



wwPDB EM Validation Summary Report ⓘ

Feb 18, 2024 – 06:56 PM JST

PDB ID : 8JZE
EMDB ID : EMD-36742
Title : PSI-AcpPCI supercomplex from Symbiodinium
Authors : Li, Z.H.; Li, X.Y.; Wang, W.D.
Deposited on : 2023-07-05
Resolution : 2.99 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

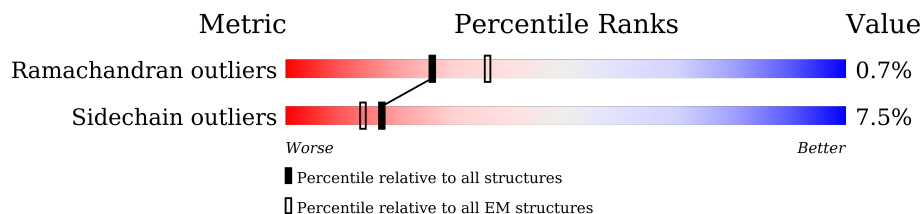
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.99 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.



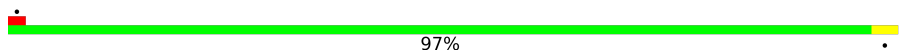
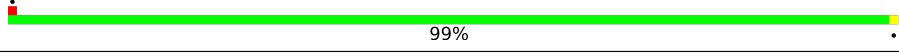
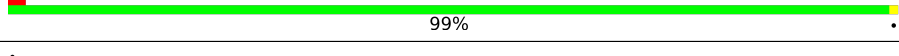
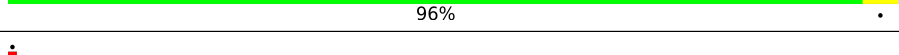
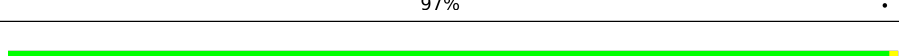
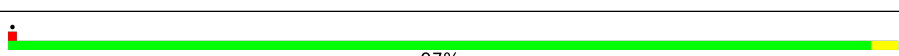
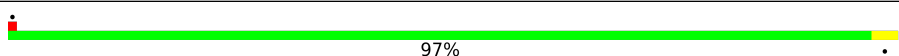
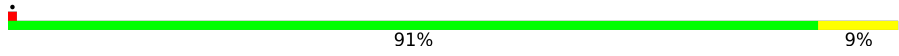


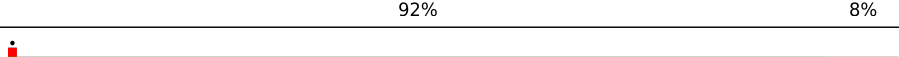
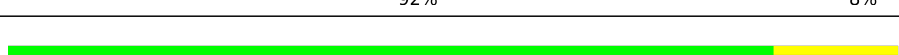
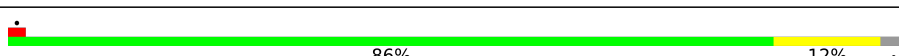


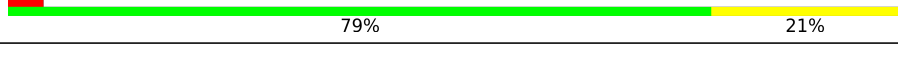


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	I	200	97%
2	K	177	96%
3	z	78	100%
4	y	131	100%
5	G	224	93%
6	A	189	93% 5%
7	c	86	99%
8	d	218	99%
9	e	73	100%

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Mol	Chain	Length	Quality of chain
10	f	184	 97%
11	h	131	 99%
12	i	119	 99%
13	j	98	 96%
14	l	250	 97%
15	m	79	 99%
16	a	670	 97%
17	b	663	 97%
18	B	192	 91% 9%
19	D	165	 82% 15%
20	F	176	 6% 86% 9%
21	H	160	 66% 92% 8%
22	J	220	 92% 8%
23	L	185	 86% 14%
24	M	173	 86% 12%
25	N	160	 36% 74% 21%
26	O	161	 7% 86% 14%
27	P	160	 79% 21%

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
30	CLA	A	307	X	-	-	-
30	CLA	A	308	X	-	-	-
30	CLA	A	309	X	-	-	-
30	CLA	A	310	X	-	-	-
30	CLA	A	311	X	-	-	-
30	CLA	A	312	X	-	-	-
30	CLA	A	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	A	315	X	-	-	-
30	CLA	A	316	X	-	-	-
30	CLA	A	317	X	-	-	-
30	CLA	A	319	X	-	-	-
30	CLA	A	320	X	-	-	-
30	CLA	B	301	X	-	-	-
30	CLA	B	307	X	-	-	-
30	CLA	B	308	X	-	-	-
30	CLA	B	309	X	-	-	-
30	CLA	B	310	X	-	-	-
30	CLA	B	311	X	-	-	-
30	CLA	B	312	X	-	-	-
30	CLA	B	313	X	-	-	-
30	CLA	B	315	X	-	-	-
30	CLA	B	316	X	-	-	-
30	CLA	B	317	X	-	-	-
30	CLA	D	308	X	-	-	-
30	CLA	D	309	X	-	-	-
30	CLA	D	311	X	-	-	-
30	CLA	D	312	X	-	-	-
30	CLA	D	313	X	-	-	-
30	CLA	D	314	X	-	-	-
30	CLA	D	316	X	-	-	-
30	CLA	F	307	X	-	-	-
30	CLA	F	308	X	-	-	-
30	CLA	F	310	X	-	-	-
30	CLA	F	311	X	-	-	-
30	CLA	F	312	X	-	-	-
30	CLA	F	313	X	-	-	-
30	CLA	F	315	X	-	-	-
30	CLA	G	509	X	-	-	-
30	CLA	G	510	X	-	-	-
30	CLA	G	511	X	-	-	-
30	CLA	G	512	X	-	-	-
30	CLA	G	513	X	-	-	-
30	CLA	G	514	X	-	-	-
30	CLA	G	516	X	-	-	-
30	CLA	G	517	X	-	-	-
30	CLA	G	518	X	-	-	-
30	CLA	G	519	X	-	-	-
30	CLA	G	520	X	-	-	-
30	CLA	H	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	H	305	X	-	-	-
30	CLA	H	307	X	-	-	-
30	CLA	H	308	X	-	-	-
30	CLA	H	309	X	-	-	-
30	CLA	H	312	X	-	-	-
30	CLA	I	306	X	-	-	-
30	CLA	I	307	X	-	-	-
30	CLA	I	308	X	-	-	-
30	CLA	I	309	X	-	-	-
30	CLA	I	310	X	-	-	-
30	CLA	I	311	X	-	-	-
30	CLA	I	312	X	-	-	-
30	CLA	I	313	X	-	-	-
30	CLA	I	315	X	-	-	-
30	CLA	I	316	X	-	-	-
30	CLA	I	319	X	-	-	-
30	CLA	I	321	X	-	-	-
30	CLA	J	301	X	-	-	-
30	CLA	J	306	X	-	-	-
30	CLA	J	307	X	-	-	-
30	CLA	J	308	X	-	-	-
30	CLA	J	309	X	-	-	-
30	CLA	J	310	X	-	-	-
30	CLA	J	311	X	-	-	-
30	CLA	J	312	X	-	-	-
30	CLA	J	314	X	-	-	-
30	CLA	J	315	X	-	-	-
30	CLA	K	306	X	-	-	-
30	CLA	K	307	X	-	-	-
30	CLA	K	308	X	-	-	-
30	CLA	K	309	X	-	-	-
30	CLA	K	310	X	-	-	-
30	CLA	K	311	X	-	-	-
30	CLA	K	312	X	-	-	-
30	CLA	K	313	X	-	-	-
30	CLA	K	315	X	-	-	-
30	CLA	K	316	X	-	-	-
30	CLA	L	308	X	-	-	-
30	CLA	L	309	X	-	-	-
30	CLA	L	310	X	-	-	-
30	CLA	L	311	X	-	-	-
30	CLA	L	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	L	313	X	-	-	-
30	CLA	L	314	X	-	-	-
30	CLA	L	316	X	-	-	-
30	CLA	L	317	X	-	-	-
30	CLA	L	318	X	-	-	-
30	CLA	M	308	X	-	-	-
30	CLA	M	309	X	-	-	-
30	CLA	M	310	X	-	-	-
30	CLA	M	311	X	-	-	-
30	CLA	M	312	X	-	-	-
30	CLA	M	313	X	-	-	-
30	CLA	M	315	X	-	-	-
30	CLA	M	316	X	-	-	-
30	CLA	M	317	X	-	-	-
30	CLA	M	318	X	-	-	-
30	CLA	N	304	X	-	-	-
30	CLA	N	305	X	-	-	-
30	CLA	N	307	X	-	-	-
30	CLA	N	309	X	-	-	-
30	CLA	N	310	X	-	-	-
30	CLA	O	308	X	-	-	-
30	CLA	O	309	X	-	-	-
30	CLA	O	311	X	-	-	-
30	CLA	O	313	X	-	-	-
30	CLA	O	314	X	-	-	-
30	CLA	O	316	X	-	-	-
30	CLA	P	209	X	-	-	-
30	CLA	P	210	X	-	-	-
30	CLA	P	212	X	-	-	-
30	CLA	P	214	X	-	-	-
30	CLA	P	215	X	-	-	-
30	CLA	P	217	X	-	-	-
30	CLA	a	701	X	-	-	-
30	CLA	a	702	X	-	-	-
30	CLA	a	703	X	-	-	-
30	CLA	a	704	X	-	-	-
30	CLA	a	705	X	-	-	-
30	CLA	a	706	X	-	-	-
30	CLA	a	707	X	-	-	-
30	CLA	a	708	X	-	-	-
30	CLA	a	709	X	-	-	-
30	CLA	a	710	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	a	711	X	-	-	-
30	CLA	a	712	X	-	-	-
30	CLA	a	713	X	-	-	-
30	CLA	a	714	X	-	-	-
30	CLA	a	715	X	-	-	-
30	CLA	a	716	X	-	-	-
30	CLA	a	717	X	-	-	-
30	CLA	a	718	X	-	-	-
30	CLA	a	719	X	-	-	-
30	CLA	a	720	X	-	-	-
30	CLA	a	721	X	-	-	-
30	CLA	a	722	X	-	-	-
30	CLA	a	723	X	-	-	-
30	CLA	a	724	X	-	-	-
30	CLA	a	725	X	-	-	-
30	CLA	a	726	X	-	-	-
30	CLA	a	727	X	-	-	-
30	CLA	a	728	X	-	-	-
30	CLA	a	729	X	-	-	-
30	CLA	a	730	X	-	-	-
30	CLA	a	731	X	-	-	-
30	CLA	a	735	X	-	-	-
30	CLA	a	738	X	-	-	-
30	CLA	b	701	X	-	-	-
30	CLA	b	703	X	-	-	-
30	CLA	b	704	X	-	-	-
30	CLA	b	705	X	-	-	-
30	CLA	b	706	X	-	-	-
30	CLA	b	707	X	-	-	-
30	CLA	b	708	X	-	-	-
30	CLA	b	709	X	-	-	-
30	CLA	b	710	X	-	-	-
30	CLA	b	711	X	-	-	-
30	CLA	b	712	X	-	-	-
30	CLA	b	713	X	-	-	-
30	CLA	b	714	X	-	-	-
30	CLA	b	715	X	-	-	-
30	CLA	b	716	X	-	-	-
30	CLA	b	717	X	-	-	-
30	CLA	b	718	X	-	-	-
30	CLA	b	719	X	-	-	-
30	CLA	b	720	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	b	721	X	-	-	-
30	CLA	b	722	X	-	-	-
30	CLA	b	723	X	-	-	-
30	CLA	b	724	X	-	-	-
30	CLA	b	725	X	-	-	-
30	CLA	b	726	X	-	-	-
30	CLA	b	727	X	-	-	-
30	CLA	b	728	X	-	-	-
30	CLA	f	301	X	-	-	-
30	CLA	f	302	X	-	-	-
30	CLA	f	303	X	-	-	-
30	CLA	h	202	X	-	-	-
30	CLA	j	104	X	-	-	-
30	CLA	j	106	X	-	-	-
30	CLA	l	303	X	-	-	-
30	CLA	l	304	X	-	-	-
30	CLA	l	305	X	-	-	-
30	CLA	l	308	X	-	-	-
30	CLA	l	309	X	-	-	-
30	CLA	l	311	X	-	-	-
30	CLA	l	312	X	-	-	-
30	CLA	l	313	X	-	-	-
30	CLA	m	202	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 55927 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 Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	I	200	1480	961	250	259	10	0	0

- Molecule 2 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	K	177	1349	872	227	238	12	0	0

- Molecule 3 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	z	78	390	234	78	78	0	0

- Molecule 4 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	y	131	655	393	131	131	0	0

- Molecule 5 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	217	1572	1004	269	289	10	0	0

- Molecule 6 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	186	Total	C	N	O	S	0	0
			1346	870	225	242	9		

- Molecule 7 is a protein called Photosystem I PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	86	Total	C	N	O	S	0	0
			653	403	109	132	9		

- Molecule 8 is a protein called Photosystem I PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	218	Total	C	N	O	S	0	0
			1731	1096	307	315	13		

- Molecule 9 is a protein called Photosystem I PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	e	73	Total	C	N	O	0	0
			587	384	99	104		

- Molecule 10 is a protein called Photosystem I PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	184	Total	C	N	O	S	0	0
			1450	930	252	260	8		

- Molecule 11 is a protein called Photosystem I PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	131	Total	C	N	O	S	0	0
			1066	704	165	193	4		

- Molecule 12 is a protein called Photosystem I PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	119	Total	C	N	O	S	0	0
			964	620	167	175	2		

- Molecule 13 is a protein called Photosystem I PsaJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	j	98	783	505	125	153	0	0

- Molecule 14 is a protein called Photosystem I PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	l	250	1943	1267	312	354	10	0	0

- Molecule 15 is a protein called Photosystem I PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	m	79	582	373	100	107	2	0	0

- Molecule 16 is a protein called Photosystem I PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	a	670	5194	3393	875	910	16	0	0

- Molecule 17 is a protein called Photosystem I PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	b	663	5199	3408	851	928	12	0	0

- Molecule 18 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	B	192	1452	934	241	265	12	0	0

- Molecule 19 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	D	160	1158	728	195	228	7	0	0

- Molecule 20 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2,

acpPCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	F	169	1237	777	209	239	12	0	0

- Molecule 21 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	H	160	1202	769	198	228	7	0	0

- Molecule 22 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	J	220	1496	938	261	290	7	0	0

- Molecule 23 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	L	185	1427	924	239	258	6	0	0

- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	M	168	1211	773	208	225	5	0	0

- Molecule 25 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	N	153	993	607	179	202	5	0	0

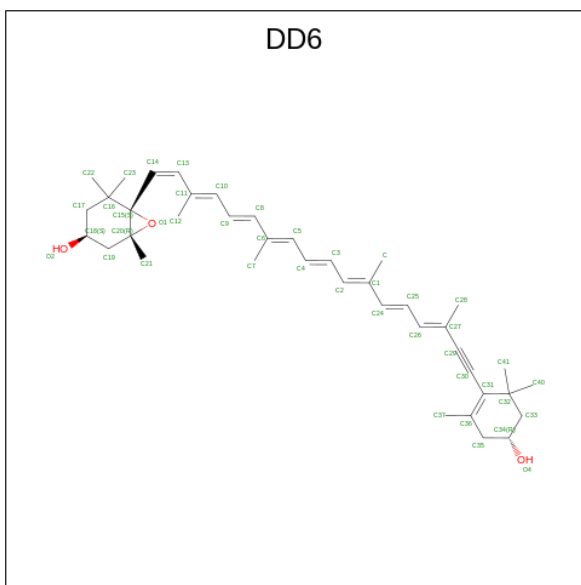
- Molecule 26 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	O	161	1073	670	189	207	7	0	0

- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	P	159	1113	693	191	223	6	0	0

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	I	1	43	40	3	0
28	I	1	43	40	3	0
28	I	1	43	40	3	0
28	I	1	43	40	3	0
28	K	1	43	40	3	0
28	K	1	43	40	3	0

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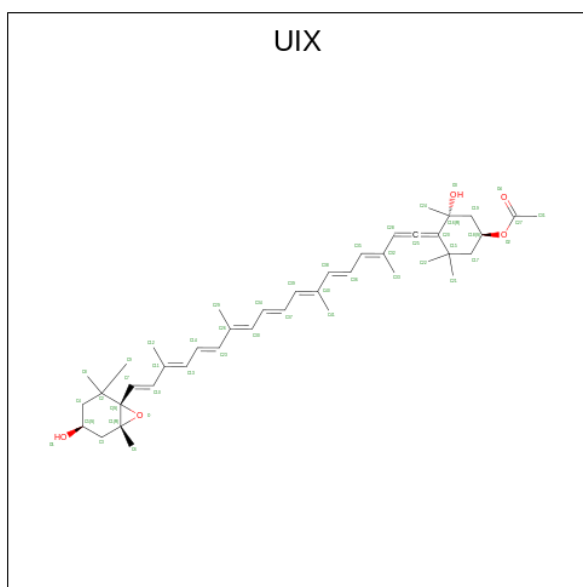
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	K	1	43	40	3	0
28	K	1	43	40	3	0
28	K	1	43	40	3	0
28	G	1	43	40	3	0
28	G	1	43	40	3	0
28	G	1	43	40	3	0
28	G	1	43	40	3	0
28	A	1	43	40	3	0
28	A	1	43	40	3	0
28	A	1	43	40	3	0
28	A	1	43	40	3	0
28	h	1	43	40	3	0
28	b	1	43	40	3	0
28	B	1	42	39	3	0
28	B	1	43	40	3	0
28	B	1	43	40	3	0
28	B	1	43	40	3	0
28	D	1	43	40	3	0
28	F	1	43	40	3	0
28	F	1	43	40	3	0
28	H	1	43	40	3	0

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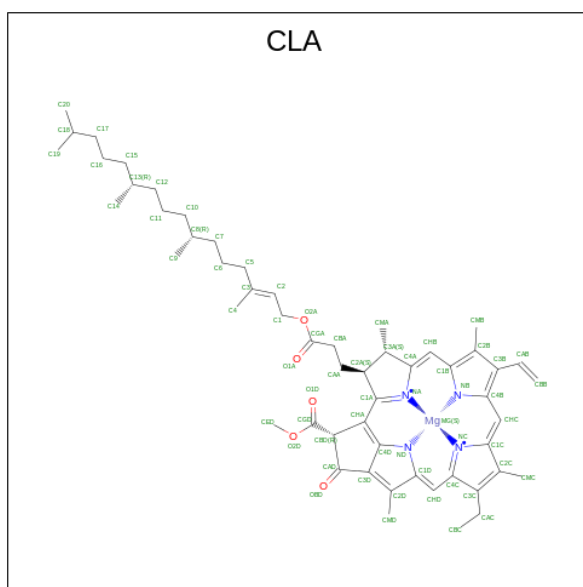
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	J	1	43	40	3	0
28	J	1	43	40	3	0
28	J	1	43	40	3	0
28	L	1	43	40	3	0
28	L	1	43	40	3	0
28	L	1	43	40	3	0
28	L	1	43	40	3	0
28	L	1	43	40	3	0
28	M	1	43	40	3	0
28	M	1	43	40	3	0
28	M	1	43	40	3	0
28	M	1	43	40	3	0
28	M	1	43	40	3	0
28	M	1	43	40	3	0
28	N	1	43	40	3	0
28	O	1	43	40	3	0
28	P	1	43	40	3	0

- Molecule 29 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyldene]cyclohexyl] ethanoate (three-letter code: UIX) (formula: C₄₂H₅₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	I	1	Total	C	O	0
			47	42	5	
29	K	1	Total	C	O	0
			47	42	5	
29	G	1	Total	C	O	0
			47	42	5	
29	A	1	Total	C	O	0
			47	42	5	
29	h	1	Total	C	O	0
			47	42	5	
29	B	1	Total	C	O	0
			47	42	5	
29	J	1	Total	C	O	0
			47	42	5	
29	O	1	Total	C	O	0
			47	42	5	
29	P	1	Total	C	O	0
			47	42	5	

- Molecule 30 is CHLOROPHYLL A (three-letter code: CLA) (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
30	I	1	49	39	1	4	5	0
30	I	1	46	36	1	4	5	0
30	I	1	60	50	1	4	5	0
30	I	1	55	45	1	4	5	0
30	I	1	48	38	1	4	5	0
30	I	1	55	45	1	4	5	0
30	I	1	65	55	1	4	5	0
30	I	1	55	45	1	4	5	0
30	I	1	52	42	1	4	5	0
30	I	1	55	45	1	4	5	0
30	I	1	45	35	1	4	5	0
30	I	1	52	42	1	4	5	0
30	K	1	49	39	1	4	5	0
30	K	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	K	1	54	44	1	4	5	0
30	K	1	50	40	1	4	5	0
30	K	1	55	45	1	4	5	0
30	K	1	52	42	1	4	5	0
30	K	1	48	38	1	4	5	0
30	K	1	55	45	1	4	5	0
30	K	1	41	33	1	4	3	0
30	K	1	46	36	1	4	5	0
30	G	1	51	41	1	4	5	0
30	G	1	65	55	1	4	5	0
30	G	1	55	45	1	4	5	0
30	G	1	60	50	1	4	5	0
30	G	1	65	55	1	4	5	0
30	G	1	53	43	1	4	5	0
30	G	1	41	33	1	4	3	0
30	G	1	46	36	1	4	5	0
30	G	1	46	36	1	4	5	0
30	G	1	61	51	1	4	5	0
30	G	1	49	39	1	4	5	0
30	A	1	45	35	1	4	5	0
30	A	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	A	1	55	45	1	4	5	0
30	A	1	65	55	1	4	5	0
30	A	1	46	36	1	4	5	0
30	A	1	55	45	1	4	5	0
30	A	1	55	45	1	4	5	0
30	A	1	41	33	1	4	3	0
30	A	1	47	37	1	4	5	0
30	A	1	41	33	1	4	3	0
30	A	1	46	36	1	4	5	0
30	A	1	46	36	1	4	5	0
30	f	1	55	45	1	4	5	0
30	f	1	46	36	1	4	5	0
30	f	1	46	36	1	4	5	0
30	h	1	55	45	1	4	5	0
30	j	1	55	45	1	4	5	0
30	j	1	58	48	1	4	5	0
30	l	1	65	55	1	4	5	0
30	l	1	60	50	1	4	5	0
30	l	1	65	55	1	4	5	0
30	l	1	41	33	1	4	3	0
30	l	1	41	33	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O		
30	l	1	Total 45	C 36	N 4	O 5	0	
30	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	l	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
30	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	b	1	48	38	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	60	50	1	4	5	0
30	b	1	52	42	1	4	5	0
30	b	1	55	45	1	4	5	0
30	b	1	54	44	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	46	36	1	4	5	0
30	b	1	60	50	1	4	5	0
30	b	1	50	40	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	51	41	1	4	5	0
30	b	1	46	36	1	4	5	0
30	b	1	53	43	1	4	5	0
30	b	1	46	36	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	50	40	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	47	37	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	b	1	65	55	1	4	5	0
30	b	1	65	55	1	4	5	0
30	B	1	60	50	1	4	5	0
30	B	1	49	39	1	4	5	0
30	B	1	45	35	1	4	5	0
30	B	1	65	55	1	4	5	0
30	B	1	55	45	1	4	5	0
30	B	1	65	55	1	4	5	0
30	B	1	51	41	1	4	5	0
30	B	1	65	55	1	4	5	0
30	B	1	41	33	1	4	3	0
30	B	1	46	36	1	4	5	0
30	B	1	45	35	1	4	5	0
30	D	1	47	37	1	4	5	0
30	D	1	46	36	1	4	5	0
30	D	1	46	36	1	4	5	0
30	D	1	46	36	1	4	5	0
30	D	1	45	35	1	4	5	0
30	D	1	46	36	1	4	5	0
30	D	1	41	33	1	4	3	0
30	F	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	F	1	46	36	1	4	5	0
30	F	1	46	36	1	4	5	0
30	F	1	46	36	1	4	5	0
30	F	1	46	36	1	4	5	0
30	F	1	46	36	1	4	5	0
30	F	1	41	33	1	4	3	0
30	H	1	47	37	1	4	5	0
30	H	1	65	55	1	4	5	0
30	H	1	51	41	1	4	5	0
30	H	1	46	36	1	4	5	0
30	H	1	47	37	1	4	5	0
30	H	1	41	33	1	4	3	0
30	H	1	46	36	1	4	5	0
30	J	1	60	50	1	4	5	0
30	J	1	46	36	1	4	5	0
30	J	1	65	55	1	4	5	0
30	J	1	46	36	1	4	5	0
30	J	1	56	46	1	4	5	0
30	J	1	46	36	1	4	5	0
30	J	1	47	37	1	4	5	0
30	J	1	53	43	1	4	5	0

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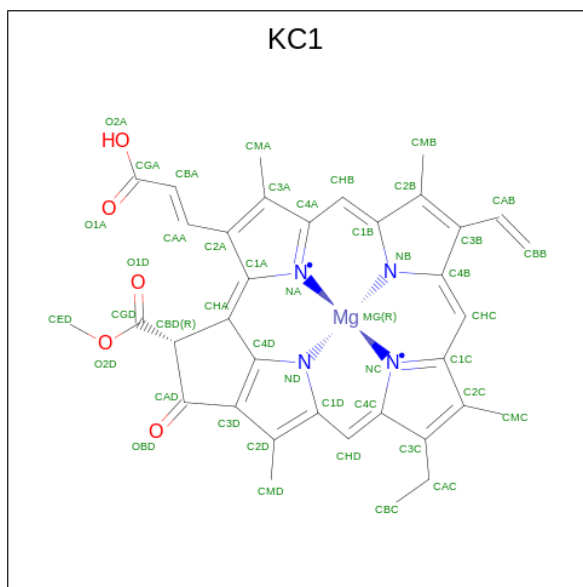
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	J	1	41	33	1	4	3	0
30	J	1	46	36	1	4	5	0
30	J	1	46	36	1	4	5	0
30	L	1	47	39	1	4	3	0
30	L	1	53	43	1	4	5	0
30	L	1	55	45	1	4	5	0
30	L	1	55	45	1	4	5	0
30	L	1	46	36	1	4	5	0
30	L	1	55	45	1	4	5	0
30	L	1	53	43	1	4	5	0
30	L	1	41	33	1	4	3	0
30	L	1	52	42	1	4	5	0
30	L	1	46	36	1	4	5	0
30	M	1	53	43	1	4	5	0
30	M	1	55	45	1	4	5	0
30	M	1	48	38	1	4	5	0
30	M	1	46	36	1	4	5	0
30	M	1	48	38	1	4	5	0
30	M	1	46	36	1	4	5	0
30	M	1	41	33	1	4	3	0
30	M	1	52	42	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	M	1	46	36	1	4	5	0
30	M	1	46	36	1	4	5	0
30	N	1	47	37	1	4	5	0
30	N	1	65	55	1	4	5	0
30	N	1	51	41	1	4	5	0
30	N	1	46	36	1	4	5	0
30	N	1	47	37	1	4	5	0
30	O	1	47	37	1	4	5	0
30	O	1	65	55	1	4	5	0
30	O	1	51	41	1	4	5	0
30	O	1	46	36	1	4	5	0
30	O	1	47	37	1	4	5	0
30	O	1	41	33	1	4	3	0
30	P	1	47	37	1	4	5	0
30	P	1	65	55	1	4	5	0
30	P	1	51	41	1	4	5	0
30	P	1	46	36	1	4	5	0
30	P	1	47	37	1	4	5	0
30	P	1	41	33	1	4	3	0

- Molecule 31 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



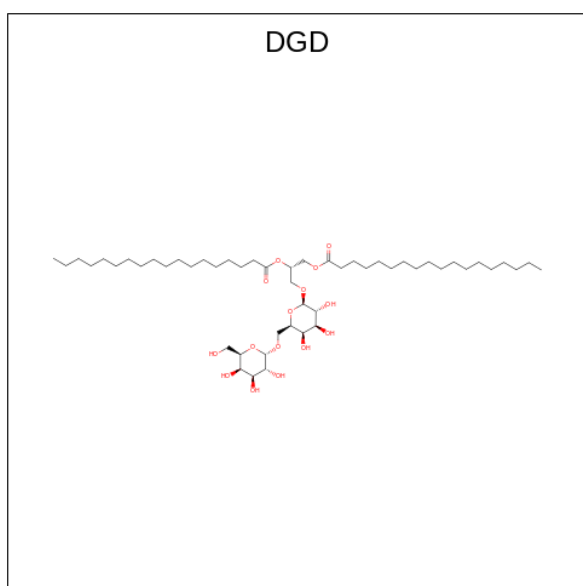
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
31	I	1	45	35	1	4	5	0
31	K	1	45	35	1	4	5	0
31	G	1	45	35	1	4	5	0
31	A	1	45	35	1	4	5	0
31	A	1	45	35	1	4	5	0
31	B	1	45	35	1	4	5	0
31	D	1	45	35	1	4	5	0
31	D	1	45	35	1	4	5	0
31	F	1	45	35	1	4	5	0
31	F	1	45	35	1	4	5	0
31	H	1	45	35	1	4	5	0
31	H	1	45	35	1	4	5	0
31	J	1	45	35	1	4	5	0
31	L	1	45	35	1	4	5	0

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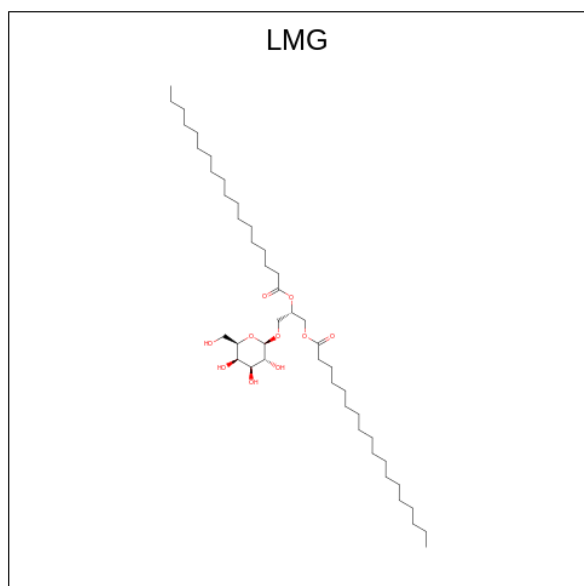
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	P	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	I	1	39	24	15	0
32	y	1	54	39	15	0
32	G	1	45	30	15	0
32	G	1	44	29	15	0
32	j	1	41	26	15	0
32	l	1	50	35	15	0
32	L	1	38	23	15	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



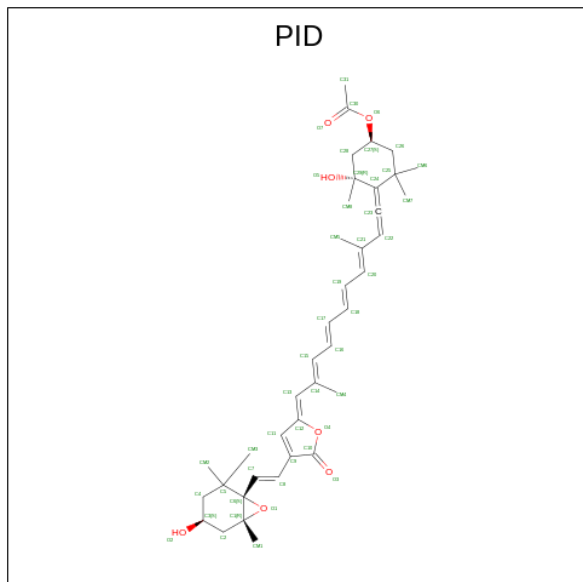
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	I	1	36	26	10	0
33	I	1	38	28	10	0
33	K	1	43	33	10	0
33	j	1	35	25	10	0

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Mol	Chain	Residues	Atoms			AltConf
33	b	1	Total	C	O	0
			44	34	10	
33	b	1	Total	C	O	0
			31	21	10	
33	B	1	Total	C	O	0
			37	27	10	
33	D	1	Total	C	O	0
			49	39	10	
33	P	1	Total	C	O	0
			27	17	10	

- Molecule 34 is PERIDININ (three-letter code: PID) (formula: C₃₉H₅₀O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	G	1	Total	C	O	0
			46	39	7	
34	G	1	Total	C	O	0
			46	39	7	
34	j	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	

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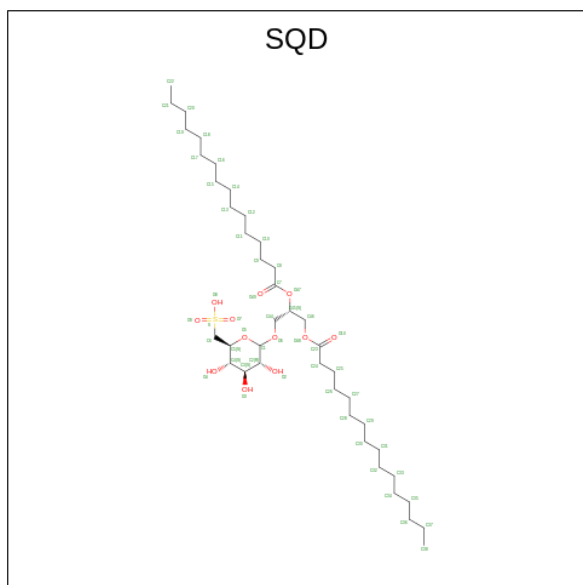
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	D	1	46	39	7	0
34	D	1	46	39	7	0
34	D	1	46	39	7	0
34	F	1	46	39	7	0
34	F	1	46	39	7	0
34	F	1	46	39	7	0
34	F	1	46	39	7	0
34	H	1	46	39	7	0
34	H	1	46	39	7	0
34	M	1	46	39	7	0
34	N	1	46	39	7	0
34	N	1	46	39	7	0
34	O	1	46	39	7	0
34	O	1	46	39	7	0
34	O	1	46	39	7	0
34	O	1	46	39	7	0
34	O	1	46	39	7	0
34	P	1	46	39	7	0
34	P	1	46	39	7	0
34	P	1	46	39	7	0
34	P	1	46	39	7	0

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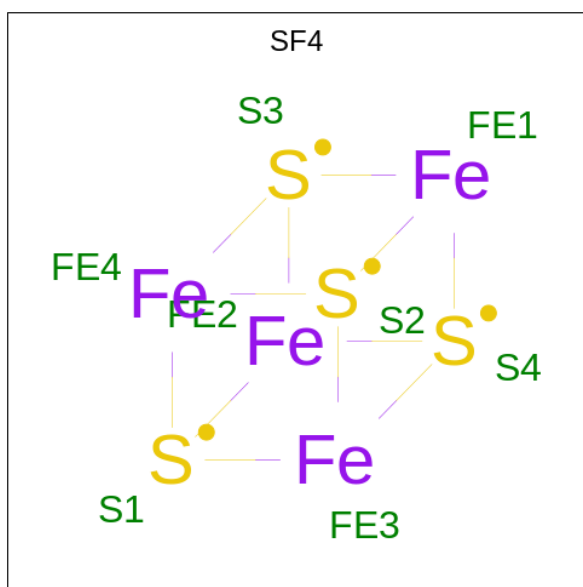
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	P	1	46	39	7	0

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



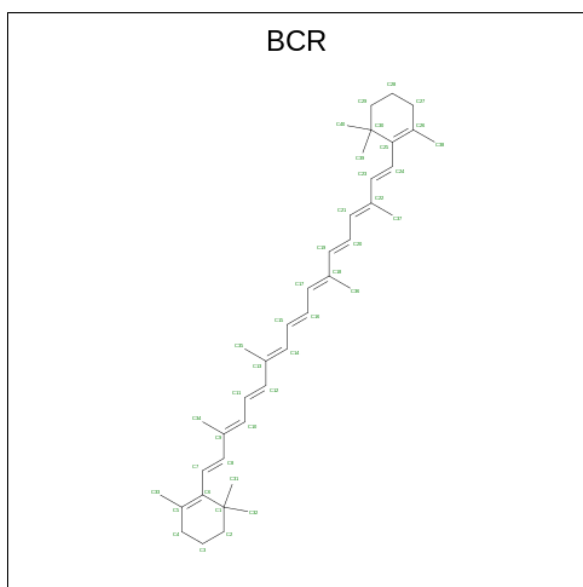
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
35	A	1	50	37	12	1	0

- Molecule 36 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms		AltConf
36	c	1	Total	Fe S	0
			8	4 4	
36	c	1	Total	Fe S	0
			8	4 4	
36	a	1	Total	Fe S	0
			8	4 4	

- Molecule 37 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



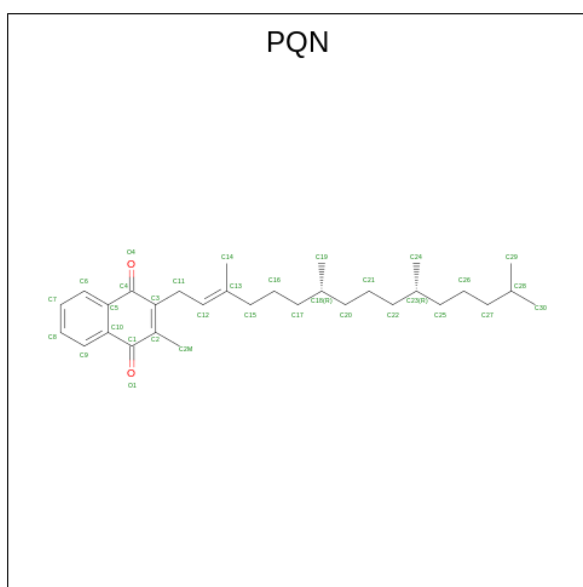
Mol	Chain	Residues	Atoms		AltConf
37	f	1	Total	C	0
			40	40	

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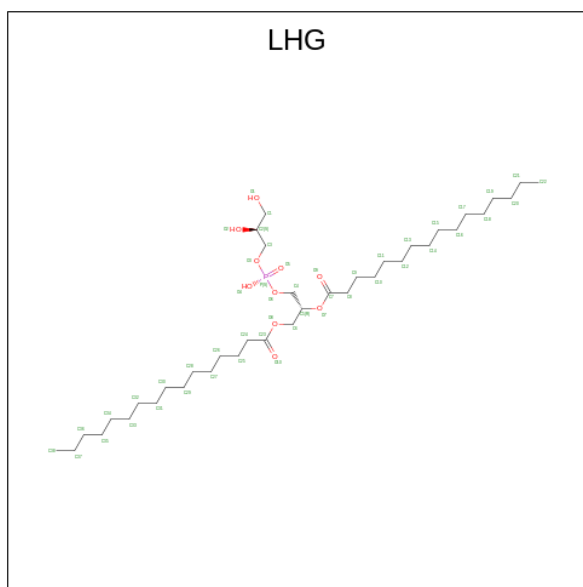
Mol	Chain	Residues	Atoms	AltConf
37	i	1	Total C 40 40	0
37	j	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	m	1	Total C 40 40	0
37	a	1	Total C 40 40	0
37	a	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	b	1	Total C 40 40	0

- Molecule 38 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

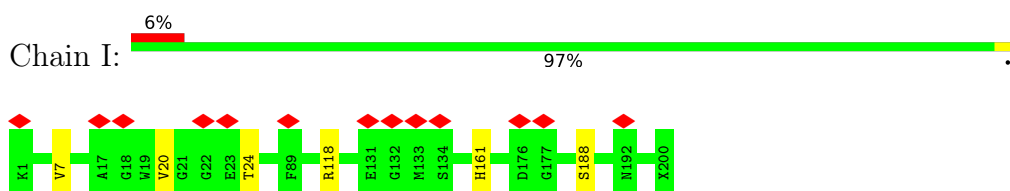


Mol	Chain	Residues	Atoms				AltConf
39	a	1	Total	C	O	P	0
			48	37	10	1	

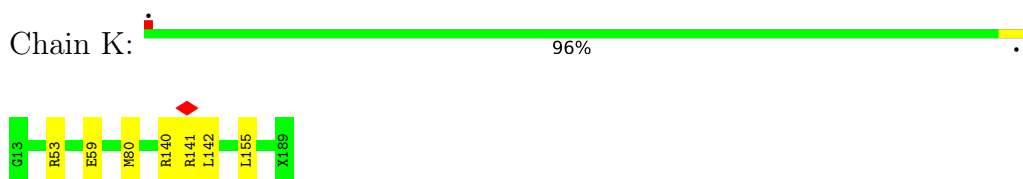
3 Residue-property plots [i](#)

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: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7



- Molecule 2: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6

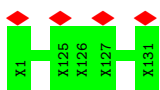


- Molecule 3: Photosystem I unk

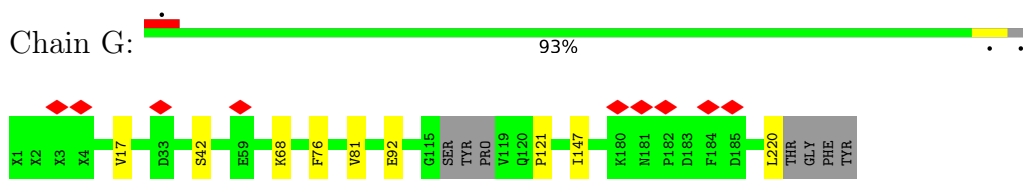


There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem I unk

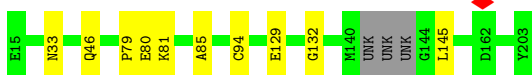


- Molecule 5: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8



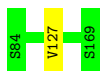
- Molecule 6: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10

Chain A:  93% 5%



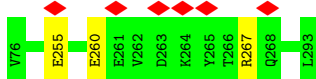
- Molecule 7: Photosystem I PsaC

Chain c:  99%



- Molecule 8: Photosystem I PsaD

Chain d:  99%



- Molecule 9: Photosystem I PsaE

Chain e:  100%

There are no outlier residues recorded for this chain.

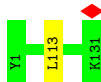
- Molecule 10: Photosystem I PsaF

Chain f:  97%



- Molecule 11: Photosystem I PsaR

Chain h:  99%



- Molecule 12: Photosystem I PsaI

Chain i:  99%



- Molecule 13: Photosystem I PsaJ

Chain j:  96%



- Molecule 14: Photosystem I PsaL

Chain l:  97%



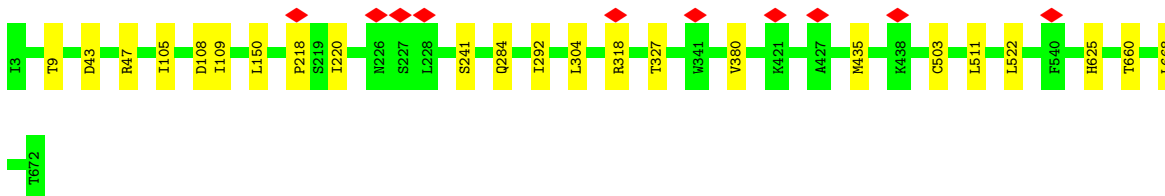
- Molecule 15: Photosystem I PsaM

Chain m:  99%



- Molecule 16: Photosystem I PsaA

Chain a:  97%



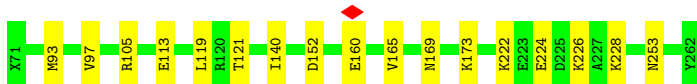
- Molecule 17: Photosystem I PsaB

Chain b:  97%




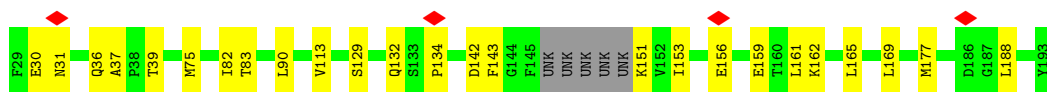
- Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11

Chain B:  91%

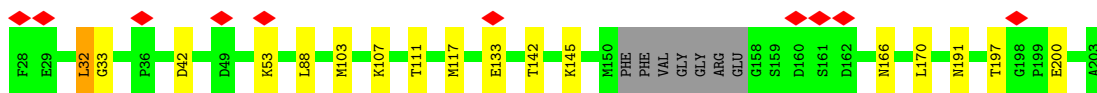
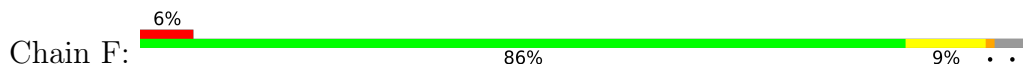


- Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9

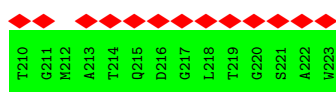
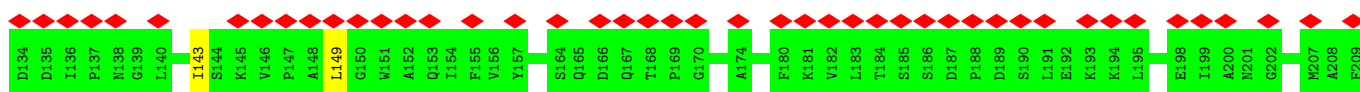
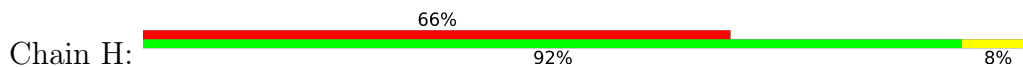
Chain D:  82%



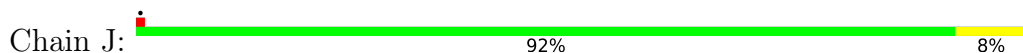
- Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2



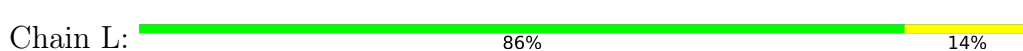
- Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12



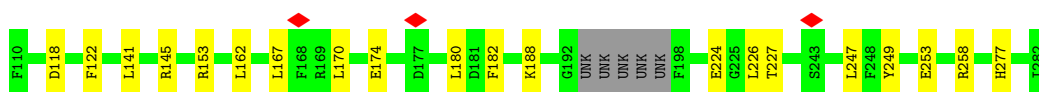
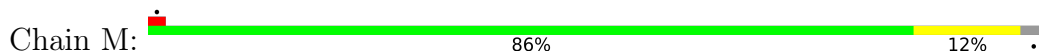
- Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3



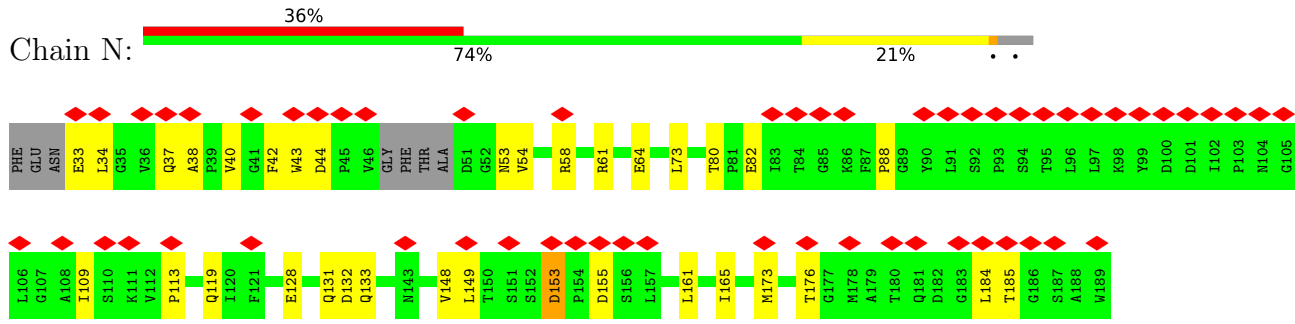
- Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5



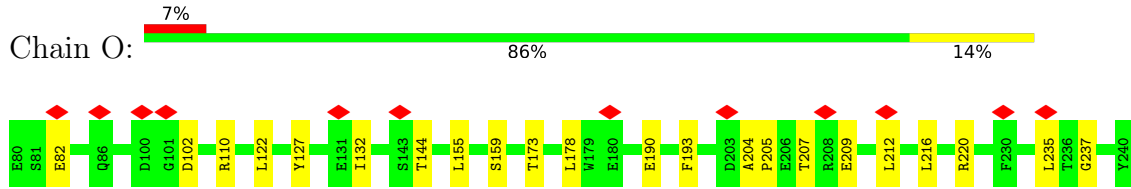
- Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4



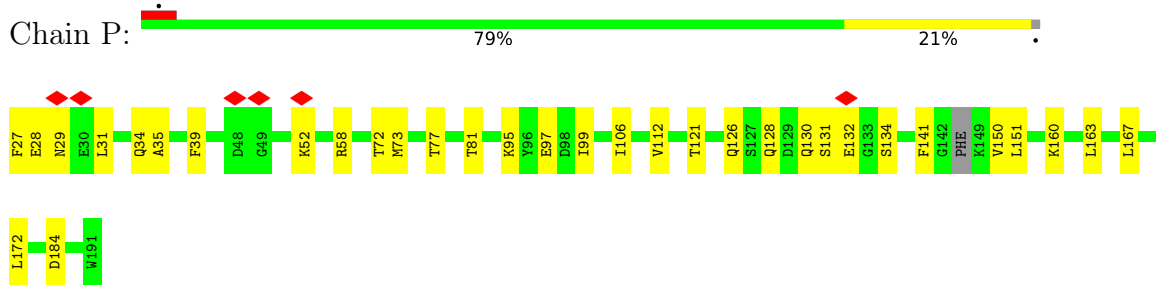
- Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13



- Molecule 26: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15



- Molecule 27: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46321	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.690	Depositor
Minimum map value	-0.344	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.235	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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, LHG, DGD, SF4, BCR, PID, KC1, SQD, DD6, LMG, UIX, CLA

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	I	0.27	0/1484	0.46	0/2019
2	K	0.27	0/1357	0.48	0/1838
5	G	0.32	0/1562	0.48	0/2122
6	A	0.33	0/1276	0.48	0/1725
7	c	0.26	0/663	0.51	0/902
8	d	0.26	0/1767	0.50	0/2375
9	e	0.33	0/608	0.42	0/833
10	f	0.26	0/1489	0.47	0/2016
11	h	0.26	0/1101	0.40	0/1493
12	i	0.26	0/992	0.48	0/1346
13	j	0.26	0/801	0.45	0/1092
14	l	0.28	0/1998	0.45	0/2706
15	m	0.27	0/590	0.48	0/793
16	a	0.30	0/5344	0.47	0/7280
17	b	0.28	0/5362	0.44	0/7335
18	B	0.27	0/1382	0.46	0/1862
19	D	0.29	0/1178	0.50	0/1592
20	F	0.28	0/1263	0.51	0/1708
21	H	0.27	0/1232	0.49	0/1665
22	J	0.27	0/1246	0.45	0/1699
23	L	0.29	0/1462	0.47	0/1985
24	M	0.27	0/1241	0.46	0/1681
25	N	0.27	0/1005	0.53	0/1370
26	O	0.25	0/1091	0.49	0/1491
27	P	0.30	0/1128	0.47	0/1523
All	All	0.28	0/38622	0.47	0/52451

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	I	191/200 (96%)	163 (85%)	28 (15%)	0	100	100
2	K	171/177 (97%)	160 (94%)	11 (6%)	0	100	100
5	G	204/224 (91%)	175 (86%)	27 (13%)	2 (1%)	15	53
6	A	162/189 (86%)	144 (89%)	14 (9%)	4 (2%)	5	28
7	c	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
8	d	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
9	e	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	f	182/184 (99%)	177 (97%)	4 (2%)	1 (0%)	29	68
11	h	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
12	i	117/119 (98%)	105 (90%)	12 (10%)	0	100	100
13	j	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
14	l	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	34	72
15	m	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
16	a	668/670 (100%)	622 (93%)	43 (6%)	3 (0%)	34	72
17	b	661/663 (100%)	613 (93%)	47 (7%)	1 (0%)	47	82
18	B	171/192 (89%)	153 (90%)	15 (9%)	3 (2%)	8	37
19	D	156/165 (94%)	131 (84%)	22 (14%)	3 (2%)	8	36
20	F	165/176 (94%)	153 (93%)	10 (6%)	2 (1%)	13	48
21	H	158/160 (99%)	140 (89%)	16 (10%)	2 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	J	164/220 (74%)	146 (89%)	17 (10%)	1 (1%)	25	64
23	L	183/185 (99%)	161 (88%)	22 (12%)	0	100	100
24	M	164/173 (95%)	151 (92%)	13 (8%)	0	100	100
25	N	149/160 (93%)	119 (80%)	24 (16%)	6 (4%)	3	17
26	O	159/161 (99%)	130 (82%)	25 (16%)	4 (2%)	5	28
27	P	155/160 (97%)	135 (87%)	19 (12%)	1 (1%)	25	64
All	All	4901/5113 (96%)	4446 (91%)	421 (9%)	34 (1%)	26	60

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	121	PRO
6	A	85	ALA
14	l	70	PRO
16	a	47	ARG
16	a	218	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	139/155 (90%)	133 (96%)	6 (4%)	29	66
2	K	133/138 (96%)	126 (95%)	7 (5%)	22	58
5	G	147/171 (86%)	140 (95%)	7 (5%)	25	62
6	A	122/129 (95%)	116 (95%)	6 (5%)	25	61
7	c	76/76 (100%)	75 (99%)	1 (1%)	69	89
8	d	182/184 (99%)	179 (98%)	3 (2%)	62	86
9	e	63/63 (100%)	63 (100%)	0	100	100
10	f	148/148 (100%)	144 (97%)	4 (3%)	44	77
11	h	112/114 (98%)	111 (99%)	1 (1%)	78	92
12	i	100/101 (99%)	99 (99%)	1 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	j	88/89 (99%)	84 (96%)	4 (4%)	27	64
14	l	199/201 (99%)	192 (96%)	7 (4%)	36	71
15	m	60/63 (95%)	59 (98%)	1 (2%)	60	85
16	a	540/592 (91%)	520 (96%)	20 (4%)	34	70
17	b	557/581 (96%)	539 (97%)	18 (3%)	39	74
18	B	142/146 (97%)	128 (90%)	14 (10%)	8	30
19	D	116/123 (94%)	94 (81%)	22 (19%)	1	8
20	F	126/140 (90%)	110 (87%)	16 (13%)	4	19
21	H	123/123 (100%)	113 (92%)	10 (8%)	11	40
22	J	124/136 (91%)	108 (87%)	16 (13%)	4	19
23	L	140/145 (97%)	115 (82%)	25 (18%)	2	9
24	M	106/128 (83%)	86 (81%)	20 (19%)	1	8
25	N	80/124 (64%)	51 (64%)	29 (36%)	0	1
26	O	89/124 (72%)	71 (80%)	18 (20%)	1	6
27	P	105/123 (85%)	73 (70%)	32 (30%)	0	1
All	All	3817/4117 (93%)	3529 (92%)	288 (8%)	17	43

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	N	155	ASP
27	P	172	LEU
26	O	82	GLU
27	P	34	GLN
18	B	226	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
27	P	128	GLN
23	L	268	GLN
19	D	55	ASN
16	a	284	GLN
20	F	166	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

342 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
30	CLA	G	516	5	41,49,73	1.88	5 (12%)	47,84,113	1.65	7 (14%)
30	CLA	I	319	30	45,53,73	1.77	6 (13%)	52,89,113	1.64	7 (13%)
30	CLA	B	312	-	51,59,73	1.69	5 (9%)	59,96,113	1.48	8 (13%)
30	CLA	j	106	-	58,66,73	1.58	6 (10%)	67,104,113	1.46	8 (11%)
30	CLA	A	320	-	46,54,73	1.78	6 (13%)	53,90,113	1.54	6 (11%)
30	CLA	b	726	-	47,55,73	1.77	5 (10%)	54,91,113	1.51	8 (14%)
34	PID	O	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.31	6 (12%)
29	UIX	B	305	-	41,49,49	1.25	3 (7%)	52,74,74	2.45	16 (30%)
37	BCR	i	201	-	41,41,41	0.82	2 (4%)	56,56,56	2.11	20 (35%)
30	CLA	K	312	-	48,56,73	1.72	7 (14%)	55,92,113	1.53	7 (12%)
30	CLA	A	317	-	41,49,73	1.86	5 (12%)	47,84,113	1.65	9 (19%)
30	CLA	a	726	-	65,73,73	1.51	7 (10%)	76,113,113	1.37	9 (11%)
30	CLA	F	311	-	46,54,73	1.77	5 (10%)	53,90,113	1.59	8 (15%)
28	DD6	D	303	-	39,45,45	1.96	2 (5%)	52,67,67	1.88	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	SQD	A	318	-	49,50,54	0.40	1 (2%)	58,61,65	0.59	0
30	CLA	A	313	-	55,63,73	1.60	5 (9%)	64,101,113	1.45	9 (14%)
34	PID	P	202	-	41,49,49	1.33	4 (9%)	49,76,76	1.60	7 (14%)
30	CLA	O	314	-	47,55,73	1.74	6 (12%)	54,91,113	1.66	8 (14%)
29	UIX	A	304	-	41,49,49	1.23	3 (7%)	52,74,74	2.44	20 (38%)
30	CLA	a	731	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	9 (11%)
30	CLA	N	307	-	51,59,73	1.73	6 (11%)	59,96,113	1.52	7 (11%)
30	CLA	I	315	-	52,60,73	1.68	5 (9%)	60,97,113	1.50	9 (15%)
28	DD6	H	303	-	39,45,45	1.97	3 (7%)	52,67,67	1.90	12 (23%)
30	CLA	O	311	-	51,59,73	1.67	5 (9%)	59,96,113	1.49	8 (13%)
28	DD6	B	306	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	19 (36%)
30	CLA	l	310	-	44,50,73	1.88	7 (15%)	48,76,113	1.38	8 (16%)
30	CLA	J	311	22	47,55,73	1.73	5 (10%)	54,91,113	1.60	8 (14%)
30	CLA	A	310	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
31	KC1	O	312	-	48,53,53	1.51	7 (14%)	55,89,89	1.87	12 (21%)
30	CLA	j	104	-	55,63,73	1.65	5 (9%)	64,101,113	1.43	9 (14%)
30	CLA	I	311	1	55,63,73	1.64	5 (9%)	64,101,113	1.46	9 (14%)
30	CLA	h	202	-	55,63,73	1.63	5 (9%)	64,101,113	1.45	8 (12%)
30	CLA	D	309	-	46,54,73	1.75	5 (10%)	53,90,113	1.60	7 (13%)
30	CLA	b	711	-	55,63,73	1.63	5 (9%)	64,101,113	1.43	8 (12%)
30	CLA	a	713	-	60,68,73	1.55	6 (10%)	70,107,113	1.41	9 (12%)
30	CLA	a	728	-	55,63,73	1.60	5 (9%)	64,101,113	1.47	9 (14%)
36	SF4	c	201	7	0,12,12	-	-	-	-	-
30	CLA	I	316	-	55,63,73	1.61	5 (9%)	64,101,113	1.51	9 (14%)
30	CLA	G	514	-	53,61,73	1.64	6 (11%)	61,98,113	1.52	9 (14%)
37	BCR	a	736	-	41,41,41	0.74	0	56,56,56	2.03	18 (32%)
30	CLA	G	518	-	46,54,73	1.79	5 (10%)	53,90,113	1.60	8 (15%)
31	KC1	D	315	19	48,53,53	1.49	7 (14%)	55,89,89	1.85	12 (21%)
30	CLA	B	316	-	46,54,73	1.77	5 (10%)	53,90,113	1.50	7 (13%)
34	PID	O	304	-	41,49,49	1.32	4 (9%)	49,76,76	1.73	8 (16%)
30	CLA	A	315	-	41,49,73	1.84	6 (14%)	47,84,113	1.66	8 (17%)
30	CLA	B	308	-	45,53,73	1.80	5 (11%)	52,89,113	1.61	8 (15%)
33	LMG	B	318	-	37,37,55	0.85	0	45,45,63	1.32	6 (13%)
32	DGD	G	501	-	46,46,67	1.02	2 (4%)	60,60,81	1.01	3 (5%)
28	DD6	M	302	-	39,45,45	2.17	4 (10%)	52,67,67	2.24	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	KC1	F	314	20	48,53,53	1.49	7 (14%)	55,89,89	1.88	10 (18%)
28	DD6	b	731	30	39,45,45	2.11	3 (7%)	52,67,67	1.96	15 (28%)
30	CLA	f	301	-	55,63,73	1.62	6 (10%)	64,101,113	1.44	8 (12%)
30	CLA	b	713	-	65,73,73	1.50	6 (9%)	76,113,113	1.34	7 (9%)
30	CLA	a	715	-	45,53,73	1.78	6 (13%)	52,89,113	1.61	7 (13%)
33	LMG	j	101	-	35,35,55	0.88	0	43,43,63	1.23	4 (9%)
30	CLA	B	310	-	55,63,73	1.63	5 (9%)	64,101,113	1.45	10 (15%)
30	CLA	G	513	5	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
31	KC1	M	307	30	48,53,53	1.51	7 (14%)	55,89,89	1.88	12 (21%)
30	CLA	P	217	-	41,49,73	1.85	7 (17%)	47,84,113	1.66	7 (14%)
30	CLA	M	318	-	46,54,73	1.78	5 (10%)	53,90,113	1.51	7 (13%)
29	UIX	G	503	-	41,49,49	1.23	3 (7%)	52,74,74	2.34	16 (30%)
30	CLA	G	510	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	8 (10%)
30	CLA	J	315	-	46,54,73	1.76	5 (10%)	53,90,113	1.56	7 (13%)
28	DD6	A	303	-	39,45,45	1.94	2 (5%)	52,67,67	1.87	13 (25%)
31	KC1	P	211	-	48,53,53	1.51	7 (14%)	55,89,89	1.89	11 (20%)
31	KC1	D	310	-	48,53,53	1.51	7 (14%)	55,89,89	1.87	11 (20%)
30	CLA	a	725	-	61,69,73	1.55	5 (8%)	71,108,113	1.40	9 (12%)
31	KC1	O	310	-	48,53,53	1.49	7 (14%)	55,89,89	1.89	11 (20%)
34	PID	G	506	-	41,49,49	1.34	4 (9%)	49,76,76	1.38	6 (12%)
30	CLA	M	310	-	48,56,73	1.73	5 (10%)	55,92,113	1.56	8 (14%)
28	DD6	G	502	-	39,45,45	1.99	2 (5%)	52,67,67	1.94	16 (30%)
30	CLA	a	738	22	46,54,73	1.78	5 (10%)	53,90,113	1.58	7 (13%)
30	CLA	J	316	-	46,54,73	1.78	5 (10%)	53,90,113	1.52	7 (13%)
30	CLA	a	716	-	47,55,73	1.76	5 (10%)	54,91,113	1.54	8 (14%)
30	CLA	I	307	-	46,54,73	1.77	5 (10%)	53,90,113	1.53	6 (11%)
30	CLA	B	317	-	45,53,73	1.80	6 (13%)	52,89,113	1.59	7 (13%)
30	CLA	A	308	-	55,63,73	1.60	5 (9%)	64,101,113	1.49	8 (12%)
33	LMG	b	733	-	44,44,55	0.81	1 (2%)	52,52,63	1.30	6 (11%)
30	CLA	O	308	-	47,55,73	1.76	5 (10%)	54,91,113	1.53	8 (14%)
30	CLA	D	314	-	46,54,73	1.80	6 (13%)	53,90,113	1.59	9 (16%)
28	DD6	A	305	31	39,45,45	1.99	2 (5%)	52,67,67	1.96	14 (26%)
32	DGD	y	201	-	55,55,67	0.92	2 (3%)	69,69,81	0.97	3 (4%)
30	CLA	a	704	-	65,73,73	1.51	6 (9%)	76,113,113	1.35	6 (7%)
30	CLA	b	701	-	65,73,73	1.50	6 (9%)	76,113,113	1.40	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DD6	J	302	-	39,45,45	2.02	2 (5%)	52,67,67	2.11	15 (28%)
30	CLA	I	310	-	48,56,73	1.71	5 (10%)	55,92,113	1.61	7 (12%)
28	DD6	K	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.69	10 (19%)
28	DD6	N	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.09	16 (30%)
28	DD6	M	306	-	39,45,45	2.17	3 (7%)	52,67,67	2.24	18 (34%)
37	BCR	a	734	-	41,41,41	0.71	0	56,56,56	2.07	19 (33%)
37	BCR	b	702	-	41,41,41	0.73	0	56,56,56	2.17	17 (30%)
30	CLA	O	313	-	46,54,73	1.72	6 (13%)	53,90,113	1.57	6 (11%)
30	CLA	a	706	16	58,66,73	1.57	6 (10%)	67,104,113	1.47	7 (10%)
29	UIX	I	304	-	41,49,49	1.32	4 (9%)	52,74,74	2.59	14 (26%)
30	CLA	H	309	-	47,55,73	1.75	5 (10%)	54,91,113	1.55	8 (14%)
28	DD6	G	504	-	39,45,45	2.24	5 (12%)	52,67,67	2.19	19 (36%)
30	CLA	B	313	18	65,73,73	1.48	5 (7%)	76,113,113	1.39	7 (9%)
30	CLA	a	719	-	47,55,73	1.76	7 (14%)	54,91,113	1.51	7 (12%)
31	KC1	A	306	28,30	48,53,53	1.49	7 (14%)	55,89,89	1.81	11 (20%)
28	DD6	B	303	-	39,45,45	2.00	2 (5%)	52,67,67	2.00	17 (32%)
30	CLA	a	707	-	65,73,73	1.52	5 (7%)	76,113,113	1.32	8 (10%)
30	CLA	M	309	24	55,63,73	1.62	5 (9%)	64,101,113	1.45	8 (12%)
31	KC1	N	306	-	48,53,53	1.50	7 (14%)	55,89,89	1.84	11 (20%)
31	KC1	P	213	-	48,53,53	1.48	7 (14%)	55,89,89	1.86	12 (21%)
31	KC1	K	314	2	48,53,53	1.50	7 (14%)	55,89,89	1.84	10 (18%)
30	CLA	b	719	-	46,54,73	1.79	5 (10%)	53,90,113	1.61	7 (13%)
31	KC1	P	216	27	48,53,53	1.51	7 (14%)	55,89,89	1.83	10 (18%)
30	CLA	l	309	-	41,49,73	1.85	5 (12%)	47,84,113	1.65	8 (17%)
30	CLA	H	305	-	65,73,73	1.49	5 (7%)	76,113,113	1.42	9 (11%)
30	CLA	K	309	-	50,58,73	1.67	5 (10%)	58,95,113	1.57	8 (13%)
30	CLA	J	309	-	56,64,73	1.59	5 (8%)	65,102,113	1.52	9 (13%)
28	DD6	L	303	-	39,45,45	1.98	2 (5%)	52,67,67	1.99	14 (26%)
34	PID	O	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.58	8 (16%)
30	CLA	L	313	-	55,63,73	1.62	5 (9%)	64,101,113	1.44	8 (12%)
28	DD6	F	301	-	39,45,45	1.99	2 (5%)	52,67,67	2.34	18 (34%)
30	CLA	H	304	-	47,55,73	1.76	5 (10%)	54,91,113	1.51	7 (12%)
30	CLA	l	304	-	60,68,73	1.54	5 (8%)	70,107,113	1.48	6 (8%)
30	CLA	O	316	-	41,49,73	1.86	5 (12%)	47,84,113	1.70	7 (14%)
28	DD6	M	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.89	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PID	F	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.77	7 (14%)
30	CLA	N	309	25	46,54,73	1.74	7 (15%)	53,90,113	1.59	6 (11%)
30	CLA	a	717	-	57,65,73	1.60	6 (10%)	66,103,113	1.45	9 (13%)
30	CLA	a	714	-	45,53,73	1.79	5 (11%)	52,89,113	1.61	7 (13%)
30	CLA	a	708	-	51,59,73	1.69	5 (9%)	59,96,113	1.50	8 (13%)
30	CLA	a	721	-	65,73,73	1.49	5 (7%)	76,113,113	1.35	9 (11%)
37	BCR	b	730	-	41,41,41	0.75	0	56,56,56	2.25	20 (35%)
28	DD6	K	305	-	39,45,45	1.98	3 (7%)	52,67,67	1.85	13 (25%)
37	BCR	l	307	-	41,41,41	0.72	0	56,56,56	2.01	19 (33%)
30	CLA	l	313	14	65,73,73	1.51	5 (7%)	76,113,113	1.40	8 (10%)
30	CLA	H	308	-	46,54,73	1.77	6 (13%)	53,90,113	1.55	6 (11%)
30	CLA	I	312	-	65,73,73	1.50	6 (9%)	76,113,113	1.34	8 (10%)
30	CLA	B	301	-	60,68,73	1.56	5 (8%)	70,107,113	1.37	8 (11%)
30	CLA	K	315	-	41,49,73	1.84	6 (14%)	47,84,113	1.71	9 (19%)
30	CLA	H	311	-	41,49,73	1.89	6 (14%)	47,84,113	1.63	8 (17%)
33	LMG	D	317	-	48,48,55	0.76	1 (2%)	55,55,63	1.28	5 (9%)
30	CLA	f	302	-	46,54,73	1.75	5 (10%)	53,90,113	1.59	7 (13%)
30	CLA	a	723	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
30	CLA	G	512	-	60,68,73	1.54	6 (10%)	70,107,113	1.44	8 (11%)
29	UIX	P	207	-	41,49,49	1.28	4 (9%)	52,74,74	2.78	20 (38%)
30	CLA	J	301	-	60,68,73	1.55	5 (8%)	70,107,113	1.39	8 (11%)
34	PID	O	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.32	5 (10%)
30	CLA	D	311	-	46,54,73	1.76	5 (10%)	53,90,113	1.57	7 (13%)
30	CLA	M	316	-	52,60,73	1.68	6 (11%)	60,97,113	1.47	6 (10%)
34	PID	D	302	-	41,49,49	1.35	4 (9%)	49,76,76	1.44	7 (14%)
30	CLA	J	310	-	46,54,73	1.81	6 (13%)	53,90,113	1.56	6 (11%)
30	CLA	M	315	-	41,49,73	1.83	5 (12%)	47,84,113	1.76	9 (19%)
34	PID	P	205	-	41,49,49	1.32	4 (9%)	49,76,76	1.70	6 (12%)
31	KC1	F	309	20	48,53,53	1.50	7 (14%)	55,89,89	1.92	12 (21%)
33	LMG	b	734	-	31,31,55	0.99	0	39,39,63	1.17	3 (7%)
30	CLA	l	303	14	65,73,73	1.53	5 (7%)	76,113,113	1.38	9 (11%)
30	CLA	a	724	-	65,73,73	1.50	6 (9%)	76,113,113	1.43	9 (11%)
30	CLA	b	714	-	46,54,73	1.75	5 (10%)	53,90,113	1.60	7 (13%)
30	CLA	b	720	-	53,61,73	1.63	5 (9%)	61,98,113	1.50	8 (13%)
30	CLA	l	305	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DD6	B	302	-	38,44,45	2.18	3 (7%)	50,65,67	2.12	20 (40%)
31	KC1	N	311	25	48,53,53	1.49	6 (12%)	55,89,89	1.85	11 (20%)
39	LHG	a	733	-	47,47,48	0.27	0	50,53,54	0.33	0
34	PID	F	302	-	41,49,49	1.33	4 (9%)	49,76,76	1.66	6 (12%)
30	CLA	H	307	-	51,59,73	1.68	5 (9%)	59,96,113	1.53	8 (13%)
30	CLA	P	215	-	47,55,73	1.74	5 (10%)	54,91,113	1.68	8 (14%)
30	CLA	F	308	-	46,54,73	1.75	6 (13%)	53,90,113	1.56	7 (13%)
30	CLA	K	313	-	55,63,73	1.61	5 (9%)	64,101,113	1.51	8 (12%)
28	DD6	G	508	-	39,45,45	2.04	3 (7%)	52,67,67	2.02	13 (25%)
30	CLA	l	308	-	41,49,73	1.86	5 (12%)	47,84,113	1.64	8 (17%)
30	CLA	b	716	-	50,58,73	1.70	5 (10%)	58,95,113	1.56	8 (13%)
30	CLA	K	310	-	55,63,73	1.62	6 (10%)	64,101,113	1.46	8 (12%)
30	CLA	A	311	6	46,54,73	1.77	5 (10%)	53,90,113	1.55	7 (13%)
30	CLA	a	709	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)
30	CLA	I	313	-	55,63,73	1.60	5 (9%)	64,101,113	1.51	8 (12%)
30	CLA	a	703	-	55,63,73	1.56	10 (18%)	64,101,113	1.59	9 (14%)
30	CLA	b	723	-	50,58,73	1.70	5 (10%)	58,95,113	1.51	10 (17%)
30	CLA	L	308	31	46,55,73	1.75	5 (10%)	55,91,113	1.53	10 (18%)
30	CLA	D	313	19	45,53,73	1.77	6 (13%)	52,89,113	1.59	7 (13%)
28	DD6	M	303	-	39,45,45	2.20	4 (10%)	52,67,67	2.20	19 (36%)
28	DD6	O	303	-	39,45,45	2.01	3 (7%)	52,67,67	2.01	14 (26%)
34	PID	P	203	-	41,49,49	1.33	4 (9%)	49,76,76	1.37	5 (10%)
34	PID	O	301	-	41,49,49	1.32	4 (9%)	49,76,76	1.53	5 (10%)
31	KC1	J	313	-	48,53,53	1.50	7 (14%)	55,89,89	1.83	9 (16%)
30	CLA	I	306	1	49,57,73	1.71	5 (10%)	55,93,113	1.57	8 (14%)
30	CLA	b	704	-	65,73,73	1.45	10 (15%)	76,113,113	1.43	9 (11%)
30	CLA	D	312	19	46,54,73	1.77	5 (10%)	53,90,113	1.49	6 (11%)
33	LMG	I	318	-	36,36,55	0.90	1 (2%)	44,44,63	1.24	3 (6%)
30	CLA	L	309	-	53,61,73	1.66	5 (9%)	61,98,113	1.51	9 (14%)
30	CLA	b	728	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
31	KC1	M	314	24	48,53,53	1.51	7 (14%)	55,89,89	1.87	11 (20%)
30	CLA	b	727	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)
33	LMG	P	201	-	27,27,55	1.00	0	35,35,63	1.19	4 (11%)
30	CLA	A	307	31	45,53,73	1.81	5 (11%)	52,89,113	1.59	6 (11%)
30	CLA	b	707	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	UIX	h	201	-	41,49,49	1.28	3 (7%)	52,74,74	2.48	19 (36%)
31	KC1	H	306	-	48,53,53	1.53	7 (14%)	55,89,89	1.87	11 (20%)
34	PID	P	206	-	41,49,49	1.33	4 (9%)	49,76,76	1.86	9 (18%)
30	CLA	D	316	-	41,49,73	1.85	6 (14%)	47,84,113	1.65	8 (17%)
30	CLA	F	312	-	46,54,73	1.69	10 (21%)	53,90,113	1.51	6 (11%)
38	PQN	b	729	-	34,34,34	1.55	2 (5%)	42,45,45	1.23	4 (9%)
28	DD6	L	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.95	12 (23%)
30	CLA	K	307	-	46,54,73	1.71	5 (10%)	53,90,113	1.60	6 (11%)
30	CLA	F	315	-	41,49,73	1.84	5 (12%)	47,84,113	1.72	8 (17%)
30	CLA	b	708	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	9 (11%)
31	KC1	L	315	-	48,53,53	1.50	7 (14%)	55,89,89	1.90	11 (20%)
34	PID	M	301	-	41,49,49	1.33	4 (9%)	49,76,76	1.74	8 (16%)
30	CLA	b	715	-	60,68,73	1.55	5 (8%)	70,107,113	1.43	8 (11%)
30	CLA	F	313	-	46,54,73	1.75	6 (13%)	53,90,113	1.64	7 (13%)
29	UIX	J	305	-	41,49,49	1.25	3 (7%)	52,74,74	2.46	17 (32%)
30	CLA	J	314	-	41,49,73	1.85	5 (12%)	47,84,113	1.67	8 (17%)
30	CLA	G	517	-	46,54,73	1.76	5 (10%)	53,90,113	1.55	7 (13%)
30	CLA	b	706	-	48,56,73	1.74	5 (10%)	55,92,113	1.57	8 (14%)
30	CLA	N	310	-	47,55,73	1.75	5 (10%)	54,91,113	1.65	8 (14%)
30	CLA	f	303	10	46,54,73	1.75	5 (10%)	53,90,113	1.55	7 (13%)
31	KC1	A	314	6	48,53,53	1.52	7 (14%)	55,89,89	1.88	12 (21%)
30	CLA	a	730	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
28	DD6	G	505	-	39,45,45	2.26	4 (10%)	52,67,67	2.31	21 (40%)
30	CLA	B	315	-	41,49,73	1.84	6 (14%)	47,84,113	1.70	7 (14%)
30	CLA	B	307	18	49,57,73	1.74	5 (10%)	55,93,113	1.52	8 (14%)
30	CLA	P	214	-	46,54,73	1.72	6 (13%)	53,90,113	1.55	6 (11%)
34	PID	D	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.78	7 (14%)
37	BCR	f	304	-	41,41,41	0.72	0	56,56,56	2.07	17 (30%)
30	CLA	A	309	-	55,63,73	1.61	5 (9%)	64,101,113	1.48	8 (12%)
30	CLA	A	319	-	46,54,73	1.77	6 (13%)	53,90,113	1.49	7 (13%)
30	CLA	G	520	-	49,57,73	1.69	6 (12%)	55,93,113	1.54	8 (14%)
34	PID	N	301	-	41,49,49	1.35	4 (9%)	49,76,76	1.50	6 (12%)
30	CLA	A	312	-	55,63,73	1.62	5 (9%)	64,101,113	1.47	7 (10%)
30	CLA	K	316	-	46,54,73	1.78	5 (10%)	53,90,113	1.56	8 (15%)
30	CLA	b	717	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	a	705	30	55,63,73	1.63	5 (9%)	64,101,113	1.53	9 (14%)
30	CLA	F	310	-	46,54,73	1.76	6 (13%)	53,90,113	1.63	8 (15%)
28	DD6	I	303	-	39,45,45	2.22	5 (12%)	52,67,67	2.03	17 (32%)
30	CLA	I	308	-	60,68,73	1.56	5 (8%)	70,107,113	1.42	10 (14%)
34	PID	N	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.68	9 (18%)
30	CLA	b	724	-	65,73,73	1.49	6 (9%)	76,113,113	1.32	7 (9%)
30	CLA	A	316	-	47,55,73	1.75	6 (12%)	54,91,113	1.53	7 (12%)
34	PID	F	306	-	41,49,49	1.33	4 (9%)	49,76,76	1.49	5 (10%)
33	LMG	I	320	-	38,38,55	0.81	0	46,46,63	1.29	6 (13%)
30	CLA	I	309	-	55,63,73	1.64	5 (9%)	64,101,113	1.45	8 (12%)
28	DD6	K	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	13 (25%)
36	SF4	c	202	7	0,12,12	-	-	-	-	-
30	CLA	P	210	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	8 (10%)
30	CLA	K	308	2	54,62,73	1.63	5 (9%)	62,99,113	1.49	8 (12%)
30	CLA	F	307	-	46,54,73	1.76	6 (13%)	53,90,113	1.60	7 (13%)
30	CLA	b	718	-	51,59,73	1.71	5 (9%)	59,96,113	1.54	7 (11%)
28	DD6	F	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.01	14 (26%)
30	CLA	K	306	2	49,57,73	1.72	5 (10%)	55,93,113	1.55	9 (16%)
30	CLA	J	306	-	46,54,73	1.76	6 (13%)	53,90,113	1.57	6 (11%)
30	CLA	M	311	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	6 (11%)
28	DD6	J	303	-	39,45,45	2.31	4 (10%)	52,67,67	2.44	18 (34%)
30	CLA	b	712	-	54,62,73	1.69	7 (12%)	67,100,113	1.55	11 (16%)
28	DD6	L	302	-	39,45,45	1.94	2 (5%)	52,67,67	2.00	14 (26%)
30	CLA	L	314	-	53,61,73	1.63	5 (9%)	61,98,113	1.51	9 (14%)
30	CLA	b	721	28	46,54,73	1.76	6 (13%)	53,90,113	1.51	6 (11%)
30	CLA	b	705	-	65,73,73	1.48	5 (7%)	76,113,113	1.36	8 (10%)
34	PID	D	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.51	6 (12%)
30	CLA	l	311	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	8 (10%)
32	DGD	G	521	-	45,45,67	1.03	2 (4%)	59,59,81	1.46	8 (13%)
30	CLA	a	720	-	62,70,73	1.52	5 (8%)	72,109,113	1.41	8 (11%)
30	CLA	I	321	30	52,60,73	1.67	5 (9%)	60,97,113	1.61	9 (15%)
30	CLA	L	317	-	52,60,73	1.69	6 (11%)	60,97,113	1.51	9 (15%)
30	CLA	D	308	-	47,55,73	1.75	5 (10%)	54,91,113	1.51	7 (12%)
30	CLA	b	710	-	52,60,73	1.70	6 (11%)	60,97,113	1.50	8 (13%)
34	PID	D	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.41	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	b	722	-	65,73,73	1.51	6 (9%)	76,113,113	1.45	9 (11%)
30	CLA	G	519	-	59,67,73	1.56	5 (8%)	68,105,113	1.44	7 (10%)
30	CLA	P	212	-	51,59,73	1.67	6 (11%)	59,96,113	1.52	7 (11%)
30	CLA	M	313	-	46,54,73	1.78	5 (10%)	53,90,113	1.55	7 (13%)
30	CLA	B	309	18	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
37	BCR	b	732	-	41,41,41	0.80	0	56,56,56	1.88	20 (35%)
36	SF4	a	737	16,17	0,12,12	-	-	-	-	-
28	DD6	A	302	-	39,45,45	2.01	3 (7%)	52,67,67	2.13	16 (30%)
34	PID	F	305	-	41,49,49	1.38	5 (12%)	49,76,76	1.87	9 (18%)
28	DD6	I	305	-	39,45,45	2.28	6 (15%)	52,67,67	2.29	17 (32%)
30	CLA	L	318	-	46,54,73	1.76	7 (15%)	53,90,113	1.58	7 (13%)
30	CLA	K	311	-	52,60,73	1.68	6 (11%)	60,97,113	1.49	7 (11%)
28	DD6	h	203	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	13 (25%)
29	UIX	K	302	-	41,49,49	1.26	3 (7%)	52,74,74	2.71	23 (44%)
30	CLA	a	727	-	46,54,73	1.79	6 (13%)	53,90,113	1.52	7 (13%)
28	DD6	L	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.82	12 (23%)
28	DD6	A	301	-	39,45,45	1.99	2 (5%)	52,67,67	2.13	14 (26%)
32	DGD	l	301	-	51,51,67	0.95	2 (3%)	65,65,81	0.89	2 (3%)
31	KC1	G	515	5	48,53,53	1.50	7 (14%)	55,89,89	1.81	12 (21%)
28	DD6	L	306	-	39,45,45	2.00	3 (7%)	52,67,67	2.04	15 (28%)
37	BCR	l	302	-	41,41,41	0.73	0	56,56,56	2.19	21 (37%)
30	CLA	b	709	-	60,68,73	1.57	6 (10%)	70,107,113	1.43	9 (12%)
34	PID	H	302	-	41,49,49	1.38	4 (9%)	49,76,76	1.37	6 (12%)
30	CLA	L	310	-	55,63,73	1.61	5 (9%)	64,101,113	1.48	7 (10%)
30	CLA	b	703	-	65,73,73	1.49	6 (9%)	76,113,113	1.32	8 (10%)
32	DGD	I	317	-	40,40,67	1.10	2 (5%)	54,54,81	1.02	4 (7%)
30	CLA	B	311	-	65,73,73	1.50	6 (9%)	76,113,113	1.30	7 (9%)
30	CLA	a	701	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	7 (13%)
32	DGD	L	301	-	39,39,67	0.95	2 (5%)	53,53,81	0.98	2 (3%)
33	LMG	K	317	-	43,43,55	0.81	1 (2%)	51,51,63	1.31	6 (11%)
31	KC1	N	308	-	48,53,53	1.52	7 (14%)	55,89,89	2.13	13 (23%)
37	BCR	j	102	-	41,41,41	0.71	0	56,56,56	2.02	16 (28%)
34	PID	j	105	-	41,49,49	1.41	4 (9%)	49,76,76	1.48	10 (20%)
31	KC1	H	310	-	48,53,53	1.49	7 (14%)	55,89,89	1.86	9 (16%)
30	CLA	L	316	-	41,49,73	1.87	5 (12%)	47,84,113	1.65	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	l	312	-	46,54,73	1.77	5 (10%)	53,90,113	1.52	7 (13%)
30	CLA	a	735	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	7 (9%)
30	CLA	a	729	-	56,64,73	1.59	6 (10%)	65,102,113	1.42	8 (12%)
34	PID	P	208	-	41,49,49	1.34	4 (9%)	49,76,76	1.46	6 (12%)
30	CLA	M	317	-	46,54,73	1.75	5 (10%)	53,90,113	1.58	7 (13%)
30	CLA	a	711	-	45,53,73	1.77	6 (13%)	52,89,113	1.65	8 (15%)
34	PID	G	507	-	41,49,49	1.33	4 (9%)	49,76,76	1.40	7 (14%)
28	DD6	P	204	-	39,45,45	2.00	3 (7%)	52,67,67	2.06	14 (26%)
34	PID	D	306	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	5 (10%)
34	PID	H	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.65	6 (12%)
30	CLA	J	307	-	65,73,73	1.48	6 (9%)	76,113,113	1.43	6 (7%)
30	CLA	O	309	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	9 (11%)
30	CLA	G	511	-	55,63,73	1.62	6 (10%)	64,101,113	1.47	7 (10%)
30	CLA	J	308	-	46,54,73	1.76	6 (13%)	53,90,113	1.57	7 (13%)
28	DD6	I	302	-	39,45,45	2.05	3 (7%)	52,67,67	2.16	17 (32%)
28	DD6	I	301	-	39,45,45	2.06	3 (7%)	52,67,67	2.20	20 (38%)
30	CLA	P	209	-	47,55,73	1.76	6 (12%)	54,91,113	1.53	8 (14%)
30	CLA	L	312	-	46,54,73	1.76	5 (10%)	53,90,113	1.55	7 (13%)
30	CLA	a	718	-	46,54,73	1.77	5 (10%)	53,90,113	1.56	7 (13%)
30	CLA	H	312	-	46,54,73	1.77	5 (10%)	53,90,113	1.56	7 (13%)
28	DD6	K	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.98	15 (28%)
28	DD6	J	304	-	39,45,45	2.20	5 (12%)	52,67,67	2.12	18 (34%)
38	PQN	a	732	-	34,34,34	1.58	2 (5%)	42,45,45	1.10	4 (9%)
30	CLA	a	712	30	60,68,73	1.55	5 (8%)	70,107,113	1.41	8 (11%)
31	KC1	L	307	30	48,53,53	1.51	7 (14%)	55,89,89	1.89	14 (25%)
30	CLA	a	702	-	65,73,73	1.47	10 (15%)	76,113,113	1.42	7 (9%)
31	KC1	O	315	26	48,53,53	1.50	6 (12%)	55,89,89	1.79	10 (18%)
30	CLA	N	304	-	47,55,73	1.76	5 (10%)	54,91,113	1.54	8 (14%)
34	PID	D	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.46	7 (14%)
30	CLA	b	725	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
30	CLA	L	311	-	55,63,73	1.62	6 (10%)	64,101,113	1.48	8 (12%)
31	KC1	B	314	18	48,53,53	1.51	7 (14%)	55,89,89	1.83	11 (20%)
30	CLA	m	202	-	60,68,73	1.55	5 (8%)	70,107,113	1.49	7 (10%)
28	DD6	M	304	-	39,45,45	2.04	3 (7%)	52,67,67	1.91	14 (26%)
30	CLA	a	710	16	55,63,73	1.64	6 (10%)	64,101,113	1.47	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	G	509	5	51,59,73	1.68	5 (9%)	59,96,113	1.52	8 (13%)
30	CLA	a	722	-	58,66,73	1.57	6 (10%)	67,104,113	1.48	8 (11%)
30	CLA	J	312	-	53,61,73	1.64	6 (11%)	61,98,113	1.56	9 (14%)
37	BCR	l	306	-	41,41,41	0.73	0	56,56,56	1.91	13 (23%)
28	DD6	B	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.89	11 (21%)
37	BCR	m	201	-	41,41,41	0.71	0	56,56,56	2.33	16 (28%)
29	UIX	O	306	-	41,49,49	1.28	3 (7%)	52,74,74	2.86	23 (44%)
28	DD6	K	318	-	39,45,45	2.02	3 (7%)	52,67,67	2.07	12 (23%)
31	KC1	I	314	1	48,53,53	1.50	7 (14%)	55,89,89	1.88	13 (23%)
30	CLA	N	305	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
30	CLA	M	312	-	48,56,73	1.74	5 (10%)	55,92,113	1.56	8 (14%)
30	CLA	M	308	31	53,61,73	1.65	5 (9%)	61,98,113	1.52	8 (13%)
32	DGD	j	103	-	42,42,67	1.05	2 (4%)	56,56,81	1.00	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	G	516	5	1/1/10/20	4/8/86/115	-
30	CLA	I	319	30	1/1/11/20	8/13/91/115	-
30	CLA	B	312	-	1/1/12/20	2/21/99/115	-
30	CLA	j	106	-	1/1/13/20	12/29/107/115	-
30	CLA	A	320	-	1/1/11/20	6/15/93/115	-
30	CLA	b	726	-	1/1/11/20	1/16/94/115	-
34	PID	O	302	-	-	2/24/93/93	0/4/4/4
29	UIX	B	305	-	-	2/31/87/87	0/3/3/3
37	BCR	i	201	-	-	8/29/63/63	0/2/2/2
30	CLA	K	312	-	1/1/11/20	4/17/95/115	-
30	CLA	A	317	-	1/1/10/20	0/8/86/115	-
30	CLA	a	726	-	1/1/15/20	11/37/115/115	-
30	CLA	F	311	-	1/1/11/20	4/15/93/115	-
28	DD6	D	303	-	-	6/26/80/80	0/3/3/3
35	SQD	A	318	-	-	6/45/65/69	0/1/1/1
30	CLA	A	313	-	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PID	P	202	-	-	3/24/93/93	0/4/4/4
30	CLA	O	314	-	1/1/11/20	9/16/94/115	-
29	UIX	A	304	-	-	0/31/87/87	0/3/3/3
30	CLA	a	731	-	1/1/15/20	13/37/115/115	-
30	CLA	N	307	-	1/1/12/20	7/21/99/115	-
30	CLA	I	315	-	1/1/12/20	7/22/100/115	-
28	DD6	H	303	-	-	1/26/80/80	0/3/3/3
30	CLA	O	311	-	1/1/12/20	5/21/99/115	-
28	DD6	B	306	-	-	2/26/80/80	0/3/3/3
30	CLA	l	310	-	-	9/26/65/115	0/5/5/9
30	CLA	J	311	22	1/1/11/20	8/16/94/115	-
30	CLA	A	310	-	1/1/15/20	15/37/115/115	-
31	KC1	O	312	-	-	8/15/71/71	-
30	CLA	j	104	-	1/1/13/20	6/25/103/115	-
30	CLA	I	311	1	1/1/13/20	10/25/103/115	-
30	CLA	h	202	-	1/1/13/20	7/25/103/115	-
30	CLA	D	309	-	1/1/11/20	7/15/93/115	-
30	CLA	b	711	-	1/1/13/20	11/25/103/115	-
30	CLA	a	713	-	1/1/14/20	10/31/109/115	-
30	CLA	a	728	-	1/1/13/20	8/25/103/115	-
36	SF4	c	201	7	-	-	0/6/5/5
30	CLA	I	316	-	1/1/13/20	14/25/103/115	-
30	CLA	G	514	-	1/1/12/20	11/23/101/115	-
37	BCR	a	736	-	-	3/29/63/63	0/2/2/2
30	CLA	G	518	-	1/1/11/20	7/15/93/115	-
31	KC1	D	315	19	-	3/15/71/71	-
30	CLA	B	316	-	1/1/11/20	7/15/93/115	-
34	PID	O	304	-	-	3/24/93/93	0/4/4/4
30	CLA	A	315	-	1/1/10/20	6/8/86/115	-
30	CLA	B	308	-	1/1/11/20	5/13/91/115	-
33	LMG	B	318	-	-	15/32/52/70	0/1/1/1
32	DGD	G	501	-	-	10/34/74/95	0/2/2/2
28	DD6	M	302	-	-	3/26/80/80	0/3/3/3
31	KC1	F	314	20	-	8/15/71/71	-
28	DD6	b	731	30	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	f	301	-	1/1/13/20	9/25/103/115	-
30	CLA	b	713	-	1/1/15/20	11/37/115/115	-
30	CLA	a	715	-	1/1/11/20	5/13/91/115	-
33	LMG	j	101	-	-	14/30/50/70	0/1/1/1
30	CLA	B	310	-	1/1/13/20	8/25/103/115	-
30	CLA	G	513	5	1/1/15/20	10/37/115/115	-
31	KC1	M	307	30	-	7/15/71/71	-
30	CLA	P	217	-	1/1/10/20	5/8/86/115	-
30	CLA	M	318	-	1/1/11/20	9/15/93/115	-
29	UIX	G	503	-	-	4/31/87/87	0/3/3/3
30	CLA	G	510	-	1/1/15/20	14/37/115/115	-
30	CLA	J	315	-	1/1/11/20	4/15/93/115	-
28	DD6	A	303	-	-	1/26/80/80	0/3/3/3
31	KC1	P	211	-	-	11/15/71/71	-
31	KC1	D	310	-	-	10/15/71/71	-
30	CLA	a	725	-	1/1/14/20	11/33/111/115	-
31	KC1	O	310	-	-	8/15/71/71	-
34	PID	G	506	-	-	3/24/93/93	0/4/4/4
30	CLA	M	310	-	1/1/11/20	7/17/95/115	-
28	DD6	G	502	-	-	6/26/80/80	0/3/3/3
30	CLA	a	738	22	1/1/11/20	2/15/93/115	-
30	CLA	J	316	-	-	2/15/93/115	-
30	CLA	a	716	-	1/1/11/20	4/16/94/115	-
30	CLA	I	307	-	1/1/11/20	6/15/93/115	-
30	CLA	B	317	-	1/1/11/20	5/13/91/115	-
30	CLA	A	308	-	1/1/13/20	5/25/103/115	-
33	LMG	b	733	-	-	19/39/59/70	0/1/1/1
30	CLA	O	308	-	1/1/11/20	5/16/94/115	-
30	CLA	D	314	-	1/1/11/20	6/15/93/115	-
28	DD6	A	305	31	-	1/26/80/80	0/3/3/3
32	DGD	y	201	-	-	7/43/83/95	0/2/2/2
30	CLA	a	704	-	1/1/15/20	6/37/115/115	-
30	CLA	b	701	-	1/1/15/20	15/37/115/115	-
28	DD6	J	302	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	I	310	-	1/1/11/20	10/17/95/115	-
28	DD6	K	303	-	-	0/26/80/80	0/3/3/3
28	DD6	N	303	-	-	0/26/80/80	0/3/3/3
28	DD6	M	306	-	-	5/26/80/80	0/3/3/3
37	BCR	a	734	-	-	4/29/63/63	0/2/2/2
37	BCR	b	702	-	-	2/29/63/63	0/2/2/2
30	CLA	O	313	-	1/1/11/20	4/15/93/115	-
30	CLA	a	706	16	1/1/13/20	17/29/107/115	-
29	UIX	I	304	-	-	4/31/87/87	0/3/3/3
30	CLA	H	309	-	1/1/11/20	7/16/94/115	-
28	DD6	G	504	-	-	5/26/80/80	0/3/3/3
30	CLA	B	313	18	1/1/15/20	11/37/115/115	-
30	CLA	a	719	-	1/1/11/20	4/16/94/115	-
31	KC1	A	306	28,30	-	6/15/71/71	-
28	DD6	B	303	-	-	2/26/80/80	0/3/3/3
30	CLA	a	707	-	1/1/15/20	16/37/115/115	-
30	CLA	M	309	24	1/1/13/20	5/25/103/115	-
31	KC1	N	306	-	-	6/15/71/71	-
31	KC1	P	213	-	-	8/15/71/71	-
31	KC1	K	314	2	-	8/15/71/71	-
30	CLA	b	719	-	1/1/11/20	11/15/93/115	-
31	KC1	P	216	27	-	8/15/71/71	-
30	CLA	l	309	-	1/1/10/20	4/8/86/115	-
30	CLA	H	305	-	1/1/15/20	8/37/115/115	-
30	CLA	K	309	-	1/1/12/20	2/19/97/115	-
30	CLA	J	309	-	1/1/13/20	8/27/105/115	-
28	DD6	L	303	-	-	0/26/80/80	0/3/3/3
34	PID	O	305	-	-	16/24/93/93	0/4/4/4
30	CLA	L	313	-	1/1/13/20	11/25/103/115	-
28	DD6	F	301	-	-	2/26/80/80	0/3/3/3
30	CLA	H	304	-	1/1/11/20	6/16/94/115	-
30	CLA	l	304	-	1/1/14/20	11/31/109/115	-
30	CLA	O	316	-	1/1/10/20	4/8/86/115	-
28	DD6	M	305	-	-	1/26/80/80	0/3/3/3
34	PID	F	304	-	-	3/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	N	309	25	1/1/11/20	3/15/93/115	-
30	CLA	a	717	-	1/1/13/20	13/28/106/115	-
30	CLA	a	714	-	1/1/11/20	4/13/91/115	-
30	CLA	a	708	-	1/1/12/20	4/21/99/115	-
30	CLA	a	721	-	1/1/15/20	18/37/115/115	-
37	BCR	b	730	-	-	8/29/63/63	0/2/2/2
28	DD6	K	305	-	-	4/26/80/80	0/3/3/3
37	BCR	l	307	-	-	0/29/63/63	0/2/2/2
30	CLA	l	313	14	1/1/15/20	19/37/115/115	-
30	CLA	H	308	-	1/1/11/20	4/15/93/115	-
30	CLA	I	312	-	1/1/15/20	14/37/115/115	-
30	CLA	B	301	-	1/1/14/20	11/31/109/115	-
30	CLA	K	315	-	1/1/10/20	3/8/86/115	-
30	CLA	H	311	-	-	6/8/86/115	-
33	LMG	D	317	-	-	17/41/61/70	0/1/1/1
30	CLA	f	302	-	1/1/11/20	6/15/93/115	-
30	CLA	a	723	-	1/1/15/20	16/37/115/115	-
30	CLA	G	512	-	1/1/14/20	13/31/109/115	-
29	UIX	P	207	-	-	8/31/87/87	0/3/3/3
30	CLA	J	301	-	1/1/14/20	11/31/109/115	-
34	PID	O	307	-	-	3/24/93/93	0/4/4/4
30	CLA	D	311	-	1/1/11/20	4/15/93/115	-
30	CLA	M	316	-	1/1/12/20	11/22/100/115	-
34	PID	D	302	-	-	2/24/93/93	0/4/4/4
30	CLA	J	310	-	1/1/11/20	6/15/93/115	-
30	CLA	M	315	-	1/1/10/20	5/8/86/115	-
34	PID	P	205	-	-	2/24/93/93	0/4/4/4
31	KC1	F	309	20	-	8/15/71/71	-
33	LMG	b	734	-	-	12/26/46/70	0/1/1/1
30	CLA	l	303	14	1/1/15/20	14/37/115/115	-
30	CLA	a	724	-	1/1/15/20	15/37/115/115	-
30	CLA	b	714	-	1/1/11/20	5/15/93/115	-
30	CLA	b	720	-	1/1/12/20	9/23/101/115	-
30	CLA	l	305	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DD6	B	302	-	-	3/24/78/80	0/3/3/3
31	KC1	N	311	25	-	7/15/71/71	-
39	LHG	a	733	-	-	18/52/52/53	-
34	PID	F	302	-	-	2/24/93/93	0/4/4/4
30	CLA	H	307	-	1/1/12/20	7/21/99/115	-
30	CLA	P	215	-	1/1/11/20	7/16/94/115	-
30	CLA	F	308	-	1/1/11/20	1/15/93/115	-
30	CLA	K	313	-	1/1/13/20	7/25/103/115	-
28	DD6	G	508	-	-	1/26/80/80	0/3/3/3
30	CLA	l	308	-	1/1/10/20	2/8/86/115	-
30	CLA	b	716	-	1/1/12/20	7/19/97/115	-
30	CLA	K	310	-	1/1/13/20	6/25/103/115	-
30	CLA	A	311	6	1/1/11/20	5/15/93/115	-
30	CLA	a	709	-	1/1/15/20	17/37/115/115	-
30	CLA	I	313	-	1/1/13/20	12/25/103/115	-
30	CLA	a	703	-	1/1/13/20	9/25/103/115	-
30	CLA	b	723	-	1/1/12/20	7/19/97/115	-
30	CLA	L	308	31	1/1/11/20	7/13/91/115	-
30	CLA	D	313	19	1/1/11/20	3/13/91/115	-
28	DD6	M	303	-	-	2/26/80/80	0/3/3/3
28	DD6	O	303	-	-	0/26/80/80	0/3/3/3
34	PID	P	203	-	-	2/24/93/93	0/4/4/4
34	PID	O	301	-	-	4/24/93/93	0/4/4/4
31	KC1	J	313	-	-	6/15/71/71	-
30	CLA	I	306	1	1/1/11/20	7/18/96/115	-
30	CLA	b	704	-	1/1/15/20	19/37/115/115	-
30	CLA	D	312	19	1/1/11/20	6/15/93/115	-
33	LMG	I	318	-	-	21/31/51/70	0/1/1/1
30	CLA	L	309	-	1/1/12/20	11/23/101/115	-
30	CLA	b	728	-	1/1/15/20	7/37/115/115	-
31	KC1	M	314	24	-	9/15/71/71	-
30	CLA	b	727	-	1/1/15/20	10/37/115/115	-
33	LMG	P	201	-	-	8/22/42/70	0/1/1/1
30	CLA	A	307	31	1/1/11/20	2/13/91/115	-
30	CLA	b	707	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	UIX	h	201	-	-	2/31/87/87	0/3/3/3
31	KC1	H	306	-	-	4/15/71/71	-
34	PID	P	206	-	-	2/24/93/93	0/4/4/4
30	CLA	D	316	-	1/1/10/20	0/8/86/115	-
30	CLA	F	312	-	1/1/11/20	4/15/93/115	-
38	PQN	b	729	-	-	4/23/43/43	0/2/2/2
30	CLA	K	307	-	1/1/11/20	0/15/93/115	-
28	DD6	L	305	-	-	3/26/80/80	0/3/3/3
30	CLA	F	315	-	1/1/10/20	4/8/86/115	-
30	CLA	b	708	-	1/1/15/20	11/37/115/115	-
31	KC1	L	315	-	-	8/15/71/71	-
34	PID	M	301	-	-	1/24/93/93	0/4/4/4
30	CLA	b	715	-	1/1/14/20	14/31/109/115	-
30	CLA	F	313	-	1/1/11/20	5/15/93/115	-
30	CLA	J	314	-	1/1/10/20	4/8/86/115	-
29	UIX	J	305	-	-	11/31/87/87	0/3/3/3
30	CLA	G	517	-	1/1/11/20	4/15/93/115	-
30	CLA	b	706	-	1/1/11/20	4/17/95/115	-
30	CLA	N	310	-	1/1/11/20	9/16/94/115	-
30	CLA	f	303	10	1/1/11/20	10/15/93/115	-
31	KC1	A	314	6	-	7/15/71/71	-
30	CLA	a	730	-	1/1/15/20	4/37/115/115	-
28	DD6	G	505	-	-	4/26/80/80	0/3/3/3
30	CLA	B	315	-	1/1/10/20	6/8/86/115	-
30	CLA	B	307	18	1/1/11/20	3/18/96/115	-
30	CLA	P	214	-	1/1/11/20	3/15/93/115	-
34	PID	D	304	-	-	3/24/93/93	0/4/4/4
37	BCR	f	304	-	-	3/29/63/63	0/2/2/2
30	CLA	A	309	-	1/1/13/20	7/25/103/115	-
30	CLA	A	319	-	1/1/11/20	8/15/93/115	-
30	CLA	G	520	-	1/1/11/20	6/18/96/115	-
34	PID	N	301	-	-	6/24/93/93	0/4/4/4
30	CLA	A	312	-	1/1/13/20	6/25/103/115	-
30	CLA	K	316	-	1/1/11/20	2/15/93/115	-
30	CLA	b	717	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	a	705	30	1/1/13/20	9/25/103/115	-
30	CLA	F	310	-	1/1/11/20	8/15/93/115	-
28	DD6	I	303	-	-	2/26/80/80	0/3/3/3
30	CLA	I	308	-	1/1/14/20	12/31/109/115	-
34	PID	N	302	-	-	2/24/93/93	0/4/4/4
30	CLA	b	724	-	1/1/15/20	14/37/115/115	-
30	CLA	A	316	-	1/1/11/20	3/16/94/115	-
34	PID	F	306	-	-	0/24/93/93	0/4/4/4
33	LMG	I	320	-	-	14/33/53/70	0/1/1/1
30	CLA	I	309	-	1/1/13/20	8/25/103/115	-
28	DD6	K	301	-	-	5/26/80/80	0/3/3/3
36	SF4	c	202	7	-	-	0/6/5/5
30	CLA	P	210	-	1/1/15/20	14/37/115/115	-
30	CLA	K	308	2	1/1/12/20	13/24/102/115	-
30	CLA	F	307	-	1/1/11/20	5/15/93/115	-
30	CLA	b	718	-	1/1/12/20	1/21/99/115	-
28	DD6	F	303	-	-	2/26/80/80	0/3/3/3
30	CLA	K	306	2	1/1/11/20	4/18/96/115	-
30	CLA	J	306	-	1/1/11/20	4/15/93/115	-
30	CLA	M	311	-	1/1/11/20	6/15/93/115	-
28	DD6	J	303	-	-	2/26/80/80	0/3/3/3
30	CLA	b	712	-	1/1/13/20	9/25/101/115	-
28	DD6	L	302	-	-	4/26/80/80	0/3/3/3
30	CLA	L	314	-	1/1/12/20	6/23/101/115	-
30	CLA	b	721	28	1/1/11/20	5/15/93/115	-
30	CLA	b	705	-	1/1/15/20	14/37/115/115	-
34	PID	D	301	-	-	2/24/93/93	0/4/4/4
30	CLA	l	311	-	1/1/15/20	17/37/115/115	-
32	DGD	G	521	-	-	18/33/73/95	0/2/2/2
30	CLA	a	720	-	1/1/14/20	6/34/112/115	-
30	CLA	I	321	30	1/1/12/20	9/22/100/115	-
30	CLA	L	317	-	1/1/12/20	11/22/100/115	-
30	CLA	D	308	-	1/1/11/20	4/16/94/115	-
30	CLA	b	710	-	1/1/12/20	6/22/100/115	-
34	PID	D	307	-	-	4/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	722	-	1/1/15/20	8/37/115/115	-
30	CLA	G	519	-	1/1/13/20	13/30/108/115	-
30	CLA	P	212	-	1/1/12/20	9/21/99/115	-
30	CLA	M	313	-	1/1/11/20	4/15/93/115	-
30	CLA	B	309	18	1/1/15/20	22/37/115/115	-
37	BCR	b	732	-	-	2/29/63/63	0/2/2/2
36	SF4	a	737	16,17	-	-	0/6/5/5
28	DD6	A	302	-	-	3/26/80/80	0/3/3/3
34	PID	F	305	-	-	8/24/93/93	0/4/4/4
28	DD6	I	305	-	-	5/26/80/80	0/3/3/3
30	CLA	L	318	-	1/1/11/20	8/15/93/115	-
30	CLA	K	311	-	1/1/12/20	9/22/100/115	-
28	DD6	h	203	-	-	1/26/80/80	0/3/3/3
30	CLA	a	727	-	1/1/11/20	8/15/93/115	-
29	UIX	K	302	-	-	4/31/87/87	0/3/3/3
28	DD6	L	304	-	-	0/26/80/80	0/3/3/3
28	DD6	A	301	-	-	3/26/80/80	0/3/3/3
32	DGD	l	301	-	-	7/39/79/95	0/2/2/2
31	KC1	G	515	5	-	8/15/71/71	-
28	DD6	L	306	-	-	3/26/80/80	0/3/3/3
37	BCR	l	302	-	-	4/29/63/63	0/2/2/2
30	CLA	b	709	-	1/1/14/20	8/31/109/115	-
34	PID	H	302	-	-	2/24/93/93	0/4/4/4
30	CLA	L	310	-	1/1/13/20	2/25/103/115	-
30	CLA	b	703	-	1/1/15/20	12/37/115/115	-
32	DGD	I	317	-	-	3/28/68/95	0/2/2/2
30	CLA	B	311	-	1/1/15/20	21/37/115/115	-
30	CLA	a	701	-	1/1/11/20	0/13/91/115	-
32	DGD	L	301	-	-	2/26/66/95	0/2/2/2
33	LMG	K	317	-	-	18/38/58/70	0/1/1/1
31	KC1	N	308	-	-	8/15/71/71	-
37	BCR	j	102	-	-	6/29/63/63	0/2/2/2
34	PID	j	105	-	-	4/24/93/93	0/4/4/4
31	KC1	H	310	-	-	6/15/71/71	-
30	CLA	L	316	-	1/1/10/20	4/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	l	312	-	1/1/11/20	8/15/93/115	-
30	CLA	a	735	-	1/1/15/20	20/37/115/115	-
30	CLA	a	729	-	1/1/13/20	9/27/105/115	-
34	PID	P	208	-	-	2/24/93/93	0/4/4/4
30	CLA	M	317	-	1/1/11/20	6/15/93/115	-
30	CLA	a	711	-	1/1/11/20	6/13/91/115	-
34	PID	G	507	-	-	0/24/93/93	1/4/4/4
28	DD6	P	204	-	-	1/26/80/80	0/3/3/3
34	PID	D	306	-	-	8/24/93/93	0/4/4/4
34	PID	H	301	-	-	4/24/93/93	0/4/4/4
30	CLA	J	307	-	1/1/15/20	21/37/115/115	-
30	CLA	O	309	-	1/1/15/20	2/37/115/115	-
30	CLA	G	511	-	1/1/13/20	4/25/103/115	-
30	CLA	J	308	-	1/1/11/20	9/15/93/115	-
28	DD6	I	302	-	-	5/26/80/80	0/3/3/3
28	DD6	I	301	-	-	3/26/80/80	0/3/3/3
30	CLA	P	209	-	1/1/11/20	4/16/94/115	-
30	CLA	L	312	-	1/1/11/20	5/15/93/115	-
30	CLA	a	718	-	1/1/11/20	8/15/93/115	-
30	CLA	H	312	-	1/1/11/20	10/15/93/115	-
28	DD6	K	304	-	-	1/26/80/80	0/3/3/3
28	DD6	J	304	-	-	2/26/80/80	0/3/3/3
38	PQN	a	732	-	-	8/23/43/43	0/2/2/2
30	CLA	a	712	30	1/1/14/20	8/31/109/115	-
31	KC1	L	307	30	-	6/15/71/71	-
30	CLA	a	702	-	1/1/15/20	12/37/115/115	-
31	KC1	O	315	26	-	5/15/71/71	-
30	CLA	N	304	-	1/1/11/20	3/16/94/115	-
34	PID	D	305	-	-	2/24/93/93	0/4/4/4
30	CLA	b	725	-	1/1/15/20	13/37/115/115	-
30	CLA	L	311	-	1/1/13/20	4/25/103/115	-
31	KC1	B	314	18	-	7/15/71/71	-
30	CLA	m	202	-	1/1/14/20	10/31/109/115	-
28	DD6	M	304	-	-	0/26/80/80	0/3/3/3
30	CLA	a	710	16	1/1/13/20	4/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	G	509	5	1/1/12/20	4/21/99/115	-
30	CLA	a	722	-	1/1/13/20	10/29/107/115	-
30	CLA	J	312	-	1/1/12/20	8/23/101/115	-
37	BCR	l	306	-	-	7/29/63/63	0/2/2/2
28	DD6	B	304	-	-	0/26/80/80	0/3/3/3
37	BCR	m	201	-	-	5/29/63/63	0/2/2/2
29	UIX	O	306	-	-	4/31/87/87	0/3/3/3
28	DD6	K	318	-	-	4/26/80/80	0/3/3/3
31	KC1	I	314	1	-	8/15/71/71	-
30	CLA	N	305	-	1/1/15/20	11/37/115/115	-
30	CLA	M	312	-	1/1/11/20	4/17/95/115	-
30	CLA	M	308	31	1/1/12/20	8/23/101/115	-
32	DGD	j	103	-	-	7/30/70/95	0/2/2/2

The worst 5 of 1591 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	l	310	CLA	CHC-C1C	9.35	1.42	1.35
28	I	305	DD6	C29-C27	-9.13	1.25	1.42
28	J	303	DD6	C29-C27	-9.10	1.25	1.42
28	M	303	DD6	C29-C27	-9.07	1.25	1.42
28	b	731	DD6	C29-C27	-9.03	1.25	1.42

The worst 5 of 3152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	304	UIX	O-C1-C3	9.22	120.31	113.38
29	J	305	UIX	O-C1-C3	8.93	120.09	113.38
29	I	304	UIX	C6-C1-C	-8.91	107.33	122.26
29	B	305	UIX	O-C1-C3	8.34	119.65	113.38
37	m	201	BCR	C7-C8-C9	-8.14	113.94	126.23

5 of 198 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	I	306	CLA	ND
30	I	307	CLA	ND
30	I	308	CLA	ND
30	I	309	CLA	ND

Continued on next page...

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Mol	Chain	Res	Type	Atom
30	I	310	CLA	ND

5 of 2300 torsion outliers are listed below:

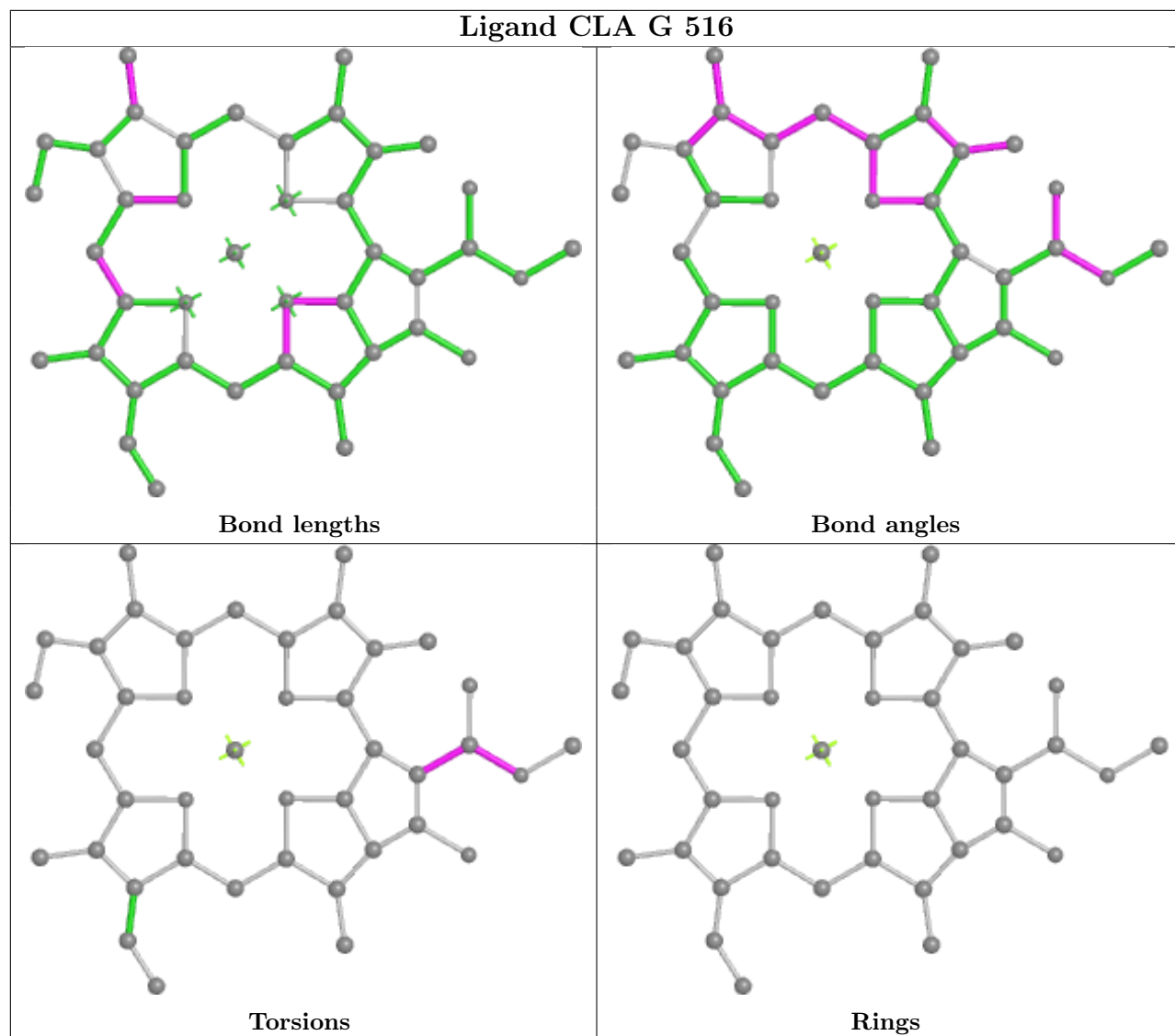
Mol	Chain	Res	Type	Atoms
28	I	302	DD6	C27-C29-C30-C31
28	K	301	DD6	C12-C11-C13-C14
28	G	502	DD6	C-C1-C24-C25
28	G	502	DD6	C2-C1-C24-C25
28	G	504	DD6	C10-C11-C13-C14

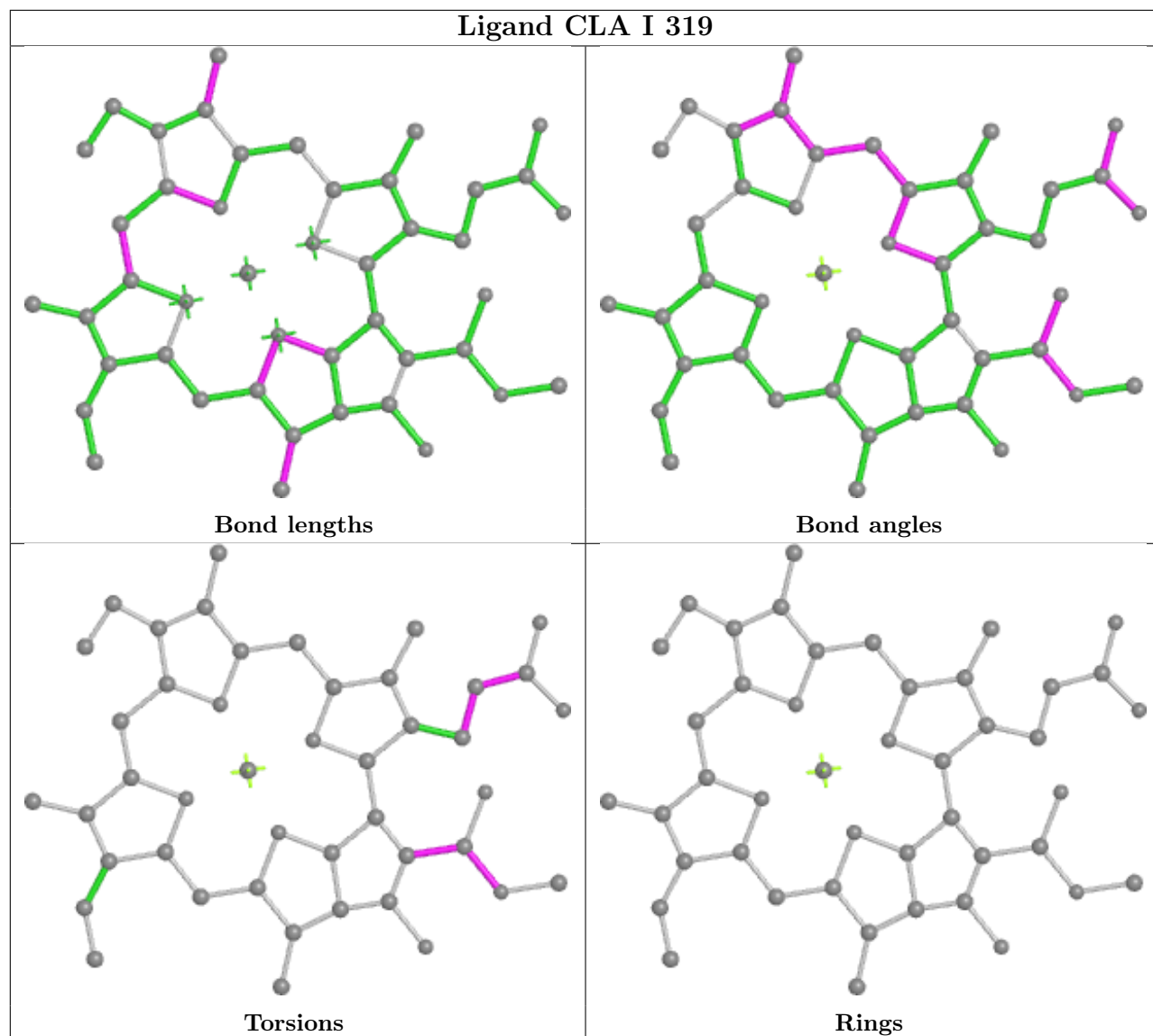
All (1) ring outliers are listed below:

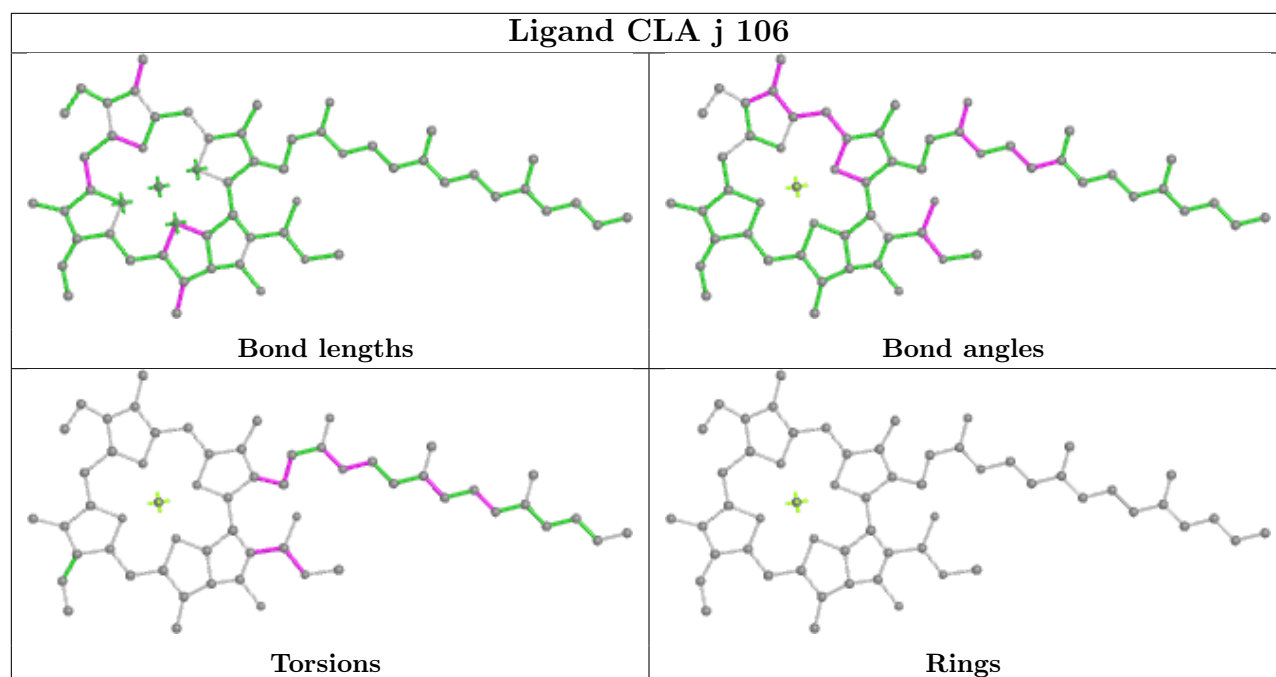
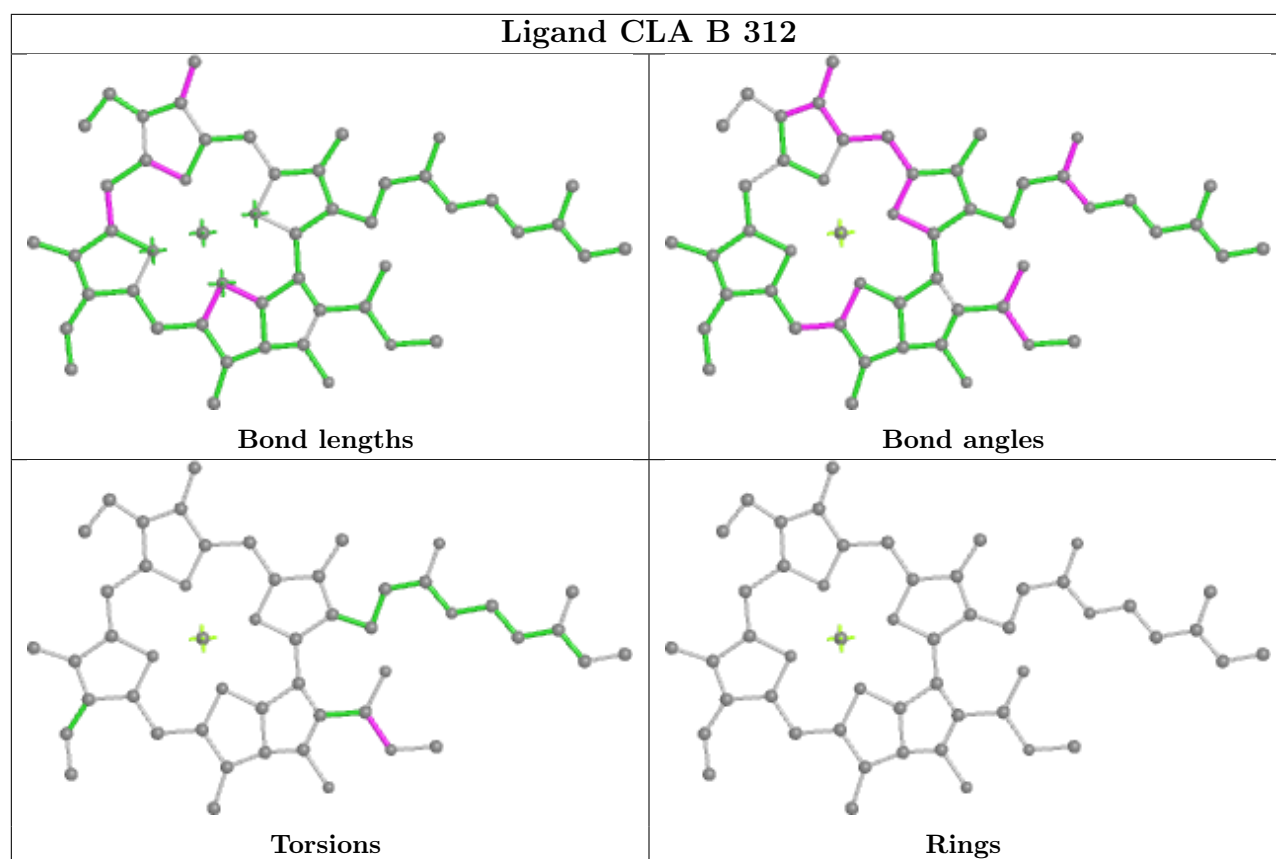
Mol	Chain	Res	Type	Atoms
34	G	507	PID	C24-C25-C26-C27-C28-C29

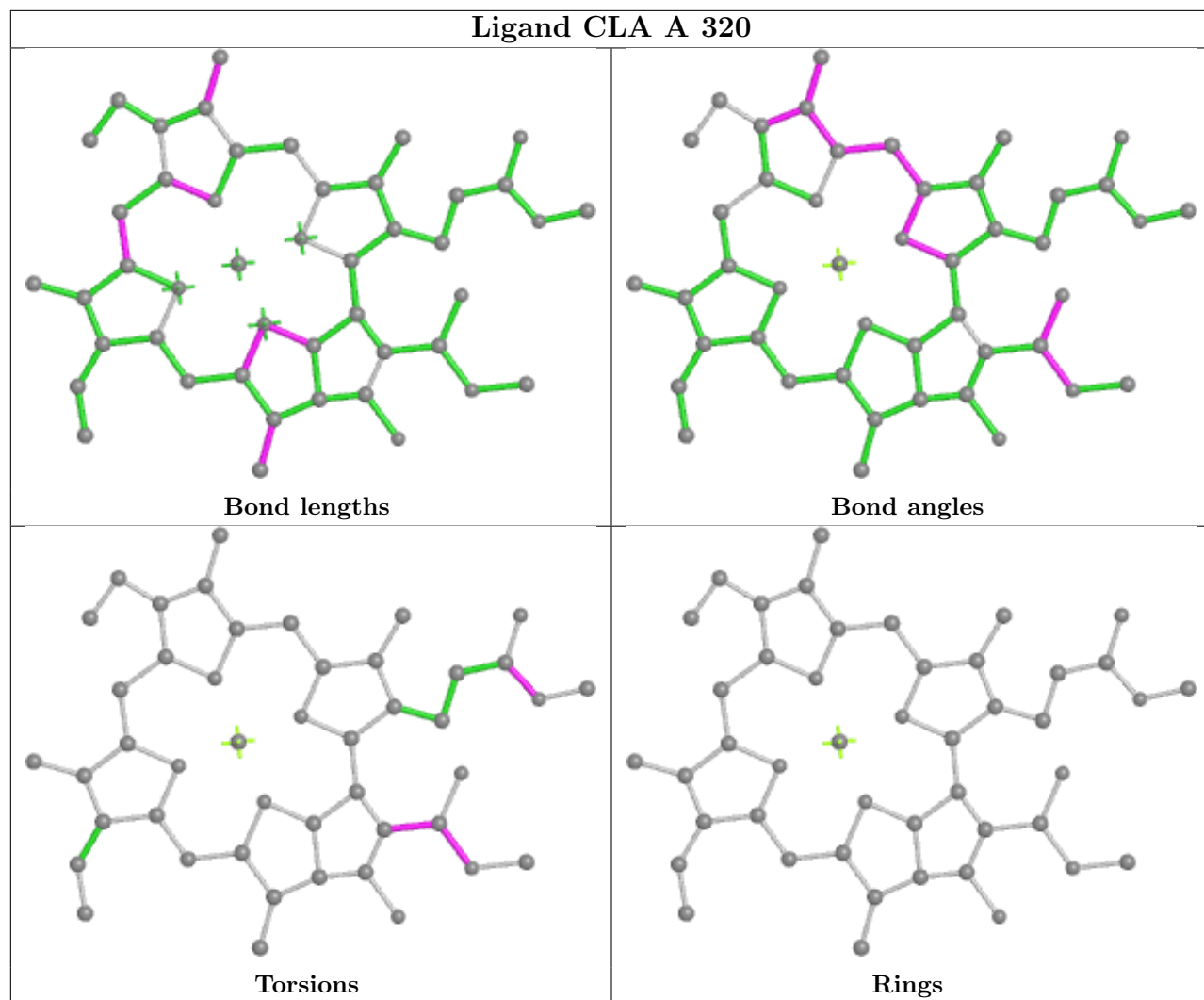
No monomer is involved in short contacts.

