



wwPDB EM Validation Summary Report ⓘ

Dec 7, 2022 – 10:36 AM JST

PDB ID : 5ZGH
EMDB ID : EMD-6930
Title : Cryo-EM structure of the red algal PSI-LHCR
Authors : Pi, X.
Deposited on : 2018-03-09
Resolution : 3.82 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

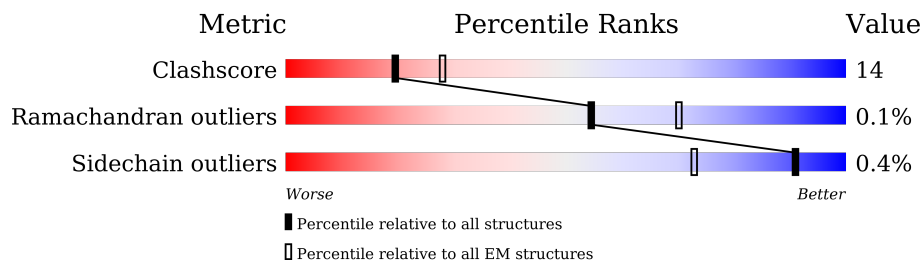
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.82 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1	175	
2	2	199	
3	3	188	
4	A	748	
5	B	732	
6	C	81	
7	D	139	
8	E	94	

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Mol	Chain	Length	Quality of chain
9	F	185	
10	I	32	
11	J	38	
12	K	60	
13	L	140	
14	M	29	
15	O	155	

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
16	CLA	1	601	X	-	-	-
16	CLA	1	602	X	-	-	-
16	CLA	1	603	X	-	-	-
16	CLA	1	604	X	-	-	-
16	CLA	1	605	X	-	-	-
16	CLA	1	606	X	-	-	-
16	CLA	1	607	X	-	-	-
16	CLA	1	608	X	-	-	-
16	CLA	1	609	X	-	-	-
16	CLA	1	610	X	-	-	-
16	CLA	1	611	X	-	-	-
16	CLA	1	612	X	-	-	-
16	CLA	2	601	X	-	-	-
16	CLA	2	602	X	-	-	-
16	CLA	2	603	X	-	-	-
16	CLA	2	604	X	-	-	-
16	CLA	2	605	X	-	-	-
16	CLA	2	606	X	-	-	-
16	CLA	2	607	X	-	-	-
16	CLA	2	608	X	-	-	-
16	CLA	2	609	X	-	-	-
16	CLA	2	610	X	-	-	-
16	CLA	2	611	X	-	-	-
16	CLA	2	612	X	-	-	-
16	CLA	2	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	3	202	X	-	-	-
16	CLA	3	203	X	-	-	-
16	CLA	3	204	X	-	-	-
16	CLA	3	205	X	-	-	-
16	CLA	3	206	X	-	-	-
16	CLA	3	207	X	-	-	-
16	CLA	3	208	X	-	-	-
16	CLA	3	209	X	-	-	-
16	CLA	3	210	X	-	-	-
16	CLA	3	211	X	-	-	-
16	CLA	3	212	X	-	-	-
16	CLA	3	213	X	-	-	-
16	CLA	A	802	X	-	-	-
16	CLA	A	803	X	-	-	-
16	CLA	A	804	X	-	-	-
16	CLA	A	805	X	-	-	-
16	CLA	A	806	X	-	-	-
16	CLA	A	807	X	-	-	-
16	CLA	A	808	X	-	-	-
16	CLA	A	809	X	-	-	-
16	CLA	A	810	X	-	-	-
16	CLA	A	811	X	-	-	-
16	CLA	A	812	X	-	-	-
16	CLA	A	813	X	-	-	-
16	CLA	A	814	X	-	-	-
16	CLA	A	815	X	-	-	-
16	CLA	A	816	X	-	-	-
16	CLA	A	817	X	-	-	-
16	CLA	A	818	X	-	-	-
16	CLA	A	819	X	-	-	-
16	CLA	A	820	X	-	-	-
16	CLA	A	821	X	-	-	-
16	CLA	A	822	X	-	-	-
16	CLA	A	823	X	-	-	-
16	CLA	A	824	X	-	-	-
16	CLA	A	825	X	-	-	-
16	CLA	A	826	X	-	-	-
16	CLA	A	827	X	-	-	-
16	CLA	A	828	X	-	-	-
16	CLA	A	829	X	-	-	-
16	CLA	A	830	X	-	-	-
16	CLA	A	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	832	X	-	-	-
16	CLA	A	833	X	-	-	-
16	CLA	A	834	X	-	-	-
16	CLA	A	835	X	-	-	-
16	CLA	A	836	X	-	-	-
16	CLA	A	837	X	-	-	-
16	CLA	A	838	X	-	-	-
16	CLA	A	839	X	-	-	-
16	CLA	A	850	X	-	-	-
16	CLA	A	851	X	-	-	-
16	CLA	A	852	X	-	-	-
16	CLA	B	801	X	-	-	-
16	CLA	B	802	X	-	X	-
16	CLA	B	803	X	-	-	-
16	CLA	B	804	X	-	-	-
16	CLA	B	805	X	-	-	-
16	CLA	B	806	X	-	-	-
16	CLA	B	807	X	-	-	-
16	CLA	B	808	X	-	-	-
16	CLA	B	809	X	-	-	-
16	CLA	B	810	X	-	-	-
16	CLA	B	811	X	-	-	-
16	CLA	B	812	X	-	-	-
16	CLA	B	813	X	-	-	-
16	CLA	B	814	X	-	-	-
16	CLA	B	815	X	-	-	-
16	CLA	B	816	X	-	-	-
16	CLA	B	817	X	-	-	-
16	CLA	B	818	X	-	-	-
16	CLA	B	819	X	-	-	-
16	CLA	B	820	X	-	-	-
16	CLA	B	821	X	-	-	-
16	CLA	B	822	X	-	-	-
16	CLA	B	823	X	-	-	-
16	CLA	B	824	X	-	-	-
16	CLA	B	825	X	-	-	-
16	CLA	B	826	X	-	-	-
16	CLA	B	827	X	-	-	-
16	CLA	B	828	X	-	-	-
16	CLA	B	829	X	-	-	-
16	CLA	B	830	X	-	-	-
16	CLA	B	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	B	832	X	-	-	-
16	CLA	B	833	X	-	-	-
16	CLA	B	834	X	-	-	-
16	CLA	B	835	X	-	-	-
16	CLA	B	836	X	-	-	-
16	CLA	B	837	X	-	-	-
16	CLA	B	838	X	-	-	-
16	CLA	B	839	X	-	-	-
16	CLA	B	840	X	-	-	-
16	CLA	B	841	X	-	-	-
16	CLA	B	842	X	-	-	-
16	CLA	F	802	X	-	-	-
16	CLA	F	803	X	-	-	-
16	CLA	J	101	X	-	-	-
16	CLA	K	101	X	-	-	-
16	CLA	K	102	X	-	-	-
16	CLA	L	201	X	-	-	-
16	CLA	L	203	X	-	-	-
16	CLA	L	204	X	-	-	-
16	CLA	L	205	X	-	-	-
16	CLA	O	201	X	-	-	-
16	CLA	O	202	X	-	-	-
16	CLA	O	203	X	-	-	-
16	CLA	O	204	X	-	-	-
17	ZEX	2	614	-	X	-	-
17	ZEX	2	616	-	X	-	-
17	ZEX	3	218	-	X	-	-
19	CLO	A	801	X	-	X	-

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 30757 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 Lhcr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	169	1351	887	227	229	8	0	0

- Molecule 2 is a protein called Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	175	1371	892	233	239	7	0	0

- Molecule 3 is a protein called Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	170	1303	845	219	232	7	0	0

- Molecule 4 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	741	5798	3792	996	983	27	0	0

- Molecule 5 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	731	5819	3827	982	991	19	0	0

- Molecule 6 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	80	597	367	104	114	12	0	0

- Molecule 7 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	119	950	600	167	179	4	0	0

- Molecule 8 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	E	61	493	322	79	92	0	0

- Molecule 9 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	154	1263	811	214	234	4	0	0

- Molecule 10 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	31	230	158	32	39	1	0	0

- Molecule 11 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	38	312	214	46	51	1	0	0

- Molecule 12 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	59	428	279	70	74	5	0	0

- Molecule 13 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	119	900	591	148	159	2	0	0

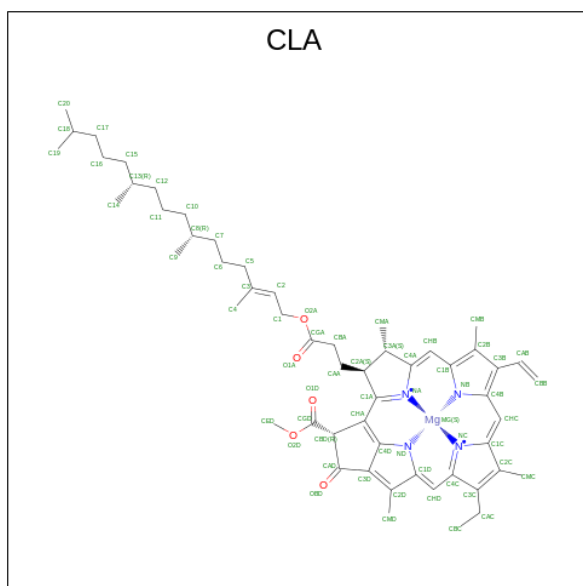
- Molecule 14 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	27	204	136	32	34	2	0	0

- Molecule 15 is a protein called PsaO.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	O	83	641	439	97	105	0	0

- Molecule 16 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	1	1	565	449	12	48	56	0
16	1	1	565	449	12	48	56	0
16	1	1	565	449	12	48	56	0
16	1	1	565	449	12	48	56	0
16	1	1	565	449	12	48	56	0
16	1	1	565	449	12	48	56	0
16	1	1	565	449	12	48	56	0
16	1	1	565	449	12	48	56	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	1	1	565	449	12	48	56	0
16	1	1	565	449	12	48	56	0
16	1	1	565	449	12	48	56	0
16	1	1	565	449	12	48	56	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	2	1	600	476	13	52	59	0
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0
16	3	1	565	449	12	48	56	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0

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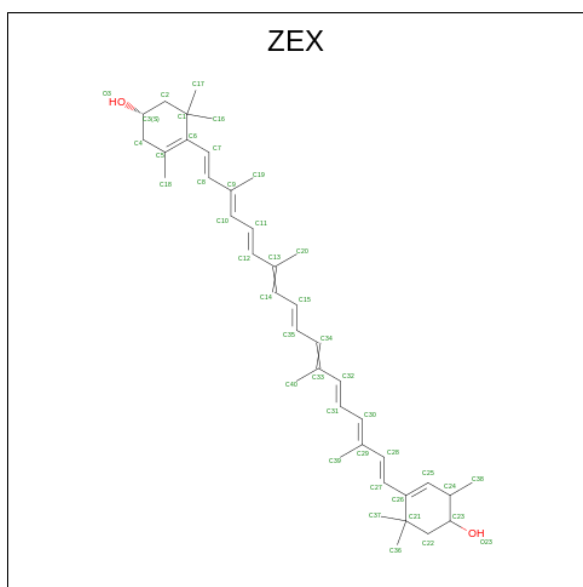
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	A	1	2423	2017	41	164	201	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0
16	B	1	2484	2068	42	168	206	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	B	1	Total 2484	C 2068	Mg 42	N 168	O 206	0
16	B	1	Total 2484	C 2068	Mg 42	N 168	O 206	0
16	B	1	Total 2484	C 2068	Mg 42	N 168	O 206	0
16	B	1	Total 2484	C 2068	Mg 42	N 168	O 206	0
16	B	1	Total 2484	C 2068	Mg 42	N 168	O 206	0
16	B	1	Total 2484	C 2068	Mg 42	N 168	O 206	0
16	B	1	Total 2484	C 2068	Mg 42	N 168	O 206	0
16	F	1	Total 86	C 68	Mg 2	N 8	O 8	0
16	F	1	Total 86	C 68	Mg 2	N 8	O 8	0
16	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
16	K	1	Total 87	C 69	Mg 2	N 8	O 8	0
16	K	1	Total 87	C 69	Mg 2	N 8	O 8	0
16	L	1	Total 228	C 188	Mg 4	N 16	O 20	0
16	L	1	Total 228	C 188	Mg 4	N 16	O 20	0
16	L	1	Total 228	C 188	Mg 4	N 16	O 20	0
16	L	1	Total 228	C 188	Mg 4	N 16	O 20	0
16	O	1	Total 188	C 150	Mg 4	N 16	O 18	0
16	O	1	Total 188	C 150	Mg 4	N 16	O 18	0
16	O	1	Total 188	C 150	Mg 4	N 16	O 18	0
16	O	1	Total 188	C 150	Mg 4	N 16	O 18	0

- Molecule 17 is (1R,2S)-4-((1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl)-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: C₄₀H₅₆O₂).



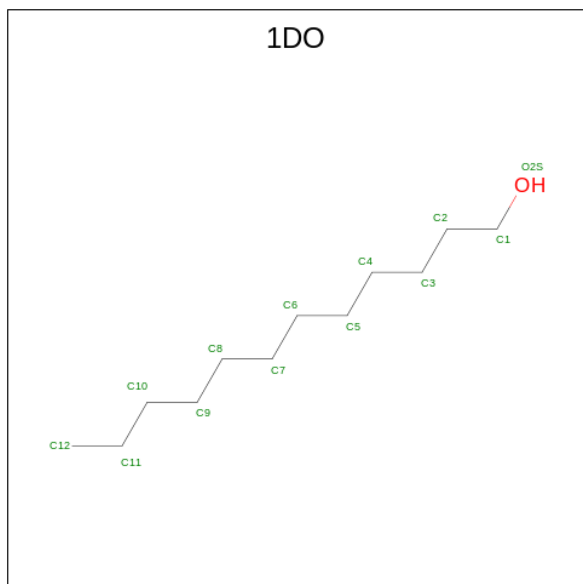
Mol	Chain	Residues	Atoms			AltConf
17	1	1	Total	C	O	0
			210	200	10	
17	1	1	Total	C	O	0
			210	200	10	
17	1	1	Total	C	O	0
			210	200	10	
17	1	1	Total	C	O	0
			210	200	10	
17	1	1	Total	C	O	0
			210	200	10	
17	2	1	Total	C	O	0
			168	160	8	
17	2	1	Total	C	O	0
			168	160	8	
17	2	1	Total	C	O	0
			168	160	8	
17	2	1	Total	C	O	0
			168	160	8	
17	3	1	Total	C	O	0
			252	240	12	
17	3	1	Total	C	O	0
			252	240	12	
17	3	1	Total	C	O	0
			252	240	12	
17	3	1	Total	C	O	0
			252	240	12	
17	3	1	Total	C	O	0
			252	240	12	

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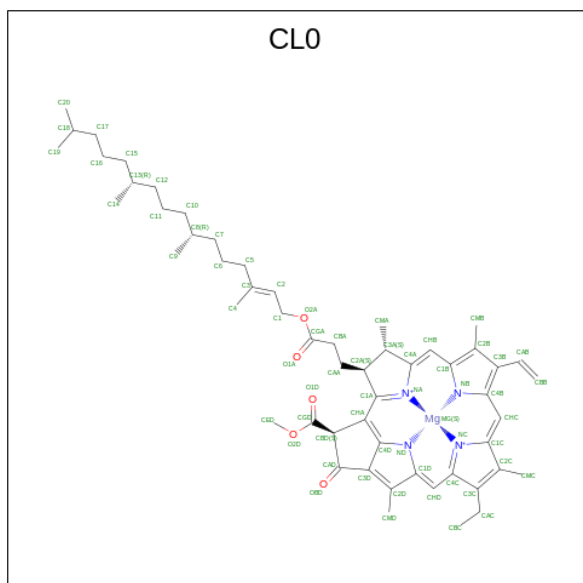
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	3	1	252	240	12	0

- Molecule 18 is 1-DODECANOL (three-letter code: 1DO) (formula: C₁₂H₂₆O).



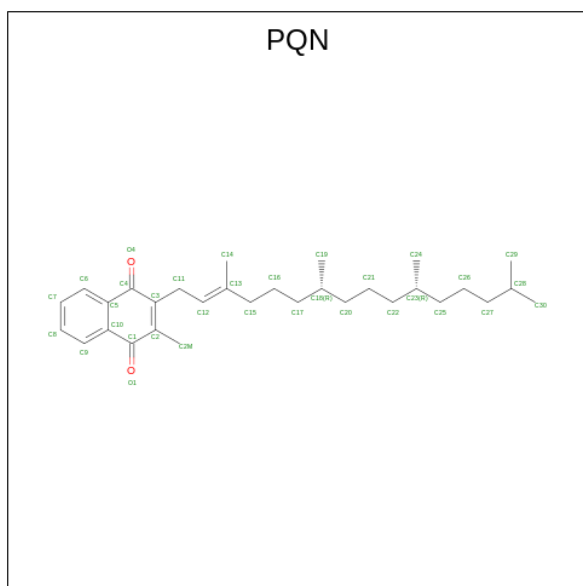
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	3	1	13	12	1	0

- Molecule 19 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



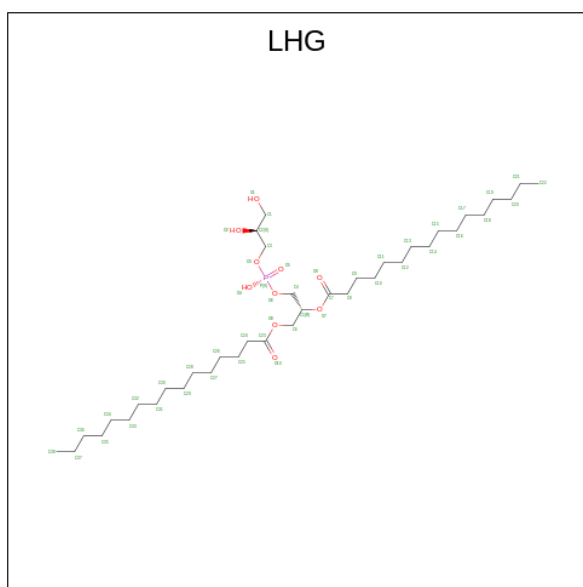
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
19	A	1	65	55	1	4	5	0

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



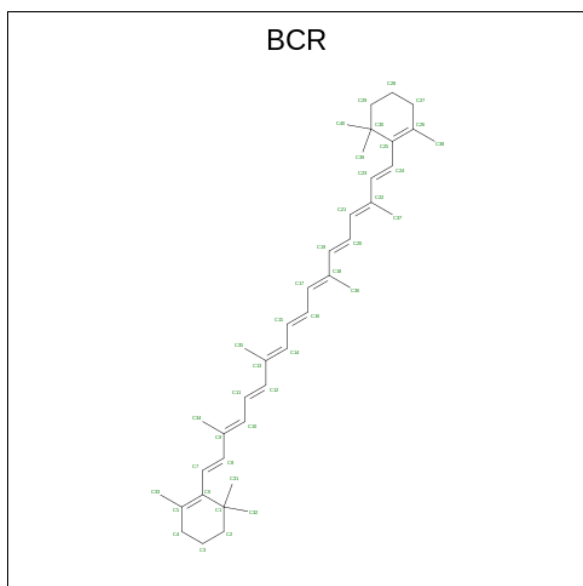
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	A	1	33	31	2	0
20	B	1	33	31	2	0

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
21	A	1	89	67	20	2	0
21	A	1	89	67	20	2	0

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



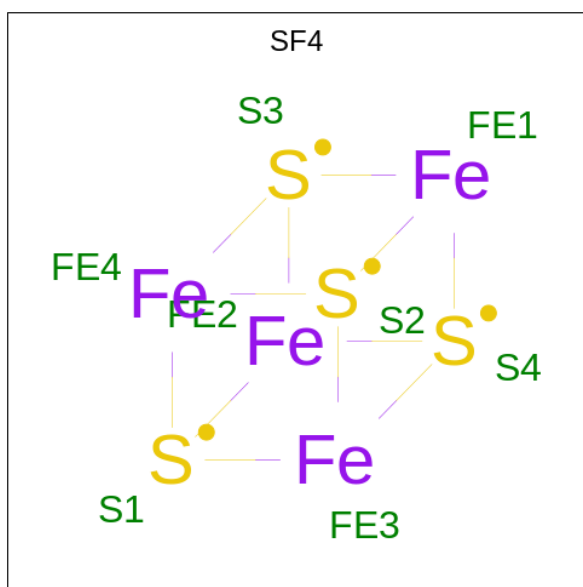
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
22	A	1	240	240	0
22	A	1	240	240	0

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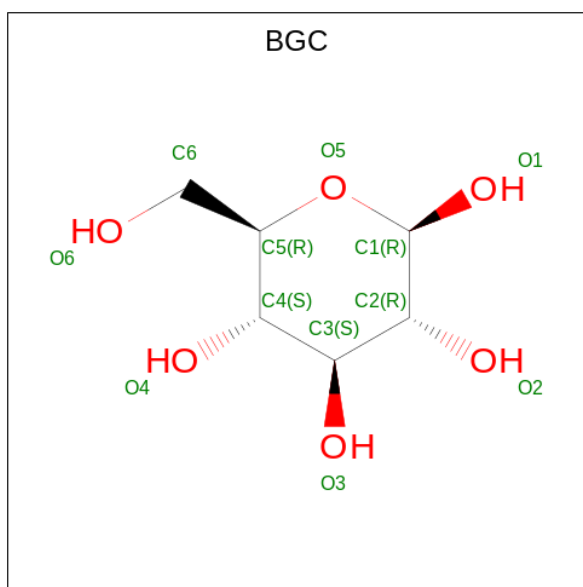
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total 240	C 240	0
22	A	1	Total 240	C 240	0
22	A	1	Total 240	C 240	0
22	A	1	Total 240	C 240	0
22	B	1	Total 240	C 240	0
22	B	1	Total 240	C 240	0
22	B	1	Total 240	C 240	0
22	B	1	Total 240	C 240	0
22	B	1	Total 240	C 240	0
22	B	1	Total 240	C 240	0
22	B	1	Total 240	C 240	0
22	F	1	Total 80	C 80	0
22	F	1	Total 80	C 80	0
22	I	1	Total 40	C 40	0
22	J	1	Total 80	C 80	0
22	J	1	Total 80	C 80	0
22	K	1	Total 40	C 40	0
22	L	1	Total 120	C 120	0
22	L	1	Total 120	C 120	0
22	L	1	Total 120	C 120	0

- Molecule 23 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



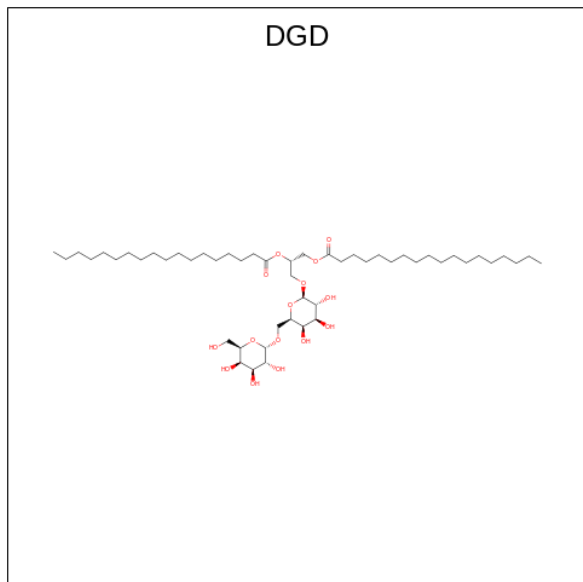
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	Fe	S	0
			8	4	4	
23	C	1	Total	Fe	S	0
			16	8	8	
23	C	1	Total	Fe	S	0
			16	8	8	

- Molecule 24 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



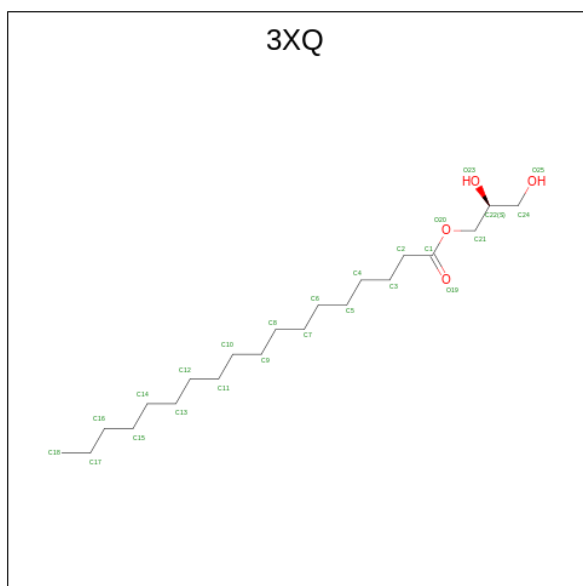
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			11	6	5	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGD) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 26 is (2S)-2,3-dihydroxypropyl octadecanoate (three-letter code: 3XQ) (formula: $C_{21}H_{42}O_4$).

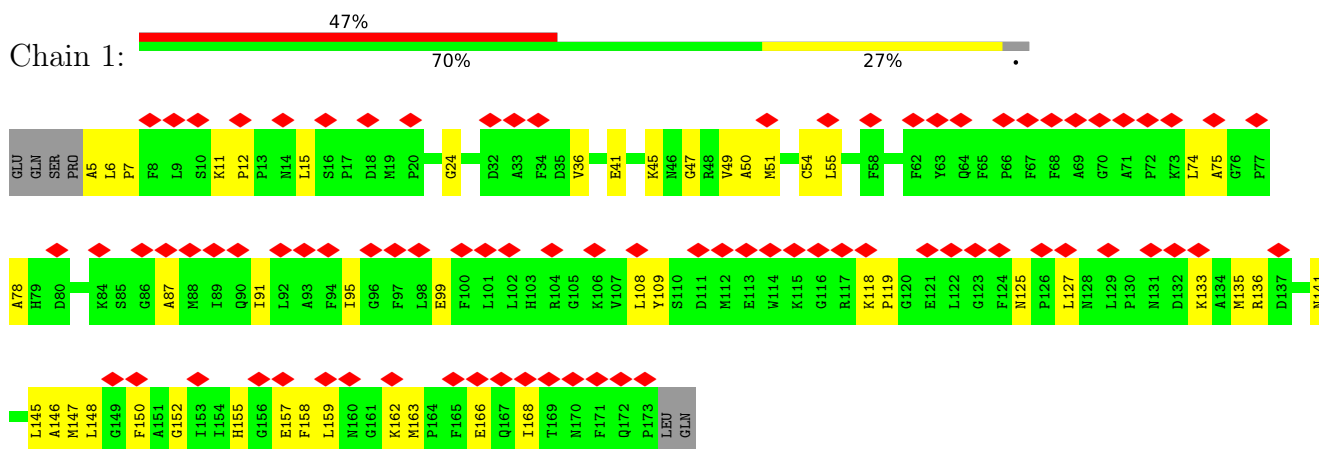


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	J	1	25	21	4	0

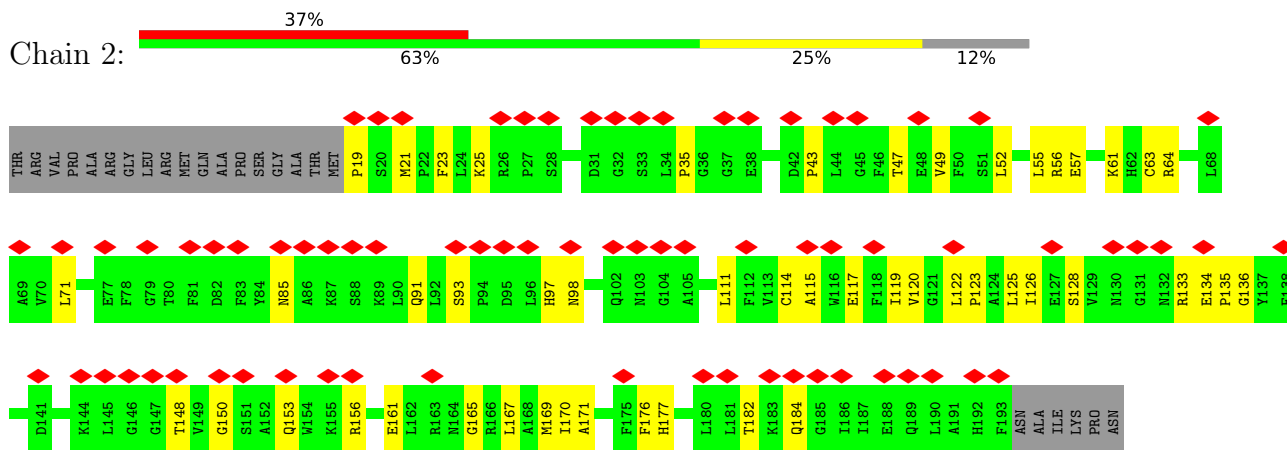
3 Residue-property plots [i](#)

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.

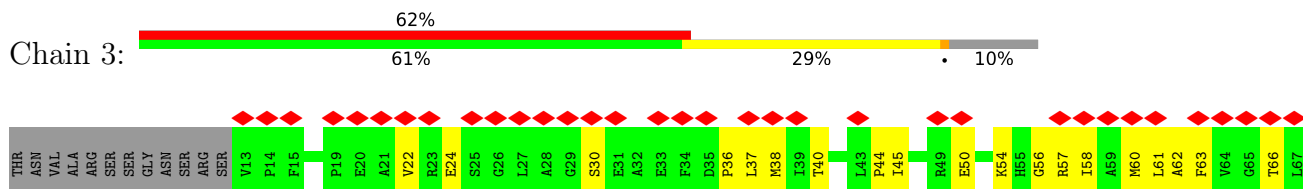
- Molecule 1: Lhcr1

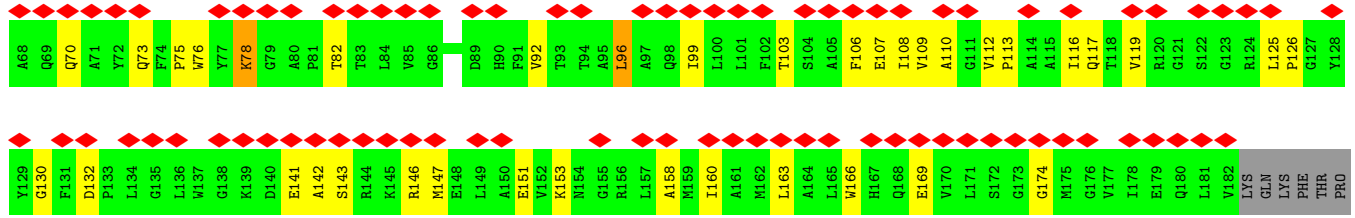


- Molecule 2: Lhcr2

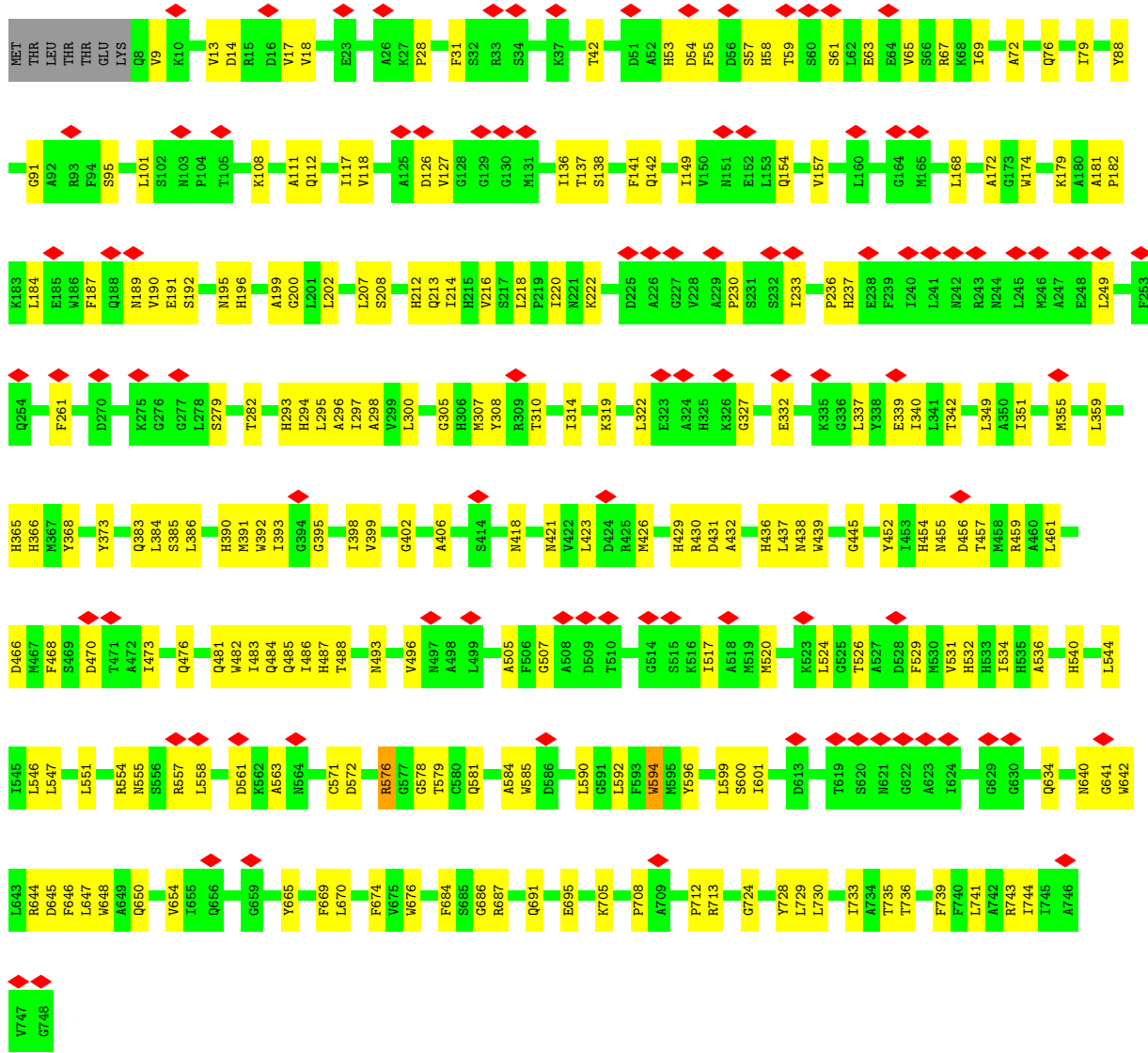


- Molecule 3: Lhcr3

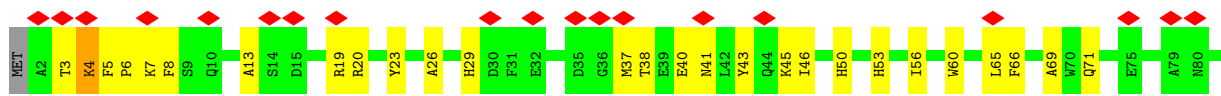
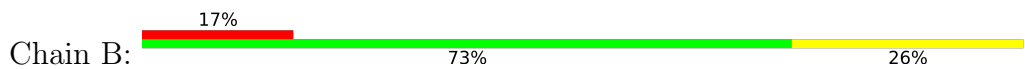


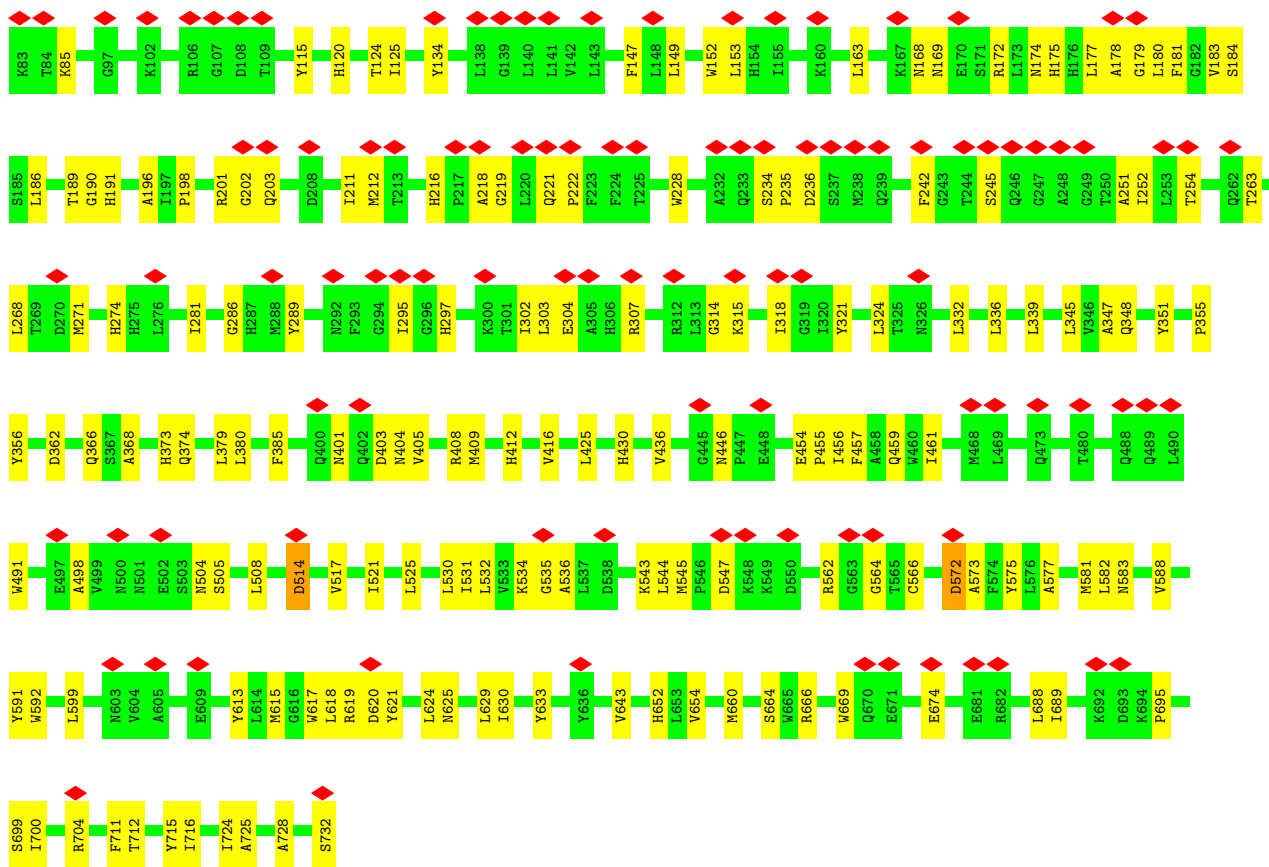


• Molecule 4: PsaA

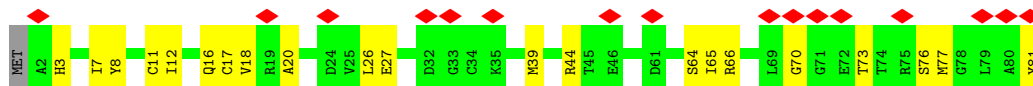
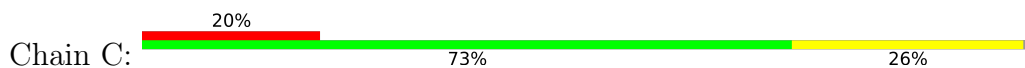


• Molecule 5: PsaB

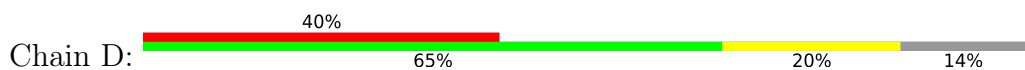




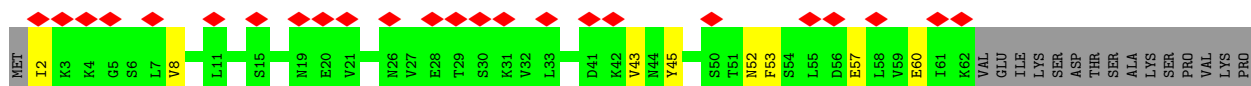
• Molecule 6: PsacC



• Molecule 7: PsadD

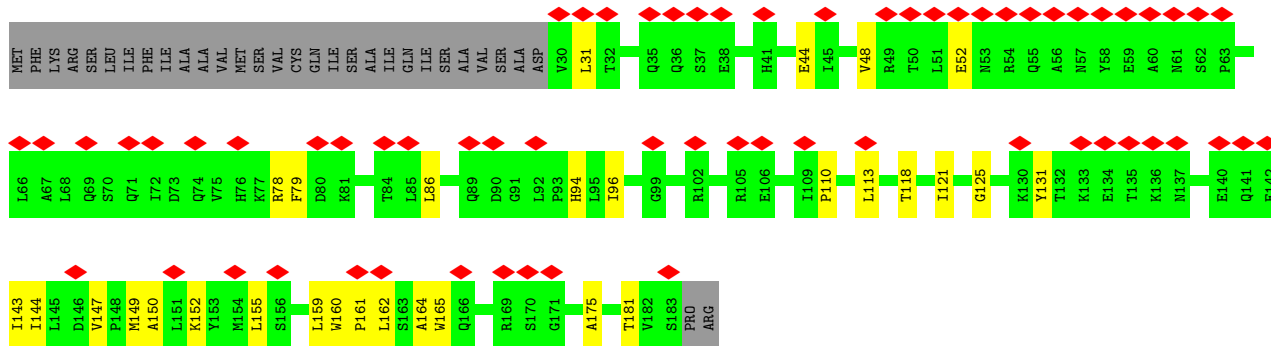


• Molecule 8: PsaeE



PRO VAL LYS SER GIU VAL LYS ALA GIU LYS ASN LYS GIU GLY ALA

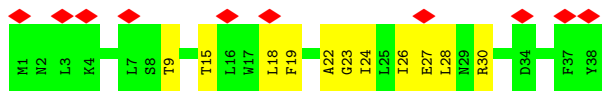
• Molecule 9: PsaF



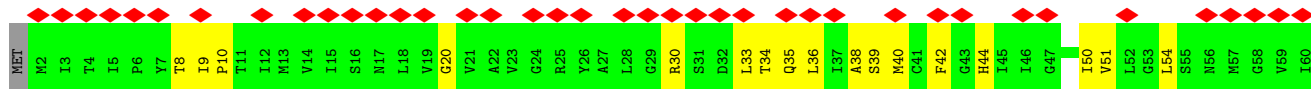
• Molecule 10: PsaI



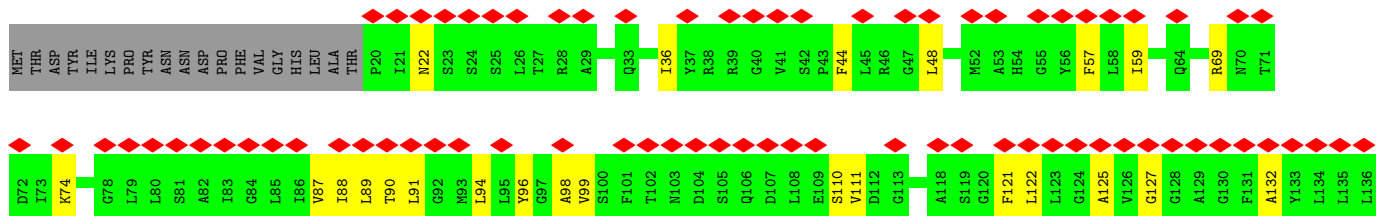
• Molecule 11: PsaJ



• Molecule 12: PsaK

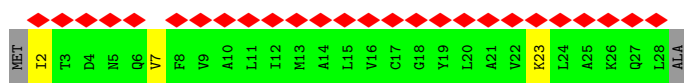
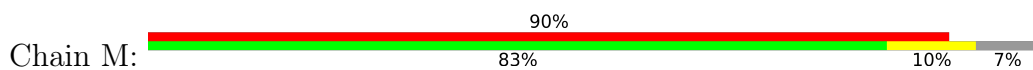


• Molecule 13: PsaL

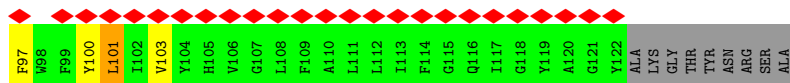




• Molecule 14: PsaM



• Molecule 15: PsaO



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76079	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.17	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.584	Depositor
Minimum map value	-0.161	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.087	Depositor
Map size (\AA)	294.0, 294.0, 294.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 1DO, DGD, SF4, ZEX, PQN, LHG, BGC, CLA, 3XQ, BCR, CLO

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	1	0.39	0/1395	0.69	1/1884 (0.1%)
2	2	0.39	0/1407	0.67	0/1898
3	3	0.38	0/1337	0.67	1/1817 (0.1%)
4	A	0.53	1/5985 (0.0%)	0.62	1/8158 (0.0%)
5	B	0.49	0/6028	0.63	3/8236 (0.0%)
6	C	0.46	0/607	0.58	0/822
7	D	0.34	0/969	0.58	0/1307
8	E	0.44	0/502	0.55	0/680
9	F	0.38	0/1296	0.59	0/1760
10	I	0.35	0/235	0.70	0/321
11	J	0.41	0/321	0.63	0/437
12	K	0.32	0/433	0.62	0/588
13	L	0.32	0/919	0.57	0/1247
14	M	0.27	0/205	0.57	0/277
15	O	0.35	0/664	0.67	1/913 (0.1%)
All	All	0.45	1/22303 (0.0%)	0.63	7/30345 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
5	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	594	TRP	CB-CG	-6.00	1.39	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	571	CYS	CA-CB-SG	-6.63	102.06	114.00
5	B	572	ASP	CB-CG-OD1	6.63	124.27	118.30
5	B	514	ASP	CB-CG-OD1	5.68	123.41	118.30
3	3	96	LEU	CA-CB-CG	5.63	128.25	115.30
1	1	159	LEU	CA-CB-CG	5.57	128.12	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	135	PRO	Peptide
5	B	430	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1351	0	1322	34	0
2	2	1371	0	1362	34	0
3	3	1303	0	1305	46	0
4	A	5798	0	5727	196	0
5	B	5819	0	5648	173	0
6	C	597	0	584	19	0
7	D	950	0	944	24	0
8	E	493	0	509	7	0
9	F	1263	0	1236	24	0
10	I	230	0	253	12	0
11	J	312	0	327	13	0
12	K	428	0	464	15	0
13	L	900	0	931	19	0
14	M	204	0	226	3	0
15	O	641	0	650	9	0
16	1	565	0	443	15	0
16	2	600	0	466	19	0
16	3	565	0	440	18	0
16	A	2423	0	2452	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	2484	0	2521	172	0
16	F	86	0	62	4	0
16	J	42	0	31	2	0
16	K	87	0	64	4	0
16	L	228	0	215	4	0
16	O	188	0	144	3	0
17	1	210	0	280	19	0
17	2	168	0	224	12	0
17	3	252	0	336	25	0
18	3	13	0	25	0	0
19	A	65	0	71	56	0
20	A	33	0	46	2	0
20	B	33	0	46	5	0
21	A	89	0	127	4	0
22	A	240	0	336	16	0
22	B	240	0	336	21	0
22	F	80	0	112	4	0
22	I	40	0	56	2	0
22	J	80	0	112	7	0
22	K	40	0	56	5	0
22	L	120	0	168	11	0
23	A	8	0	0	0	0
23	C	16	0	0	1	0
24	A	11	0	9	0	0
25	B	66	0	96	4	0
26	J	25	0	0	0	0
All	All	30757	0	30762	859	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 14.

The worst 5 of 859 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)
19:A:801:CL0:C19	16:B:802:CLA:HMB3	1.45	1.42
19:A:801:CL0:H66	16:B:802:CLA:CMB	1.58	1.33
4:A:642:TRP:CD1	19:A:801:CL0:H50	1.63	1.32
19:A:801:CL0:C19	16:B:802:CLA:CMB	2.13	1.26
5:B:4:LYS:HB2	5:B:13:ALA:HB1	1.25	1.11

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	167/175 (95%)	129 (77%)	37 (22%)	1 (1%)	25	62
2	2	173/199 (87%)	134 (78%)	39 (22%)	0	100	100
3	3	168/188 (89%)	141 (84%)	27 (16%)	0	100	100
4	A	739/748 (99%)	686 (93%)	52 (7%)	1 (0%)	51	83
5	B	729/732 (100%)	663 (91%)	65 (9%)	1 (0%)	51	83
6	C	78/81 (96%)	67 (86%)	11 (14%)	0	100	100
7	D	117/139 (84%)	103 (88%)	14 (12%)	0	100	100
8	E	59/94 (63%)	53 (90%)	6 (10%)	0	100	100
9	F	152/185 (82%)	136 (90%)	16 (10%)	0	100	100
10	I	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
11	J	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	K	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
13	L	117/140 (84%)	107 (92%)	10 (8%)	0	100	100
14	M	25/29 (86%)	23 (92%)	2 (8%)	0	100	100
15	O	81/155 (52%)	67 (83%)	14 (17%)	0	100	100
All	All	2727/2995 (91%)	2421 (89%)	303 (11%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	12	PRO
5	B	7	LYS
4	A	526	THR

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	1	139/145 (96%)	138 (99%)	1 (1%)	84	91
2	2	142/160 (89%)	141 (99%)	1 (1%)	84	91
3	3	132/148 (89%)	131 (99%)	1 (1%)	81	89
4	A	598/605 (99%)	595 (100%)	3 (0%)	88	94
5	B	598/599 (100%)	596 (100%)	2 (0%)	92	96
6	C	66/67 (98%)	66 (100%)	0	100	100
7	D	101/118 (86%)	101 (100%)	0	100	100
8	E	58/87 (67%)	58 (100%)	0	100	100
9	F	136/162 (84%)	136 (100%)	0	100	100
10	I	26/27 (96%)	26 (100%)	0	100	100
11	J	34/34 (100%)	34 (100%)	0	100	100
12	K	48/49 (98%)	48 (100%)	0	100	100
13	L	94/113 (83%)	93 (99%)	1 (1%)	73	85
14	M	22/23 (96%)	22 (100%)	0	100	100
15	O	64/121 (53%)	63 (98%)	1 (2%)	62	79
All	All	2258/2458 (92%)	2248 (100%)	10 (0%)	91	95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	4	LYS
13	L	22	ASN
15	O	82	ARG
4	A	69	ILE
4	A	438	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	374	GLN
8	E	52	ASN
13	L	22	ASN
12	K	44	HIS
4	A	320	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

