	D	58	0	0	0	0
31	E	22	0	0	0	0
31	F	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	G	2	0	0	1	0
31	H	7	0	0	0	0
31	I	5	0	0	0	0
31	J	8	0	0	0	0
31	K	2	0	0	0	0
31	L	12	0	0	0	0
All	All	37485	0	36713	311	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 4.

The worst 5 of 311 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)
18:4:609:CLA:HAB	26:4:616:LUT:H12	1.60	0.81
13:1:146:ILE:HG22	18:1:309:CLA:HAB	1.66	0.77
13:1:95:VAL:HG11	26:1:316:LUT:H32	1.65	0.76
13:1:87:HIS:HD2	28:1:317:XAT:H35	1.49	0.75
18:A:823:CLA:HAB	18:A:845:CLA:HBB1	1.72	0.72

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	740/750 (99%)	717 (97%)	22 (3%)	1 (0%)	48	57
2	B	731/734 (100%)	715 (98%)	16 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/206 (68%)	136 (96%)	5 (4%)	0	100	100
5	E	65/143 (46%)	65 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	92/94 (98%)	92 (100%)	0	0	100	100
7	I	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
8	L	155/213 (73%)	152 (98%)	3 (2%)	0	100	100
9	F	156/178 (88%)	153 (98%)	3 (2%)	0	100	100
10	G	92/144 (64%)	86 (94%)	6 (6%)	0	100	100
11	J	41/52 (79%)	41 (100%)	0	0	100	100
12	K	84/130 (65%)	82 (98%)	2 (2%)	0	100	100
13	1	193/242 (80%)	186 (96%)	7 (4%)	0	100	100
14	2	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
15	3	220/269 (82%)	205 (93%)	15 (7%)	0	100	100
16	4	197/256 (77%)	189 (96%)	8 (4%)	0	100	100
All	All	3221/3735 (86%)	3126 (97%)	94 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	VAL

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	600/608 (99%)	597 (100%)	3 (0%)	81	90
2	B	598/599 (100%)	595 (100%)	3 (0%)	81	90
3	C	70/71 (99%)	70 (100%)	0	100	100
4	D	120/163 (74%)	119 (99%)	1 (1%)	73	85
5	E	59/115 (51%)	58 (98%)	1 (2%)	53	69
6	H	76/76 (100%)	75 (99%)	1 (1%)	61	76
7	I	30/33 (91%)	30 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	L	123/168 (73%)	122 (99%)	1 (1%)	73	85
9	F	128/142 (90%)	125 (98%)	3 (2%)	44	59
10	G	77/112 (69%)	76 (99%)	1 (1%)	61	76
11	J	37/44 (84%)	35 (95%)	2 (5%)	20	25
12	K	66/102 (65%)	63 (96%)	3 (4%)	24	33
13	1	155/192 (81%)	150 (97%)	5 (3%)	34	47
14	2	165/165 (100%)	162 (98%)	3 (2%)	51	68
15	3	176/216 (82%)	171 (97%)	5 (3%)	38	52
16	4	160/203 (79%)	160 (100%)	0	100	100
All	All	2640/3009 (88%)	2608 (99%)	32 (1%)	61	78

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	3	121	VAL
15	3	175	MET
9	F	155	ILE
9	F	137	ARG
15	3	208	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
14	2	233	ASN
16	4	174	HIS
16	4	237	ASN
16	4	236	HIS
2	B	83	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](#)

224 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMU	G	203	-	36,36,36	0.09	0	47,47,47	0.29	0
26	LUT	3	315	-	42,43,43	0.19	0	51,60,60	0.35	0
18	CLA	4	610	-	49,53,73	1.40	4 (8%)	58,89,113	0.95	2 (3%)
18	CLA	3	311	-	49,53,73	1.40	4 (8%)	58,89,113	0.95	2 (3%)
30	QDL	4	617	-	42,45,45	0.14	0	55,67,67	0.68	3 (5%)
24	LMU	4	621	-	23,23,36	0.13	0	28,28,47	0.26	0
18	CLA	A	856	-	49,53,73	1.38	4 (8%)	58,89,113	0.97	2 (3%)
18	CLA	B	837	-	69,73,73	1.07	4 (5%)	82,113,113	0.82	2 (2%)
24	LMU	2	618	-	36,36,36	0.09	0	47,47,47	0.15	0
18	CLA	3	310	15	59,63,73	1.25	4 (6%)	70,101,113	0.88	2 (2%)
18	CLA	B	813	-	69,73,73	1.15	4 (5%)	82,113,113	0.82	2 (2%)
20	LHG	A	847	18	30,30,48	0.28	0	33,36,54	0.34	0
24	LMU	1	320	-	36,36,36	0.10	0	47,47,47	0.17	0
18	CLA	A	841	-	69,73,73	1.09	4 (5%)	82,113,113	0.82	2 (2%)
23	LMG	4	619	-	46,46,55	0.18	0	54,54,63	0.14	0
25	DGD	J	104	-	59,59,67	0.16	0	73,73,81	0.16	0
18	CLA	A	826	31	69,73,73	1.15	4 (5%)	82,113,113	0.84	2 (2%)
21	BCR	B	840	-	41,41,41	0.28	0	56,56,56	0.44	0
27	CHL	4	607	-	45,59,74	2.24	10 (22%)	40,96,114	1.21	5 (12%)
18	CLA	L	304	-	64,68,73	1.15	5 (7%)	76,107,113	0.87	3 (3%)
18	CLA	A	842	-	69,73,73	1.07	4 (5%)	82,113,113	0.88	4 (4%)
18	CLA	1	312	13	49,53,73	1.38	4 (8%)	58,89,113	0.97	3 (5%)
21	BCR	L	307	-	41,41,41	0.13	0	56,56,56	0.31	0
18	CLA	A	820	-	69,73,73	1.17	5 (7%)	82,113,113	0.80	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	830	-	69,73,73	1.12	4 (5%)	82,113,113	0.80	2 (2%)
18	CLA	B	811	-	56,60,73	1.30	4 (7%)	65,97,113	0.91	2 (3%)
20	LHG	B	846	18	38,38,48	0.25	0	41,44,54	0.31	0
18	CLA	1	311	-	49,53,73	1.37	4 (8%)	58,89,113	0.96	2 (3%)
18	CLA	A	825	-	64,68,73	1.20	4 (6%)	76,107,113	0.83	2 (2%)
18	CLA	B	807	-	69,73,73	1.11	4 (5%)	82,113,113	0.81	2 (2%)
18	CLA	A	803	31	69,73,73	1.16	4 (5%)	82,113,113	0.84	2 (2%)
23	LMG	F	810	-	30,30,55	0.20	0	38,38,63	0.19	0
27	CHL	2	605	31	45,59,74	2.22	10 (22%)	40,96,114	1.32	5 (12%)
18	CLA	1	310	13	59,63,73	1.32	4 (6%)	70,101,113	0.94	2 (2%)
18	CLA	1	314	-	49,53,73	1.39	4 (8%)	58,89,113	0.96	3 (5%)
23	LMG	4	620	-	45,45,55	0.19	0	53,53,63	0.22	0
18	CLA	B	819	-	62,66,73	1.20	4 (6%)	73,104,113	0.91	3 (4%)
28	XAT	2	616	-	41,47,47	0.12	0	54,74,74	0.49	0
18	CLA	B	825	-	69,73,73	1.19	4 (5%)	82,113,113	0.87	3 (3%)
24	LMU	F	809	-	36,36,36	0.11	0	47,47,47	0.36	0
21	BCR	B	843	-	41,41,41	0.17	0	56,56,56	0.34	0
21	BCR	I	101	-	41,41,41	0.15	0	56,56,56	0.41	0
21	BCR	F	801	-	41,41,41	0.34	0	56,56,56	0.49	0
24	LMU	4	623	-	36,36,36	0.10	0	47,47,47	0.42	0
28	XAT	1	317	-	41,47,47	0.13	0	54,74,74	0.58	0
18	CLA	A	807	1	69,73,73	1.15	4 (5%)	82,113,113	0.79	2 (2%)
18	CLA	1	306	-	49,53,73	1.39	4 (8%)	58,89,113	0.99	3 (5%)
27	CHL	4	606	31	40,54,74	2.38	10 (25%)	34,90,114	1.36	5 (14%)
18	CLA	A	828	-	69,73,73	1.16	4 (5%)	82,113,113	0.82	2 (2%)
18	CLA	B	818	-	64,68,73	1.21	4 (6%)	76,107,113	0.83	2 (2%)
25	DGD	B	845	-	62,62,67	0.17	0	76,76,81	0.29	0
18	CLA	A	813	-	49,53,73	1.39	4 (8%)	58,89,113	0.97	2 (3%)
18	CLA	2	604	-	49,53,73	1.39	4 (8%)	58,89,113	0.96	2 (3%)
21	BCR	3	313	-	41,41,41	0.14	0	56,56,56	0.40	0
26	LUT	3	314	-	42,43,43	0.18	0	51,60,60	0.56	0
18	CLA	2	612	14	69,73,73	1.18	4 (5%)	82,113,113	0.81	2 (2%)
18	CLA	2	613	-	54,58,73	1.30	4 (7%)	64,95,113	0.93	3 (4%)
24	LMU	1	321	-	24,24,36	0.11	0	29,29,47	0.24	0
21	BCR	F	806	-	41,41,41	0.24	0	56,56,56	0.39	0
18	CLA	B	830	-	69,73,73	1.13	5 (7%)	82,113,113	0.80	2 (2%)
18	CLA	A	818	-	64,68,73	1.19	4 (6%)	76,107,113	0.92	4 (5%)
24	LMU	F	807	-	36,36,36	0.11	0	47,47,47	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	808	-	51,55,73	1.30	4 (7%)	60,91,113	0.95	2 (3%)
18	CLA	B	814	-	49,53,73	1.31	4 (8%)	58,89,113	0.96	3 (5%)
18	CLA	B	833	-	65,69,73	1.14	4 (6%)	77,108,113	0.87	2 (2%)
18	CLA	K	203	31	64,68,73	1.23	5 (7%)	76,107,113	0.85	2 (2%)
18	CLA	2	602	14	69,73,73	1.17	4 (5%)	82,113,113	0.81	3 (3%)
24	LMU	H	201	-	24,24,36	0.11	0	29,29,47	0.24	0
18	CLA	B	836	31	69,73,73	1.10	4 (5%)	82,113,113	0.84	3 (3%)
18	CLA	3	305	15	65,69,73	1.20	4 (6%)	77,108,113	0.84	2 (2%)
21	BCR	B	842	-	41,41,41	0.17	0	56,56,56	0.46	0
21	BCR	J	103	-	41,41,41	0.27	0	56,56,56	0.45	0
18	CLA	A	832	-	49,53,73	1.32	4 (8%)	58,89,113	0.97	2 (3%)
18	CLA	3	307	15	64,68,73	1.23	4 (6%)	76,107,113	0.85	2 (2%)
18	CLA	B	820	-	69,73,73	1.14	4 (5%)	82,113,113	0.85	3 (3%)
21	BCR	A	850	-	41,41,41	0.14	0	56,56,56	0.39	0
18	CLA	1	308	31	49,53,73	1.40	4 (8%)	58,89,113	0.98	2 (3%)
18	CLA	4	614	-	54,58,73	1.27	4 (7%)	64,95,113	0.91	2 (3%)
18	CLA	B	816	-	69,73,73	1.14	4 (5%)	82,113,113	0.81	2 (2%)
18	CLA	4	604	31	49,53,73	1.40	4 (8%)	58,89,113	0.98	2 (3%)
18	CLA	B	824	-	69,73,73	1.16	4 (5%)	82,113,113	0.82	2 (2%)
21	BCR	A	851	-	41,41,41	0.17	0	56,56,56	0.34	0
18	CLA	A	819	-	60,64,73	1.24	4 (6%)	71,102,113	0.87	2 (2%)
18	CLA	A	823	-	56,60,73	1.29	4 (7%)	65,97,113	0.94	3 (4%)
18	CLA	3	304	31	49,53,73	1.41	4 (8%)	58,89,113	0.99	2 (3%)
18	CLA	K	204	-	49,53,73	1.40	4 (8%)	58,89,113	0.99	2 (3%)
23	LMG	A	857	-	43,43,55	0.18	0	51,51,63	0.16	0
18	CLA	A	838	-	55,59,73	1.25	4 (7%)	64,96,113	0.94	2 (3%)
18	CLA	B	803	-	49,53,73	1.36	4 (8%)	58,89,113	0.92	2 (3%)
18	CLA	B	834	-	69,73,73	1.08	4 (5%)	82,113,113	0.87	4 (4%)
18	CLA	B	817	31	59,63,73	1.24	4 (6%)	70,101,113	0.89	3 (4%)
18	CLA	2	601	14	69,73,73	1.18	4 (5%)	82,113,113	0.83	2 (2%)
18	CLA	B	810	-	60,64,73	1.22	4 (6%)	71,102,113	0.88	2 (2%)
17	CL0	H	202	6	48,63,73	1.50	6 (12%)	48,101,113	1.83	5 (10%)
24	LMU	1	301	-	36,36,36	0.12	0	47,47,47	0.39	0
18	CLA	A	811	-	49,53,73	1.33	4 (8%)	58,89,113	1.00	3 (5%)
21	BCR	G	202	-	41,41,41	0.17	0	56,56,56	0.37	0
27	CHL	2	606	31	40,54,74	2.35	10 (25%)	34,90,114	1.43	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	831	-	69,73,73	1.11	4 (5%)	82,113,113	0.80	2 (2%)
18	CLA	A	802	-	69,73,73	1.04	4 (5%)	82,113,113	0.76	2 (2%)
21	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.30	0
18	CLA	B	826	-	69,73,73	1.14	4 (5%)	82,113,113	0.81	2 (2%)
18	CLA	A	815	-	58,62,73	1.23	4 (6%)	68,99,113	0.91	2 (2%)
18	CLA	A	834	-	69,73,73	1.13	4 (5%)	82,113,113	0.85	2 (2%)
18	CLA	A	845	20	49,53,73	1.41	4 (8%)	58,89,113	0.97	2 (3%)
18	CLA	B	827	-	69,73,73	1.12	4 (5%)	82,113,113	0.83	2 (2%)
21	BCR	B	841	-	41,41,41	0.15	0	56,56,56	0.35	0
18	CLA	A	810	1	54,58,73	1.31	4 (7%)	64,95,113	0.95	2 (3%)
21	BCR	B	844	-	41,41,41	0.16	0	56,56,56	0.30	0
24	LMU	F	803	-	36,36,36	0.12	0	47,47,47	0.42	0
18	CLA	B	812	-	69,73,73	1.14	4 (5%)	82,113,113	0.83	2 (2%)
18	CLA	F	802	-	69,73,73	1.14	4 (5%)	82,113,113	0.90	3 (3%)
18	CLA	A	829	-	69,73,73	1.15	4 (5%)	82,113,113	0.84	2 (2%)
20	LHG	2	617	18	42,42,48	0.23	0	45,48,54	0.29	0
21	BCR	K	205	-	41,41,41	0.15	0	56,56,56	0.28	0
18	CLA	B	802	-	69,73,73	1.10	4 (5%)	82,113,113	0.76	2 (2%)
18	CLA	A	816	-	64,68,73	1.16	4 (6%)	76,107,113	0.85	3 (3%)
18	CLA	1	305	31	54,58,73	1.32	4 (7%)	64,95,113	0.93	2 (3%)
18	CLA	1	313	13	69,73,73	1.16	4 (5%)	82,113,113	0.89	2 (2%)
18	CLA	A	821	-	49,53,73	1.37	4 (8%)	58,89,113	0.95	2 (3%)
18	CLA	A	804	-	69,73,73	1.14	4 (5%)	82,113,113	0.86	3 (3%)
18	CLA	B	809	-	69,73,73	1.13	4 (5%)	82,113,113	0.79	2 (2%)
18	CLA	B	831	-	69,73,73	1.12	4 (5%)	82,113,113	0.84	2 (2%)
24	LMU	A	858	-	24,24,36	0.10	0	29,29,47	0.25	0
18	CLA	A	827	31	59,63,73	1.20	5 (8%)	70,101,113	0.89	2 (2%)
24	LMU	B	848	-	24,24,36	0.13	0	29,29,47	0.22	0
26	LUT	4	616	-	42,43,43	0.22	0	51,60,60	0.46	0
18	CLA	3	308	15	59,63,73	1.24	4 (6%)	70,101,113	0.89	3 (4%)
19	PQN	B	838	-	34,34,34	0.33	0	43,45,45	0.41	0
27	CHL	4	615	16	40,54,74	2.34	10 (25%)	34,90,114	1.42	5 (14%)
18	CLA	B	835	-	54,58,73	1.27	4 (7%)	64,95,113	0.92	2 (3%)
18	CLA	B	822	31	69,73,73	1.20	4 (5%)	82,113,113	0.85	2 (2%)
26	LUT	J	101	-	42,43,43	0.19	0	51,60,60	0.59	1 (1%)
18	CLA	B	808	2	69,73,73	1.16	4 (5%)	82,113,113	0.82	2 (2%)
18	CLA	4	612	16	69,73,73	1.16	4 (5%)	82,113,113	0.83	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	J	102	11	49,53,73	1.37	4 (8%)	58,89,113	0.95	2 (3%)
26	LUT	2	615	-	42,43,43	0.26	0	51,60,60	0.36	0
26	LUT	1	316	-	42,43,43	0.20	0	51,60,60	0.45	0
18	CLA	A	809	1	69,73,73	1.14	4 (5%)	82,113,113	0.97	4 (4%)
18	CLA	4	613	-	50,54,73	1.34	4 (8%)	59,90,113	0.95	3 (5%)
21	BCR	K	202	-	41,41,41	0.26	0	56,56,56	0.51	1 (1%)
18	CLA	A	833	-	59,63,73	1.24	4 (6%)	70,101,113	0.87	2 (2%)
18	CLA	B	823	31	69,73,73	1.10	4 (5%)	82,113,113	0.83	2 (2%)
18	CLA	4	602	16	64,68,73	1.22	4 (6%)	76,107,113	0.85	2 (2%)
27	CHL	1	302	13	60,74,74	1.93	10 (16%)	58,114,114	1.02	4 (6%)
18	CLA	L	305	31	49,53,73	1.38	4 (8%)	58,89,113	0.97	2 (3%)
27	CHL	1	307	13	40,54,74	2.39	10 (25%)	34,90,114	1.27	4 (11%)
27	CHL	2	614	14	41,55,74	2.31	10 (24%)	35,91,114	1.43	5 (14%)
18	CLA	4	603	16	69,73,73	1.12	4 (5%)	82,113,113	0.84	4 (4%)
22	SF4	C	101	3	0,12,12	-	-	-	-	-
18	CLA	A	805	18	54,58,73	1.26	4 (7%)	64,95,113	0.93	2 (3%)
20	LHG	A	846	-	48,48,48	0.24	0	51,54,54	0.29	0
24	LMU	F	808	-	36,36,36	0.10	0	47,47,47	0.20	0
27	CHL	3	306	31	45,59,74	2.23	10 (22%)	40,96,114	1.38	5 (12%)
27	CHL	3	301	15	60,74,74	1.92	10 (16%)	58,114,114	1.12	5 (8%)
18	CLA	A	855	31	69,73,73	1.09	4 (5%)	82,113,113	0.83	3 (3%)
18	CLA	3	303	-	49,53,73	1.39	4 (8%)	58,89,113	0.97	3 (5%)
18	CLA	A	840	-	59,63,73	1.23	4 (6%)	70,101,113	0.93	2 (2%)
18	CLA	1	309	13	69,73,73	1.15	4 (5%)	82,113,113	0.77	2 (2%)
18	CLA	3	309	15	49,53,73	1.36	4 (8%)	58,89,113	0.98	3 (5%)
18	CLA	3	302	15	59,63,73	1.27	4 (6%)	70,101,113	0.88	2 (2%)
18	CLA	4	601	16	54,58,73	1.31	4 (7%)	64,95,113	0.94	2 (3%)
18	CLA	4	608	16	69,73,73	1.18	4 (5%)	82,113,113	0.90	3 (3%)
21	BCR	L	306	-	41,41,41	0.24	0	56,56,56	0.53	1 (1%)
18	CLA	A	814	-	69,73,73	1.14	4 (5%)	82,113,113	0.81	2 (2%)
18	CLA	B	815	-	64,68,73	1.20	4 (6%)	76,107,113	0.86	2 (2%)
27	CHL	2	607	-	45,59,74	2.22	11 (24%)	40,96,114	1.30	5 (12%)
18	CLA	K	201	12	49,53,73	1.41	4 (8%)	58,89,113	0.99	3 (5%)
18	CLA	F	804	31	69,73,73	1.16	4 (5%)	82,113,113	0.84	2 (2%)
18	CLA	2	609	14	64,68,73	1.21	4 (6%)	76,107,113	0.84	2 (2%)
21	BCR	A	848	-	41,41,41	0.15	0	56,56,56	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	SF4	C	102	3	0,12,12	-	-	-		
18	CLA	B	839	20	69,73,73	1.17	4 (5%)	82,113,113	0.82	2 (2%)
21	BCR	L	302	-	41,41,41	0.15	0	56,56,56	0.33	0
25	DGD	4	622	-	50,50,67	0.17	0	64,64,81	0.36	0
18	CLA	G	205	10	50,54,73	1.38	4 (8%)	59,90,113	0.95	3 (5%)
18	CLA	1	303	13	69,73,73	1.16	4 (5%)	82,113,113	0.82	3 (3%)
24	LMU	L	301	-	20,20,36	0.13	0	25,25,47	0.32	0
18	CLA	G	204	-	49,53,73	1.40	4 (8%)	58,89,113	0.98	3 (5%)
18	CLA	A	822	31	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
18	CLA	B	804	-	69,73,73	1.10	4 (5%)	82,113,113	0.82	3 (3%)
18	CLA	B	821	-	49,53,73	1.39	4 (8%)	58,89,113	0.95	2 (3%)
18	CLA	4	609	16	64,68,73	1.23	4 (6%)	76,107,113	0.81	2 (2%)
19	PQN	A	844	-	34,34,34	0.36	0	43,45,45	0.41	0
24	LMU	G	207	-	36,36,36	0.11	0	47,47,47	0.25	0
18	CLA	B	806	-	64,68,73	1.17	4 (6%)	76,107,113	0.84	2 (2%)
18	CLA	A	839	-	69,73,73	1.11	4 (5%)	82,113,113	0.84	2 (2%)
21	BCR	4	618	-	41,41,41	0.18	0	56,56,56	0.46	0
17	CL0	A	801	-	58,73,73	1.26	7 (12%)	60,113,113	1.72	5 (8%)
18	CLA	A	836	-	69,73,73	1.14	4 (5%)	82,113,113	0.82	2 (2%)
18	CLA	G	201	-	61,65,73	1.22	4 (6%)	72,103,113	0.87	2 (2%)
22	SF4	A	853	1,2	0,12,12	-	-	-		
18	CLA	1	304	-	64,68,73	1.19	4 (6%)	76,107,113	0.85	3 (3%)
18	CLA	B	828	-	49,53,73	1.30	4 (8%)	58,89,113	0.94	2 (3%)
18	CLA	A	806	-	69,73,73	1.10	4 (5%)	82,113,113	0.82	2 (2%)
18	CLA	A	835	-	69,73,73	1.13	4 (5%)	82,113,113	0.83	3 (3%)
18	CLA	A	824	-	49,53,73	1.37	5 (10%)	58,89,113	0.97	3 (5%)
18	CLA	F	805	9	54,58,73	1.25	4 (7%)	64,95,113	0.90	2 (3%)
18	CLA	A	843	31	69,73,73	1.12	4 (5%)	82,113,113	0.85	3 (3%)
24	LMU	A	859	-	36,36,36	0.10	0	47,47,47	0.21	0
18	CLA	1	315	13	49,53,73	1.37	4 (8%)	58,89,113	0.95	2 (3%)
18	CLA	A	812	18	69,73,73	1.12	5 (7%)	82,113,113	0.82	3 (3%)
18	CLA	L	303	8	49,53,73	1.37	4 (8%)	58,89,113	0.98	3 (5%)
27	CHL	4	605	31	60,74,74	1.90	10 (16%)	58,114,114	1.12	6 (10%)
18	CLA	2	610	20	64,68,73	1.22	4 (6%)	76,107,113	0.84	2 (2%)
18	CLA	B	829	-	69,73,73	1.17	4 (5%)	82,113,113	0.81	2 (2%)
18	CLA	3	312	-	49,53,73	1.38	4 (8%)	58,89,113	0.95	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	2	611	14	49,53,73	1.36	4 (8%)	58,89,113	0.96	3 (5%)
20	LHG	1	319	-	48,48,48	0.22	0	51,54,54	0.27	0
21	BCR	G	206	-	41,41,41	0.14	0	56,56,56	0.37	0
29	C7Z	1	322	-	43,43,43	0.11	0	56,60,60	0.28	0
18	CLA	2	603	-	69,73,73	1.15	4 (5%)	82,113,113	0.80	2 (2%)
18	CLA	B	801	-	69,73,73	1.12	4 (5%)	82,113,113	0.81	2 (2%)
18	CLA	B	805	2	69,73,73	1.17	4 (5%)	82,113,113	0.78	2 (2%)
26	LUT	1	318	-	42,43,43	0.21	0	51,60,60	0.41	0
20	LHG	B	847	-	48,48,48	0.22	0	51,54,54	0.26	0
18	CLA	A	854	31	69,73,73	1.15	4 (5%)	82,113,113	0.82	2 (2%)
18	CLA	4	611	16	51,55,73	1.35	4 (7%)	60,91,113	0.97	2 (3%)
21	BCR	A	852	-	41,41,41	0.22	0	56,56,56	0.43	0
24	LMU	4	624	-	24,24,36	0.12	0	29,29,47	0.25	0
18	CLA	A	817	31	49,53,73	1.39	4 (8%)	58,89,113	0.97	2 (3%)
18	CLA	B	832	31	49,53,73	1.40	4 (8%)	58,89,113	0.98	2 (3%)
18	CLA	2	608	14	49,53,73	1.37	4 (8%)	58,89,113	0.96	3 (5%)
18	CLA	A	837	1	49,53,73	1.35	4 (8%)	58,89,113	0.98	3 (5%)

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
24	LMU	G	203	-	-	3/21/61/61	0/2/2/2
26	LUT	3	315	-	-	0/29/67/67	0/2/2/2
18	CLA	4	610	-	1/1/11/20	3/15/91/115	-
18	CLA	3	311	-	1/1/11/20	6/15/91/115	-
30	QDL	4	617	-	-	0/30/80/80	0/3/3/3
24	LMU	4	621	-	-	2/14/34/61	0/1/1/2
18	CLA	A	856	-	1/1/11/20	5/15/91/115	-
18	CLA	B	837	-	1/1/15/20	5/39/115/115	-
24	LMU	2	618	-	-	2/21/61/61	0/2/2/2
18	CLA	3	310	15	1/1/13/20	5/27/103/115	-
18	CLA	B	813	-	1/1/15/20	2/39/115/115	-
27	CHL	4	607	-	3/3/17/26	1/21/119/137	-
20	LHG	A	847	18	-	12/35/35/53	-
18	CLA	A	841	-	1/1/15/20	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMG	4	619	-	-	1/41/61/70	0/1/1/1
24	LMU	1	320	-	-	3/21/61/61	0/2/2/2
18	CLA	A	826	31	1/1/15/20	6/39/115/115	-
21	BCR	B	840	-	-	2/29/63/63	0/2/2/2
25	DGD	J	104	-	-	5/47/87/95	0/2/2/2
18	CLA	L	304	-	1/1/14/20	3/33/109/115	-
18	CLA	A	842	-	1/1/15/20	8/39/115/115	-
18	CLA	1	312	13	1/1/11/20	6/15/91/115	-
21	BCR	L	307	-	-	2/29/63/63	0/2/2/2
18	CLA	A	820	-	1/1/15/20	7/39/115/115	-
18	CLA	A	830	-	1/1/15/20	2/39/115/115	-
18	CLA	B	811	-	1/1/12/20	2/24/100/115	-
20	LHG	B	846	18	-	7/43/43/53	-
18	CLA	1	311	-	1/1/11/20	4/15/91/115	-
18	CLA	A	825	-	1/1/14/20	2/33/109/115	-
18	CLA	B	807	-	1/1/15/20	10/39/115/115	-
18	CLA	A	803	31	1/1/15/20	2/39/115/115	-
27	CHL	2	605	31	3/3/17/26	1/21/119/137	-
23	LMG	F	810	-	-	2/25/45/70	0/1/1/1
18	CLA	1	310	13	1/1/13/20	3/27/103/115	-
18	CLA	1	314	-	1/1/11/20	4/15/91/115	-
23	LMG	4	620	-	-	4/40/60/70	0/1/1/1
18	CLA	B	819	-	1/1/13/20	6/31/107/115	-
28	XAT	2	616	-	-	0/31/93/93	0/4/4/4
18	CLA	B	825	-	1/1/15/20	5/39/115/115	-
24	LMU	F	809	-	-	1/21/61/61	0/2/2/2
21	BCR	B	843	-	-	1/29/63/63	0/2/2/2
21	BCR	I	101	-	-	0/29/63/63	0/2/2/2
21	BCR	F	801	-	-	0/29/63/63	0/2/2/2
24	LMU	4	623	-	-	4/21/61/61	0/2/2/2
28	XAT	1	317	-	-	0/31/93/93	0/4/4/4
18	CLA	A	807	1	1/1/15/20	8/39/115/115	-
18	CLA	1	306	-	1/1/11/20	1/15/91/115	-
27	CHL	4	606	31	3/3/16/26	0/15/113/137	-
18	CLA	A	828	-	1/1/15/20	2/39/115/115	-
18	CLA	B	818	-	1/1/14/20	6/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	B	845	-	-	10/50/90/95	0/2/2/2
18	CLA	A	813	-	1/1/11/20	2/15/91/115	-
18	CLA	2	604	-	1/1/11/20	0/15/91/115	-
21	BCR	3	313	-	-	4/29/63/63	0/2/2/2
26	LUT	3	314	-	-	0/29/67/67	0/2/2/2
18	CLA	2	612	14	1/1/15/20	3/39/115/115	-
18	CLA	2	613	-	1/1/12/20	2/21/97/115	-
24	LMU	1	321	-	-	0/15/35/61	0/1/1/2
21	BCR	F	806	-	-	2/29/63/63	0/2/2/2
18	CLA	B	830	-	1/1/15/20	4/39/115/115	-
18	CLA	A	818	-	1/1/14/20	2/33/109/115	-
24	LMU	F	807	-	-	4/21/61/61	0/2/2/2
18	CLA	A	808	-	1/1/11/20	0/18/94/115	-
18	CLA	B	814	-	1/1/11/20	2/15/91/115	-
18	CLA	B	833	-	1/1/14/20	2/35/111/115	-
18	CLA	K	203	31	1/1/14/20	5/33/109/115	-
18	CLA	2	602	14	1/1/15/20	2/39/115/115	-
24	LMU	H	201	-	-	3/15/35/61	0/1/1/2
18	CLA	B	836	31	1/1/15/20	5/39/115/115	-
18	CLA	3	305	15	1/1/14/20	6/35/111/115	-
21	BCR	B	842	-	-	2/29/63/63	0/2/2/2
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2
18	CLA	A	832	-	1/1/11/20	2/15/91/115	-
18	CLA	3	307	15	1/1/14/20	5/33/109/115	-
18	CLA	B	820	-	1/1/15/20	5/39/115/115	-
21	BCR	A	850	-	-	2/29/63/63	0/2/2/2
18	CLA	1	308	31	1/1/11/20	3/15/91/115	-
18	CLA	4	614	-	1/1/12/20	2/21/97/115	-
18	CLA	B	816	-	1/1/15/20	2/39/115/115	-
18	CLA	4	604	31	1/1/11/20	8/15/91/115	-
18	CLA	B	824	-	1/1/15/20	2/39/115/115	-
21	BCR	A	851	-	-	2/29/63/63	0/2/2/2
18	CLA	A	819	-	1/1/13/20	6/29/105/115	-
18	CLA	A	823	-	1/1/12/20	5/24/100/115	-
18	CLA	3	304	31	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	K	204	-	1/1/11/20	6/15/91/115	-
23	LMG	A	857	-	-	4/38/58/70	0/1/1/1
18	CLA	A	838	-	1/1/12/20	0/23/99/115	-
18	CLA	B	803	-	1/1/11/20	4/15/91/115	-
18	CLA	B	834	-	1/1/15/20	0/39/115/115	-
18	CLA	B	817	31	1/1/13/20	2/27/103/115	-
18	CLA	2	601	14	1/1/15/20	7/39/115/115	-
18	CLA	B	810	-	1/1/13/20	4/29/105/115	-
17	CL0	H	202	6	3/3/18/25	5/25/123/135	-
24	LMU	1	301	-	-	2/21/61/61	0/2/2/2
18	CLA	A	811	-	1/1/11/20	0/15/91/115	-
27	CHL	2	606	31	3/3/16/26	2/15/113/137	-
21	BCR	G	202	-	-	0/29/63/63	0/2/2/2
18	CLA	A	831	-	1/1/15/20	4/39/115/115	-
18	CLA	A	802	-	1/1/15/20	1/39/115/115	-
21	BCR	A	849	-	-	2/29/63/63	0/2/2/2
18	CLA	B	826	-	1/1/15/20	0/39/115/115	-
18	CLA	A	815	-	1/1/12/20	2/26/102/115	-
18	CLA	A	834	-	1/1/15/20	5/39/115/115	-
18	CLA	A	845	20	1/1/11/20	7/15/91/115	-
18	CLA	B	827	-	1/1/15/20	4/39/115/115	-
21	BCR	B	841	-	-	4/29/63/63	0/2/2/2
18	CLA	A	810	1	1/1/12/20	2/21/97/115	-
21	BCR	B	844	-	-	2/29/63/63	0/2/2/2
24	LMU	F	803	-	-	3/21/61/61	0/2/2/2
18	CLA	B	812	-	1/1/15/20	3/39/115/115	-
18	CLA	F	802	-	1/1/15/20	0/39/115/115	-
18	CLA	A	829	-	1/1/15/20	5/39/115/115	-
20	LHG	2	617	18	-	14/47/47/53	-
21	BCR	K	205	-	-	2/29/63/63	0/2/2/2
18	CLA	B	802	-	1/1/15/20	1/39/115/115	-
18	CLA	A	816	-	1/1/14/20	2/33/109/115	-
18	CLA	1	305	31	1/1/12/20	2/21/97/115	-
18	CLA	1	313	13	1/1/15/20	9/39/115/115	-
18	CLA	A	821	-	1/1/11/20	5/15/91/115	-
18	CLA	A	804	-	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	809	-	1/1/15/20	2/39/115/115	-
18	CLA	B	831	-	1/1/15/20	5/39/115/115	-
24	LMU	A	858	-	-	2/15/35/61	0/1/1/2
18	CLA	A	827	31	1/1/13/20	3/27/103/115	-
24	LMU	B	848	-	-	1/15/35/61	0/1/1/2
26	LUT	4	616	-	-	2/29/67/67	0/2/2/2
18	CLA	3	308	15	1/1/13/20	6/27/103/115	-
19	PQN	B	838	-	-	2/23/43/43	0/2/2/2
27	CHL	4	615	16	3/3/16/26	1/15/113/137	-
18	CLA	B	835	-	1/1/12/20	0/21/97/115	-
18	CLA	B	822	31	1/1/15/20	7/39/115/115	-
26	LUT	J	101	-	-	4/29/67/67	0/2/2/2
18	CLA	B	808	2	1/1/15/20	3/39/115/115	-
18	CLA	4	612	16	1/1/15/20	5/39/115/115	-
18	CLA	J	102	11	1/1/11/20	2/15/91/115	-
26	LUT	2	615	-	-	2/29/67/67	0/2/2/2
26	LUT	1	316	-	-	0/29/67/67	0/2/2/2
18	CLA	A	809	1	1/1/15/20	8/39/115/115	-
18	CLA	4	613	-	1/1/11/20	2/17/93/115	-
21	BCR	K	202	-	-	0/29/63/63	0/2/2/2
18	CLA	A	833	-	1/1/13/20	1/27/103/115	-
18	CLA	B	823	31	1/1/15/20	2/39/115/115	-
18	CLA	4	602	16	1/1/14/20	2/33/109/115	-
27	CHL	1	302	13	3/3/20/26	3/39/137/137	-
18	CLA	L	305	31	1/1/11/20	0/15/91/115	-
27	CHL	1	307	13	3/3/16/26	2/15/113/137	-
27	CHL	2	614	14	3/3/16/26	2/17/115/137	-
18	CLA	4	603	16	1/1/15/20	6/39/115/115	-
22	SF4	C	101	3	-	-	0/6/5/5
18	CLA	A	805	18	1/1/12/20	3/21/97/115	-
20	LHG	A	846	-	-	6/53/53/53	-
24	LMU	F	808	-	-	4/21/61/61	0/2/2/2
27	CHL	3	306	31	3/3/17/26	3/21/119/137	-
27	CHL	3	301	15	3/3/20/26	7/39/137/137	-
18	CLA	A	855	31	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	303	-	1/1/11/20	4/15/91/115	-
18	CLA	A	840	-	1/1/13/20	0/27/103/115	-
18	CLA	1	309	13	1/1/15/20	5/39/115/115	-
18	CLA	3	309	15	1/1/11/20	6/15/91/115	-
18	CLA	3	302	15	1/1/13/20	2/27/103/115	-
18	CLA	4	601	16	1/1/12/20	3/21/97/115	-
18	CLA	4	608	16	1/1/15/20	12/39/115/115	-
21	BCR	L	306	-	-	2/29/63/63	0/2/2/2
18	CLA	A	814	-	1/1/15/20	7/39/115/115	-
18	CLA	B	815	-	1/1/14/20	4/33/109/115	-
27	CHL	2	607	-	3/3/17/26	5/21/119/137	-
18	CLA	K	201	12	1/1/11/20	6/15/91/115	-
18	CLA	F	804	31	1/1/15/20	6/39/115/115	-
18	CLA	2	609	14	1/1/14/20	6/33/109/115	-
21	BCR	A	848	-	-	2/29/63/63	0/2/2/2
22	SF4	C	102	3	-	-	0/6/5/5
18	CLA	B	839	20	1/1/15/20	6/39/115/115	-
21	BCR	L	302	-	-	3/29/63/63	0/2/2/2
25	DGD	4	622	-	-	5/38/78/95	0/2/2/2
18	CLA	G	205	10	1/1/11/20	3/17/93/115	-
18	CLA	1	303	13	1/1/15/20	2/39/115/115	-
24	LMU	L	301	-	-	0/11/31/61	0/1/1/2
18	CLA	G	204	-	1/1/11/20	4/15/91/115	-
18	CLA	A	822	31	1/1/15/20	5/39/115/115	-
18	CLA	B	804	-	1/1/15/20	7/39/115/115	-
18	CLA	B	821	-	1/1/11/20	2/15/91/115	-
18	CLA	4	609	16	1/1/14/20	4/33/109/115	-
19	PQN	A	844	-	-	0/23/43/43	0/2/2/2
24	LMU	G	207	-	-	2/21/61/61	0/2/2/2
18	CLA	B	806	-	1/1/14/20	3/33/109/115	-
18	CLA	A	839	-	1/1/15/20	3/39/115/115	-
21	BCR	4	618	-	-	2/29/63/63	0/2/2/2
17	CL0	A	801	-	3/3/20/25	3/37/135/135	-
18	CLA	A	836	-	1/1/15/20	1/39/115/115	-
18	CLA	G	201	-	1/1/13/20	5/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	SF4	A	853	1,2	-	-	0/6/5/5
18	CLA	1	304	-	1/1/14/20	2/33/109/115	-
18	CLA	B	828	-	1/1/11/20	0/15/91/115	-
18	CLA	A	806	-	1/1/15/20	2/39/115/115	-
18	CLA	A	835	-	1/1/15/20	5/39/115/115	-
18	CLA	A	824	-	1/1/11/20	4/15/91/115	-
18	CLA	F	805	9	1/1/12/20	4/21/97/115	-
18	CLA	A	843	31	1/1/15/20	7/39/115/115	-
24	LMU	A	859	-	-	3/21/61/61	0/2/2/2
18	CLA	1	315	13	1/1/11/20	0/15/91/115	-
18	CLA	A	812	18	1/1/15/20	6/39/115/115	-
18	CLA	L	303	8	1/1/11/20	4/15/91/115	-
27	CHL	4	605	31	3/3/20/26	5/39/137/137	-
18	CLA	2	610	20	1/1/14/20	1/33/109/115	-
18	CLA	B	829	-	1/1/15/20	3/39/115/115	-
18	CLA	3	312	-	1/1/11/20	2/15/91/115	-
18	CLA	2	611	14	1/1/11/20	4/15/91/115	-
20	LHG	1	319	-	-	9/53/53/53	-
21	BCR	G	206	-	-	4/29/63/63	0/2/2/2
29	C7Z	1	322	-	-	4/29/67/67	0/2/2/2
18	CLA	2	603	-	1/1/15/20	5/39/115/115	-
18	CLA	B	801	-	1/1/15/20	3/39/115/115	-
18	CLA	B	805	2	1/1/15/20	4/39/115/115	-
26	LUT	1	318	-	-	0/29/67/67	0/2/2/2
20	LHG	B	847	-	-	12/53/53/53	-
18	CLA	A	854	31	1/1/15/20	5/39/115/115	-
18	CLA	4	611	16	1/1/11/20	5/18/94/115	-
21	BCR	A	852	-	-	4/29/63/63	0/2/2/2
24	LMU	4	624	-	-	1/15/35/61	0/1/1/2
18	CLA	A	817	31	1/1/11/20	5/15/91/115	-
18	CLA	B	832	31	1/1/11/20	0/15/91/115	-
18	CLA	2	608	14	1/1/11/20	0/15/91/115	-
18	CLA	A	837	1	1/1/11/20	0/15/91/115	-

The worst 5 of 701 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	607	CHL	MG-NB	-7.28	1.91	2.05
27	3	306	CHL	MG-NB	-7.28	1.91	2.05
27	2	607	CHL	MG-NB	-7.23	1.91	2.05
27	1	307	CHL	MG-NB	-7.21	1.91	2.05
27	1	302	CHL	MG-NB	-7.18	1.91	2.05

The worst 5 of 403 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	801	CL0	C1B-CHB-C4A	11.30	128.59	121.32
17	H	202	CL0	C1B-CHB-C4A	10.68	128.20	121.32
27	4	605	CHL	C1B-CHB-C4A	4.96	124.51	121.32
27	3	306	CHL	C1B-CHB-C4A	4.93	124.50	121.32
27	2	614	CHL	C1B-CHB-C4A	4.82	124.42	121.32

5 of 182 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CL0	ND
17	A	801	CL0	NA
17	A	801	CL0	NC
17	H	202	CL0	ND
17	H	202	CL0	NA

5 of 743 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	809	CLA	O2A-C1-C2-C3
18	A	812	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

141 monomers are involved in 216 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	203	LMU	2	0
26	3	315	LUT	3	0
18	3	311	CLA	1	0
18	A	856	CLA	1	0
24	2	618	LMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	847	LHG	1	0
24	1	320	LMU	1	0
18	A	841	CLA	2	0
23	4	619	LMG	2	0
25	J	104	DGD	3	0
18	A	826	CLA	1	0
18	1	312	CLA	3	0
21	L	307	BCR	1	0
18	A	820	CLA	3	0
20	B	846	LHG	1	0
18	1	311	CLA	1	0
18	A	825	CLA	1	0
18	B	807	CLA	2	0
23	F	810	LMG	2	0
18	1	310	CLA	6	0
23	4	620	LMG	3	0
18	B	819	CLA	1	0
28	2	616	XAT	1	0
24	F	809	LMU	2	0
21	B	843	BCR	1	0
24	4	623	LMU	2	0
28	1	317	XAT	2	0
18	1	306	CLA	2	0
27	4	606	CHL	2	0
18	A	828	CLA	1	0
18	B	818	CLA	1	0
18	A	813	CLA	1	0
21	3	313	BCR	4	0
26	3	314	LUT	1	0
24	1	321	LMU	1	0
21	F	806	BCR	2	0
18	B	830	CLA	1	0
18	A	818	CLA	3	0
24	F	807	LMU	2	0
18	B	833	CLA	1	0
24	H	201	LMU	1	0
18	B	836	CLA	1	0
18	3	305	CLA	1	0
21	J	103	BCR	1	0
18	3	307	CLA	3	0
18	B	820	CLA	5	0
21	A	850	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	308	CLA	1	0
18	4	614	CLA	1	0
18	B	824	CLA	3	0
21	A	851	BCR	2	0
18	A	819	CLA	2	0
18	A	823	CLA	2	0
18	3	304	CLA	2	0
23	A	857	LMG	3	0
18	A	838	CLA	2	0
18	B	817	CLA	2	0
18	2	601	CLA	2	0
18	B	810	CLA	2	0
17	H	202	CL0	2	0
24	1	301	LMU	2	0
18	A	811	CLA	3	0
21	G	202	BCR	2	0
27	2	606	CHL	1	0
21	A	849	BCR	2	0
18	A	815	CLA	2	0
18	A	845	CLA	1	0
21	B	844	BCR	3	0
24	F	803	LMU	1	0
18	F	802	CLA	1	0
18	A	829	CLA	4	0
20	2	617	LHG	2	0
18	A	816	CLA	1	0
18	1	313	CLA	3	0
18	A	804	CLA	1	0
18	A	827	CLA	1	0
24	B	848	LMU	1	0
26	4	616	LUT	4	0
18	3	308	CLA	4	0
18	B	822	CLA	4	0
26	J	101	LUT	3	0
18	4	612	CLA	1	0
26	2	615	LUT	1	0
26	1	316	LUT	4	0
21	K	202	BCR	2	0
18	B	823	CLA	1	0
18	4	602	CLA	1	0
27	1	302	CHL	3	0
18	L	305	CLA	1	0

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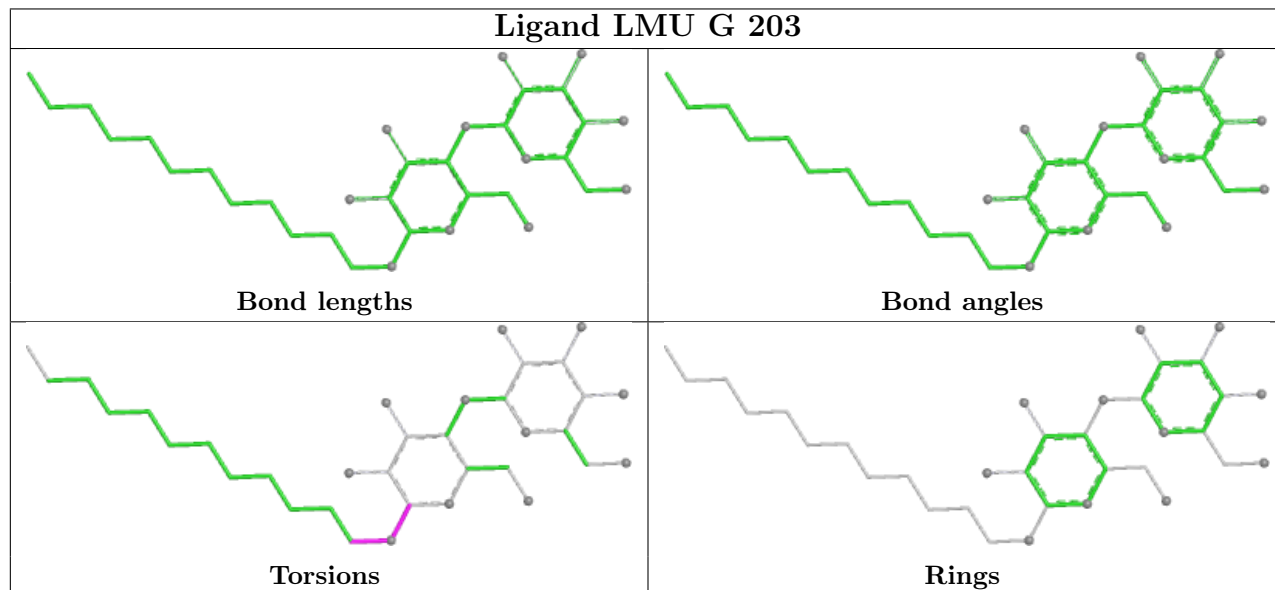
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	1	307	CHL	2	0
18	4	603	CLA	1	0
18	A	805	CLA	1	0
20	A	846	LHG	3	0
24	F	808	LMU	1	0
27	3	301	CHL	5	0
18	A	855	CLA	5	0
18	3	303	CLA	2	0
18	1	309	CLA	6	0
18	3	302	CLA	4	0
18	4	601	CLA	1	0
18	4	608	CLA	2	0
21	L	306	BCR	2	0
18	B	815	CLA	3	0
18	F	804	CLA	4	0
18	2	609	CLA	1	0
21	A	848	BCR	4	0
18	B	839	CLA	1	0
25	4	622	DGD	1	0
18	G	205	CLA	2	0
18	1	303	CLA	2	0
24	L	301	LMU	2	0
18	A	822	CLA	2	0
18	B	804	CLA	1	0
18	4	609	CLA	4	0
24	G	207	LMU	2	0
18	B	806	CLA	1	0
18	A	839	CLA	1	0
21	4	618	BCR	3	0
18	A	836	CLA	1	0
18	G	201	CLA	4	0
18	A	806	CLA	1	0
18	A	824	CLA	1	0
18	F	805	CLA	1	0
18	A	843	CLA	3	0
24	A	859	LMU	1	0
18	1	315	CLA	1	0
18	A	812	CLA	2	0
18	L	303	CLA	2	0
27	4	605	CHL	1	0
18	2	610	CLA	2	0
18	B	829	CLA	3	0

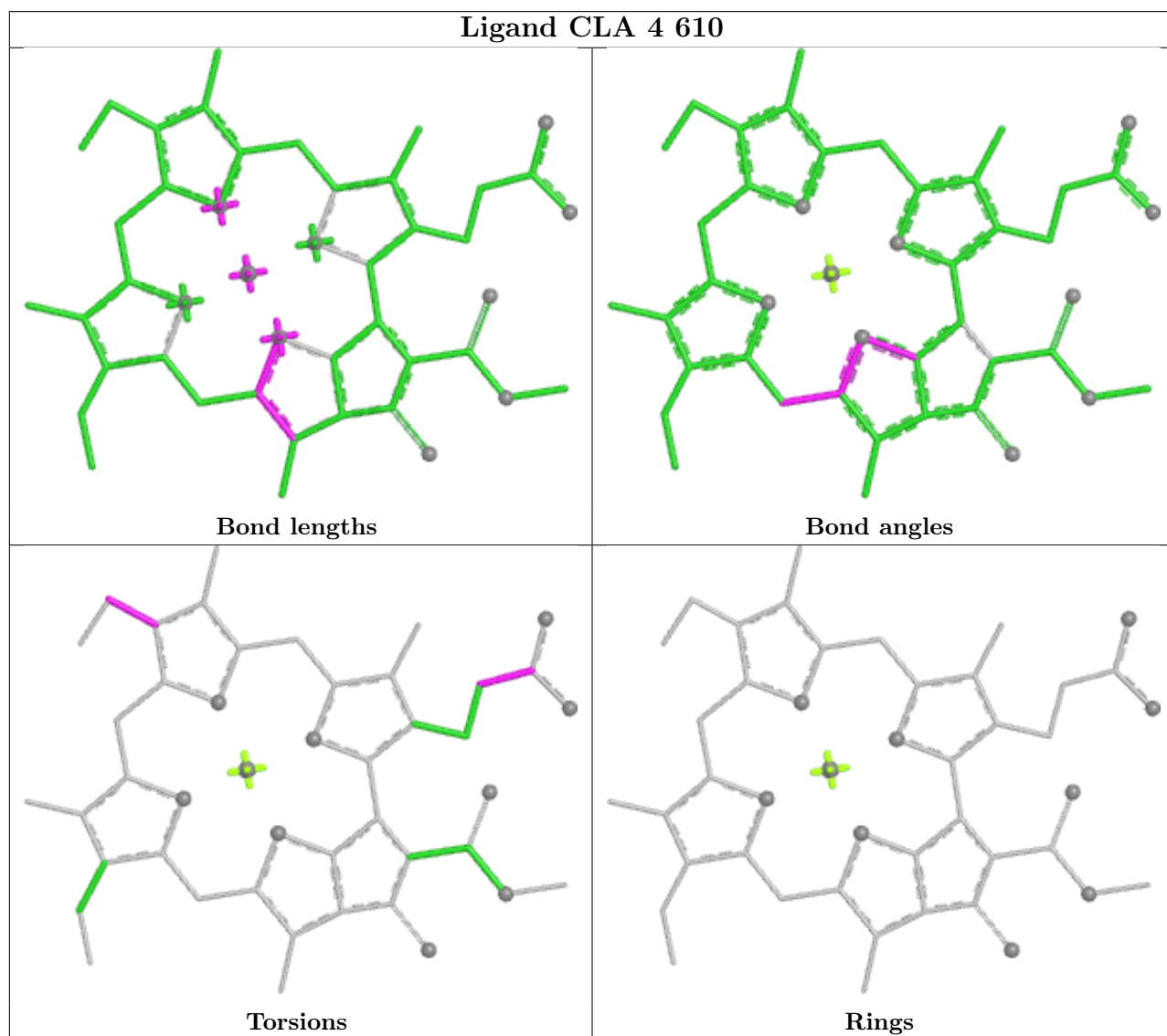
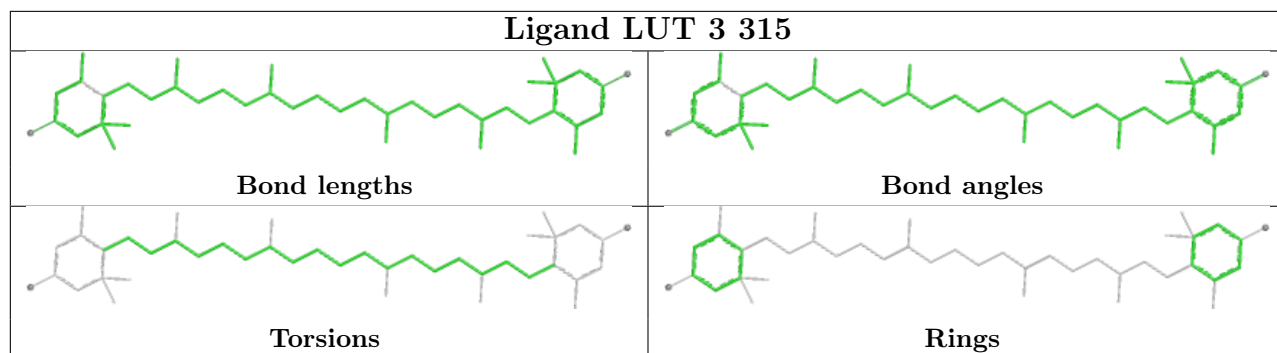
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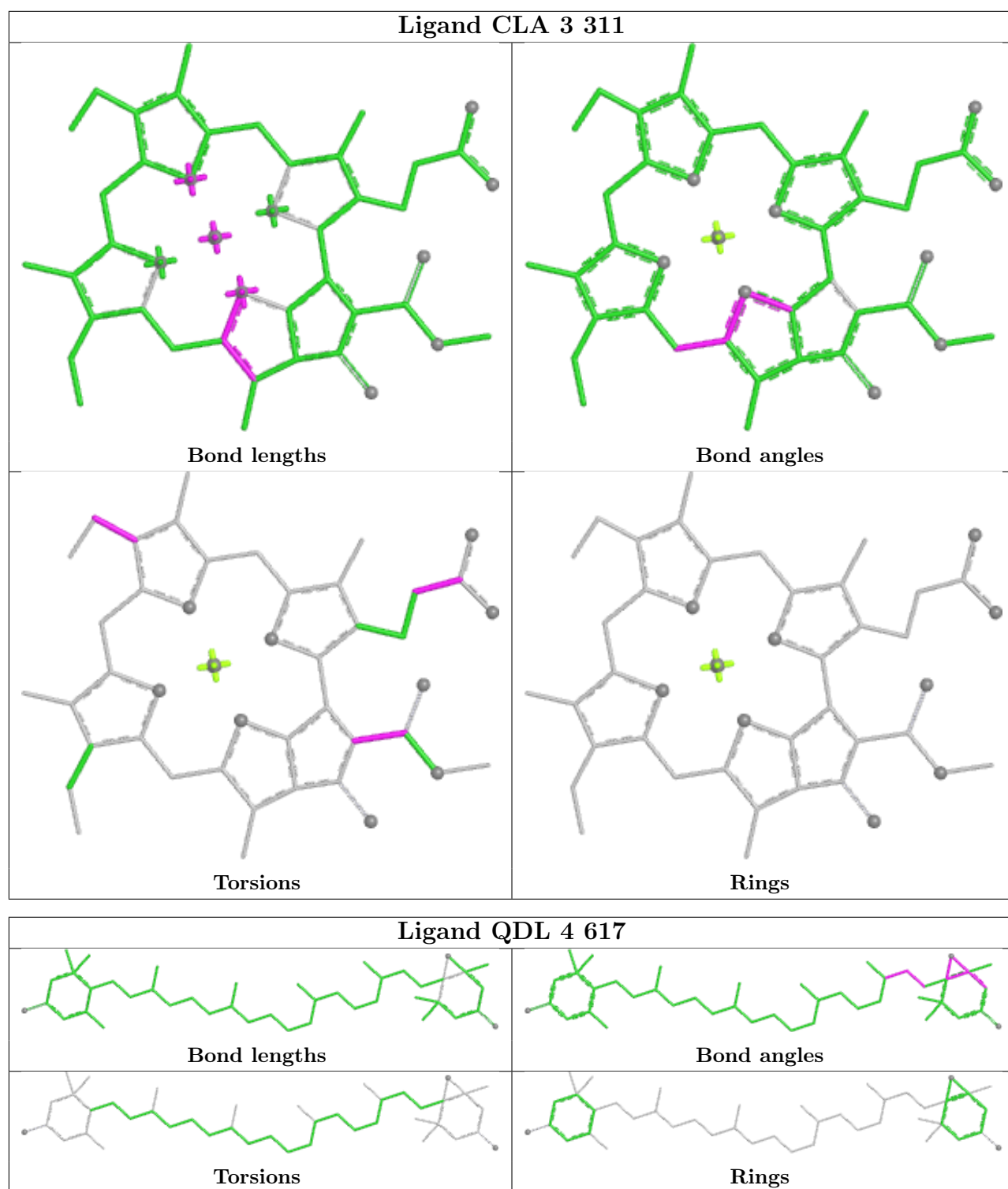
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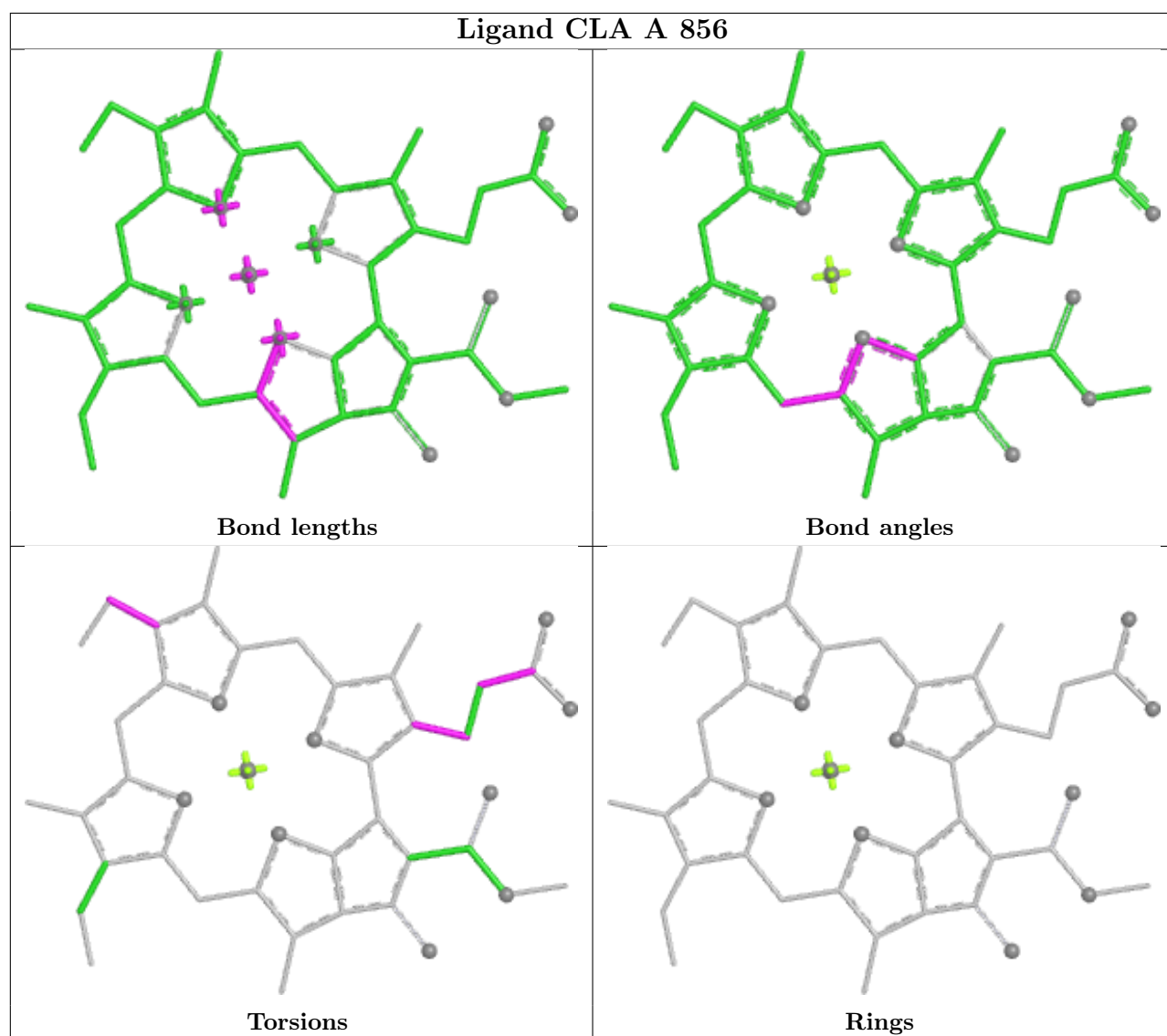
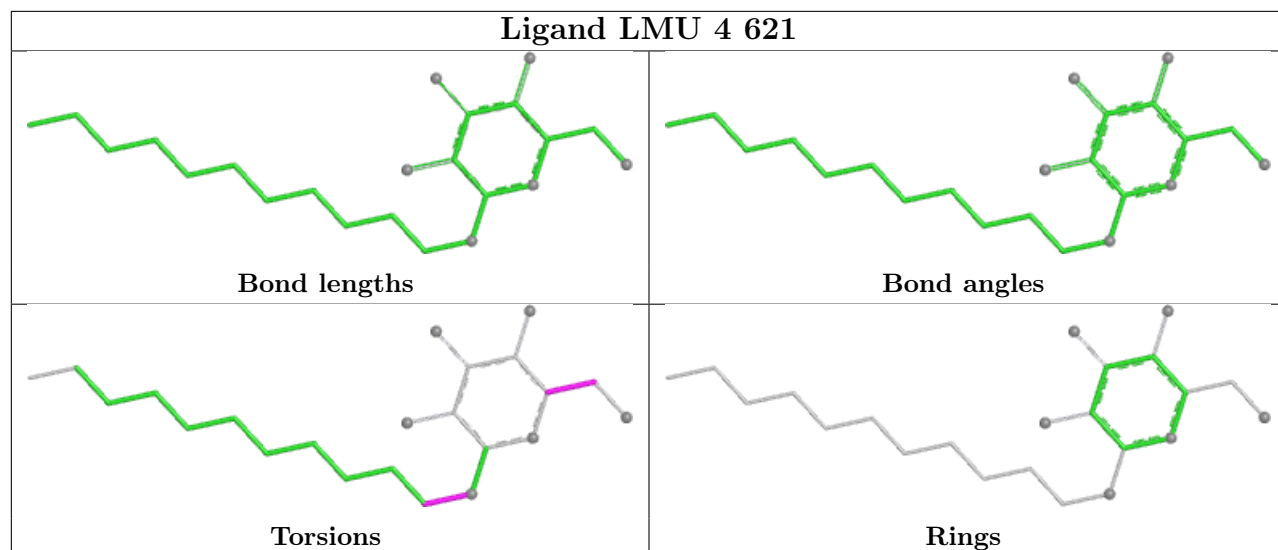
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	319	LHG	5	0
21	G	206	BCR	2	0
18	2	603	CLA	1	0
26	1	318	LUT	1	0
20	B	847	LHG	1	0
18	A	854	CLA	1	0
18	4	611	CLA	1	0
21	A	852	BCR	1	0
24	4	624	LMU	1	0
18	A	817	CLA	3	0

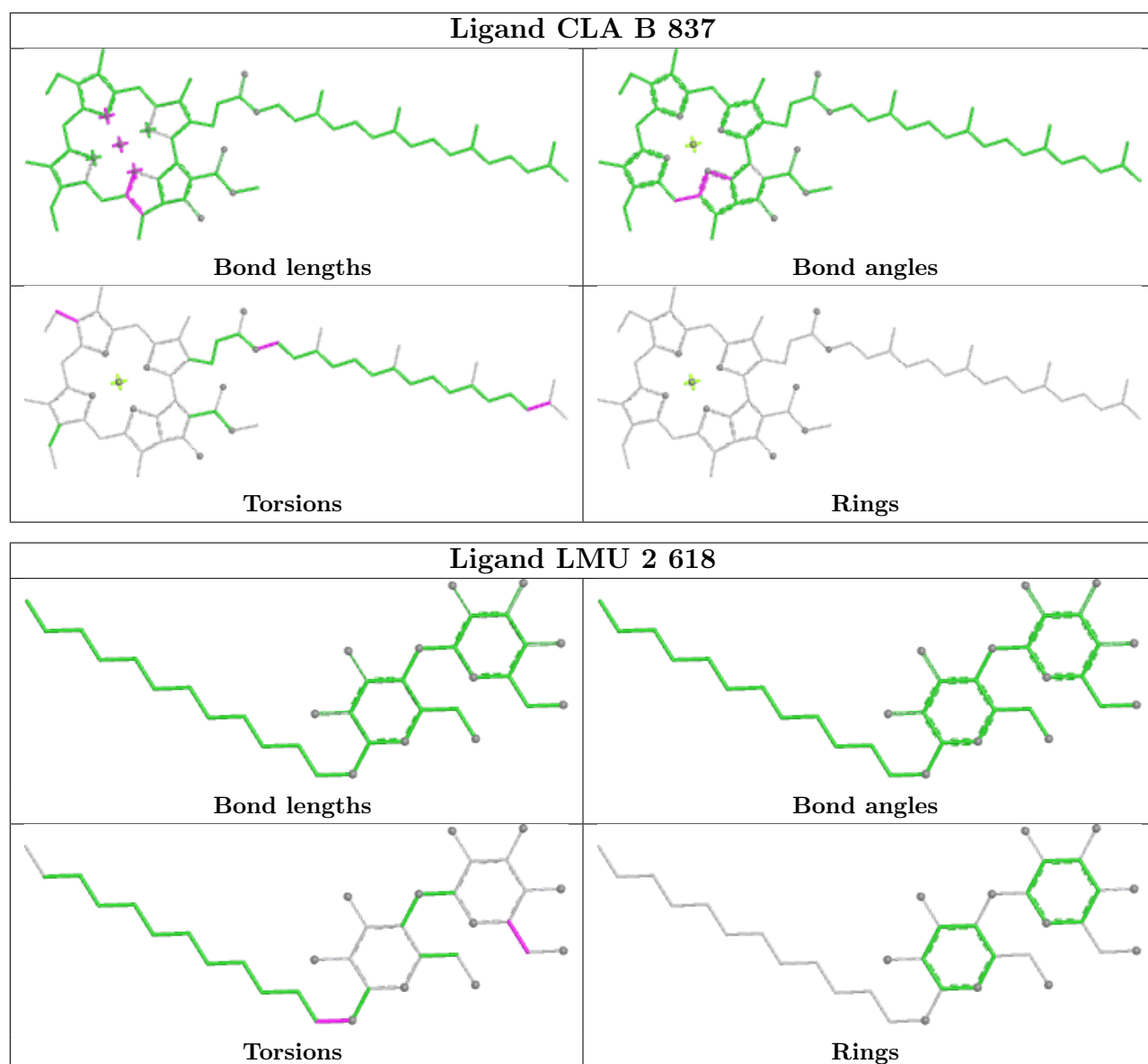
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

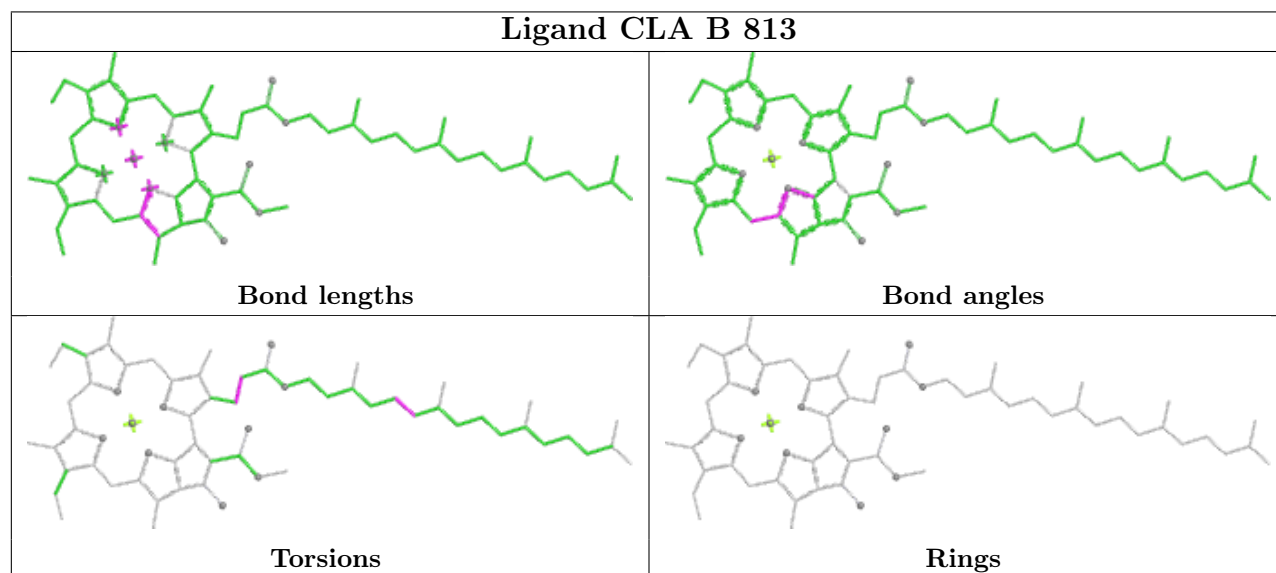
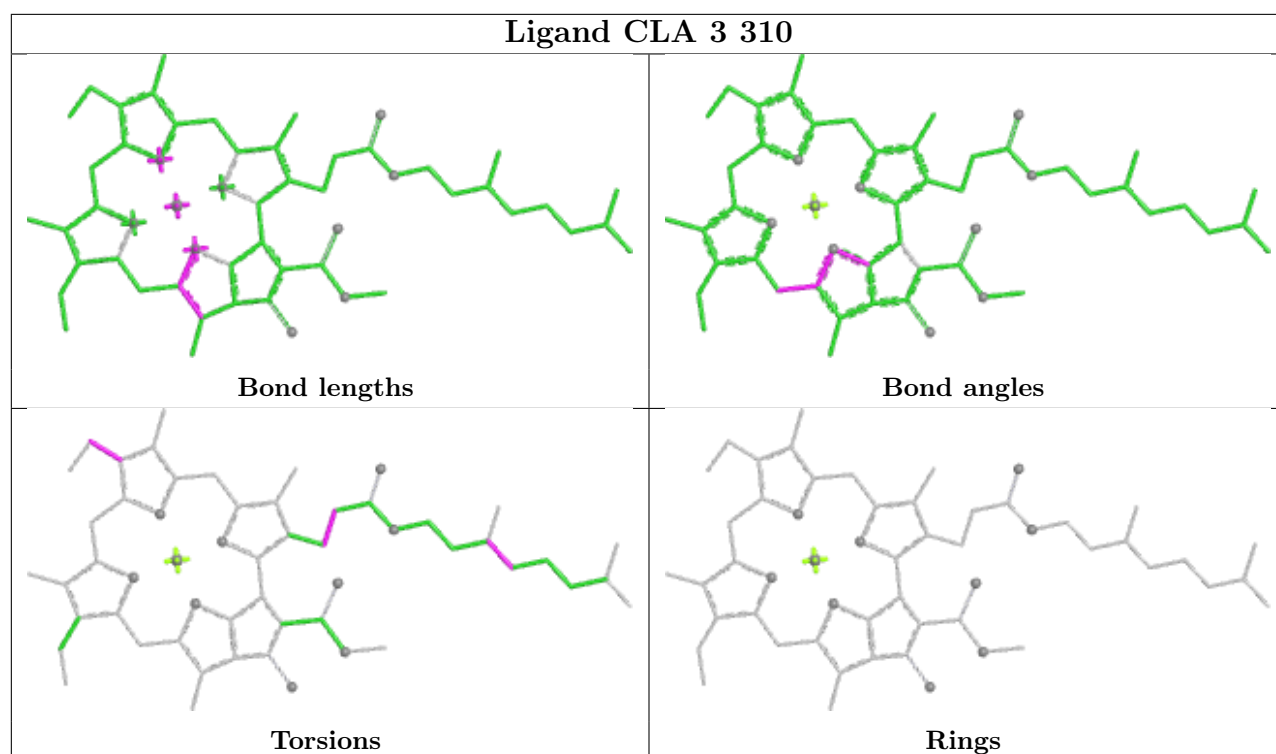