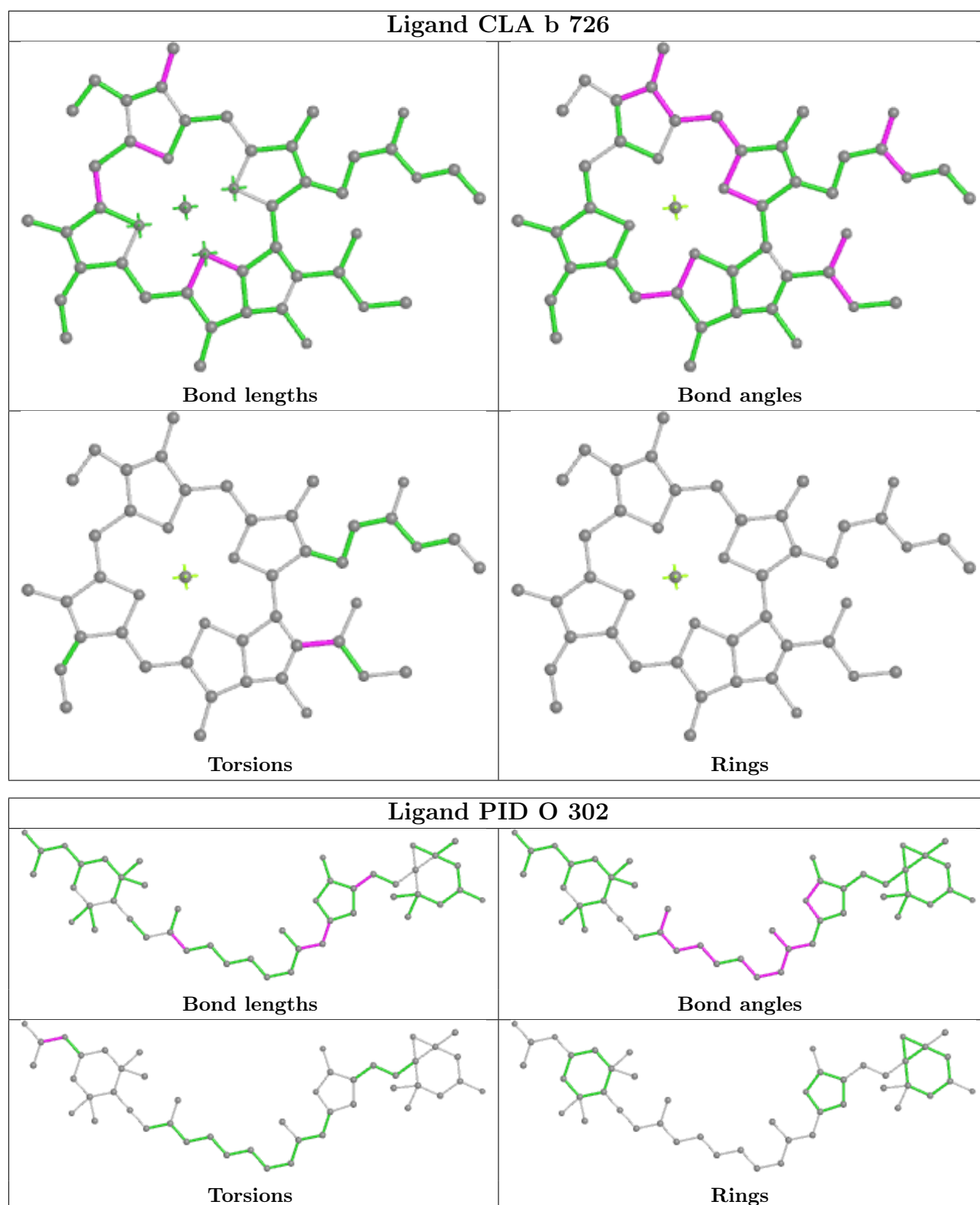
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

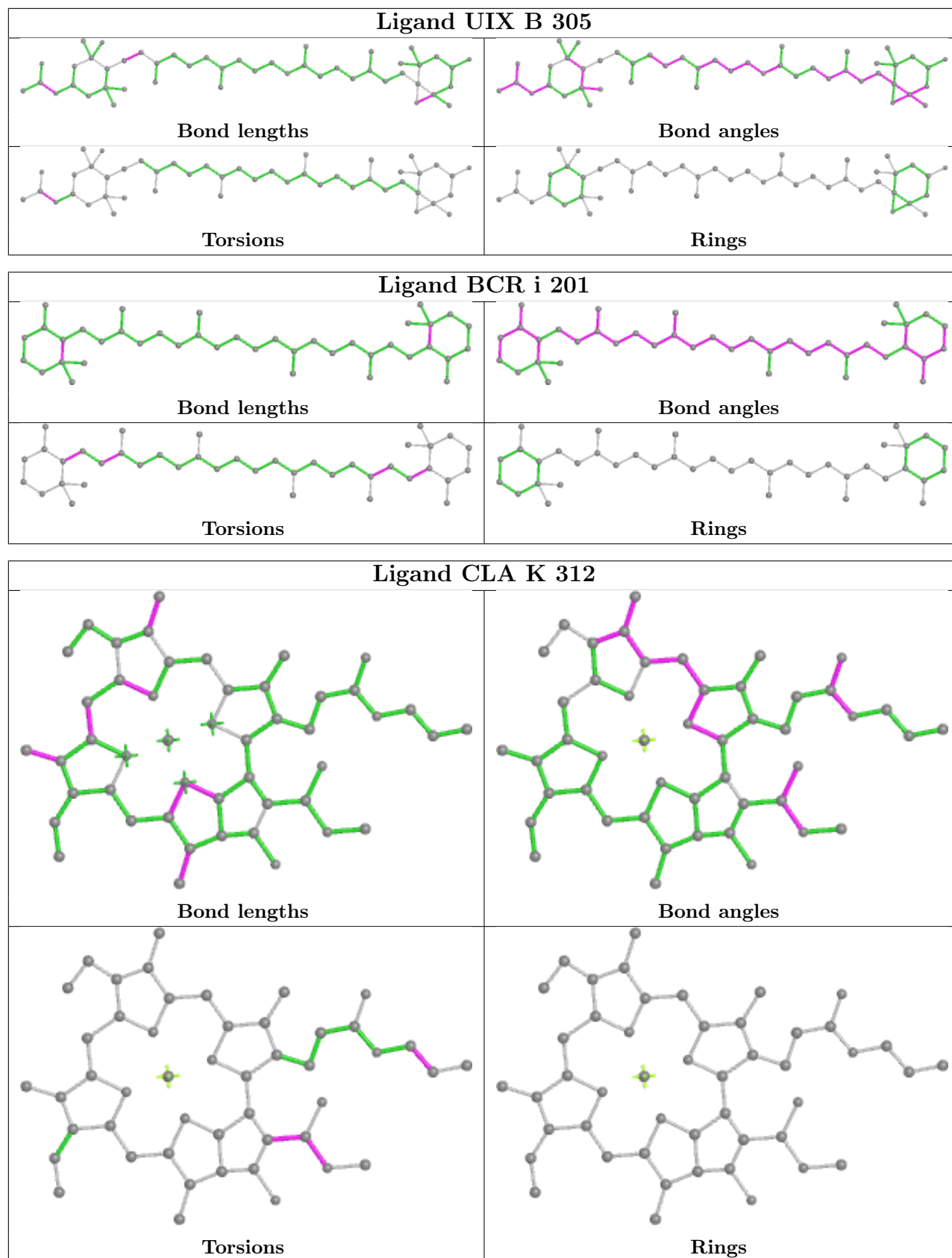


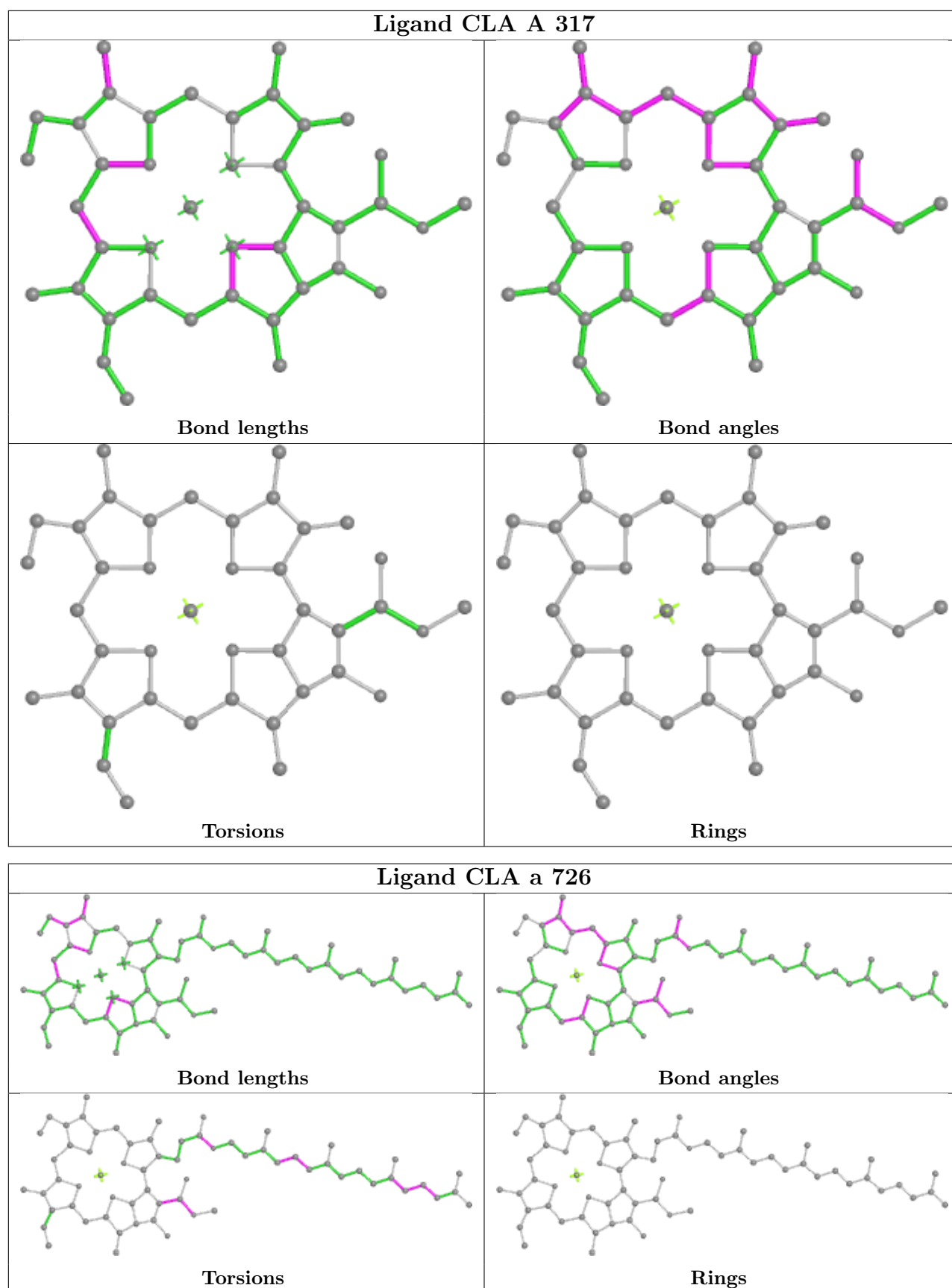


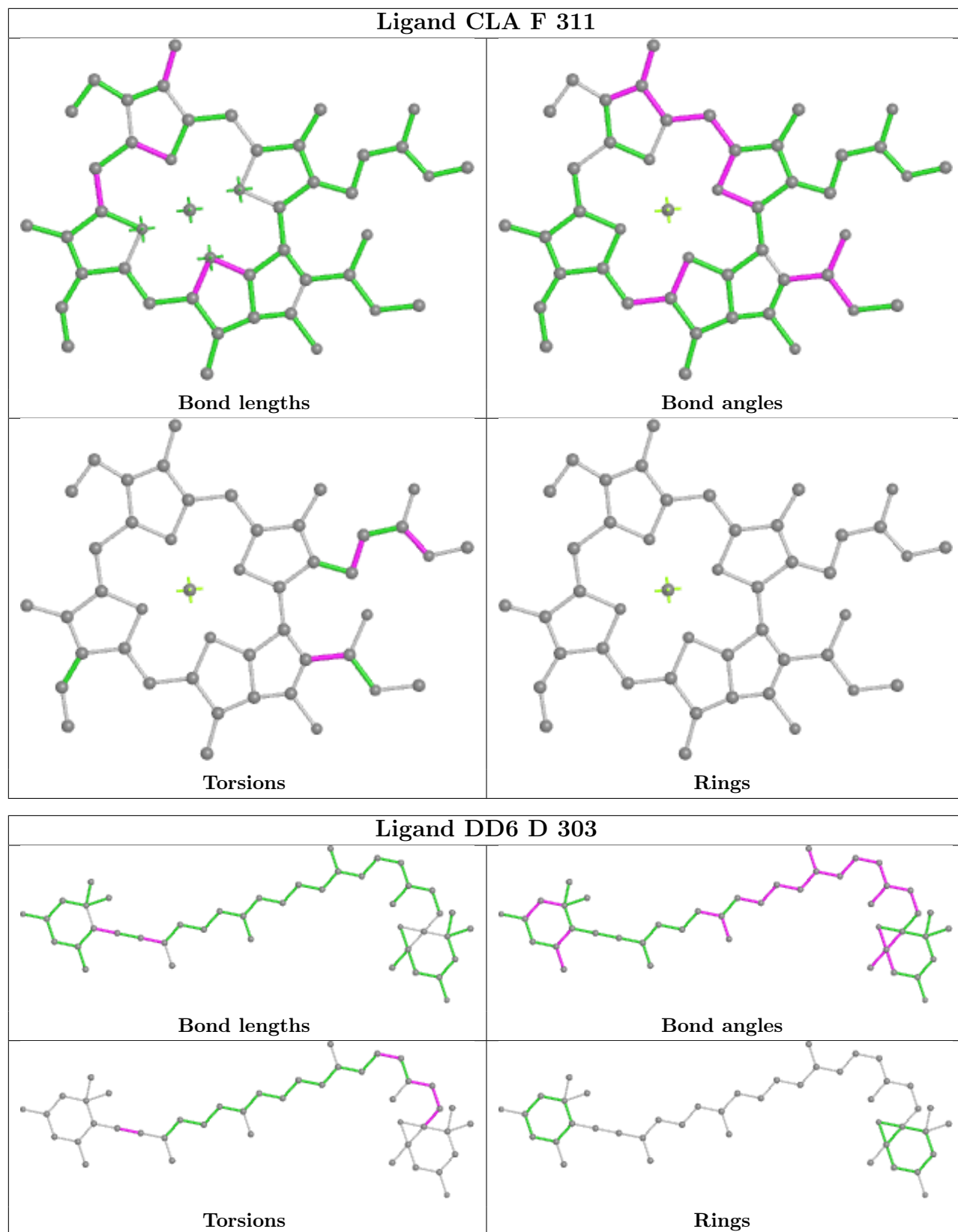


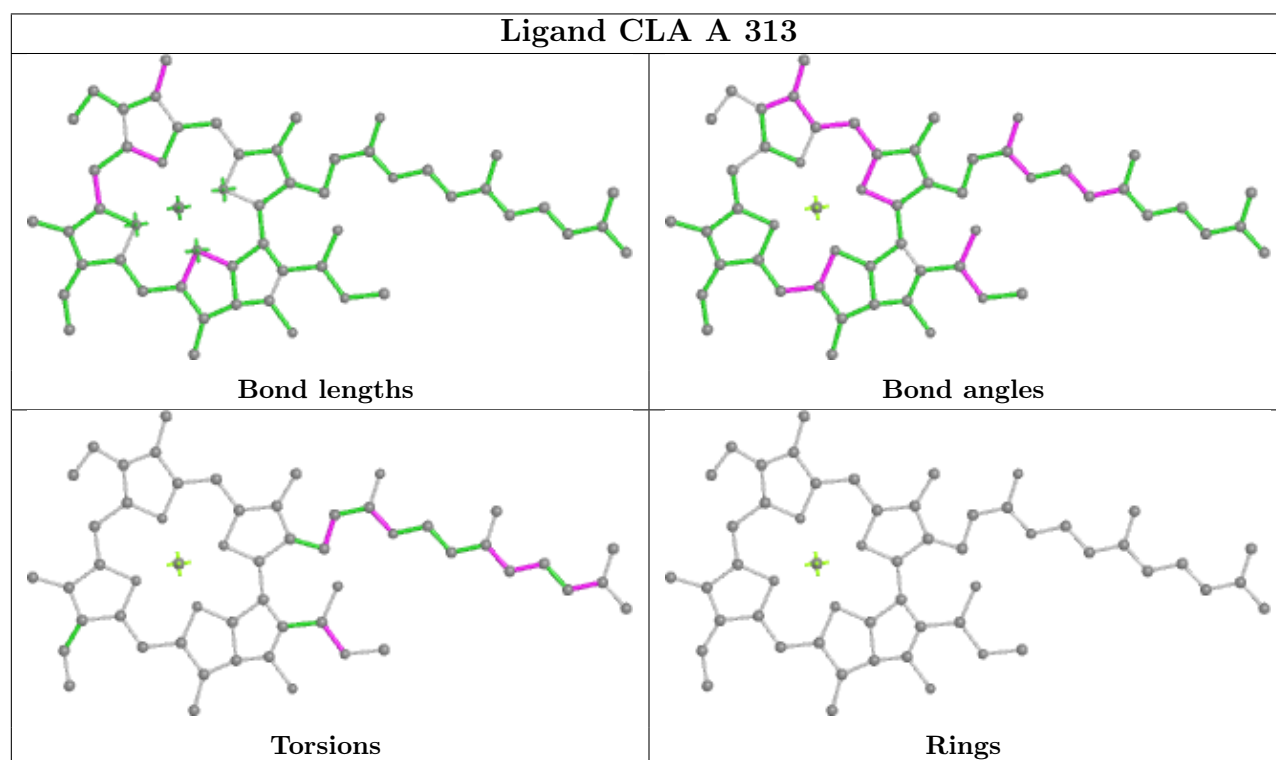
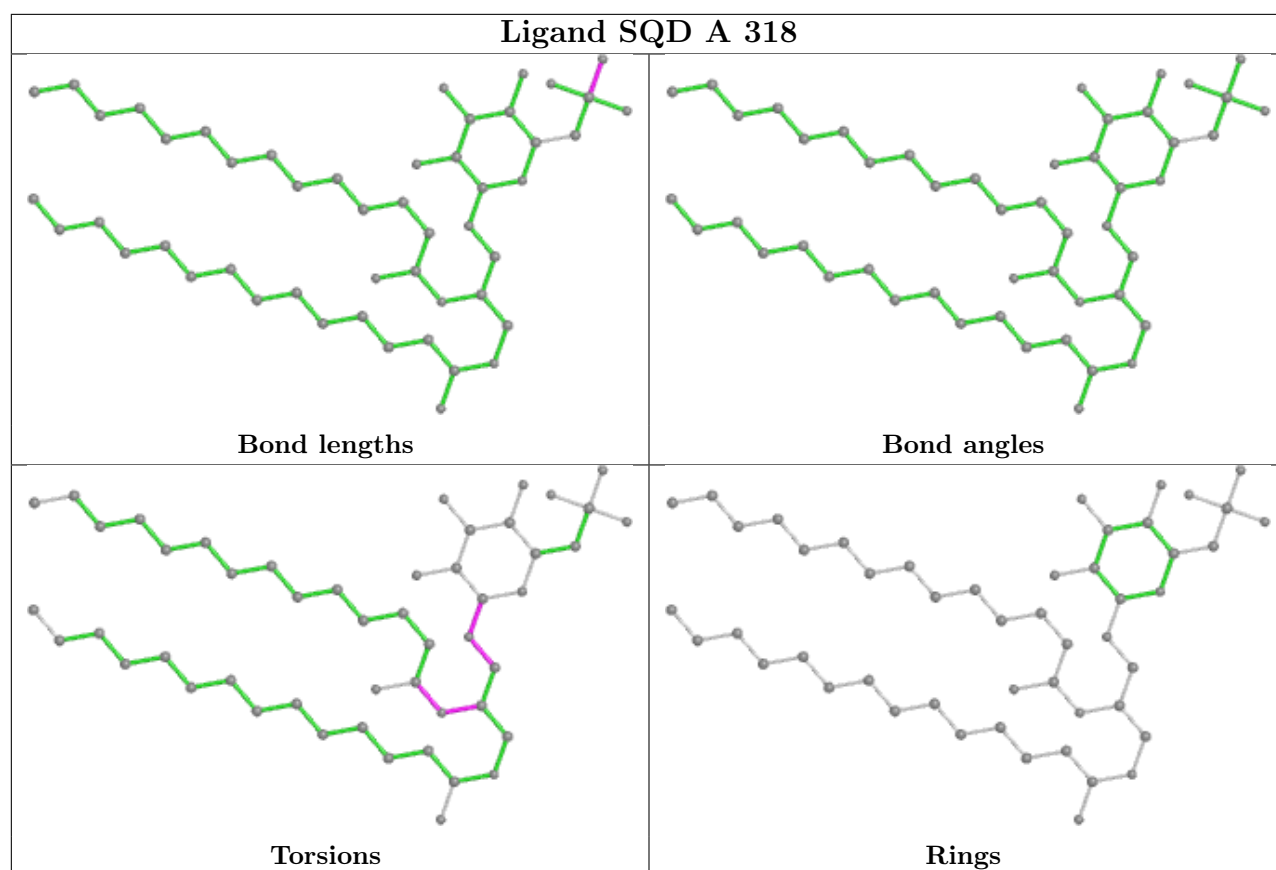


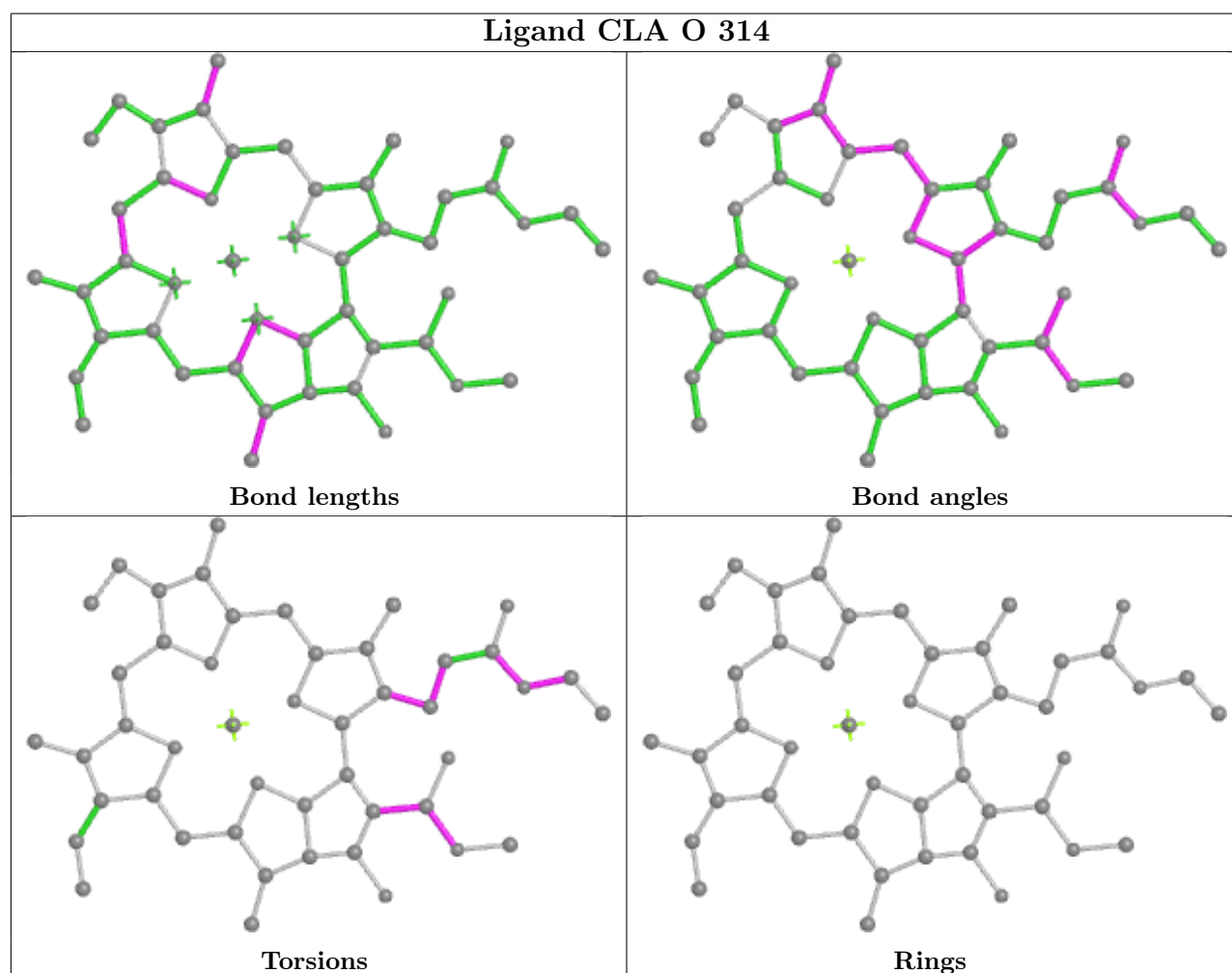
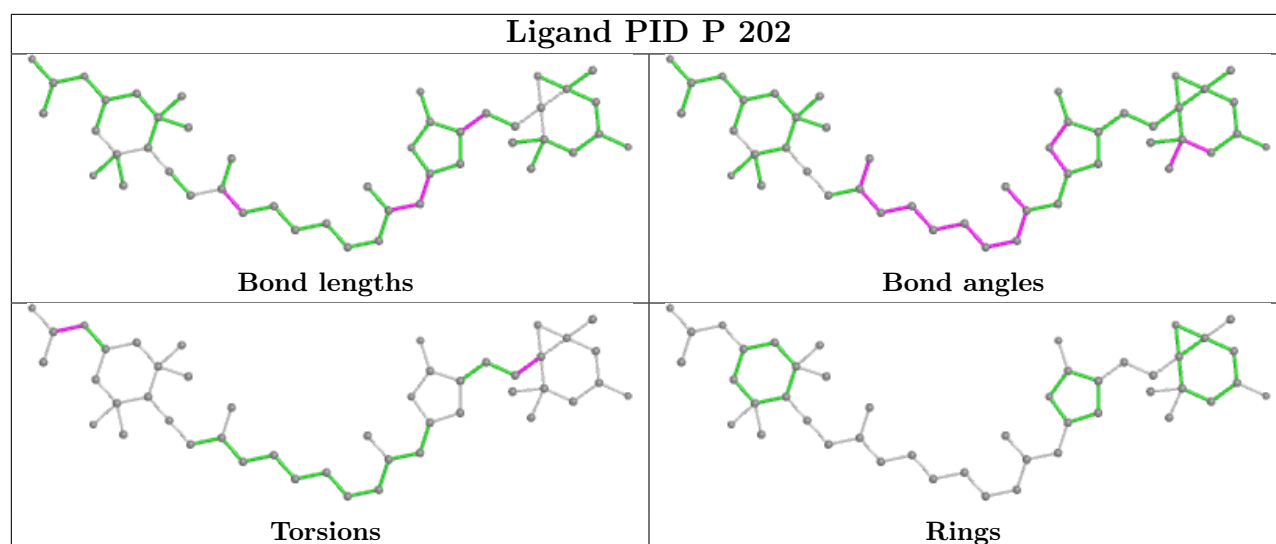


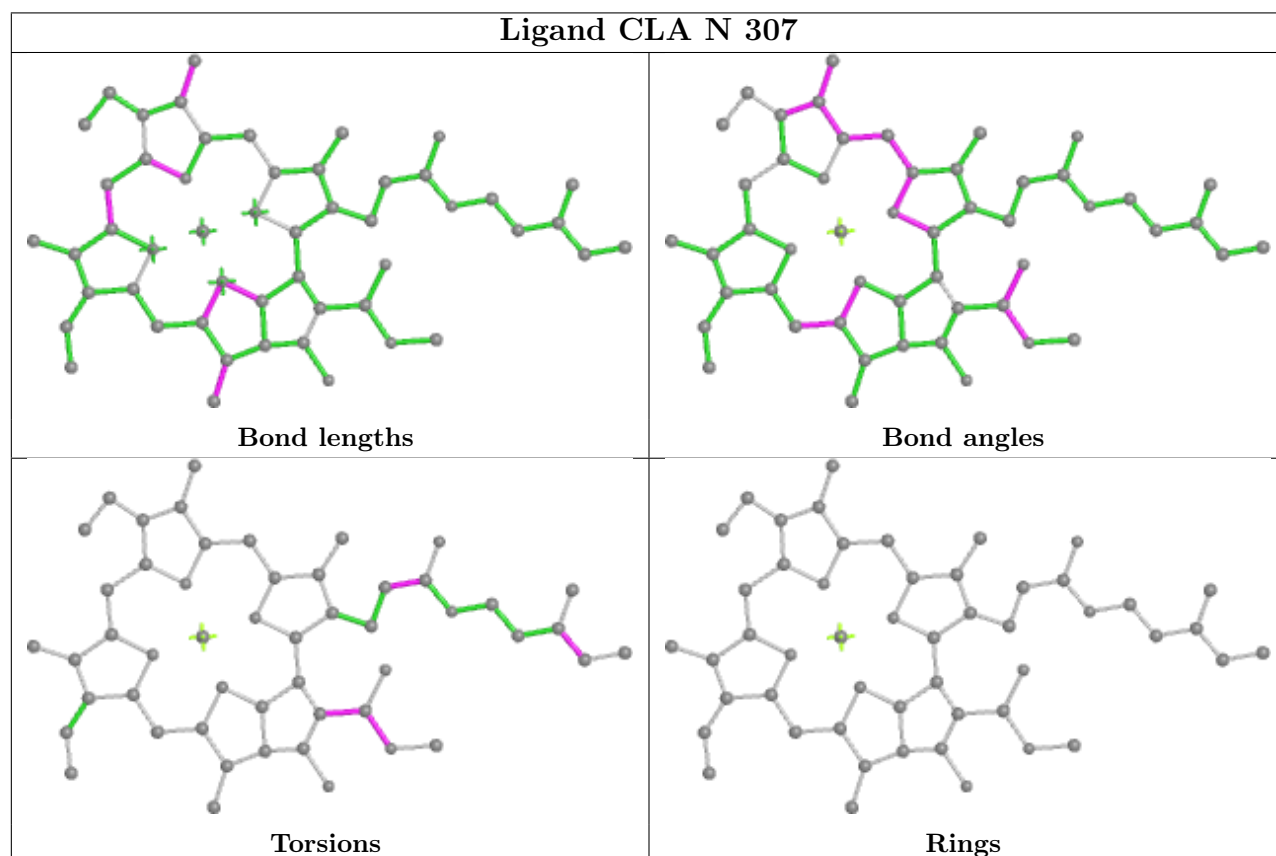
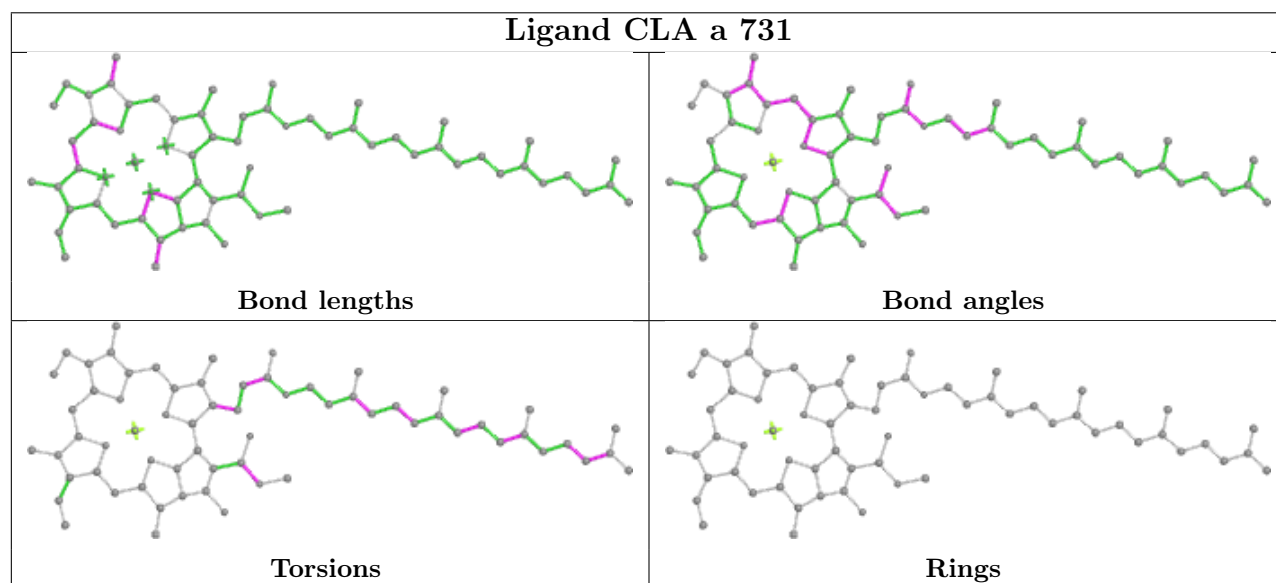
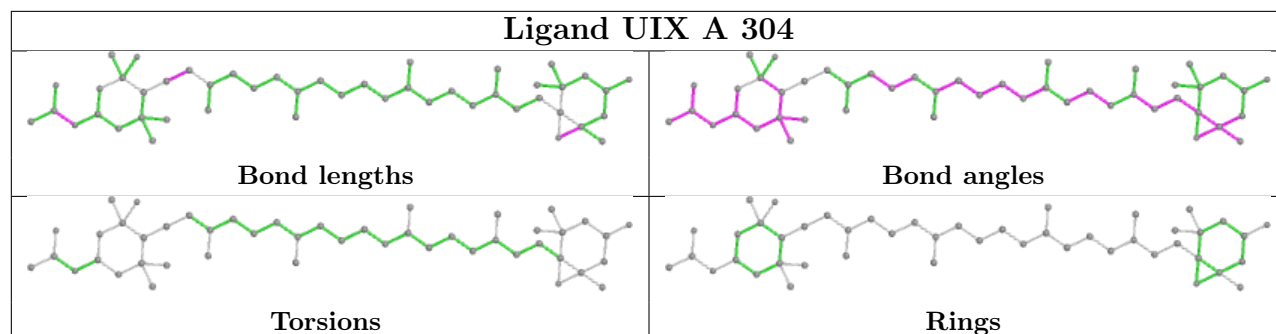


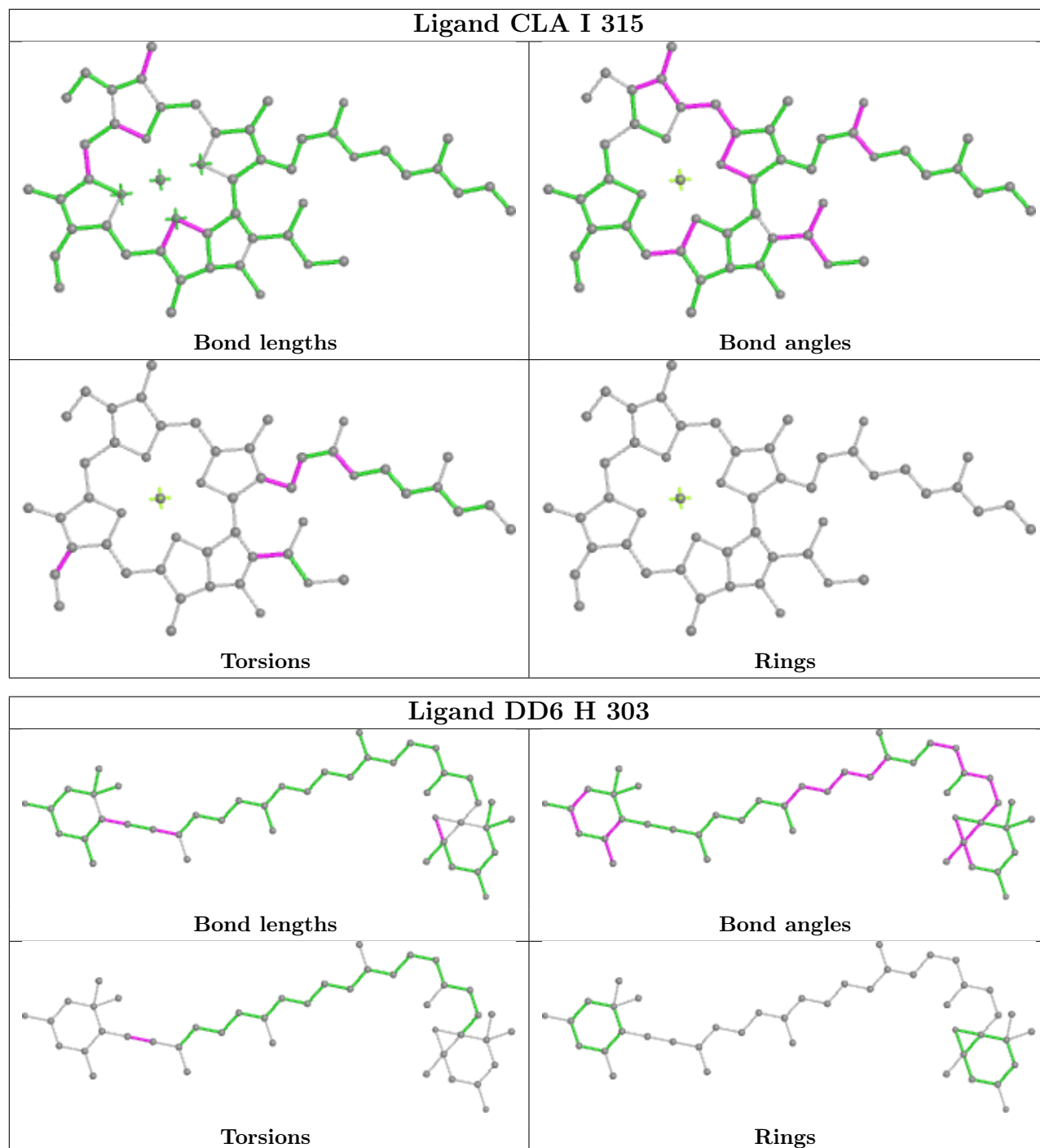


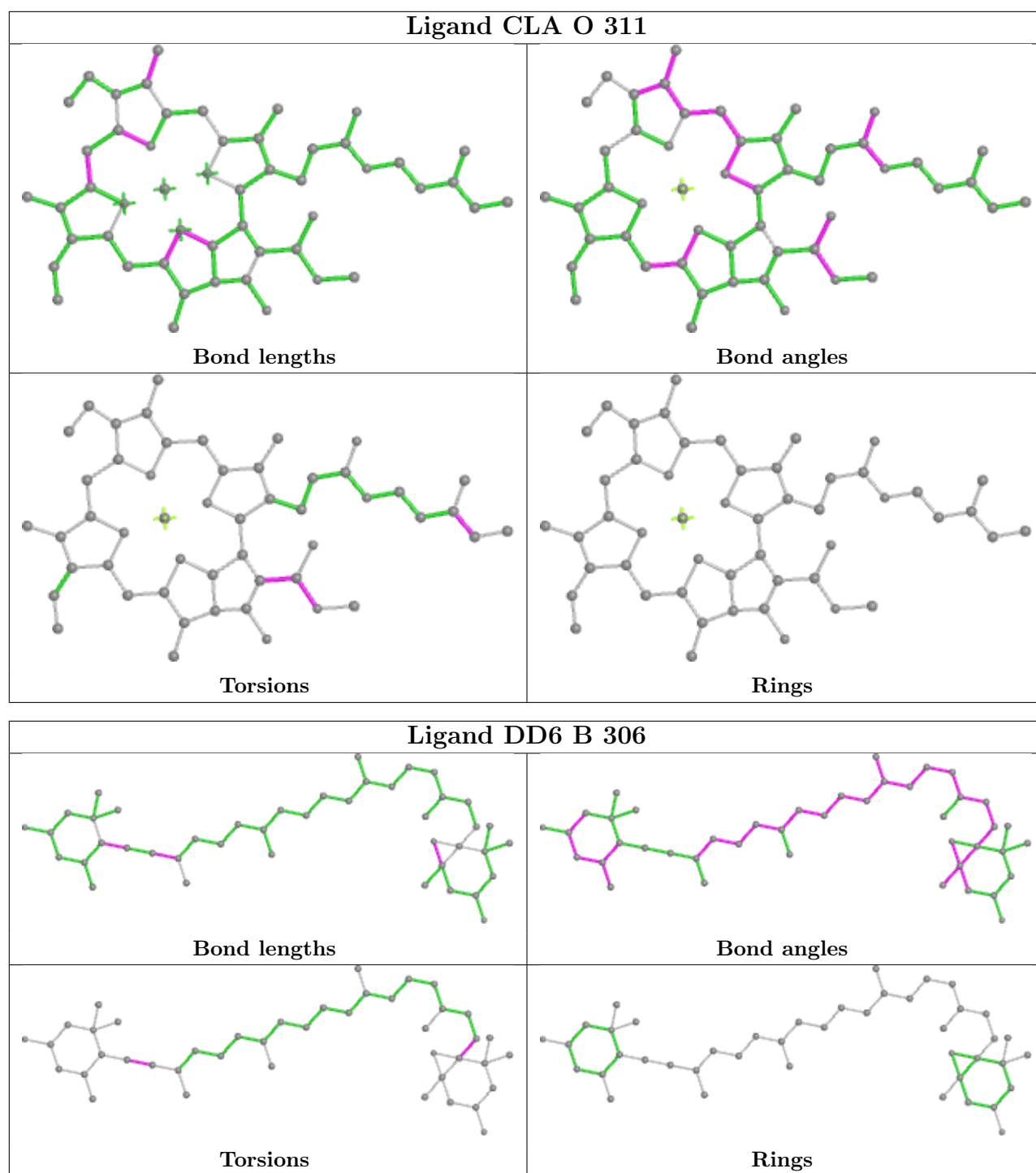


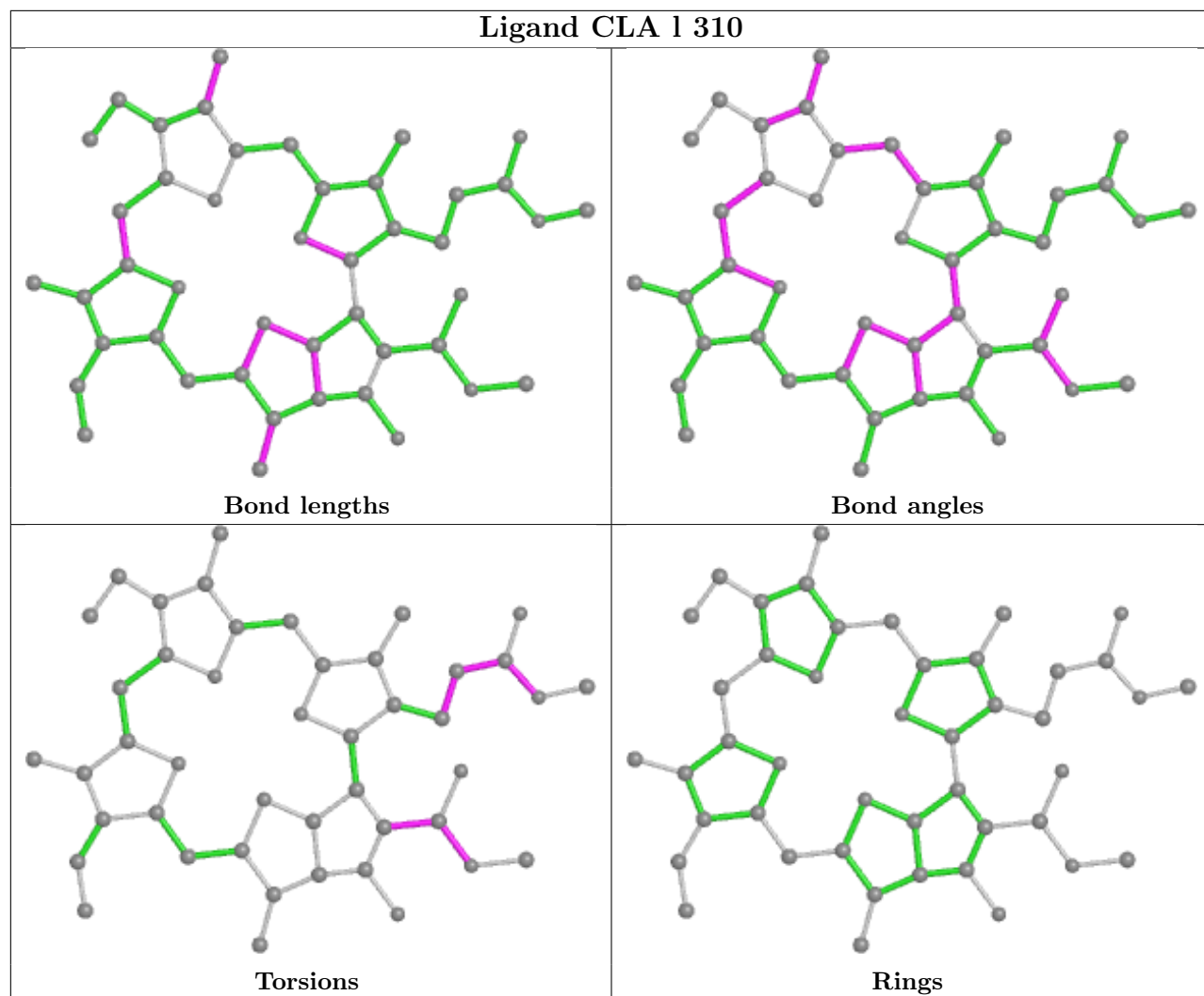


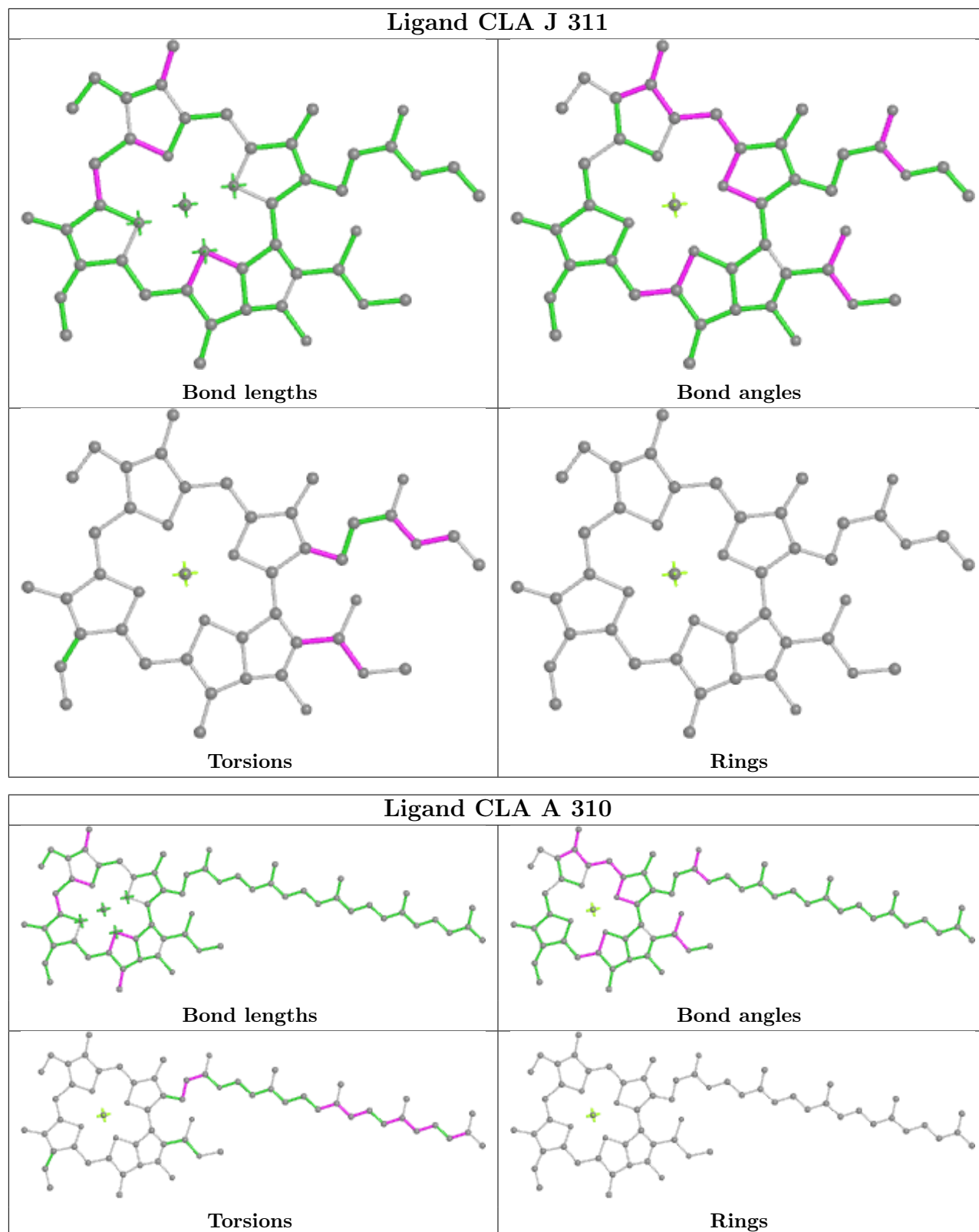


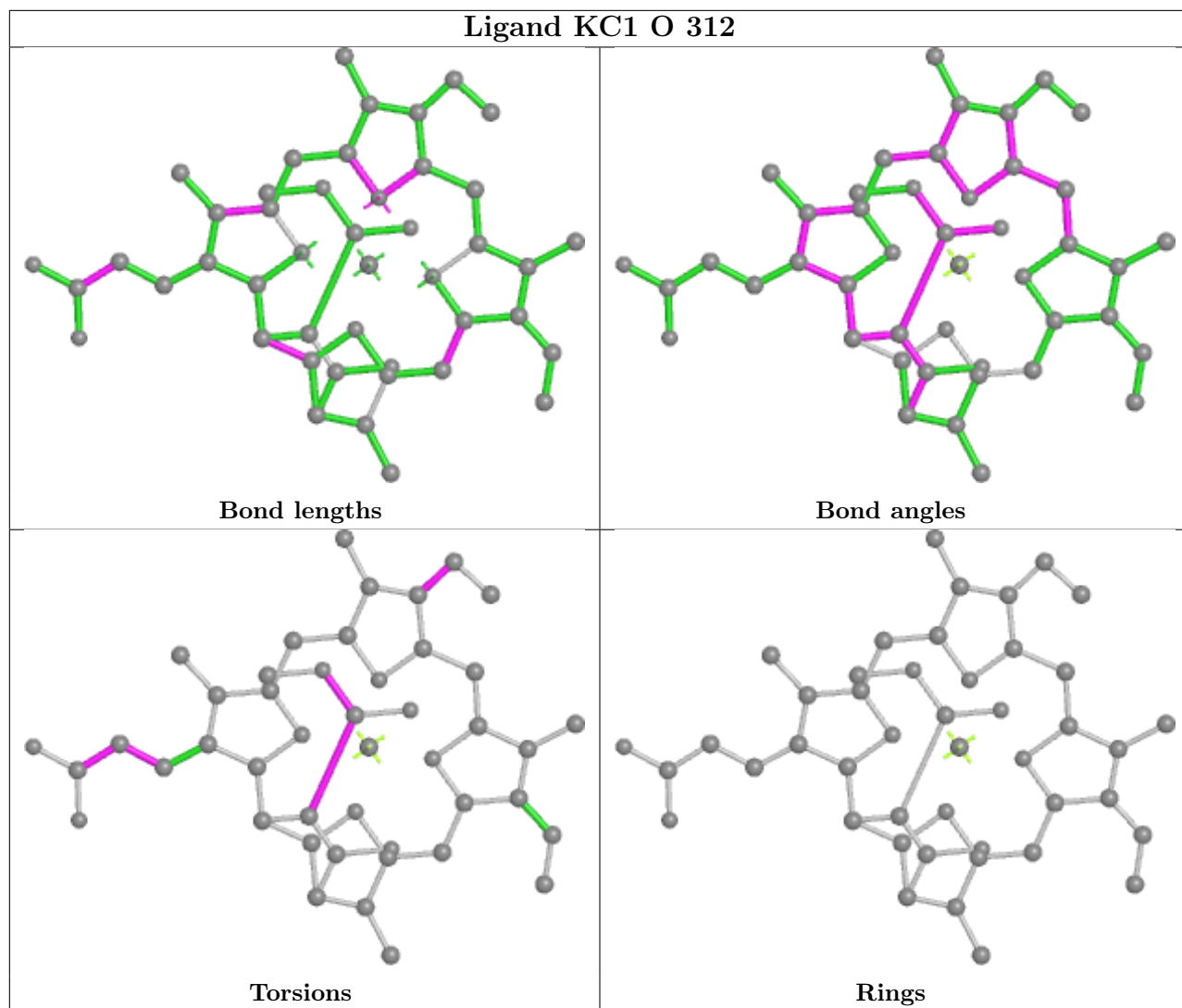


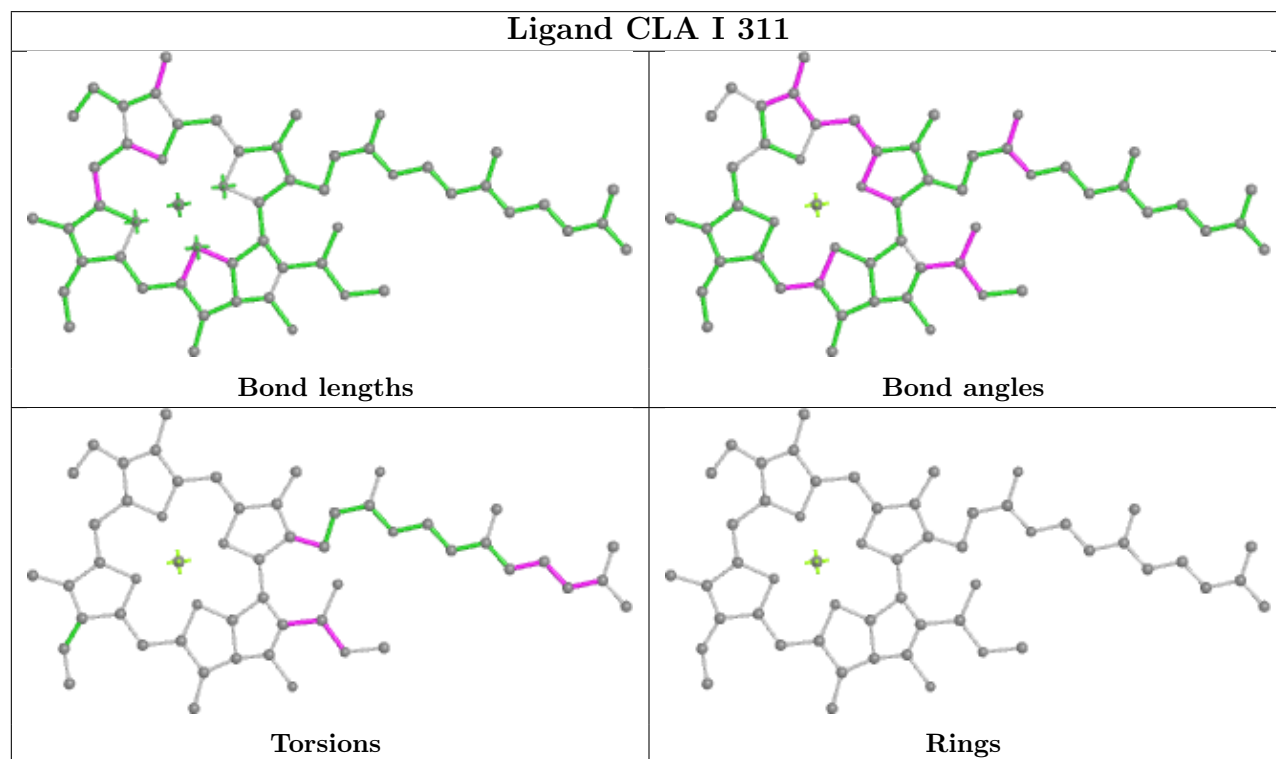
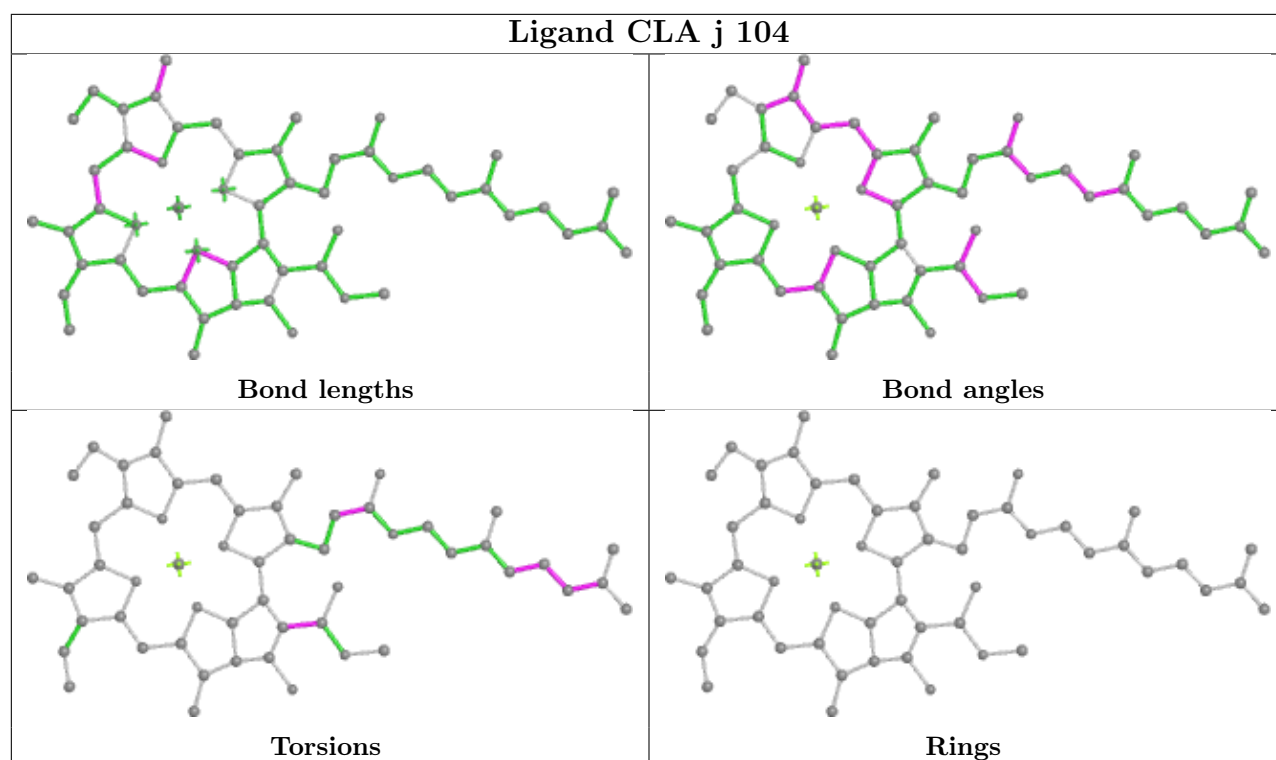


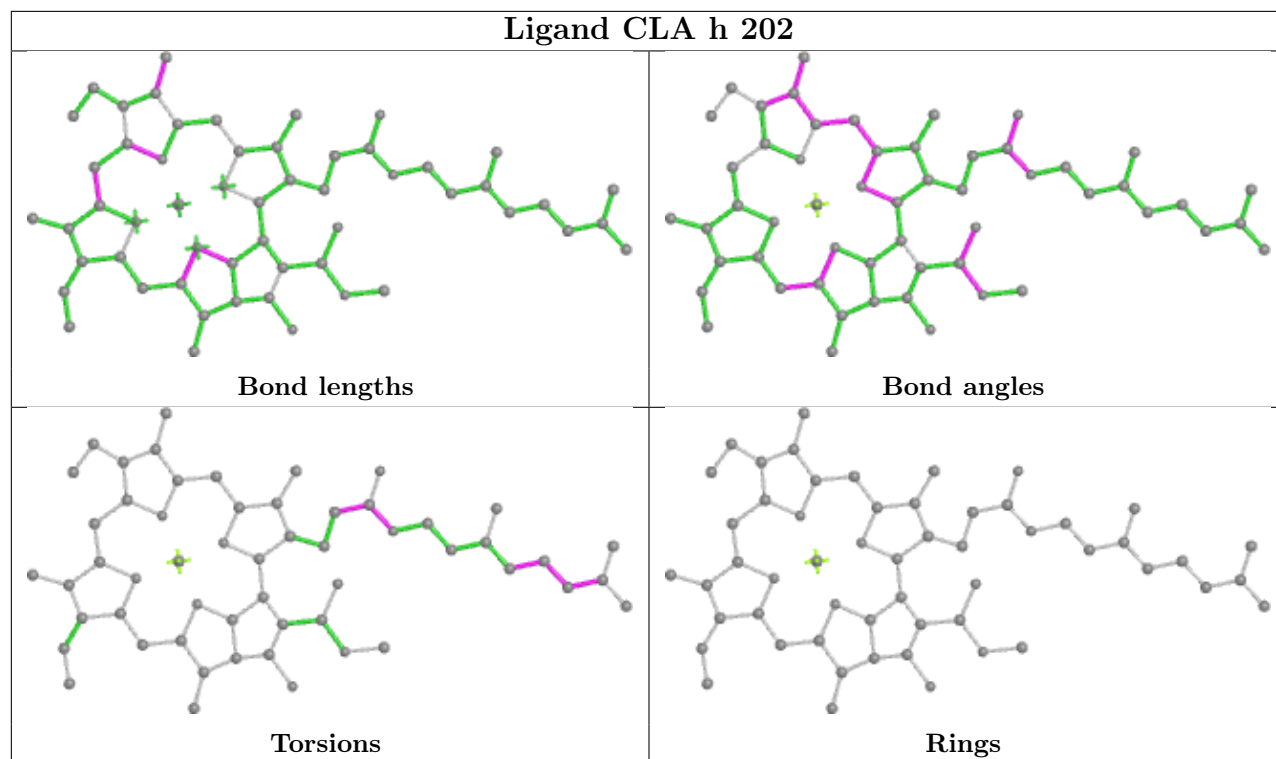


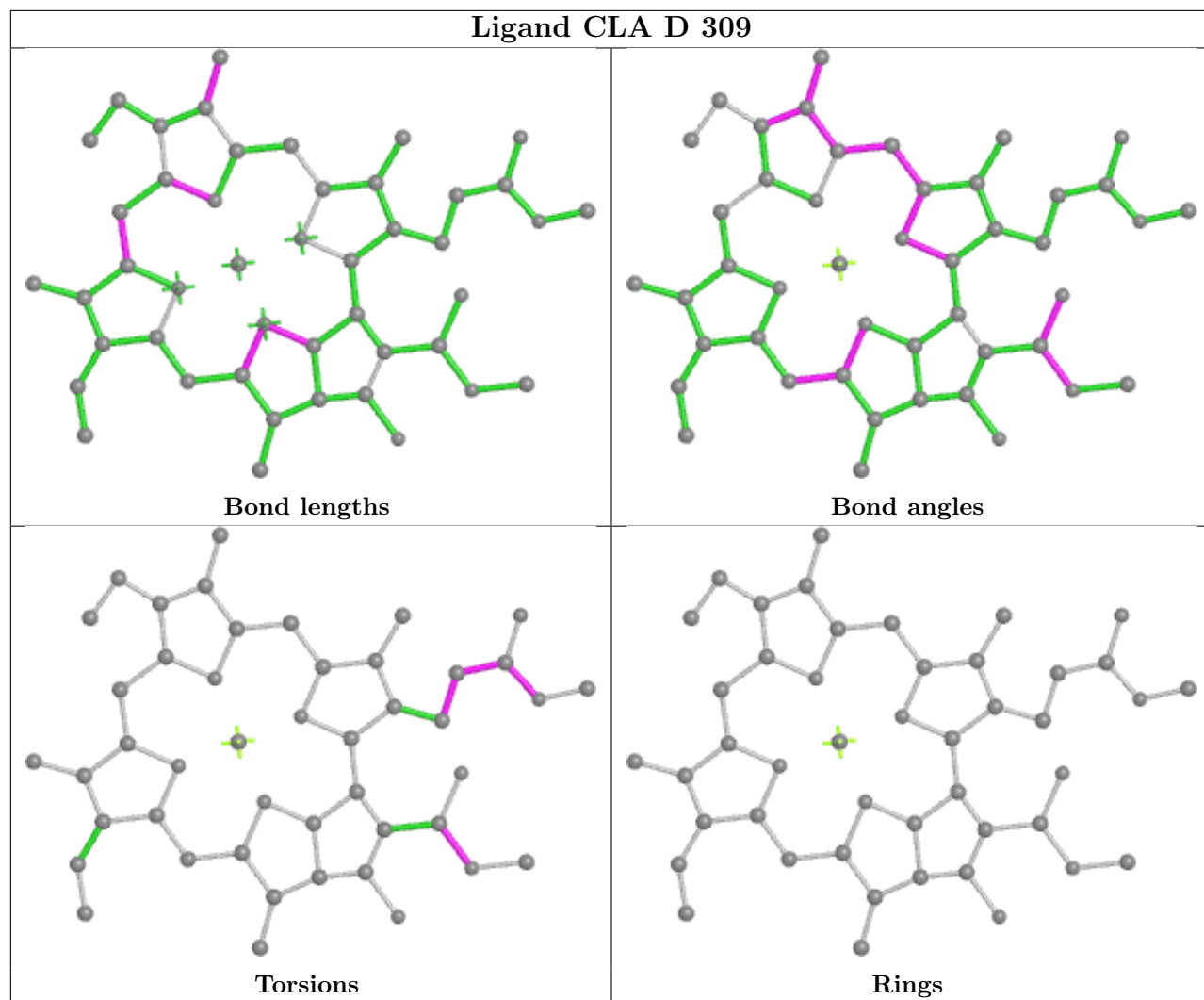


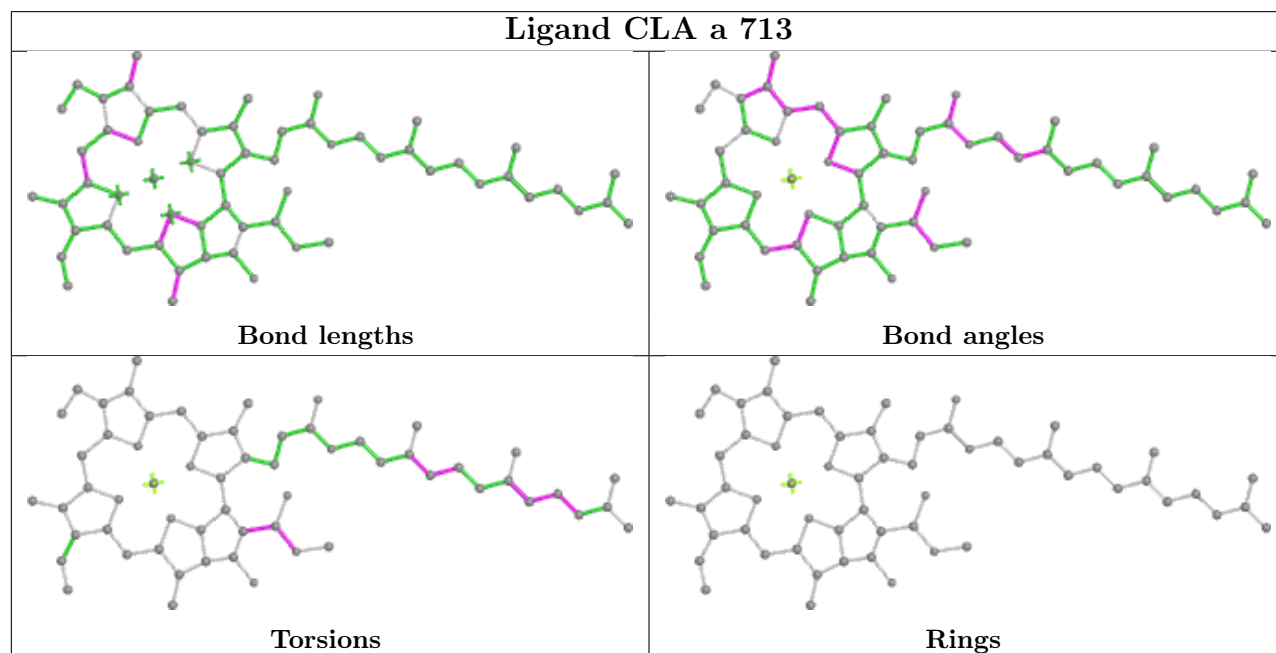
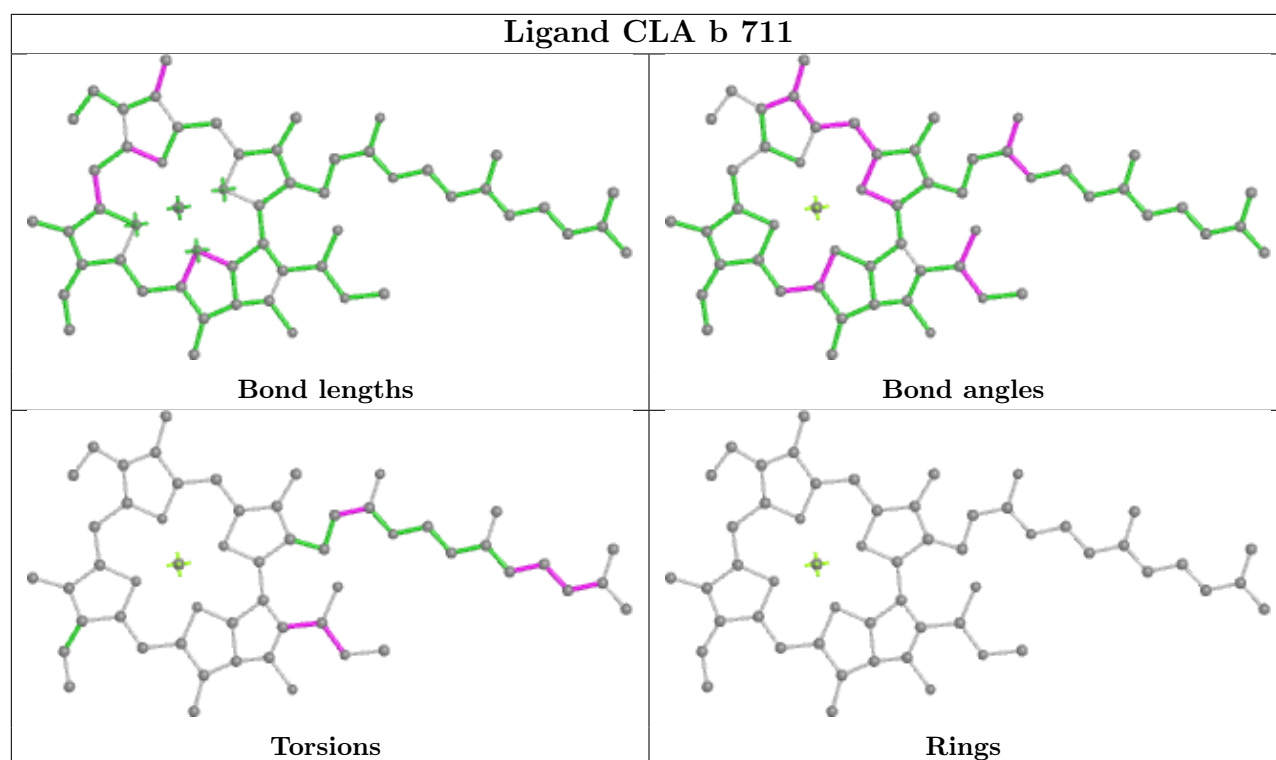


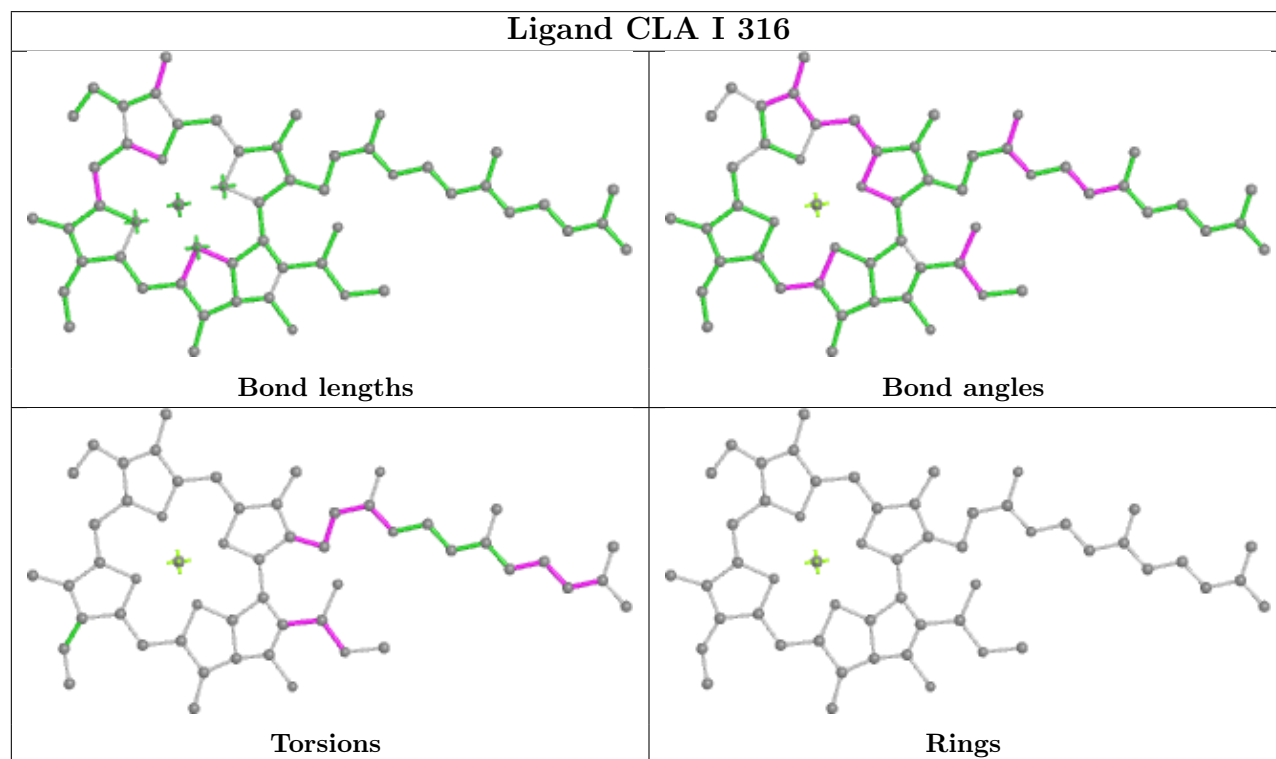
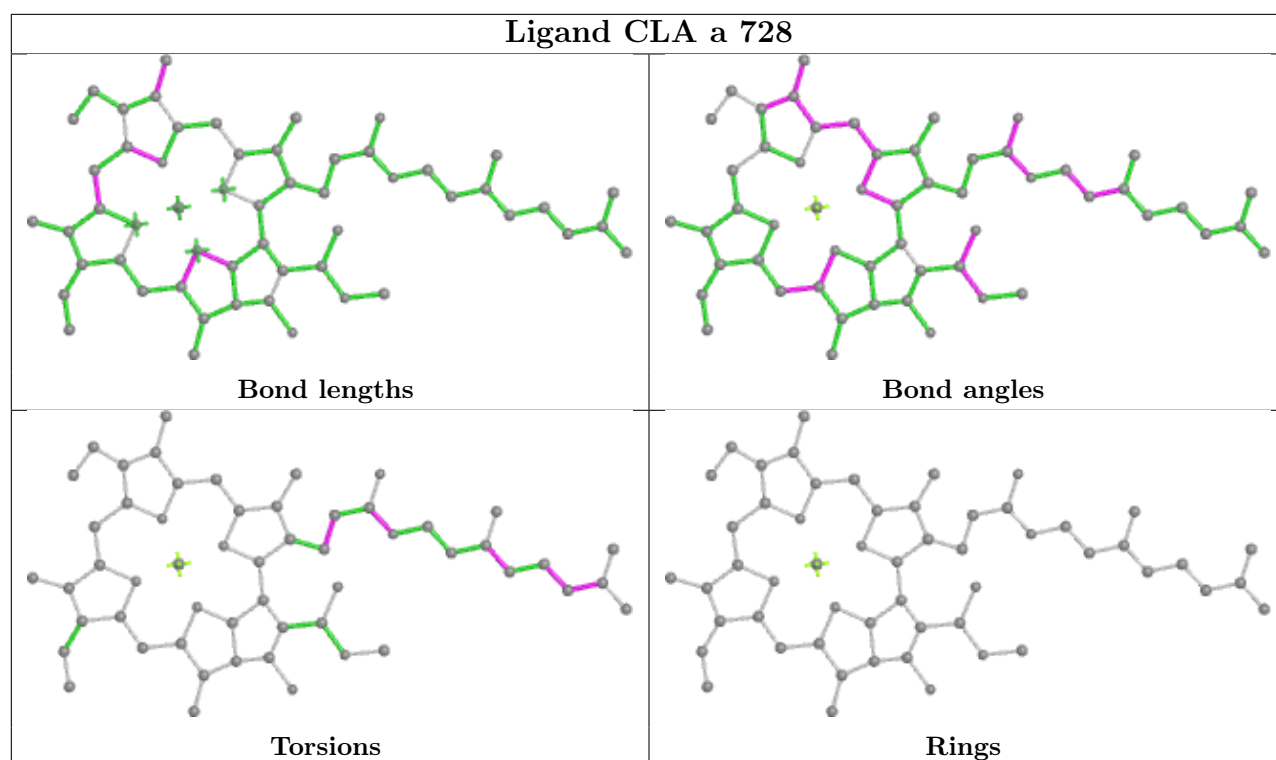


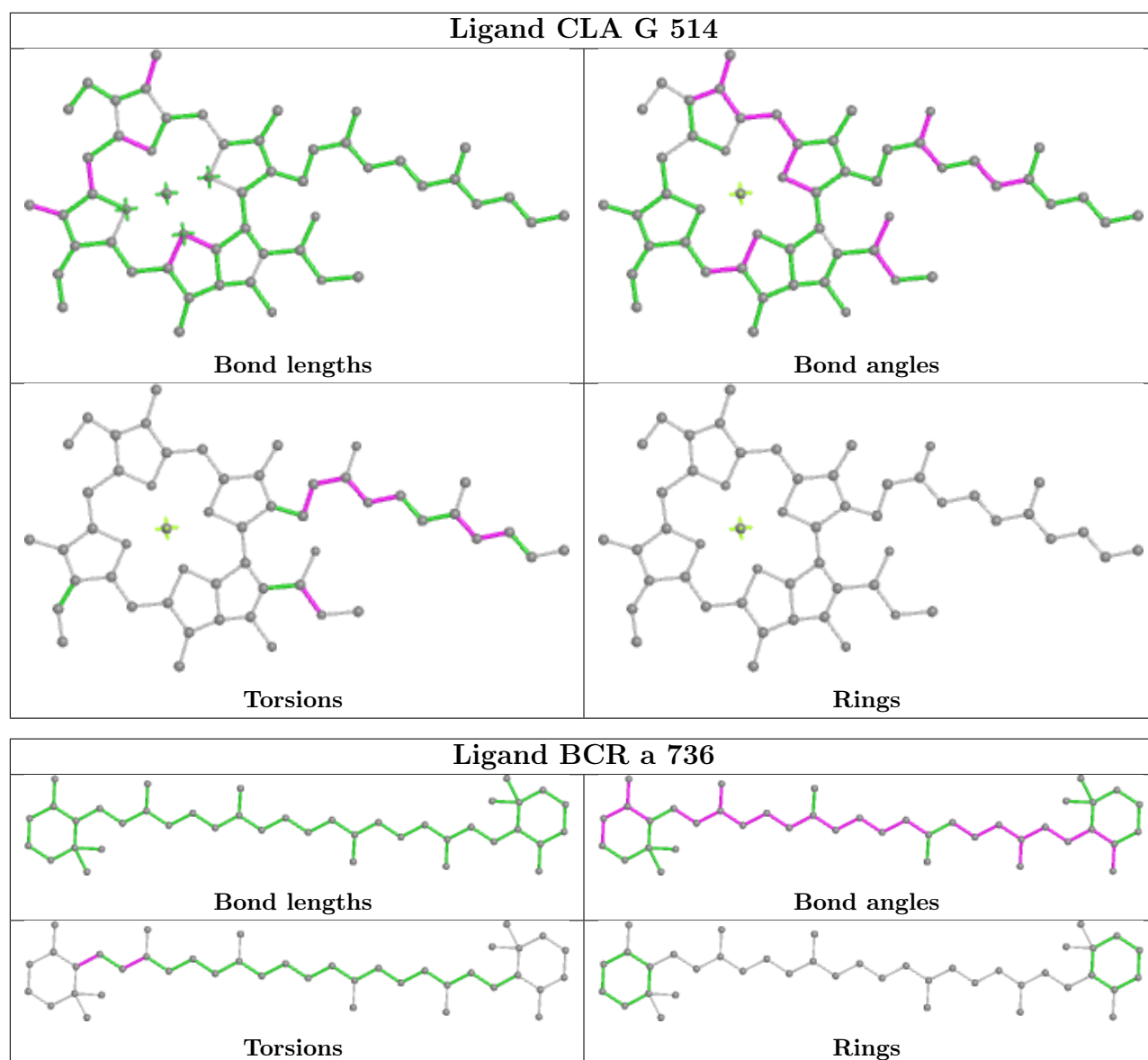


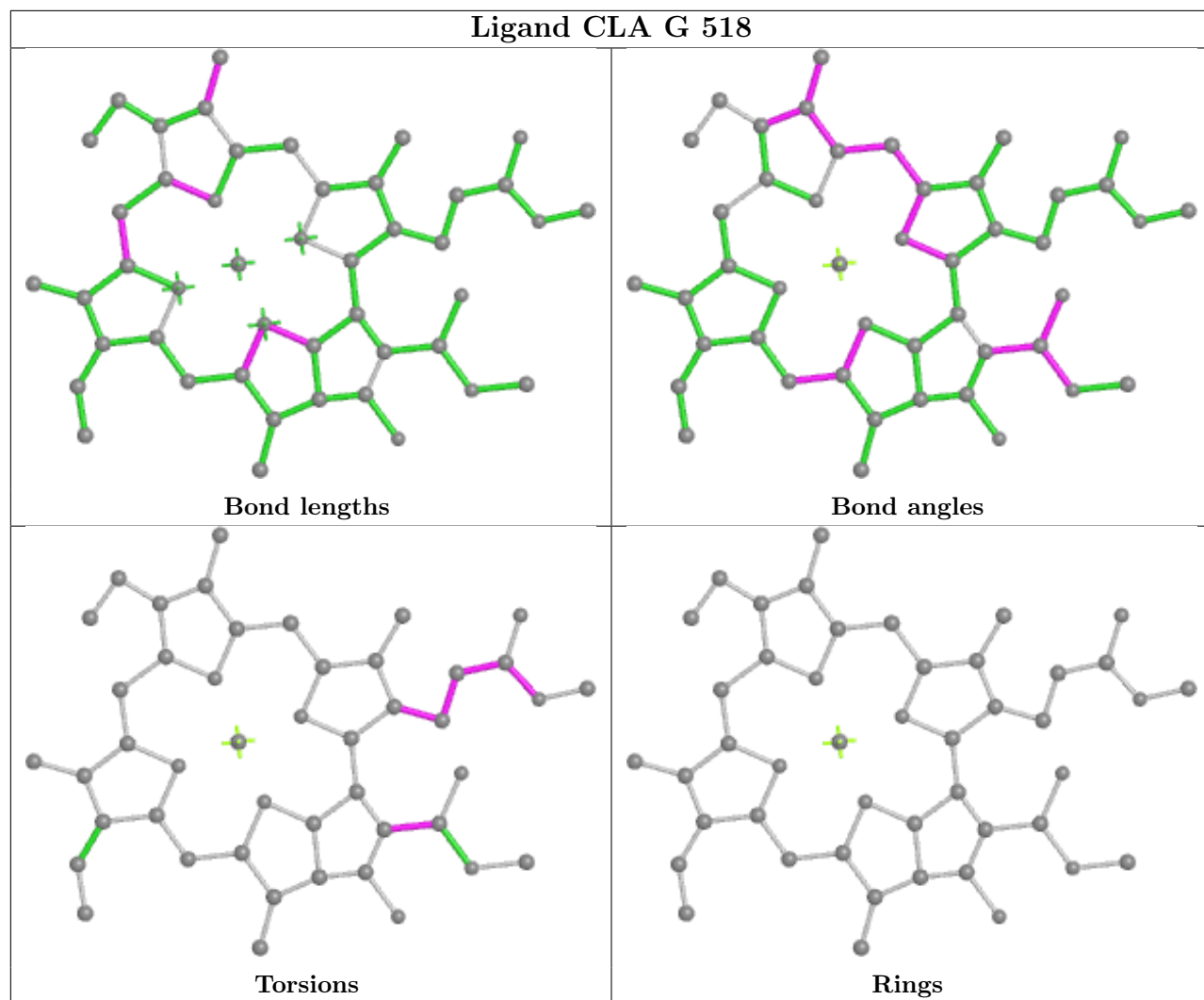


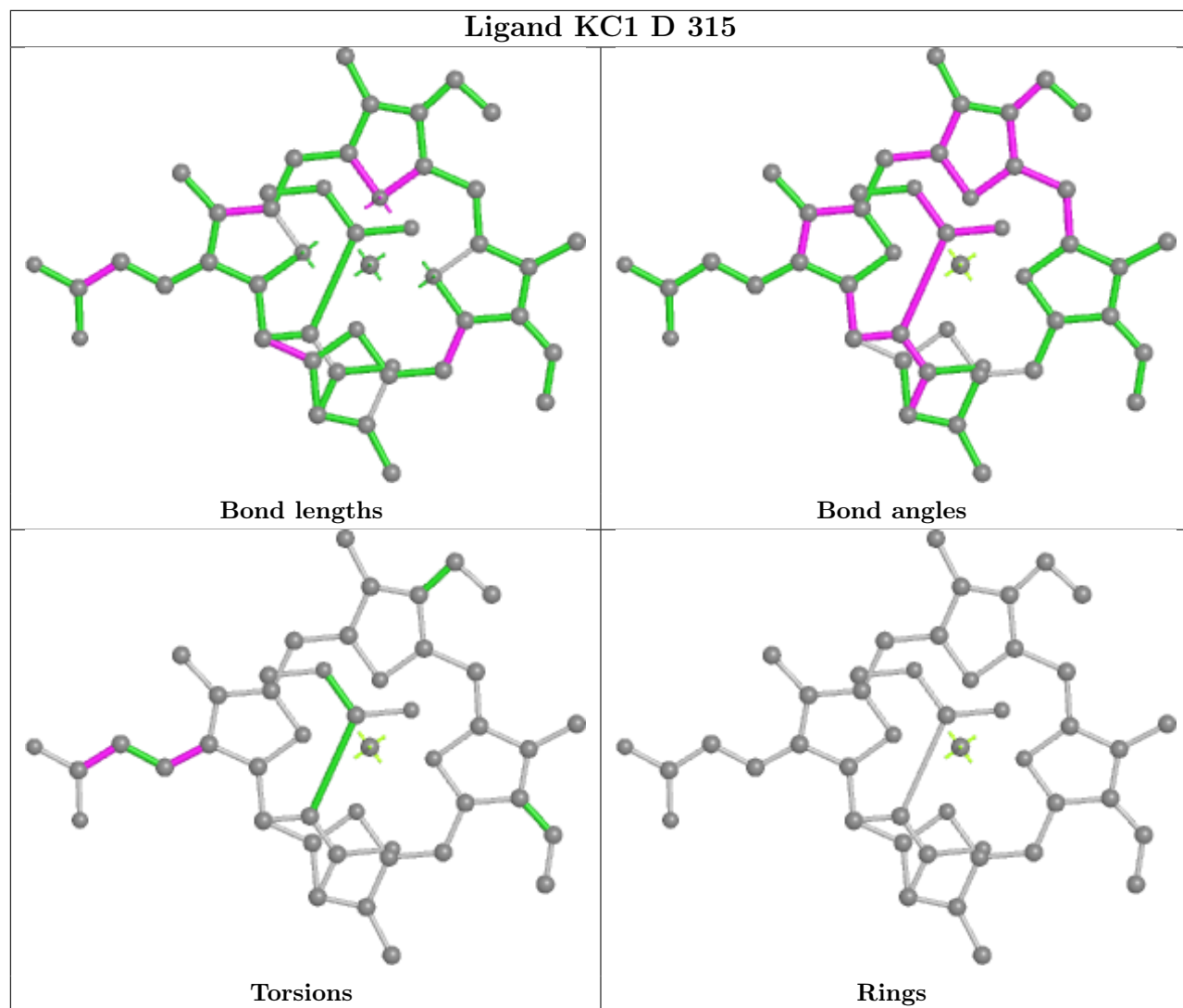


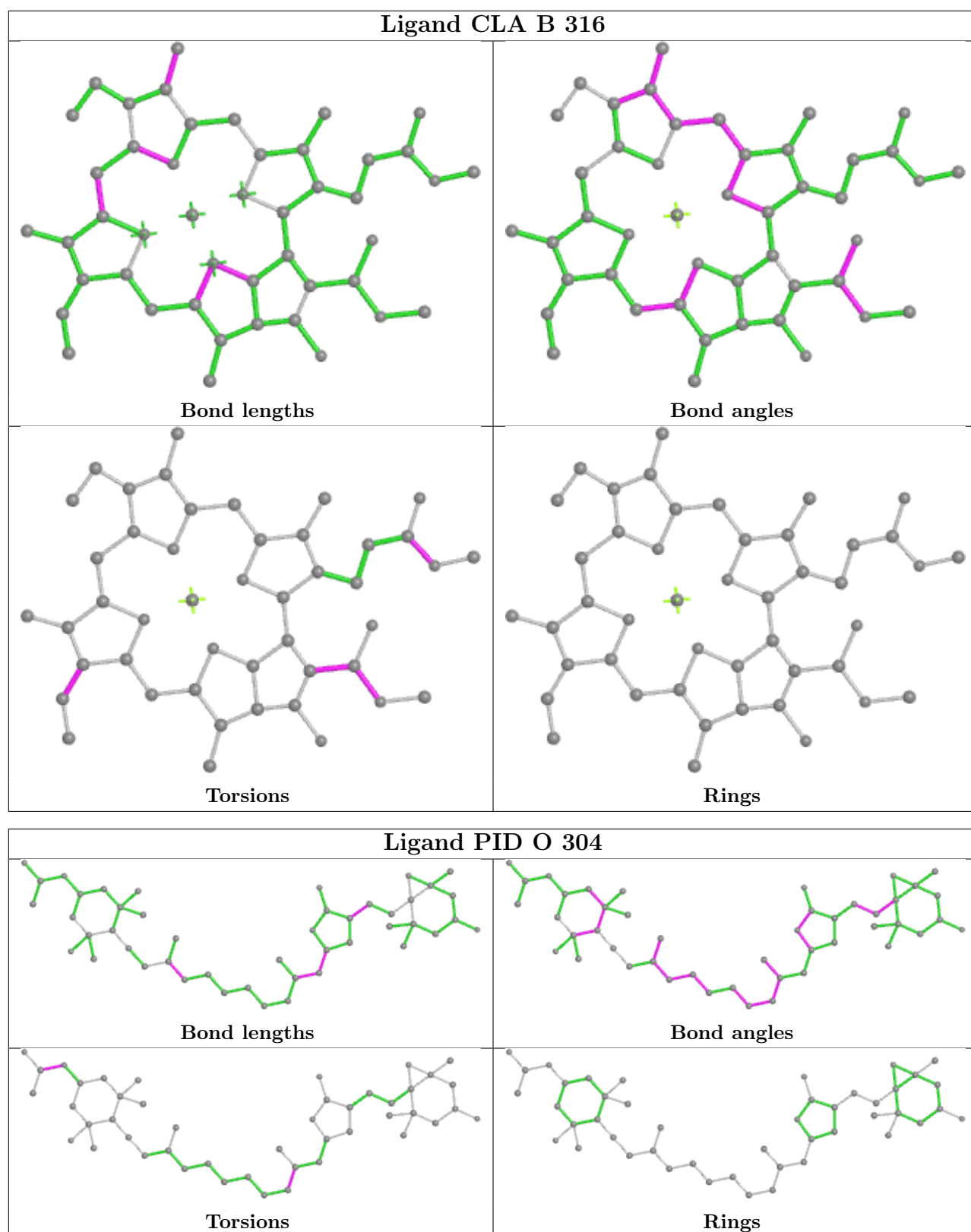


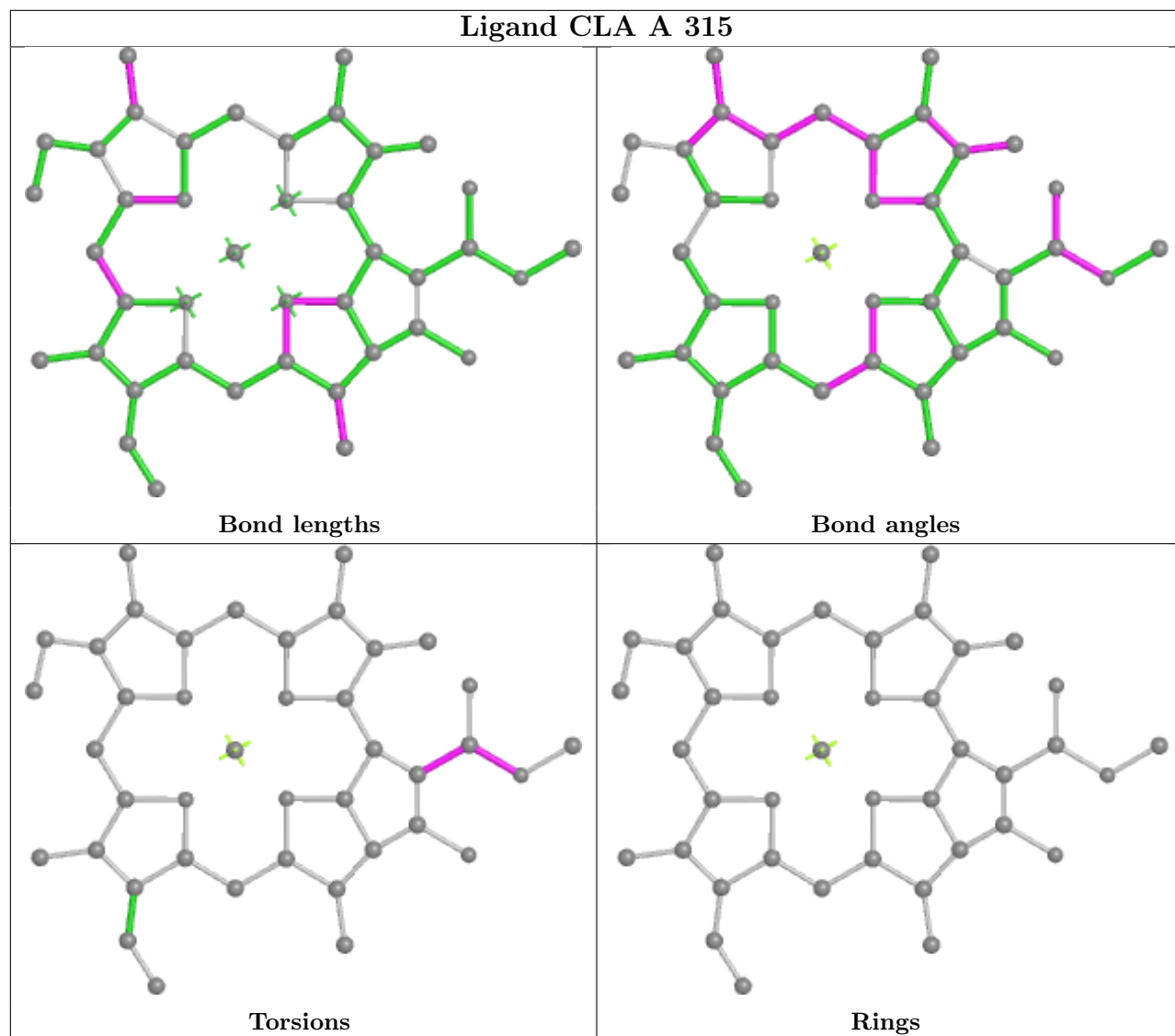


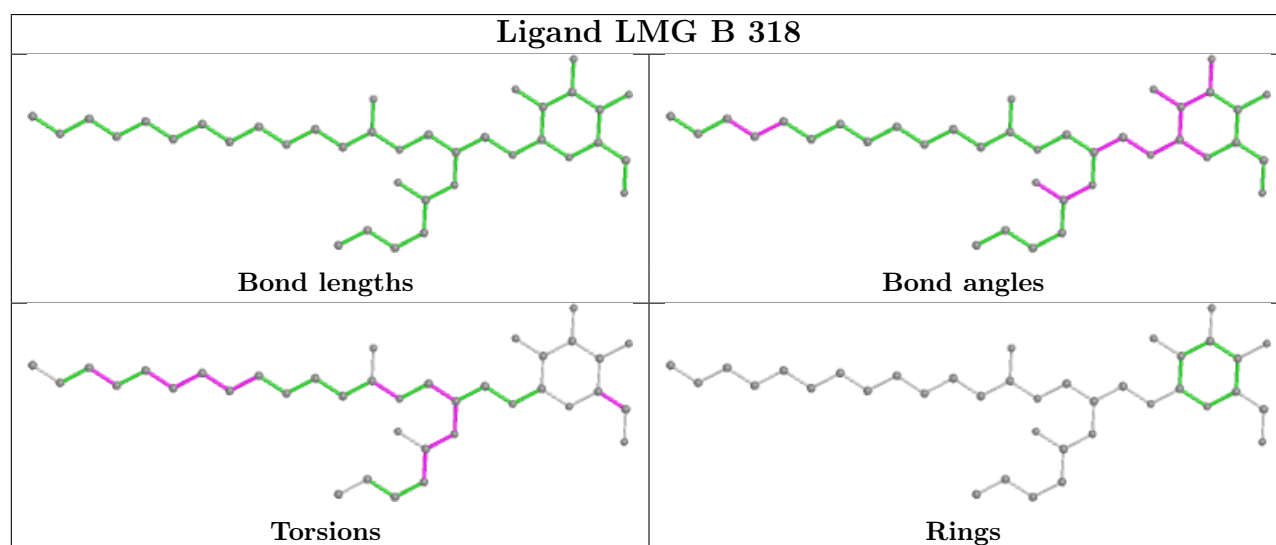
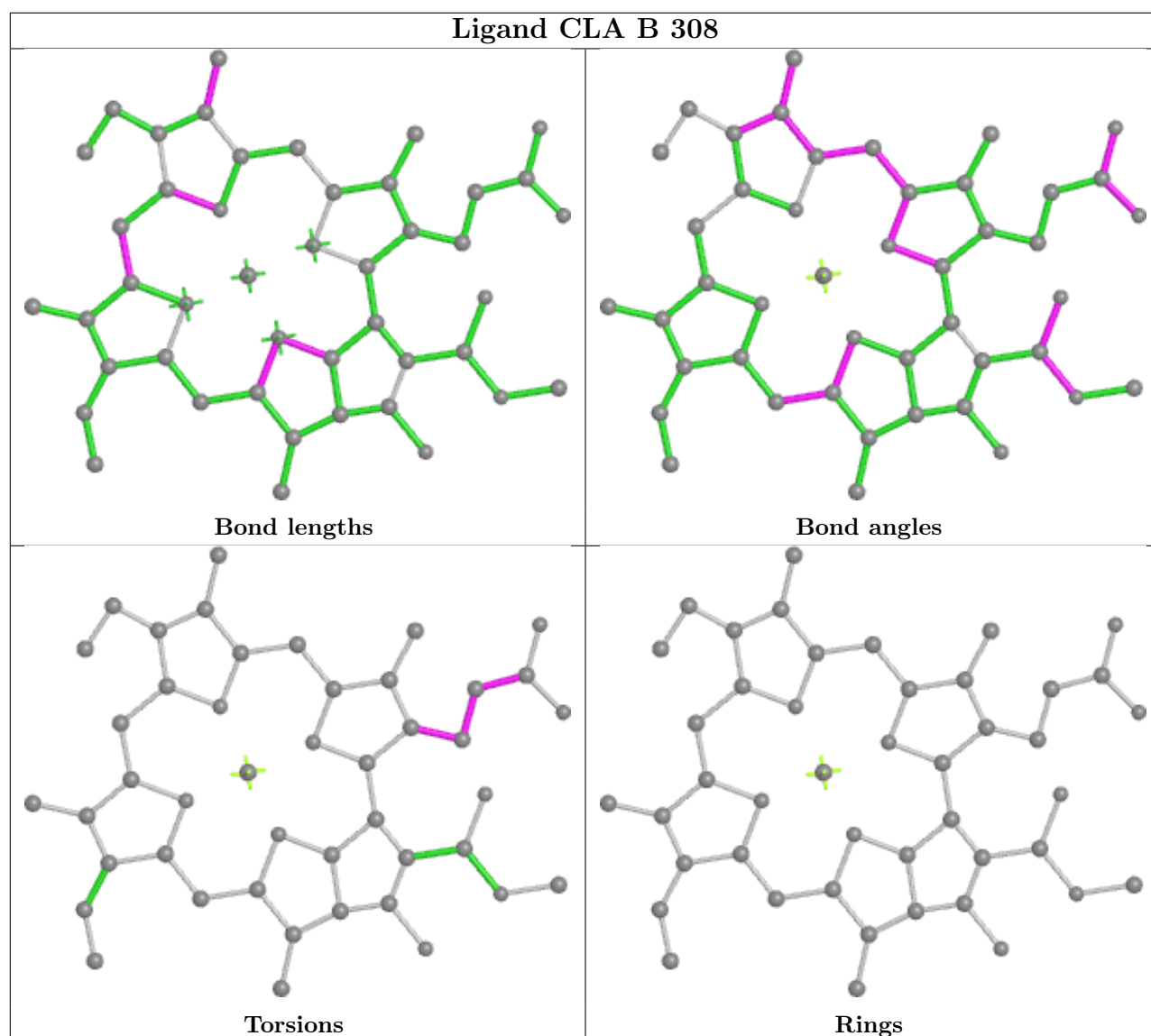


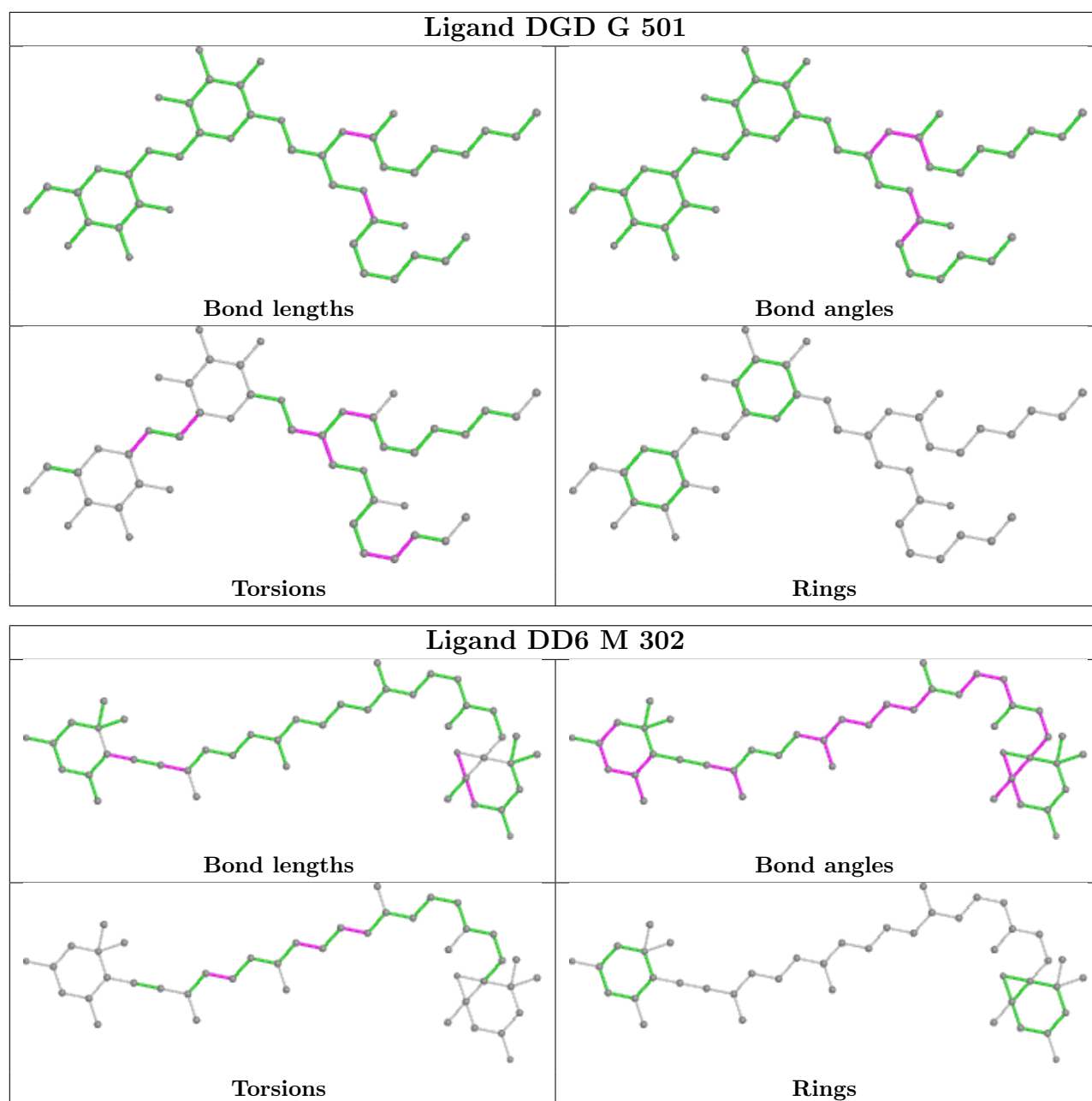


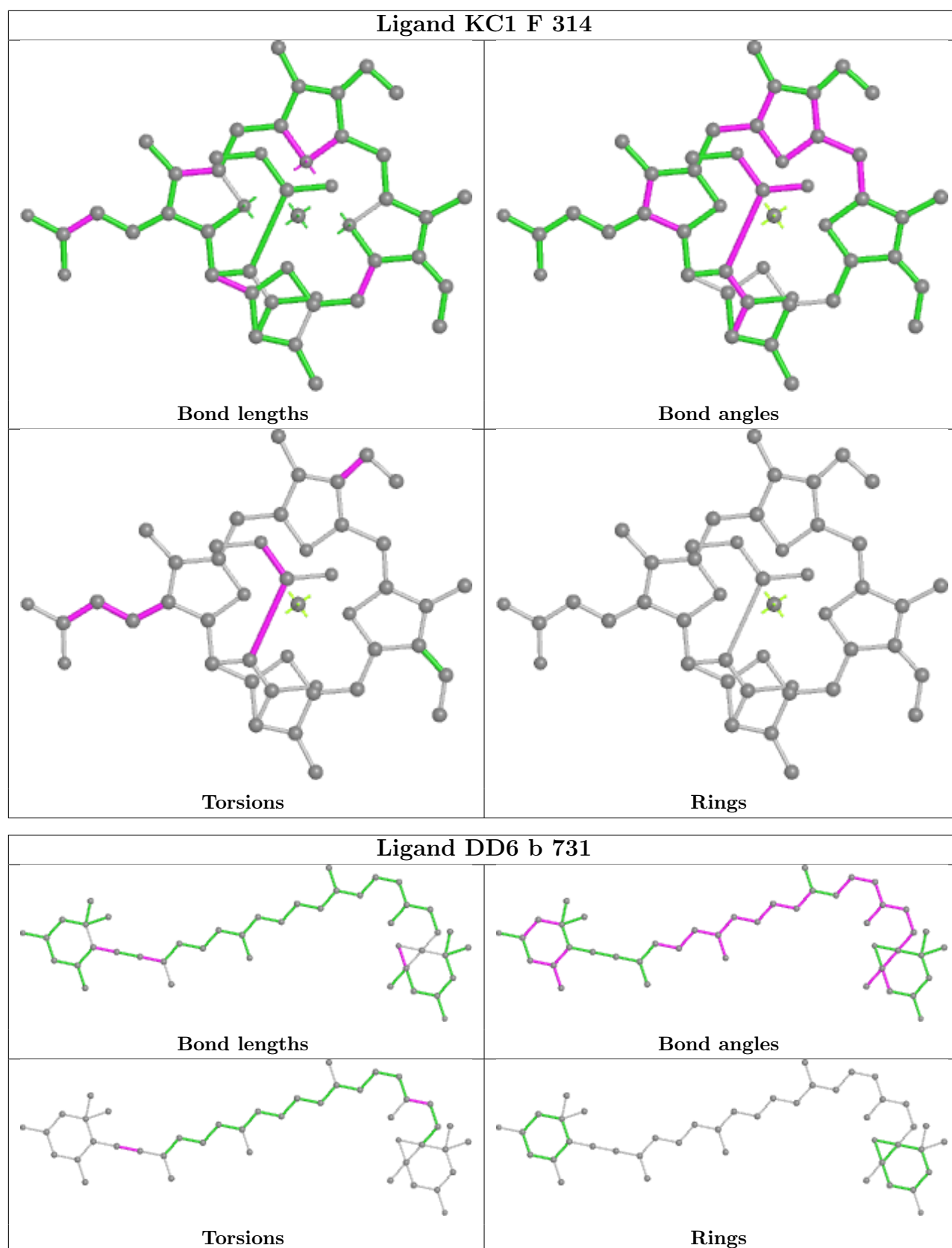


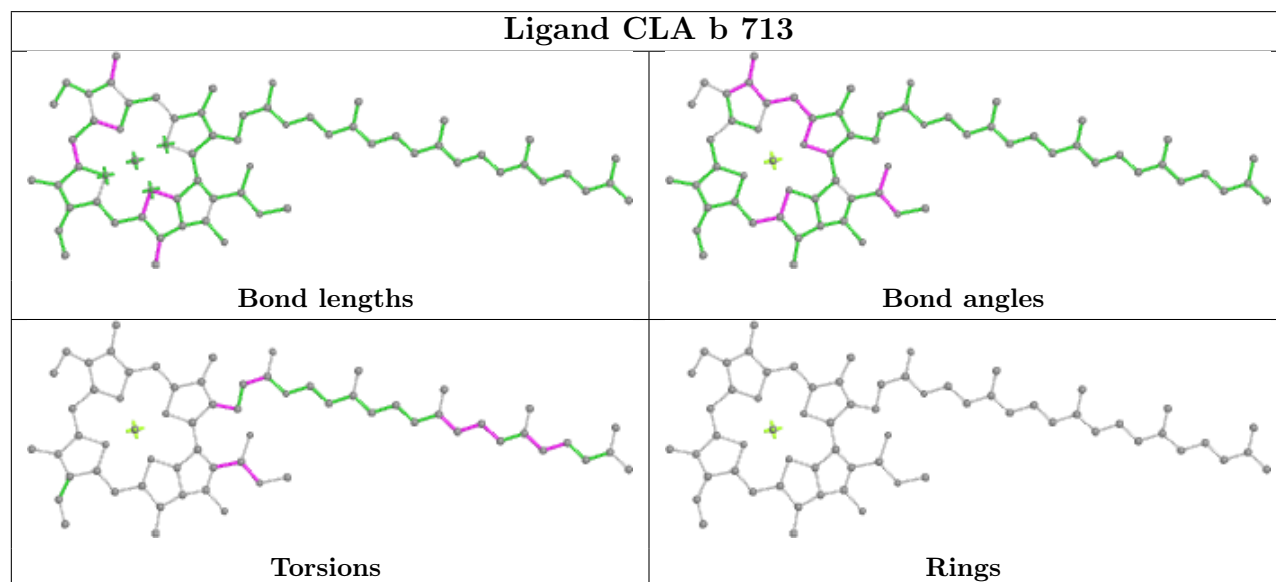
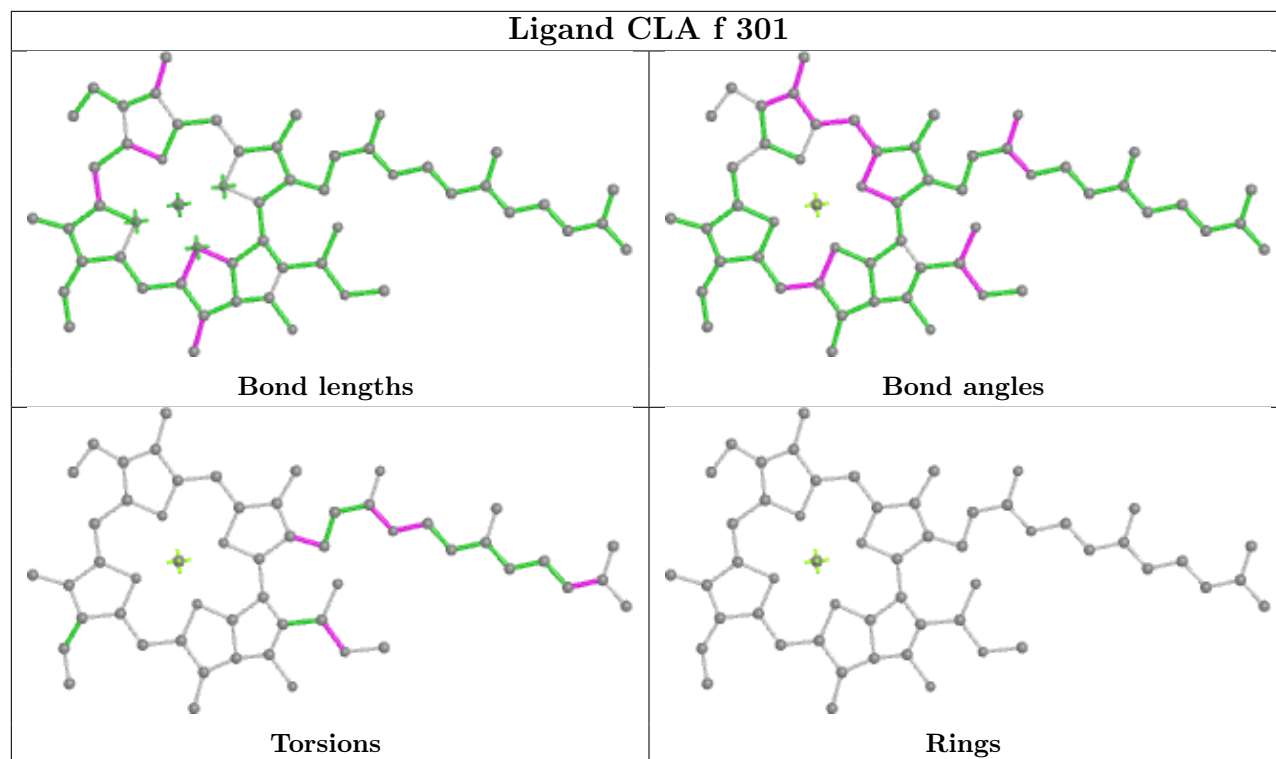


