



# wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 03:44 am GMT

PDB ID : 8C29  
EMDB ID : EMD-16389  
Title : Cryo-EM structure of photosystem II C2S2 supercomplex from Norway spruce (Picea abies) at 2.8 Angstrom resolution  
Authors : Kopecny, D.; Semchonok, D.A.; Kouril, R.  
Deposited on : 2022-12-21  
Resolution : 2.79 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

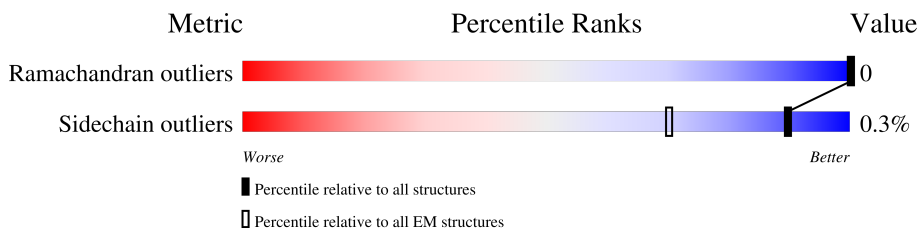
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.79 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	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	353	
1	a	353	
2	B	508	
2	b	508	
3	C	473	
3	c	473	
4	D	353	
4	d	353	
5	E	83	

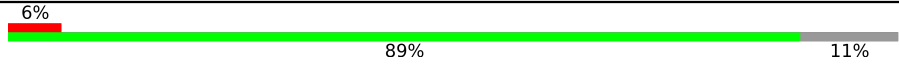
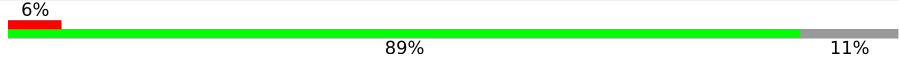


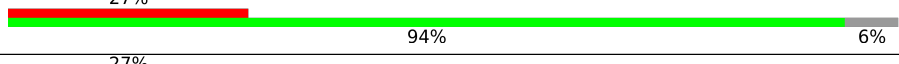
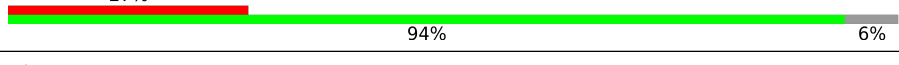
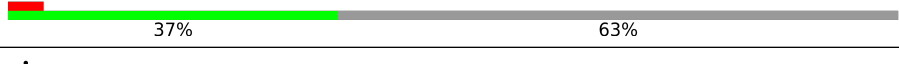



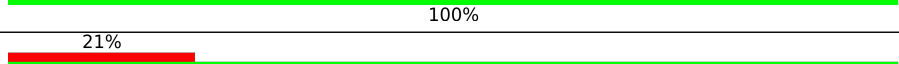
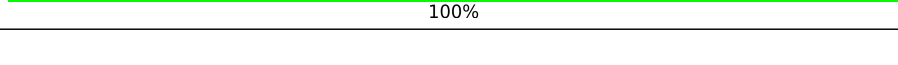
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Mol	Chain	Length	Quality of chain	
5	e	83	5%	78% 22%
6	F	39	5%	77% 23%
6	f	39	8%	77% 23%
7	G	275	9%	79% 21%
7	N	275	5%	79% 21%
7	Y	275	•	79% 21%
7	g	275	10%	79% 21%
7	n	275	6%	79% 21%
7	y	275	•	79% 21%
8	H	75	•	81% 17%
8	h	75	•	81% 17%
9	I	36	8%	100%
9	i	36	8%	100%
10	K	59	•	63% 37%
10	k	59	•	63% 37%
11	L	38	5%	95% 5%
11	l	38	5%	95% 5%
12	M	37	•	84% 16%
12	m	37	5%	84% 16%
13	O	341	10%	56% 44%
13	o	341	11%	56% 44%
14	R	300	•	73% 27%
14	r	300	5%	73% 27%
15	S	303	18%	69% 30%
15	s	303	18%	69% 30%

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Mol	Chain	Length	Quality of chain
16	T	35	
16	t	35	
17	U	133	
17	u	133	
18	V	33	
18	v	33	
19	W	146	
19	w	146	
20	X	129	
20	x	129	
21	Z	62	
21	z	62	

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
23	CLA	A	402	X	-	-	-
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	G	602	X	-	-	-
23	CLA	G	603	X	-	-	-
23	CLA	G	604	X	-	-	-
23	CLA	G	610	X	-	-	-
23	CLA	G	611	X	-	-	-
23	CLA	G	612	X	-	-	-
23	CLA	G	613	X	-	-	-
23	CLA	G	614	X	-	-	-
23	CLA	N	602	X	-	-	-
23	CLA	N	603	X	-	-	-
23	CLA	N	604	X	-	-	-
23	CLA	N	610	X	-	-	-
23	CLA	N	611	X	-	-	-
23	CLA	N	612	X	-	-	-
23	CLA	N	613	X	-	-	-
23	CLA	N	614	X	-	-	-
23	CLA	R	601	X	-	-	-
23	CLA	R	602	X	-	-	-
23	CLA	R	603	X	-	-	-
23	CLA	R	604	X	-	-	-
23	CLA	R	608	X	-	-	-
23	CLA	R	609	X	-	-	-
23	CLA	R	610	X	-	-	-
23	CLA	R	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	R	612	X	-	-	-
23	CLA	S	602	X	-	-	-
23	CLA	S	603	X	-	-	-
23	CLA	S	604	X	-	-	-
23	CLA	S	608	X	-	-	-
23	CLA	S	609	X	-	-	-
23	CLA	S	610	X	-	-	-
23	CLA	S	611	X	-	-	-
23	CLA	S	612	X	-	-	-
23	CLA	S	613	X	-	-	-
23	CLA	Y	303	X	-	-	-
23	CLA	Y	304	X	-	-	-
23	CLA	Y	305	X	-	-	-
23	CLA	Y	310	X	-	-	-
23	CLA	Y	311	X	-	-	-
23	CLA	Y	312	X	-	-	-
23	CLA	Y	313	X	-	-	-
23	CLA	Y	314	X	-	-	-
23	CLA	a	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	405	X	-	-	-
23	CLA	d	406	X	-	-	-
23	CLA	g	602	X	-	-	-
23	CLA	g	603	X	-	-	-
23	CLA	g	604	X	-	-	-
23	CLA	g	610	X	-	-	-
23	CLA	g	611	X	-	-	-
23	CLA	g	612	X	-	-	-
23	CLA	g	613	X	-	-	-
23	CLA	g	614	X	-	-	-
23	CLA	n	602	X	-	-	-
23	CLA	n	603	X	-	-	-
23	CLA	n	604	X	-	-	-
23	CLA	n	610	X	-	-	-
23	CLA	n	611	X	-	-	-
23	CLA	n	612	X	-	-	-
23	CLA	n	613	X	-	-	-
23	CLA	n	614	X	-	-	-
23	CLA	r	601	X	-	-	-
23	CLA	r	602	X	-	-	-
23	CLA	r	603	X	-	-	-
23	CLA	r	604	X	-	-	-
23	CLA	r	608	X	-	-	-
23	CLA	r	609	X	-	-	-
23	CLA	r	610	X	-	-	-
23	CLA	r	611	X	-	-	-
23	CLA	r	612	X	-	-	-
23	CLA	s	602	X	-	-	-
23	CLA	s	603	X	-	-	-
23	CLA	s	604	X	-	-	-
23	CLA	s	608	X	-	-	-
23	CLA	s	609	X	-	-	-
23	CLA	s	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	s	611	X	-	-	-
23	CLA	s	612	X	-	-	-
23	CLA	s	613	X	-	-	-
23	CLA	y	304	X	-	-	-
23	CLA	y	305	X	-	-	-
23	CLA	y	306	X	-	-	-
23	CLA	y	311	X	-	-	-
23	CLA	y	312	X	-	-	-
23	CLA	y	313	X	-	-	-
23	CLA	y	314	X	-	-	-
23	CLA	y	315	X	-	-	-
39	CHL	G	601	X	-	-	-
39	CHL	G	605	X	-	-	-
39	CHL	G	606	X	-	-	-
39	CHL	G	607	X	-	-	-
39	CHL	G	608	X	-	-	-
39	CHL	G	609	X	-	-	-
39	CHL	G	620	X	-	-	-
39	CHL	N	601	X	-	-	-
39	CHL	N	605	X	-	-	-
39	CHL	N	606	X	-	-	-
39	CHL	N	607	X	-	-	-
39	CHL	N	608	X	-	-	-
39	CHL	N	609	X	-	-	-
39	CHL	R	605	X	-	-	-
39	CHL	R	606	X	-	-	-
39	CHL	R	607	X	-	-	-
39	CHL	S	601	X	-	-	-
39	CHL	S	605	X	-	-	-
39	CHL	S	606	X	-	-	-
39	CHL	S	607	X	-	-	-
39	CHL	Y	302	X	-	-	-
39	CHL	Y	306	X	-	-	-
39	CHL	Y	307	X	-	-	-
39	CHL	Y	308	X	-	-	-
39	CHL	Y	309	X	-	-	-
39	CHL	g	601	X	-	-	-
39	CHL	g	605	X	-	-	-
39	CHL	g	606	X	-	-	-
39	CHL	g	607	X	-	-	-
39	CHL	g	608	X	-	-	-
39	CHL	g	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CHL	g	619	X	-	-	-
39	CHL	n	601	X	-	-	-
39	CHL	n	605	X	-	-	-
39	CHL	n	606	X	-	-	-
39	CHL	n	607	X	-	-	-
39	CHL	n	608	X	-	-	-
39	CHL	n	609	X	-	-	-
39	CHL	r	605	X	-	-	-
39	CHL	r	606	X	-	-	-
39	CHL	r	607	X	-	-	-
39	CHL	s	601	X	-	-	-
39	CHL	s	605	X	-	-	-
39	CHL	s	606	X	-	-	-
39	CHL	s	607	X	-	-	-
39	CHL	y	303	X	-	-	-
39	CHL	y	307	X	-	-	-
39	CHL	y	308	X	-	-	-
39	CHL	y	309	X	-	-	-
39	CHL	y	310	X	-	-	-

## 2 Entry composition [i](#)

There are 43 unique types of molecules in this entry. The entry contains 71174 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	321	Total	C	N	O	S	0	0
			2502	1637	412	440	13		
1	a	321	Total	C	N	O	S	0	0
			2502	1637	412	440	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	295	PHE	LEU	conflict	UNP P50155
a	295	PHE	LEU	conflict	UNP P50155

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	485	Total	C	N	O	S	0	0
			3812	2503	638	657	14		
2	b	485	Total	C	N	O	S	0	0
			3812	2503	638	657	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	464	PHE	SER	conflict	UNP R4ZGX1
b	464	PHE	SER	conflict	UNP R4ZGX1

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	433	Total	C	N	O	S	0	0
			3377	2224	565	578	10		
3	c	433	Total	C	N	O	S	0	0
			3377	2224	565	578	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	175	LEU	PRO	conflict	UNP R4ZGZ0
C	433	LEU	PRO	conflict	UNP R4ZGZ0
c	175	LEU	PRO	conflict	UNP R4ZGZ0
c	433	LEU	PRO	conflict	UNP R4ZGZ0

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	337	2686	1781	439	455	11	0	0
4	d	337	2685	1781	439	454	11	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	280	LEU	SER	conflict	UNP R4ZGX6
D	312	PHE	SER	conflict	UNP R4ZGX6
d	280	LEU	SER	conflict	UNP R4ZGX6
d	312	PHE	SER	conflict	UNP R4ZGX6

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	65	537	353	84	100	0	0
5	e	65	537	353	84	100	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	30	240	160	41	38	1	0	0
6	f	30	240	160	41	38	1	0	0

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total 1659	C 1080	N 268	O 305	S 6	0	0
7	N	218	Total 1659	C 1080	N 268	O 305	S 6	0	0
7	Y	218	Total 1659	C 1080	N 268	O 305	S 6	0	0
7	g	218	Total 1659	C 1080	N 268	O 305	S 6	0	0
7	n	218	Total 1659	C 1080	N 268	O 305	S 6	0	0
7	y	218	Total 1659	C 1080	N 268	O 305	S 6	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	224	ILE	LEU	conflict	UNP Q40771
G	249	LEU	ILE	conflict	UNP Q40771
G	261	ASN	THR	conflict	UNP Q40771
N	224	ILE	LEU	conflict	UNP Q40771
N	249	LEU	ILE	conflict	UNP Q40771
N	261	ASN	THR	conflict	UNP Q40771
Y	224	ILE	LEU	conflict	UNP Q40771
Y	249	LEU	ILE	conflict	UNP Q40771
Y	261	ASN	THR	conflict	UNP Q40771
g	224	ILE	LEU	conflict	UNP Q40771
g	249	LEU	ILE	conflict	UNP Q40771
g	261	ASN	THR	conflict	UNP Q40771
n	224	ILE	LEU	conflict	UNP Q40771
n	249	LEU	ILE	conflict	UNP Q40771
n	261	ASN	THR	conflict	UNP Q40771
y	224	ILE	LEU	conflict	UNP Q40771
y	249	LEU	ILE	conflict	UNP Q40771
y	261	ASN	THR	conflict	UNP Q40771

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	62	Total 462	C 305	N 71	O 84	S 2	0	0
8	h	62	Total 462	C 305	N 71	O 84	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	36	Total	C	N	O	S	0	0
			297	202	46	48	1		
9	i	36	Total	C	N	O	S	0	0
			297	202	46	48	1		

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	37	Total	C	N	O	S	0	0
			302	211	43	47	1		
10	k	37	Total	C	N	O	S	0	0
			302	211	43	47	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	31	PHE	SER	conflict	UNP R4ZGX8
K	45	PHE	SER	conflict	UNP R4ZGX8
k	31	PHE	SER	conflict	UNP R4ZGX8
k	45	PHE	SER	conflict	UNP R4ZGX8

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	36	Total	C	N	O	0	0
			302	200	49	53		
11	l	36	Total	C	N	O	0	0
			302	200	49	53		

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	31	Total	C	N	O	0	0
			238	165	33	40		
12	m	31	Total	C	N	O	0	0
			238	165	33	40		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	25	LEU	PRO	conflict	UNP A2CHR7

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Chain	Residue	Modelled	Actual	Comment	Reference
m	25	LEU	PRO	conflict	UNP A2CHR7

- Molecule 13 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	190	Total	C	N	O	S	0	0
			1470	936	236	293	5		
13	o	190	Total	C	N	O	S	0	0
			1470	936	236	293	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	219	Total	C	N	O	S	0	0
			1722	1132	272	314	4		
14	r	219	Total	C	N	O	S	0	0
			1722	1132	272	314	4		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	54	THR	PRO	conflict	UNP A9NKX0
R	56	ALA	-	insertion	UNP A9NKX0
R	57	VAL	-	insertion	UNP A9NKX0
R	58	ALA	-	insertion	UNP A9NKX0
R	59	LYS	-	insertion	UNP A9NKX0
R	60	PRO	-	insertion	UNP A9NKX0
R	61	LYS	-	insertion	UNP A9NKX0
R	62	THR	-	insertion	UNP A9NKX0
R	63	LYS	-	insertion	UNP A9NKX0
R	64	ALA	-	insertion	UNP A9NKX0
R	65	VAL	-	insertion	UNP A9NKX0
R	66	ALA	-	insertion	UNP A9NKX0
R	67	LYS	-	insertion	UNP A9NKX0
r	54	THR	PRO	conflict	UNP A9NKX0
r	56	ALA	-	insertion	UNP A9NKX0
r	57	VAL	-	insertion	UNP A9NKX0
r	58	ALA	-	insertion	UNP A9NKX0
r	59	LYS	-	insertion	UNP A9NKX0
r	60	PRO	-	insertion	UNP A9NKX0
r	61	LYS	-	insertion	UNP A9NKX0
r	62	THR	-	insertion	UNP A9NKX0

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Chain	Residue	Modelled	Actual	Comment	Reference
r	63	LYS	-	insertion	UNP A9NKX0
r	64	ALA	-	insertion	UNP A9NKX0
r	65	VAL	-	insertion	UNP A9NKX0
r	66	ALA	-	insertion	UNP A9NKX0
r	67	LYS	-	insertion	UNP A9NKX0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	S	211	1626	1067	261	294	4	0	0
15	s	211	1626	1067	261	294	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	213	LEU	ALA	conflict	UNP A9NKM0
s	213	LEU	ALA	conflict	UNP A9NKM0

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	T	31	254	177	36	40	1	0	0
16	t	31	254	177	36	40	1	0	0

- Molecule 17 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	U	27	205	127	39	36	3	0	0
17	u	27	205	127	39	36	3	0	0

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	V	31	228	151	37	40	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	v	31	228	151	37	40	0	0

- Molecule 19 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	W	54	415	271	61	82	1	0	0
19	w	54	415	271	61	82	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	98	MET	LEU	conflict	UNP A9NLC2
w	98	MET	LEU	conflict	UNP A9NLC2

- Molecule 20 is a protein called Photosystem II PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	X	34	226	146	37	43	0	0
20	x	34	226	146	37	43	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	80	ALA	VAL	conflict	UNP A9NTS2
x	80	ALA	VAL	conflict	UNP A9NTS2

- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Z	62	453	305	68	79	1	0	0
21	z	62	453	305	68	79	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

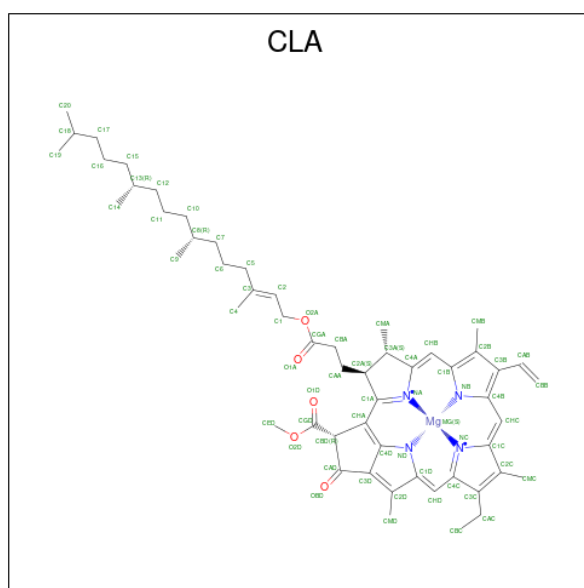


Chain	Residue	Modelled	Actual	Comment	Reference
Z	17	LEU	PHE	conflict	UNP R4ZGT1
z	17	LEU	PHE	conflict	UNP R4ZGT1

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total Fe 1 1	0
22	a	1	Total Fe 1 1	0

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C Mg N O 65 55 1 4 5	0
23	A	1	Total C Mg N O 65 55 1 4 5	0
23	A	1	Total C Mg N O 49 39 1 4 5	0
23	A	1	Total C Mg N O 60 50 1 4 5	0
23	B	1	Total C Mg N O 49 39 1 4 5	0
23	B	1	Total C Mg N O 65 55 1 4 5	0
23	B	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	B	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	55	45	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	C	1	65	55	1	4	5	0
23	D	1	65	55	1	4	5	0
23	D	1	65	55	1	4	5	0
23	G	1	65	55	1	4	5	0
23	G	1	60	50	1	4	5	0
23	G	1	49	39	1	4	5	0
23	G	1	65	55	1	4	5	0
23	G	1	49	39	1	4	5	0
23	G	1	49	39	1	4	5	0
23	G	1	65	55	1	4	5	0
23	G	1	49	39	1	4	5	0
23	N	1	65	55	1	4	5	0
23	N	1	65	55	1	4	5	0
23	N	1	49	39	1	4	5	0
23	N	1	65	55	1	4	5	0
23	N	1	65	55	1	4	5	0
23	N	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	N	1	65	55	1	4	5	0
23	N	1	49	39	1	4	5	0
23	R	1	49	39	1	4	5	0
23	R	1	65	55	1	4	5	0
23	R	1	60	50	1	4	5	0
23	R	1	55	45	1	4	5	0
23	R	1	65	55	1	4	5	0
23	R	1	65	55	1	4	5	0
23	R	1	65	55	1	4	5	0
23	R	1	49	39	1	4	5	0
23	R	1	49	39	1	4	5	0
23	S	1	57	47	1	4	5	0
23	S	1	49	39	1	4	5	0
23	S	1	49	39	1	4	5	0
23	S	1	49	39	1	4	5	0
23	S	1	56	46	1	4	5	0
23	S	1	65	55	1	4	5	0
23	S	1	49	39	1	4	5	0
23	S	1	55	45	1	4	5	0
23	S	1	65	55	1	4	5	0
23	Y	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	Y	1	65	55	1	4	5	0
23	Y	1	65	55	1	4	5	0
23	Y	1	65	55	1	4	5	0
23	Y	1	65	55	1	4	5	0
23	Y	1	65	55	1	4	5	0
23	Y	1	65	55	1	4	5	0
23	Y	1	65	55	1	4	5	0
23	a	1	65	55	1	4	5	0
23	a	1	65	55	1	4	5	0
23	a	1	49	39	1	4	5	0
23	a	1	60	50	1	4	5	0
23	b	1	50	40	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	b	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	65	55	1	4	5	0
23	c	1	60	50	1	4	5	0
23	d	1	65	55	1	4	5	0
23	d	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	g	1	65	55	1	4	5	0
23	g	1	65	55	1	4	5	0
23	g	1	49	39	1	4	5	0
23	g	1	65	55	1	4	5	0
23	g	1	65	55	1	4	5	0
23	g	1	49	39	1	4	5	0
23	g	1	65	55	1	4	5	0
23	g	1	49	39	1	4	5	0
23	n	1	65	55	1	4	5	0
23	n	1	65	55	1	4	5	0
23	n	1	49	39	1	4	5	0
23	n	1	65	55	1	4	5	0
23	n	1	49	39	1	4	5	0
23	n	1	65	55	1	4	5	0
23	n	1	49	39	1	4	5	0
23	n	1	65	55	1	4	5	0
23	n	1	49	39	1	4	5	0
23	r	1	49	39	1	4	5	0
23	r	1	65	55	1	4	5	0
23	r	1	60	50	1	4	5	0
23	r	1	55	45	1	4	5	0
23	r	1	65	55	1	4	5	0

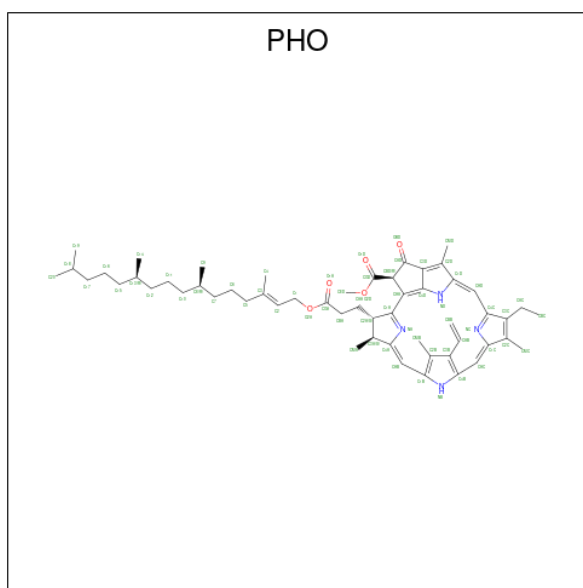
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Mol	Chain	Residues	Atoms					AltConf
23	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

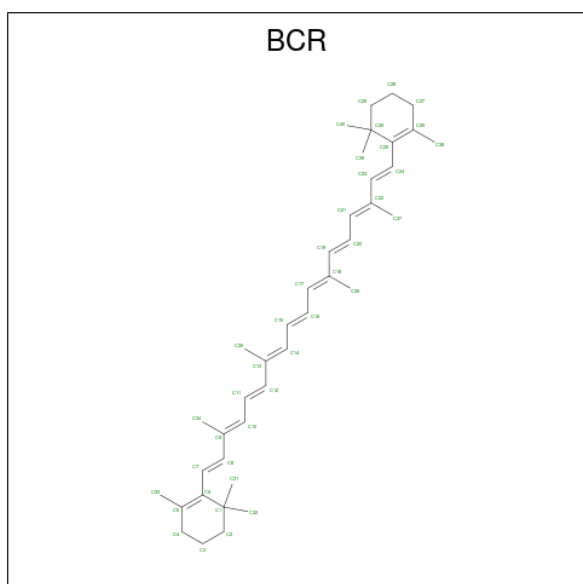


- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



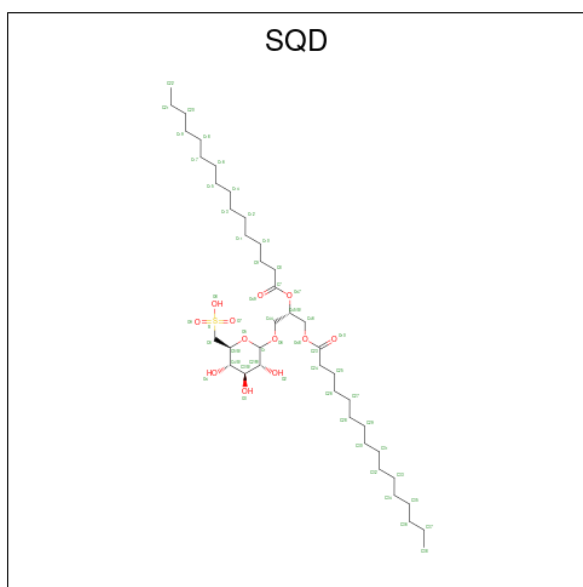
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



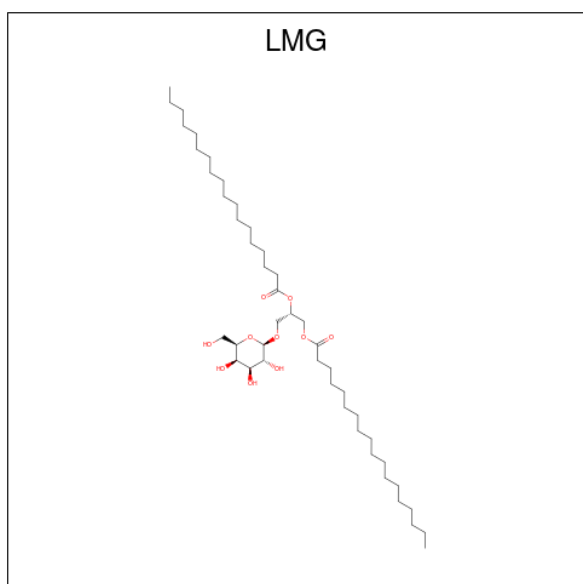
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 39 39	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	H	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	V	1	Total C 40 40	0
25	Z	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	d	1	Total C 40 40	0
25	h	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	v	1	Total C 40 40	0
25	z	1	Total C 40 40	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



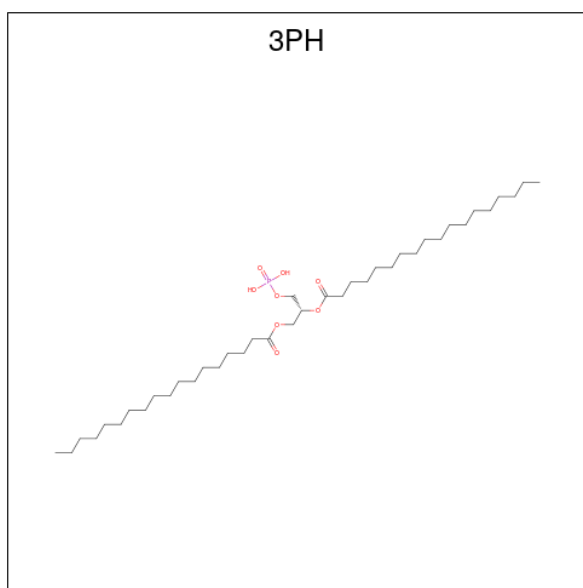
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
26	A	1	50	37	12	1	0
26	L	1	54	41	12	1	0
26	M	1	50	37	12	1	0
26	a	1	48	35	12	1	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



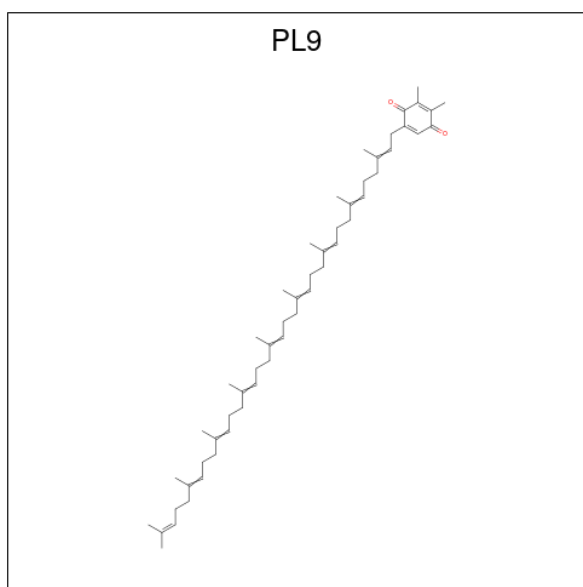
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			53	43	10	
27	B	1	Total	C	O	0
			48	38	10	
27	B	1	Total	C	O	0
			49	39	10	
27	C	1	Total	C	O	0
			45	35	10	
27	D	1	Total	C	O	0
			36	26	10	
27	R	1	Total	C	O	0
			51	41	10	
27	b	1	Total	C	O	0
			51	41	10	
27	b	1	Total	C	O	0
			50	40	10	
27	c	1	Total	C	O	0
			46	36	10	
27	d	1	Total	C	O	0
			46	36	10	
27	r	1	Total	C	O	0
			51	41	10	
27	w	1	Total	C	O	0
			48	38	10	

- Molecule 28 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).



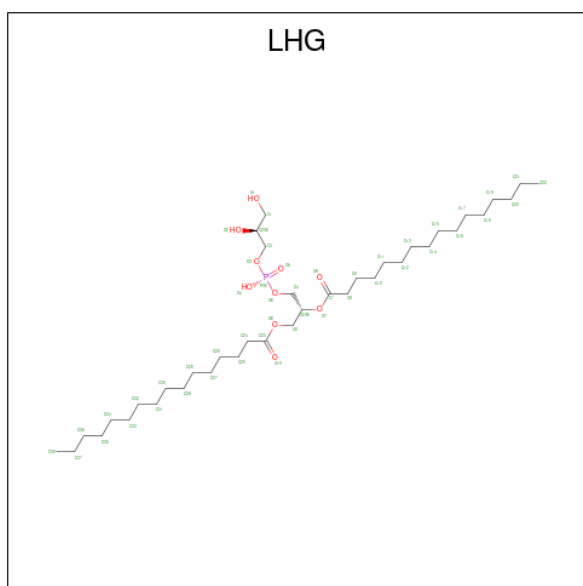
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			48	39	8	1	
28	C	1	Total	C	O	P	0
			48	39	8	1	
28	D	1	Total	C	O	P	0
			38	29	8	1	
28	L	1	Total	C	O	P	0
			41	32	8	1	
28	T	1	Total	C	O	P	0
			48	39	8	1	
28	W	1	Total	C	O	P	0
			46	37	8	1	
28	X	1	Total	C	O	P	0
			46	37	8	1	
28	a	1	Total	C	O	P	0
			48	39	8	1	
28	d	1	Total	C	O	P	0
			38	29	8	1	
28	s	1	Total	C	O	P	0
			38	29	8	1	
28	w	1	Total	C	O	P	0
			48	39	8	1	
28	x	1	Total	C	O	P	0
			46	37	8	1	

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



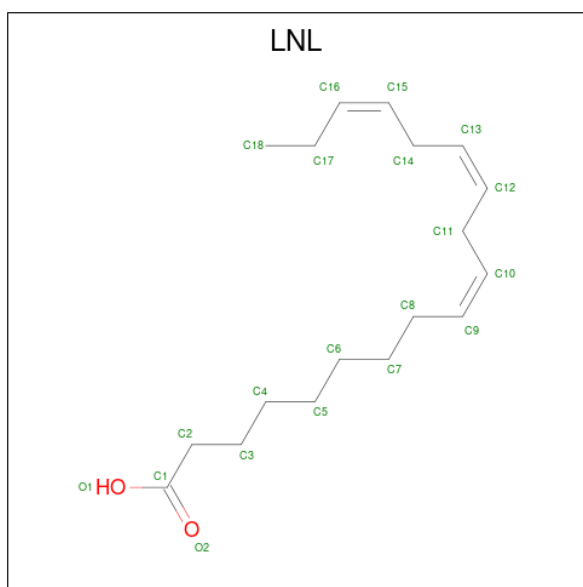
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	A	1	55	53	2	0
29	D	1	55	53	2	0
29	a	1	55	53	2	0
29	d	1	55	53	2	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			37	26	10	1	
30	D	1	Total	C	O	P	0
			43	32	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	G	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	R	1	Total	C	O	P	0
			38	27	10	1	
30	S	1	Total	C	O	P	0
			49	38	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	a	1	Total	C	O	P	0
			49	38	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	g	1	Total	C	O	P	0
			49	38	10	1	
30	n	1	Total	C	O	P	0
			45	34	10	1	
30	r	1	Total	C	O	P	0
			37	26	10	1	
30	s	1	Total	C	O	P	0
			49	38	10	1	
30	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is ALPHA-LINOLENIC ACID (three-letter code: LNL) (formula: C<sub>18</sub>H<sub>30</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			20	18	2	
31	A	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	I	1	Total	C	O	0
			20	18	2	
31	a	1	Total	C	O	0
			20	18	2	

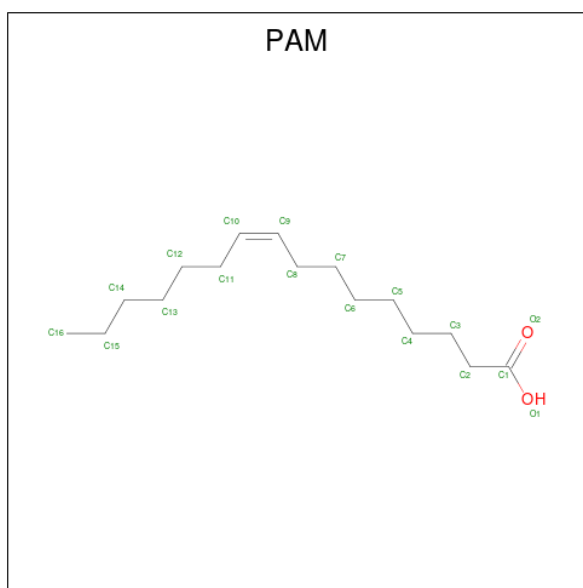
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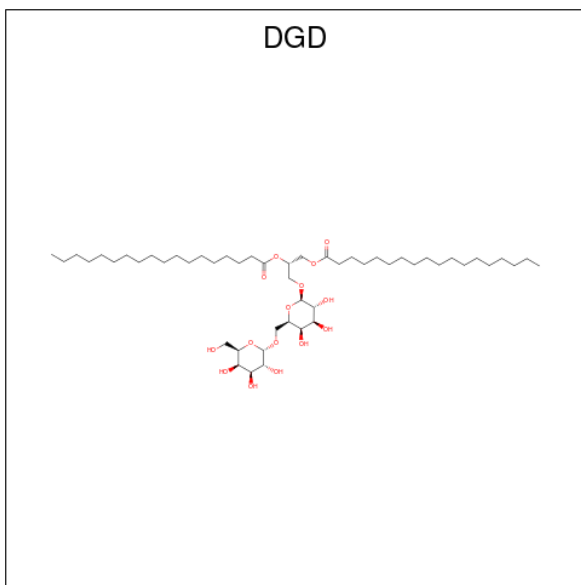
Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	i	1	Total	C	O	0
			20	18	2	

- Molecule 32 is PALMITOLEIC ACID (three-letter code: PAM) (formula:  $C_{16}H_{30}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			18	16	2	
32	b	1	Total	C	O	0
			18	16	2	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



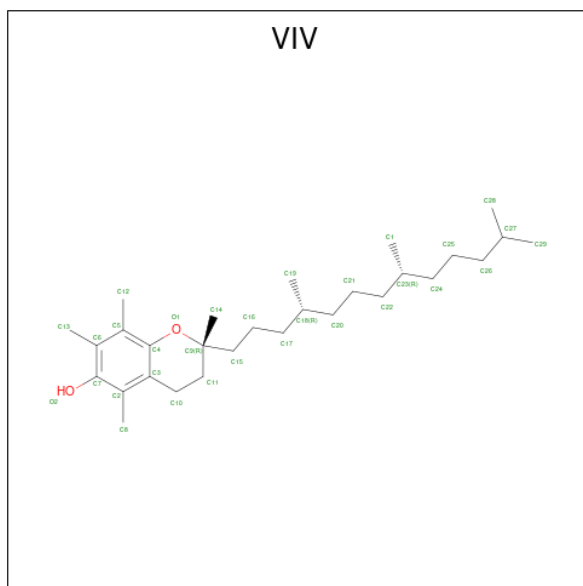
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			66	51	15	
33	H	1	Total	C	O	0
			62	47	15	
33	c	1	Total	C	O	0
			55	40	15	
33	d	1	Total	C	O	0
			62	47	15	

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	C	1	Total	Mg	0
			1	1	
34	c	1	Total	Mg	0
			1	1	

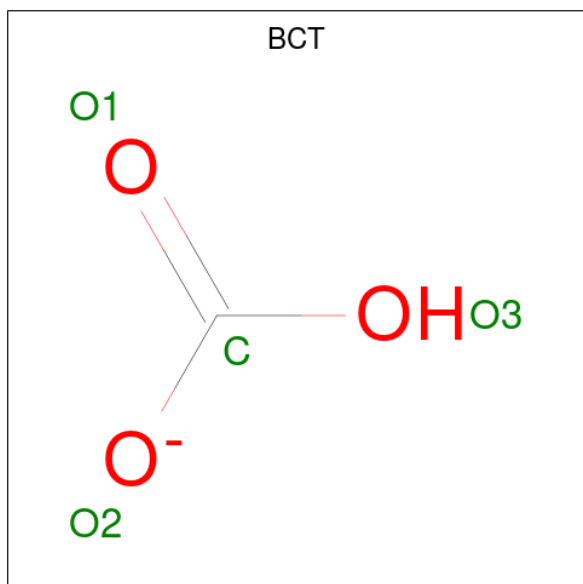
- Molecule 35 is (2R)-2,5,7,8-TETRAMETHYL-2-[(4R,8R)-4,8,12-TRIMETHYLTRIDECYL

]CHROMAN-6-OL (three-letter code: VIV) (formula: C<sub>29</sub>H<sub>50</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			31	29	2	
35	y	1	Total	C	O	0
			31	29	2	

- Molecule 36 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



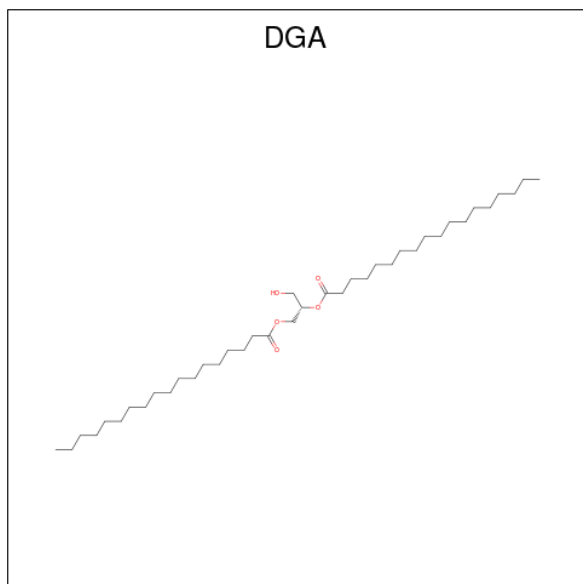
Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total	C	O	0
			4	1	3	

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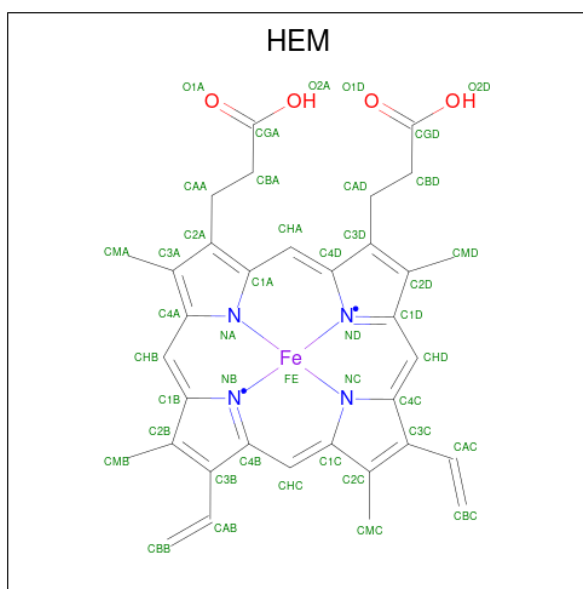
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	d	1	4	1	3	0

- Molecule 37 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ).



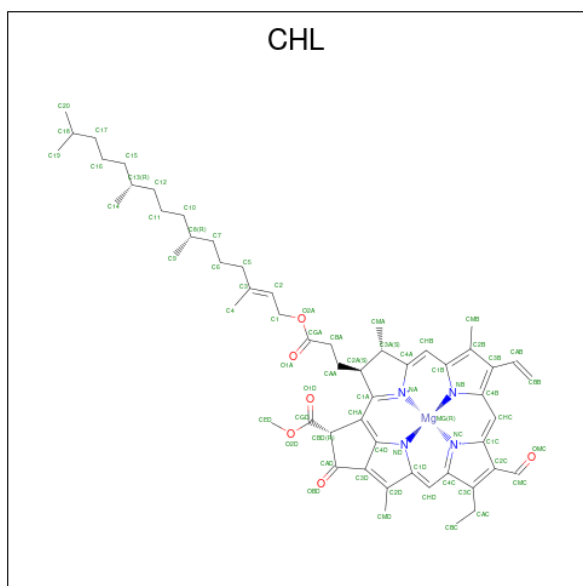
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	D	1	40	35	5	0
37	b	1	44	39	5	0

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
38	F	1	43	34	1	4	4	0
38	f	1	43	34	1	4	4	0

- Molecule 39 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
39	G	1	66	55	1	4	6	0
39	G	1	48	37	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
39	G	1	50	39	1	4	6	0
39	G	1	66	55	1	4	6	0
39	G	1	50	39	1	4	6	0
39	G	1	66	55	1	4	6	0
39	G	1	66	55	1	4	6	0
39	N	1	66	55	1	4	6	0
39	N	1	50	39	1	4	6	0
39	N	1	66	55	1	4	6	0
39	N	1	66	55	1	4	6	0
39	N	1	50	39	1	4	6	0
39	N	1	66	55	1	4	6	0
39	R	1	50	39	1	4	6	0
39	R	1	66	55	1	4	6	0
39	R	1	66	55	1	4	6	0
39	S	1	52	41	1	4	6	0
39	S	1	50	39	1	4	6	0
39	S	1	50	39	1	4	6	0
39	S	1	49	38	1	4	6	0
39	Y	1	66	55	1	4	6	0
39	Y	1	48	37	1	4	6	0
39	Y	1	66	55	1	4	6	0

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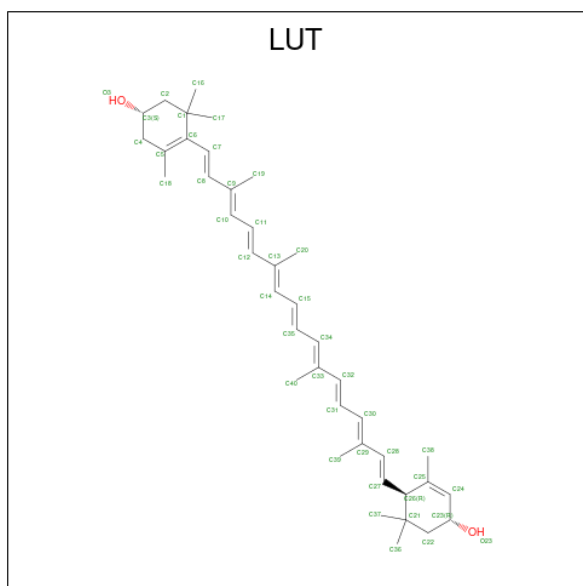
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
39	Y	1	50	39	1	4	6	0
39	Y	1	66	55	1	4	6	0
39	g	1	66	55	1	4	6	0
39	g	1	48	37	1	4	6	0
39	g	1	50	39	1	4	6	0
39	g	1	66	55	1	4	6	0
39	g	1	50	39	1	4	6	0
39	g	1	66	55	1	4	6	0
39	g	1	66	55	1	4	6	0
39	n	1	66	55	1	4	6	0
39	n	1	48	37	1	4	6	0
39	n	1	66	55	1	4	6	0
39	n	1	66	55	1	4	6	0
39	n	1	50	39	1	4	6	0
39	n	1	66	55	1	4	6	0
39	r	1	50	39	1	4	6	0
39	r	1	66	55	1	4	6	0
39	r	1	66	55	1	4	6	0
39	s	1	52	41	1	4	6	0
39	s	1	50	39	1	4	6	0
39	s	1	50	39	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
39	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 40 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	G	1	Total	C	O	0
			42	40	2	
40	G	1	Total	C	O	0
			42	40	2	
40	N	1	Total	C	O	0
			42	40	2	
40	N	1	Total	C	O	0
			42	40	2	
40	R	1	Total	C	O	0
			42	40	2	

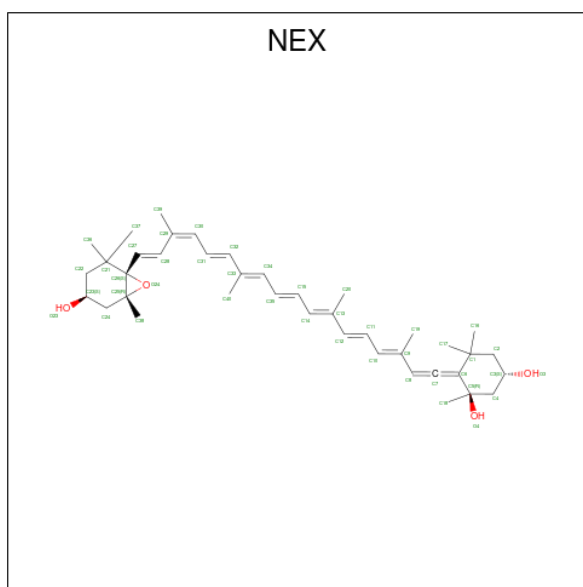
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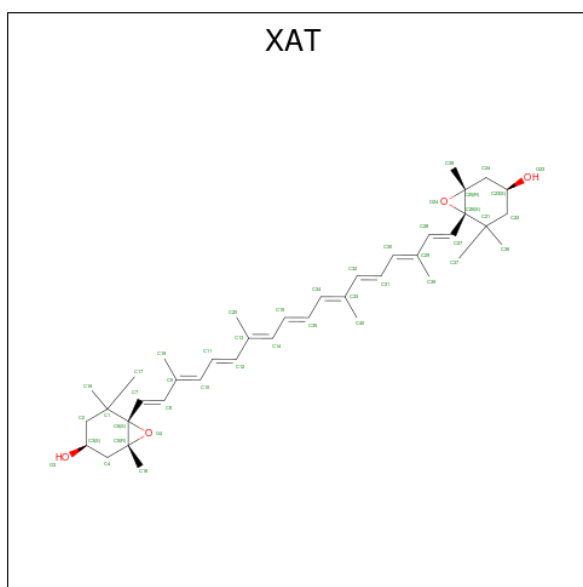
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	S	1	42	40	2	0
40	S	1	42	40	2	0
40	Y	1	42	40	2	0
40	Y	1	42	40	2	0
40	g	1	42	40	2	0
40	g	1	42	40	2	0
40	n	1	42	40	2	0
40	n	1	42	40	2	0
40	r	1	42	40	2	0
40	s	1	42	40	2	0
40	s	1	42	40	2	0
40	y	1	42	40	2	0
40	y	1	42	40	2	0

- Molecule 41 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
41	G	1	Total	C	O	0
			24	22	2	
41	N	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	S	1	Total	C	O	0
			23	21	2	
41	Y	1	Total	C	O	0
			44	40	4	
41	g	1	Total	C	O	0
			44	40	4	
41	n	1	Total	C	O	0
			44	40	4	
41	r	1	Total	C	O	0
			44	40	4	
41	s	1	Total	C	O	0
			27	25	2	

- Molecule 42 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
42	G	1	Total	C	O	0
			44	40	4	
42	N	1	Total	C	O	0
			44	40	4	
42	R	1	Total	C	O	0
			44	40	4	
42	Y	1	Total	C	O	0
			44	40	4	
42	n	1	Total	C	O	0
			44	40	4	
42	n	1	Total	C	O	0
			44	40	4	
42	r	1	Total	C	O	0
			44	40	4	
42	y	1	Total	C	O	0
			44	40	4	

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		AltConf
43	A	28	Total	O	0
			28	28	
43	B	31	Total	O	0
			31	31	
43	C	10	Total	O	0
			10	10	
43	D	18	Total	O	0
			18	18	

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Mol	Chain	Residues	Atoms	AltConf
43	E	4	Total O 4 4	0
43	H	10	Total O 10 10	0
43	I	1	Total O 1 1	0
43	L	2	Total O 2 2	0
43	N	4	Total O 4 4	0
43	O	4	Total O 4 4	0
43	R	8	Total O 8 8	0
43	S	1	Total O 1 1	0
43	T	5	Total O 5 5	0
43	U	1	Total O 1 1	0
43	V	1	Total O 1 1	0
43	Y	8	Total O 8 8	0
43	Z	1	Total O 1 1	0
43	a	20	Total O 20 20	0
43	b	31	Total O 31 31	0
43	c	14	Total O 14 14	0
43	d	25	Total O 25 25	0
43	e	4	Total O 4 4	0
43	f	1	Total O 1 1	0
43	g	1	Total O 1 1	0
43	h	11	Total O 11 11	0

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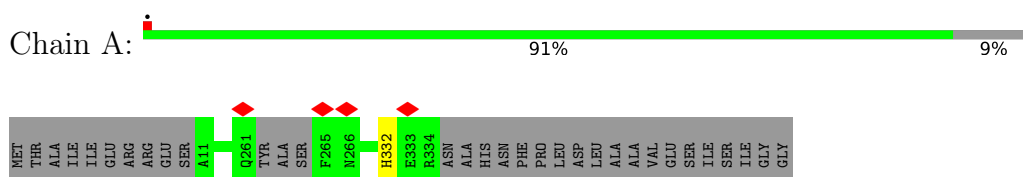
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Mol	Chain	Residues	Atoms	AltConf
43	i	2	Total O 2 2	0
43	l	4	Total O 4 4	0
43	n	1	Total O 1 1	0
43	o	2	Total O 2 2	0
43	r	7	Total O 7 7	0
43	t	4	Total O 4 4	0
43	v	2	Total O 2 2	0
43	x	1	Total O 1 1	0
43	y	13	Total O 13 13	0

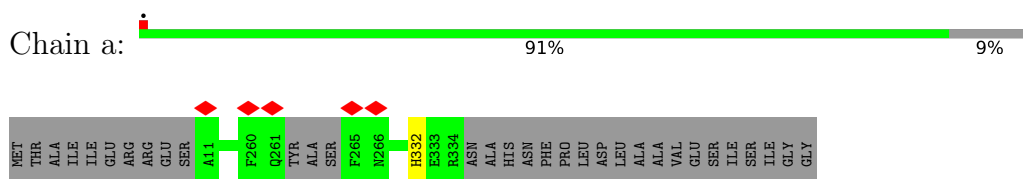
### 3 Residue-property plots [i](#)

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

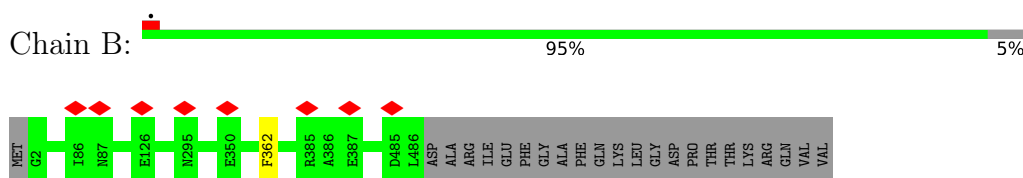
- Molecule 1: Photosystem II protein D1



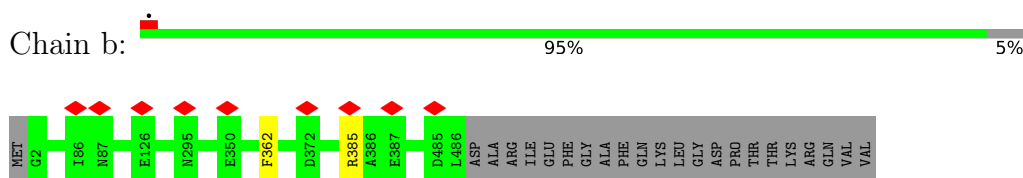
- Molecule 1: Photosystem II protein D1



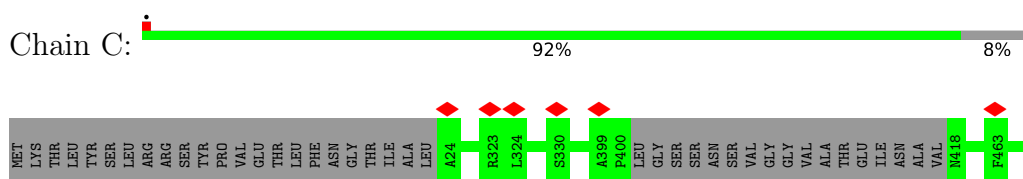
- Molecule 2: Photosystem II CP47 reaction center protein



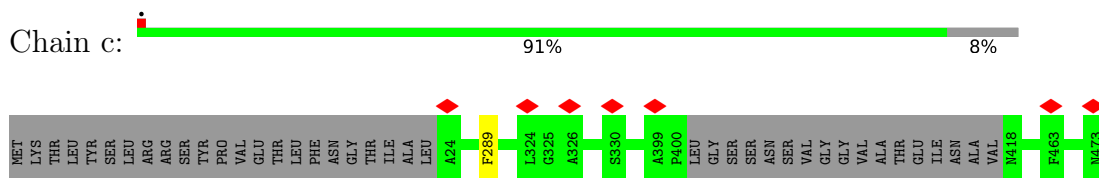
- Molecule 2: Photosystem II CP47 reaction center protein



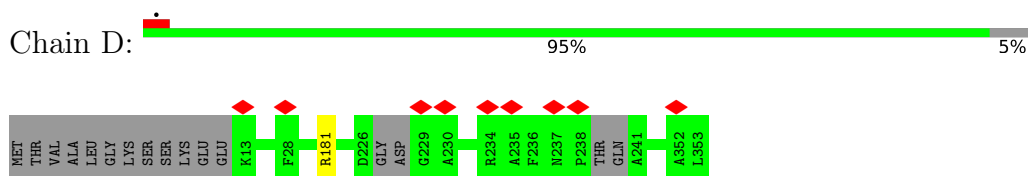
- Molecule 3: Photosystem II CP43 reaction center protein



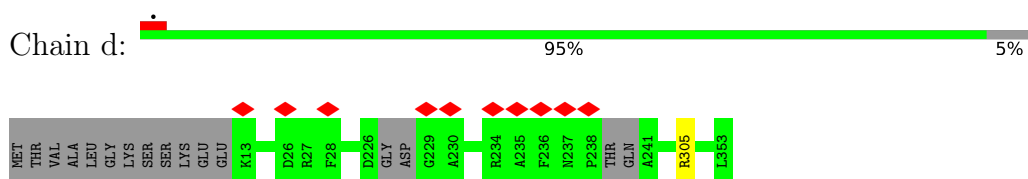
• Molecule 3: Photosystem II CP43 reaction center protein



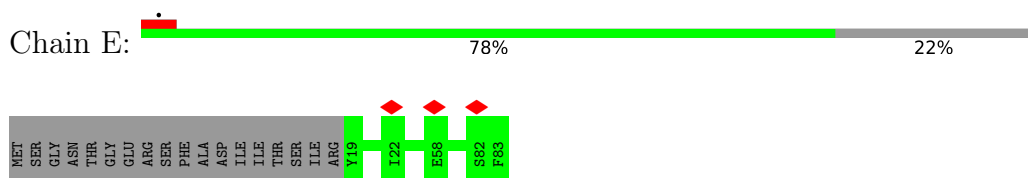
• Molecule 4: Photosystem II D2 protein



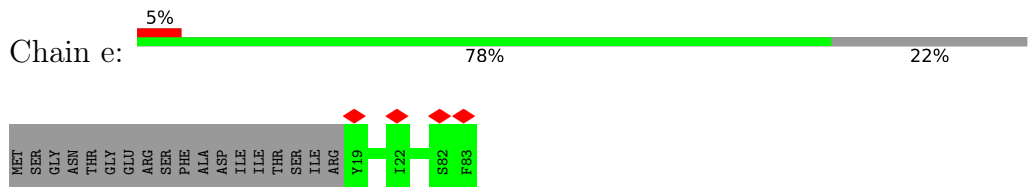
• Molecule 4: Photosystem II D2 protein



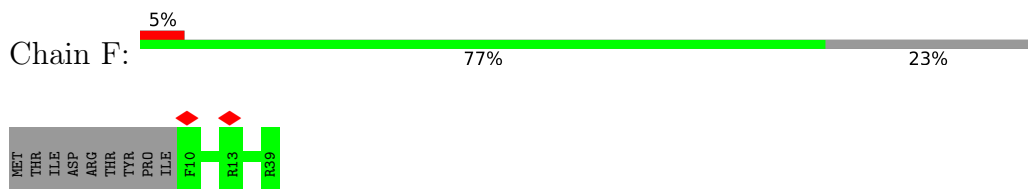
• Molecule 5: Cytochrome b559 subunit alpha



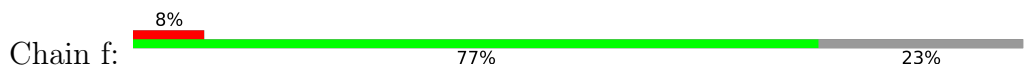
• Molecule 5: Cytochrome b559 subunit alpha

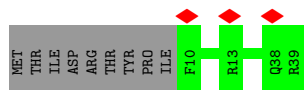


• Molecule 6: Cytochrome b559 subunit beta

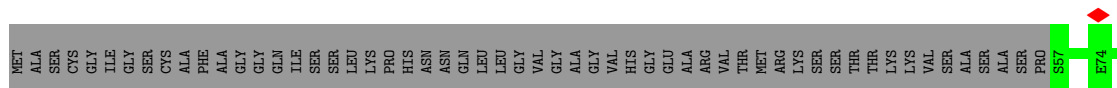
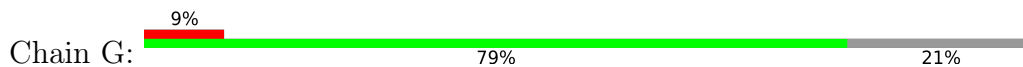


• Molecule 6: Cytochrome b559 subunit beta

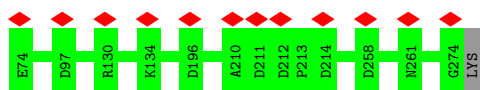
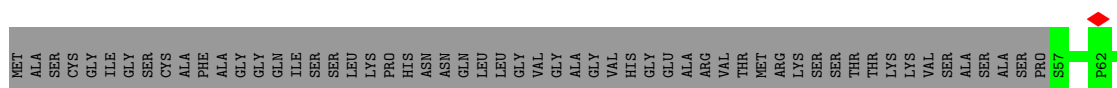
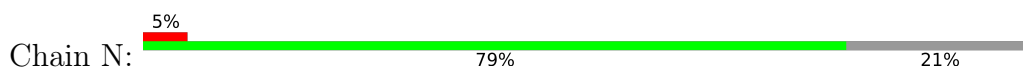




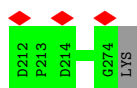
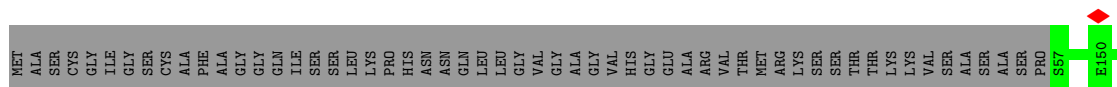
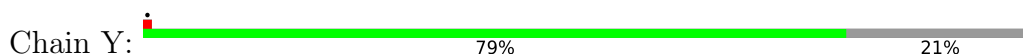
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic



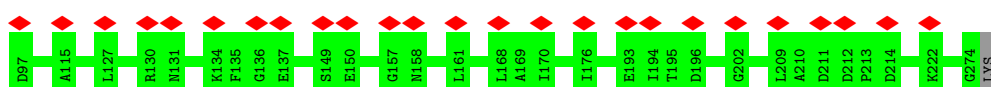
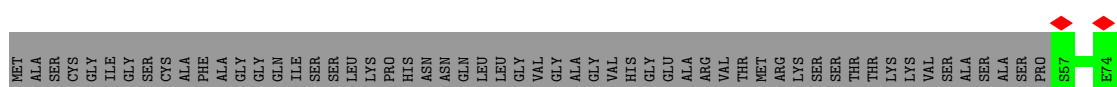
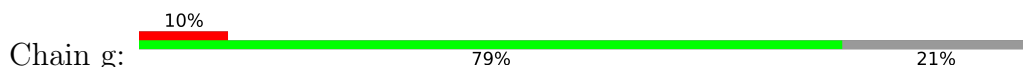
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic



• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

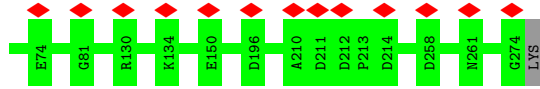
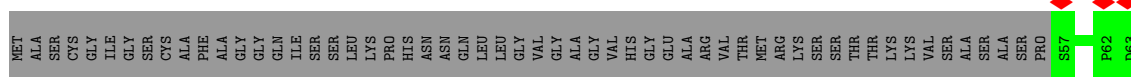
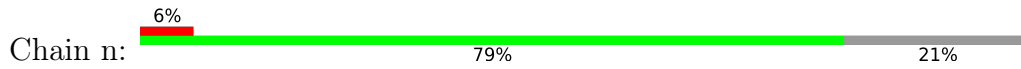


• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

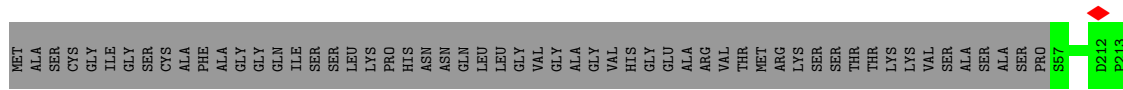
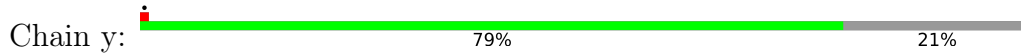


• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

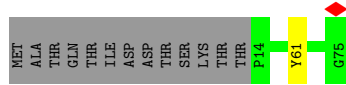
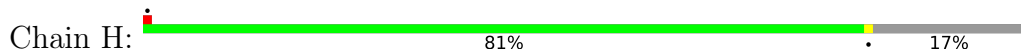




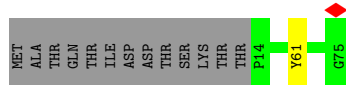
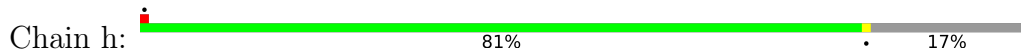
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



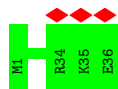
- Molecule 8: Photosystem II reaction center protein H



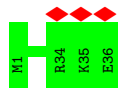
- Molecule 8: Photosystem II reaction center protein H



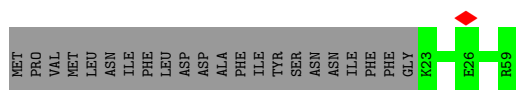
- Molecule 9: Photosystem II reaction center protein I



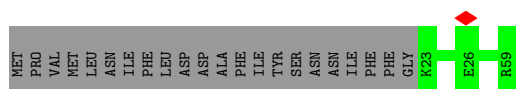
- Molecule 9: Photosystem II reaction center protein I



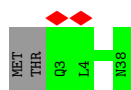
• Molecule 10: Photosystem II reaction center protein K



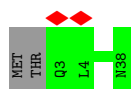
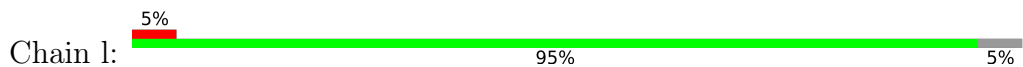
• Molecule 10: Photosystem II reaction center protein K



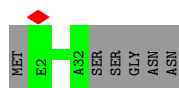
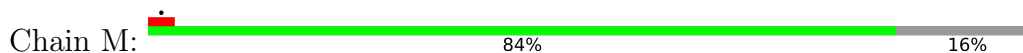
• Molecule 11: Photosystem II reaction center protein L



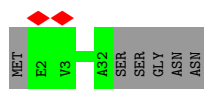
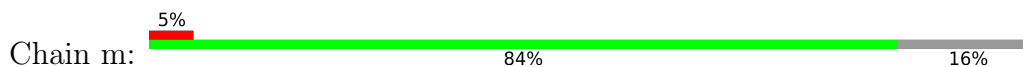
• Molecule 11: Photosystem II reaction center protein L



• Molecule 12: Photosystem II reaction center protein M

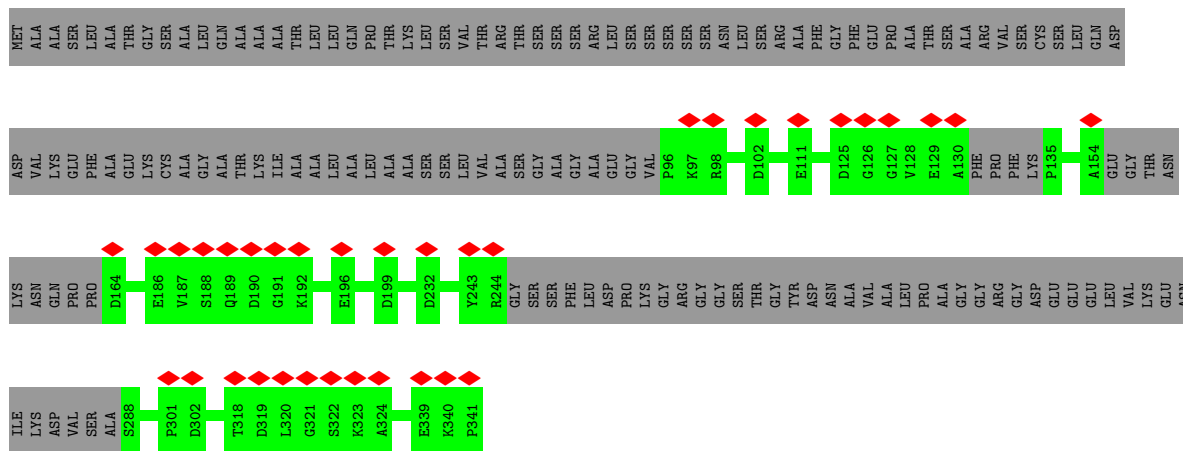


• Molecule 12: Photosystem II reaction center protein M

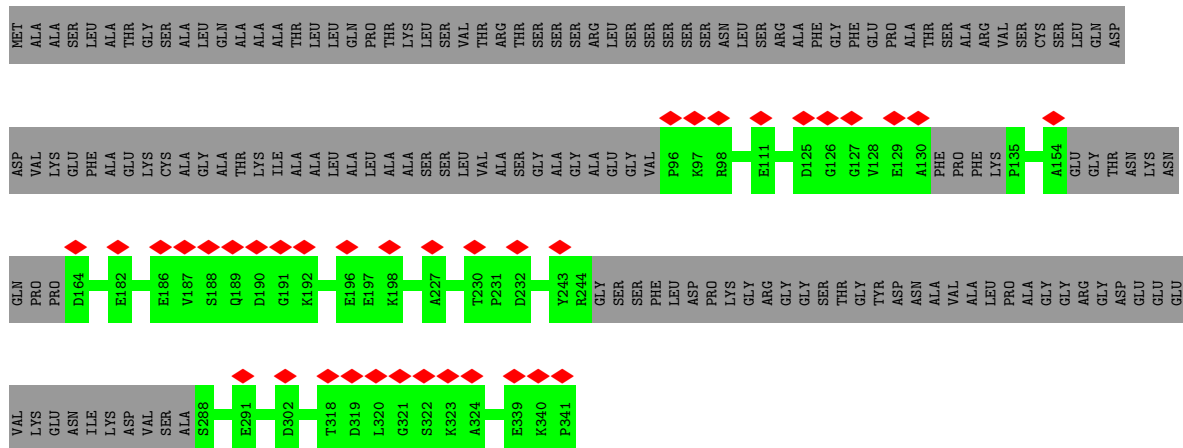


• Molecule 13: Oxygen-evolving enhancer protein 1, chloroplastic

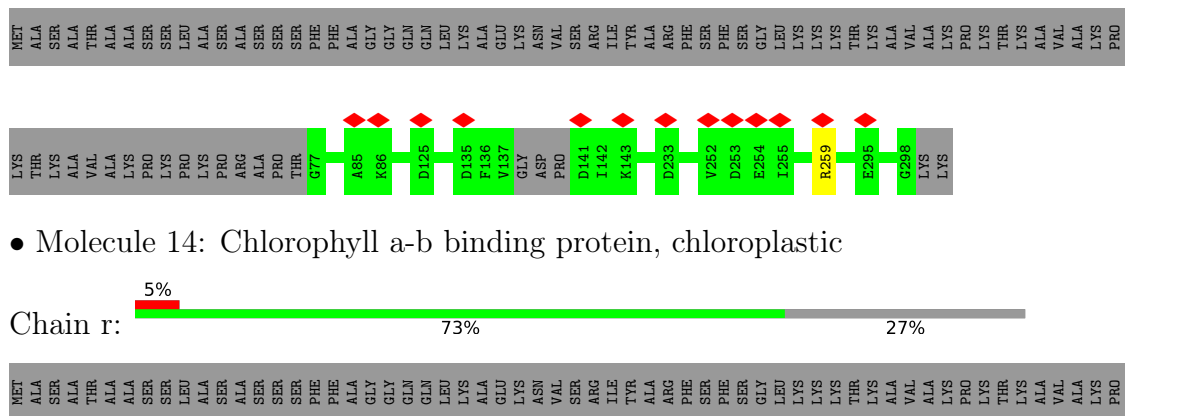




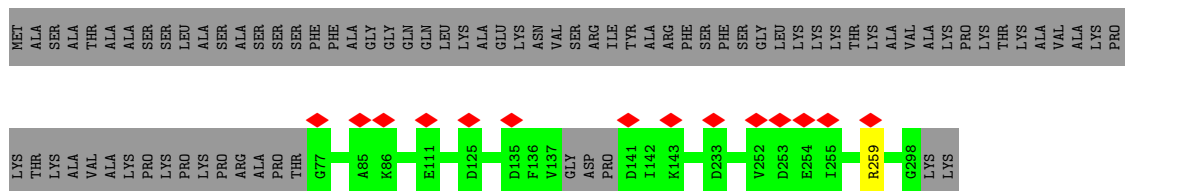
• Molecule 13: Oxygen-evolving enhancer protein 1, chloroplastic



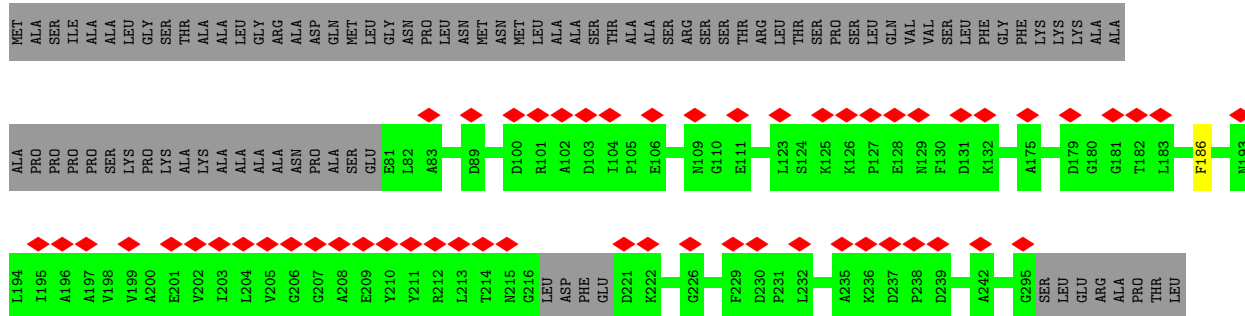
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic



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



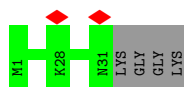
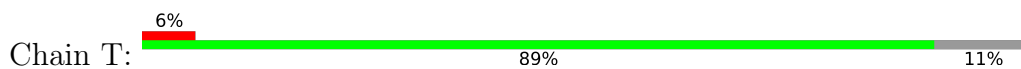
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



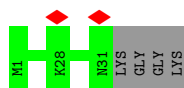
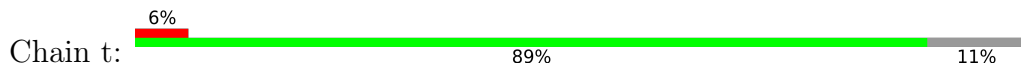
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



• Molecule 16: Photosystem II reaction center protein T



• Molecule 16: Photosystem II reaction center protein T



• Molecule 17: Photosystem II 5 kDa protein, chloroplastic







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	60956	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	120	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	7.081	Depositor
Minimum map value	-3.771	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.210	Depositor
Recommended contour level	0.886	Depositor
Map size (Å)	430.64896, 430.64896, 430.64896	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96127, 0.96127, 0.96127	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, DGA, LNL, PHO, LUT, BCR, XAT, SQD, NEX, FE2, PL9, CHL, CLA, MG, VIV, LHG, LMG, PAM, HEM, 3PH, DGD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/2578	0.46	0/3513
1	a	0.26	0/2578	0.47	0/3513
2	B	0.26	0/3940	0.48	0/5363
2	b	0.27	0/3940	0.49	0/5363
3	C	0.29	0/3493	0.47	0/4757
3	c	0.29	0/3493	0.48	0/4757
4	D	0.26	0/2778	0.47	0/3786
4	d	0.27	0/2777	0.47	0/3786
5	E	0.27	0/555	0.46	0/756
5	e	0.27	0/555	0.47	0/756
6	F	0.25	0/247	0.44	0/333
6	f	0.25	0/247	0.46	0/333
7	G	0.29	0/1712	0.48	0/2335
7	N	0.26	0/1712	0.43	0/2335
7	Y	0.29	0/1712	0.45	0/2335
7	g	0.27	0/1712	0.46	0/2335
7	n	0.26	0/1712	0.43	0/2335
7	y	0.26	0/1712	0.43	0/2335
8	H	0.28	0/475	0.49	0/647
8	h	0.29	0/475	0.49	0/647
9	I	0.28	0/305	0.49	0/409
9	i	0.28	0/305	0.49	0/409
10	K	0.28	0/313	0.44	0/428
10	k	0.28	0/313	0.44	0/428
11	L	0.25	0/309	0.40	0/421
11	l	0.26	0/309	0.42	0/421
12	M	0.25	0/242	0.37	0/330
12	m	0.26	0/242	0.42	0/330
13	O	0.24	0/1497	0.47	0/2017
13	o	0.25	0/1497	0.48	0/2017
14	R	0.25	0/1767	0.42	0/2397



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
14	r	0.26	0/1767	0.44	0/2397
15	S	0.28	0/1673	0.43	0/2272
15	s	0.27	0/1673	0.45	0/2272
16	T	0.27	0/262	0.41	0/356
16	t	0.27	0/262	0.39	0/356
17	U	0.23	0/209	0.49	0/280
17	u	0.24	0/209	0.47	0/280
18	V	0.22	0/228	0.45	0/311
18	v	0.22	0/228	0.43	0/311
19	W	0.25	0/423	0.49	0/574
19	w	0.24	0/423	0.42	0/574
20	X	0.24	0/228	0.33	0/310
20	x	0.24	0/228	0.34	0/310
21	Z	0.26	0/463	0.38	0/633
21	z	0.25	0/463	0.35	0/633
All	All	0.27	0/54241	0.46	0/73796

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	A	317/353 (90%)	312 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
2	B	483/508 (95%)	473 (98%)	10 (2%)	0	100	100
2	b	483/508 (95%)	473 (98%)	10 (2%)	0	100	100
3	C	429/473 (91%)	420 (98%)	9 (2%)	0	100	100
3	c	429/473 (91%)	419 (98%)	10 (2%)	0	100	100
4	D	331/353 (94%)	319 (96%)	12 (4%)	0	100	100
4	d	331/353 (94%)	322 (97%)	9 (3%)	0	100	100
5	E	63/83 (76%)	61 (97%)	2 (3%)	0	100	100
5	e	63/83 (76%)	62 (98%)	1 (2%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	0	100	100
6	f	28/39 (72%)	28 (100%)	0	0	100	100
7	G	216/275 (78%)	206 (95%)	10 (5%)	0	100	100
7	N	216/275 (78%)	209 (97%)	7 (3%)	0	100	100
7	Y	216/275 (78%)	211 (98%)	5 (2%)	0	100	100
7	g	216/275 (78%)	207 (96%)	9 (4%)	0	100	100
7	n	216/275 (78%)	209 (97%)	7 (3%)	0	100	100
7	y	216/275 (78%)	212 (98%)	4 (2%)	0	100	100
8	H	60/75 (80%)	58 (97%)	2 (3%)	0	100	100
8	h	60/75 (80%)	59 (98%)	1 (2%)	0	100	100
9	I	34/36 (94%)	34 (100%)	0	0	100	100
9	i	34/36 (94%)	34 (100%)	0	0	100	100
10	K	35/59 (59%)	33 (94%)	2 (6%)	0	100	100
10	k	35/59 (59%)	32 (91%)	3 (9%)	0	100	100
11	L	34/38 (90%)	34 (100%)	0	0	100	100
11	l	34/38 (90%)	34 (100%)	0	0	100	100
12	M	29/37 (78%)	29 (100%)	0	0	100	100
12	m	29/37 (78%)	29 (100%)	0	0	100	100
13	O	182/341 (53%)	175 (96%)	7 (4%)	0	100	100
13	o	182/341 (53%)	173 (95%)	9 (5%)	0	100	100
14	R	215/300 (72%)	213 (99%)	2 (1%)	0	100	100
14	r	215/300 (72%)	211 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	S	207/303 (68%)	196 (95%)	11 (5%)	0	100	100
15	s	207/303 (68%)	196 (95%)	11 (5%)	0	100	100
16	T	29/35 (83%)	29 (100%)	0	0	100	100
16	t	29/35 (83%)	29 (100%)	0	0	100	100
17	U	25/133 (19%)	25 (100%)	0	0	100	100
17	u	25/133 (19%)	25 (100%)	0	0	100	100
18	V	29/33 (88%)	26 (90%)	3 (10%)	0	100	100
18	v	29/33 (88%)	29 (100%)	0	0	100	100
19	W	52/146 (36%)	51 (98%)	1 (2%)	0	100	100
19	w	52/146 (36%)	51 (98%)	1 (2%)	0	100	100
20	X	32/129 (25%)	31 (97%)	1 (3%)	0	100	100
20	x	32/129 (25%)	32 (100%)	0	0	100	100
21	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
21	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	6644/8722 (76%)	6469 (97%)	175 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/282 (91%)	256 (100%)	1 (0%)	89	96
1	a	257/282 (91%)	256 (100%)	1 (0%)	89	96
2	B	387/406 (95%)	386 (100%)	1 (0%)	91	97
2	b	387/406 (95%)	385 (100%)	2 (0%)	86	95
3	C	338/371 (91%)	338 (100%)	0	100	100
3	c	338/371 (91%)	337 (100%)	1 (0%)	91	97
4	D	271/284 (95%)	270 (100%)	1 (0%)	89	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	271/284 (95%)	270 (100%)	1 (0%)	89	96
5	E	59/74 (80%)	59 (100%)	0	100	100
5	e	59/74 (80%)	59 (100%)	0	100	100
6	F	25/34 (74%)	25 (100%)	0	100	100
6	f	25/34 (74%)	25 (100%)	0	100	100
7	G	166/208 (80%)	166 (100%)	0	100	100
7	N	166/208 (80%)	166 (100%)	0	100	100
7	Y	166/208 (80%)	166 (100%)	0	100	100
7	g	166/208 (80%)	166 (100%)	0	100	100
7	n	166/208 (80%)	166 (100%)	0	100	100
7	y	166/208 (80%)	166 (100%)	0	100	100
8	H	50/62 (81%)	49 (98%)	1 (2%)	50	78
8	h	50/62 (81%)	49 (98%)	1 (2%)	50	78
9	I	33/33 (100%)	33 (100%)	0	100	100
9	i	33/33 (100%)	33 (100%)	0	100	100
10	K	32/52 (62%)	32 (100%)	0	100	100
10	k	32/52 (62%)	32 (100%)	0	100	100
11	L	34/36 (94%)	34 (100%)	0	100	100
11	l	34/36 (94%)	34 (100%)	0	100	100
12	M	25/30 (83%)	25 (100%)	0	100	100
12	m	25/30 (83%)	25 (100%)	0	100	100
13	O	164/275 (60%)	164 (100%)	0	100	100
13	o	164/275 (60%)	164 (100%)	0	100	100
14	R	180/241 (75%)	179 (99%)	1 (1%)	84	94
14	r	180/241 (75%)	179 (99%)	1 (1%)	84	94
15	S	162/230 (70%)	161 (99%)	1 (1%)	84	94
15	s	162/230 (70%)	161 (99%)	1 (1%)	84	94
16	T	28/30 (93%)	28 (100%)	0	100	100
16	t	28/30 (93%)	28 (100%)	0	100	100
17	U	23/103 (22%)	23 (100%)	0	100	100
17	u	23/103 (22%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	V	27/29 (93%)	27 (100%)	0	100	100
18	v	27/29 (93%)	27 (100%)	0	100	100
19	W	46/116 (40%)	46 (100%)	0	100	100
19	w	46/116 (40%)	46 (100%)	0	100	100
20	X	23/94 (24%)	23 (100%)	0	100	100
20	x	23/94 (24%)	23 (100%)	0	100	100
21	Z	51/51 (100%)	51 (100%)	0	100	100
21	z	51/51 (100%)	51 (100%)	0	100	100
All	All	5426/6914 (78%)	5412 (100%)	14 (0%)	90	97

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	362	PHE
2	b	385	ARG
15	s	186	PHE
8	h	61	TYR
14	r	259	ARG