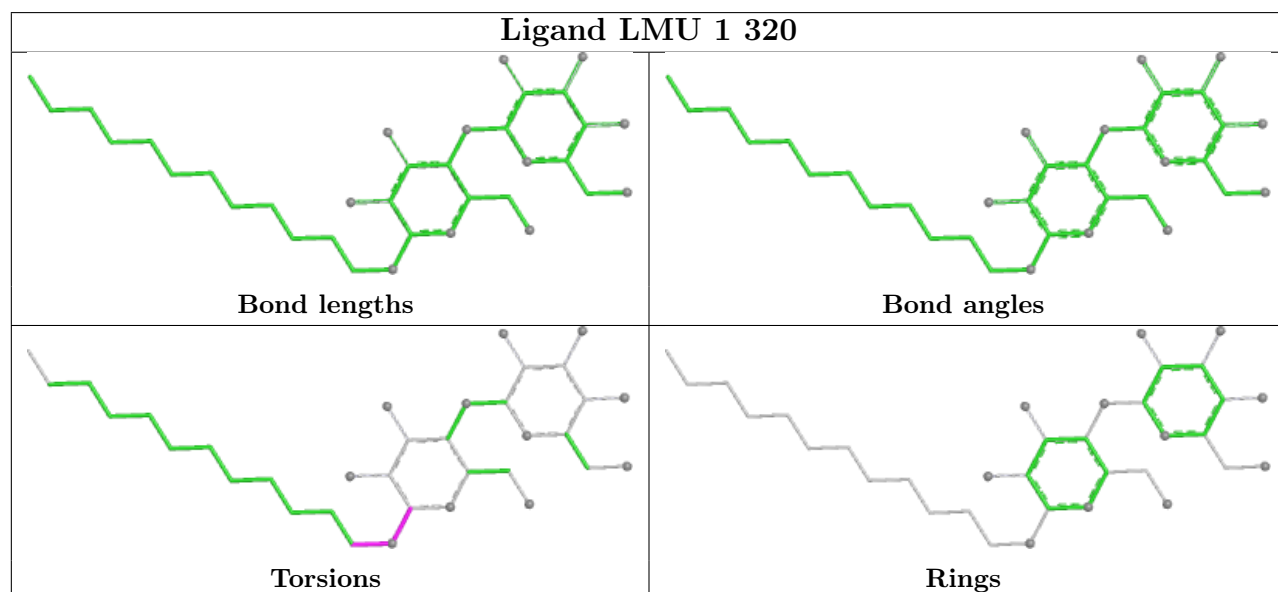
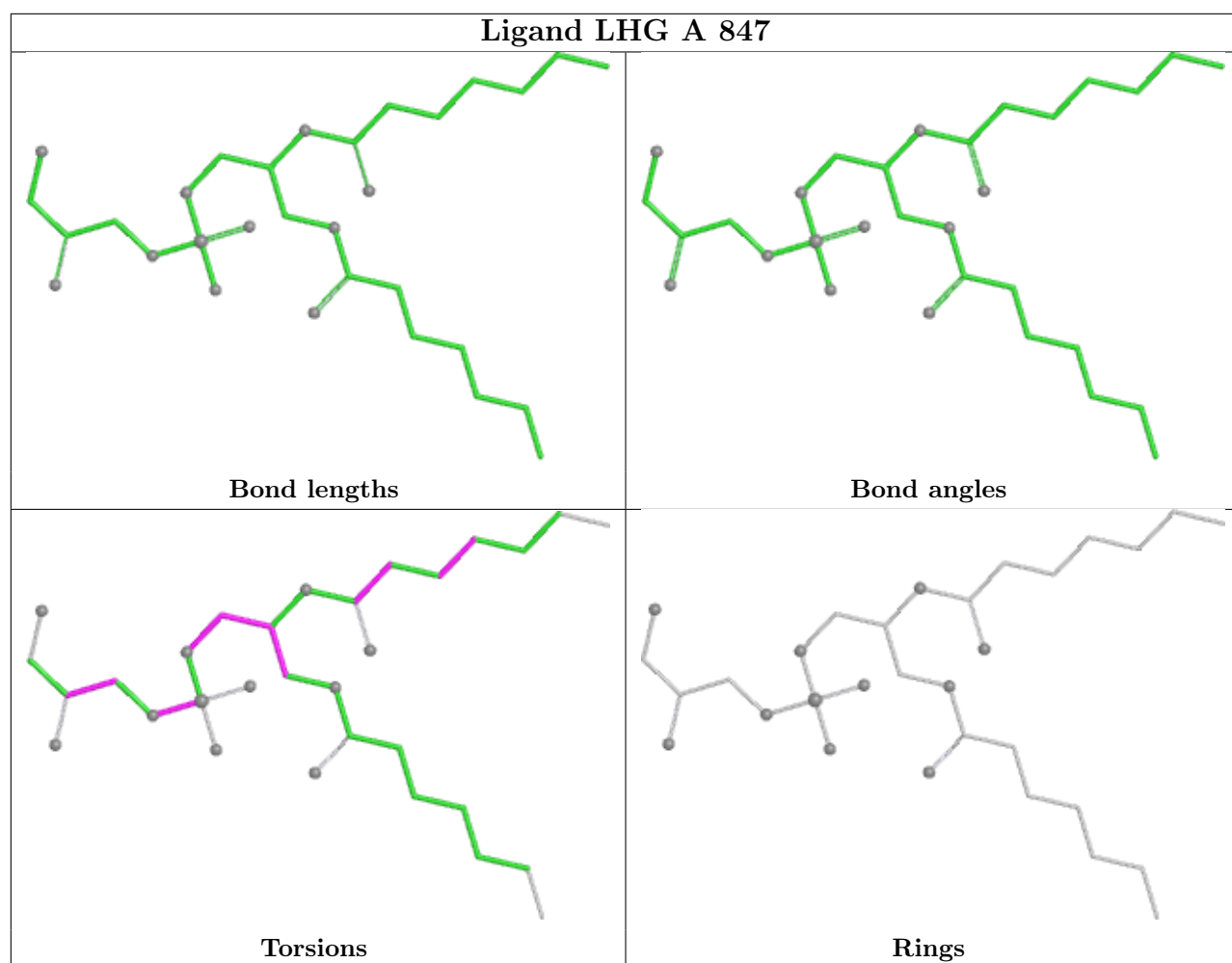


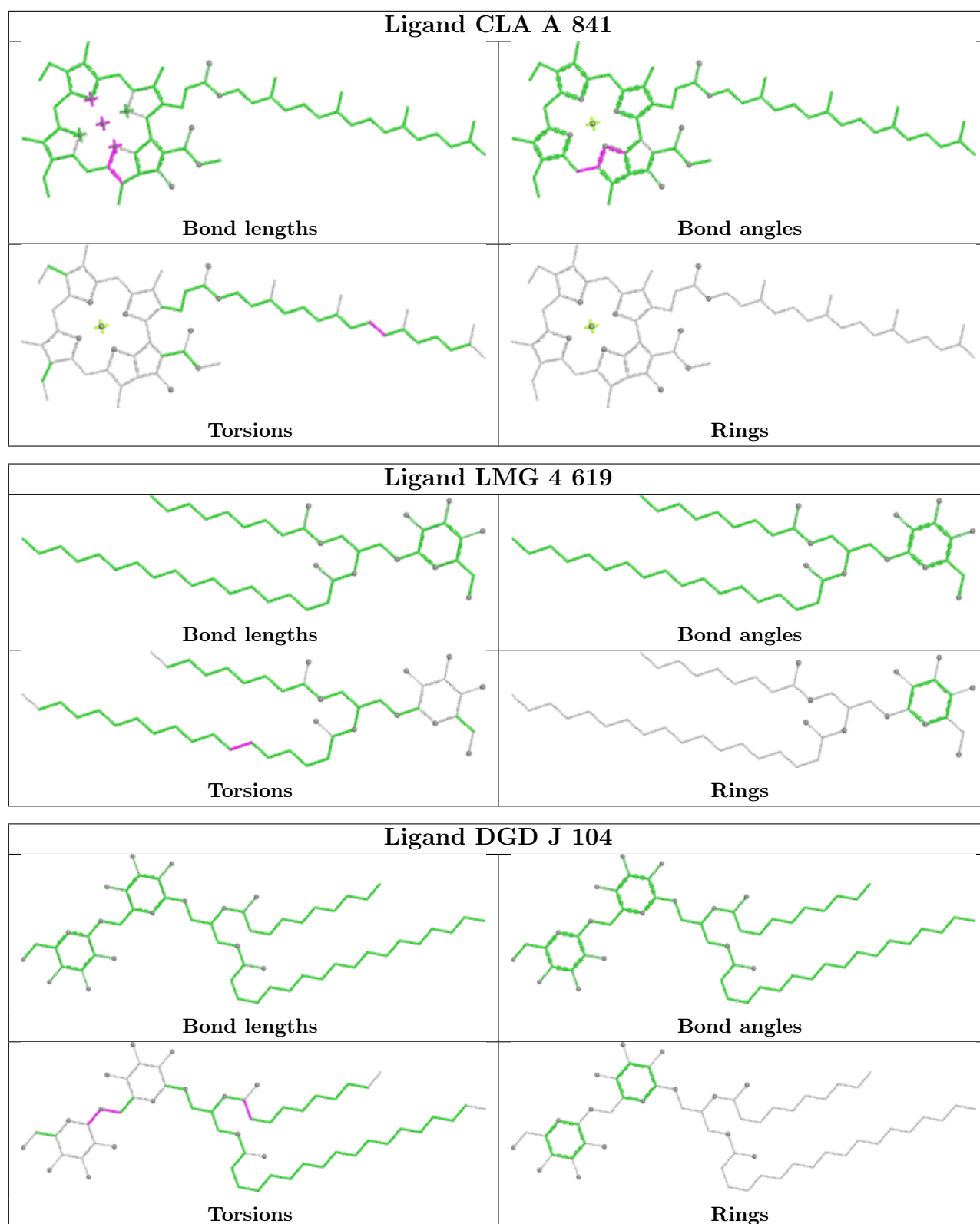


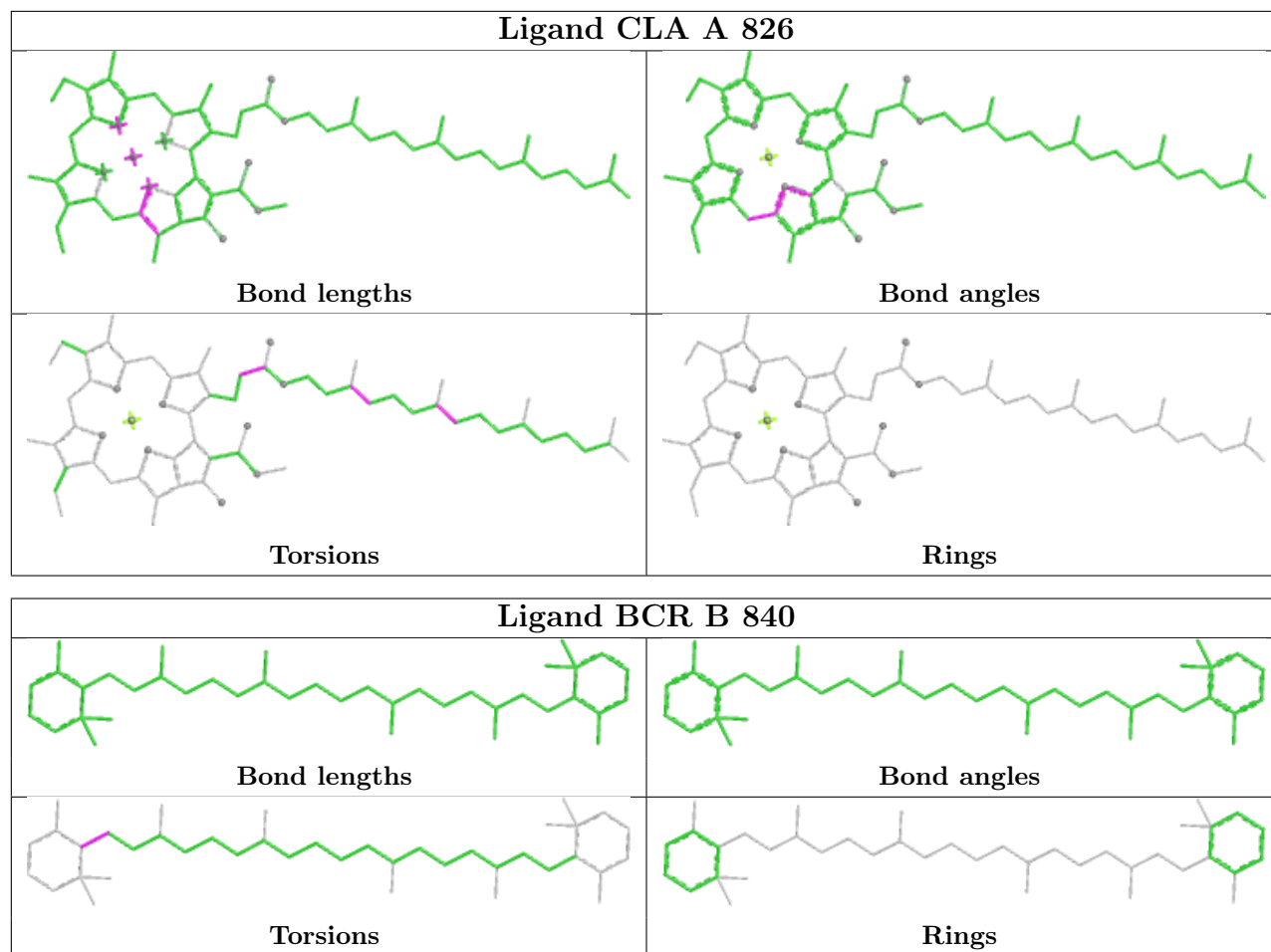


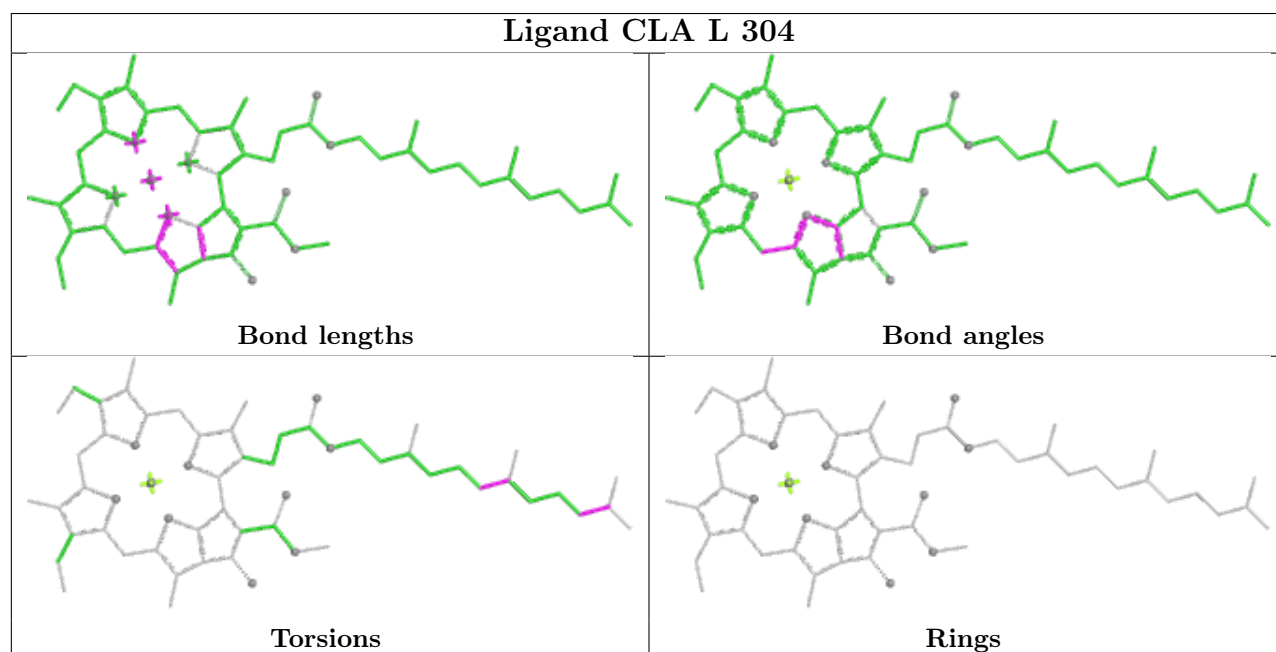
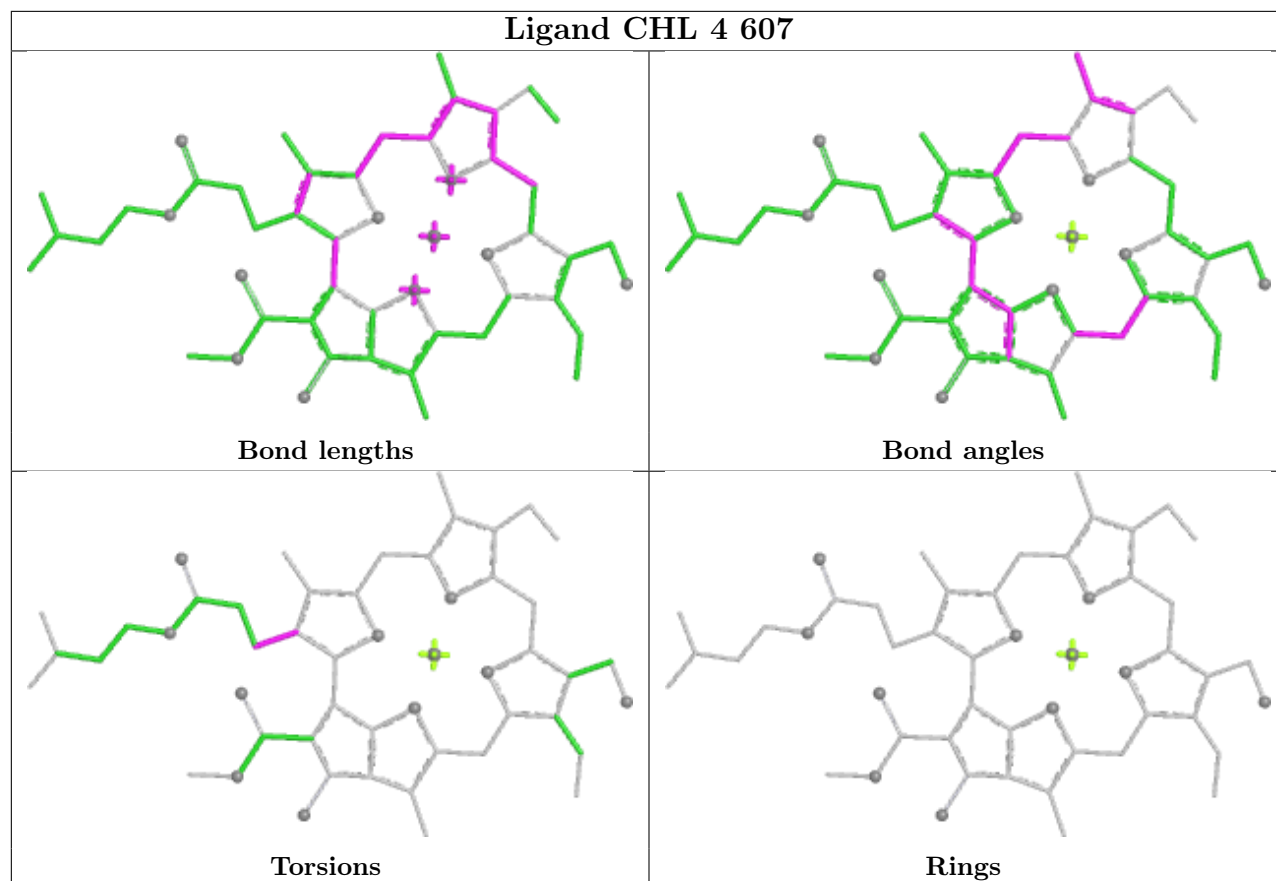


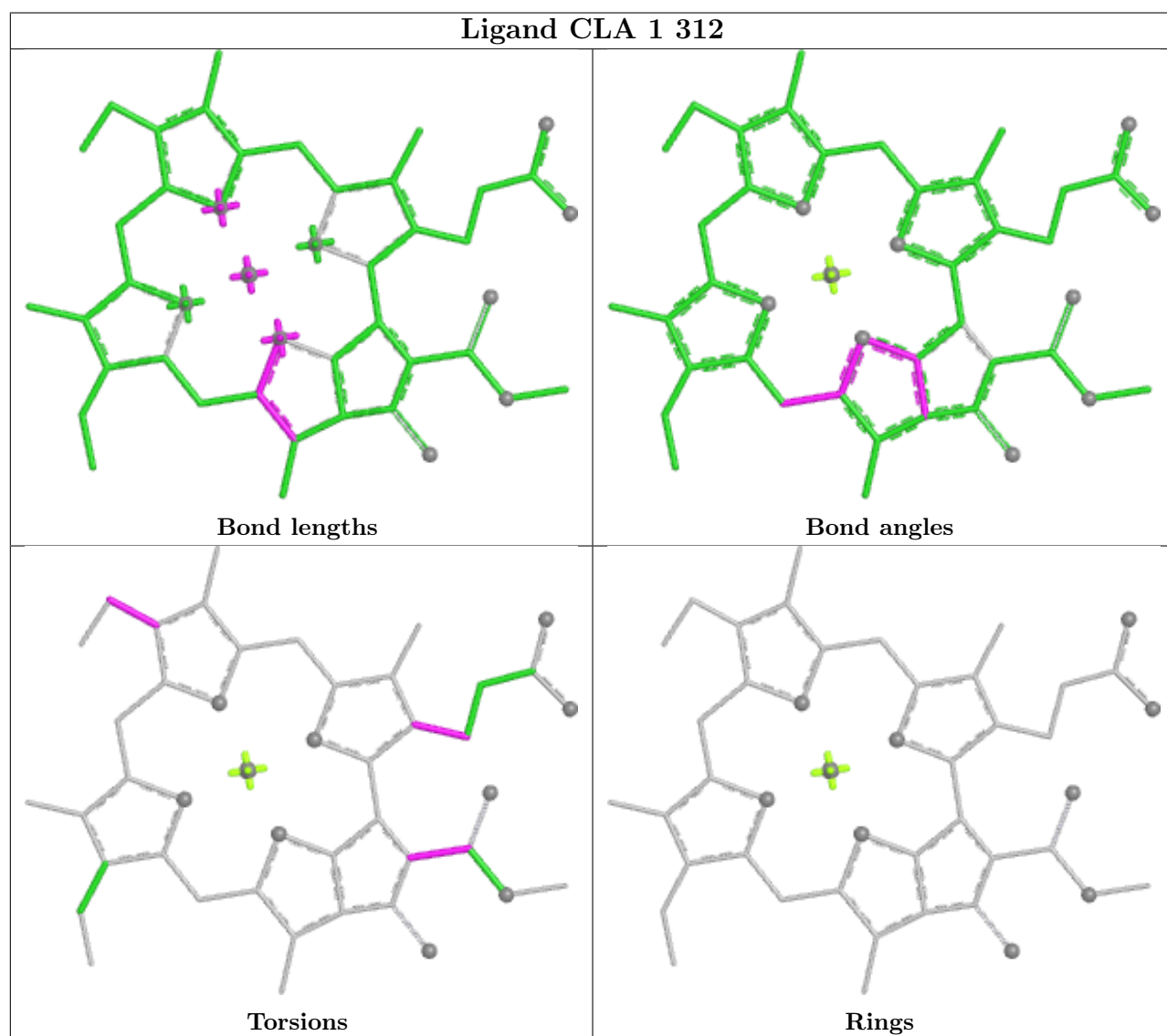
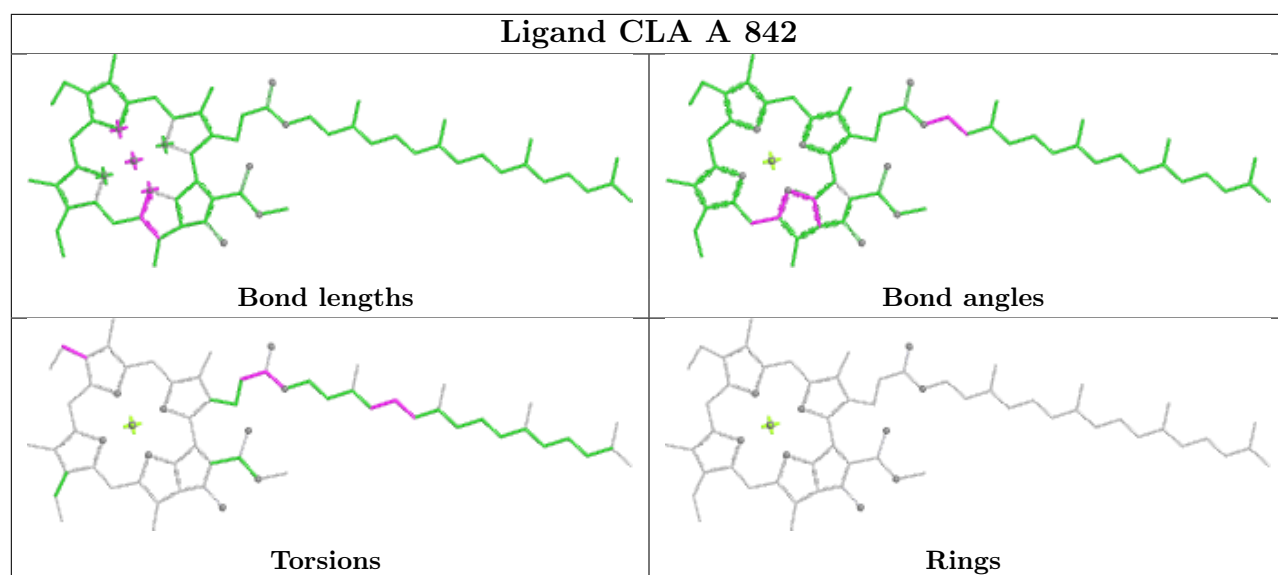


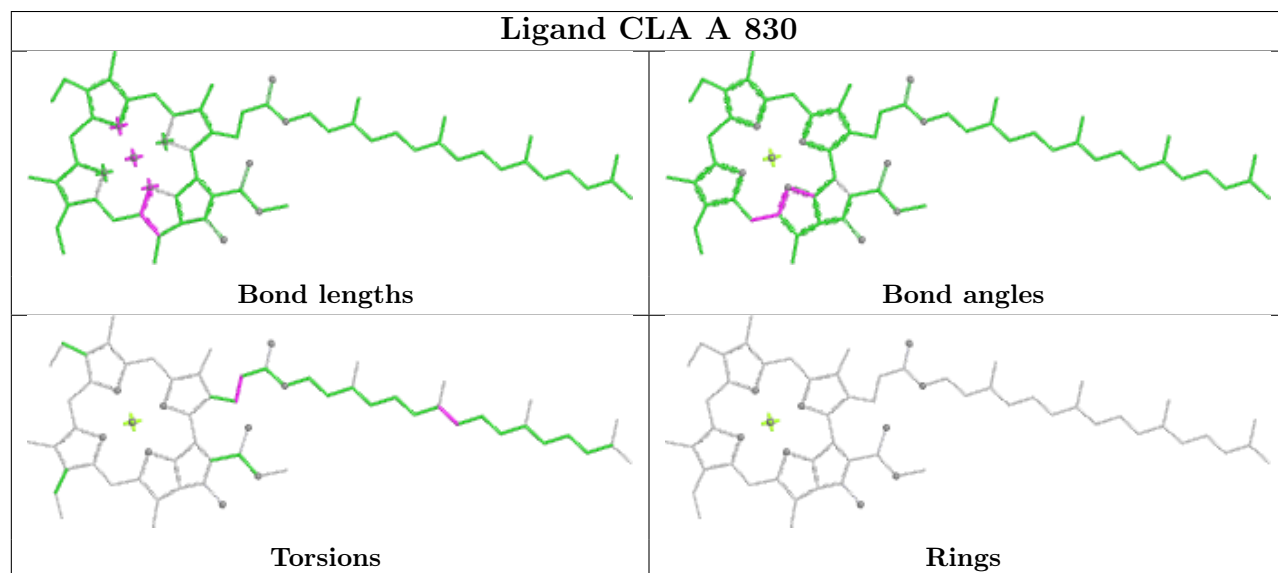
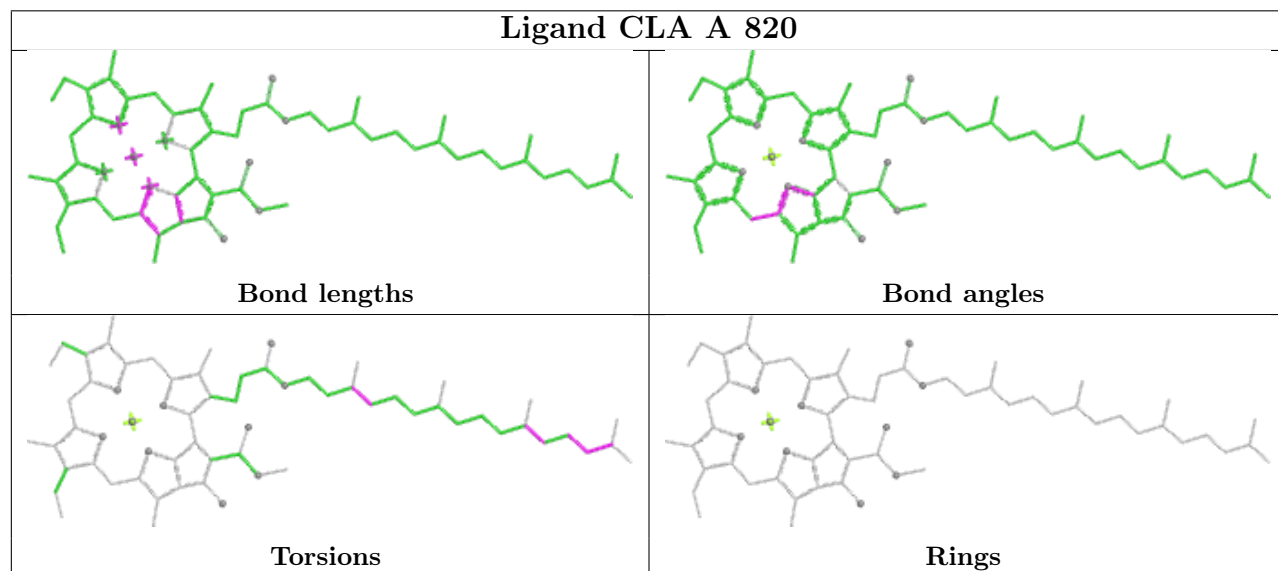
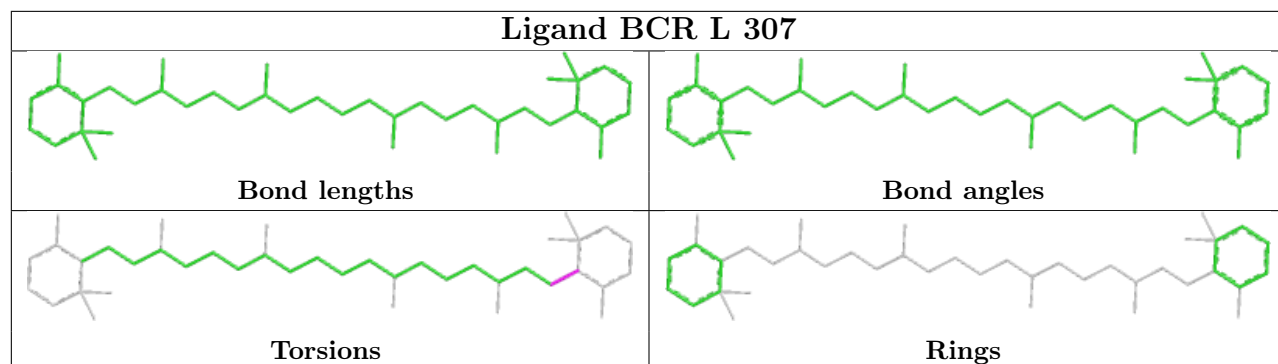


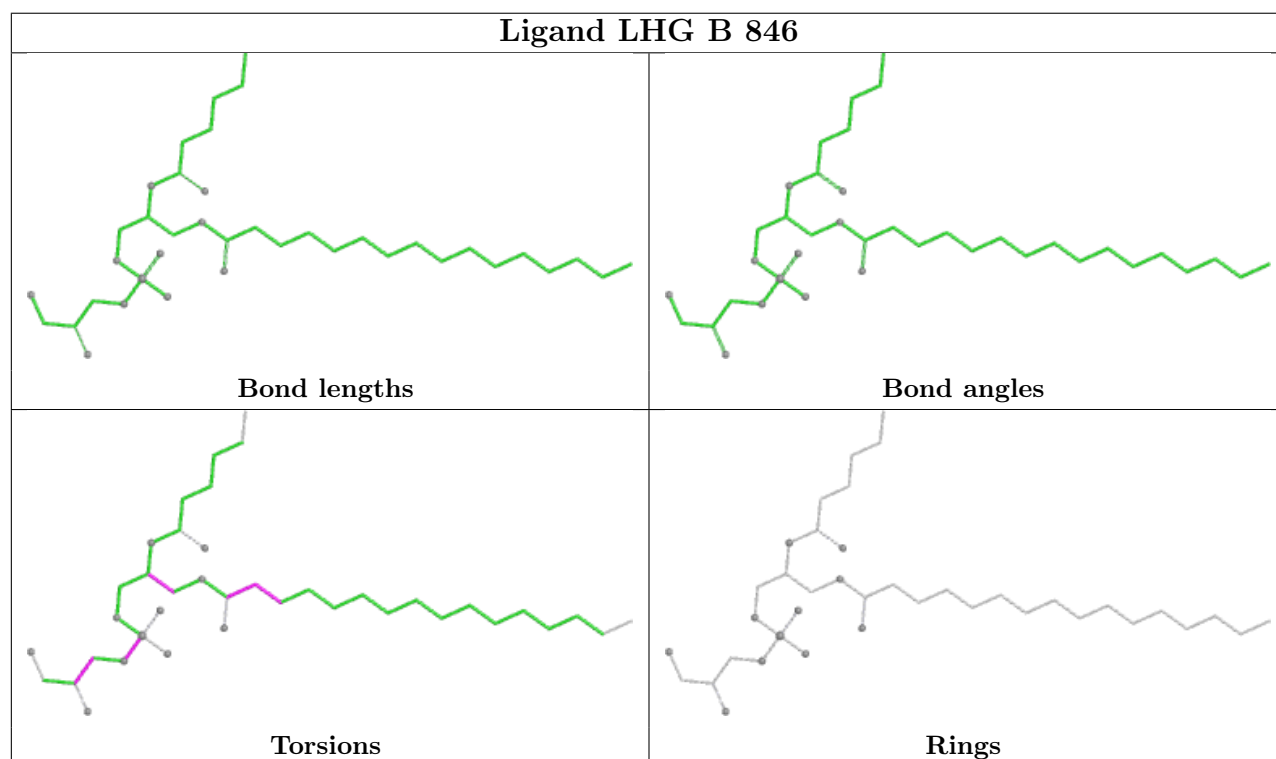
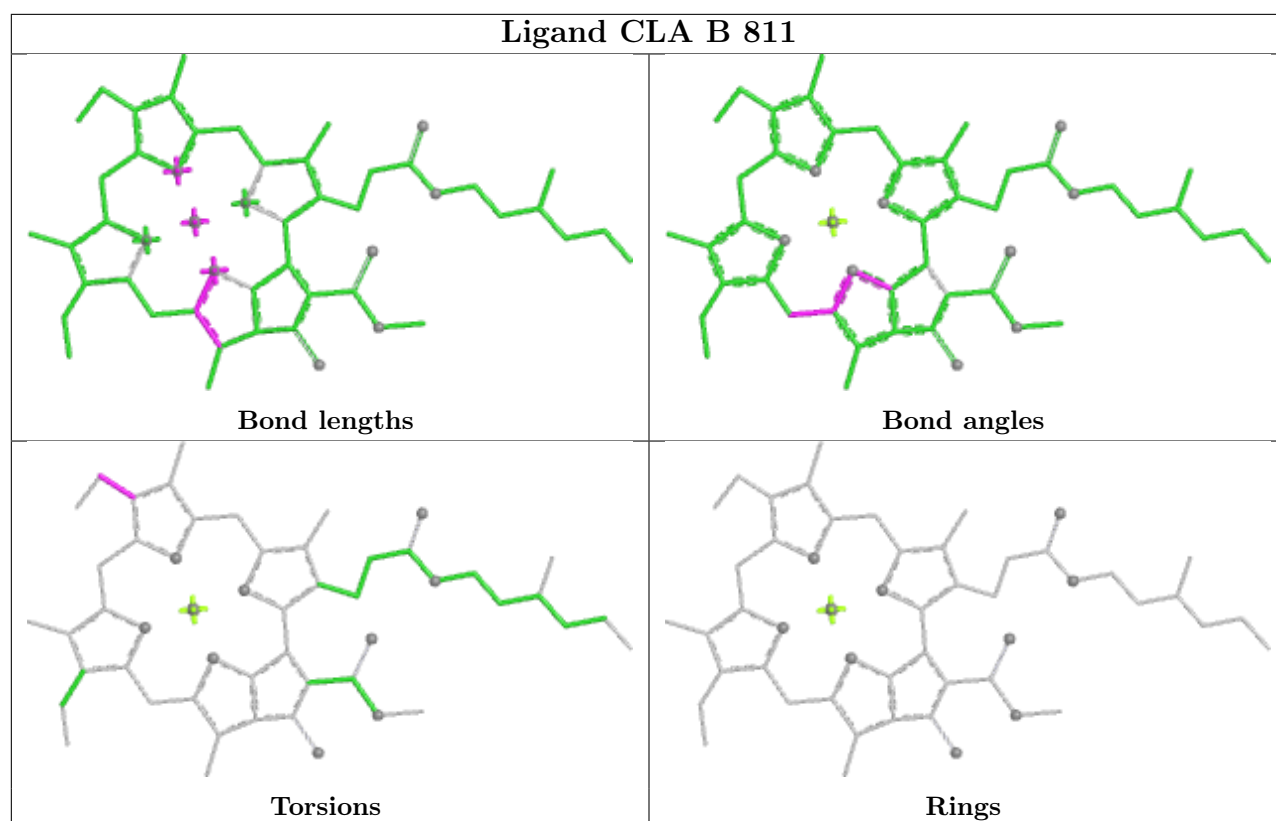


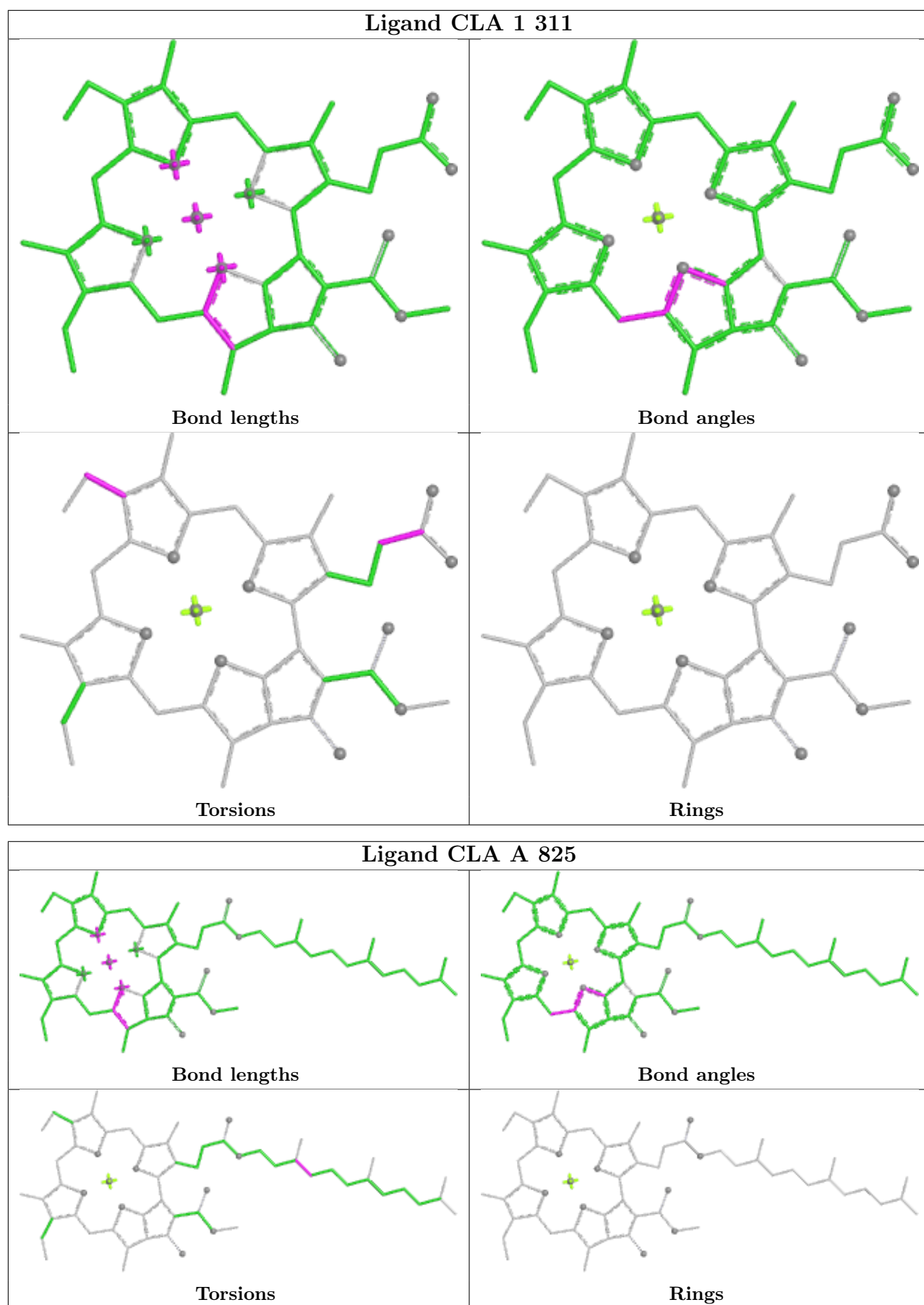


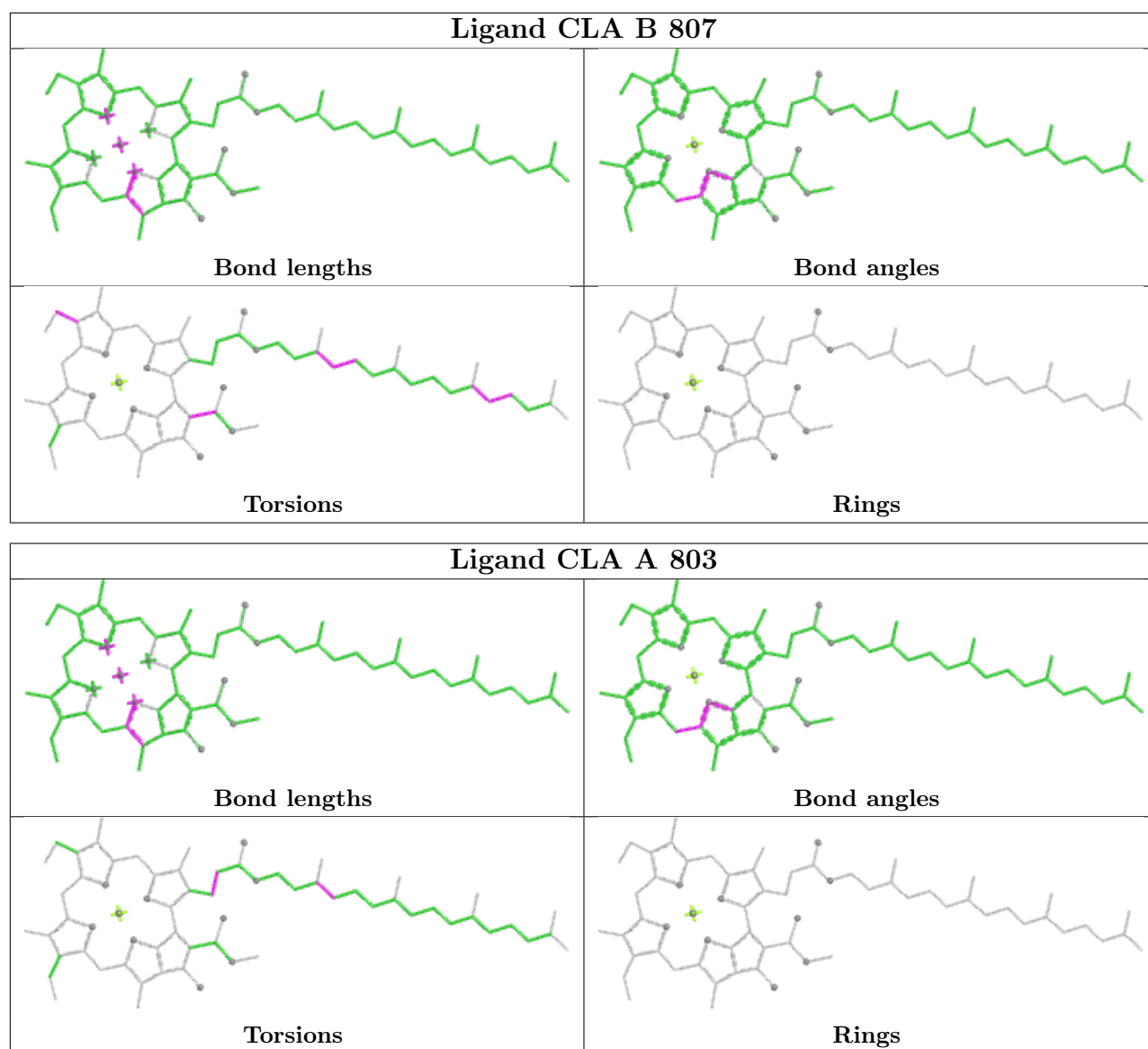


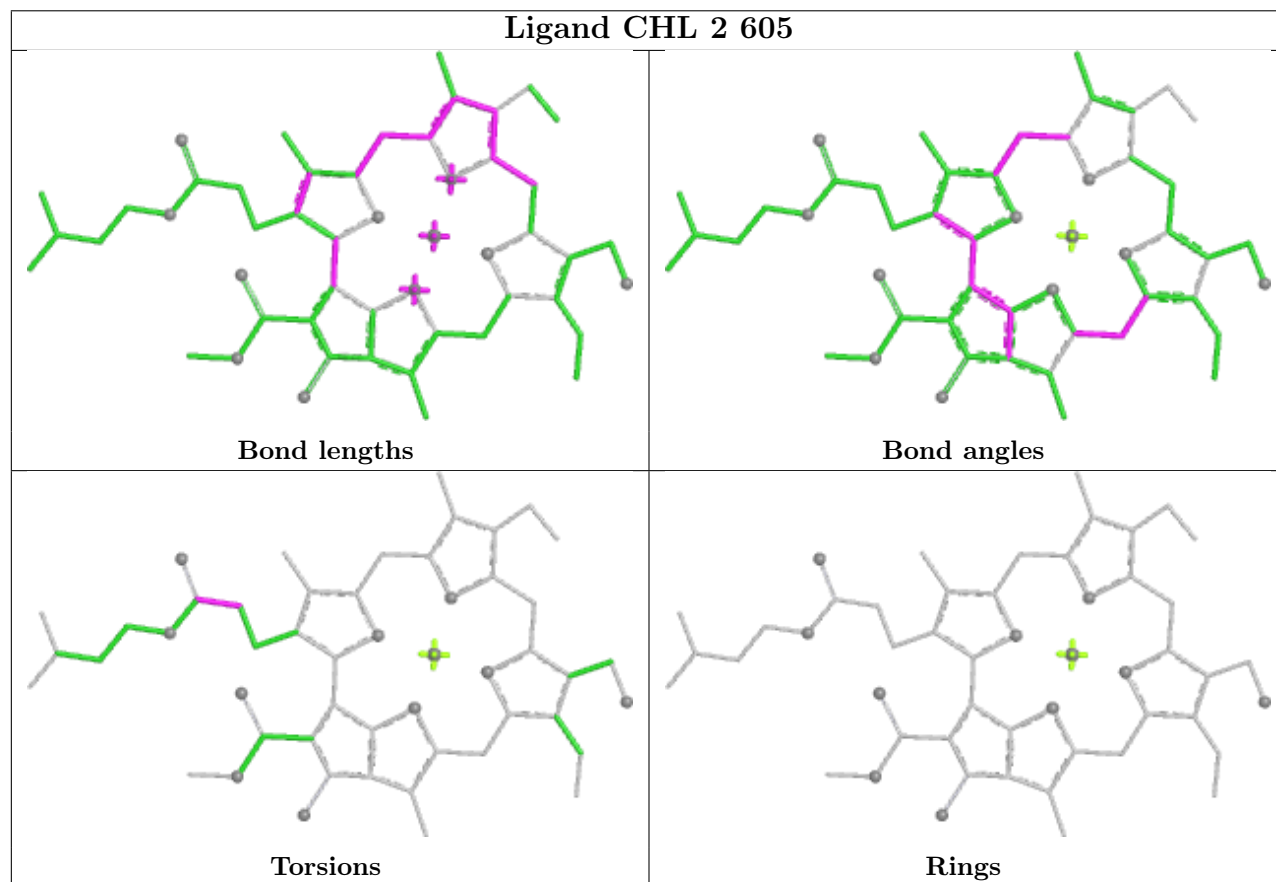
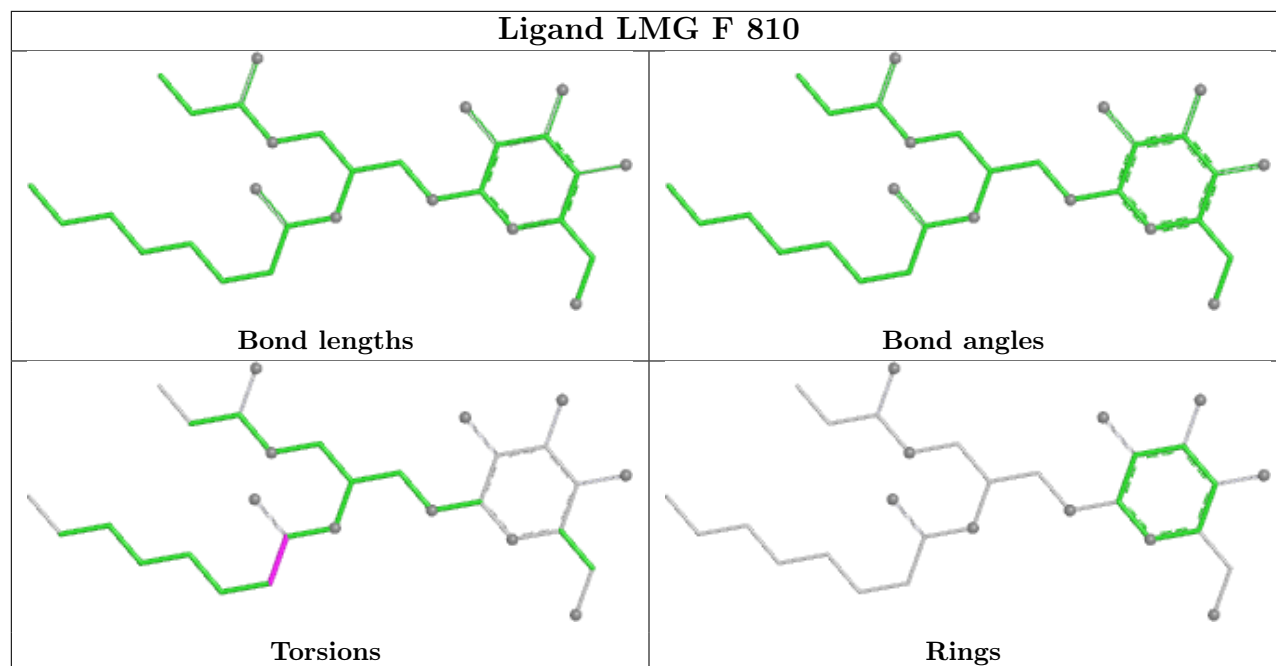