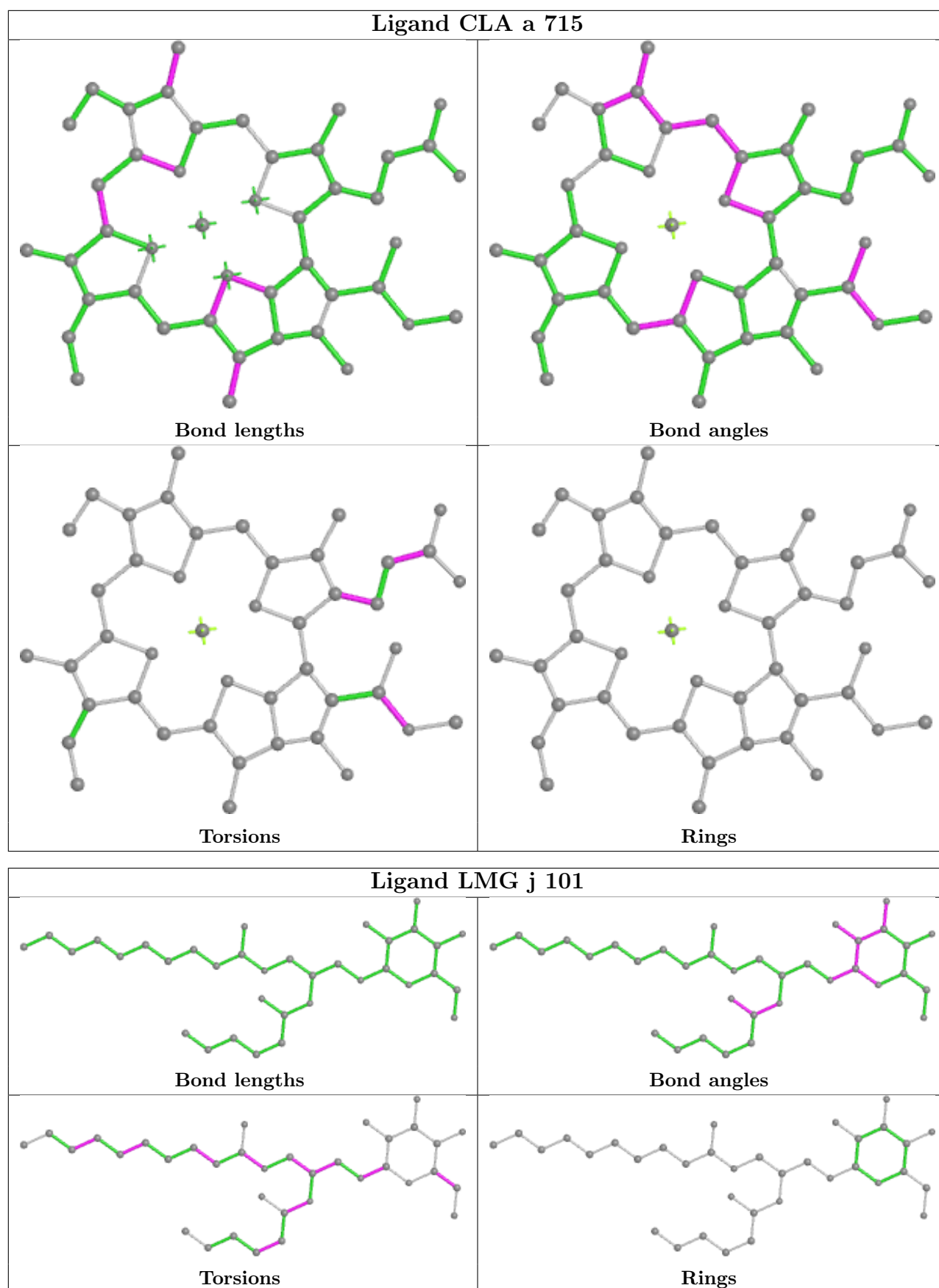


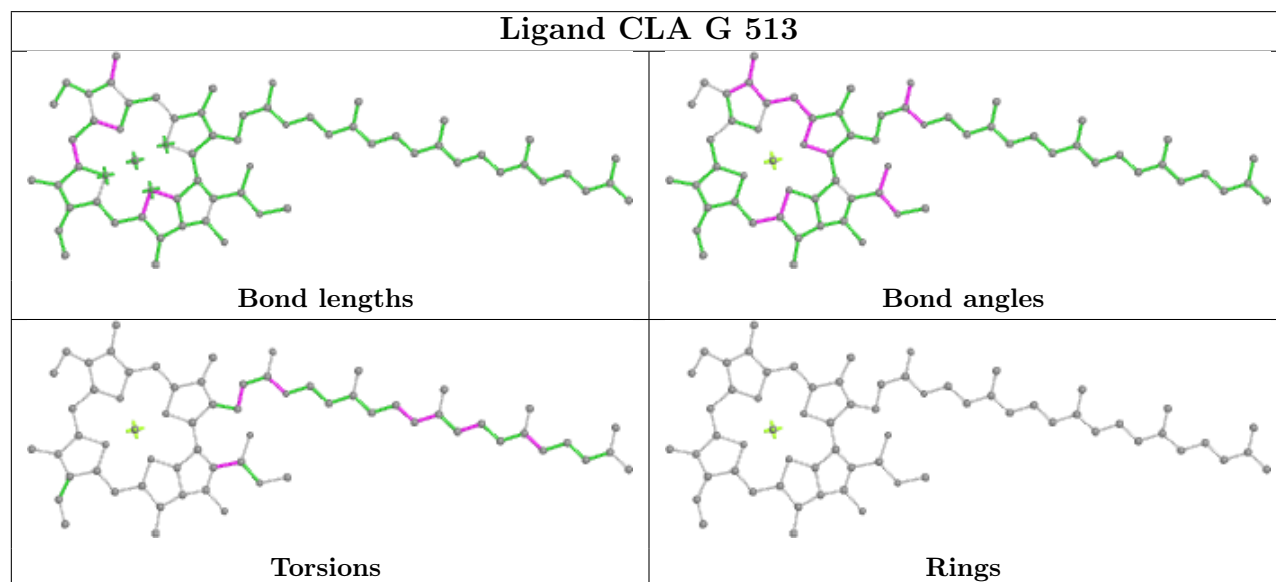
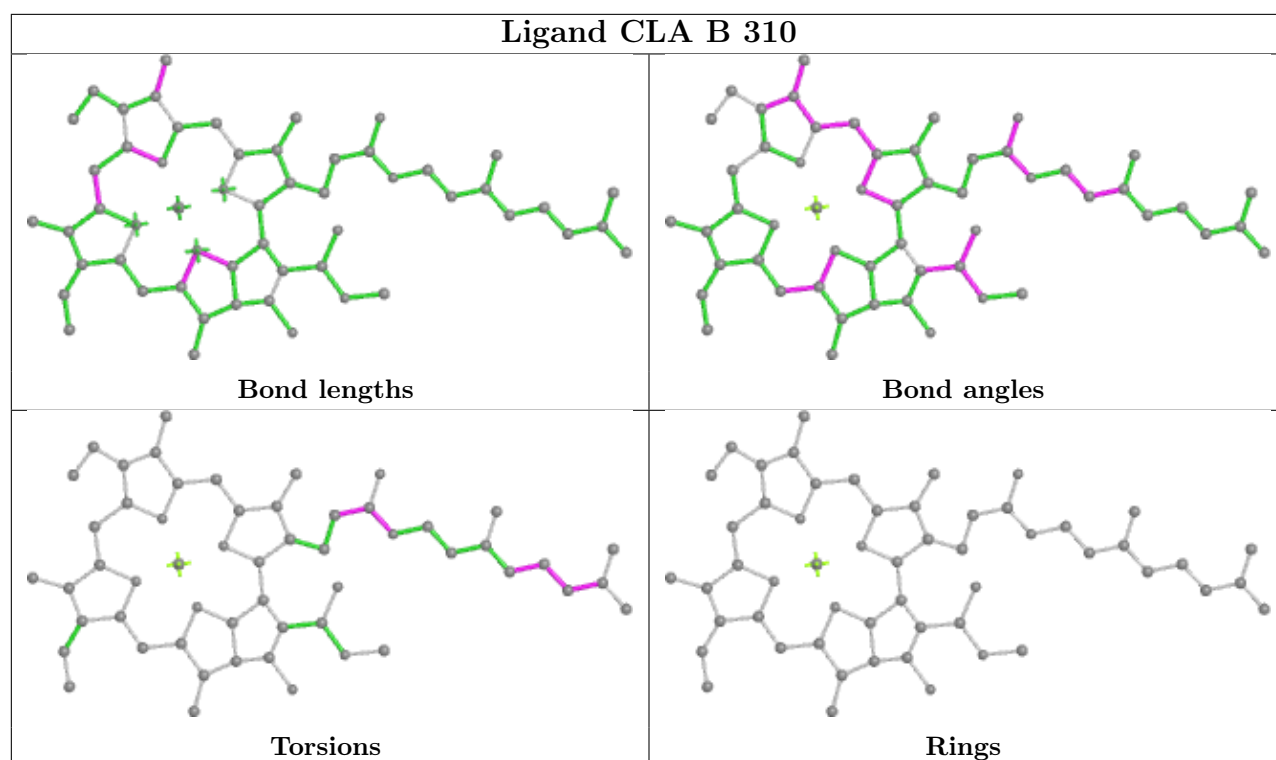


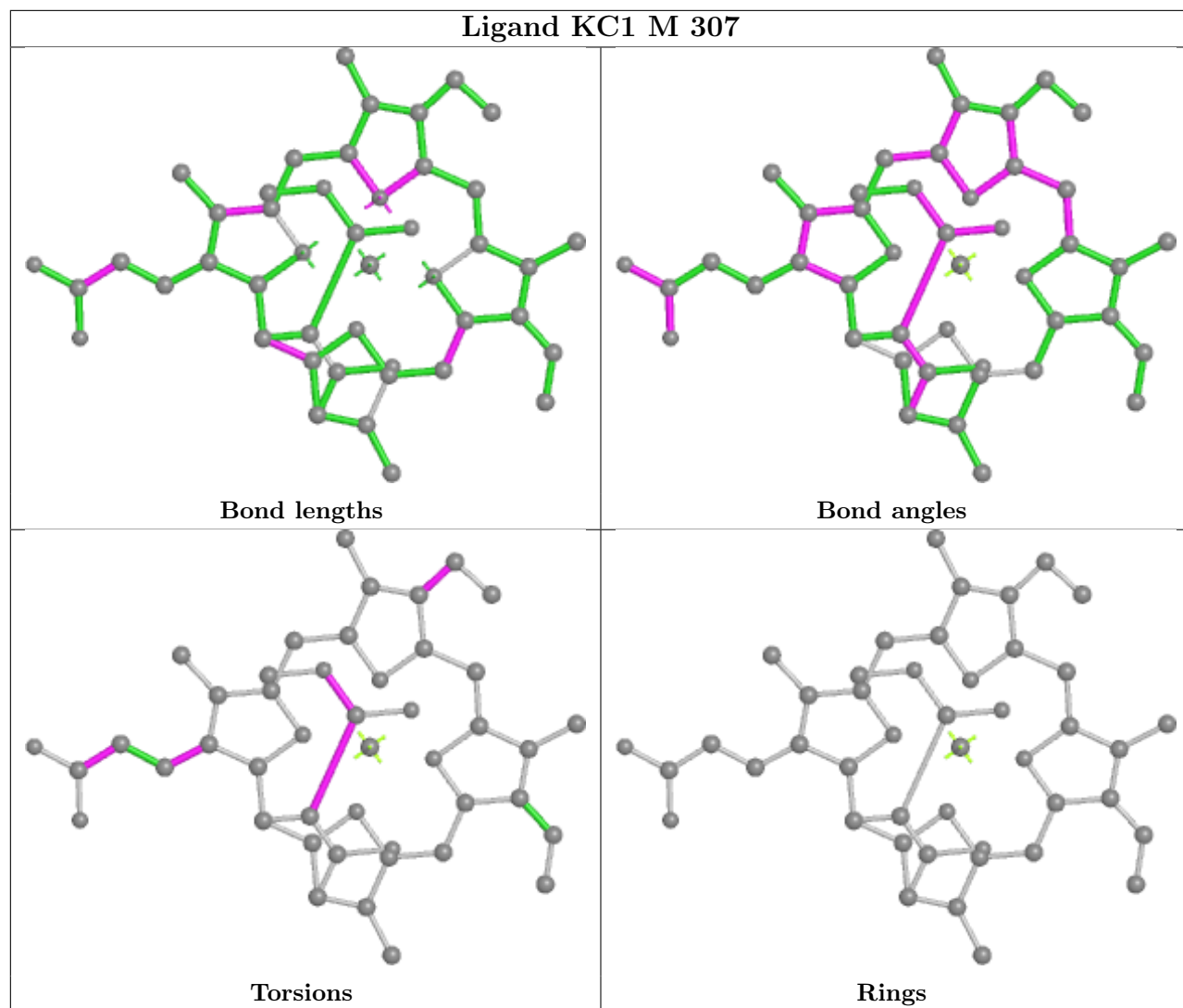


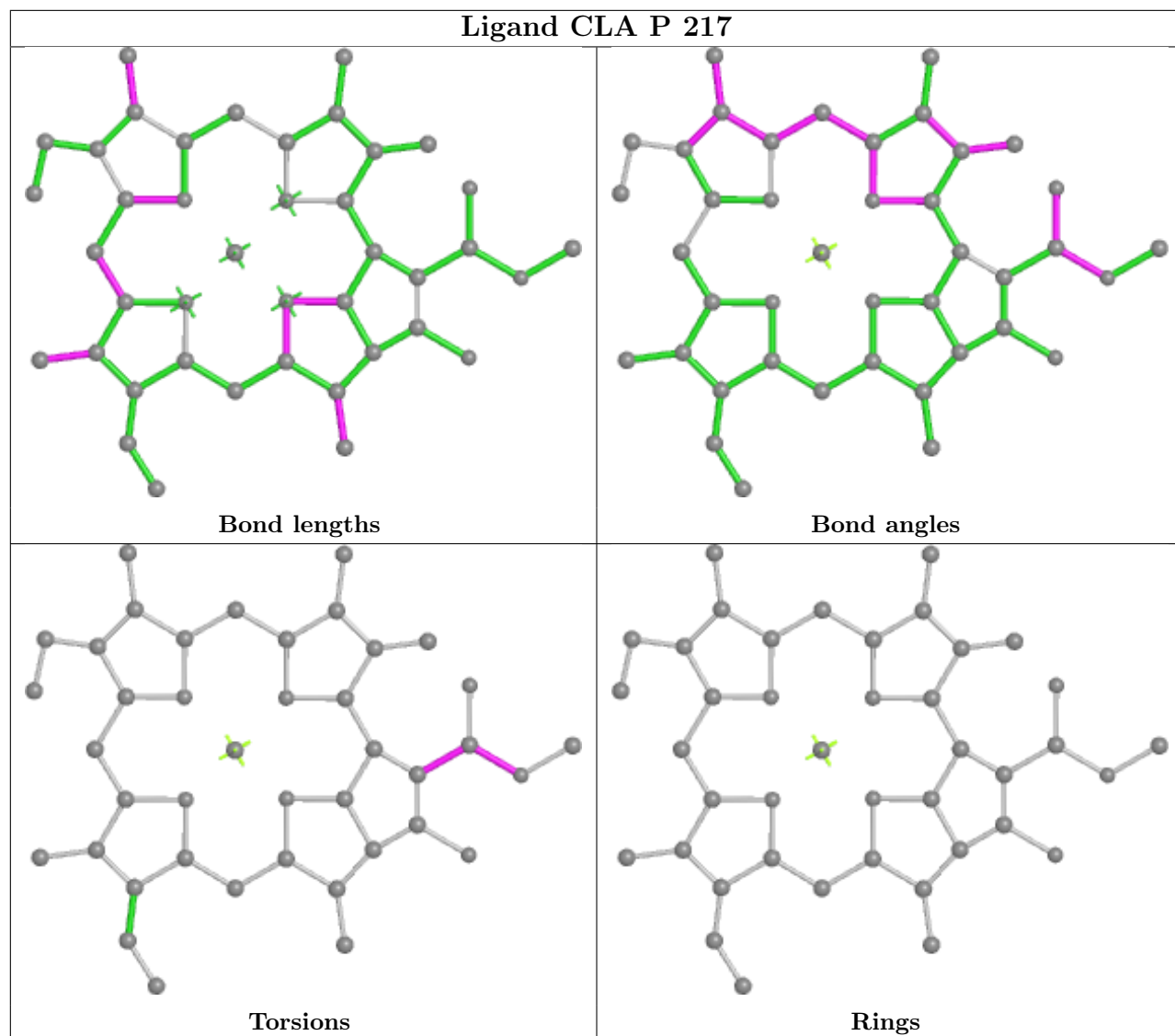


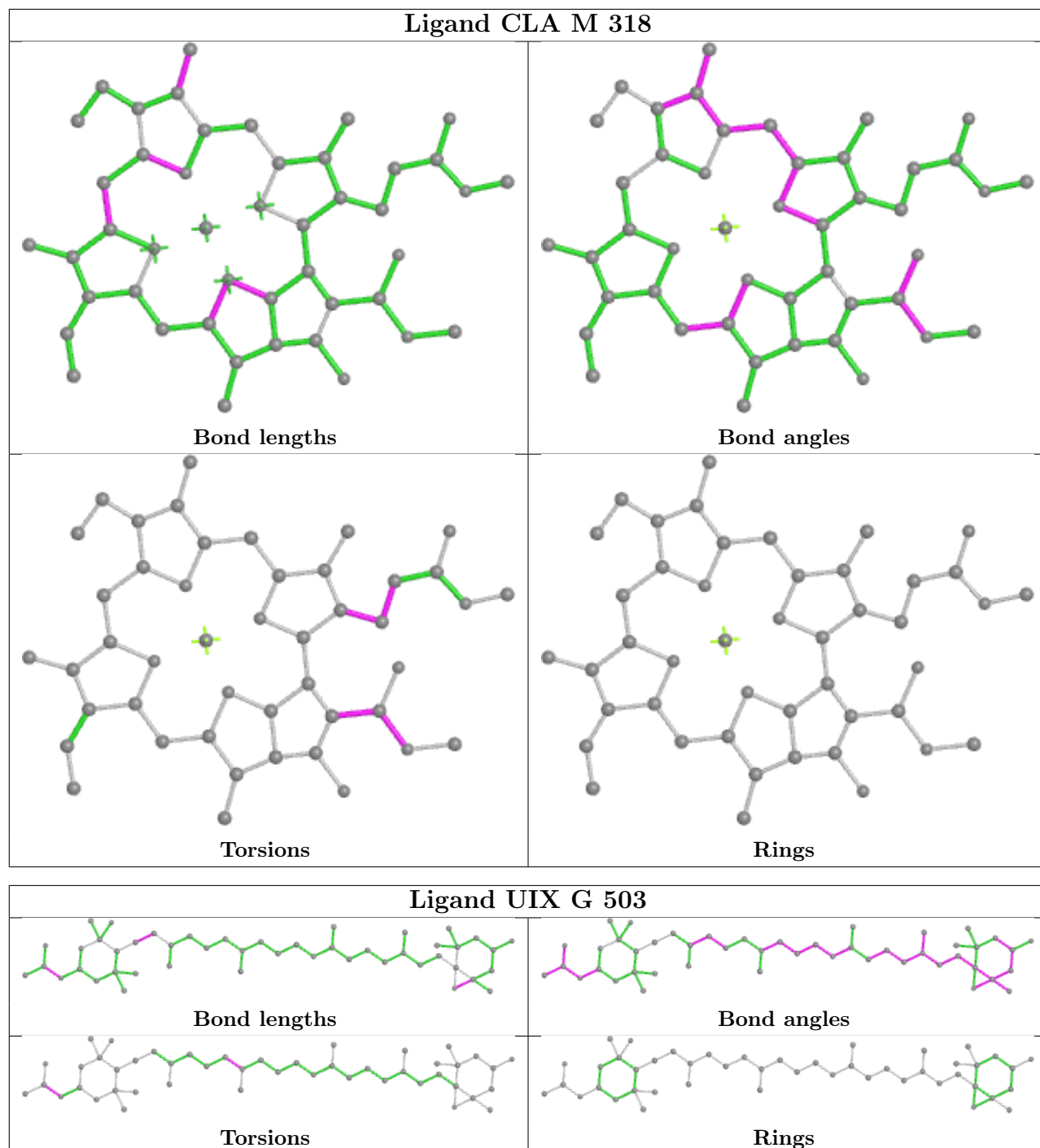


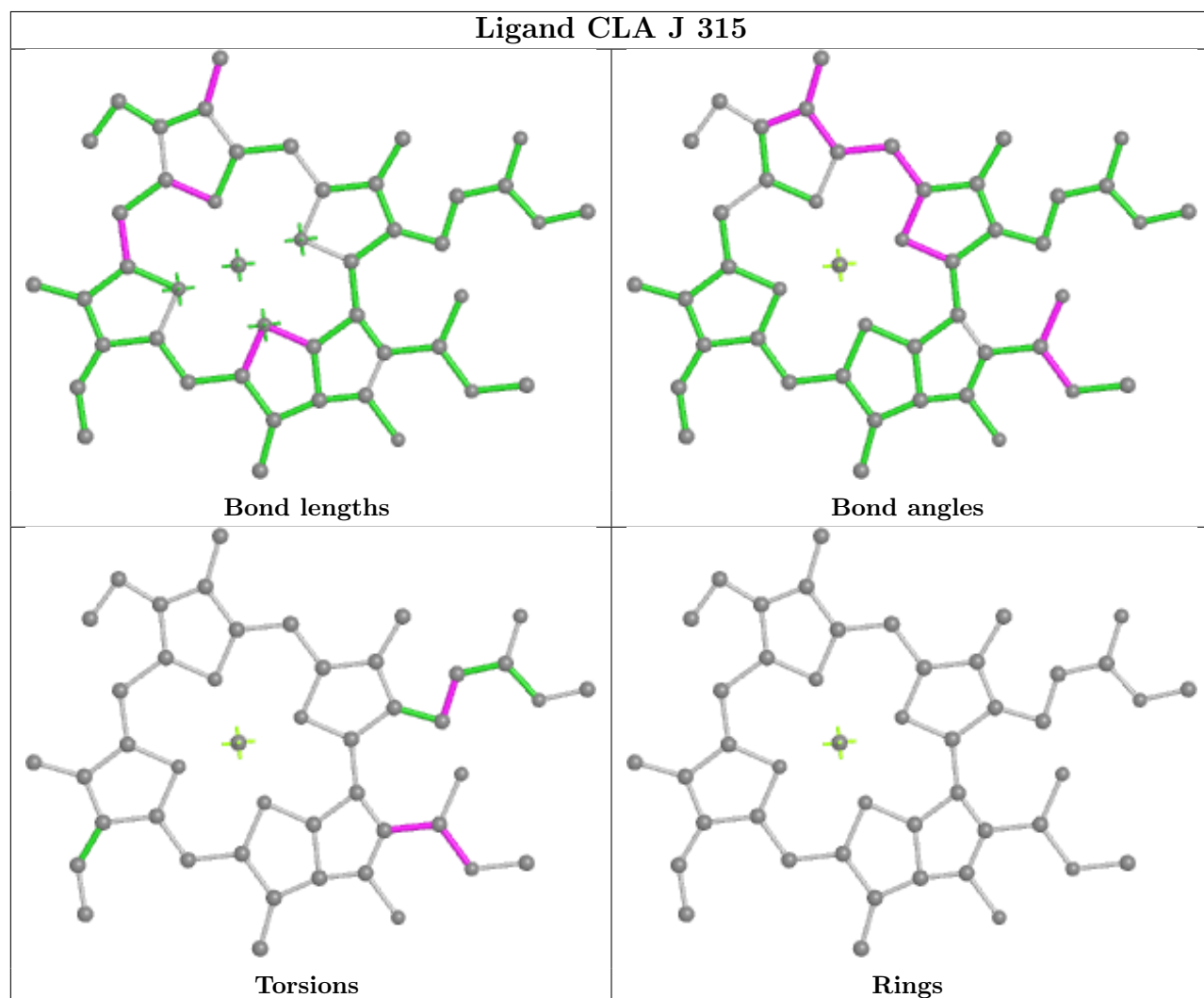
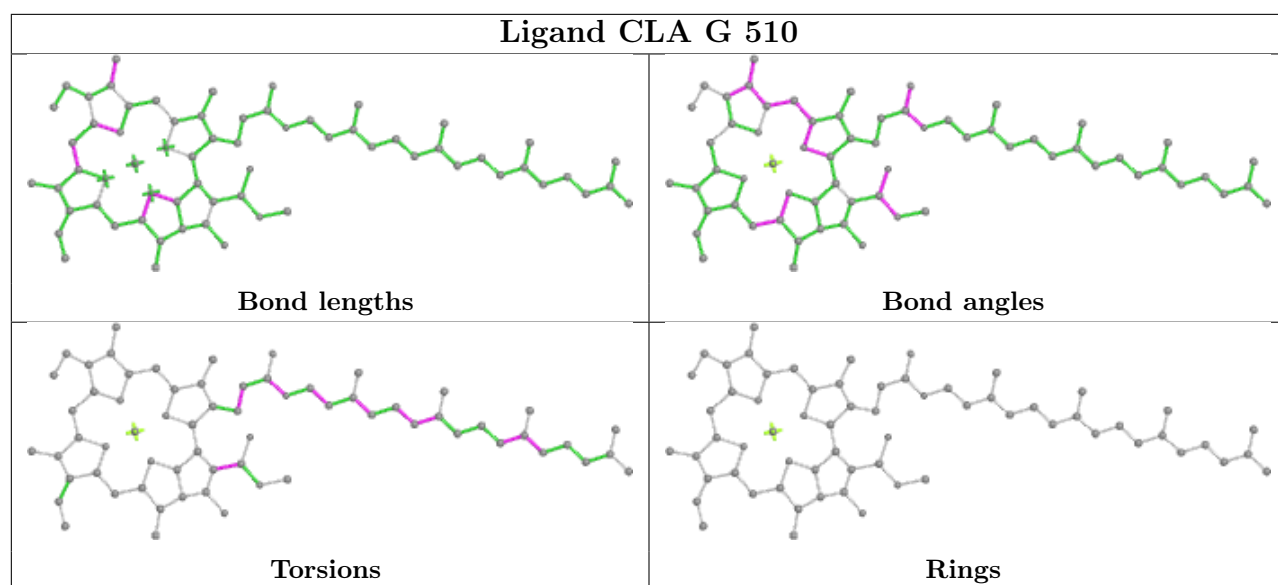


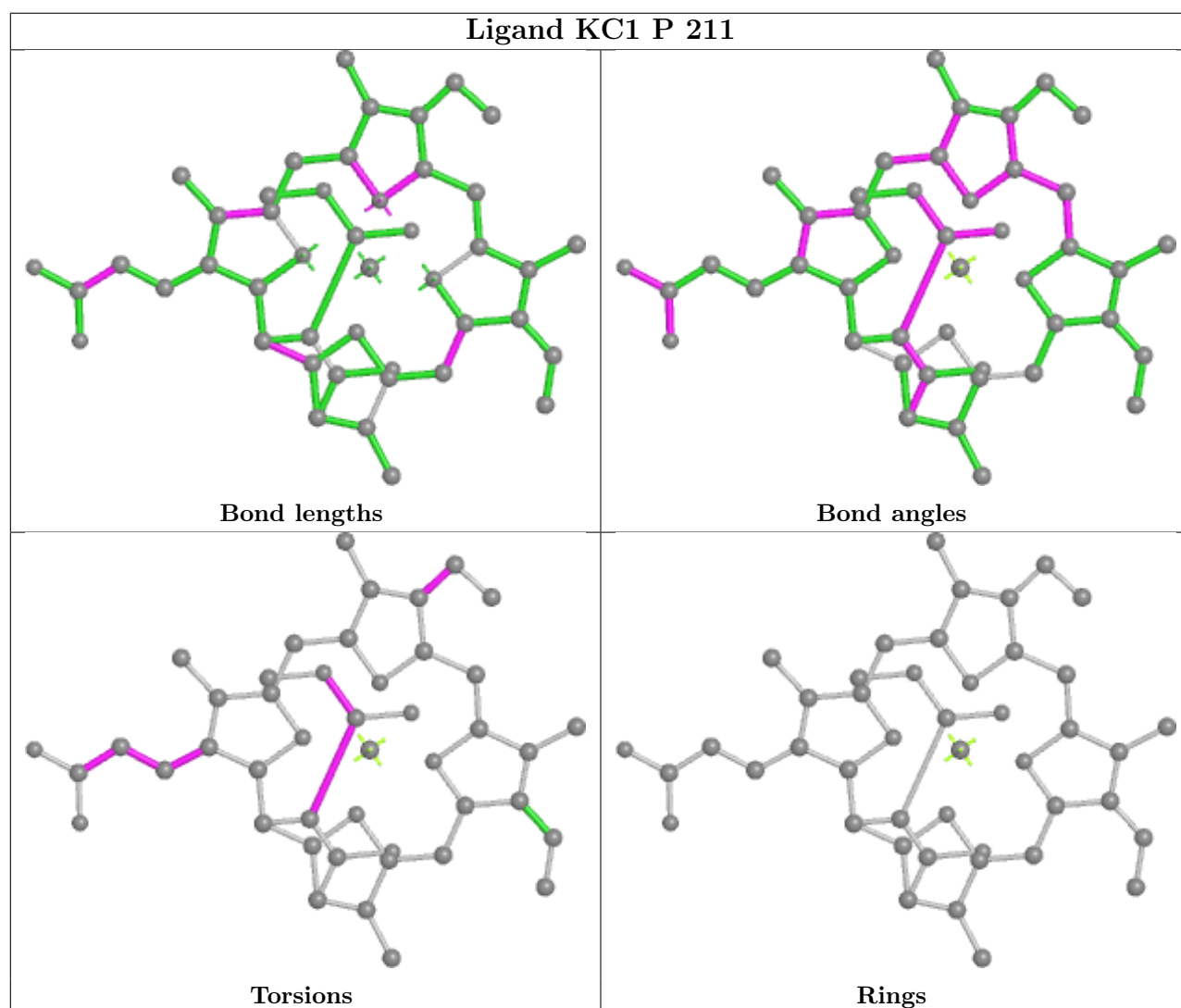
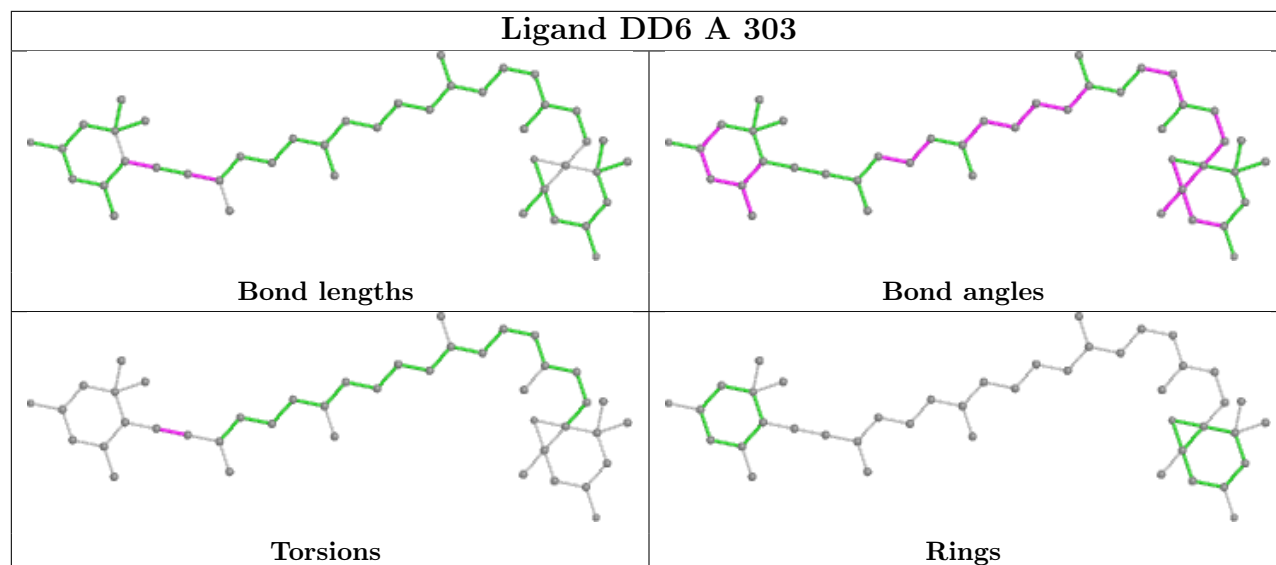


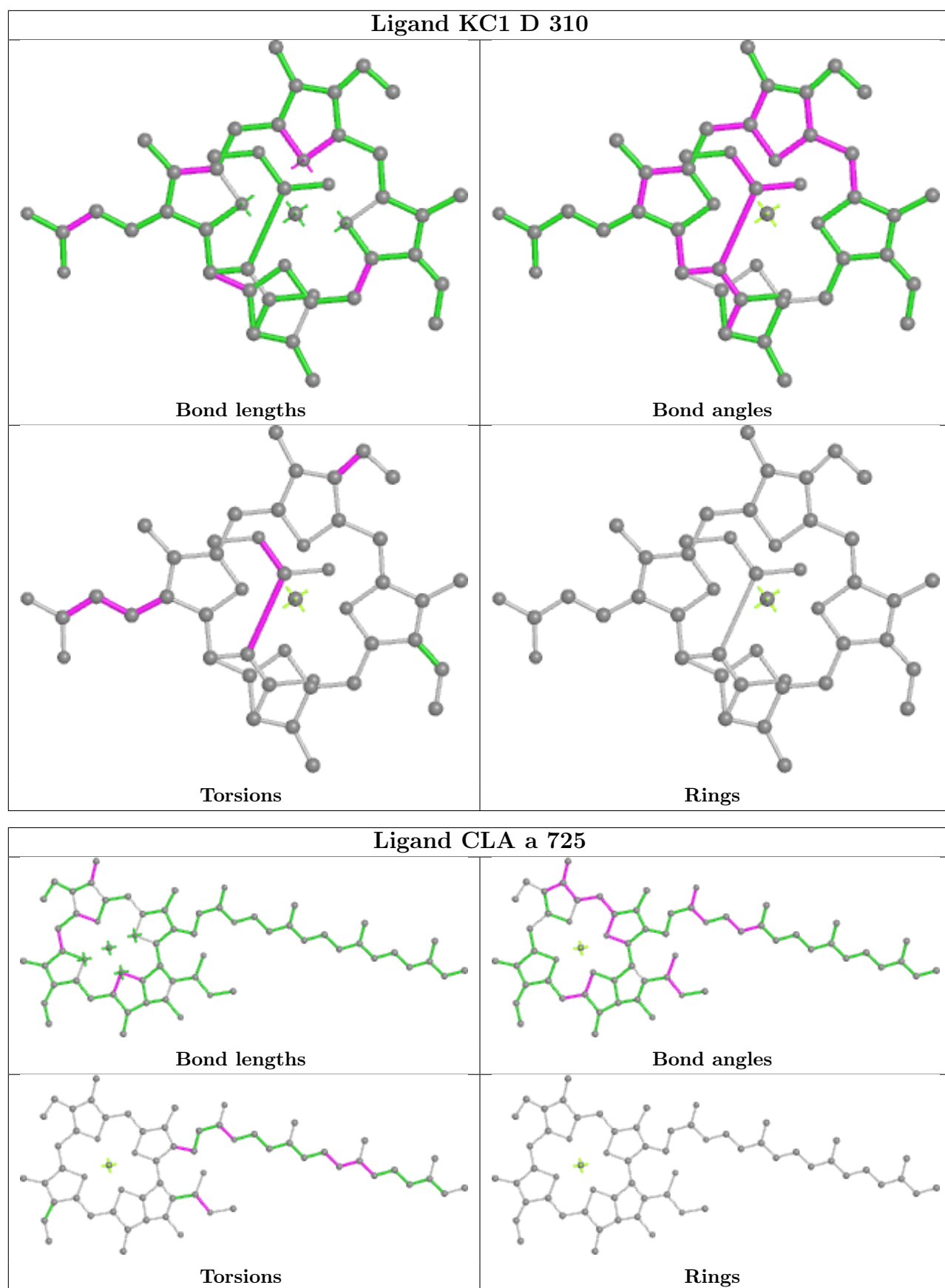


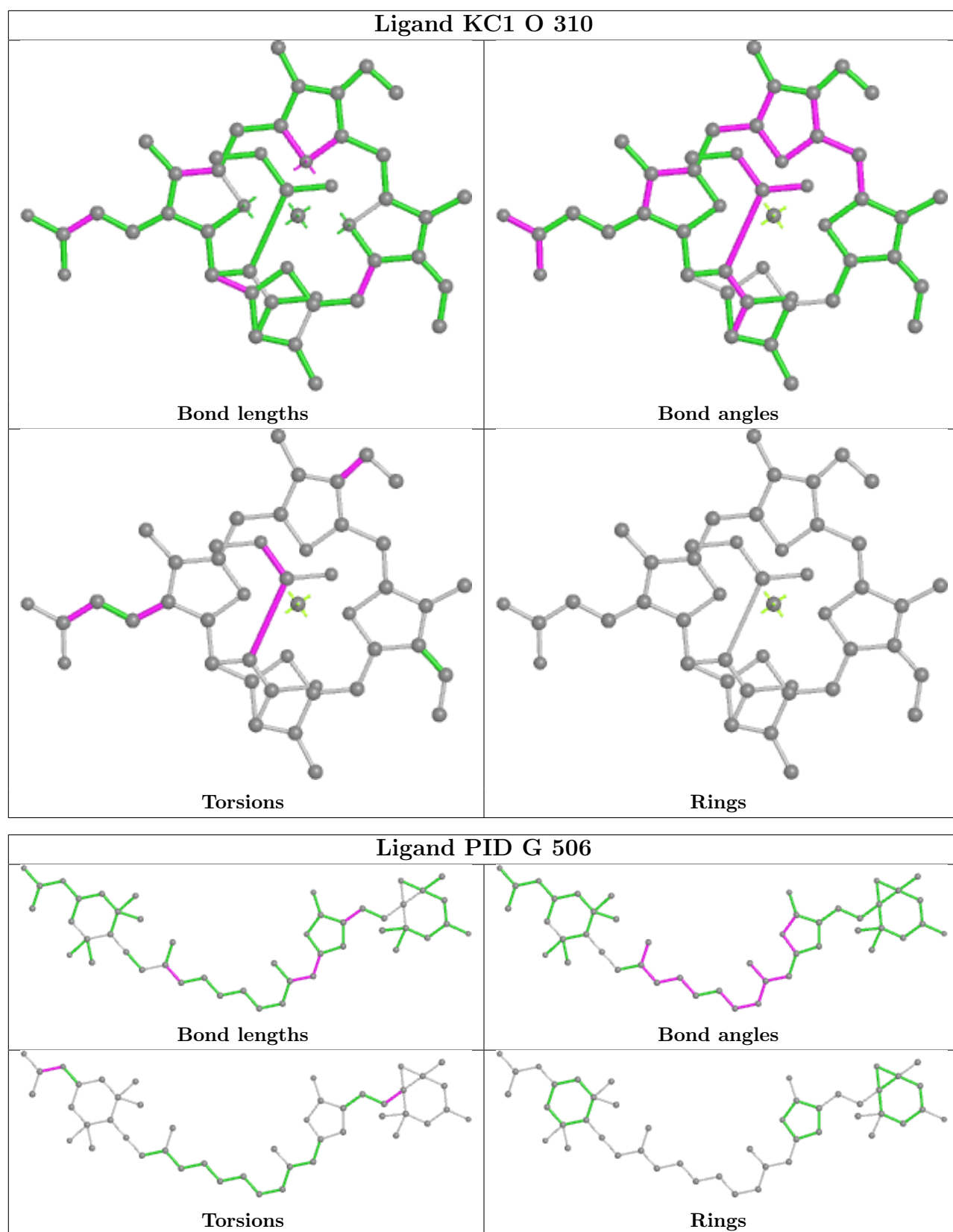


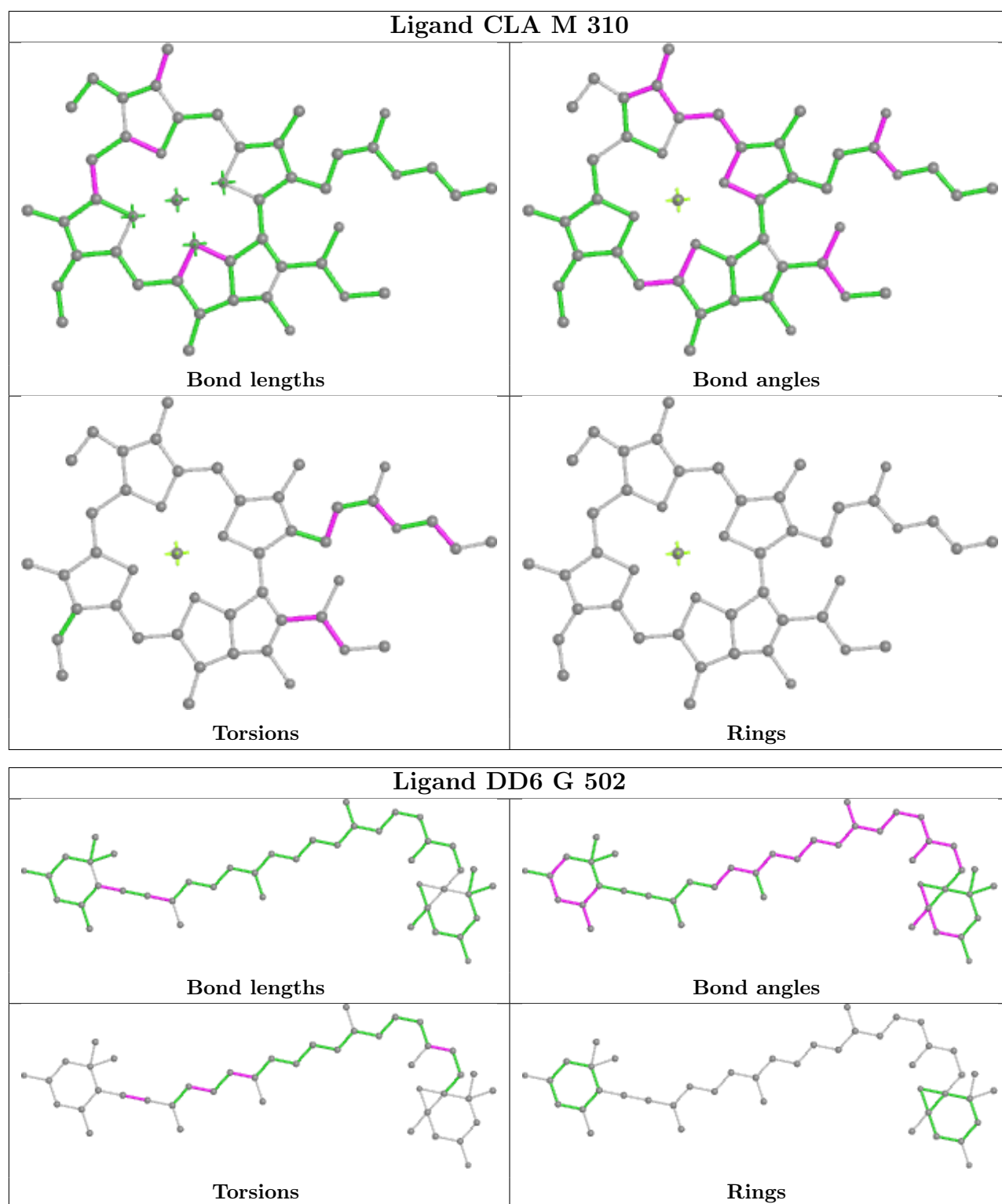


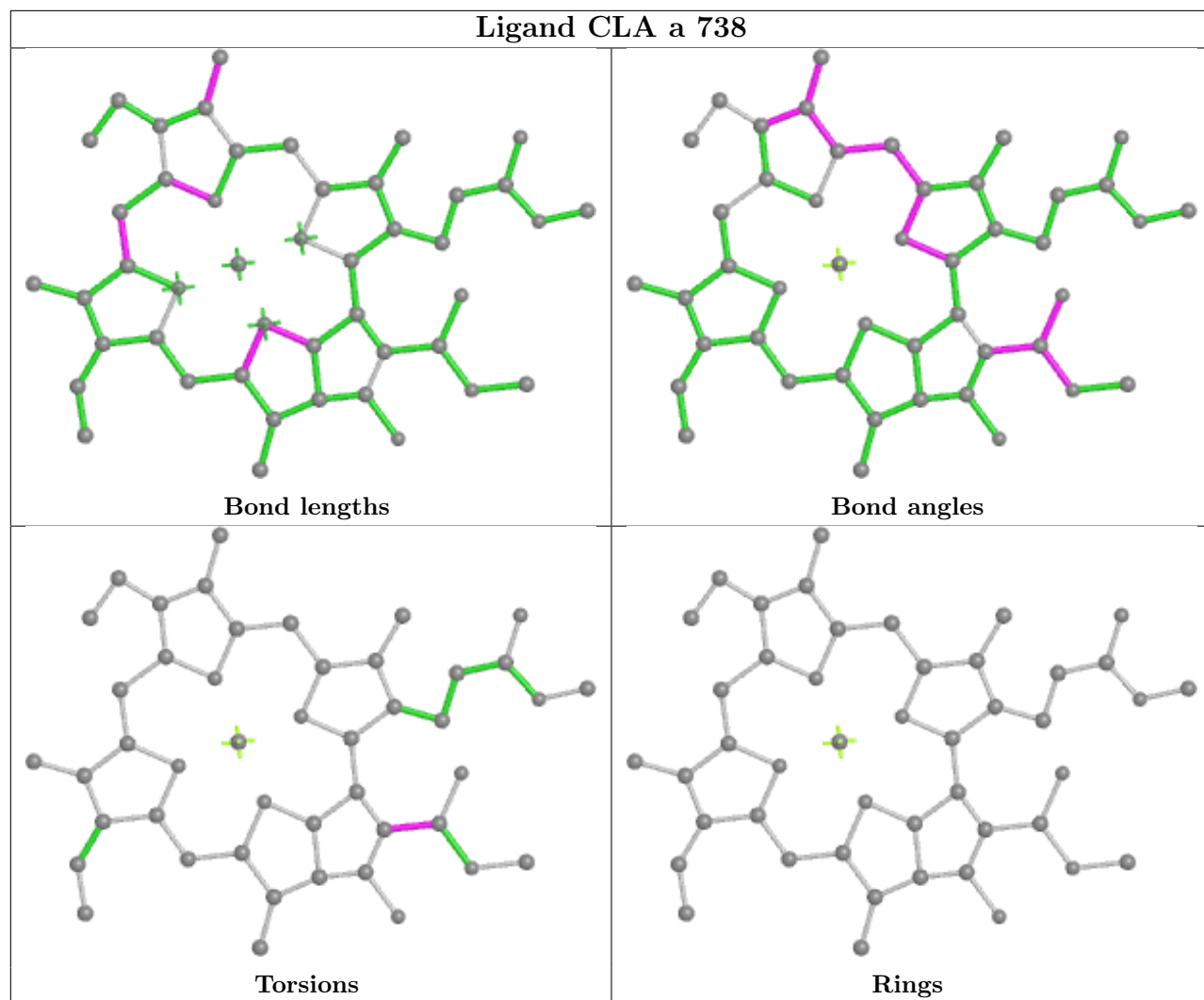


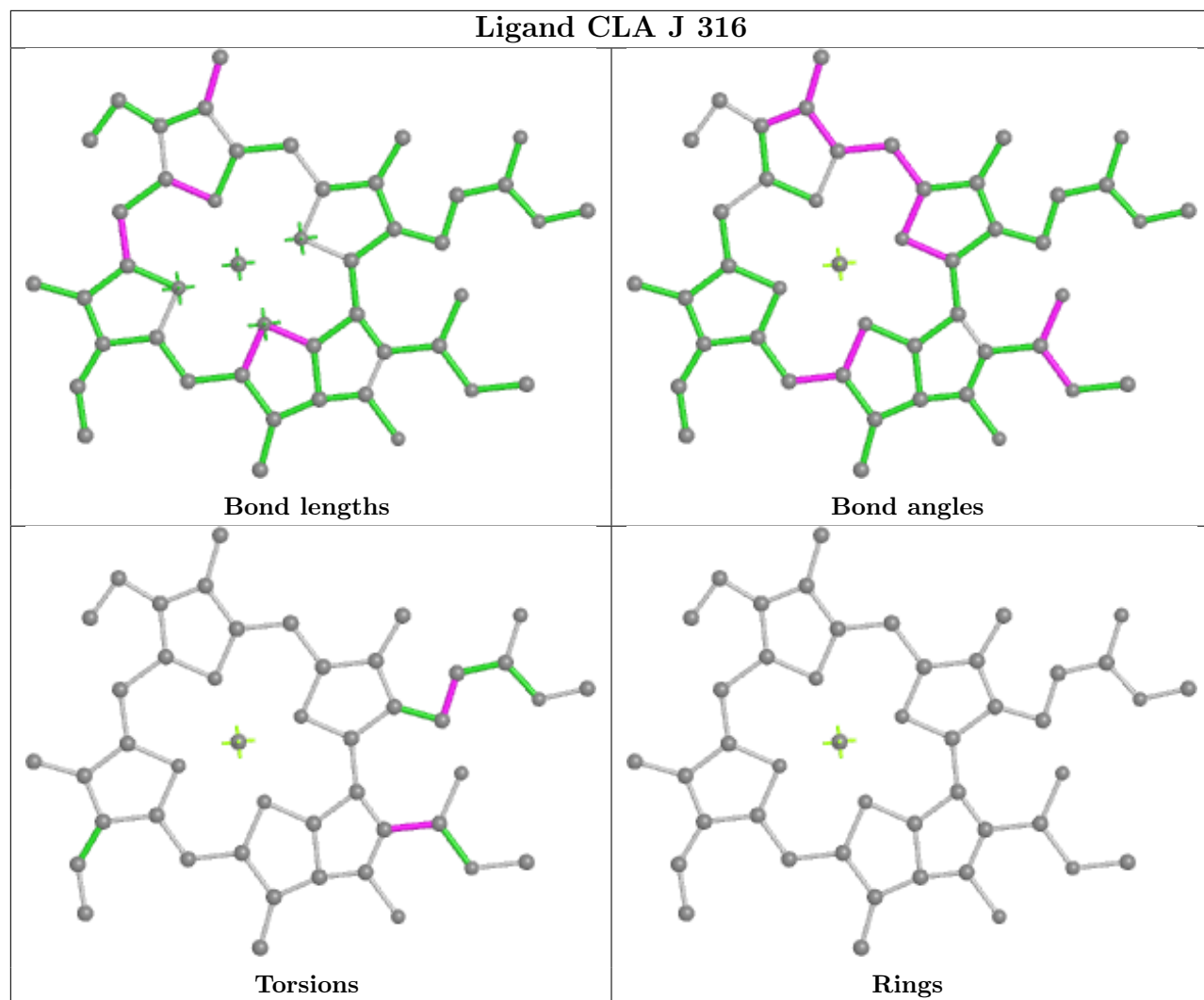


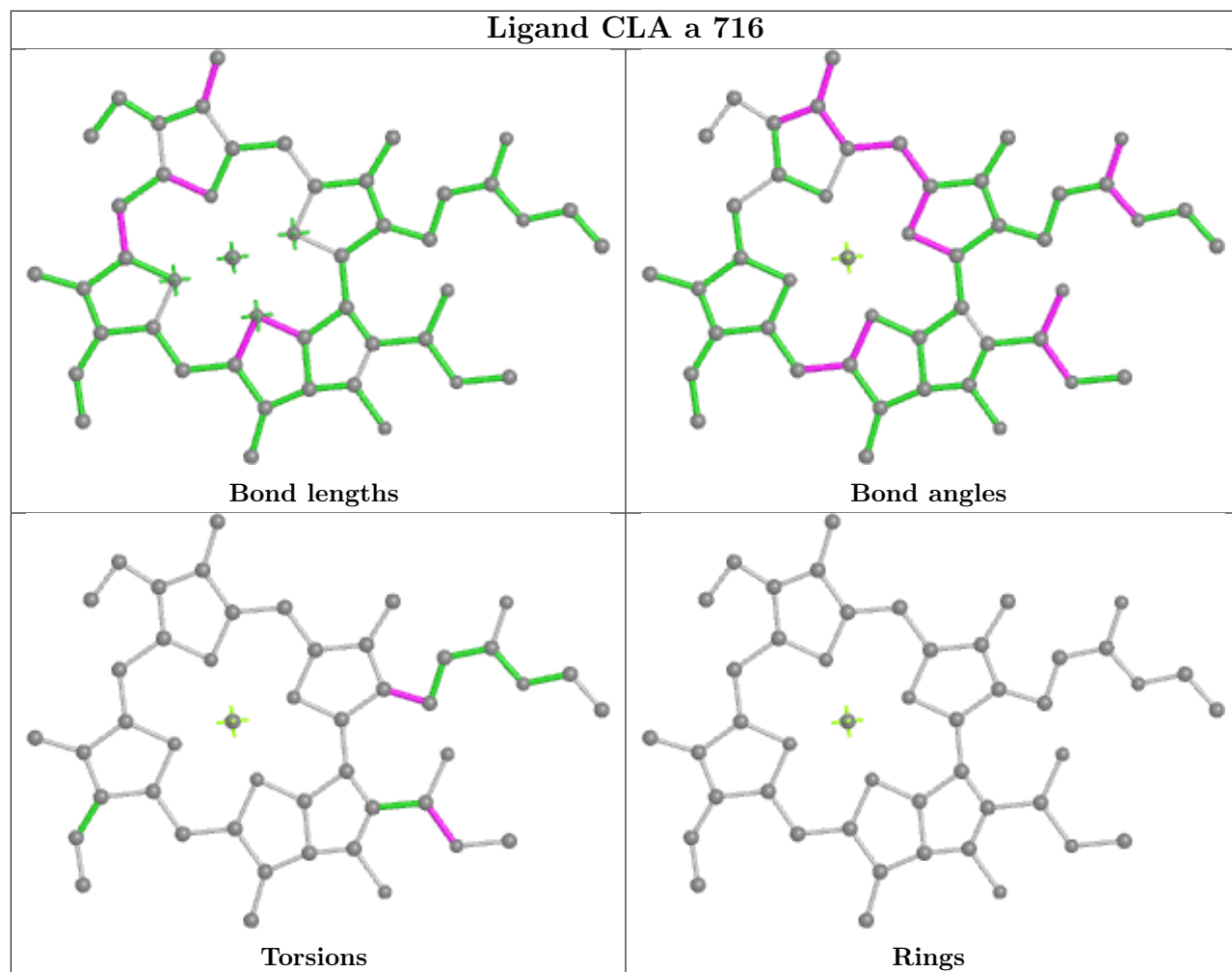


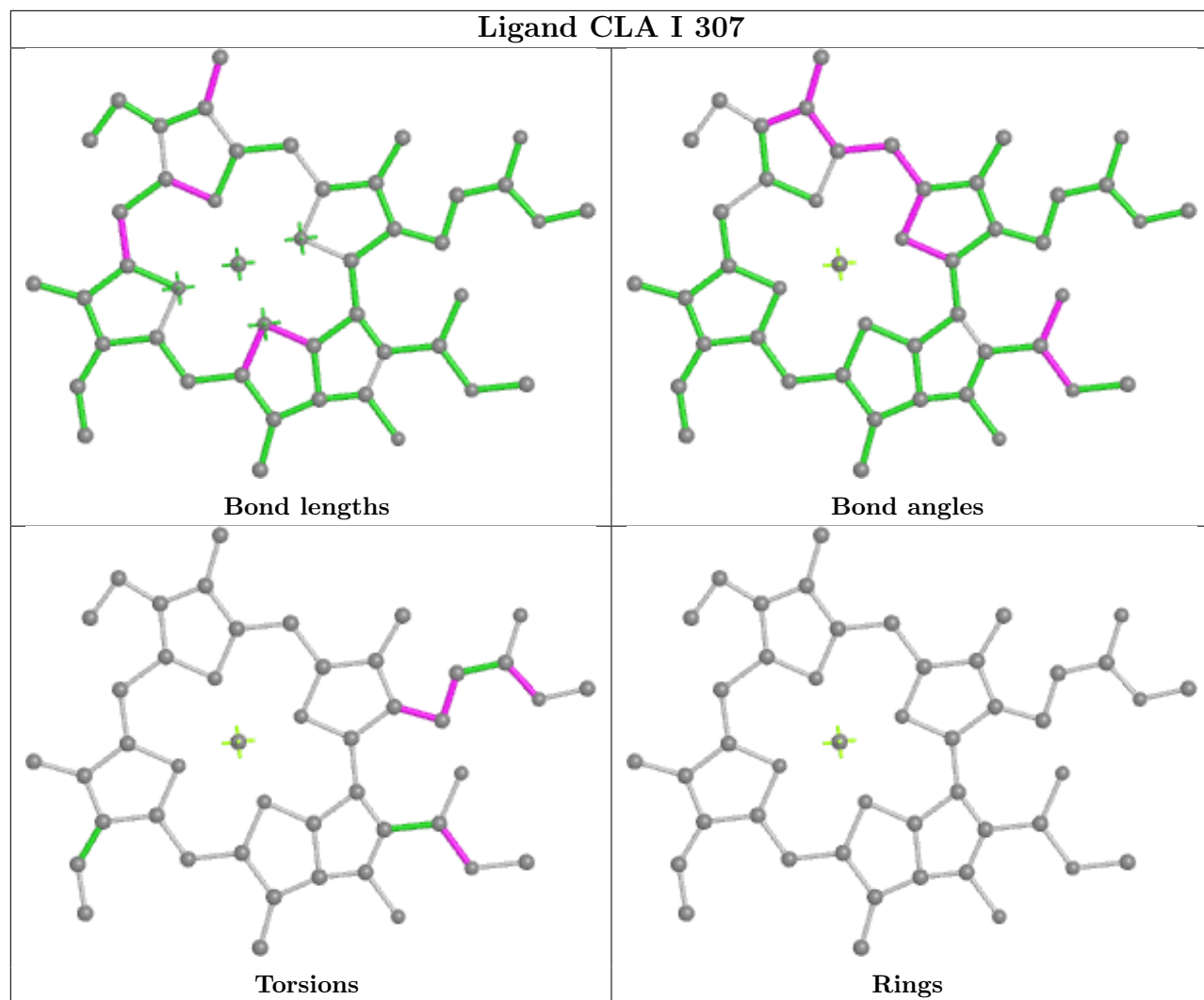


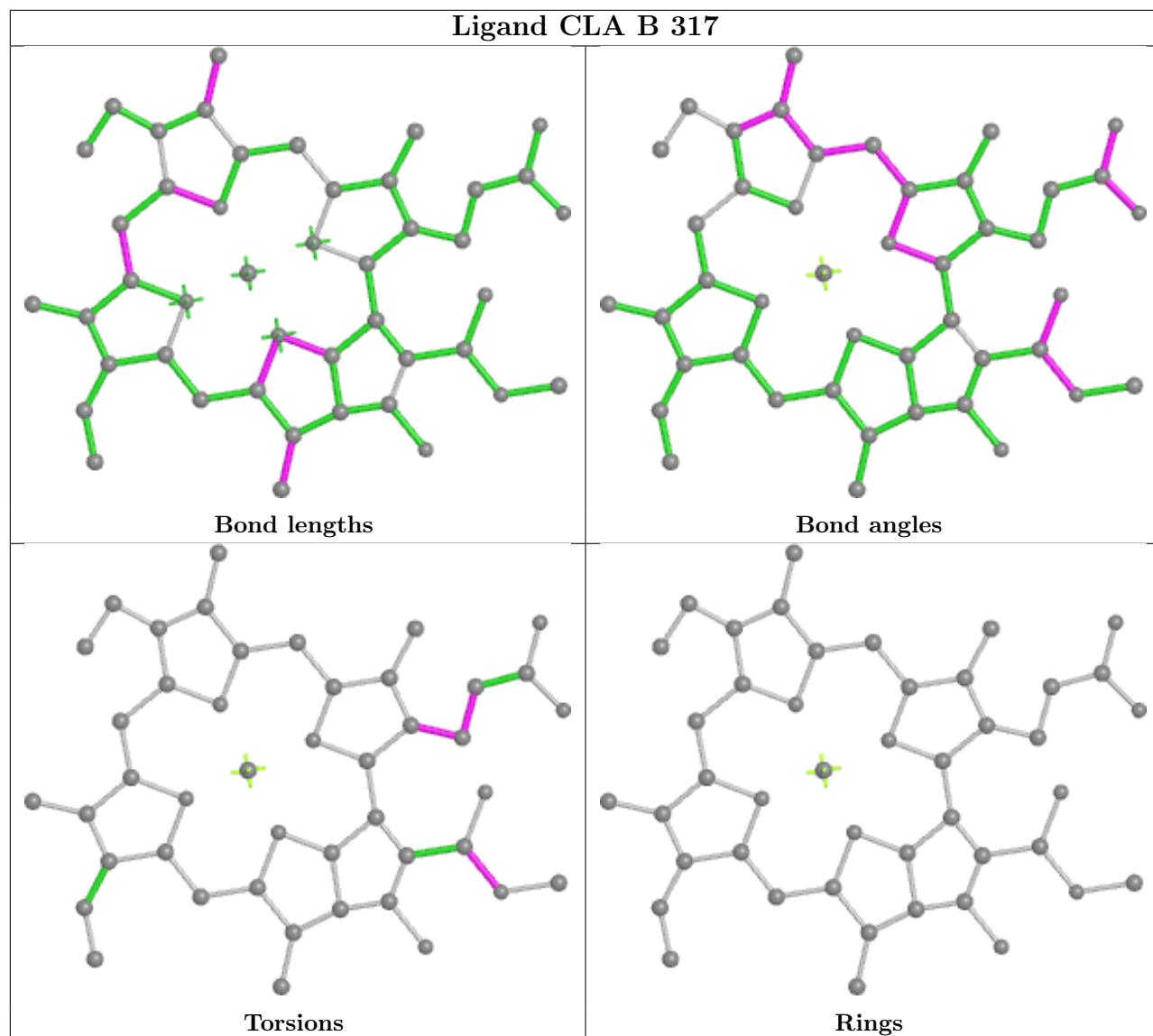


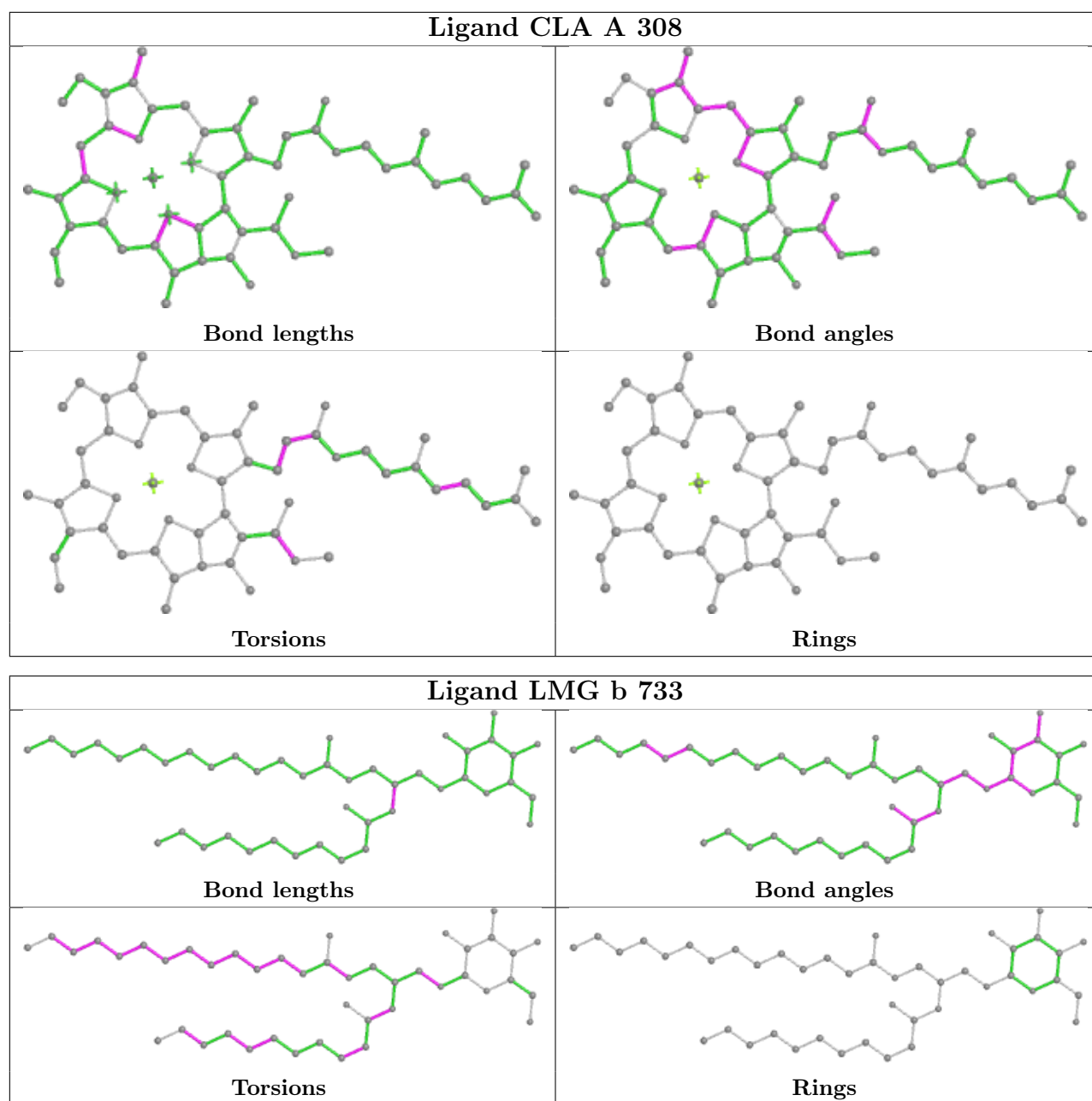


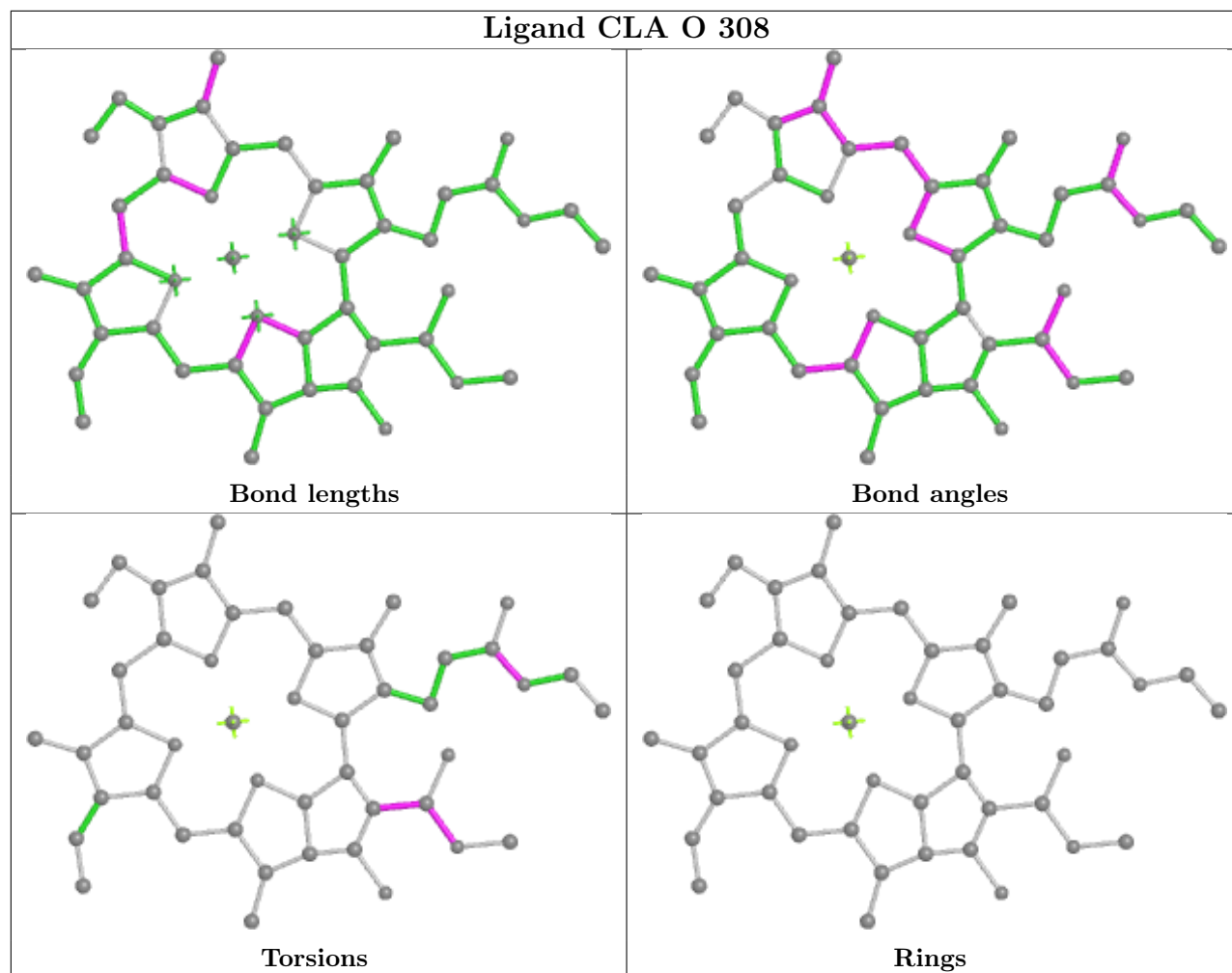


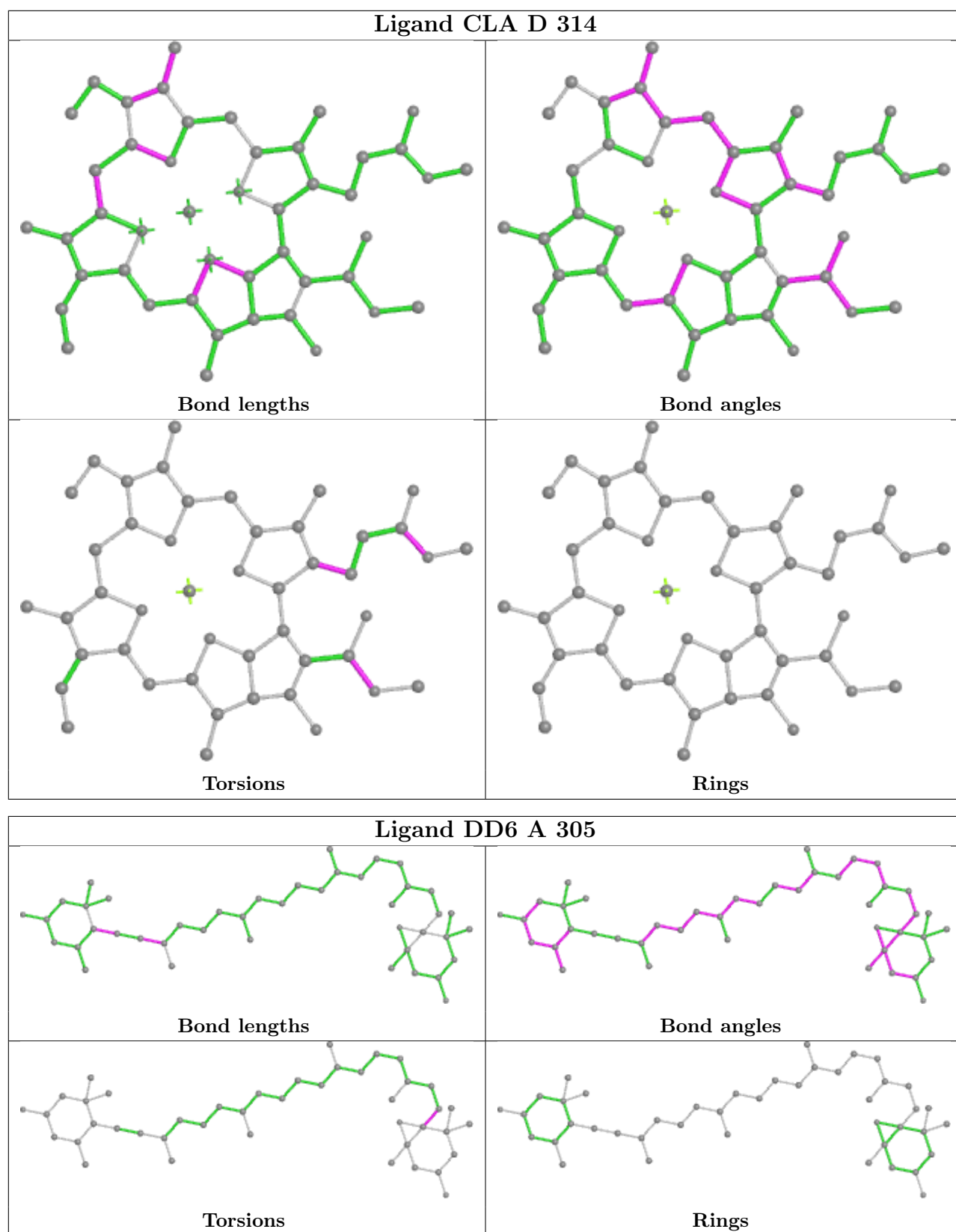


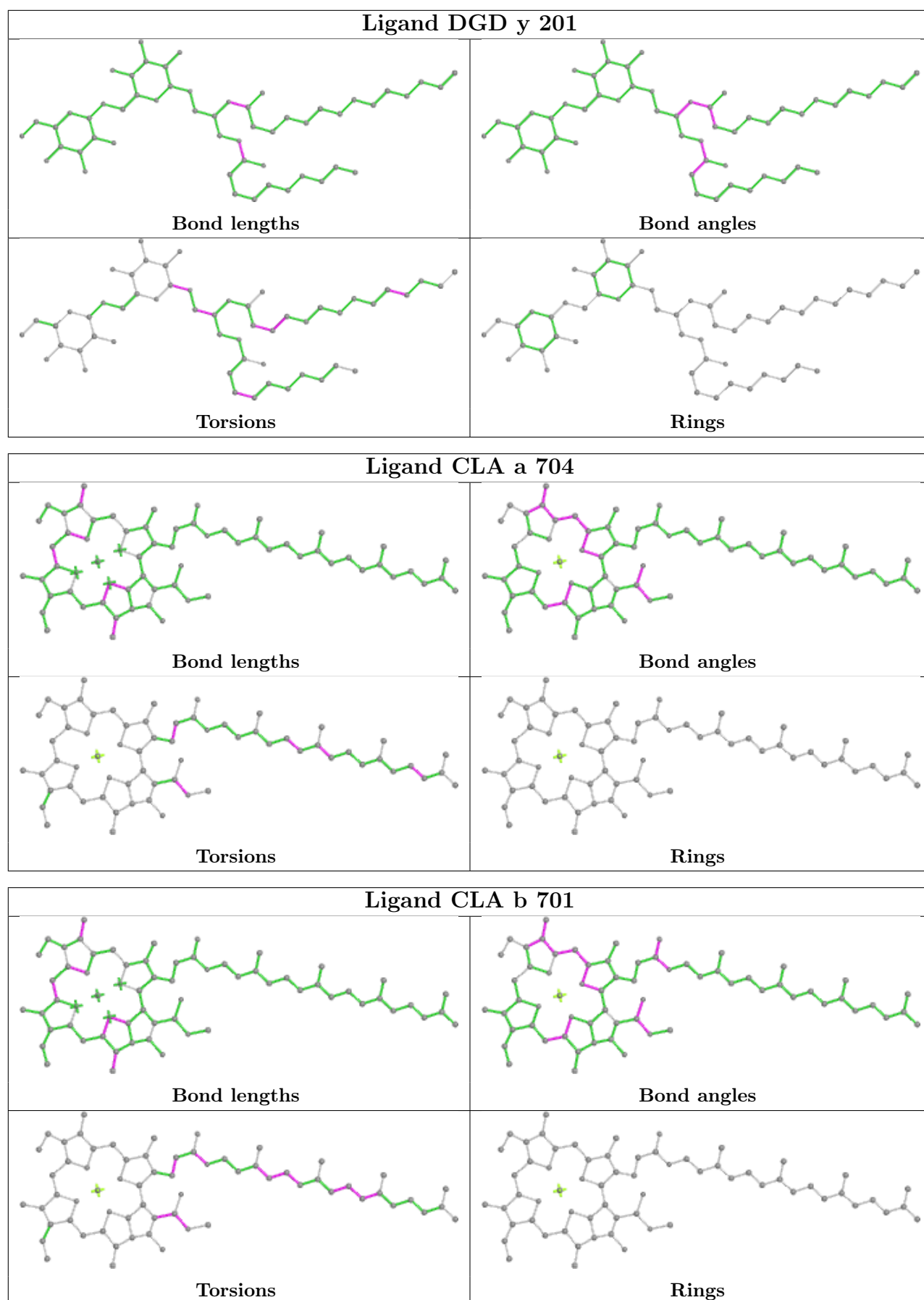


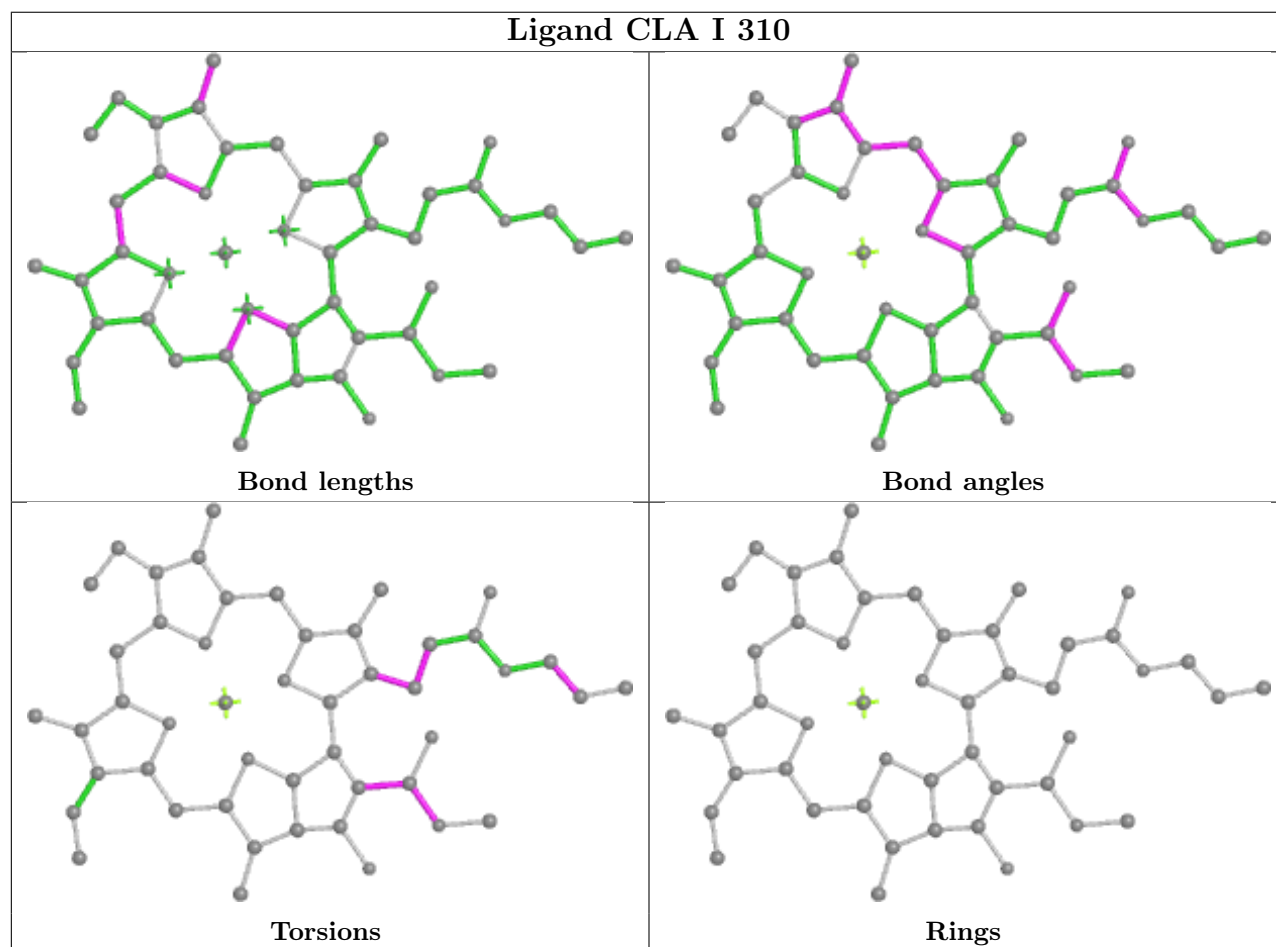
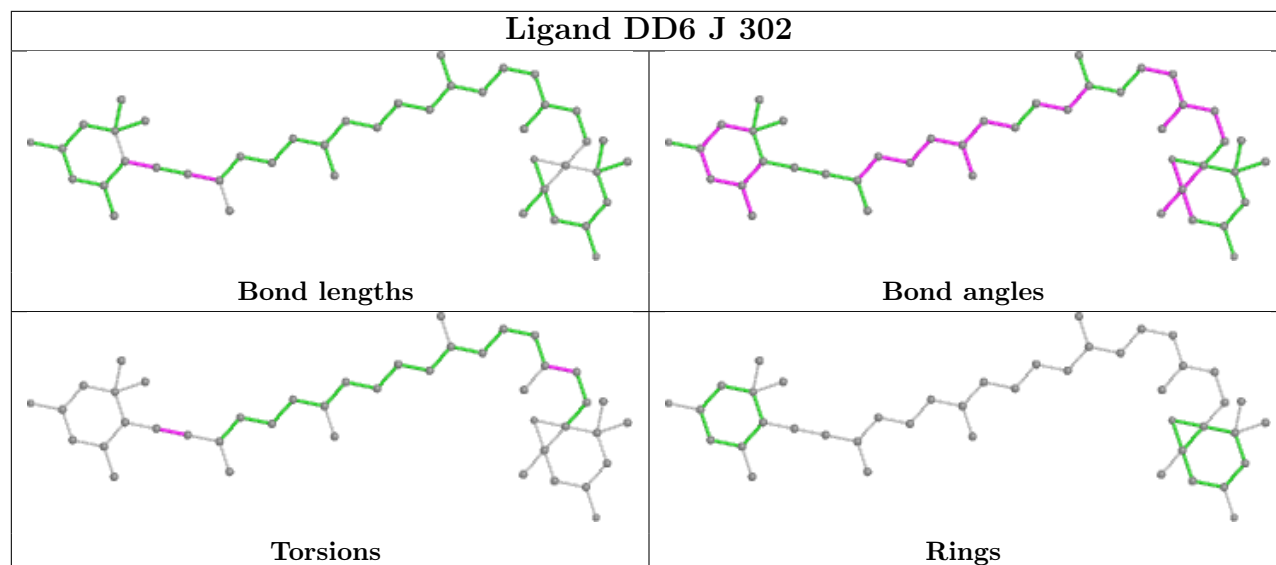


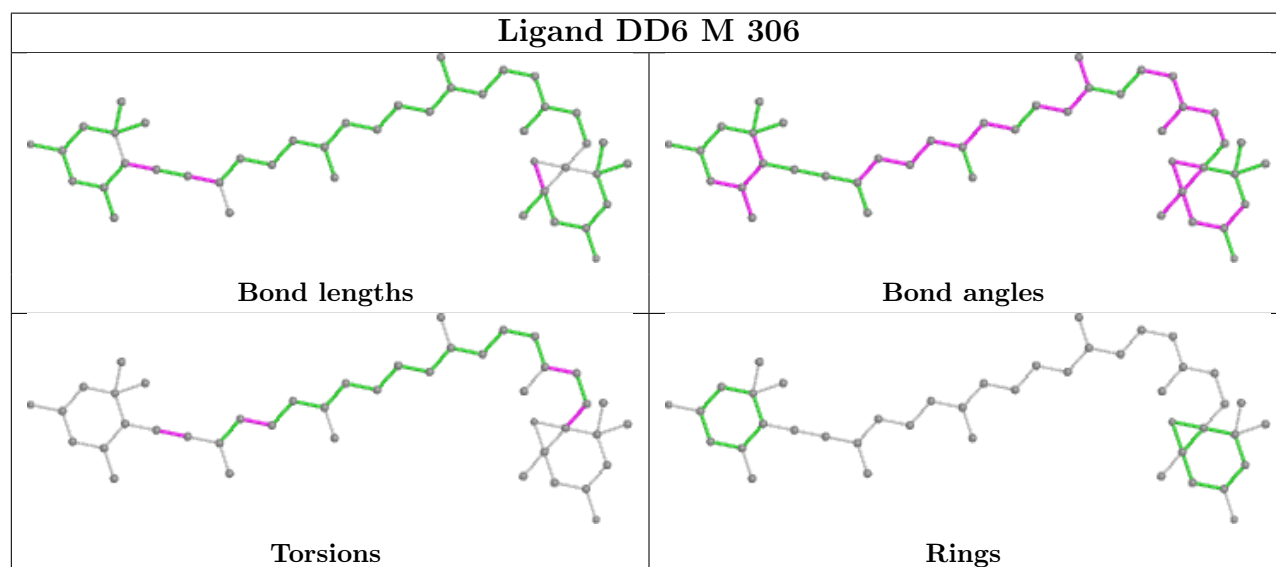
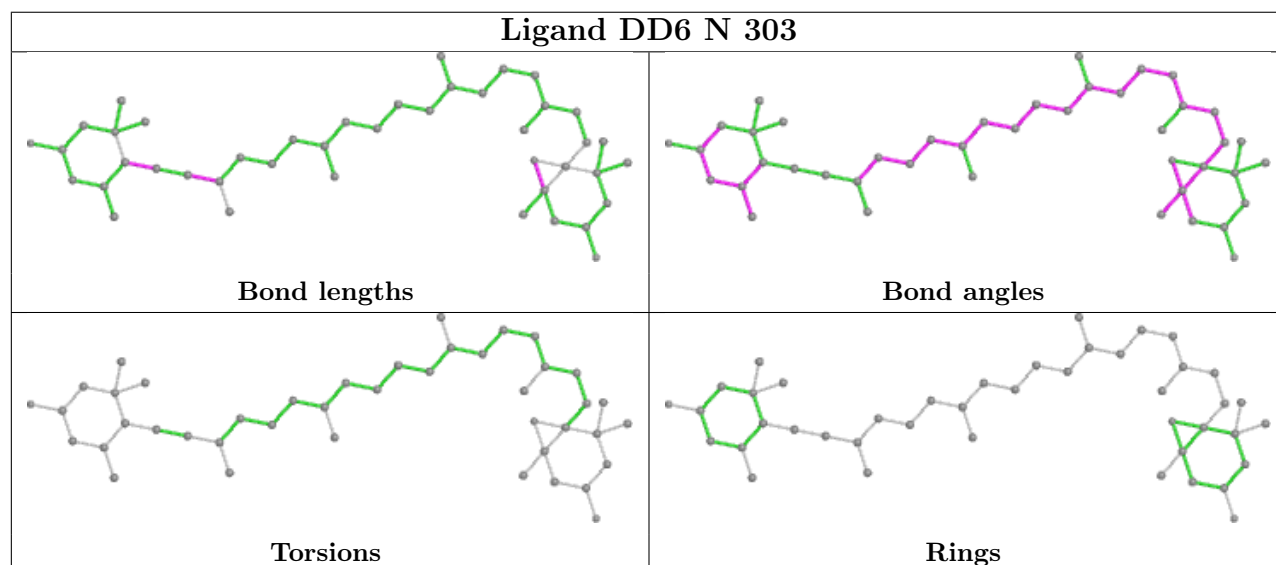
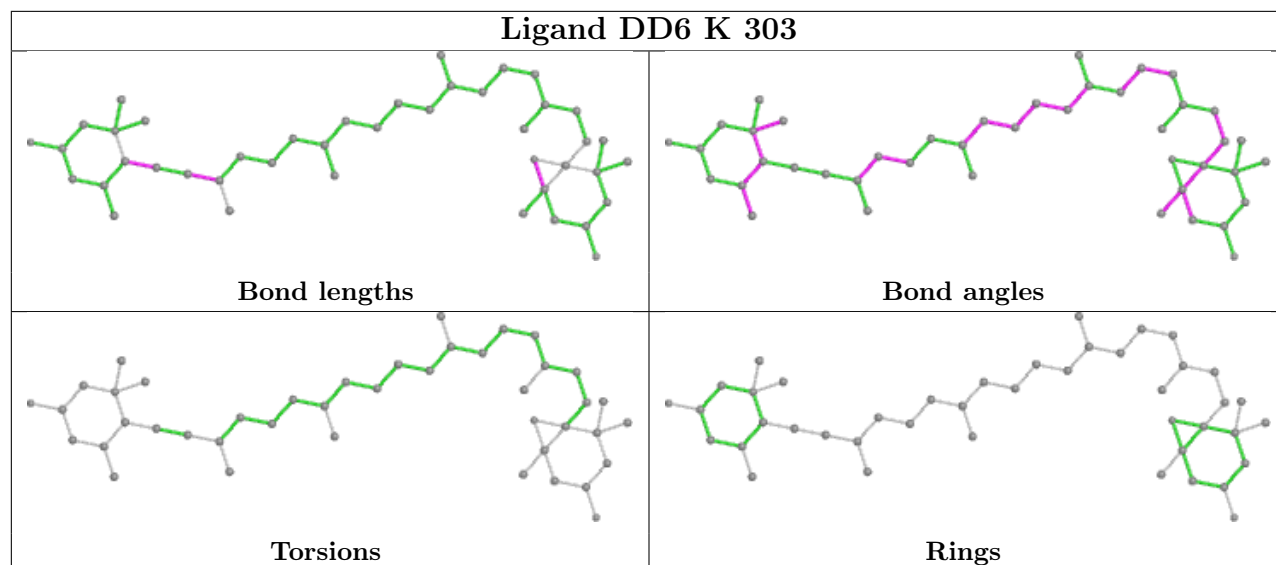


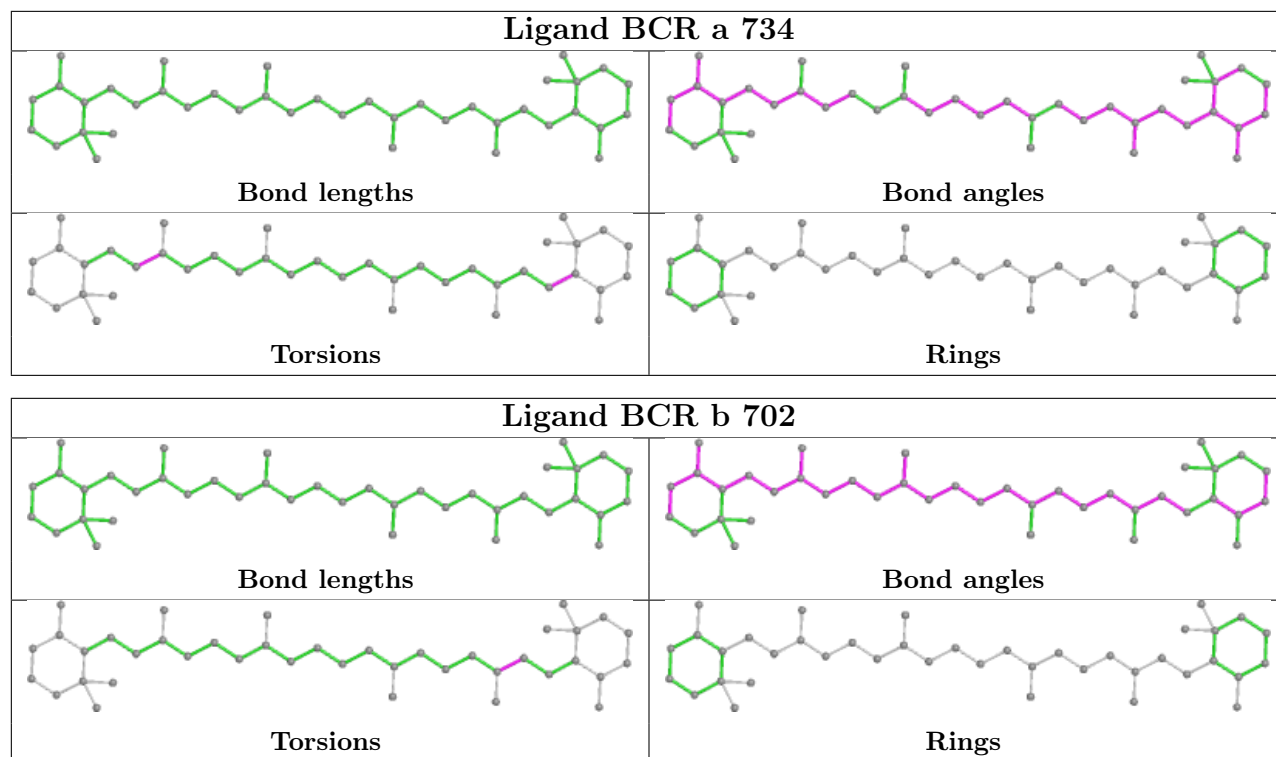


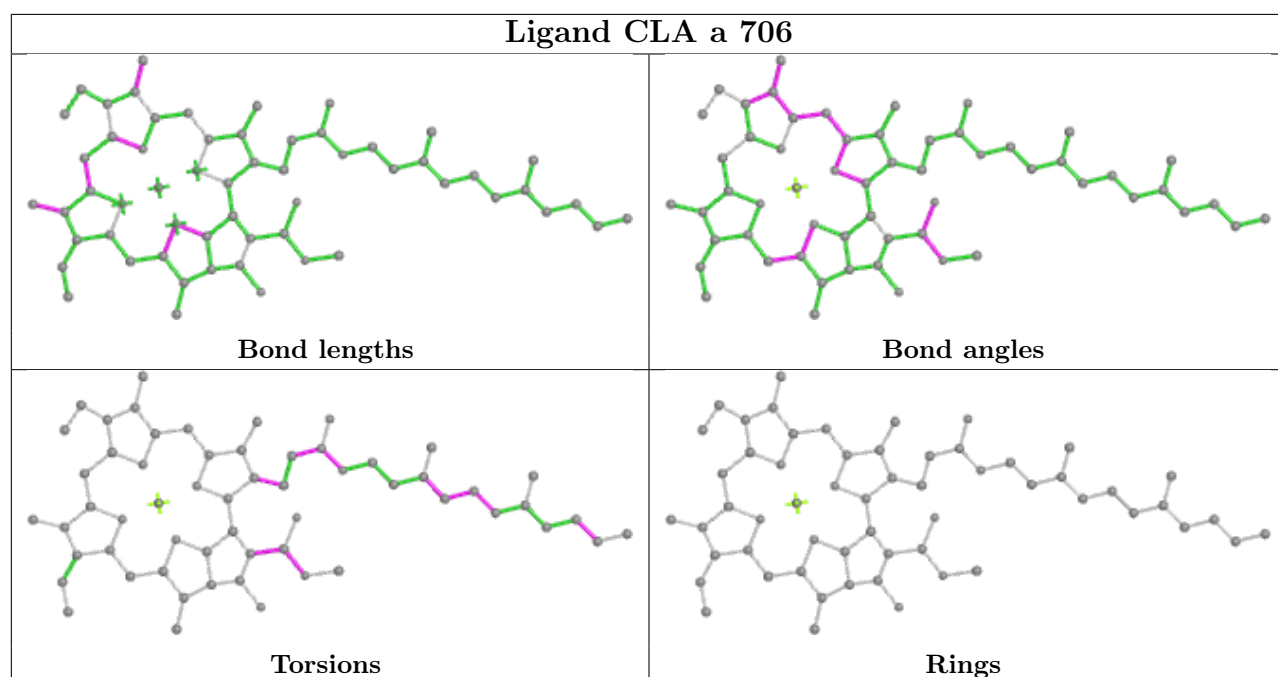
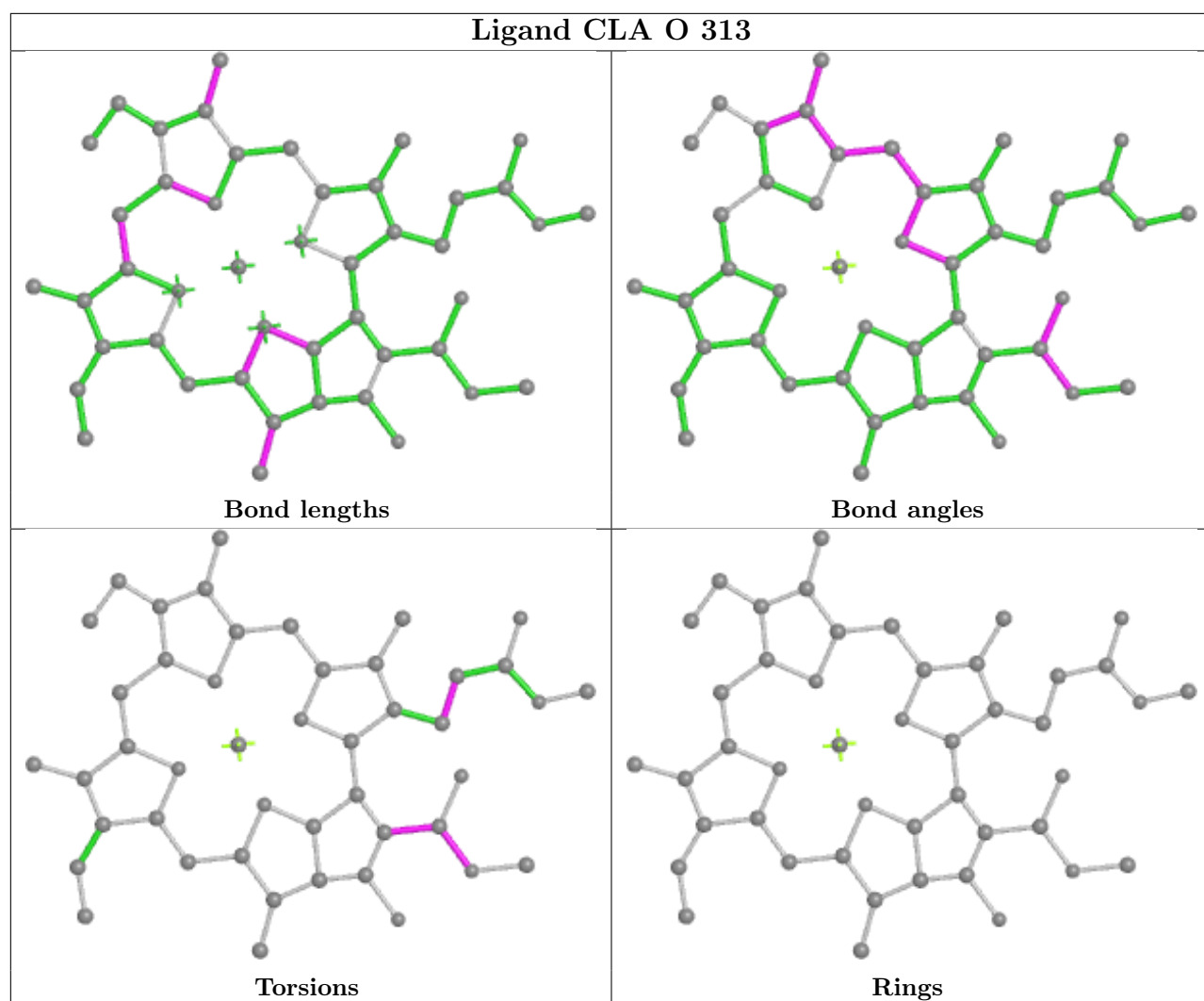


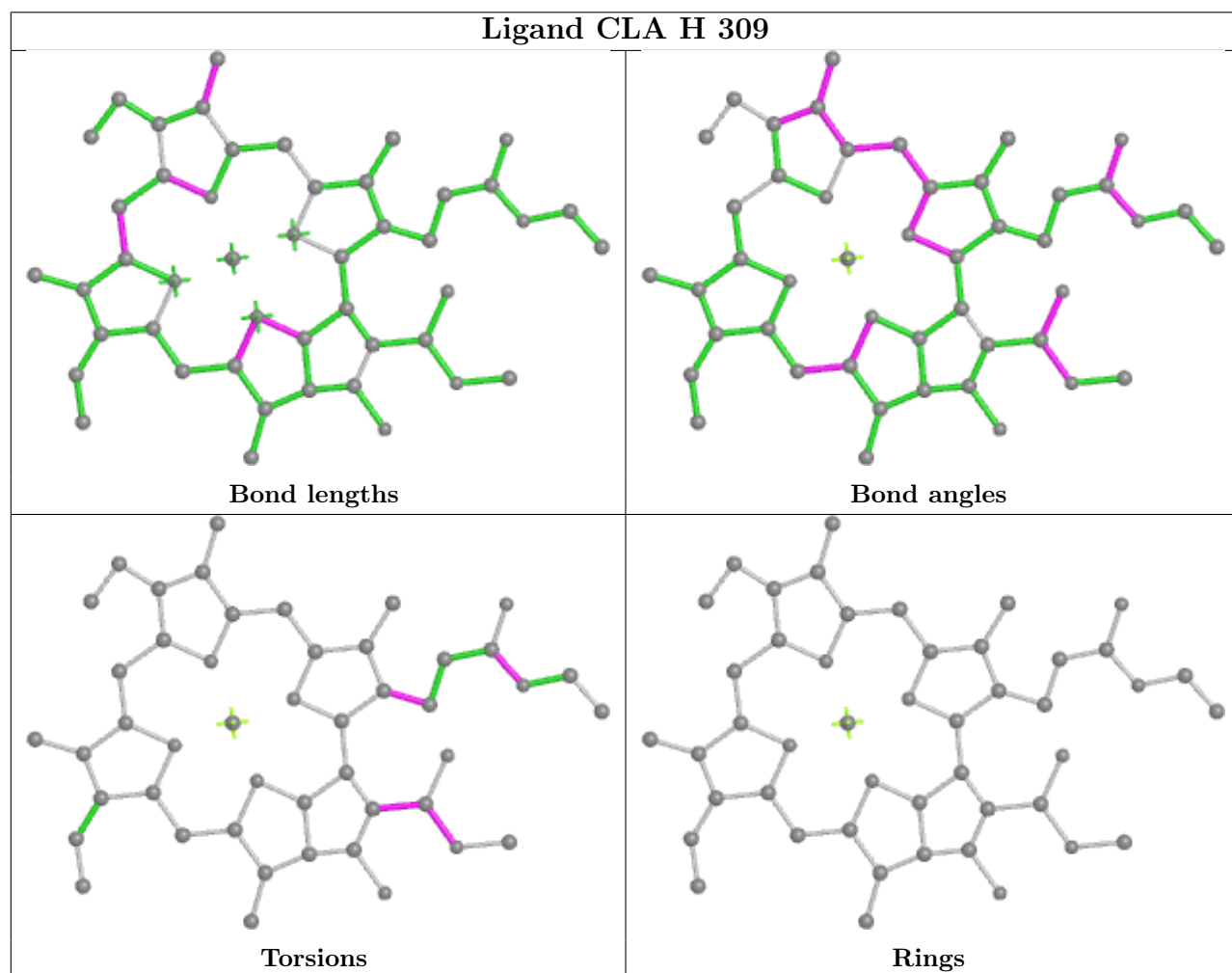
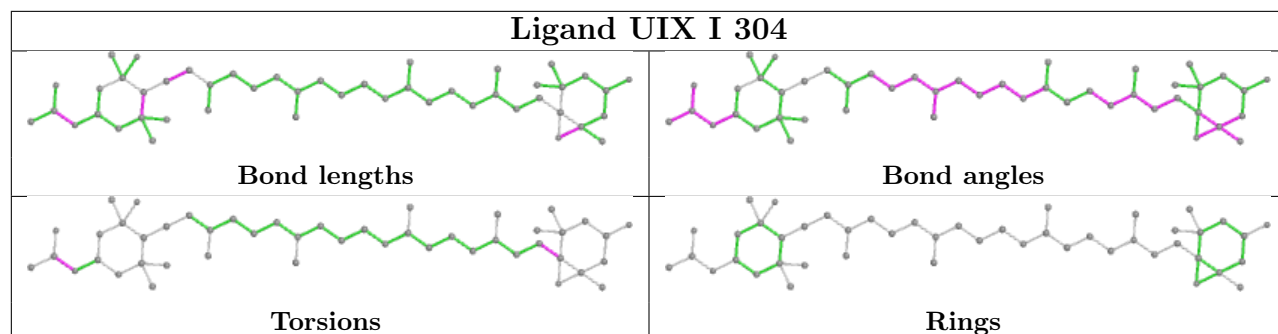


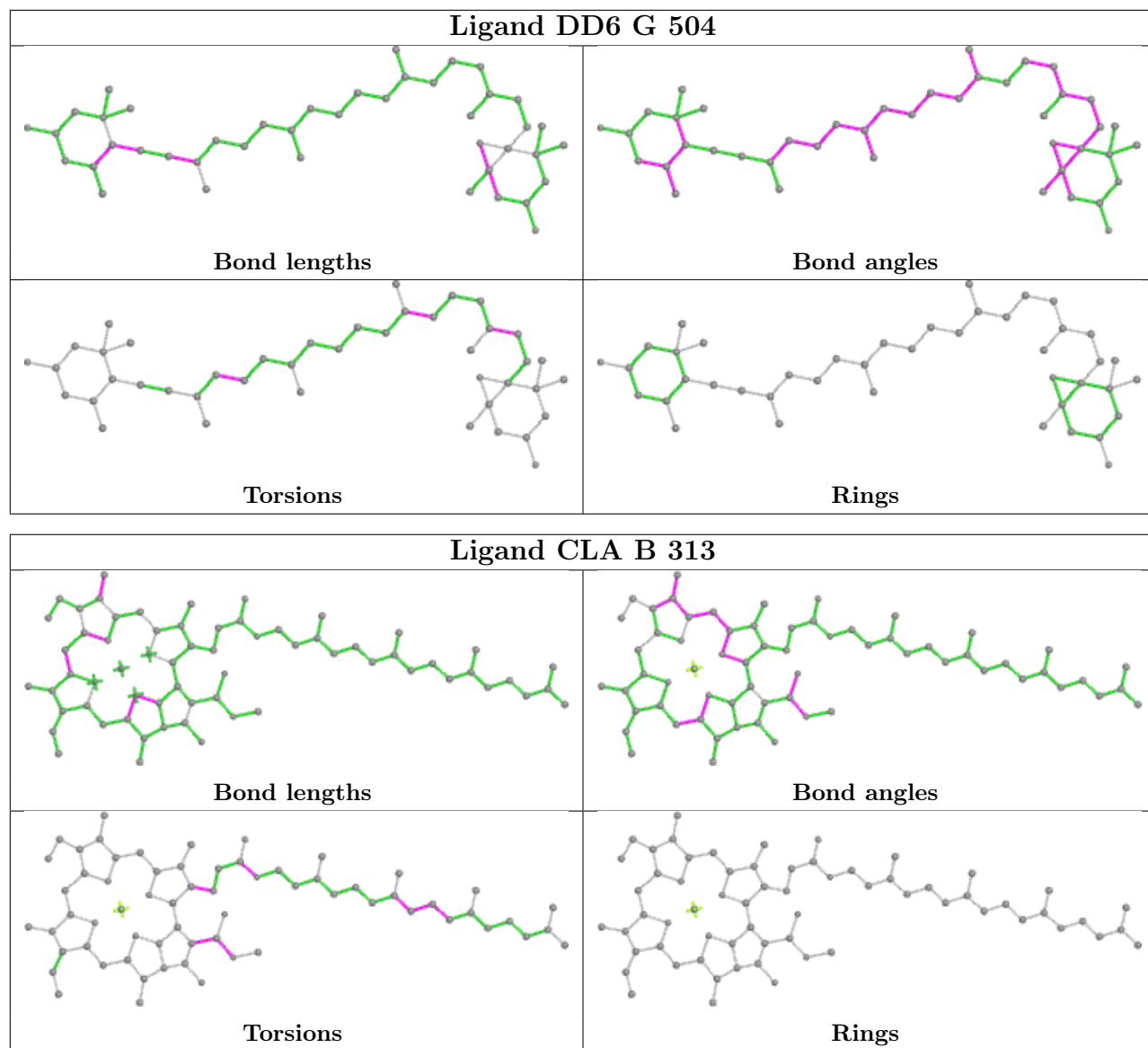


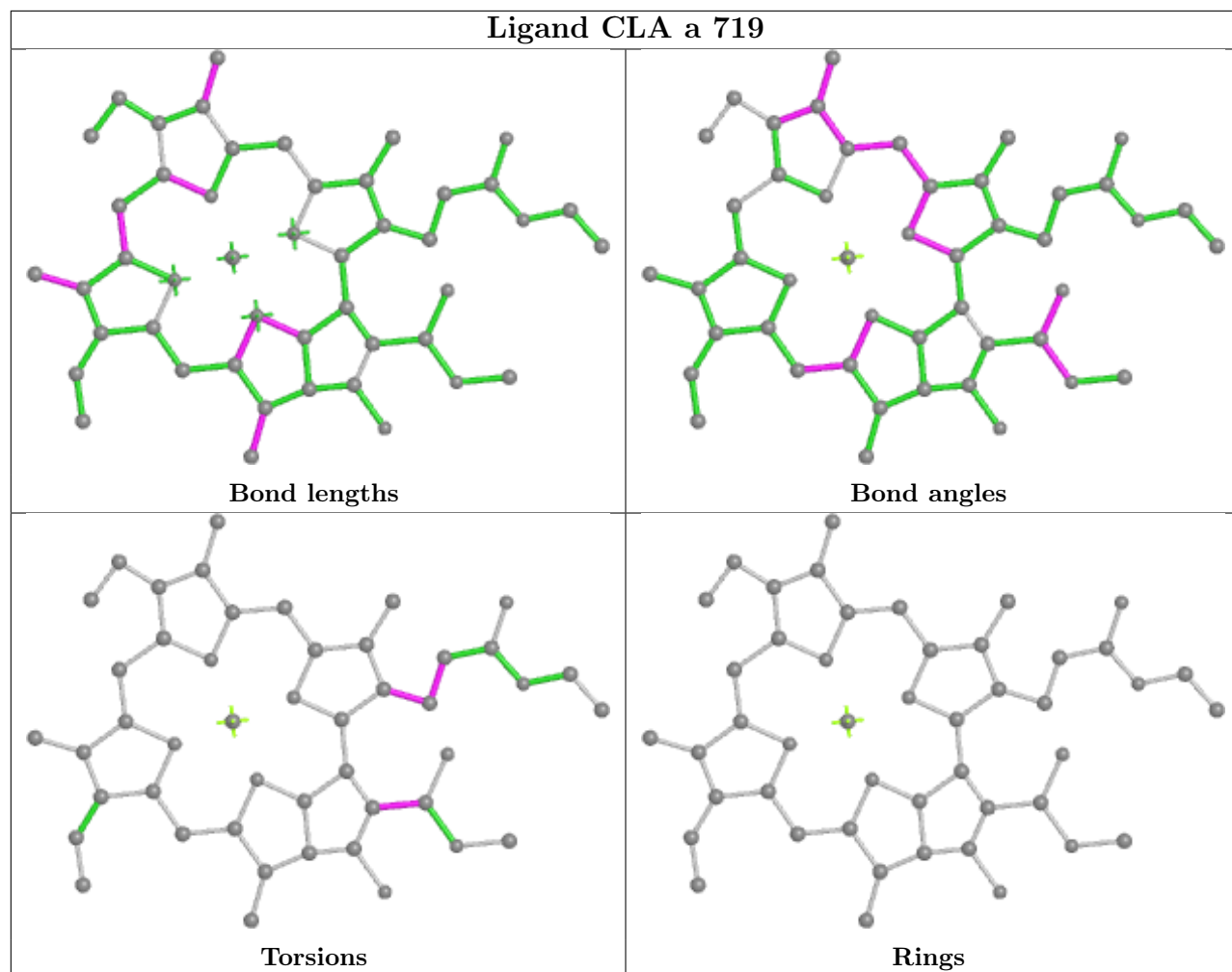


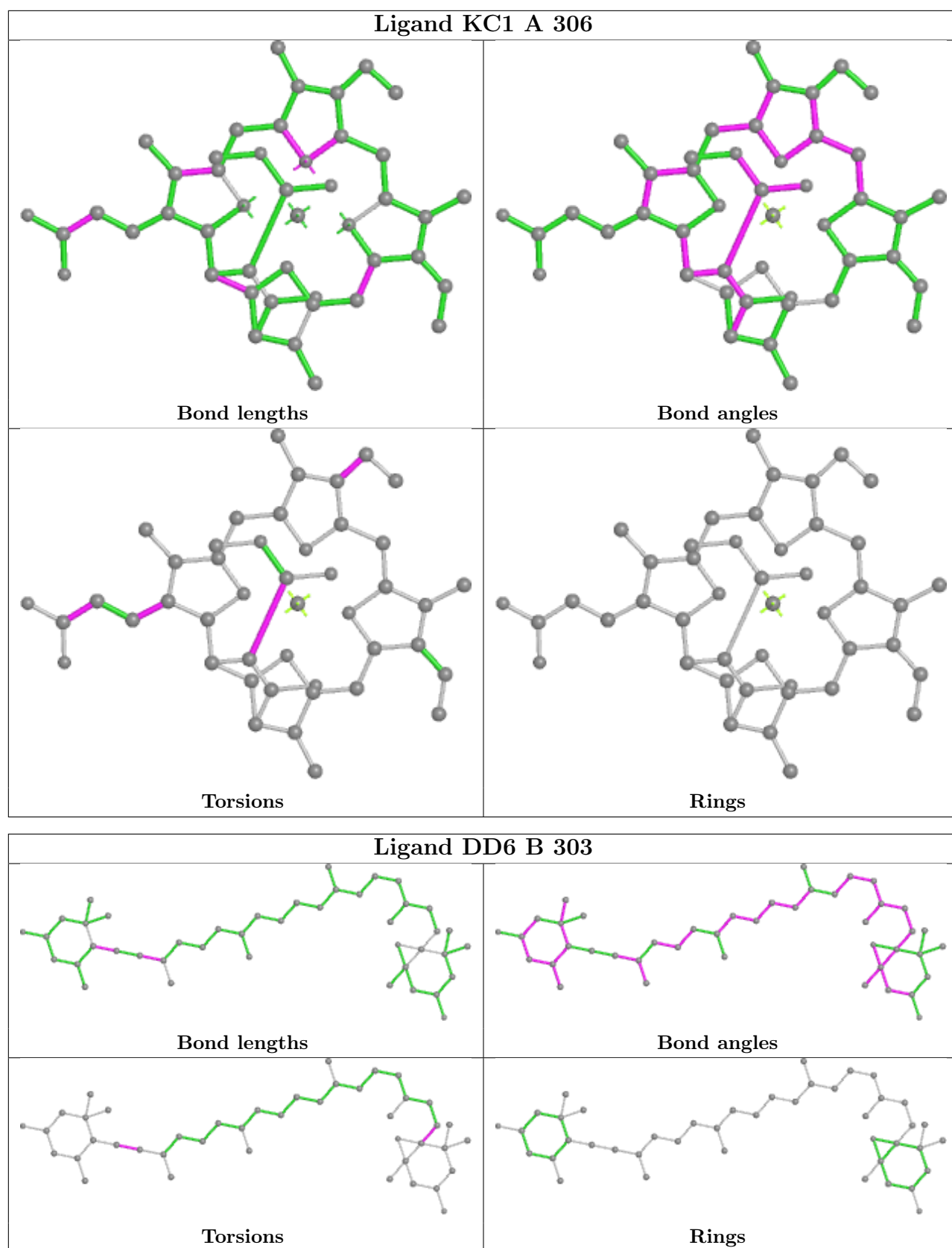


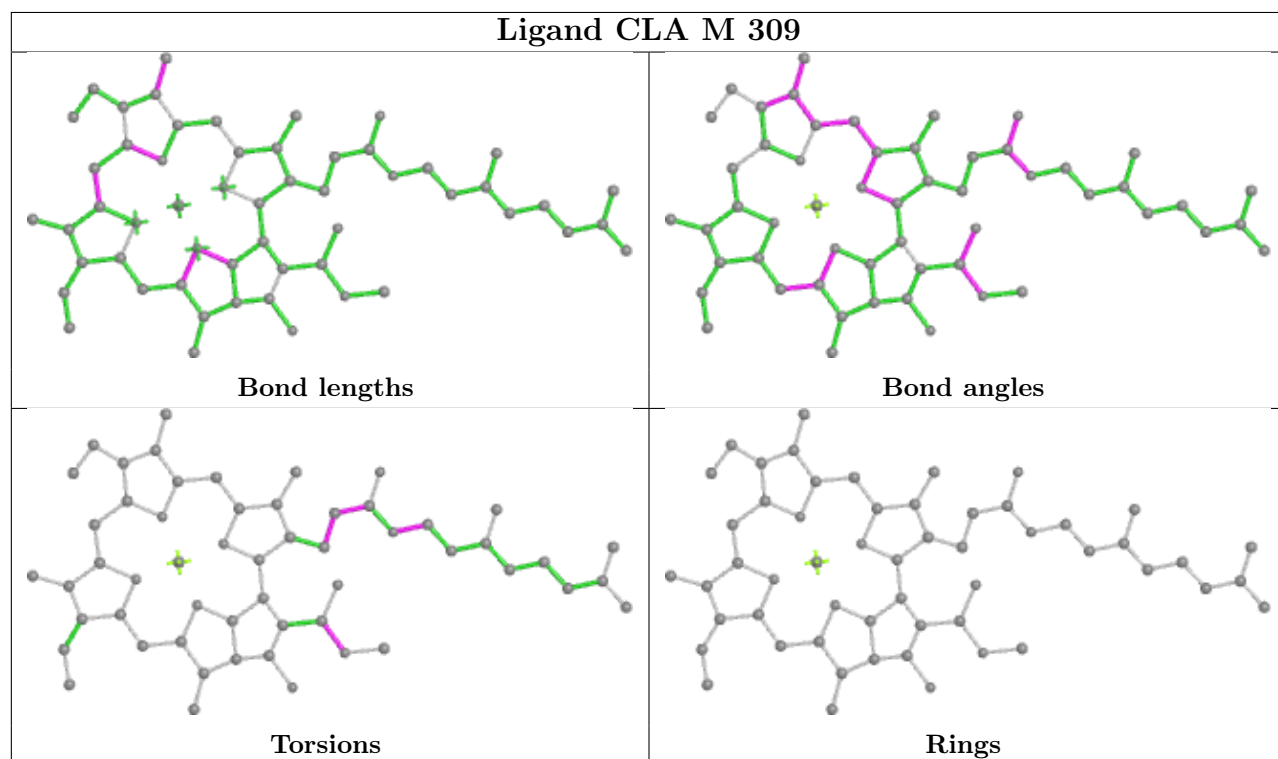
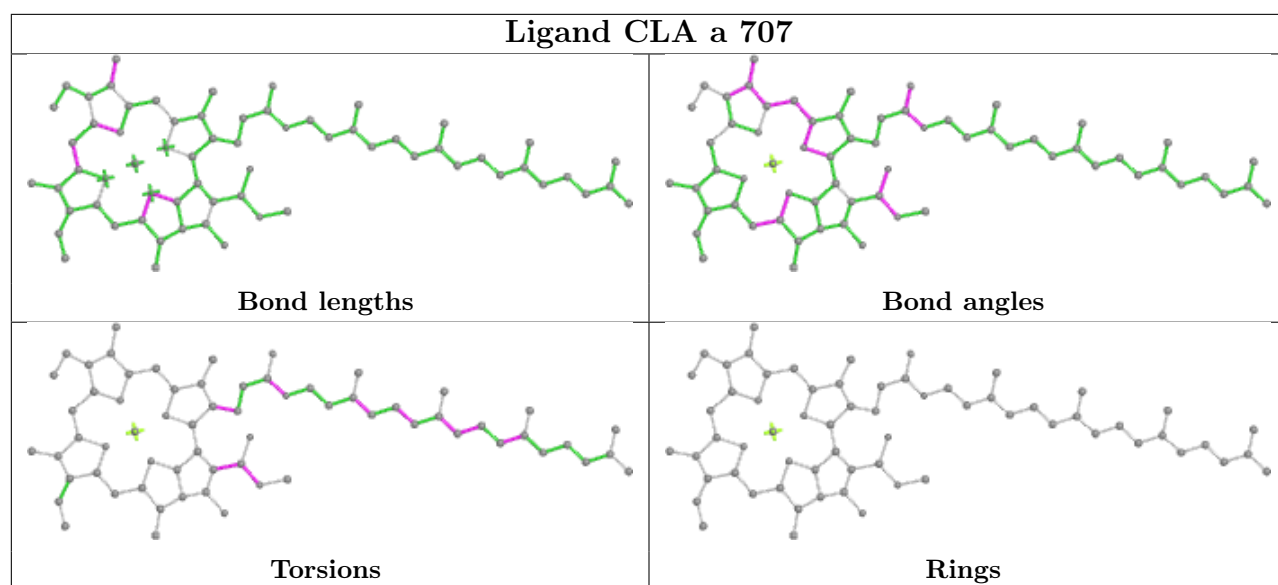