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

Mol	Chain	Res	Type
3	c	28	GLN
3	c	313	GLN
15	s	224	HIS
14	r	156	GLN
3	C	313	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 358 ligands modelled in this entry, 4 are monoatomic - leaving 354 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	Y	311	30	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
23	CLA	n	602	7	65,73,73	1.48	6 (9%)	76,113,113	1.40	9 (11%)
28	3PH	L	102	-	40,40,47	0.68	1 (2%)	44,45,52	0.64	1 (2%)
23	CLA	G	613	7	65,73,73	1.48	6 (9%)	76,113,113	1.42	7 (9%)
39	CHL	G	609	7	66,74,74	1.66	5 (7%)	73,114,114	1.72	9 (12%)
23	CLA	Y	304	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
38	HEM	f	501	6,5	41,50,50	1.50	5 (12%)	45,82,82	1.41	7 (15%)
23	CLA	N	604	-	49,57,73	1.71	6 (12%)	55,93,113	1.58	8 (14%)
28	3PH	w	202	-	47,47,47	0.63	1 (2%)	51,52,52	0.59	1 (1%)
28	3PH	x	201	-	45,45,47	0.65	1 (2%)	49,50,52	0.60	1 (2%)
27	LMG	C	525	-	45,45,55	0.20	0	53,53,63	0.14	0
39	CHL	N	608	-	50,58,74	1.81	5 (10%)	52,94,114	1.94	10 (19%)
23	CLA	G	604	-	49,57,73	1.71	5 (10%)	55,93,113	1.55	8 (14%)
24	PHO	D	402	-	51,69,69	0.98	3 (5%)	47,99,99	1.19	4 (8%)
28	3PH	a	410	-	47,47,47	0.63	1 (2%)	51,52,52	0.56	1 (1%)
23	CLA	B	611	-	65,73,73	1.46	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	s	611	15	49,57,73	1.70	5 (10%)	55,93,113	1.54	6 (10%)
31	LNL	i	101	-	19,19,19	0.45	0	18,19,19	0.89	1 (5%)
42	XAT	N	619	-	39,47,47	3.16	23 (58%)	54,74,74	4.58	32 (59%)
28	3PH	D	403	-	37,37,47	0.70	1 (2%)	41,42,52	0.65	1 (2%)
23	CLA	R	611	-	49,57,73	1.70	6 (12%)	55,93,113	1.52	7 (12%)
23	CLA	r	611	-	49,57,73	1.70	5 (10%)	55,93,113	1.56	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	s	603	-	49,57,73	1.71	6 (12%)	55,93,113	1.54	8 (14%)
23	CLA	s	608	-	49,57,73	1.74	5 (10%)	55,93,113	1.49	7 (12%)
23	CLA	N	611	30	65,73,73	1.50	5 (7%)	76,113,113	1.34	8 (10%)
23	CLA	r	603	-	60,68,73	1.53	6 (10%)	70,107,113	1.44	8 (11%)
23	CLA	c	513	-	60,68,73	1.52	6 (10%)	70,107,113	1.43	8 (11%)
23	CLA	c	508	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	8 (10%)
25	BCR	b	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
23	CLA	b	602	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
41	NEX	G	617	-	21,25,46	4.26	19 (90%)	28,38,70	5.44	11 (39%)
25	BCR	b	617	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	8 (14%)
39	CHL	Y	306	7	48,56,74	1.84	5 (10%)	51,92,114	2.12	9 (17%)
23	CLA	n	613	7	65,73,73	1.48	5 (7%)	76,113,113	1.41	7 (9%)
25	BCR	k	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	6 (10%)
31	LNL	B	622	-	19,19,19	0.45	0	18,19,19	0.93	1 (5%)
39	CHL	Y	307	-	66,74,74	1.57	5 (7%)	73,114,114	1.63	10 (13%)
31	LNL	B	625	-	19,19,19	0.45	0	18,19,19	0.91	1 (5%)
39	CHL	y	307	7	48,56,74	1.83	5 (10%)	51,92,114	2.10	9 (17%)
31	LNL	c	518	-	19,19,19	0.44	0	18,19,19	0.92	1 (5%)
28	3PH	X	201	-	45,45,47	0.65	1 (2%)	49,50,52	0.60	1 (2%)
23	CLA	S	608	-	49,57,73	1.72	5 (10%)	55,93,113	1.48	7 (12%)
33	DGD	H	502	-	63,63,67	0.87	1 (1%)	77,77,81	1.33	7 (9%)
23	CLA	B	616	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
26	SQD	M	101	-	49,50,54	1.59	8 (16%)	58,61,65	1.38	6 (10%)
23	CLA	n	610	7	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
27	LMG	b	620	-	51,51,55	0.19	0	59,59,63	0.22	0
31	LNL	c	519	-	19,19,19	0.43	0	18,19,19	0.93	1 (5%)
23	CLA	N	602	7	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
23	CLA	B	607	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
32	PAM	B	621	-	17,17,17	0.61	0	17,17,17	0.78	0
39	CHL	n	606	-	66,74,74	1.58	5 (7%)	73,114,114	1.58	11 (15%)
40	LUT	Y	316	-	42,43,43	2.36	20 (47%)	51,60,60	3.15	23 (45%)
40	LUT	Y	315	-	42,43,43	1.78	10 (23%)	51,60,60	2.77	20 (39%)
25	BCR	d	410	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	6 (10%)
42	XAT	n	617	-	39,47,47	3.04	21 (53%)	54,74,74	4.50	30 (55%)
42	XAT	n	620	-	39,47,47	3.15	23 (58%)	54,74,74	4.56	31 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LNL	c	521	-	19,19,19	0.43	0	18,19,19	0.94	1 (5%)
23	CLA	C	503	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
39	CHL	N	606	-	66,74,74	1.58	5 (7%)	73,114,114	1.59	10 (13%)
40	LUT	G	616	-	42,43,43	2.41	20 (47%)	51,60,60	3.11	21 (41%)
30	LHG	b	627	-	48,48,48	1.36	8 (16%)	51,54,54	0.73	2 (3%)
23	CLA	C	504	43	65,73,73	1.49	6 (9%)	76,113,113	1.39	6 (7%)
23	CLA	C	501	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
23	CLA	B	615	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
30	LHG	S	616	23	48,48,48	1.43	8 (16%)	51,54,54	0.73	2 (3%)
31	LNL	c	517	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
37	DGA	D	410	-	39,39,43	0.20	0	41,41,45	0.15	0
41	NEX	g	617	-	38,46,46	4.18	33 (86%)	50,70,70	4.94	24 (48%)
23	CLA	B	608	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
39	CHL	y	310	7	66,74,74	1.57	4 (6%)	73,114,114	1.58	10 (13%)
23	CLA	r	604	43	55,63,73	1.61	5 (9%)	64,101,113	1.49	8 (12%)
31	LNL	b	624	-	19,19,19	0.43	0	18,19,19	0.88	1 (5%)
39	CHL	R	607	-	66,74,74	1.59	4 (6%)	73,114,114	1.67	12 (16%)
23	CLA	N	613	-	65,73,73	1.49	5 (7%)	76,113,113	1.50	9 (11%)
25	BCR	D	411	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
27	LMG	d	409	-	46,46,55	0.19	0	54,54,63	0.15	0
30	LHG	R	616	23	37,37,48	1.56	8 (21%)	40,43,54	0.86	2 (5%)
23	CLA	R	601	14	49,57,73	1.73	6 (12%)	55,93,113	1.51	7 (12%)
39	CHL	G	608	-	50,58,74	1.85	5 (10%)	52,94,114	1.87	9 (17%)
23	CLA	g	614	-	49,57,73	1.71	5 (10%)	55,93,113	1.52	8 (14%)
31	LNL	b	625	-	19,19,19	0.44	0	18,19,19	0.92	1 (5%)
23	CLA	N	610	7	65,73,73	1.47	6 (9%)	76,113,113	1.37	9 (11%)
23	CLA	n	603	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
40	LUT	y	317	-	42,43,43	2.38	20 (47%)	51,60,60	3.16	23 (45%)
25	BCR	Z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
23	CLA	c	511	3	65,73,73	1.48	6 (9%)	76,113,113	1.43	8 (10%)
23	CLA	b	604	-	65,73,73	1.48	6 (9%)	76,113,113	1.47	8 (10%)
23	CLA	b	616	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
31	LNL	C	520	-	19,19,19	0.44	0	18,19,19	0.90	1 (5%)
25	BCR	B	618	-	40,40,41	1.09	2 (5%)	52,54,56	1.25	6 (11%)
23	CLA	r	602	14	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LNL	a	401	-	19,19,19	0.43	0	18,19,19	0.93	1 (5%)
23	CLA	S	610	30	65,73,73	1.51	5 (7%)	76,113,113	1.37	8 (10%)
23	CLA	n	614	-	49,57,73	1.71	6 (12%)	55,93,113	1.54	8 (14%)
23	CLA	r	608	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	7 (9%)
23	CLA	c	512	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
25	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
39	CHL	G	606	-	50,58,74	1.88	4 (8%)	52,94,114	1.96	9 (17%)
23	CLA	B	602	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	10 (13%)
28	3PH	A	410	-	47,47,47	0.62	1 (2%)	51,52,52	0.60	1 (1%)
30	LHG	G	618	23	48,48,48	1.39	8 (16%)	51,54,54	0.75	2 (3%)
23	CLA	C	509	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	G	614	-	49,57,73	1.73	5 (10%)	55,93,113	1.49	8 (14%)
23	CLA	Y	312	7	65,73,73	1.52	5 (7%)	76,113,113	1.35	7 (9%)
23	CLA	C	507	43	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)
29	PL9	d	407	-	55,55,55	0.08	0	68,69,69	0.22	0
24	PHO	A	405	-	51,69,69	0.99	3 (5%)	47,99,99	1.15	6 (12%)
39	CHL	r	605	-	50,58,74	1.78	4 (8%)	52,94,114	1.95	10 (19%)
23	CLA	c	506	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	8 (10%)
23	CLA	B	609	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	9 (11%)
23	CLA	C	508	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	7 (9%)
42	XAT	G	619	-	39,47,47	3.01	22 (56%)	54,74,74	4.57	30 (55%)
23	CLA	S	613	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	9 (11%)
23	CLA	Y	310	7	65,73,73	1.47	5 (7%)	76,113,113	1.38	9 (11%)
30	LHG	s	616	23	48,48,48	1.39	8 (16%)	51,54,54	0.74	2 (3%)
23	CLA	G	611	30	49,57,73	1.72	5 (10%)	55,93,113	1.52	7 (12%)
40	LUT	n	615	-	42,43,43	1.89	11 (26%)	51,60,60	2.97	19 (37%)
35	VIV	y	301	-	32,32,32	0.88	1 (3%)	41,45,45	1.13	5 (12%)
28	3PH	s	618	-	37,37,47	0.70	1 (2%)	41,42,52	0.64	1 (2%)
31	LNL	C	522	-	19,19,19	0.44	0	18,19,19	0.91	1 (5%)
28	3PH	C	524	-	47,47,47	0.63	1 (2%)	51,52,52	0.60	1 (1%)
30	LHG	N	618	23	48,48,48	1.45	8 (16%)	51,54,54	0.69	2 (3%)
30	LHG	D	408	-	48,48,48	1.13	4 (8%)	51,54,54	0.93	3 (5%)
23	CLA	b	613	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
25	BCR	a	408	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	6 (10%)
23	CLA	N	614	-	49,57,73	1.70	5 (10%)	55,93,113	1.54	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	510	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
25	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	8 (14%)
30	LHG	a	412	-	48,48,48	1.40	8 (16%)	51,54,54	0.73	2 (3%)
23	CLA	s	602	15	57,65,73	1.59	6 (10%)	66,103,113	1.45	7 (10%)
23	CLA	B	613	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	7 (9%)
24	PHO	d	402	-	51,69,69	0.99	4 (7%)	47,99,99	1.13	5 (10%)
41	NEX	s	617	-	23,27,46	4.08	19 (82%)	28,38,70	3.76	14 (50%)
23	CLA	d	406	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)
41	NEX	R	618	-	38,46,46	3.93	31 (81%)	50,70,70	4.85	20 (40%)
23	CLA	c	509	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
42	XAT	r	615	-	39,47,47	3.22	20 (51%)	54,74,74	4.70	31 (57%)
23	CLA	B	606	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	8 (10%)
23	CLA	D	406	-	65,73,73	1.50	5 (7%)	76,113,113	1.39	8 (10%)
31	LNL	C	517	-	19,19,19	0.43	0	18,19,19	0.92	1 (5%)
31	LNL	b	623	-	19,19,19	0.45	0	18,19,19	0.89	1 (5%)
23	CLA	a	404	43	65,73,73	1.47	6 (9%)	76,113,113	1.44	8 (10%)
23	CLA	r	601	14	49,57,73	1.73	5 (10%)	55,93,113	1.50	6 (10%)
23	CLA	G	602	7	65,73,73	1.48	6 (9%)	76,113,113	1.40	9 (11%)
40	LUT	r	613	-	42,43,43	2.49	20 (47%)	51,60,60	3.11	24 (47%)
27	LMG	B	626	-	49,49,55	0.19	0	57,57,63	0.14	0
33	DGD	c	515	-	56,56,67	0.95	2 (3%)	70,70,81	1.45	9 (12%)
39	CHL	S	607	-	49,57,74	1.85	5 (10%)	52,93,114	1.88	10 (19%)
39	CHL	s	601	-	52,60,74	1.78	5 (9%)	56,97,114	1.86	11 (19%)
23	CLA	y	305	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
36	BCT	D	401	22	2,3,3	1.16	0	2,3,3	4.53	2 (100%)
23	CLA	b	609	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	9 (11%)
40	LUT	s	614	-	42,43,43	2.74	23 (54%)	51,60,60	3.28	24 (47%)
40	LUT	N	615	-	42,43,43	2.58	21 (50%)	51,60,60	3.25	24 (47%)
40	LUT	S	615	-	42,43,43	2.65	22 (52%)	51,60,60	3.22	24 (47%)
23	CLA	S	604	-	49,57,73	1.70	5 (10%)	55,93,113	1.58	7 (12%)
25	BCR	v	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	4 (7%)
39	CHL	n	601	7	66,74,74	1.59	5 (7%)	73,114,114	1.67	9 (12%)
23	CLA	G	612	7	49,57,73	1.72	6 (12%)	55,93,113	1.55	7 (12%)
40	LUT	G	615	-	42,43,43	1.97	12 (28%)	51,60,60	2.89	22 (43%)
39	CHL	y	303	7	66,74,74	1.58	4 (6%)	73,114,114	1.66	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LNL	b	622	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
31	LNL	I	101	-	19,19,19	0.43	0	18,19,19	0.91	1 (5%)
41	NEX	N	617	-	38,46,46	4.10	32 (84%)	50,70,70	4.96	22 (44%)
23	CLA	C	510	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
23	CLA	C	512	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	7 (9%)
23	CLA	N	603	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
23	CLA	R	604	43	55,63,73	1.61	6 (10%)	64,101,113	1.50	7 (10%)
23	CLA	R	612	14	49,57,73	1.73	5 (10%)	55,93,113	1.53	7 (12%)
40	LUT	R	613	-	42,43,43	2.53	21 (50%)	51,60,60	3.16	25 (49%)
23	CLA	b	605	-	65,73,73	1.48	7 (10%)	76,113,113	1.36	7 (9%)
24	PHO	a	406	-	51,69,69	0.98	3 (5%)	47,99,99	1.14	4 (8%)
23	CLA	a	405	43	49,57,73	1.69	5 (10%)	55,93,113	1.57	8 (14%)
42	XAT	Y	301	-	39,47,47	3.30	24 (61%)	54,74,74	4.45	32 (59%)
27	LMG	B	620	-	48,48,55	0.19	0	56,56,63	0.19	0
39	CHL	G	601	7	66,74,74	1.57	4 (6%)	73,114,114	1.65	8 (10%)
23	CLA	y	315	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	9 (11%)
27	LMG	A	409	-	53,53,55	0.19	0	61,61,63	0.19	0
27	LMG	R	617	-	51,51,55	0.18	0	59,59,63	0.26	0
23	CLA	A	402	-	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
23	CLA	s	609	15	56,64,73	1.62	5 (8%)	65,102,113	1.48	7 (10%)
23	CLA	a	403	-	65,73,73	1.47	7 (10%)	76,113,113	1.43	7 (9%)
23	CLA	g	603	-	65,73,73	1.50	6 (9%)	76,113,113	1.40	8 (10%)
23	CLA	g	612	7	49,57,73	1.71	6 (12%)	55,93,113	1.60	7 (12%)
40	LUT	g	615	-	42,43,43	1.88	10 (23%)	51,60,60	2.93	21 (41%)
23	CLA	D	405	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	6 (7%)
23	CLA	r	612	14	49,57,73	1.72	6 (12%)	55,93,113	1.50	7 (12%)
39	CHL	g	606	-	50,58,74	1.87	5 (10%)	52,94,114	1.98	11 (21%)
39	CHL	r	607	-	66,74,74	1.60	4 (6%)	73,114,114	1.67	12 (16%)
23	CLA	B	601	-	49,57,73	1.70	5 (10%)	55,93,113	1.58	8 (14%)
23	CLA	b	612	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
23	CLA	y	304	7	65,73,73	1.48	5 (7%)	76,113,113	1.40	9 (11%)
26	SQD	L	101	-	53,54,54	1.53	8 (15%)	62,65,65	1.40	6 (9%)
23	CLA	c	502	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
25	BCR	H	501	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	4 (7%)
30	LHG	r	616	23	36,36,48	1.60	8 (22%)	39,42,54	0.82	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CHL	G	605	7	48,56,74	1.87	4 (8%)	51,92,114	2.09	12 (23%)
39	CHL	S	606	-	50,58,74	1.83	4 (8%)	52,94,114	1.96	11 (21%)
23	CLA	b	607	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
23	CLA	y	312	30	65,73,73	1.48	5 (7%)	76,113,113	1.37	9 (11%)
39	CHL	n	609	7	66,74,74	1.56	4 (6%)	73,114,114	1.61	10 (13%)
23	CLA	C	513	-	65,73,73	1.47	6 (9%)	76,113,113	1.45	9 (11%)
27	LMG	w	201	-	48,48,55	0.19	0	56,56,63	0.18	0
40	LUT	y	316	-	42,43,43	1.80	10 (23%)	51,60,60	2.77	19 (37%)
23	CLA	S	611	15	49,57,73	1.71	5 (10%)	55,93,113	1.53	7 (12%)
30	LHG	d	408	-	48,48,48	1.36	8 (16%)	51,54,54	0.74	2 (3%)
30	LHG	A	412	-	36,36,48	1.52	8 (22%)	39,42,54	0.89	2 (5%)
39	CHL	Y	308	-	50,58,74	1.82	5 (10%)	52,94,114	1.93	8 (15%)
31	LNL	C	521	-	19,19,19	0.45	0	18,19,19	0.93	1 (5%)
23	CLA	g	604	-	49,57,73	1.71	5 (10%)	55,93,113	1.55	8 (14%)
23	CLA	y	311	7	65,73,73	1.47	5 (7%)	76,113,113	1.38	9 (11%)
23	CLA	s	604	-	49,57,73	1.70	6 (12%)	55,93,113	1.58	8 (14%)
23	CLA	R	603	-	60,68,73	1.53	6 (10%)	70,107,113	1.45	8 (11%)
40	LUT	g	616	-	42,43,43	2.40	19 (45%)	51,60,60	3.11	21 (41%)
28	3PH	T	101	-	47,47,47	0.63	1 (2%)	51,52,52	0.61	1 (1%)
31	LNL	C	518	-	19,19,19	0.44	0	18,19,19	0.97	1 (5%)
39	CHL	R	605	-	50,58,74	1.81	4 (8%)	52,94,114	1.91	11 (21%)
39	CHL	g	605	7	48,56,74	1.83	4 (8%)	51,92,114	2.11	11 (21%)
29	PL9	A	411	-	55,55,55	0.11	0	68,69,69	0.42	0
23	CLA	S	609	15	56,64,73	1.60	5 (8%)	65,102,113	1.43	8 (12%)
27	LMG	c	523	-	46,46,55	0.19	0	54,54,63	0.17	0
33	DGD	d	411	-	63,63,67	0.85	1 (1%)	77,77,81	1.35	7 (9%)
23	CLA	R	602	14	65,73,73	1.48	5 (7%)	76,113,113	1.38	6 (7%)
23	CLA	a	407	-	60,68,73	1.54	5 (8%)	70,107,113	1.46	9 (12%)
39	CHL	g	607	-	66,74,74	1.57	4 (6%)	73,114,114	1.71	9 (12%)
23	CLA	Y	313	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	8 (10%)
23	CLA	B	614	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
28	3PH	d	403	-	37,37,47	0.71	1 (2%)	41,42,52	0.66	1 (2%)
39	CHL	G	620	-	66,74,74	1.58	5 (7%)	73,114,114	1.71	12 (16%)
30	LHG	d	404	-	48,48,48	1.36	8 (16%)	51,54,54	0.78	2 (3%)
38	HEM	F	501	-	41,50,50	1.47	3 (7%)	45,82,82	1.42	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	CHL	g	619	43	66,74,74	1.58	5 (7%)	73,114,114	1.70	11 (15%)
30	LHG	n	619	23	44,44,48	1.45	8 (18%)	47,50,54	0.75	2 (4%)
40	LUT	s	615	-	42,43,43	2.55	21 (50%)	51,60,60	3.15	24 (47%)
30	LHG	g	618	-	48,48,48	1.40	8 (16%)	51,54,54	0.77	2 (3%)
30	LHG	Y	318	23	48,48,48	1.39	8 (16%)	51,54,54	0.69	2 (3%)
25	BCR	V	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	4 (7%)
23	CLA	R	609	14	65,73,73	1.49	5 (7%)	76,113,113	1.36	7 (9%)
39	CHL	R	606	-	66,74,74	1.56	5 (7%)	73,114,114	1.67	13 (17%)
23	CLA	C	502	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
39	CHL	N	601	7	66,74,74	1.59	5 (7%)	73,114,114	1.67	10 (13%)
23	CLA	b	611	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)
31	LNL	A	413	-	19,19,19	0.44	0	18,19,19	0.89	1 (5%)
39	CHL	g	609	7	66,74,74	1.60	4 (6%)	73,114,114	1.68	12 (16%)
23	CLA	A	406	-	60,68,73	1.53	5 (8%)	70,107,113	1.44	9 (12%)
39	CHL	G	607	-	66,74,74	1.58	4 (6%)	73,114,114	1.71	10 (13%)
31	LNL	c	520	-	19,19,19	0.43	0	18,19,19	0.95	1 (5%)
26	SQD	a	409	-	47,48,54	1.61	7 (14%)	56,59,65	1.45	6 (10%)
39	CHL	n	607	-	66,74,74	1.58	4 (6%)	73,114,114	1.69	9 (12%)
23	CLA	g	611	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
27	LMG	r	617	-	51,51,55	0.19	0	59,59,63	0.16	0
23	CLA	s	613	-	65,73,73	1.50	5 (7%)	76,113,113	1.40	9 (11%)
23	CLA	c	507	43	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
40	LUT	S	614	-	42,43,43	2.60	21 (50%)	51,60,60	3.23	25 (49%)
39	CHL	y	308	43	50,58,74	1.80	5 (10%)	52,94,114	1.92	10 (19%)
23	CLA	b	610	43	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)
23	CLA	b	615	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
23	CLA	b	603	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	8 (10%)
39	CHL	g	608	-	50,58,74	1.85	5 (10%)	52,94,114	1.84	9 (17%)
36	BCT	d	401	22	2,3,3	1.15	0	2,3,3	4.51	2 (100%)
23	CLA	c	504	43	65,73,73	1.49	6 (9%)	76,113,113	1.38	6 (7%)
30	LHG	y	318	23	48,48,48	1.39	8 (16%)	51,54,54	0.71	2 (3%)
39	CHL	S	601	-	52,60,74	1.77	5 (9%)	56,97,114	1.87	11 (19%)
23	CLA	b	614	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	c	501	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
39	CHL	n	608	-	50,58,74	1.82	5 (10%)	52,94,114	1.94	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	605	-	65,73,73	1.49	7 (10%)	76,113,113	1.36	8 (10%)
39	CHL	Y	309	7	66,74,74	1.60	4 (6%)	73,114,114	1.61	9 (12%)
40	LUT	n	616	-	42,43,43	2.36	19 (45%)	51,60,60	3.07	21 (41%)
25	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
30	LHG	D	404	-	42,42,48	1.43	8 (19%)	45,48,54	0.80	2 (4%)
23	CLA	B	610	43	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
31	LNL	a	413	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
23	CLA	s	610	30	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
29	PL9	D	407	-	55,55,55	0.08	0	68,69,69	0.21	0
23	CLA	R	608	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	8 (10%)
41	NEX	n	618	-	38,46,46	4.08	32 (84%)	50,70,70	4.99	22 (44%)
39	CHL	n	605	7	48,56,74	1.86	5 (10%)	51,92,114	2.06	10 (19%)
39	CHL	s	605	-	50,58,74	1.81	3 (6%)	52,94,114	1.94	10 (19%)
23	CLA	Y	303	7	65,73,73	1.47	5 (7%)	76,113,113	1.40	9 (11%)
31	LNL	B	623	-	19,19,19	0.45	0	18,19,19	0.86	1 (5%)
39	CHL	g	601	7	66,74,74	1.56	4 (6%)	73,114,114	1.64	8 (10%)
27	LMG	b	628	-	50,50,55	0.19	0	58,58,63	0.18	0
41	NEX	Y	317	-	38,46,46	4.00	31 (81%)	50,70,70	4.95	22 (44%)
39	CHL	s	606	-	50,58,74	1.81	5 (10%)	52,94,114	1.89	10 (19%)
23	CLA	s	612	15	55,63,73	1.61	6 (10%)	64,101,113	1.48	7 (10%)
31	LNL	C	519	-	19,19,19	0.43	0	18,19,19	0.95	1 (5%)
39	CHL	s	607	-	49,57,74	1.85	5 (10%)	52,93,114	1.87	11 (21%)
28	3PH	W	201	-	45,45,47	0.64	1 (2%)	49,50,52	0.60	1 (2%)
35	VIV	C	523	-	32,32,32	0.93	2 (6%)	41,45,45	1.14	4 (9%)
23	CLA	N	612	7	49,57,73	1.71	6 (12%)	55,93,113	1.54	7 (12%)
42	XAT	y	302	-	39,47,47	3.39	24 (61%)	54,74,74	4.46	31 (57%)
23	CLA	S	612	15	55,63,73	1.62	6 (10%)	64,101,113	1.49	7 (10%)
23	CLA	Y	314	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	9 (11%)
23	CLA	g	602	7	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
25	BCR	h	501	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	4 (7%)
27	LMG	D	409	-	36,36,55	0.20	0	44,44,63	0.14	0
30	LHG	L	103	-	48,48,48	1.36	8 (16%)	51,54,54	0.71	2 (3%)
25	BCR	C	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
23	CLA	B	604	-	65,73,73	1.48	6 (9%)	76,113,113	1.46	8 (10%)
23	CLA	C	506	-	55,63,73	1.62	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
23	CLA	B	612	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	8 (10%)
23	CLA	c	505	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	A	404	43	49,57,73	1.70	6 (12%)	55,93,113	1.57	8 (14%)
39	CHL	Y	302	7	66,74,74	1.59	5 (7%)	73,114,114	1.63	10 (13%)
39	CHL	r	606	-	66,74,74	1.56	4 (6%)	73,114,114	1.65	12 (16%)
25	BCR	b	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
37	DGA	b	626	-	43,43,43	0.19	0	45,45,45	0.15	0
41	NEX	R	614	-	38,46,46	4.09	32 (84%)	50,70,70	4.87	22 (44%)
40	LUT	N	616	-	42,43,43	2.59	22 (52%)	51,60,60	3.21	22 (43%)
26	SQD	A	408	-	49,50,54	1.57	7 (14%)	58,61,65	1.45	7 (12%)
23	CLA	c	503	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	7 (9%)
23	CLA	S	603	-	49,57,73	1.70	5 (10%)	55,93,113	1.56	7 (12%)
23	CLA	G	610	7	65,73,73	1.46	5 (7%)	76,113,113	1.44	8 (10%)
42	XAT	R	615	-	39,47,47	3.21	20 (51%)	54,74,74	4.68	31 (57%)
39	CHL	N	605	7	50,58,74	1.82	5 (10%)	52,94,114	2.16	9 (17%)
39	CHL	S	605	-	50,58,74	1.80	3 (6%)	52,94,114	1.99	9 (17%)
23	CLA	g	613	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	9 (11%)
23	CLA	n	612	7	49,57,73	1.72	6 (12%)	55,93,113	1.55	7 (12%)
32	PAM	b	621	-	17,17,17	0.63	0	17,17,17	0.78	0
23	CLA	S	602	15	57,65,73	1.60	6 (10%)	66,103,113	1.45	8 (12%)
23	CLA	Y	305	-	65,73,73	1.50	5 (7%)	76,113,113	1.40	8 (10%)
33	DGD	C	515	-	67,67,67	0.88	2 (2%)	81,81,81	1.46	10 (12%)
23	CLA	r	609	14	65,73,73	1.47	6 (9%)	76,113,113	1.35	8 (10%)
23	CLA	y	313	7	65,73,73	1.51	5 (7%)	76,113,113	1.35	7 (9%)
41	NEX	S	617	-	19,23,46	4.24	16 (84%)	23,33,70	4.24	11 (47%)
23	CLA	b	601	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	9 (15%)
23	CLA	R	610	30	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
23	CLA	C	505	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	C	511	3	65,73,73	1.48	5 (7%)	76,113,113	1.43	7 (9%)
23	CLA	g	610	7	65,73,73	1.46	5 (7%)	76,113,113	1.43	8 (10%)
31	LNL	B	624	-	19,19,19	0.44	0	18,19,19	0.90	1 (5%)
23	CLA	y	306	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	9 (11%)
23	CLA	G	603	-	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
23	CLA	d	405	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	6 (7%)
23	CLA	n	611	30	49,57,73	1.73	5 (10%)	55,93,113	1.52	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	608	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
23	CLA	r	610	30	65,73,73	1.49	5 (7%)	76,113,113	1.42	8 (10%)
23	CLA	n	604	-	49,57,73	1.71	6 (12%)	55,93,113	1.58	8 (14%)
25	BCR	A	407	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	5 (8%)
39	CHL	y	309	-	50,58,74	1.82	4 (8%)	52,94,114	1.89	8 (15%)
23	CLA	b	606	-	65,73,73	1.50	7 (10%)	76,113,113	1.38	9 (11%)
23	CLA	A	403	43	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
39	CHL	N	607	-	66,74,74	1.58	4 (6%)	73,114,114	1.68	9 (12%)
25	BCR	z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
23	CLA	B	603	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)
31	LNL	A	414	-	19,19,19	0.43	0	18,19,19	0.92	1 (5%)
29	PL9	a	411	-	55,55,55	0.11	0	68,69,69	0.28	0
23	CLA	y	314	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	8 (10%)
41	NEX	r	614	-	38,46,46	3.97	31 (81%)	50,70,70	4.87	22 (44%)
39	CHL	N	609	7	66,74,74	1.57	4 (6%)	73,114,114	1.62	10 (13%)
25	BCR	c	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
31	LNL	c	522	-	19,19,19	0.43	0	18,19,19	0.94	1 (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
23	CLA	Y	311	30	1/1/15/20	7/37/115/115	-
23	CLA	n	602	7	1/1/15/20	11/37/115/115	-
28	3PH	L	102	-	-	14/42/42/49	-
23	CLA	G	613	7	1/1/15/20	12/37/115/115	-
39	CHL	G	609	7	3/3/20/26	12/39/137/137	-
23	CLA	Y	304	-	1/1/15/20	12/37/115/115	-
38	HEM	f	501	6,5	-	1/12/54/54	-
23	CLA	N	604	-	1/1/11/20	7/18/96/115	-
28	3PH	w	202	-	-	17/49/49/49	-
28	3PH	x	201	-	-	13/47/47/49	-
27	LMG	C	525	-	-	10/40/60/70	0/1/1/1
39	CHL	N	608	-	3/3/16/26	6/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	G	604	-	1/1/11/20	6/18/96/115	-
24	PHO	D	402	-	-	9/37/103/103	0/5/6/6
28	3PH	a	410	-	-	21/49/49/49	-
23	CLA	B	611	-	1/1/15/20	10/37/115/115	-
23	CLA	s	611	15	1/1/11/20	8/18/96/115	-
31	LNL	i	101	-	-	9/17/17/17	-
42	XAT	N	619	-	-	13/31/93/93	0/4/4/4
28	3PH	D	403	-	-	13/39/39/49	-
23	CLA	R	611	-	1/1/11/20	6/18/96/115	-
23	CLA	r	611	-	1/1/11/20	6/18/96/115	-
23	CLA	s	603	-	1/1/11/20	12/18/96/115	-
23	CLA	s	608	-	1/1/11/20	7/18/96/115	-
23	CLA	N	611	30	1/1/15/20	9/37/115/115	-
23	CLA	r	603	-	1/1/14/20	5/31/109/115	-
23	CLA	c	513	-	1/1/14/20	8/31/109/115	-
23	CLA	c	508	-	1/1/15/20	3/37/115/115	-
25	BCR	b	619	-	-	6/29/63/63	0/2/2/2
23	CLA	b	602	-	1/1/15/20	12/37/115/115	-
41	NEX	G	617	-	-	7/16/47/83	0/2/2/3
25	BCR	b	617	-	-	11/29/63/63	0/2/2/2
39	CHL	Y	306	7	3/3/16/26	2/18/116/137	-
23	CLA	n	613	7	1/1/15/20	6/37/115/115	-
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
31	LNL	B	622	-	-	7/17/17/17	-
39	CHL	Y	307	-	3/3/20/26	3/39/137/137	-
31	LNL	B	625	-	-	7/17/17/17	-
39	CHL	y	307	7	3/3/16/26	2/18/116/137	-
31	LNL	c	518	-	-	12/17/17/17	-
28	3PH	X	201	-	-	13/47/47/49	-
23	CLA	S	608	-	1/1/11/20	1/18/96/115	-
33	DGD	H	502	-	-	24/51/91/95	0/2/2/2
23	CLA	B	616	-	1/1/15/20	11/37/115/115	-
26	SQD	M	101	-	-	24/45/65/69	0/1/1/1
23	CLA	n	610	7	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	b	620	-	-	8/46/66/70	0/1/1/1
31	LNL	c	519	-	-	11/17/17/17	-
23	CLA	N	602	7	1/1/15/20	4/37/115/115	-
23	CLA	B	607	-	1/1/15/20	21/37/115/115	-
32	PAM	B	621	-	-	5/15/15/15	-
39	CHL	n	606	-	3/3/20/26	8/39/137/137	-
40	LUT	Y	316	-	-	15/29/67/67	0/2/2/2
40	LUT	Y	315	-	-	17/29/67/67	0/2/2/2
25	BCR	d	410	-	-	9/29/63/63	0/2/2/2
42	XAT	n	617	-	-	6/31/93/93	0/4/4/4
42	XAT	n	620	-	-	9/31/93/93	0/4/4/4
31	LNL	c	521	-	-	7/17/17/17	-
23	CLA	C	503	-	1/1/15/20	8/37/115/115	-
39	CHL	N	606	-	3/3/20/26	9/39/137/137	-
40	LUT	G	616	-	-	9/29/67/67	0/2/2/2
30	LHG	b	627	-	-	22/53/53/53	-
23	CLA	C	504	43	1/1/15/20	8/37/115/115	-
23	CLA	C	501	-	1/1/15/20	12/37/115/115	-
23	CLA	B	615	-	1/1/15/20	7/37/115/115	-
30	LHG	S	616	23	-	14/53/53/53	-
31	LNL	c	517	-	-	5/17/17/17	-
37	DGA	D	410	-	-	12/41/41/45	-
41	NEX	g	617	-	-	14/27/83/83	0/3/3/3
23	CLA	B	608	-	1/1/15/20	10/37/115/115	-
39	CHL	y	310	7	3/3/20/26	8/39/137/137	-
23	CLA	r	604	43	1/1/13/20	8/25/103/115	-
31	LNL	b	624	-	-	9/17/17/17	-
39	CHL	R	607	-	3/3/20/26	9/39/137/137	-
23	CLA	N	613	-	1/1/15/20	12/37/115/115	-
25	BCR	D	411	-	-	5/29/63/63	0/2/2/2
27	LMG	d	409	-	-	6/41/61/70	0/1/1/1
30	LHG	R	616	23	-	17/42/42/53	-
23	CLA	R	601	14	1/1/11/20	10/18/96/115	-
39	CHL	G	608	-	3/3/16/26	8/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	g	614	-	1/1/11/20	6/18/96/115	-
31	LNL	b	625	-	-	9/17/17/17	-
23	CLA	N	610	7	1/1/15/20	10/37/115/115	-
23	CLA	n	603	-	1/1/15/20	11/37/115/115	-
40	LUT	y	317	-	-	15/29/67/67	0/2/2/2
25	BCR	Z	101	-	-	5/29/63/63	0/2/2/2
23	CLA	c	511	3	1/1/15/20	12/37/115/115	-
23	CLA	b	604	-	1/1/15/20	6/37/115/115	-
23	CLA	b	616	-	1/1/15/20	12/37/115/115	-
31	LNL	C	520	-	-	11/17/17/17	-
25	BCR	B	618	-	-	3/29/60/63	0/2/2/2
23	CLA	r	602	14	1/1/15/20	13/37/115/115	-
31	LNL	a	401	-	-	11/17/17/17	-
23	CLA	S	610	30	1/1/15/20	14/37/115/115	-
23	CLA	n	614	-	1/1/11/20	10/18/96/115	-
23	CLA	r	608	-	1/1/15/20	9/37/115/115	-
23	CLA	c	512	-	1/1/15/20	21/37/115/115	-
25	BCR	B	619	-	-	4/29/63/63	0/2/2/2
39	CHL	G	606	-	3/3/16/26	4/20/118/137	-
23	CLA	B	602	-	1/1/15/20	14/37/115/115	-
28	3PH	A	410	-	-	18/49/49/49	-
30	LHG	G	618	23	-	19/53/53/53	-
23	CLA	C	509	-	1/1/15/20	10/37/115/115	-
23	CLA	G	614	-	1/1/11/20	6/18/96/115	-
23	CLA	Y	312	7	1/1/15/20	9/37/115/115	-
23	CLA	C	507	43	1/1/15/20	9/37/115/115	-
29	PL9	d	407	-	-	10/53/73/73	0/1/1/1
39	CHL	r	605	-	3/3/16/26	6/20/118/137	-
24	PHO	A	405	-	-	10/37/103/103	0/5/6/6
23	CLA	c	506	-	1/1/15/20	15/37/115/115	-
23	CLA	B	609	-	1/1/15/20	8/37/115/115	-
23	CLA	C	508	-	1/1/15/20	7/37/115/115	-
42	XAT	G	619	-	-	11/31/93/93	0/4/4/4
23	CLA	S	613	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	Y	310	7	1/1/15/20	13/37/115/115	-
30	LHG	s	616	23	-	19/53/53/53	-
23	CLA	G	611	30	1/1/11/20	8/18/96/115	-
40	LUT	n	615	-	-	14/29/67/67	0/2/2/2
35	VIV	y	301	-	-	15/19/30/30	0/2/2/2
28	3PH	s	618	-	-	14/39/39/49	-
31	LNL	C	522	-	-	11/17/17/17	-
28	3PH	C	524	-	-	19/49/49/49	-
30	LHG	N	618	23	-	25/53/53/53	-
30	LHG	D	408	-	-	29/53/53/53	-
23	CLA	b	613	-	1/1/15/20	13/37/115/115	-
25	BCR	a	408	-	-	4/29/63/63	0/2/2/2
23	CLA	N	614	-	1/1/11/20	7/18/96/115	-
23	CLA	c	510	-	1/1/15/20	14/37/115/115	-
25	BCR	B	617	-	-	10/29/63/63	0/2/2/2
30	LHG	a	412	-	-	26/53/53/53	-
23	CLA	s	602	15	1/1/13/20	9/28/106/115	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-
24	PHO	d	402	-	-	5/37/103/103	0/5/6/6
41	NEX	s	617	-	-	8/15/40/83	0/1/1/3
23	CLA	d	406	-	1/1/15/20	7/37/115/115	-
41	NEX	R	618	-	-	12/27/83/83	0/3/3/3
23	CLA	c	509	-	1/1/15/20	10/37/115/115	-
42	XAT	r	615	-	-	14/31/93/93	0/4/4/4
23	CLA	B	606	-	1/1/15/20	9/37/115/115	-
23	CLA	D	406	-	1/1/15/20	15/37/115/115	-
31	LNL	C	517	-	-	12/17/17/17	-
31	LNL	b	623	-	-	10/17/17/17	-
23	CLA	a	404	43	1/1/15/20	11/37/115/115	-
23	CLA	r	601	14	1/1/11/20	10/18/96/115	-
23	CLA	G	602	7	1/1/15/20	5/37/115/115	-
40	LUT	r	613	-	-	11/29/67/67	0/2/2/2
27	LMG	B	626	-	-	8/44/64/70	0/1/1/1
33	DGD	c	515	-	-	13/44/84/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	S	607	-	3/3/16/26	5/19/117/137	-
39	CHL	s	601	-	3/3/17/26	6/23/121/137	-
23	CLA	y	305	-	1/1/15/20	12/37/115/115	-
23	CLA	b	609	-	1/1/15/20	10/37/115/115	-
40	LUT	s	614	-	-	18/29/67/67	0/2/2/2
40	LUT	N	615	-	-	13/29/67/67	0/2/2/2
40	LUT	S	615	-	-	16/29/67/67	0/2/2/2
23	CLA	S	604	-	1/1/11/20	7/18/96/115	-
25	BCR	v	101	-	-	10/29/63/63	0/2/2/2
39	CHL	n	601	7	3/3/20/26	8/39/137/137	-
23	CLA	G	612	7	1/1/11/20	6/18/96/115	-
40	LUT	G	615	-	-	22/29/67/67	0/2/2/2
39	CHL	y	303	7	3/3/20/26	13/39/137/137	-
31	LNL	b	622	-	-	8/17/17/17	-
31	LNL	I	101	-	-	11/17/17/17	-
41	NEX	N	617	-	-	12/27/83/83	0/3/3/3
23	CLA	C	510	-	1/1/15/20	12/37/115/115	-
23	CLA	C	512	-	1/1/15/20	17/37/115/115	-
23	CLA	N	603	-	1/1/15/20	10/37/115/115	-
23	CLA	R	604	43	1/1/13/20	9/25/103/115	-
23	CLA	R	612	14	1/1/11/20	8/18/96/115	-
40	LUT	R	613	-	-	16/29/67/67	0/2/2/2
23	CLA	b	605	-	1/1/15/20	15/37/115/115	-
24	PHO	a	406	-	-	10/37/103/103	0/5/6/6
23	CLA	a	405	43	1/1/11/20	1/18/96/115	-
42	XAT	Y	301	-	-	17/31/93/93	0/4/4/4
27	LMG	B	620	-	-	7/43/63/70	0/1/1/1
39	CHL	G	601	7	3/3/20/26	9/39/137/137	-
23	CLA	y	315	-	1/1/15/20	18/37/115/115	-
27	LMG	A	409	-	-	11/48/68/70	0/1/1/1
27	LMG	R	617	-	-	14/46/66/70	0/1/1/1
23	CLA	A	402	-	1/1/15/20	10/37/115/115	-
23	CLA	s	609	15	1/1/13/20	11/27/105/115	-
23	CLA	a	403	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	g	603	-	1/1/15/20	10/37/115/115	-
23	CLA	g	612	7	1/1/11/20	6/18/96/115	-
40	LUT	g	615	-	-	19/29/67/67	0/2/2/2
23	CLA	D	405	-	1/1/15/20	9/37/115/115	-
23	CLA	r	612	14	1/1/11/20	5/18/96/115	-
39	CHL	g	606	-	3/3/16/26	4/20/118/137	-
39	CHL	r	607	-	3/3/20/26	9/39/137/137	-
23	CLA	B	601	-	1/1/11/20	10/18/96/115	-
23	CLA	b	612	-	1/1/15/20	12/37/115/115	-
23	CLA	y	304	7	1/1/15/20	13/37/115/115	-
26	SQD	L	101	-	-	24/49/69/69	0/1/1/1
23	CLA	c	502	-	1/1/15/20	12/37/115/115	-
25	BCR	H	501	-	-	7/29/63/63	0/2/2/2
39	CHL	S	606	-	3/3/16/26	6/20/118/137	-
39	CHL	G	605	7	3/3/16/26	6/18/116/137	-
30	LHG	r	616	23	-	19/41/41/53	-
23	CLA	b	607	-	1/1/15/20	16/37/115/115	-
23	CLA	y	312	30	1/1/15/20	7/37/115/115	-
39	CHL	n	609	7	3/3/20/26	8/39/137/137	-
23	CLA	C	513	-	1/1/15/20	12/37/115/115	-
27	LMG	w	201	-	-	5/43/63/70	0/1/1/1
40	LUT	y	316	-	-	17/29/67/67	0/2/2/2
23	CLA	S	611	15	1/1/11/20	9/18/96/115	-
30	LHG	d	408	-	-	15/53/53/53	-
30	LHG	A	412	-	-	21/41/41/53	-
39	CHL	Y	308	-	3/3/16/26	6/20/118/137	-
31	LNL	C	521	-	-	11/17/17/17	-
23	CLA	g	604	-	1/1/11/20	8/18/96/115	-
23	CLA	y	311	7	1/1/15/20	10/37/115/115	-
23	CLA	s	604	-	1/1/11/20	8/18/96/115	-
23	CLA	R	603	-	1/1/14/20	5/31/109/115	-
40	LUT	g	616	-	-	10/29/67/67	0/2/2/2
28	3PH	T	101	-	-	22/49/49/49	-
31	LNL	C	518	-	-	8/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	R	605	-	3/3/16/26	2/20/118/137	-
39	CHL	g	605	7	3/3/16/26	5/18/116/137	-
29	PL9	A	411	-	-	7/53/73/73	0/1/1/1
23	CLA	S	609	15	1/1/13/20	12/27/105/115	-
27	LMG	c	523	-	-	9/41/61/70	0/1/1/1
33	DGD	d	411	-	-	18/51/91/95	0/2/2/2
23	CLA	R	602	14	1/1/15/20	6/37/115/115	-
23	CLA	a	407	-	1/1/14/20	5/31/109/115	-
39	CHL	g	607	-	3/3/20/26	13/39/137/137	-
23	CLA	Y	313	-	1/1/15/20	10/37/115/115	-
23	CLA	B	614	-	1/1/15/20	13/37/115/115	-
28	3PH	d	403	-	-	10/39/39/49	-
39	CHL	G	620	-	3/3/20/26	12/39/137/137	-
30	LHG	d	404	-	-	20/53/53/53	-
38	HEM	F	501	-	-	3/12/54/54	-
39	CHL	g	619	43	3/3/20/26	8/39/137/137	-
30	LHG	n	619	23	-	23/49/49/53	-
40	LUT	s	615	-	-	11/29/67/67	0/2/2/2
30	LHG	g	618	-	-	15/53/53/53	-
30	LHG	Y	318	23	-	21/53/53/53	-
25	BCR	V	101	-	-	11/29/63/63	0/2/2/2
23	CLA	R	609	14	1/1/15/20	6/37/115/115	-
39	CHL	R	606	-	3/3/20/26	9/39/137/137	-
23	CLA	C	502	-	1/1/15/20	12/37/115/115	-
39	CHL	N	601	7	3/3/20/26	7/39/137/137	-
23	CLA	b	611	-	1/1/15/20	6/37/115/115	-
31	LNL	A	413	-	-	10/17/17/17	-
39	CHL	g	609	7	3/3/20/26	11/39/137/137	-
23	CLA	A	406	-	1/1/14/20	1/31/109/115	-
39	CHL	G	607	-	3/3/20/26	9/39/137/137	-
31	LNL	c	520	-	-	6/17/17/17	-
26	SQD	a	409	-	-	18/43/63/69	0/1/1/1
39	CHL	n	607	-	3/3/20/26	8/39/137/137	-
23	CLA	g	611	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	r	617	-	-	11/46/66/70	0/1/1/1
23	CLA	s	613	-	1/1/15/20	16/37/115/115	-
23	CLA	c	507	43	1/1/15/20	6/37/115/115	-
40	LUT	S	614	-	-	15/29/67/67	0/2/2/2
39	CHL	y	308	43	3/3/16/26	3/20/118/137	-
23	CLA	b	610	43	1/1/15/20	10/37/115/115	-
23	CLA	b	615	-	1/1/15/20	6/37/115/115	-
23	CLA	b	603	-	1/1/15/20	11/37/115/115	-
39	CHL	g	608	-	3/3/16/26	8/20/118/137	-
23	CLA	c	504	43	1/1/15/20	8/37/115/115	-
30	LHG	y	318	23	-	22/53/53/53	-
39	CHL	S	601	-	3/3/17/26	4/23/121/137	-
23	CLA	b	614	-	1/1/15/20	12/37/115/115	-
23	CLA	c	501	-	1/1/15/20	15/37/115/115	-
39	CHL	n	608	-	3/3/16/26	4/20/118/137	-
23	CLA	B	605	-	1/1/15/20	13/37/115/115	-
39	CHL	Y	309	7	3/3/20/26	4/39/137/137	-
40	LUT	n	616	-	-	14/29/67/67	0/2/2/2
25	BCR	K	101	-	-	4/29/63/63	0/2/2/2
30	LHG	D	404	-	-	10/47/47/53	-
23	CLA	B	610	43	1/1/15/20	8/37/115/115	-
31	LNL	a	413	-	-	9/17/17/17	-
23	CLA	s	610	30	1/1/15/20	14/37/115/115	-
29	PL9	D	407	-	-	10/53/73/73	0/1/1/1
23	CLA	R	608	-	1/1/15/20	7/37/115/115	-
41	NEX	n	618	-	-	14/27/83/83	0/3/3/3
39	CHL	n	605	7	3/3/16/26	4/18/116/137	-
39	CHL	s	605	-	3/3/16/26	5/20/118/137	-
23	CLA	Y	303	7	1/1/15/20	13/37/115/115	-
31	LNL	B	623	-	-	10/17/17/17	-
39	CHL	g	601	7	3/3/20/26	6/39/137/137	-
27	LMG	b	628	-	-	11/45/65/70	0/1/1/1
41	NEX	Y	317	-	-	14/27/83/83	0/3/3/3
39	CHL	s	606	-	3/3/16/26	4/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	s	612	15	1/1/13/20	7/25/103/115	-
31	LNL	C	519	-	-	5/17/17/17	-
39	CHL	s	607	-	3/3/16/26	6/19/117/137	-
28	3PH	W	201	-	-	23/47/47/49	-
35	VIV	C	523	-	-	12/19/30/30	0/2/2/2
23	CLA	N	612	7	1/1/11/20	9/18/96/115	-
42	XAT	y	302	-	-	18/31/93/93	0/4/4/4
23	CLA	S	612	15	1/1/13/20	9/25/103/115	-
23	CLA	Y	314	-	1/1/15/20	11/37/115/115	-
23	CLA	g	602	7	1/1/15/20	5/37/115/115	-
25	BCR	h	501	-	-	7/29/63/63	0/2/2/2
27	LMG	D	409	-	-	1/31/51/70	0/1/1/1
30	LHG	L	103	-	-	25/53/53/53	-
25	BCR	C	514	-	-	7/29/63/63	0/2/2/2
23	CLA	B	604	-	1/1/15/20	9/37/115/115	-
23	CLA	C	506	-	1/1/13/20	9/25/103/115	-
23	CLA	B	612	-	1/1/15/20	11/37/115/115	-
23	CLA	c	505	-	1/1/15/20	8/37/115/115	-
23	CLA	A	404	43	1/1/11/20	4/18/96/115	-
39	CHL	Y	302	7	3/3/20/26	11/39/137/137	-
39	CHL	r	606	-	3/3/20/26	10/39/137/137	-
25	BCR	b	618	-	-	5/29/63/63	0/2/2/2
37	DGA	b	626	-	-	14/45/45/45	-
41	NEX	R	614	-	-	13/27/83/83	0/3/3/3
40	LUT	N	616	-	-	20/29/67/67	0/2/2/2
26	SQD	A	408	-	-	29/45/65/69	0/1/1/1
23	CLA	c	503	-	1/1/15/20	7/37/115/115	-
23	CLA	S	603	-	1/1/11/20	12/18/96/115	-
23	CLA	G	610	7	1/1/15/20	10/37/115/115	-
42	XAT	R	615	-	-	14/31/93/93	0/4/4/4
39	CHL	N	605	7	3/3/16/26	5/20/118/137	-
39	CHL	S	605	-	3/3/16/26	6/20/118/137	-
23	CLA	g	613	-	1/1/15/20	10/37/115/115	-
23	CLA	n	612	7	1/1/11/20	5/18/96/115	-

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PAM	b	621	-	-	3/15/15/15	-
23	CLA	S	602	15	1/1/13/20	10/28/106/115	-
23	CLA	Y	305	-	1/1/15/20	12/37/115/115	-
33	DGD	C	515	-	-	20/55/95/95	0/2/2/2
23	CLA	r	609	14	1/1/15/20	7/37/115/115	-
23	CLA	y	313	7	1/1/15/20	9/37/115/115	-
41	NEX	S	617	-	-	6/11/36/83	0/1/1/3
23	CLA	b	601	-	1/1/12/20	5/19/97/115	-
23	CLA	R	610	30	1/1/15/20	9/37/115/115	-
23	CLA	C	505	-	1/1/15/20	6/37/115/115	-
23	CLA	C	511	3	1/1/15/20	11/37/115/115	-
23	CLA	g	610	7	1/1/15/20	10/37/115/115	-
31	LNL	B	624	-	-	8/17/17/17	-
23	CLA	y	306	-	1/1/15/20	20/37/115/115	-
23	CLA	G	603	-	1/1/14/20	3/31/109/115	-
23	CLA	d	405	-	1/1/15/20	7/37/115/115	-
23	CLA	n	611	30	1/1/11/20	5/18/96/115	-
23	CLA	b	608	-	1/1/15/20	10/37/115/115	-
23	CLA	r	610	30	1/1/15/20	10/37/115/115	-
23	CLA	n	604	-	1/1/11/20	7/18/96/115	-
39	CHL	y	309	-	3/3/16/26	3/20/118/137	-
25	BCR	A	407	-	-	4/29/63/63	0/2/2/2
23	CLA	b	606	-	1/1/15/20	10/37/115/115	-
23	CLA	A	403	43	1/1/15/20	10/37/115/115	-
39	CHL	N	607	-	3/3/20/26	7/39/137/137	-
25	BCR	z	101	-	-	5/29/63/63	0/2/2/2
23	CLA	B	603	-	1/1/15/20	10/37/115/115	-
31	LNL	A	414	-	-	8/17/17/17	-
29	PL9	a	411	-	-	12/53/73/73	0/1/1/1
23	CLA	y	314	-	1/1/15/20	14/37/115/115	-
41	NEX	r	614	-	-	9/27/83/83	0/3/3/3
39	CHL	N	609	7	3/3/20/26	7/39/137/137	-
25	BCR	c	514	-	-	7/29/63/63	0/2/2/2
31	LNL	c	522	-	-	7/17/17/17	-

The worst 5 of 2109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	609	CHL	C4B-NB	11.99	1.45	1.35
39	G	606	CHL	C4B-NB	11.72	1.45	1.35
39	g	606	CHL	C4B-NB	11.72	1.45	1.35
39	g	608	CHL	C4B-NB	11.53	1.45	1.35
39	G	608	CHL	C4B-NB	11.52	1.45	1.35

The worst 5 of 2825 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	N	617	NEX	O24-C25-C24	23.84	131.29	113.38
41	n	618	NEX	O24-C25-C24	23.64	131.14	113.38
41	g	617	NEX	O24-C25-C24	23.37	130.94	113.38
41	R	618	NEX	O24-C25-C24	23.16	130.78	113.38
41	r	614	NEX	O24-C25-C24	23.13	130.76	113.38

5 of 304 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	402	CLA	ND
23	A	403	CLA	ND
23	A	404	CLA	ND
23	A	406	CLA	ND
23	B	601	CLA	ND

5 of 3614 torsion outliers are listed below:

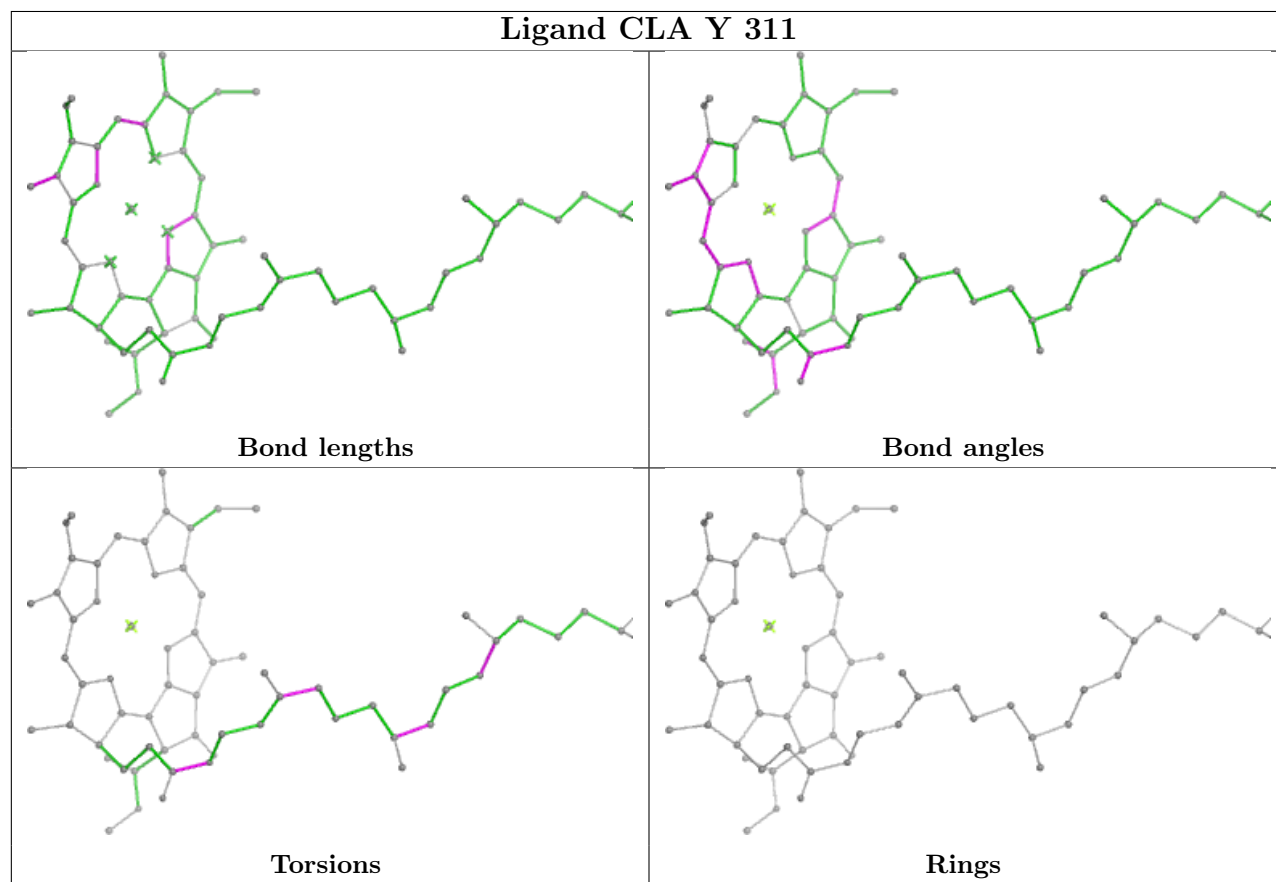
Mol	Chain	Res	Type	Atoms
23	A	403	CLA	C2A-CAA-CBA-CGA
23	A	403	CLA	CHA-CBD-CGD-O1D
23	A	403	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	C1A-C2A-CAA-CBA
23	B	601	CLA	CHA-CBD-CGD-O1D

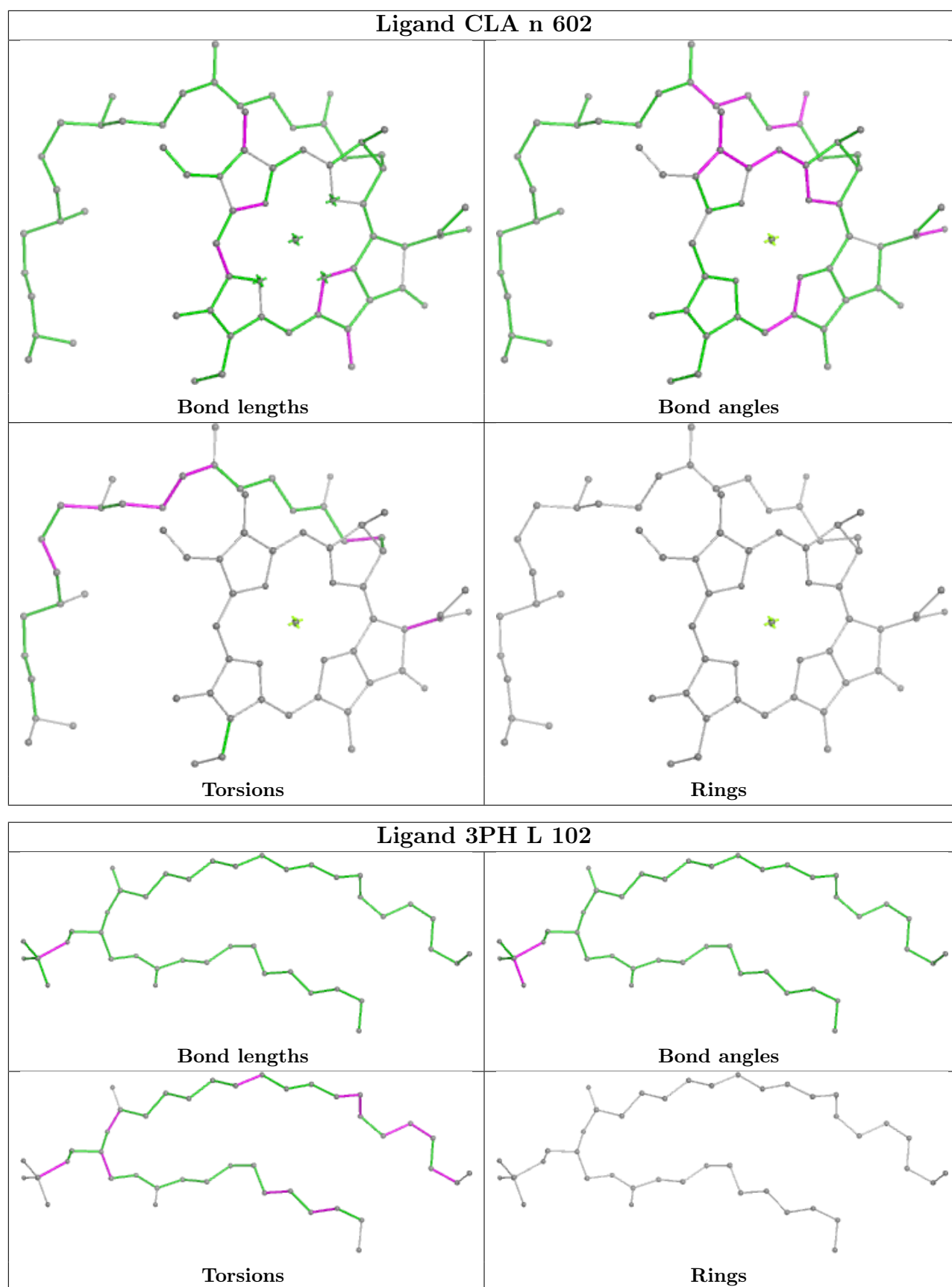
There are no ring outliers.

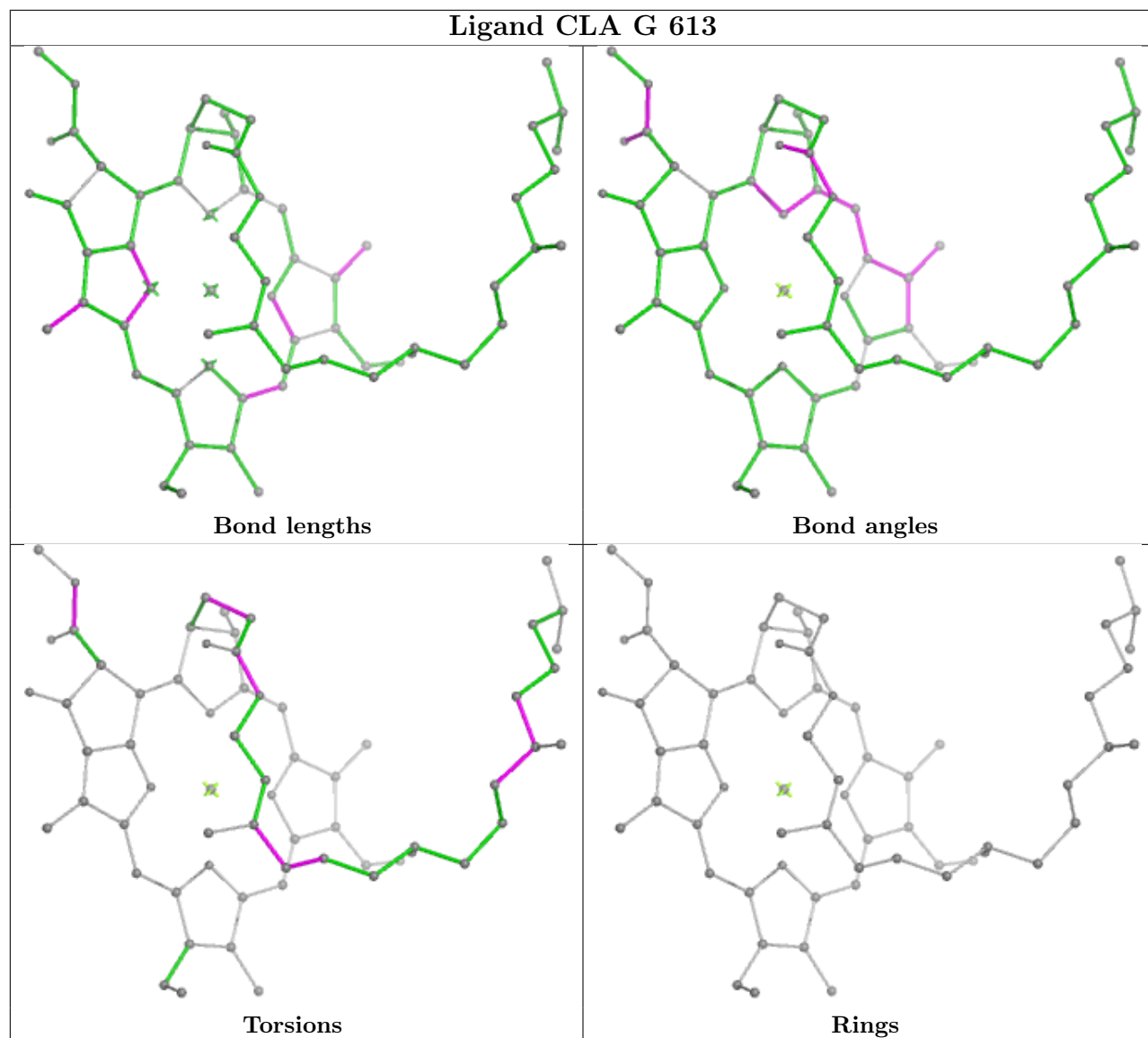
No monomer is involved in short contacts.

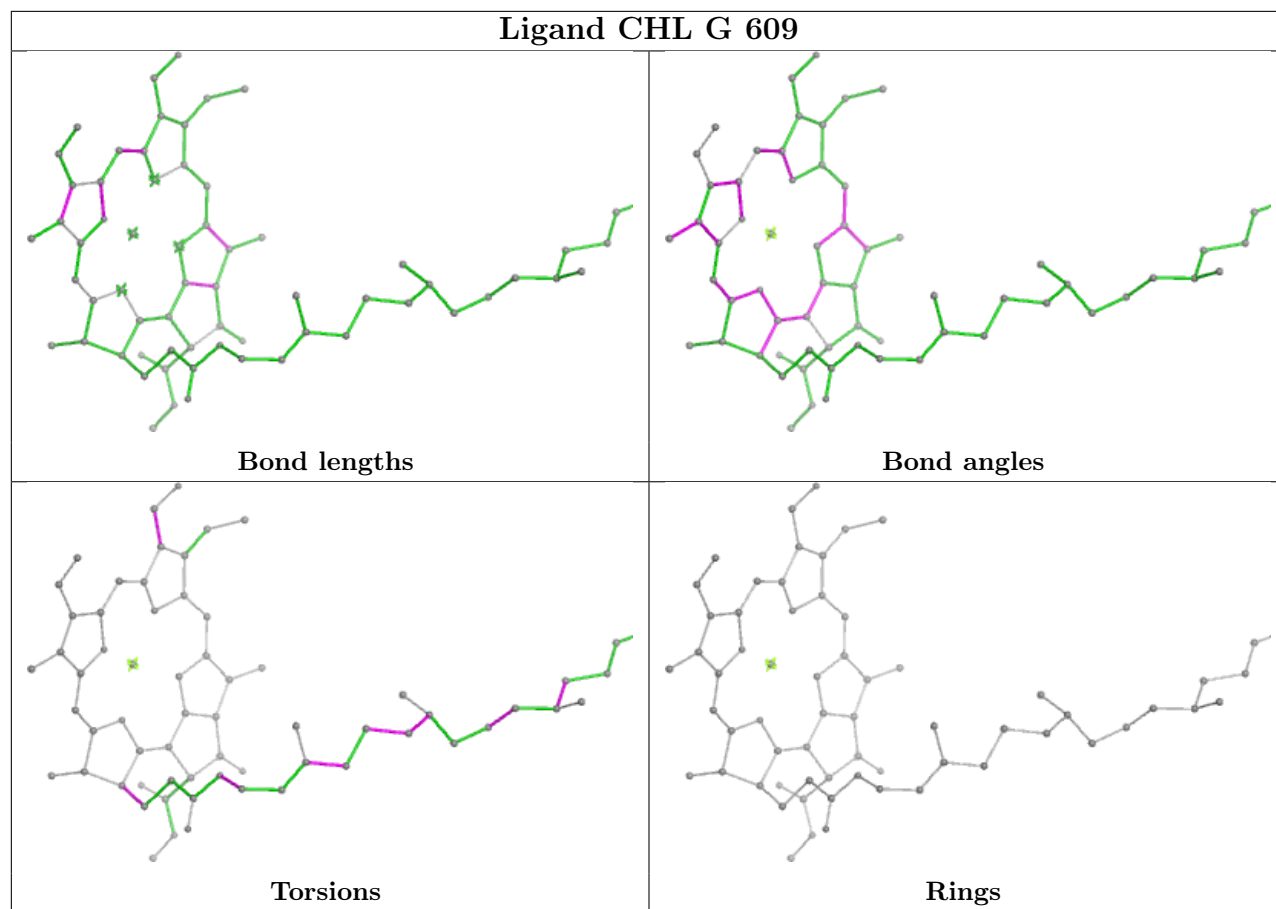
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

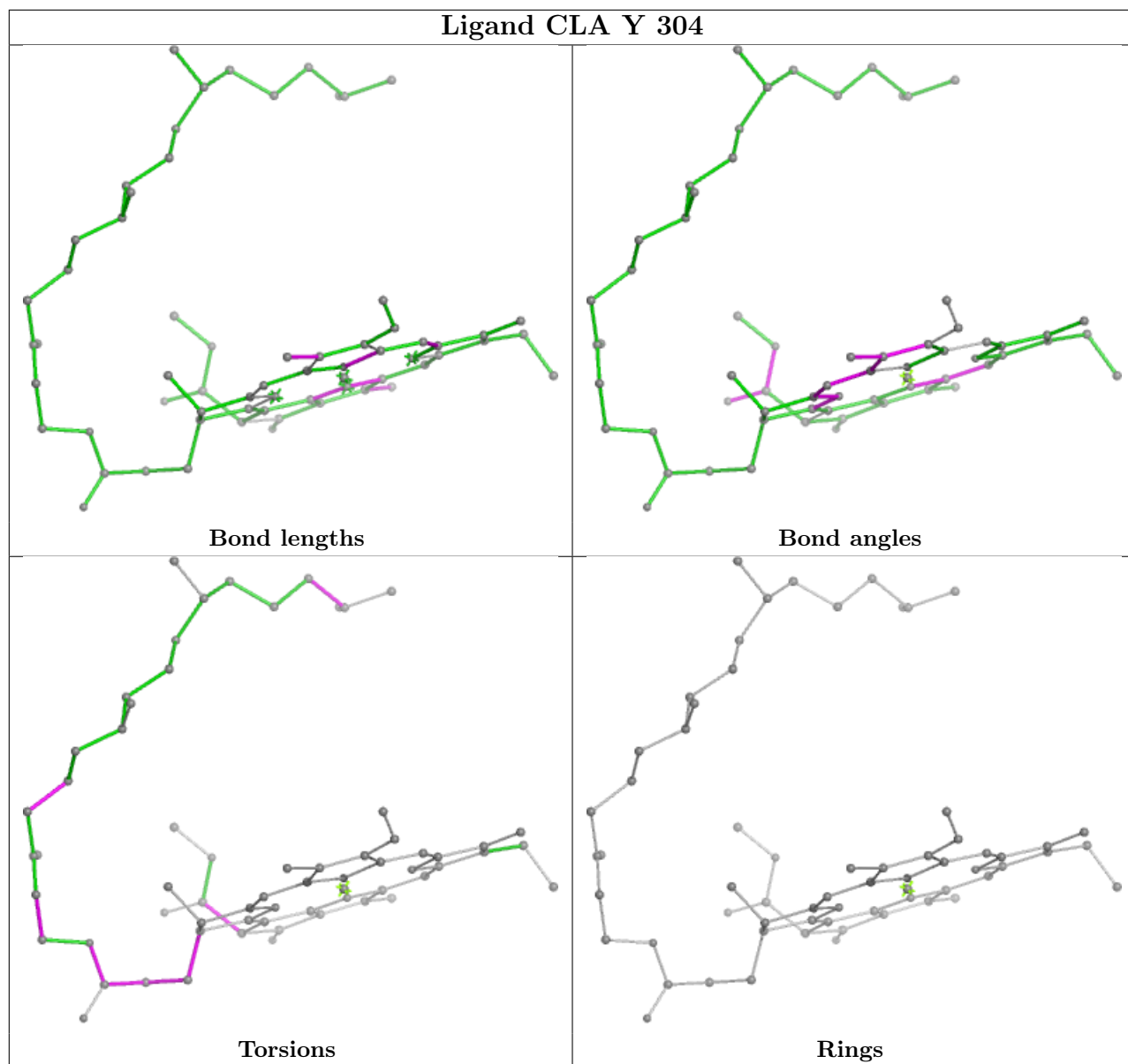
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



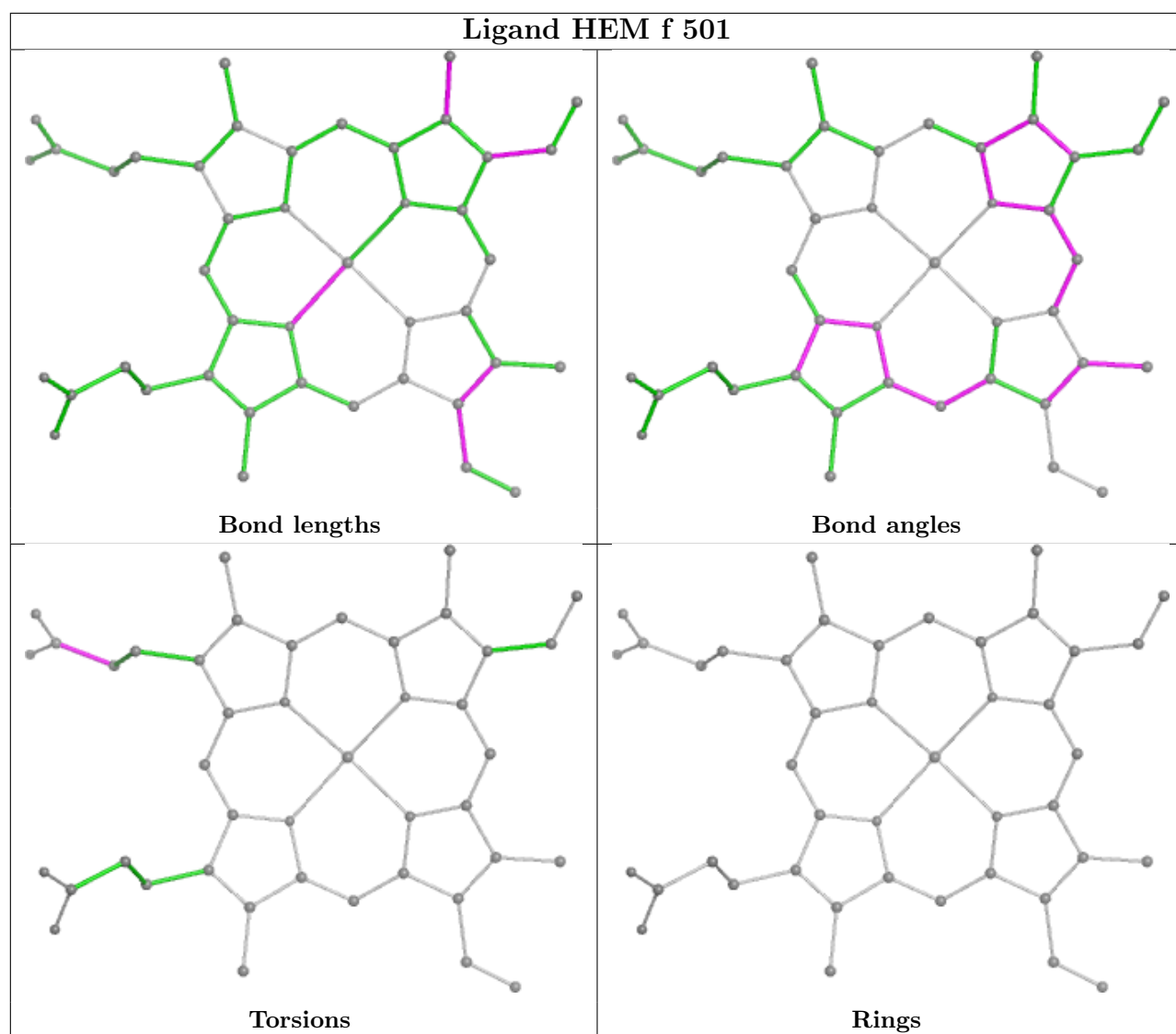


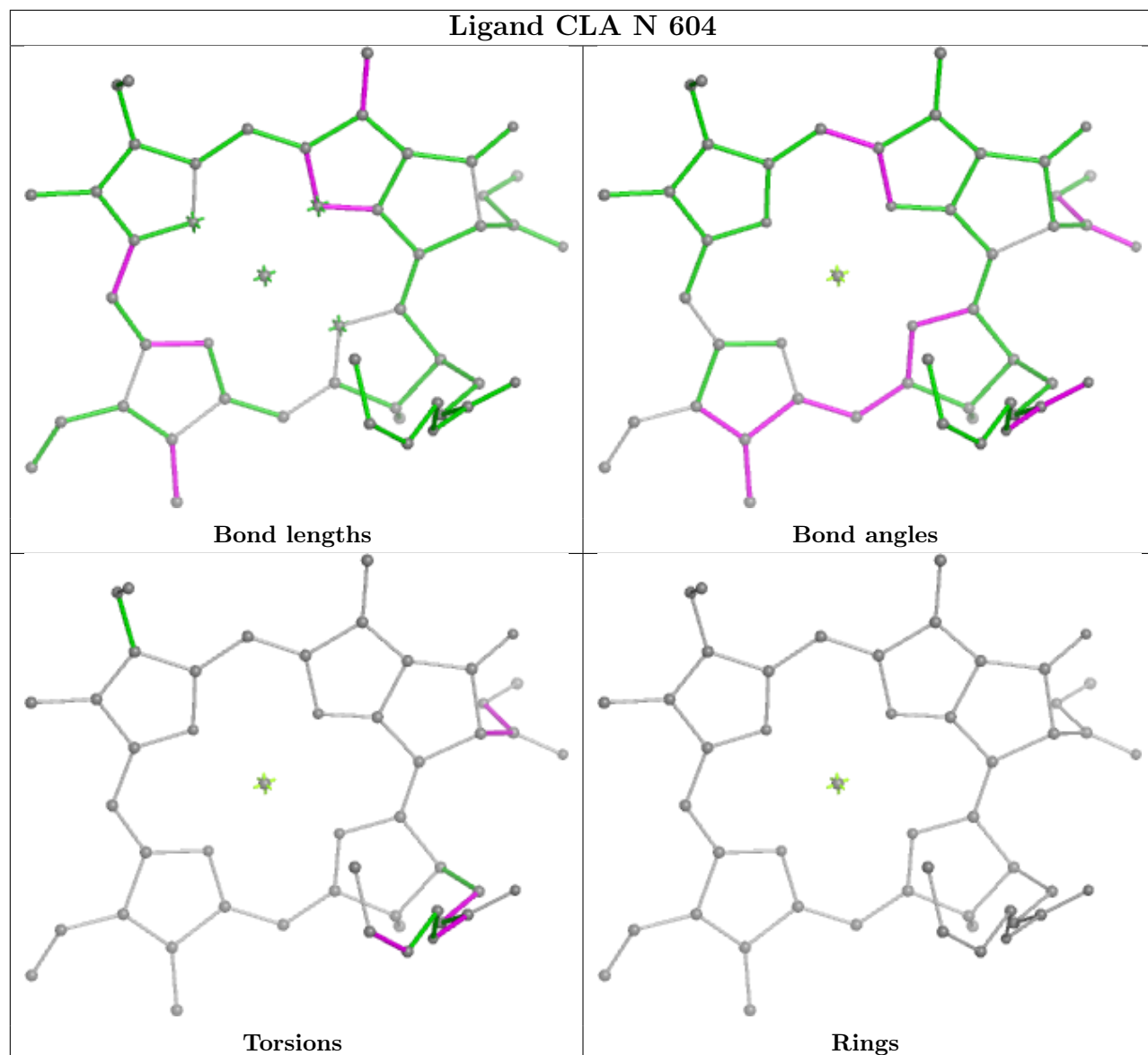


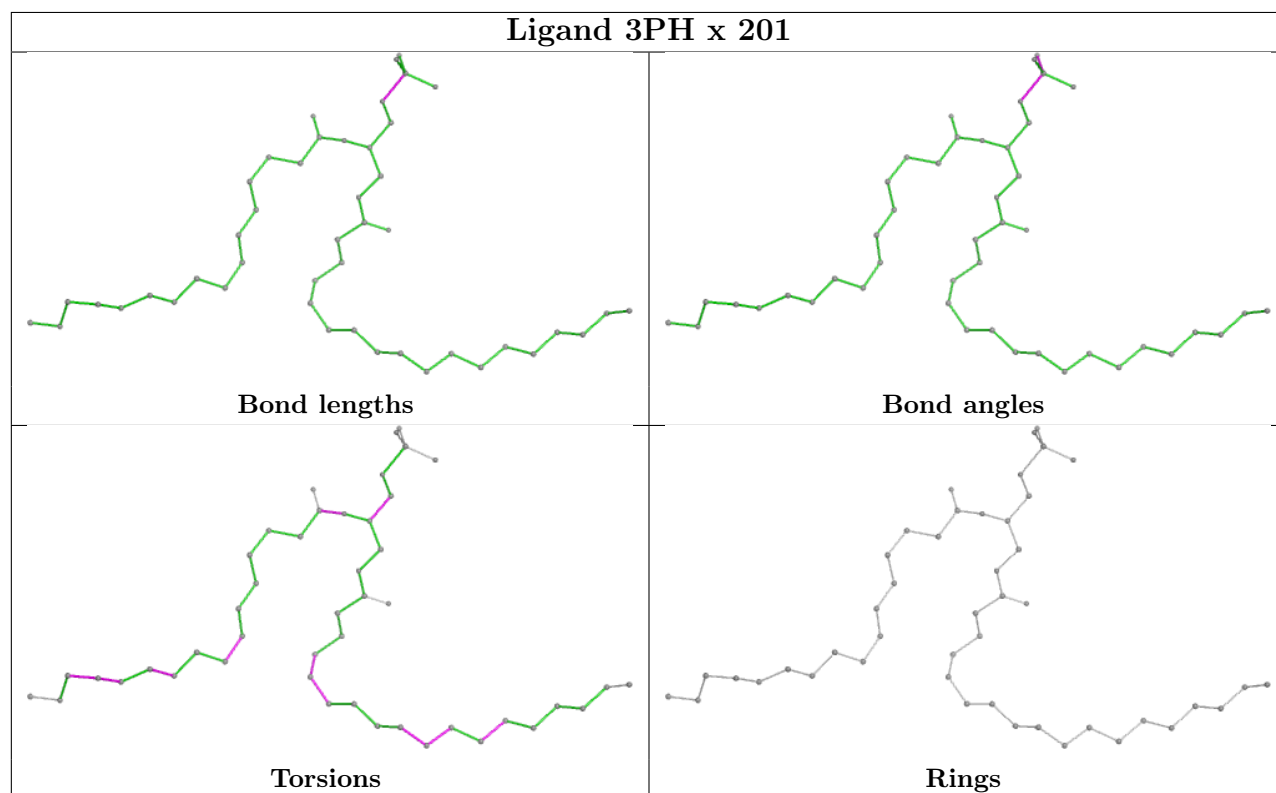
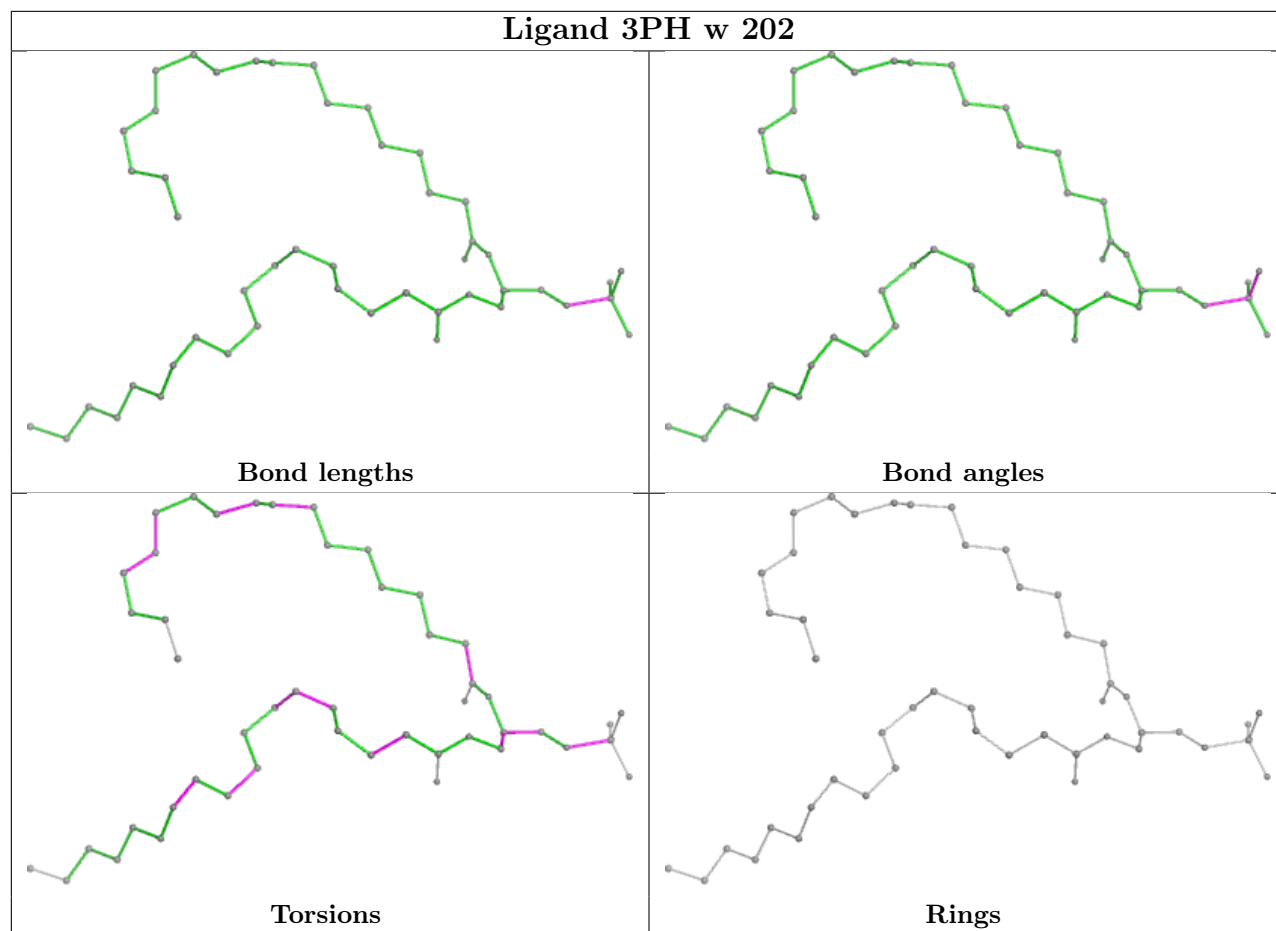