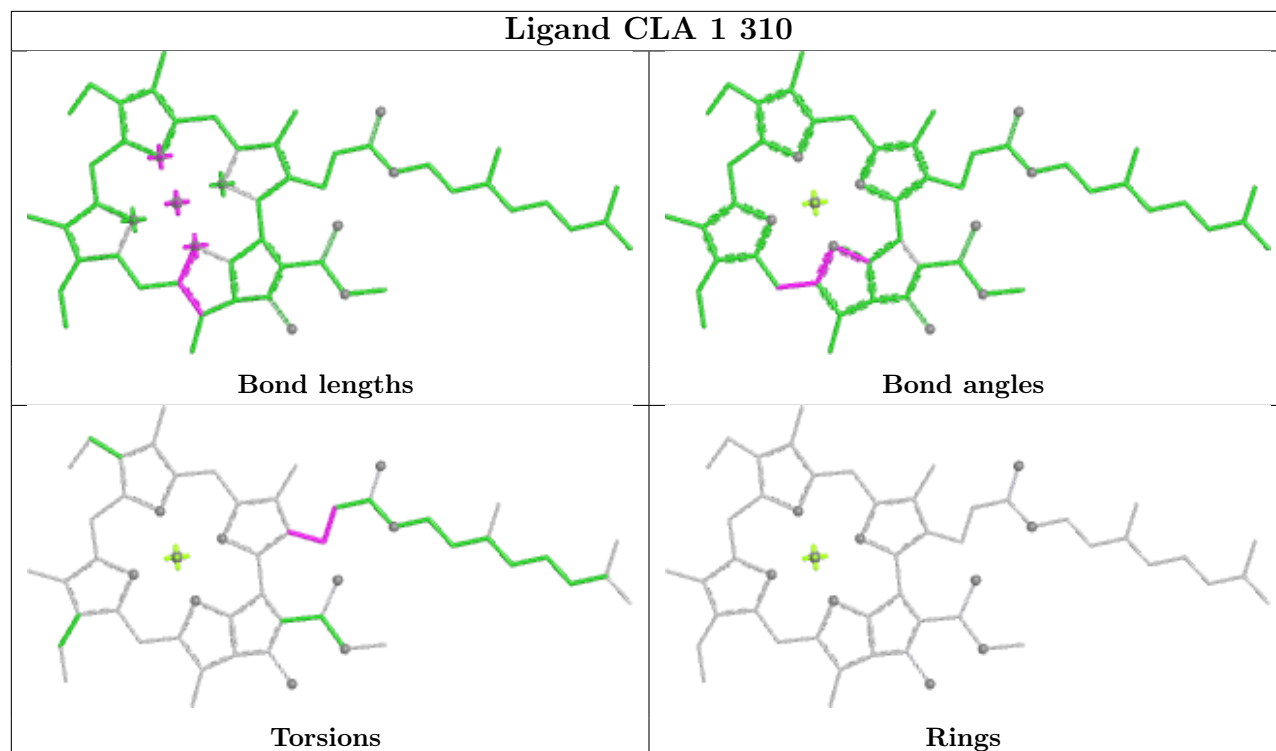


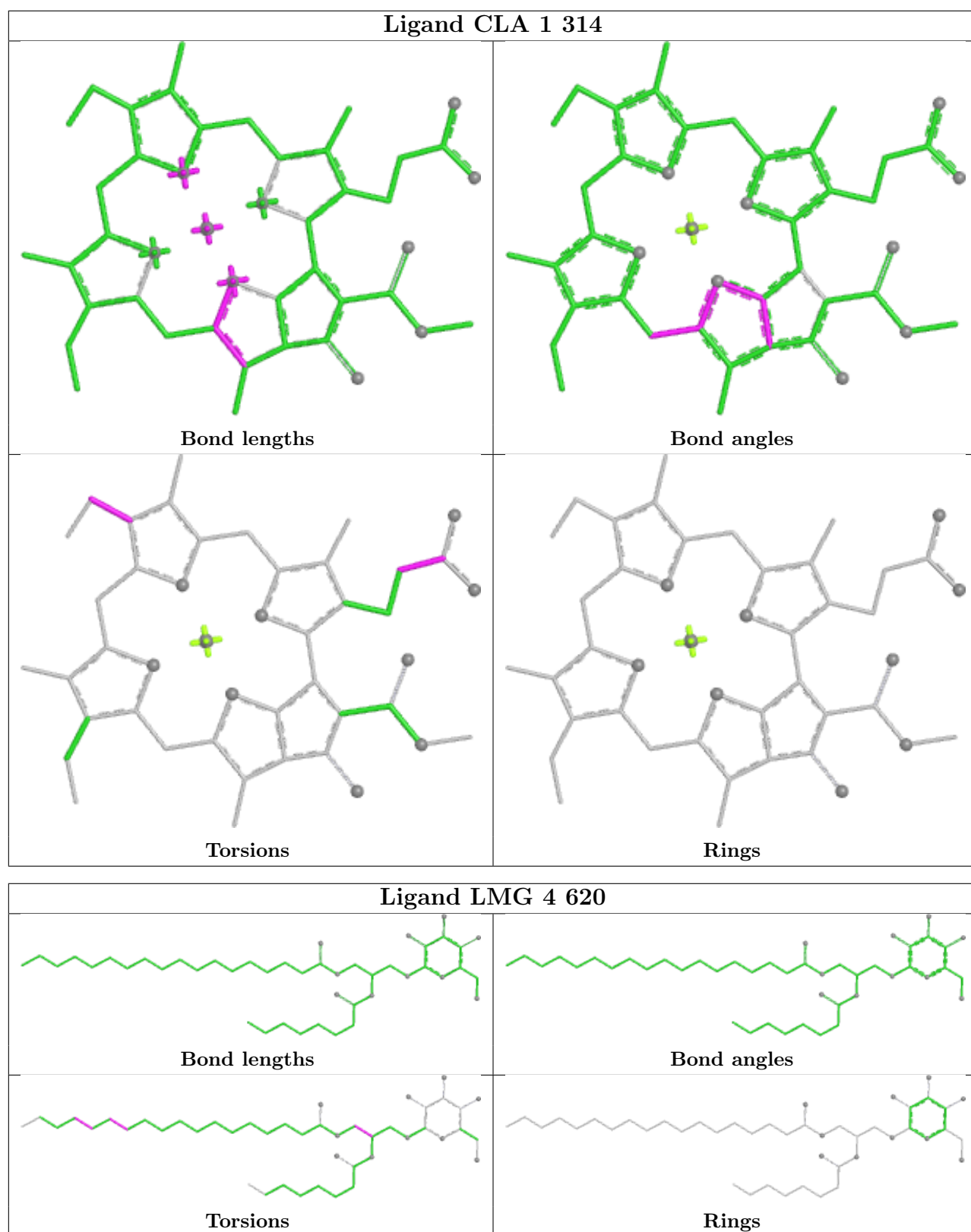


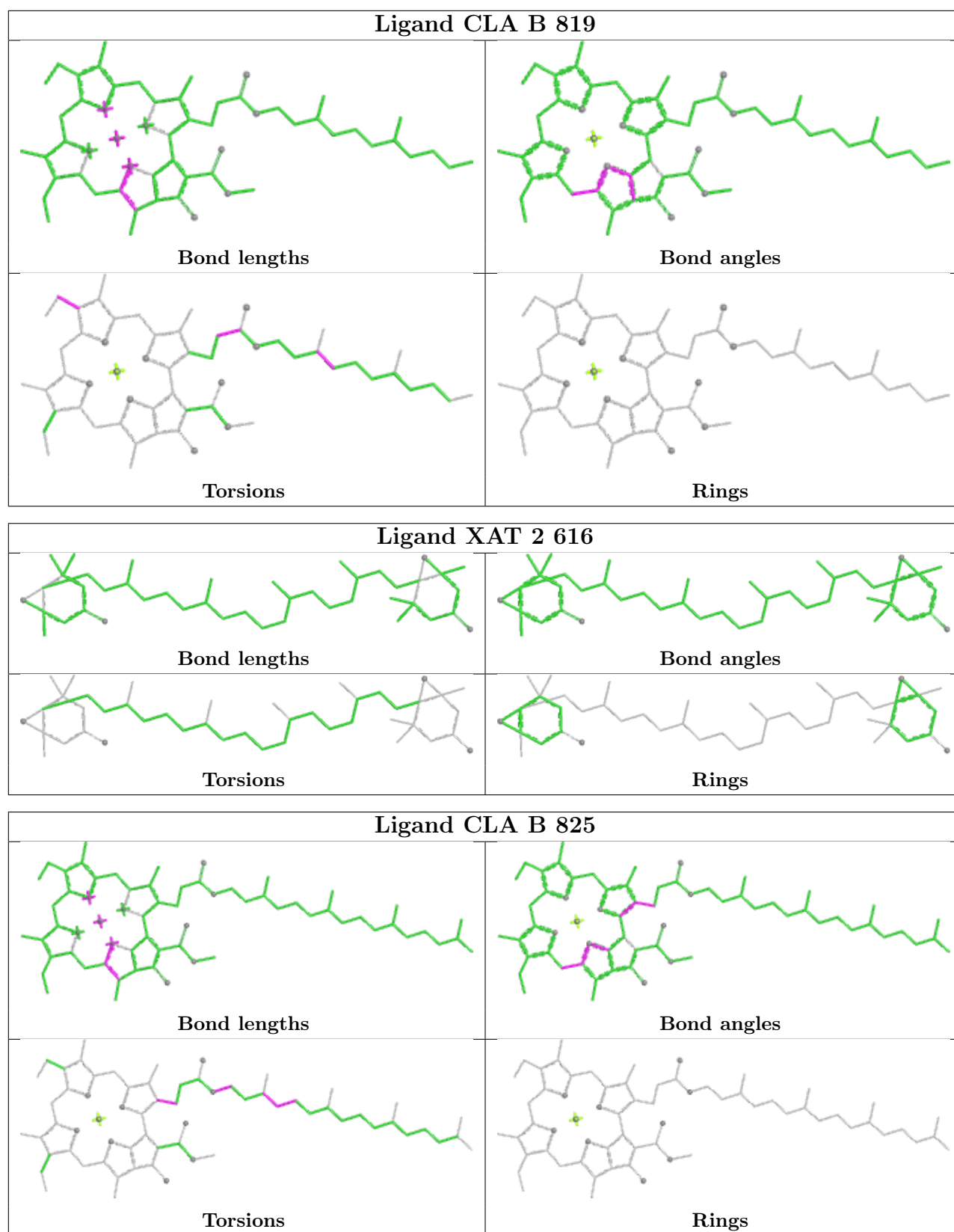


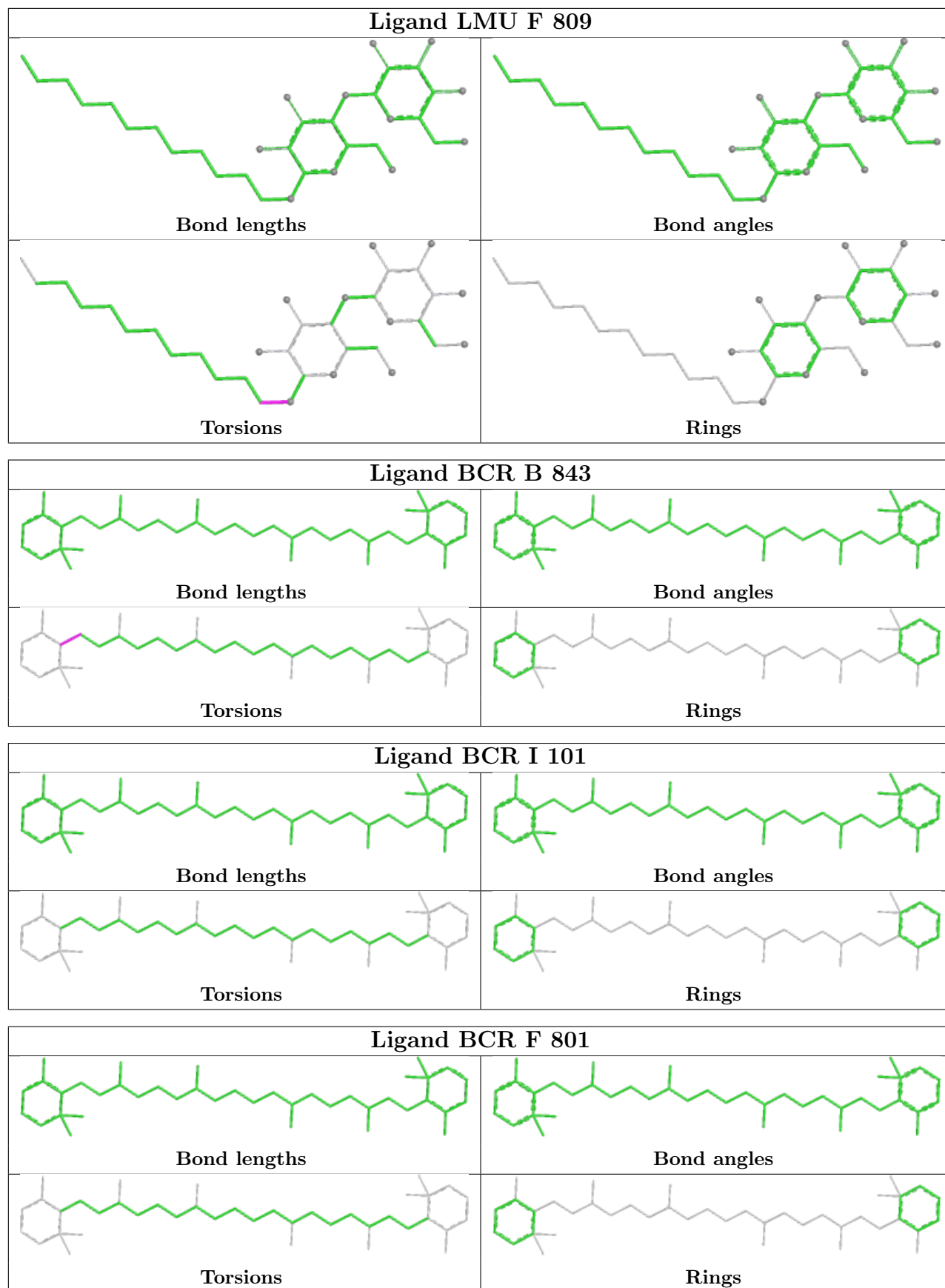


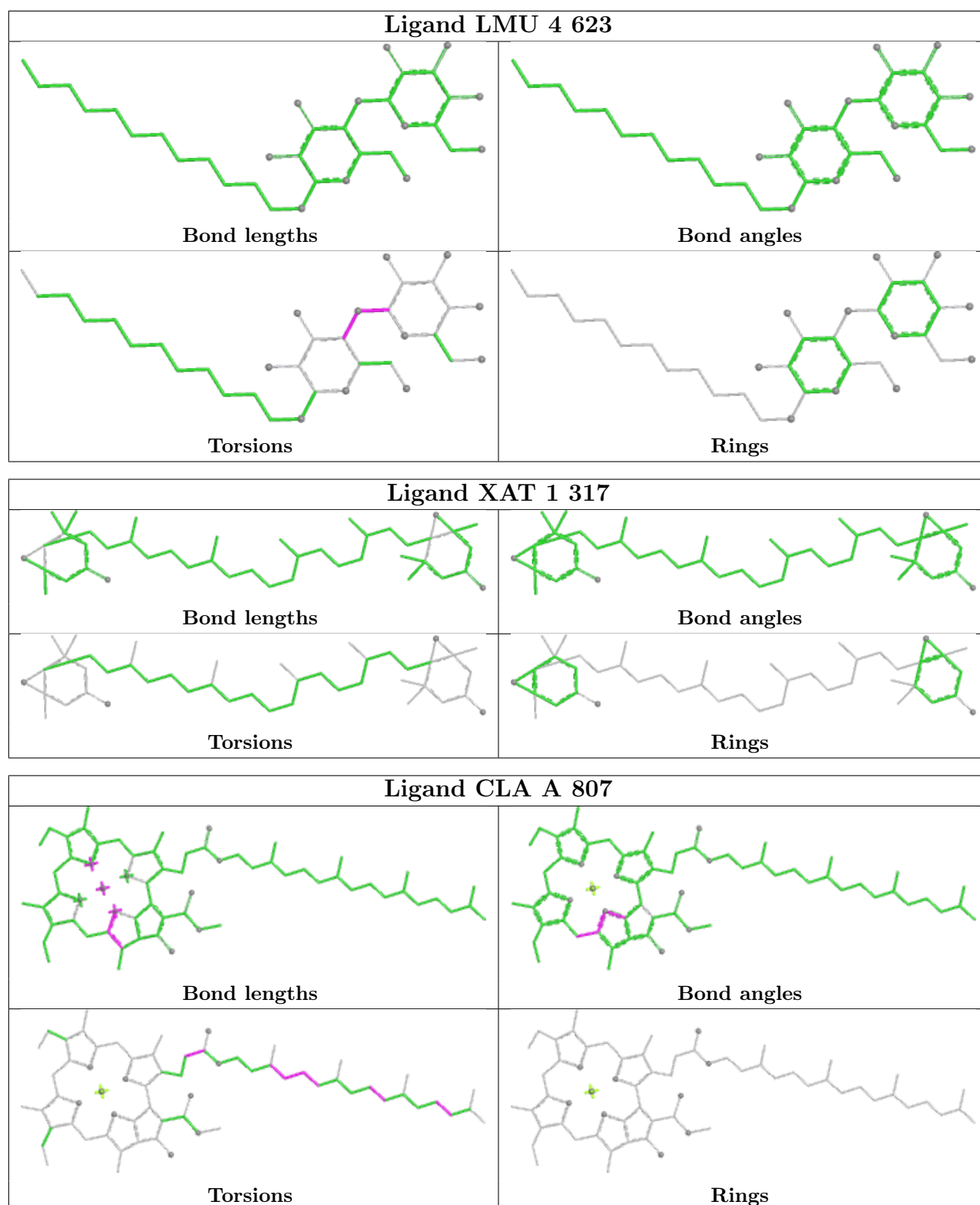


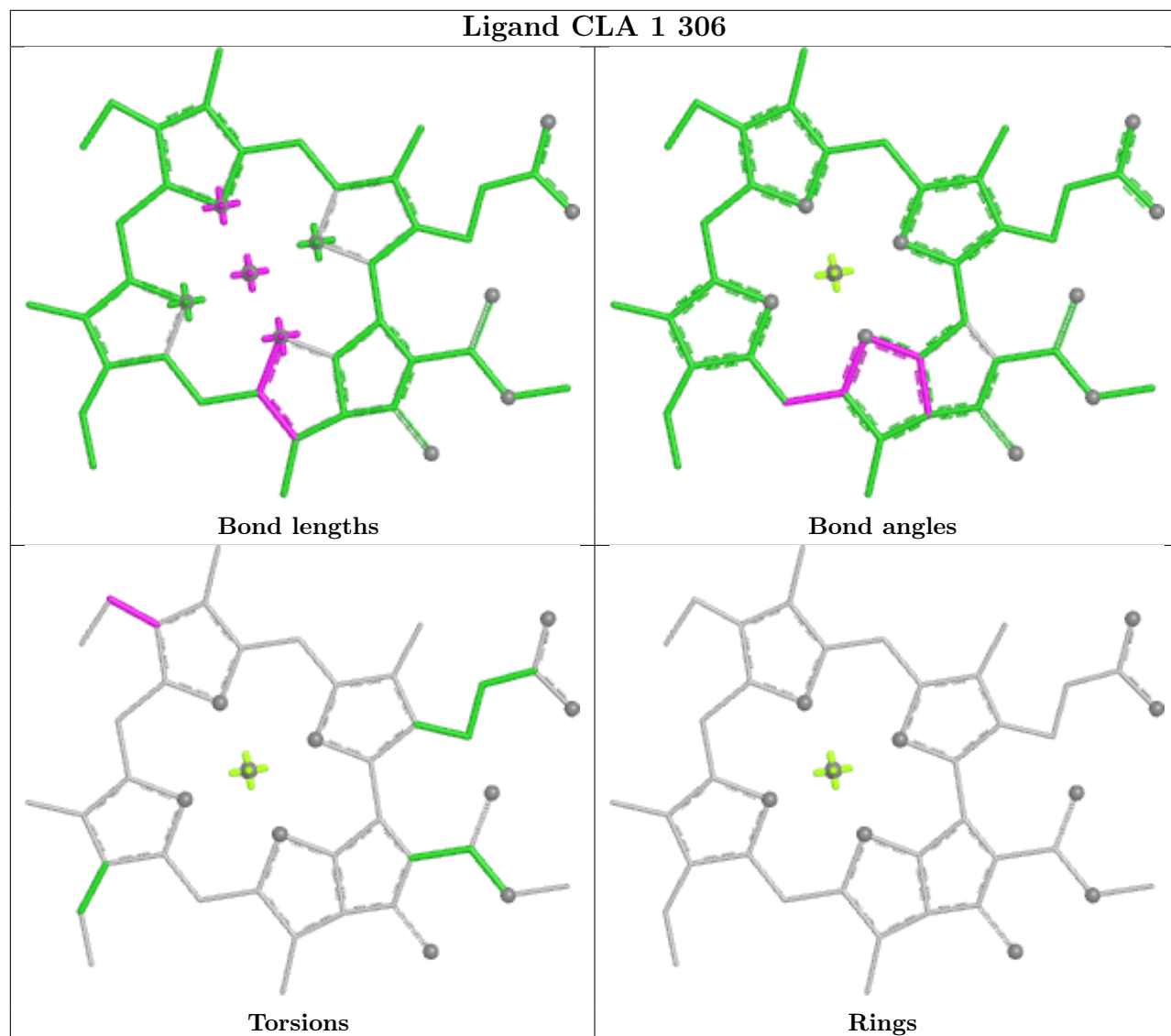


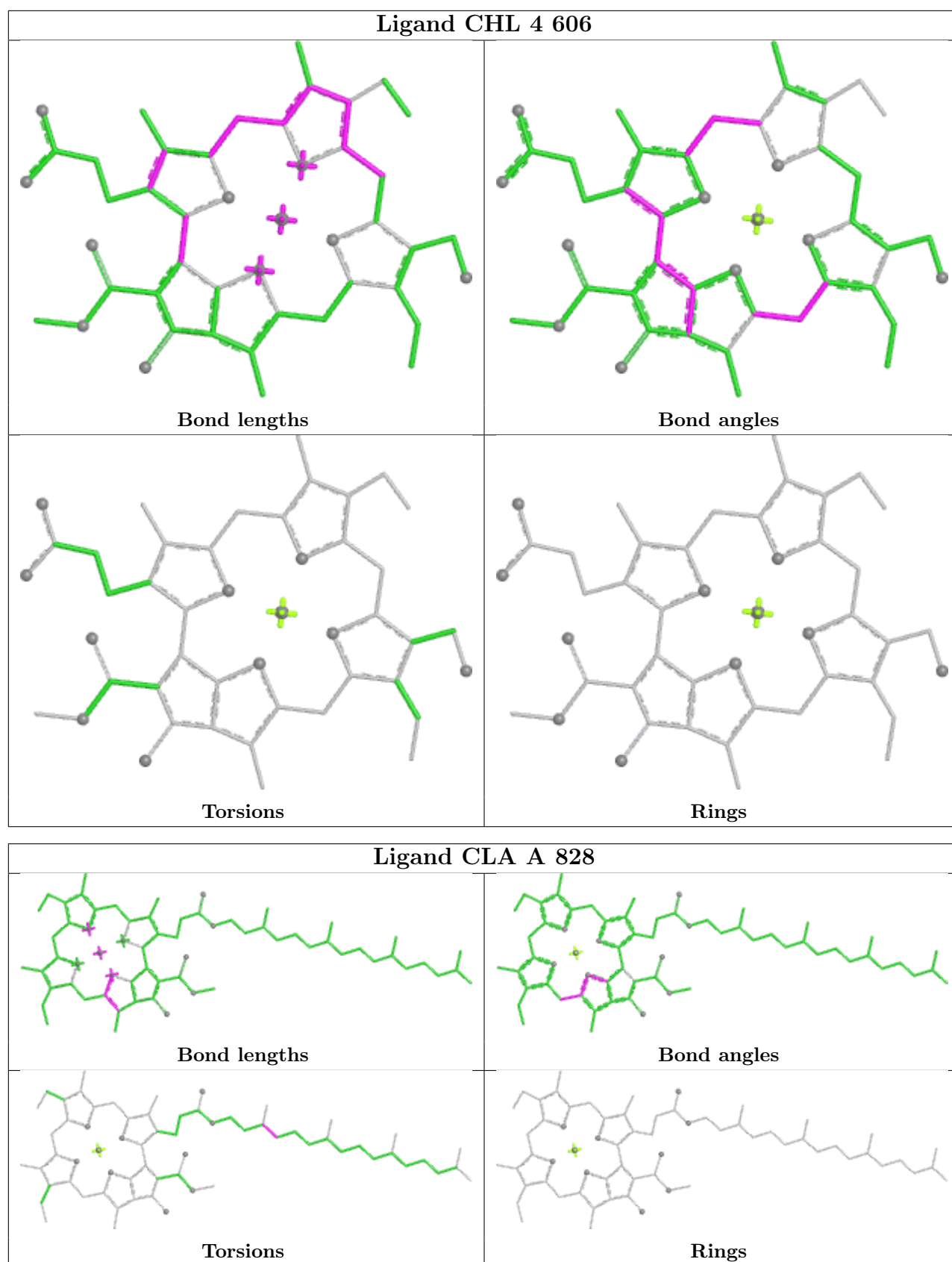


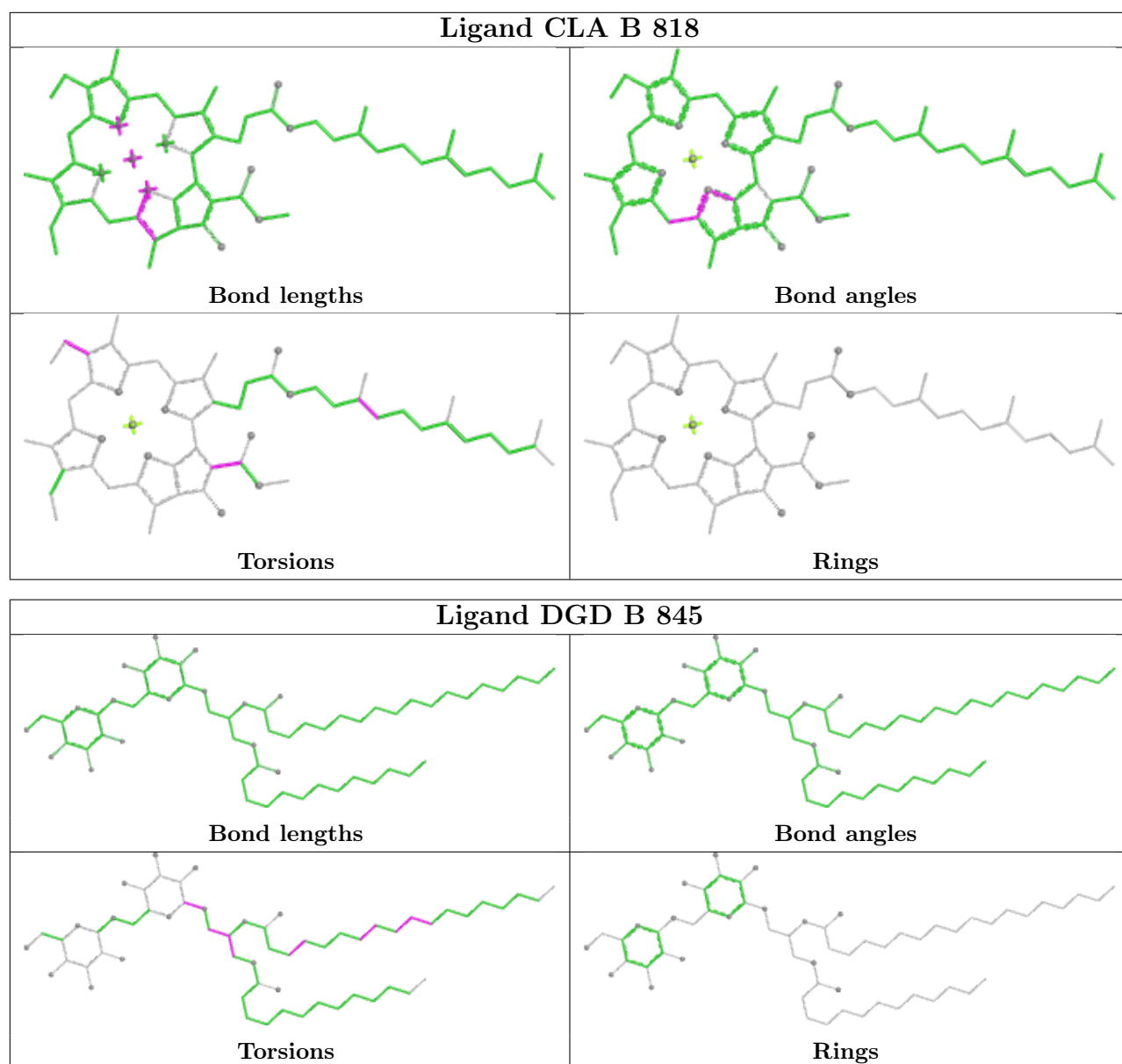


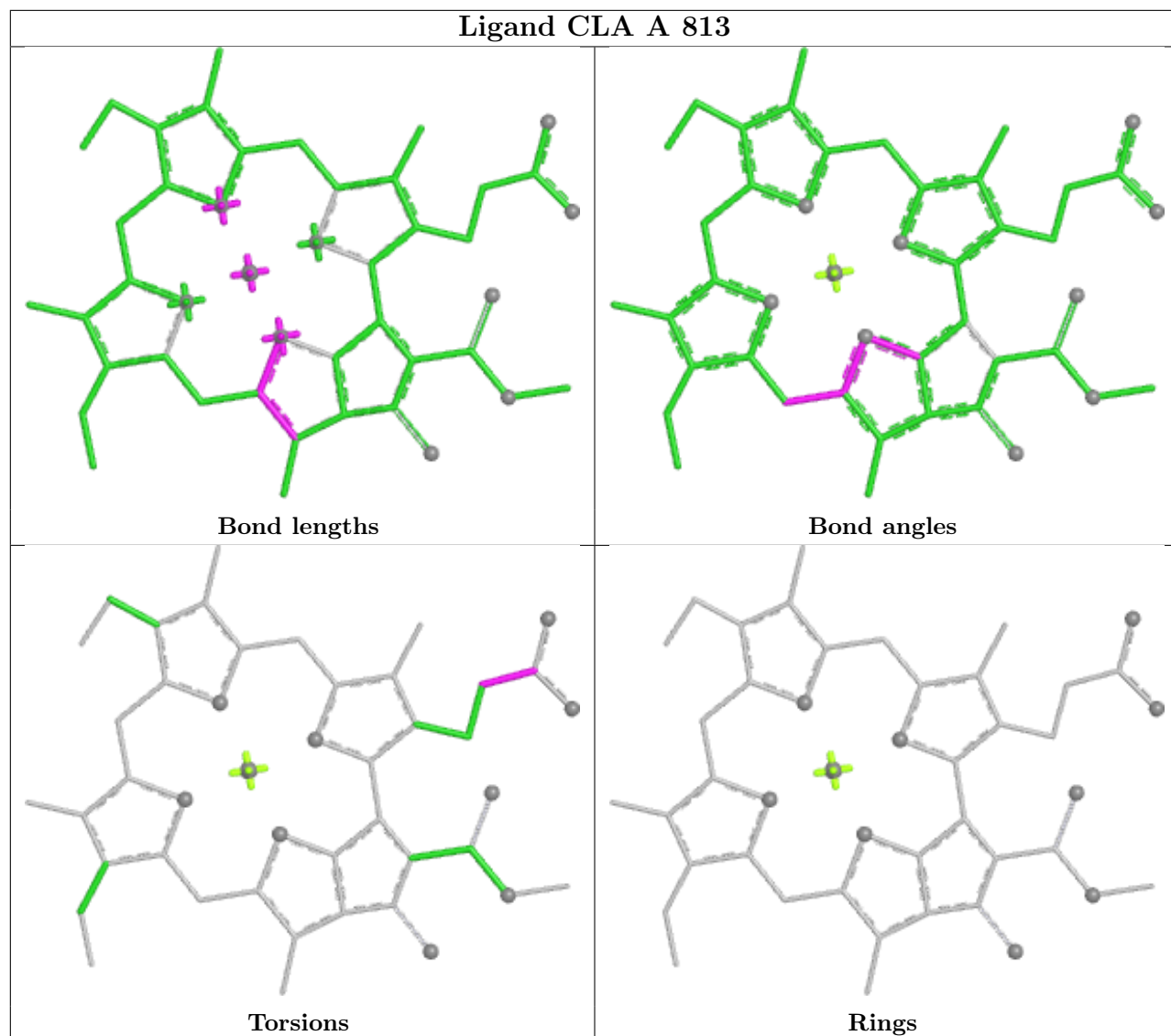


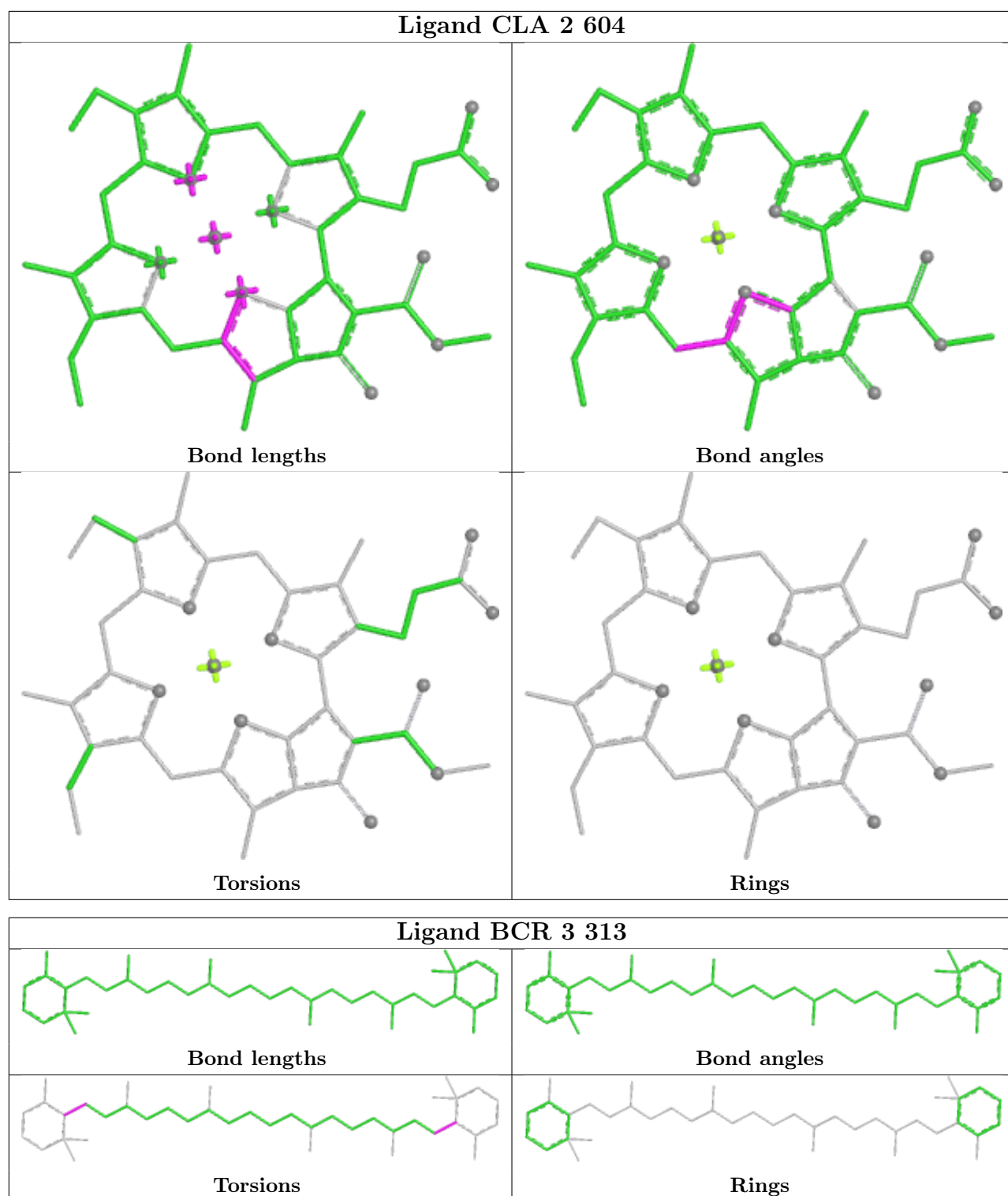


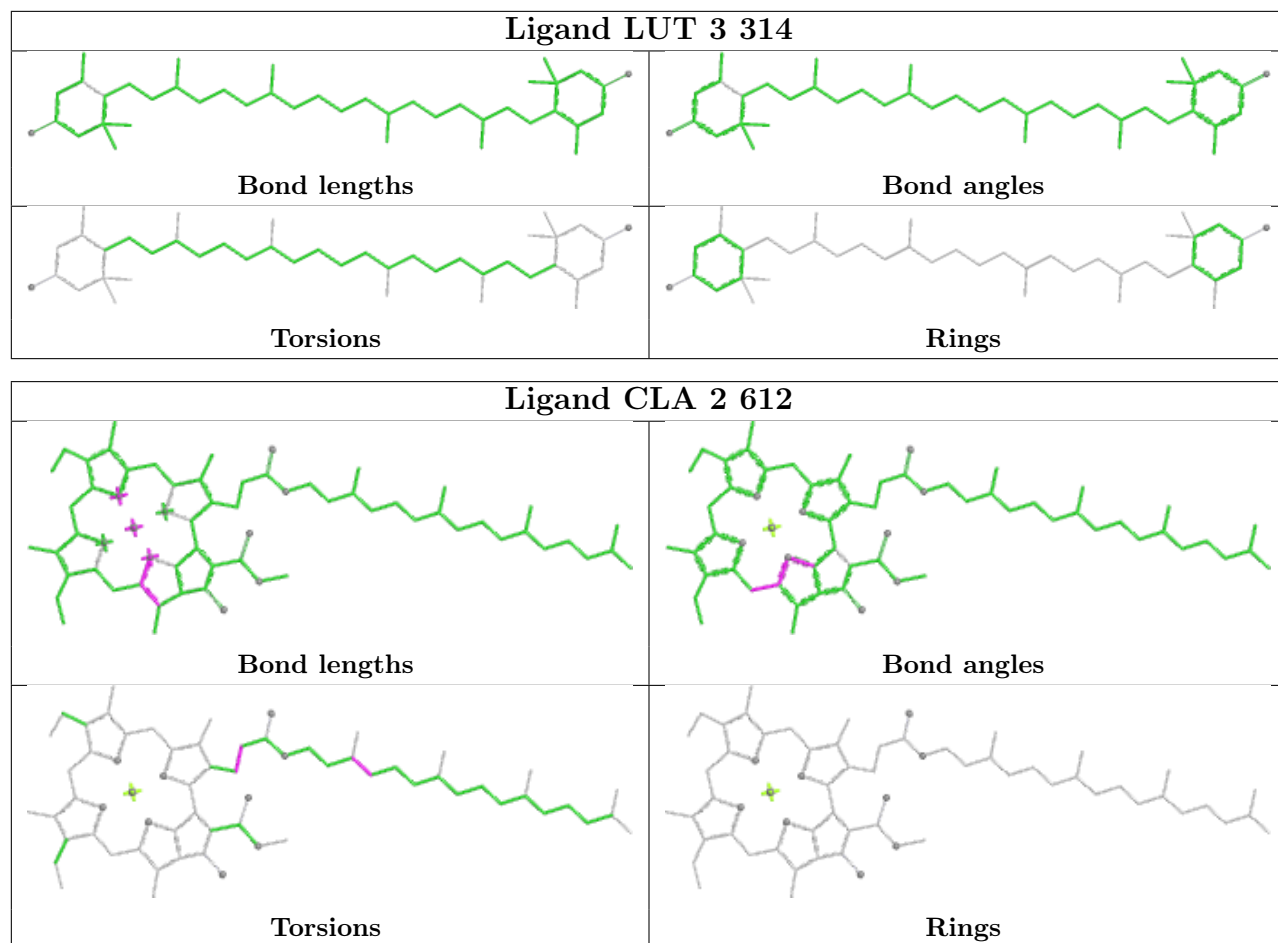


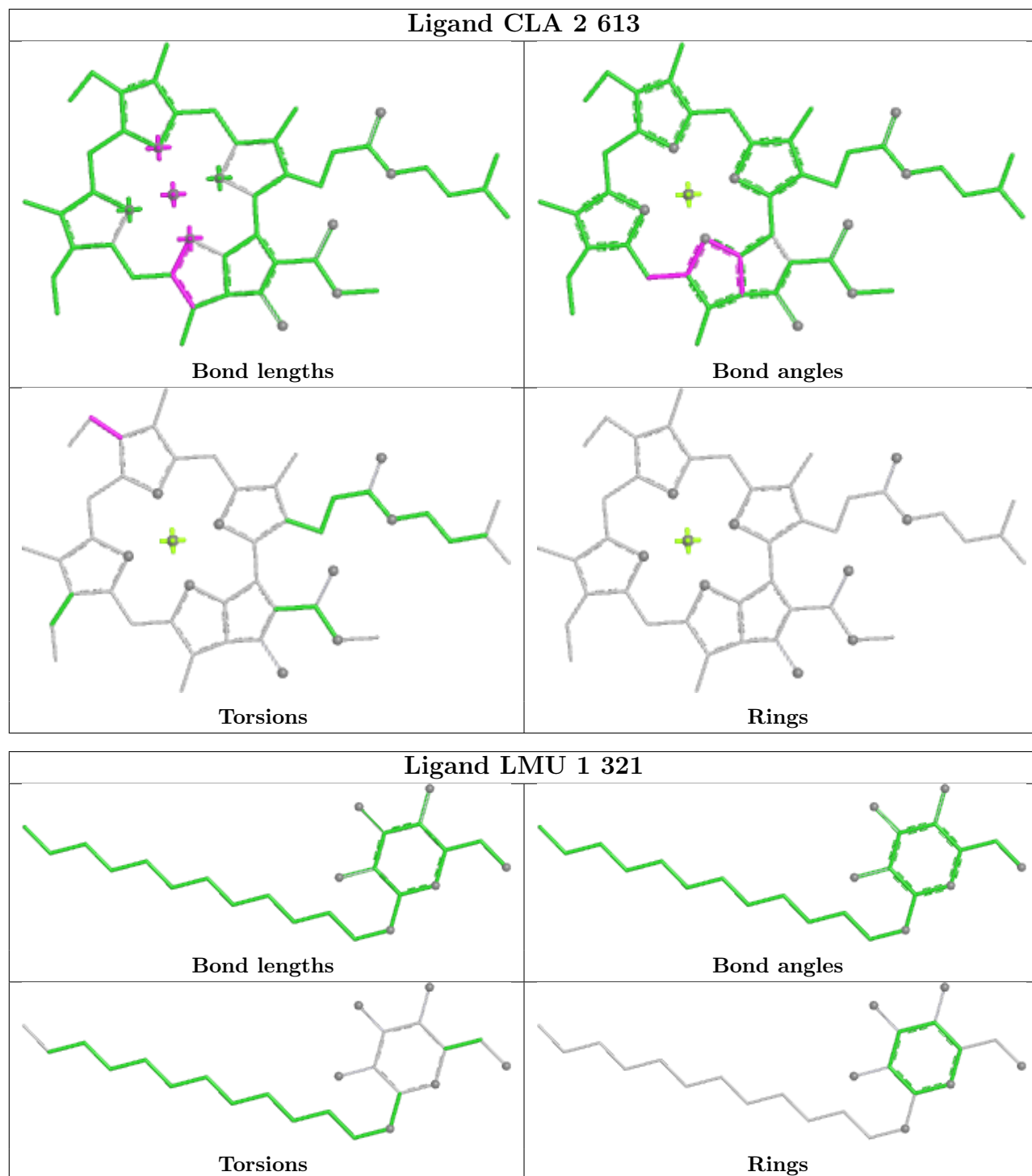


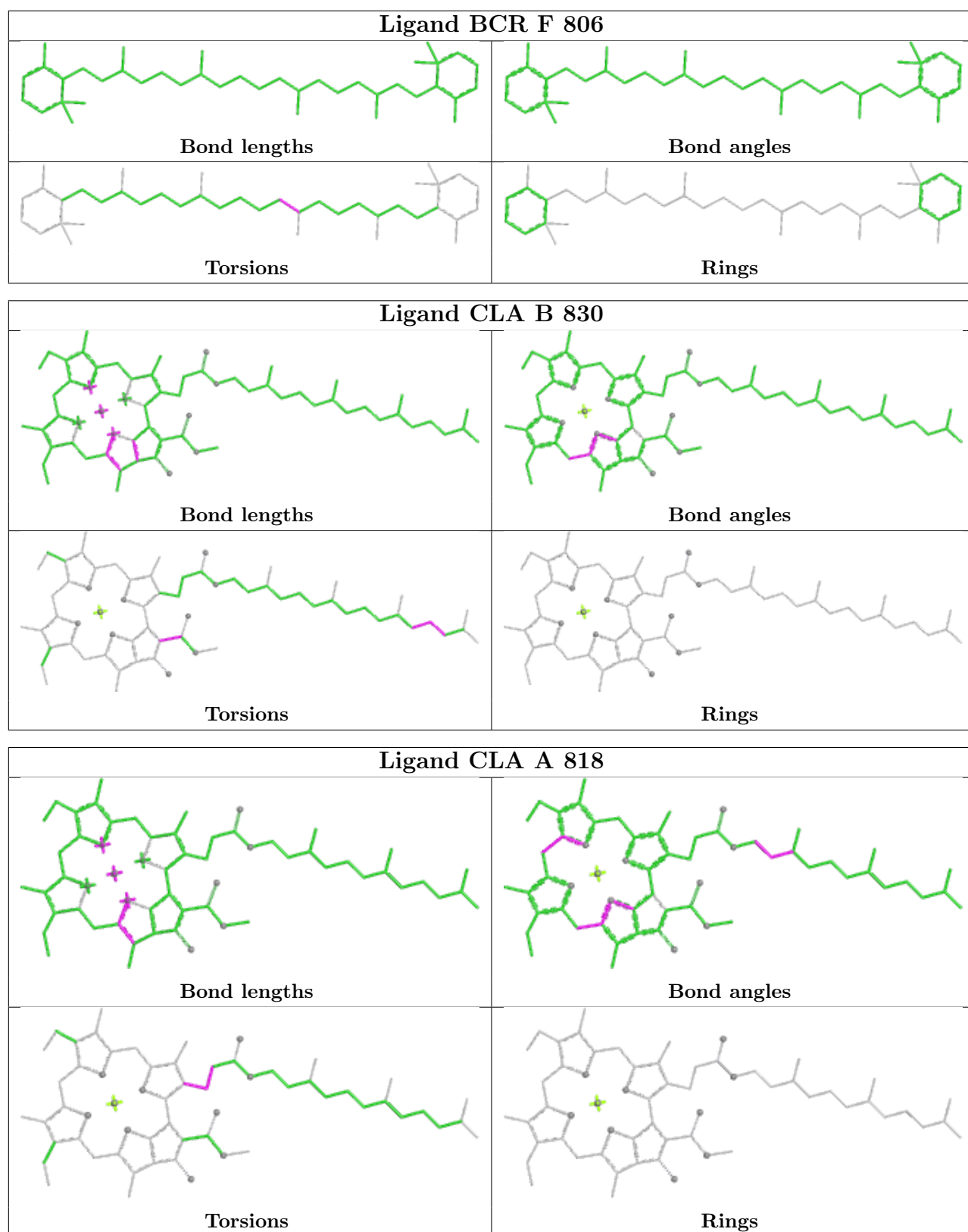


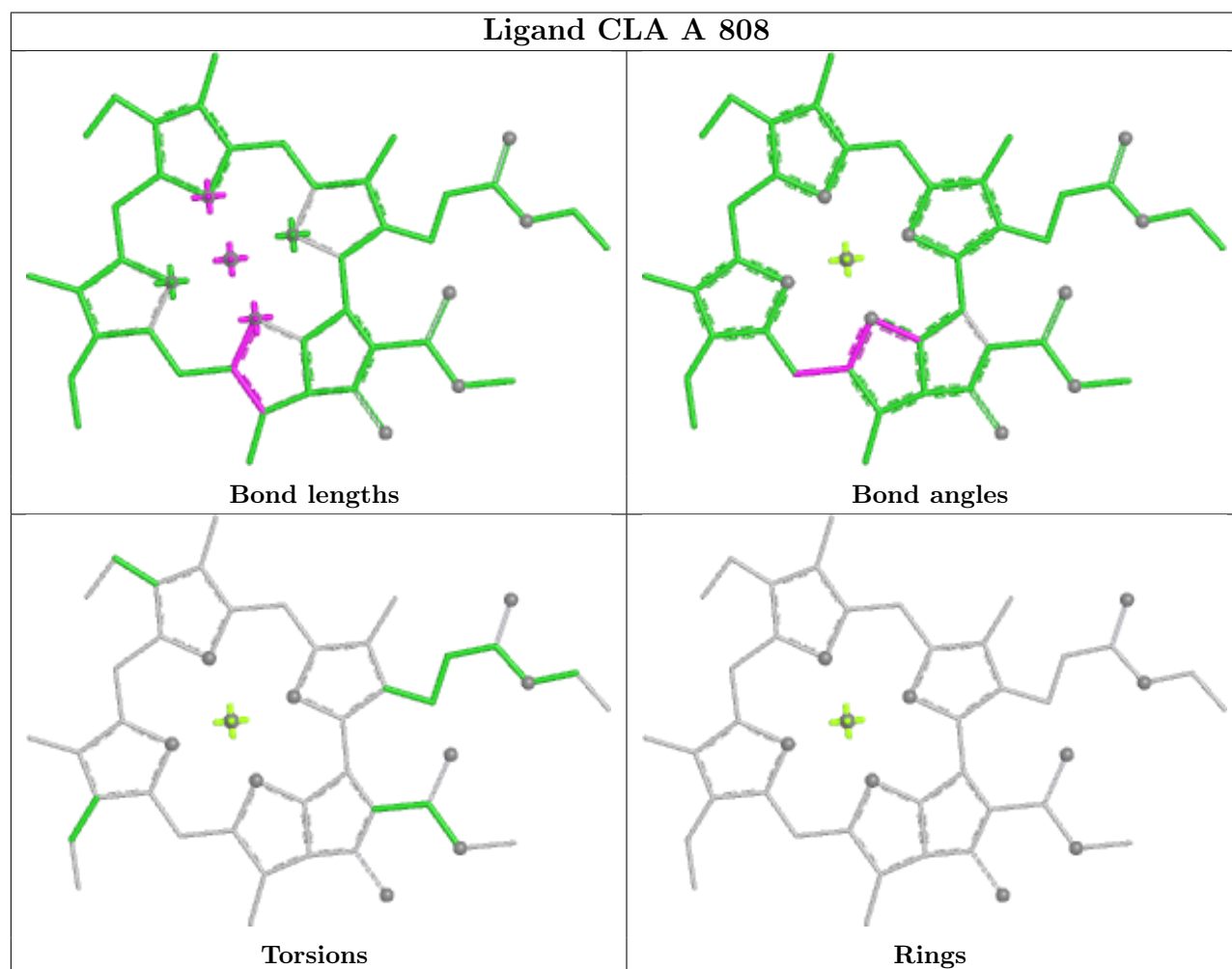
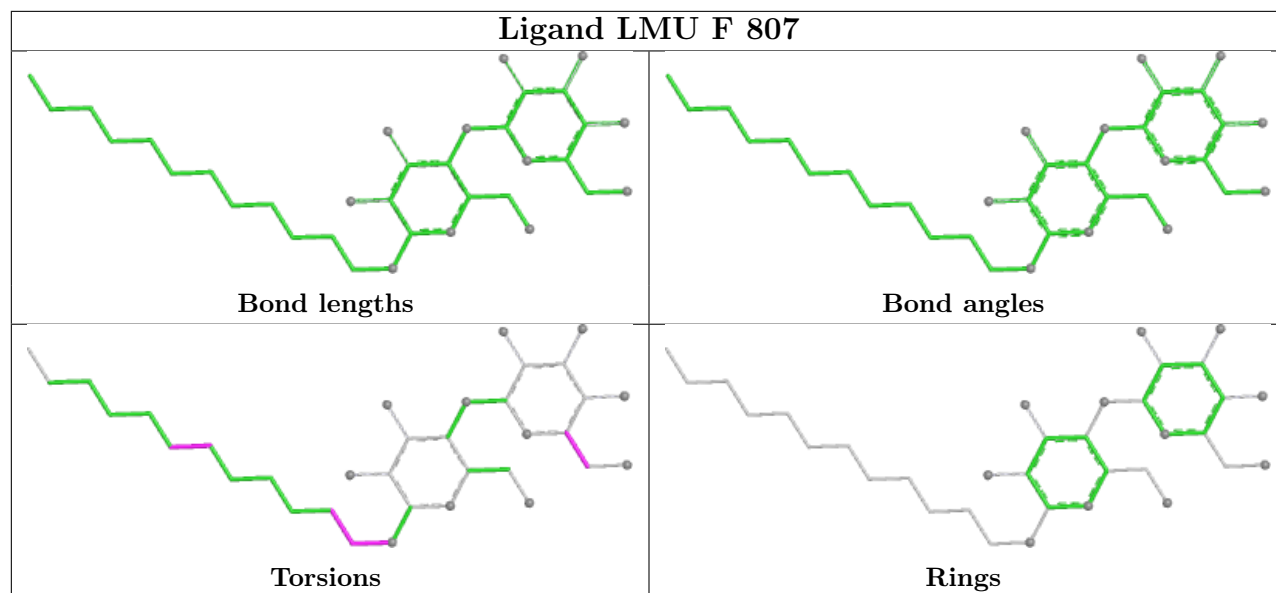


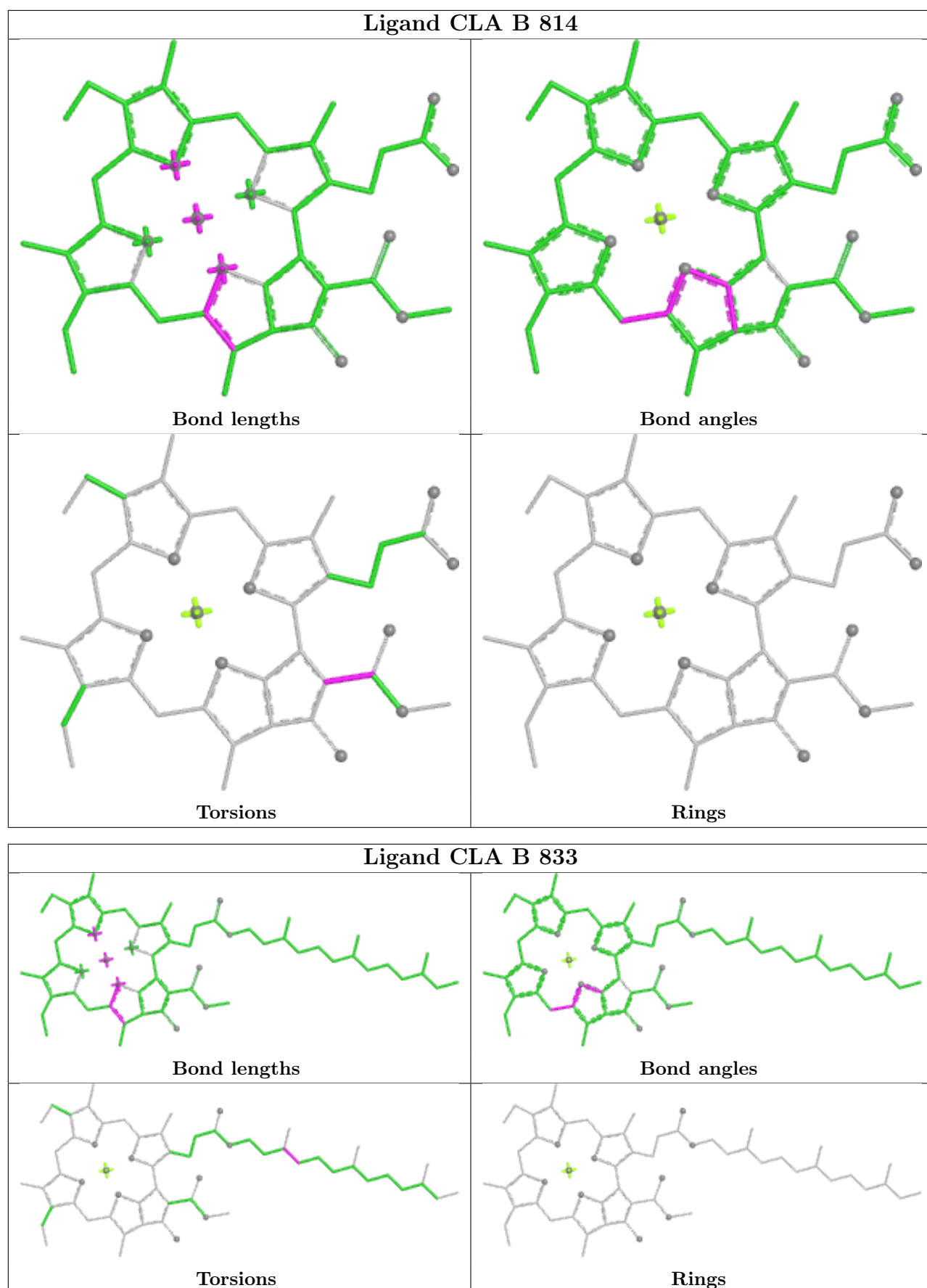


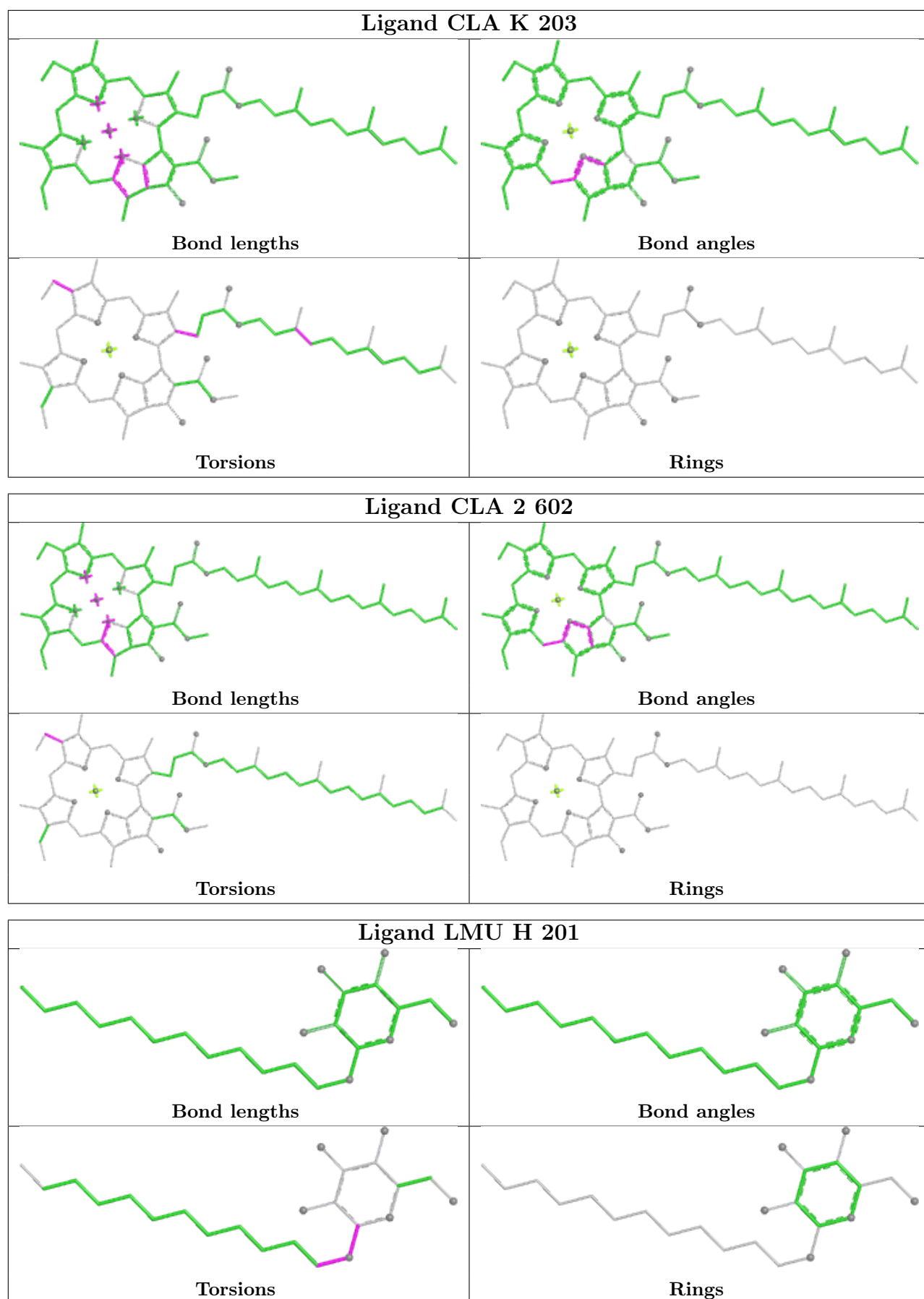


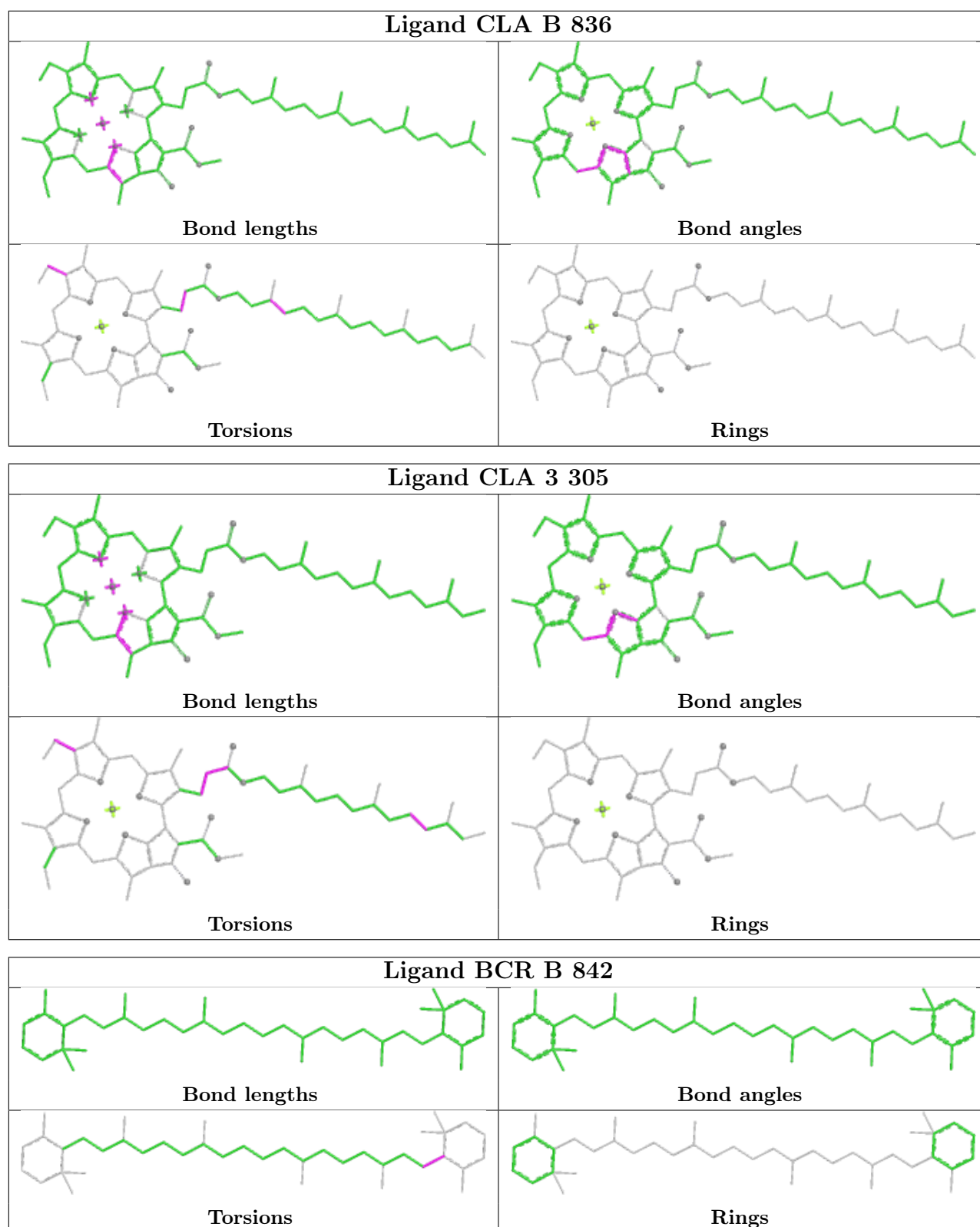


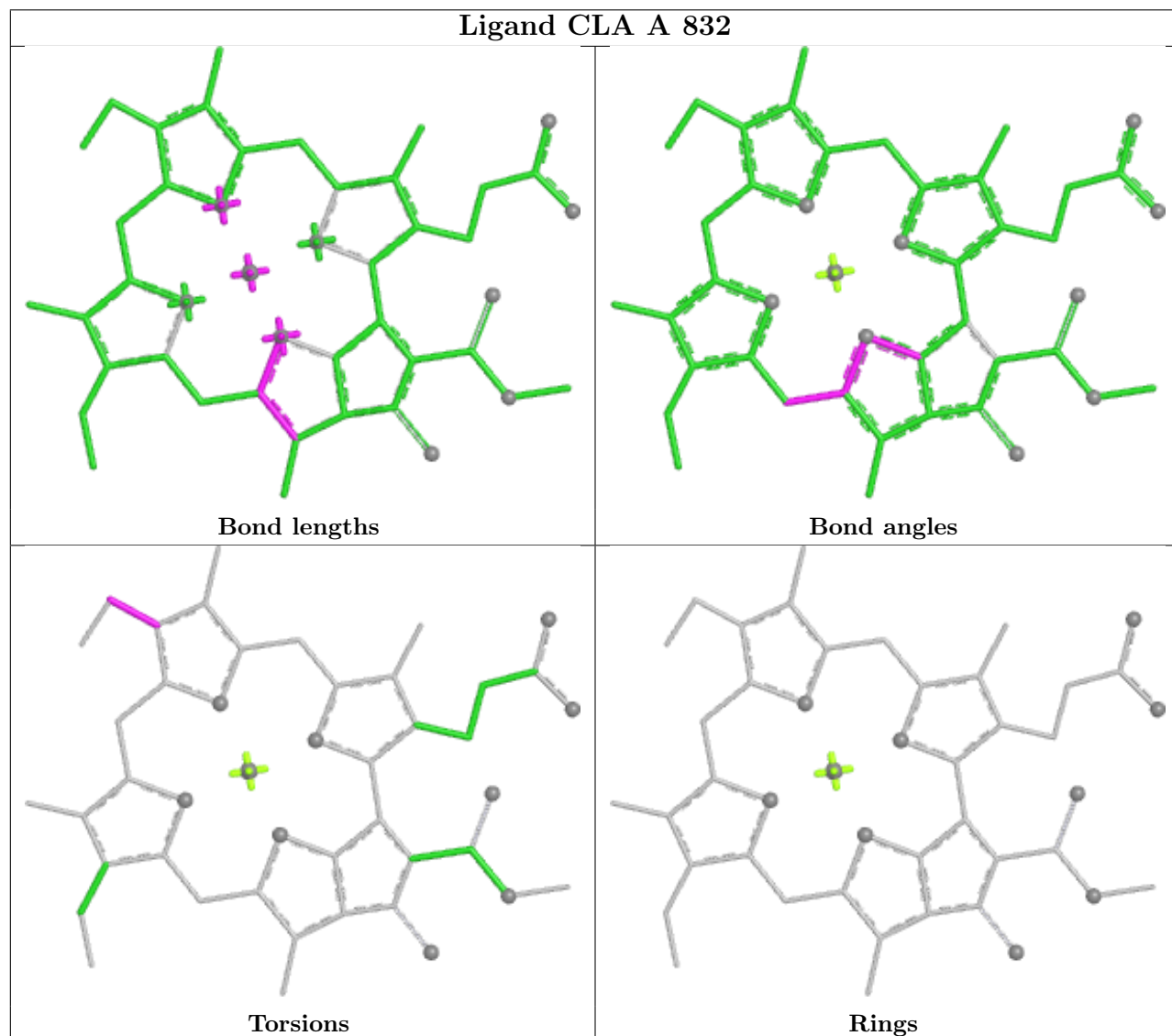
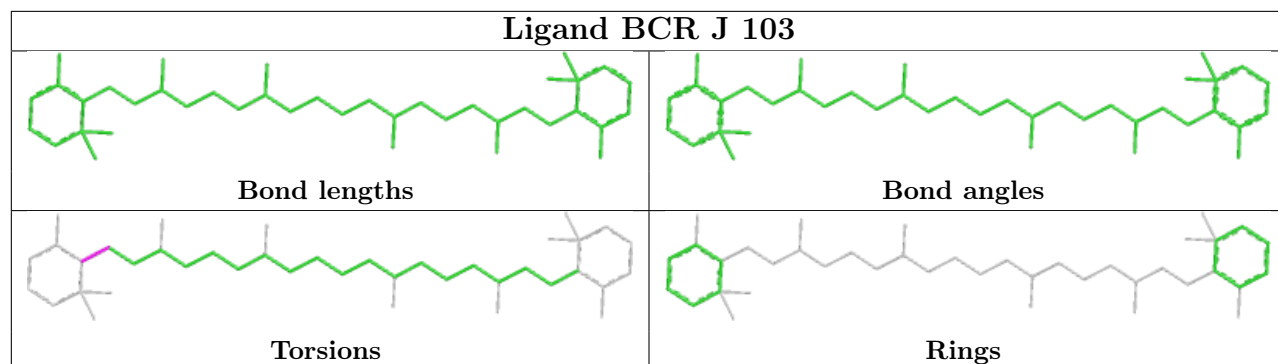


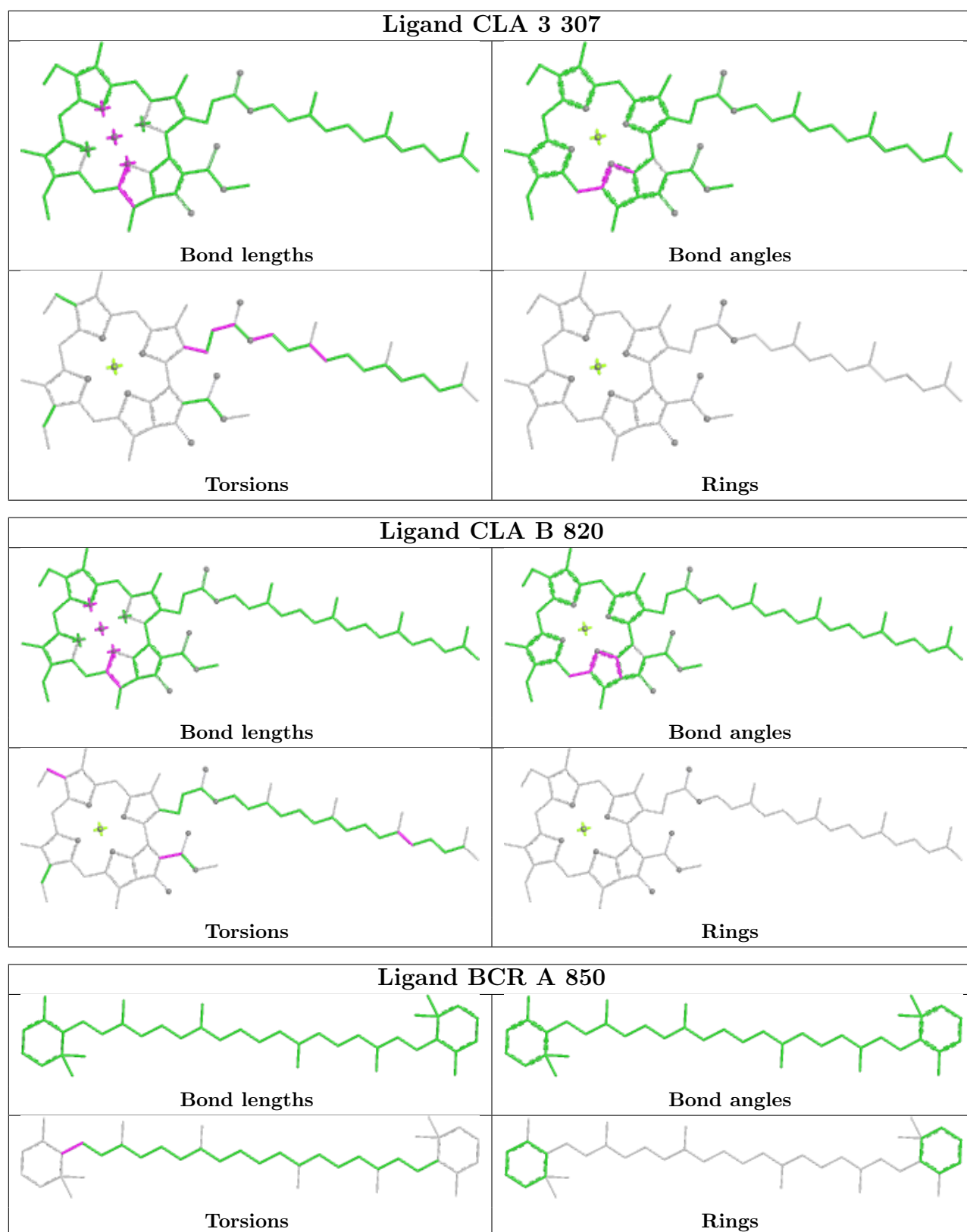


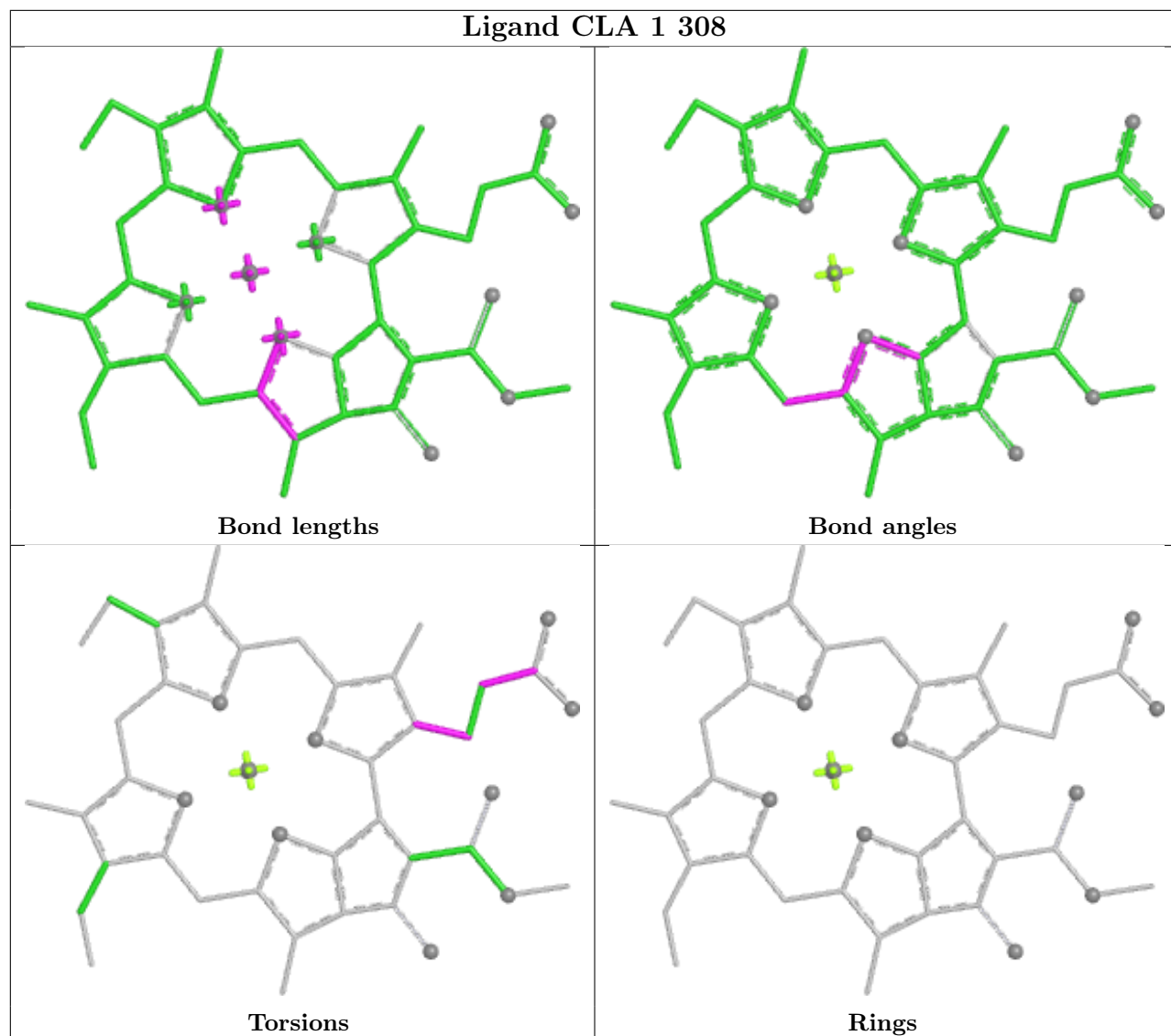


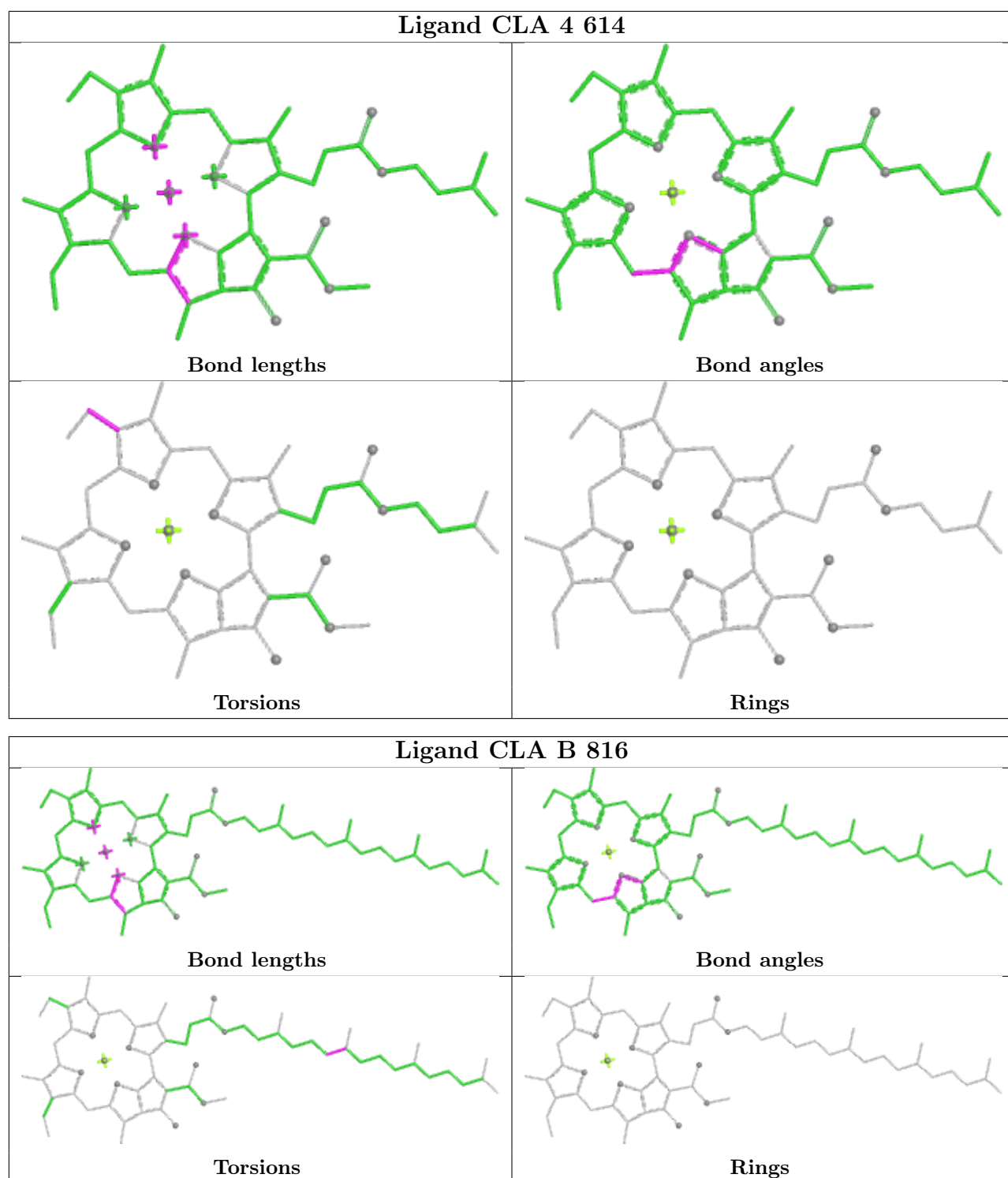


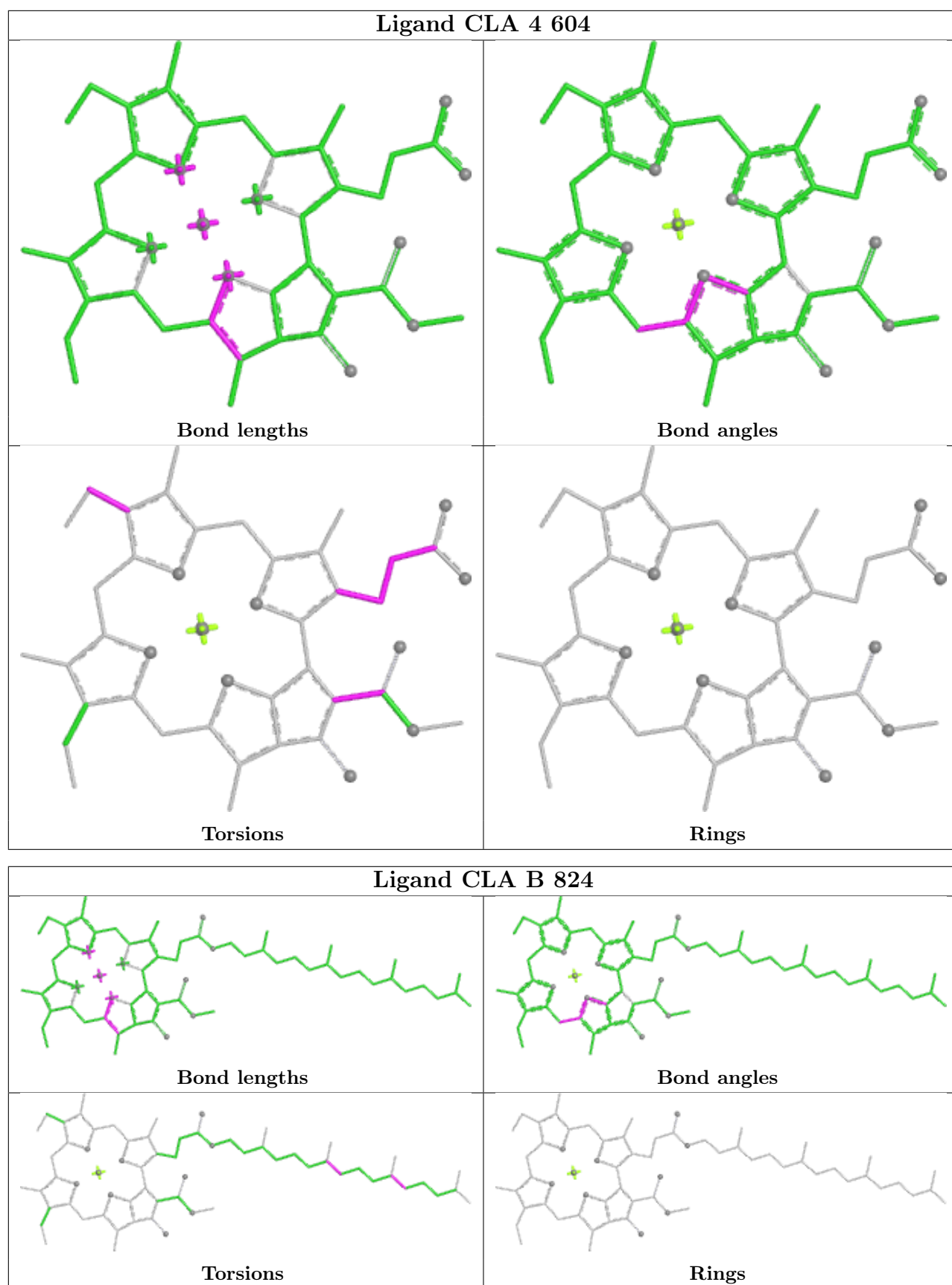


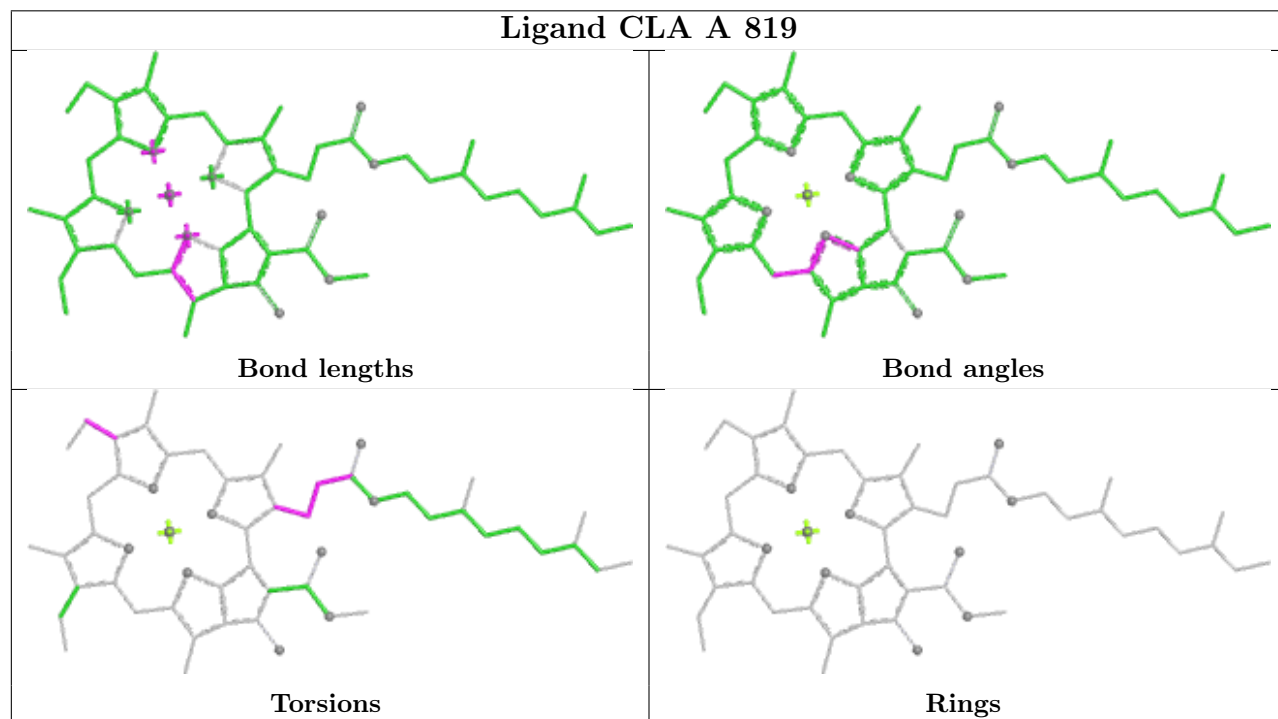
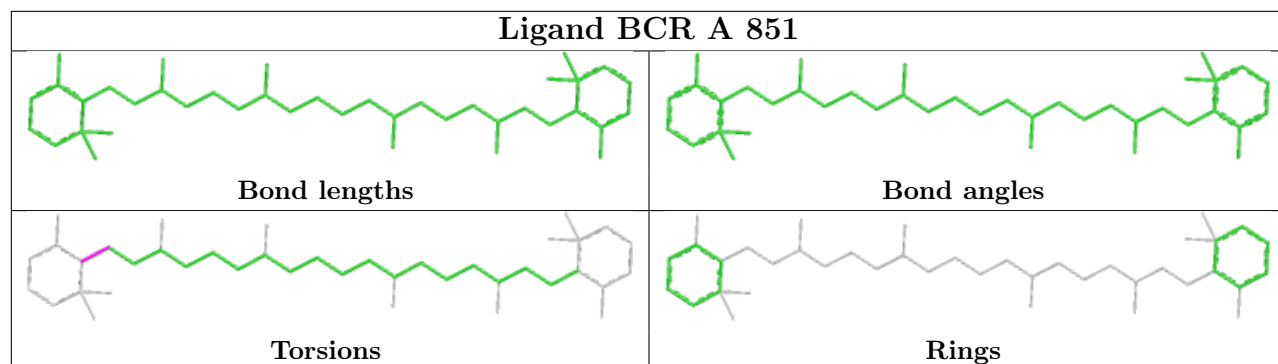