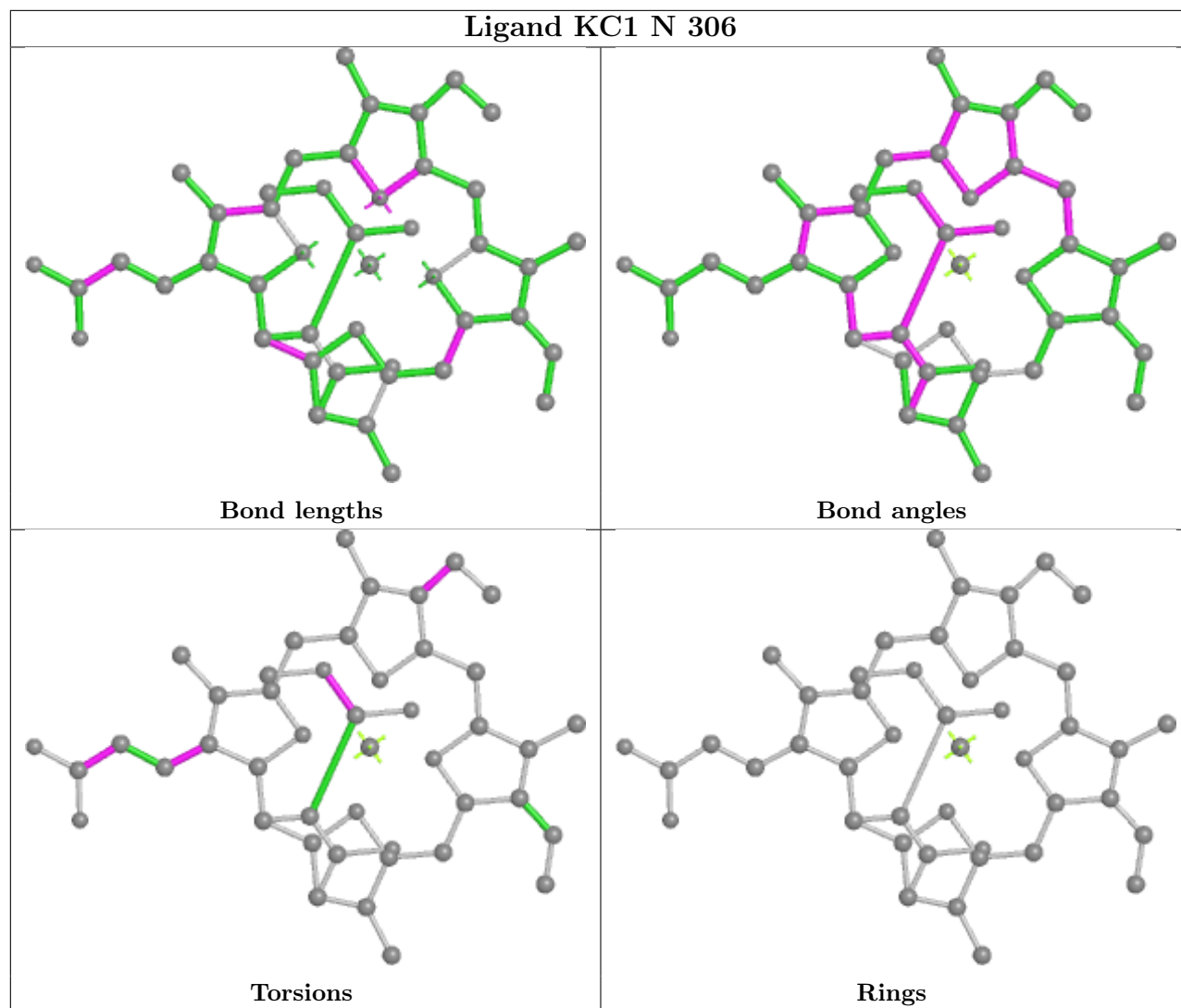


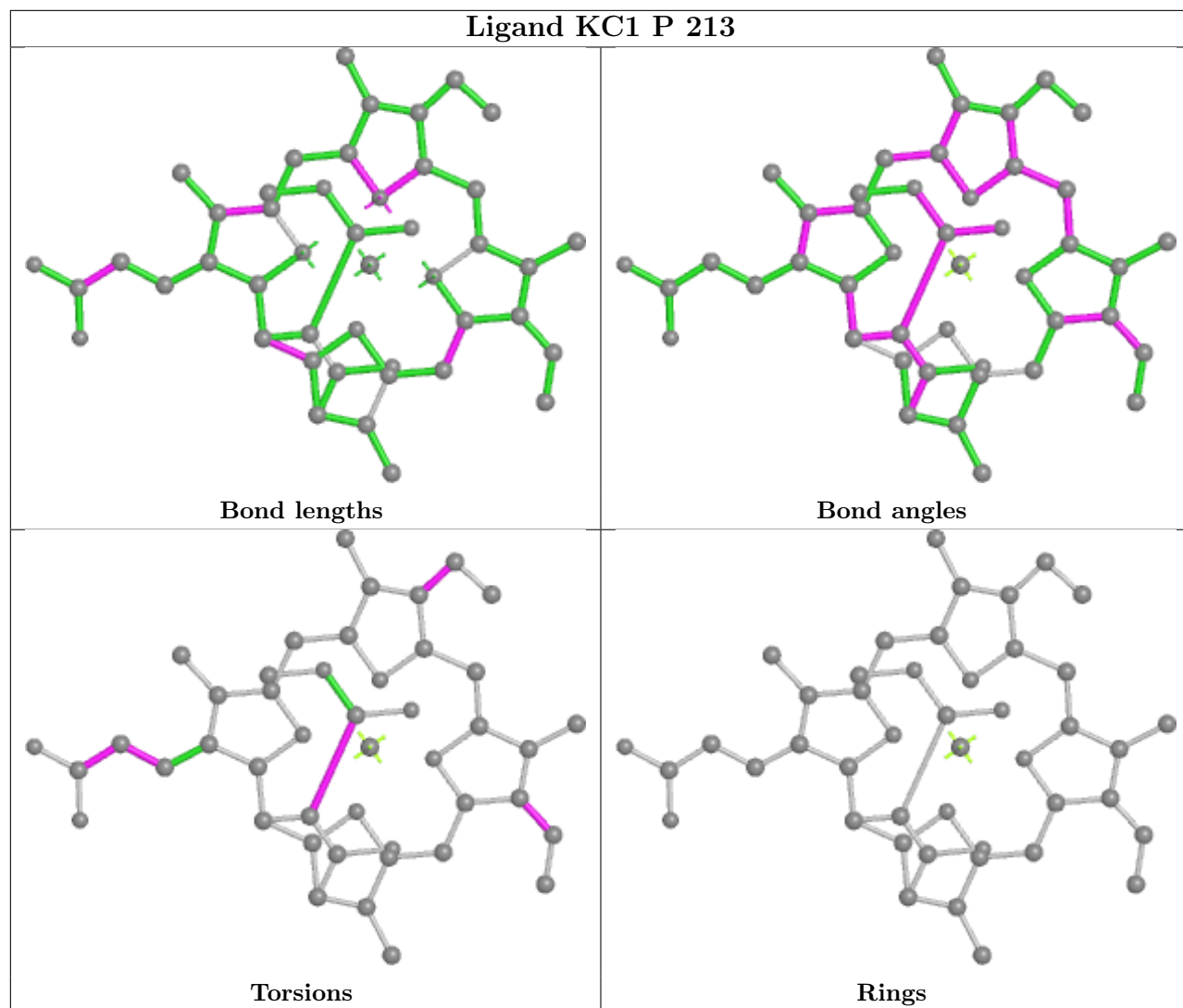


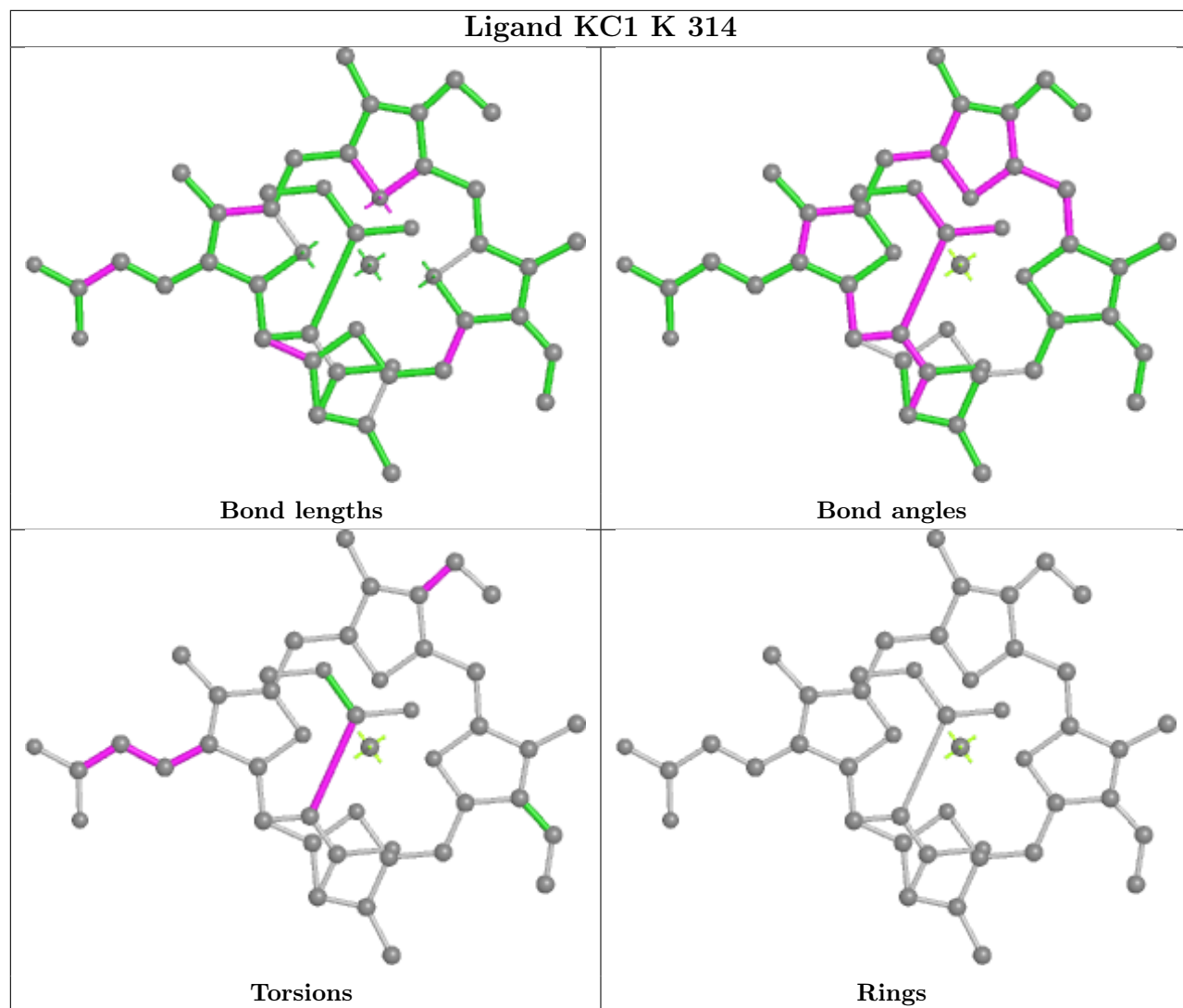


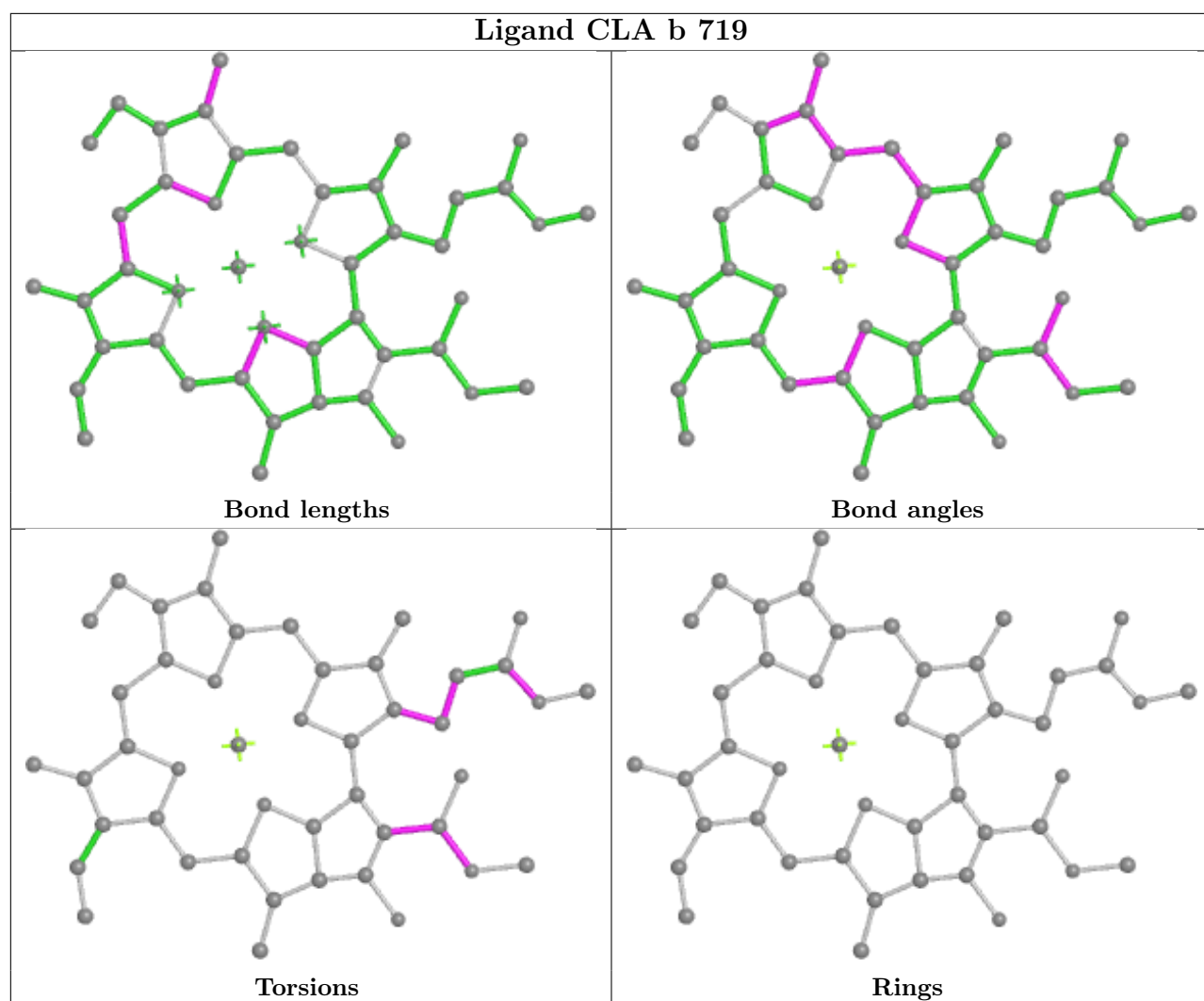


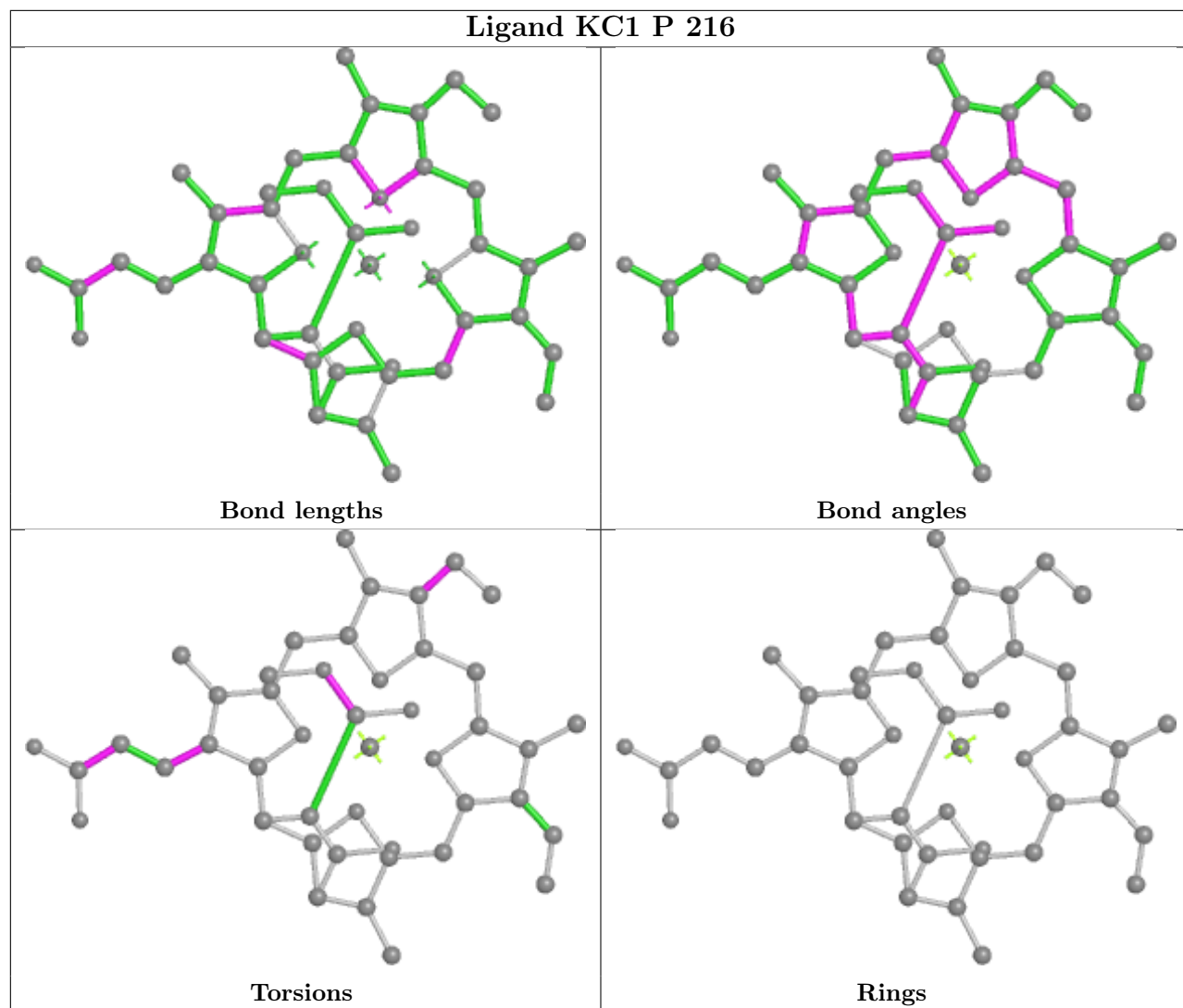


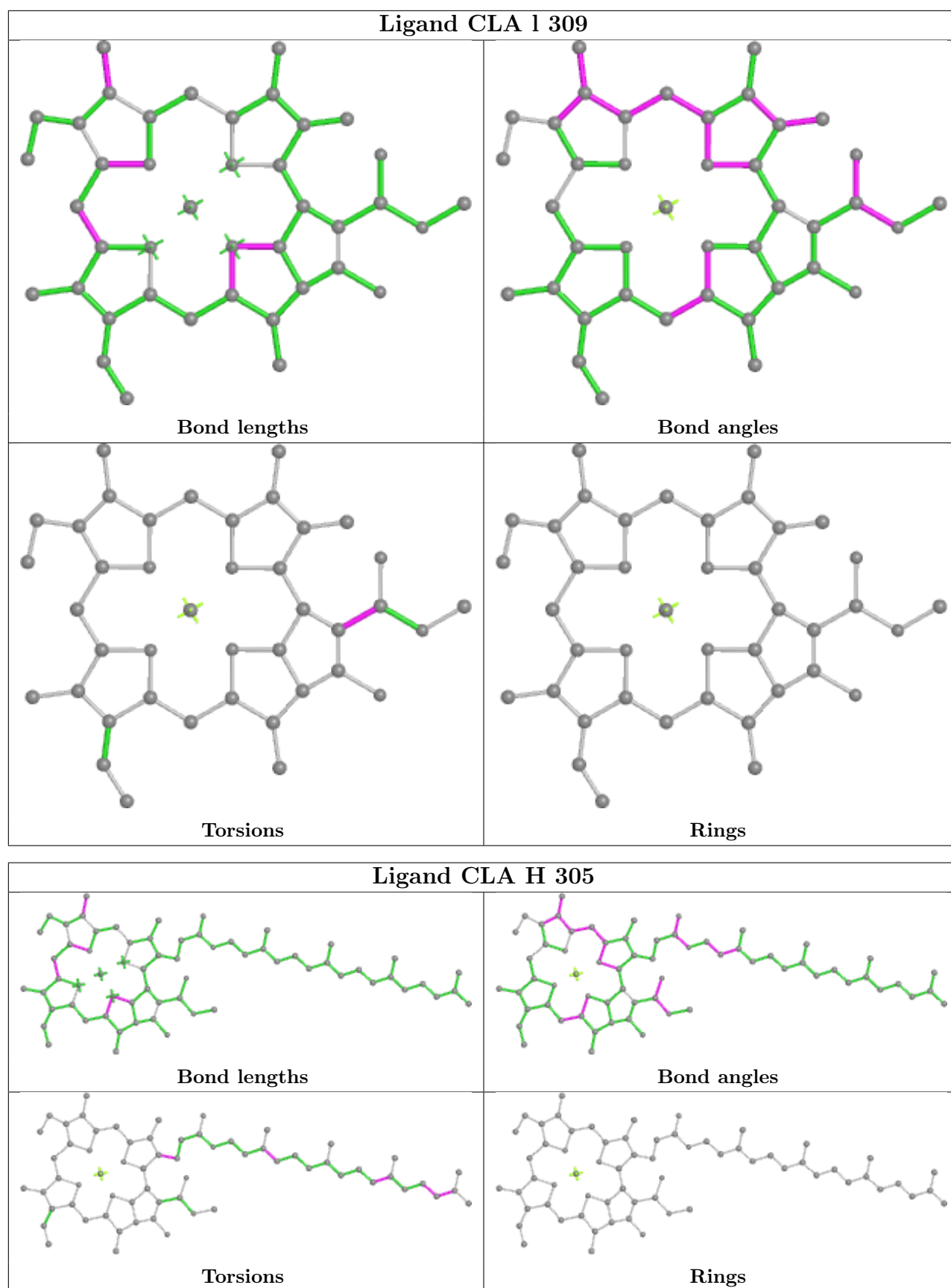


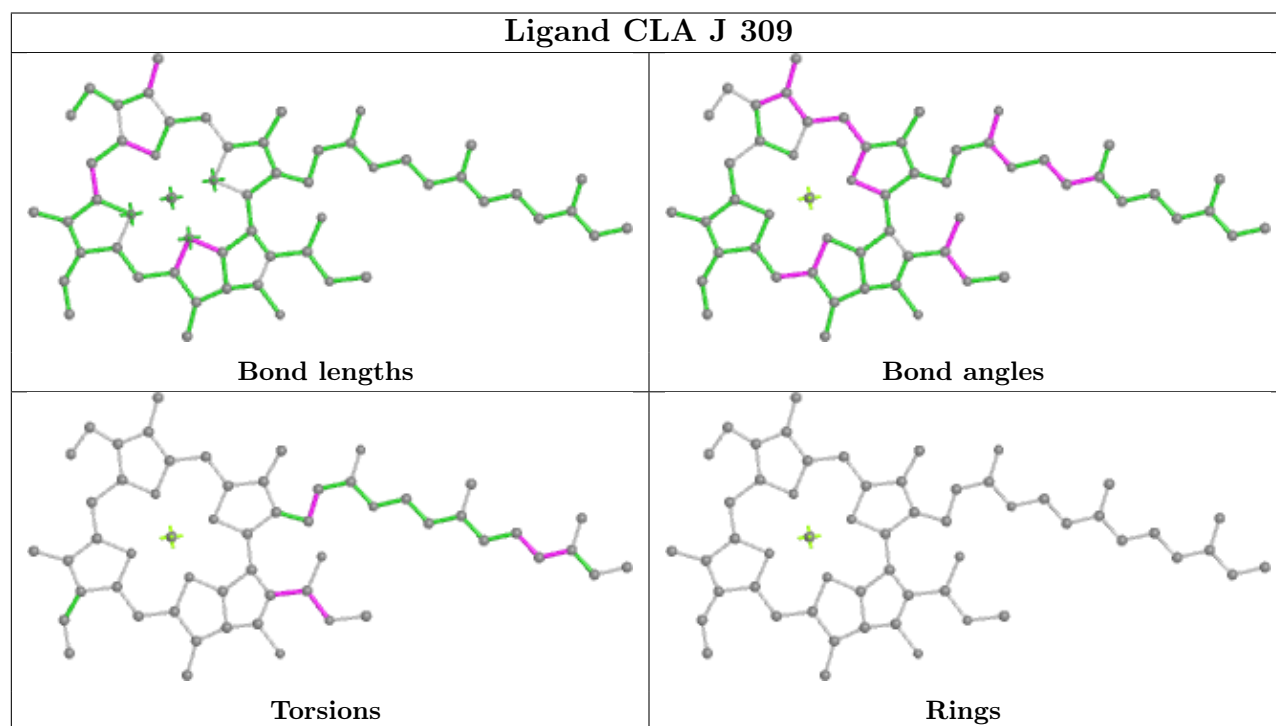
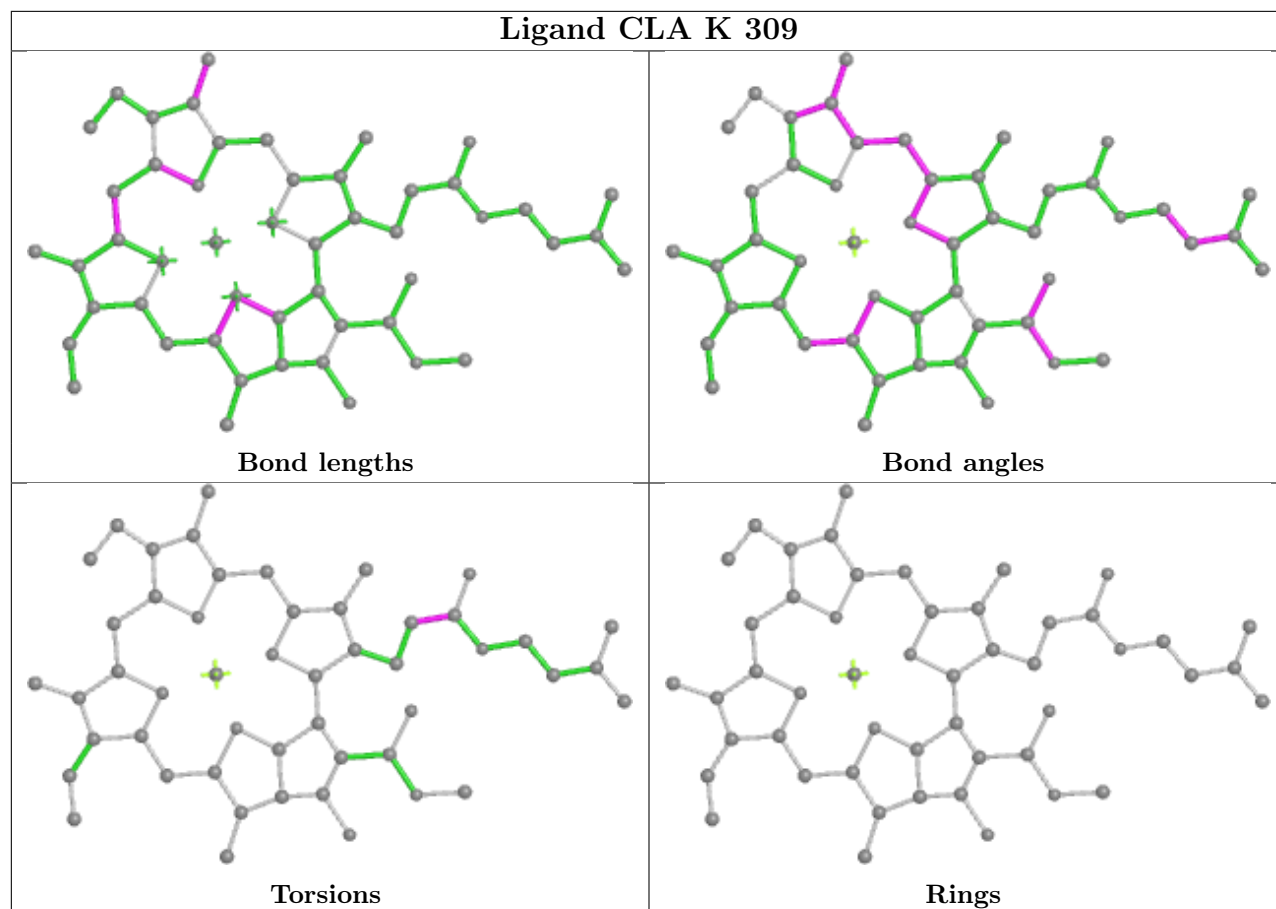


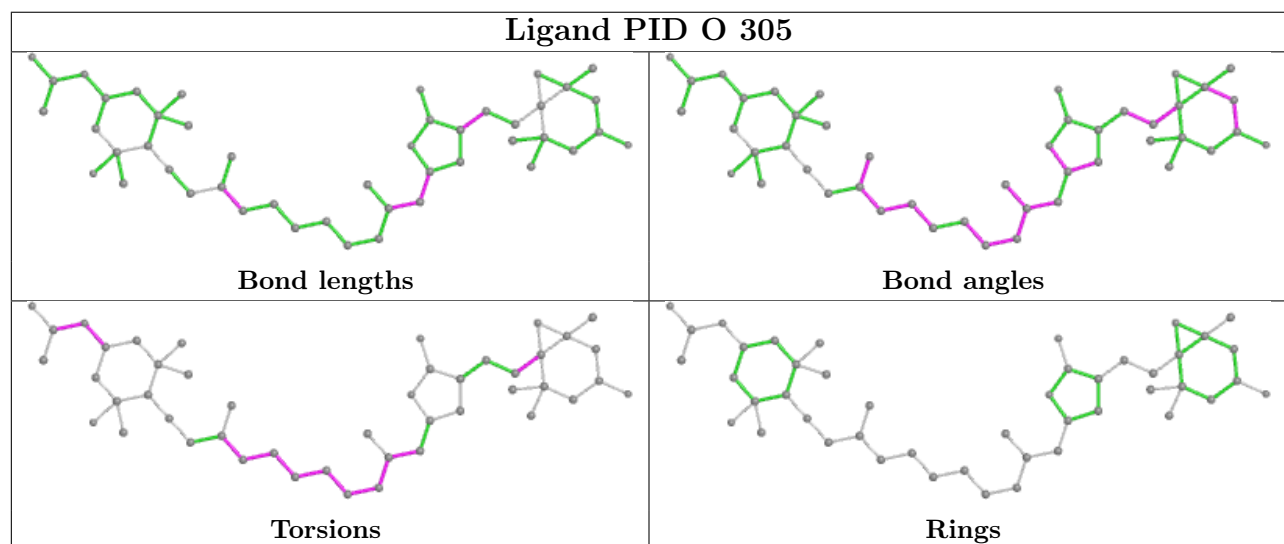
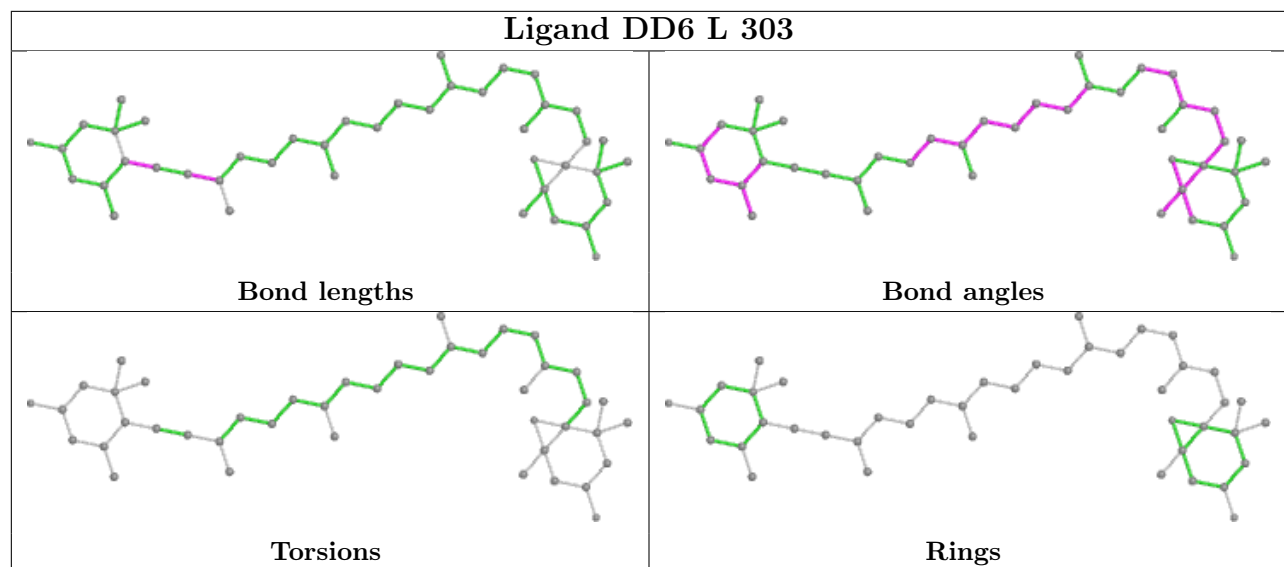


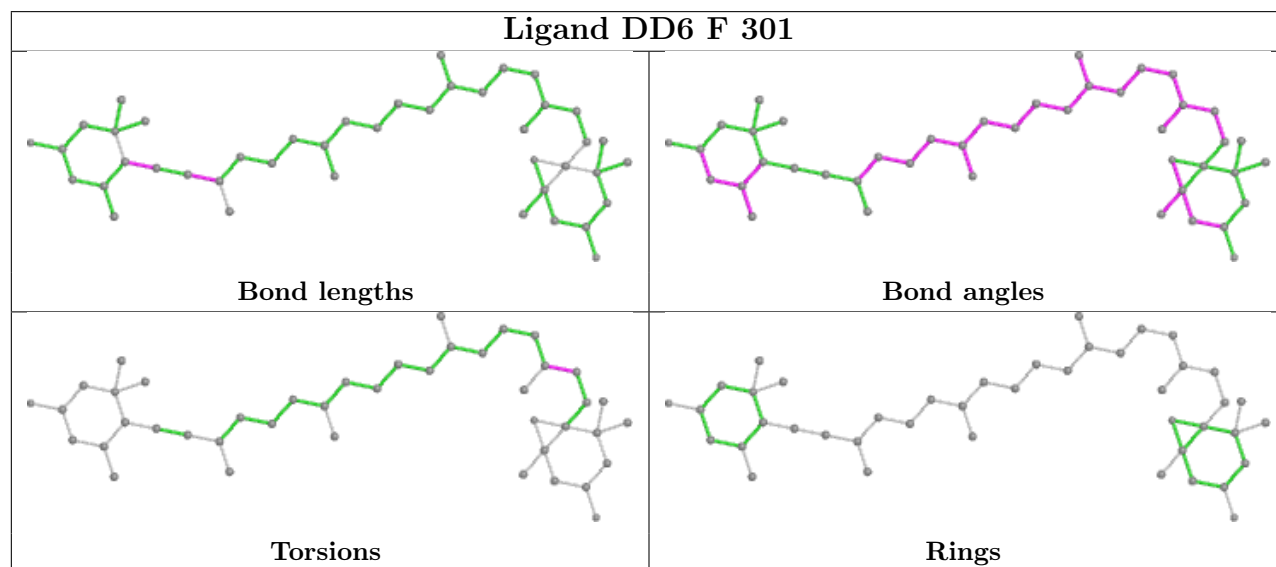
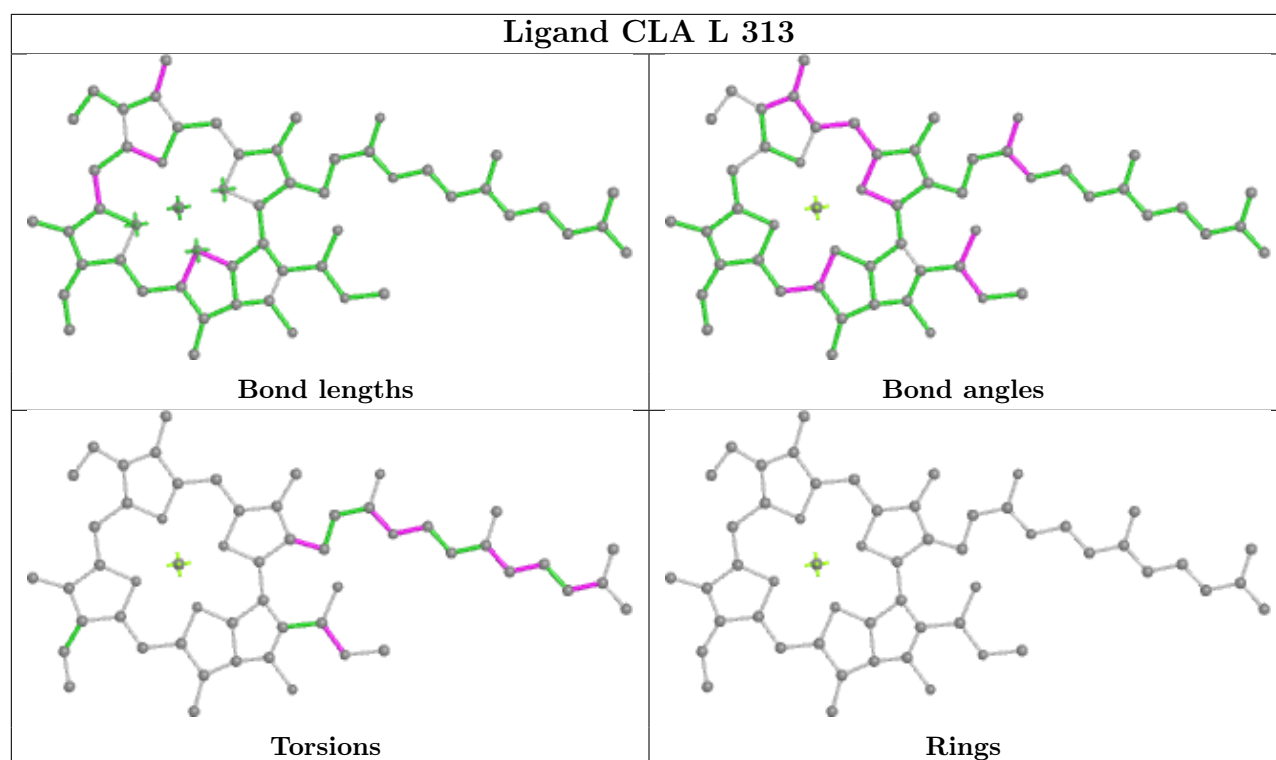


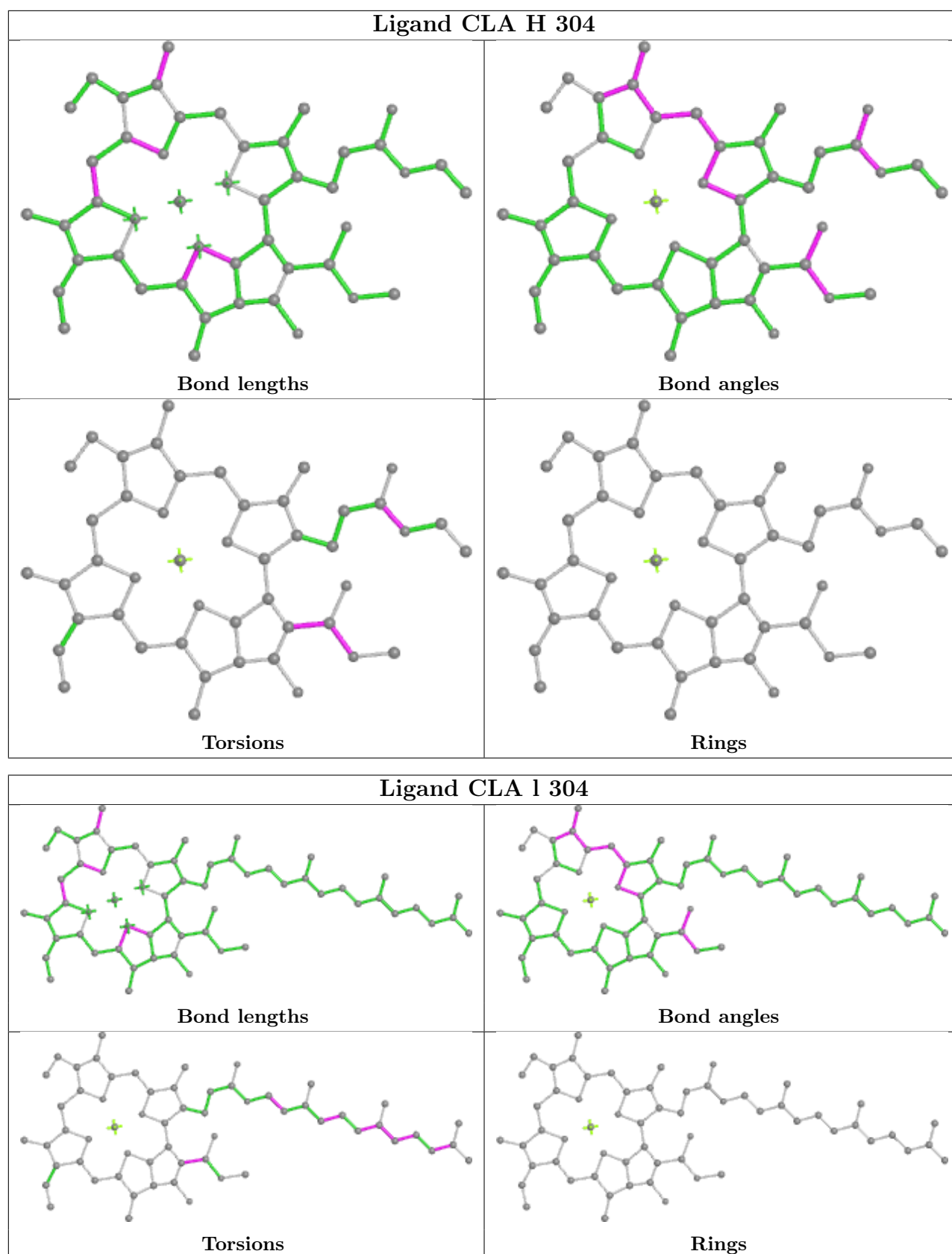


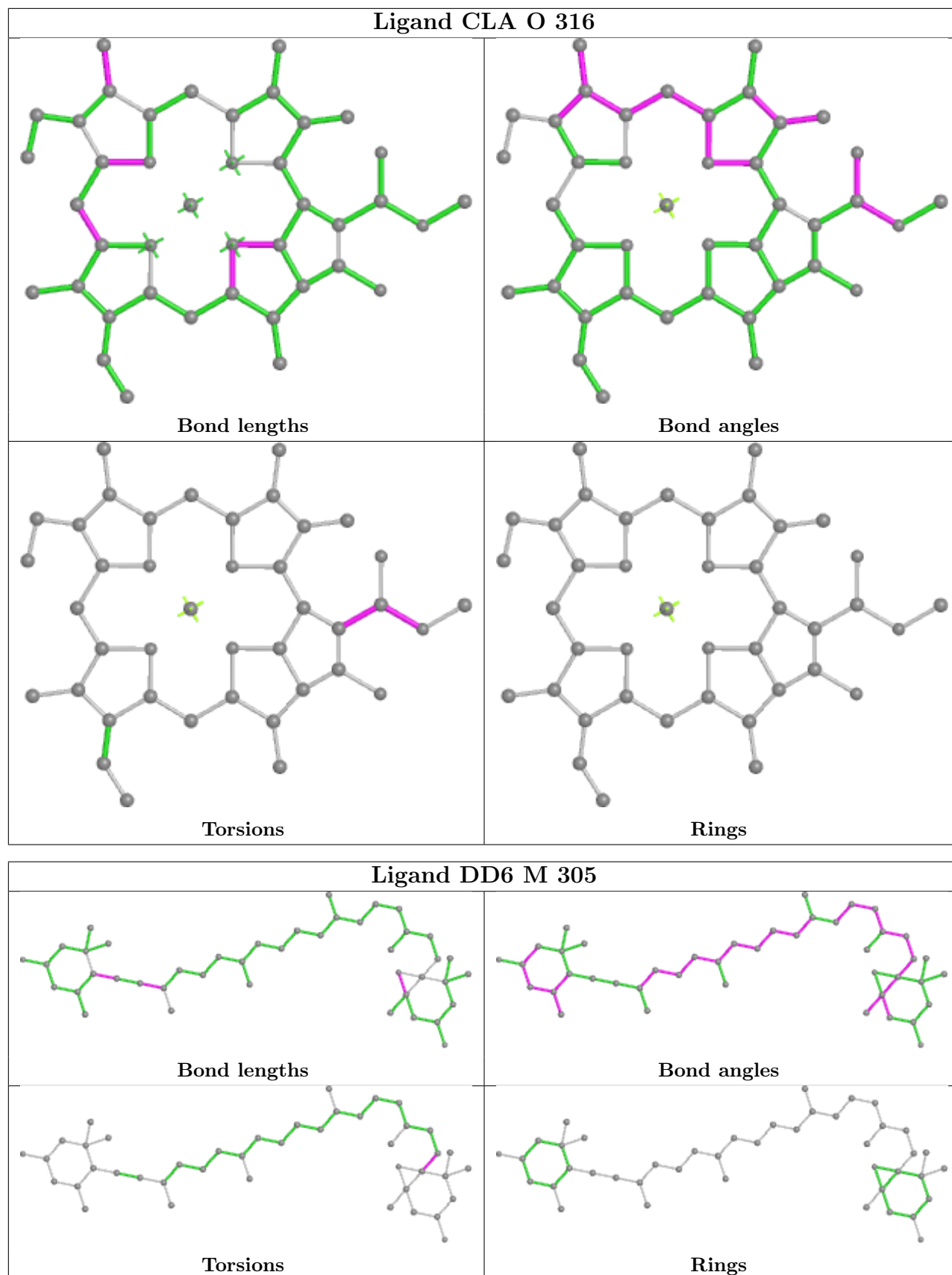


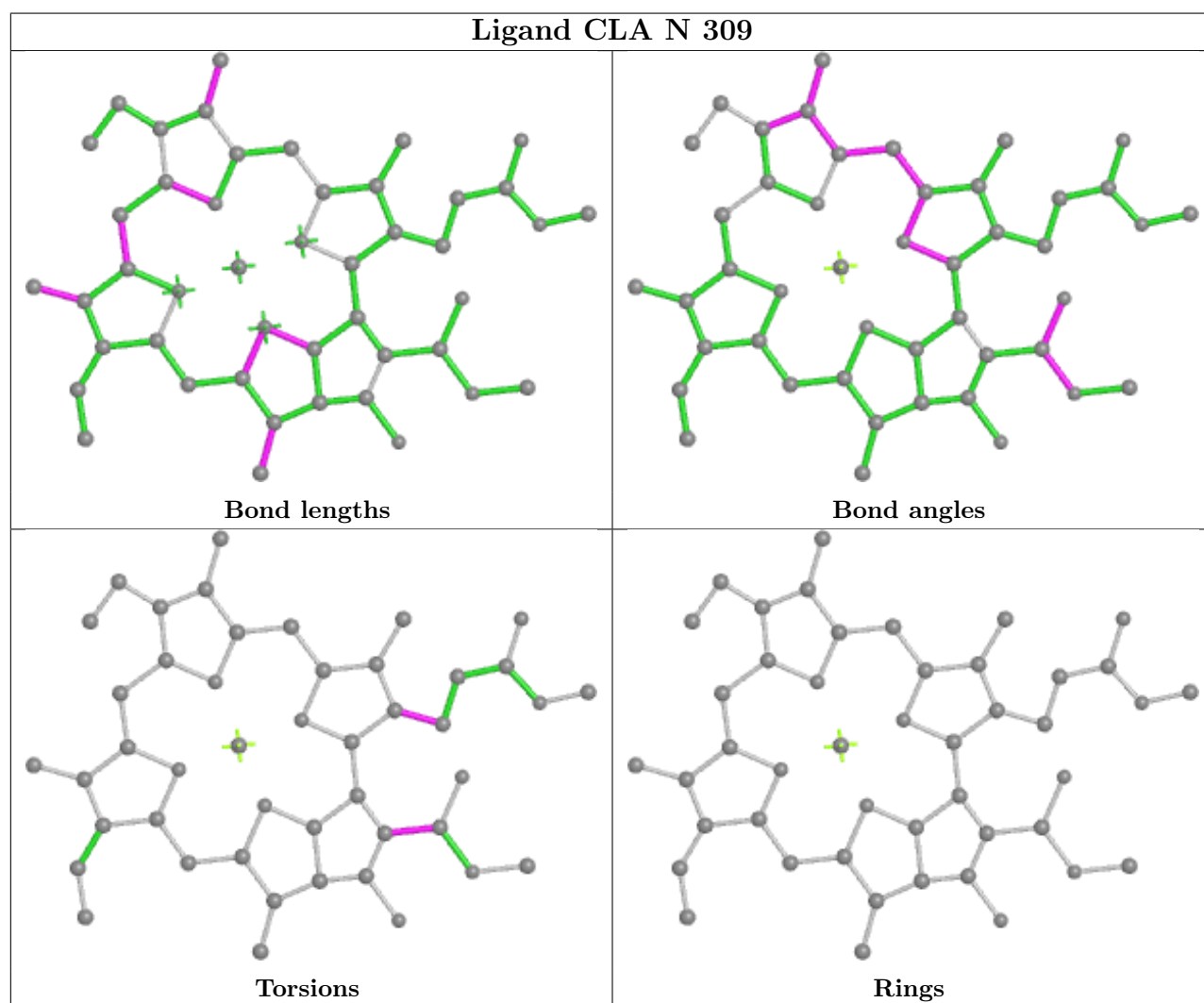
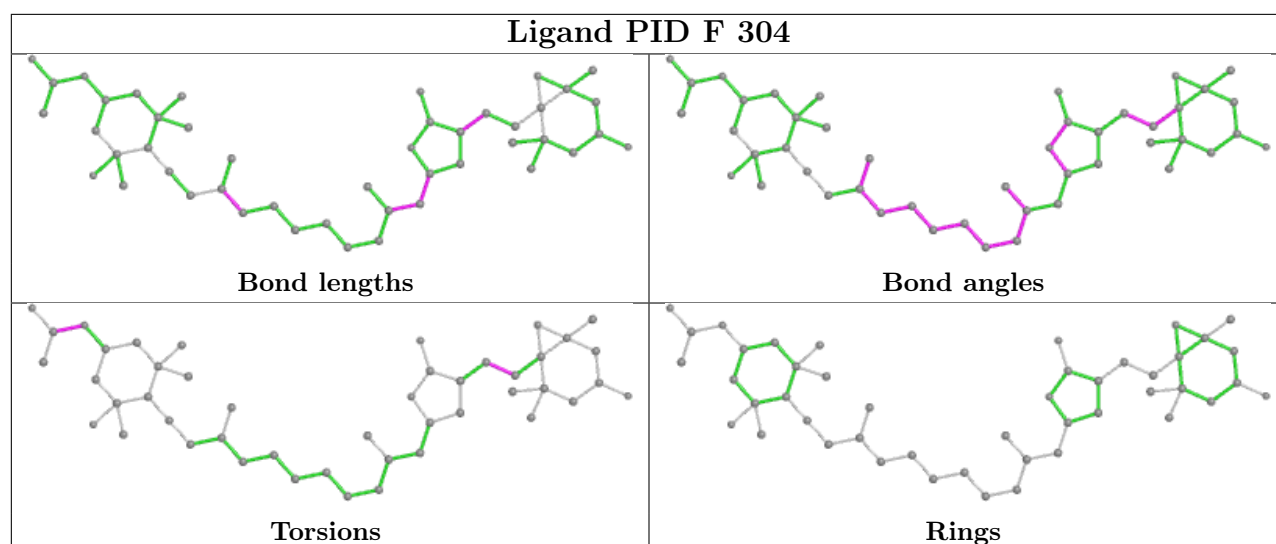


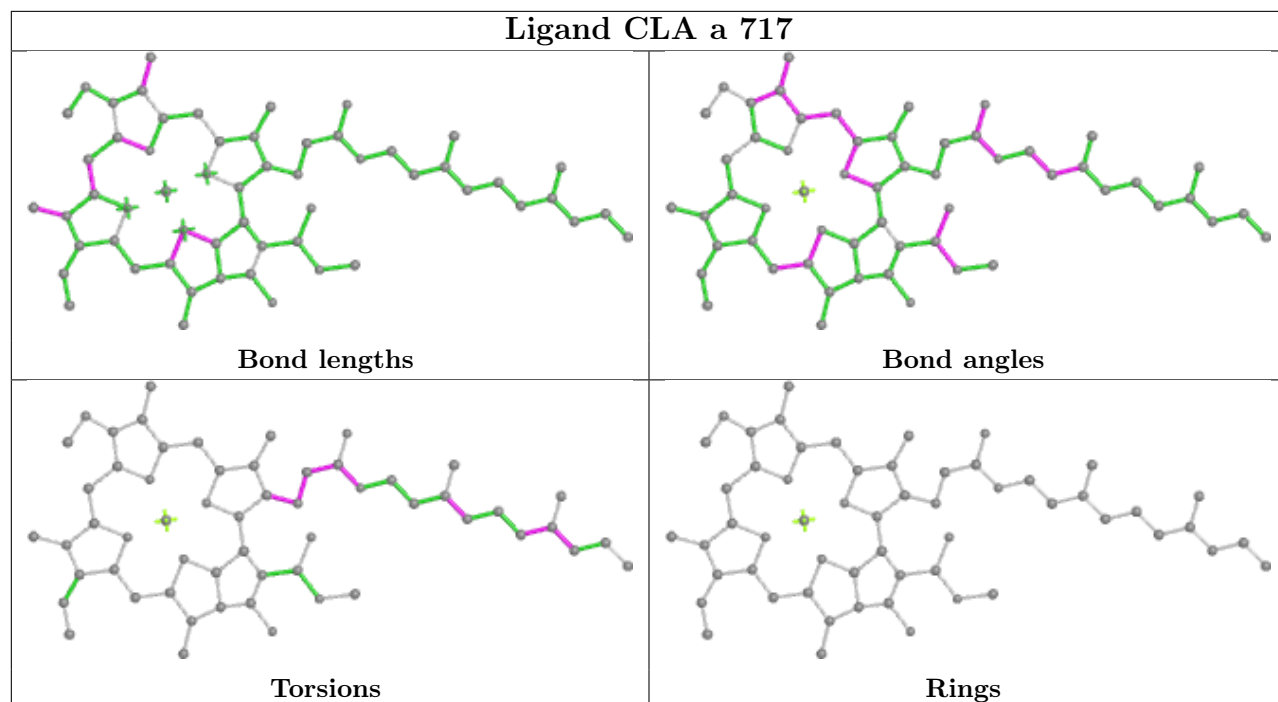


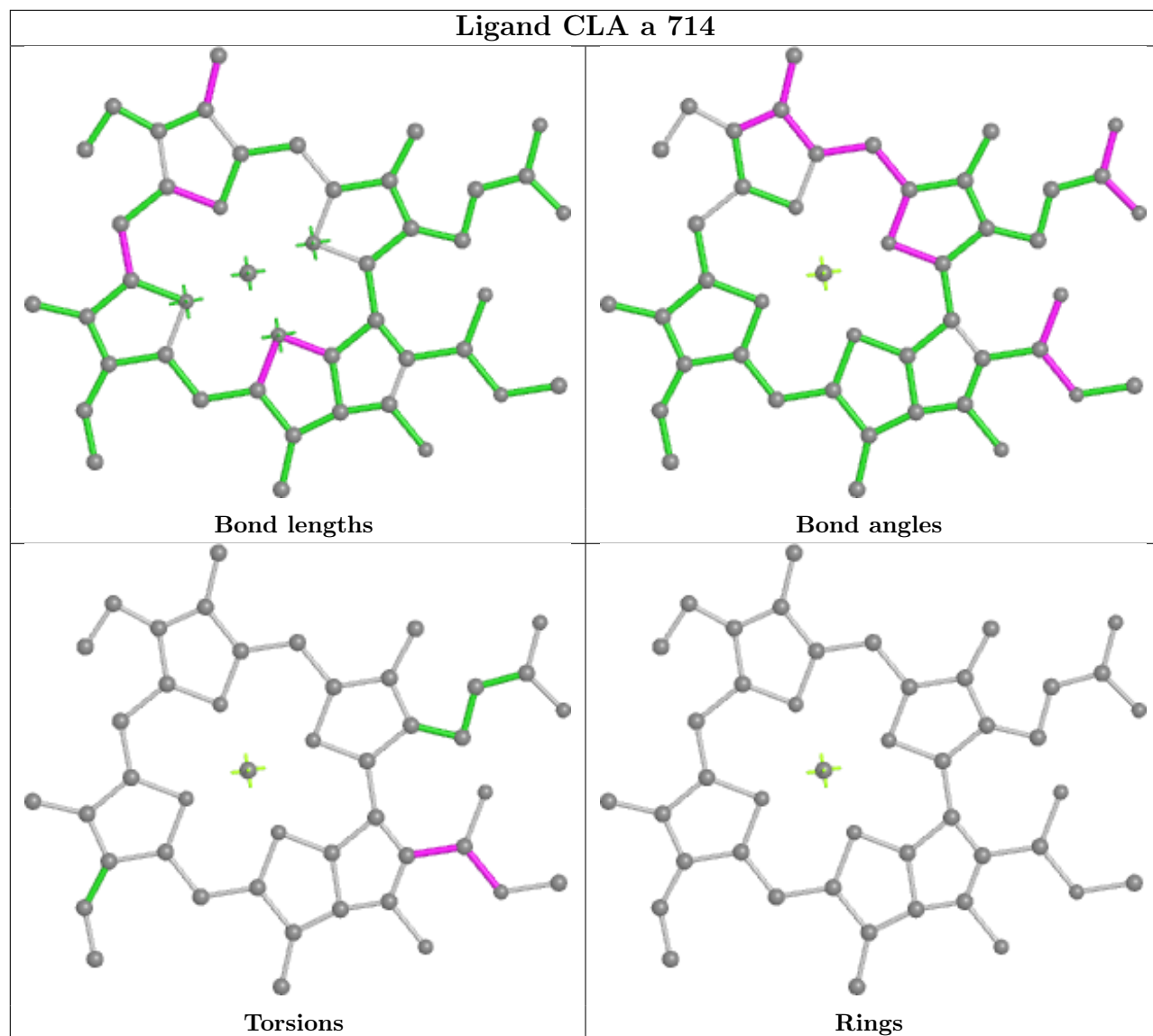


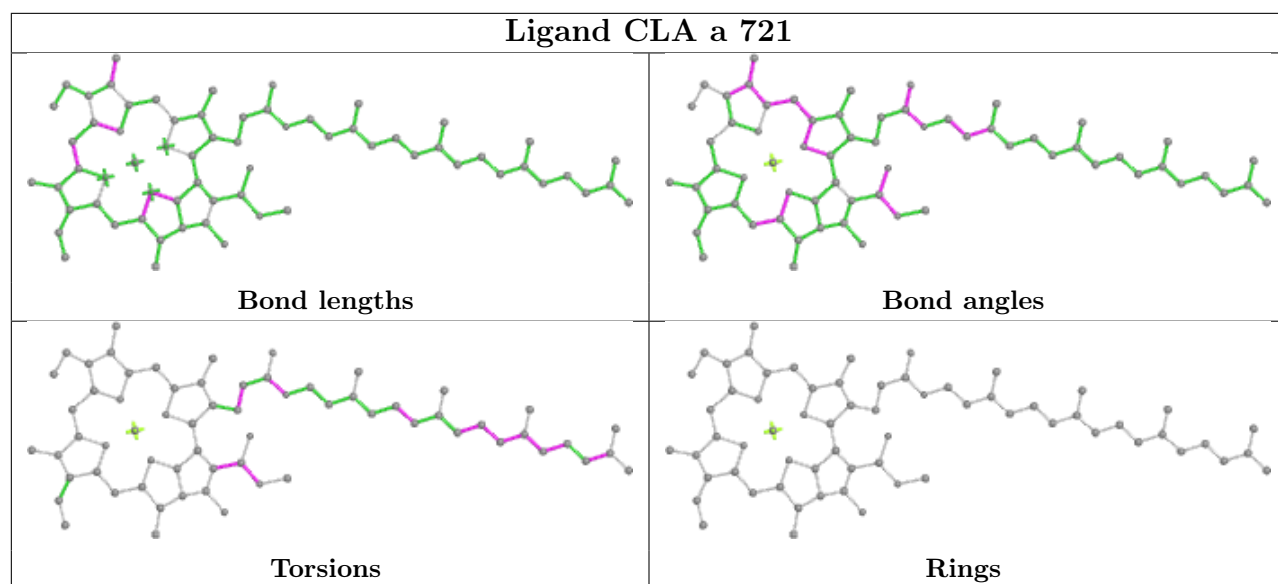
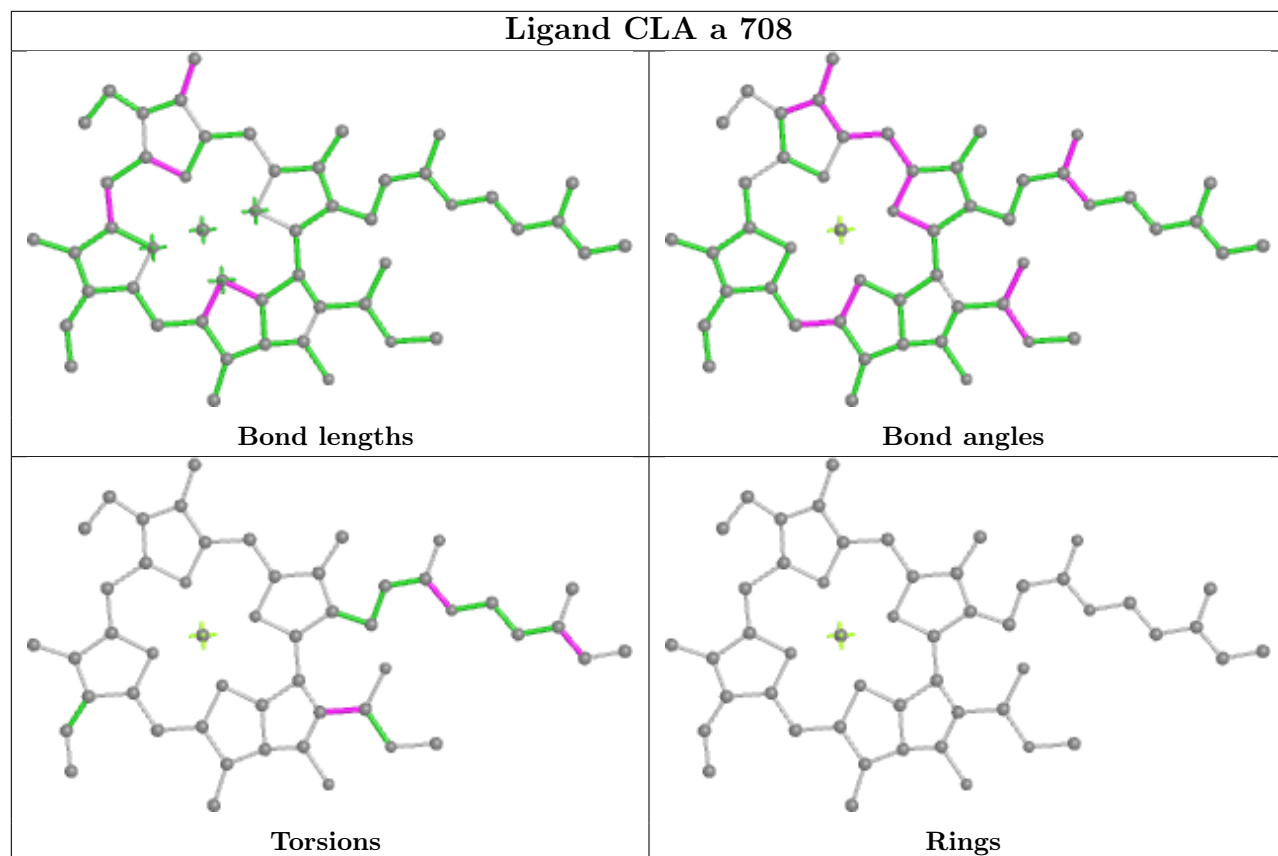


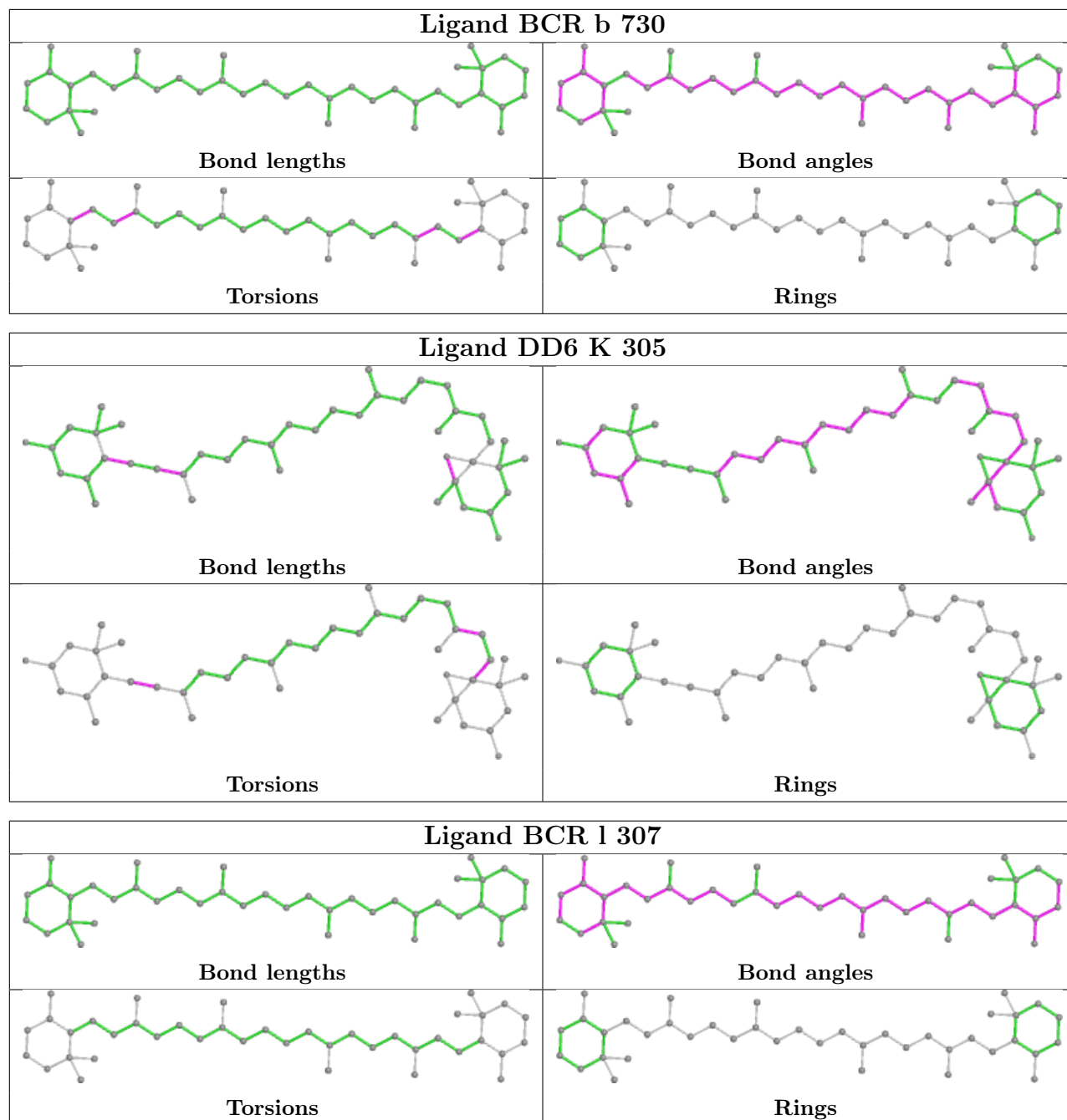


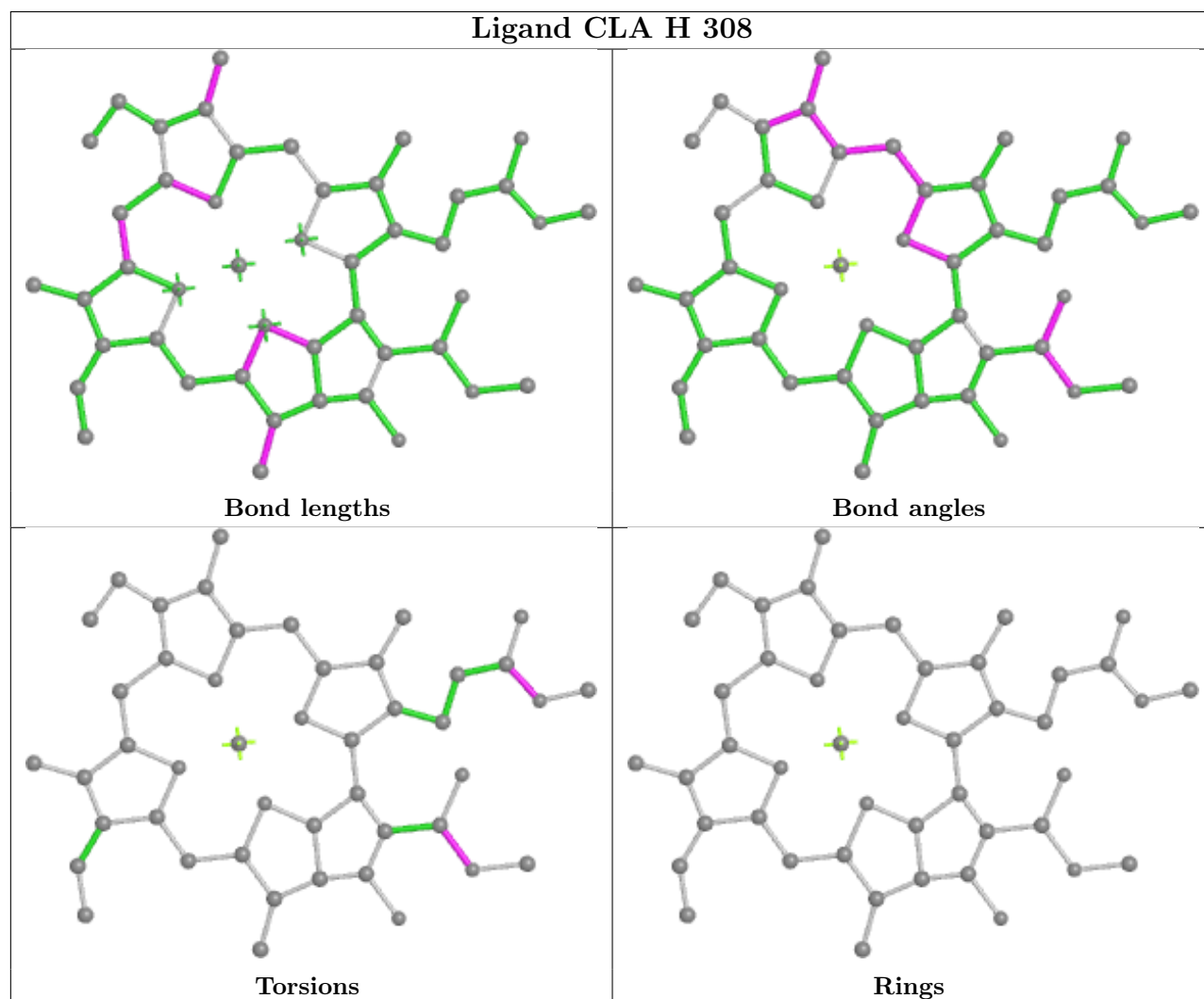
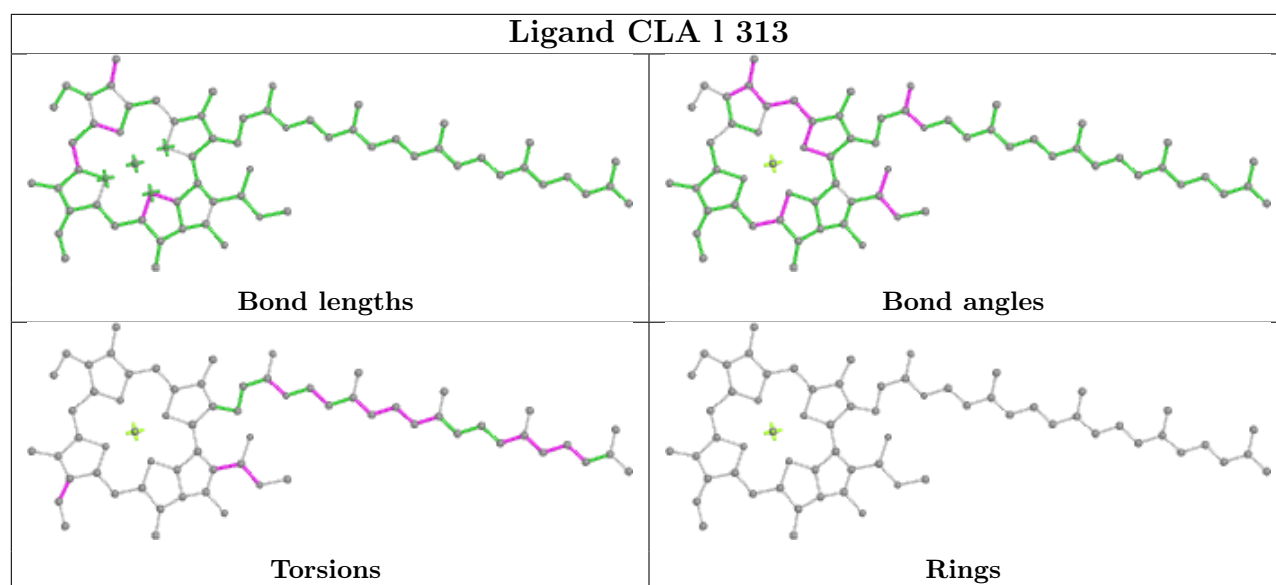


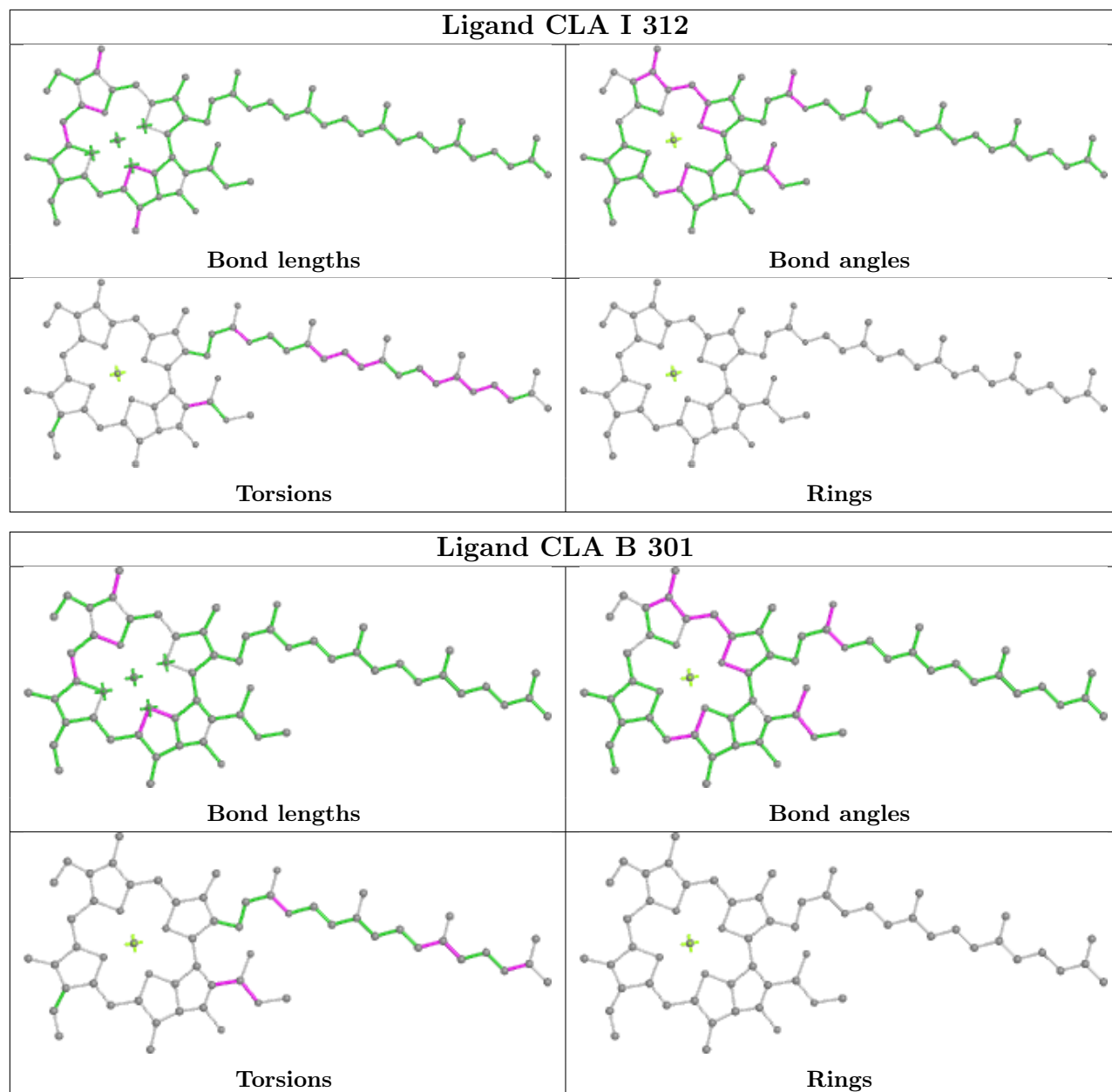


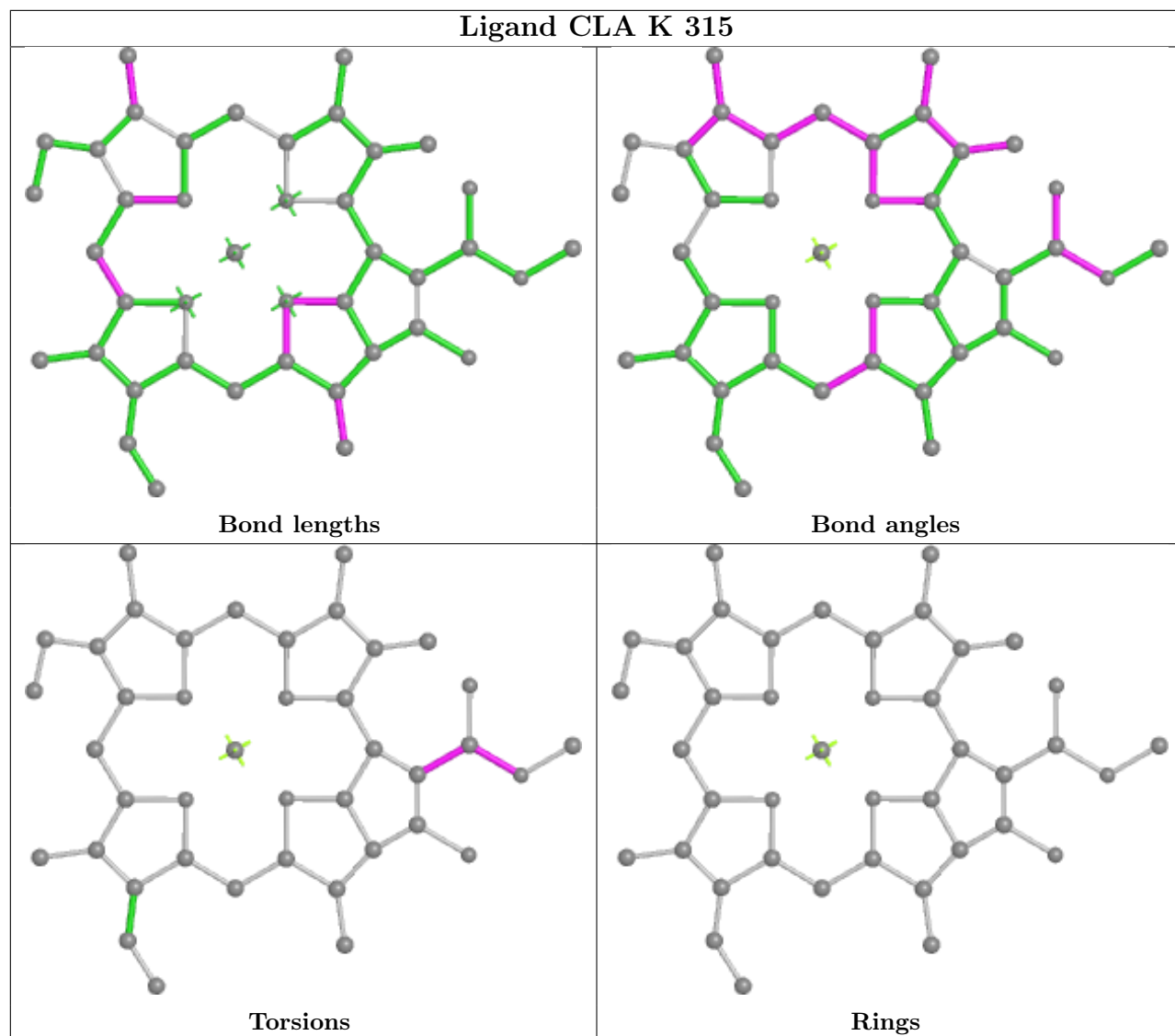


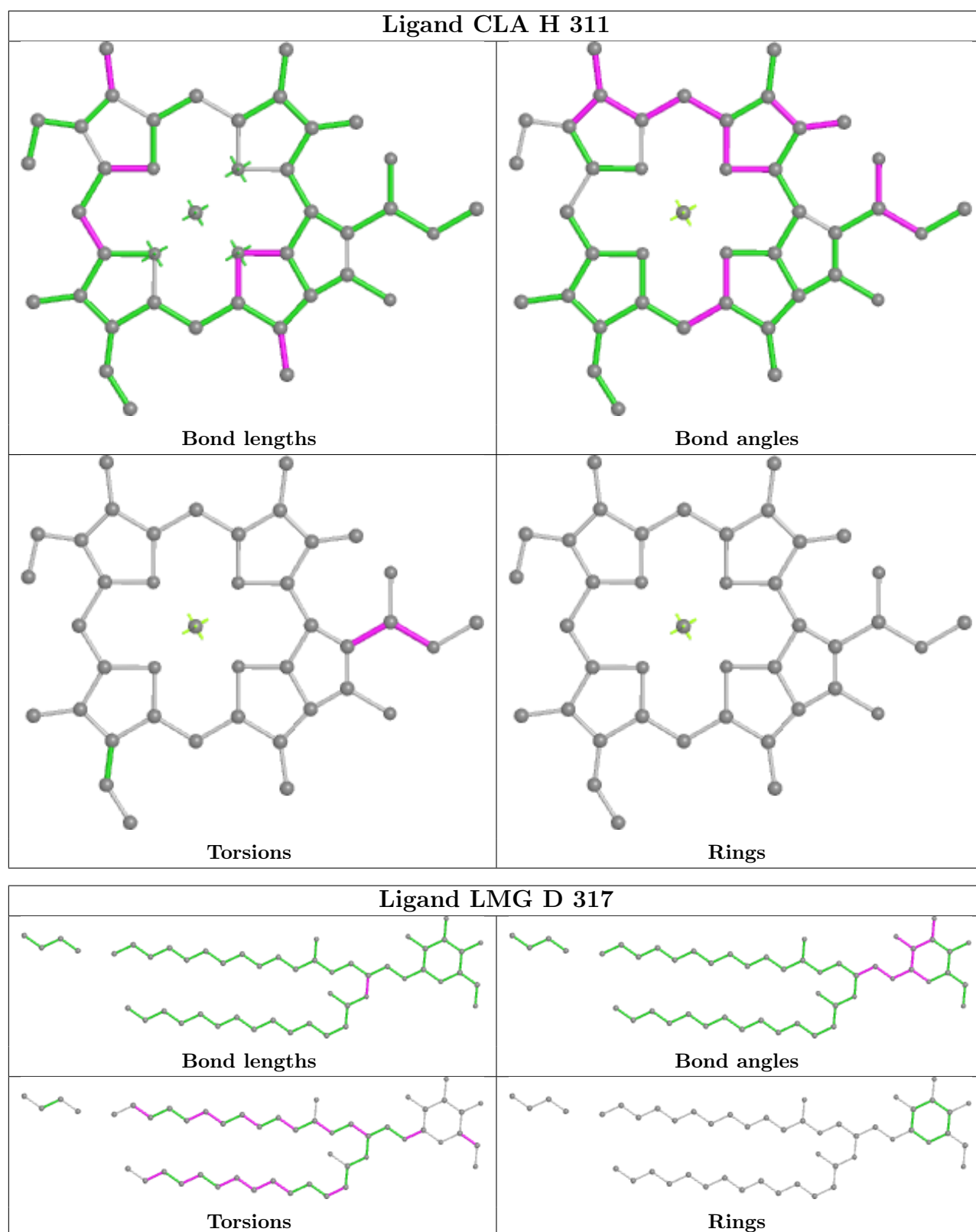


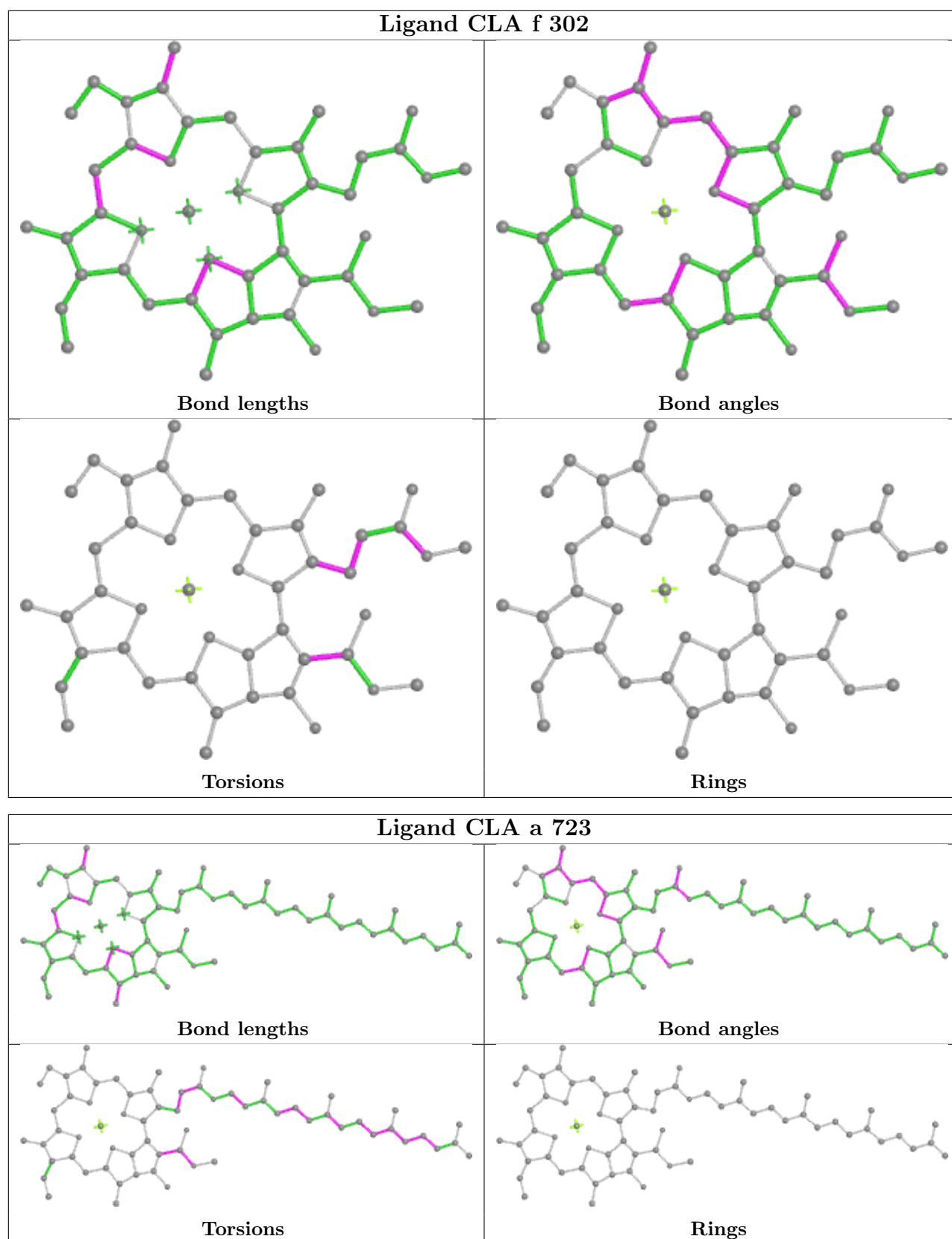


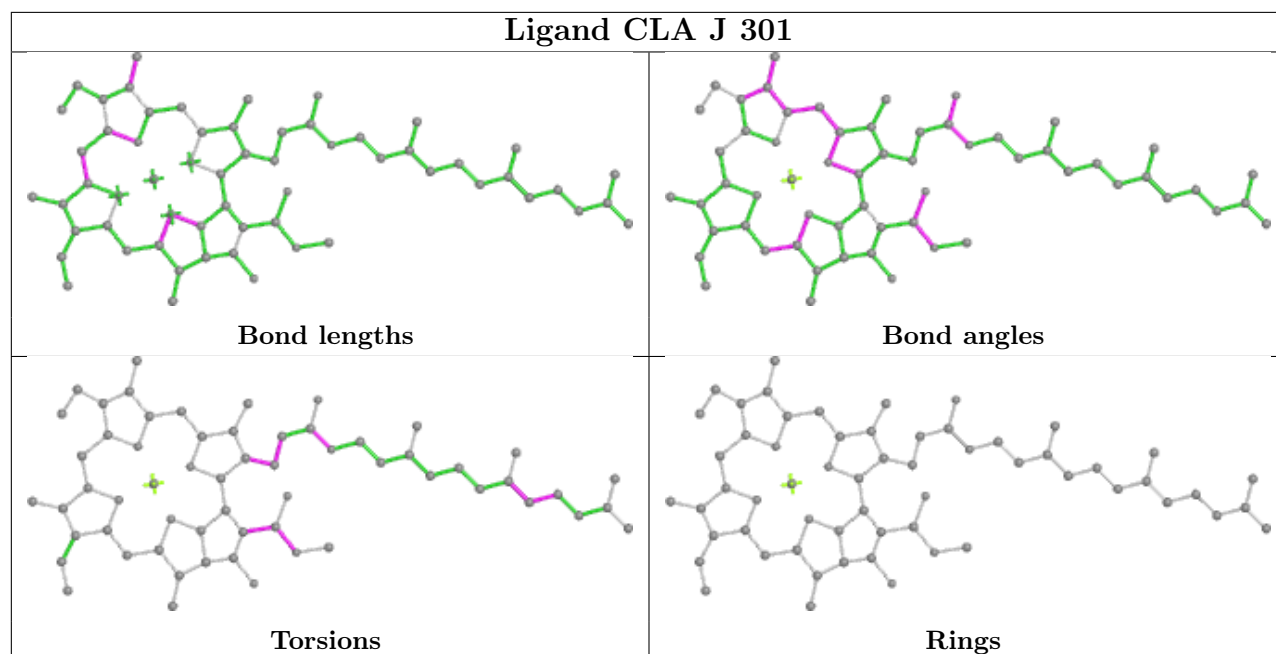
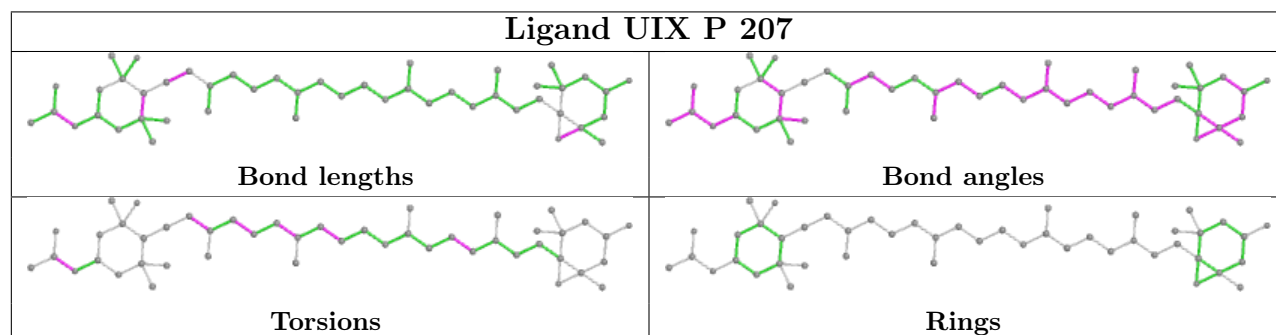
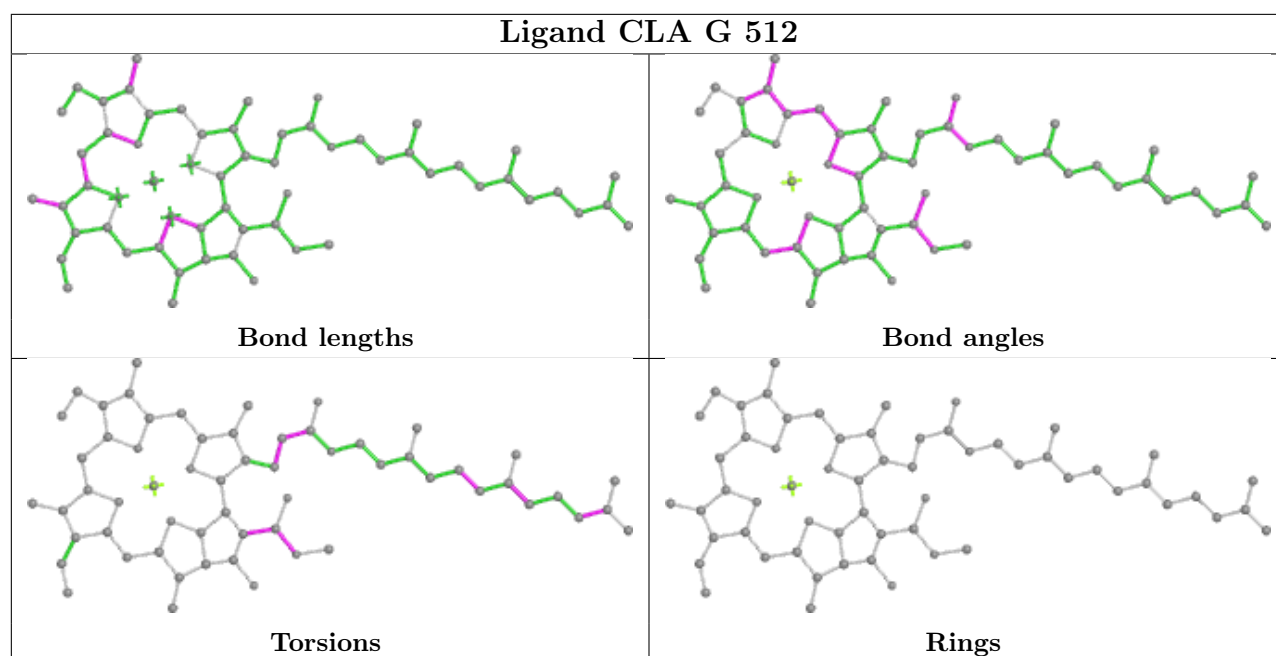


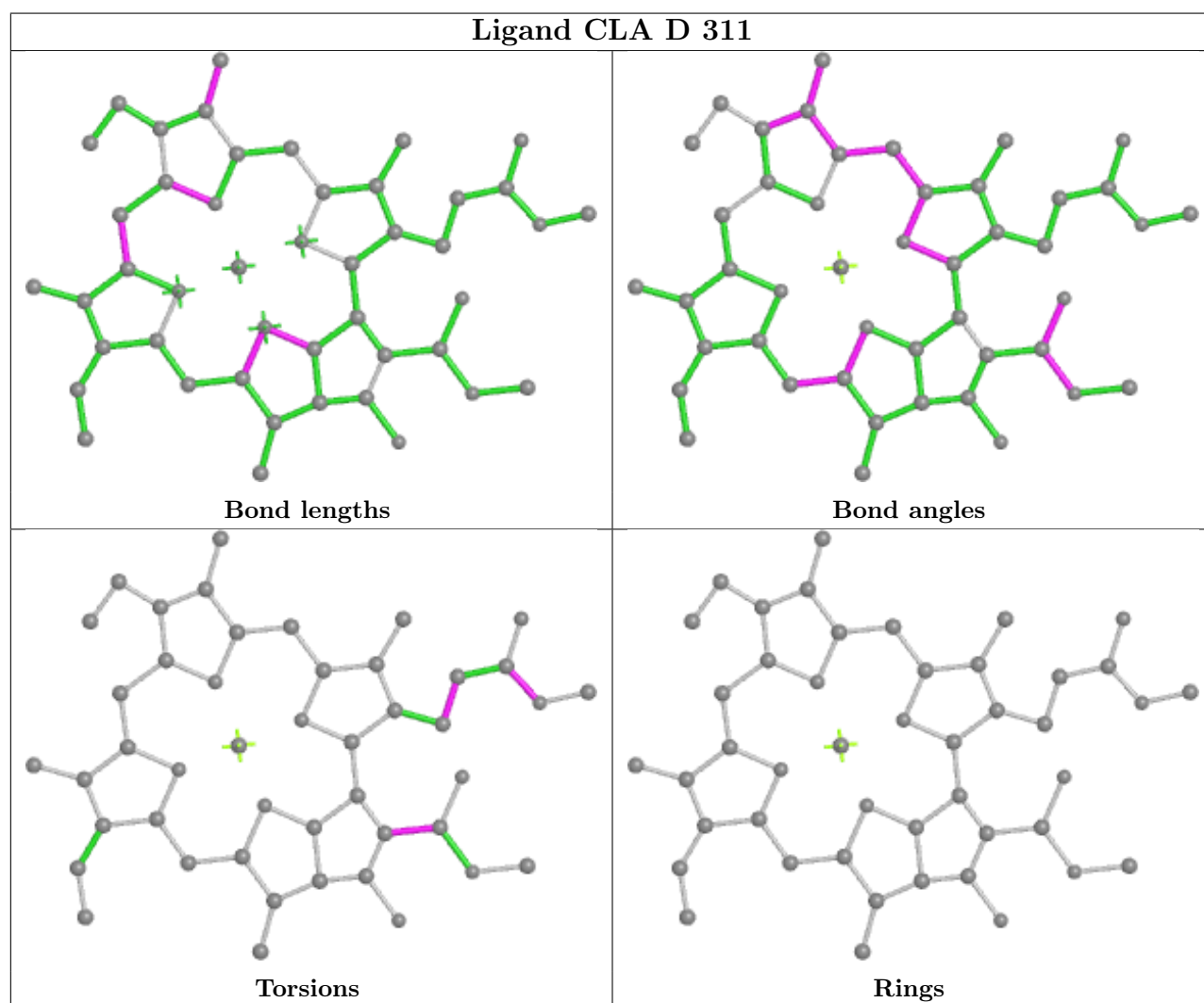
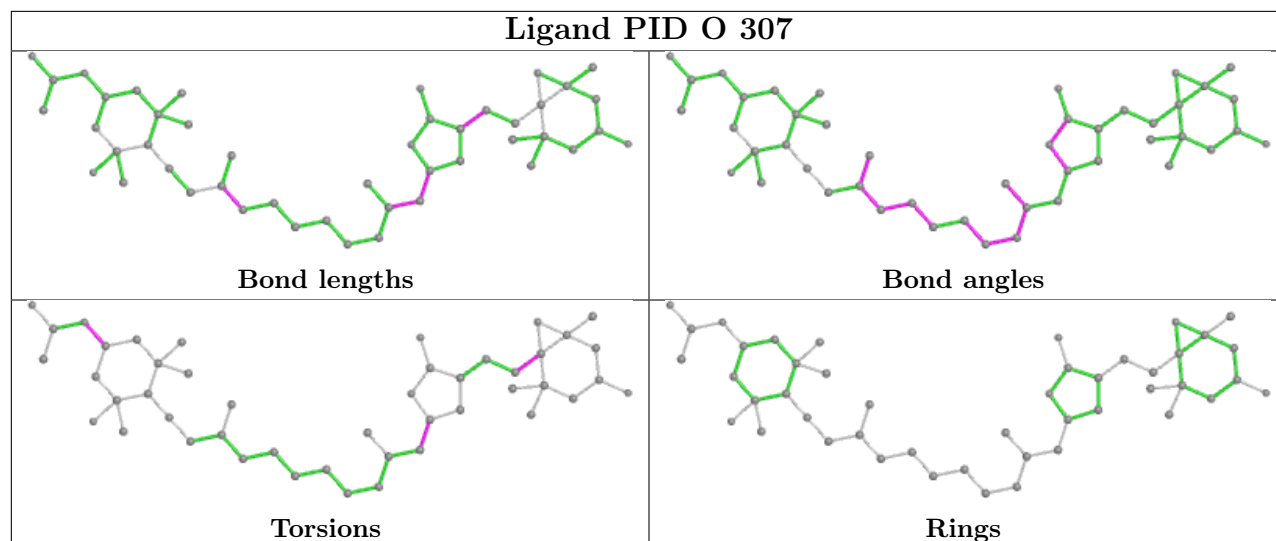


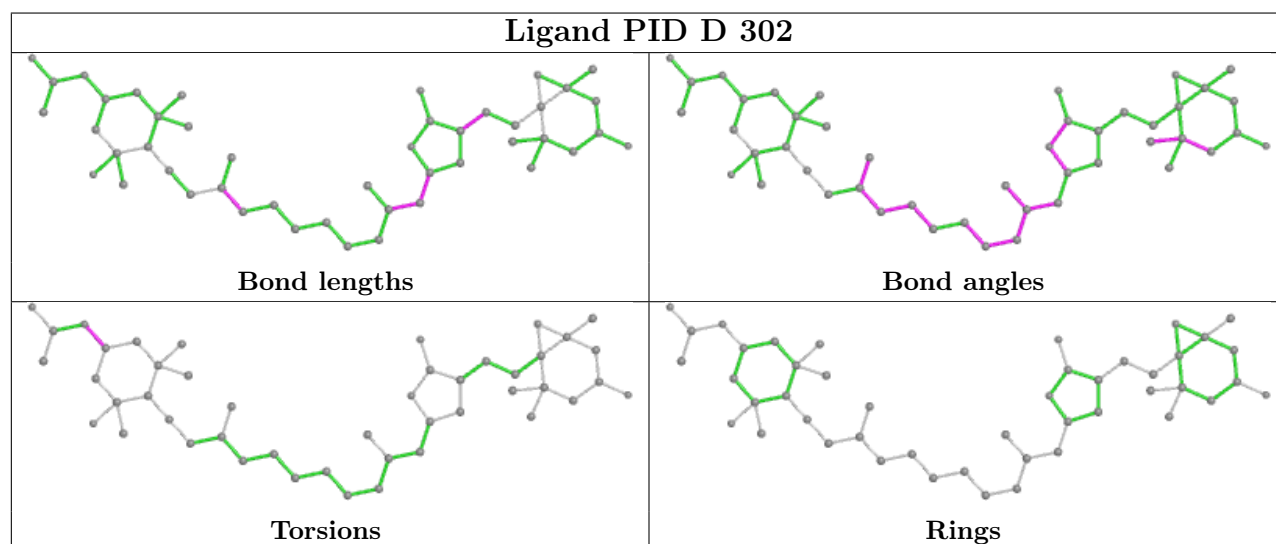
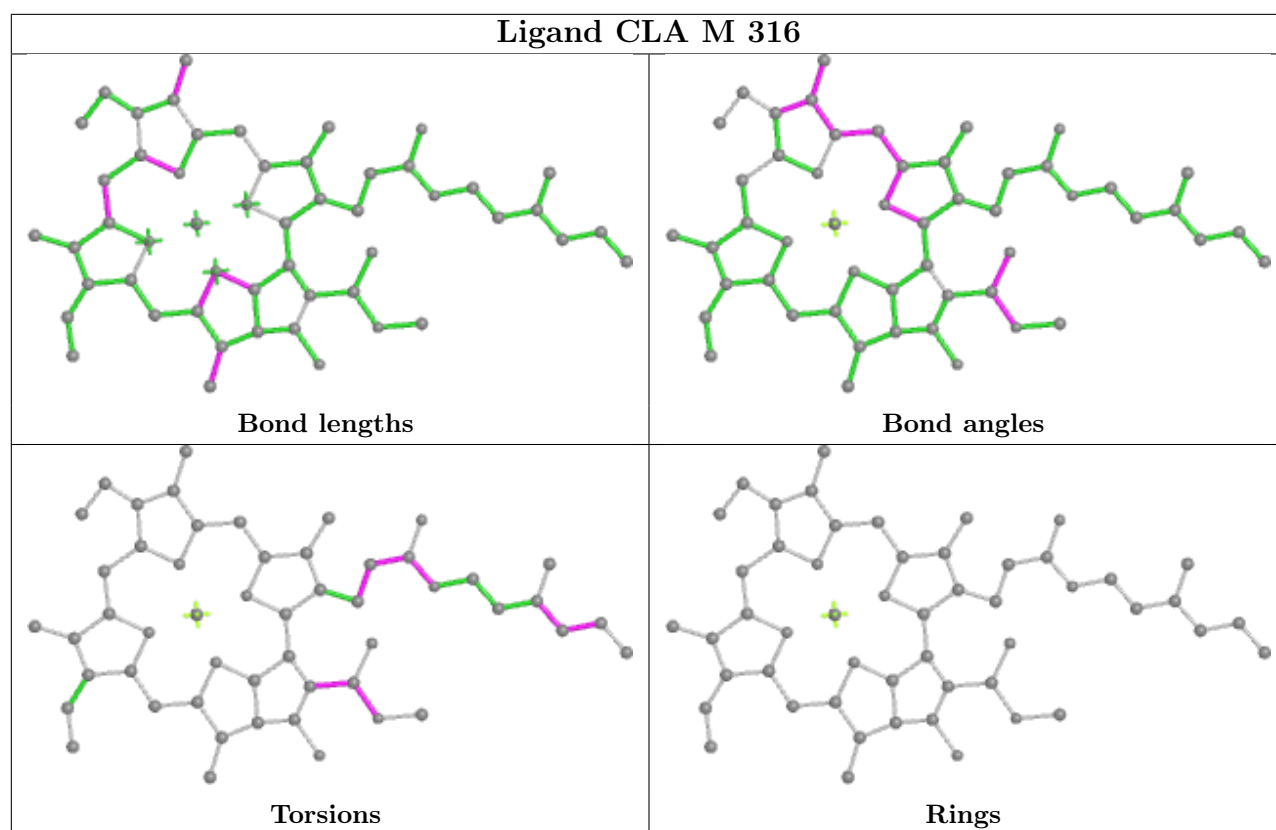


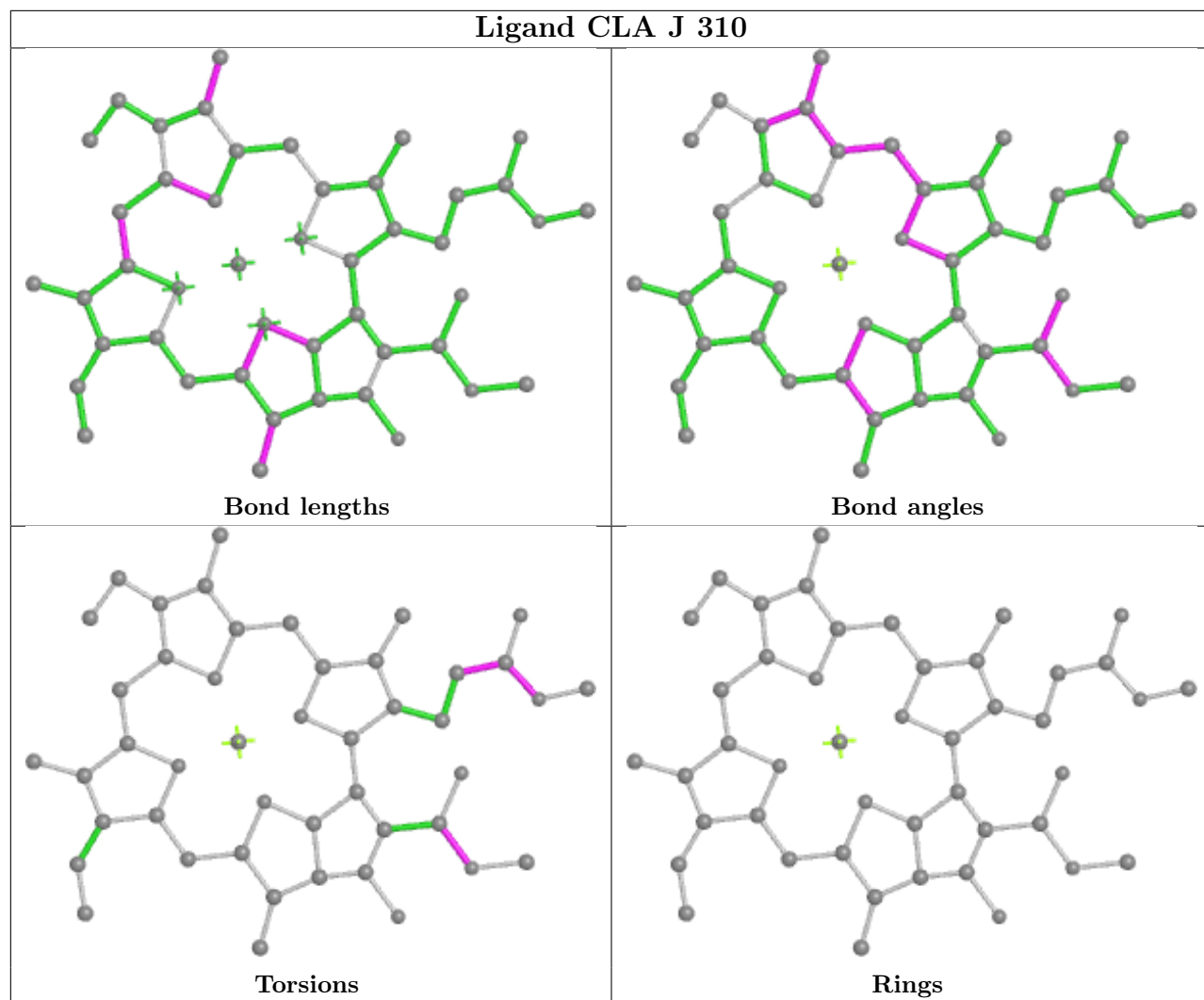


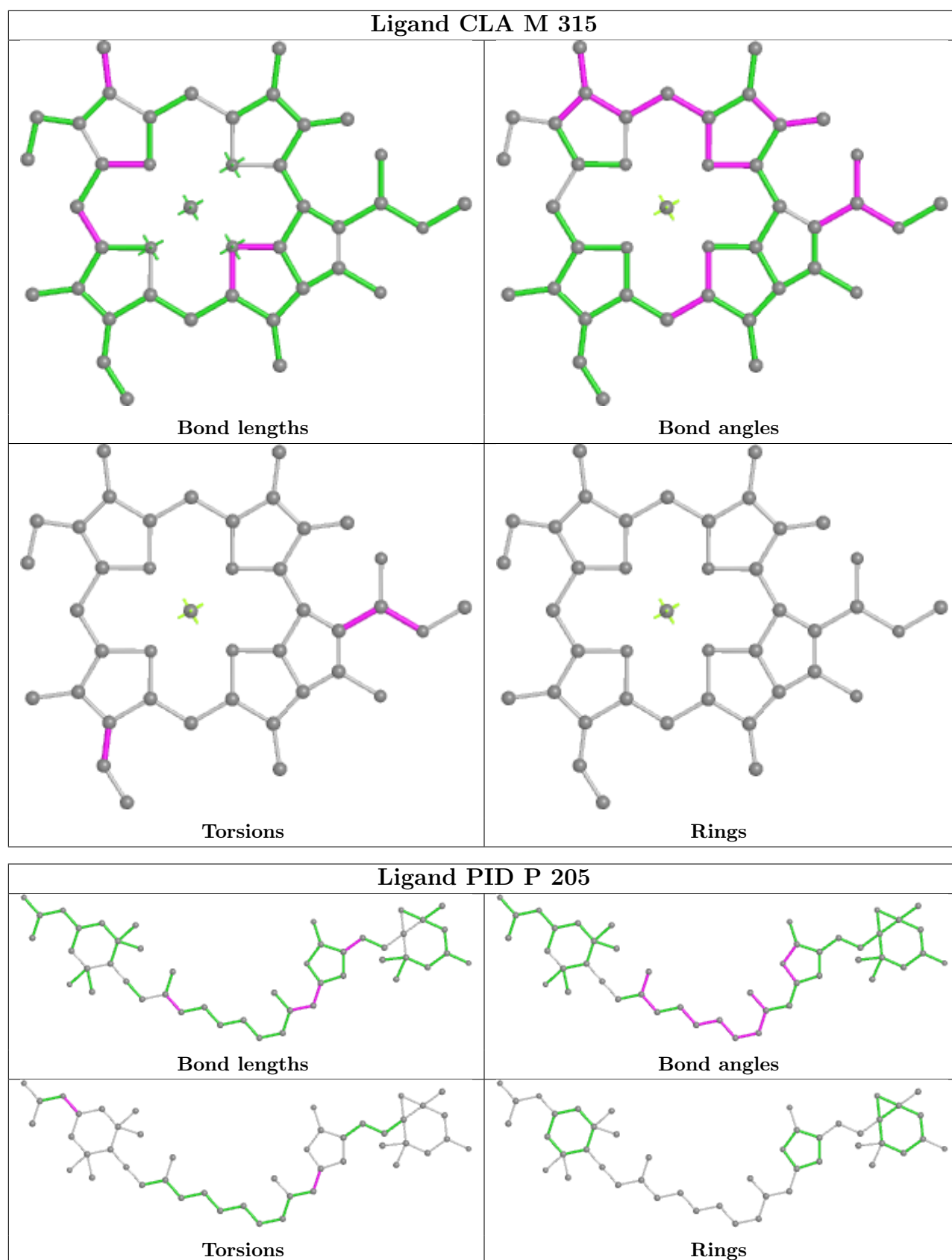


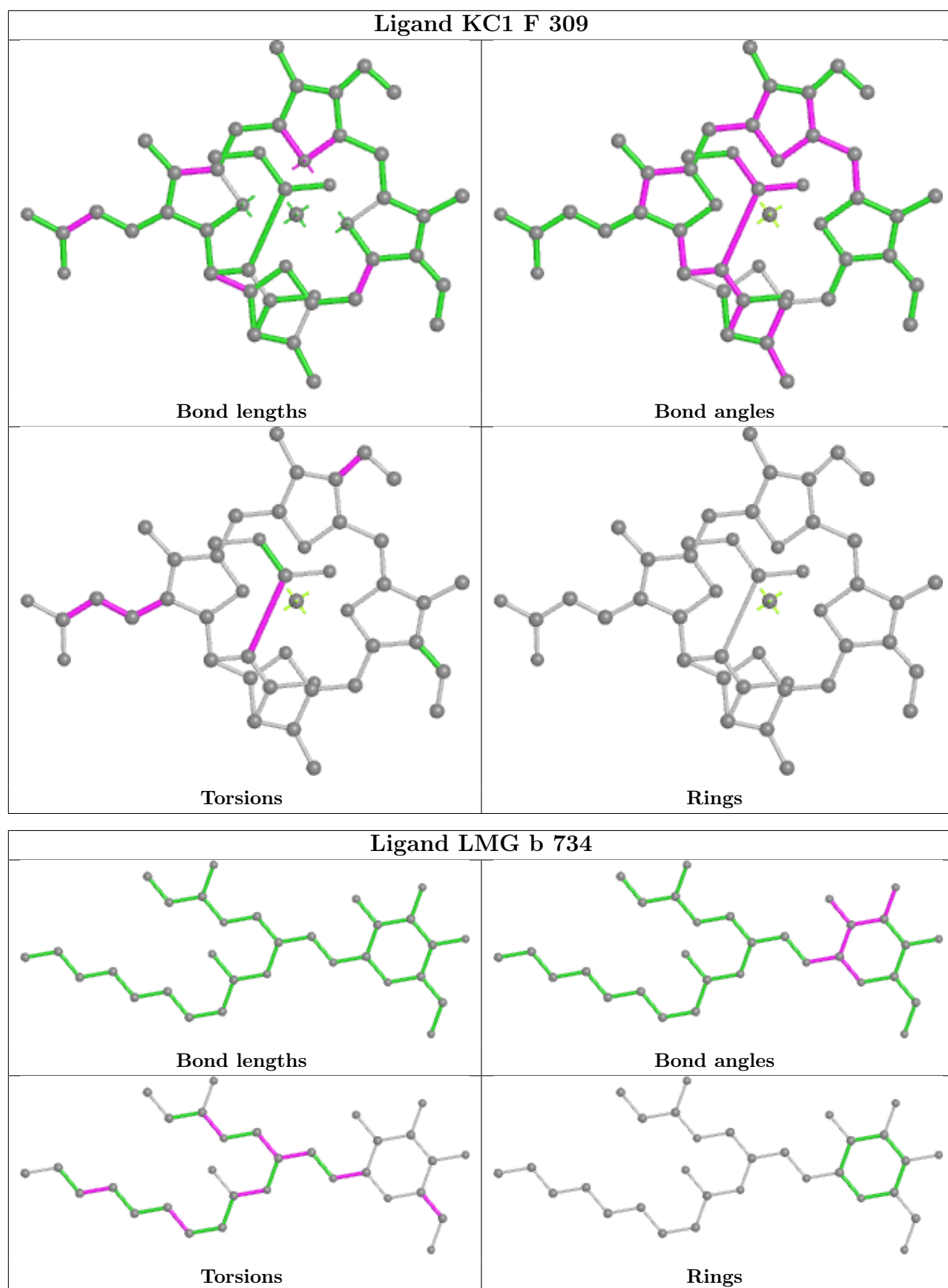


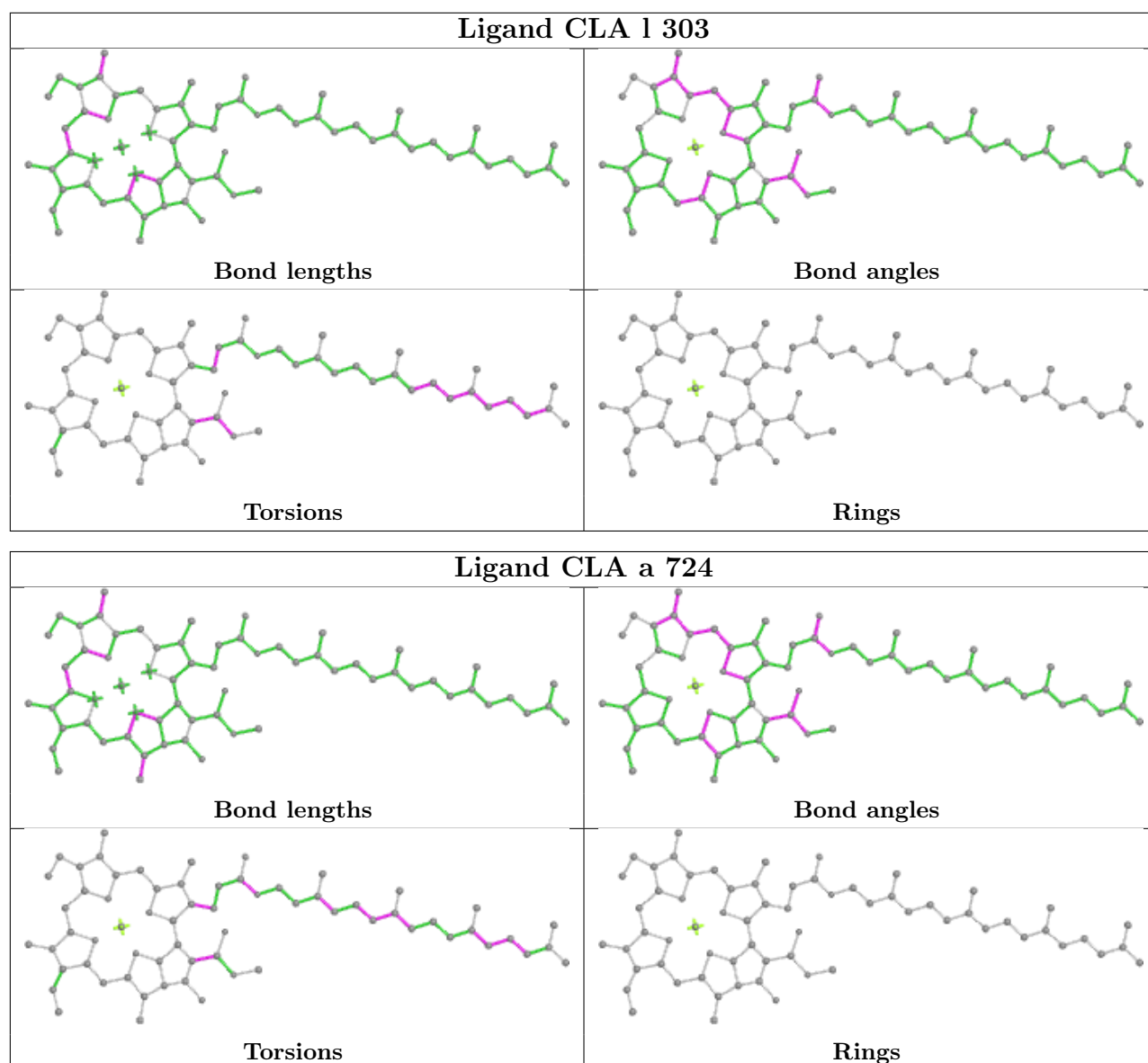


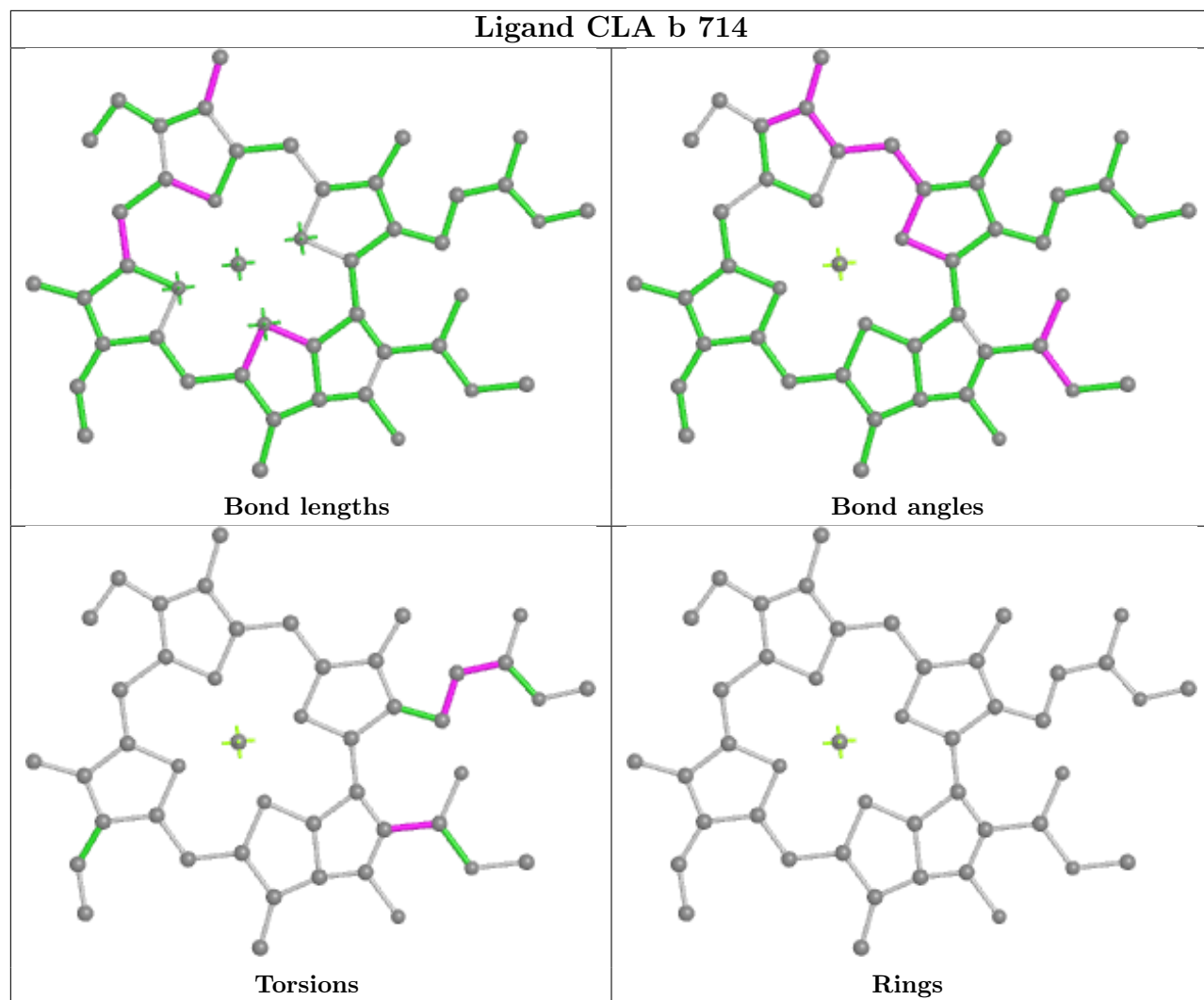


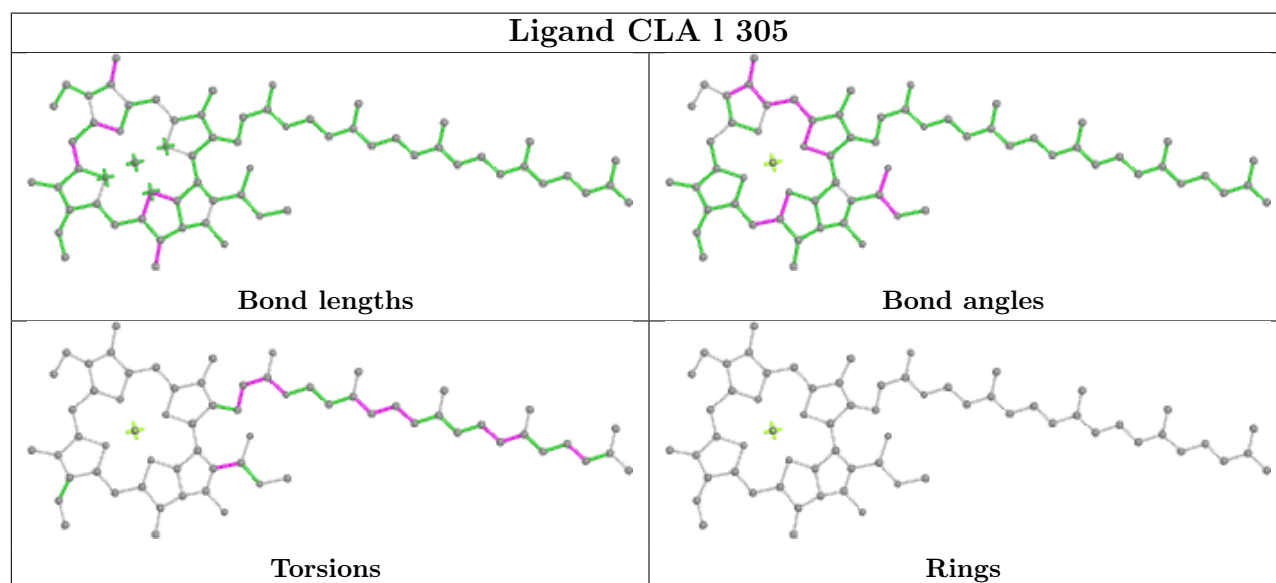
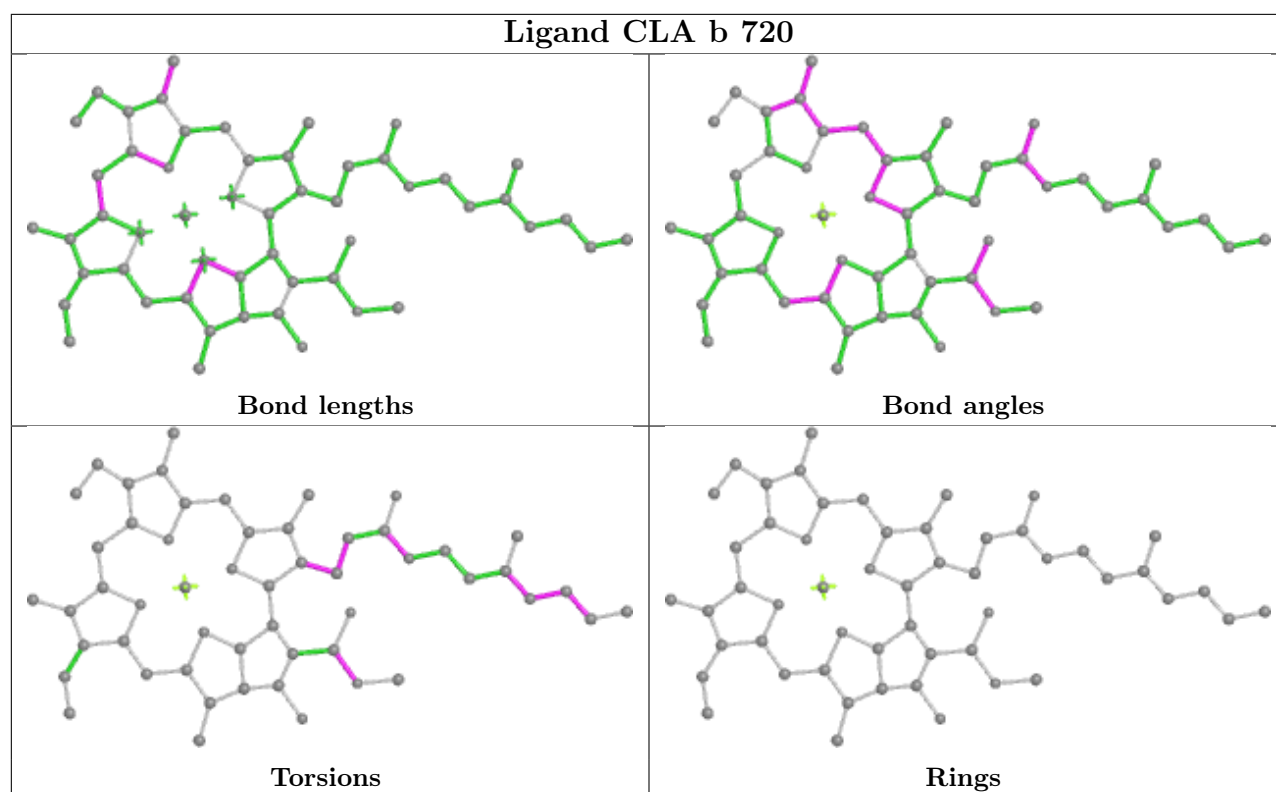