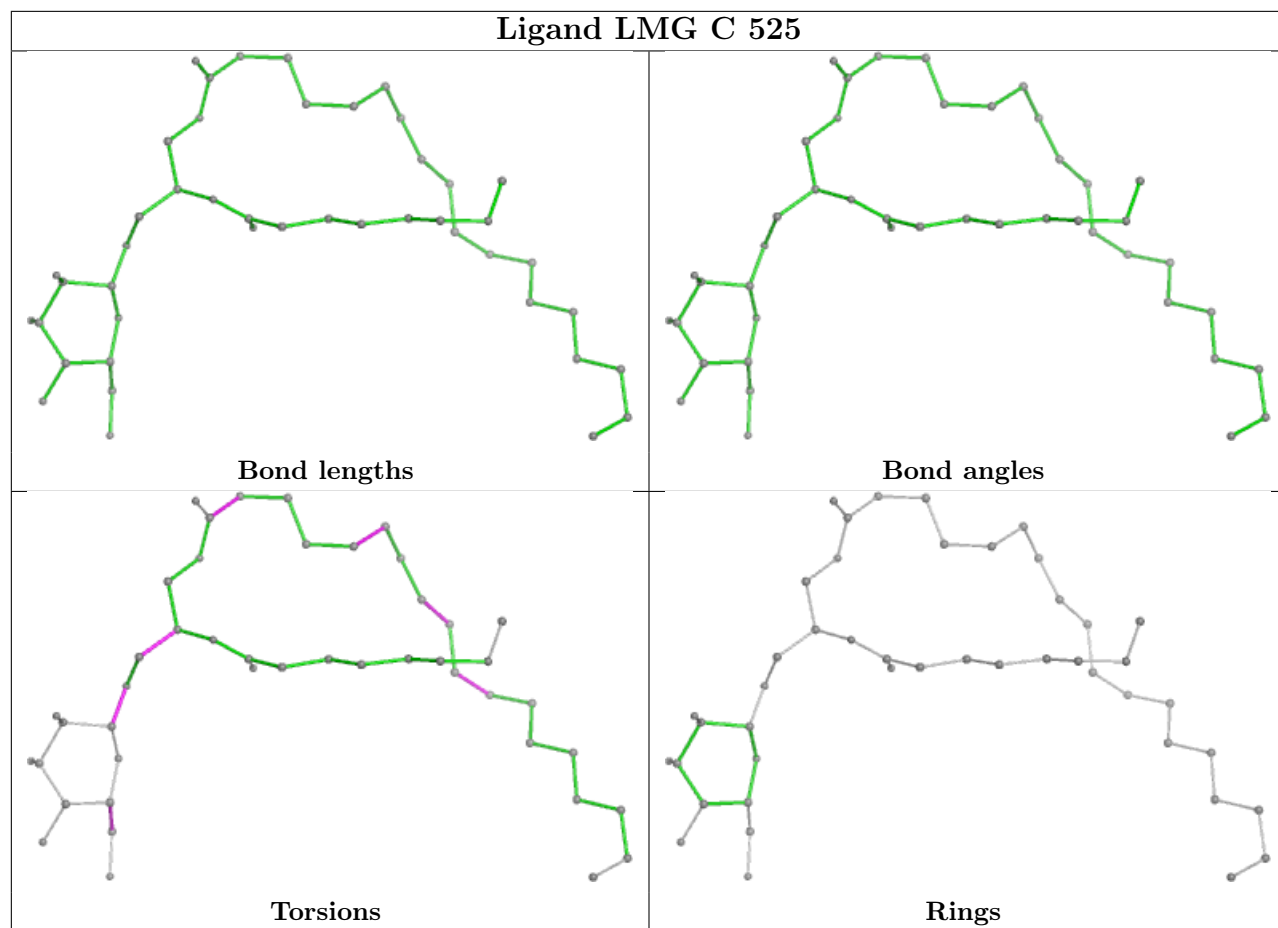


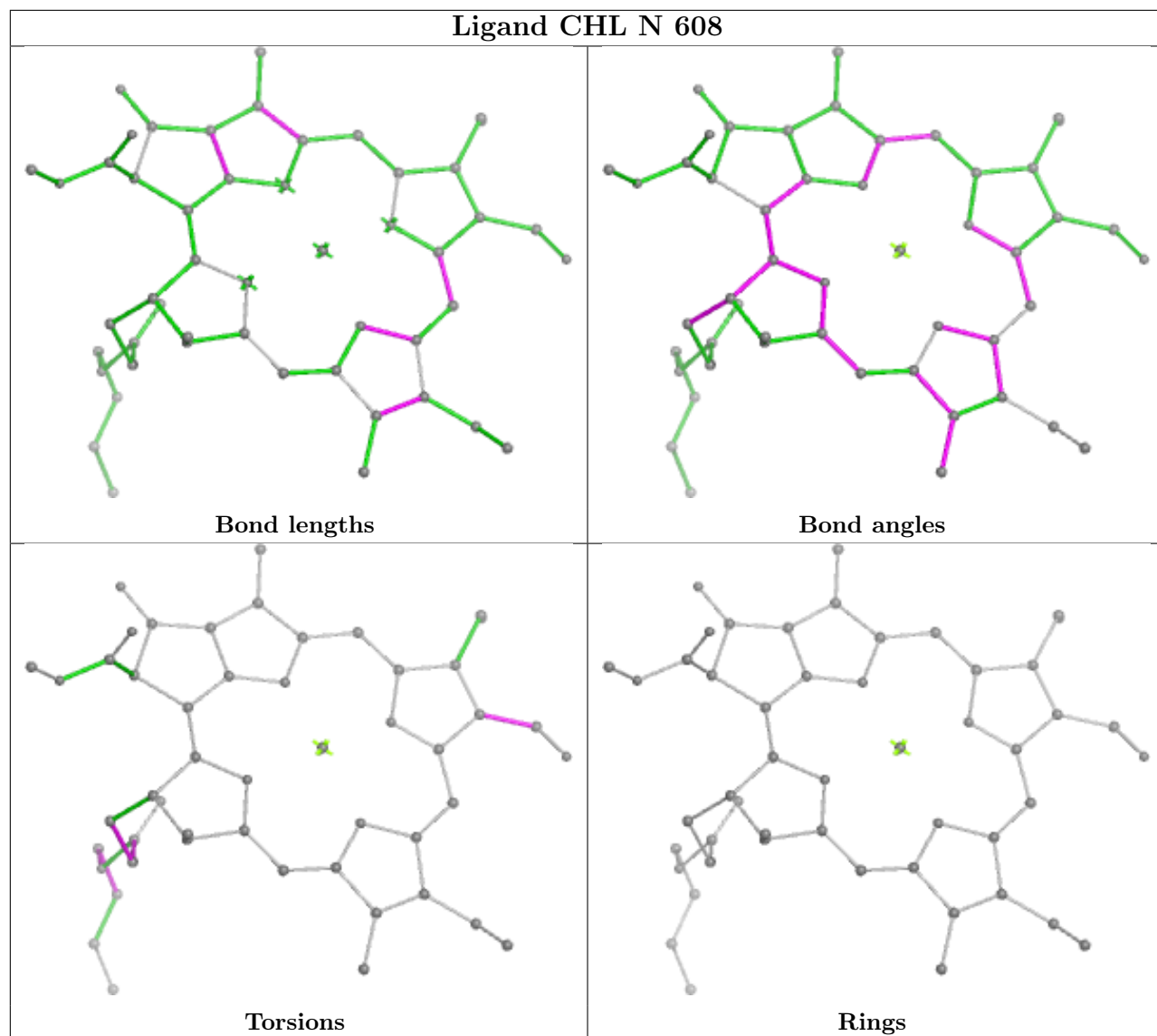


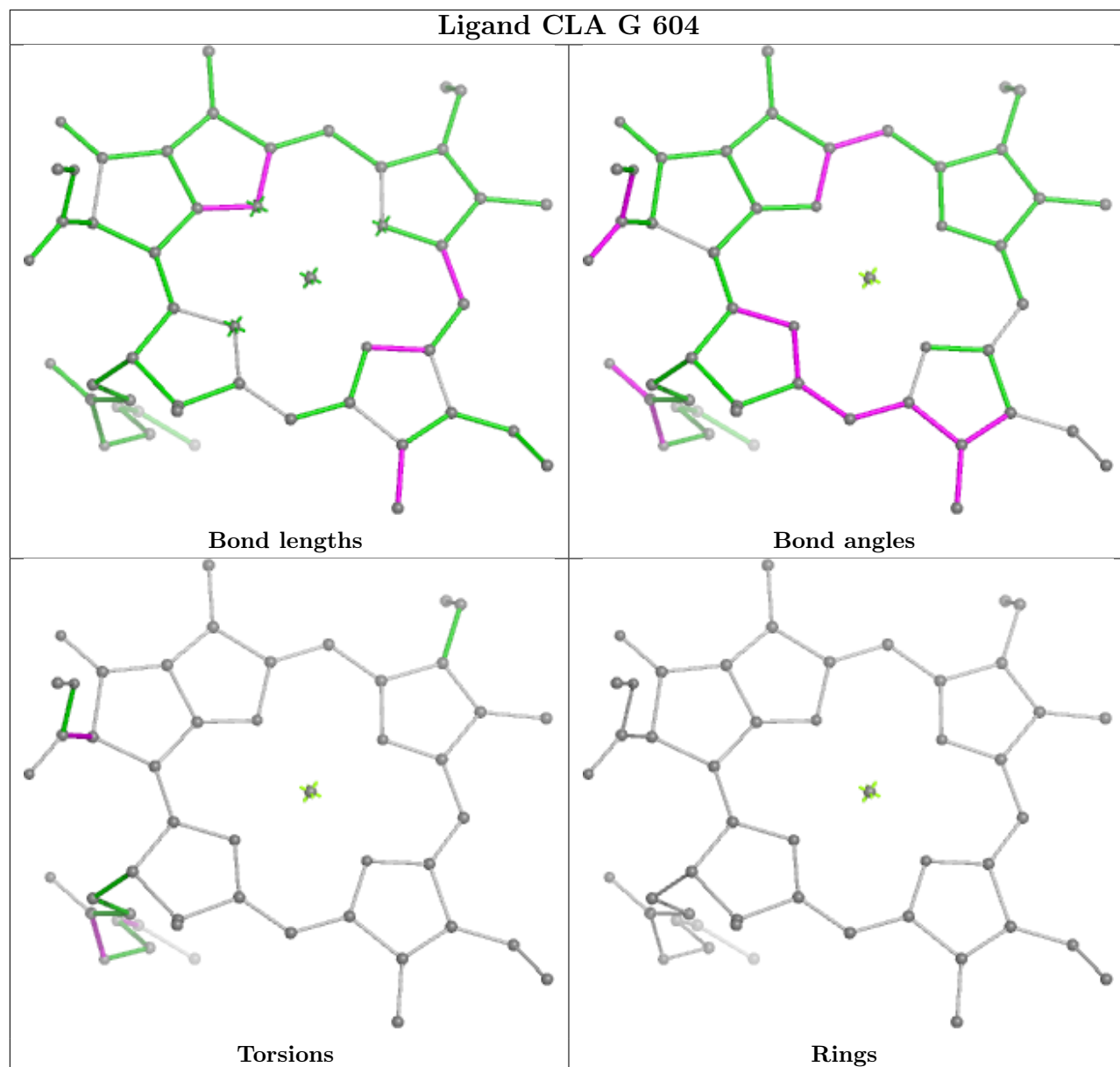


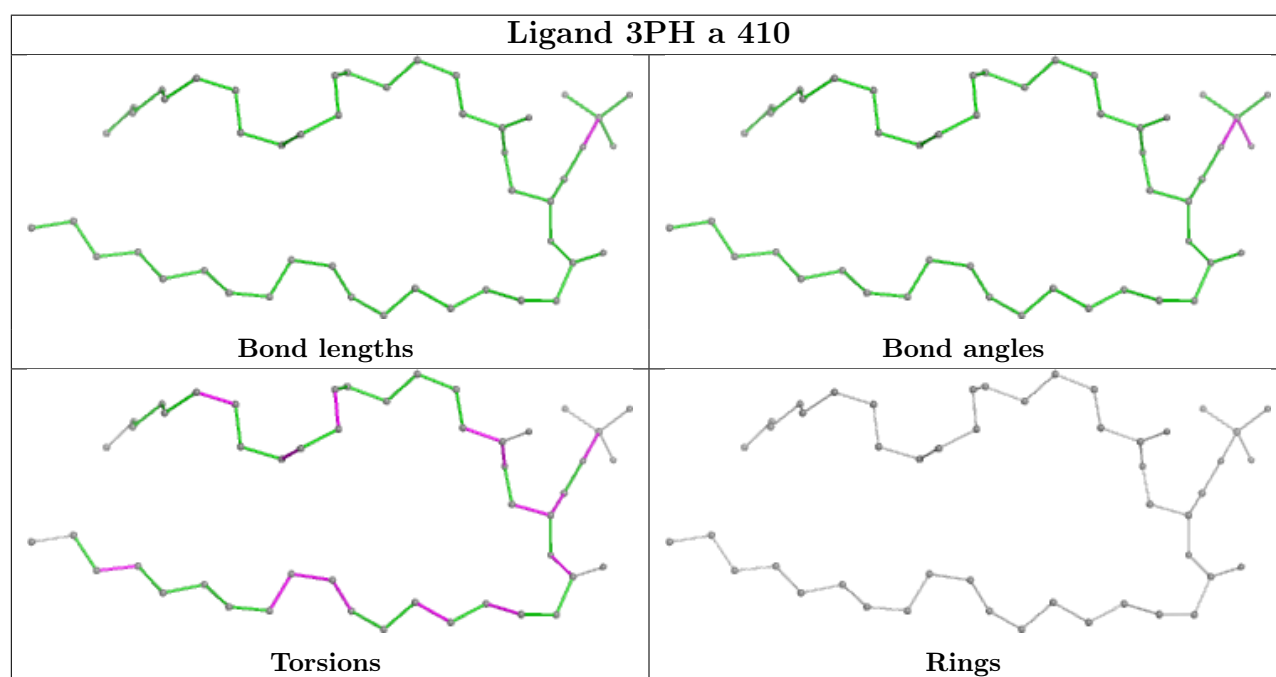
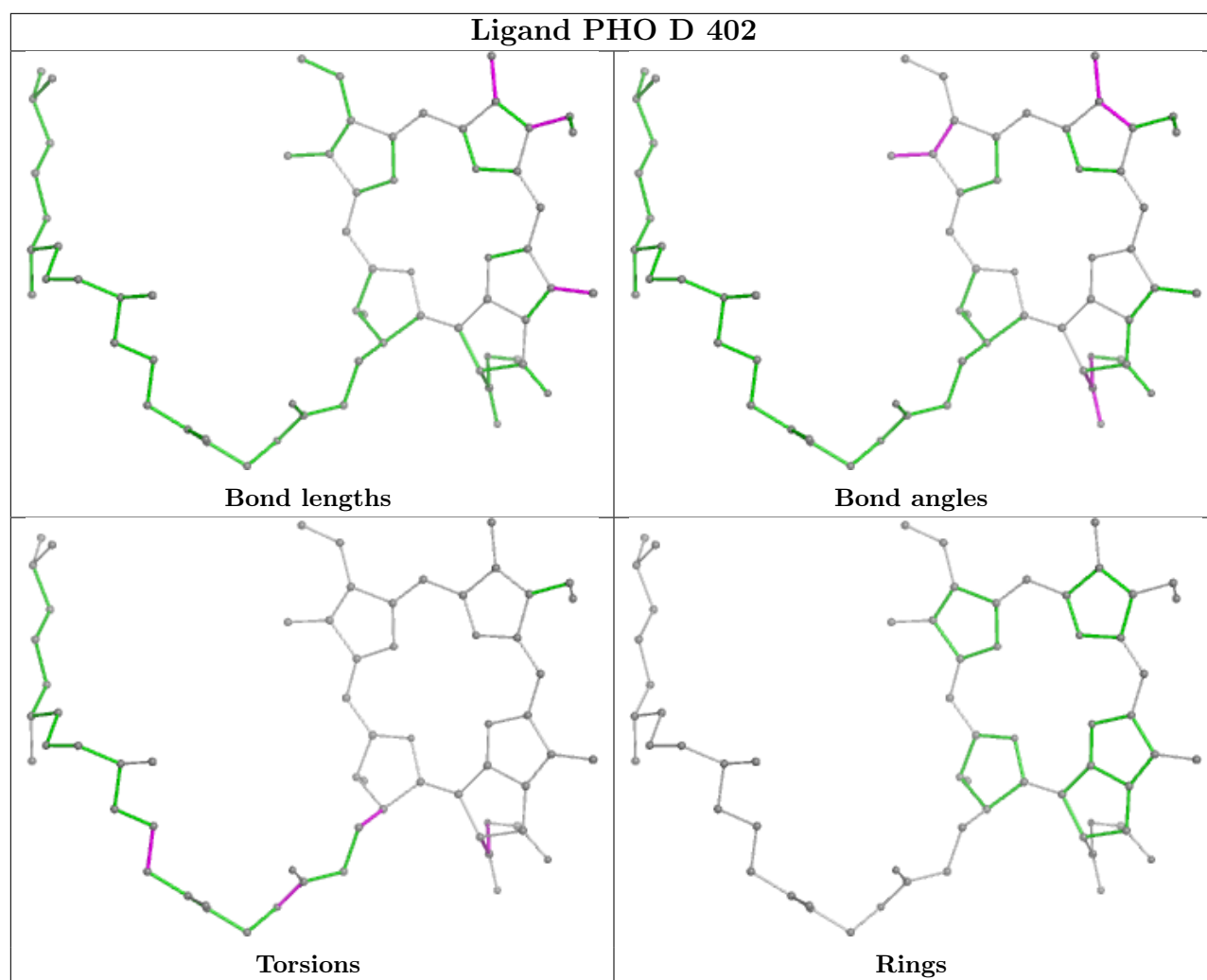


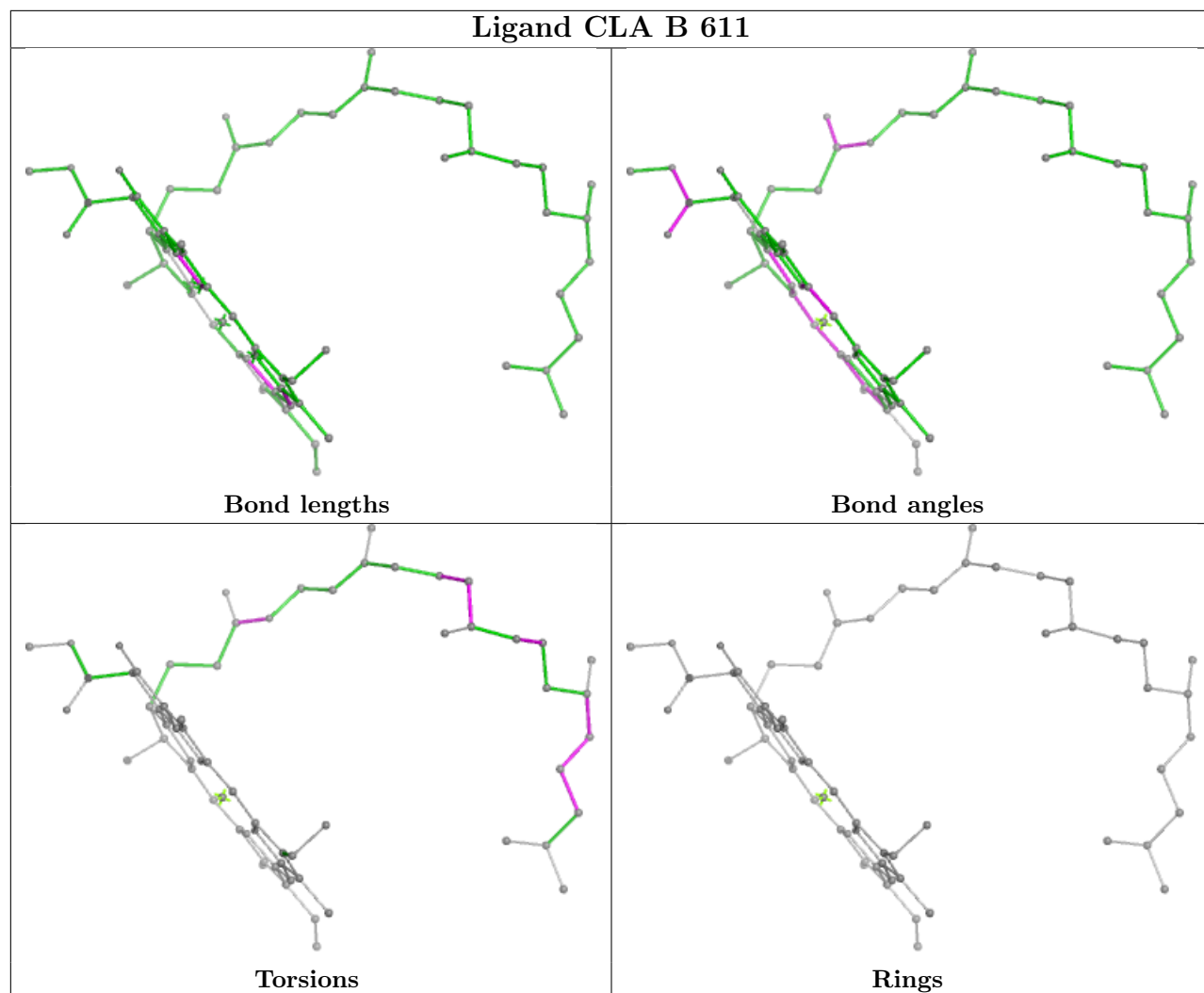




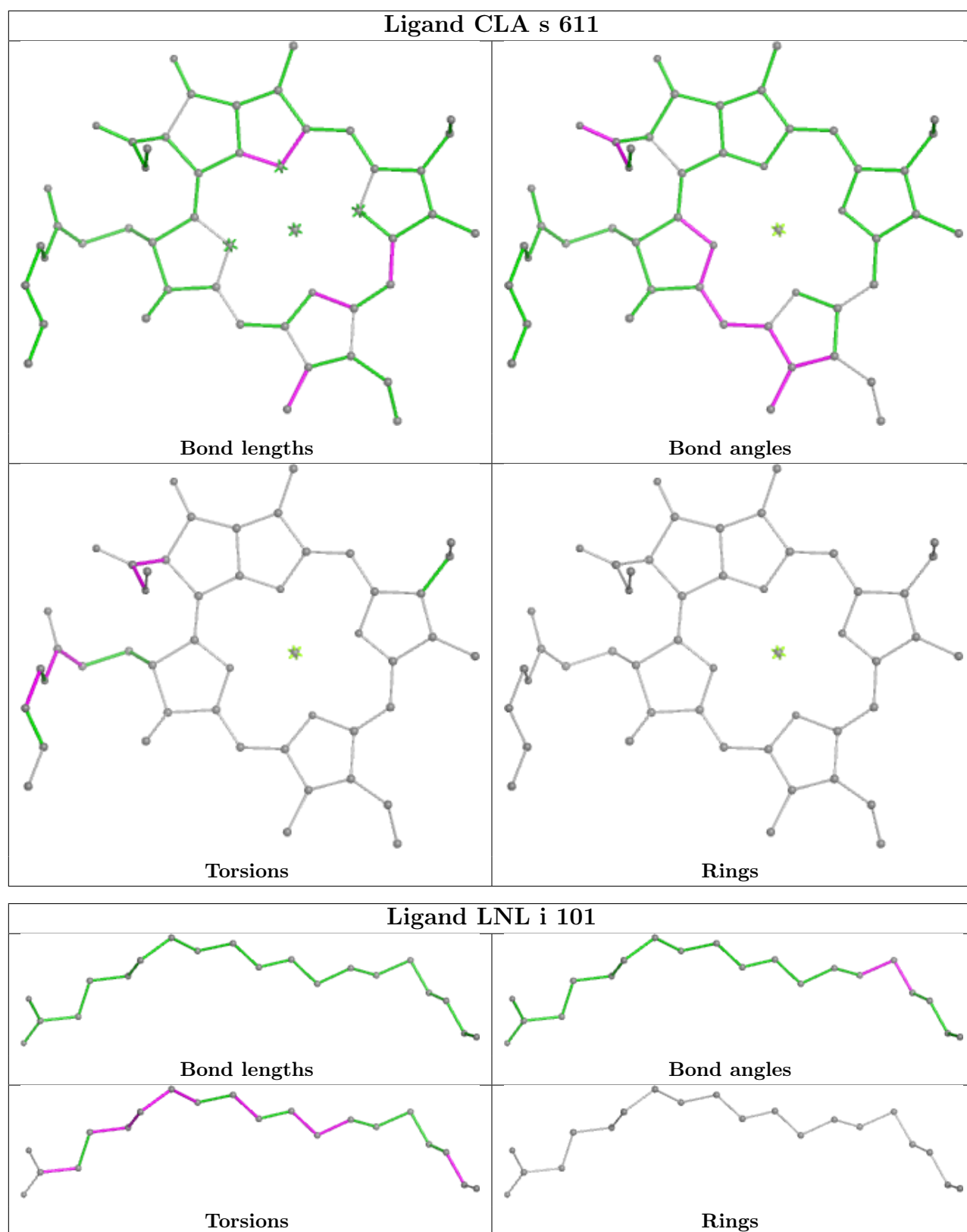


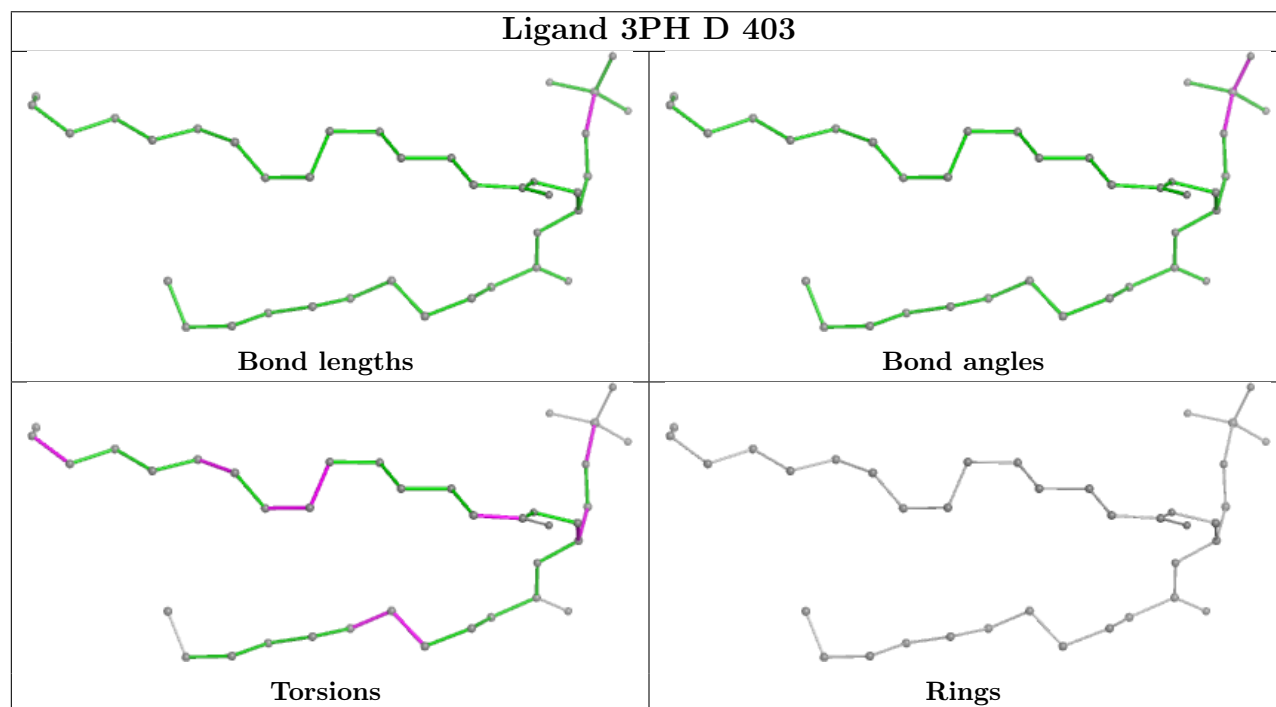
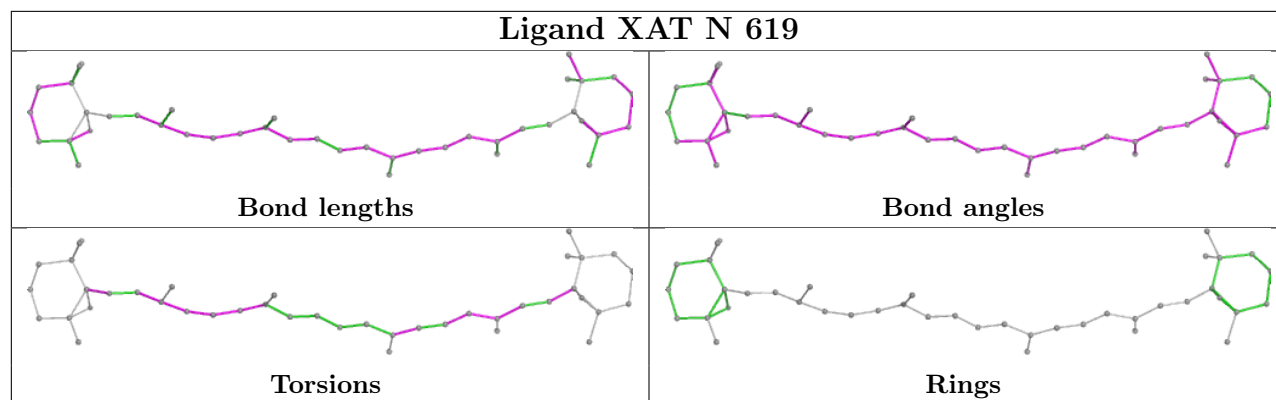


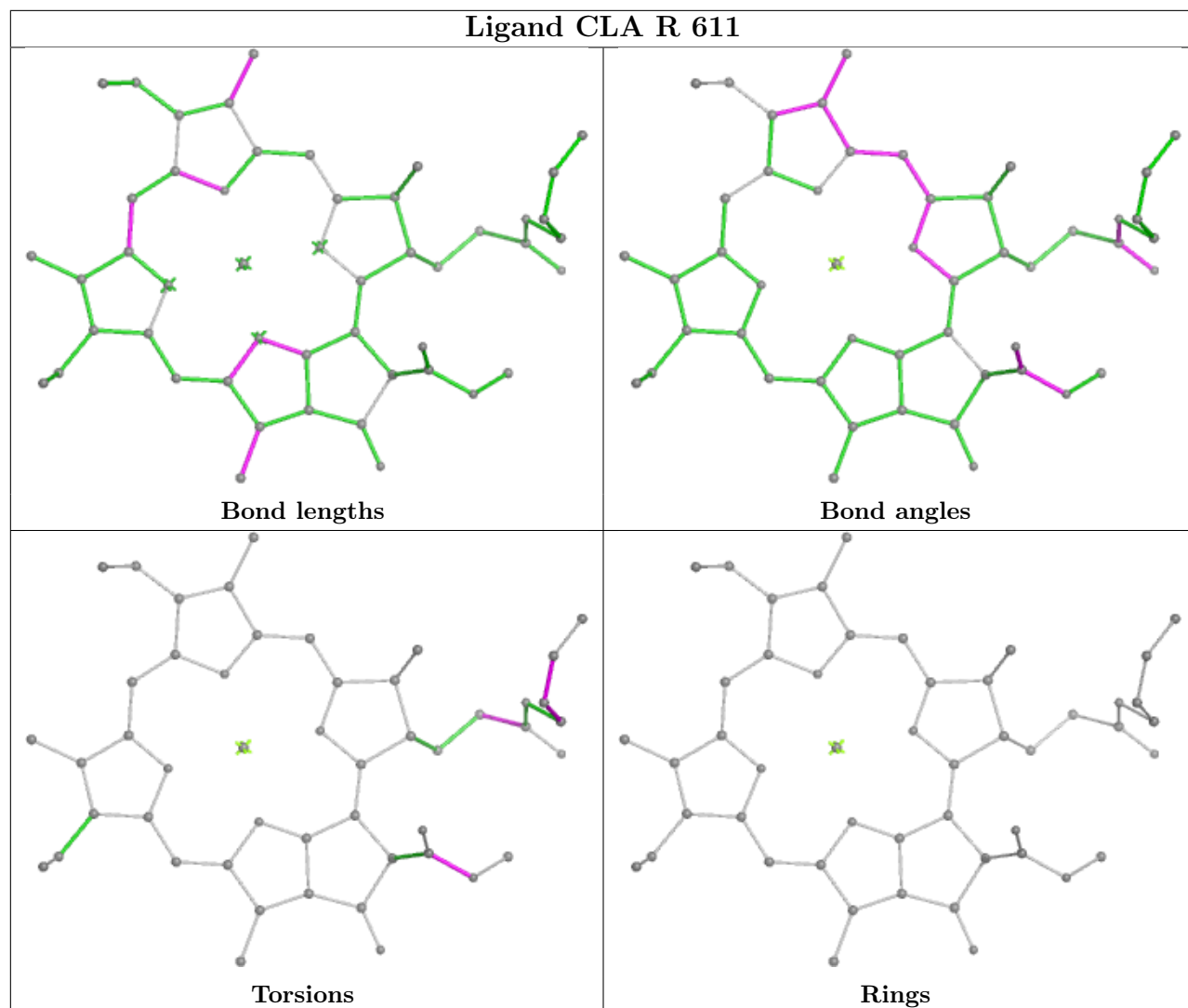


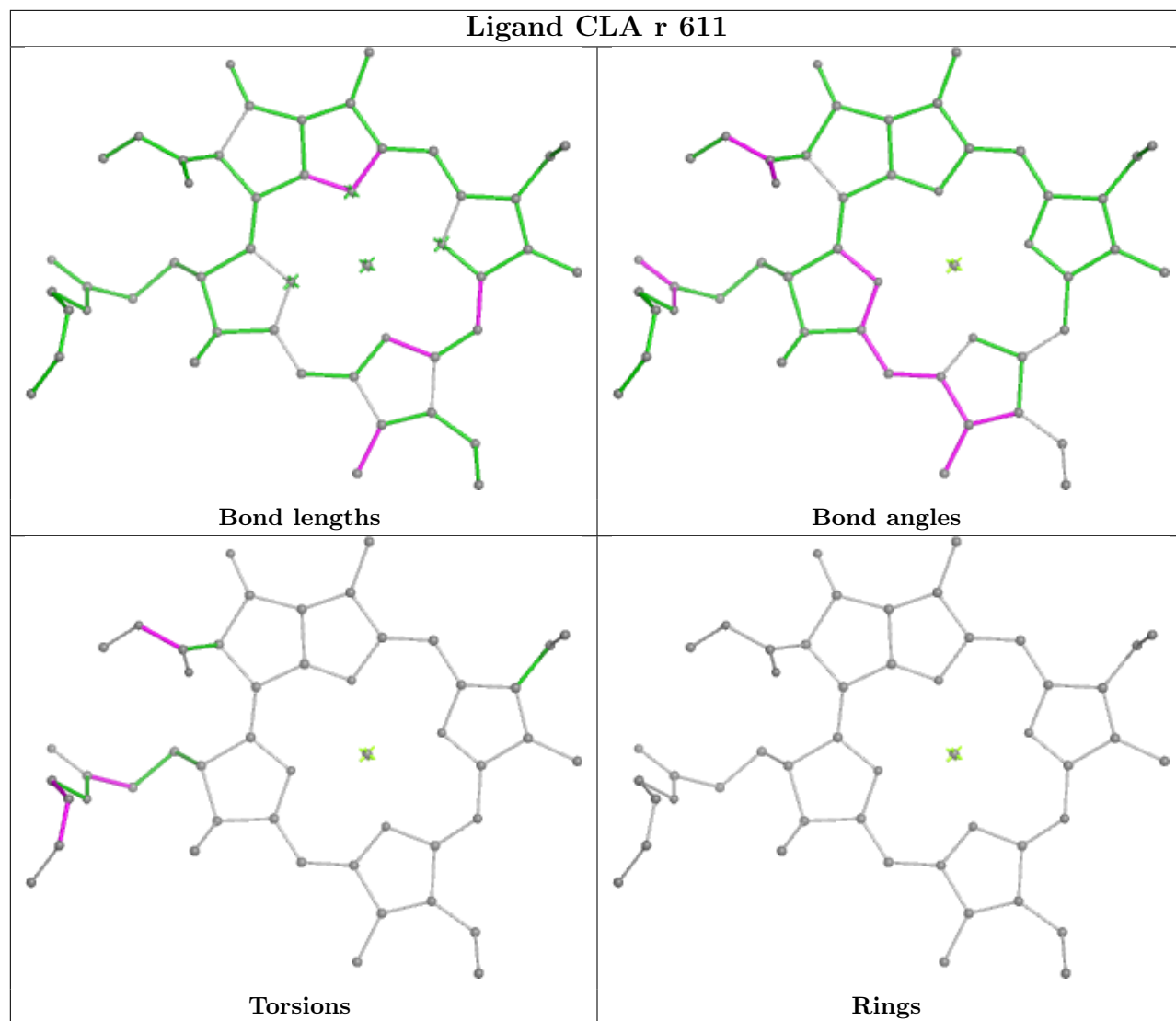


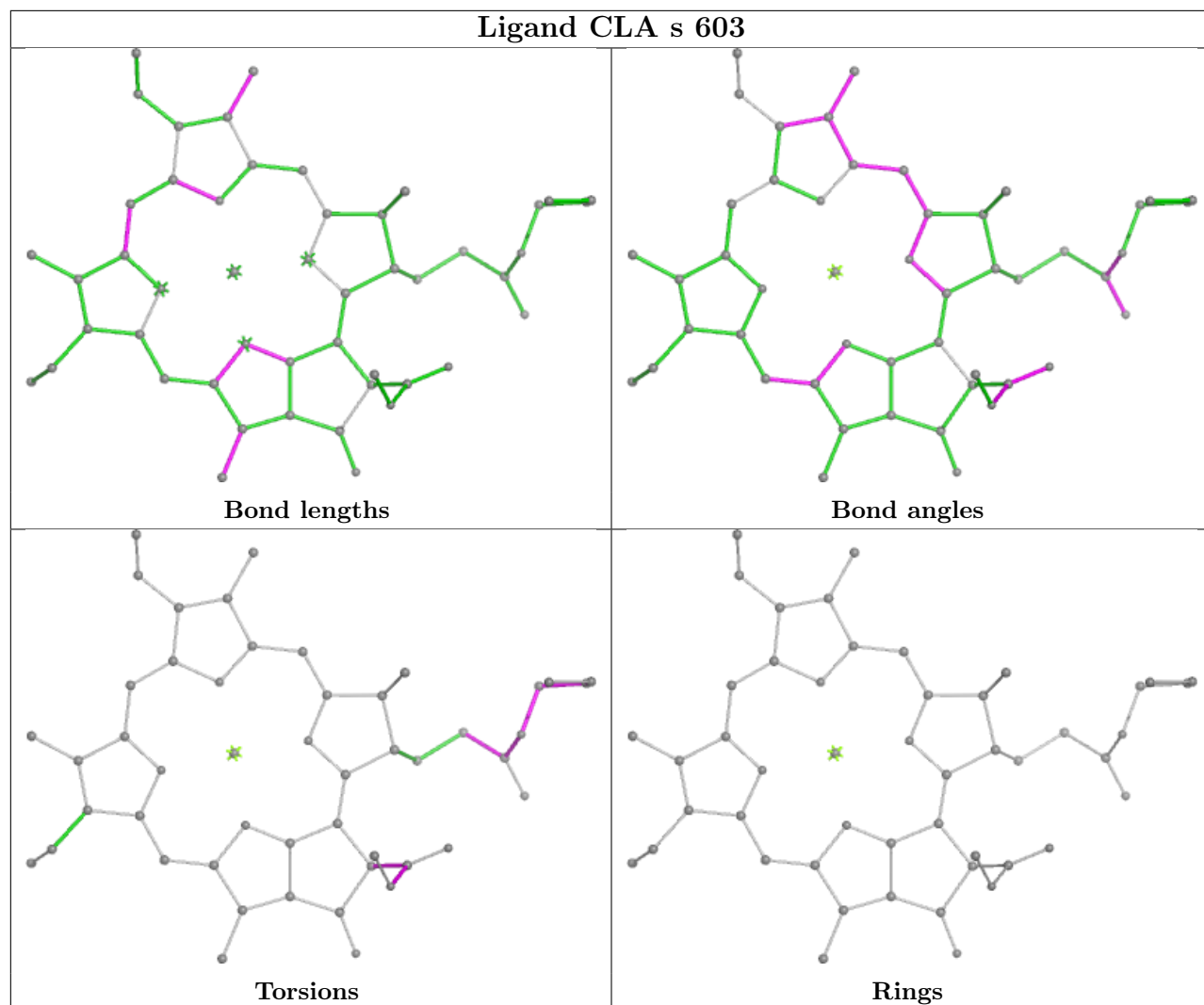


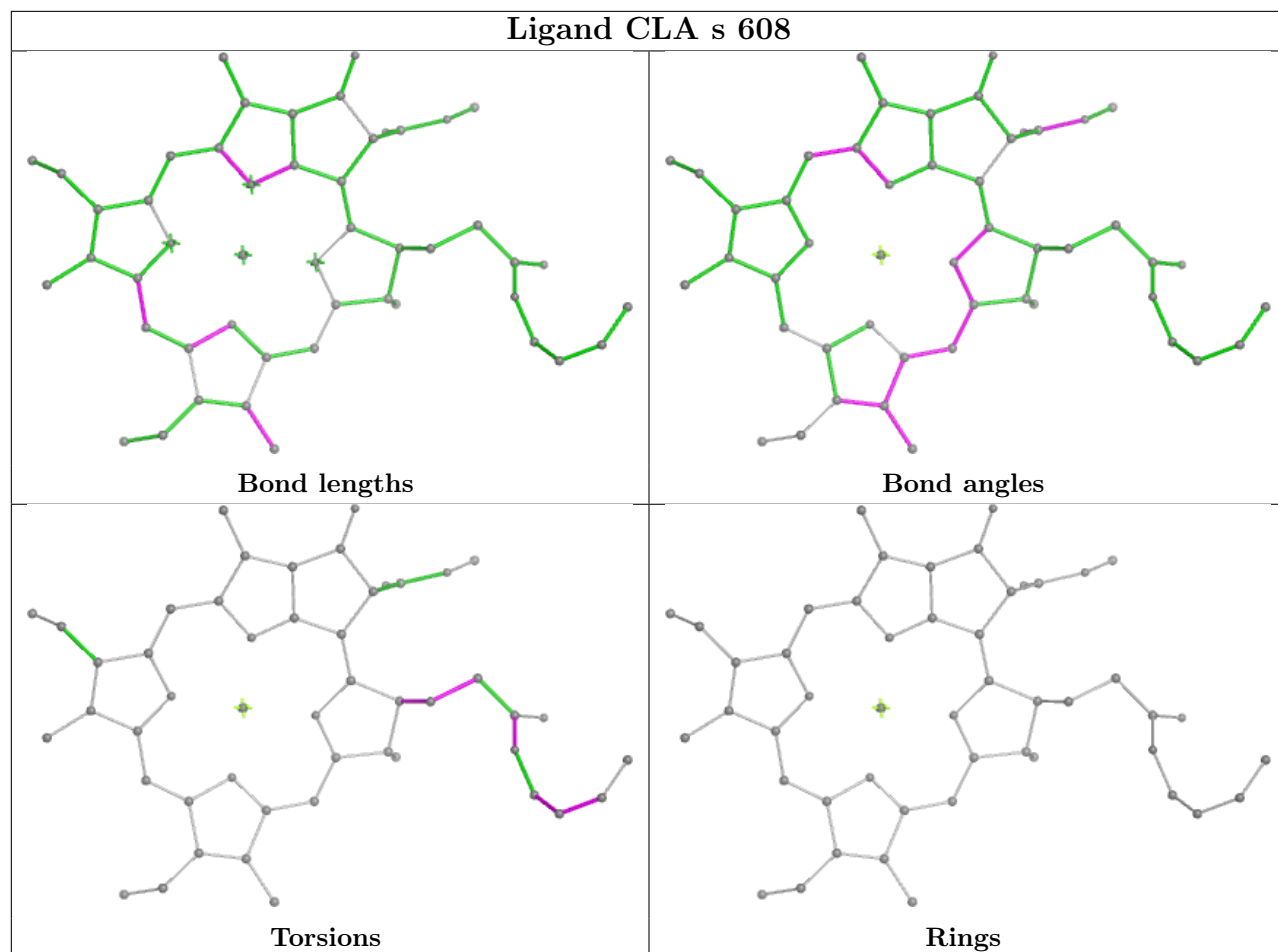


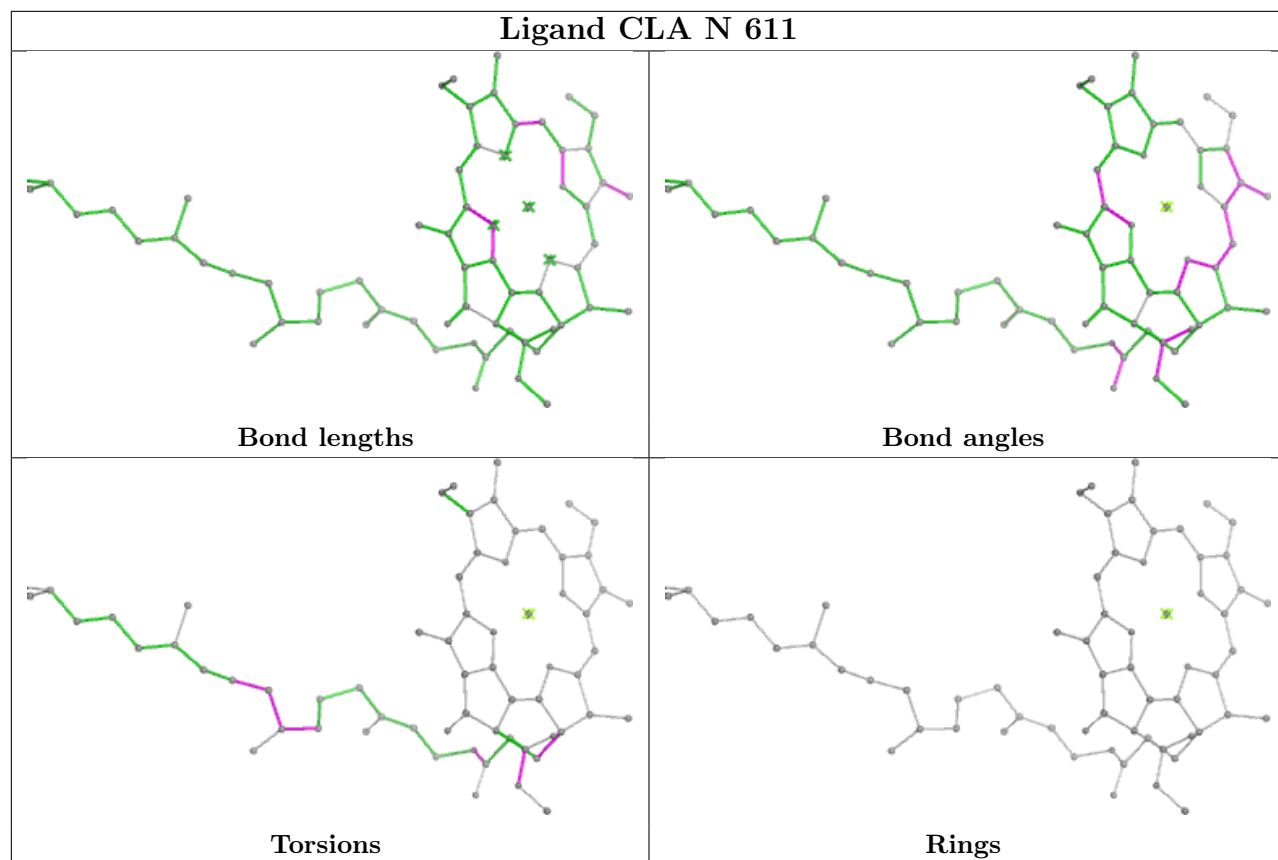


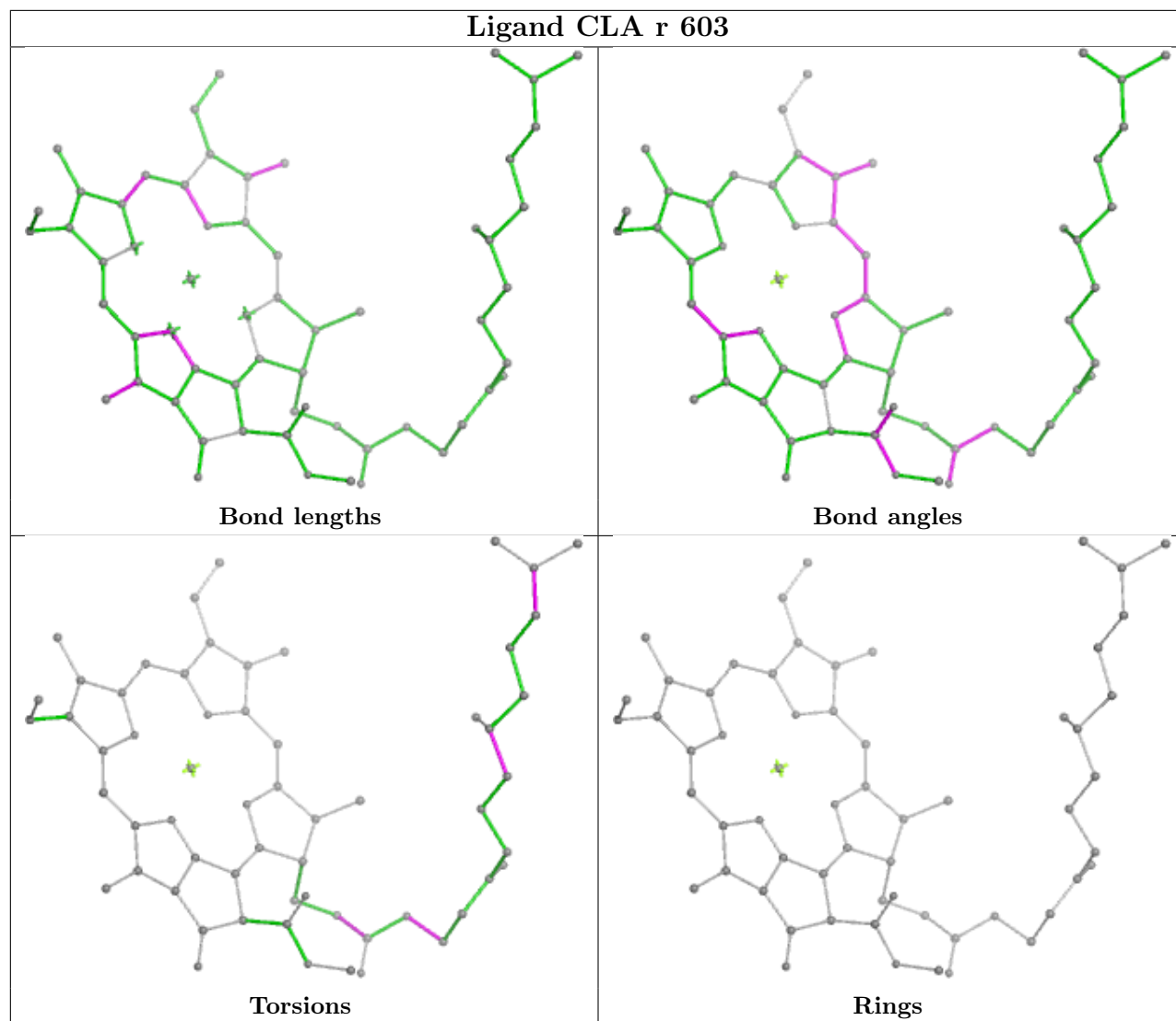




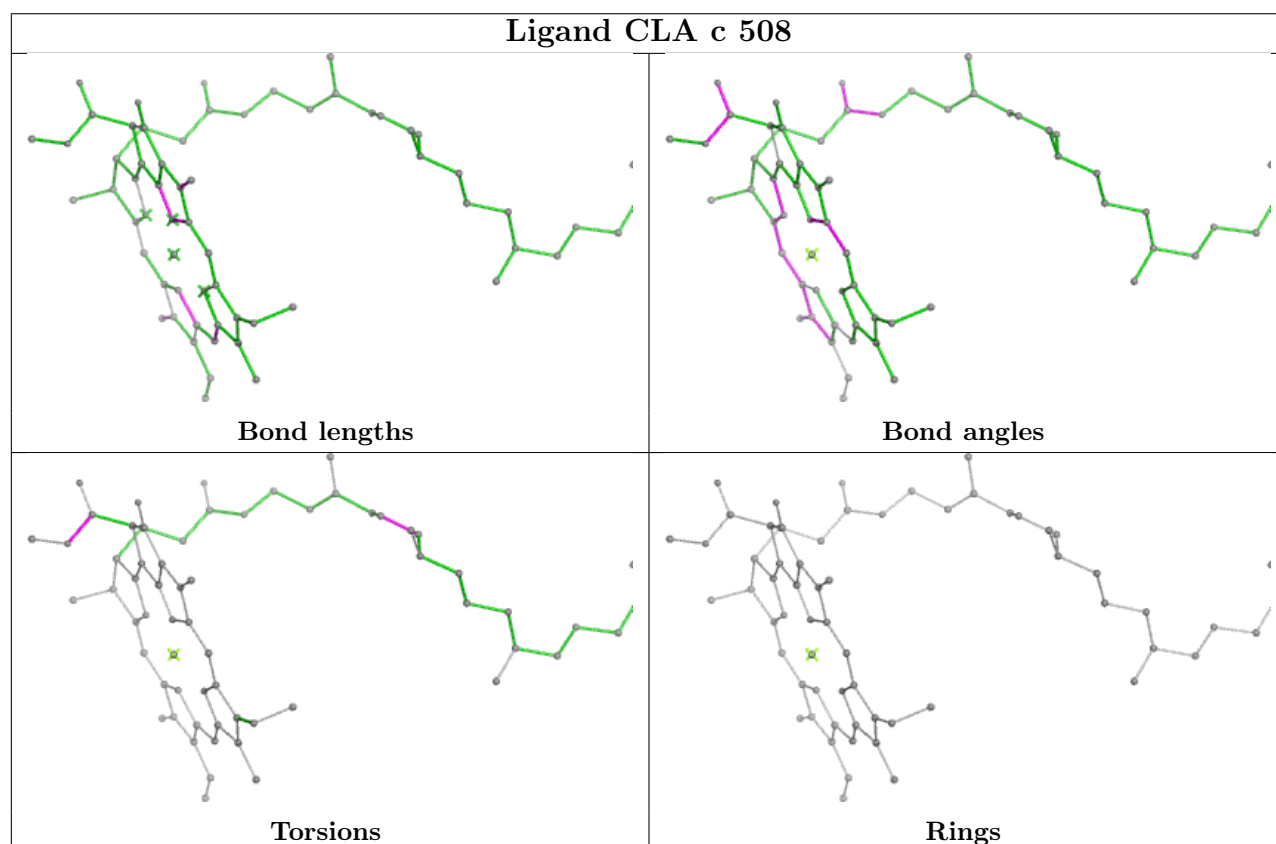
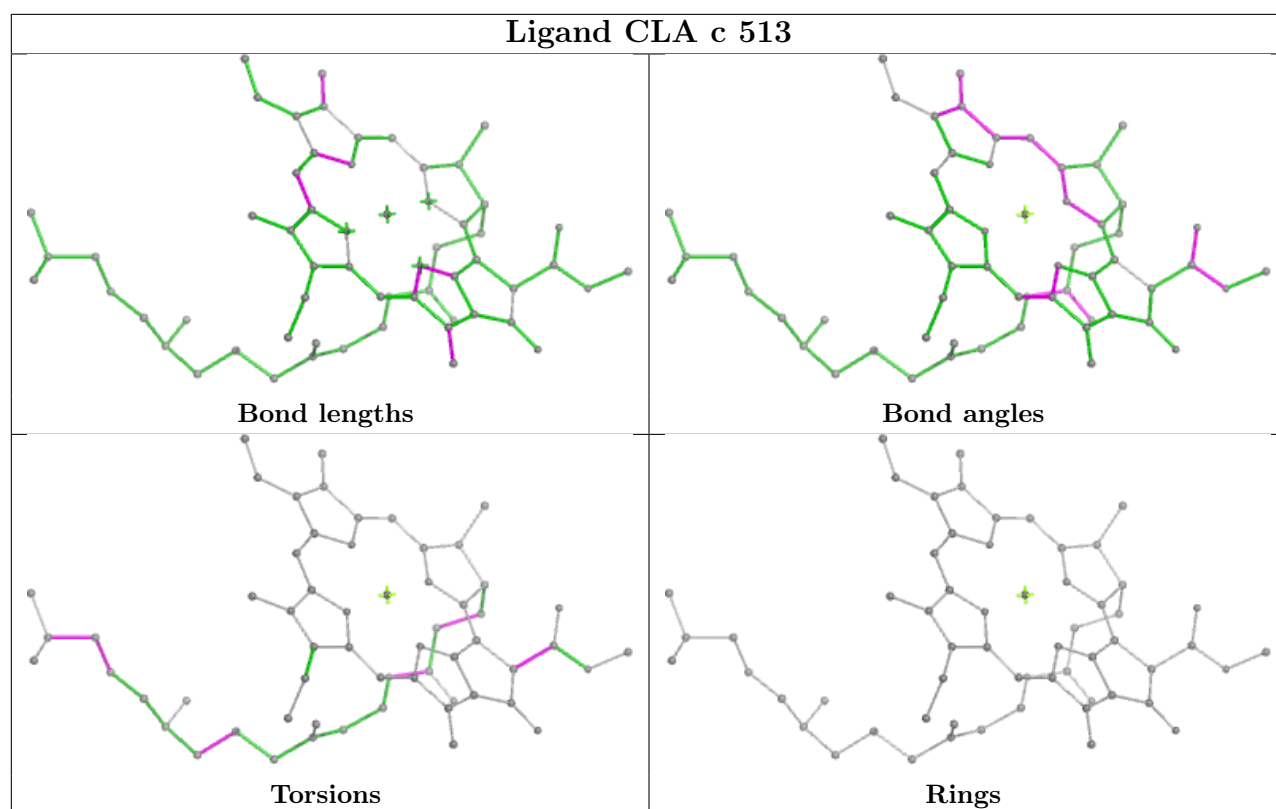


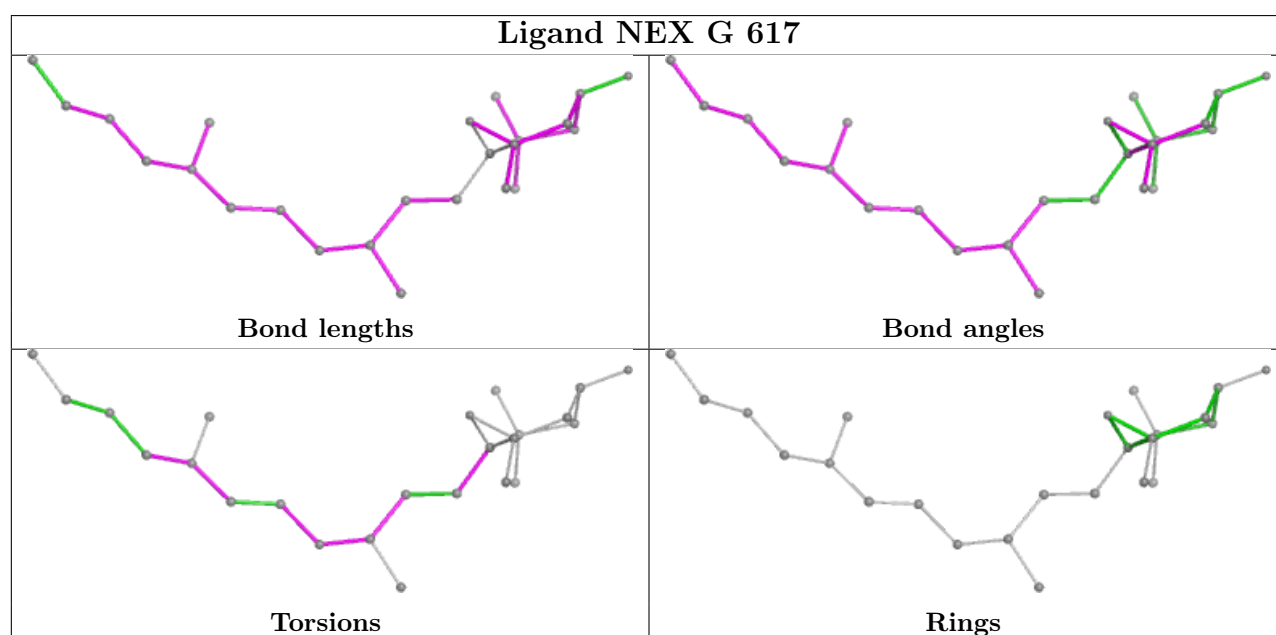
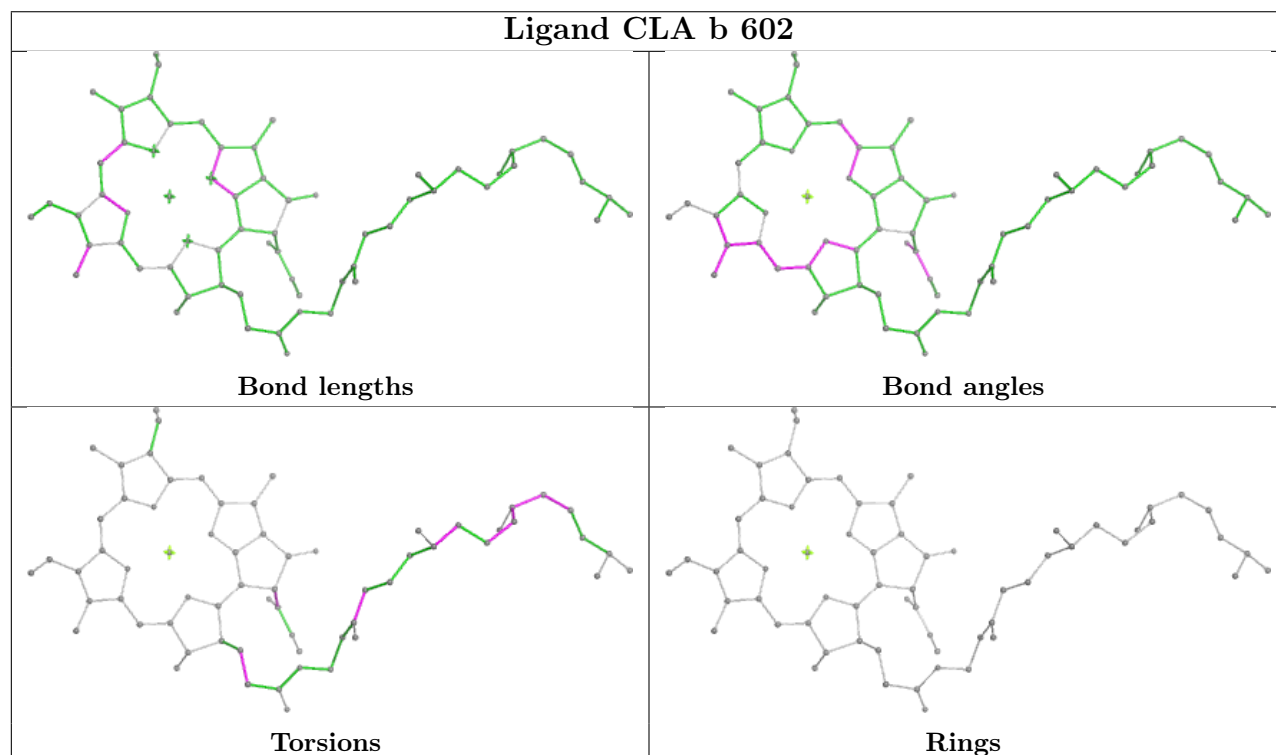
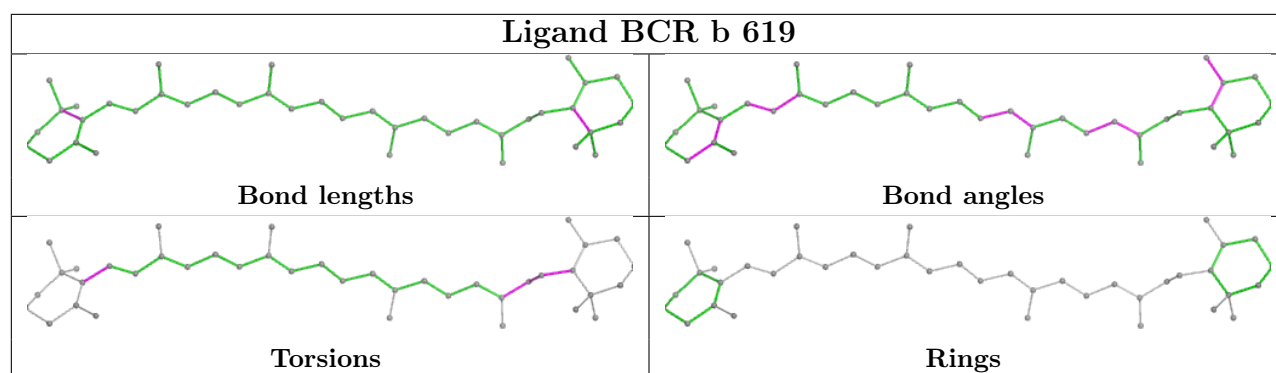


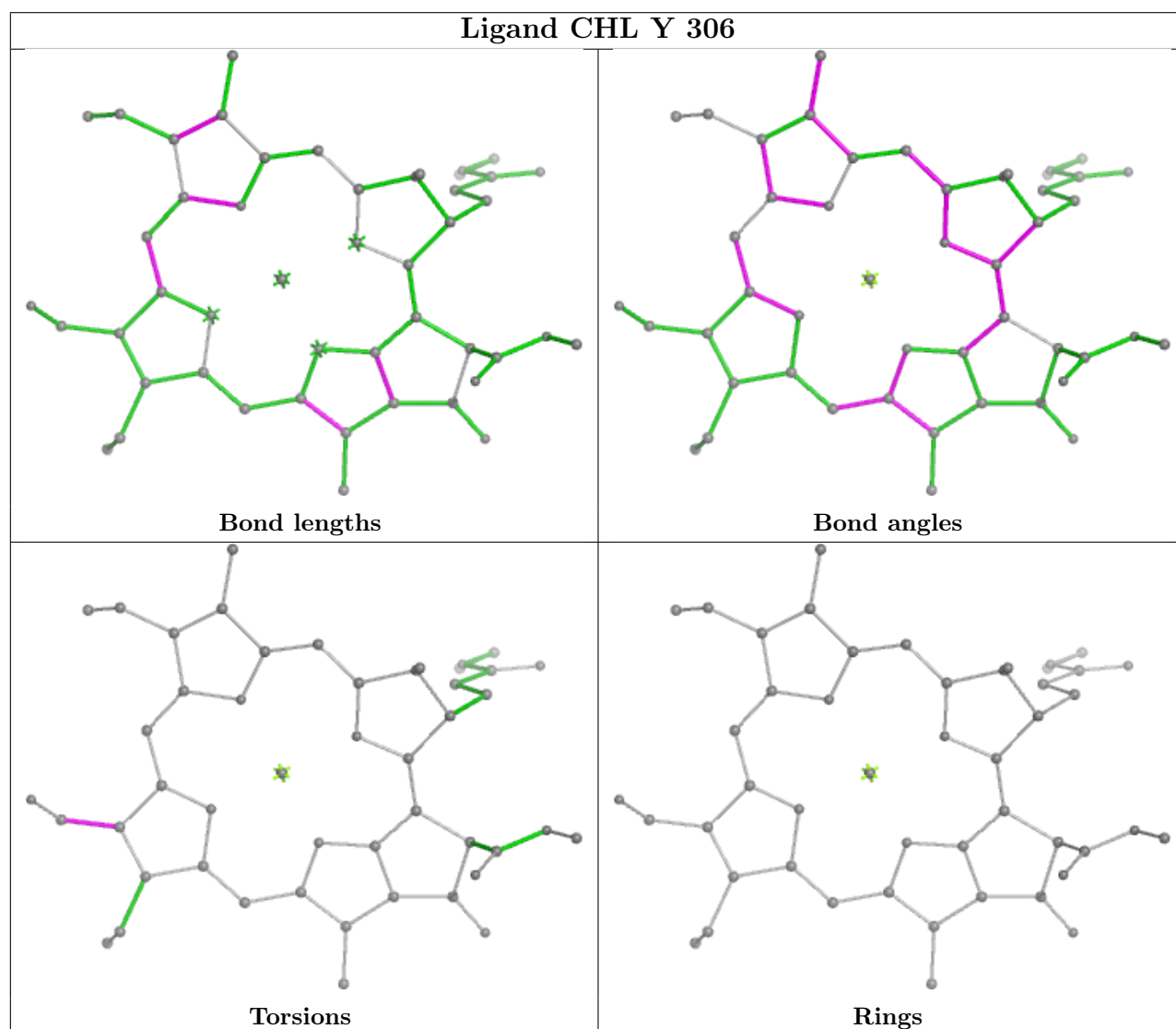
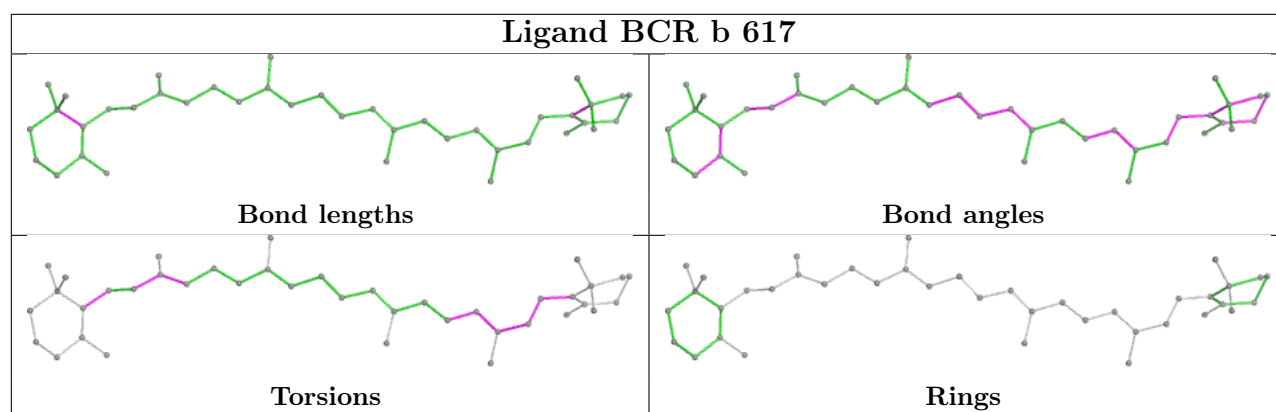


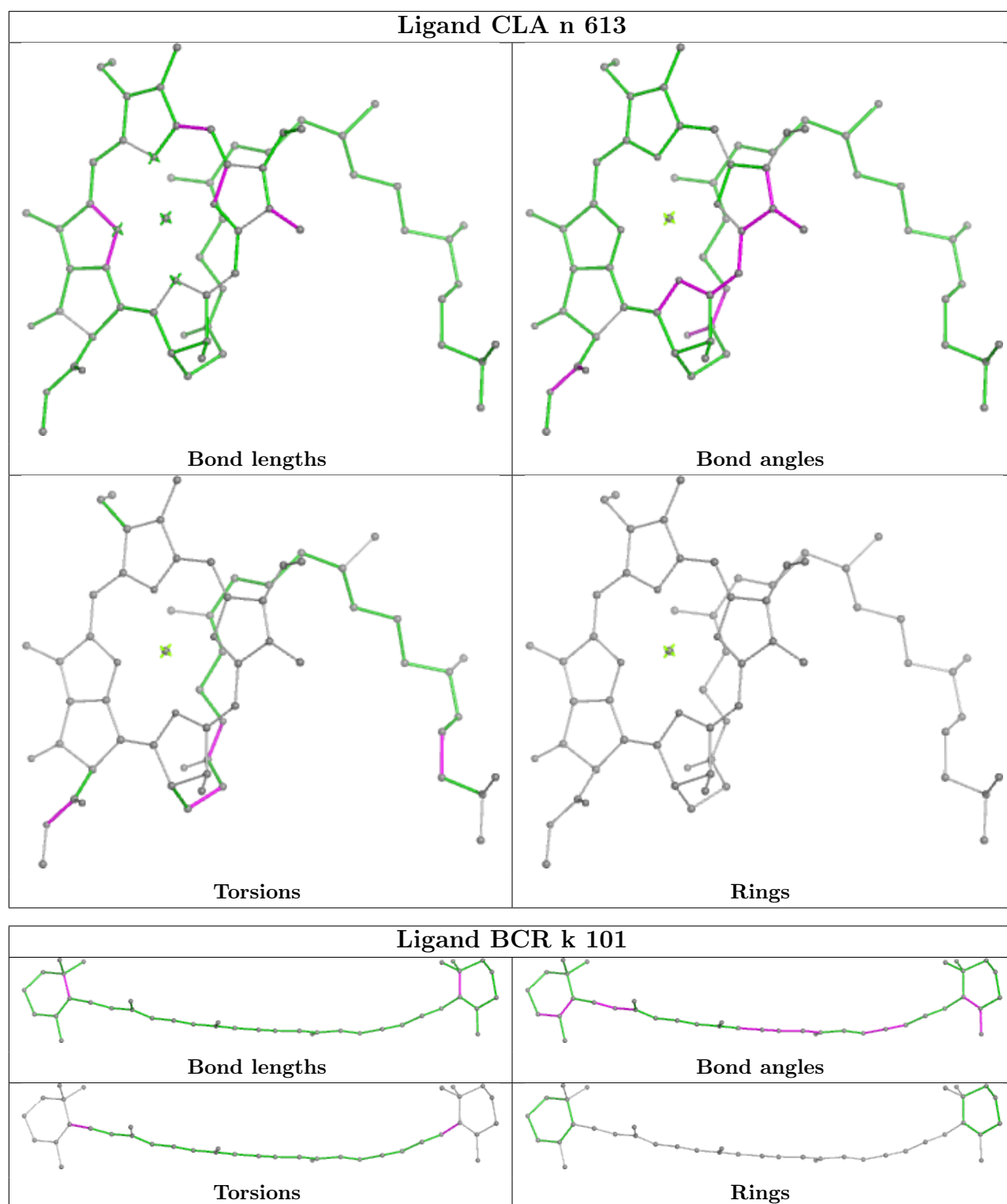


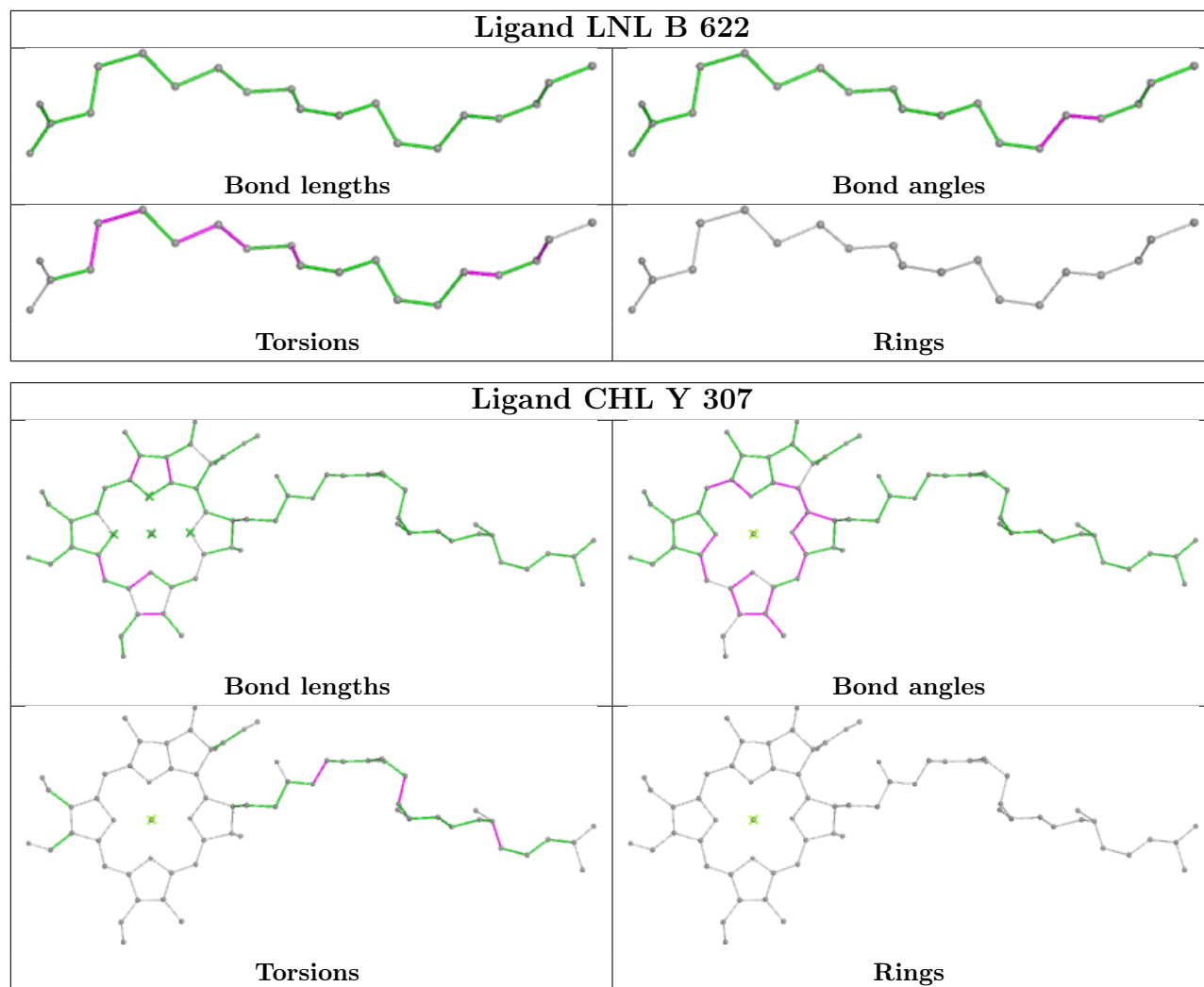


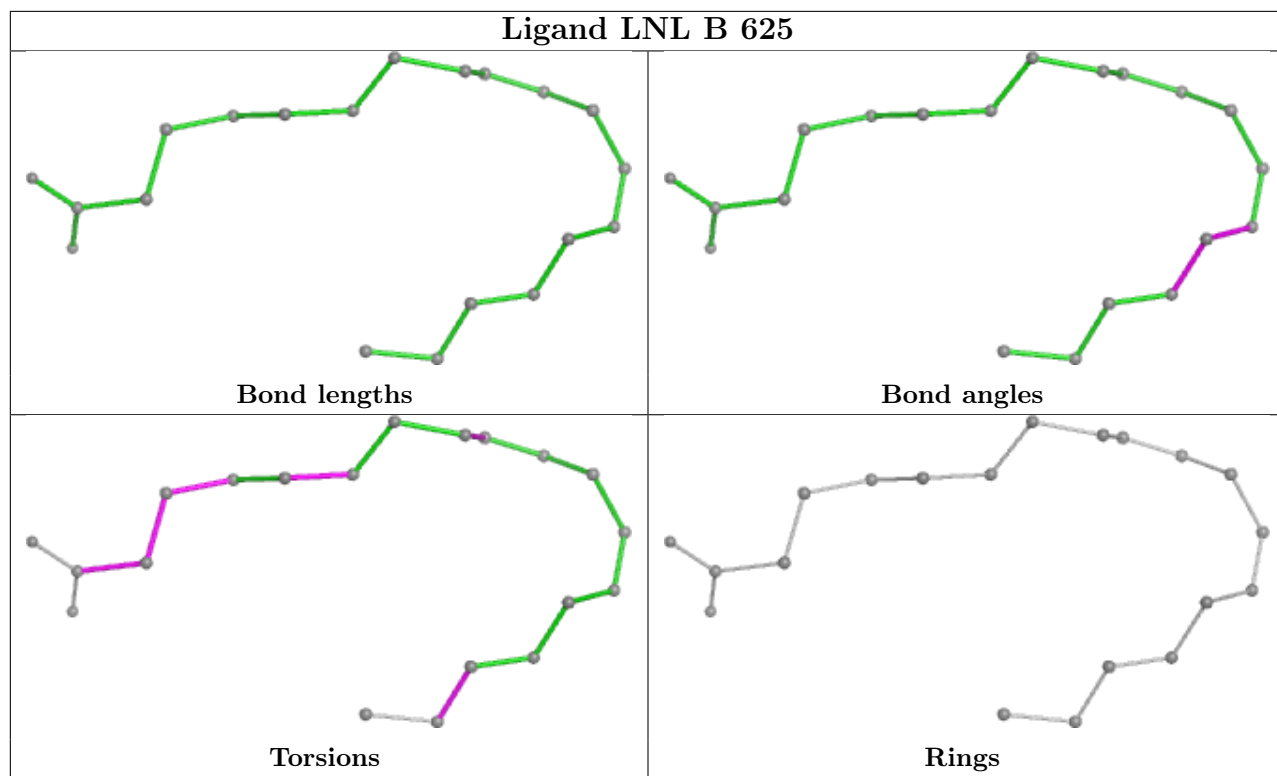


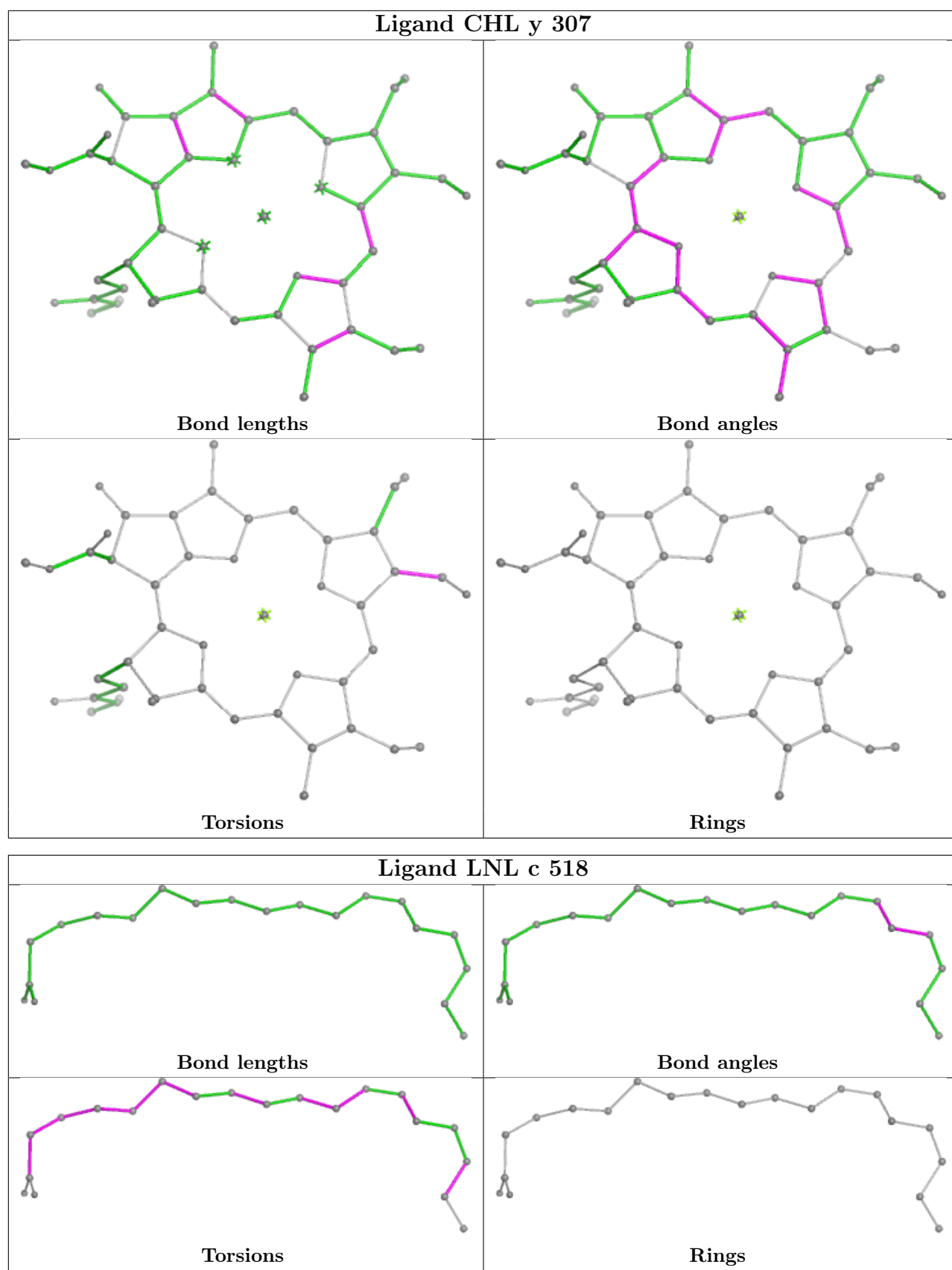


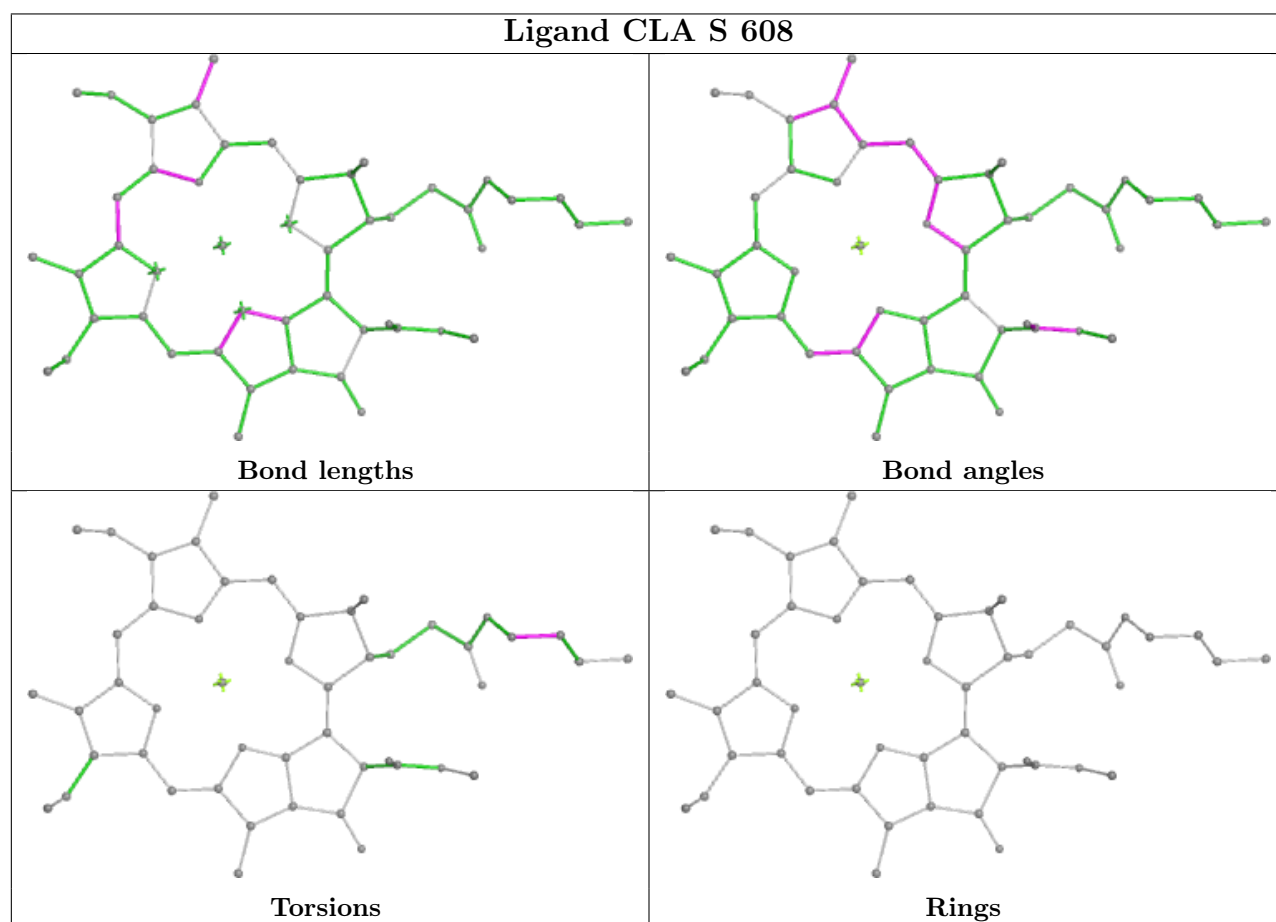
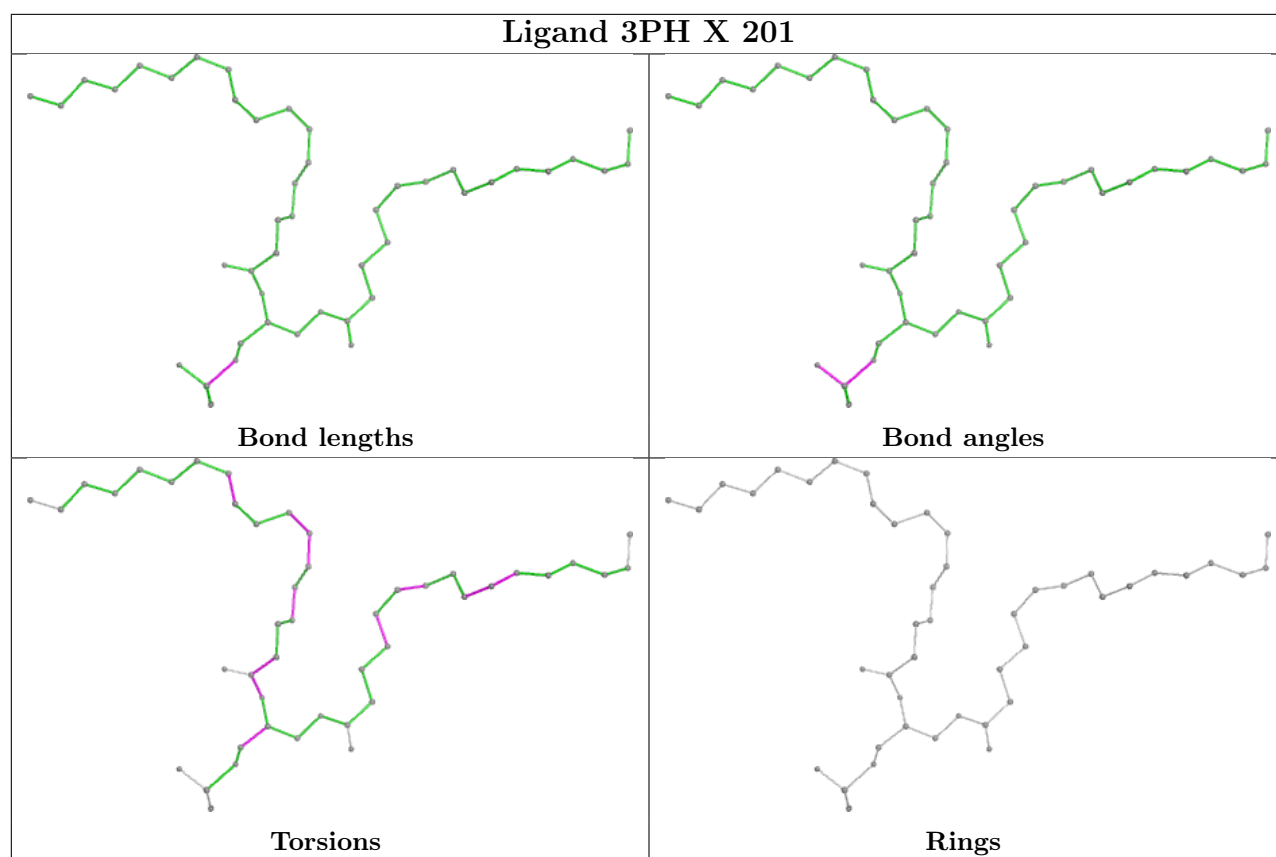