181 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
22	BCR	J	103	-	41,41,41	1.27	3 (7%)	56,56,56	1.29	5 (8%)
16	CLA	1	611	-	45,53,73	1.70	8 (17%)	52,89,113	1.73	8 (15%)
16	CLA	A	834	-	45,53,73	1.76	9 (20%)	52,89,113	1.82	9 (17%)
17	ZEX	2	614	-	42,43,43	4.96	19 (45%)	55,60,60	5.27	34 (61%)
16	CLA	B	804	-	65,73,73	1.51	10 (15%)	76,113,113	1.61	14 (18%)
16	CLA	2	605	-	45,53,73	1.71	9 (20%)	52,89,113	1.86	9 (17%)
16	CLA	3	204	-	45,53,73	1.73	9 (20%)	52,89,113	1.76	8 (15%)
16	CLA	B	822	-	45,53,73	1.75	10 (22%)	52,89,113	1.72	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	823	-	46,54,73	1.70	8 (17%)	53,90,113	1.64	7 (13%)
18	1DO	3	219	24	12,12,12	0.23	0	11,11,11	0.83	0
16	CLA	B	816	-	45,53,73	1.70	9 (20%)	52,89,113	1.69	8 (15%)
16	CLA	3	211	-	42,50,73	1.76	6 (14%)	48,85,113	1.75	8 (16%)
16	CLA	A	802	-	65,73,73	1.46	9 (13%)	76,113,113	1.65	9 (11%)
16	CLA	1	608	-	60,68,73	1.50	9 (15%)	70,107,113	1.57	9 (12%)
17	ZEX	2	615	-	42,43,43	4.82	18 (42%)	55,60,60	5.28	30 (54%)
16	CLA	B	811	-	65,73,73	1.45	11 (16%)	76,113,113	1.54	12 (15%)
21	LHG	A	841	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	6 (11%)
16	CLA	1	610	-	45,53,73	1.76	9 (20%)	52,89,113	1.76	9 (17%)
26	3XQ	J	104	-	24,24,24	0.58	1 (4%)	25,25,25	1.12	1 (4%)
16	CLA	B	817	-	42,50,73	1.77	9 (21%)	48,85,113	1.75	8 (16%)
16	CLA	B	840	-	65,73,73	1.45	10 (15%)	76,113,113	1.53	9 (11%)
23	SF4	A	848	-	0,12,12	-	-	-	-	-
16	CLA	B	819	-	59,67,73	1.54	10 (16%)	68,105,113	1.60	10 (14%)
22	BCR	J	102	-	41,41,41	1.23	4 (9%)	56,56,56	1.34	7 (12%)
16	CLA	B	826	-	65,73,73	1.49	10 (15%)	76,113,113	1.51	10 (13%)
16	CLA	B	818	-	55,63,73	1.53	8 (14%)	64,101,113	1.60	9 (14%)
16	CLA	A	851	-	43,51,73	1.77	9 (20%)	49,86,113	1.81	8 (16%)
17	ZEX	1	614	-	42,43,43	5.04	19 (45%)	55,60,60	5.49	29 (52%)
16	CLA	B	829	-	65,73,73	1.42	10 (15%)	76,113,113	1.48	11 (14%)
16	CLA	B	837	-	60,68,73	1.55	11 (18%)	70,107,113	1.63	13 (18%)
16	CLA	A	805	-	65,73,73	1.45	10 (15%)	76,113,113	1.66	10 (13%)
16	CLA	1	601	-	48,56,73	1.68	9 (18%)	55,92,113	2.08	12 (21%)
16	CLA	L	203	-	57,65,73	1.54	7 (12%)	66,103,113	1.54	8 (12%)
17	ZEX	1	613	-	42,43,43	5.00	18 (42%)	55,60,60	5.30	32 (58%)
22	BCR	F	804	-	41,41,41	1.13	2 (4%)	56,56,56	1.41	11 (19%)
16	CLA	A	852	-	61,69,73	1.45	11 (18%)	71,108,113	1.58	9 (12%)
17	ZEX	3	214	-	42,43,43	5.09	19 (45%)	55,60,60	5.14	32 (58%)
16	CLA	B	827	-	65,73,73	1.43	10 (15%)	76,113,113	1.52	11 (14%)
16	CLA	1	606	-	45,53,73	1.73	10 (22%)	52,89,113	1.70	11 (21%)
16	CLA	B	824	-	43,51,73	1.76	10 (23%)	49,86,113	1.70	8 (16%)
22	BCR	B	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	7 (12%)
16	CLA	2	612	-	45,53,73	1.74	10 (22%)	52,89,113	1.70	8 (15%)
16	CLA	B	820	-	60,68,73	1.47	11 (18%)	70,107,113	1.68	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	2	602	-	65,73,73	1.48	8 (12%)	76,113,113	1.52	7 (9%)
16	CLA	2	606	-	45,53,73	1.72	9 (20%)	52,89,113	1.69	9 (17%)
23	SF4	C	101	-	0,12,12	-	-	-	-	-
16	CLA	A	818	-	65,73,73	1.48	11 (16%)	76,113,113	1.58	11 (14%)
16	CLA	2	613	-	45,53,73	1.75	7 (15%)	52,89,113	1.68	7 (13%)
16	CLA	A	811	-	54,62,73	1.55	9 (16%)	62,99,113	1.56	9 (14%)
16	CLA	A	808	4	65,73,73	1.50	10 (15%)	76,113,113	1.63	12 (15%)
16	CLA	2	607	-	45,53,73	1.72	10 (22%)	52,89,113	1.61	11 (21%)
16	CLA	3	205	-	45,53,73	1.76	9 (20%)	52,89,113	1.77	10 (19%)
16	CLA	B	821	-	65,73,73	1.48	10 (15%)	76,113,113	1.45	8 (10%)
16	CLA	A	809	-	55,63,73	1.57	9 (16%)	64,101,113	1.55	8 (12%)
22	BCR	I	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.34	7 (12%)
16	CLA	L	201	-	56,64,73	1.53	10 (17%)	65,102,113	1.52	7 (10%)
16	CLA	1	607	-	45,53,73	1.71	8 (17%)	52,89,113	1.78	9 (17%)
16	CLA	A	803	-	55,63,73	1.54	10 (18%)	64,101,113	1.77	9 (14%)
16	CLA	3	212	-	46,54,73	1.70	7 (15%)	53,90,113	1.65	7 (13%)
16	CLA	A	813	-	45,53,73	1.66	8 (17%)	52,89,113	1.81	10 (19%)
24	BGC	A	853	18	11,11,12	1.60	3 (27%)	15,15,17	1.00	0
17	ZEX	1	615	-	42,43,43	5.00	19 (45%)	55,60,60	5.04	29 (52%)
22	BCR	B	848	-	41,41,41	1.20	2 (4%)	56,56,56	1.53	10 (17%)
16	CLA	B	808	-	65,73,73	1.48	11 (16%)	76,113,113	1.48	11 (14%)
17	ZEX	3	215	-	42,43,43	5.04	19 (45%)	55,60,60	5.26	30 (54%)
16	CLA	1	612	-	45,53,73	1.73	7 (15%)	52,89,113	1.67	8 (15%)
16	CLA	B	802	-	65,73,73	1.57	10 (15%)	76,113,113	1.60	17 (22%)
16	CLA	3	207	-	45,53,73	1.73	9 (20%)	52,89,113	1.71	7 (13%)
16	CLA	A	815	-	45,53,73	1.72	9 (20%)	52,89,113	1.84	10 (19%)
16	CLA	B	839	-	47,55,73	1.64	9 (19%)	54,91,113	1.73	9 (16%)
16	CLA	K	102	-	42,50,73	1.79	9 (21%)	48,85,113	1.75	7 (14%)
16	CLA	B	814	-	55,63,73	1.53	8 (14%)	64,101,113	1.72	7 (10%)
16	CLA	2	611	-	45,53,73	1.71	9 (20%)	52,89,113	1.85	10 (19%)
16	CLA	B	828	-	65,73,73	1.47	10 (15%)	76,113,113	1.49	9 (11%)
16	CLA	A	837	-	65,73,73	1.39	8 (12%)	76,113,113	1.52	9 (11%)
22	BCR	B	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	6 (10%)
16	CLA	B	831	-	65,73,73	1.51	10 (15%)	76,113,113	1.85	15 (19%)
16	CLA	A	806	-	65,73,73	1.49	10 (15%)	76,113,113	1.69	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	812	-	65,73,73	1.43	10 (15%)	76,113,113	1.54	10 (13%)
17	ZEX	3	201	-	42,43,43	5.24	19 (45%)	55,60,60	5.24	28 (50%)
16	CLA	3	206	-	45,53,73	1.84	9 (20%)	52,89,113	1.87	12 (23%)
16	CLA	F	802	-	45,53,73	1.76	9 (20%)	52,89,113	1.72	11 (21%)
22	BCR	B	849	-	41,41,41	1.24	3 (7%)	56,56,56	1.51	9 (16%)
16	CLA	B	809	-	65,73,73	1.42	10 (15%)	76,113,113	1.46	10 (13%)
16	CLA	2	608	-	50,58,73	1.62	9 (18%)	58,95,113	1.77	11 (18%)
20	PQN	B	843	-	34,34,34	2.79	10 (29%)	42,45,45	2.16	5 (11%)
16	CLA	A	822	-	51,59,73	1.67	9 (17%)	59,96,113	1.57	7 (11%)
22	BCR	A	843	-	41,41,41	1.15	2 (4%)	56,56,56	1.30	6 (10%)
22	BCR	L	202	-	41,41,41	1.24	2 (4%)	56,56,56	1.34	6 (10%)
16	CLA	A	817	-	65,73,73	1.44	11 (16%)	76,113,113	1.53	11 (14%)
20	PQN	A	840	-	34,34,34	2.79	10 (29%)	42,45,45	2.16	6 (14%)
22	BCR	B	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
16	CLA	2	604	-	42,50,73	1.70	10 (23%)	48,85,113	1.81	8 (16%)
16	CLA	B	813	-	54,62,73	1.66	7 (12%)	67,100,113	1.59	11 (16%)
17	ZEX	2	617	-	42,43,43	4.87	19 (45%)	55,60,60	5.24	30 (54%)
22	BCR	A	845	-	41,41,41	1.27	3 (7%)	56,56,56	1.43	8 (14%)
22	BCR	A	846	-	41,41,41	1.27	2 (4%)	56,56,56	1.33	7 (12%)
17	ZEX	1	616	-	42,43,43	5.08	19 (45%)	55,60,60	5.13	28 (50%)
16	CLA	A	820	-	65,73,73	1.49	10 (15%)	76,113,113	1.60	9 (11%)
22	BCR	L	206	-	41,41,41	1.13	2 (4%)	56,56,56	1.49	10 (17%)
22	BCR	A	849	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	8 (14%)
17	ZEX	1	617	-	42,43,43	4.93	19 (45%)	55,60,60	5.31	27 (49%)
16	CLA	B	803	-	65,73,73	1.42	10 (15%)	76,113,113	1.59	11 (14%)
16	CLA	2	601	-	45,53,73	1.75	10 (22%)	52,89,113	1.79	9 (17%)
16	CLA	B	833	-	65,73,73	1.51	9 (13%)	76,113,113	1.46	9 (11%)
22	BCR	A	847	-	41,41,41	1.31	3 (7%)	56,56,56	1.29	7 (12%)
16	CLA	B	835	-	65,73,73	1.42	10 (15%)	76,113,113	1.52	9 (11%)
16	CLA	A	821	-	49,57,73	1.62	9 (18%)	55,93,113	1.72	9 (16%)
23	SF4	C	102	-	0,12,12	-	-	-	-	-
16	CLA	B	810	-	65,73,73	1.44	10 (15%)	76,113,113	1.67	11 (14%)
16	CLA	B	801	-	65,73,73	1.46	12 (18%)	76,113,113	2.01	15 (19%)
22	BCR	A	844	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	9 (16%)
16	CLA	A	826	-	65,73,73	1.45	10 (15%)	76,113,113	1.56	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	825	-	55,63,73	1.59	10 (18%)	64,101,113	1.53	9 (14%)
16	CLA	B	836	-	45,53,73	1.78	10 (22%)	52,89,113	1.67	7 (13%)
16	CLA	O	204	-	45,53,73	1.76	7 (15%)	52,89,113	1.60	8 (15%)
16	CLA	A	804	-	65,73,73	1.51	11 (16%)	76,113,113	1.67	11 (14%)
16	CLA	A	829	-	65,73,73	1.61	13 (20%)	76,113,113	1.84	22 (28%)
16	CLA	L	204	-	65,73,73	1.42	10 (15%)	76,113,113	1.46	8 (10%)
16	CLA	3	202	-	45,53,73	1.74	7 (15%)	52,89,113	1.72	10 (19%)
16	CLA	A	823	-	55,63,73	1.55	10 (18%)	64,101,113	1.67	8 (12%)
16	CLA	O	201	-	52,60,73	1.62	8 (15%)	60,97,113	1.63	9 (15%)
16	CLA	A	816	-	62,70,73	1.47	10 (16%)	72,109,113	1.53	9 (12%)
16	CLA	K	101	-	45,53,73	1.72	10 (22%)	52,89,113	1.72	7 (13%)
16	CLA	B	834	-	58,66,73	1.54	11 (18%)	67,104,113	1.59	10 (14%)
16	CLA	A	835	-	51,59,73	1.56	9 (17%)	59,96,113	1.82	11 (18%)
16	CLA	3	203	-	63,71,73	1.47	9 (14%)	73,110,113	1.58	9 (12%)
16	CLA	B	806	-	45,53,73	1.72	9 (20%)	52,89,113	1.80	8 (15%)
16	CLA	B	807	-	65,73,73	1.43	10 (15%)	76,113,113	1.60	11 (14%)
16	CLA	A	827	-	65,73,73	1.47	10 (15%)	76,113,113	1.63	11 (14%)
16	CLA	B	805	-	65,73,73	1.53	10 (15%)	76,113,113	1.87	14 (18%)
22	BCR	L	207	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	5 (8%)
16	CLA	1	604	-	45,53,73	1.64	8 (17%)	52,89,113	1.86	8 (15%)
16	CLA	B	815	-	65,73,73	1.42	10 (15%)	76,113,113	1.53	11 (14%)
16	CLA	A	839	-	65,73,73	1.43	11 (16%)	76,113,113	1.61	9 (11%)
16	CLA	B	838	-	65,73,73	1.52	10 (15%)	76,113,113	1.51	9 (11%)
16	CLA	A	810	-	65,73,73	1.44	10 (15%)	76,113,113	1.57	11 (14%)
22	BCR	B	844	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	8 (14%)
16	CLA	1	605	-	41,50,73	1.84	5 (12%)	46,85,113	1.72	8 (17%)
16	CLA	A	836	-	65,73,73	1.46	10 (15%)	76,113,113	1.58	11 (14%)
16	CLA	L	205	-	50,58,73	1.64	9 (18%)	58,95,113	1.70	10 (17%)
16	CLA	A	833	-	65,73,73	1.44	9 (13%)	76,113,113	1.57	11 (14%)
16	CLA	2	610	-	42,50,73	1.79	9 (21%)	48,85,113	1.77	8 (16%)
16	CLA	A	814	-	42,50,73	1.73	8 (19%)	48,85,113	2.01	8 (16%)
16	CLA	A	828	-	65,73,73	1.53	10 (15%)	76,113,113	1.58	13 (17%)
16	CLA	B	830	-	65,73,73	1.50	9 (13%)	76,113,113	1.52	10 (13%)
16	CLA	A	830	-	50,58,73	1.67	10 (20%)	58,95,113	1.52	10 (17%)
16	CLA	B	841	-	65,73,73	1.49	11 (16%)	76,113,113	1.49	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	K	103	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	5 (8%)
16	CLA	A	850	-	65,73,73	1.48	11 (16%)	76,113,113	2.15	17 (22%)
16	CLA	1	602	-	59,67,73	1.44	8 (13%)	68,105,113	1.63	7 (10%)
16	CLA	A	825	-	55,63,73	1.57	10 (18%)	64,101,113	1.70	11 (17%)
17	ZEX	3	216	-	42,43,43	5.10	19 (45%)	55,60,60	5.10	30 (54%)
16	CLA	A	807	4	65,73,73	1.39	10 (15%)	76,113,113	1.53	10 (13%)
16	CLA	A	824	-	65,73,73	1.49	10 (15%)	76,113,113	1.55	13 (17%)
16	CLA	F	803	-	41,49,73	1.80	8 (19%)	47,84,113	1.76	7 (14%)
19	CL0	A	801	-	65,73,73	2.87	20 (30%)	76,113,113	3.27	39 (51%)
16	CLA	B	842	-	65,73,73	1.43	7 (10%)	76,113,113	1.41	7 (9%)
16	CLA	A	838	-	65,73,73	1.43	10 (15%)	76,113,113	1.56	9 (11%)
16	CLA	B	812	-	65,73,73	1.46	9 (13%)	76,113,113	1.49	8 (10%)
16	CLA	O	202	-	41,49,73	1.84	6 (14%)	47,84,113	1.79	9 (19%)
17	ZEX	2	616	-	42,43,43	5.14	20 (47%)	55,60,60	5.01	29 (52%)
25	DGD	B	850	-	67,67,67	0.98	4 (5%)	81,81,81	1.51	13 (16%)
17	ZEX	3	217	-	42,43,43	5.10	19 (45%)	55,60,60	4.92	29 (52%)
17	ZEX	3	218	-	42,43,43	5.46	20 (47%)	55,60,60	4.43	32 (58%)
16	CLA	3	210	-	41,49,73	1.81	6 (14%)	47,84,113	1.80	8 (17%)
16	CLA	O	203	-	50,58,73	1.68	6 (12%)	58,95,113	1.59	9 (15%)
21	LHG	A	842	-	39,39,48	0.75	1 (2%)	42,45,54	1.30	6 (14%)
22	BCR	F	801	-	41,41,41	1.26	3 (7%)	56,56,56	1.47	8 (14%)
16	CLA	B	832	-	45,53,73	1.74	10 (22%)	52,89,113	1.68	9 (17%)
16	CLA	J	101	-	42,50,73	1.75	10 (23%)	48,85,113	1.70	9 (18%)
16	CLA	A	819	-	45,53,73	1.73	9 (20%)	52,89,113	1.74	7 (13%)
16	CLA	3	209	-	52,60,73	1.58	6 (11%)	60,97,113	1.70	8 (13%)
16	CLA	A	832	-	65,73,73	1.42	11 (16%)	76,113,113	1.64	12 (15%)
16	CLA	1	609	-	41,49,73	1.76	7 (17%)	47,84,113	1.85	8 (17%)
16	CLA	A	831	-	65,73,73	1.44	10 (15%)	76,113,113	1.55	10 (13%)
16	CLA	3	213	-	51,59,73	1.64	7 (13%)	59,96,113	1.60	8 (13%)
16	CLA	3	208	-	45,53,73	1.78	8 (17%)	52,89,113	1.64	8 (15%)
16	CLA	2	609	-	41,49,73	1.76	6 (14%)	47,84,113	1.87	7 (14%)
16	CLA	2	603	-	45,53,73	1.73	10 (22%)	52,89,113	1.71	8 (15%)
16	CLA	1	603	-	45,53,73	1.76	10 (22%)	52,89,113	1.61	8 (15%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	J	103	-	-	15/29/63/63	0/2/2/2
16	CLA	1	611	-	1/1/11/20	8/13/91/115	-
16	CLA	A	834	-	1/1/11/20	6/13/91/115	-
17	ZEX	2	614	-	-	17/29/67/67	0/2/2/2
16	CLA	B	804	-	1/1/15/20	14/37/115/115	-
16	CLA	2	605	-	1/1/11/20	5/13/91/115	-
16	CLA	3	204	-	1/1/11/20	10/13/91/115	-
16	CLA	B	822	-	1/1/11/20	5/13/91/115	-
16	CLA	B	823	-	1/1/11/20	6/15/93/115	-
18	1DO	3	219	24	-	1/10/10/10	-
16	CLA	B	816	-	1/1/11/20	4/13/91/115	-
16	CLA	3	211	-	1/1/10/20	0/10/88/115	-
16	CLA	A	802	-	1/1/15/20	21/37/115/115	-
16	CLA	1	608	-	1/1/14/20	9/31/109/115	-
17	ZEX	2	615	-	-	20/29/67/67	0/2/2/2
16	CLA	B	811	-	1/1/15/20	13/37/115/115	-
21	LHG	A	841	-	-	27/53/53/53	-
16	CLA	1	610	-	1/1/11/20	4/13/91/115	-
26	3XQ	J	104	-	-	14/24/24/24	-
16	CLA	B	817	-	1/1/10/20	4/10/88/115	-
16	CLA	B	840	-	1/1/15/20	13/37/115/115	-
23	SF4	A	848	-	-	-	0/6/5/5
16	CLA	B	819	-	1/1/13/20	13/30/108/115	-
22	BCR	J	102	-	-	16/29/63/63	0/2/2/2
16	CLA	B	826	-	1/1/15/20	10/37/115/115	-
16	CLA	B	818	-	1/1/13/20	15/25/103/115	-
16	CLA	A	851	-	1/1/10/20	2/11/89/115	-
17	ZEX	1	614	-	-	17/29/67/67	0/2/2/2
16	CLA	B	829	-	1/1/15/20	20/37/115/115	-
16	CLA	B	837	-	1/1/14/20	16/31/109/115	-
16	CLA	A	805	-	1/1/15/20	18/37/115/115	-
16	CLA	1	601	-	1/1/11/20	6/17/95/115	-
16	CLA	L	203	-	1/1/13/20	15/28/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ZEX	1	613	-	-	18/29/67/67	0/2/2/2
22	BCR	F	804	-	-	19/29/63/63	0/2/2/2
16	CLA	A	852	-	1/1/14/20	13/33/111/115	-
17	ZEX	3	214	-	-	15/29/67/67	0/2/2/2
16	CLA	B	827	-	1/1/15/20	10/37/115/115	-
16	CLA	1	606	-	1/1/11/20	6/13/91/115	-
16	CLA	B	824	-	1/1/10/20	4/11/89/115	-
22	BCR	B	847	-	-	18/29/63/63	0/2/2/2
16	CLA	2	612	-	1/1/11/20	7/13/91/115	-
16	CLA	B	820	-	1/1/14/20	11/31/109/115	-
16	CLA	2	602	-	1/1/15/20	11/37/115/115	-
16	CLA	2	606	-	1/1/11/20	5/13/91/115	-
23	SF4	C	101	-	-	-	0/6/5/5
16	CLA	A	818	-	1/1/15/20	15/37/115/115	-
16	CLA	2	613	-	1/1/11/20	1/13/91/115	-
16	CLA	A	811	-	1/1/12/20	6/24/102/115	-
16	CLA	A	808	4	1/1/15/20	19/37/115/115	-
16	CLA	2	607	-	1/1/11/20	7/13/91/115	-
16	CLA	3	205	-	1/1/11/20	6/13/91/115	-
16	CLA	B	821	-	1/1/15/20	13/37/115/115	-
16	CLA	A	809	-	1/1/13/20	6/25/103/115	-
22	BCR	I	101	-	-	18/29/63/63	0/2/2/2
16	CLA	L	201	-	1/1/13/20	5/27/105/115	-
16	CLA	1	607	-	1/1/11/20	7/13/91/115	-
16	CLA	A	803	-	1/1/13/20	7/25/103/115	-
16	CLA	3	212	-	1/1/11/20	8/15/93/115	-
16	CLA	A	813	-	1/1/11/20	8/13/91/115	-
24	BGC	A	853	18	-	2/2/19/22	0/1/1/1
17	ZEX	1	615	-	-	18/29/67/67	0/2/2/2
22	BCR	B	848	-	-	23/29/63/63	0/2/2/2
16	CLA	B	808	-	1/1/15/20	16/37/115/115	-
17	ZEX	3	215	-	-	16/29/67/67	0/2/2/2
16	CLA	1	612	-	1/1/11/20	4/13/91/115	-
16	CLA	B	802	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	3	207	-	1/1/11/20	4/13/91/115	-
16	CLA	A	815	-	1/1/11/20	6/13/91/115	-
16	CLA	B	839	-	1/1/11/20	2/16/94/115	-
16	CLA	K	102	-	1/1/10/20	3/10/88/115	-
16	CLA	B	814	-	1/1/13/20	6/25/103/115	-
16	CLA	2	611	-	1/1/11/20	6/13/91/115	-
16	CLA	B	828	-	1/1/15/20	12/37/115/115	-
16	CLA	A	837	-	1/1/15/20	13/37/115/115	-
22	BCR	B	845	-	-	11/29/63/63	0/2/2/2
16	CLA	B	831	-	1/1/15/20	14/37/115/115	-
16	CLA	A	806	-	1/1/15/20	18/37/115/115	-
16	CLA	A	812	-	1/1/15/20	9/37/115/115	-
17	ZEX	3	201	-	-	18/29/67/67	0/2/2/2
16	CLA	3	206	-	1/1/11/20	6/13/91/115	-
16	CLA	F	802	-	1/1/11/20	4/13/91/115	-
22	BCR	B	849	-	-	14/29/63/63	0/2/2/2
16	CLA	B	809	-	1/1/15/20	15/37/115/115	-
16	CLA	2	608	-	1/1/12/20	8/19/97/115	-
20	PQN	B	843	-	-	7/23/43/43	0/2/2/2
16	CLA	A	822	-	1/1/12/20	11/21/99/115	-
22	BCR	A	843	-	-	13/29/63/63	0/2/2/2
22	BCR	L	202	-	-	20/29/63/63	0/2/2/2
16	CLA	A	817	-	1/1/15/20	12/37/115/115	-
20	PQN	A	840	-	-	9/23/43/43	0/2/2/2
22	BCR	B	846	-	-	20/29/63/63	0/2/2/2
16	CLA	2	604	-	1/1/10/20	4/10/88/115	-
16	CLA	B	813	-	1/1/13/20	6/25/101/115	-
17	ZEX	2	617	-	-	19/29/67/67	0/2/2/2
22	BCR	A	845	-	-	18/29/63/63	0/2/2/2
22	BCR	A	846	-	-	16/29/63/63	0/2/2/2
17	ZEX	1	616	-	-	18/29/67/67	0/2/2/2
16	CLA	A	820	-	1/1/15/20	15/37/115/115	-
22	BCR	L	206	-	-	18/29/63/63	0/2/2/2
22	BCR	A	849	-	-	17/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ZEX	1	617	-	-	17/29/67/67	0/2/2/2
16	CLA	B	803	-	1/1/15/20	16/37/115/115	-
16	CLA	2	601	-	1/1/11/20	7/13/91/115	-
16	CLA	B	833	-	1/1/15/20	21/37/115/115	-
22	BCR	A	847	-	-	18/29/63/63	0/2/2/2
16	CLA	B	835	-	1/1/15/20	15/37/115/115	-
16	CLA	A	821	-	1/1/11/20	6/18/96/115	-
23	SF4	C	102	-	-	-	0/6/5/5
16	CLA	B	810	-	1/1/15/20	8/37/115/115	-
16	CLA	B	801	-	1/1/15/20	15/37/115/115	-
22	BCR	A	844	-	-	17/29/63/63	0/2/2/2
16	CLA	A	826	-	1/1/15/20	10/37/115/115	-
16	CLA	B	825	-	1/1/13/20	10/25/103/115	-
16	CLA	B	836	-	1/1/11/20	9/13/91/115	-
16	CLA	O	204	-	1/1/11/20	4/13/91/115	-
16	CLA	A	804	-	1/1/15/20	5/37/115/115	-
16	CLA	A	829	-	1/1/15/20	10/37/115/115	-
16	CLA	L	204	-	1/1/15/20	17/37/115/115	-
16	CLA	3	202	-	1/1/11/20	7/13/91/115	-
16	CLA	A	823	-	1/1/13/20	7/25/103/115	-
16	CLA	O	201	-	1/1/12/20	8/22/100/115	-
16	CLA	A	816	-	1/1/14/20	11/34/112/115	-
16	CLA	K	101	-	1/1/11/20	4/13/91/115	-
16	CLA	B	834	-	1/1/13/20	8/29/107/115	-
16	CLA	A	835	-	1/1/12/20	9/21/99/115	-
16	CLA	3	203	-	1/1/14/20	19/35/113/115	-
16	CLA	B	806	-	1/1/11/20	7/13/91/115	-
16	CLA	B	807	-	1/1/15/20	14/37/115/115	-
16	CLA	A	827	-	1/1/15/20	12/37/115/115	-
16	CLA	B	805	-	1/1/15/20	17/37/115/115	-
22	BCR	L	207	-	-	16/29/63/63	0/2/2/2
16	CLA	1	604	-	1/1/11/20	7/13/91/115	-
16	CLA	B	815	-	1/1/15/20	21/37/115/115	-
16	CLA	A	839	-	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	838	-	1/1/15/20	8/37/115/115	-
16	CLA	A	810	-	1/1/15/20	16/37/115/115	-
22	BCR	B	844	-	-	13/29/63/63	0/2/2/2
16	CLA	1	605	-	1/1/10/20	4/9/87/115	-
16	CLA	A	836	-	1/1/15/20	15/37/115/115	-
16	CLA	L	205	-	1/1/12/20	6/19/97/115	-
16	CLA	A	833	-	1/1/15/20	9/37/115/115	-
16	CLA	2	610	-	1/1/10/20	6/10/88/115	-
16	CLA	A	814	-	1/1/10/20	5/10/88/115	-
16	CLA	A	828	-	1/1/15/20	19/37/115/115	-
16	CLA	B	830	-	1/1/15/20	15/37/115/115	-
16	CLA	A	830	-	1/1/12/20	4/19/97/115	-
16	CLA	B	841	-	1/1/15/20	12/37/115/115	-
22	BCR	K	103	-	-	18/29/63/63	0/2/2/2
16	CLA	A	850	-	1/1/15/20	11/37/115/115	-
16	CLA	1	602	-	1/1/13/20	9/30/108/115	-
16	CLA	A	825	-	1/1/13/20	4/25/103/115	-
19	CL0	A	801	-	3/3/20/25	11/37/135/135	-
16	CLA	A	807	4	1/1/15/20	13/37/115/115	-
16	CLA	A	824	-	1/1/15/20	12/37/115/115	-
16	CLA	F	803	-	1/1/10/20	3/8/86/115	-
17	ZEX	3	216	-	-	15/29/67/67	0/2/2/2
16	CLA	B	842	-	1/1/15/20	12/37/115/115	-
16	CLA	A	838	-	1/1/15/20	11/37/115/115	-
16	CLA	B	812	-	1/1/15/20	16/37/115/115	-
16	CLA	O	202	-	1/1/10/20	3/8/86/115	-
17	ZEX	2	616	-	-	20/29/67/67	0/2/2/2
25	DGD	B	850	-	-	31/55/95/95	0/2/2/2
17	ZEX	3	217	-	-	17/29/67/67	0/2/2/2
17	ZEX	3	218	-	-	17/29/67/67	0/2/2/2
16	CLA	3	210	-	1/1/10/20	4/8/86/115	-
16	CLA	O	203	-	1/1/12/20	6/19/97/115	-
21	LHG	A	842	-	-	19/44/44/53	-
22	BCR	F	801	-	-	17/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	832	-	1/1/11/20	4/13/91/115	-
16	CLA	J	101	-	1/1/10/20	7/10/88/115	-
16	CLA	A	819	-	1/1/11/20	9/13/91/115	-
16	CLA	3	209	-	1/1/12/20	6/22/100/115	-
16	CLA	A	832	-	1/1/15/20	13/37/115/115	-
16	CLA	1	609	-	1/1/10/20	0/8/86/115	-
16	CLA	A	831	-	1/1/15/20	18/37/115/115	-
16	CLA	3	213	-	1/1/12/20	7/21/99/115	-
16	CLA	3	208	-	1/1/11/20	8/13/91/115	-
16	CLA	2	609	-	1/1/10/20	4/8/86/115	-
16	CLA	2	603	-	1/1/11/20	4/13/91/115	-
16	CLA	1	603	-	1/1/11/20	7/13/91/115	-

The worst 5 of 1611 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	218	ZEX	C14-C13	15.79	1.56	1.35
17	1	616	ZEX	C14-C13	14.77	1.55	1.35
17	3	201	ZEX	C14-C13	14.74	1.55	1.35
17	3	217	ZEX	C14-C13	14.51	1.55	1.35
17	2	616	ZEX	C14-C13	14.43	1.54	1.35

The worst 5 of 1960 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	614	ZEX	C31-C30-C29	-16.56	103.68	127.31
19	A	801	CL0	C4A-NA-C1A	14.24	113.11	106.71
17	1	617	ZEX	C31-C30-C29	-13.77	107.66	127.31
17	3	201	ZEX	C31-C30-C29	-13.19	108.48	127.31
17	1	615	ZEX	C18-C5-C6	-13.08	109.84	124.53

5 of 136 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	1	601	CLA	ND
16	1	602	CLA	ND
16	1	603	CLA	ND
16	1	604	CLA	ND
16	1	605	CLA	ND

5 of 1990 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	601	CLA	CBD-CGD-O2D-CED
16	1	602	CLA	CBD-CGD-O2D-CED
16	1	603	CLA	CBD-CGD-O2D-CED
16	1	604	CLA	C1A-C2A-CAA-CBA
16	1	604	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

158 monomers are involved in 473 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	J	103	BCR	5	0
16	1	611	CLA	1	0
16	A	834	CLA	6	0
17	2	614	ZEX	3	0
16	B	804	CLA	10	0
16	2	605	CLA	1	0
16	3	204	CLA	1	0
16	B	823	CLA	2	0
16	B	816	CLA	2	0
16	A	802	CLA	9	0
17	2	615	ZEX	4	0
16	B	811	CLA	8	0
21	A	841	LHG	2	0
16	1	610	CLA	1	0
16	B	817	CLA	2	0
16	B	840	CLA	7	0
16	B	819	CLA	1	0
22	J	102	BCR	3	0
16	B	826	CLA	4	0
16	B	818	CLA	2	0
16	A	851	CLA	2	0
17	1	614	ZEX	6	0
16	B	829	CLA	10	0
16	B	837	CLA	3	0
16	A	805	CLA	5	0
17	1	613	ZEX	7	0
16	A	852	CLA	3	0
17	3	214	ZEX	4	0
16	B	827	CLA	6	0
16	1	606	CLA	1	0
16	B	824	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	847	BCR	5	0
16	B	820	CLA	3	0
16	2	602	CLA	4	0
16	2	606	CLA	1	0
16	A	818	CLA	8	0
16	A	808	CLA	5	0
16	2	607	CLA	4	0
16	3	205	CLA	2	0
16	B	821	CLA	3	0
16	A	809	CLA	3	0
22	I	101	BCR	2	0
16	L	201	CLA	1	0
16	1	607	CLA	3	0
16	A	803	CLA	2	0
16	3	212	CLA	1	0
17	1	615	ZEX	2	0
22	B	848	BCR	5	0
16	B	808	CLA	5	0
17	3	215	ZEX	5	0
16	1	612	CLA	1	0
16	B	802	CLA	22	0
16	3	207	CLA	1	0
16	A	815	CLA	2	0
16	B	839	CLA	6	0
16	K	102	CLA	3	0
16	2	611	CLA	2	0
16	B	828	CLA	6	0
16	A	837	CLA	2	0
22	B	845	BCR	4	0
16	B	831	CLA	5	0
16	A	806	CLA	2	0
16	A	812	CLA	6	0
17	3	201	ZEX	7	0
16	3	206	CLA	5	0
16	F	802	CLA	3	0
22	B	849	BCR	3	0
16	B	809	CLA	3	0
16	2	608	CLA	1	0
20	B	843	PQN	5	0
16	A	822	CLA	1	0
22	A	843	BCR	3	0
22	L	202	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	817	CLA	5	0
20	A	840	PQN	2	0
22	B	846	BCR	4	0
16	2	604	CLA	1	0
17	2	617	ZEX	4	0
22	A	845	BCR	4	0
22	A	846	BCR	4	0
17	1	616	ZEX	2	0
16	A	820	CLA	3	0
22	L	206	BCR	9	0
22	A	849	BCR	1	0
17	1	617	ZEX	2	0
16	B	803	CLA	6	0
16	2	601	CLA	4	0
16	B	833	CLA	9	0
22	A	847	BCR	4	0
16	B	835	CLA	6	0
16	A	821	CLA	1	0
23	C	102	SF4	1	0
16	B	810	CLA	5	0
16	B	801	CLA	6	0
16	A	826	CLA	7	0
16	B	825	CLA	6	0
16	B	836	CLA	2	0
16	O	204	CLA	1	0
16	A	804	CLA	7	0
16	A	829	CLA	7	0
16	L	204	CLA	2	0
16	A	823	CLA	2	0
16	O	201	CLA	1	0
16	A	816	CLA	4	0
16	K	101	CLA	1	0
16	B	834	CLA	3	0
16	A	835	CLA	1	0
16	3	203	CLA	5	0
16	B	807	CLA	10	0
16	A	827	CLA	10	0
16	B	805	CLA	6	0
22	L	207	BCR	1	0
16	1	604	CLA	2	0
16	B	815	CLA	9	0
16	A	839	CLA	3	0

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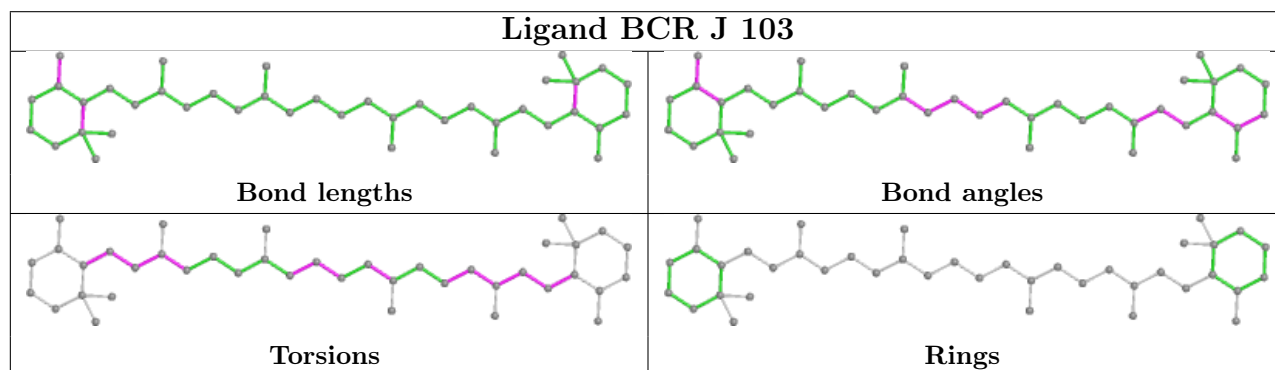
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	838	CLA	1	0
16	A	810	CLA	5	0
22	B	844	BCR	1	0
16	1	605	CLA	2	0
16	A	836	CLA	9	0
16	L	205	CLA	1	0
16	A	833	CLA	5	0
16	2	610	CLA	1	0
16	A	814	CLA	1	0
16	A	828	CLA	3	0
16	B	830	CLA	4	0
16	A	830	CLA	1	0
16	B	841	CLA	9	0
22	K	103	BCR	5	0
16	A	850	CLA	6	0
16	1	602	CLA	1	0
16	A	825	CLA	4	0
17	3	216	ZEX	3	0
16	A	807	CLA	5	0
16	A	824	CLA	4	0
16	F	803	CLA	1	0
19	A	801	CL0	56	0
16	B	842	CLA	4	0
16	A	838	CLA	4	0
16	B	812	CLA	3	0
17	2	616	ZEX	1	0
25	B	850	DGD	4	0
17	3	217	ZEX	2	0
17	3	218	ZEX	6	0
16	3	210	CLA	1	0
16	O	203	CLA	1	0
21	A	842	LHG	2	0
22	F	801	BCR	4	0
16	B	832	CLA	6	0
16	J	101	CLA	2	0
16	A	819	CLA	3	0
16	3	209	CLA	2	0
16	A	832	CLA	3	0
16	1	609	CLA	2	0
16	A	831	CLA	9	0
16	3	208	CLA	1	0
16	2	603	CLA	1	0

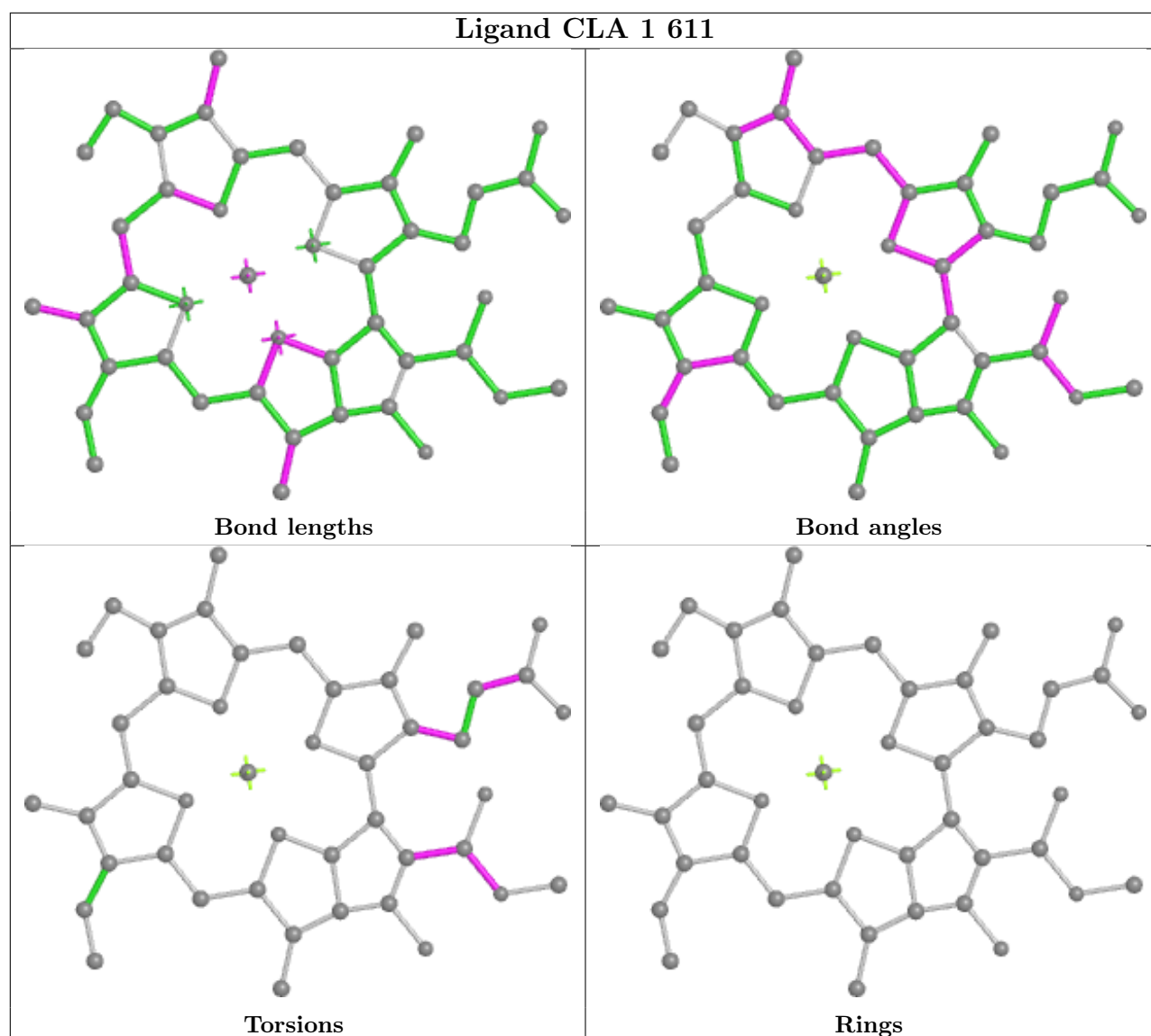
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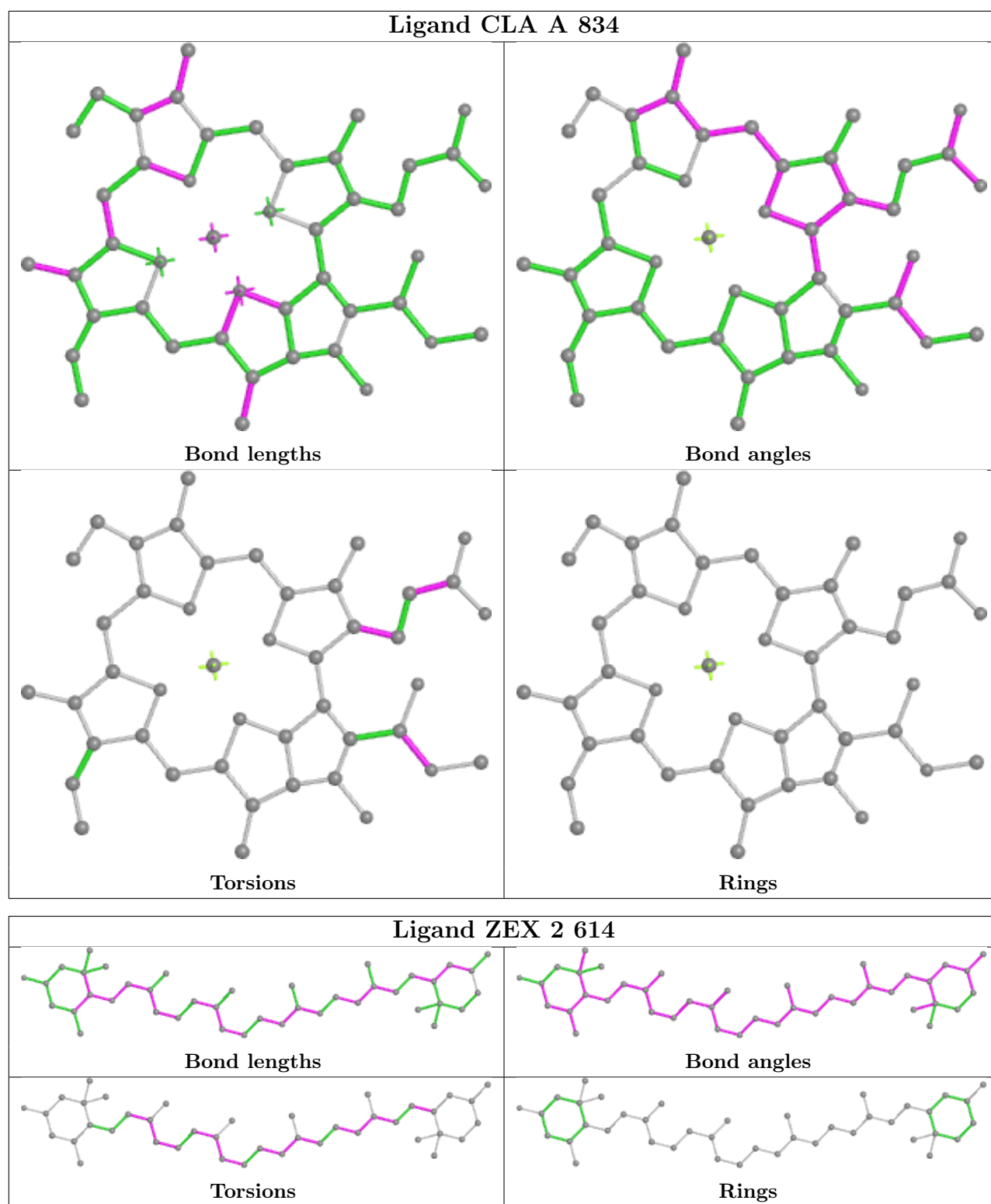
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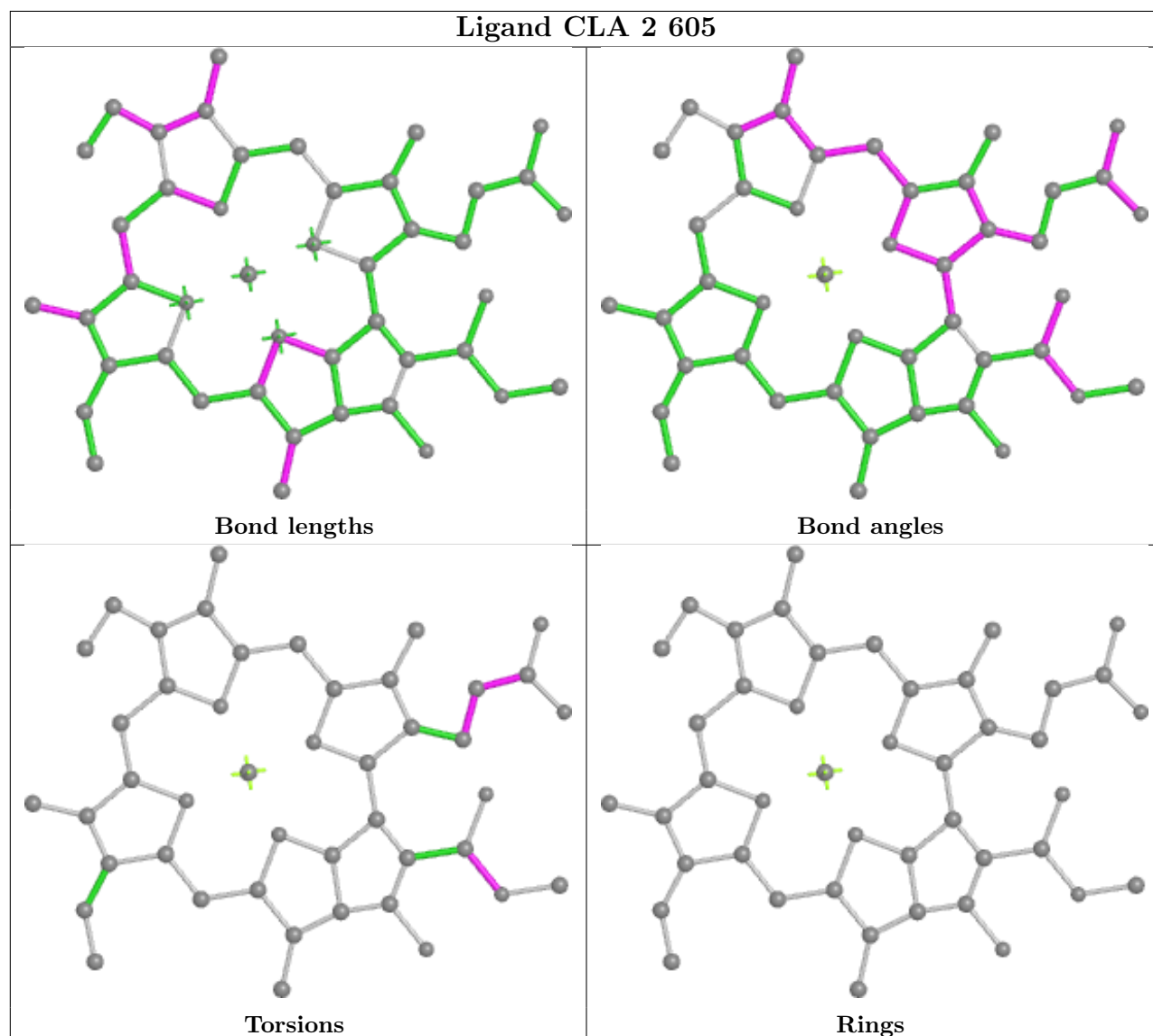
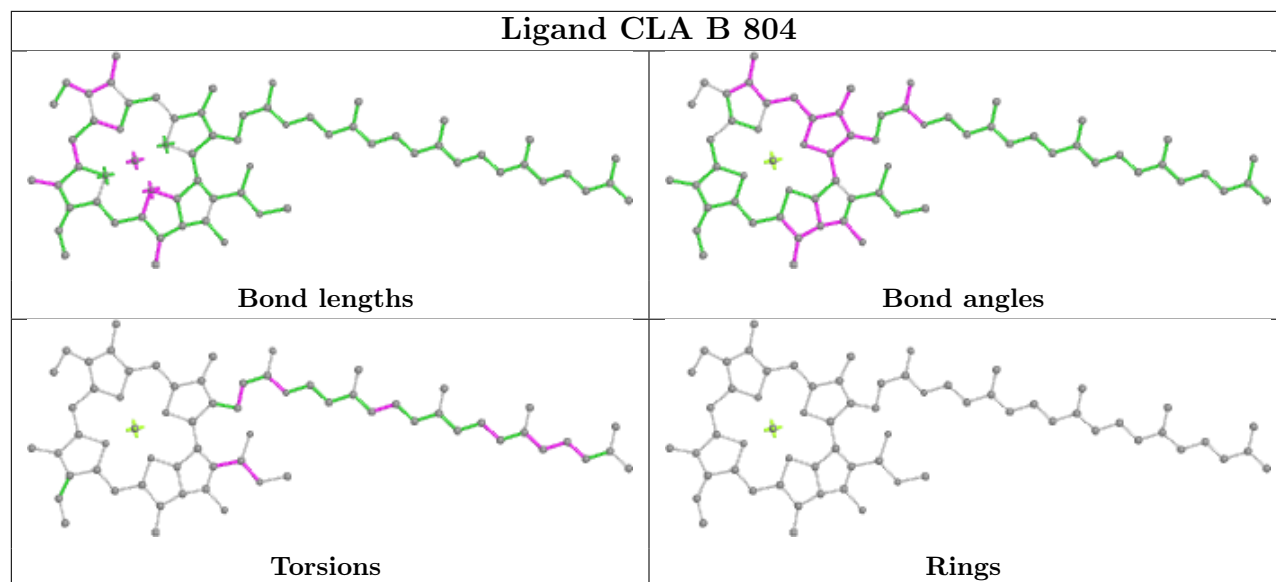
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	603	CLA	2	0

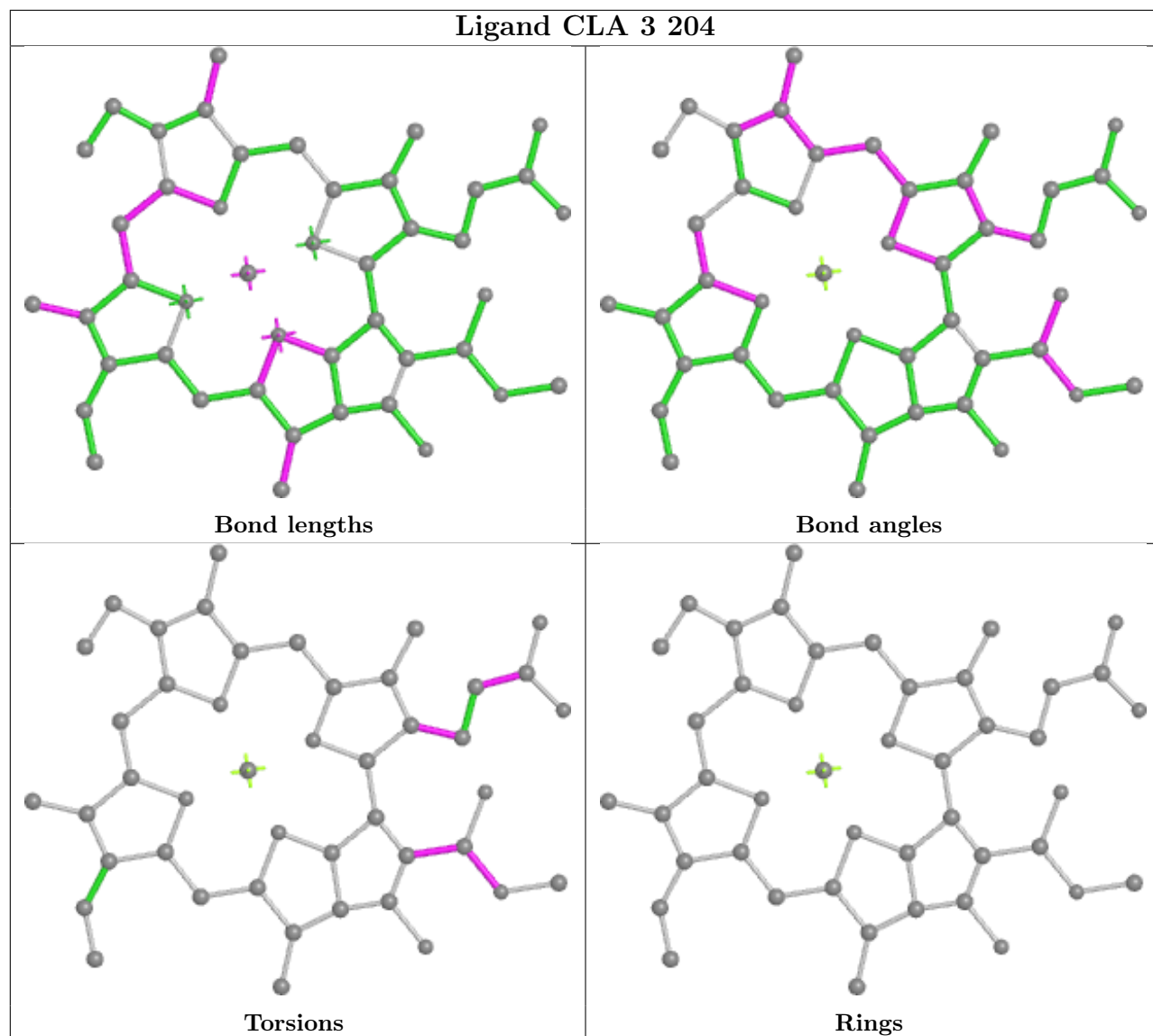
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

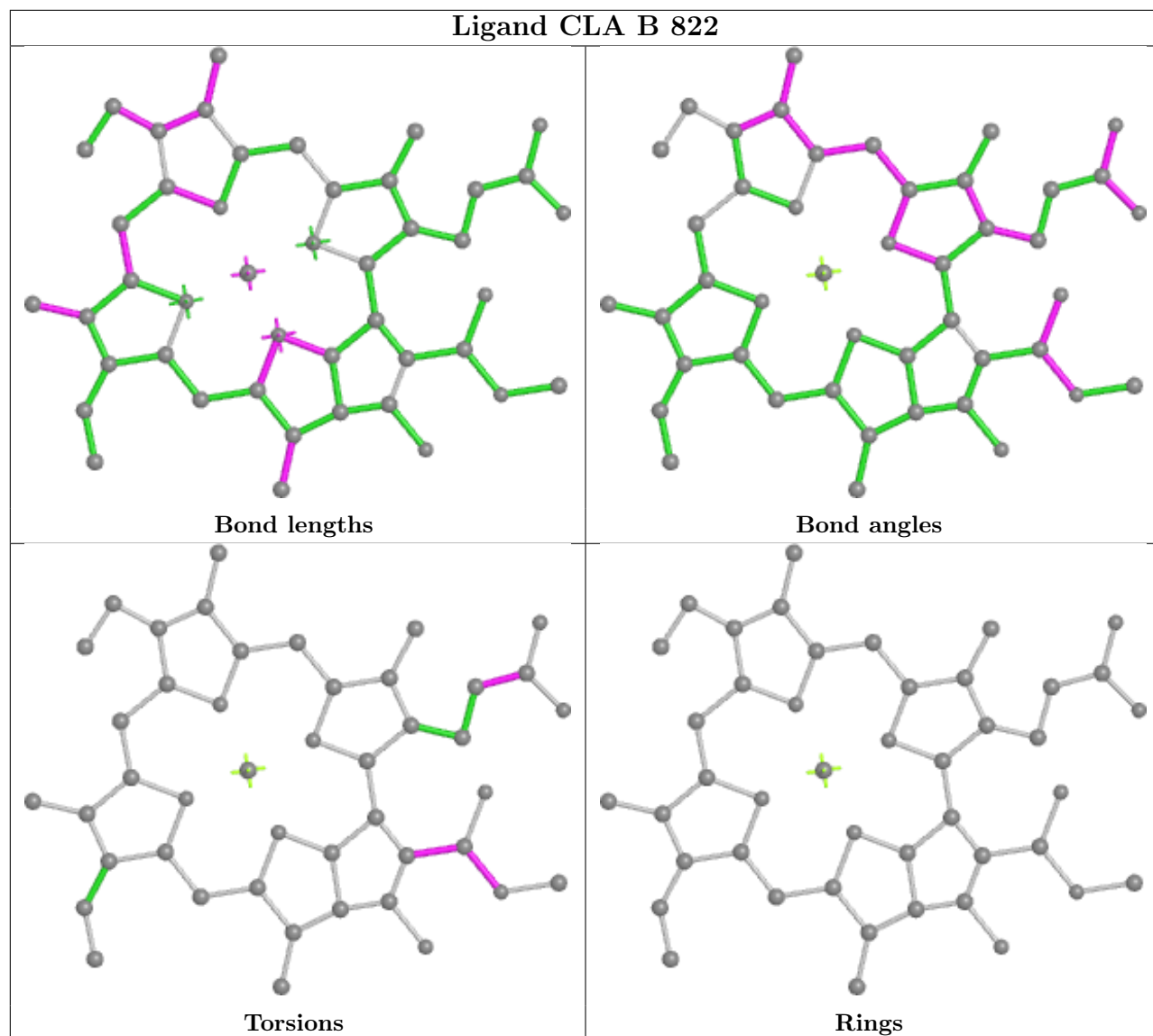


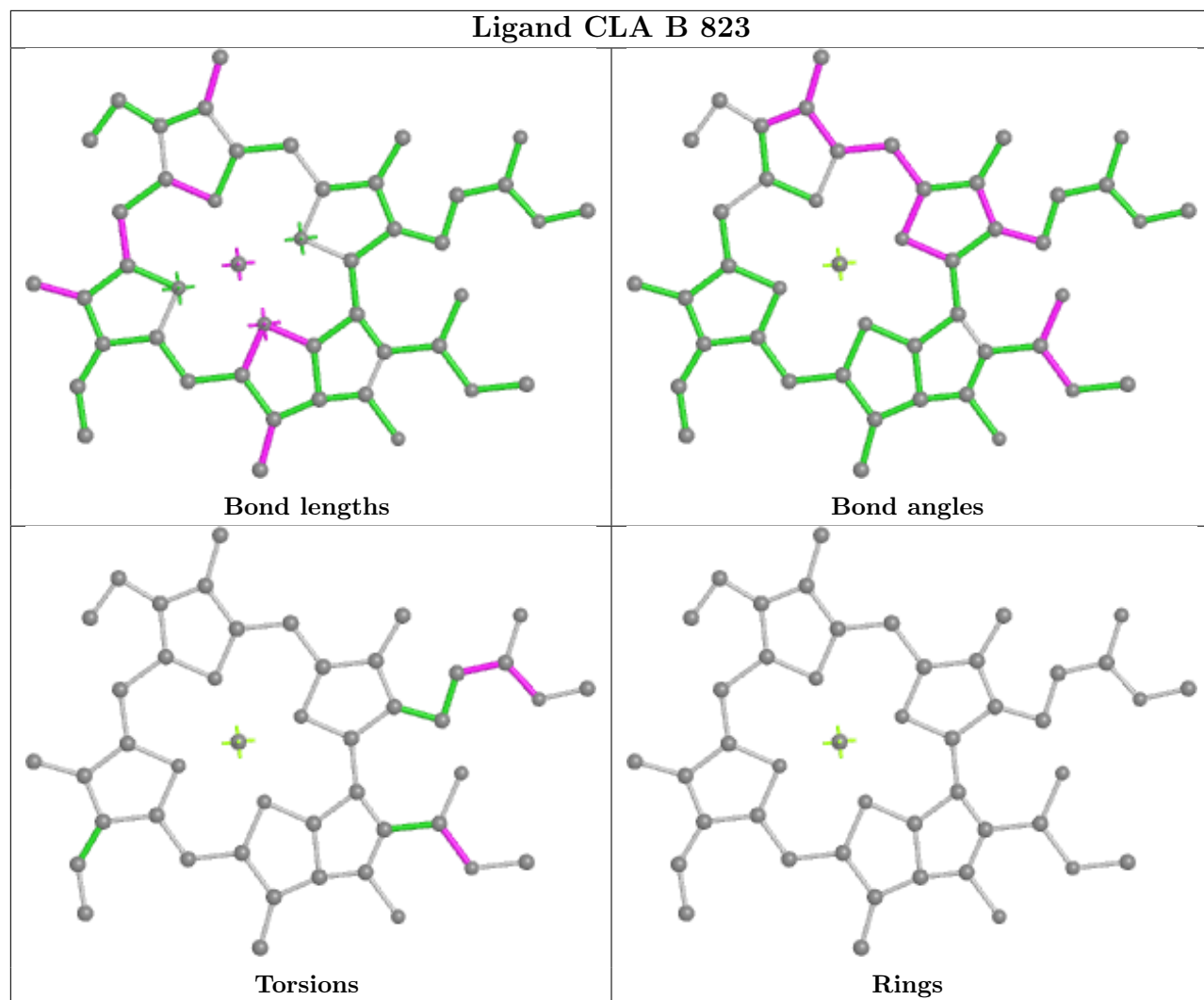


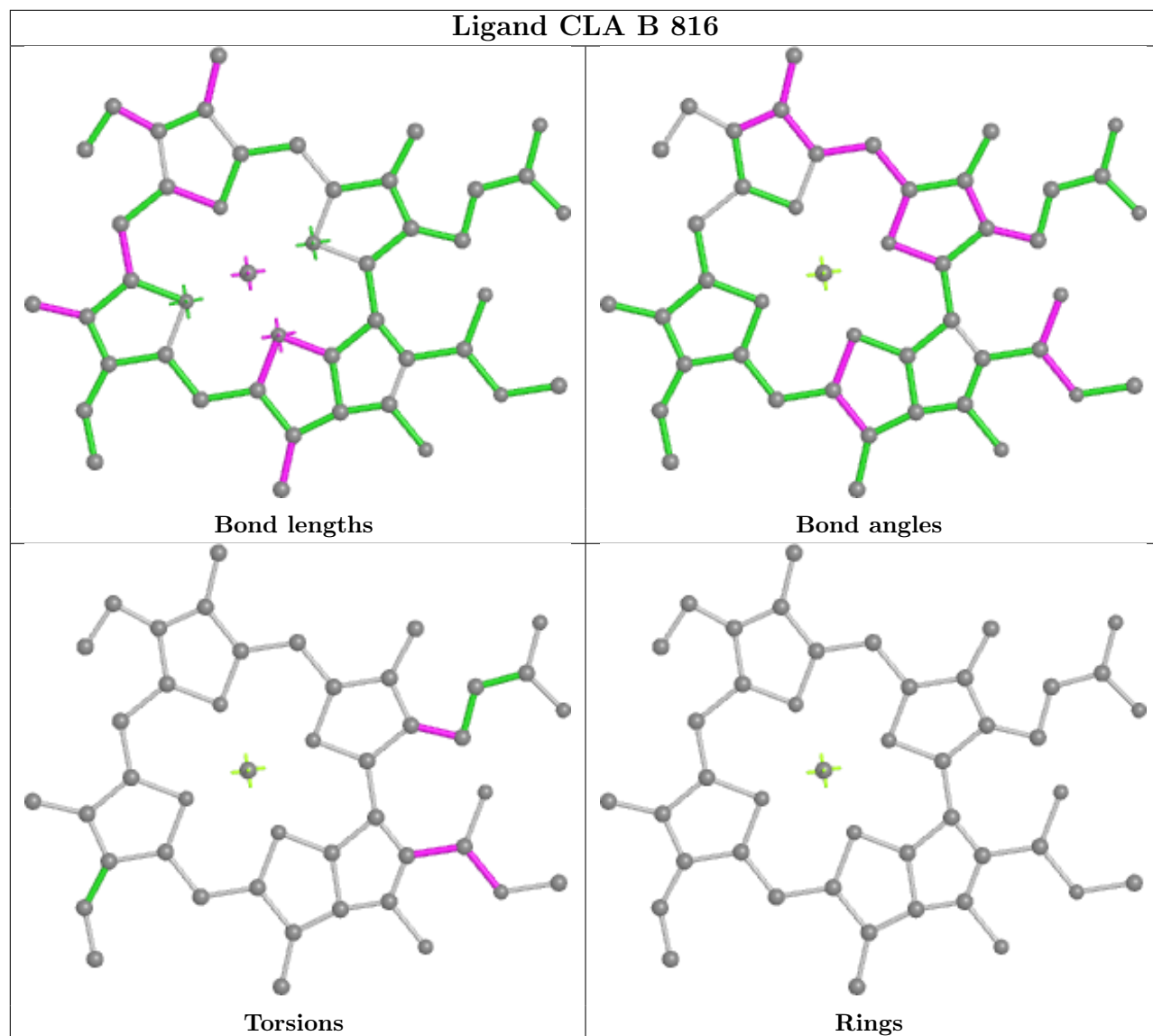


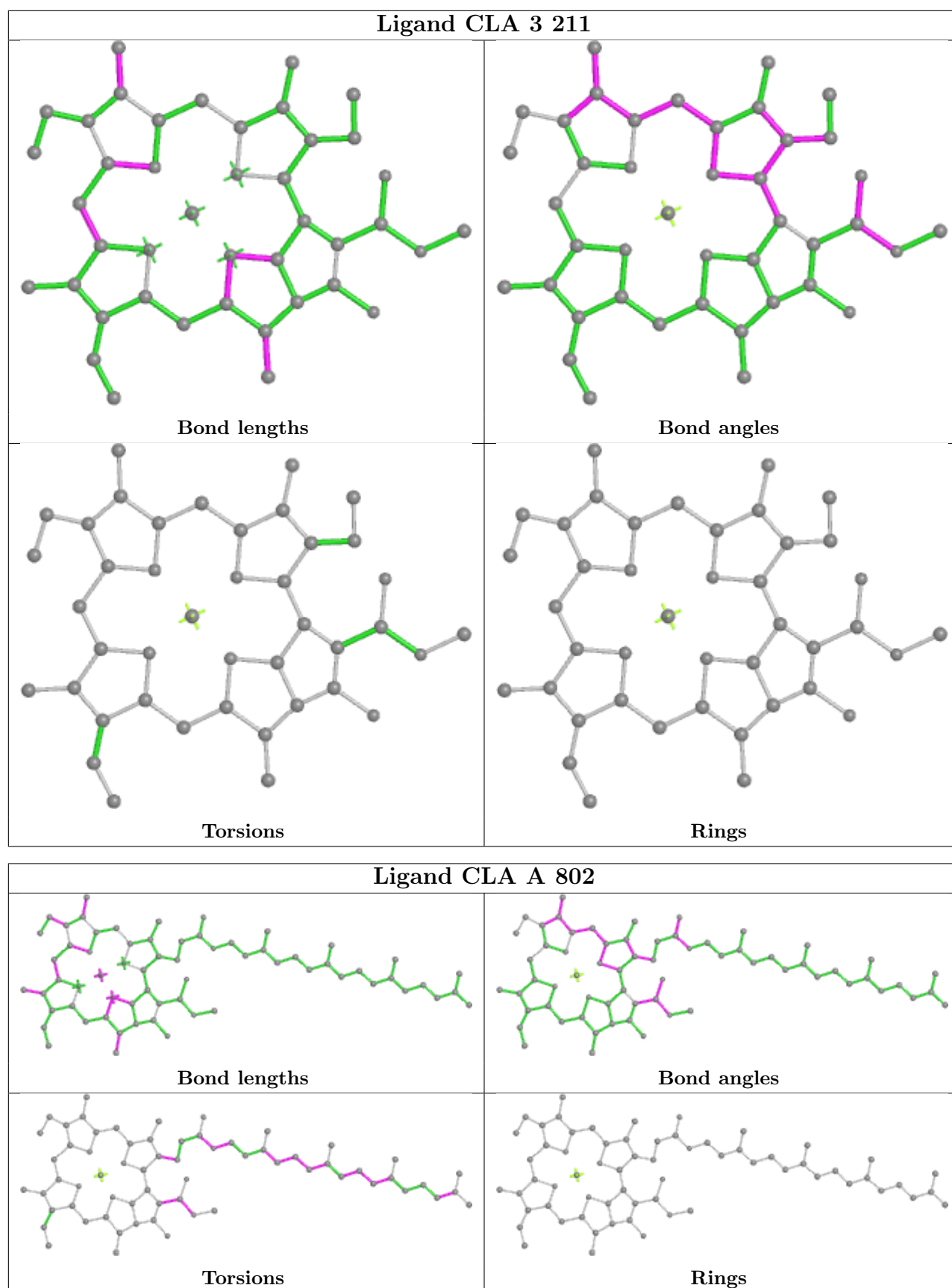


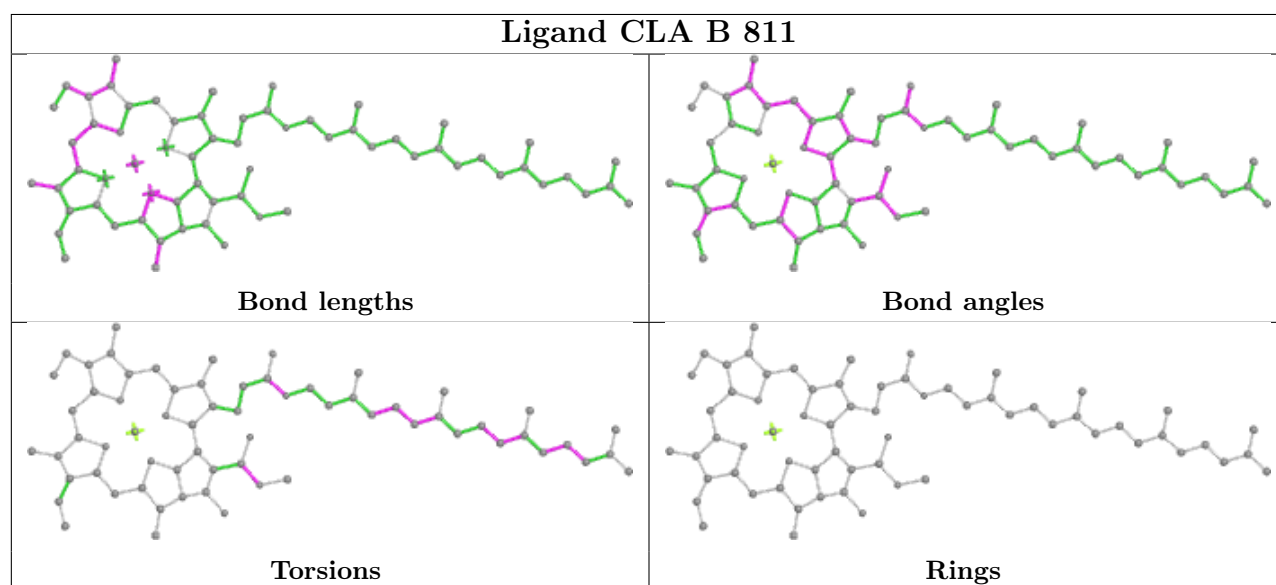
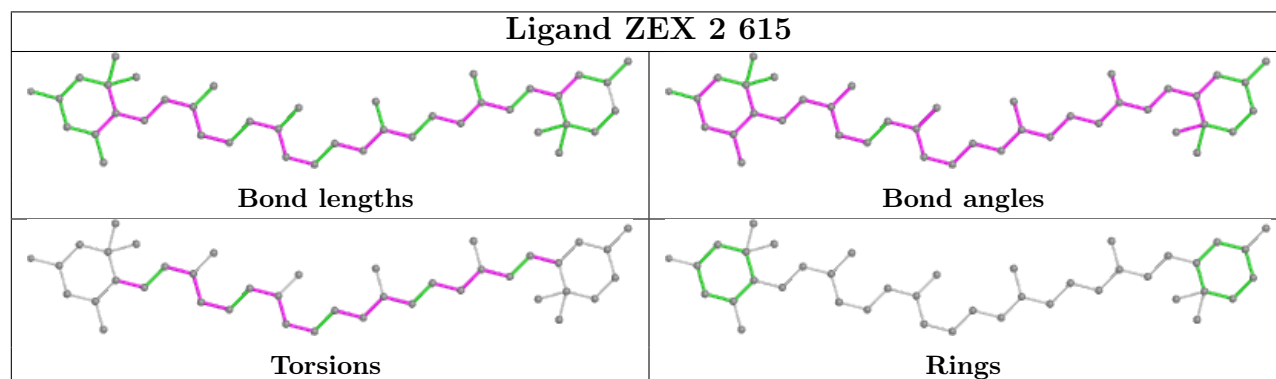
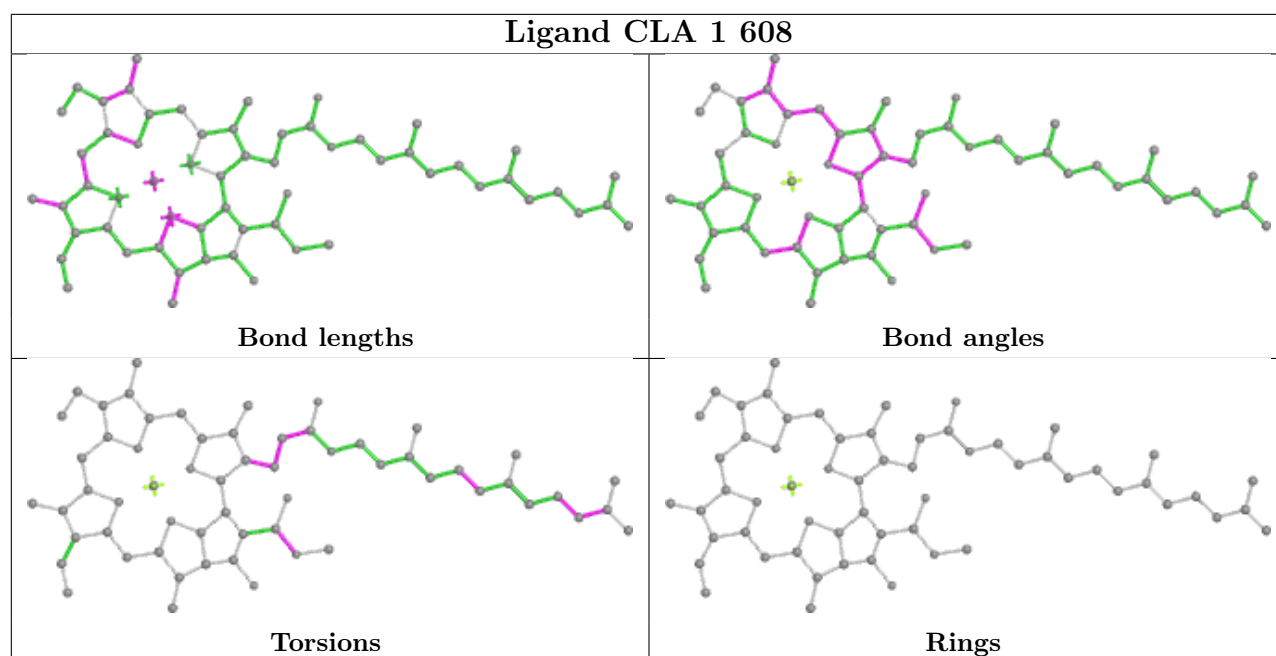