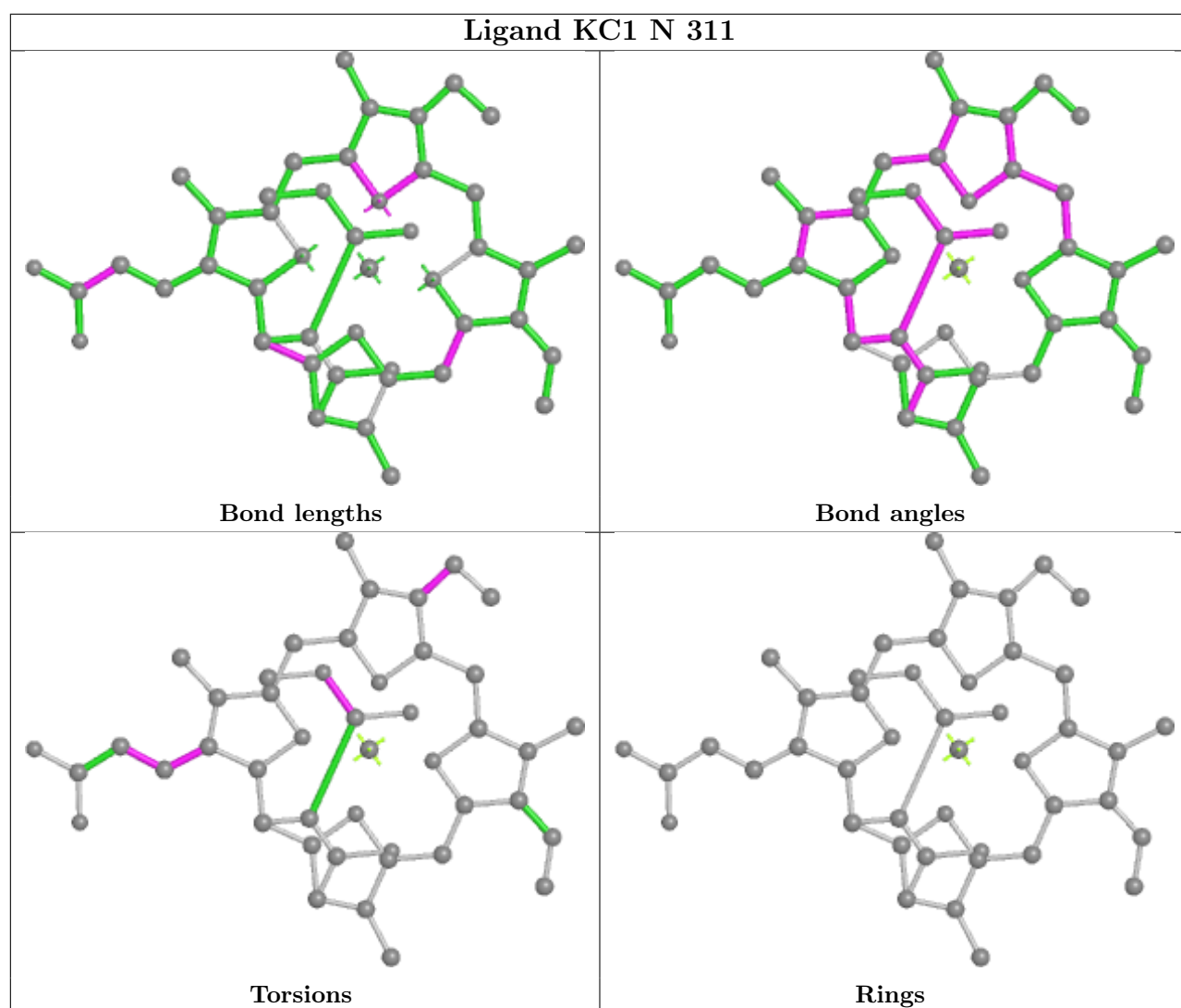
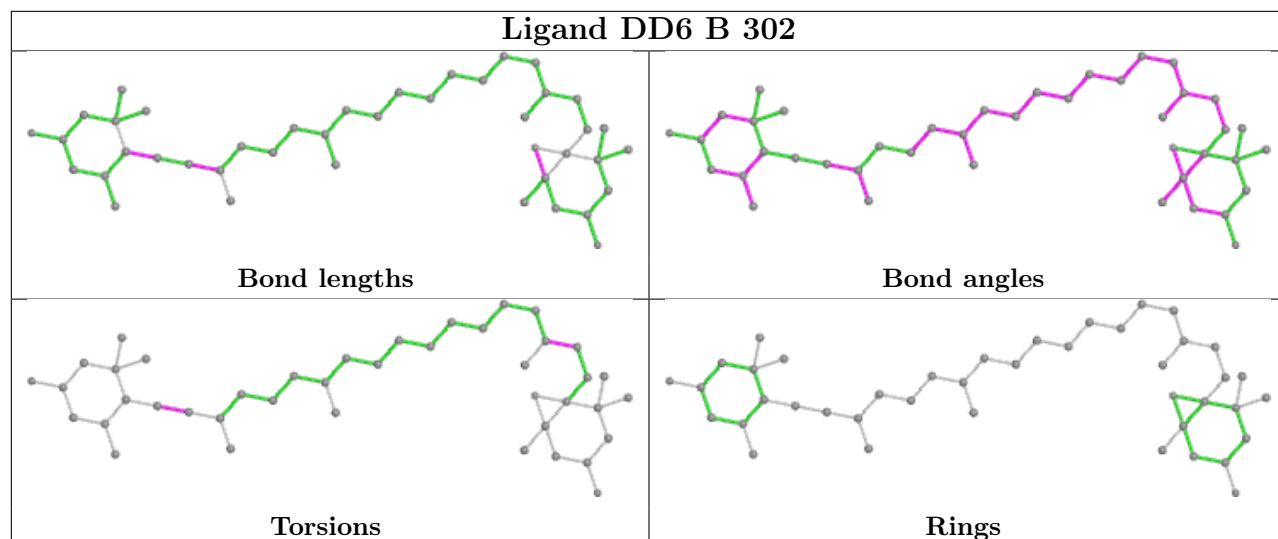


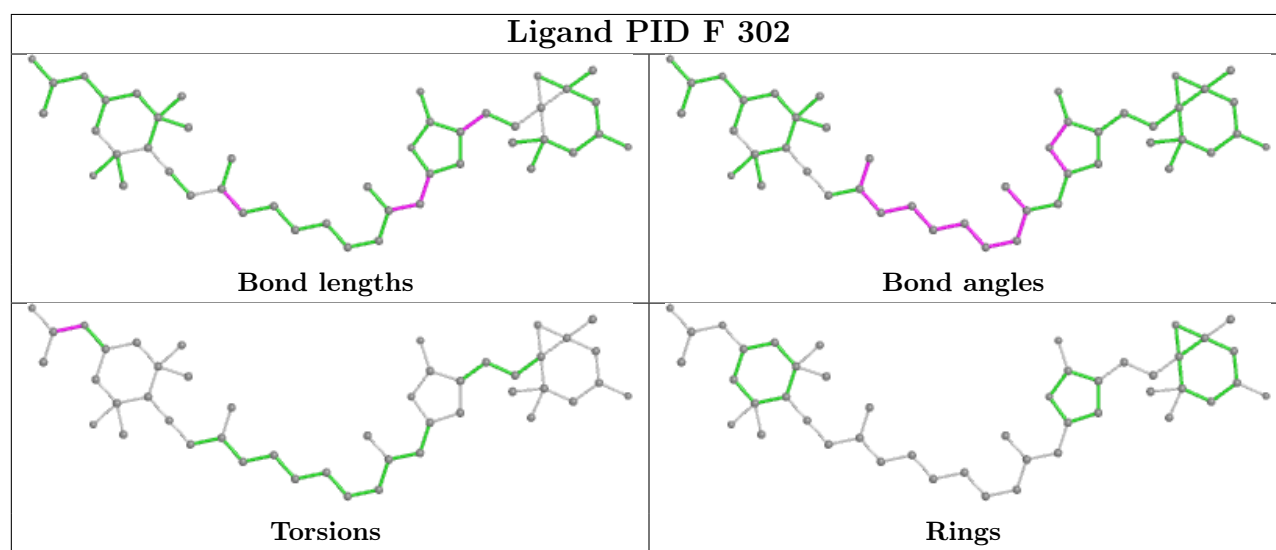
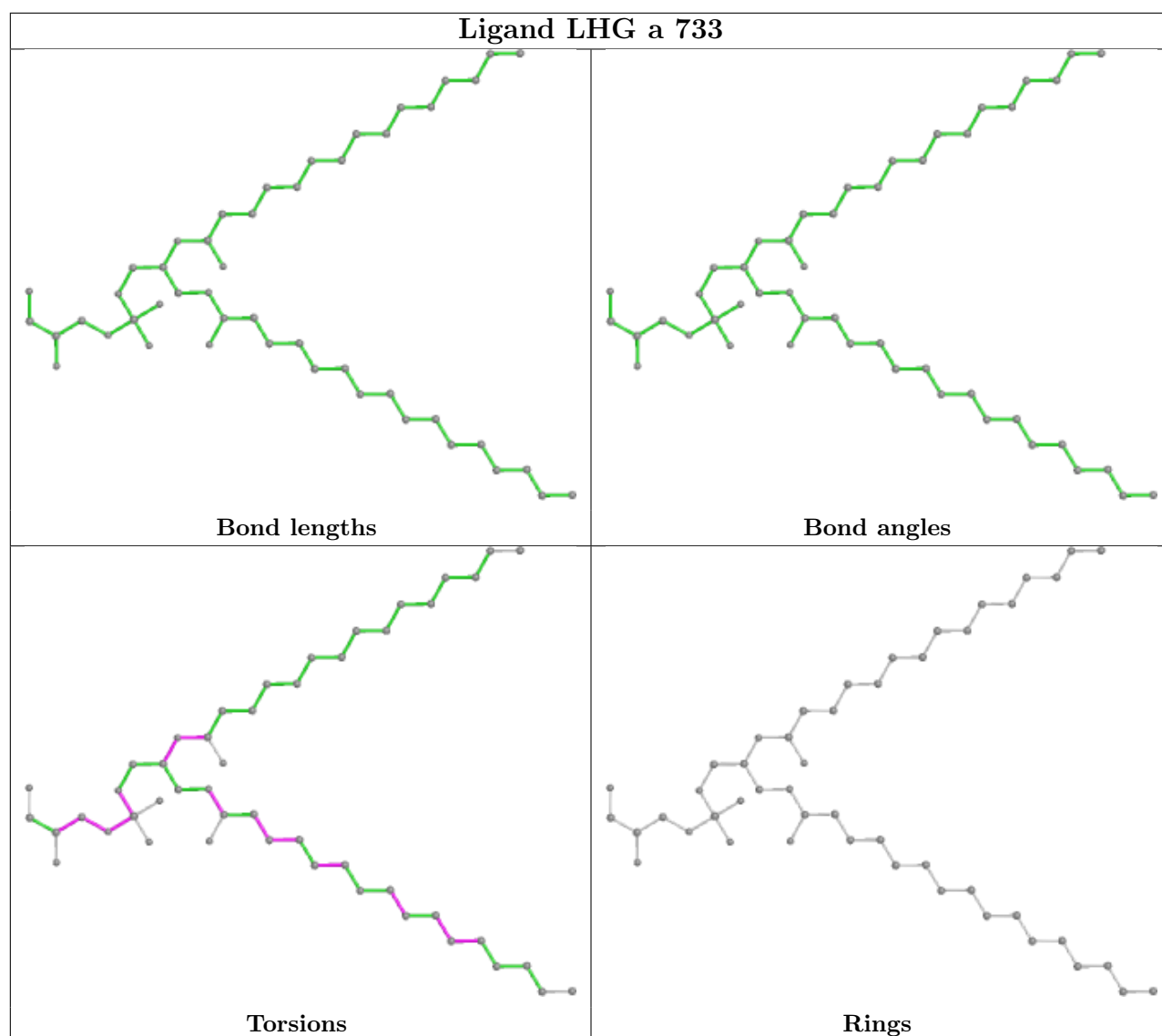


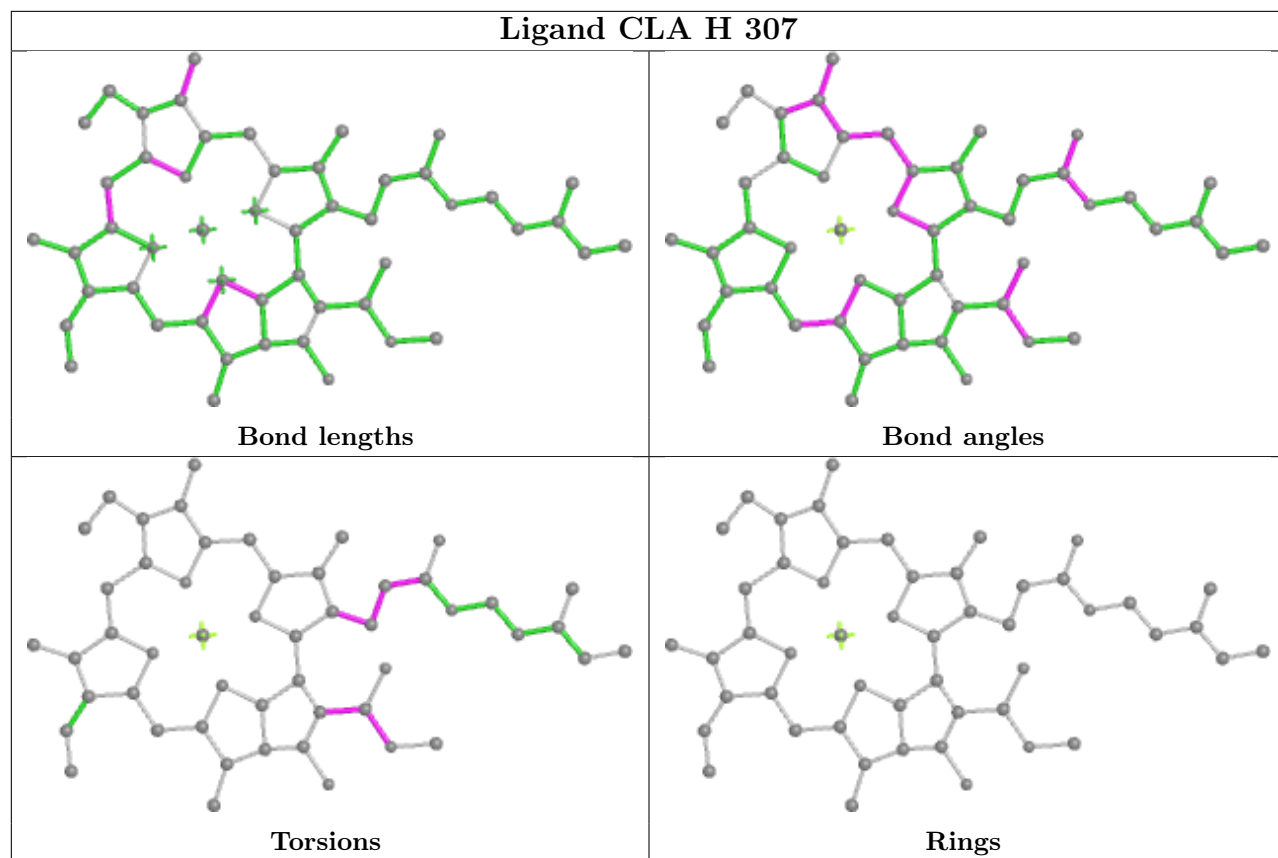


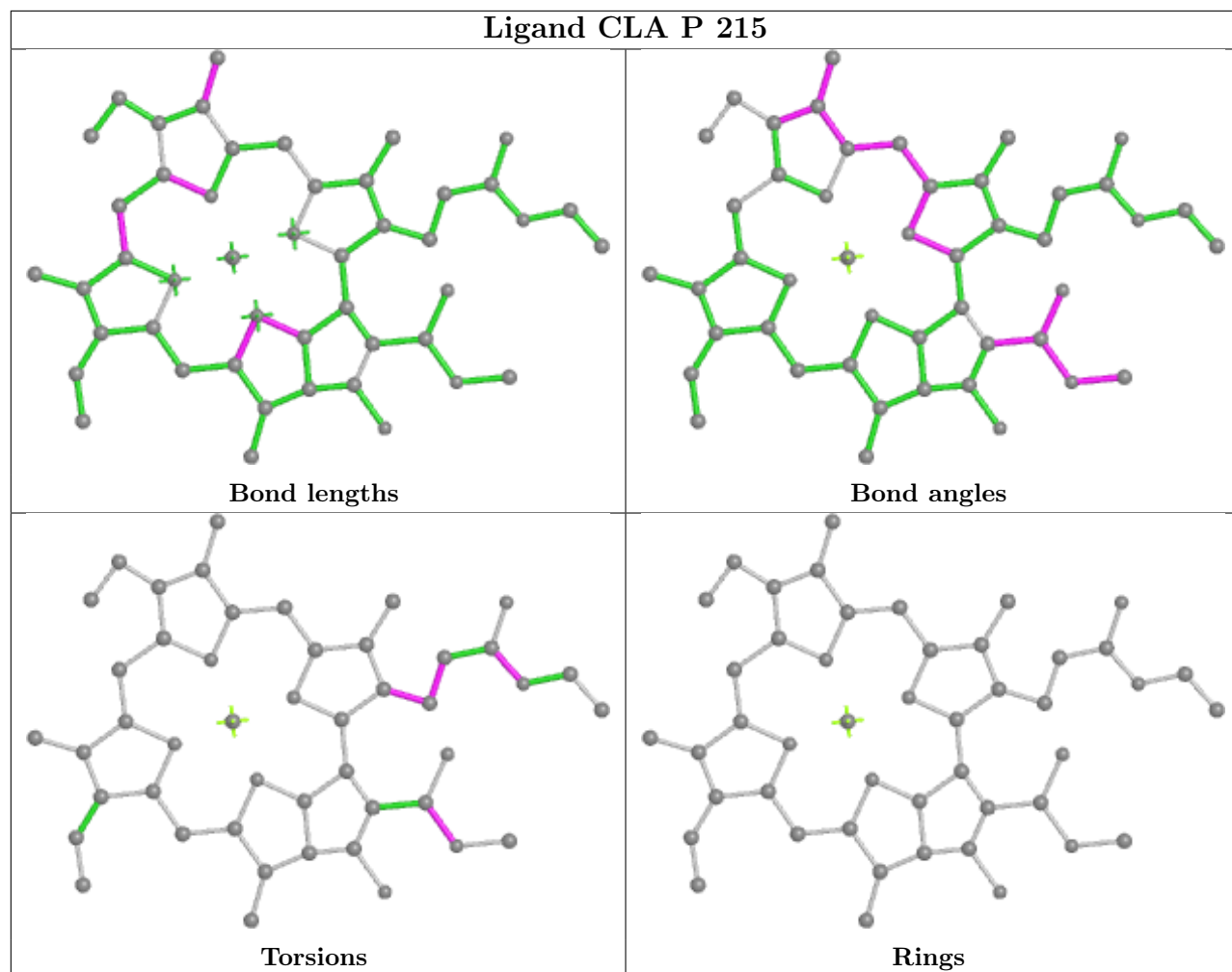


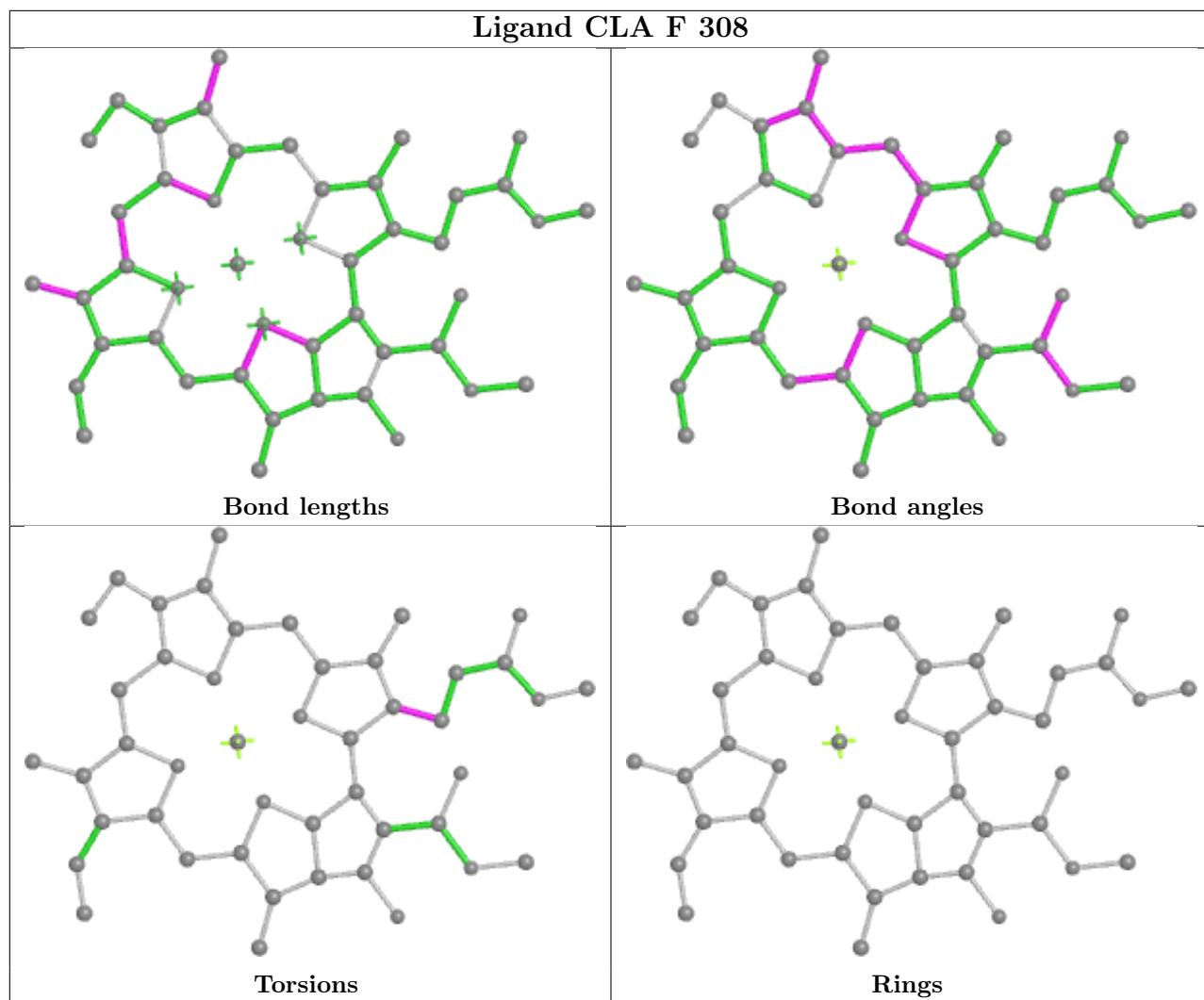


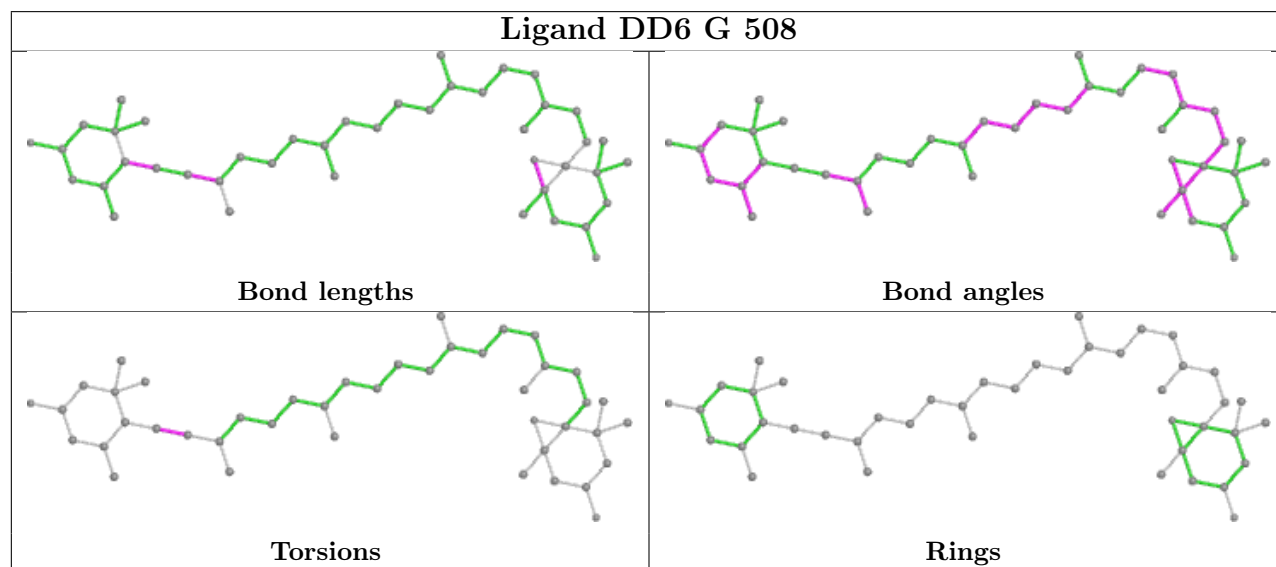
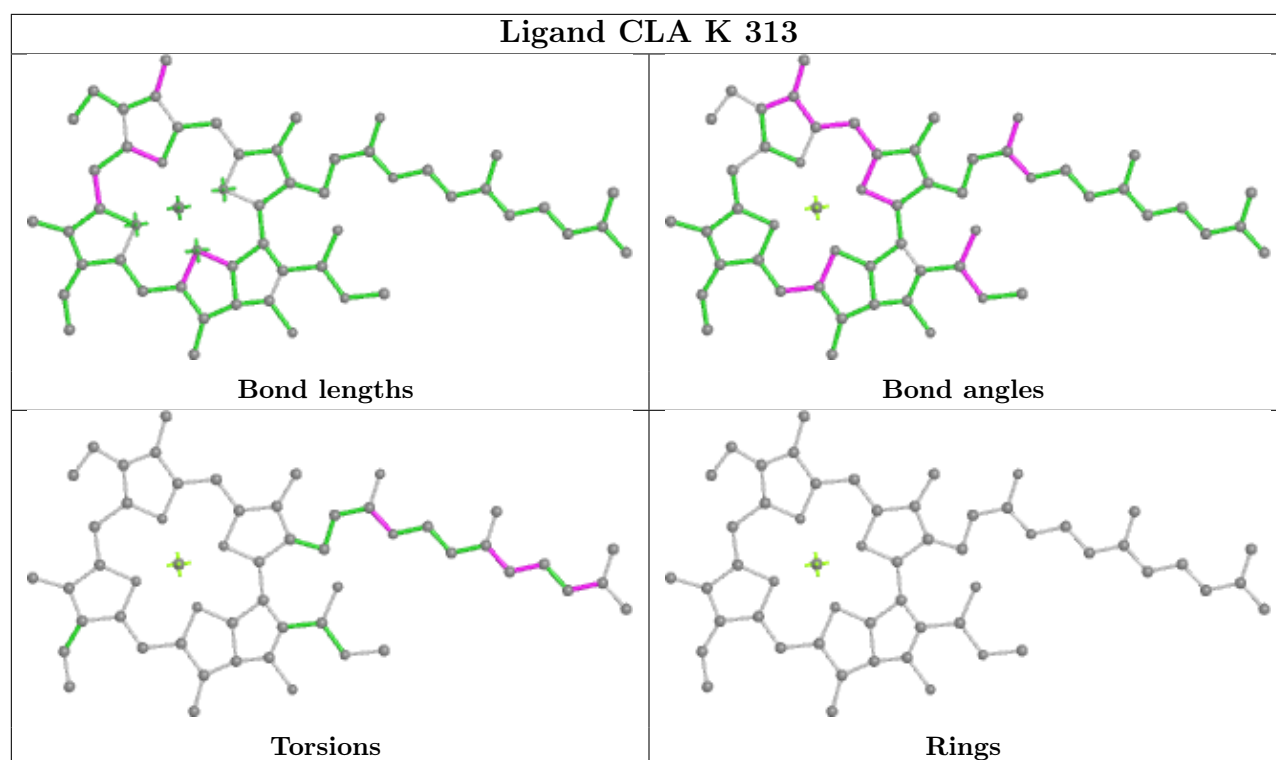


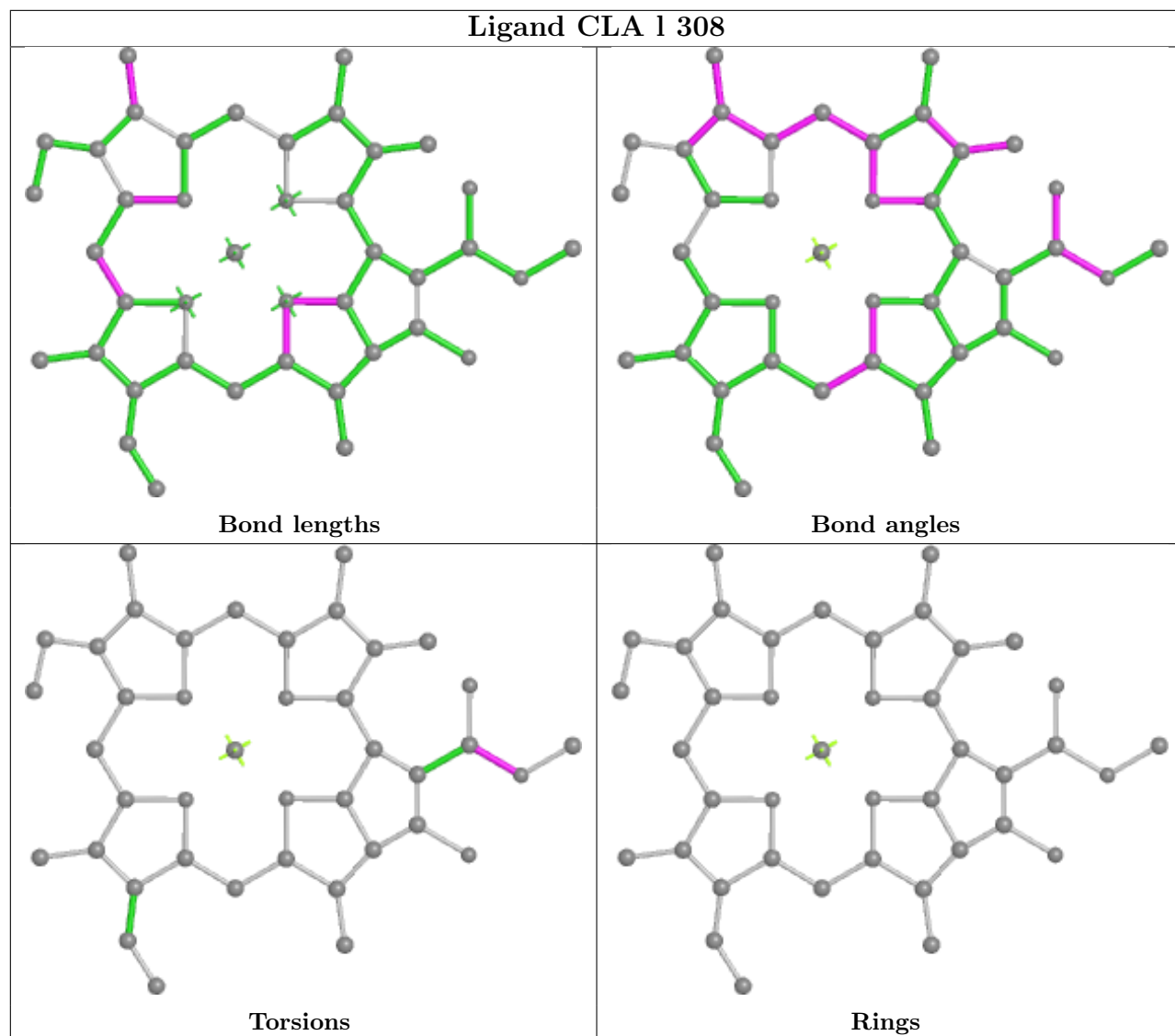


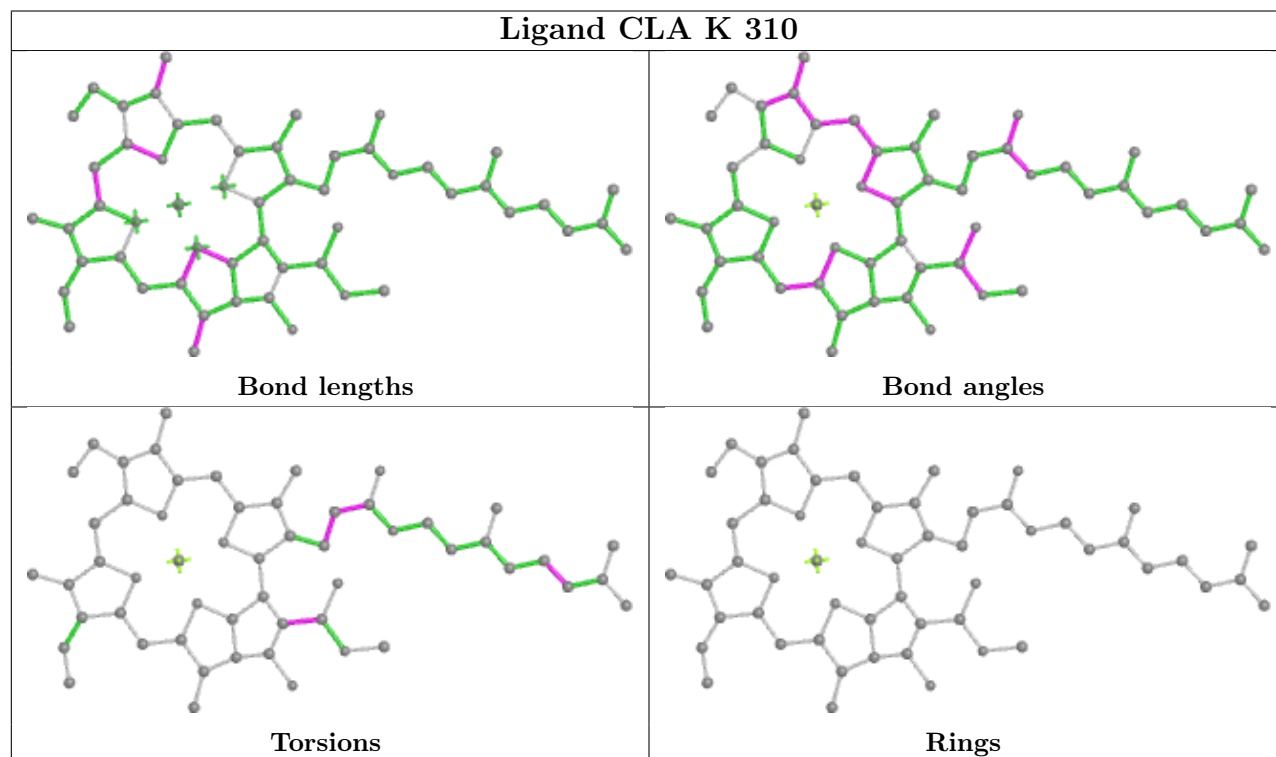
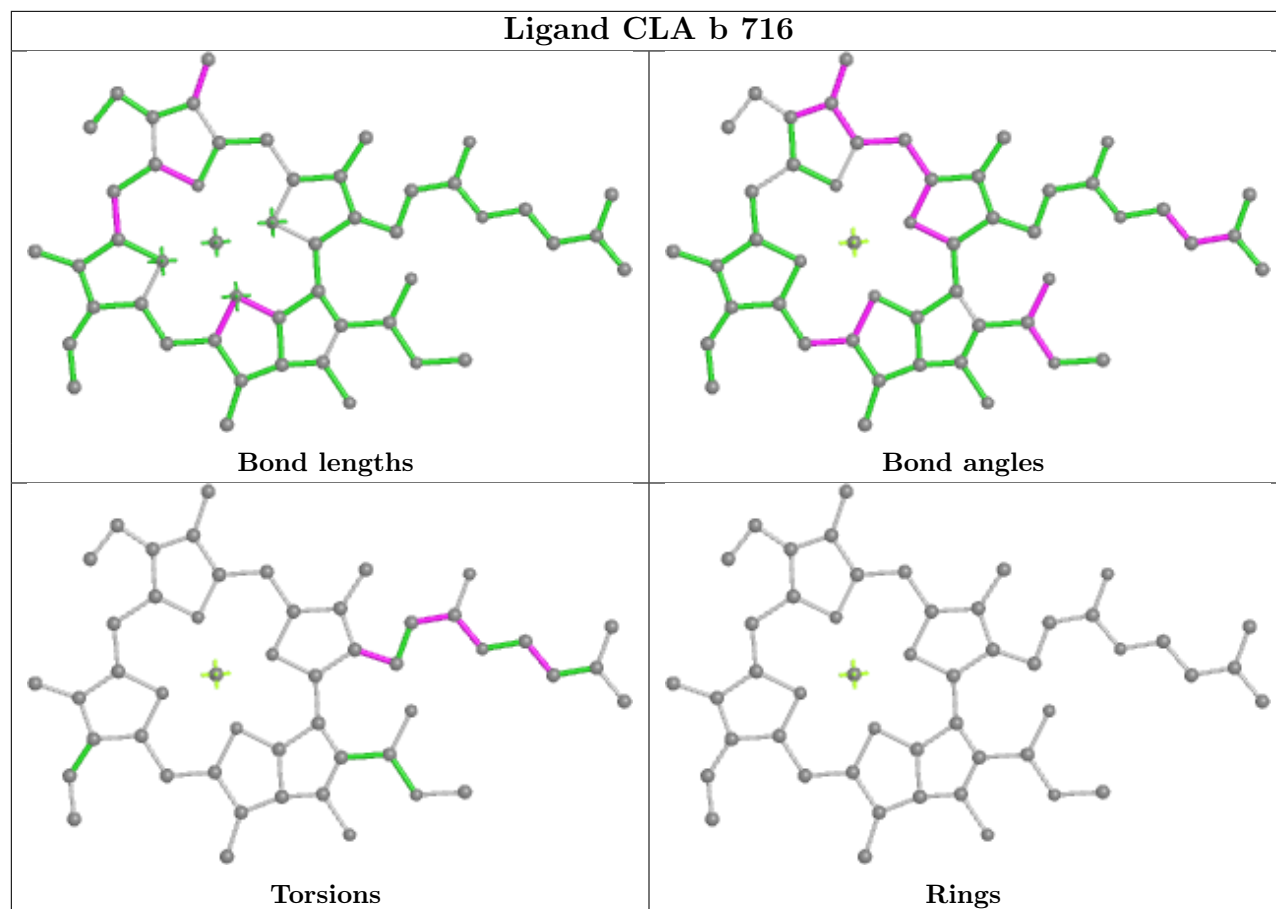


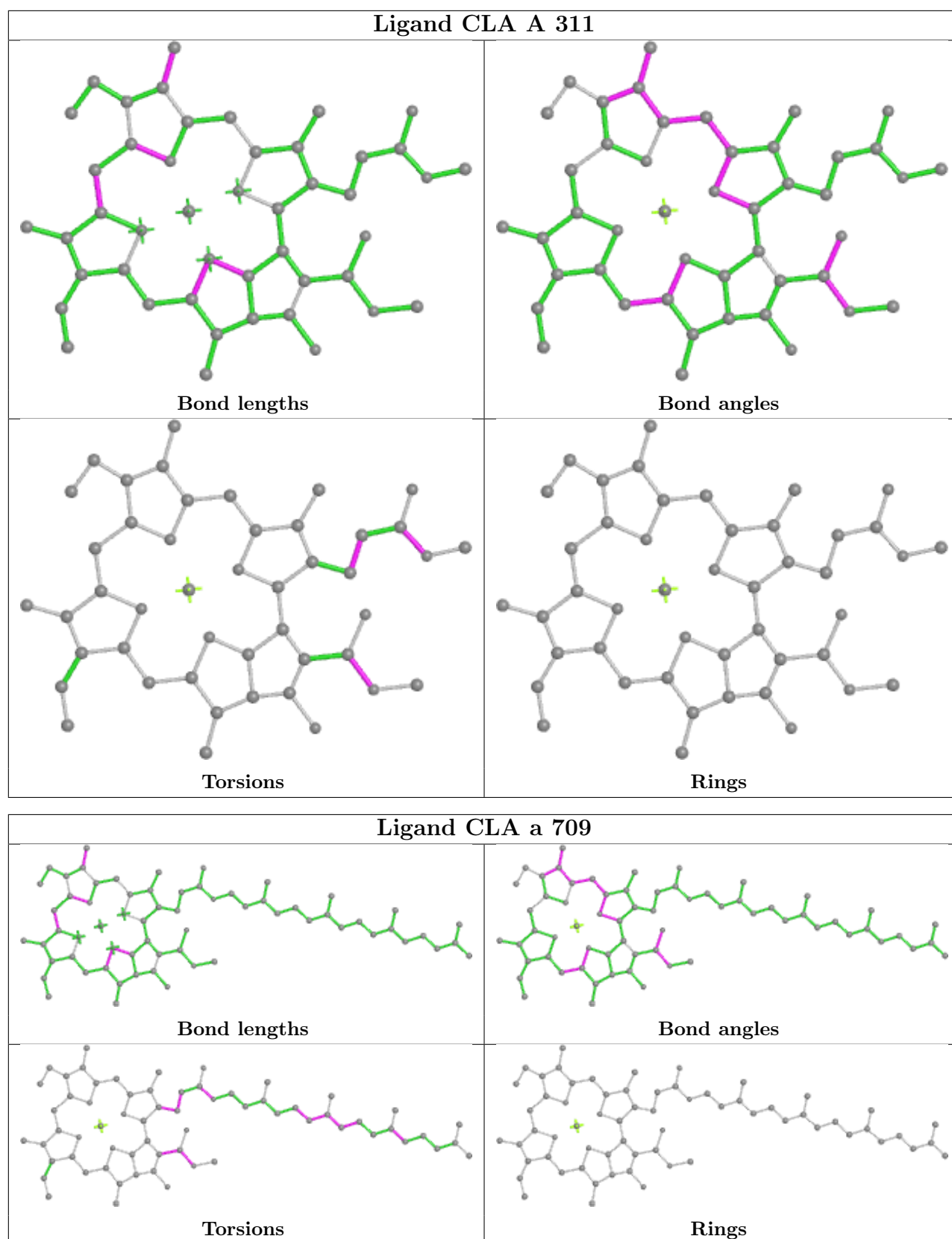


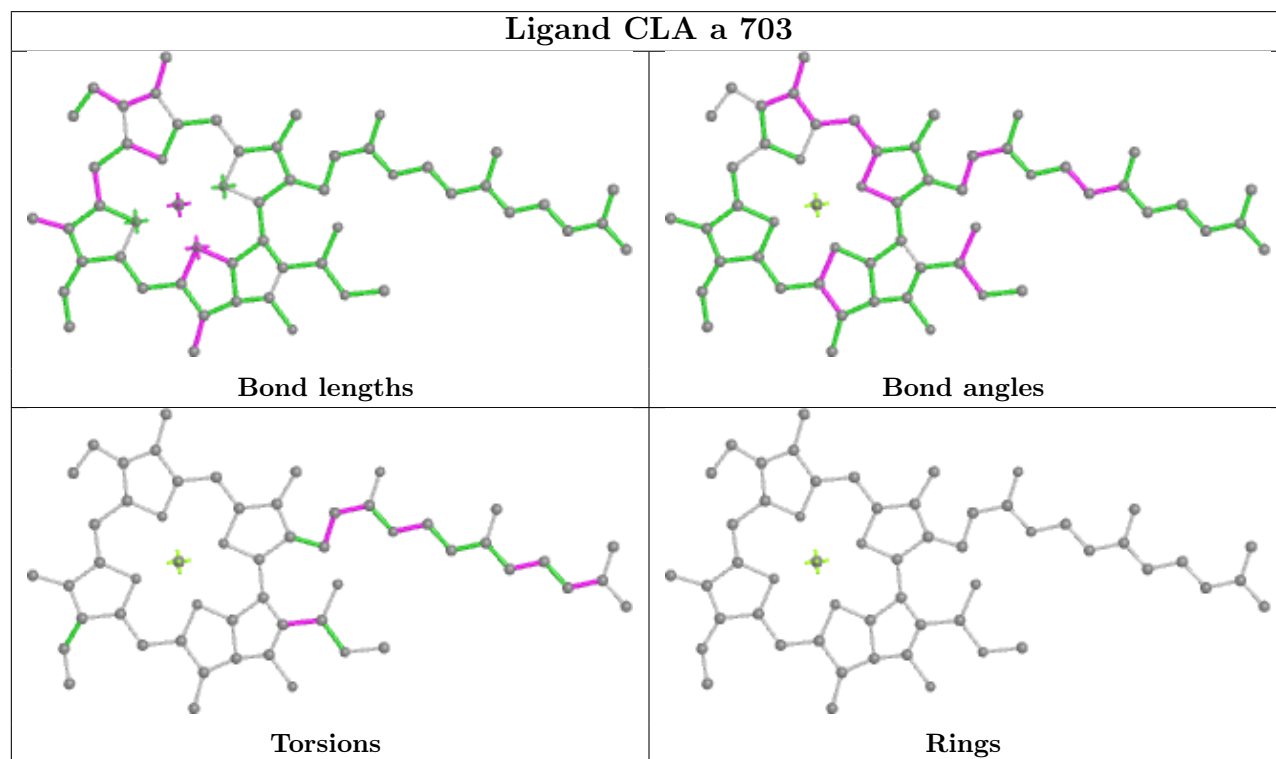
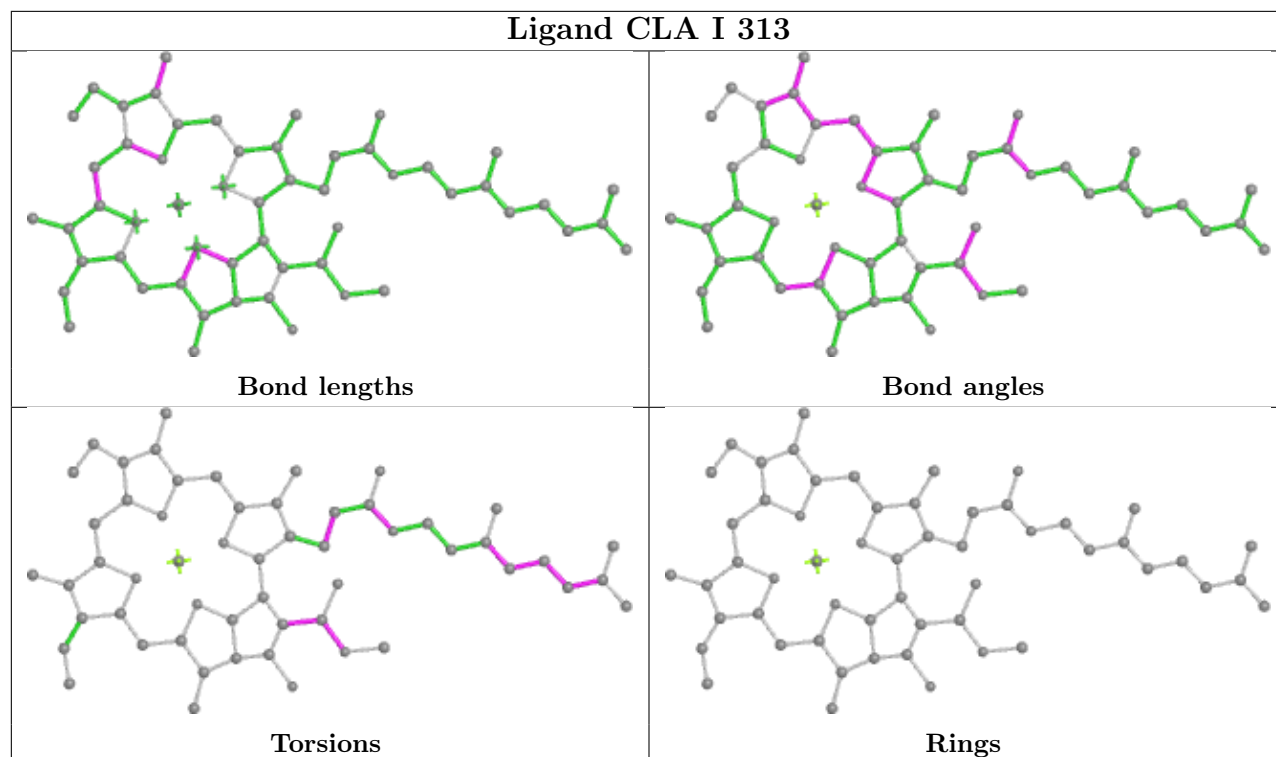


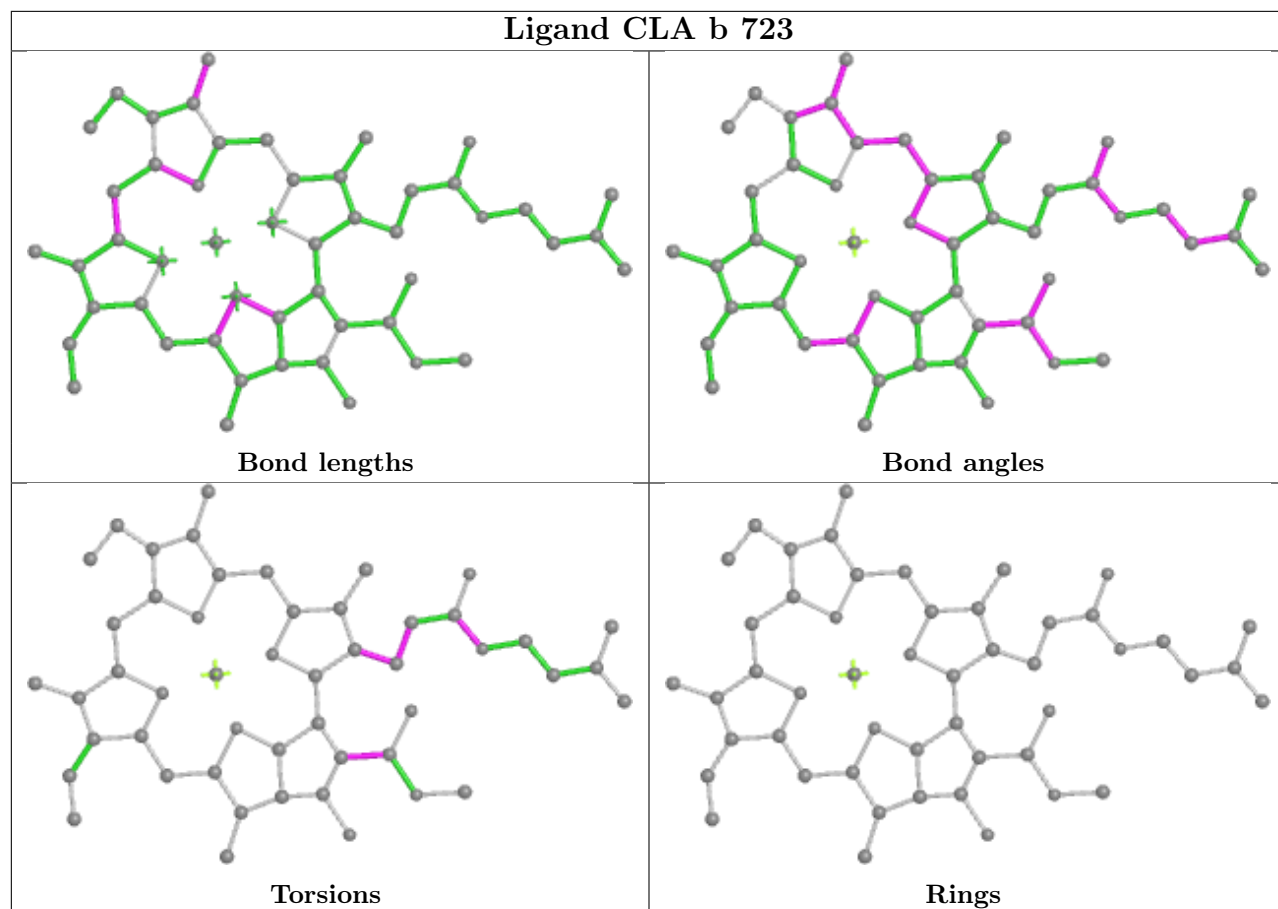


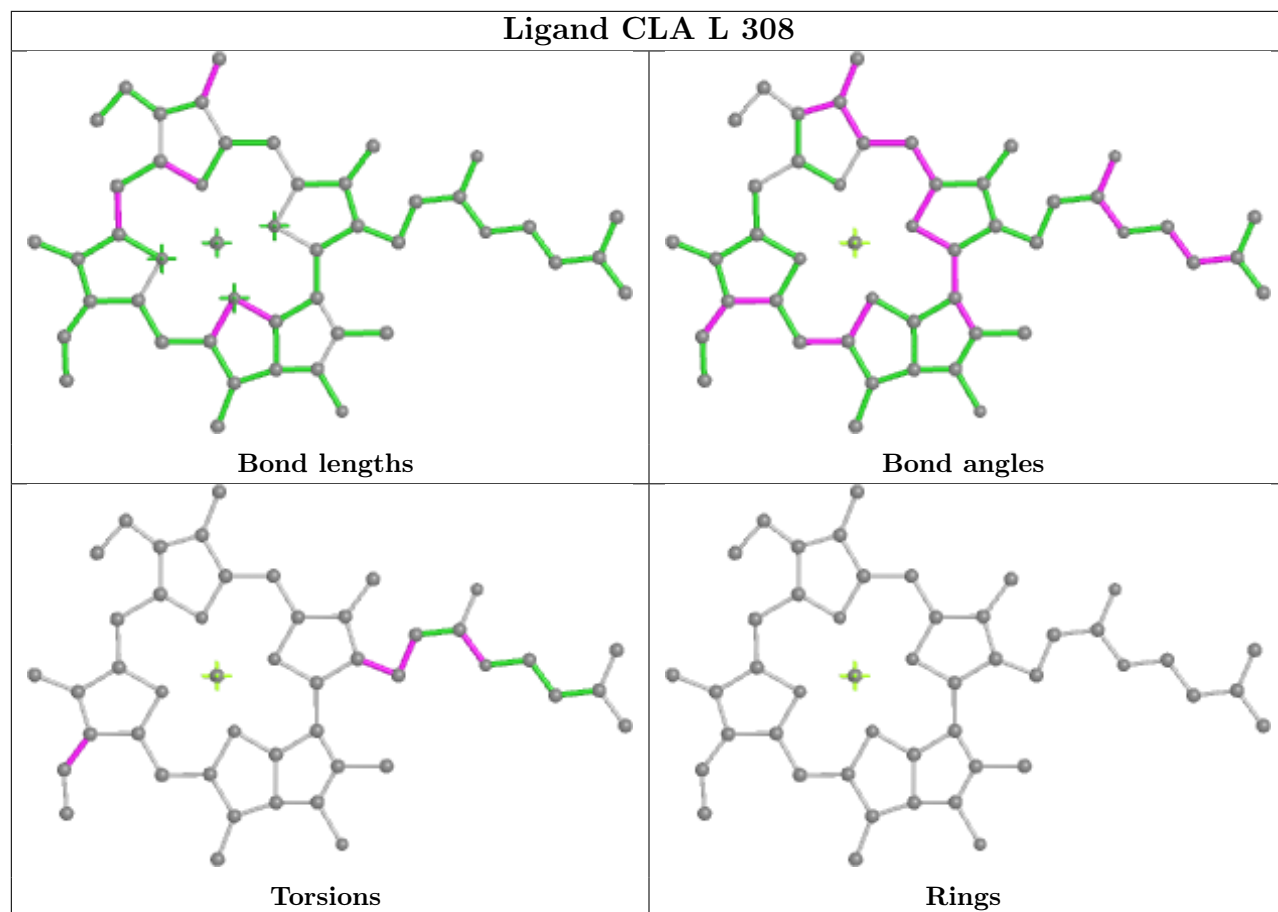


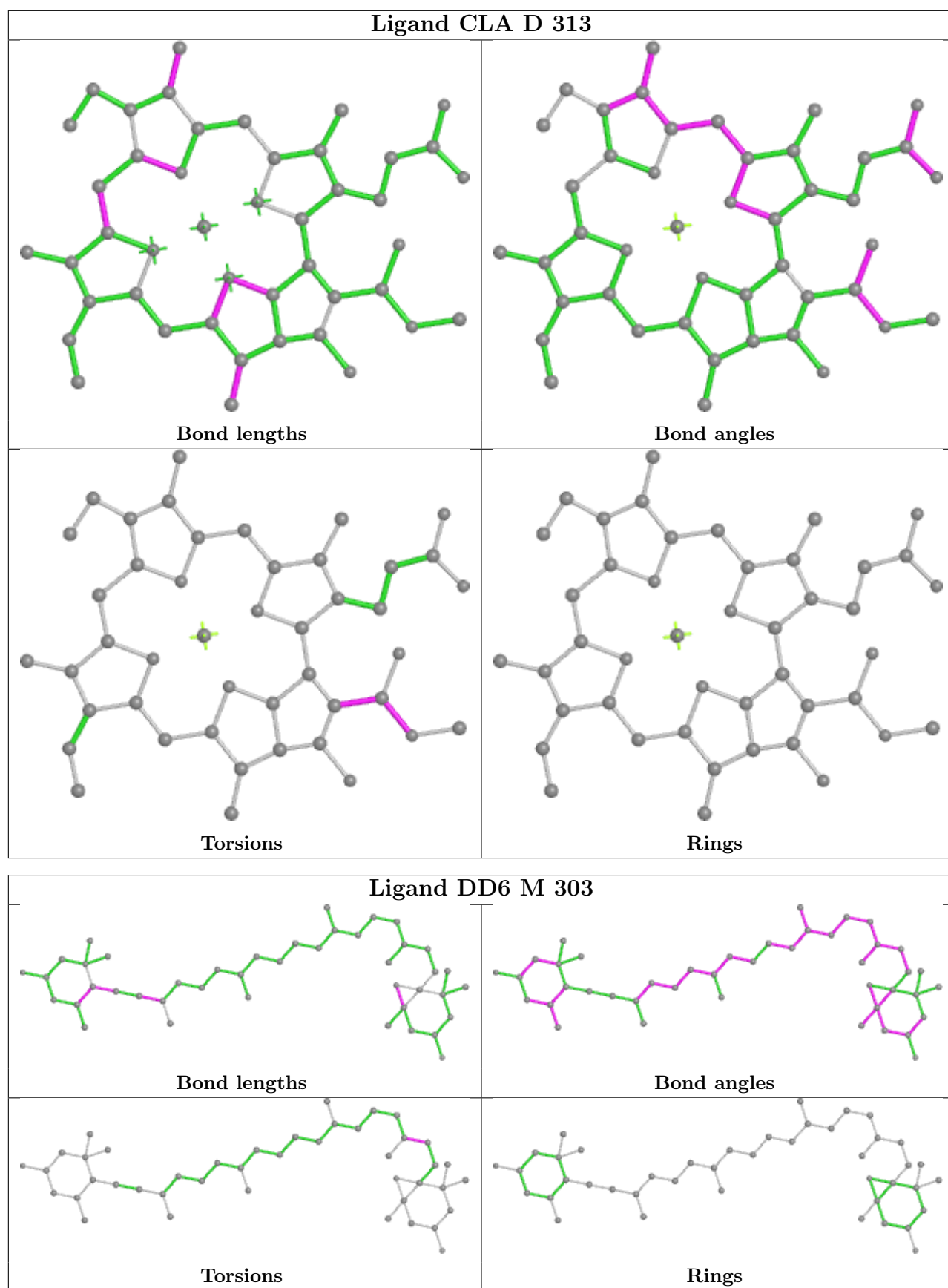


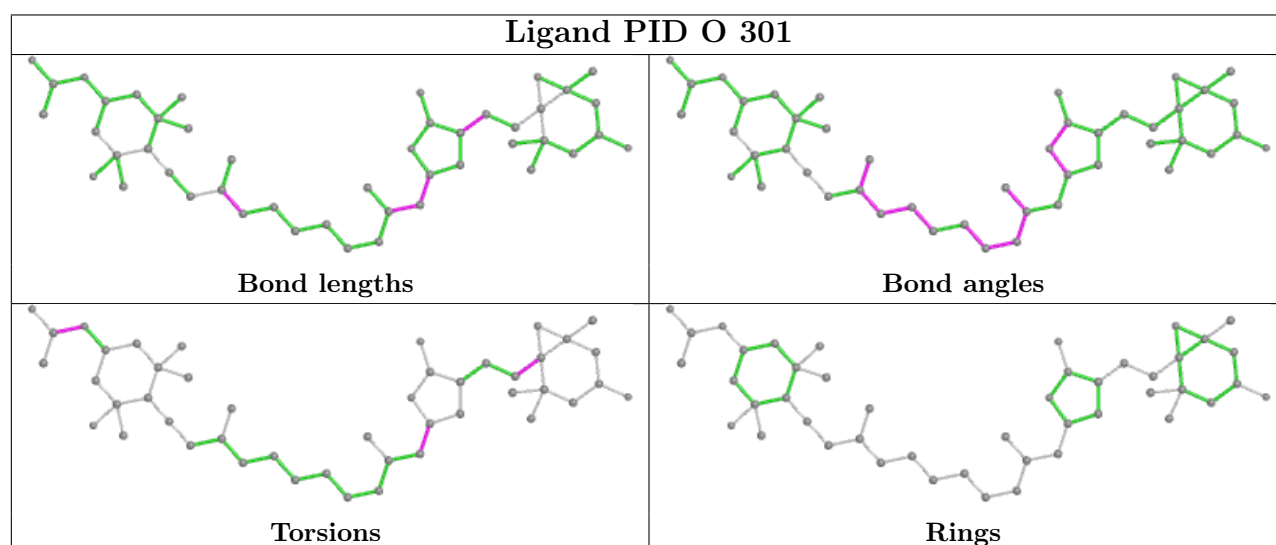
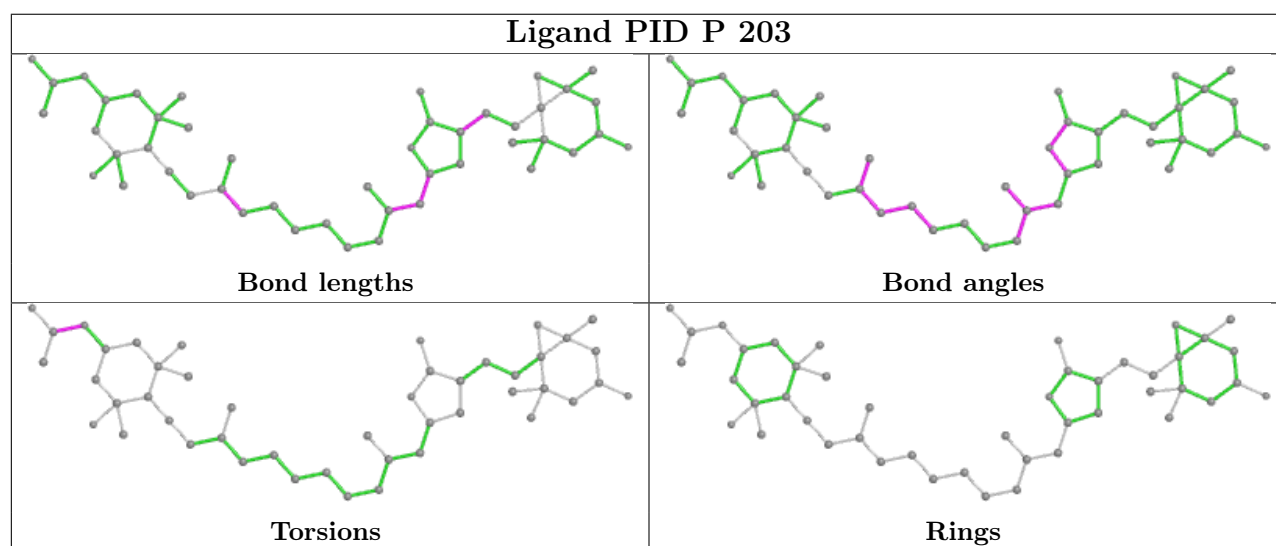
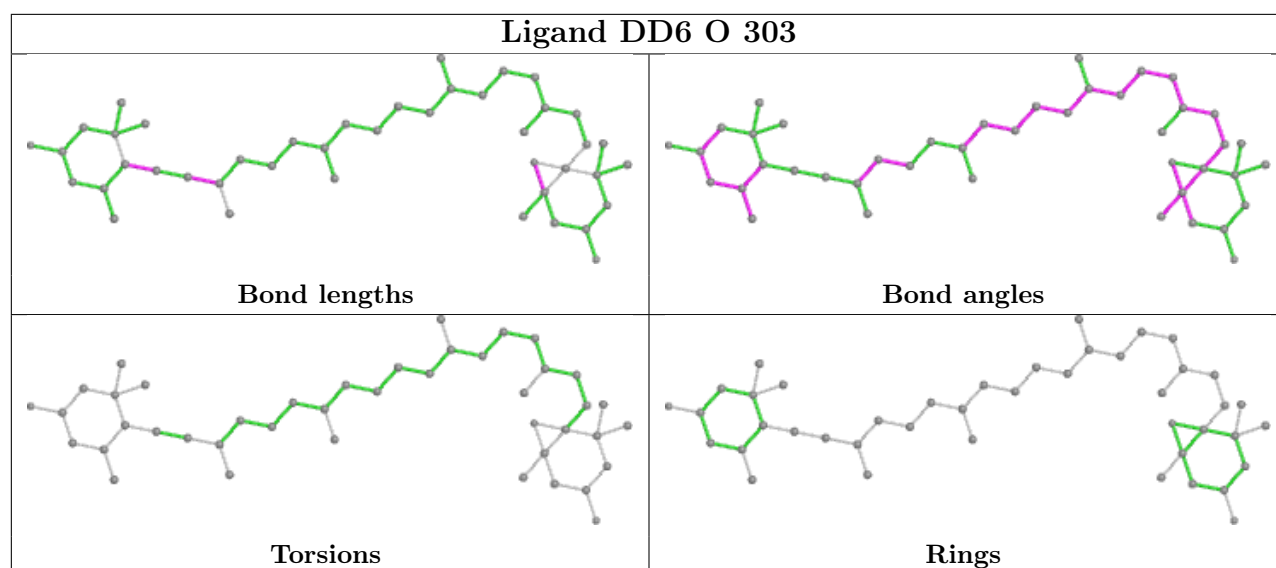


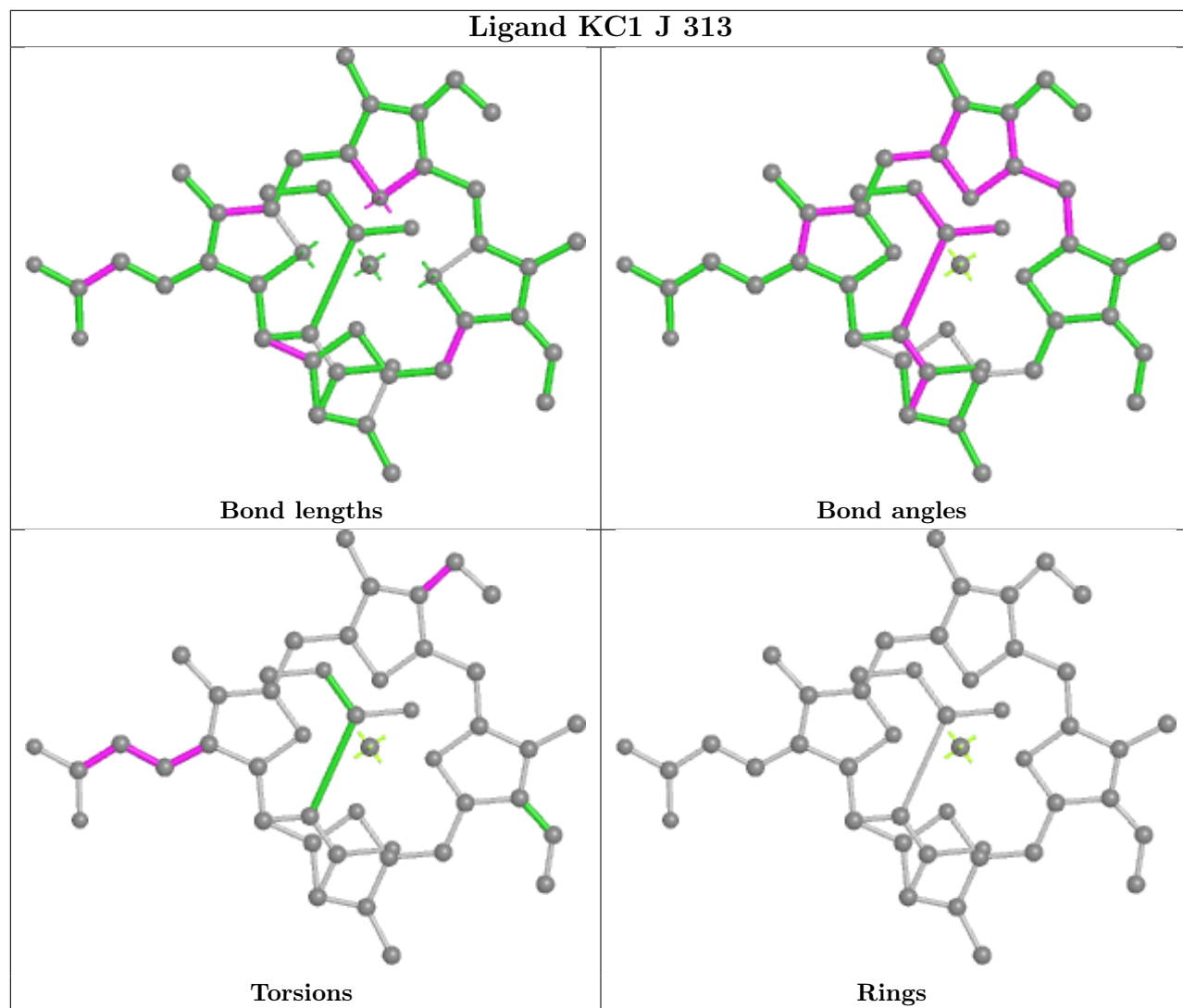


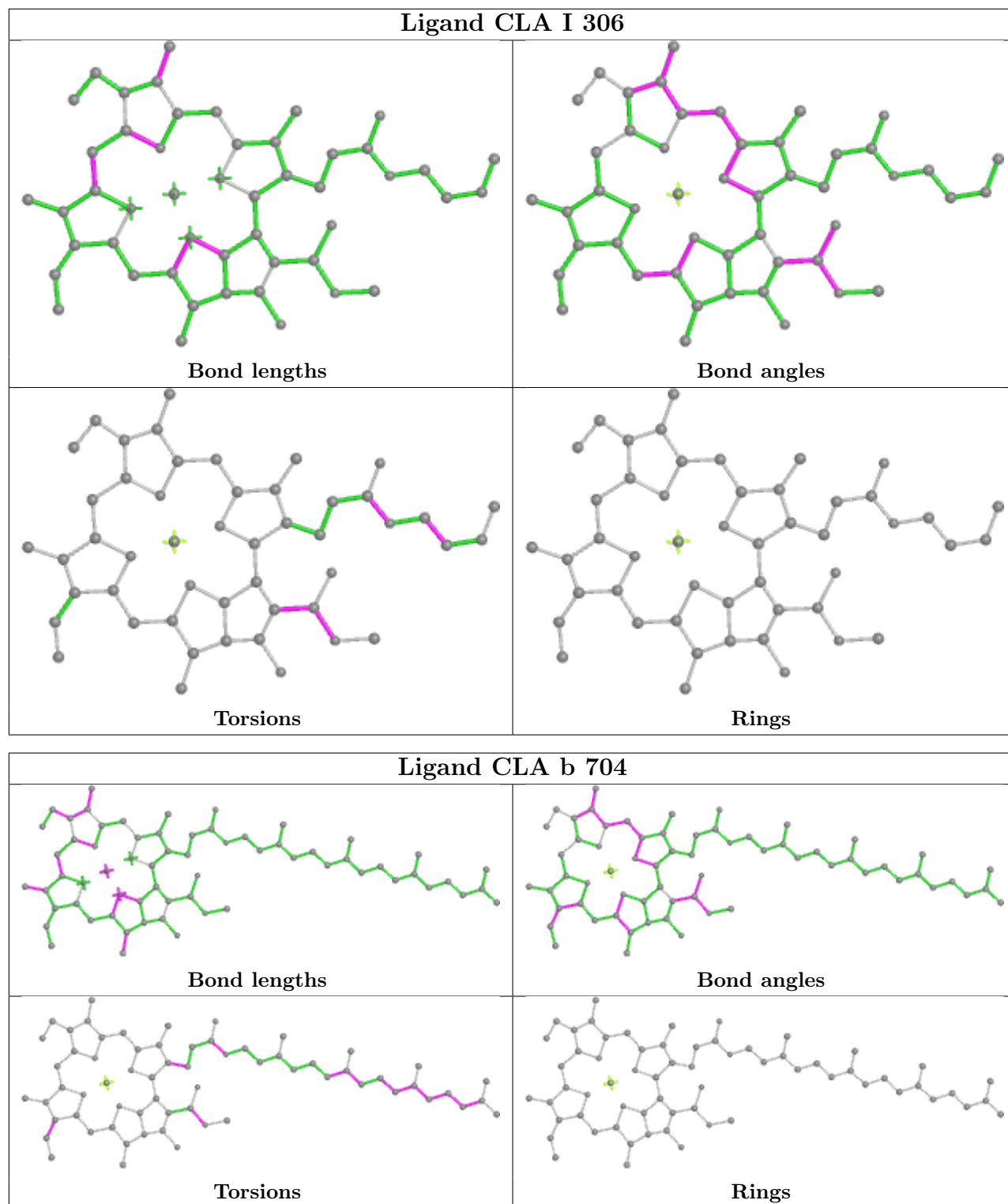


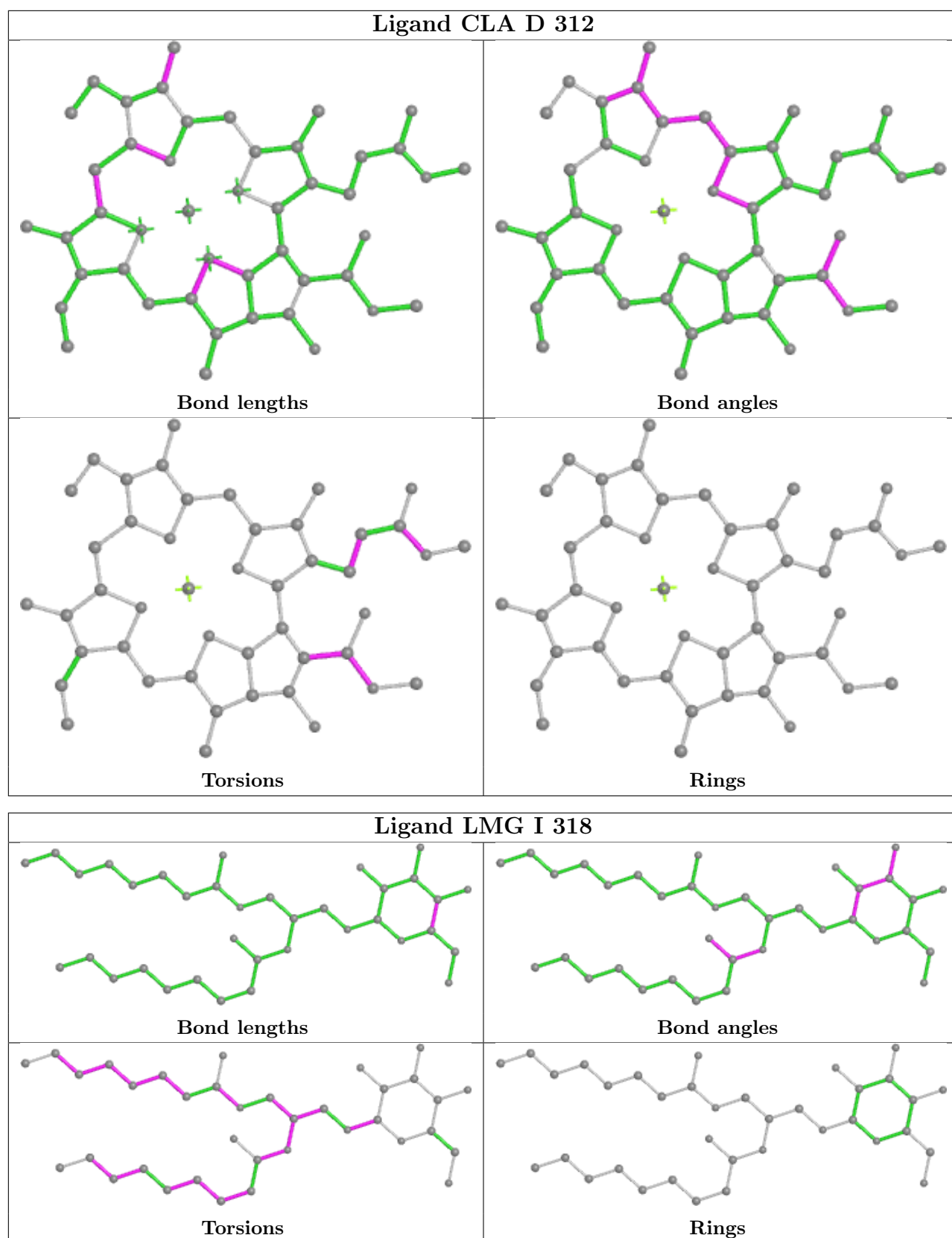


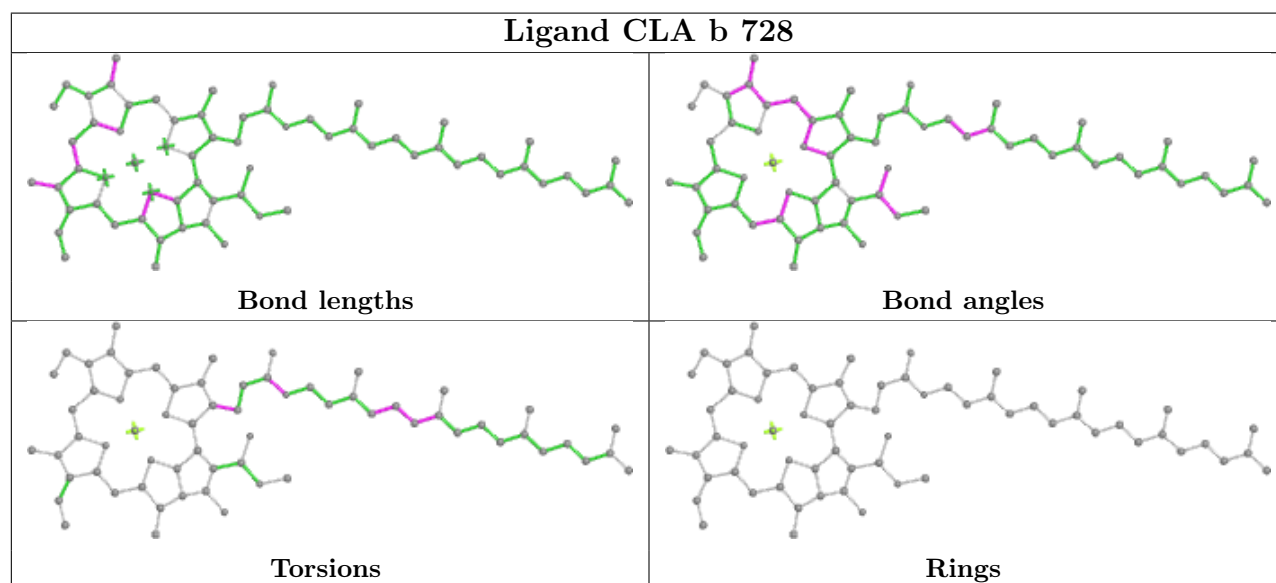
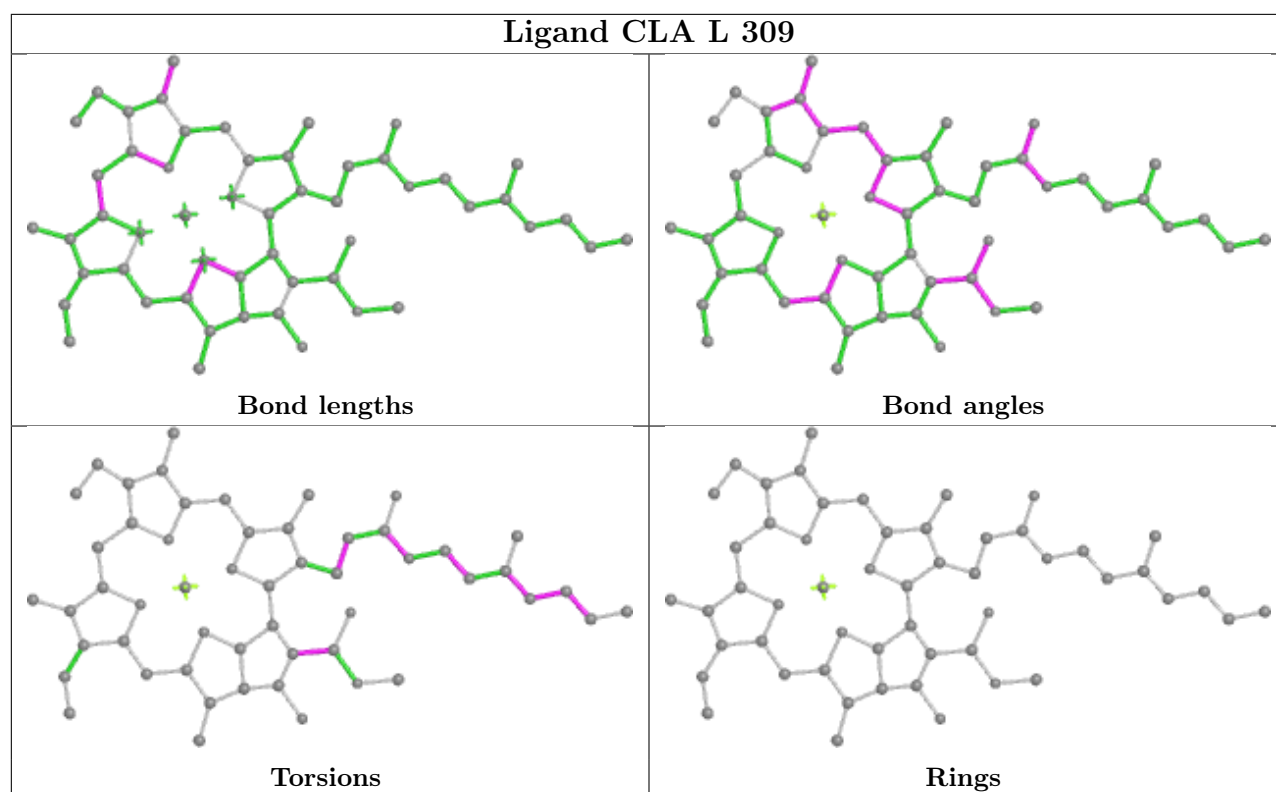


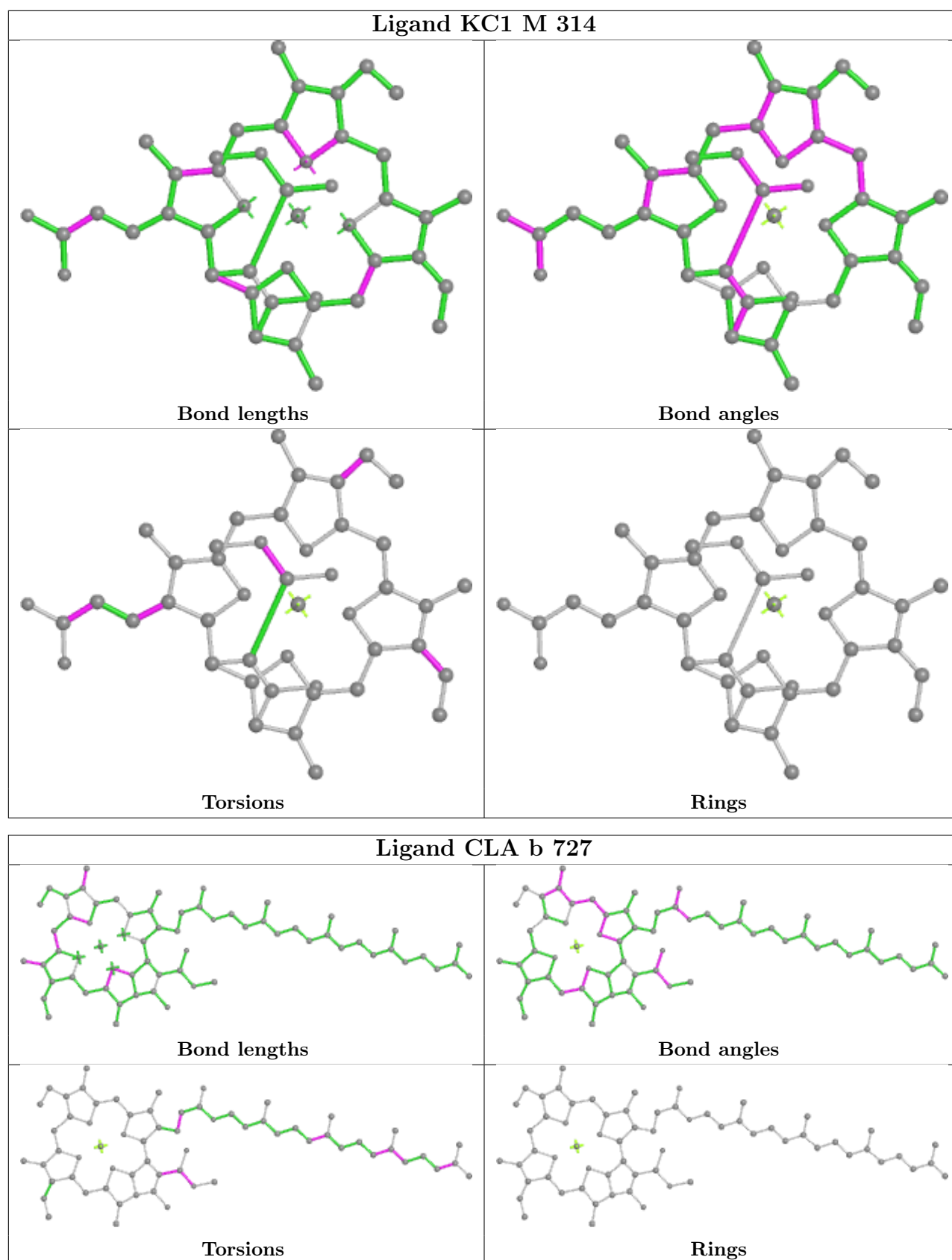


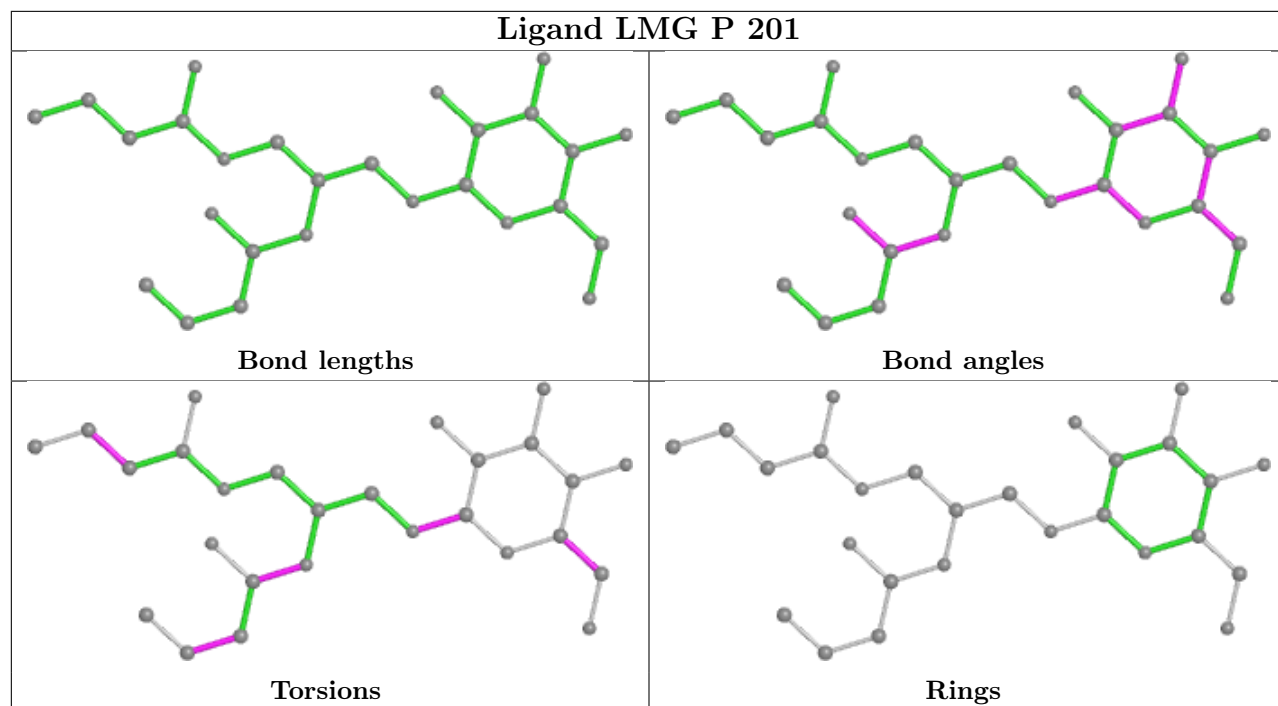


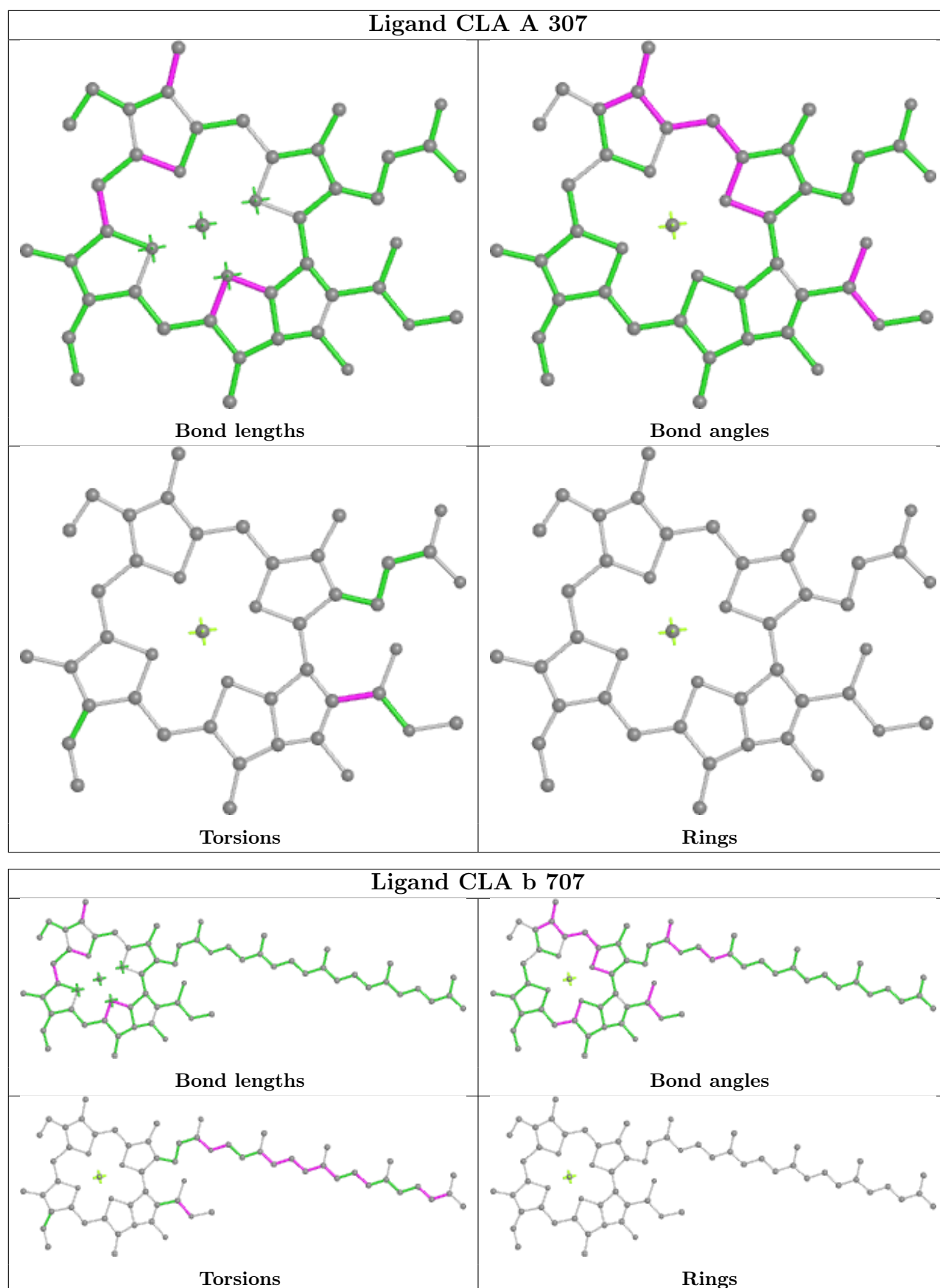


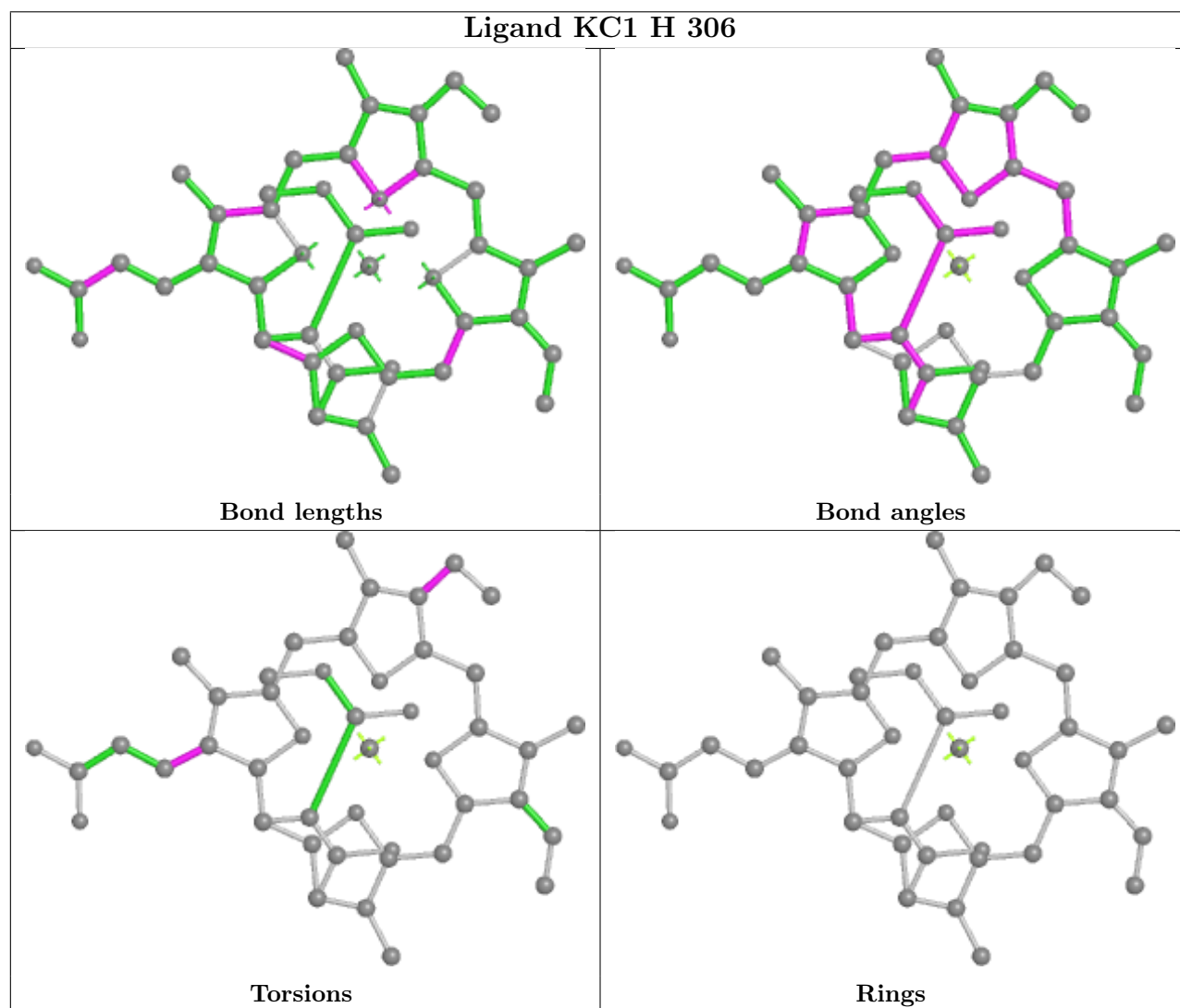
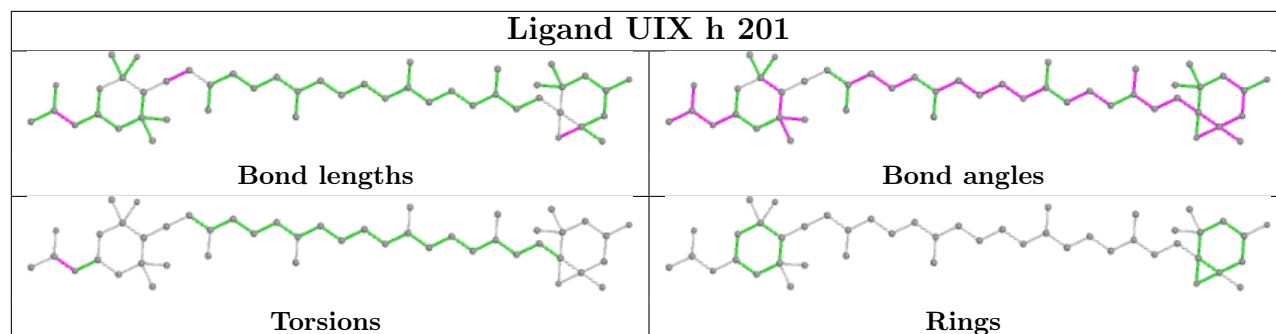


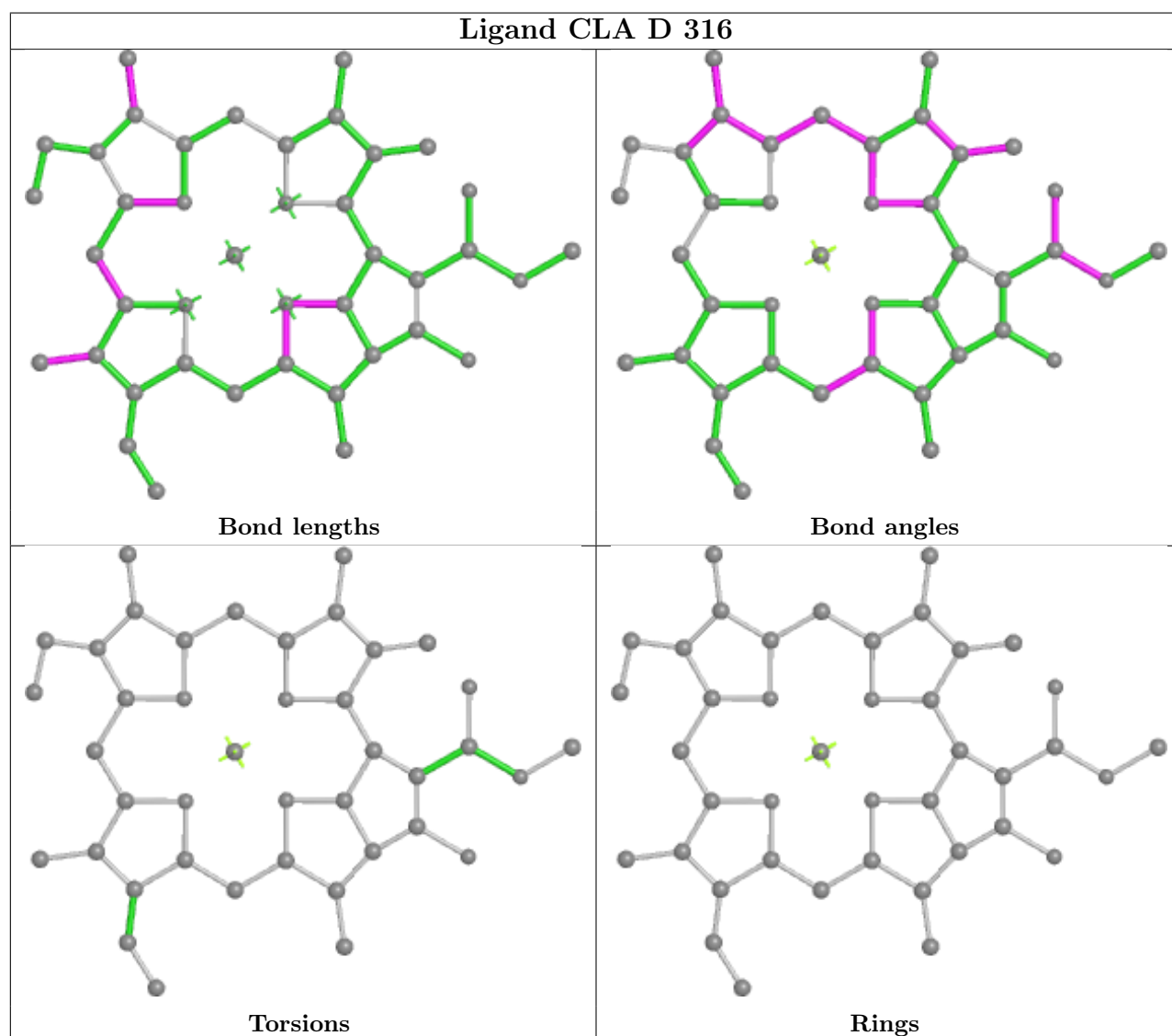
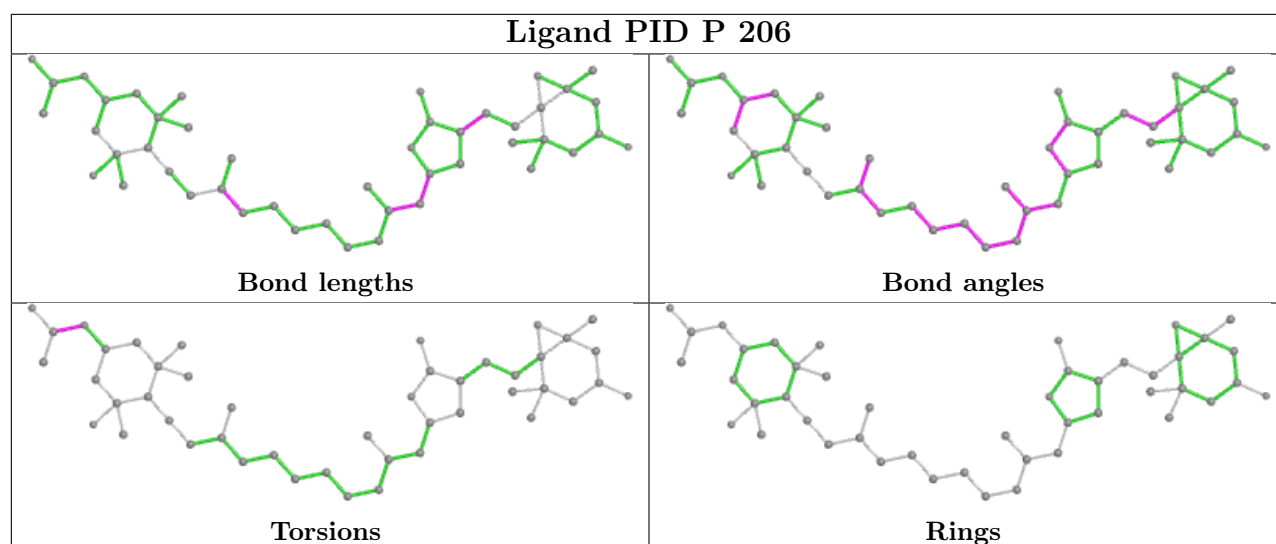


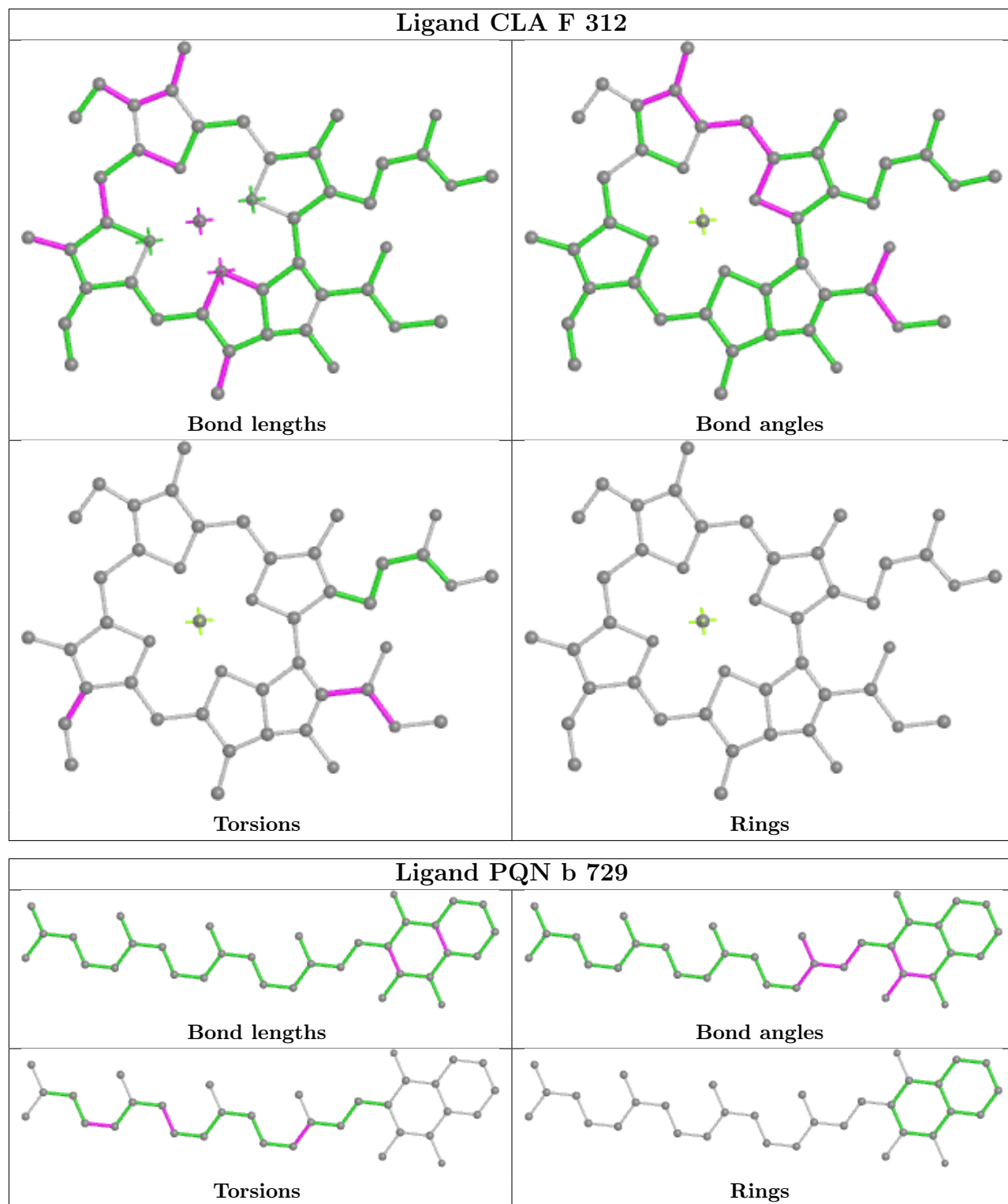


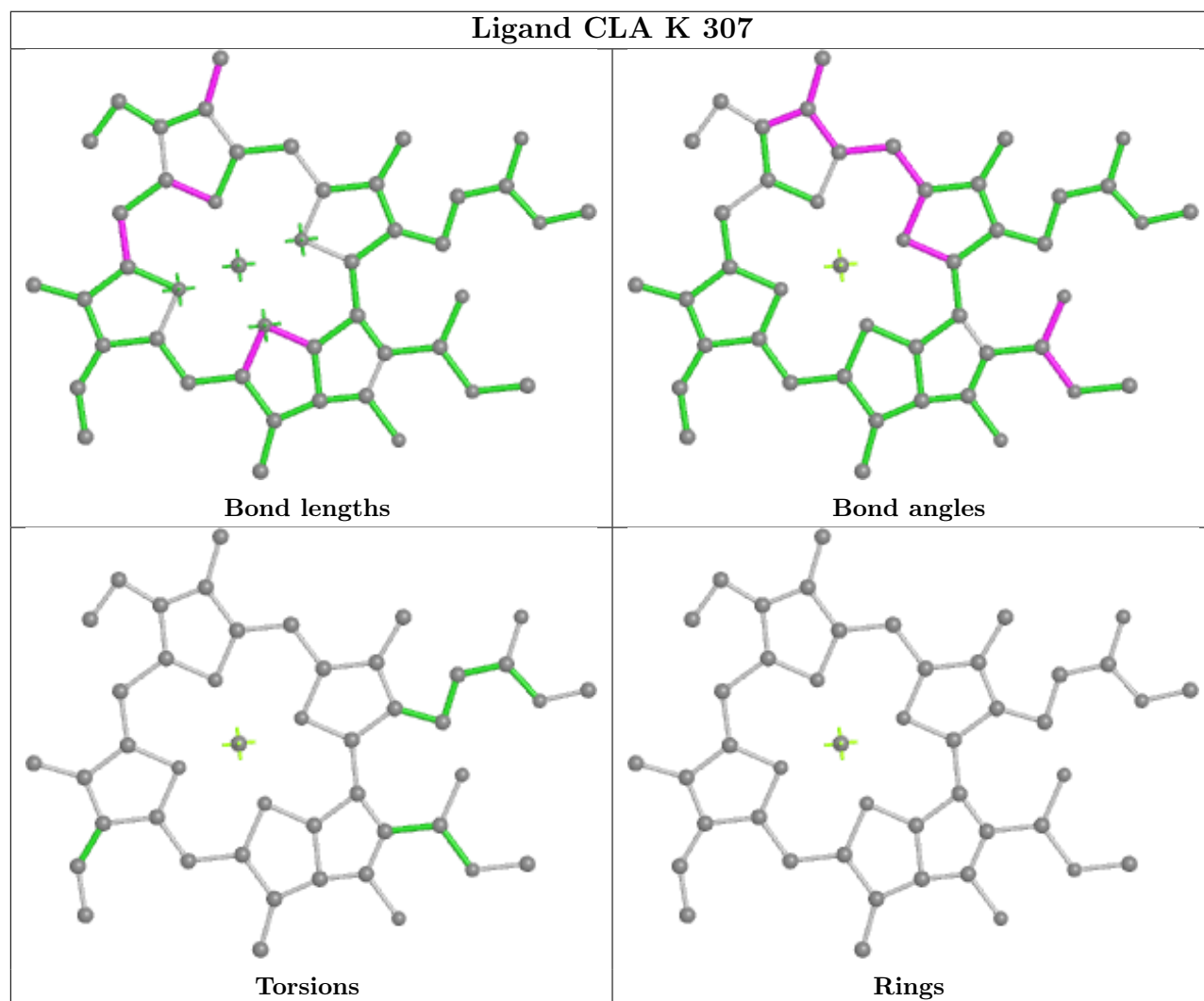
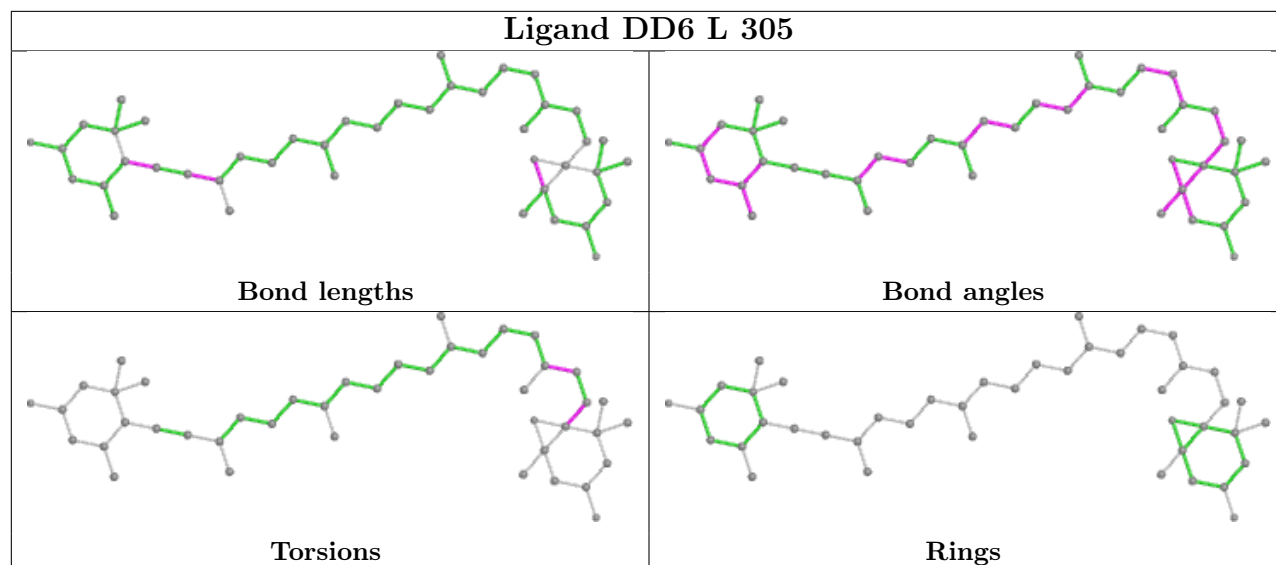


