



# wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 11:18 AM UTC

PDB ID : 9GRX / pdb\_00009grx  
EMDB ID : EMD-51527  
Title : NDH-PSI-LHCI supercomplex from *S. oleracea*  
Authors : Introini, B.; Hahn, A.; Kuehlbrandt, W.  
Deposited on : 2024-09-13  
Resolution : 3.19 Å(reported)  
Based on initial models : 4y28, 6khj, .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

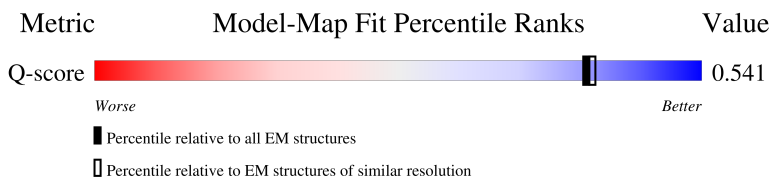
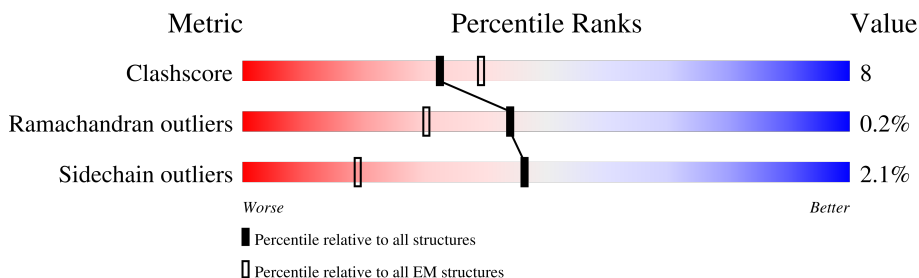
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.19 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14455 ( 2.69 - 3.69 )

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

Mol	Chain	Length	Quality of chain
1	0	157	82% (green), 17% (yellow), 1% (red), 1% (orange), 1% (grey)
2	1	403	83% (green), 17% (yellow)
3	2	372	63% (green), 17% (yellow), 19% (grey), 1% (red), 1% (orange)
4	3	139	79% (green), 20% (yellow), 1% (red), 1% (orange)



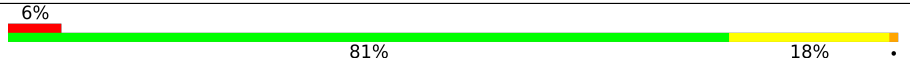
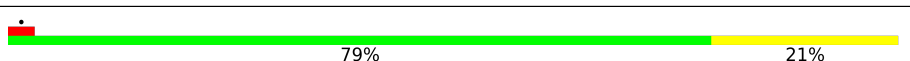
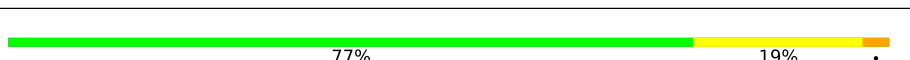
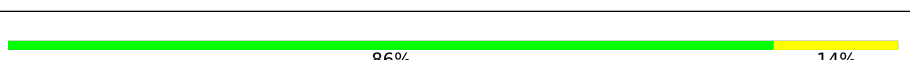
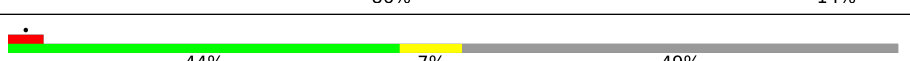
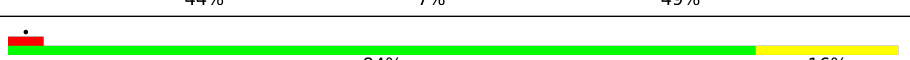
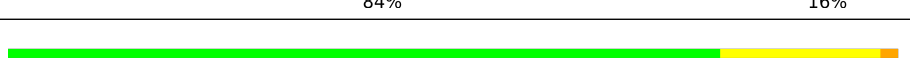
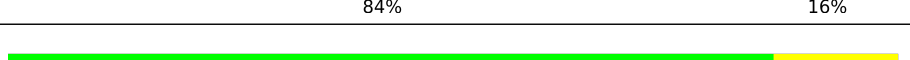
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Mol	Chain	Length	Quality of chain
5	4	93	86% 14%
6	5	154	91% 8%
7	6	125	82% 18%
8	7	144	92% 8%
9	8	143	81% 18%
10	9	174	83% 16%
11	A	350	81% 18%
12	B	488	75% 24%
13	C	115	82% 17%
14	D	498	80% 20%
15	E	100	81% 18%
16	F	742	77% 20%
17	G	176	79% 19%
18	H	389	77% 18% 5%
19	I	163	85% 15%
20	J	158	77% 22%
21	K	202	74% 23%
22	L	109	88% 11%
23	M	141	78% 21%
24	N	165	85% 15%
25	O	95	86% 12%
26	U	240	58% 9% 32%
27	a	742	84% 16%
28	b	733	84% 16%
29	c	81	85% 12%

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Mol	Chain	Length	Quality of chain
30	d	143	
31	e	68	
32	f	153	
33	g	97	
34	h	95	
35	i	31	
36	j	42	
37	k	130	
38	l	160	
39	w	215	
40	x	198	
41	y	221	
42	z	193	

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
50	CLA	a	801	X	-	-	-
50	CLA	a	802	X	-	-	-
50	CLA	a	809	X	-	-	-
50	CLA	a	811	X	-	-	-
50	CLA	a	812	X	-	-	-
50	CLA	a	813	X	-	-	-
50	CLA	a	814	X	-	-	-
50	CLA	a	815	X	-	-	-
50	CLA	a	816	X	-	-	-
50	CLA	a	817	X	-	-	-
50	CLA	a	818	X	-	-	-
50	CLA	a	819	X	-	-	-
50	CLA	a	820	X	-	-	-
50	CLA	a	821	X	-	-	-
50	CLA	a	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	CLA	a	823	X	-	-	-
50	CLA	a	824	X	-	-	-
50	CLA	a	826	X	-	-	-
50	CLA	a	833	X	-	-	-
50	CLA	a	834	X	-	-	-
50	CLA	a	835	X	-	-	-
50	CLA	a	836	X	-	-	-
50	CLA	a	837	X	-	-	-
50	CLA	a	838	X	-	-	-
50	CLA	a	839	X	-	-	-
50	CLA	a	840	X	-	-	-
50	CLA	a	841	X	-	-	-
50	CLA	a	842	X	-	-	-
50	CLA	a	843	X	-	-	-
50	CLA	a	844	X	-	-	-
50	CLA	a	845	X	-	-	-
50	CLA	a	846	X	-	-	-
50	CLA	a	847	X	-	-	-
50	CLA	a	848	X	-	-	-
50	CLA	a	849	X	-	-	-
50	CLA	a	850	X	-	-	-
50	CLA	a	851	X	-	-	-
50	CLA	a	852	X	-	-	-
50	CLA	a	853	X	-	-	-
50	CLA	a	854	X	-	-	-
50	CLA	a	855	X	-	-	-
50	CLA	a	856	X	-	-	-
50	CLA	a	857	X	-	-	-
50	CLA	a	858	X	-	-	-
50	CLA	b	801	X	-	-	-
50	CLA	b	802	X	-	-	-
50	CLA	b	803	X	-	-	-
50	CLA	b	804	X	-	-	-
50	CLA	b	805	X	-	-	-
50	CLA	b	806	X	-	-	-
50	CLA	b	807	X	-	-	-
50	CLA	b	808	X	-	-	-
50	CLA	b	809	X	-	-	-
50	CLA	b	810	X	-	-	-
50	CLA	b	811	X	-	-	-
50	CLA	b	812	X	-	-	-
50	CLA	b	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	CLA	b	814	X	-	-	-
50	CLA	b	815	X	-	-	-
50	CLA	b	822	X	-	-	-
50	CLA	b	823	X	-	-	-
50	CLA	b	824	X	-	-	-
50	CLA	b	825	X	-	-	-
50	CLA	b	826	X	-	-	-
50	CLA	b	828	X	-	-	-
50	CLA	b	832	X	-	-	-
50	CLA	b	833	X	-	-	-
50	CLA	b	834	X	-	-	-
50	CLA	b	835	X	-	-	-
50	CLA	b	836	X	-	-	-
50	CLA	b	837	X	-	-	-
50	CLA	b	838	X	-	-	-
50	CLA	b	839	X	-	-	-
50	CLA	b	840	X	-	-	-
50	CLA	b	841	X	-	-	-
50	CLA	b	842	X	-	-	-
50	CLA	b	843	X	-	-	-
50	CLA	b	844	X	-	-	-
50	CLA	b	845	X	-	-	-
50	CLA	b	846	X	-	-	-
50	CLA	b	847	X	-	-	-
50	CLA	b	848	X	-	-	-
50	CLA	b	849	X	-	-	-
50	CLA	b	851	X	-	-	-
50	CLA	f	301	X	-	-	-
50	CLA	f	302	X	-	-	-
50	CLA	f	303	X	-	-	-
50	CLA	g	201	X	-	-	-
50	CLA	g	203	X	-	-	-
50	CLA	g	204	X	-	-	-
50	CLA	h	201	X	-	-	-
50	CLA	j	102	X	-	-	-
50	CLA	k	203	X	-	-	-
50	CLA	k	204	X	-	-	-
50	CLA	k	205	X	-	-	-
50	CLA	l	301	X	-	-	-
50	CLA	l	305	X	-	-	-
50	CLA	l	306	X	-	-	-
50	CLA	w	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	CLA	w	303	X	-	-	-
50	CLA	w	305	X	-	-	-
50	CLA	w	306	X	-	-	-
50	CLA	w	307	X	-	-	-
50	CLA	w	308	X	-	-	-
50	CLA	w	310	X	-	-	-
50	CLA	w	314	X	-	-	-
50	CLA	w	315	X	-	-	-
50	CLA	w	316	X	-	-	-
50	CLA	x	302	X	-	-	-
50	CLA	x	303	X	-	-	-
50	CLA	x	304	X	-	-	-
50	CLA	x	306	X	-	-	-
50	CLA	x	307	X	-	-	-
50	CLA	x	308	X	-	-	-
50	CLA	x	309	X	-	-	-
50	CLA	x	310	X	-	-	-
50	CLA	x	312	X	-	-	-
50	CLA	x	313	X	-	-	-
50	CLA	x	316	X	-	-	-
50	CLA	x	318	X	-	-	-
50	CLA	y	302	X	-	-	-
50	CLA	y	303	X	-	-	-
50	CLA	y	304	X	-	-	-
50	CLA	y	305	X	-	-	-
50	CLA	y	306	X	-	-	-
50	CLA	y	307	X	-	-	-
50	CLA	y	308	X	-	-	-
50	CLA	y	309	X	-	-	-
50	CLA	y	310	X	-	-	-
50	CLA	y	311	X	-	-	-
50	CLA	y	312	X	-	-	-
50	CLA	y	313	X	-	-	-
50	CLA	y	314	X	-	-	-
50	CLA	z	302	X	-	-	-
50	CLA	z	303	X	-	-	-
50	CLA	z	305	X	-	-	-
50	CLA	z	306	X	-	-	-
50	CLA	z	307	X	-	-	-
50	CLA	z	308	X	-	-	-
50	CLA	z	309	X	-	-	-
50	CLA	z	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	CLA	z	311	X	-	-	-
50	CLA	z	316	X	-	-	-
50	CLA	z	319	X	-	-	-
52	CLO	a	808	X	-	-	-
54	CHL	w	304	X	-	-	-
54	CHL	w	309	X	-	-	-
54	CHL	w	311	X	-	-	-
54	CHL	x	301	X	-	-	-
54	CHL	x	305	X	-	-	-
54	CHL	x	311	X	-	-	-
54	CHL	x	319	X	-	-	-
54	CHL	z	304	X	-	-	-
54	CHL	z	312	X	-	-	-
55	LUT	w	320	-	-	X	-
55	LUT	y	315	-	-	X	-
55	LUT	y	316	-	-	X	-
55	LUT	z	320	-	-	X	-

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 83864 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 Photosynthetic NDH subunit of lumenal location 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	157	1317	840	227	248	2	0	0

- Molecule 2 is a protein called Photosynthetic NDH subunit of subcomplex B 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	403	3133	1994	515	607	17	0	0

- Molecule 3 is a protein called Photosynthetic NDH subunit of subcomplex B 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	300	2305	1463	383	452	7	0	0

- Molecule 4 is a protein called Photosynthetic NDH subunit of subcomplex B 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	139	1093	690	185	210	8	0	0

- Molecule 5 is a protein called Photosynthetic NDH subunit of subcomplex B 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	93	756	482	125	143	6	0	0

- Molecule 6 is a protein called Photosynthetic NDH subunit of subcomplex B 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	154	1258	816	194	242	6	0	0

- Molecule 7 is a protein called Photosynthetic NDH subunit of luminal location 2, chloroplast.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	125	1048	675	174	193	6	0	0

- Molecule 8 is a protein called Photosynthetic NDH subunit of luminal location 3, chloroplast.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	144	1156	739	198	213	6	0	0

- Molecule 9 is a protein called peptidylprolyl isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	143	1075	680	187	201	7	0	0

- Molecule 10 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	174	1326	836	233	251	6	0	0

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit 1, chloroplast.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	350	2728	1821	420	482	5	0	0

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit 2 A, chloroplast.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	B	488	3799	2506	583	683	27	0	0

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit 3, chloroplast.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	C	115	944	653	133	155	3	0	0

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	D	498	3955	2660	607	665	23	0	0

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	E	100	780	509	133	135	3	0	0

- Molecule 16 is a protein called NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	F	722	5796	3885	889	990	32	0	0

- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	G	176	1357	910	204	238	5	0	0

- Molecule 18 is a protein called NAD(P)H-quinone oxidoreductase subunit H, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	H	371	3008	1948	506	535	19	0	0

- Molecule 19 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	I	163	1329	845	226	246	12	0	0

- Molecule 20 is a protein called NAD(P)H-quinone oxidoreductase subunit J, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	J	158	1324	864	224	231	5	0	0

- Molecule 21 is a protein called NAD(P)H-quinone oxidoreductase subunit K, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	K	202	1597	1020	272	294	11	0	0

- Molecule 22 is a protein called NAD(P)H-quinone oxidoreductase subunit L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	L	109	936	639	147	144	6	0	0

- Molecule 23 is a protein called NAD(P)H-quinone oxidoreductase subunit M, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	M	141	1169	743	196	221	9	0	0

- Molecule 24 is a protein called NAD(P)H-quinone oxidoreductase subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	N	165	1323	862	228	228	5	0	0

- Molecule 25 is a protein called NAD(P)H-quinone oxidoreductase subunit O, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	O	95	786	515	127	142	2	0	0

- Molecule 26 is a protein called NAD(P)H-quinone oxidoreductase subunit U, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	163	1266	802	218	243	3	0	0

- Molecule 27 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	742	5827	3817	991	1001	18	0	0

- Molecule 28 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	b	733	5855	3841	996	1003	15	0	0

- Molecule 29 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	81	623	385	108	118	12	0	0

- Molecule 30 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	d	143	1132	729	194	205	4	0	0

- Molecule 31 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	e	68	546	348	98	99	1	0	0

- Molecule 32 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	f	153	1211	785	206	217	3	0	0

- Molecule 33 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	g	97	759	493	123	141	2	0	0

- Molecule 34 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	h	95	737	479	120	138	0	0

- Molecule 35 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	31	Total	C	N	O	S	0	0
			244	168	36	38	2		

- Molecule 36 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	42	Total	C	N	O	S	0	0
			345	236	51	57	1		

- Molecule 37 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	66	Total	C	N	O	S	0	0
			462	294	78	87	3		

- Molecule 38 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	160	Total	C	N	O	S	0	0
			1200	791	192	212	5		

- Molecule 39 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	w	215	Total	C	N	O	S	0	0
			1689	1096	281	300	12		

- Molecule 40 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	x	198	Total	C	N	O	S	0	0
			1568	1023	256	284	5		

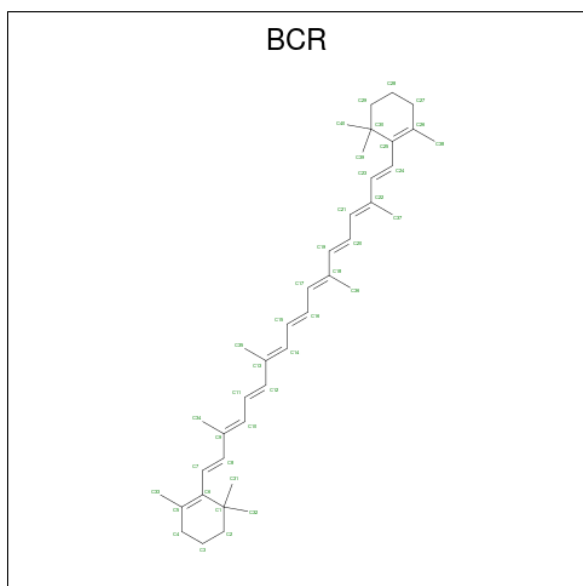
- Molecule 41 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	y	221	Total	C	N	O	S	0	0
			1713	1125	277	306	5		

- Molecule 42 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	z	193	1498	973	250	270	5	0	0

- Molecule 43 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



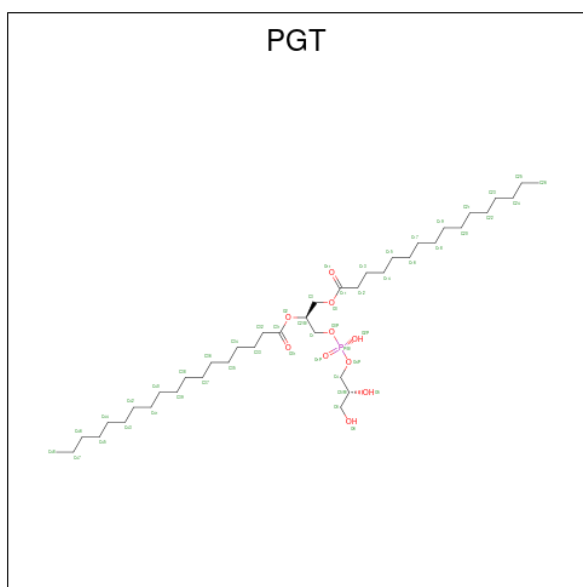
Mol	Chain	Residues	Atoms		AltConf
43	4	1	Total	C	0
			40	40	
43	a	1	Total	C	0
			27	27	
43	a	1	Total	C	0
			30	30	
43	a	1	Total	C	0
			39	39	
43	a	1	Total	C	0
			40	40	
43	a	1	Total	C	0
			40	40	
43	a	1	Total	C	0
			40	40	
43	a	1	Total	C	0
			39	39	
43	b	1	Total	C	0
			40	40	
43	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	f	1	Total C 40 40	0
43	g	1	Total C 40 40	0
43	i	1	Total C 40 40	0
43	j	1	Total C 40 40	0
43	j	1	Total C 40 40	0
43	k	1	Total C 40 40	0
43	k	1	Total C 40 40	0
43	l	1	Total C 40 40	0
43	l	1	Total C 40 40	0
43	l	1	Total C 40 40	0
43	w	1	Total C 40 40	0
43	x	1	Total C 40 40	0
43	y	1	Total C 40 40	0
43	z	1	Total C 40 40	0

- Molecule 44 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



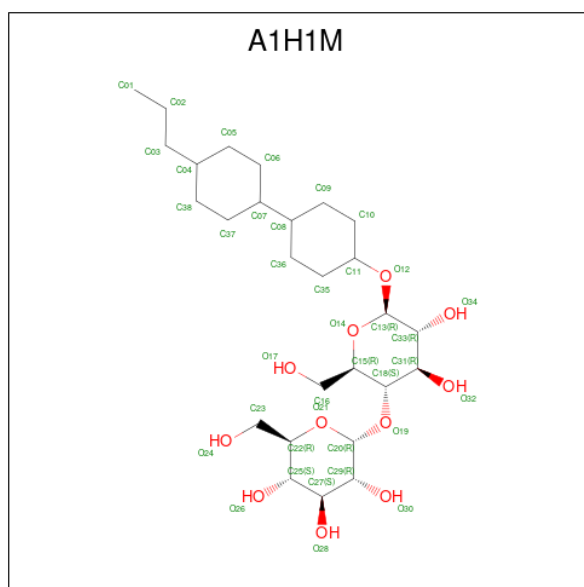
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
44	5	1	35	24	10	1	0
44	A	1	32	21	10	1	0
44	A	1	37	26	10	1	0
44	A	1	38	27	10	1	0
44	A	1	44	33	10	1	0
44	B	1	34	23	10	1	0
44	B	1	42	31	10	1	0
44	B	1	46	35	10	1	0
44	B	1	35	24	10	1	0
44	D	1	34	23	10	1	0
44	F	1	43	32	10	1	0
44	I	1	44	33	10	1	0
44	L	1	40	29	10	1	0
44	N	1	26	15	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
44	a	1	Total 32	C 21	O 10	P 1	0
44	a	1	Total 33	C 22	O 10	P 1	0
44	a	1	Total 46	C 35	O 10	P 1	0
44	b	1	Total 48	C 37	O 10	P 1	0
44	b	1	Total 39	C 28	O 10	P 1	0
44	f	1	Total 39	C 28	O 10	P 1	0
44	w	1	Total 40	C 29	O 10	P 1	0
44	z	1	Total 45	C 34	O 10	P 1	0
44	z	1	Total 33	C 22	O 10	P 1	0
44	z	1	Total 46	C 35	O 10	P 1	0

- Molecule 45 is 4-trans-(4-trans-Propylcyclohexyl)-cyclohexyl alpha-maltoside (CCD ID: A1H1M) (formula: C<sub>27</sub>H<sub>48</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



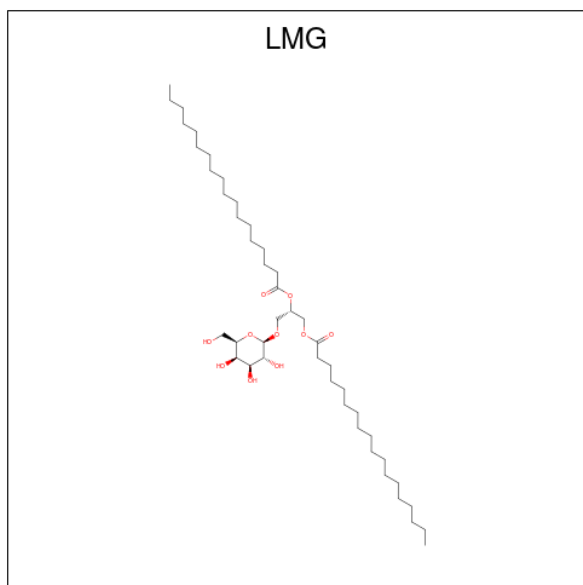
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	5	1	Total 38	C 27	O 11	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	F	1	38	27	11	0

- Molecule 46 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



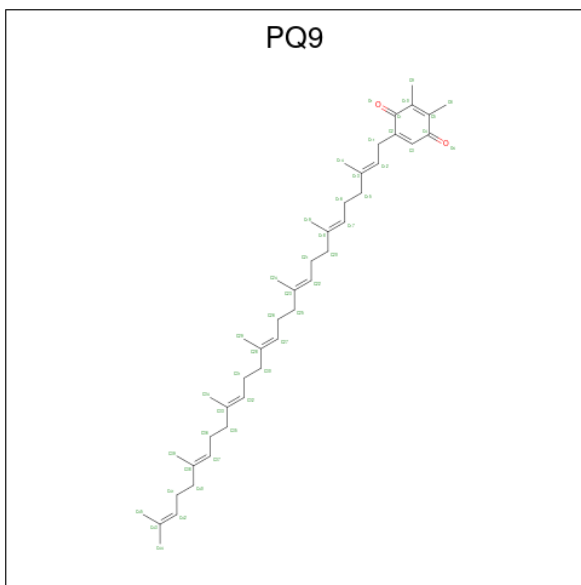
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
46	7	1	41	31	10	0
46	B	1	37	27	10	0
46	D	1	34	24	10	0
46	F	1	28	18	10	0
46	H	1	33	23	10	0
46	f	1	34	24	10	0
46	j	1	34	24	10	0
46	j	1	37	27	10	0
46	w	1	40	30	10	0
46	x	1	48	38	10	0

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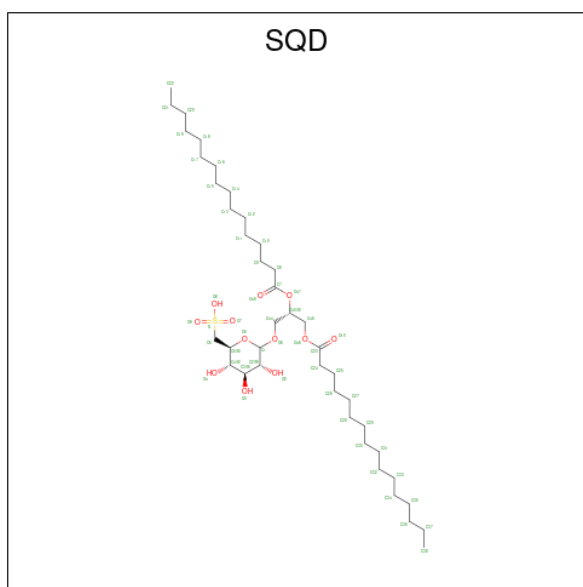
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
46	z	1	40	30	10	0
46	z	1	36	26	10	0

- Molecule 47 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: C<sub>43</sub>H<sub>64</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



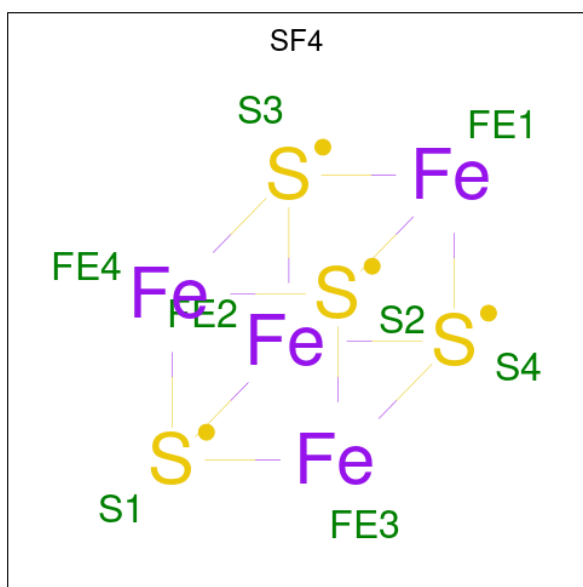
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
47	A	1	36	34	2	0

- Molecule 48 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S) (labeled as "Ligand of Interest" by depositor).



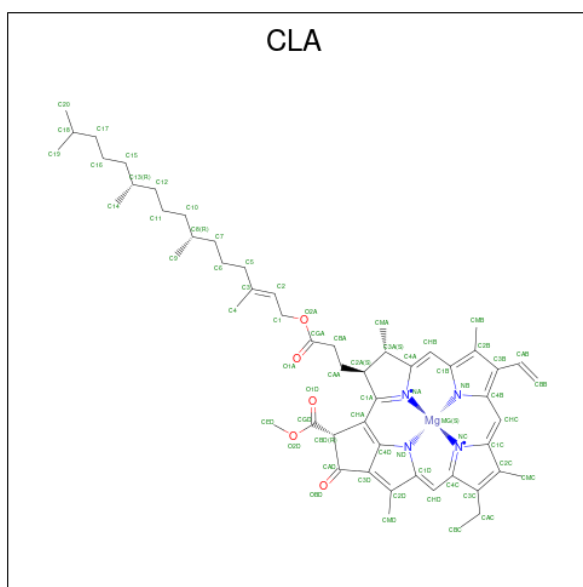
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
48	B	1	40	27	12	1	0
48	F	1	41	28	12	1	0
48	F	1	43	30	12	1	0
48	a	1	36	23	12	1	0
48	j	1	42	29	12	1	0
48	w	1	31	18	12	1	0
48	w	1	41	28	12	1	0

- Molecule 49 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
49	I	1	Total	Fe	S	0
			8	4	4	
49	I	1	Total	Fe	S	0
			8	4	4	
49	K	1	Total	Fe	S	0
			8	4	4	
49	a	1	Total	Fe	S	0
			8	4	4	
49	c	1	Total	Fe	S	0
			8	4	4	
49	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 50 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
50	a	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
50	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
50	a	1	Total	C	Mg	N	O	0
			63	53	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
50	a	1	51	41	1	4	5	0
50	a	1	55	45	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	45	35	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	58	48	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	42	34	1	4	3	0
50	a	1	55	45	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	57	47	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	42	35	1	3	3	0
50	a	1	52	42	1	4	5	0
50	a	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
50	a	1	65	55	1	4	5	0
50	a	1	46	36	1	4	5	0
50	a	1	51	41	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	42	34	1	4	3	0
50	a	1	64	54	1	4	5	0
50	a	1	65	55	1	4	5	0
50	a	1	65	55	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	41	33	1	4	3	0
50	b	1	65	55	1	4	5	0
50	b	1	52	42	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	43	35	1	4	3	0
50	b	1	59	49	1	4	5	0
50	b	1	50	40	1	4	5	0
50	b	1	45	35	1	4	5	0
50	b	1	62	52	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
50	b	1	43	35	1	4	3	0
50	b	1	65	55	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	58	48	1	4	5	0
50	b	1	55	45	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	55	45	1	4	5	0
50	b	1	60	50	1	4	5	0
50	b	1	54	44	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	45	35	1	4	5	0
50	b	1	59	49	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	52	42	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	55	45	1	4	5	0
50	b	1	57	47	1	4	5	0
50	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
50	b	1	65	55	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	65	55	1	4	5	0
50	b	1	60	50	1	4	5	0
50	b	1	42	34	1	4	3	0
50	b	1	50	40	1	4	5	0
50	b	1	47	37	1	4	5	0
50	f	1	57	47	1	4	5	0
50	f	1	42	34	1	4	3	0
50	f	1	41	33	1	4	3	0
50	g	1	49	39	1	4	5	0
50	g	1	52	42	1	4	5	0
50	g	1	43	35	1	4	3	0
50	h	1	46	36	1	4	5	0
50	j	1	42	34	1	4	3	0
50	k	1	41	33	1	4	3	0
50	k	1	57	47	1	4	5	0
50	k	1	42	34	1	4	3	0
50	l	1	45	35	1	4	5	0
50	l	1	40	32	1	4	3	0
50	l	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
50	w	1	50	40	1	4	5	0
50	w	1	45	35	1	4	5	0
50	w	1	51	41	1	4	5	0
50	w	1	65	55	1	4	5	0
50	w	1	45	35	1	4	5	0
50	w	1	65	55	1	4	5	0
50	w	1	65	55	1	4	5	0
50	w	1	44	35	1	4	4	0
50	w	1	46	36	1	4	5	0
50	w	1	50	40	1	4	5	0
50	x	1	41	33	1	4	3	0
50	x	1	57	47	1	4	5	0
50	x	1	47	37	1	4	5	0
50	x	1	60	50	1	4	5	0
50	x	1	60	50	1	4	5	0
50	x	1	50	40	1	4	5	0
50	x	1	42	34	1	4	3	0
50	x	1	43	35	1	4	3	0
50	x	1	65	55	1	4	5	0
50	x	1	53	43	1	4	5	0
50	x	1	45	35	1	4	5	0

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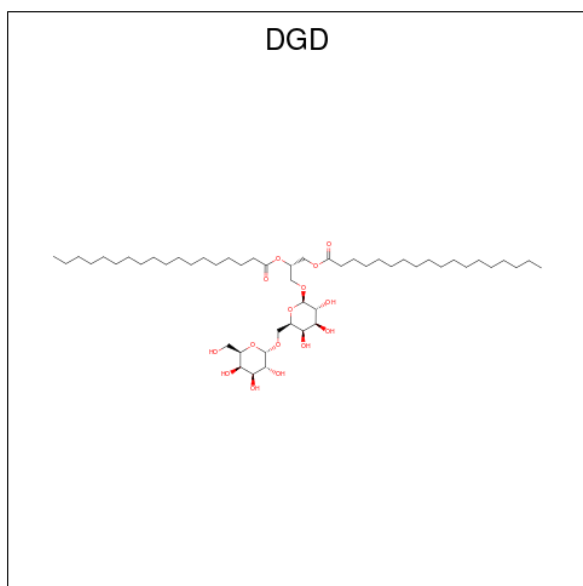
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
50	x	1	45	35	1	4	5	0
50	y	1	52	42	1	4	5	0
50	y	1	55	45	1	4	5	0
50	y	1	39	33	1	4	1	0
50	y	1	45	35	1	4	5	0
50	y	1	40	32	1	4	3	0
50	y	1	41	33	1	4	3	0
50	y	1	65	55	1	4	5	0
50	y	1	42	34	1	4	3	0
50	y	1	65	55	1	4	5	0
50	y	1	51	41	1	4	5	0
50	y	1	51	41	1	4	5	0
50	y	1	65	55	1	4	5	0
50	y	1	65	55	1	4	5	0
50	z	1	55	45	1	4	5	0
50	z	1	41	33	1	4	3	0
50	z	1	50	40	1	4	5	0
50	z	1	56	46	1	4	5	0
50	z	1	60	50	1	4	5	0
50	z	1	43	33	1	4	5	0
50	z	1	42	34	1	4	3	0

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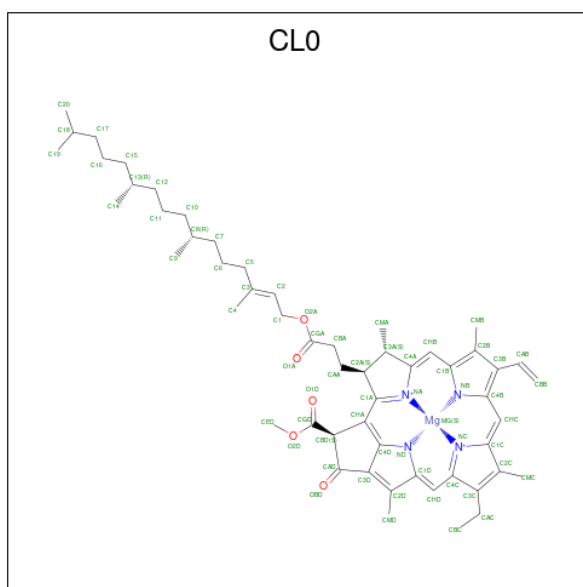
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
50	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
50	z	1	Total 55	C 45	Mg 1	N 4	O 5	0
50	z	1	Total 47	C 37	Mg 1	N 4	O 5	0
50	z	1	Total 42	C 34	Mg 1	N 4	O 3	0

- Molecule 51 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



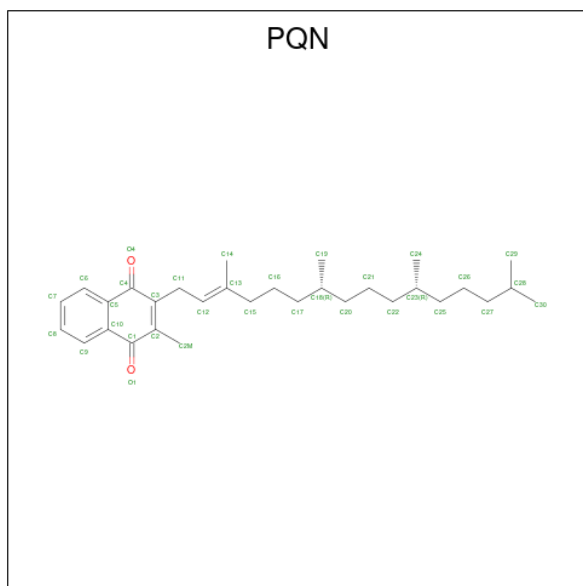
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
51	a	1	Total 66	C 51	O 15	0
51	b	1	Total 59	C 44	O 15	0
51	x	1	Total 48	C 33	O 15	0

- Molecule 52 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



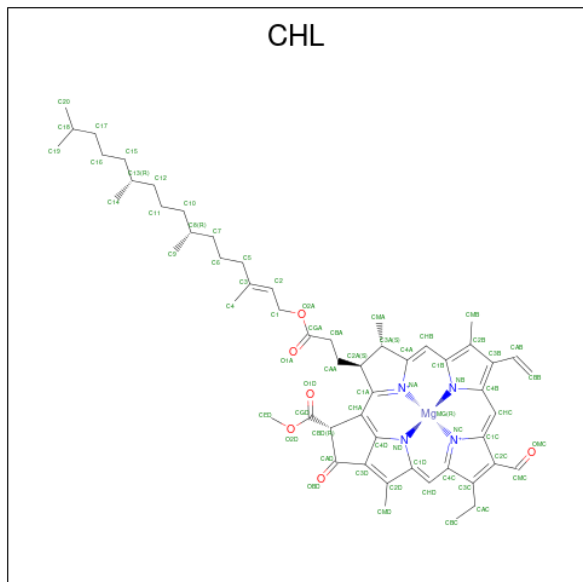
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
52	a	1	61	52	1	4	4	0

- Molecule 53 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



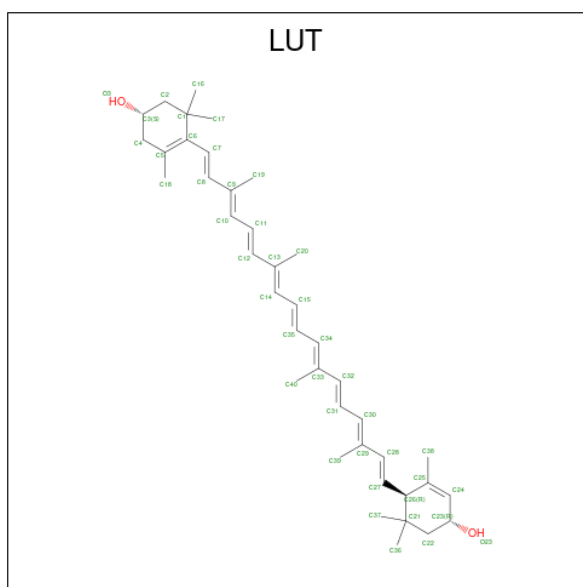
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
53	a	1	33	31	2	0
53	b	1	33	31	2	0

- Molecule 54 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
54	w	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
54	w	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	w	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
54	x	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	x	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
54	x	1	Total	C	Mg	N	O	0
			40	31	1	4	4	
54	x	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
54	z	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
54	z	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 55 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula:  $C_{40}H_{56}O_2$ ) (labeled as "Ligand of Interest" by depositor).

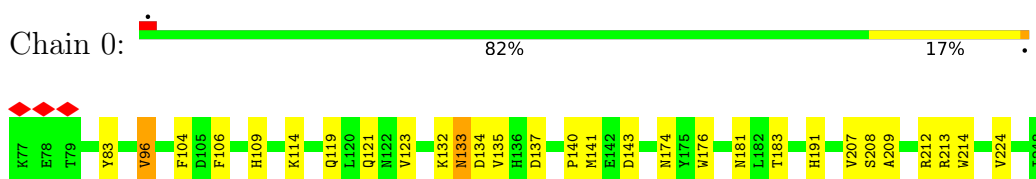


Mol	Chain	Residues	Atoms			AltConf
55	w	1	Total	C	O	0
			42	40	2	
55	w	1	Total	C	O	0
			42	40	2	
55	x	1	Total	C	O	0
			42	40	2	
55	x	1	Total	C	O	0
			42	40	2	
55	y	1	Total	C	O	0
			42	40	2	
55	y	1	Total	C	O	0
			42	40	2	
55	z	1	Total	C	O	0
			42	40	2	
55	z	1	Total	C	O	0
			42	40	2	

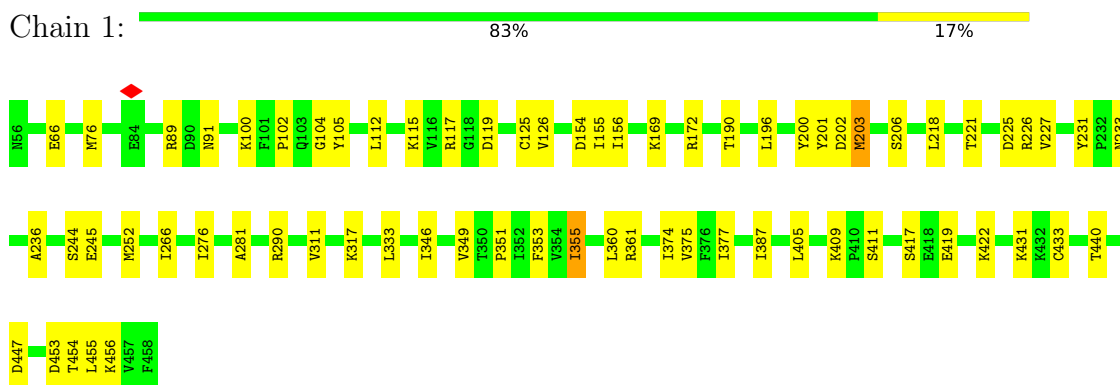
### 3 Residue-property plots [i](#)

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.

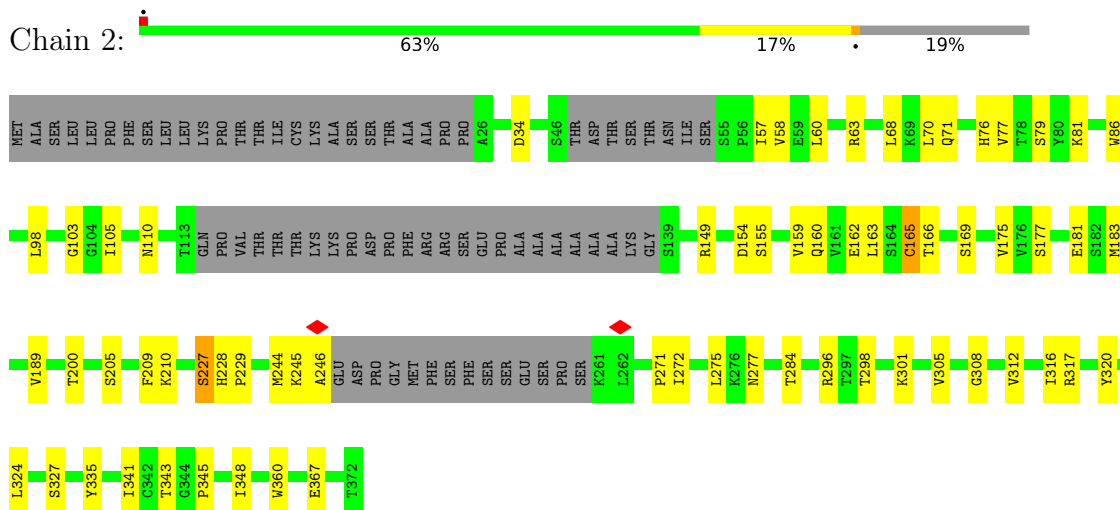
- Molecule 1: Photosynthetic NDH subunit of luminal location 1, chloroplactic



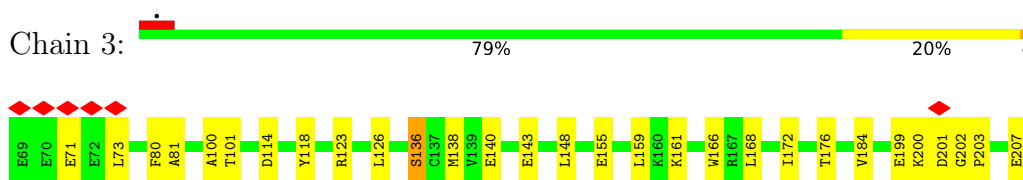
- Molecule 2: Photosynthetic NDH subunit of subcomplex B 1, chloroplactic



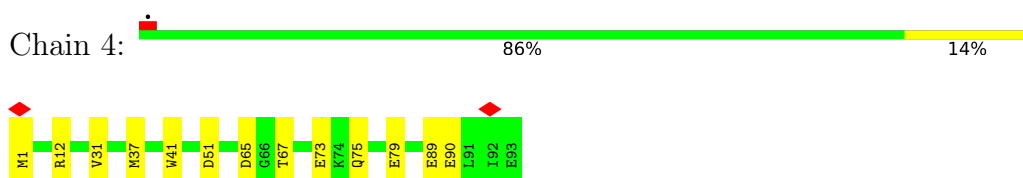
- Molecule 3: Photosynthetic NDH subunit of subcomplex B 2, chloroplactic



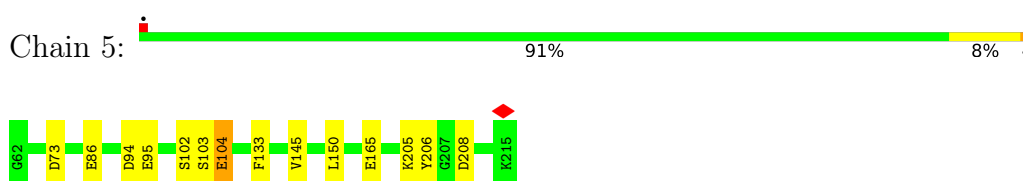
- Molecule 4: Photosynthetic NDH subunit of subcomplex B 3, chloroplactic



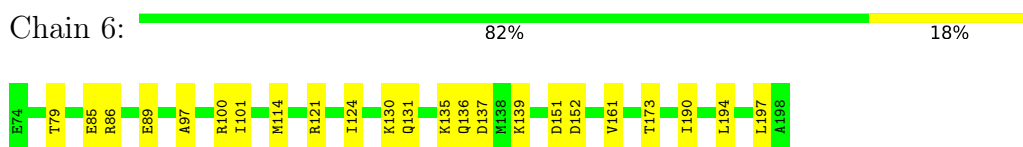
- Molecule 5: Photosynthetic NDH subunit of subcomplex B 4, chloroplactic



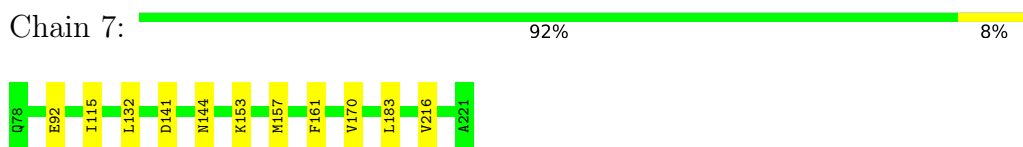
- Molecule 6: Photosynthetic NDH subunit of subcomplex B 5, chloroplactic



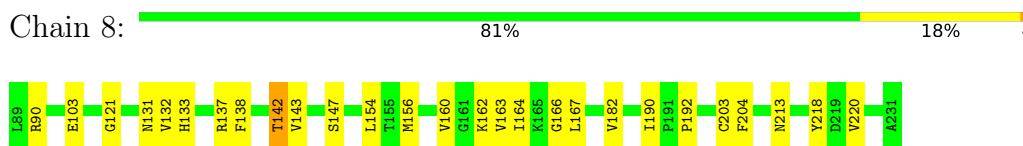
- Molecule 7: Photosynthetic NDH subunit of luminal location 2, chloroplactic



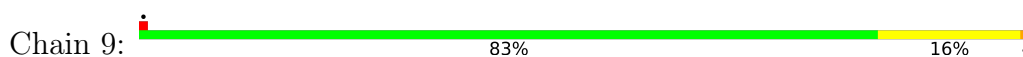
- Molecule 8: Photosynthetic NDH subunit of luminal location 3, chloroplactic



- Molecule 9: peptidylprolyl isomerase

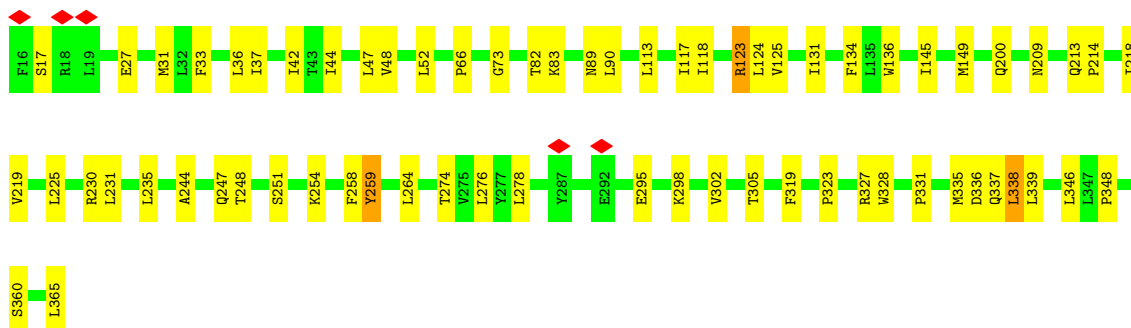
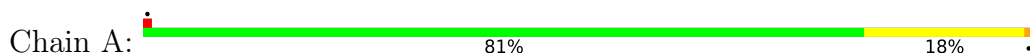


- Molecule 10: Peptidyl-prolyl cis-trans isomerase

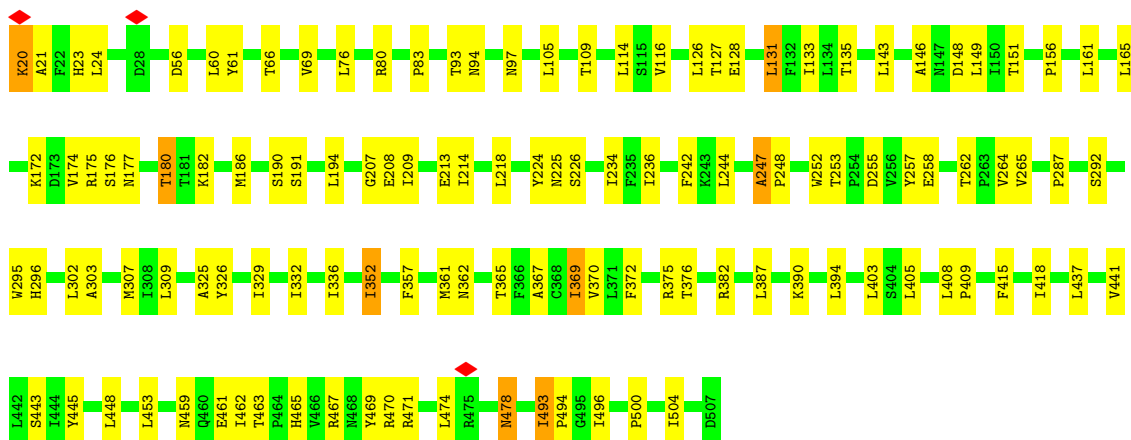
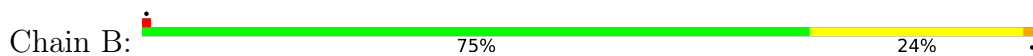




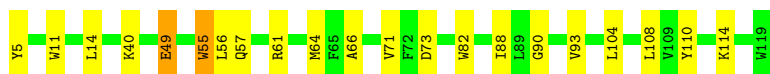
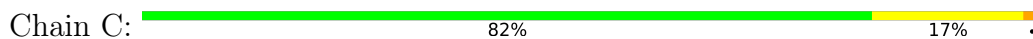
• Molecule 11: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic



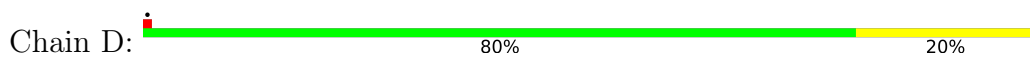
• Molecule 12: NAD(P)H-quinone oxidoreductase subunit 2 A, chloroplastic

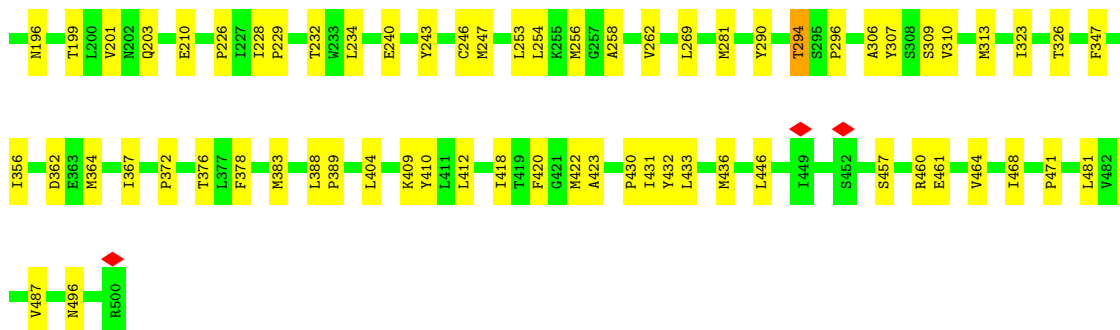


• Molecule 13: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic

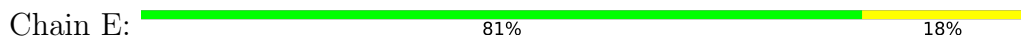


• Molecule 14: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic

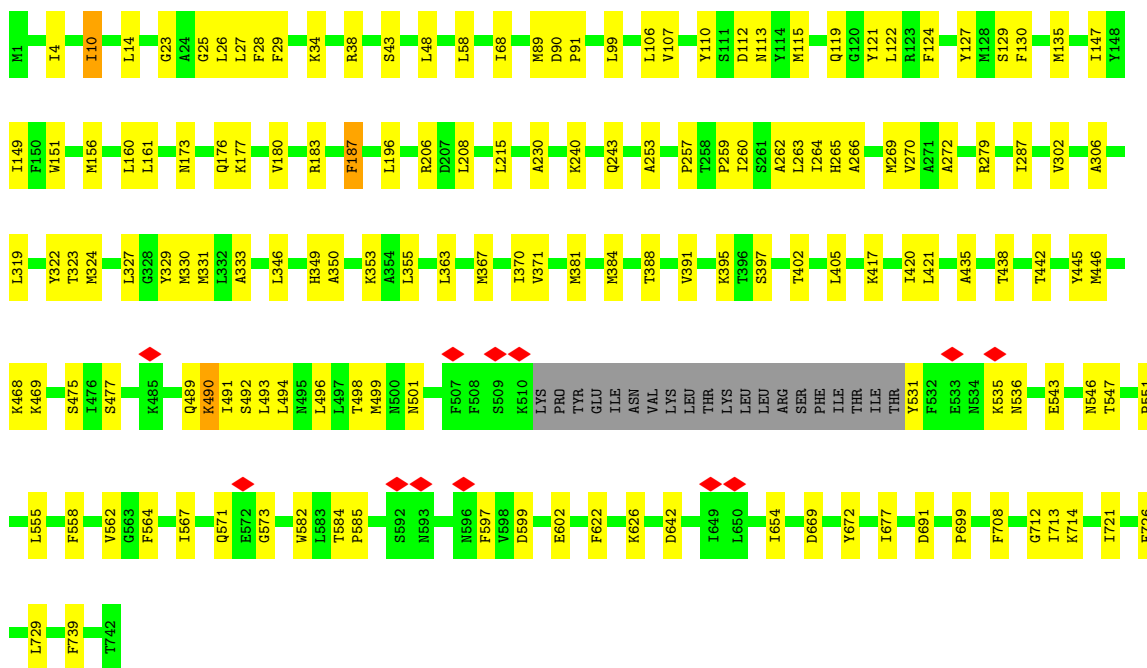
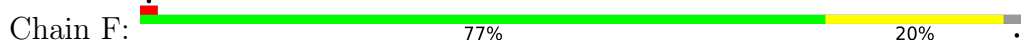




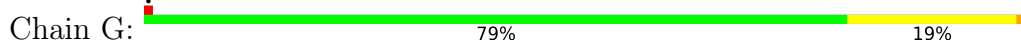
- Molecule 15: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic



- Molecule 16: NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic



- Molecule 17: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic





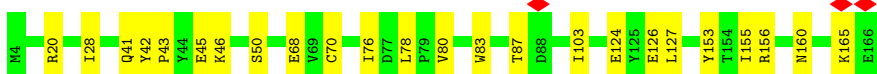
- Molecule 18: NAD(P)H-quinone oxidoreductase subunit H, chloroplactic

Chain H: 77% 18% 5%



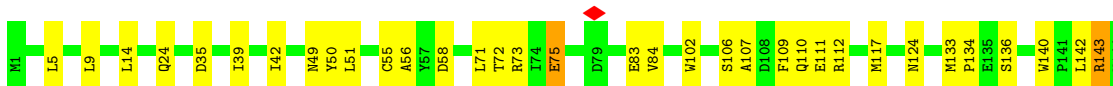
- Molecule 19: NAD(P)H-quinone oxidoreductase subunit I, chloroplactic

Chain I: 85% 15%



- Molecule 20: NAD(P)H-quinone oxidoreductase subunit J, chloroplactic

Chain J: 77% 22%



- Molecule 21: NAD(P)H-quinone oxidoreductase subunit K, chloroplactic

Chain K: 74% 23%

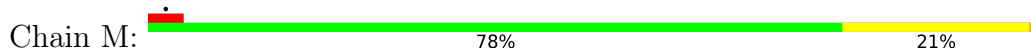


- Molecule 22: NAD(P)H-quinone oxidoreductase subunit L, chloroplactic

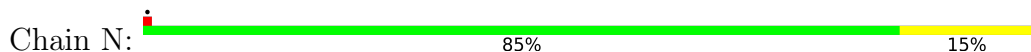
Chain L: 88% 11%



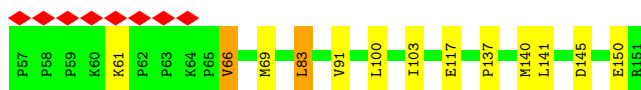
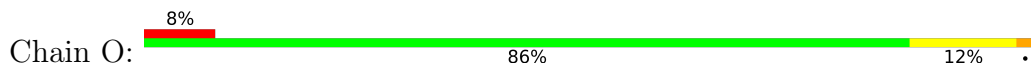
- Molecule 23: NAD(P)H-quinone oxidoreductase subunit M, chloroplastic



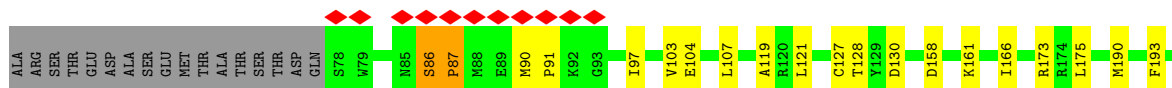
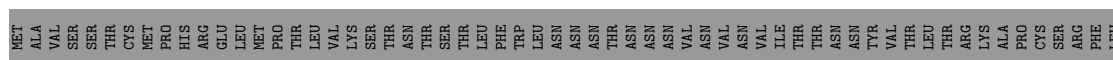
- Molecule 24: NAD(P)H-quinone oxidoreductase subunit N, chloroplastic



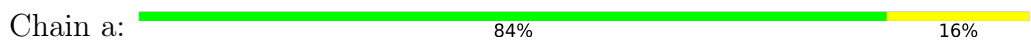
- Molecule 25: NAD(P)H-quinone oxidoreductase subunit O, chloroplastic

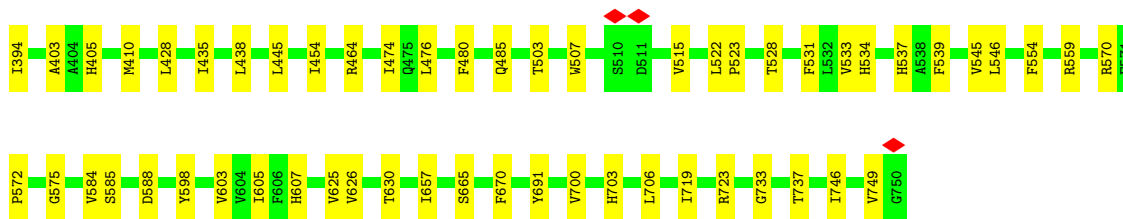


- Molecule 26: NAD(P)H-quinone oxidoreductase subunit U, chloroplastic



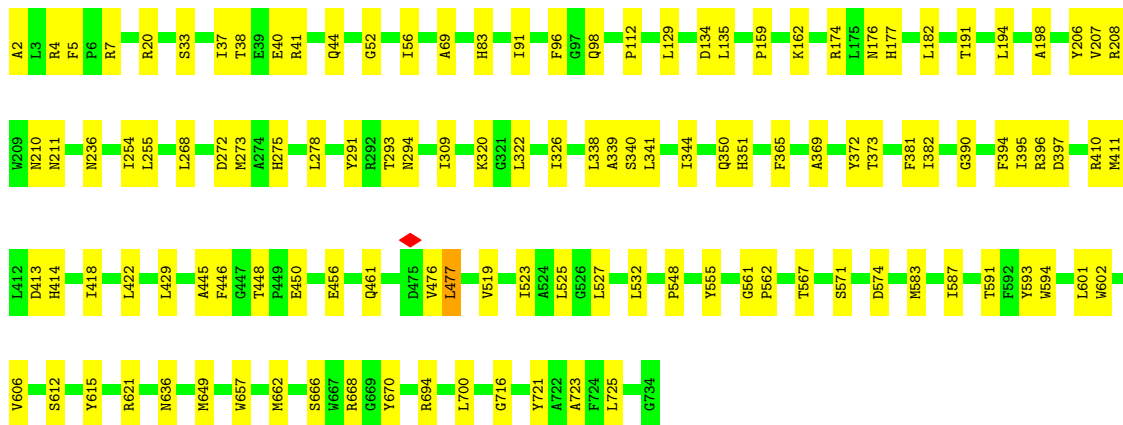
- Molecule 27: Photosystem I P700 chlorophyll a apoprotein A1





- Molecule 28: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 84% 16%



- Molecule 29: Photosystem I iron-sulfur center

Chain c: 85% 12%



- Molecule 30: Photosystem I reaction center subunit II, chloroplastic

Chain d: 83% 17%



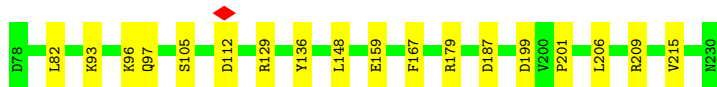
- Molecule 31: Photosystem I reaction center subunit IV, chloroplastic

Chain e: 6% 87% 13%

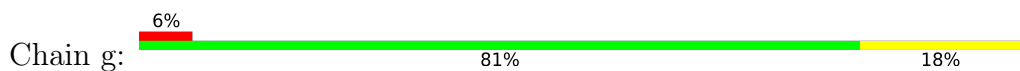


- Molecule 32: Photosystem I reaction center subunit III, chloroplastic

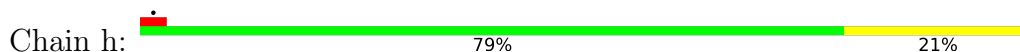
Chain f: 88% 12%



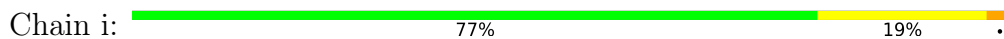
- Molecule 33: Photosystem I reaction center subunit V, chloroplastic



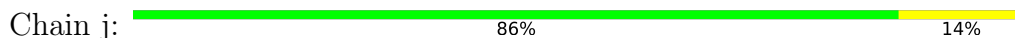
- Molecule 34: Photosystem I reaction center subunit VI, chloroplastic



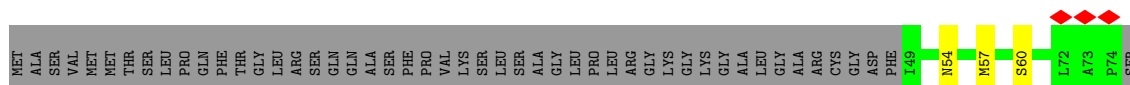
- Molecule 35: Photosystem I reaction center subunit VIII



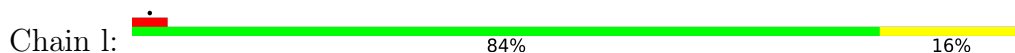
- Molecule 36: Photosystem I reaction center subunit IX

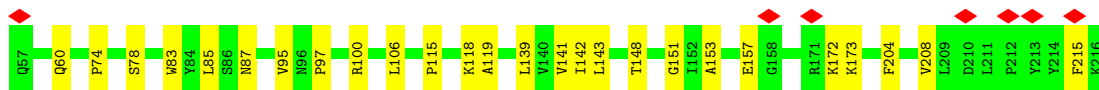


- Molecule 37: PSI-K

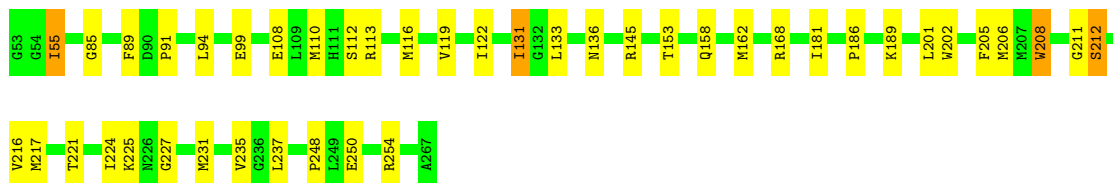
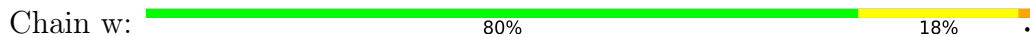


- Molecule 38: Photosystem I reaction center subunit XI, chloroplastic

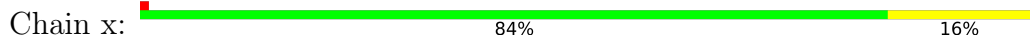




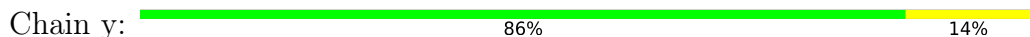
• Molecule 39: Chlorophyll a-b binding protein, chloroplastic



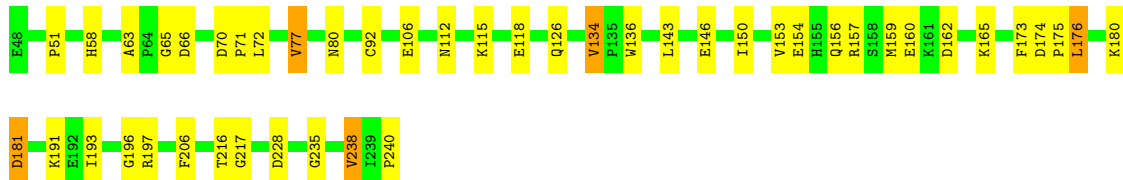
• Molecule 40: Chlorophyll a-b binding protein, chloroplastic



• Molecule 41: Chlorophyll a-b binding protein, chloroplastic



• Molecule 42: Chlorophyll a-b binding protein, chloroplastic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38385	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.744	Depositor
Minimum map value	-0.387	Depositor
Average map value	0.043	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, SQD, PGT, A1H1M, CHL, LUT, SF4, PQ9, CL0, LMG, DGD, CLA, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.15	0/1351	0.40	0/1831
2	1	0.13	0/3200	0.35	0/4340
3	2	0.13	0/2350	0.35	0/3186
4	3	0.15	0/1118	0.41	0/1512
5	4	0.17	0/777	0.38	0/1051
6	5	0.23	0/1301	0.44	0/1770
7	6	0.17	0/1075	0.40	0/1448
8	7	0.18	0/1178	0.38	0/1589
9	8	0.14	0/1101	0.34	0/1494
10	9	0.11	0/1352	0.35	1/1821 (0.1%)
11	A	0.21	0/2795	0.45	1/3810 (0.0%)
12	B	0.22	0/3890	0.48	0/5290
13	C	0.25	0/977	0.48	0/1333
14	D	0.16	0/4072	0.36	0/5535
15	E	0.18	0/791	0.42	0/1070
16	F	0.20	0/5965	0.43	1/8100 (0.0%)
17	G	0.17	0/1388	0.37	0/1893
18	H	0.17	0/3081	0.39	0/4170
19	I	0.15	0/1357	0.38	0/1839
20	J	0.13	0/1369	0.32	0/1862
21	K	0.18	0/1633	0.44	0/2212
22	L	0.17	0/975	0.43	0/1328
23	M	0.20	0/1193	0.46	0/1611
24	N	0.13	0/1363	0.33	0/1852
25	O	0.16	0/811	0.42	0/1100
26	U	0.22	0/1297	0.61	4/1764 (0.2%)
27	a	0.13	0/6024	0.31	0/8220
28	b	0.13	0/6067	0.31	0/8282
29	c	0.13	0/636	0.34	0/860
30	d	0.14	0/1162	0.37	0/1569
31	e	0.15	0/559	0.36	0/757
32	f	0.14	0/1239	0.30	0/1671

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	g	0.14	0/779	0.35	0/1055
34	h	0.13	0/758	0.32	0/1029
35	i	0.17	0/251	0.38	0/339
36	j	0.14	0/357	0.31	0/484
37	k	0.10	0/467	0.27	0/630
38	l	0.15	0/1235	0.35	0/1685
39	w	0.20	0/1750	0.45	0/2389
40	x	0.14	0/1619	0.32	0/2206
41	y	0.17	0/1768	0.39	0/2400
42	z	0.15	0/1546	0.35	1/2104 (0.0%)
All	All	0.17	0/73977	0.39	8/100491 (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
11	A	0	1
18	H	0	1
21	K	0	2
39	w	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U	91	PRO	N-CA-CB	13.58	110.53	102.92
26	U	87	PRO	N-CA-CB	8.01	111.67	103.25
10	9	80	PRO	N-CA-CB	6.78	110.46	103.00
11	A	258	PHE	CA-CB-CG	6.34	120.14	113.80
16	F	499	MET	CA-CB-CG	6.20	126.51	114.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	A	123	ARG	Sidechain
18	H	195	ARG	Sidechain
21	K	139	CYS	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
21	K	91	ARG	Sidechain
39	w	212	SER	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	0	1317	0	1268	16	0
2	1	3133	0	3096	43	0
3	2	2305	0	2298	37	0
4	3	1093	0	1078	18	0
5	4	756	0	700	15	0
6	5	1258	0	1147	11	0
7	6	1048	0	1020	19	0
8	7	1156	0	1172	6	0
9	8	1075	0	1051	16	0
10	9	1326	0	1307	16	0
11	A	2728	0	2807	53	0
12	B	3799	0	3881	88	0
13	C	944	0	951	21	0
14	D	3955	0	4064	68	0
15	E	780	0	824	17	0
16	F	5796	0	5847	113	0
17	G	1357	0	1415	32	0
18	H	3008	0	3025	57	0
19	I	1329	0	1310	17	0
20	J	1324	0	1283	21	0
21	K	1597	0	1619	42	0
22	L	936	0	930	10	0
23	M	1169	0	1155	24	0
24	N	1323	0	1334	16	0
25	O	786	0	789	7	0
26	U	1266	0	1182	15	0
27	a	5827	0	5685	90	0
28	b	5855	0	5629	89	0
29	c	623	0	602	10	0
30	d	1132	0	1145	17	0
31	e	546	0	555	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	f	1211	0	1236	14	0
33	g	759	0	736	13	0
34	h	737	0	733	18	0
35	i	244	0	262	7	0
36	j	345	0	347	6	0
37	k	462	0	474	7	0
38	l	1200	0	1208	22	0
39	w	1689	0	1617	45	0
40	x	1568	0	1516	32	0
41	y	1713	0	1679	51	0
42	z	1498	0	1471	48	0
43	4	40	0	56	4	0
43	a	255	0	348	18	0
43	b	280	0	392	22	0
43	f	40	0	56	2	0
43	g	40	0	56	2	0
43	i	40	0	56	2	0
43	j	80	0	112	10	0
43	k	80	0	112	0	0
43	l	120	0	168	5	0
43	w	40	0	56	1	0
43	x	40	0	55	1	0
43	y	40	0	56	1	0
43	z	40	0	55	1	0
44	5	35	0	40	2	0
44	A	151	0	185	3	0
44	B	157	0	200	6	0
44	D	34	0	38	1	0
44	F	43	0	59	0	0
44	I	44	0	61	0	0
44	L	40	0	50	2	0
44	N	26	0	22	2	0
44	a	111	0	132	6	0
44	b	87	0	117	2	0
44	f	39	0	48	0	0
44	w	40	0	53	1	0
44	z	124	0	164	9	0
45	5	38	0	0	0	0
45	F	38	0	0	6	0
46	7	41	0	52	0	0
46	B	37	0	44	1	0
46	D	34	0	38	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	F	28	0	26	2	0
46	H	33	0	36	1	0
46	f	34	0	38	1	0
46	j	71	0	82	3	0
46	w	40	0	50	2	0
46	x	48	0	66	4	0
46	z	76	0	92	7	0
47	A	36	0	45	15	0
48	B	40	0	44	10	0
48	F	84	0	96	18	0
48	a	36	0	36	3	0
48	j	42	0	51	0	0
48	w	72	0	72	15	0
49	I	16	0	0	1	0
49	K	8	0	0	0	0
49	a	8	0	0	0	0
49	c	16	0	0	0	0
50	a	2583	0	2598	106	0
50	b	2314	0	2287	91	0
50	f	140	0	113	3	0
50	g	144	0	115	4	0
50	h	46	0	33	2	0
50	j	42	0	31	0	0
50	k	140	0	108	5	0
50	l	145	0	116	5	0
50	w	526	0	461	29	0
50	x	608	0	518	19	0
50	y	676	0	603	40	0
50	z	532	0	432	26	0
51	a	66	0	96	2	0
51	b	59	0	79	3	0
51	x	48	0	54	2	0
52	a	61	0	62	0	0
53	a	33	0	46	1	0
53	b	33	0	46	3	0
54	w	135	0	88	13	0
54	x	179	0	115	9	0
54	z	103	0	84	7	0
55	w	84	0	112	30	0
55	x	84	0	112	21	0
55	y	84	0	112	60	0
55	z	84	0	112	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	83864	0	83596	1415	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 8.

The worst 5 of 1415 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)
50:y:302:CLA:H42	55:y:315:LUT:C37	1.52	1.37
41:y:240:TYR:CE1	55:y:315:LUT:H162	1.60	1.34
42:z:174:ASP:HA	55:z:320:LUT:O23	1.30	1.30
11:A:259:TYR:CE2	47:A:405:PQ9:H161	1.65	1.29
11:A:259:TYR:CD2	47:A:405:PQ9:H161	1.74	1.21

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	155/157 (99%)	152 (98%)	3 (2%)	0	100	100
2	1	401/403 (100%)	393 (98%)	8 (2%)	0	100	100
3	2	292/372 (78%)	286 (98%)	5 (2%)	1 (0%)	36	68
4	3	137/139 (99%)	129 (94%)	8 (6%)	0	100	100
5	4	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
6	5	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
7	6	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
8	7	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
9	8	141/143 (99%)	136 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	9	172/174 (99%)	167 (97%)	5 (3%)	0	100	100
11	A	348/350 (99%)	340 (98%)	8 (2%)	0	100	100
12	B	486/488 (100%)	453 (93%)	32 (7%)	1 (0%)	43	73
13	C	113/115 (98%)	103 (91%)	9 (8%)	1 (1%)	14	47
14	D	496/498 (100%)	483 (97%)	12 (2%)	1 (0%)	43	73
15	E	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
16	F	718/742 (97%)	683 (95%)	33 (5%)	2 (0%)	36	68
17	G	174/176 (99%)	165 (95%)	9 (5%)	0	100	100
18	H	367/389 (94%)	352 (96%)	15 (4%)	0	100	100
19	I	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
20	J	156/158 (99%)	152 (97%)	4 (3%)	0	100	100
21	K	200/202 (99%)	189 (94%)	8 (4%)	3 (2%)	8	37
22	L	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
23	M	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18	52
24	N	163/165 (99%)	156 (96%)	6 (4%)	1 (1%)	21	56
25	O	93/95 (98%)	90 (97%)	1 (1%)	2 (2%)	5	29
26	U	161/240 (67%)	151 (94%)	7 (4%)	3 (2%)	6	33
27	a	740/742 (100%)	721 (97%)	19 (3%)	0	100	100
28	b	731/733 (100%)	716 (98%)	15 (2%)	0	100	100
29	c	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
30	d	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
31	e	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
32	f	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
33	g	95/97 (98%)	91 (96%)	2 (2%)	2 (2%)	5	31
34	h	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
35	i	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
36	j	40/42 (95%)	40 (100%)	0	0	100	100
37	k	62/130 (48%)	61 (98%)	1 (2%)	0	100	100
38	l	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
39	w	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
40	x	196/198 (99%)	194 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	y	219/221 (99%)	214 (98%)	5 (2%)	0	100	100
42	z	191/193 (99%)	188 (98%)	3 (2%)	0	100	100
All	All	8990/9337 (96%)	8691 (97%)	281 (3%)	18 (0%)	44	73

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	F	501	ASN
21	K	140	PRO
23	M	94	LEU
25	O	61	LYS
26	U	86	SER

### 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	0	143/143 (100%)	140 (98%)	3 (2%)	47	71
2	1	340/340 (100%)	334 (98%)	6 (2%)	51	74
3	2	260/321 (81%)	253 (97%)	7 (3%)	39	68
4	3	120/120 (100%)	116 (97%)	4 (3%)	33	65
5	4	76/76 (100%)	76 (100%)	0	100	100
6	5	131/131 (100%)	127 (97%)	4 (3%)	35	66
7	6	112/112 (100%)	112 (100%)	0	100	100
8	7	123/123 (100%)	120 (98%)	3 (2%)	43	70
9	8	114/115 (99%)	112 (98%)	2 (2%)	51	74
10	9	143/144 (99%)	138 (96%)	5 (4%)	32	64
11	A	296/304 (97%)	289 (98%)	7 (2%)	43	70
12	B	424/424 (100%)	408 (96%)	16 (4%)	29	62
13	C	99/99 (100%)	96 (97%)	3 (3%)	36	66
14	D	430/430 (100%)	421 (98%)	9 (2%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	E	86/86 (100%)	83 (96%)	3 (4%)	32	64
16	F	626/652 (96%)	614 (98%)	12 (2%)	50	73
17	G	153/153 (100%)	148 (97%)	5 (3%)	33	65
18	H	321/339 (95%)	318 (99%)	3 (1%)	70	81
19	I	150/150 (100%)	147 (98%)	3 (2%)	48	72
20	J	140/140 (100%)	135 (96%)	5 (4%)	31	63
21	K	180/180 (100%)	173 (96%)	7 (4%)	28	62
22	L	99/99 (100%)	94 (95%)	5 (5%)	21	54
23	M	129/129 (100%)	127 (98%)	2 (2%)	55	75
24	N	139/139 (100%)	138 (99%)	1 (1%)	76	83
25	O	87/87 (100%)	83 (95%)	4 (5%)	24	58
26	U	127/212 (60%)	124 (98%)	3 (2%)	43	70
27	a	598/598 (100%)	586 (98%)	12 (2%)	48	72
28	b	599/599 (100%)	591 (99%)	8 (1%)	61	78
29	c	71/71 (100%)	69 (97%)	2 (3%)	38	68
30	d	122/122 (100%)	119 (98%)	3 (2%)	42	69
31	e	60/60 (100%)	60 (100%)	0	100	100
32	f	126/126 (100%)	125 (99%)	1 (1%)	73	82
33	g	82/82 (100%)	82 (100%)	0	100	100
34	h	79/79 (100%)	79 (100%)	0	100	100
35	i	27/27 (100%)	26 (96%)	1 (4%)	30	63
36	j	37/37 (100%)	37 (100%)	0	100	100
37	k	49/97 (50%)	48 (98%)	1 (2%)	48	72
38	l	123/123 (100%)	122 (99%)	1 (1%)	73	82
39	w	177/177 (100%)	171 (97%)	6 (3%)	32	64
40	x	166/166 (100%)	164 (99%)	2 (1%)	63	79
41	y	173/173 (100%)	173 (100%)	0	100	100
42	z	154/154 (100%)	148 (96%)	6 (4%)	28	62
All	All	7691/7939 (97%)	7526 (98%)	165 (2%)	46	71

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	O	66	VAL
29	c	73	THR
26	U	128	THR
27	a	626	VAL
38	l	60	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
27	a	214	GLN
30	d	112	GLN
27	a	721	GLN
28	b	333	GLN
33	g	107	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