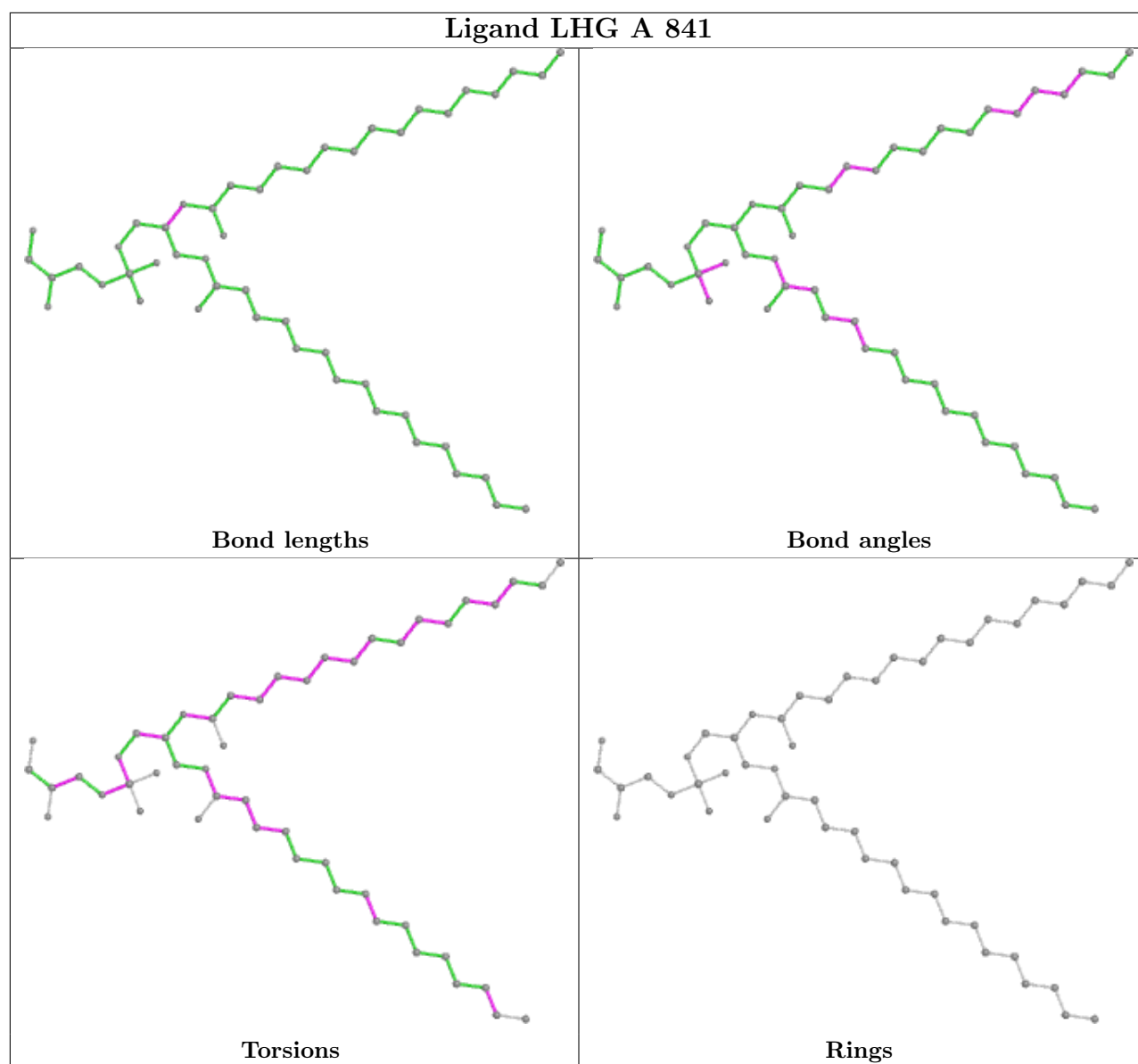


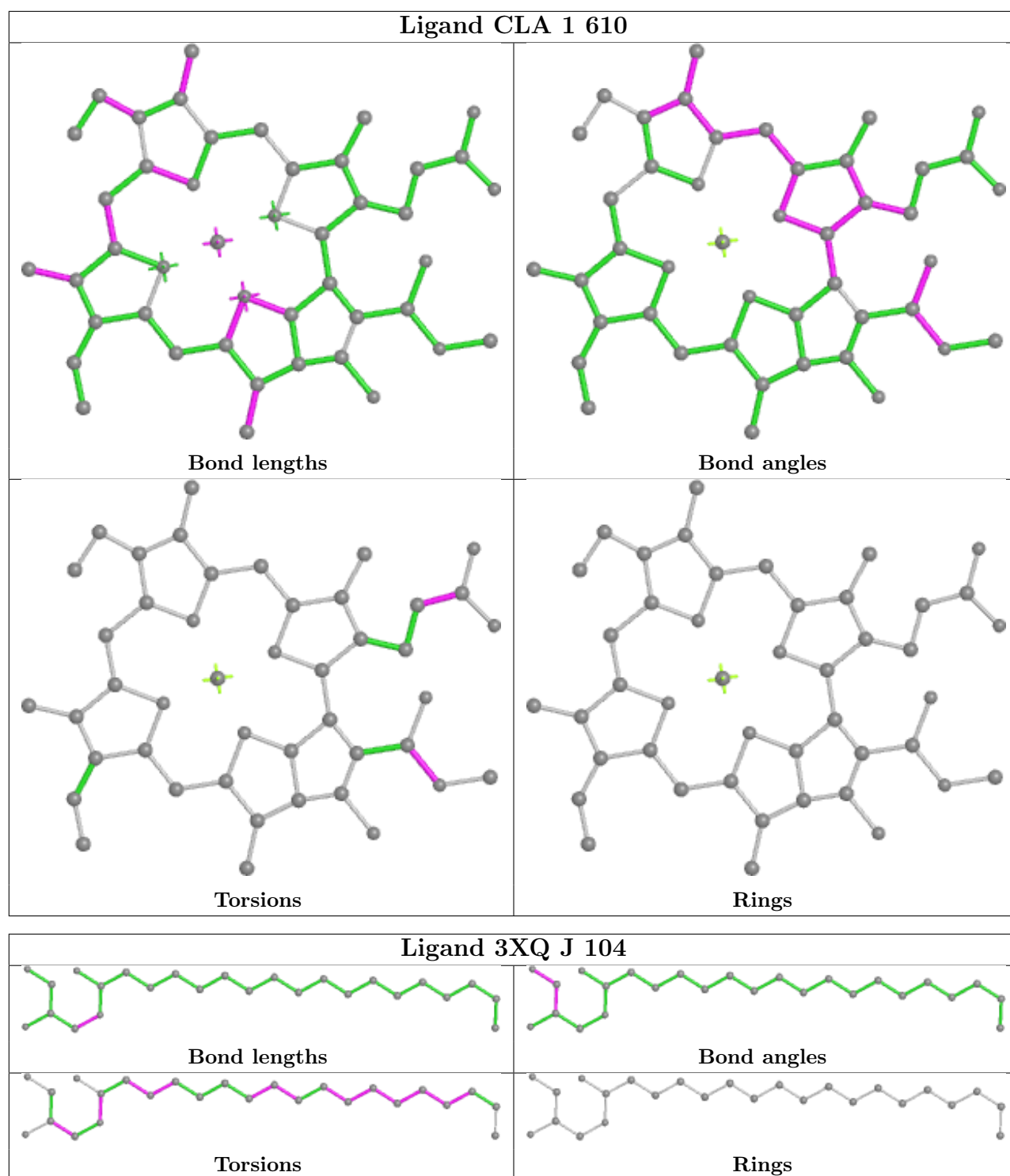


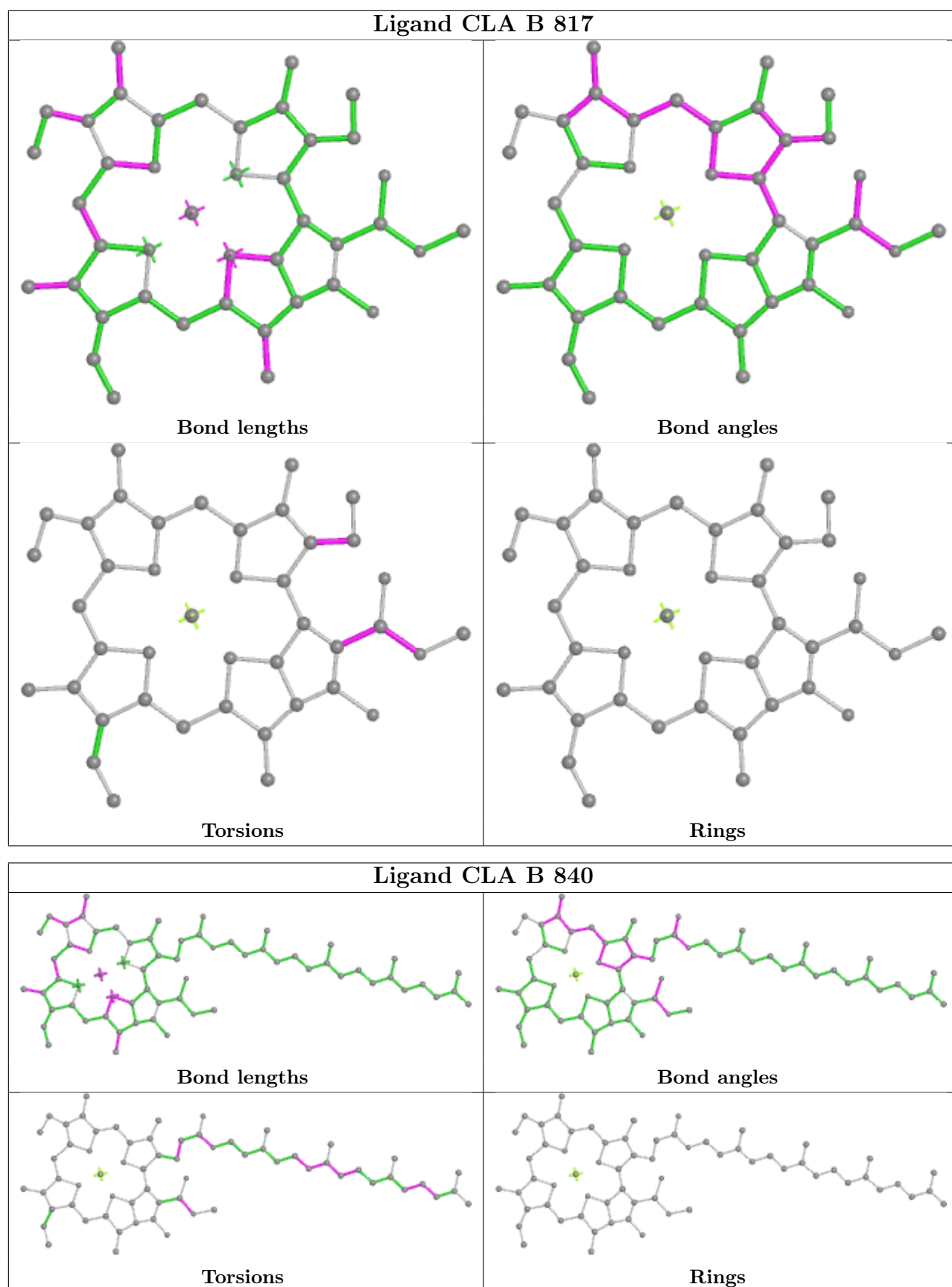


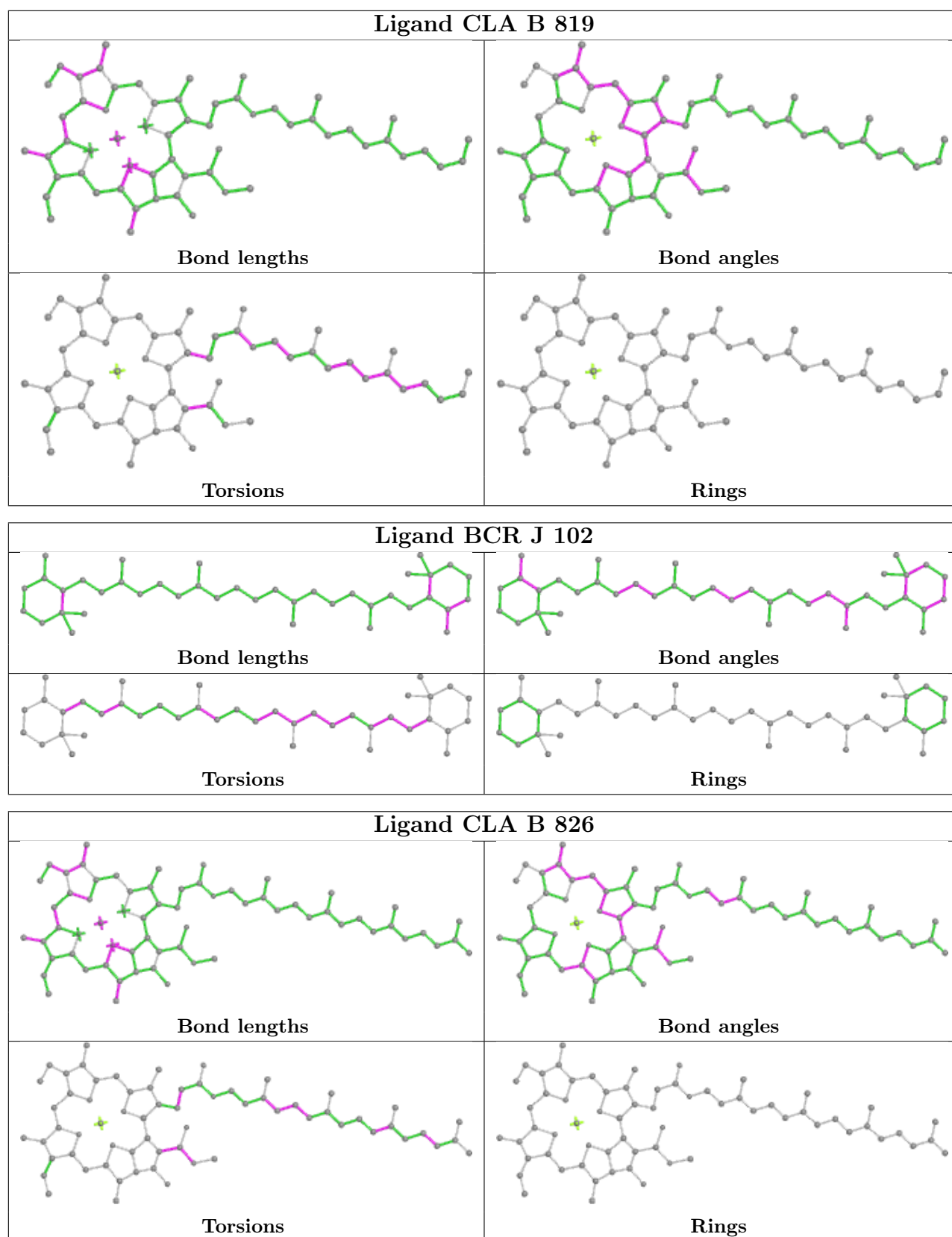


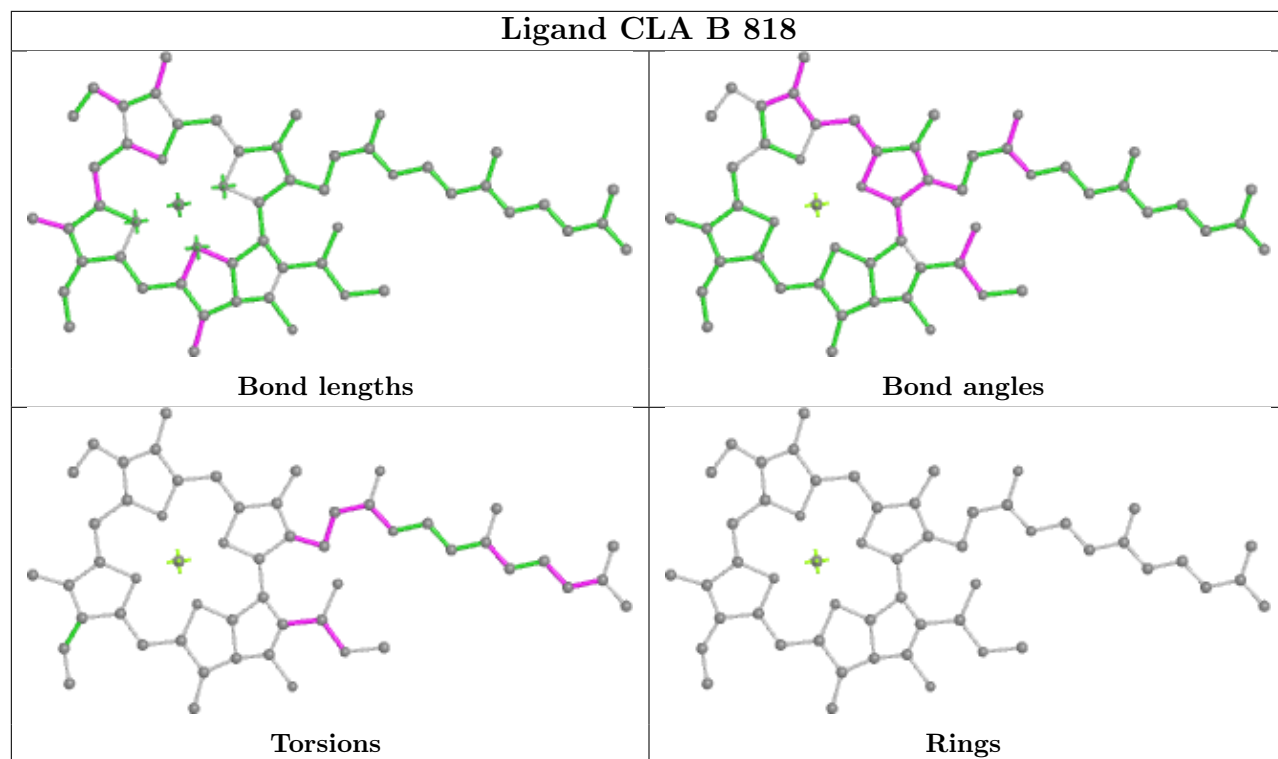


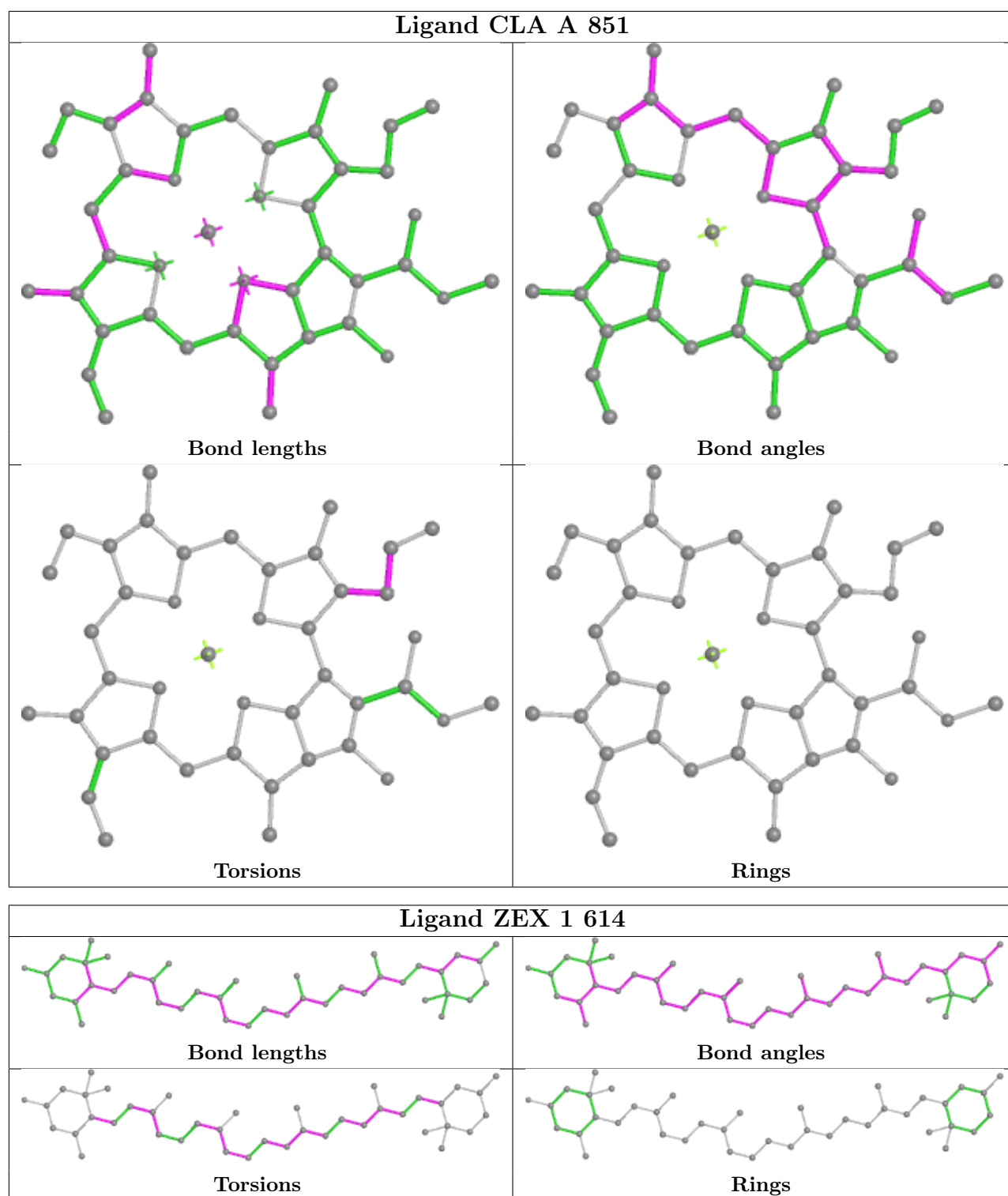


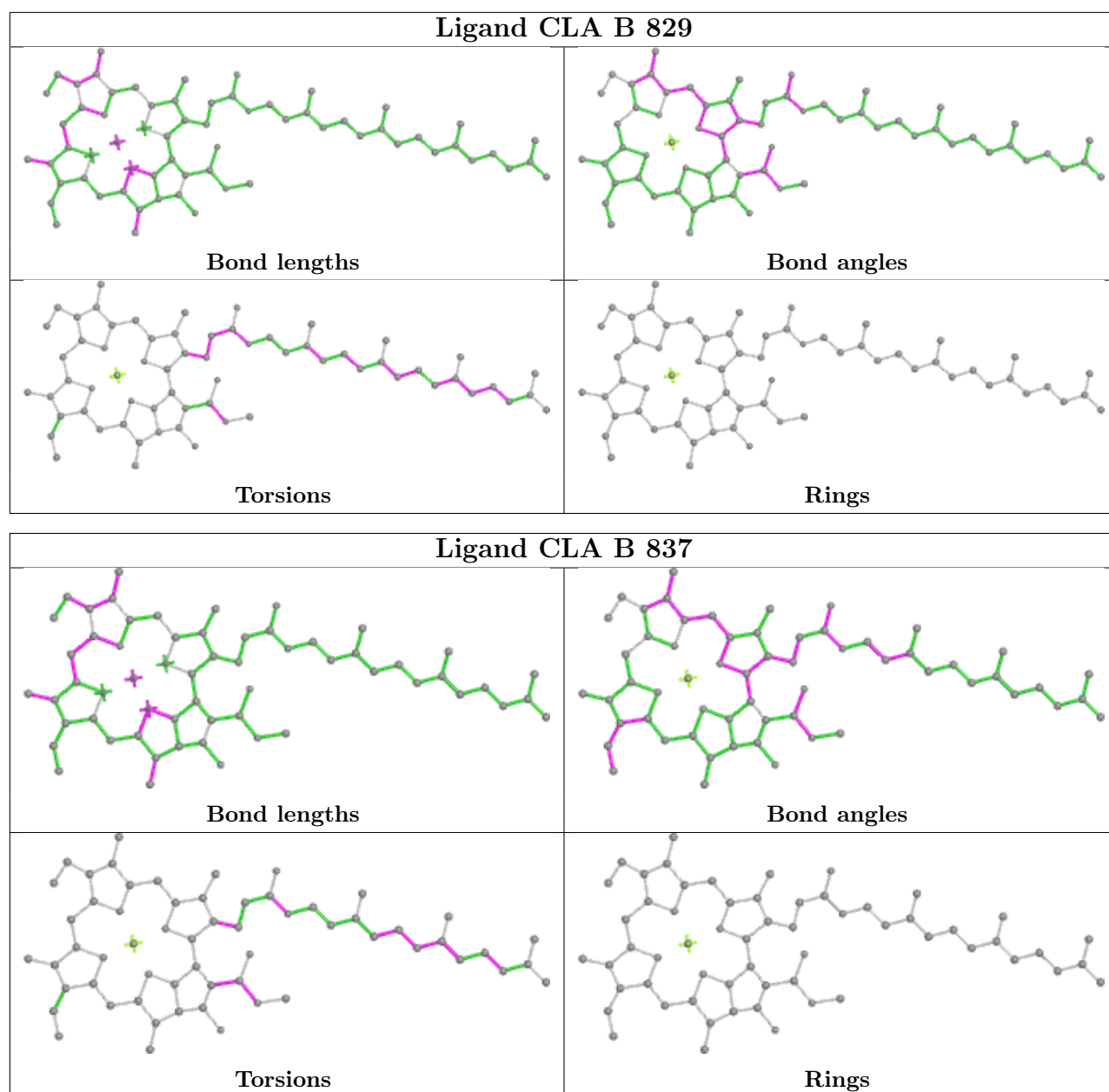


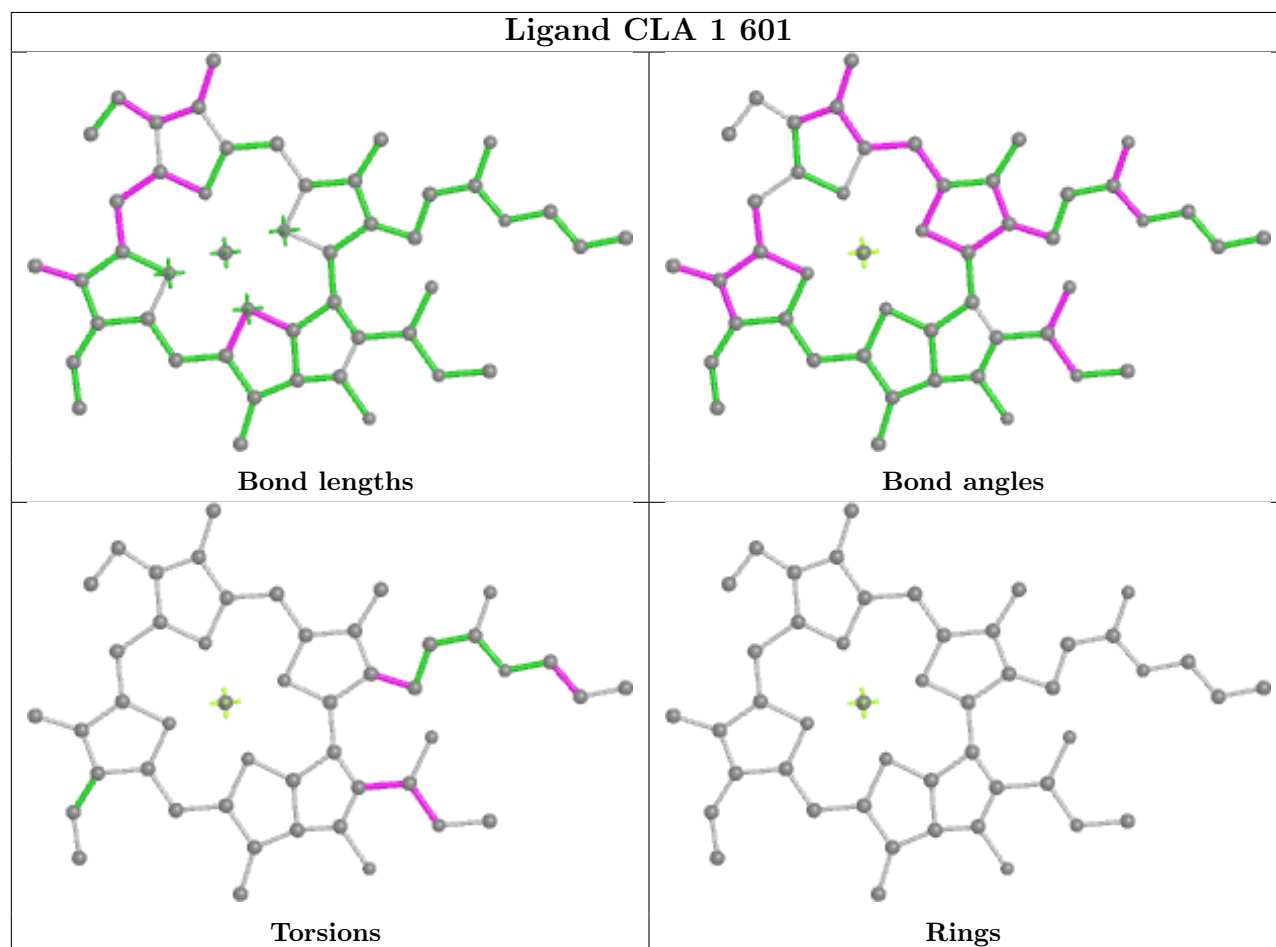
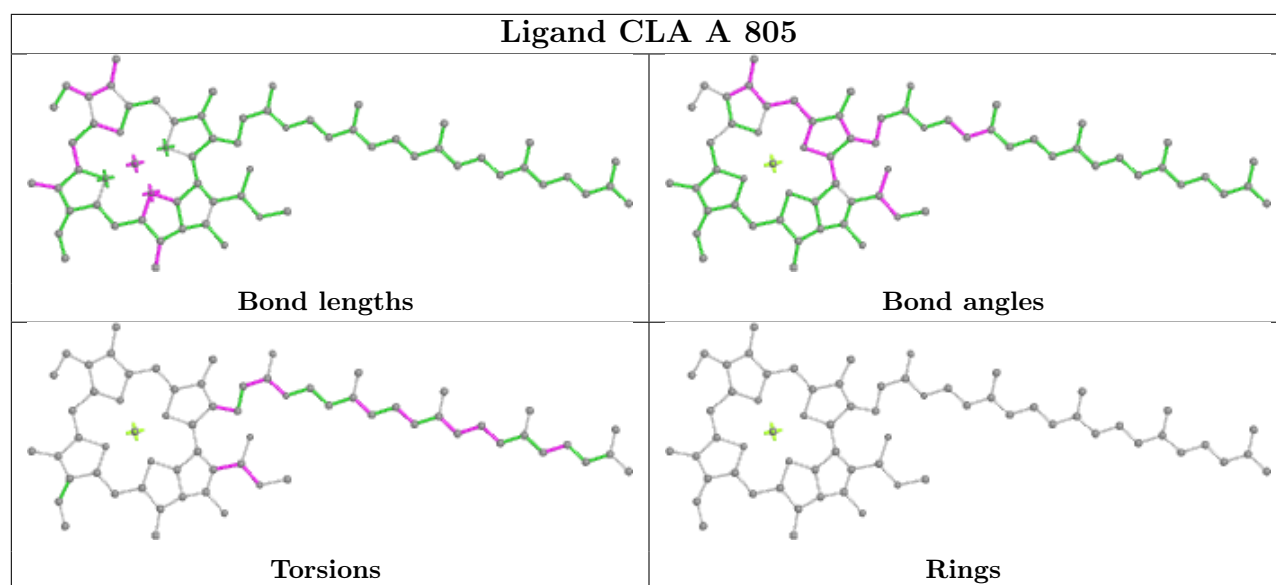


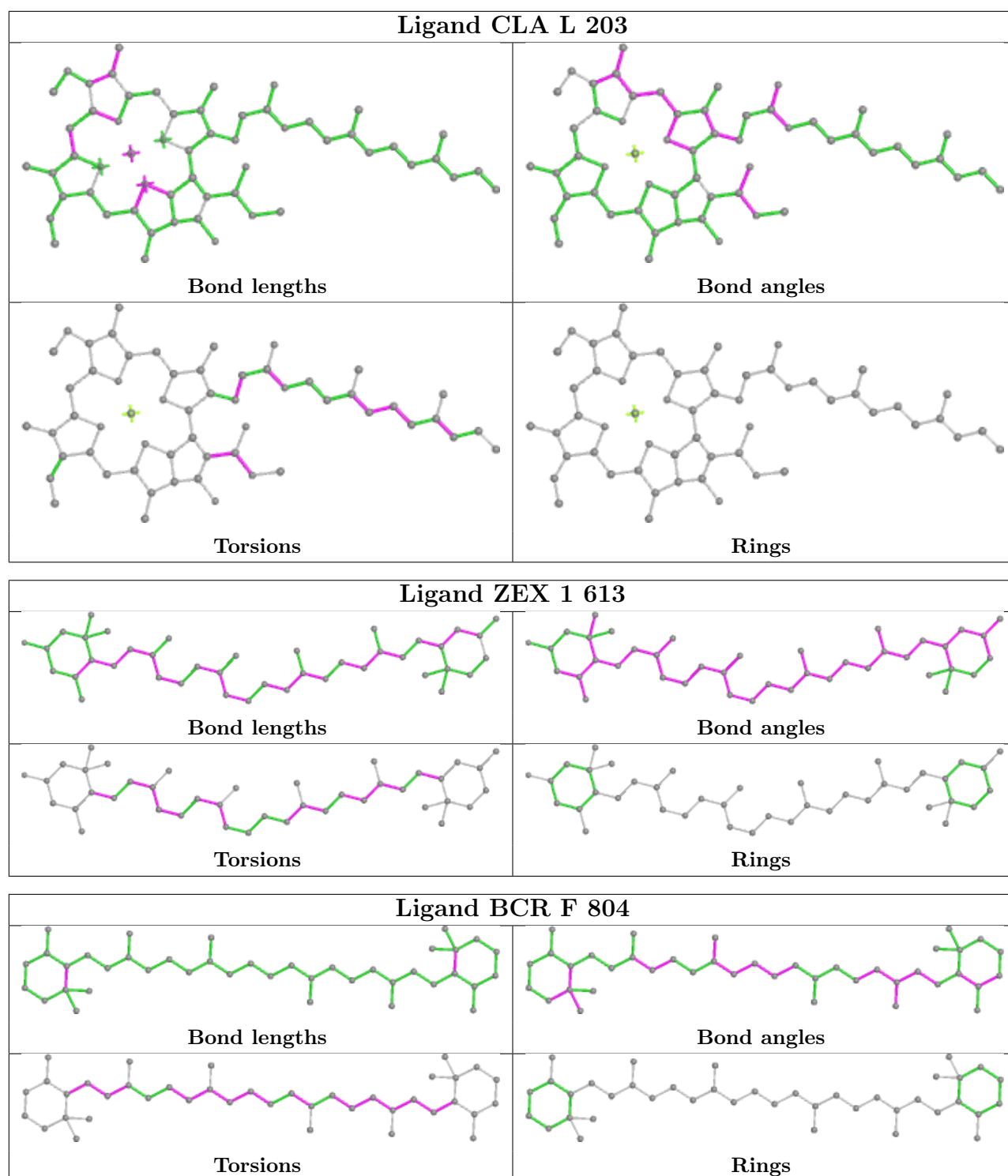


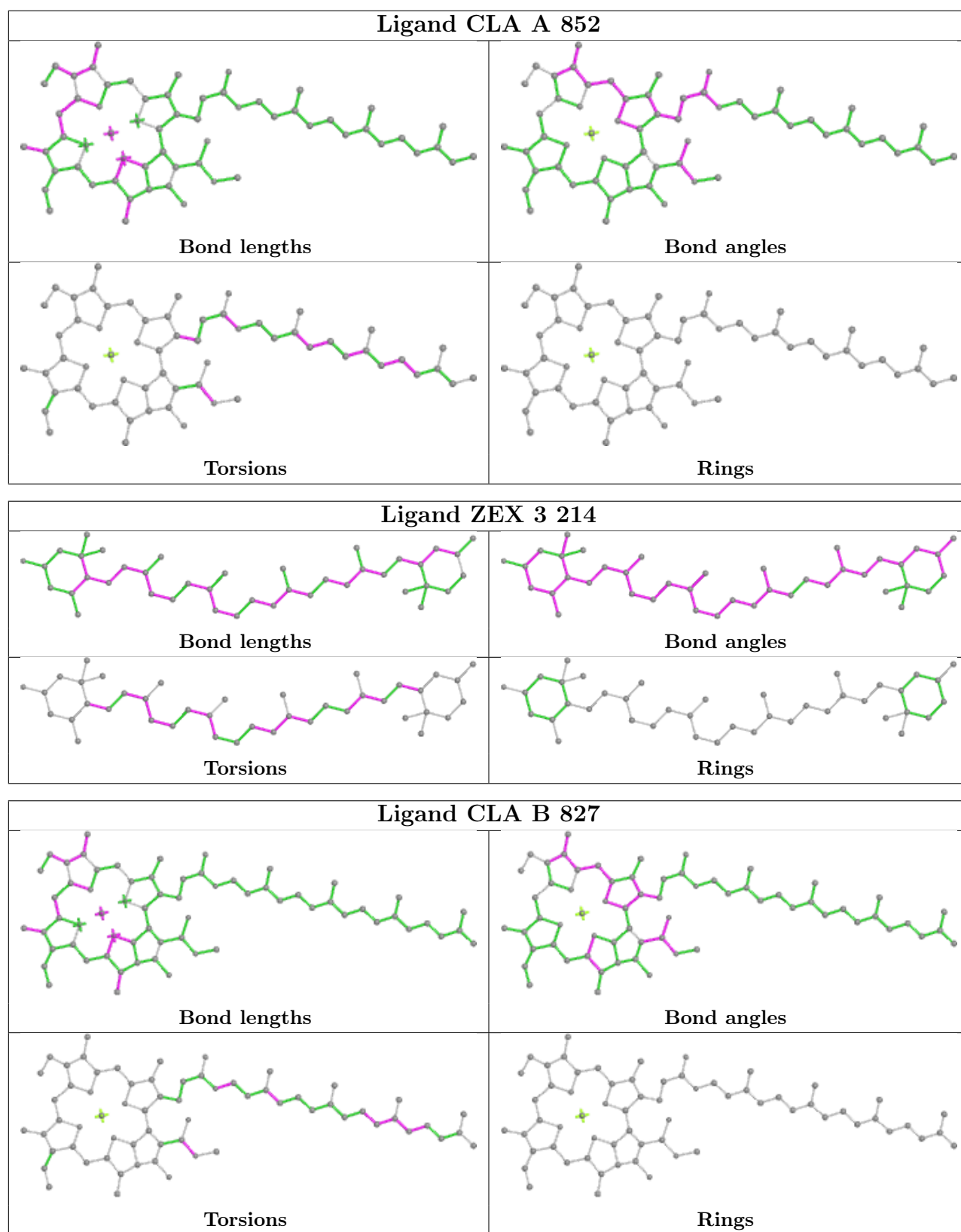


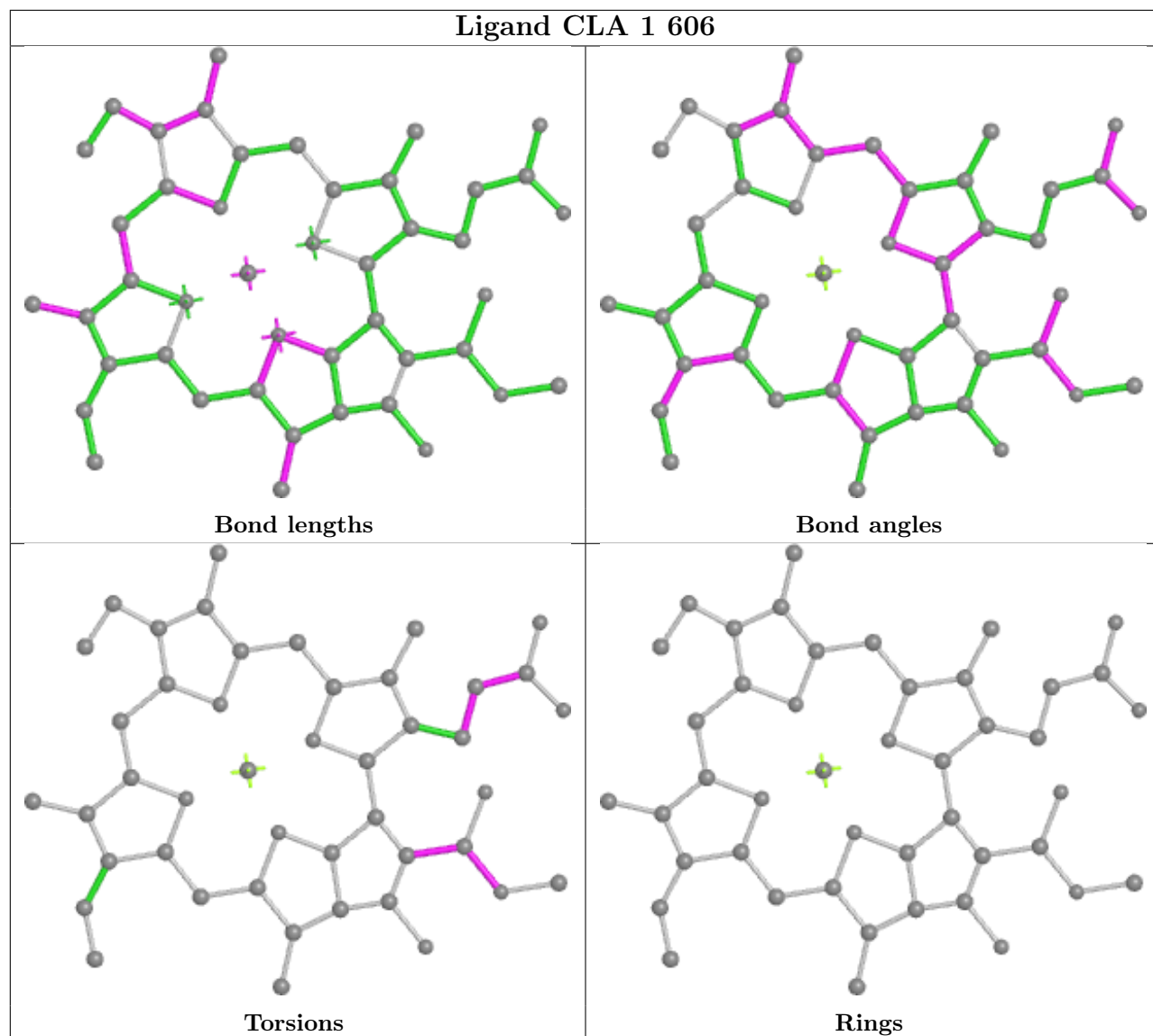


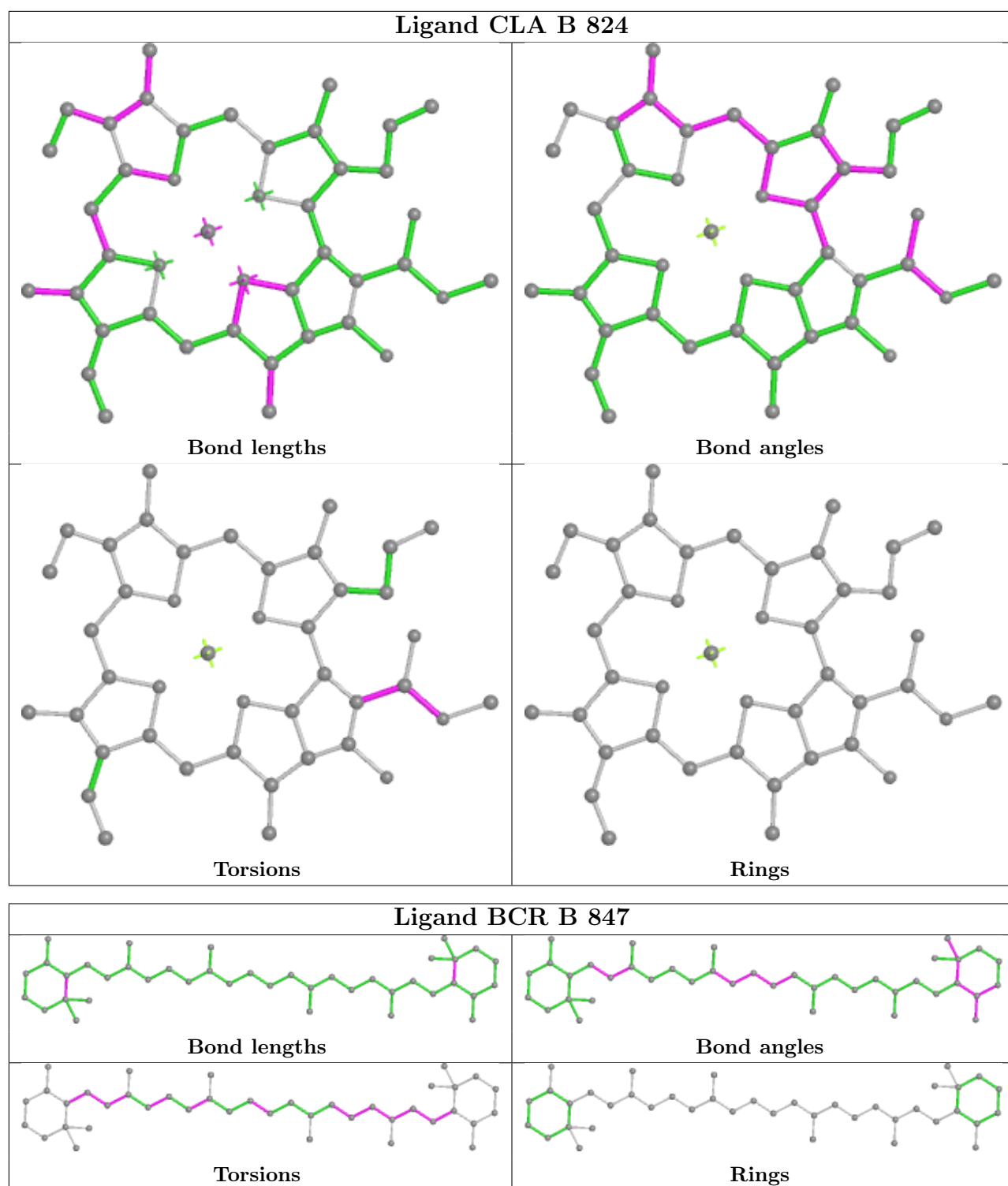


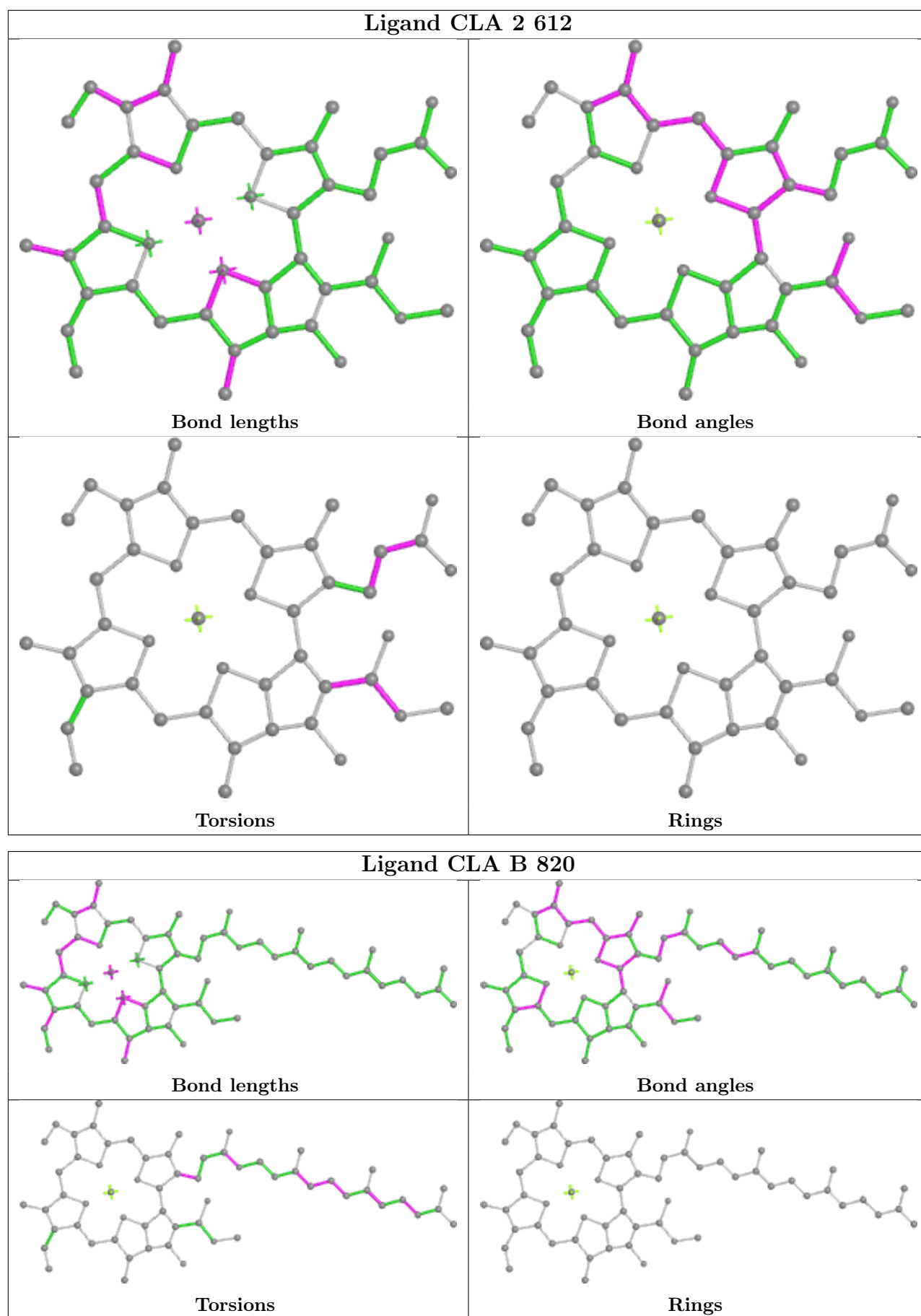


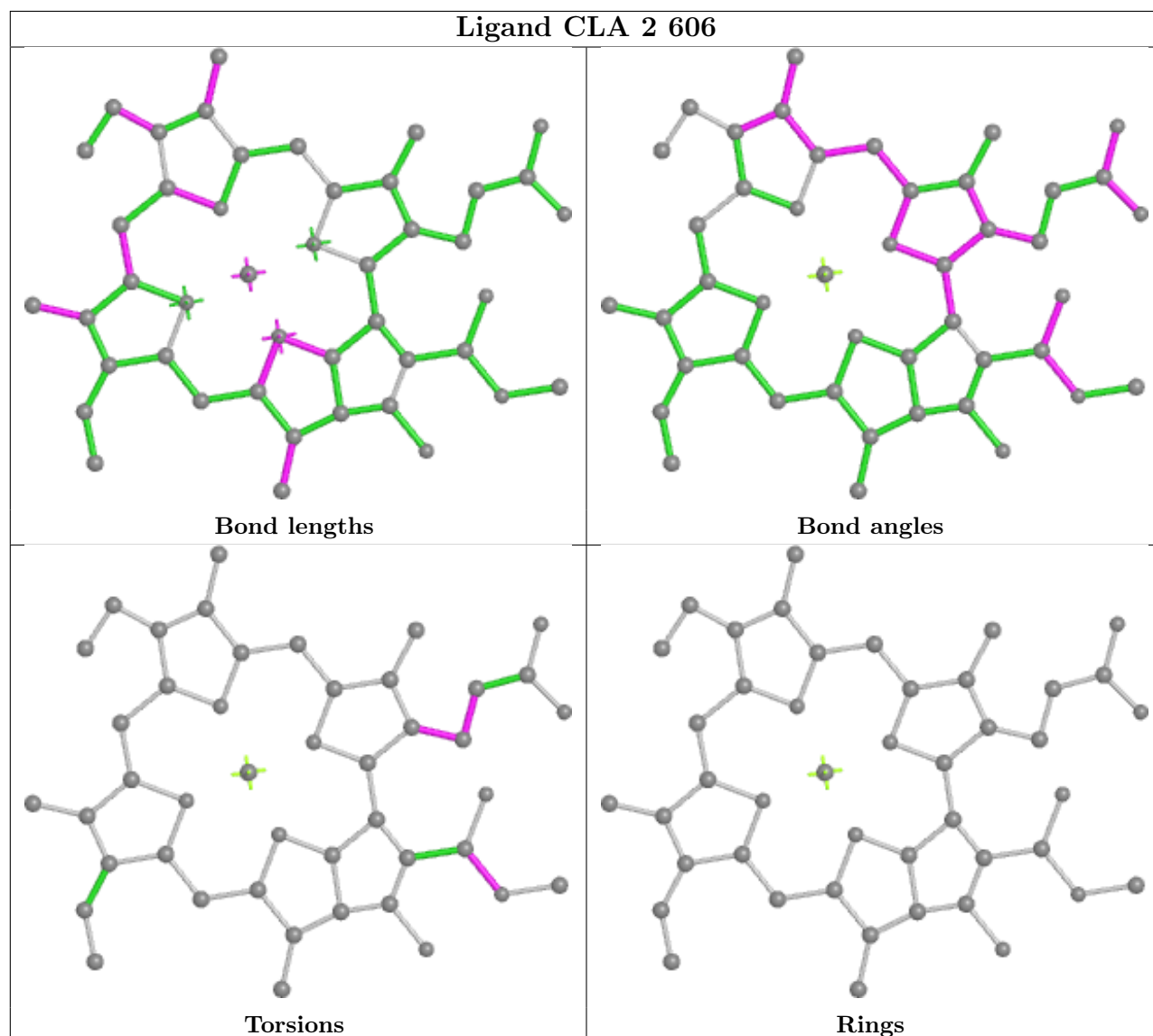
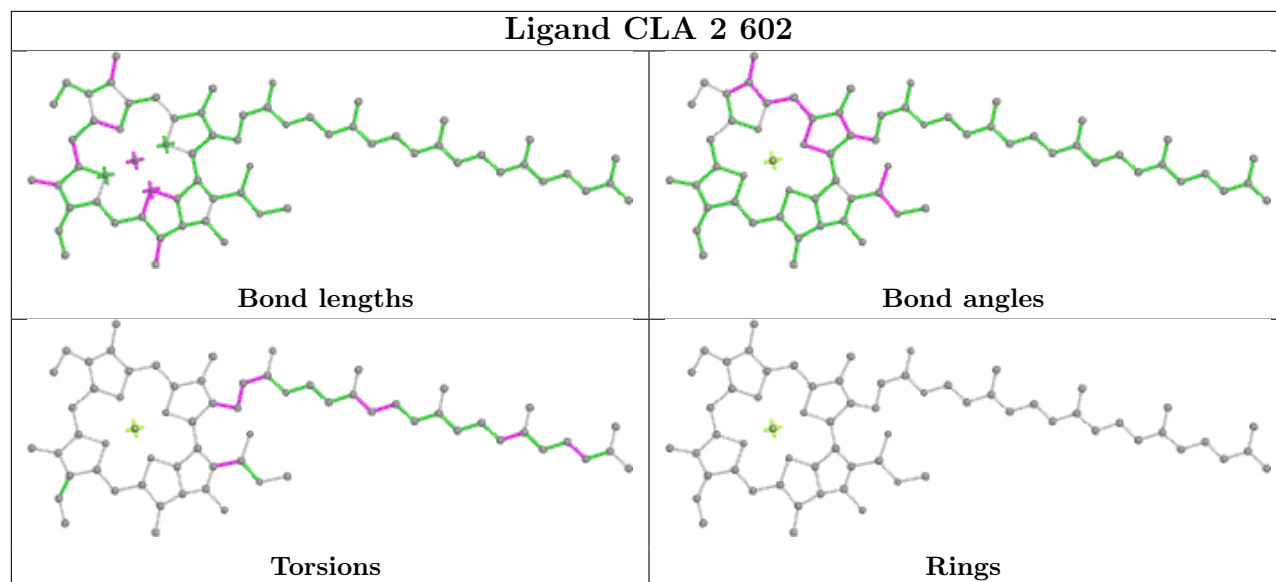


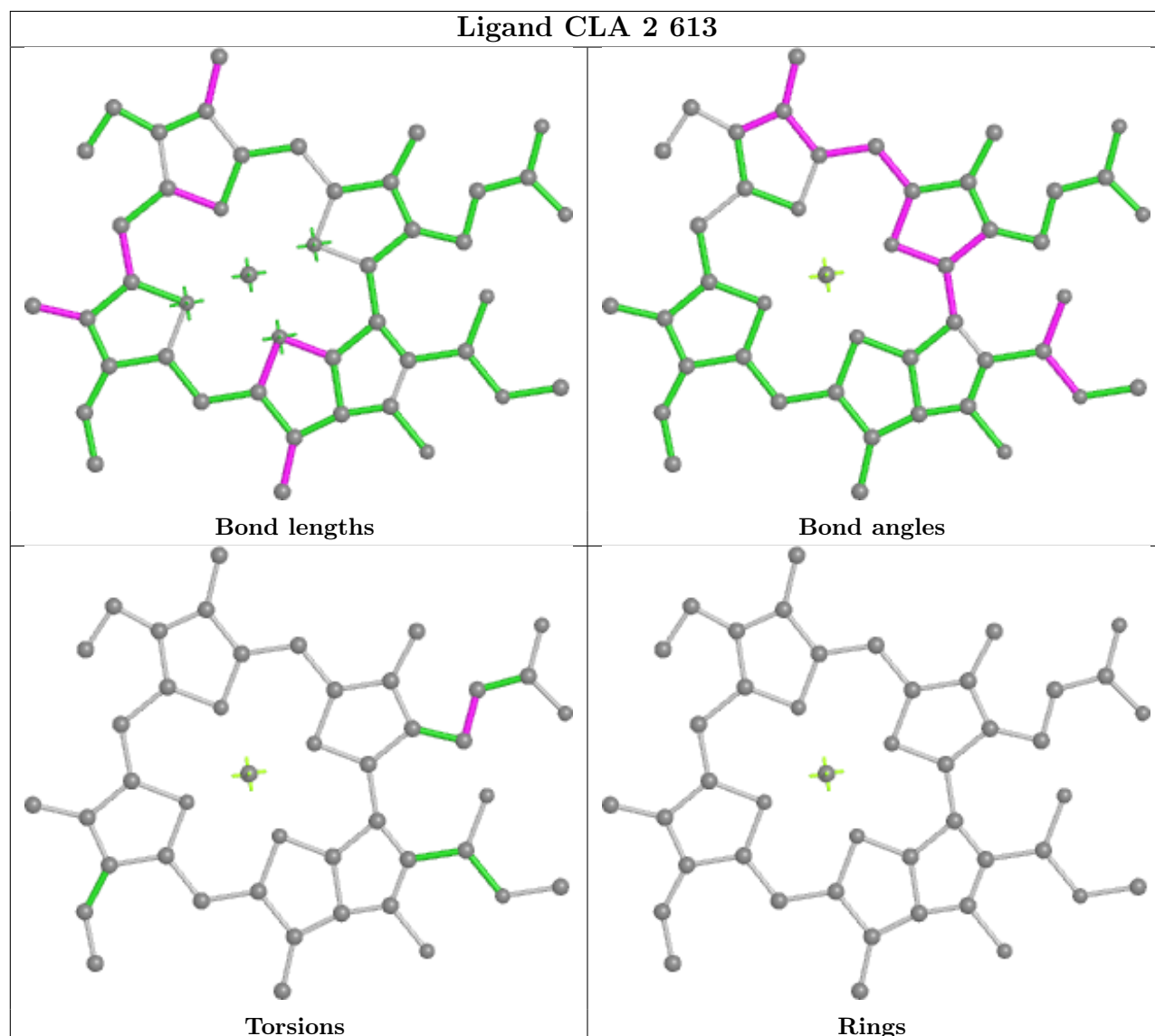
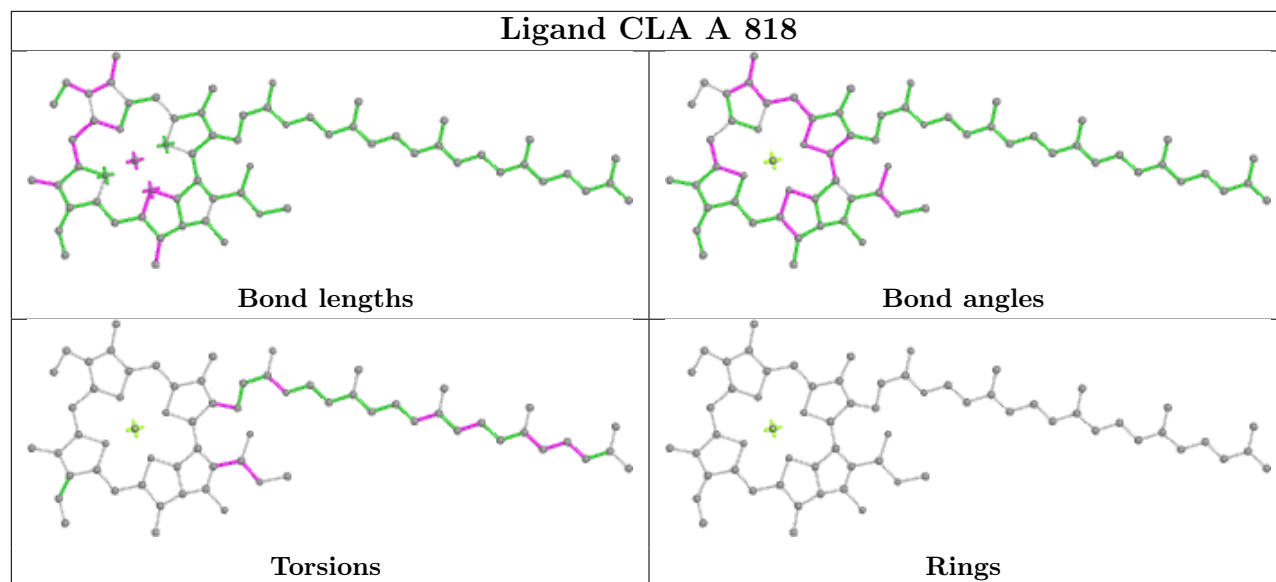


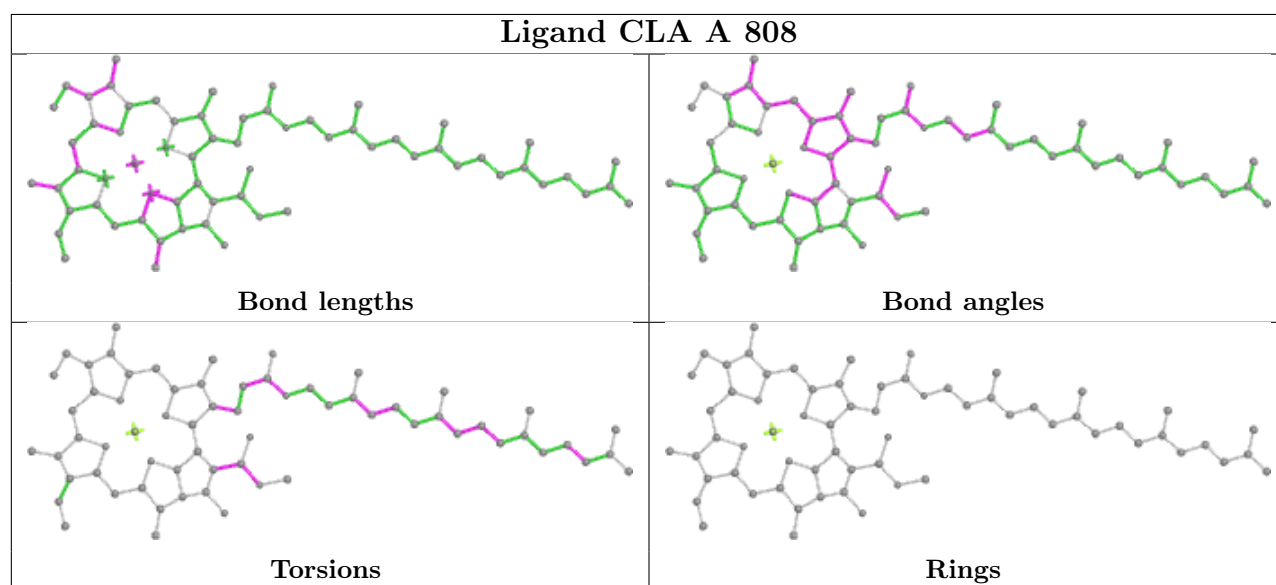
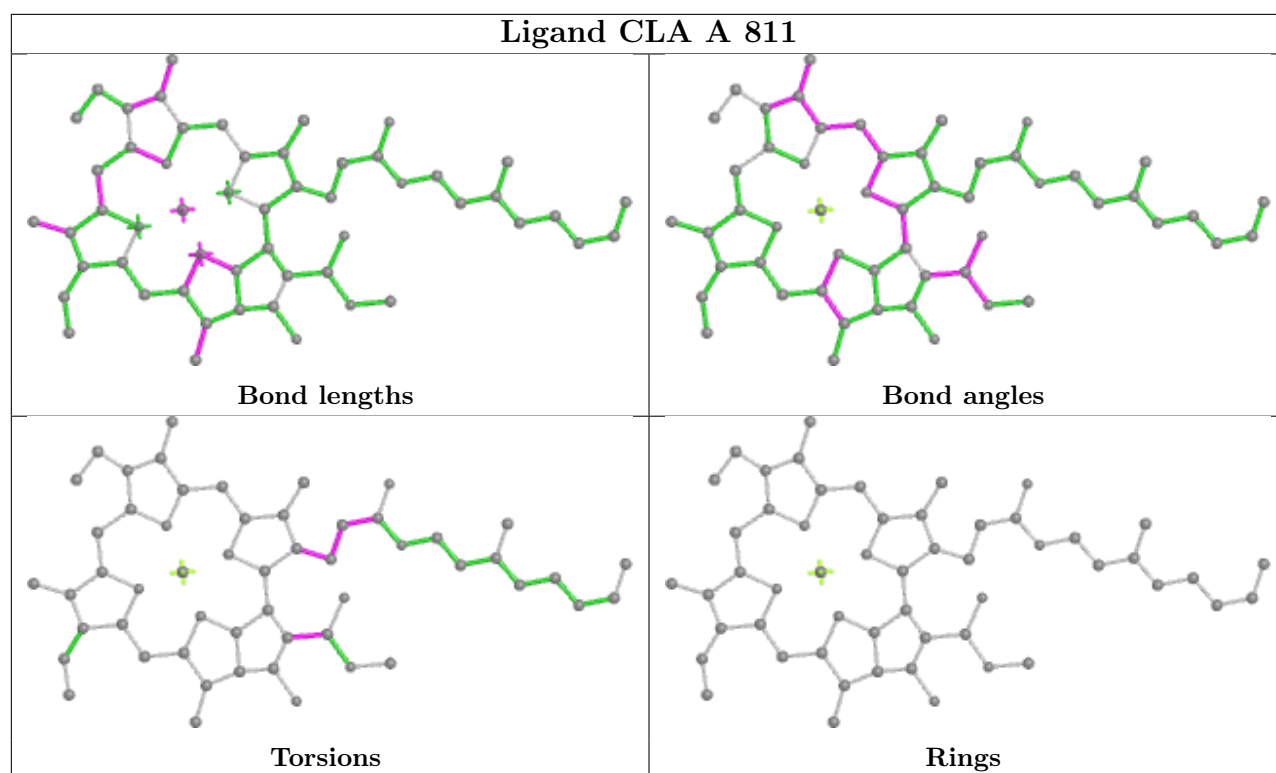