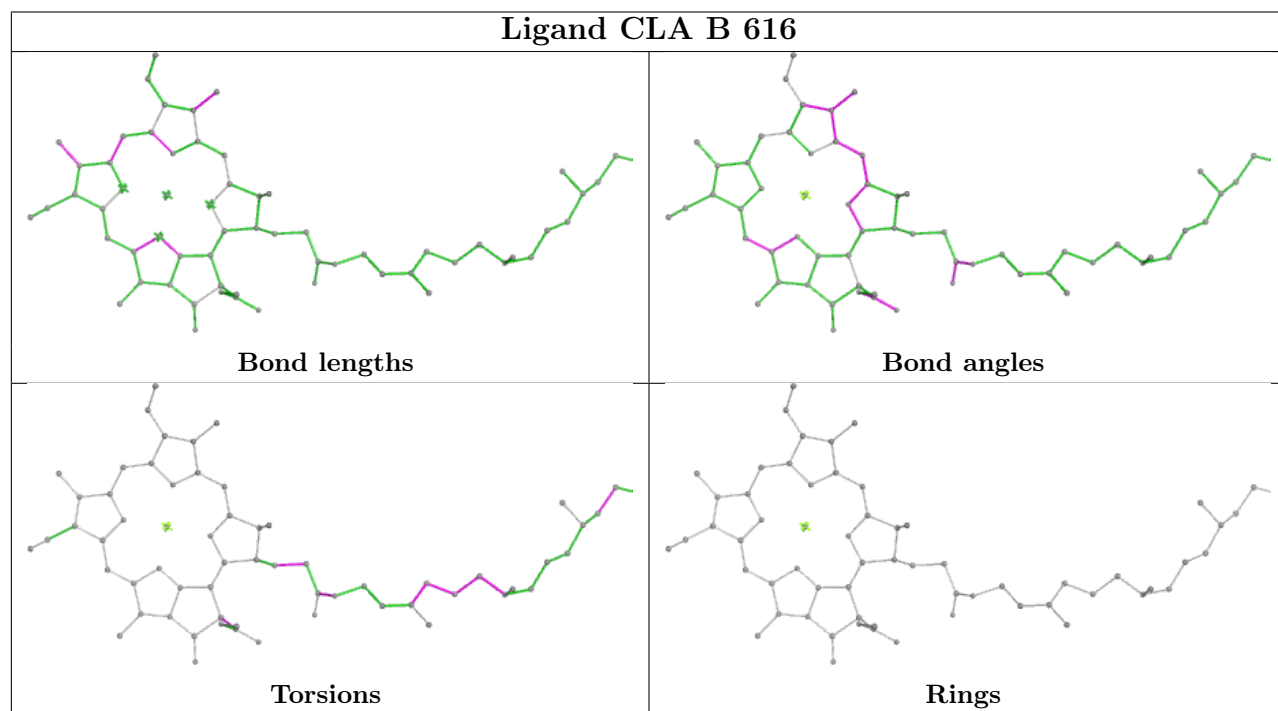
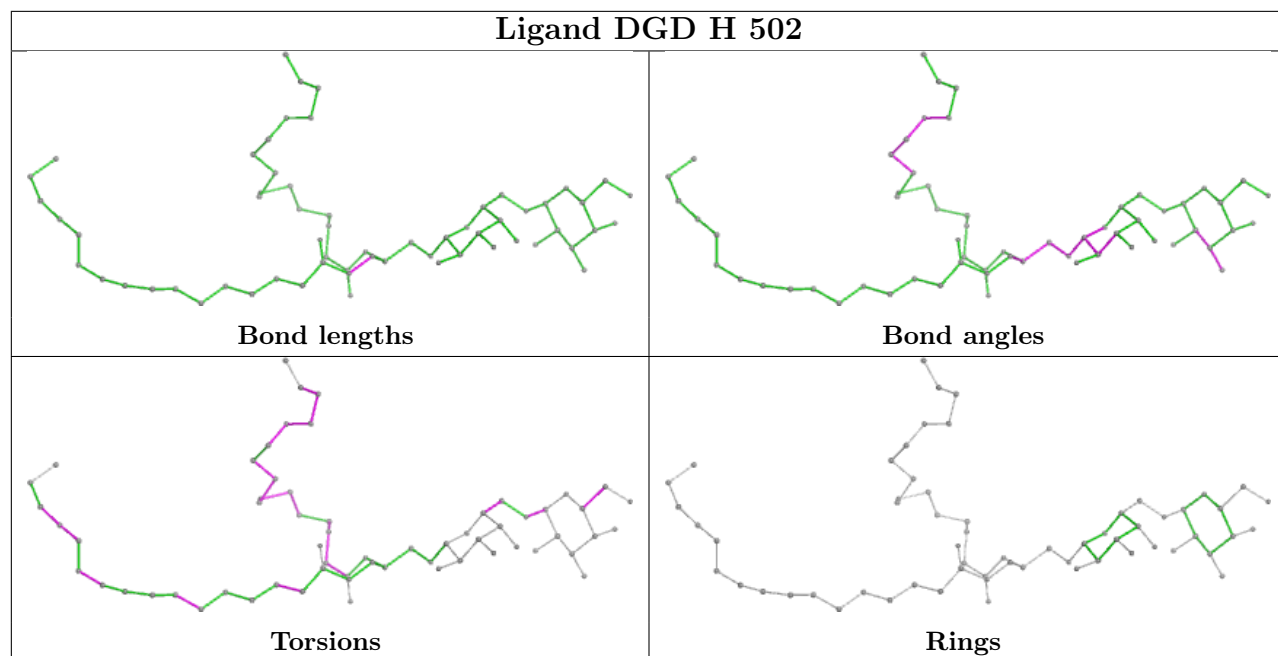


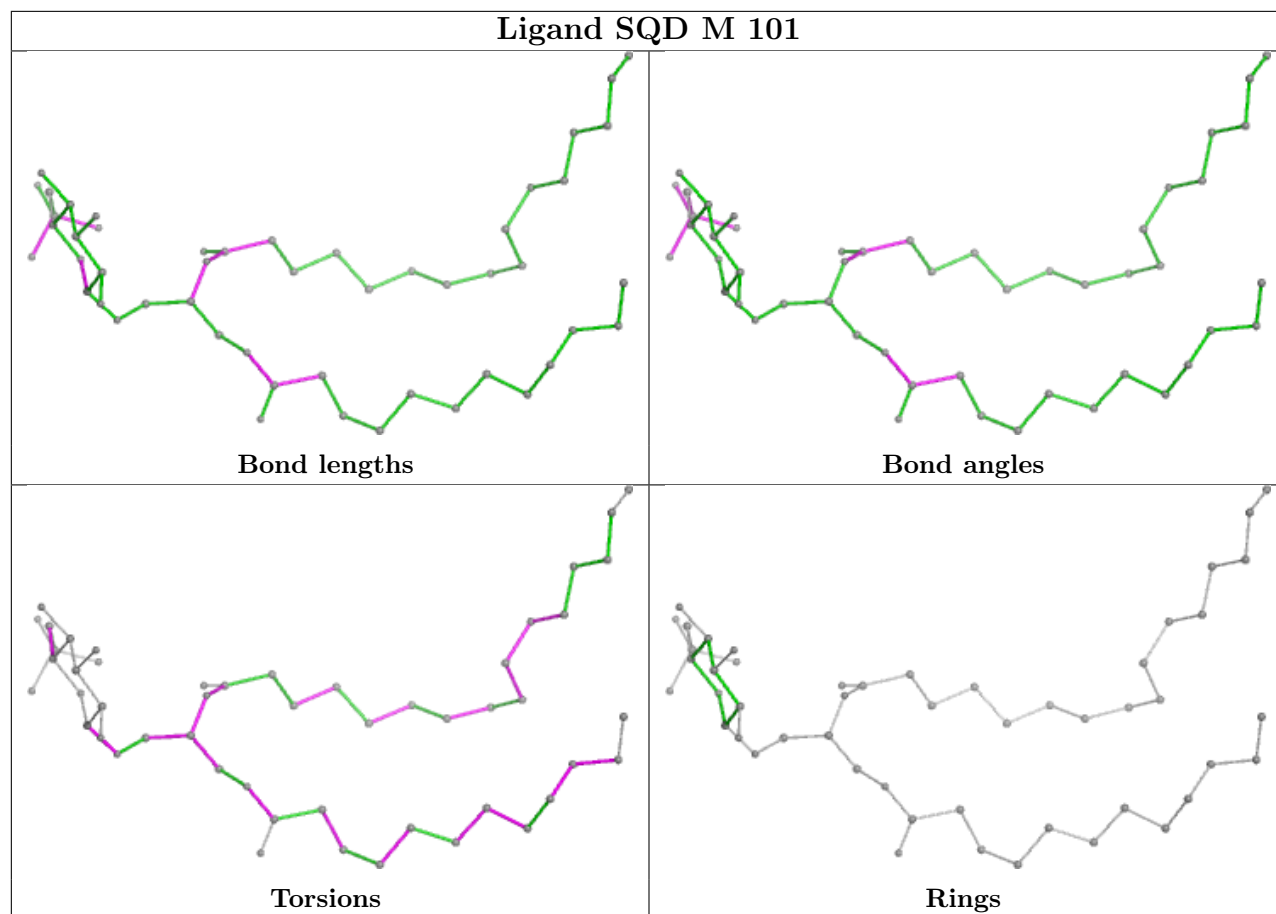


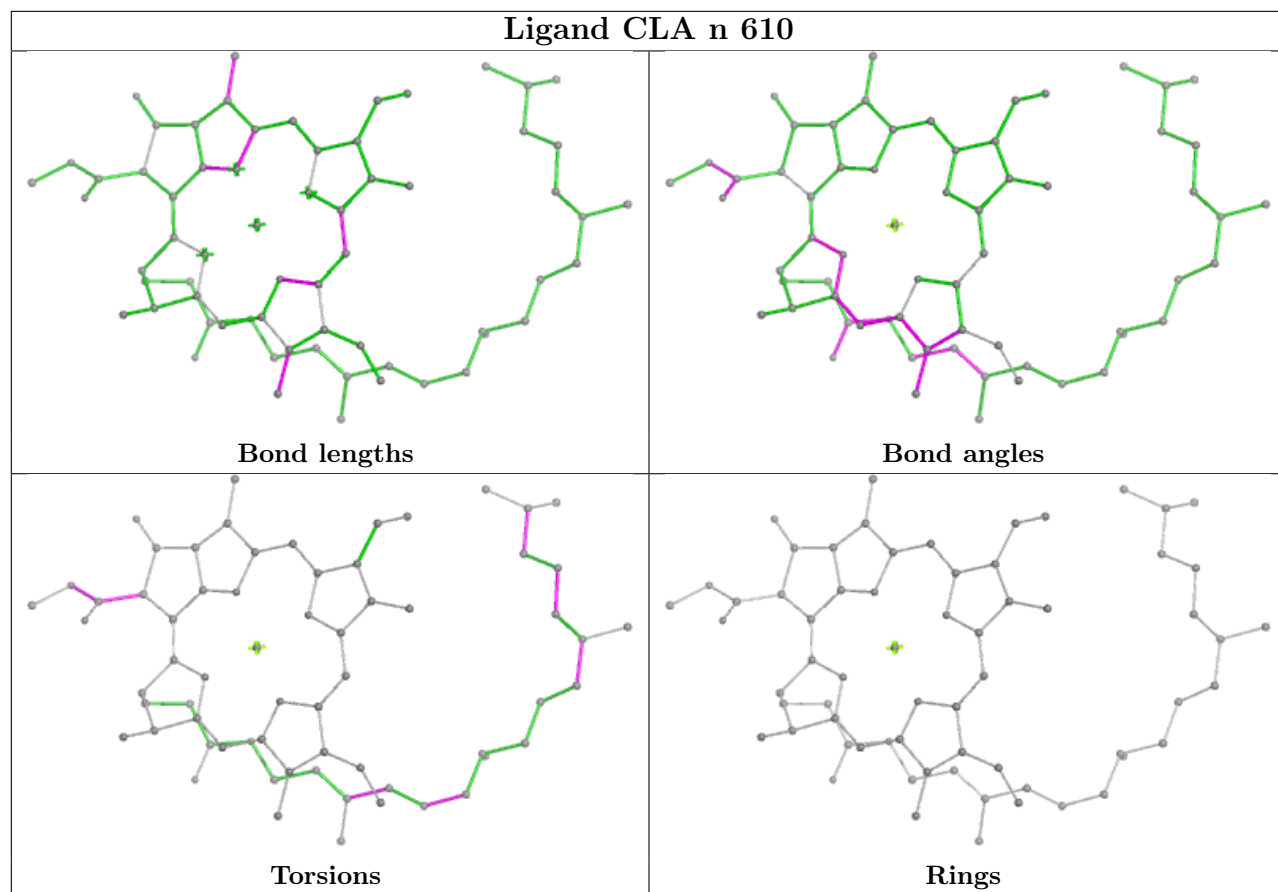


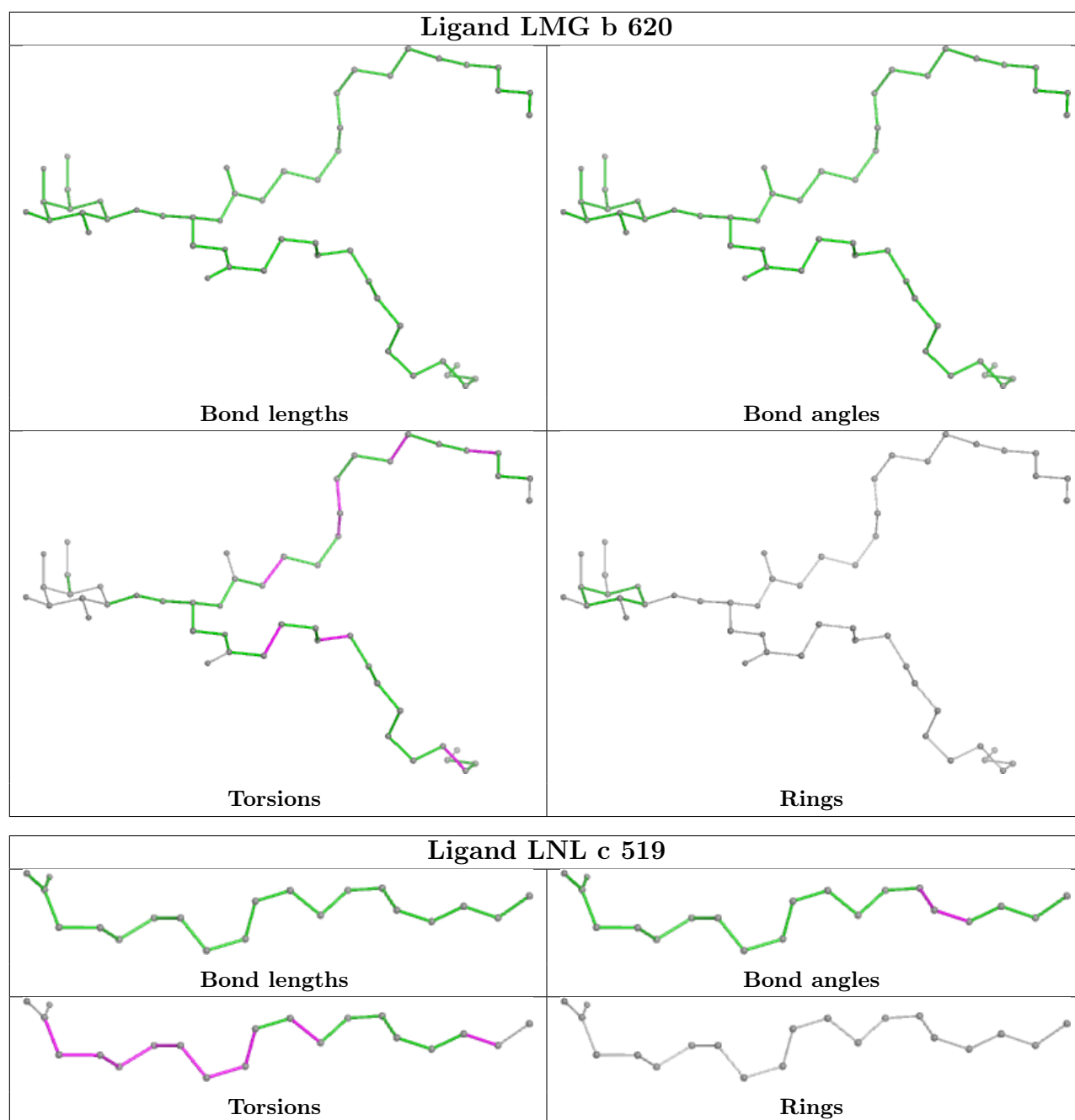


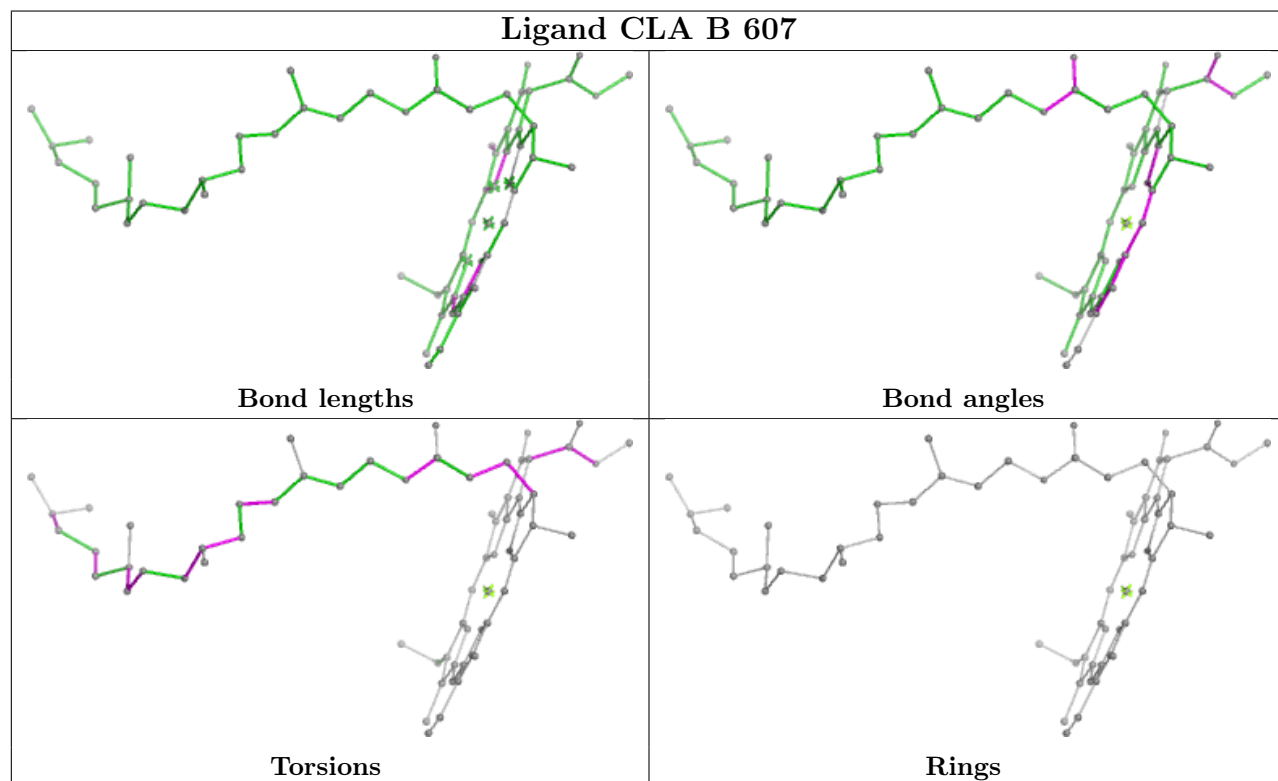
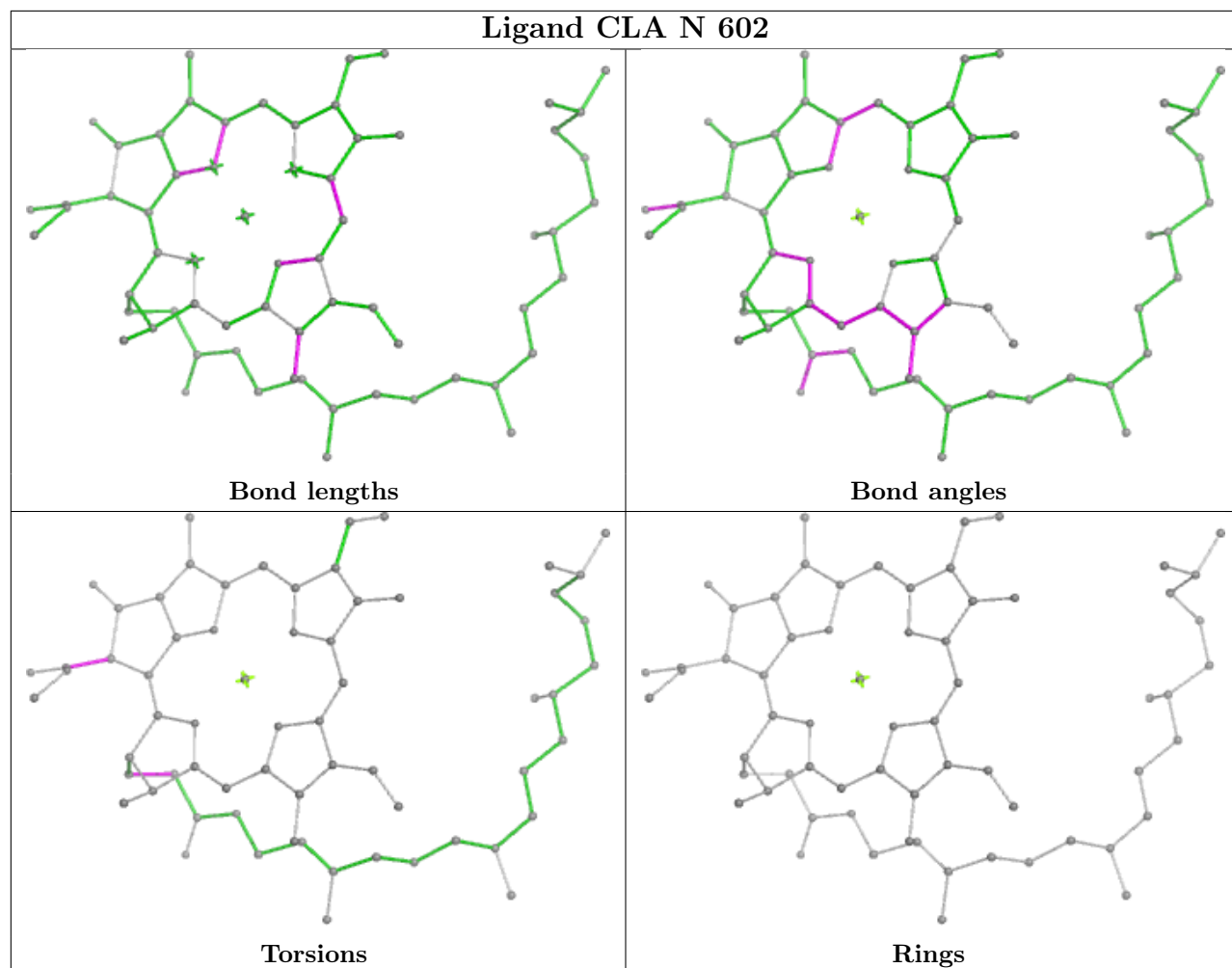


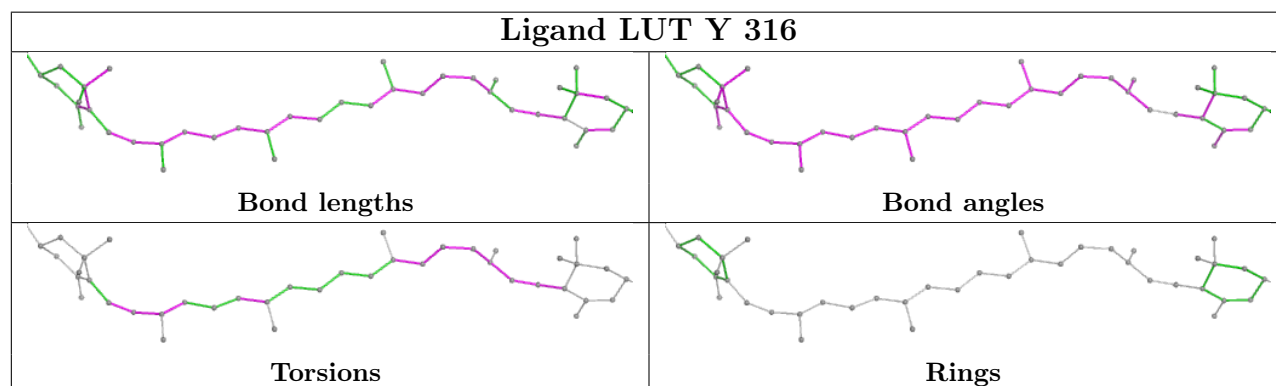
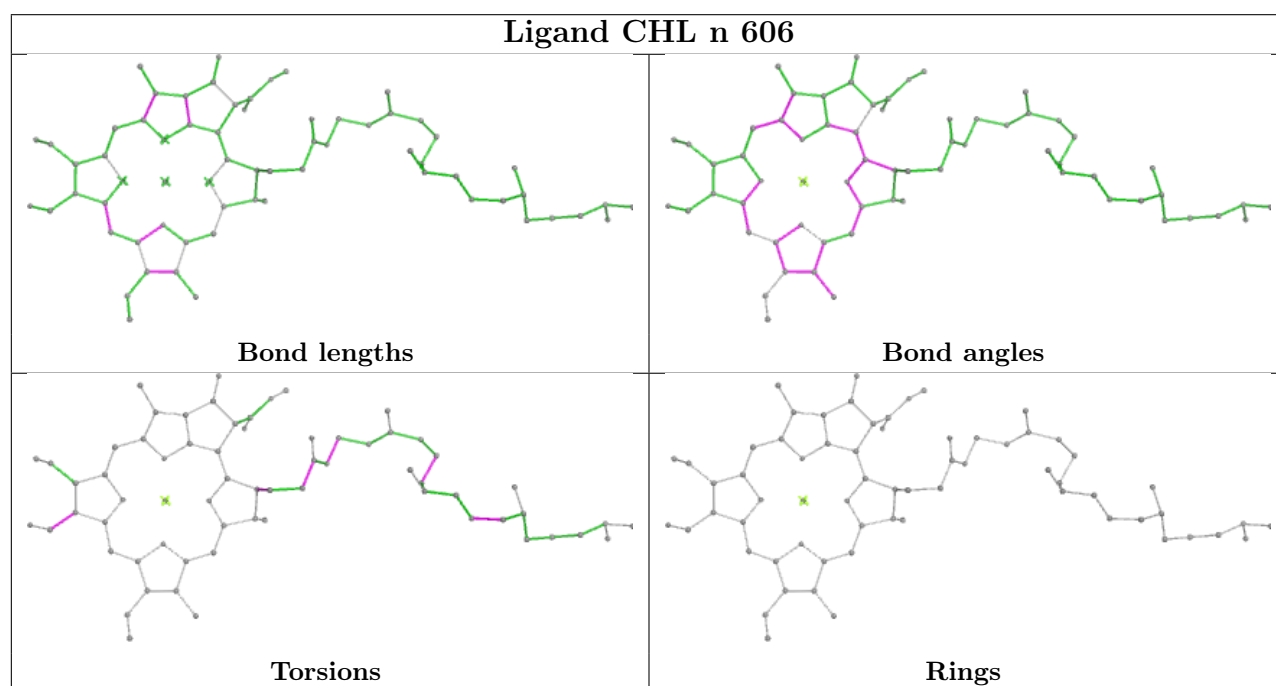
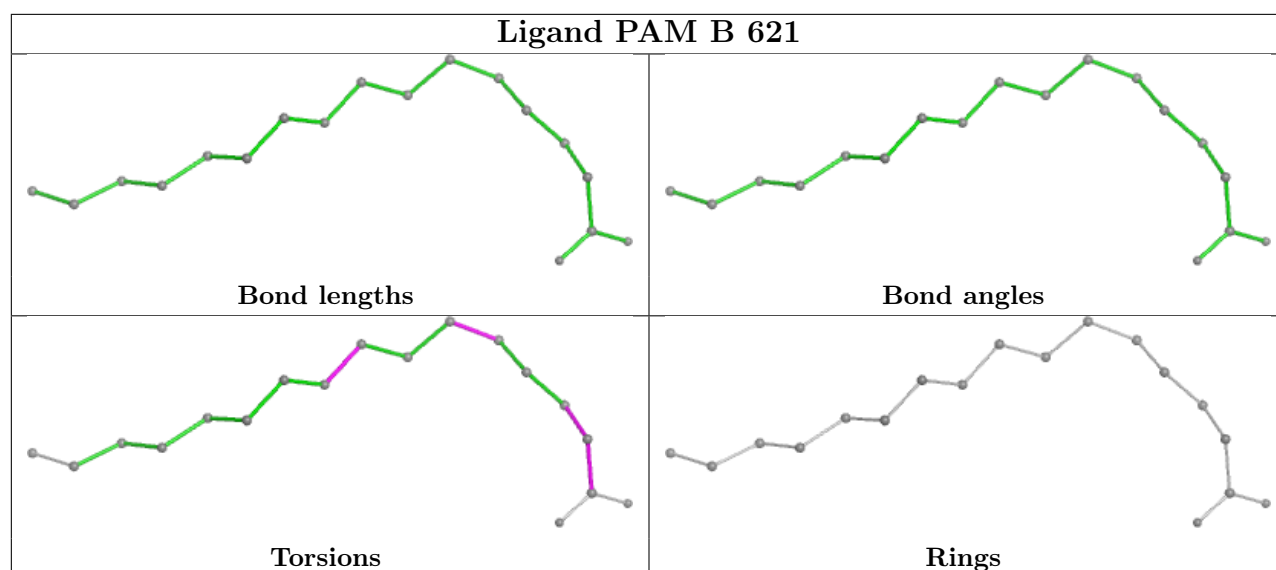


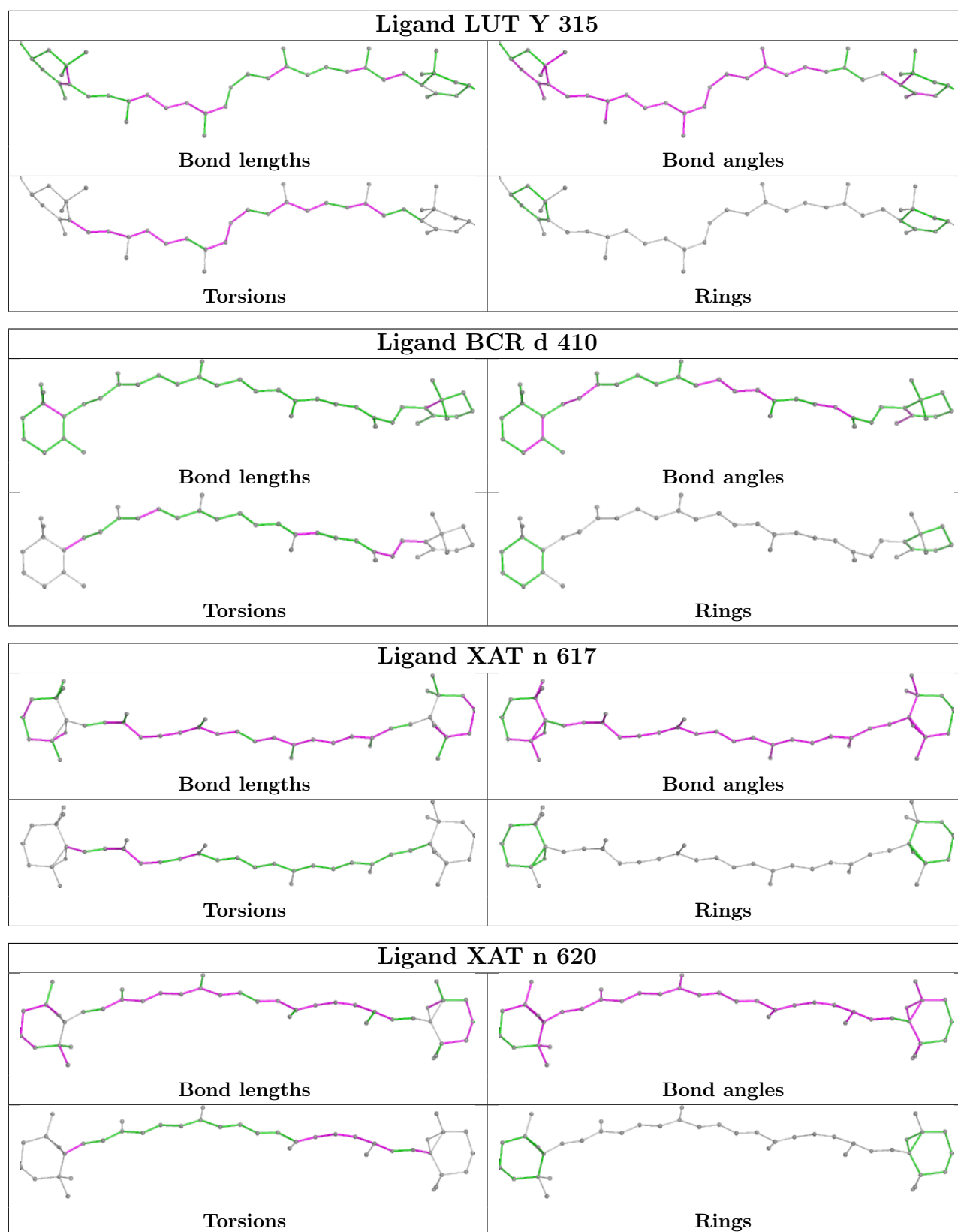


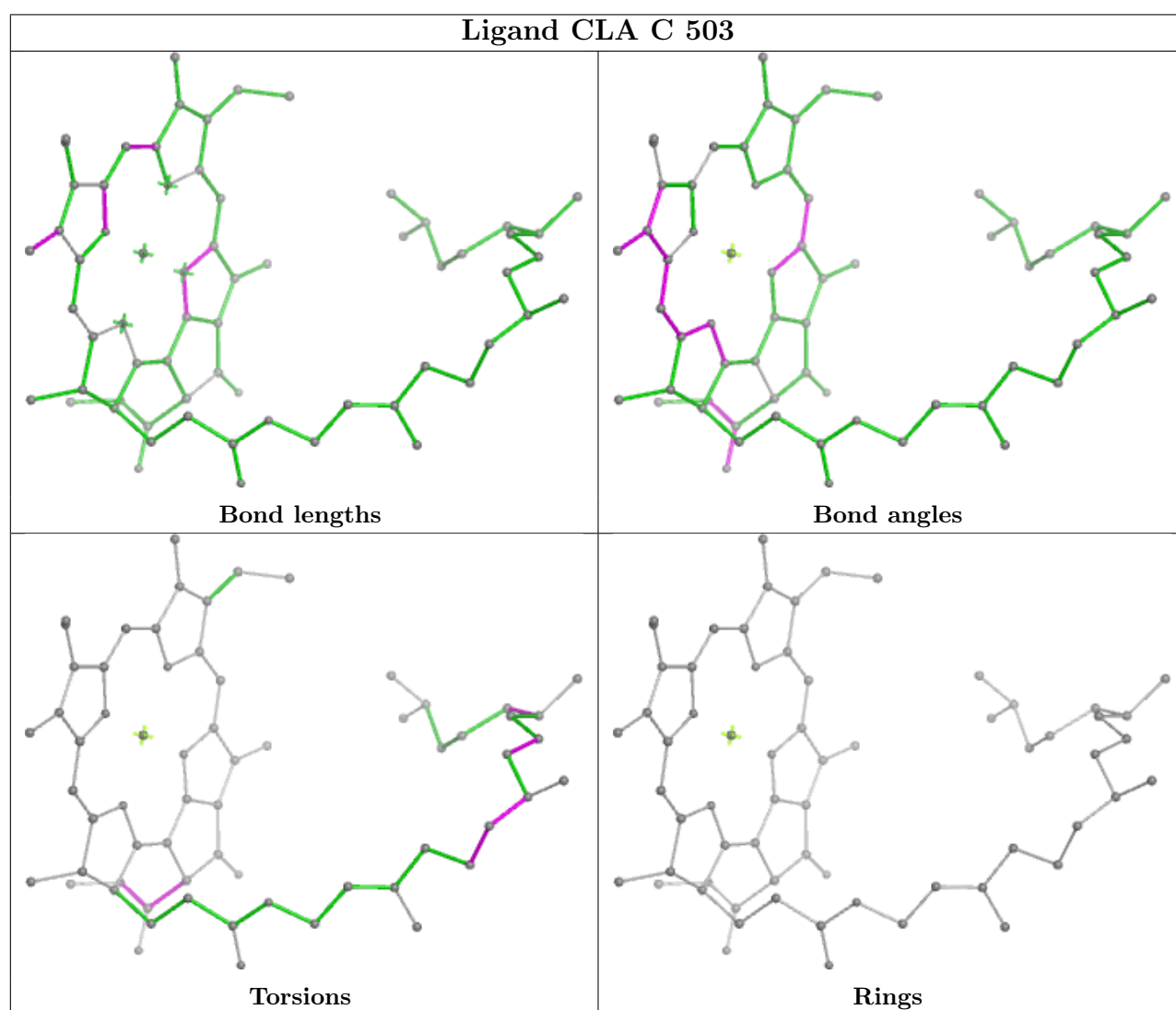
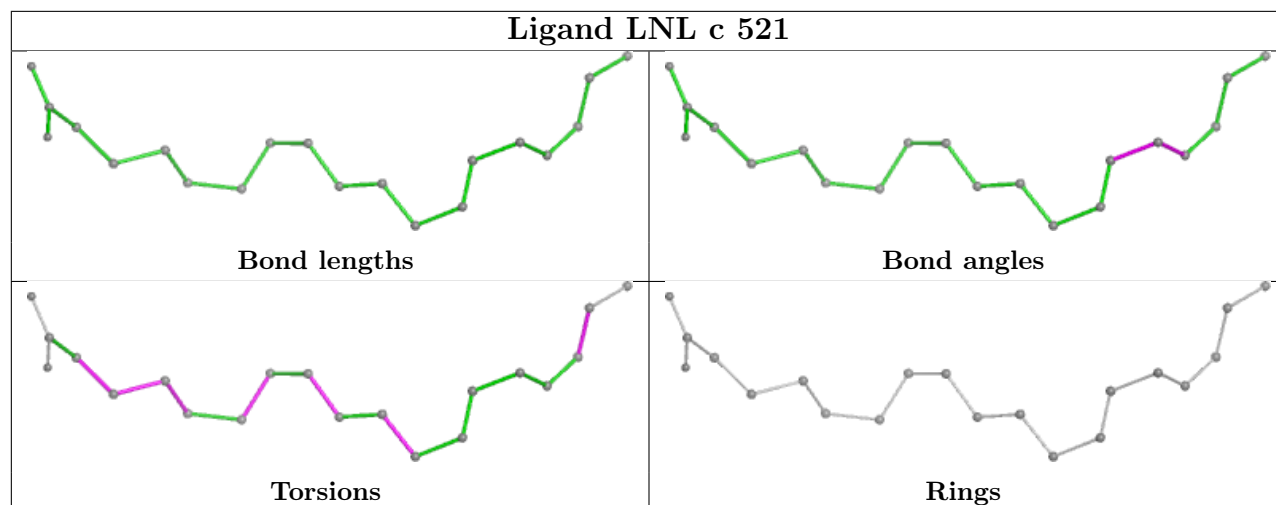




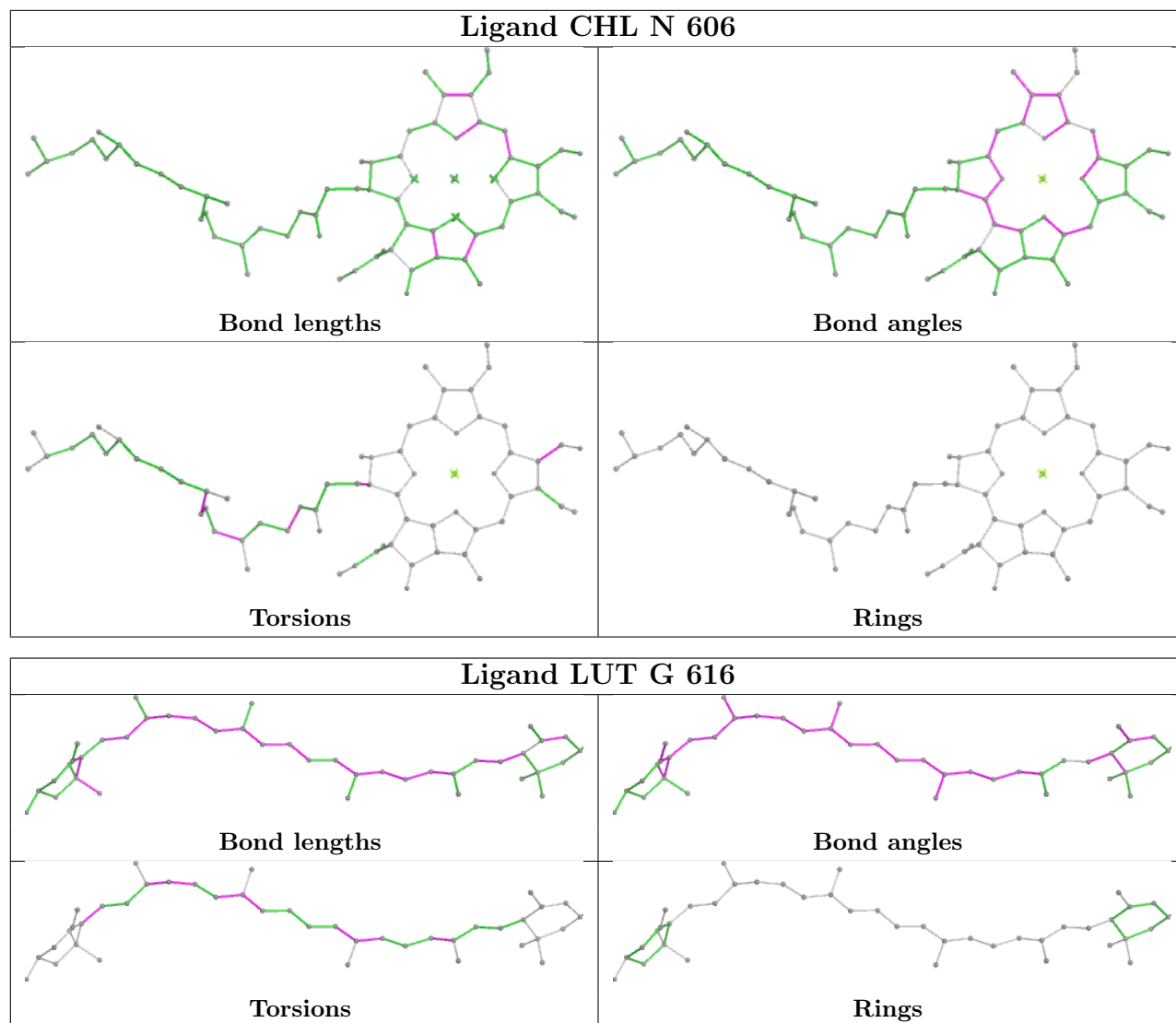


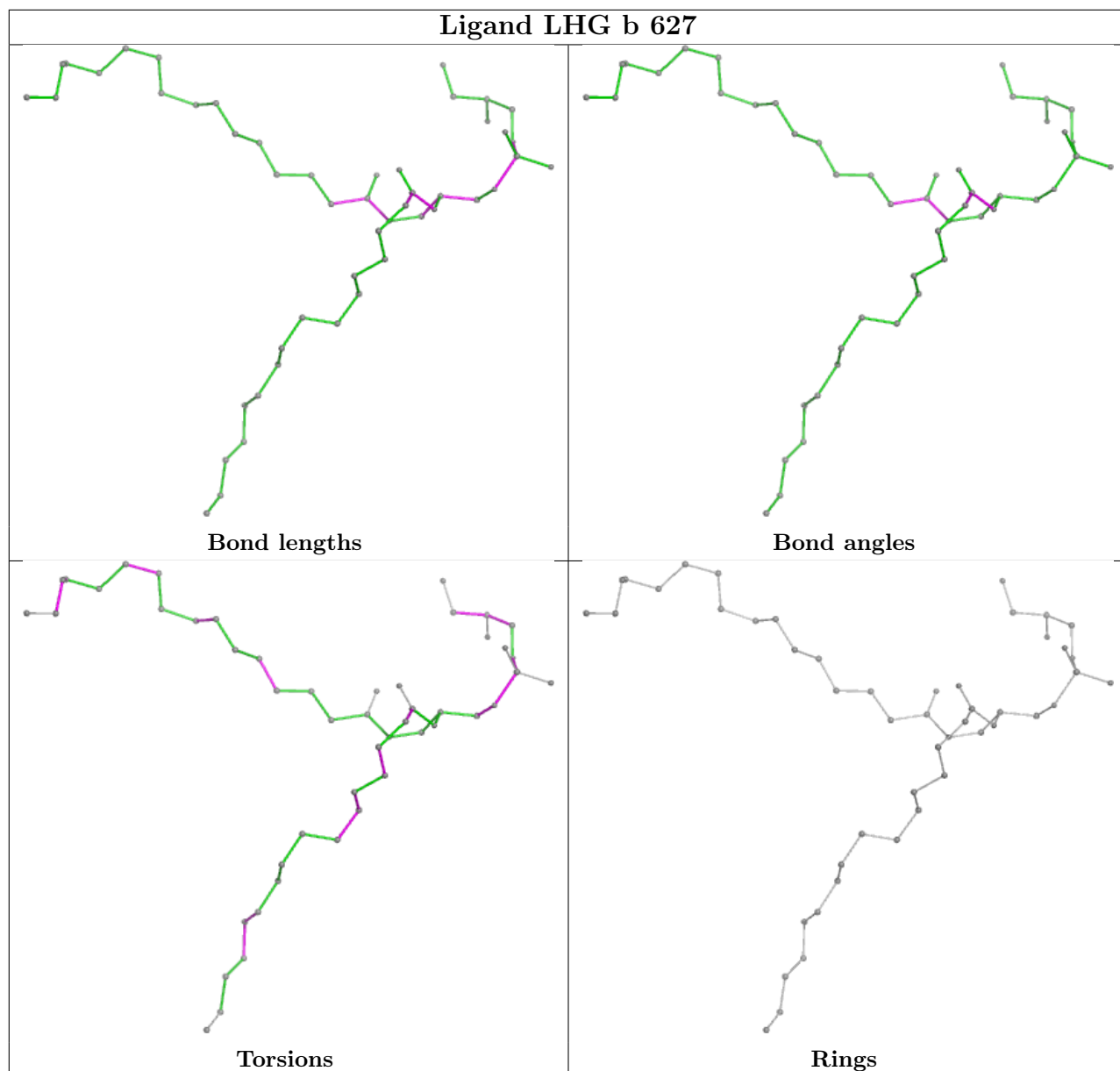


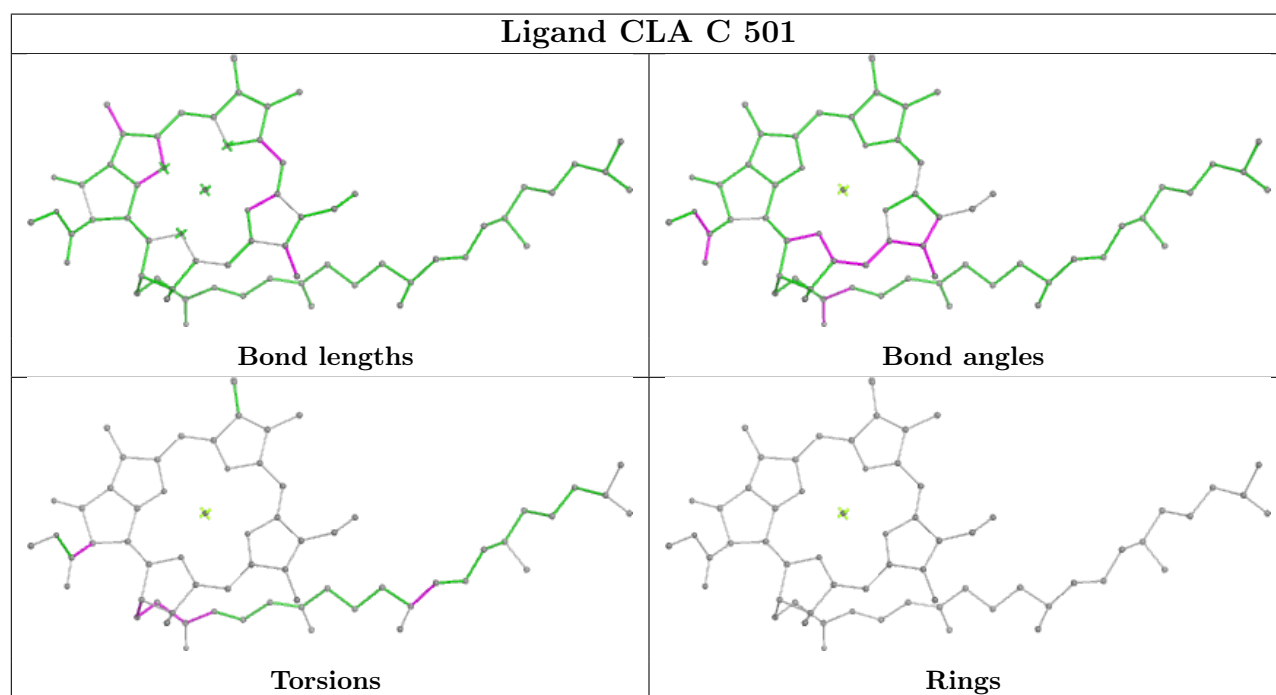
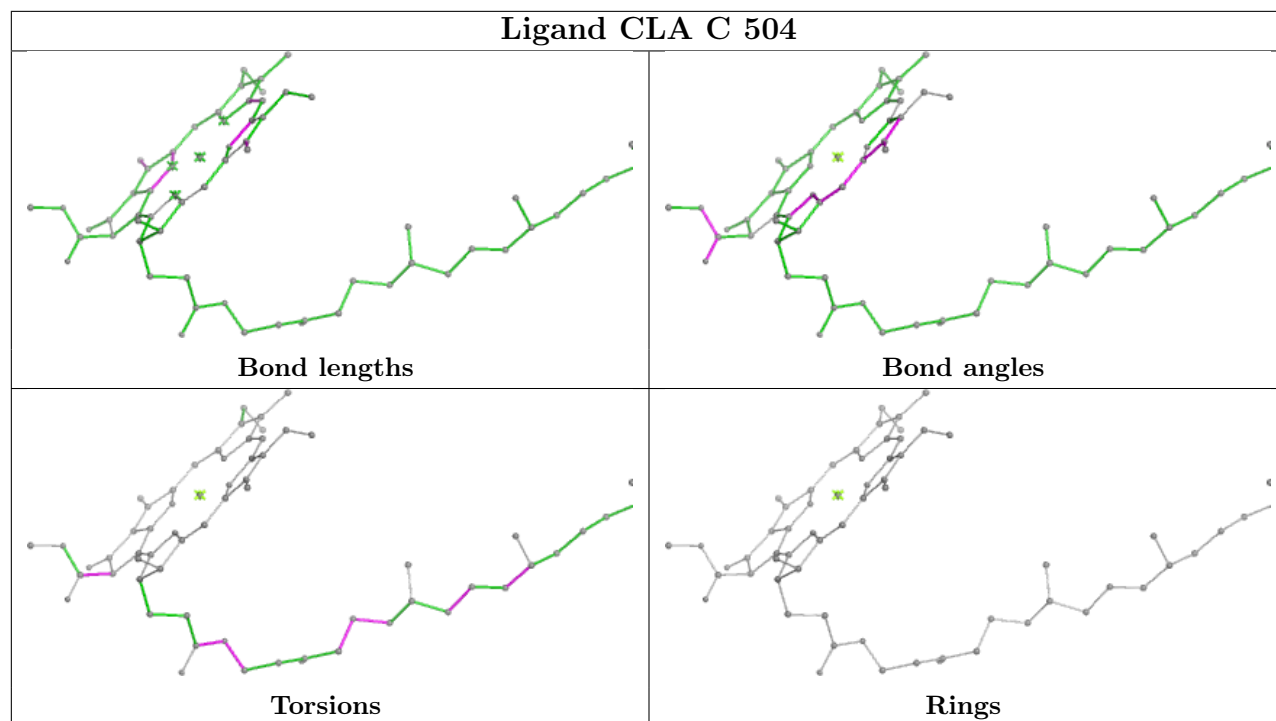


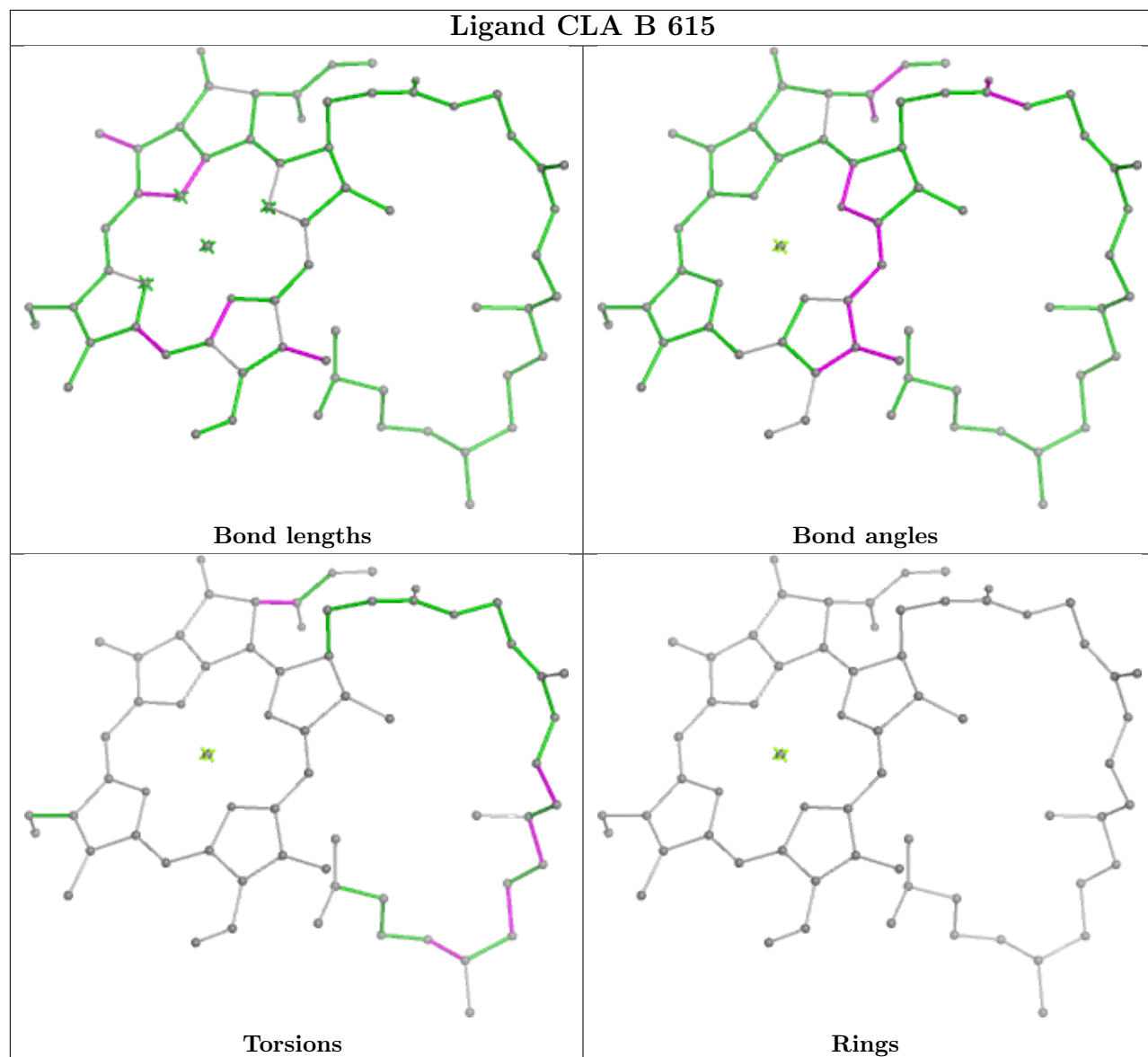


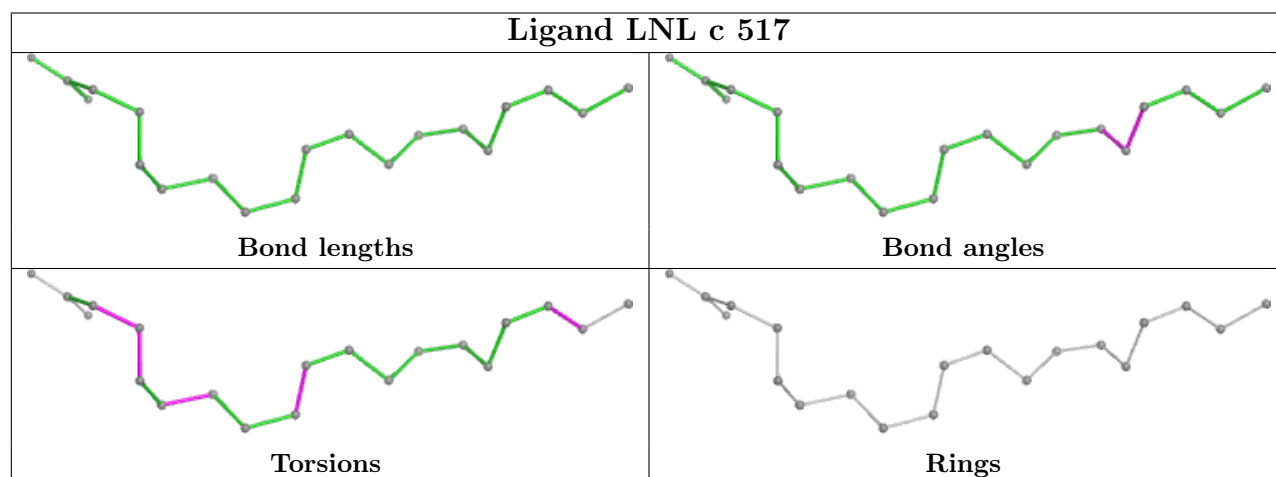
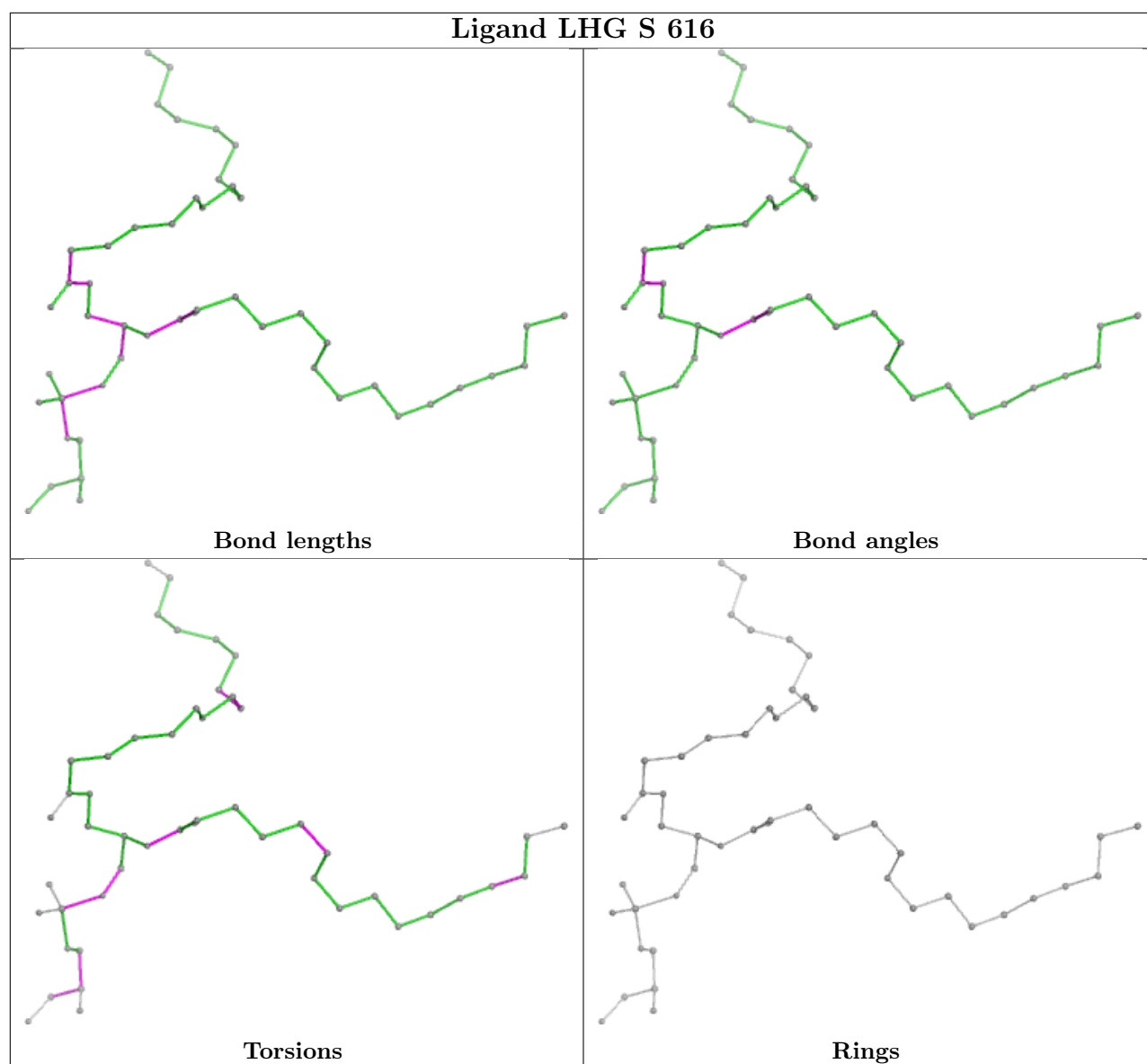


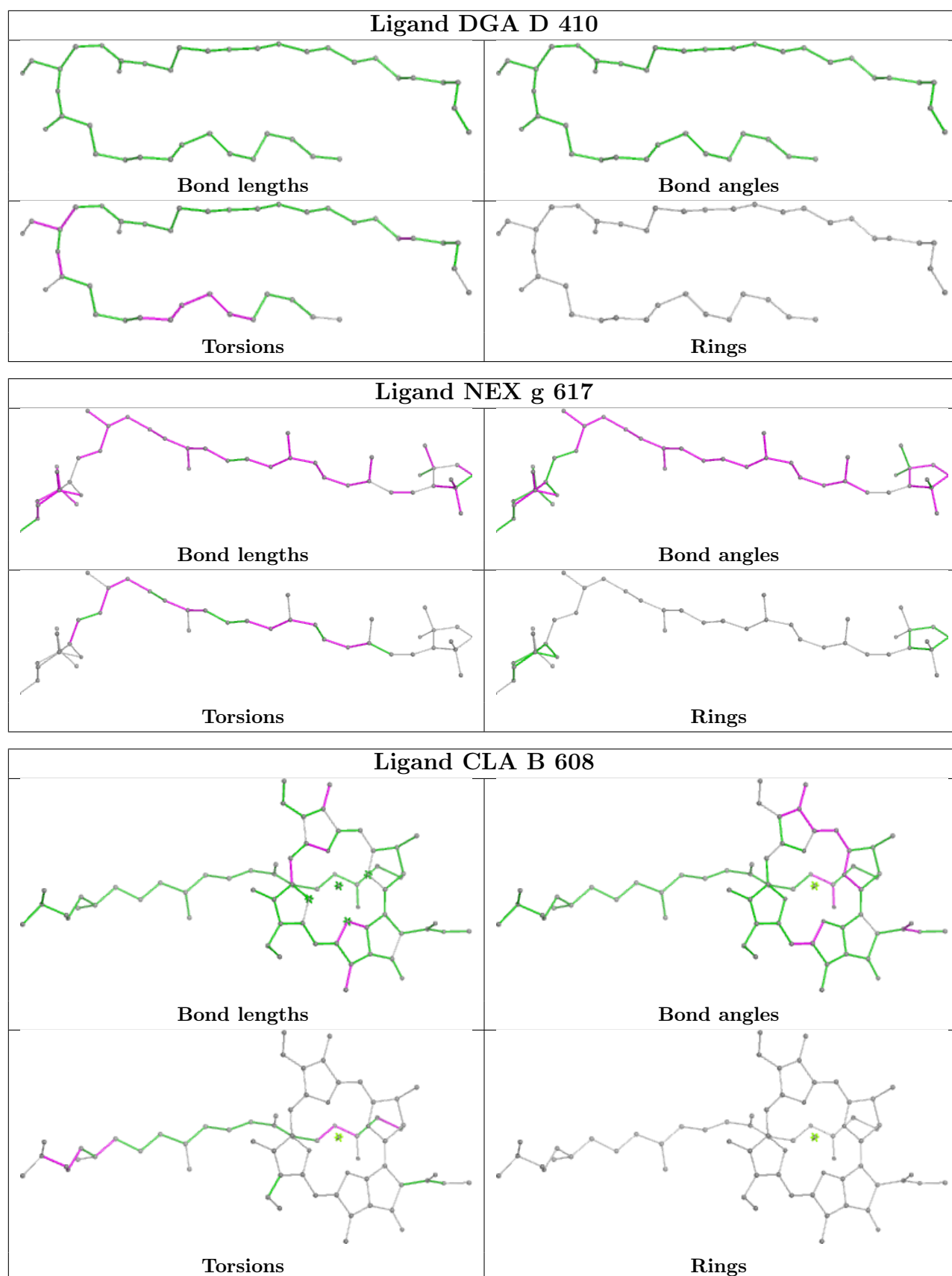


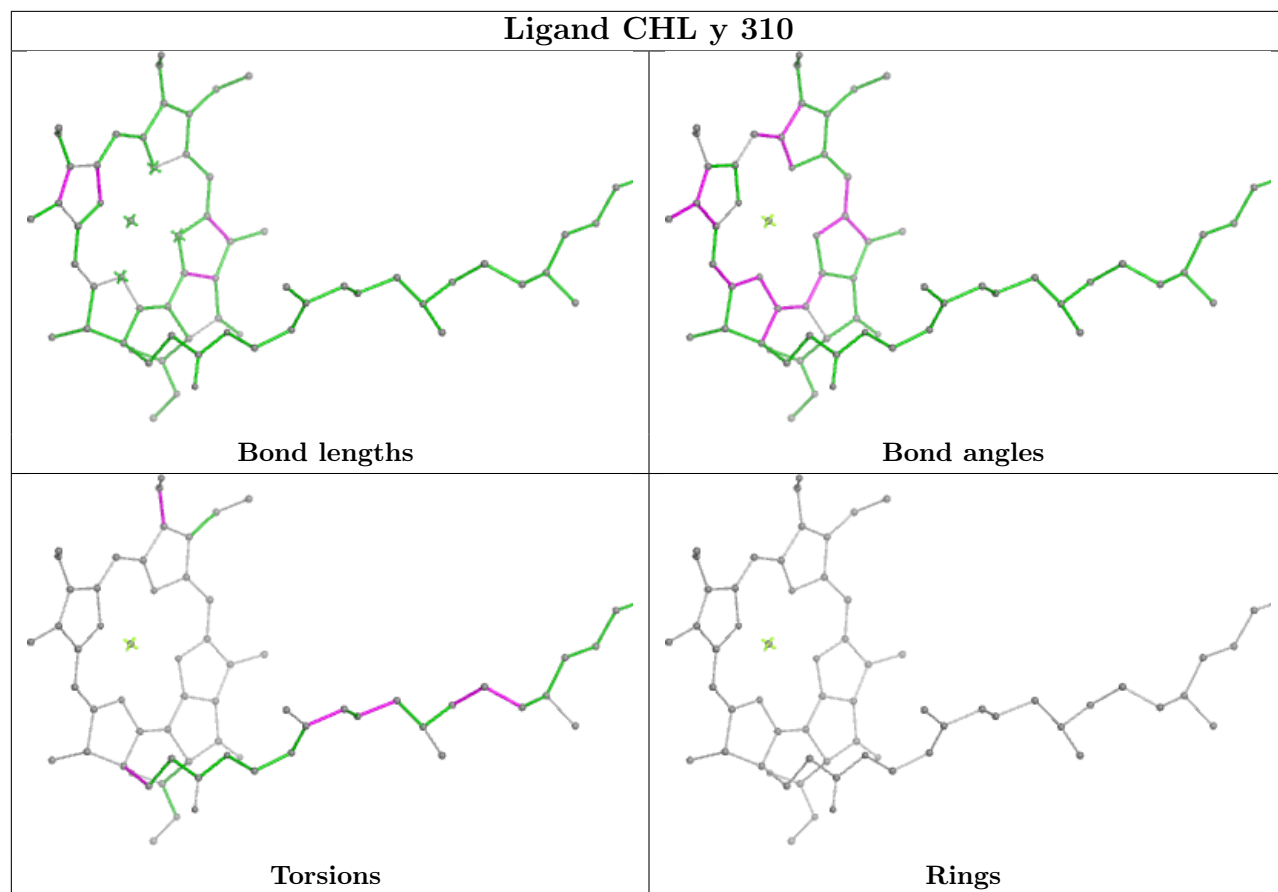


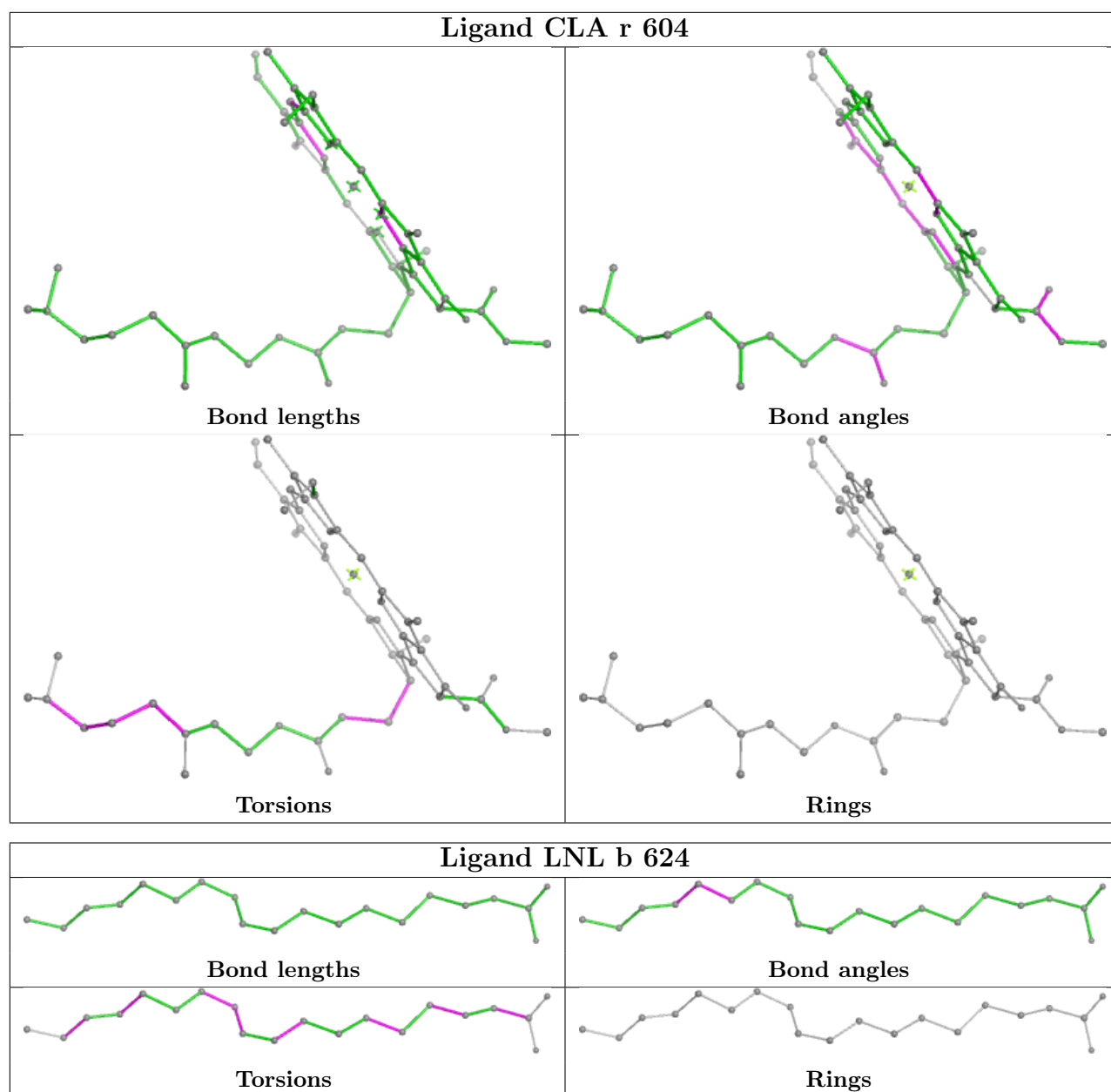




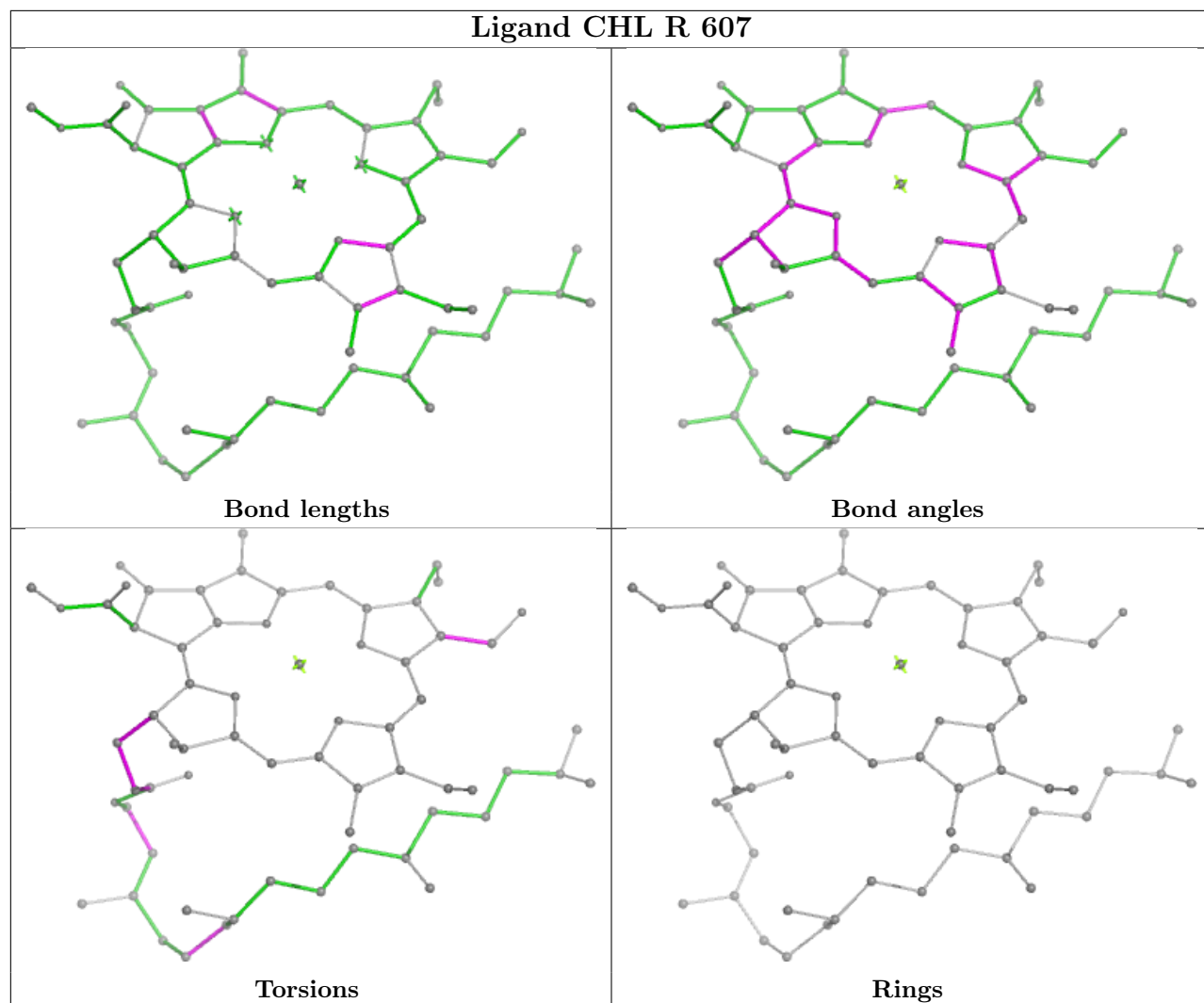


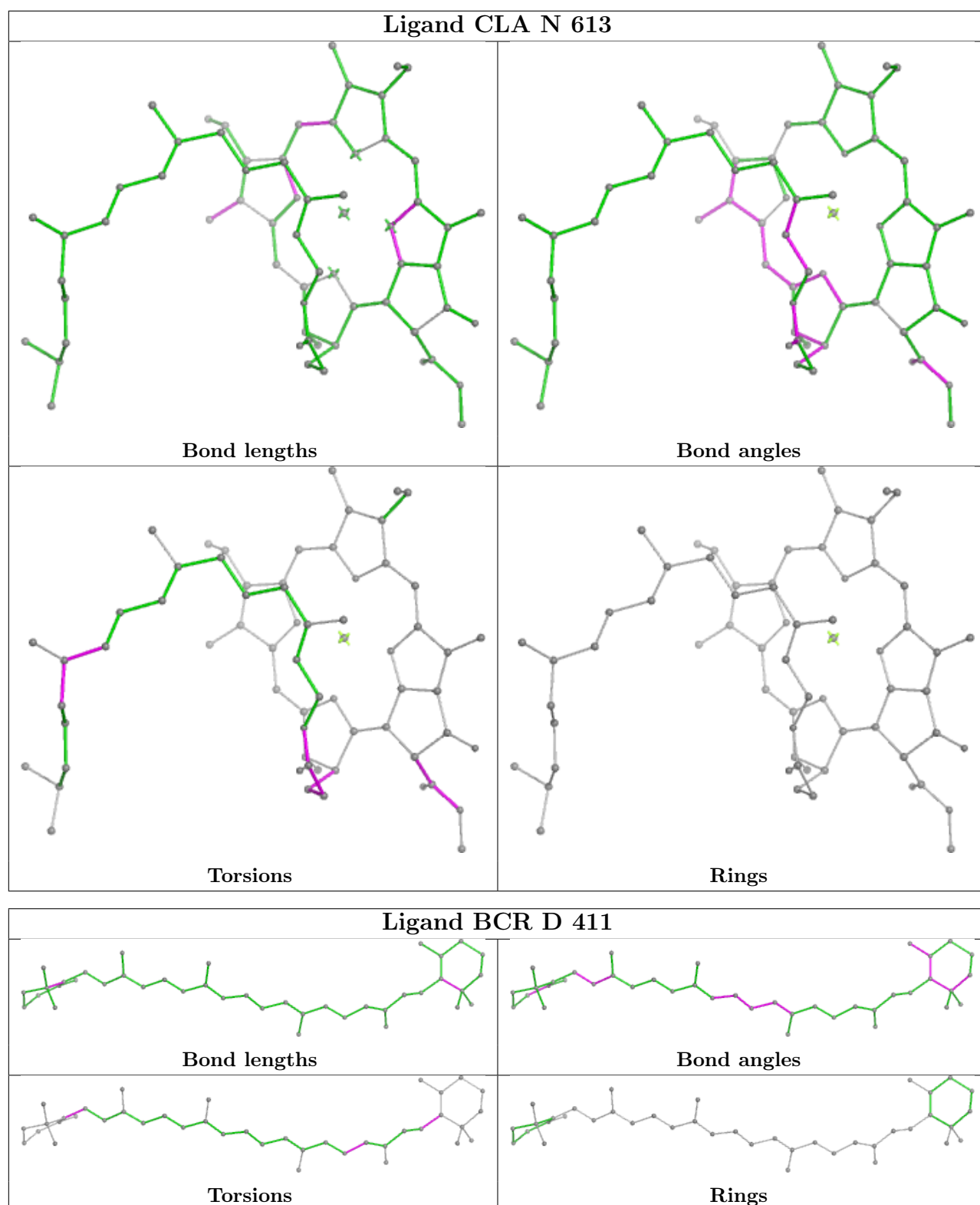


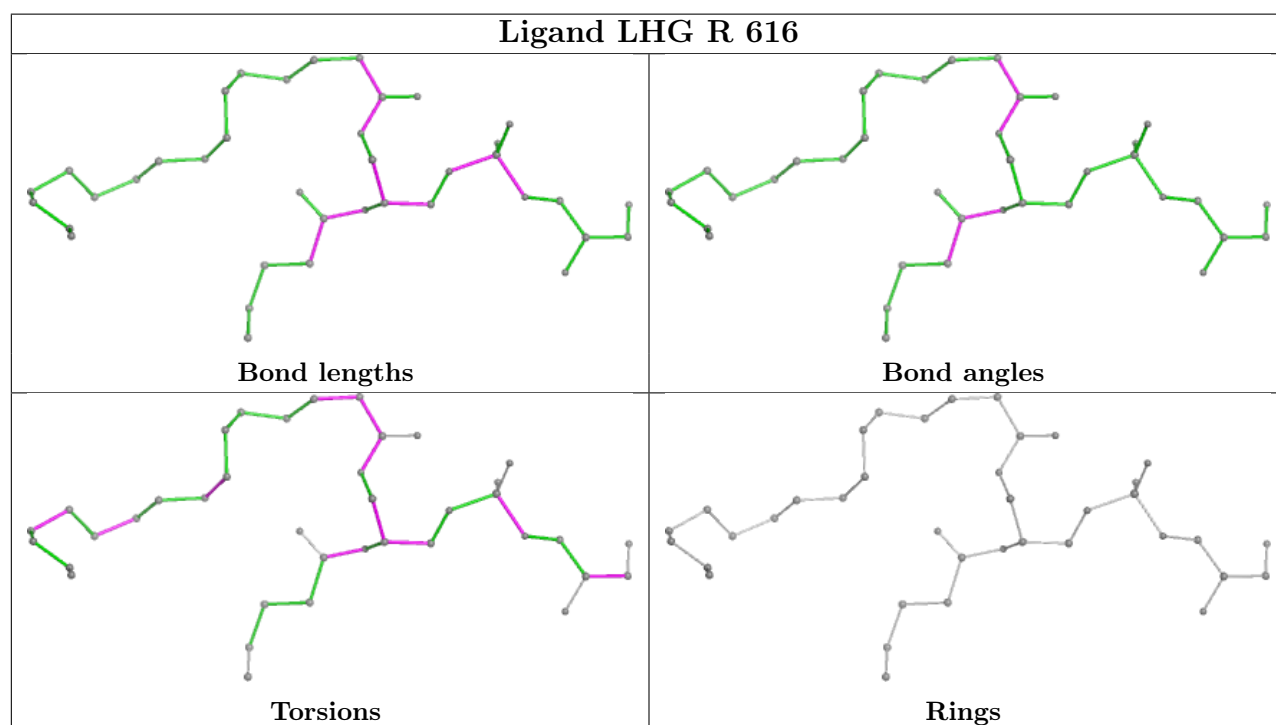
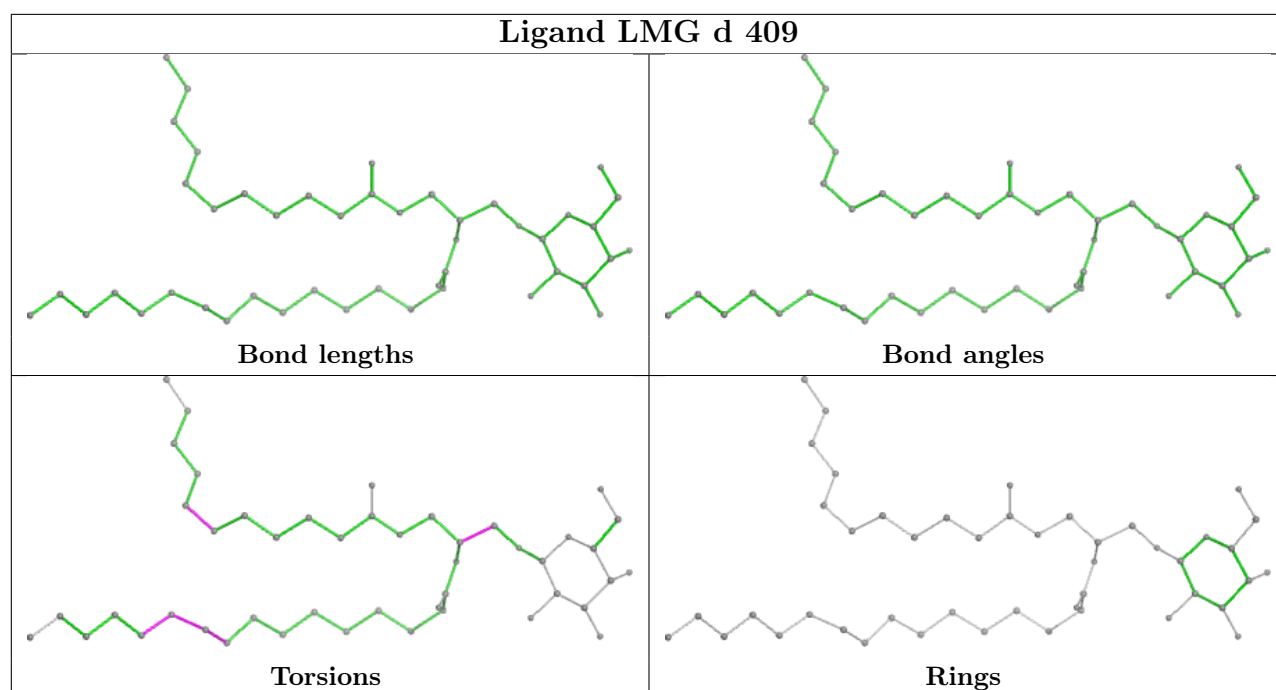