248 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
55	LUT	y	316	-	42,43,43	0.87	0	51,60,60	0.77	1 (1%)
43	BCR	l	302	-	41,41,41	0.66	0	56,56,56	1.04	3 (5%)
54	CHL	z	312	42	55,69,74	2.04	12 (21%)	52,108,114	2.66	19 (36%)
50	CLA	a	856	-	68,72,73	1.20	7 (10%)	80,111,113	1.46	9 (11%)
46	LMG	f	306	-	34,34,55	1.01	1 (2%)	42,42,63	1.15	2 (4%)
51	DGD	a	804	-	67,67,67	1.01	2 (2%)	81,81,81	1.00	1 (1%)
50	CLA	a	824	-	69,73,73	1.23	6 (8%)	82,113,113	1.68	9 (10%)
44	PGT	B	602	-	41,41,50	0.53	0	44,47,56	0.45	0
50	CLA	x	306	-	64,68,73	1.28	7 (10%)	76,107,113	1.66	9 (11%)
43	BCR	b	816	-	41,41,41	0.69	0	56,56,56	1.17	6 (10%)
43	BCR	y	301	-	41,41,41	0.67	0	56,56,56	1.06	3 (5%)
50	CLA	w	302	-	54,58,73	1.40	8 (14%)	64,95,113	1.78	7 (10%)
44	PGT	a	805	-	31,31,50	0.60	0	34,37,56	0.57	0
50	CLA	y	302	41	56,60,73	1.44	11 (19%)	69,97,113	2.09	13 (18%)
50	CLA	a	815	27	69,73,73	1.23	9 (13%)	82,113,113	1.65	8 (9%)
50	CLA	b	811	-	49,53,73	1.41	7 (14%)	58,89,113	1.77	7 (12%)
50	CLA	a	834	-	69,73,73	1.23	7 (10%)	82,113,113	1.60	6 (7%)
51	DGD	x	317	-	49,49,67	1.11	0	63,63,81	1.04	1 (1%)
50	CLA	g	203	-	56,60,73	1.36	7 (12%)	65,97,113	1.66	8 (12%)
44	PGT	5	301	-	34,34,50	0.58	0	37,40,56	0.59	0
46	LMG	j	105	-	37,37,55	0.95	1 (2%)	45,45,63	1.07	1 (2%)
43	BCR	w	301	-	41,41,41	0.64	0	56,56,56	1.06	4 (7%)
43	BCR	a	810	-	30,30,41	0.88	1 (3%)	39,39,56	1.34	5 (12%)
50	CLA	b	807	-	69,73,73	1.22	6 (8%)	82,113,113	1.66	8 (9%)
50	CLA	b	810	-	54,58,73	1.39	6 (11%)	64,95,113	1.74	6 (9%)
50	CLA	y	310	41	69,73,73	1.22	6 (8%)	82,113,113	1.66	9 (10%)
46	LMG	H	401	-	33,33,55	1.06	2 (6%)	41,41,63	1.26	4 (9%)
50	CLA	a	823	-	59,63,73	1.32	7 (11%)	70,101,113	1.68	7 (10%)
43	BCR	a	827	-	40,40,41	0.69	0	54,54,56	1.14	5 (9%)
50	CLA	b	823	-	59,63,73	1.33	7 (11%)	70,101,113	1.68	8 (11%)
50	CLA	b	849	-	54,58,73	1.40	8 (14%)	64,95,113	1.75	7 (10%)
43	BCR	a	829	-	41,41,41	0.76	0	56,56,56	1.17	6 (10%)
50	CLA	z	307	42	64,68,73	1.29	8 (12%)	76,107,113	1.67	7 (9%)
50	CLA	x	308	-	54,58,73	1.38	6 (11%)	64,95,113	1.80	9 (14%)
50	CLA	y	308	-	69,73,73	1.24	7 (10%)	82,113,113	1.65	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	SF4	K	301	21	0,12,12	-	-	-	-	-
50	CLA	b	808	-	47,51,73	1.39	7 (14%)	55,86,113	1.78	5 (9%)
43	BCR	b	820	-	41,41,41	0.70	0	56,56,56	1.15	6 (10%)
46	LMG	F	802	-	28,28,55	1.09	2 (7%)	36,36,63	1.16	2 (5%)
50	CLA	y	307	-	45,49,73	1.44	8 (17%)	54,84,113	2.06	6 (11%)
50	CLA	b	838	-	56,60,73	1.37	7 (12%)	65,97,113	1.79	8 (12%)
50	CLA	b	848	-	46,50,73	1.42	7 (15%)	53,85,113	1.88	6 (11%)
50	CLA	a	846	-	69,73,73	1.24	7 (10%)	82,113,113	1.68	9 (10%)
50	CLA	y	314	41	69,73,73	1.24	8 (11%)	82,113,113	1.58	10 (12%)
50	CLA	z	316	44	51,55,73	1.38	7 (13%)	60,91,113	1.73	6 (10%)
50	CLA	a	812	-	60,66,73	1.79	9 (15%)	69,101,113	2.08	11 (15%)
44	PGT	B	606	-	34,34,50	0.54	0	37,40,56	0.74	1 (2%)
50	CLA	l	301	-	49,53,73	1.42	7 (14%)	58,89,113	1.79	6 (10%)
50	CLA	w	308	39	69,73,73	1.23	5 (7%)	82,113,113	1.69	11 (13%)
50	CLA	b	805	28	69,73,73	1.23	6 (8%)	82,113,113	1.69	10 (12%)
45	A1H1M	5	302	-	41,41,41	1.07	3 (7%)	58,58,58	1.91	13 (22%)
44	PGT	b	830	50	38,38,50	0.55	0	41,44,56	0.51	0
50	CLA	b	847	-	64,68,73	1.28	6 (9%)	76,107,113	1.74	9 (11%)
50	CLA	b	851	-	51,55,73	1.38	7 (13%)	60,91,113	1.77	7 (11%)
50	CLA	f	301	-	61,65,73	1.30	6 (9%)	72,103,113	1.78	9 (12%)
50	CLA	f	303	-	45,49,73	1.44	8 (17%)	54,84,113	1.83	7 (12%)
50	CLA	x	312	40	69,73,73	1.23	7 (10%)	82,113,113	1.60	9 (10%)
46	LMG	w	312	-	40,40,55	0.94	1 (2%)	48,48,63	1.11	2 (4%)
50	CLA	a	842	-	69,73,73	1.23	6 (8%)	82,113,113	1.57	9 (10%)
49	SF4	I	202	19	0,12,12	-	-	-	-	-
50	CLA	b	814	-	69,73,73	1.25	7 (10%)	82,113,113	1.73	10 (12%)
50	CLA	z	308	-	44,50,73	1.54	9 (20%)	47,82,113	2.12	7 (14%)
50	CLA	a	849	-	69,73,73	1.24	6 (8%)	82,113,113	1.56	10 (12%)
54	CHL	w	311	-	41,55,74	2.14	10 (24%)	34,90,114	3.29	15 (44%)
50	CLA	f	302	-	46,50,73	1.41	6 (13%)	53,85,113	1.90	5 (9%)
44	PGT	D	602	-	33,33,50	0.57	0	36,39,56	0.62	0
50	CLA	b	826	-	59,63,73	1.33	7 (11%)	70,101,113	1.75	8 (11%)
50	CLA	a	826	44	49,53,73	1.40	7 (14%)	58,89,113	1.75	6 (10%)
54	CHL	x	305	-	40,54,74	2.26	11 (27%)	34,90,114	3.26	17 (50%)
50	CLA	a	848	-	56,60,73	1.36	6 (10%)	65,97,113	1.70	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	CLA	z	309	-	46,50,73	1.41	7 (15%)	53,85,113	1.79	4 (7%)
50	CLA	w	303	39	49,53,73	1.41	8 (16%)	58,89,113	1.81	7 (12%)
50	CLA	x	316	-	49,53,73	1.41	6 (12%)	58,89,113	1.77	5 (8%)
50	CLA	a	801	-	69,73,73	1.23	6 (8%)	82,113,113	1.63	7 (8%)
46	LMG	x	315	-	48,48,55	0.83	2 (4%)	56,56,63	1.10	2 (3%)
50	CLA	a	811	-	69,73,73	1.23	6 (8%)	82,113,113	1.66	9 (10%)
46	LMG	z	314	-	40,40,55	1.11	4 (10%)	48,48,63	1.07	1 (2%)
55	LUT	x	320	-	42,43,43	0.86	0	51,60,60	0.56	0
55	LUT	x	321	-	42,43,43	0.87	0	51,60,60	0.86	2 (3%)
50	CLA	b	844	28	69,73,73	1.23	7 (10%)	82,113,113	1.63	9 (10%)
44	PGT	z	301	-	44,44,50	0.51	0	47,50,56	0.51	0
50	CLA	y	305	41	49,53,73	1.41	6 (12%)	58,89,113	1.76	5 (8%)
43	BCR	b	819	-	41,41,41	0.75	1 (2%)	56,56,56	1.26	6 (10%)
43	BCR	g	202	-	41,41,41	0.72	0	56,56,56	1.01	3 (5%)
43	BCR	f	304	-	41,41,41	0.69	1 (2%)	56,56,56	1.05	5 (8%)
50	CLA	x	302	-	45,49,73	1.44	8 (17%)	54,84,113	1.94	9 (16%)
50	CLA	z	306	42	60,64,73	1.30	6 (10%)	71,102,113	1.78	12 (16%)
50	CLA	x	318	-	47,53,73	1.34	5 (10%)	54,88,113	1.86	6 (11%)
50	CLA	z	310	42	45,49,73	1.42	7 (15%)	54,84,113	1.94	9 (16%)
50	CLA	k	205	-	46,50,73	1.40	6 (13%)	53,85,113	1.84	7 (13%)
43	BCR	j	101	-	41,41,41	0.73	0	56,56,56	1.17	3 (5%)
43	BCR	a	830	-	41,41,41	0.70	0	56,56,56	1.04	4 (7%)
50	CLA	x	304	40	51,55,73	1.37	5 (9%)	60,91,113	1.73	6 (10%)
50	CLA	a	858	-	69,73,73	1.22	6 (8%)	82,113,113	1.49	8 (9%)
44	PGT	b	829	-	47,47,50	0.50	0	50,53,56	0.45	0
50	CLA	b	837	-	69,73,73	1.23	7 (10%)	82,113,113	1.66	7 (8%)
43	BCR	4	101	-	41,41,41	0.66	0	56,56,56	1.21	4 (7%)
43	BCR	b	817	-	41,41,41	0.69	0	56,56,56	1.19	6 (10%)
50	CLA	b	828	-	64,68,73	1.29	7 (10%)	76,107,113	1.59	8 (10%)
50	CLA	b	840	-	69,73,73	1.22	6 (8%)	82,113,113	1.62	7 (8%)
50	CLA	w	306	39	69,73,73	1.24	8 (11%)	82,113,113	1.60	9 (10%)
44	PGT	z	317	50	45,45,50	0.51	0	48,51,56	0.48	0
49	SF4	I	201	19	0,12,12	-	-	-	-	-
50	CLA	a	819	-	64,68,73	1.28	7 (10%)	76,107,113	1.65	8 (10%)
50	CLA	a	841	-	59,63,73	1.33	6 (10%)	70,101,113	1.69	7 (10%)
43	BCR	b	831	-	41,41,41	0.65	0	56,56,56	1.35	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	PQ9	A	405	-	36,36,45	2.92	20 (55%)	44,46,57	10.90	22 (50%)
50	CLA	b	841	-	59,63,73	1.33	8 (13%)	70,101,113	1.76	7 (10%)
54	CHL	w	304	-	40,53,74	2.39	12 (30%)	35,89,114	3.21	17 (48%)
49	SF4	c	101	29	0,12,12	-	-	-	-	-
50	CLA	x	307	40	64,68,73	1.27	8 (12%)	76,107,113	1.72	9 (11%)
53	PQN	a	825	-	34,34,34	1.02	3 (8%)	43,45,45	1.76	10 (23%)
50	CLA	a	821	-	67,71,73	1.27	8 (11%)	81,110,113	1.88	10 (12%)
50	CLA	a	814	-	69,73,73	1.23	6 (8%)	82,113,113	1.67	8 (9%)
50	CLA	w	316	39	54,58,73	1.37	6 (11%)	64,95,113	1.88	9 (14%)
50	CLA	z	302	-	59,63,73	1.33	7 (11%)	70,101,113	1.68	8 (11%)
54	CHL	x	311	-	34,48,74	2.39	9 (26%)	32,82,114	2.95	12 (37%)
55	LUT	y	315	-	42,43,43	0.89	0	51,60,60	0.62	0
50	CLA	z	303	-	45,49,73	1.45	8 (17%)	54,84,113	1.76	8 (14%)
44	PGT	I	203	-	43,43,50	0.52	0	46,49,56	0.48	0
50	CLA	w	307	-	49,53,73	1.44	7 (14%)	58,89,113	1.71	6 (10%)
50	CLA	a	852	-	55,59,73	1.36	6 (10%)	64,96,113	1.77	8 (12%)
50	CLA	a	843	-	69,73,73	1.24	7 (10%)	82,113,113	1.66	9 (10%)
50	CLA	b	839	-	69,73,73	1.23	7 (10%)	82,113,113	1.63	9 (10%)
43	BCR	l	303	-	41,41,41	0.65	0	56,56,56	1.22	5 (8%)
50	CLA	a	844	-	61,65,73	1.30	6 (9%)	72,103,113	1.64	10 (13%)
50	CLA	b	803	-	69,73,73	1.23	6 (8%)	82,113,113	1.78	10 (12%)
44	PGT	f	305	-	38,38,50	0.54	0	41,44,56	0.51	0
50	CLA	b	822	-	62,66,73	1.30	7 (11%)	73,104,113	1.72	8 (10%)
50	CLA	a	833	-	69,73,73	1.23	7 (10%)	82,113,113	1.58	11 (13%)
50	CLA	a	820	-	69,73,73	1.21	7 (10%)	82,113,113	1.59	10 (12%)
50	CLA	b	804	-	45,49,73	1.43	7 (15%)	54,84,113	1.81	8 (14%)
50	CLA	b	832	-	58,62,73	1.34	6 (10%)	68,99,113	1.72	8 (11%)
44	PGT	a	806	50	32,32,50	0.60	0	35,38,56	0.54	0
55	LUT	w	319	-	42,43,43	0.83	0	51,60,60	0.94	2 (3%)
44	PGT	A	403	-	37,37,50	0.32	0	40,43,56	0.38	0
44	PGT	w	313	50	39,39,50	0.54	0	42,45,56	0.51	0
55	LUT	w	320	-	42,43,43	0.78	0	51,60,60	0.69	1 (1%)
46	LMG	D	601	-	34,34,55	1.00	1 (2%)	42,42,63	1.14	3 (7%)
53	PQN	b	827	-	34,34,34	1.03	3 (8%)	43,45,45	1.82	10 (23%)
50	CLA	b	836	-	69,73,73	1.23	7 (10%)	82,113,113	1.62	9 (10%)
49	SF4	c	102	29	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	CLA	w	310	-	69,73,73	1.24	6 (8%)	82,113,113	1.72	15 (18%)
50	CLA	a	851	27	50,54,73	1.40	7 (14%)	59,90,113	1.78	6 (10%)
43	BCR	b	818	-	41,41,41	0.68	0	56,56,56	1.04	3 (5%)
50	CLA	a	850	-	69,73,73	1.22	6 (8%)	82,113,113	1.55	9 (10%)
50	CLA	w	305	-	55,59,73	1.37	7 (12%)	64,96,113	1.88	7 (10%)
50	CLA	a	816	-	46,50,73	1.40	6 (13%)	53,85,113	1.72	4 (7%)
43	BCR	a	803	-	27,27,41	0.70	0	34,35,56	1.23	2 (5%)
49	SF4	a	832	28,27	0,12,12	-	-	-		
50	CLA	a	838	-	69,73,73	1.22	6 (8%)	82,113,113	1.69	10 (12%)
43	BCR	a	831	-	40,40,41	0.66	0	54,54,56	1.16	5 (9%)
50	CLA	w	314	44	47,52,73	1.41	7 (14%)	55,87,113	1.88	7 (12%)
44	PGT	z	313	-	32,32,50	0.58	0	35,38,56	0.54	0
44	PGT	a	807	-	45,45,50	0.51	0	48,51,56	0.51	0
50	CLA	a	854	-	69,73,73	1.22	6 (8%)	82,113,113	1.54	10 (12%)
50	CLA	a	809	-	61,65,73	1.30	7 (11%)	72,103,113	1.73	10 (13%)
50	CLA	a	817	-	45,49,73	1.45	7 (15%)	54,84,113	1.75	5 (9%)
50	CLA	b	824	44	69,73,73	1.23	6 (8%)	82,113,113	1.70	8 (9%)
44	PGT	B	603	-	45,45,50	0.51	0	48,51,56	0.46	0
50	CLA	b	801	-	69,73,73	1.23	6 (8%)	82,113,113	1.60	8 (9%)
50	CLA	b	812	-	66,70,73	1.25	7 (10%)	78,109,113	1.63	11 (14%)
50	CLA	y	309	-	46,50,73	1.44	7 (15%)	53,85,113	1.64	4 (7%)
50	CLA	a	818	-	63,67,73	1.28	7 (11%)	74,105,113	1.62	10 (13%)
50	CLA	a	853	-	69,73,73	1.23	6 (8%)	82,113,113	1.64	9 (10%)
44	PGT	A	404	-	43,43,50	0.52	0	46,49,56	0.47	0
50	CLA	y	306	-	42,48,73	1.38	8 (19%)	49,82,113	1.92	7 (14%)
46	LMG	B	605	-	37,37,55	0.98	2 (5%)	45,45,63	1.05	2 (4%)
52	CL0	a	808	-	55,69,73	3.19	17 (30%)	58,107,113	2.17	14 (24%)
46	LMG	z	315	-	36,36,55	0.97	1 (2%)	44,44,63	1.13	2 (4%)
50	CLA	a	847	-	40,48,73	1.63	4 (10%)	48,76,113	1.41	8 (16%)
46	LMG	7	301	-	41,41,55	0.99	1 (2%)	49,49,63	1.23	4 (8%)
50	CLA	x	310	-	47,51,73	1.39	6 (12%)	55,86,113	1.71	5 (9%)
54	CHL	x	301	-	37,51,74	2.31	11 (29%)	30,86,114	3.27	14 (46%)
48	SQD	w	317	-	29,31,54	0.54	1 (3%)	39,42,65	0.58	0
50	CLA	b	835	-	63,67,73	1.28	6 (9%)	74,105,113	1.63	7 (9%)
50	CLA	b	809	-	63,67,73	1.28	7 (11%)	74,105,113	1.65	9 (12%)
44	PGT	L	201	-	39,39,50	0.55	0	42,45,56	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	PGT	B	601	-	33,33,50	0.58	0	36,39,56	0.57	0
45	A1H1M	F	804	-	41,41,41	1.27	5 (12%)	58,58,58	1.83	16 (27%)
50	CLA	a	840	-	46,50,73	1.40	7 (15%)	53,85,113	1.77	5 (9%)
50	CLA	a	855	-	46,50,73	1.41	6 (13%)	53,85,113	1.85	6 (11%)
50	CLA	l	306	-	64,68,73	1.30	9 (14%)	76,107,113	1.67	10 (13%)
50	CLA	k	204	-	61,65,73	1.31	6 (9%)	72,103,113	1.76	8 (11%)
48	SQD	a	859	-	34,36,54	0.51	1 (2%)	44,47,65	0.83	1 (2%)
50	CLA	b	842	-	61,65,73	1.30	6 (9%)	72,103,113	1.60	8 (11%)
50	CLA	x	313	40	57,61,73	1.38	8 (14%)	67,98,113	1.66	9 (13%)
50	CLA	g	201	-	53,57,73	1.37	7 (13%)	61,93,113	1.60	6 (9%)
55	LUT	z	320	-	42,43,43	0.96	1 (2%)	51,60,60	0.67	0
50	CLA	b	802	-	69,73,73	1.21	6 (8%)	82,113,113	1.54	8 (9%)
50	CLA	a	802	-	64,68,73	1.29	7 (10%)	76,107,113	1.63	9 (11%)
50	CLA	b	815	-	69,73,73	1.23	8 (11%)	82,113,113	1.68	9 (10%)
50	CLA	h	201	34	50,54,73	1.40	6 (12%)	59,90,113	1.83	5 (8%)
50	CLA	b	833	-	69,73,73	1.22	7 (10%)	82,113,113	1.67	9 (10%)
48	SQD	B	604	-	38,40,54	0.52	1 (2%)	48,51,65	0.62	0
43	BCR	i	101	-	41,41,41	0.66	0	56,56,56	1.14	3 (5%)
48	SQD	w	318	-	39,41,54	0.44	1 (2%)	49,52,65	0.92	3 (6%)
50	CLA	b	813	-	47,51,73	1.40	7 (14%)	55,86,113	1.65	6 (10%)
50	CLA	y	304	-	41,47,73	1.49	8 (19%)	51,81,113	1.82	4 (7%)
44	PGT	F	803	-	42,42,50	0.52	0	45,48,56	0.48	0
51	DGD	b	821	-	60,60,67	1.01	1 (1%)	74,74,81	1.02	3 (4%)
50	CLA	a	822	-	55,59,73	1.37	7 (12%)	64,96,113	1.92	9 (14%)
50	CLA	x	303	40	61,65,73	1.34	6 (9%)	72,103,113	1.63	12 (16%)
50	CLA	b	834	-	49,53,73	1.41	7 (14%)	58,89,113	1.69	6 (10%)
50	CLA	a	857	-	69,73,73	1.23	6 (8%)	82,113,113	1.65	8 (9%)
50	CLA	b	845	-	69,73,73	1.25	6 (8%)	82,113,113	1.43	8 (9%)
50	CLA	y	313	41	69,73,73	1.23	8 (11%)	82,113,113	1.75	8 (9%)
50	CLA	a	839	-	69,73,73	1.22	7 (10%)	82,113,113	1.55	9 (10%)
50	CLA	j	102	36	46,50,73	1.41	6 (13%)	53,85,113	1.88	6 (11%)
50	CLA	a	836	27	69,73,73	1.22	5 (7%)	82,113,113	1.58	8 (9%)
54	CHL	x	319	42	44,58,74	2.21	11 (25%)	37,94,114	3.10	17 (45%)
50	CLA	a	835	-	62,66,73	1.30	6 (9%)	73,104,113	1.71	9 (12%)
48	SQD	F	801	-	39,41,54	0.45	1 (2%)	49,52,65	1.05	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
43	BCR	j	103	-	41,41,41	0.71	0	56,56,56	1.16	4 (7%)
50	CLA	g	204	33	47,51,73	1.41	7 (14%)	55,86,113	1.71	5 (9%)
48	SQD	j	106	-	40,42,54	0.45	1 (2%)	50,53,65	0.57	1 (2%)
54	CHL	w	309	-	37,51,74	2.31	10 (27%)	30,86,114	3.27	13 (43%)
44	PGT	A	401	-	31,31,50	0.59	0	34,37,56	0.61	0
50	CLA	b	846	-	69,73,73	1.22	6 (8%)	82,113,113	1.61	8 (9%)
50	CLA	l	305	38	44,48,73	1.46	7 (15%)	53,83,113	1.77	7 (13%)
50	CLA	b	806	-	56,60,73	1.36	6 (10%)	65,97,113	1.79	8 (12%)
43	BCR	z	318	-	41,41,41	0.71	0	56,56,56	1.40	5 (8%)
43	BCR	k	201	-	41,41,41	0.70	0	56,56,56	1.48	10 (17%)
44	PGT	N	301	-	25,25,50	0.65	0	28,31,56	0.60	0
43	BCR	a	828	-	41,41,41	0.70	0	56,56,56	1.10	3 (5%)
46	LMG	j	104	-	34,34,55	1.02	1 (2%)	42,42,63	1.15	2 (4%)
43	BCR	b	850	-	41,41,41	0.72	0	56,56,56	1.18	5 (8%)
50	CLA	k	203	-	45,49,73	1.47	8 (17%)	54,84,113	1.81	6 (11%)
50	CLA	x	309	-	46,50,73	1.41	7 (15%)	53,85,113	1.83	5 (9%)
54	CHL	z	304	42	36,50,74	2.36	10 (27%)	29,85,114	3.50	15 (51%)
50	CLA	y	311	-	55,59,73	1.38	9 (16%)	64,96,113	1.87	8 (12%)
48	SQD	F	805	-	41,43,54	0.46	0	51,54,65	0.79	2 (3%)
50	CLA	w	315	39	50,54,73	1.41	6 (12%)	59,90,113	1.80	6 (10%)
43	BCR	k	202	-	41,41,41	0.72	1 (2%)	56,56,56	1.14	3 (5%)
43	BCR	x	314	-	41,41,41	0.62	0	56,56,56	1.18	4 (7%)
50	CLA	a	813	-	56,60,73	1.35	7 (12%)	65,97,113	1.67	8 (12%)
50	CLA	z	305	-	54,58,73	1.38	6 (11%)	64,95,113	1.73	7 (10%)
50	CLA	b	825	-	69,73,73	1.24	6 (8%)	82,113,113	1.58	10 (12%)
50	CLA	y	312	-	55,59,73	1.35	6 (10%)	64,96,113	1.74	8 (12%)
50	CLA	y	303	-	59,63,73	1.33	6 (10%)	70,101,113	1.75	7 (10%)
55	LUT	z	321	-	42,43,43	0.86	0	51,60,60	0.73	1 (1%)
50	CLA	z	311	-	59,63,73	1.32	6 (10%)	70,101,113	1.59	6 (8%)
50	CLA	b	843	-	69,73,73	1.22	7 (10%)	82,113,113	1.68	8 (9%)
44	PGT	A	402	-	36,36,50	0.57	0	39,42,56	0.52	0
50	CLA	a	845	-	69,73,73	1.24	6 (8%)	82,113,113	1.62	8 (9%)
50	CLA	z	319	-	46,50,73	1.44	6 (13%)	53,85,113	1.75	4 (7%)
43	BCR	l	304	-	41,41,41	0.68	0	56,56,56	1.09	4 (7%)
50	CLA	a	837	-	69,73,73	1.24	6 (8%)	82,113,113	1.61	8 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	LUT	y	316	-	-	4/29/67/67	0/2/2/2
43	BCR	l	302	-	-	8/29/63/63	0/2/2/2
54	CHL	z	312	42	3/3/19/26	12/33/131/137	-
50	CLA	a	856	-	1/1/14/20	8/37/113/115	-
46	LMG	f	306	-	-	12/29/49/70	0/1/1/1
51	DGD	a	804	-	-	32/55/95/95	0/2/2/2
50	CLA	a	824	-	1/1/15/20	15/39/115/115	-
50	CLA	x	306	-	1/1/14/20	12/33/109/115	-
44	PGT	B	602	-	-	10/46/46/55	-
43	BCR	b	816	-	-	6/29/63/63	0/2/2/2
43	BCR	y	301	-	-	5/29/63/63	0/2/2/2
50	CLA	w	302	-	1/1/12/20	12/21/97/115	-
50	CLA	y	302	41	1/1/13/20	5/23/99/115	-
44	PGT	a	805	-	-	14/36/36/55	-
50	CLA	a	815	27	1/1/15/20	16/39/115/115	-
50	CLA	b	811	-	1/1/11/20	4/15/91/115	-
50	CLA	a	834	-	1/1/15/20	11/39/115/115	-
51	DGD	x	317	-	-	24/37/77/95	0/2/2/2
50	CLA	g	203	-	1/1/12/20	4/24/100/115	-
50	CLA	b	807	-	1/1/15/20	19/39/115/115	-
50	CLA	z	308	-	1/1/11/20	6/15/88/115	-
43	BCR	w	301	-	-	3/29/63/63	0/2/2/2
43	BCR	a	810	-	-	11/24/41/63	0/1/1/2
50	CLA	b	810	-	1/1/12/20	4/21/97/115	-
50	CLA	y	310	41	1/1/15/20	11/39/115/115	-
50	CLA	z	307	42	1/1/14/20	11/33/109/115	-
50	CLA	b	823	-	1/1/13/20	10/27/103/115	-
50	CLA	a	823	-	1/1/13/20	7/27/103/115	-
50	CLA	b	849	-	1/1/12/20	8/21/97/115	-
43	BCR	a	827	-	-	3/27/61/63	0/2/2/2
46	LMG	H	401	-	-	10/28/48/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	BCR	a	829	-	-	2/29/63/63	0/2/2/2
50	CLA	x	308	-	1/1/12/20	9/21/97/115	-
50	CLA	y	308	-	1/1/15/20	15/39/115/115	-
50	CLA	b	808	-	1/1/10/20	7/13/89/115	-
50	CLA	y	307	-	1/1/10/20	4/10/86/115	-
50	CLA	z	316	44	1/1/11/20	3/18/94/115	-
50	CLA	y	314	41	1/1/15/20	18/39/115/115	-
43	BCR	b	820	-	-	2/29/63/63	0/2/2/2
50	CLA	b	838	-	1/1/12/20	9/24/100/115	-
50	CLA	b	848	-	1/1/10/20	3/12/88/115	-
50	CLA	a	846	-	1/1/15/20	15/39/115/115	-
46	LMG	F	802	-	-	5/23/43/70	0/1/1/1
49	SF4	K	301	21	-	-	0/6/5/5
50	CLA	a	812	-	1/1/14/20	17/36/109/115	-
50	CLA	l	301	-	1/1/11/20	5/15/91/115	-
50	CLA	w	308	39	1/1/15/20	19/39/115/115	-
44	PGT	B	606	-	-	24/39/39/55	-
50	CLA	b	805	28	1/1/15/20	23/39/115/115	-
45	A1H1M	5	302	-	-	10/19/79/79	0/4/4/4
44	PGT	b	830	50	-	16/43/43/55	-
50	CLA	b	847	-	1/1/14/20	11/33/109/115	-
50	CLA	b	851	-	1/1/11/20	3/18/94/115	-
50	CLA	f	301	-	1/1/13/20	11/30/106/115	-
50	CLA	f	303	-	1/1/10/20	2/10/86/115	-
50	CLA	x	312	40	1/1/15/20	20/39/115/115	-
50	CLA	a	842	-	1/1/15/20	24/39/115/115	-
46	LMG	w	312	-	-	15/35/55/70	0/1/1/1
50	CLA	b	814	-	1/1/15/20	13/39/115/115	-
49	SF4	I	202	19	-	-	0/6/5/5
50	CLA	a	849	-	1/1/15/20	17/39/115/115	-
54	CHL	w	311	-	3/3/15/26	5/16/114/137	-
50	CLA	f	302	-	1/1/10/20	1/12/88/115	-
44	PGT	D	602	-	-	10/38/38/55	-
50	CLA	b	826	-	1/1/13/20	12/27/103/115	-
50	CLA	a	826	44	1/1/11/20	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	CHL	x	305	-	3/3/16/26	4/15/113/137	-
50	CLA	a	848	-	1/1/12/20	6/24/100/115	-
50	CLA	z	309	-	1/1/10/20	2/12/88/115	-
50	CLA	w	303	39	1/1/11/20	3/15/91/115	-
50	CLA	x	316	-	1/1/11/20	4/15/91/115	-
50	CLA	a	801	-	1/1/15/20	13/39/115/115	-
50	CLA	a	811	-	1/1/15/20	21/39/115/115	-
46	LMG	x	315	-	-	16/43/63/70	0/1/1/1
46	LMG	z	314	-	-	13/35/55/70	0/1/1/1
55	LUT	x	320	-	-	1/29/67/67	0/2/2/2
55	LUT	x	321	-	-	6/29/67/67	0/2/2/2
50	CLA	b	844	28	1/1/15/20	22/39/115/115	-
44	PGT	z	301	-	-	18/49/49/55	-
50	CLA	y	305	41	1/1/11/20	2/15/91/115	-
43	BCR	b	819	-	-	5/29/63/63	0/2/2/2
43	BCR	g	202	-	-	6/29/63/63	0/2/2/2
50	CLA	x	302	-	1/1/10/20	2/10/86/115	-
43	BCR	f	304	-	-	2/29/63/63	0/2/2/2
50	CLA	z	306	42	1/1/13/20	8/29/105/115	-
50	CLA	x	318	-	1/1/11/20	6/17/93/115	-
50	CLA	z	310	42	1/1/10/20	4/10/86/115	-
50	CLA	k	205	-	1/1/10/20	4/12/88/115	-
43	BCR	j	101	-	-	10/29/63/63	0/2/2/2
43	BCR	a	830	-	-	7/29/63/63	0/2/2/2
50	CLA	x	304	40	1/1/11/20	3/18/94/115	-
50	CLA	a	858	-	1/1/15/20	14/39/115/115	-
44	PGT	b	829	-	-	19/52/52/55	-
50	CLA	b	837	-	1/1/15/20	17/39/115/115	-
43	BCR	4	101	-	-	8/29/63/63	0/2/2/2
50	CLA	b	828	-	1/1/14/20	14/33/109/115	-
43	BCR	b	817	-	-	3/29/63/63	0/2/2/2
50	CLA	b	840	-	1/1/15/20	16/39/115/115	-
50	CLA	w	306	39	1/1/15/20	17/39/115/115	-
50	CLA	a	819	-	1/1/14/20	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CLA	a	841	-	1/1/13/20	9/27/103/115	-
50	CLA	b	841	-	1/1/13/20	9/27/103/115	-
44	PGT	z	317	50	-	16/50/50/55	-
54	CHL	w	304	-	3/3/16/26	7/15/111/137	-
43	BCR	b	831	-	-	4/29/63/63	0/2/2/2
47	PQ9	A	405	-	-	4/31/51/61	0/1/1/1
49	SF4	I	201	19	-	-	0/6/5/5
49	SF4	c	101	29	-	-	0/6/5/5
50	CLA	x	307	40	1/1/14/20	13/33/109/115	-
53	PQN	a	825	-	-	8/23/43/43	0/2/2/2
50	CLA	a	821	-	1/1/14/20	12/35/111/115	-
50	CLA	a	814	-	1/1/15/20	20/39/115/115	-
50	CLA	w	316	39	1/1/12/20	8/21/97/115	-
50	CLA	z	302	-	1/1/13/20	8/27/103/115	-
54	CHL	x	311	-	3/3/14/26	5/8/102/137	-
55	LUT	y	315	-	-	0/29/67/67	0/2/2/2
50	CLA	z	303	-	1/1/10/20	2/10/86/115	-
44	PGT	I	203	-	-	14/48/48/55	-
50	CLA	w	307	-	1/1/11/20	6/15/91/115	-
50	CLA	a	852	-	1/1/12/20	5/23/99/115	-
50	CLA	a	843	-	1/1/15/20	17/39/115/115	-
50	CLA	b	839	-	1/1/15/20	21/39/115/115	-
43	BCR	l	303	-	-	6/29/63/63	0/2/2/2
50	CLA	a	844	-	1/1/13/20	8/30/106/115	-
50	CLA	b	803	-	1/1/15/20	16/39/115/115	-
44	PGT	f	305	-	-	10/43/43/55	-
50	CLA	b	822	-	1/1/13/20	10/31/107/115	-
50	CLA	a	833	-	1/1/15/20	18/39/115/115	-
50	CLA	a	820	-	1/1/15/20	17/39/115/115	-
50	CLA	b	804	-	1/1/10/20	0/10/86/115	-
50	CLA	b	832	-	1/1/12/20	12/26/102/115	-
44	PGT	a	806	50	-	14/37/37/55	-
55	LUT	w	319	-	-	6/29/67/67	0/2/2/2
44	PGT	A	403	-	-	18/42/42/55	-
44	PGT	w	313	50	-	10/44/44/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	LUT	w	320	-	-	1/29/67/67	0/2/2/2
46	LMG	D	601	-	-	13/29/49/70	0/1/1/1
53	PQN	b	827	-	-	8/23/43/43	0/2/2/2
50	CLA	b	836	-	1/1/15/20	11/39/115/115	-
49	SF4	c	102	29	-	-	0/6/5/5
50	CLA	w	310	-	1/1/15/20	18/39/115/115	-
50	CLA	a	851	27	1/1/11/20	4/17/93/115	-
50	CLA	a	850	-	1/1/15/20	14/39/115/115	-
43	BCR	b	818	-	-	6/29/63/63	0/2/2/2
50	CLA	w	305	-	1/1/12/20	4/23/99/115	-
50	CLA	a	816	-	1/1/10/20	3/12/88/115	-
43	BCR	a	803	-	-	5/21/38/63	0/1/1/2
49	SF4	a	832	28,27	-	-	0/6/5/5
50	CLA	a	838	-	1/1/15/20	14/39/115/115	-
43	BCR	a	831	-	-	8/27/61/63	0/2/2/2
50	CLA	w	314	44	1/1/10/20	8/14/90/115	-
44	PGT	z	313	-	-	13/37/37/55	-
50	CLA	a	854	-	1/1/15/20	15/39/115/115	-
44	PGT	a	807	-	-	15/50/50/55	-
50	CLA	a	809	-	1/1/13/20	5/30/106/115	-
50	CLA	a	817	-	1/1/10/20	0/10/86/115	-
50	CLA	b	824	44	1/1/15/20	17/39/115/115	-
44	PGT	B	603	-	-	19/50/50/55	-
50	CLA	b	801	-	1/1/15/20	17/39/115/115	-
50	CLA	b	812	-	1/1/14/20	9/36/112/115	-
50	CLA	y	309	-	1/1/10/20	3/12/88/115	-
50	CLA	a	818	-	1/1/13/20	12/32/108/115	-
50	CLA	a	853	-	1/1/15/20	11/39/115/115	-
50	CLA	y	306	-	1/1/10/20	2/10/86/115	-
44	PGT	A	404	-	-	15/48/48/55	-
46	LMG	B	605	-	-	17/32/52/70	0/1/1/1
52	CL0	a	808	-	3/3/18/25	5/33/125/135	-
46	LMG	z	315	-	-	8/31/51/70	0/1/1/1
50	CLA	a	847	-	1/1/7/20	11/26/62/115	-
46	LMG	7	301	-	-	14/36/56/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CLA	x	310	-	1/1/10/20	3/13/89/115	-
54	CHL	x	301	-	3/3/15/26	4/12/110/137	-
48	SQD	w	317	-	-	5/26/46/69	0/1/1/1
50	CLA	b	835	-	1/1/13/20	9/32/108/115	-
50	CLA	b	809	-	1/1/13/20	12/32/108/115	-
44	PGT	L	201	-	-	12/44/44/55	-
50	CLA	a	855	-	1/1/10/20	2/12/88/115	-
50	CLA	a	840	-	1/1/10/20	2/12/88/115	-
50	CLA	l	306	-	1/1/14/20	19/33/109/115	-
44	PGT	B	601	-	-	15/38/38/55	-
45	A1H1M	F	804	-	-	13/19/79/79	0/4/4/4
50	CLA	k	204	-	1/1/13/20	7/30/106/115	-
50	CLA	b	842	-	1/1/13/20	22/30/106/115	-
44	PGT	5	301	-	-	16/39/39/55	-
48	SQD	a	859	-	-	6/31/51/69	0/1/1/1
50	CLA	x	313	40	1/1/12/20	6/25/101/115	-
50	CLA	g	201	-	1/1/11/20	10/20/96/115	-
55	LUT	z	320	-	-	6/29/67/67	0/2/2/2
50	CLA	b	802	-	1/1/15/20	20/39/115/115	-
50	CLA	a	802	-	1/1/14/20	8/33/109/115	-
50	CLA	b	815	-	1/1/15/20	11/39/115/115	-
50	CLA	h	201	34	1/1/11/20	8/17/93/115	-
50	CLA	b	833	-	1/1/15/20	16/39/115/115	-
50	CLA	y	304	-	1/1/9/20	0/6/82/115	-
50	CLA	b	813	-	1/1/10/20	4/13/89/115	-
43	BCR	i	101	-	-	6/29/63/63	0/2/2/2
48	SQD	B	604	-	-	6/35/55/69	0/1/1/1
48	SQD	w	318	-	-	8/36/56/69	0/1/1/1
44	PGT	F	803	-	-	12/47/47/55	-
51	DGD	b	821	-	-	22/48/88/95	0/2/2/2
50	CLA	a	822	-	1/1/12/20	8/23/99/115	-
50	CLA	x	303	40	1/1/13/20	9/30/106/115	-
50	CLA	b	834	-	1/1/11/20	4/15/91/115	-
50	CLA	a	857	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CLA	b	845	-	1/1/15/20	18/39/115/115	-
50	CLA	y	313	41	1/1/15/20	18/39/115/115	-
50	CLA	a	839	-	1/1/15/20	16/39/115/115	-
50	CLA	j	102	36	1/1/10/20	2/12/88/115	-
50	CLA	a	836	27	1/1/15/20	15/39/115/115	-
54	CHL	x	319	42	3/3/16/26	7/20/118/137	-
50	CLA	a	835	-	1/1/13/20	15/31/107/115	-
48	SQD	F	801	-	-	2/36/56/69	0/1/1/1
50	CLA	g	204	33	1/1/10/20	5/13/89/115	-
43	BCR	j	103	-	-	8/29/63/63	0/2/2/2
48	SQD	j	106	-	-	8/37/57/69	0/1/1/1
54	CHL	w	309	-	3/3/15/26	5/12/110/137	-
50	CLA	b	846	-	1/1/15/20	16/39/115/115	-
44	PGT	A	401	-	-	9/36/36/55	-
50	CLA	l	305	38	1/1/10/20	0/8/84/115	-
50	CLA	b	806	-	1/1/12/20	5/24/100/115	-
43	BCR	z	318	-	-	8/29/63/63	0/2/2/2
54	CHL	z	304	42	3/3/15/26	6/10/108/137	-
50	CLA	k	203	-	1/1/10/20	2/10/86/115	-
43	BCR	a	828	-	-	0/29/63/63	0/2/2/2
43	BCR	k	201	-	-	5/29/63/63	0/2/2/2
43	BCR	b	850	-	-	2/29/63/63	0/2/2/2
44	PGT	N	301	-	-	15/30/30/55	-
50	CLA	x	309	-	1/1/10/20	2/12/88/115	-
46	LMG	j	104	-	-	10/29/49/70	0/1/1/1
50	CLA	y	311	-	1/1/12/20	7/23/99/115	-
48	SQD	F	805	-	-	7/38/58/69	0/1/1/1
50	CLA	w	315	39	1/1/11/20	4/17/93/115	-
50	CLA	a	813	-	1/1/12/20	8/24/100/115	-
50	CLA	z	305	-	1/1/12/20	5/21/97/115	-
43	BCR	k	202	-	-	4/29/63/63	0/2/2/2
43	BCR	x	314	-	-	11/29/63/63	0/2/2/2
50	CLA	b	825	-	1/1/15/20	16/39/115/115	-
50	CLA	y	312	-	1/1/12/20	6/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	LMG	j	105	-	-	18/32/52/70	0/1/1/1
50	CLA	y	303	-	1/1/13/20	8/27/103/115	-
55	LUT	z	321	-	-	0/29/67/67	0/2/2/2
50	CLA	z	311	-	1/1/13/20	10/27/103/115	-
50	CLA	b	843	-	1/1/15/20	19/39/115/115	-
44	PGT	A	402	-	-	11/41/41/55	-
50	CLA	a	845	-	1/1/15/20	15/39/115/115	-
50	CLA	z	319	-	1/1/10/20	3/12/88/115	-
43	BCR	l	304	-	-	7/29/63/63	0/2/2/2
50	CLA	a	837	-	1/1/15/20	10/39/115/115	-

The worst 5 of 1152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	808	CL0	C1A-CHA	9.95	1.51	1.40
52	a	808	CL0	C1B-C2B	8.55	1.49	1.39
52	a	808	CL0	C1D-C2D	8.41	1.49	1.39
47	A	405	PQ9	C3-C2	8.05	1.54	1.34
52	a	808	CL0	C4B-C3B	7.70	1.48	1.39

The worst 5 of 1538 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	405	PQ9	C34-C33-C35	-27.40	83.87	116.13
47	A	405	PQ9	C19-C18-C20	-26.51	69.21	115.23
47	A	405	PQ9	C24-C23-C25	-26.42	69.37	115.23
47	A	405	PQ9	C14-C13-C15	-26.12	69.88	115.23
47	A	405	PQ9	C29-C28-C27	17.84	169.45	123.63

5 of 174 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
50	a	801	CLA	ND
50	a	802	CLA	ND
50	a	809	CLA	ND
50	a	811	CLA	ND
50	a	812	CLA	ND

5 of 2336 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	4	101	BCR	C5-C6-C7-C8
43	4	101	BCR	C21-C22-C23-C24
43	a	803	BCR	C5-C6-C7-C8
43	a	803	BCR	C7-C8-C9-C10
43	a	803	BCR	C7-C8-C9-C34

There are no ring outliers.

201 monomers are involved in 576 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	y	316	LUT	28	0
43	l	302	BCR	2	0
54	z	312	CHL	7	0
50	a	856	CLA	3	0
46	f	306	LMG	1	0
51	a	804	DGD	2	0
50	a	824	CLA	4	0
44	B	602	PGT	2	0
50	x	306	CLA	1	0
43	b	816	BCR	3	0
43	y	301	BCR	1	0
44	a	805	PGT	3	0
50	y	302	CLA	7	0
50	a	815	CLA	3	0
50	b	811	CLA	2	0
50	a	834	CLA	3	0
51	x	317	DGD	2	0
50	g	203	CLA	2	0
44	5	301	PGT	2	0
46	j	105	LMG	2	0
43	w	301	BCR	1	0
43	a	810	BCR	4	0
50	b	807	CLA	4	0
50	b	810	CLA	1	0
50	y	310	CLA	5	0
46	H	401	LMG	1	0
50	a	823	CLA	3	0
43	a	827	BCR	4	0
50	b	823	CLA	1	0
50	b	849	CLA	4	0
43	a	829	BCR	1	0
50	z	307	CLA	2	0
50	x	308	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	y	308	CLA	4	0
43	b	820	BCR	4	0
46	F	802	LMG	2	0
50	b	838	CLA	1	0
50	b	848	CLA	1	0
50	a	846	CLA	6	0
50	y	314	CLA	3	0
50	z	316	CLA	1	0
50	a	812	CLA	2	0
44	B	606	PGT	1	0
50	l	301	CLA	3	0
50	w	308	CLA	9	0
50	b	805	CLA	6	0
50	b	847	CLA	4	0
50	b	851	CLA	5	0
50	f	301	CLA	2	0
50	f	303	CLA	1	0
50	x	312	CLA	7	0
46	w	312	LMG	2	0
50	a	842	CLA	3	0
49	I	202	SF4	1	0
50	b	814	CLA	1	0
50	a	849	CLA	4	0
54	w	311	CHL	9	0
44	D	602	PGT	1	0
50	b	826	CLA	1	0
50	a	826	CLA	2	0
54	x	305	CHL	1	0
50	a	848	CLA	1	0
50	z	309	CLA	4	0
50	w	303	CLA	3	0
50	x	316	CLA	2	0
50	a	801	CLA	5	0
46	x	315	LMG	4	0
50	a	811	CLA	4	0
46	z	314	LMG	4	0
55	x	320	LUT	10	0
55	x	321	LUT	11	0
50	b	844	CLA	4	0
44	z	301	PGT	5	0
43	b	819	BCR	6	0
43	g	202	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	f	304	BCR	2	0
50	z	306	CLA	10	0
50	x	318	CLA	1	0
50	z	310	CLA	3	0
50	k	205	CLA	3	0
43	j	101	BCR	6	0
43	a	830	BCR	3	0
50	a	858	CLA	6	0
44	b	829	PGT	2	0
50	b	837	CLA	2	0
43	4	101	BCR	4	0
43	b	817	BCR	1	0
50	b	828	CLA	5	0
50	b	840	CLA	6	0
50	w	306	CLA	7	0
44	z	317	PGT	3	0
50	a	841	CLA	2	0
43	b	831	BCR	5	0
47	A	405	PQ9	15	0
50	b	841	CLA	3	0
54	w	304	CHL	1	0
50	x	307	CLA	3	0
53	a	825	PQN	1	0
50	a	814	CLA	5	0
50	w	316	CLA	2	0
50	z	302	CLA	3	0
54	x	311	CHL	3	0
55	y	315	LUT	32	0
50	w	307	CLA	5	0
50	a	852	CLA	1	0
50	a	843	CLA	3	0
50	b	839	CLA	2	0
43	l	303	BCR	2	0
50	a	844	CLA	3	0
50	b	803	CLA	5	0
50	b	822	CLA	3	0
50	a	833	CLA	3	0
50	a	820	CLA	5	0
50	b	804	CLA	3	0
44	a	806	PGT	1	0
55	w	319	LUT	9	0
44	A	403	PGT	2	0

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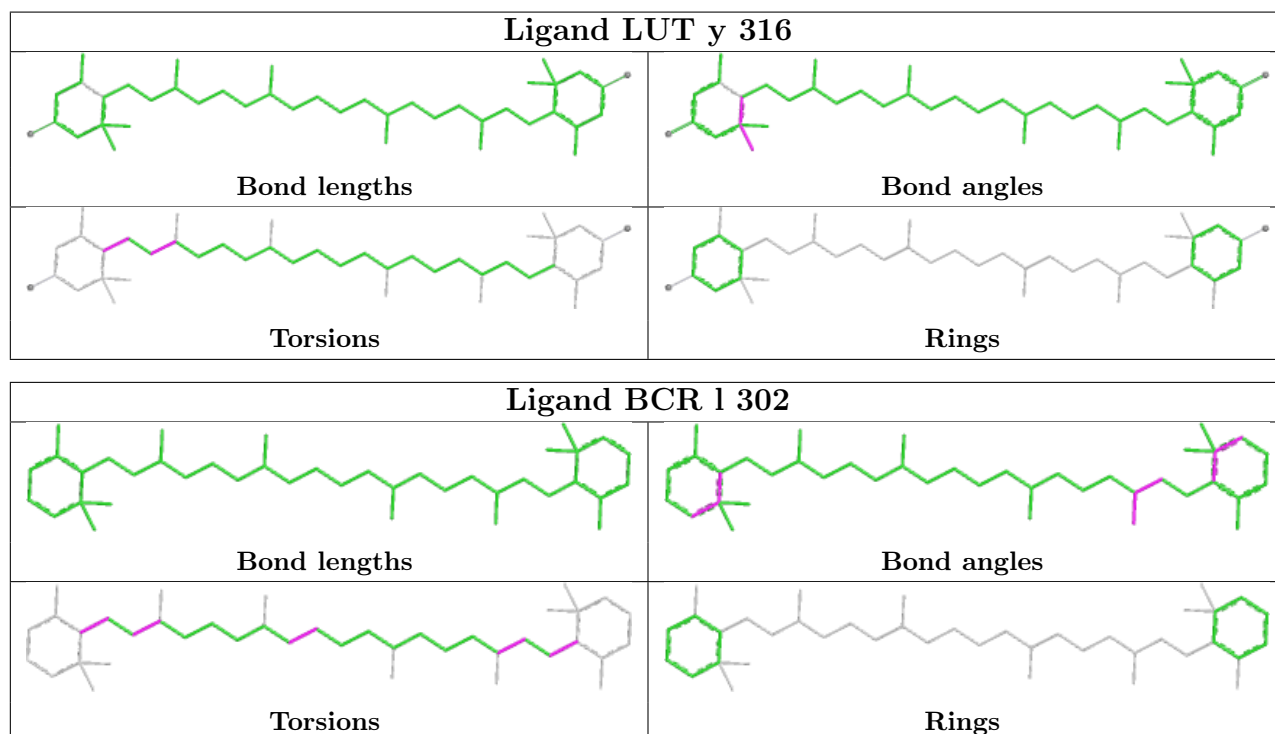
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	w	313	PGT	1	0
55	w	320	LUT	21	0
46	D	601	LMG	1	0
53	b	827	PQN	3	0
50	b	836	CLA	4	0
50	w	310	CLA	4	0
43	b	818	BCR	1	0
50	a	850	CLA	2	0
43	a	803	BCR	1	0
50	a	838	CLA	8	0
43	a	831	BCR	2	0
50	w	314	CLA	1	0
44	z	313	PGT	1	0
44	a	807	PGT	2	0
50	a	854	CLA	4	0
50	a	809	CLA	3	0
44	B	603	PGT	3	0
50	b	801	CLA	6	0
50	b	812	CLA	2	0
50	a	818	CLA	1	0
50	a	853	CLA	2	0
46	B	605	LMG	1	0
46	z	315	LMG	3	0
50	x	310	CLA	1	0
54	x	301	CHL	1	0
48	w	317	SQD	2	0
50	b	835	CLA	1	0
50	b	809	CLA	2	0
44	L	201	PGT	2	0
45	F	804	A1H1M	6	0
50	l	306	CLA	2	0
50	k	204	CLA	1	0
48	a	859	SQD	3	0
50	b	842	CLA	2	0
50	g	201	CLA	2	0
55	z	320	LUT	27	0
50	b	802	CLA	3	0
50	a	802	CLA	2	0
50	b	815	CLA	3	0
50	h	201	CLA	2	0
50	b	833	CLA	5	0
48	B	604	SQD	10	0

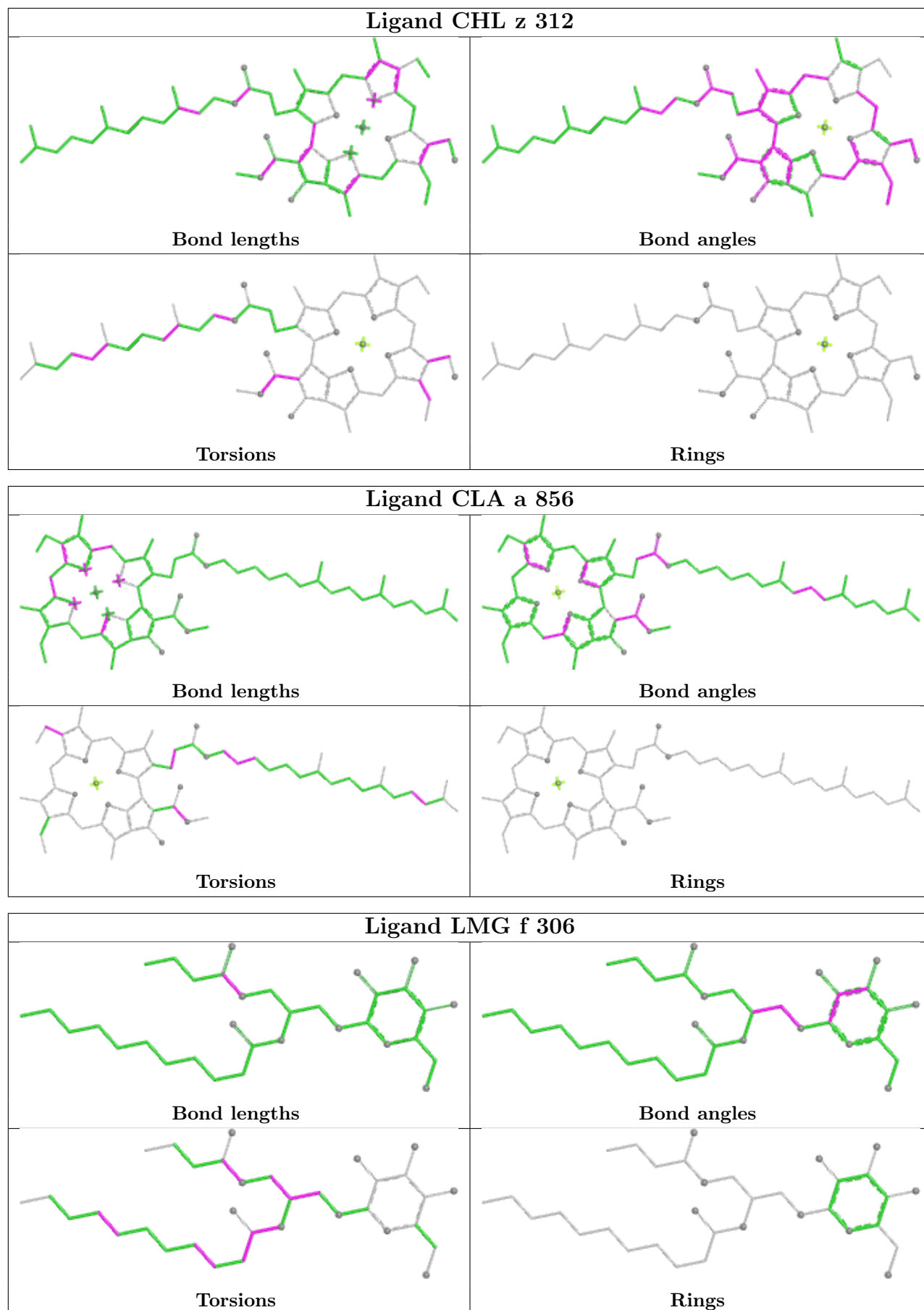
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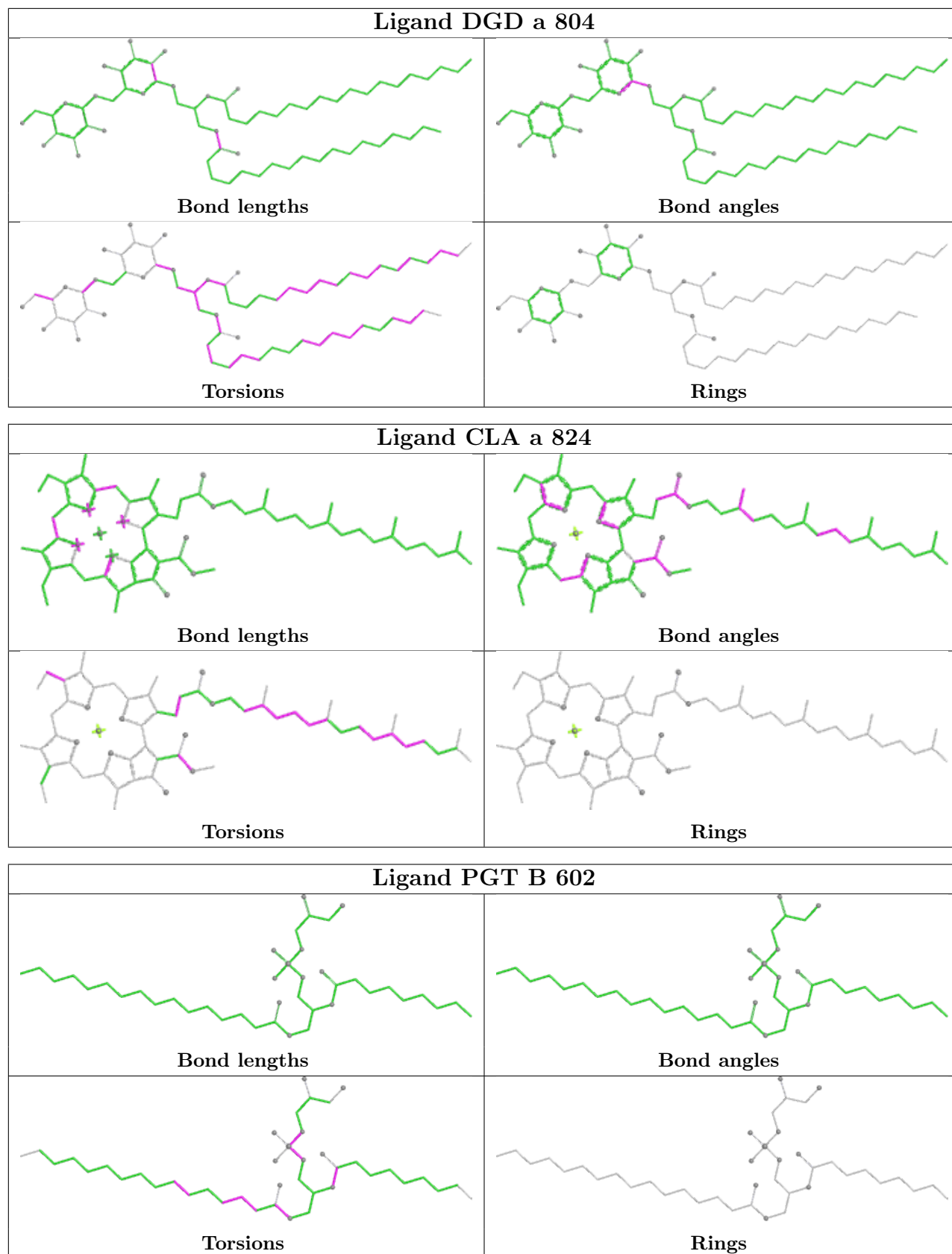
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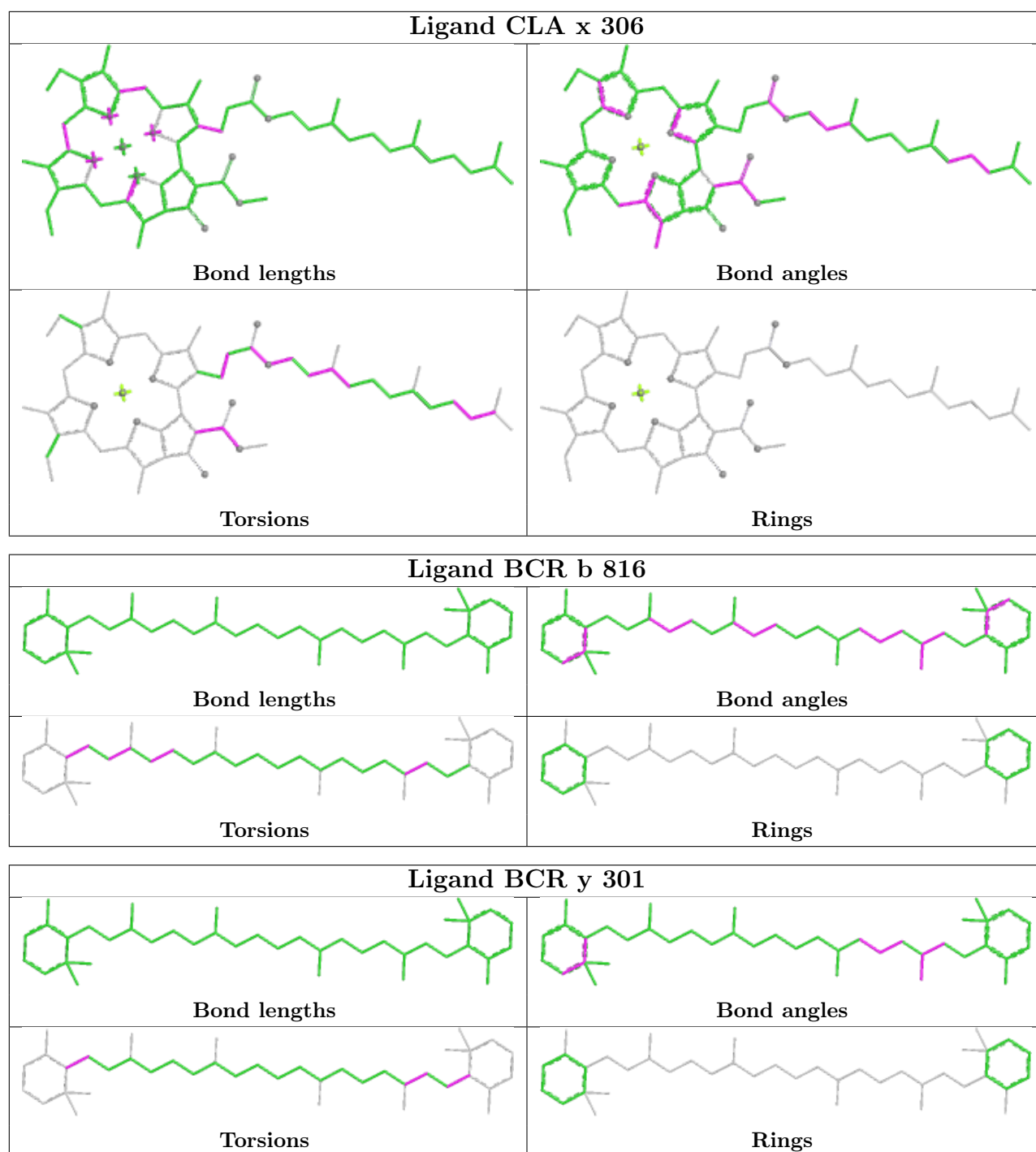
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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48	w	318	SQD	13	0
50	b	813	CLA	1	0
51	b	821	DGD	3	0
50	a	822	CLA	2	0
50	x	303	CLA	2	0
50	b	834	CLA	1	0
50	a	857	CLA	5	0
50	b	845	CLA	5	0
50	y	313	CLA	5	0
50	a	839	CLA	5	0
50	a	836	CLA	4	0
54	x	319	CHL	5	0
50	a	835	CLA	5	0
48	F	801	SQD	7	0
43	j	103	BCR	4	0
54	w	309	CHL	3	0
50	b	846	CLA	1	0
50	l	305	CLA	1	0
50	b	806	CLA	1	0
43	z	318	BCR	1	0
44	N	301	PGT	2	0
43	a	828	BCR	4	0
46	j	104	LMG	1	0
43	b	850	BCR	3	0
50	k	203	CLA	1	0
54	z	304	CHL	1	0
50	y	311	CLA	5	0
48	F	805	SQD	11	0
43	x	314	BCR	1	0
50	a	813	CLA	2	0
50	z	305	CLA	1	0
50	b	825	CLA	3	0
50	y	312	CLA	3	0
50	y	303	CLA	11	0
55	z	321	LUT	7	0
50	b	843	CLA	2	0
44	A	402	PGT	1	0
50	a	845	CLA	5	0
50	z	319	CLA	3	0
43	l	304	BCR	1	0
50	a	837	CLA	1	0

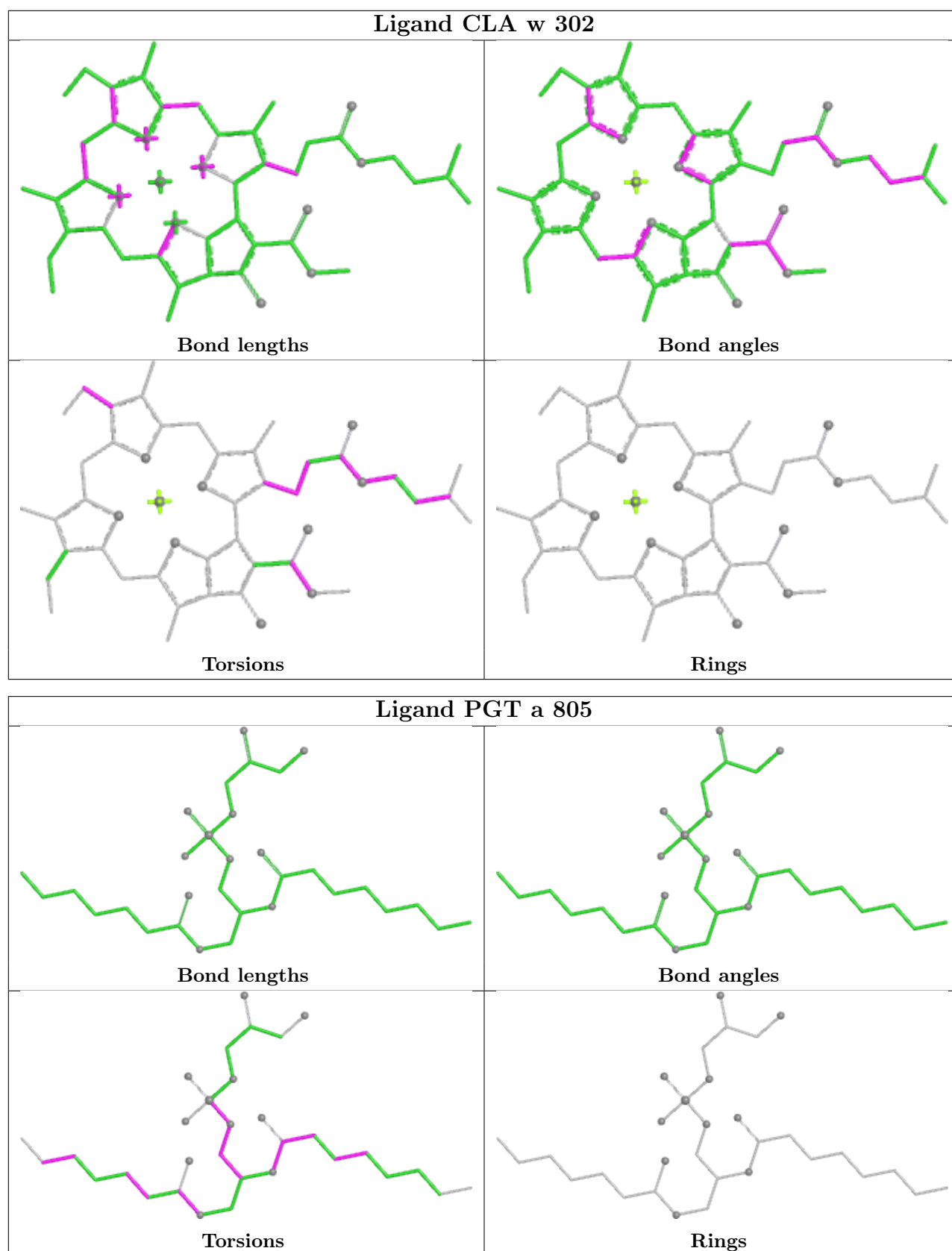
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

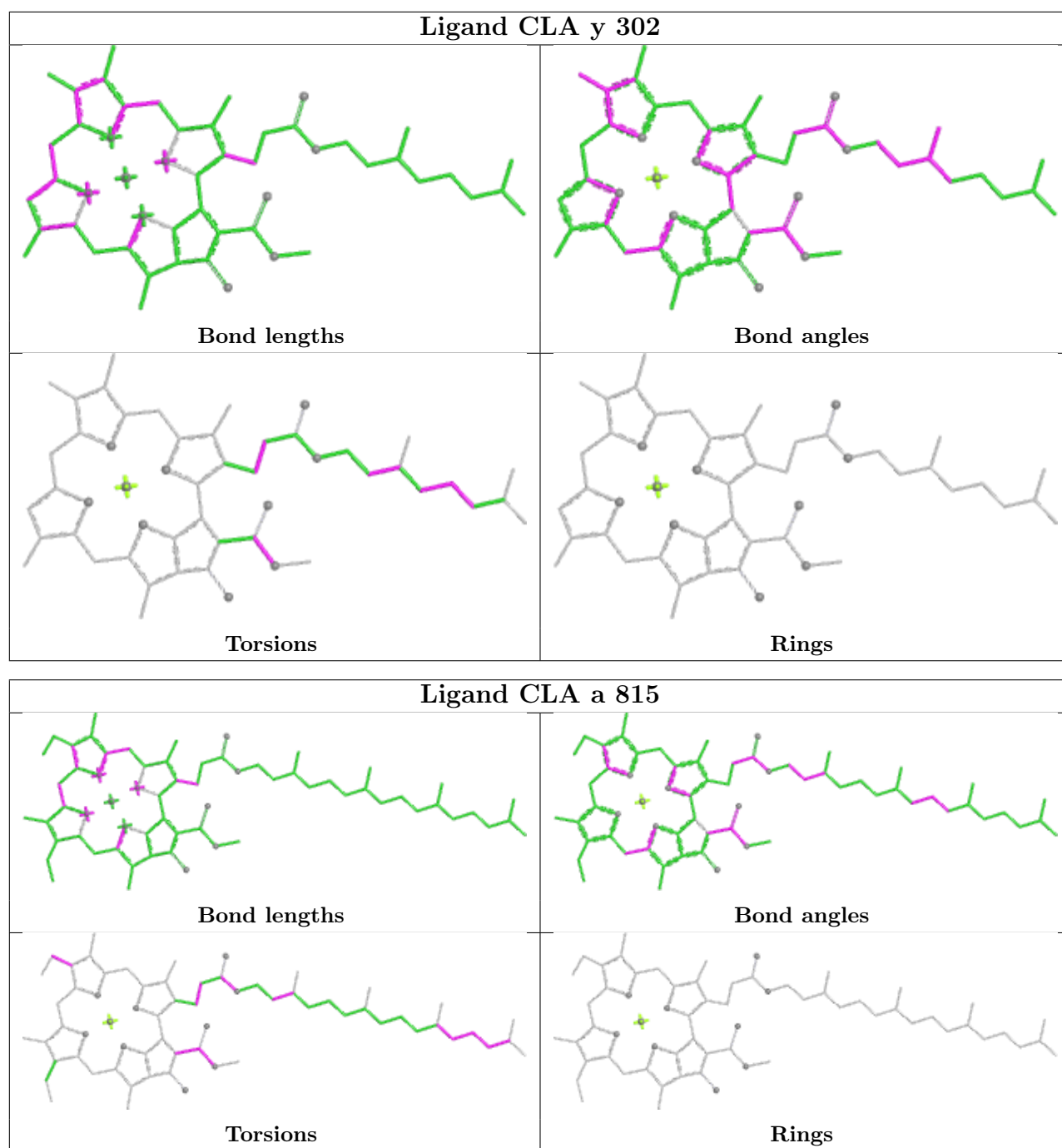


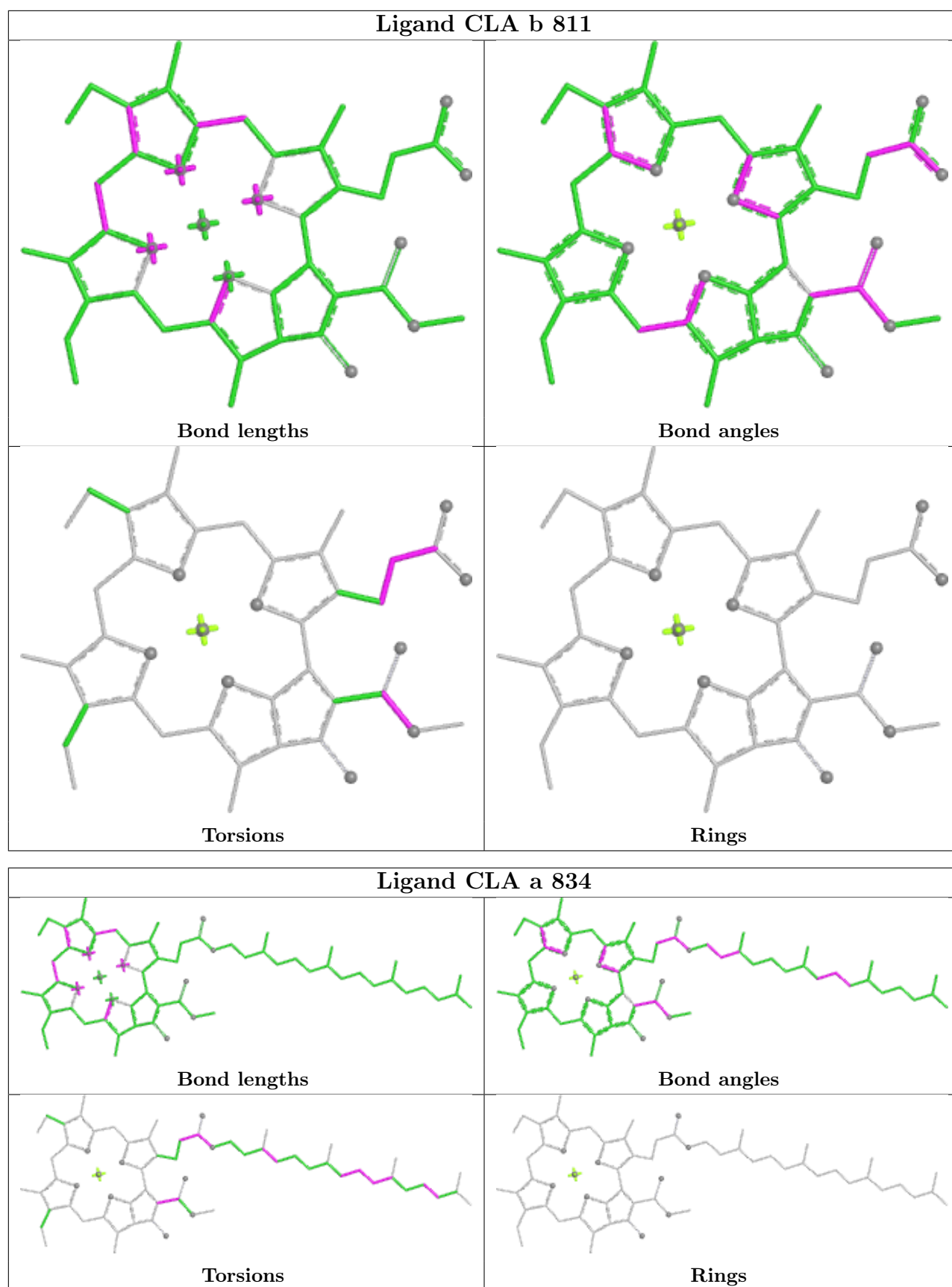


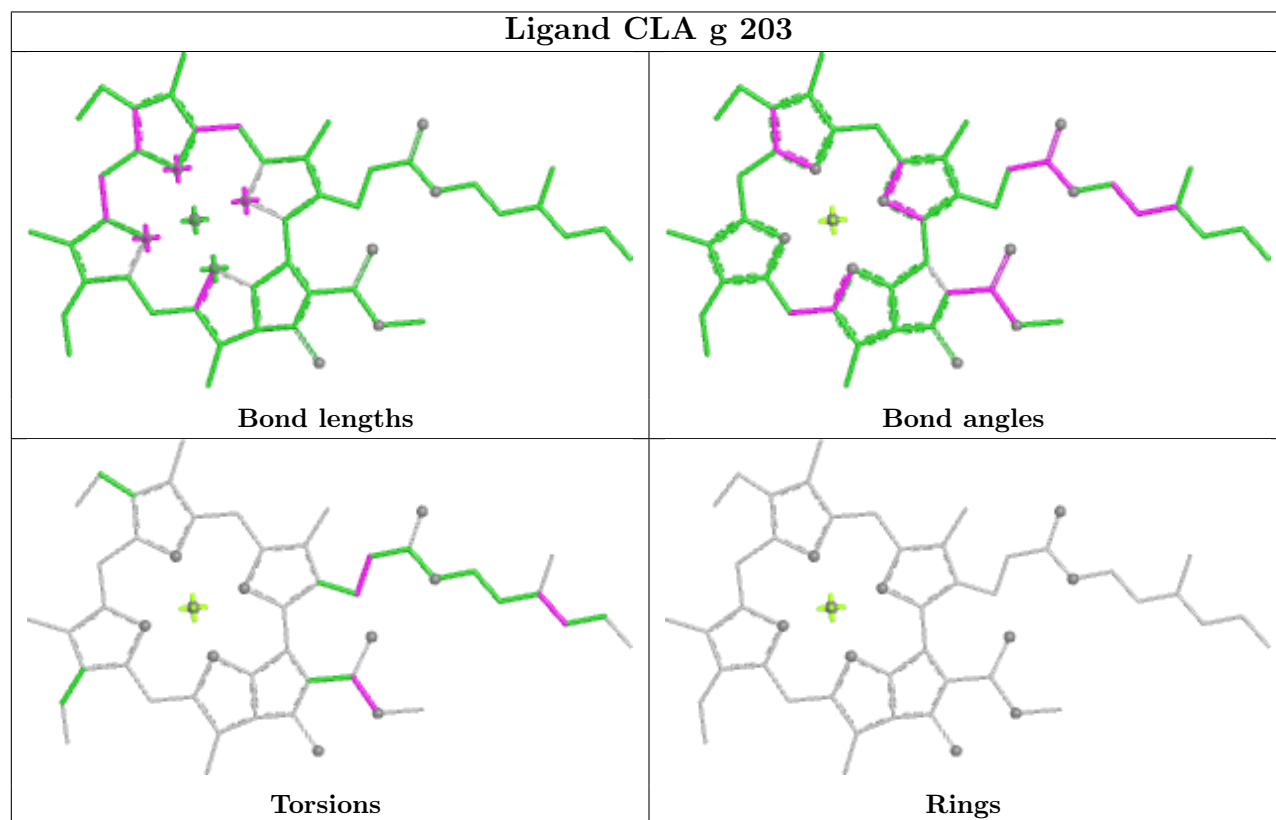
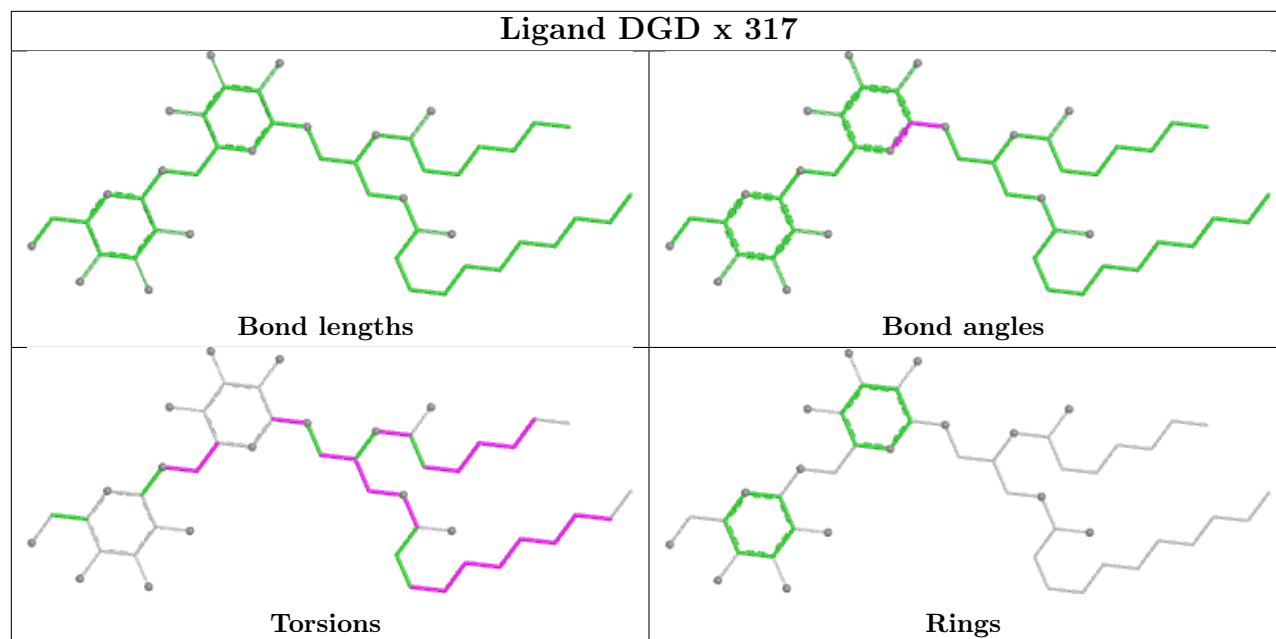


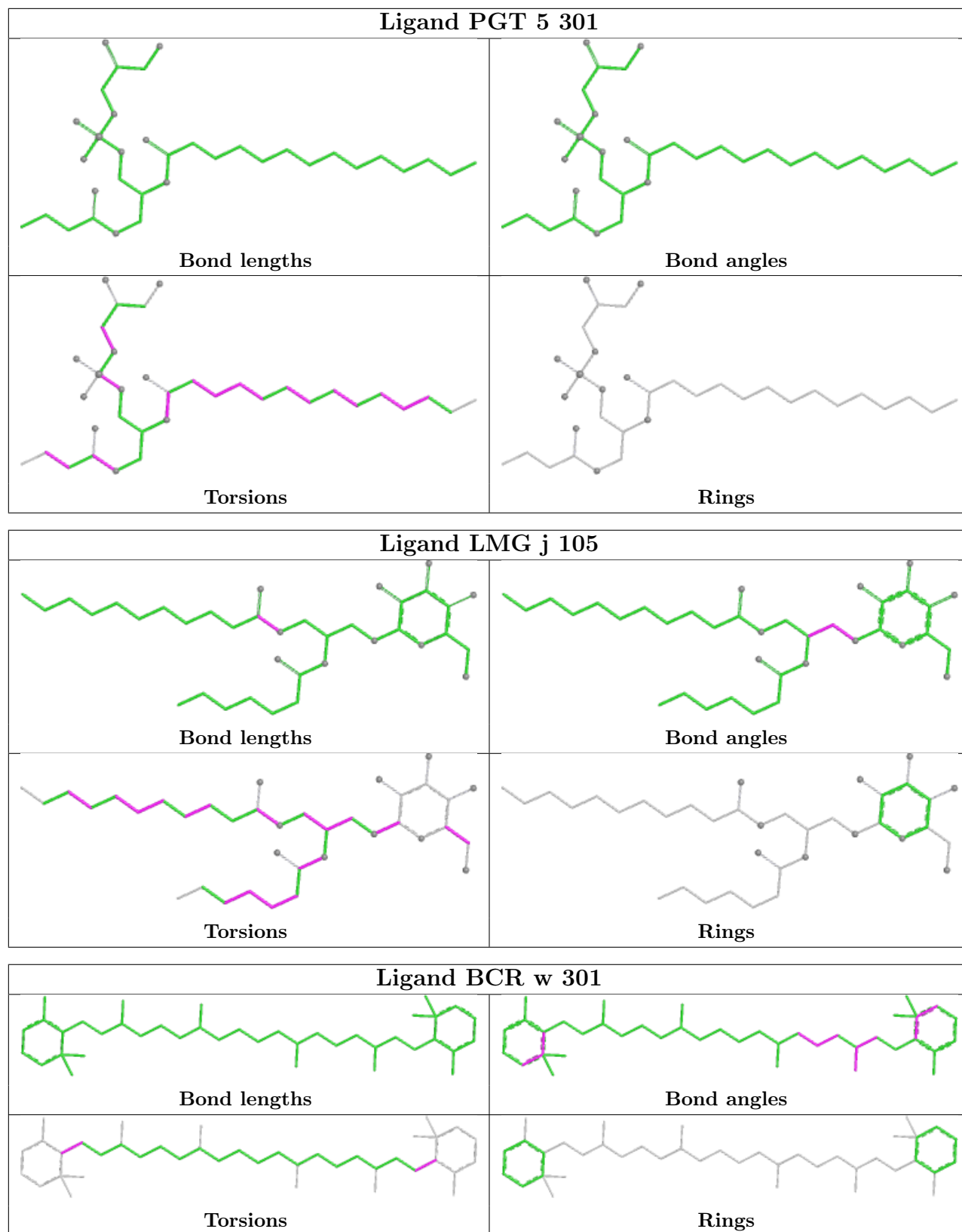


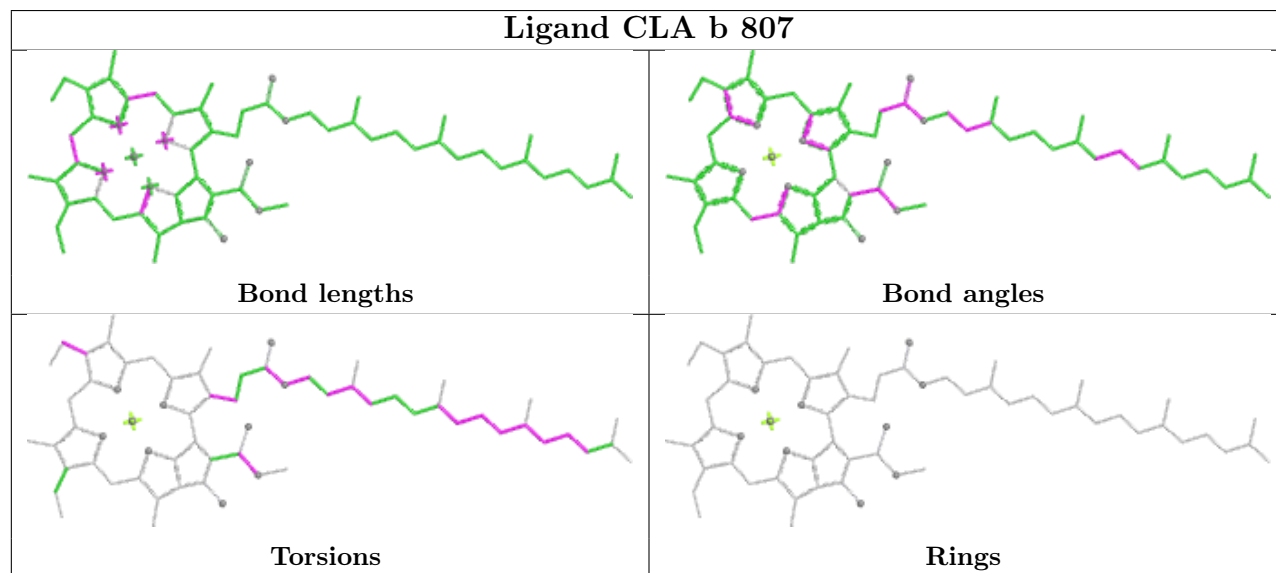
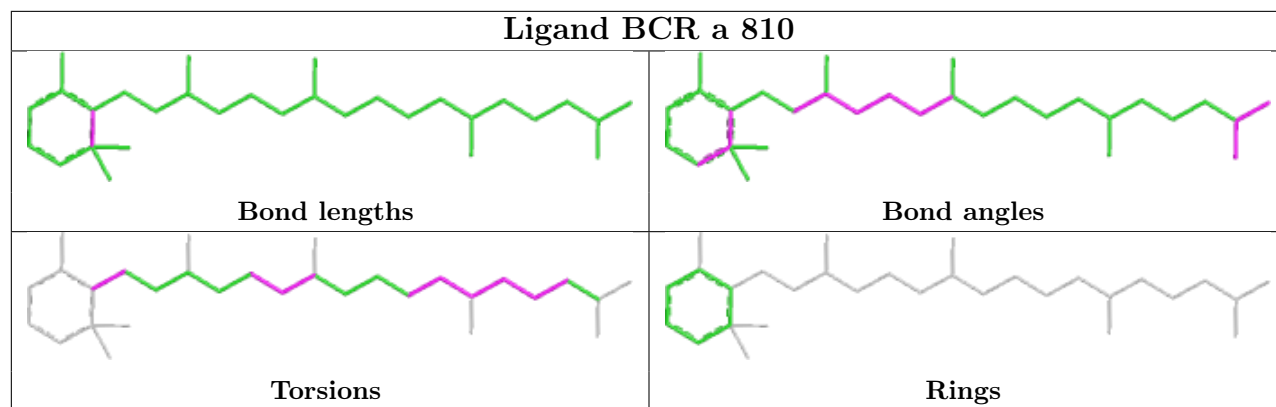


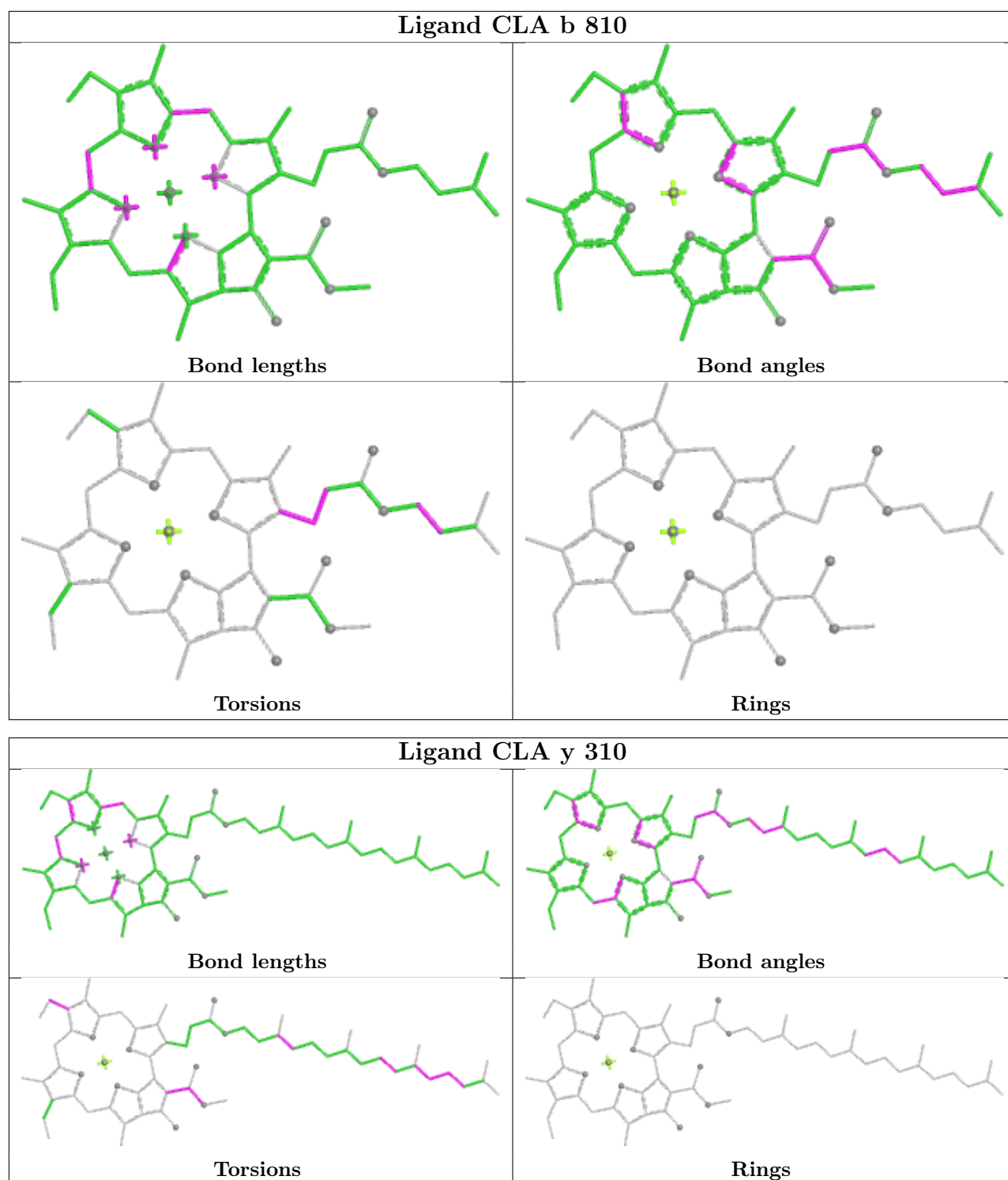


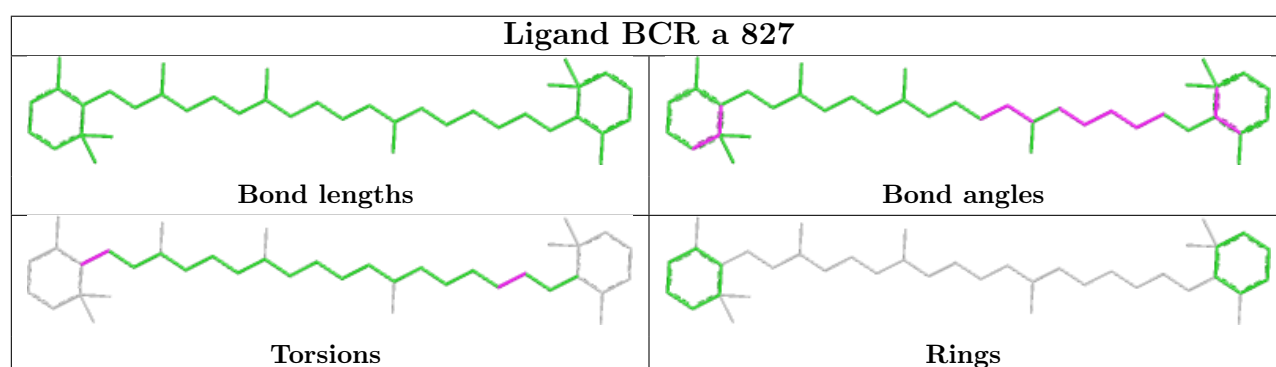
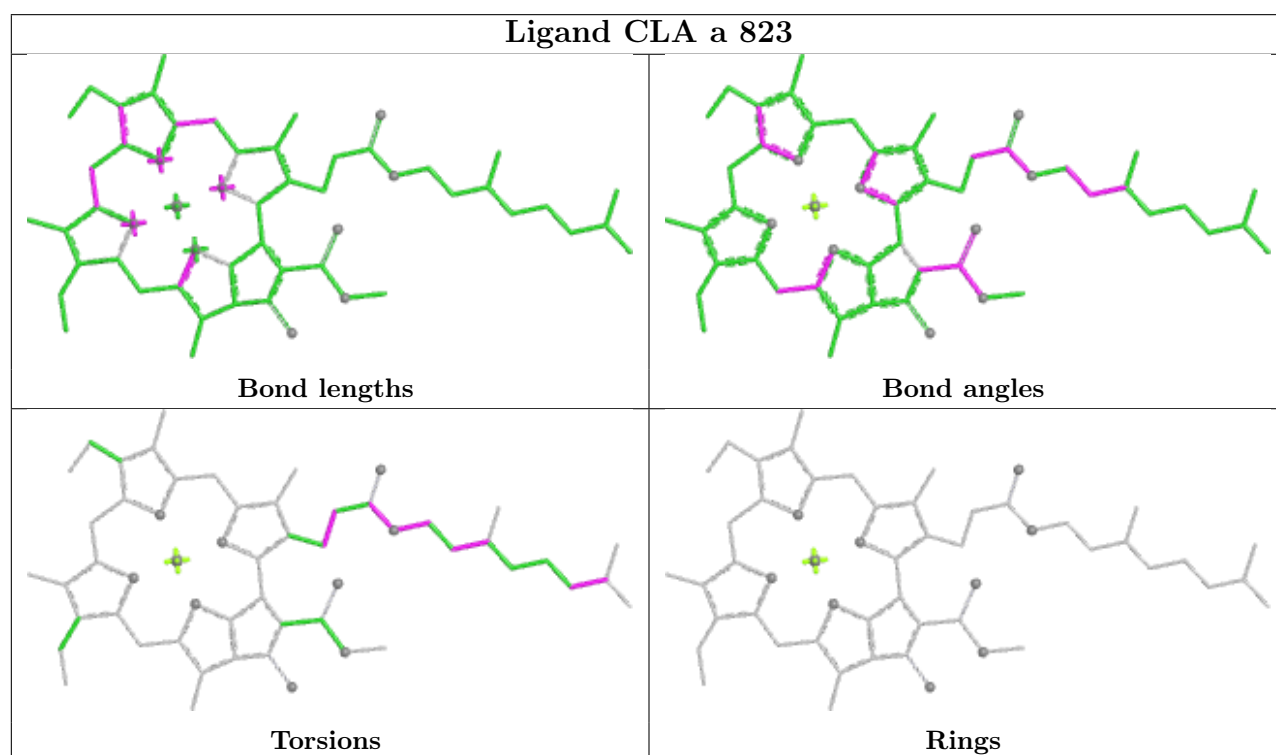
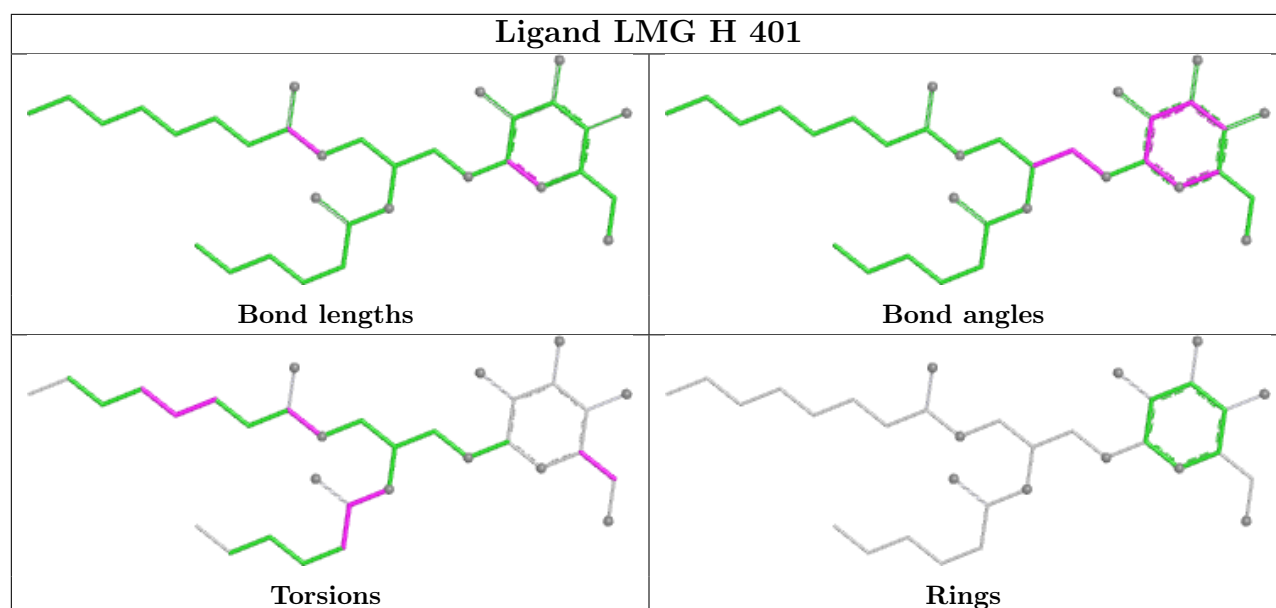