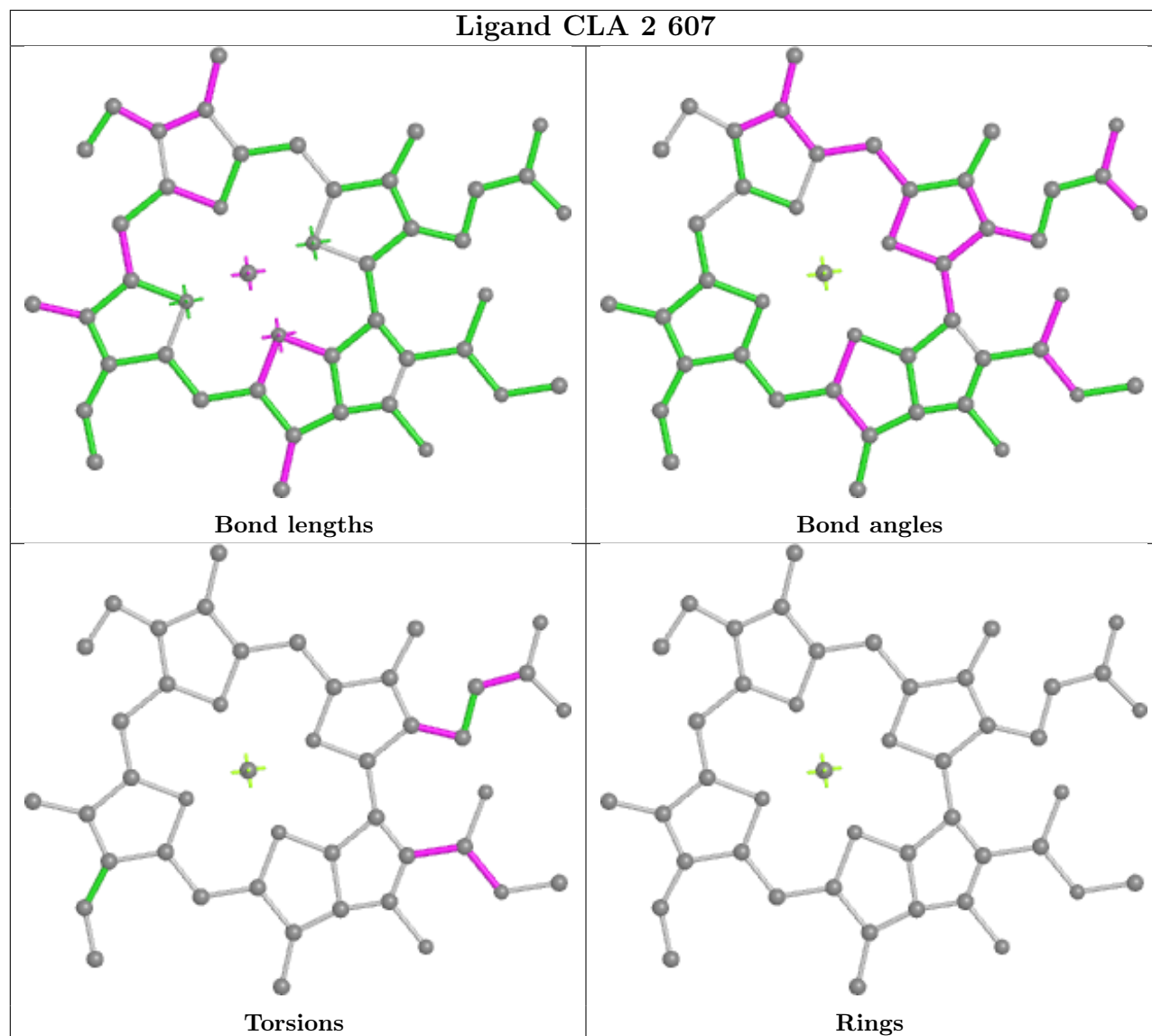


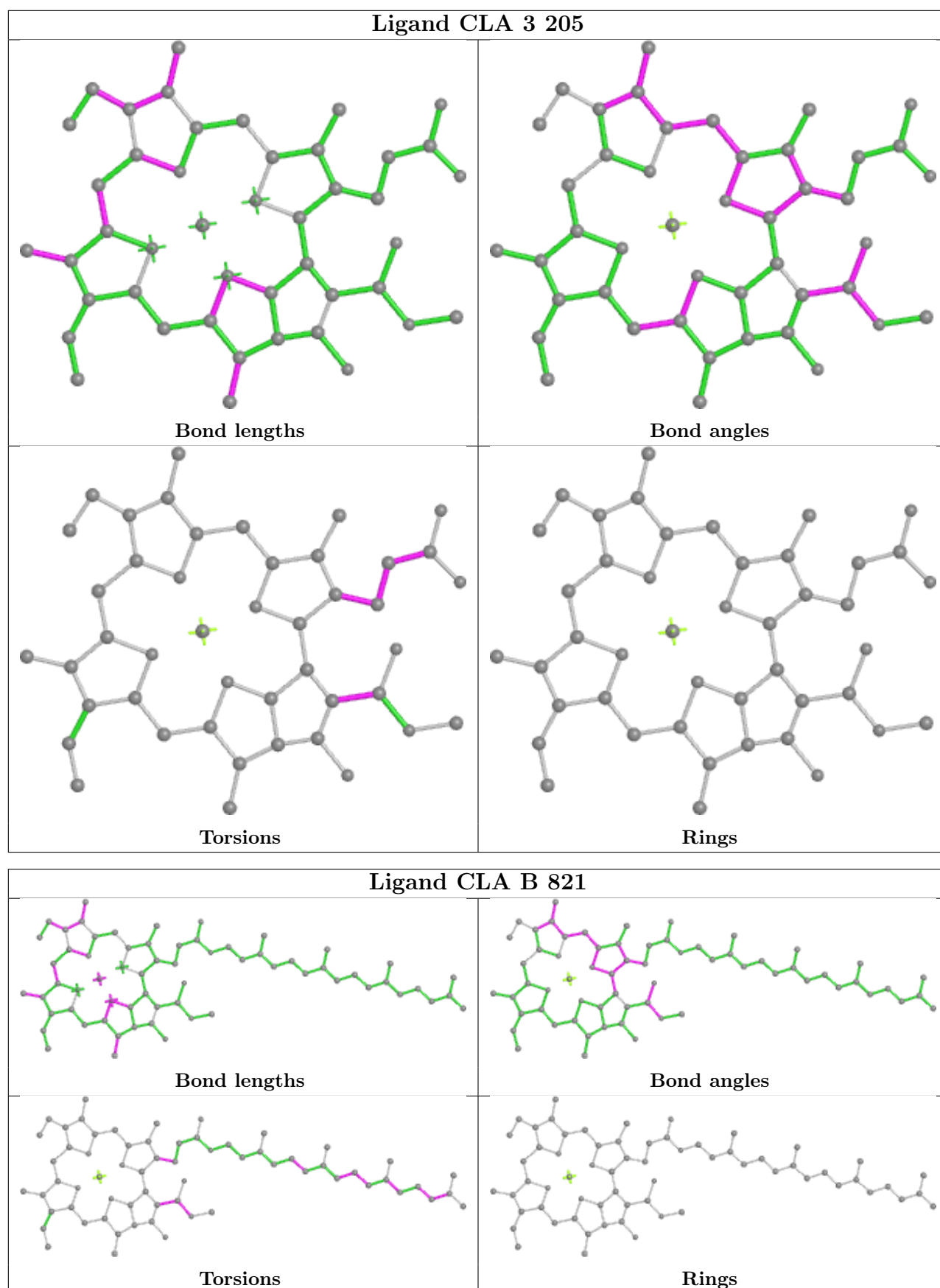


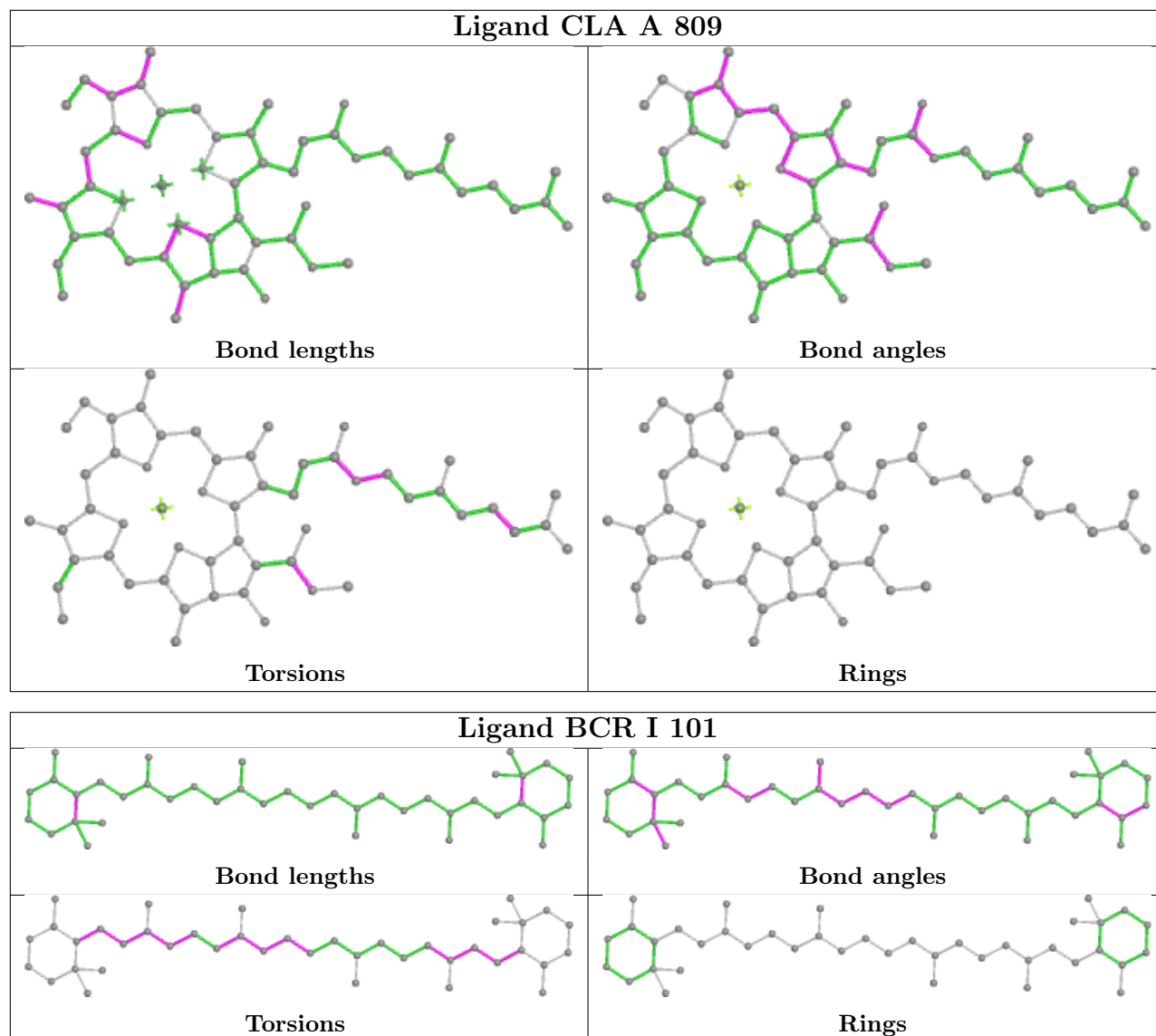


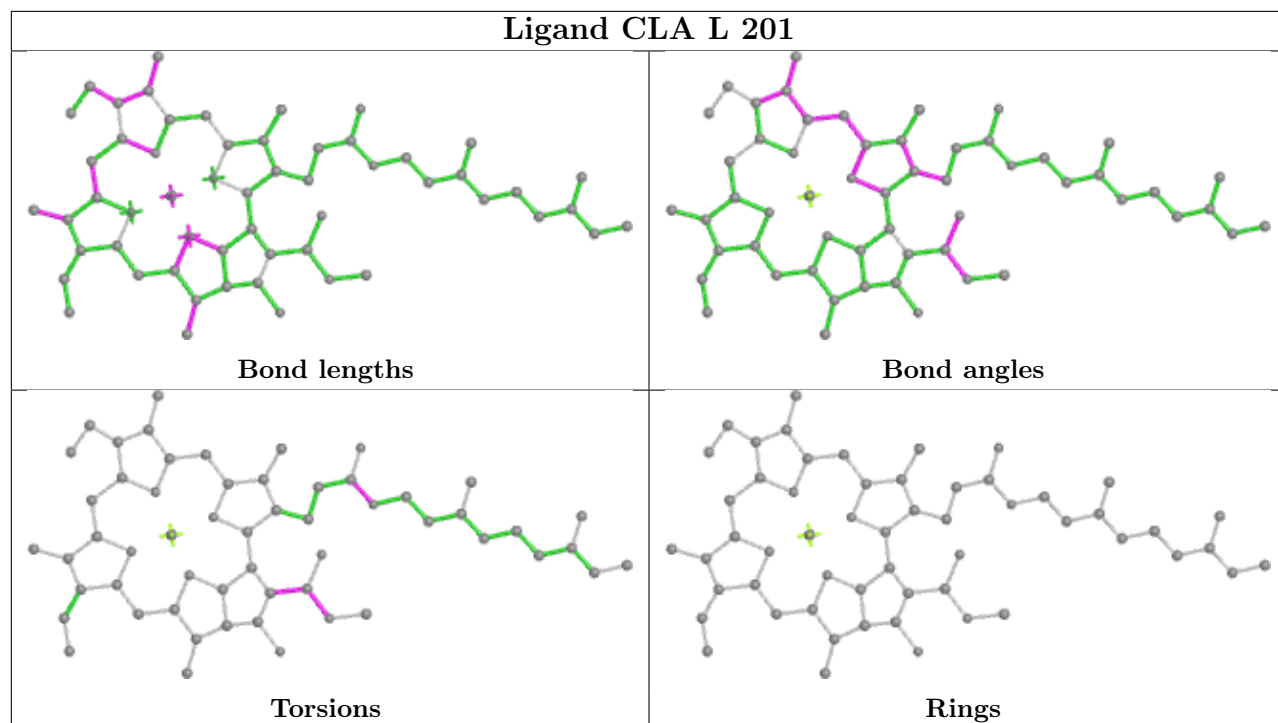


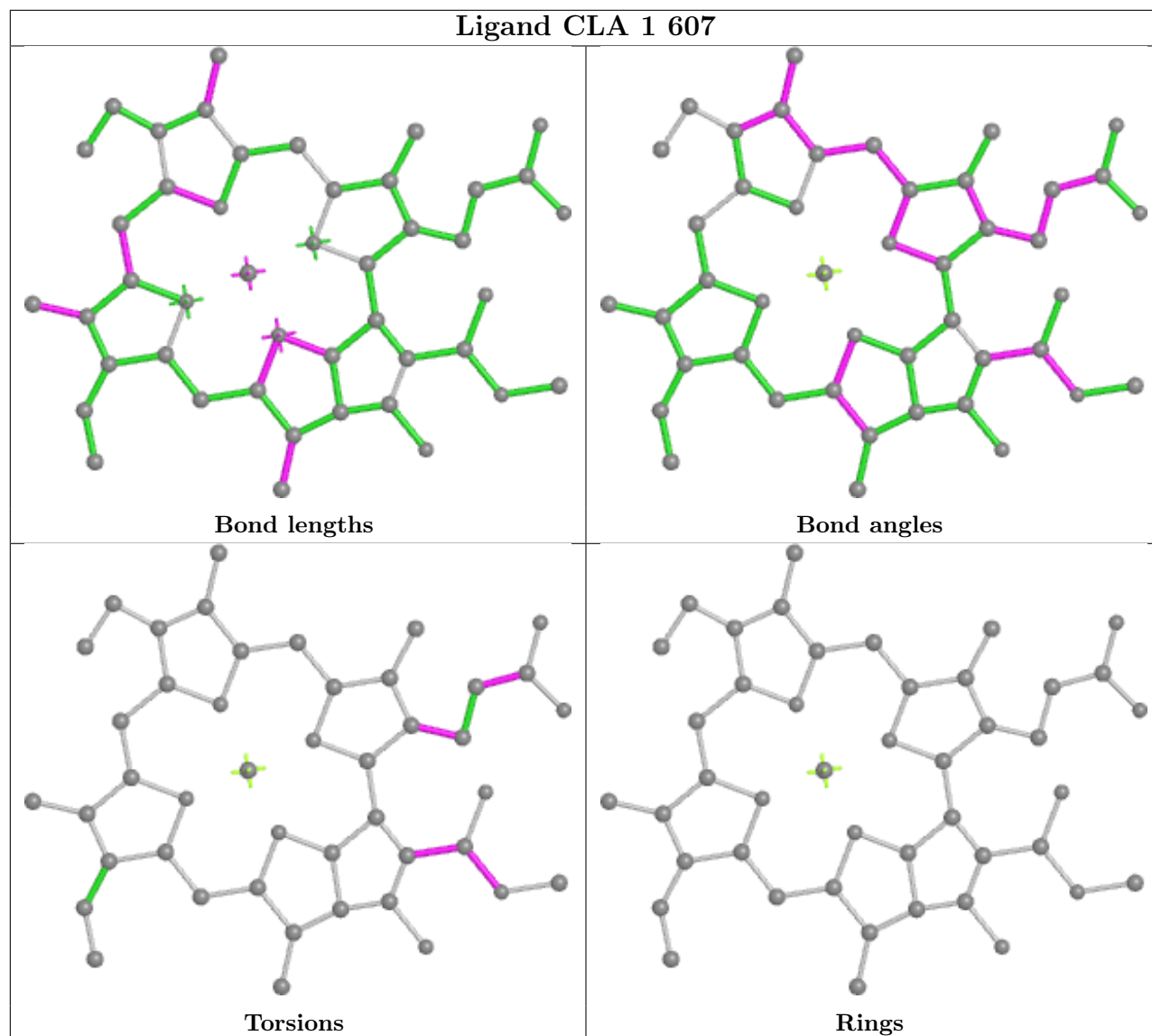


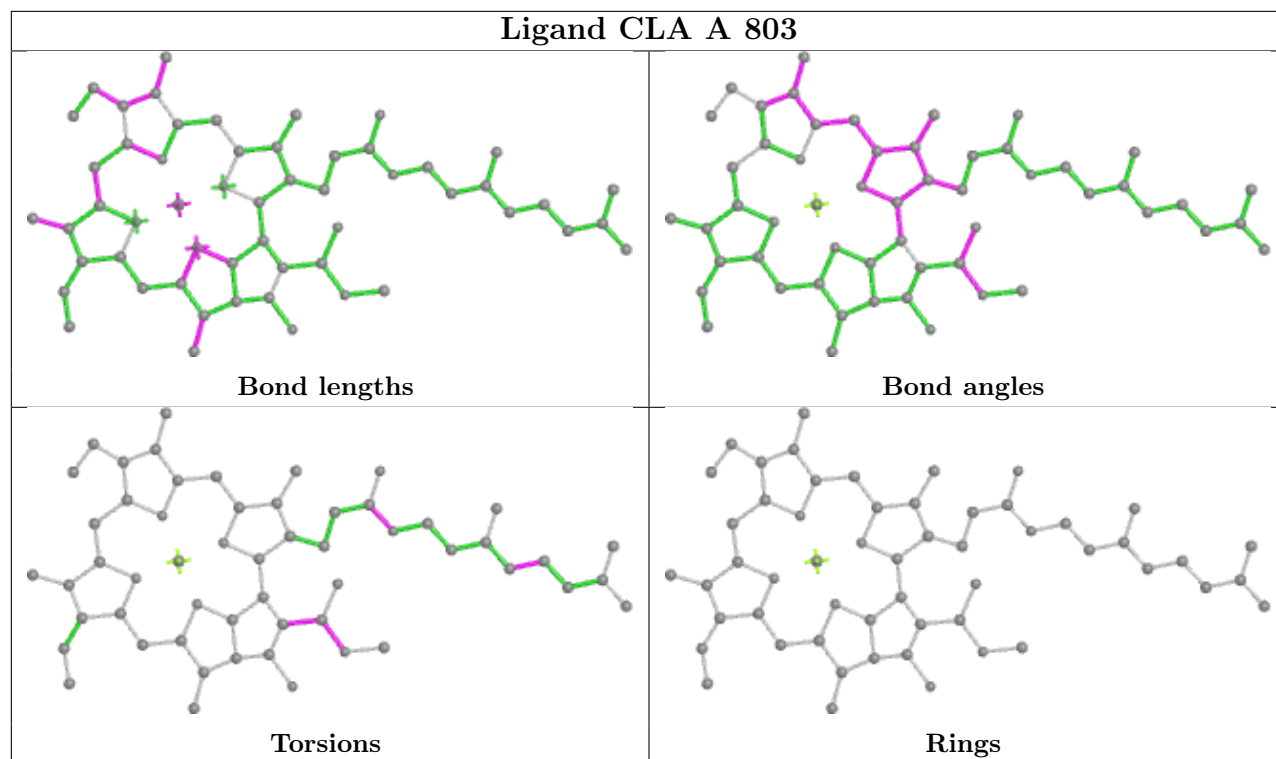


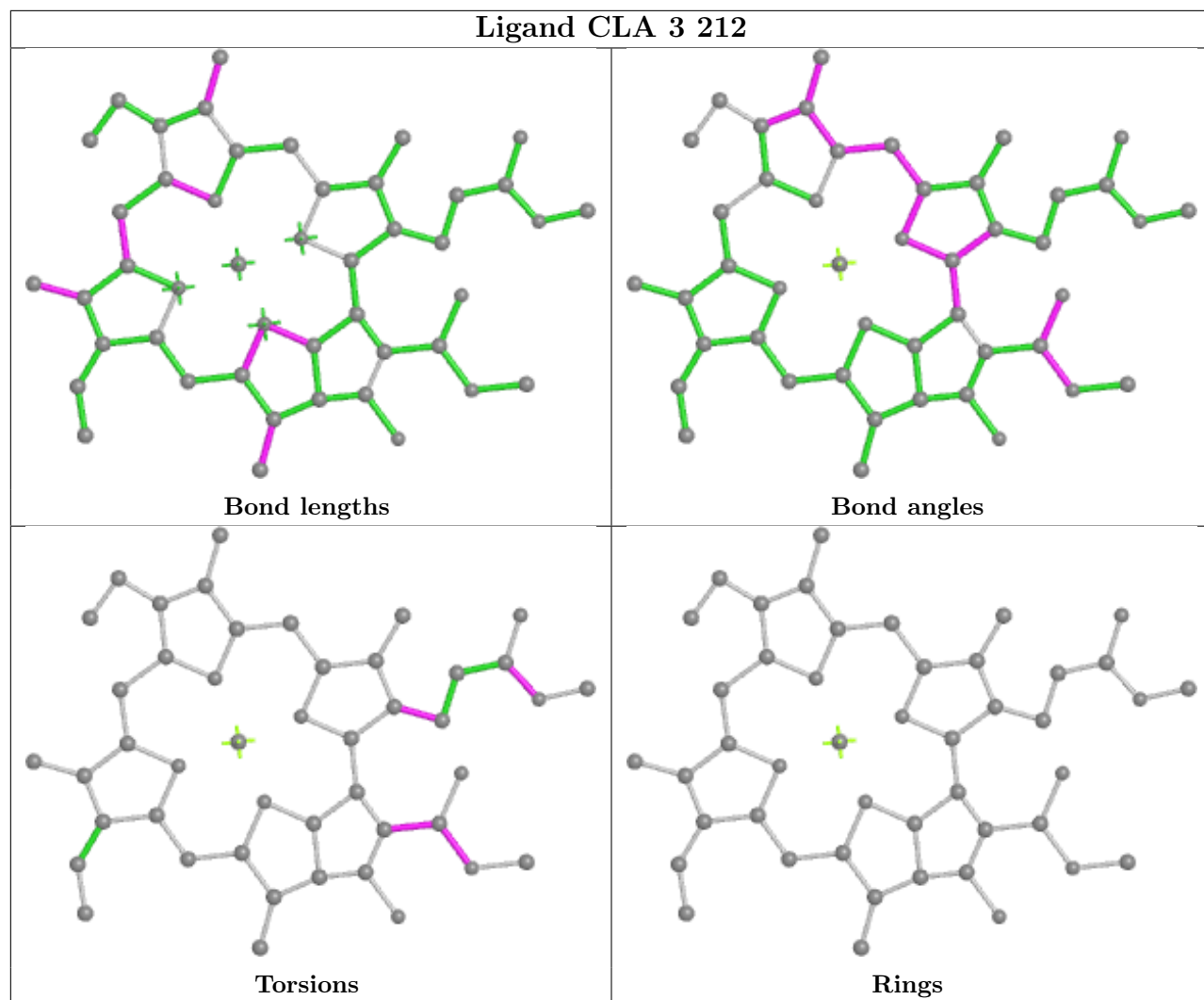


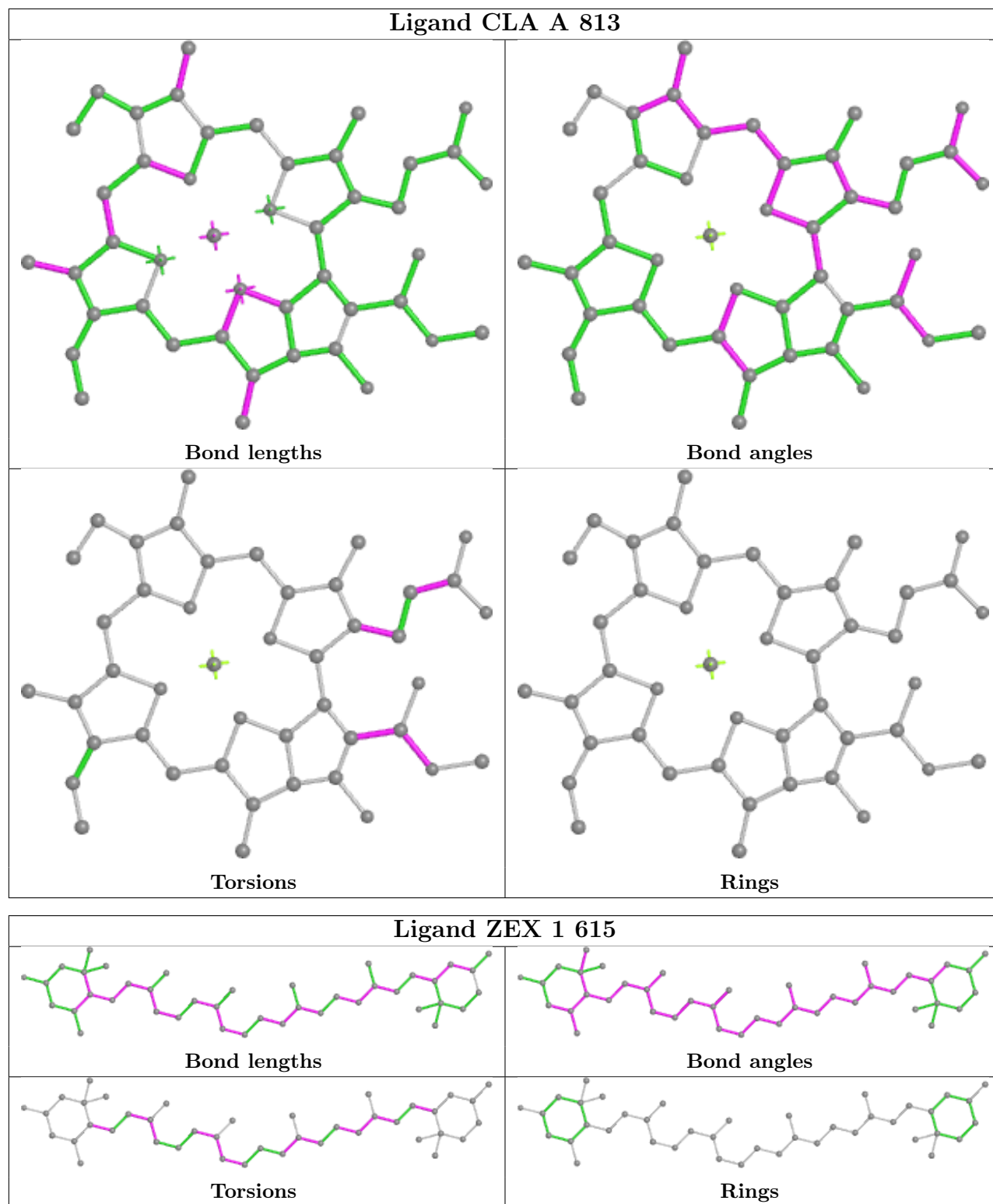


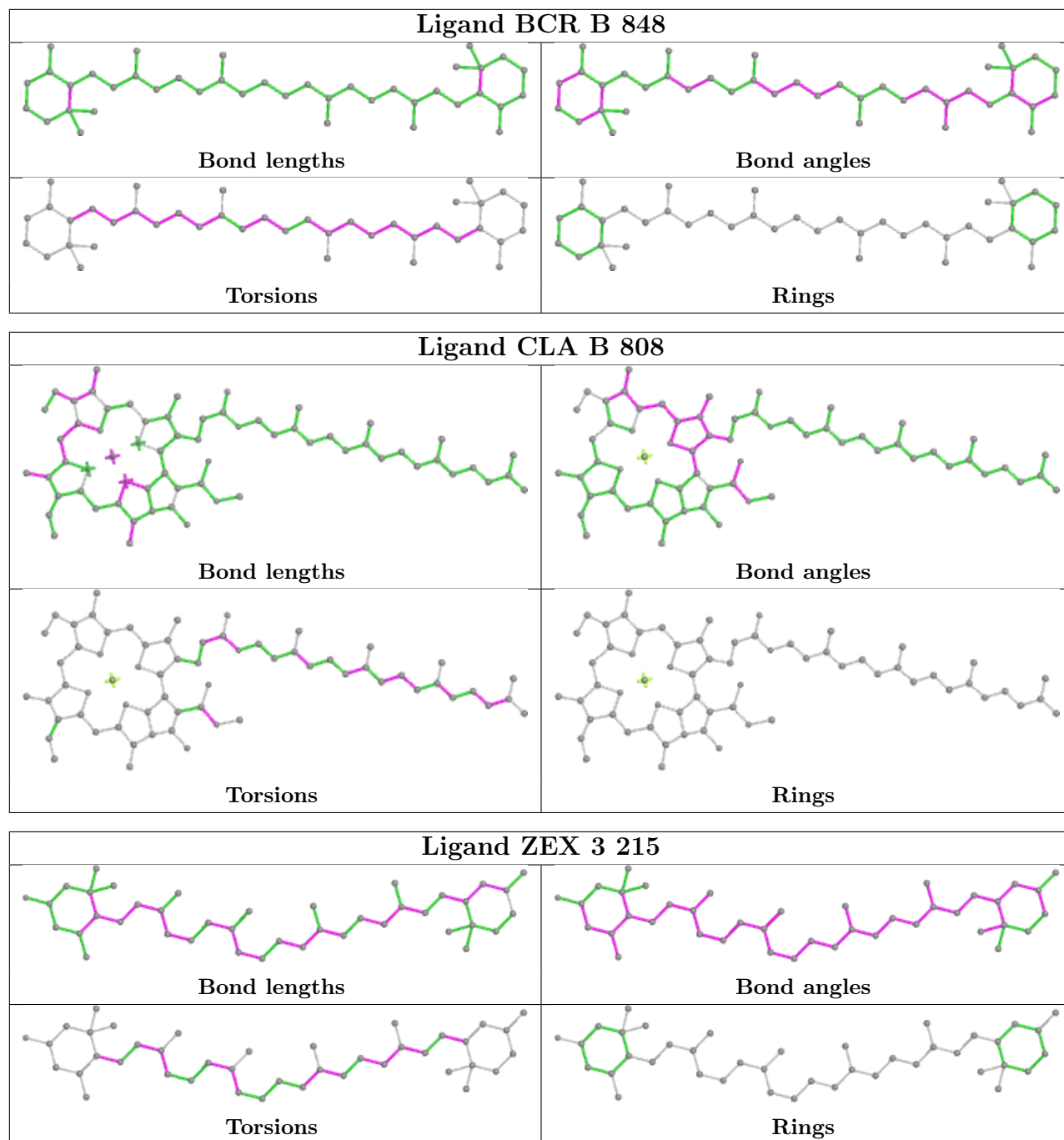


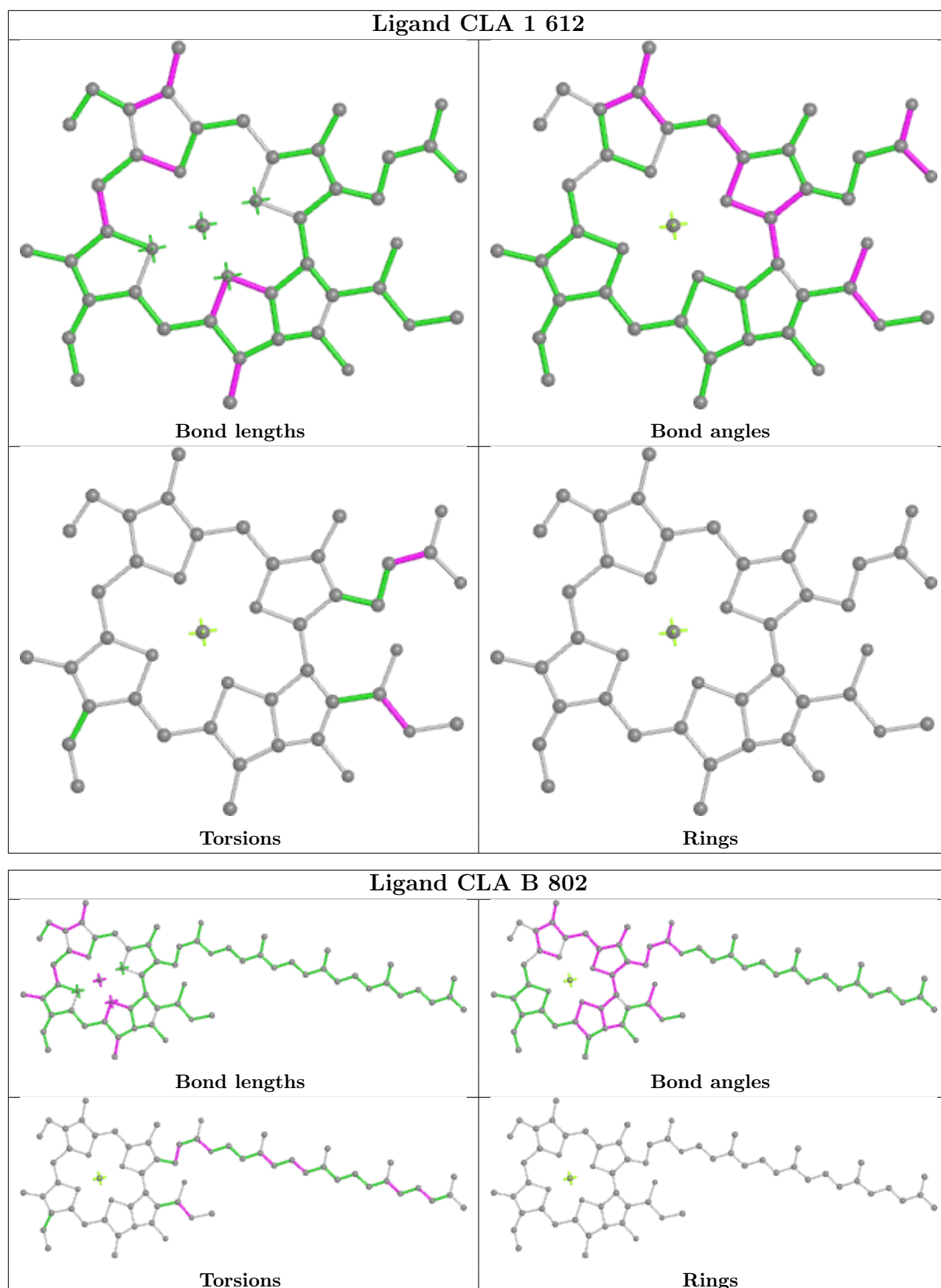


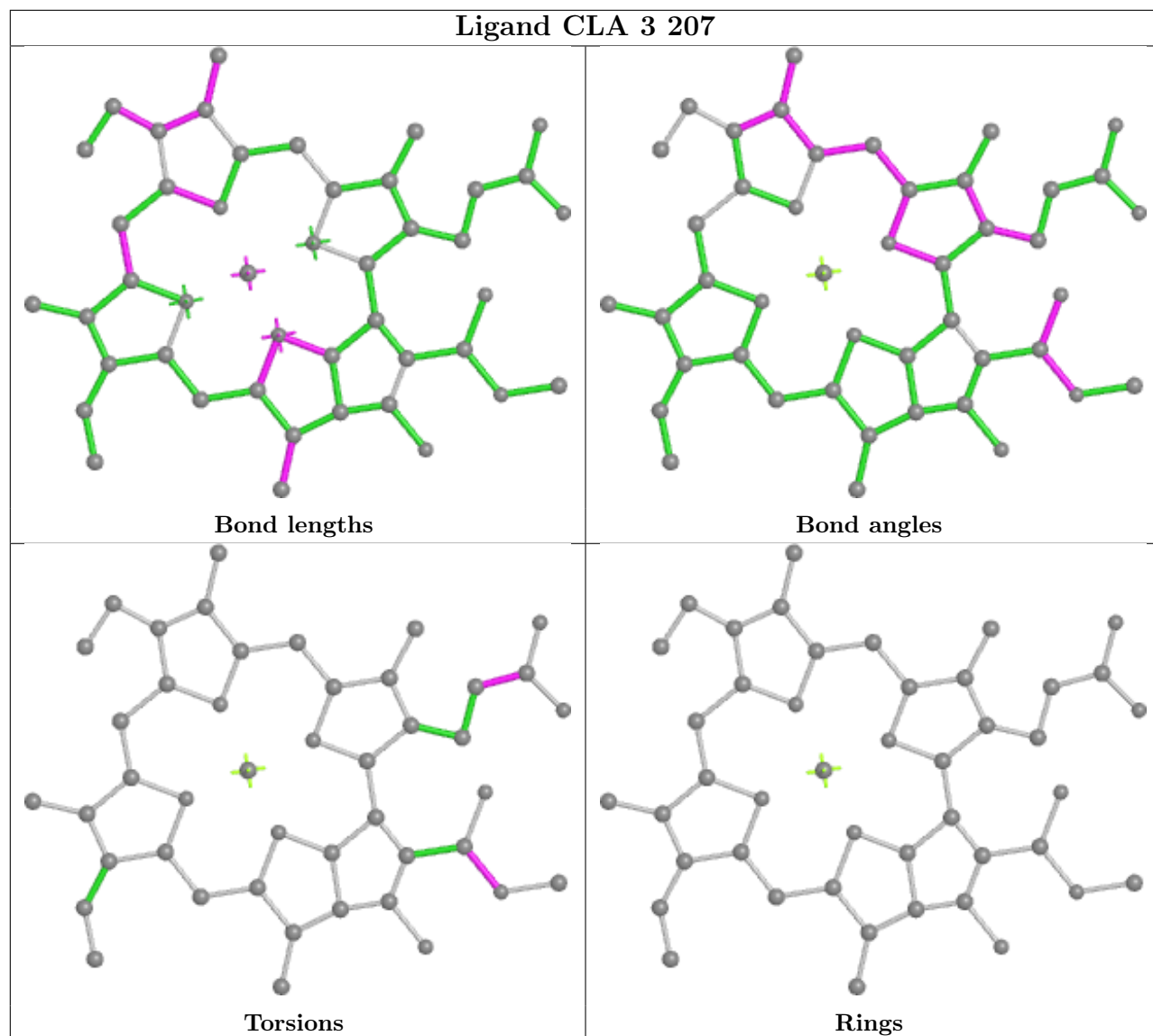


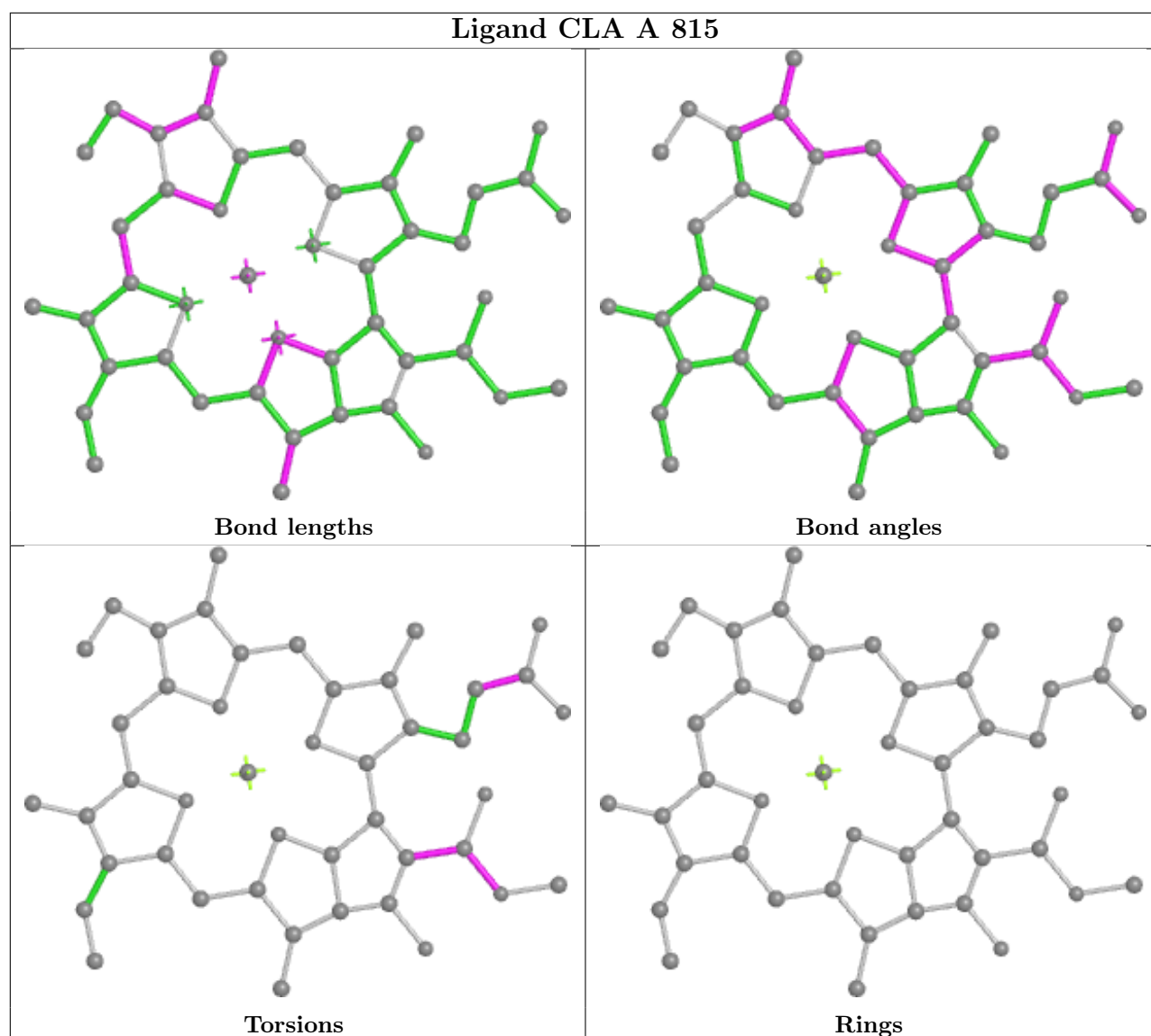


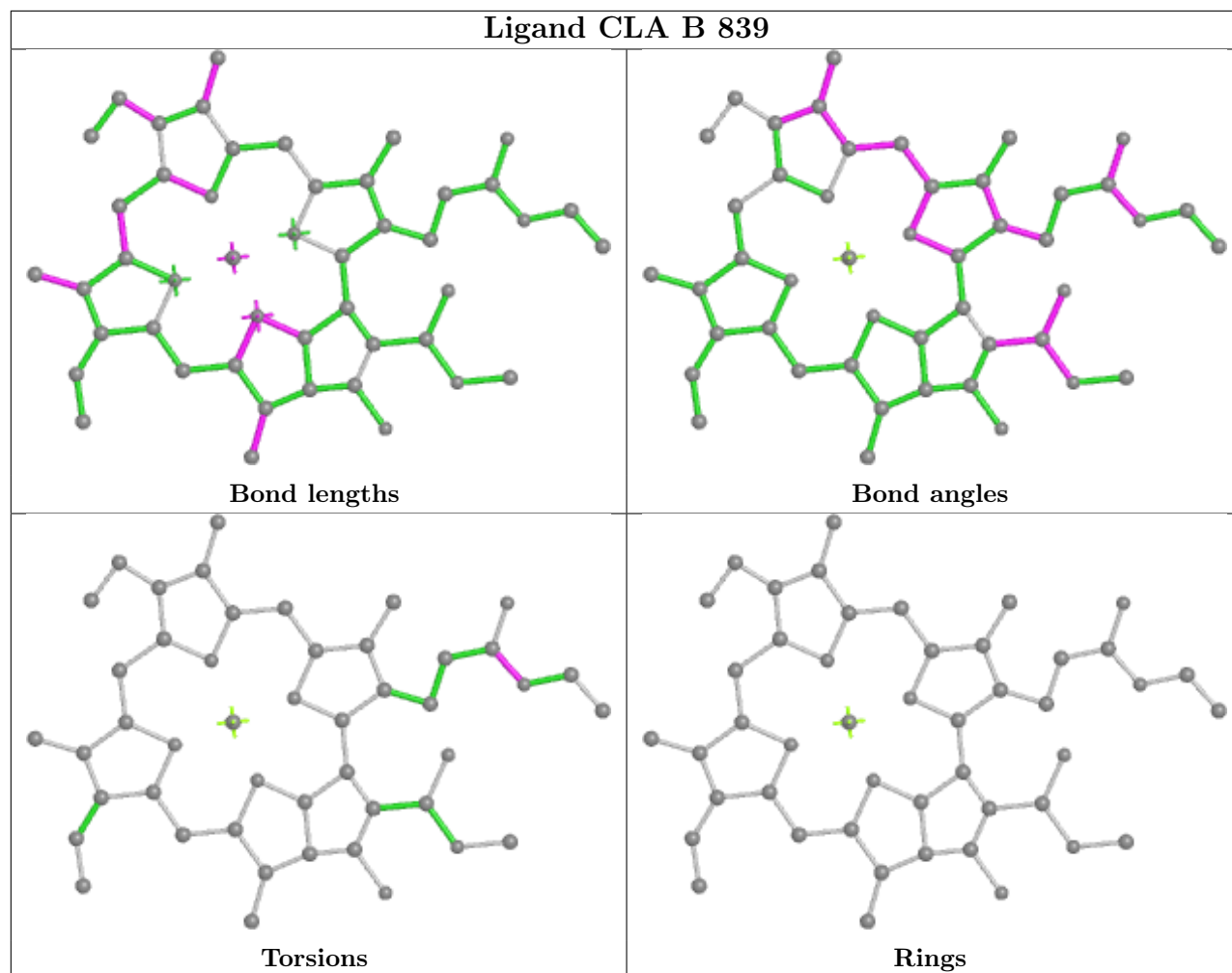


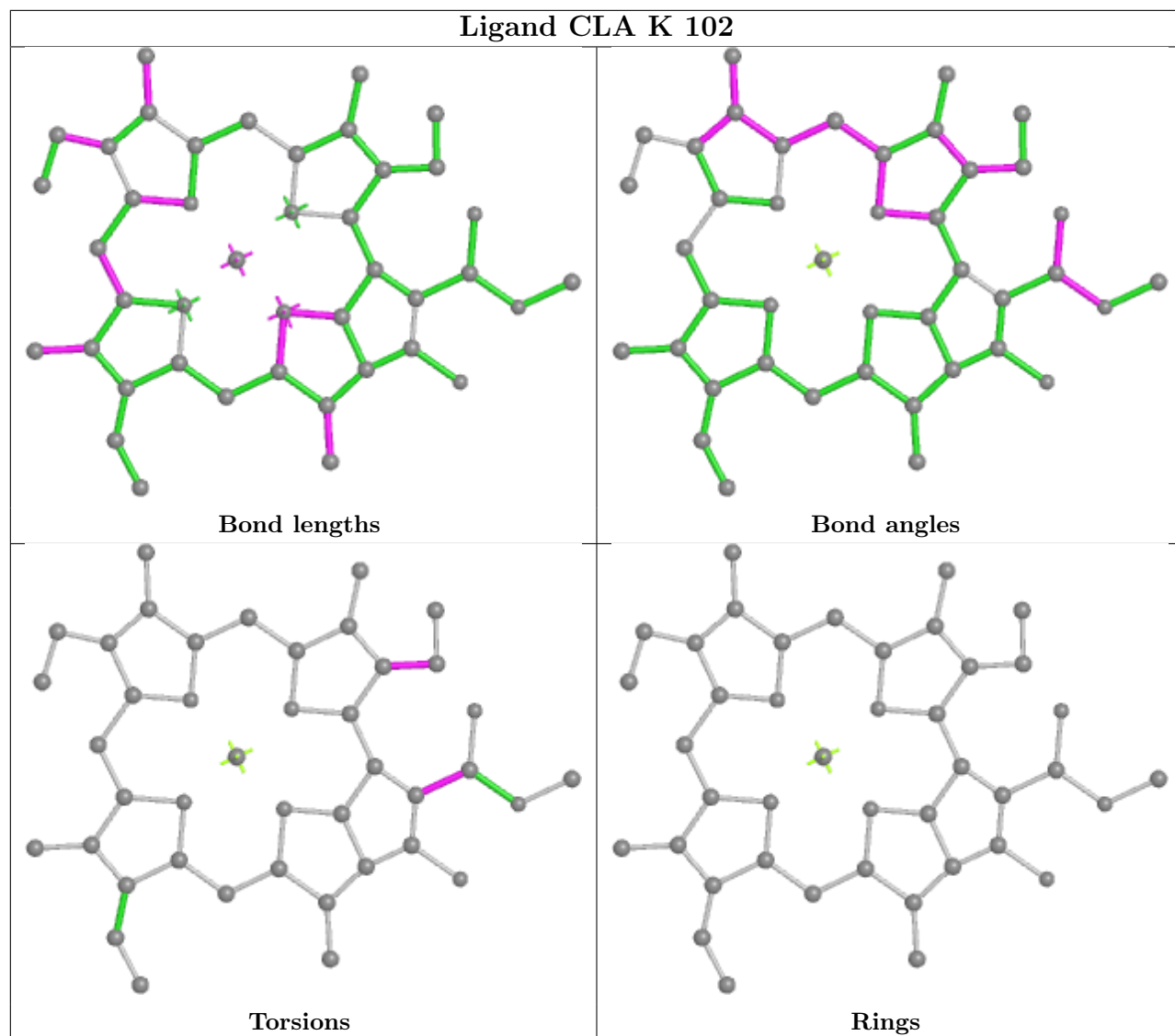


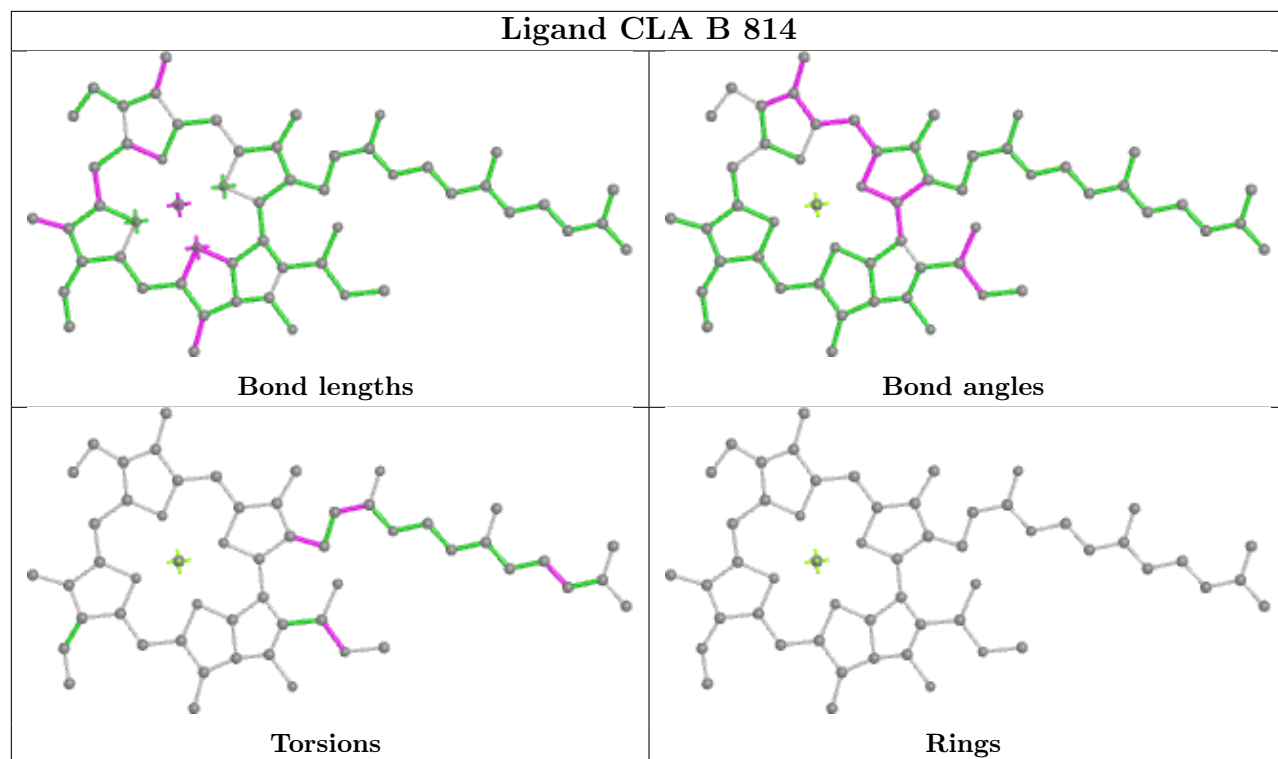


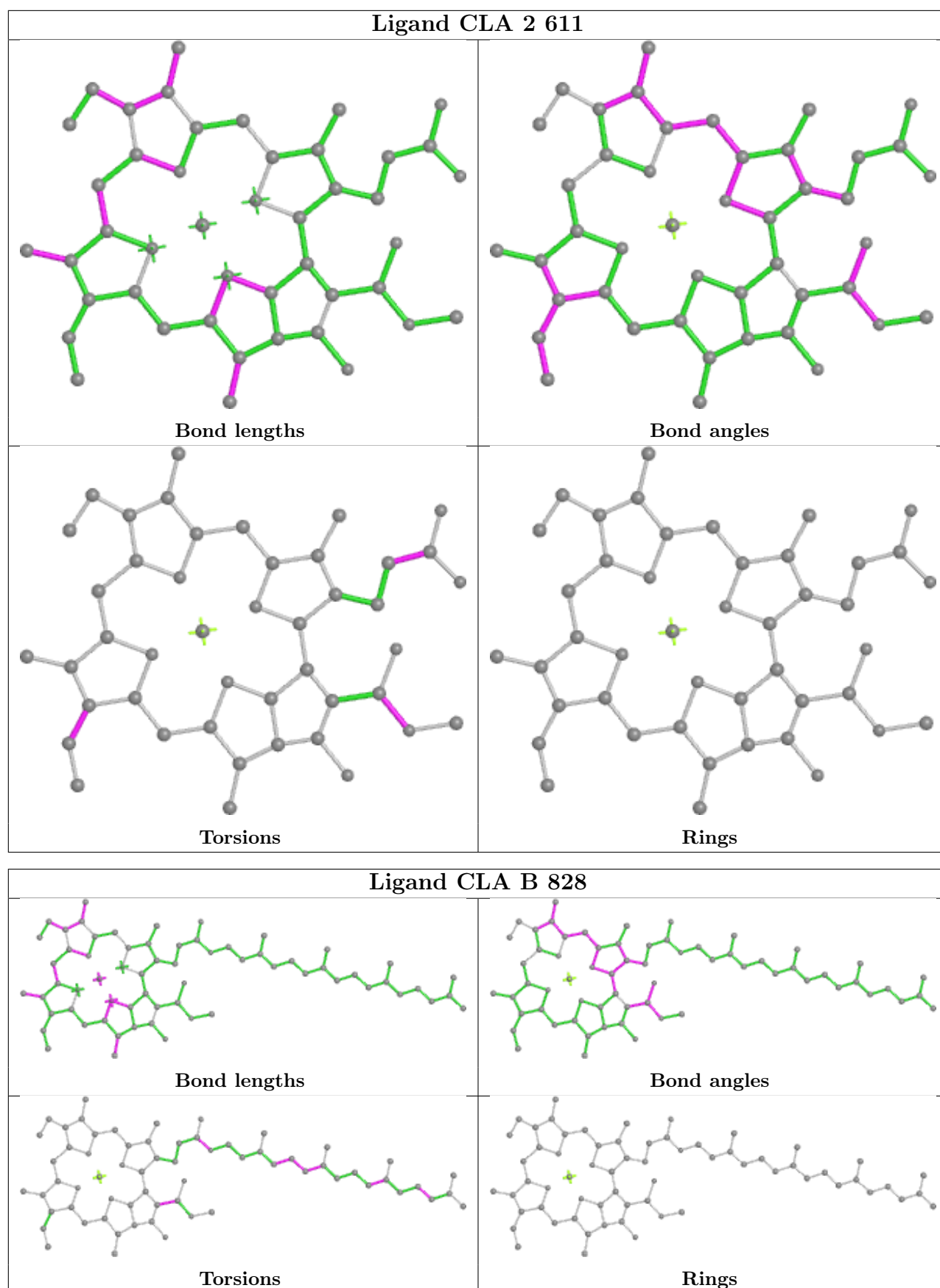


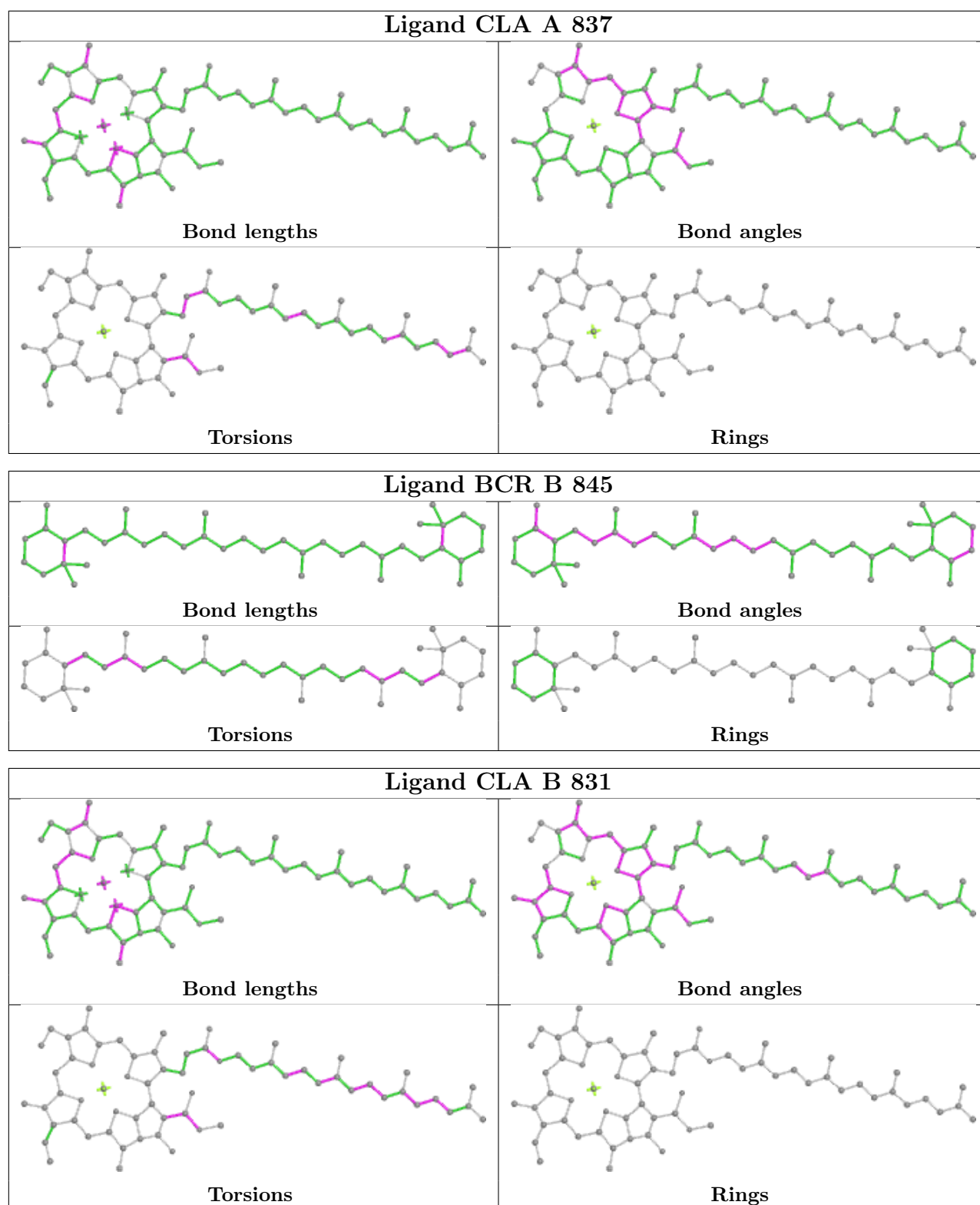


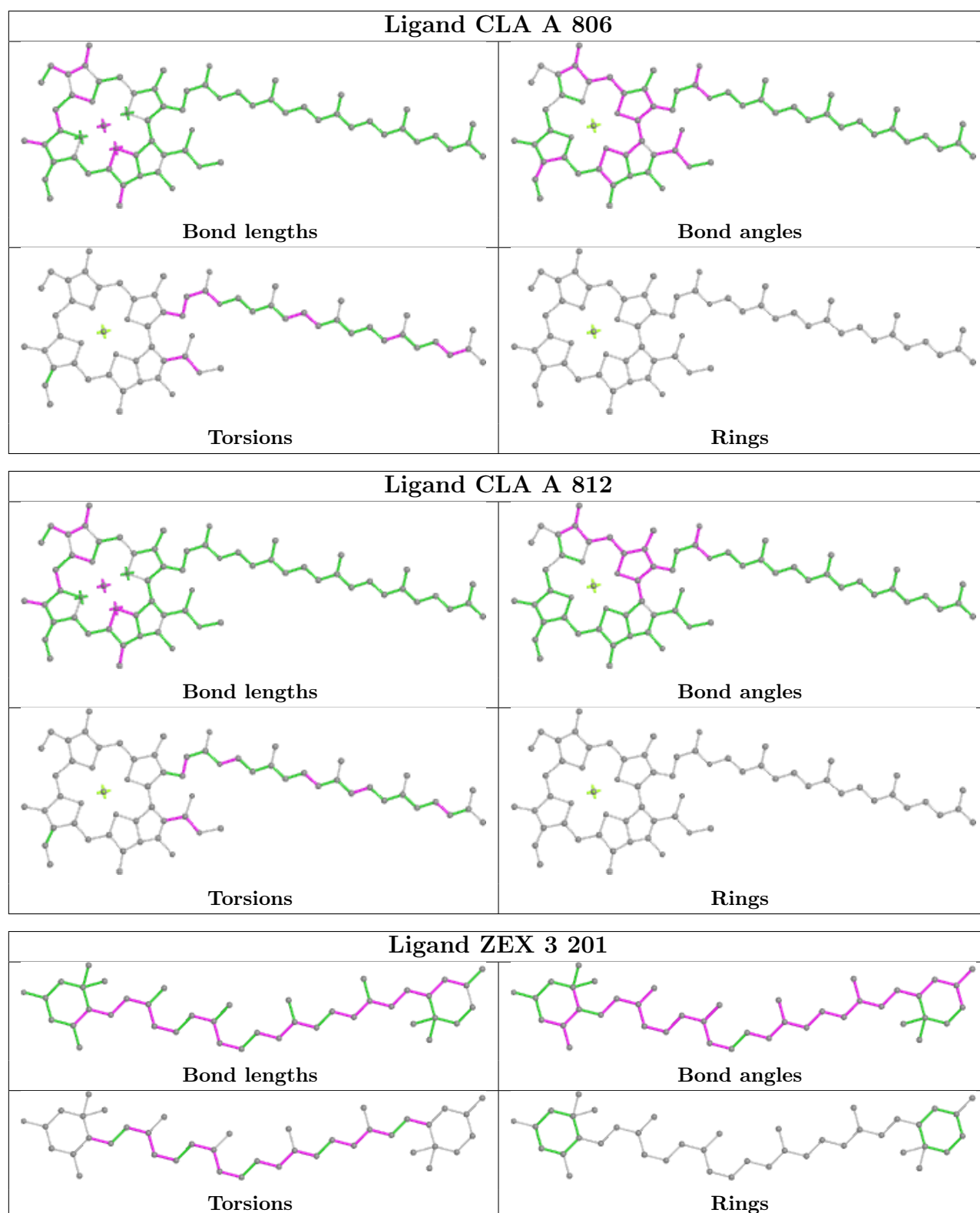


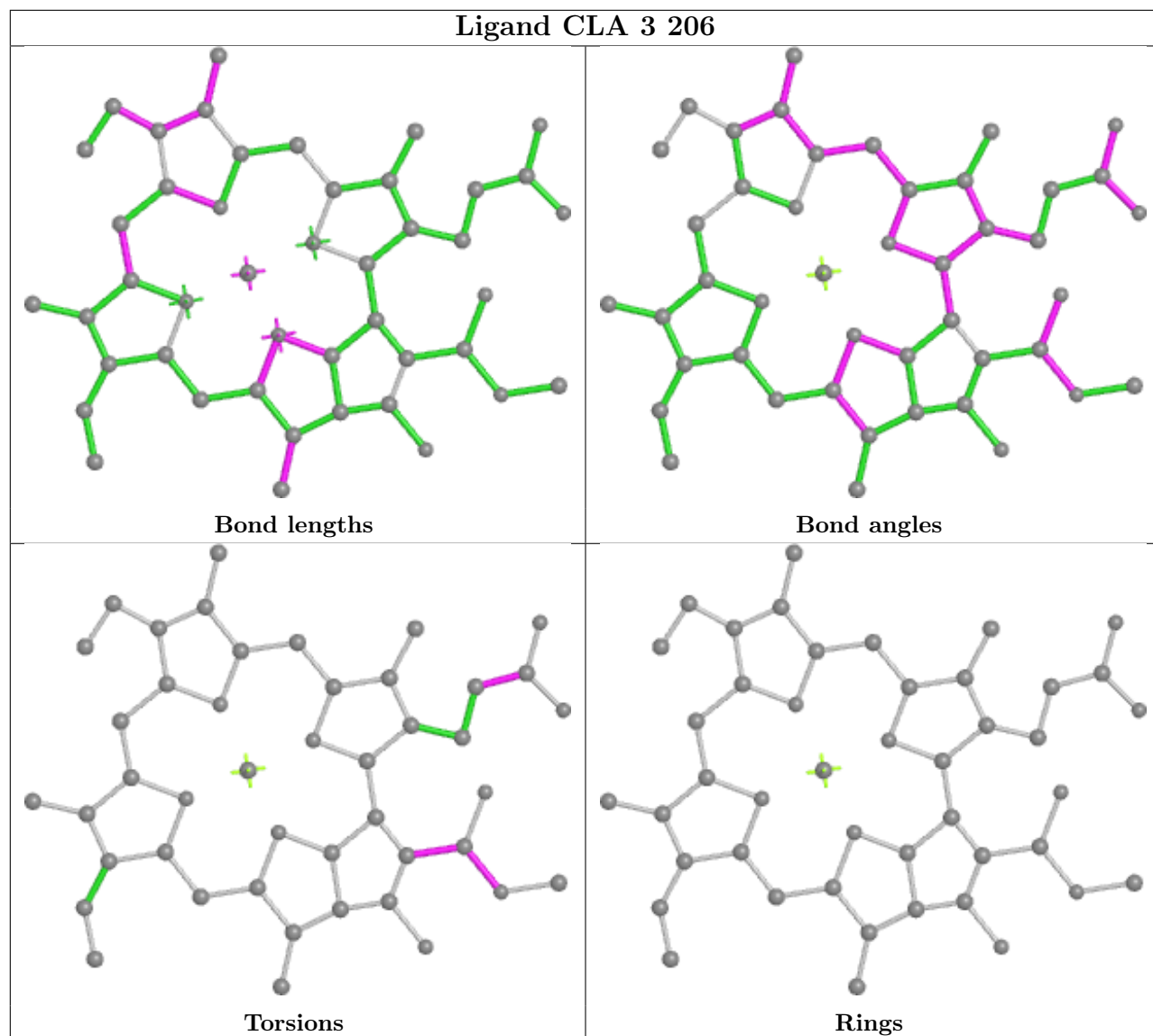


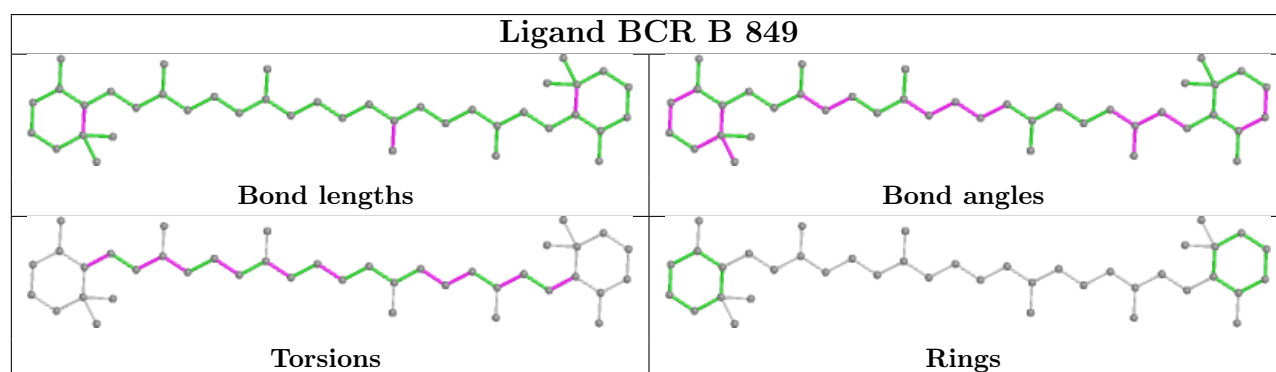