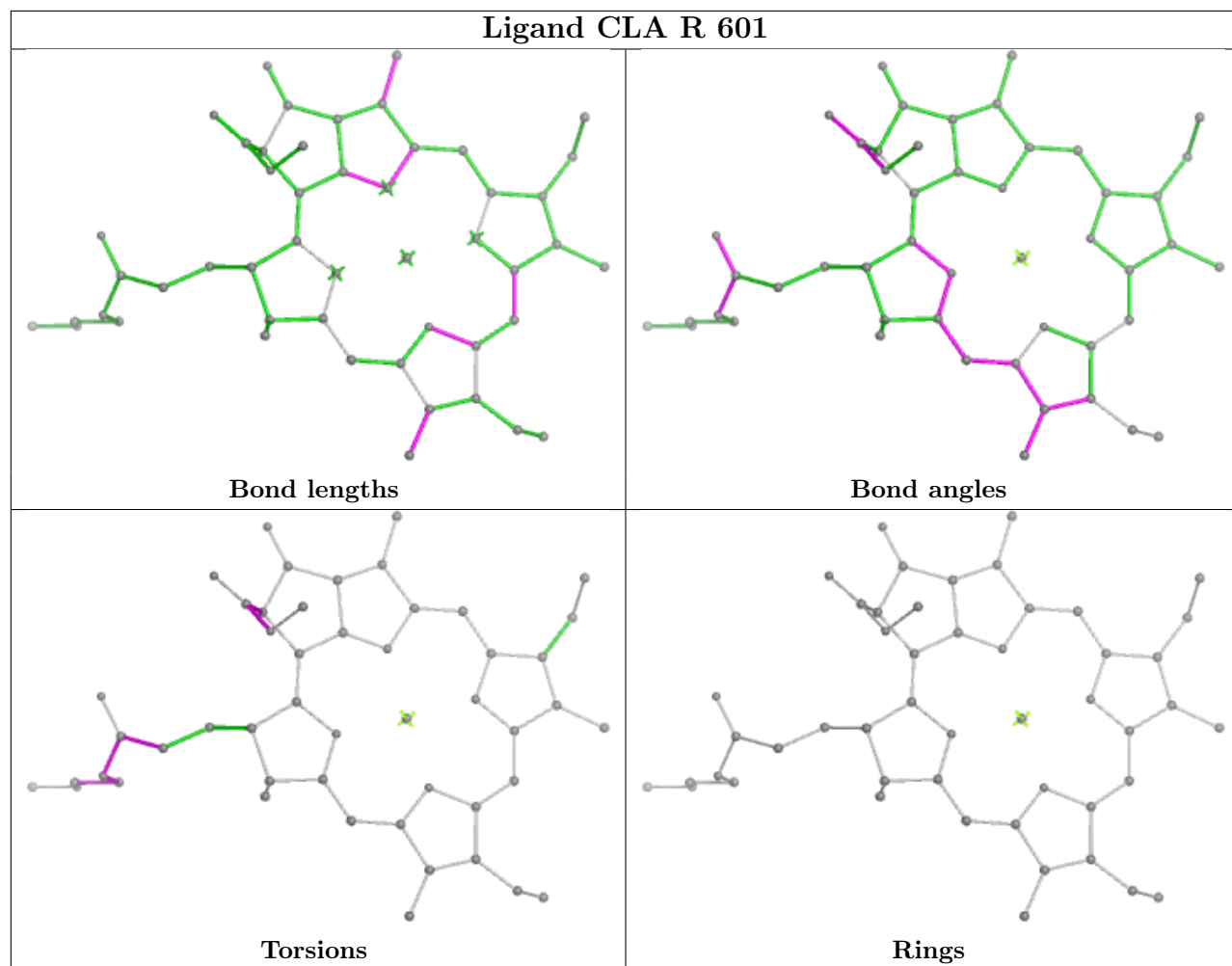


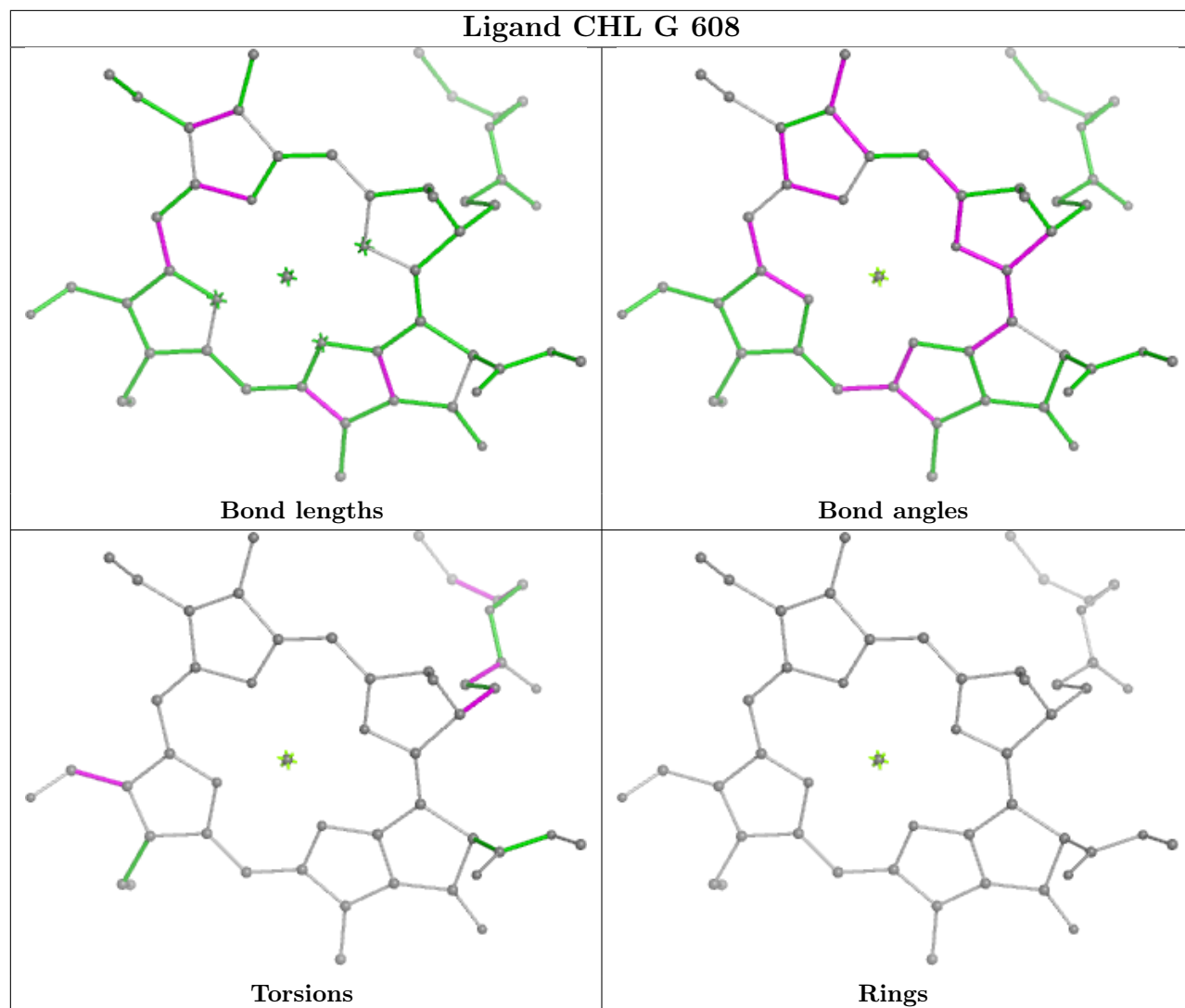


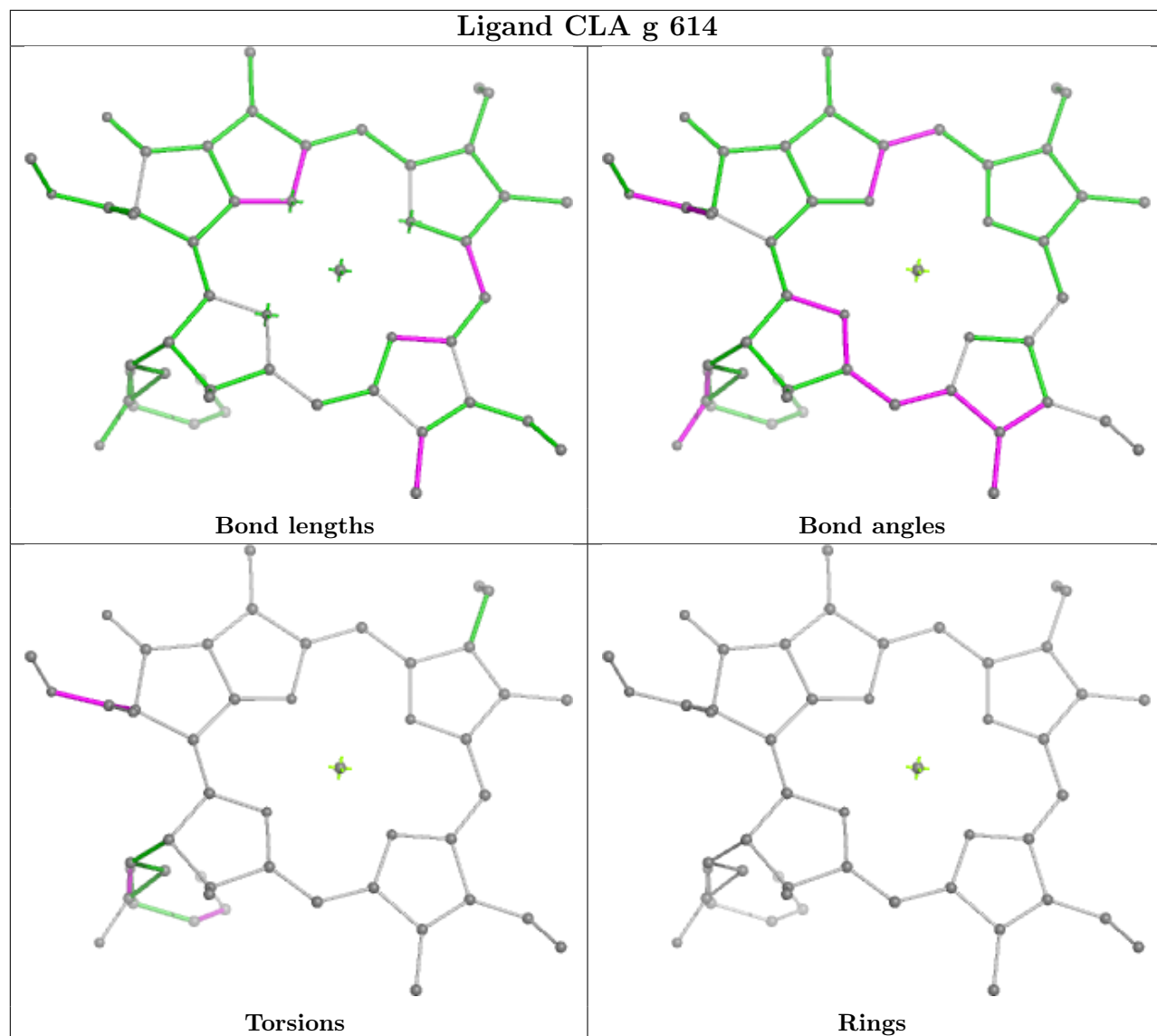


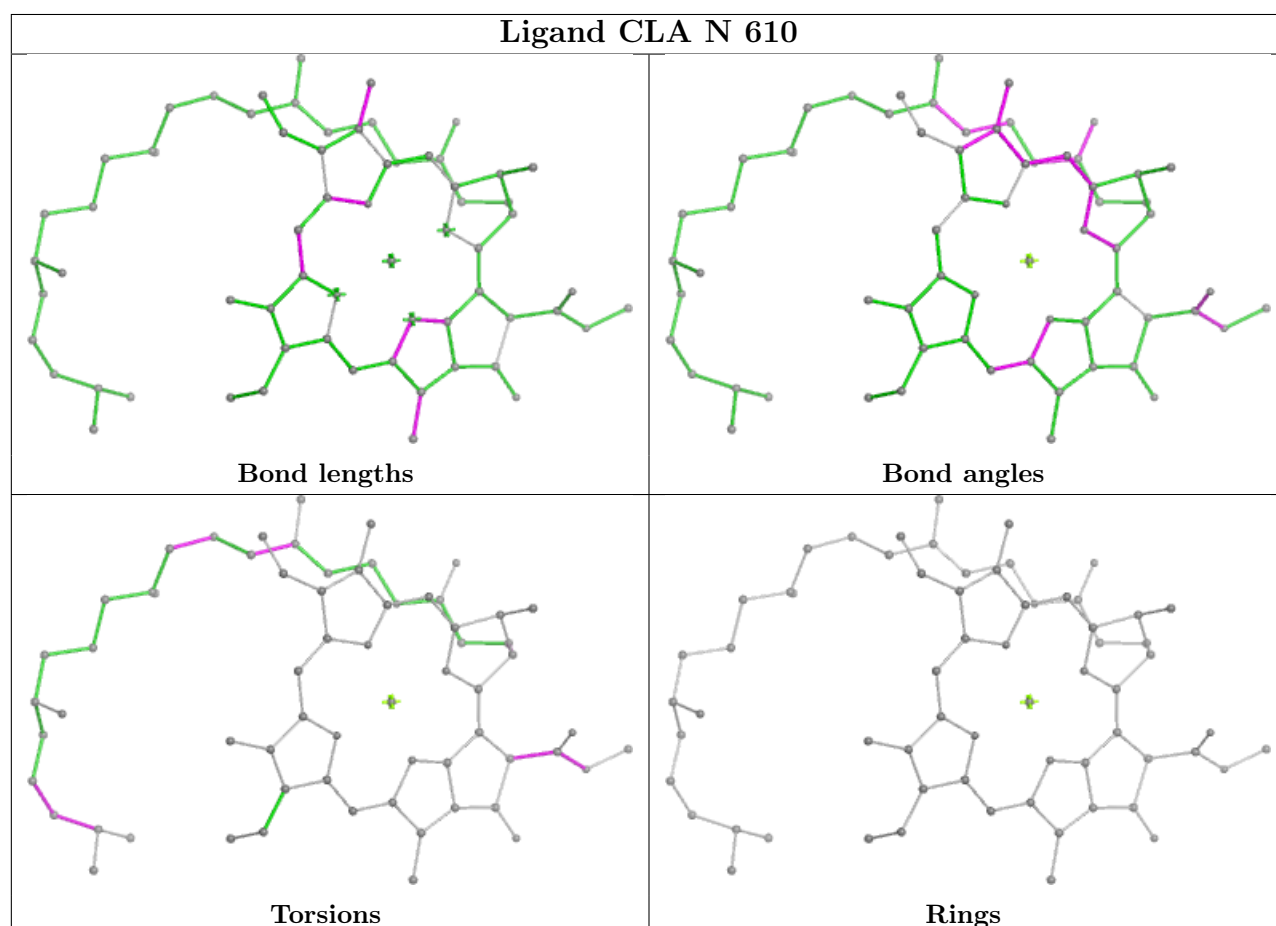
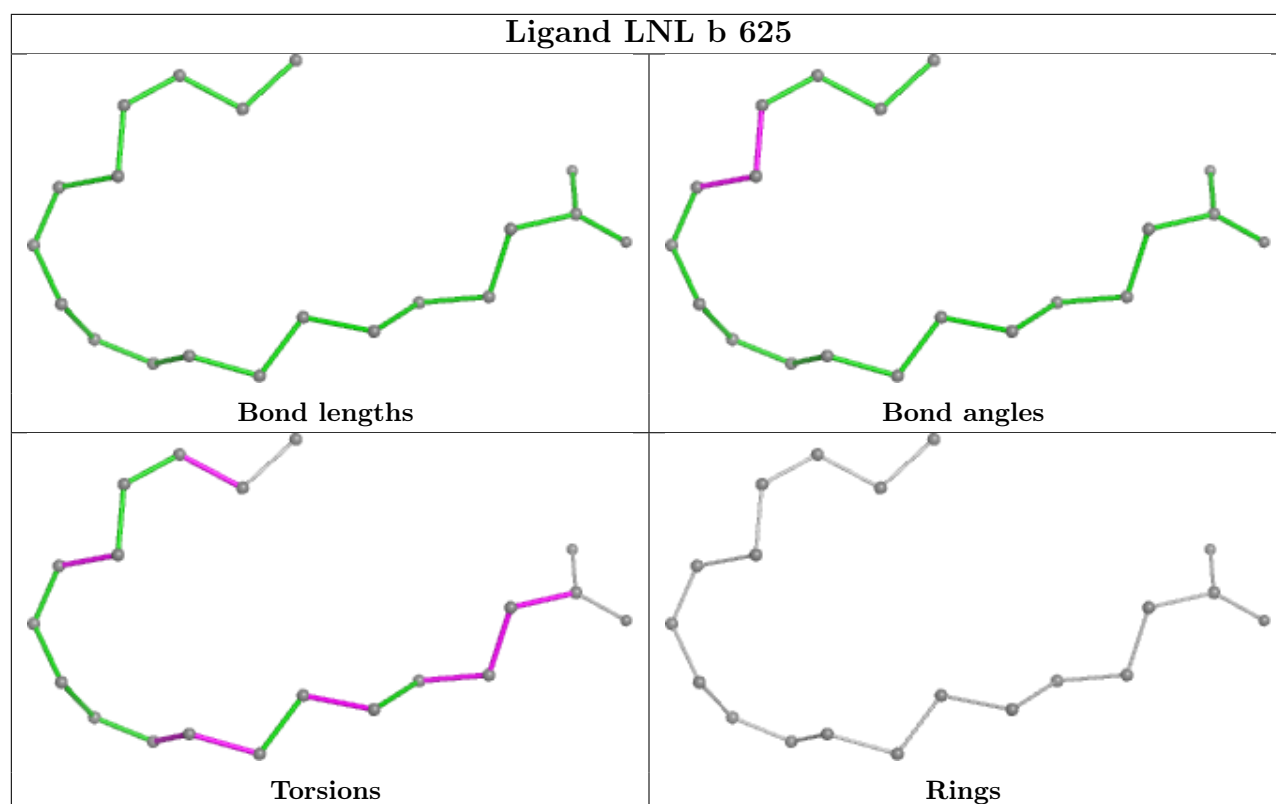


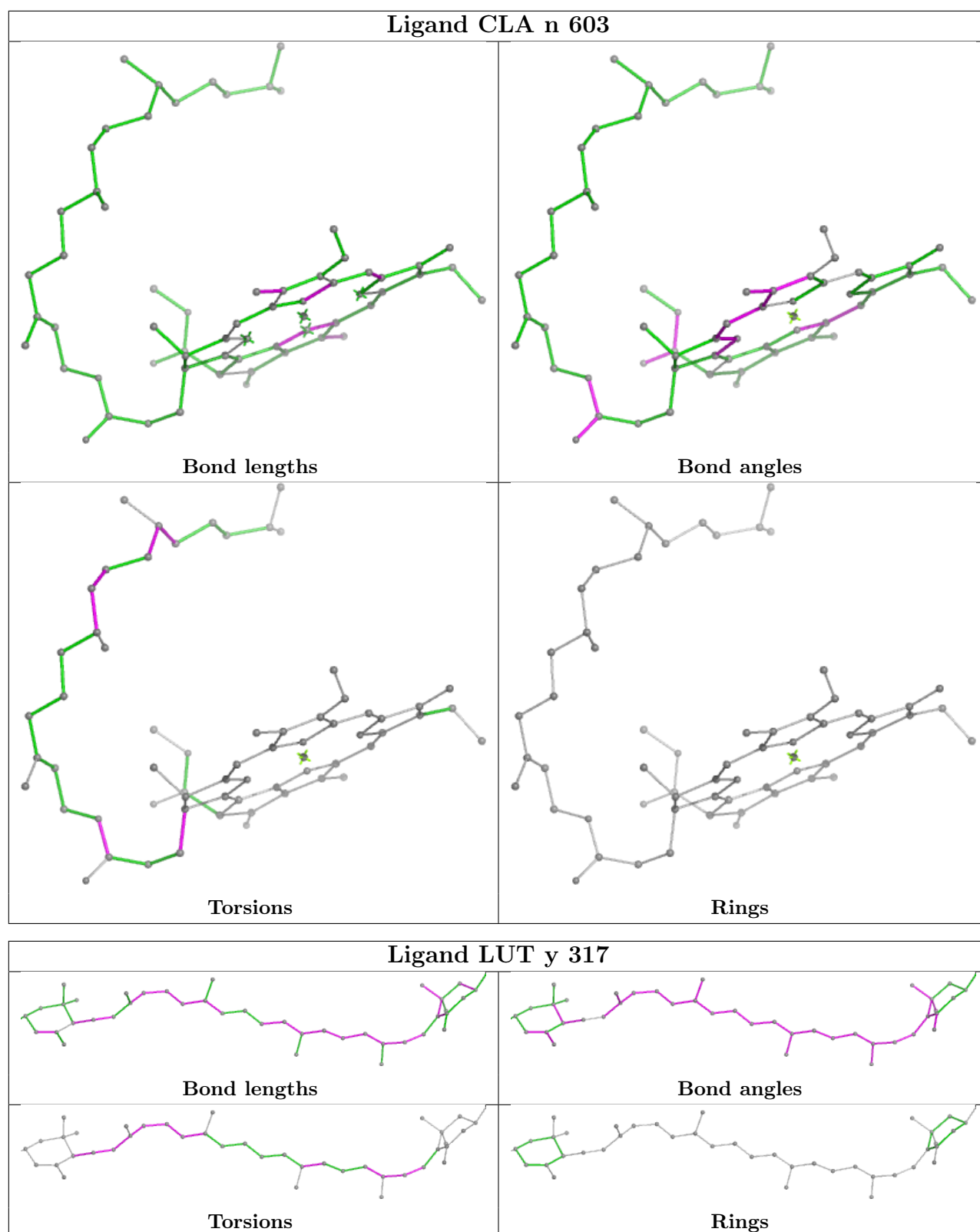




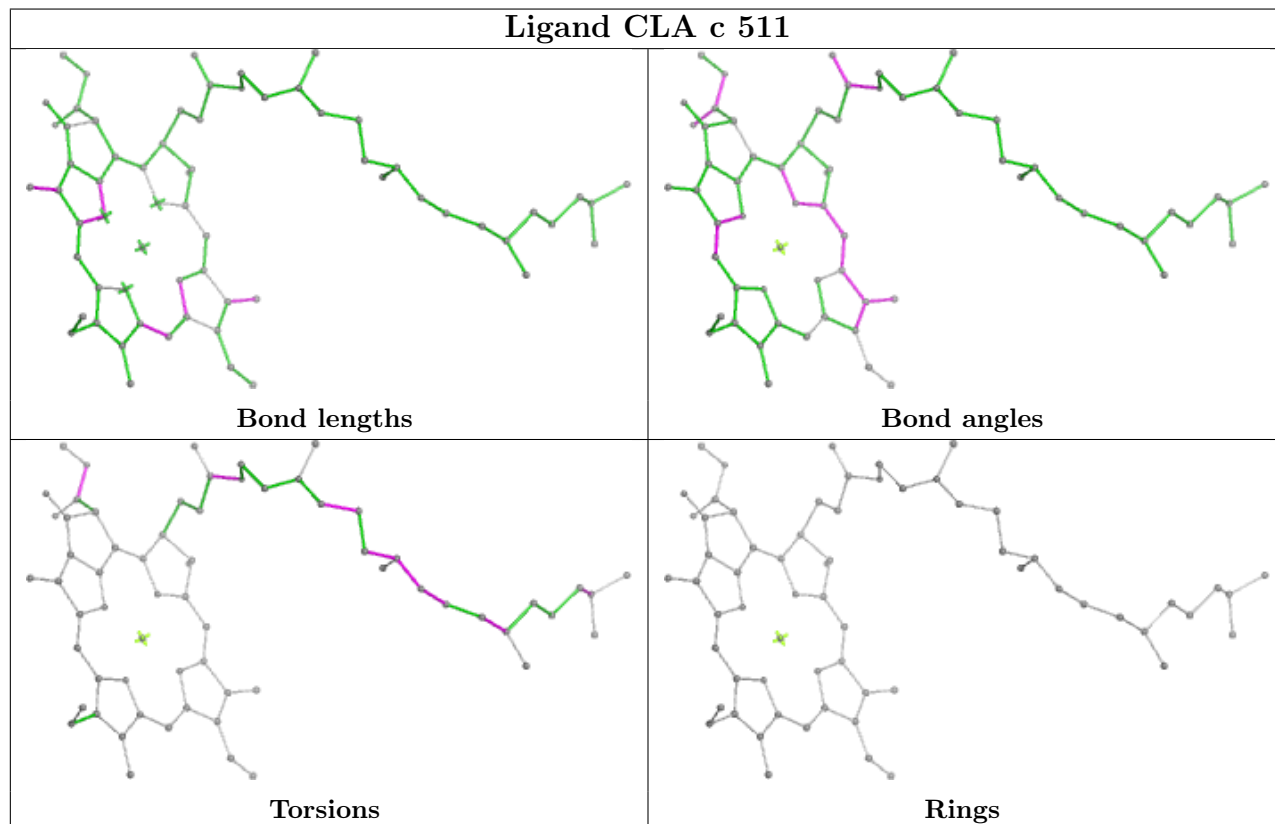
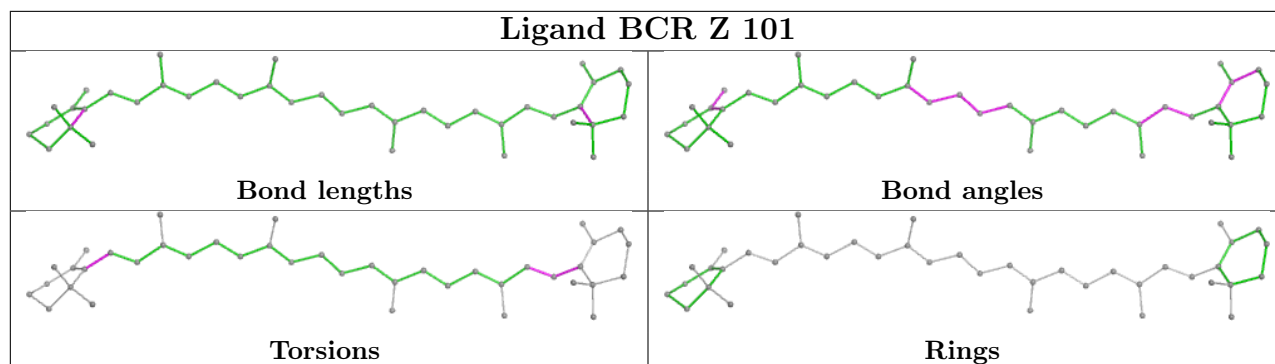


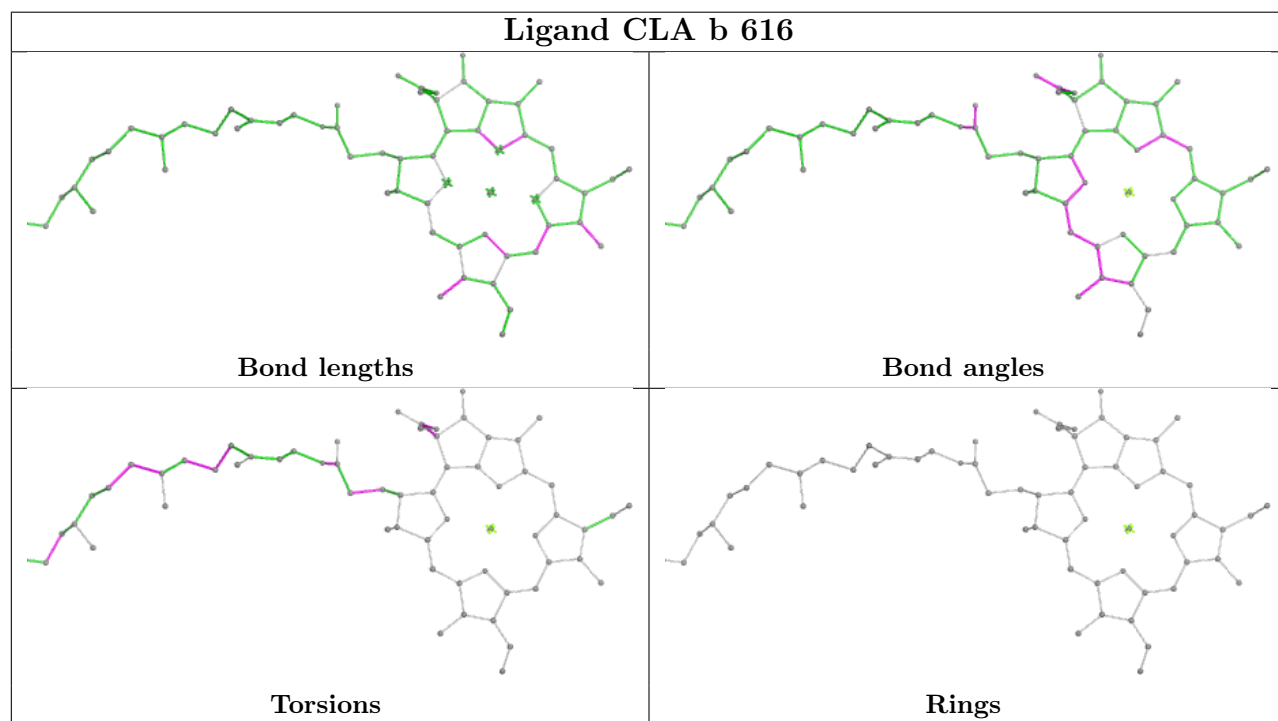
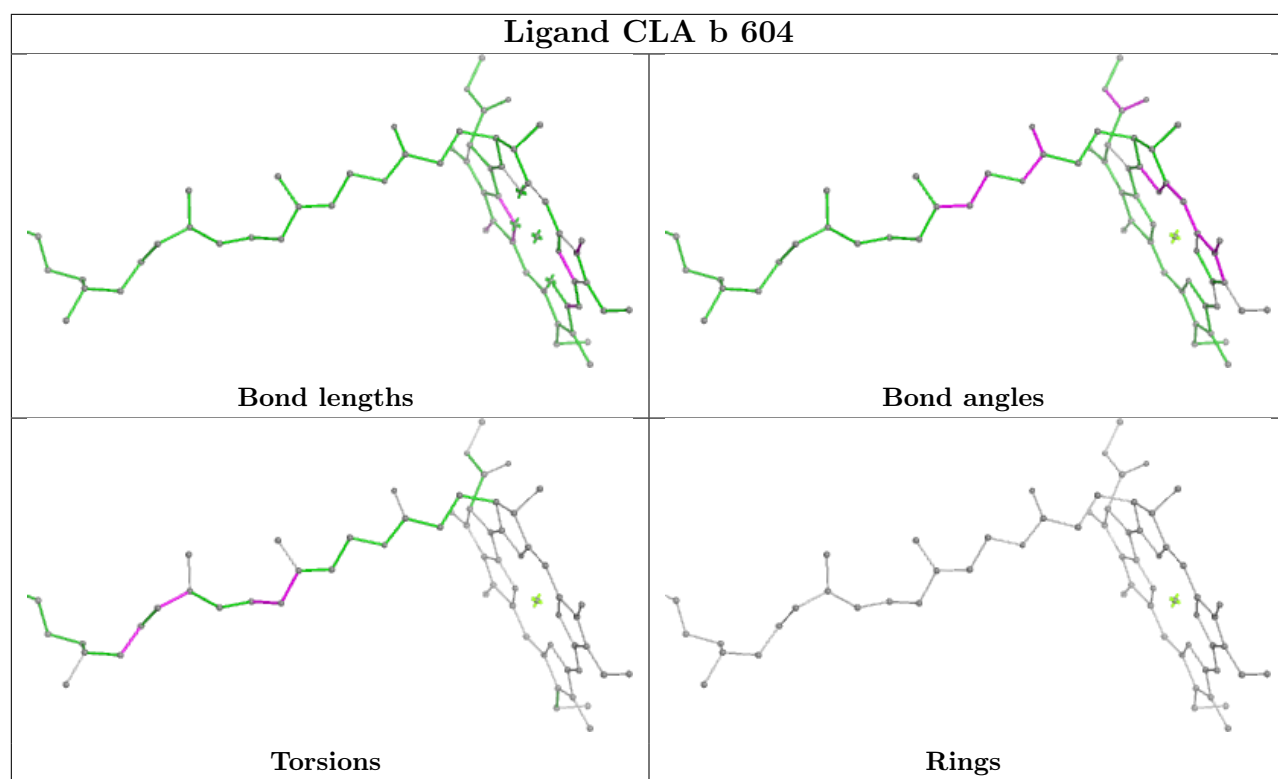


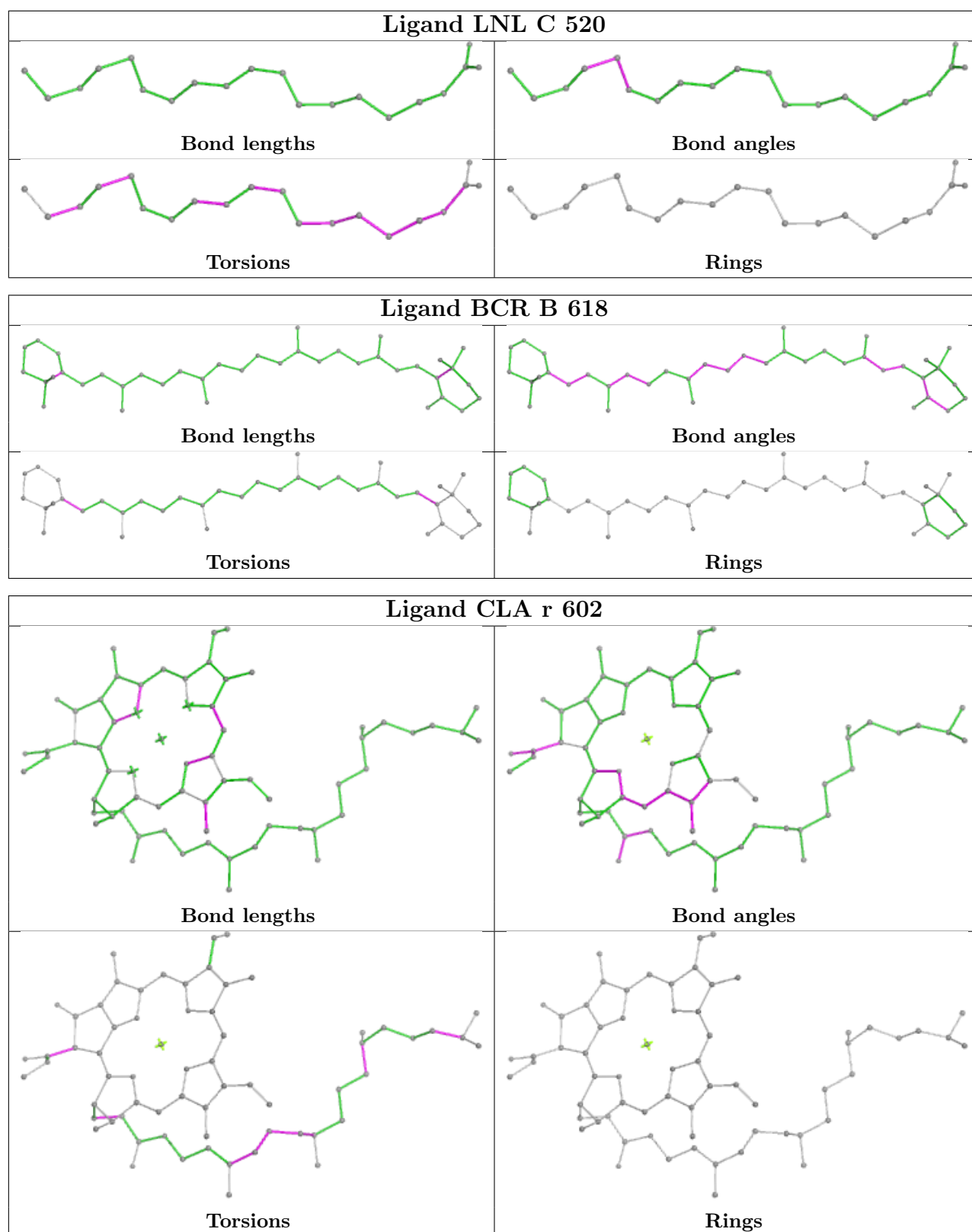


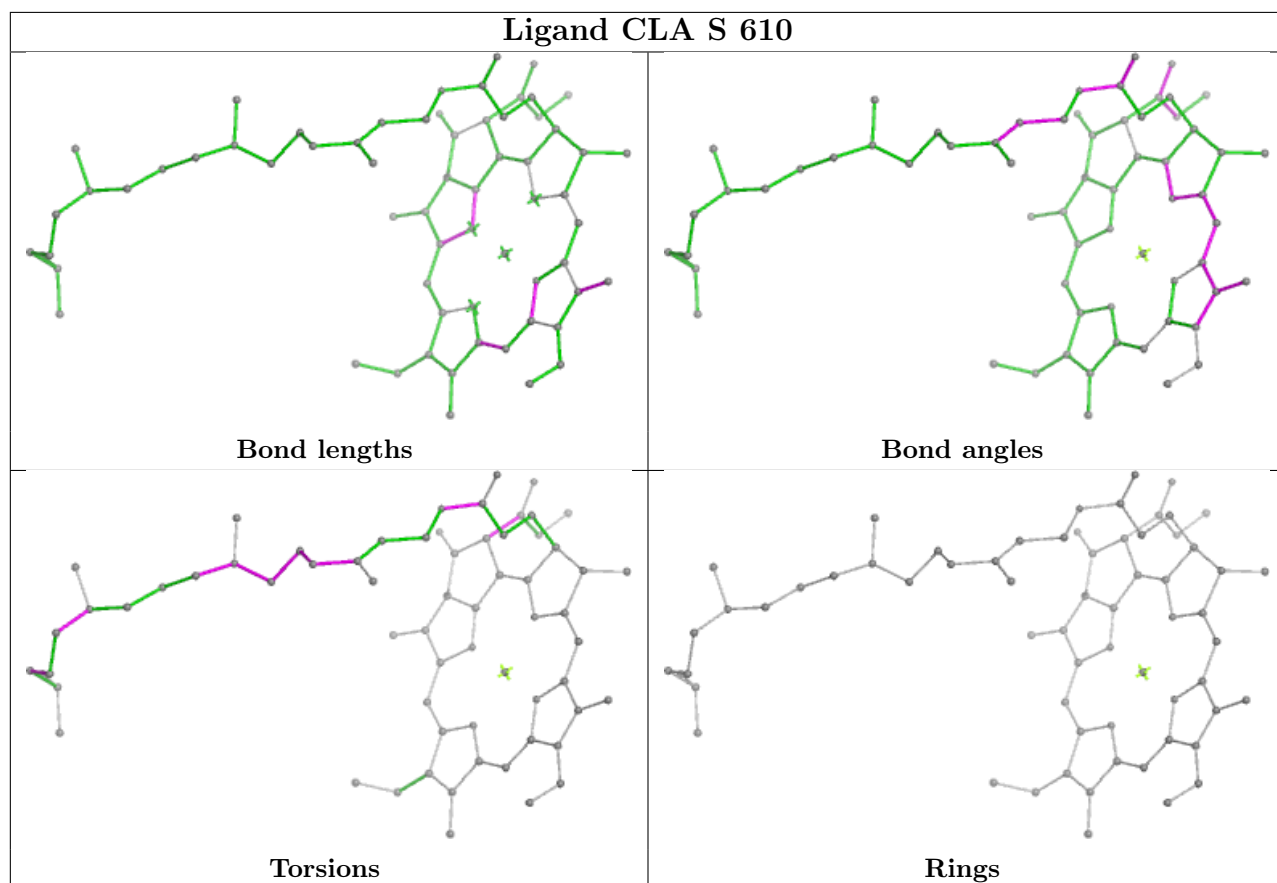
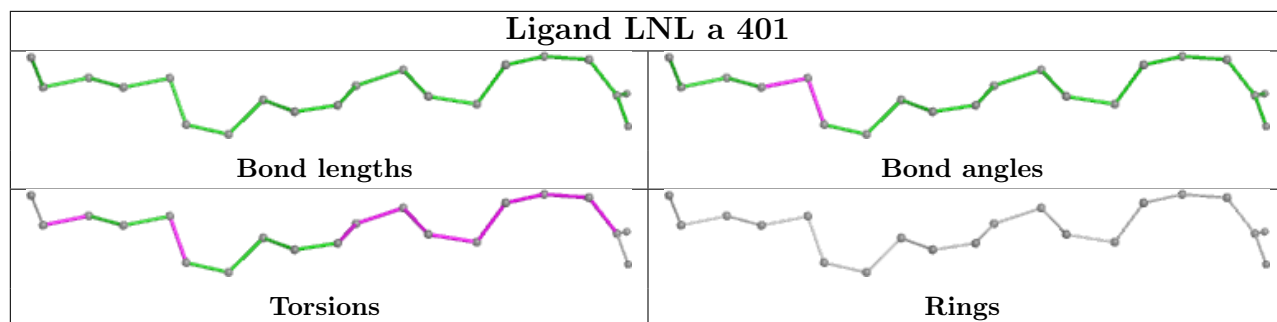


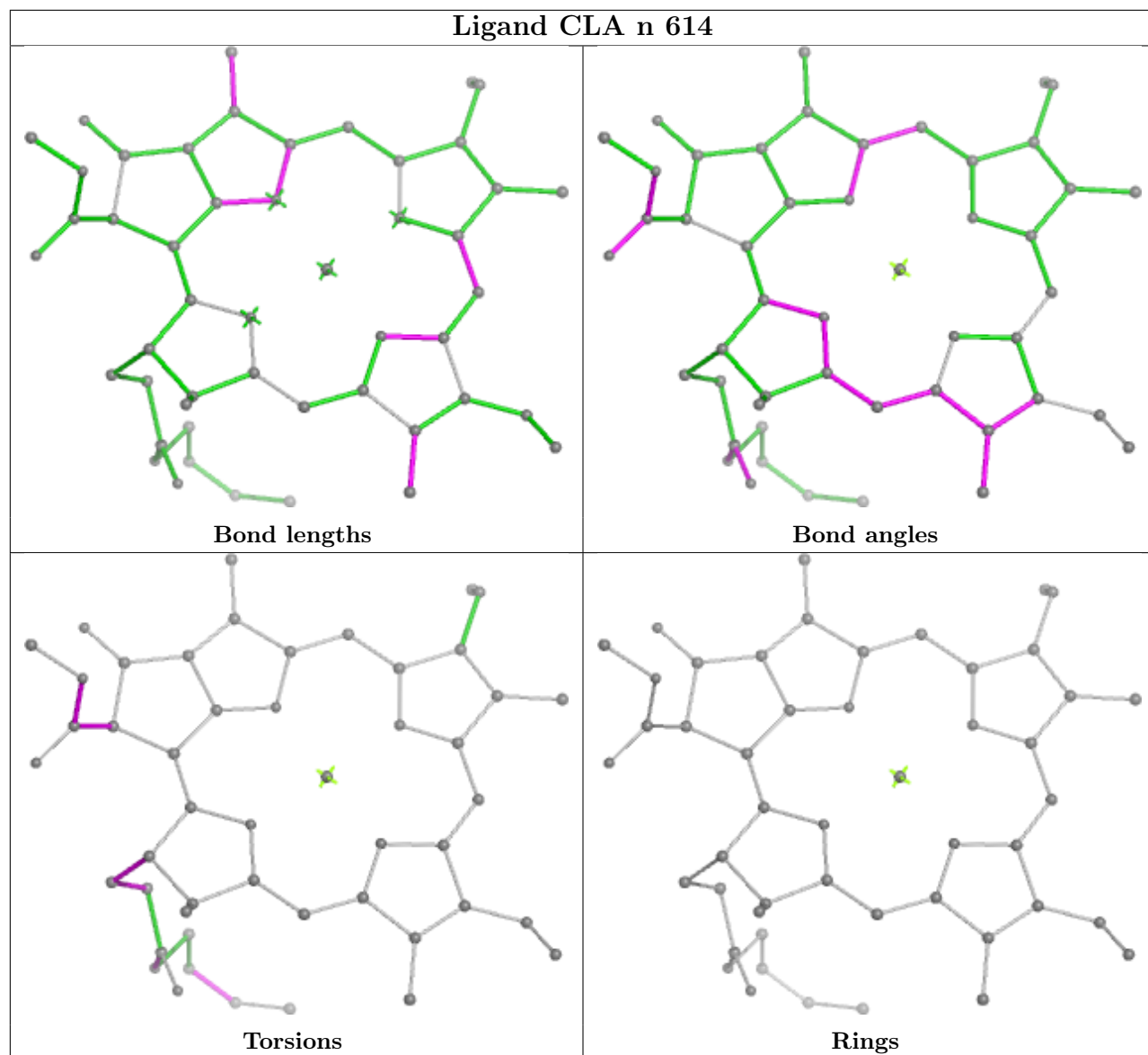


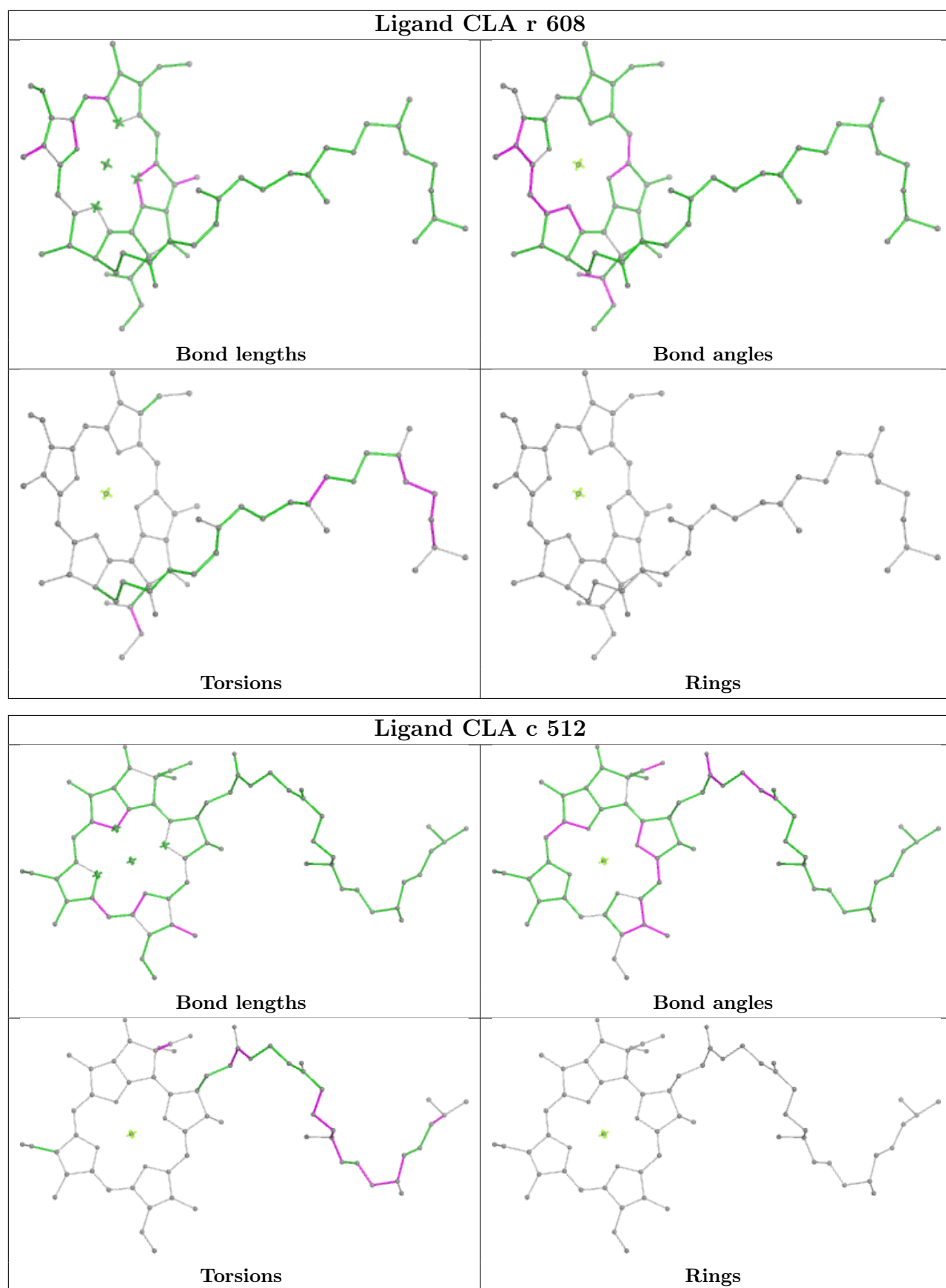


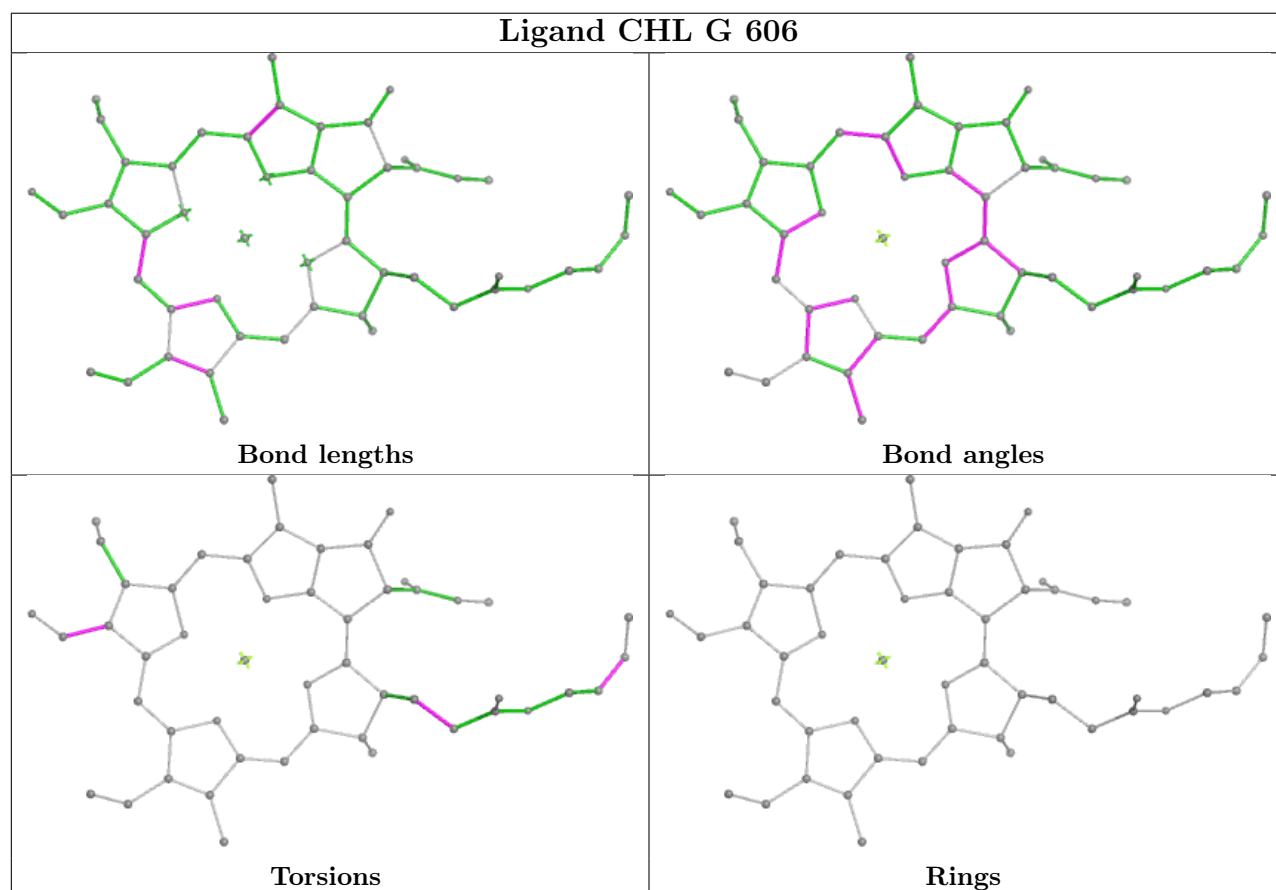
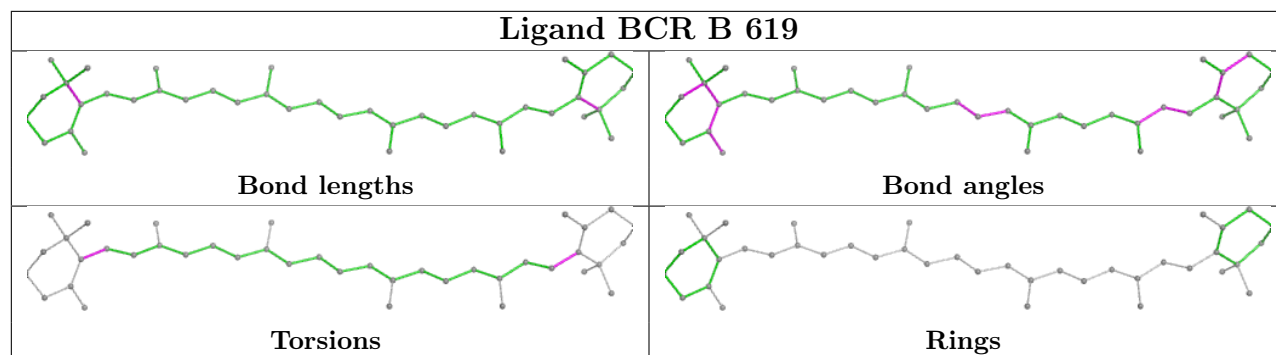


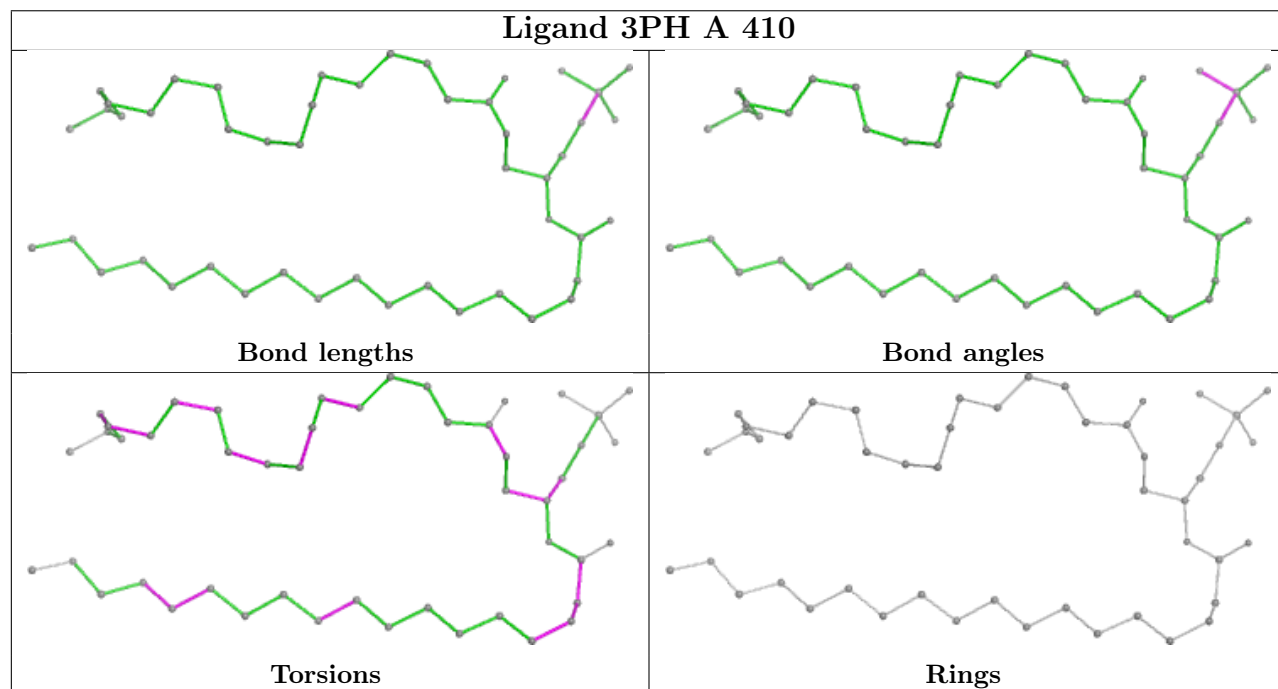
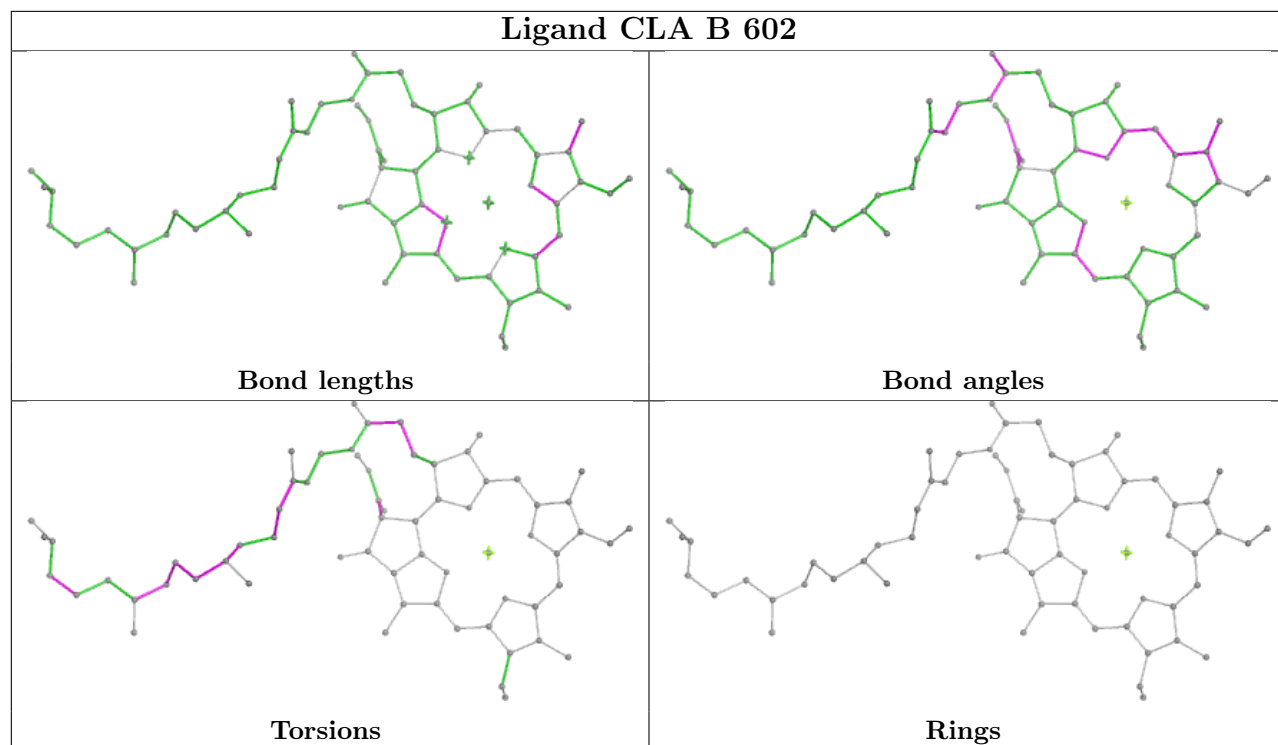




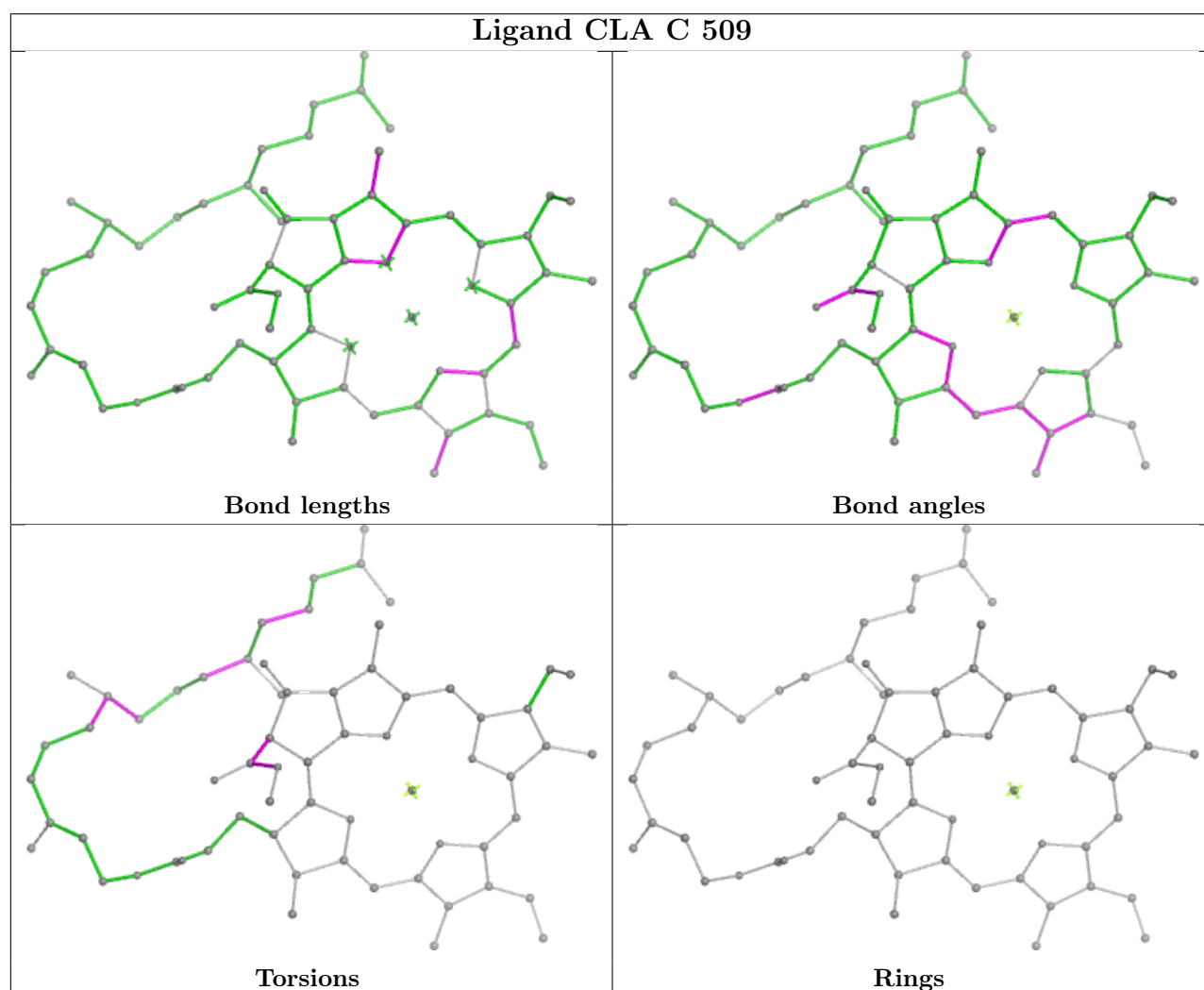
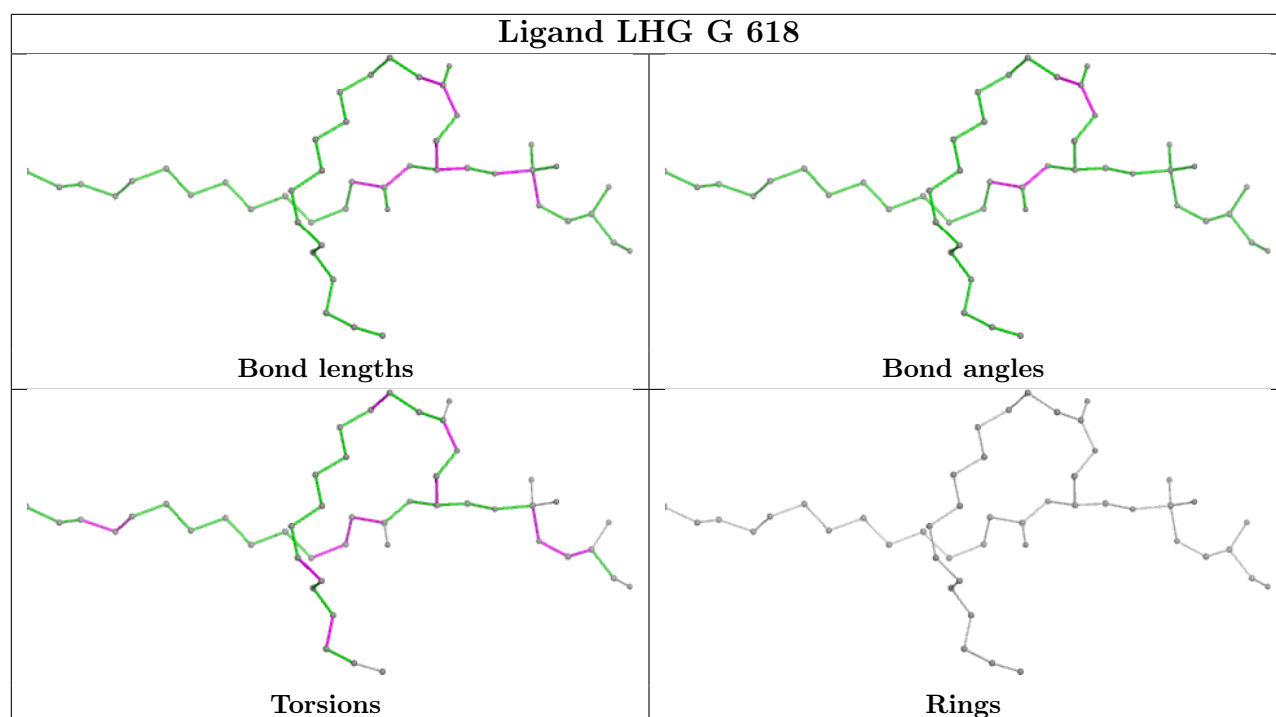