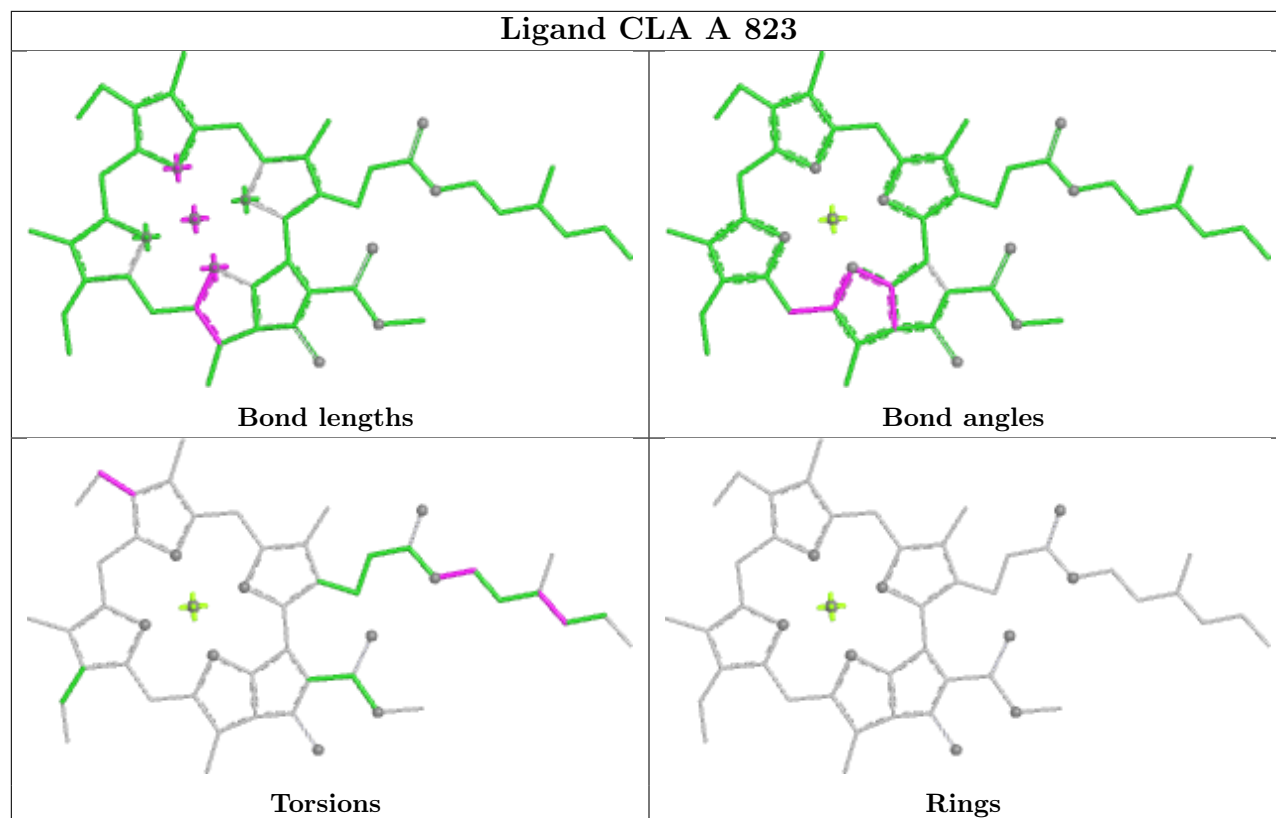


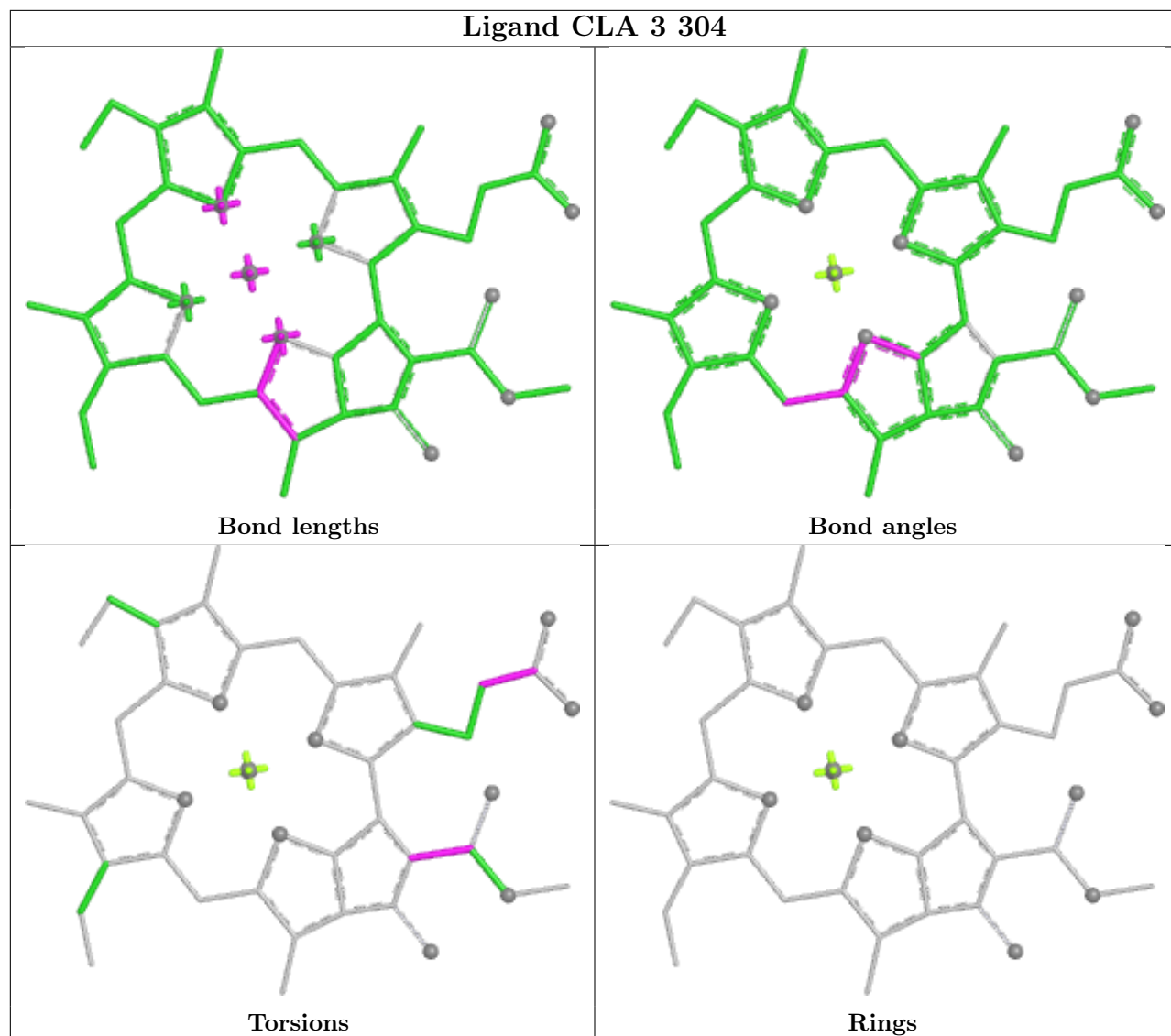


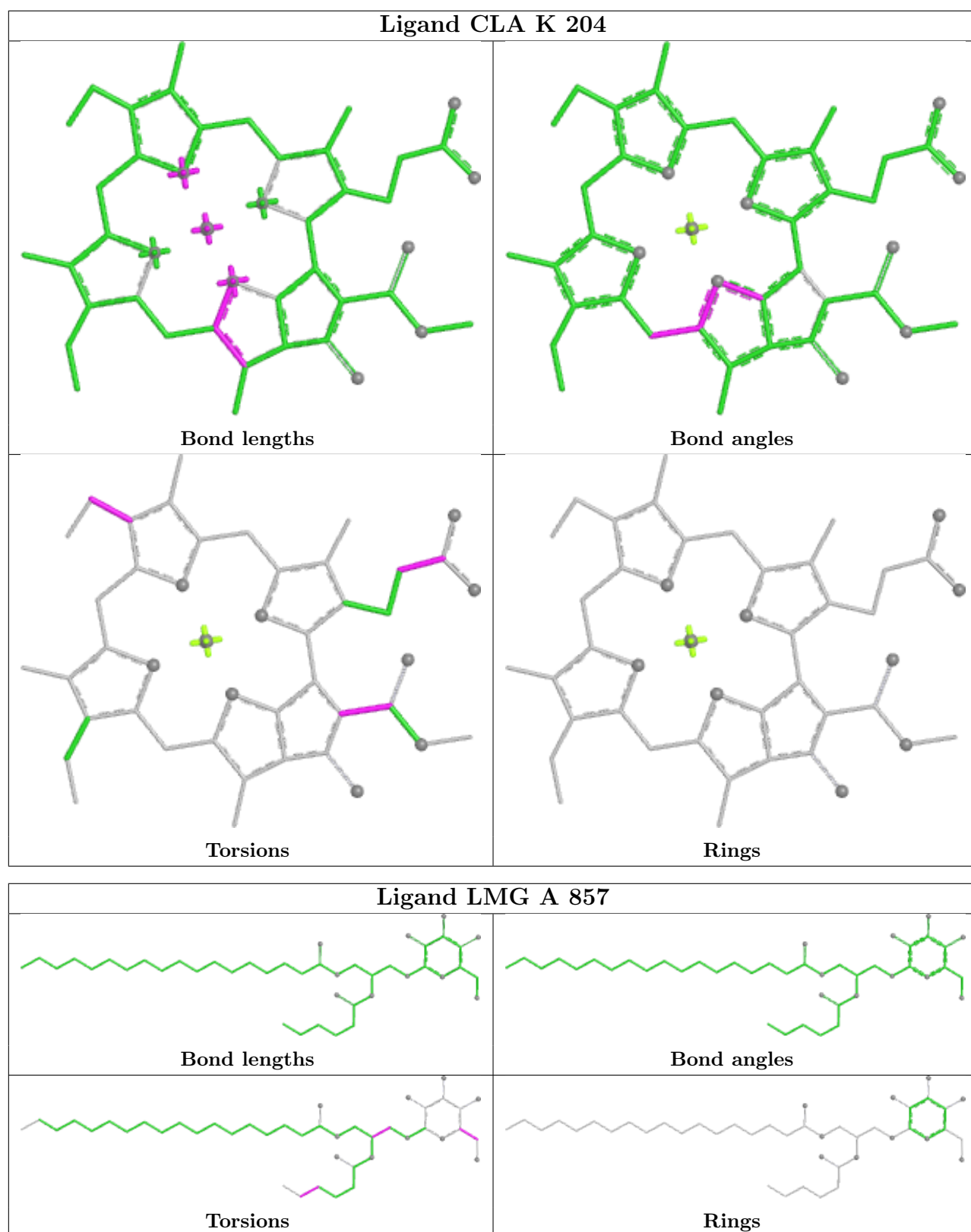


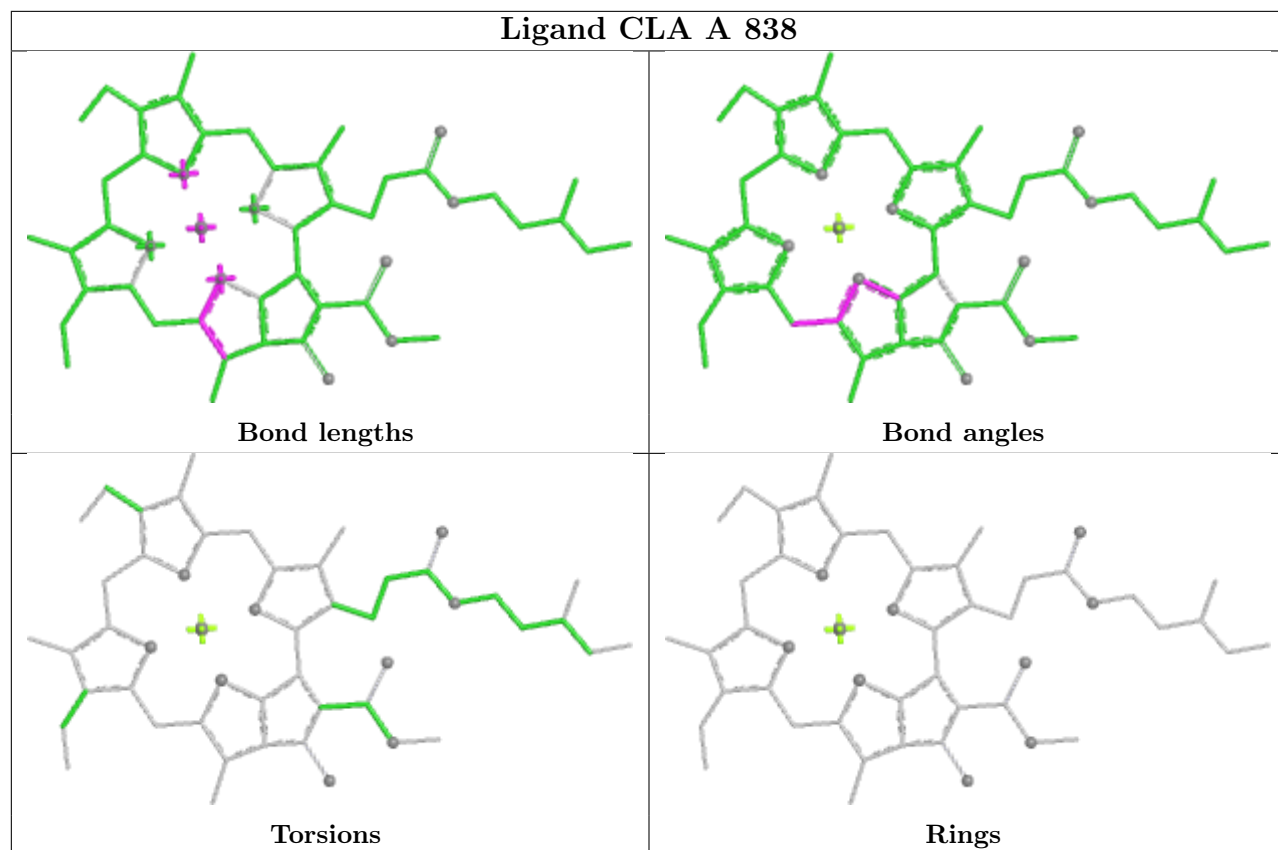


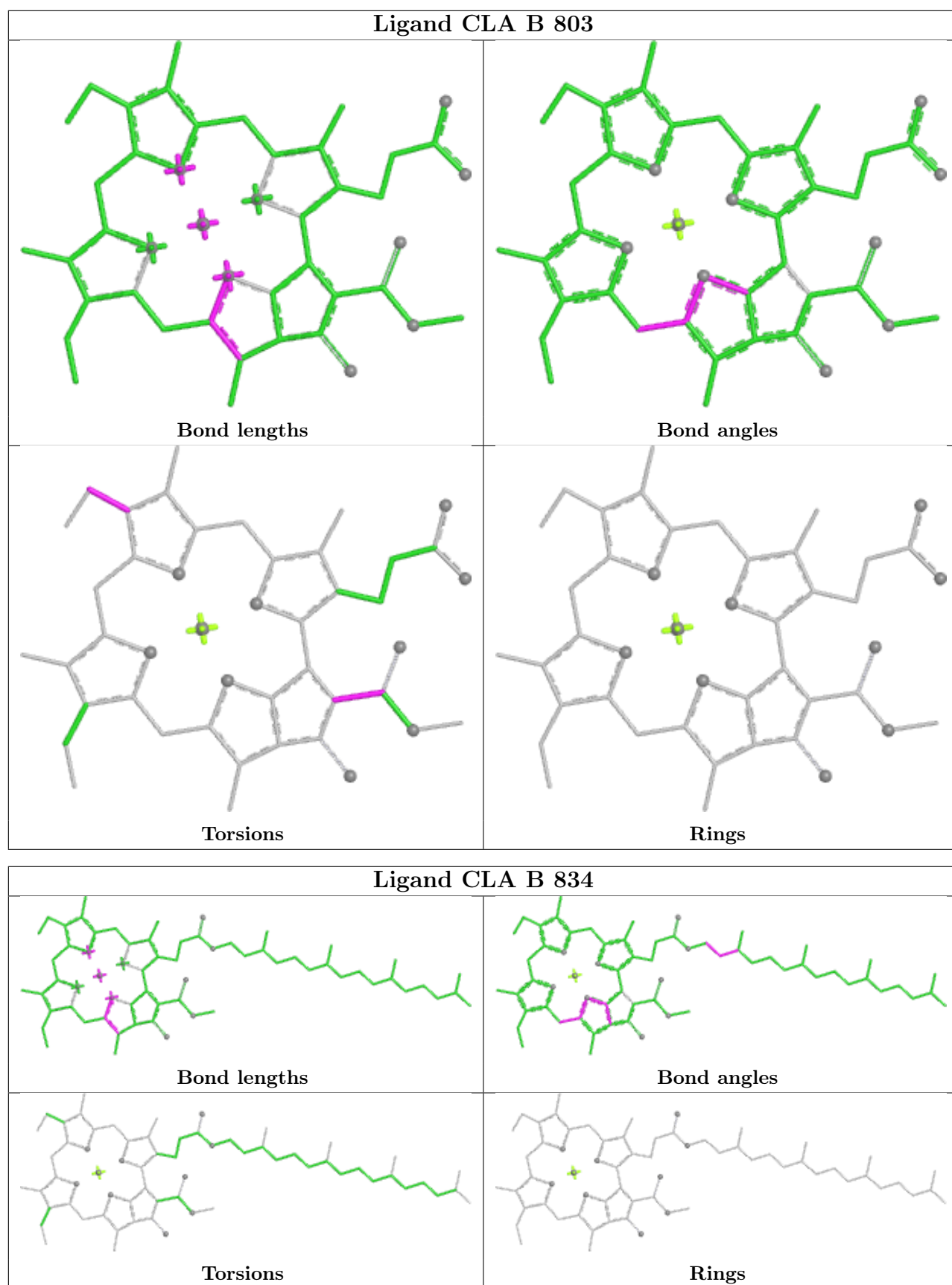


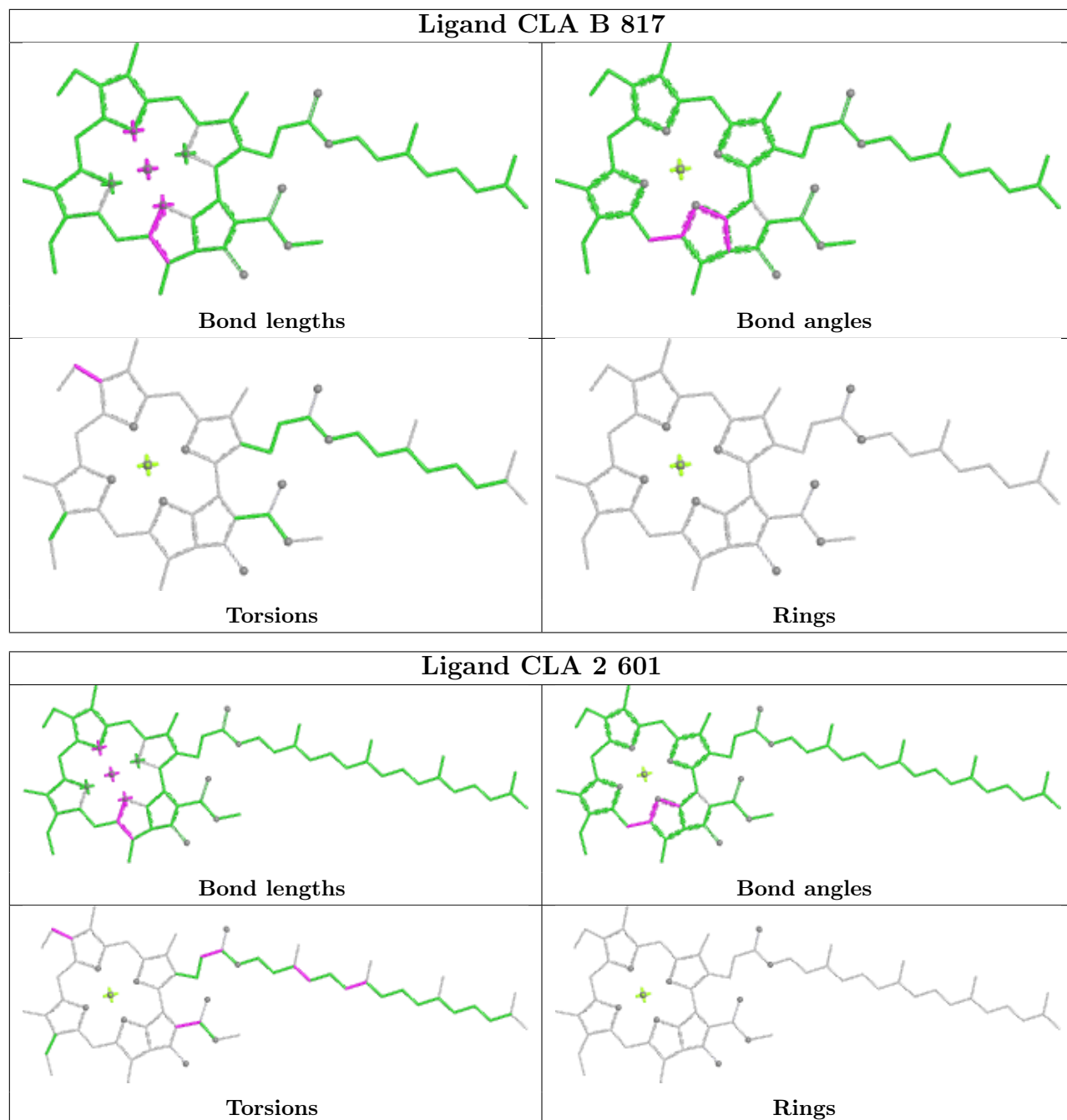


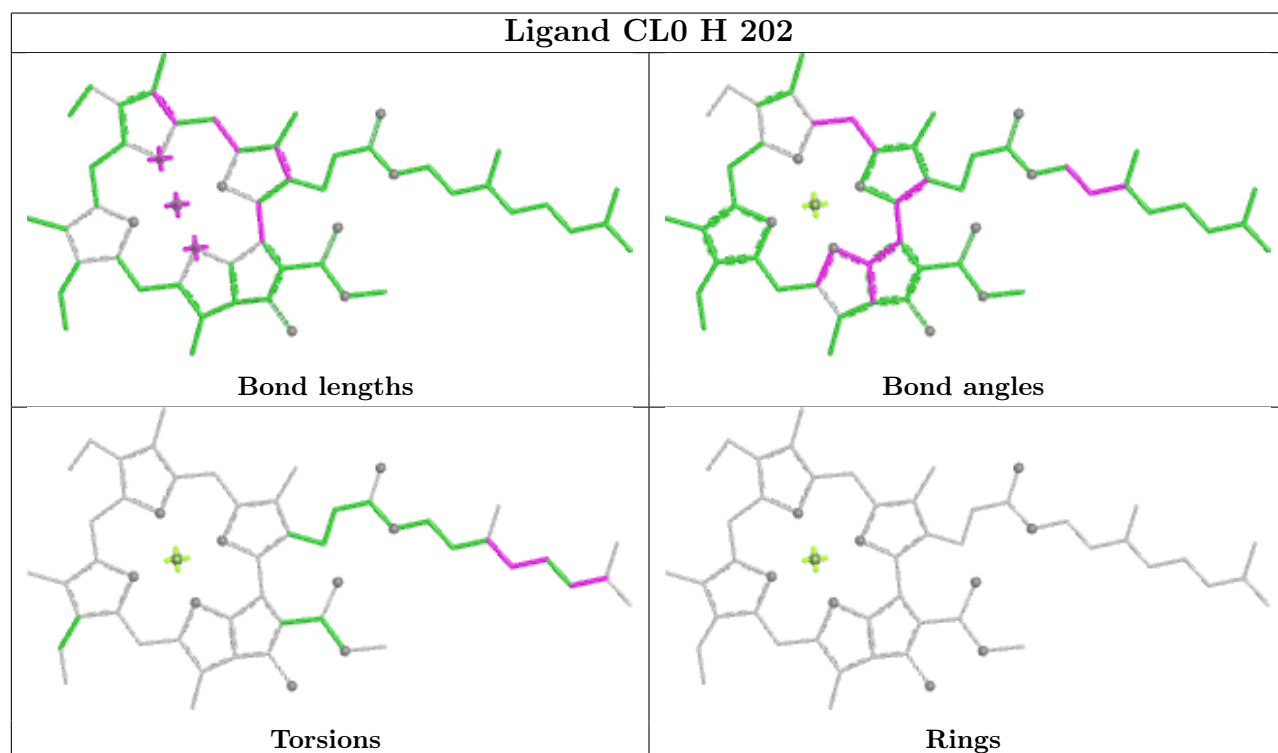
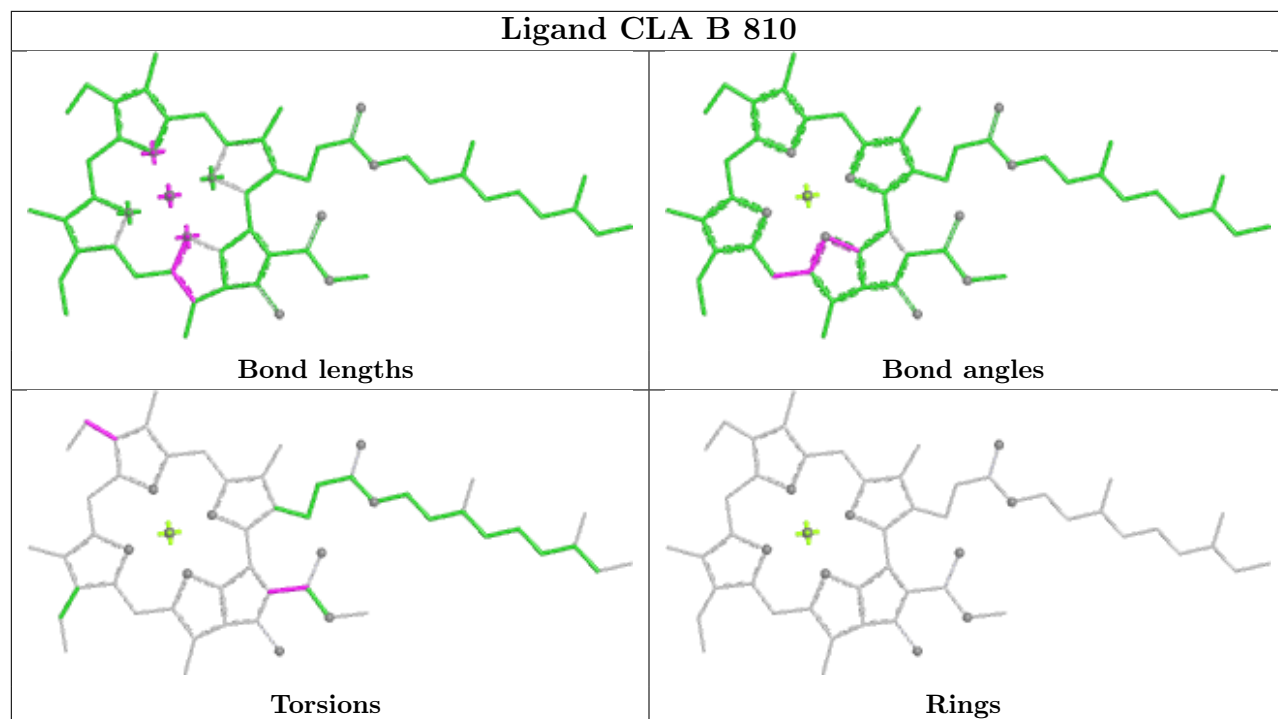


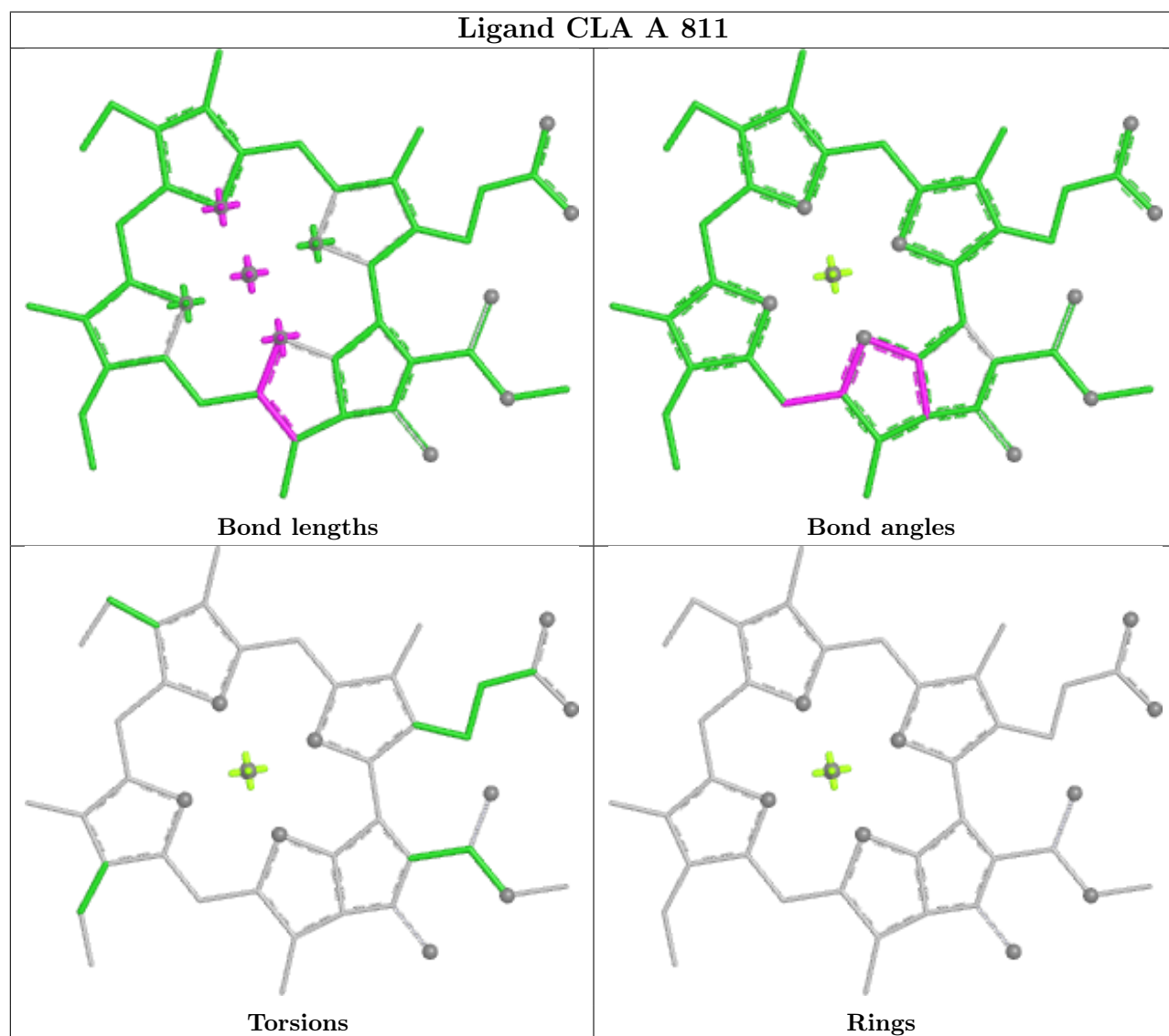
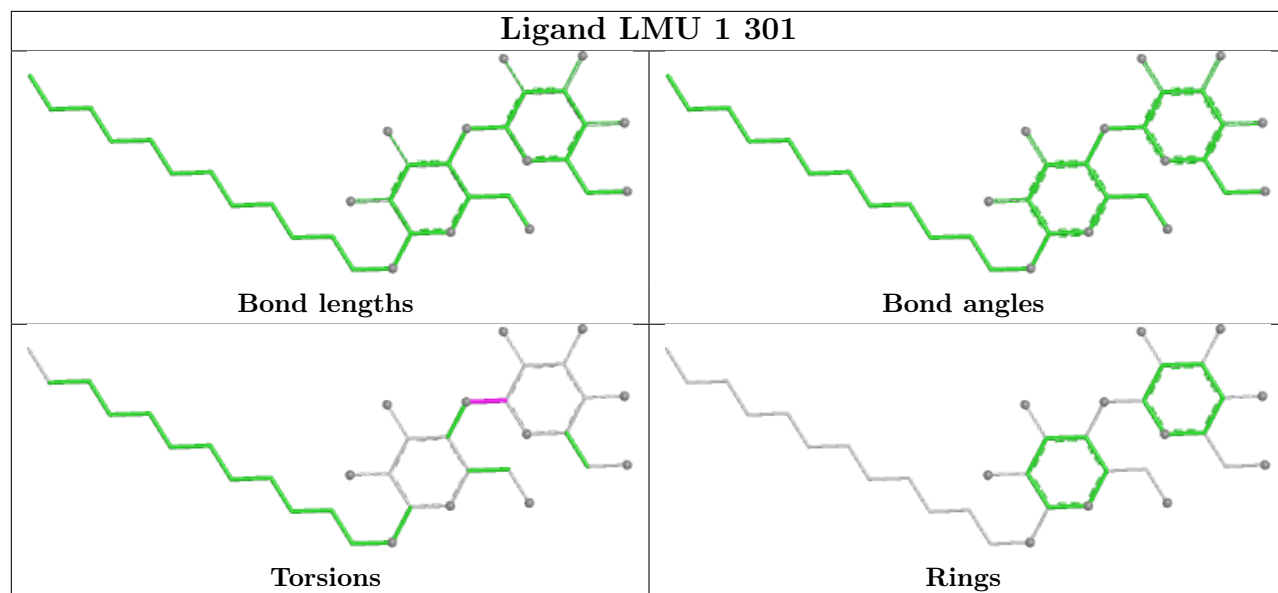


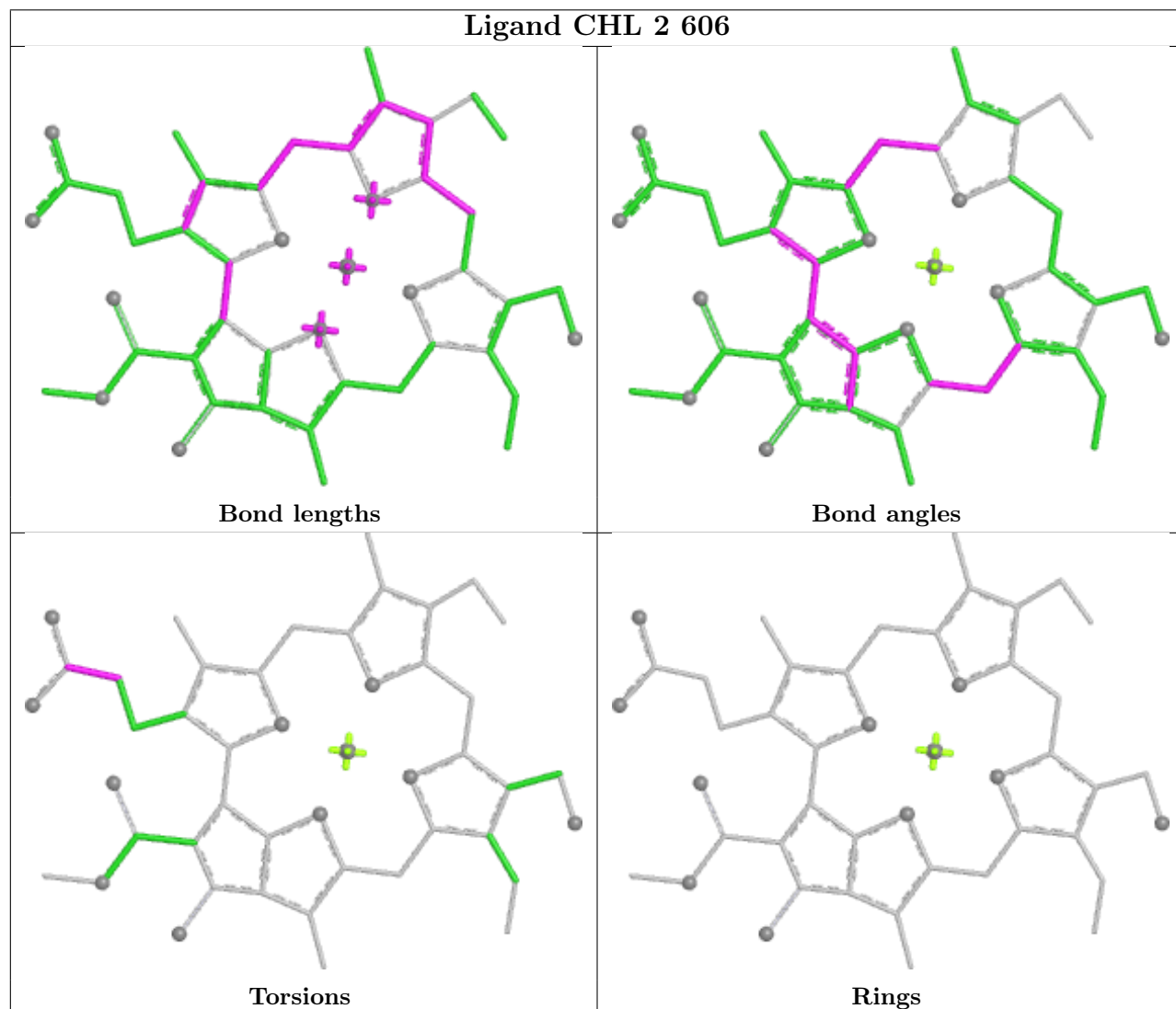
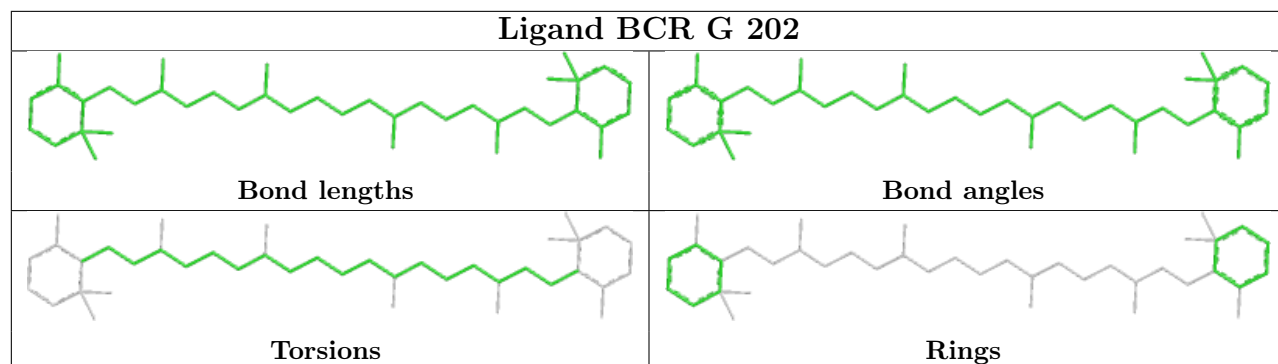


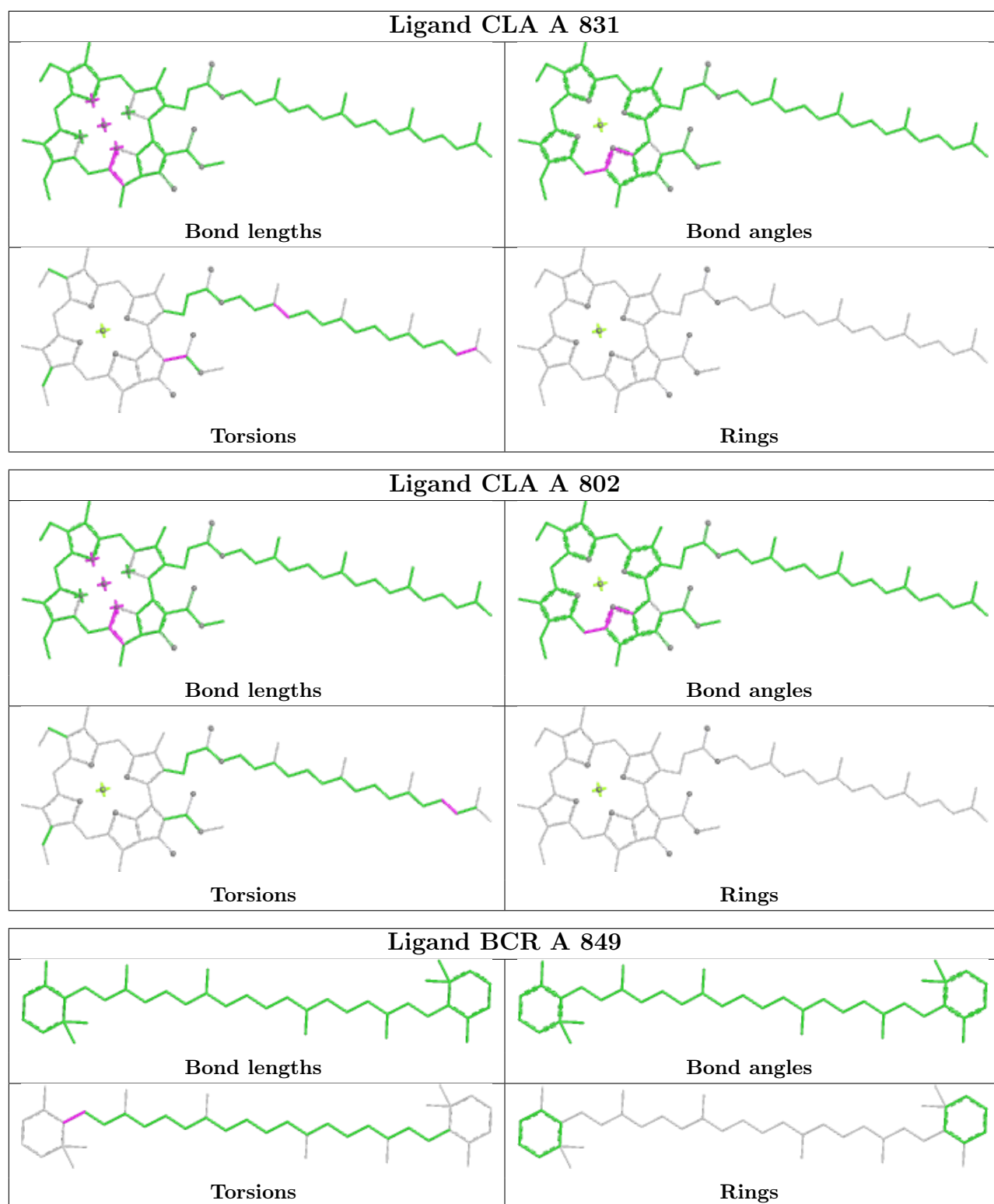


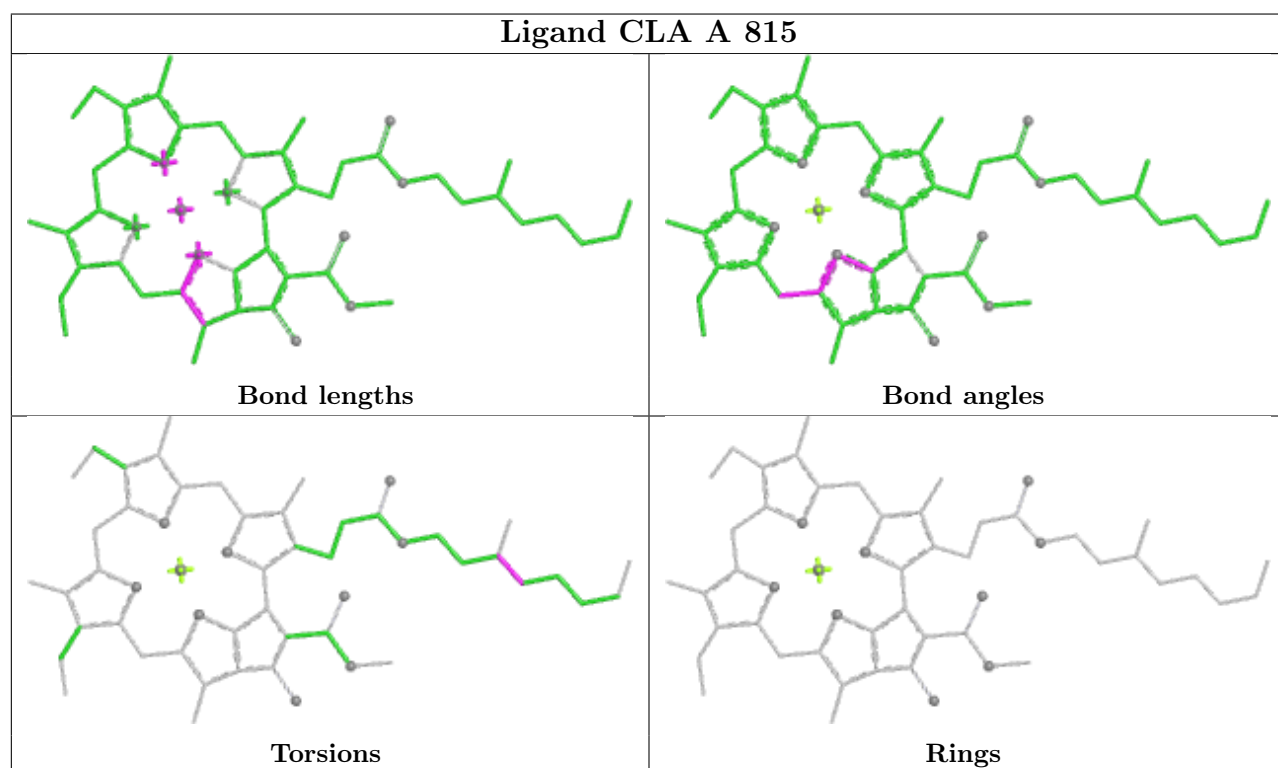
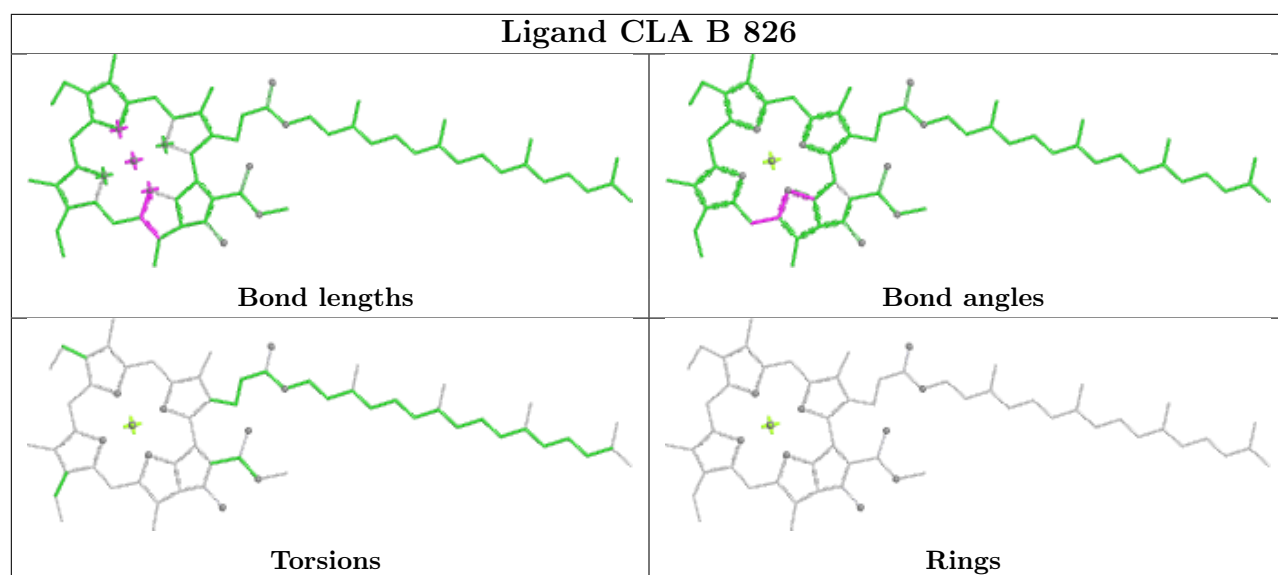


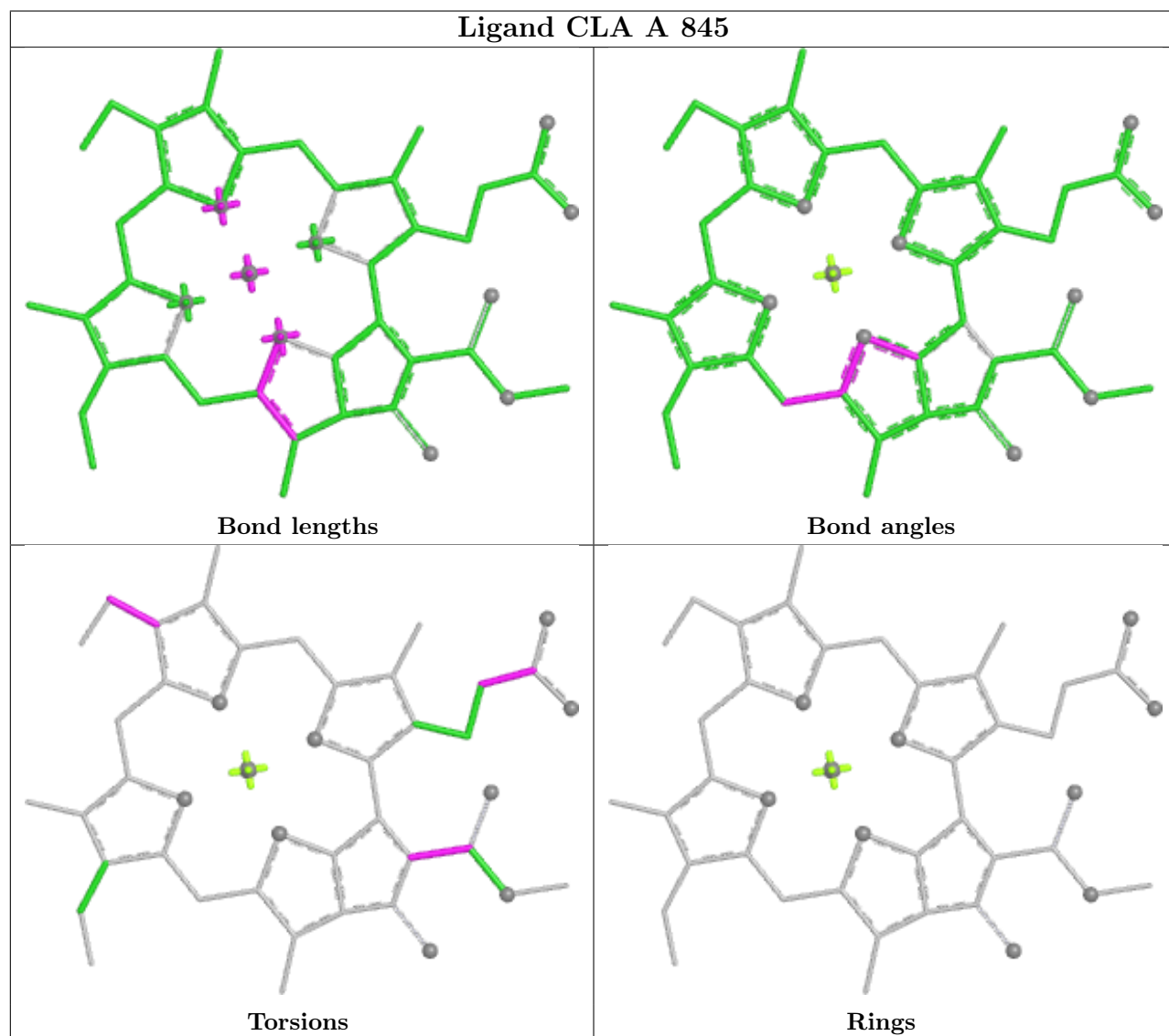
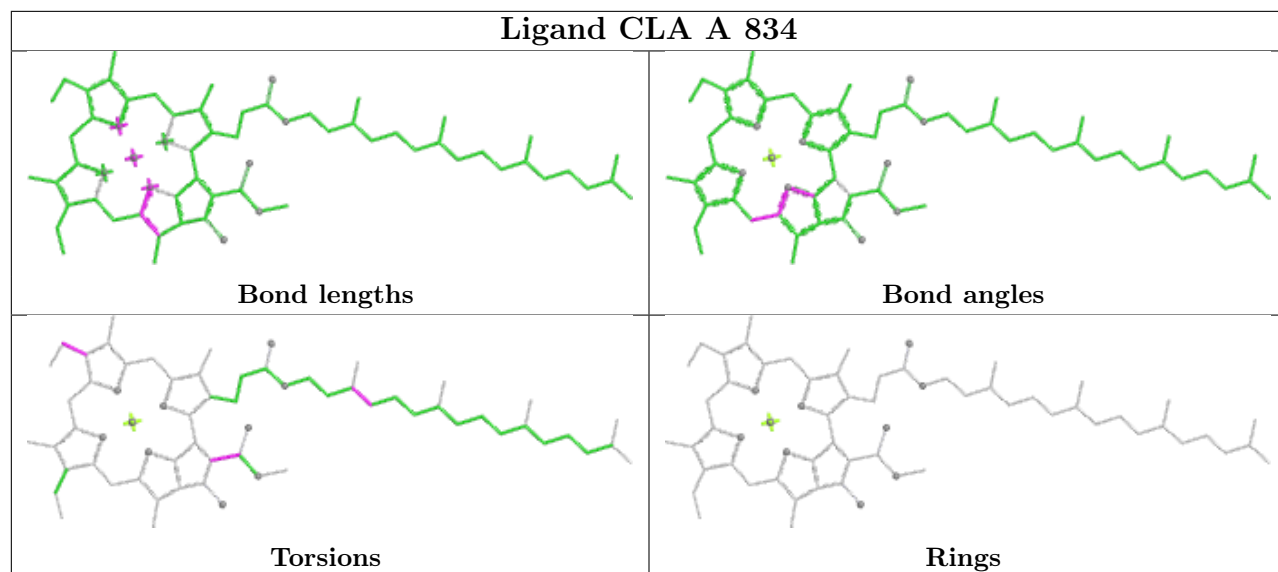


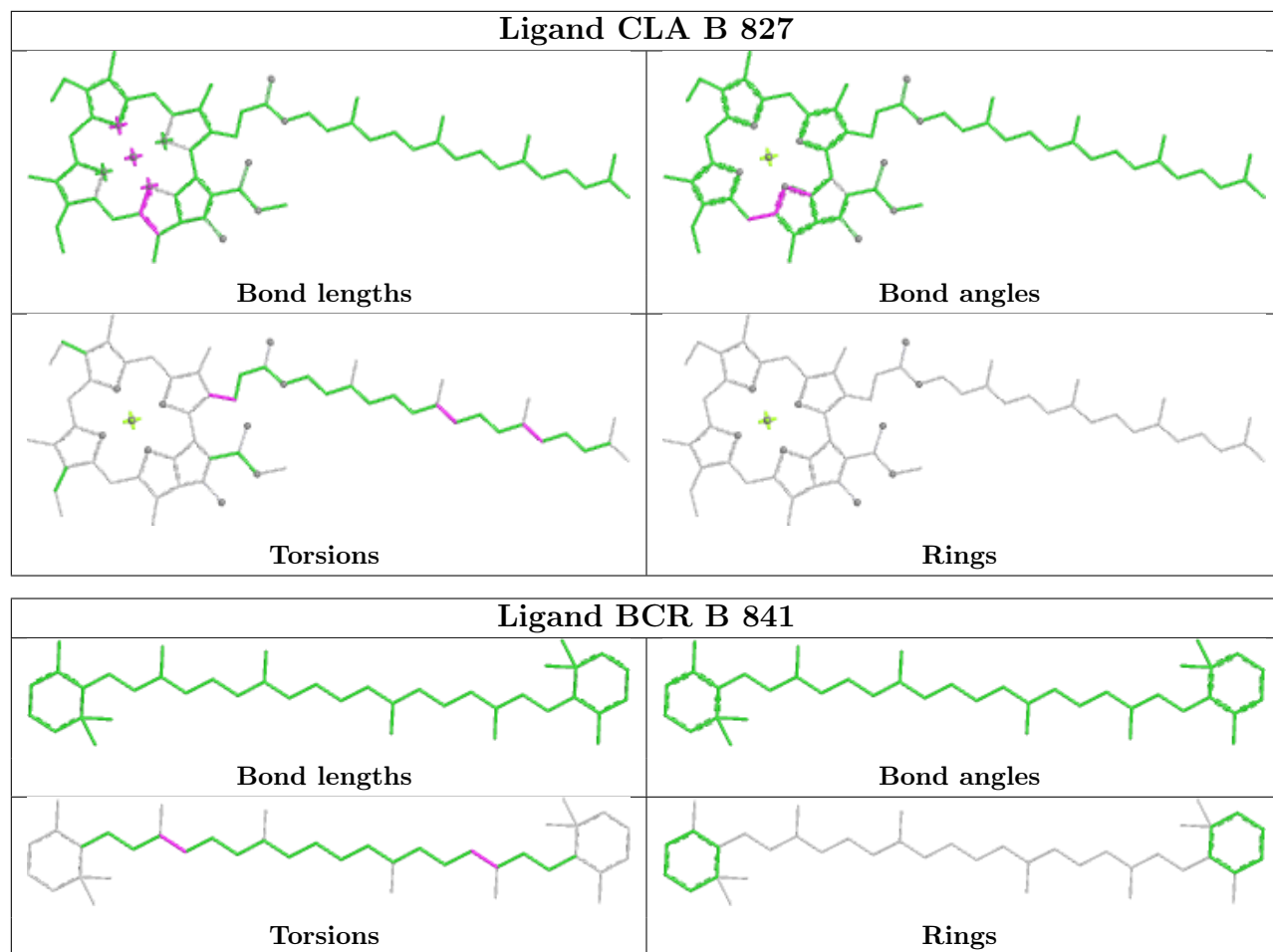


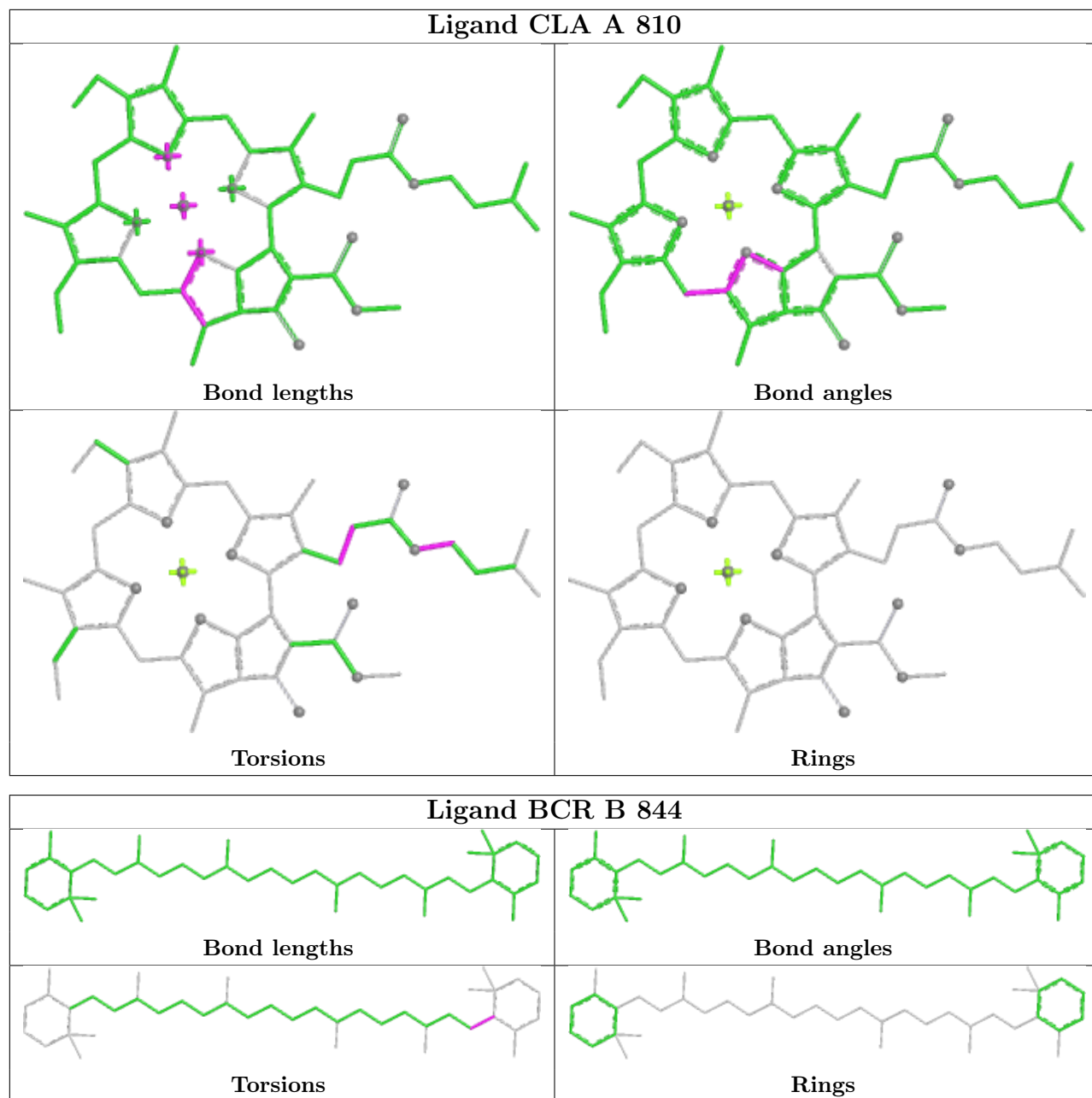


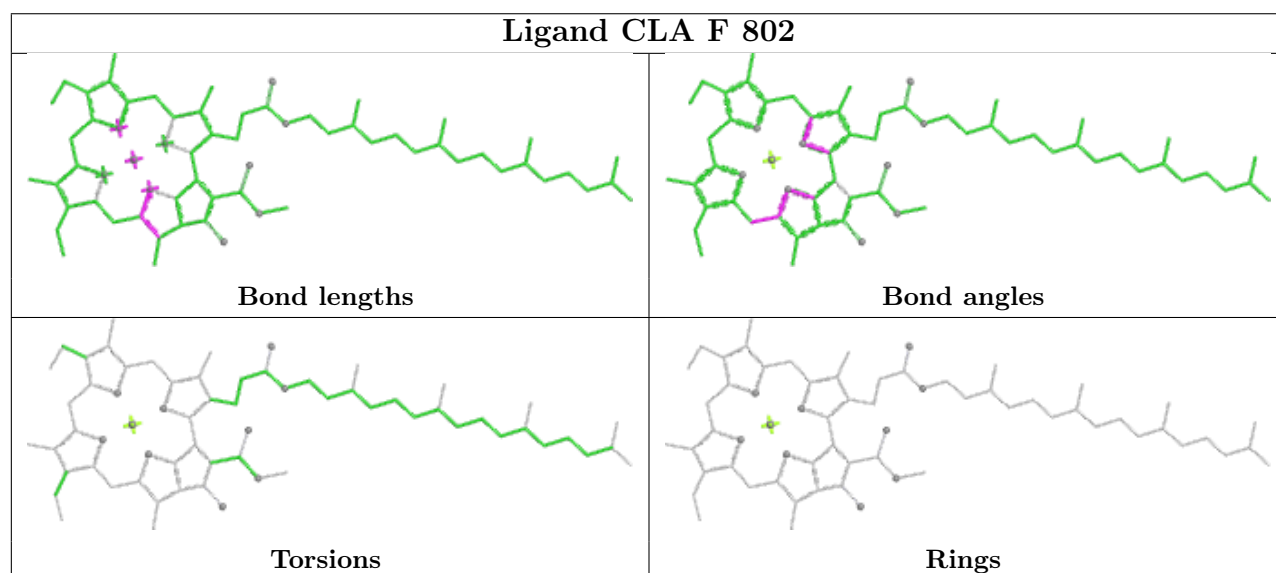
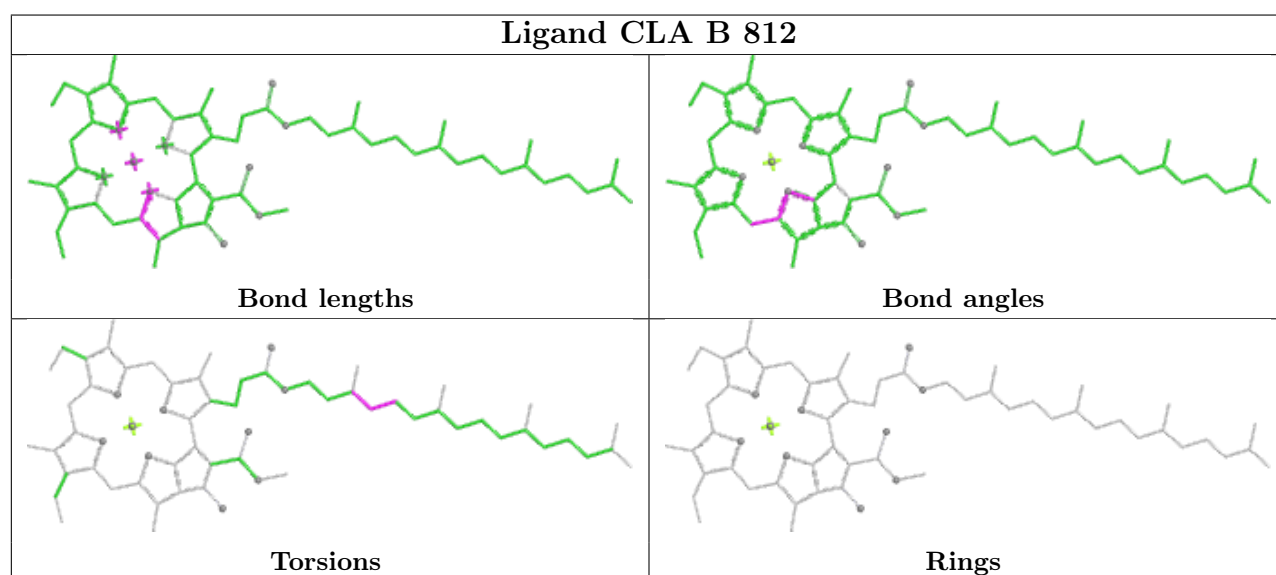
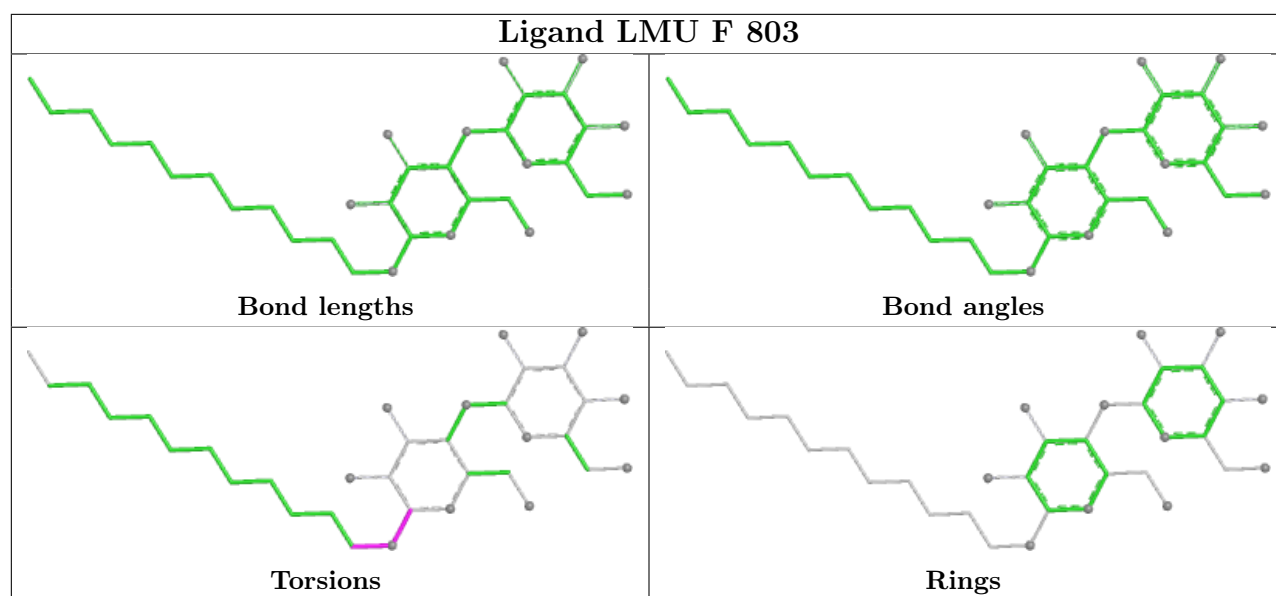


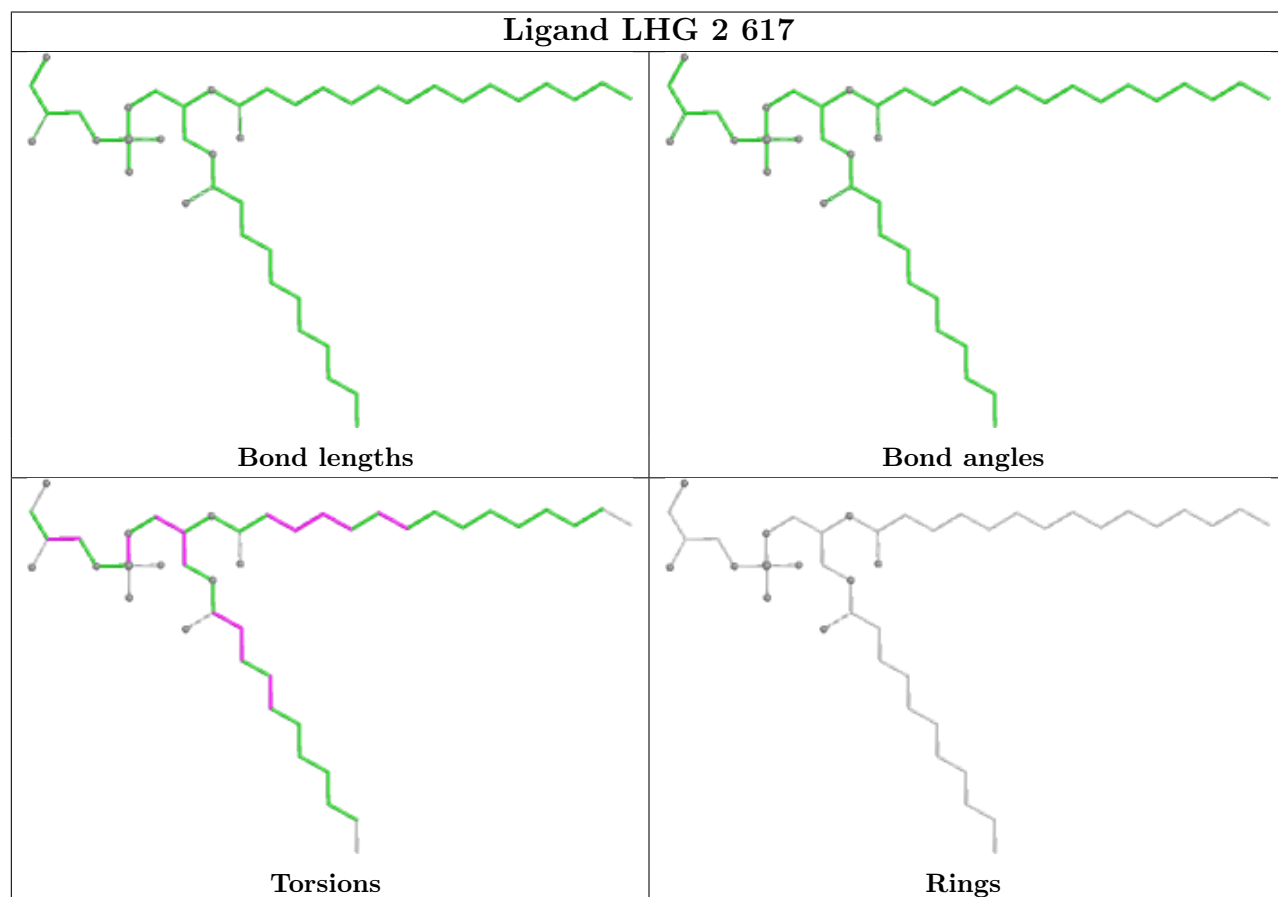
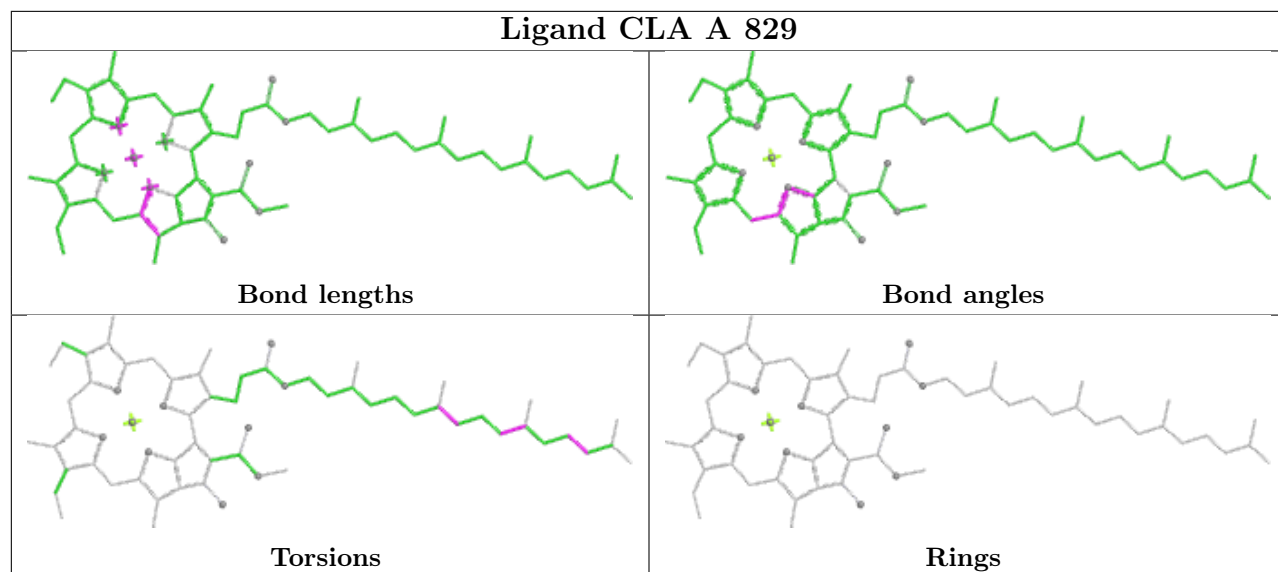