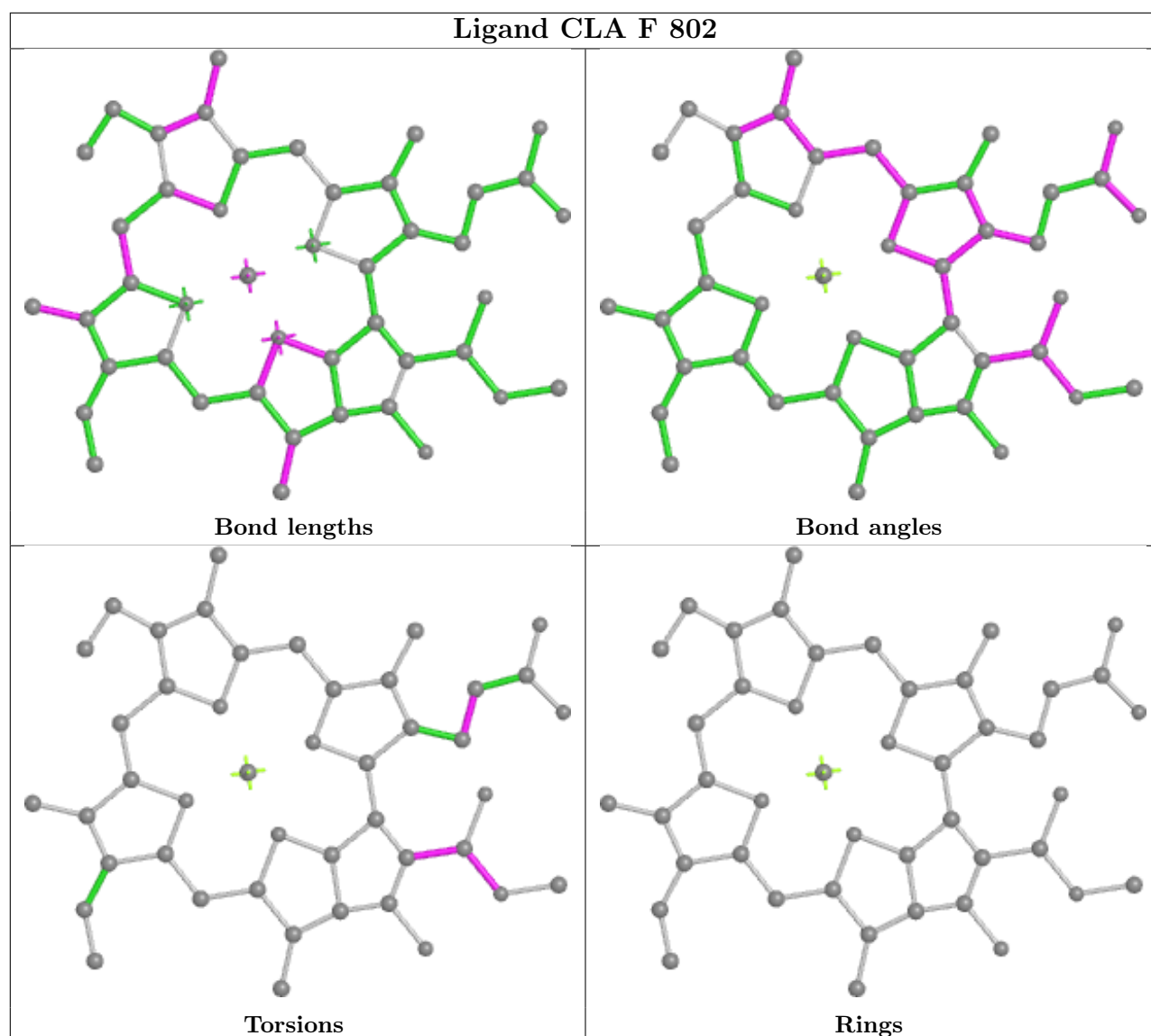


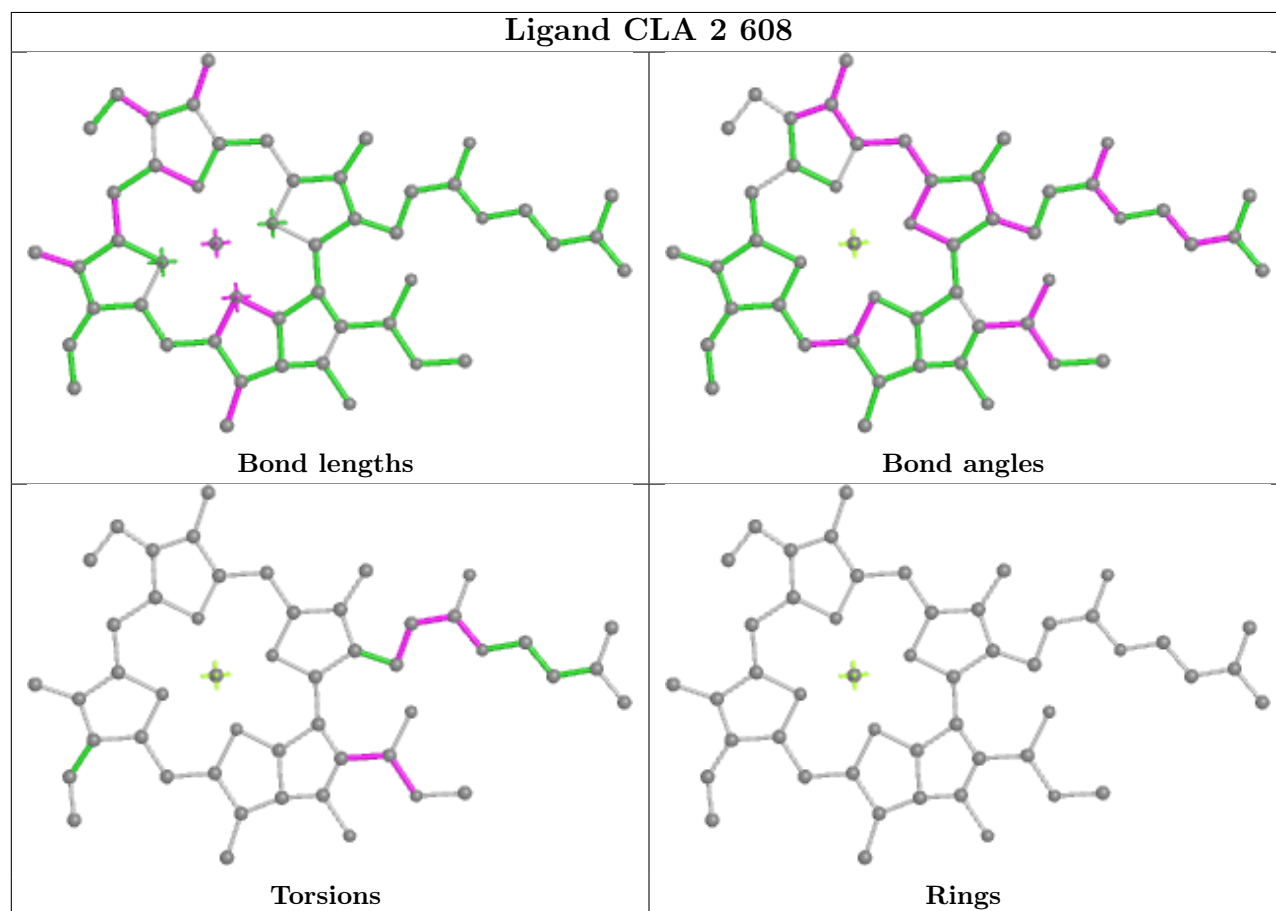
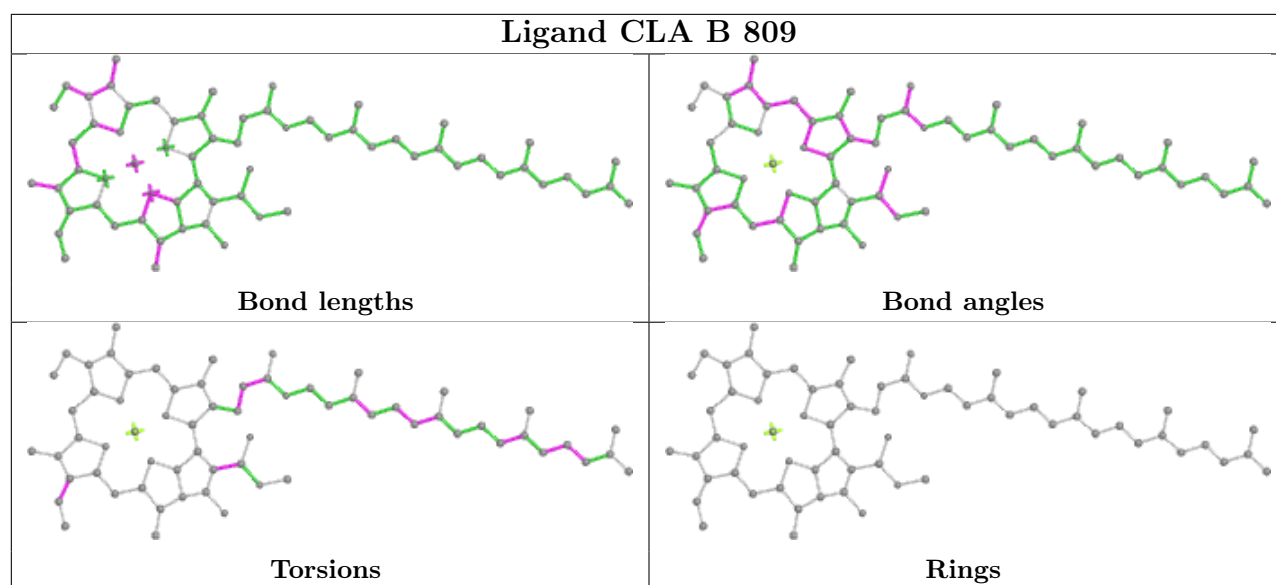


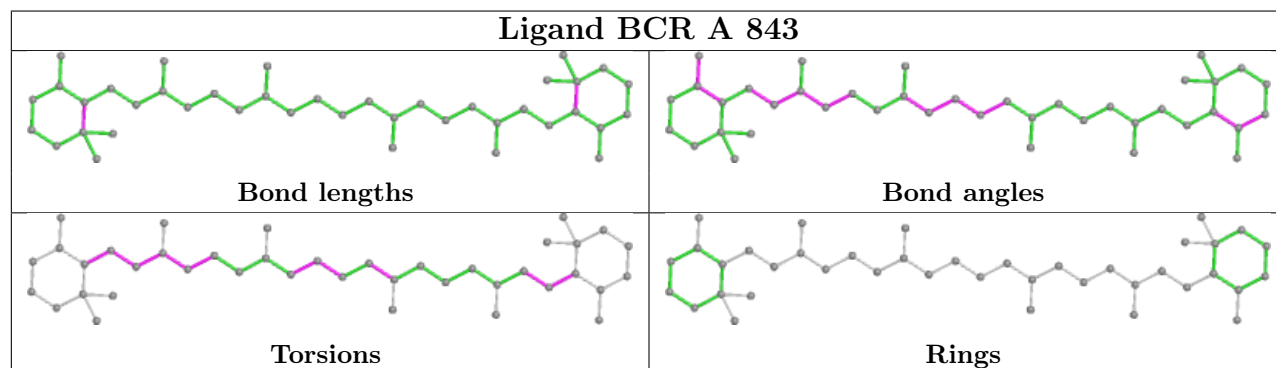
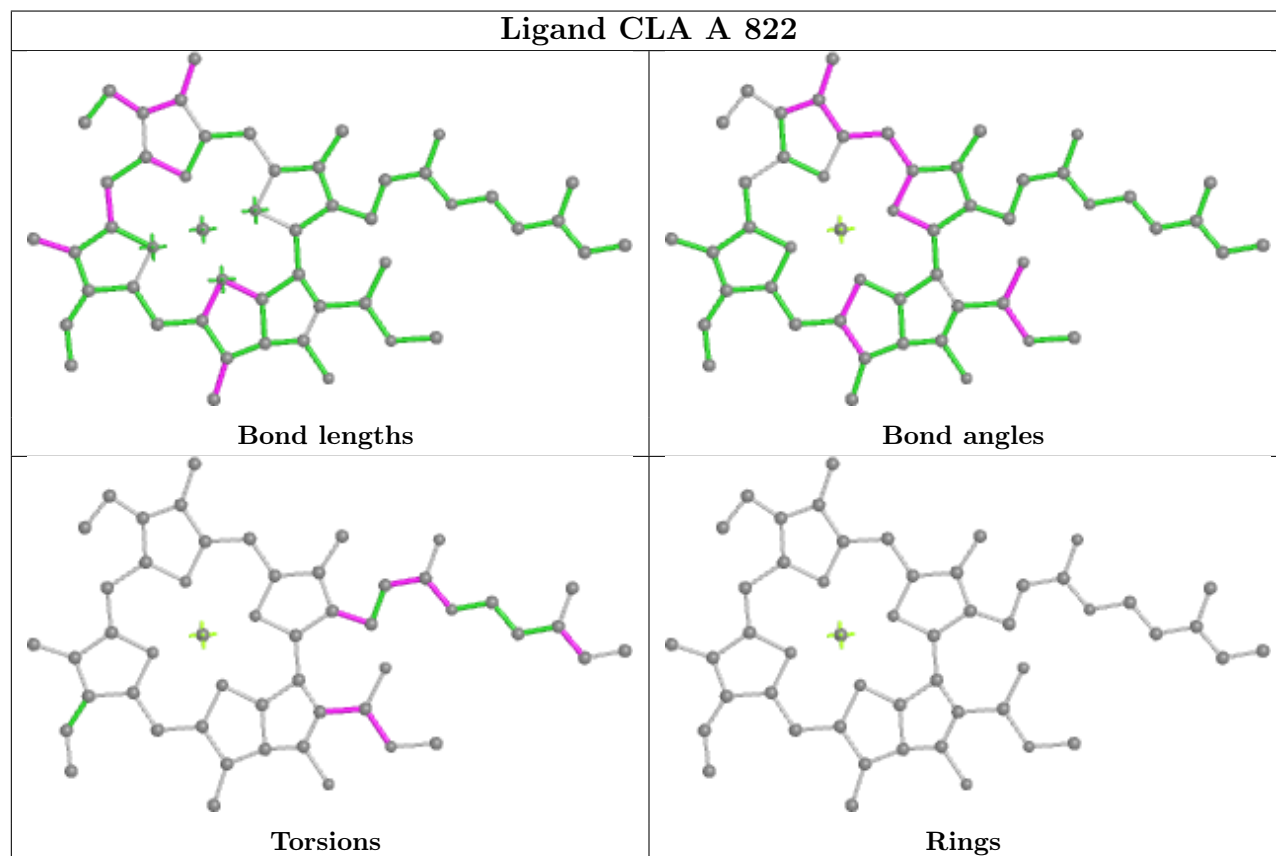
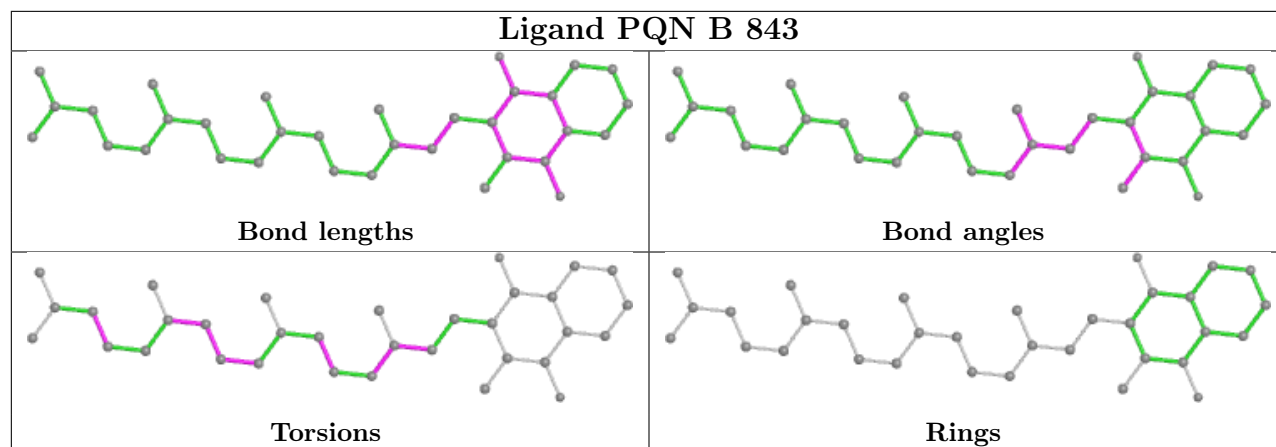


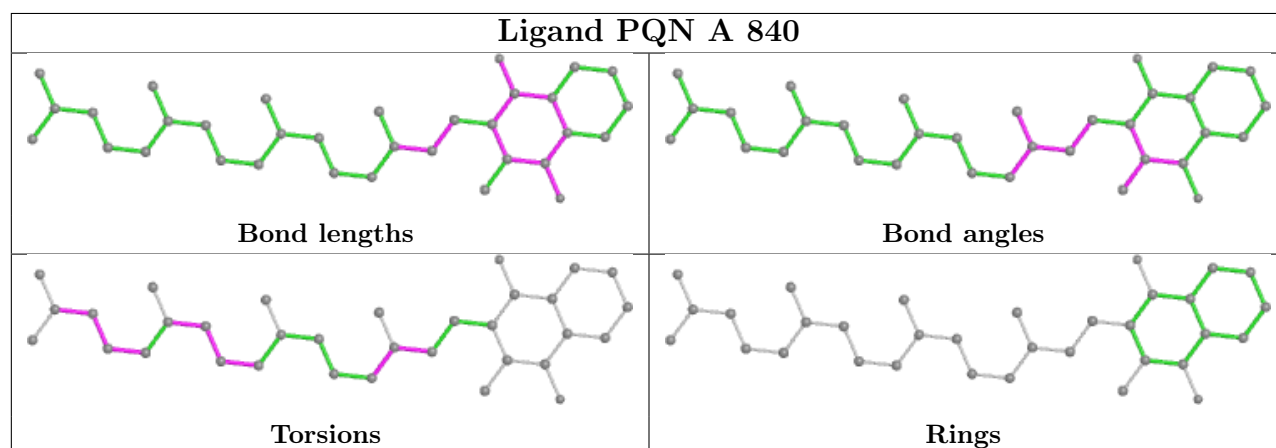
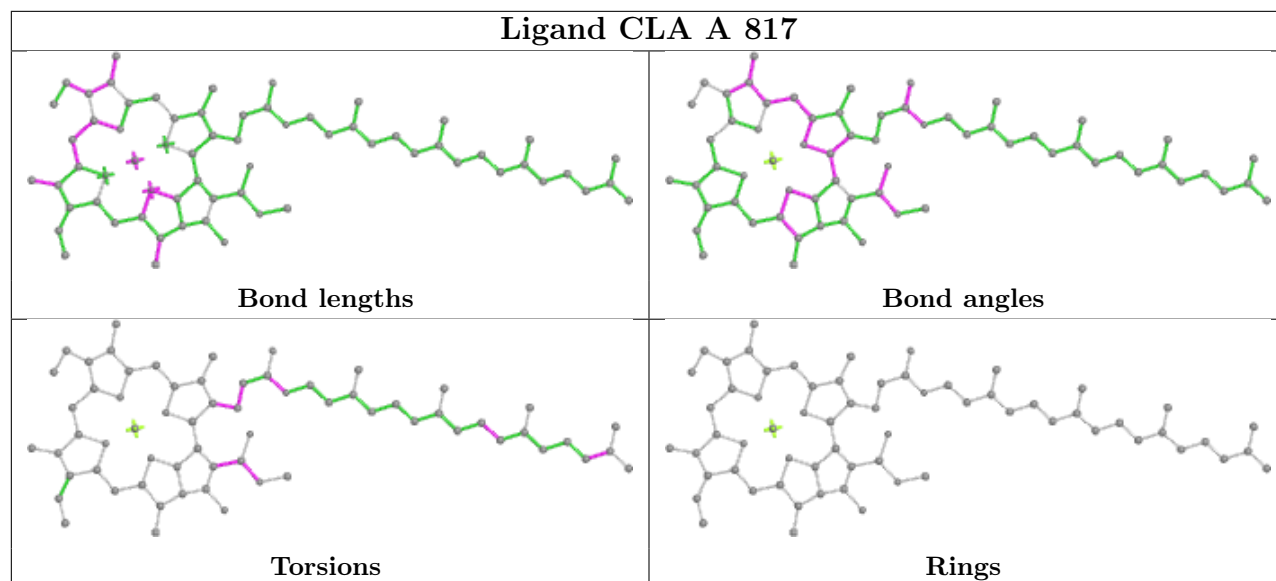
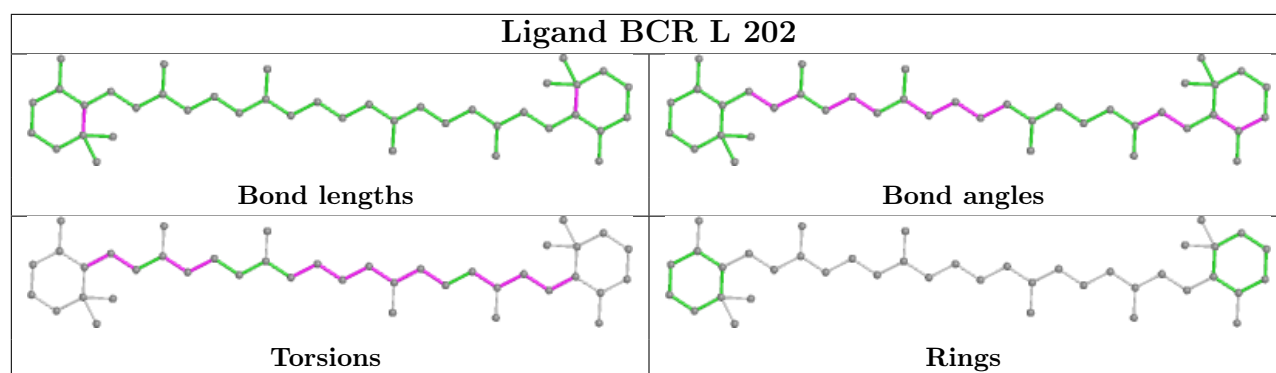


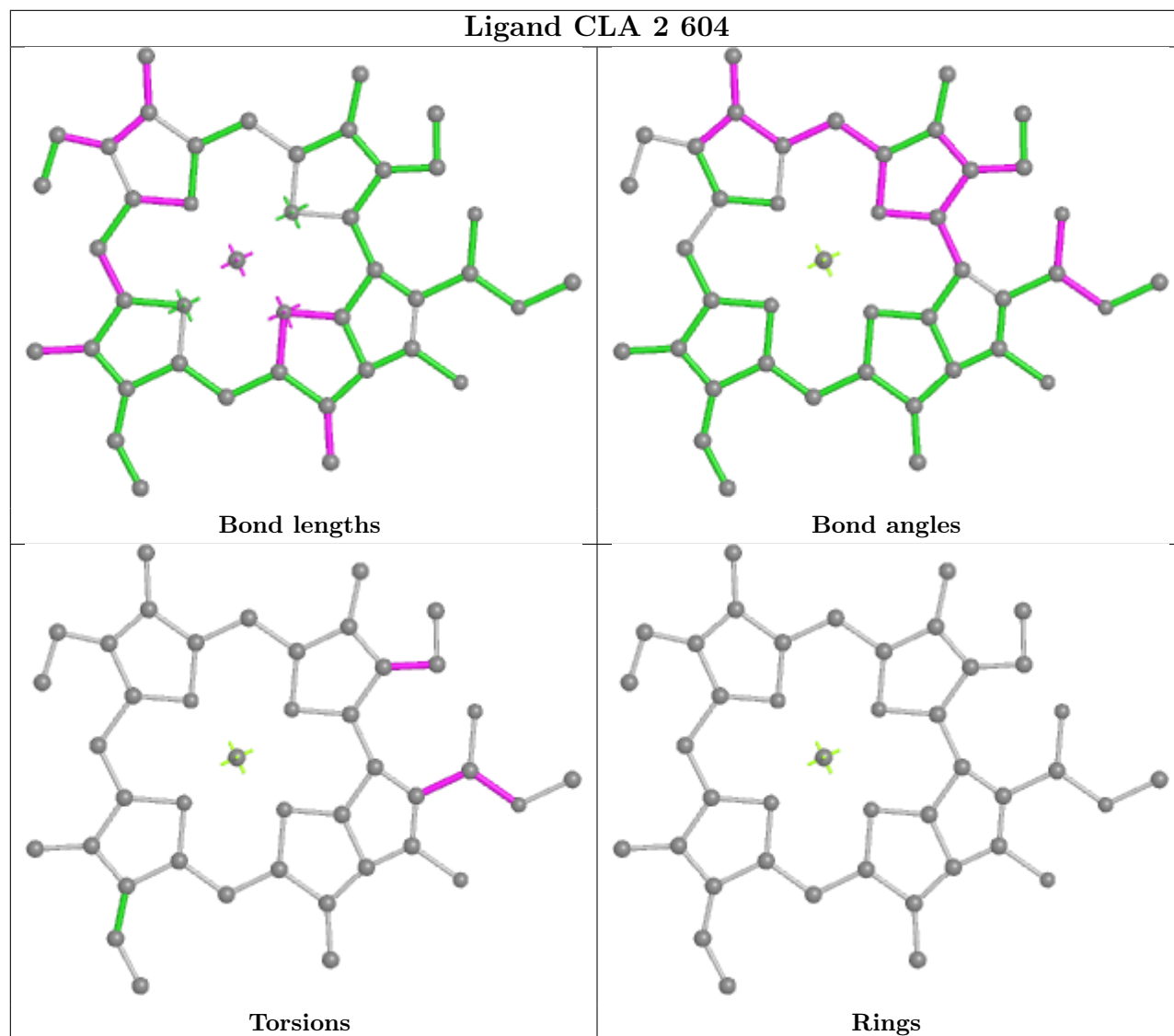
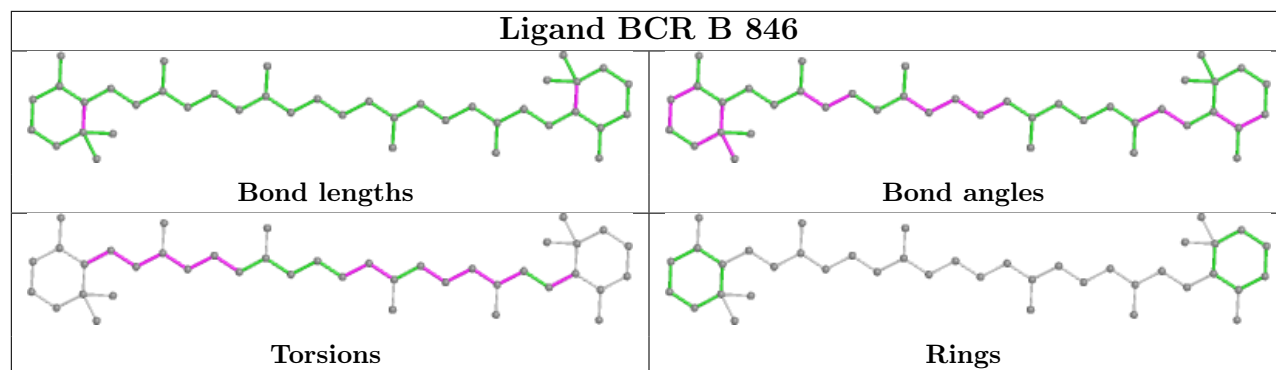


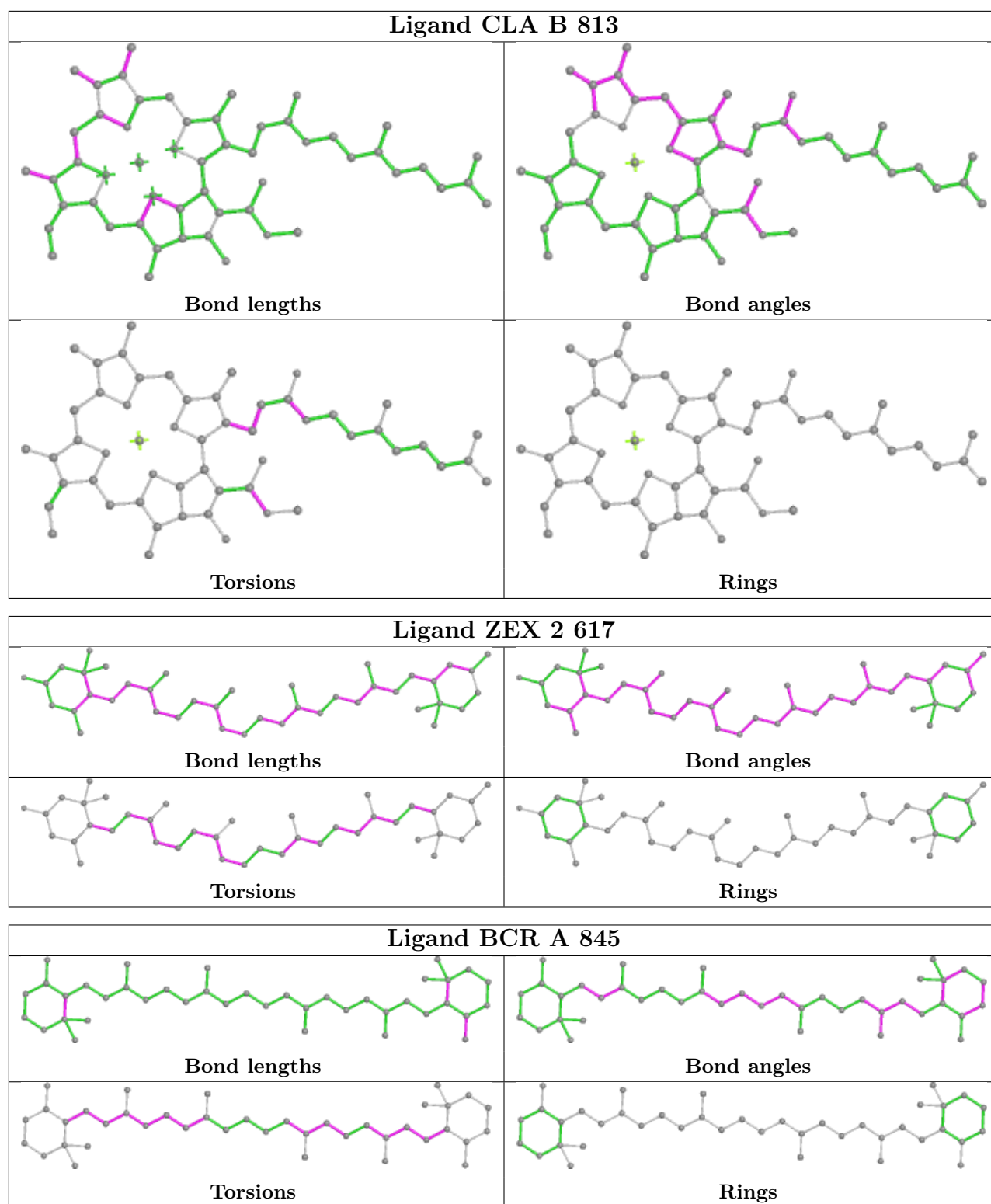


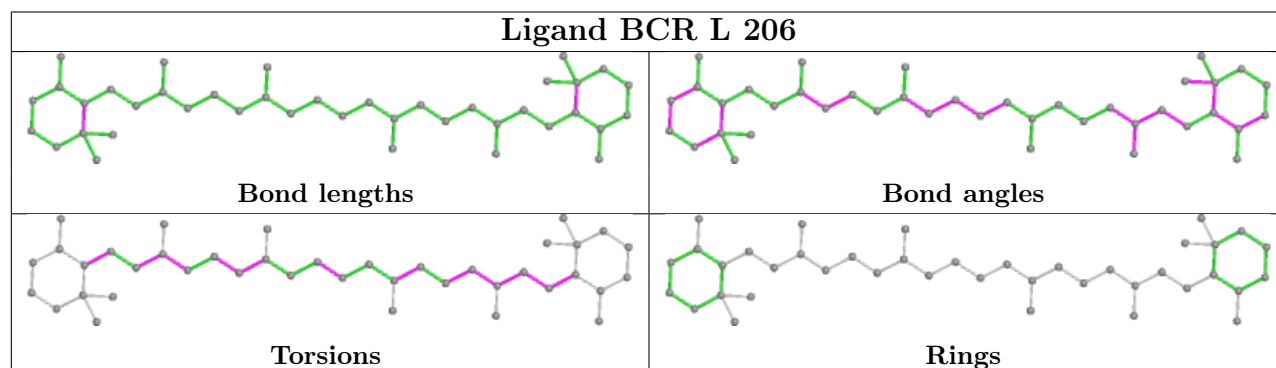
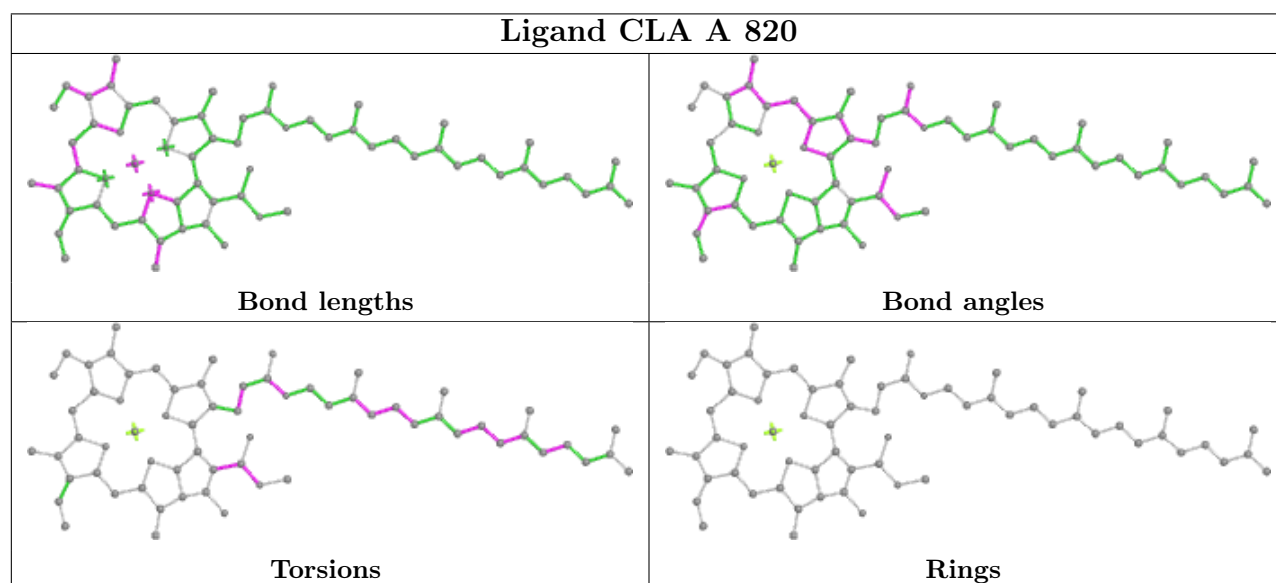
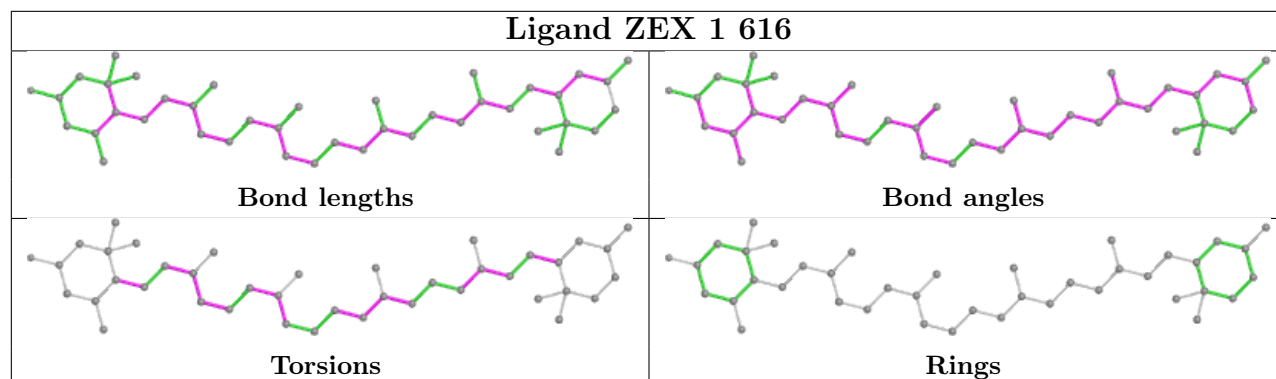
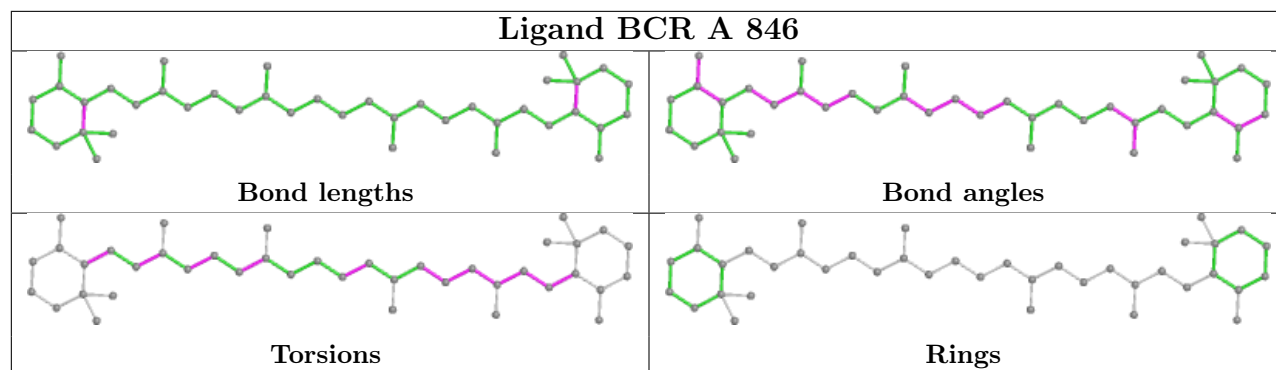


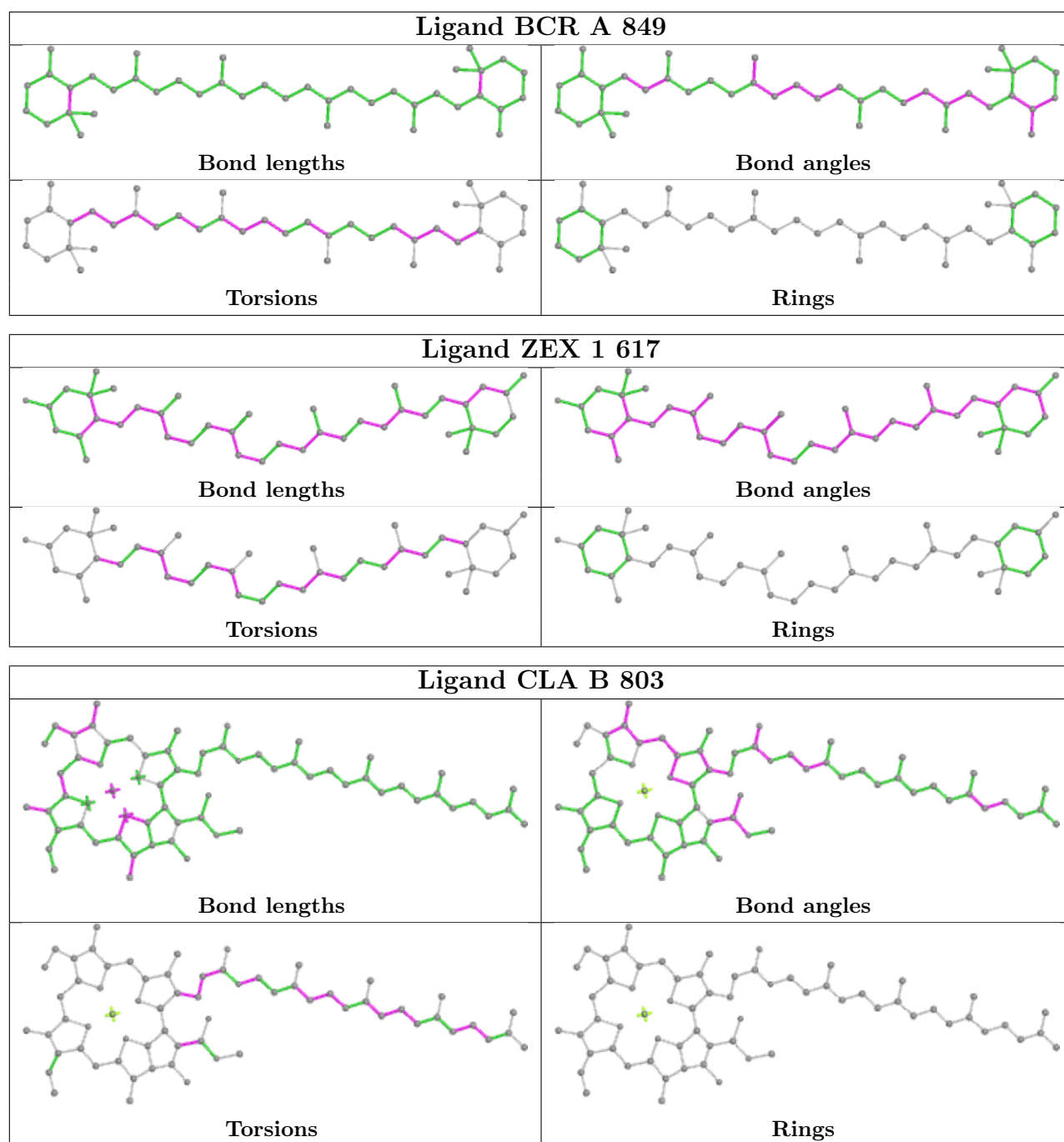


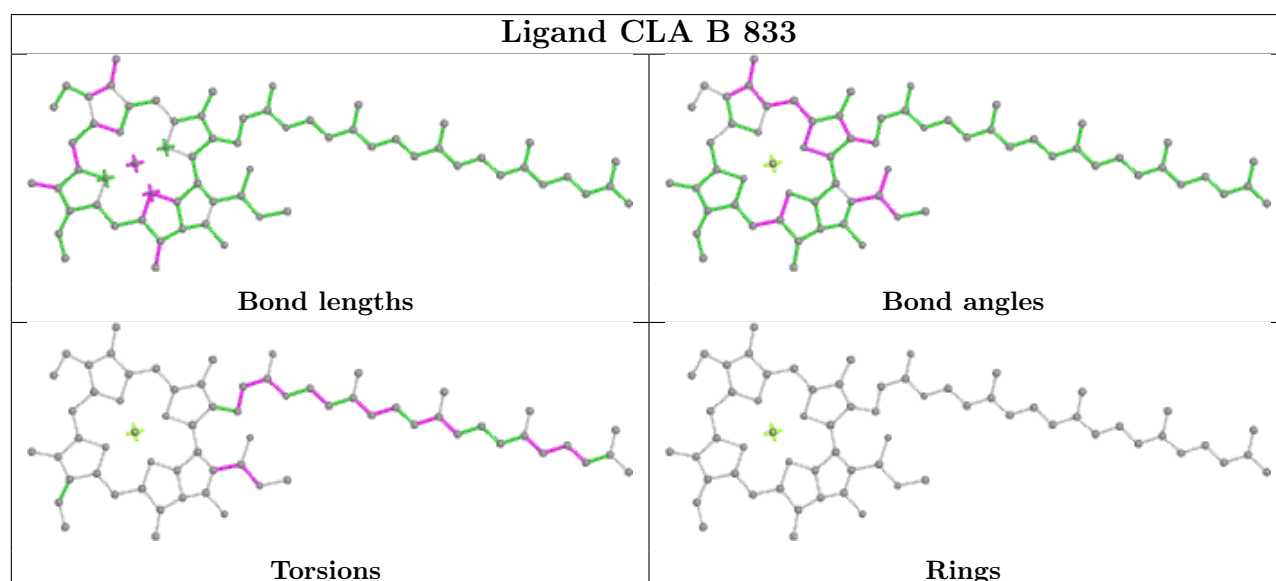
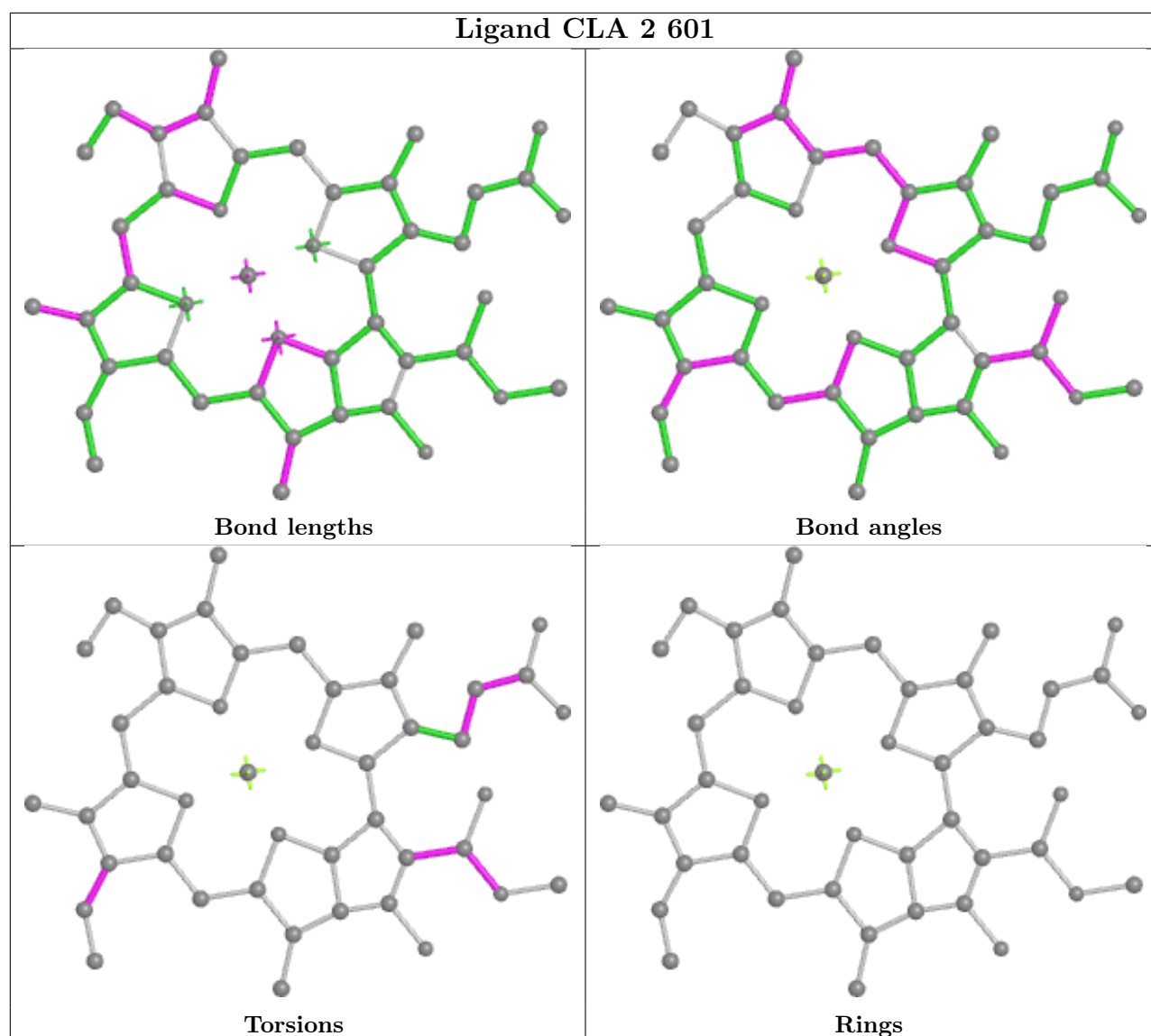


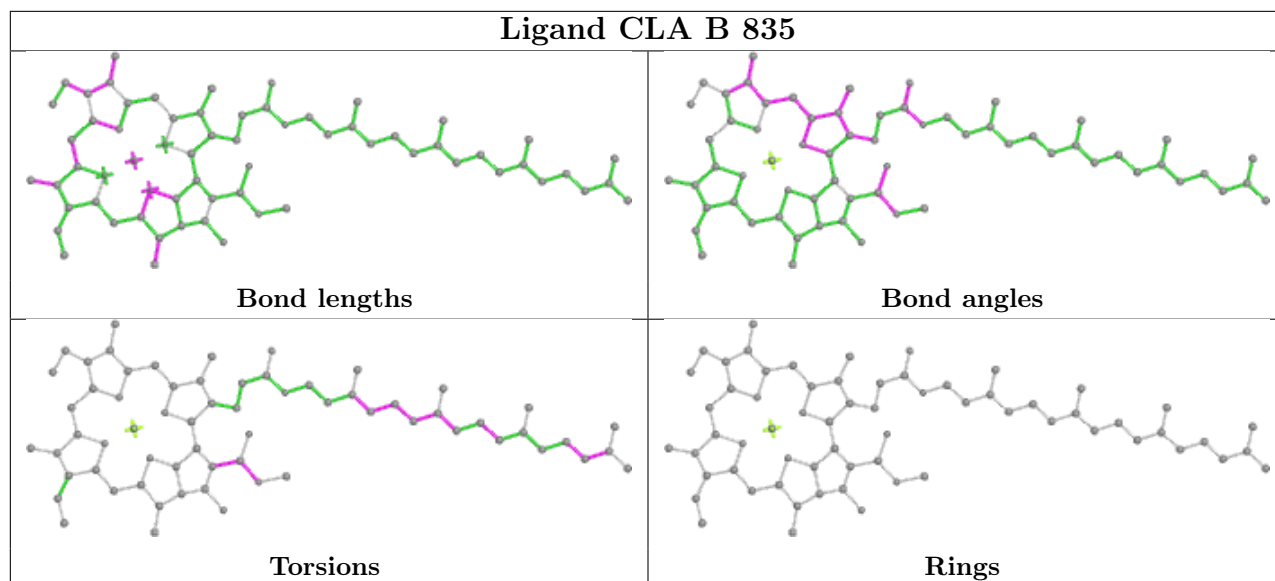
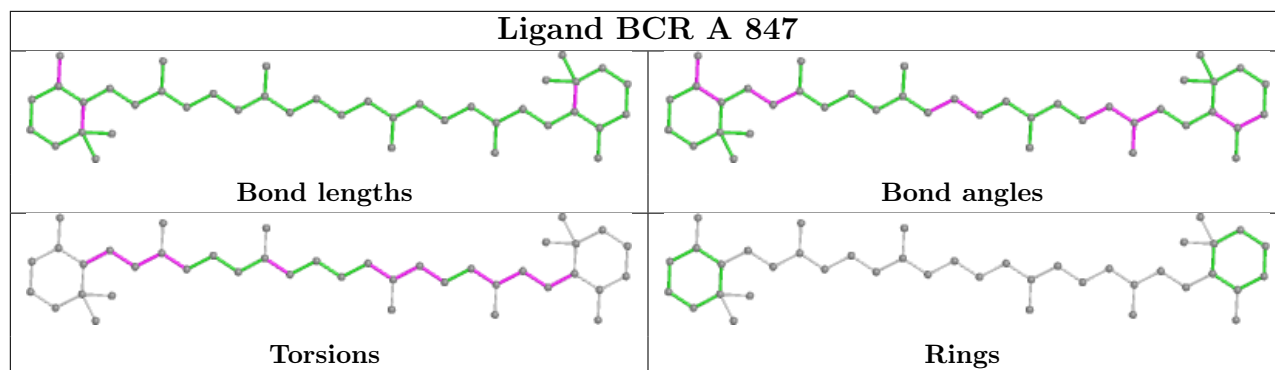