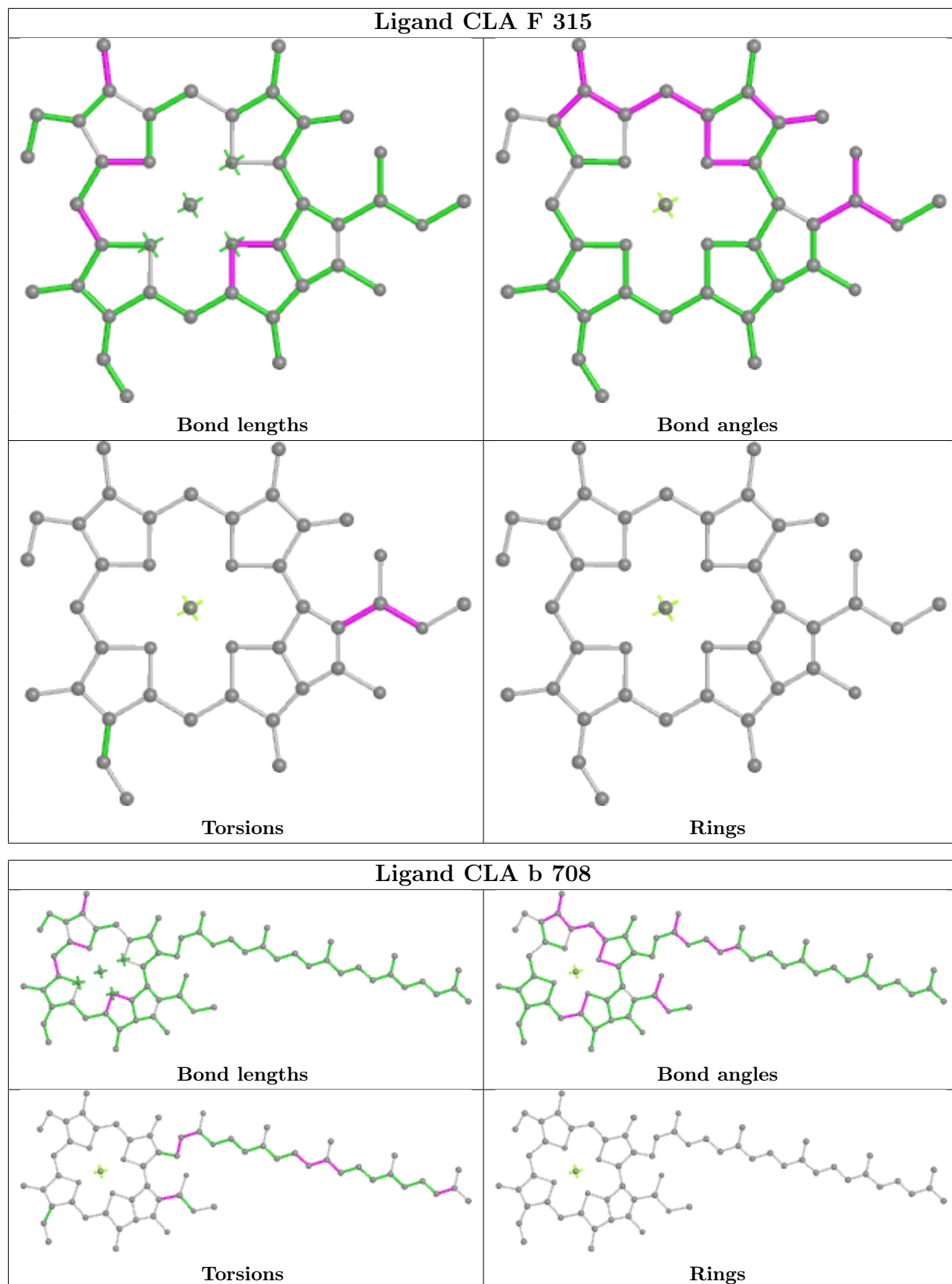


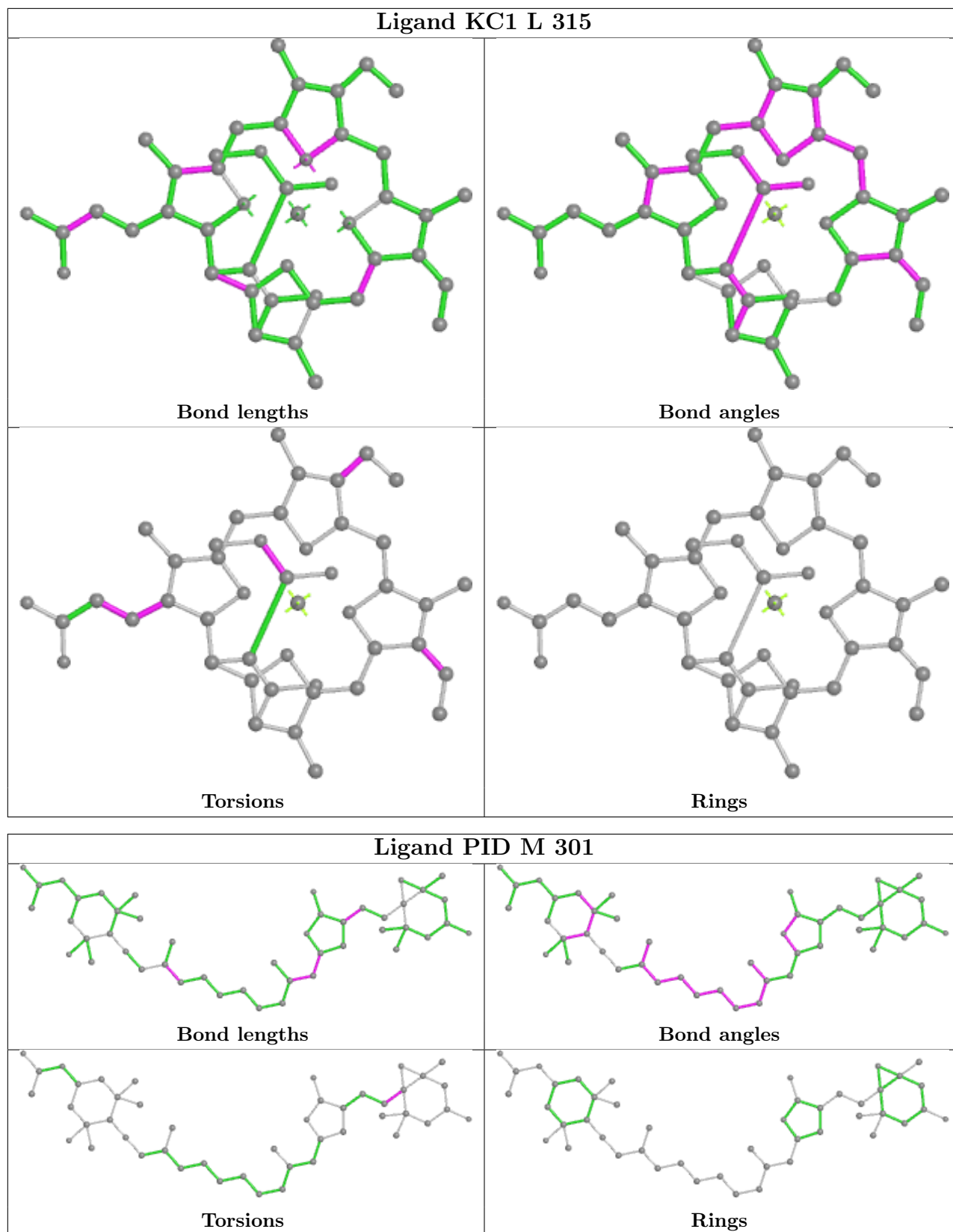


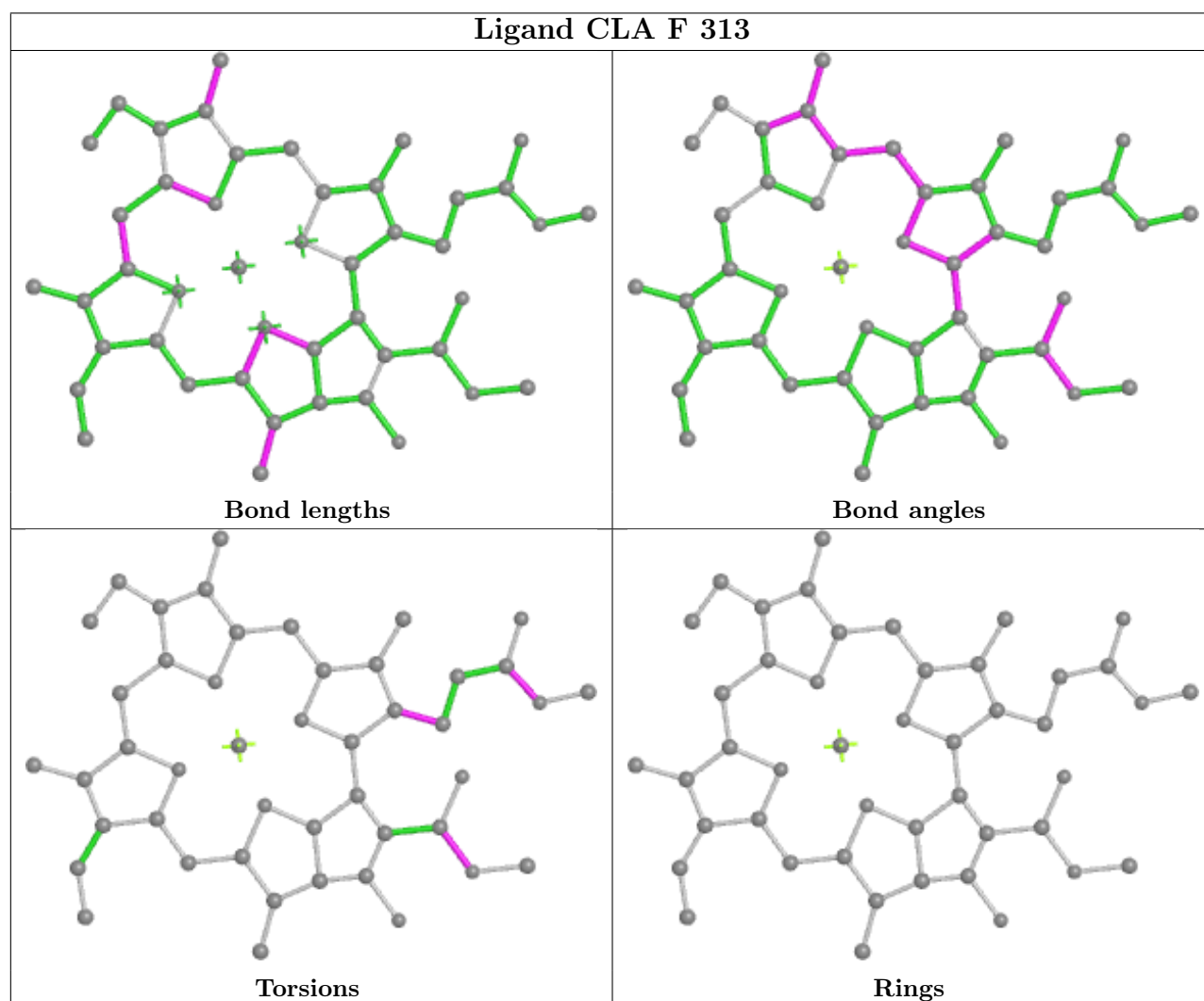
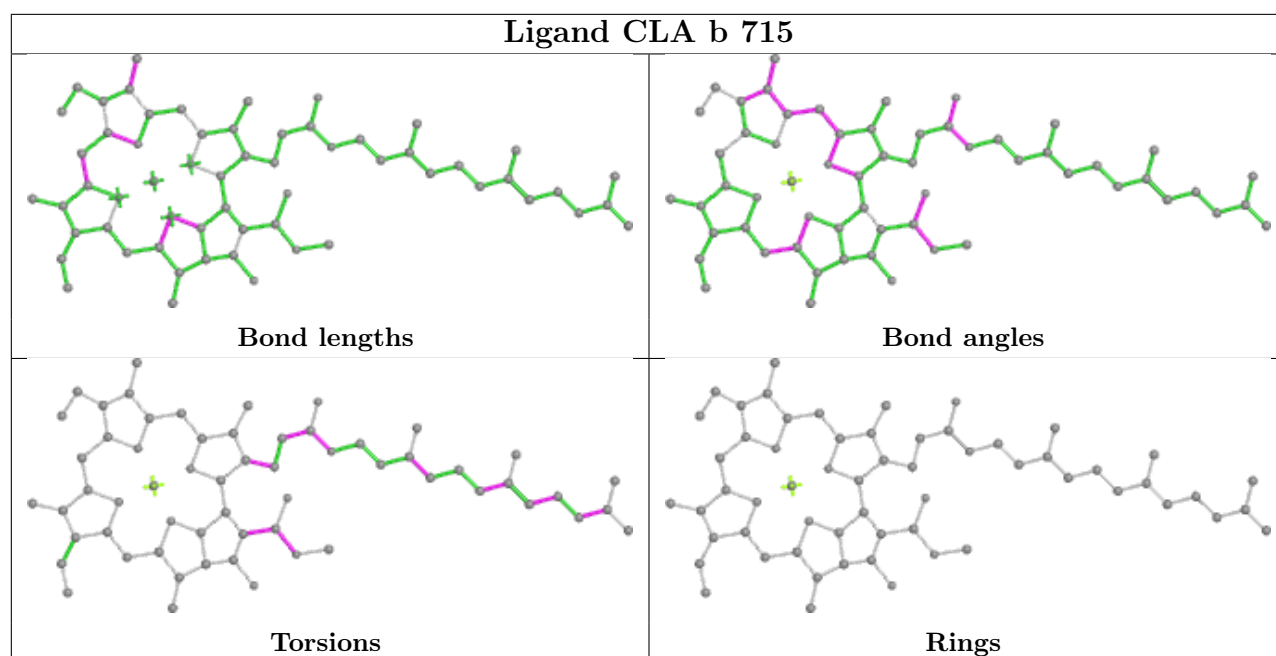


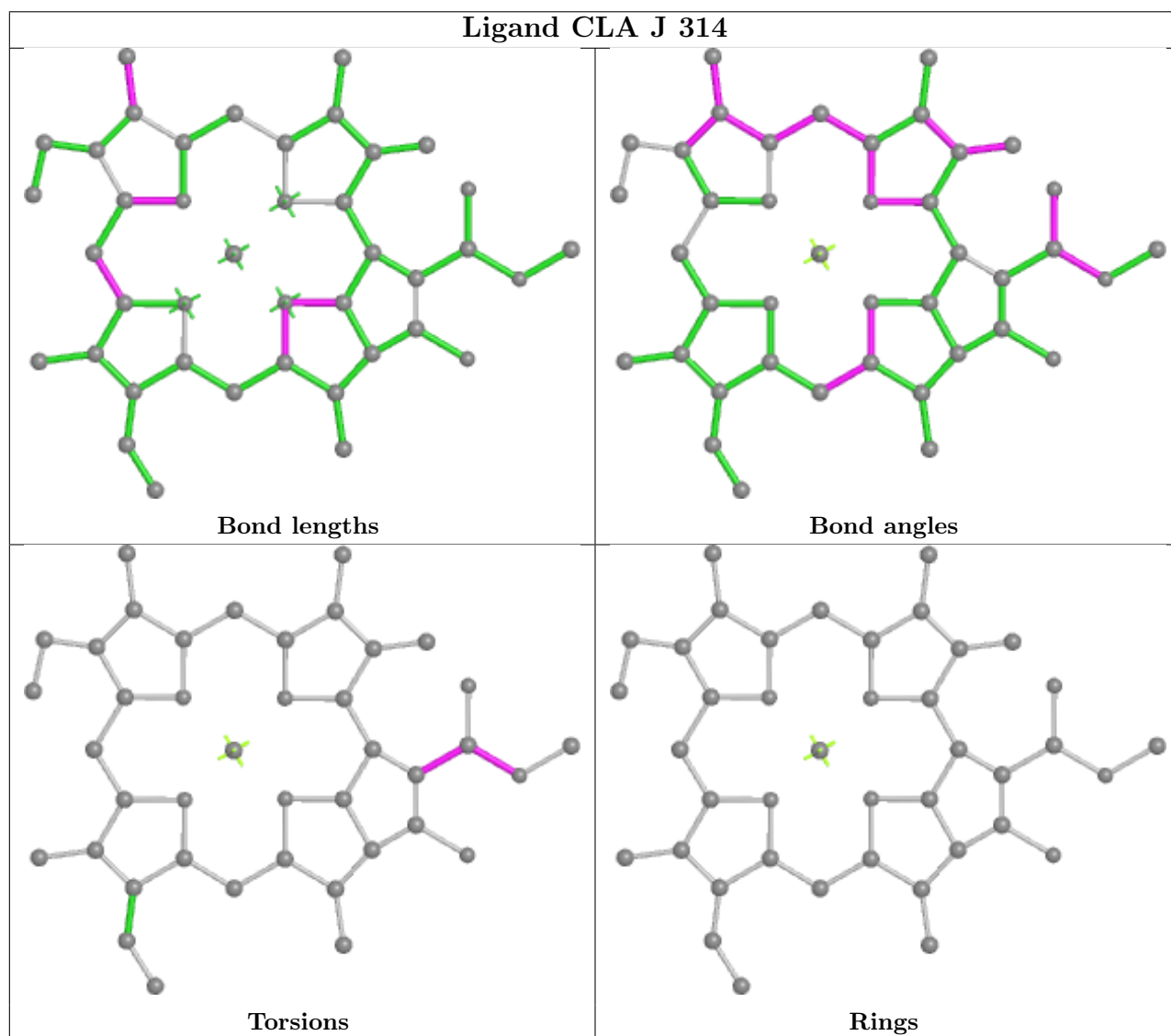
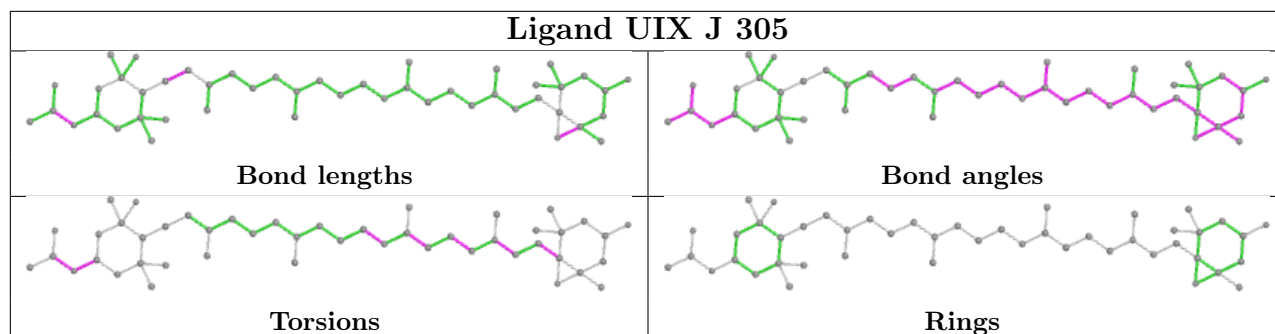


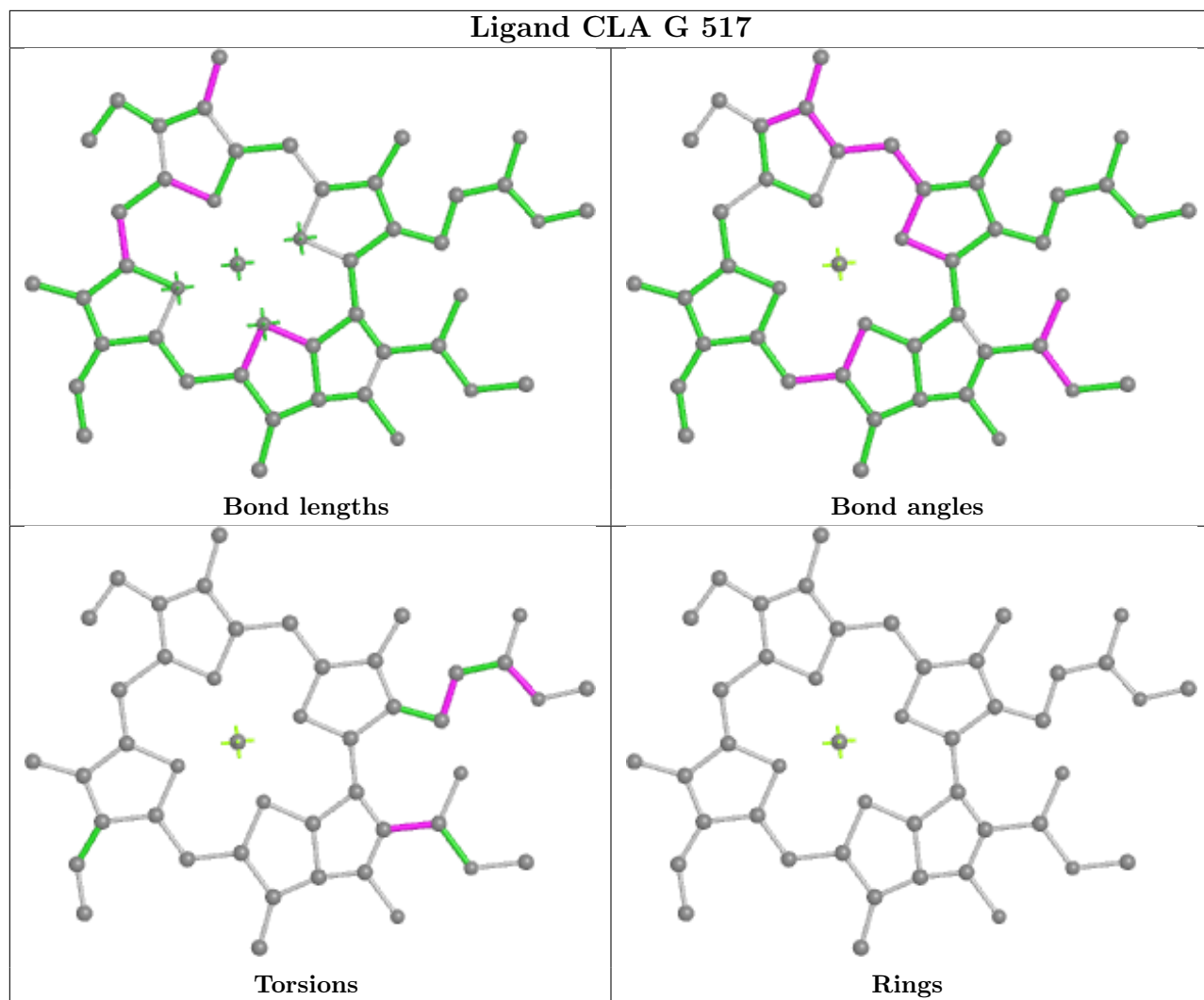


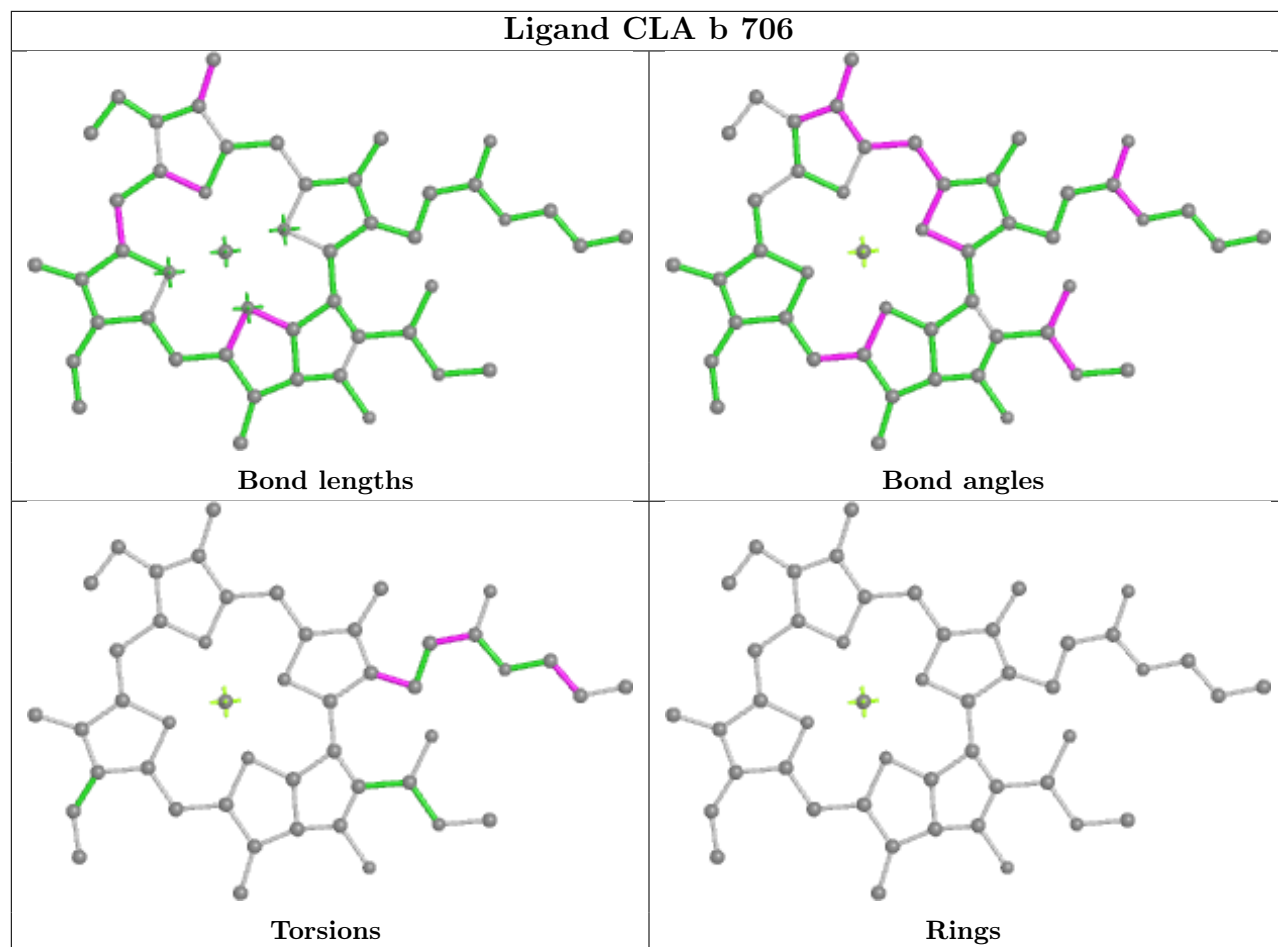


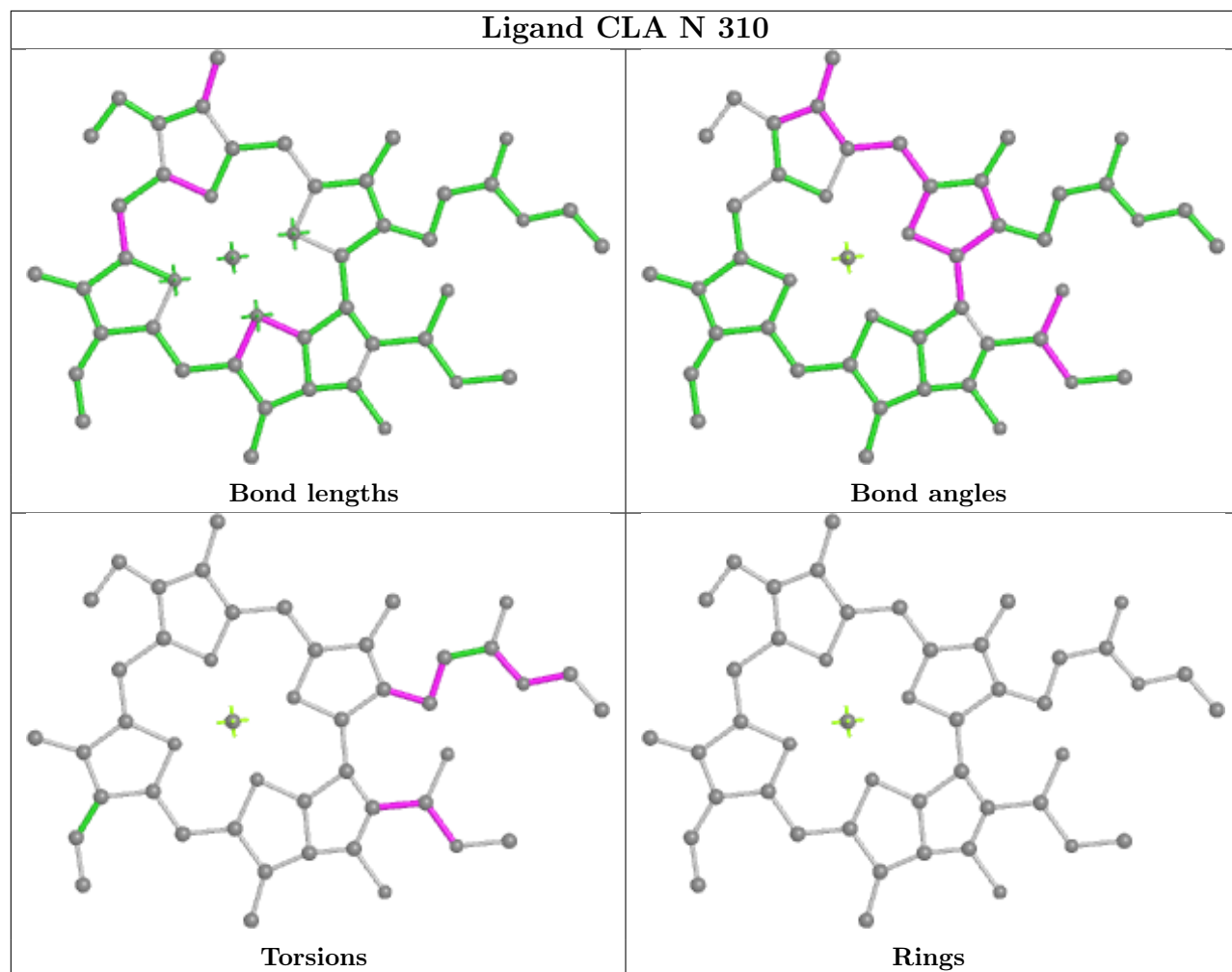


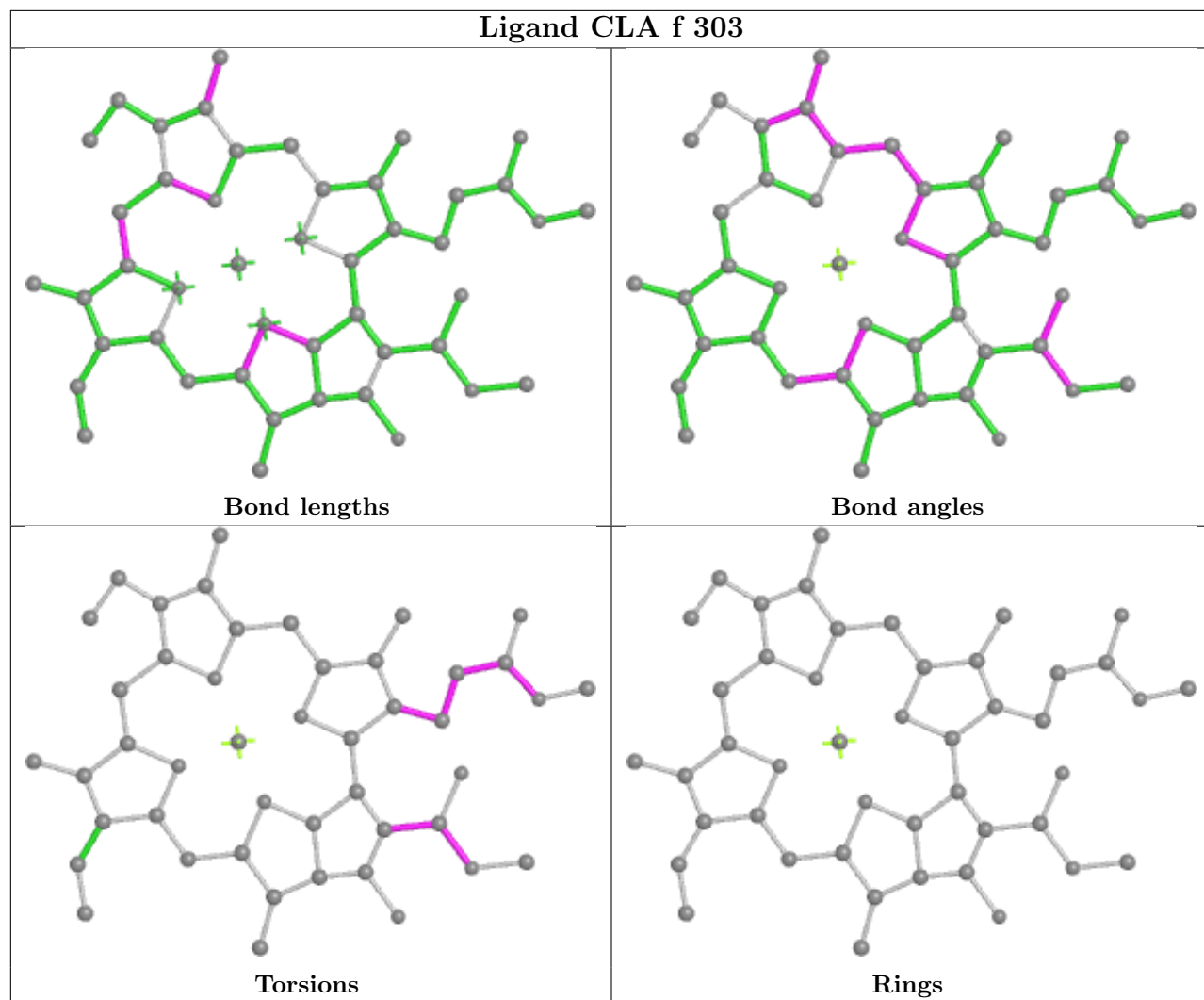


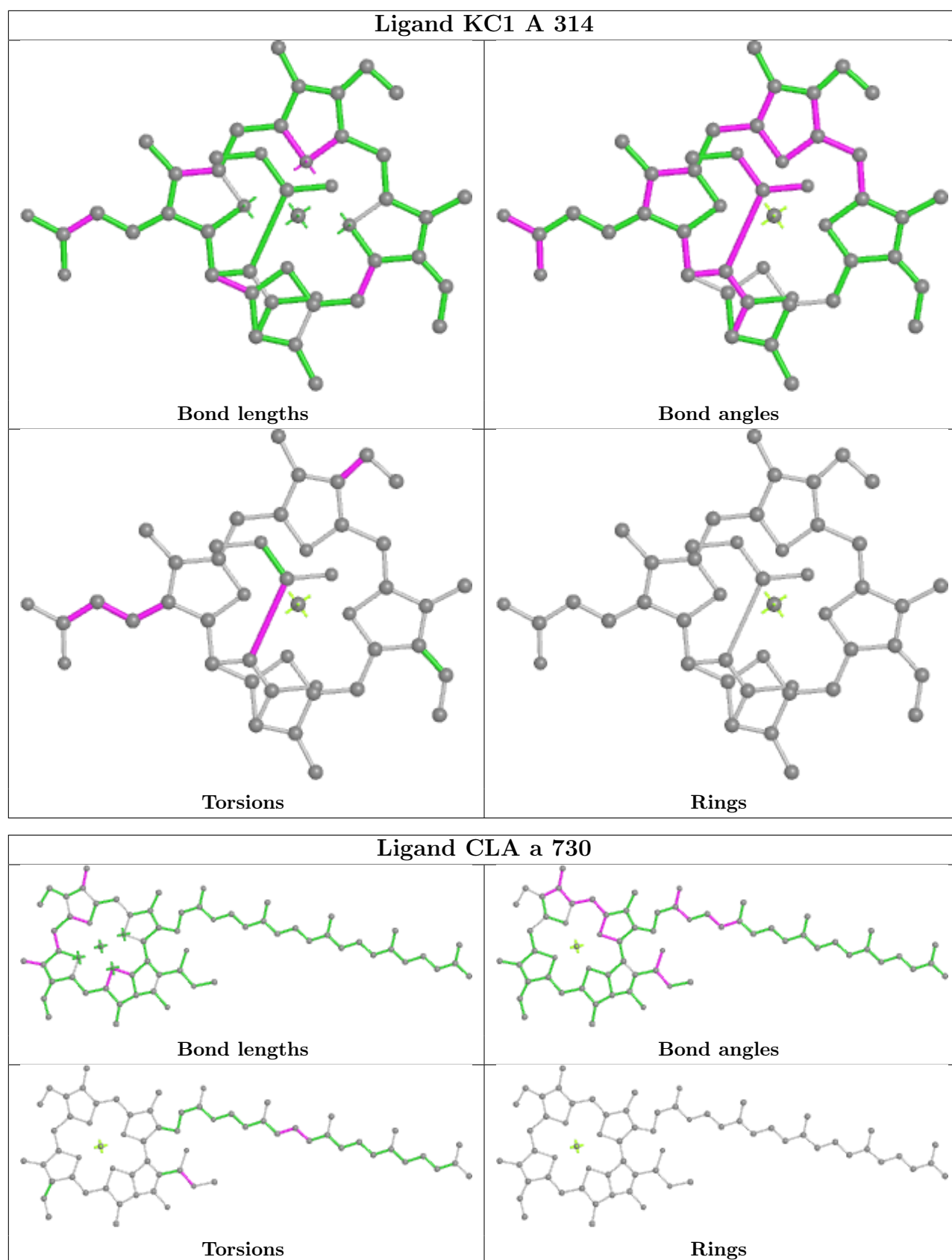


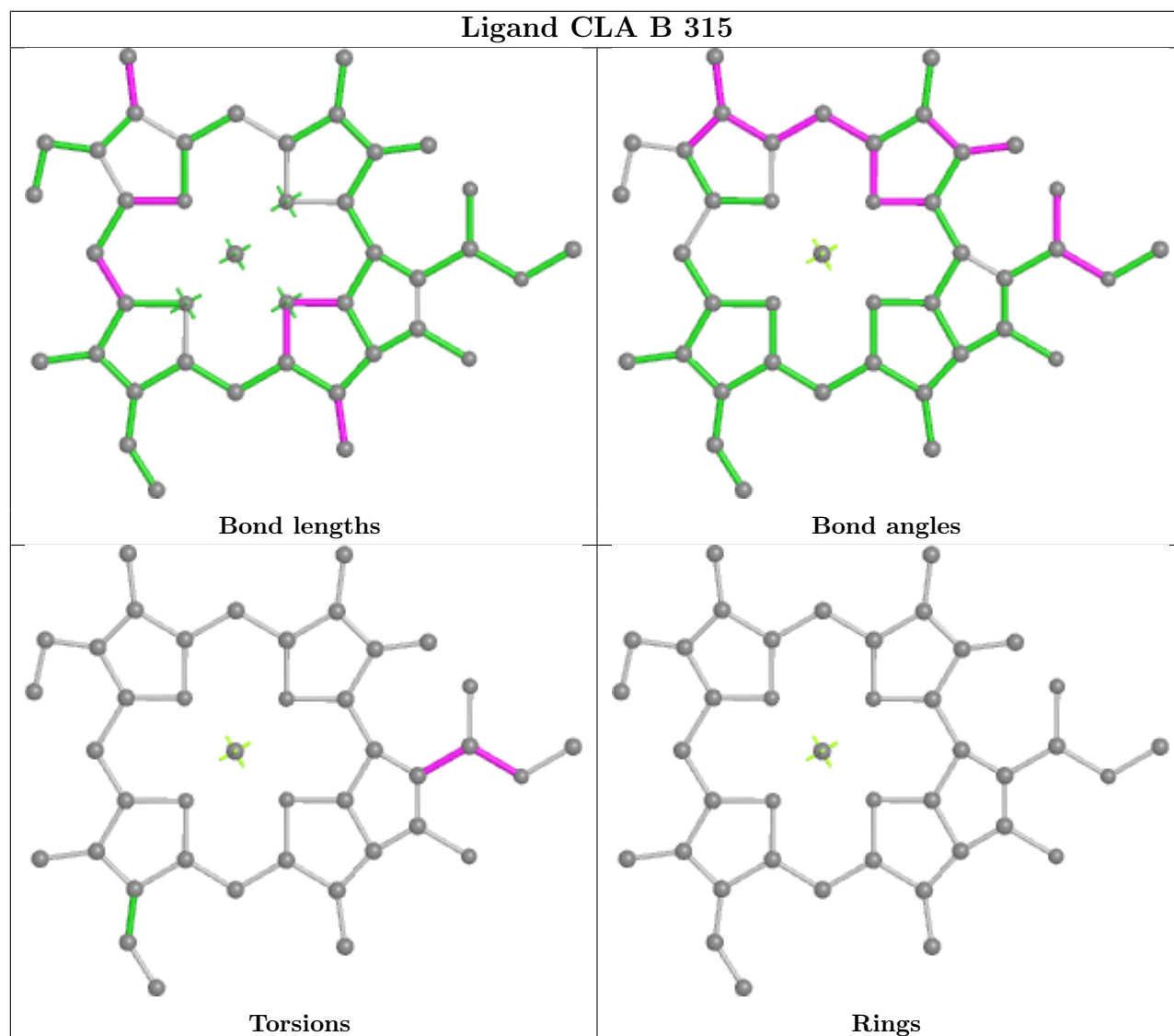
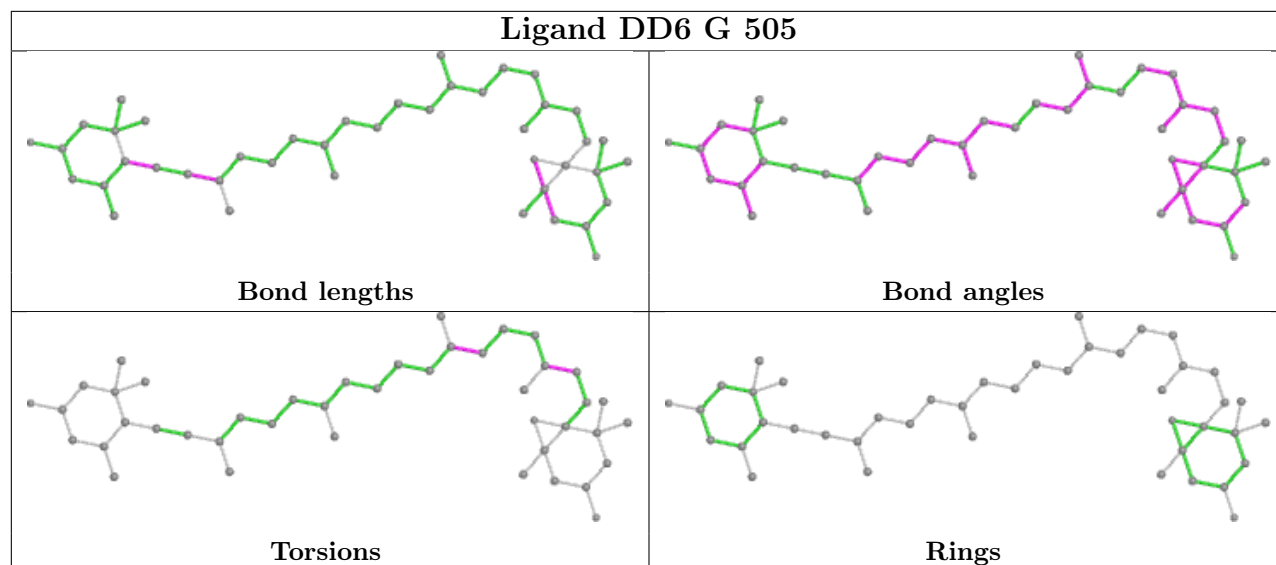


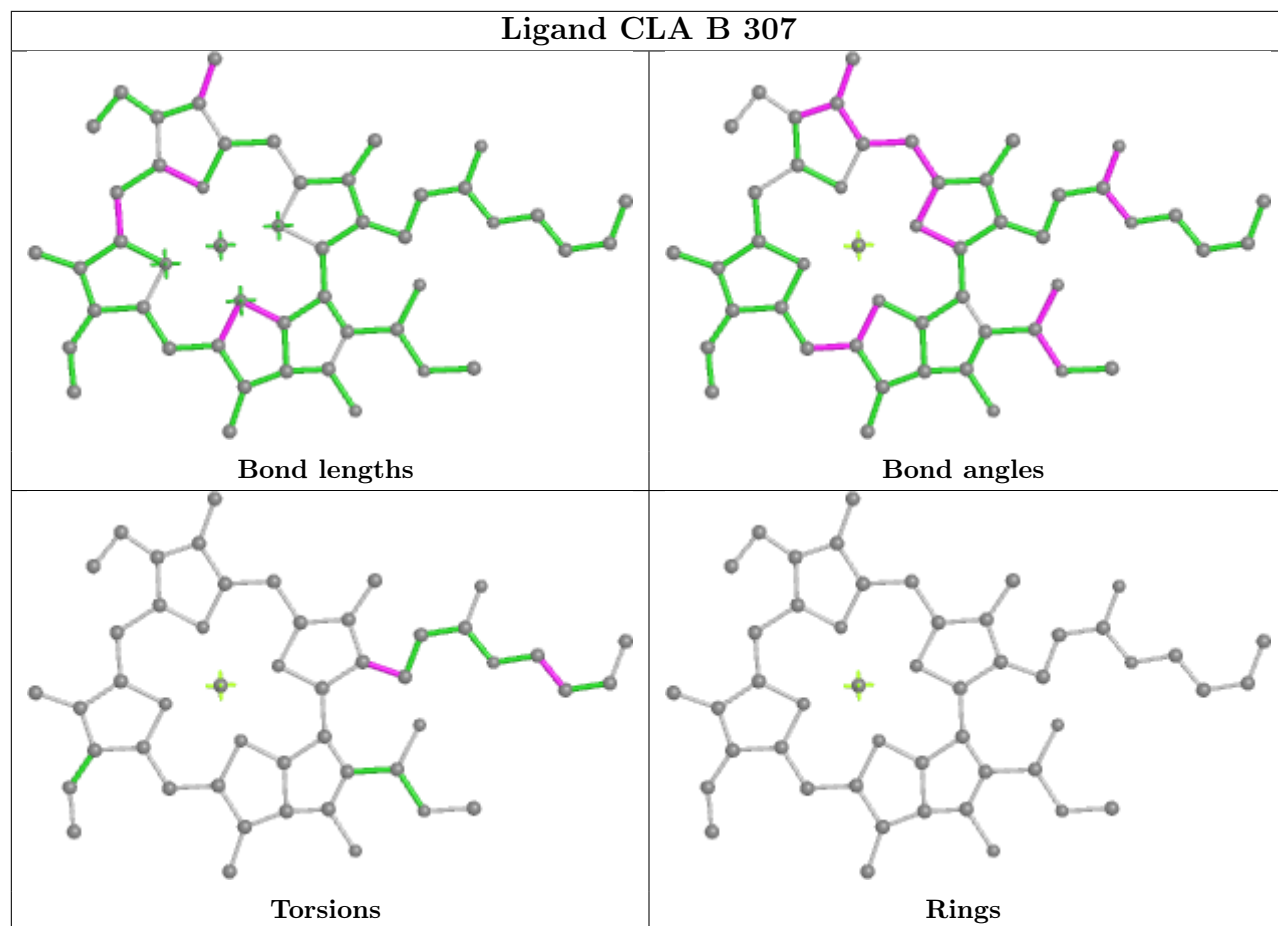


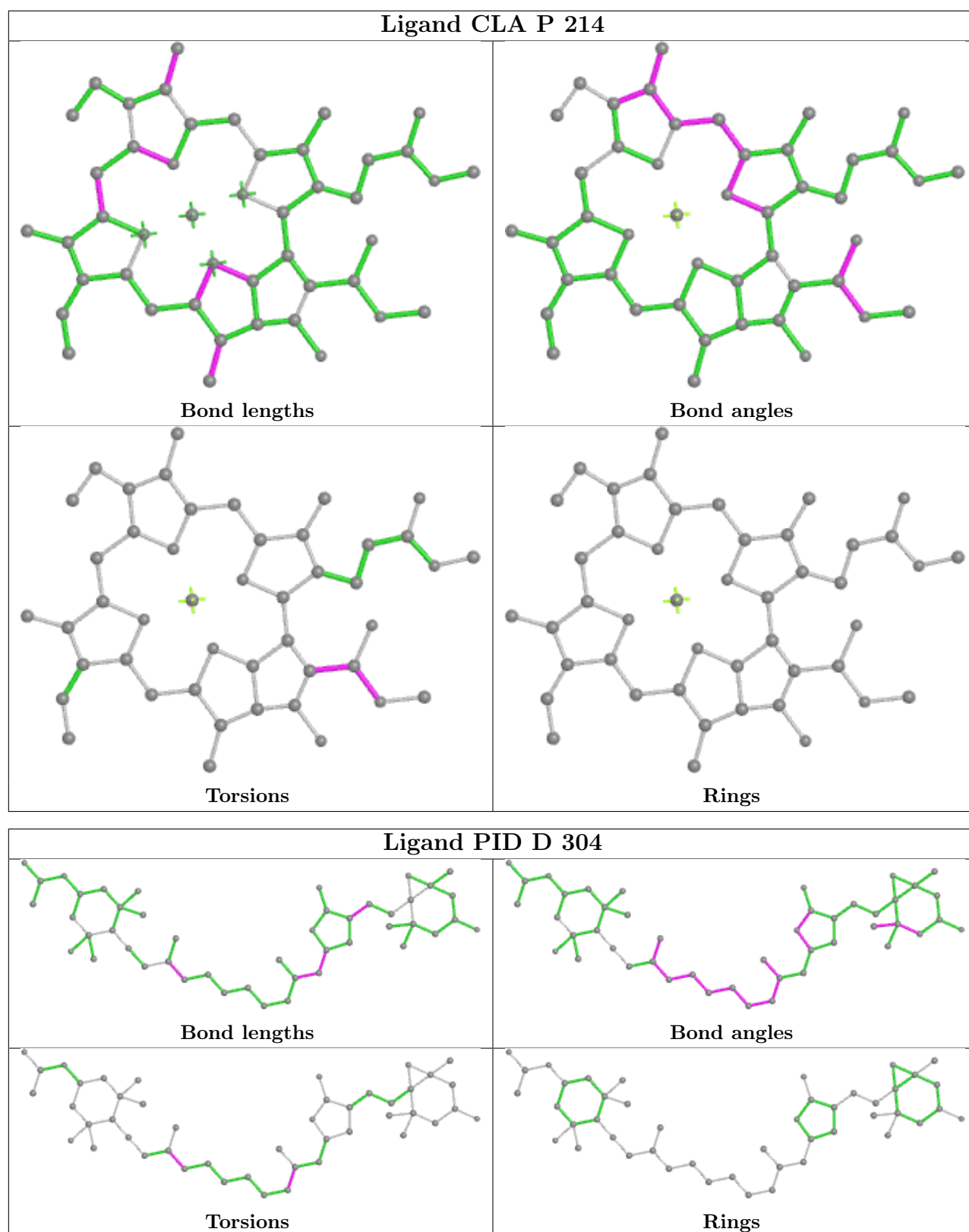


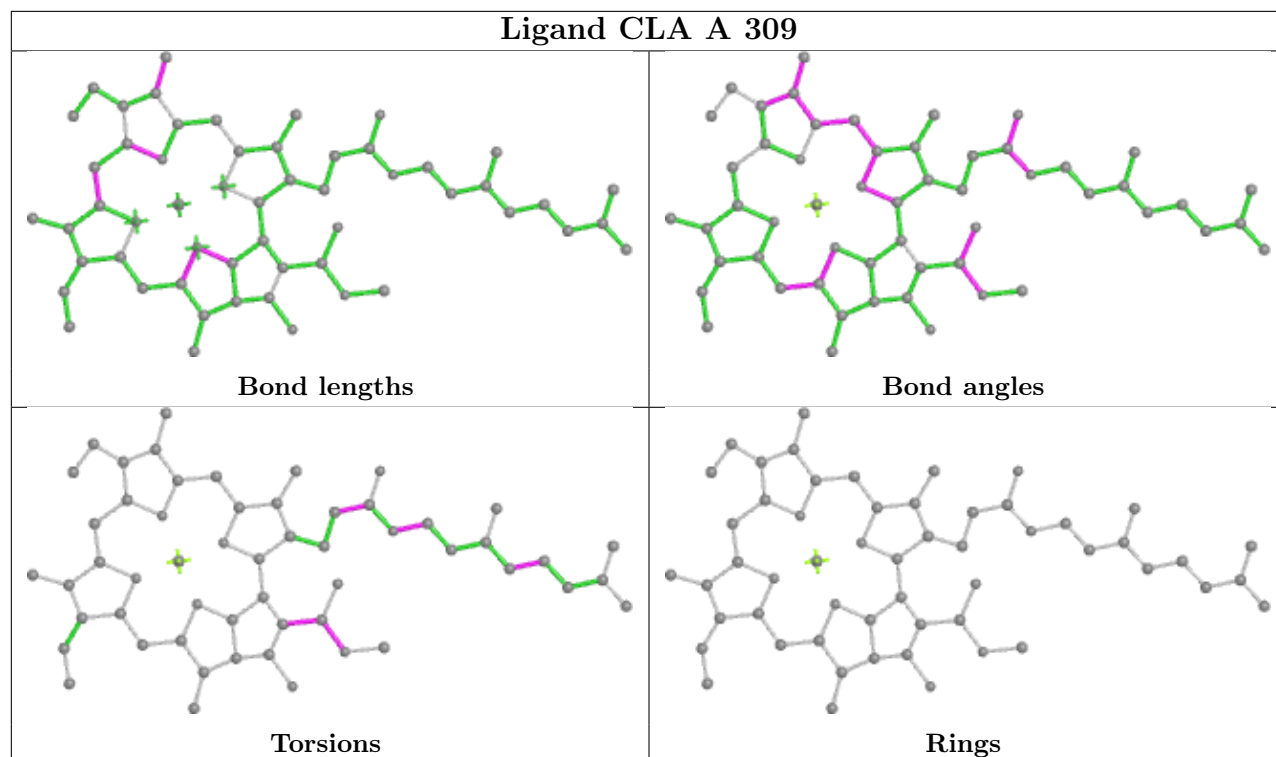
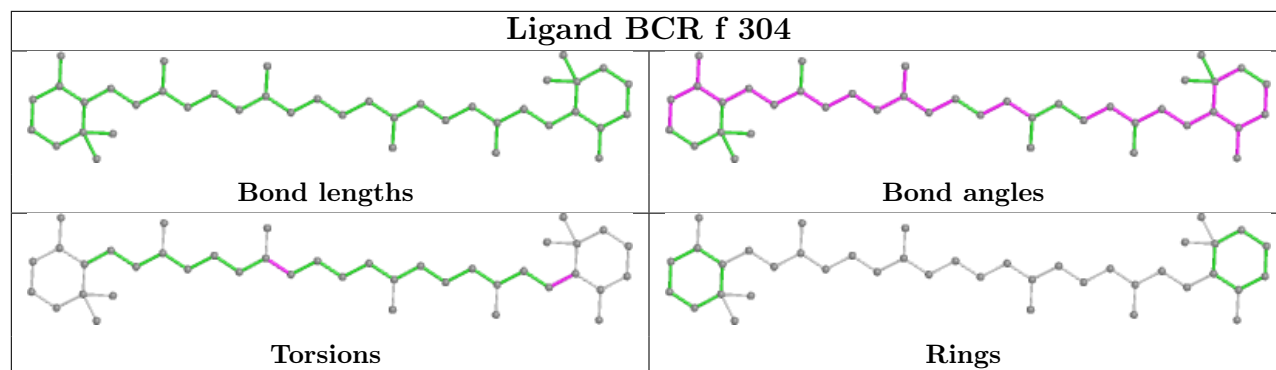


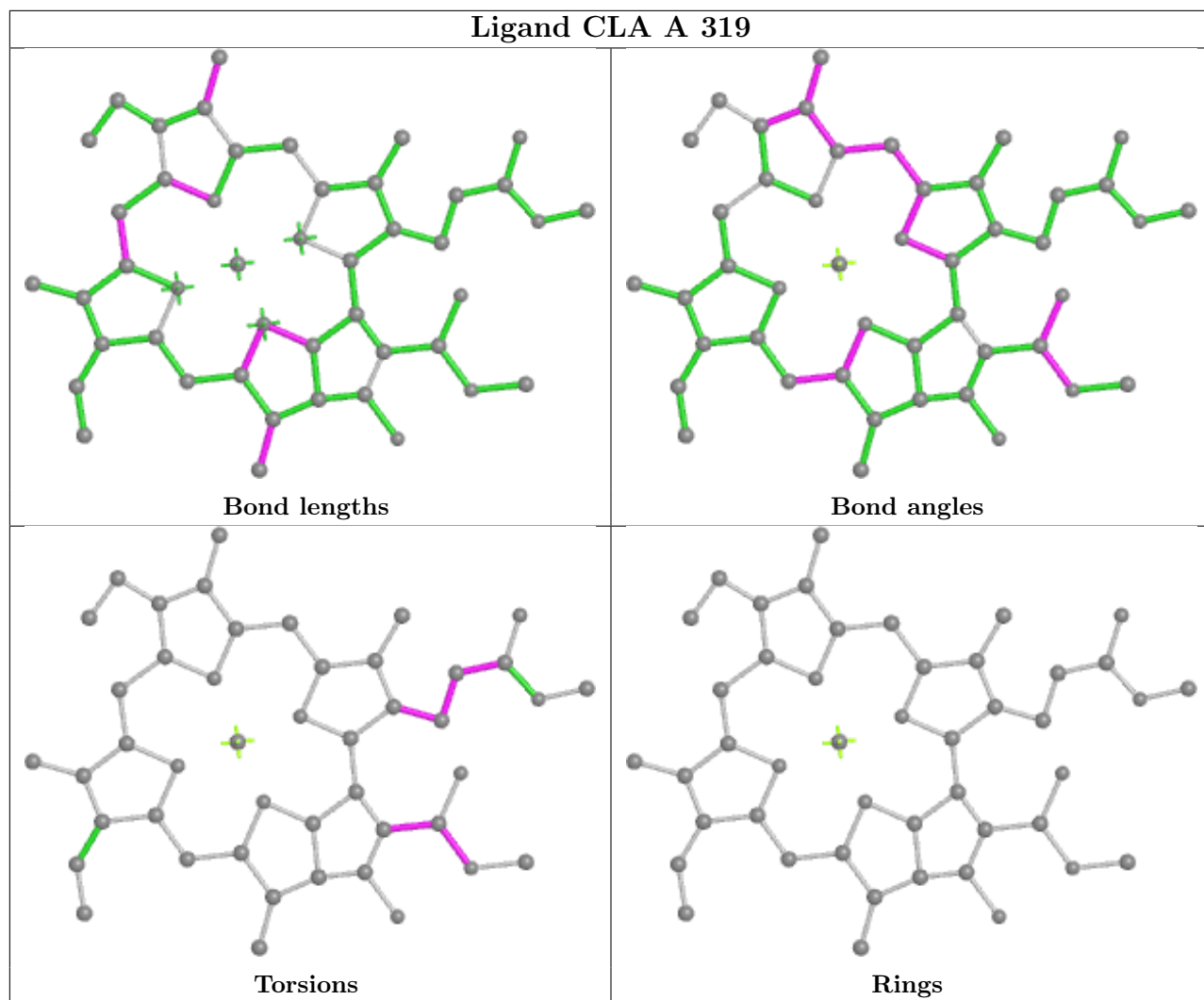


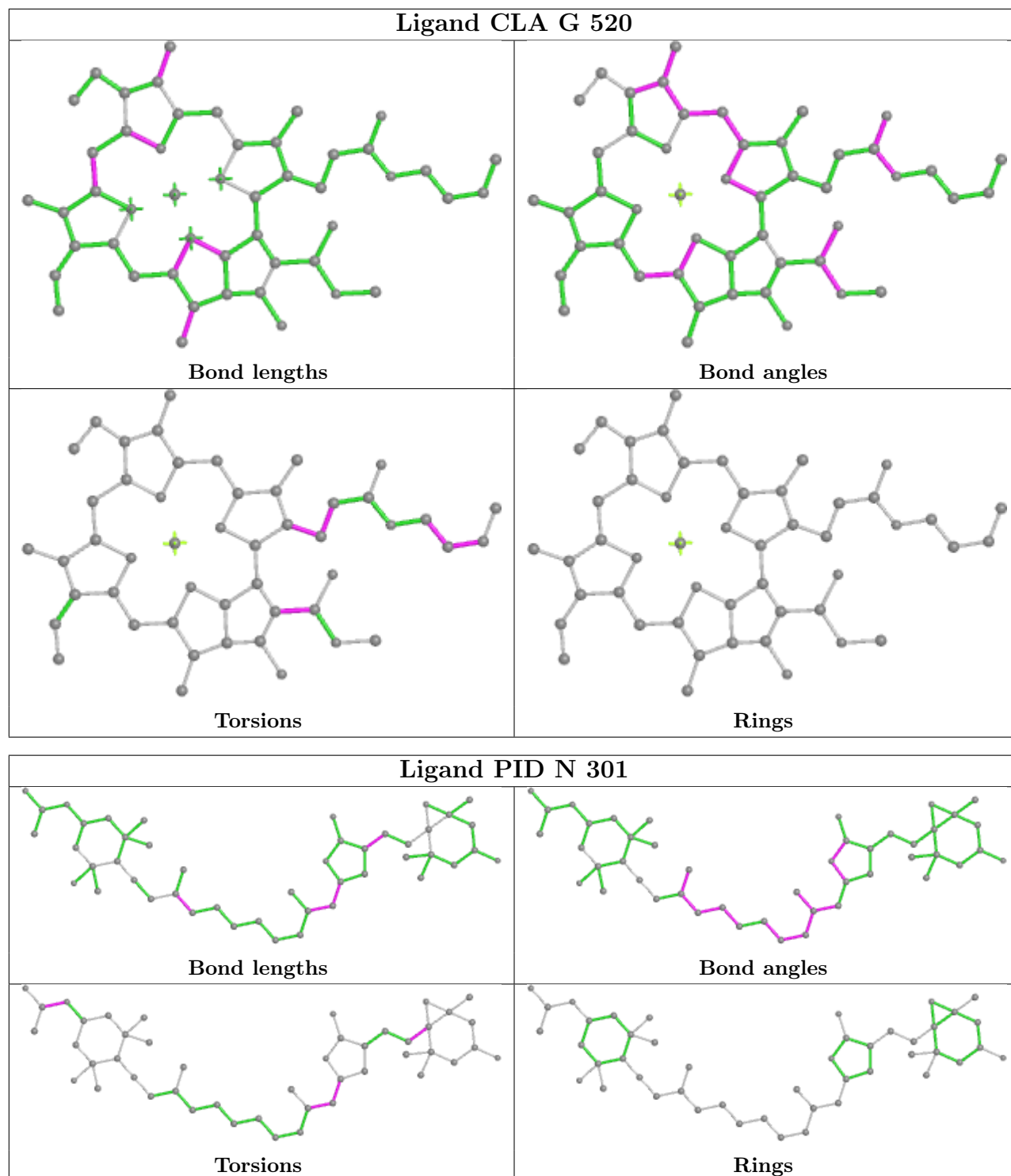


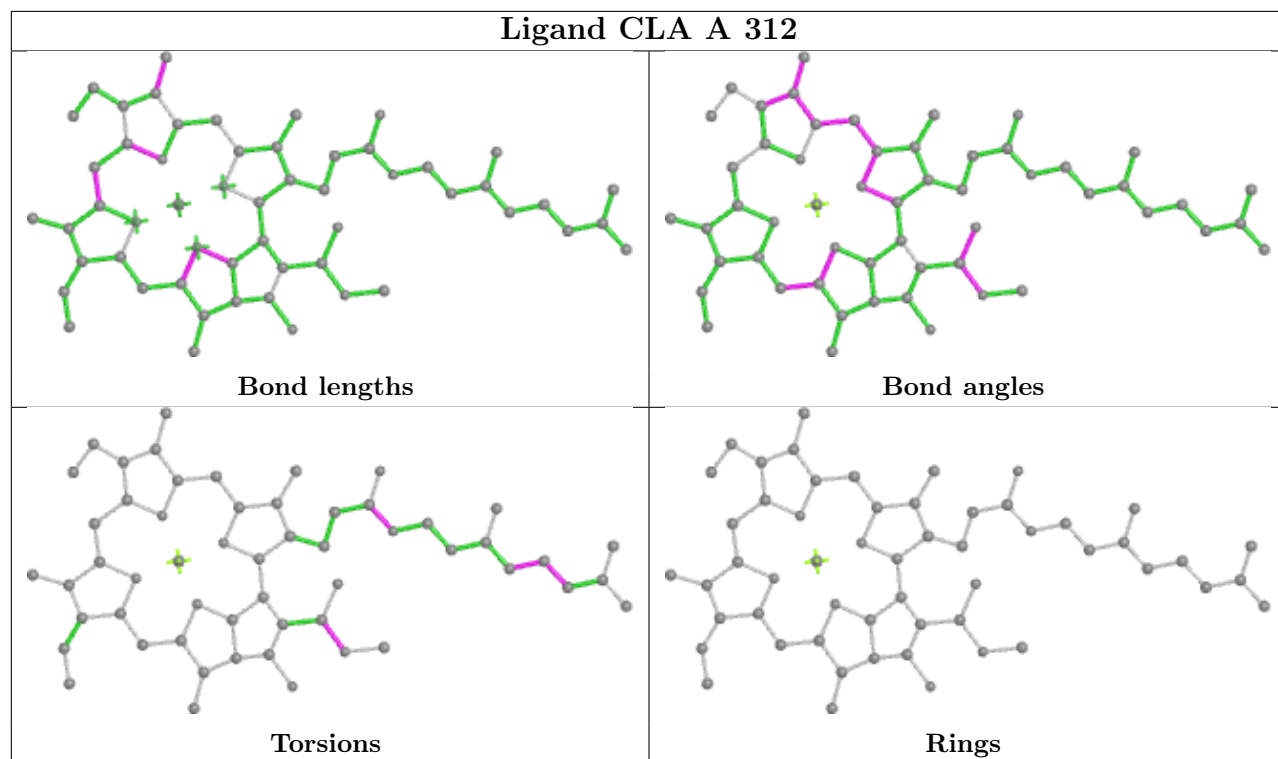


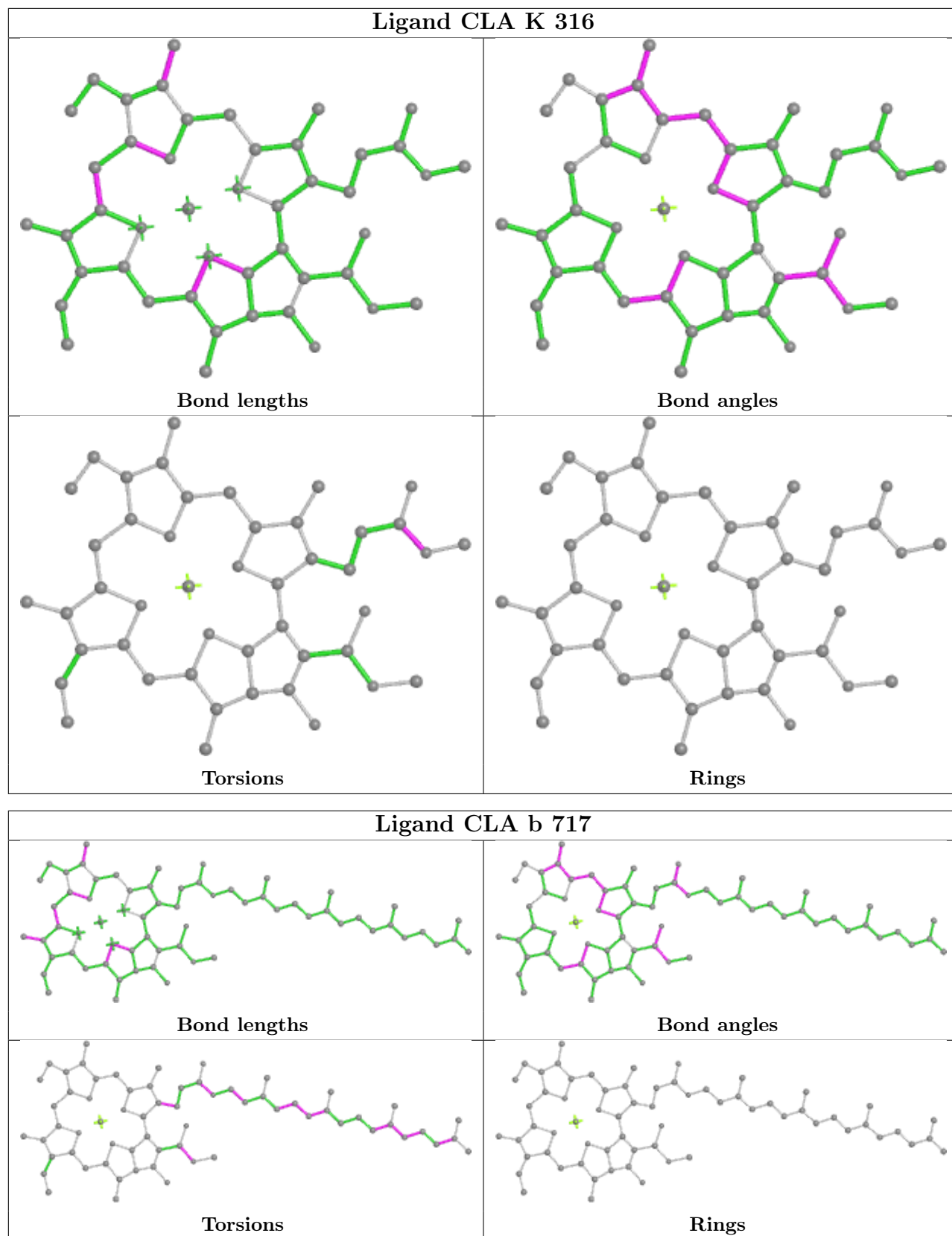


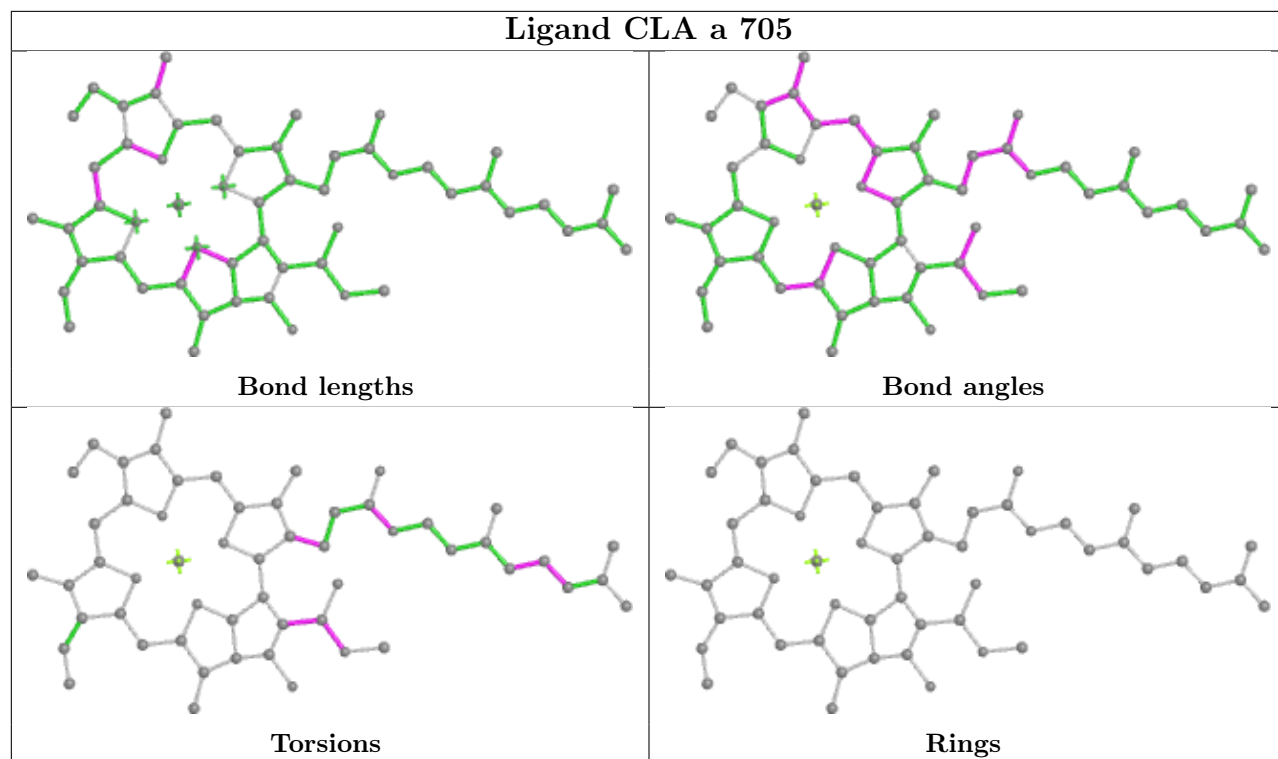


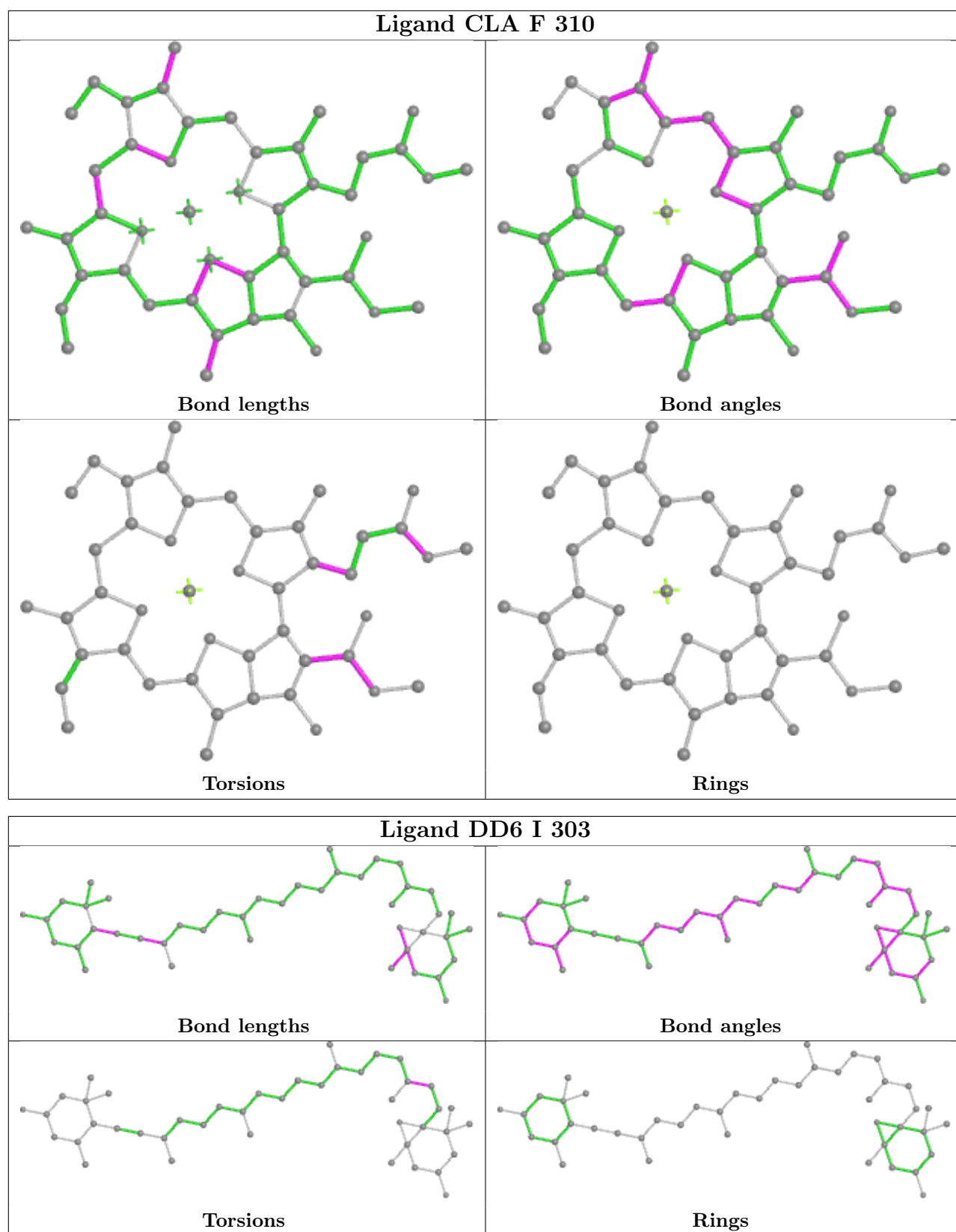


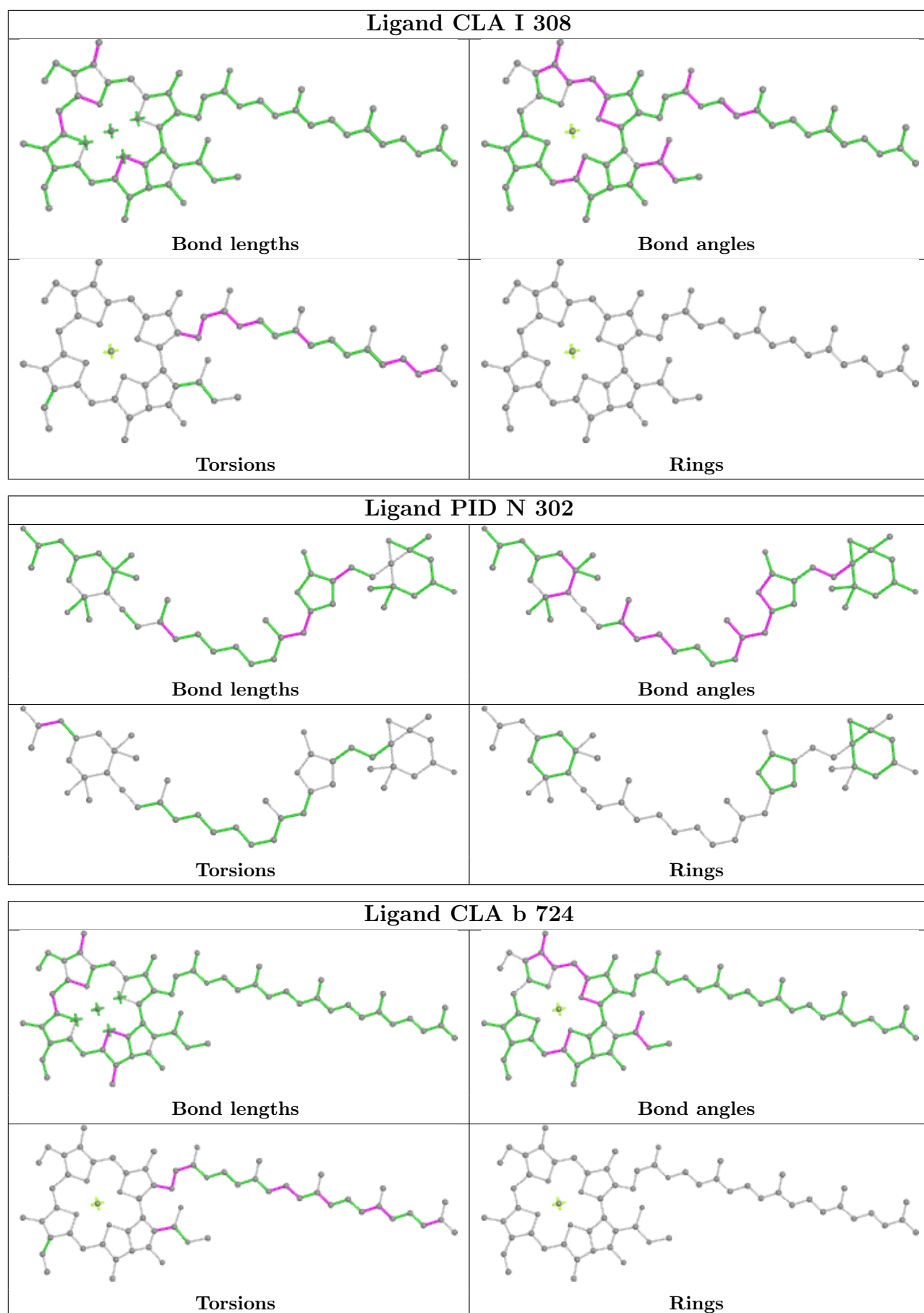


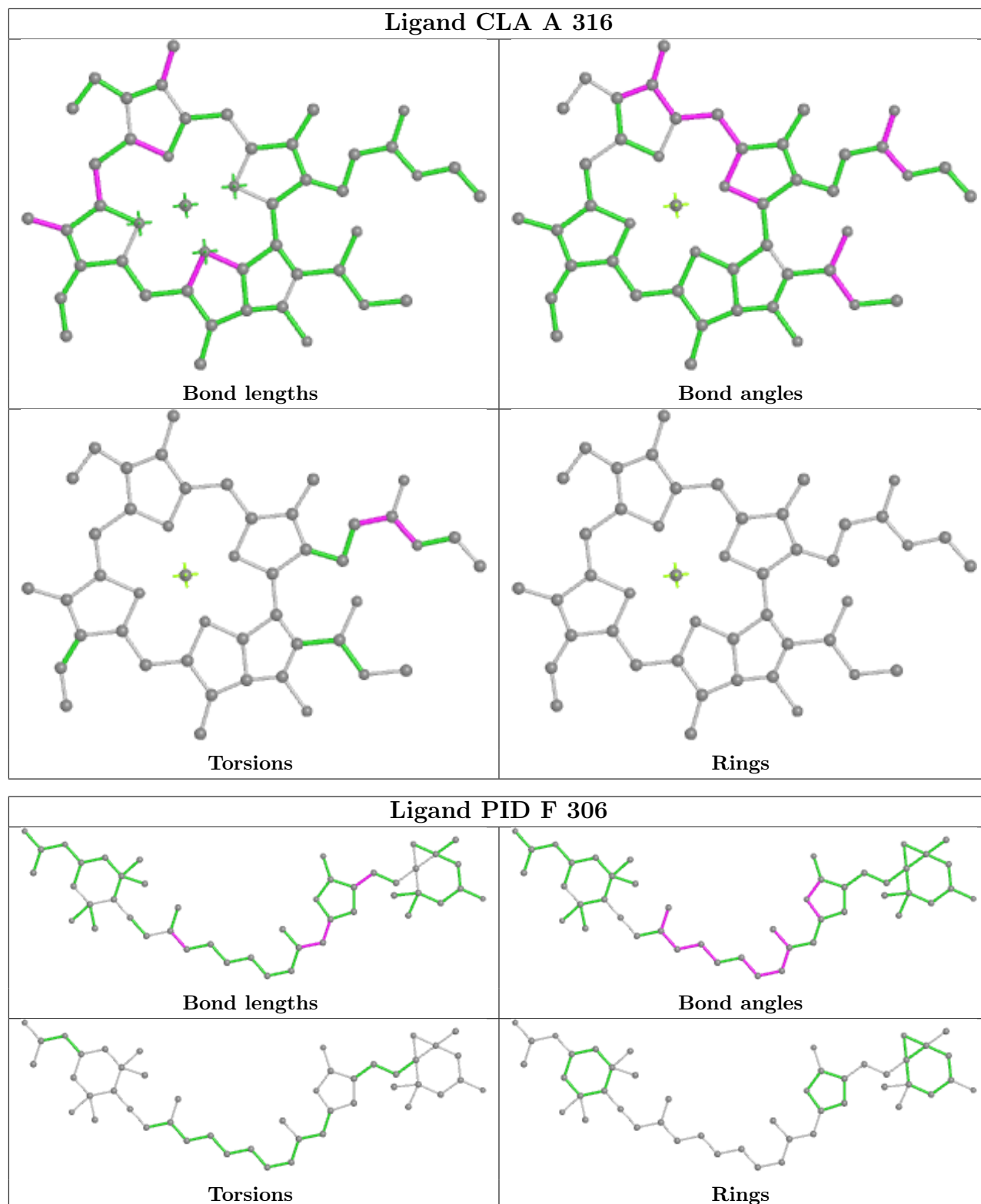


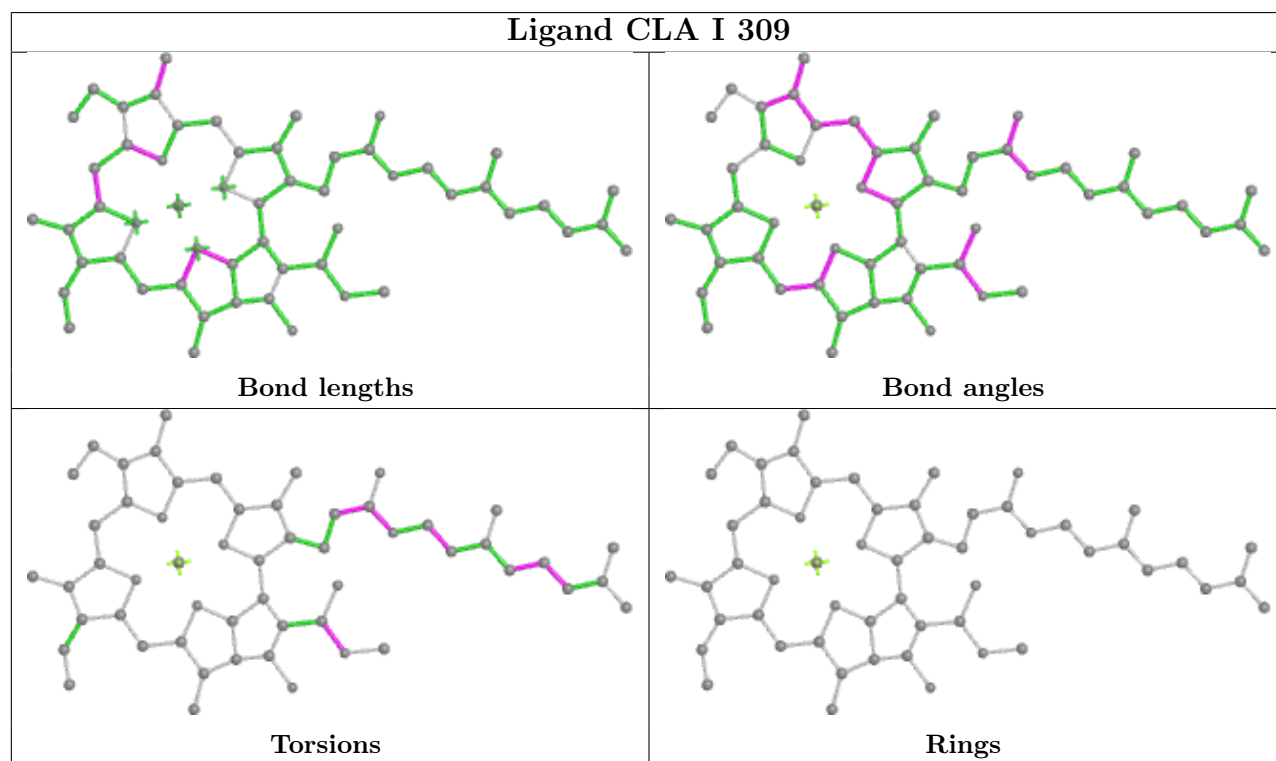
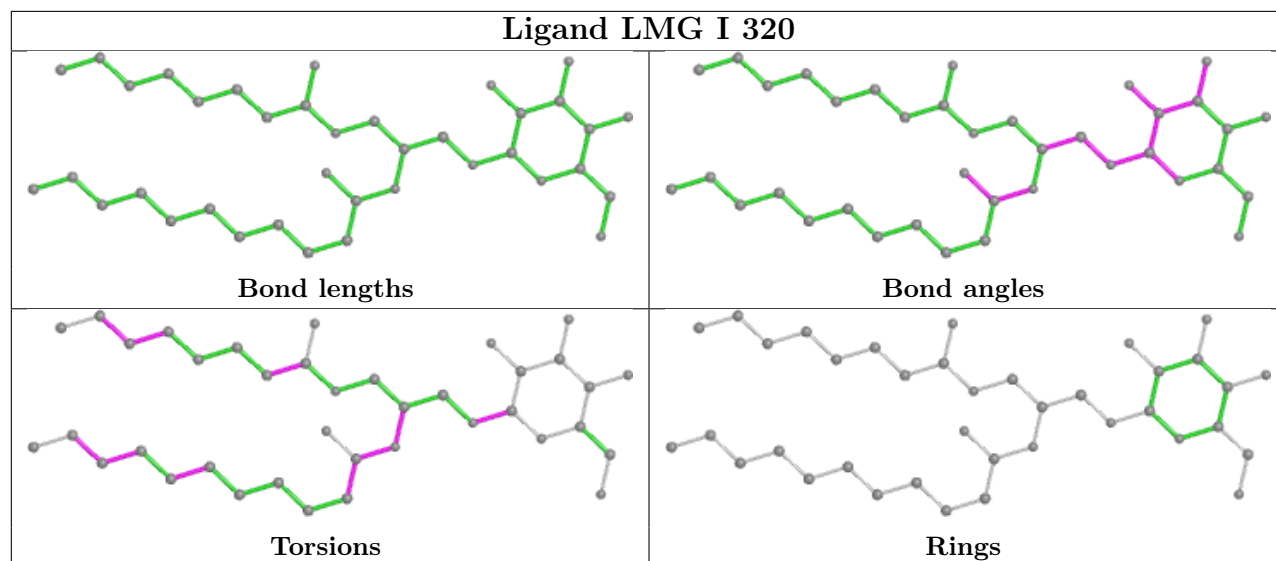


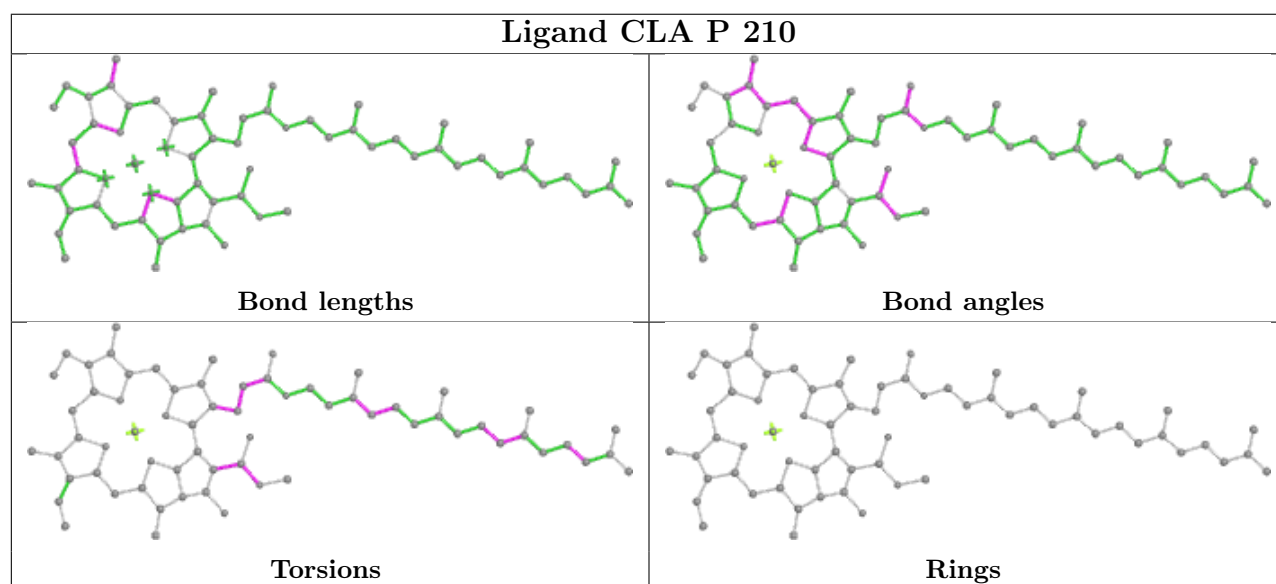
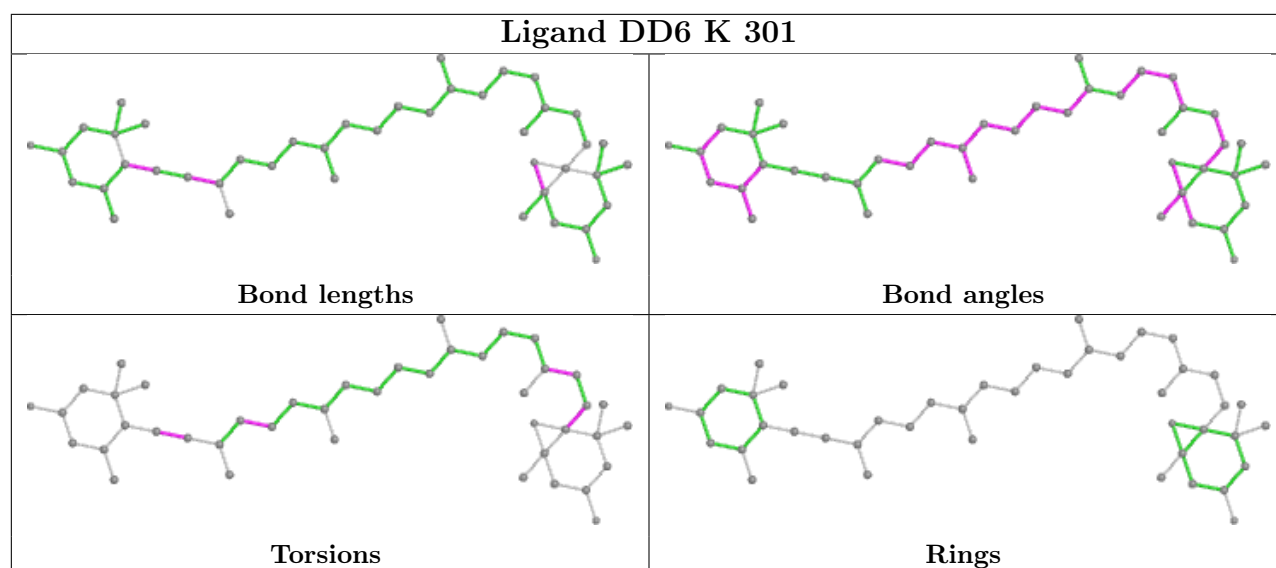


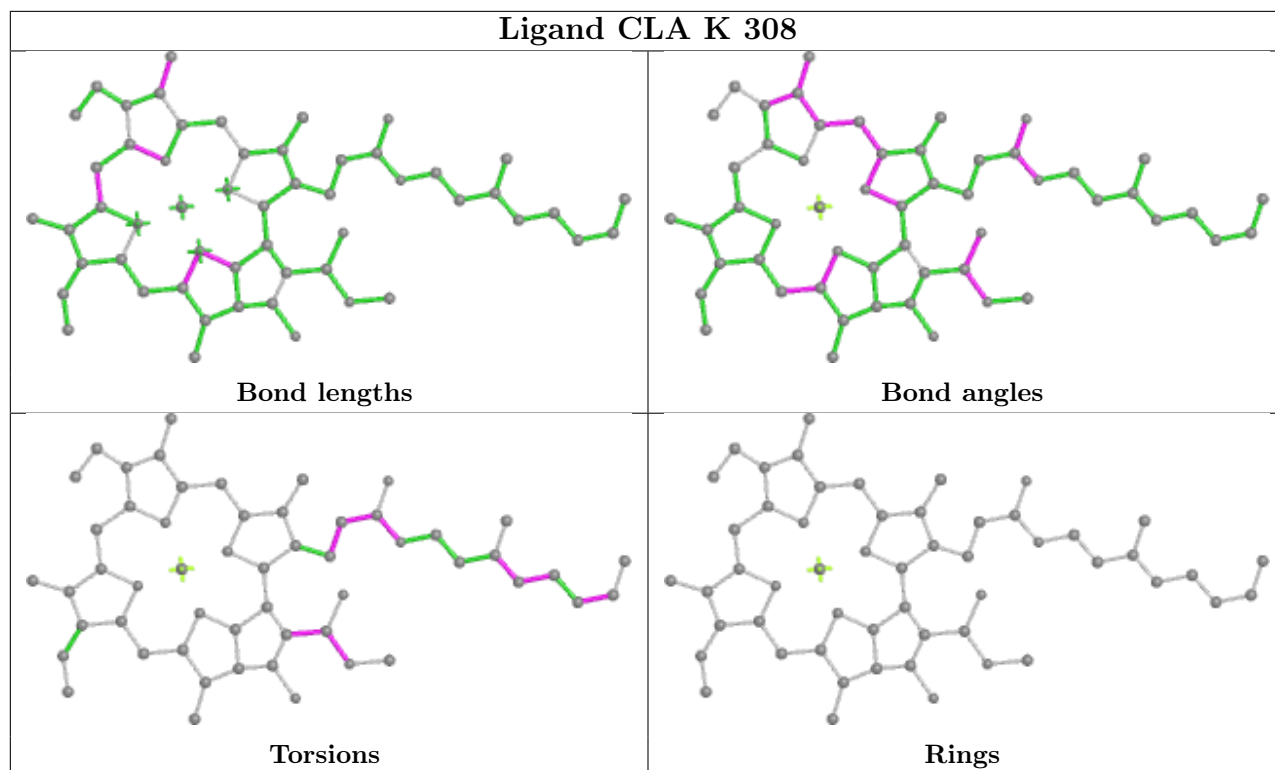


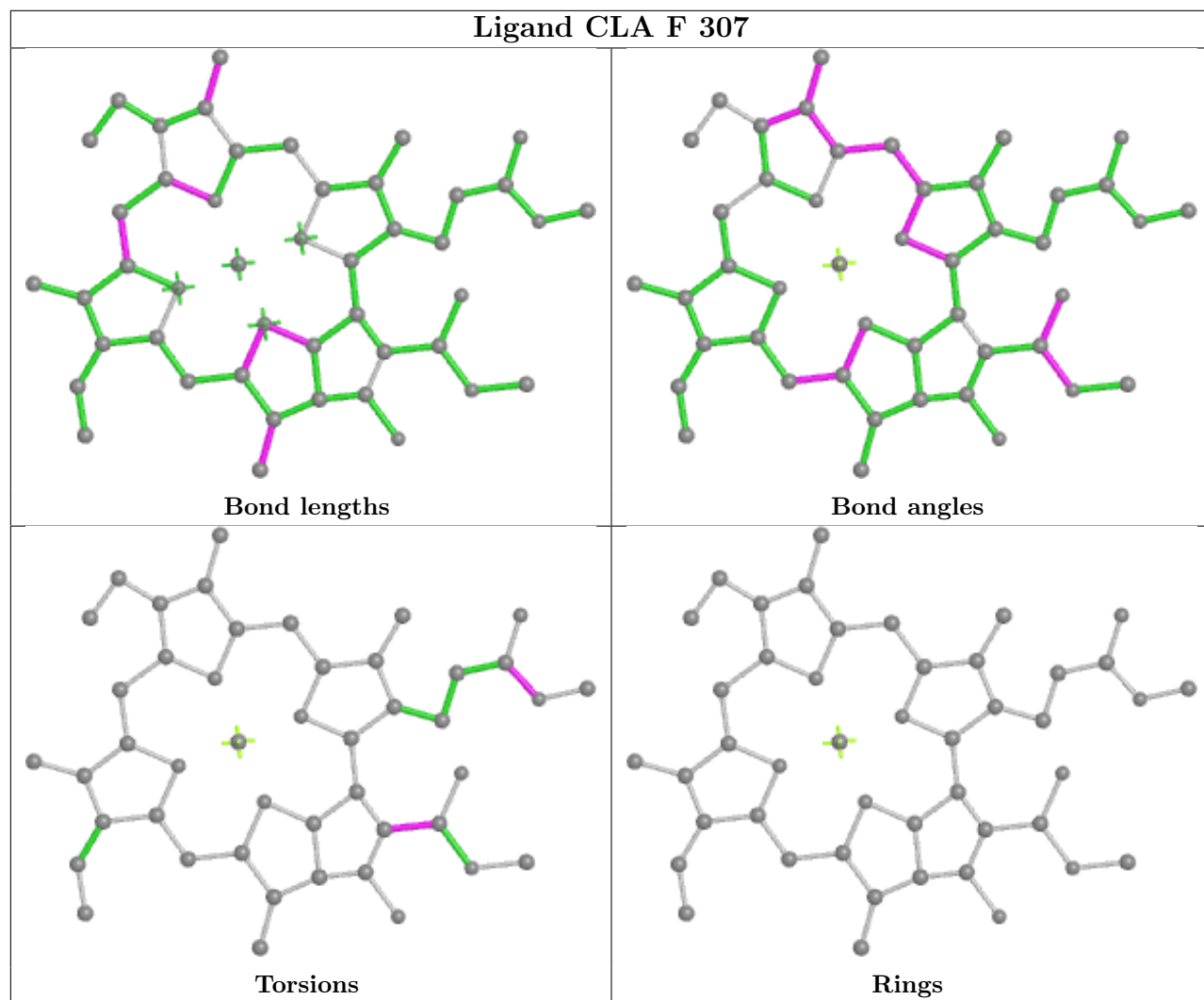


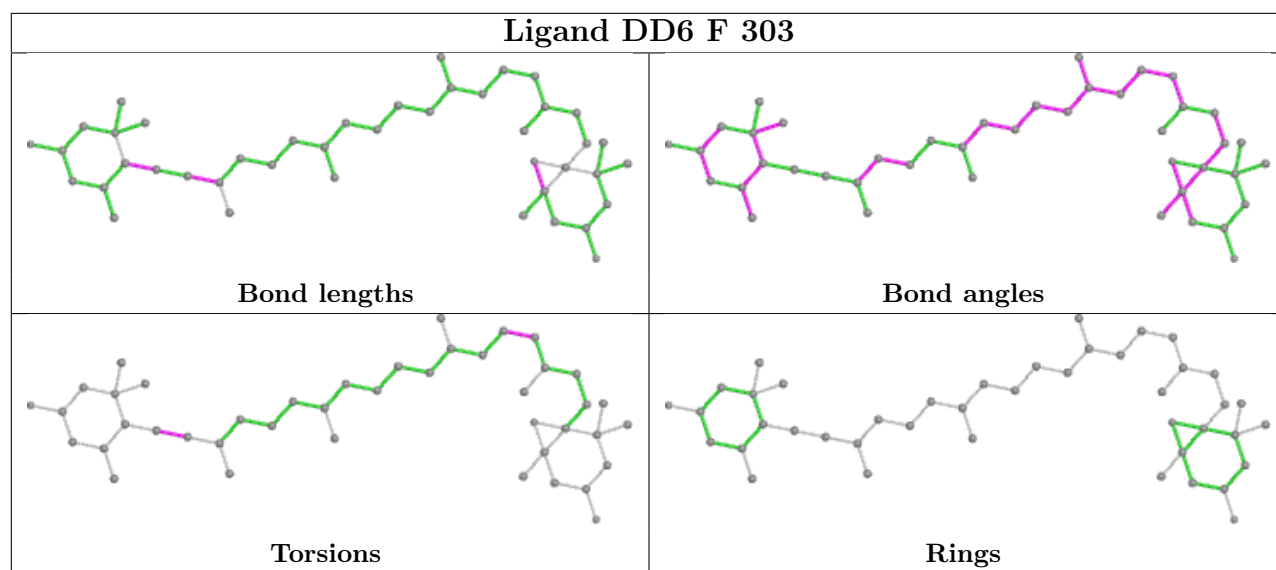
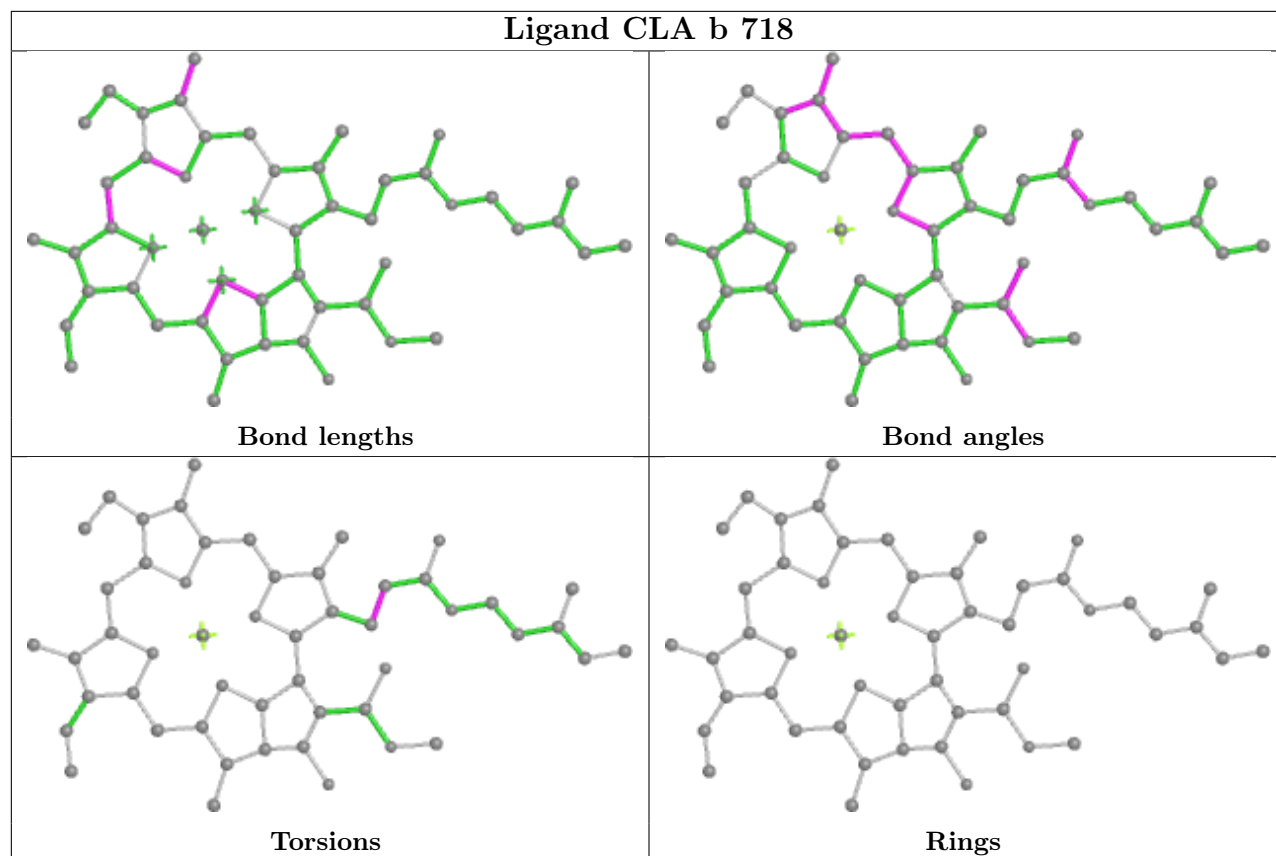


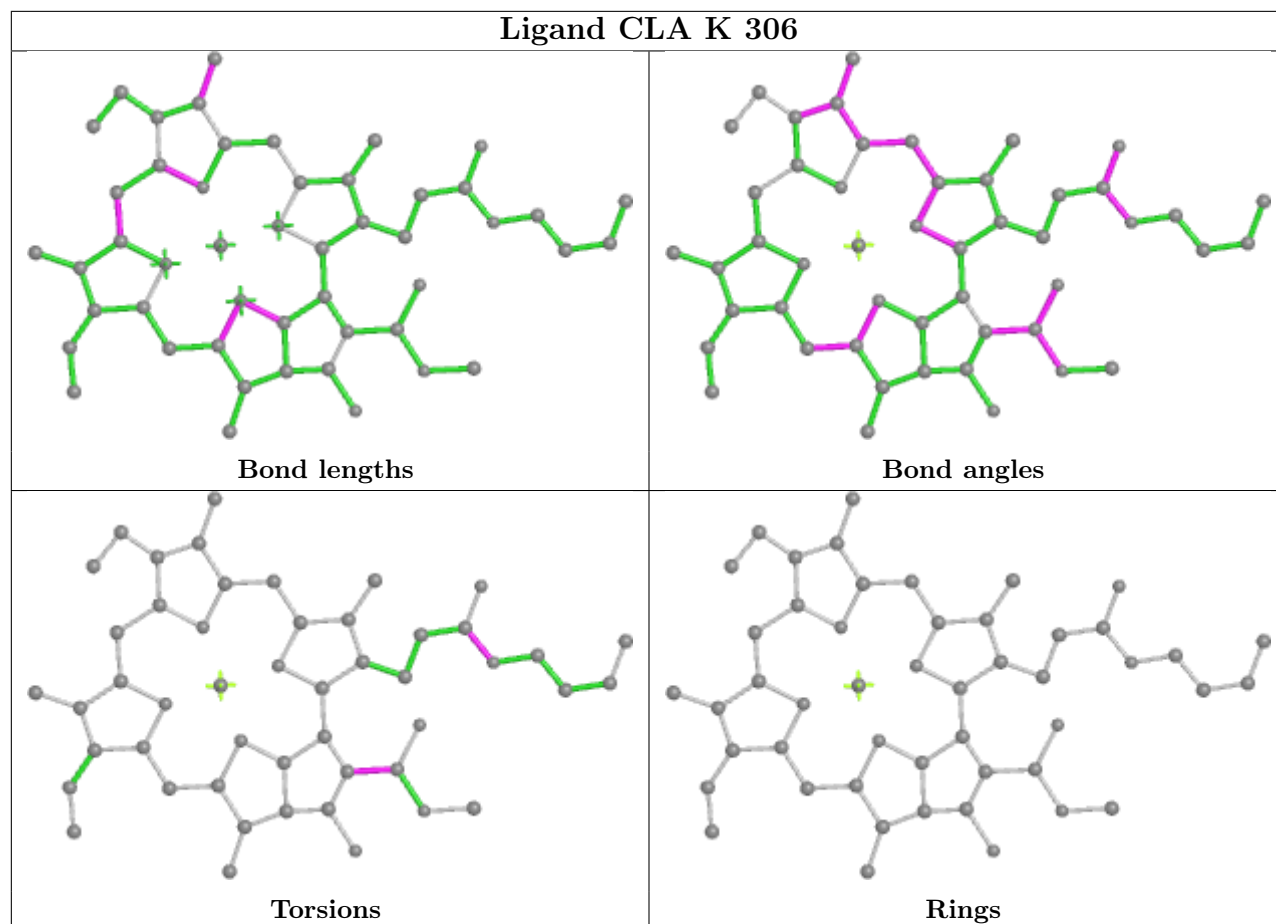


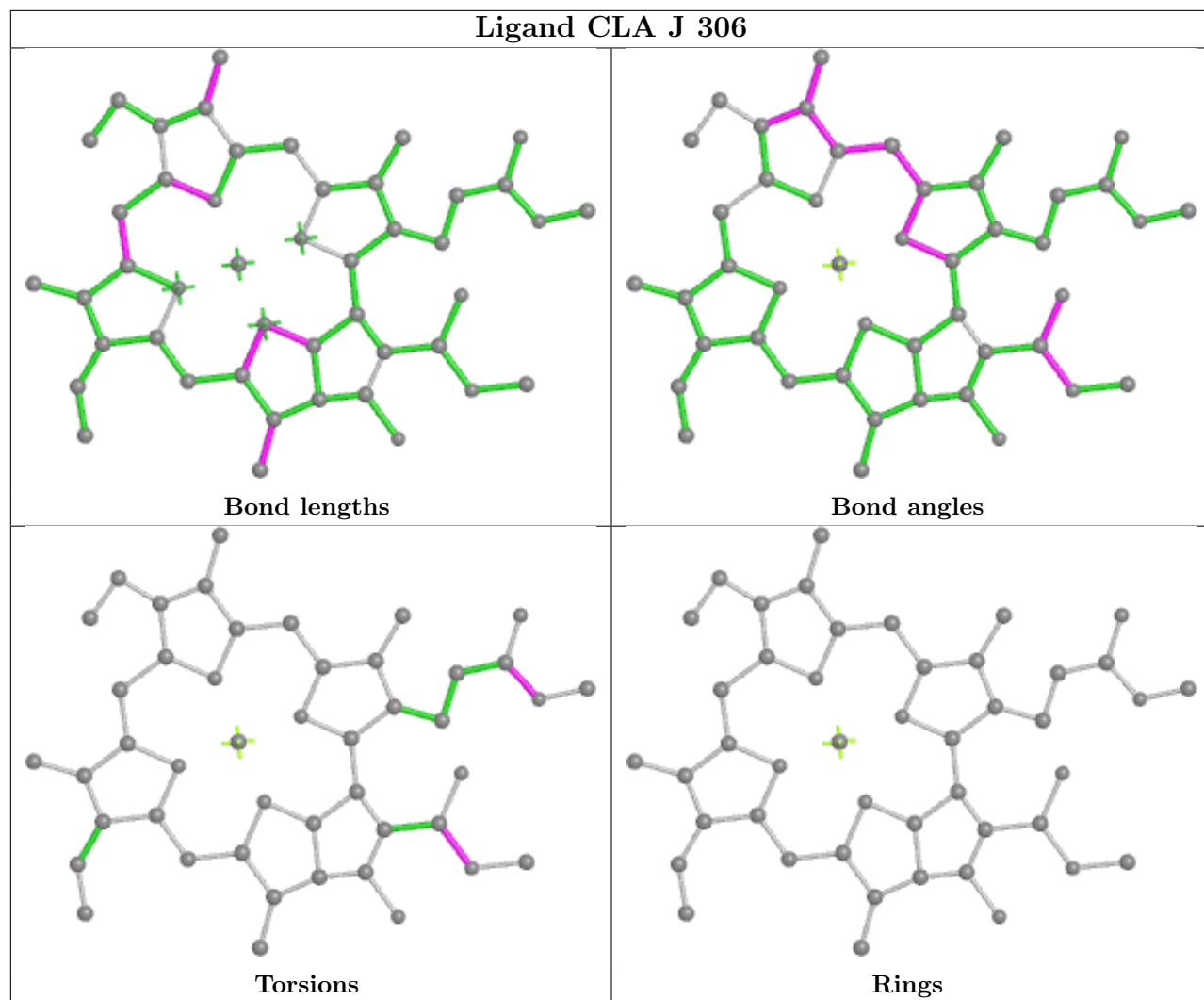


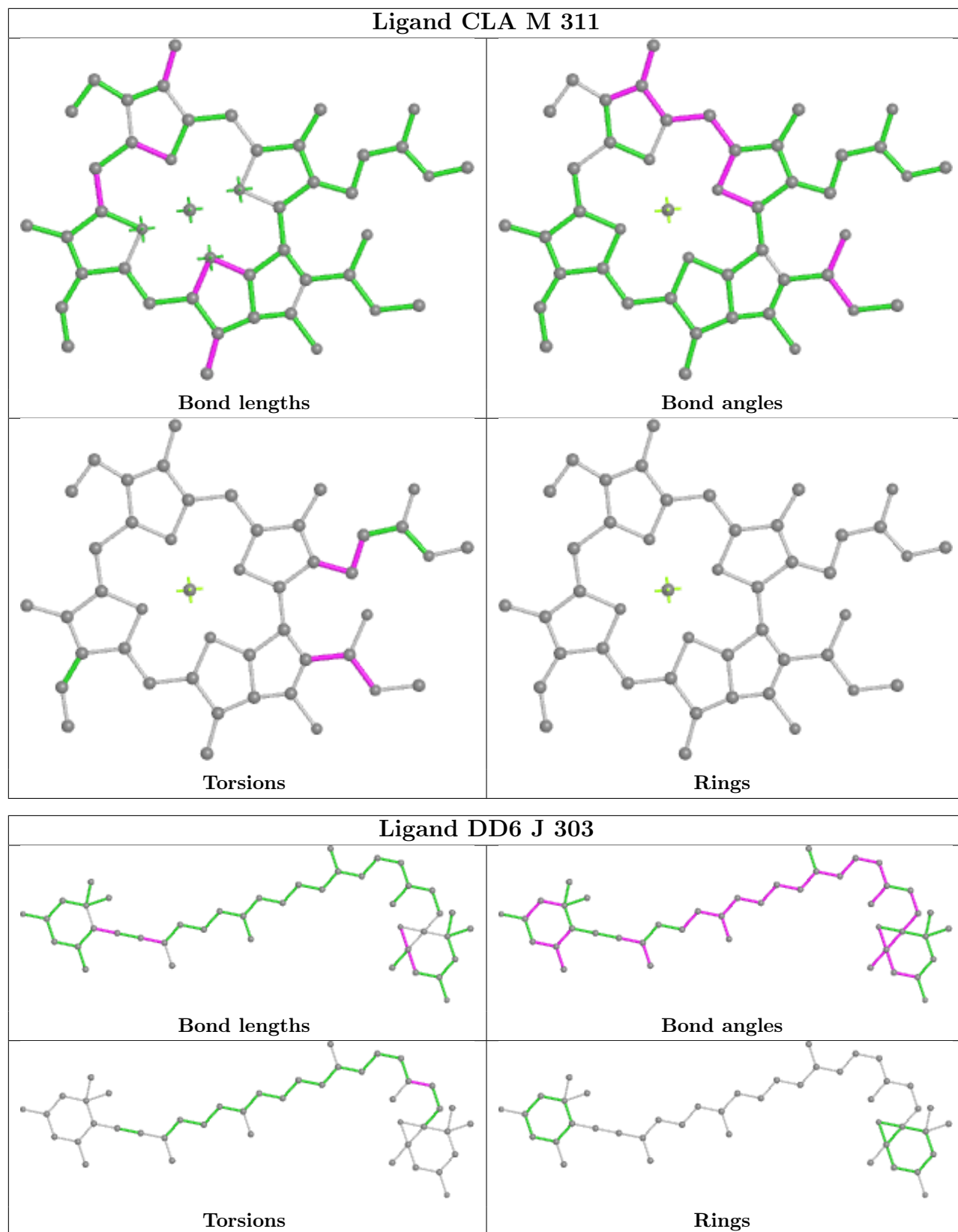


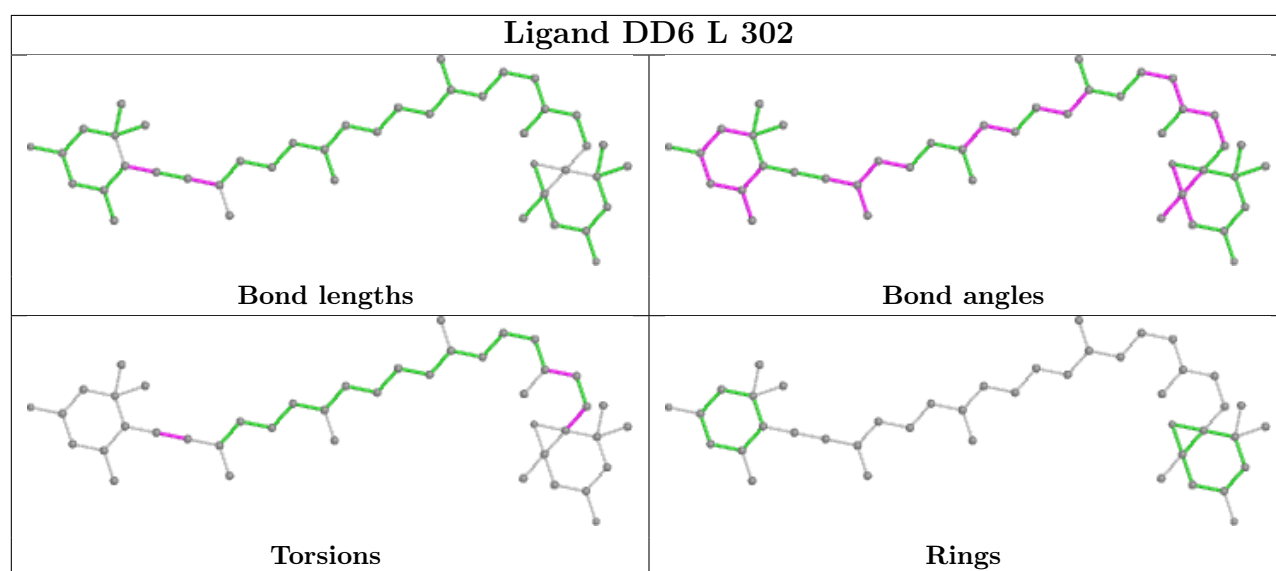
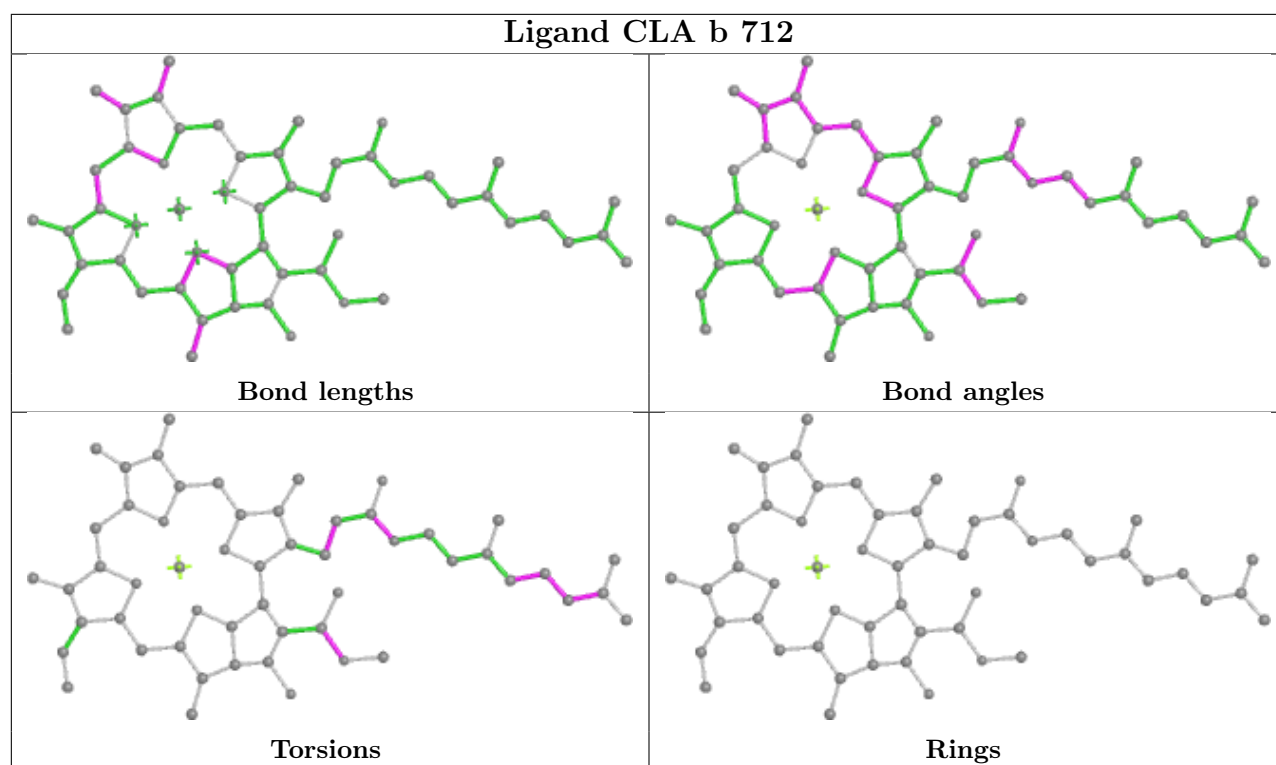