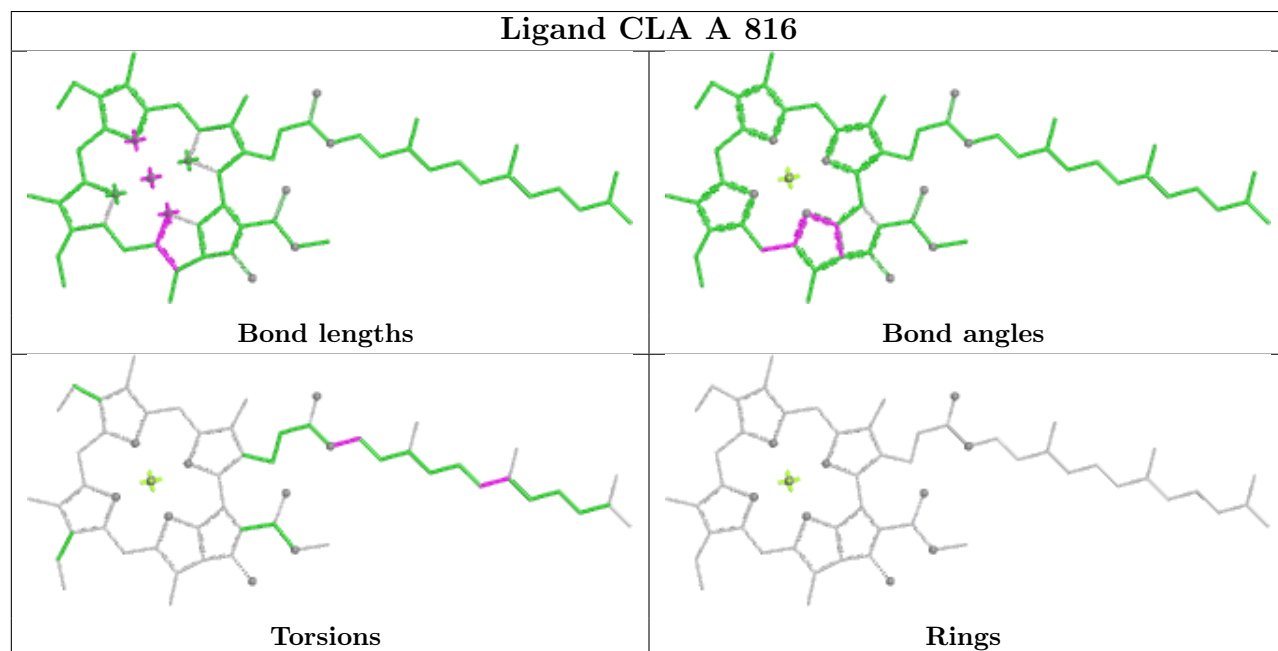
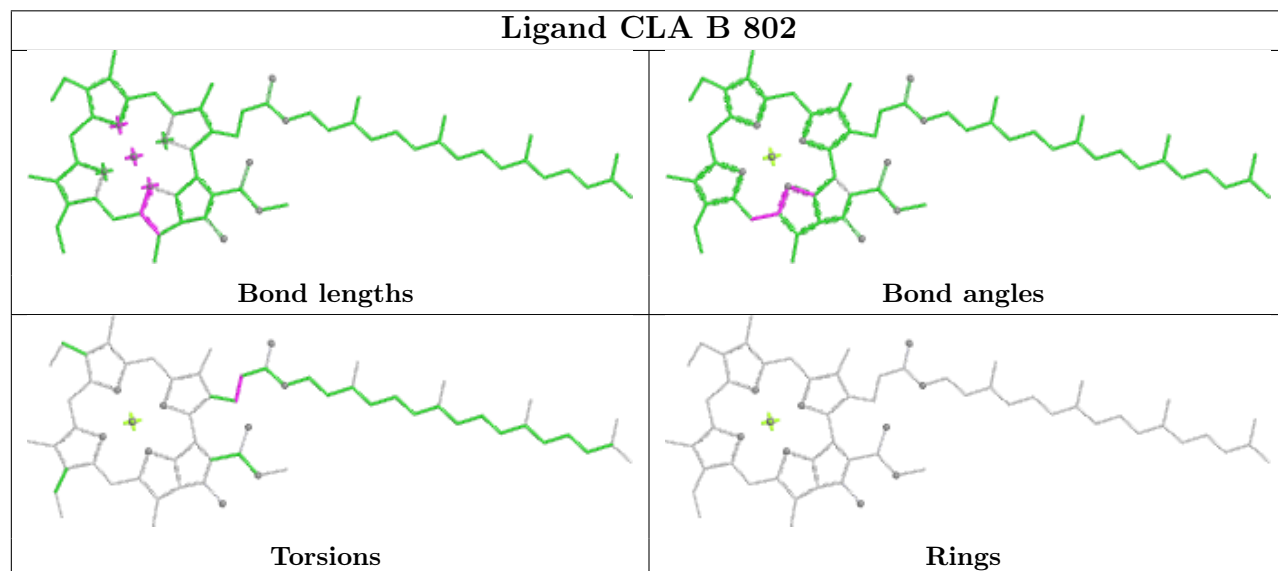
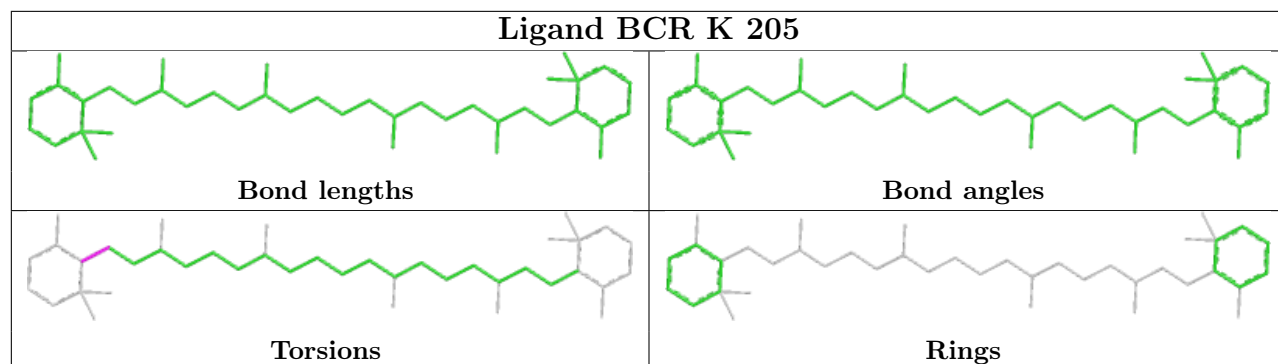


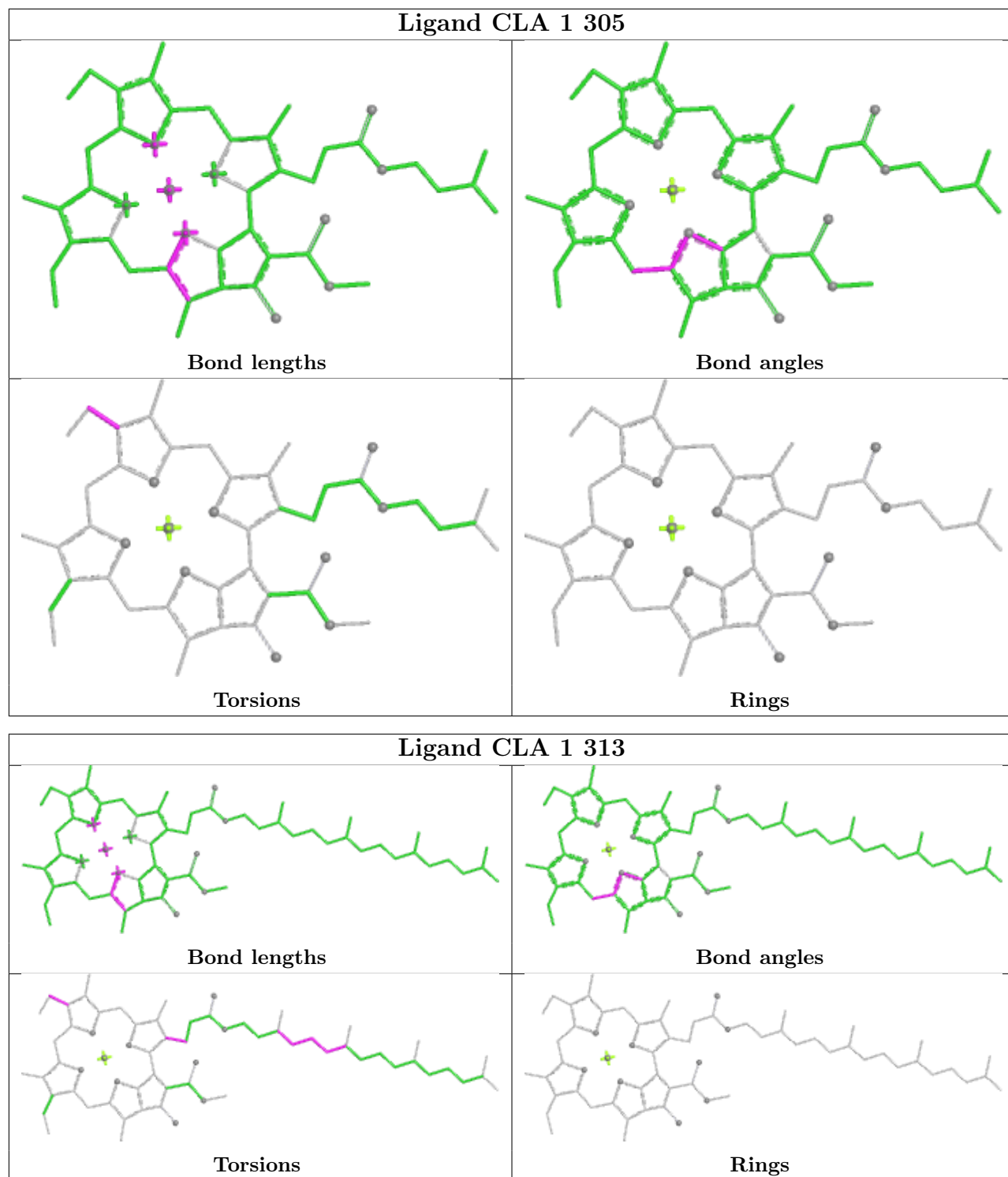


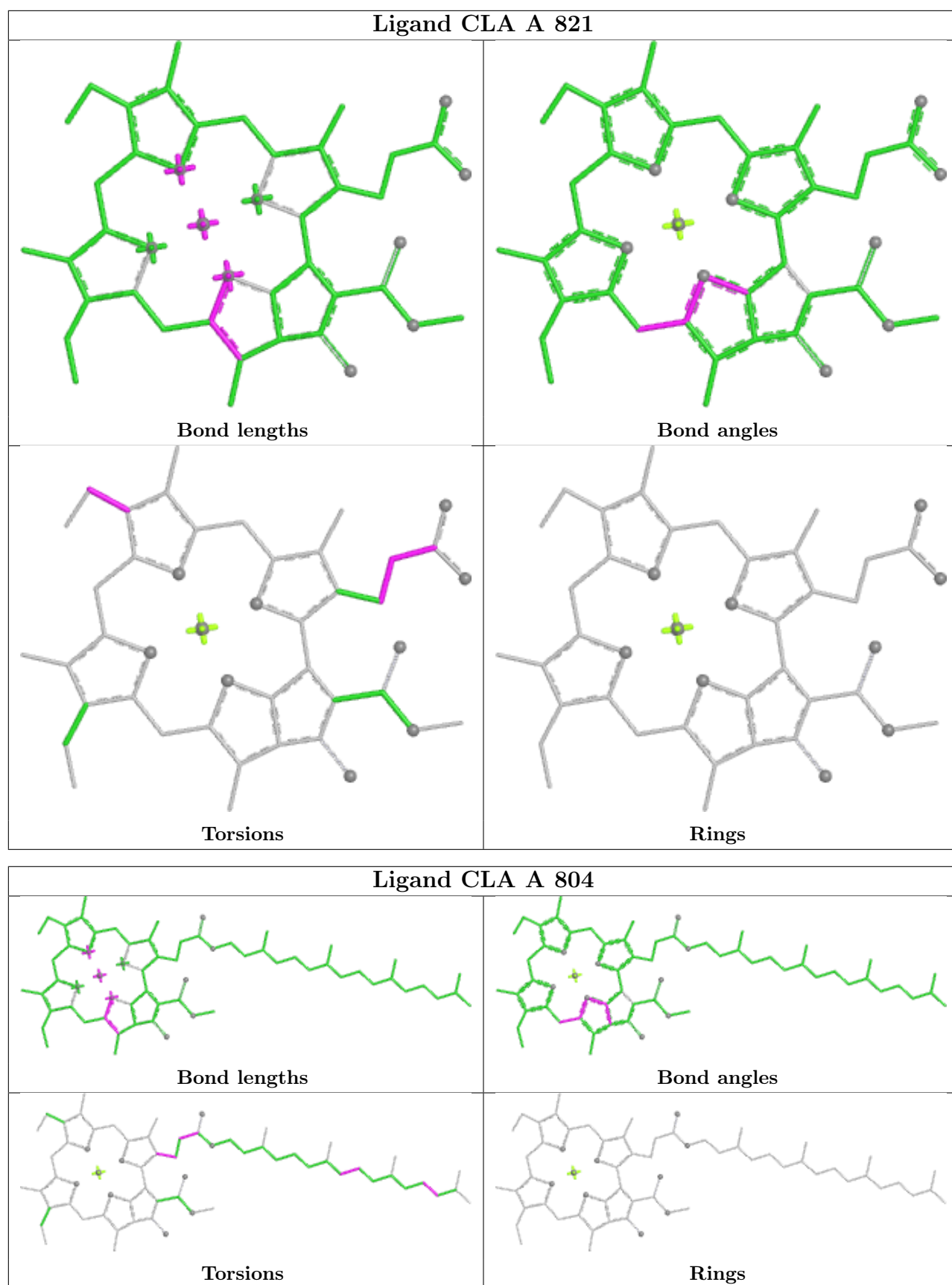


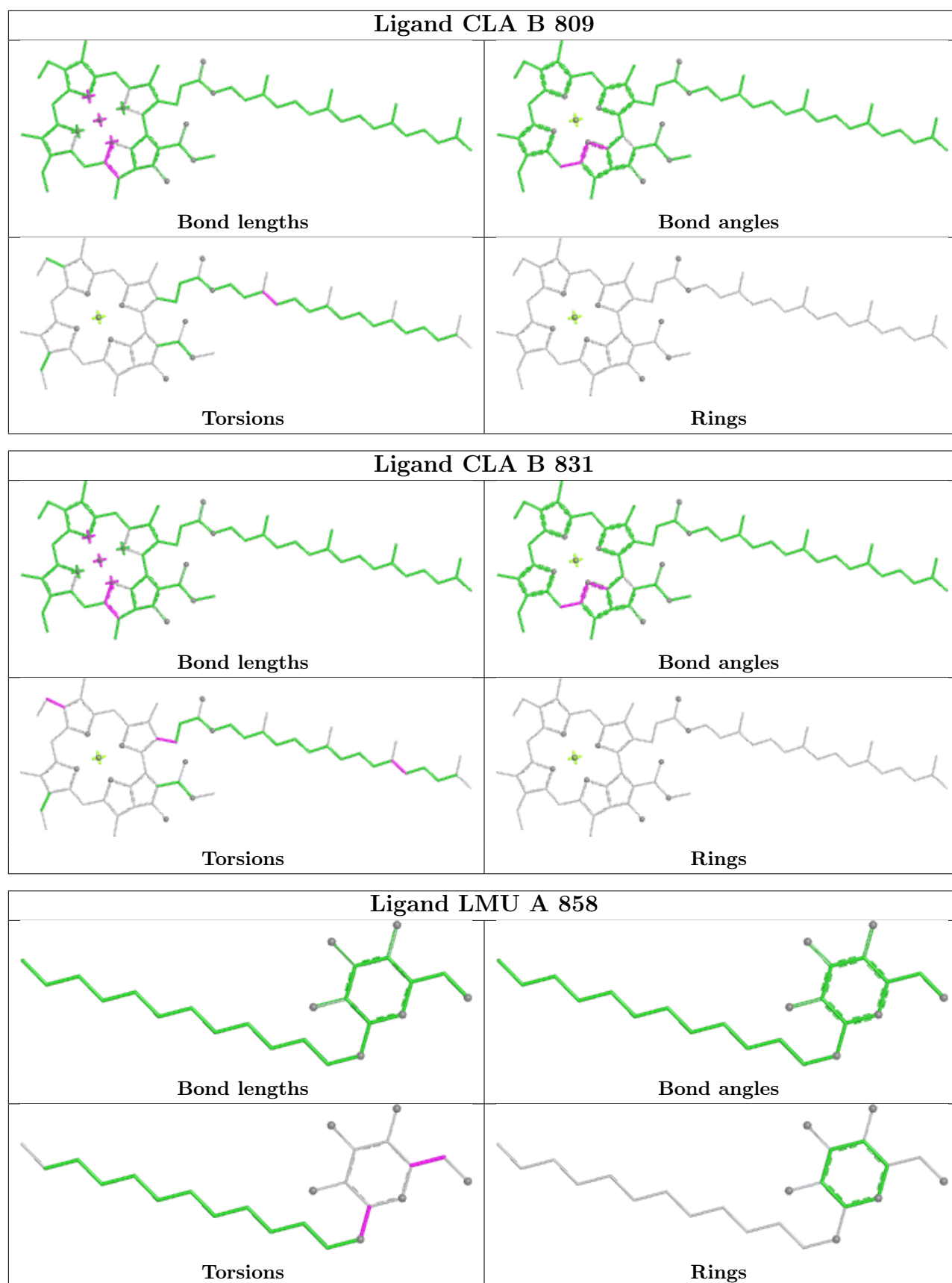


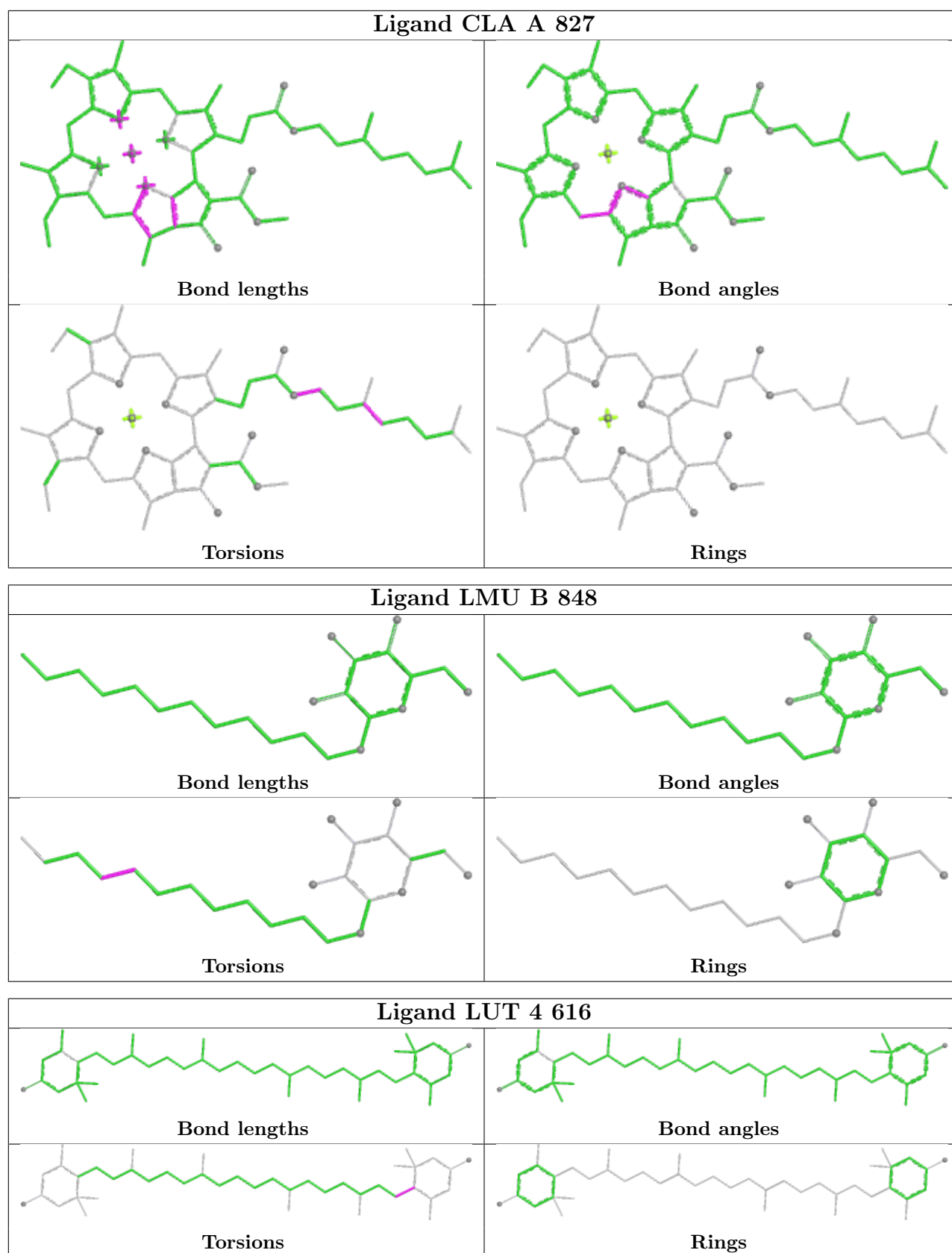


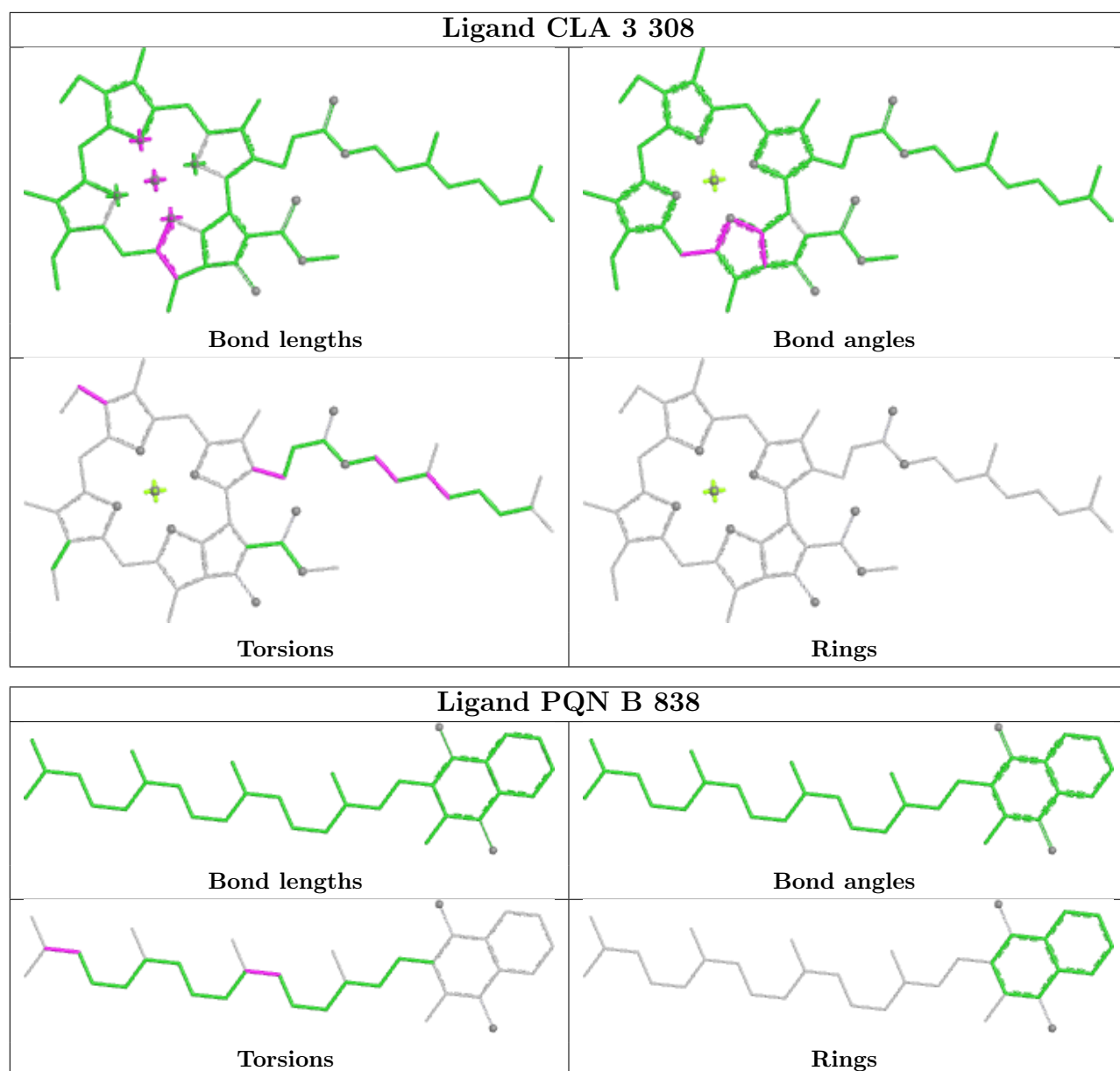


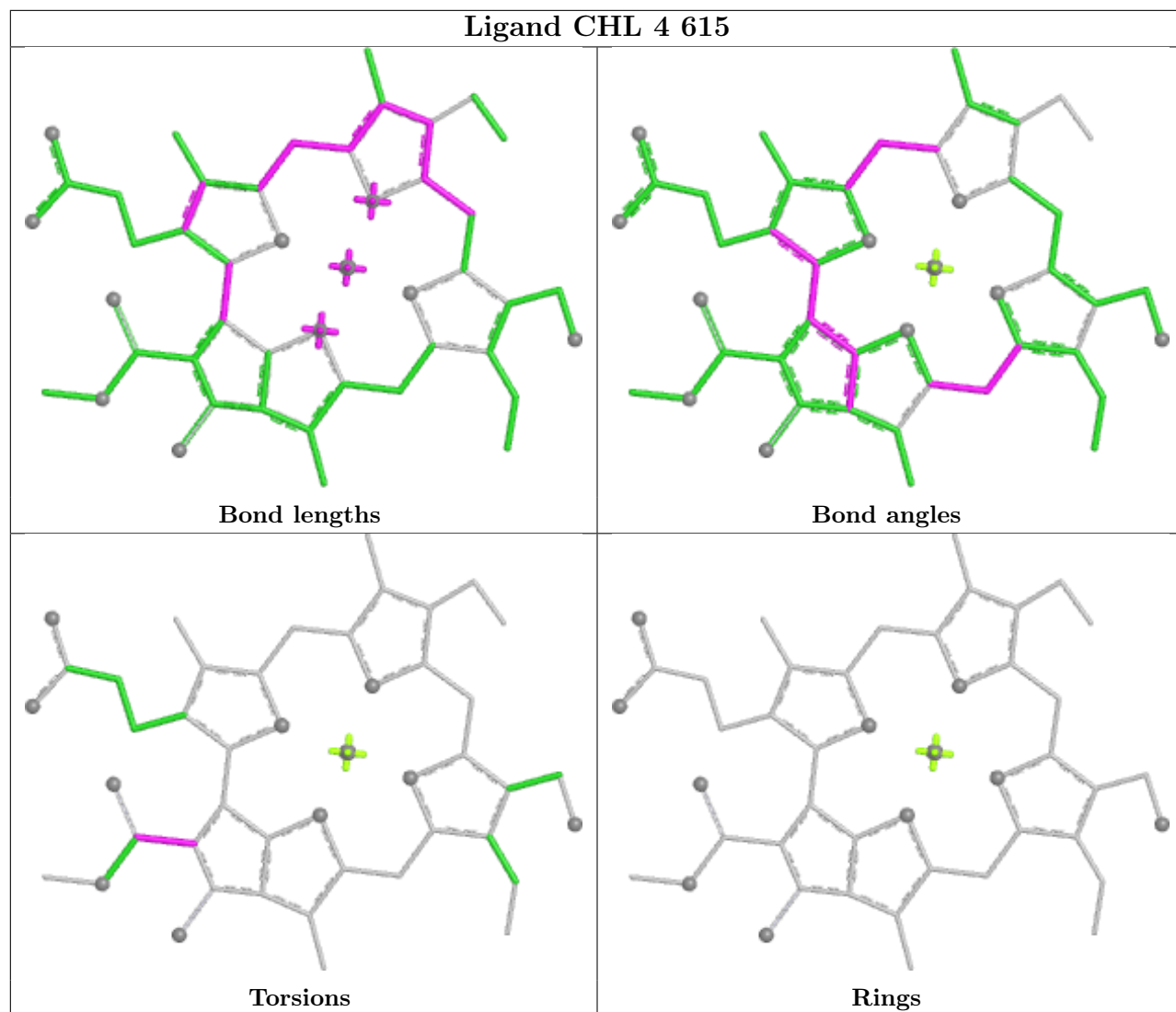


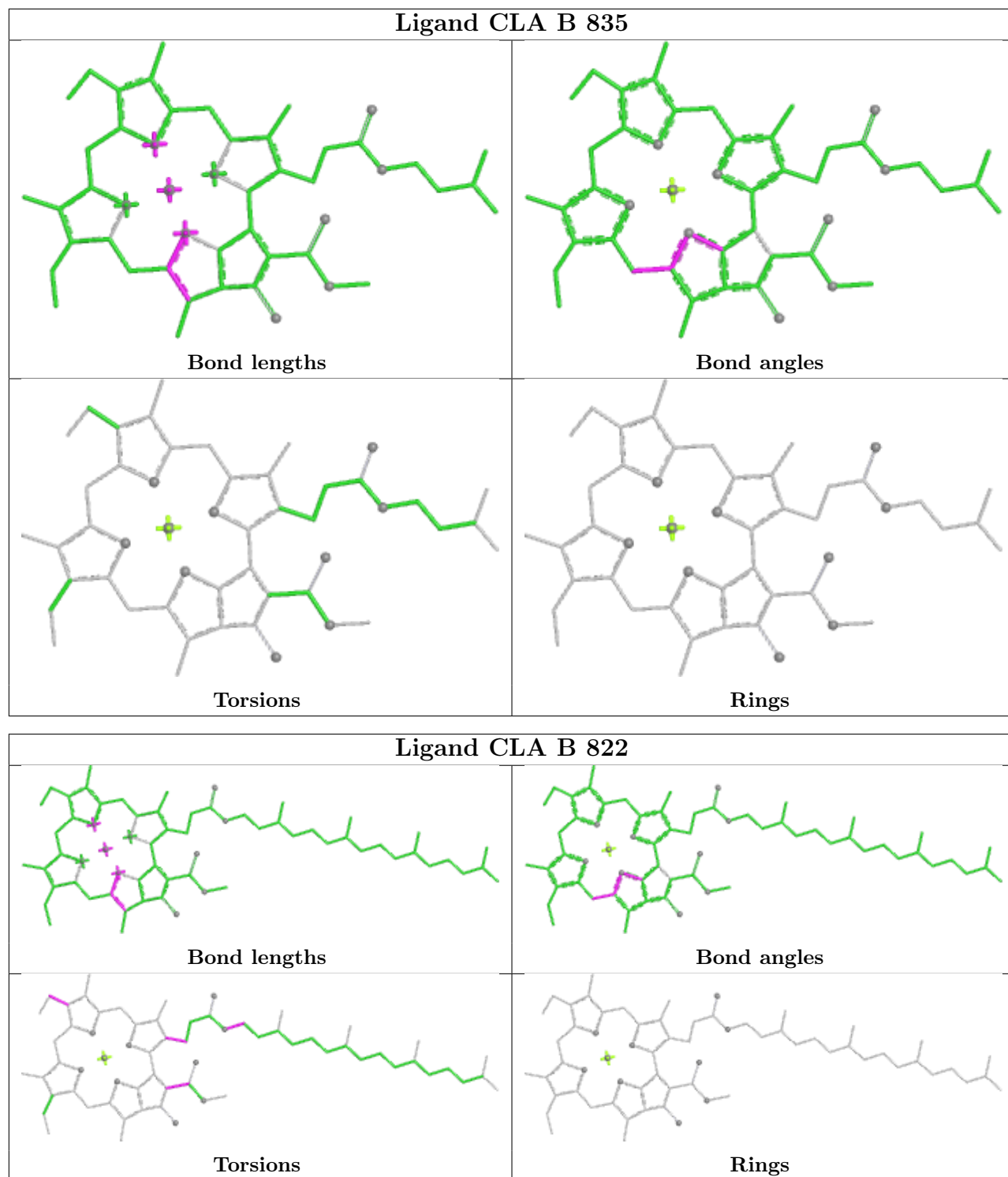


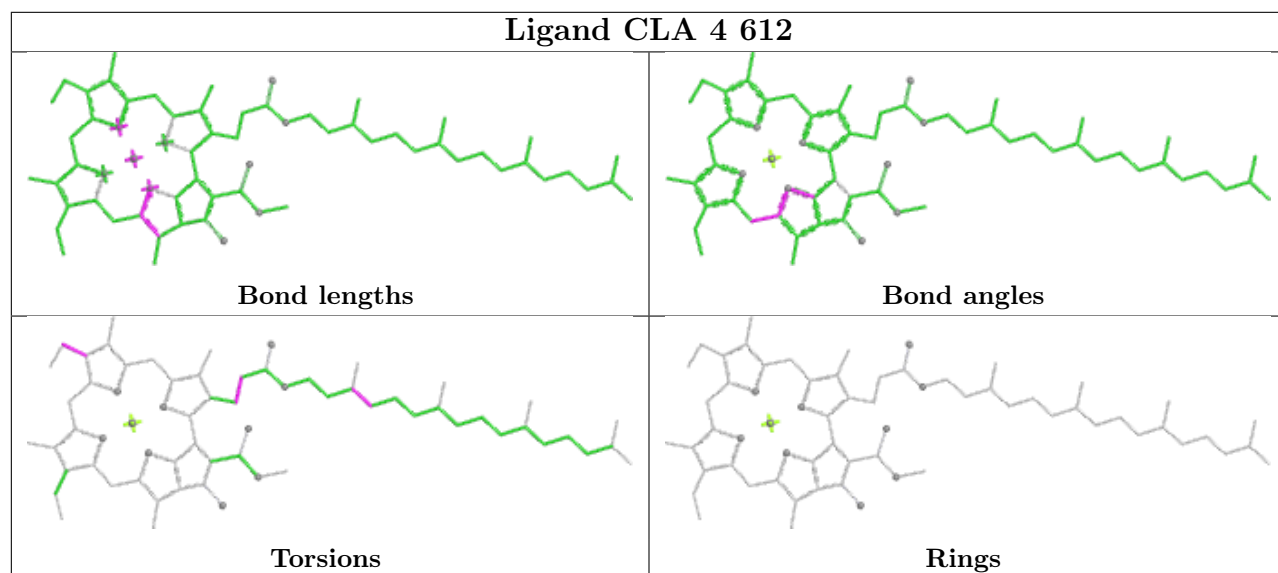
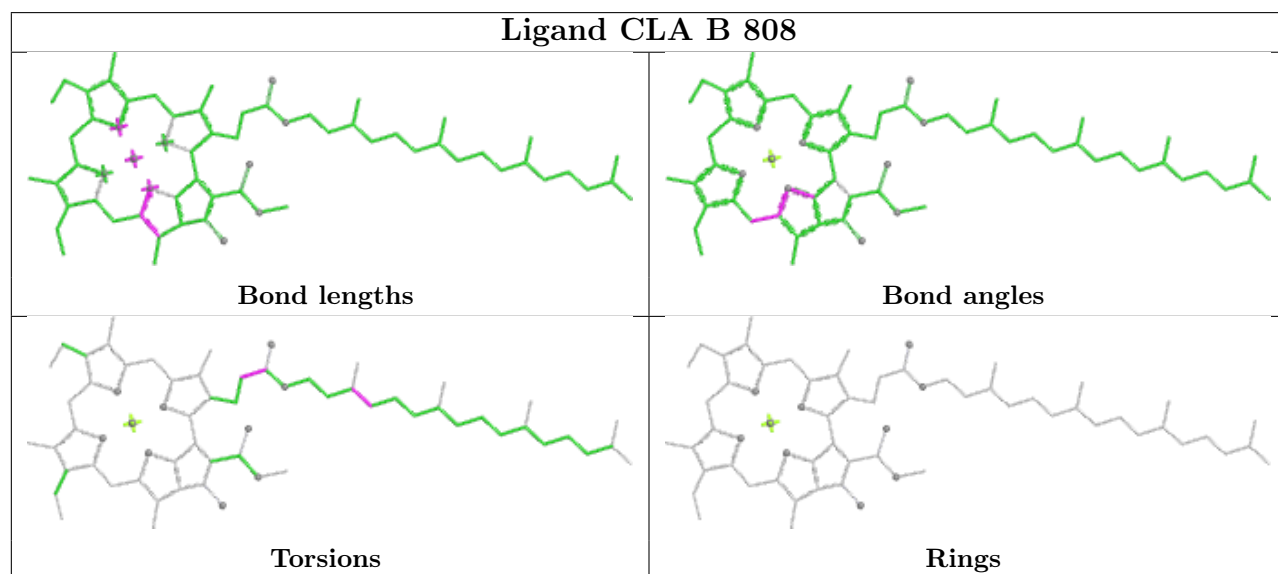
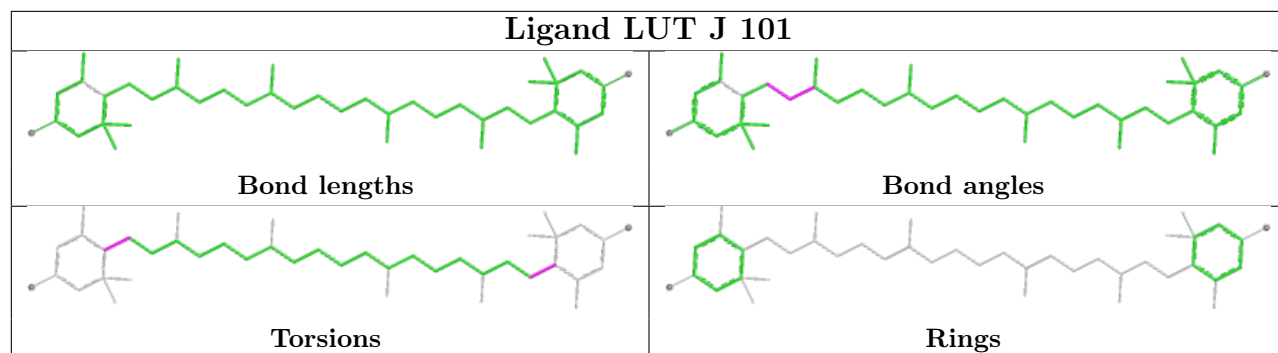


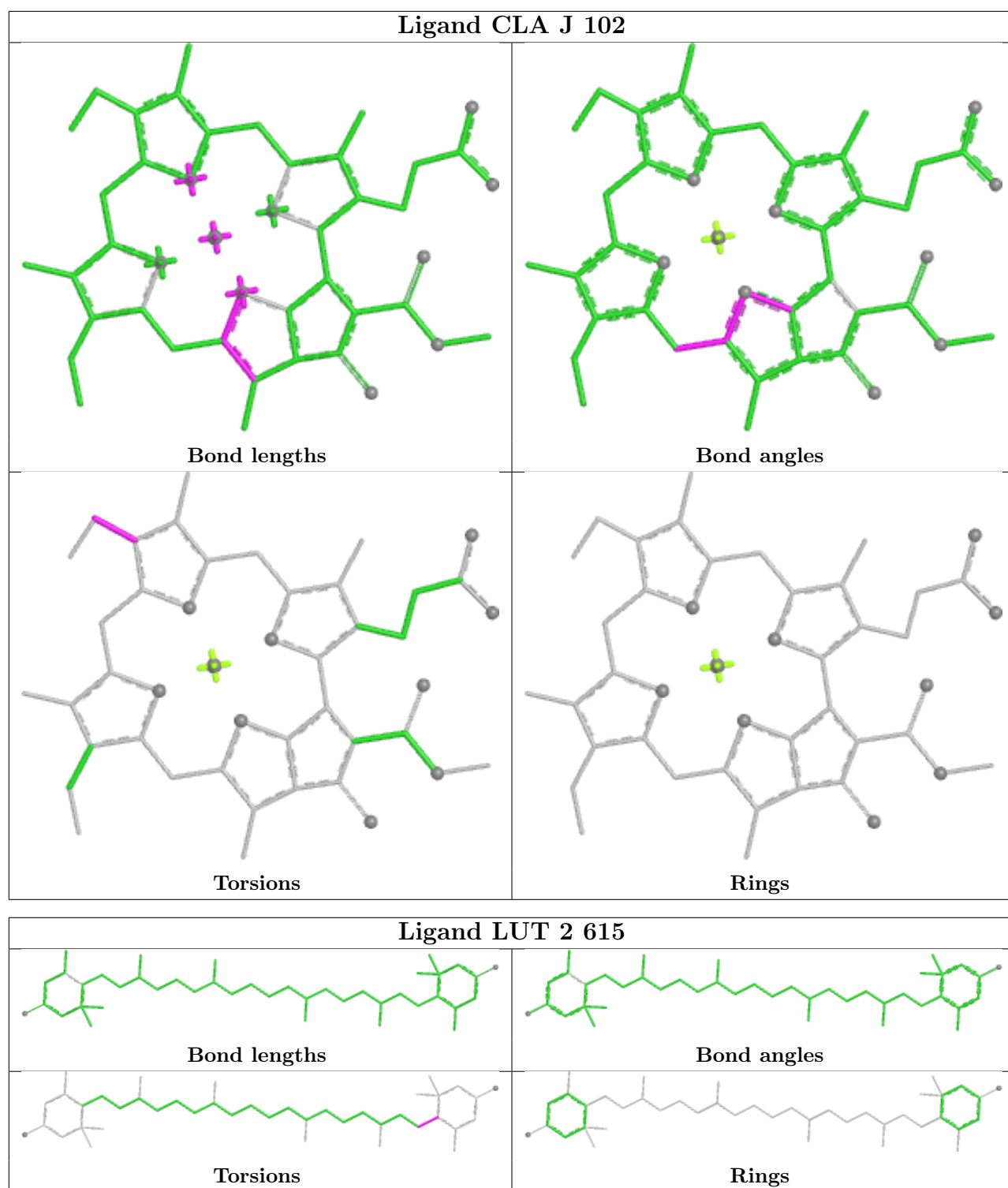


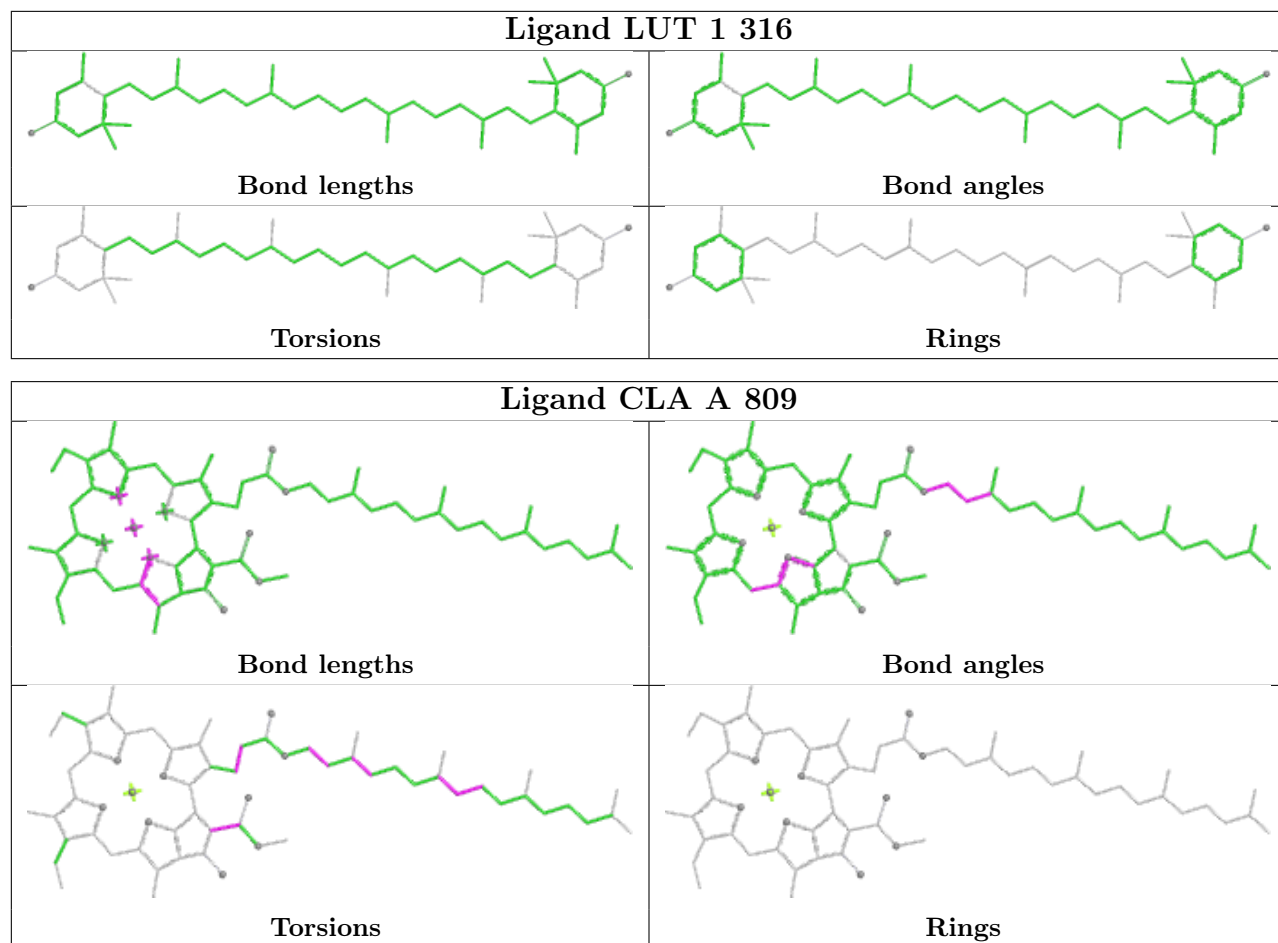


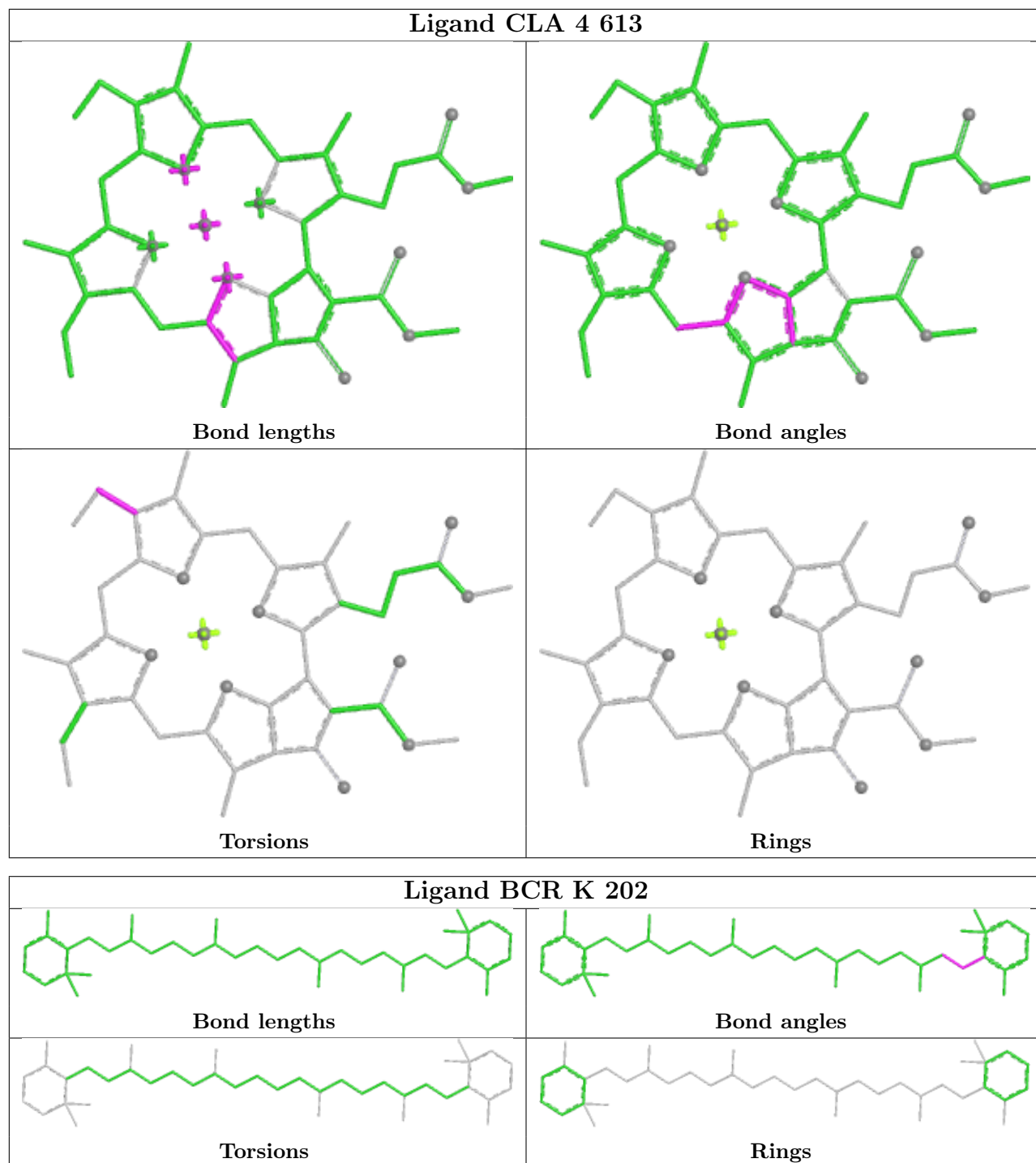


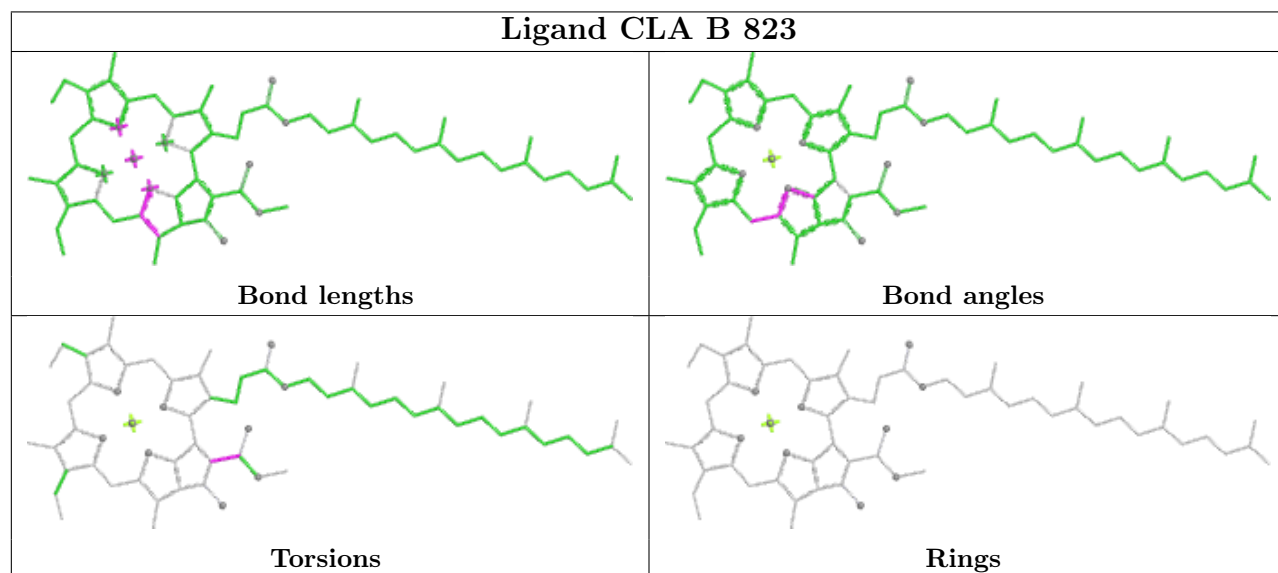
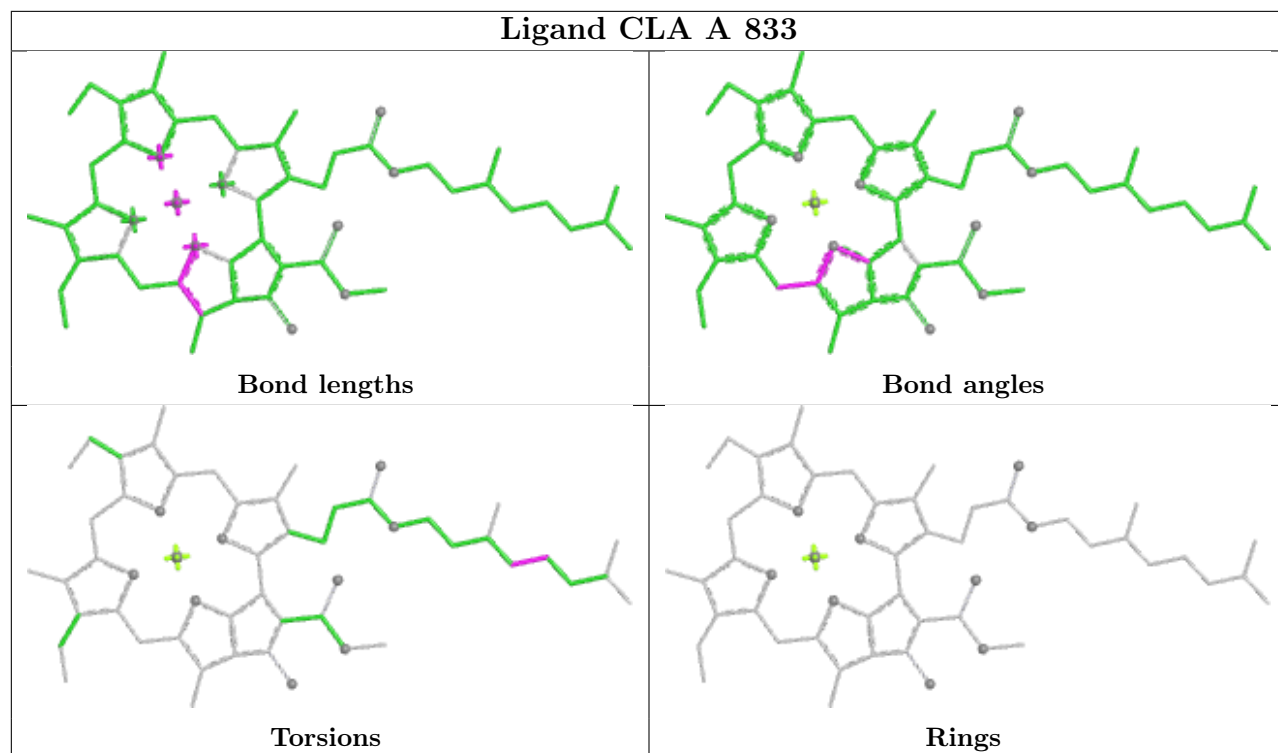


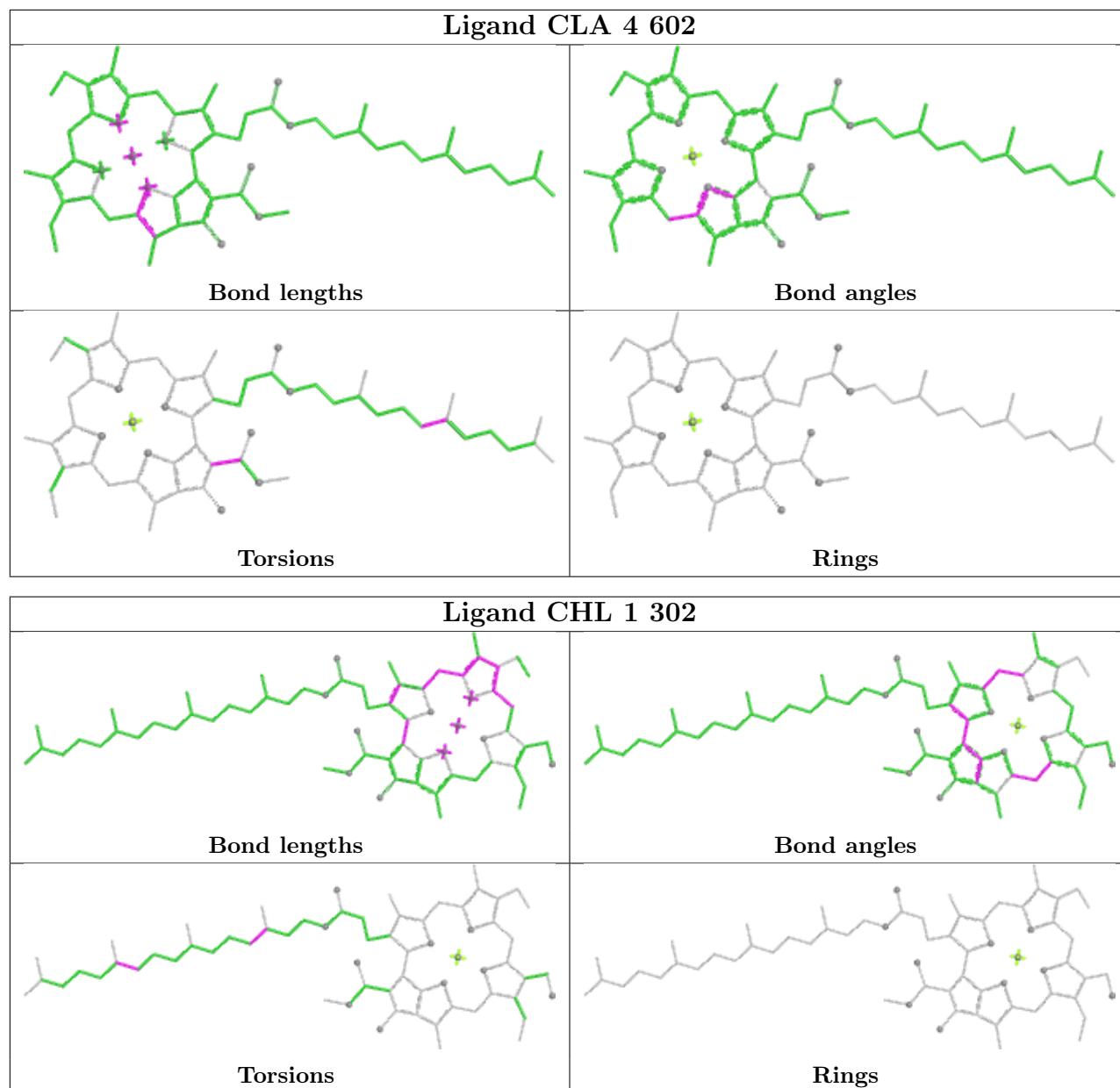


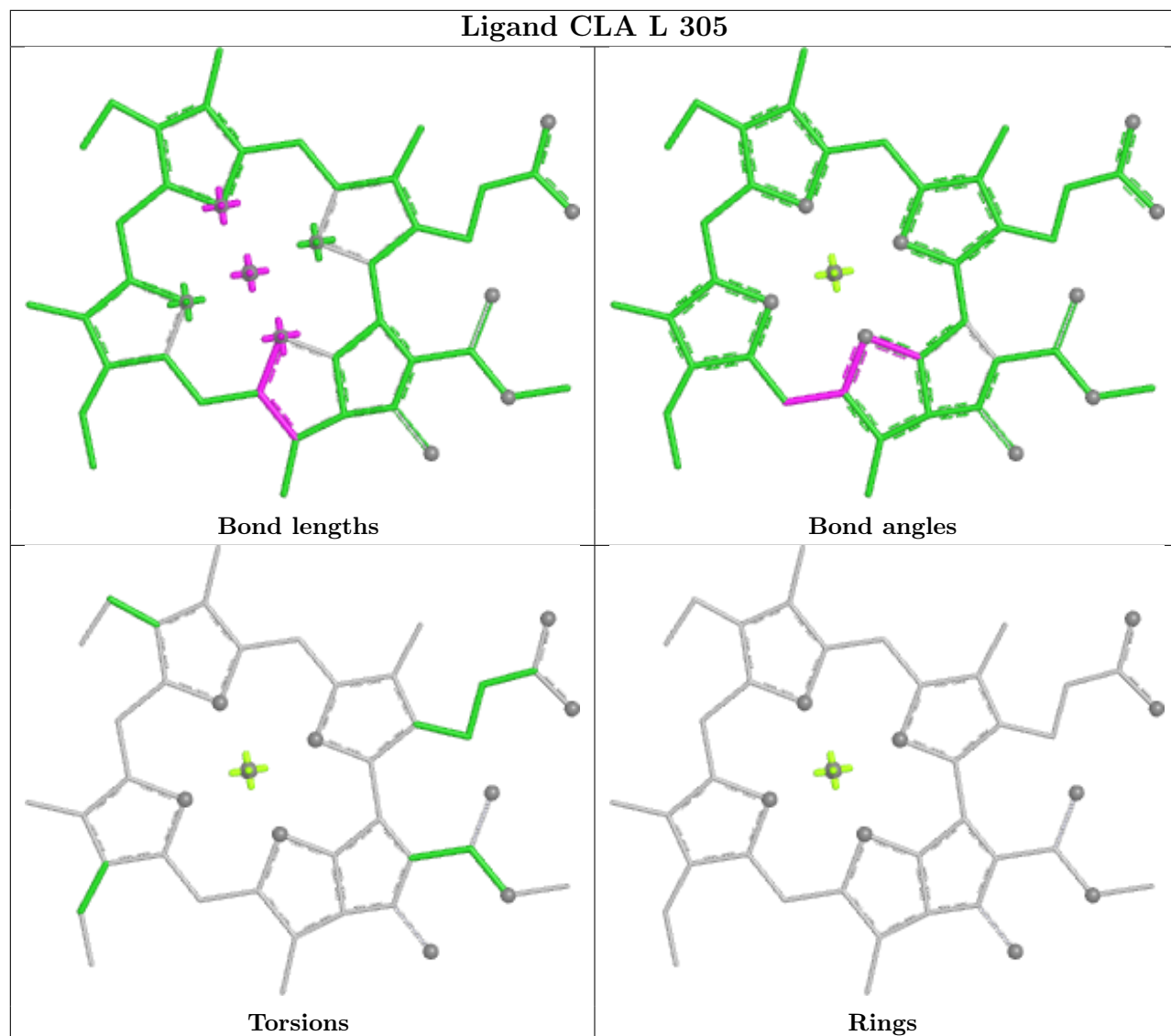


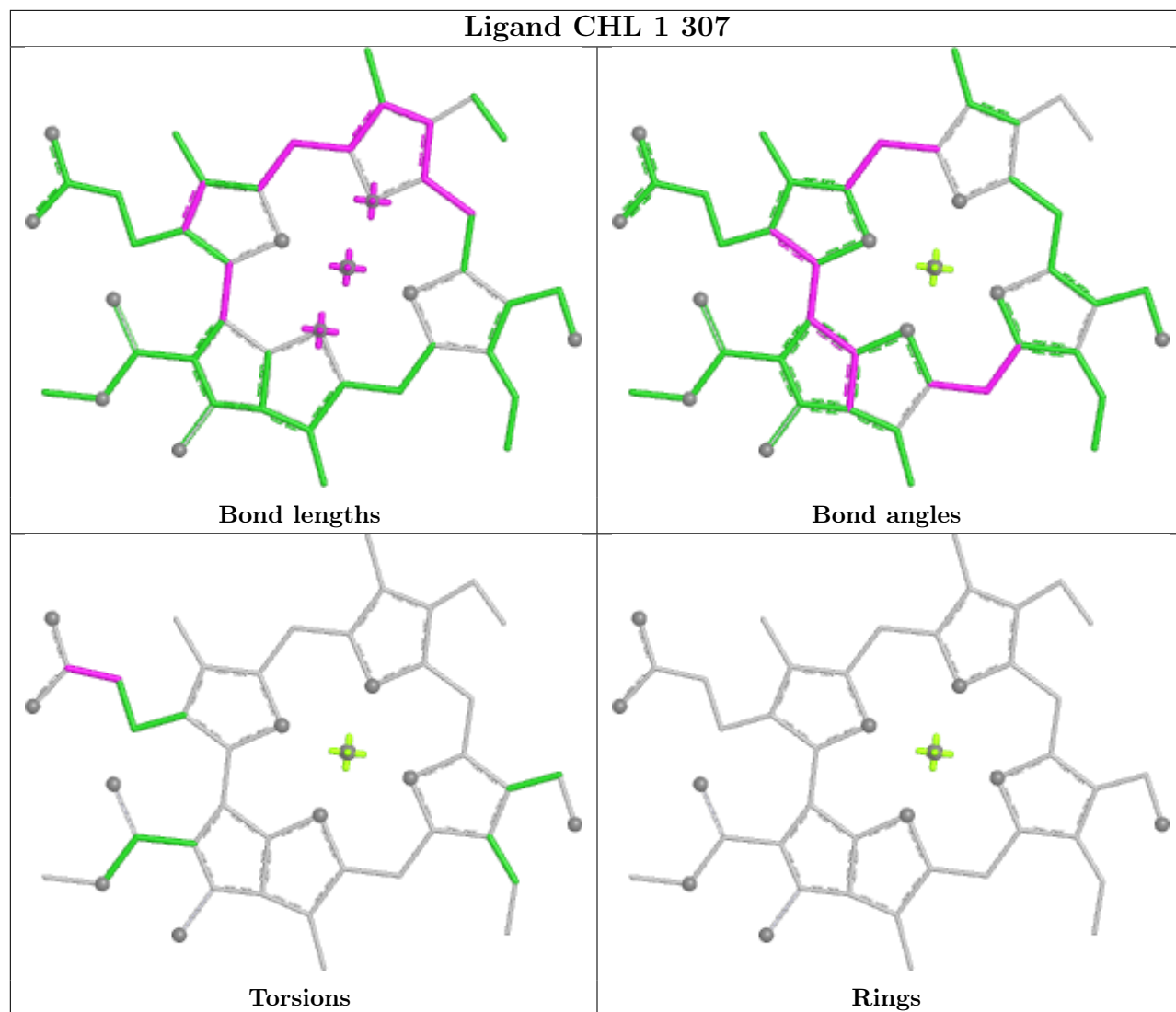


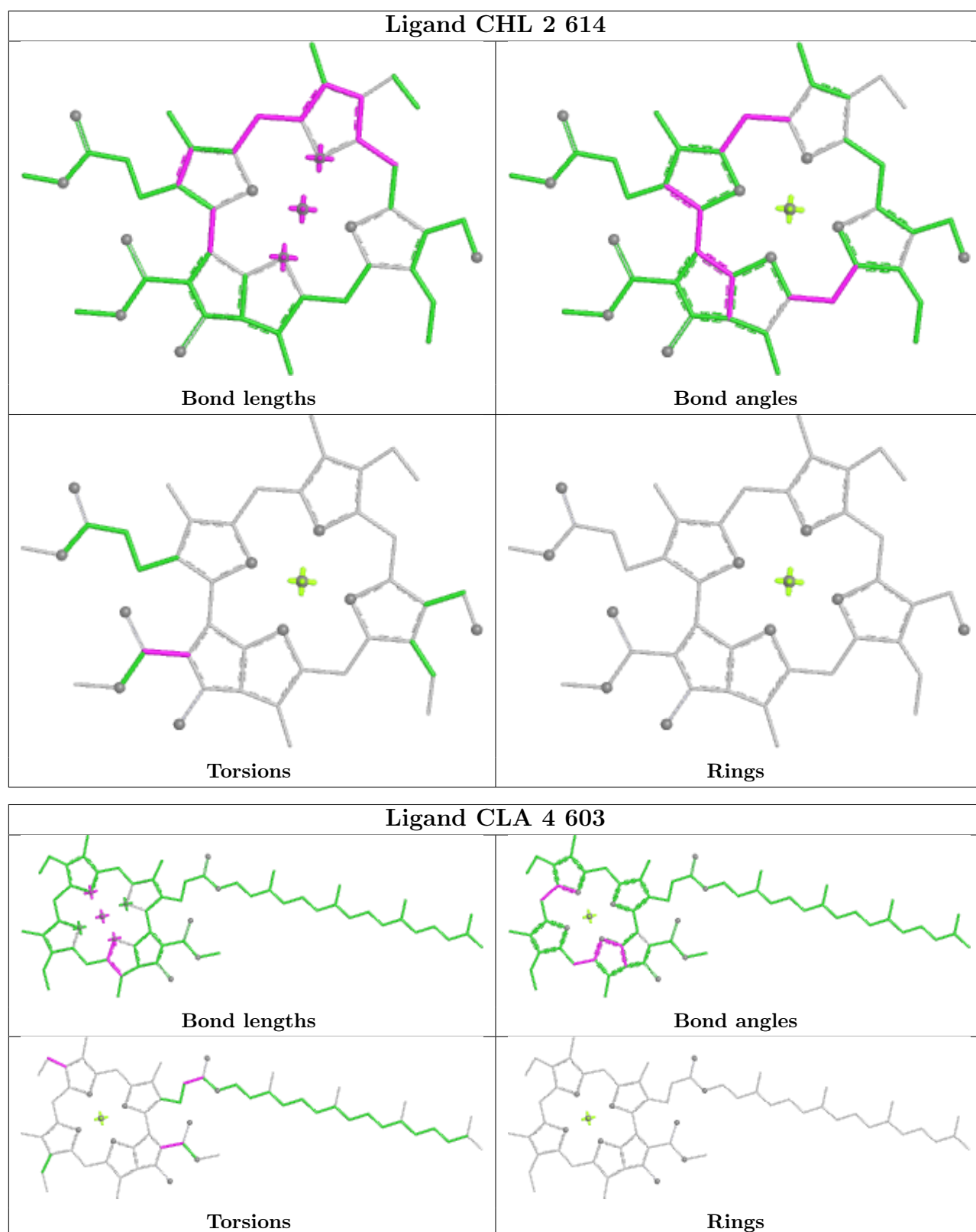


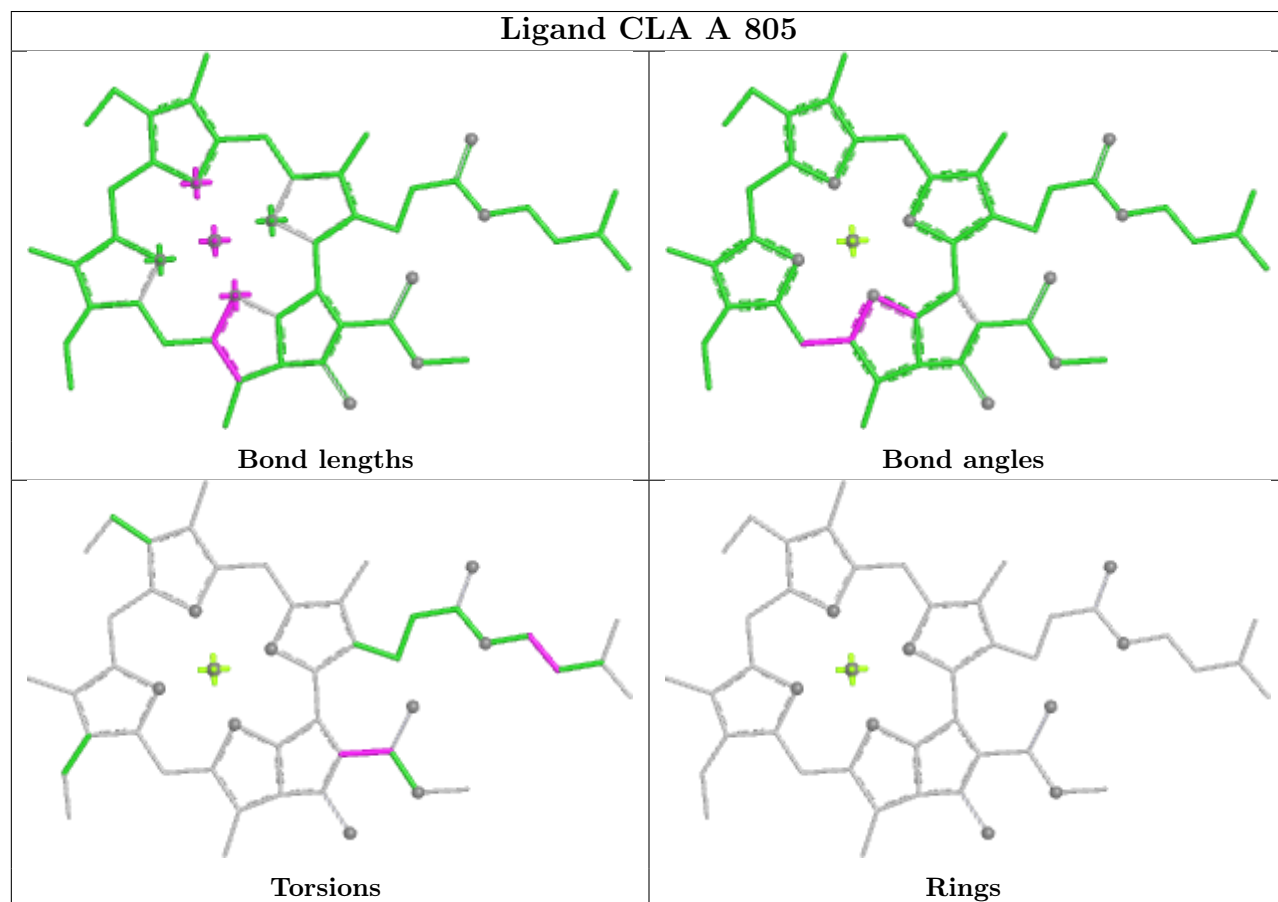
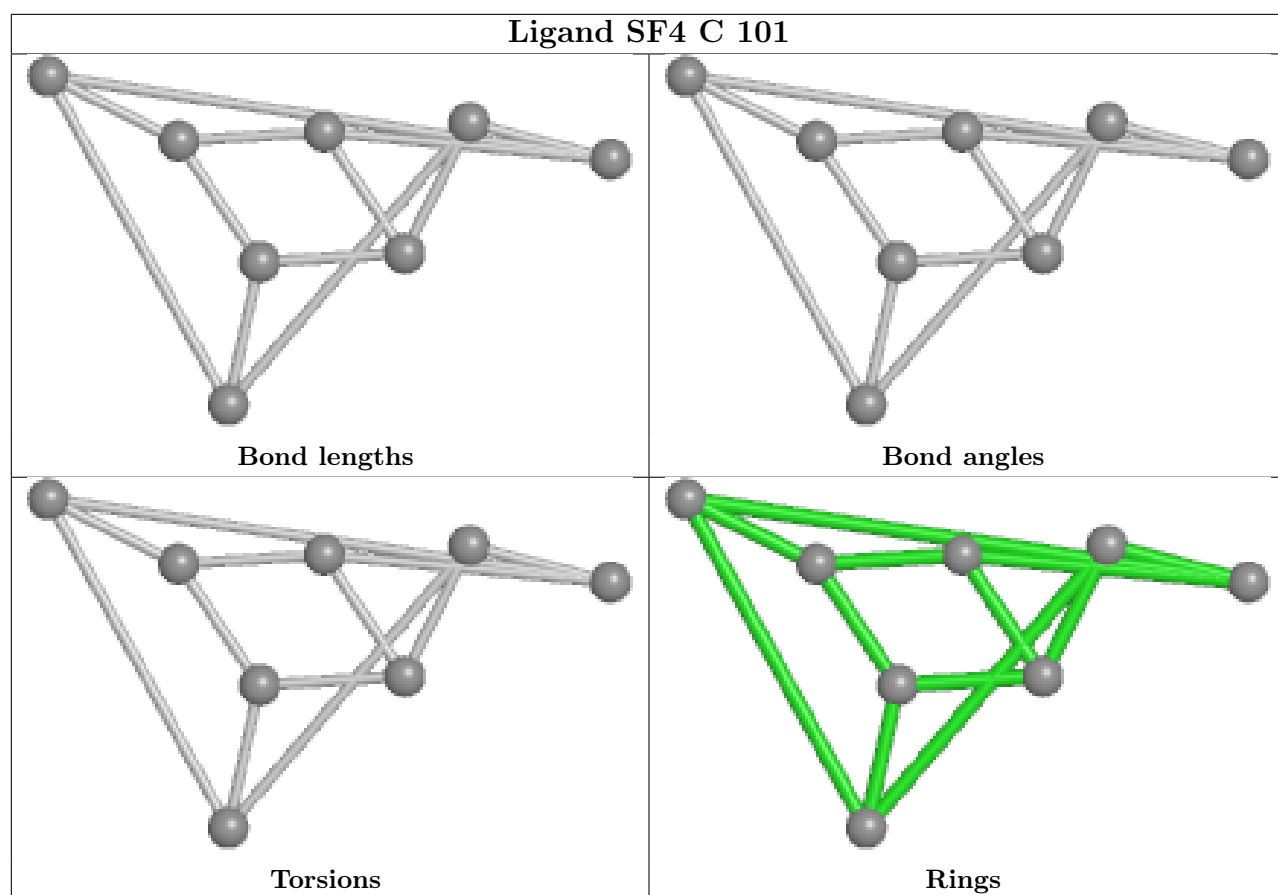