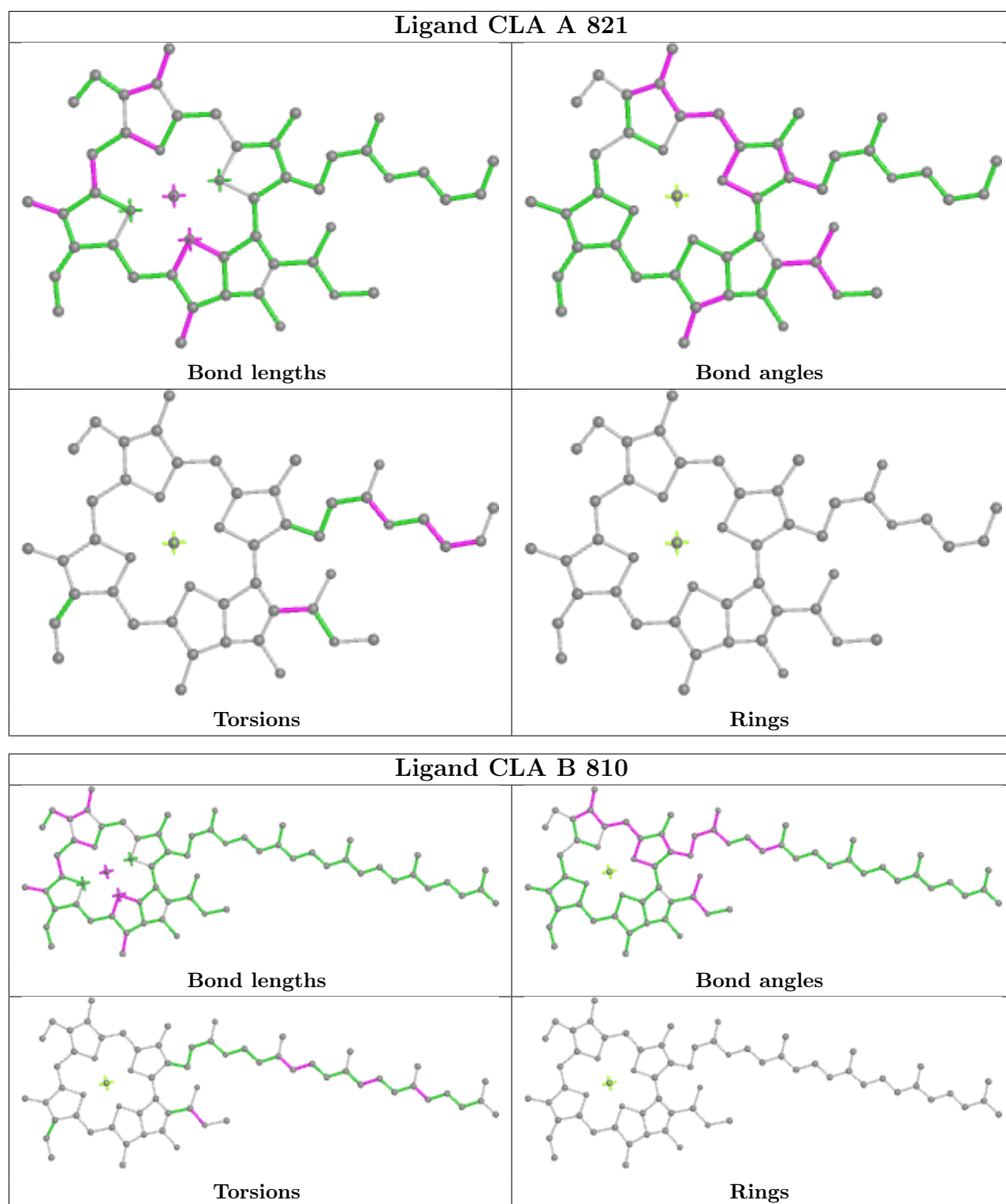


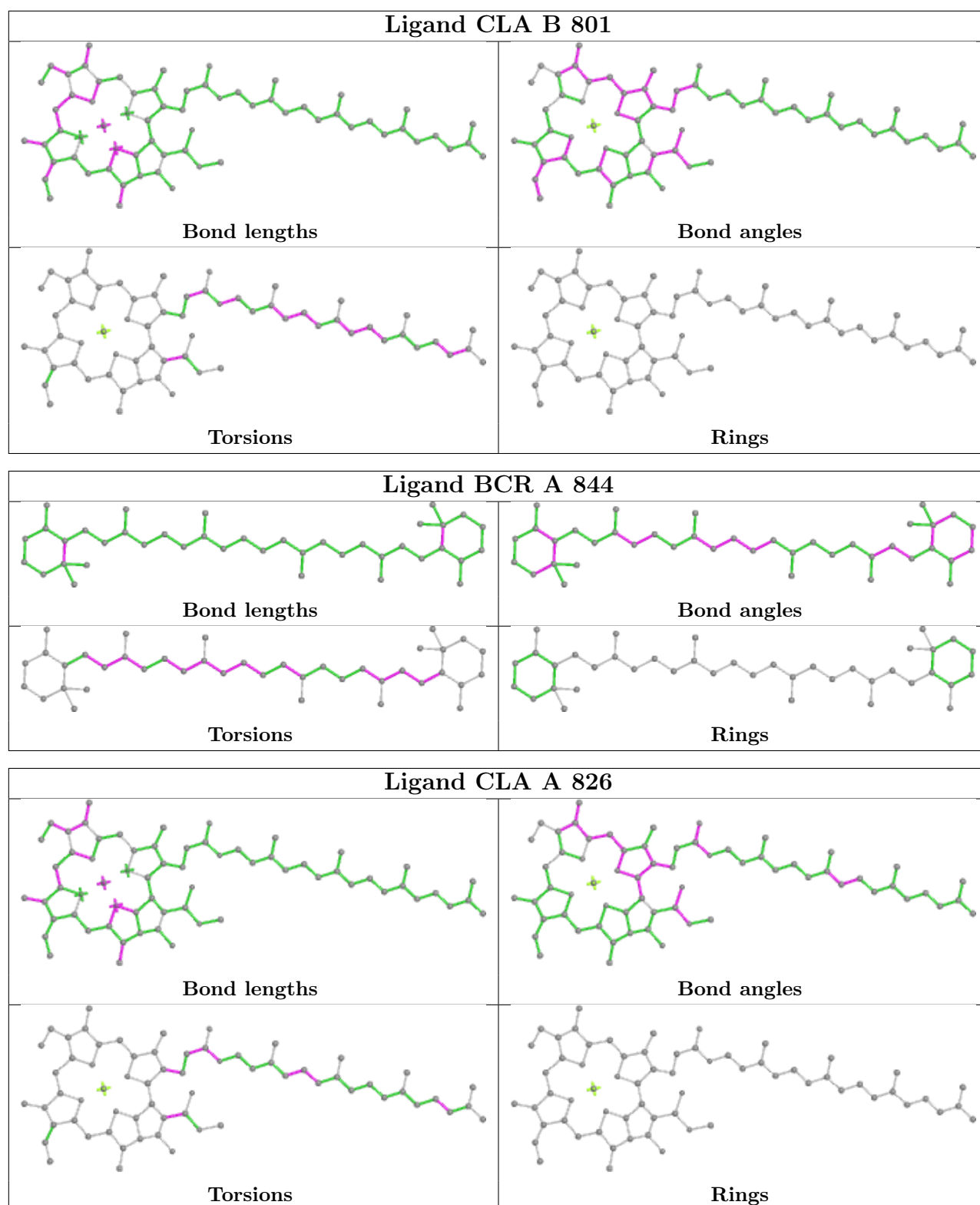


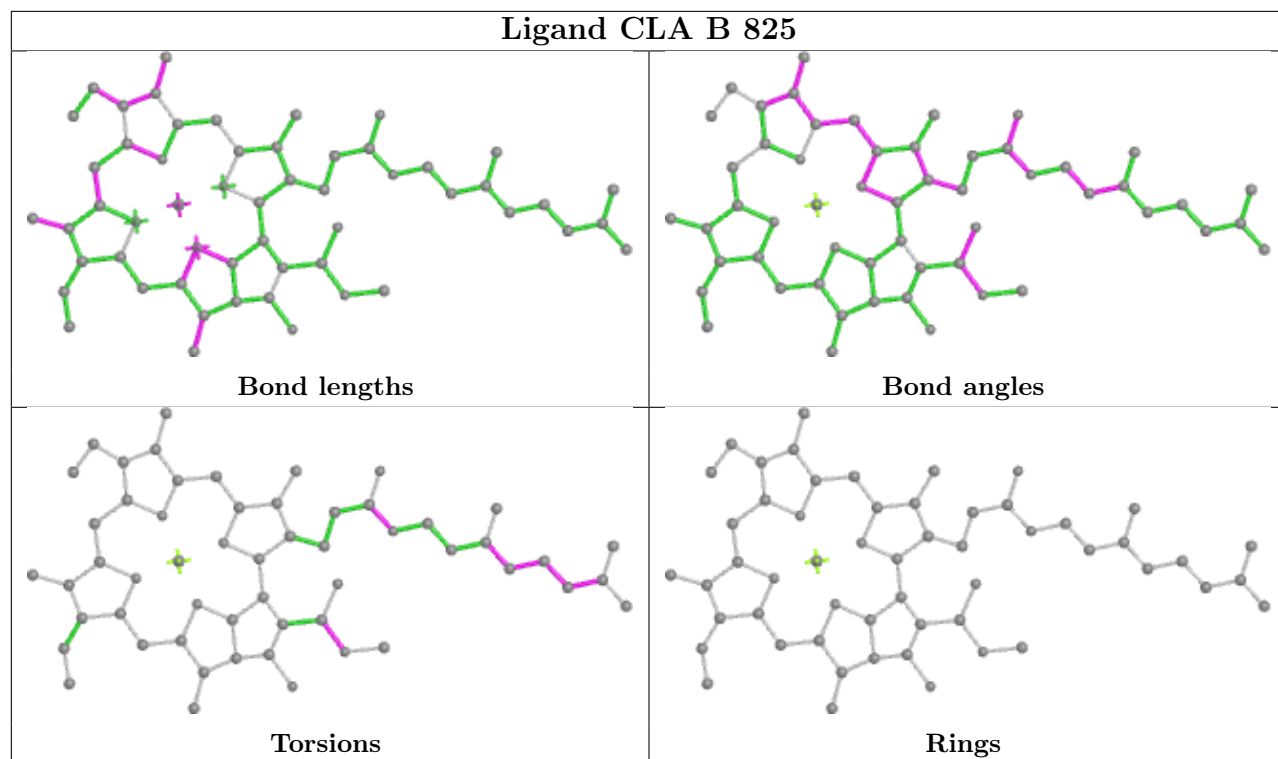


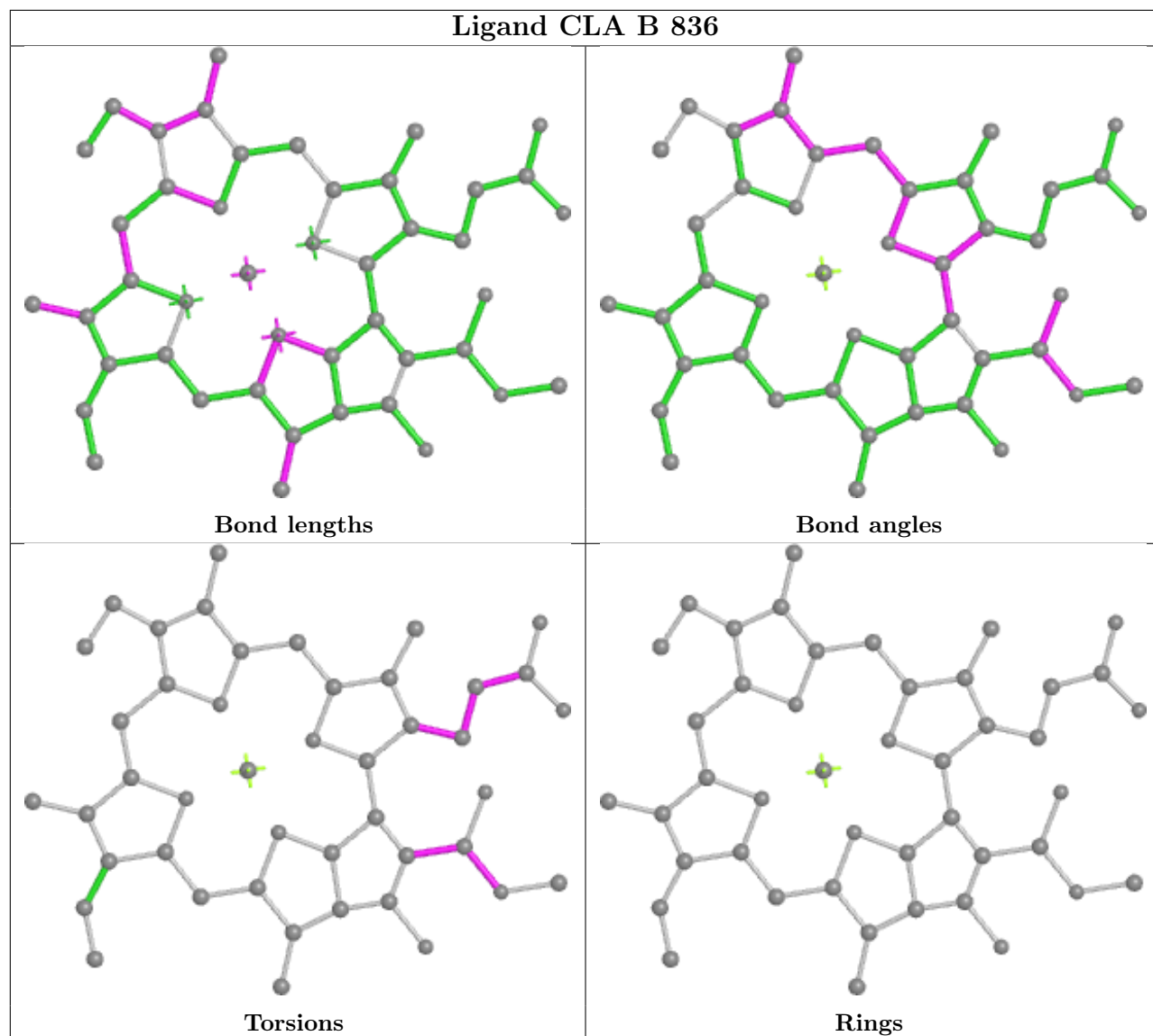


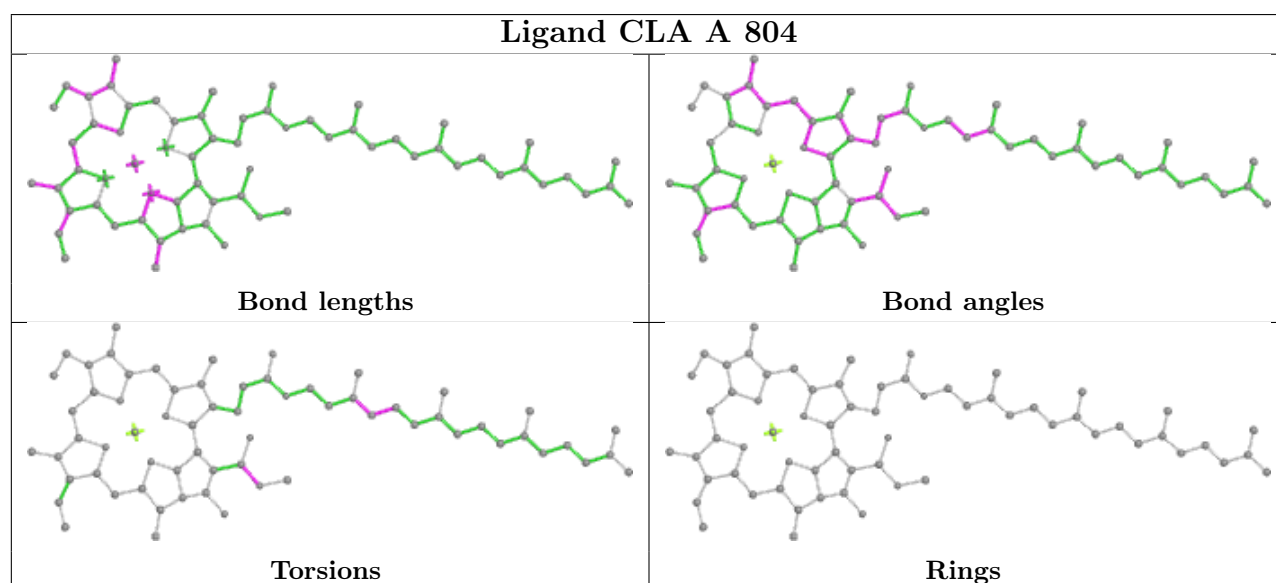
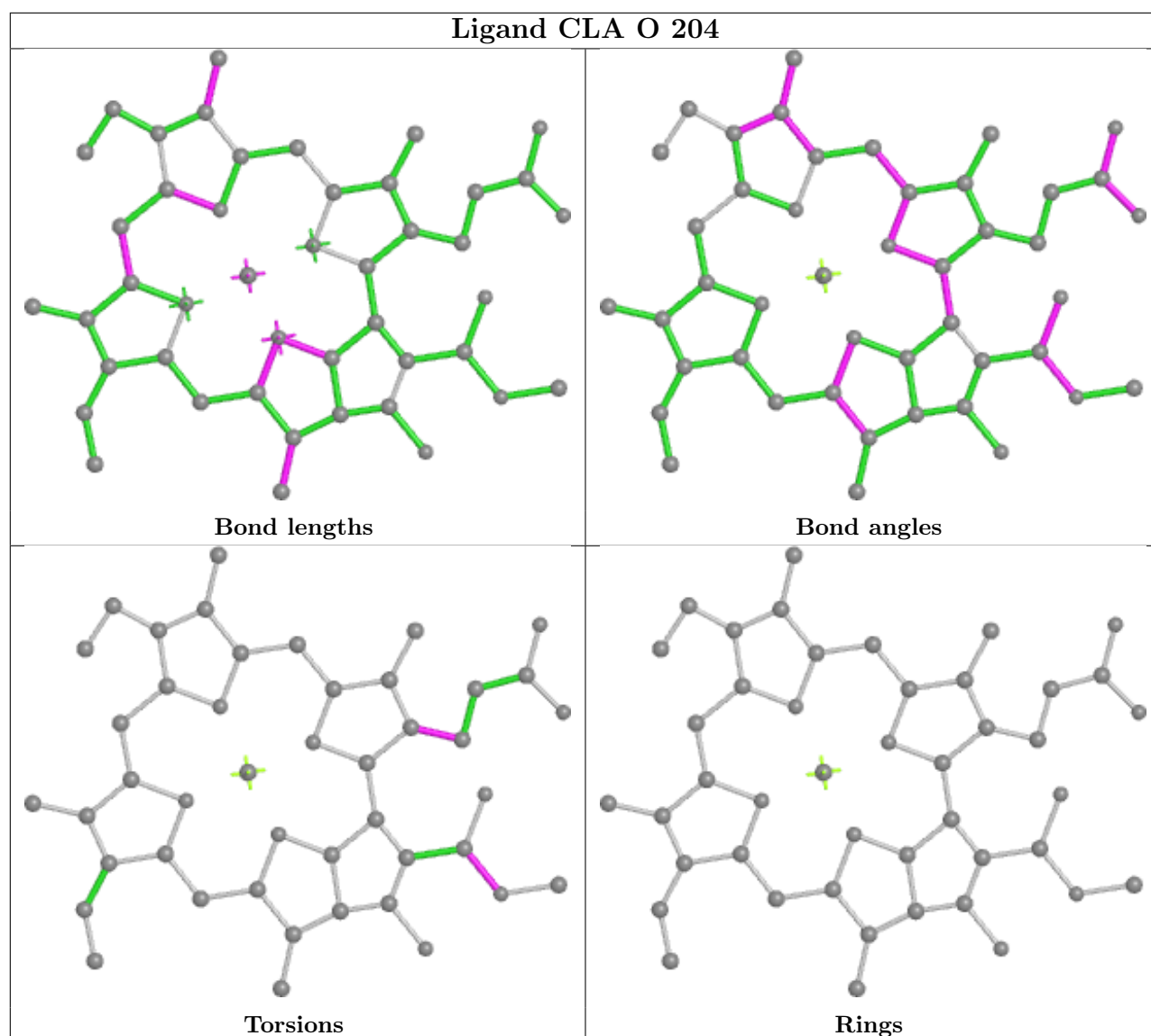


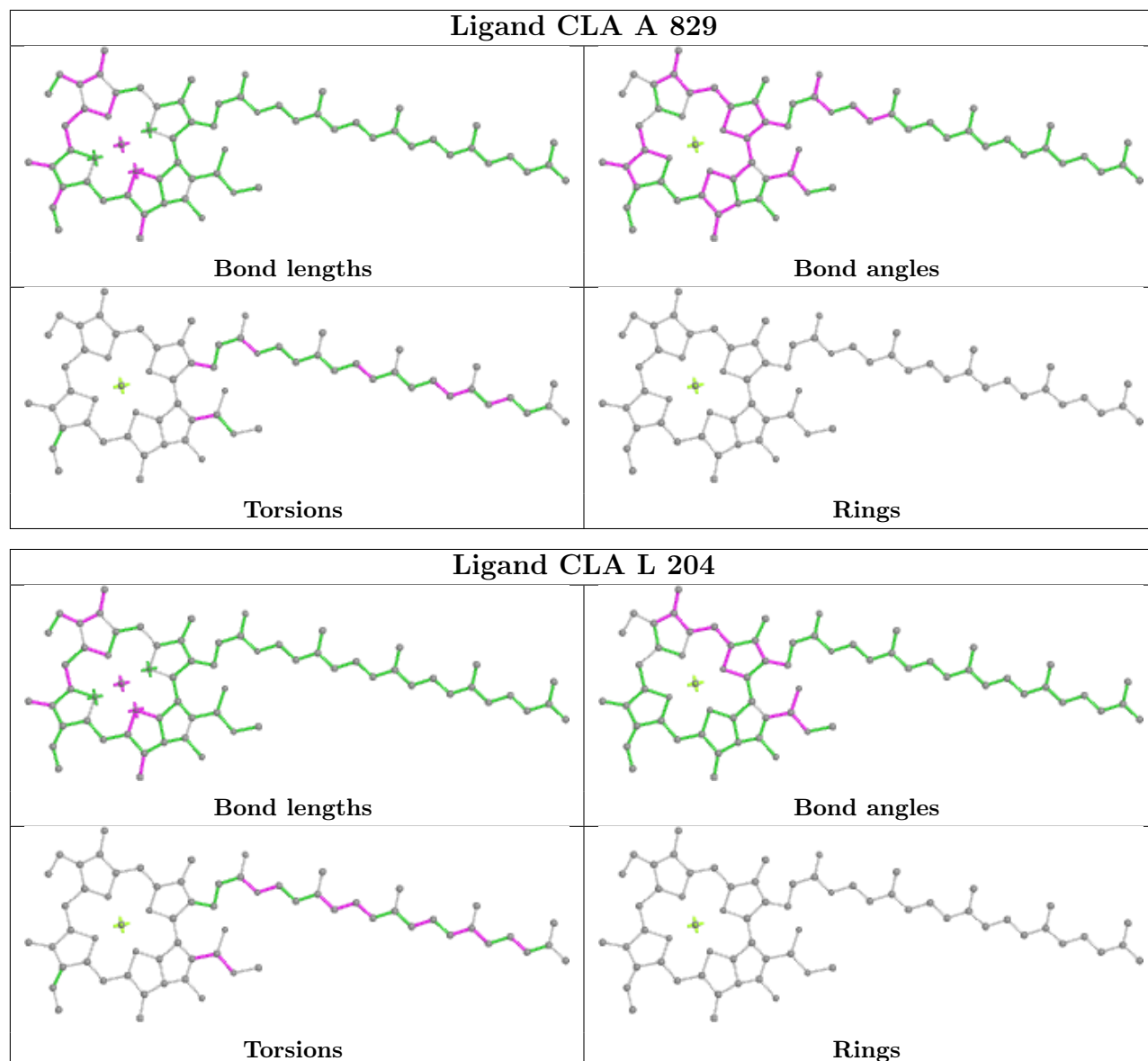


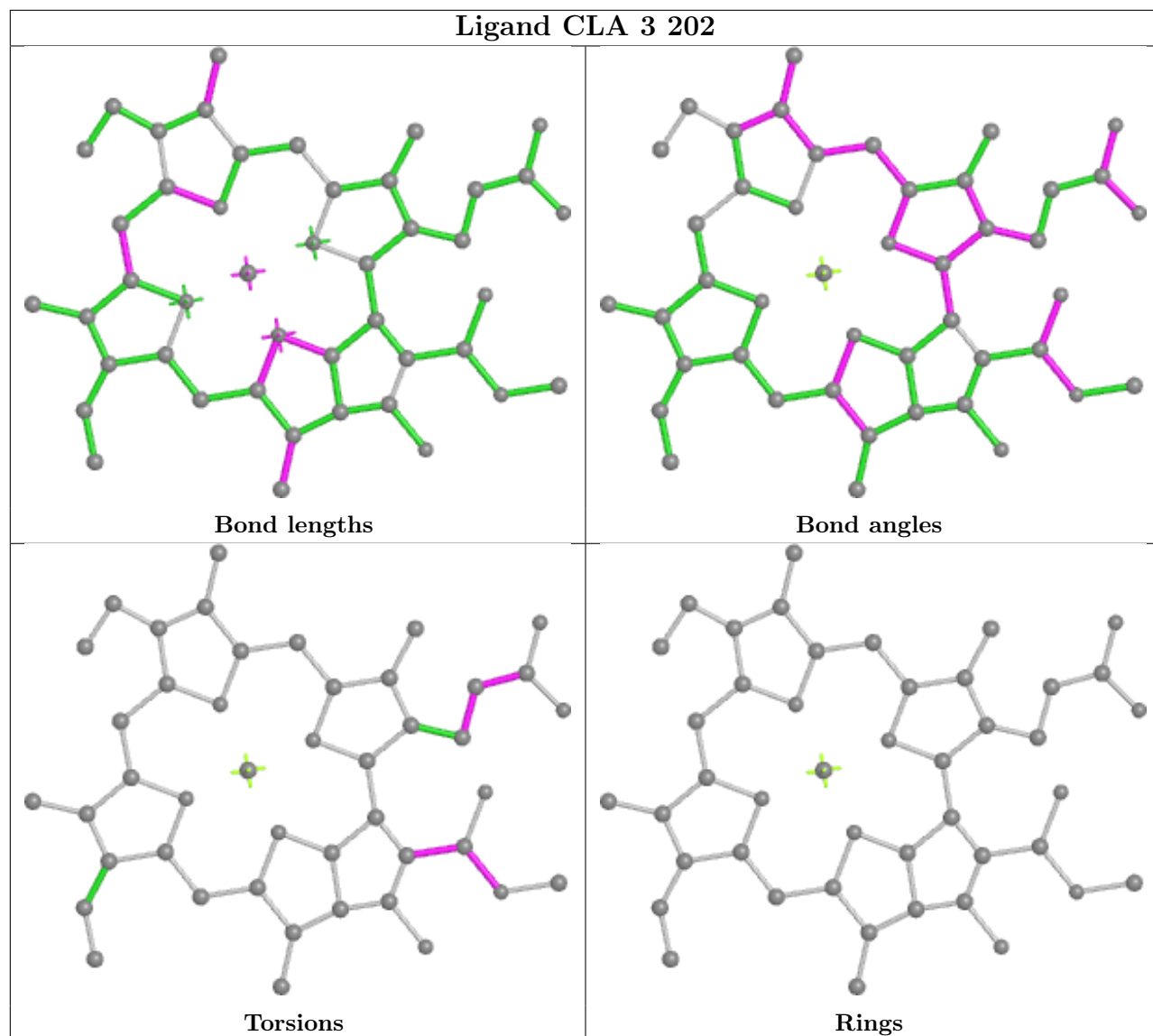


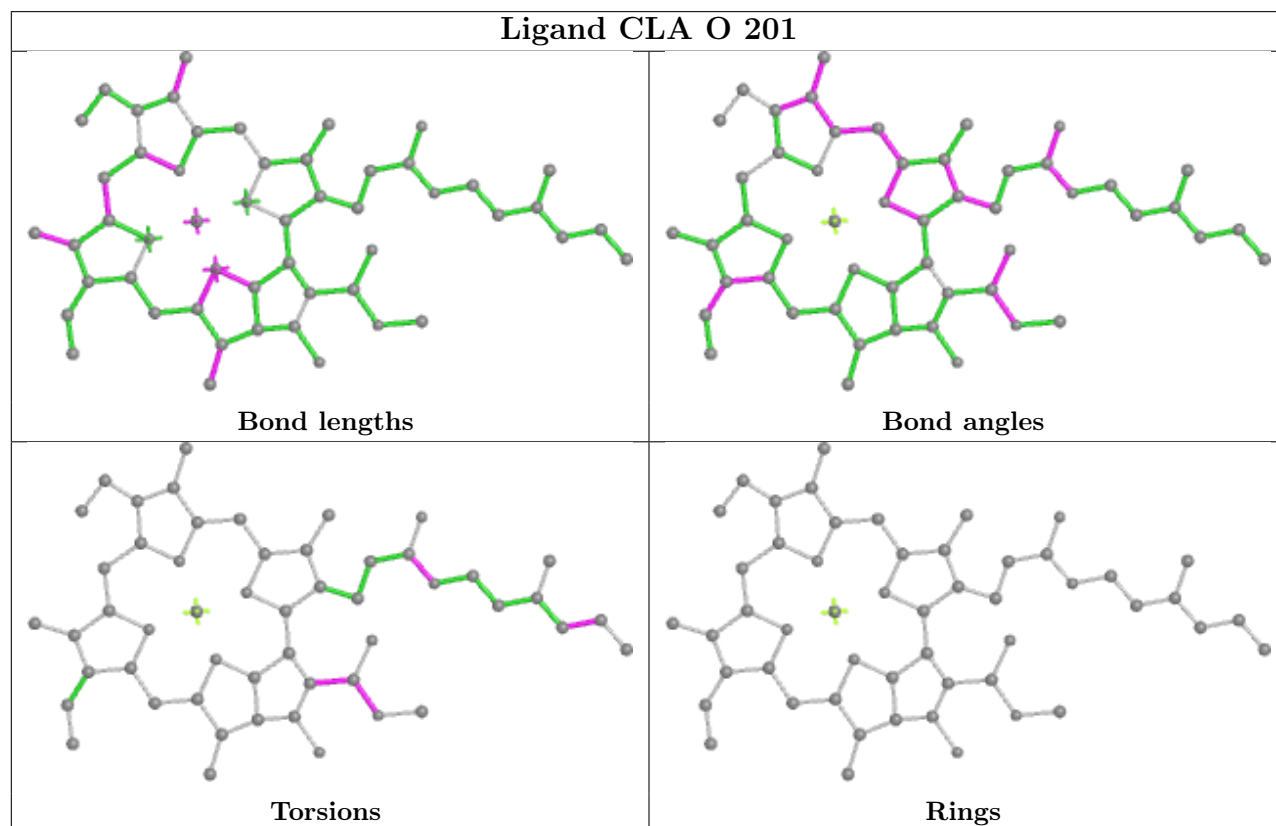
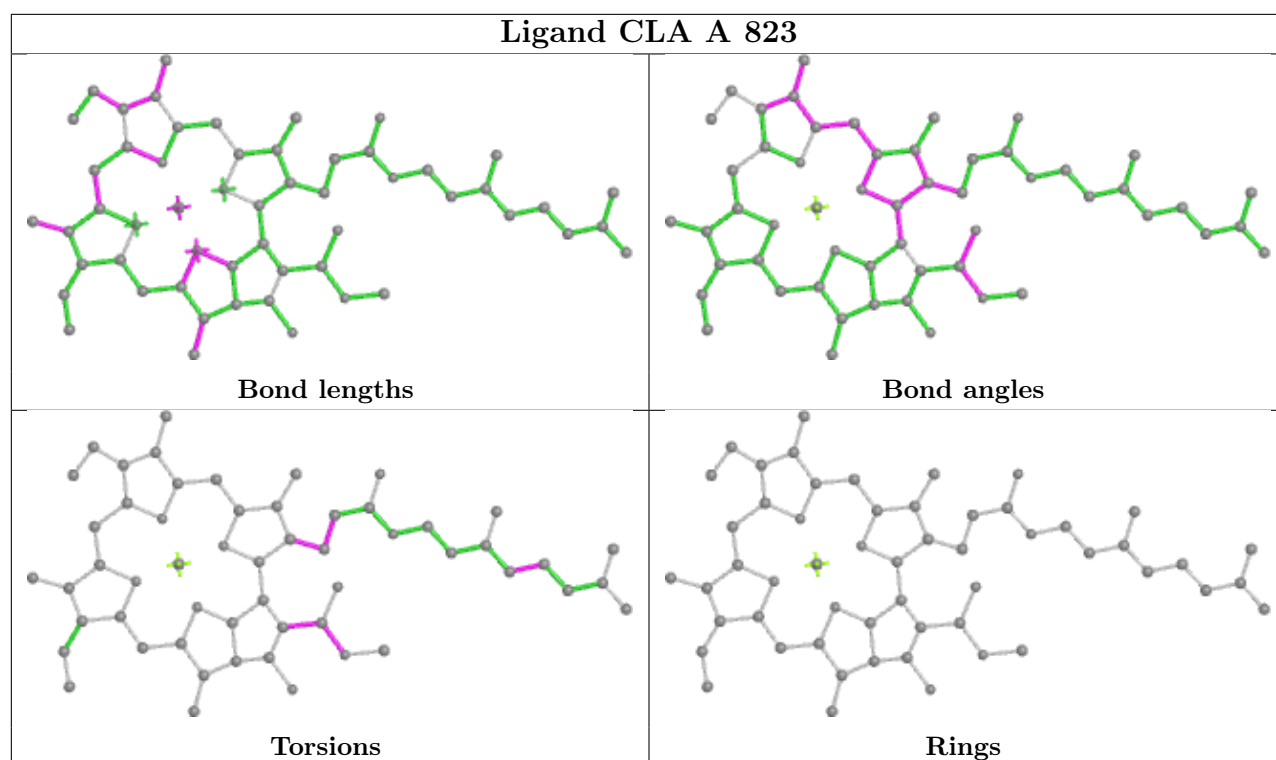


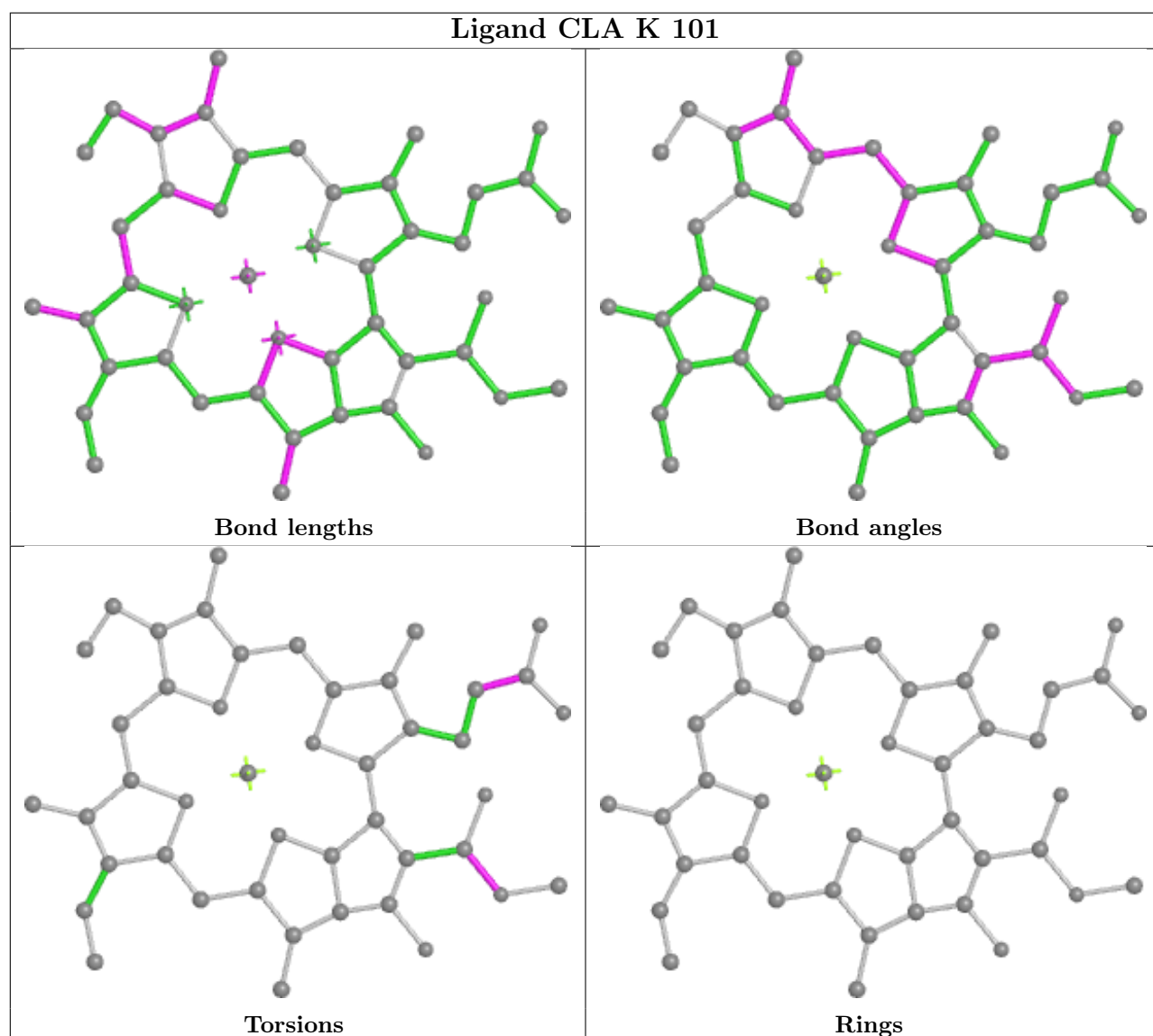
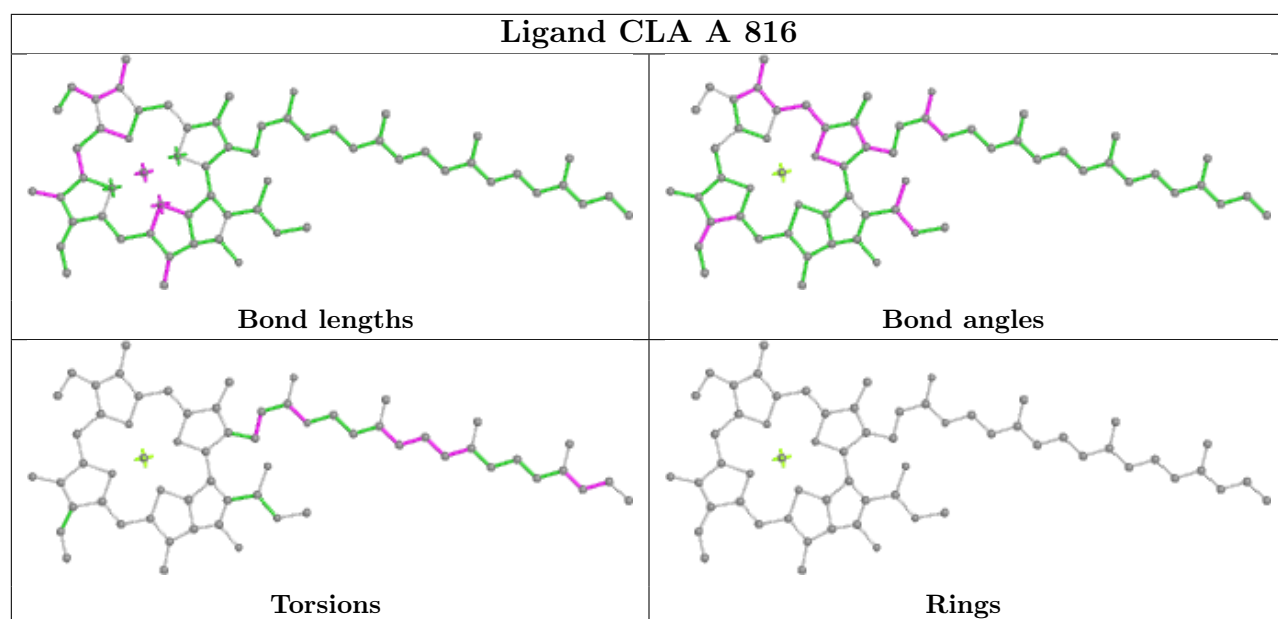


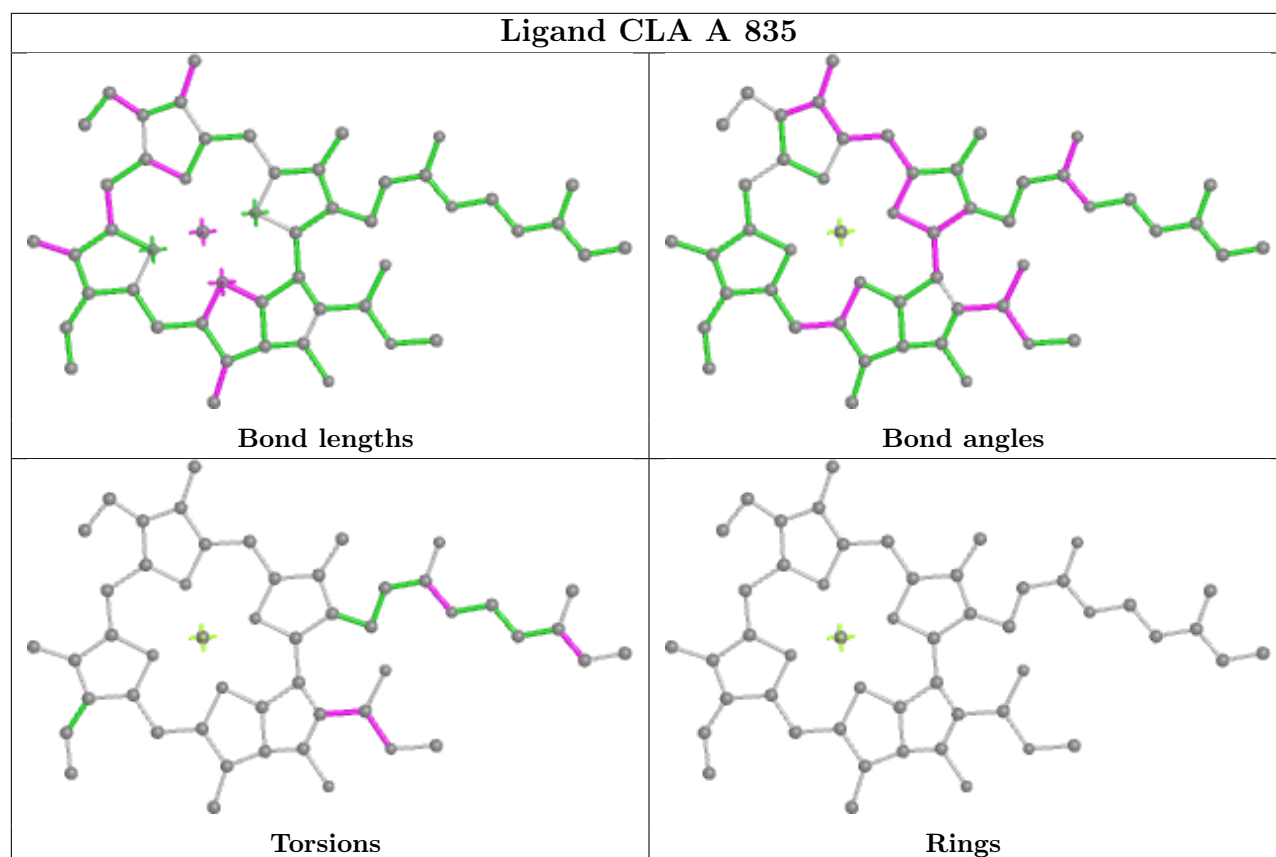
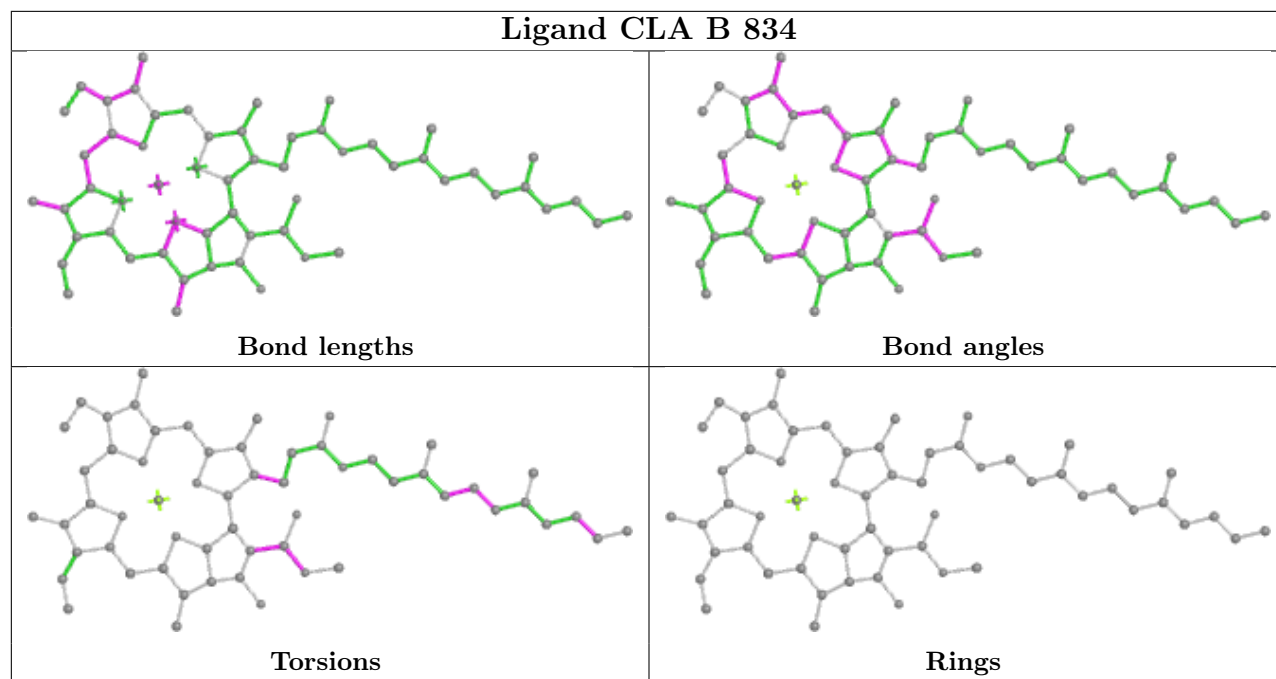


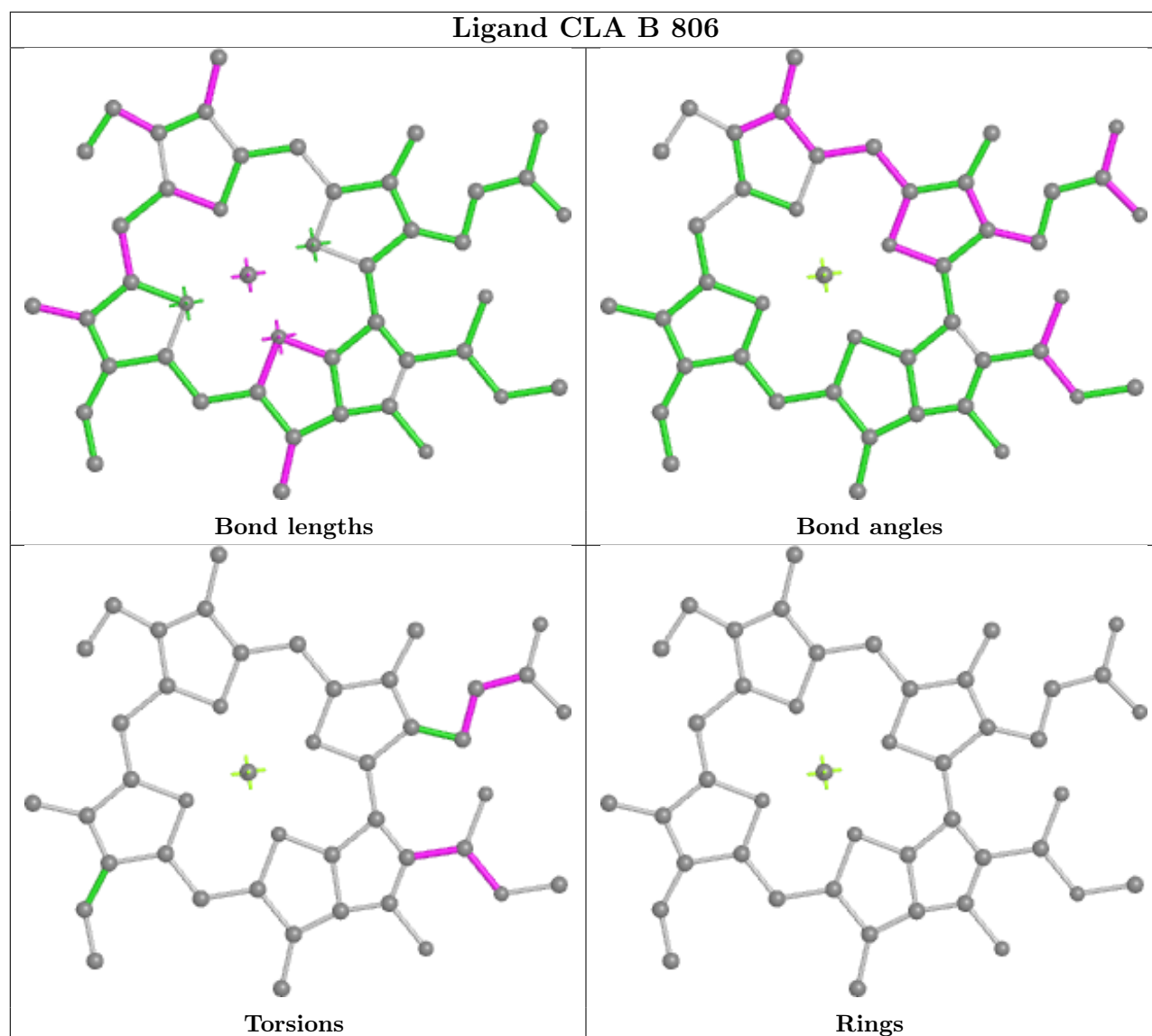
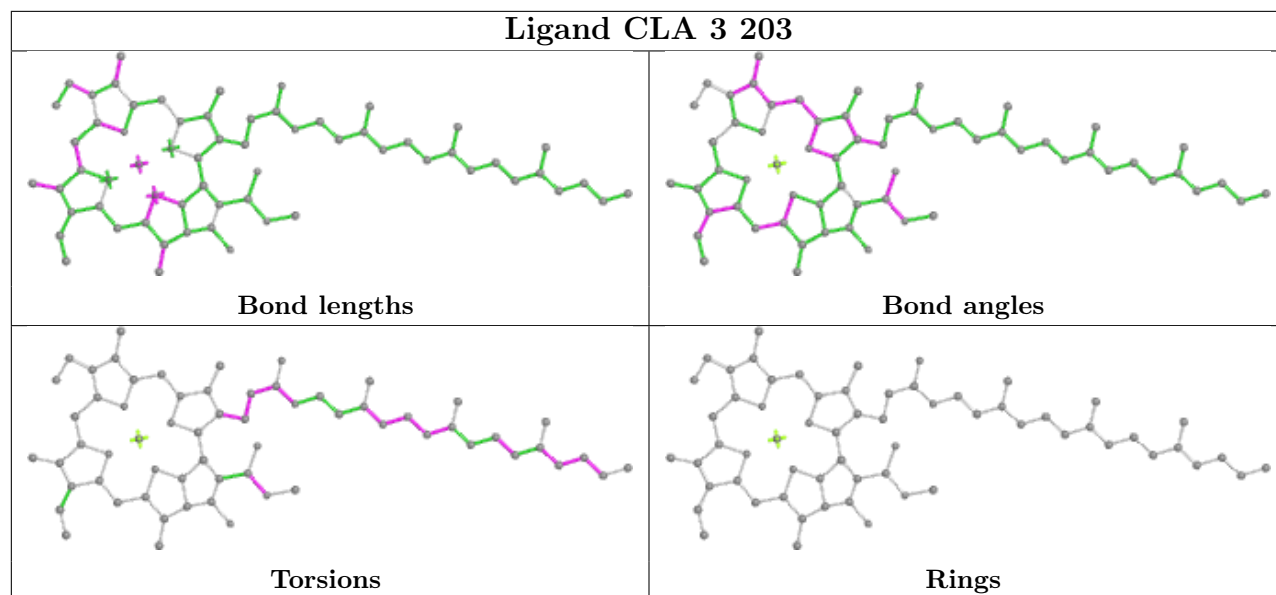


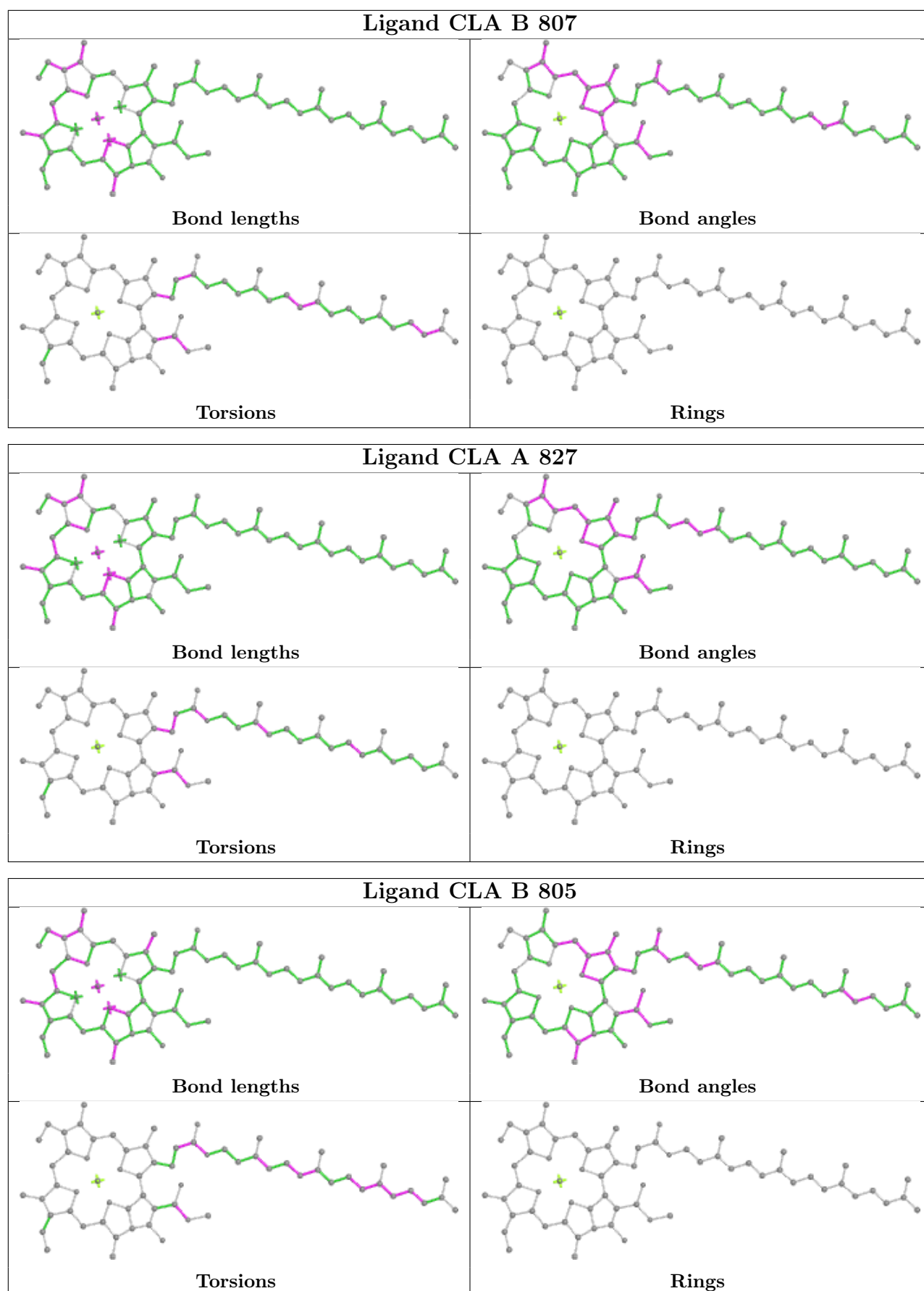


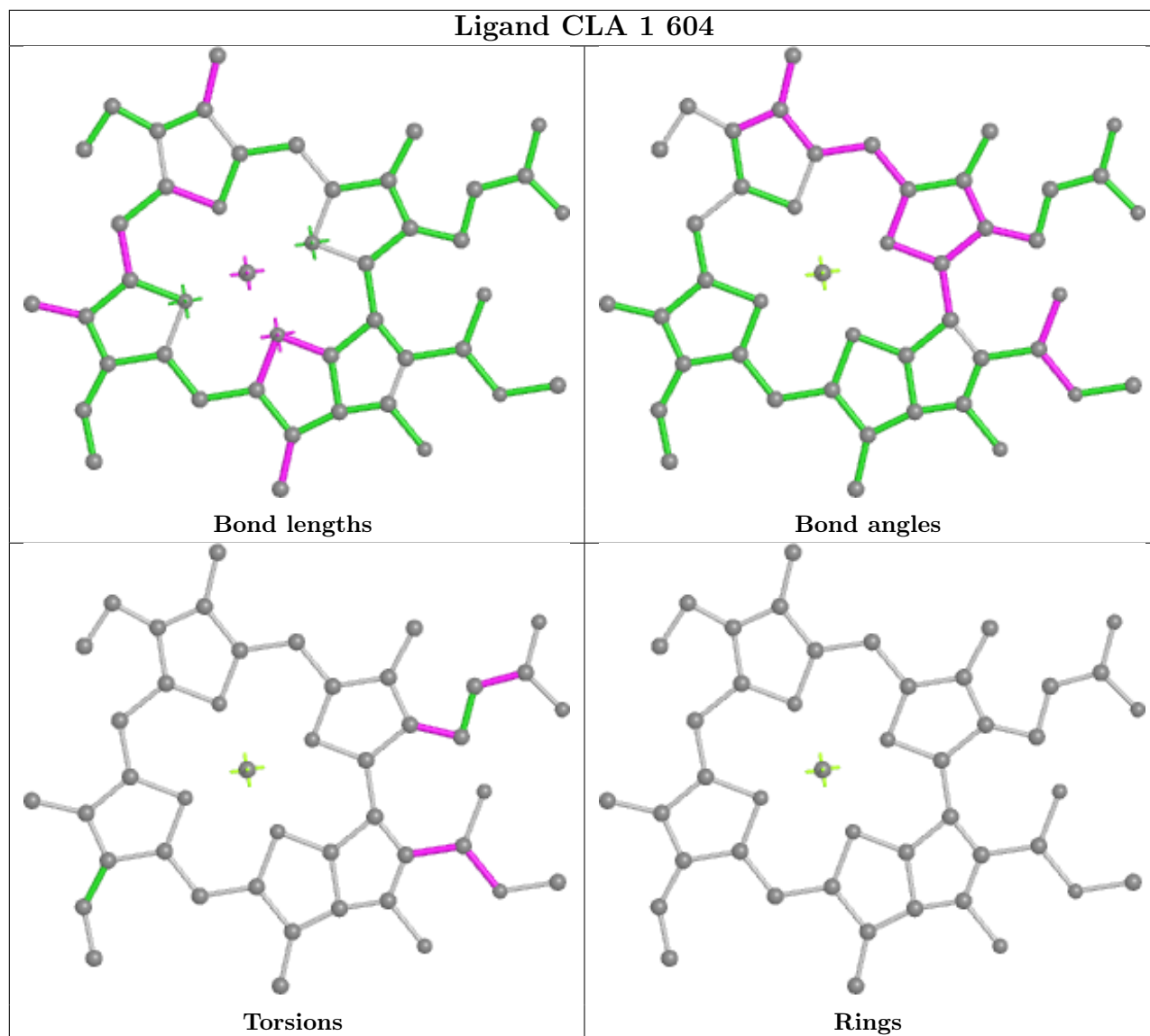
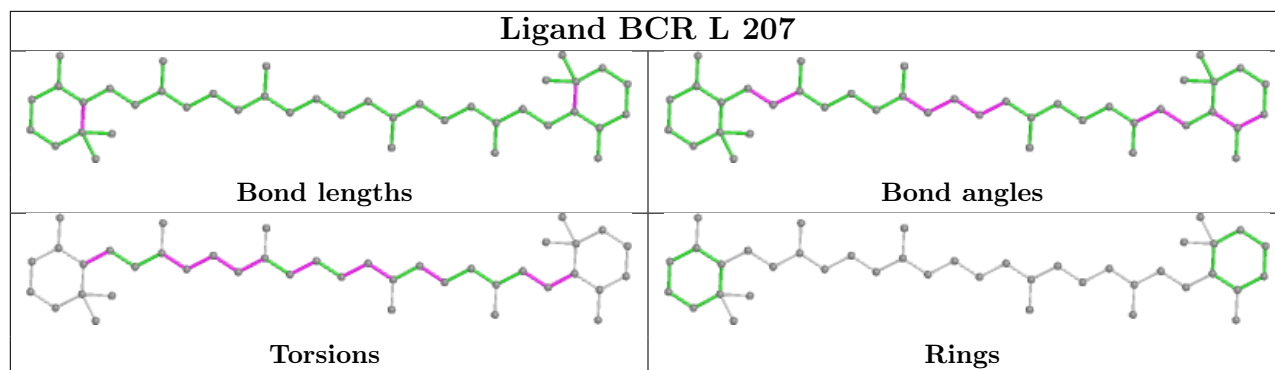


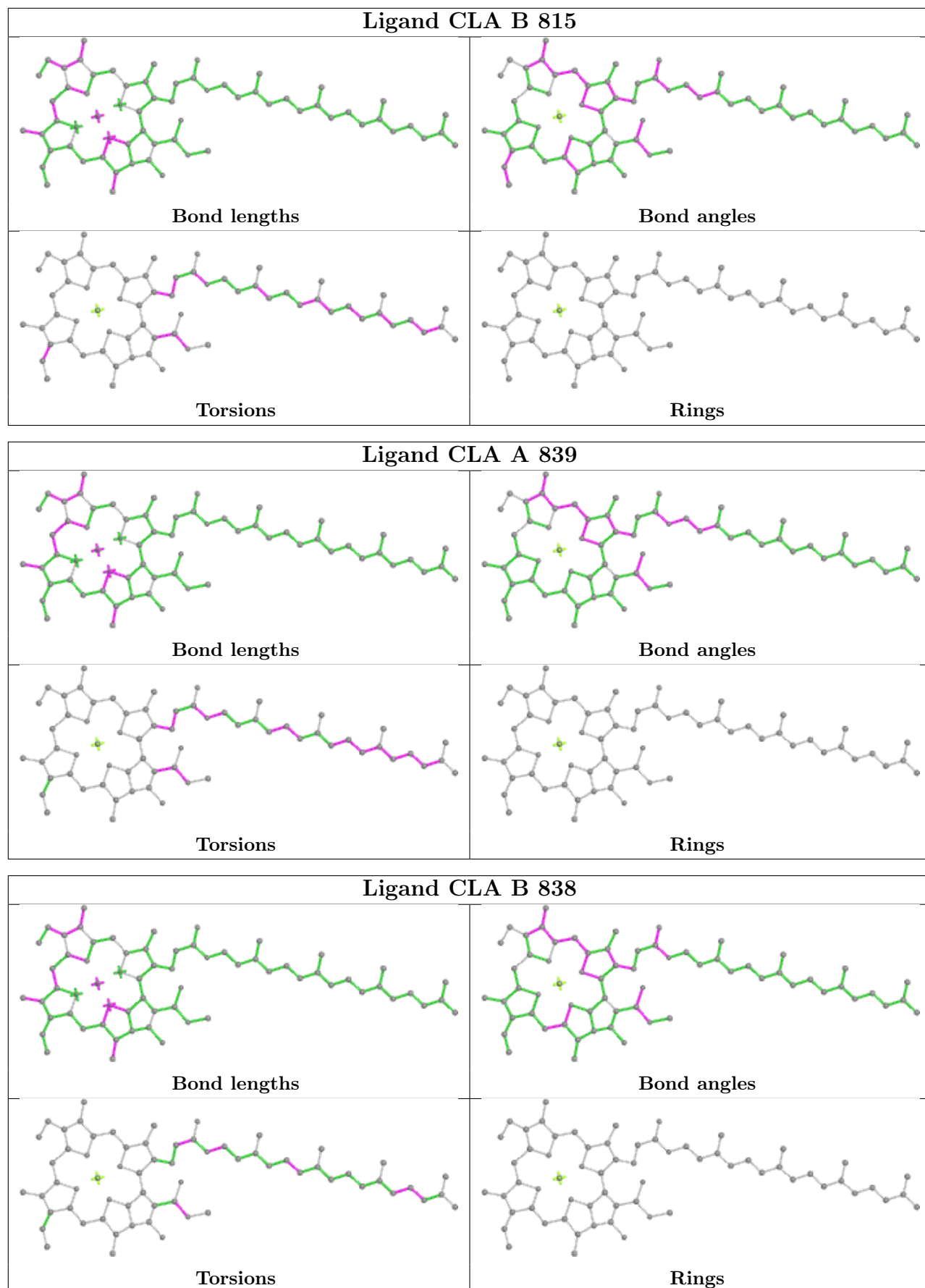


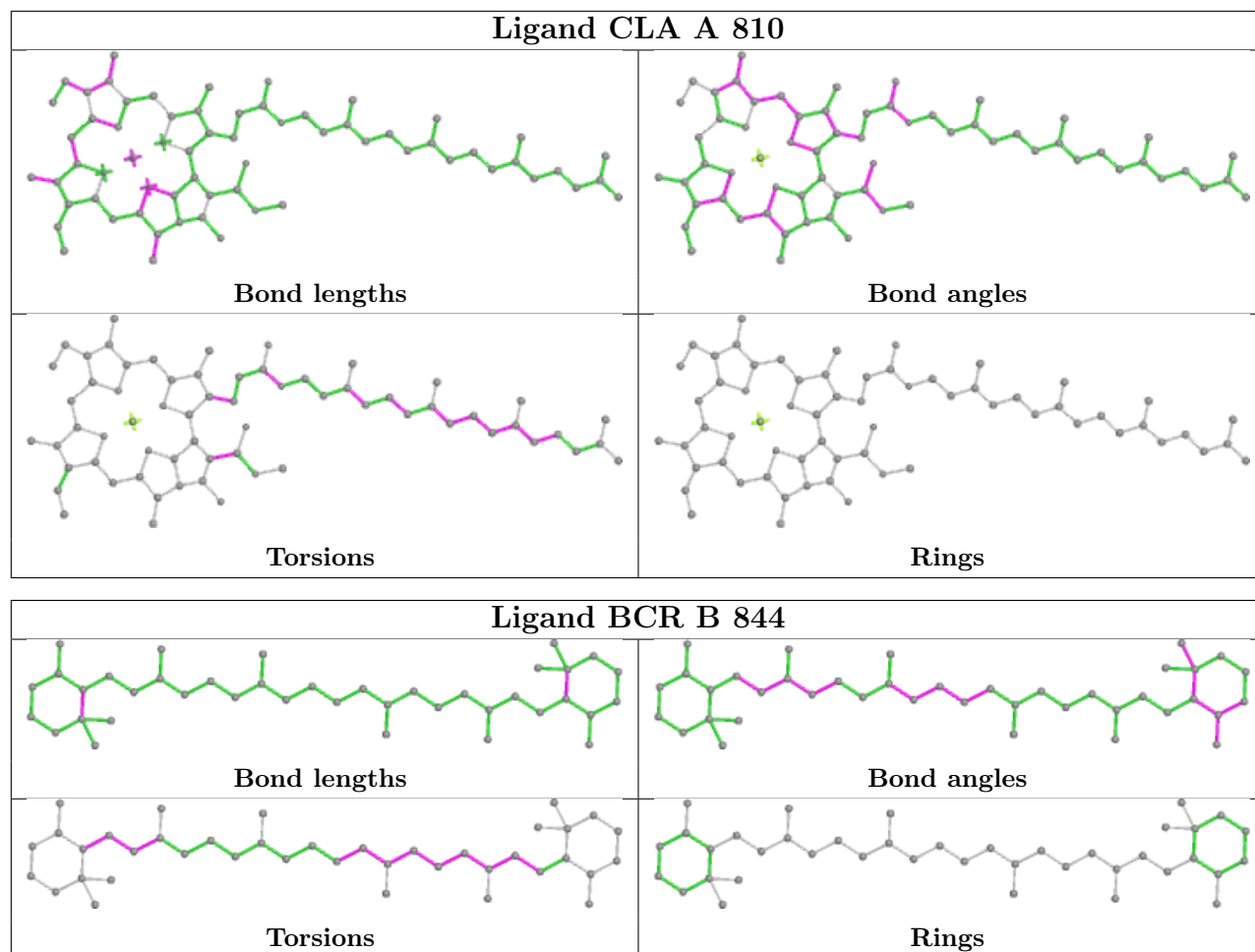


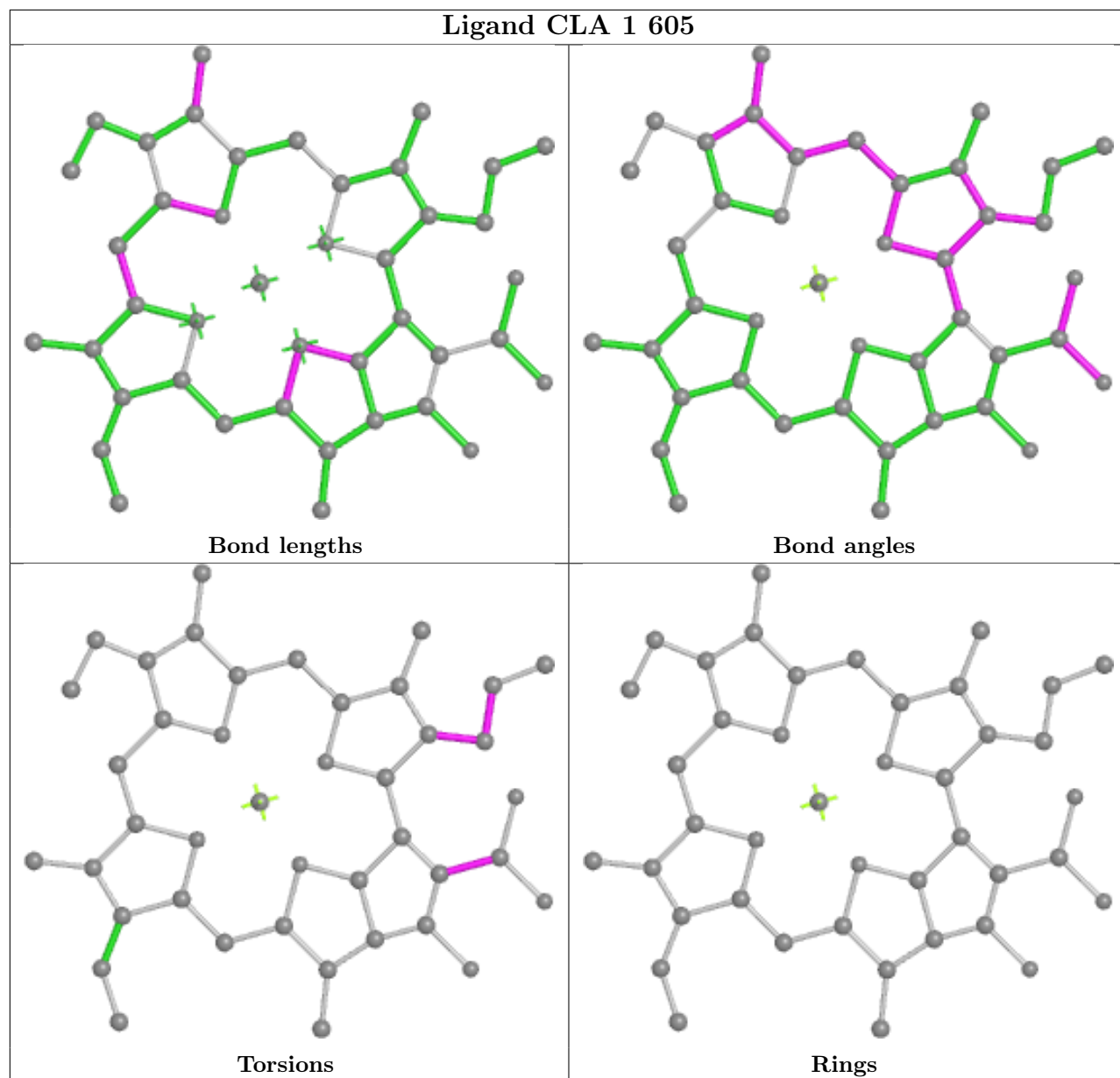


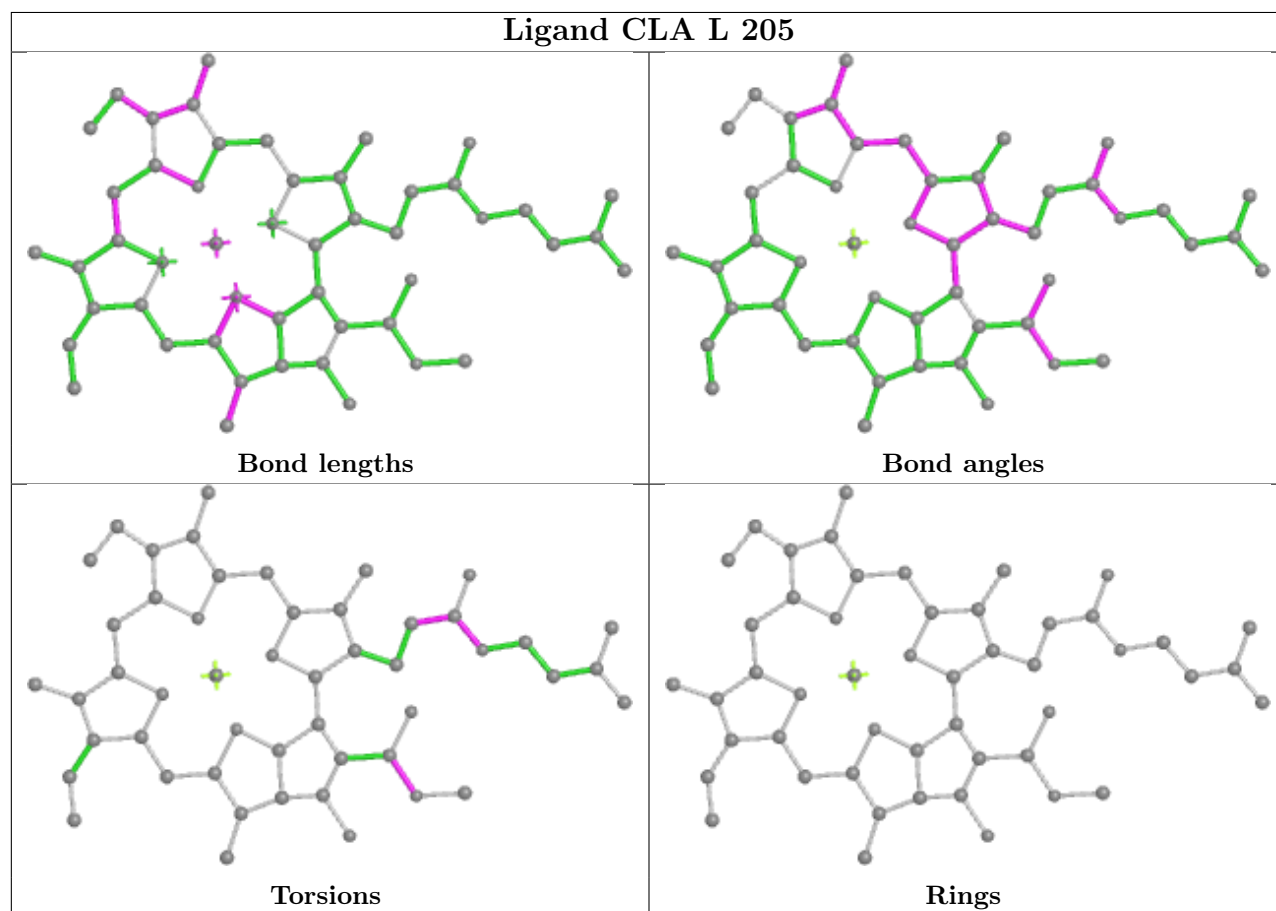
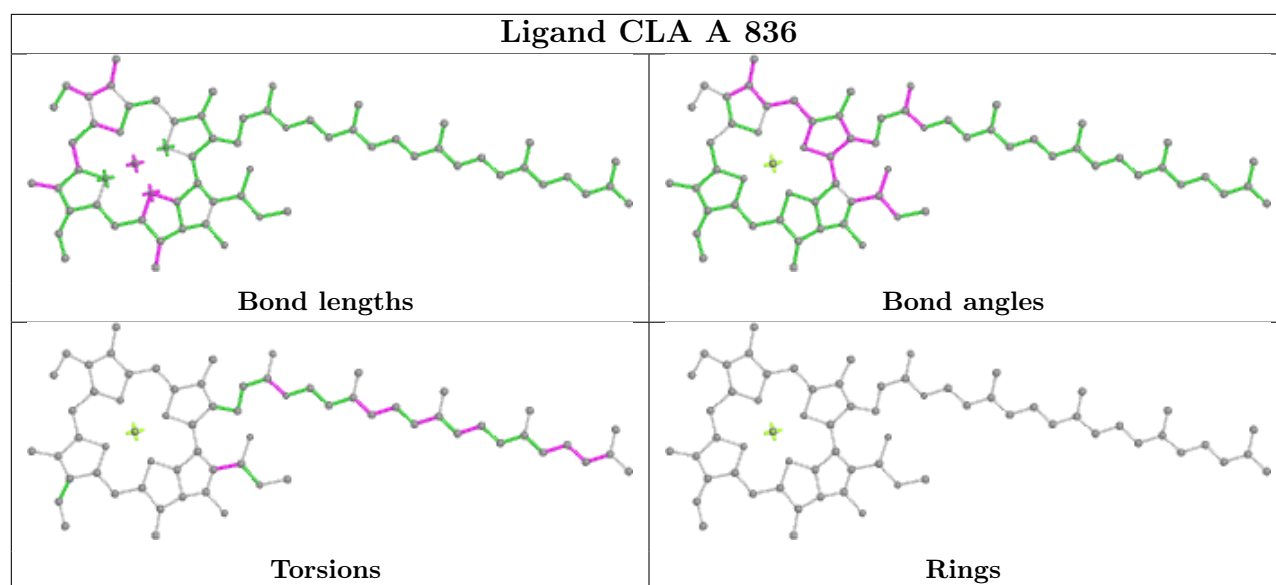