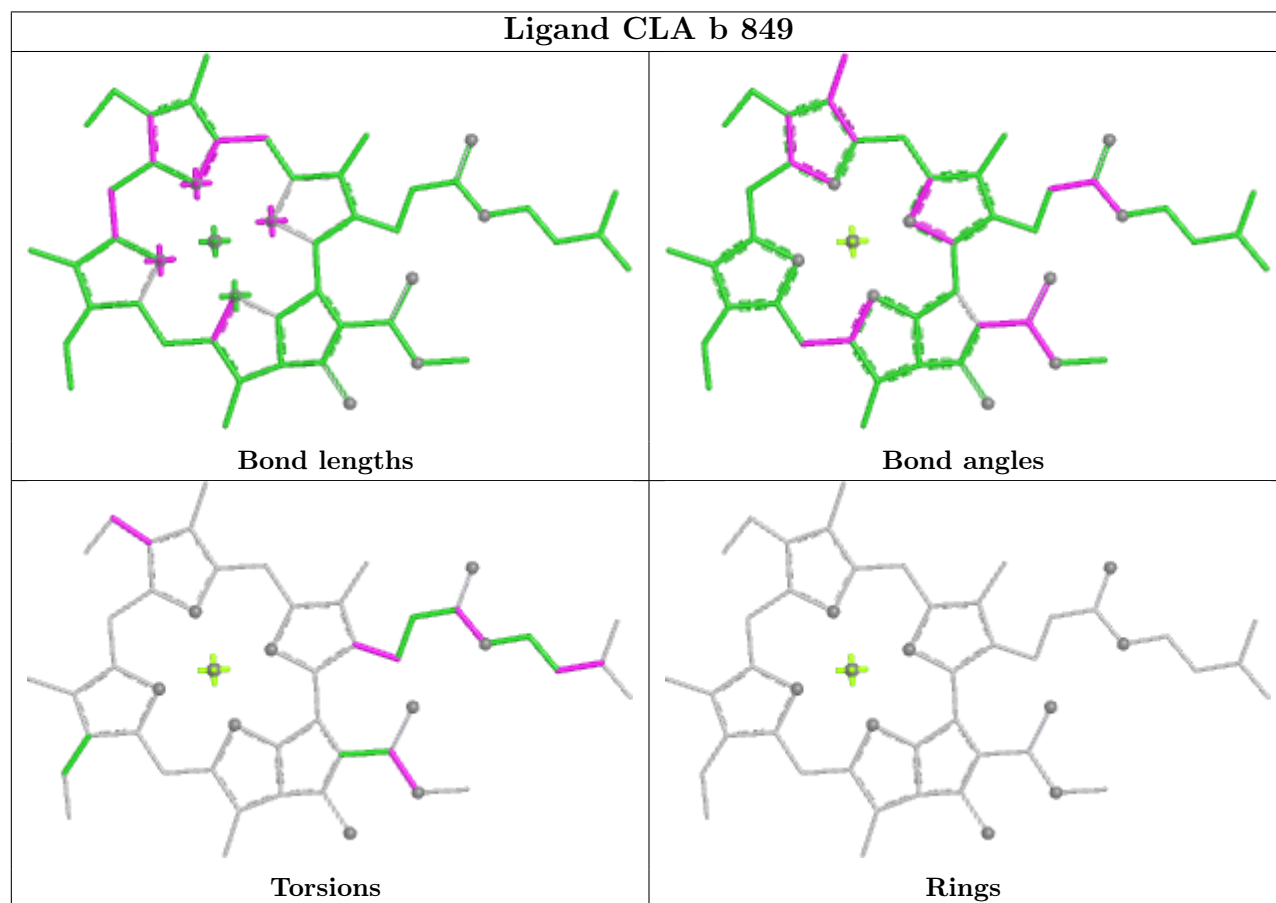
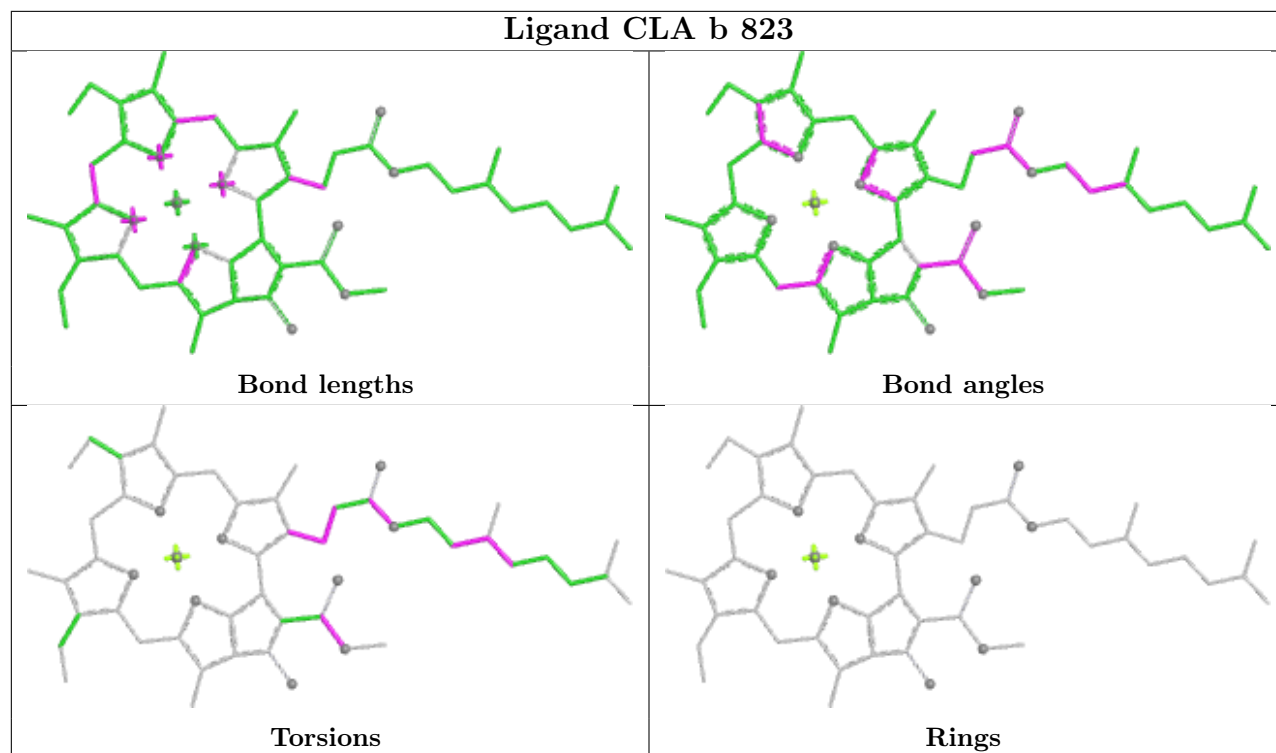


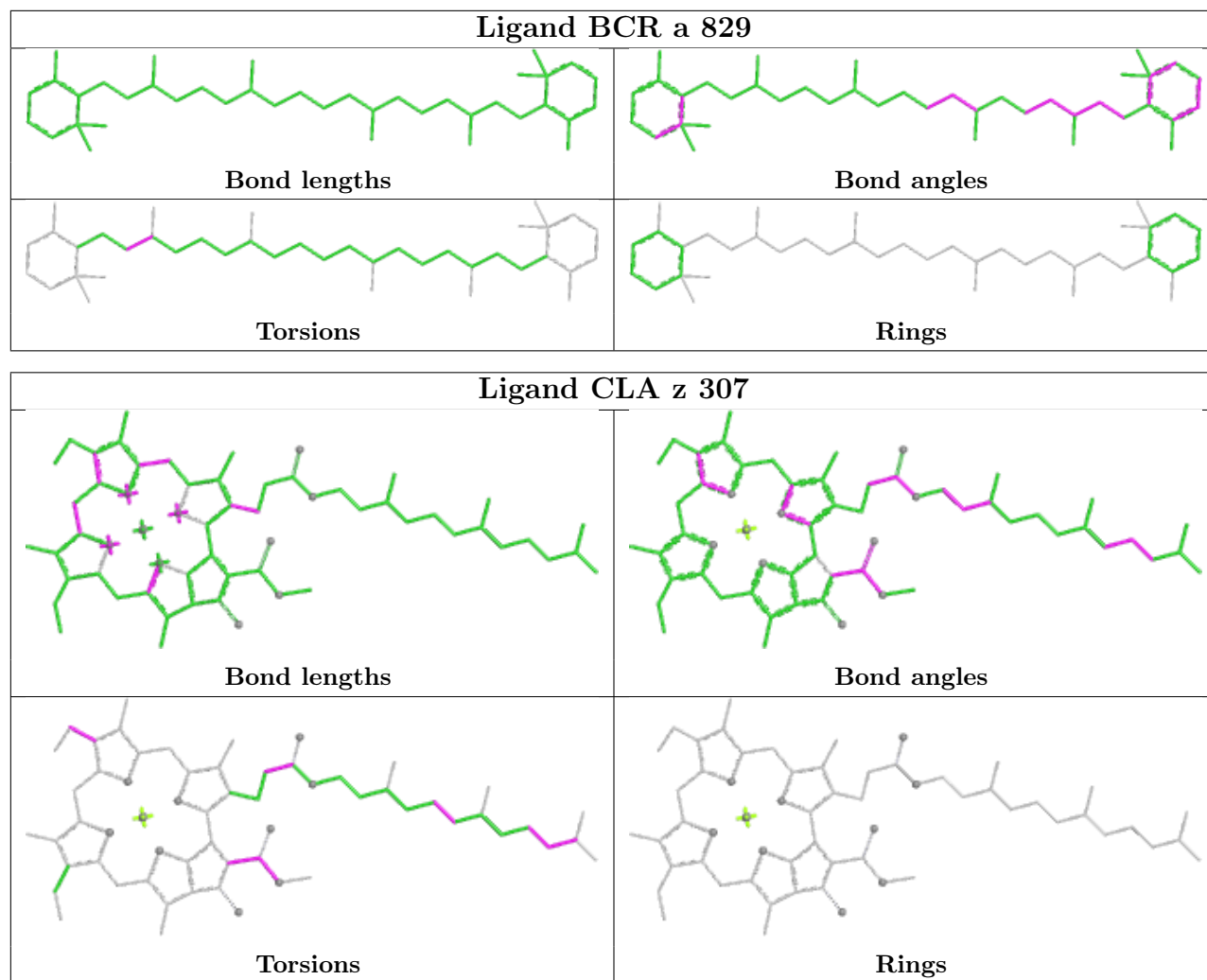


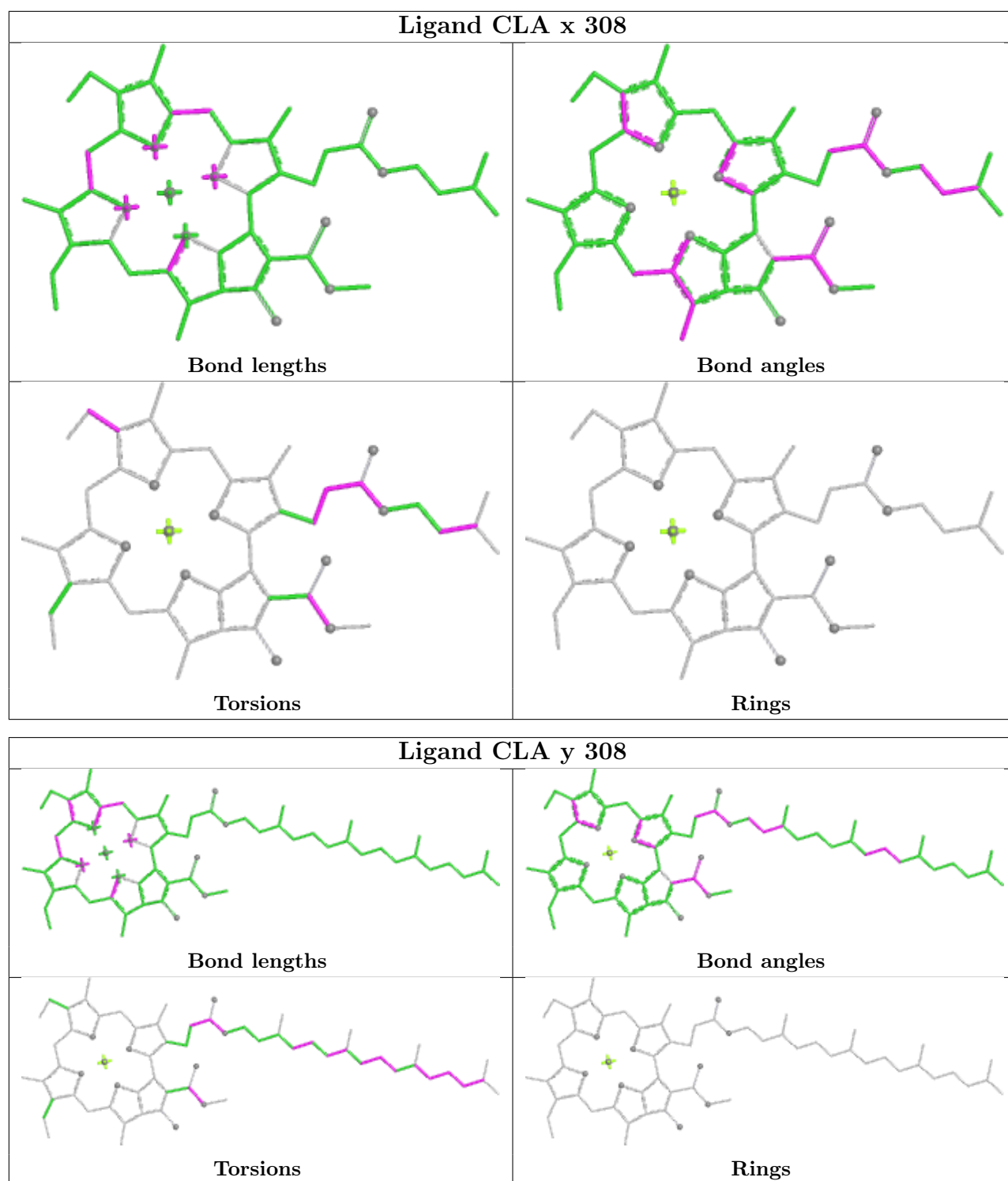


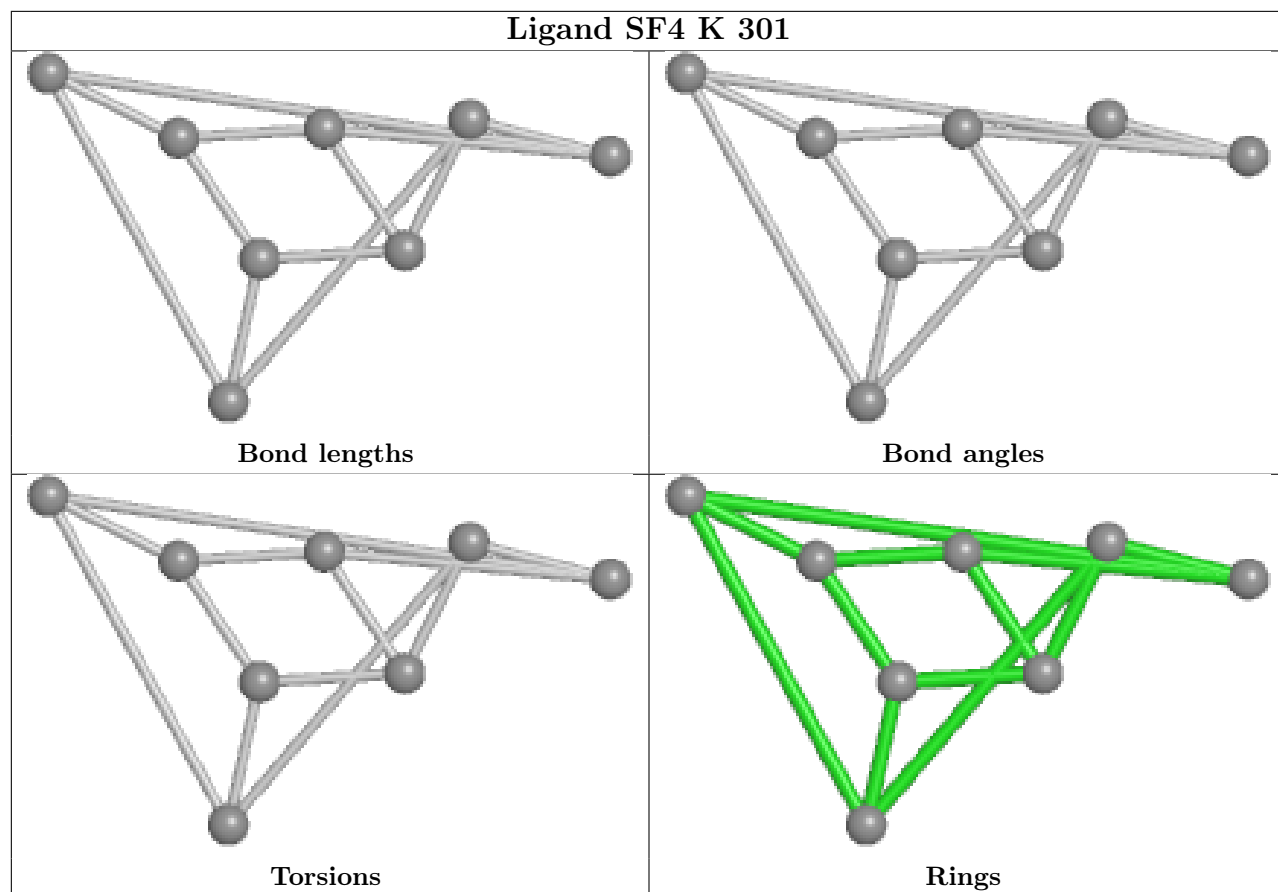


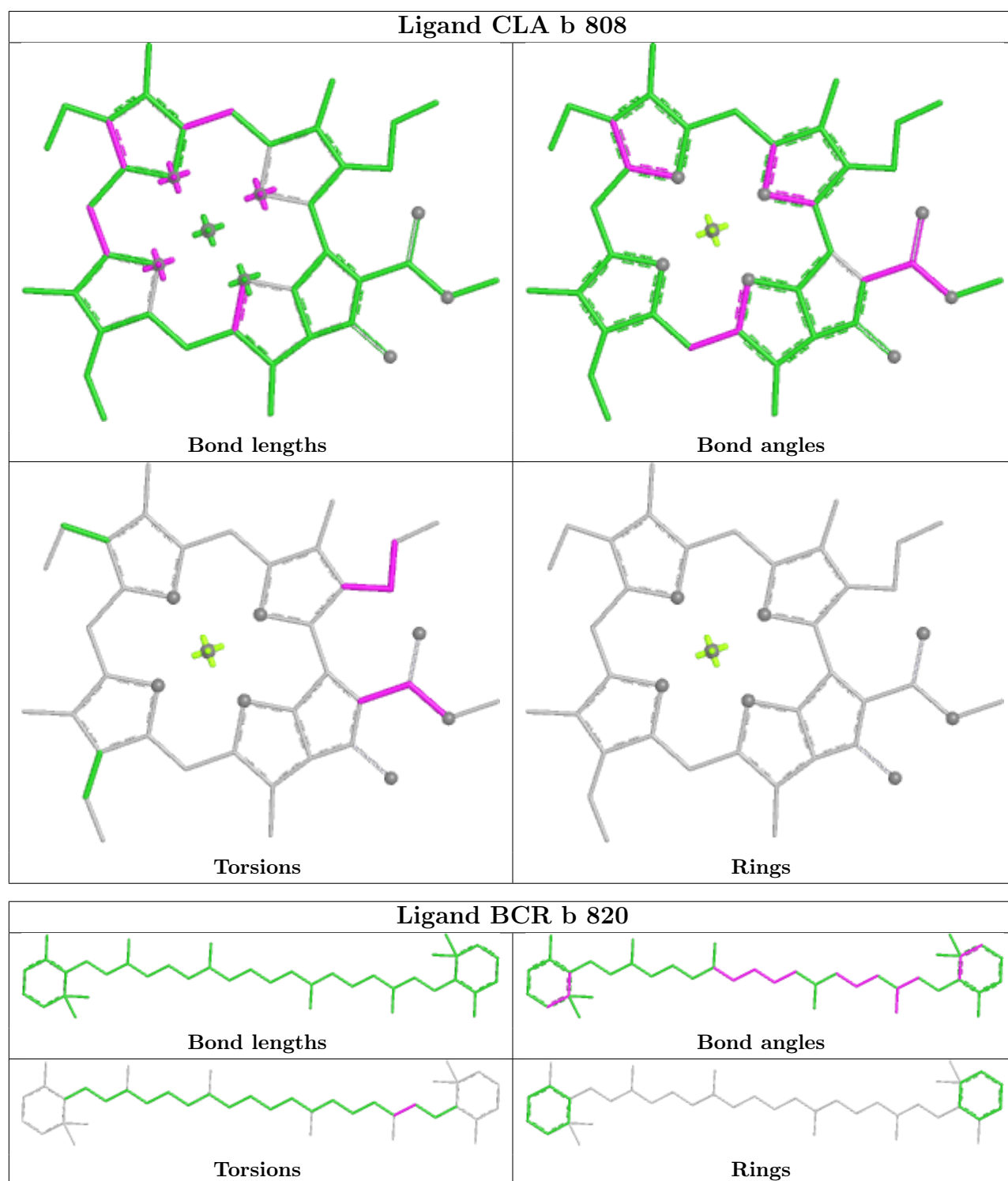


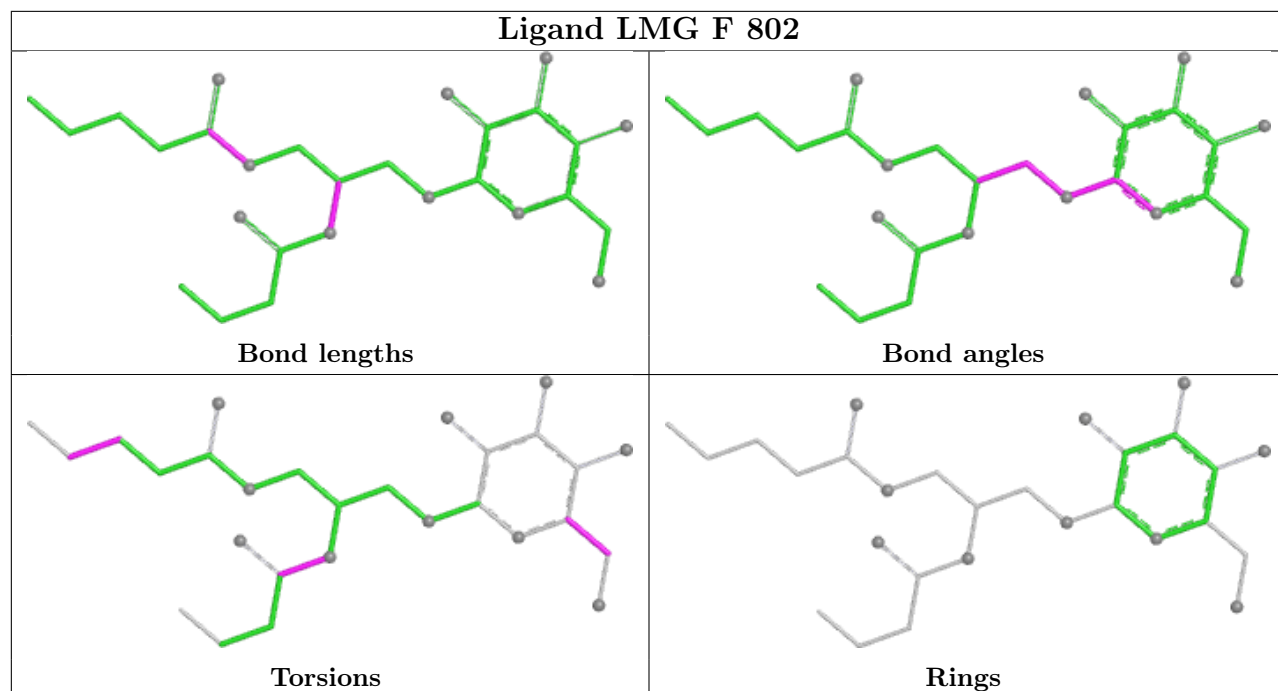


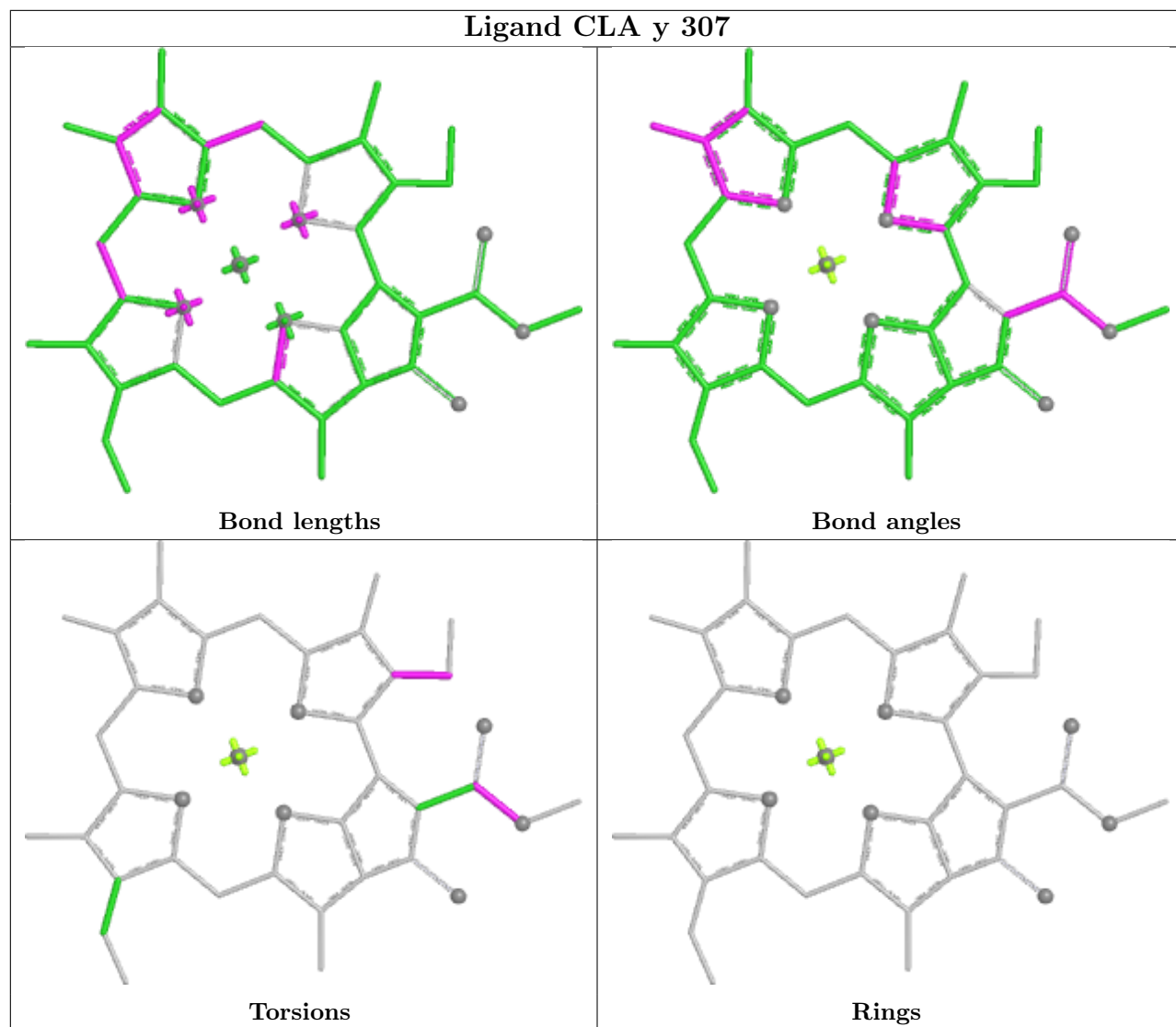


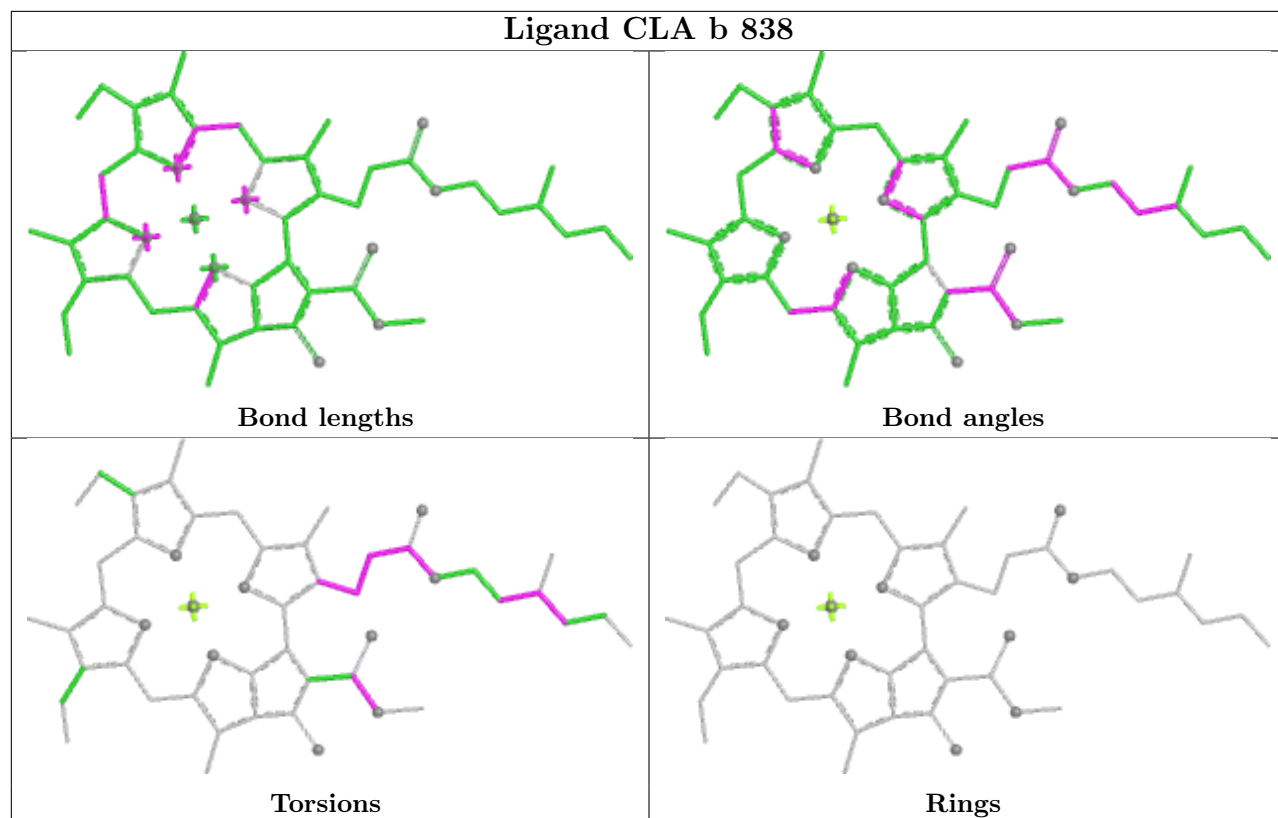


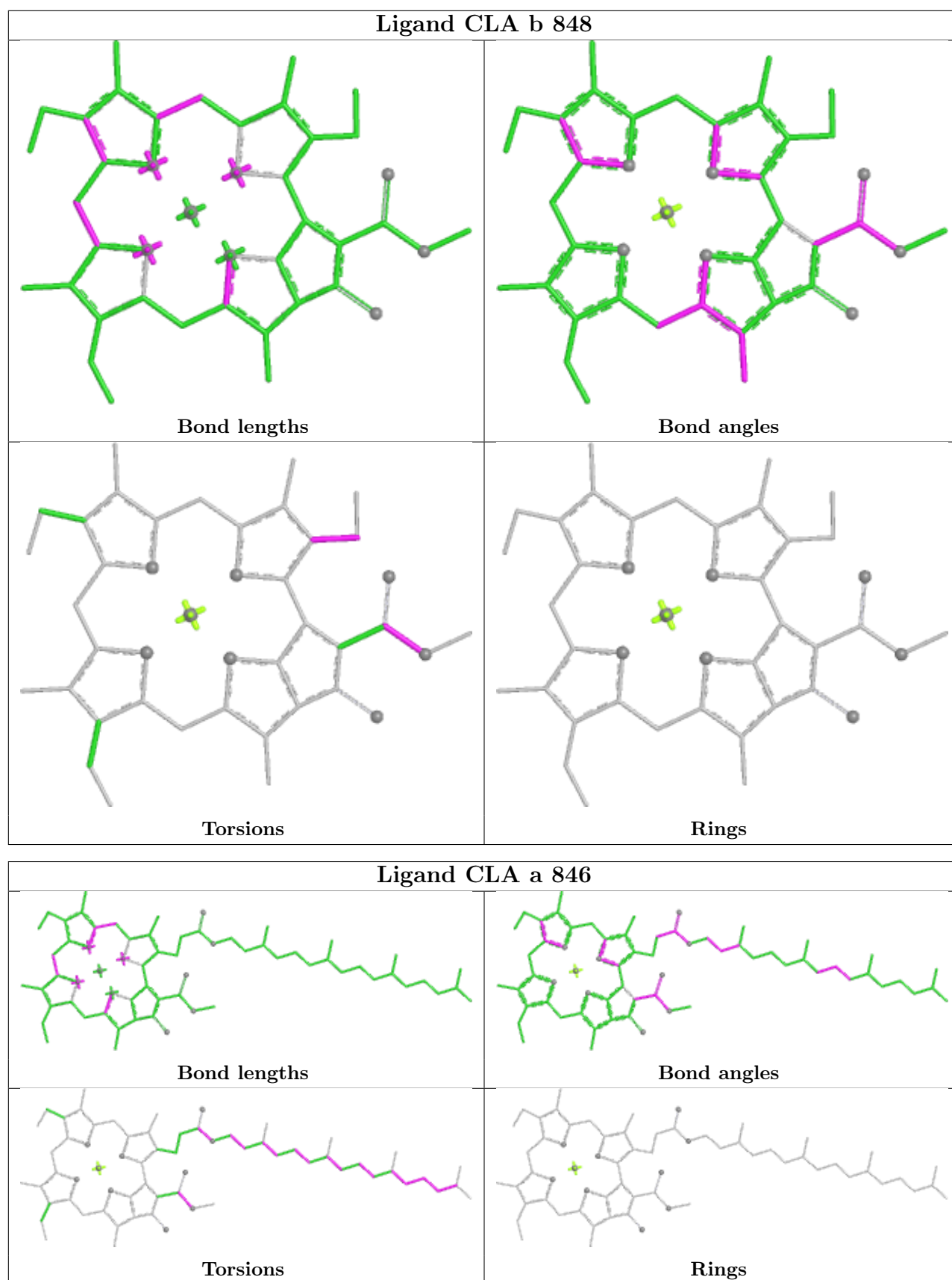


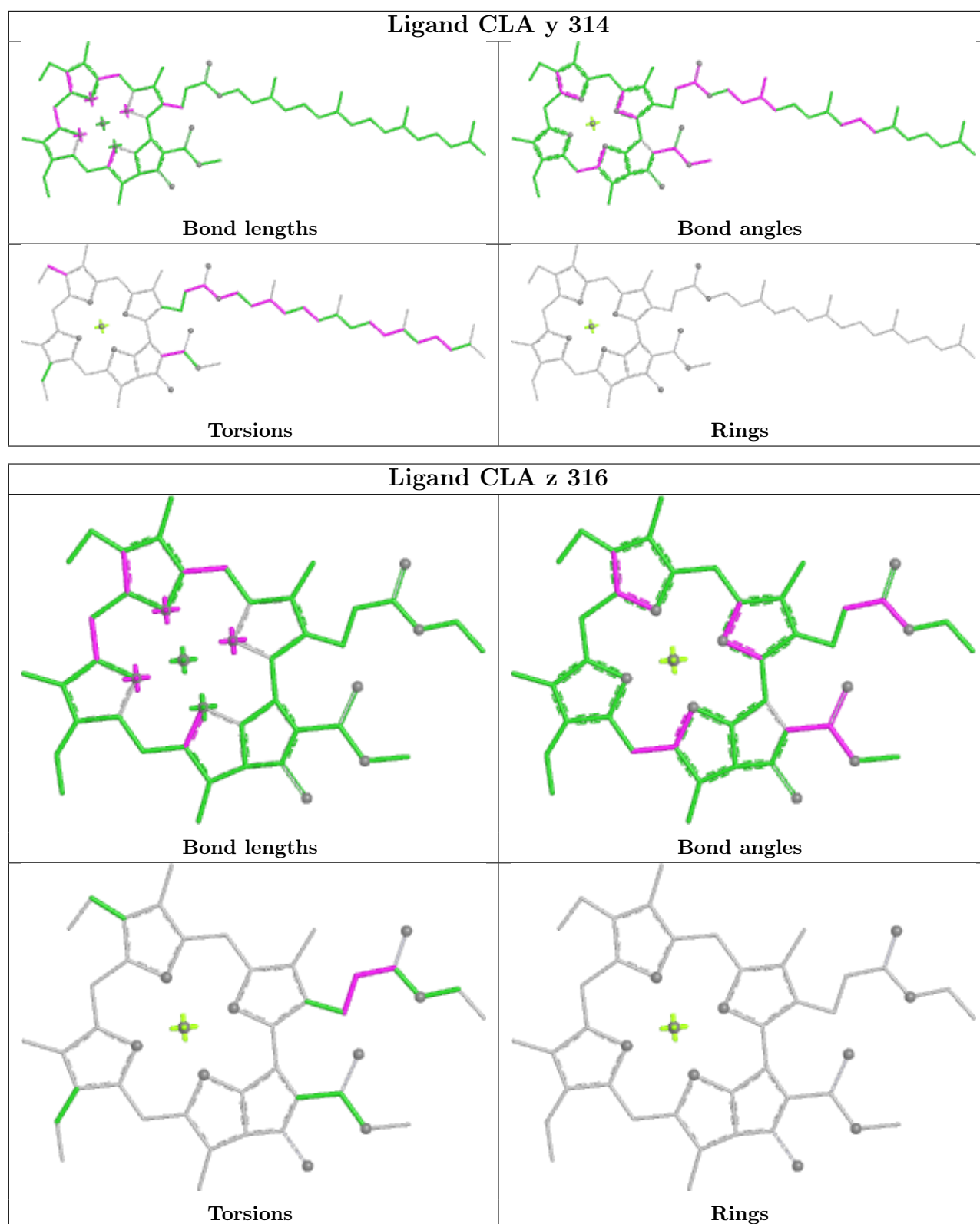


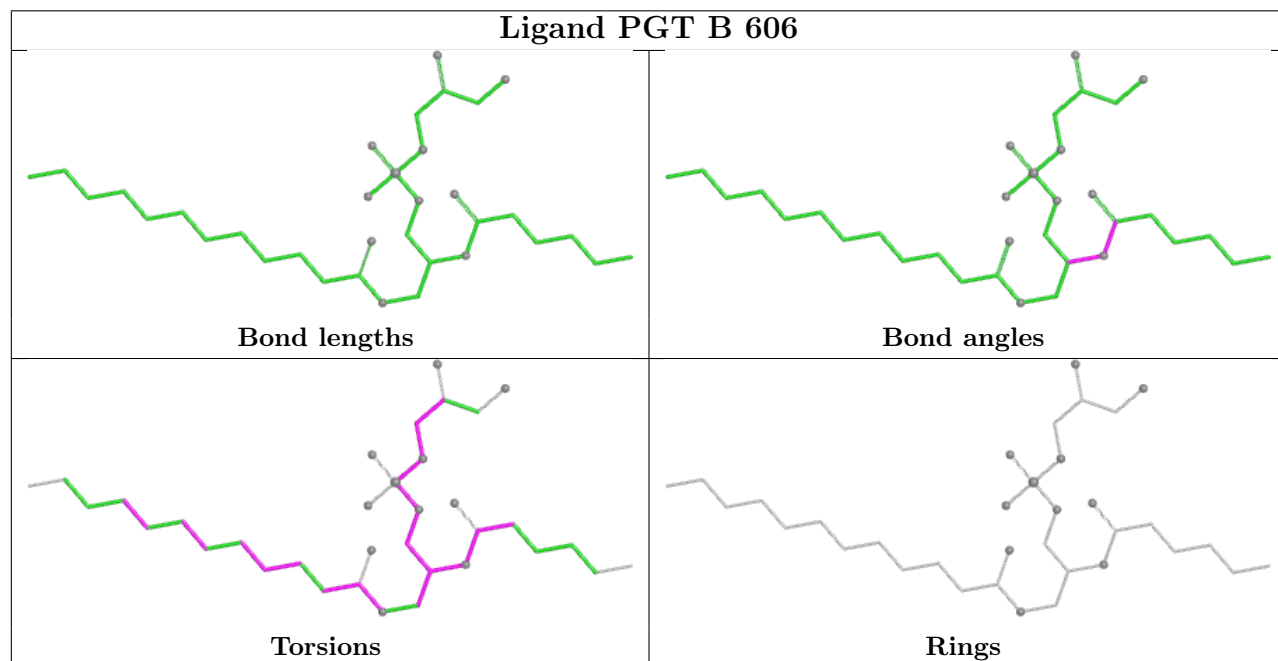
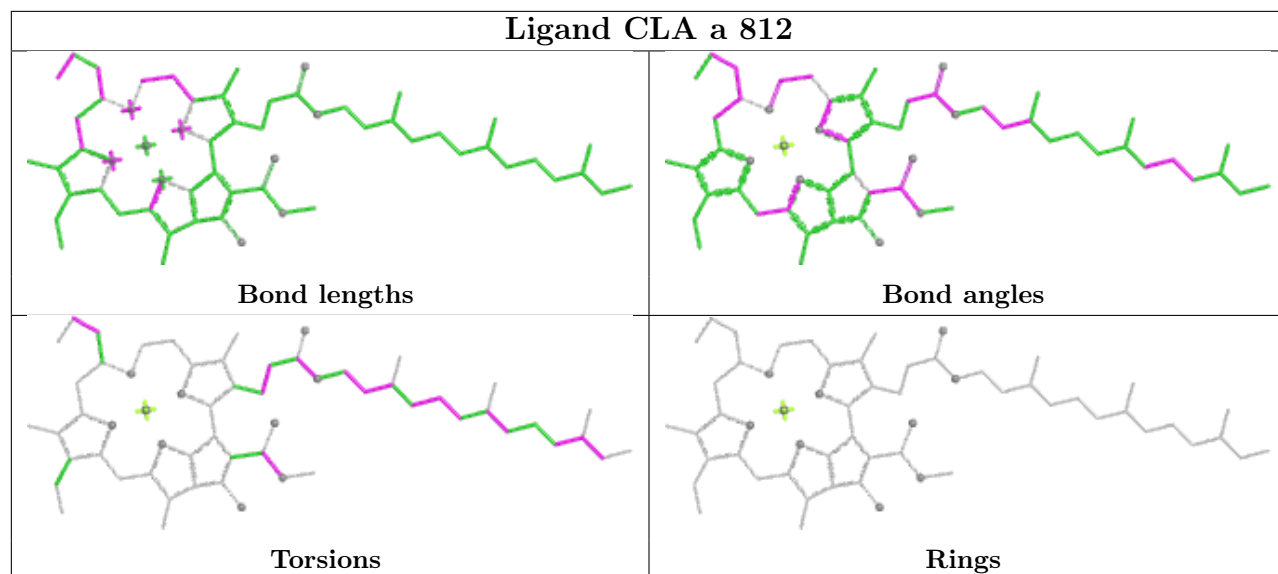


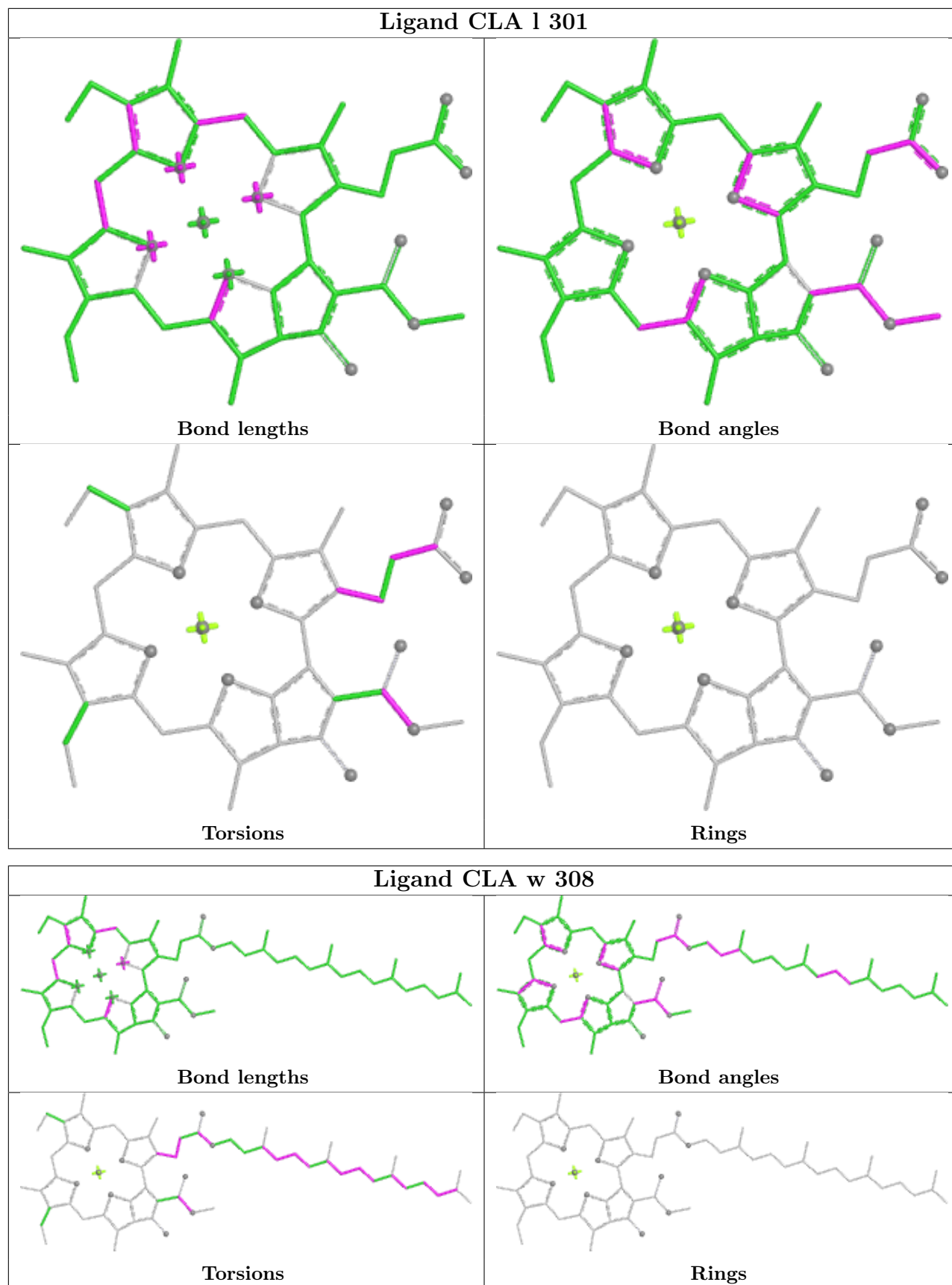


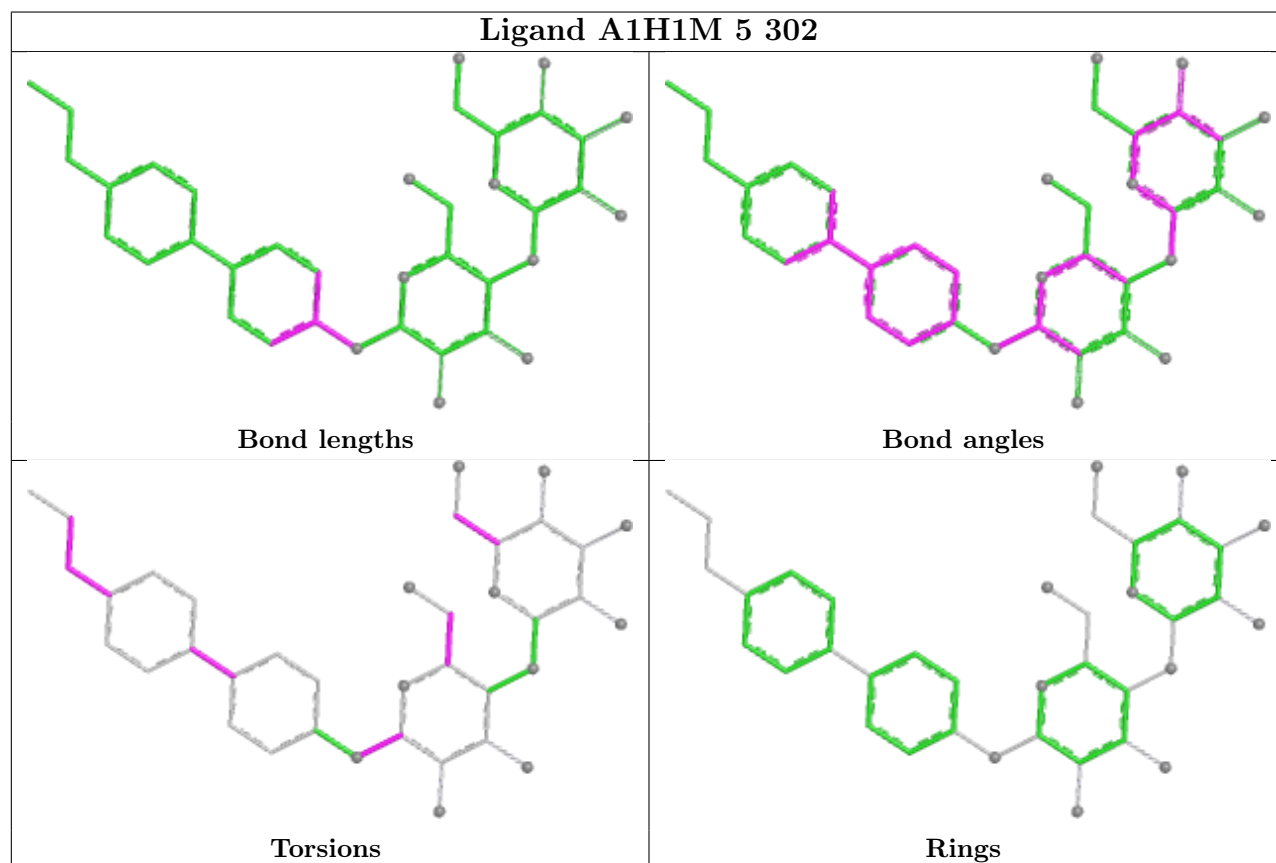
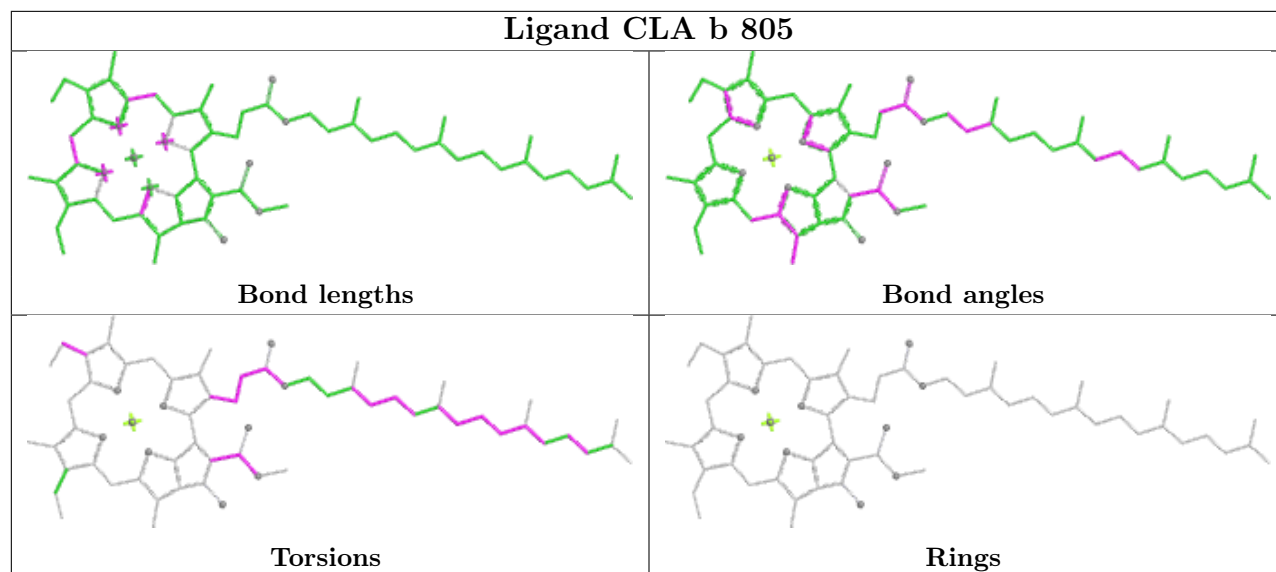


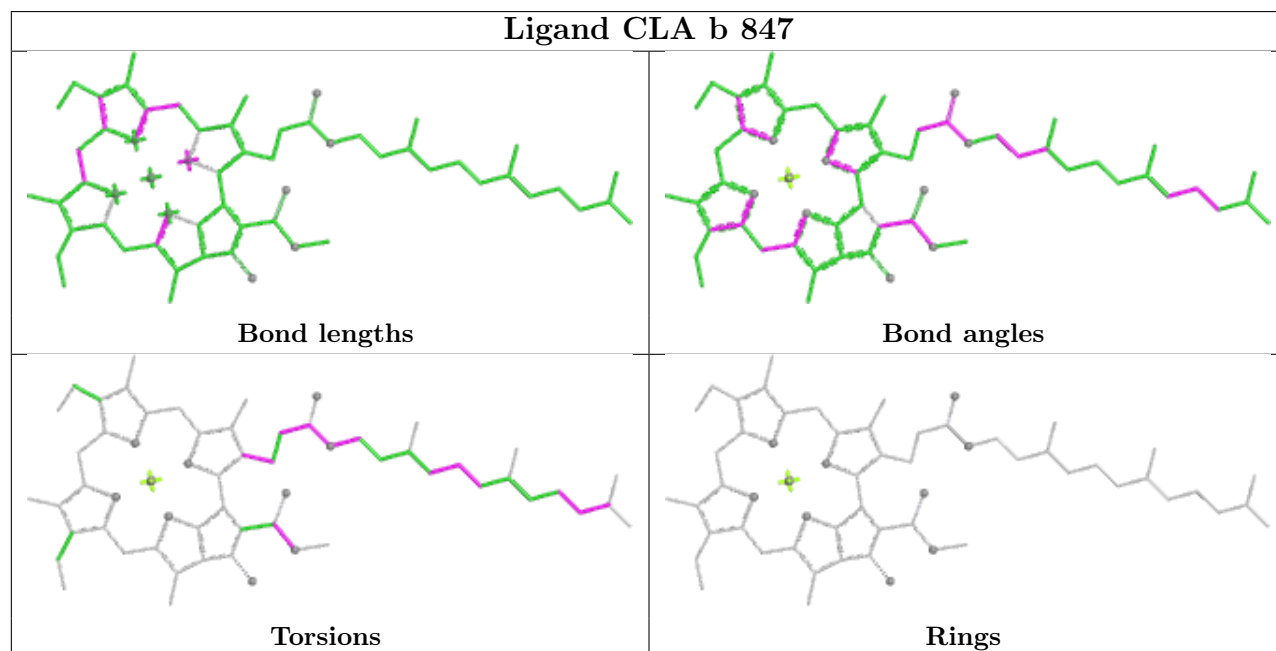
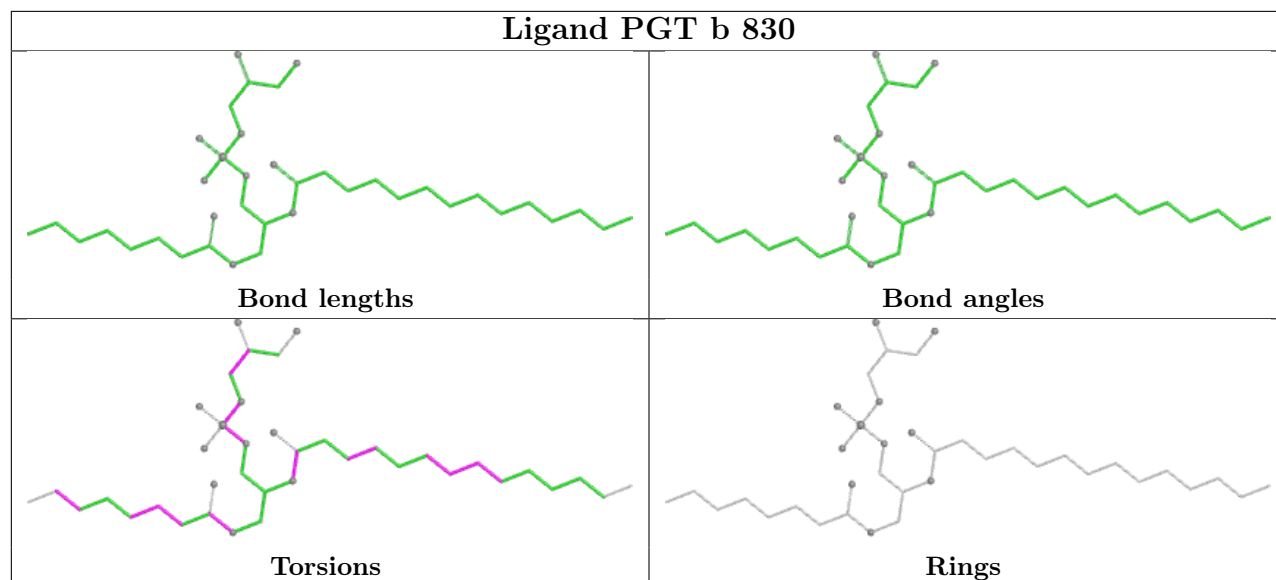


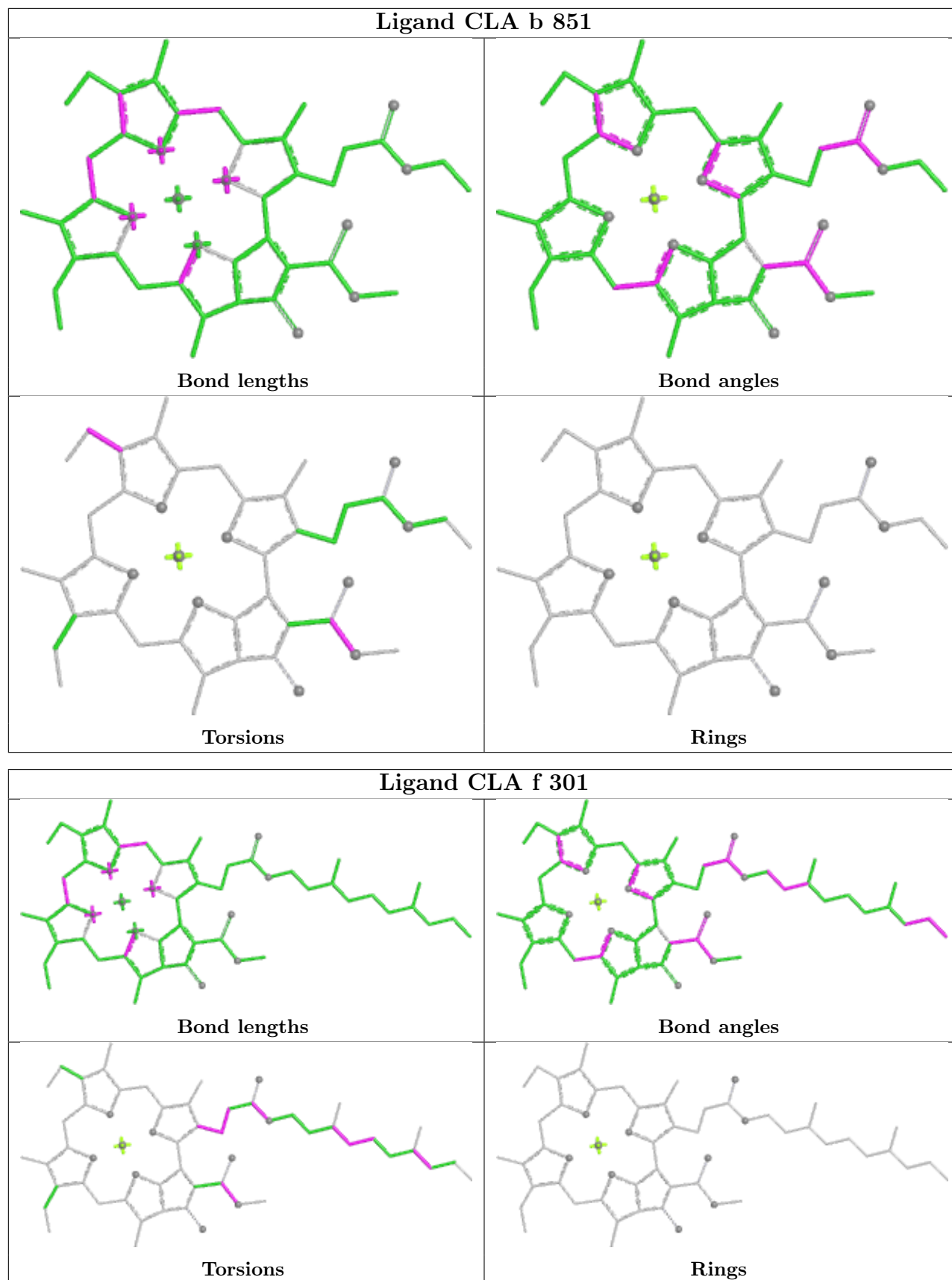


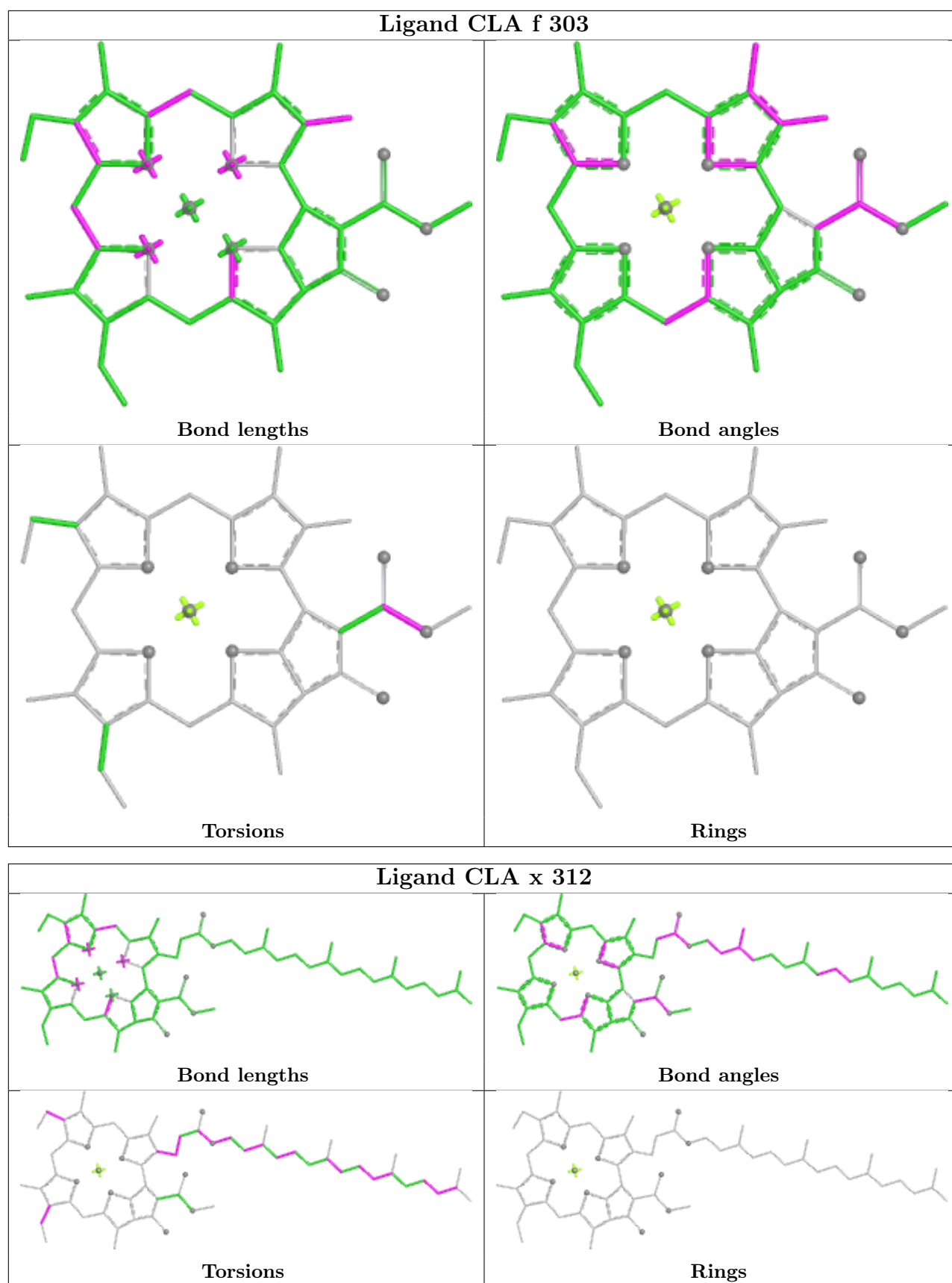


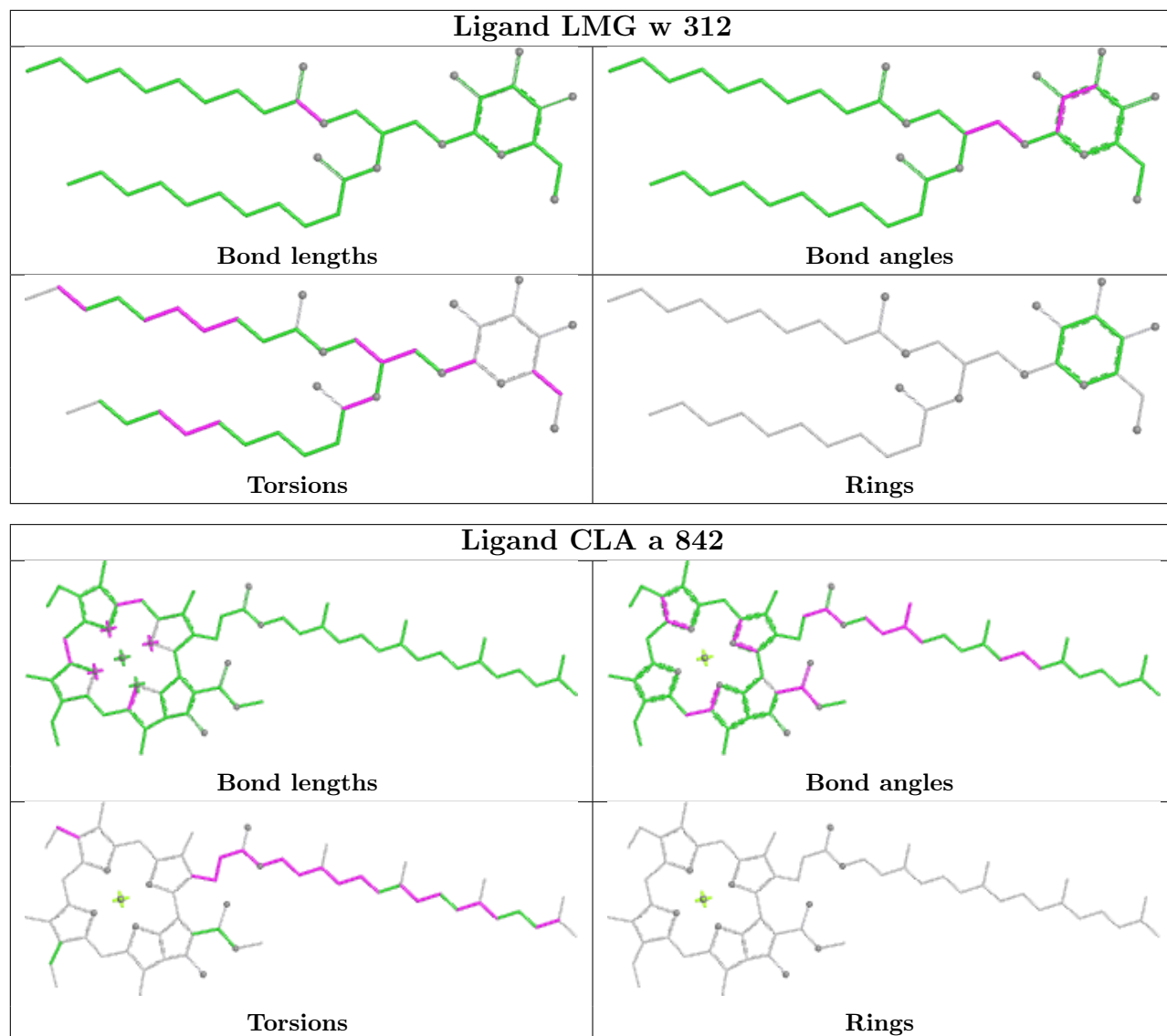


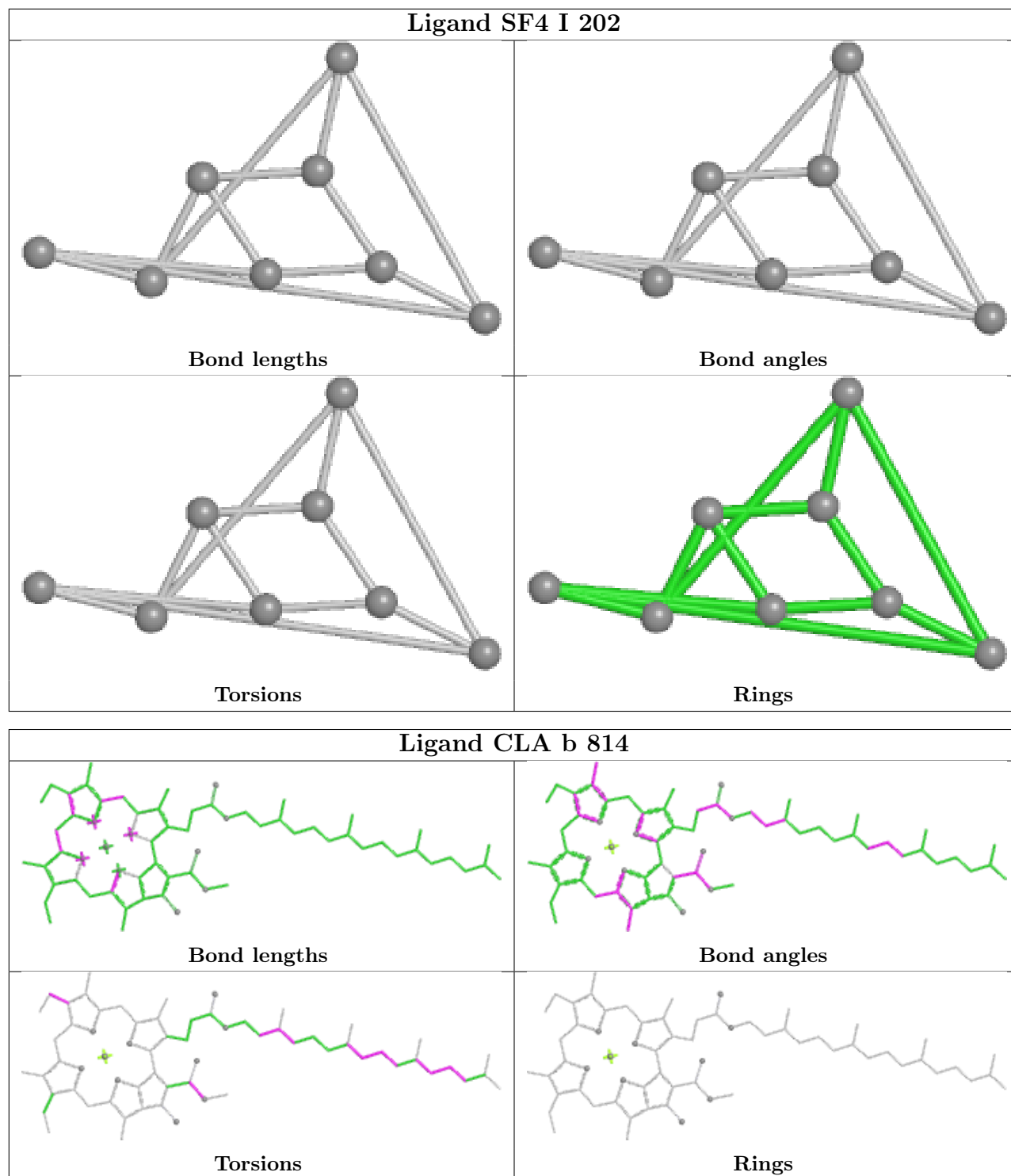


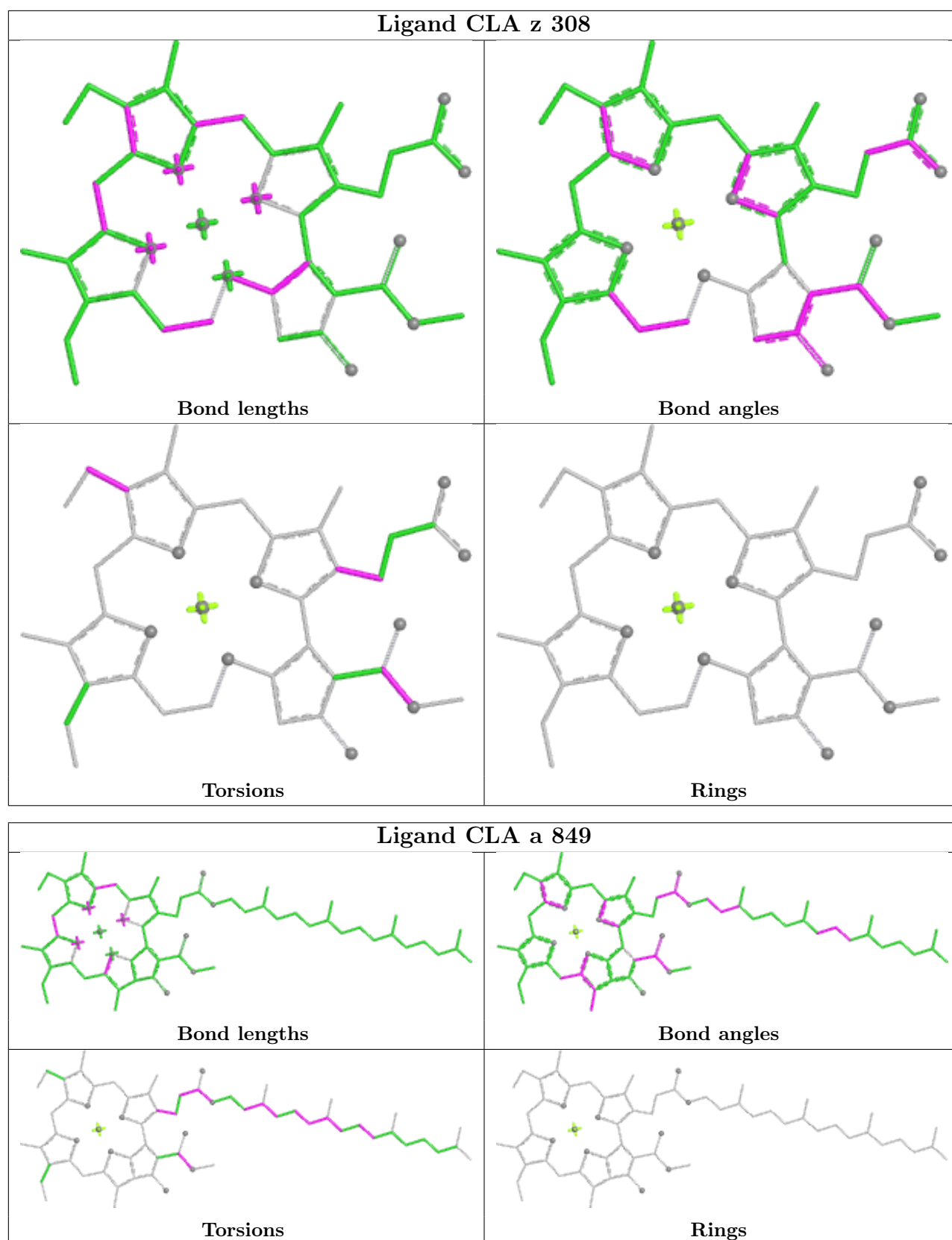


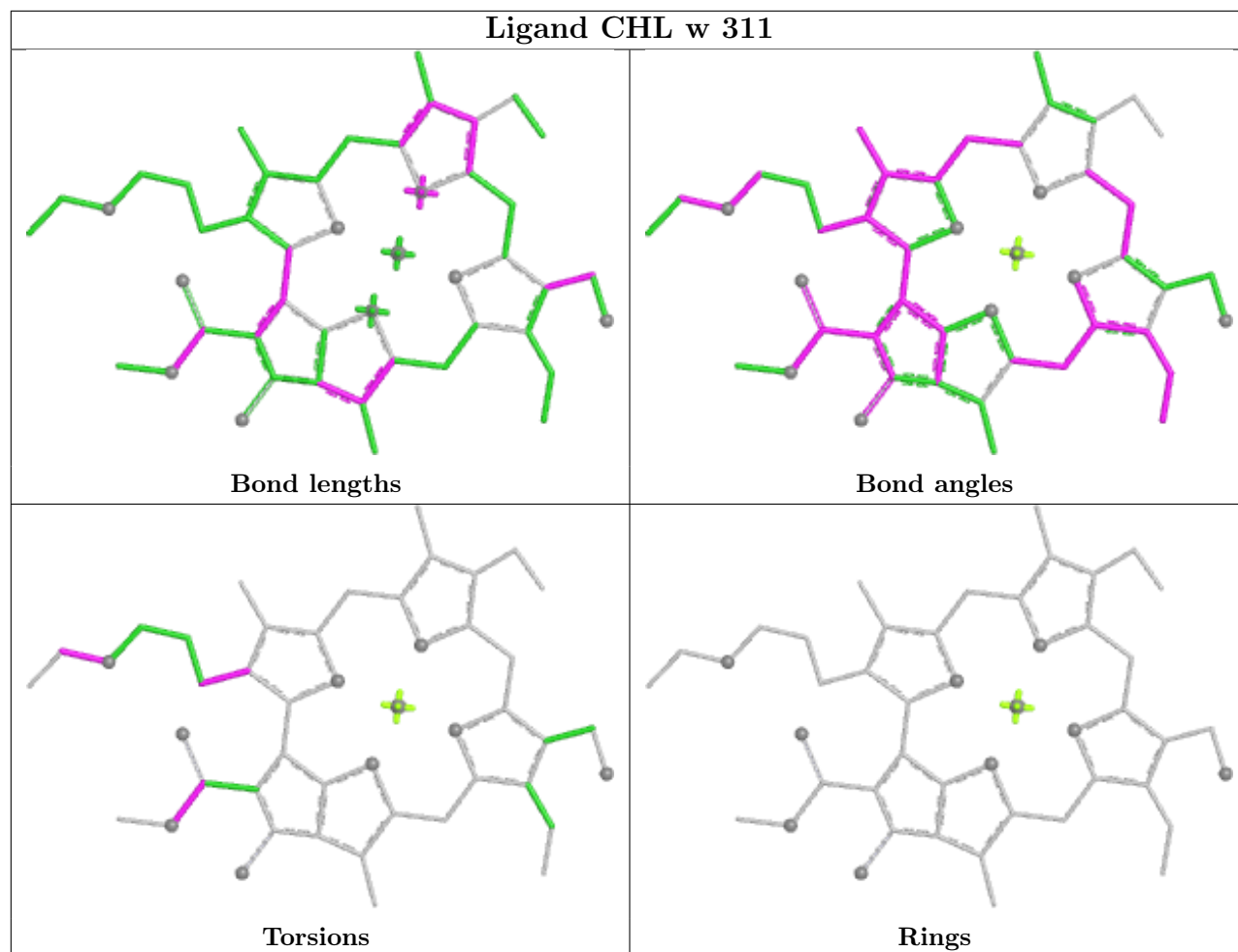


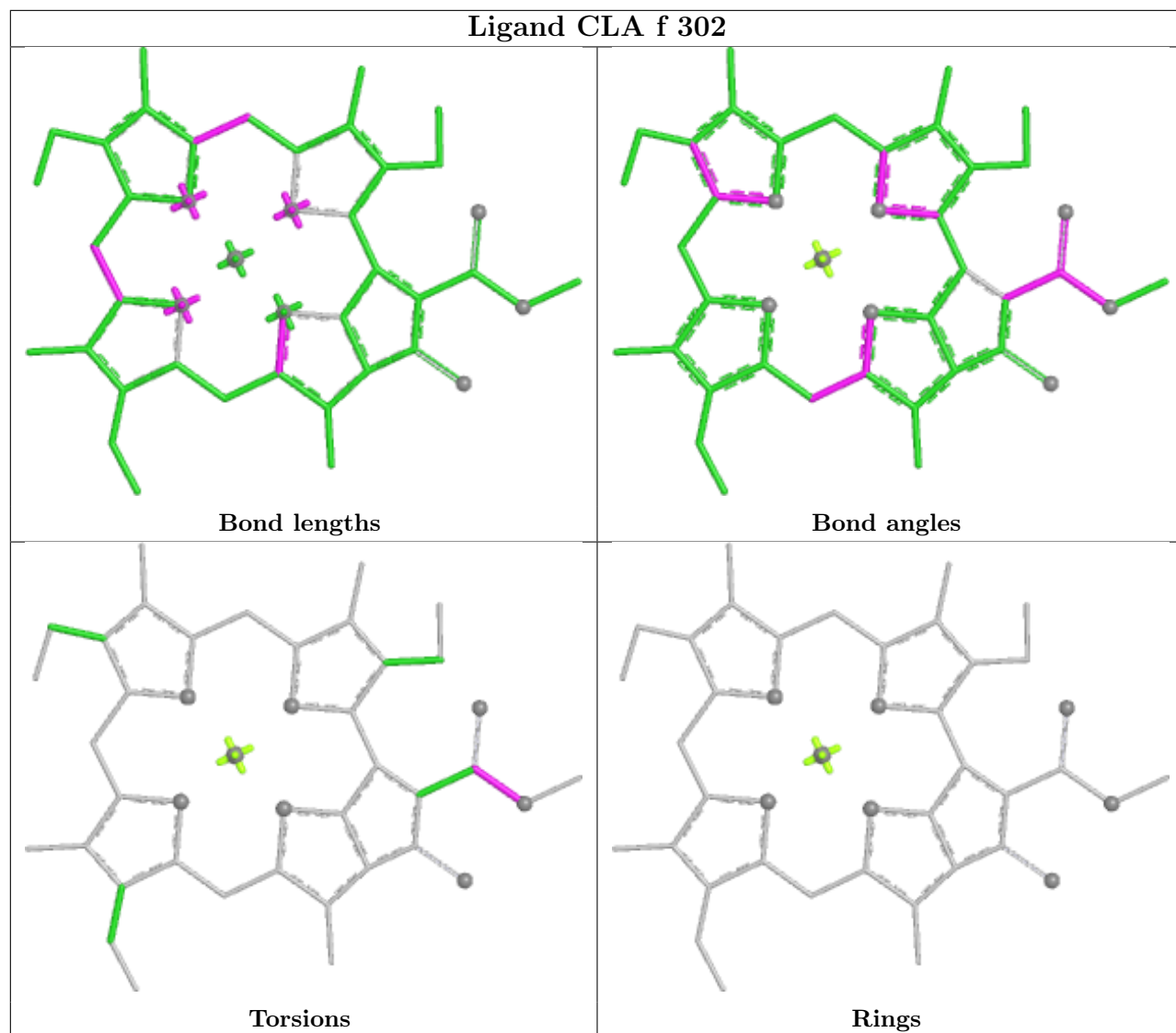


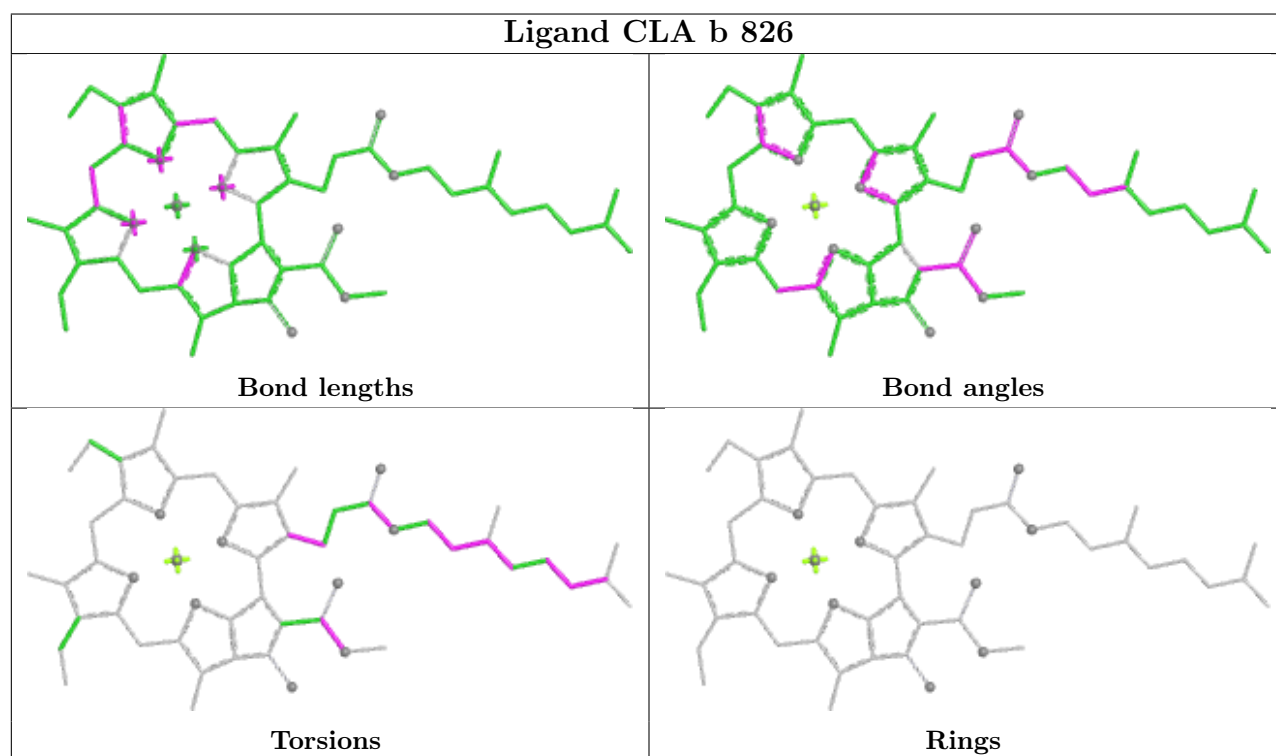
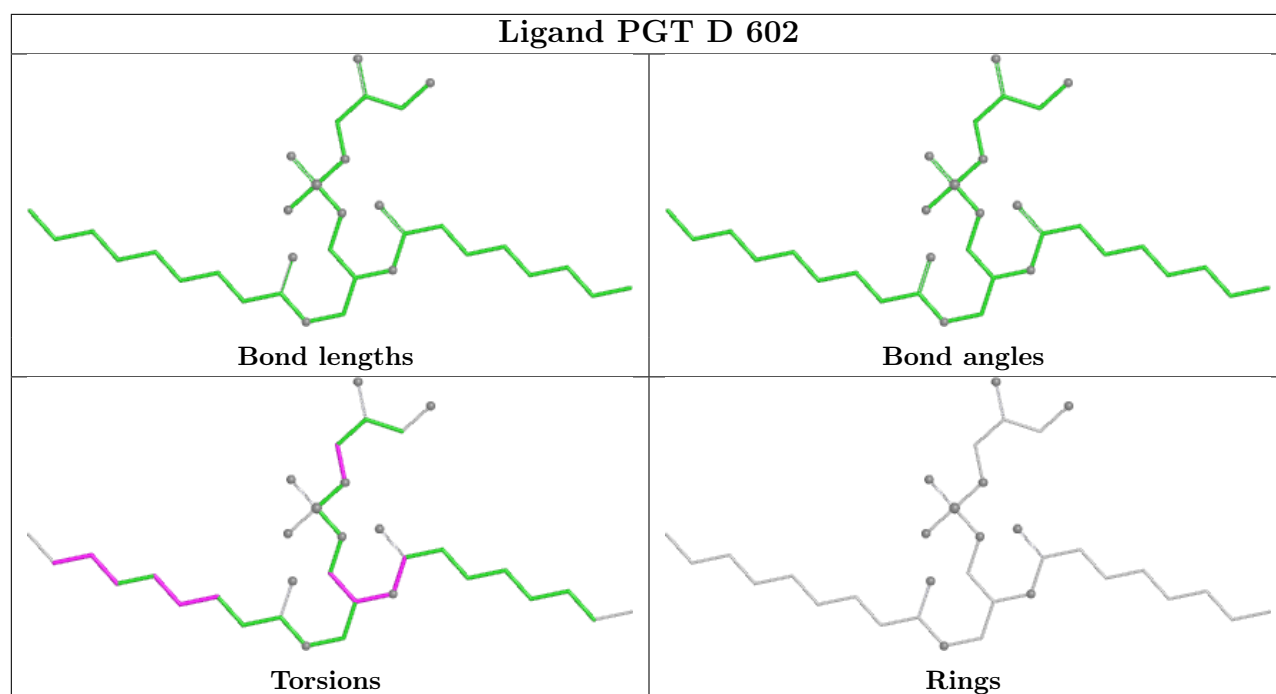