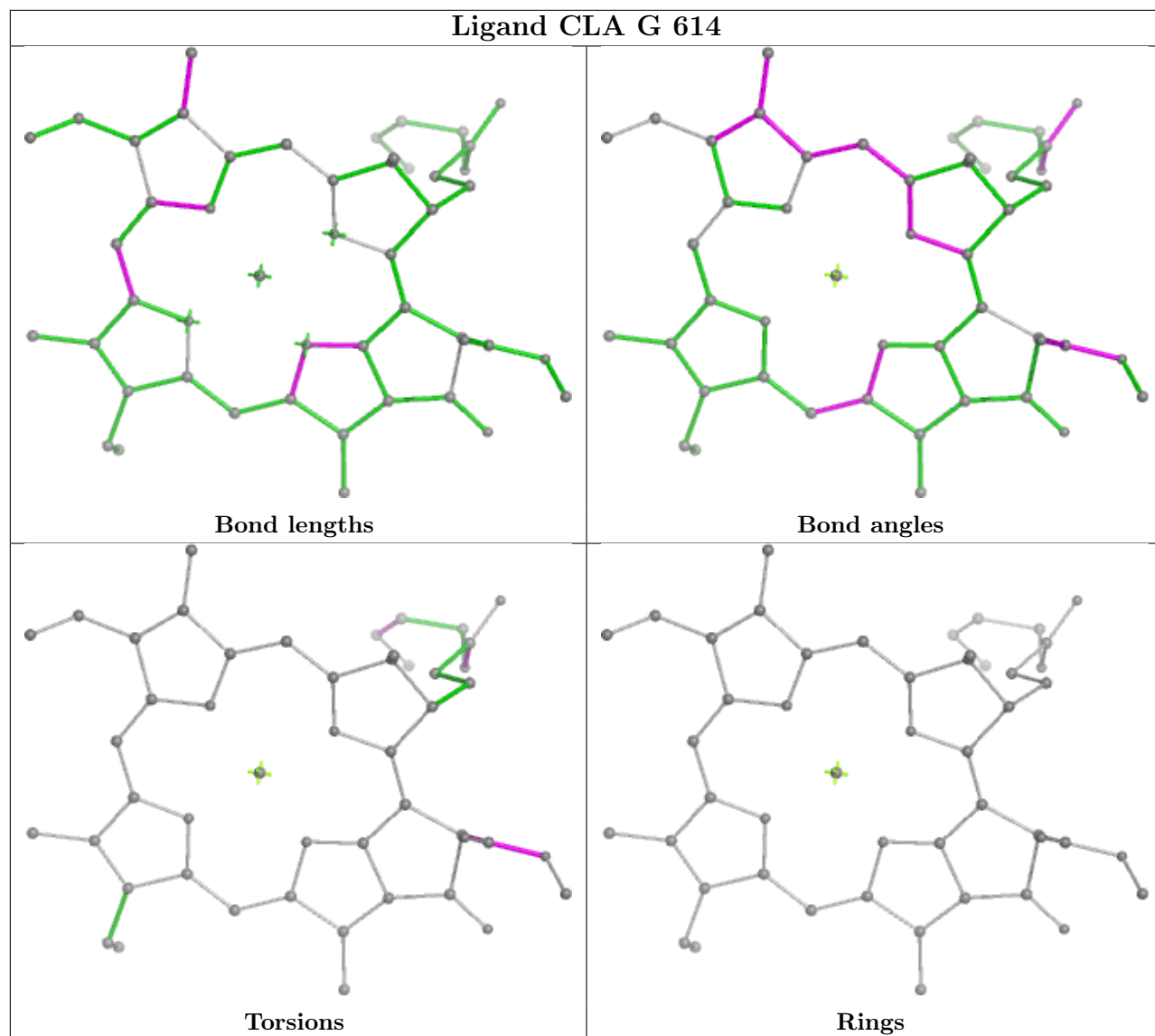


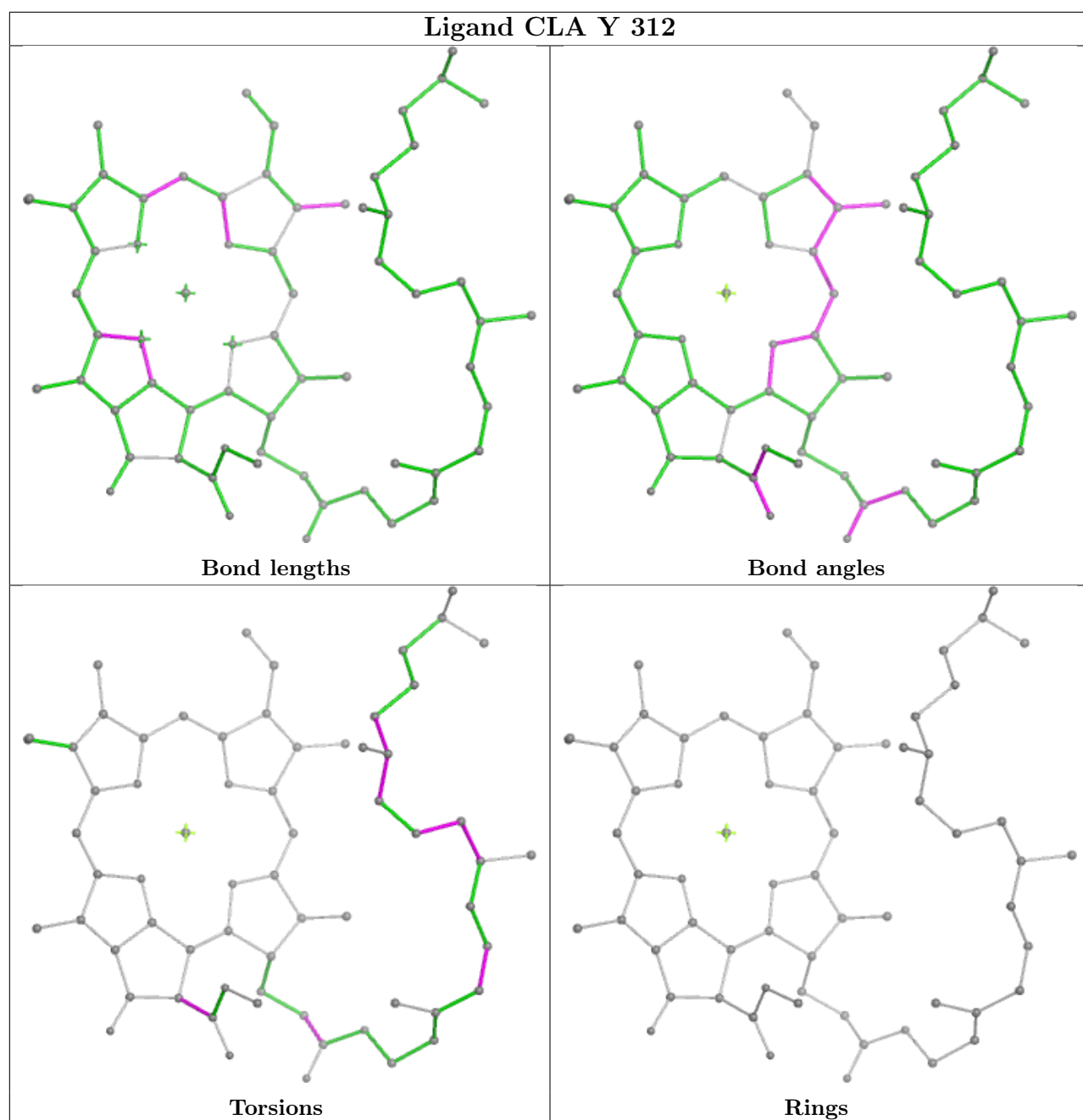


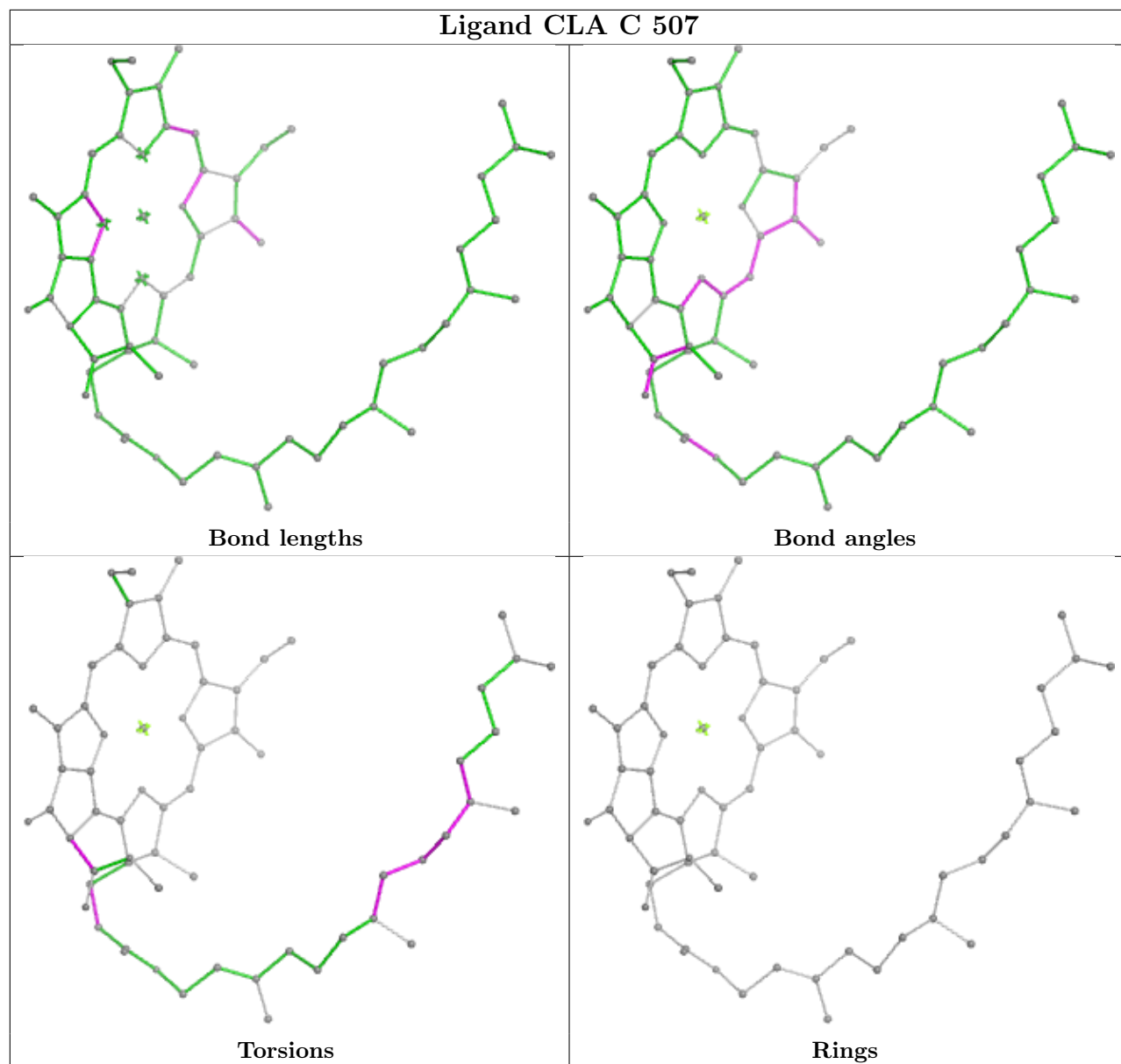


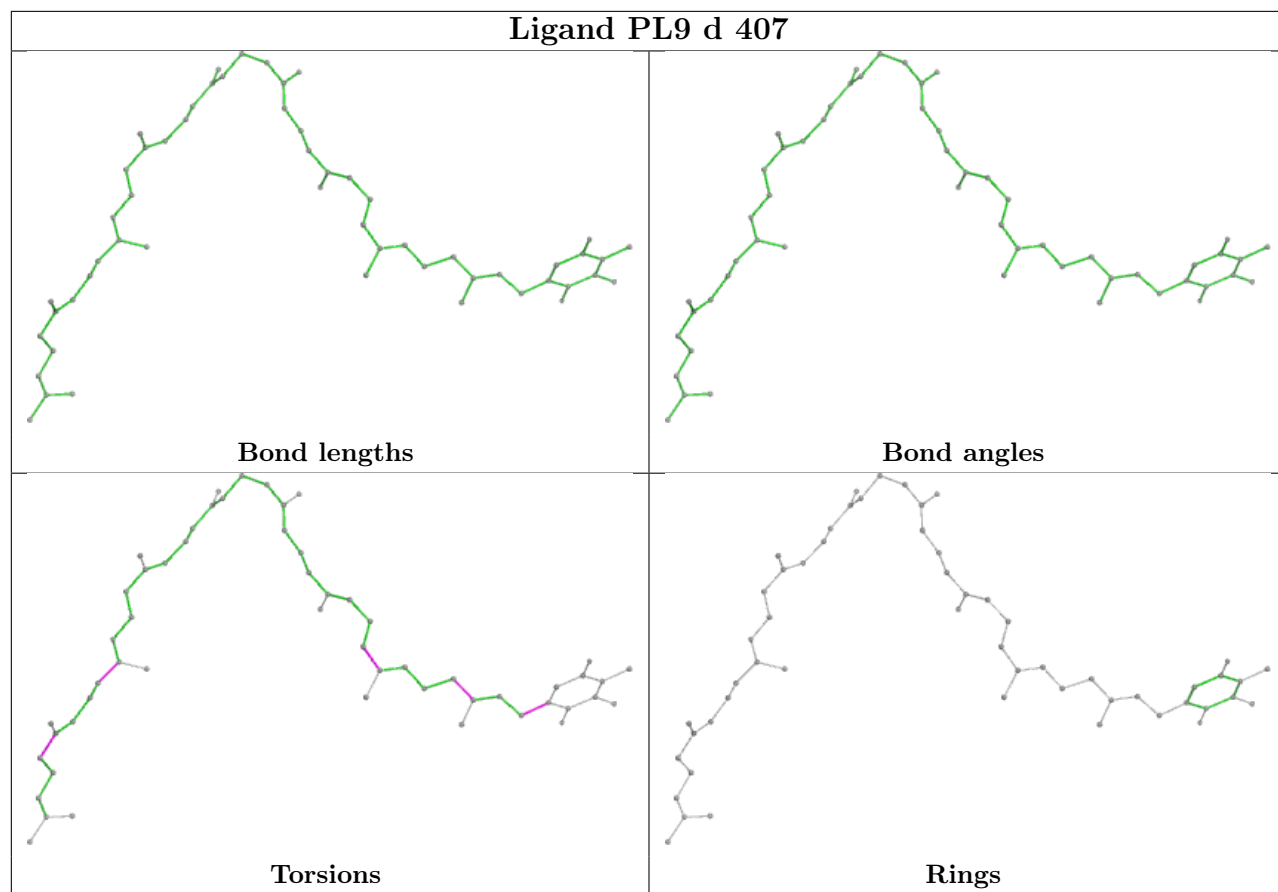


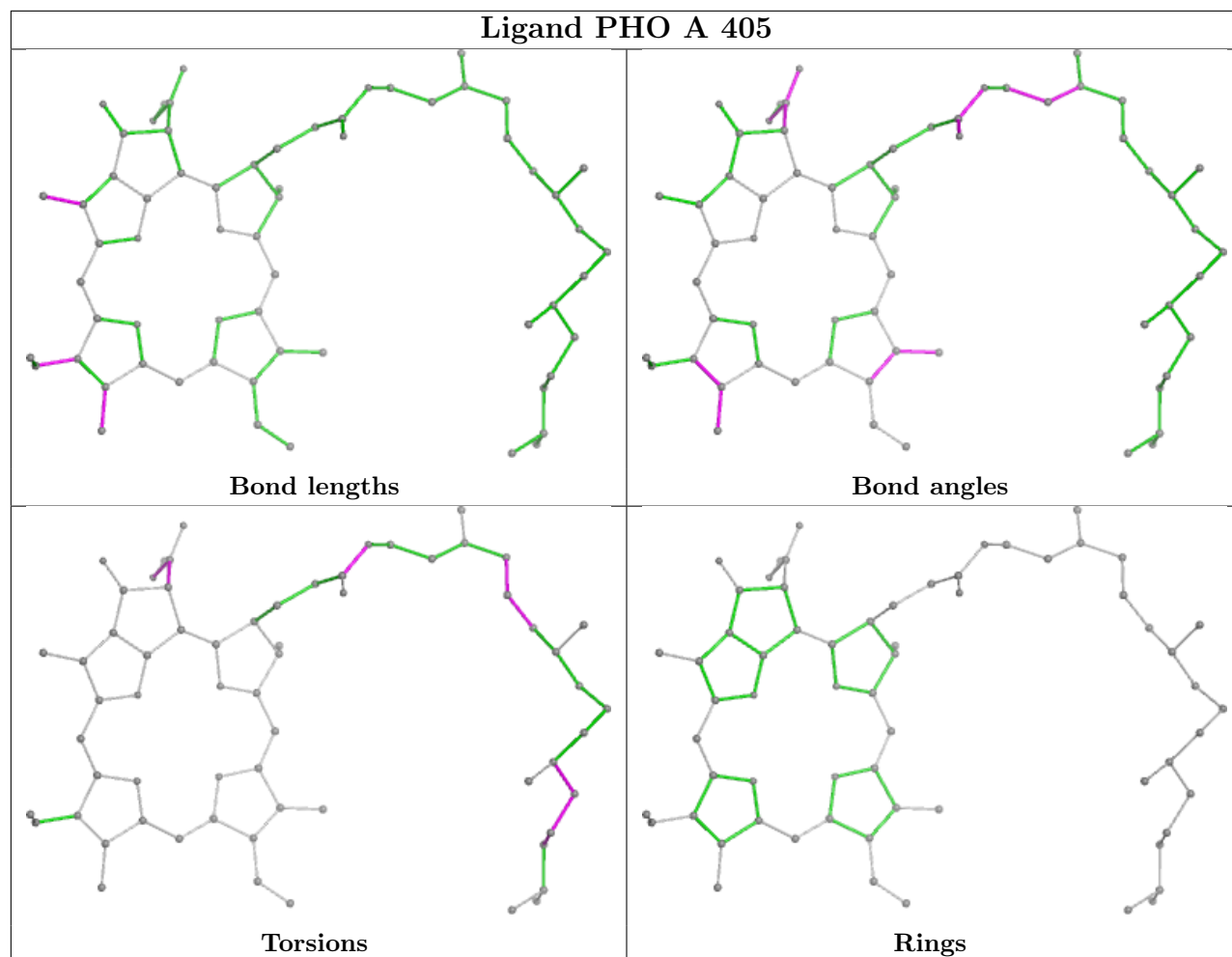


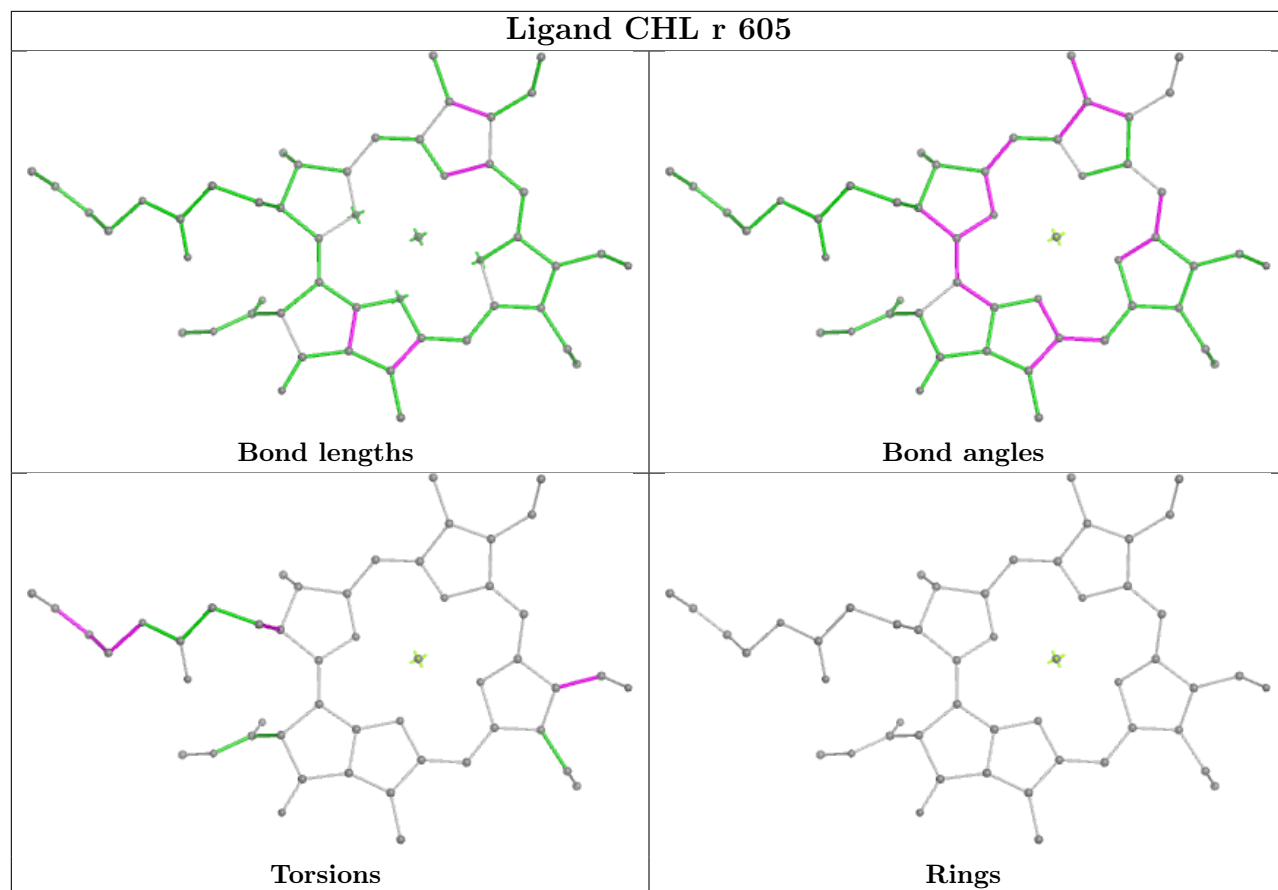


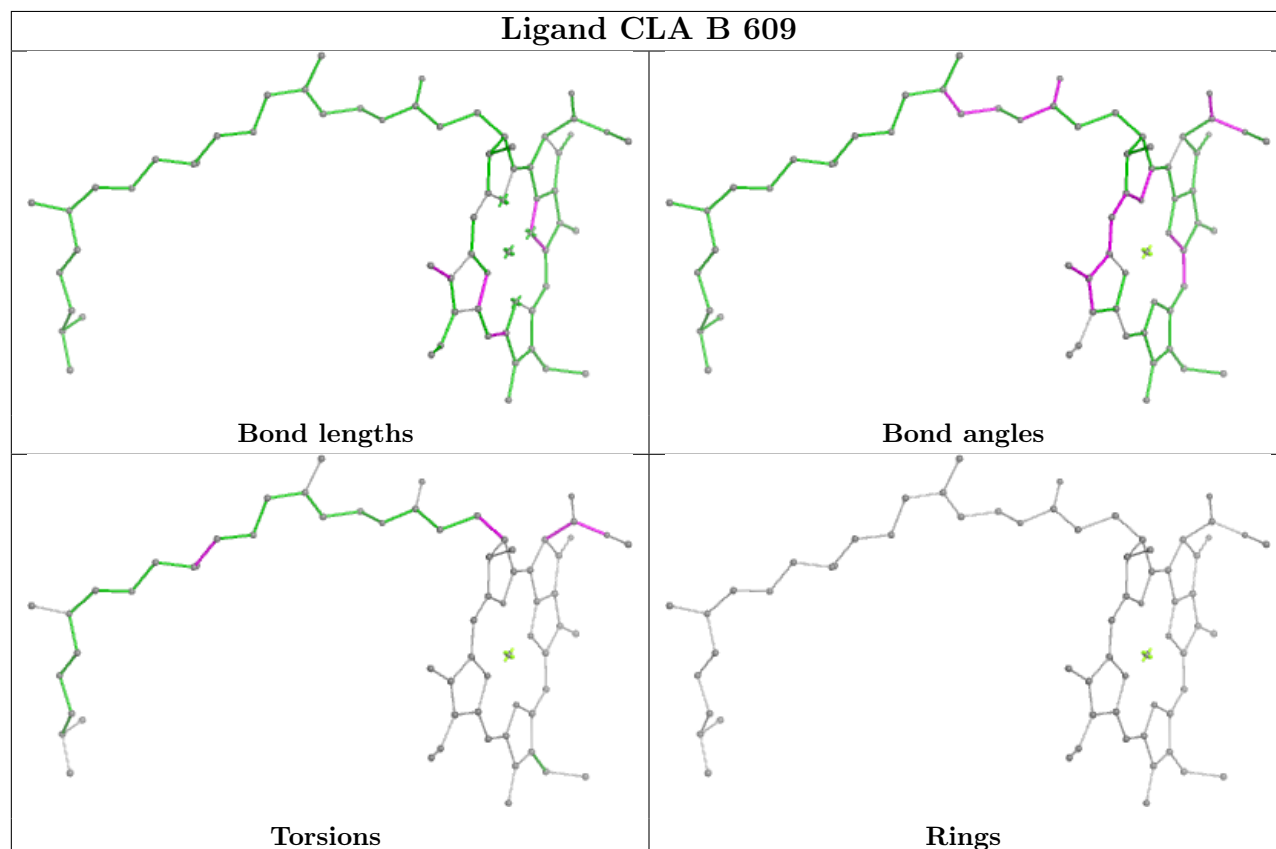
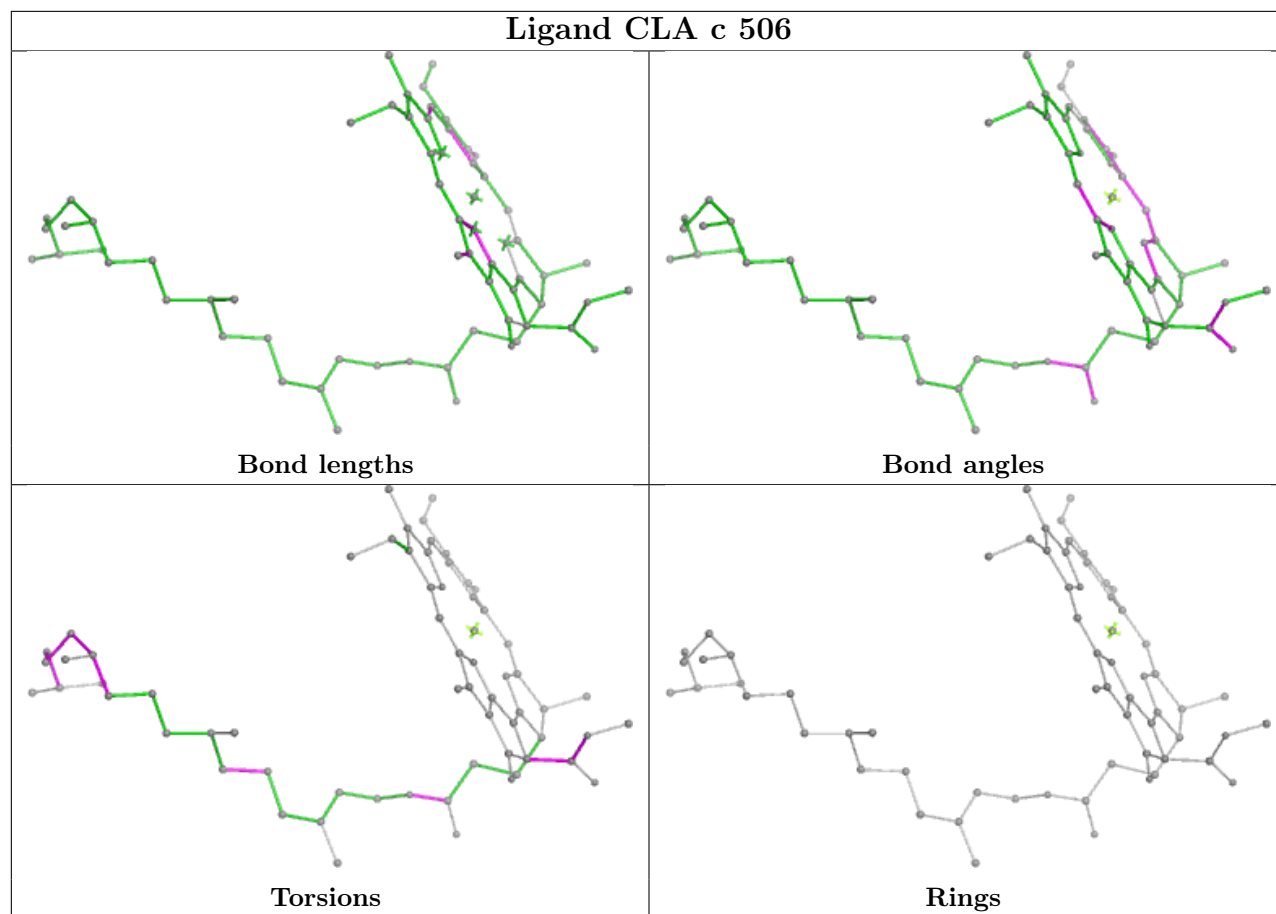




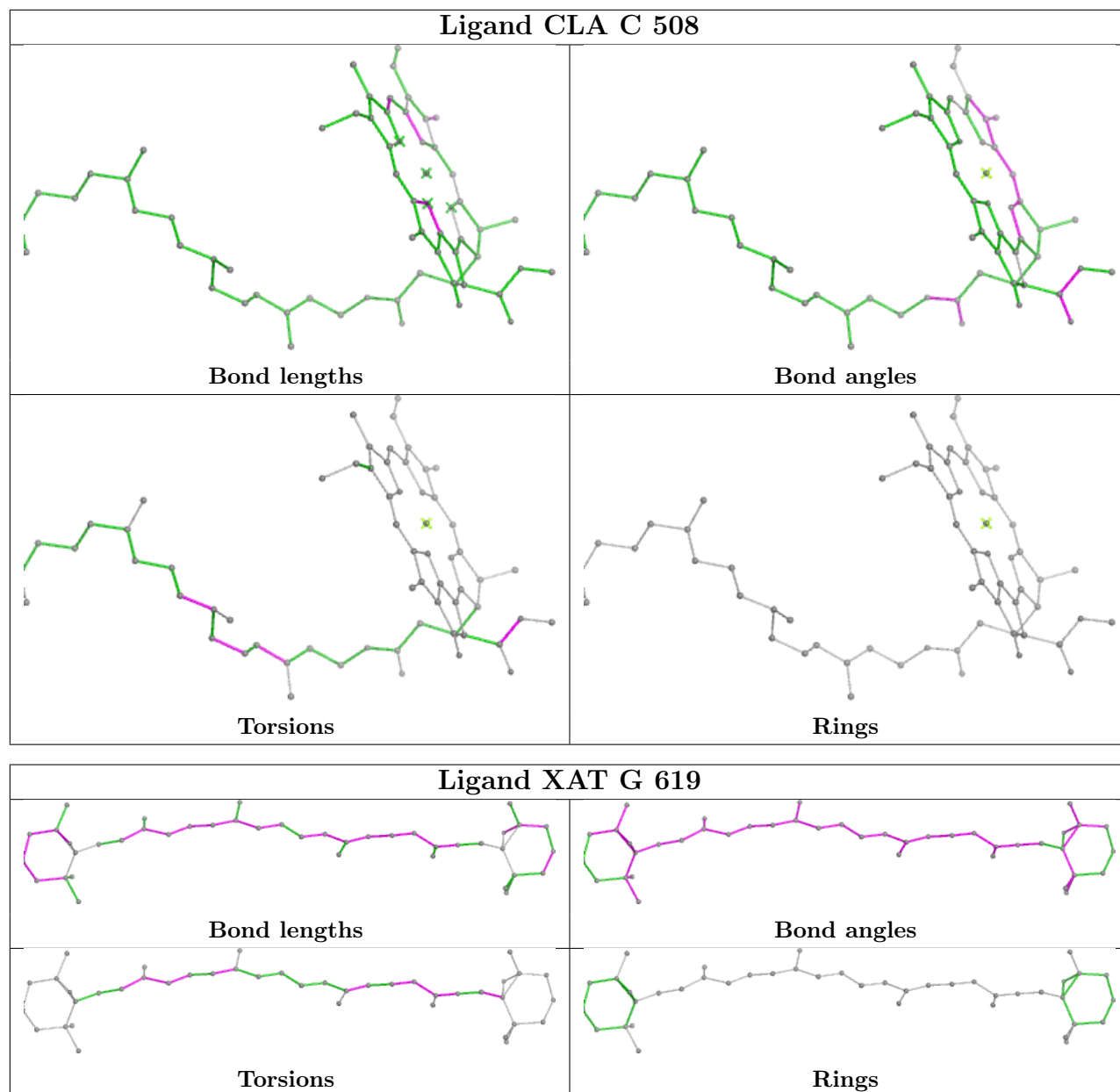


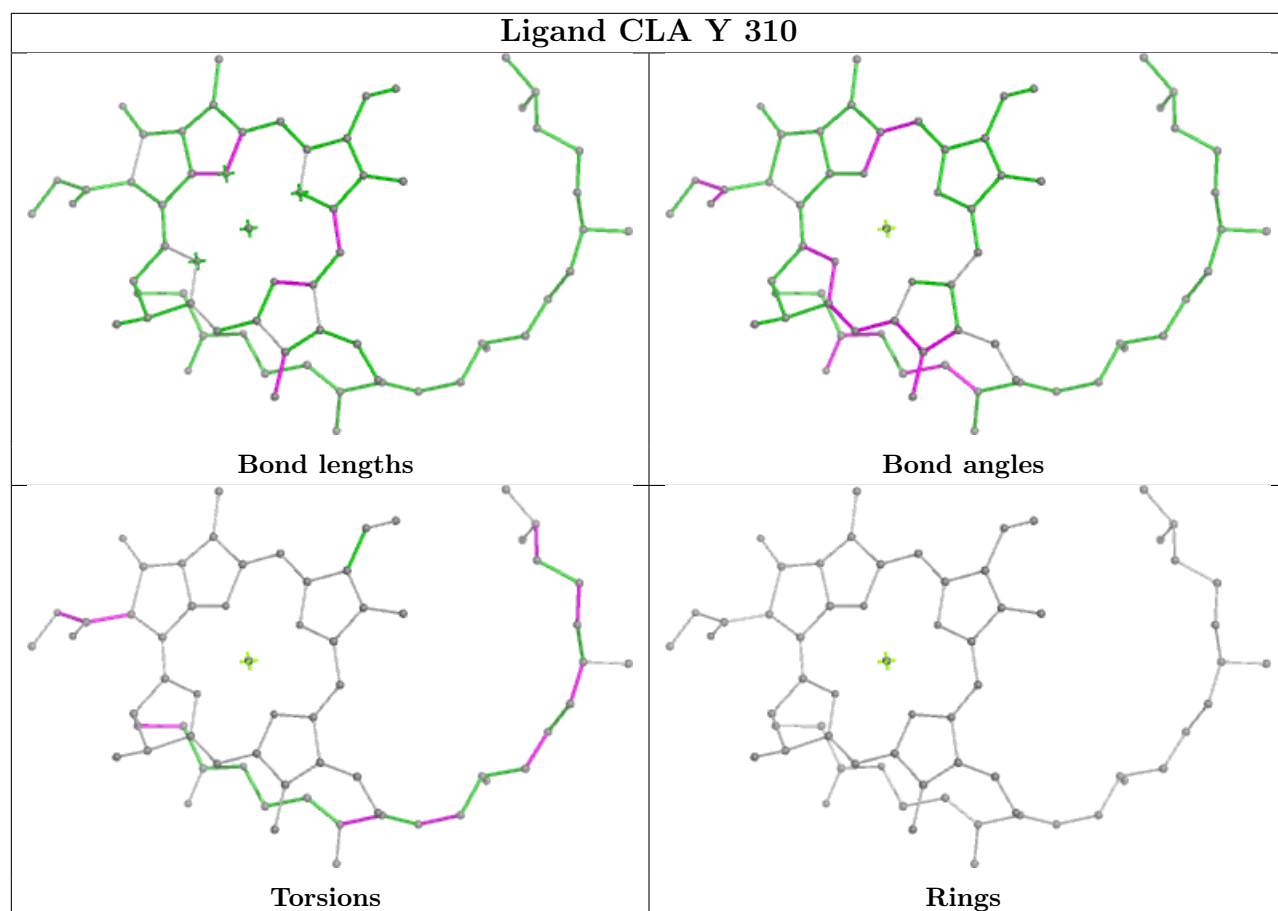
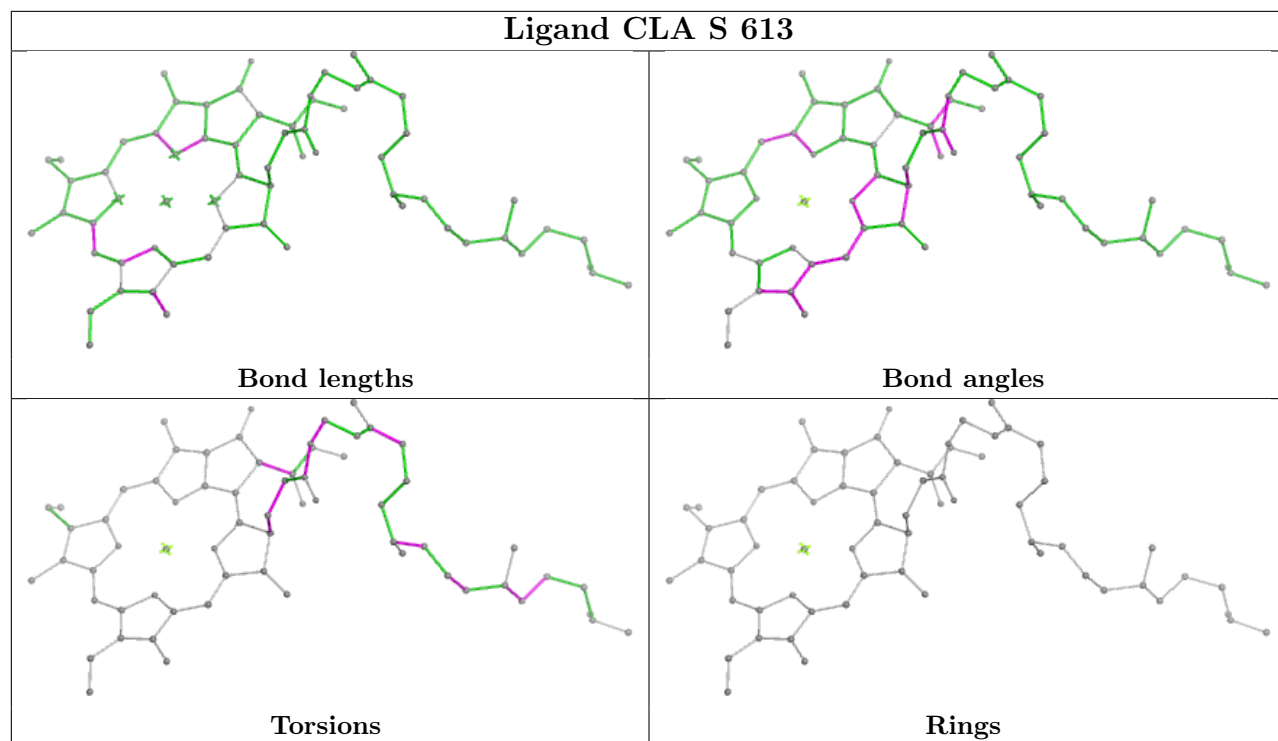


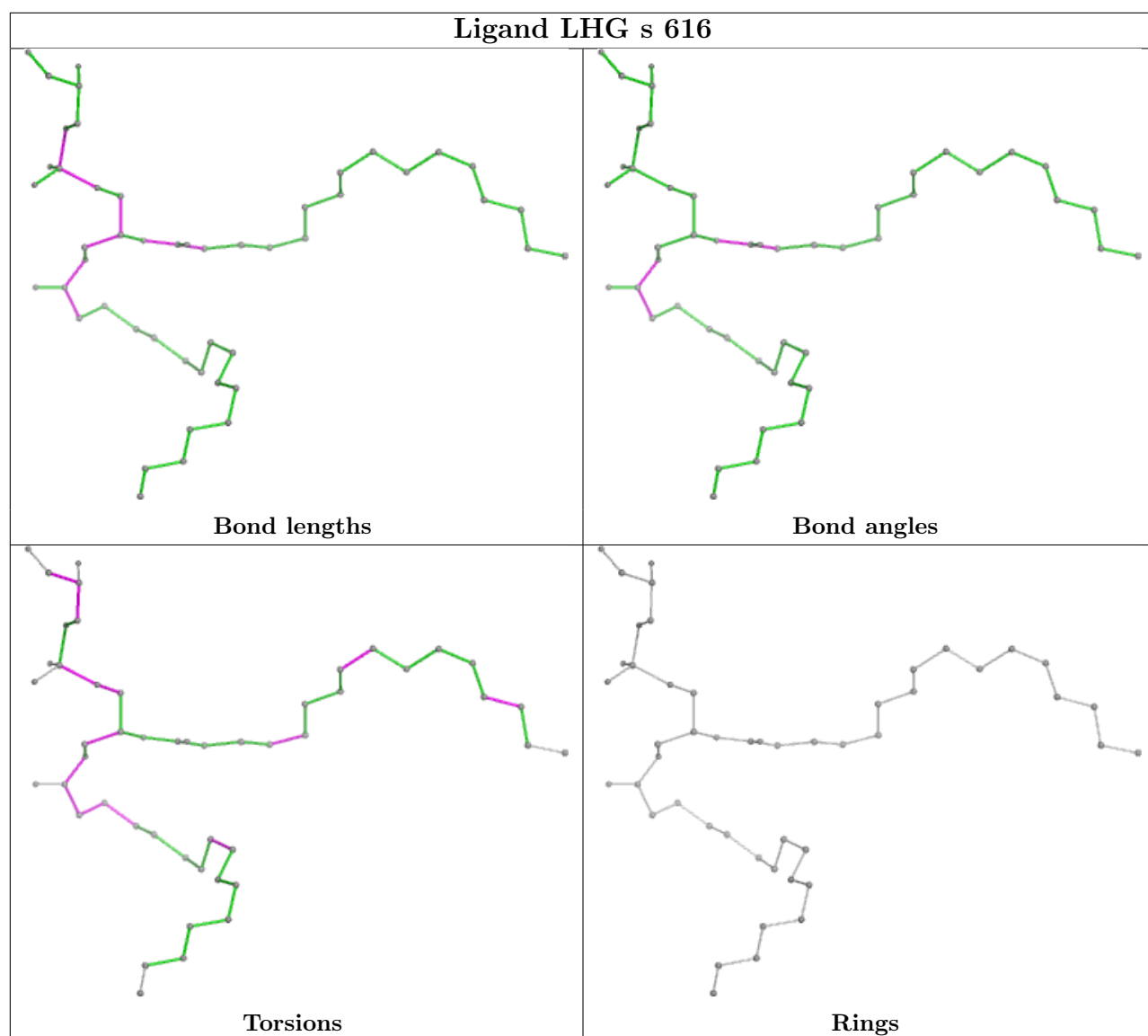


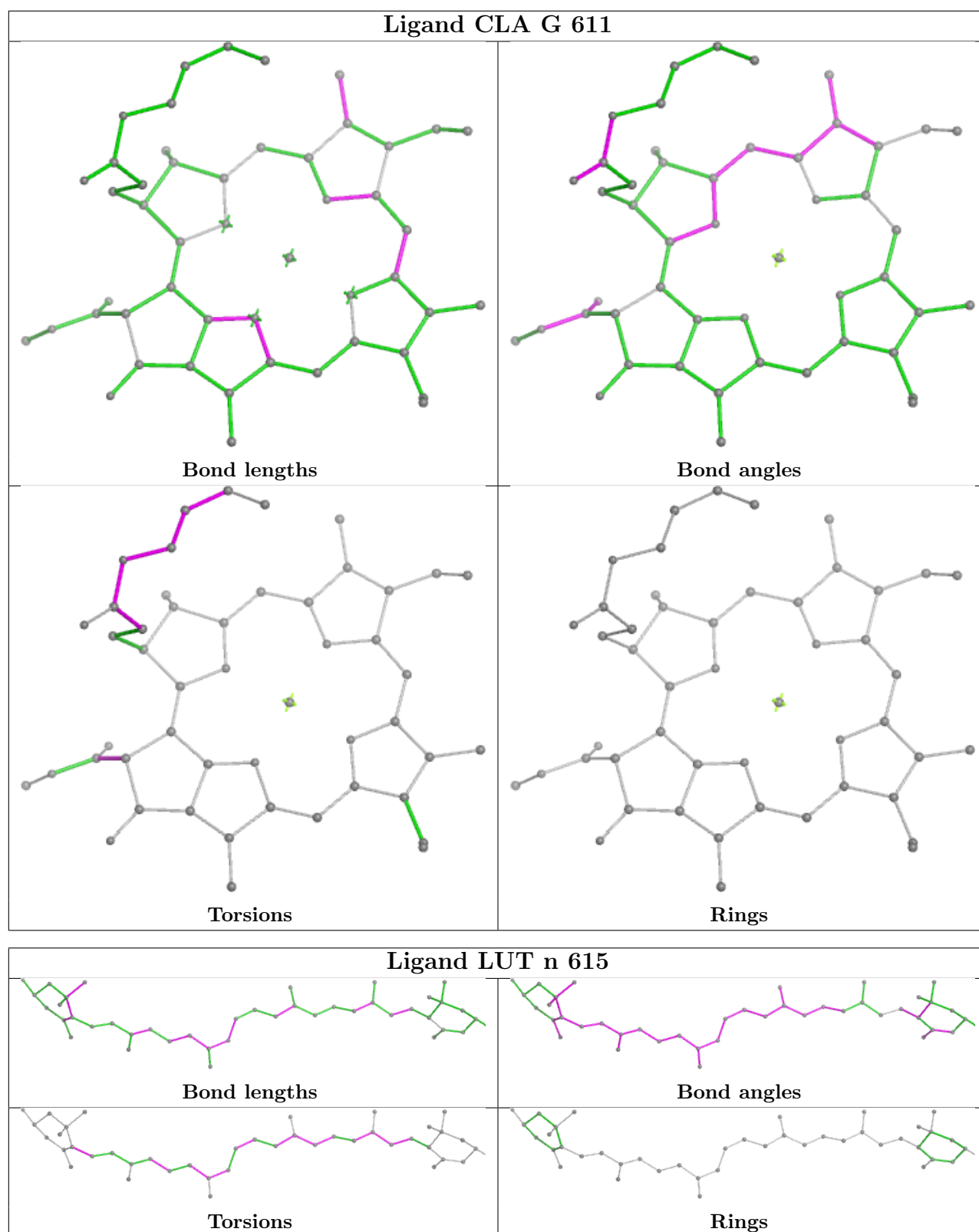


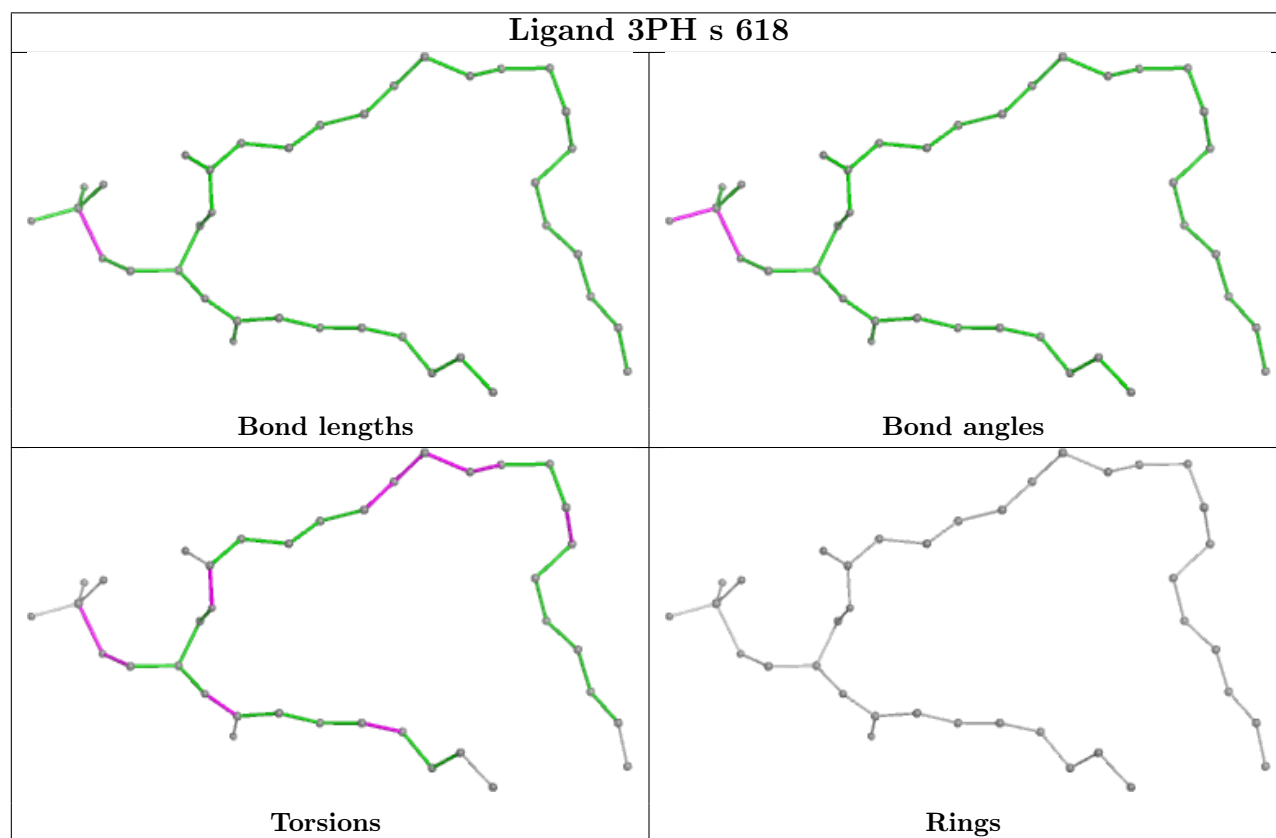
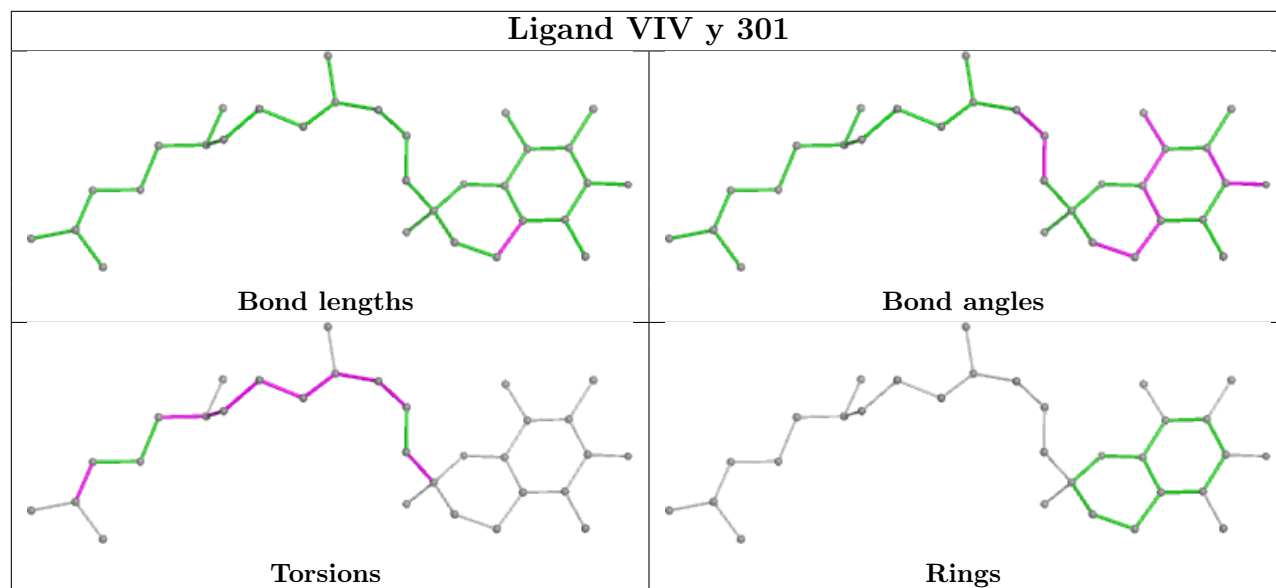


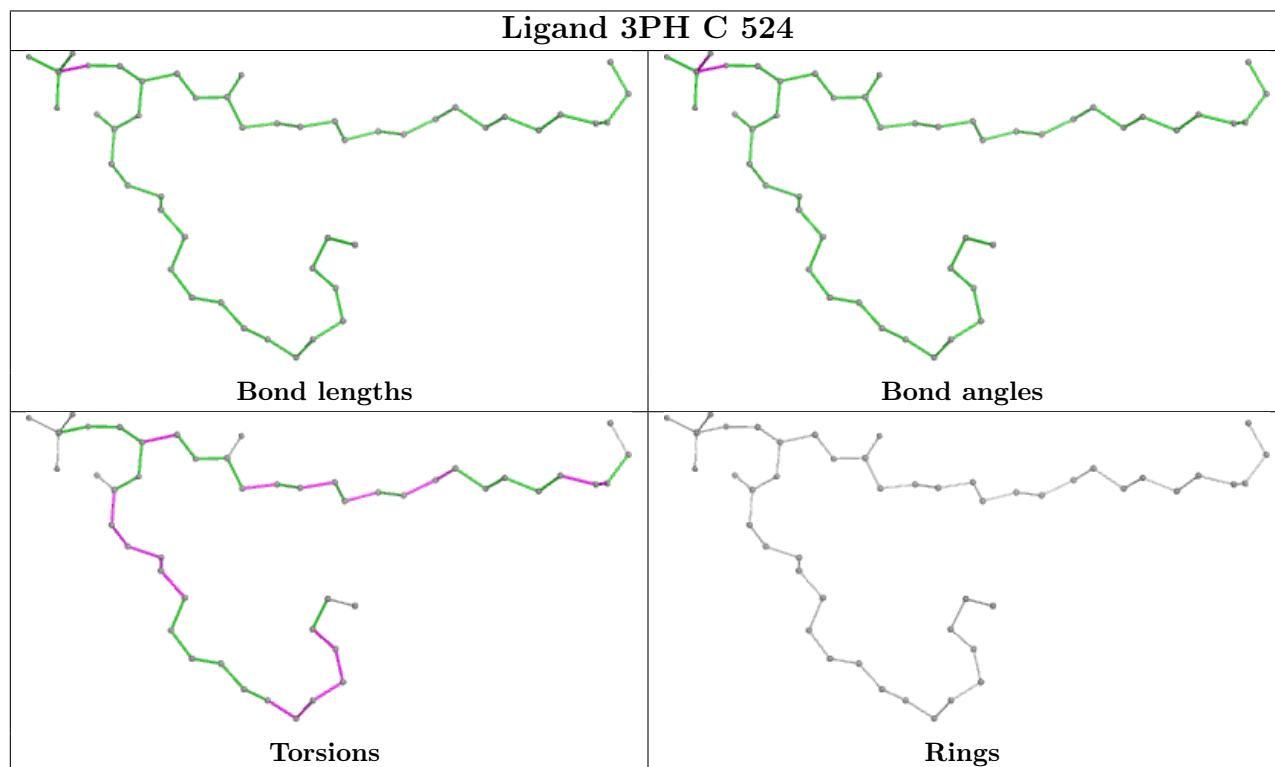
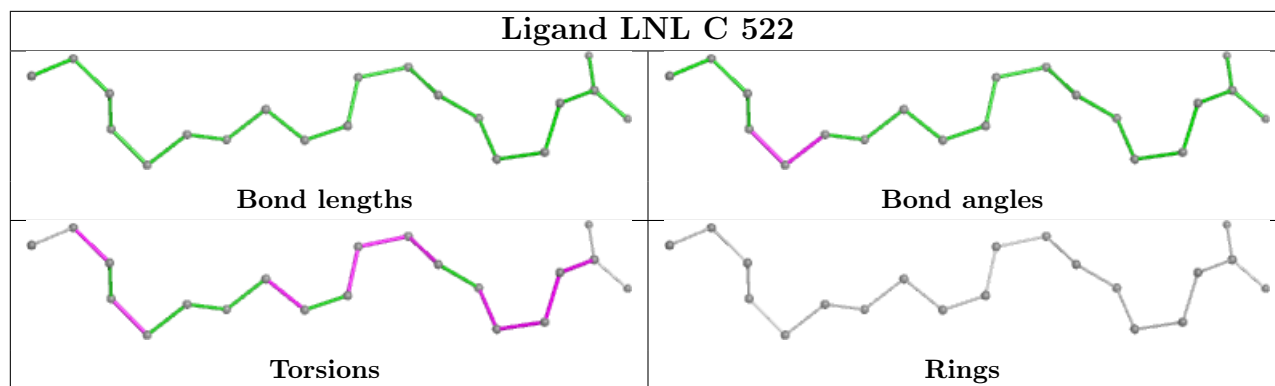


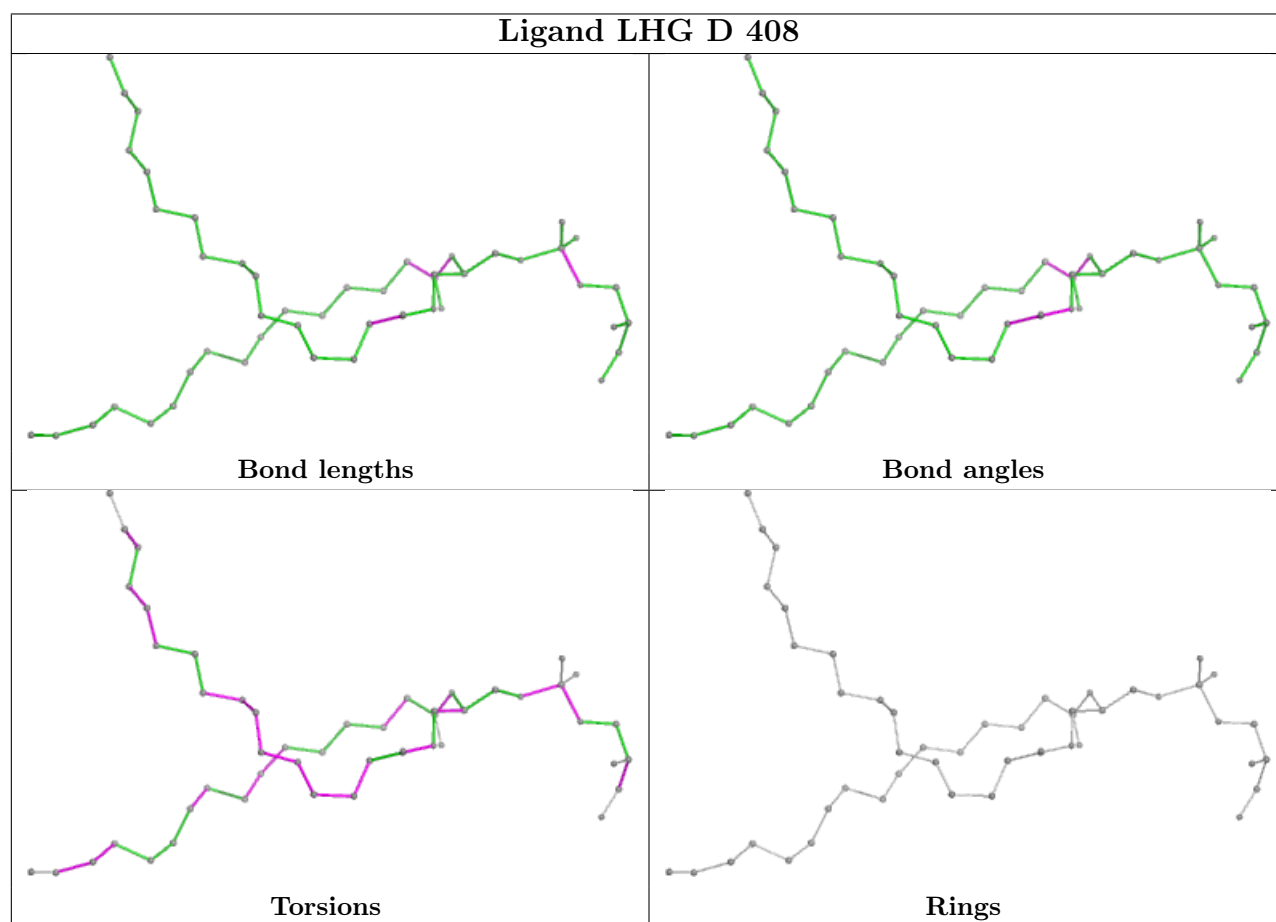
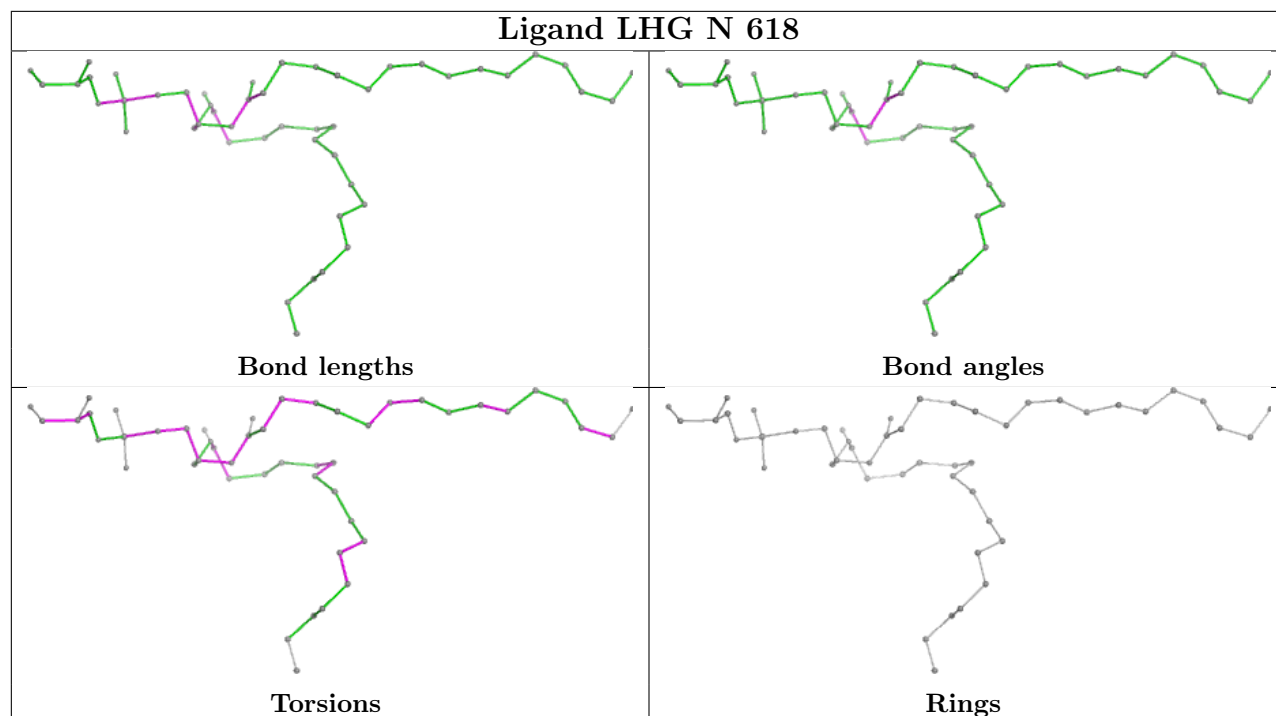


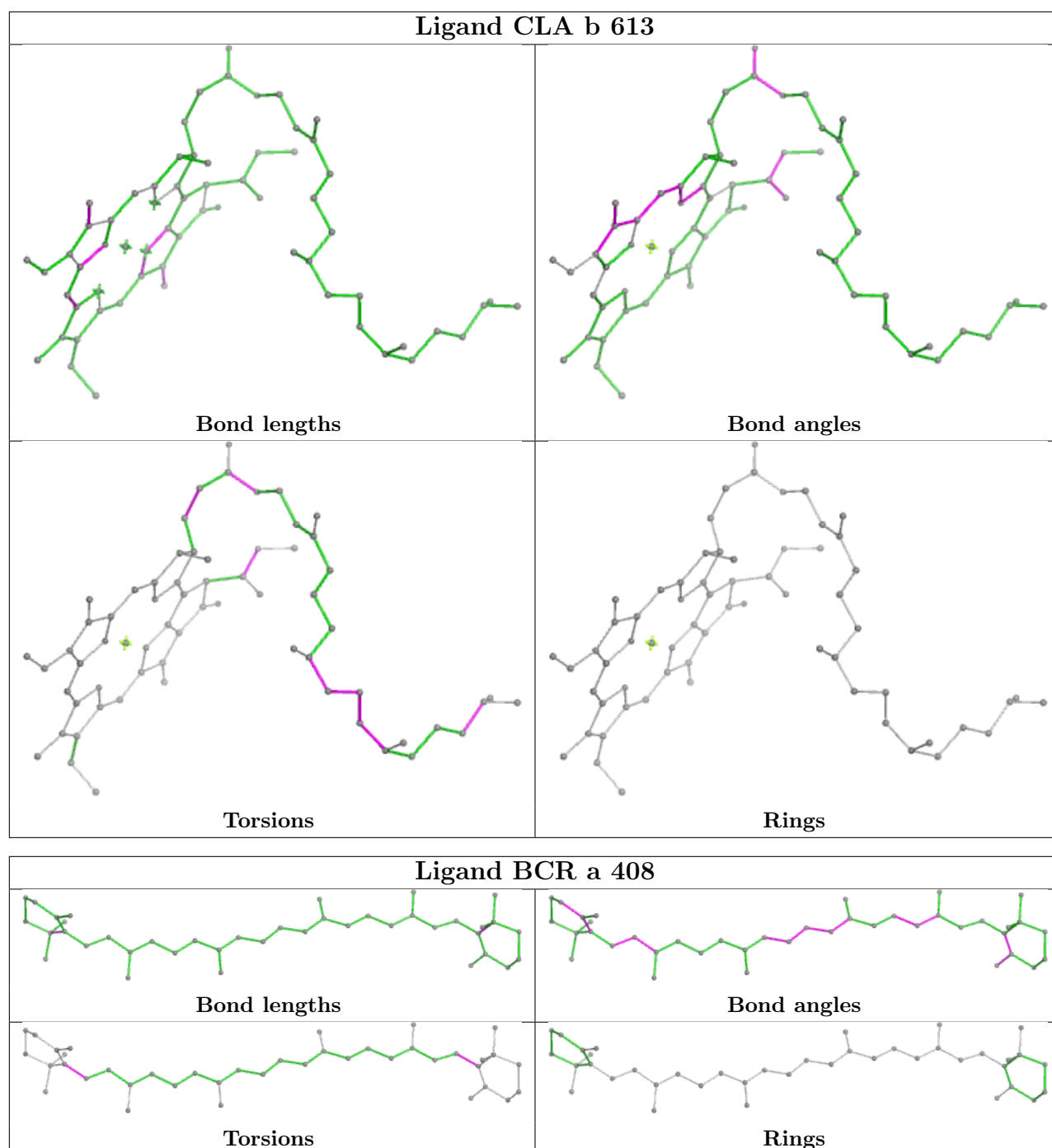




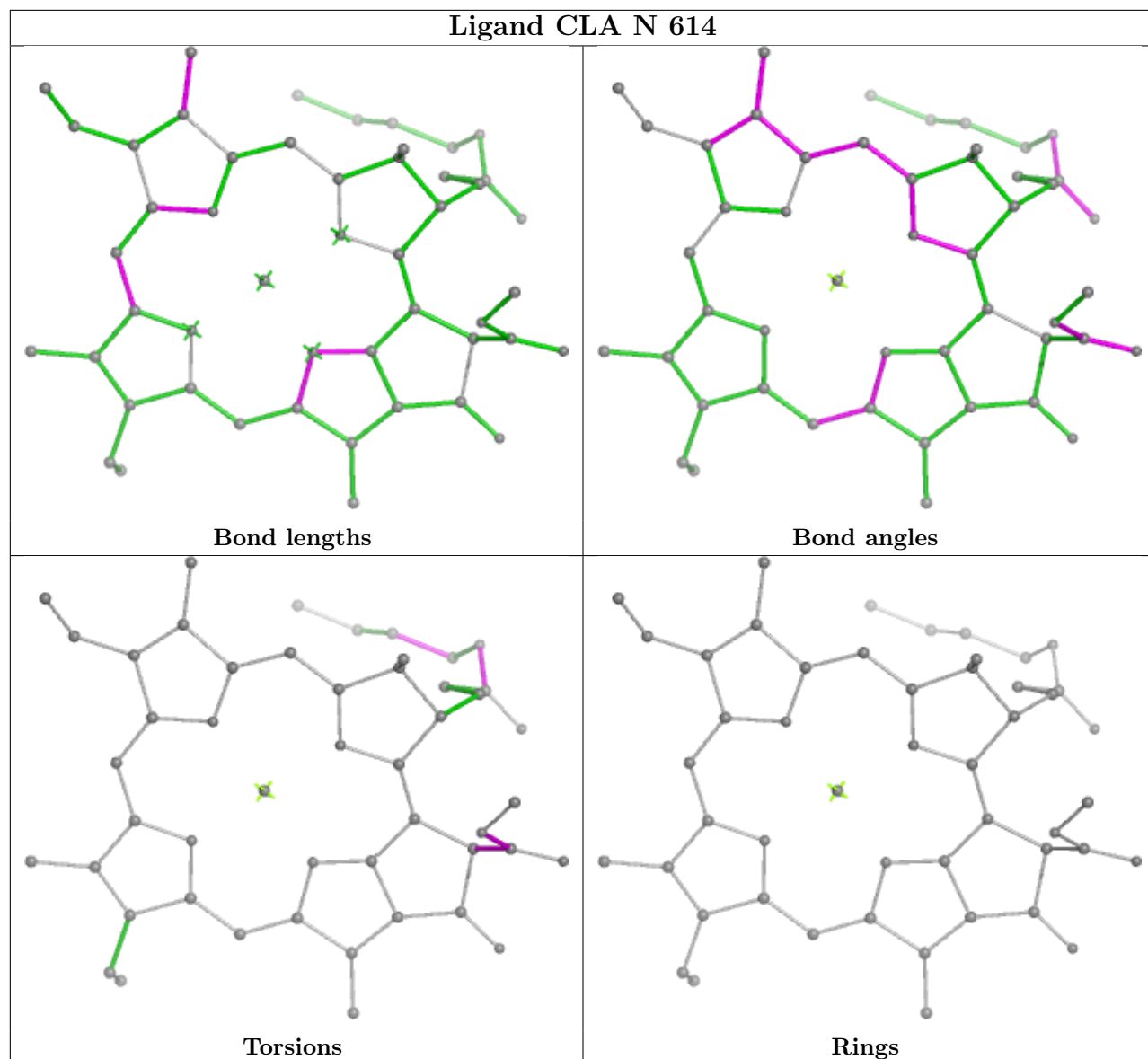


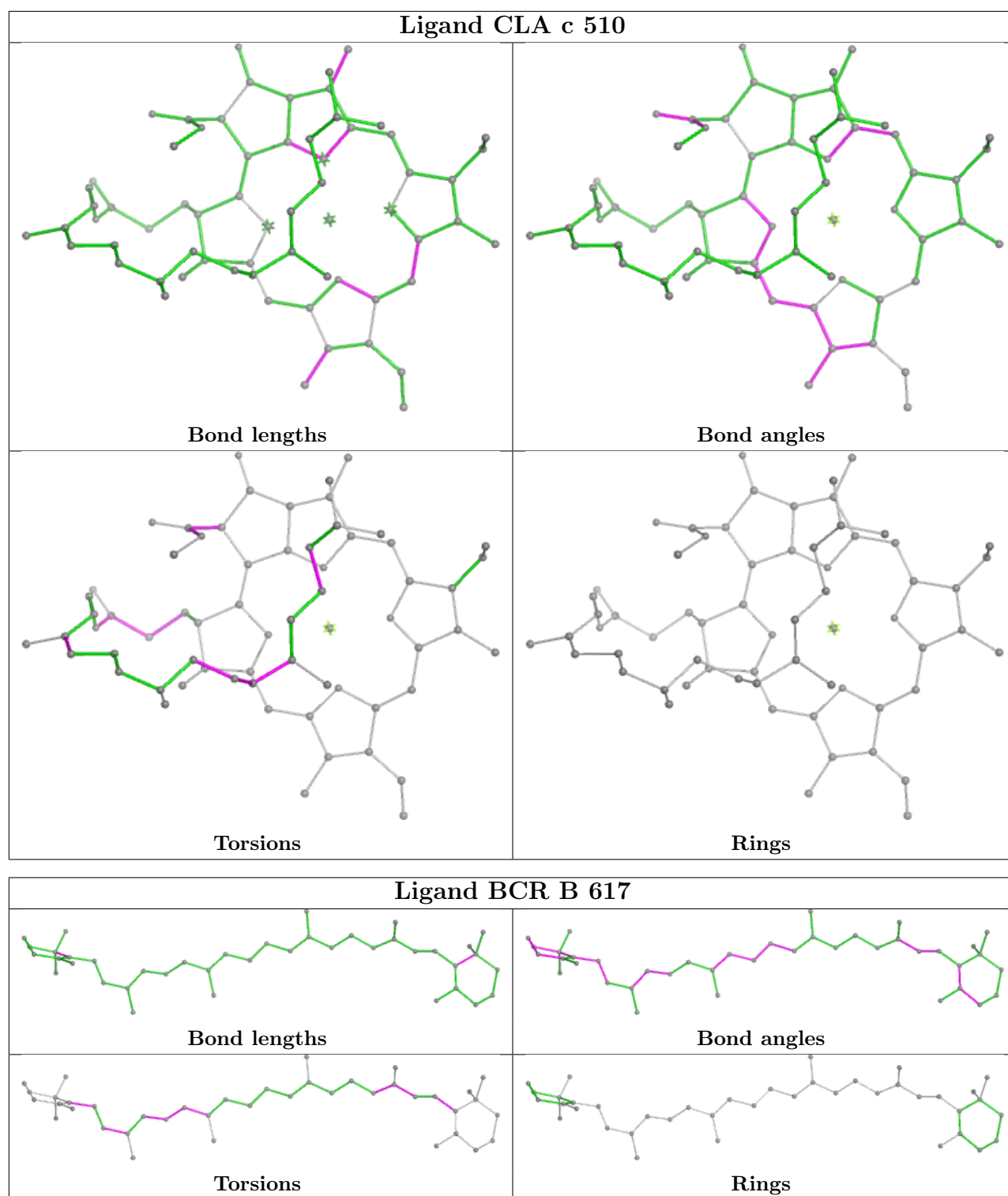


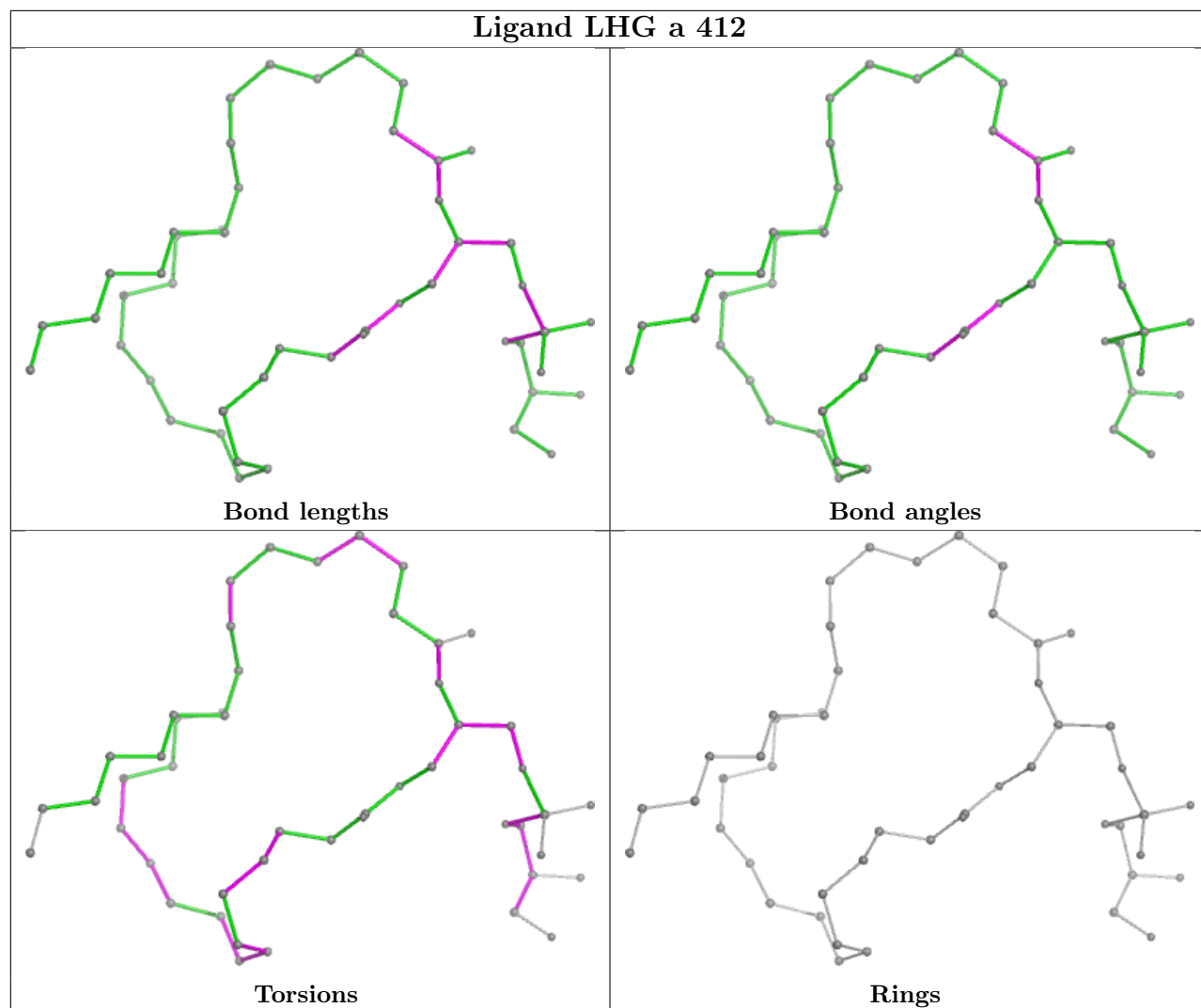


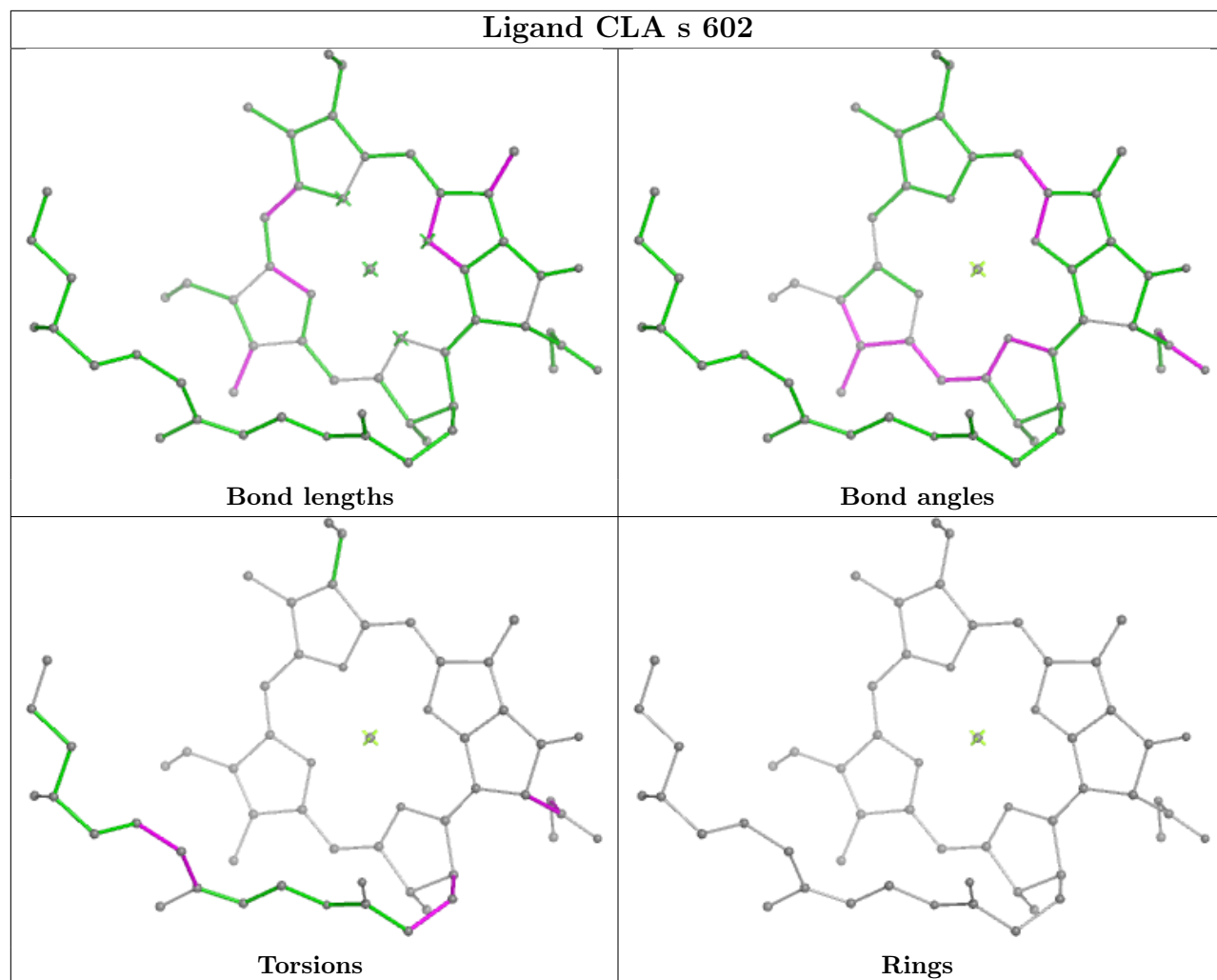


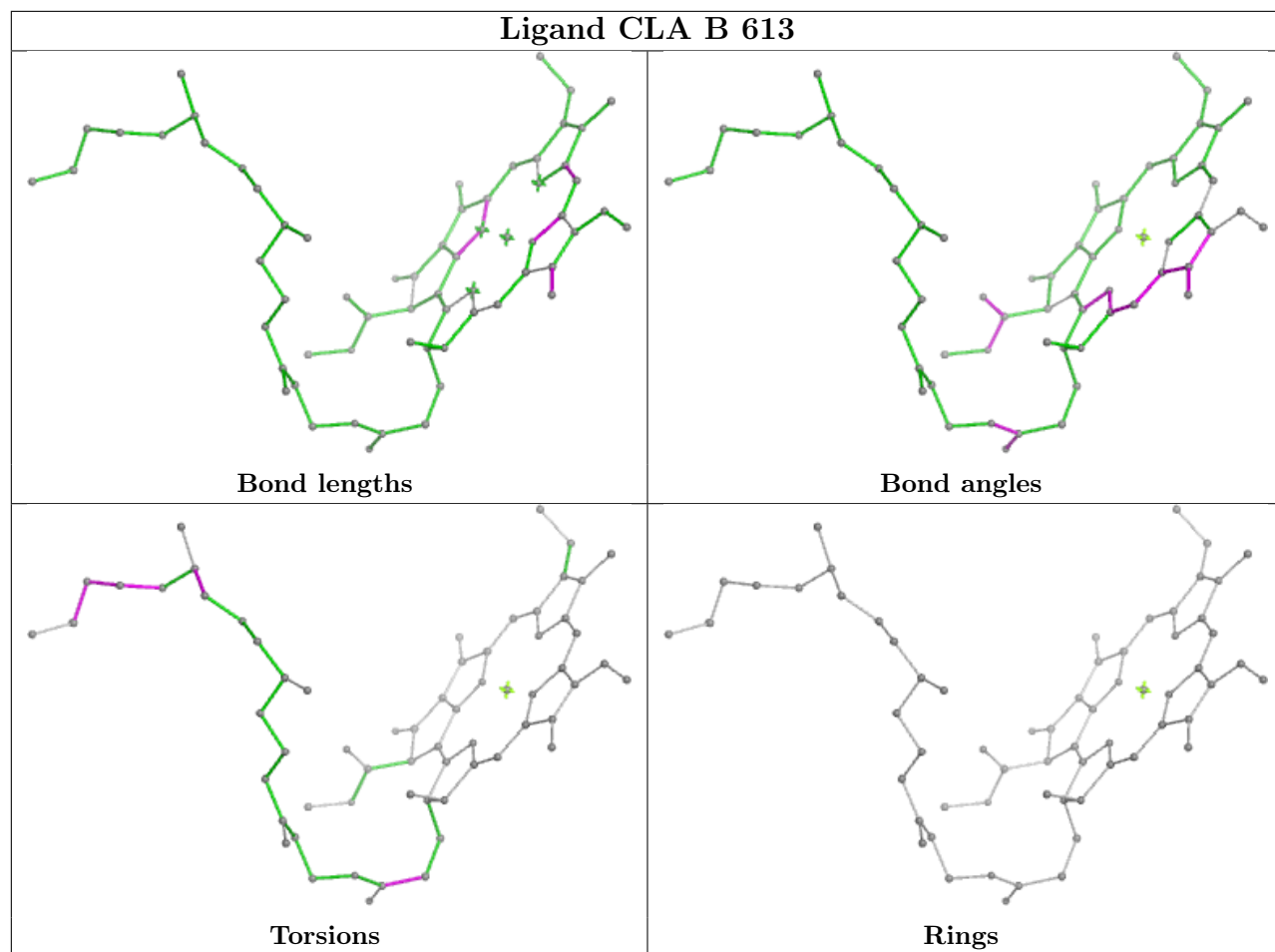


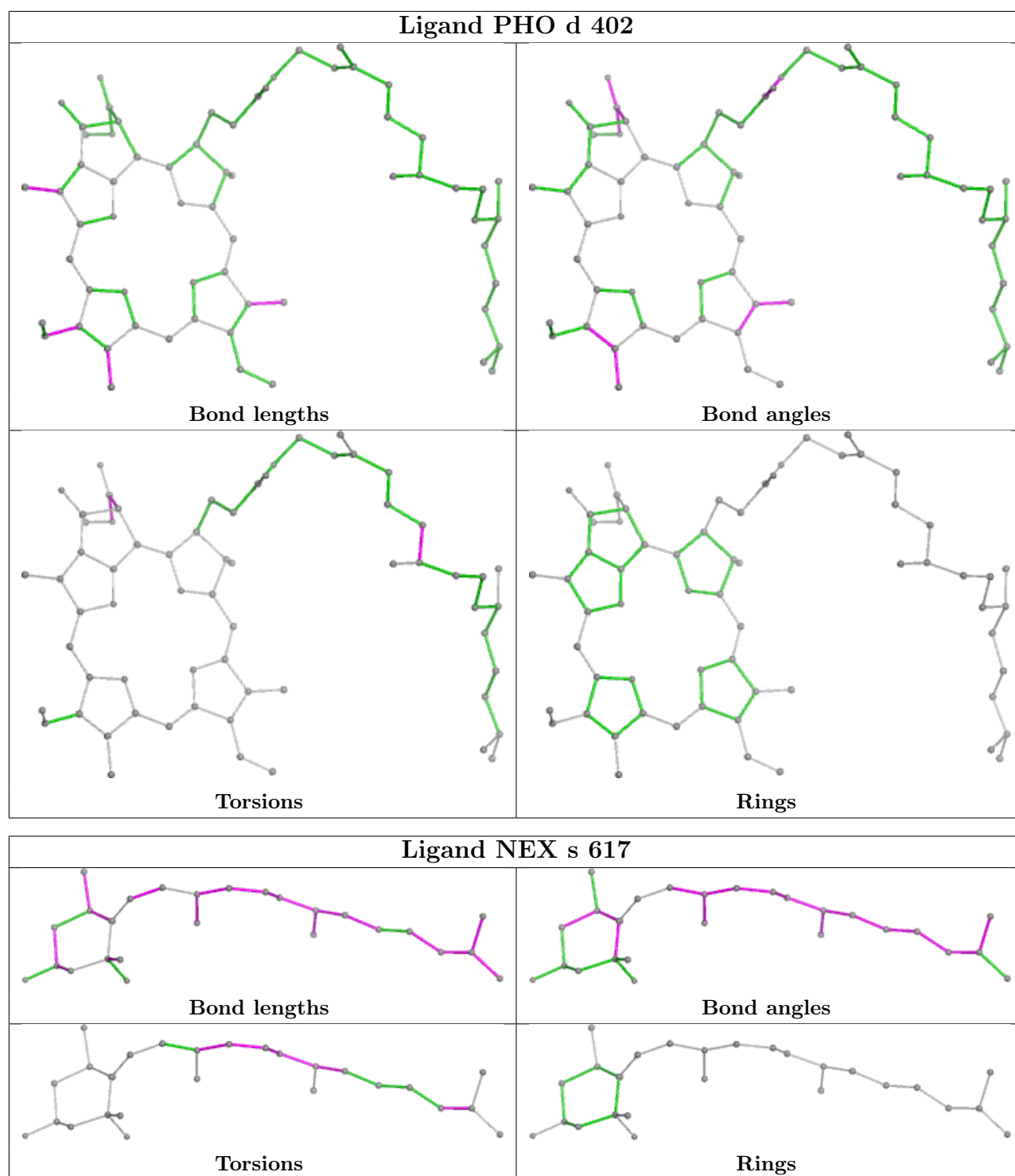


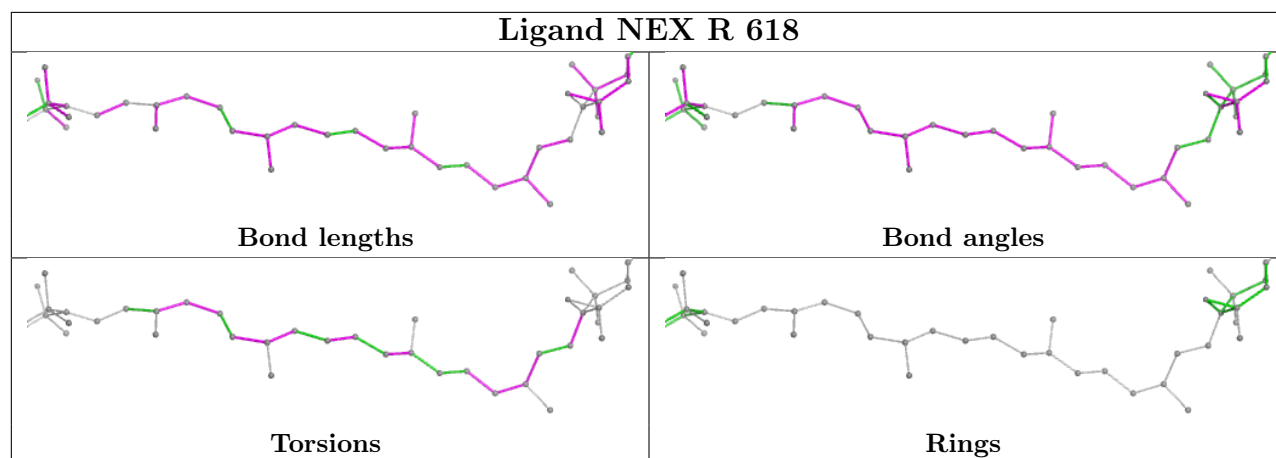
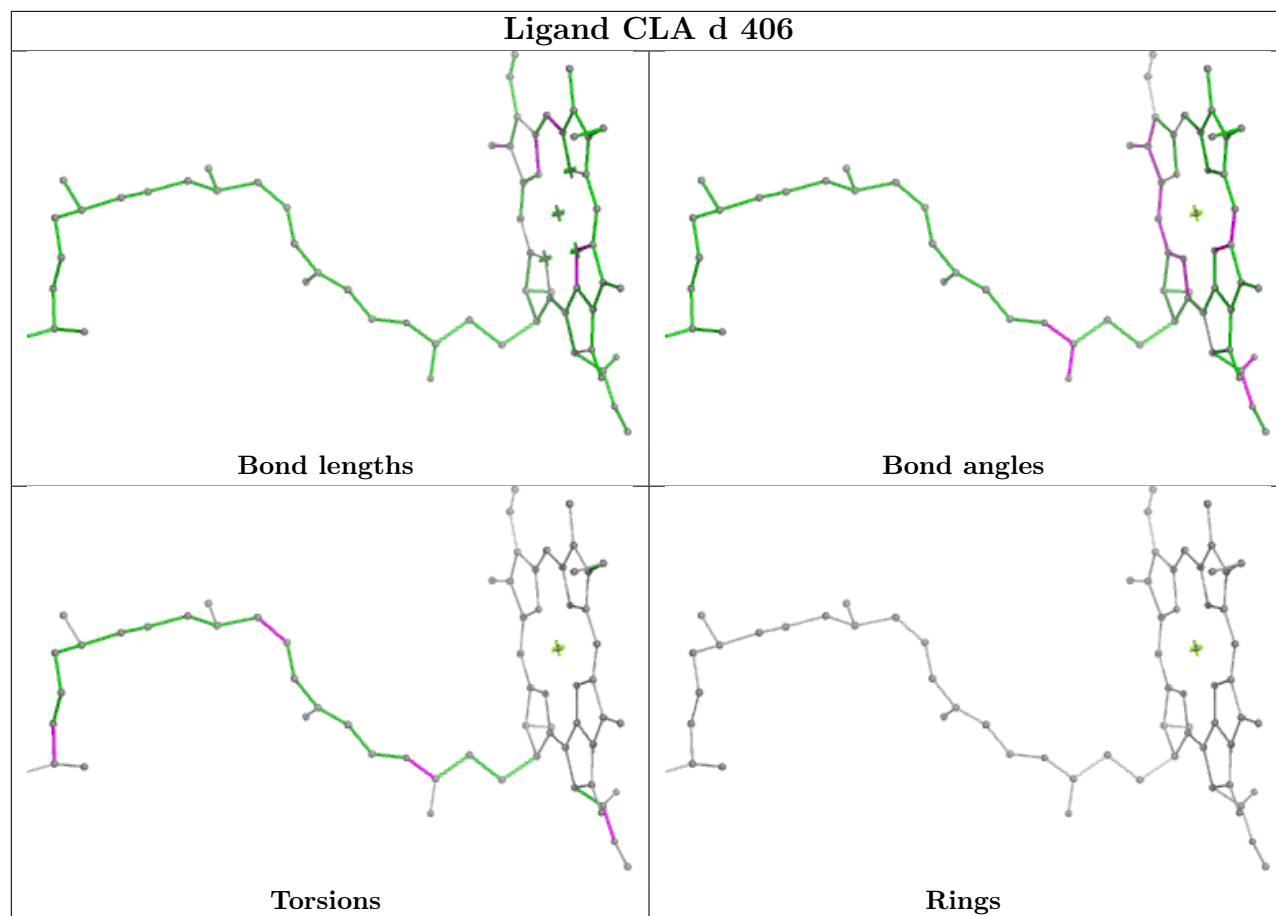