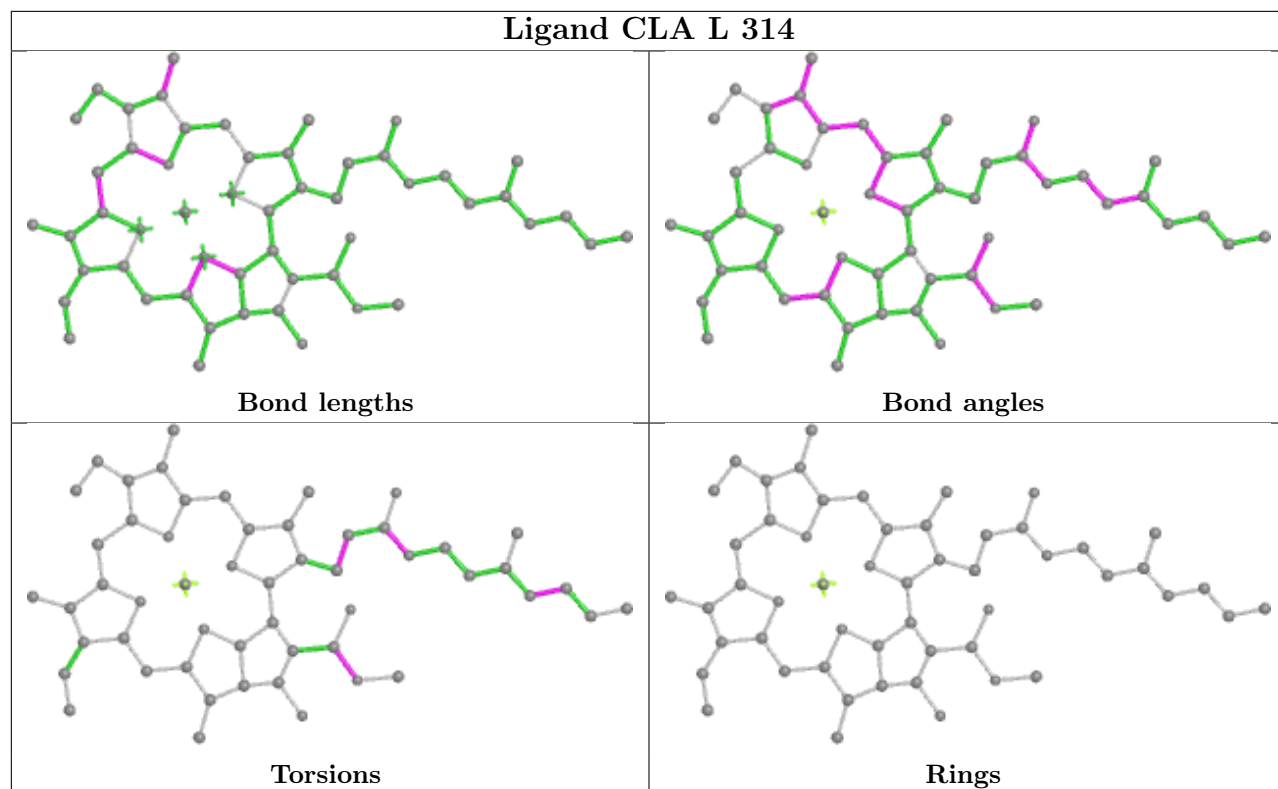


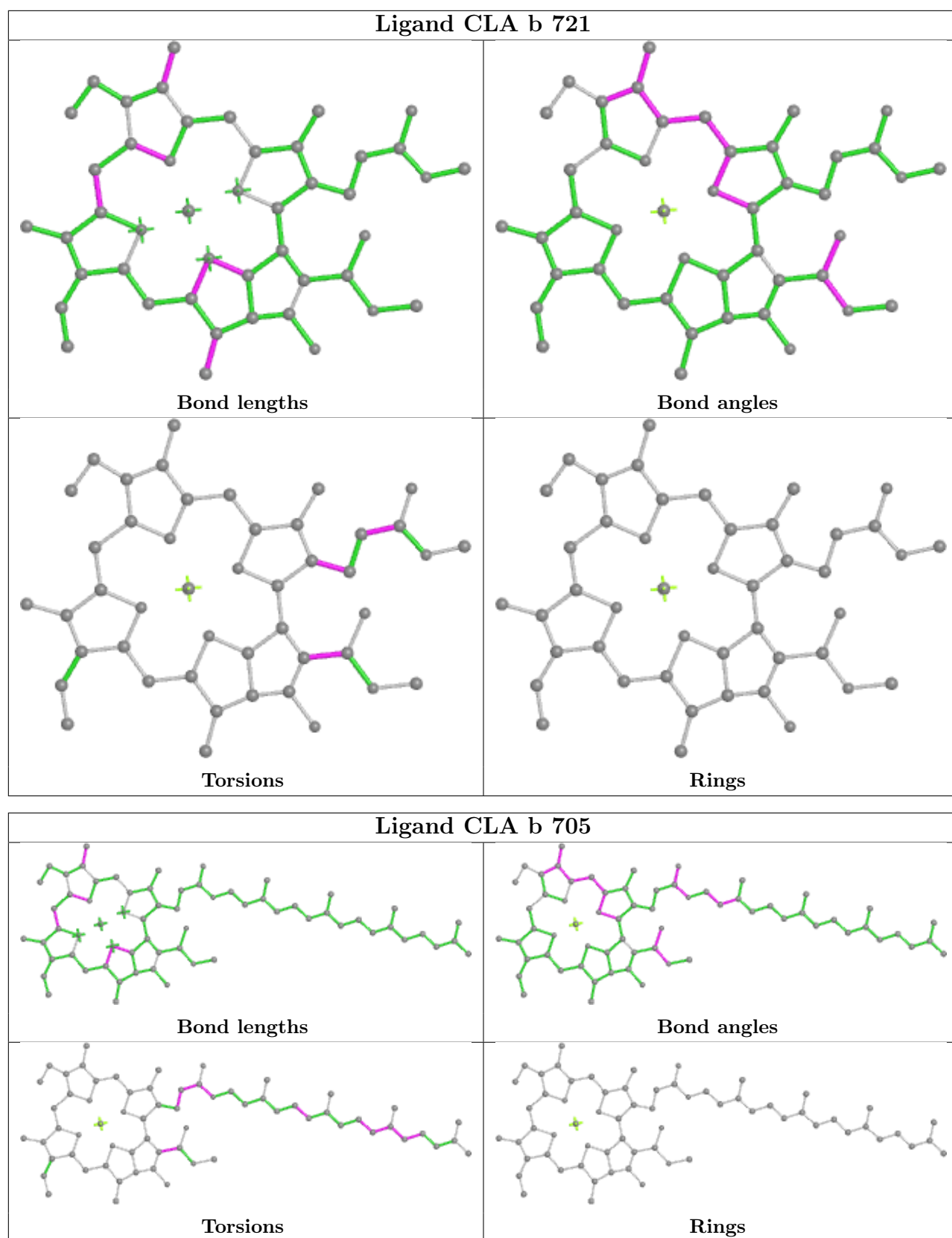


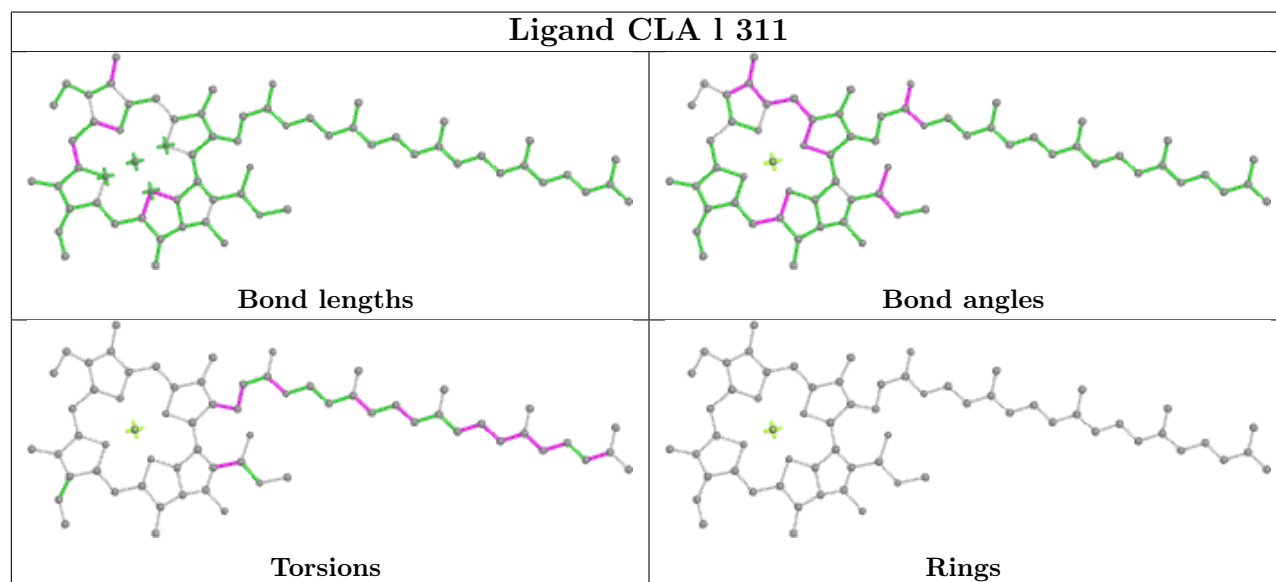
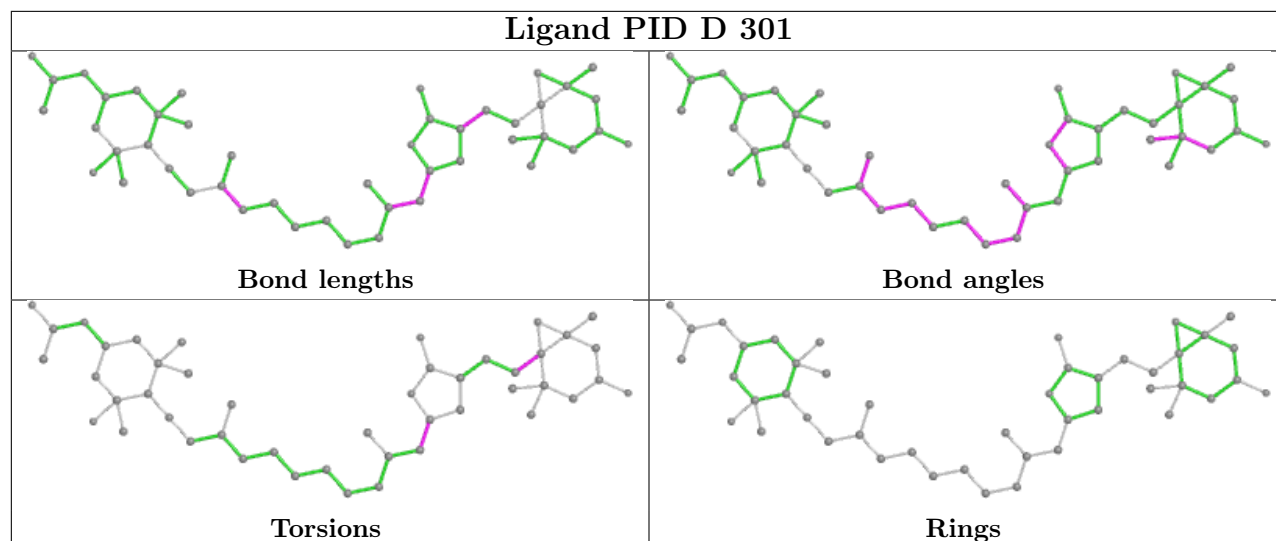


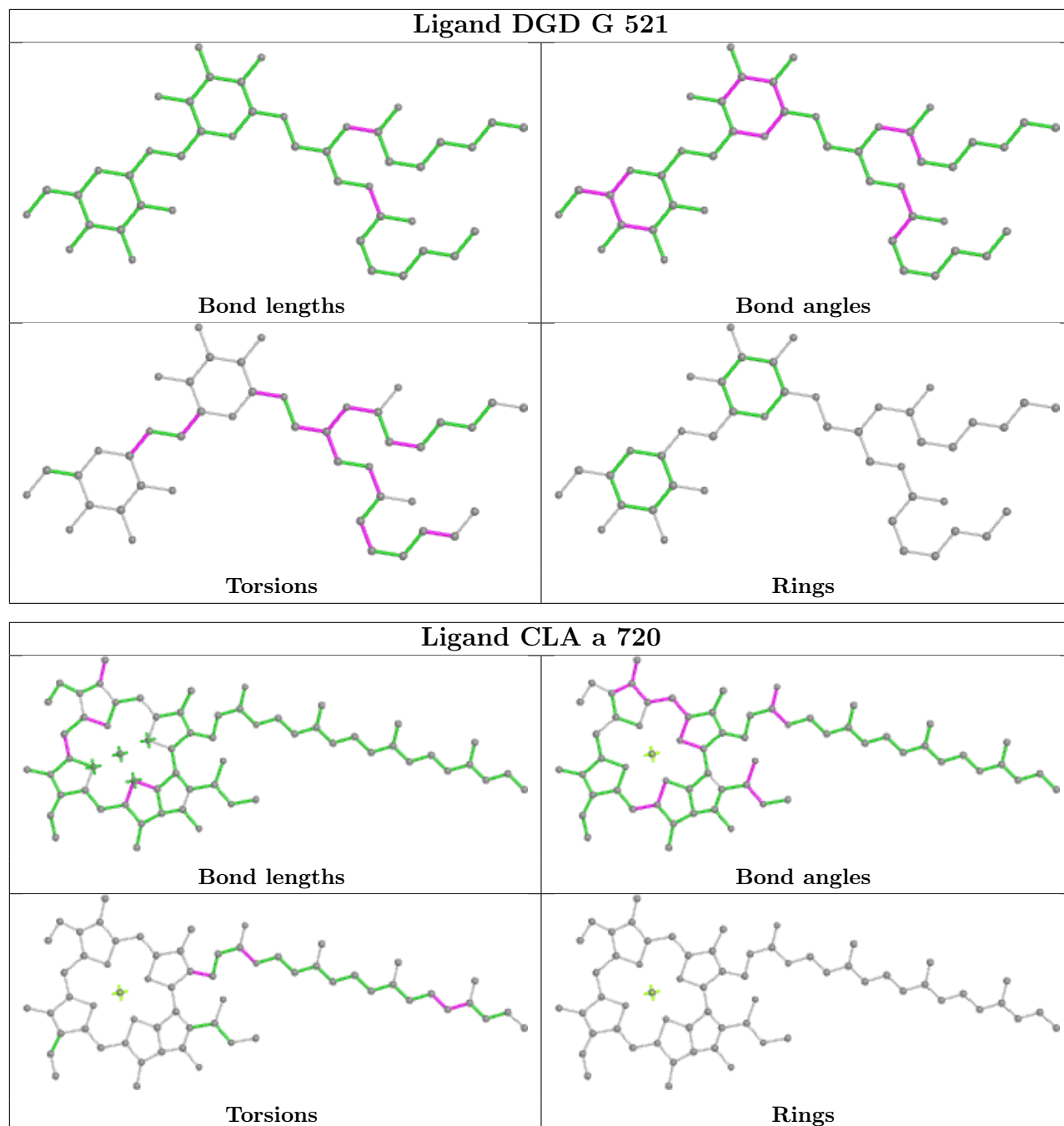


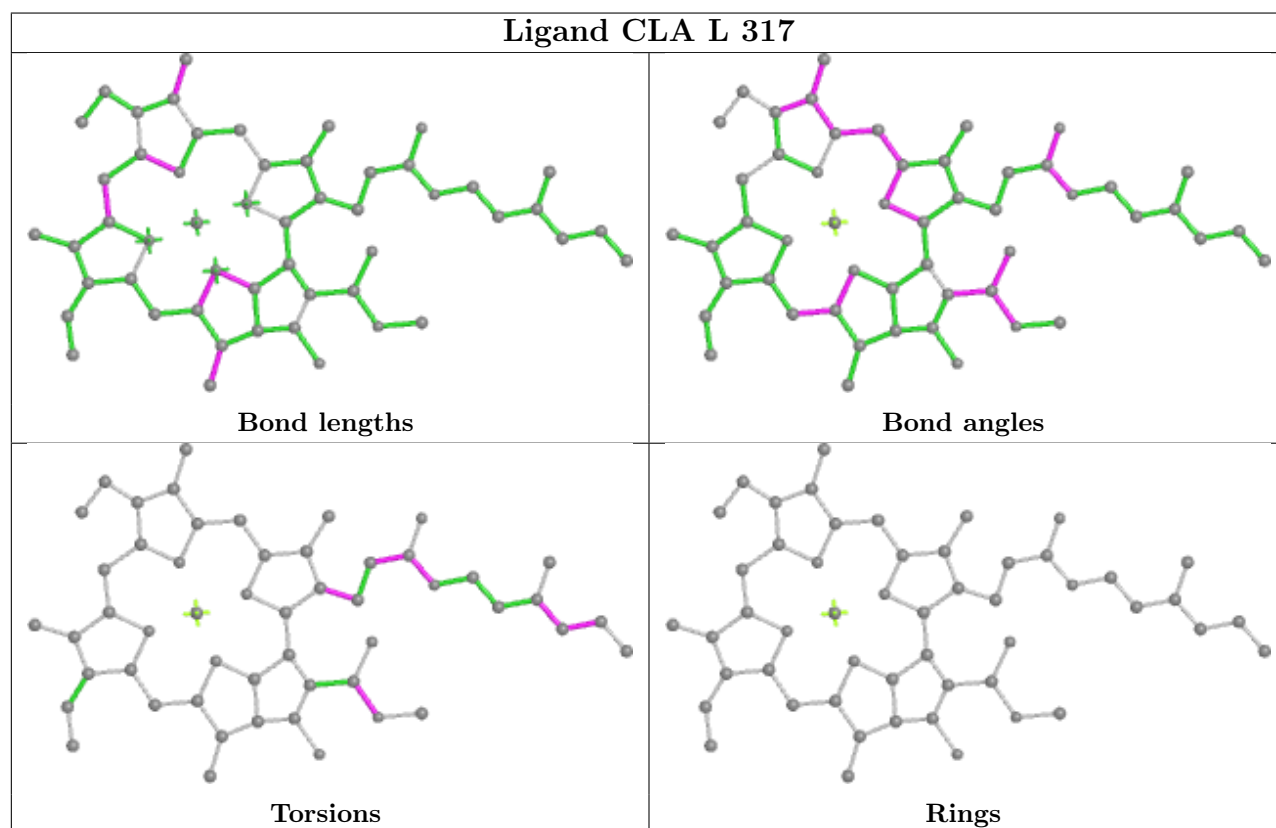
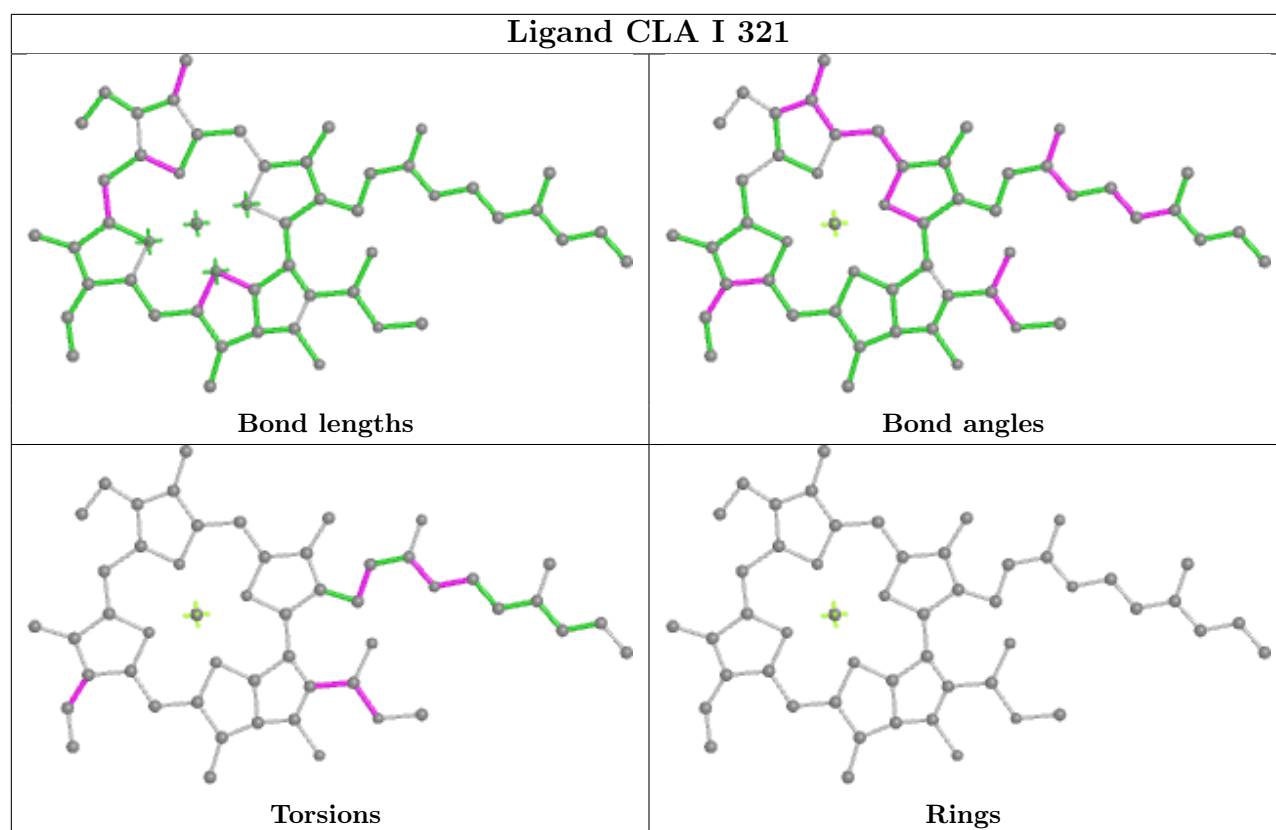


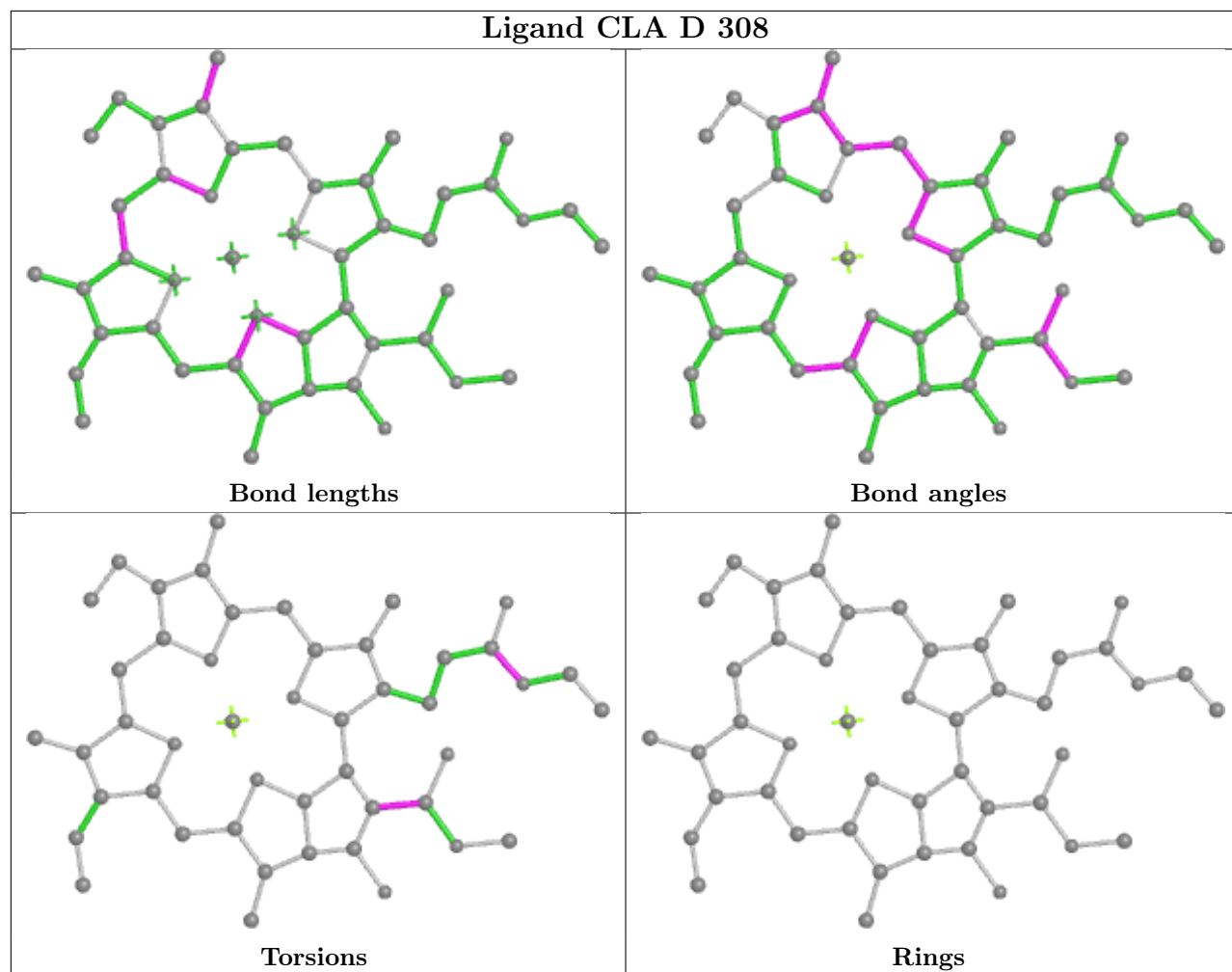


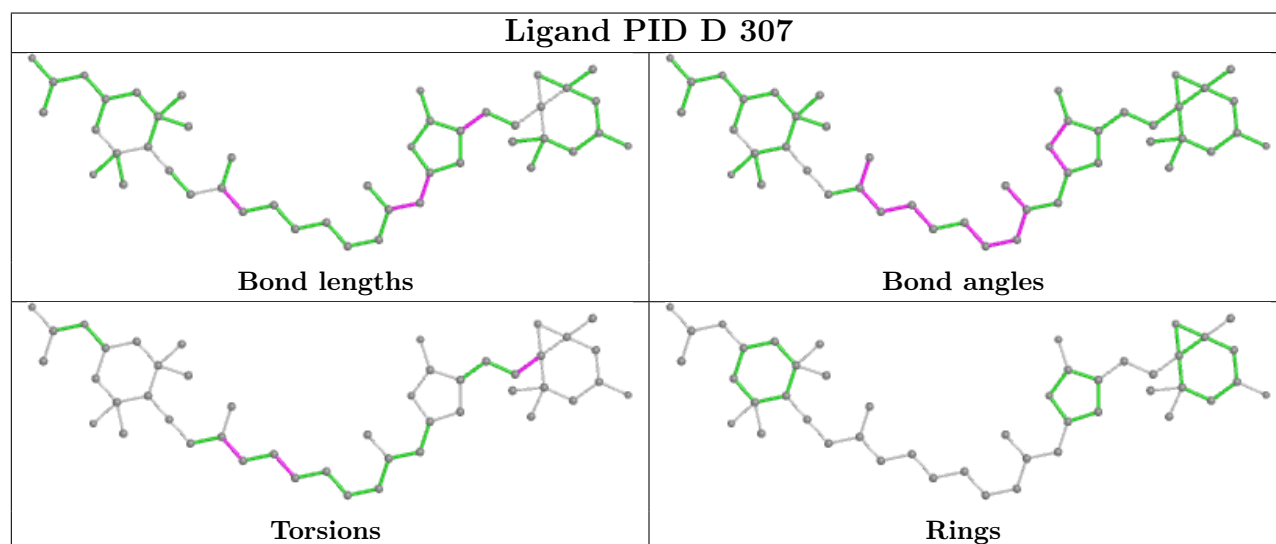
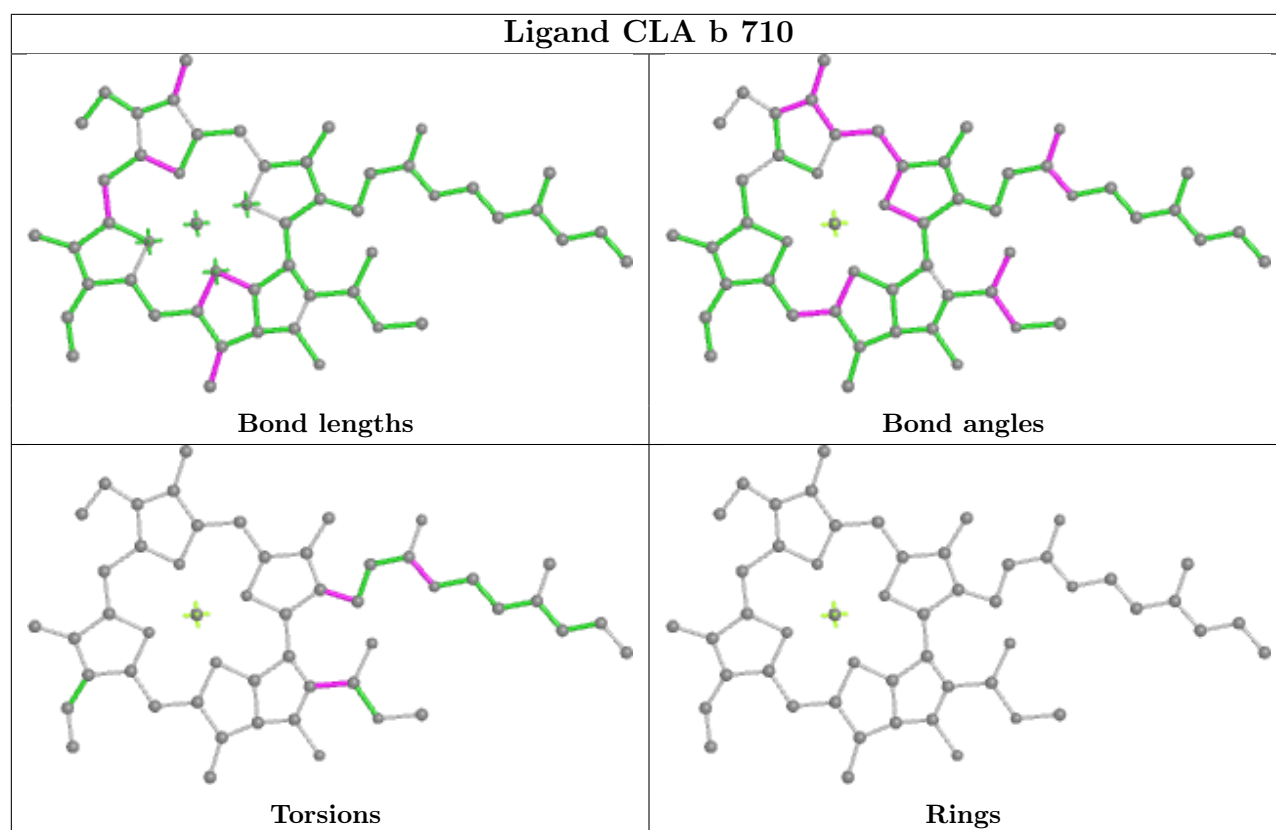


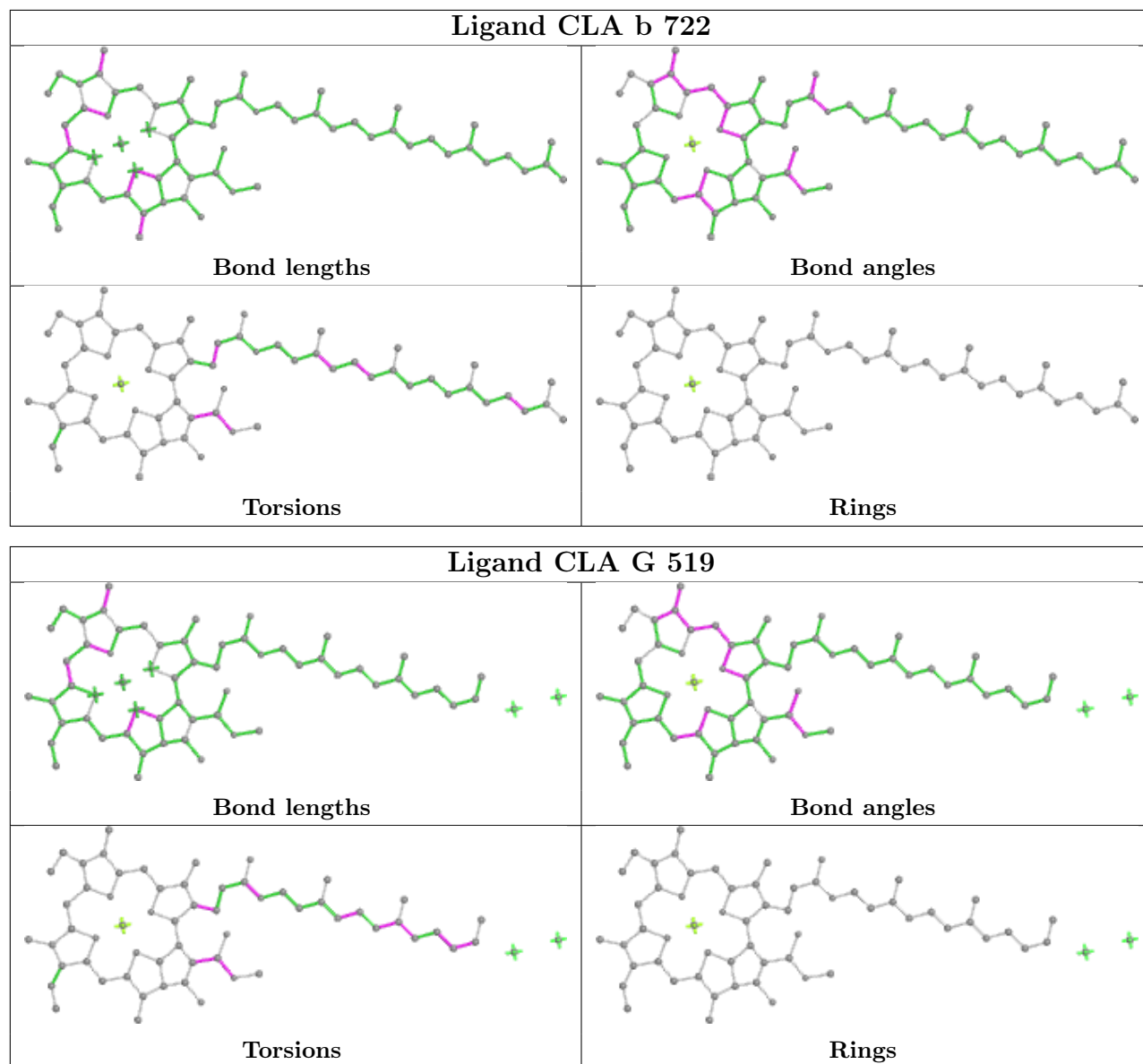


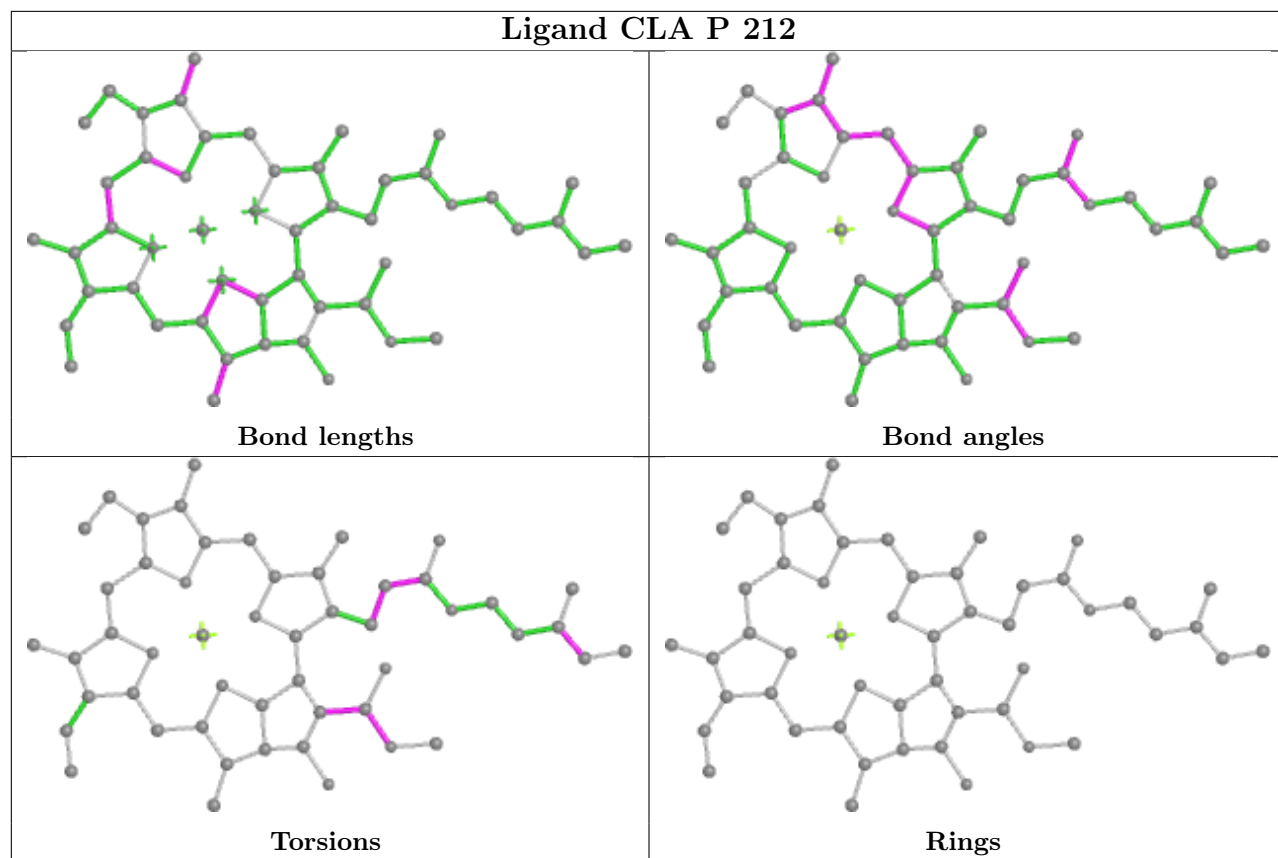


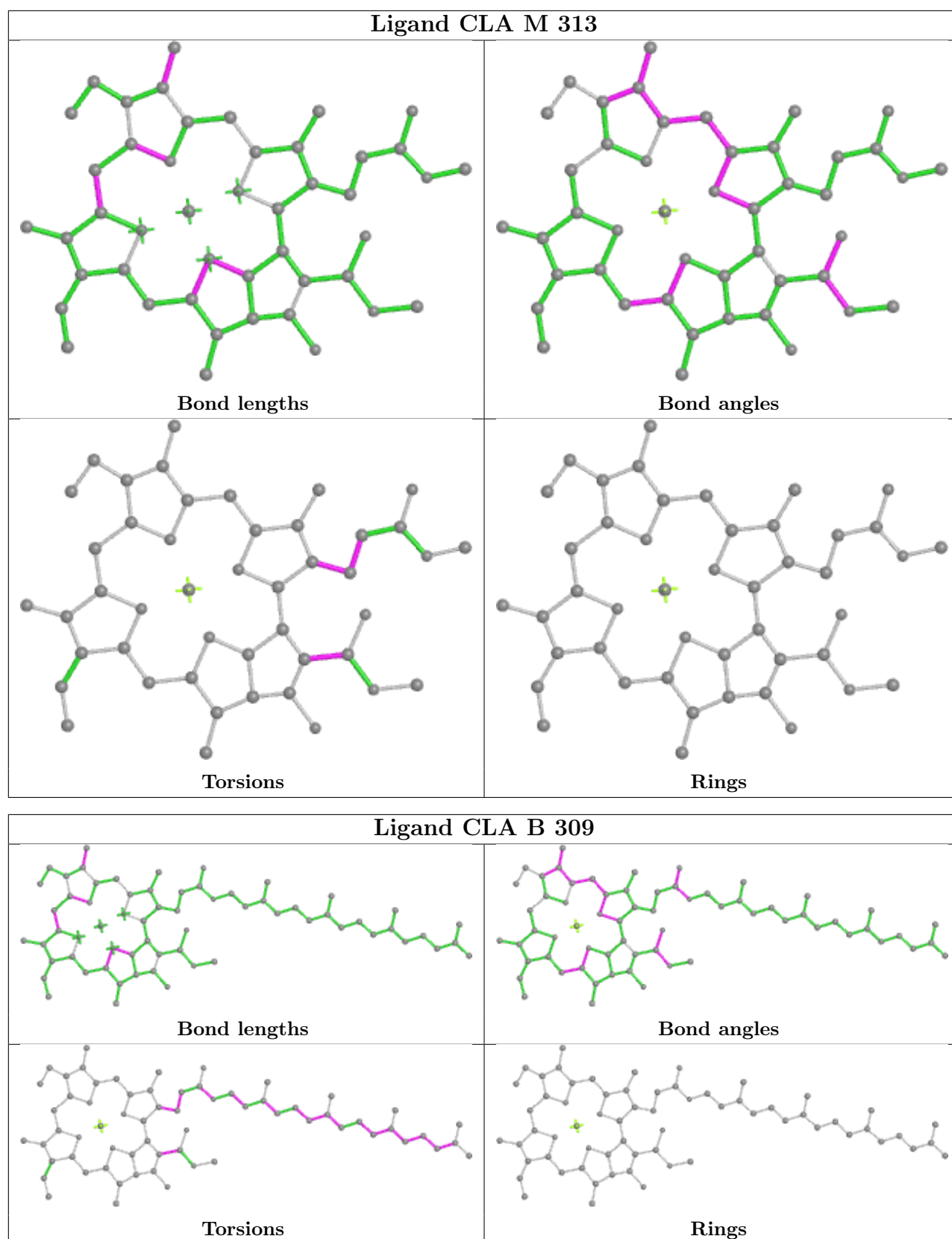


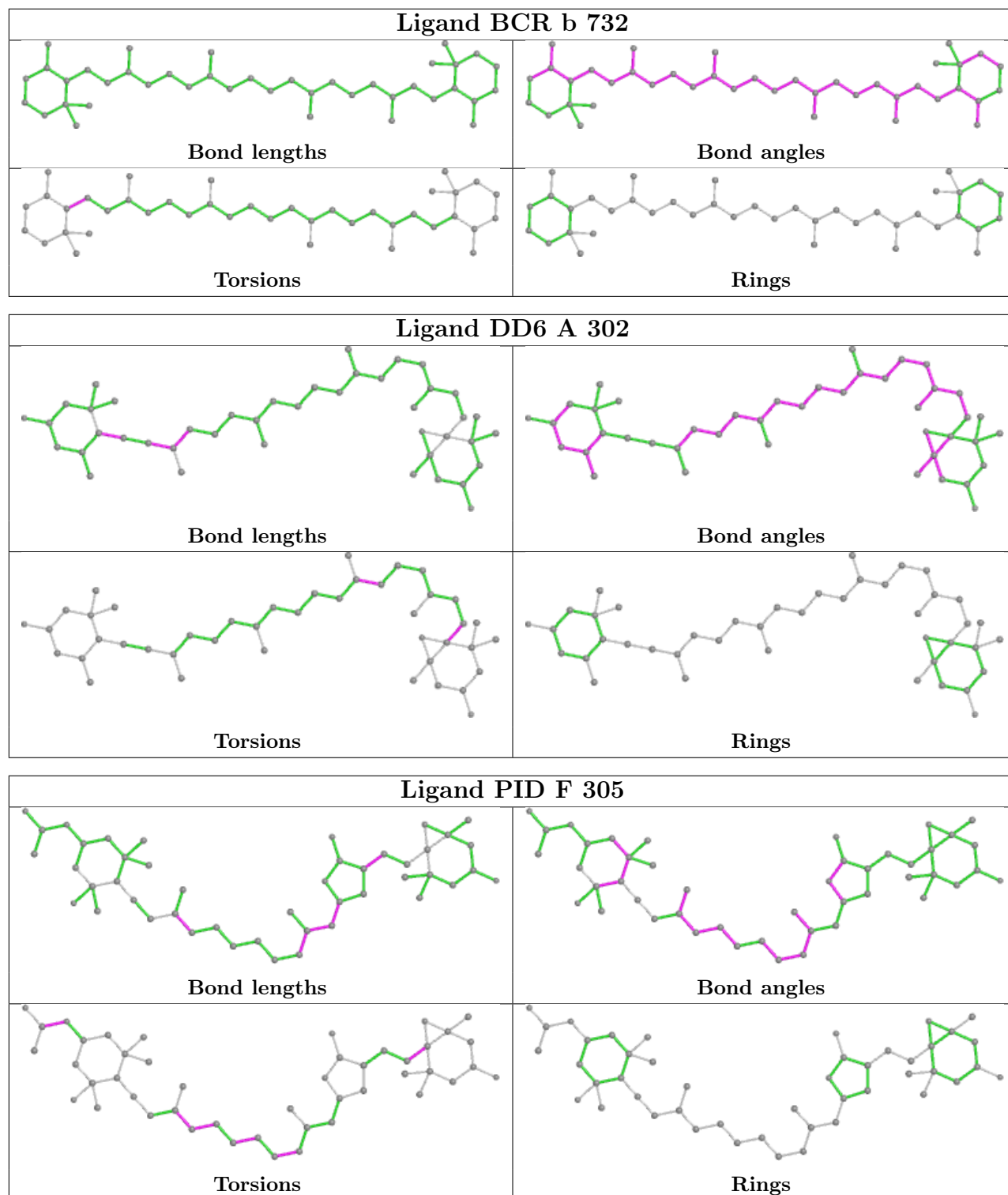


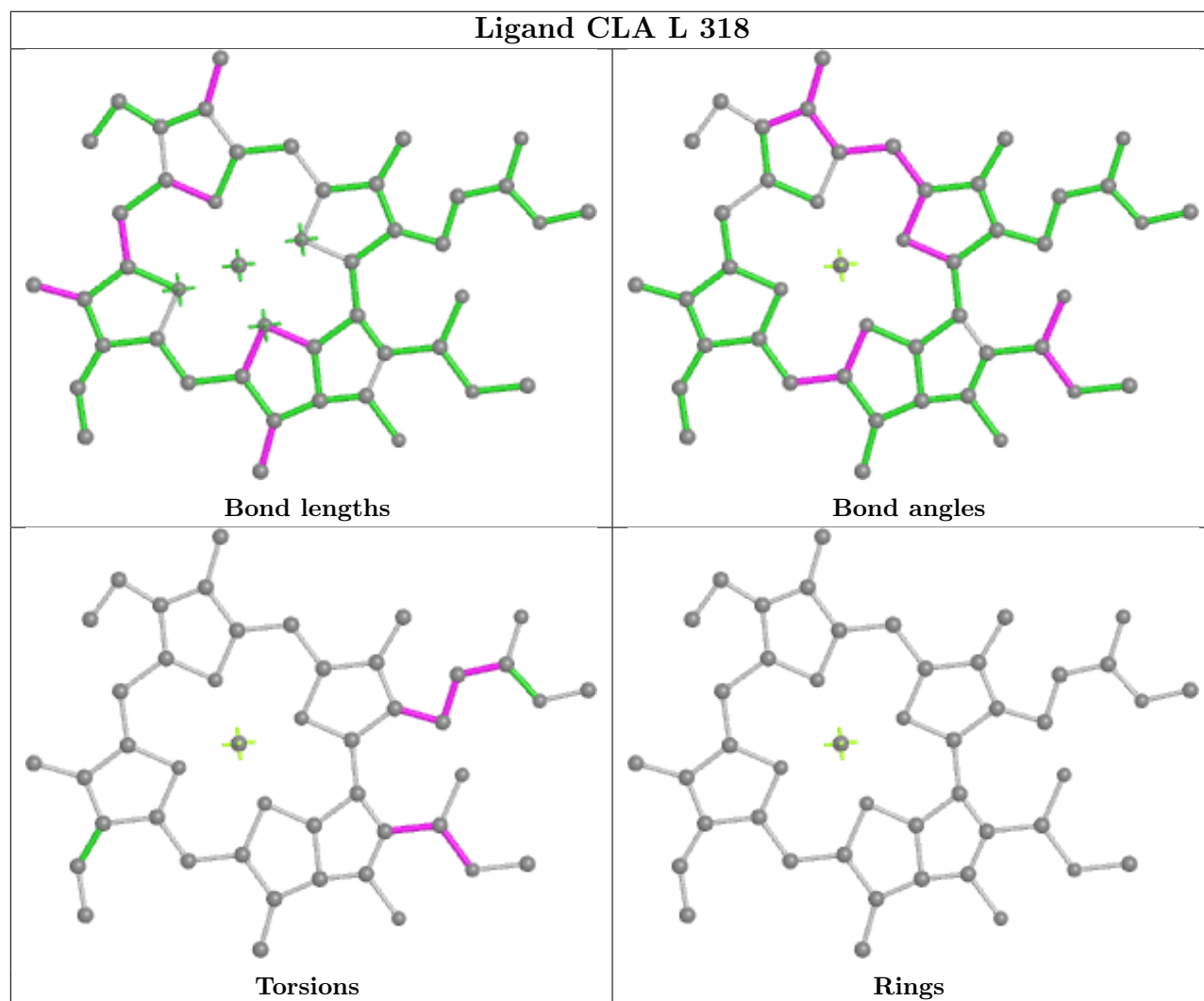
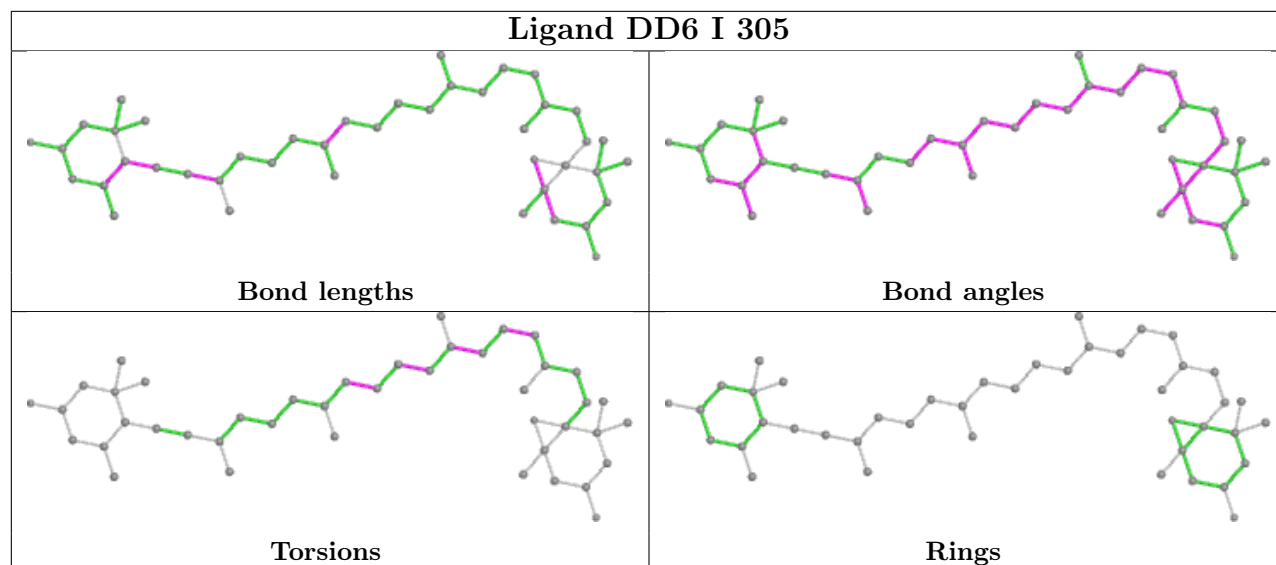


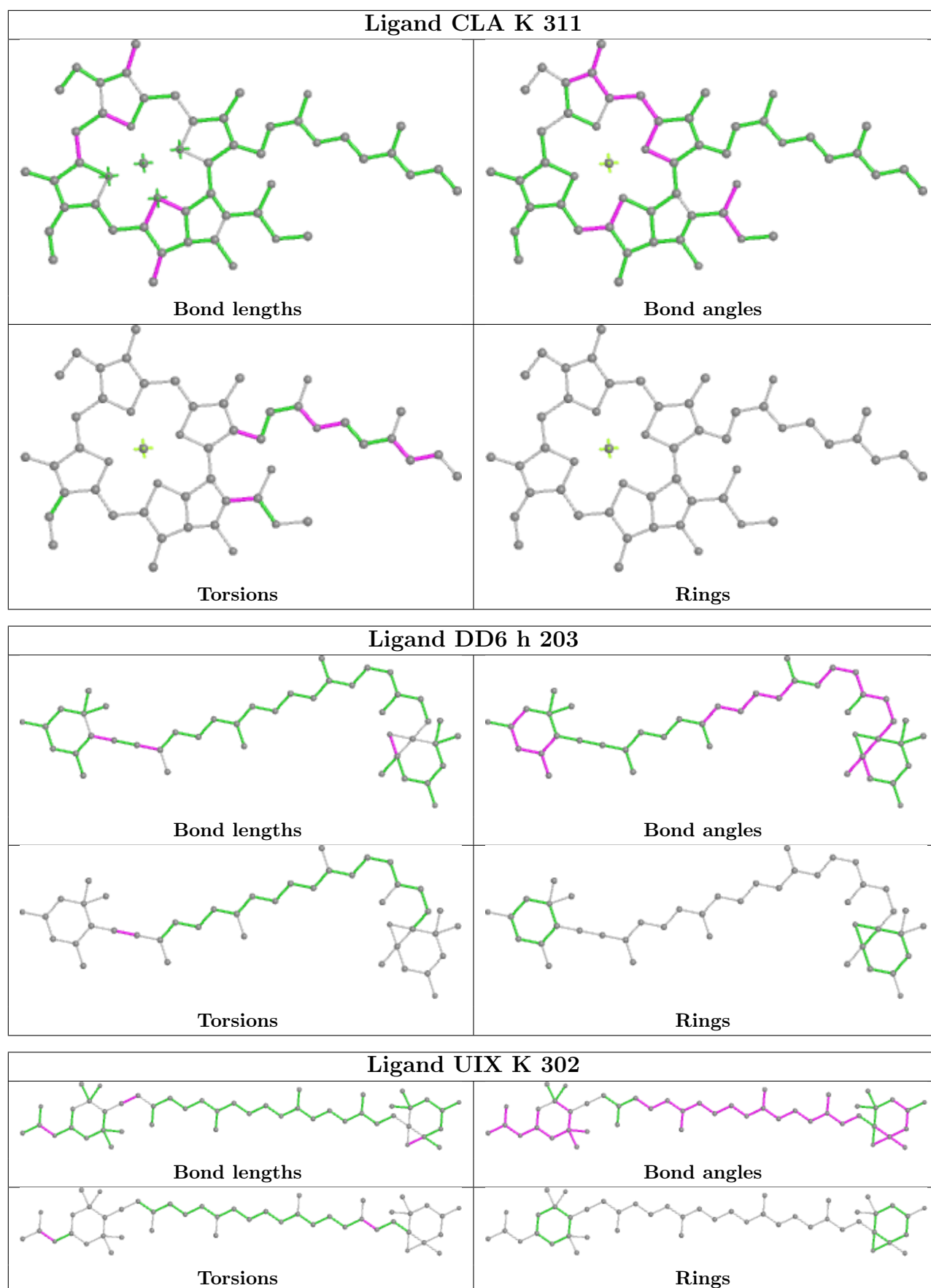


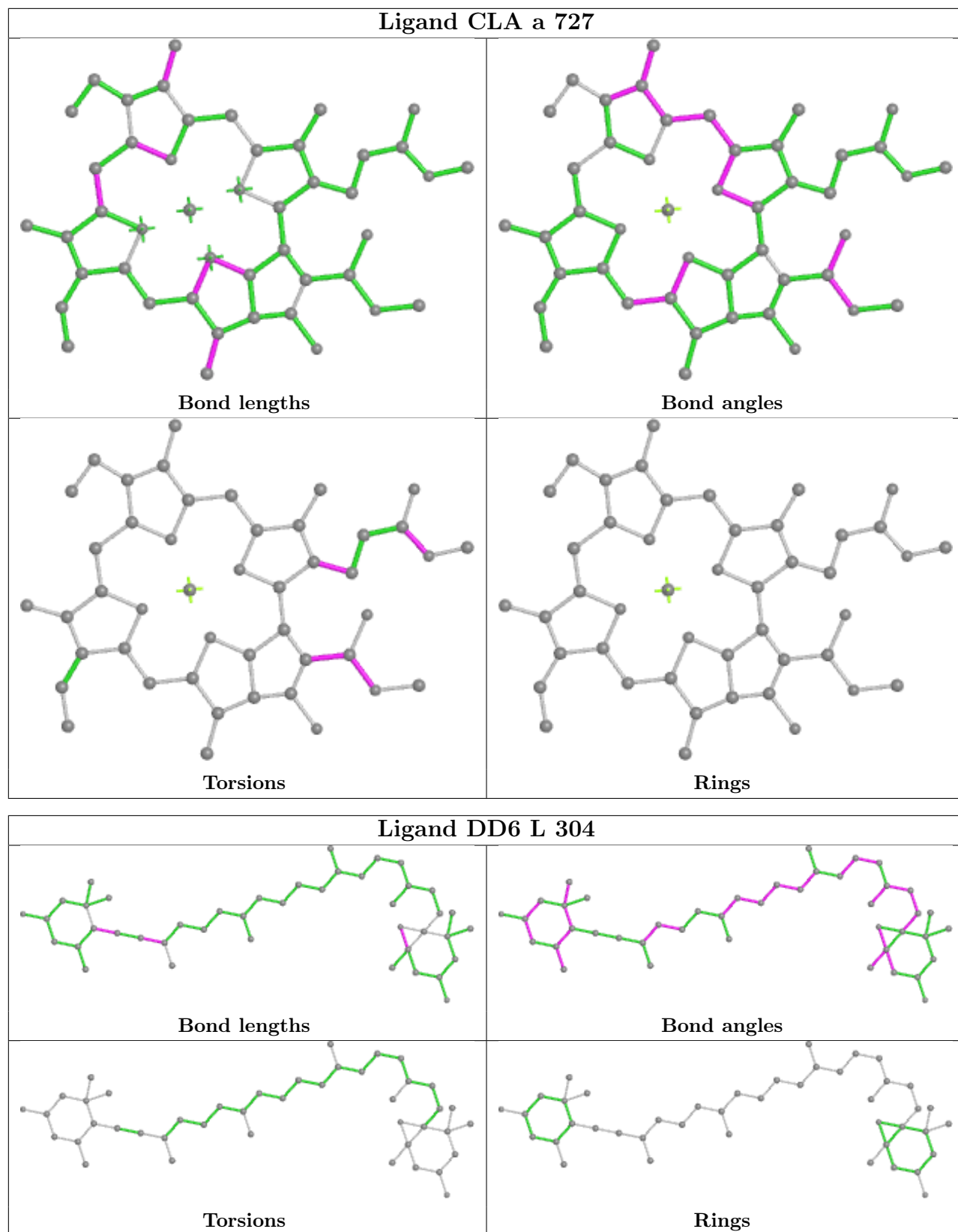


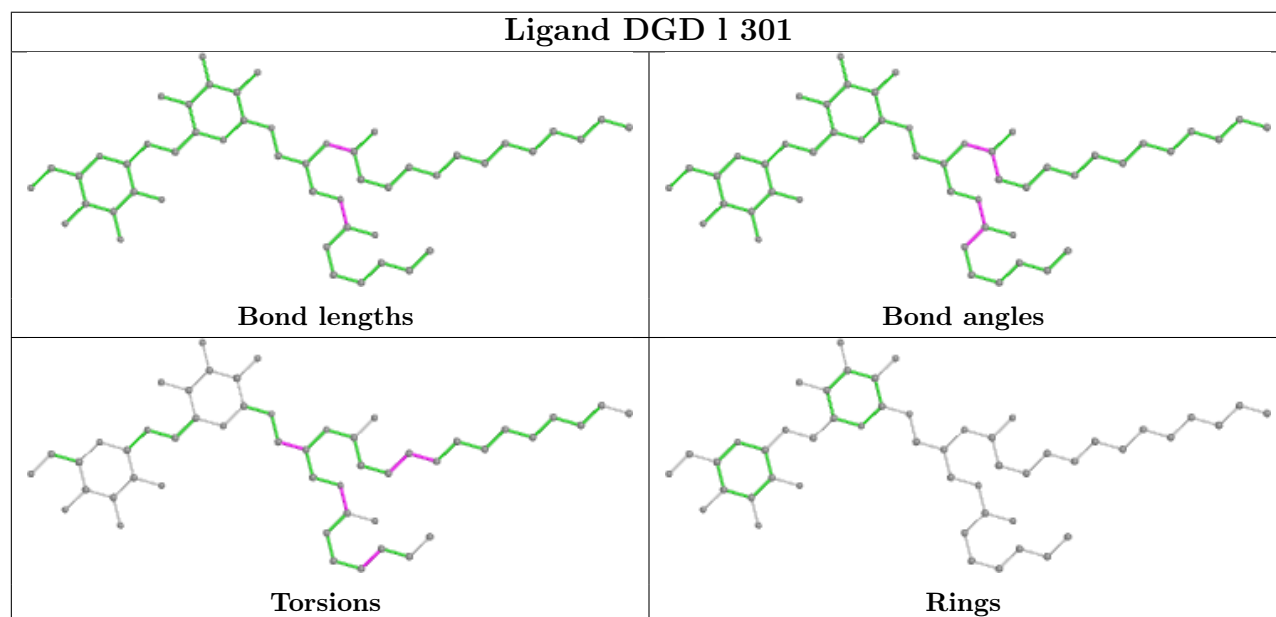
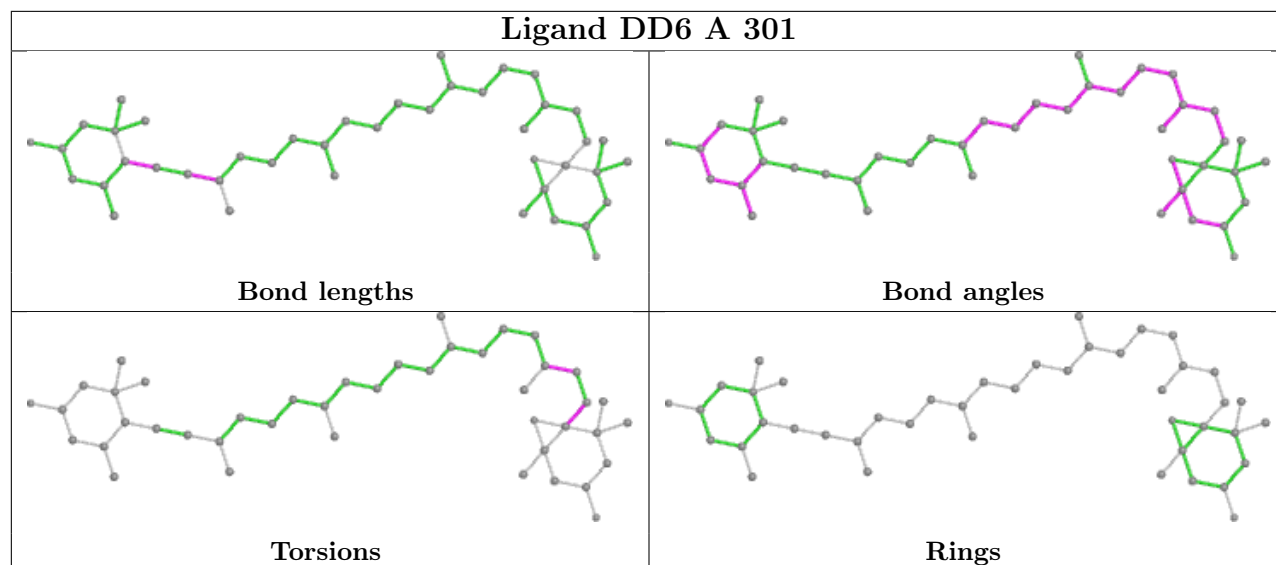


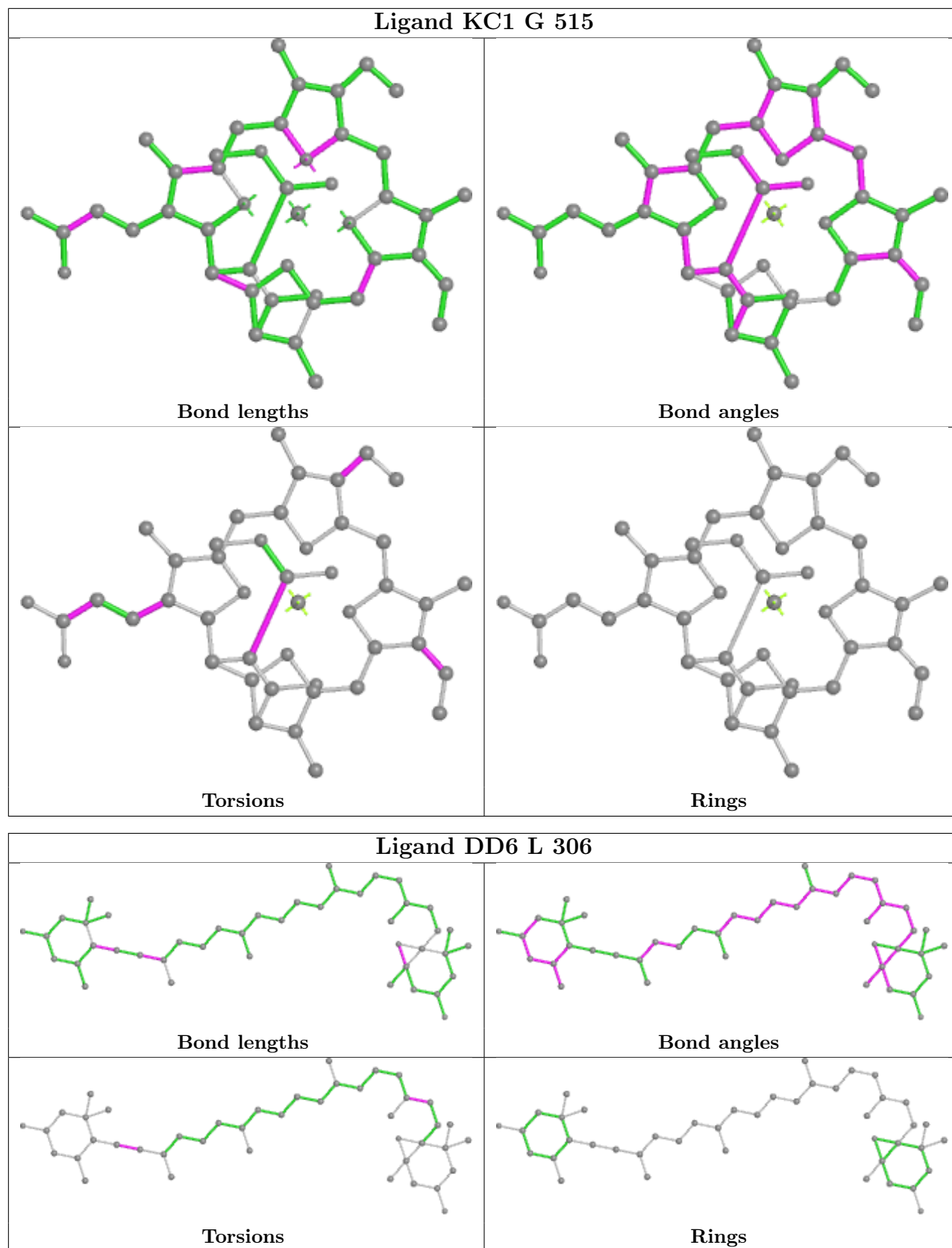


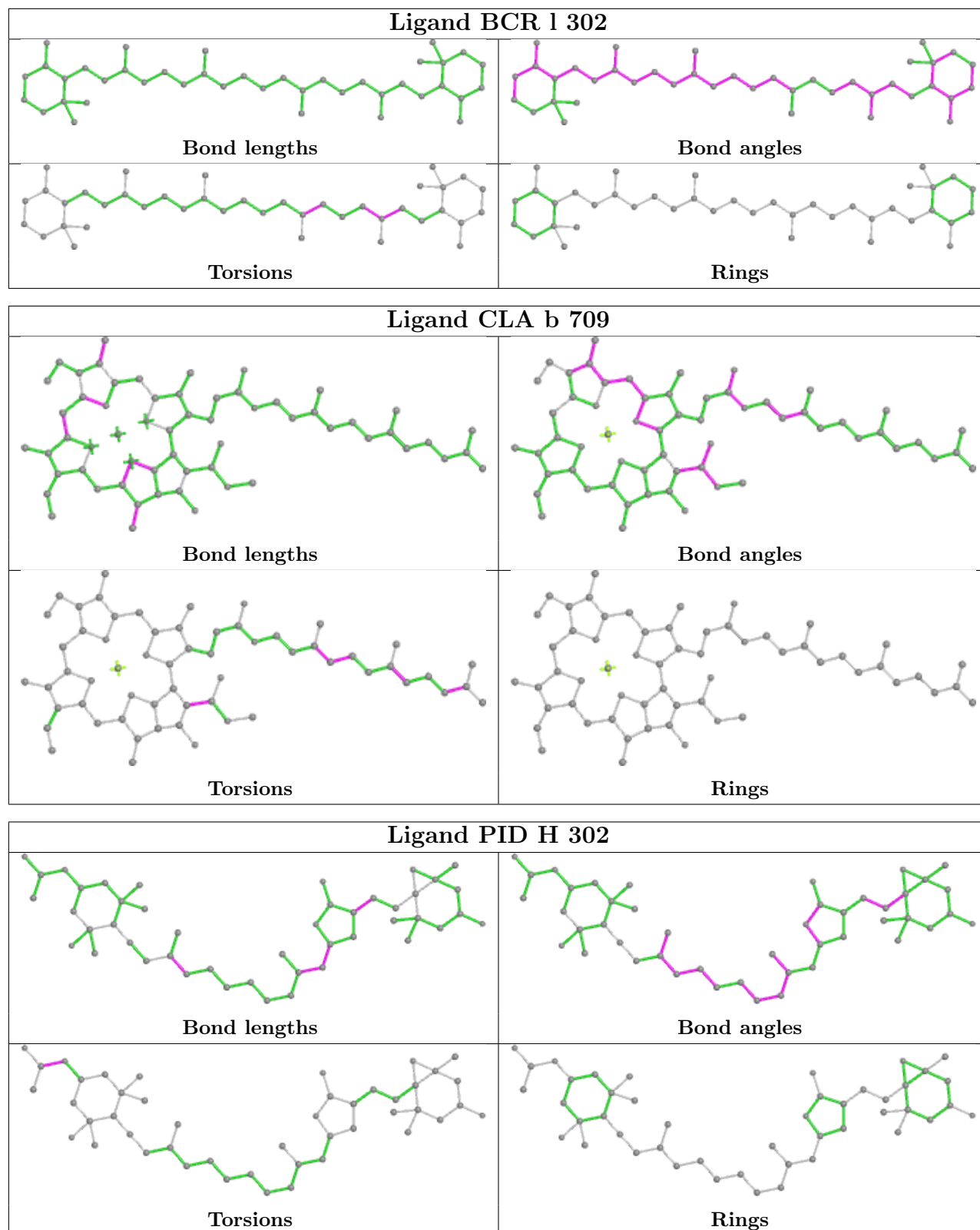


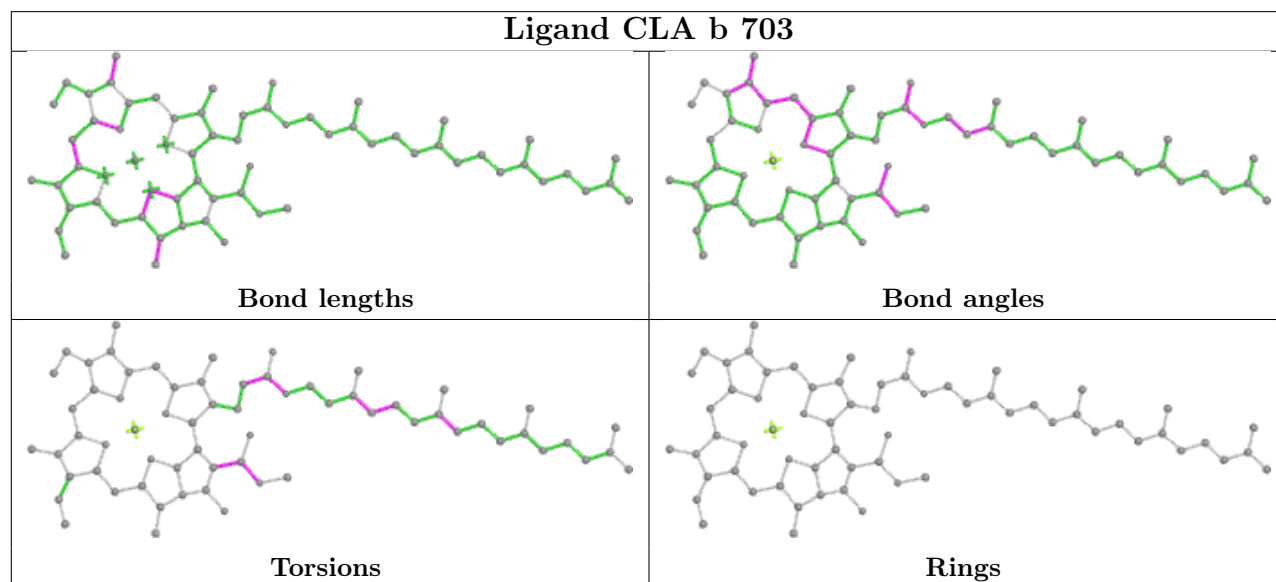
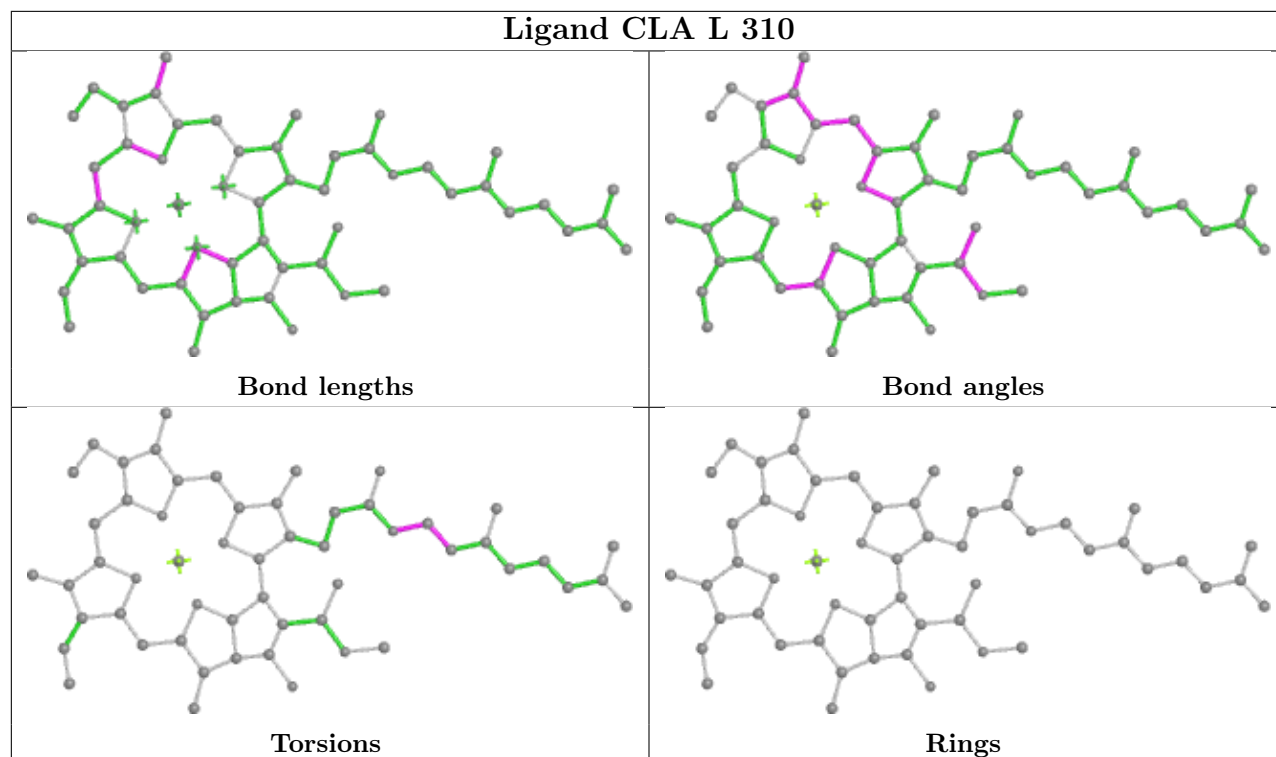


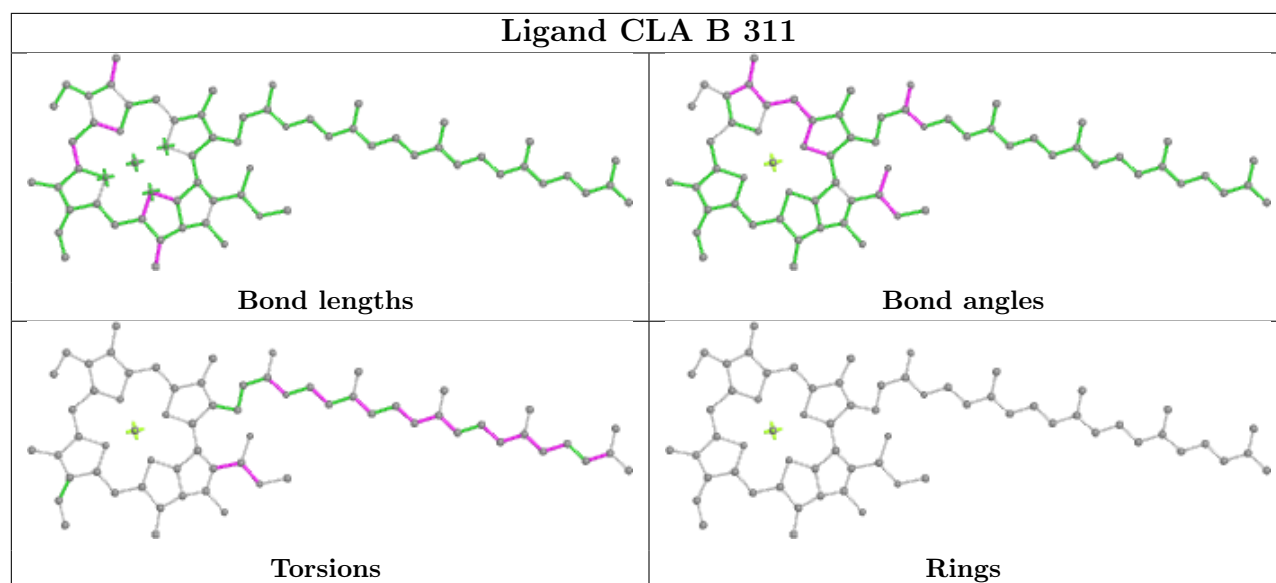
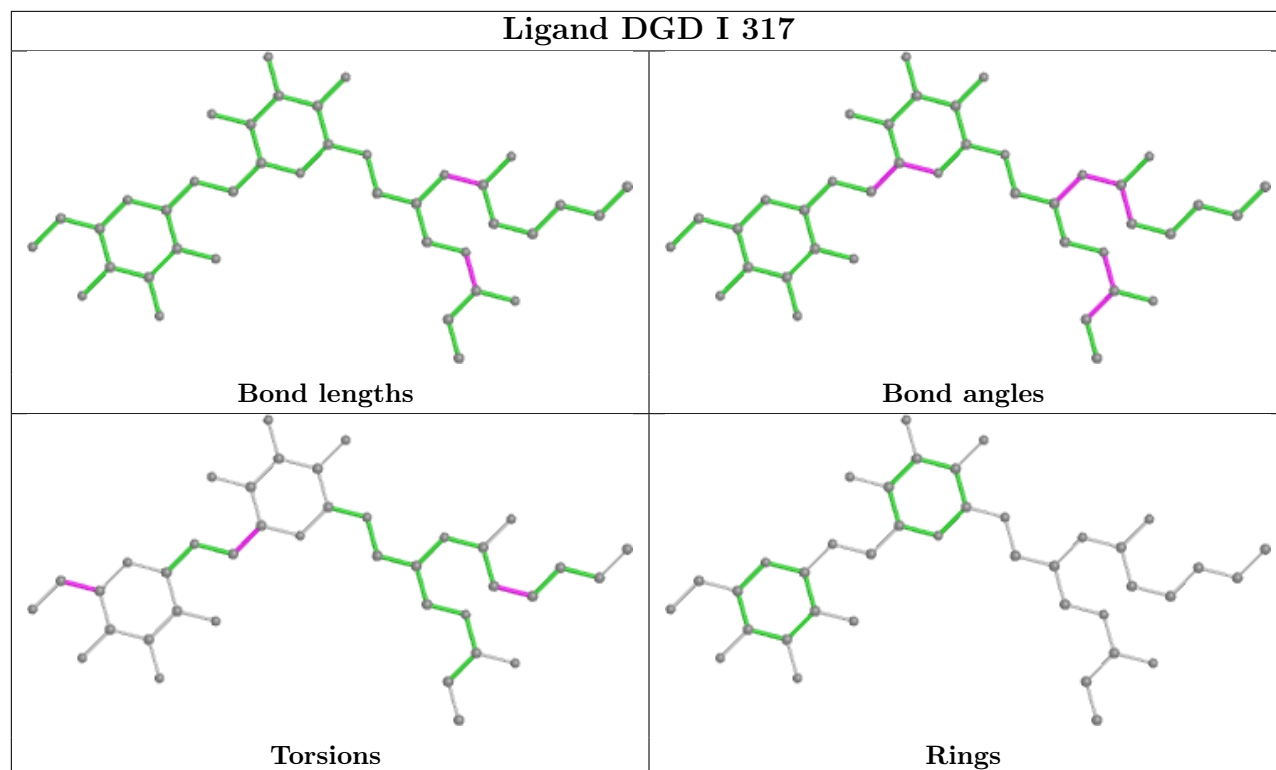


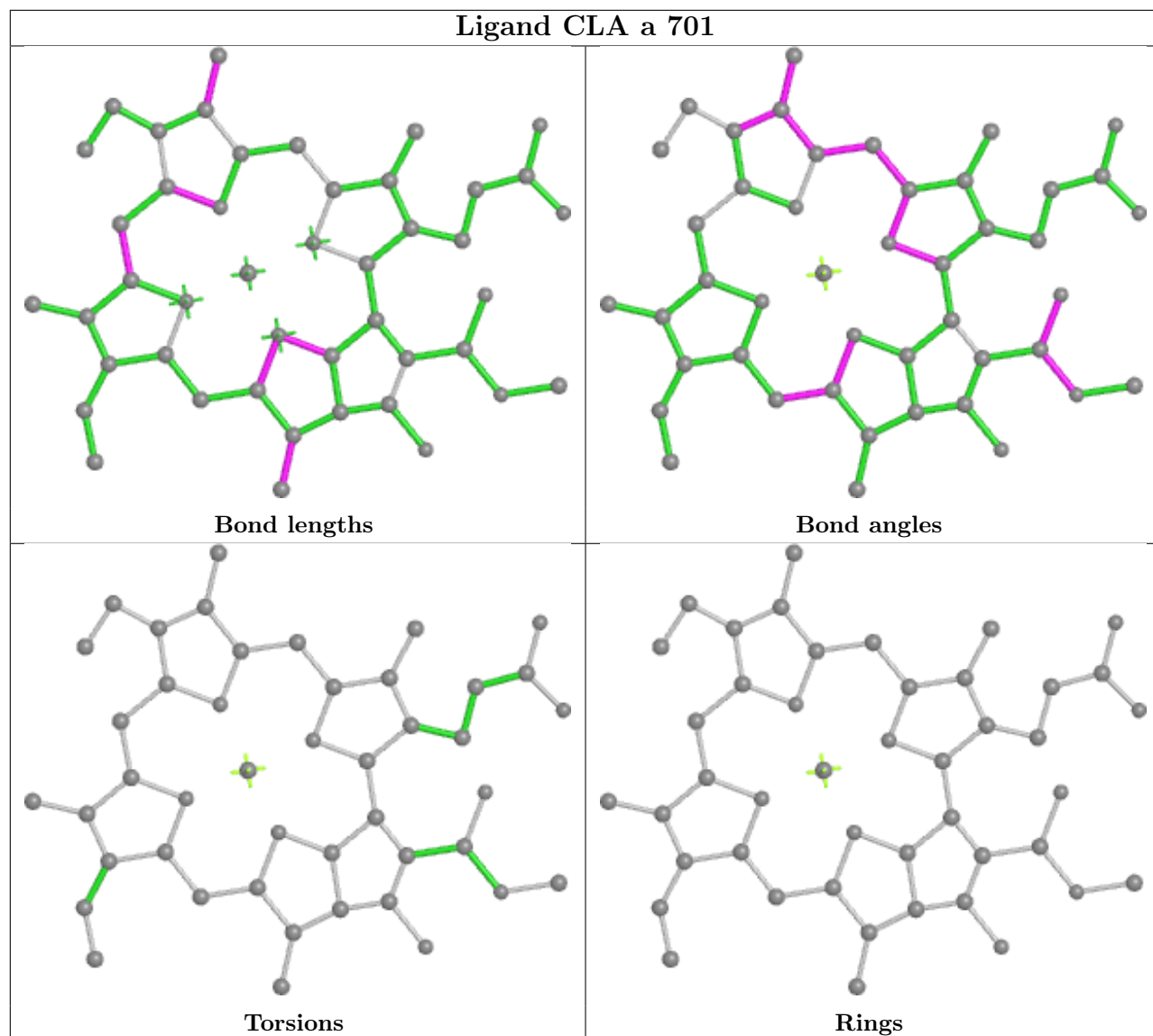


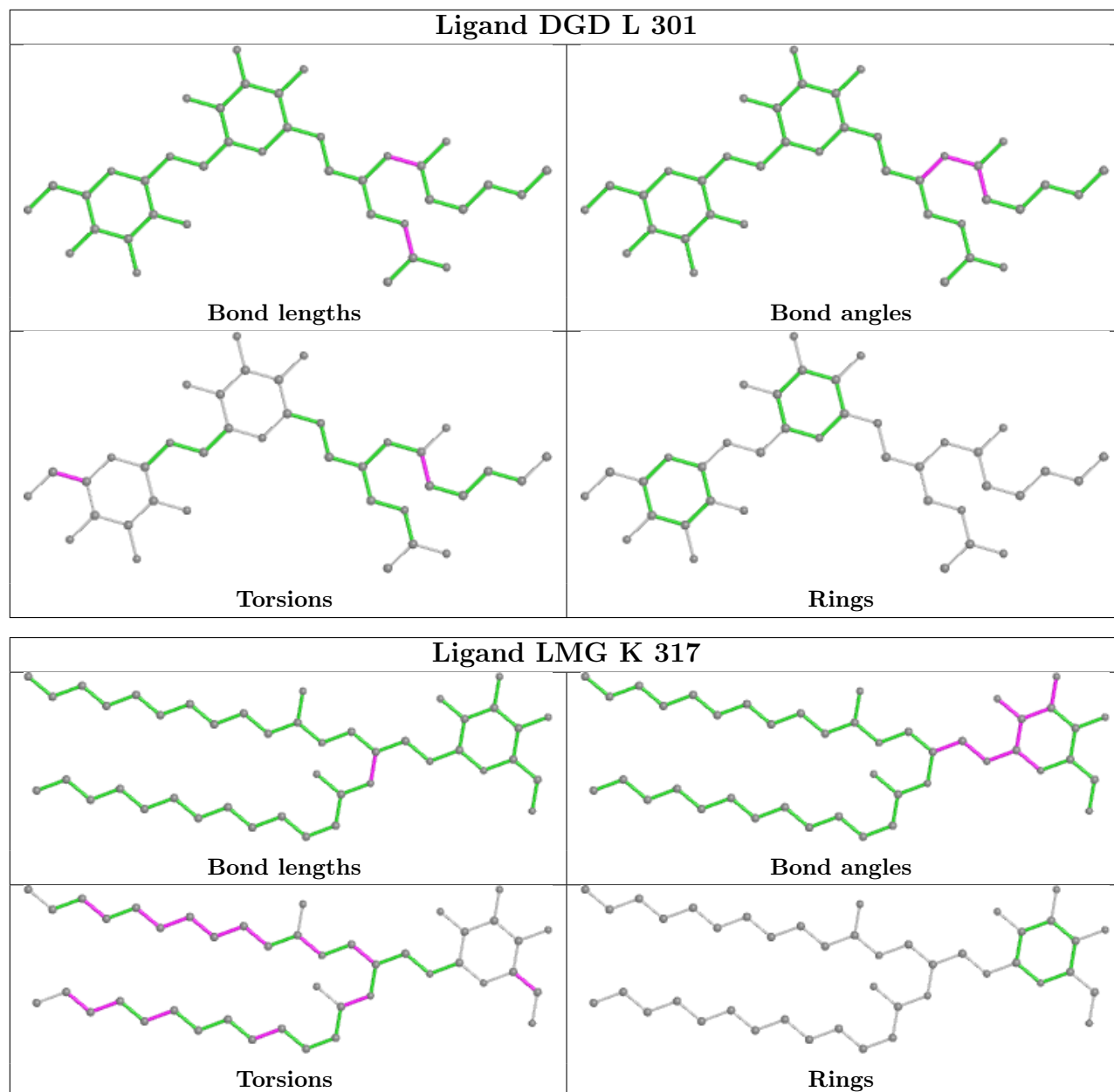


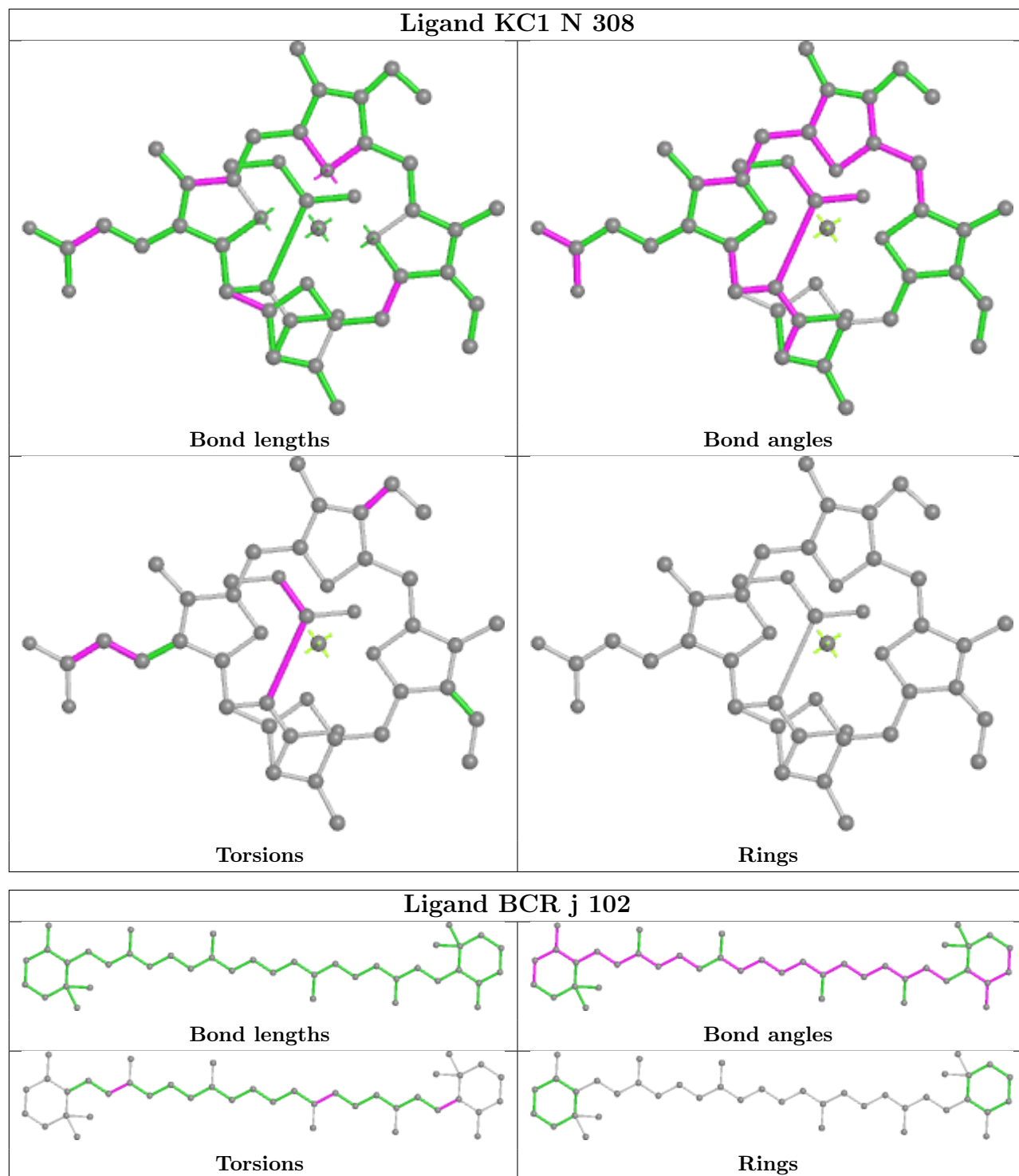


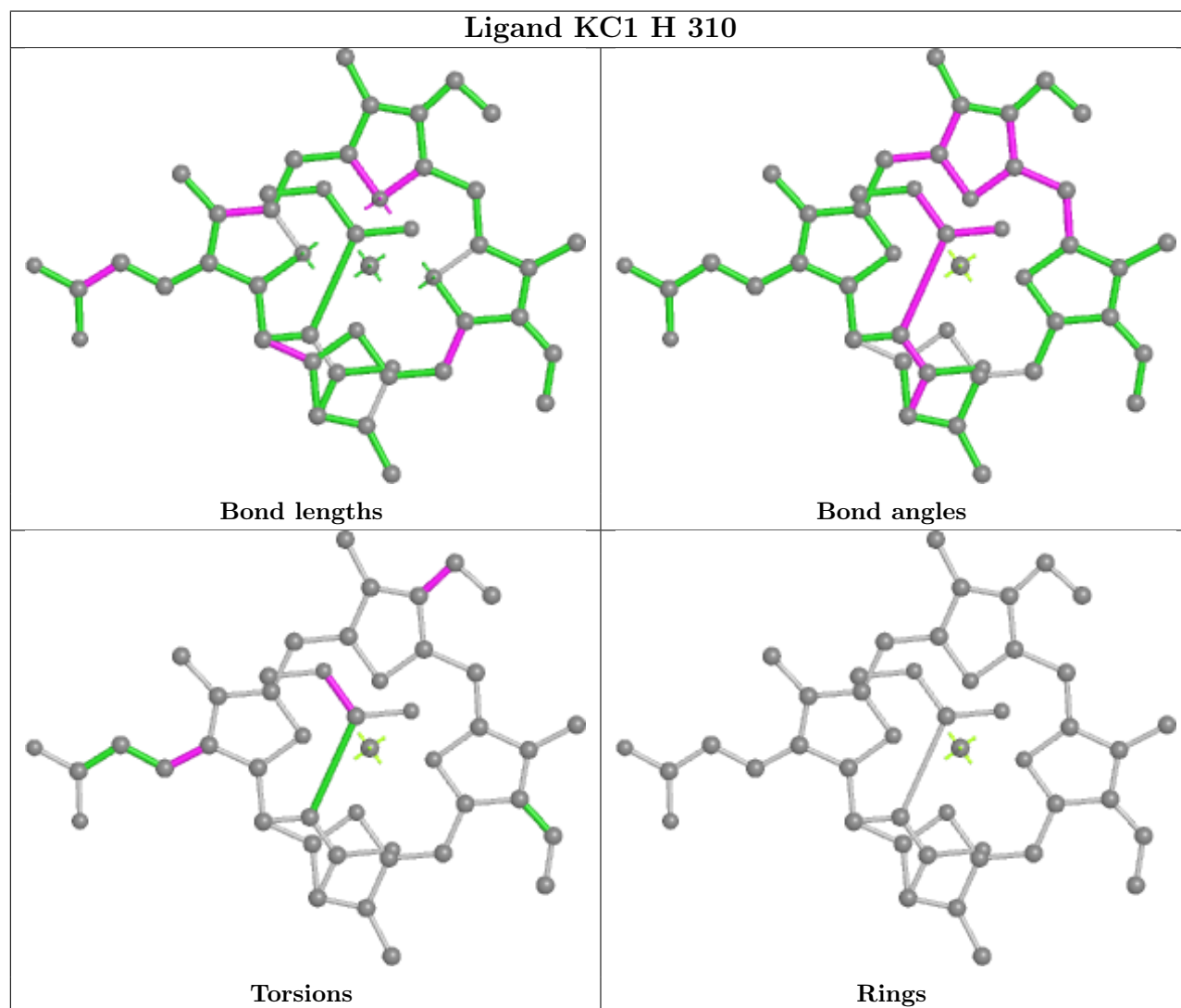
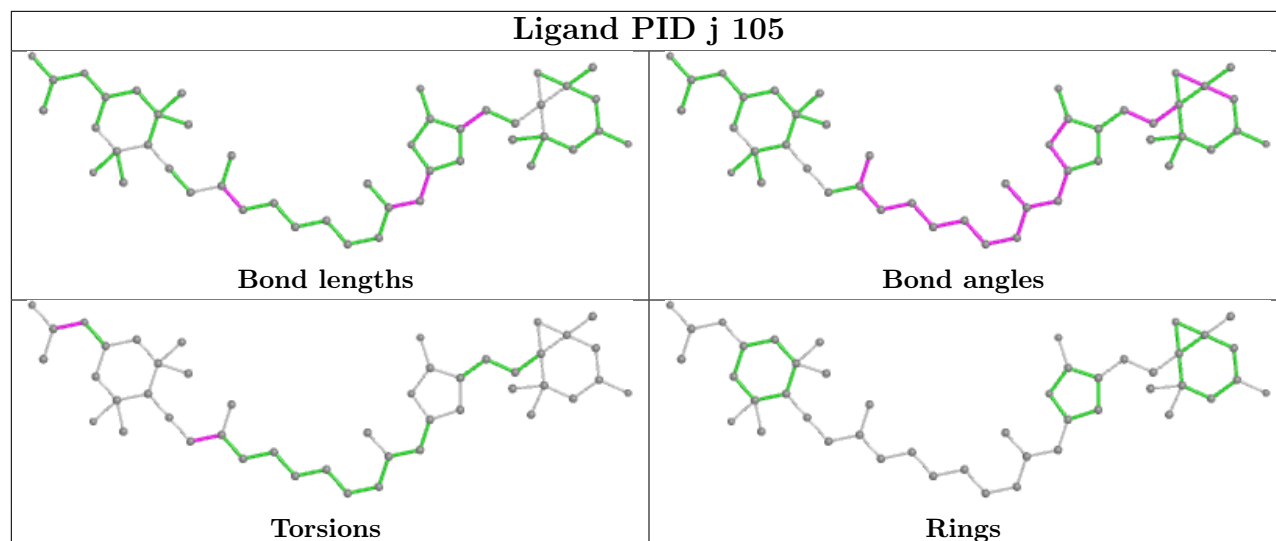


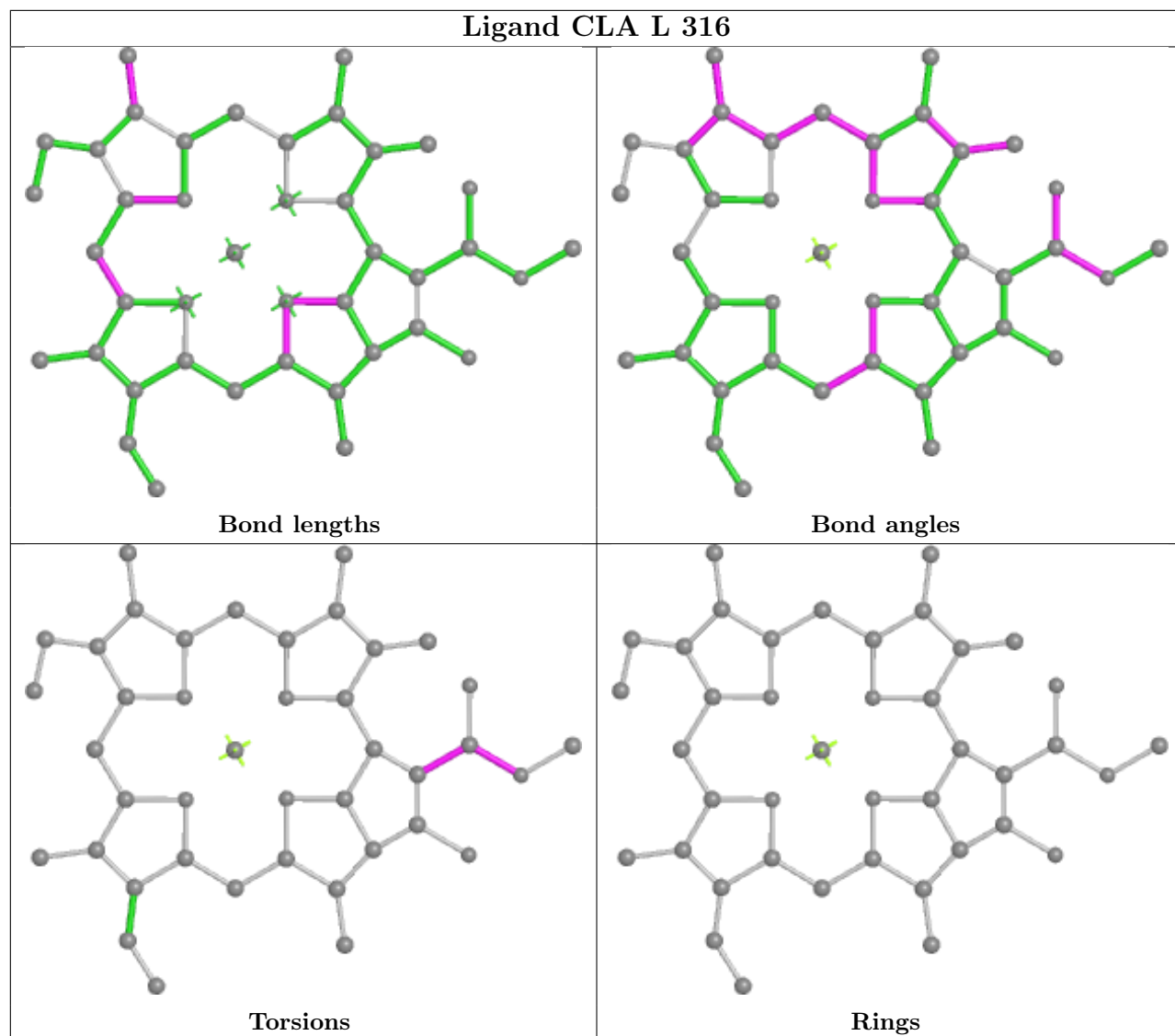


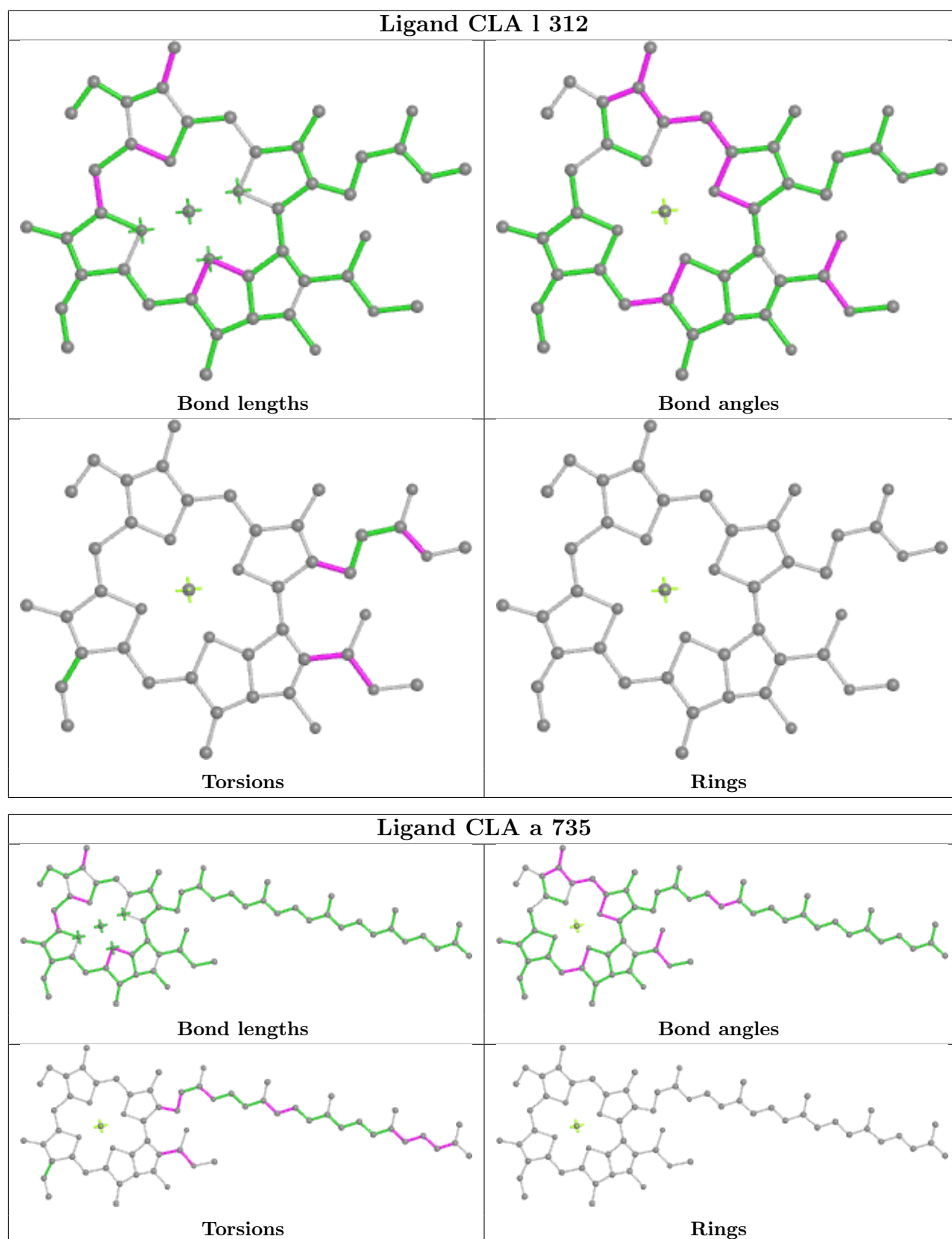


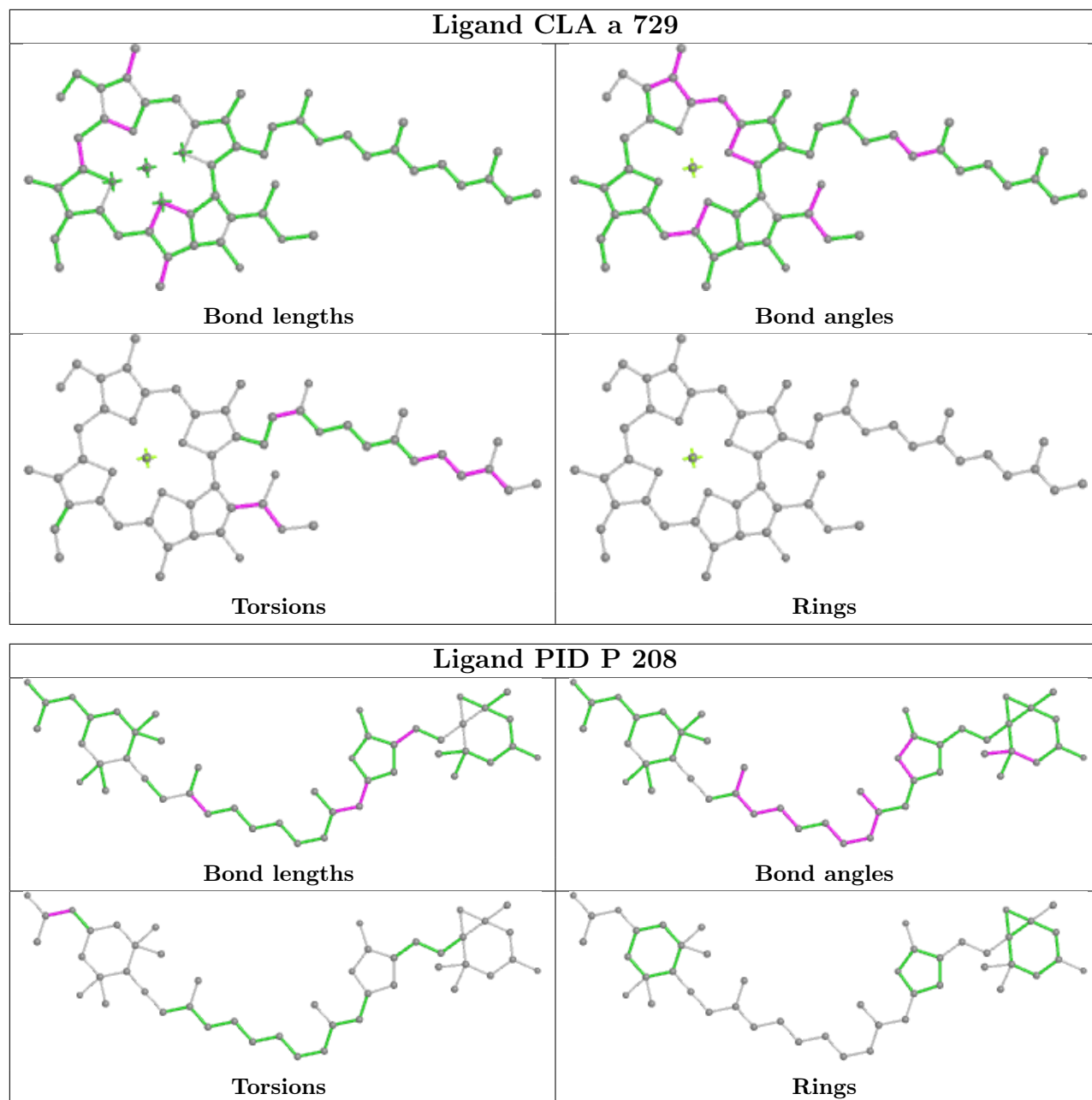


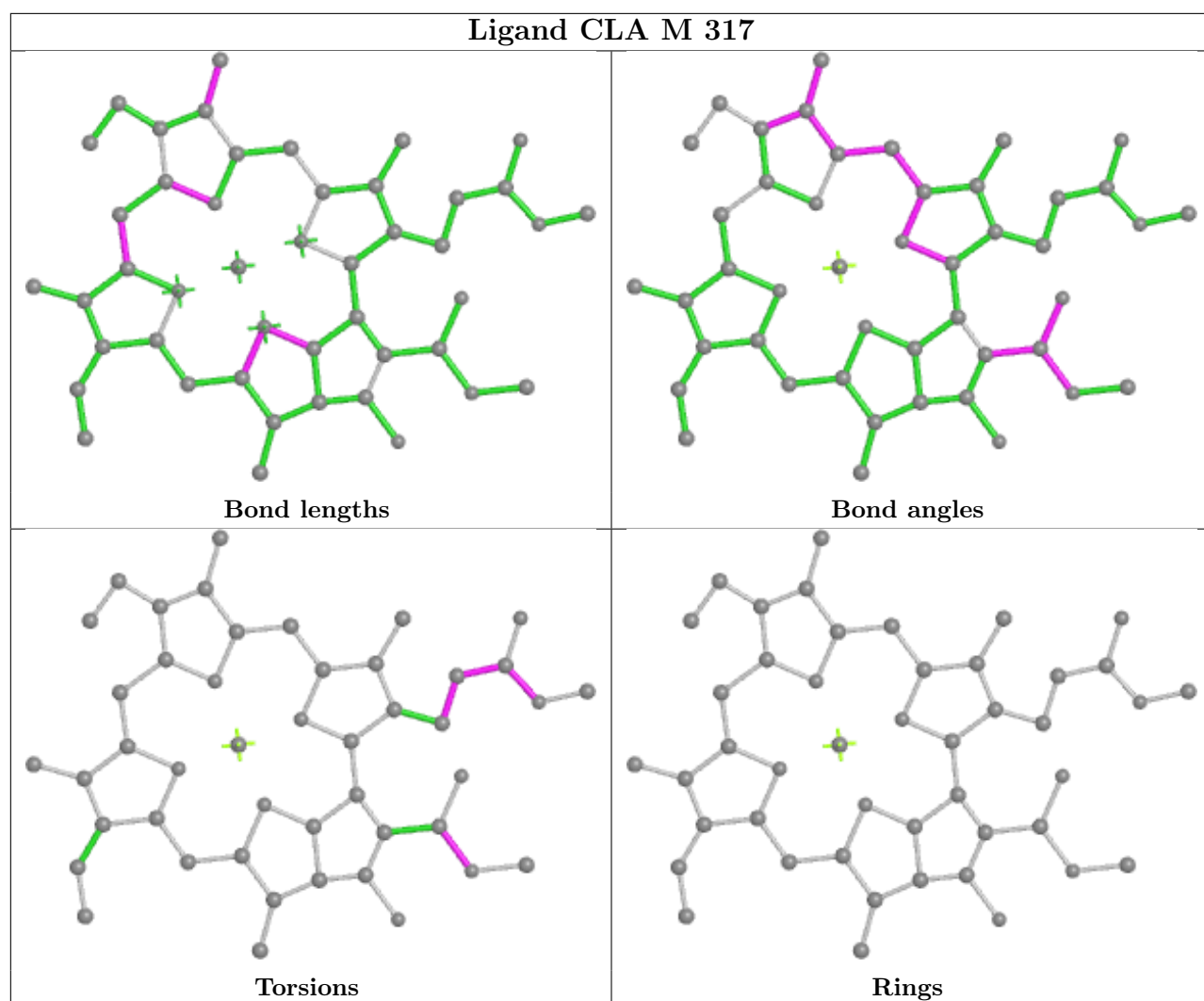


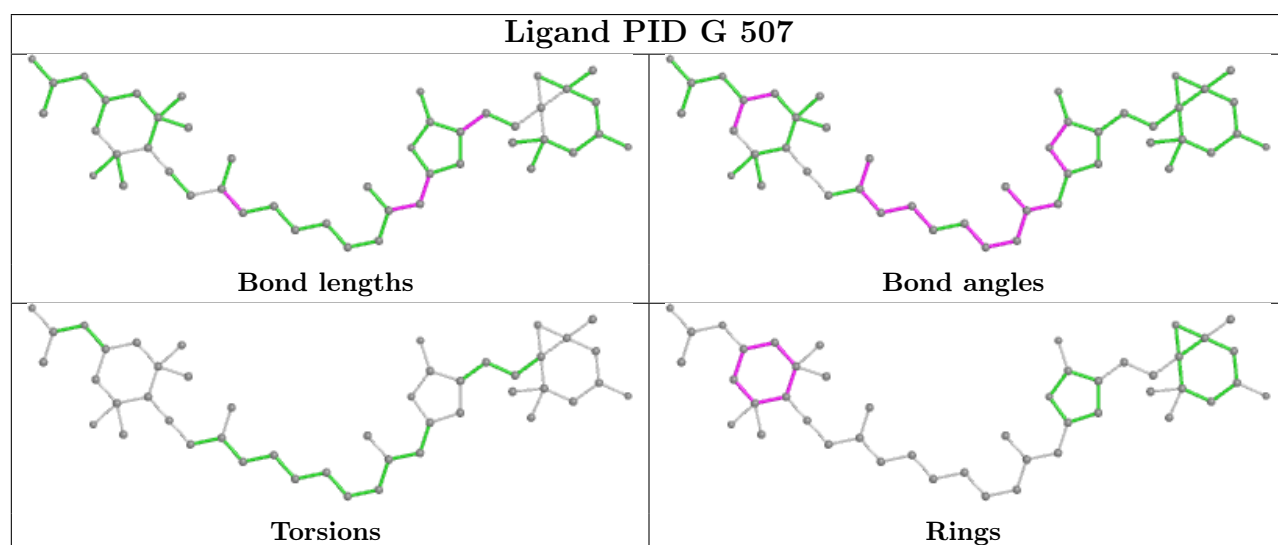
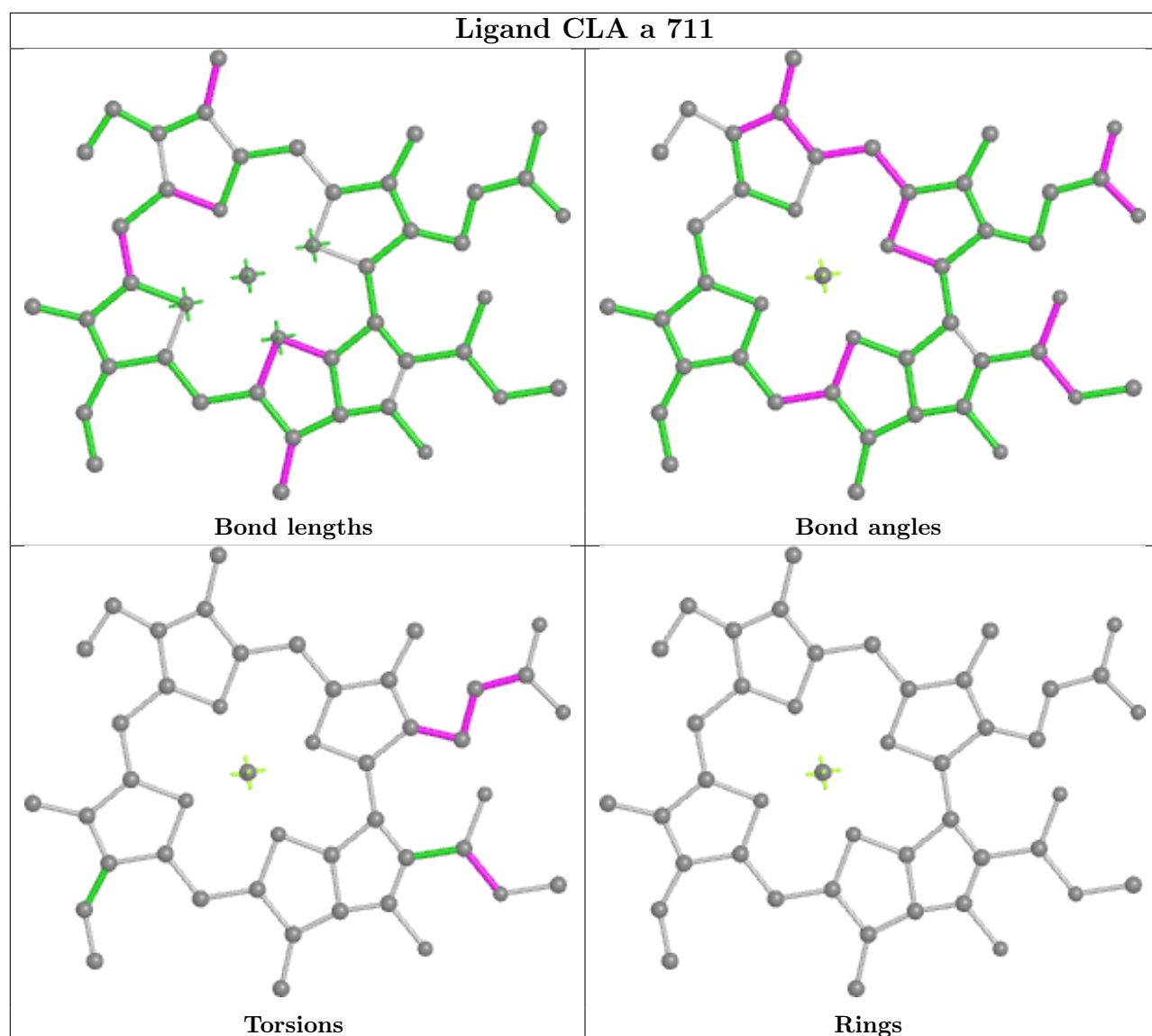