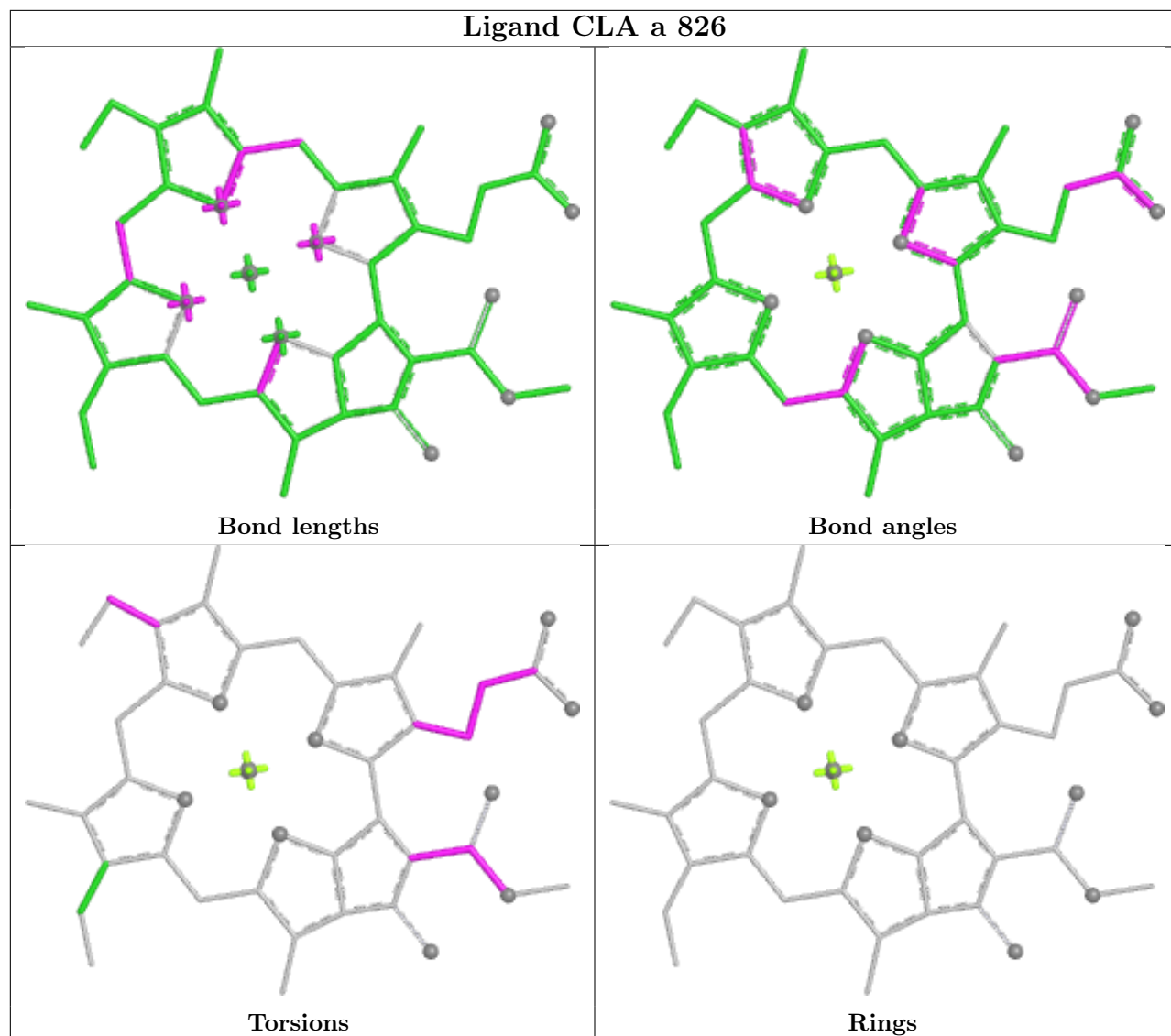


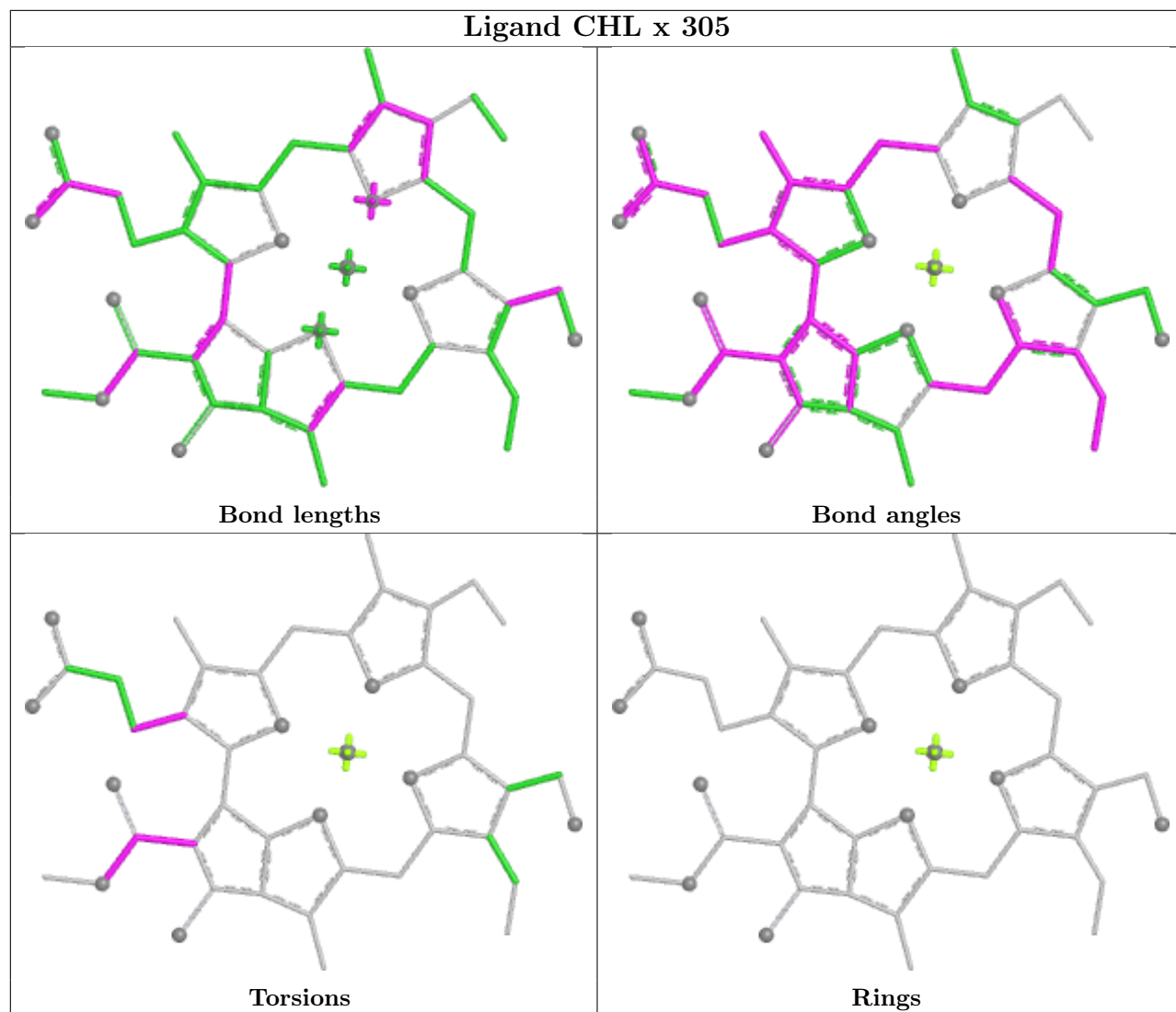


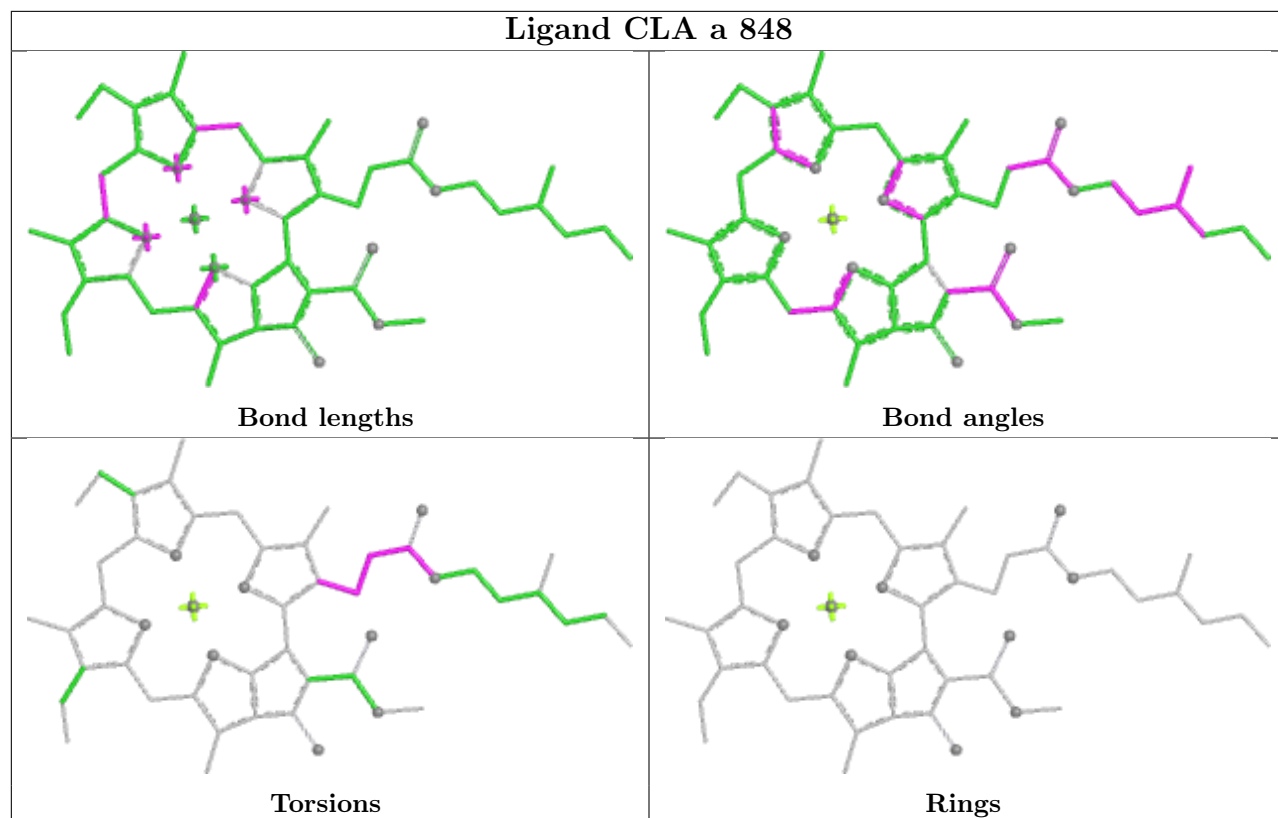


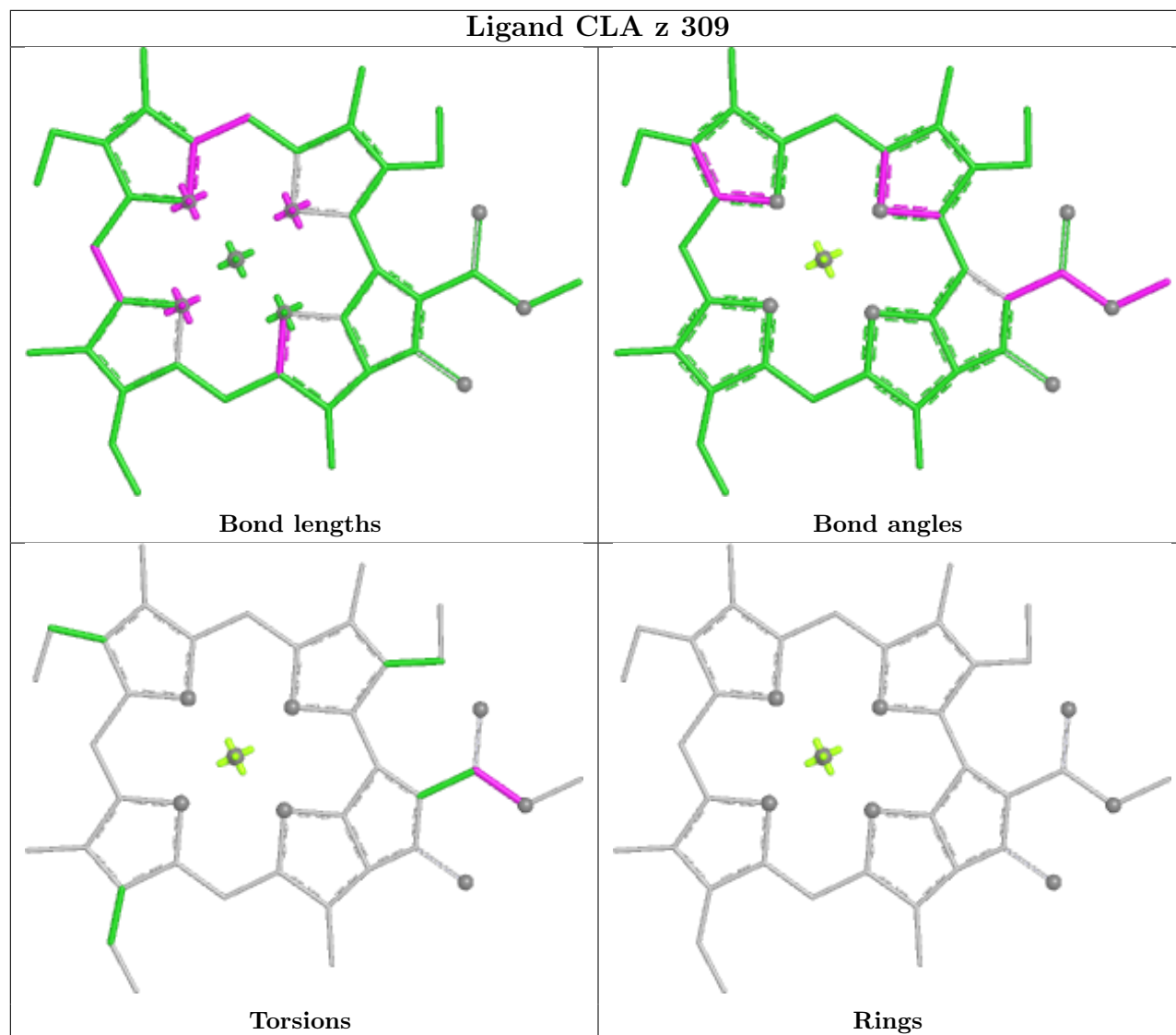


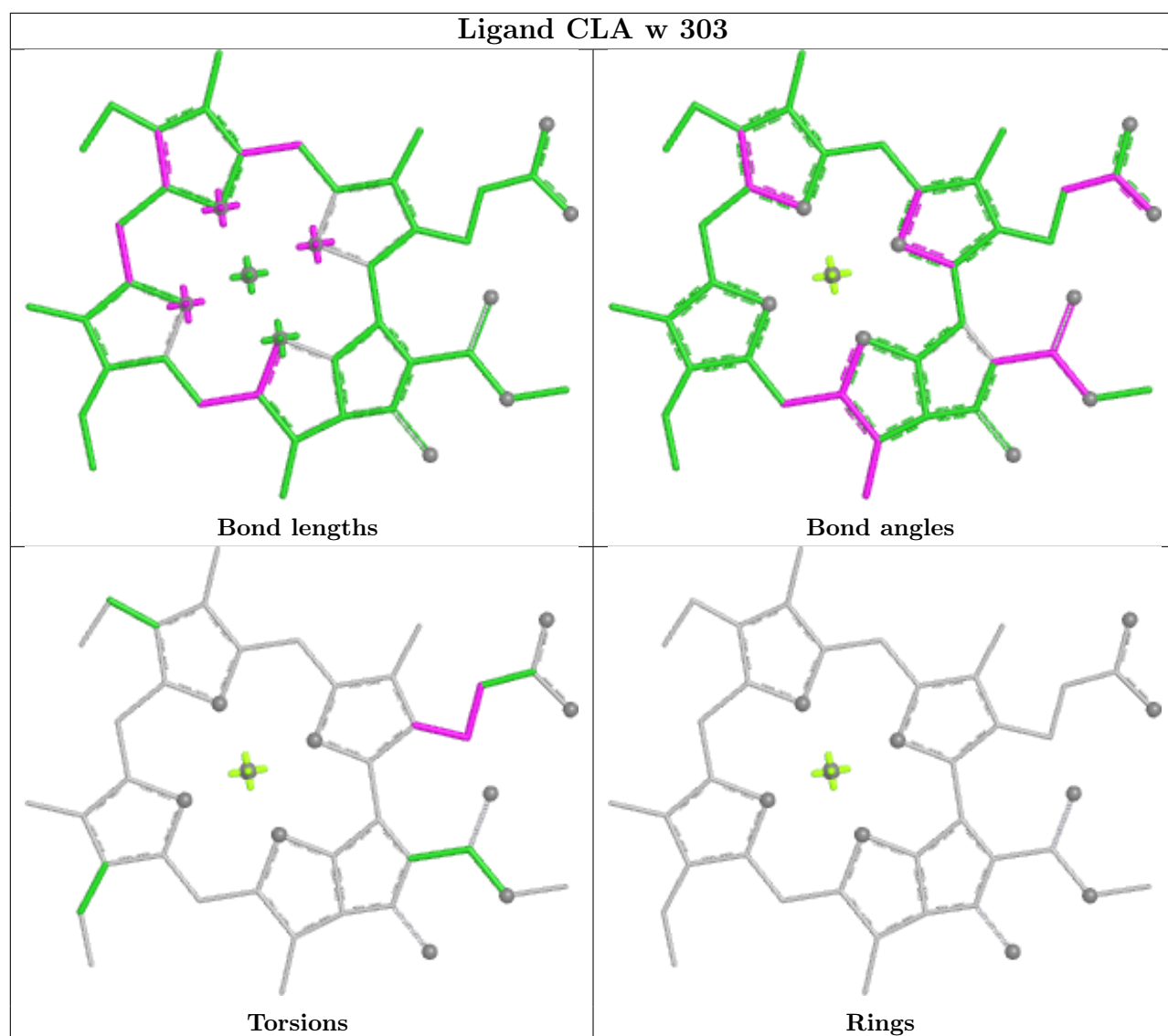


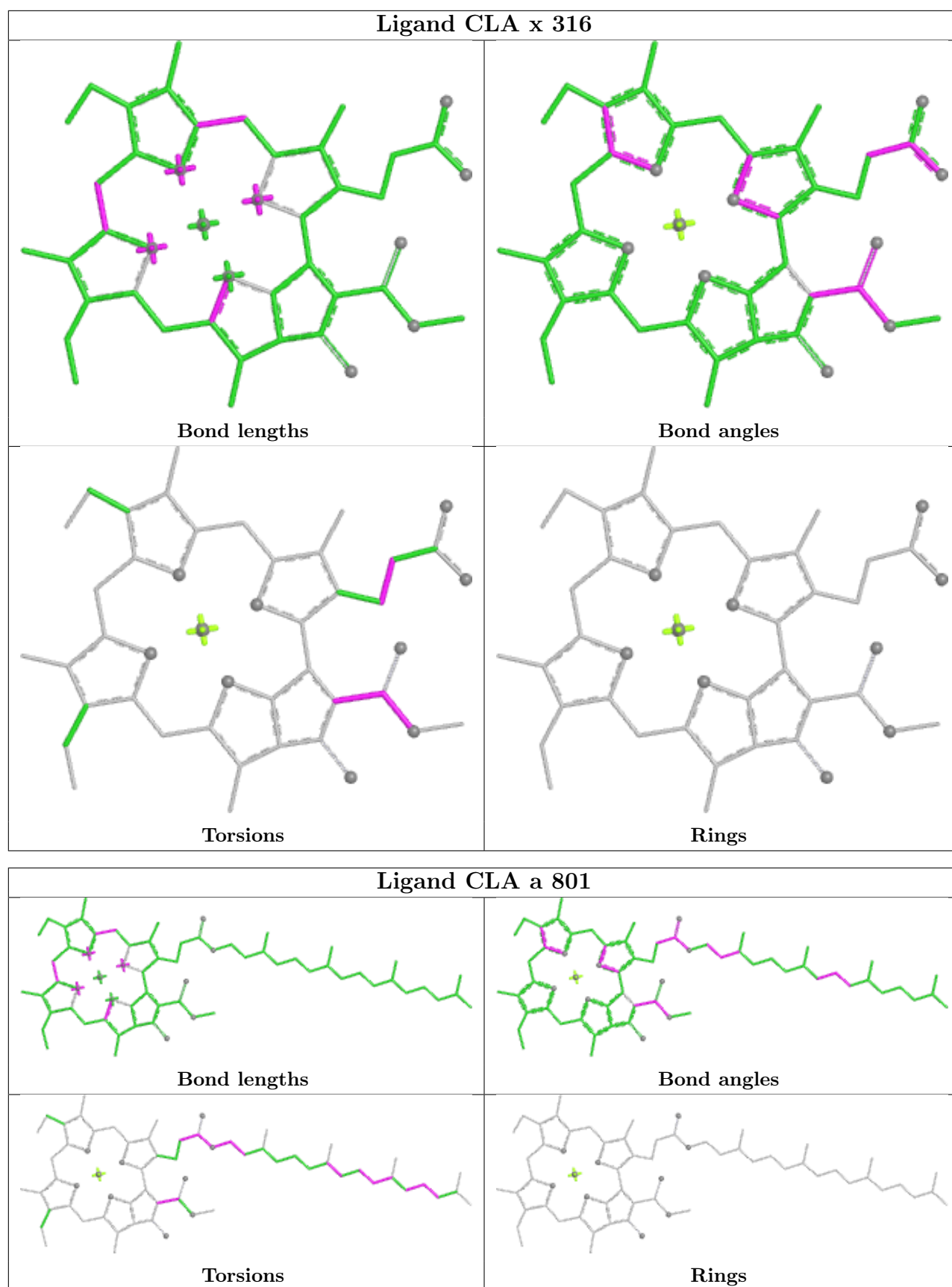


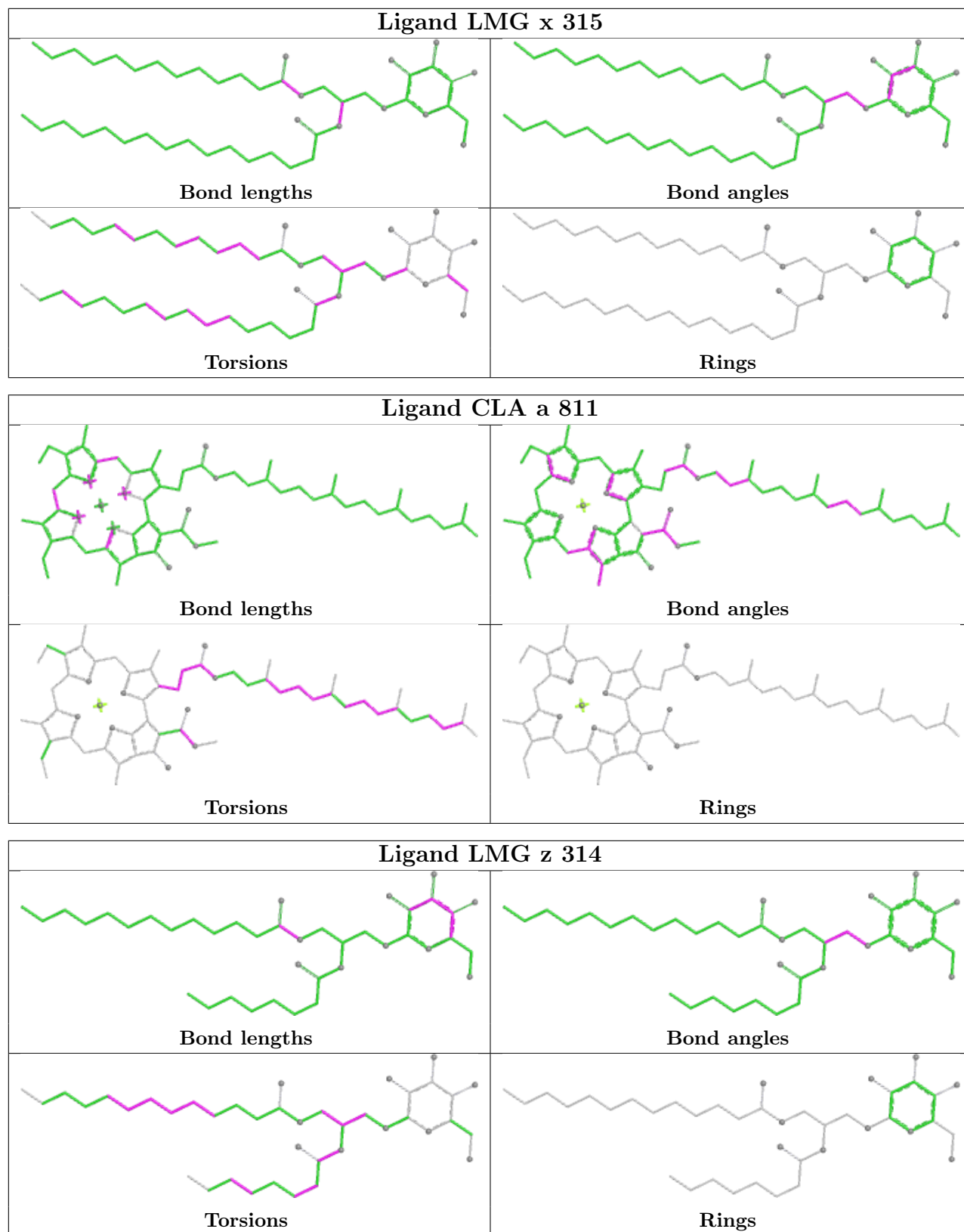


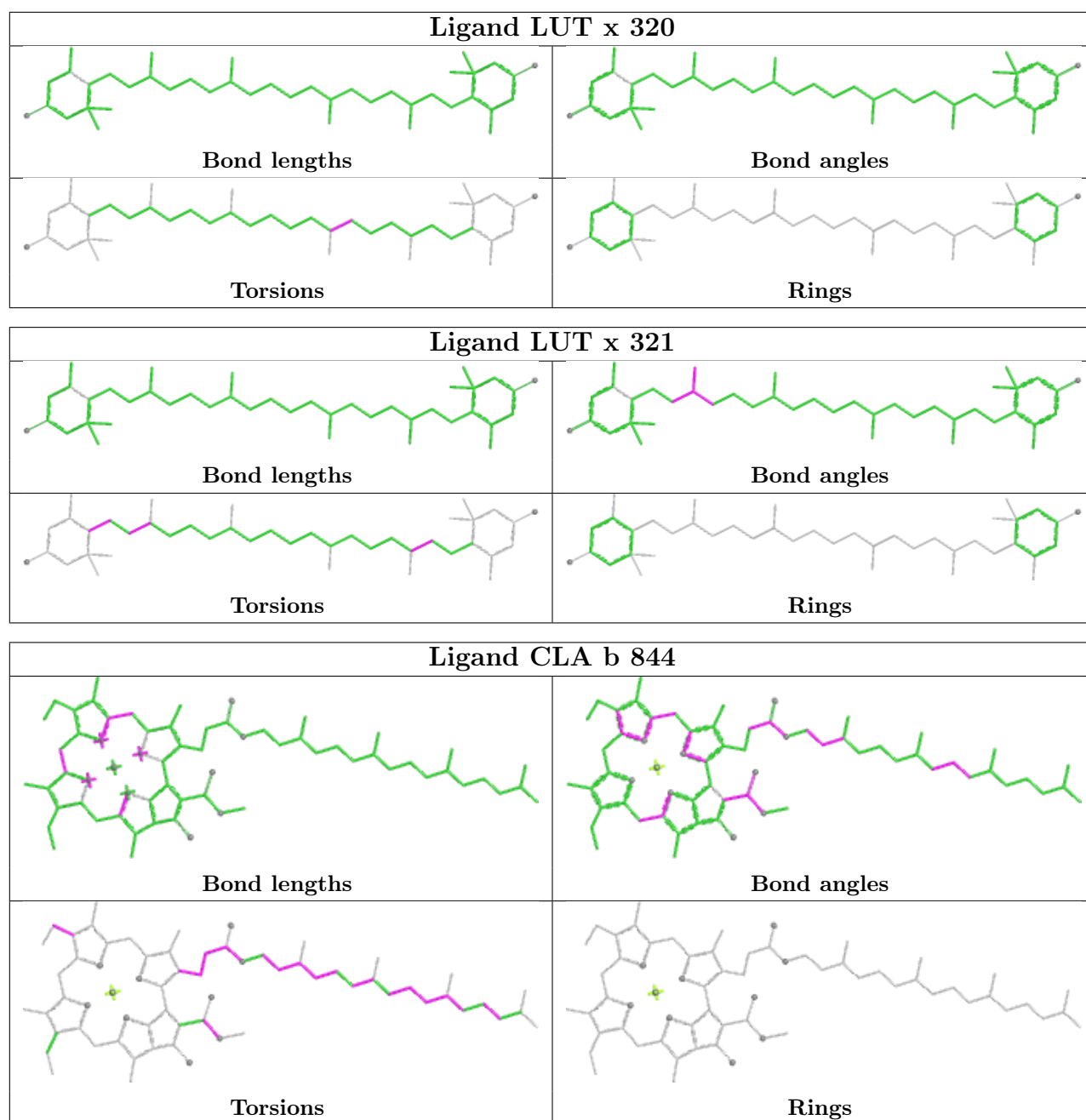


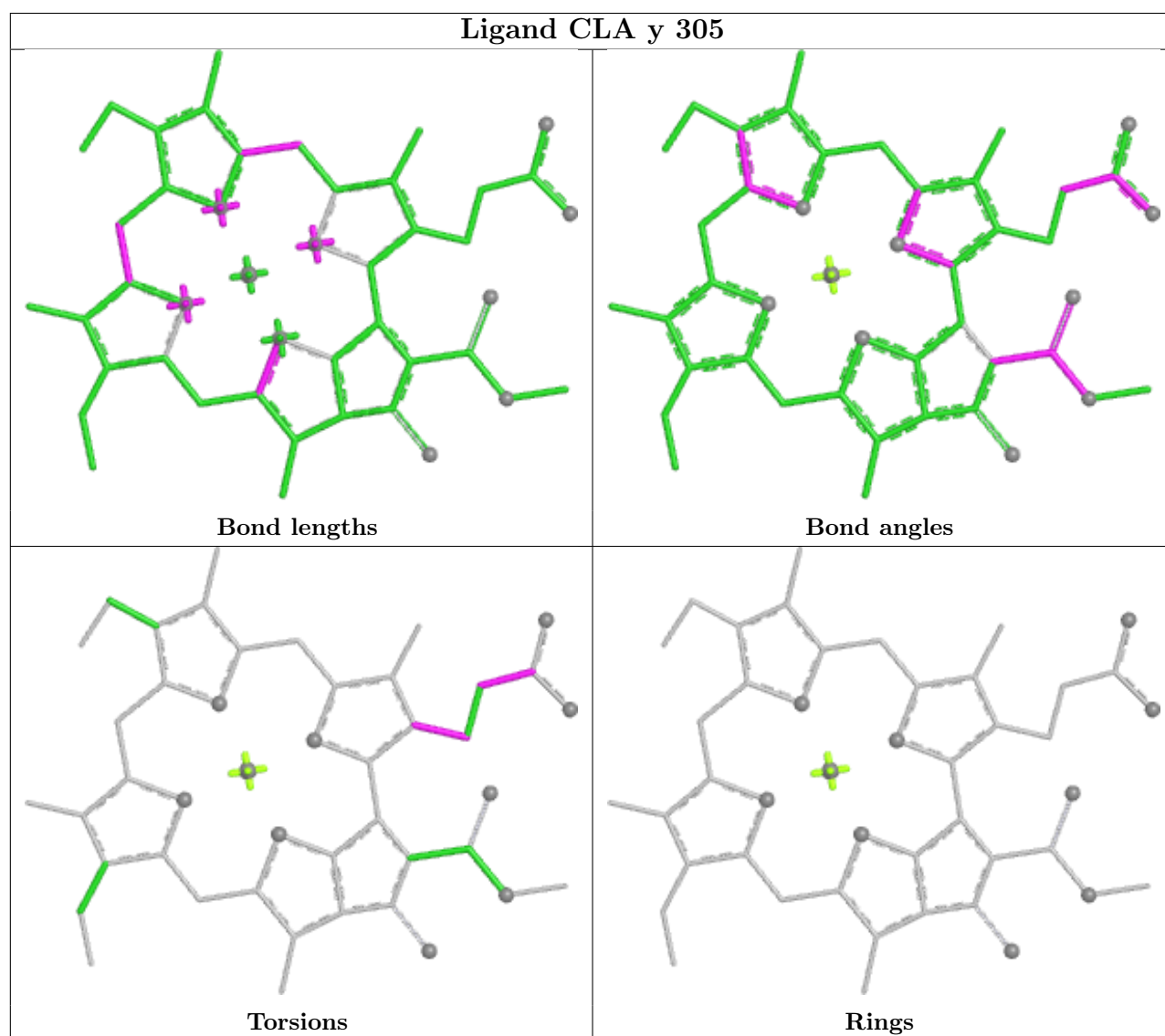
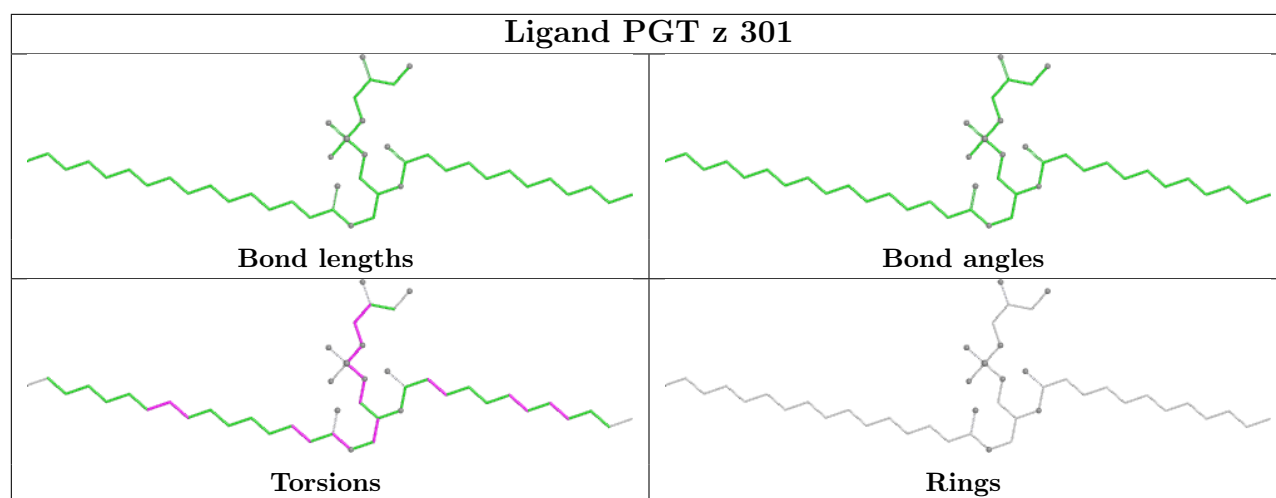


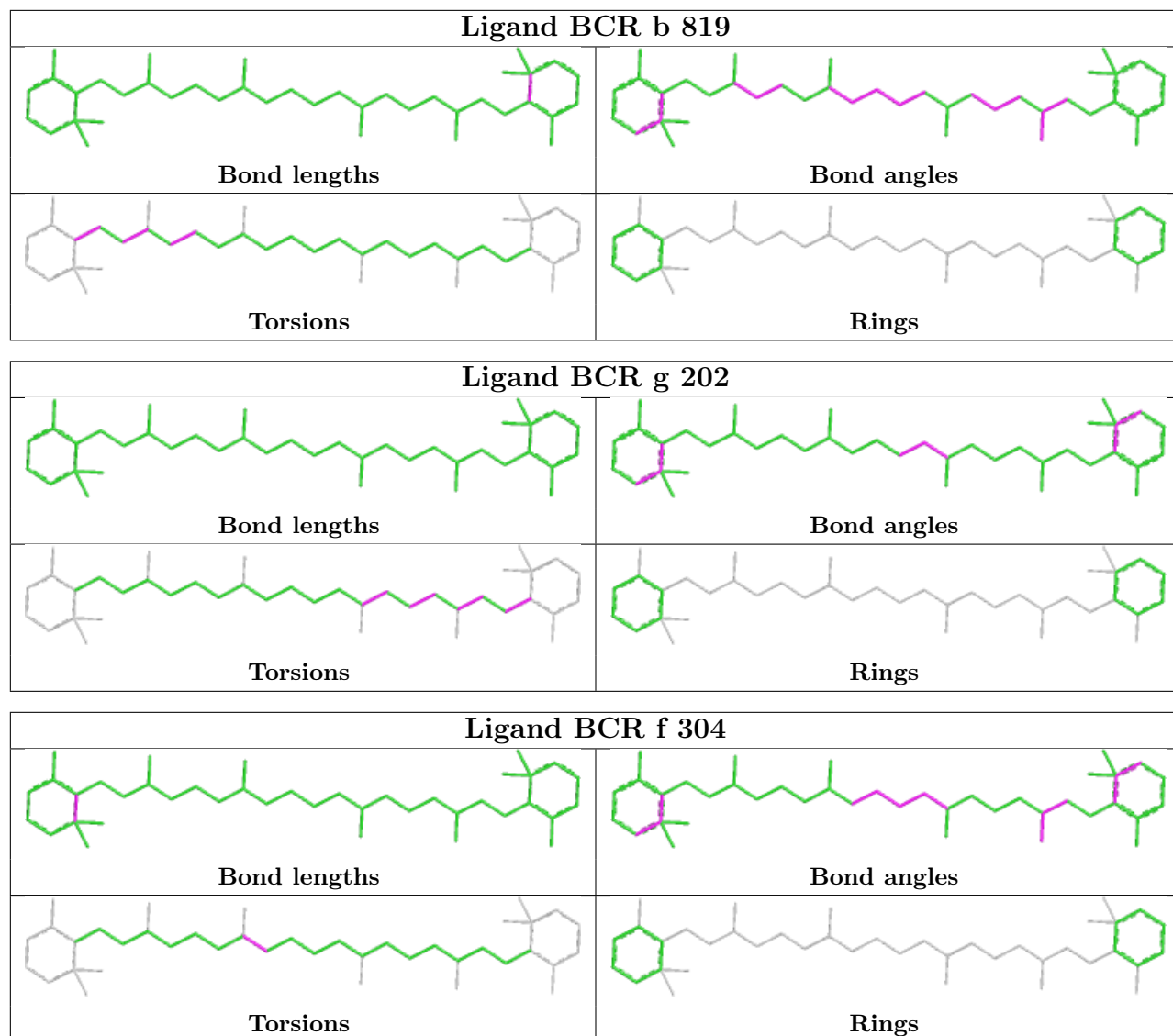


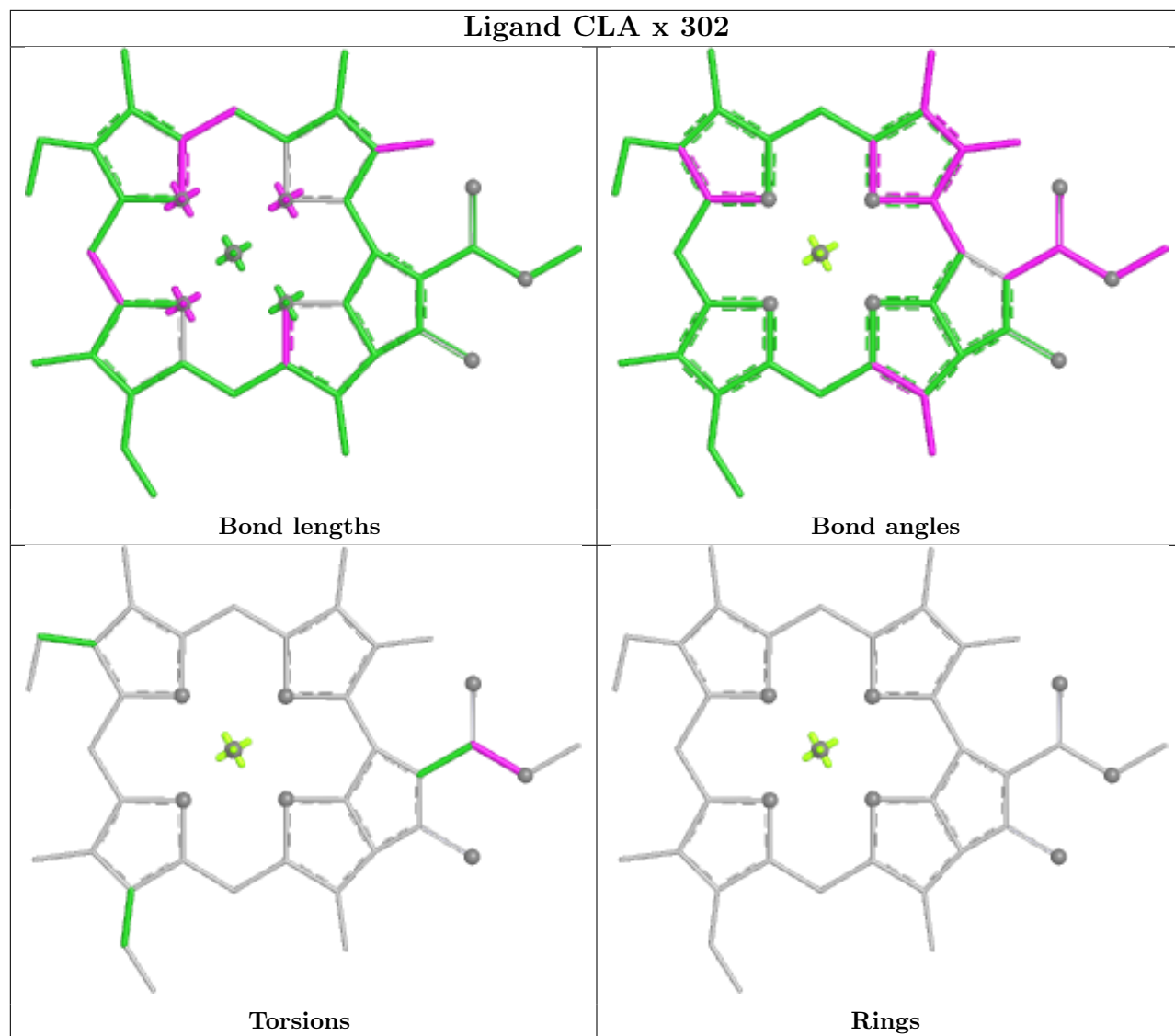


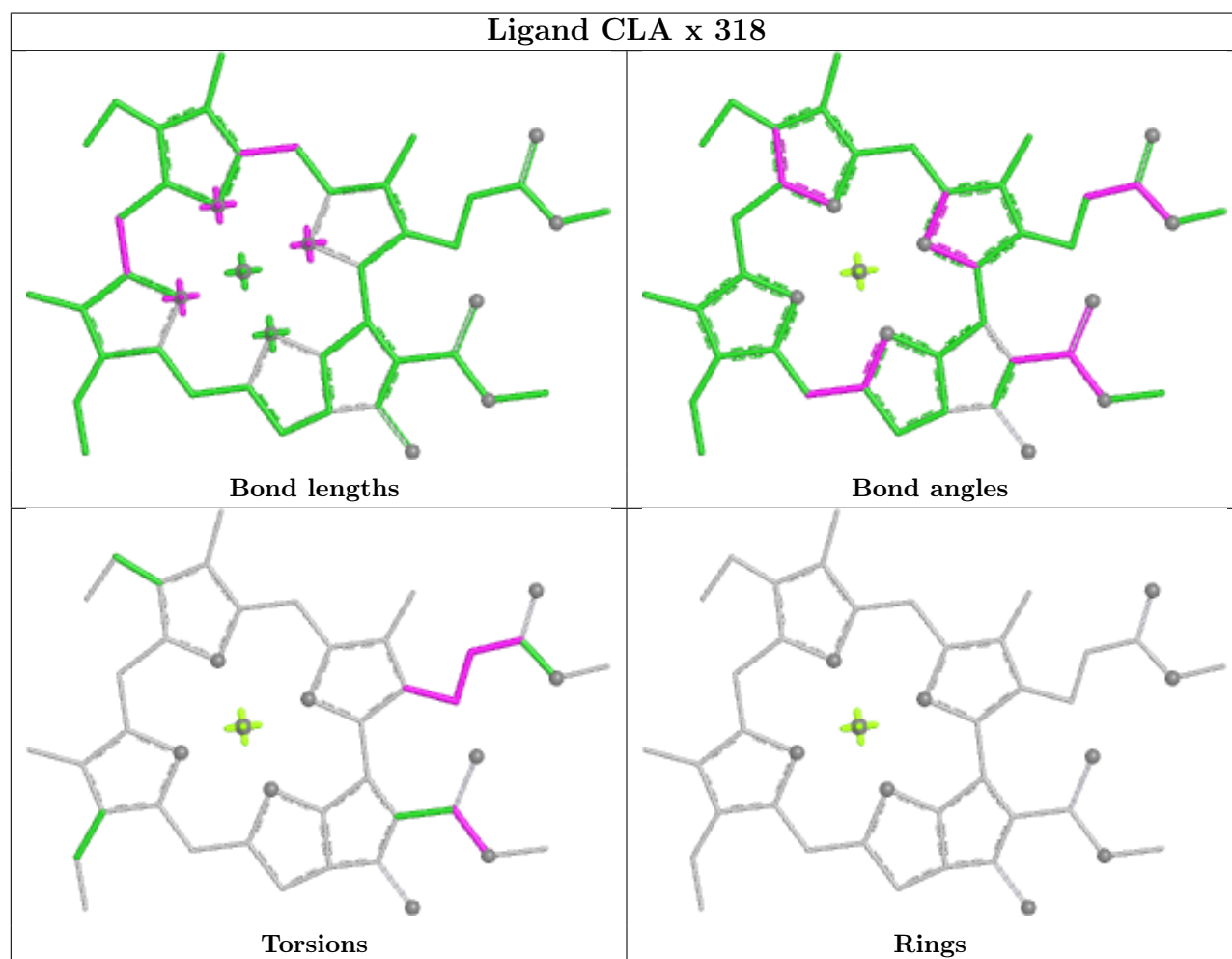
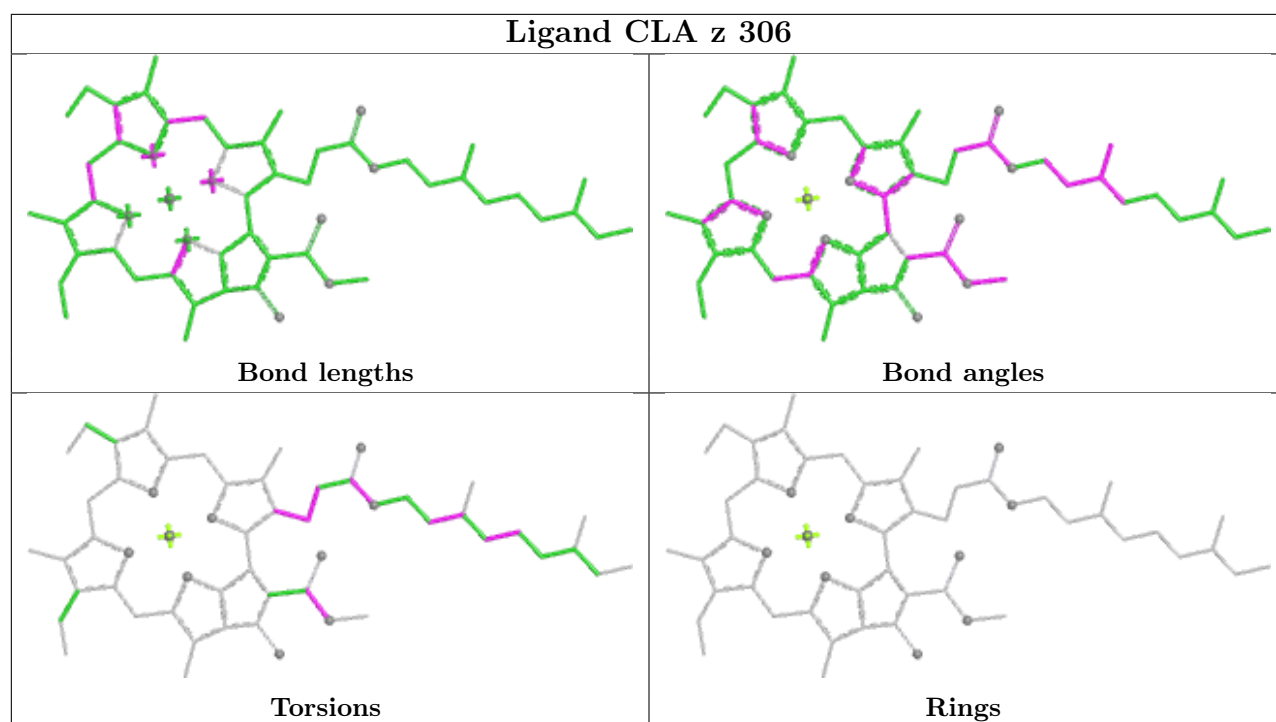


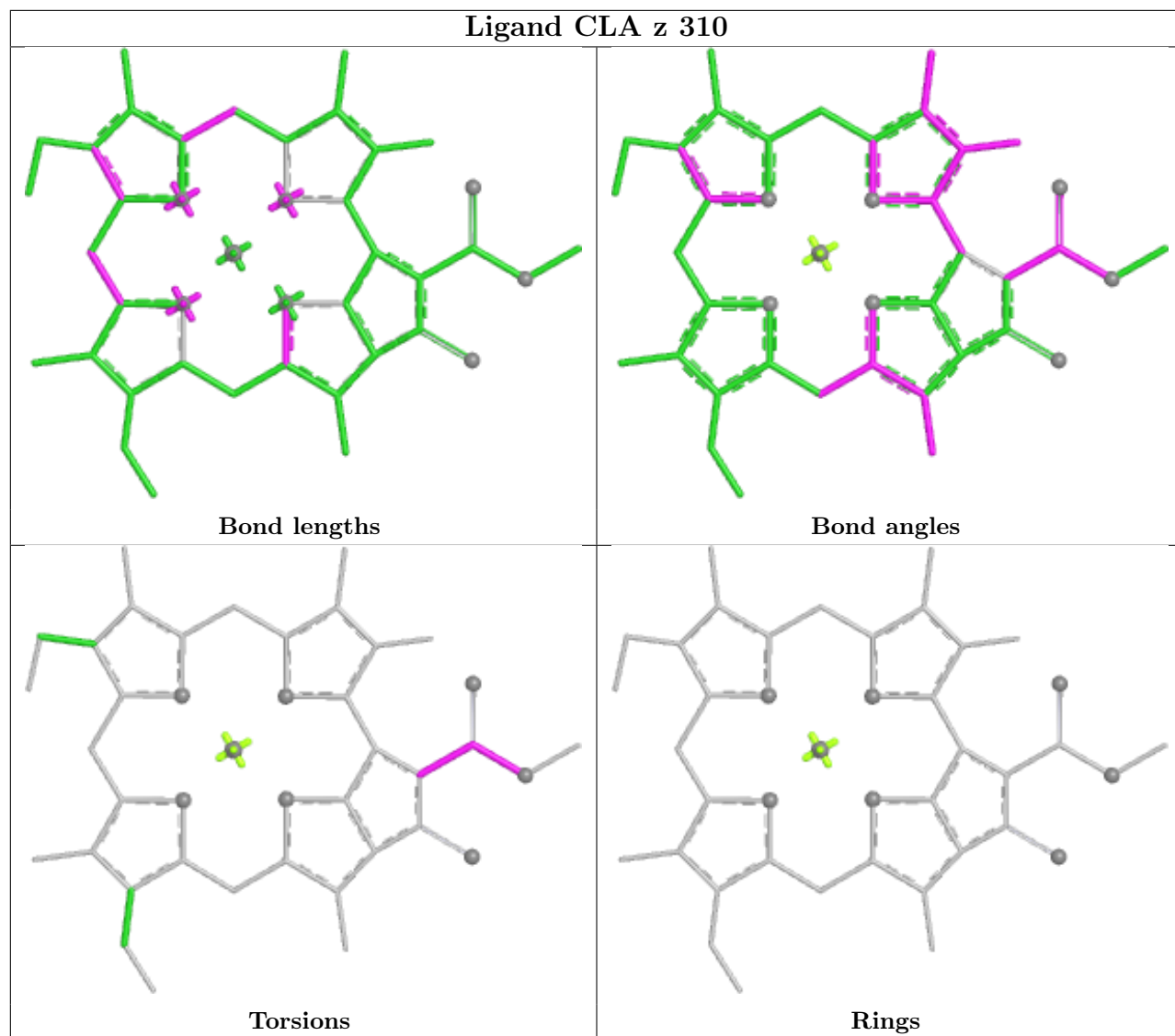


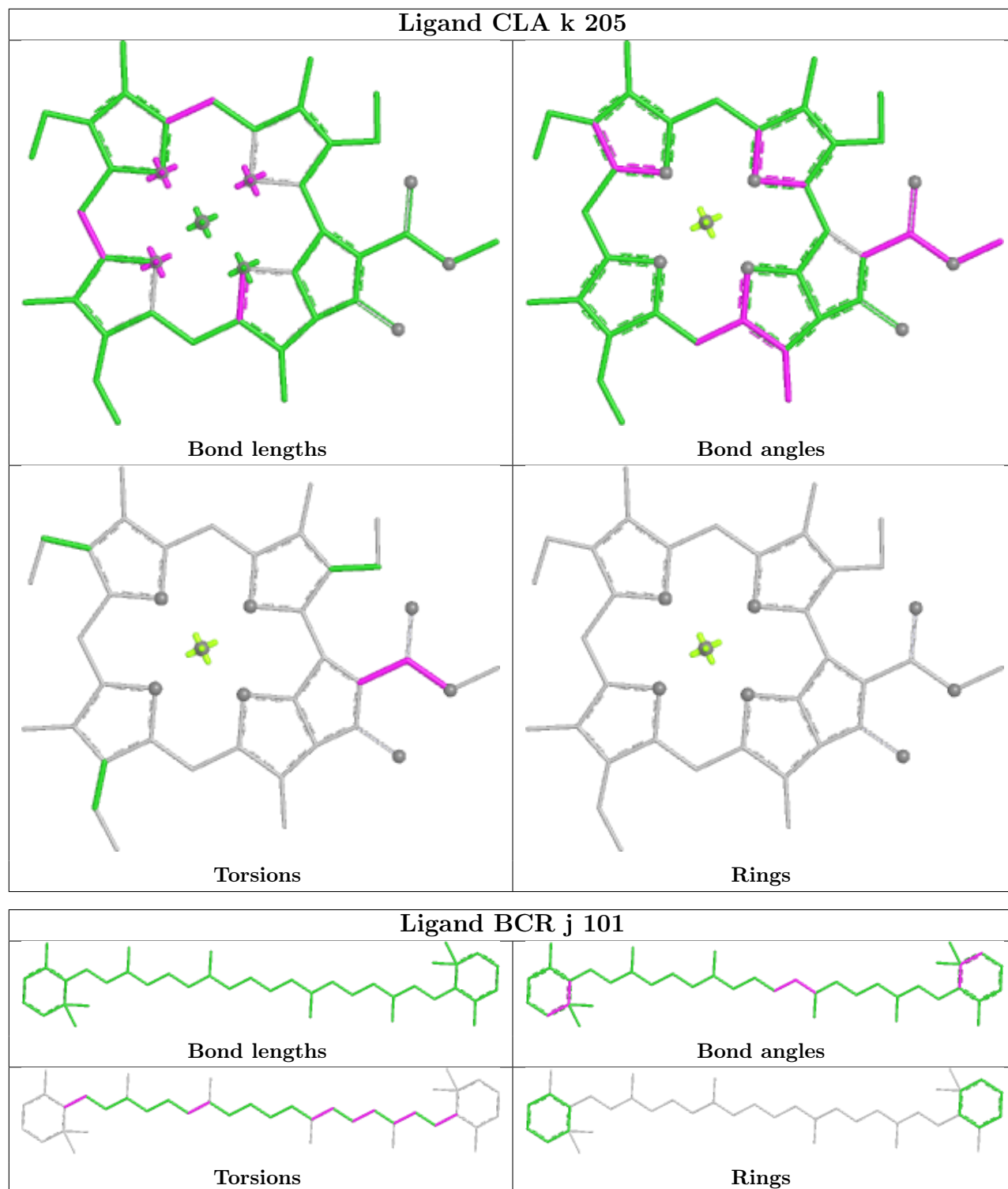


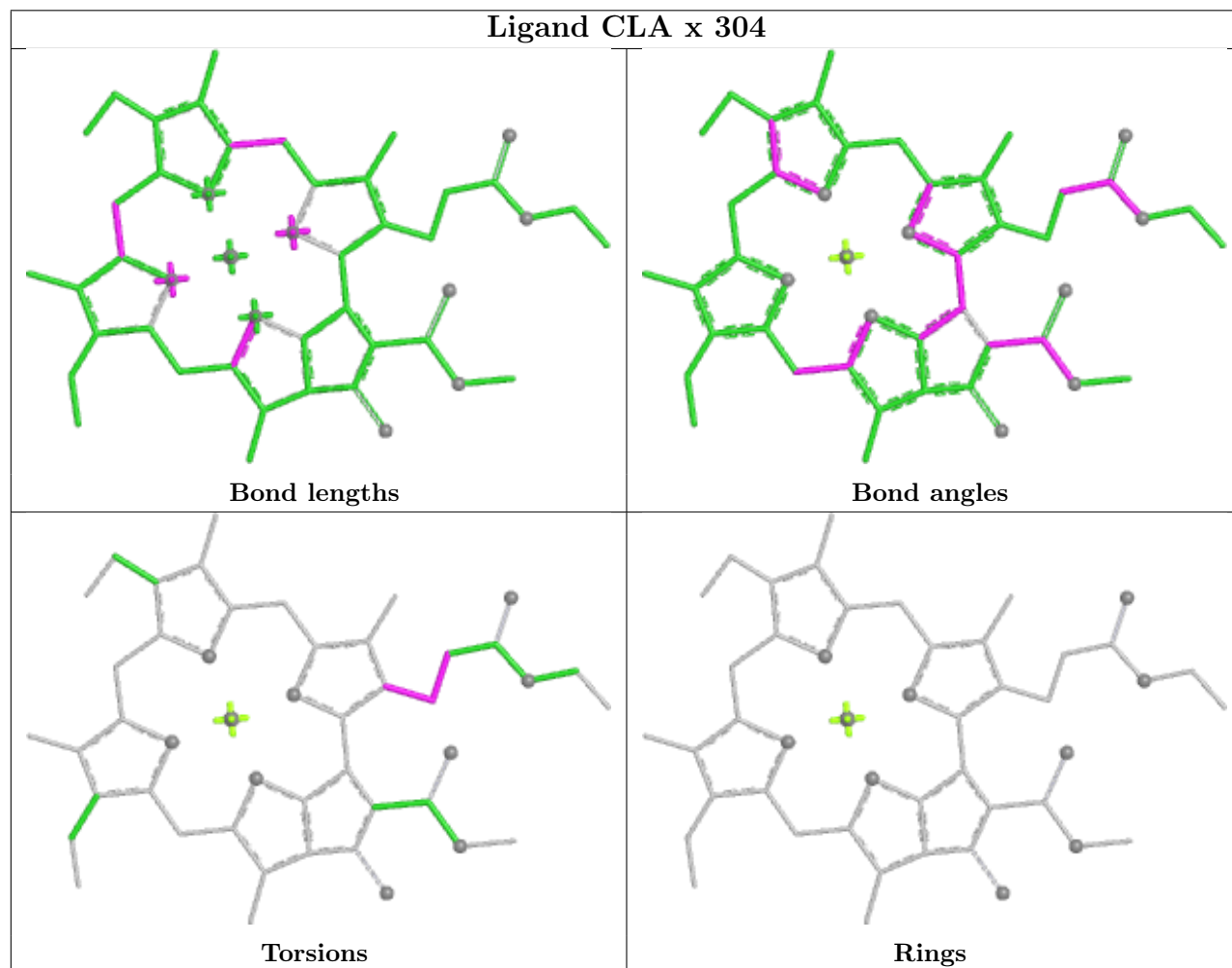
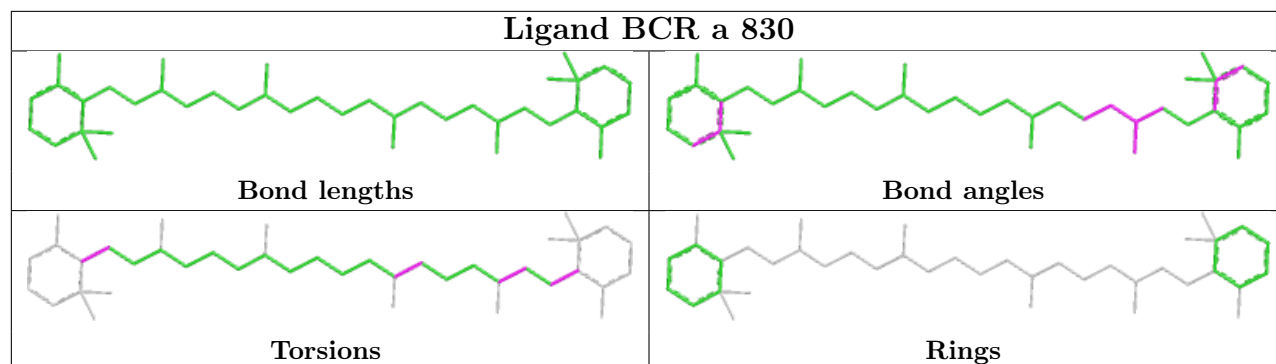


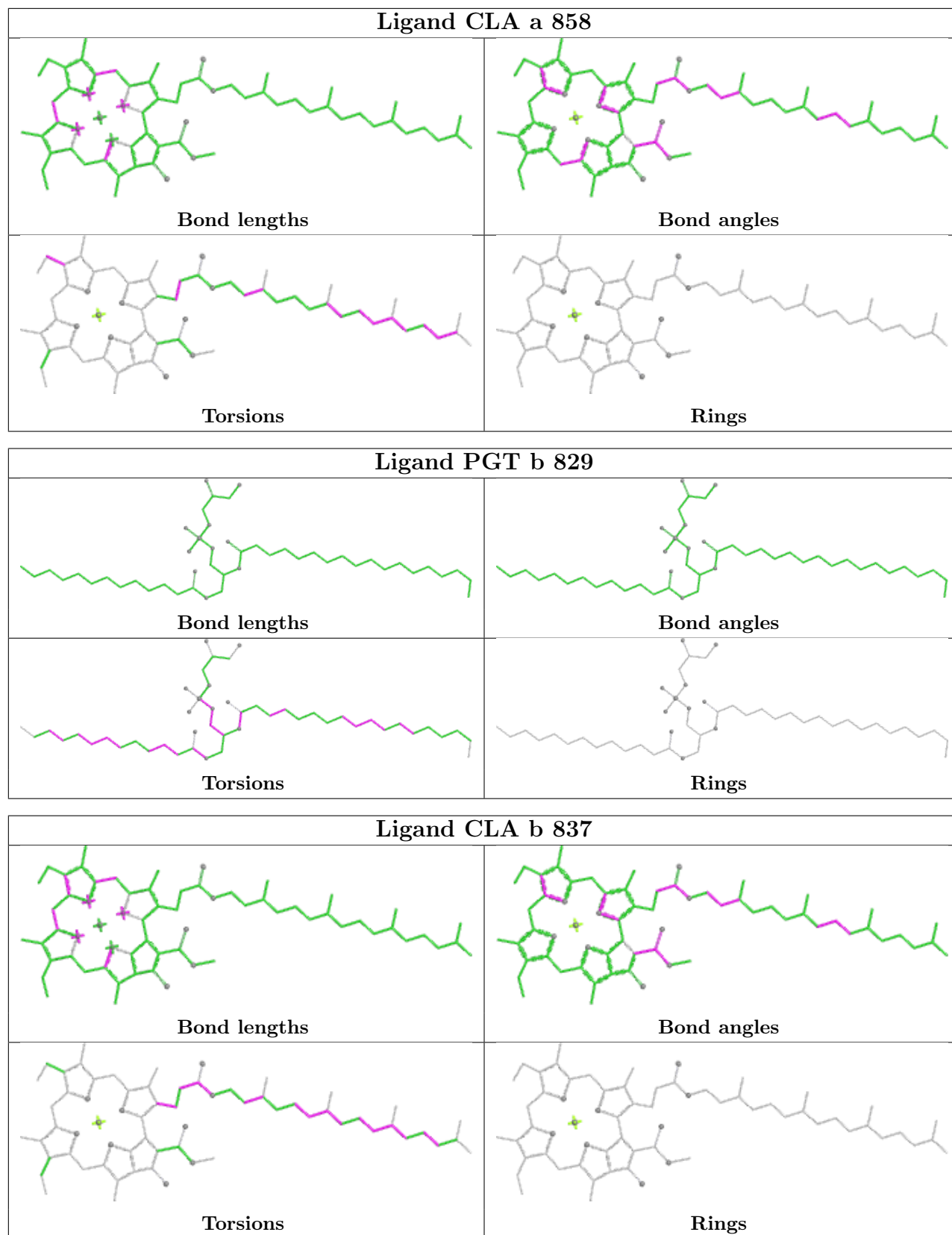


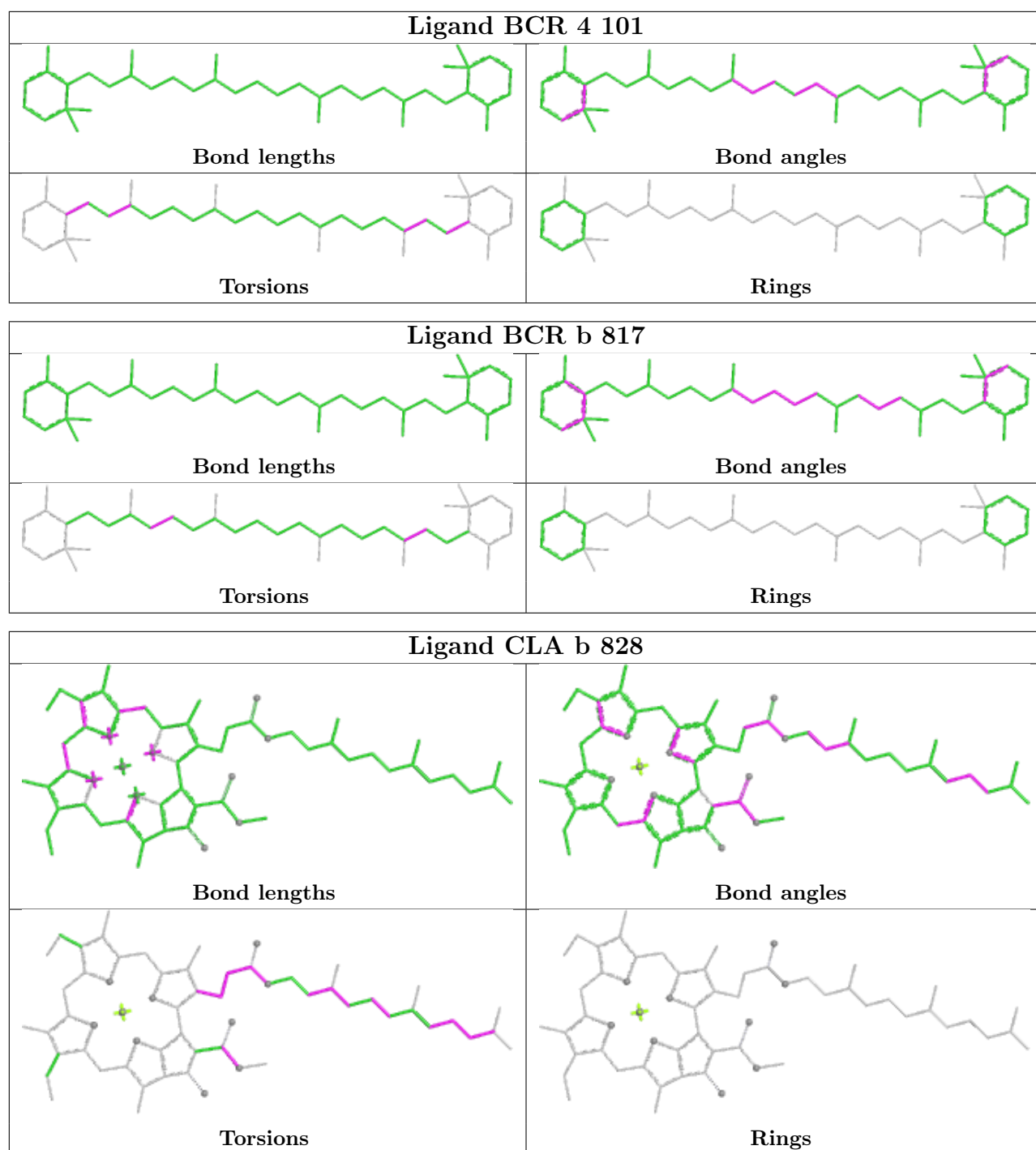


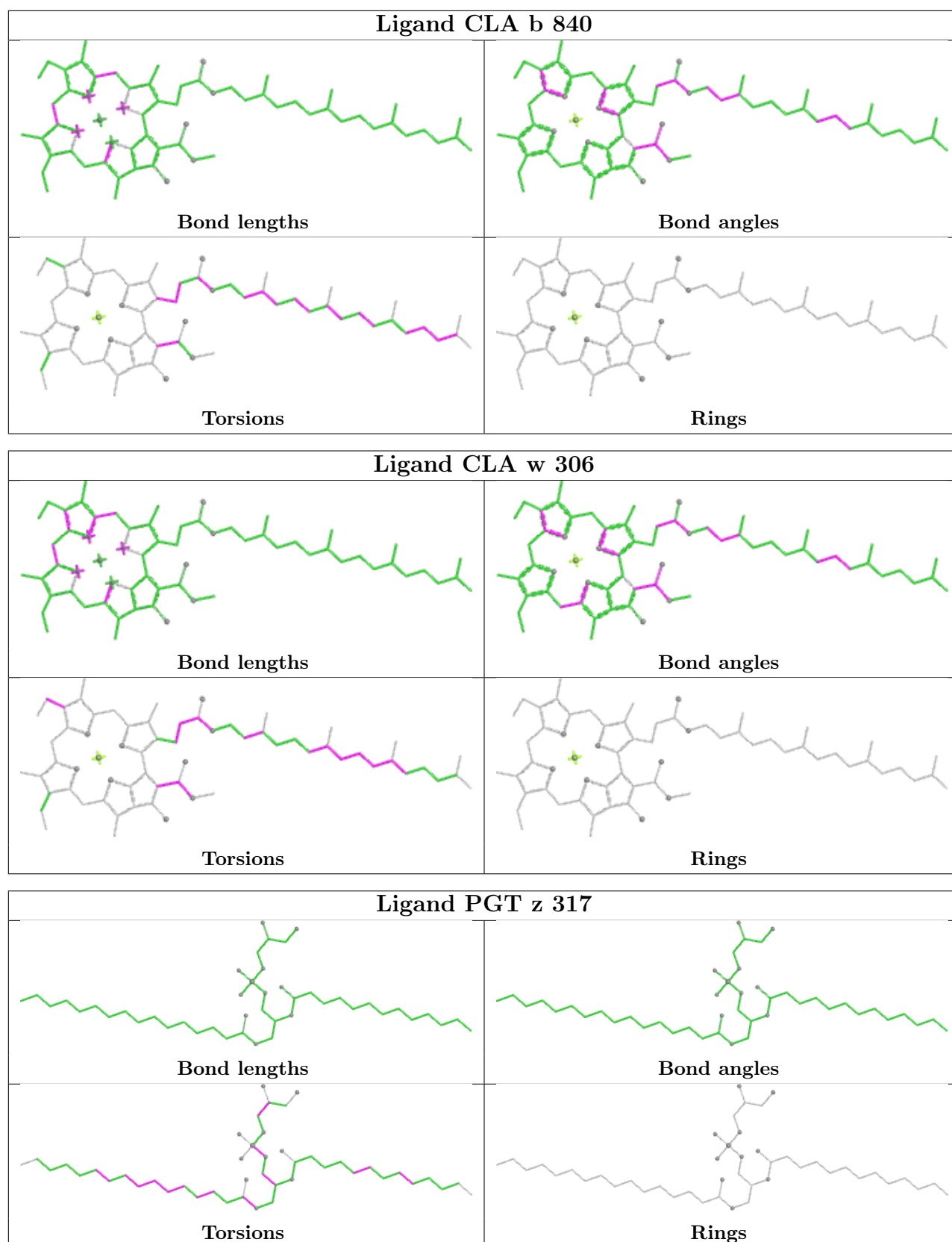


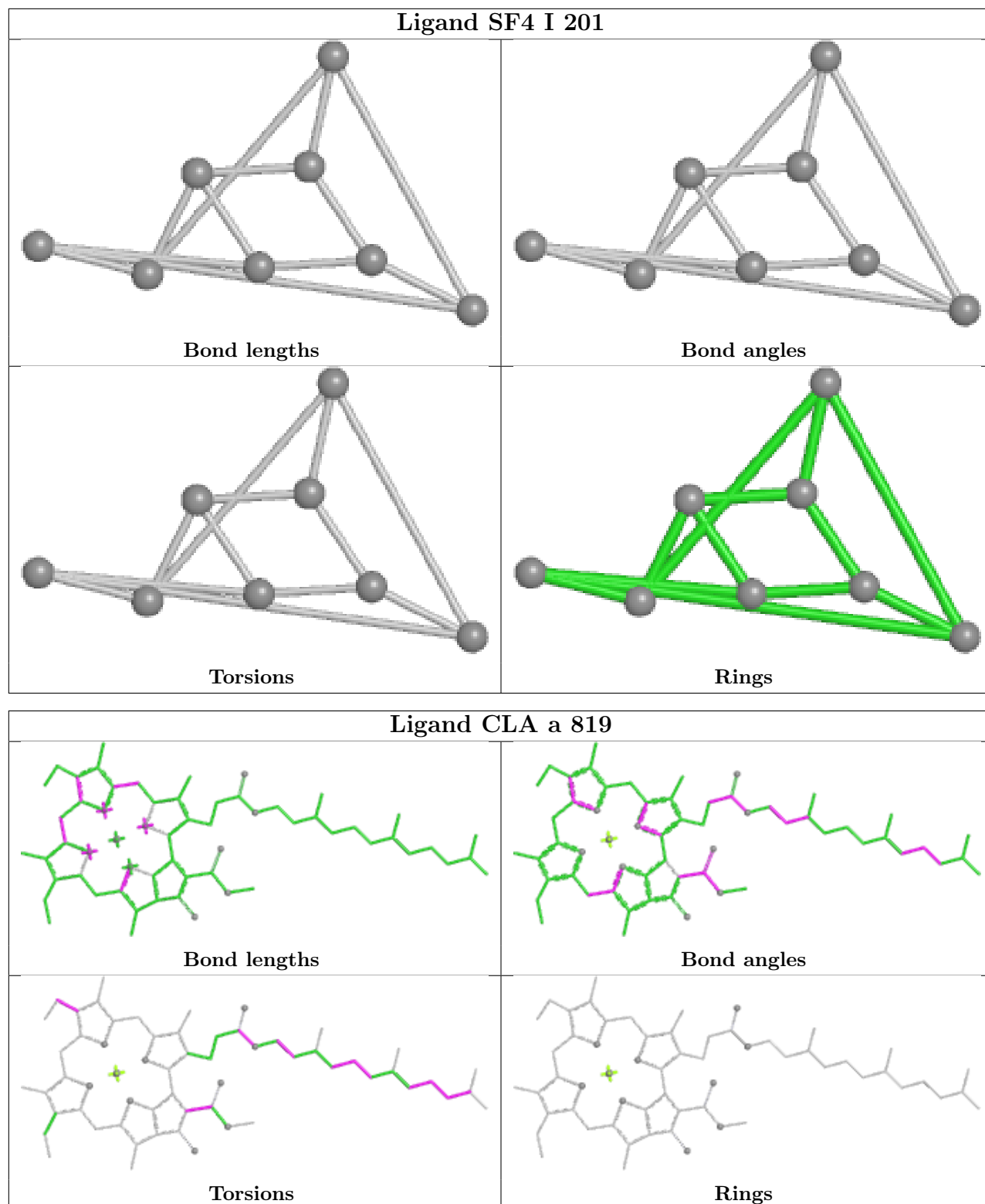


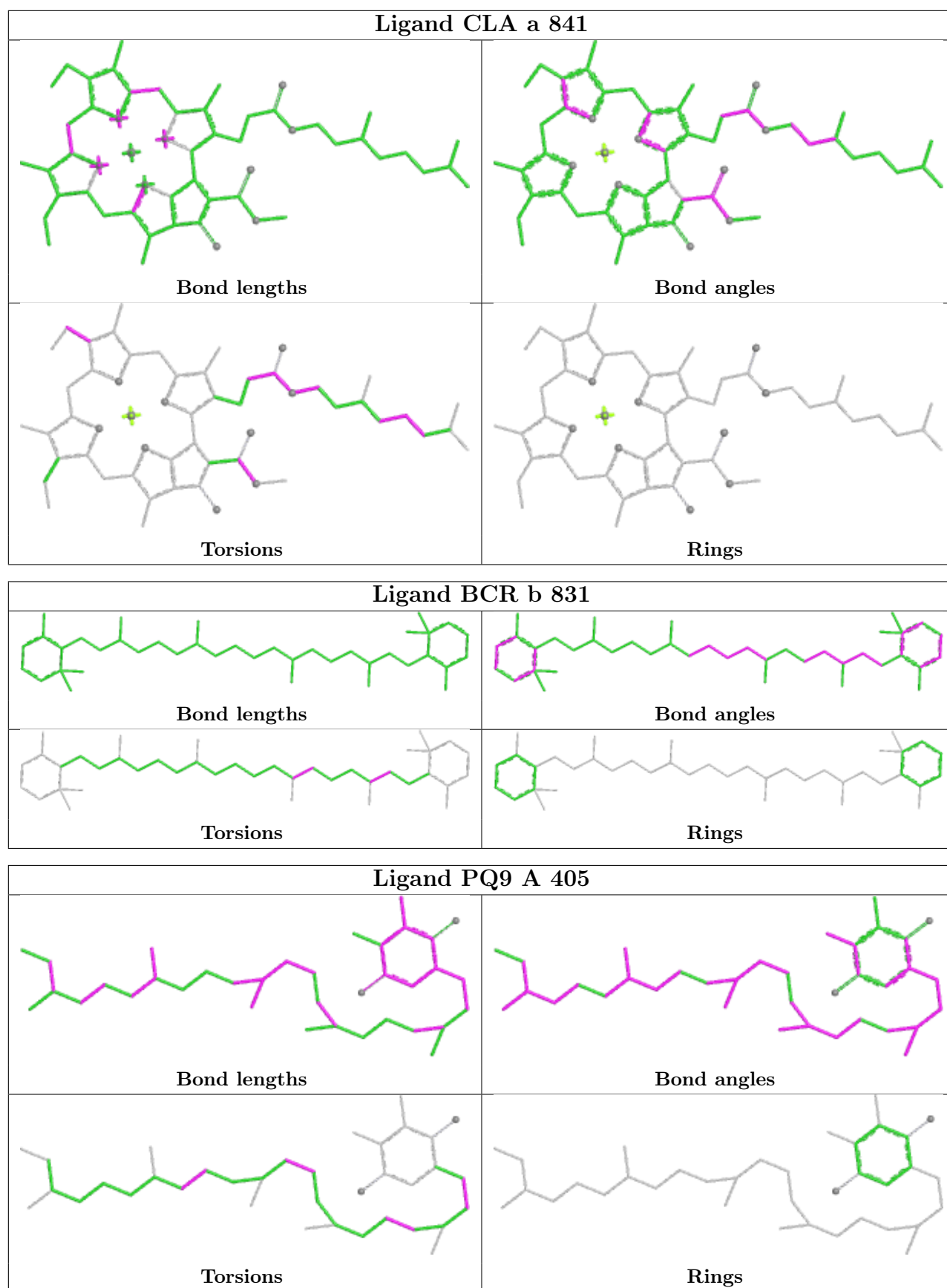


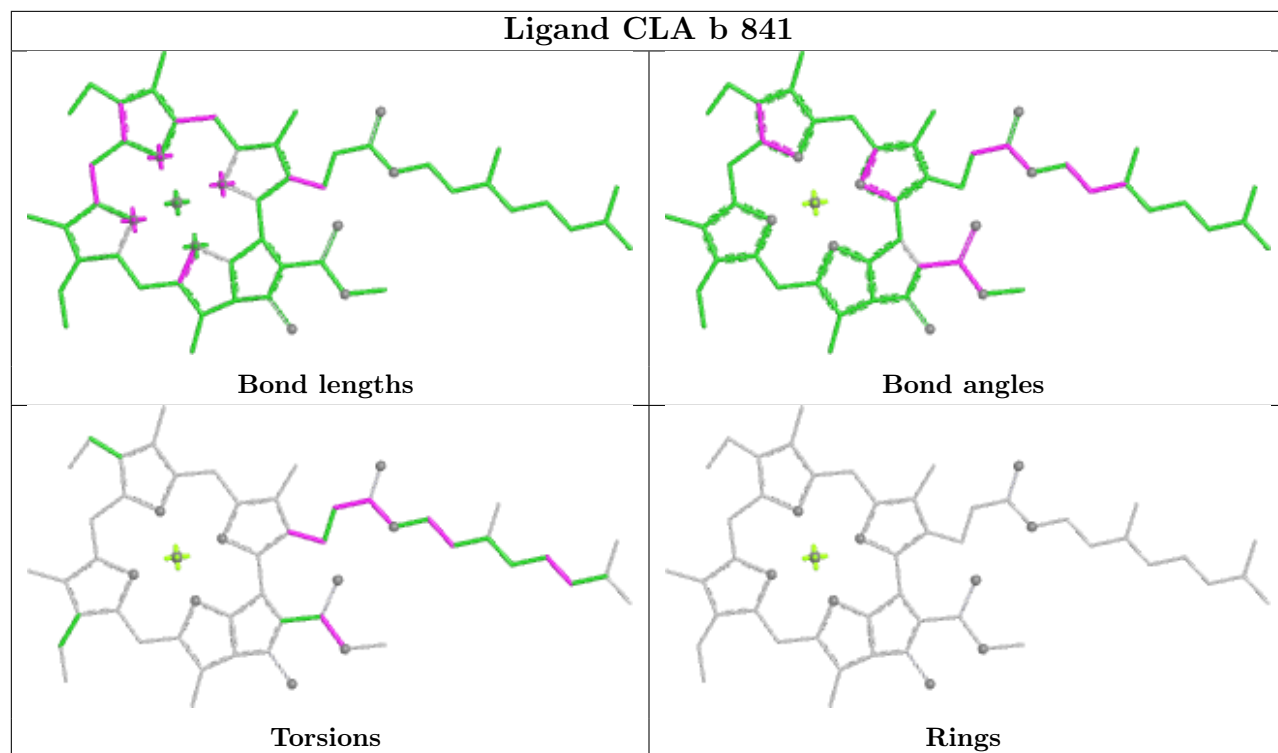


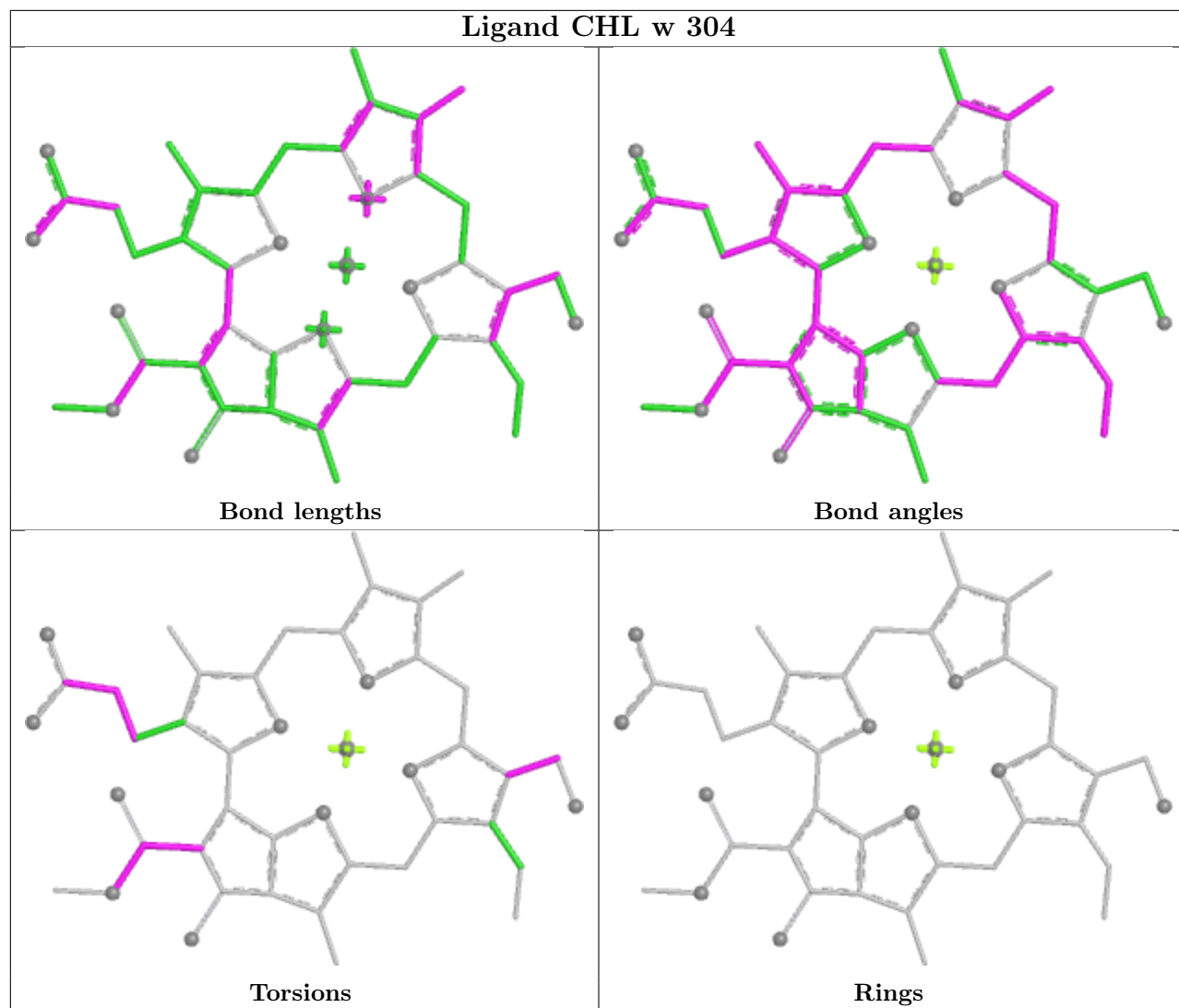


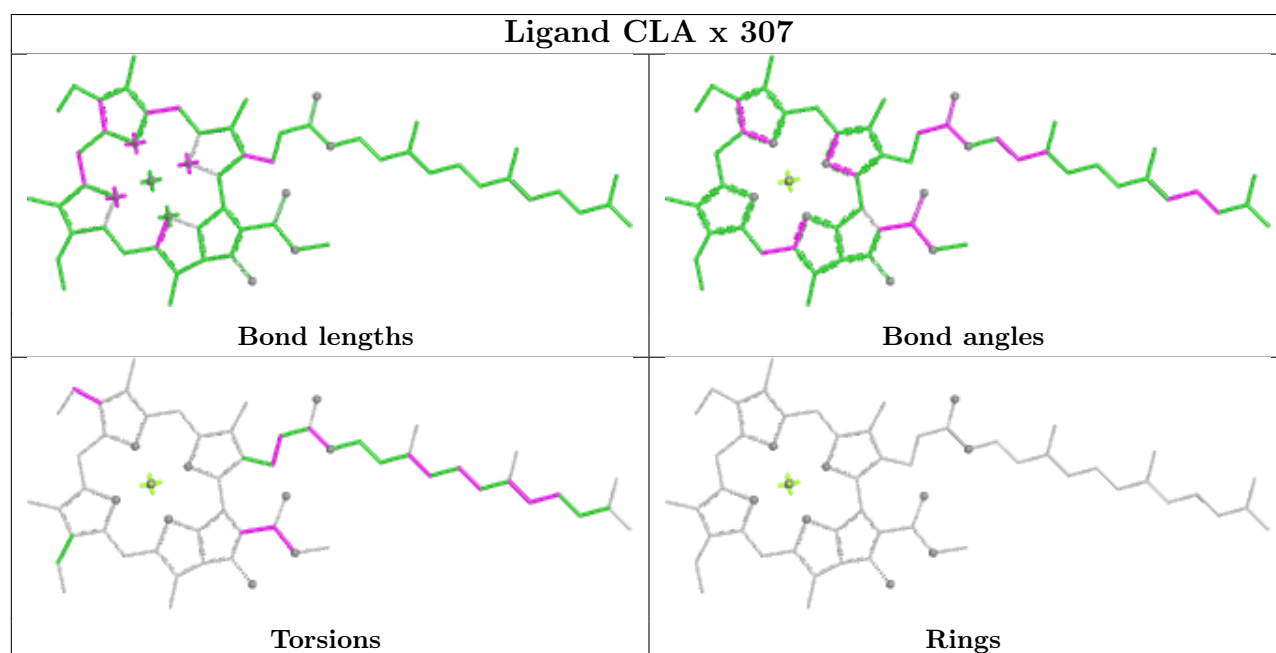
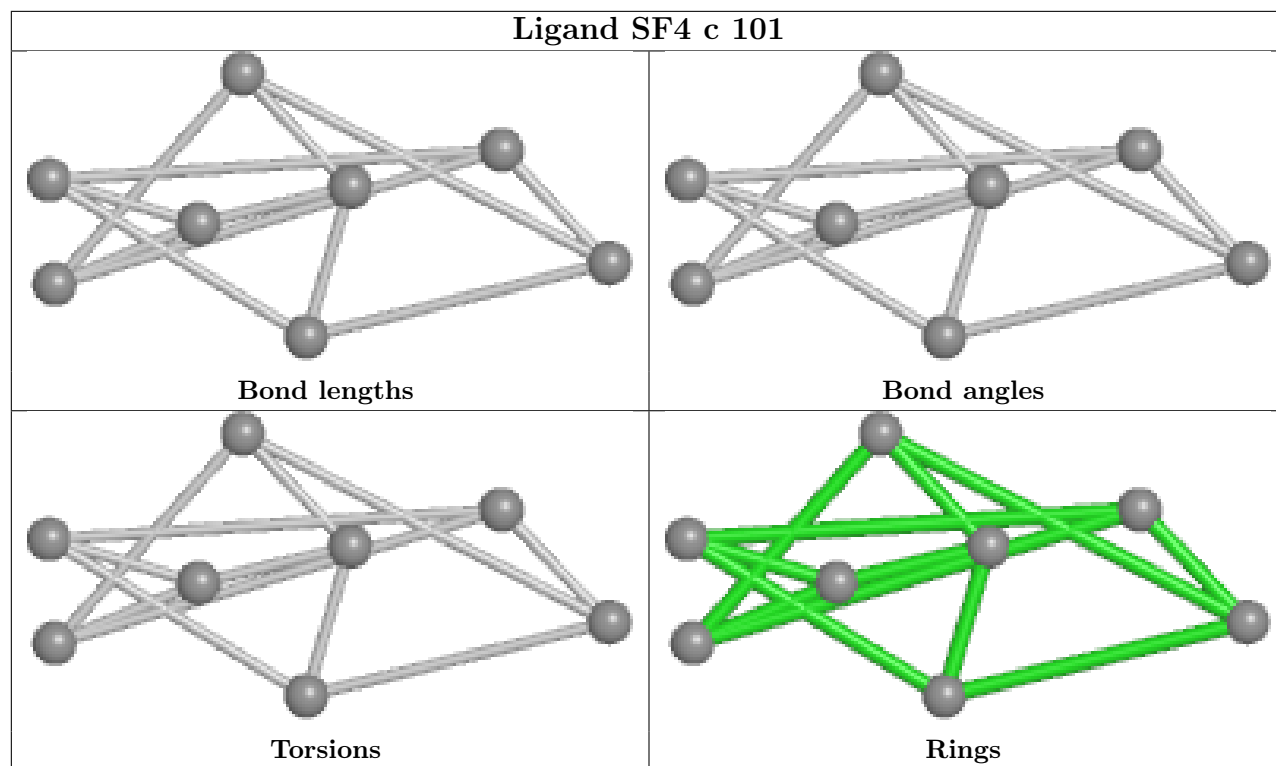