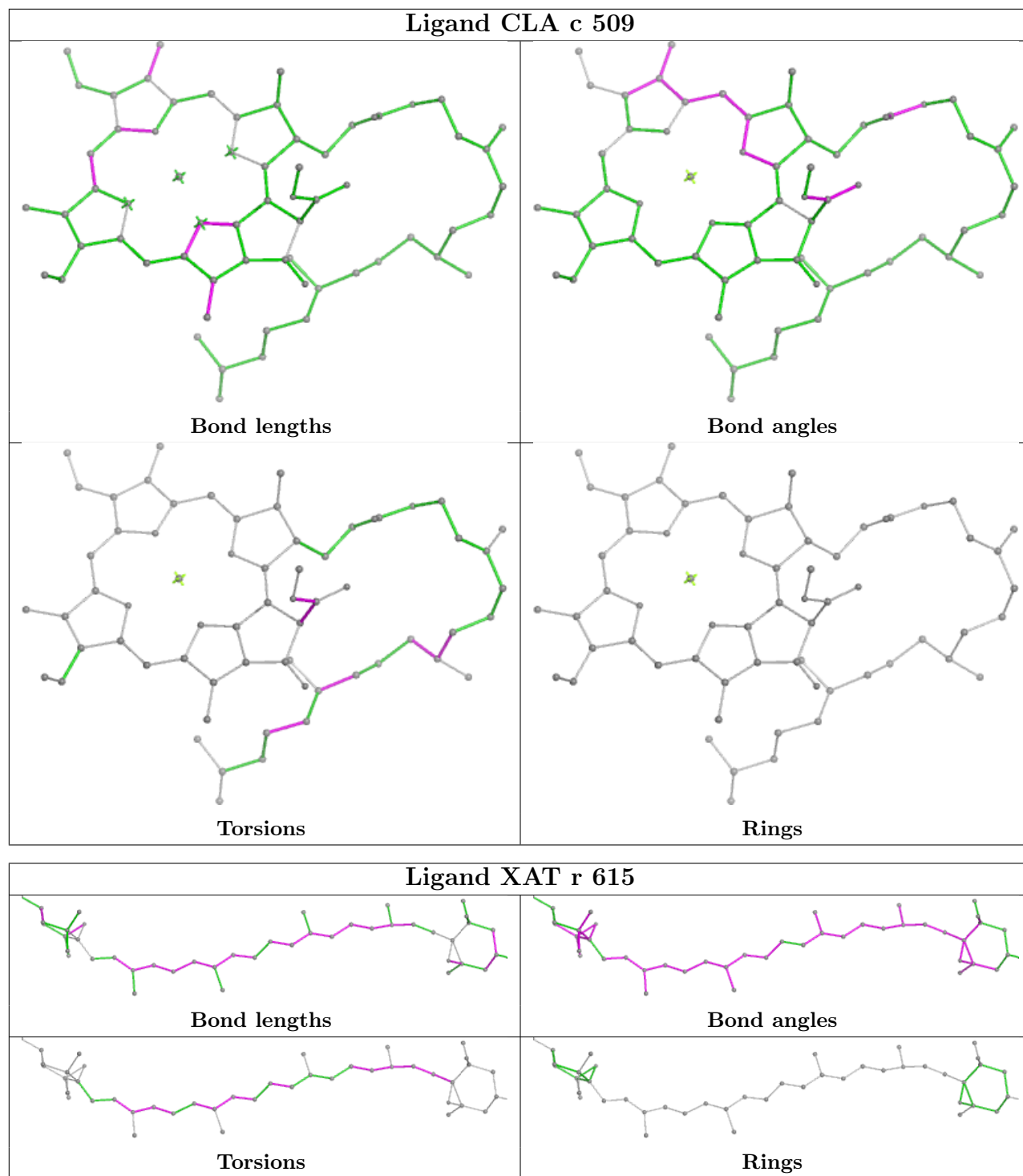




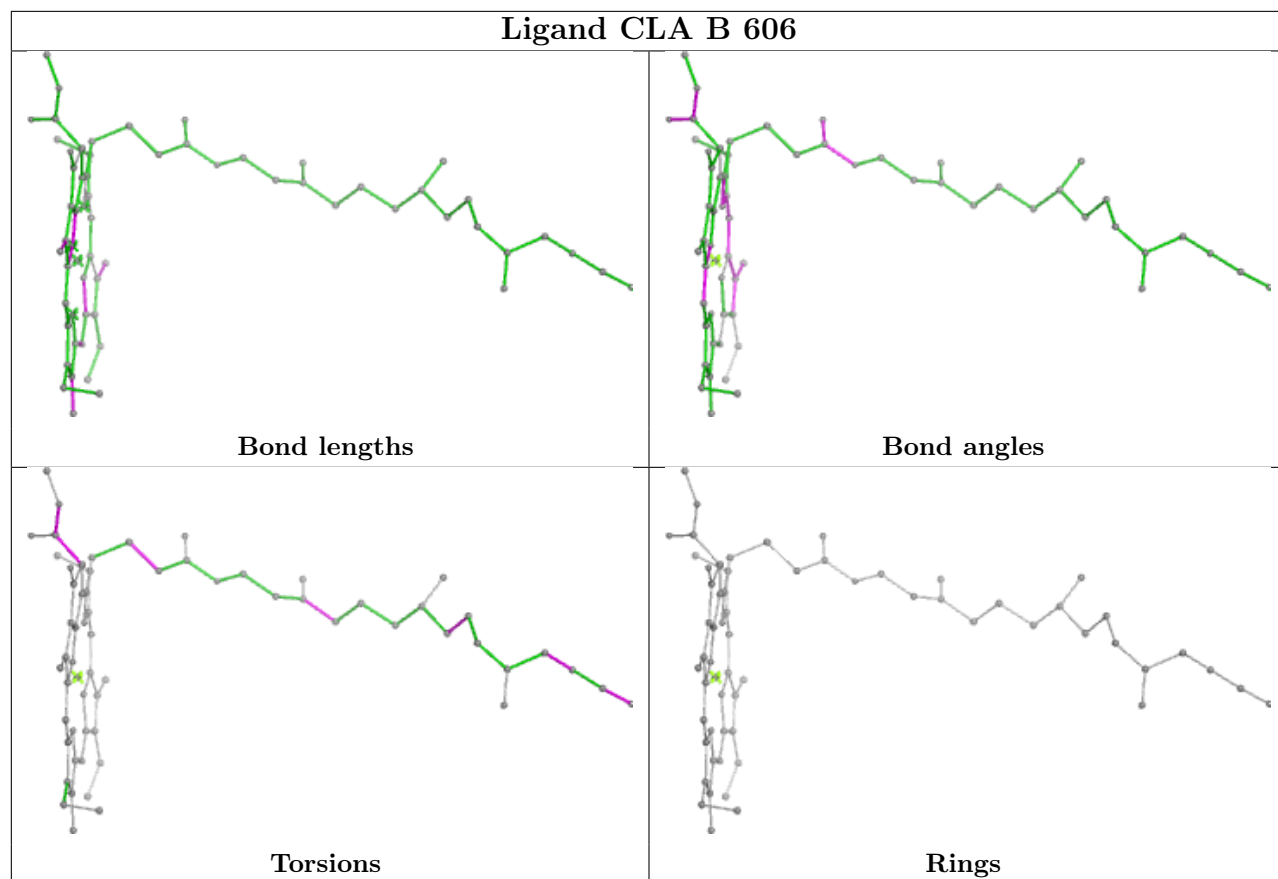


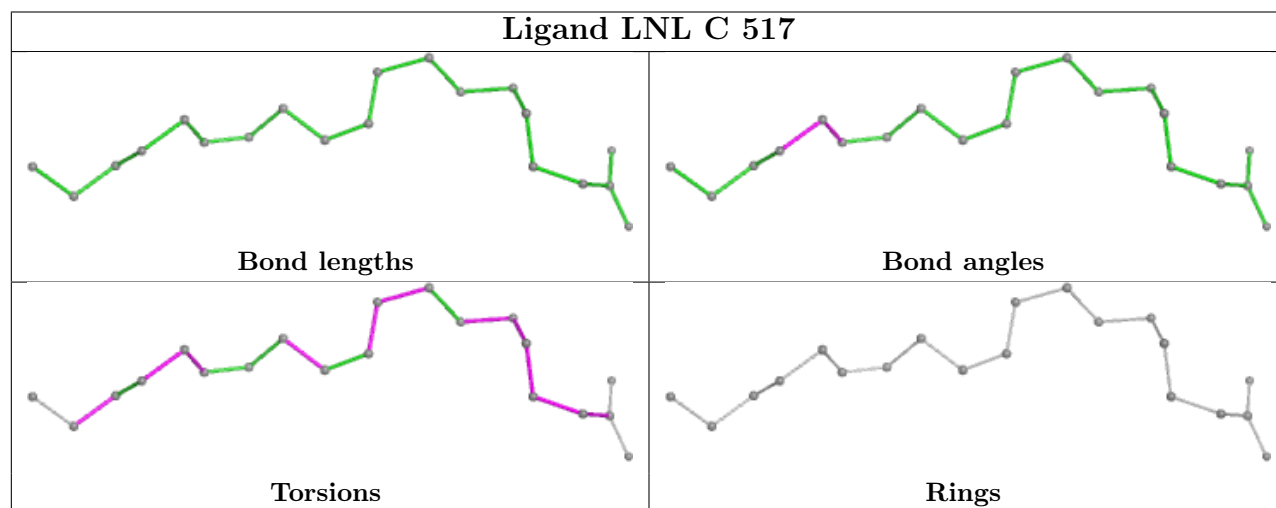
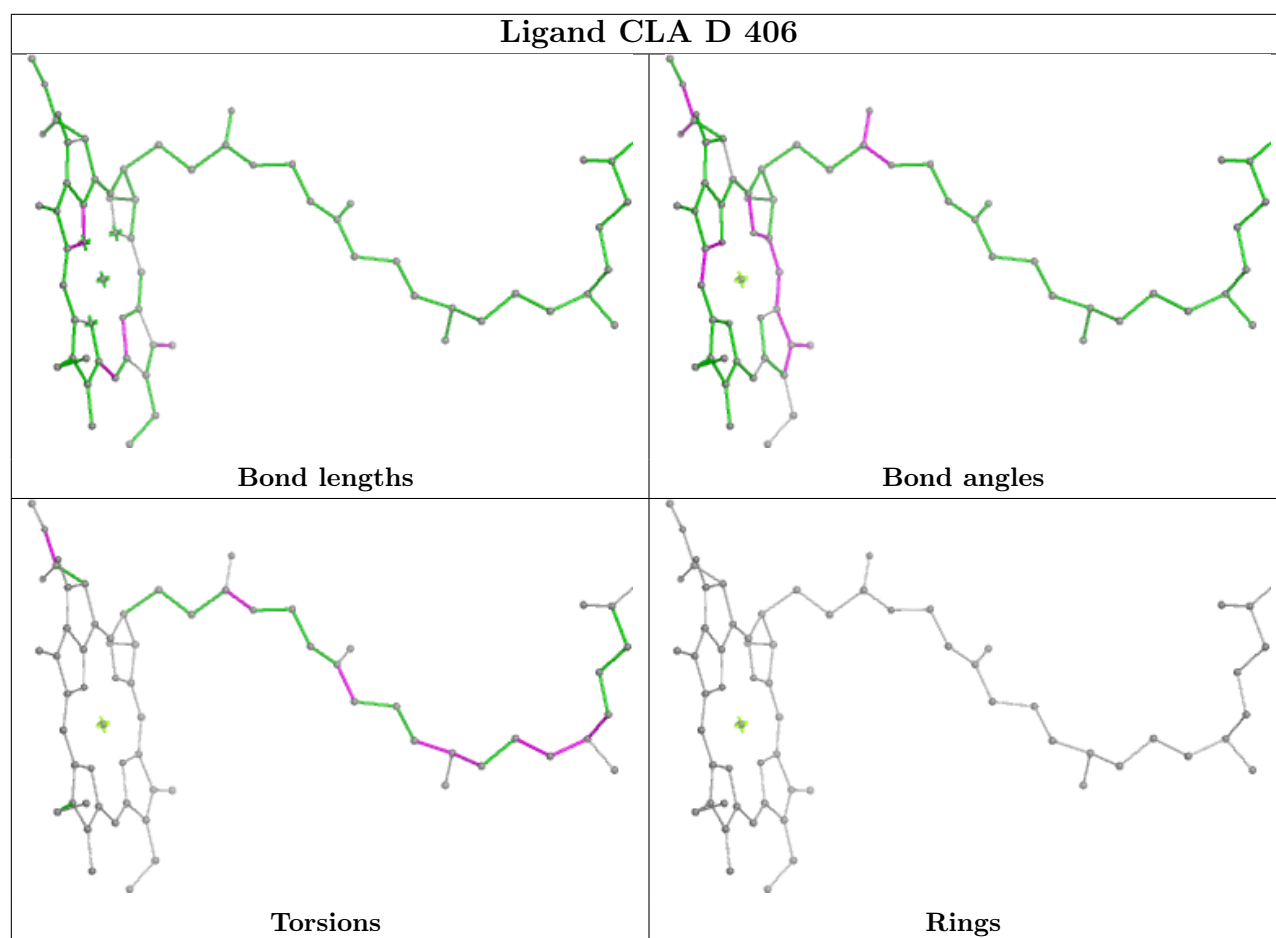


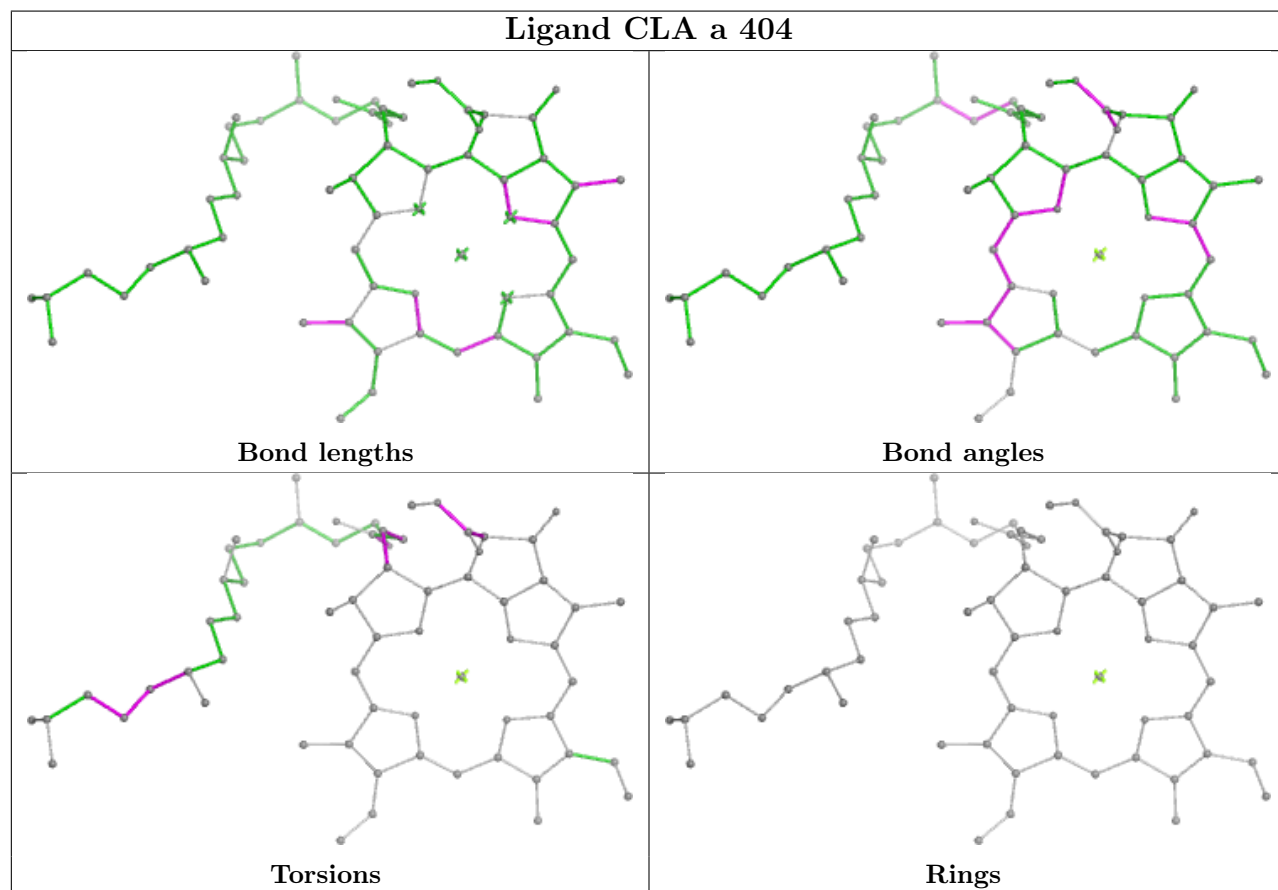
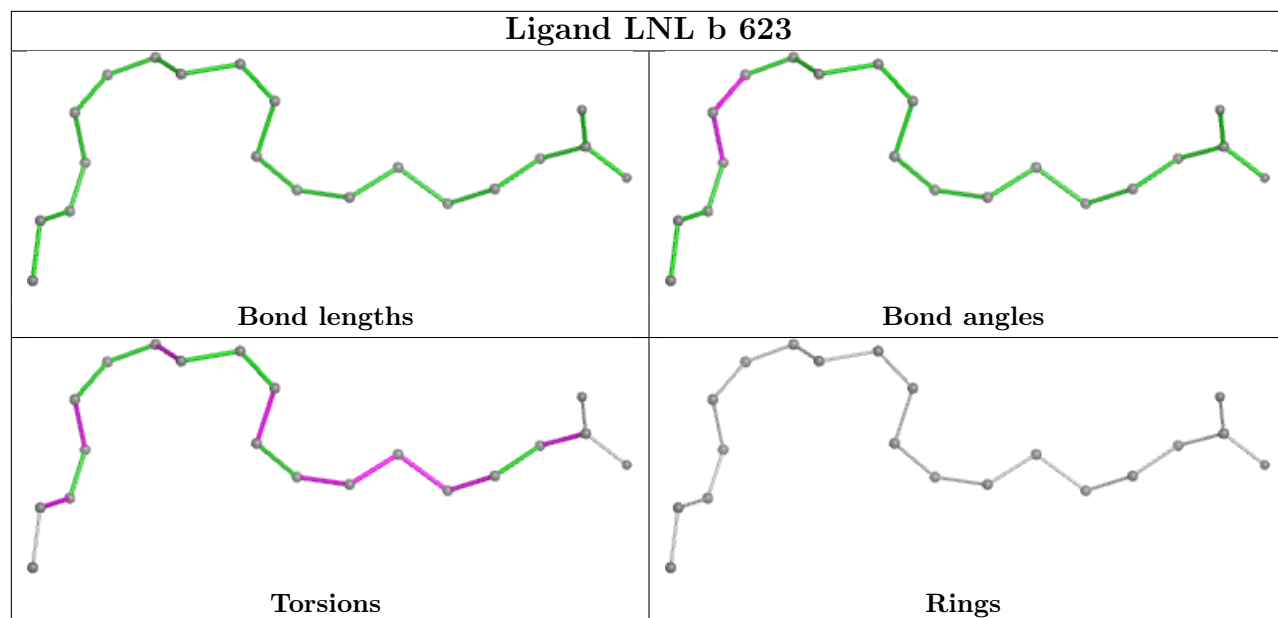


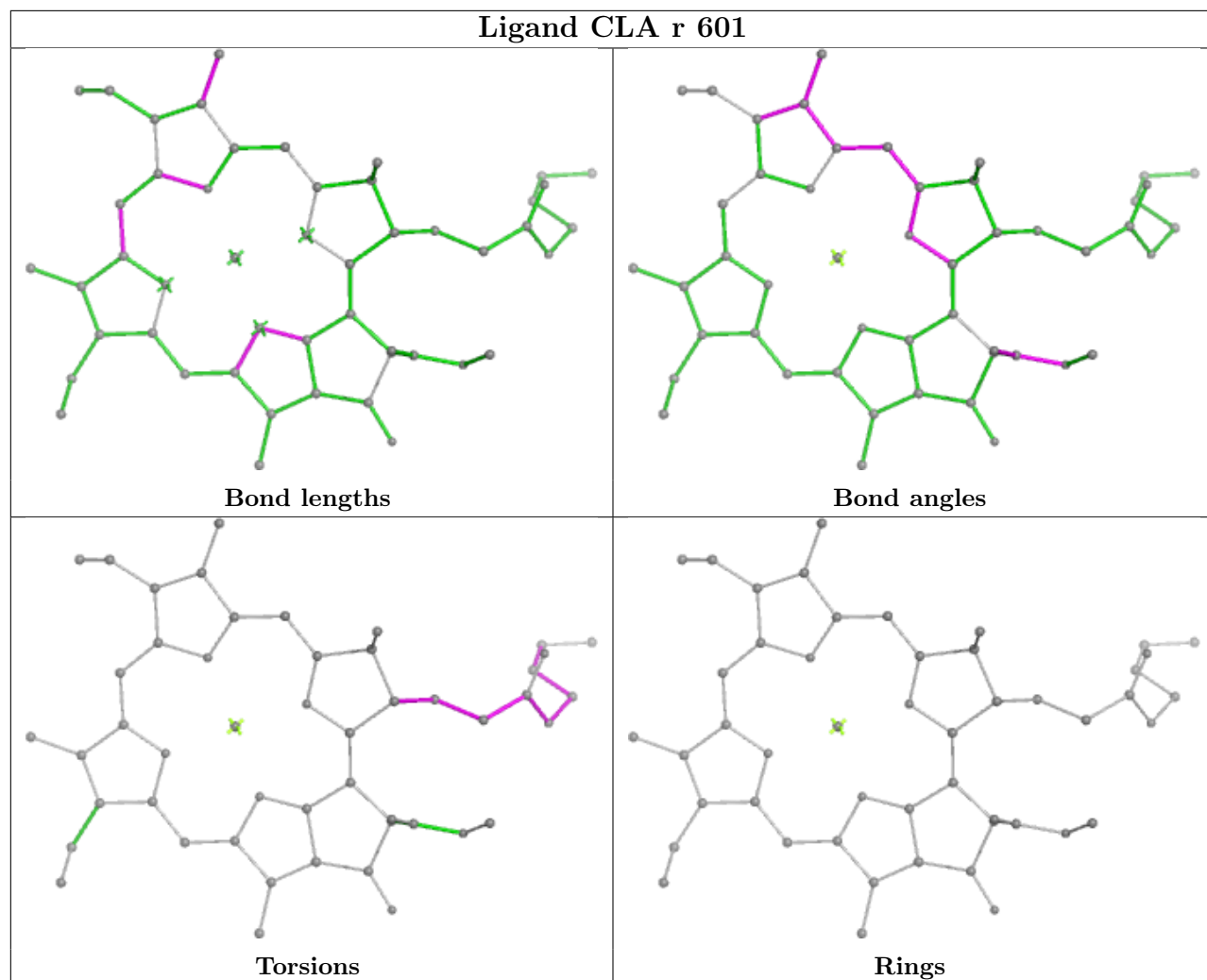


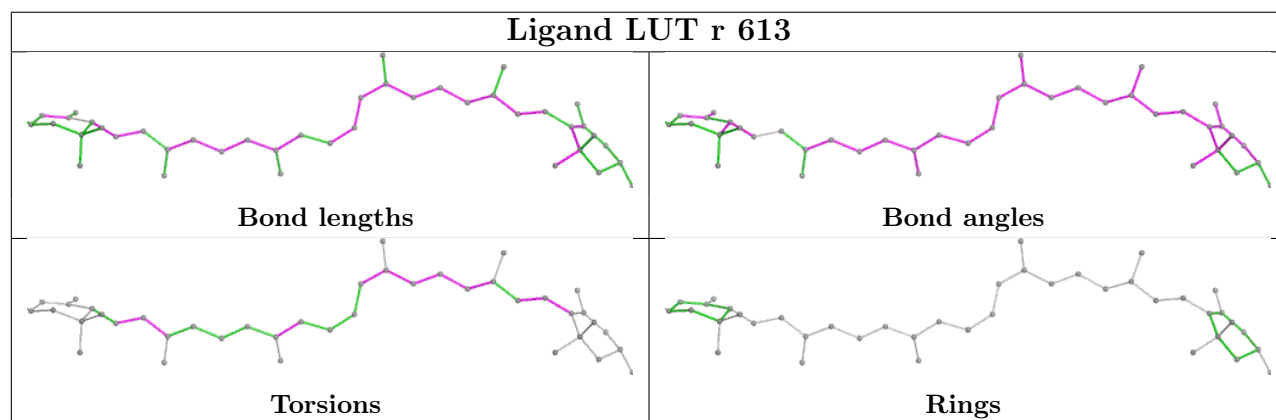
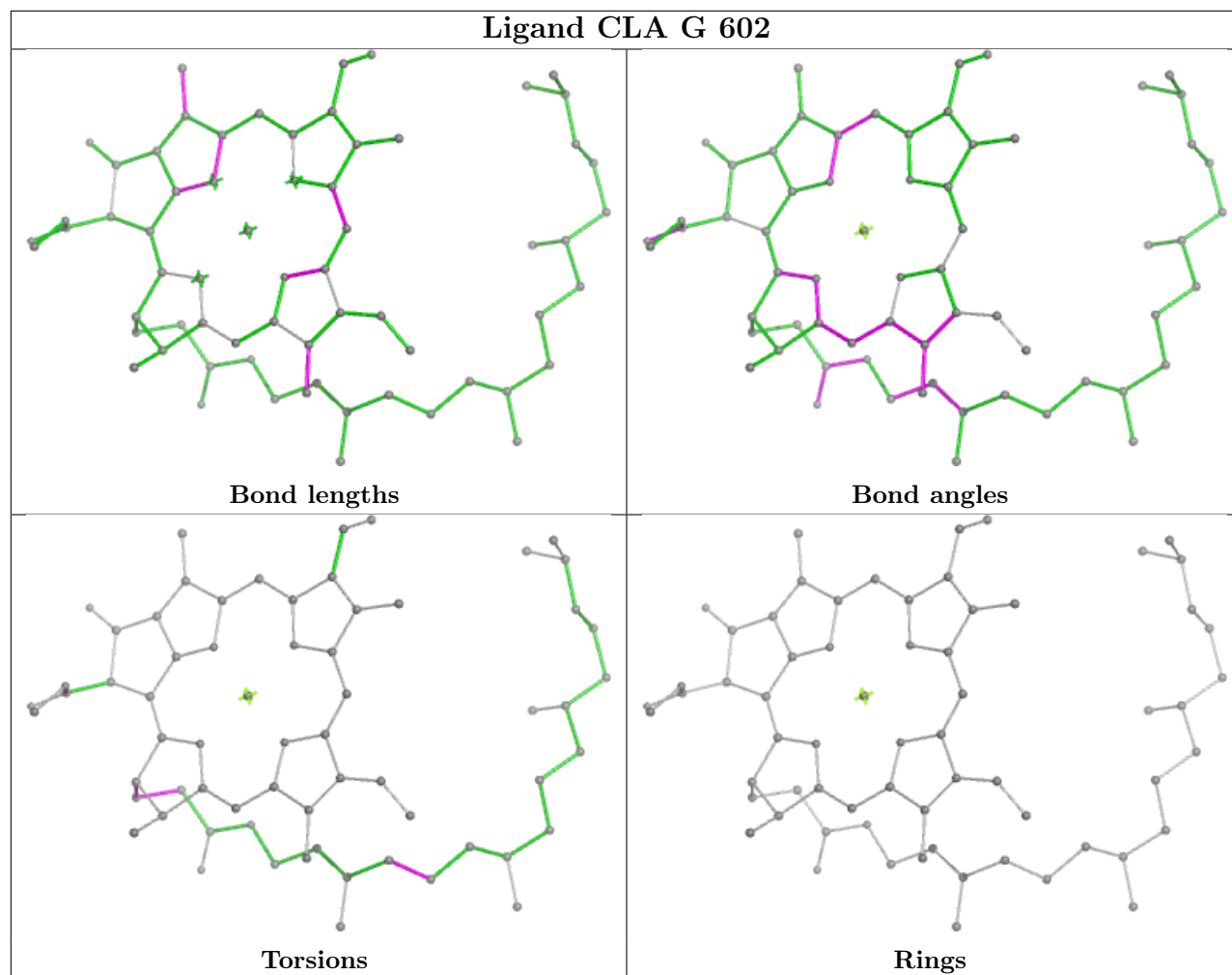


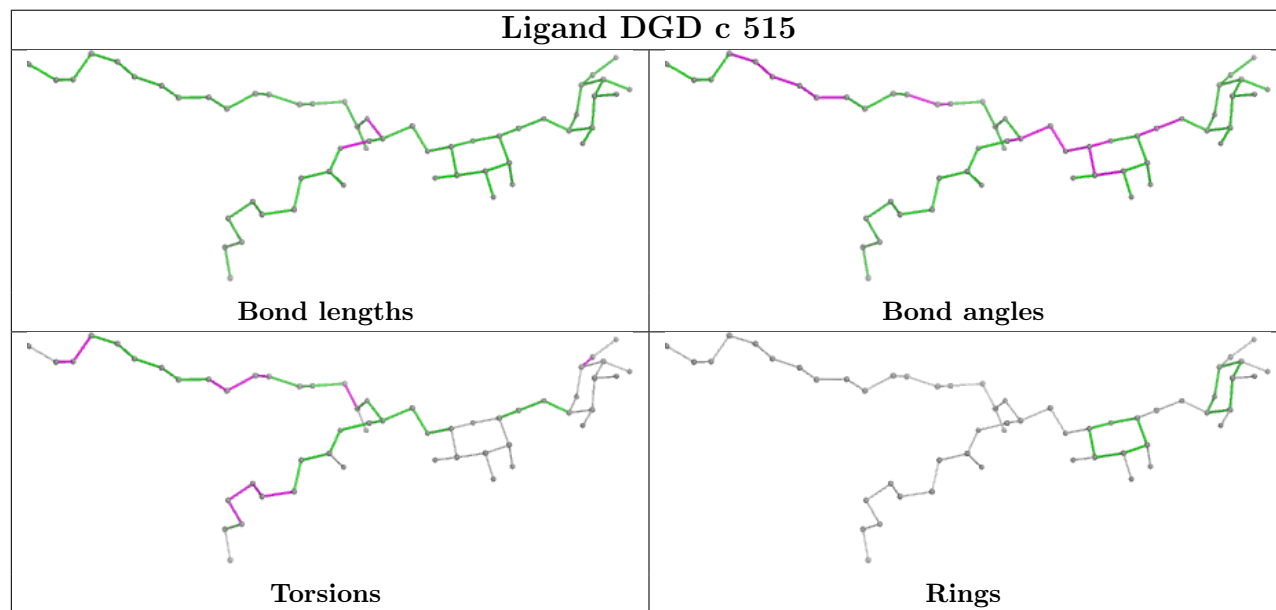
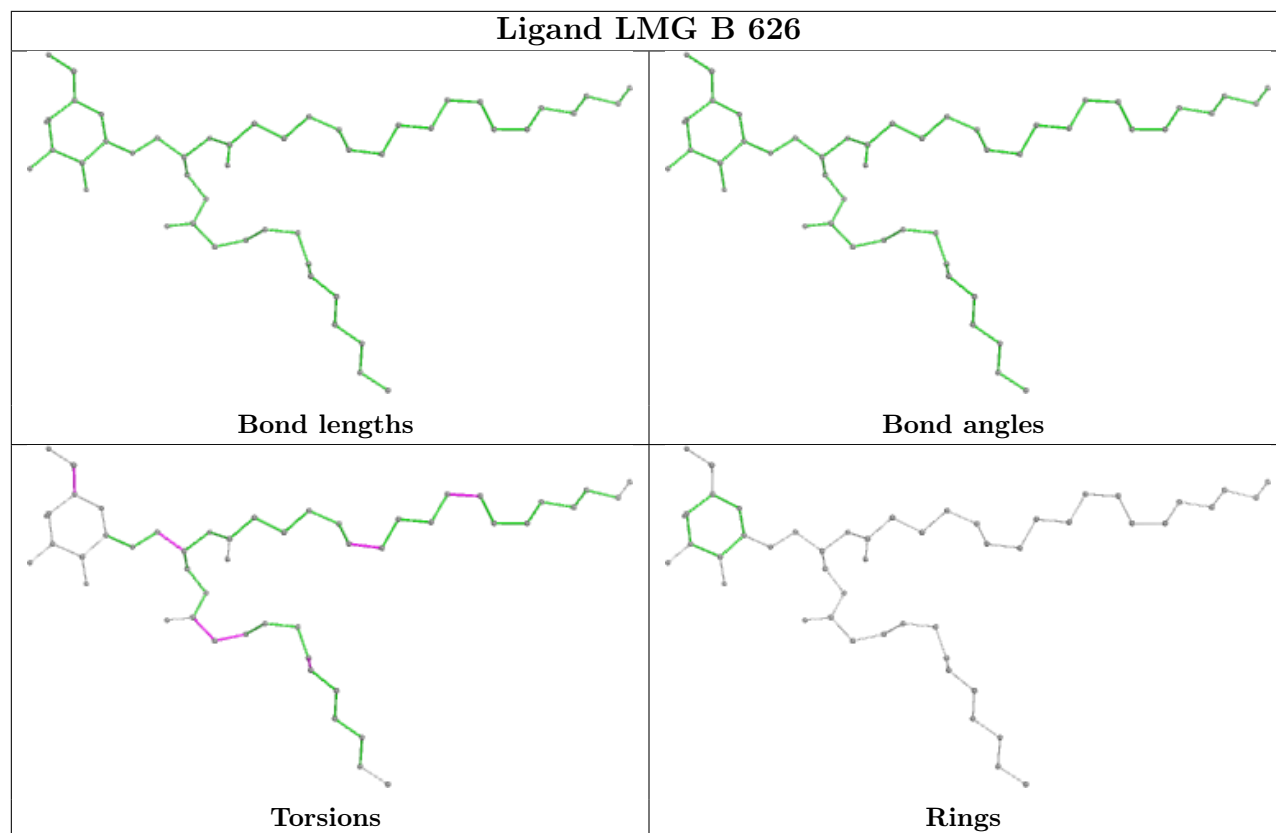


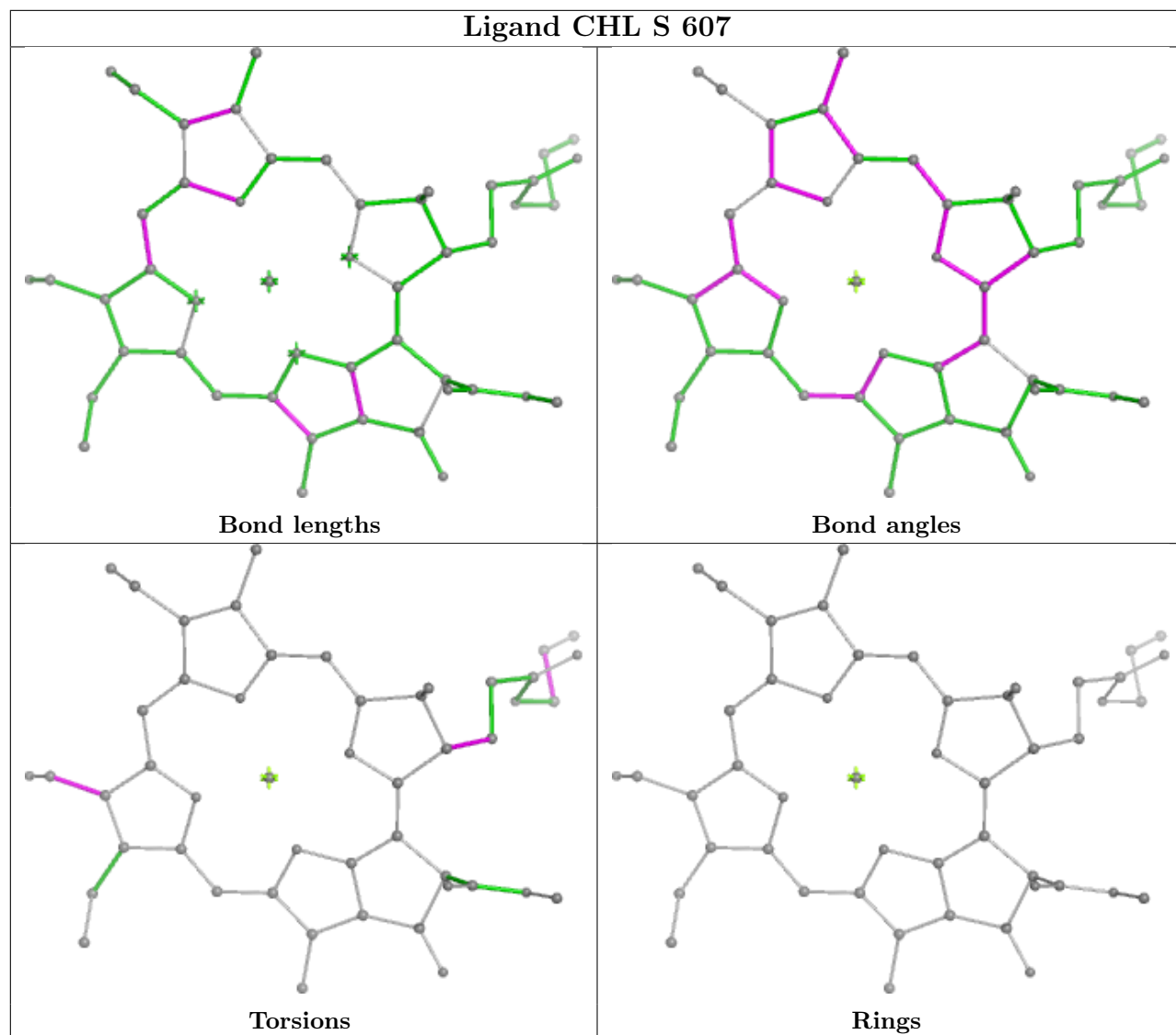


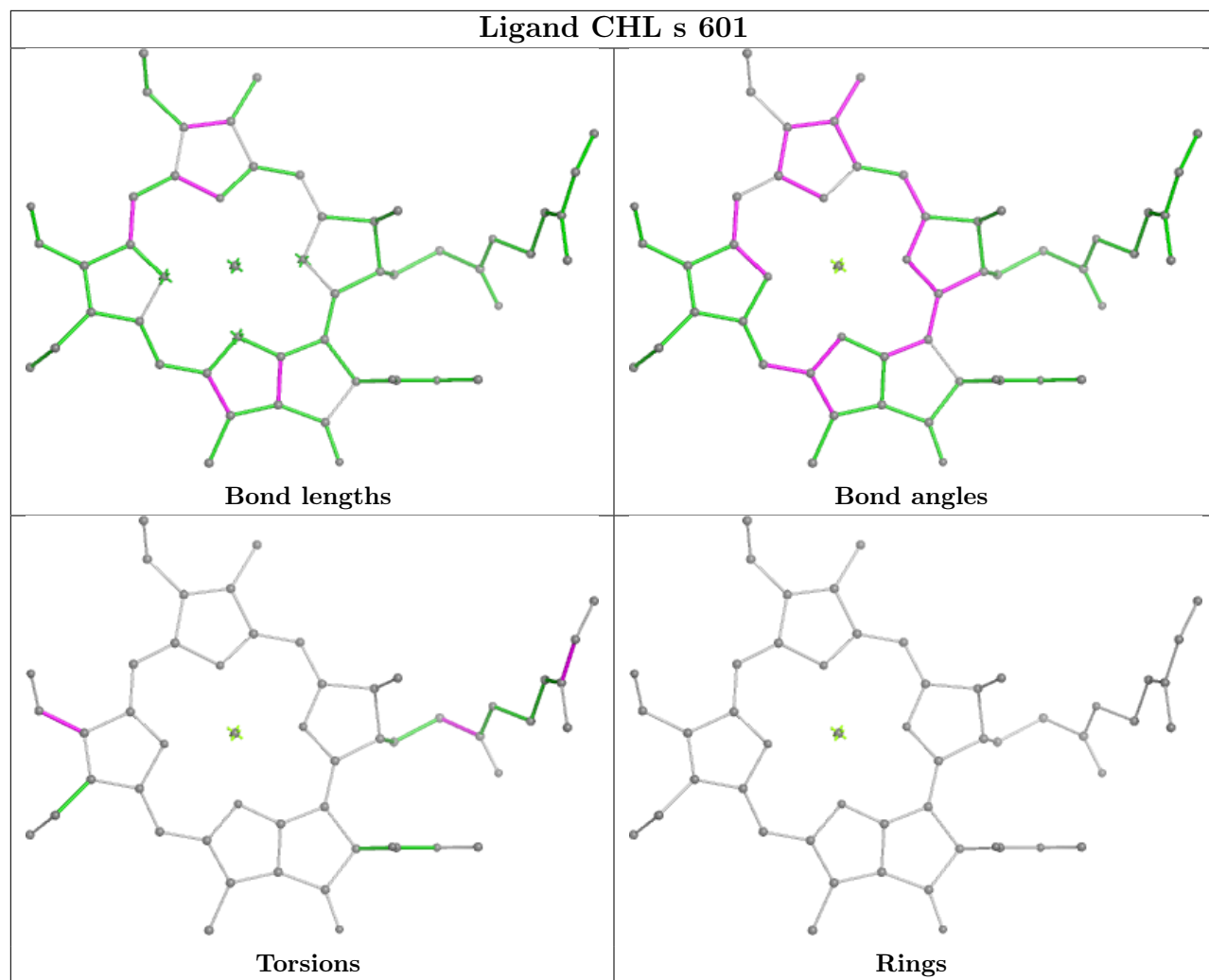




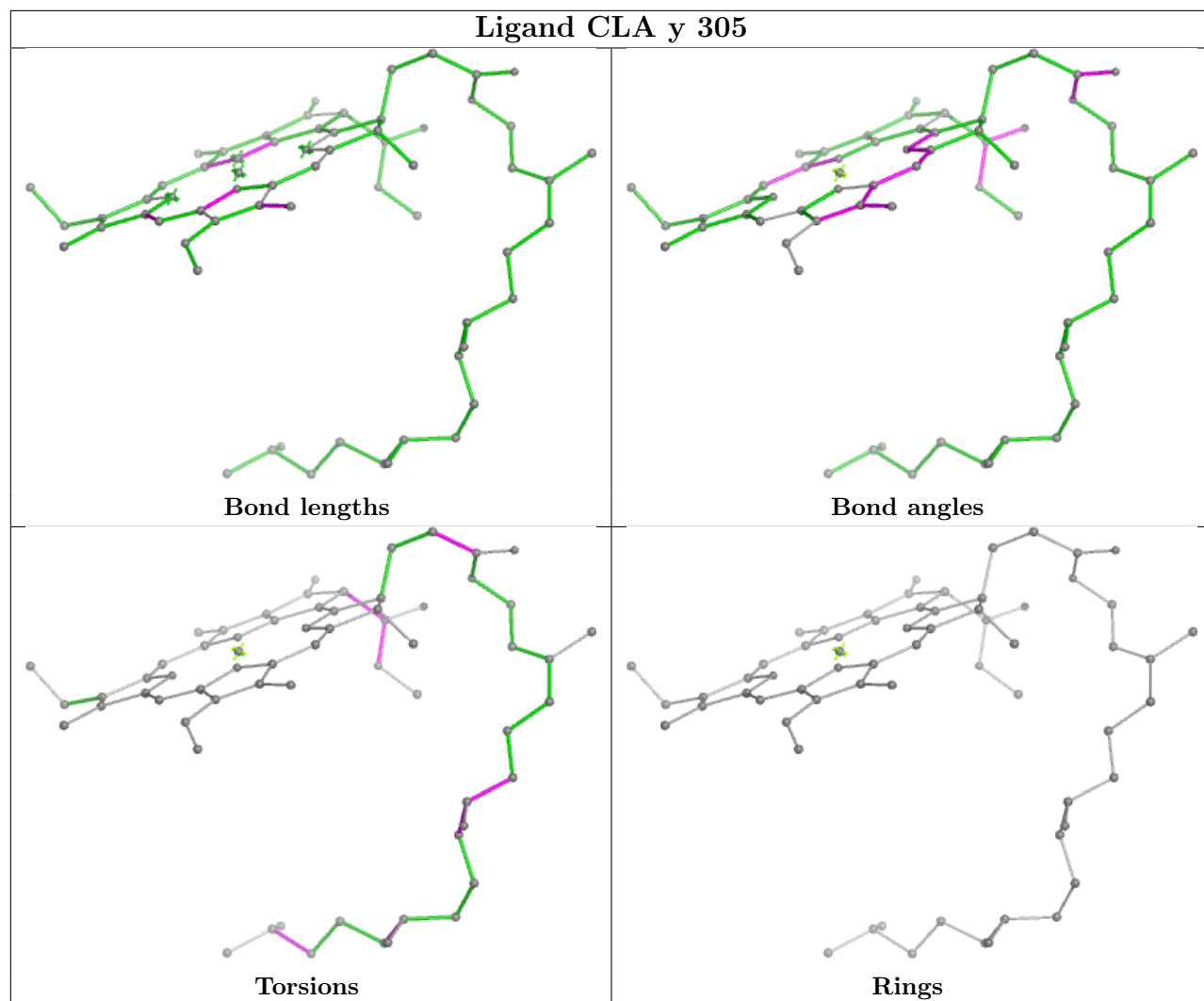


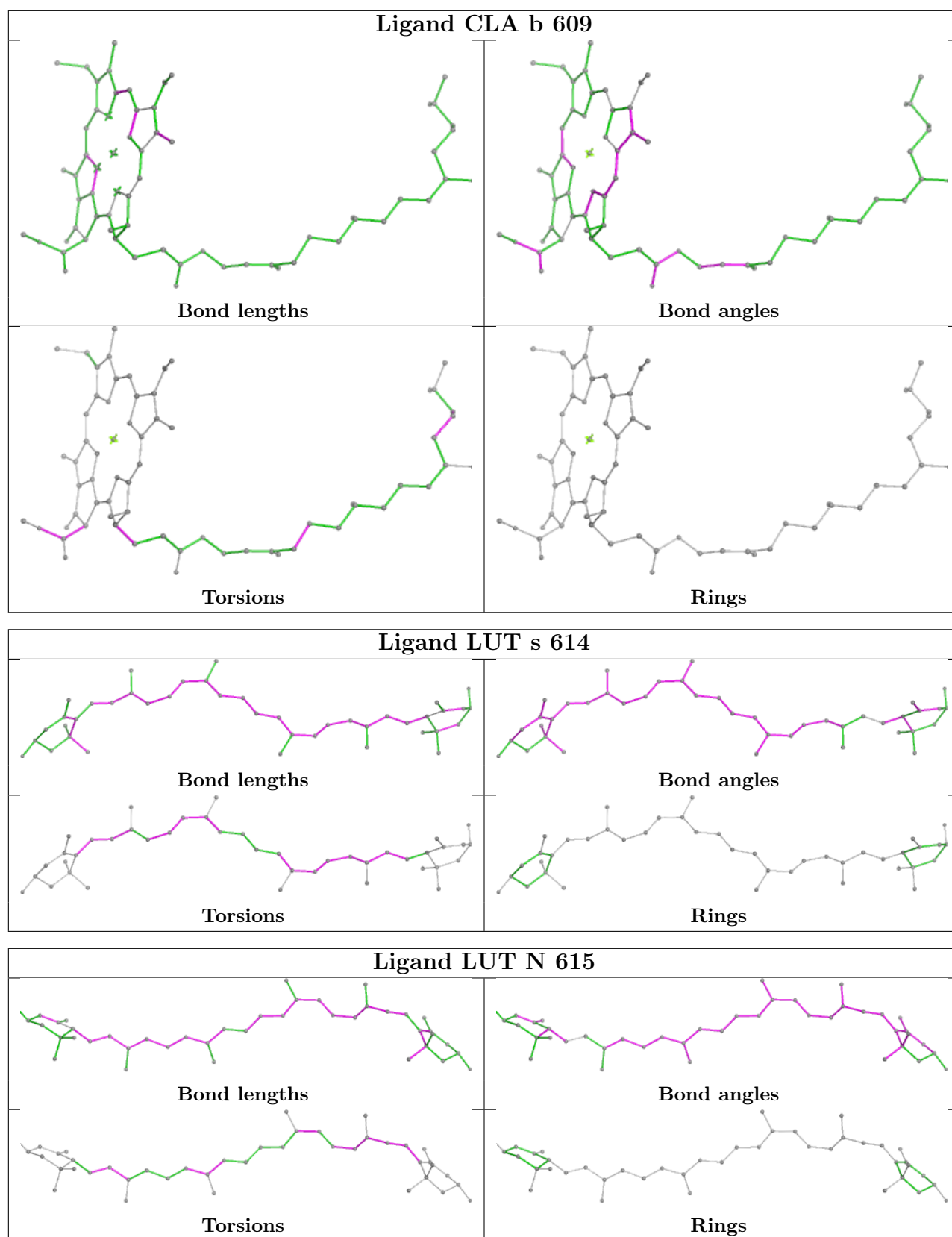


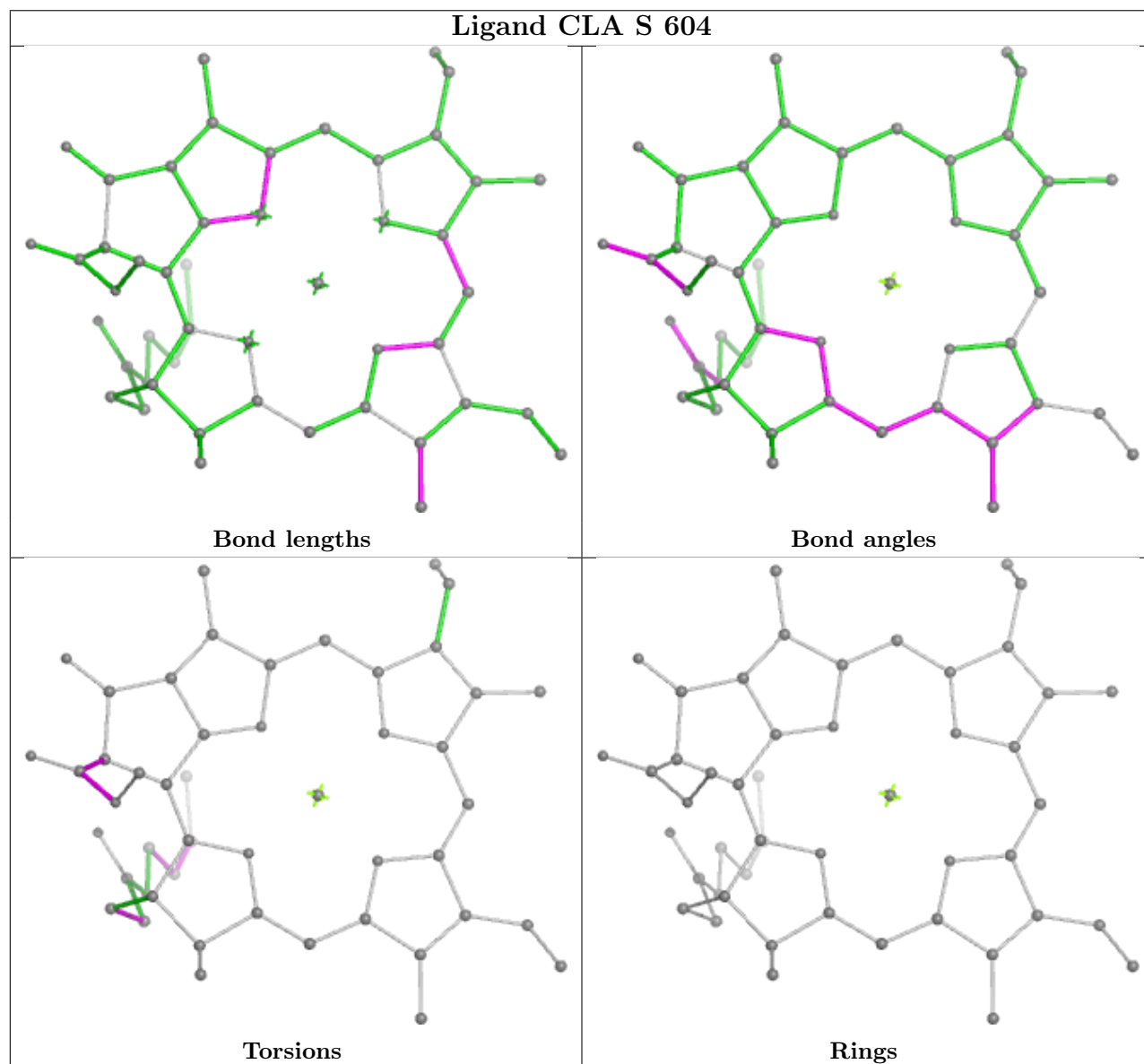
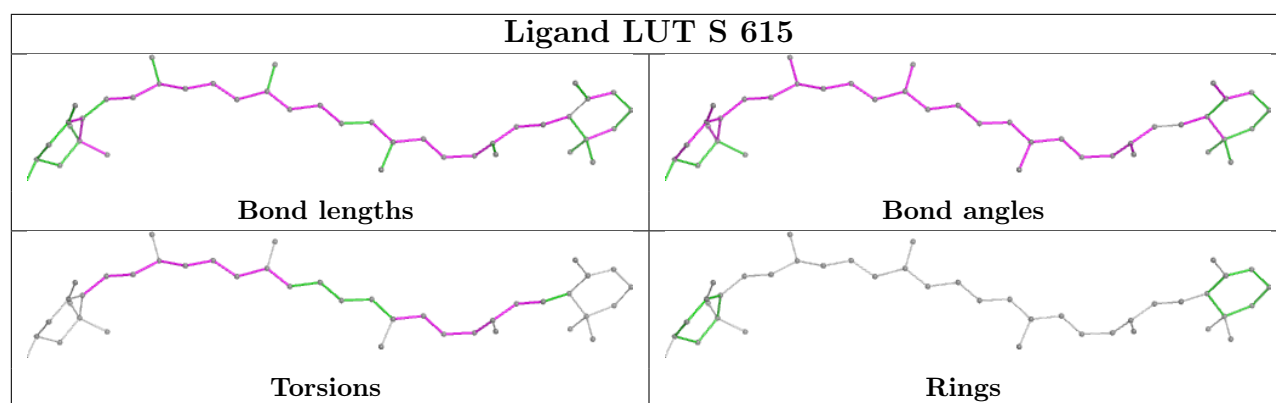


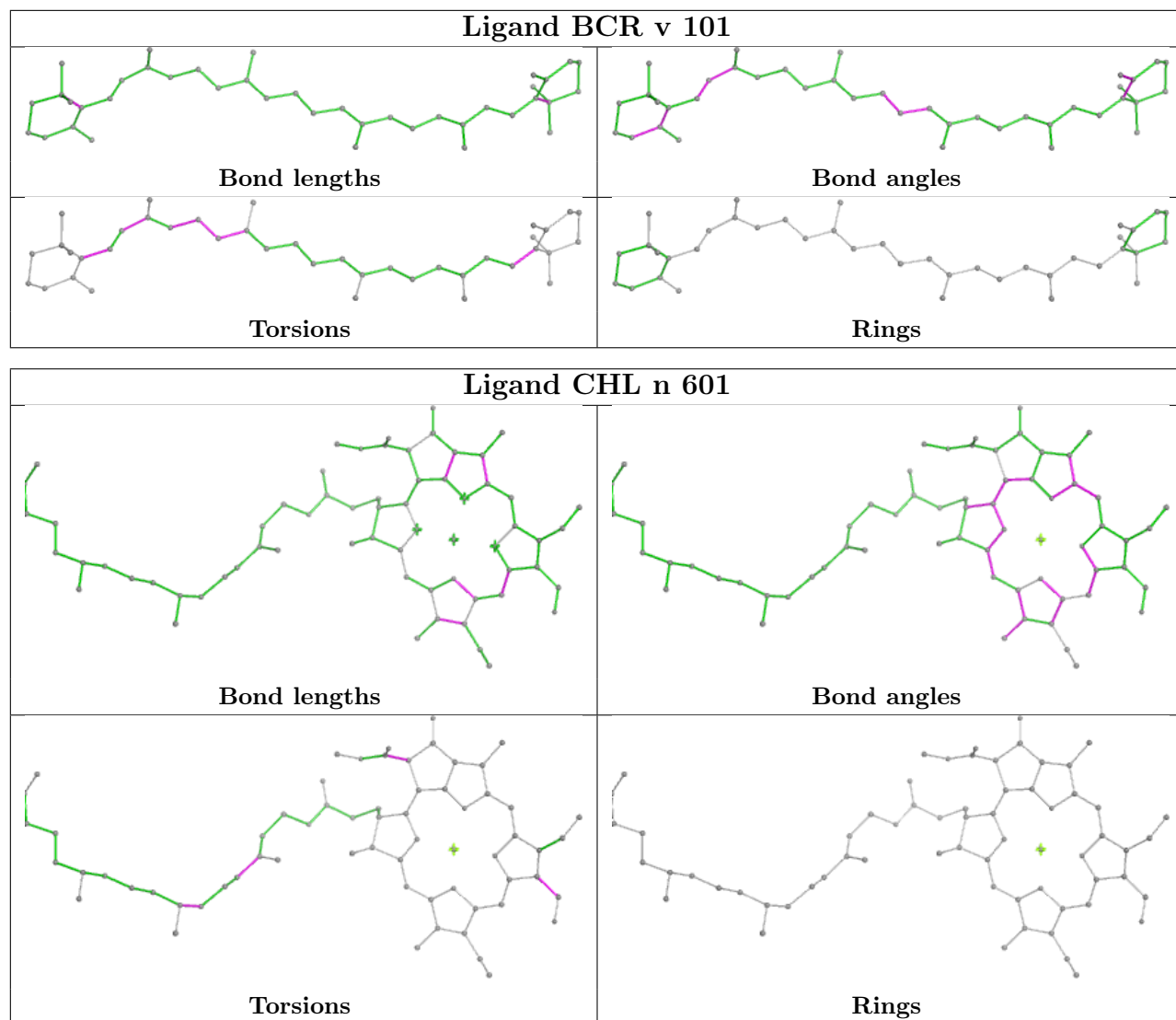


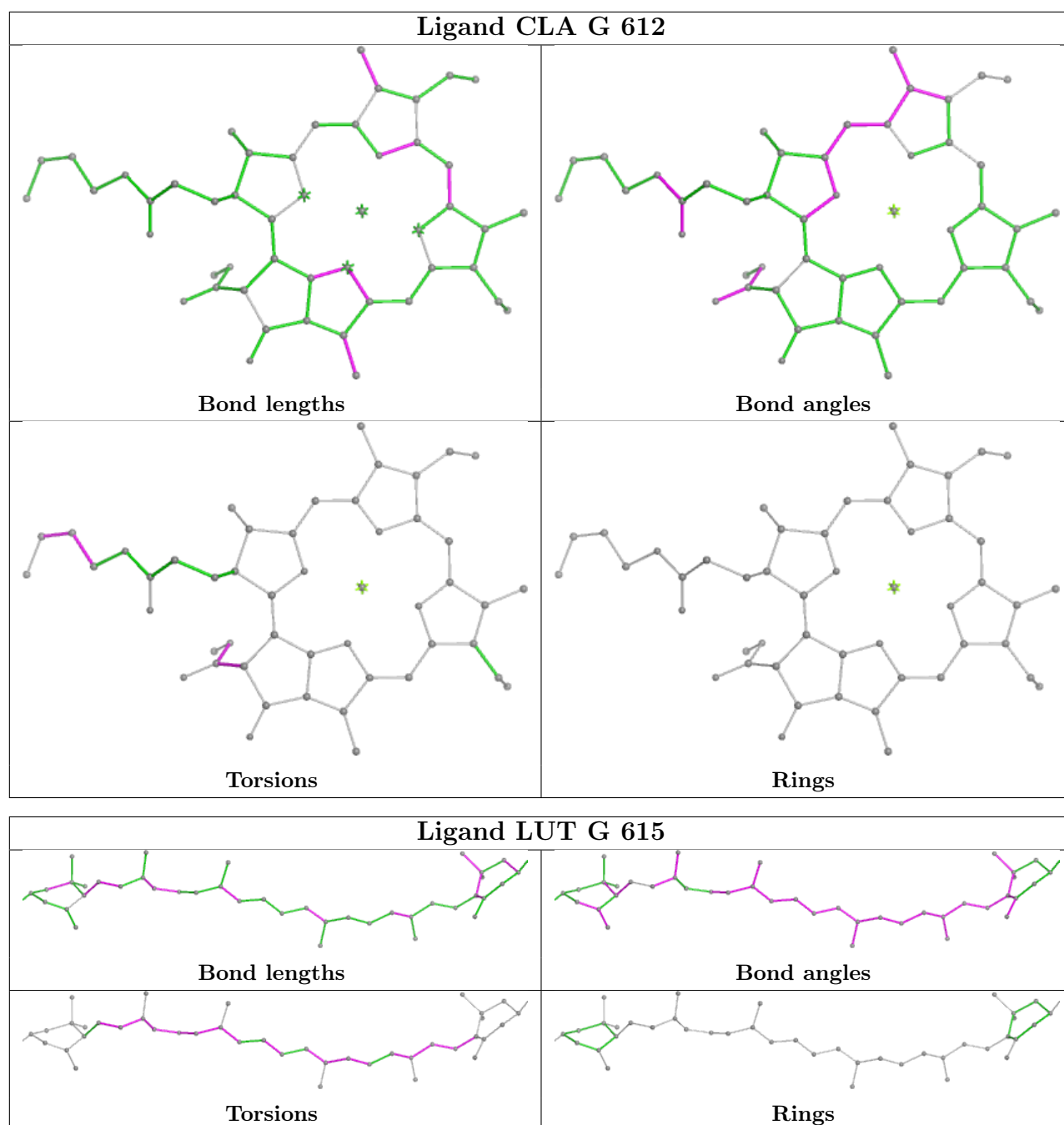


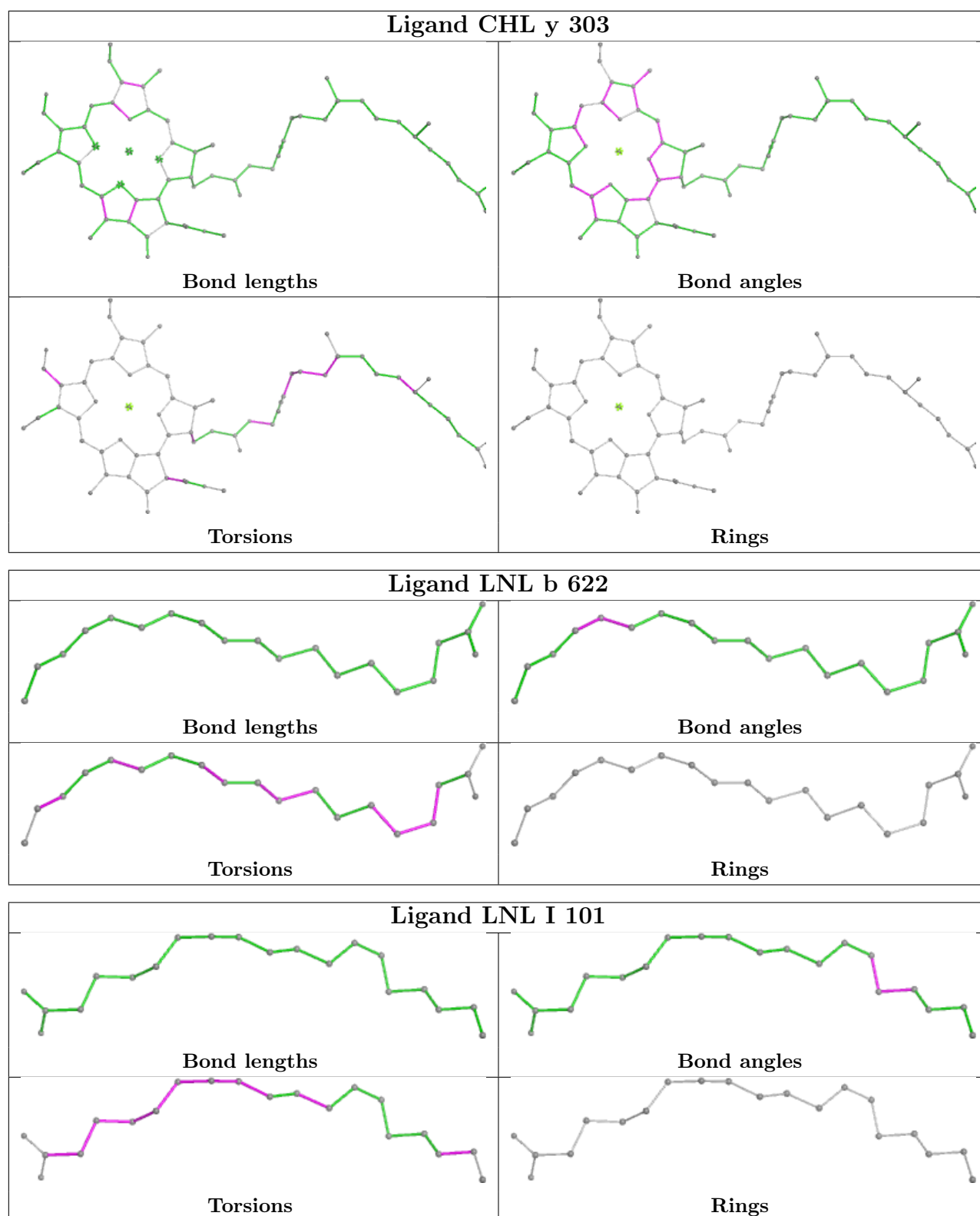


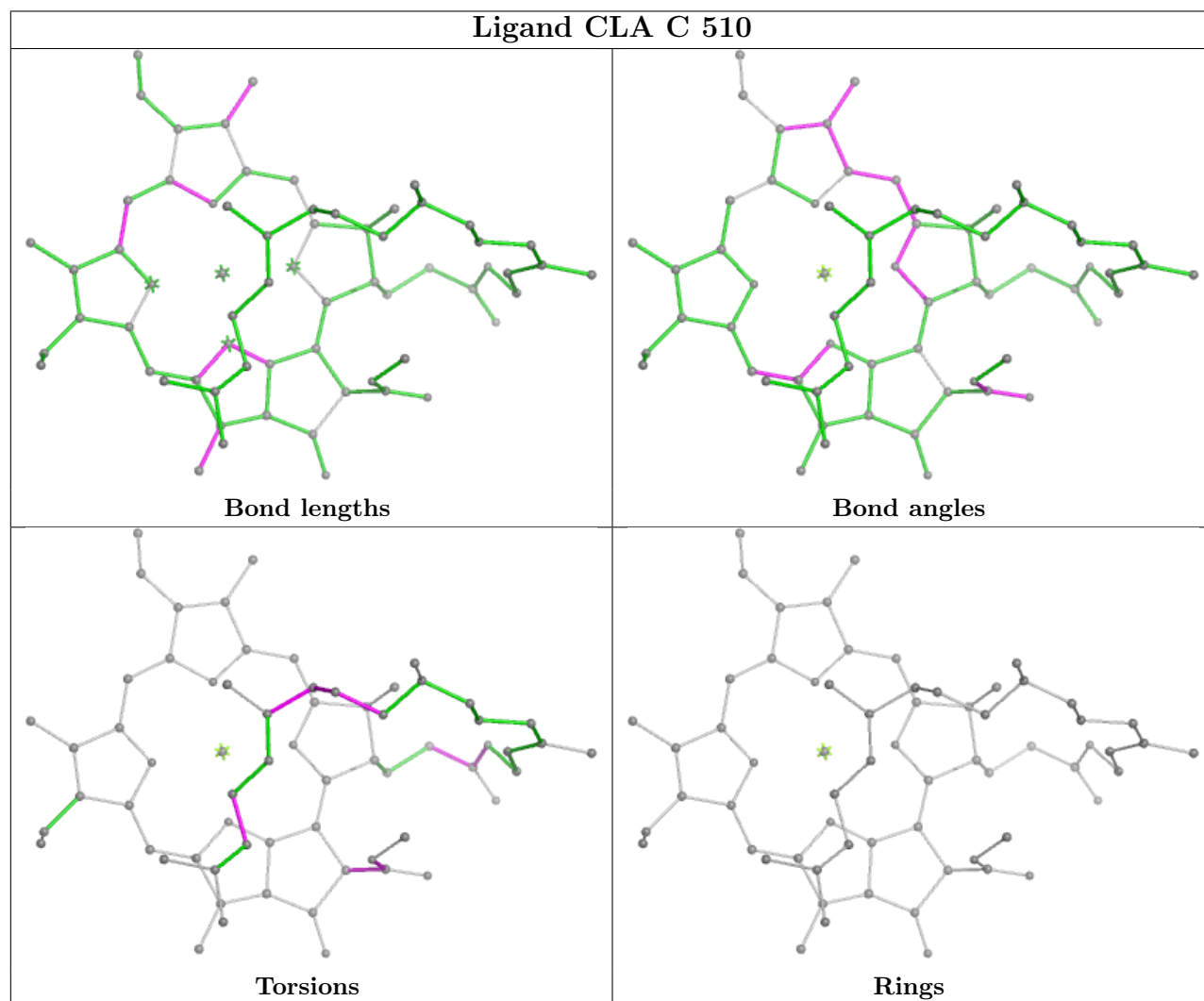
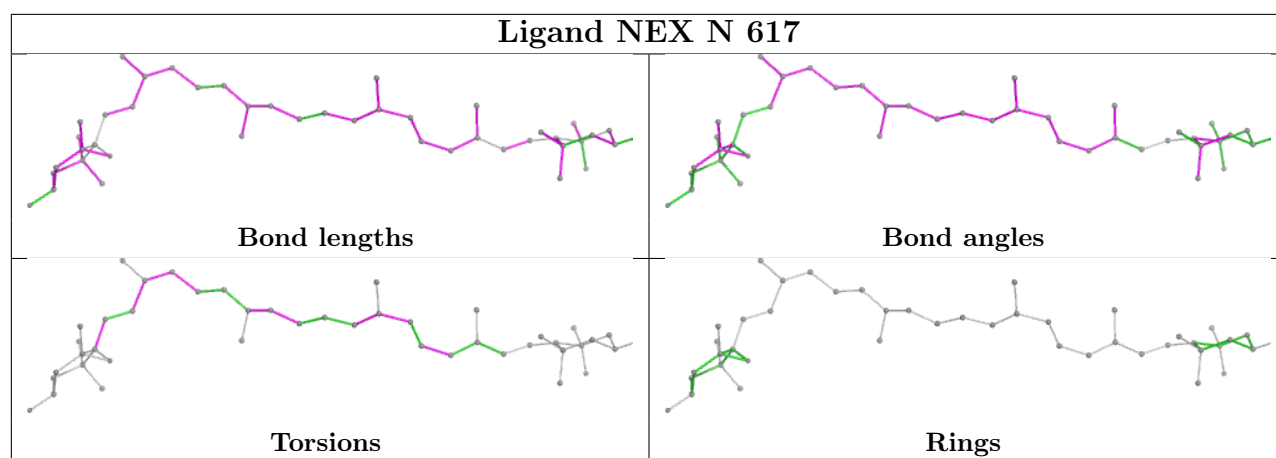


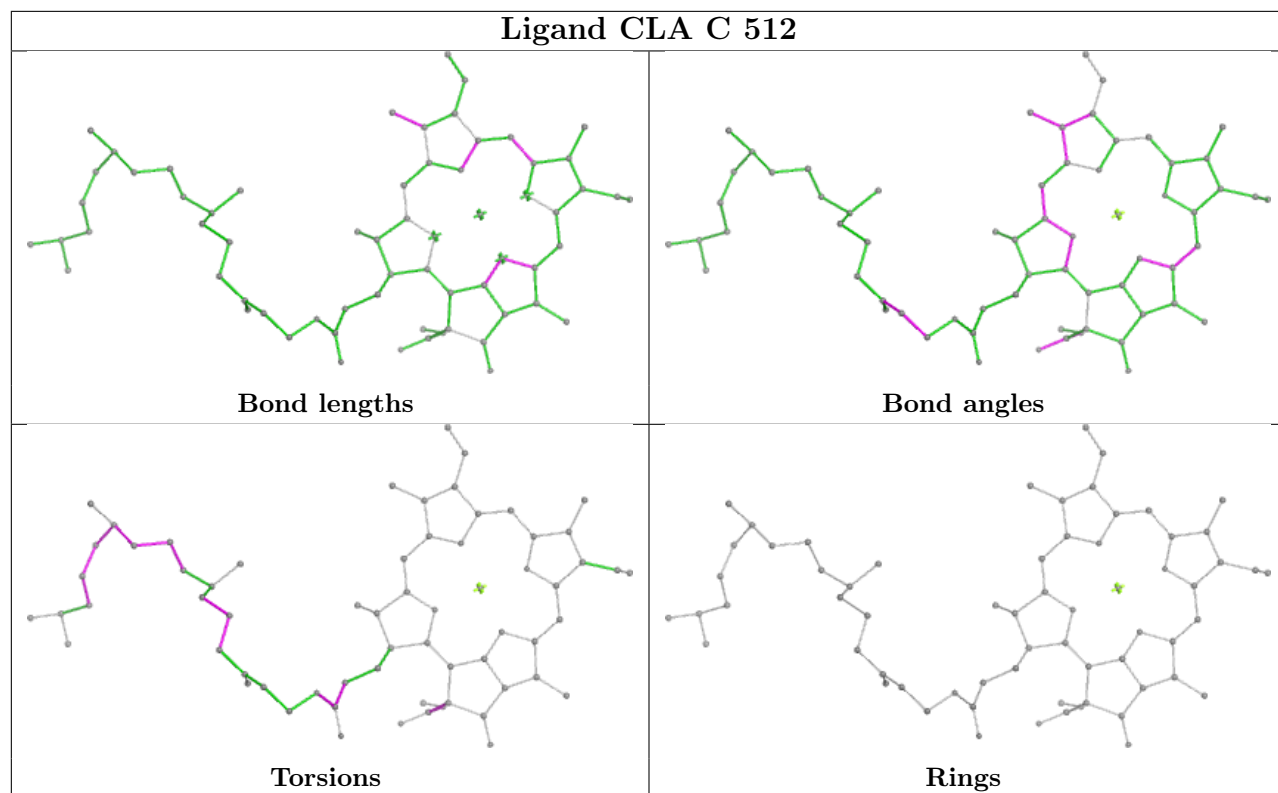




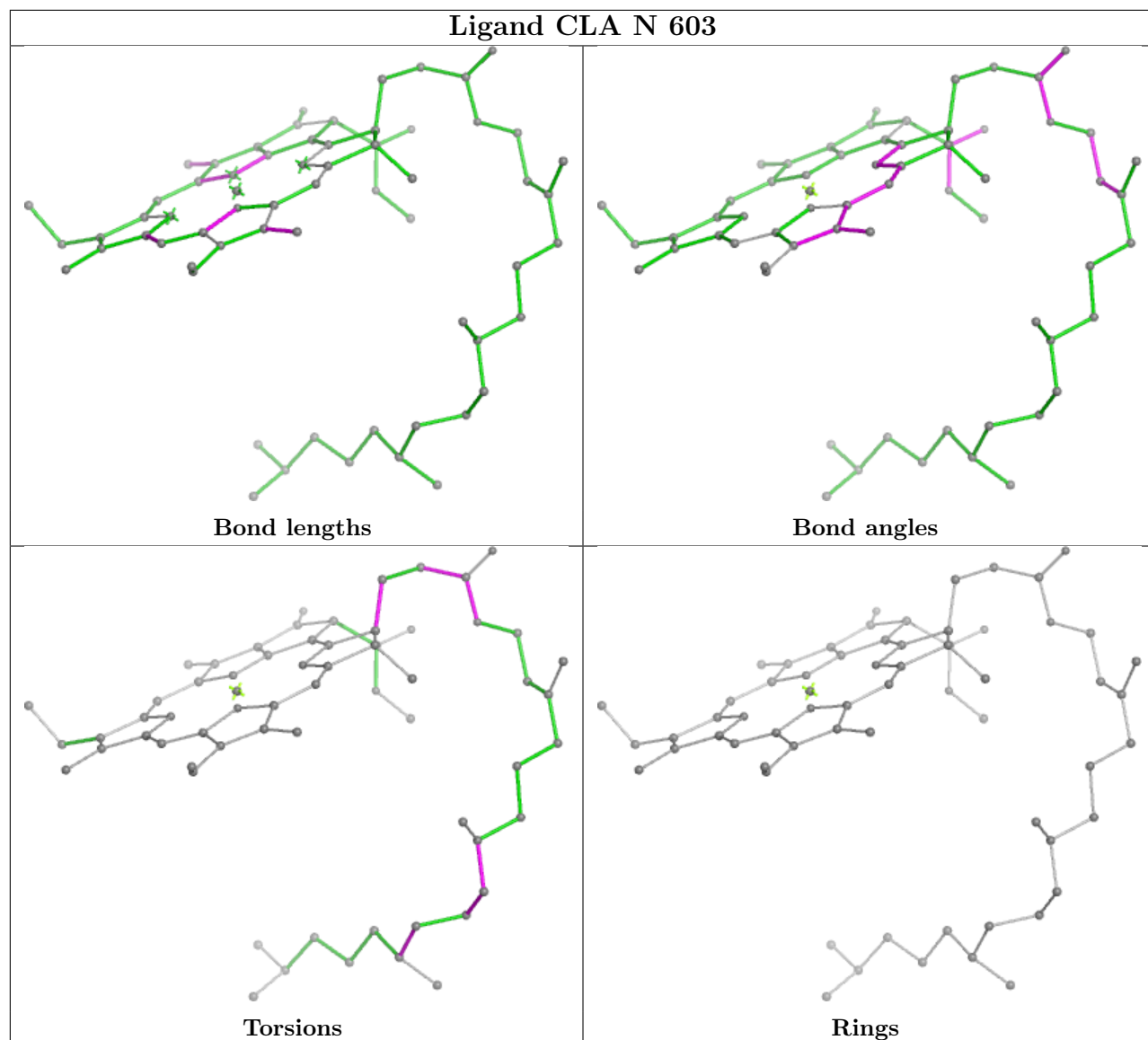


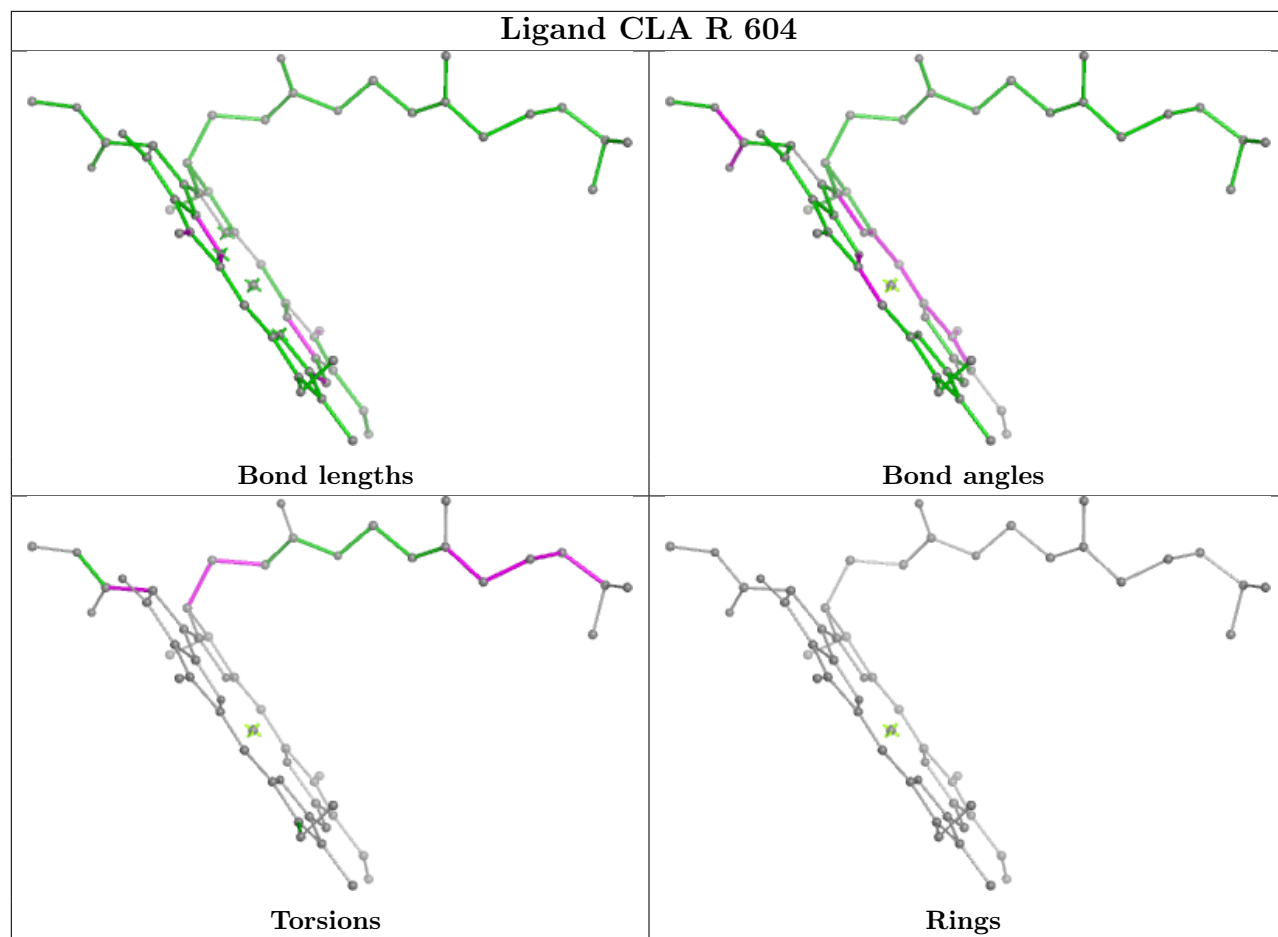


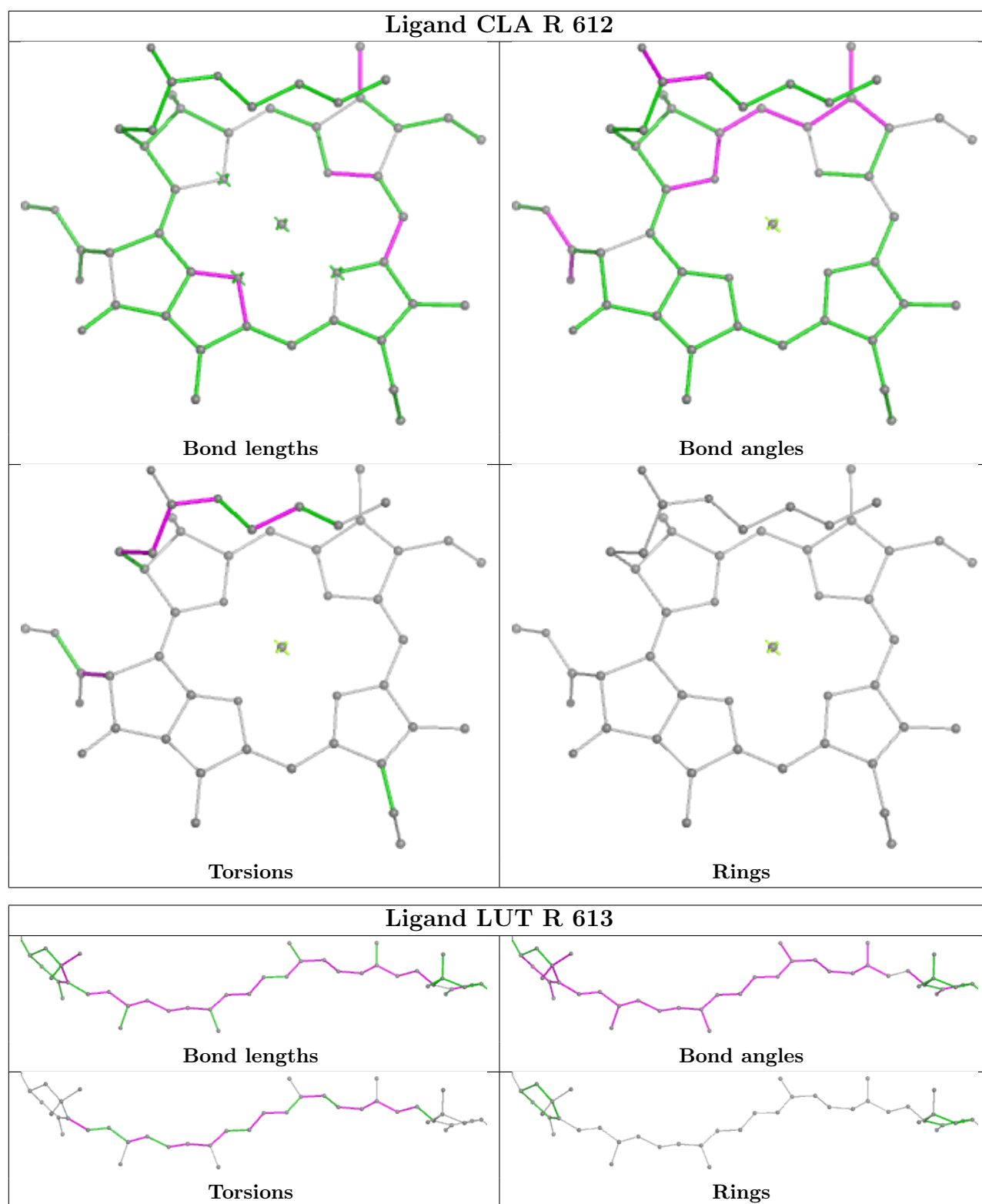


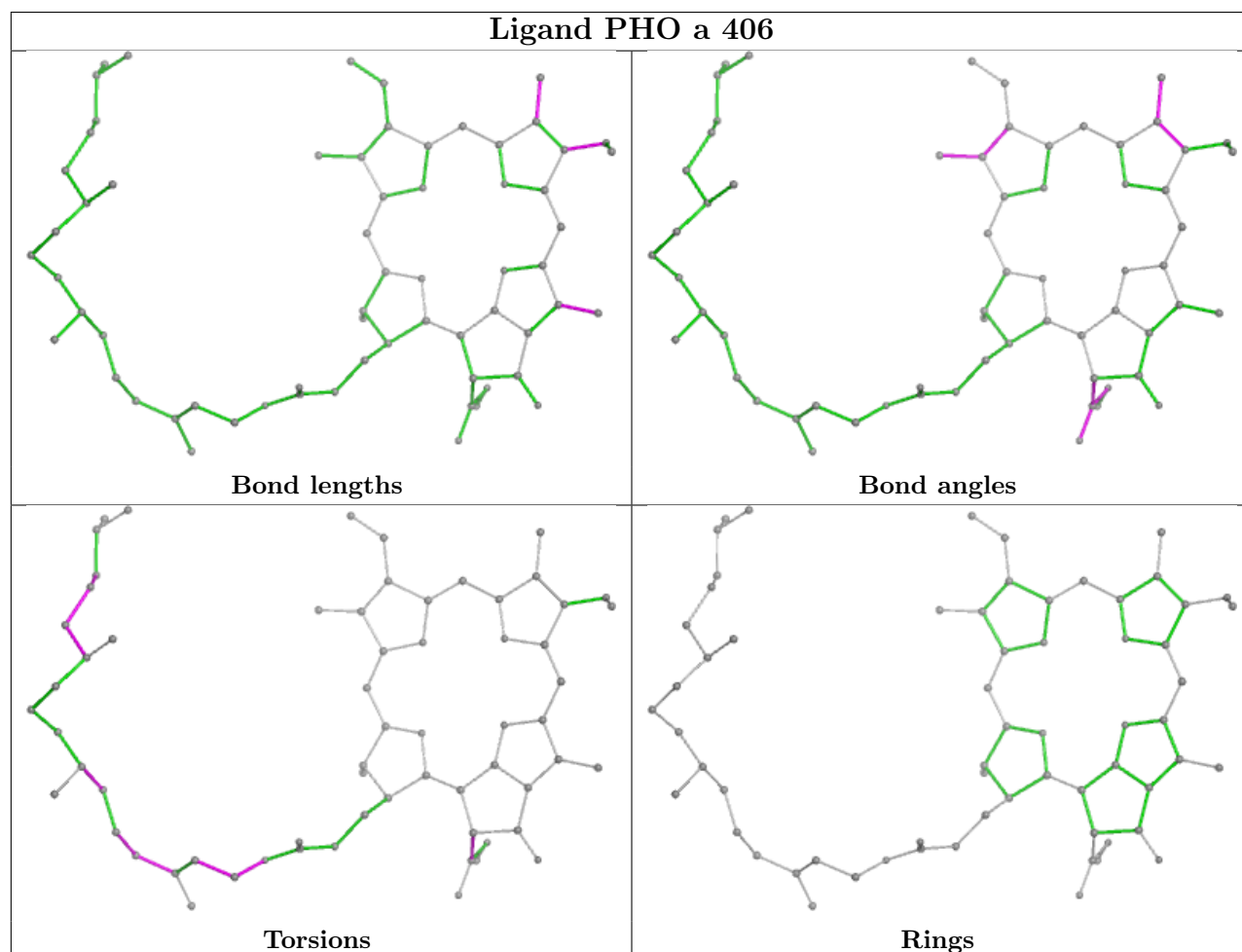
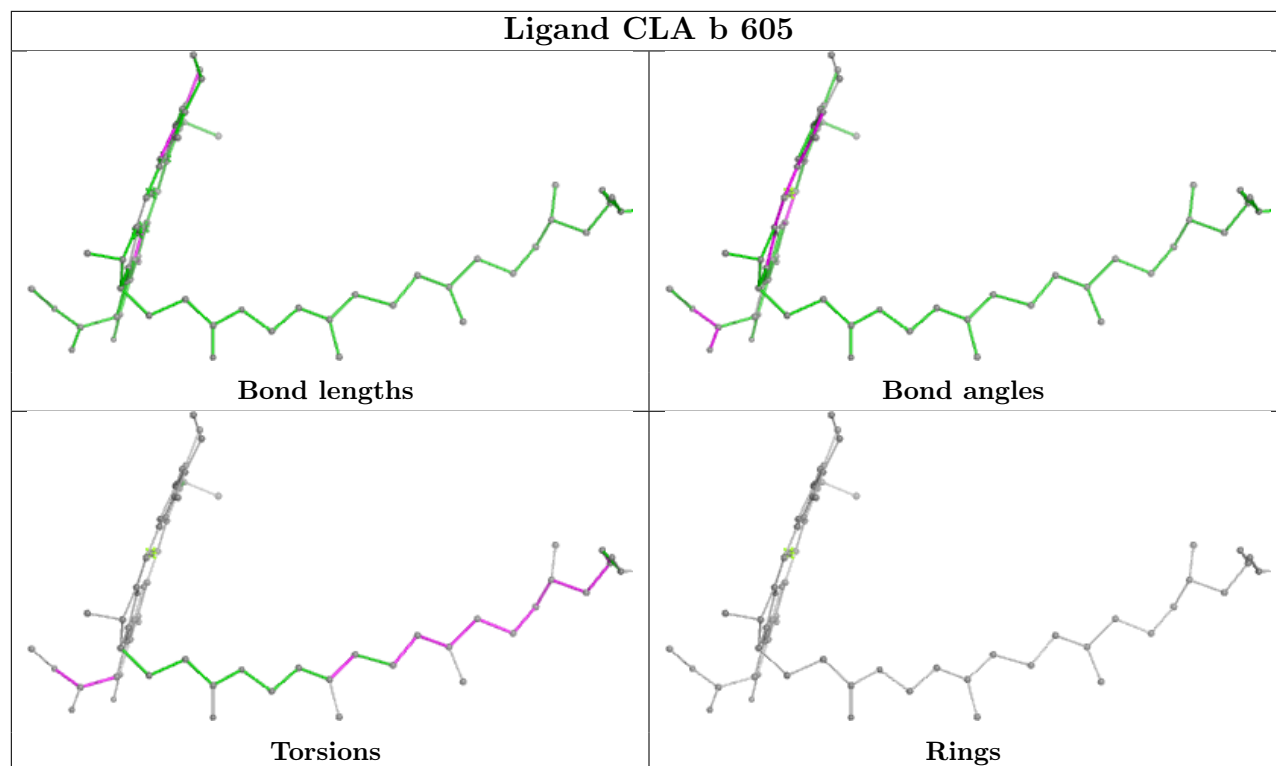