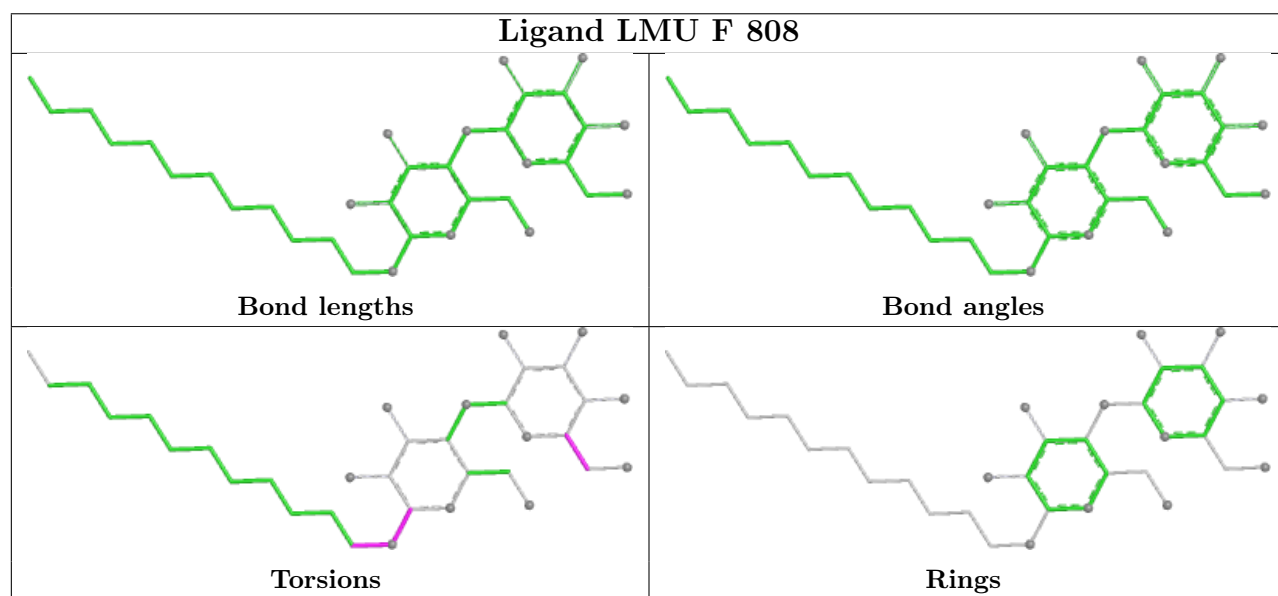
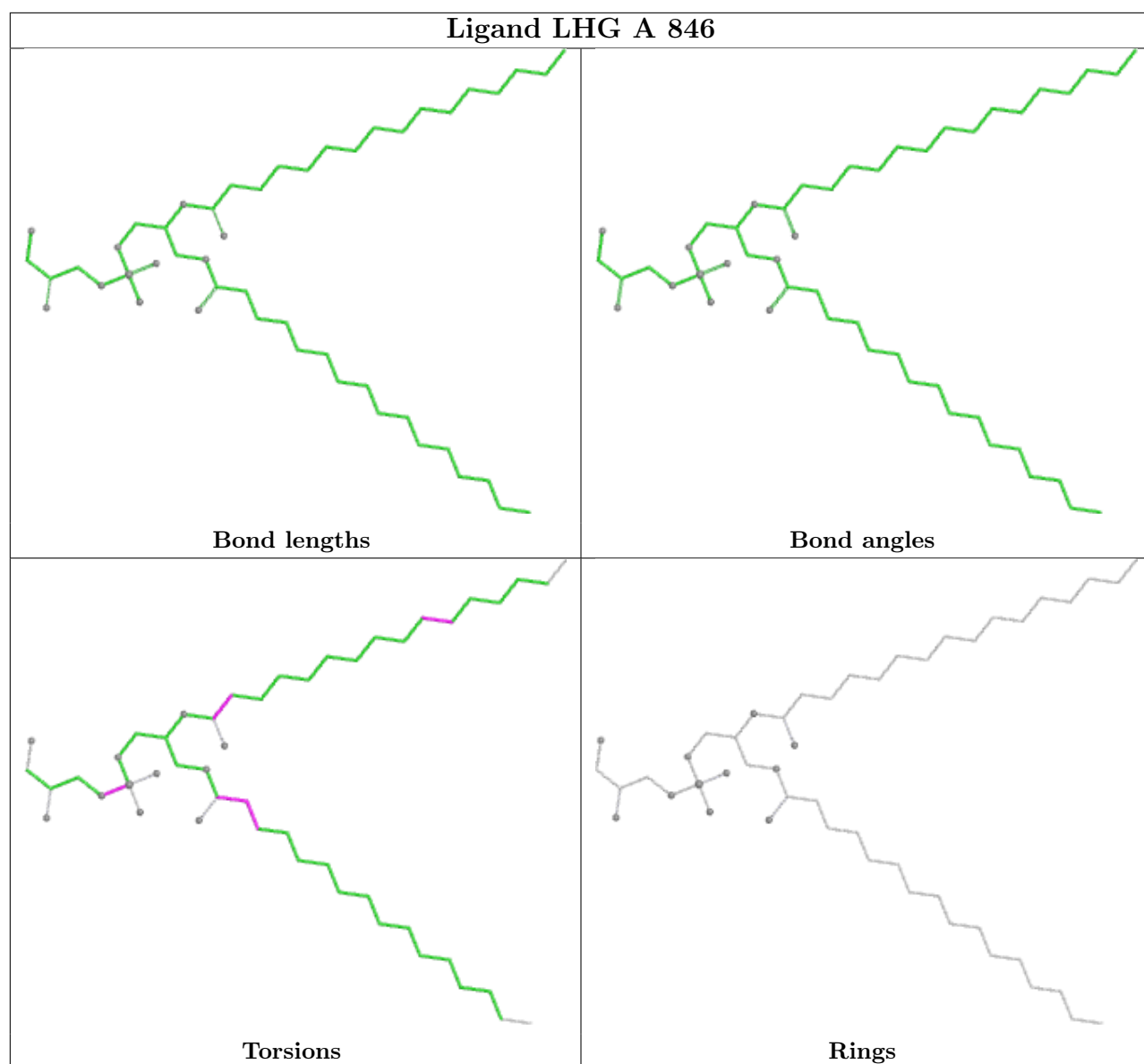


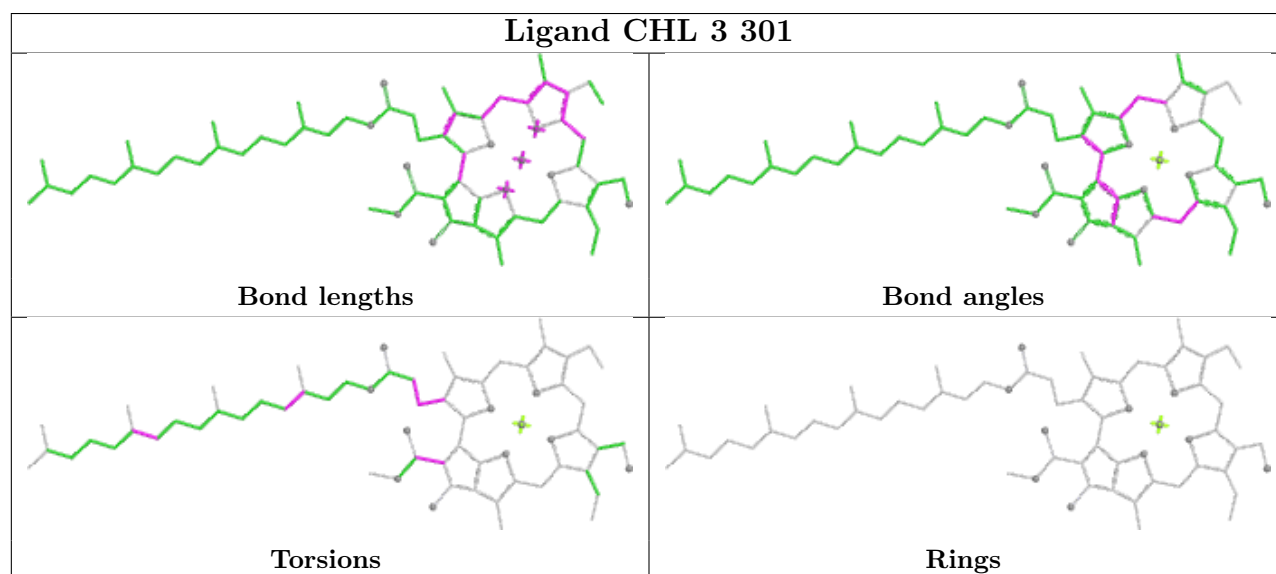
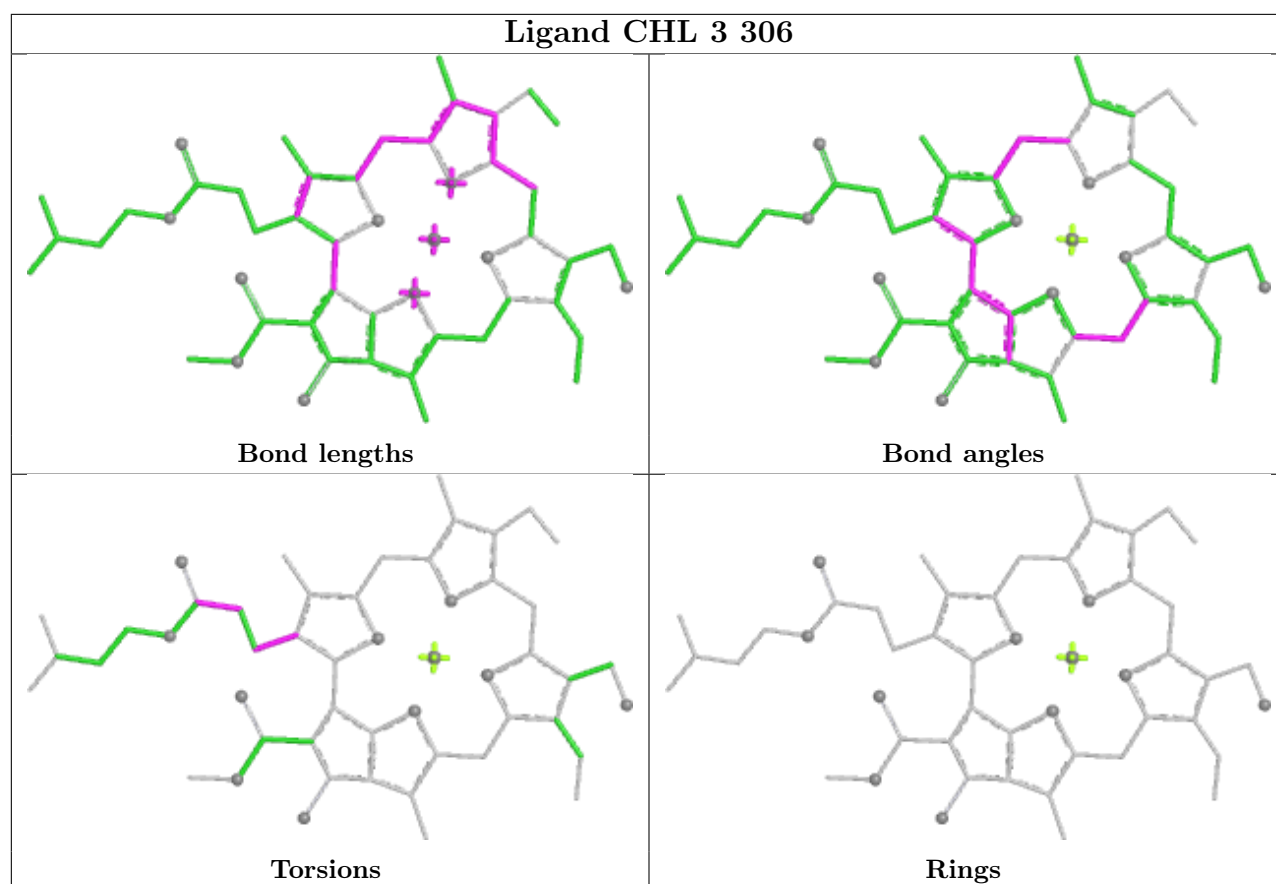


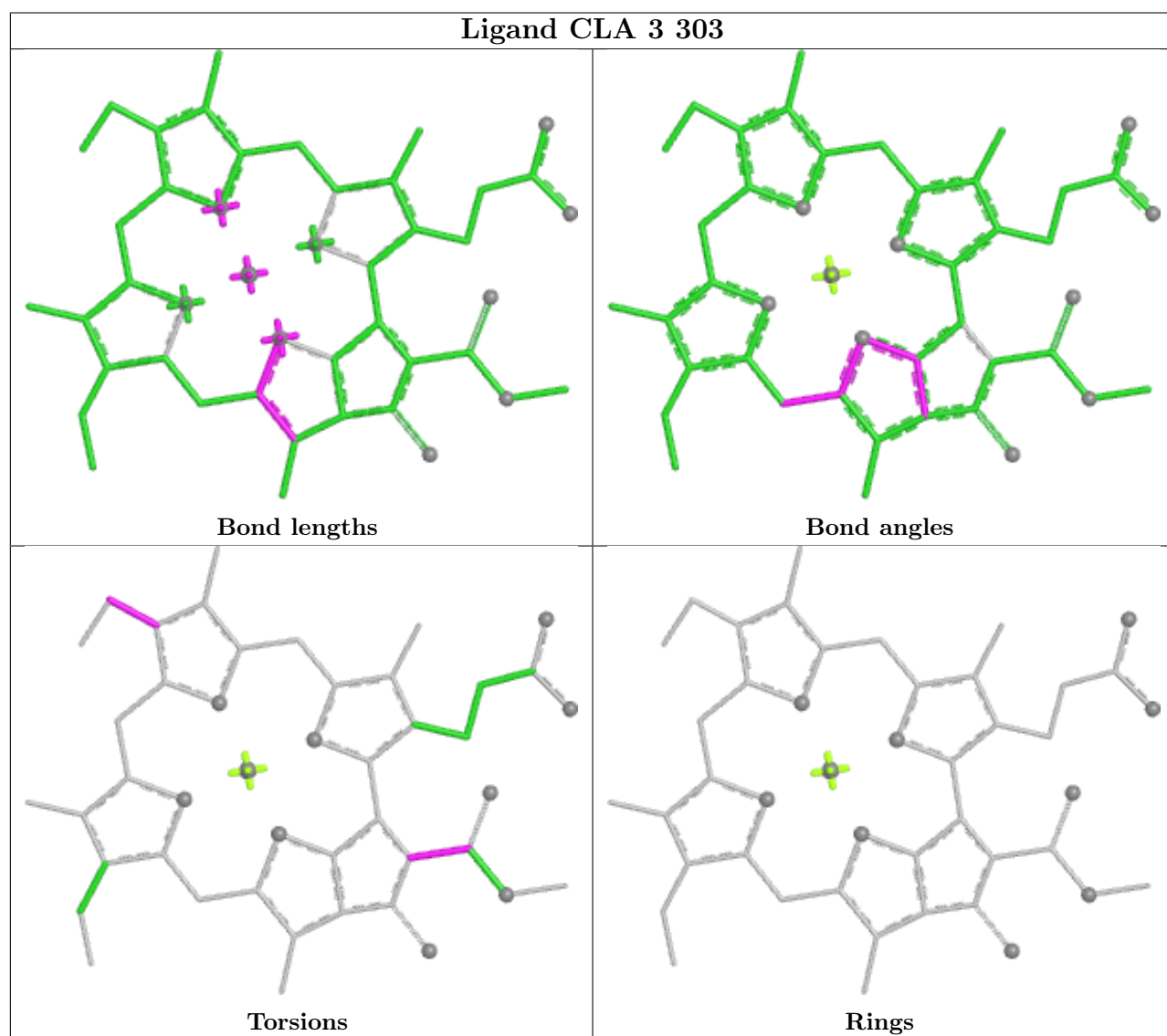
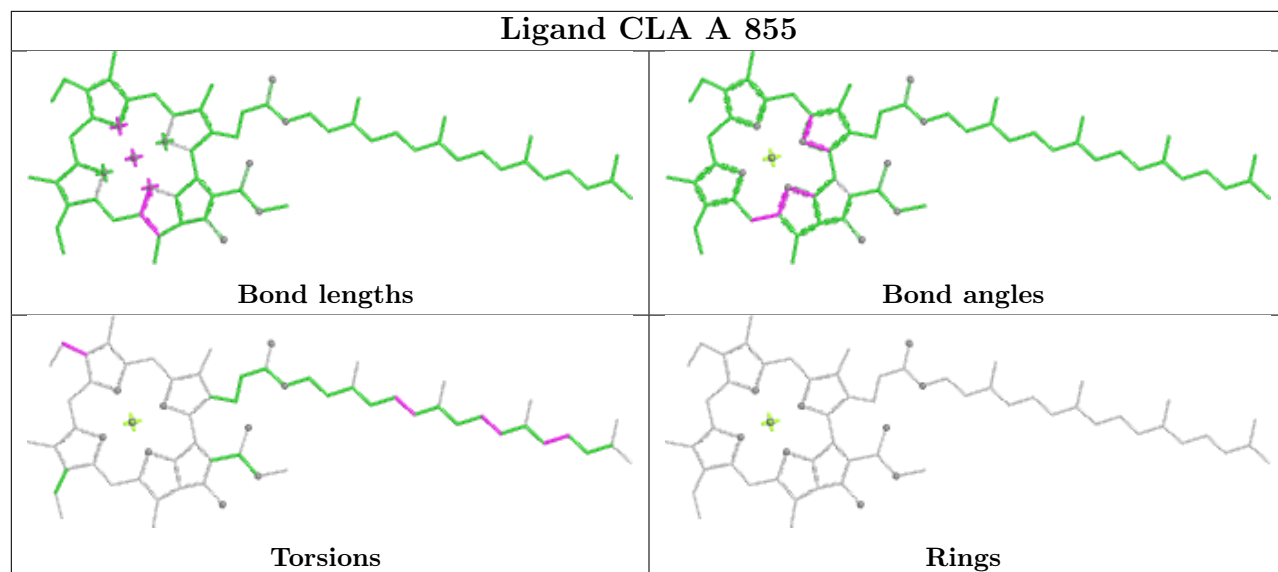


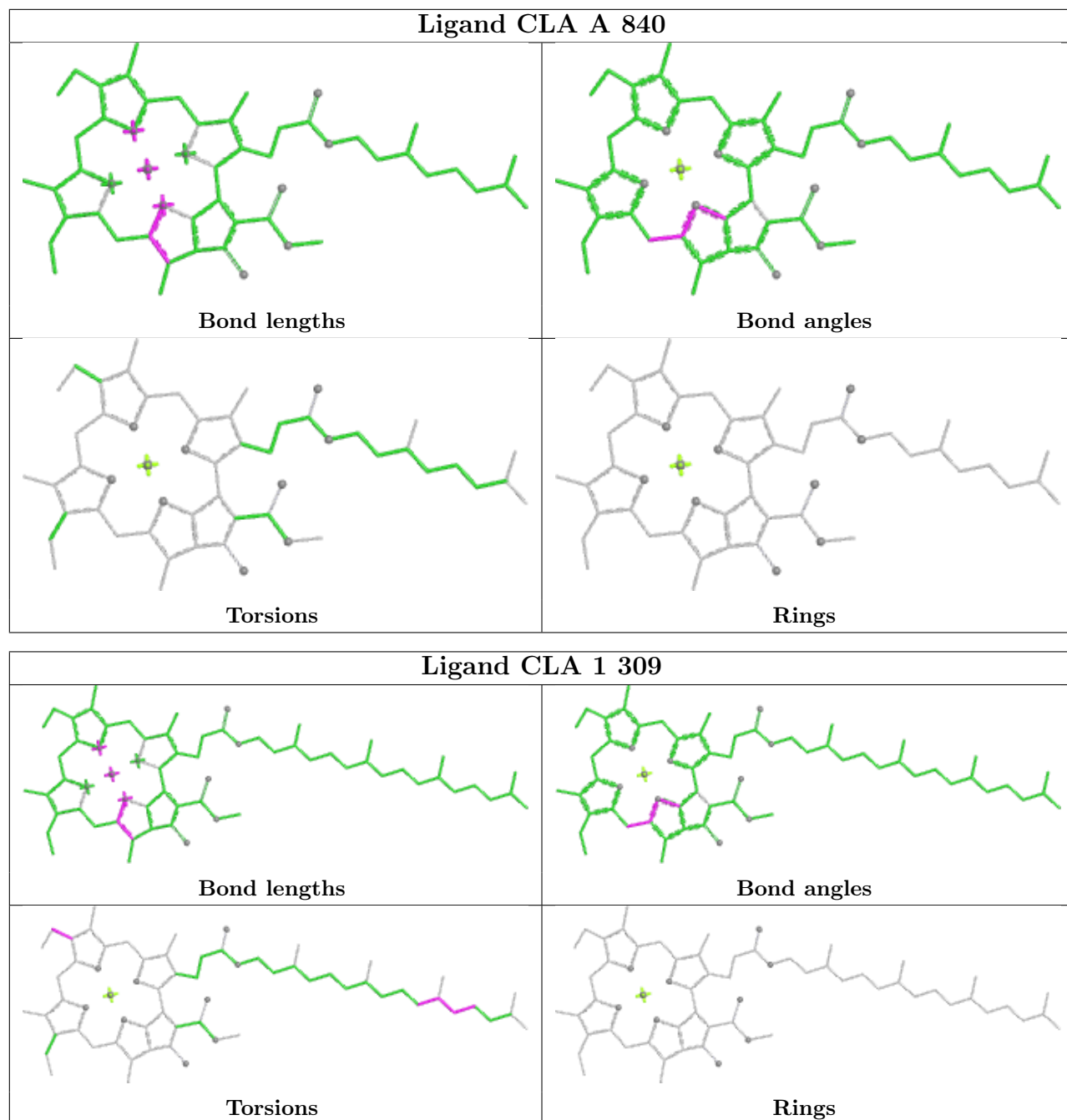


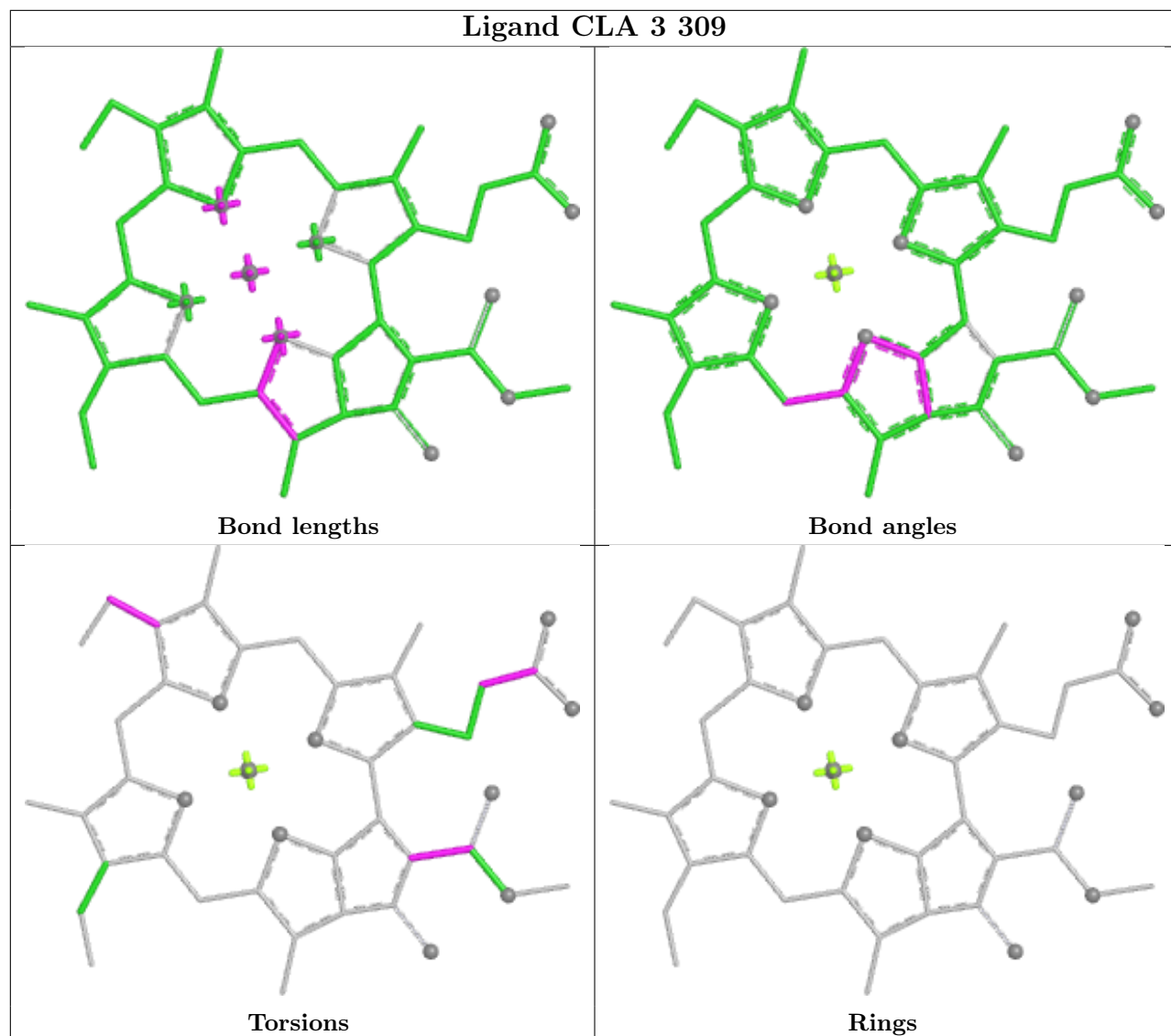


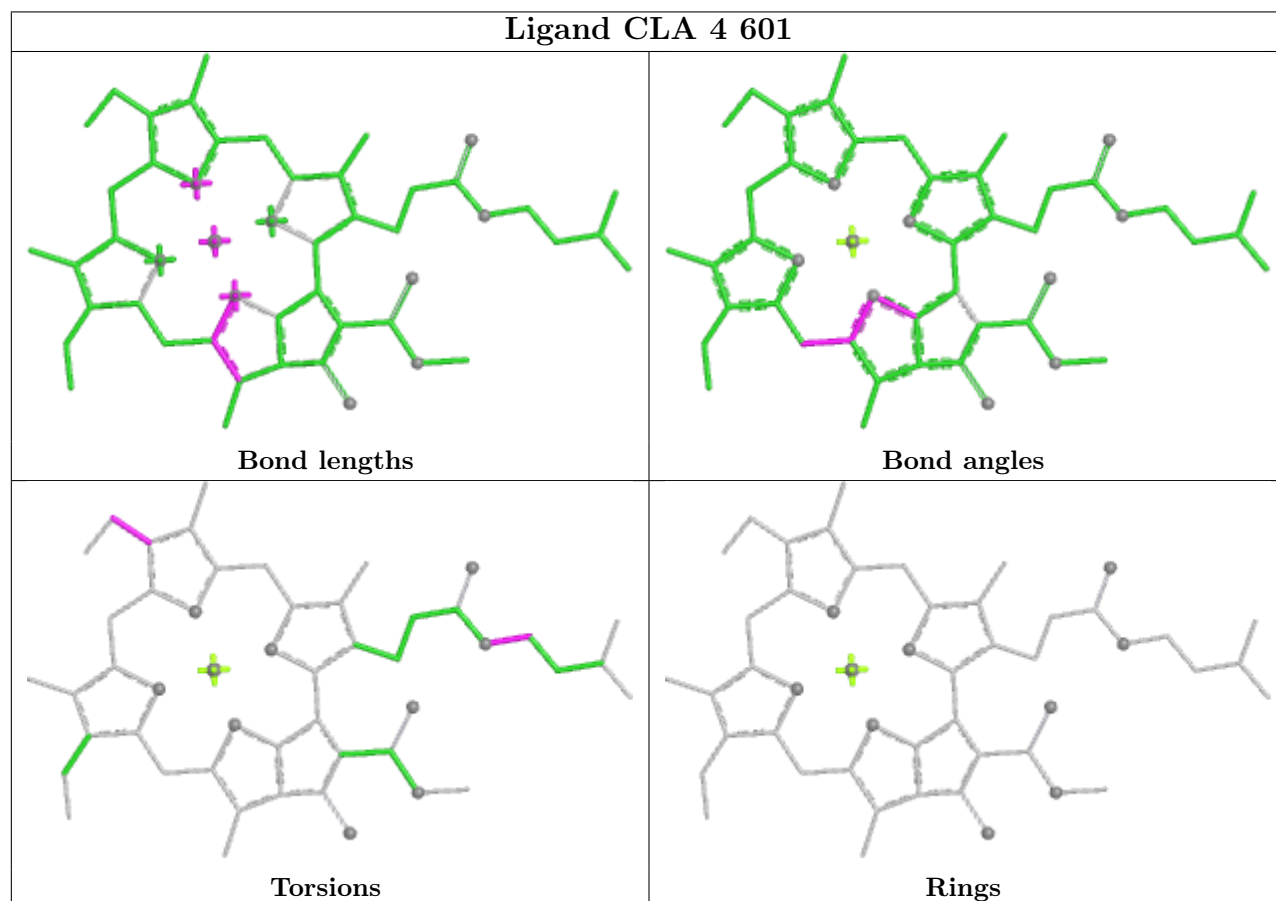
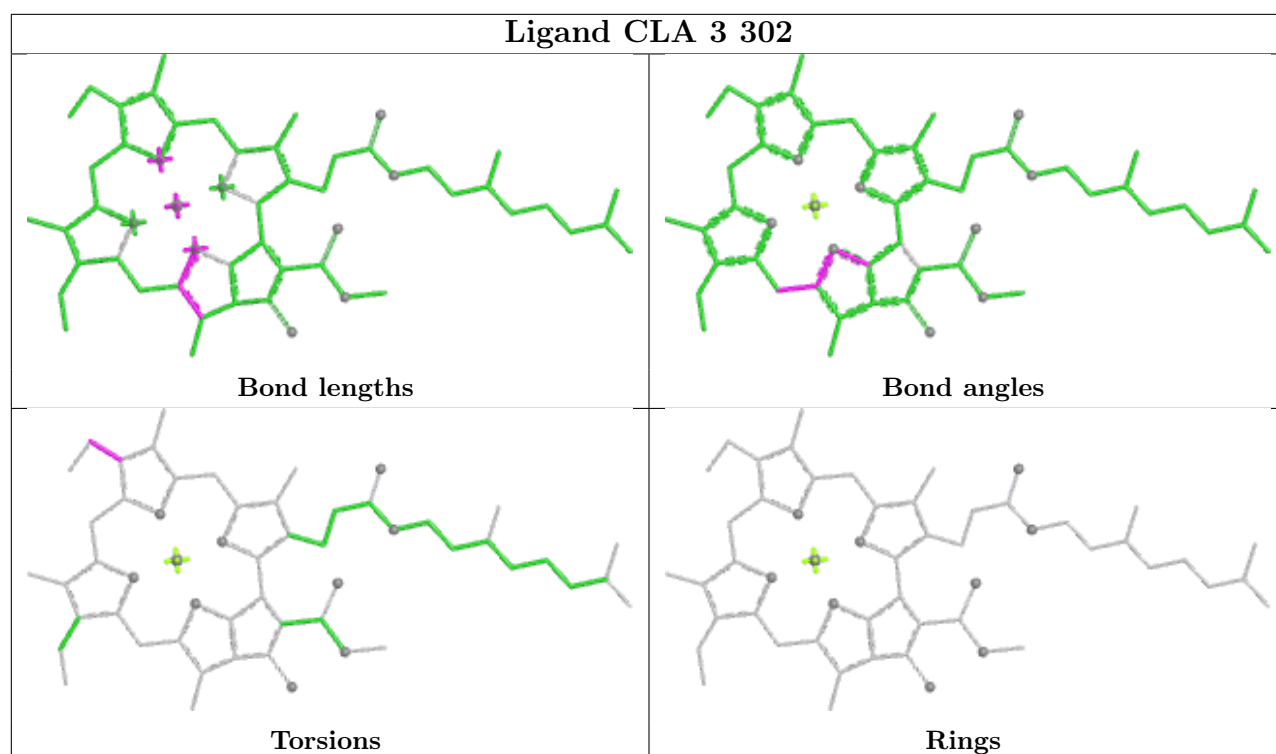


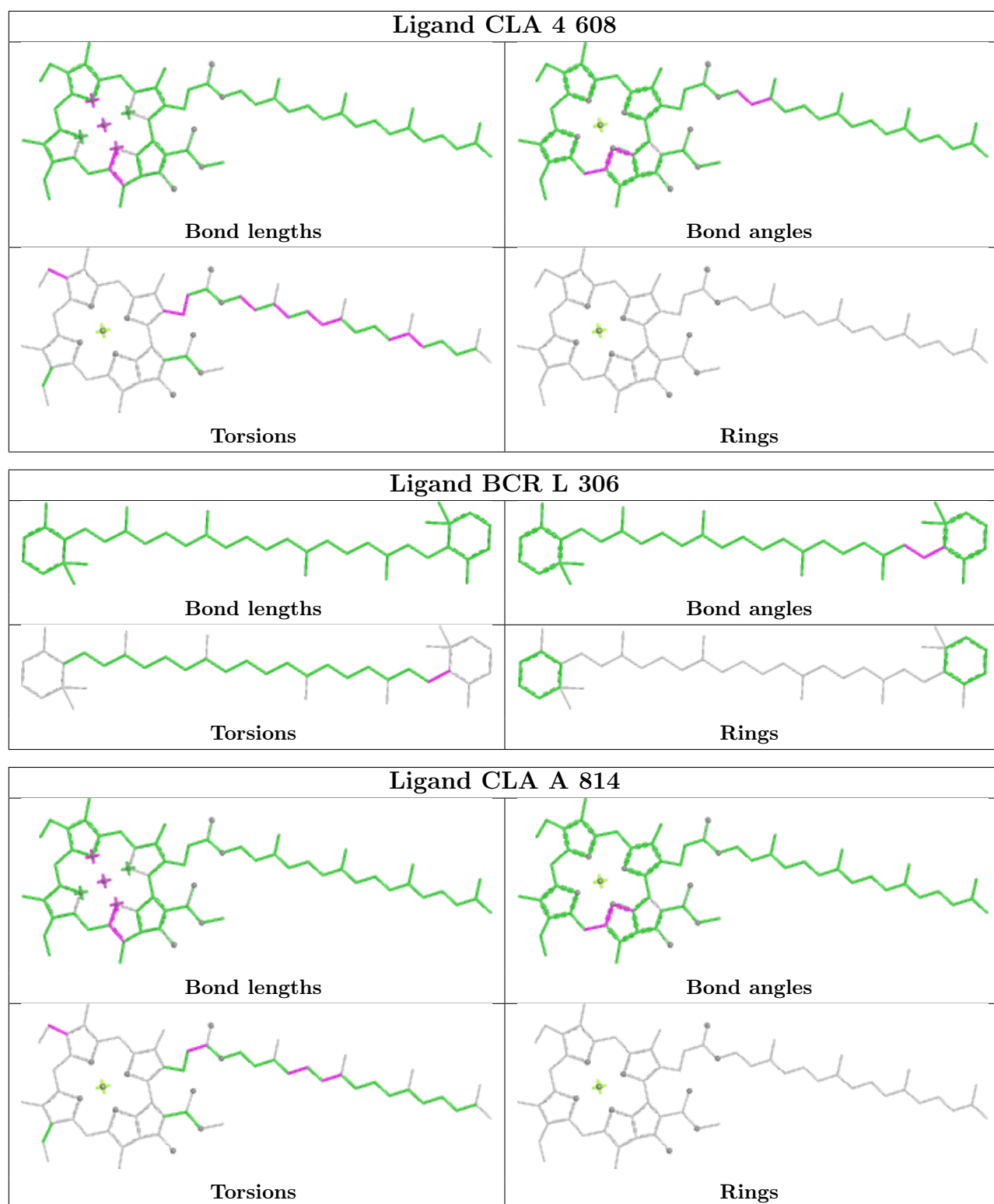


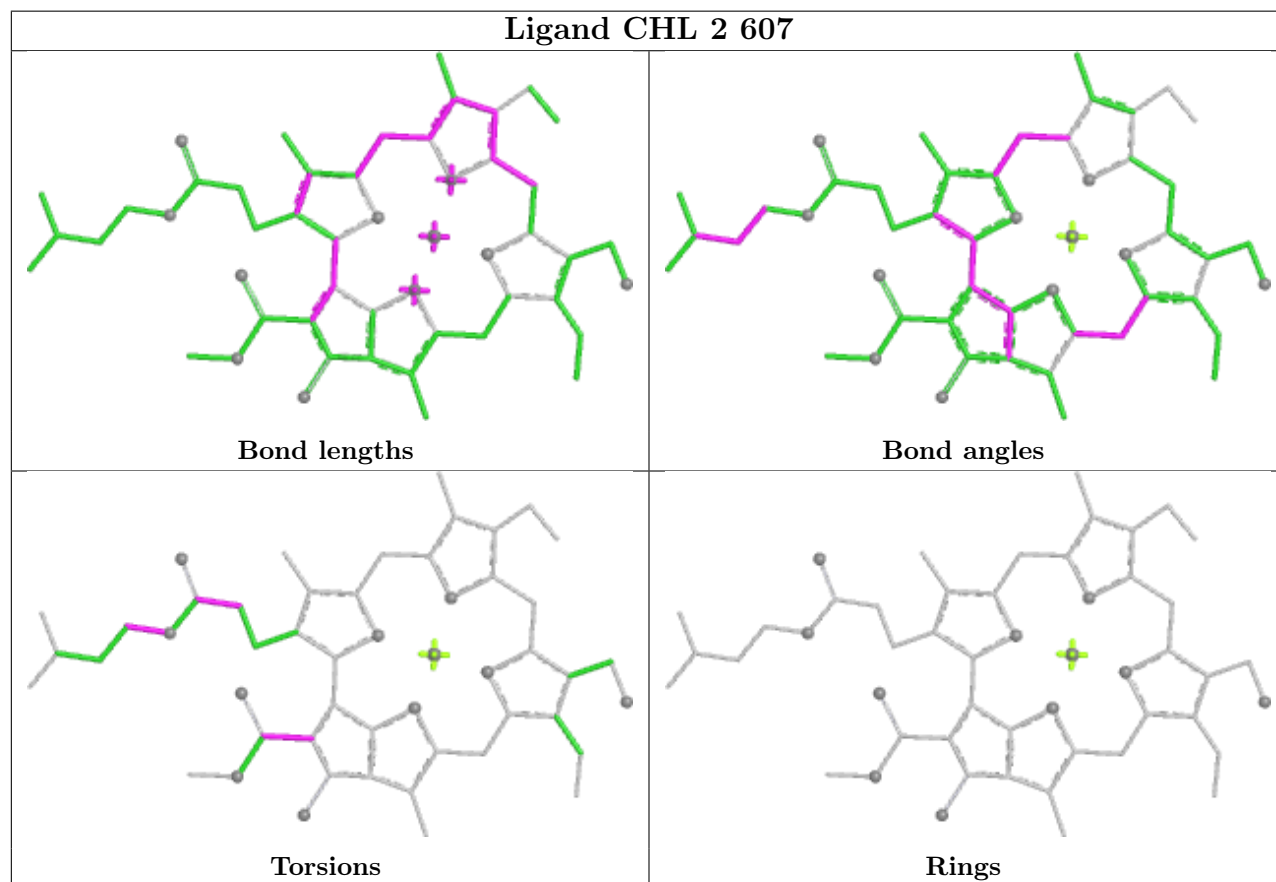
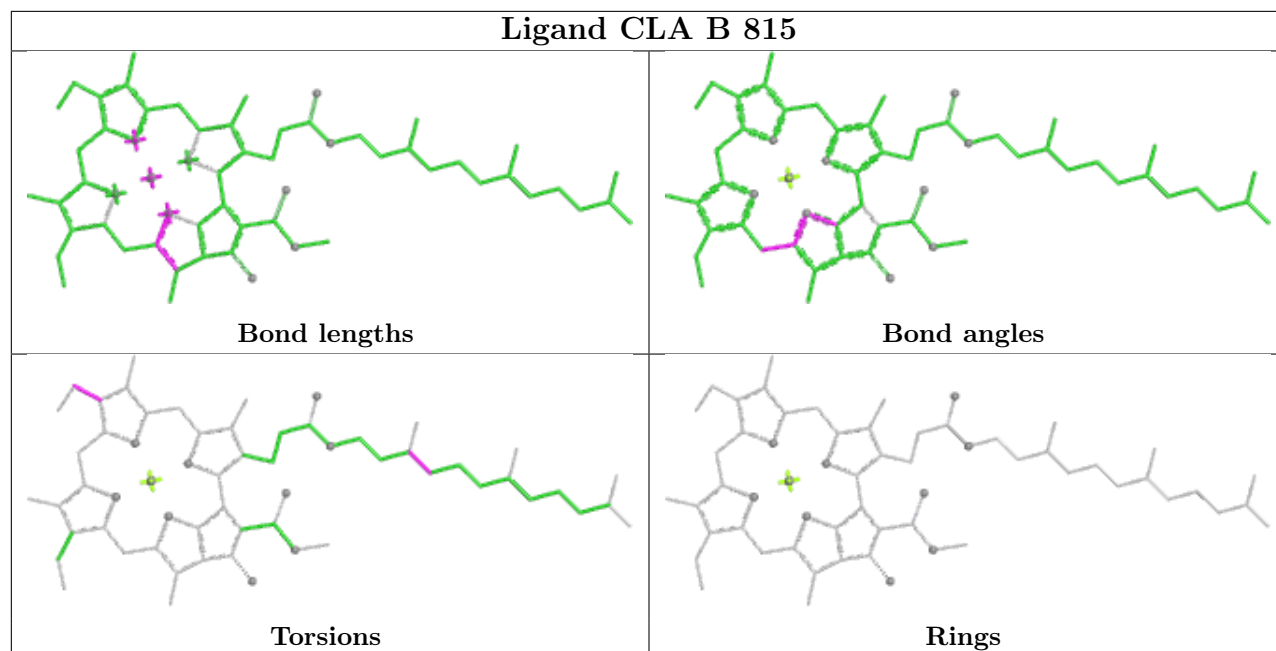


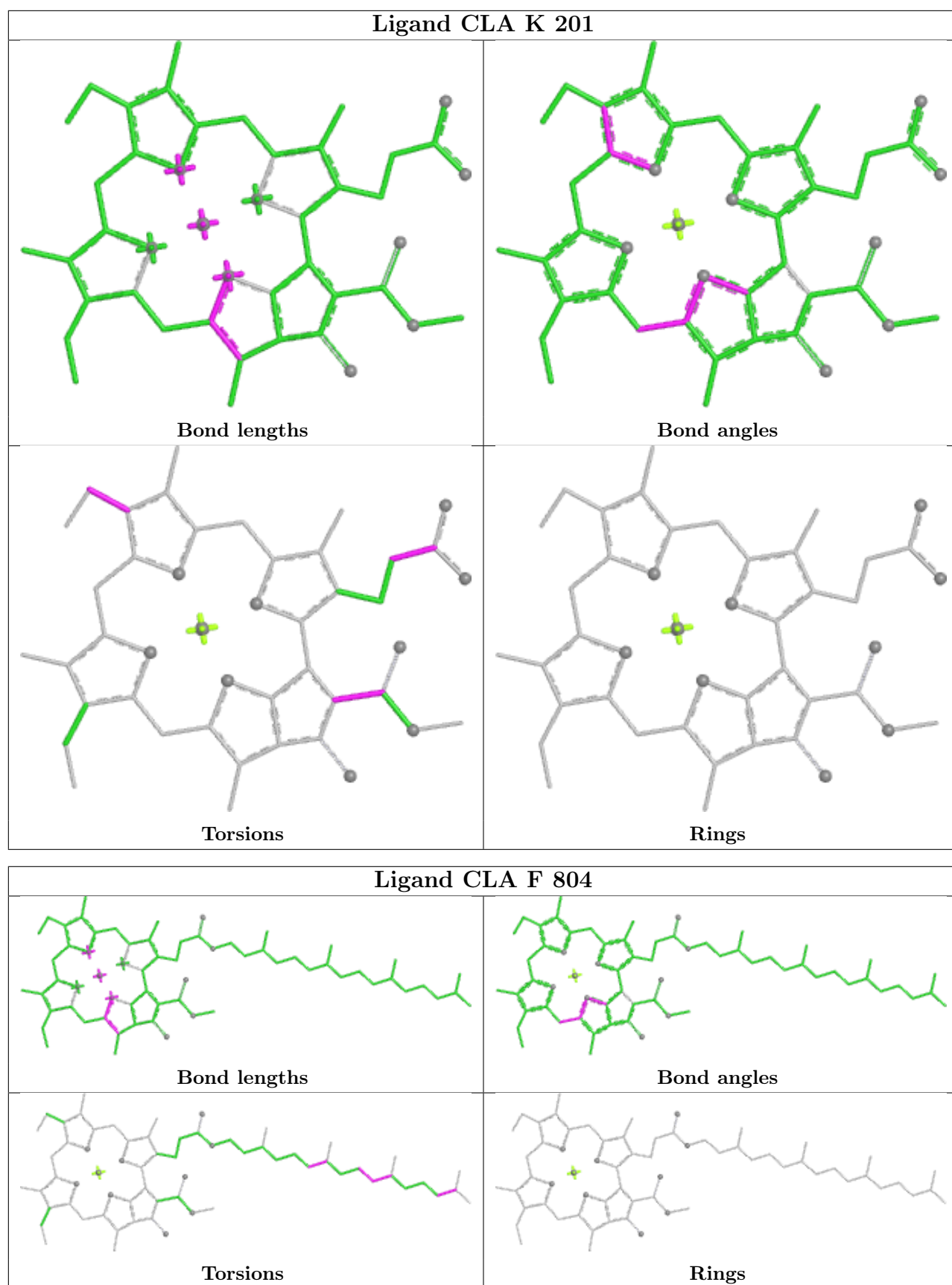


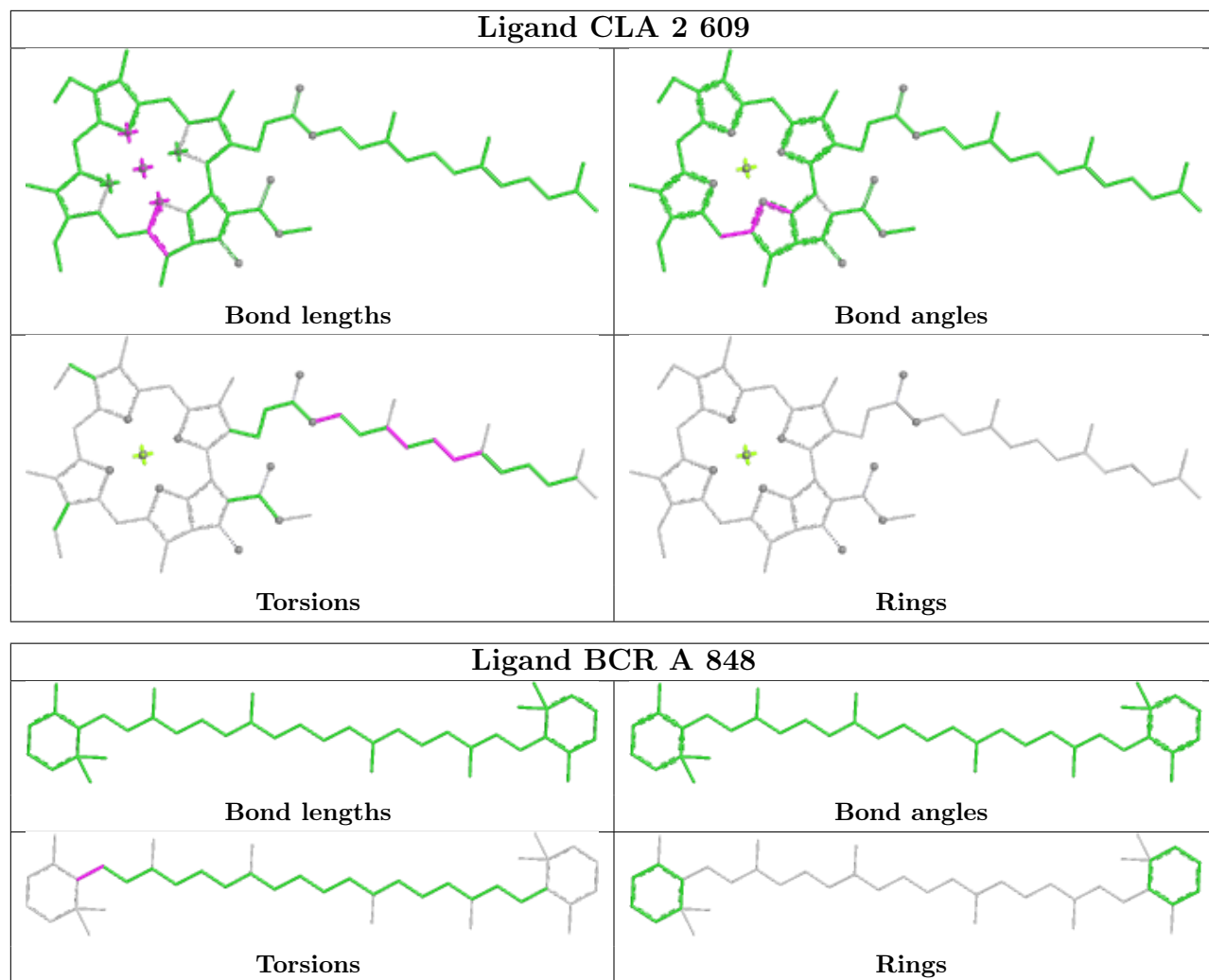


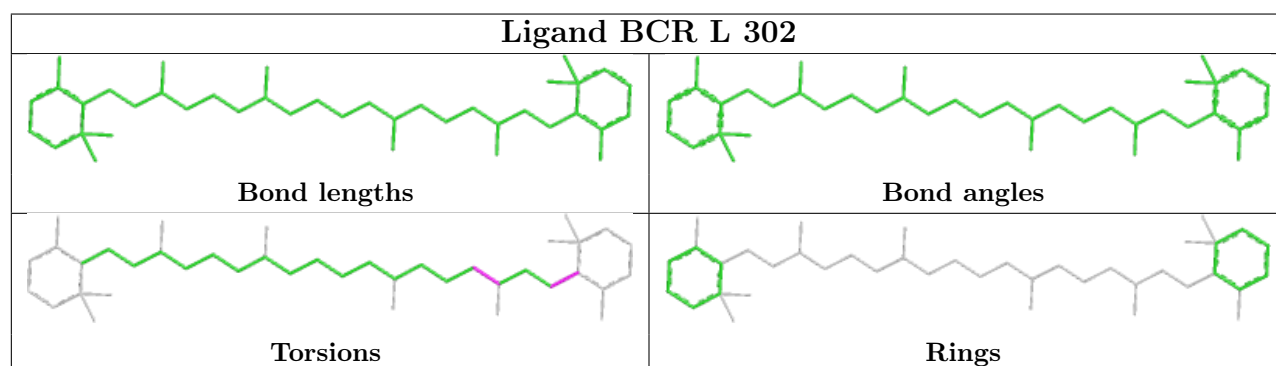
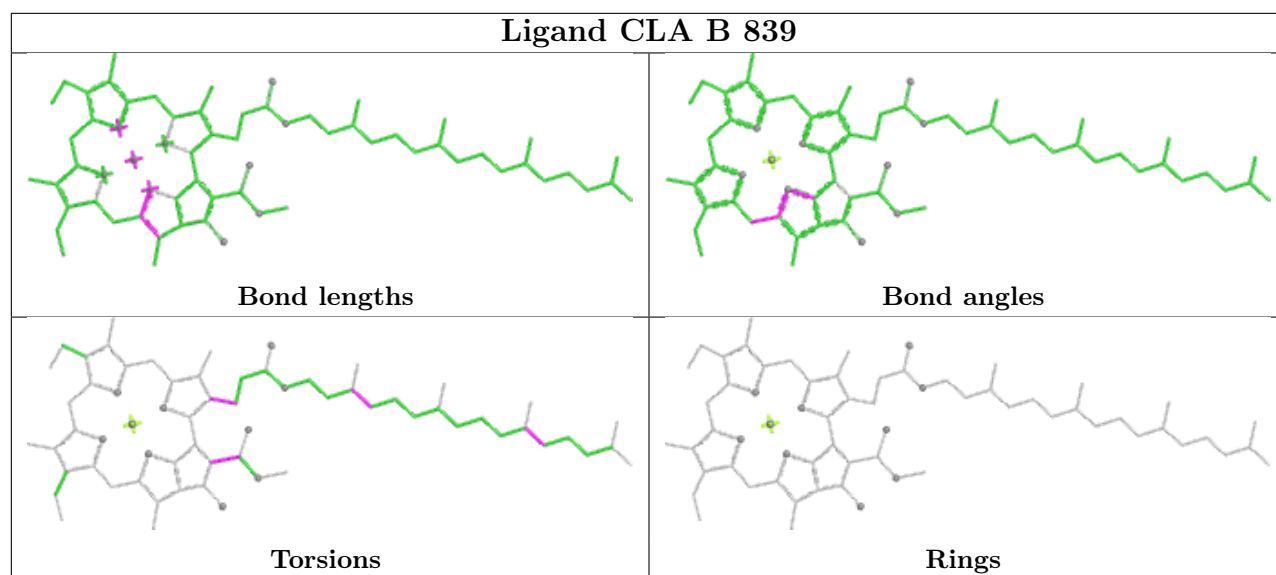
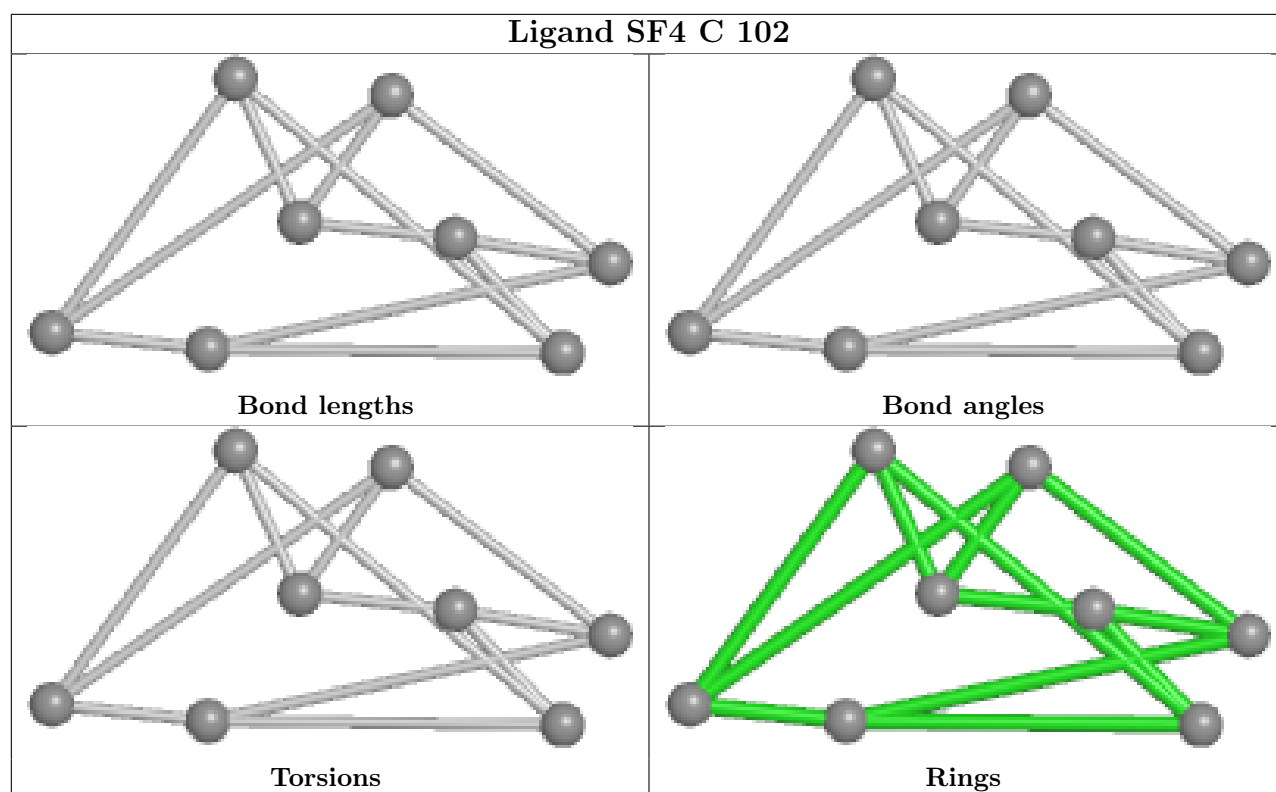


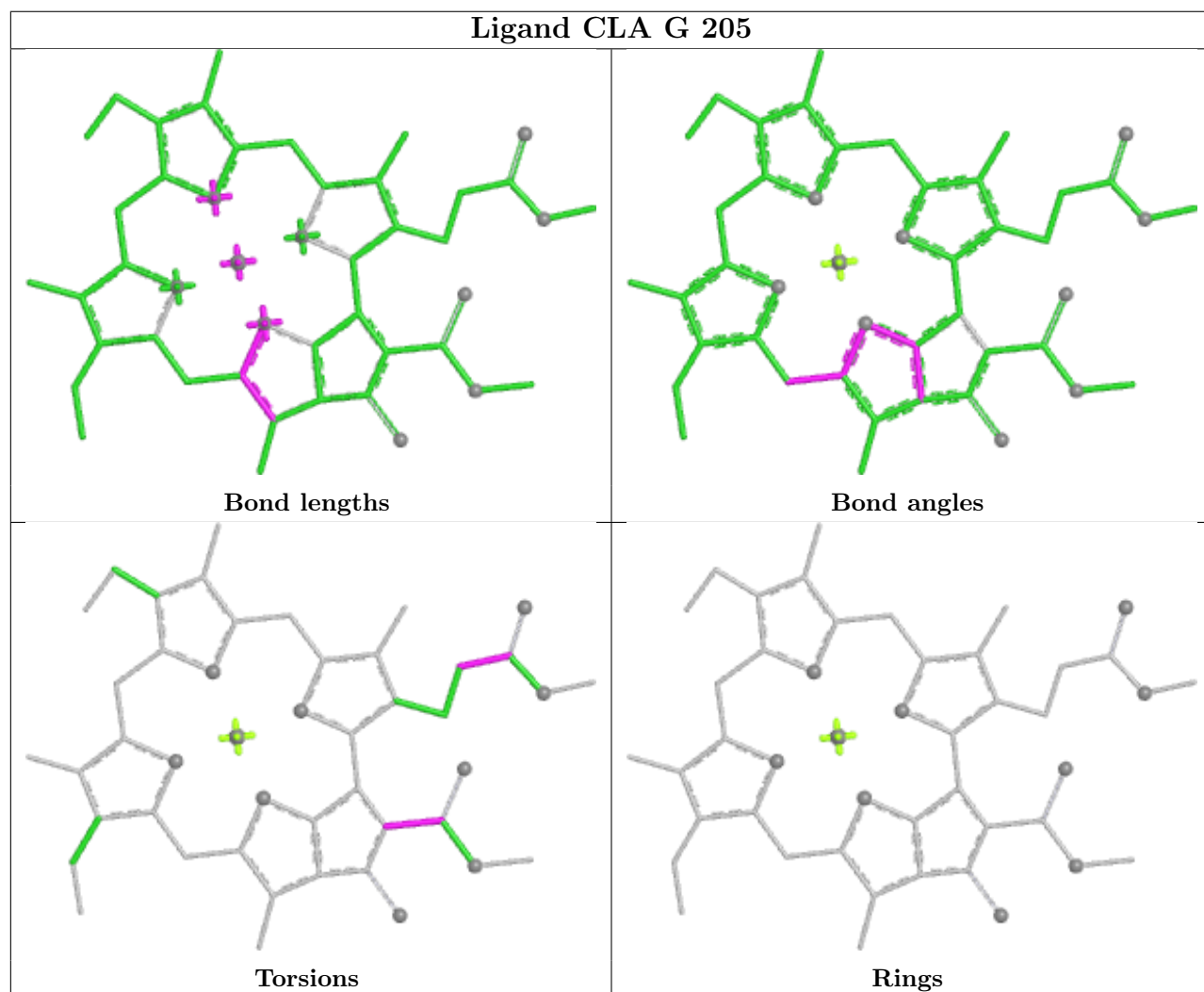
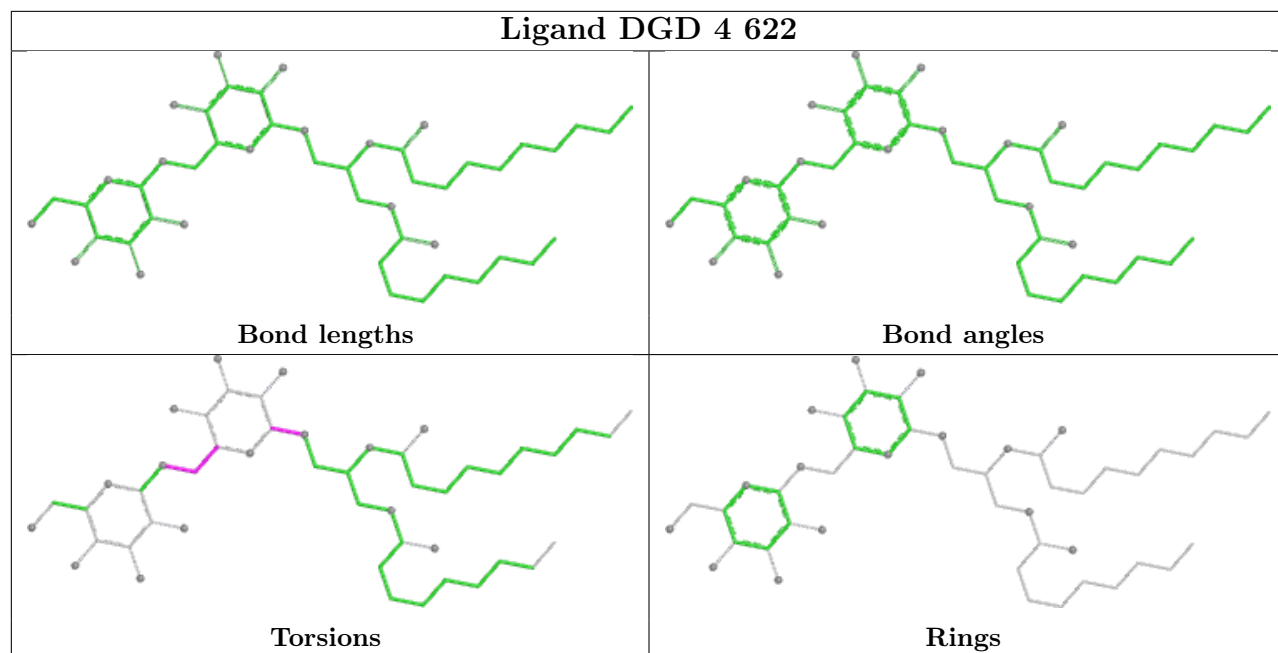


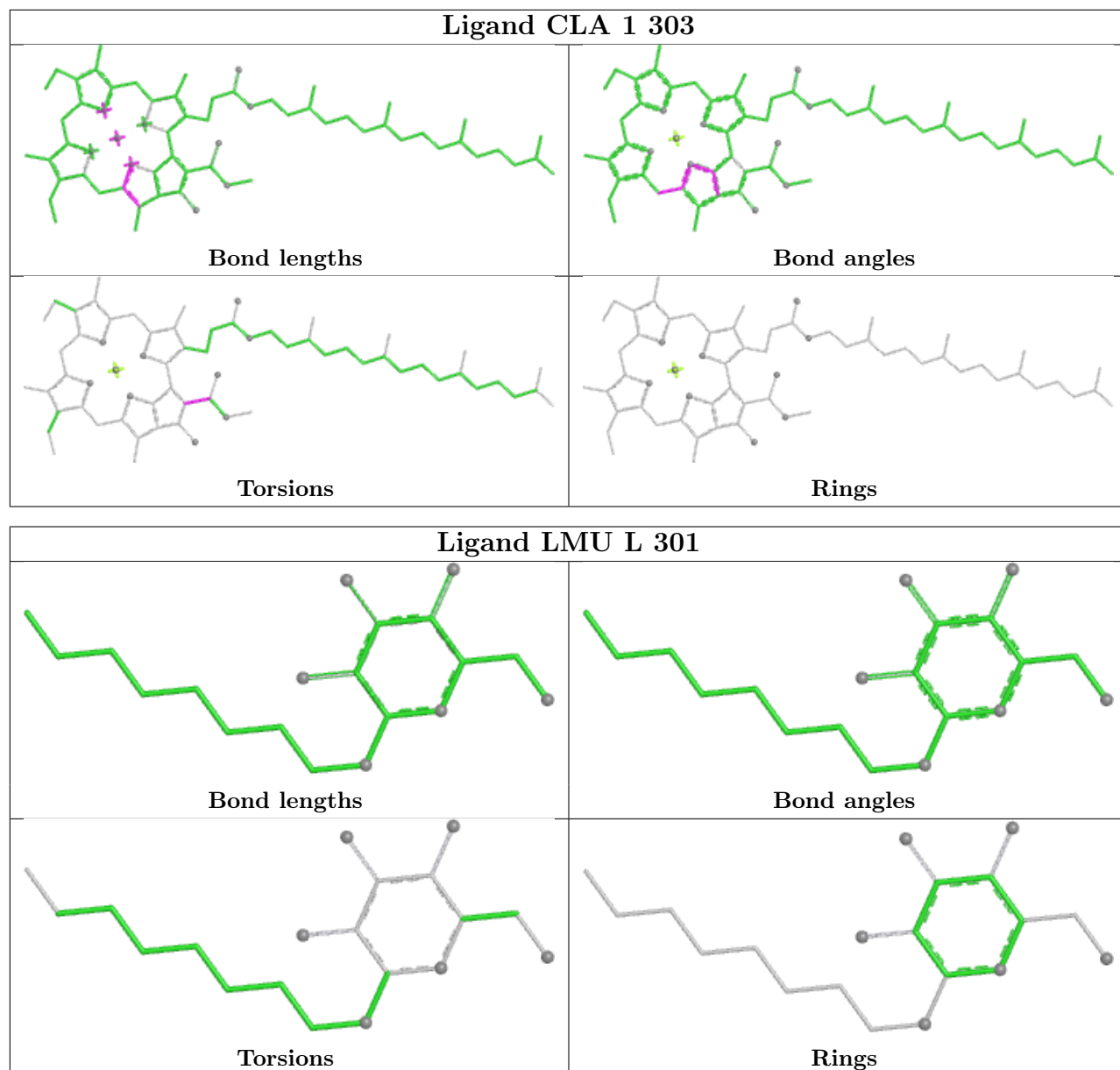


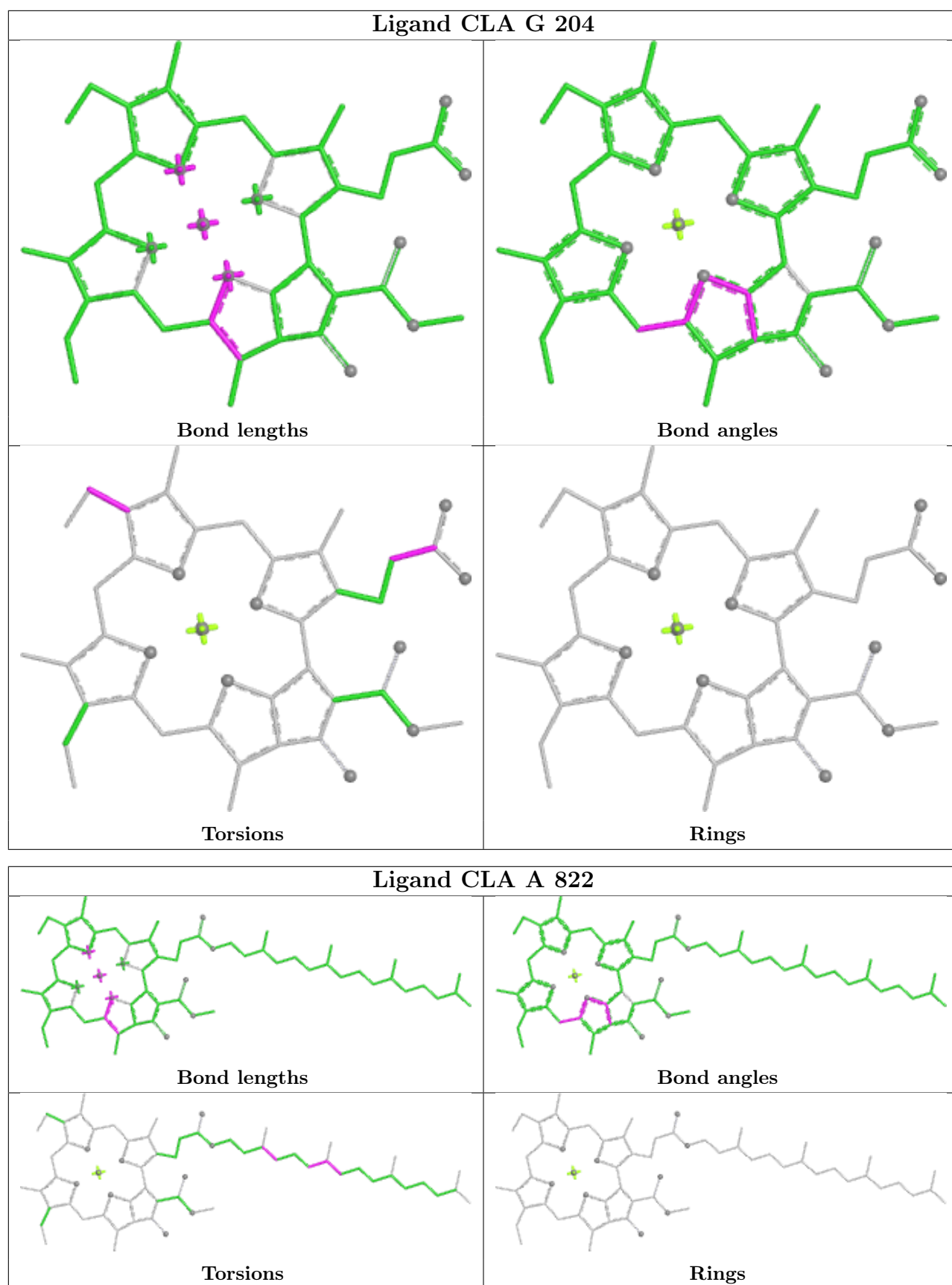


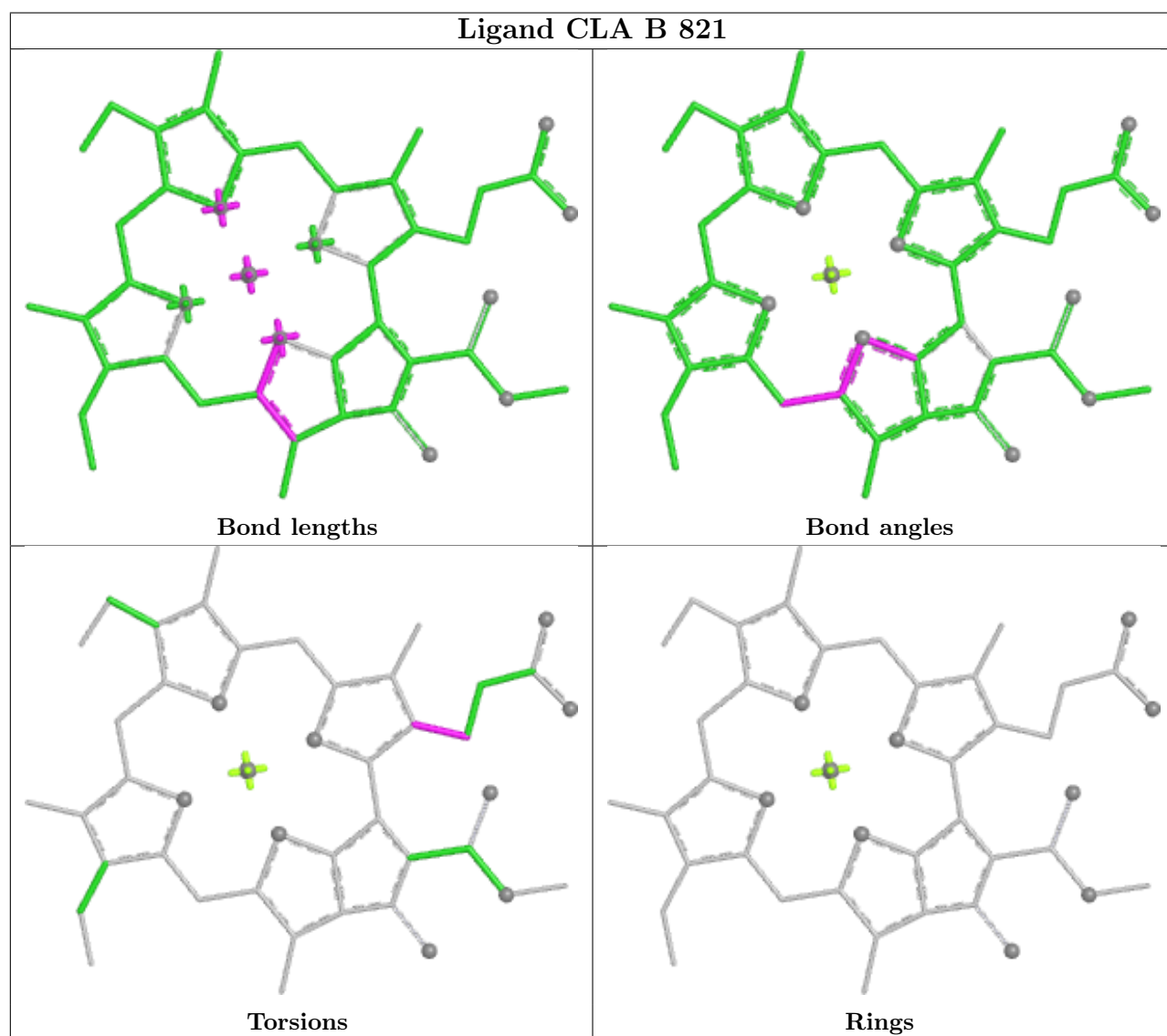
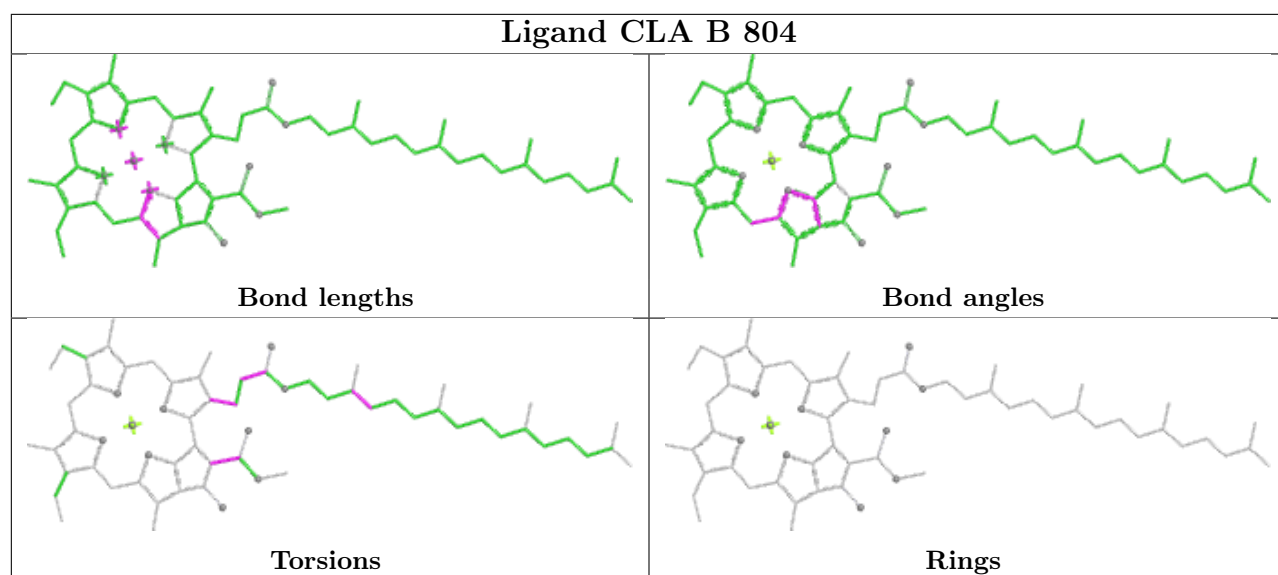