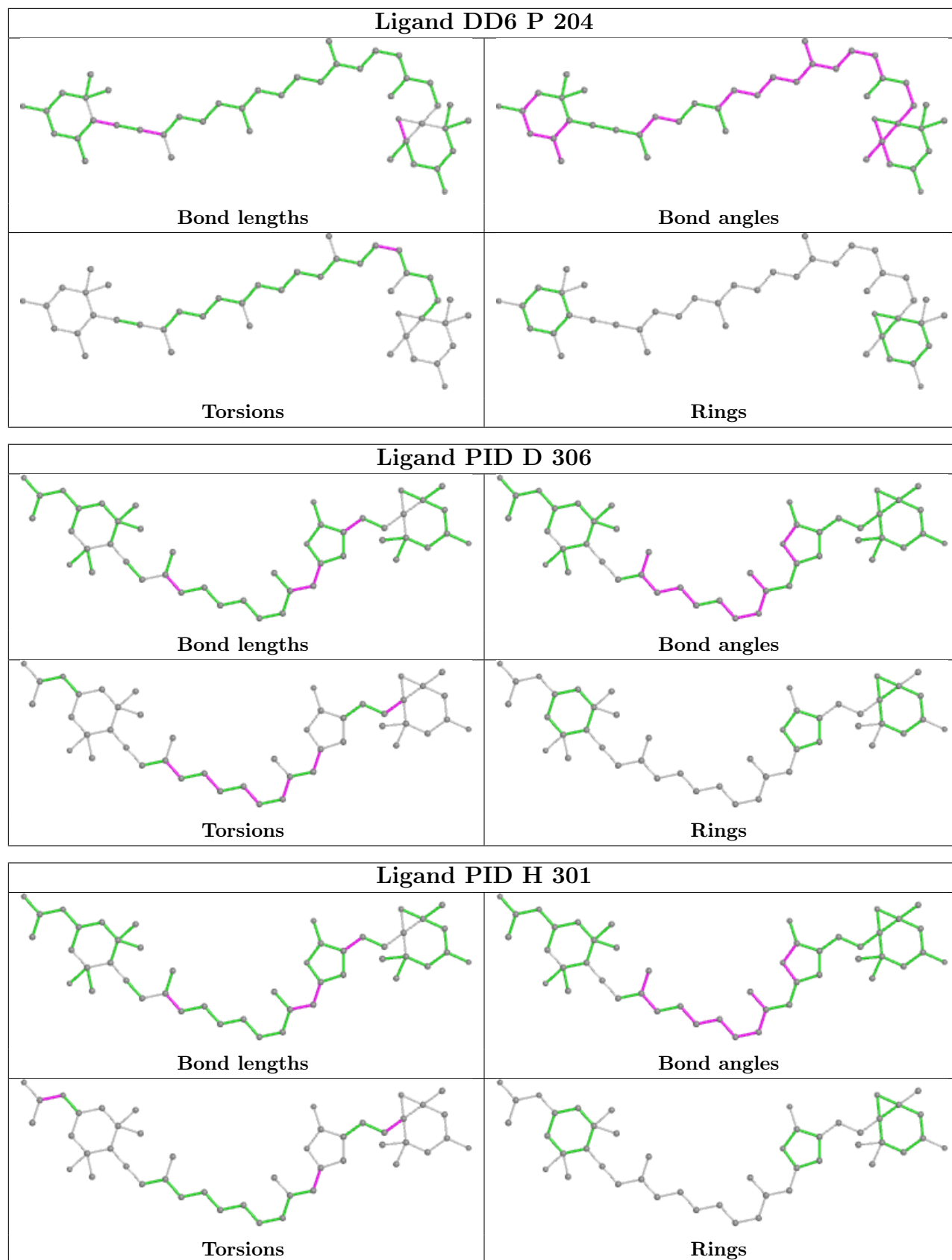


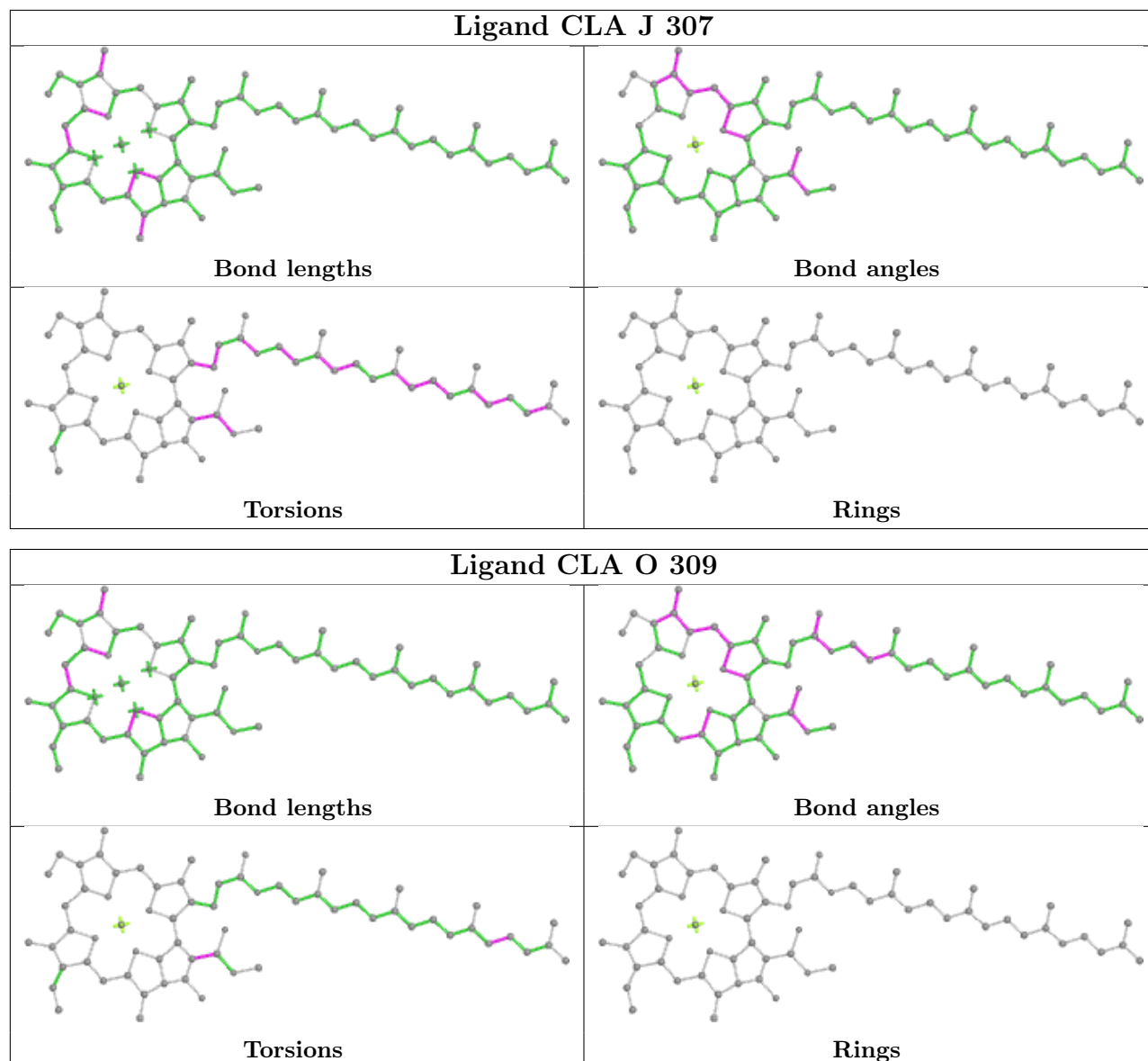


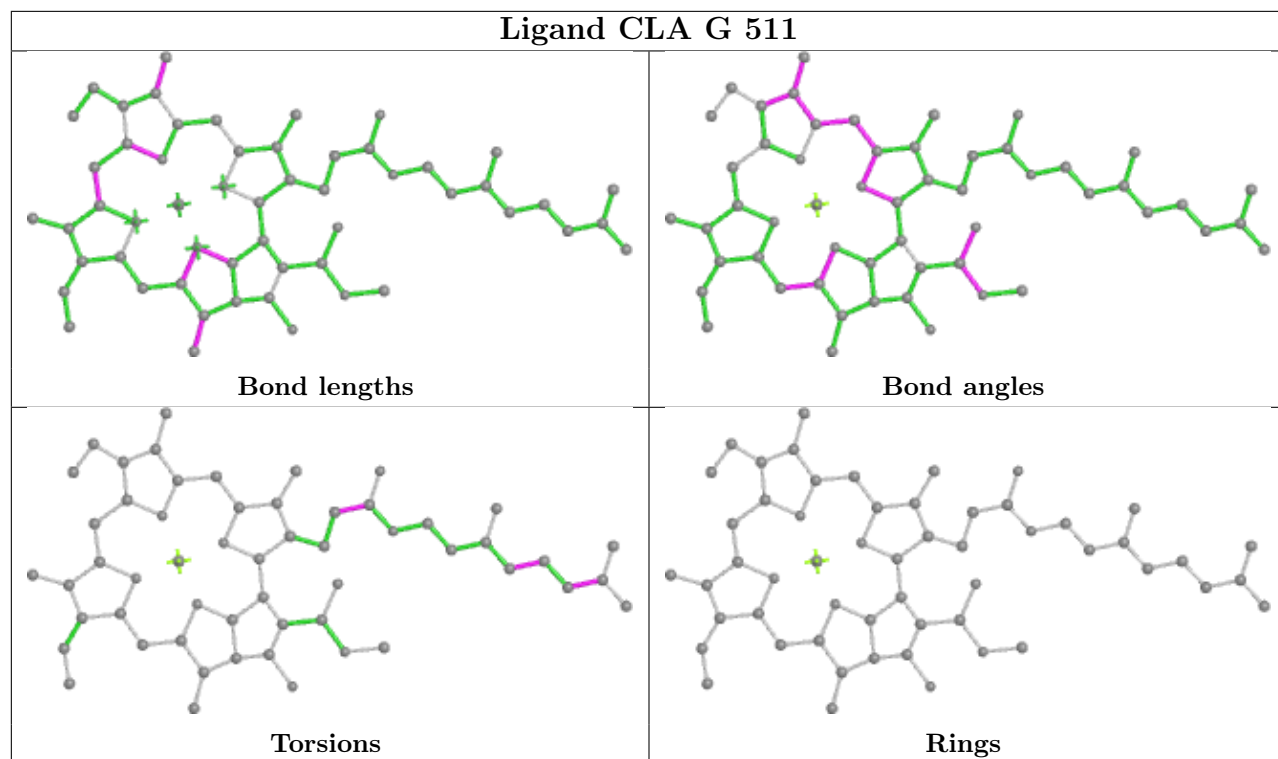


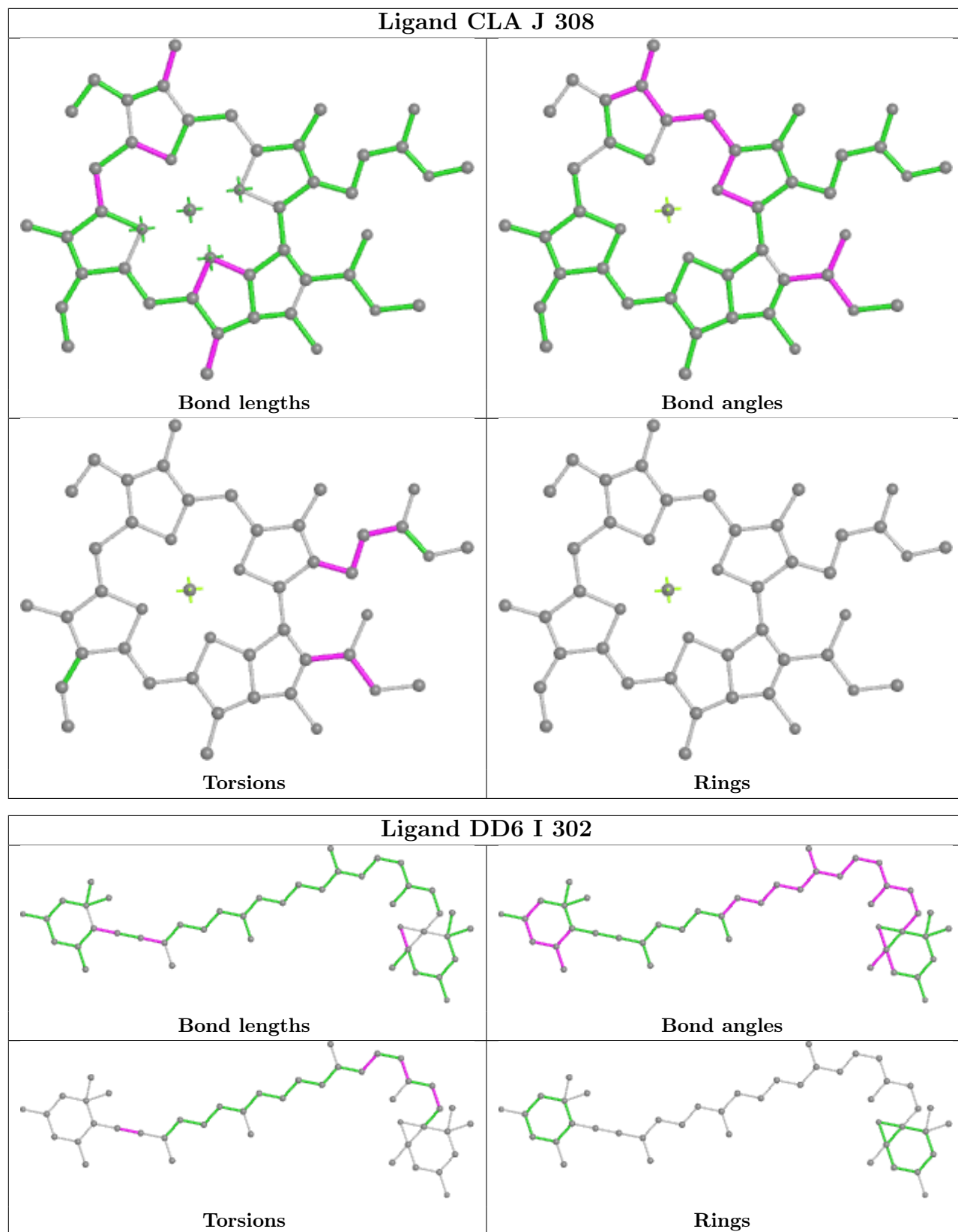


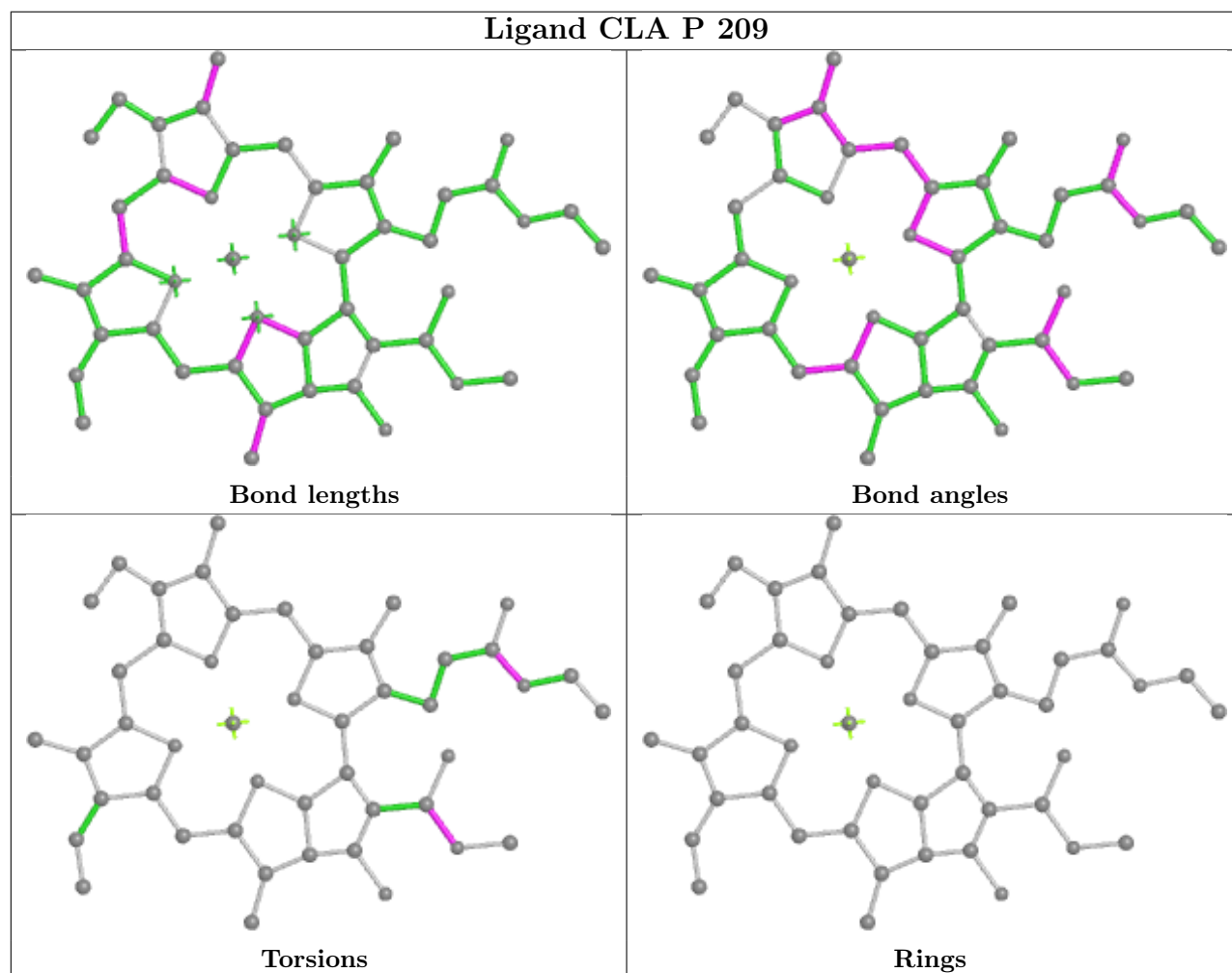
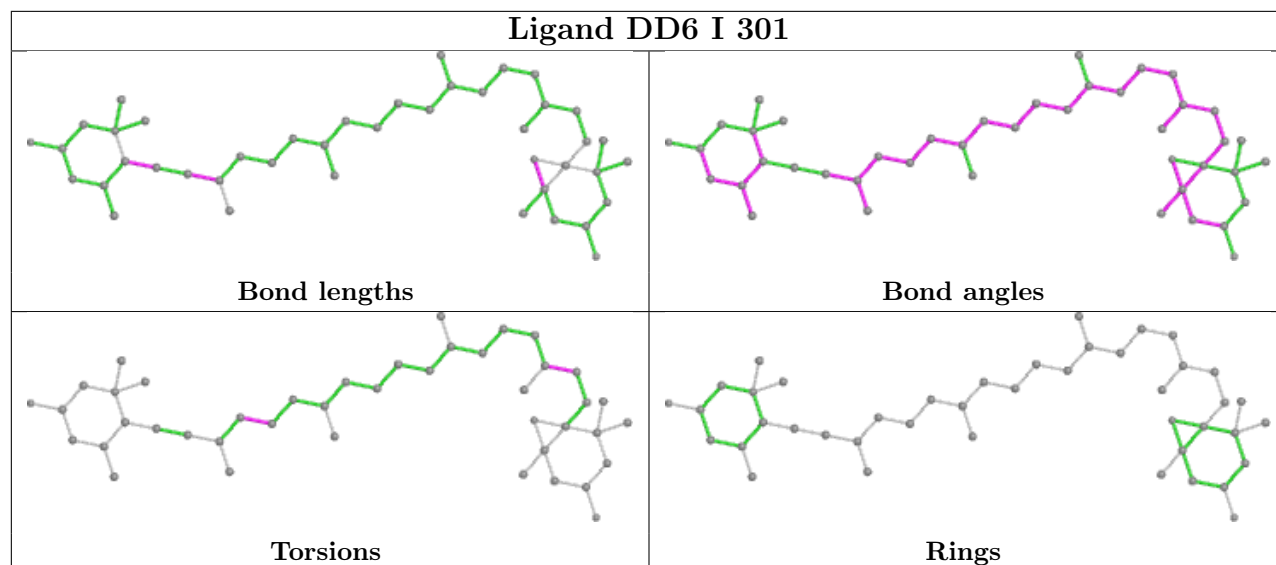


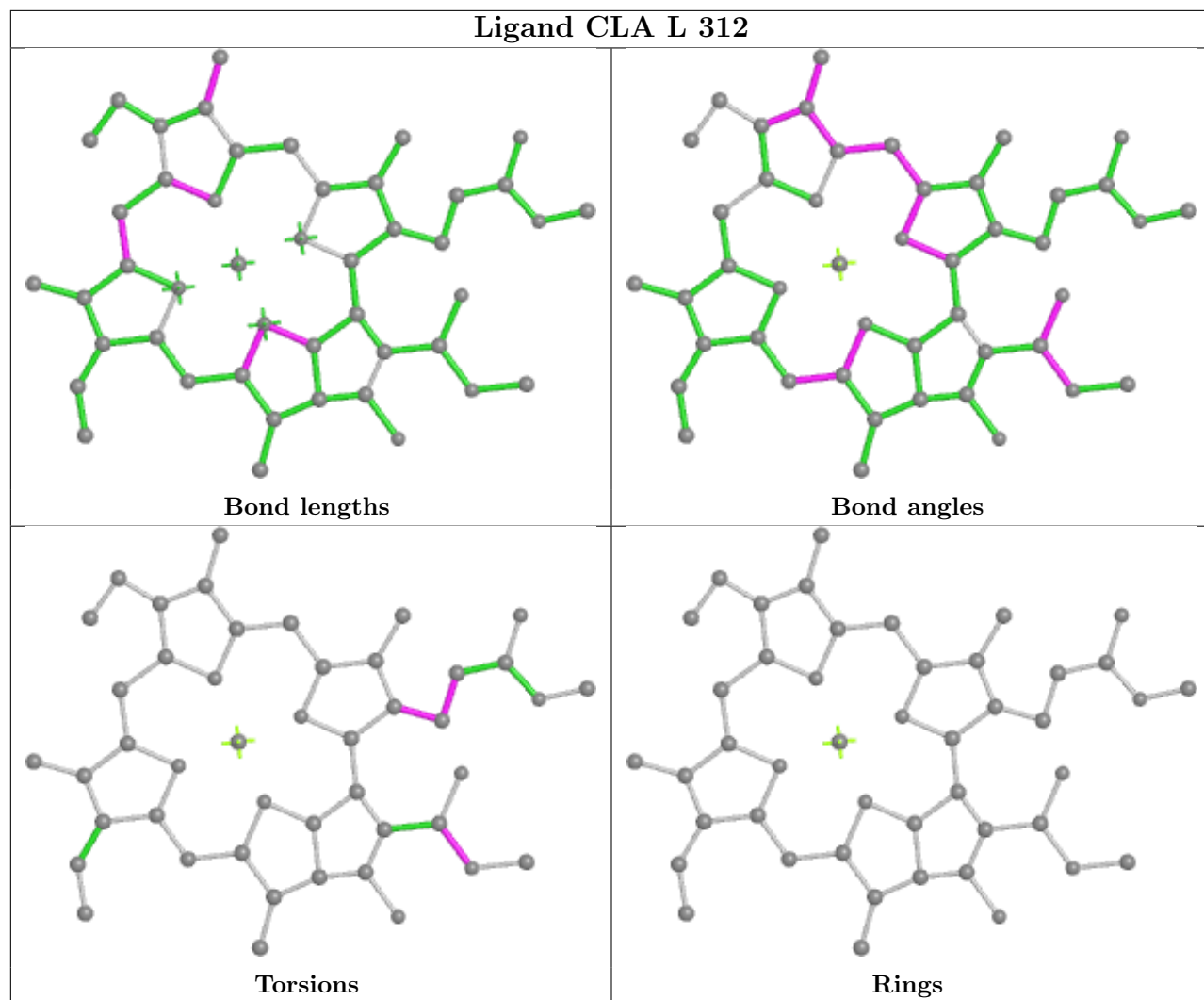


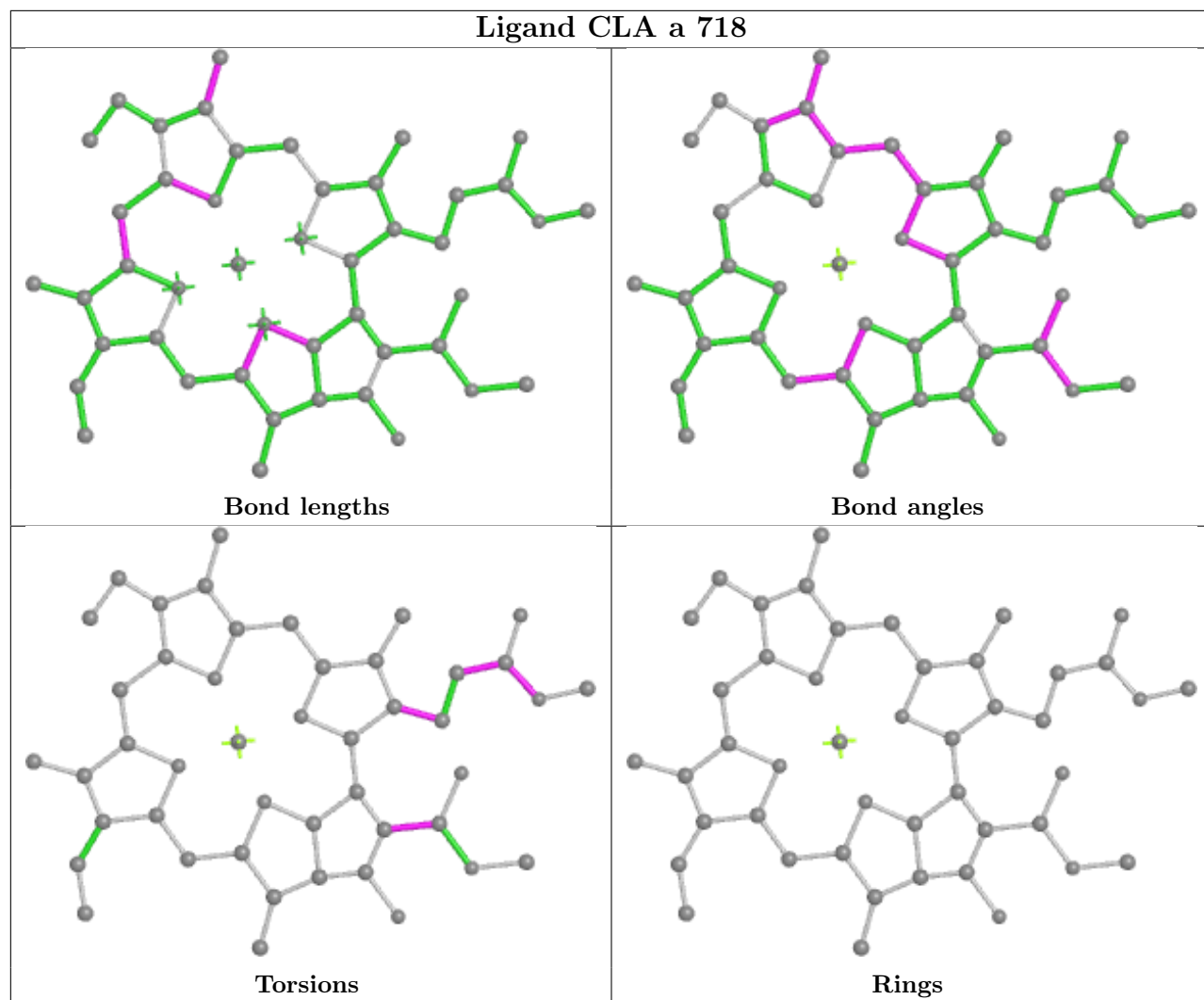


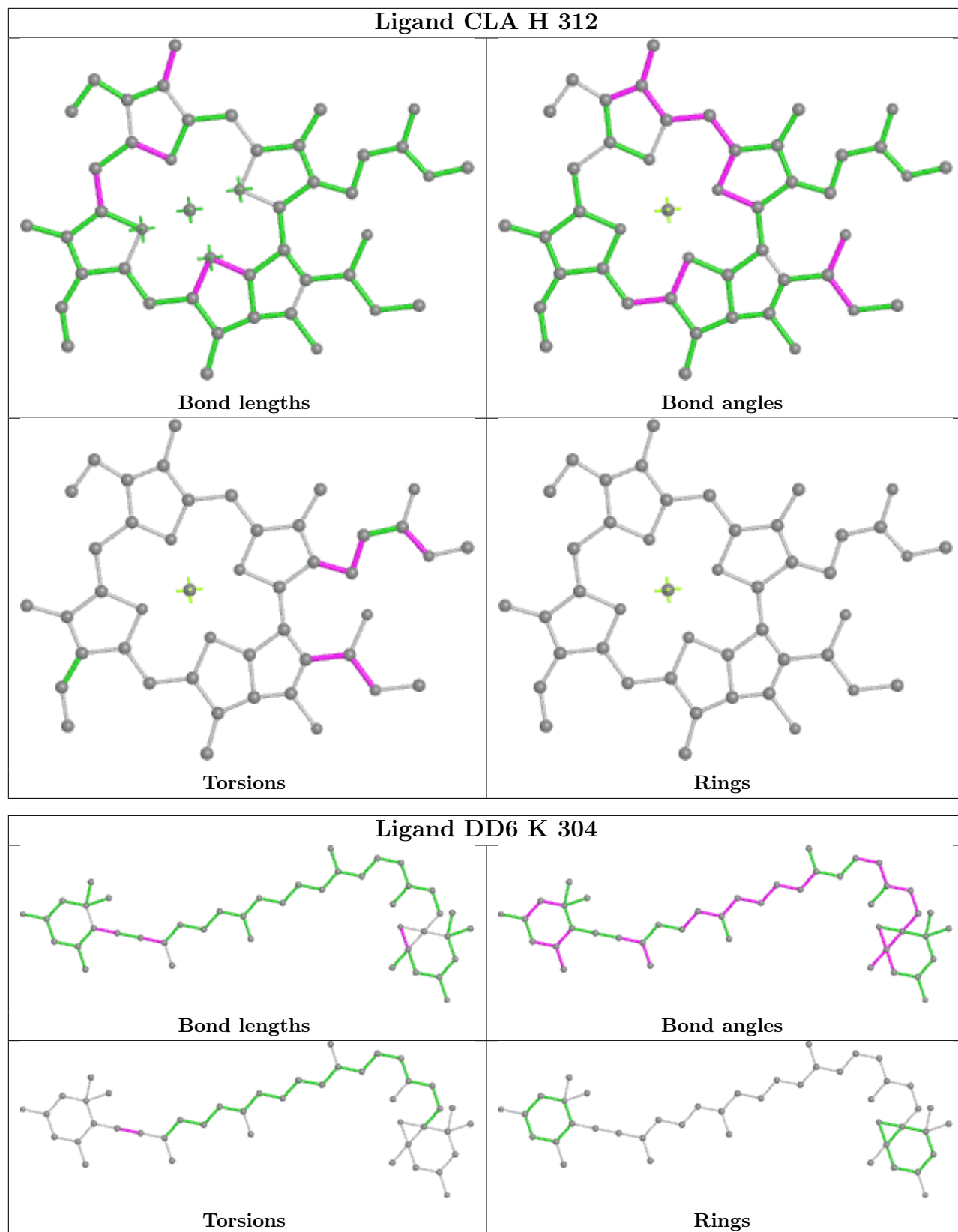


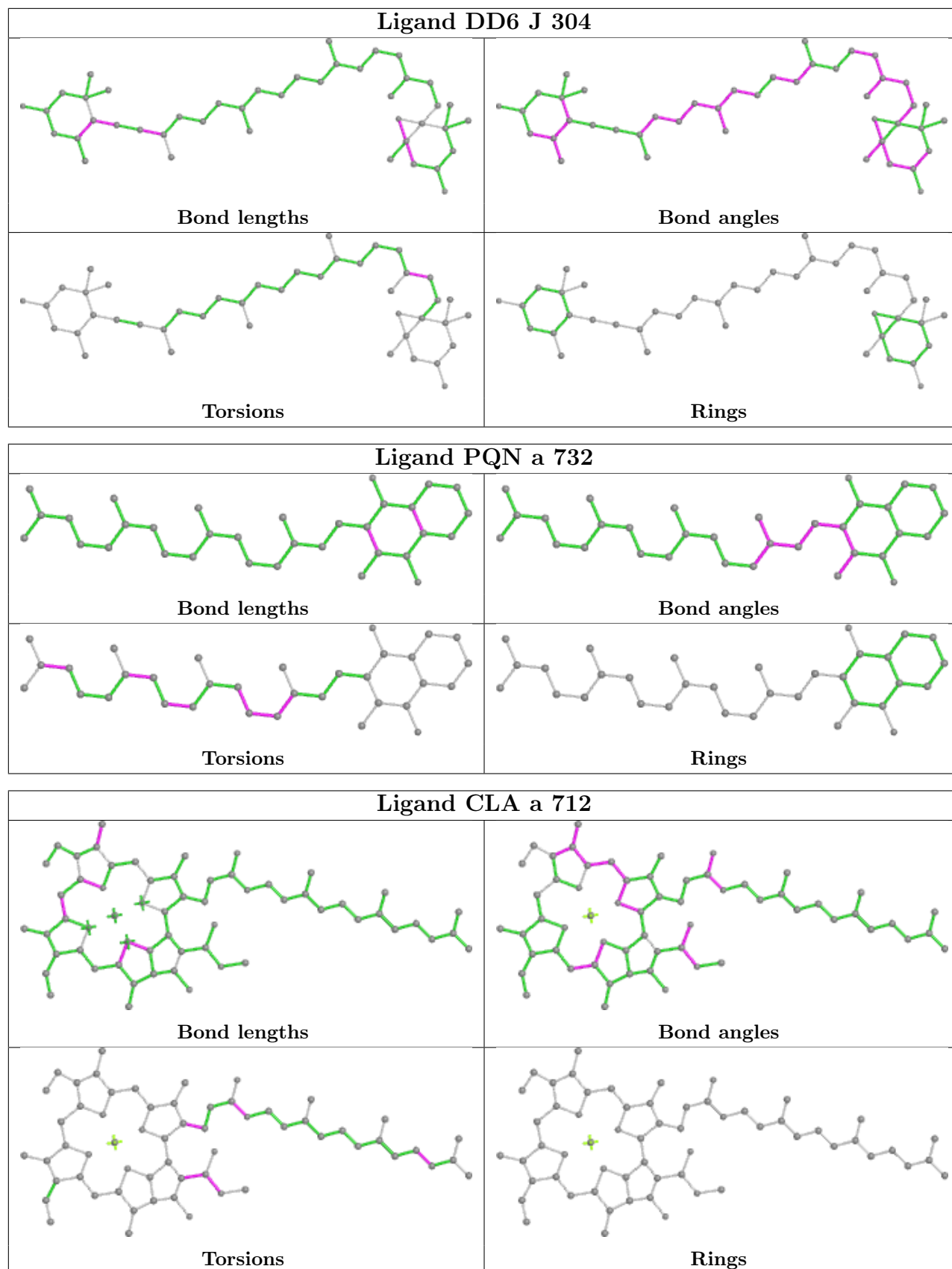


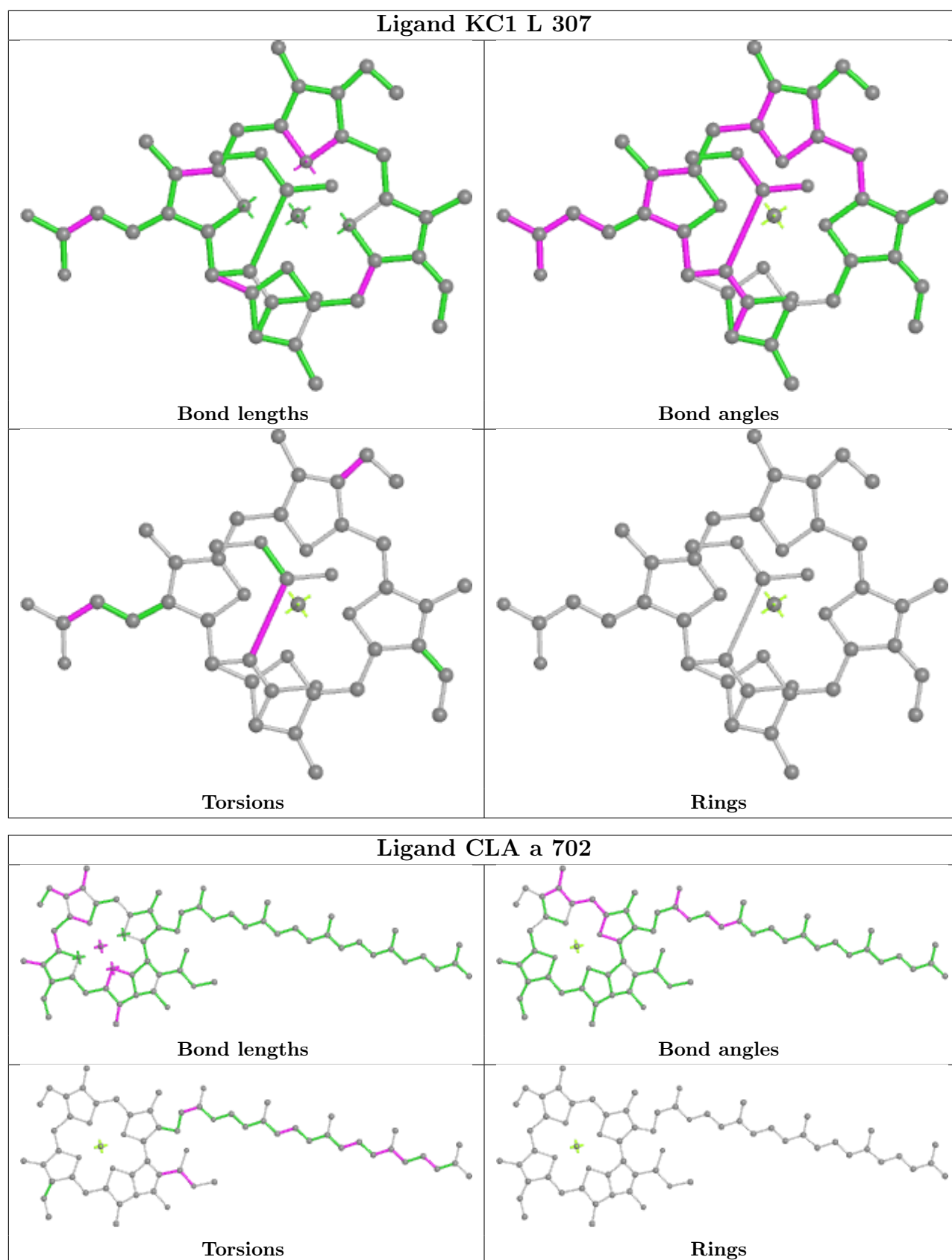


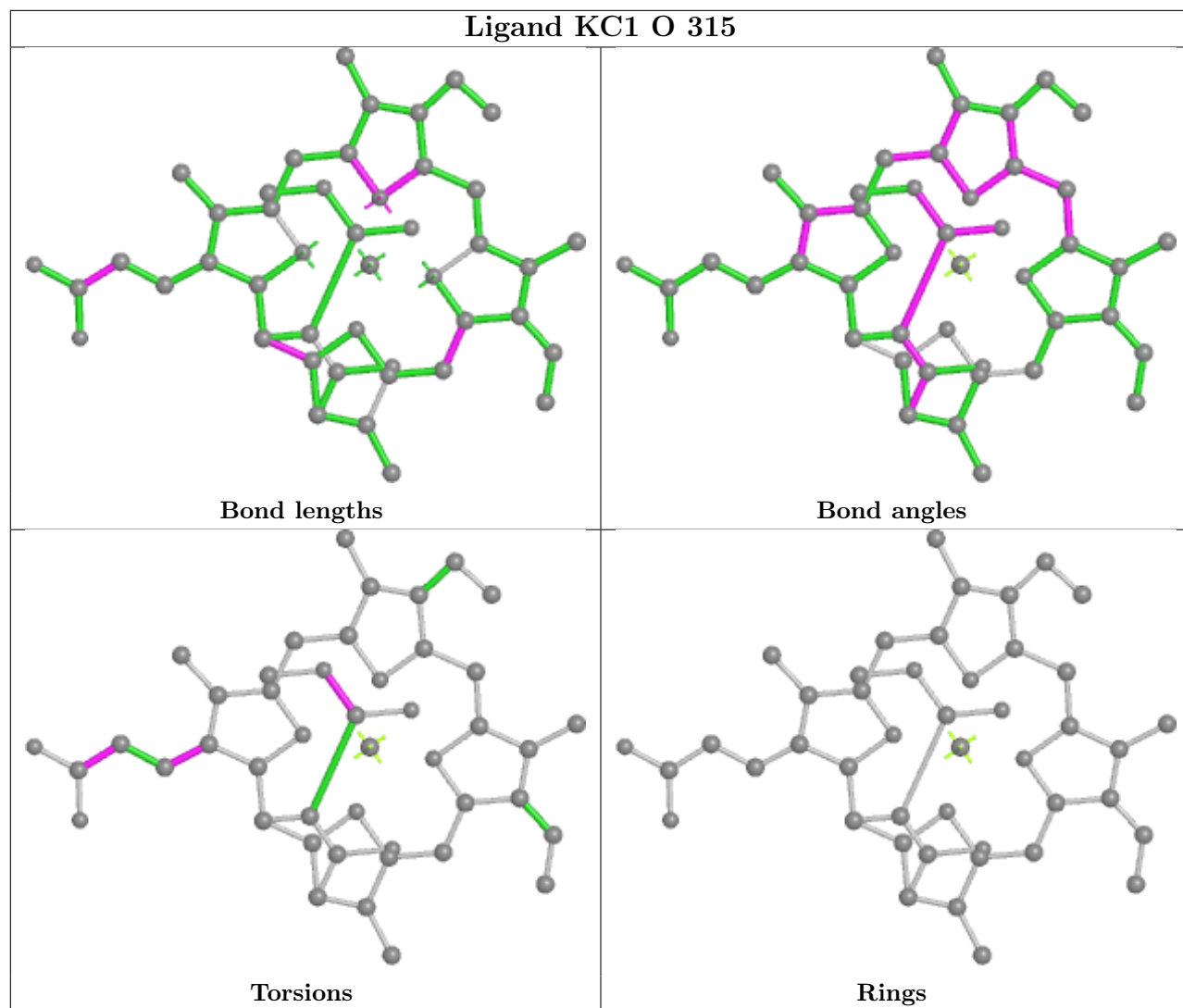


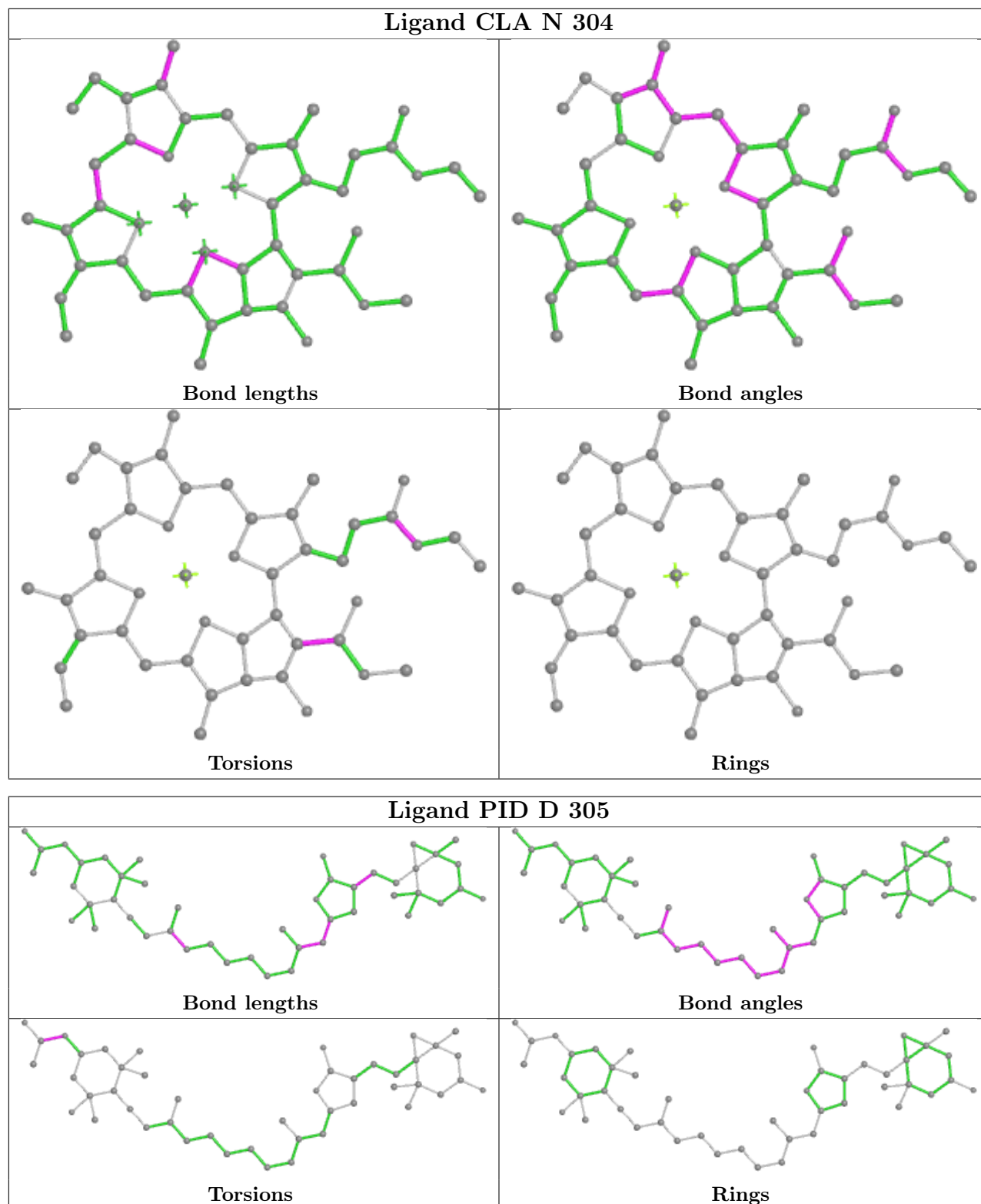


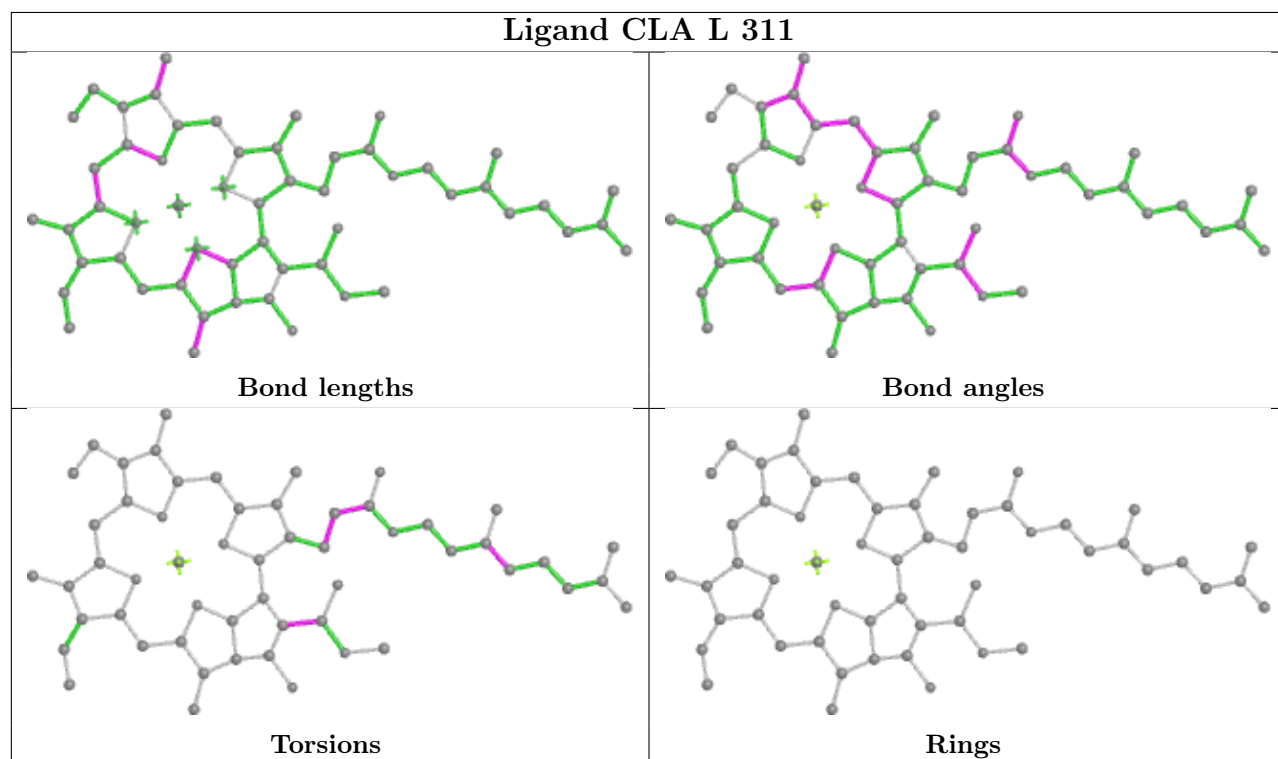
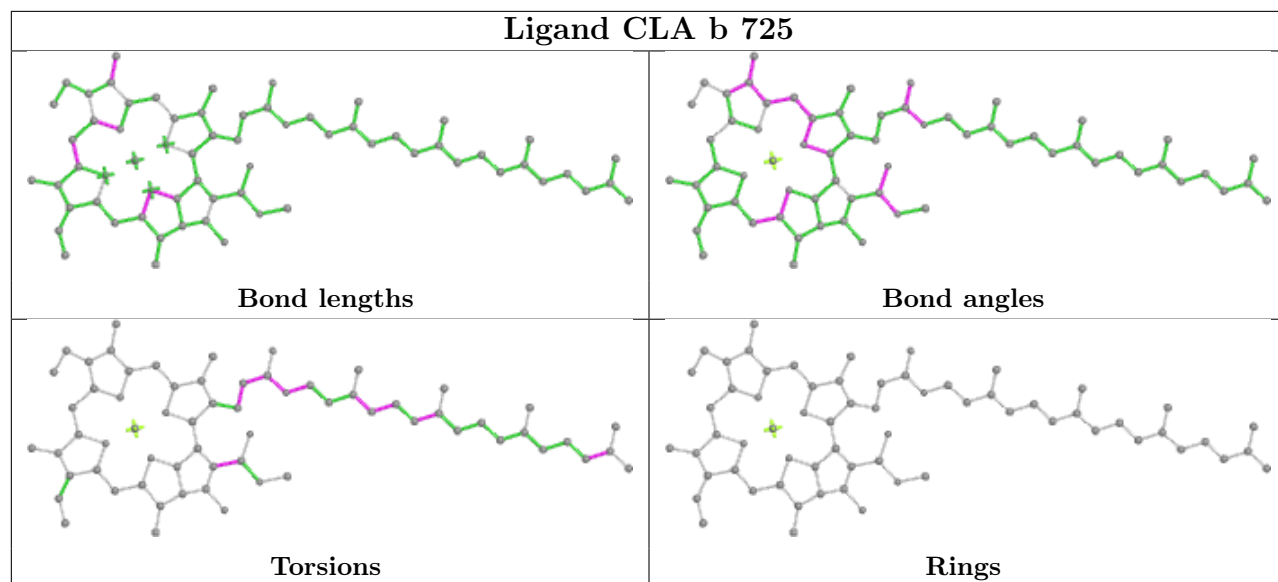


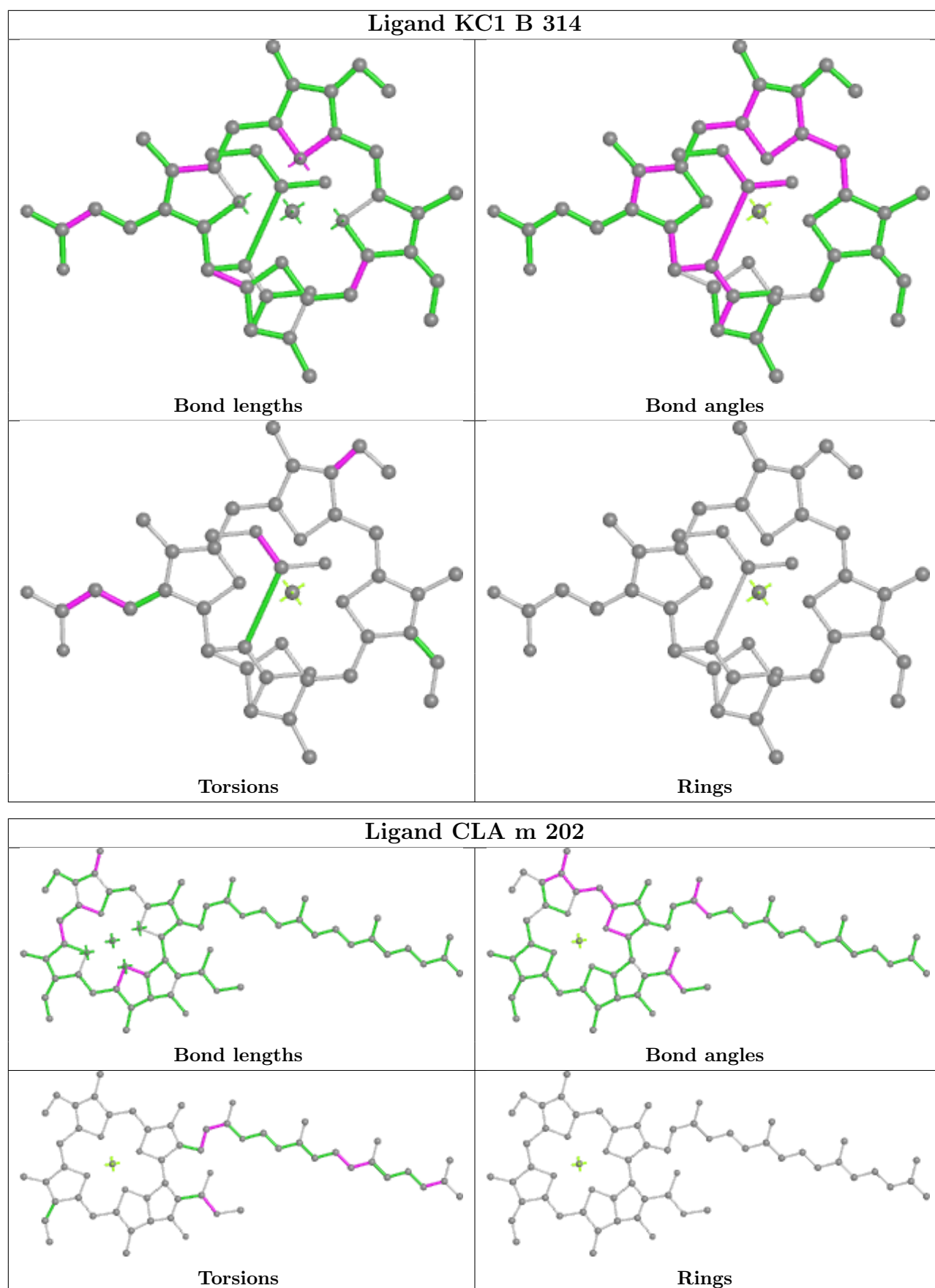


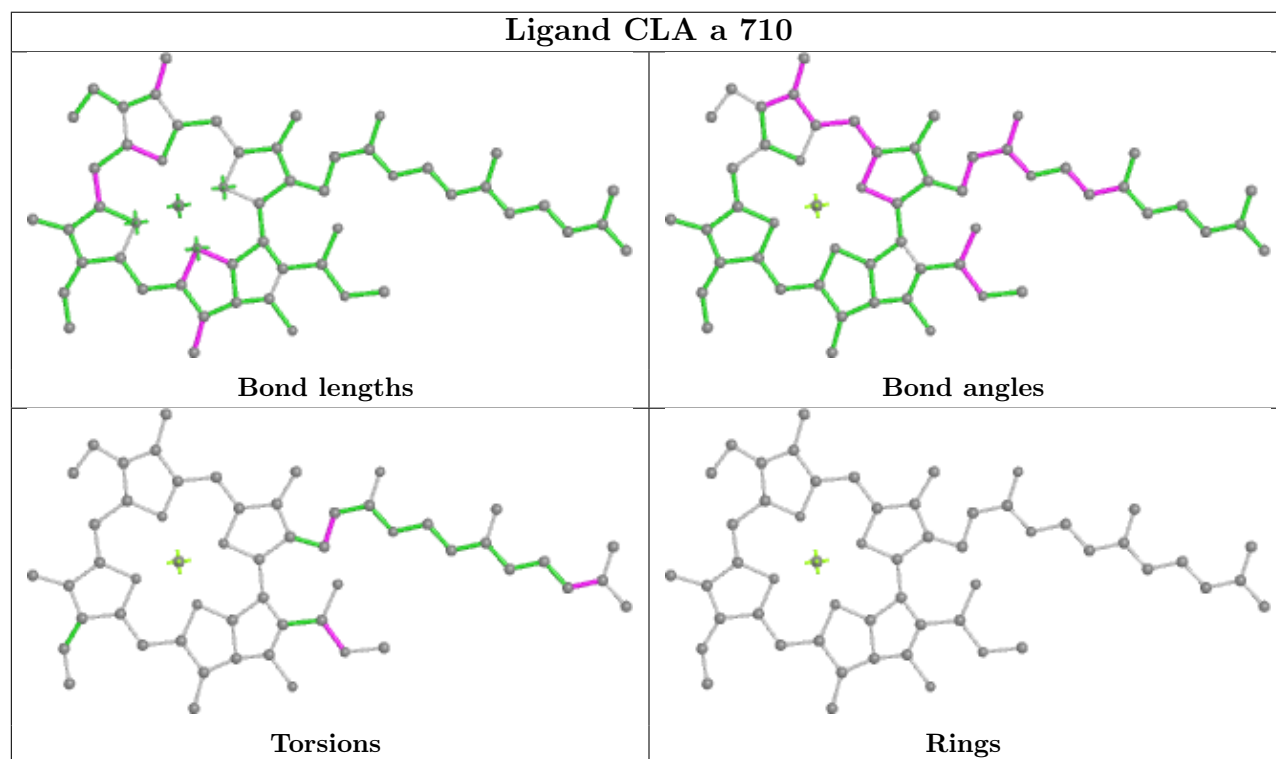
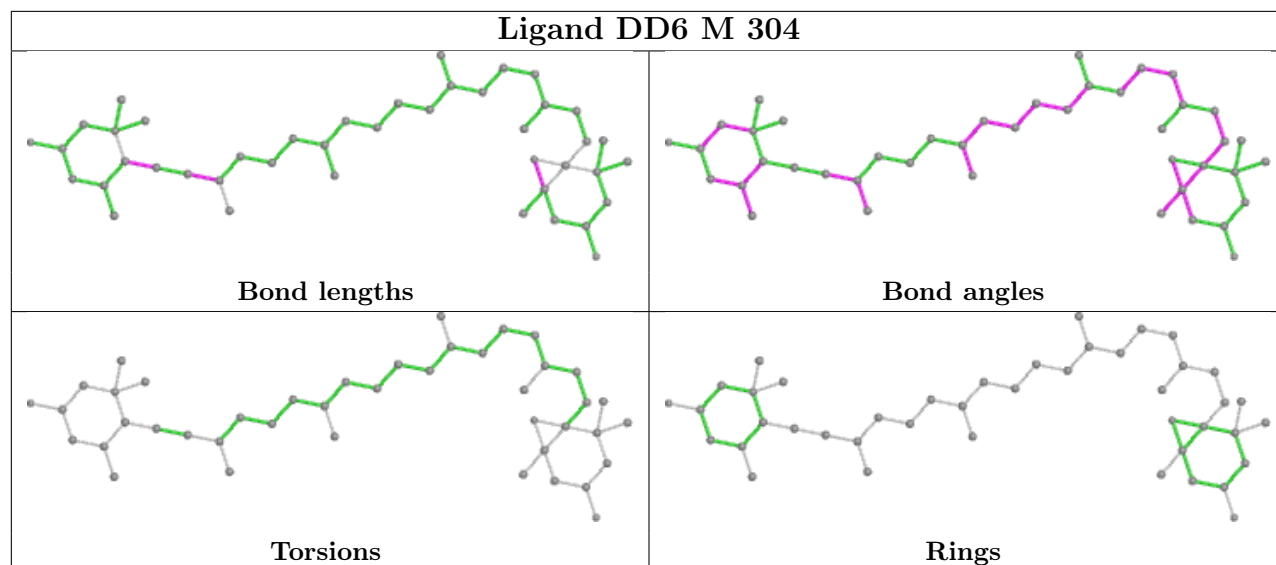


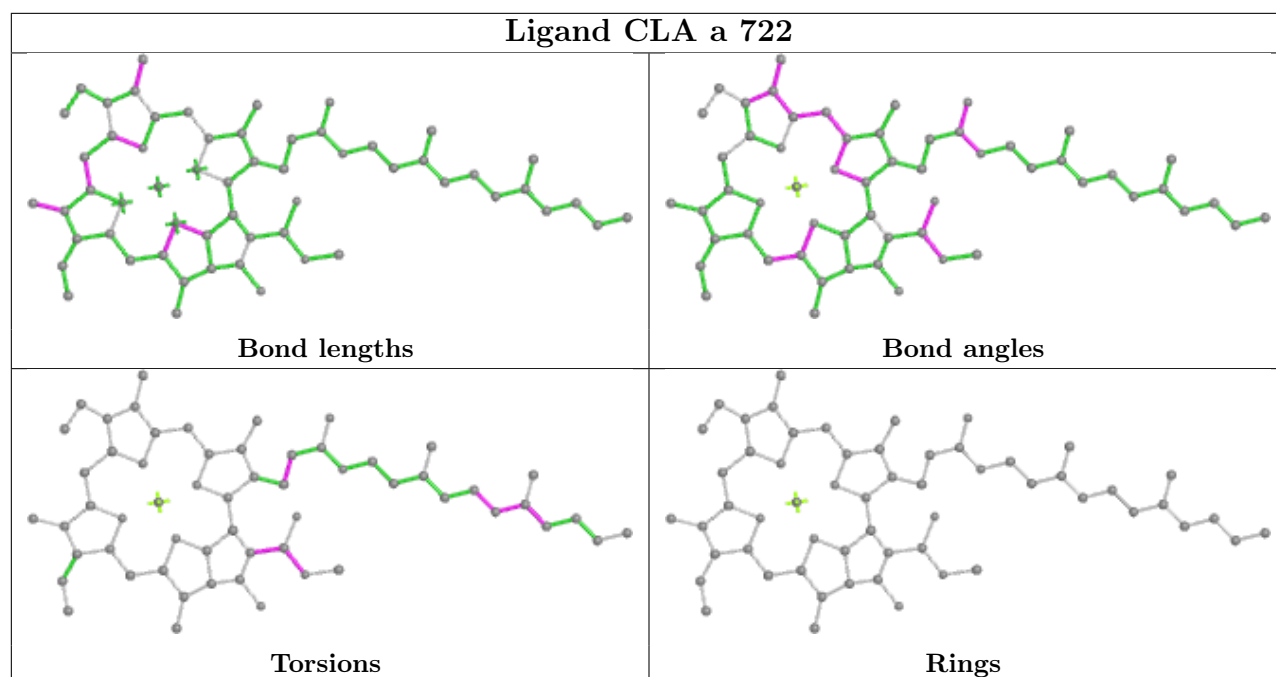
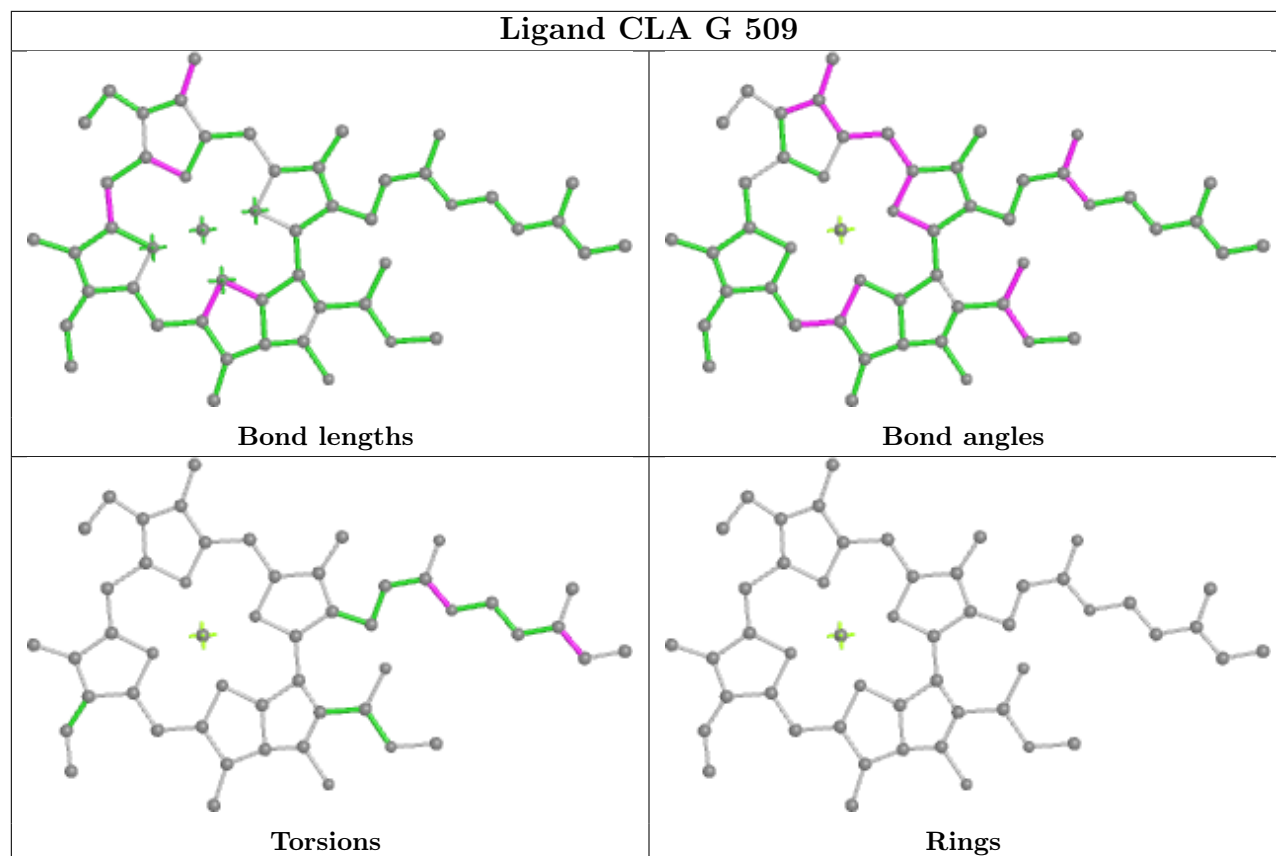


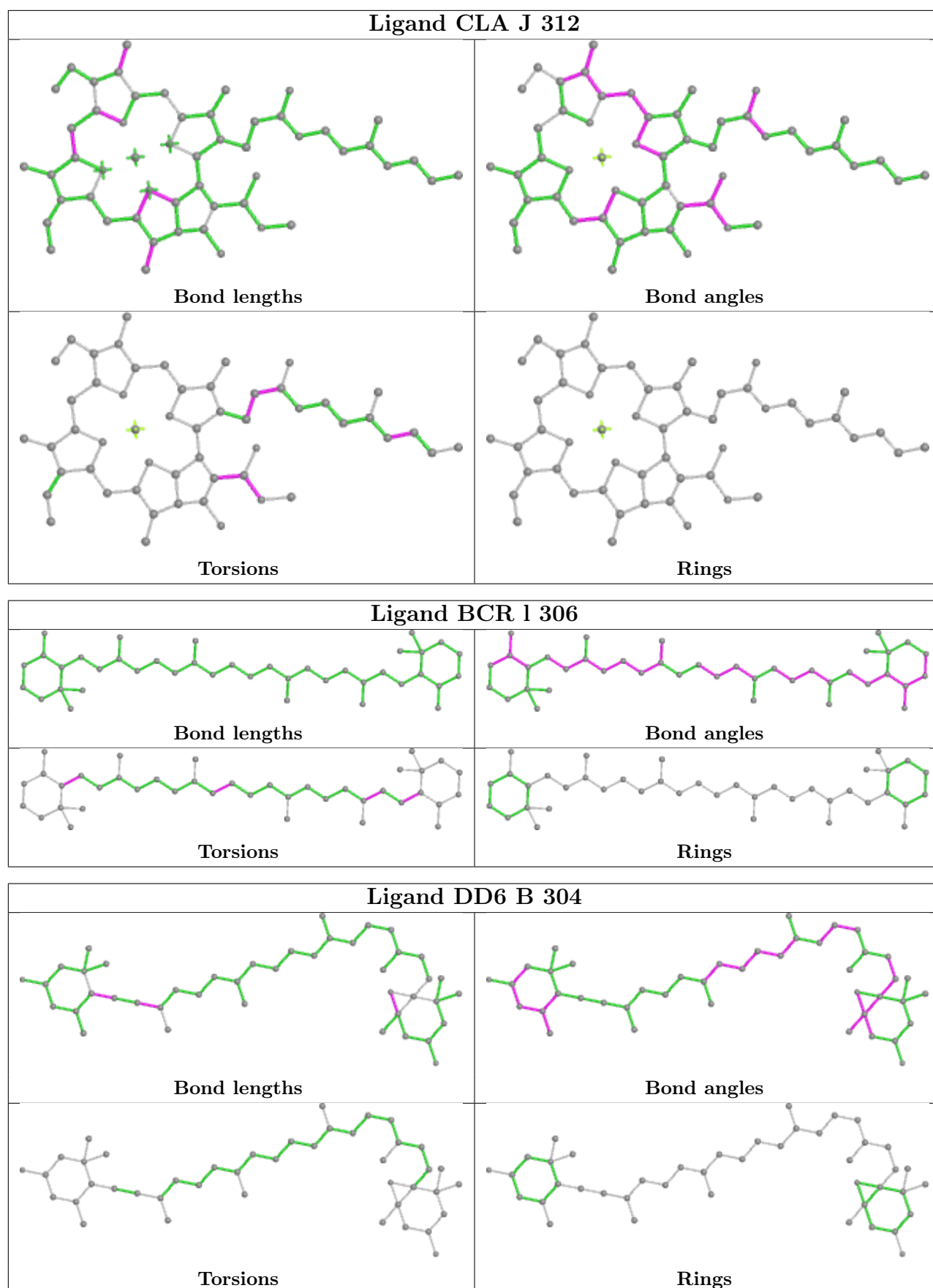


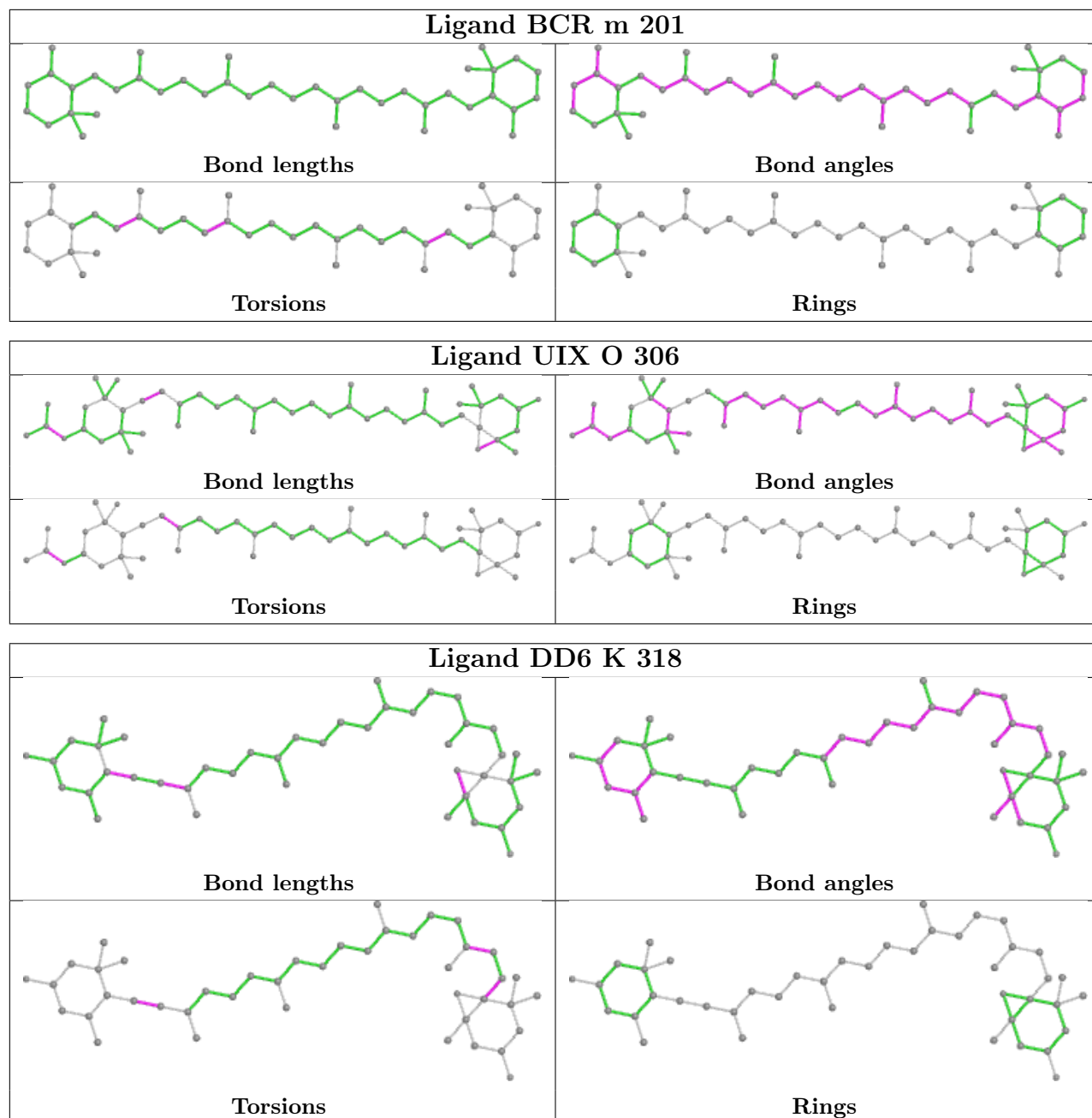


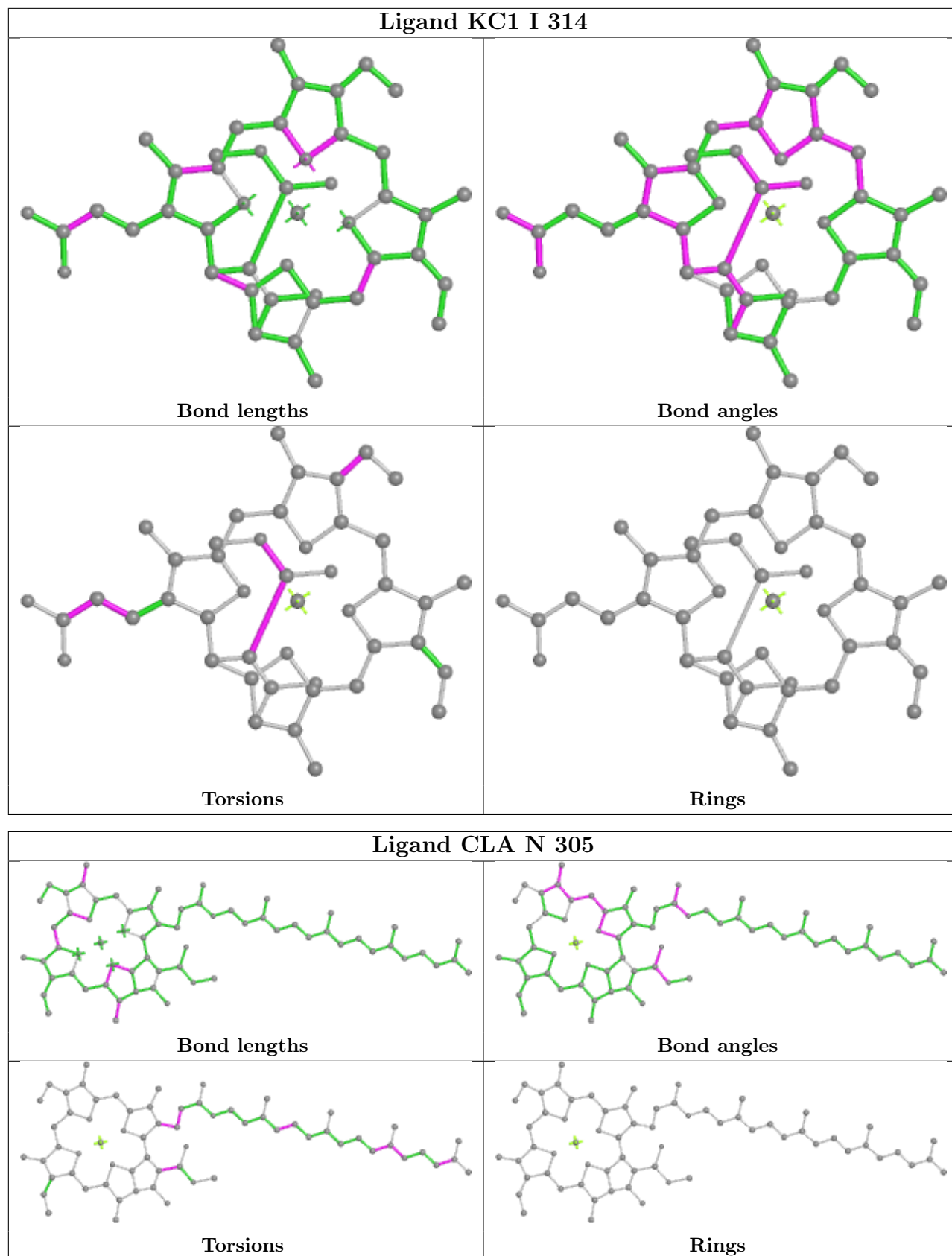


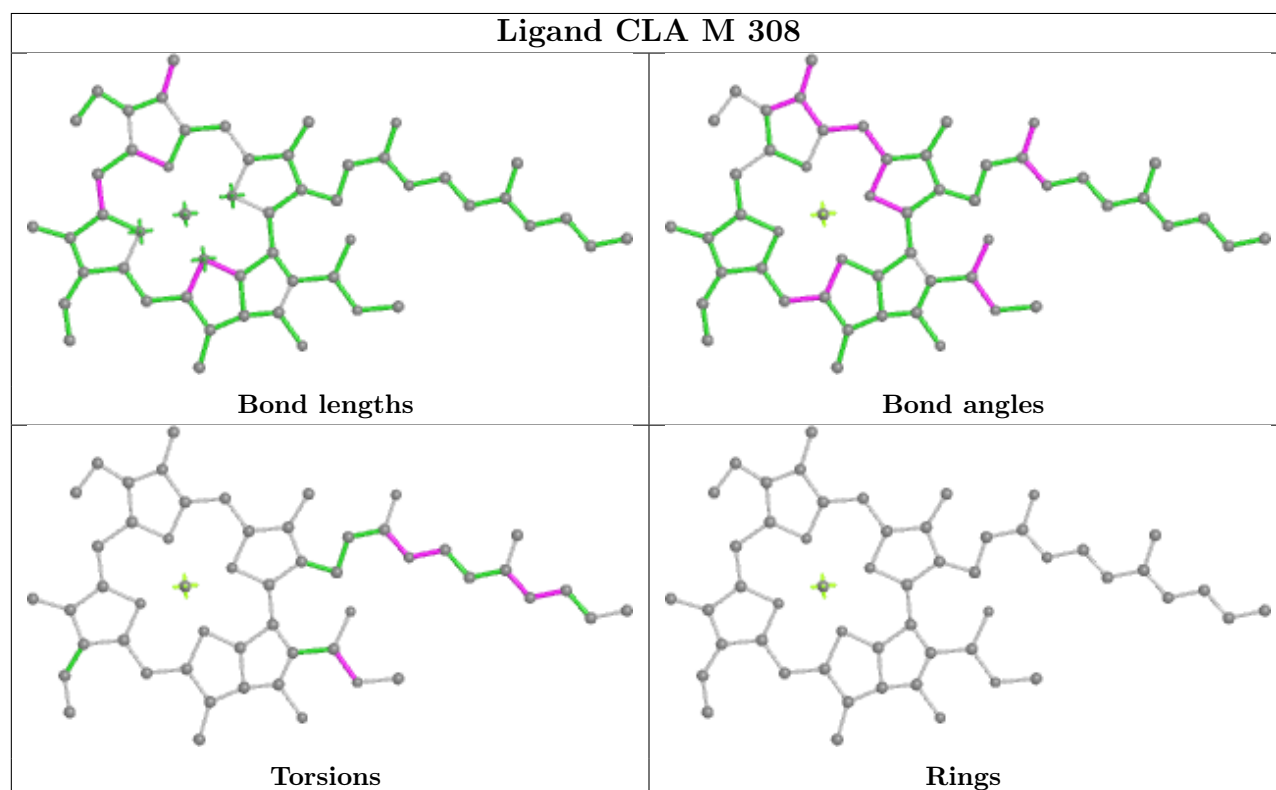
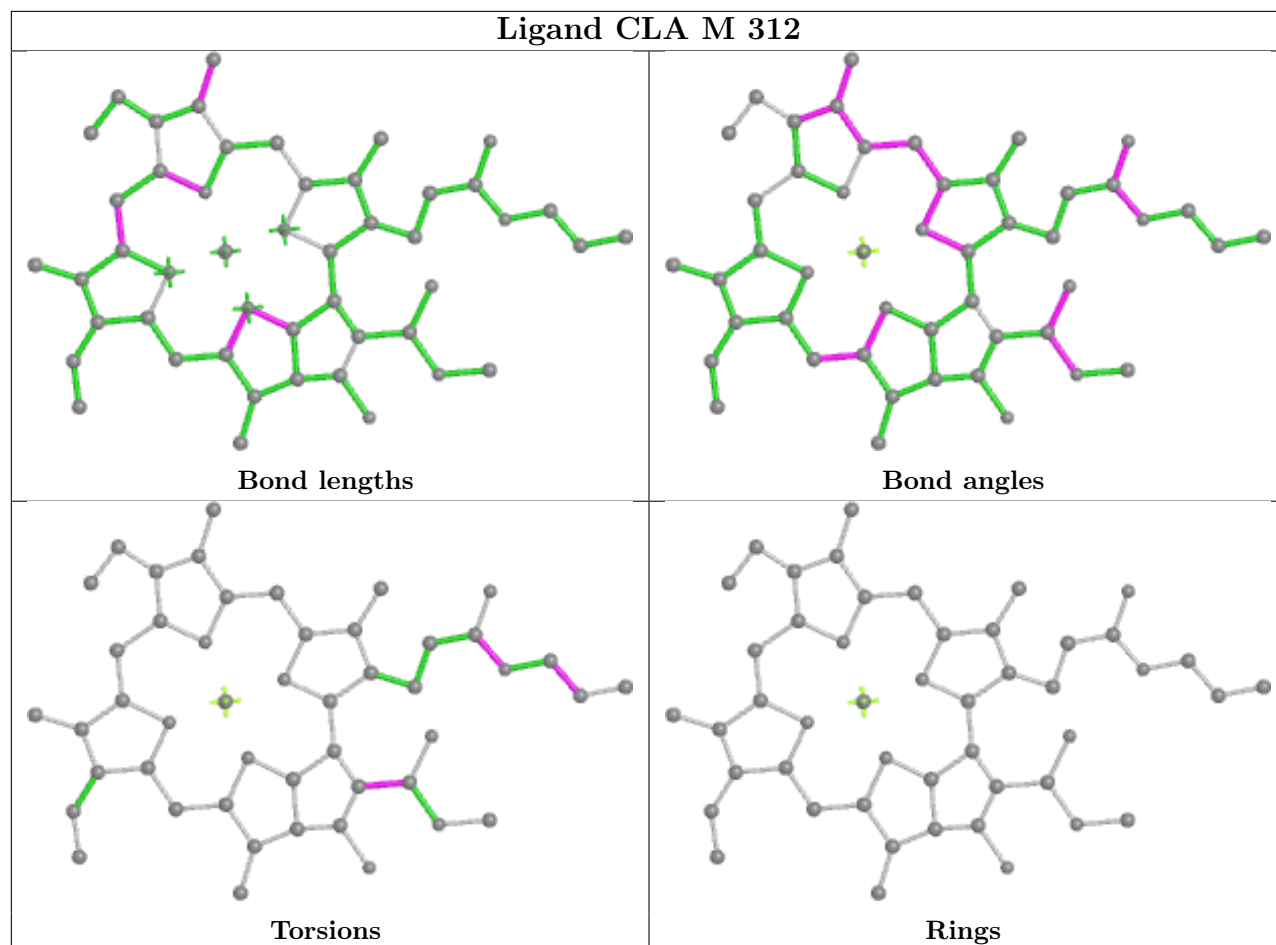


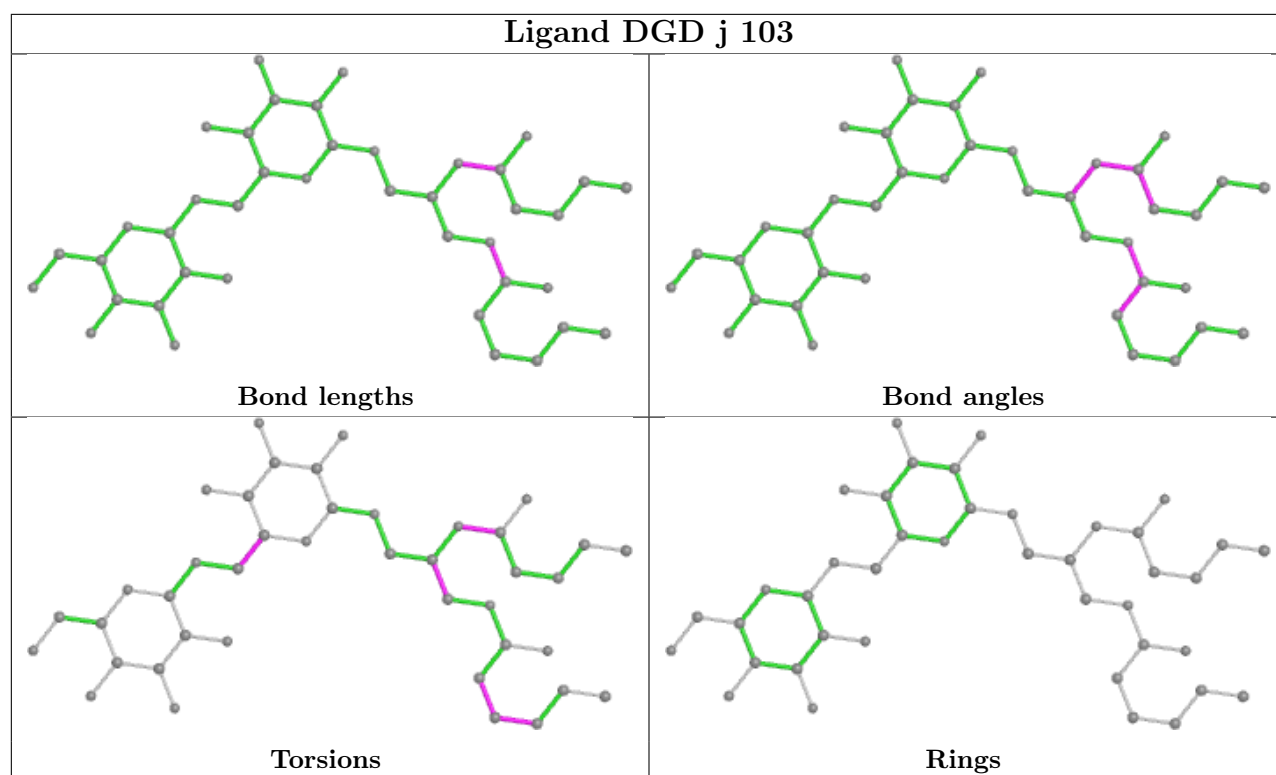












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

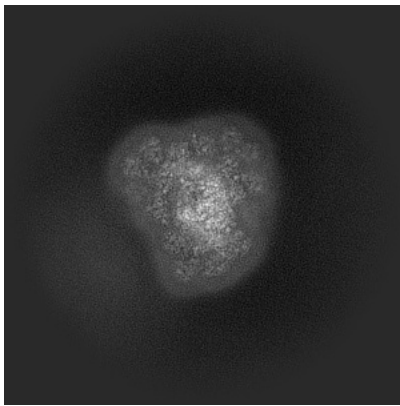
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36742. These allow visual inspection of the internal detail of the map and identification of artifacts.

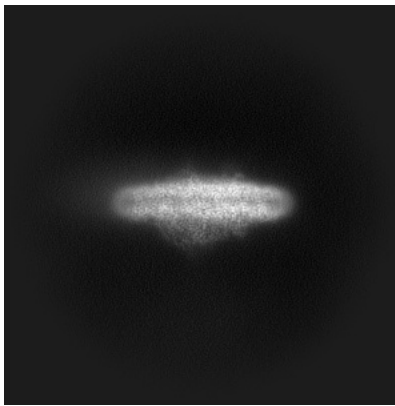
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

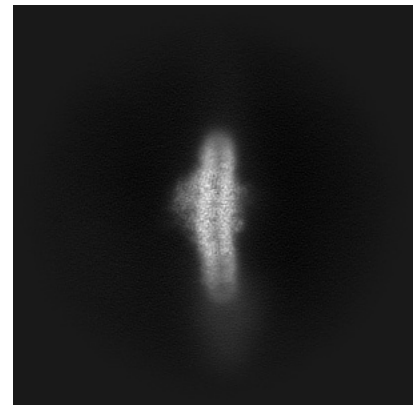
6.1.1 Primary map



X

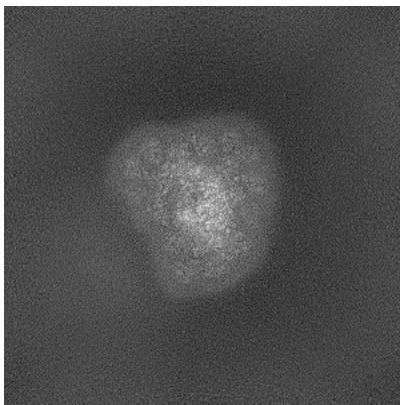


Y

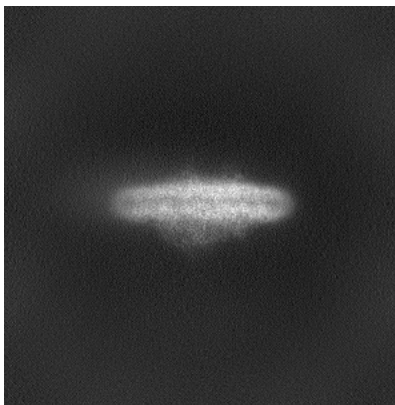


Z

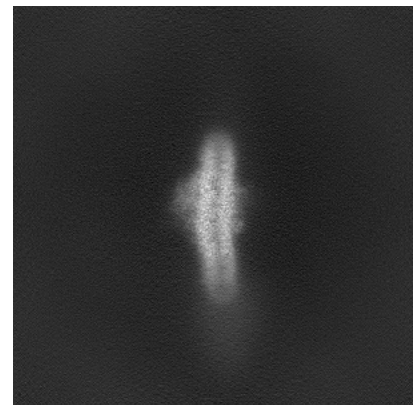
6.1.2 Raw map



X



Y

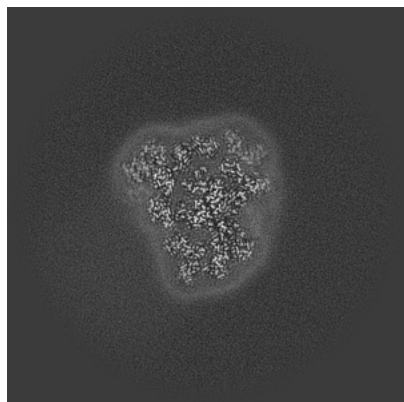


Z

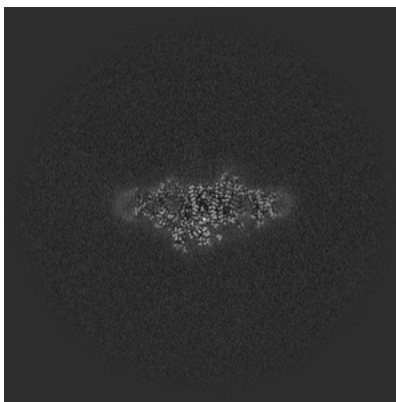
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

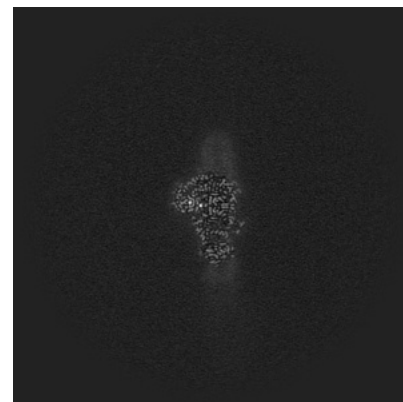
6.2.1 Primary map



X Index: 256

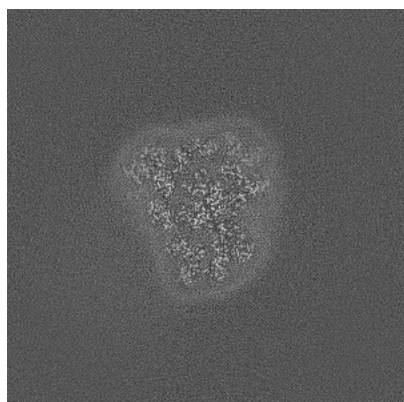


Y Index: 256

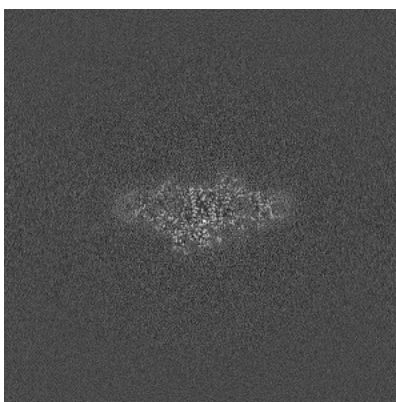


Z Index: 256

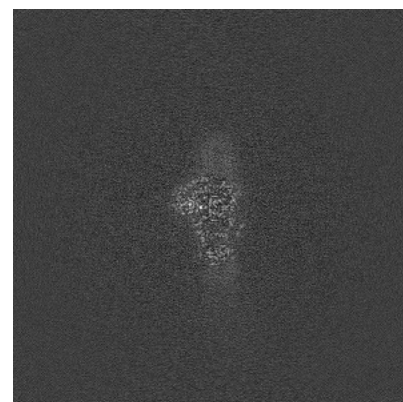
6.2.2 Raw map



X Index: 256



Y Index: 256

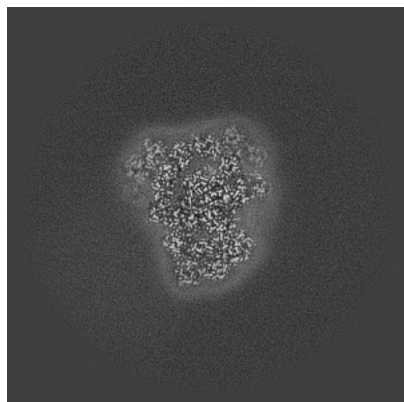


Z Index: 256

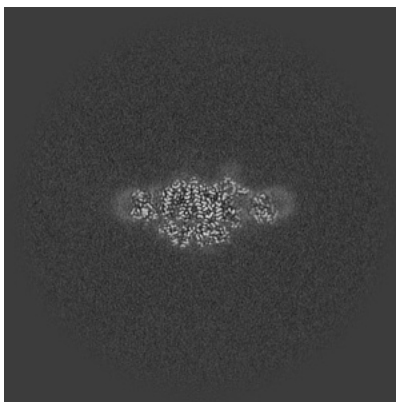
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

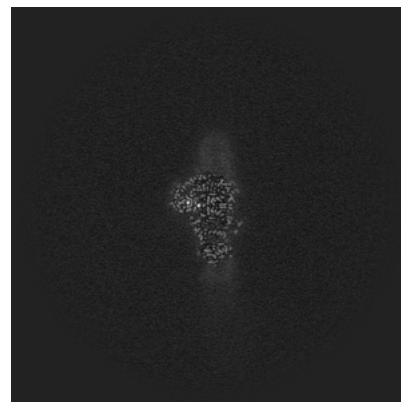
6.3.1 Primary map



X Index: 250

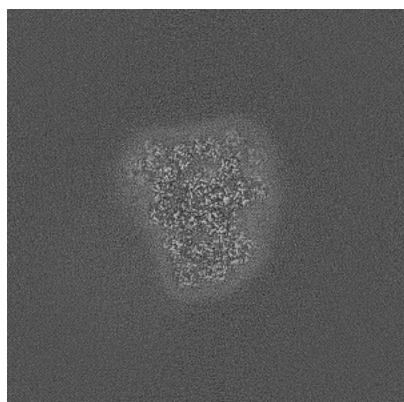


Y Index: 264

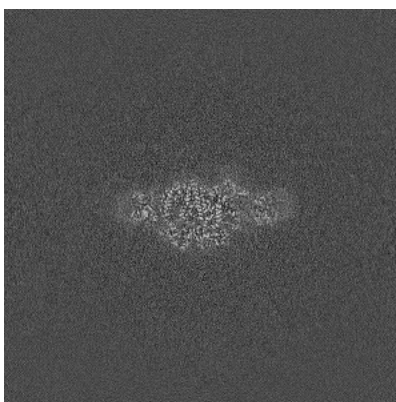


Z Index: 256

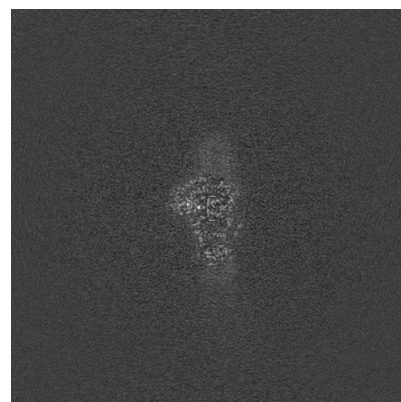
6.3.2 Raw map



X Index: 250



Y Index: 264

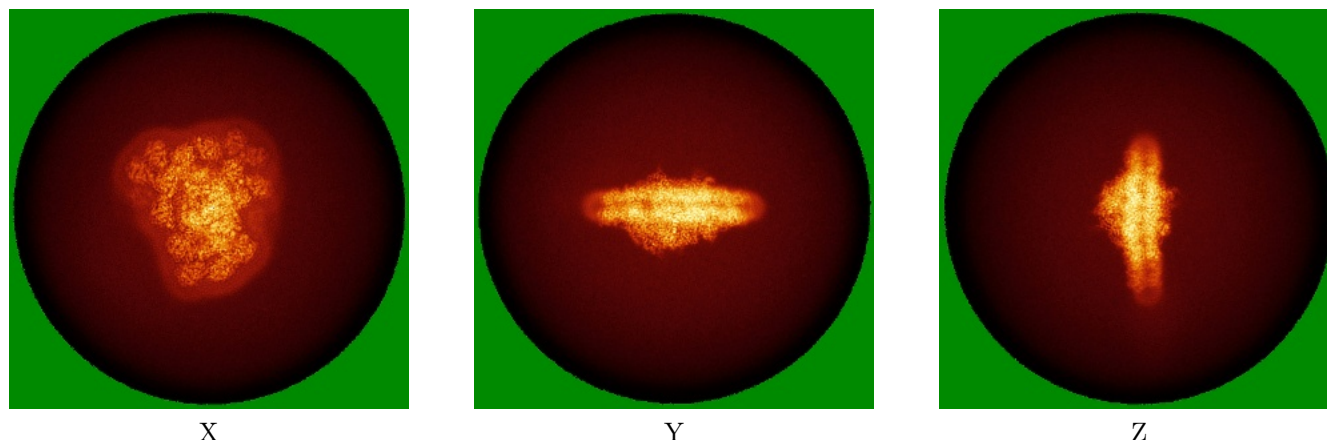


Z Index: 256

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

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

6.4.1 Primary map

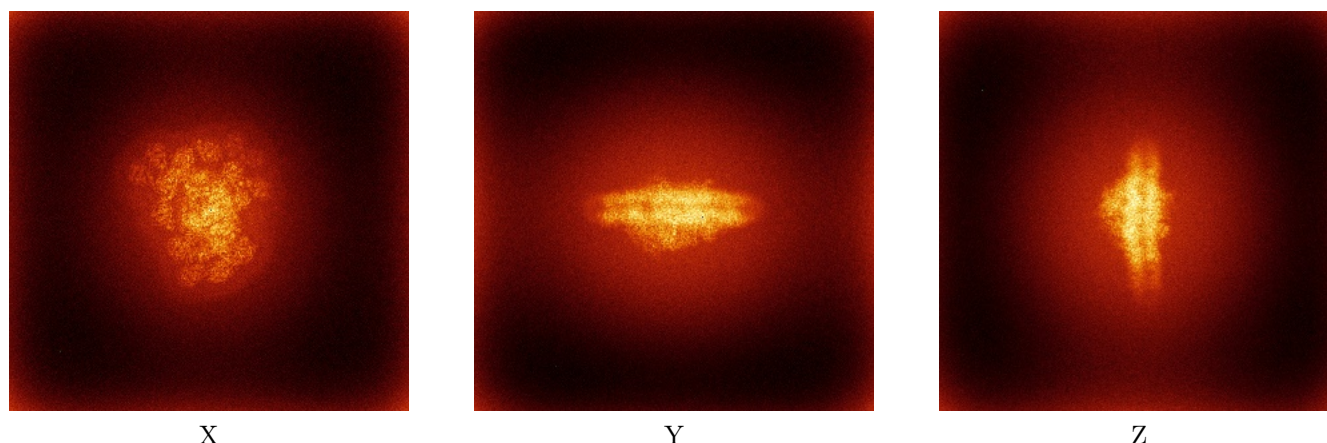


X

Y

Z

6.4.2 Raw map



X

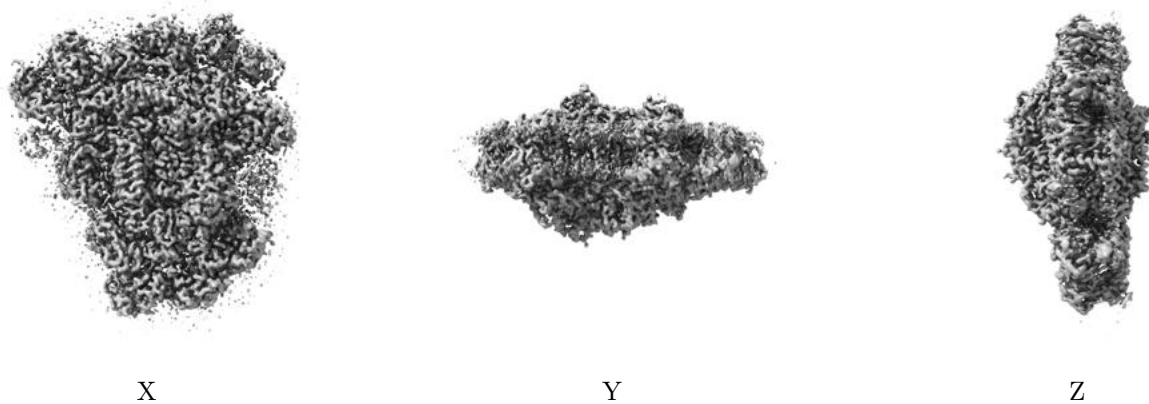
Y

Z

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

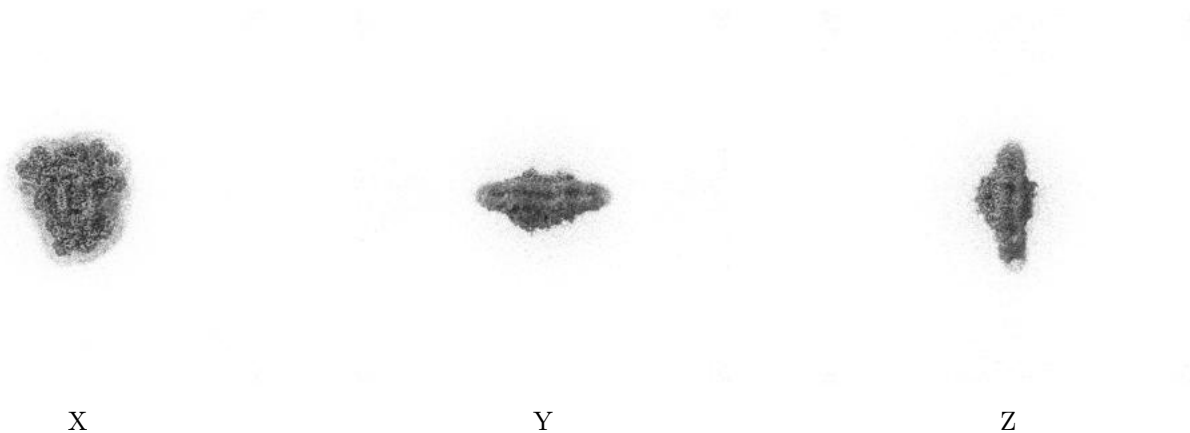
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.235. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

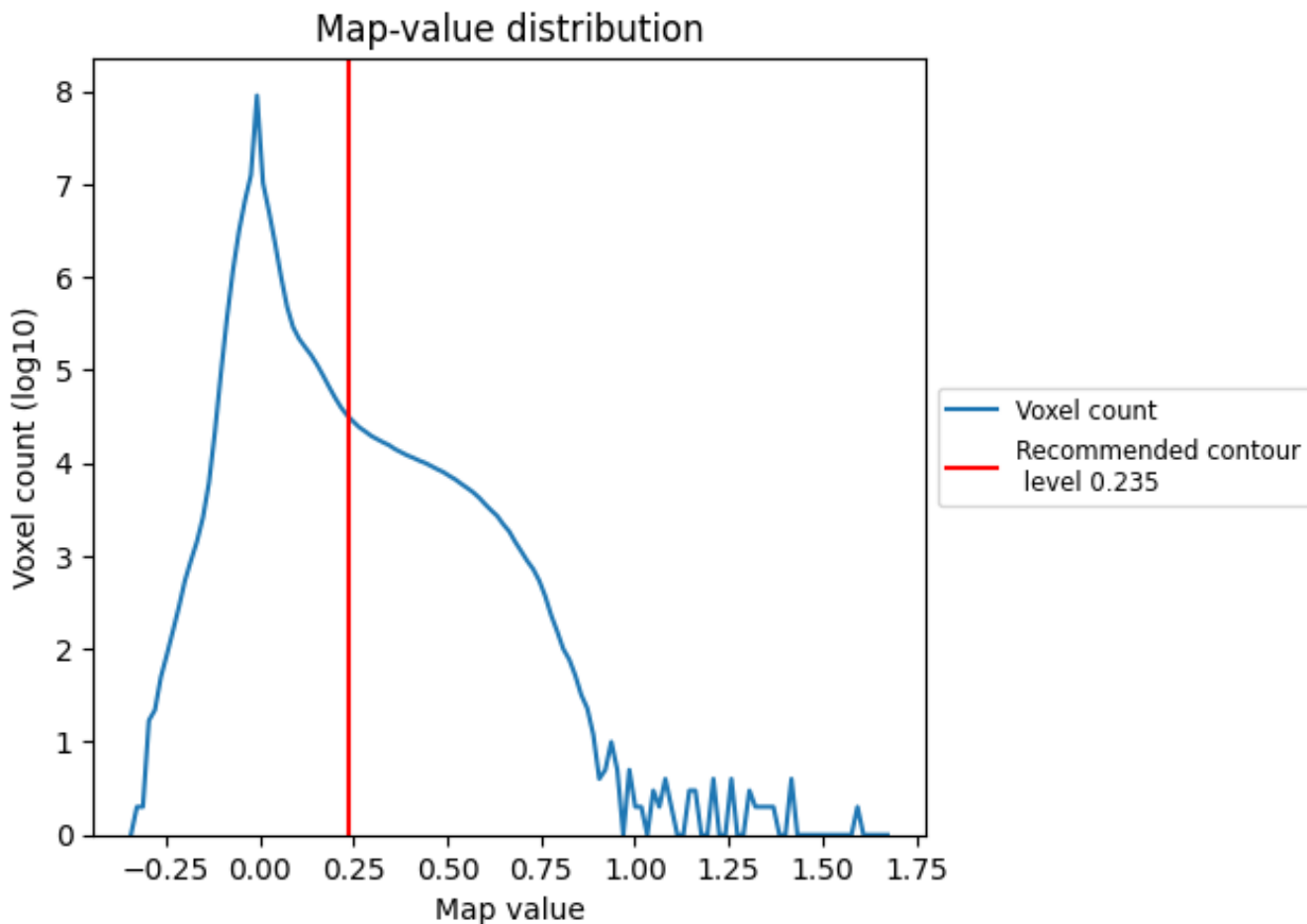
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

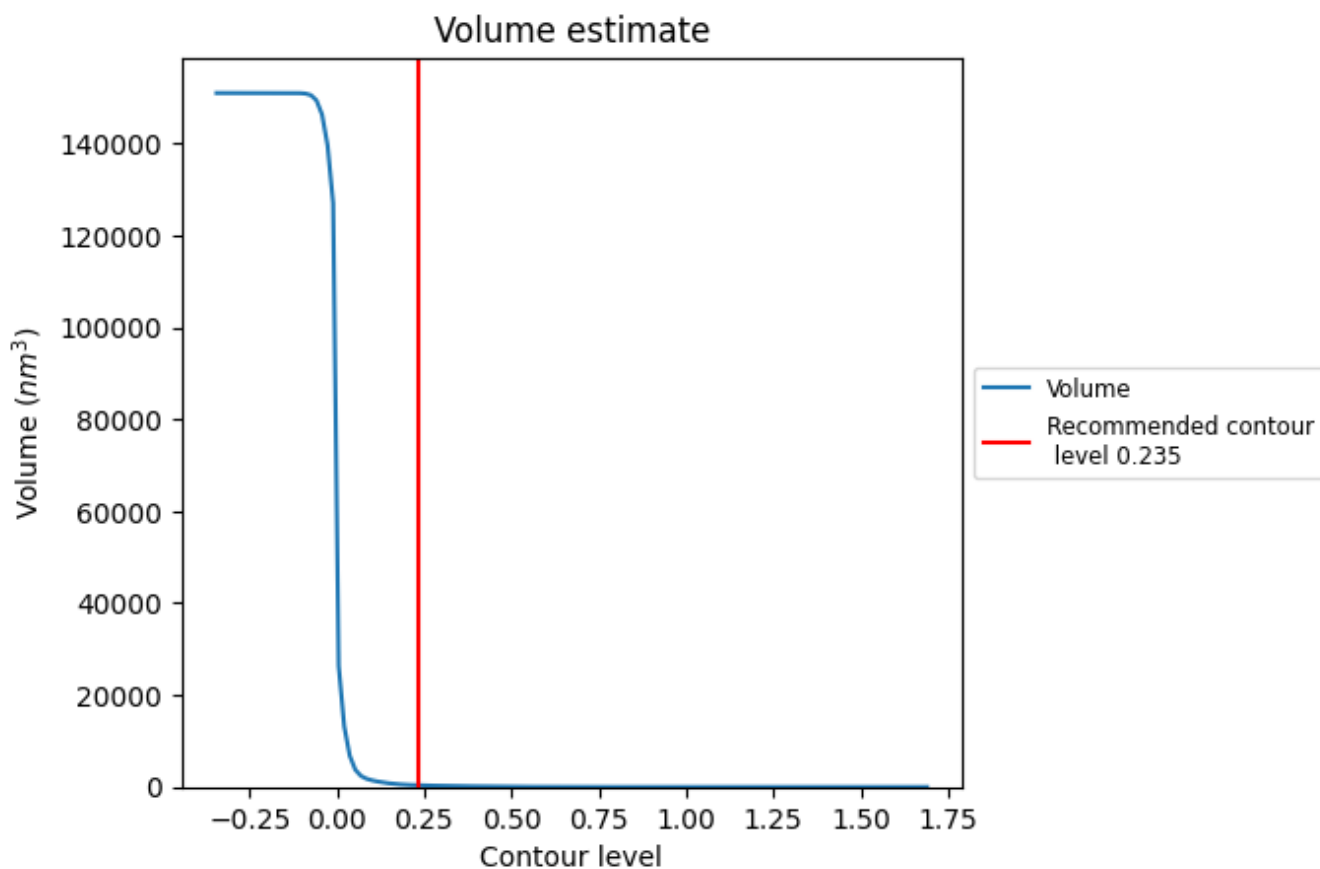
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

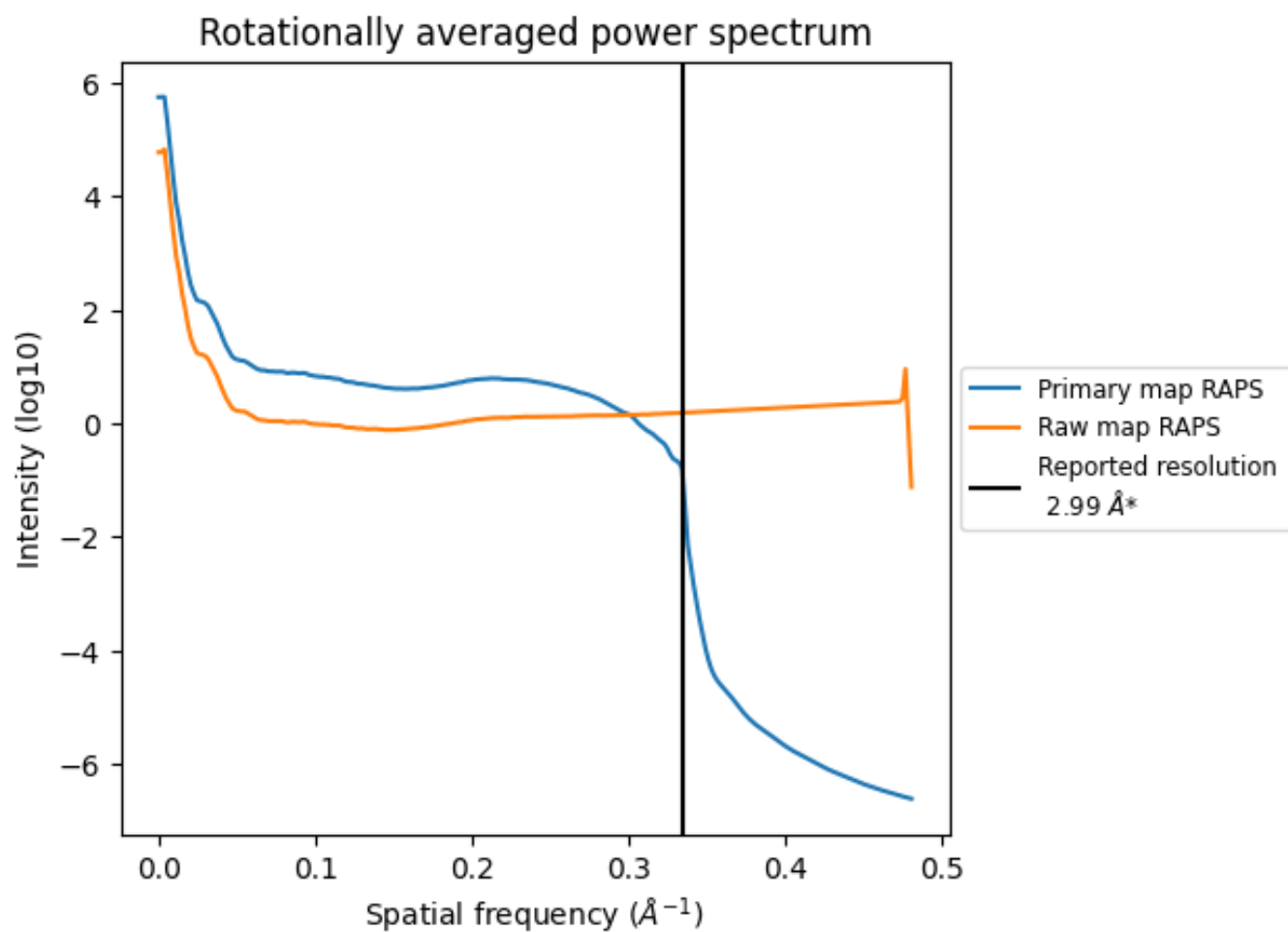
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 363 nm^3 ; this corresponds to an approximate mass of 328 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

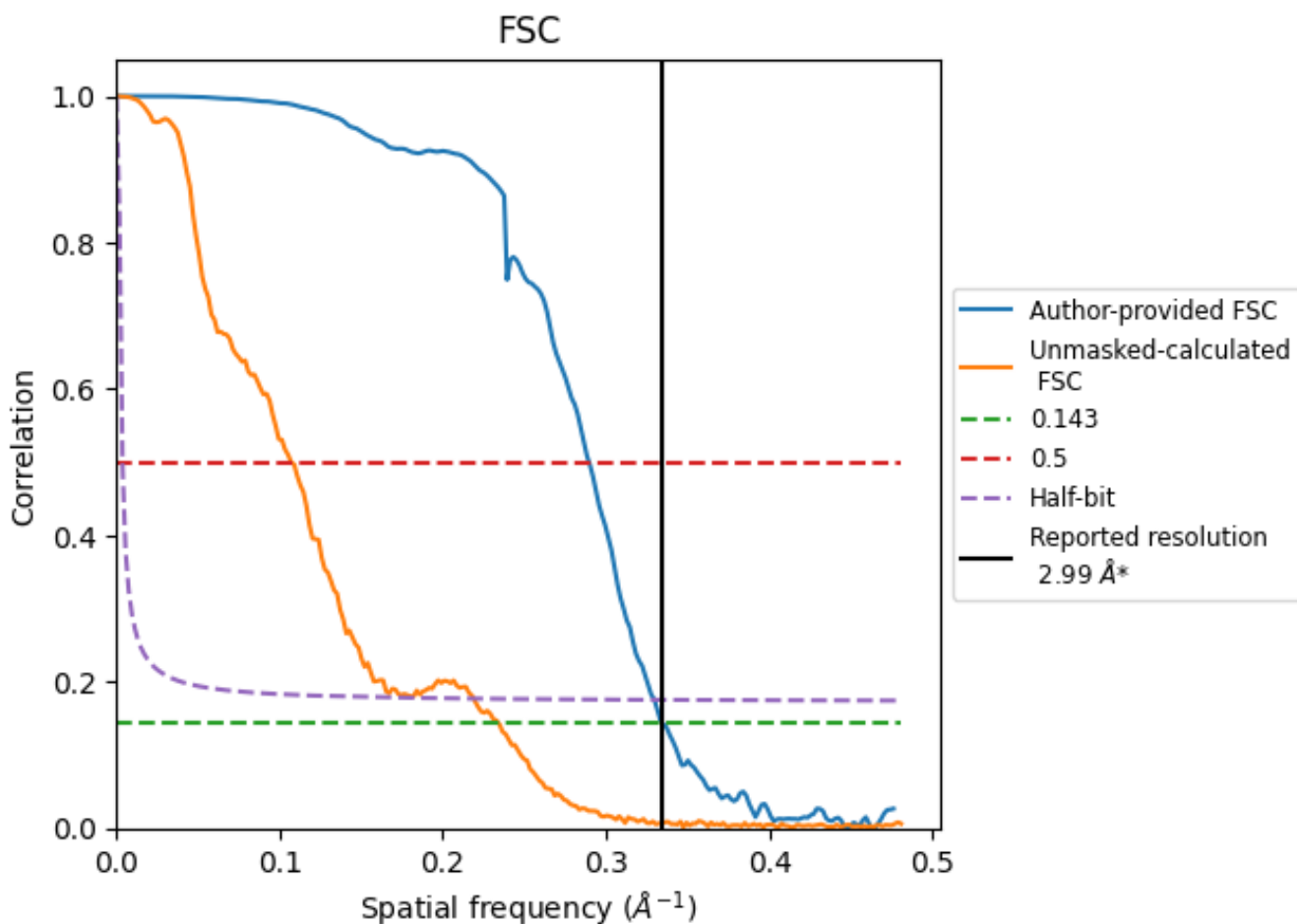


*Reported resolution corresponds to spatial frequency of 0.334 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.334 Å⁻¹

8.2 Resolution estimates [i](#)

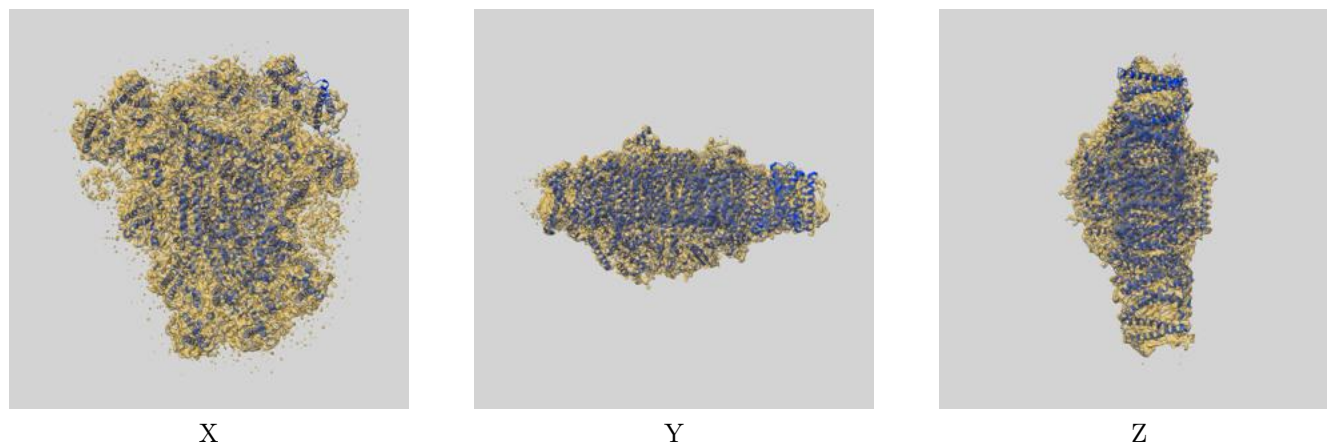
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.45	3.03
Unmasked-calculated*	4.27	9.35	4.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 2.99 by more than 10 %

9 Map-model fit [i](#)

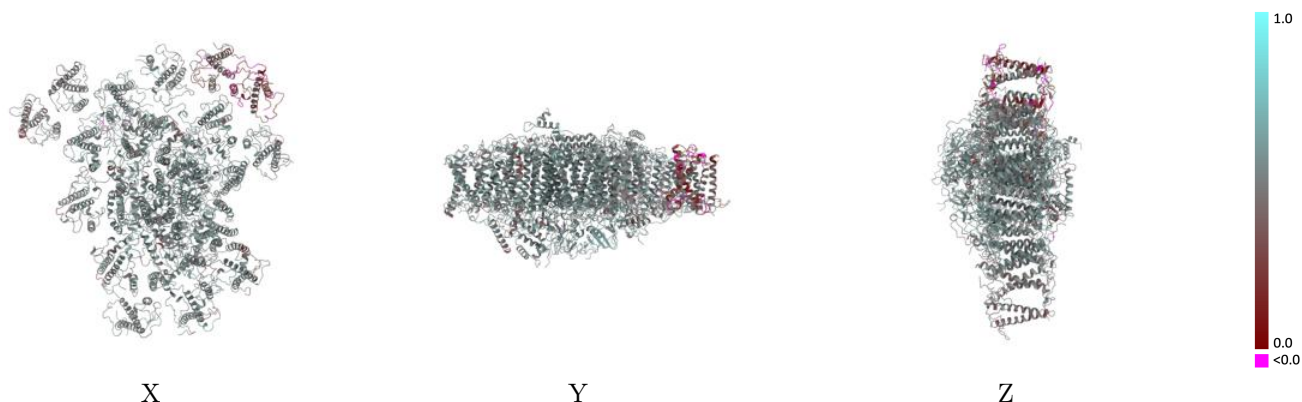
This section contains information regarding the fit between EMDB map EMD-36742 and PDB model 8JZE. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



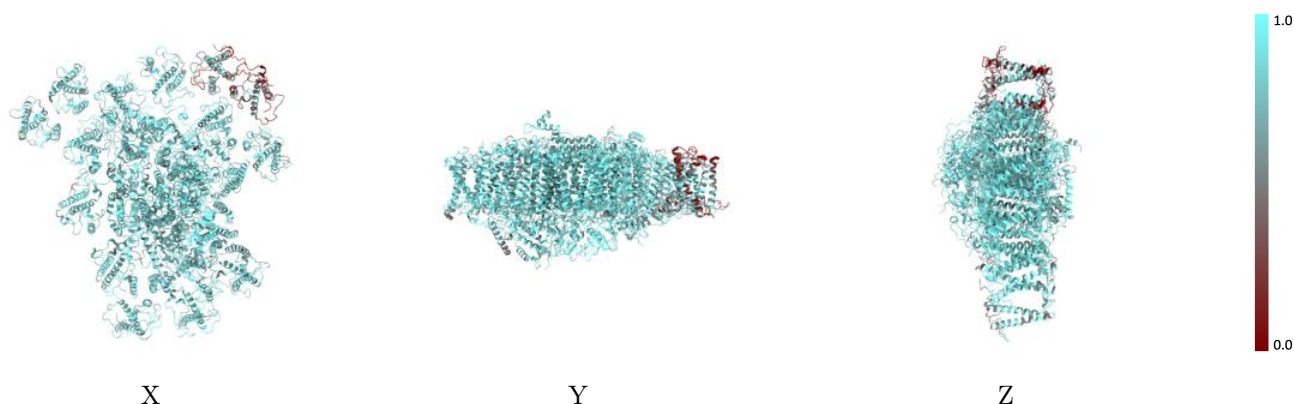
The images above show the 3D surface view of the map at the recommended contour level 0.235 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



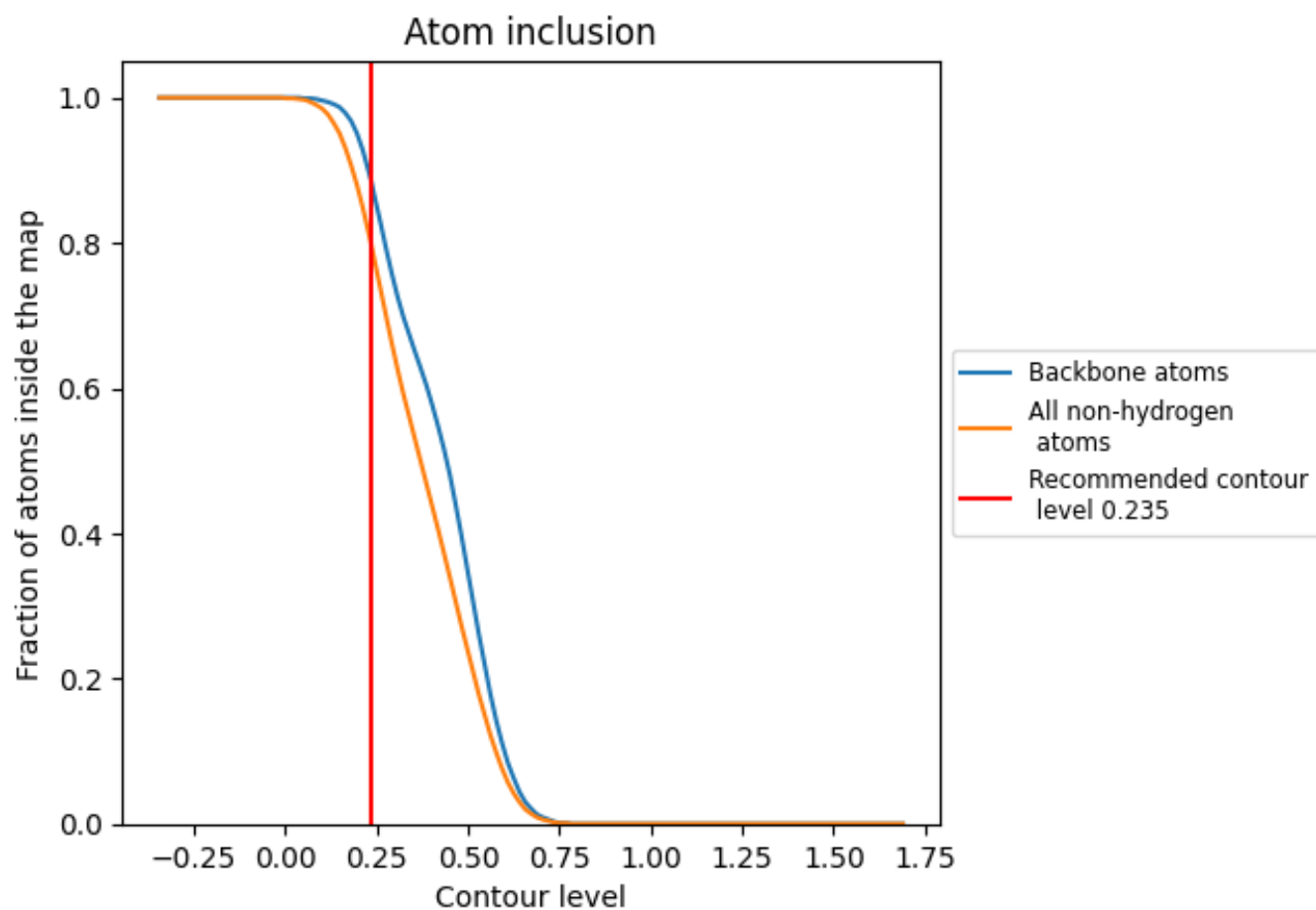
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.235).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.5180
A	 0.8360	 0.5390
B	 0.7940	 0.5260
D	 0.7490	 0.5080
F	 0.7320	 0.4980
G	 0.8000	 0.5170
H	 0.3060	 0.2340
I	 0.7850	 0.5140
J	 0.8410	 0.5330
K	 0.8600	 0.5510
L	 0.8440	 0.5460
M	 0.7800	 0.5200
N	 0.4940	 0.3650
O	 0.6780	 0.4560
P	 0.7250	 0.4850
a	 0.8560	 0.5470
b	 0.8710	 0.5530
c	 0.9280	 0.5570
d	 0.8550	 0.5450
e	 0.8990	 0.5640
f	 0.8330	 0.5420
h	 0.8660	 0.5480
i	 0.8360	 0.5320
j	 0.7800	 0.5310
l	 0.8610	 0.5490
m	 0.8270	 0.5380
y	 0.8670	 0.5260
z	 0.9150	 0.5230