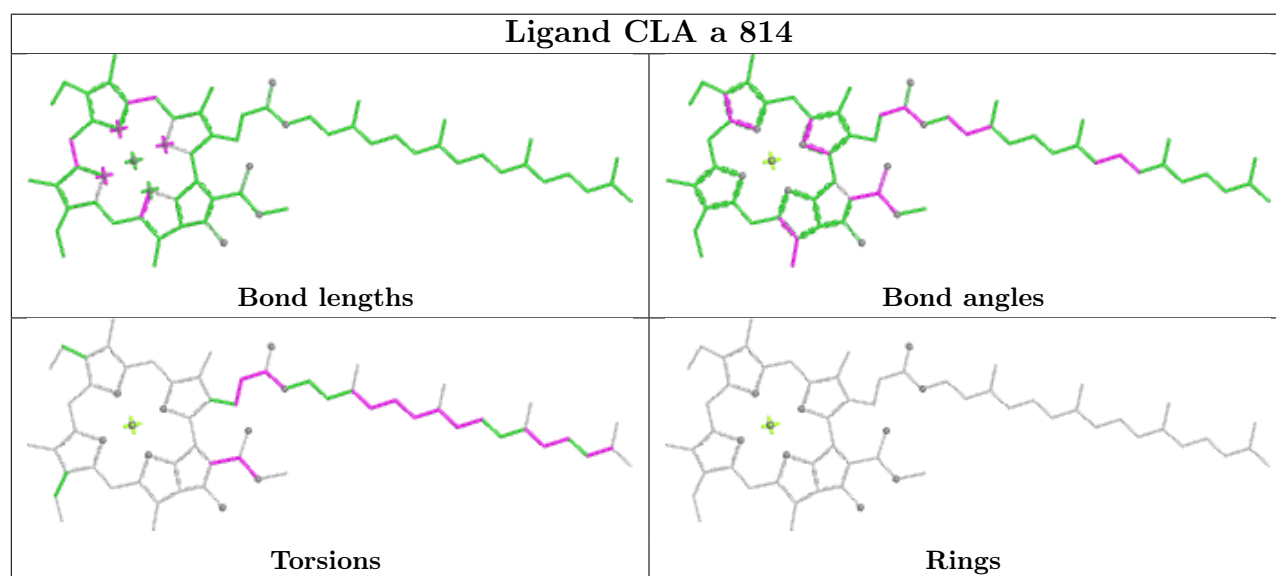
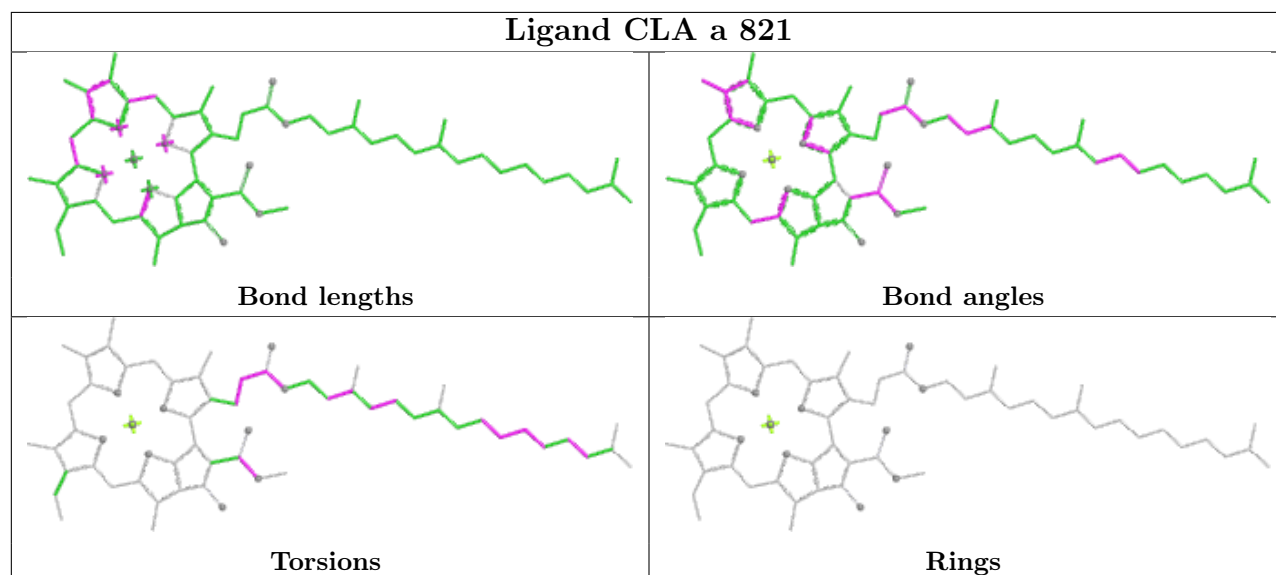
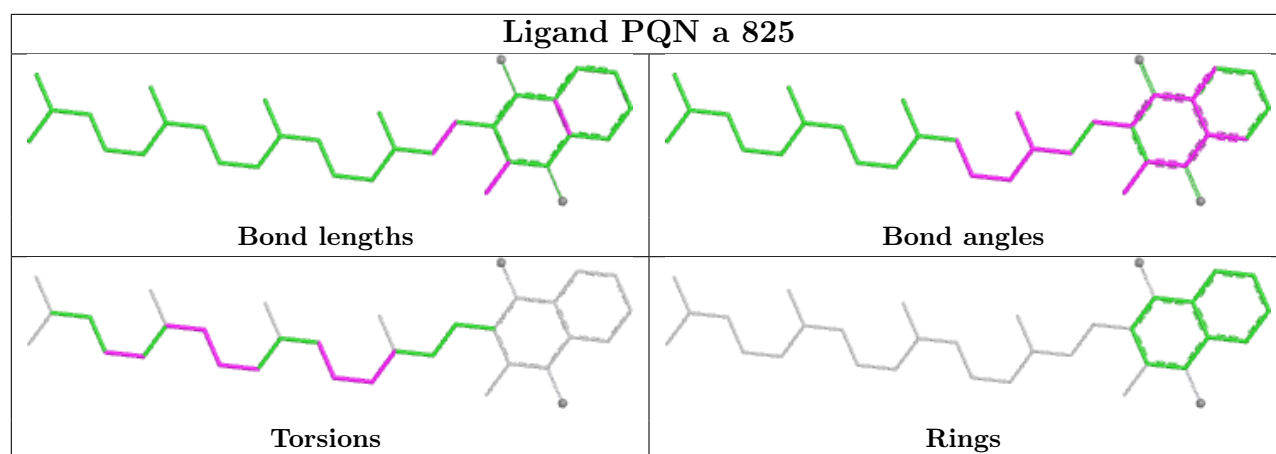


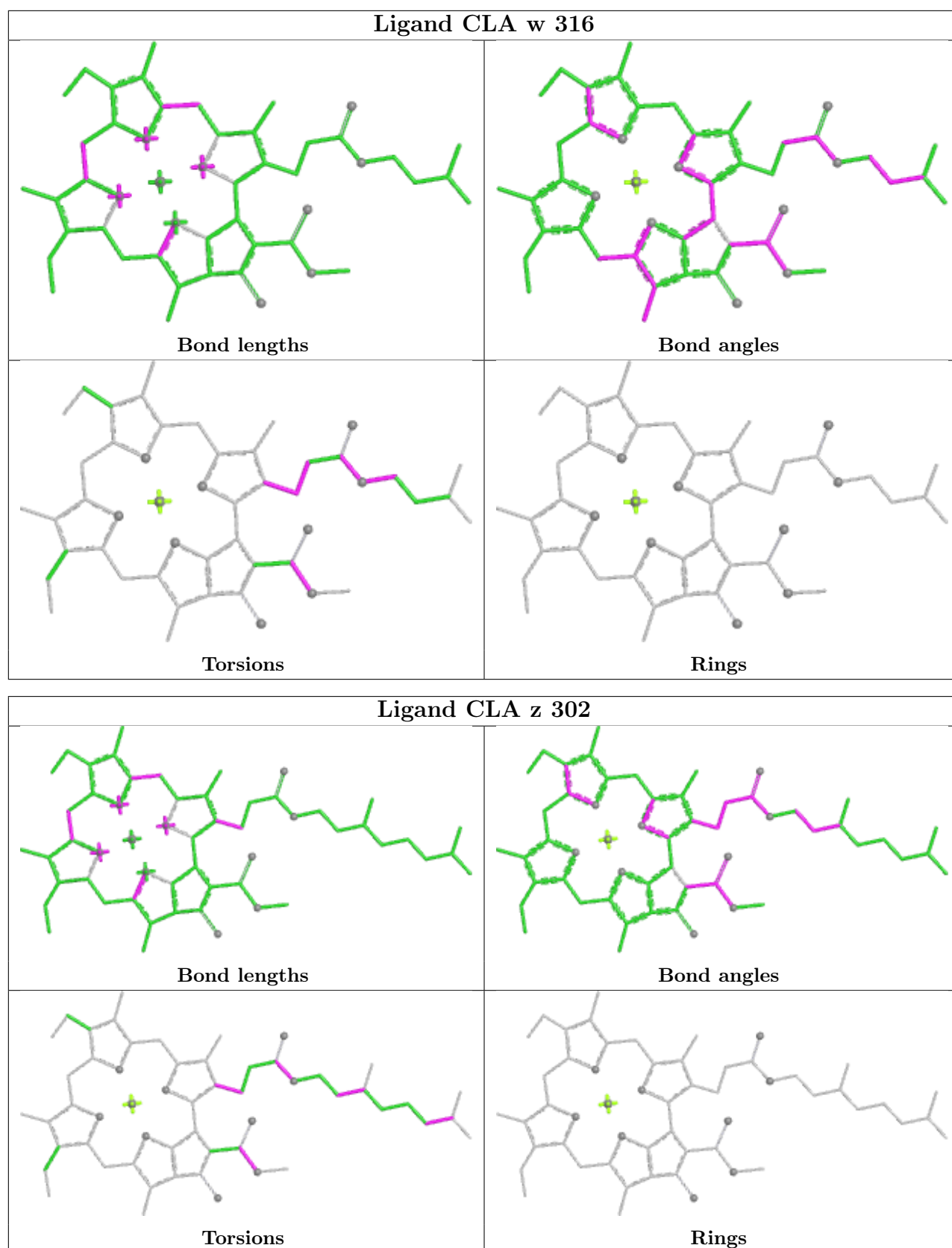


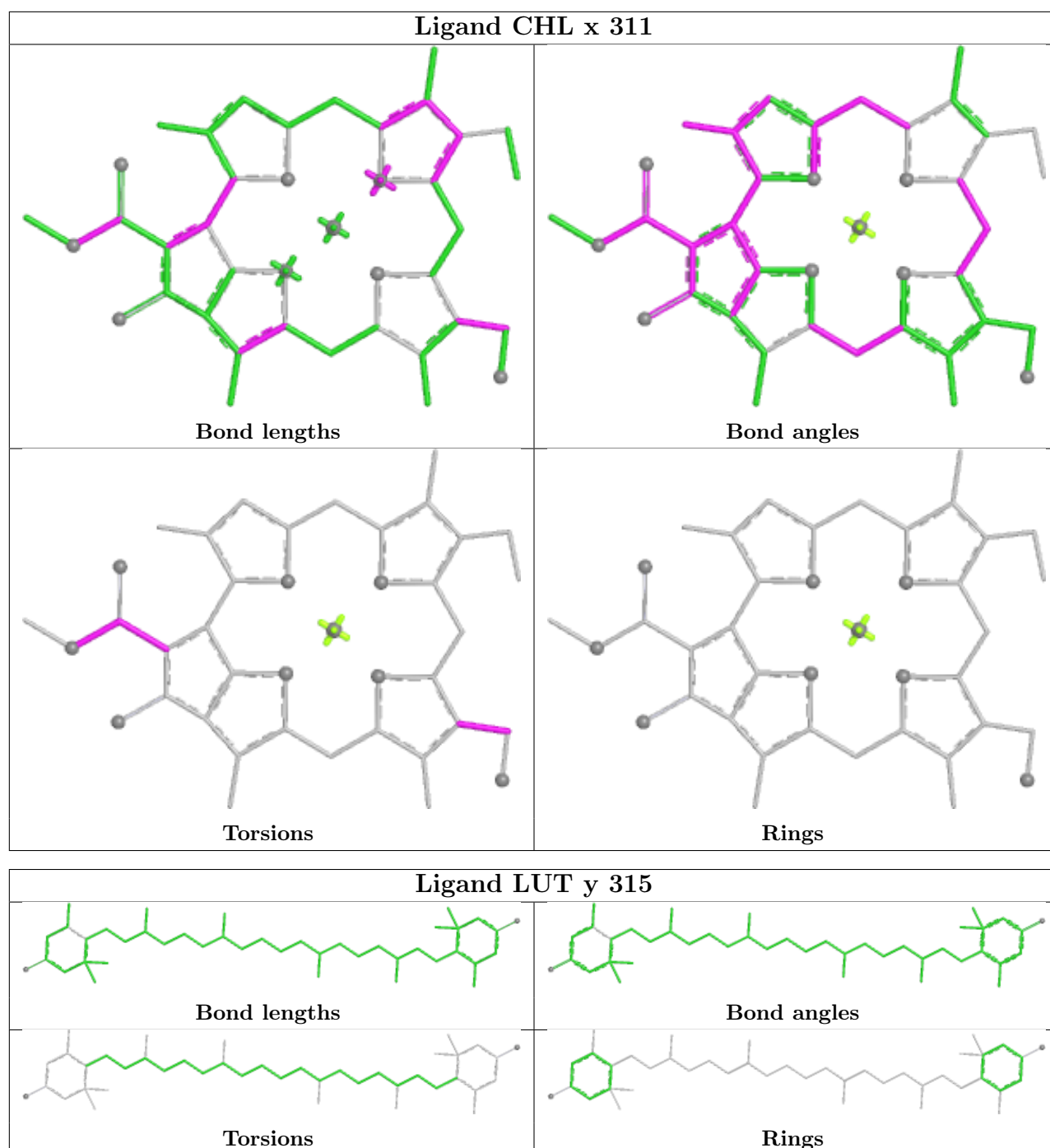


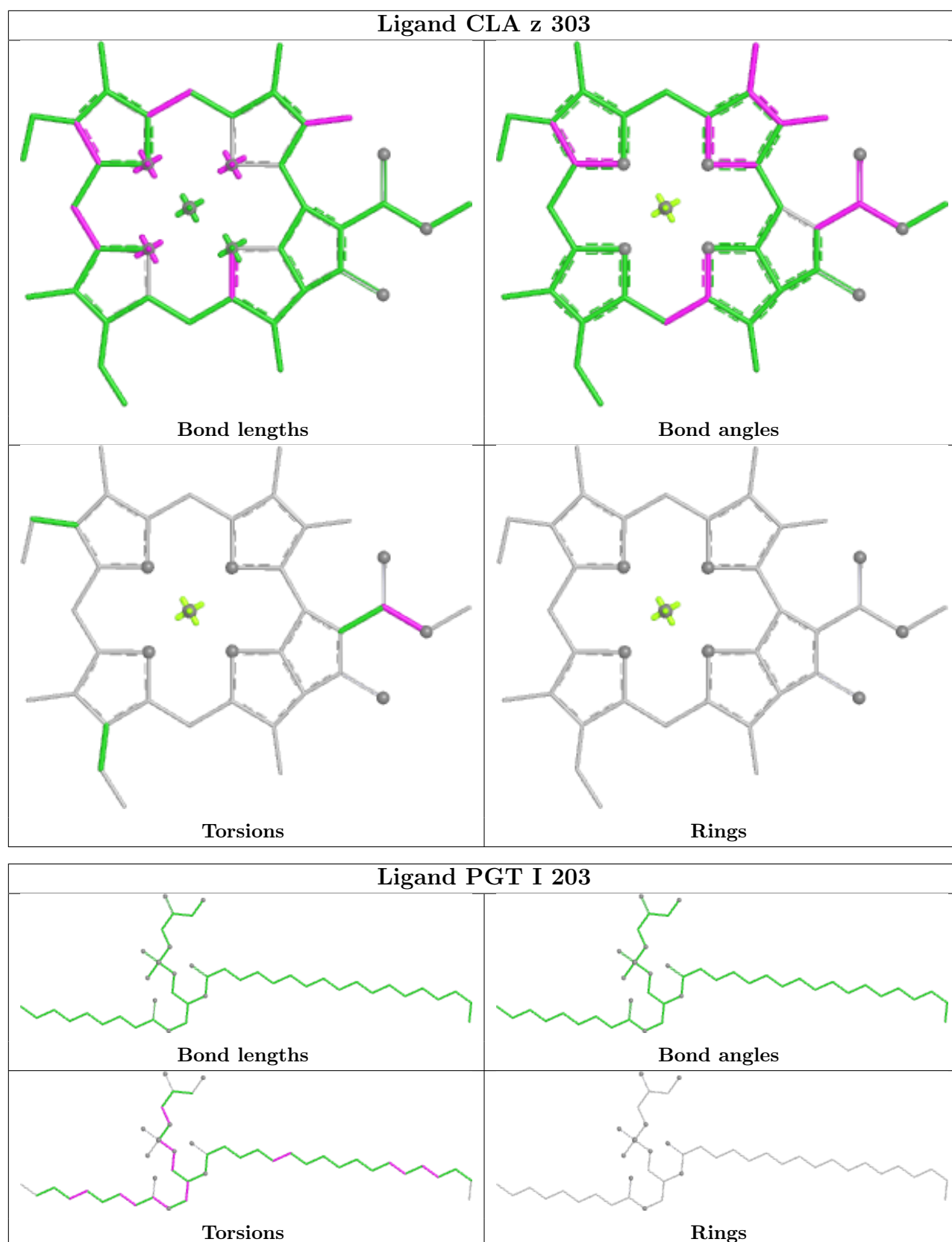


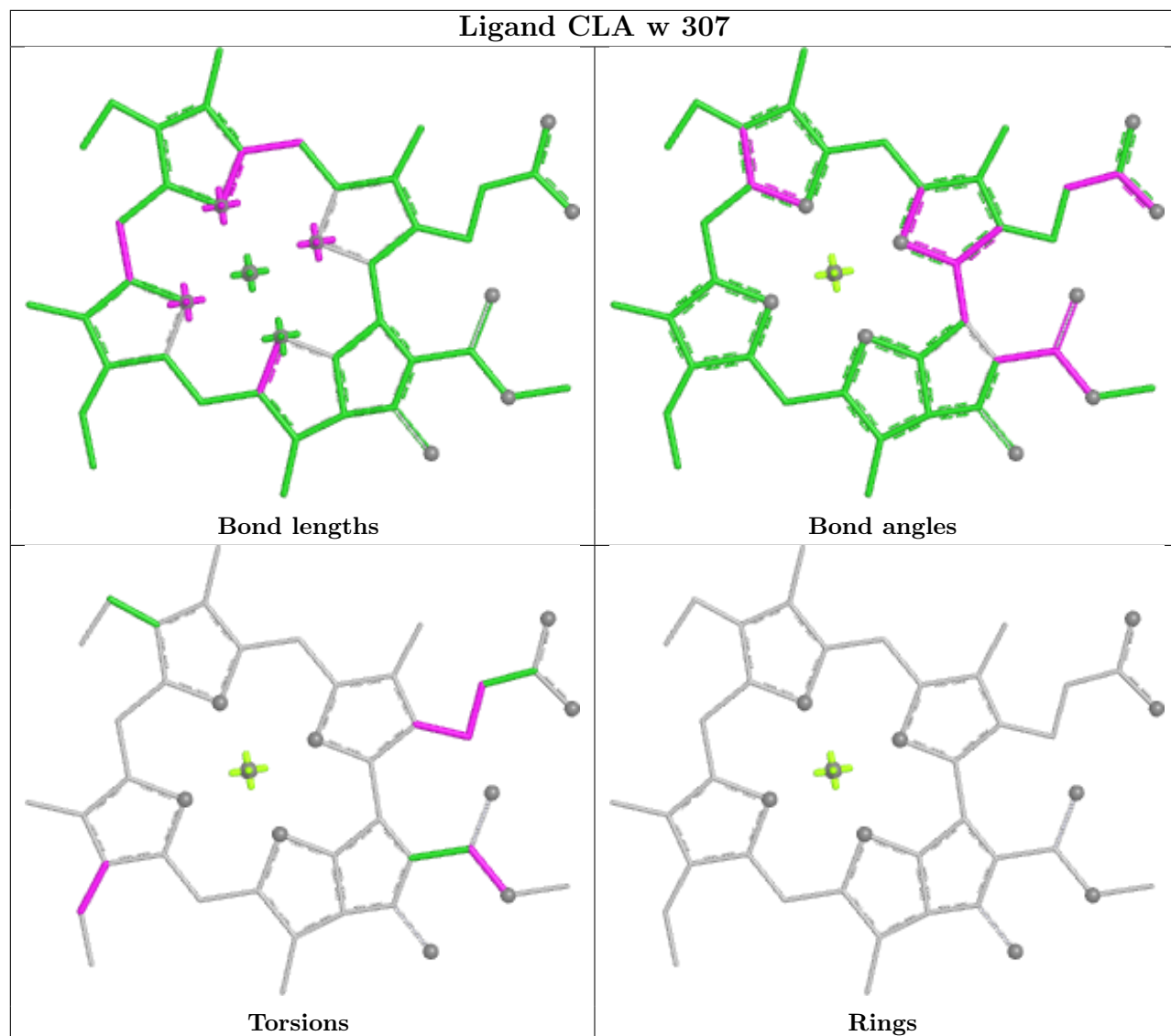


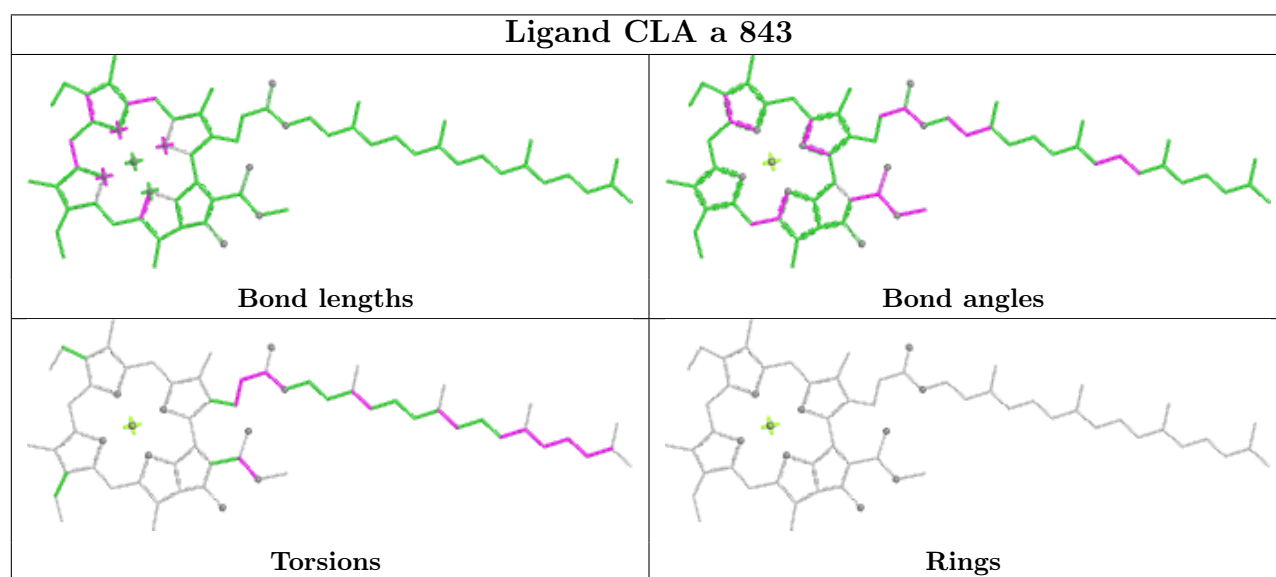
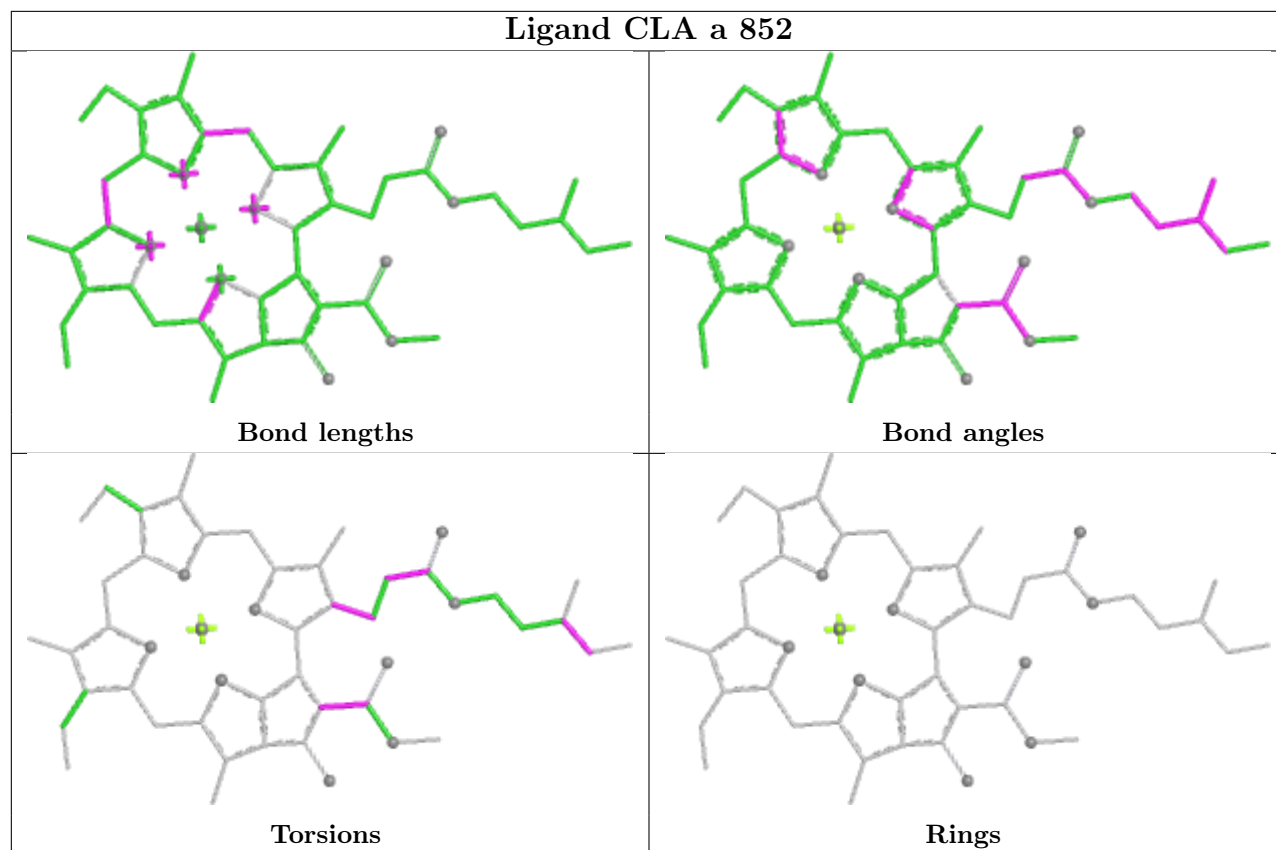


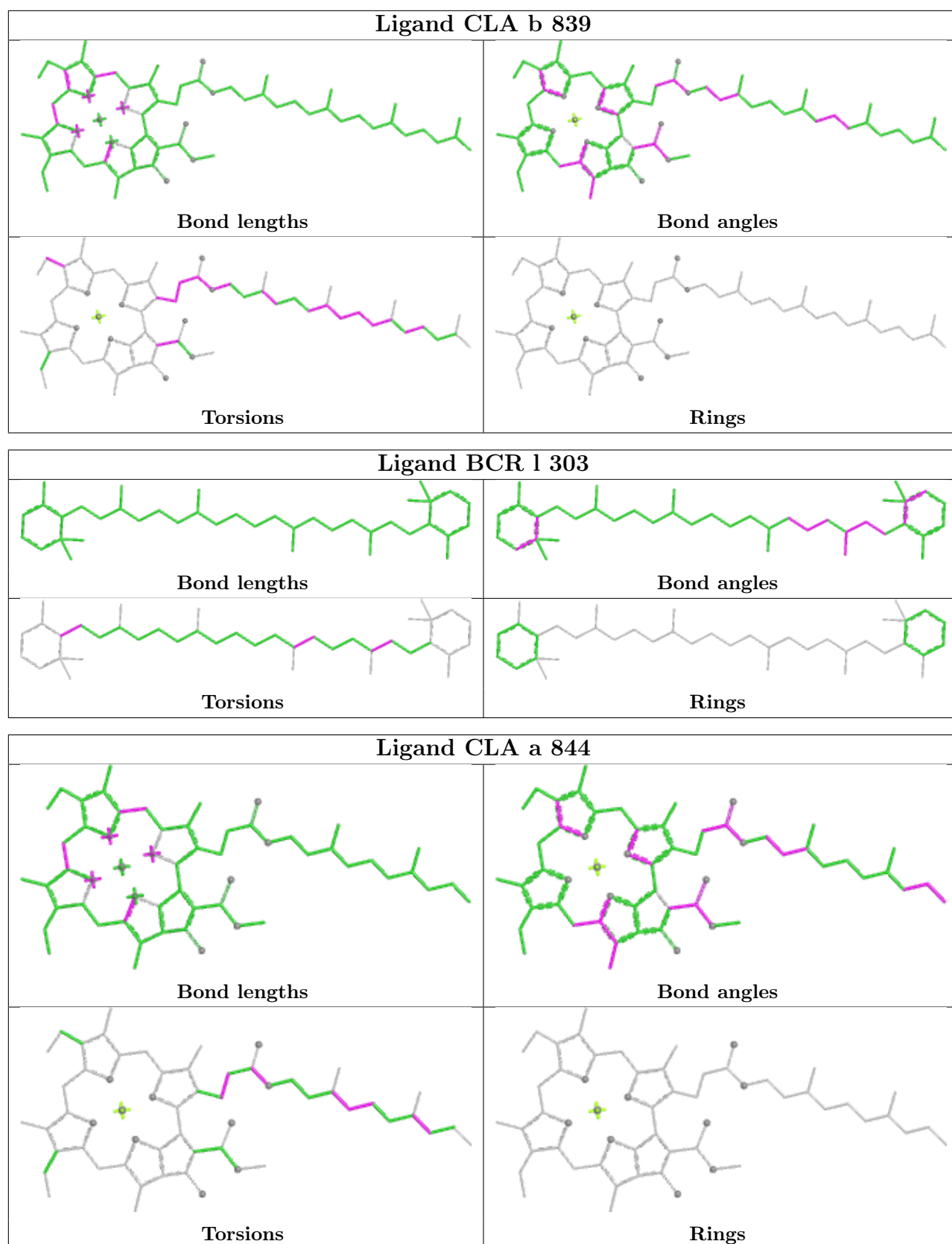


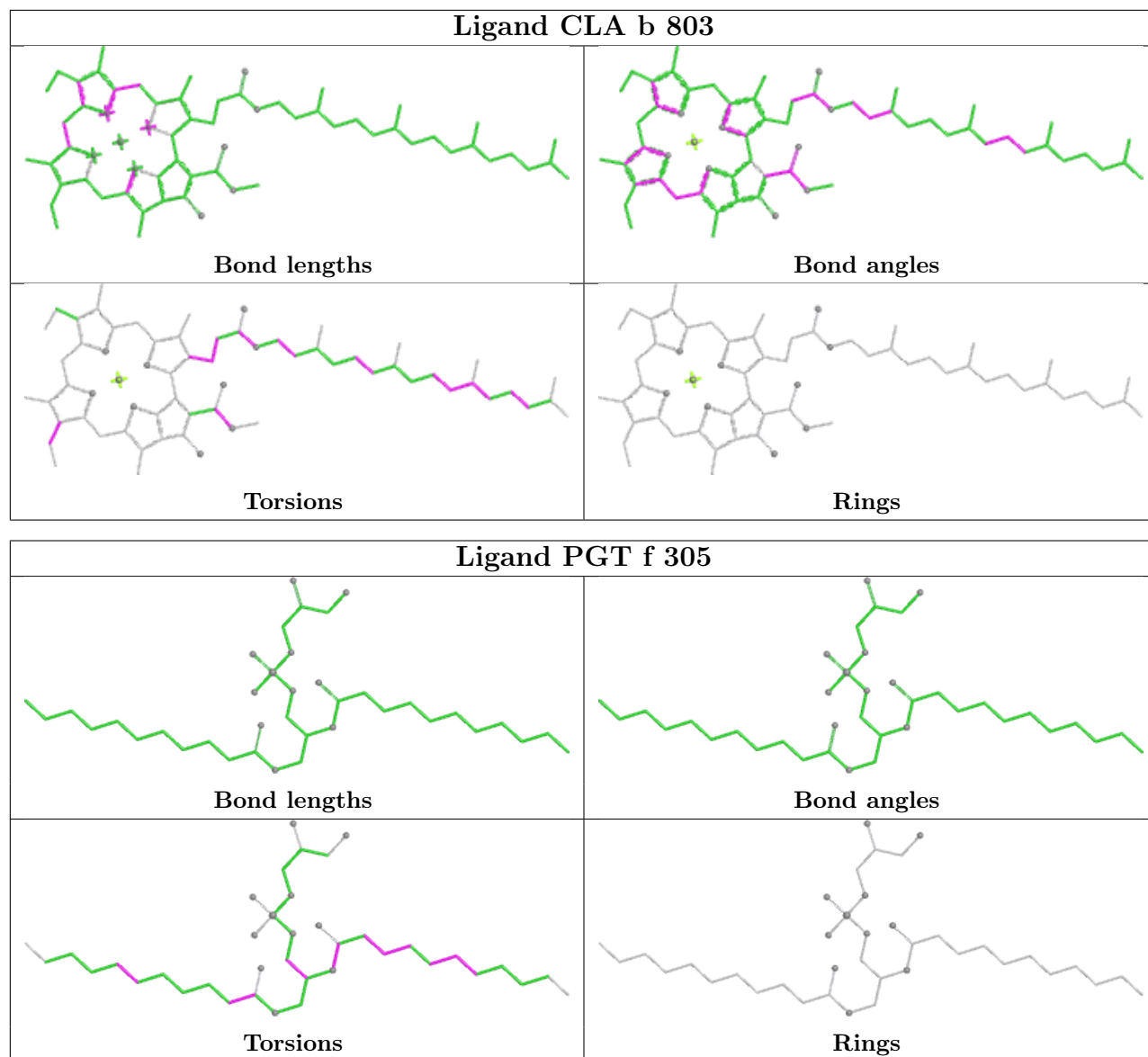


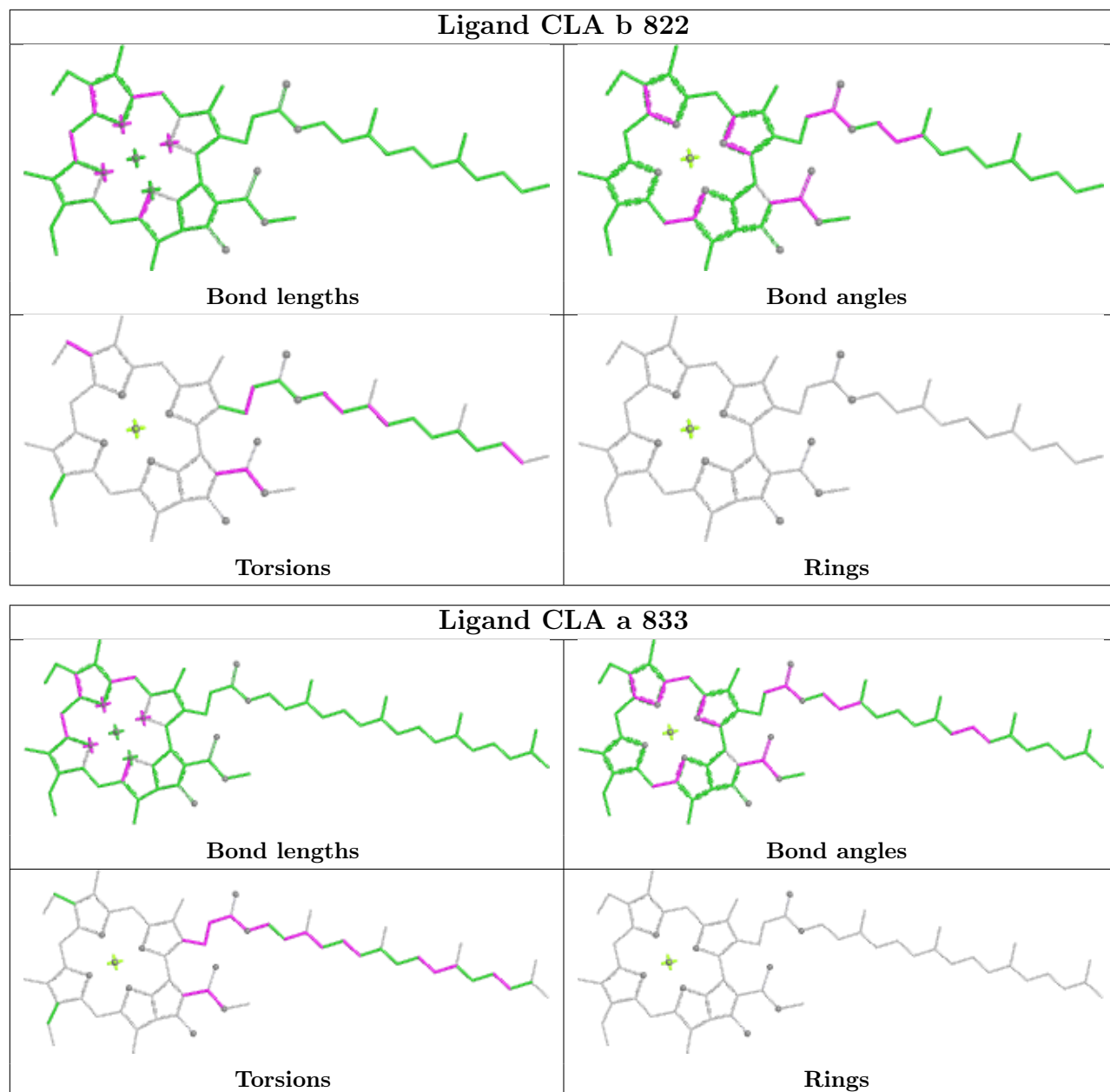


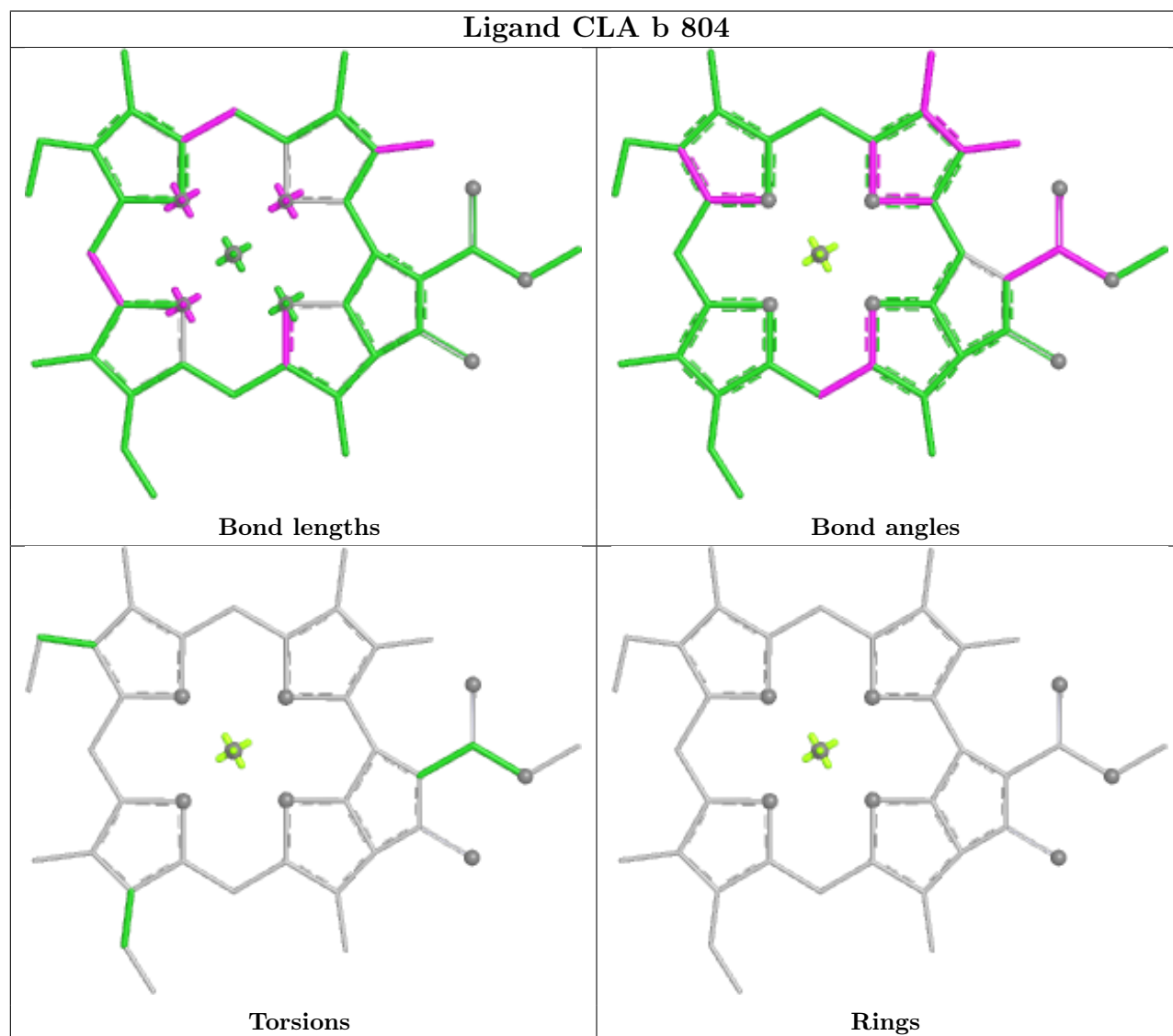
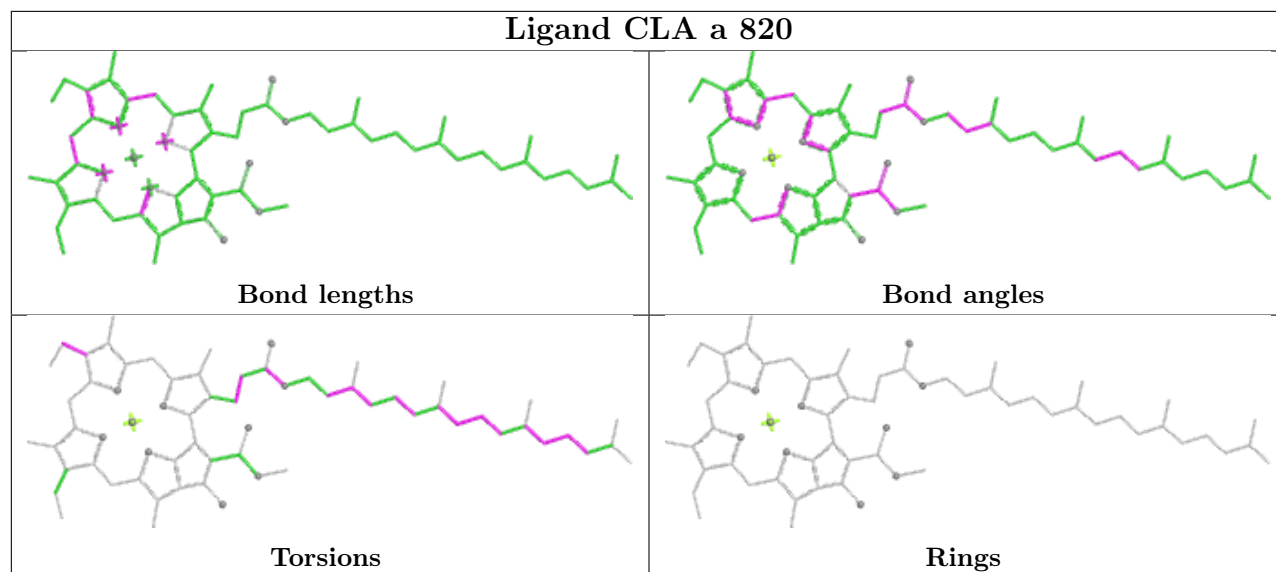


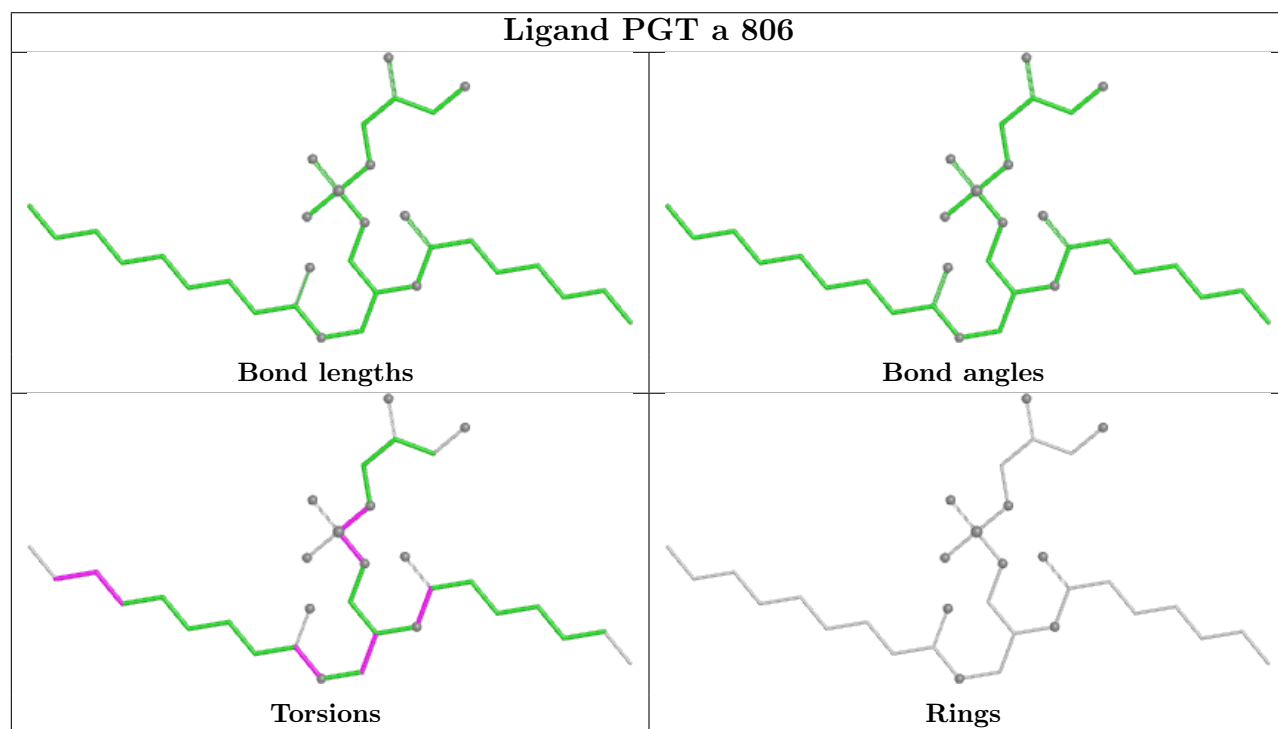
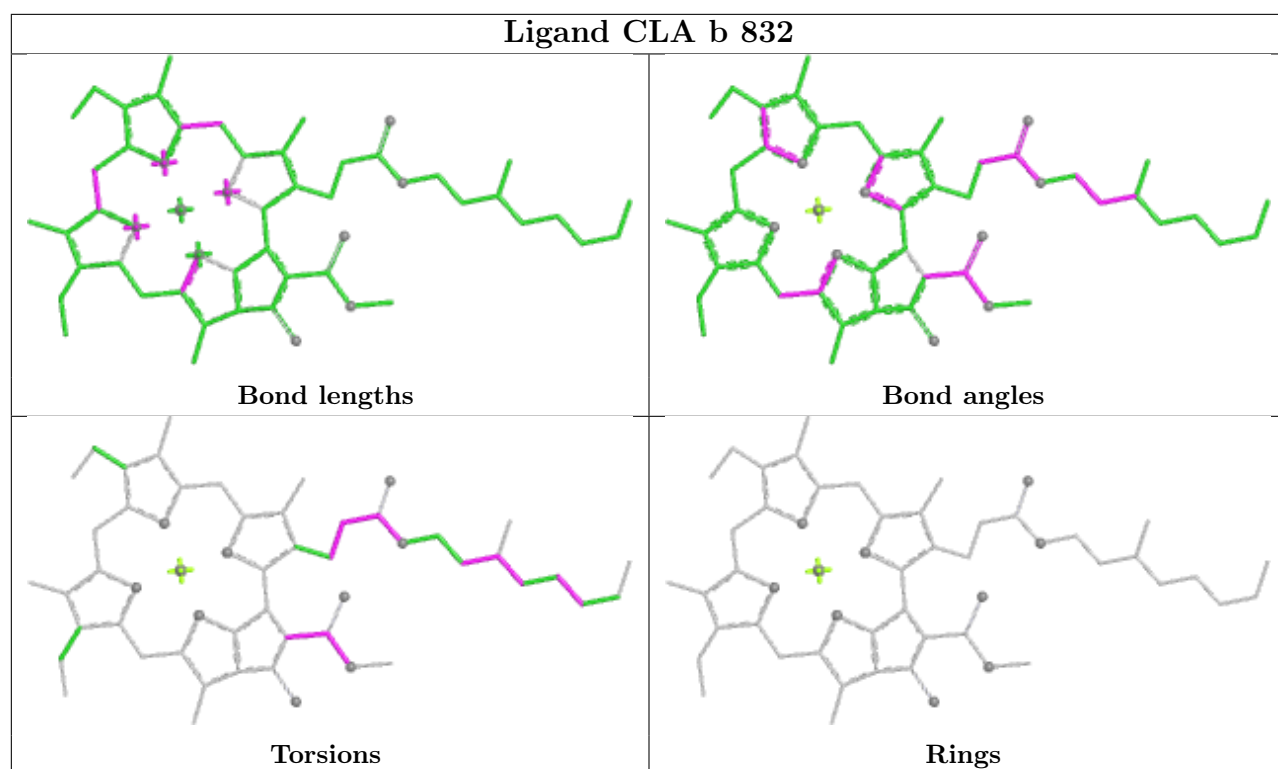


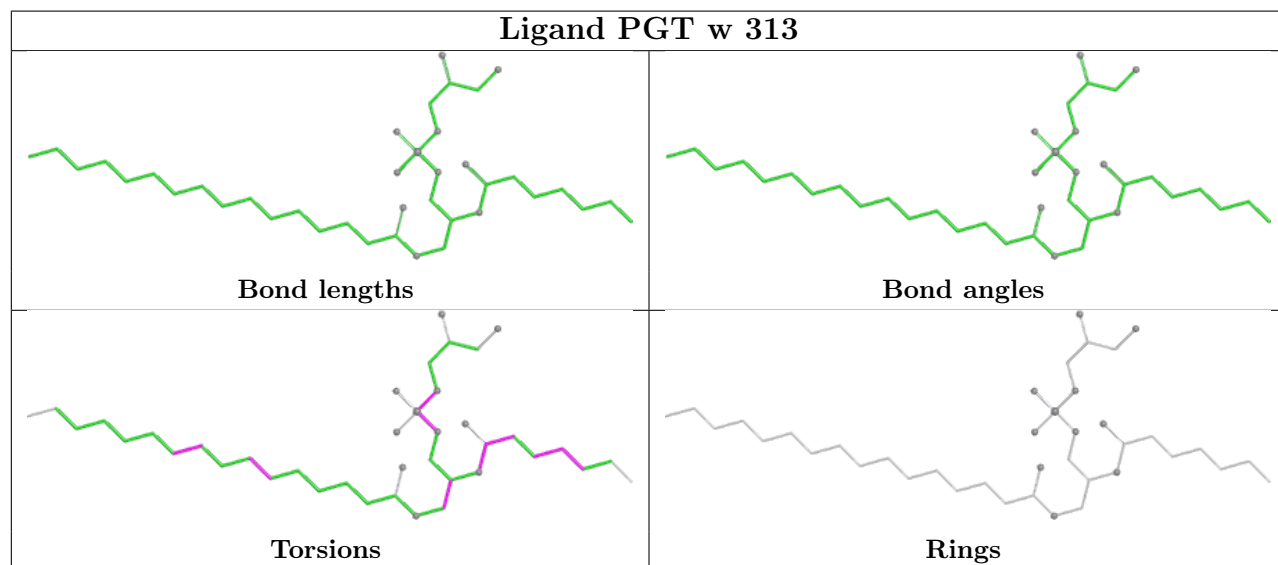
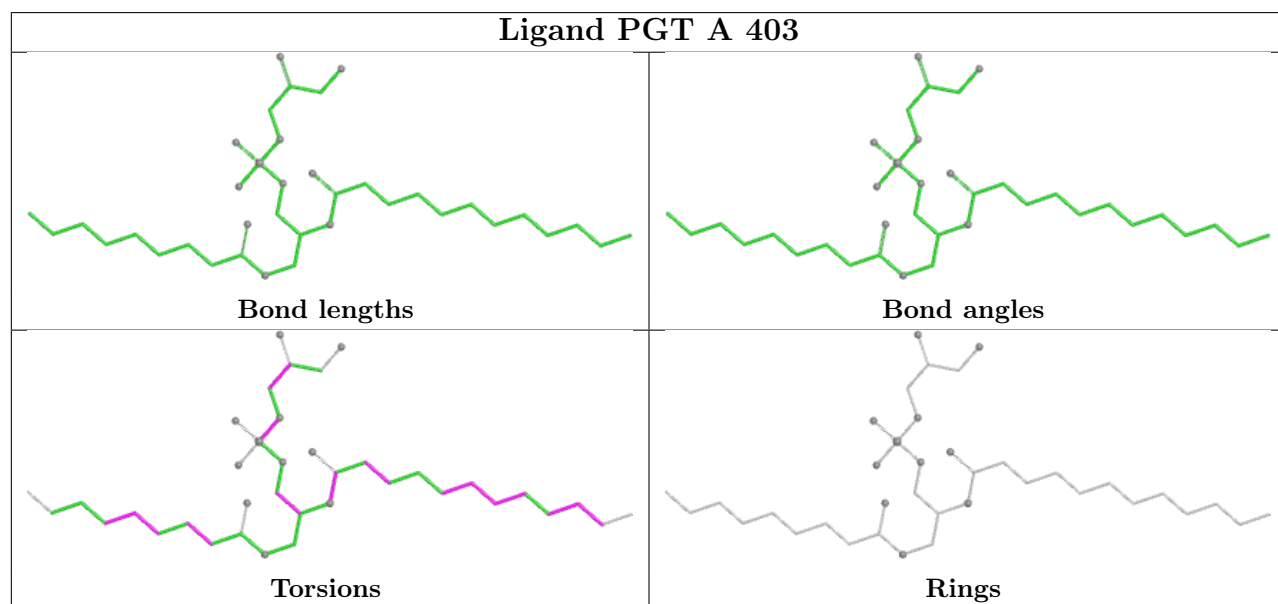
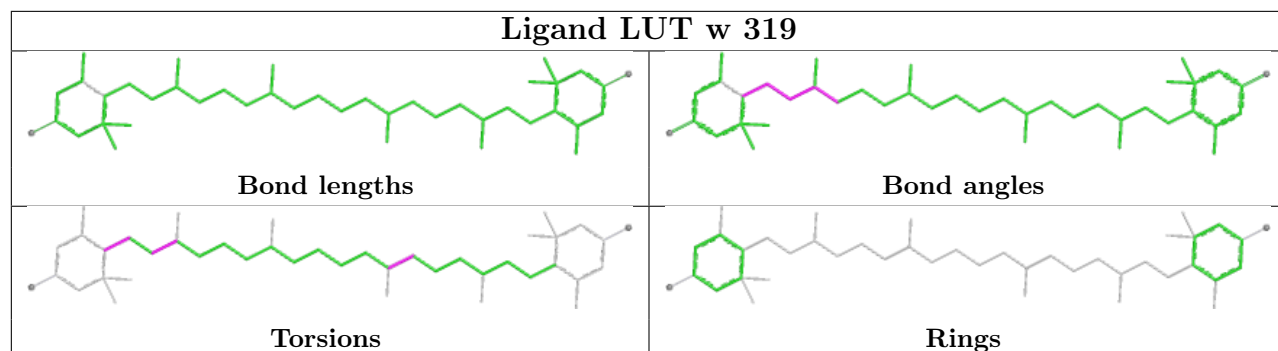


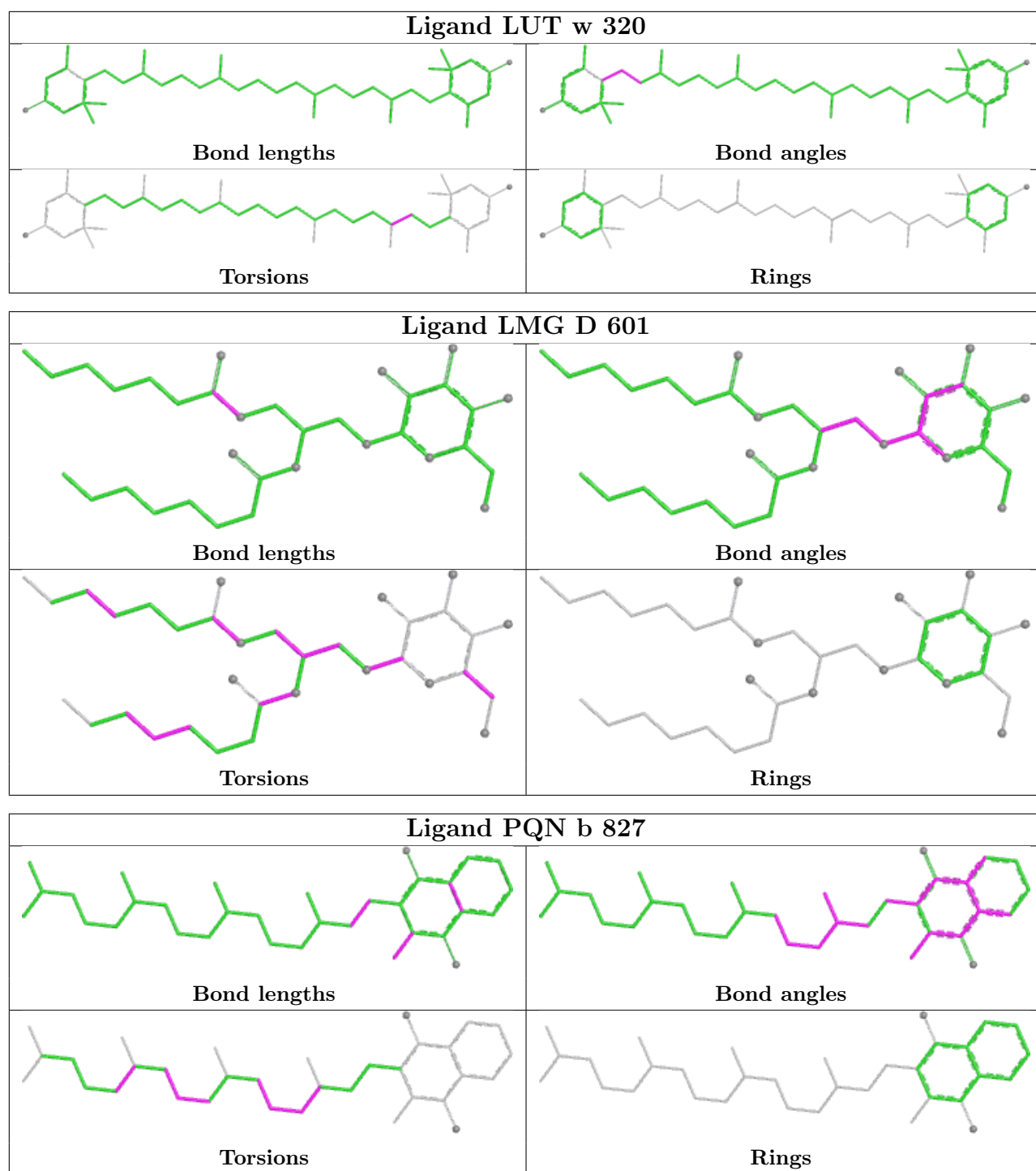


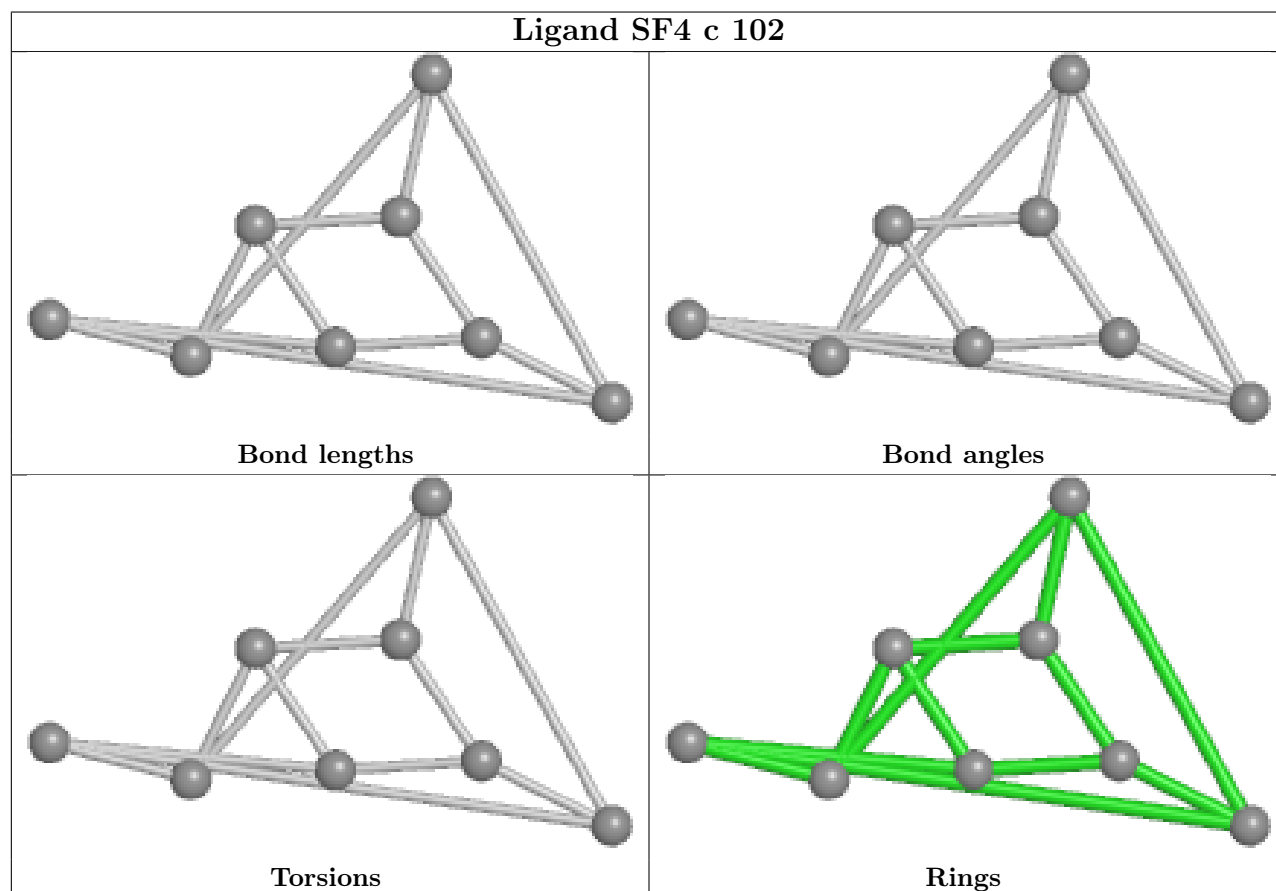
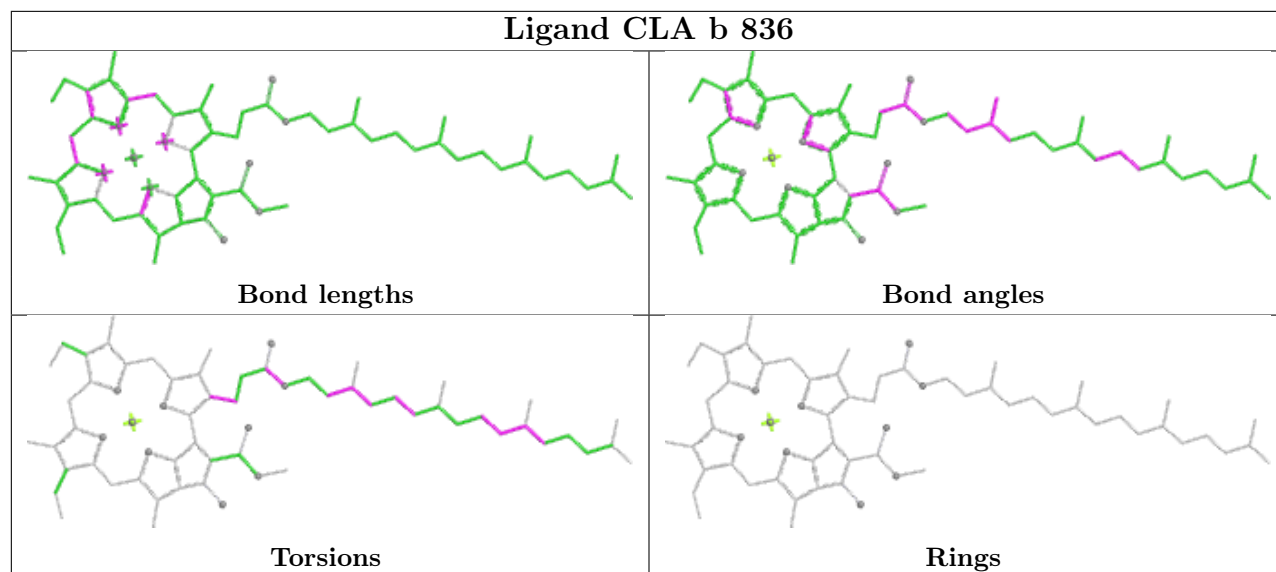


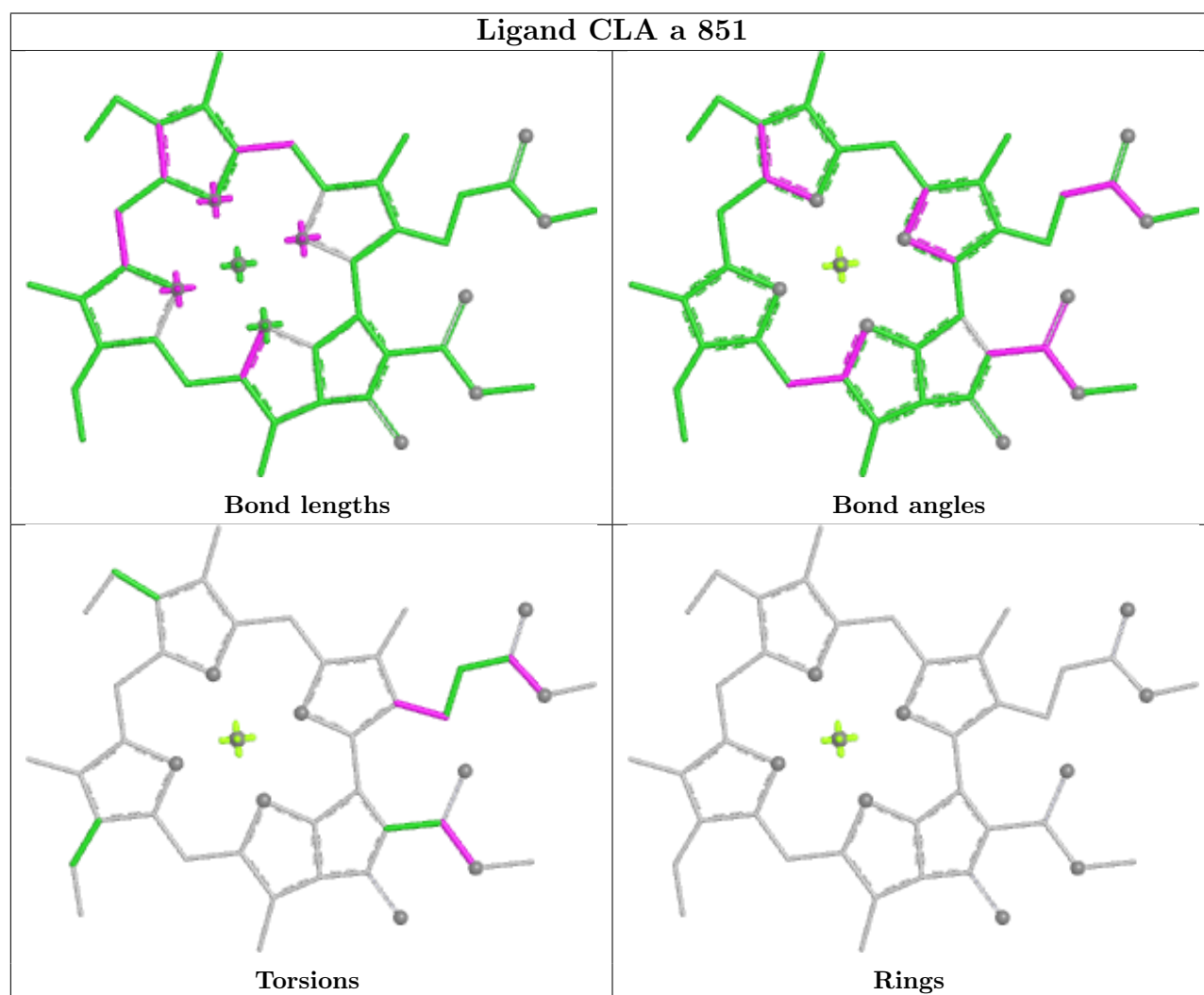
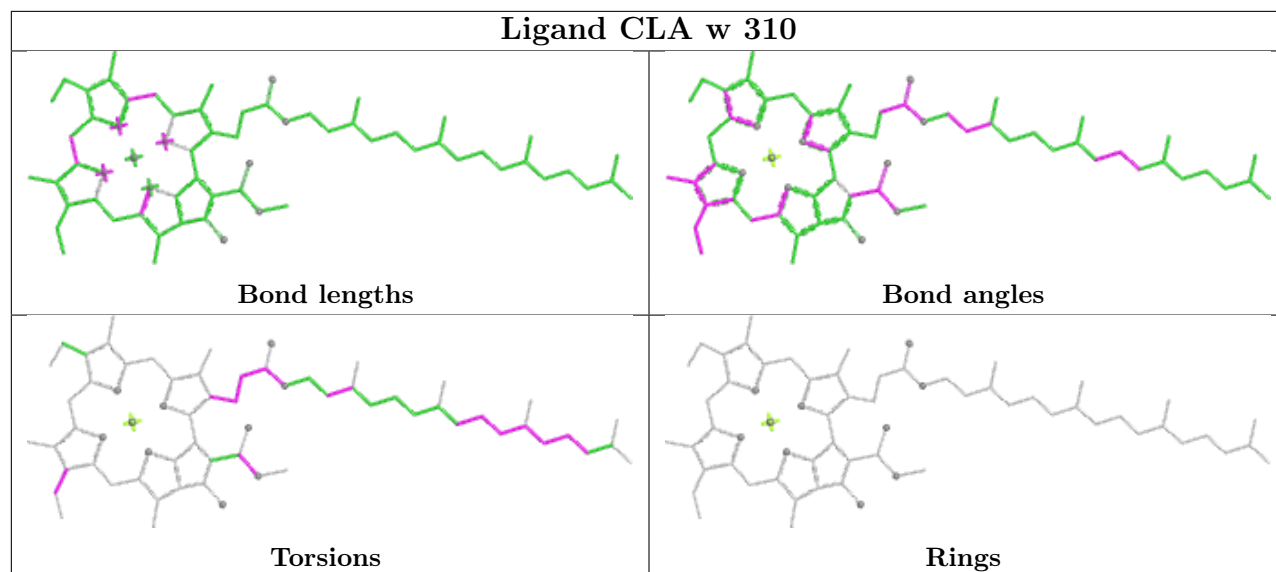