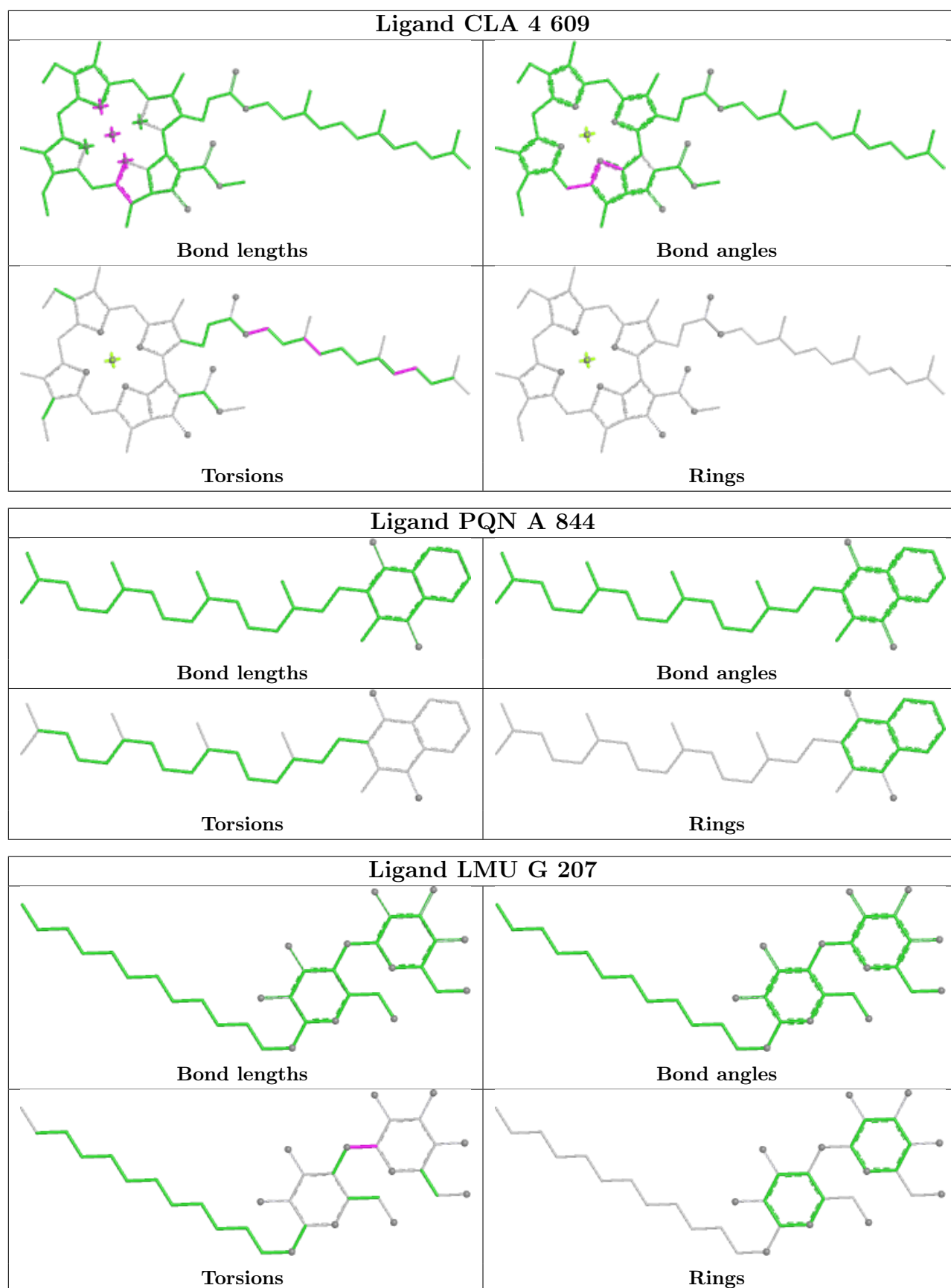


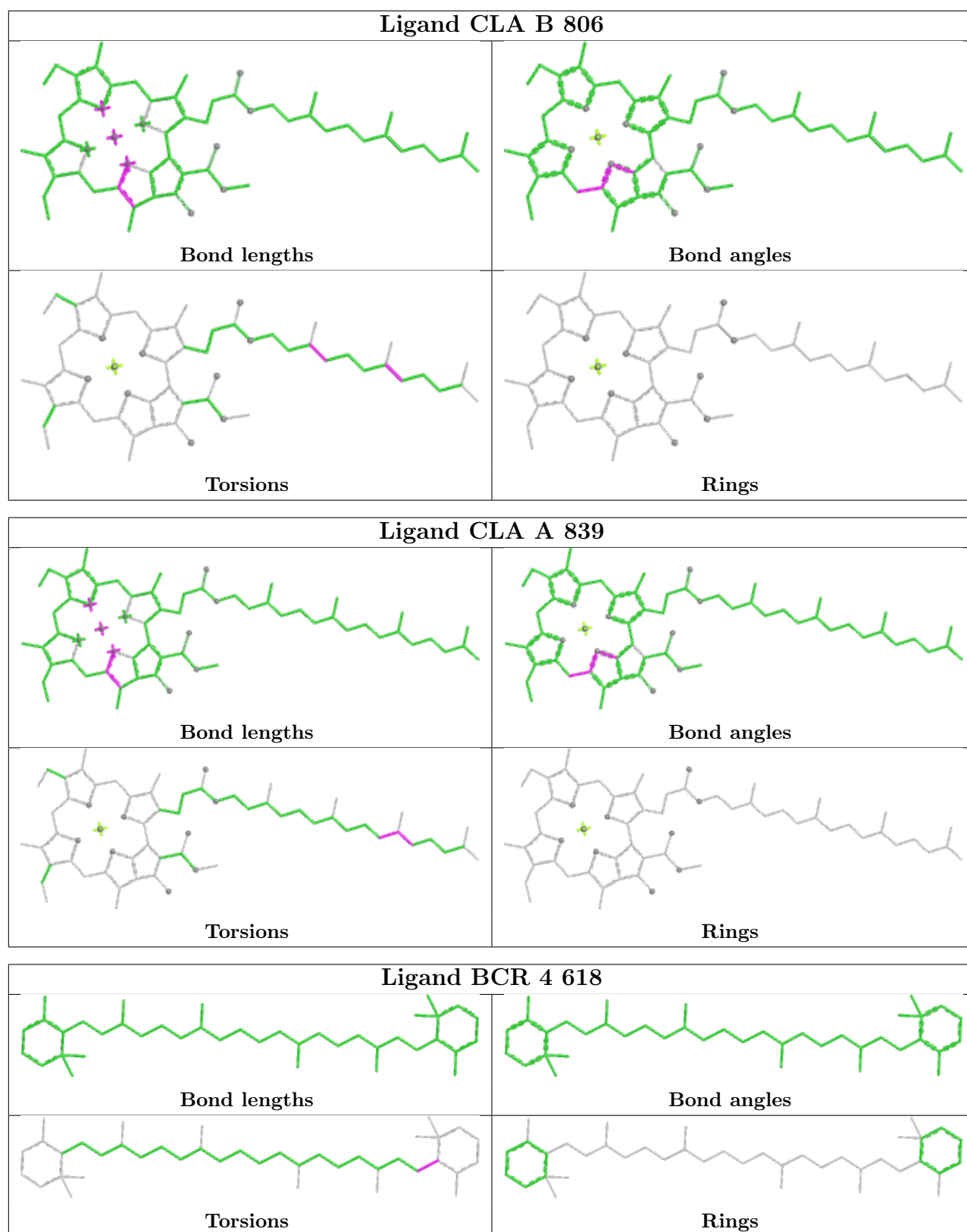


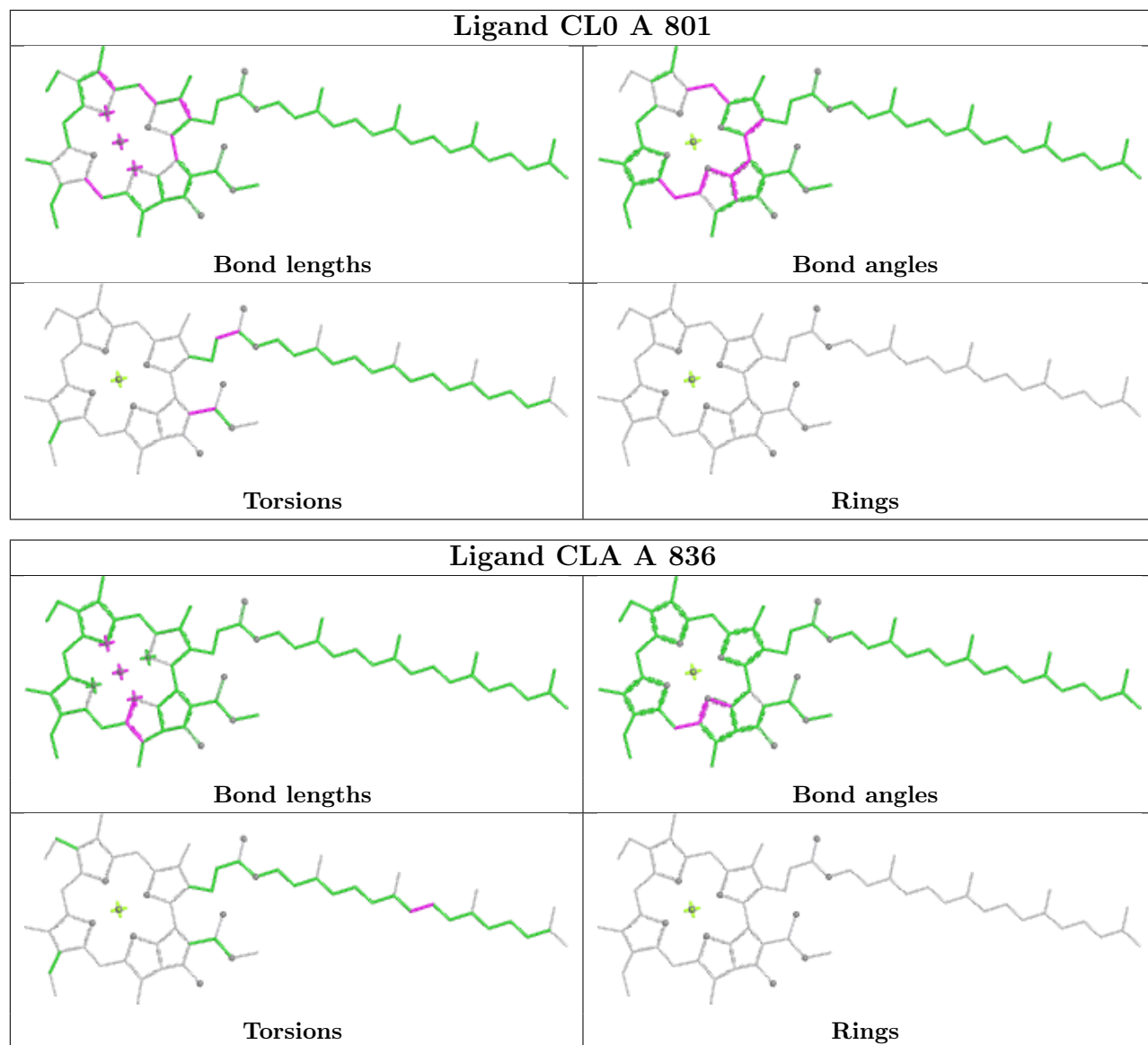


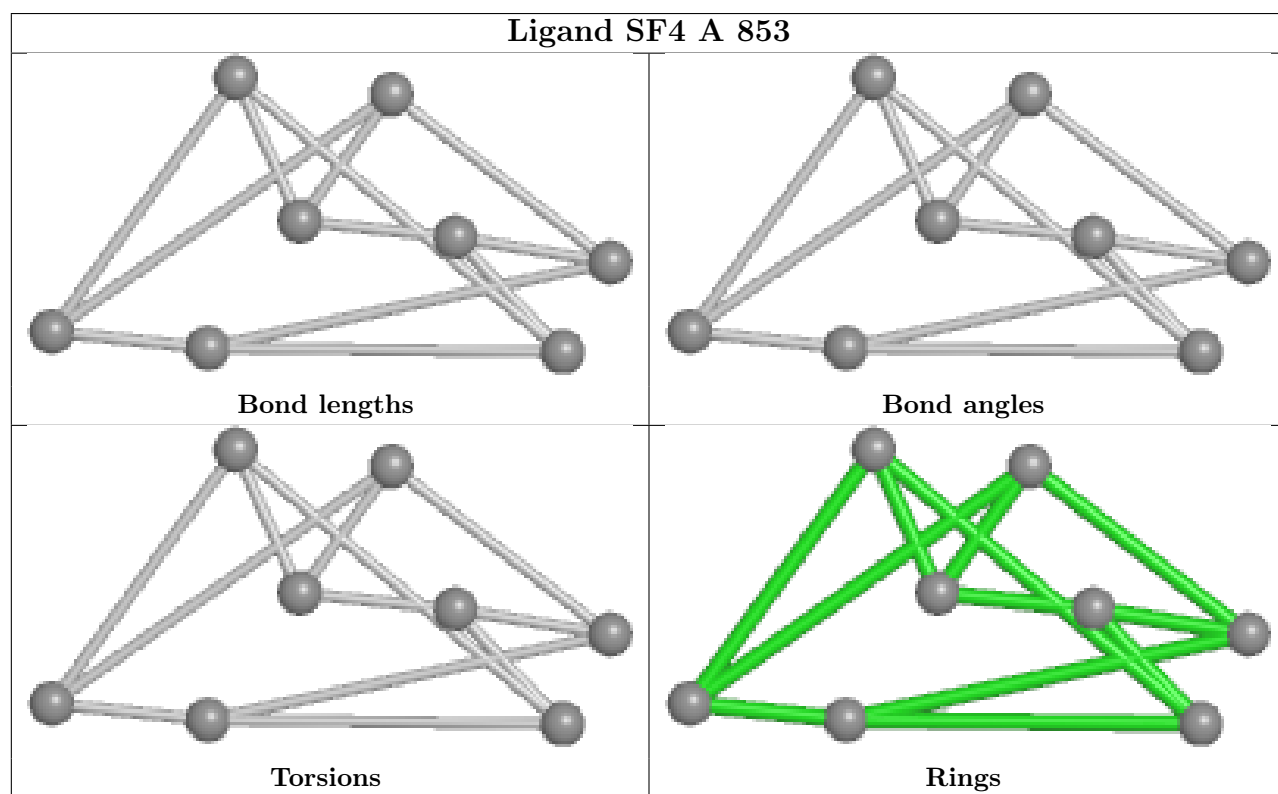
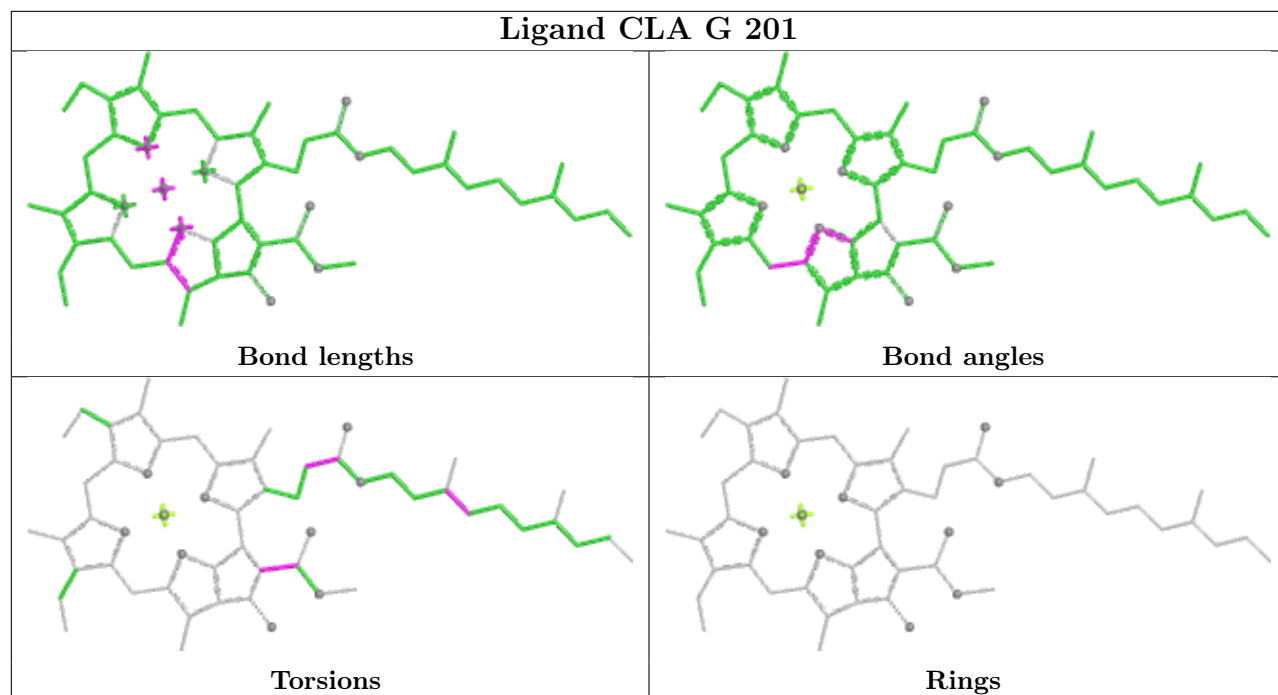


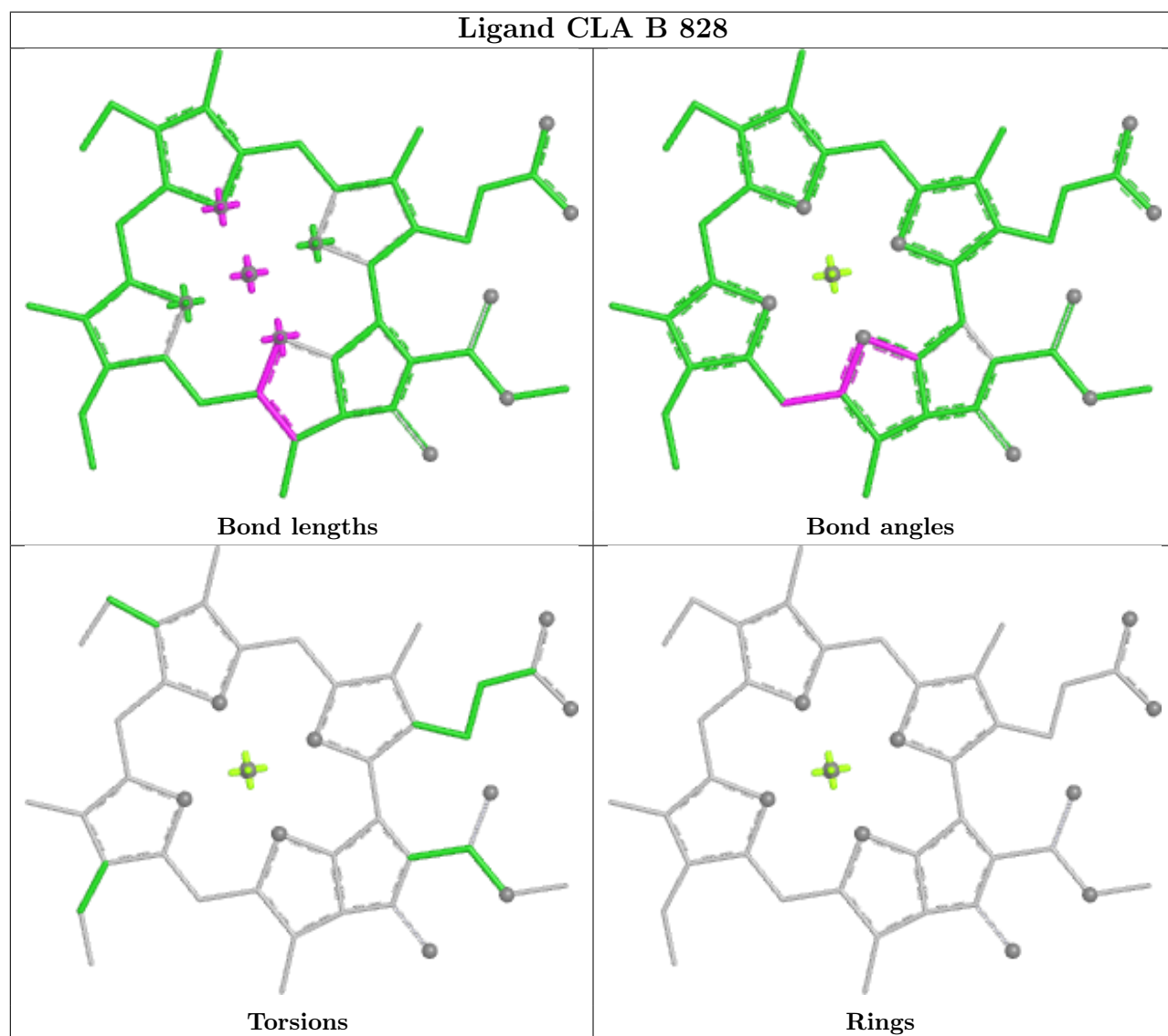
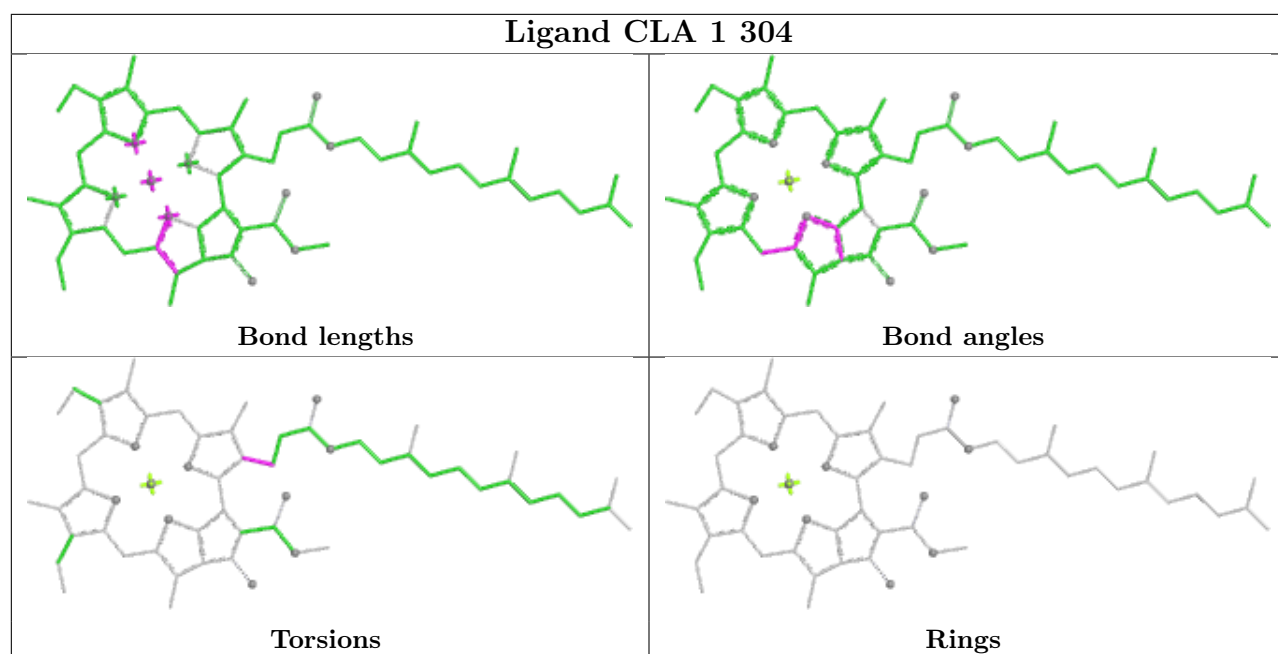


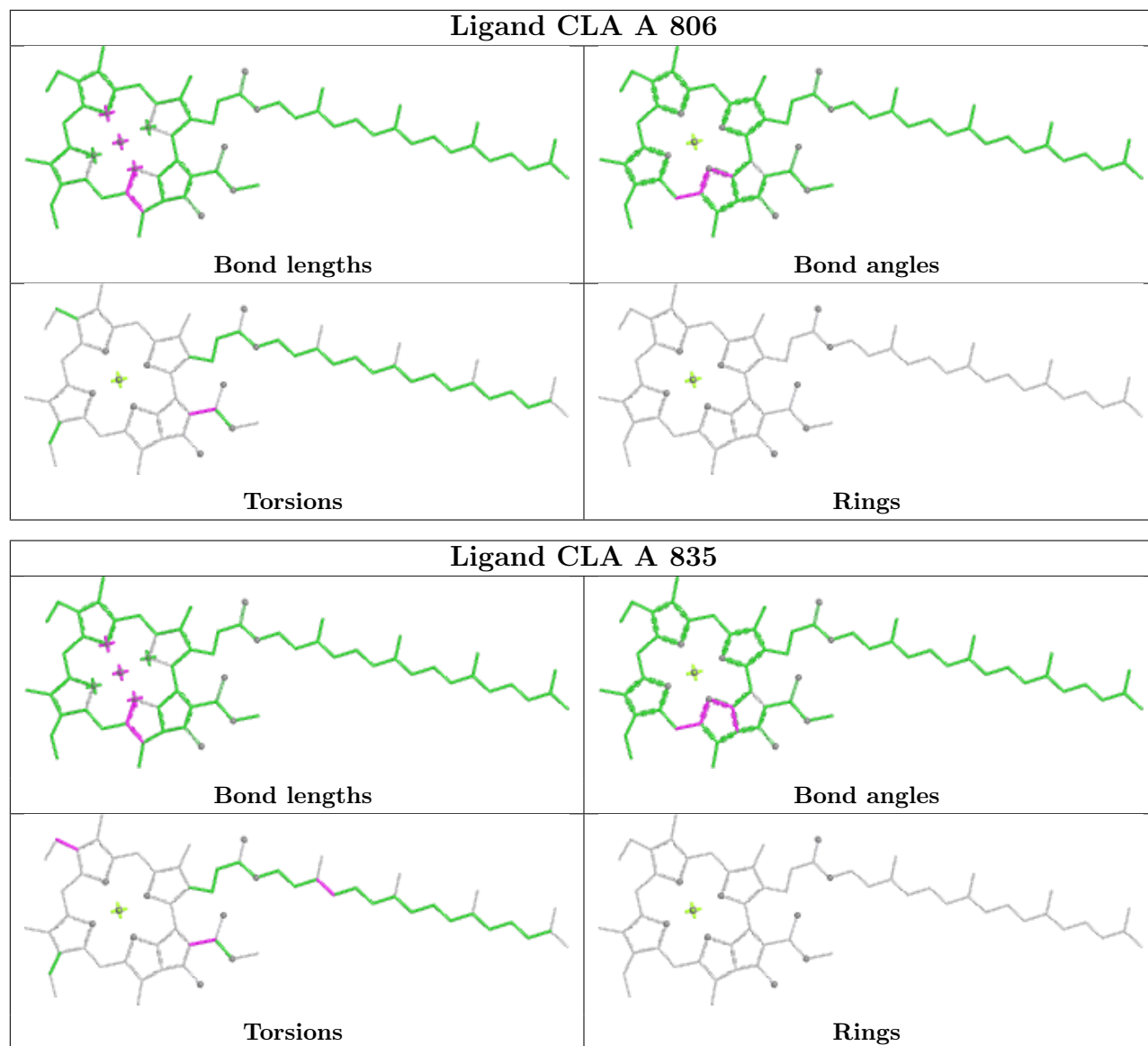


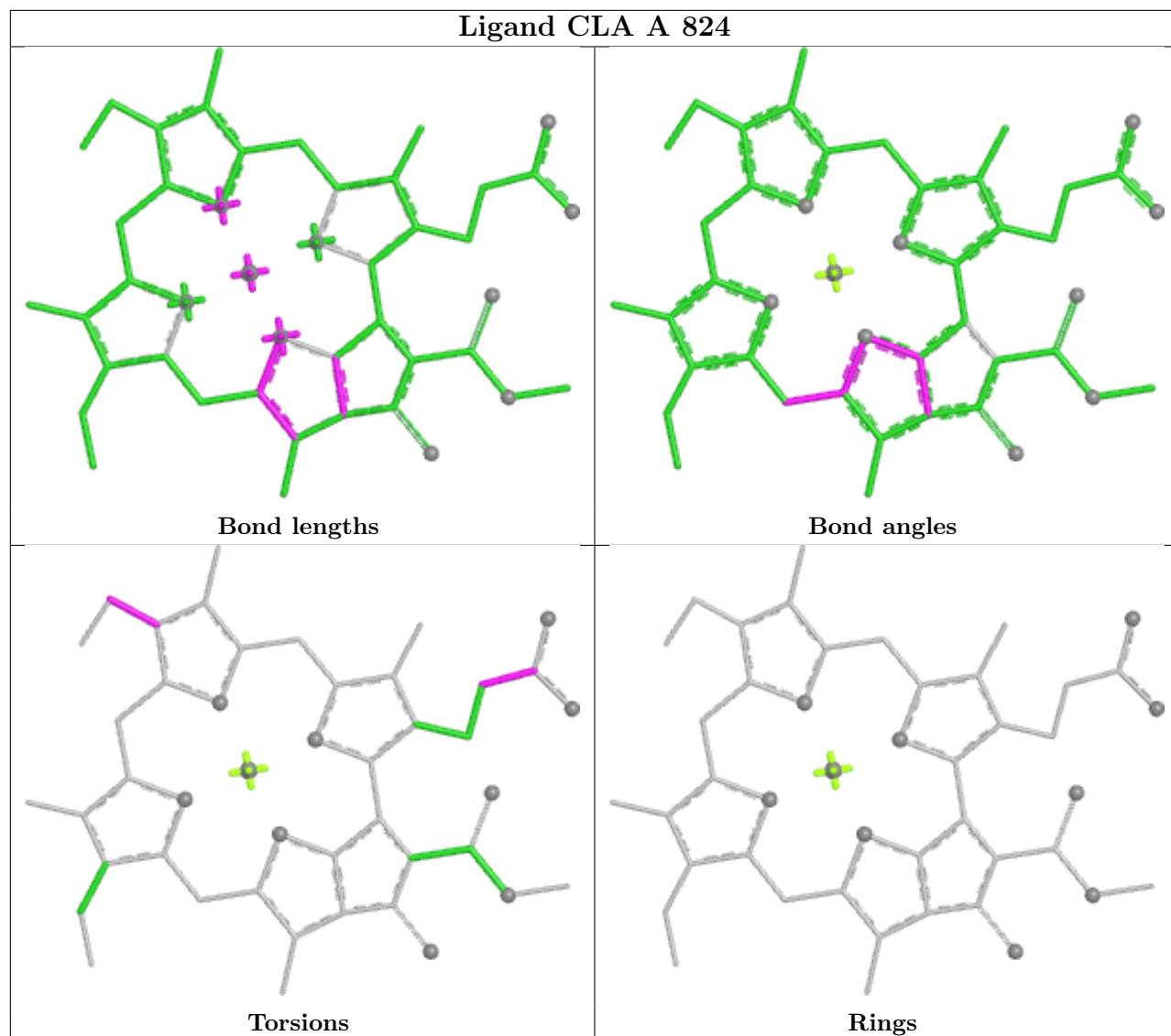


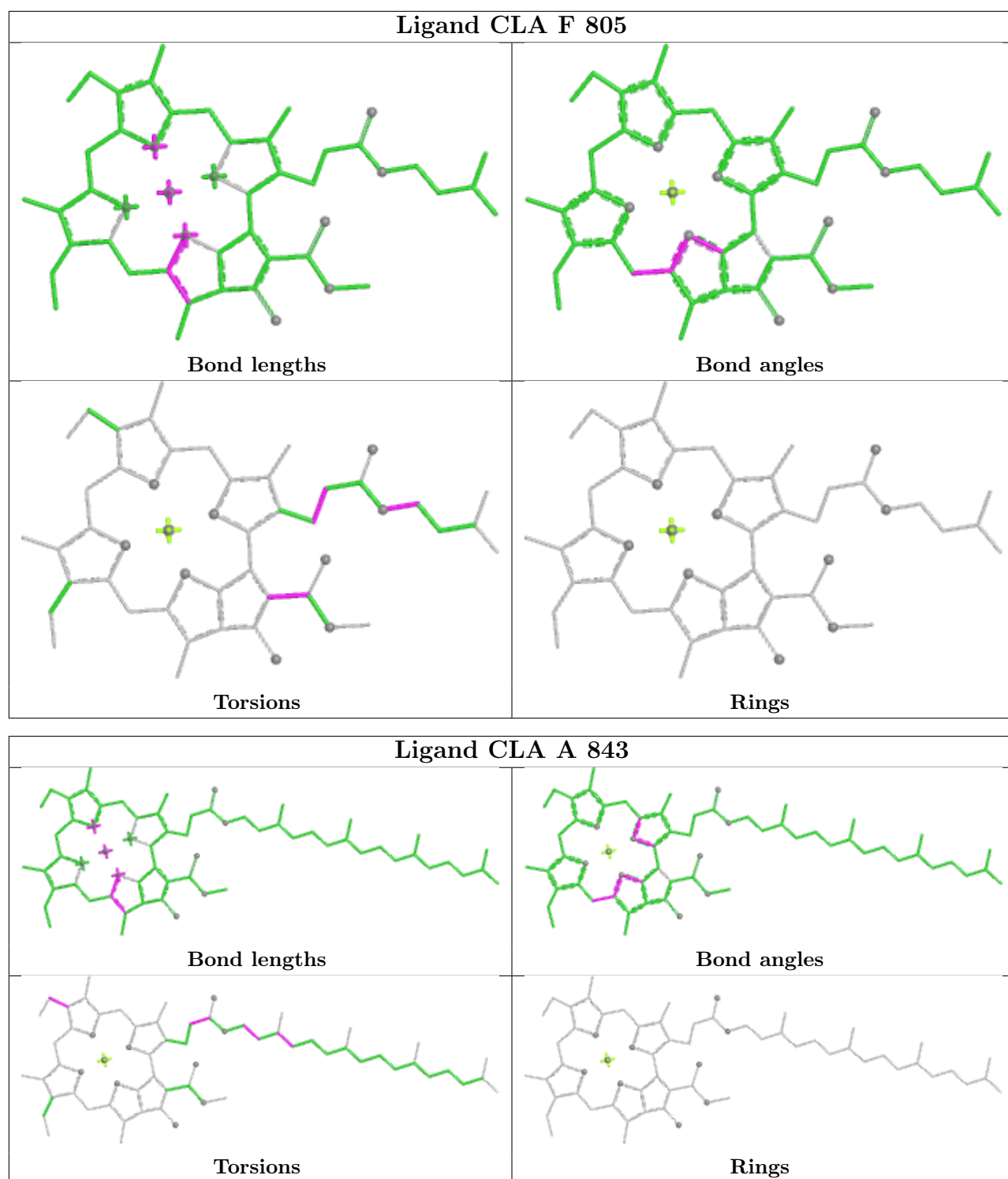


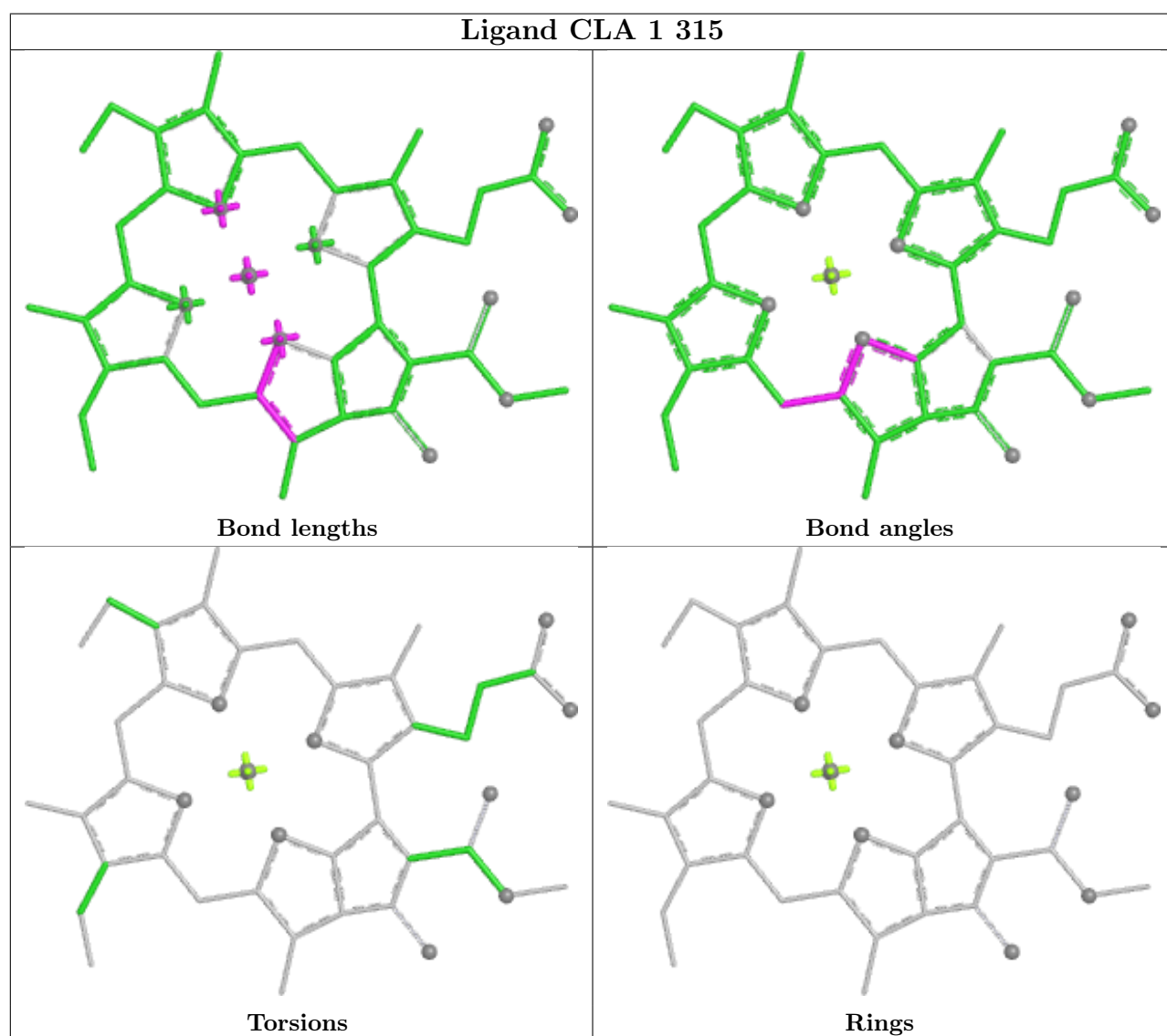
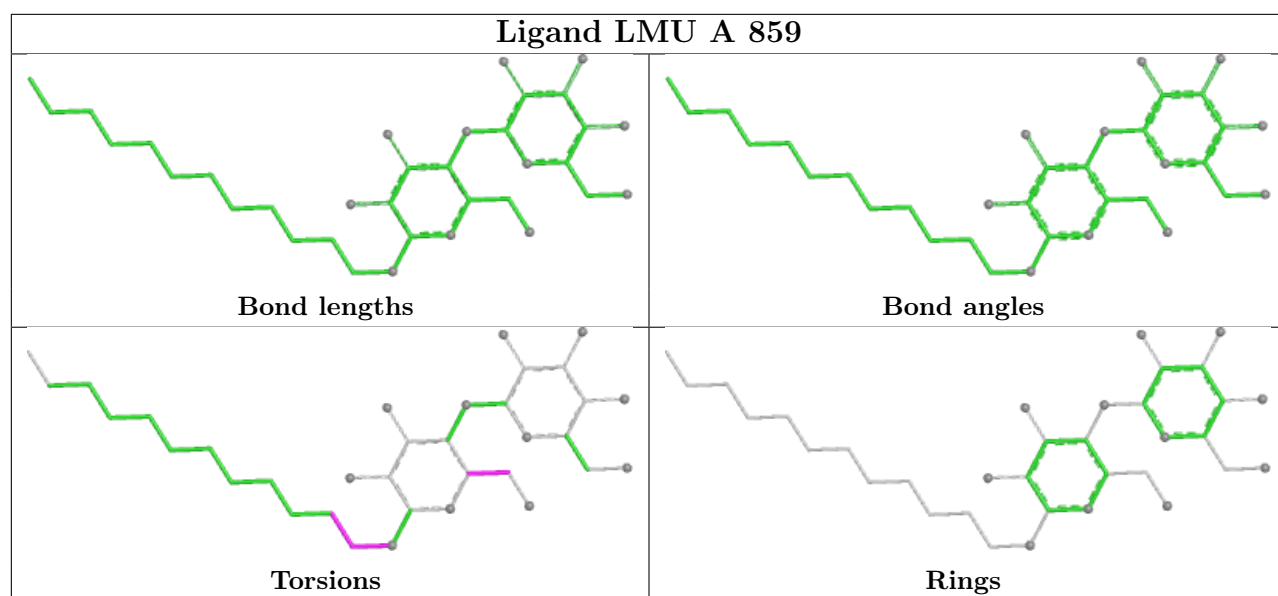


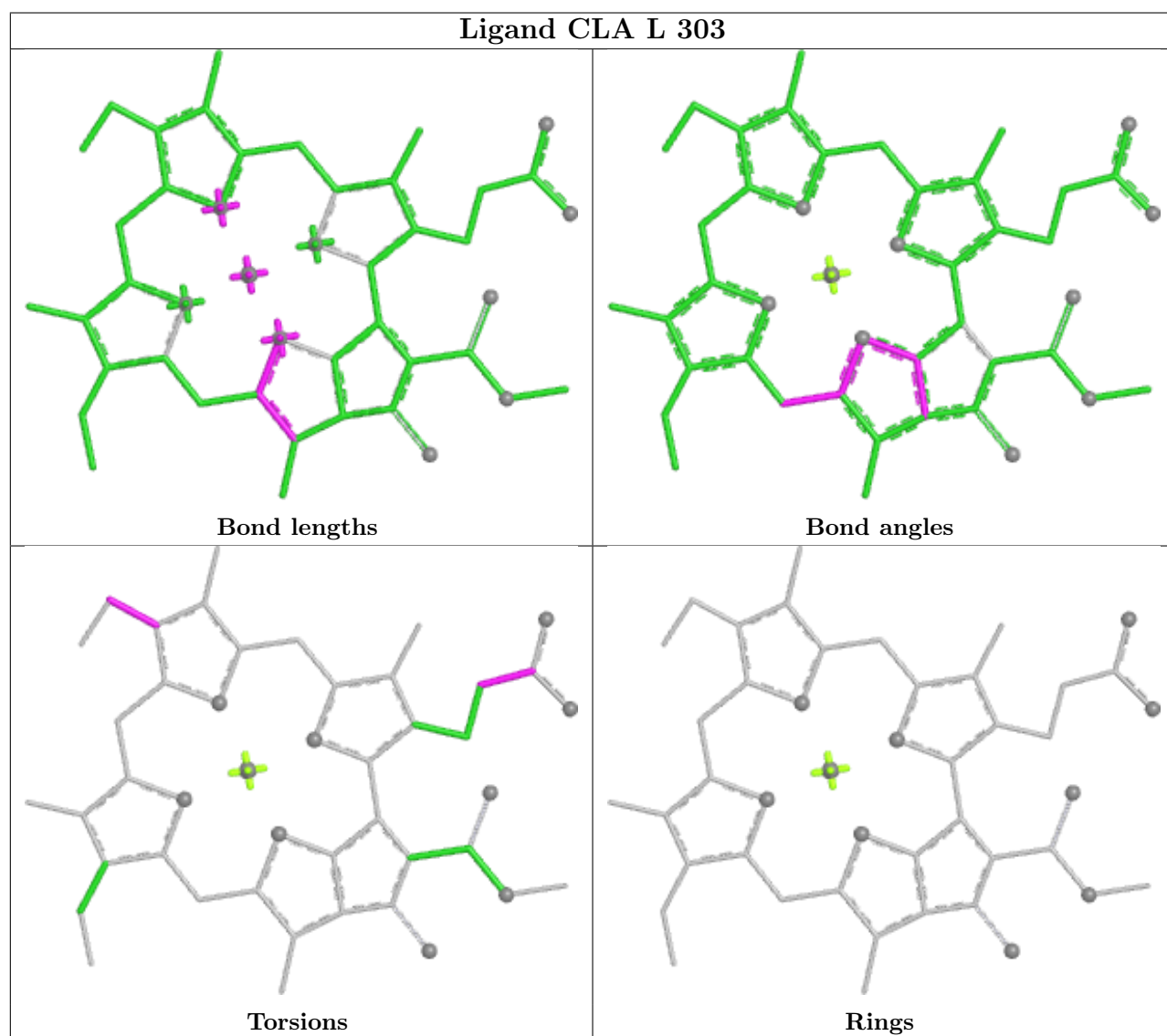
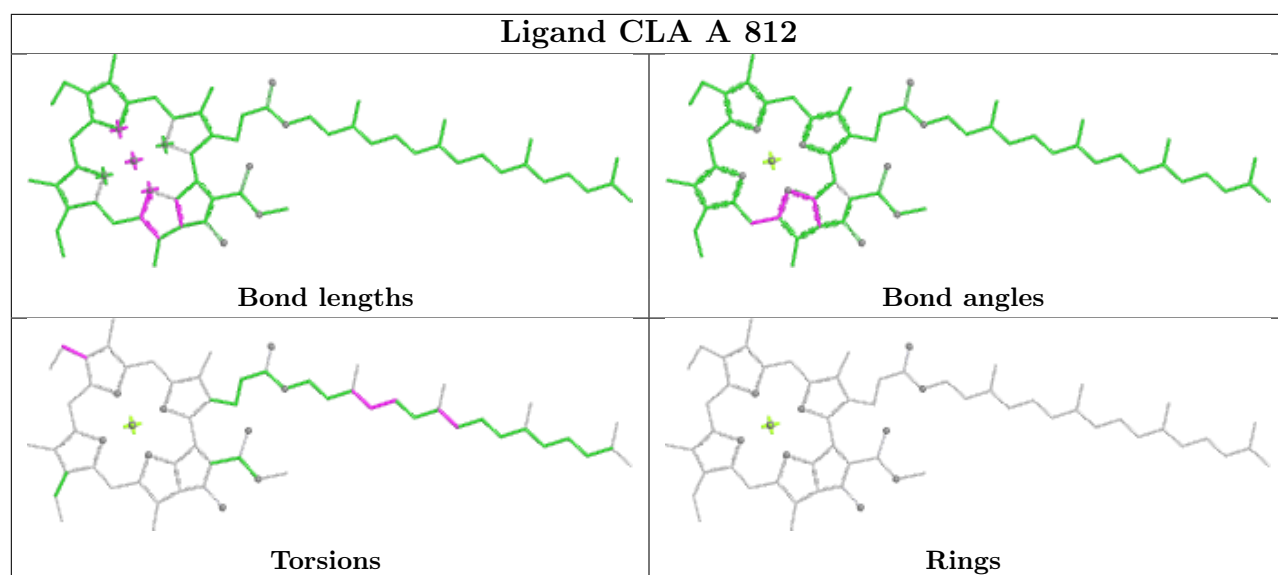


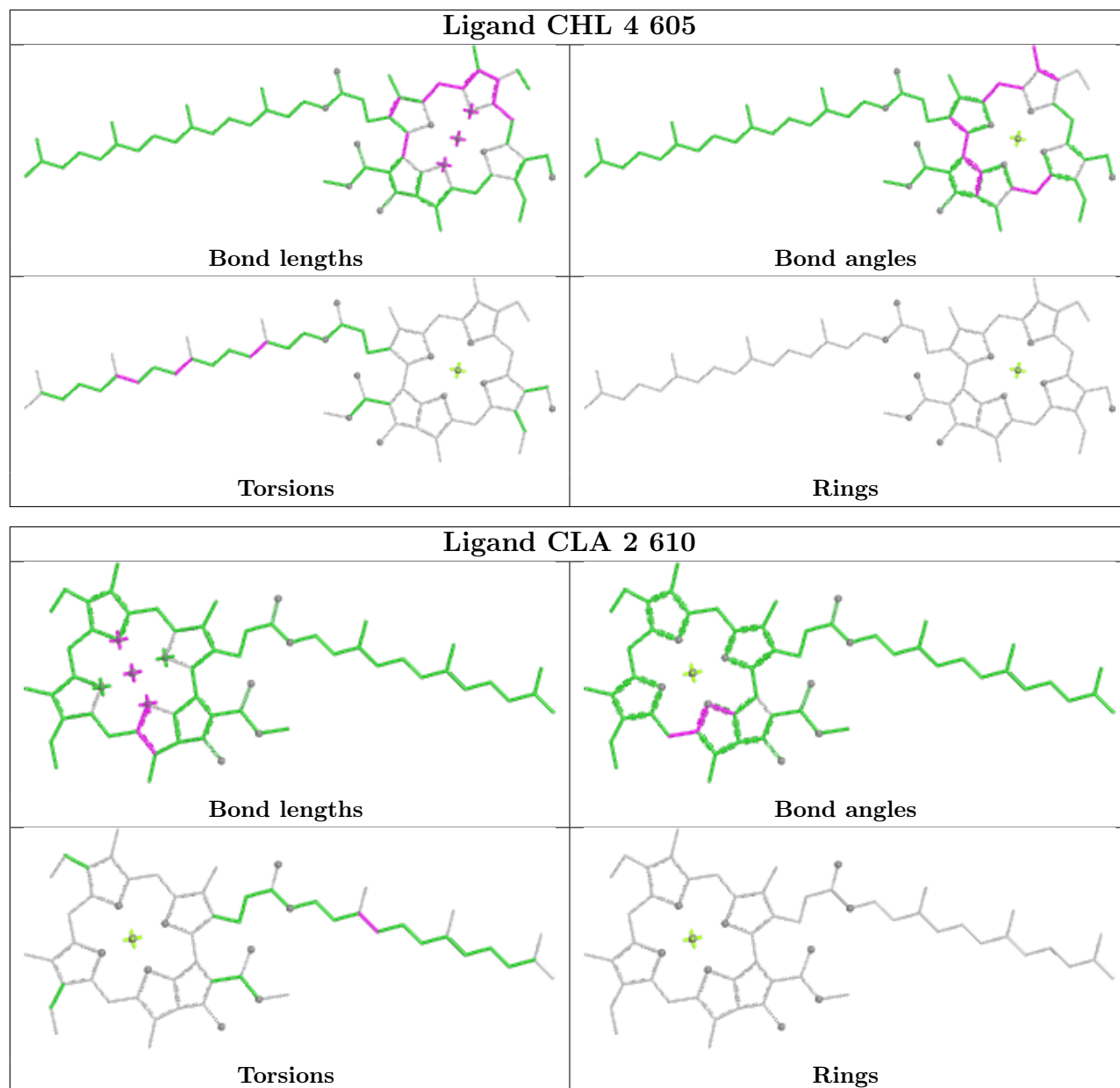


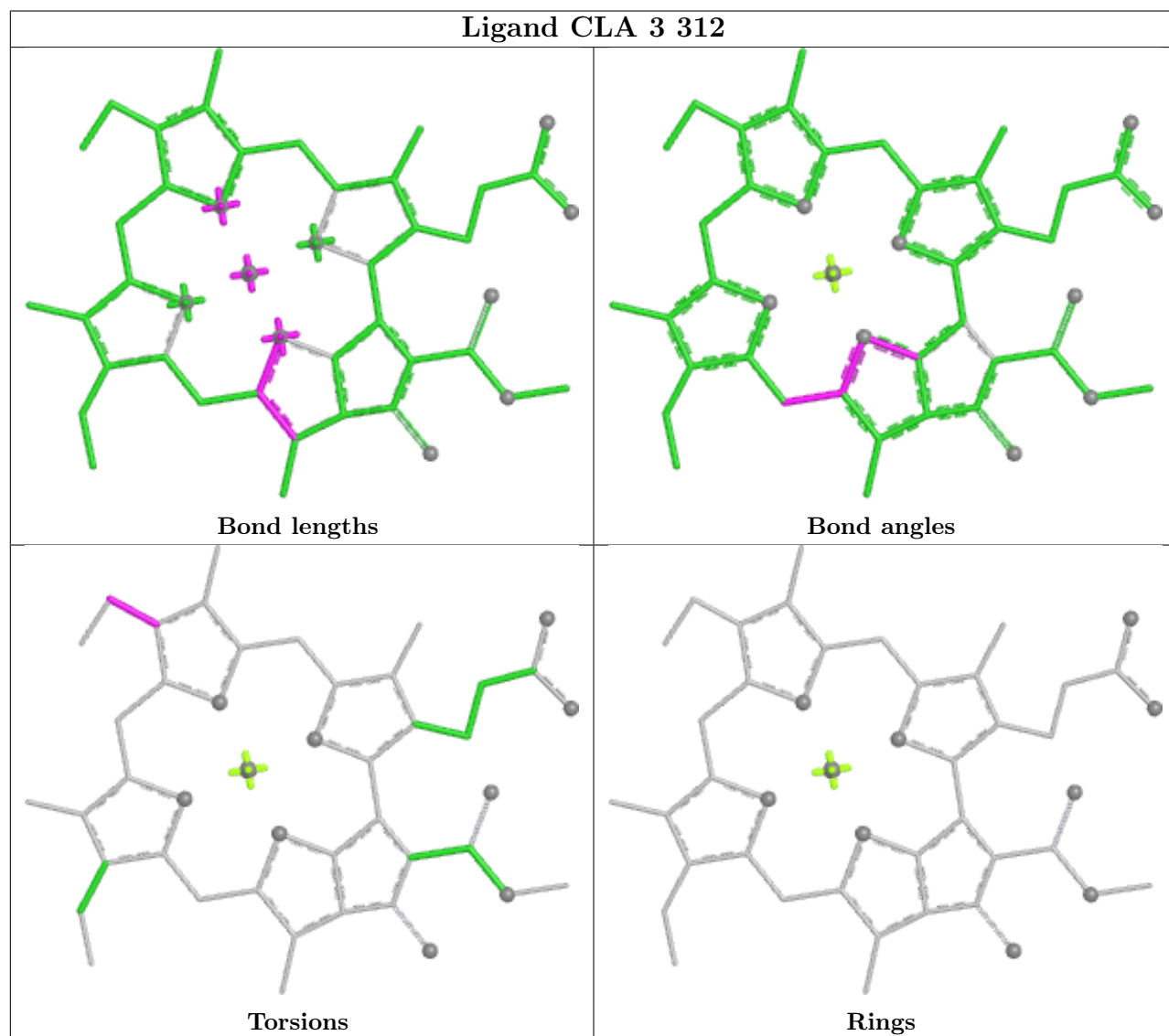
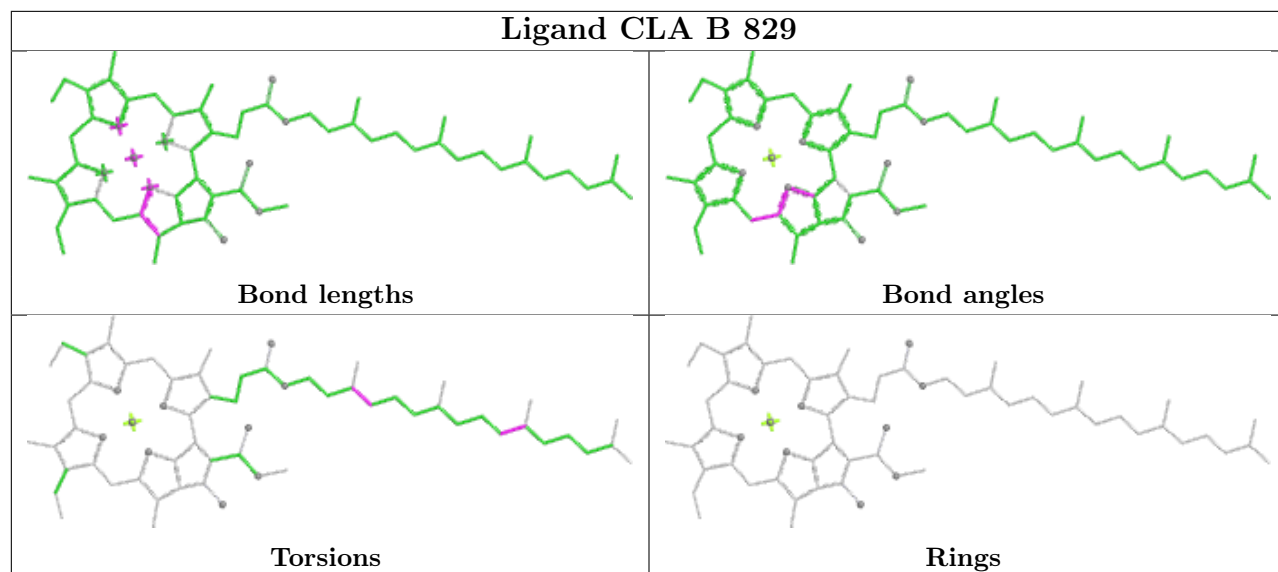


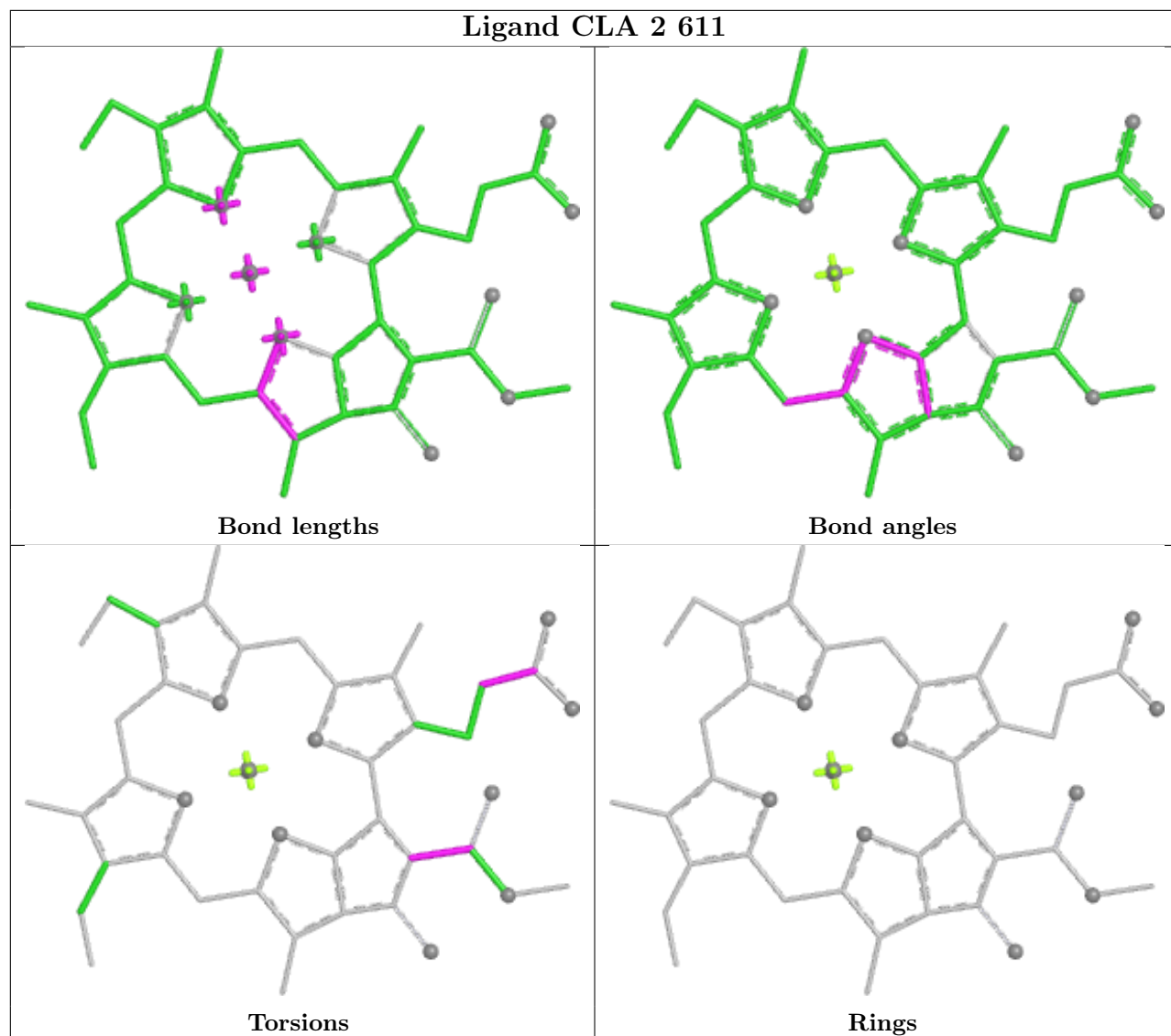


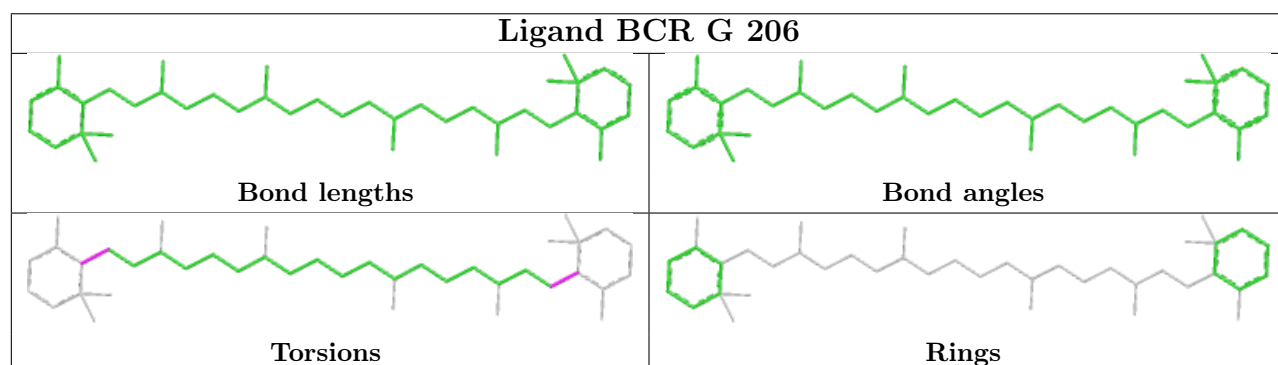
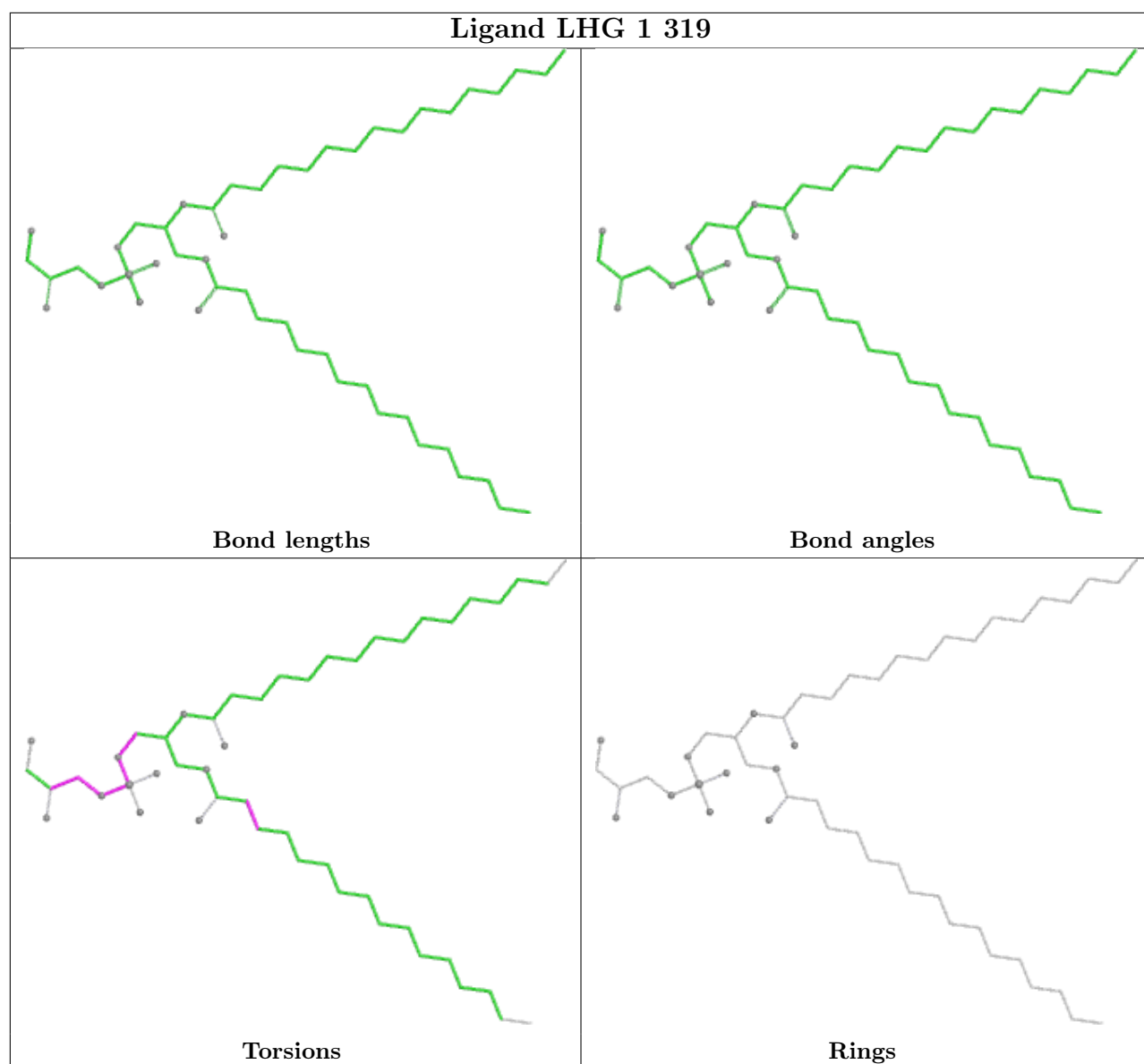