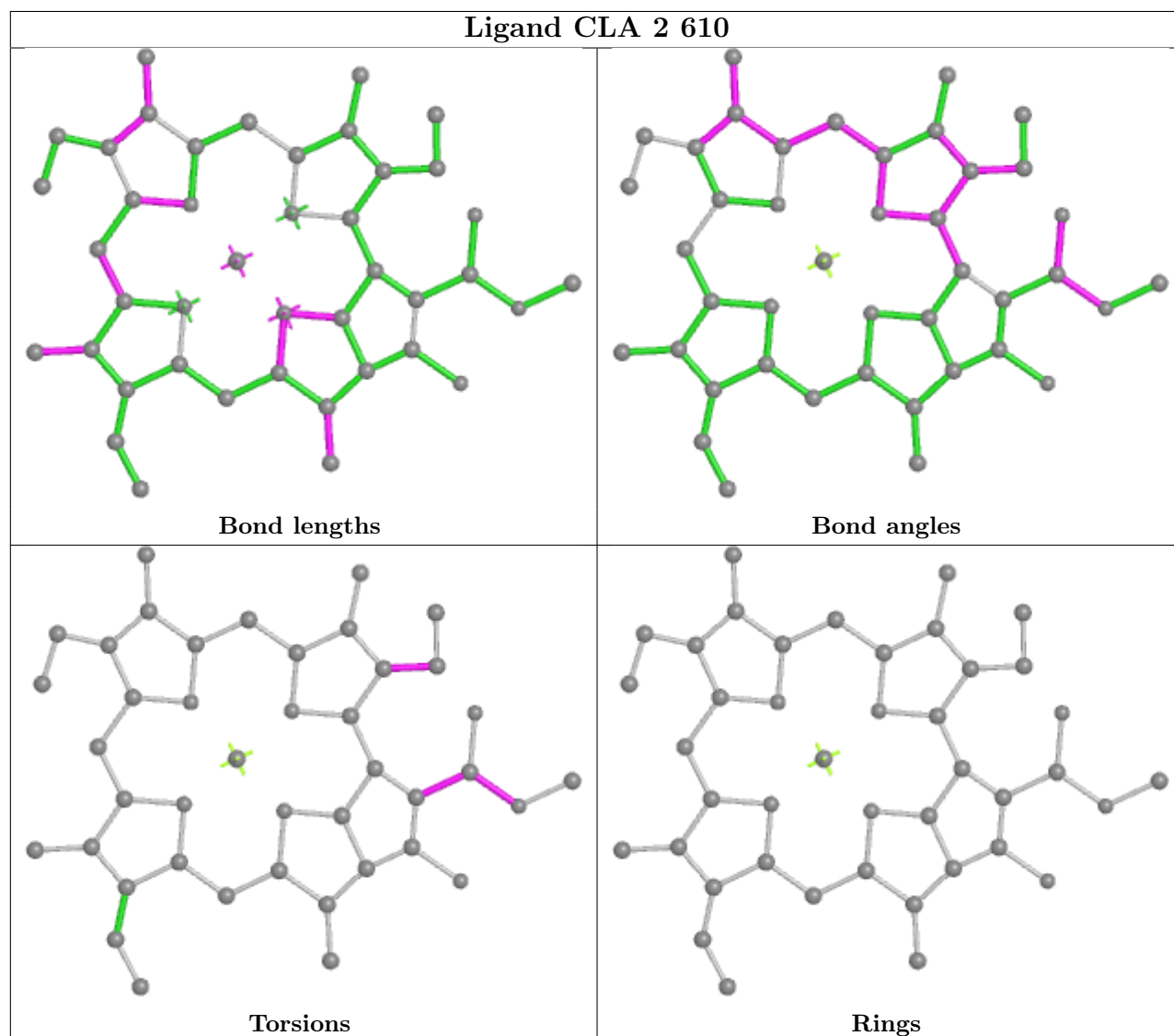
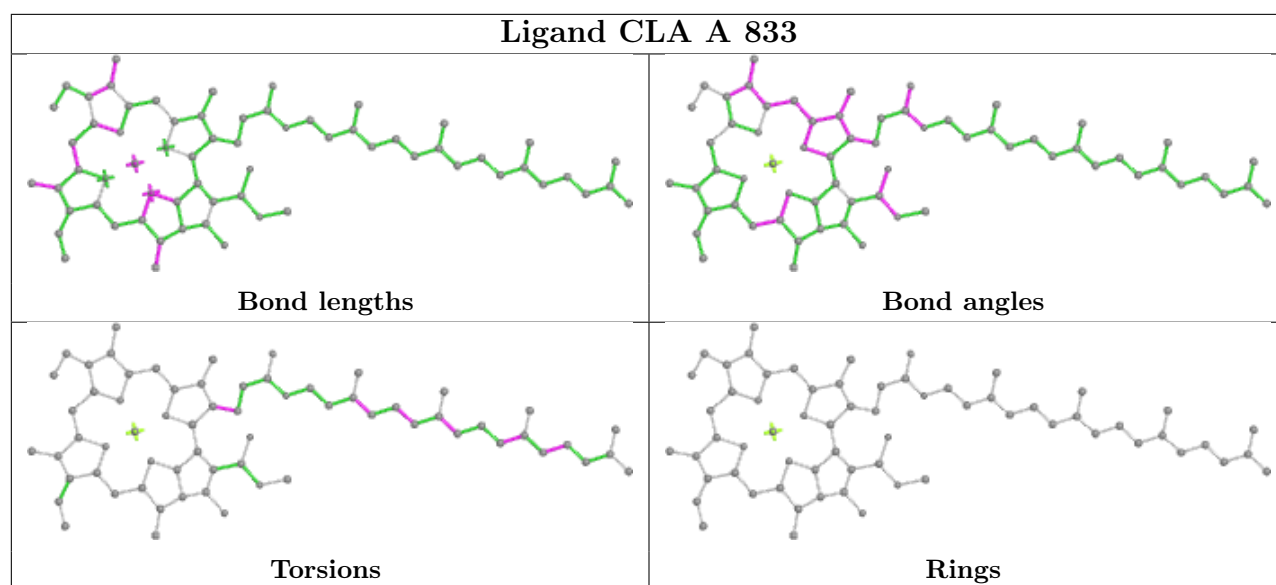


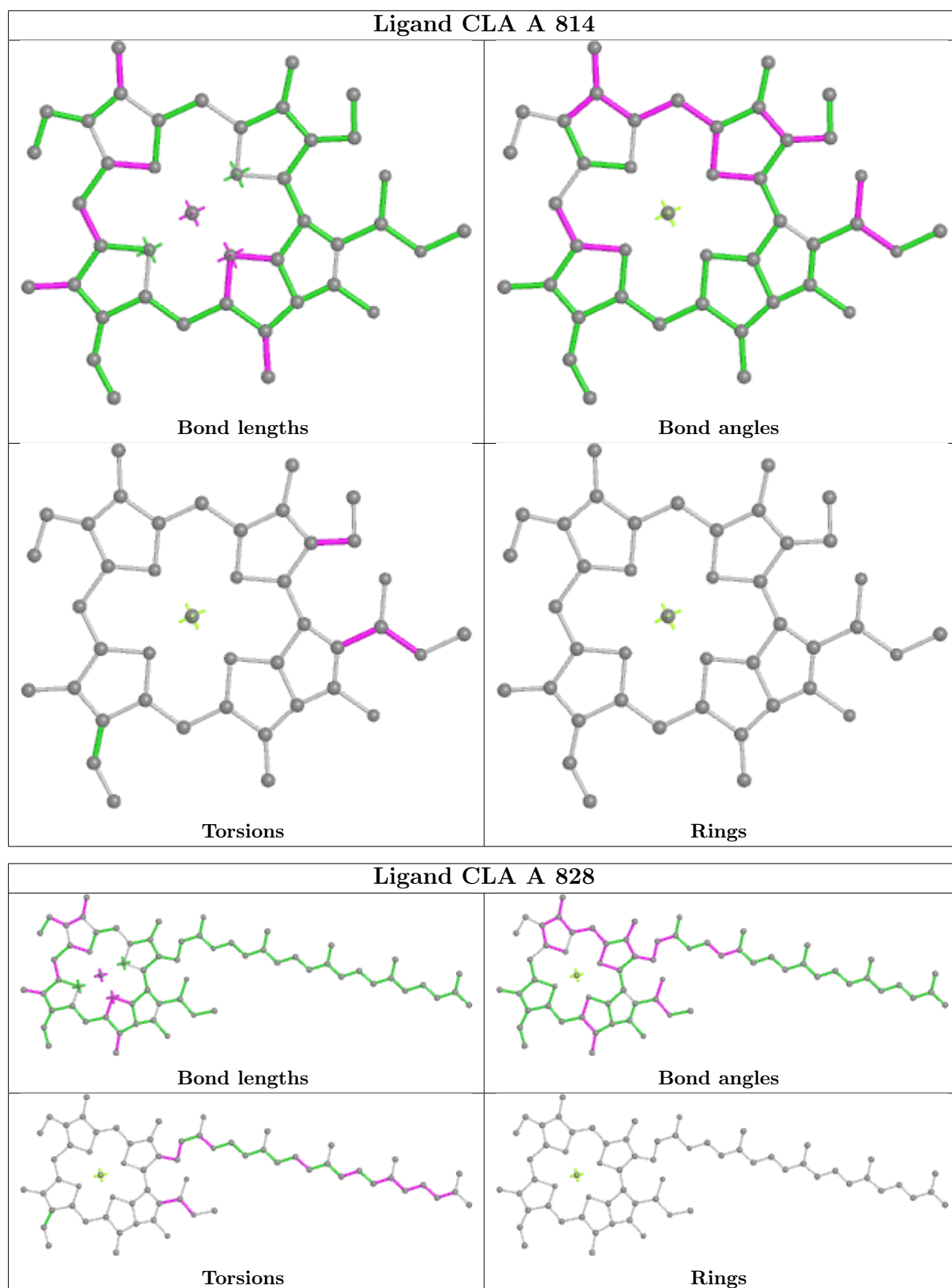


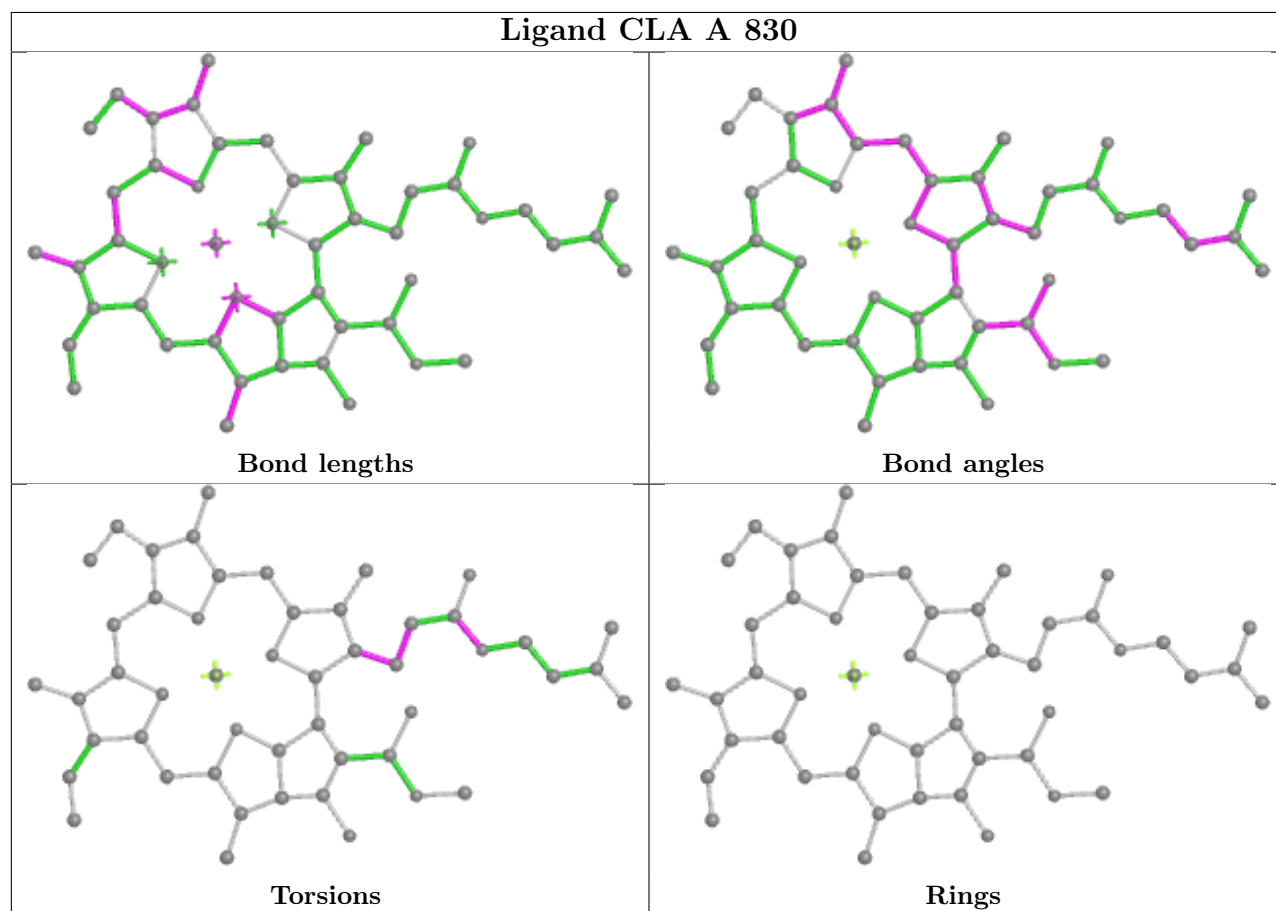
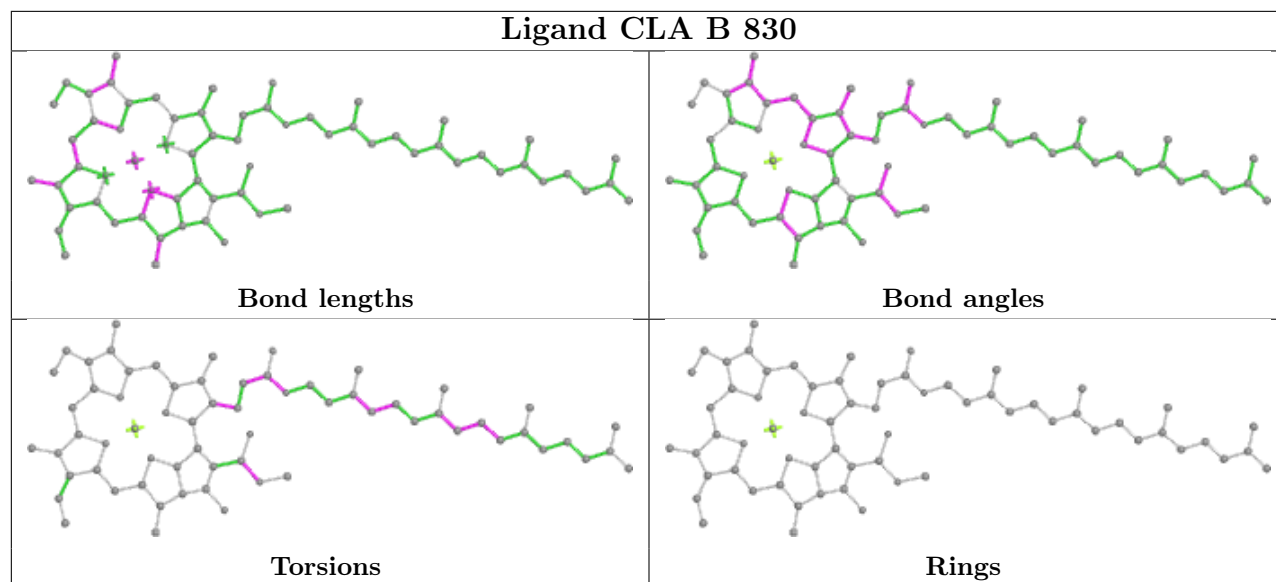


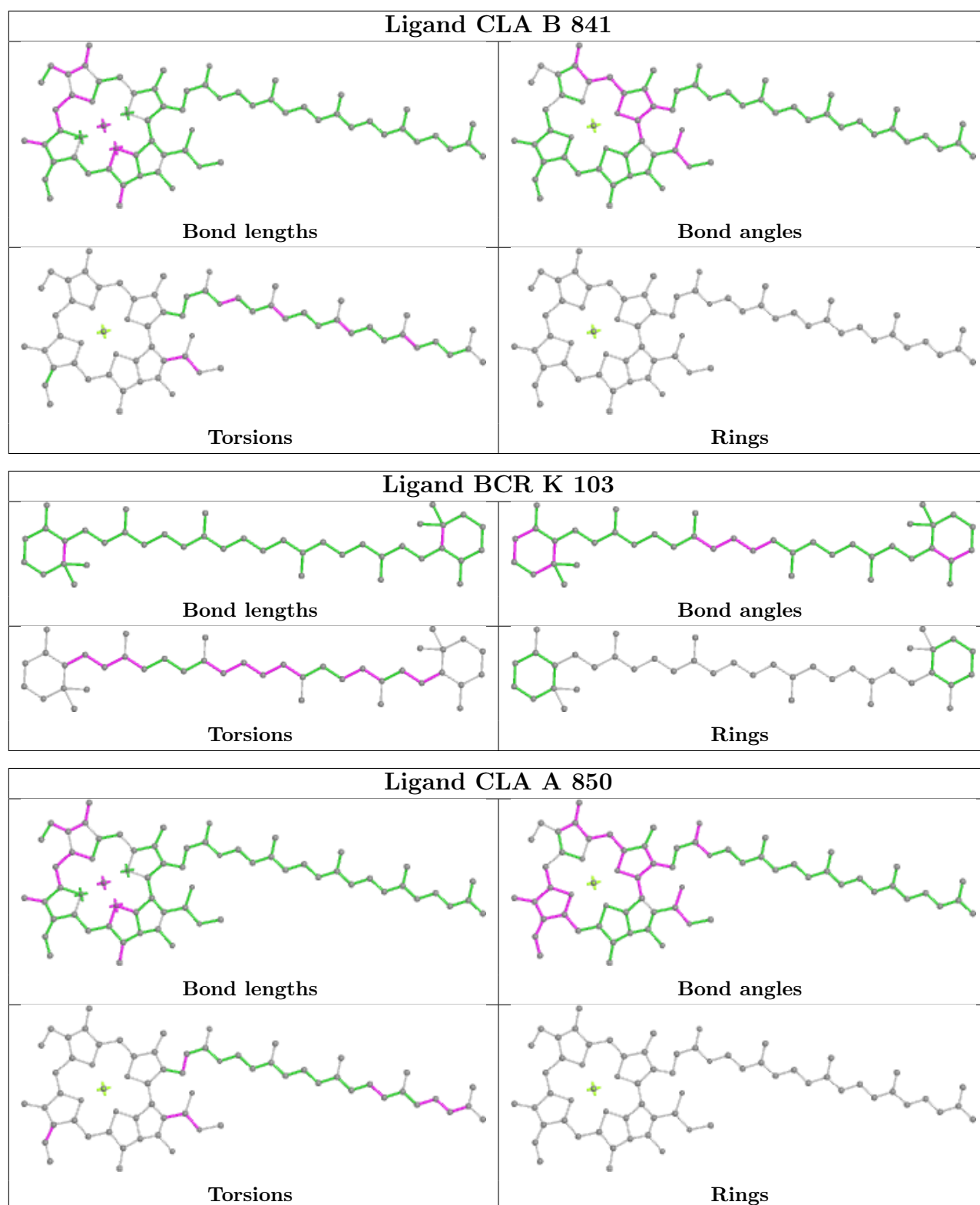


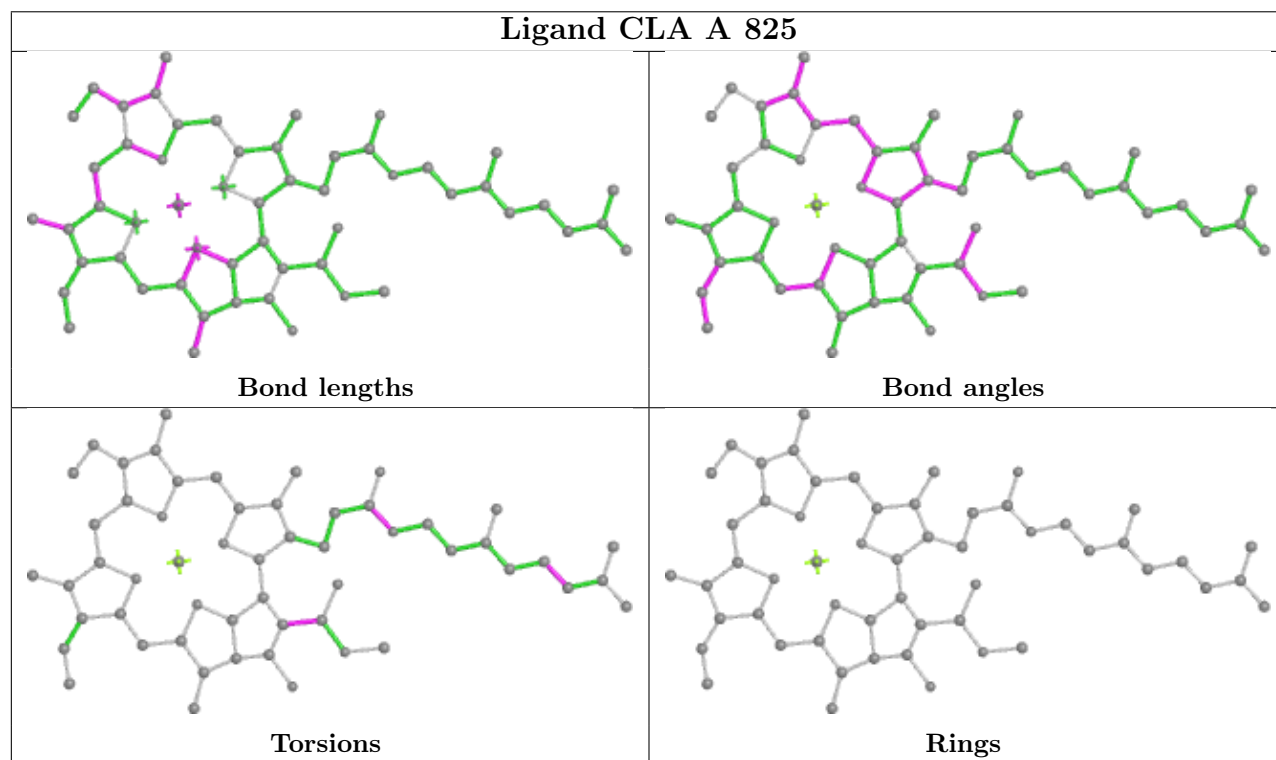
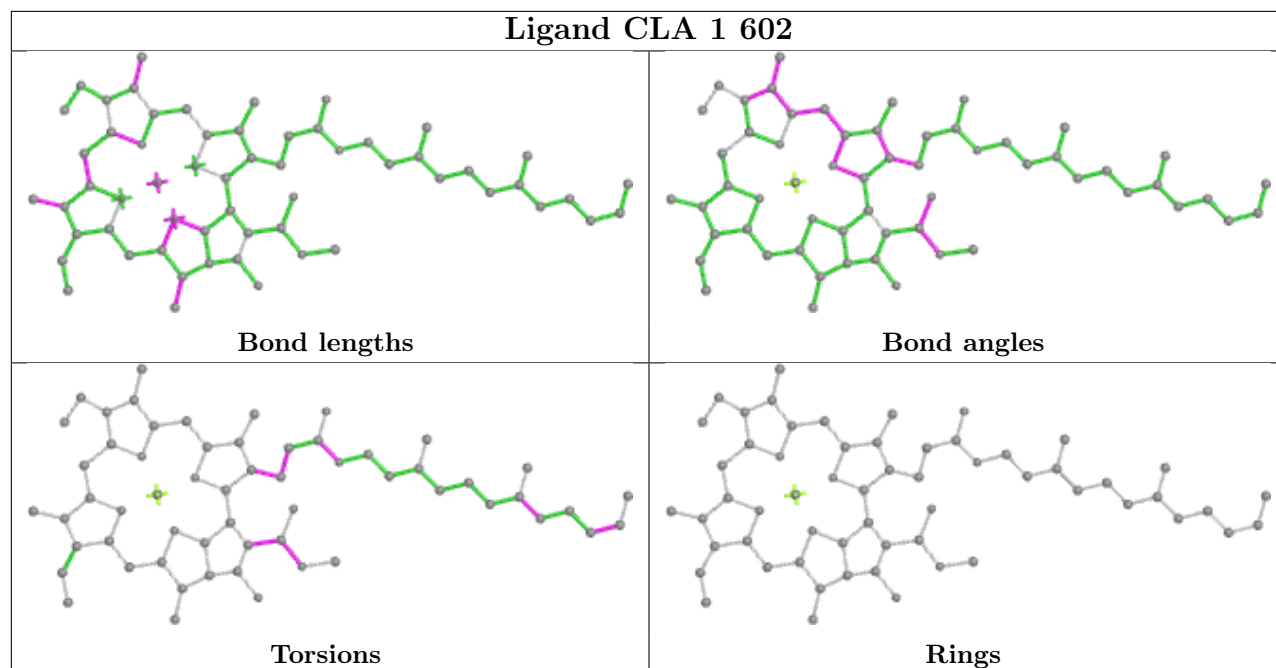


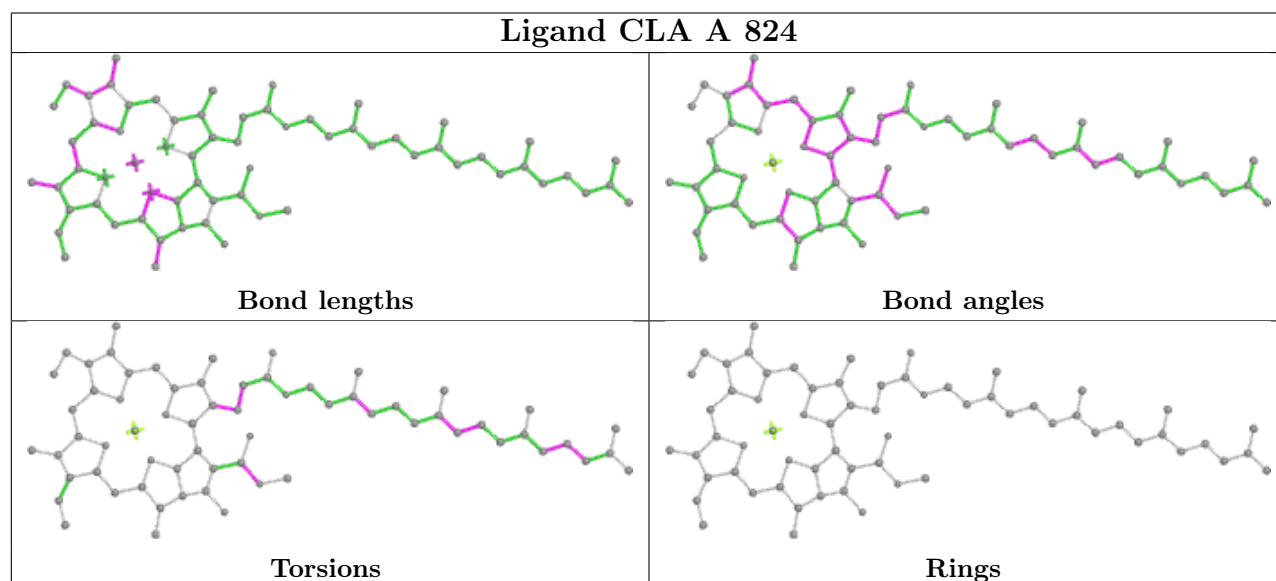
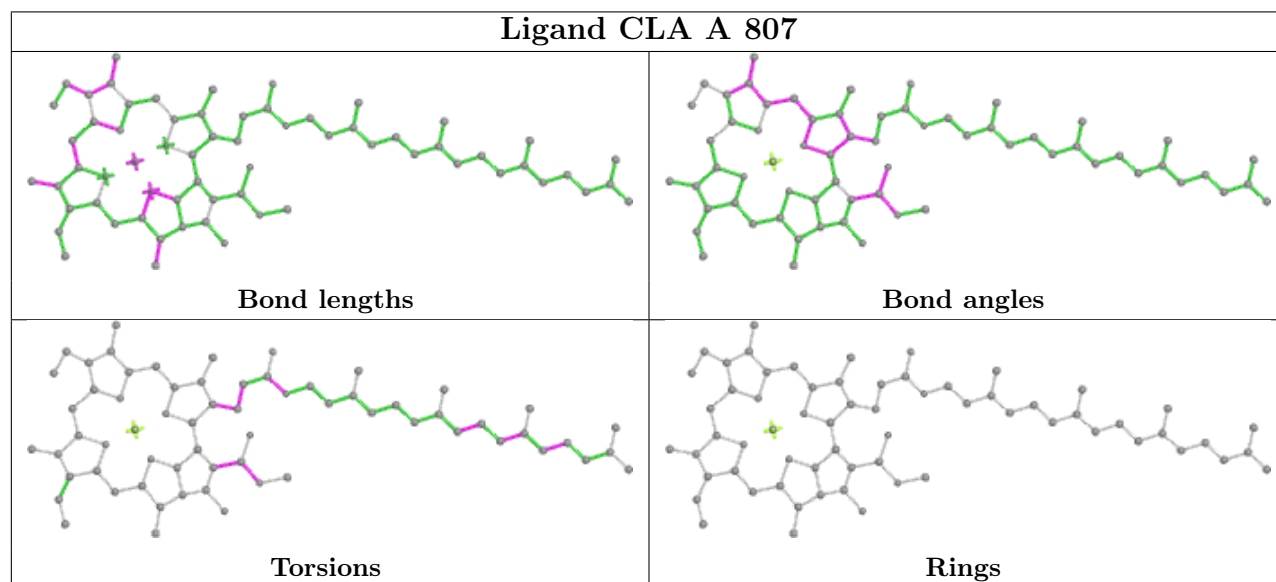
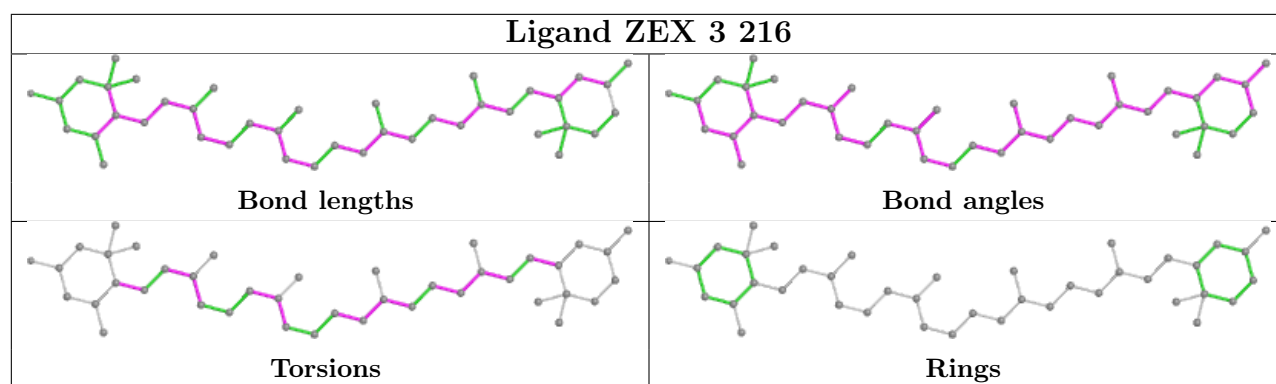


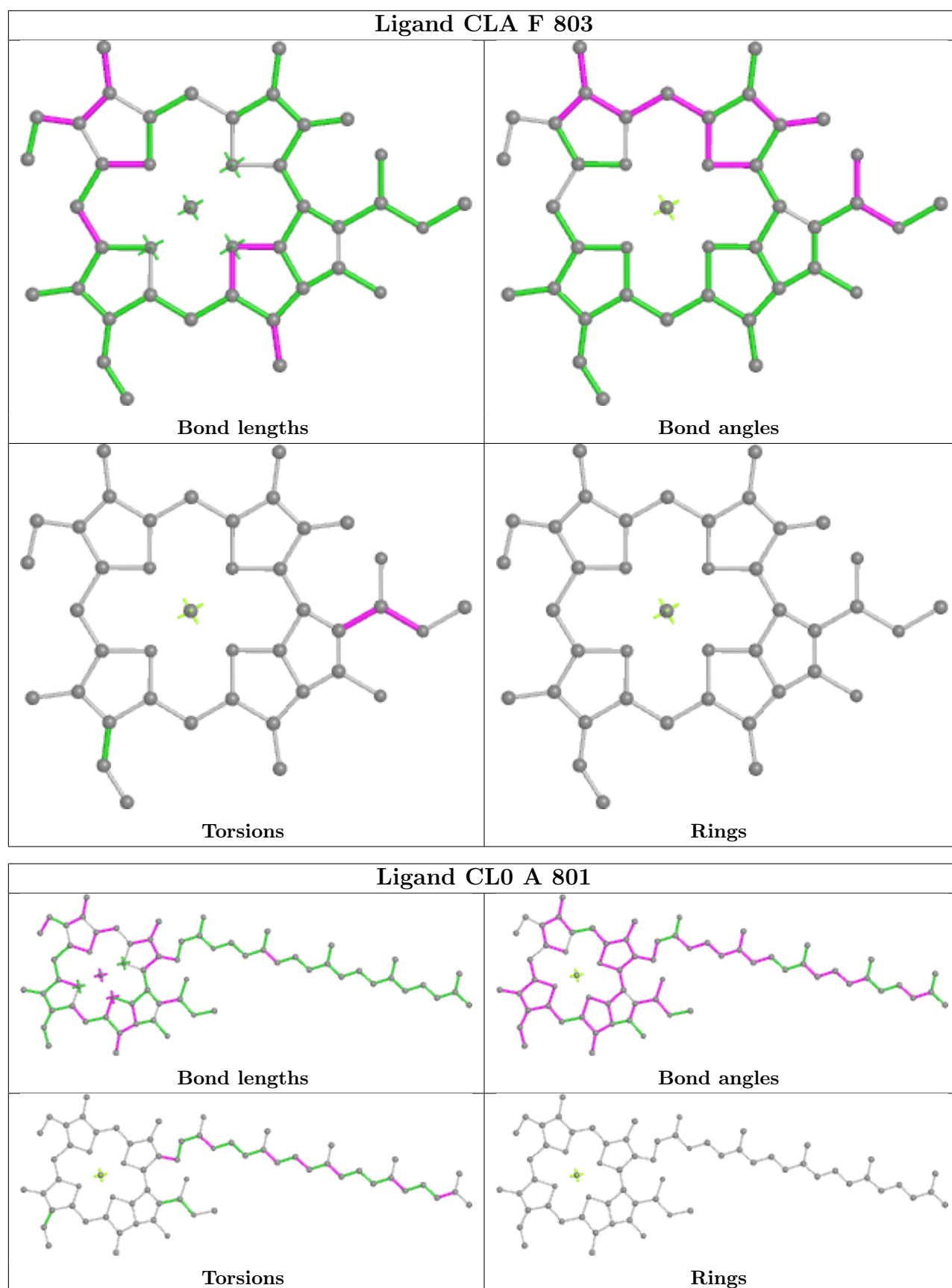


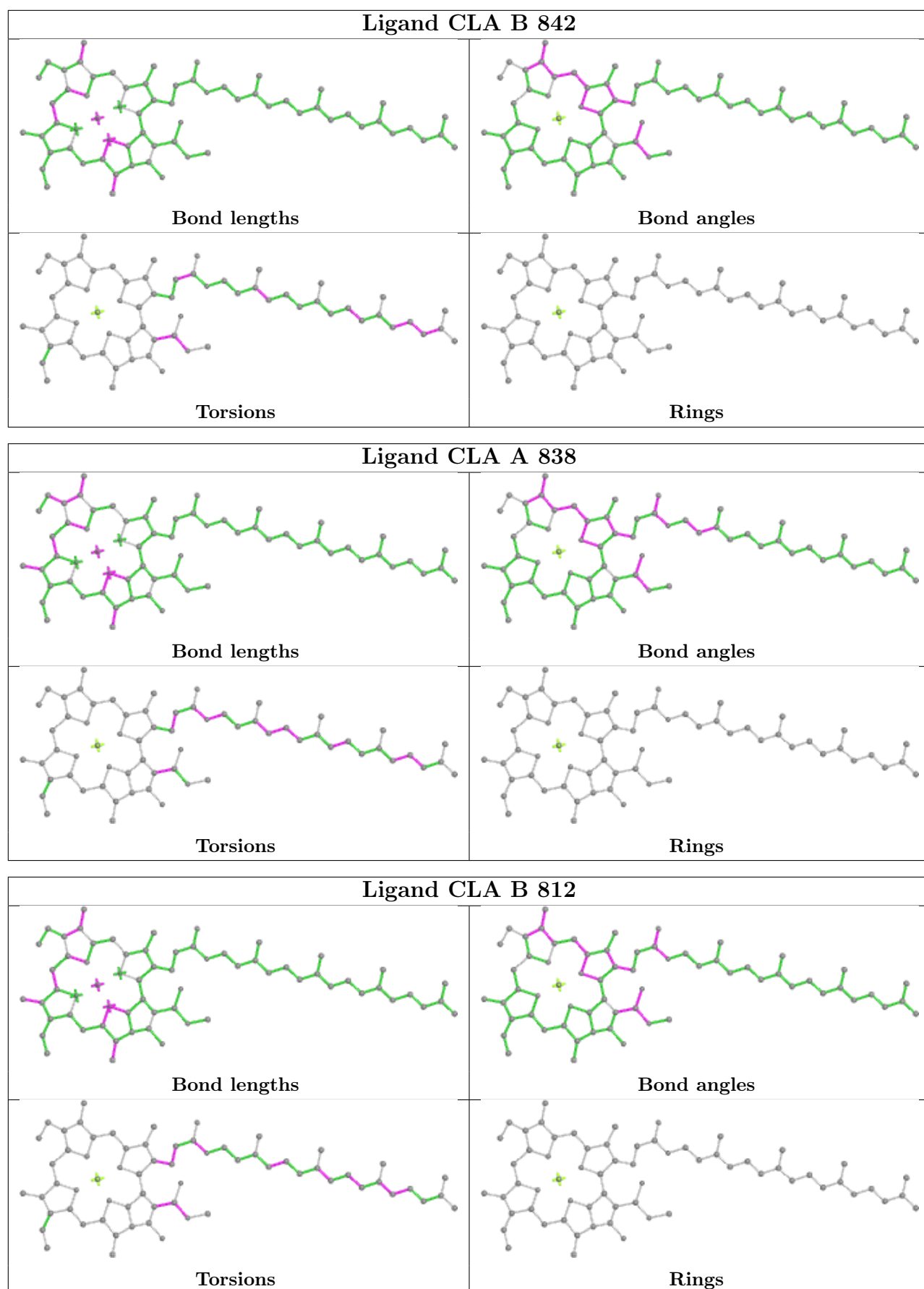


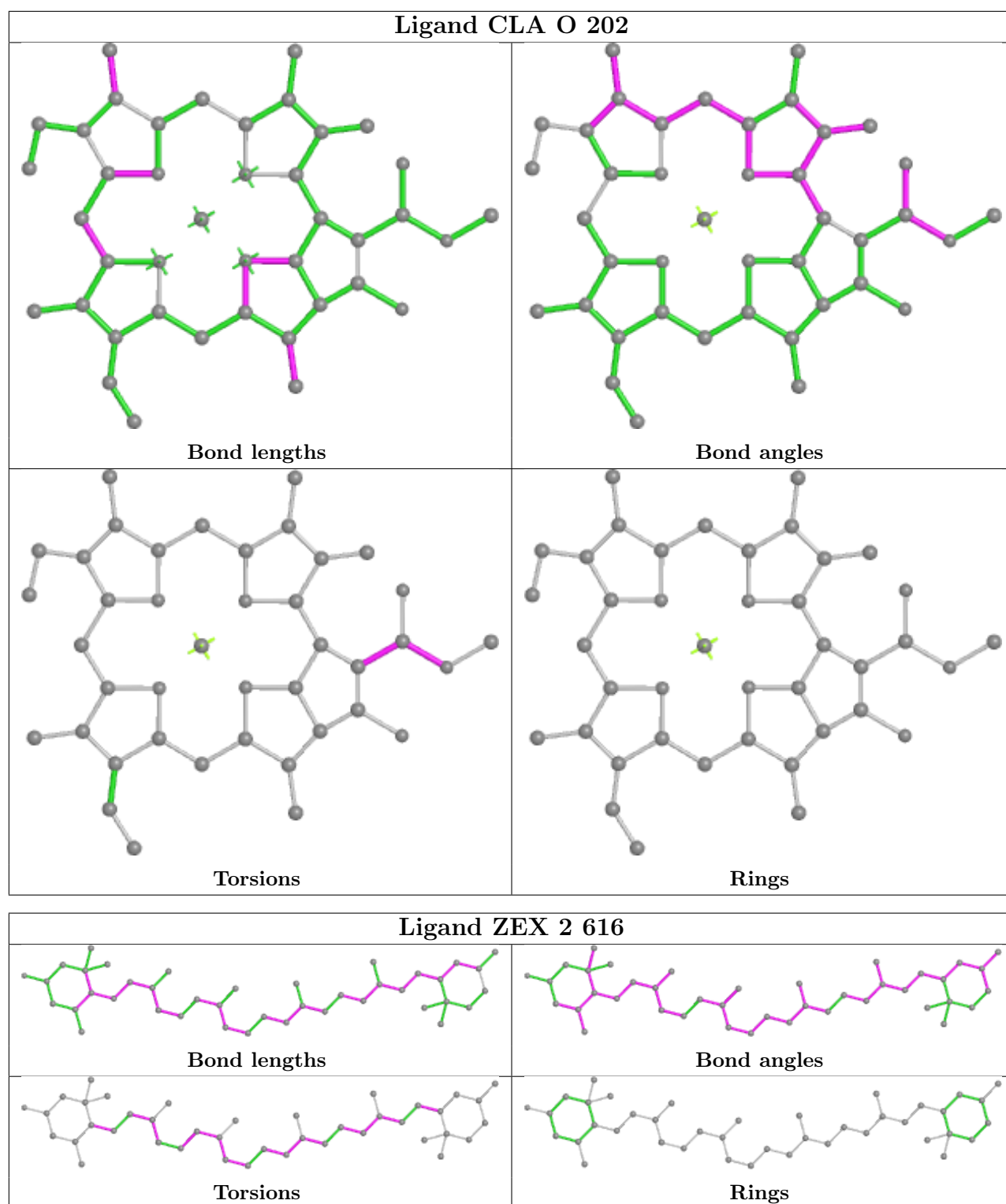


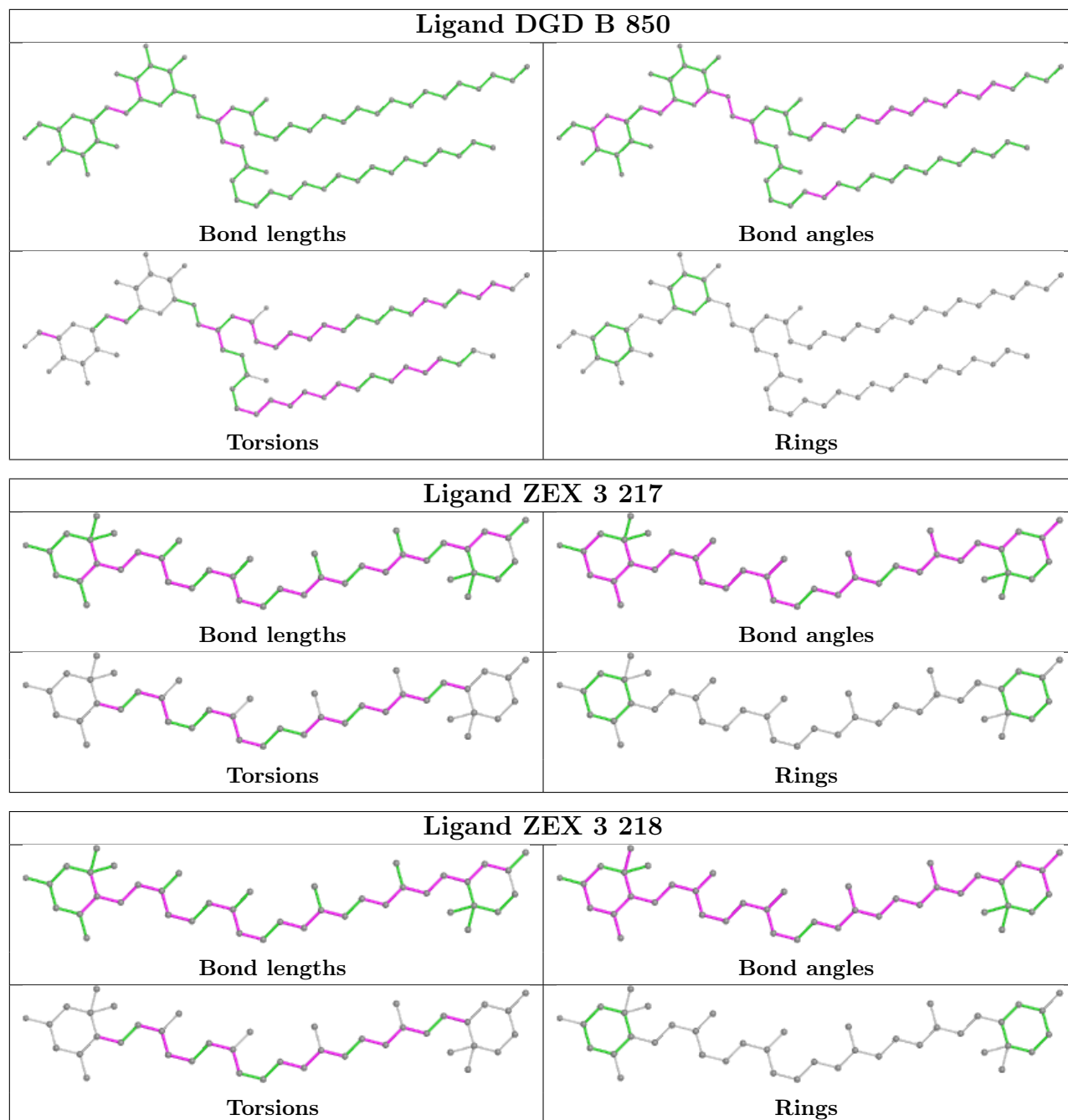


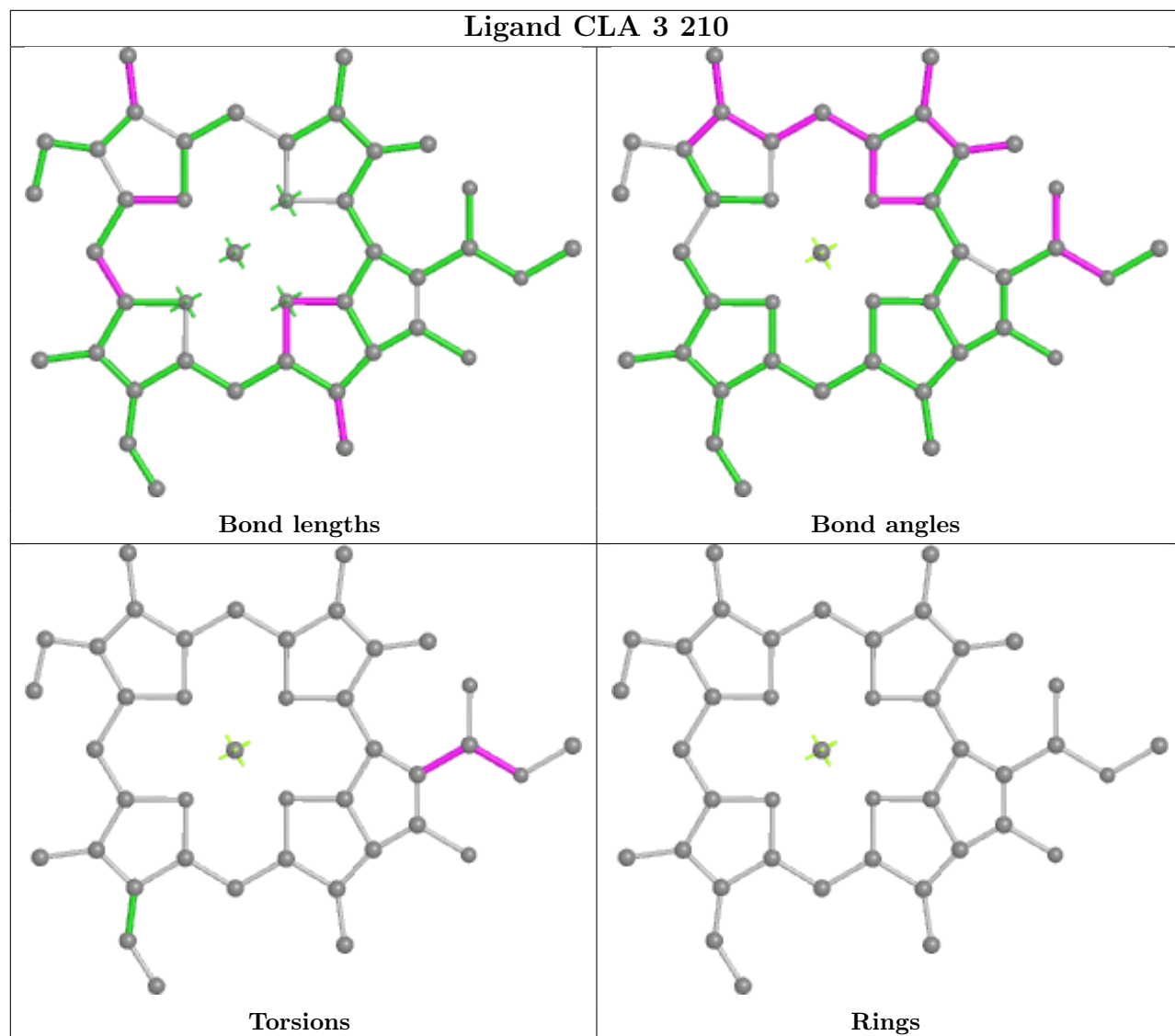


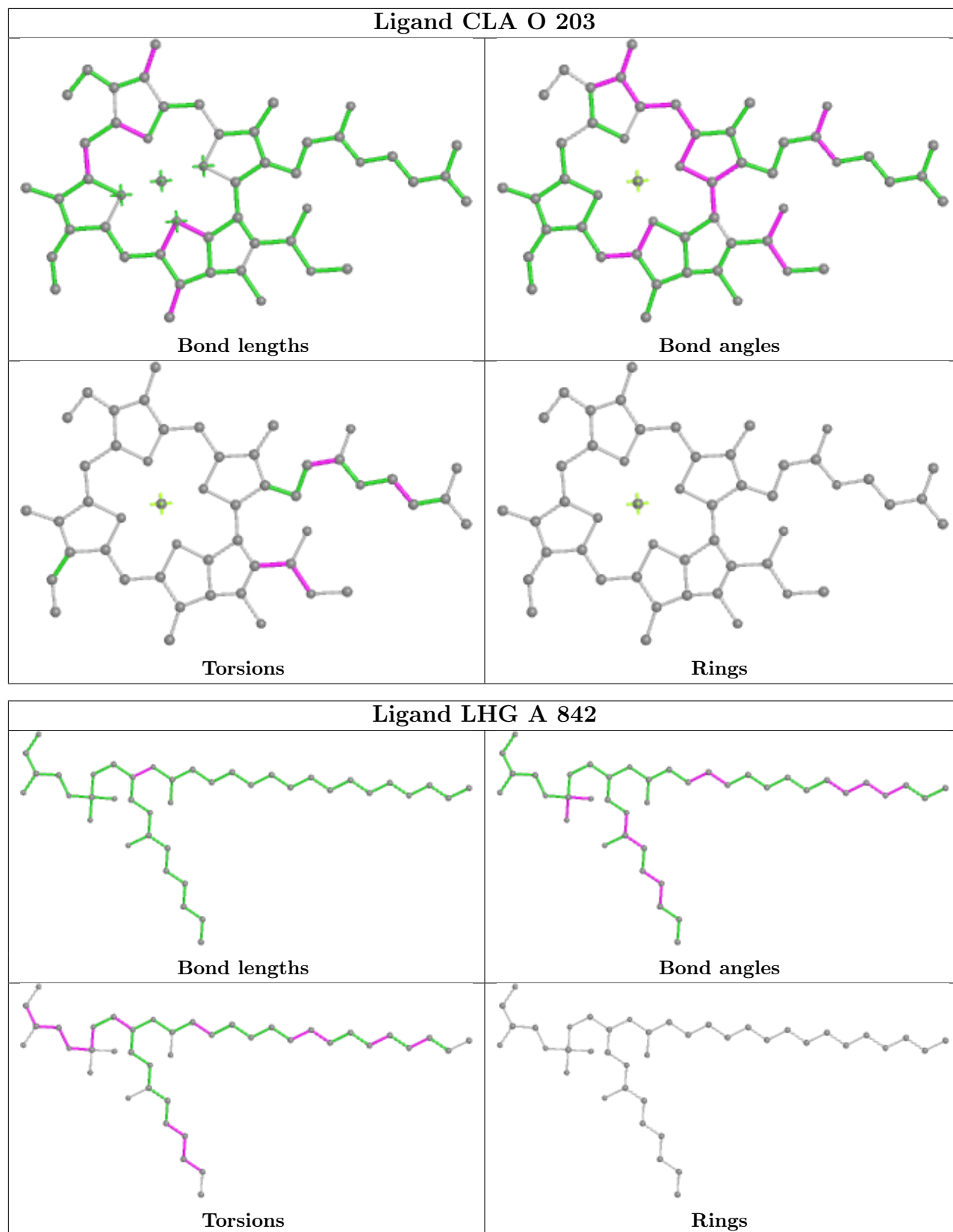


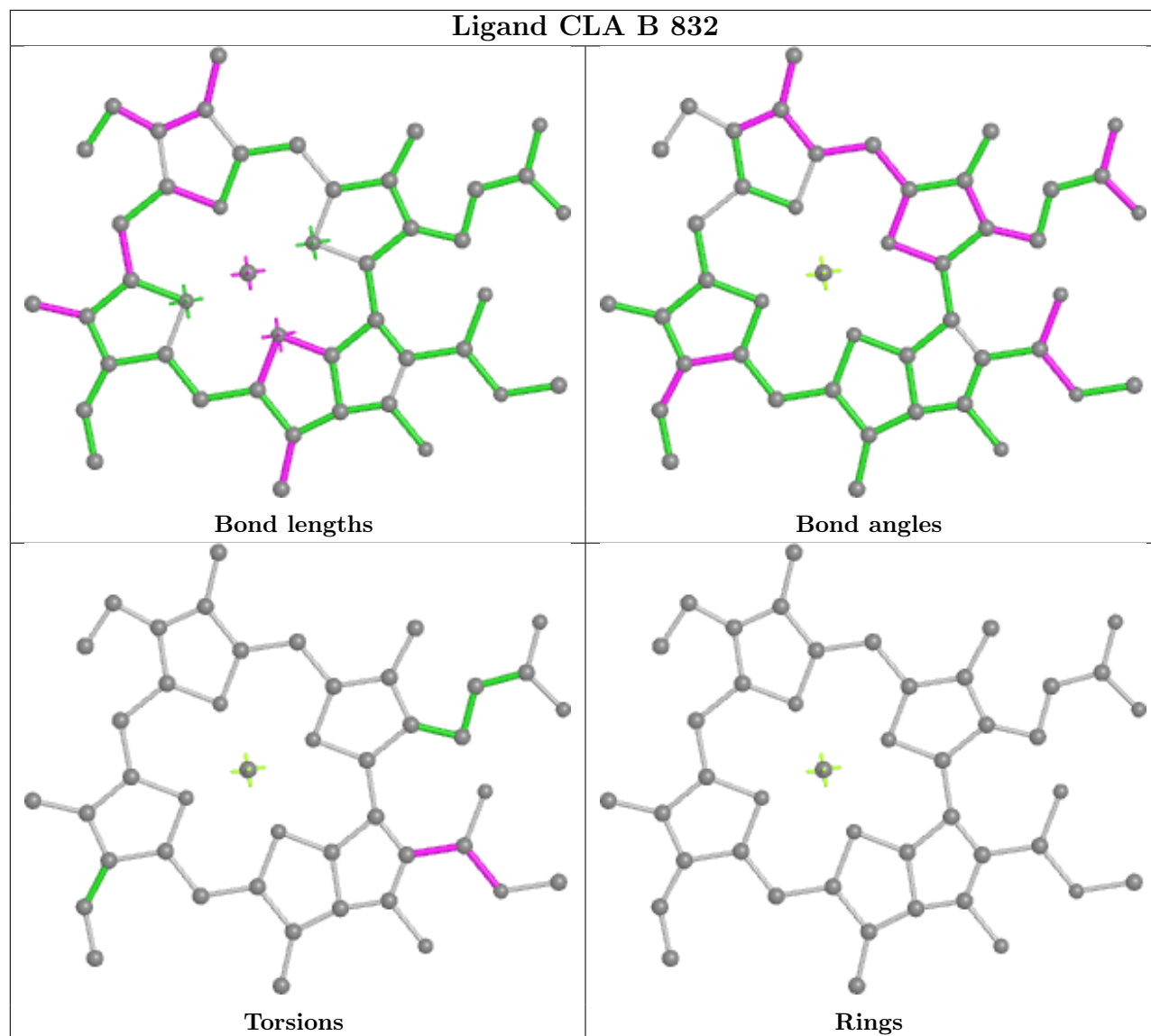
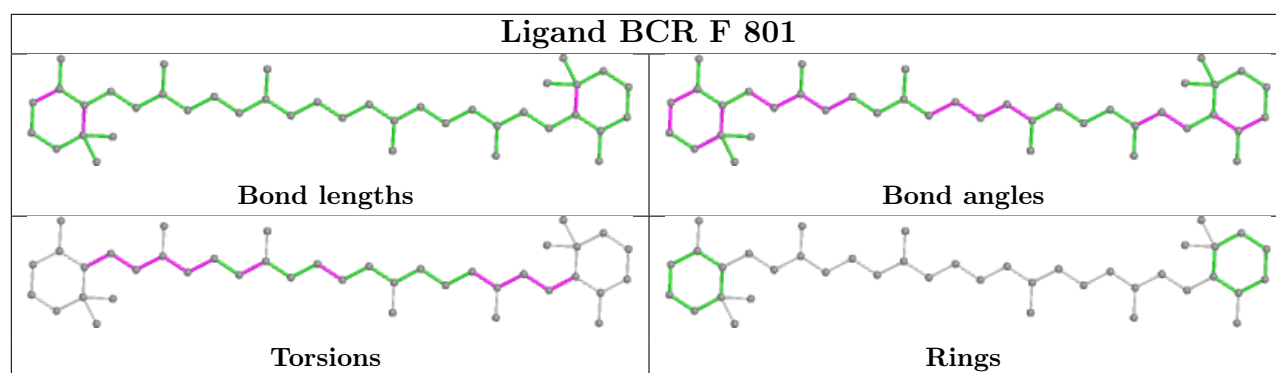