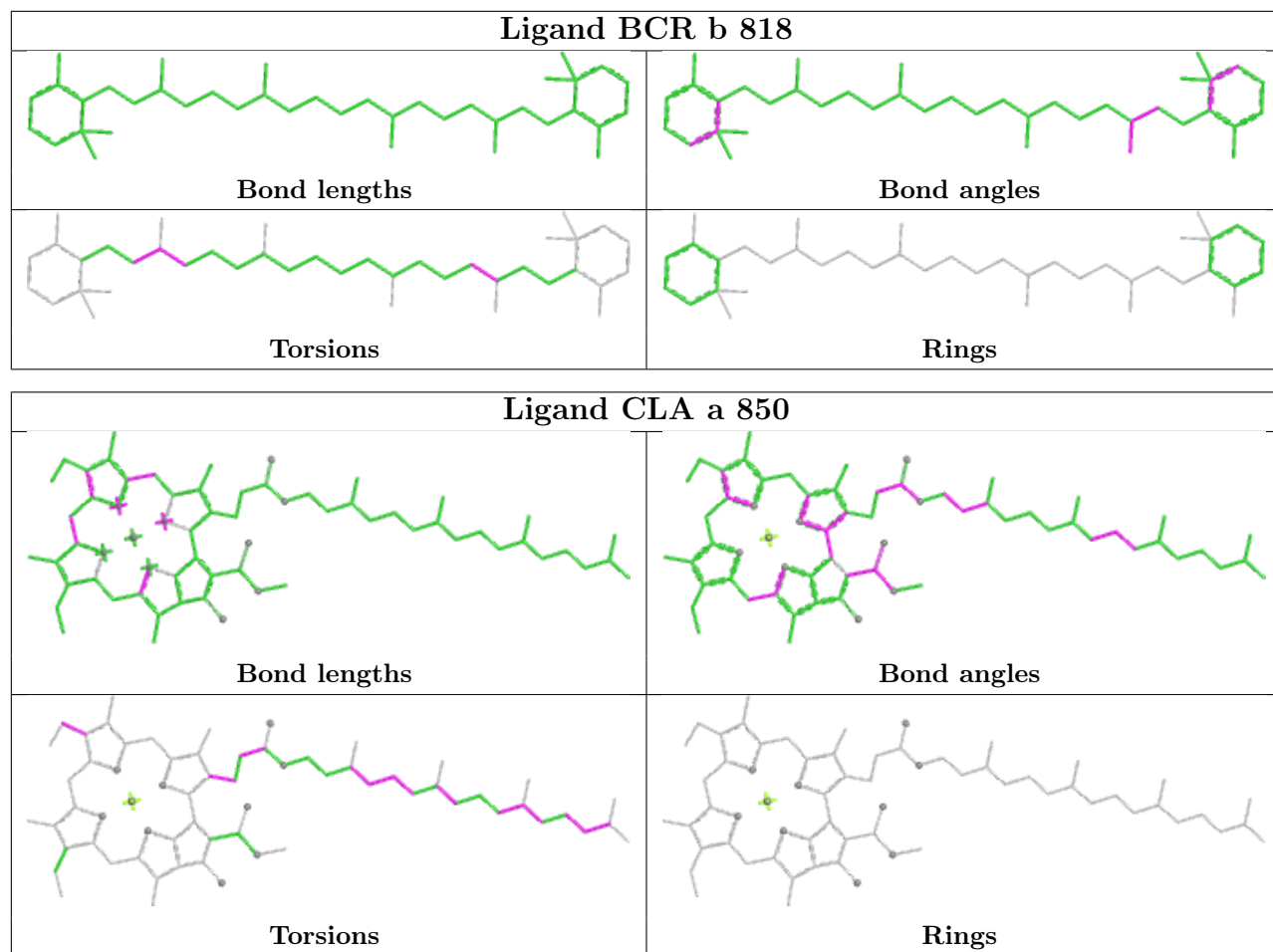


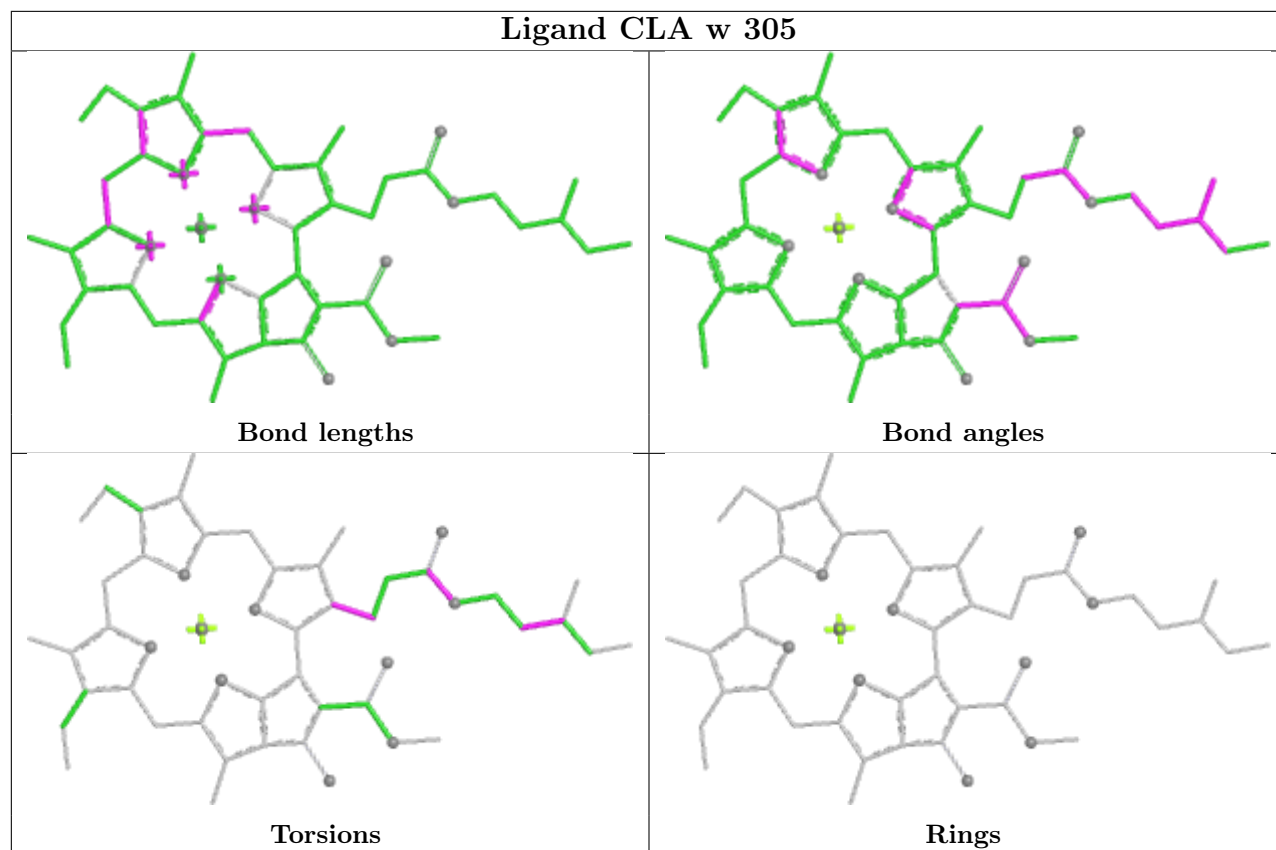


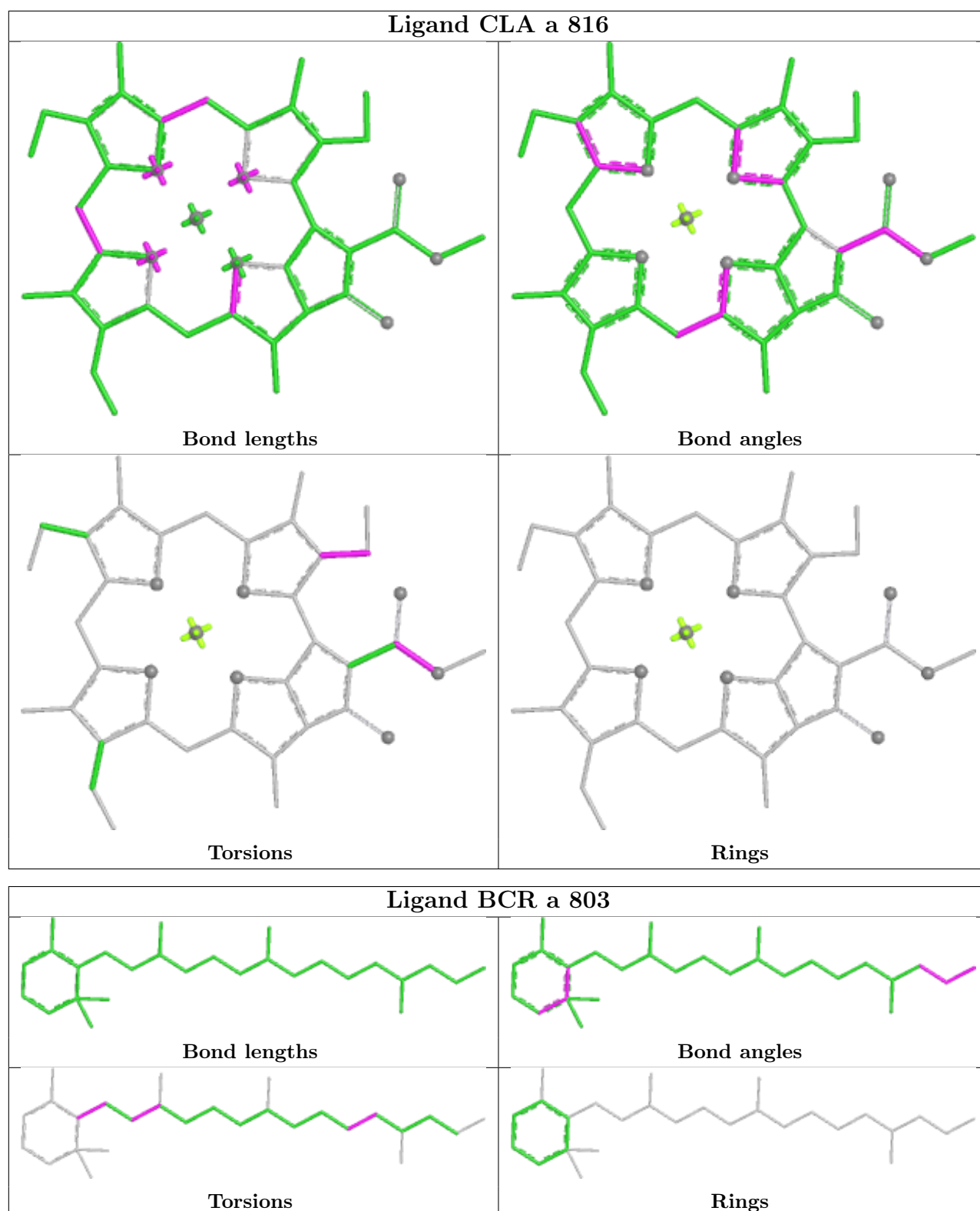


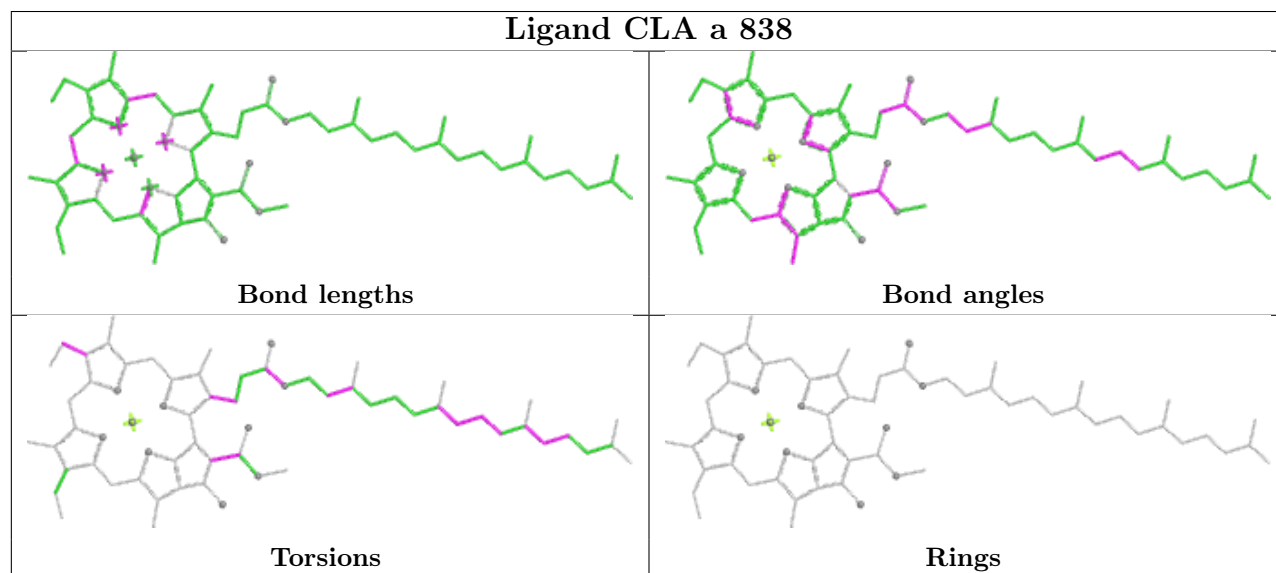
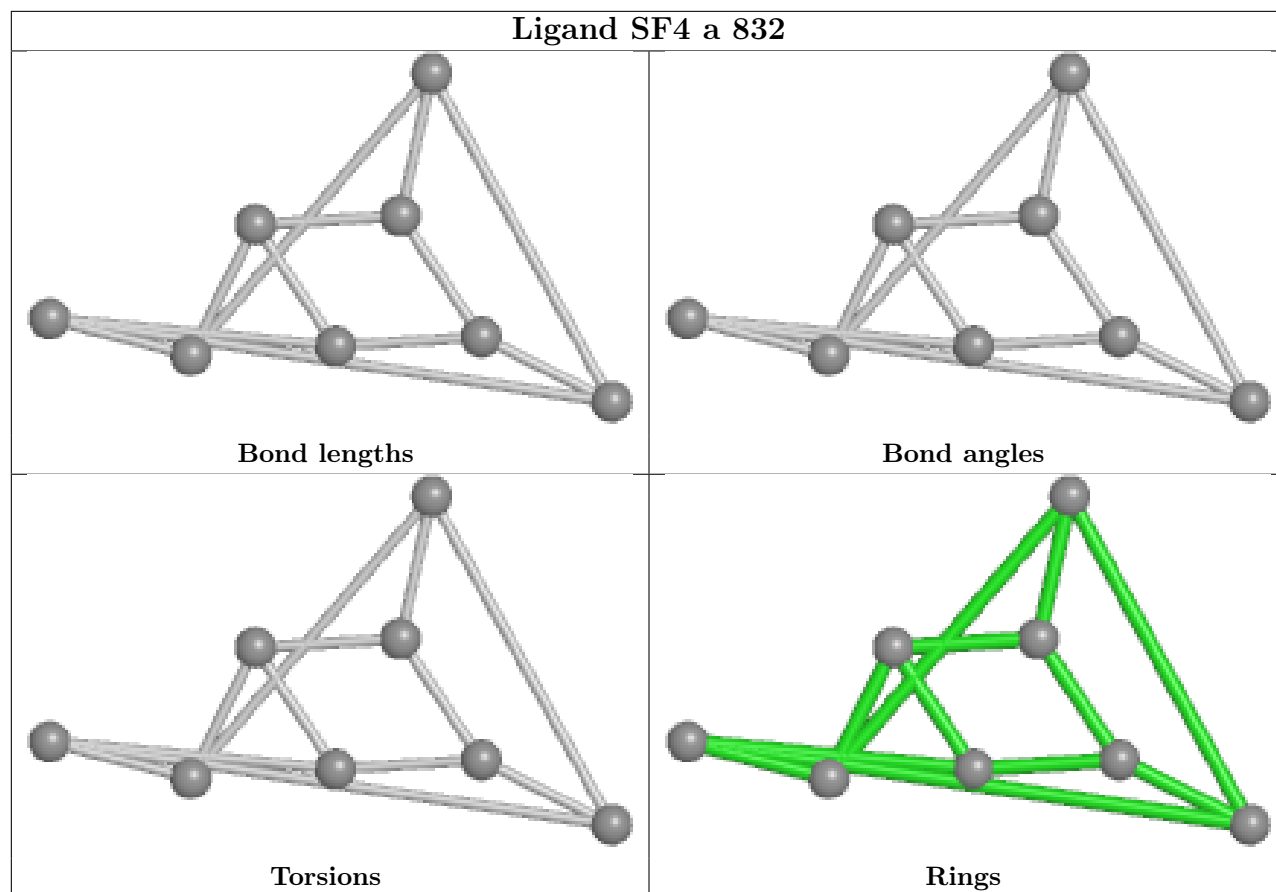


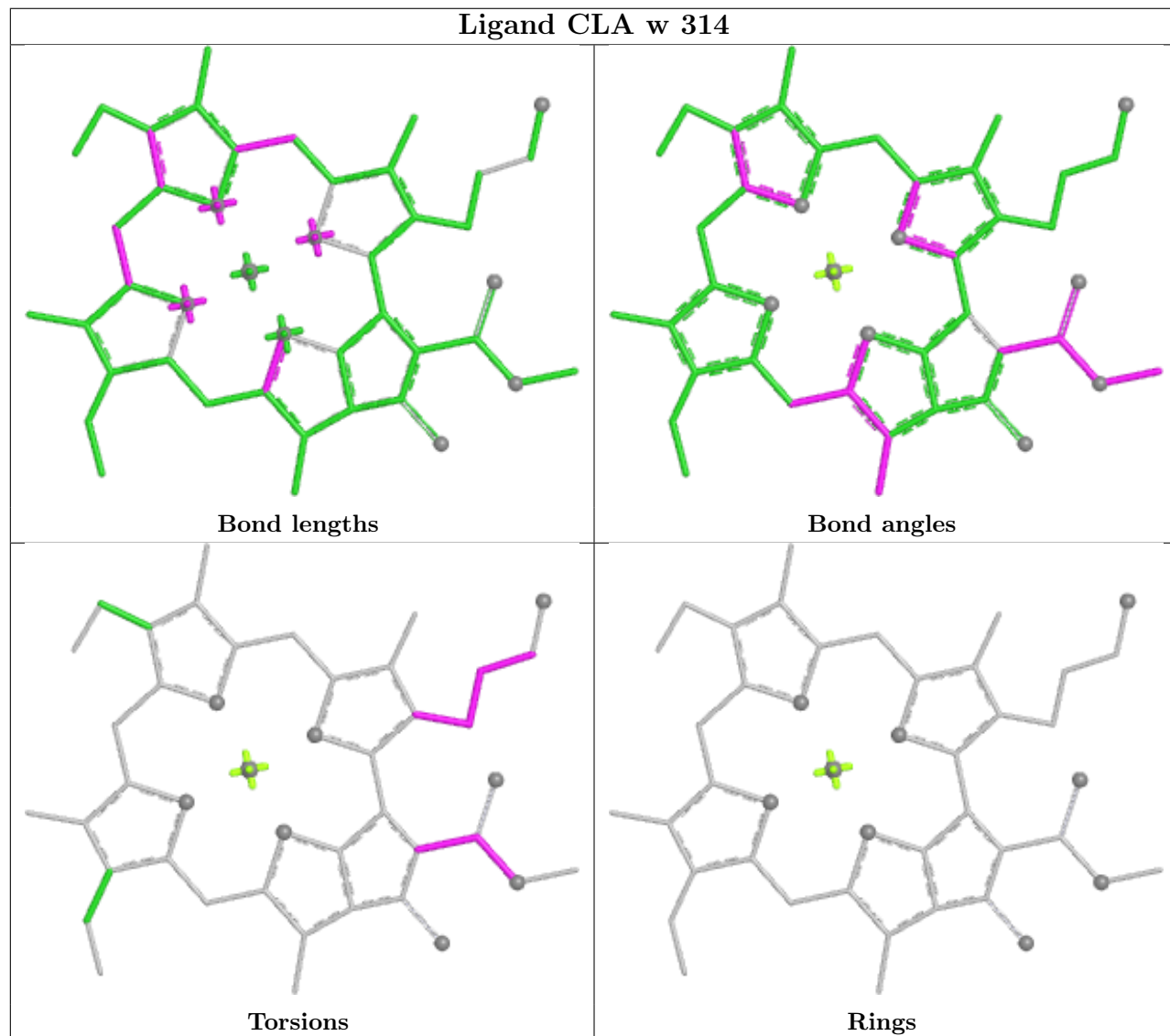
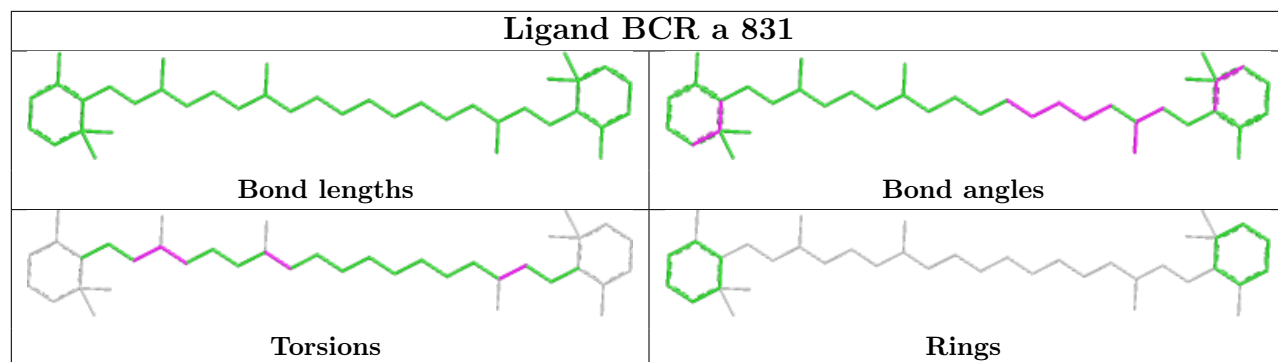


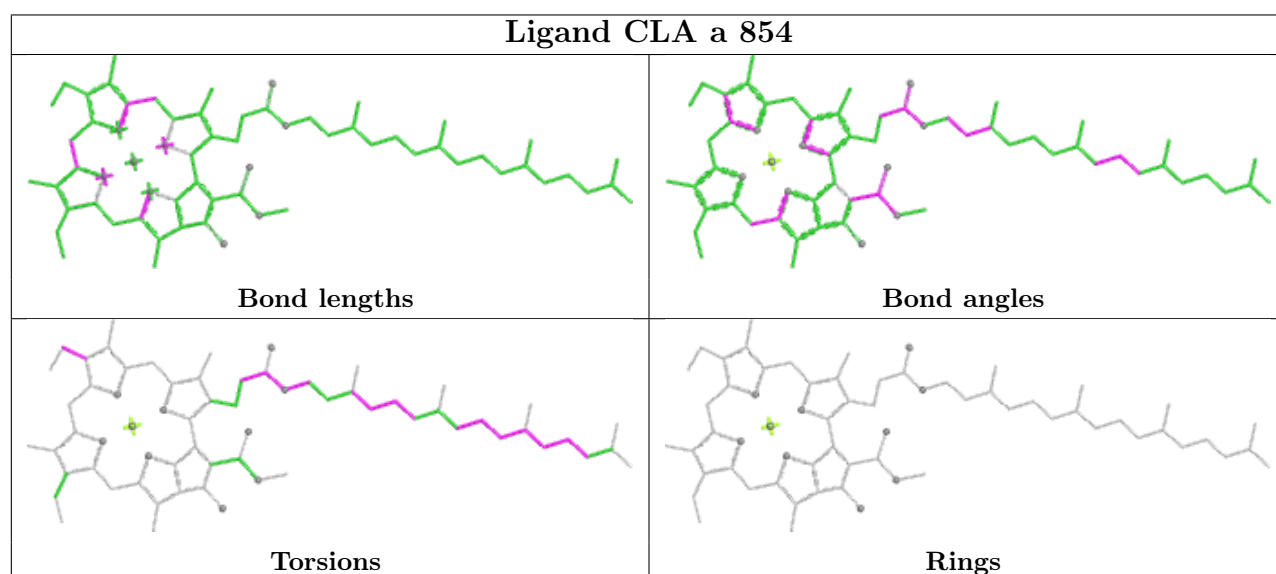
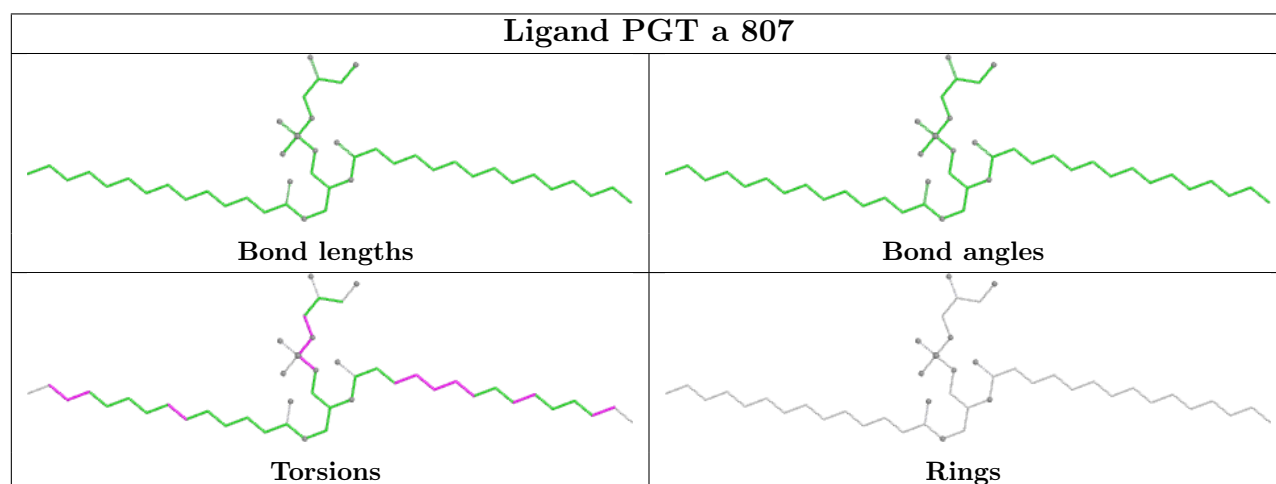
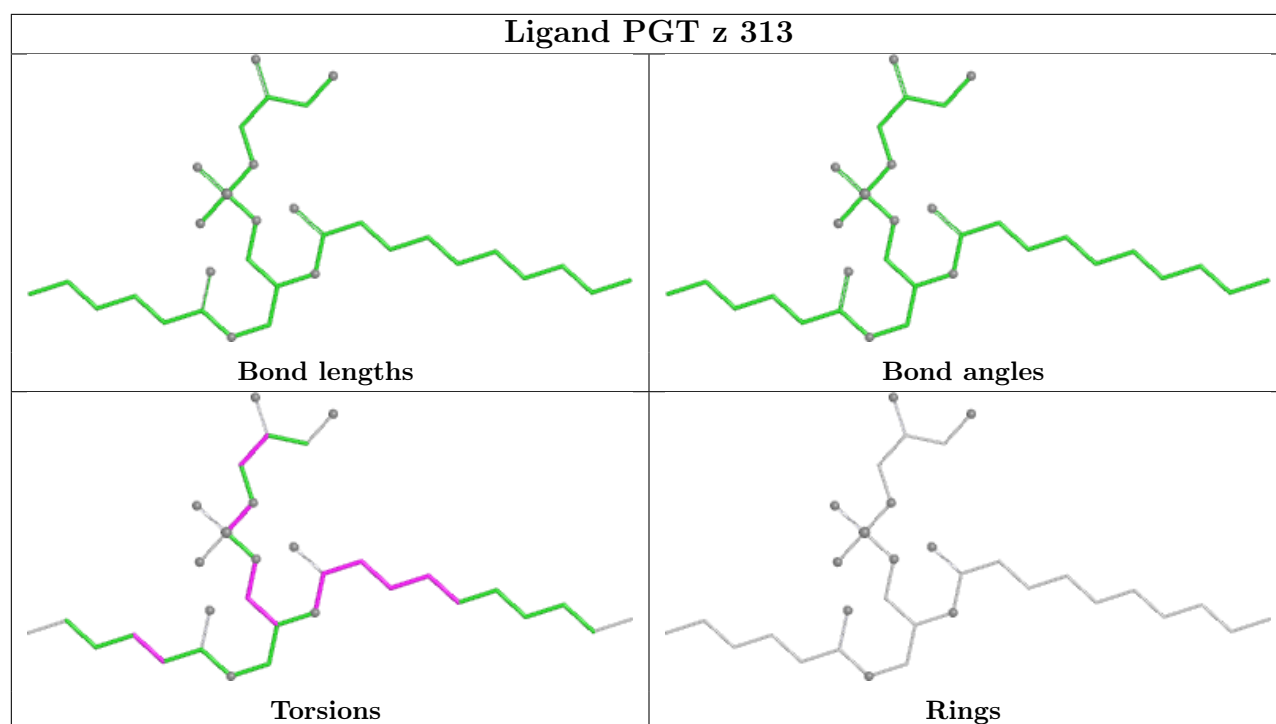


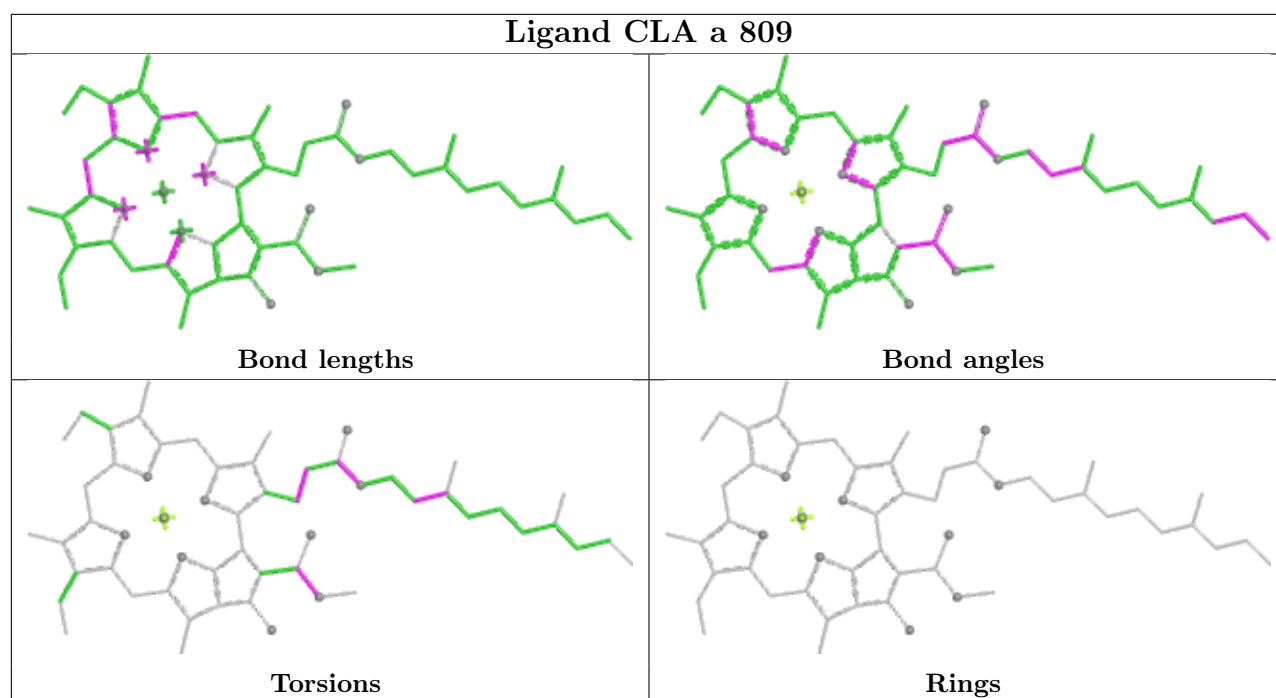


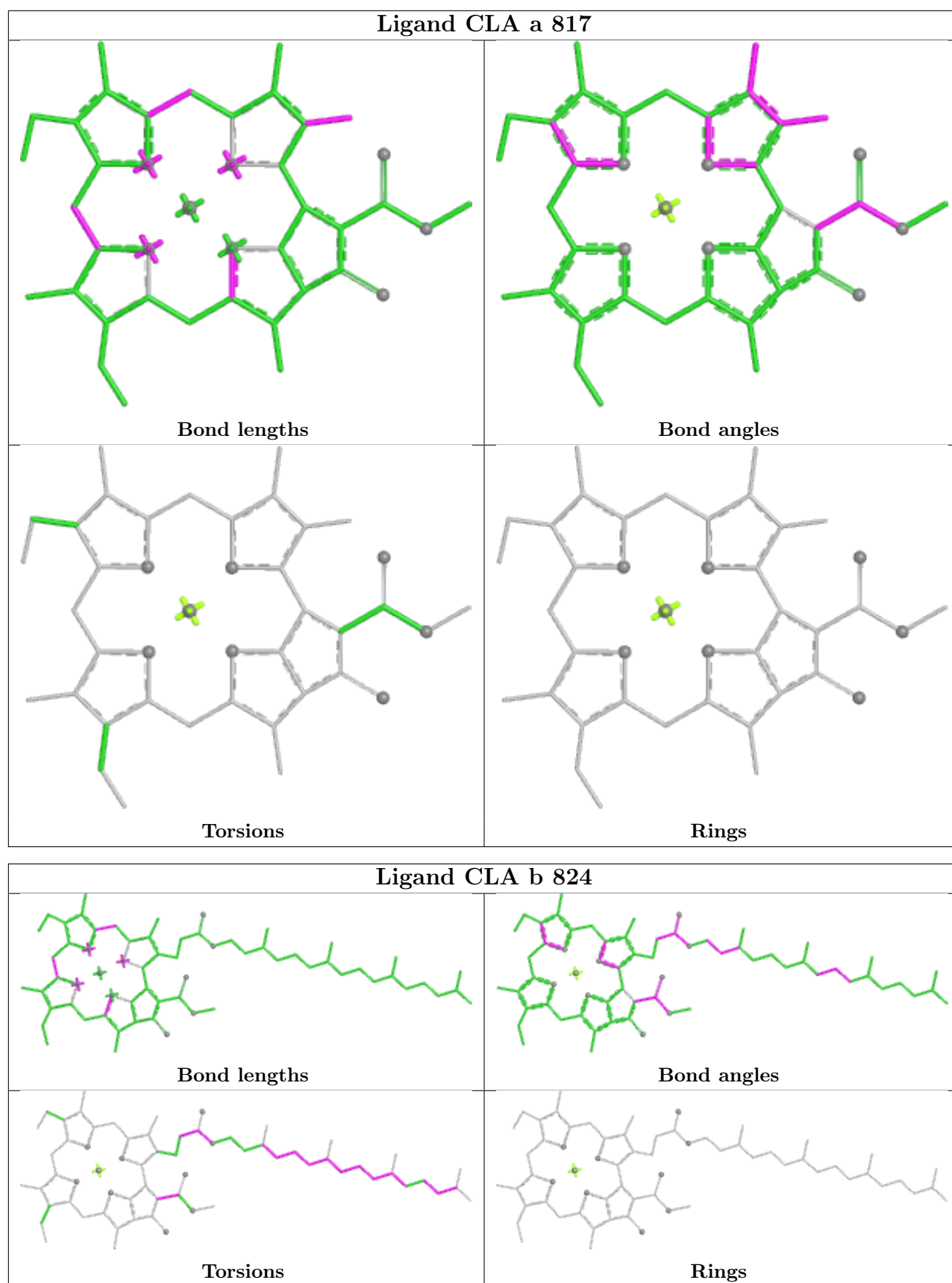


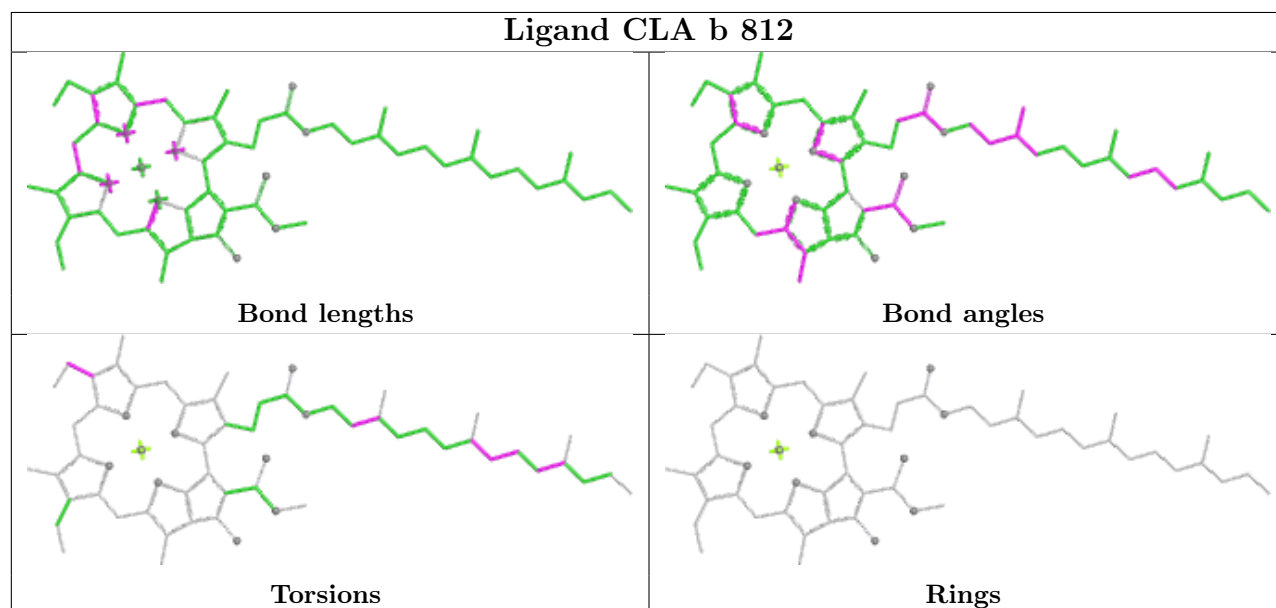
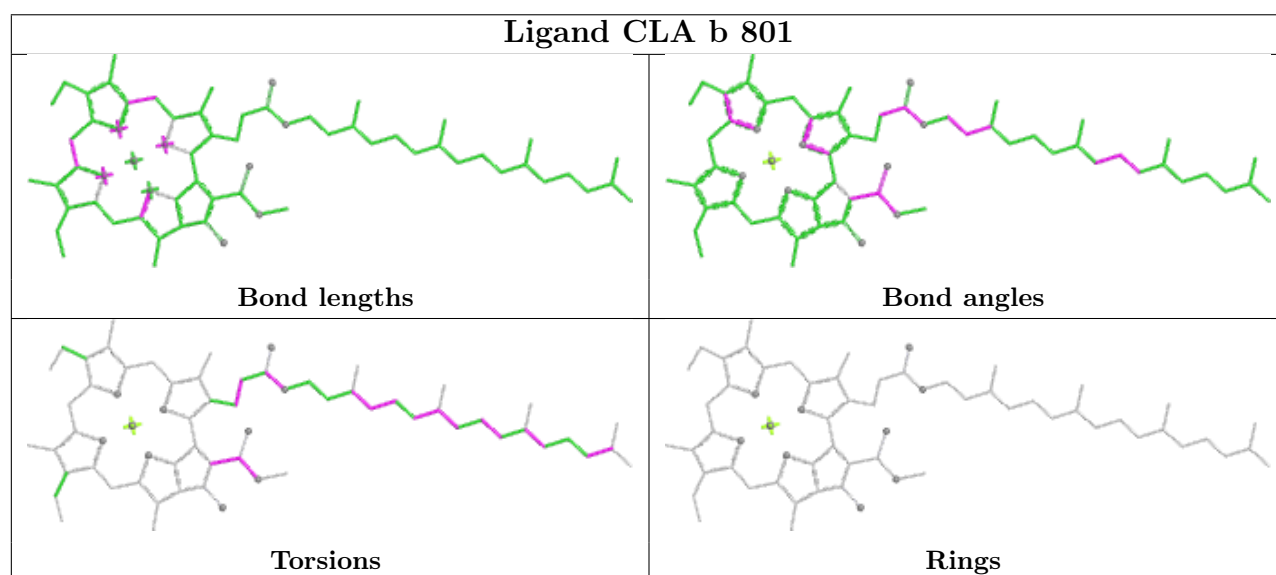
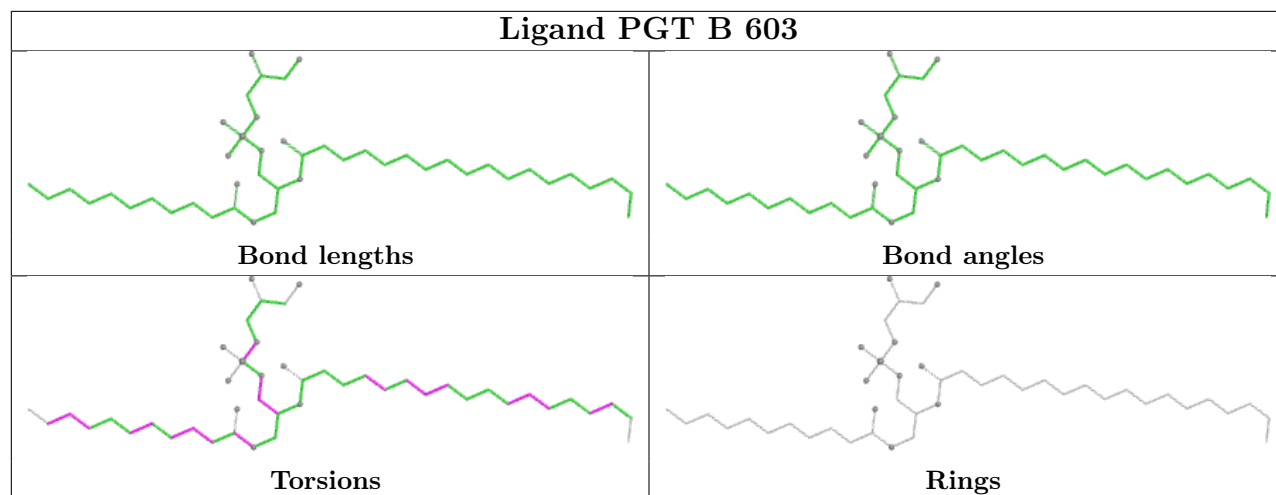