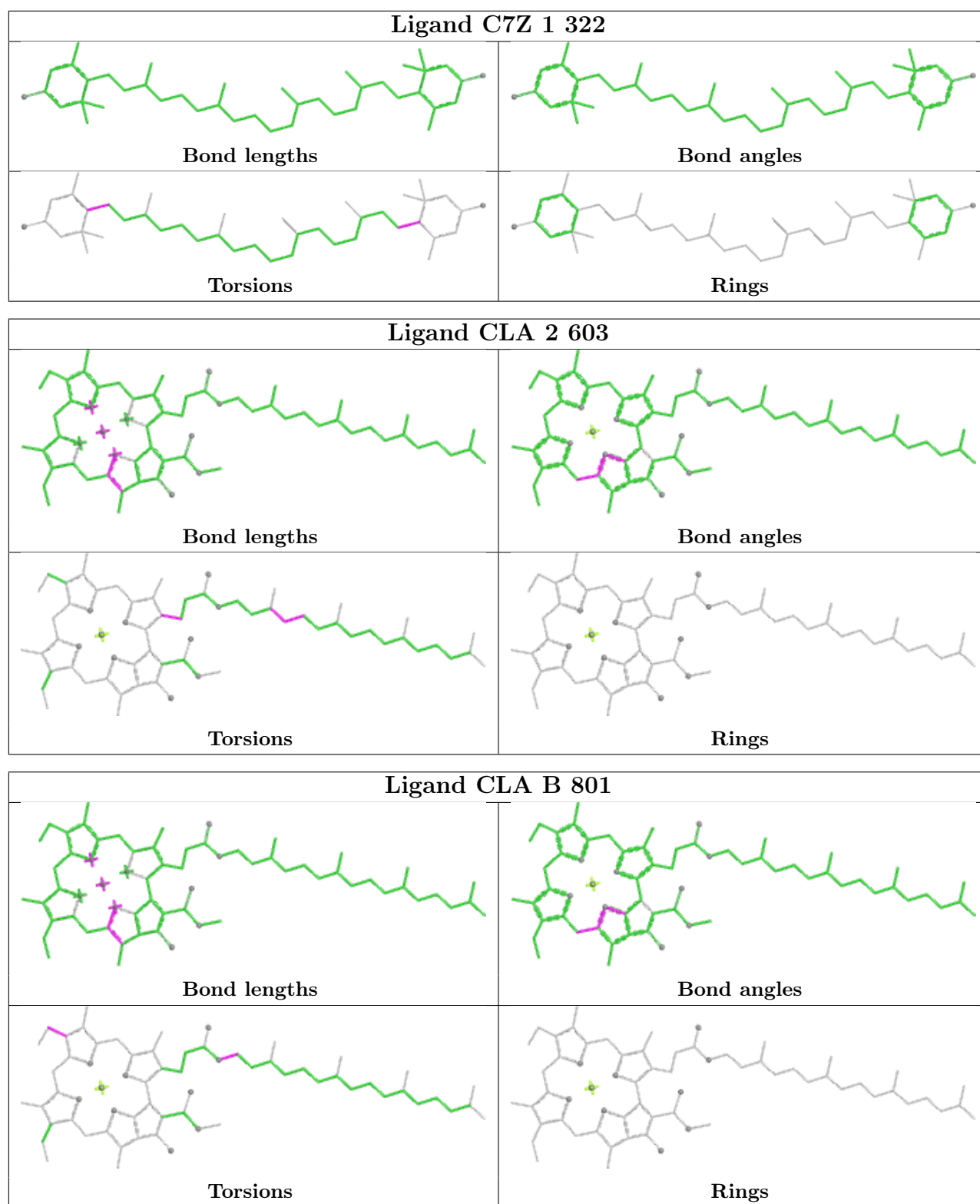


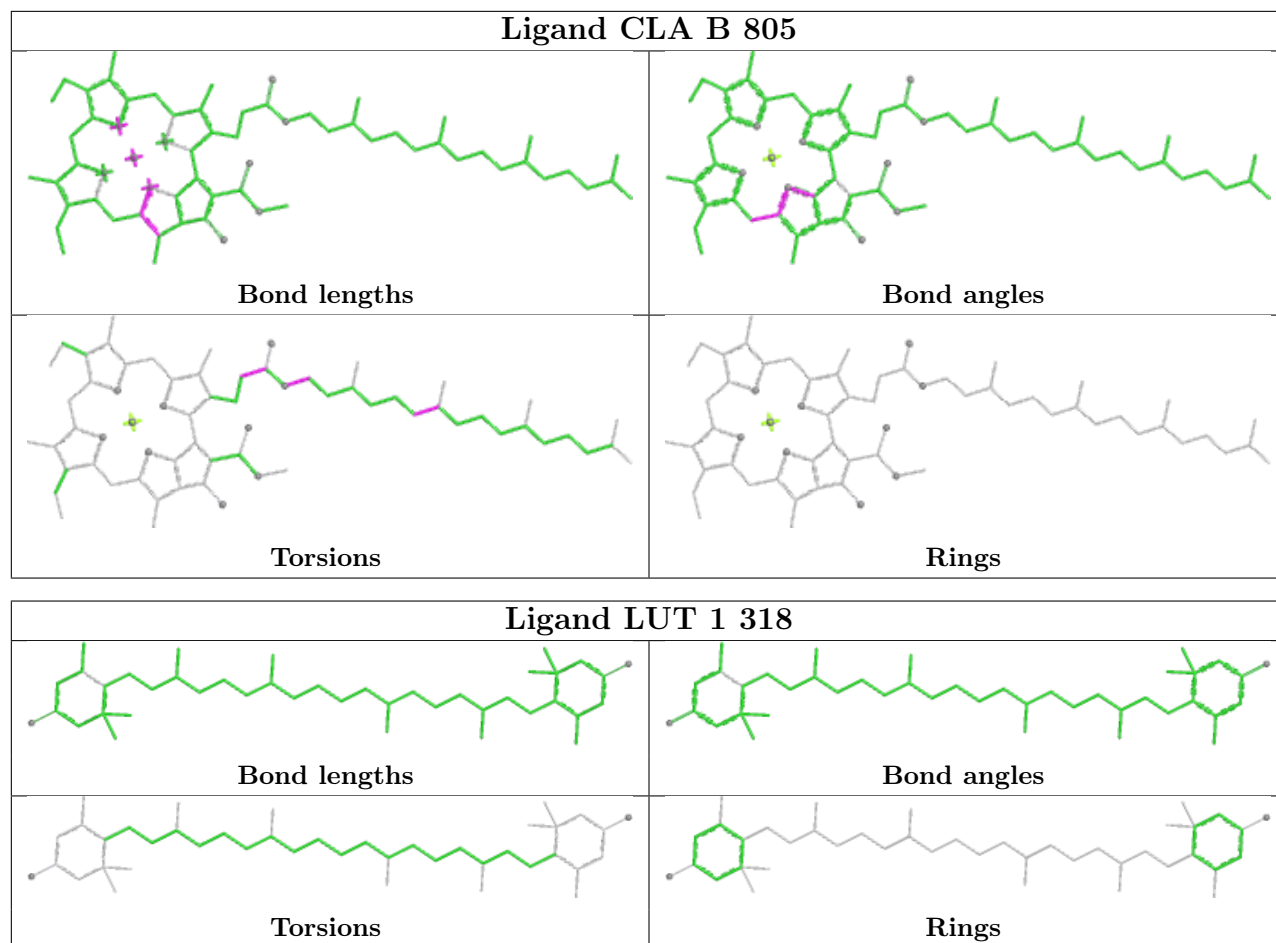


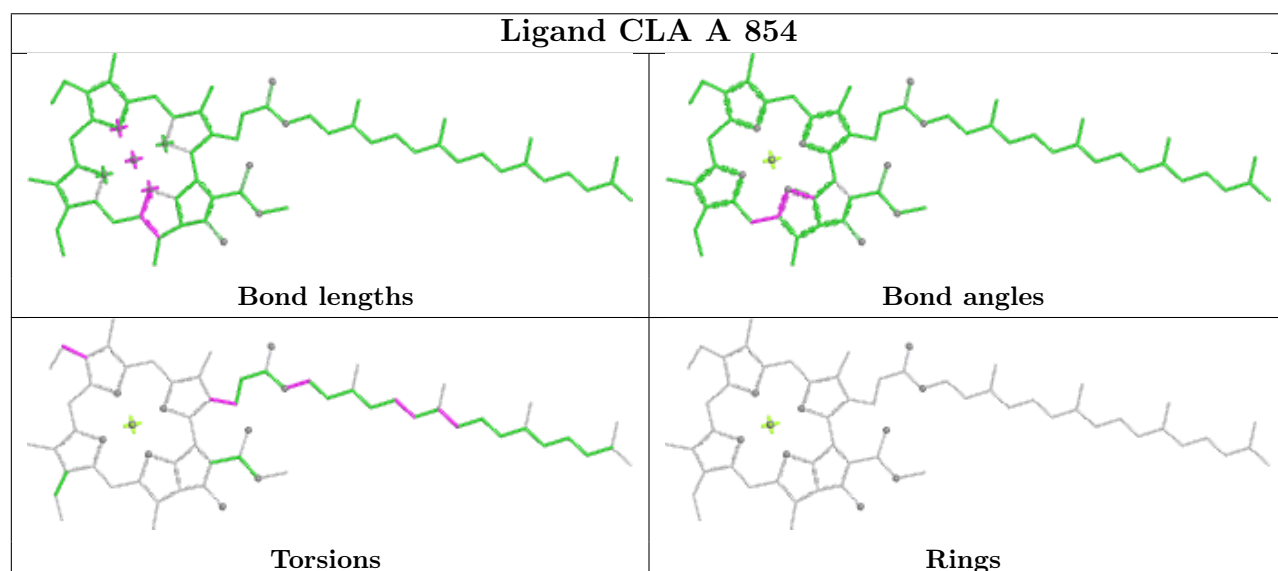
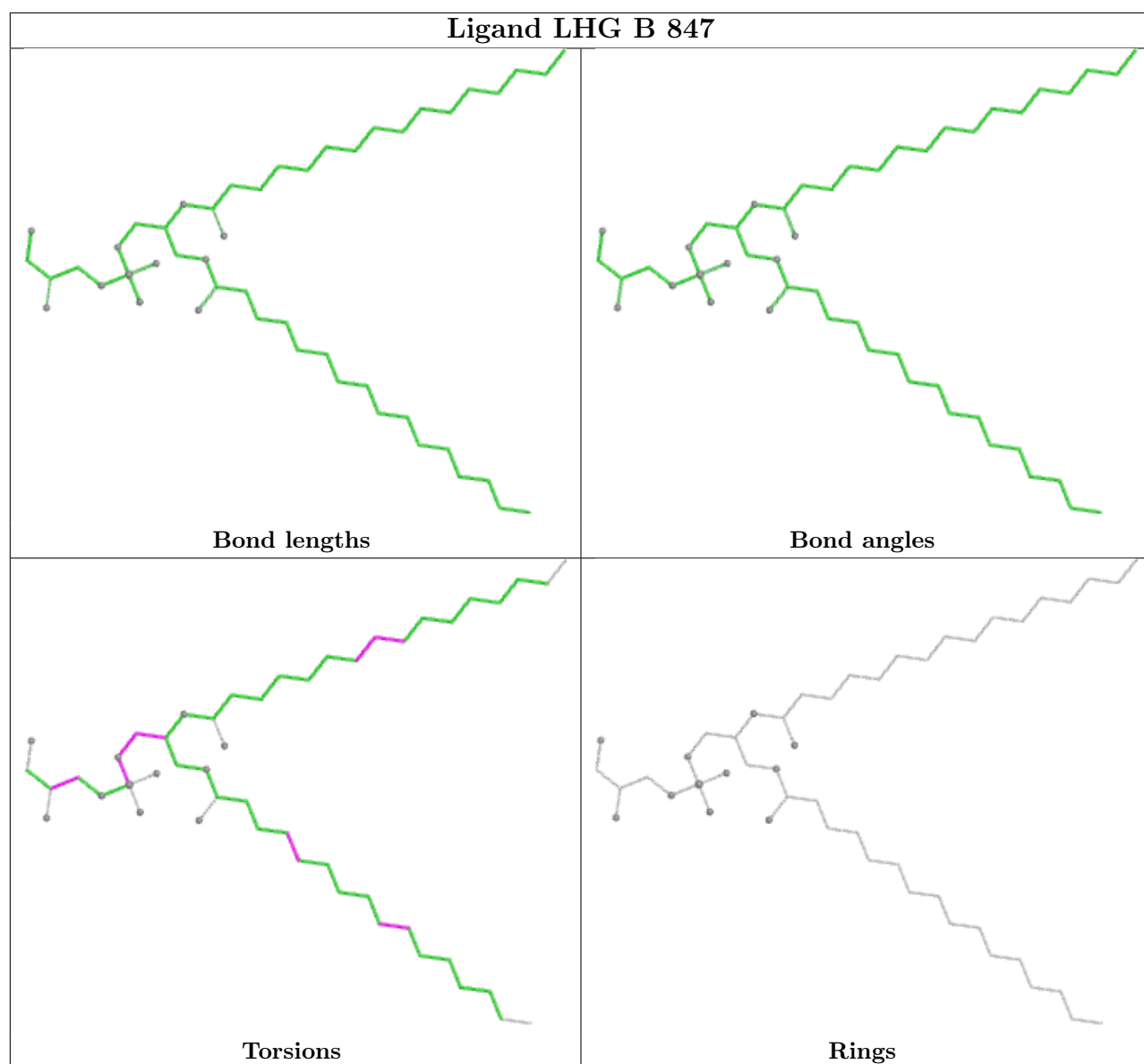


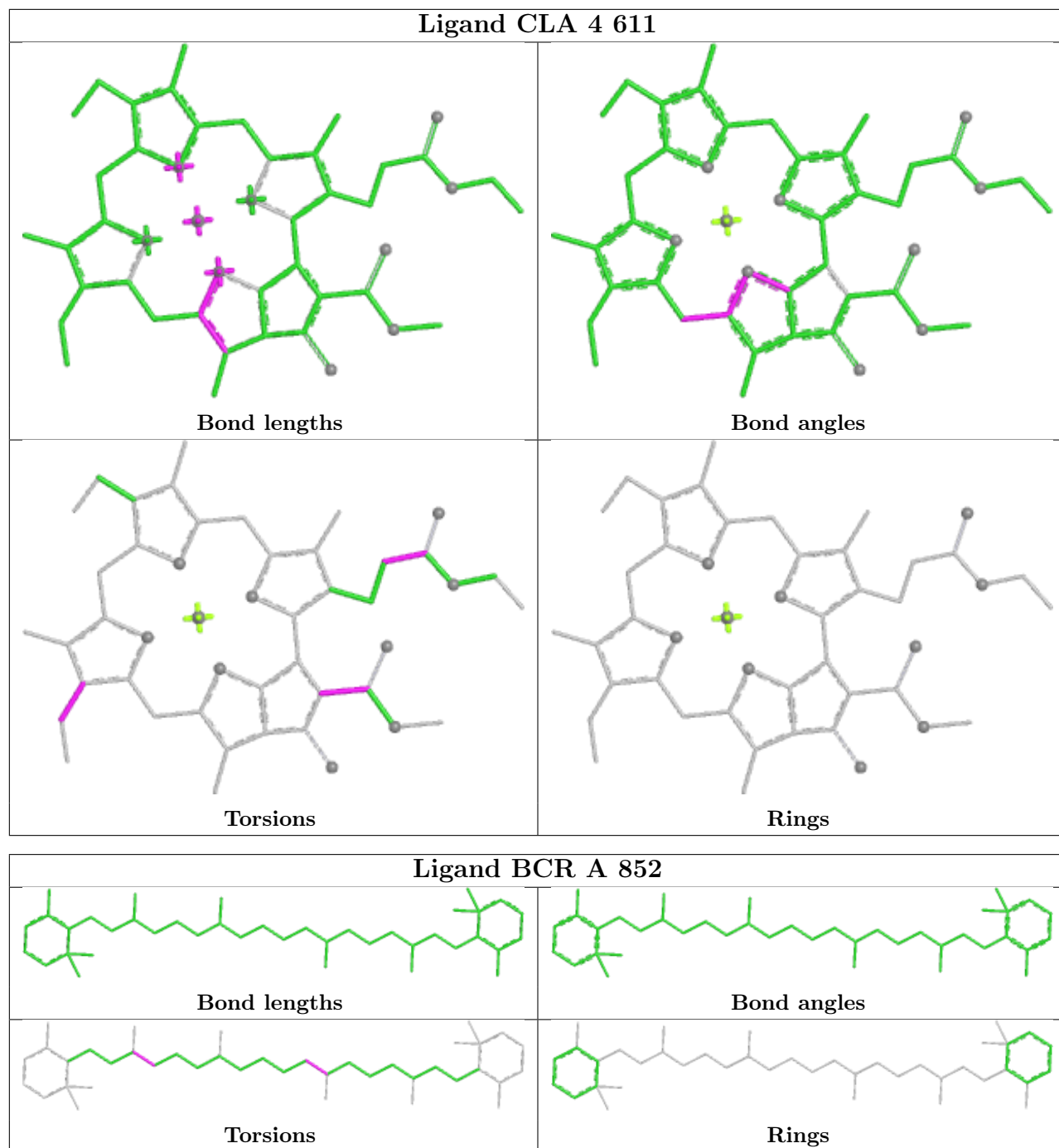


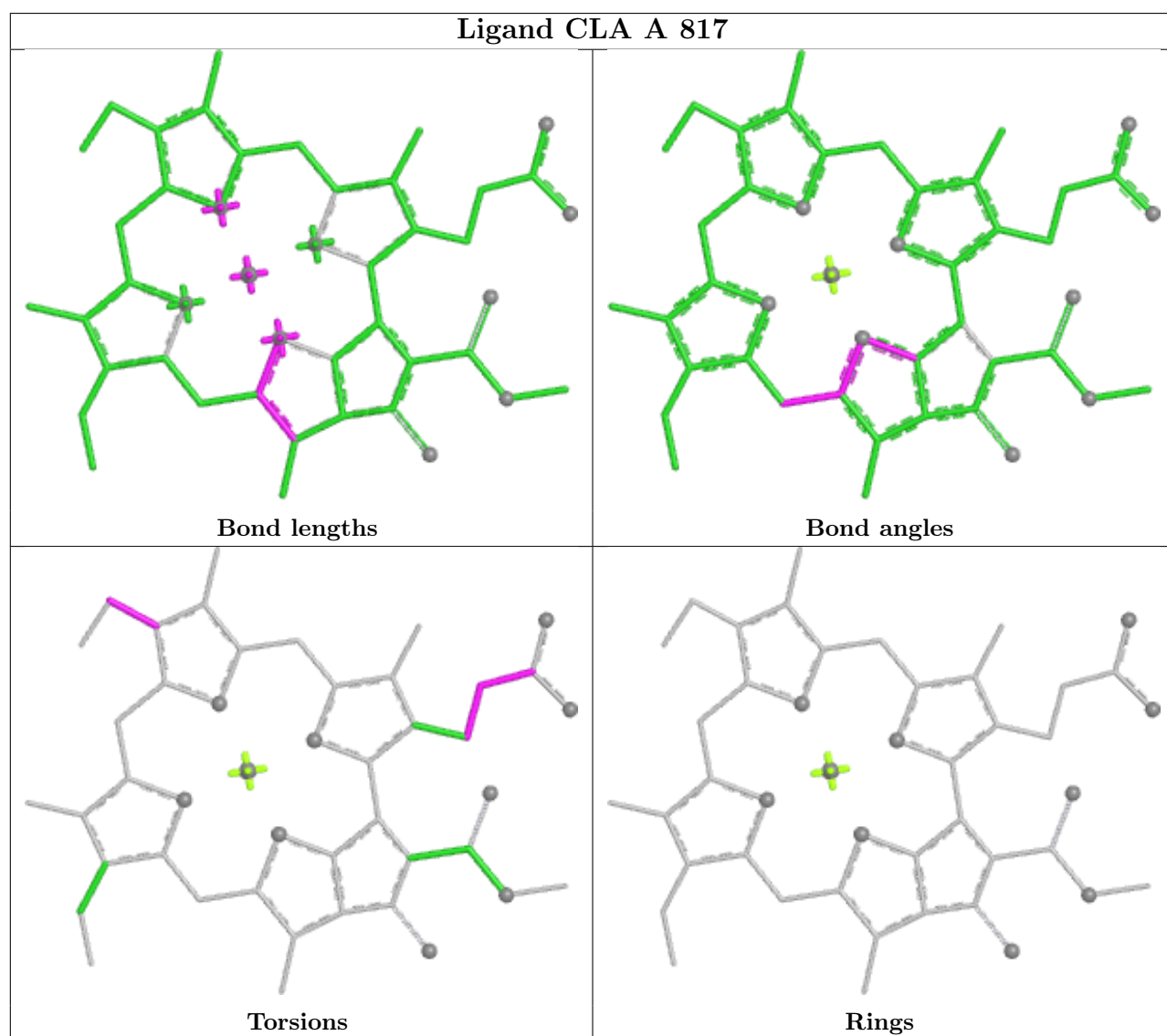
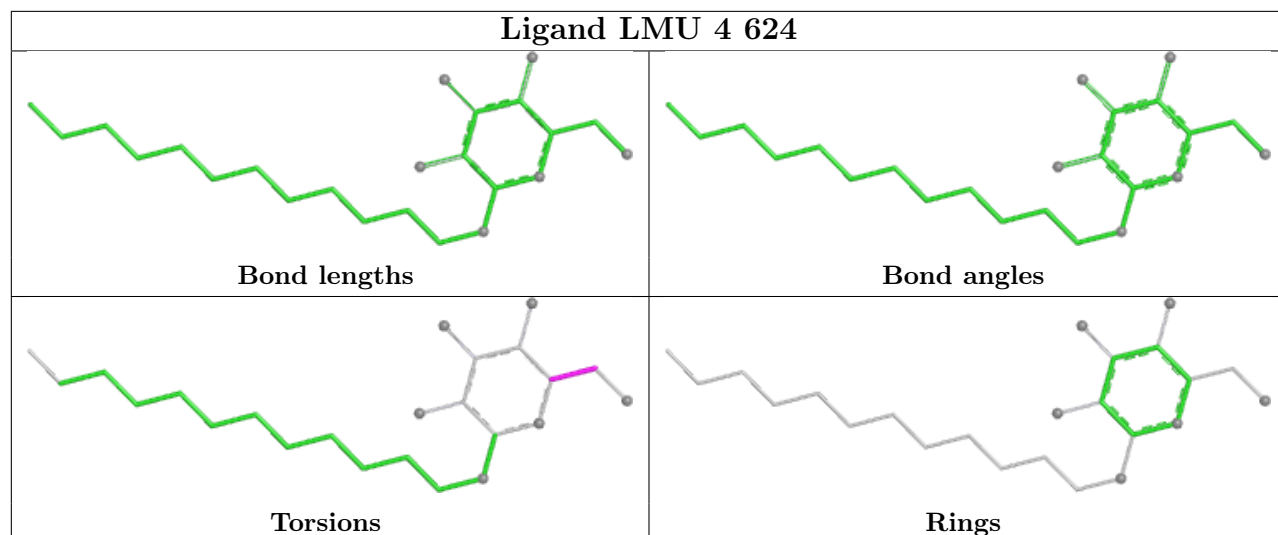


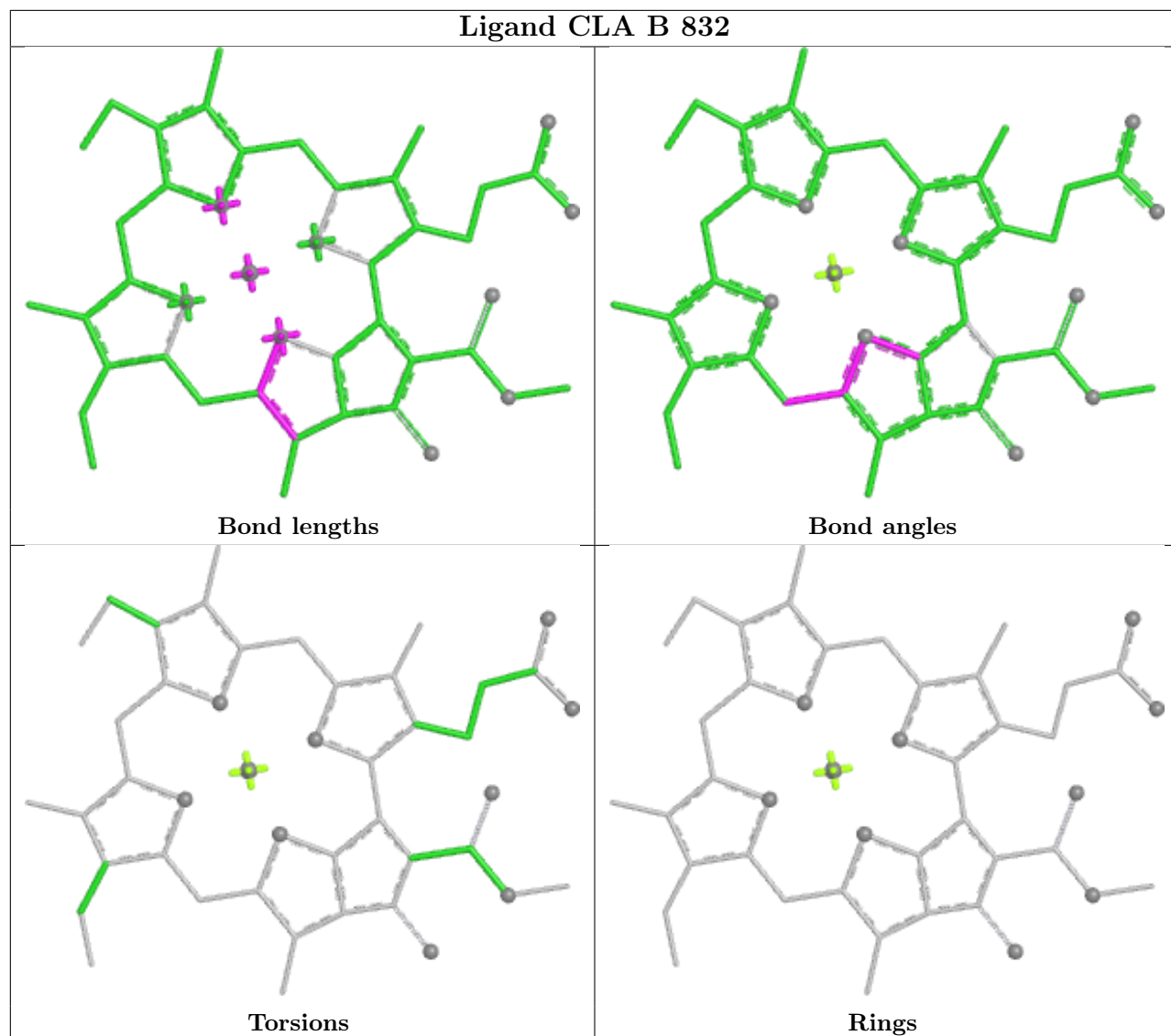


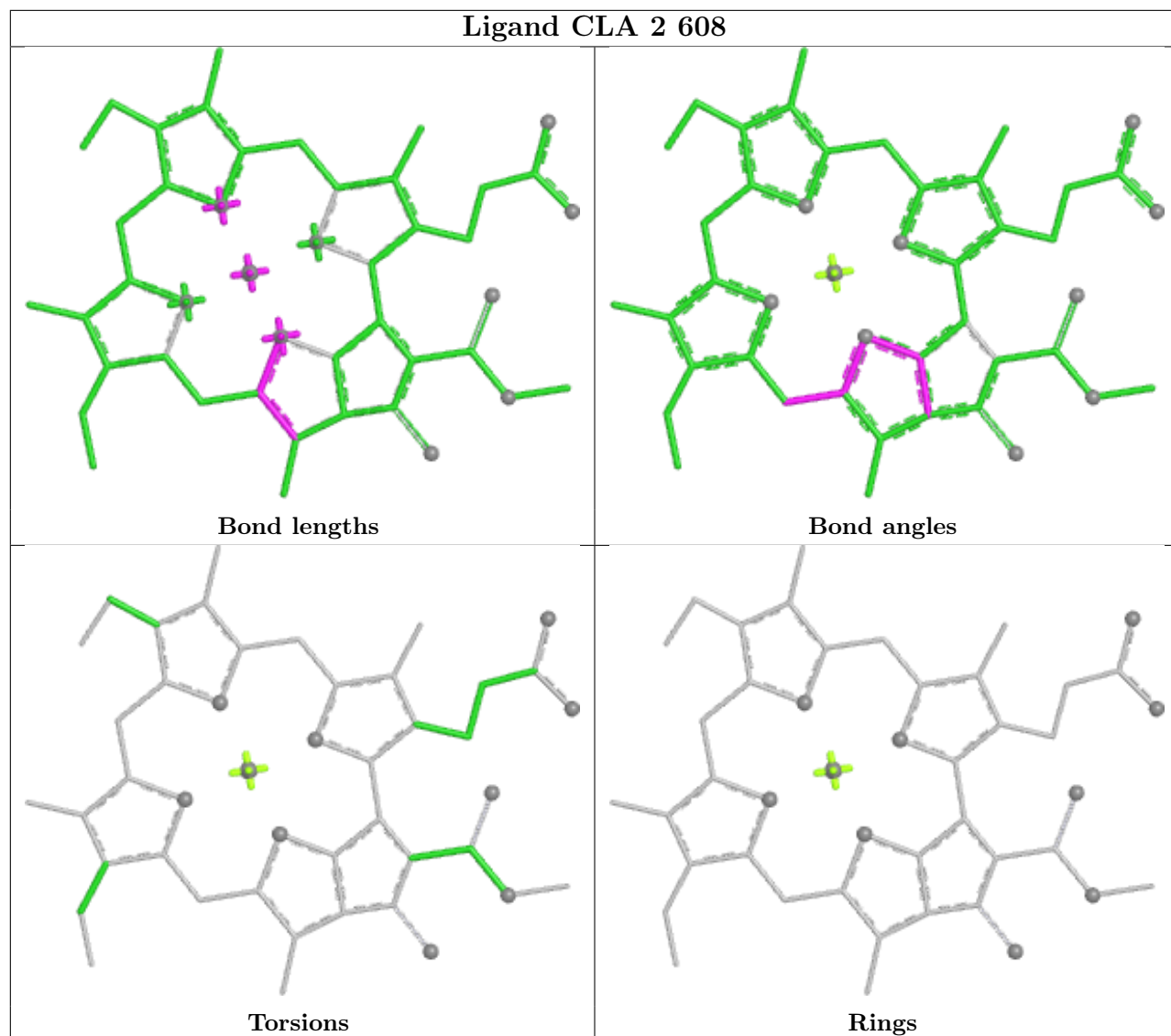


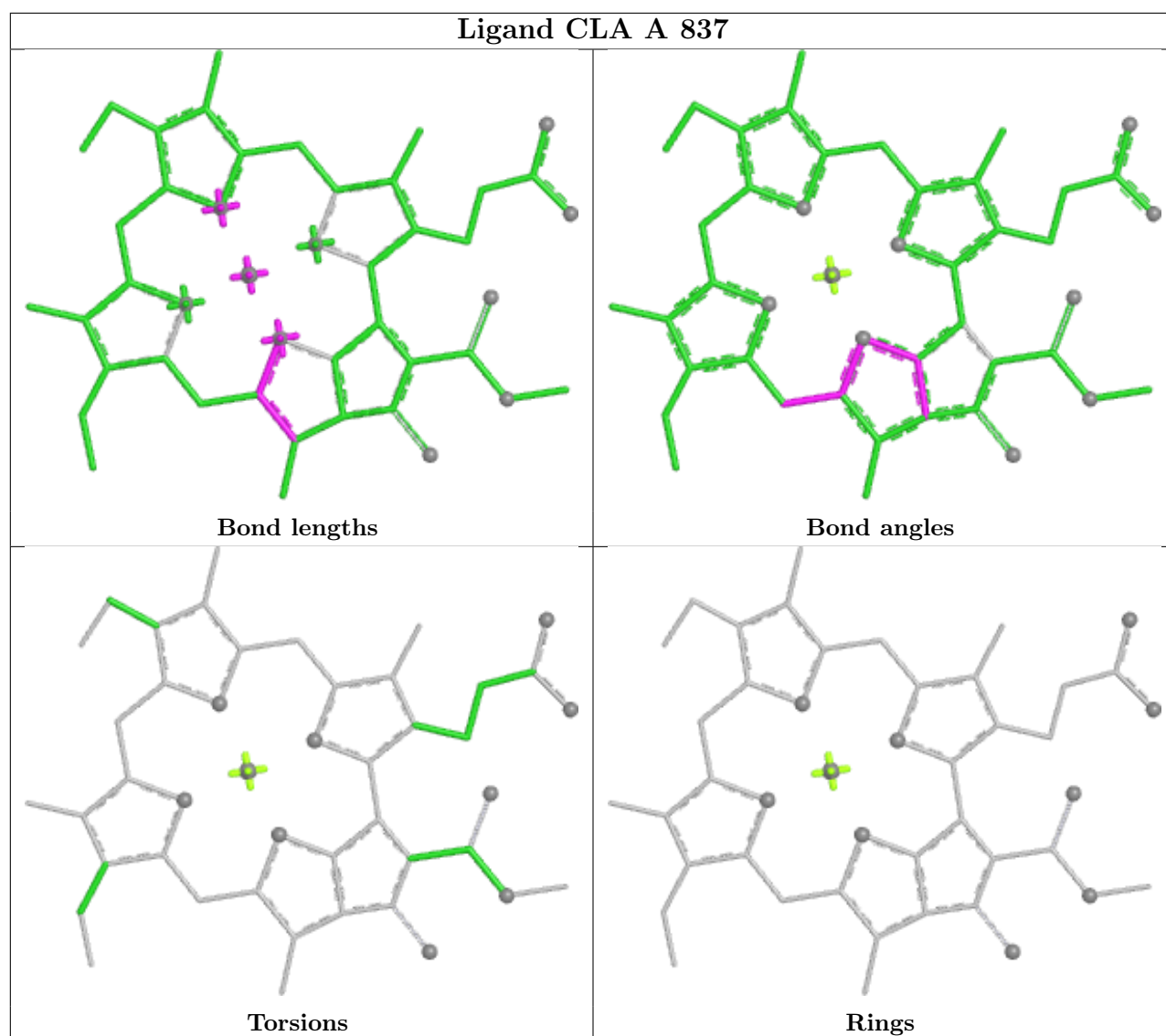












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	L	1
12	K	1
13	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	209:PRO	C	210:TYR	N	3.43
1	K	123:GLY	C	124:VAL	N	3.22
1	1	236:PRO	C	237:ARG	N	3.17

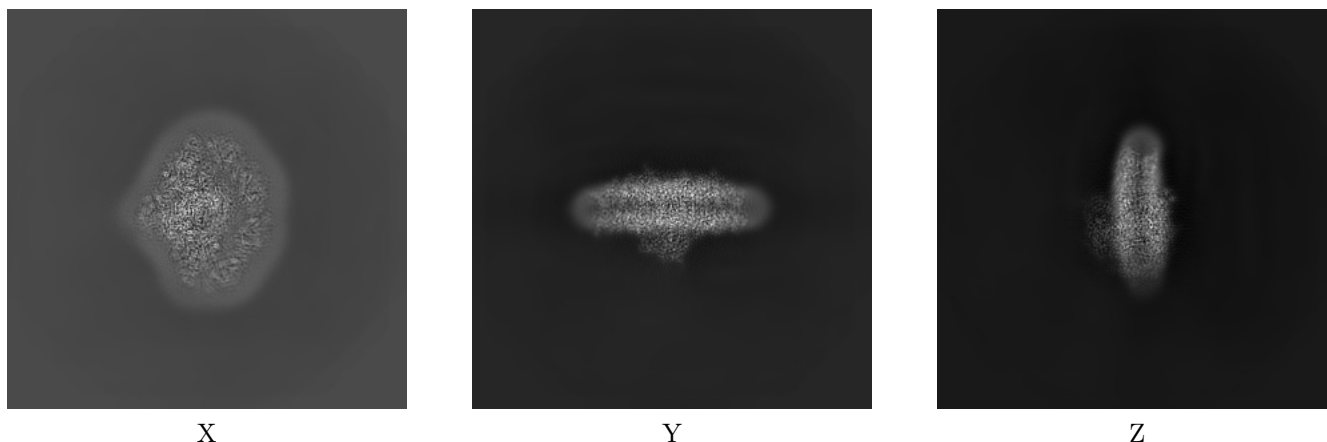
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15969. These allow visual inspection of the internal detail of the map and identification of artifacts.

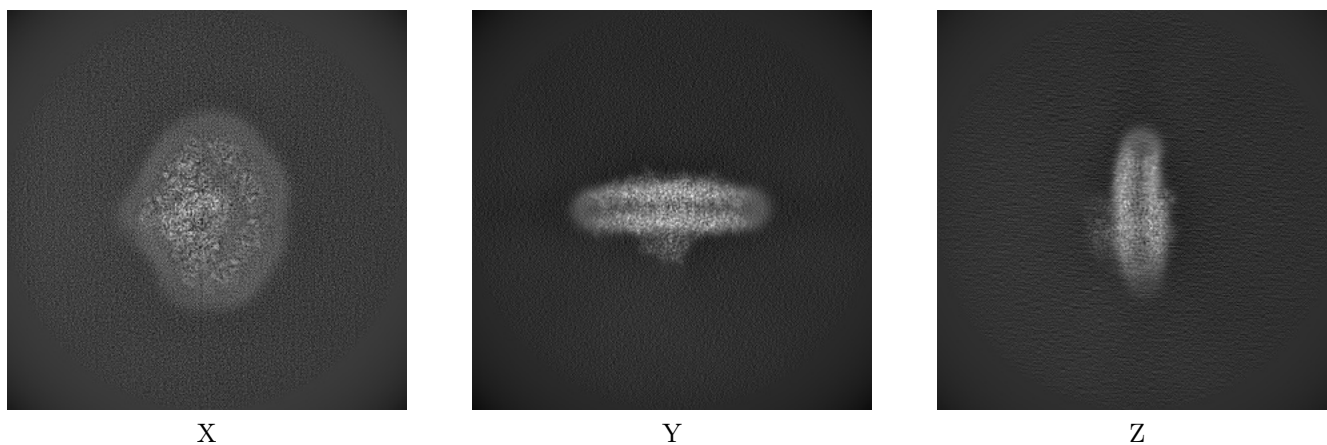
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



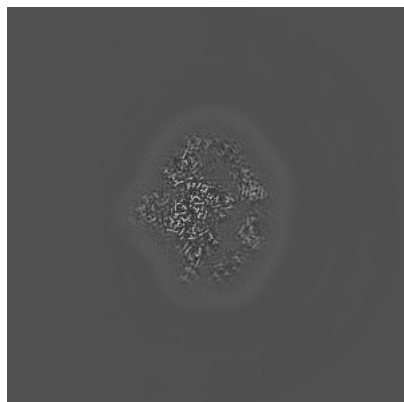
6.1.2 Raw map



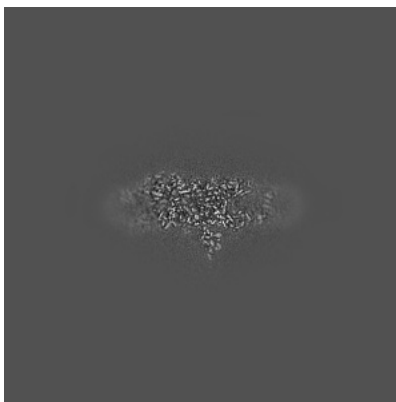
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

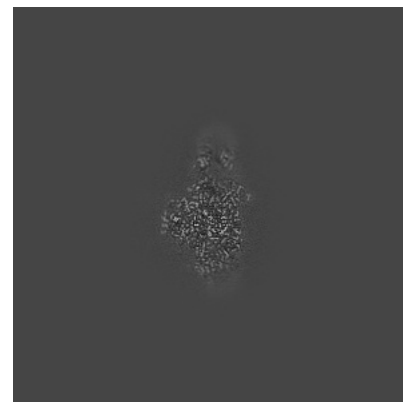
6.2.1 Primary map



X Index: 250

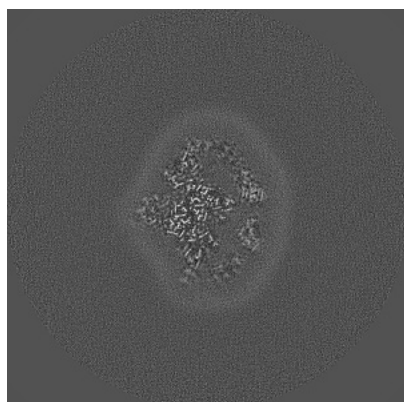


Y Index: 250

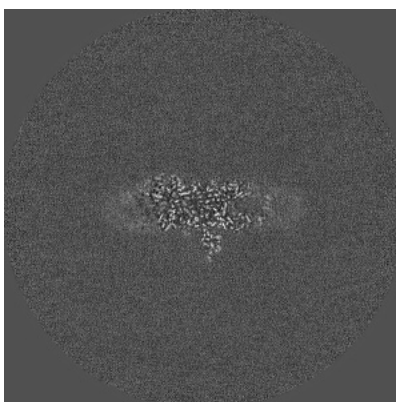


Z Index: 250

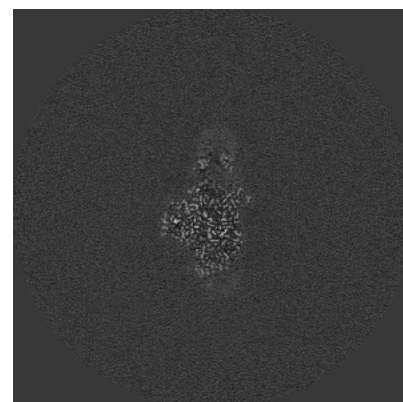
6.2.2 Raw map



X Index: 250



Y Index: 250

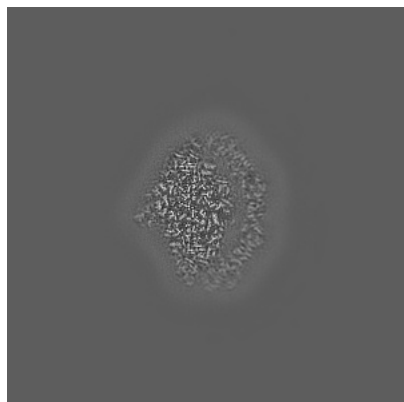


Z Index: 250

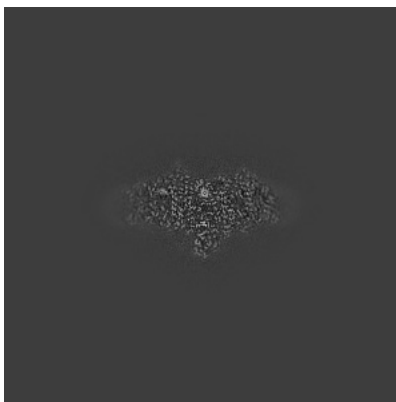
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

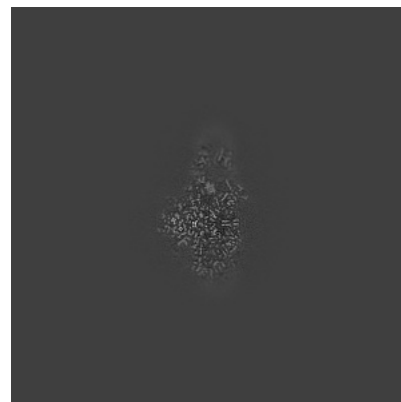
6.3.1 Primary map



X Index: 267

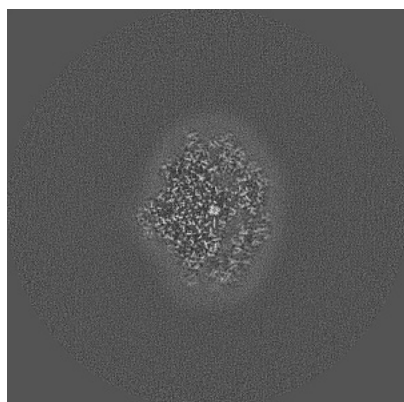


Y Index: 227

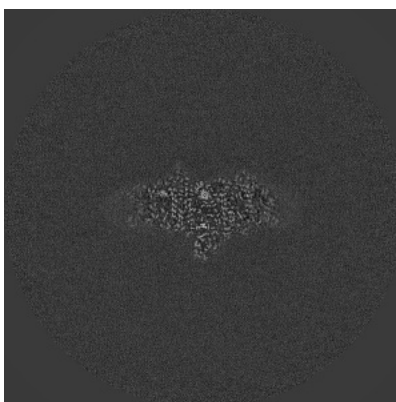


Z Index: 248

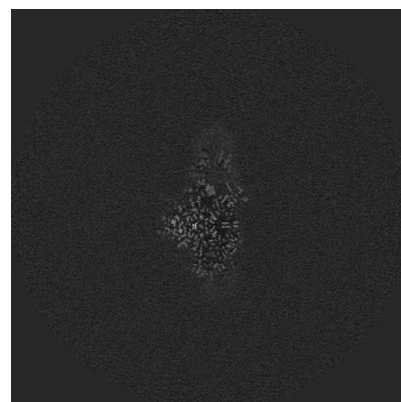
6.3.2 Raw map



X Index: 235



Y Index: 227

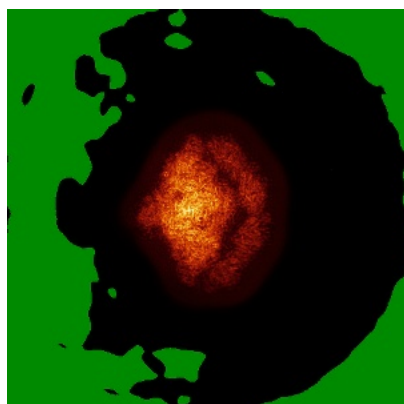


Z Index: 248

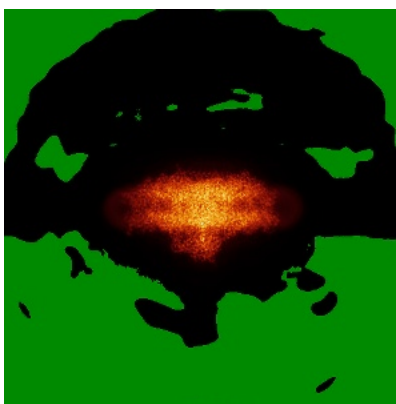
The images above show the largest variance slices of the map in three orthogonal directions.

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

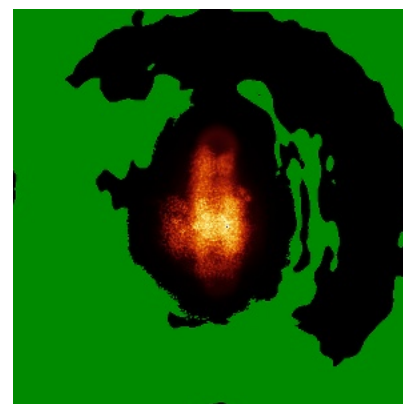
6.4.1 Primary map



X

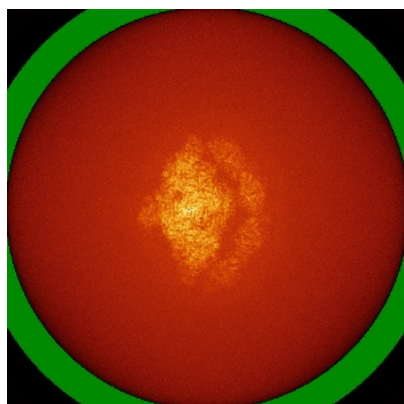


Y

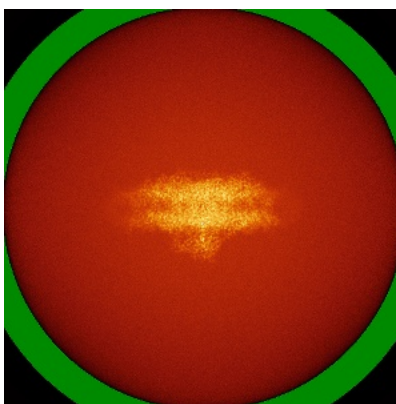


Z

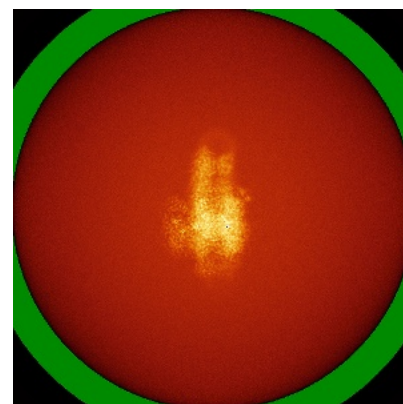
6.4.2 Raw map



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](#)

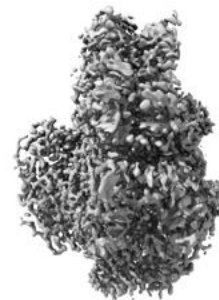
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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



X



Y



Z

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.

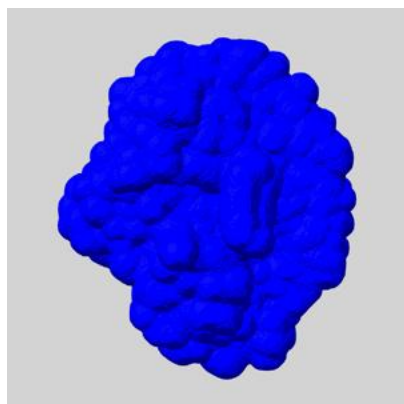
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

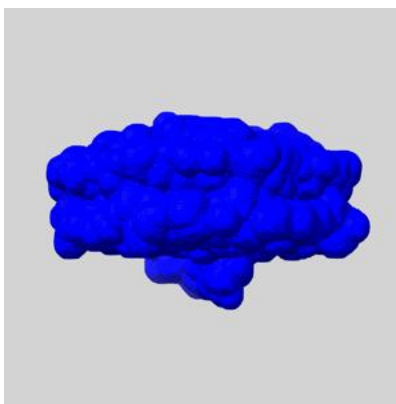
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

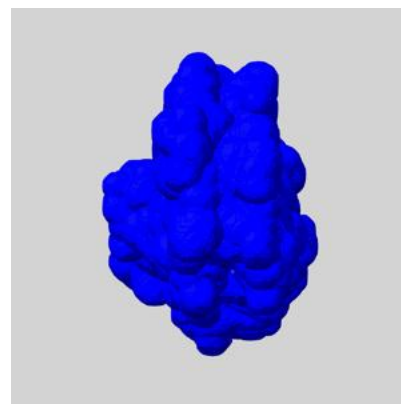
6.6.1 emd_15969_msk_1.map [i](#)



X



Y

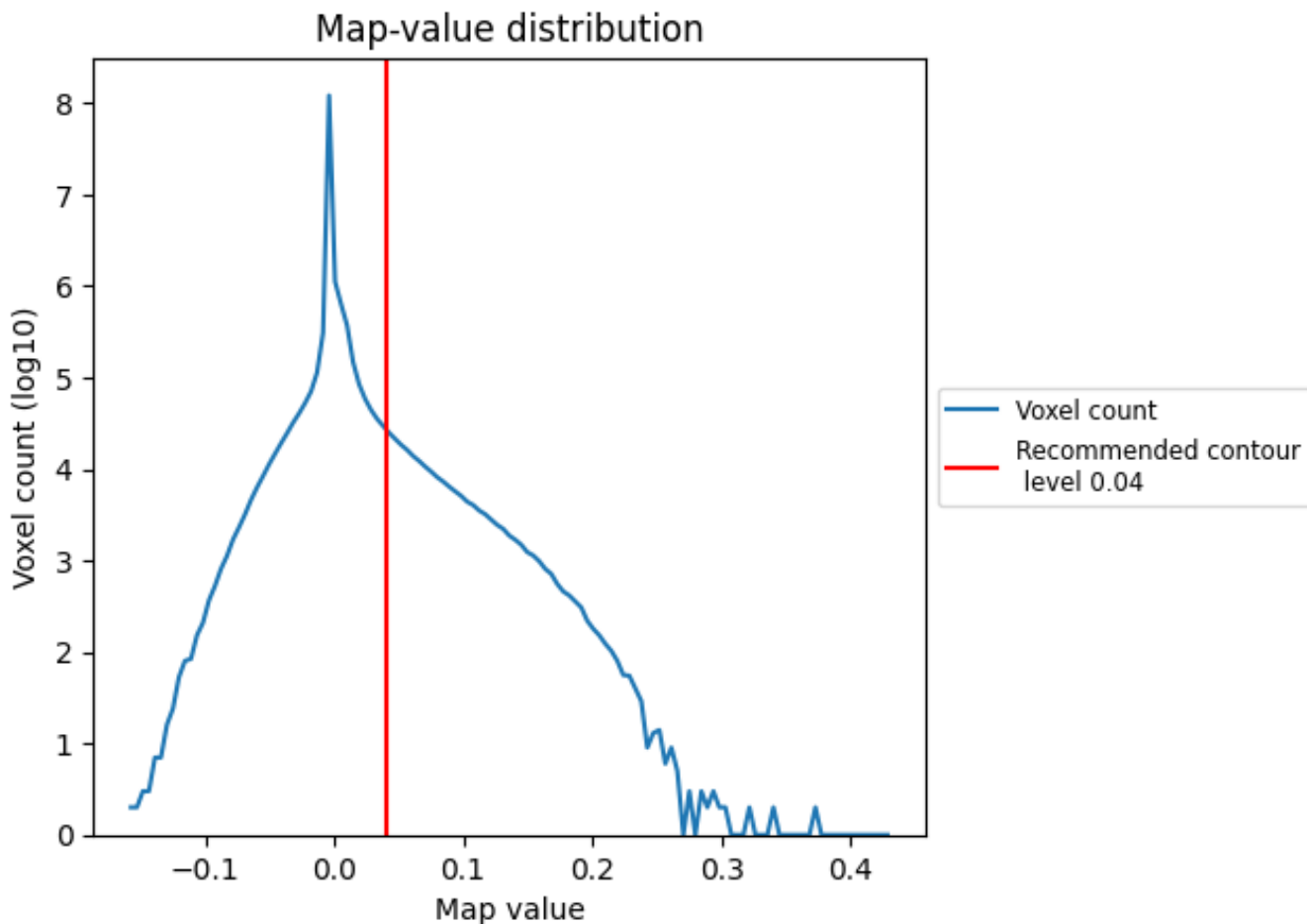


Z

7 Map analysis [i](#)

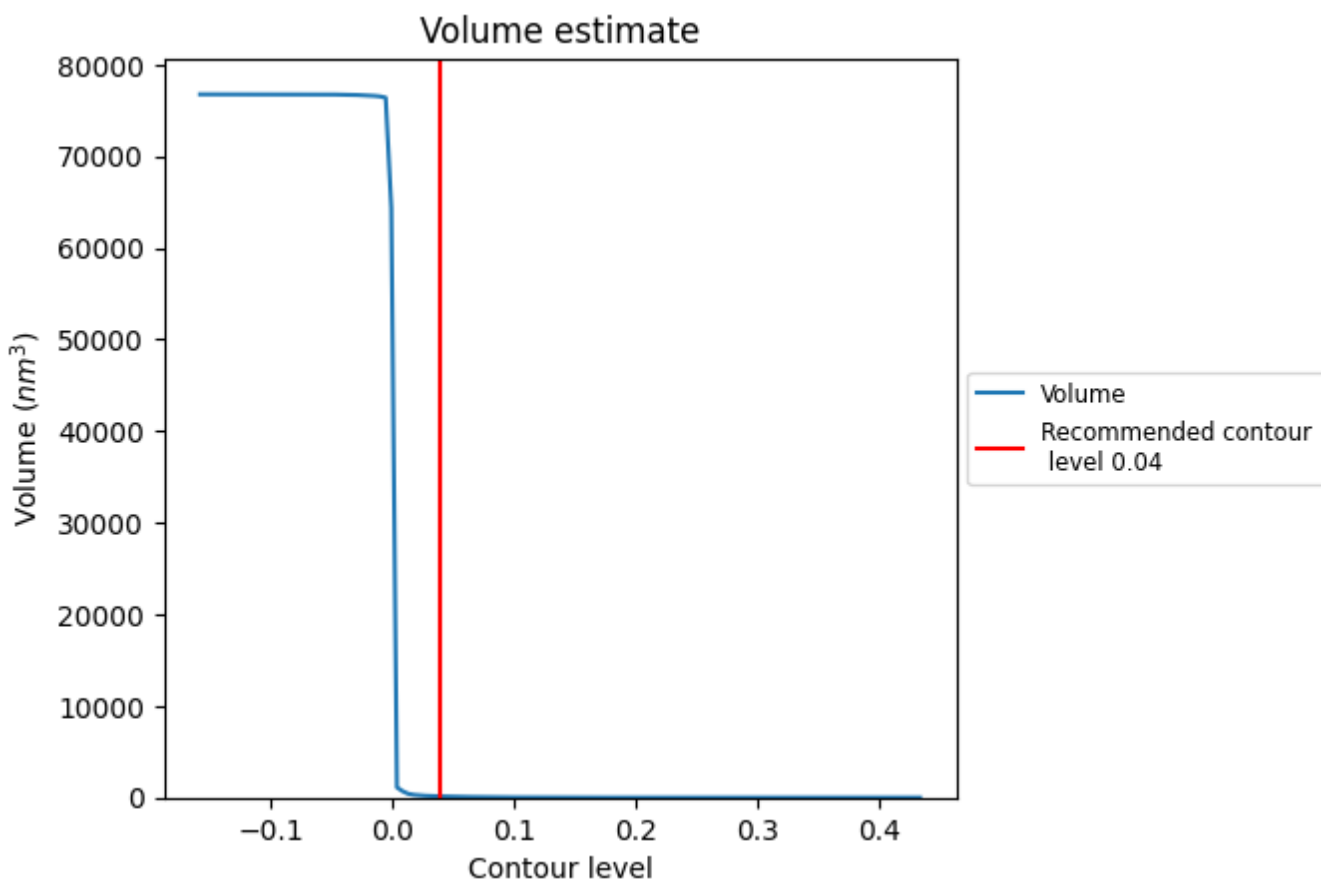
This section contains the results of statistical analysis of the map.

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.

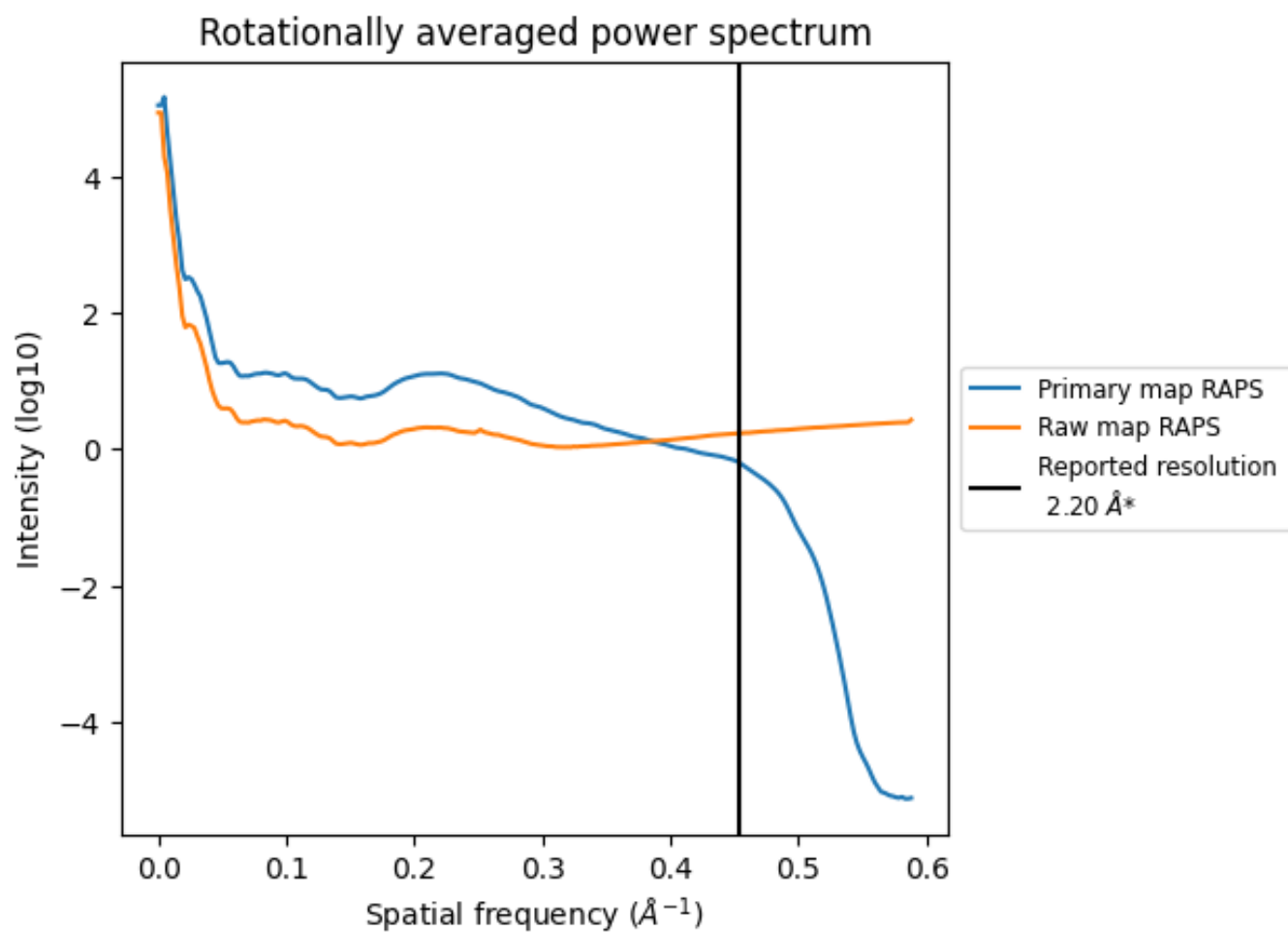
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm³; this corresponds to an approximate mass of 118 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](#)

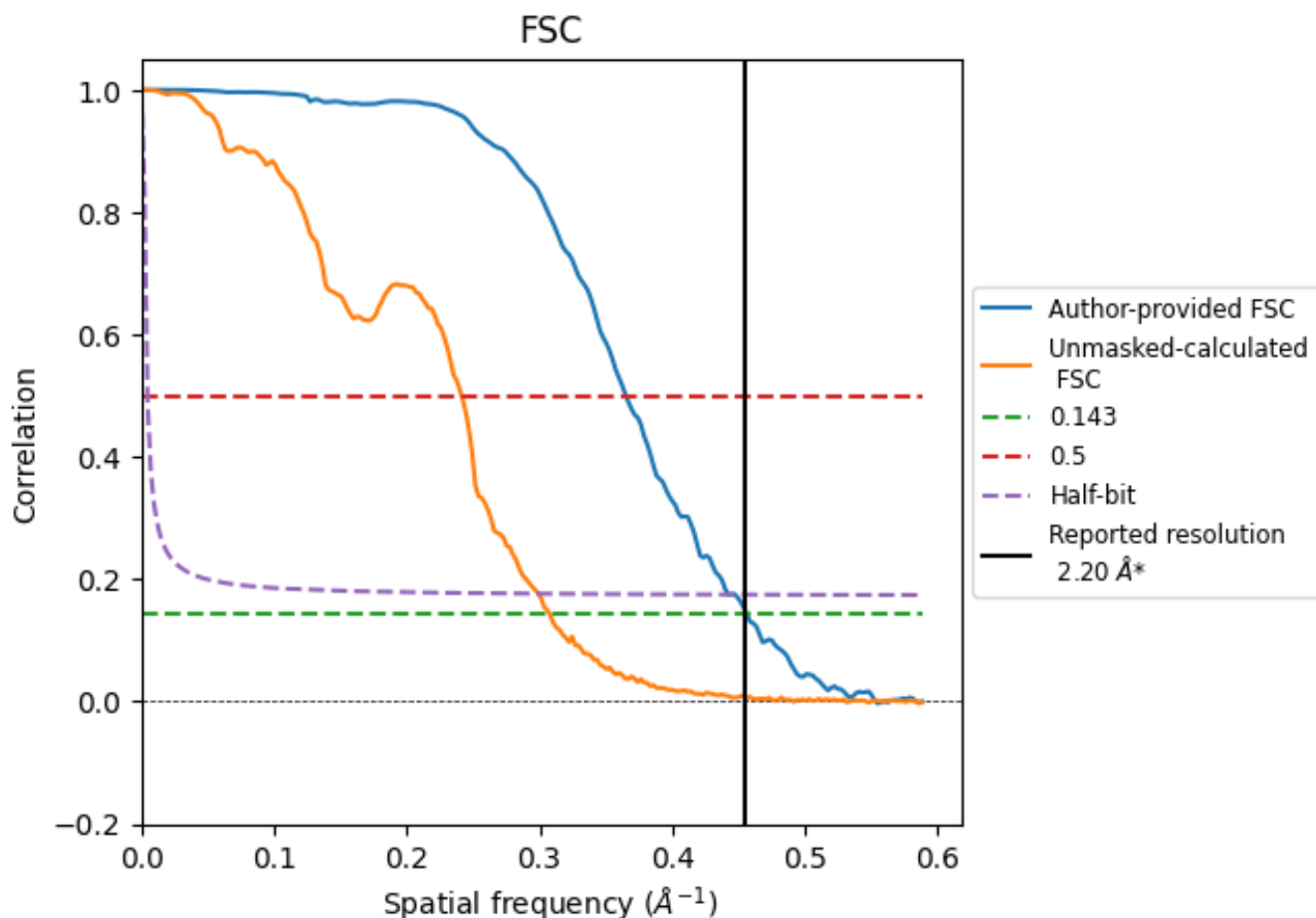


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

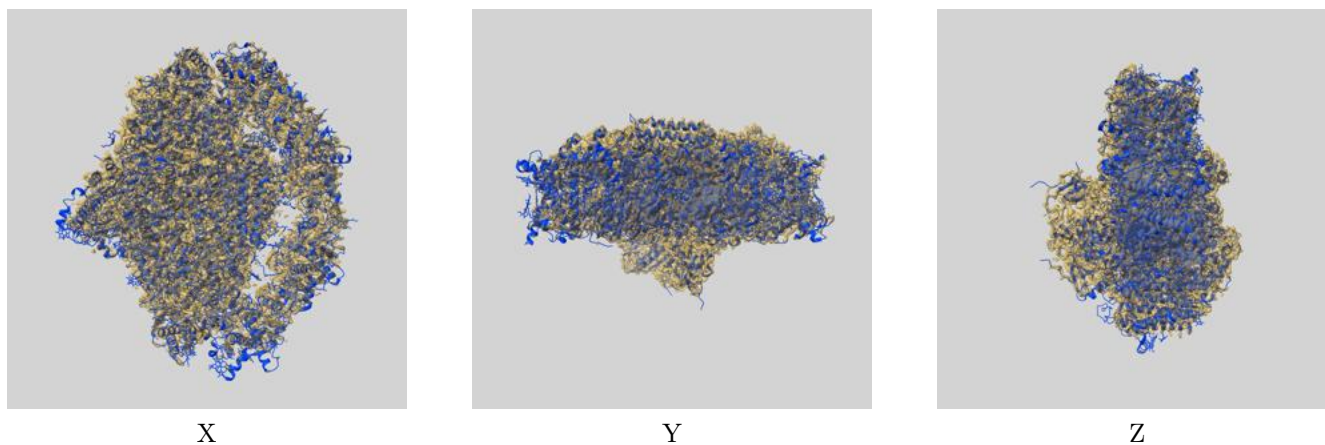
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.19	2.74	2.26
Unmasked-calculated*	3.25	4.14	3.34

*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 3.25 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

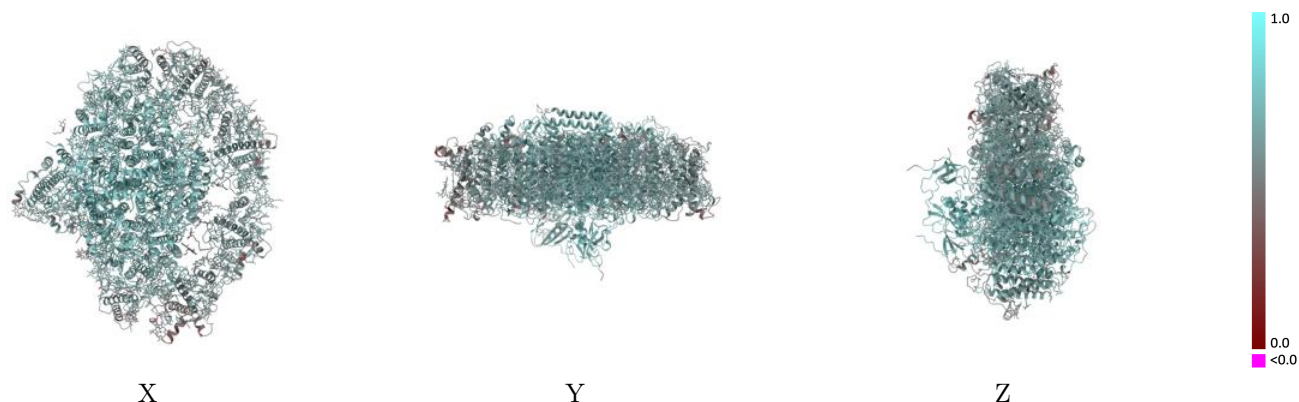
This section contains information regarding the fit between EMDB map EMD-15969 and PDB model 8BCV. Per-residue inclusion information can be found in section 3 on page 29.

9.1 Map-model overlay [i](#)



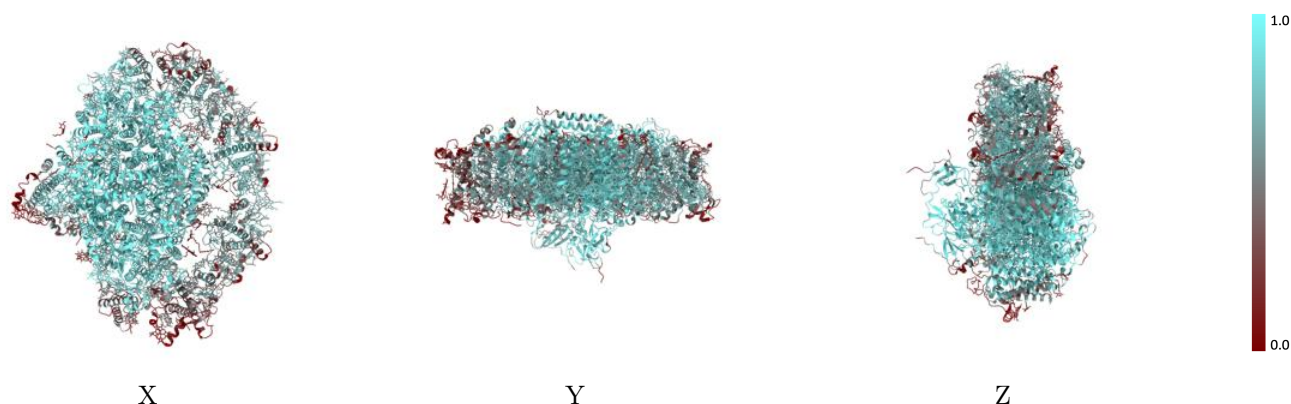
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



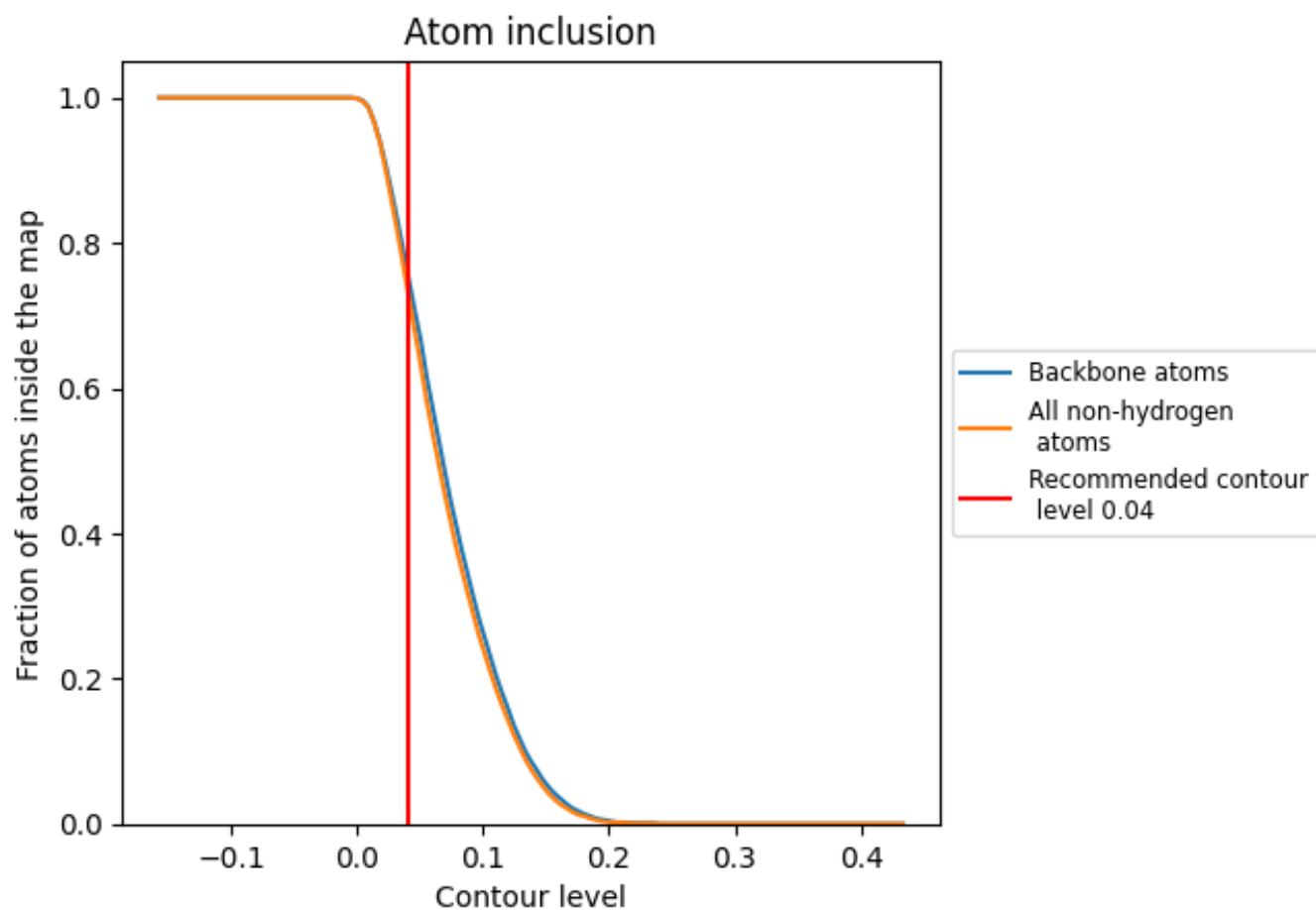
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 73% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7340	 0.6450
1	 0.5320	 0.5570
2	 0.5720	 0.5760
3	 0.3100	 0.5110
4	 0.6350	 0.5870
A	 0.8860	 0.7030
B	 0.9140	 0.7110
C	 0.9770	 0.7440
D	 0.8570	 0.6840
E	 0.7640	 0.6740
F	 0.7910	 0.6720
G	 0.6000	 0.5730
H	 0.2460	 0.5230
I	 0.7910	 0.6630
J	 0.7580	 0.6520
K	 0.2930	 0.4840
L	 0.5770	 0.5950