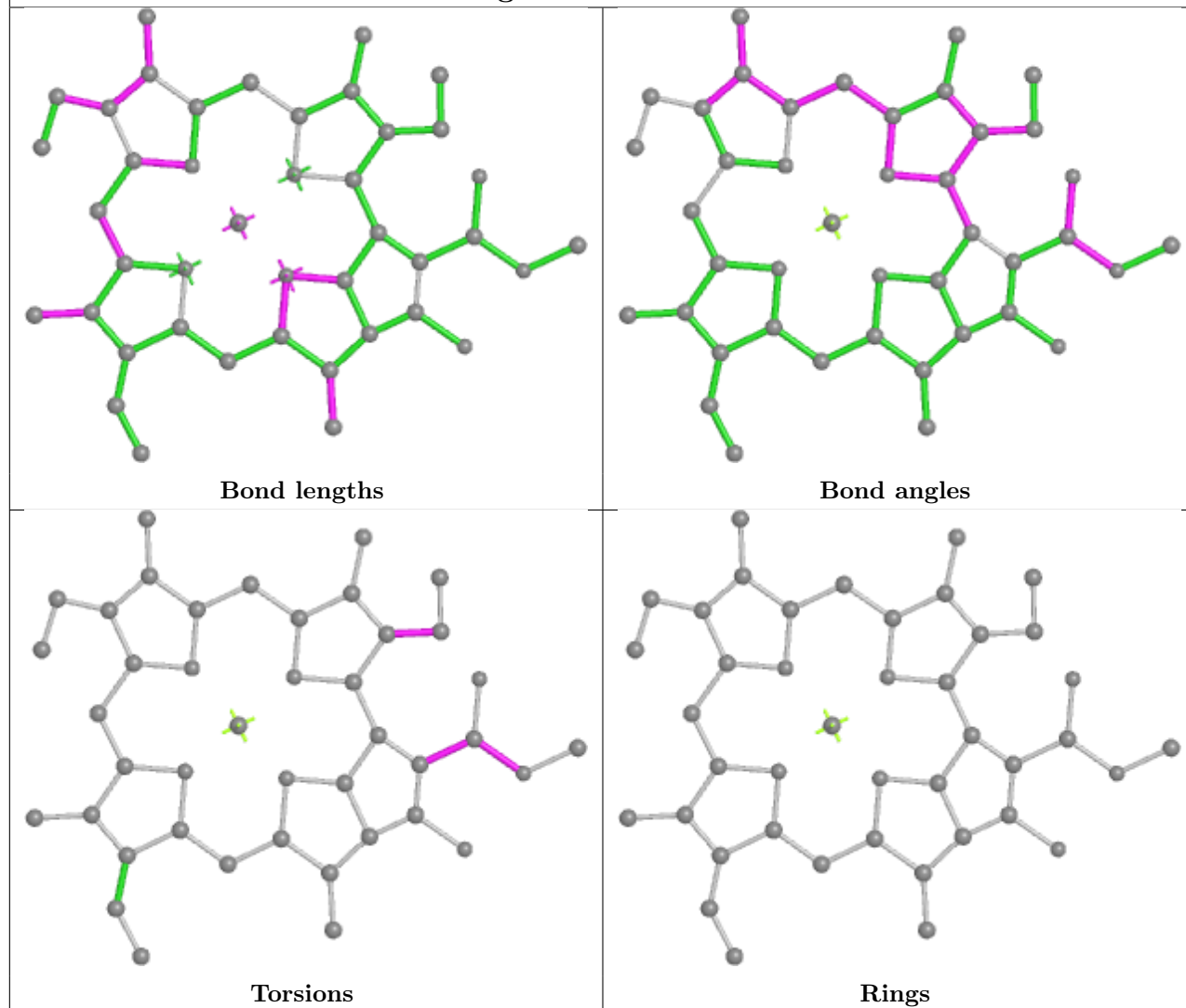


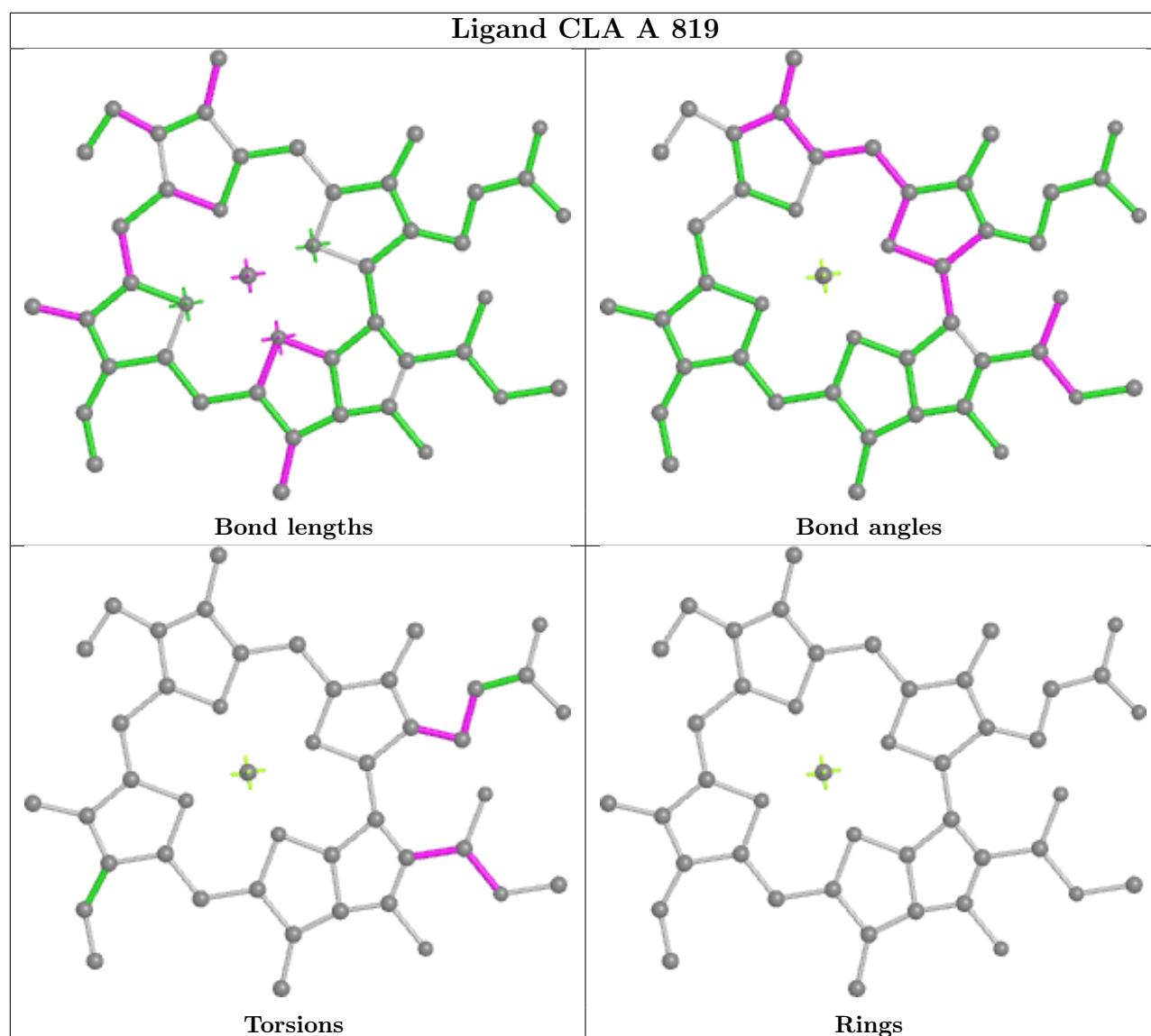


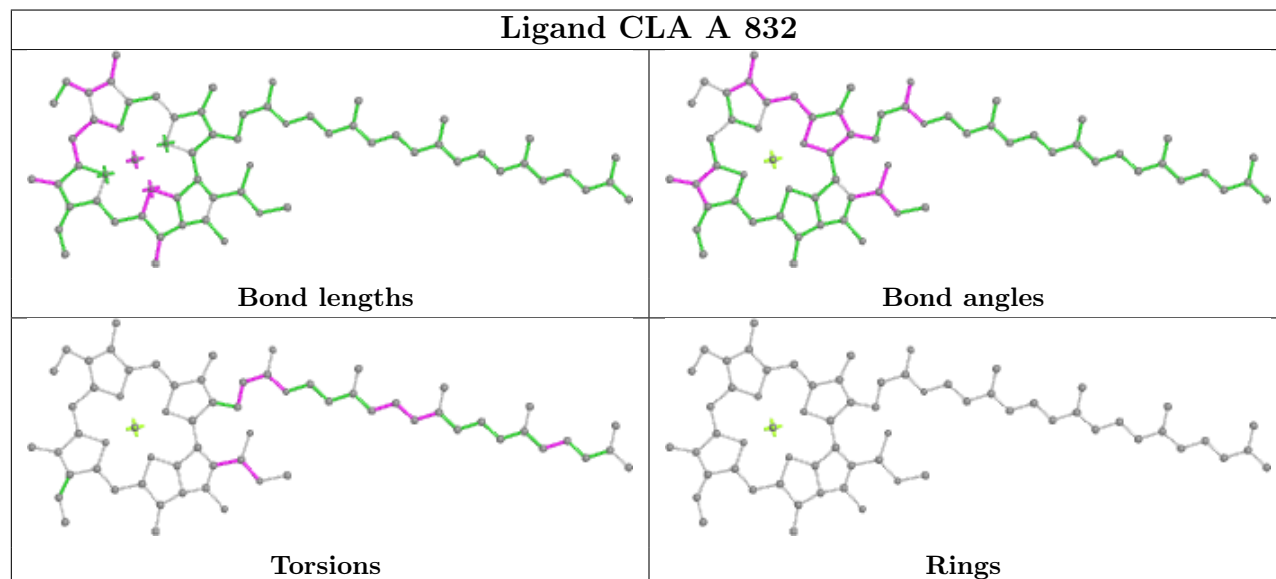
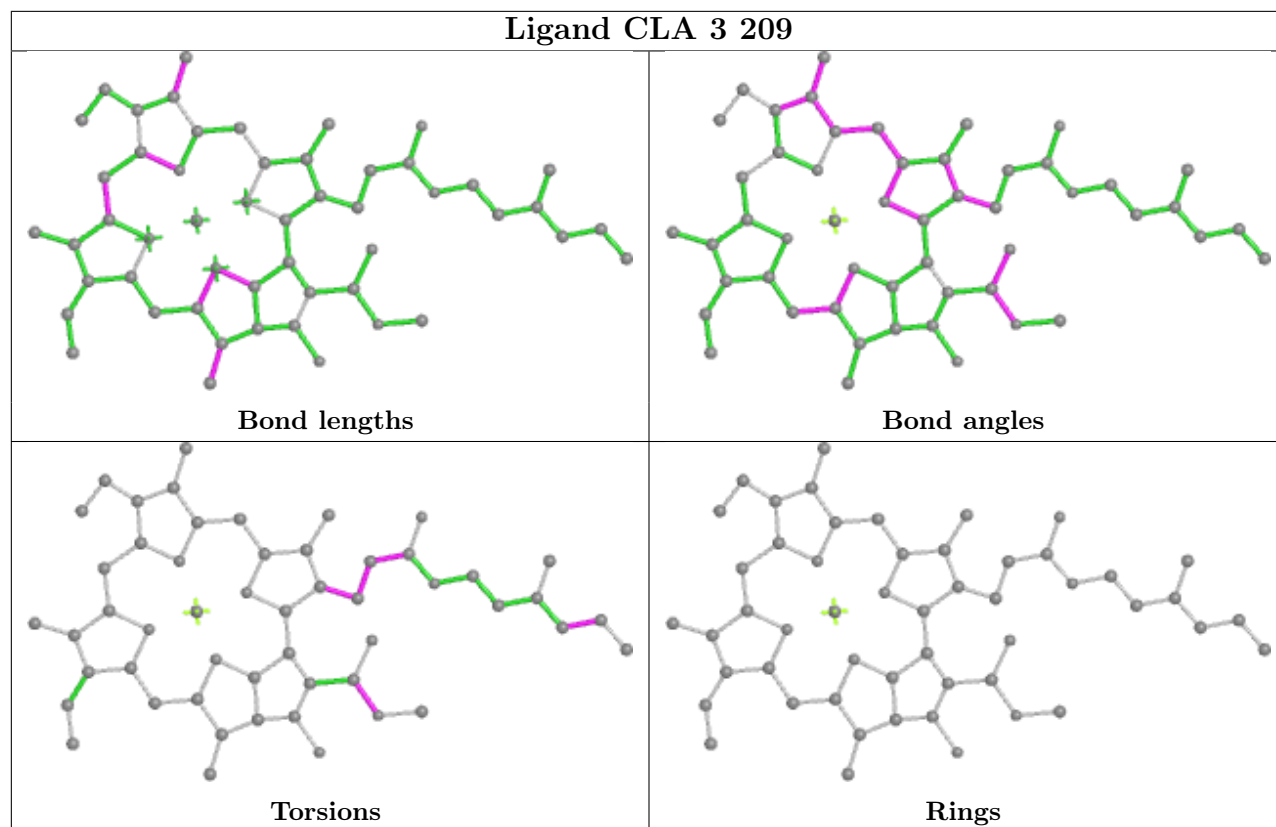


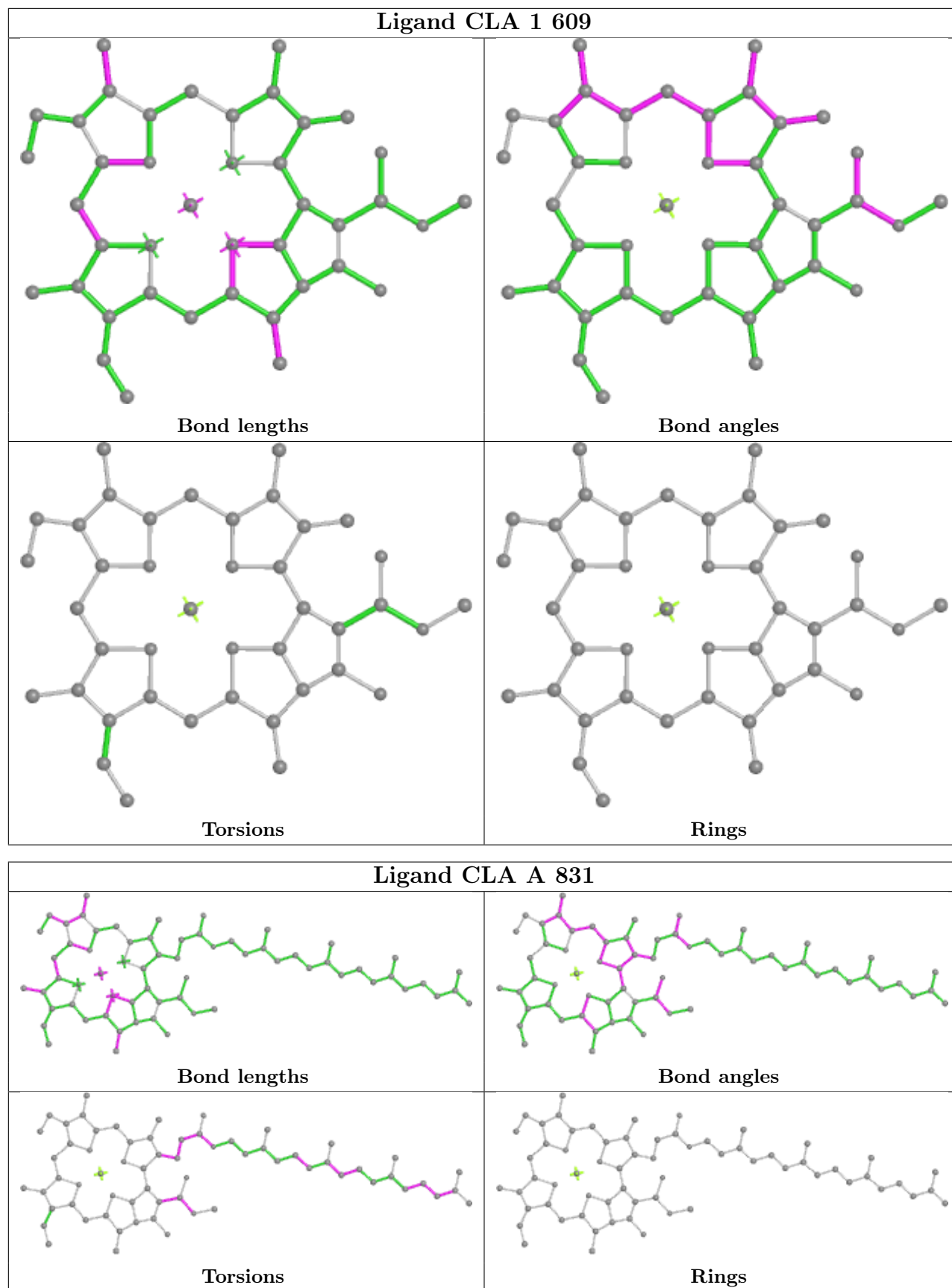


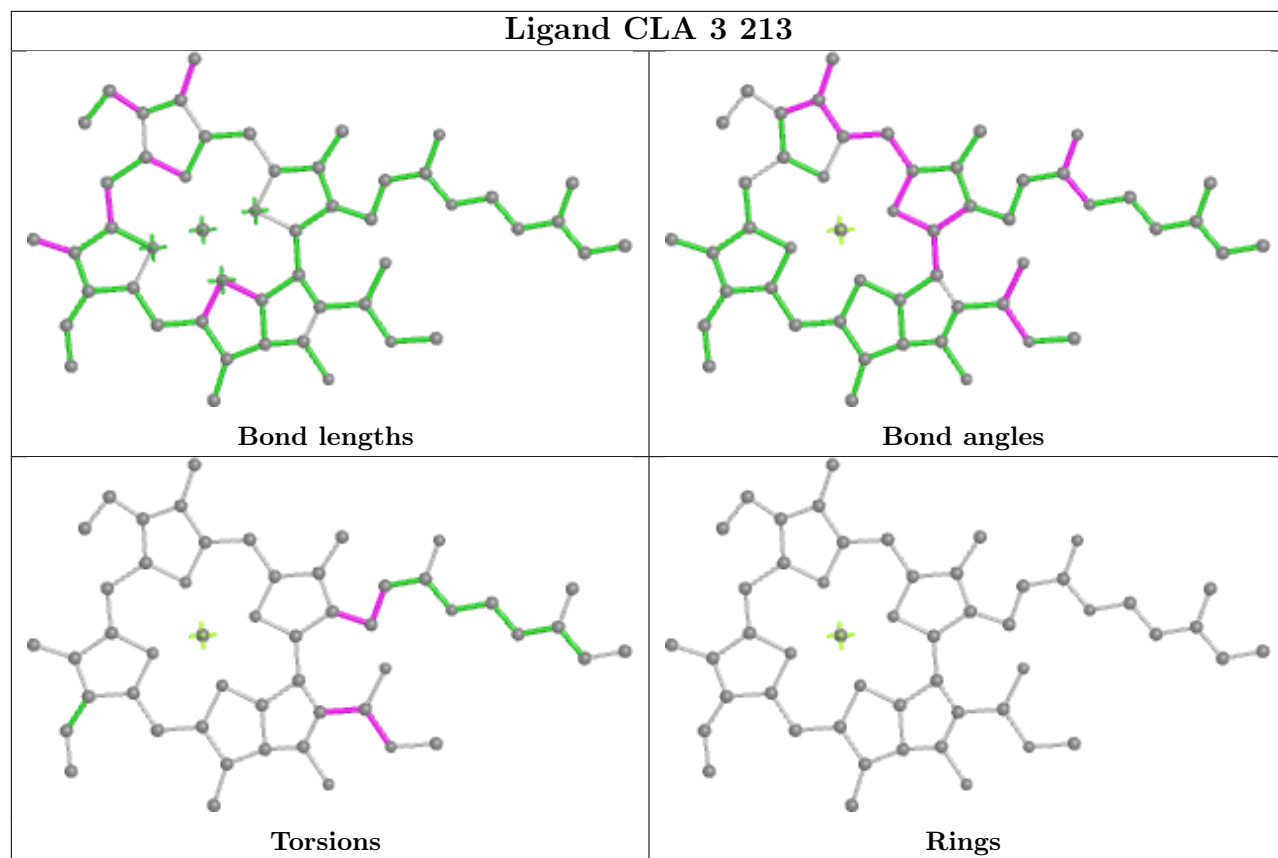
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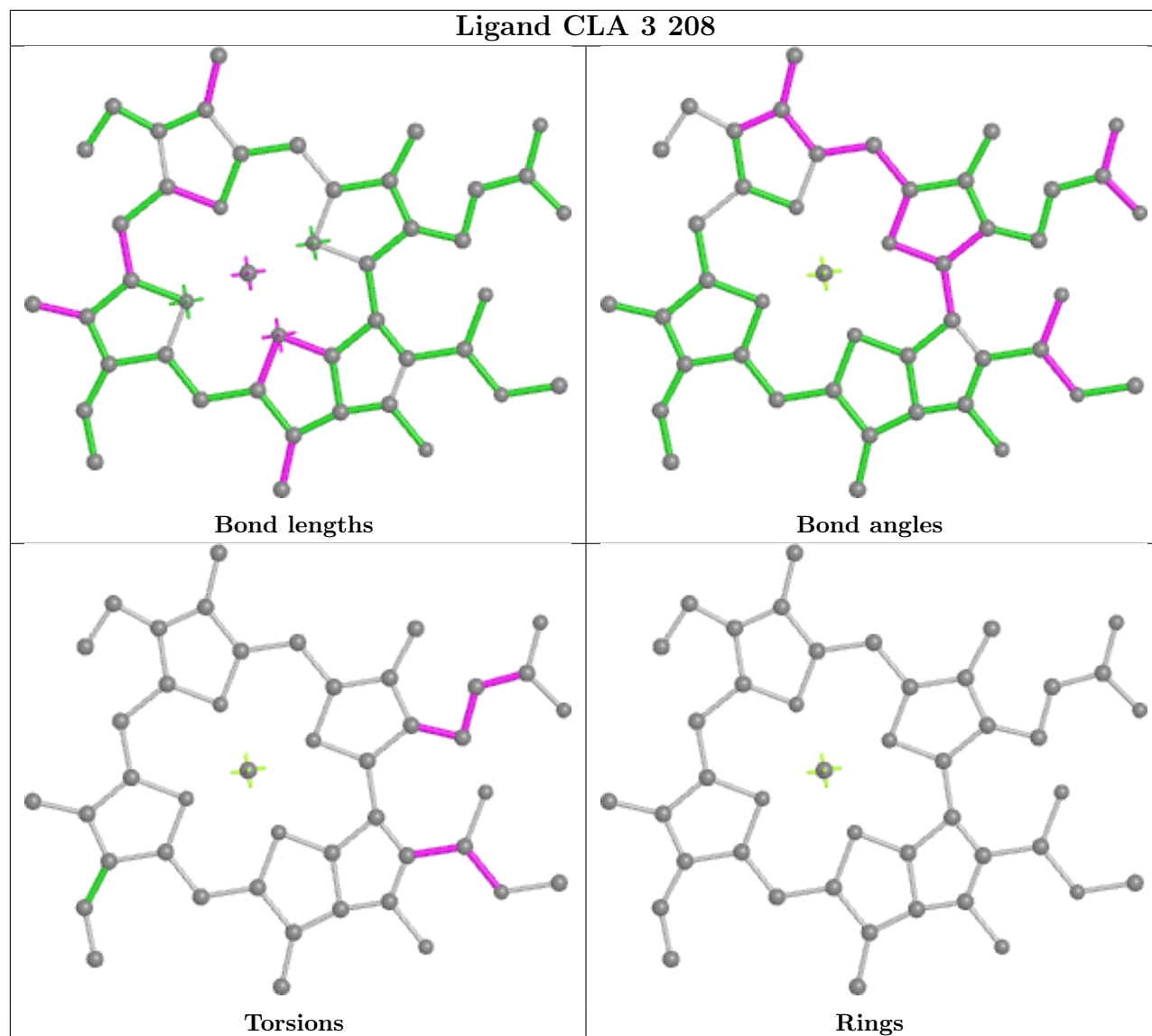


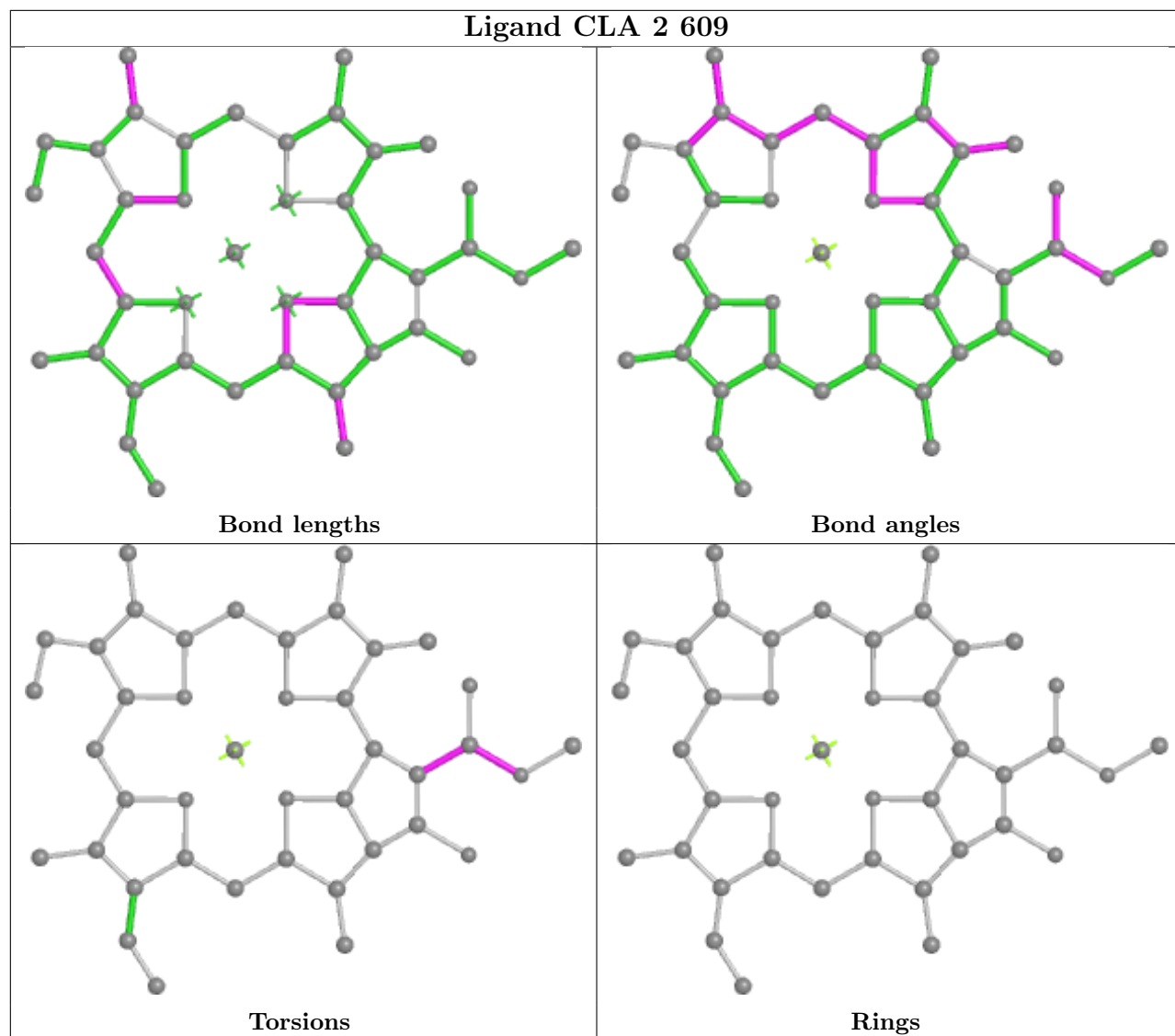


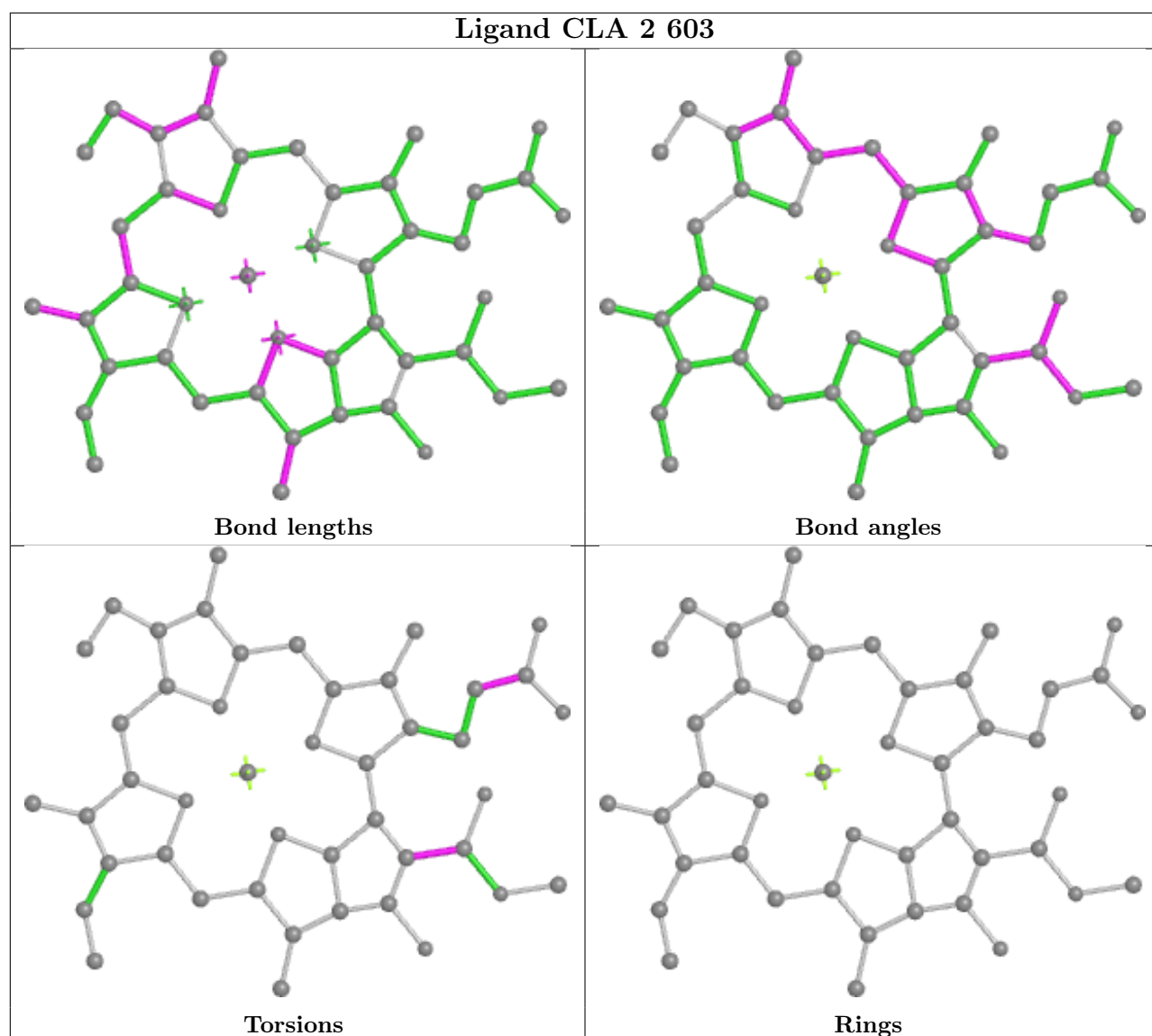


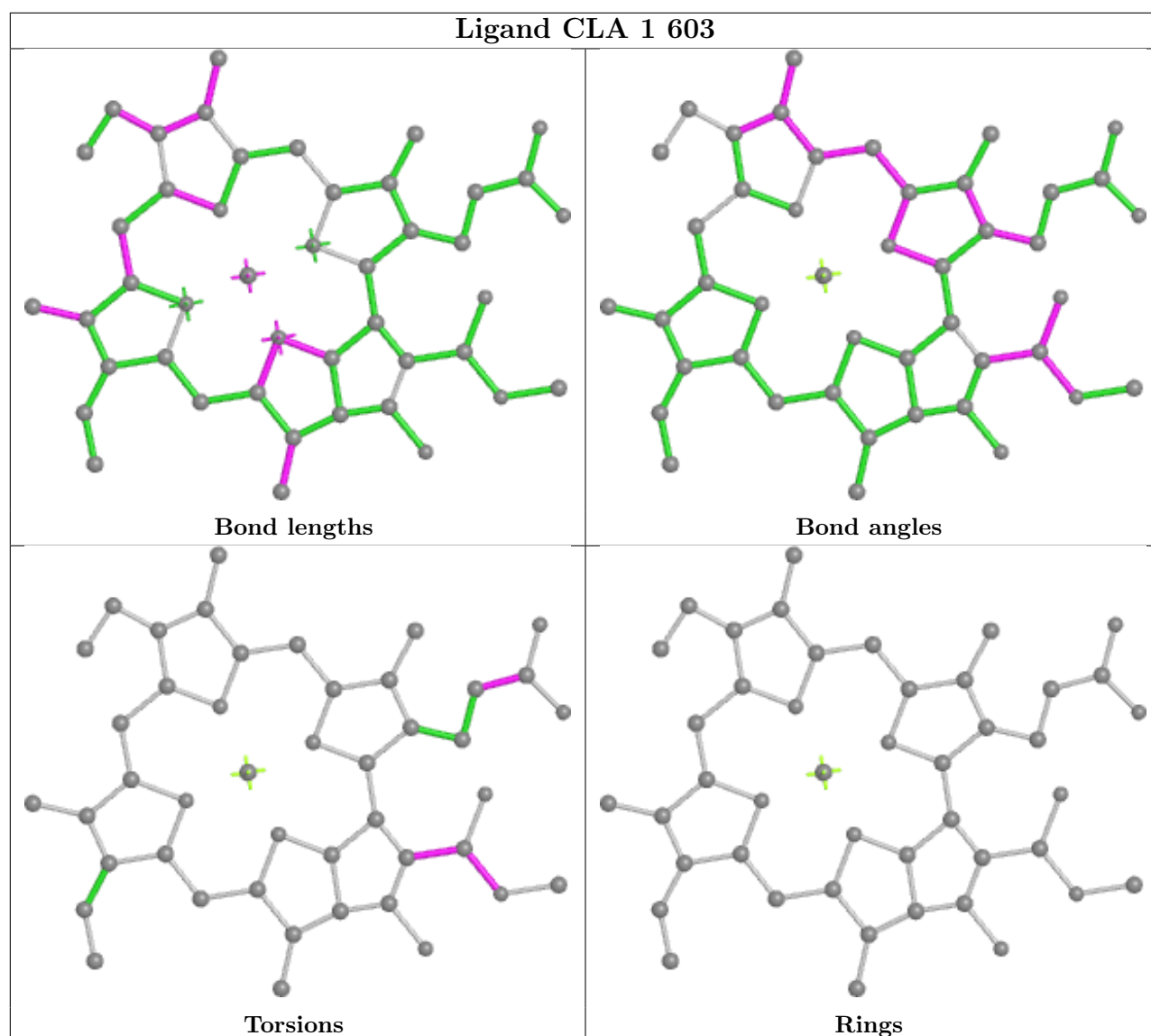












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

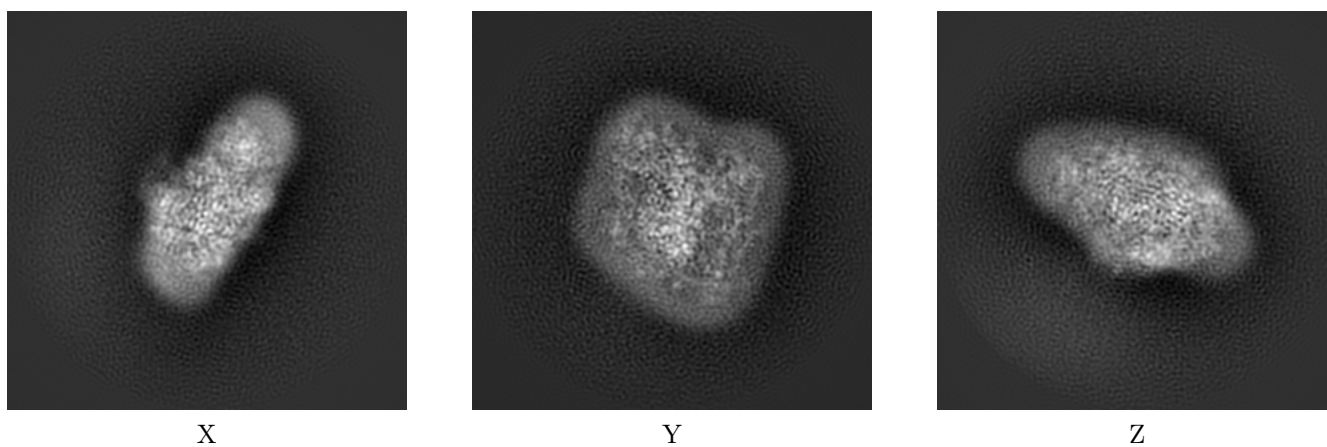
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6930. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

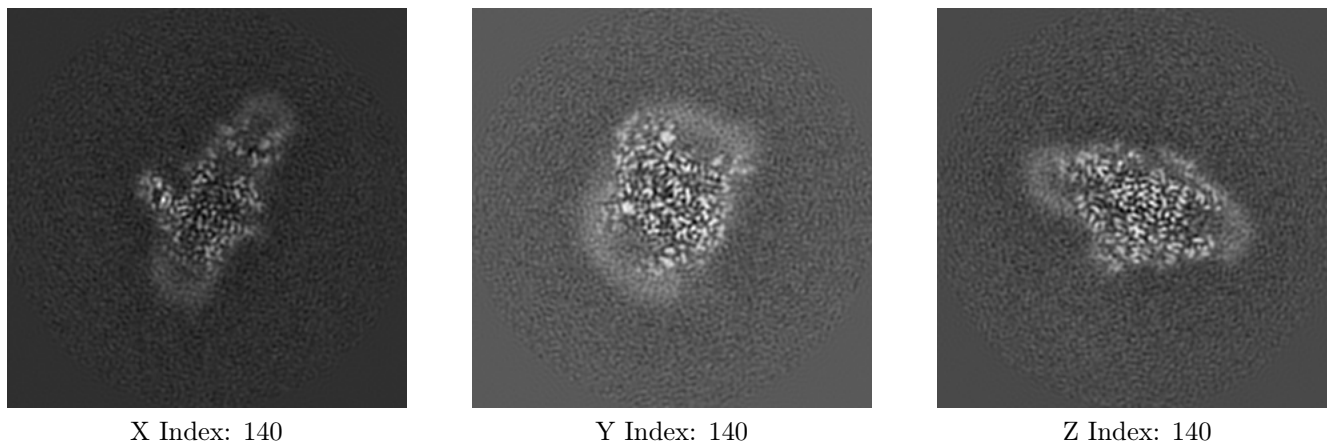
6.1.1 Primary map



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

6.2 Central slices [i](#)

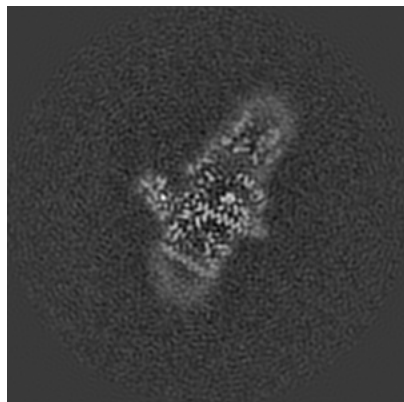
6.2.1 Primary map



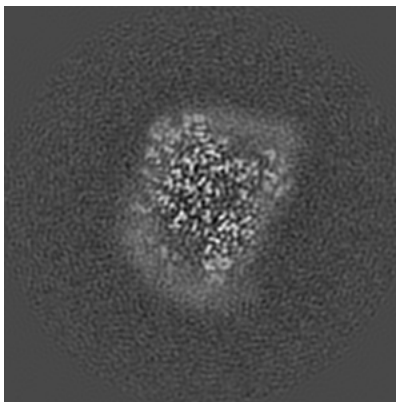
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

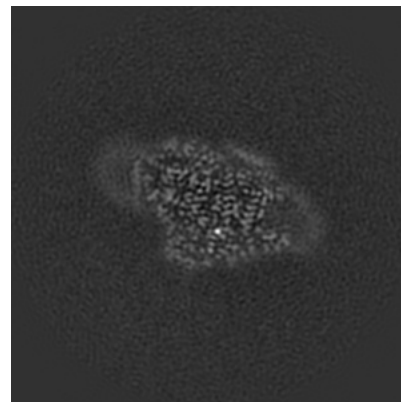
6.3.1 Primary map



X Index: 137



Y Index: 145

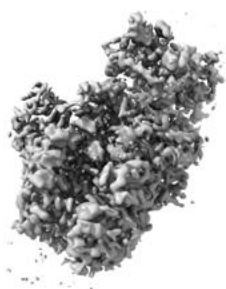


Z Index: 143

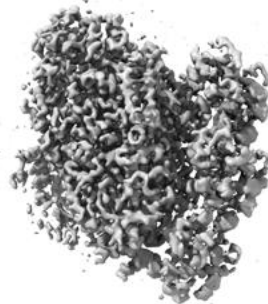
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.087. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

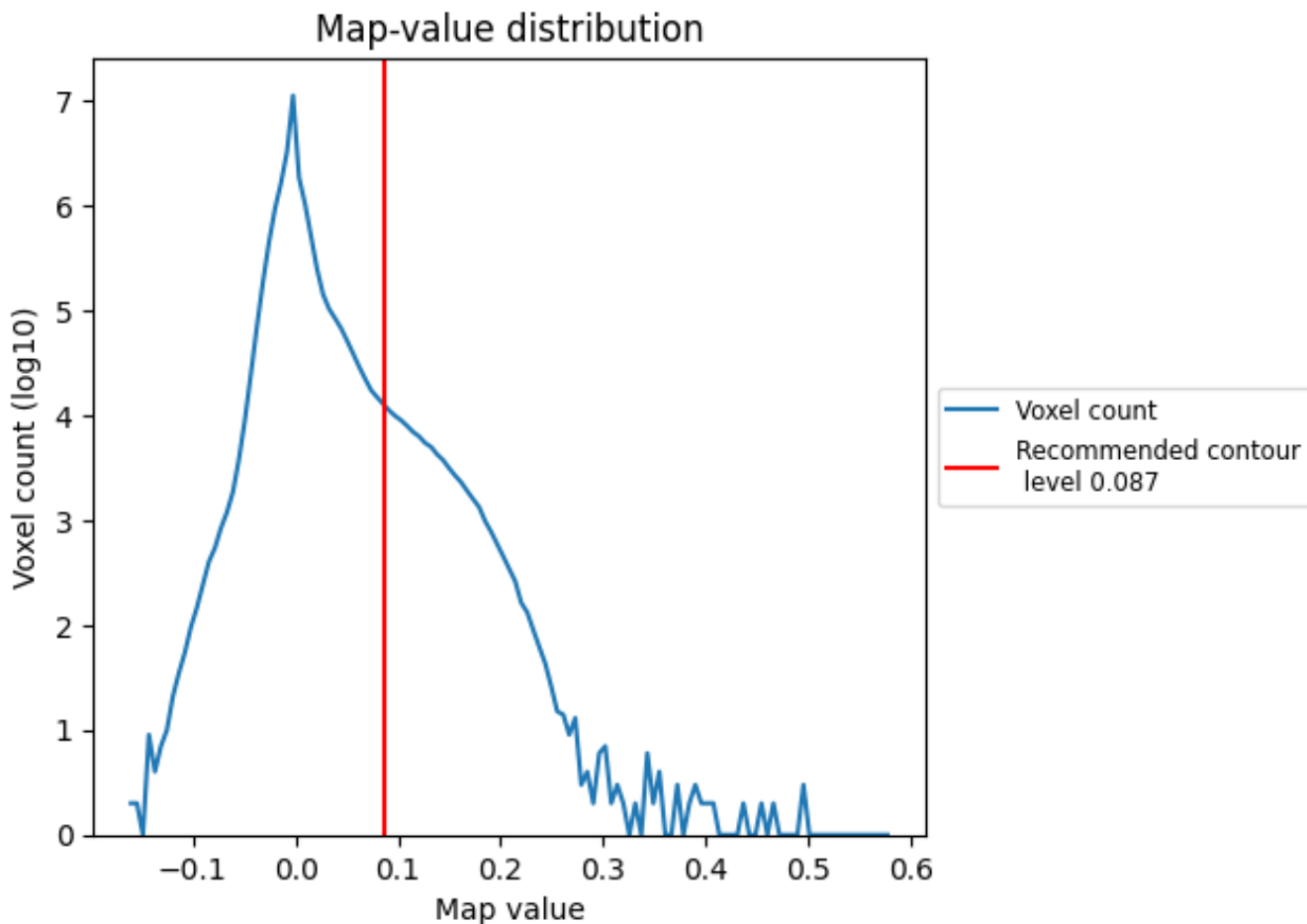
6.5 Mask visualisation

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

7 Map analysis [i](#)

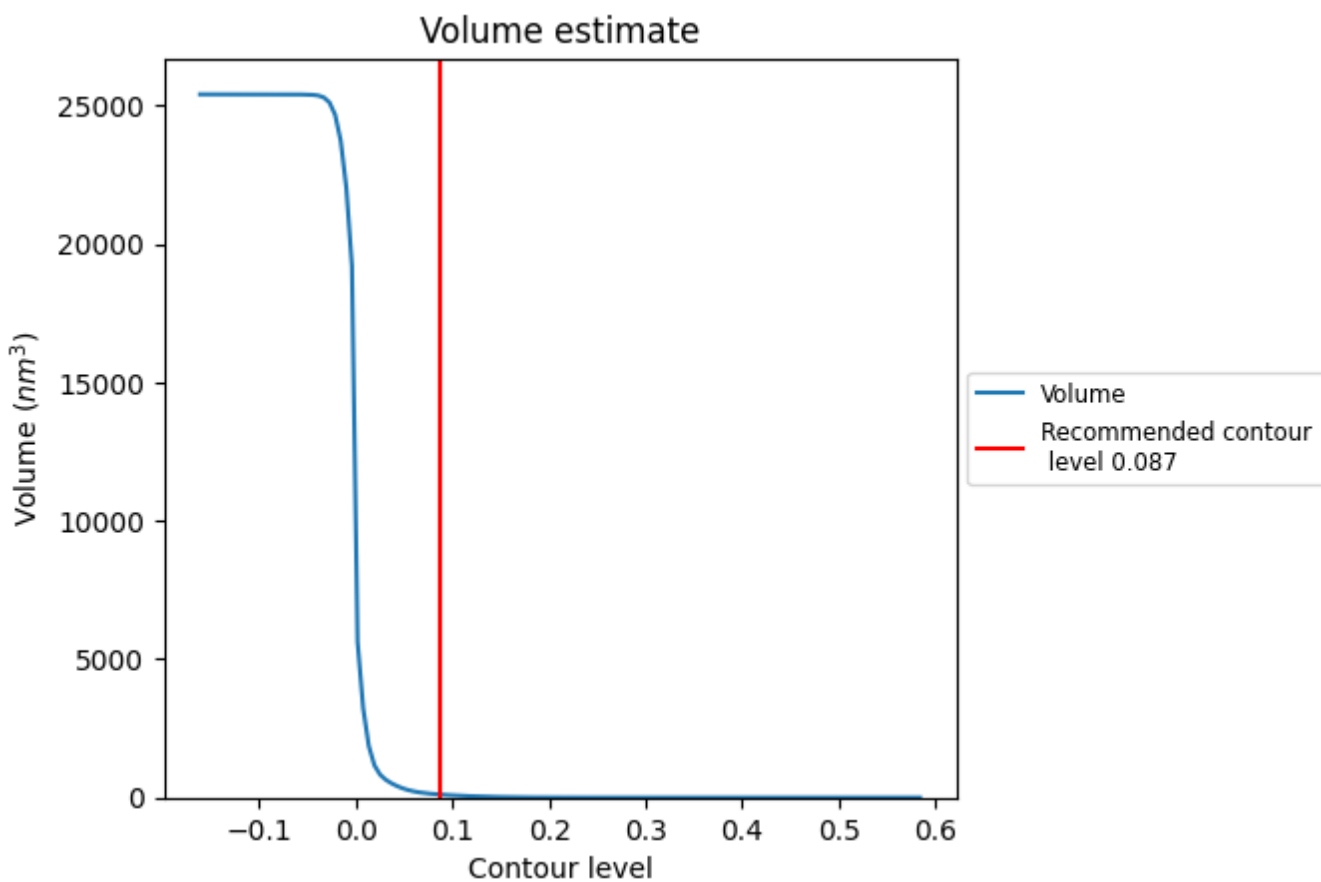
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

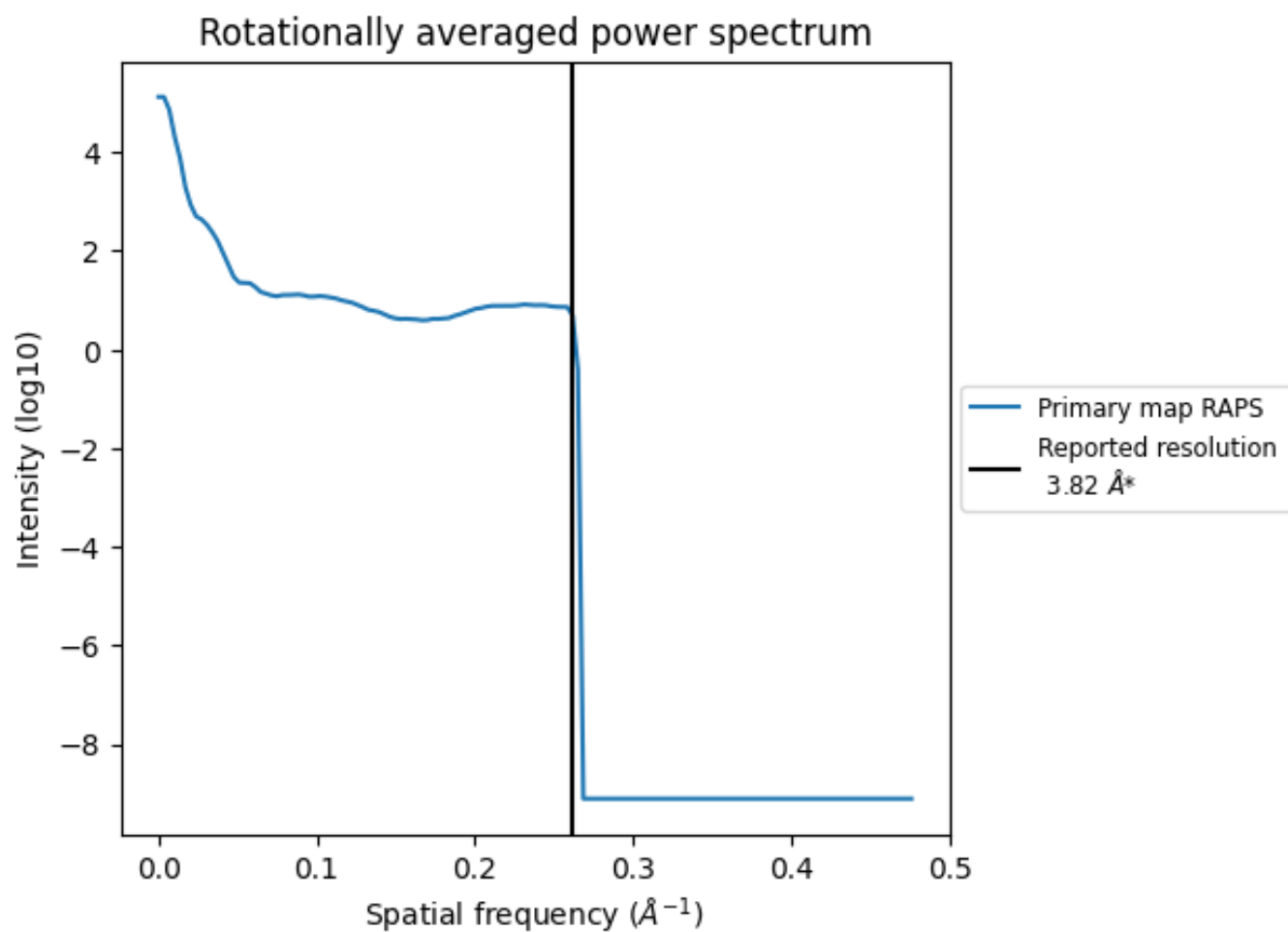
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm^3 ; this corresponds to an approximate mass of 100 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 0.262 Å⁻¹

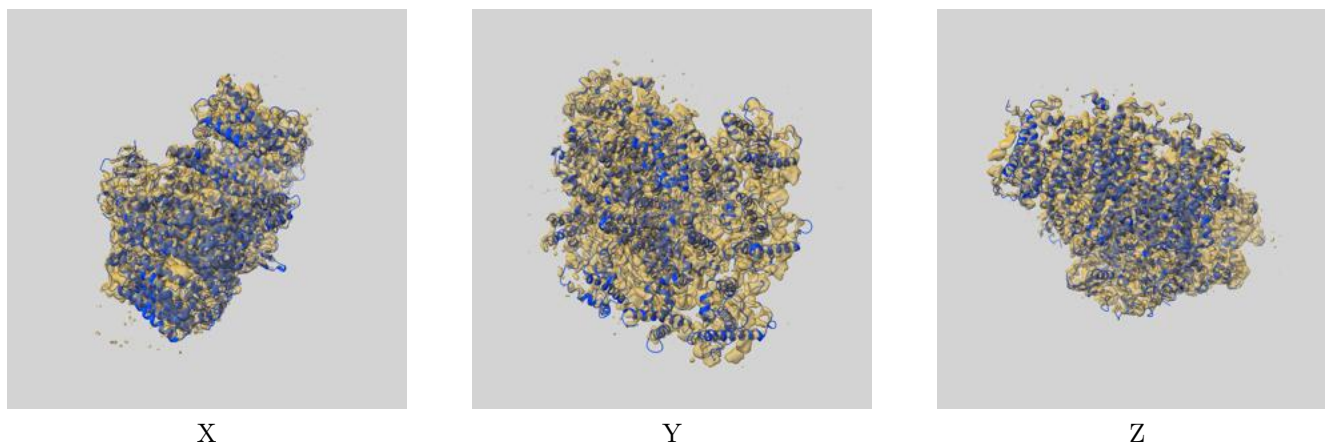
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

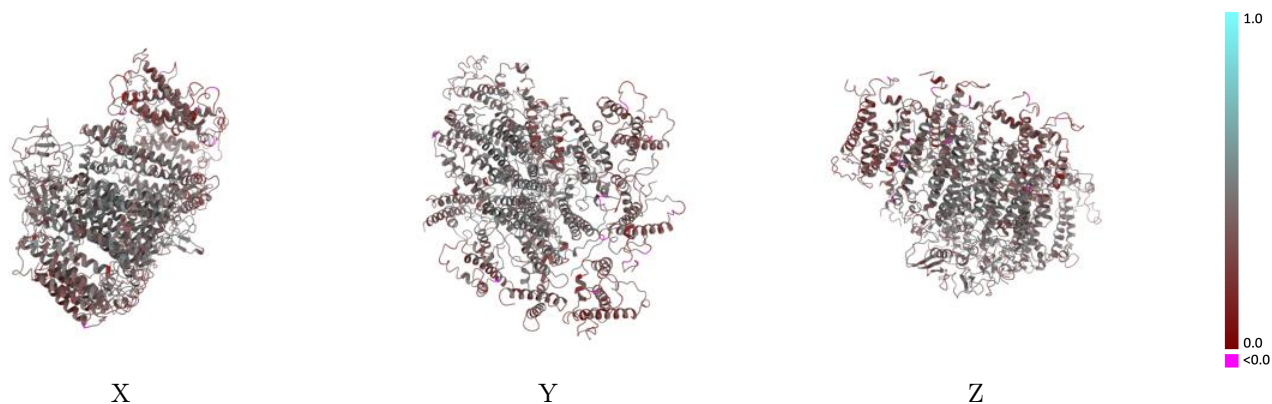
This section contains information regarding the fit between EMDB map EMD-6930 and PDB model 5ZGH. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



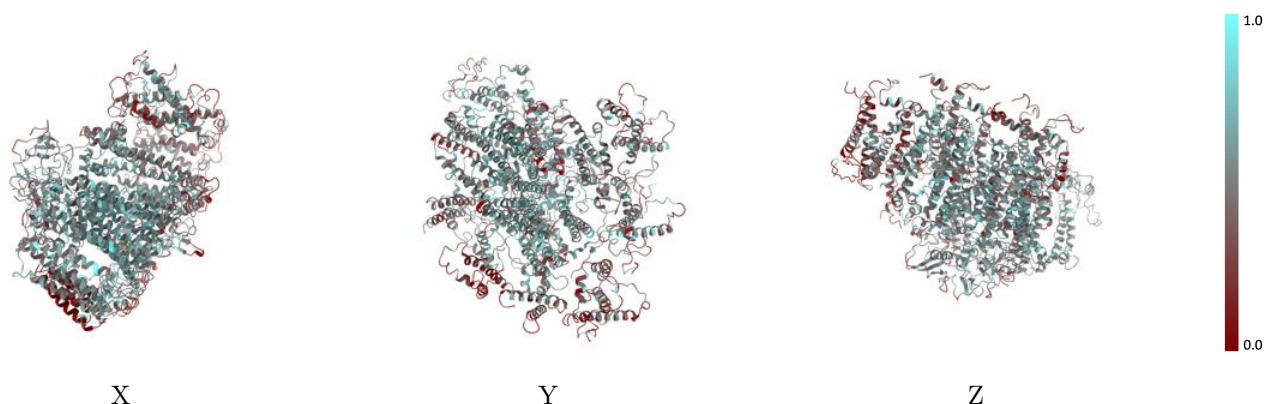
The images above show the 3D surface view of the map at the recommended contour level 0.087 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



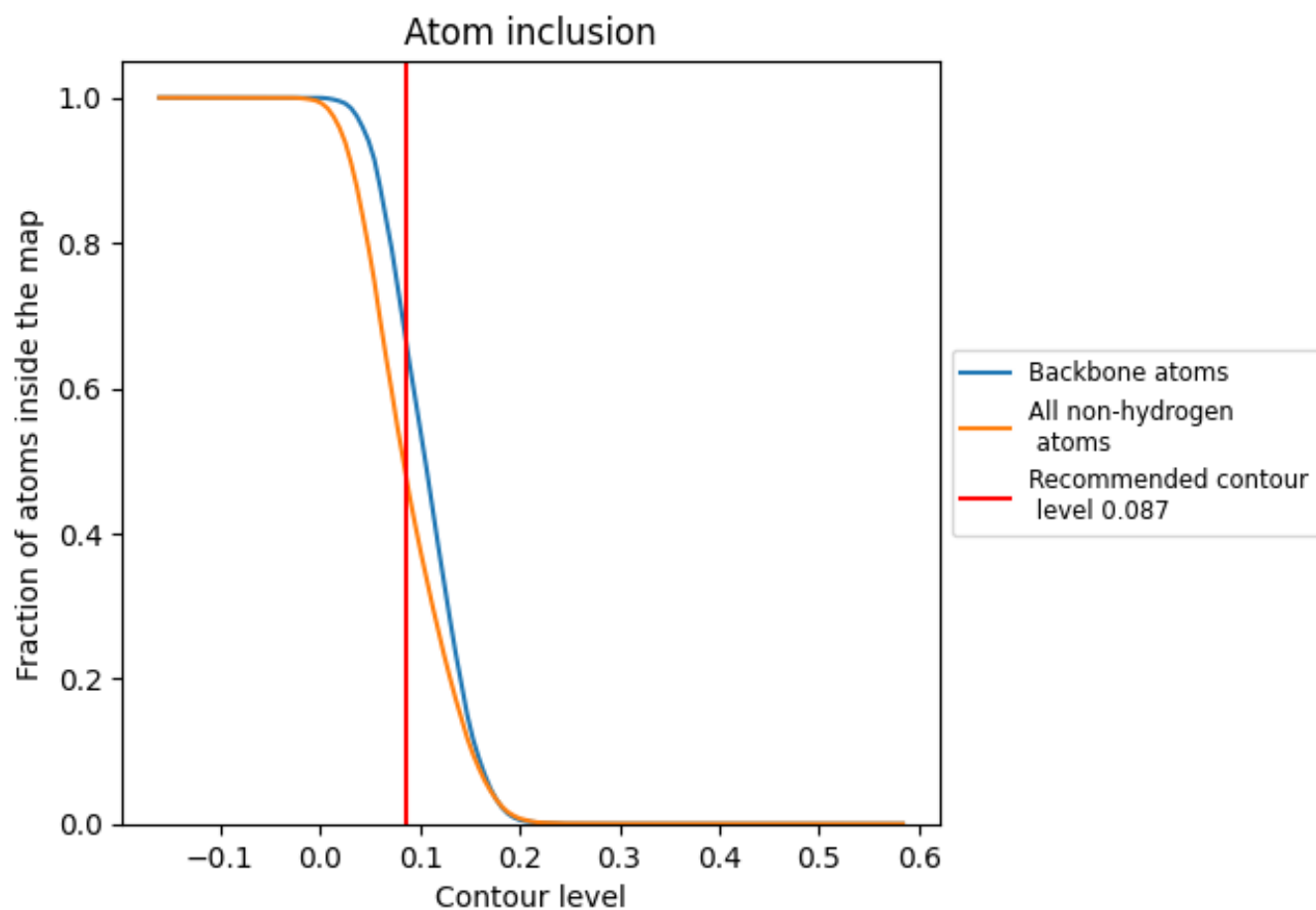
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.087).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 47% 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 (0.087) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4717	 0.4070
1	 0.3974	 0.3350
2	 0.4376	 0.3490
3	 0.3078	 0.3220
A	 0.5528	 0.4540
B	 0.5327	 0.4330
C	 0.5693	 0.4290
D	 0.4151	 0.3880
E	 0.4454	 0.3930
F	 0.4483	 0.3970
I	 0.3420	 0.3860
J	 0.4422	 0.4570
K	 0.3346	 0.3470
L	 0.3462	 0.3750
M	 0.0443	 0.2930
O	 0.1856	 0.3230