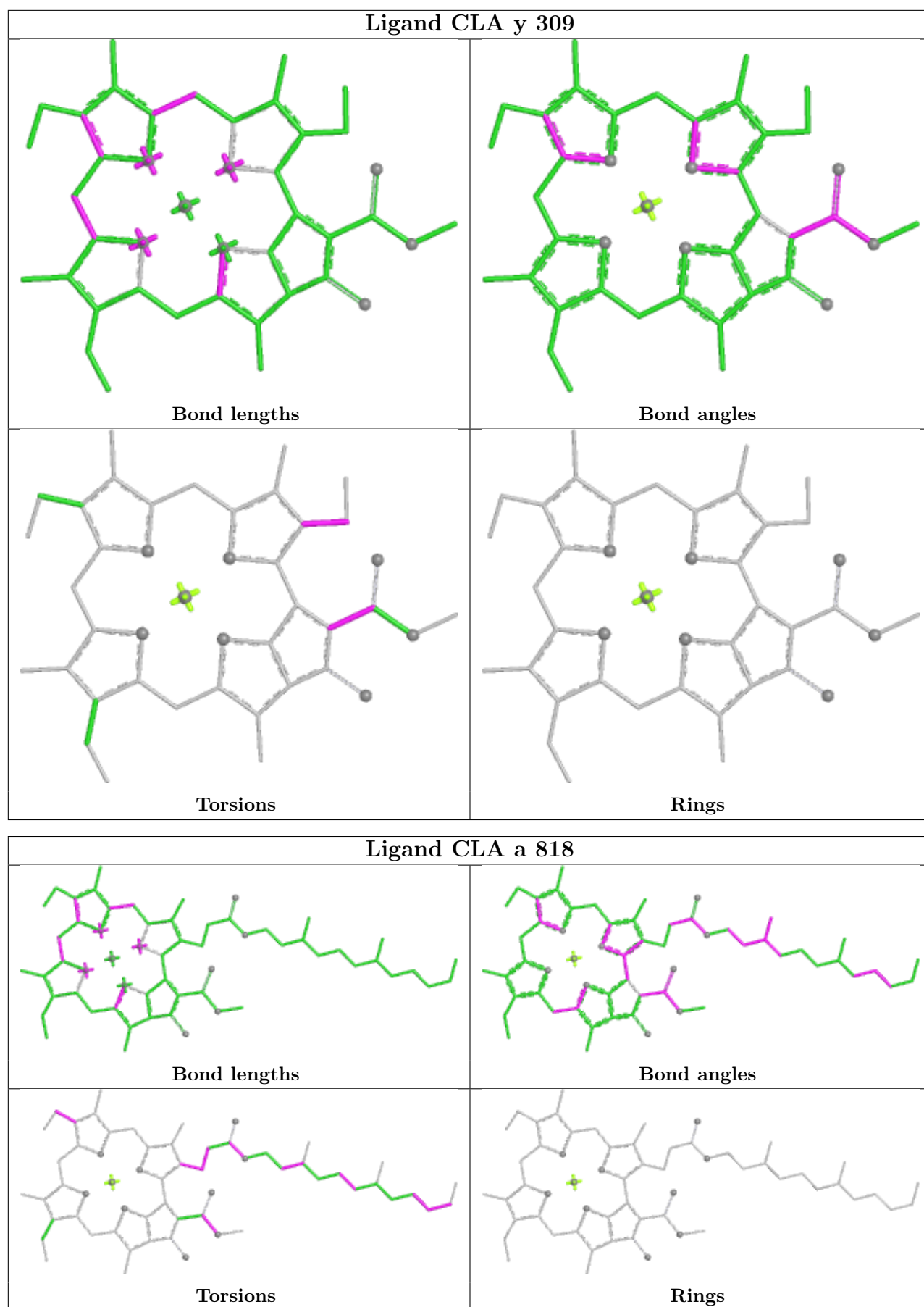


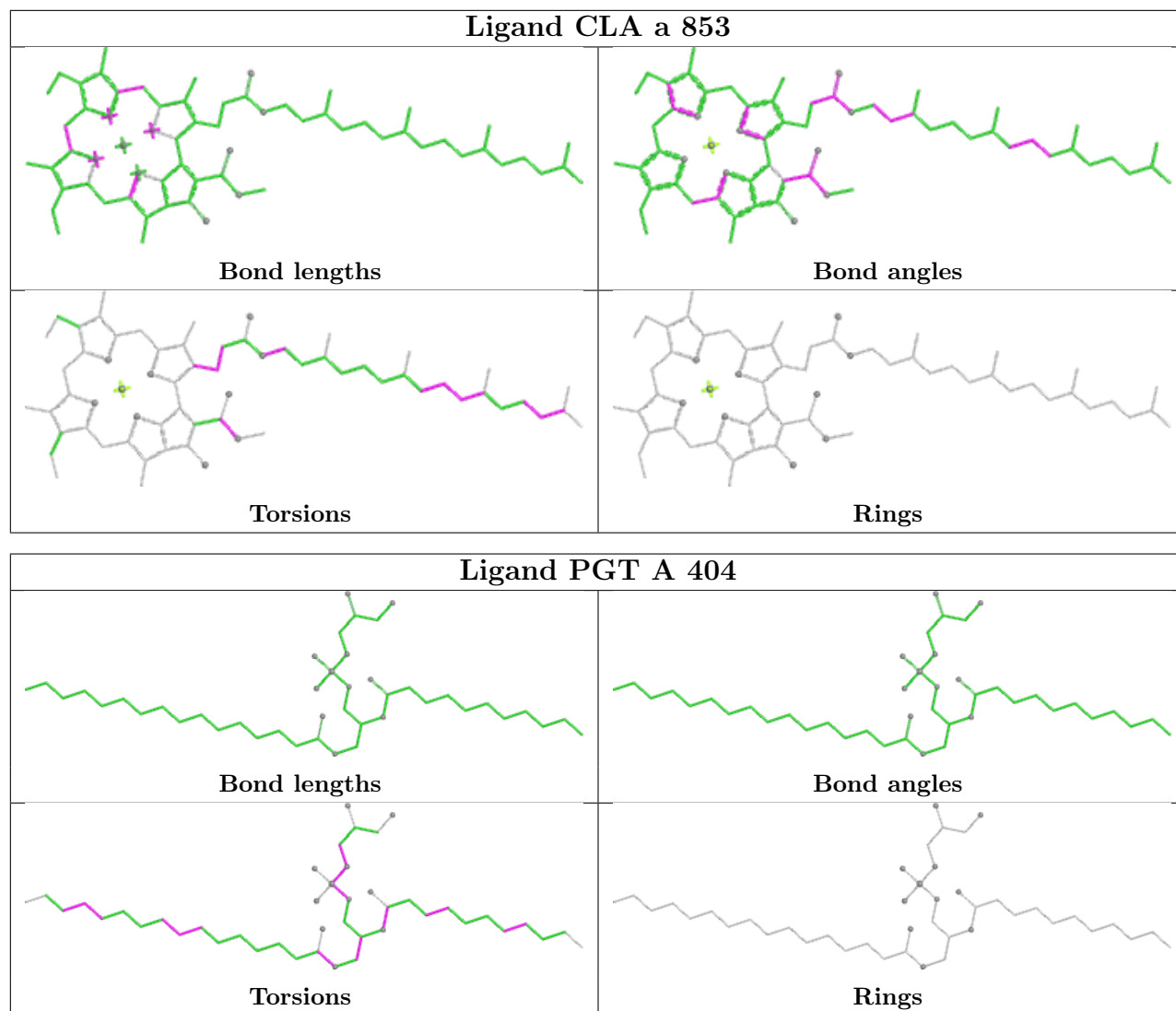


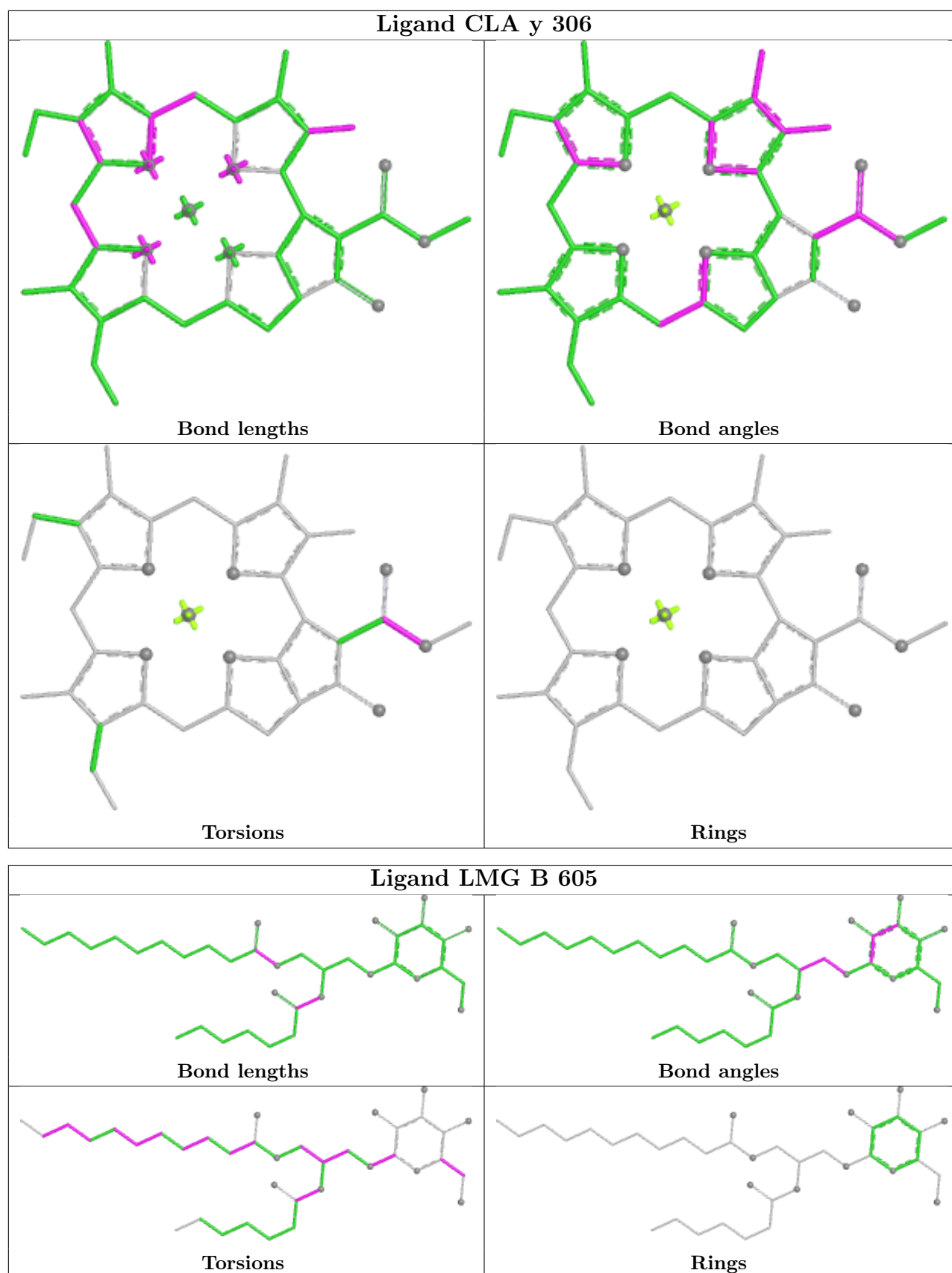


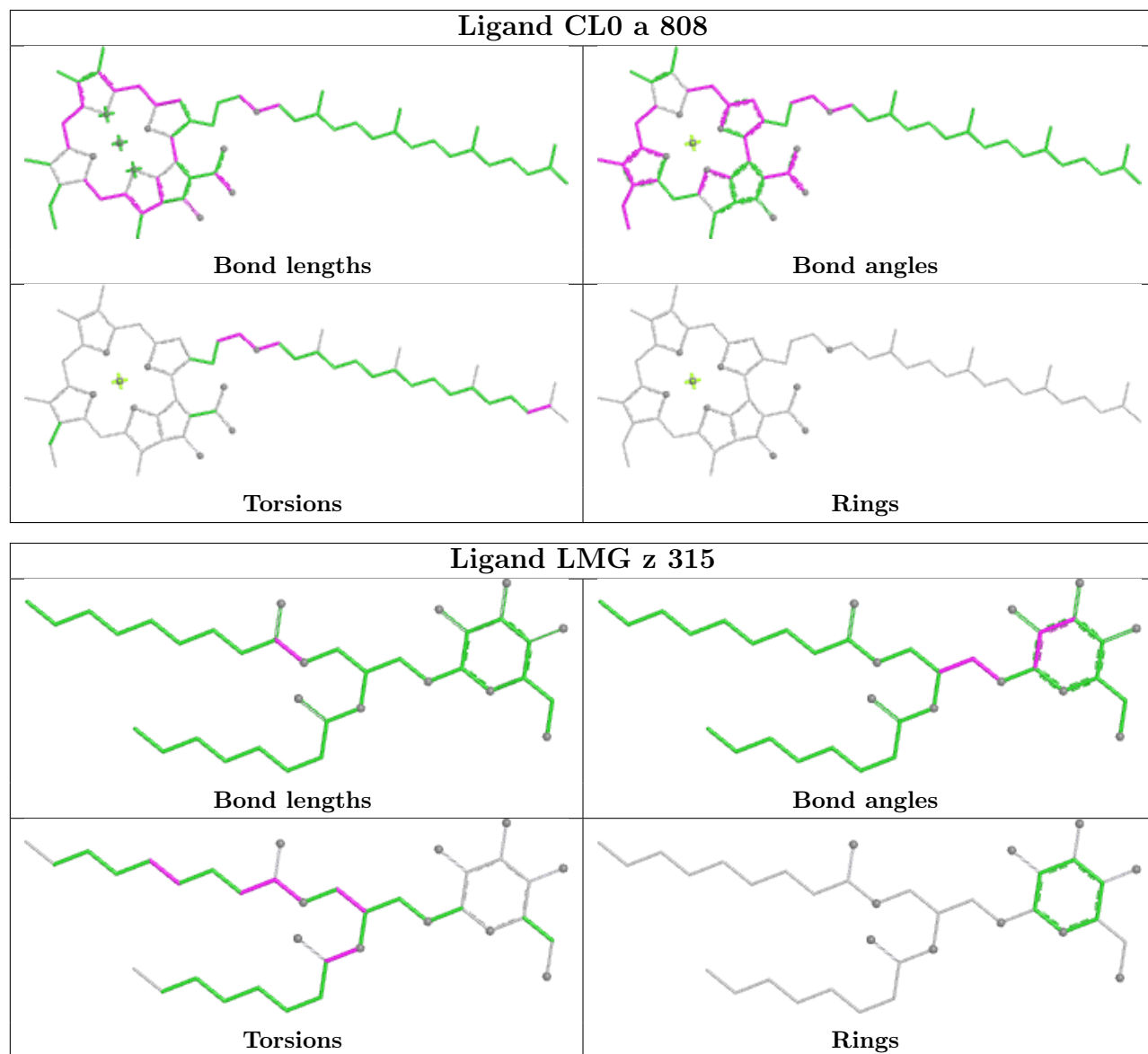


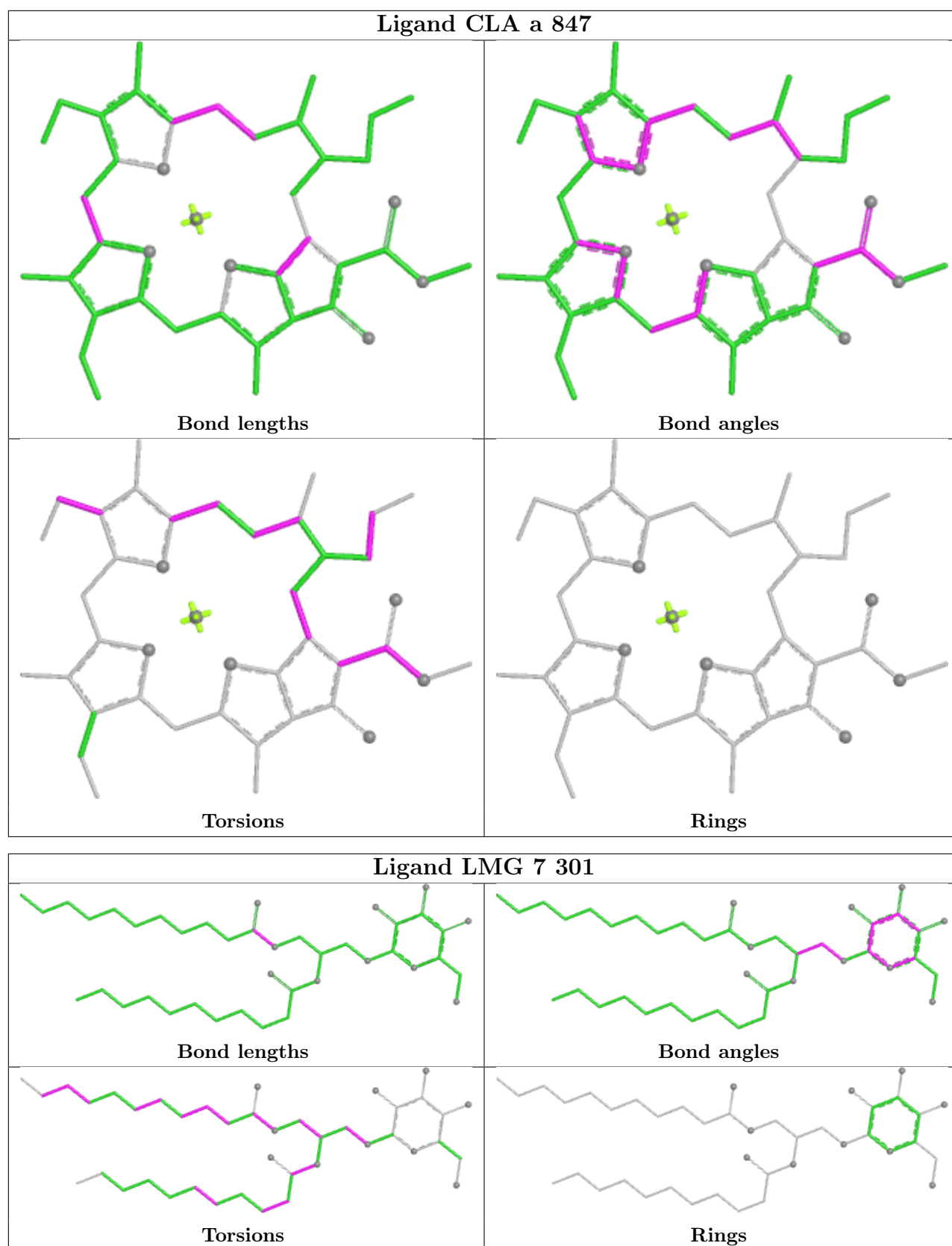


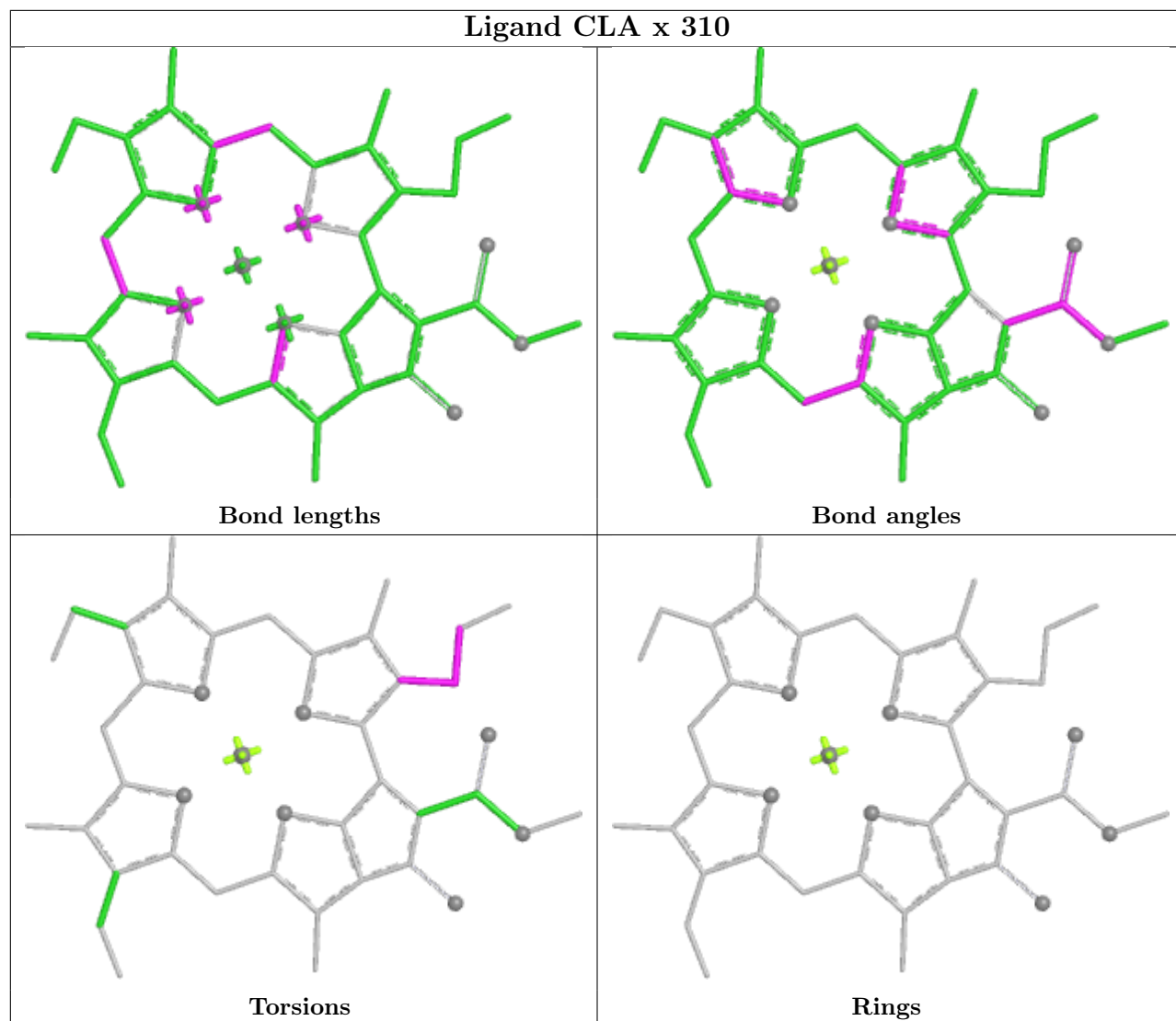


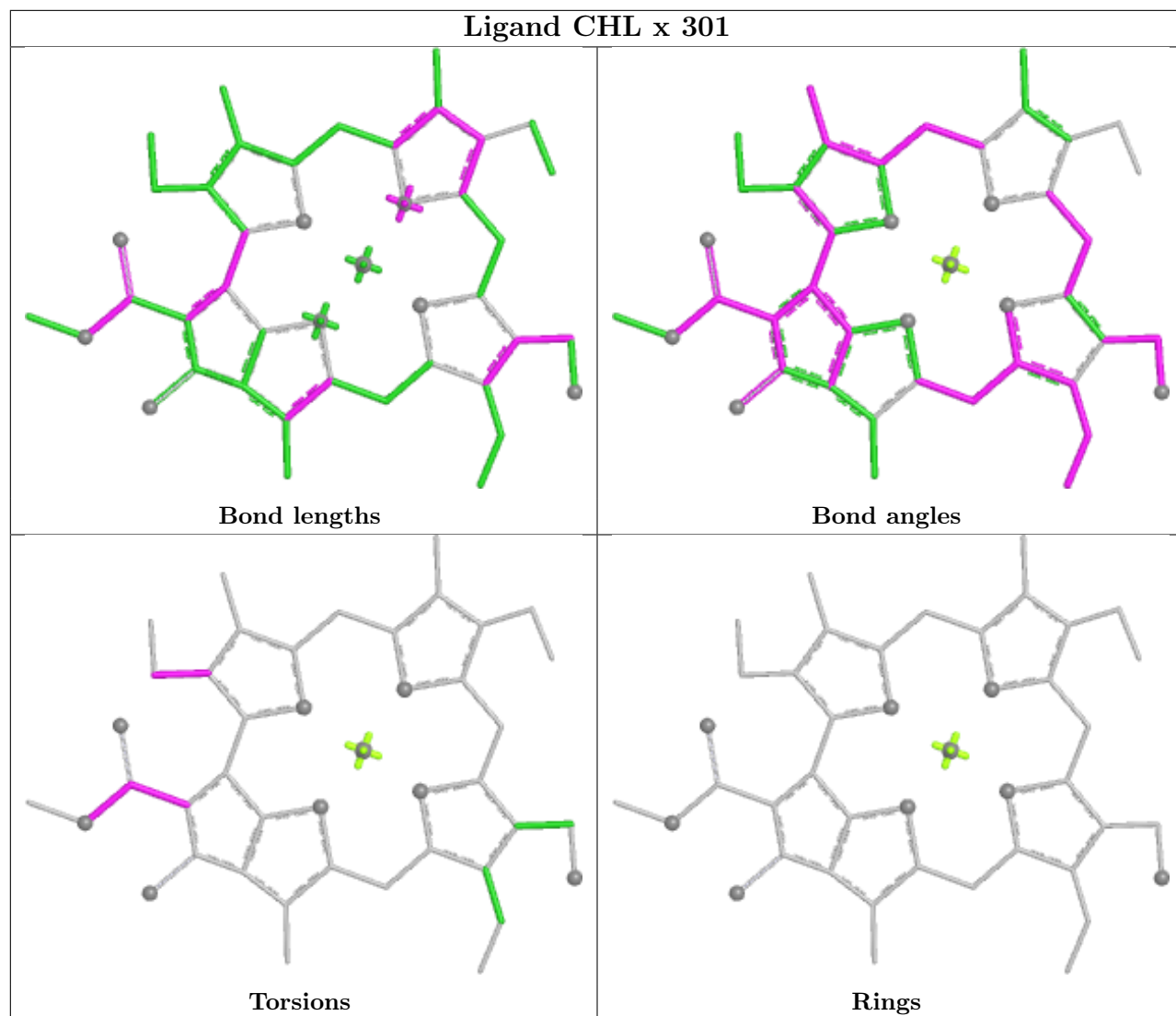


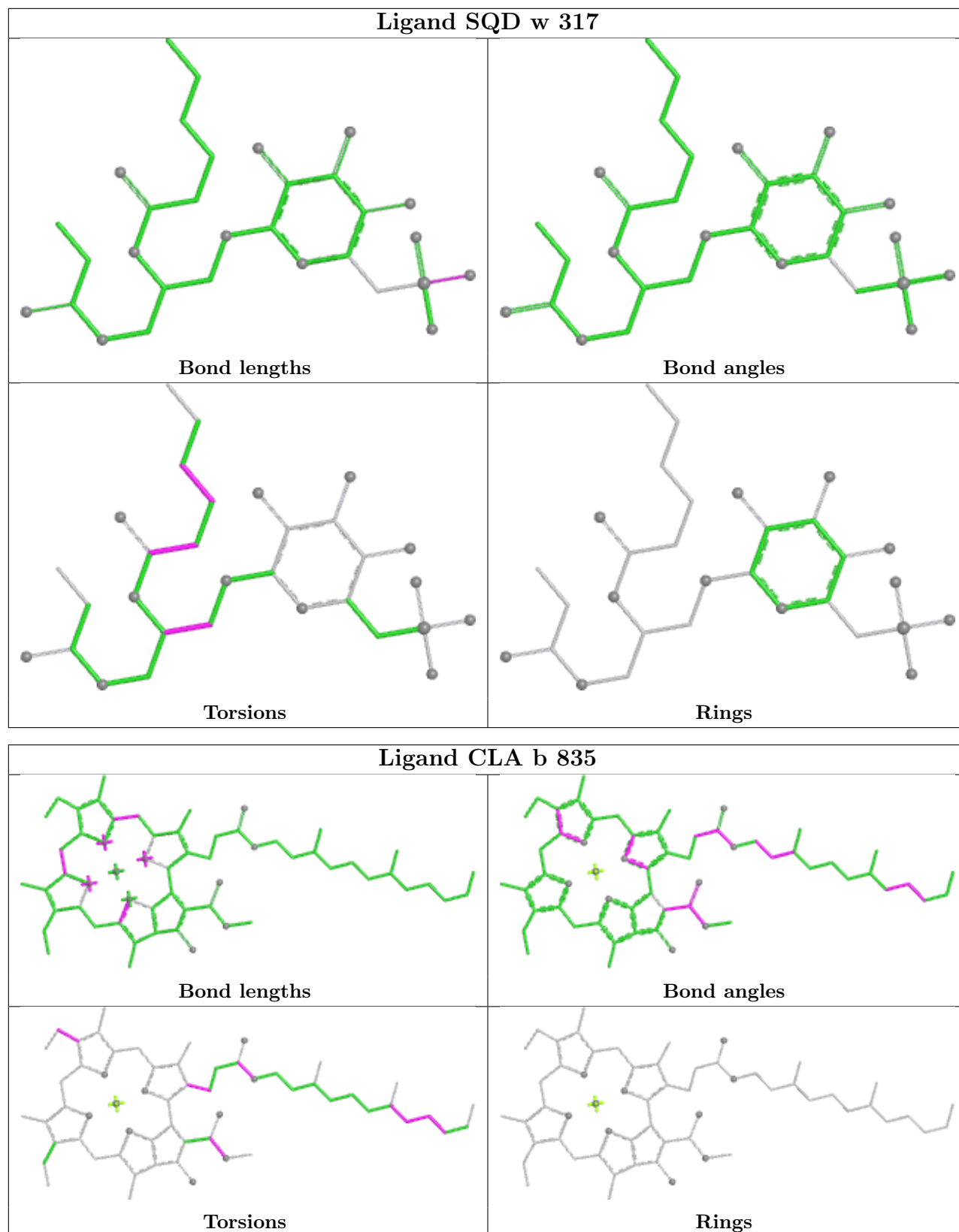


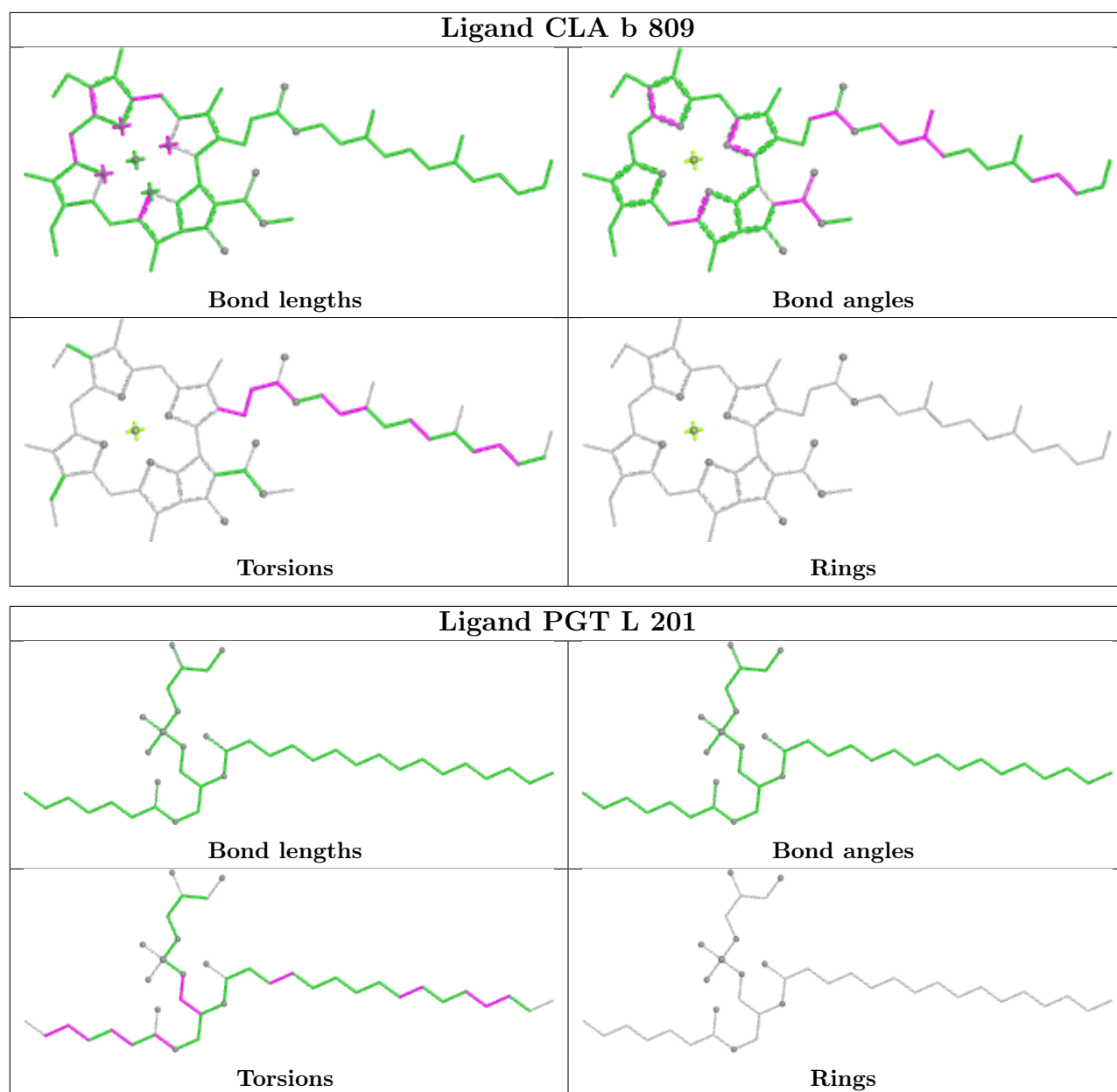


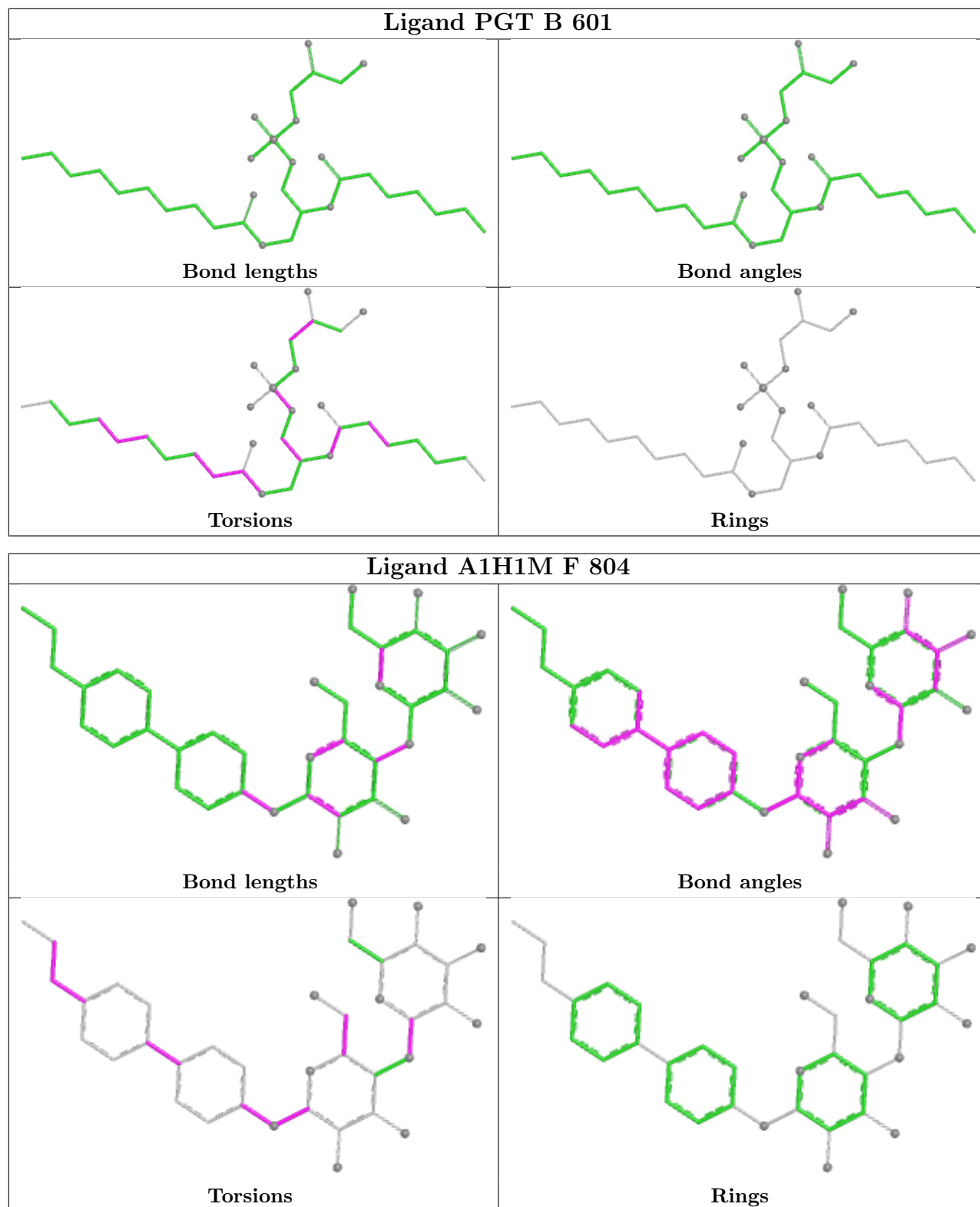


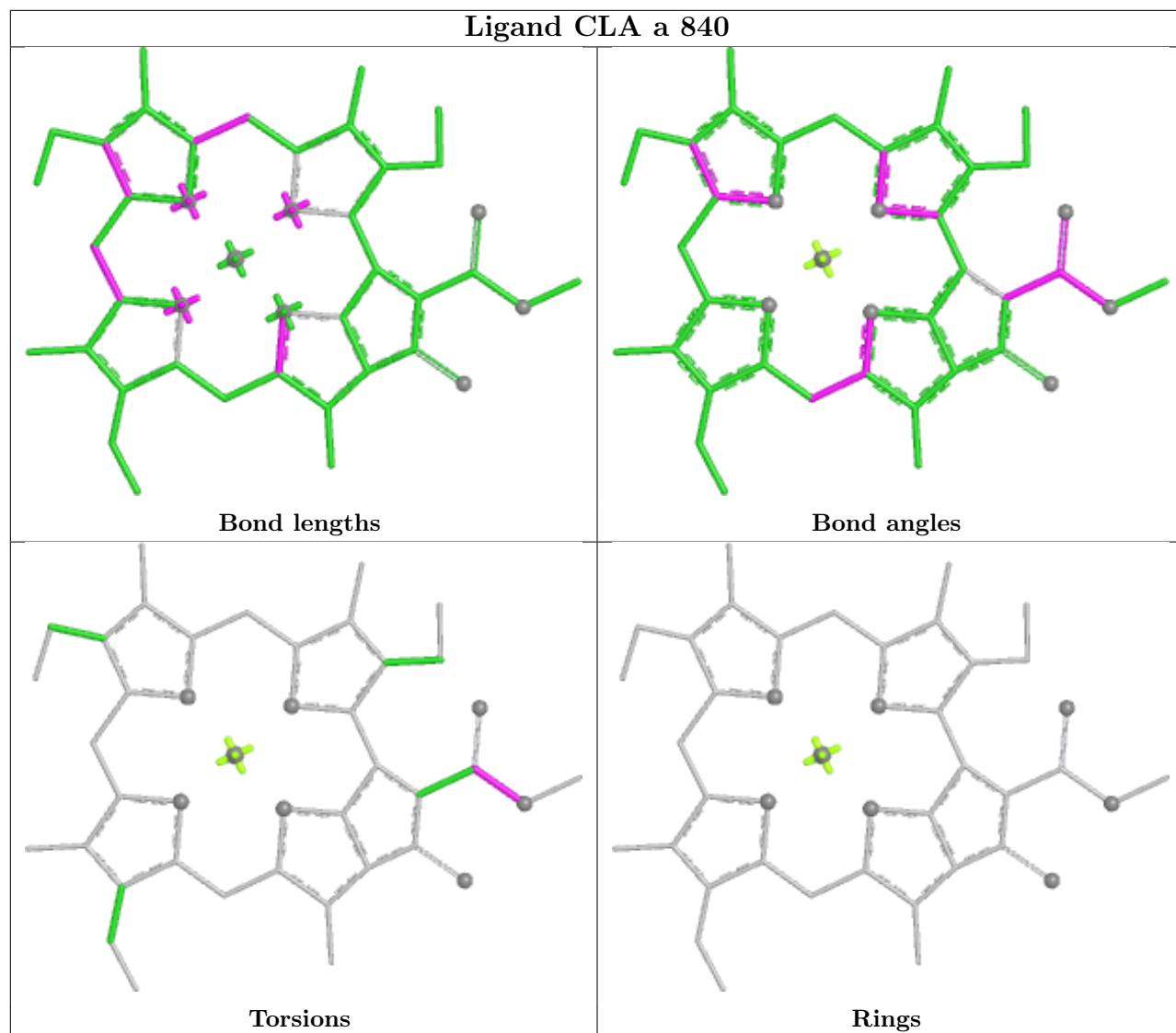


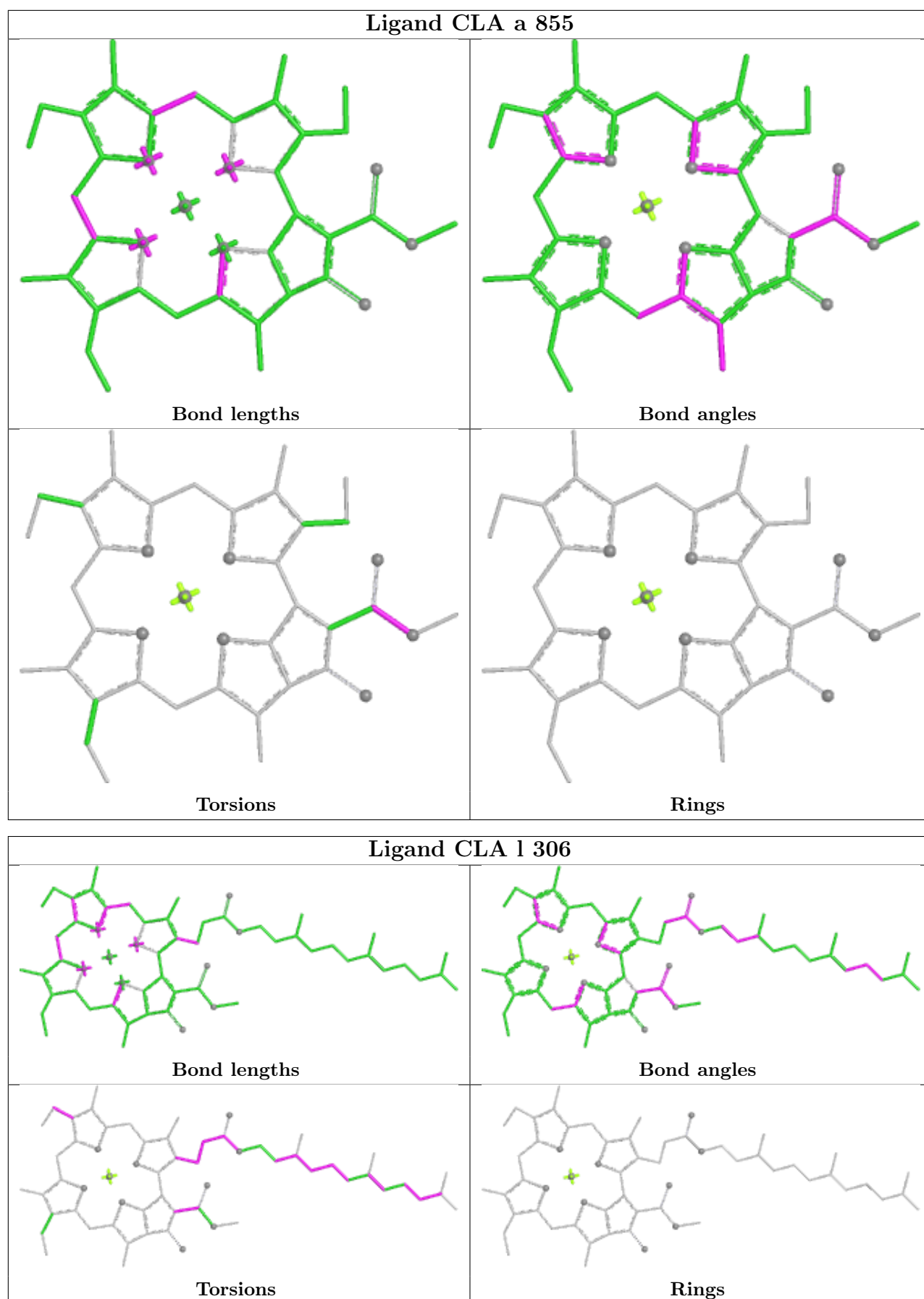


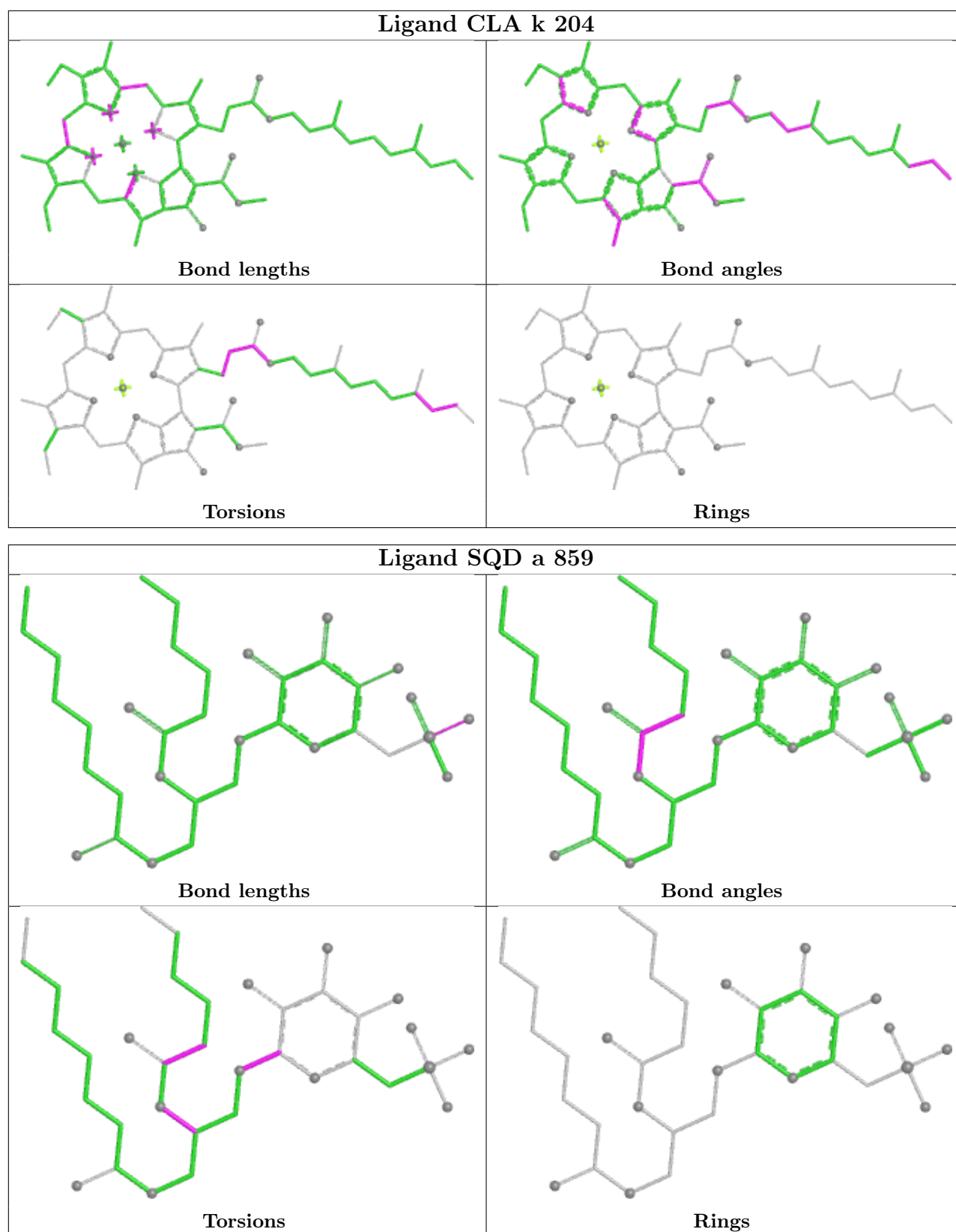


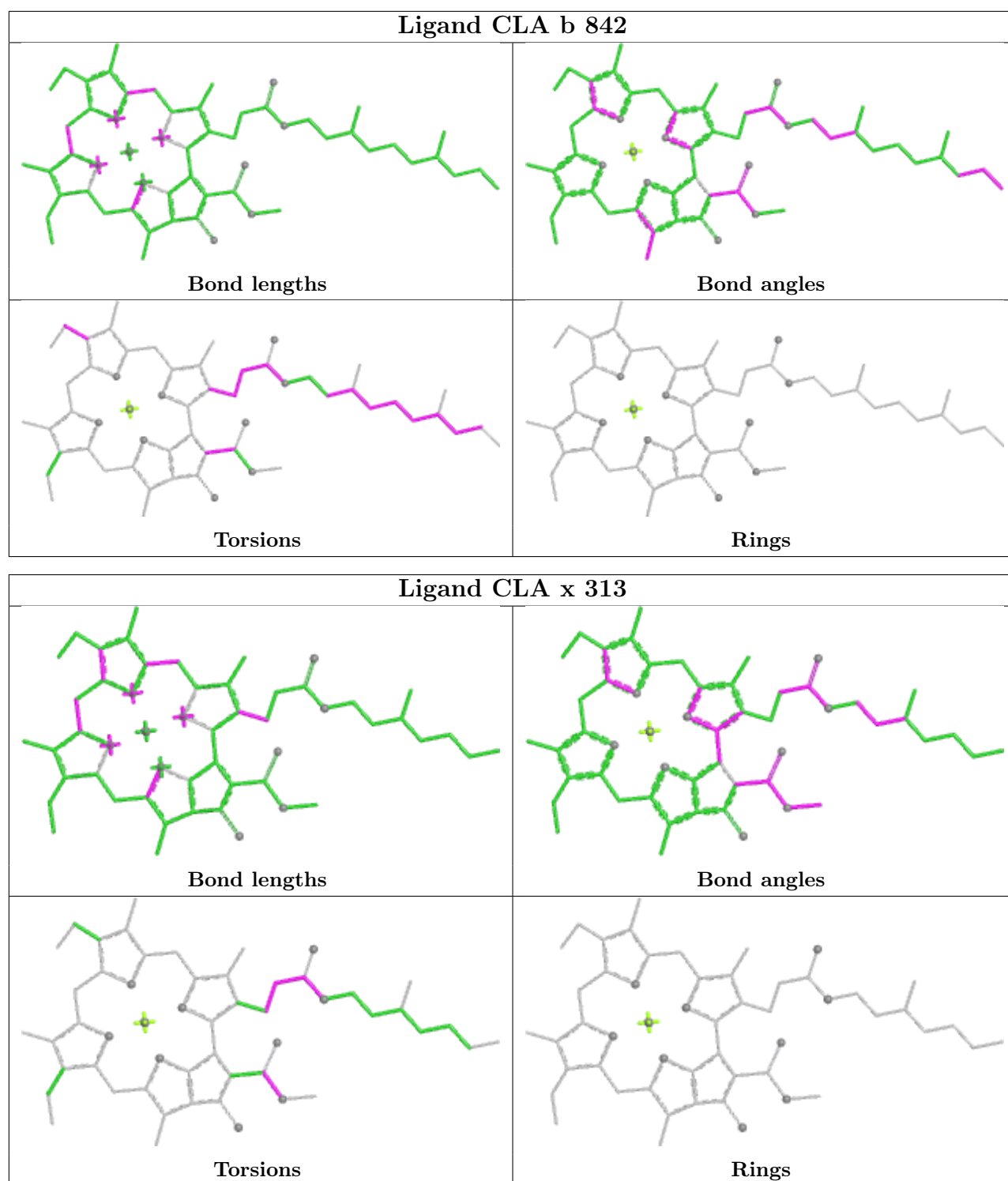


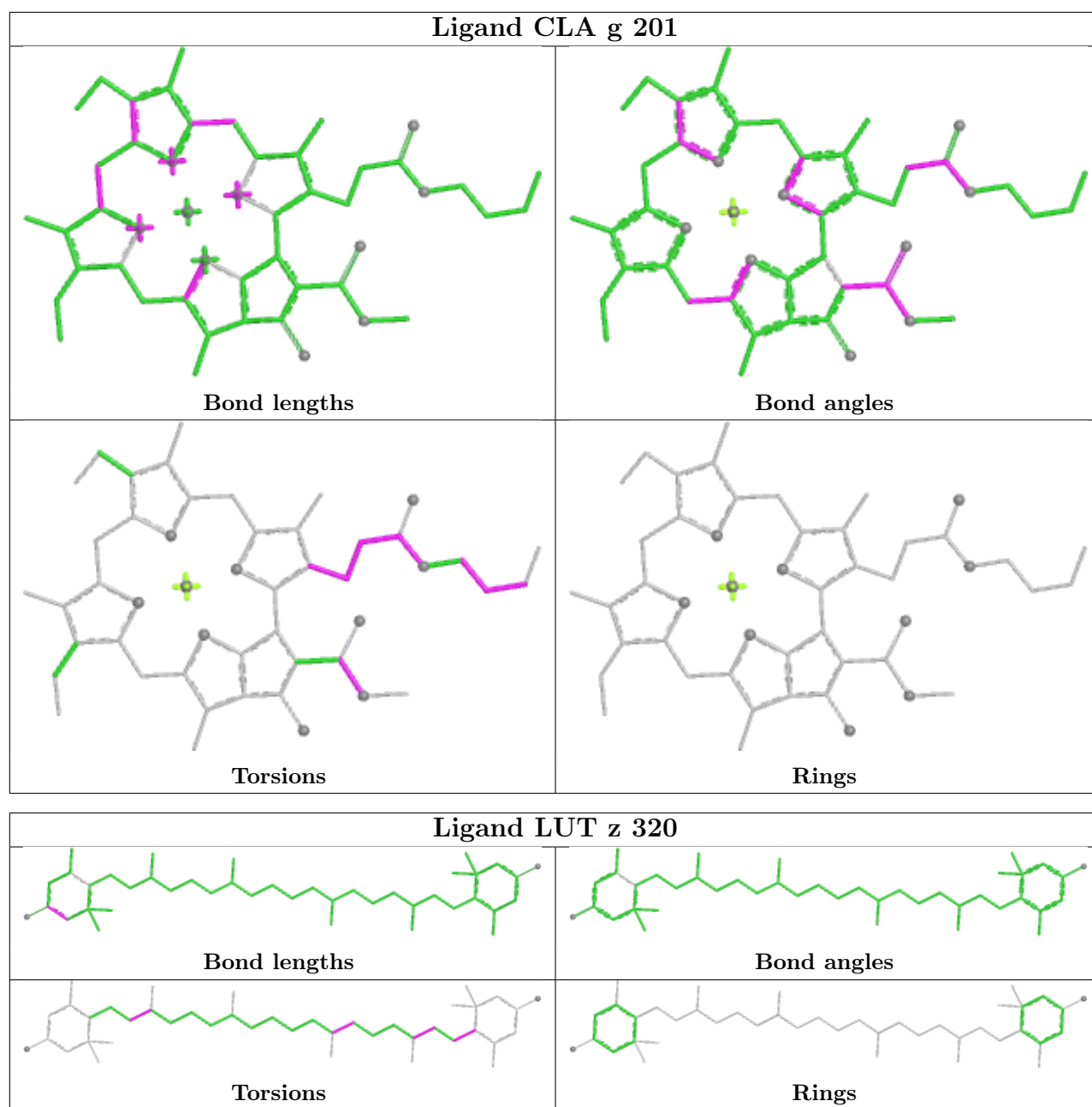


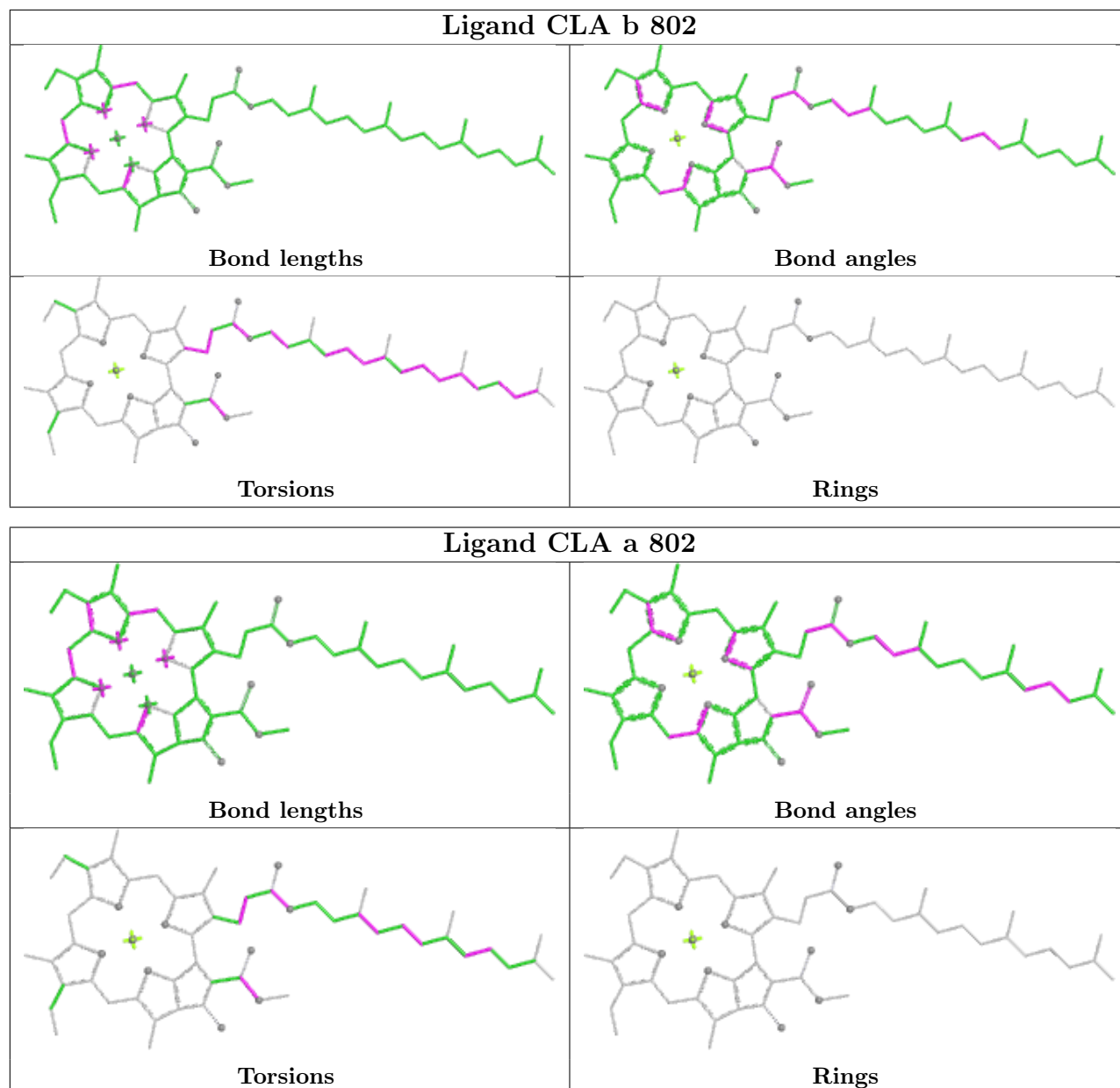


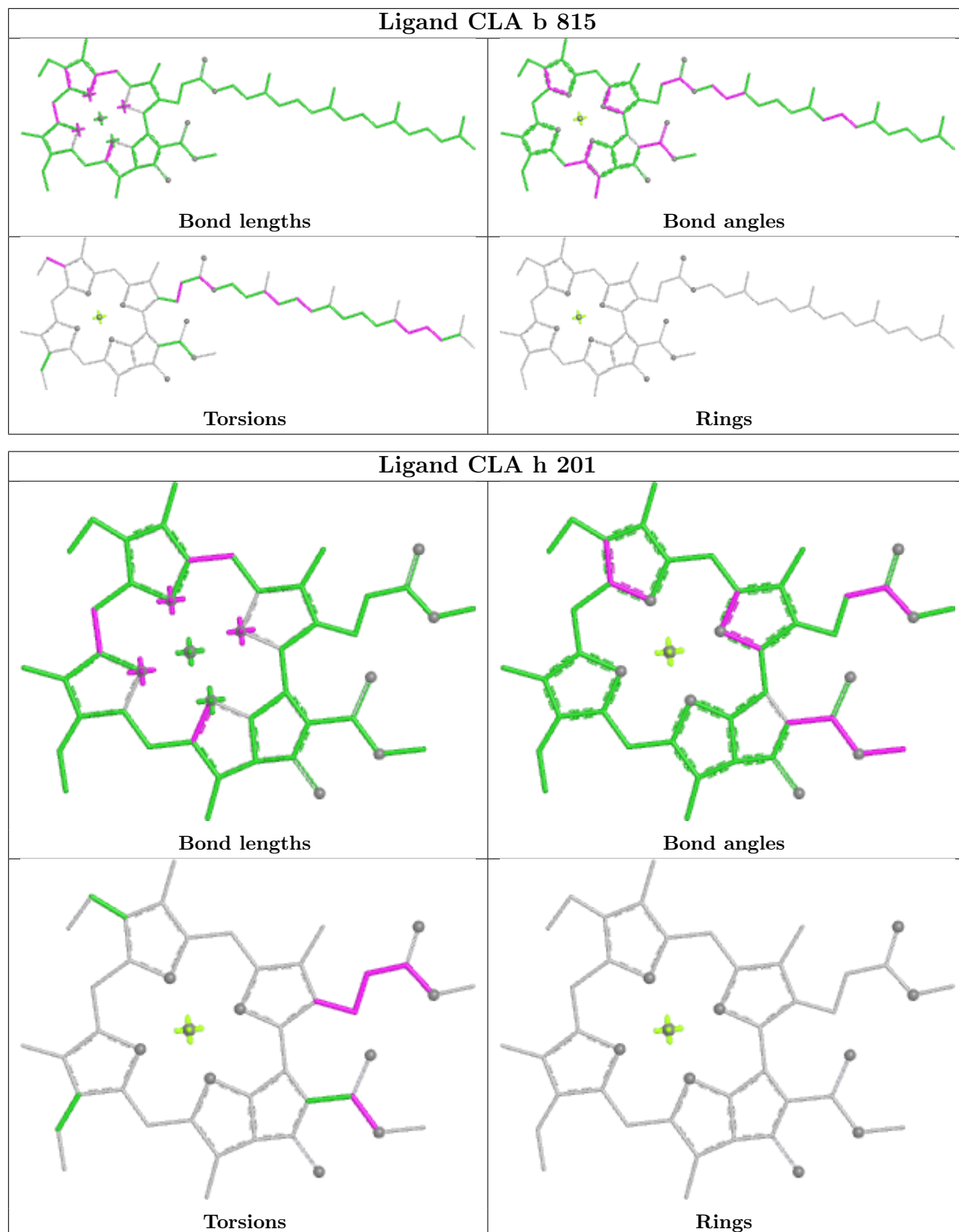


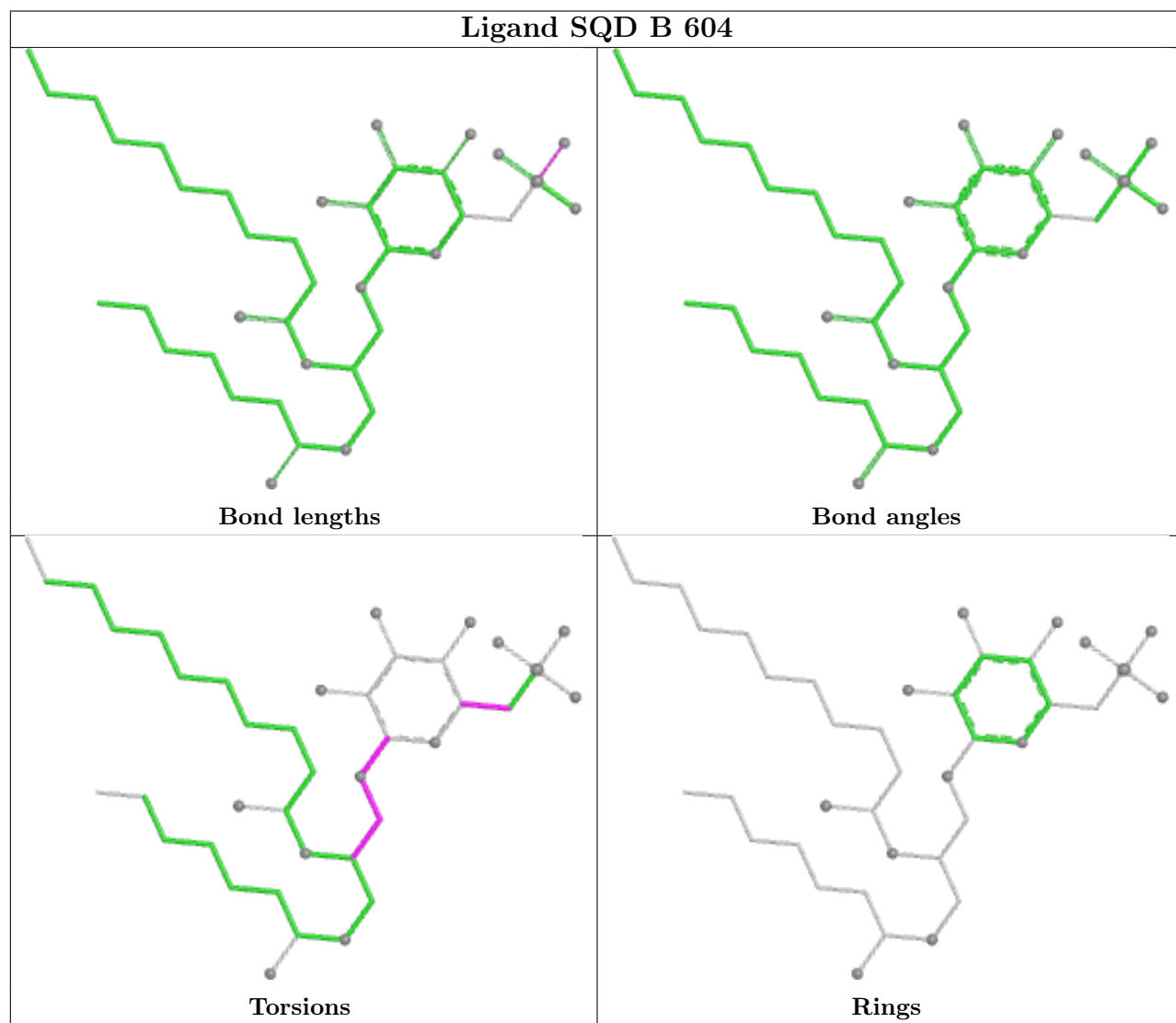
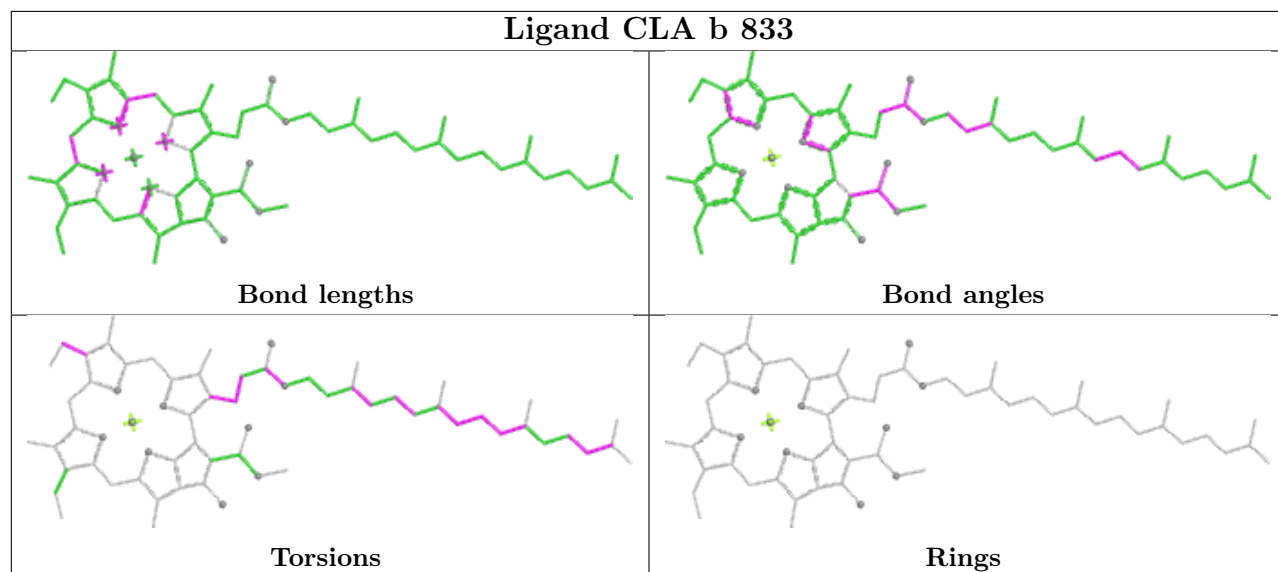


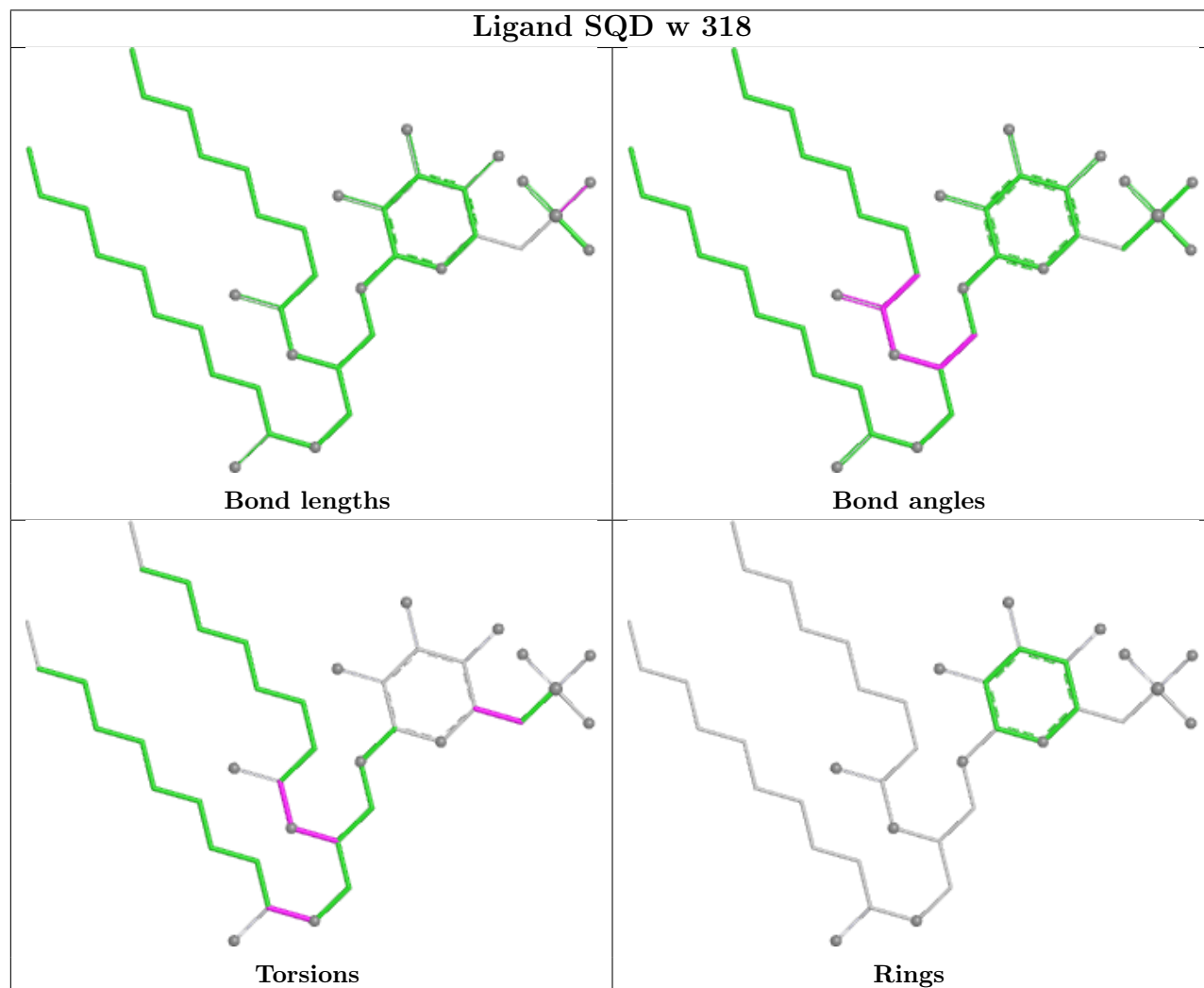
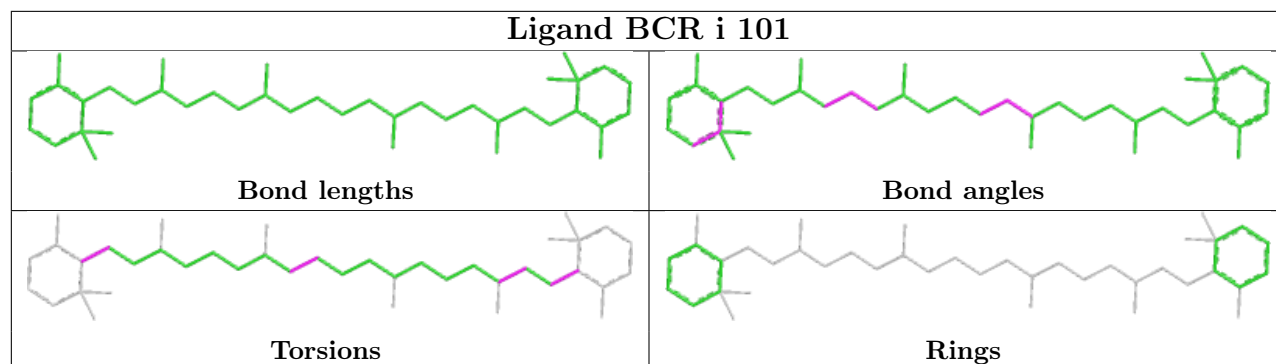


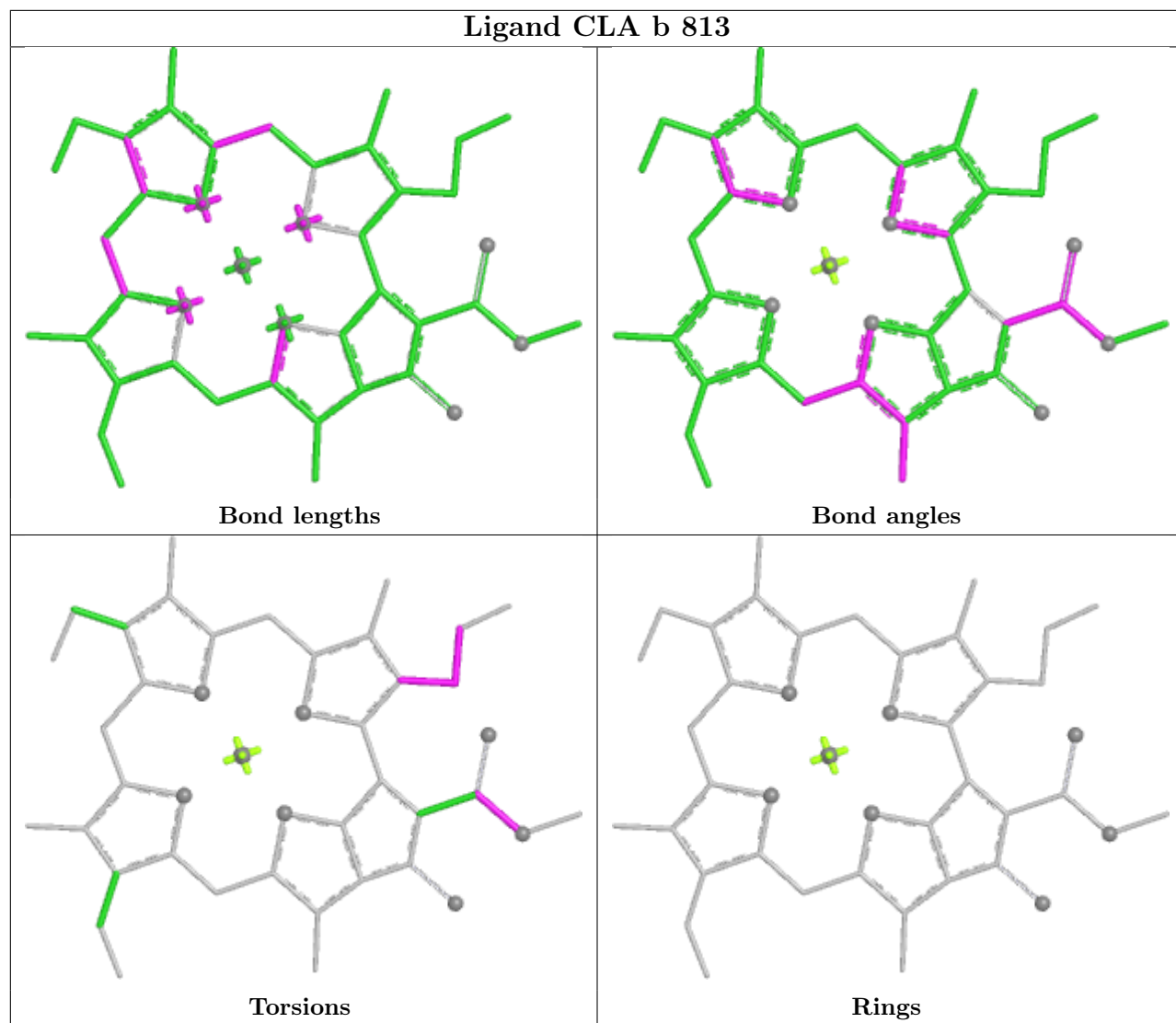


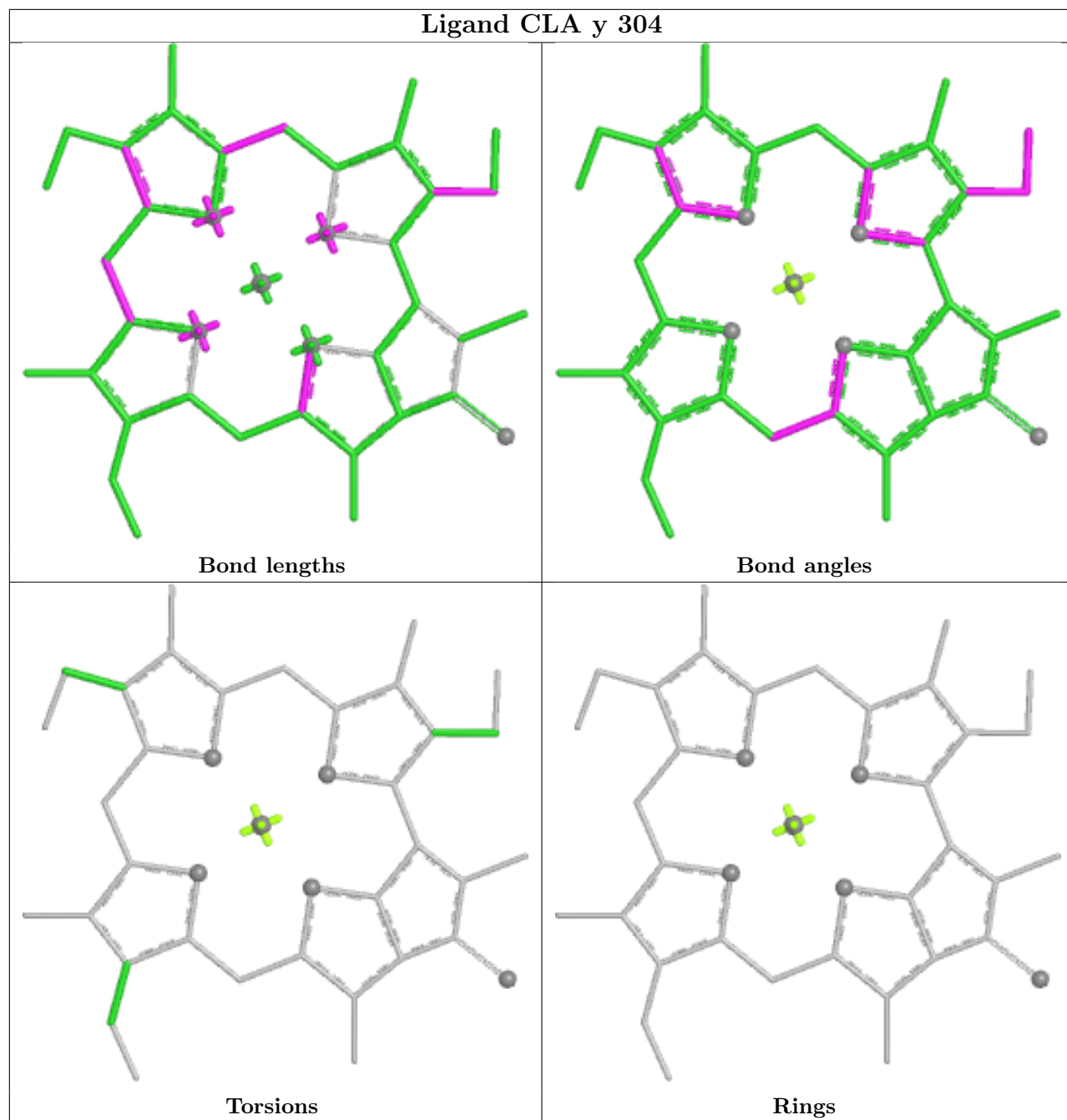


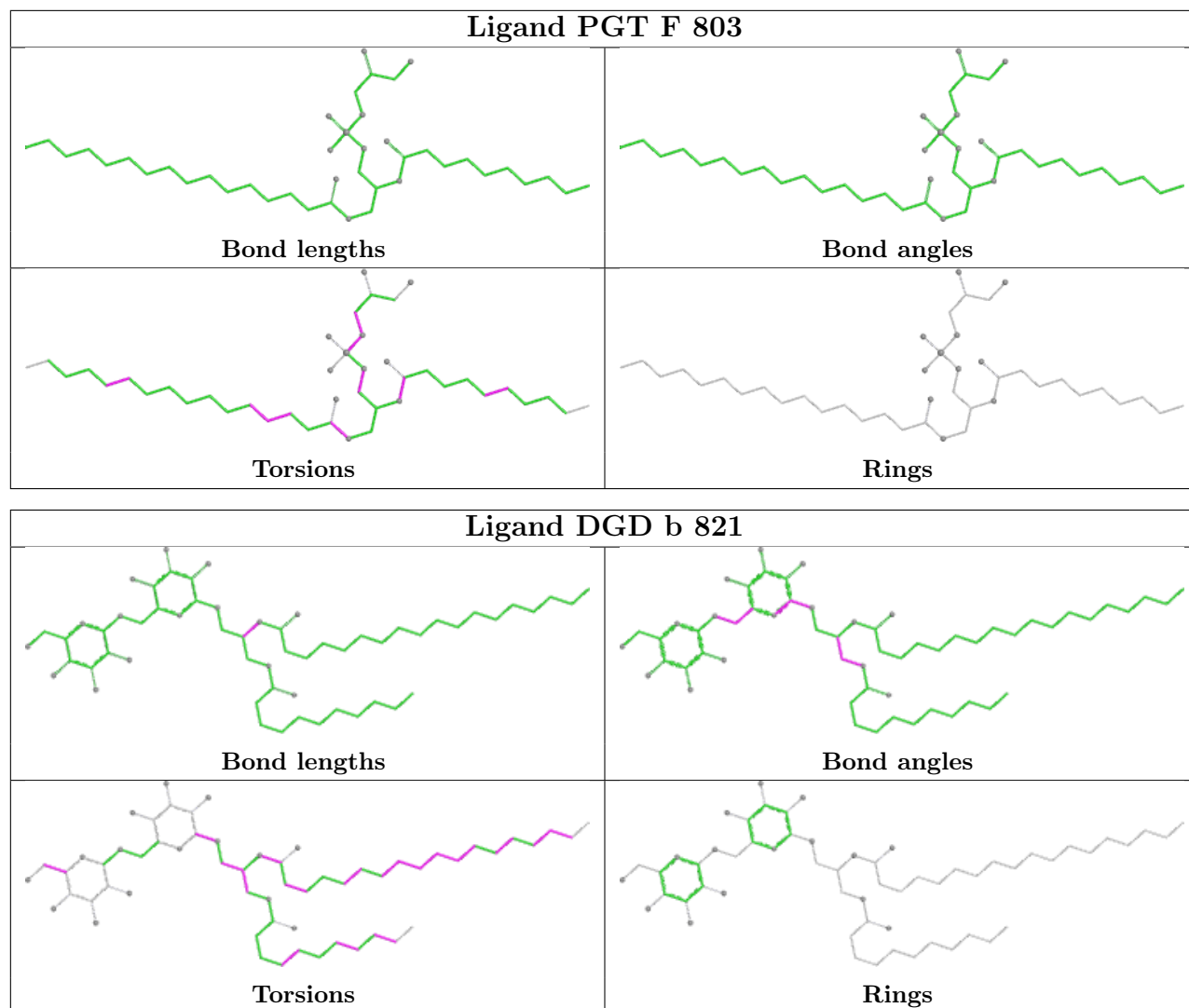


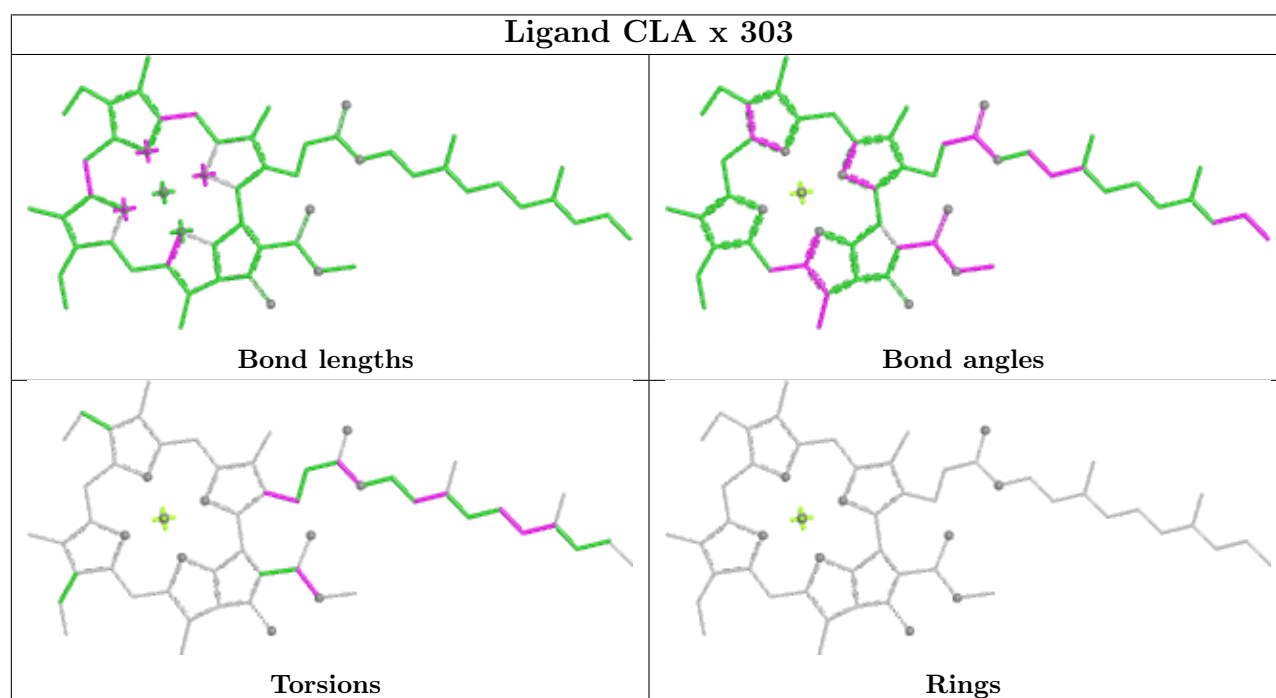
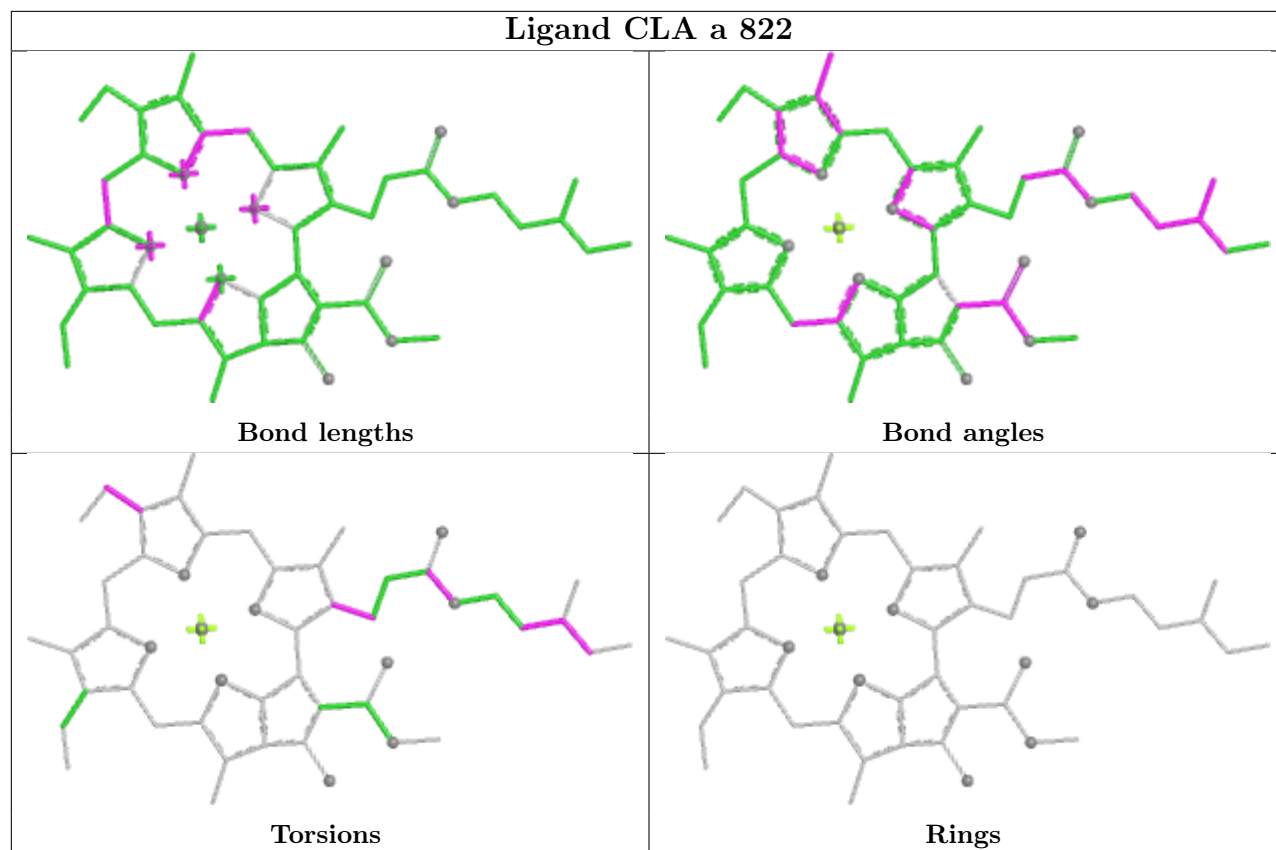


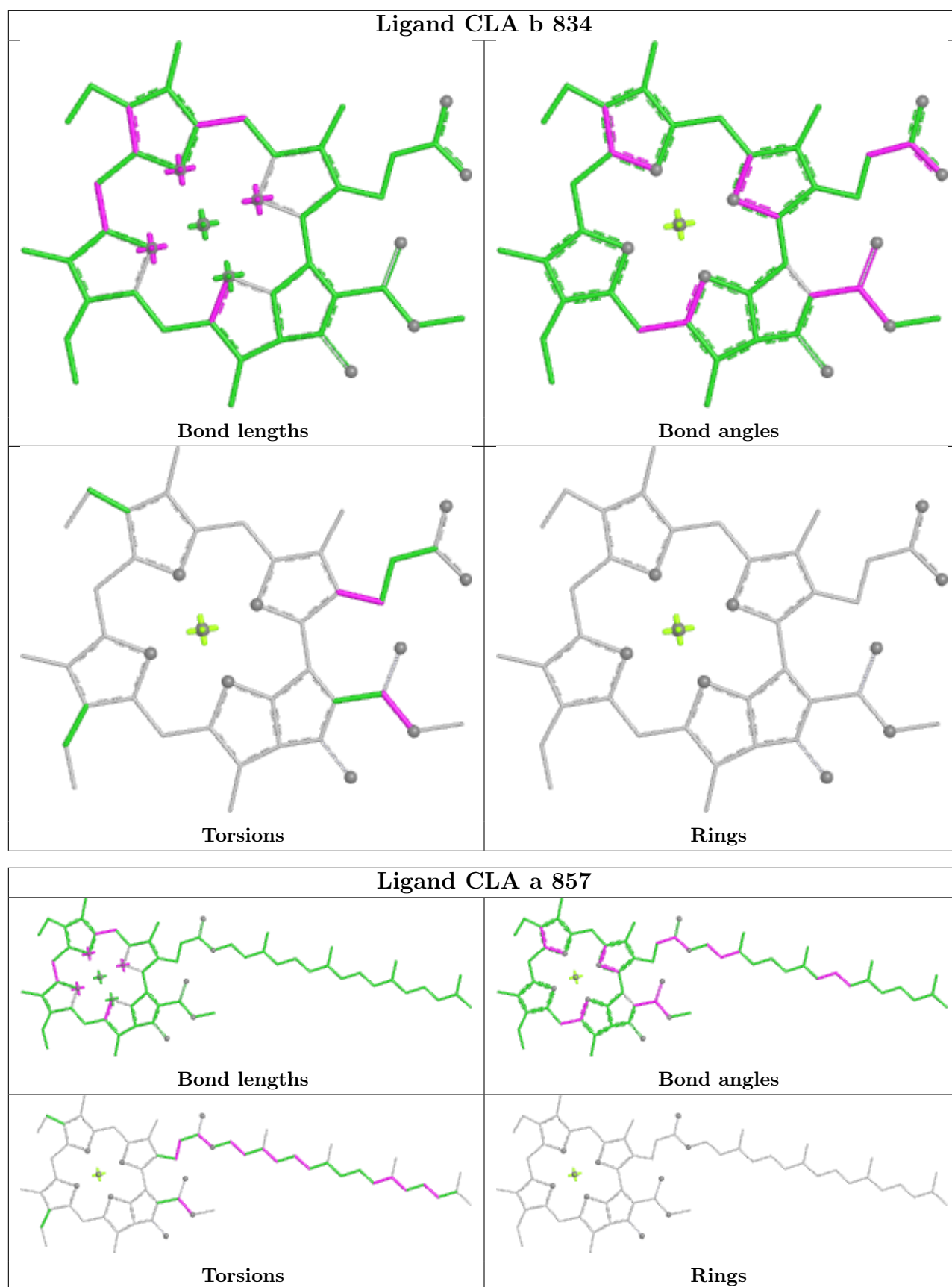


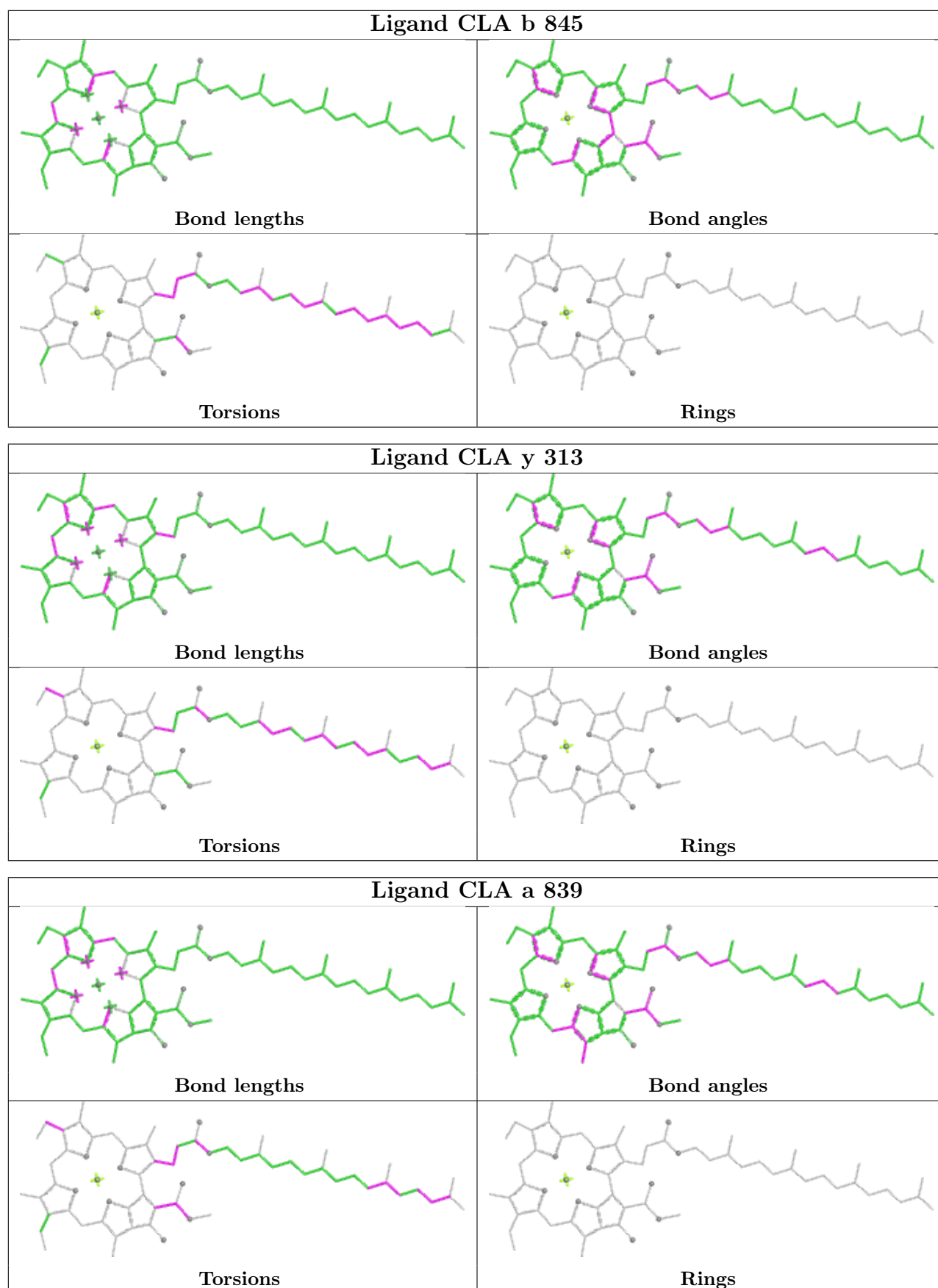


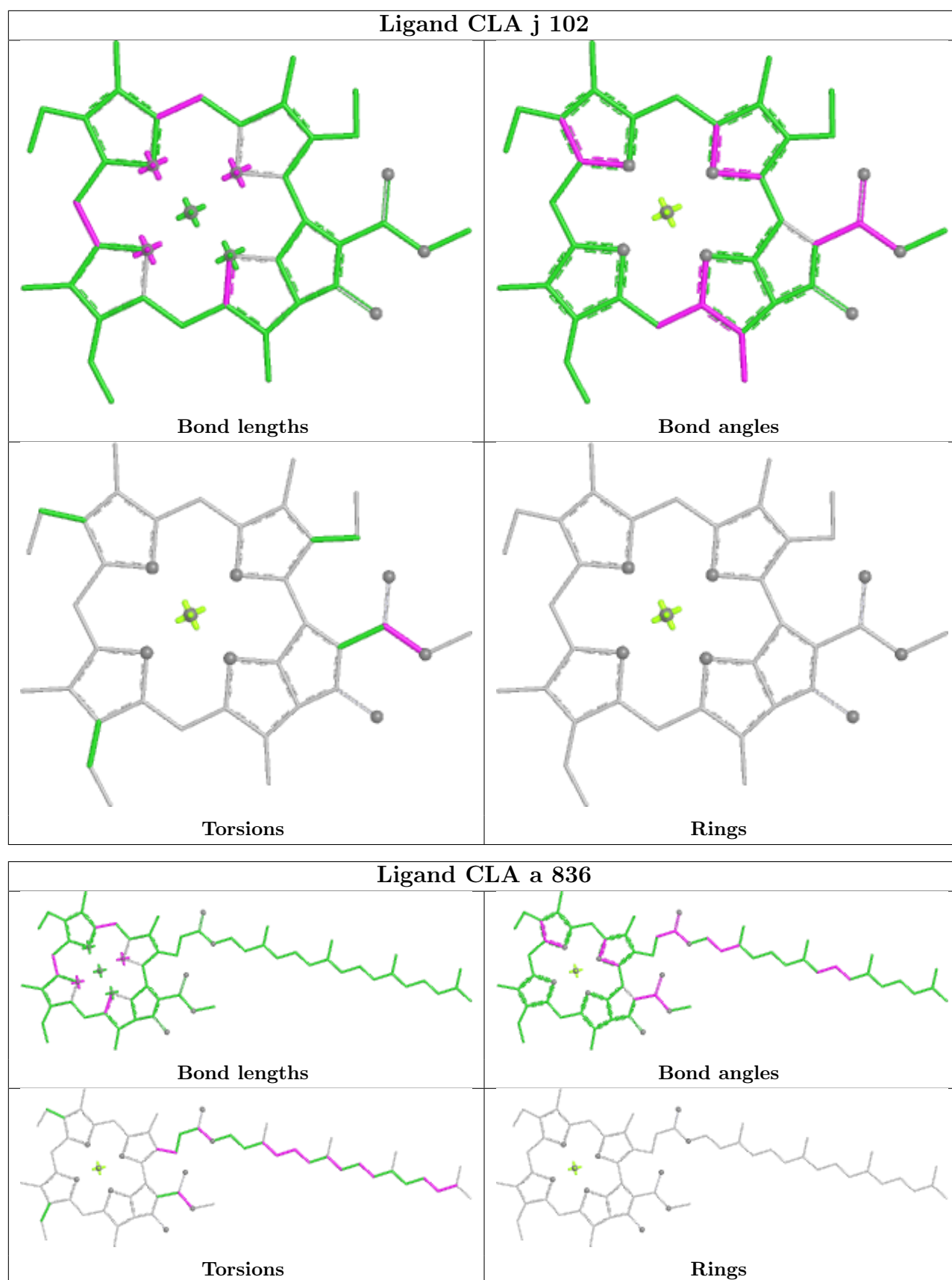


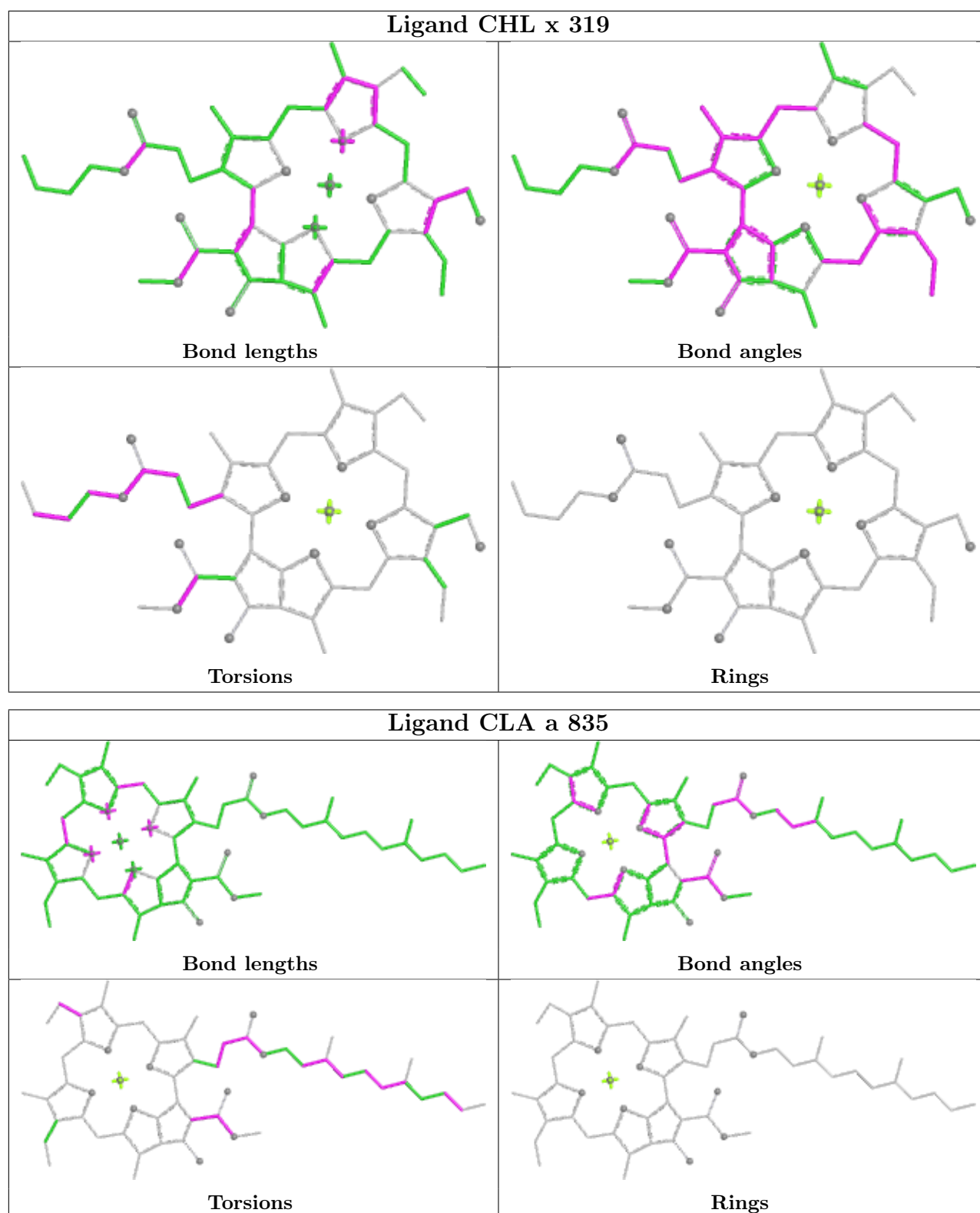


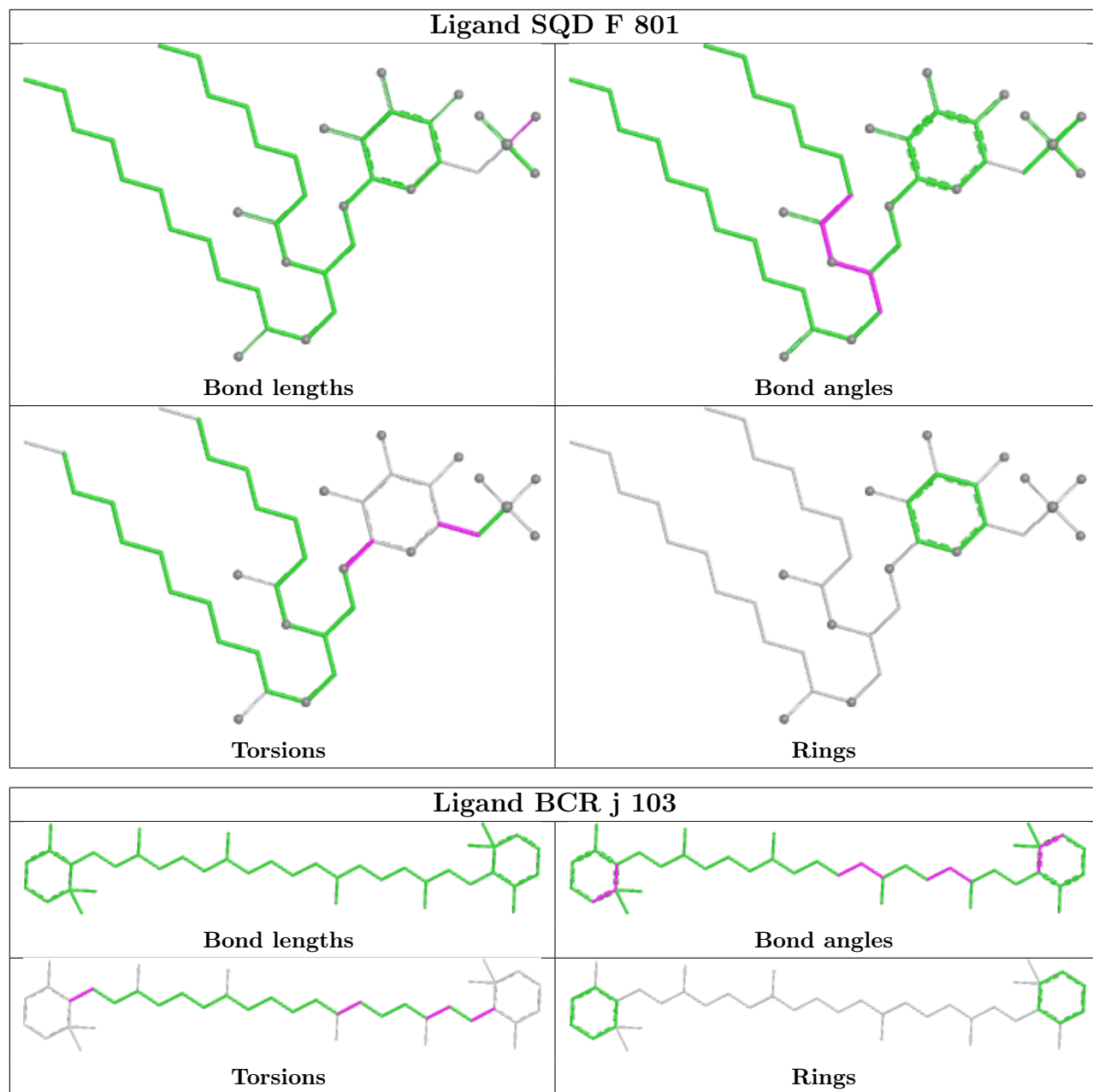


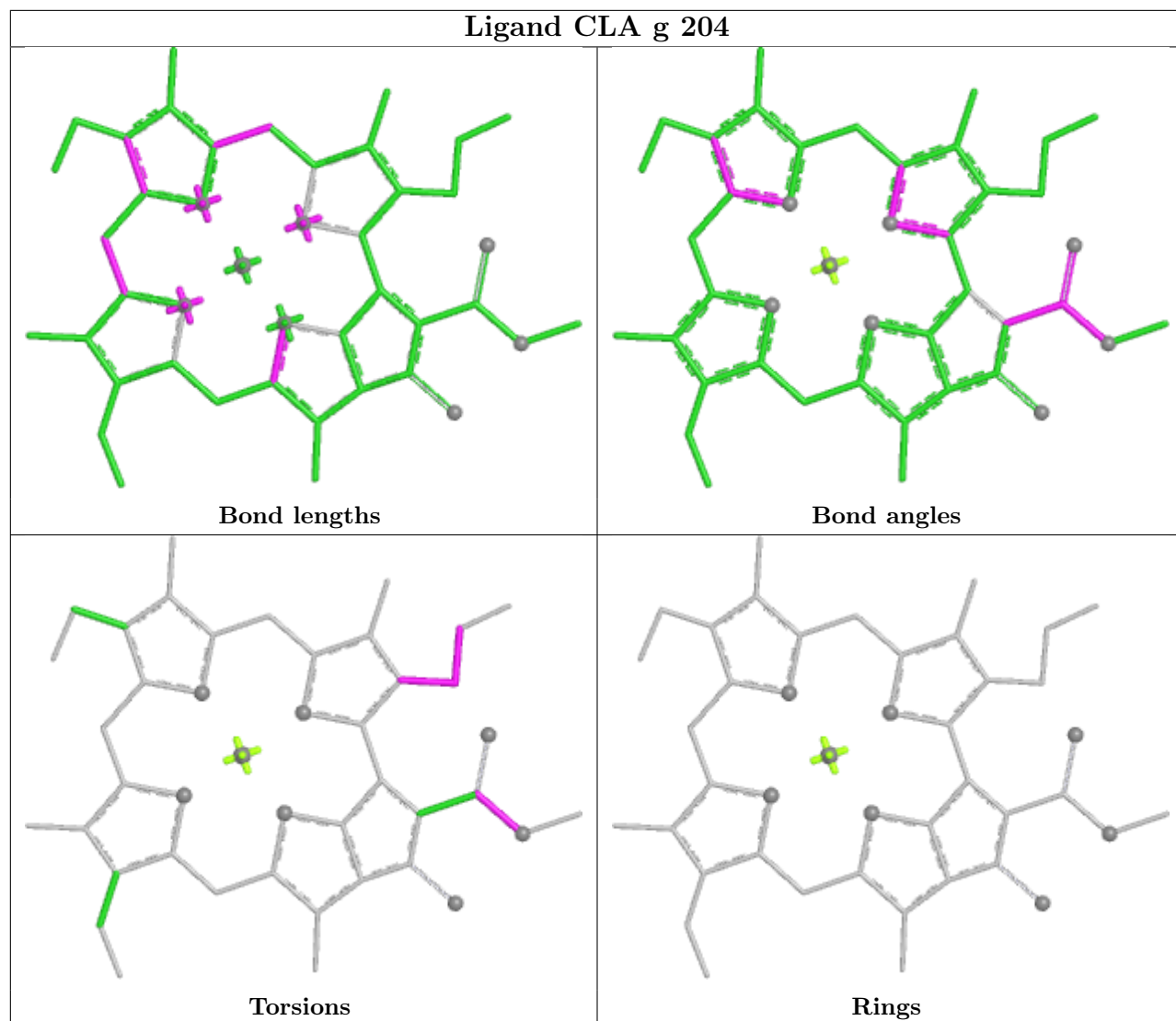


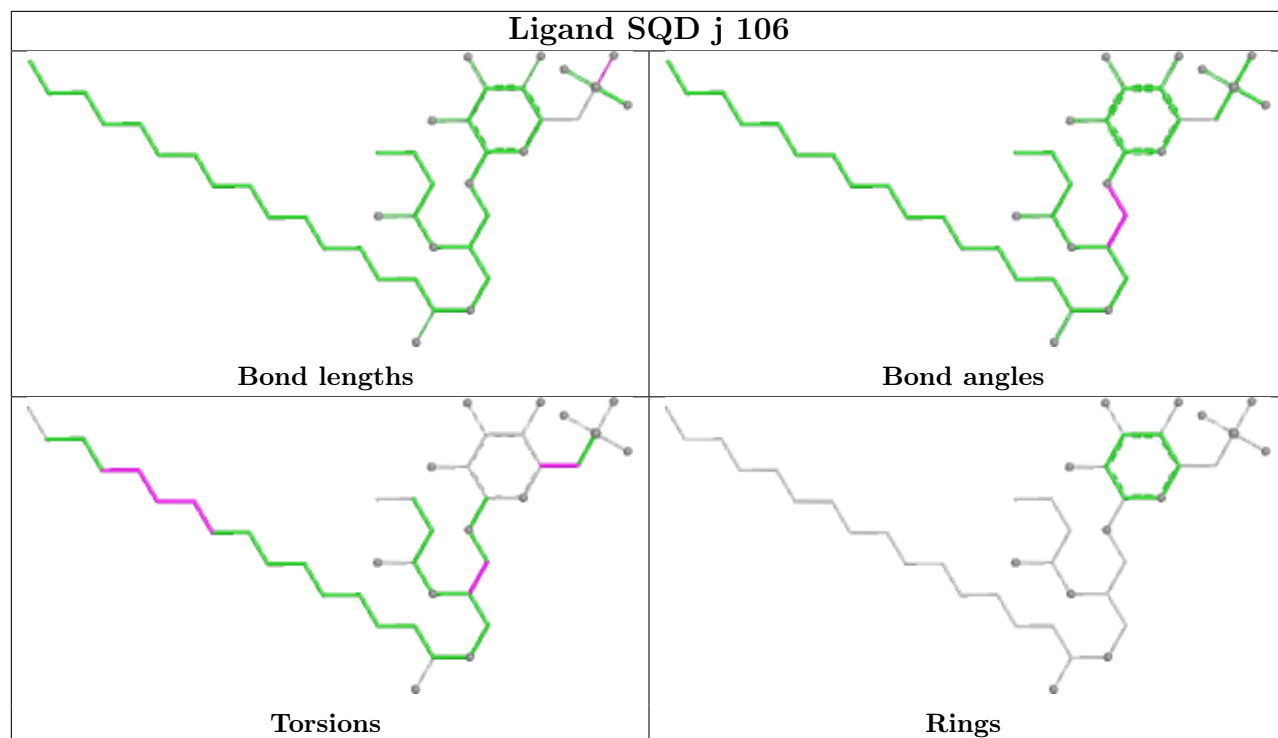


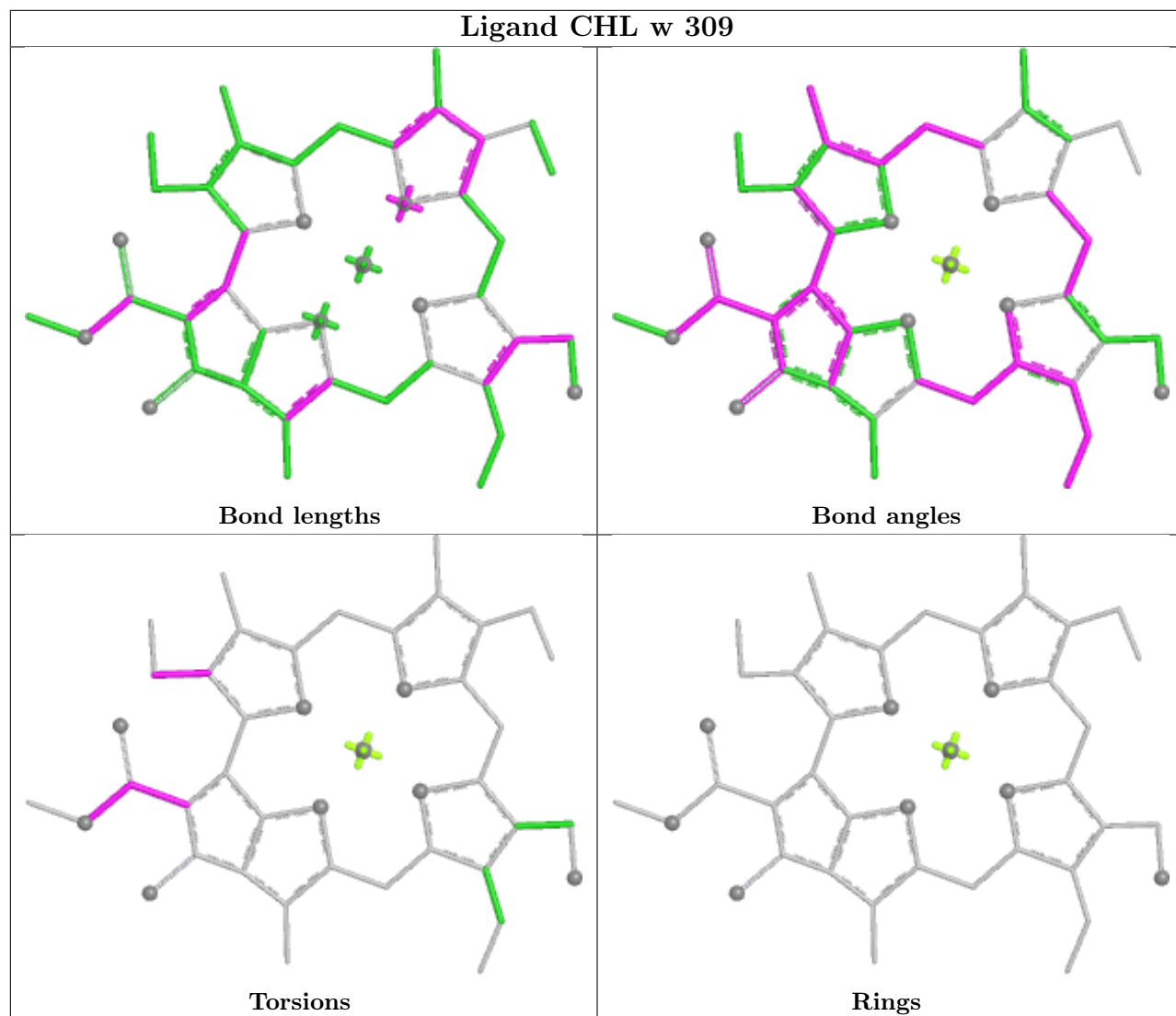


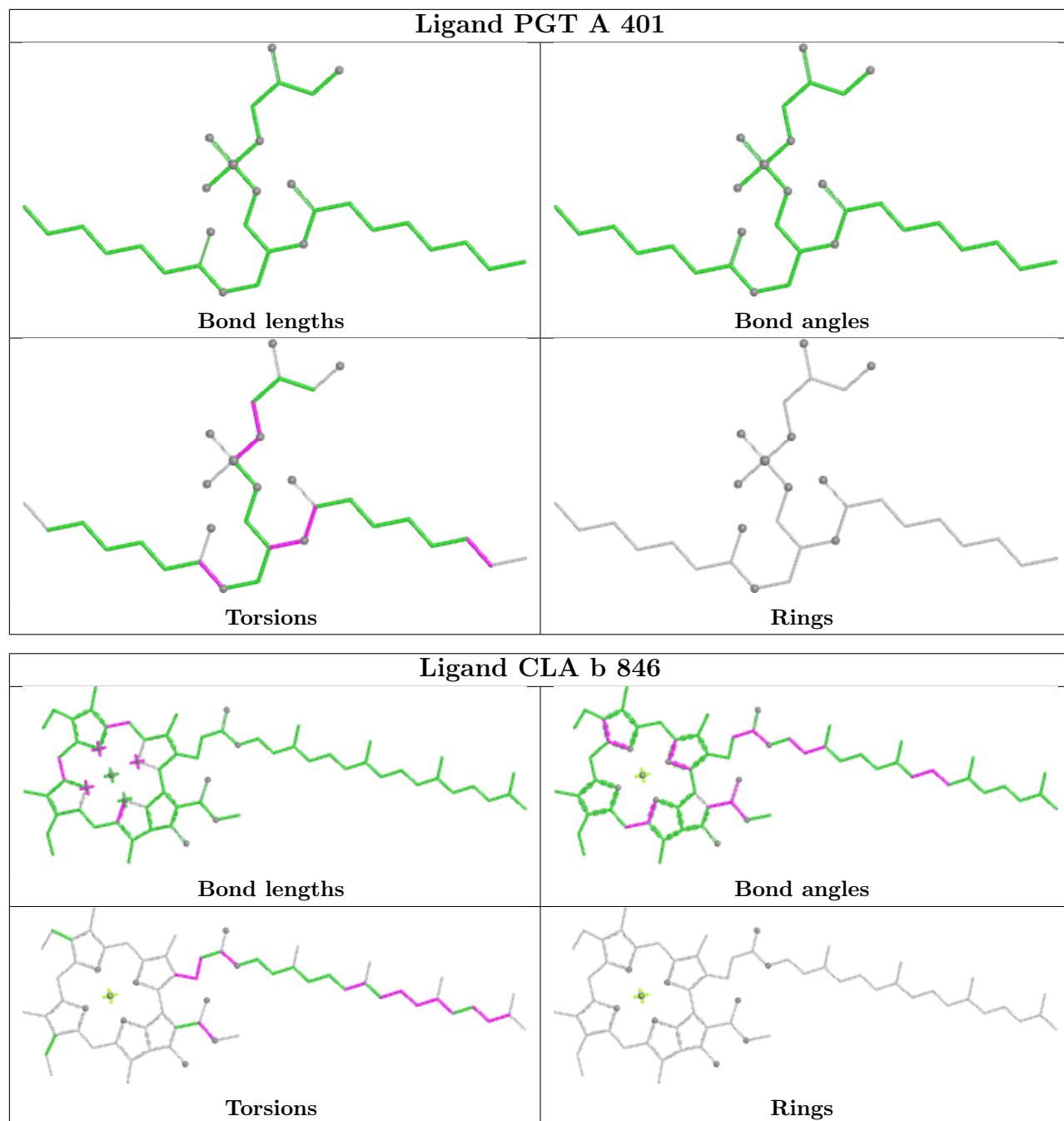


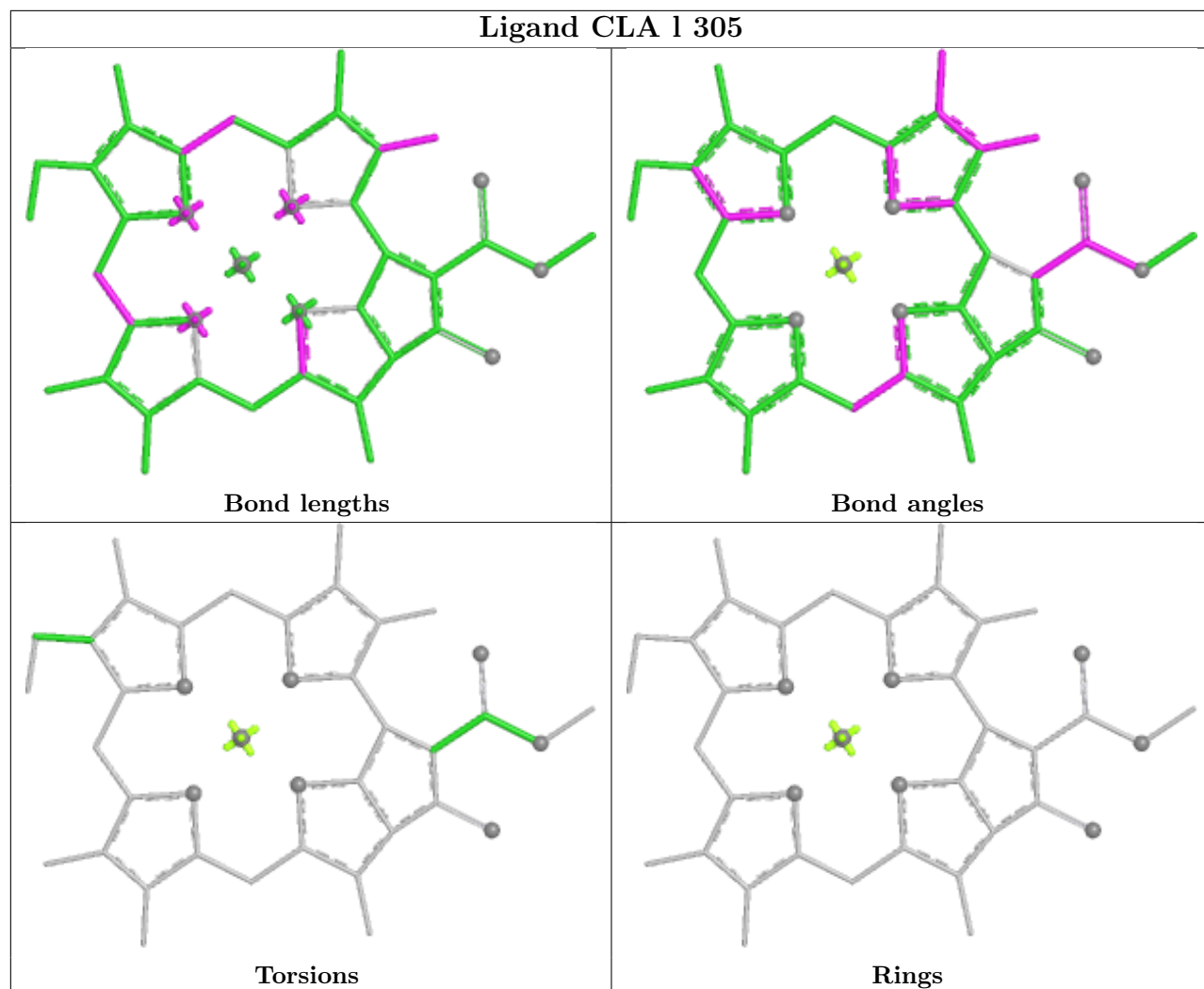


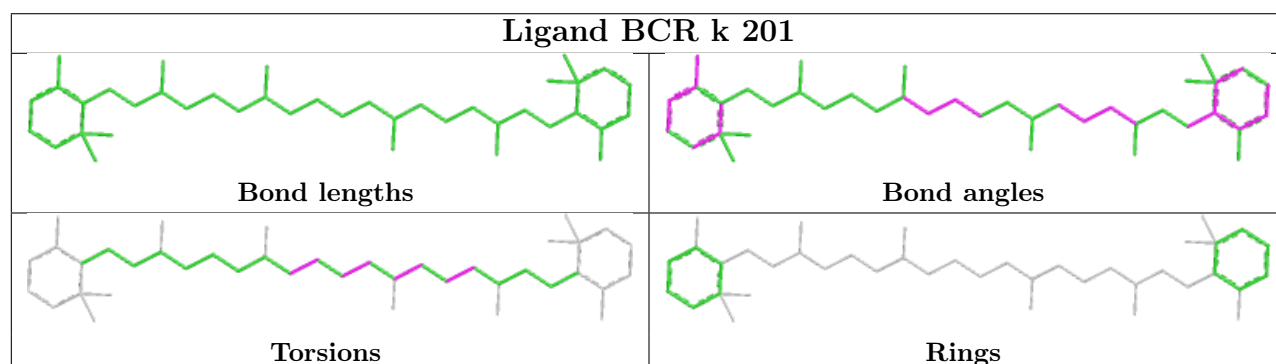
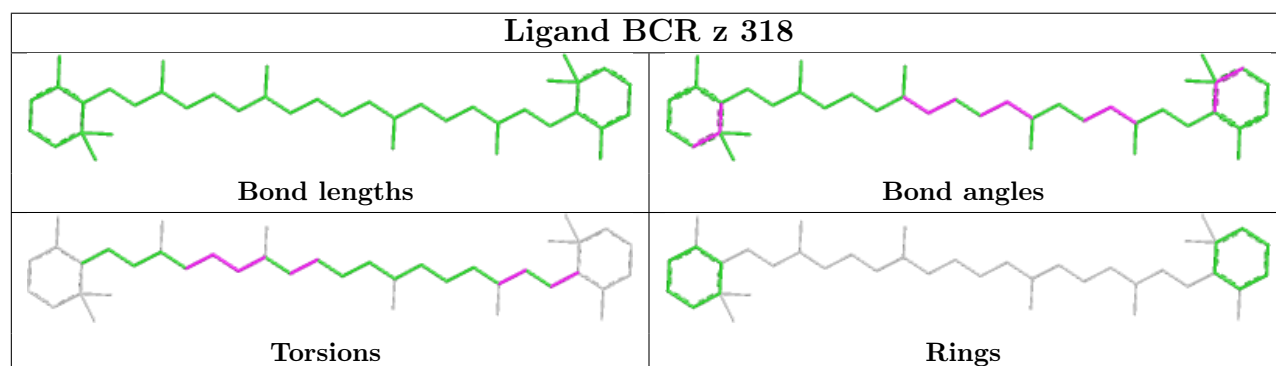
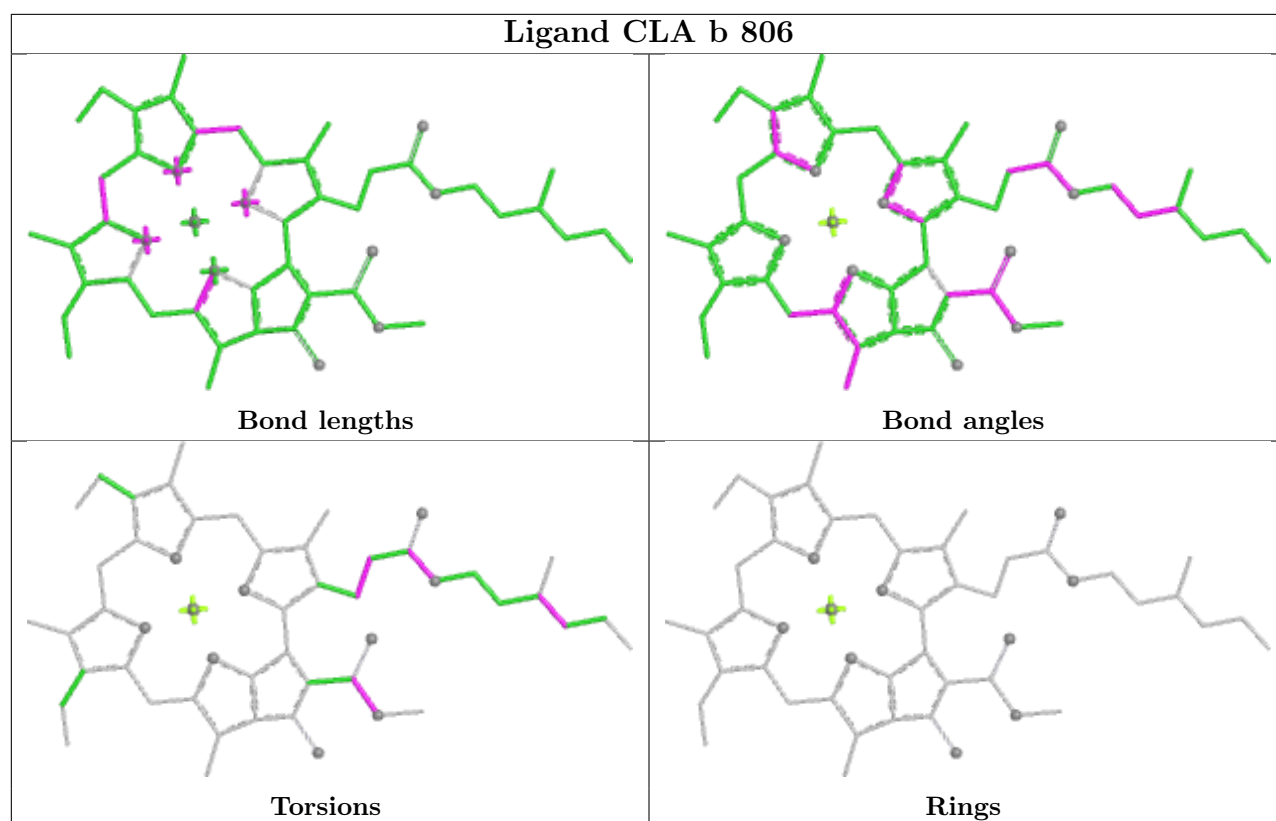


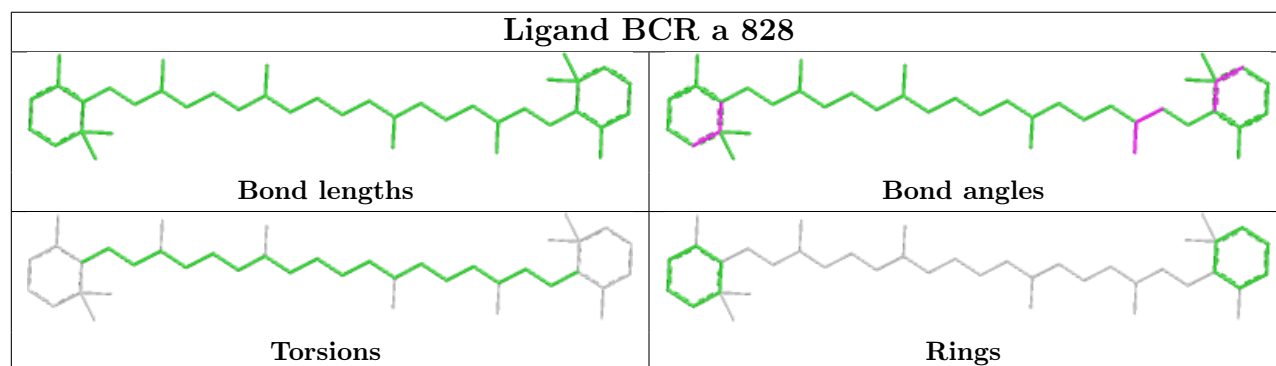
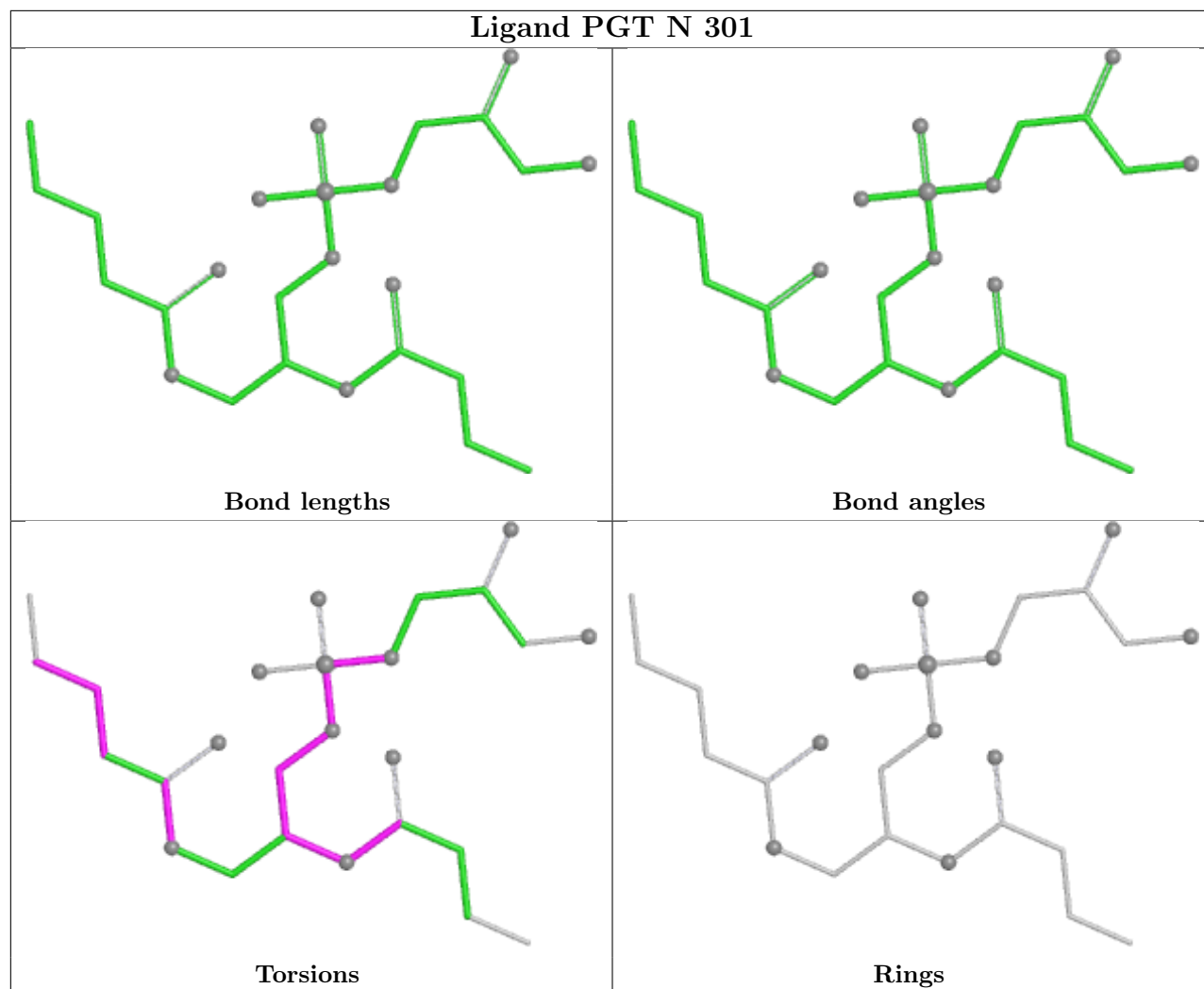


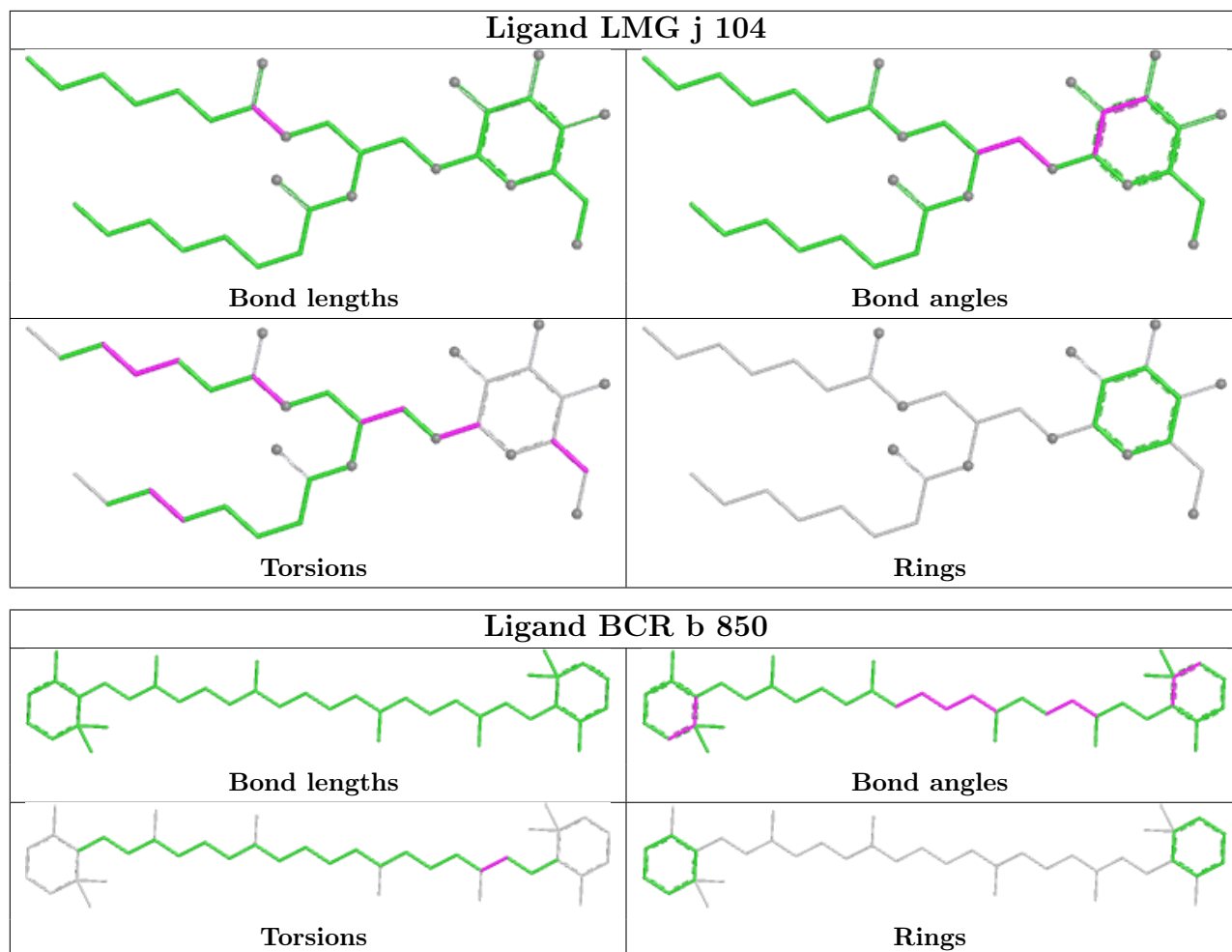


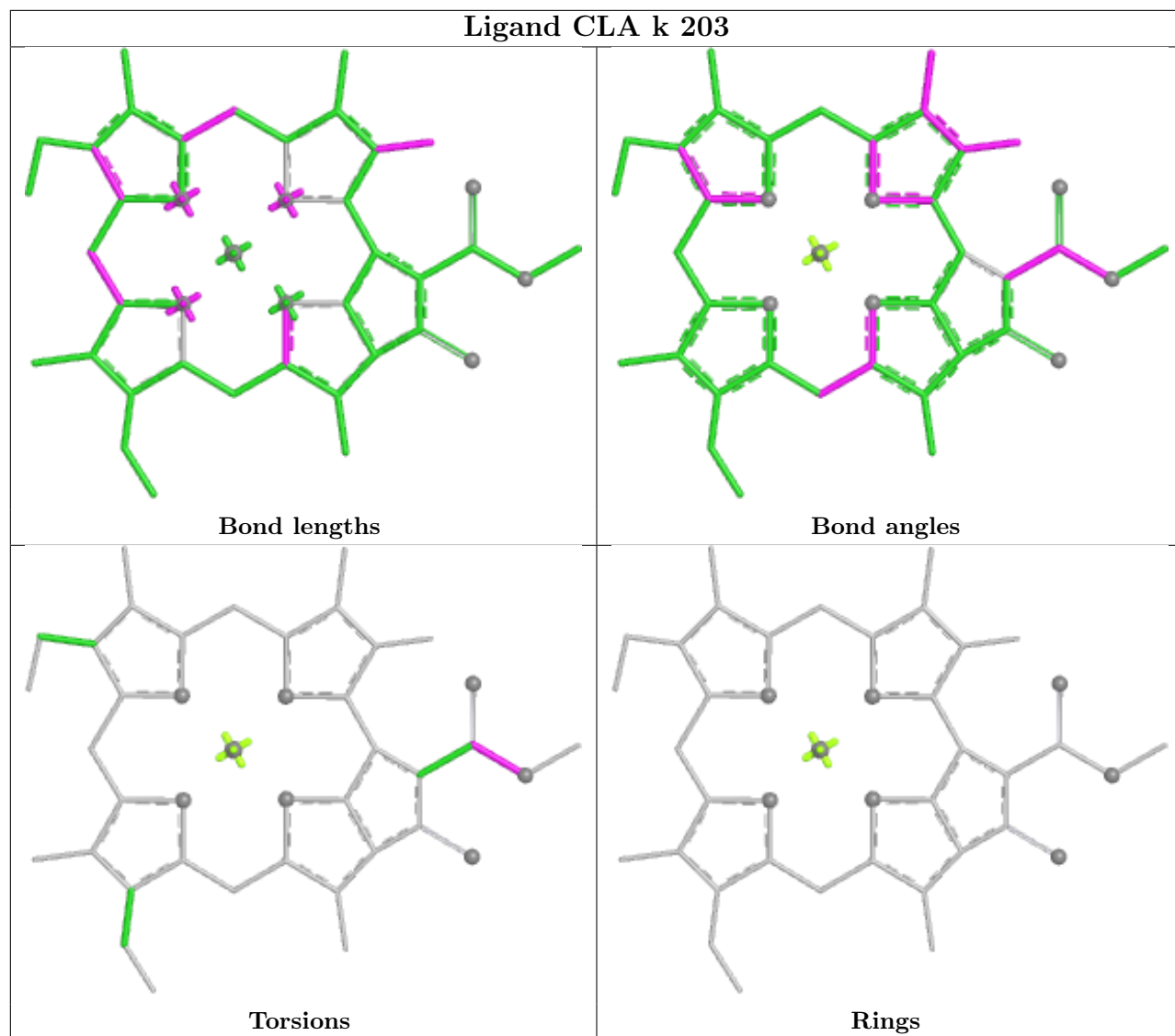


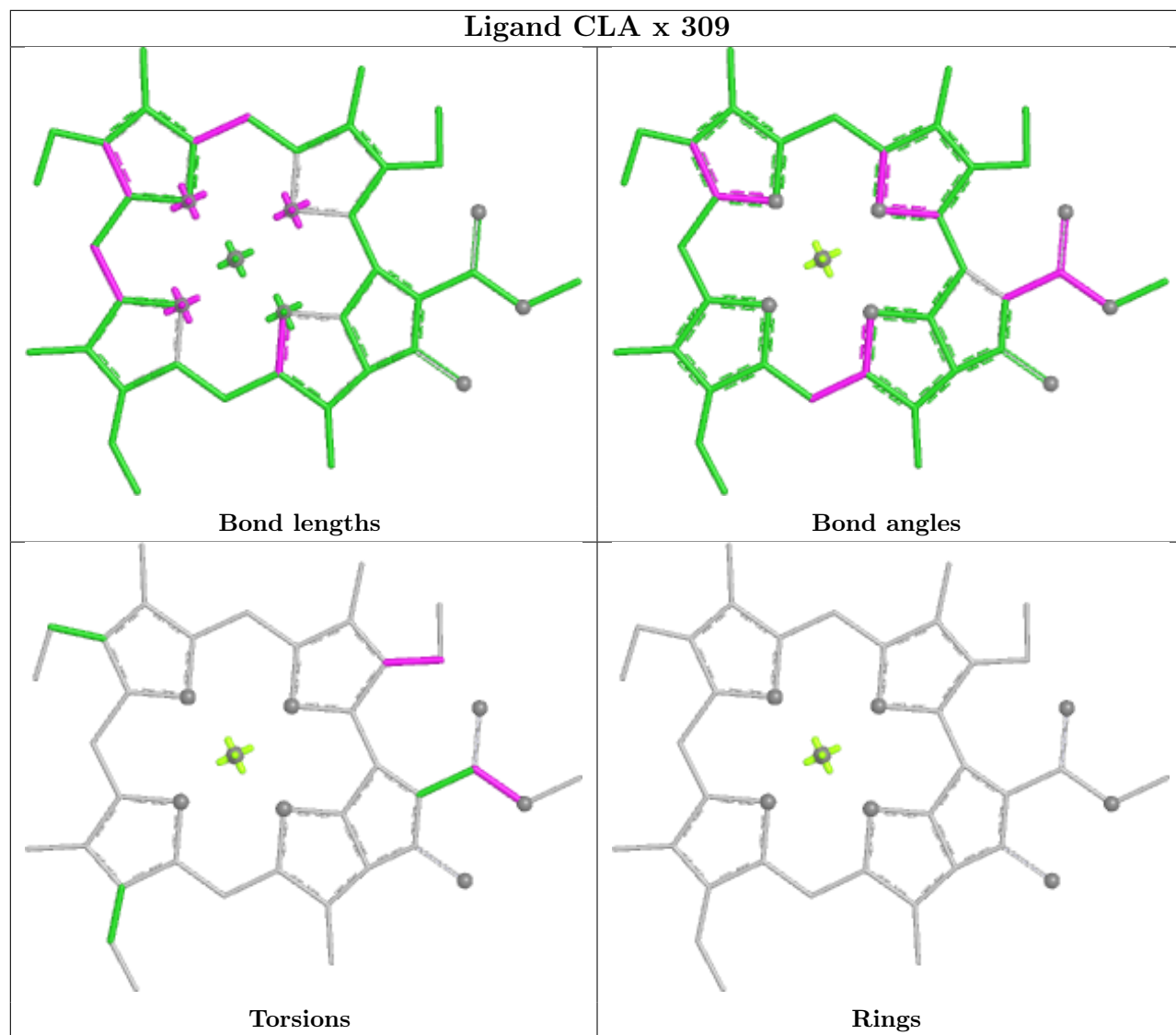


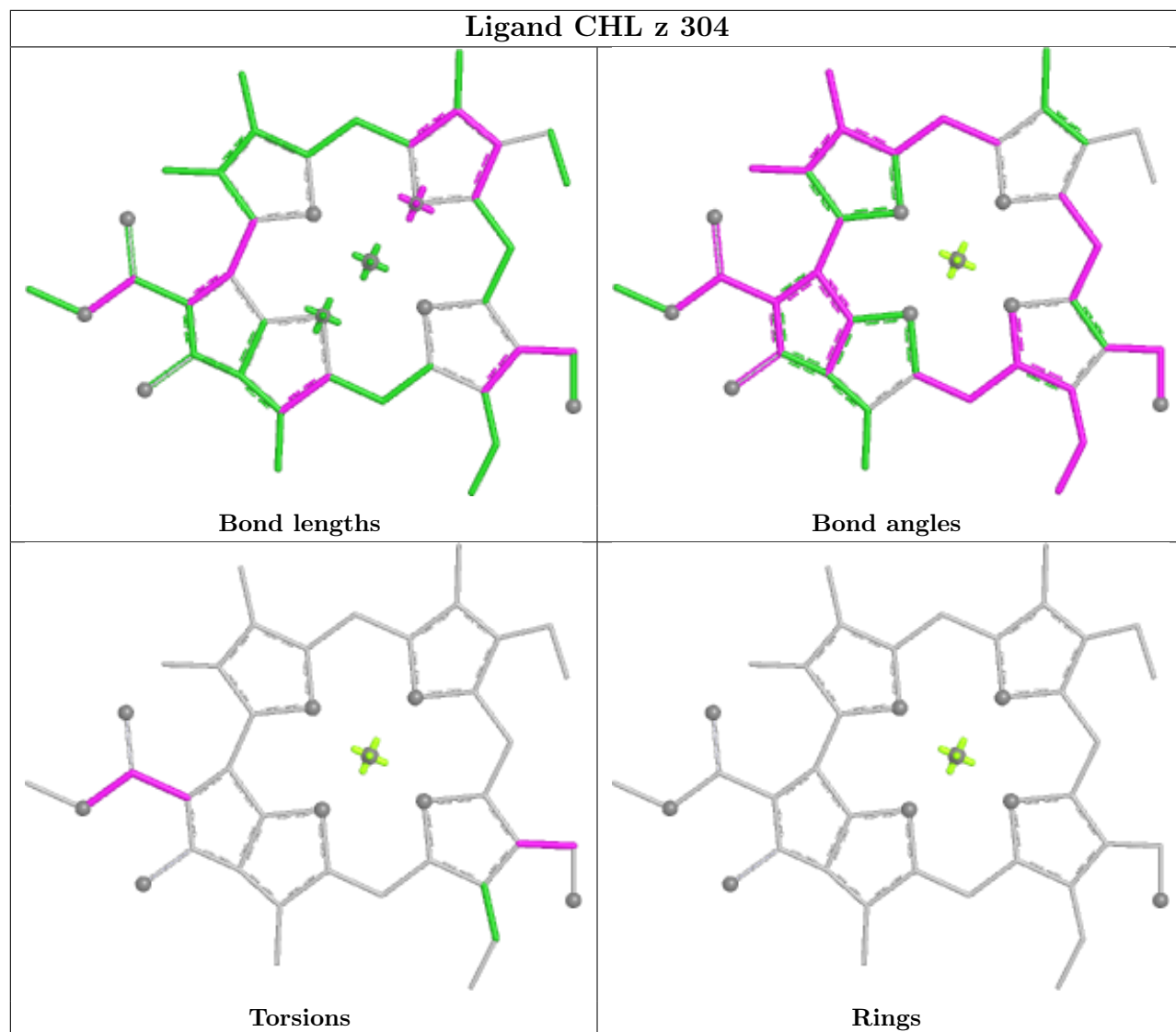


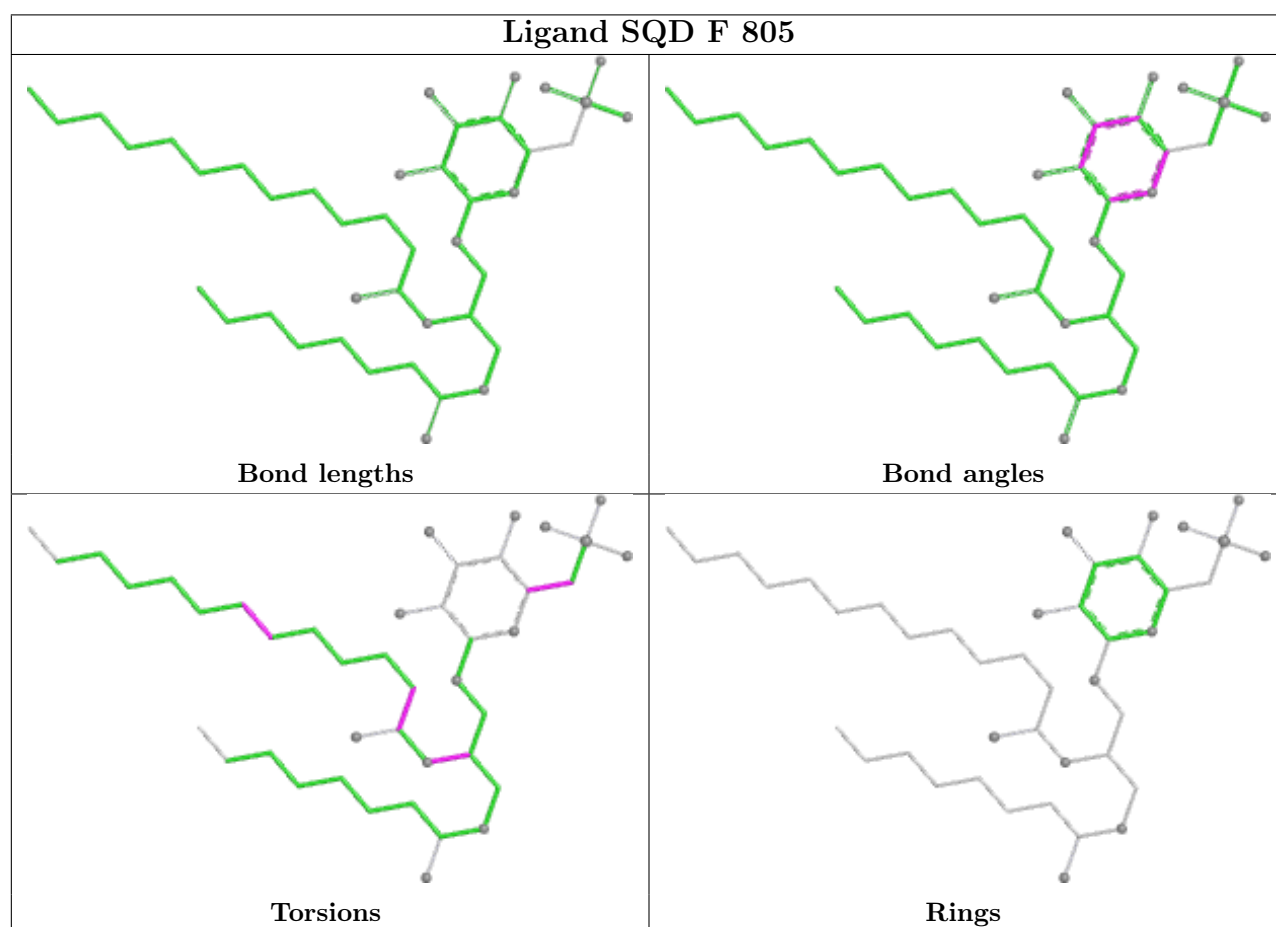
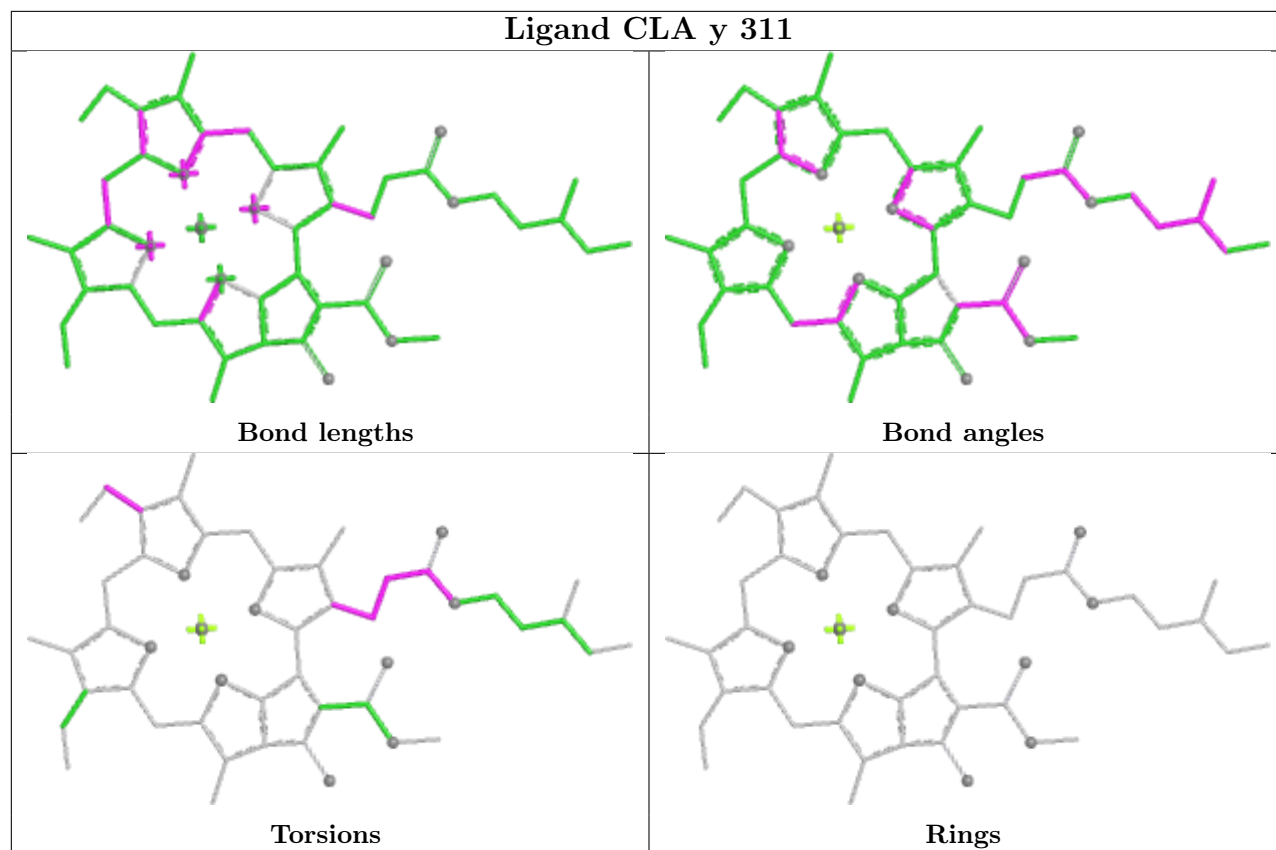


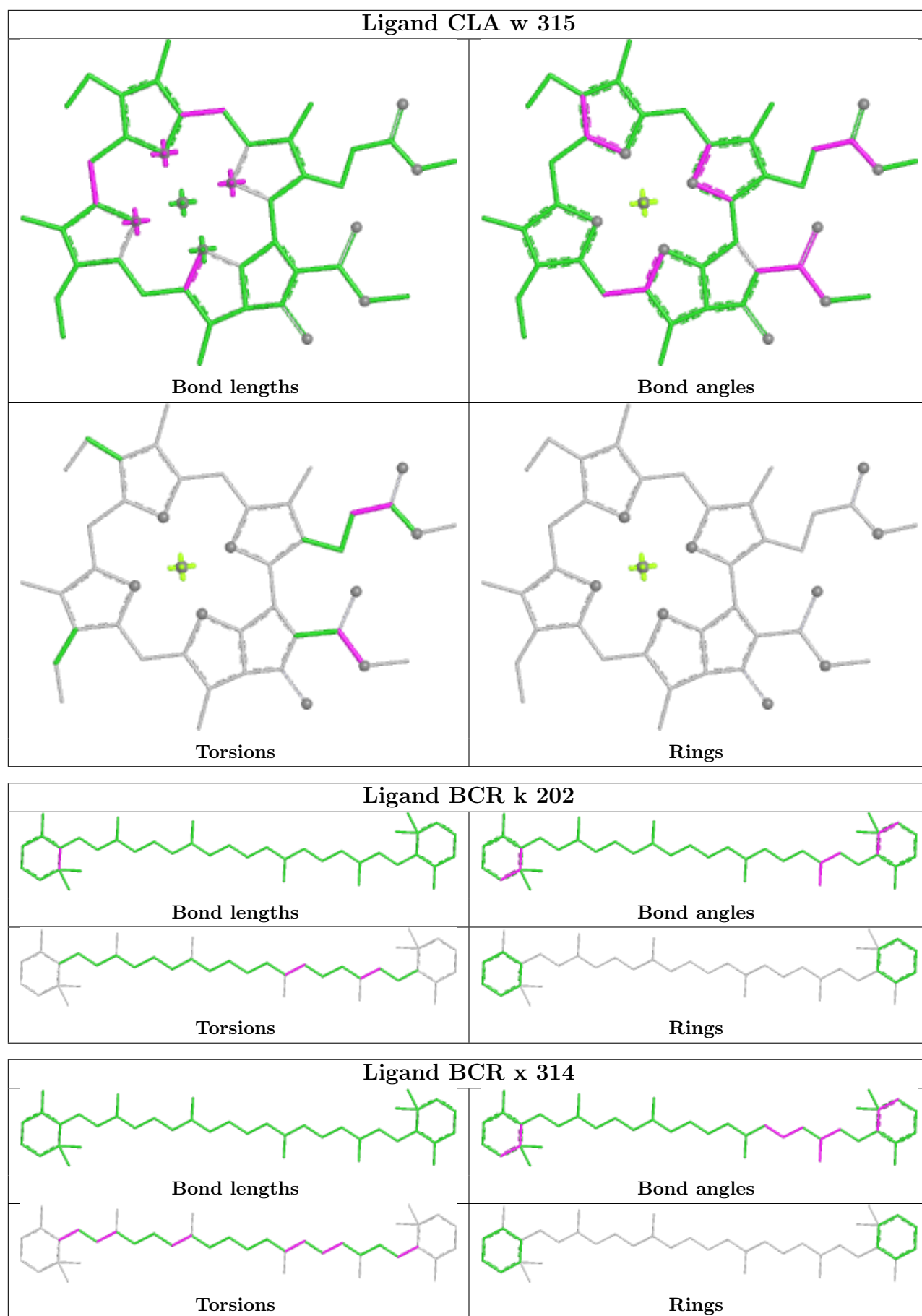


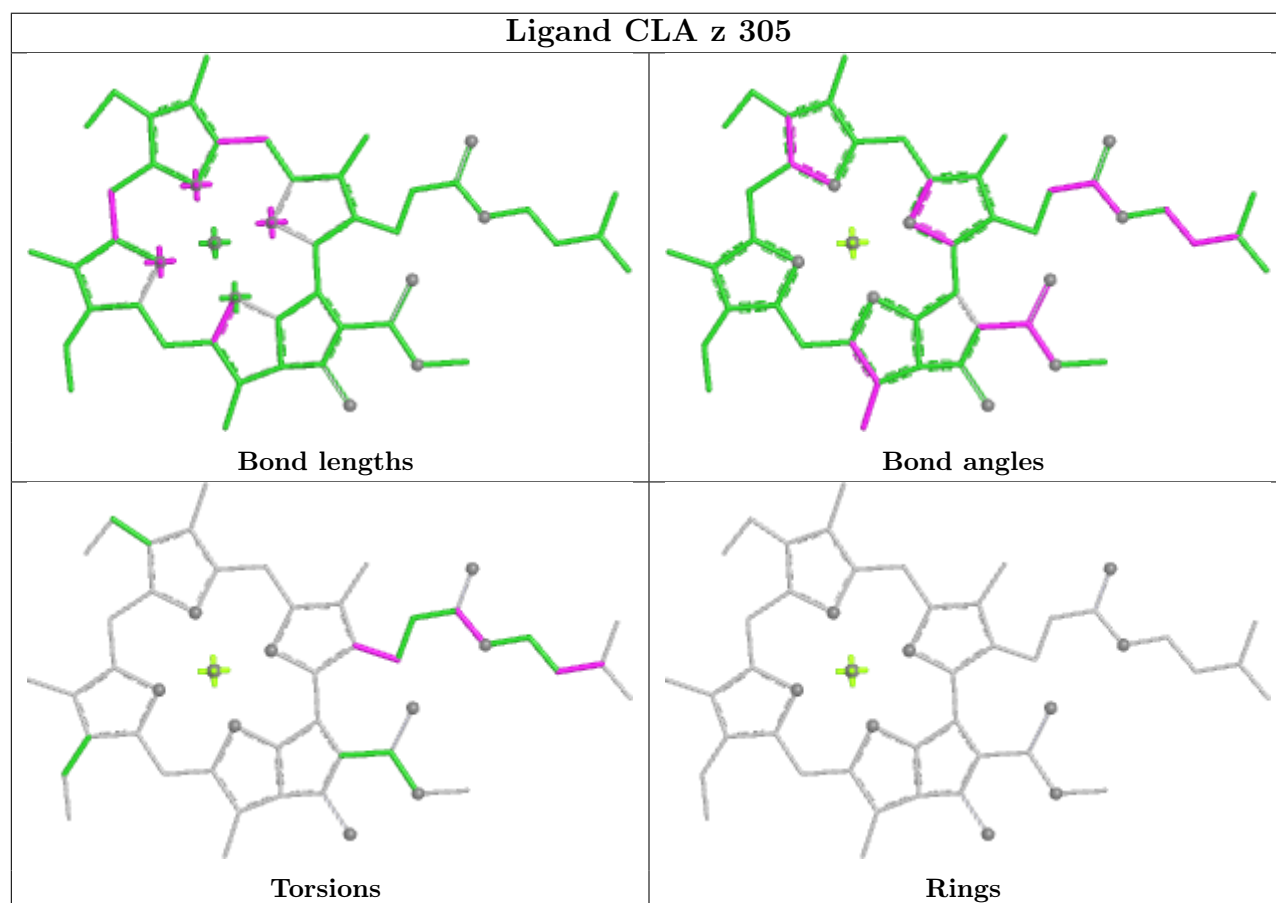
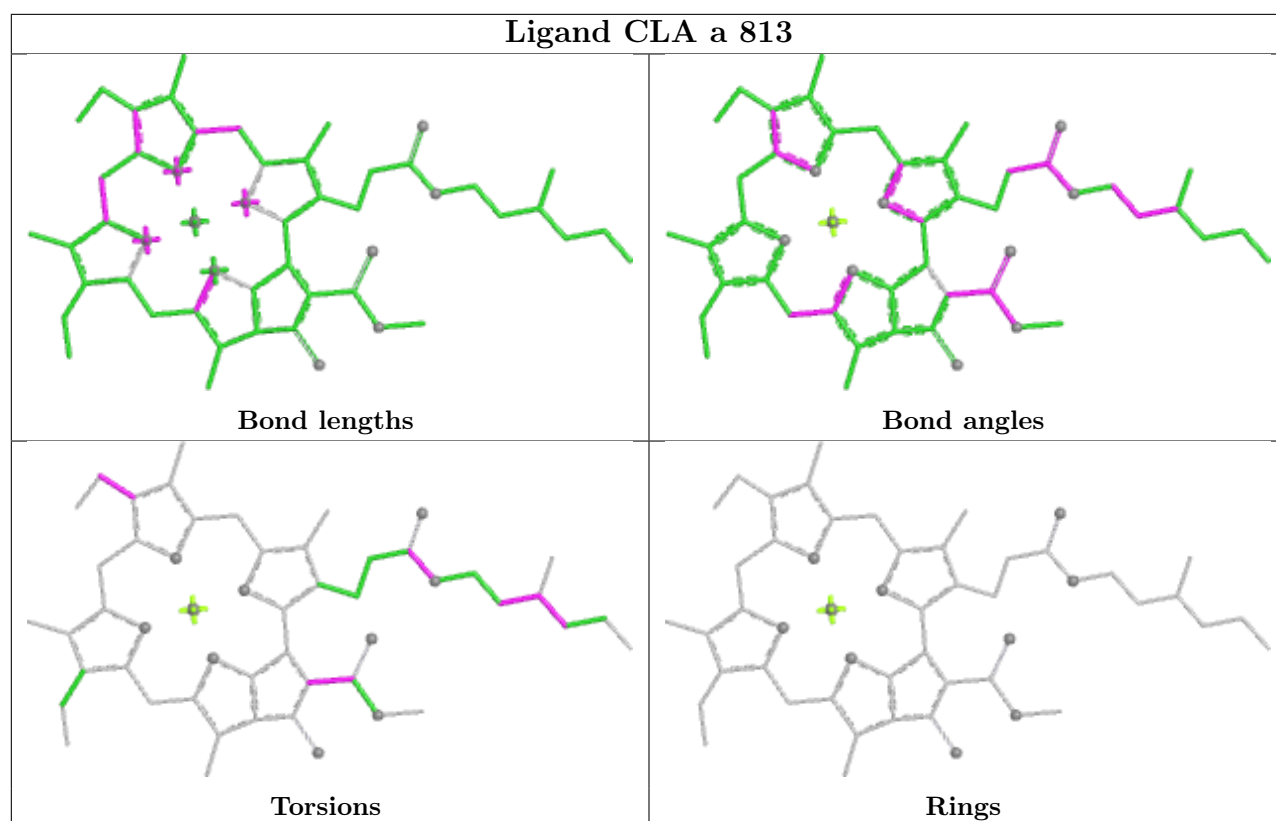


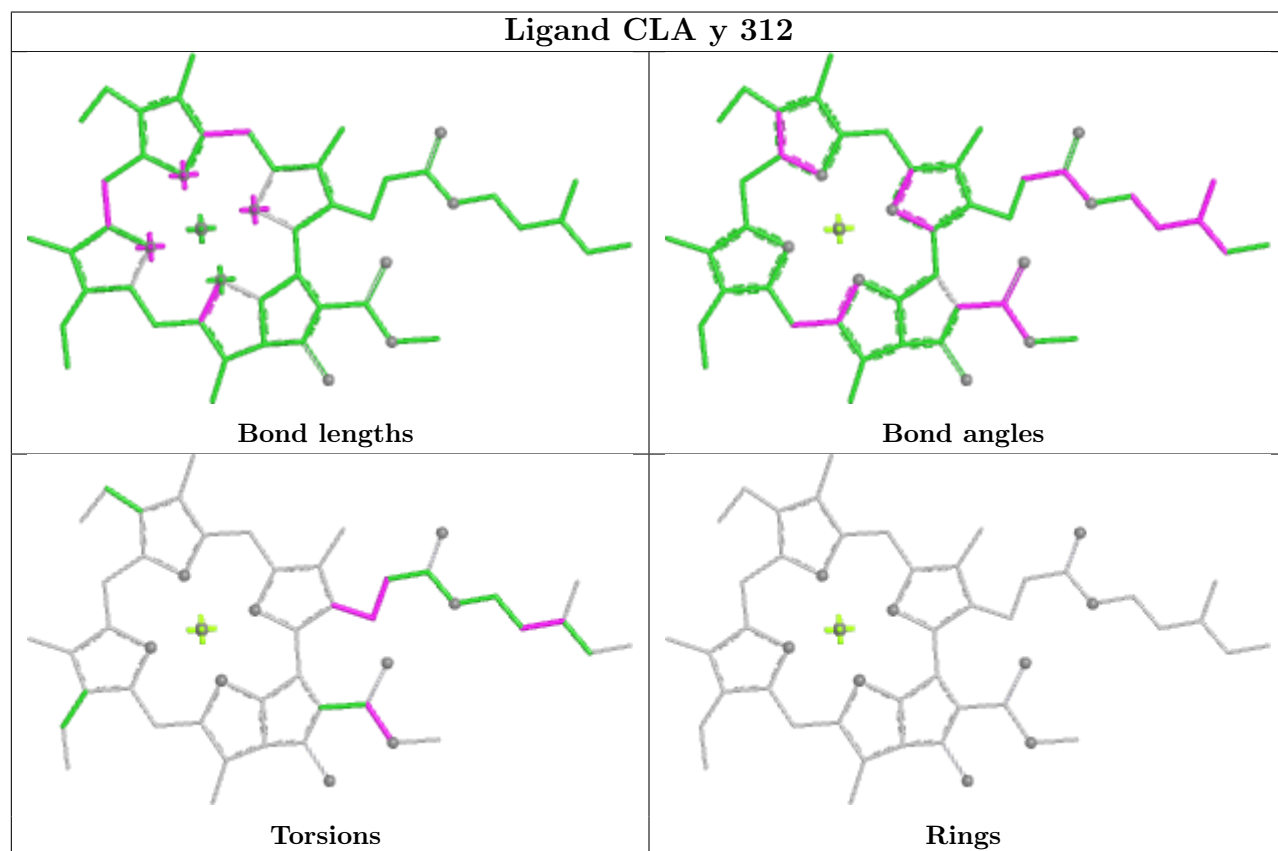
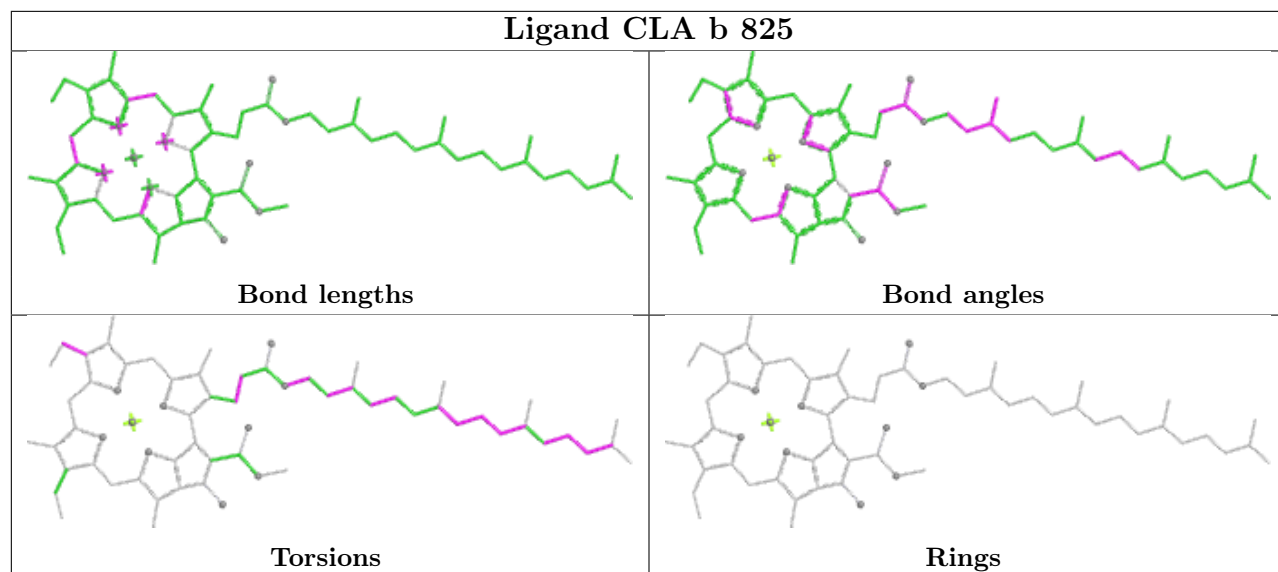


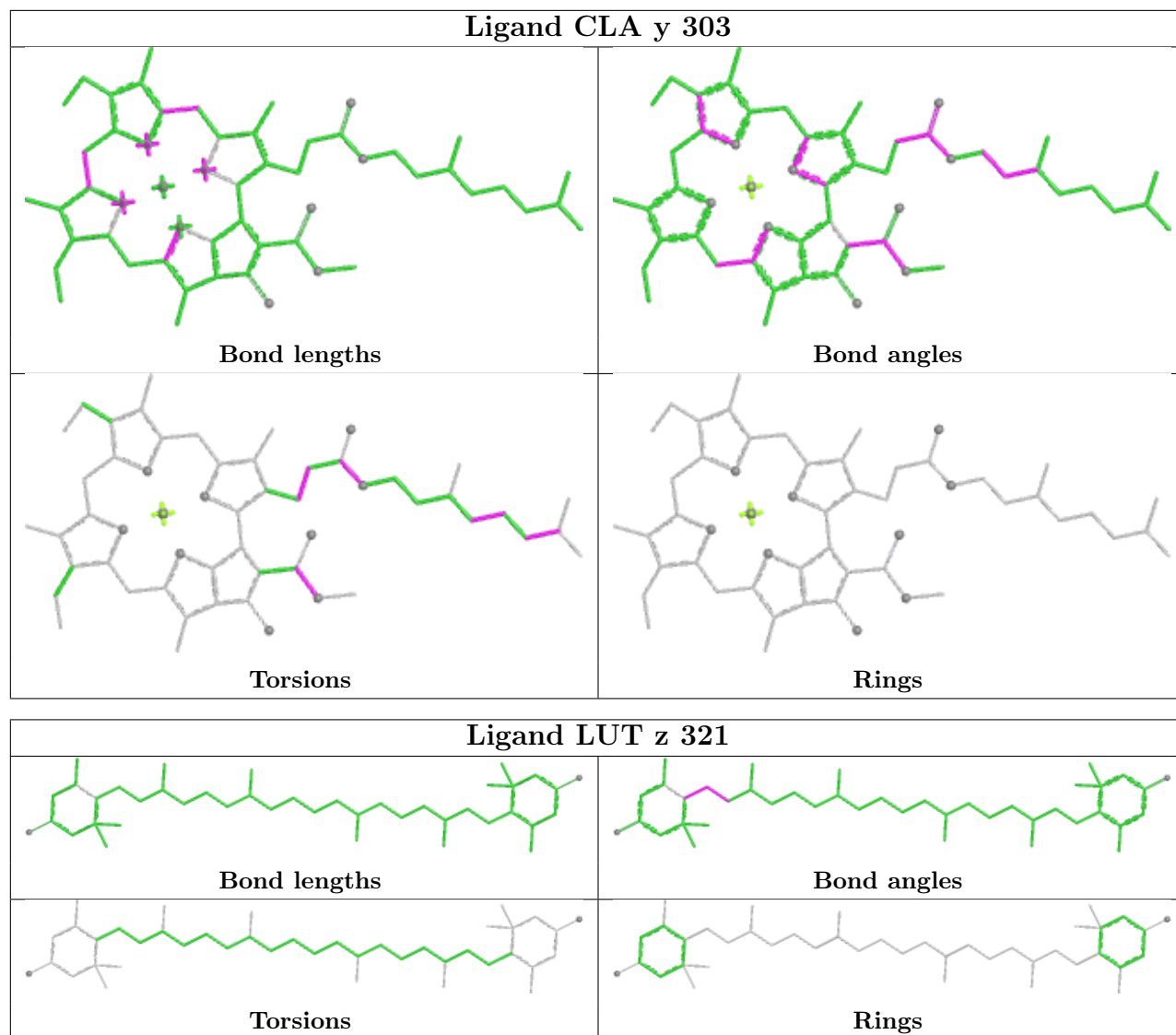


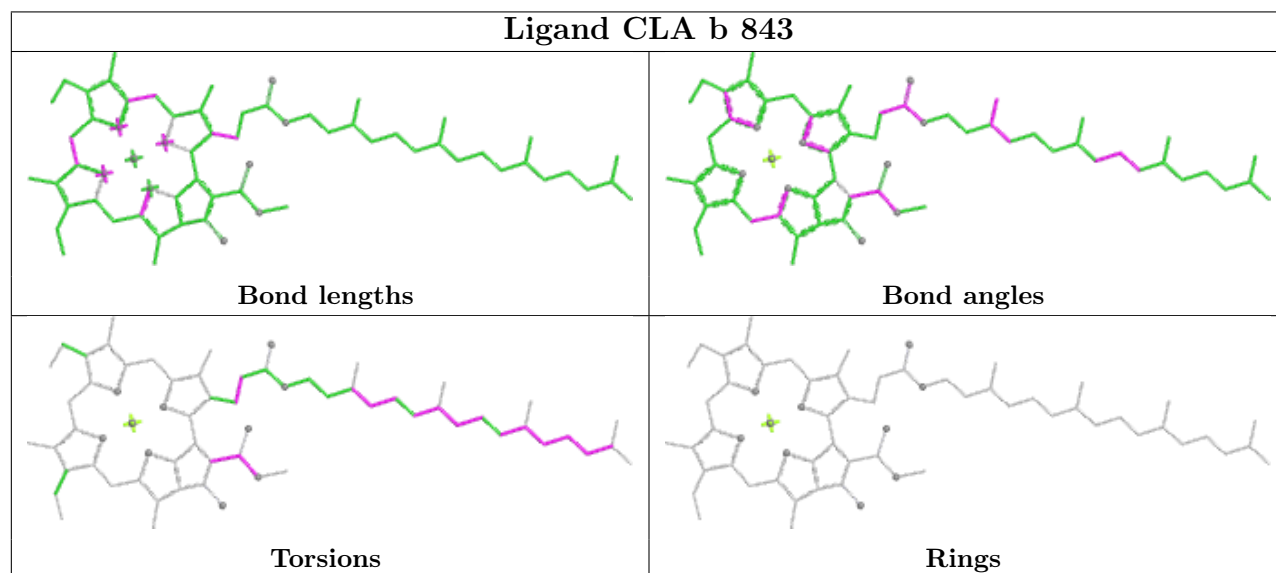
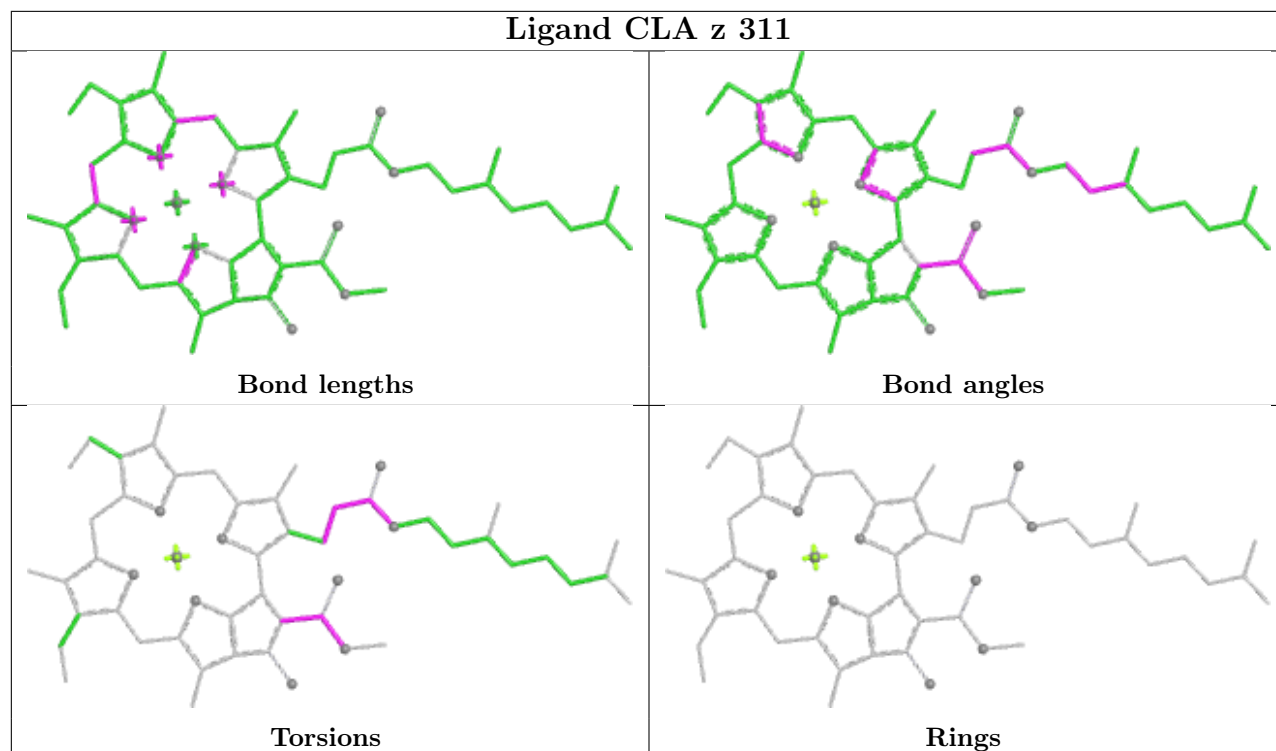


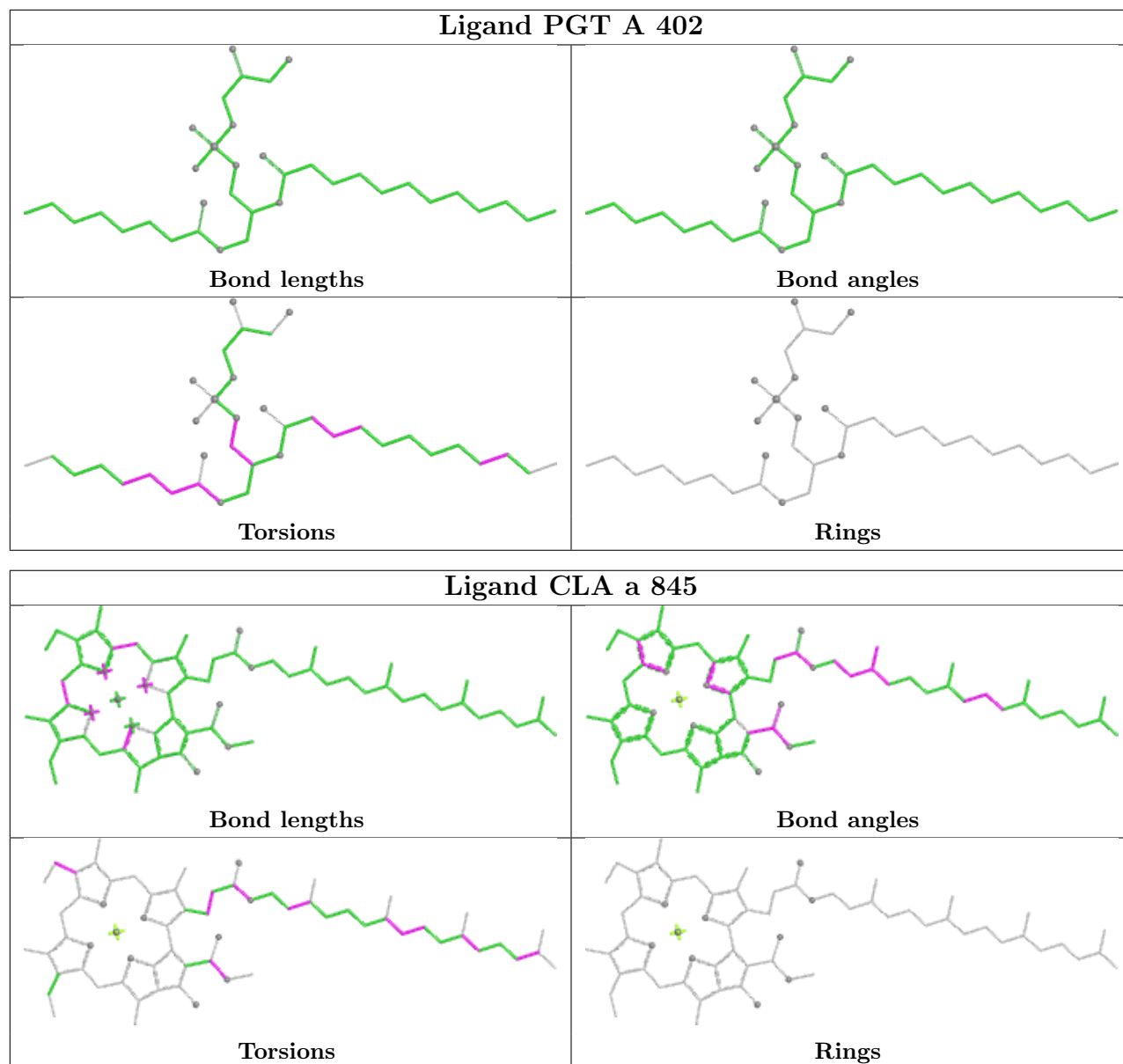


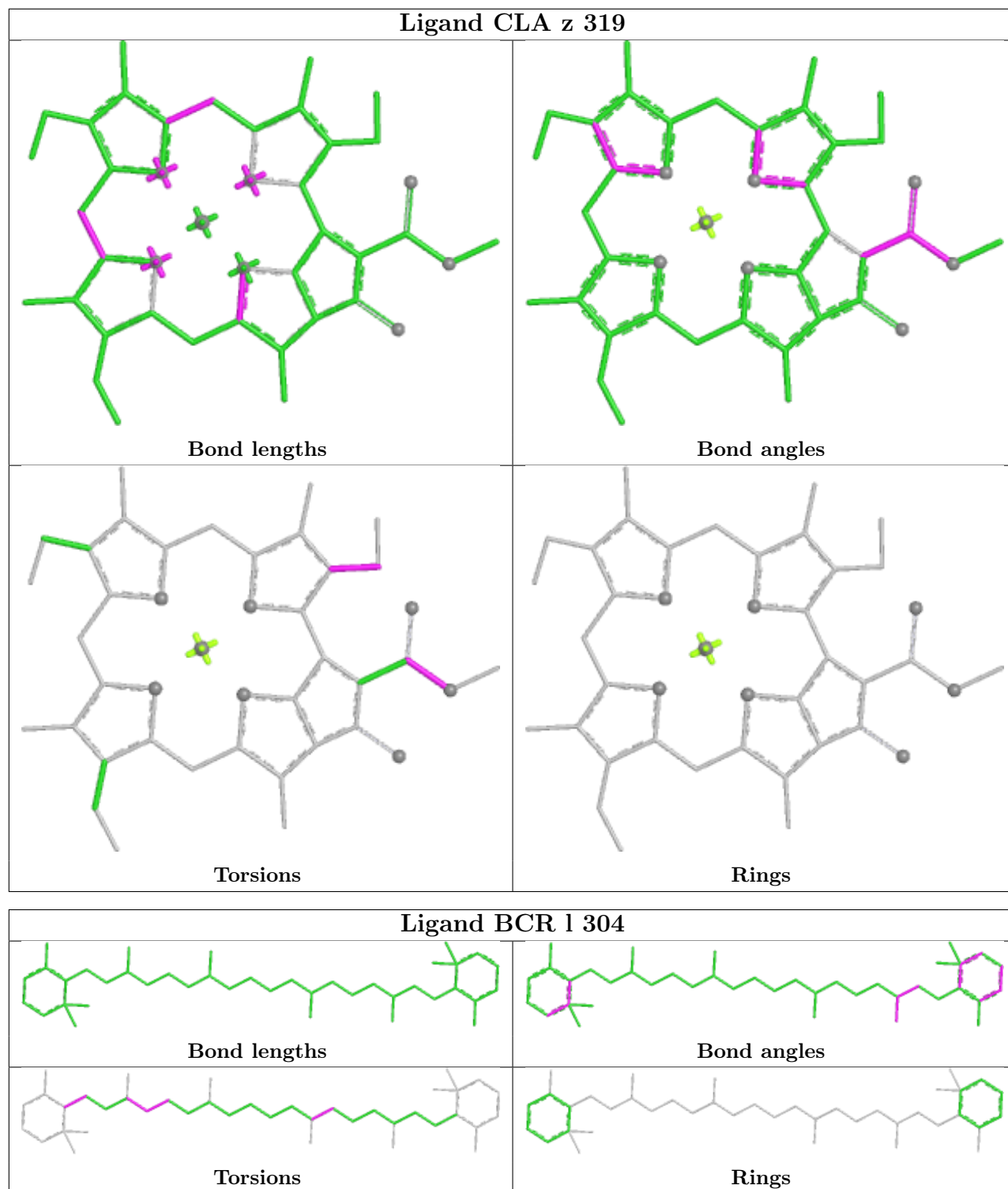


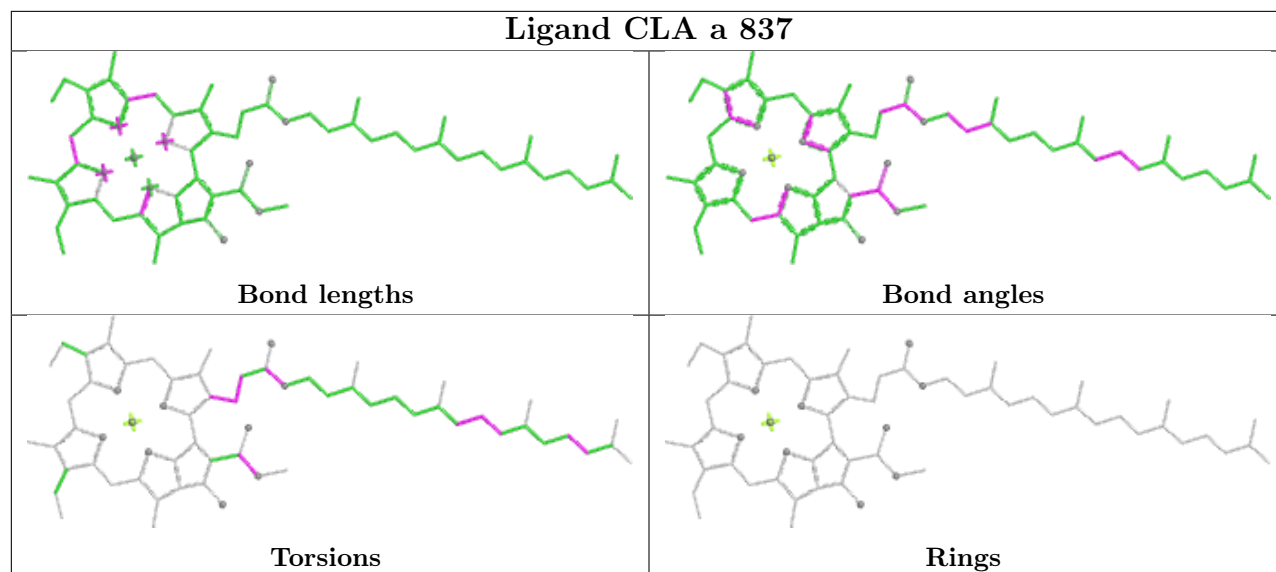












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

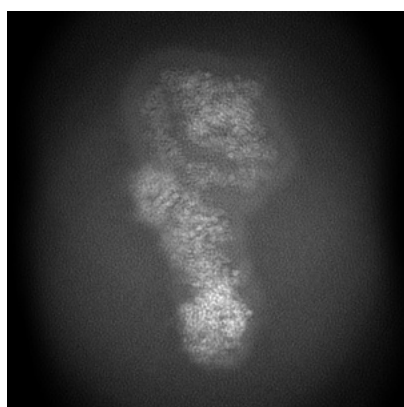
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51527. These allow visual inspection of the internal detail of the map and identification of artifacts.

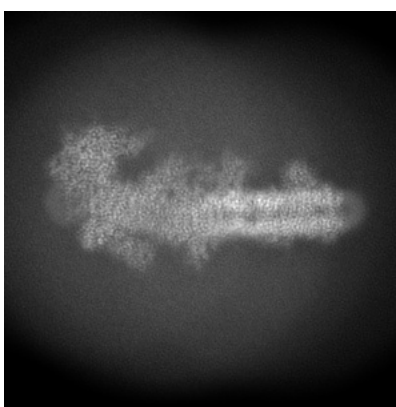
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

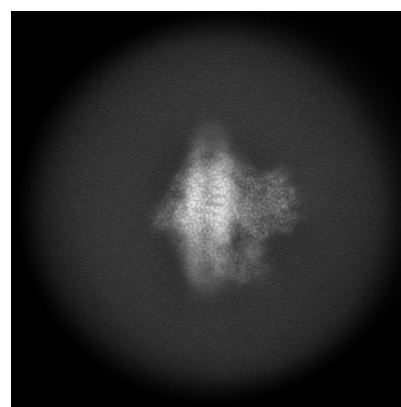
#### 6.1.1 Primary map



X



Y

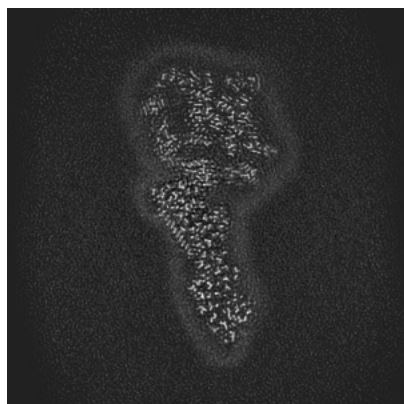


Z

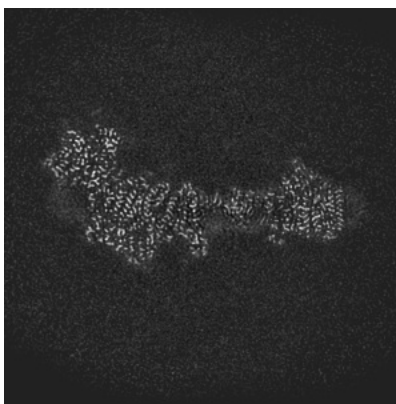
The images above show the map projected in three orthogonal directions.

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

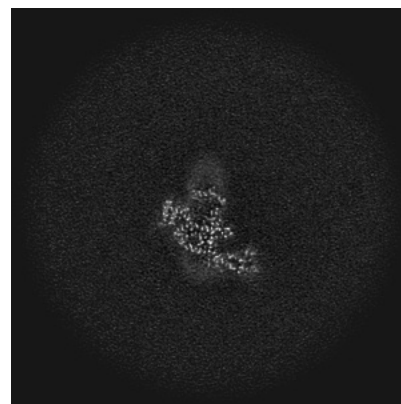
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

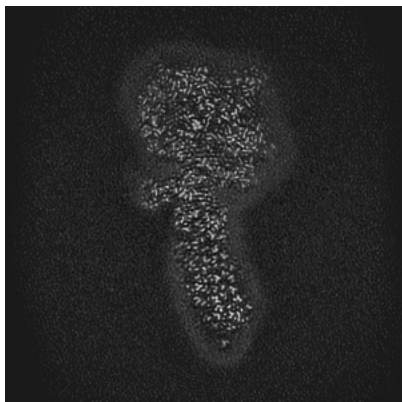


Z Index: 256

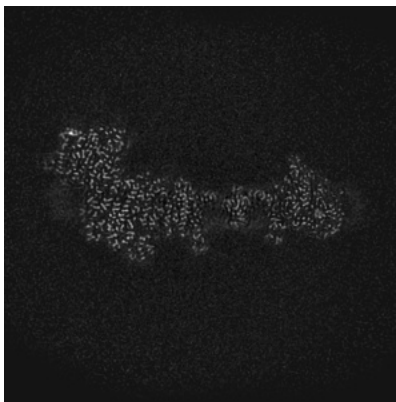
The images above show central slices of the map in three orthogonal directions.

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

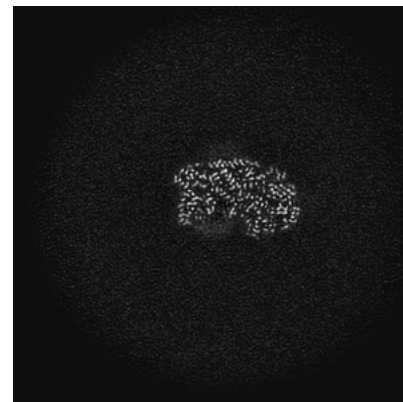
### 6.3.1 Primary map



X Index: 265



Y Index: 260

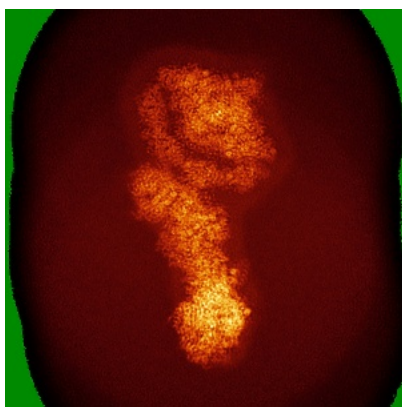


Z Index: 125

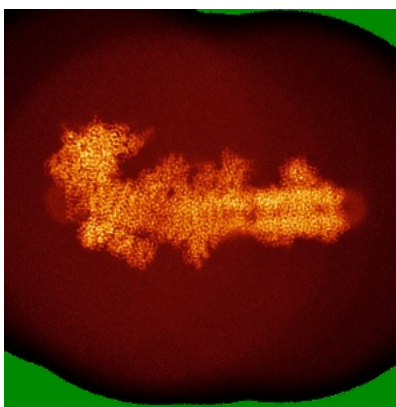
The images above show the largest variance slices of the map in three orthogonal directions.

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

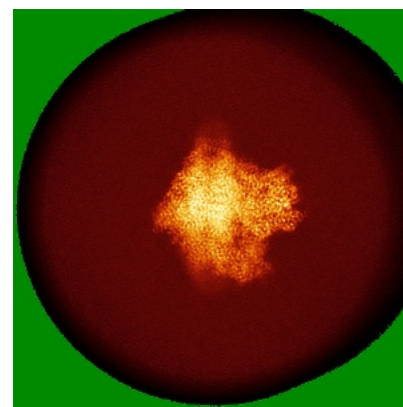
### 6.4.1 Primary map



X



Y

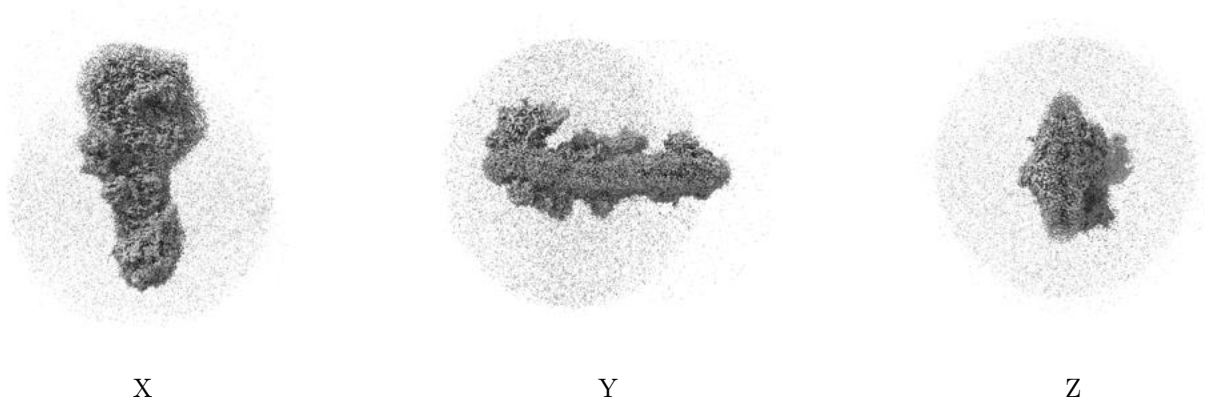


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

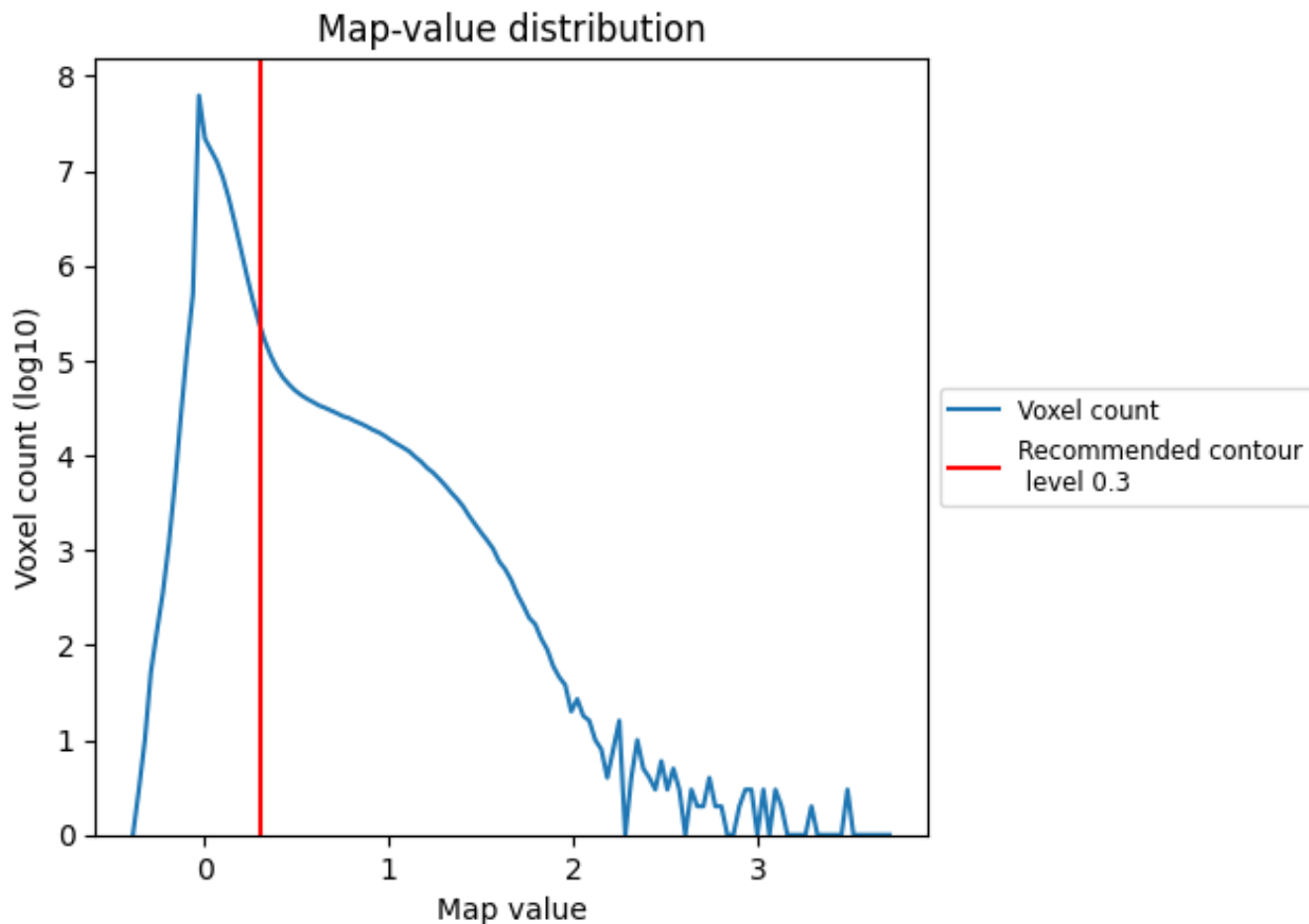
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

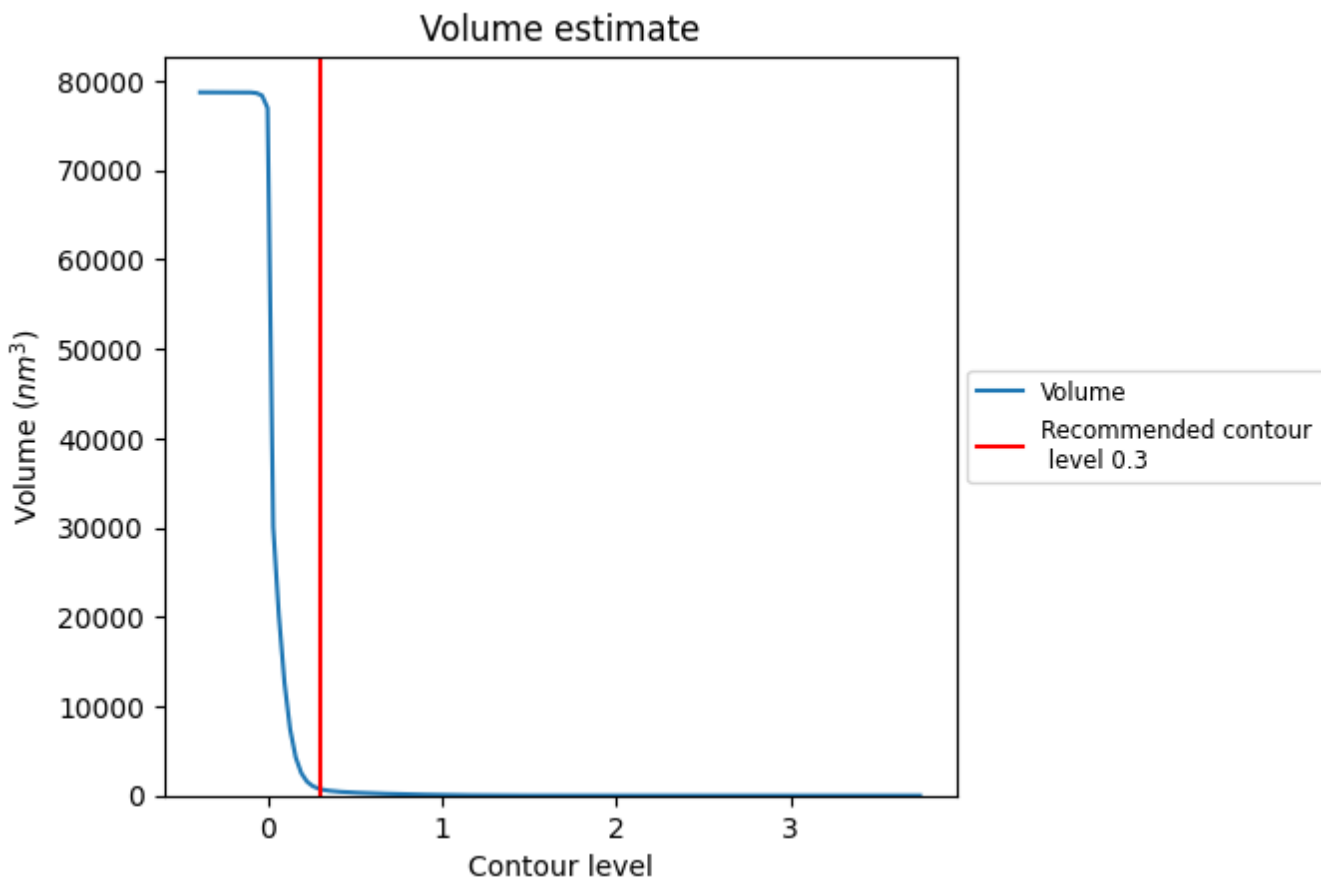
This section contains the results of statistical analysis of the map.

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



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

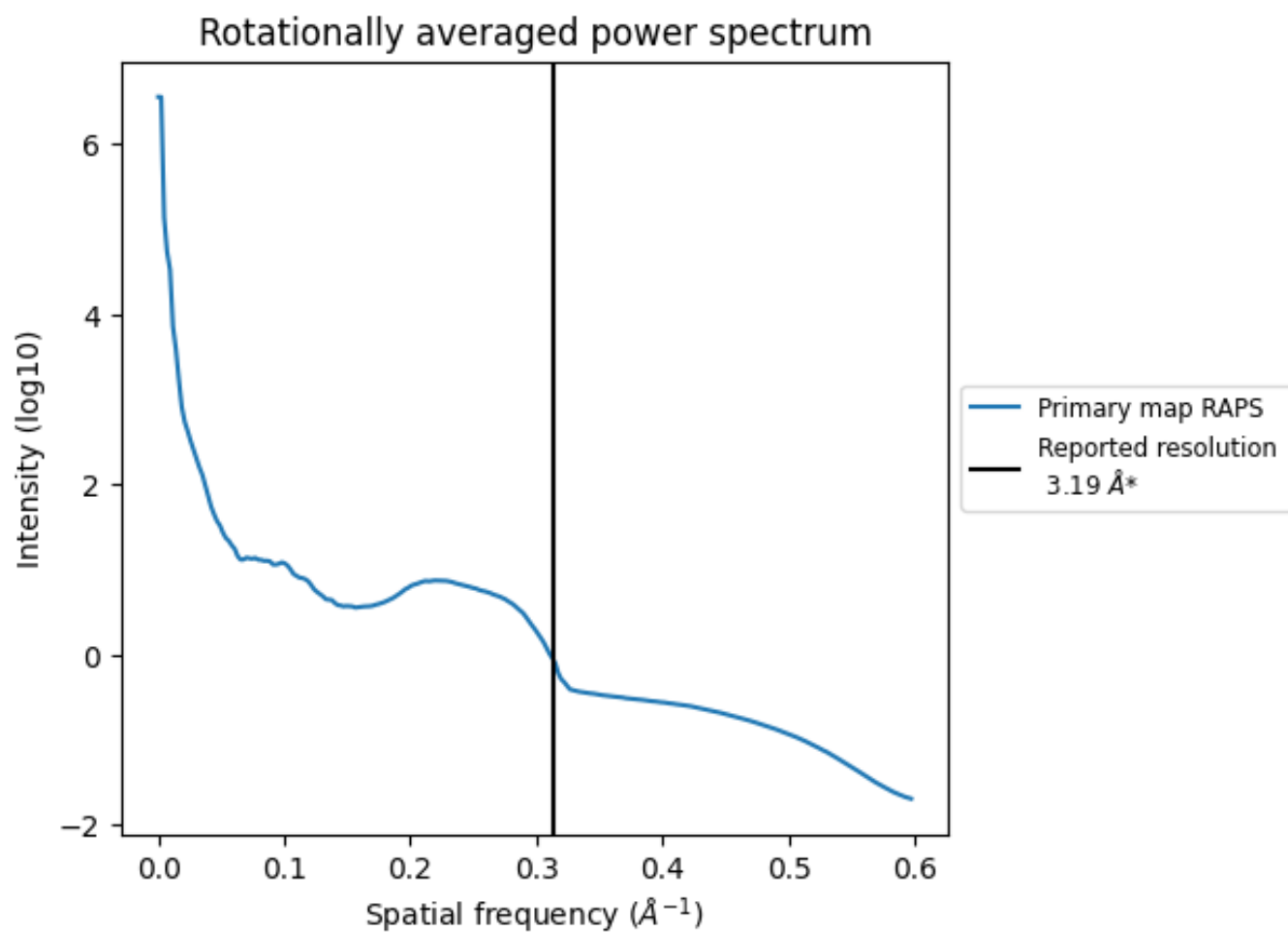
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747  $\text{nm}^3$ ; this corresponds to an approximate mass of 675 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  $0.313 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation

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

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

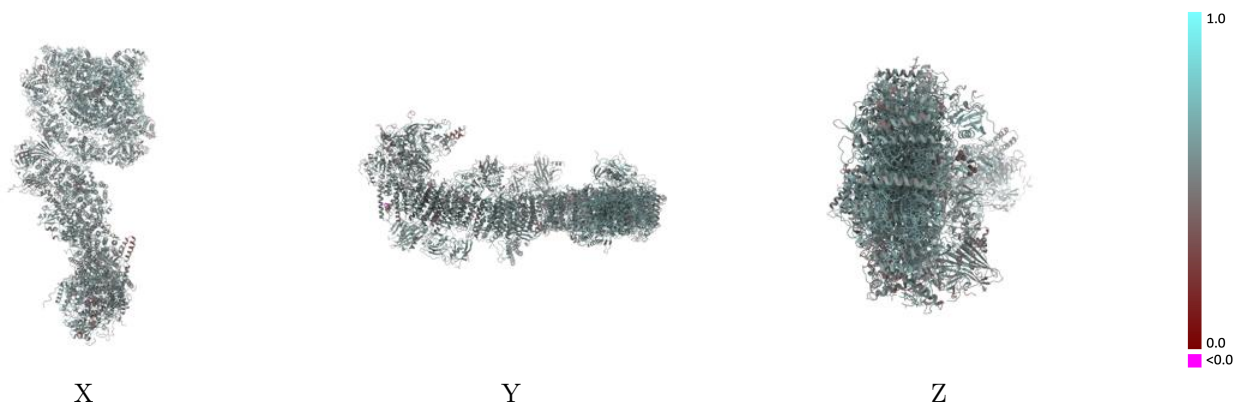
This section contains information regarding the fit between EMDB map EMD-51527 and PDB model 9GRX. Per-residue inclusion information can be found in section [3](#) on page [34](#).

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



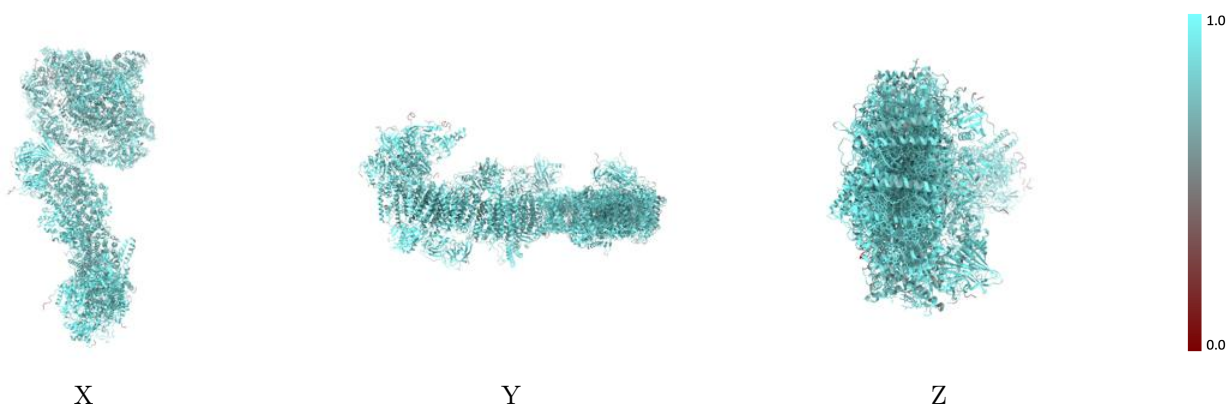
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



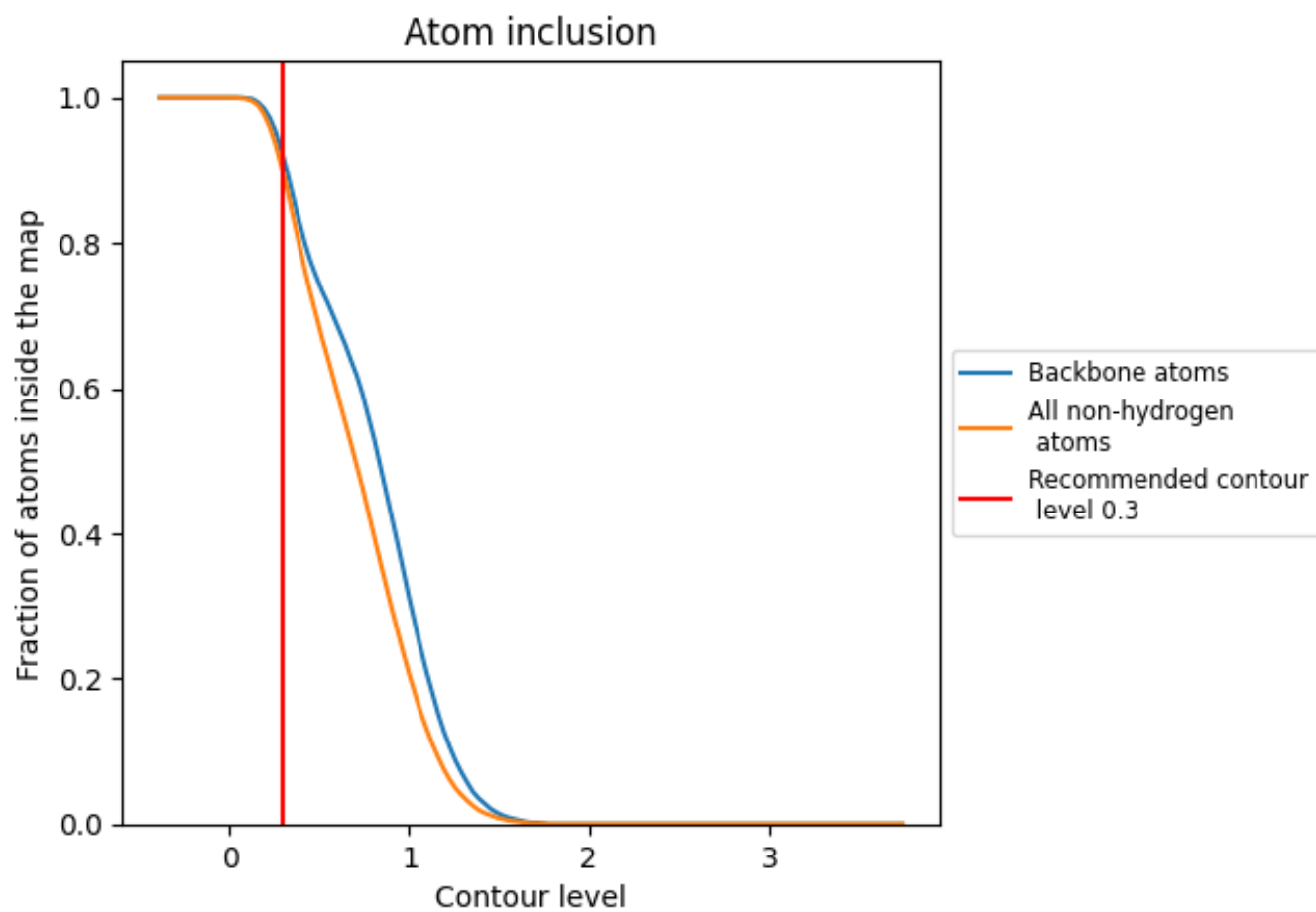
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.5410
0	 0.9360	 0.5380
1	 0.9010	 0.5310
2	 0.9130	 0.5190
3	 0.8660	 0.5090
4	 0.9060	 0.5410
5	 0.9090	 0.5360
6	 0.9370	 0.5290
7	 0.9390	 0.5360
8	 0.9580	 0.5540
9	 0.9370	 0.5460
A	 0.8730	 0.5200
B	 0.8910	 0.5230
C	 0.8800	 0.5150
D	 0.9330	 0.5510
E	 0.9290	 0.5410
F	 0.9090	 0.5240
G	 0.8980	 0.5220
H	 0.8970	 0.5250
I	 0.9000	 0.5250
J	 0.9310	 0.5430
K	 0.8970	 0.5220
L	 0.9000	 0.5250
M	 0.8910	 0.5260
N	 0.9000	 0.5150
O	 0.8800	 0.5110
U	 0.8480	 0.4840
a	 0.9150	 0.5790
b	 0.9070	 0.5780
c	 0.9210	 0.5590
d	 0.9030	 0.5710
e	 0.8230	 0.5320
f	 0.8740	 0.5640
g	 0.7850	 0.5270
h	 0.7260	 0.5120



*Continued on next page...*

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Chain	Atom inclusion	Q-score
i	 0.8970	 0.5740
j	 0.8510	 0.5490
k	 0.8000	 0.4920
l	 0.8070	 0.5390
w	 0.9280	 0.5470
x	 0.8710	 0.5420
y	 0.9030	 0.5330
z	 0.8010	 0.5160