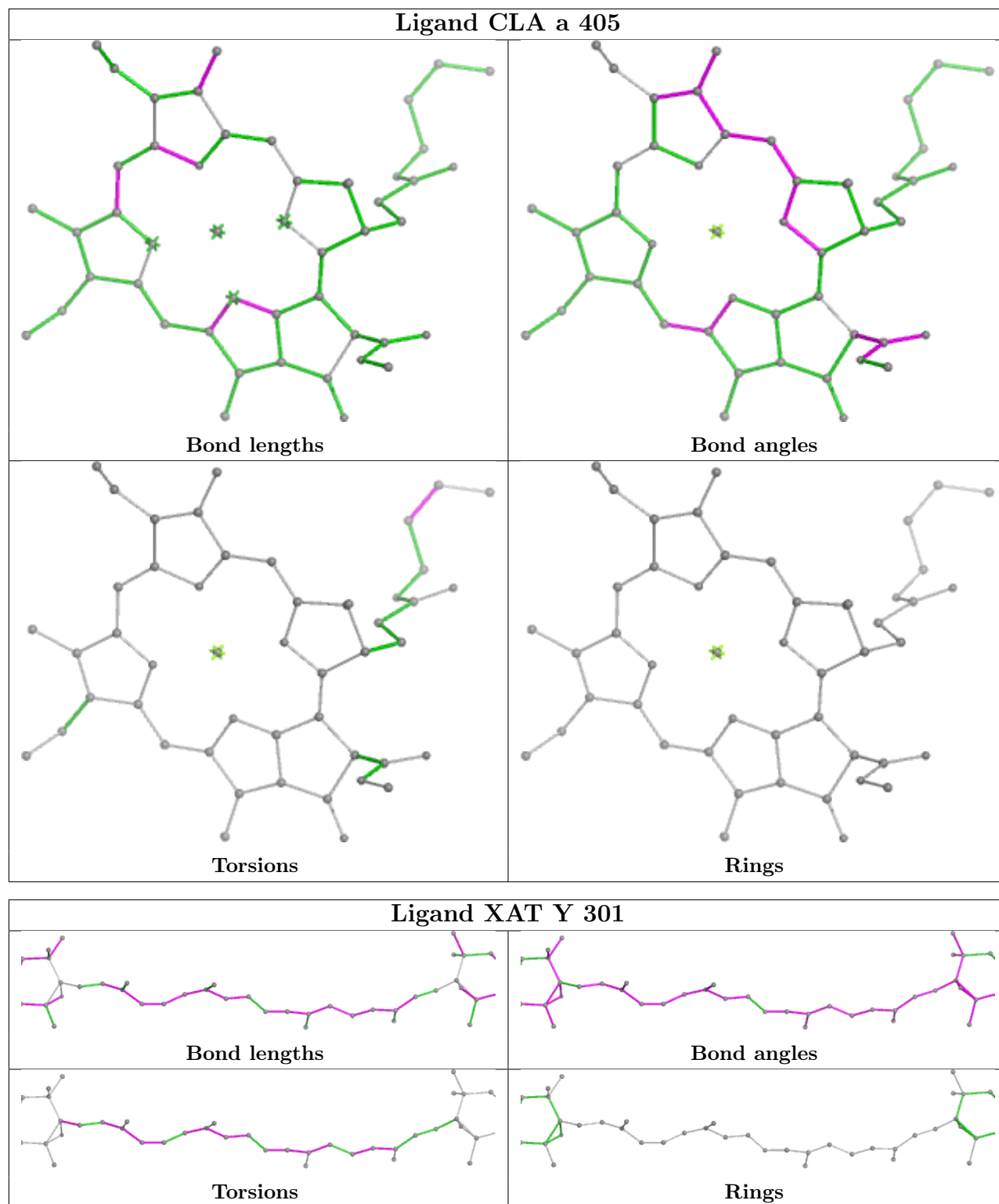


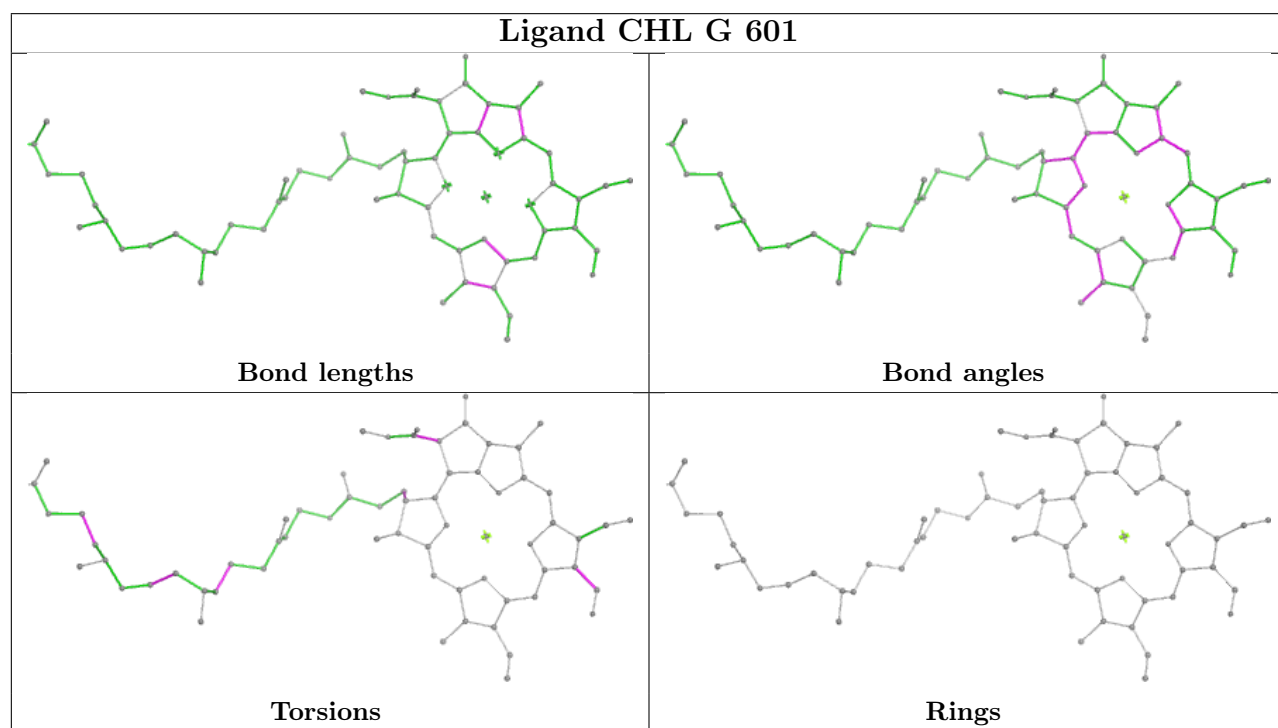
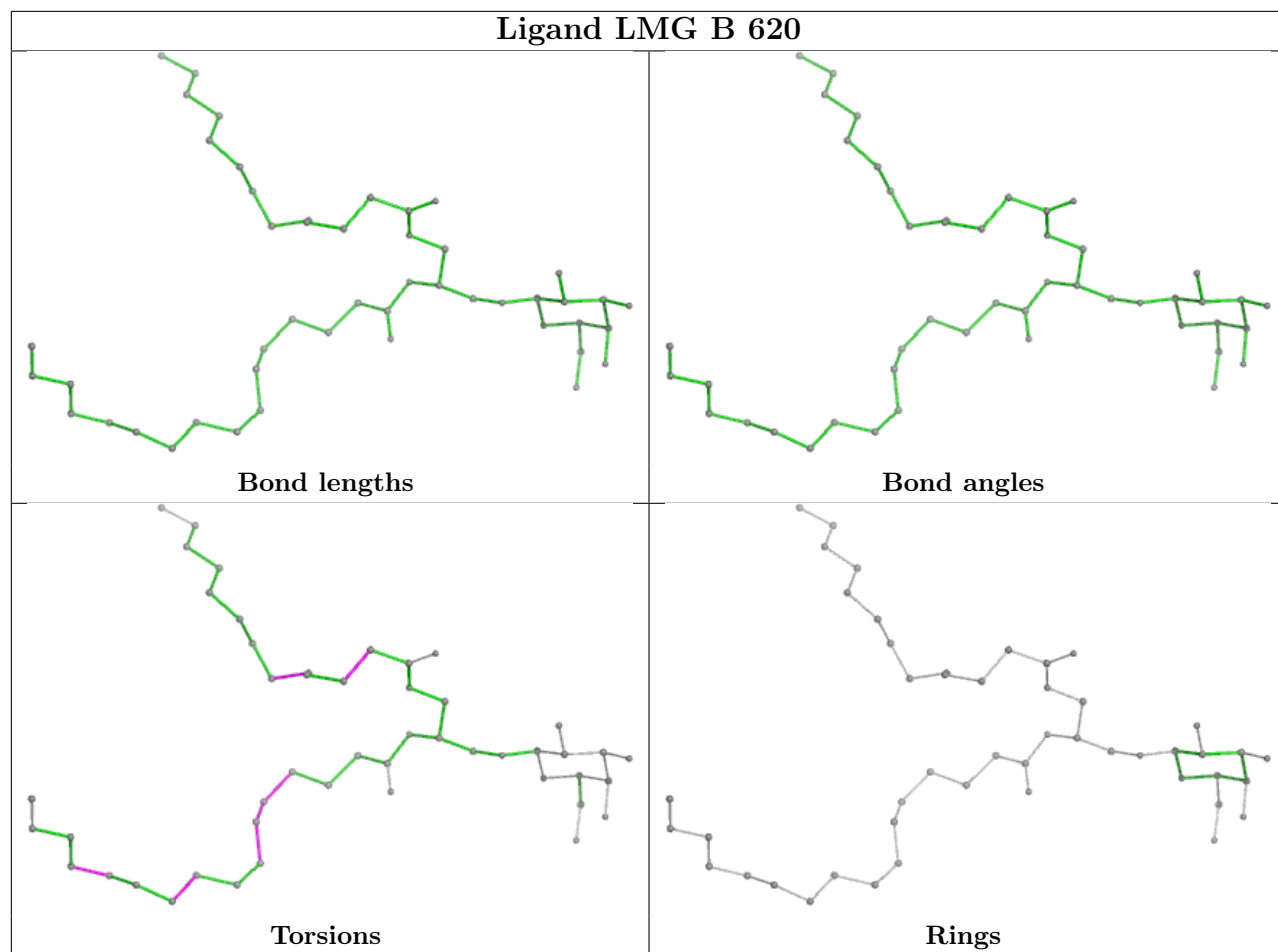


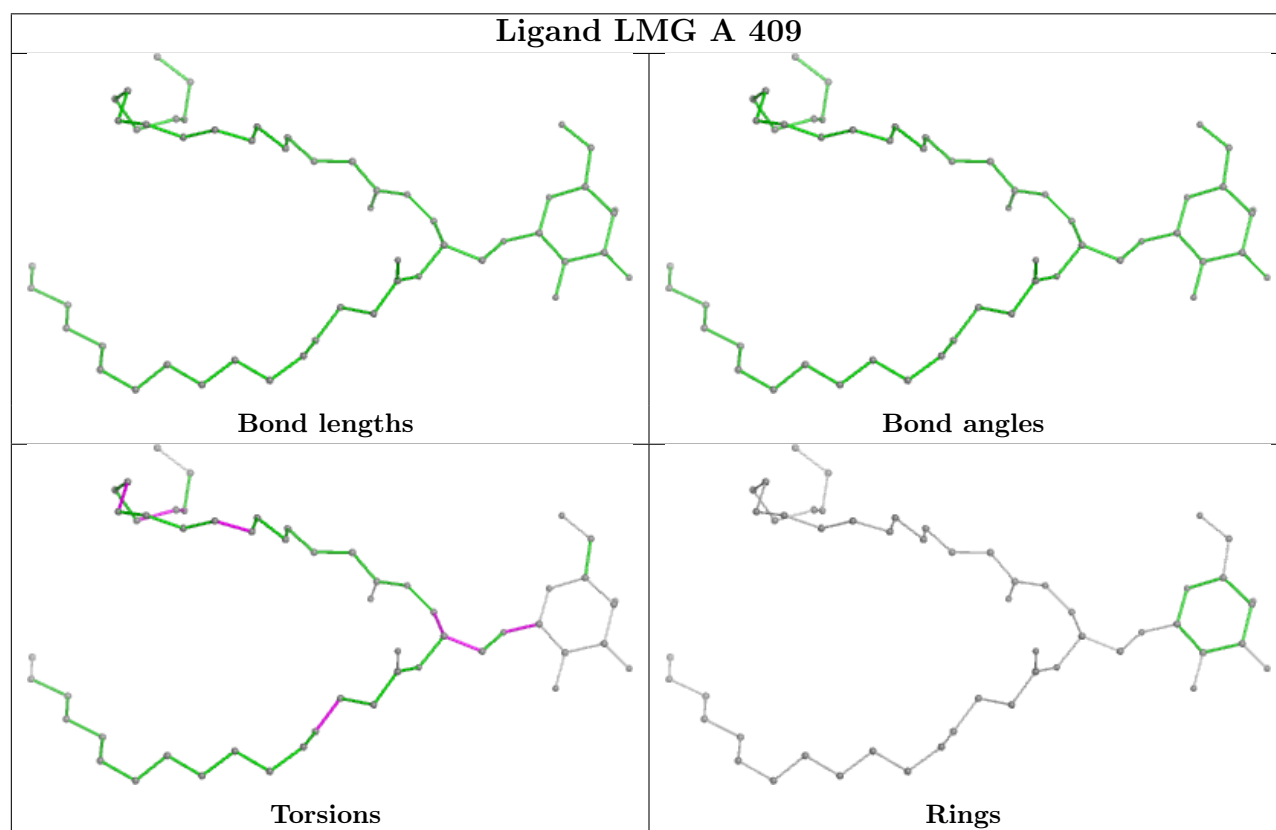
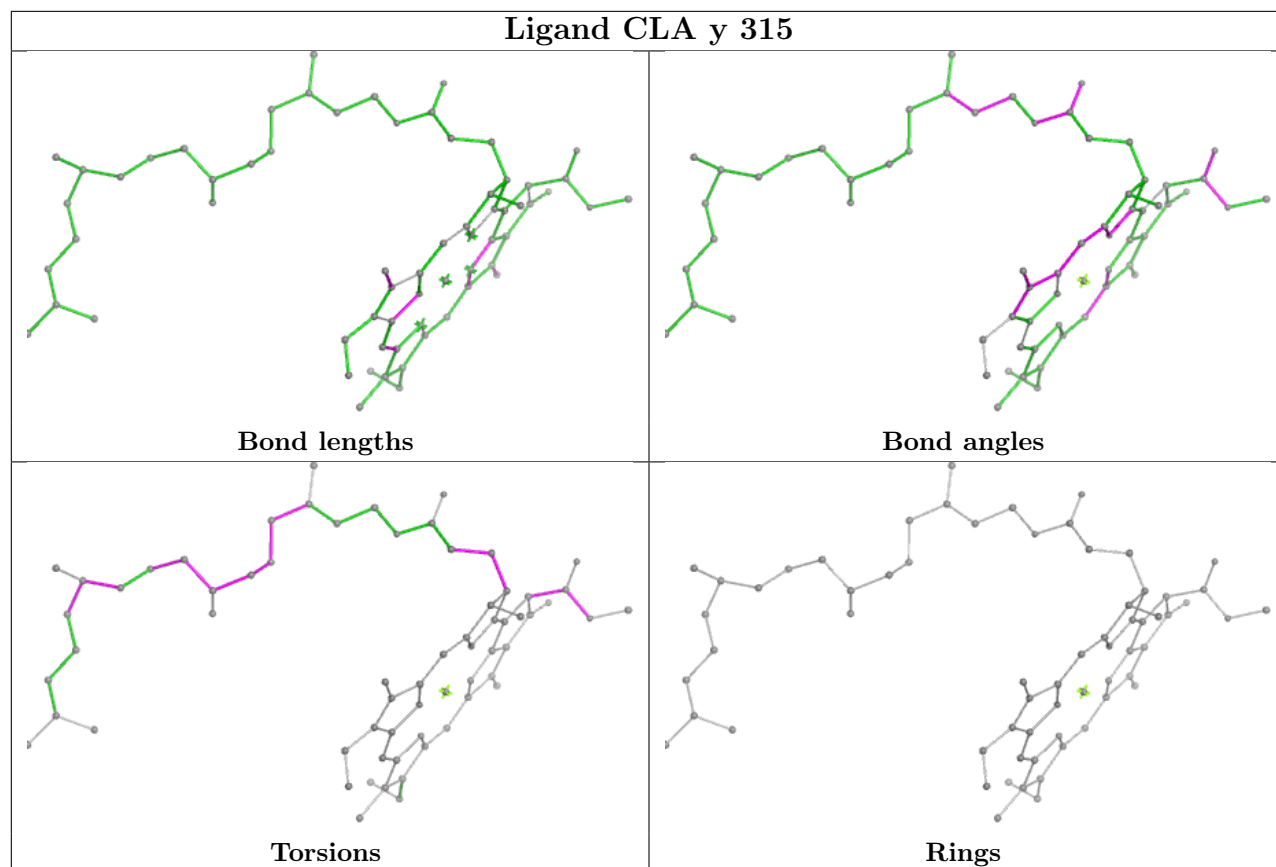


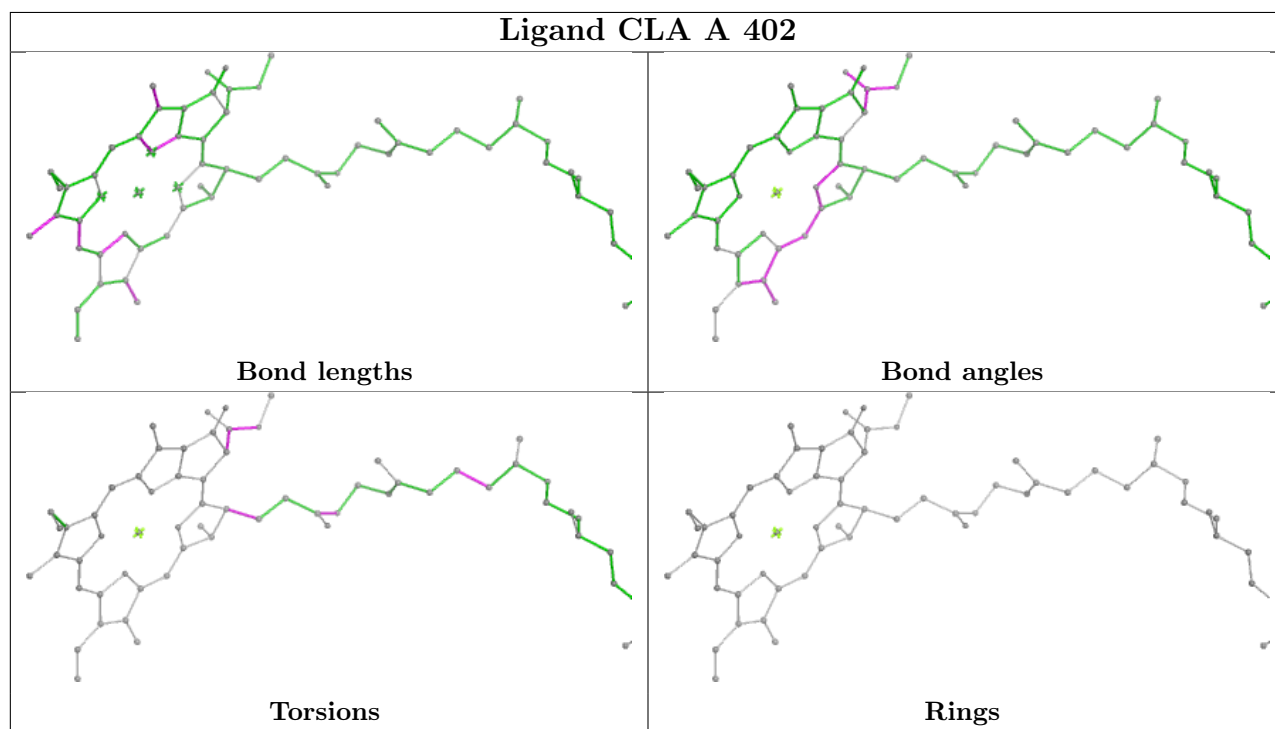
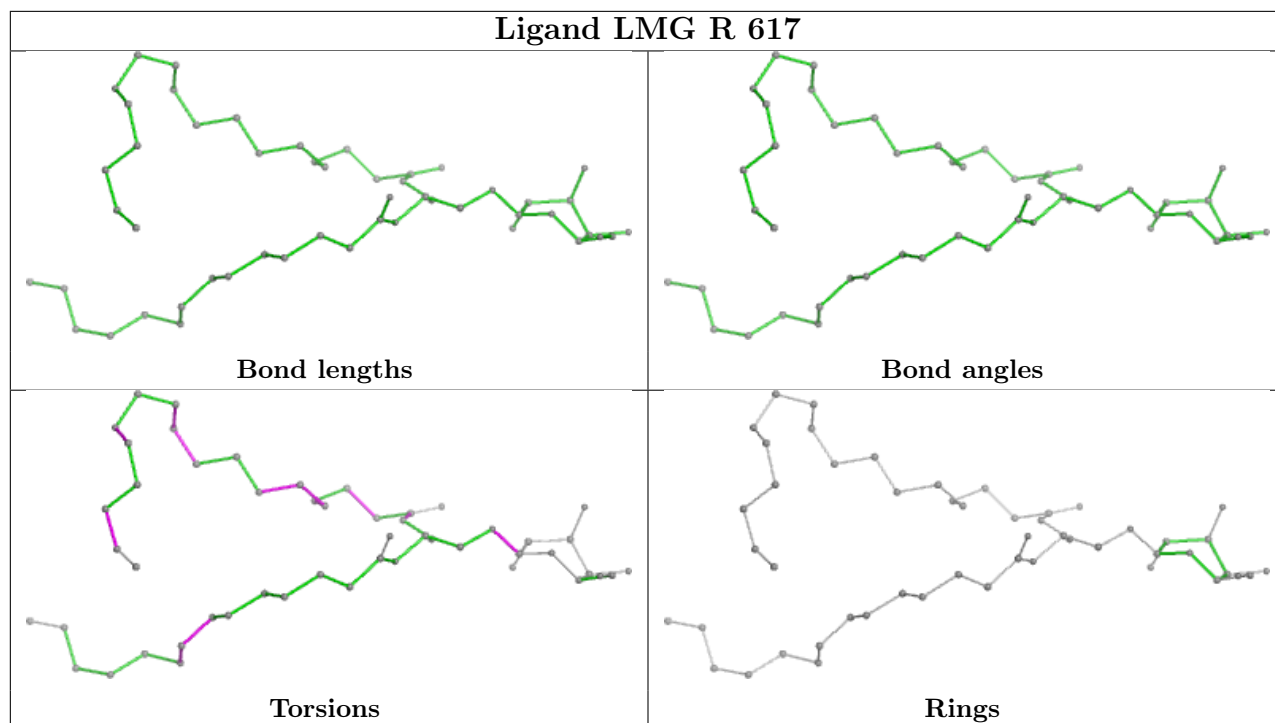




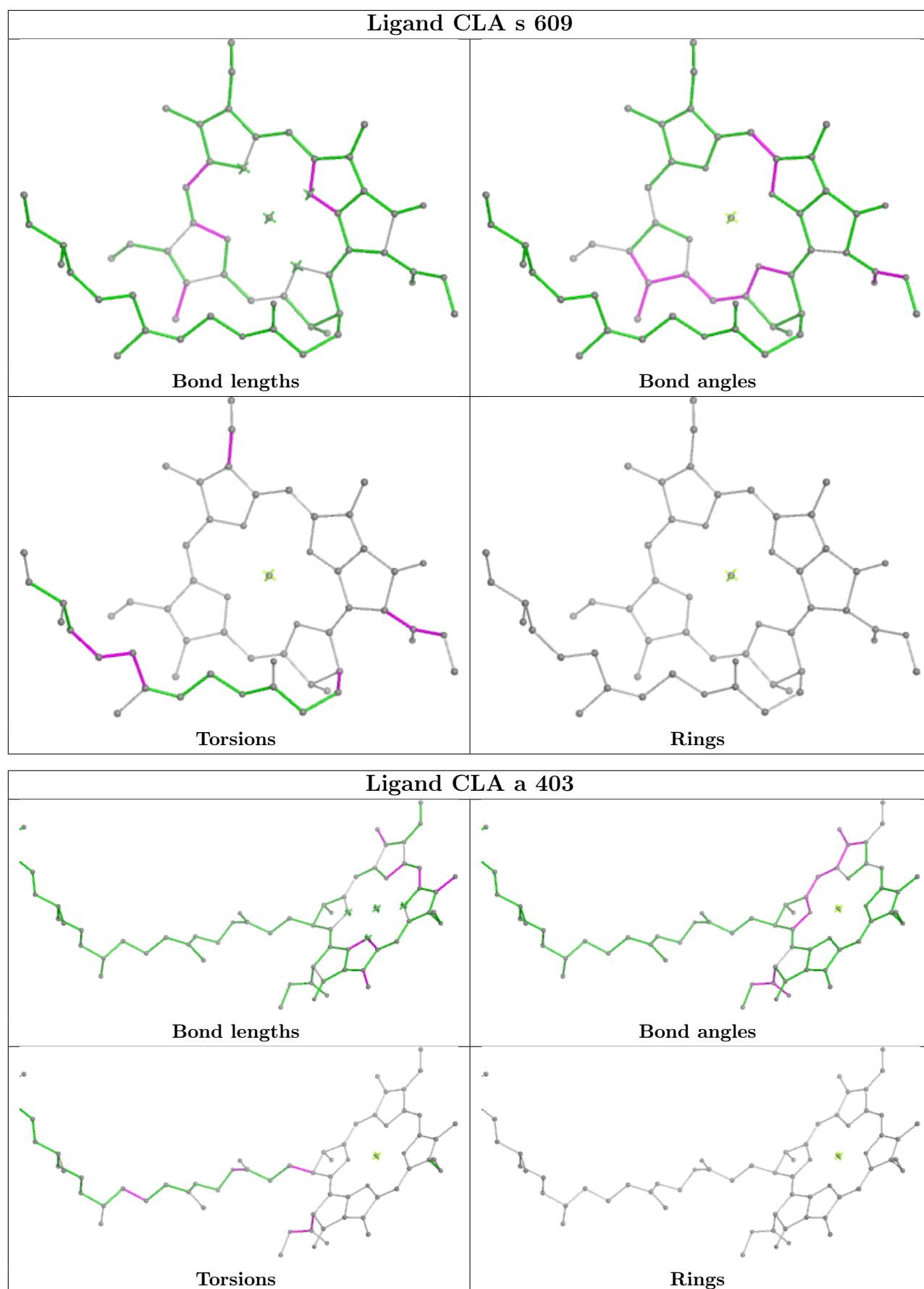


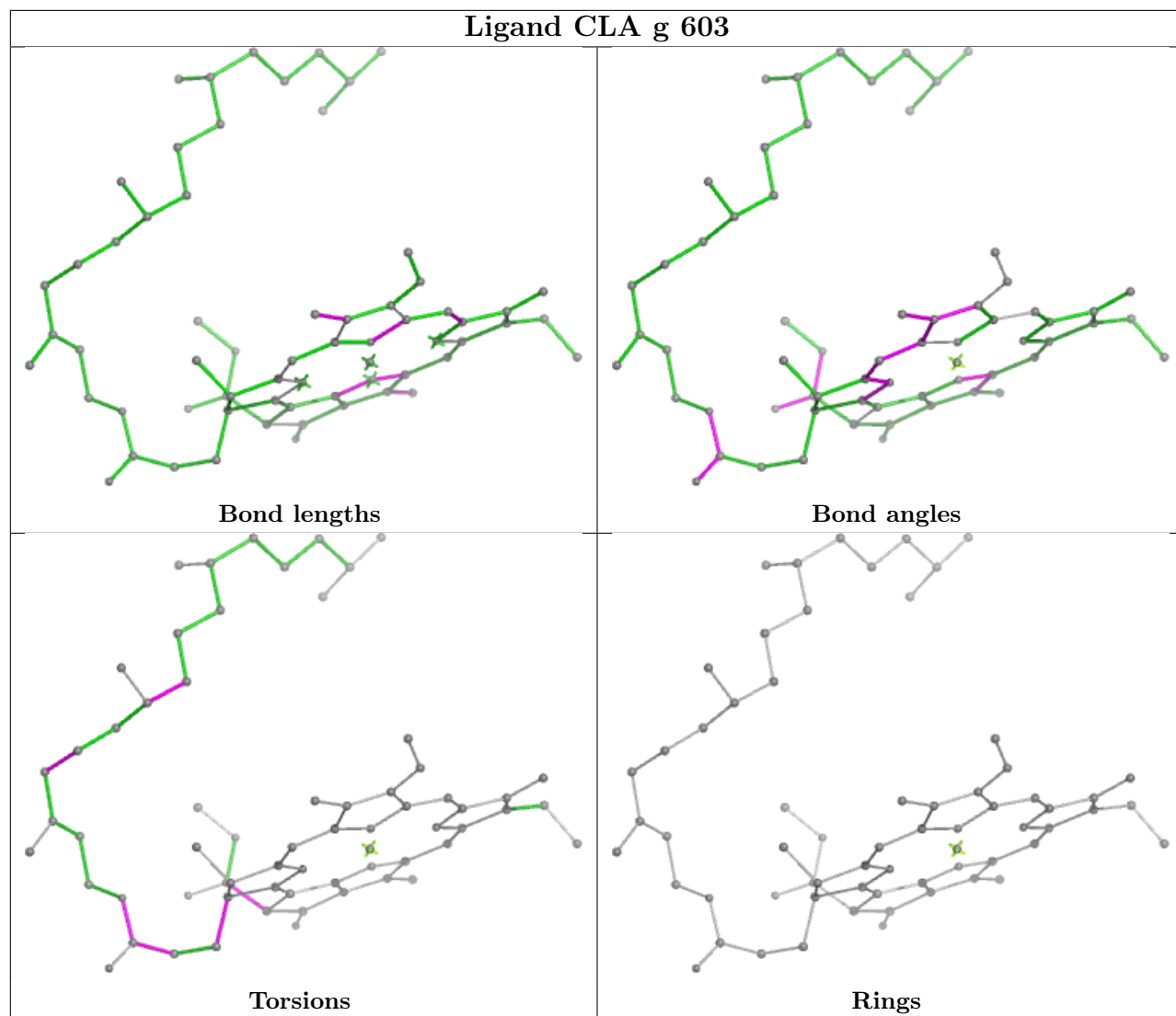


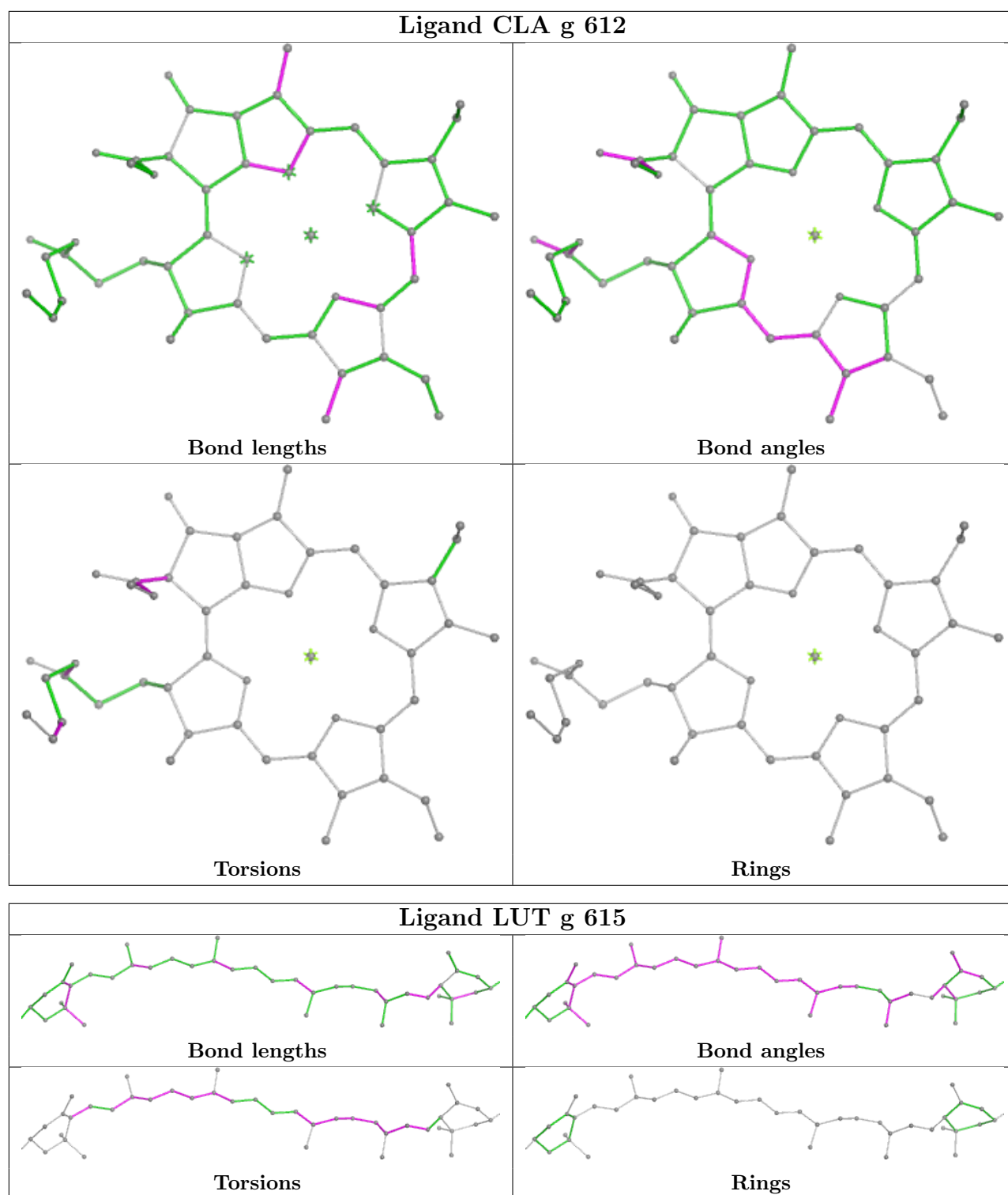


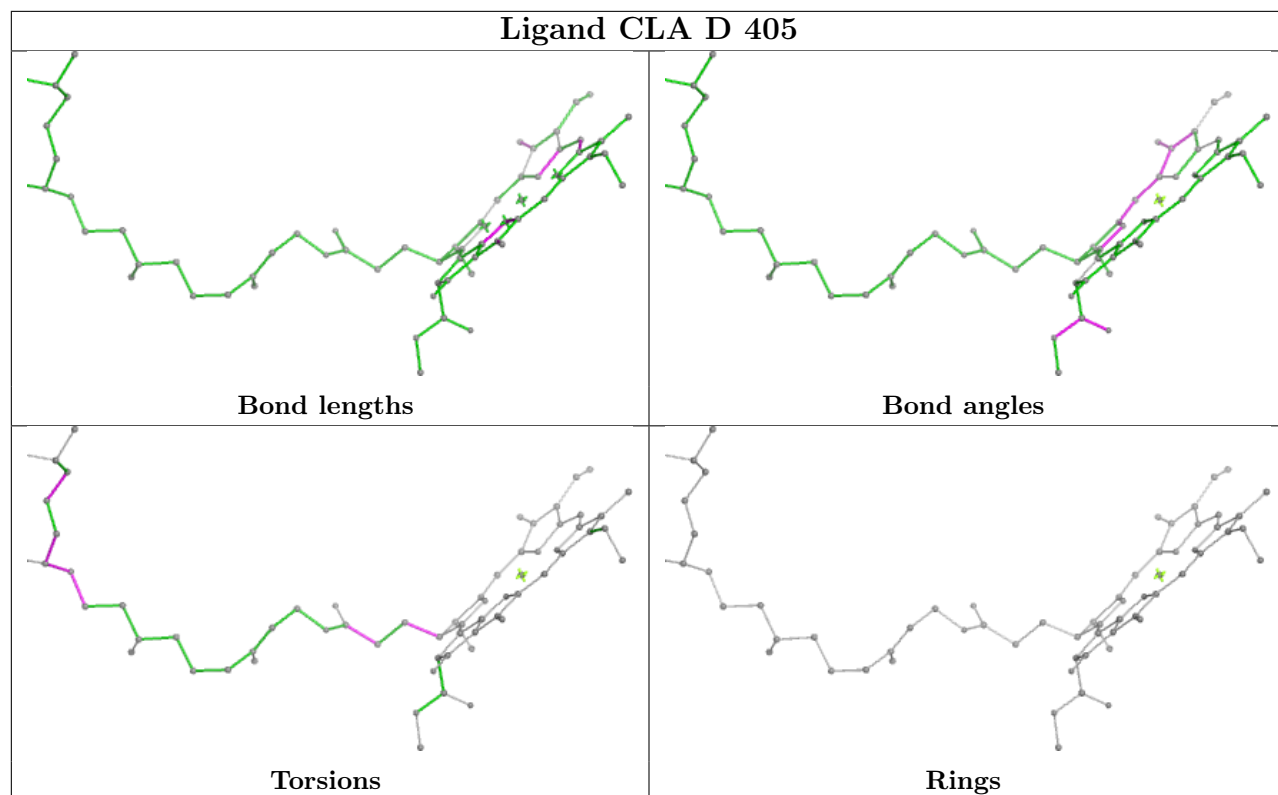


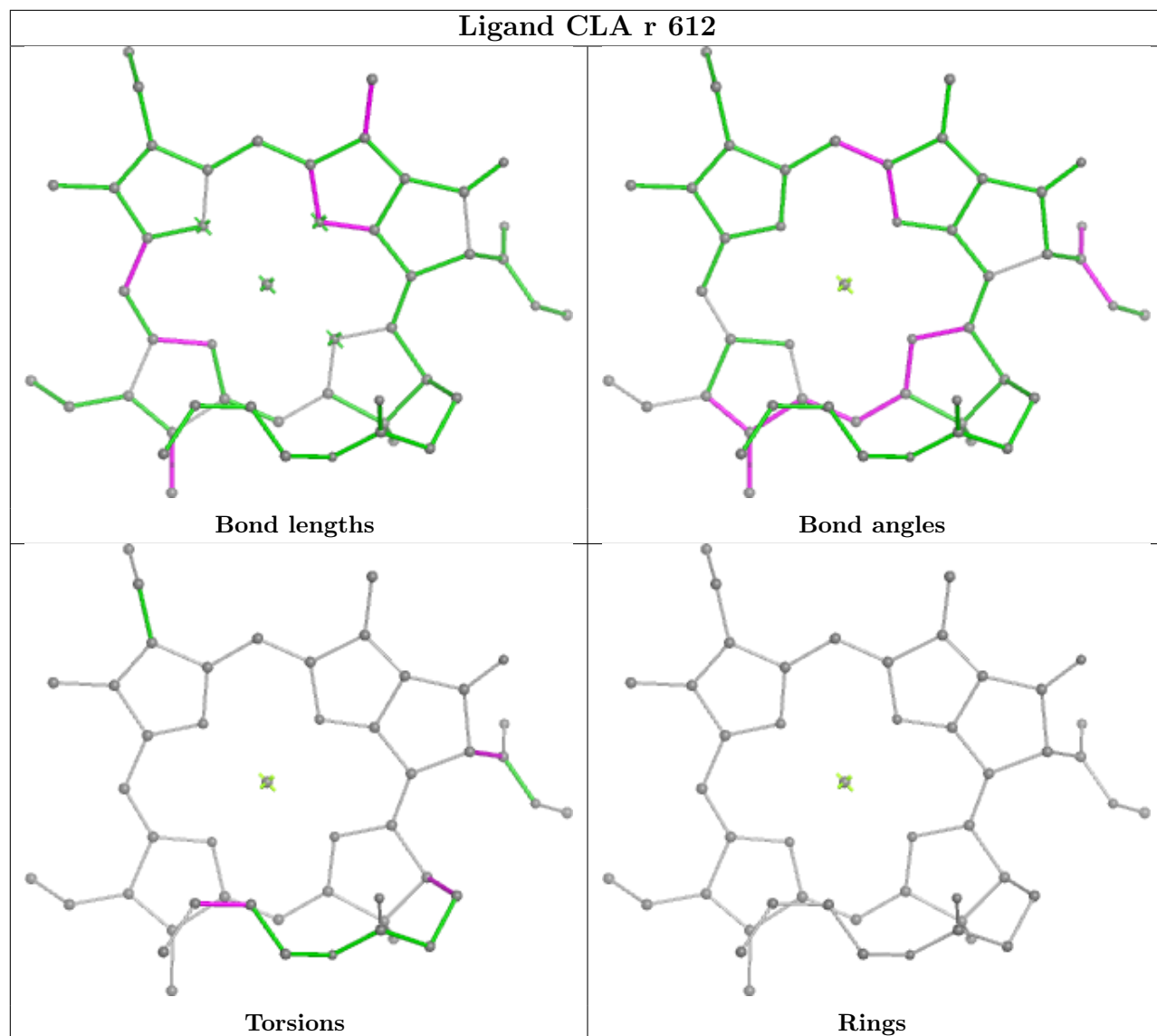


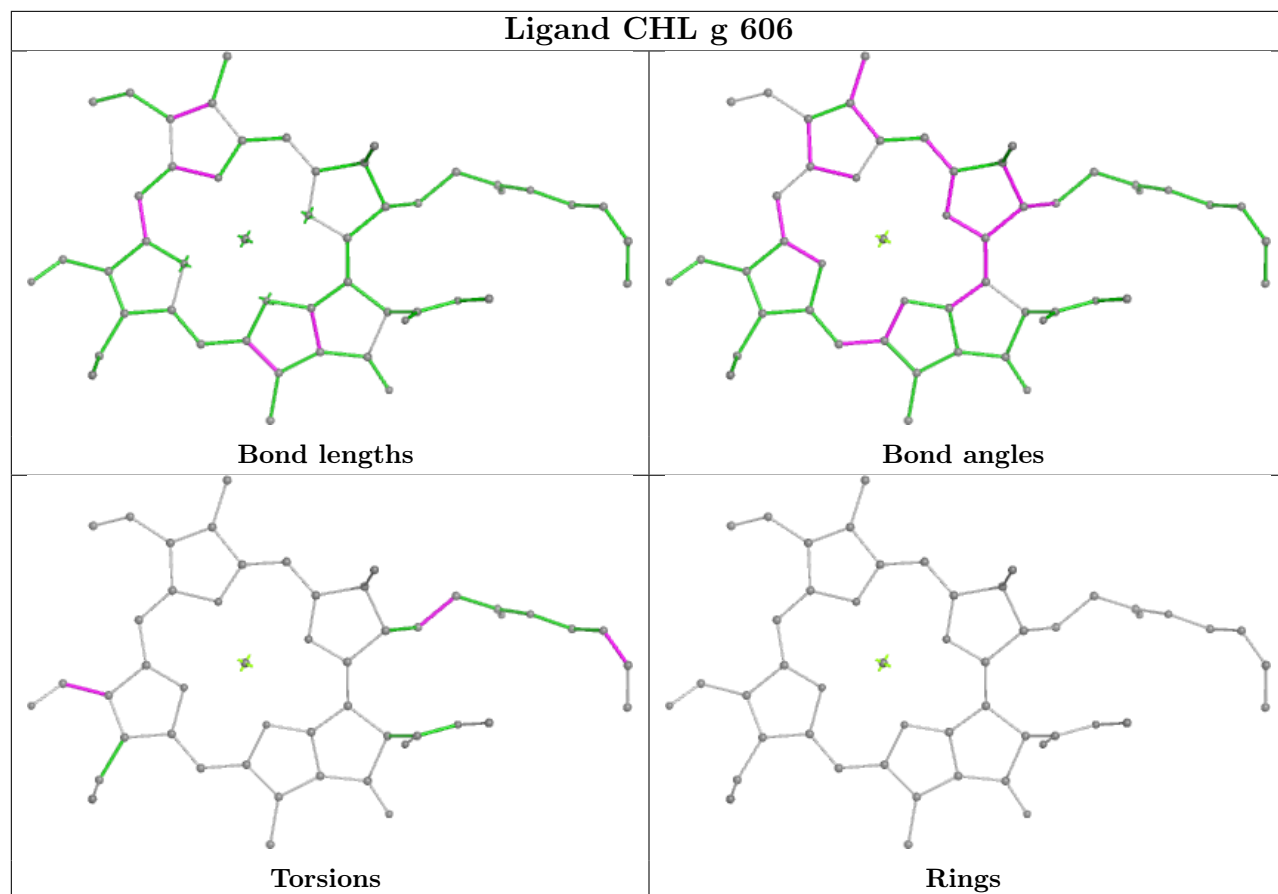


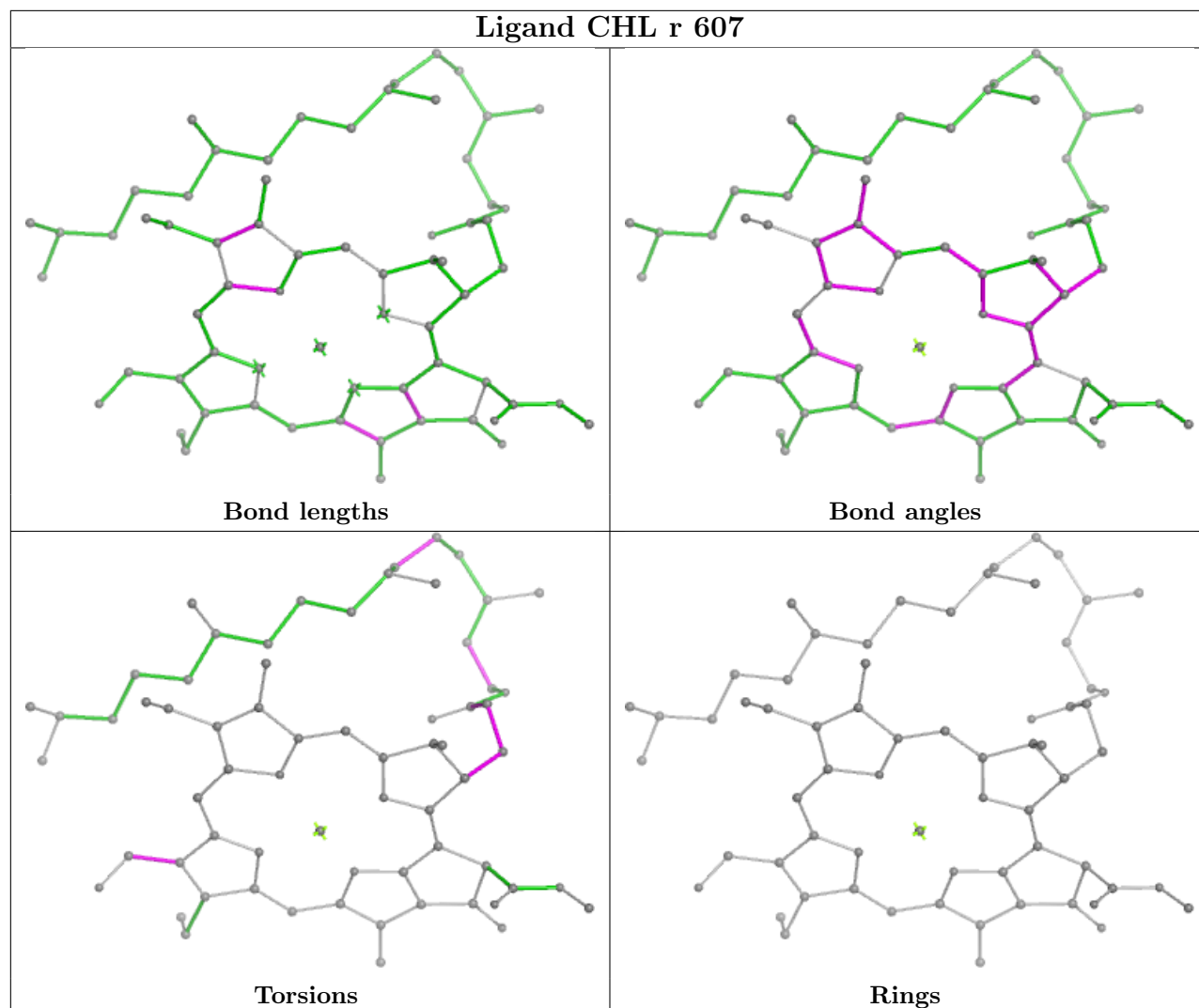


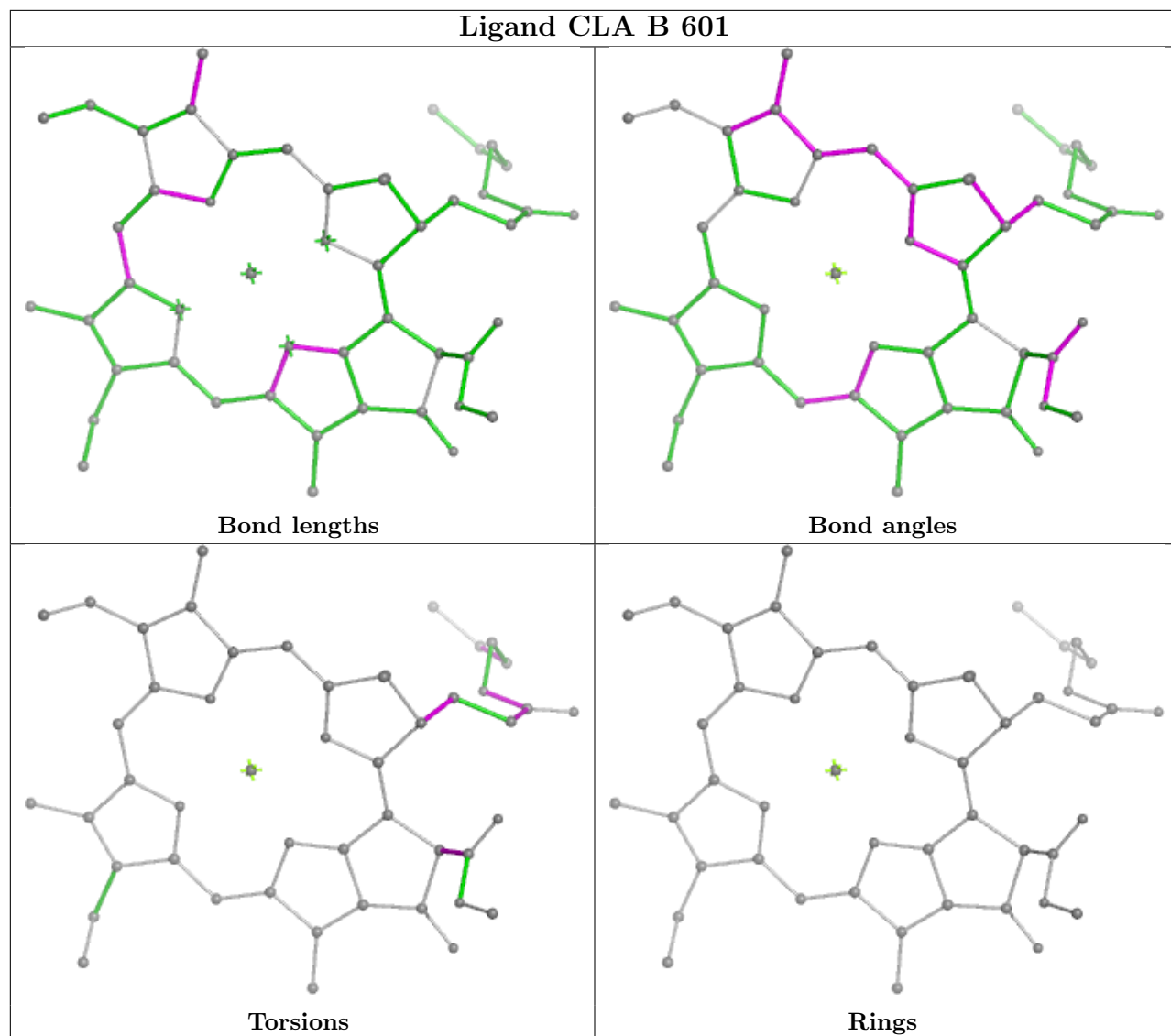




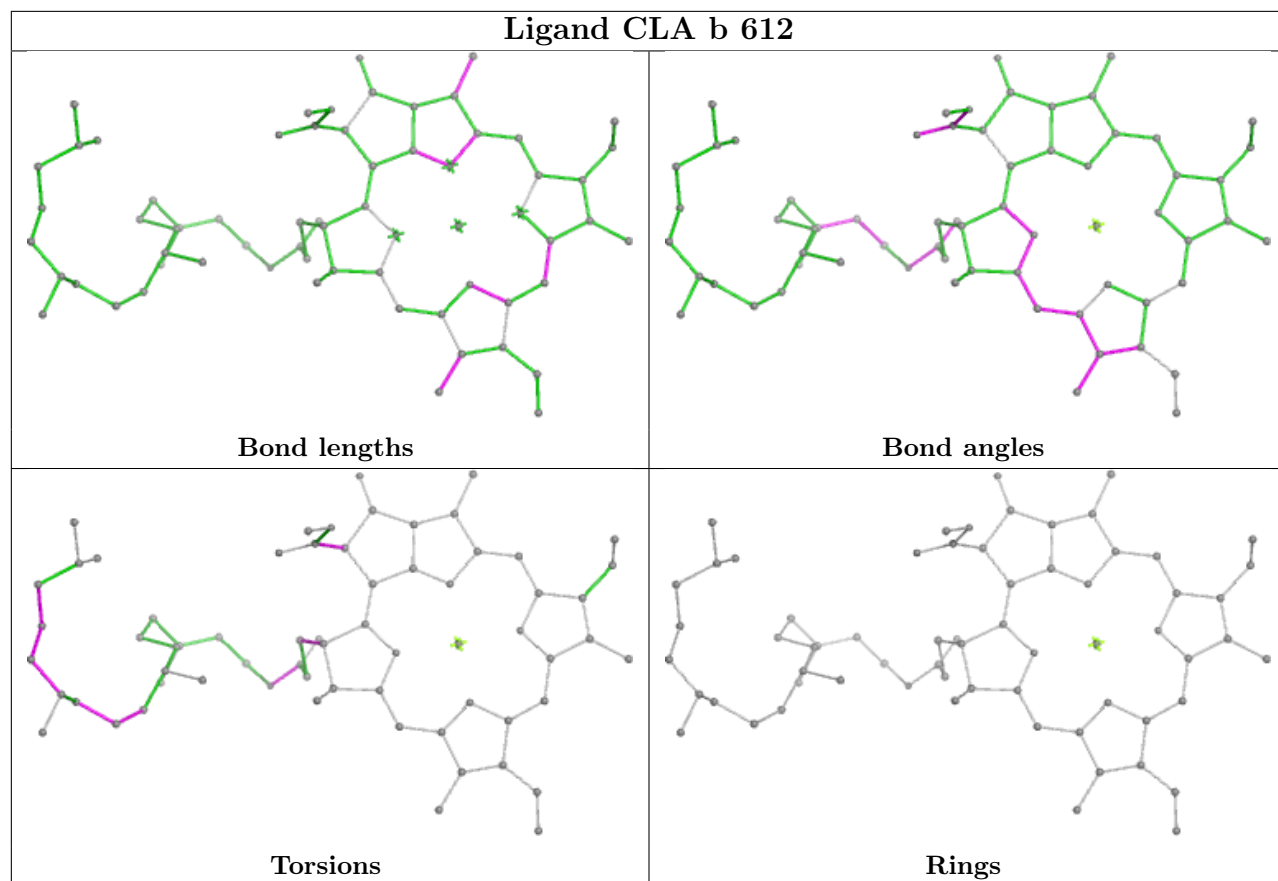


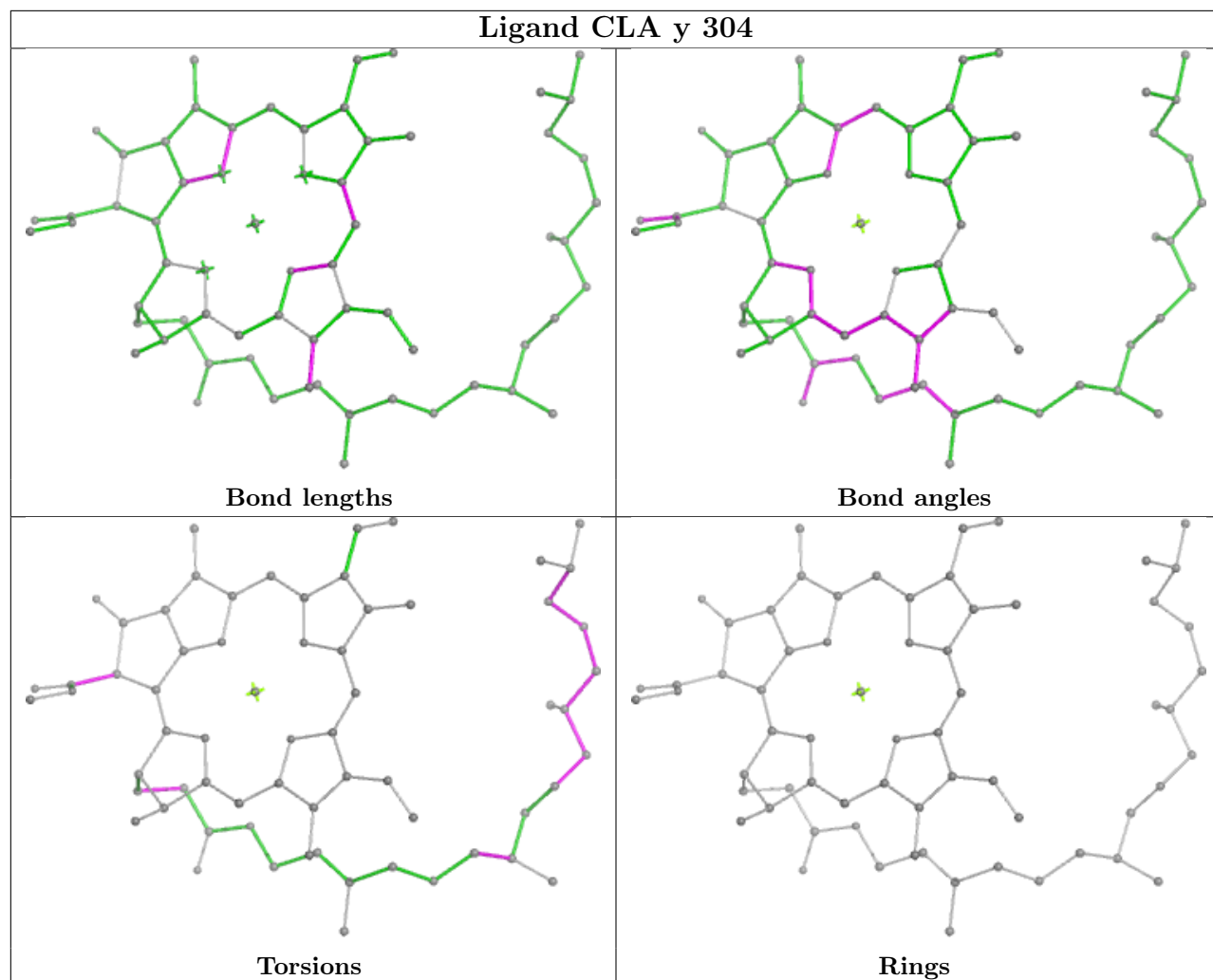


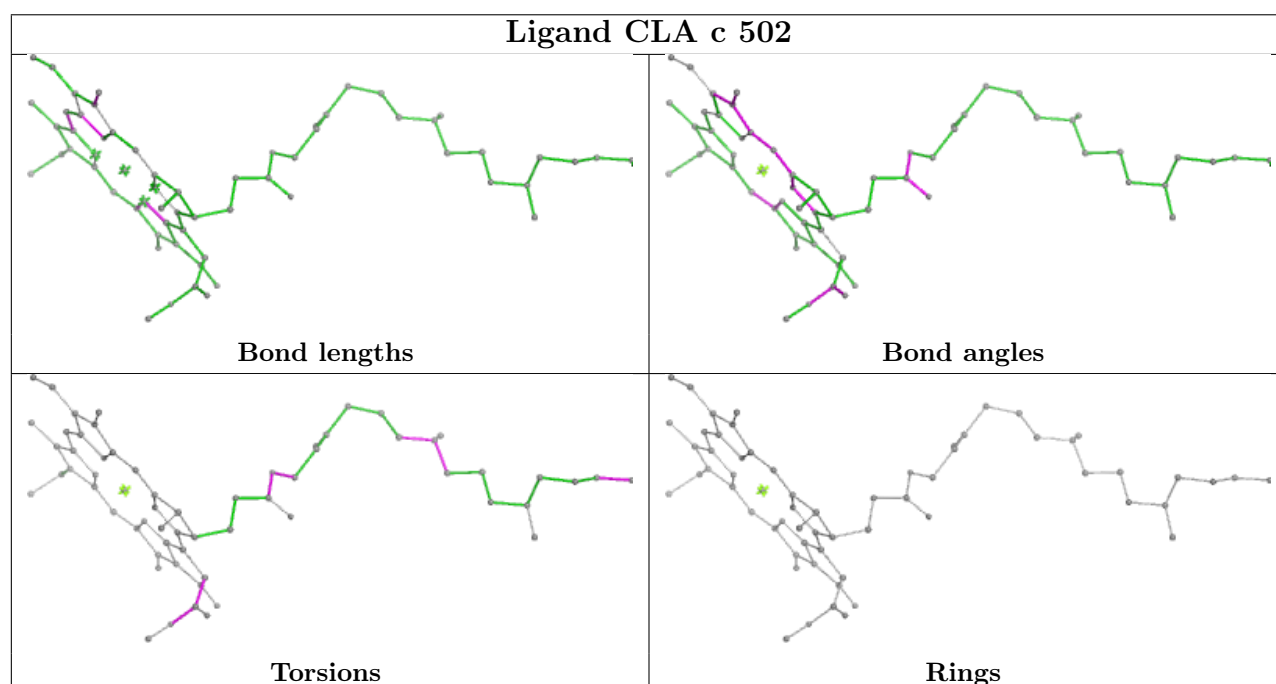
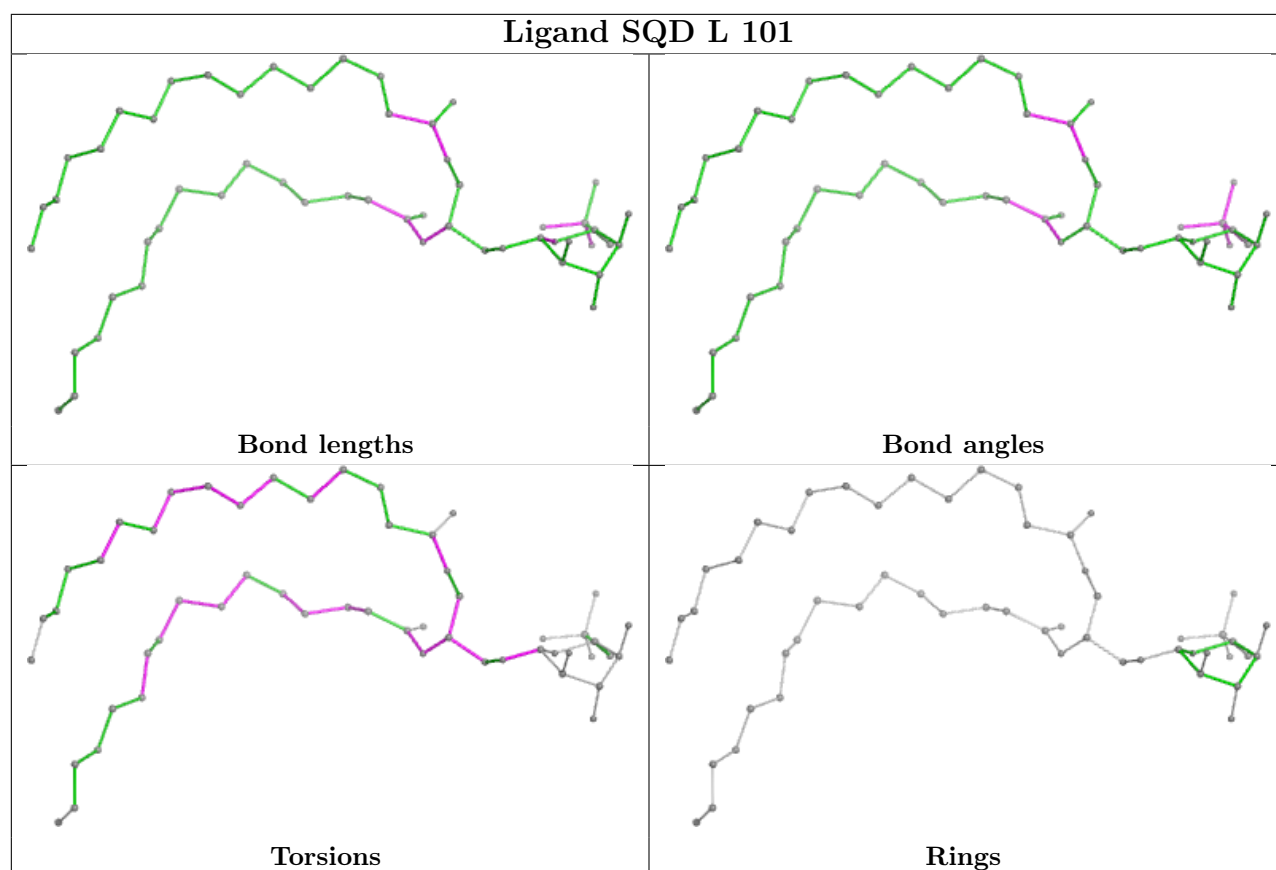


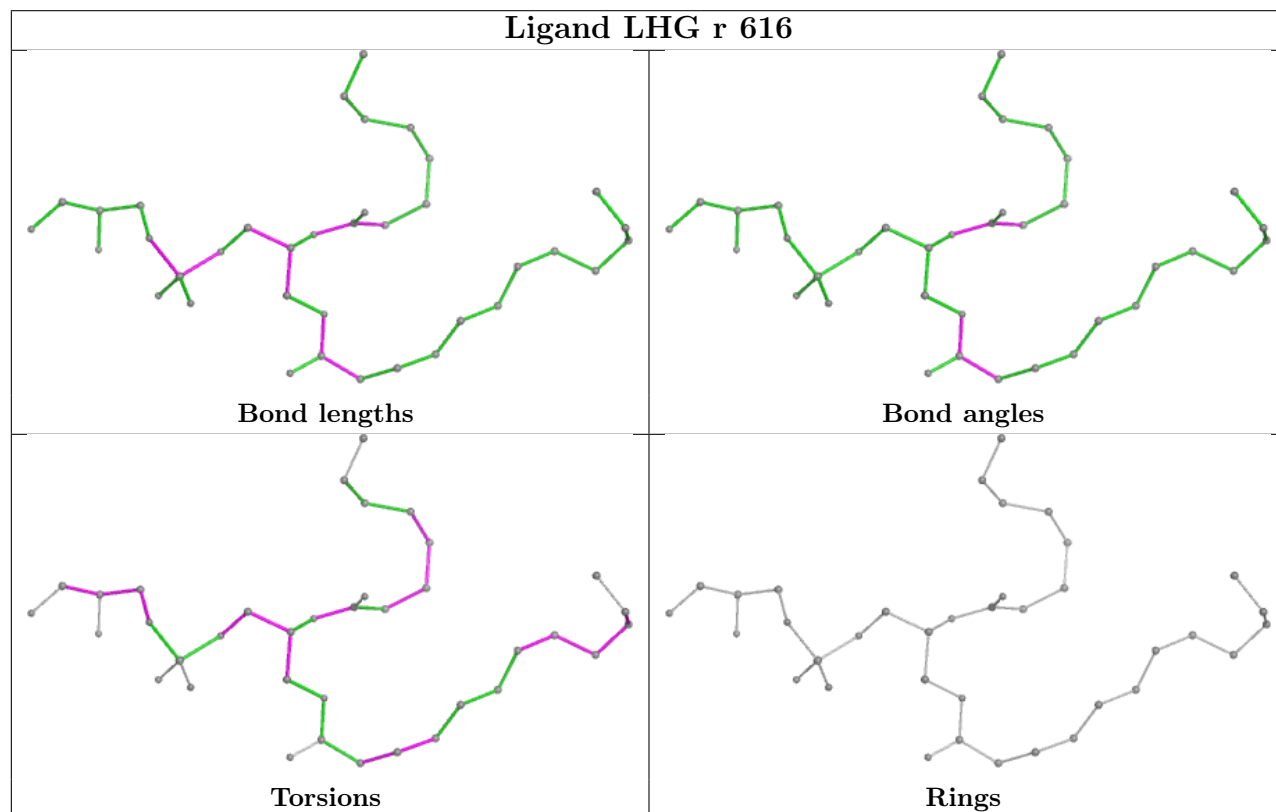
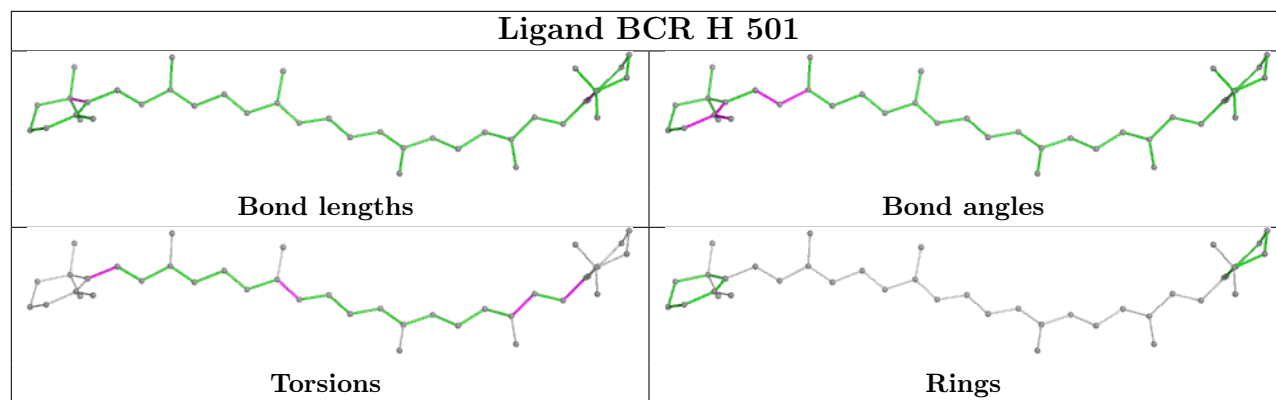


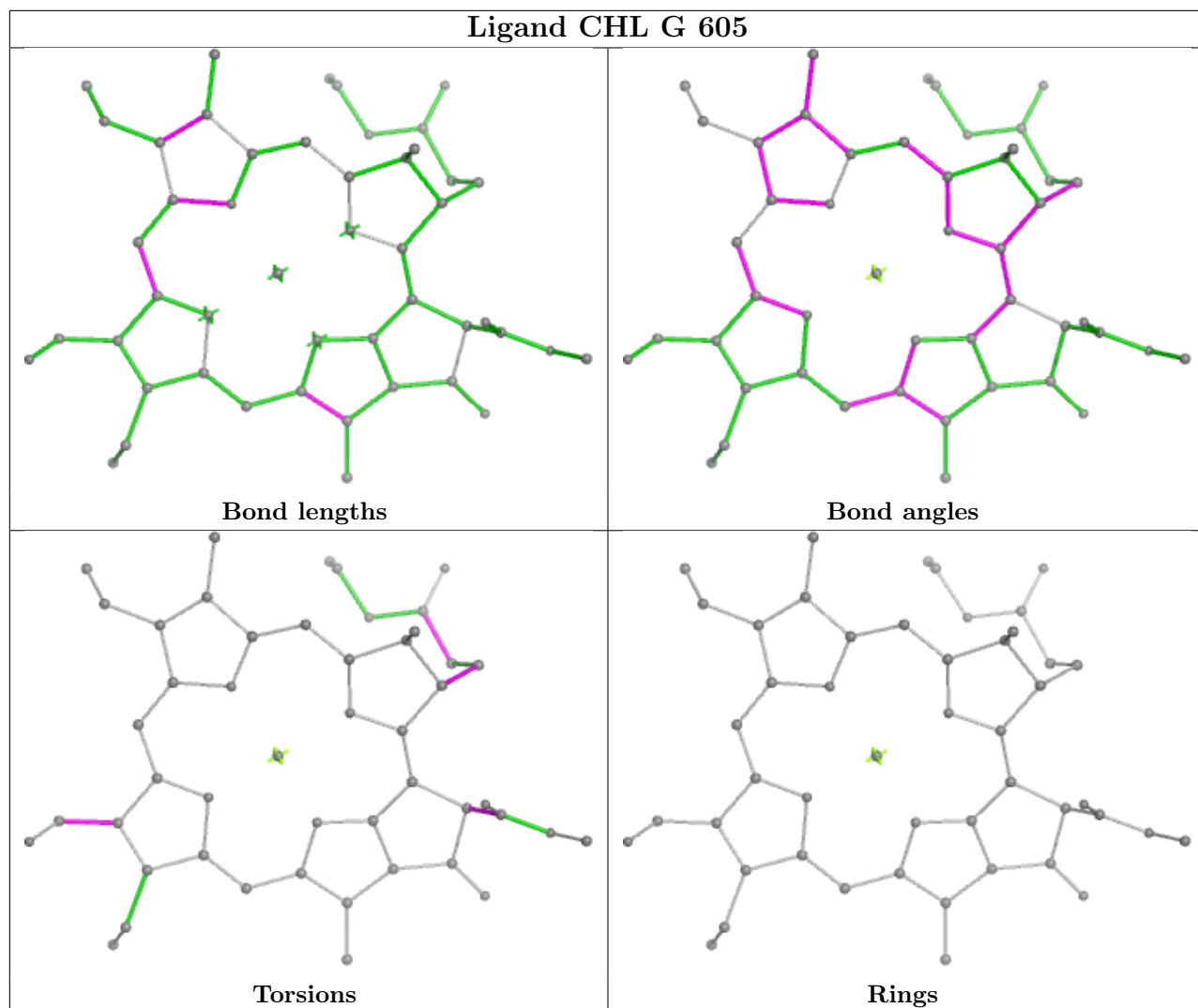


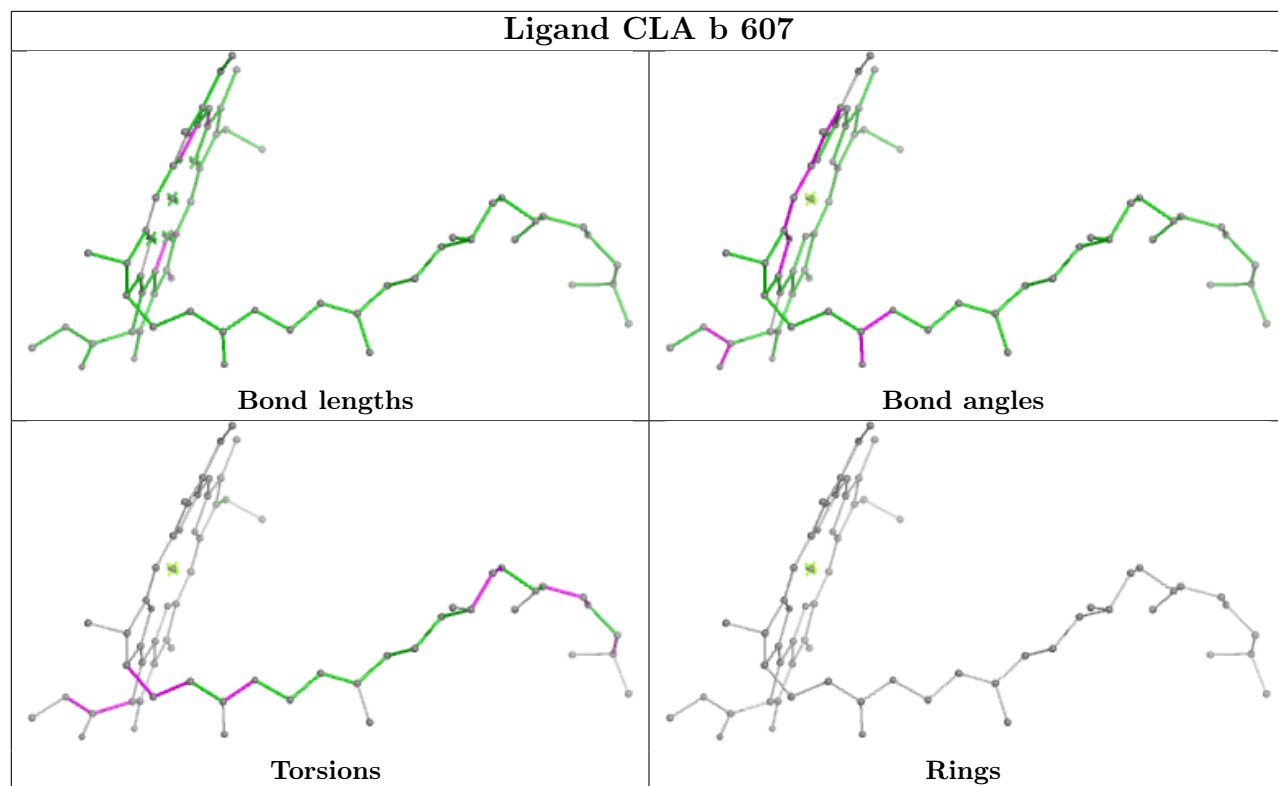
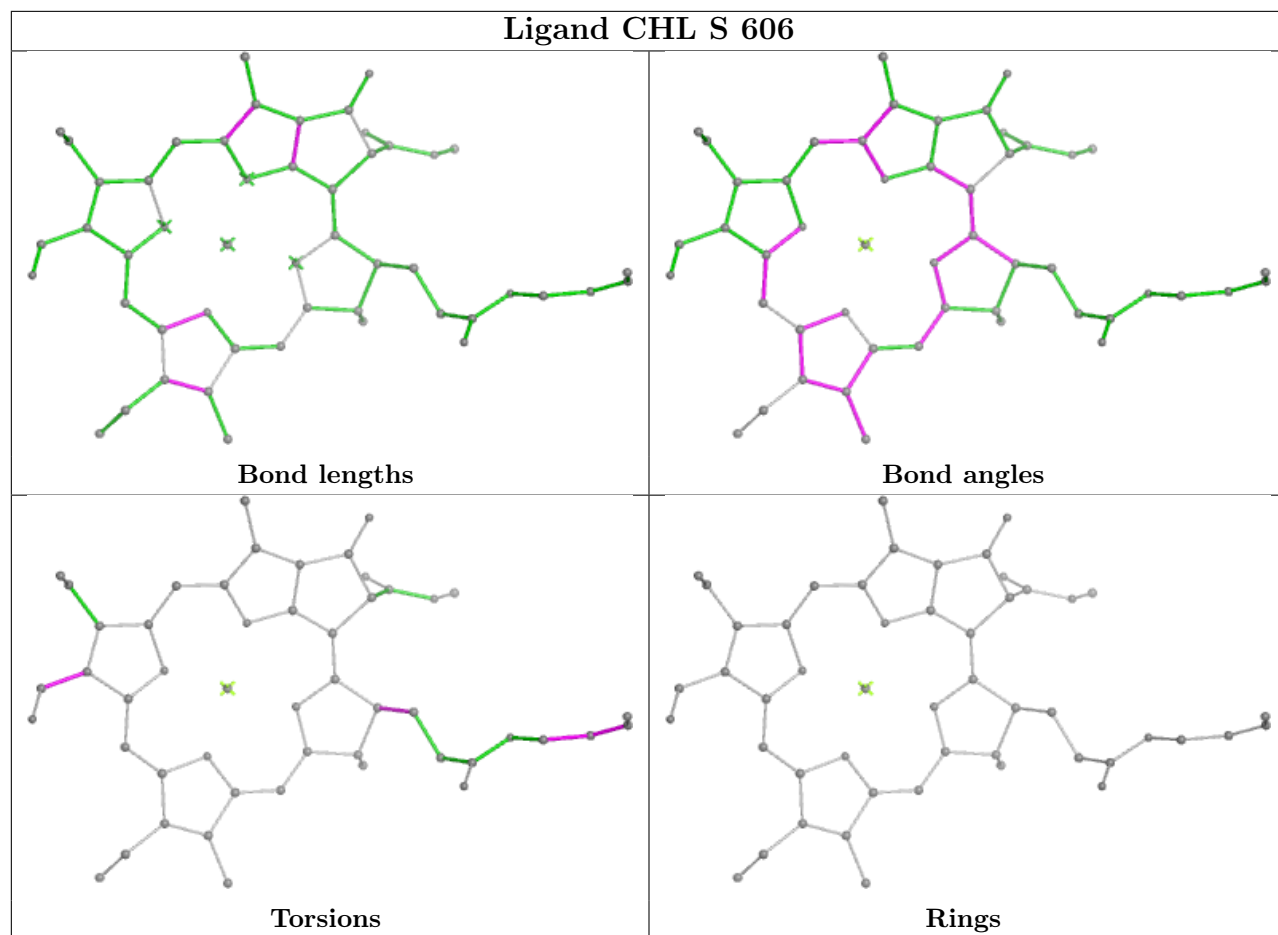


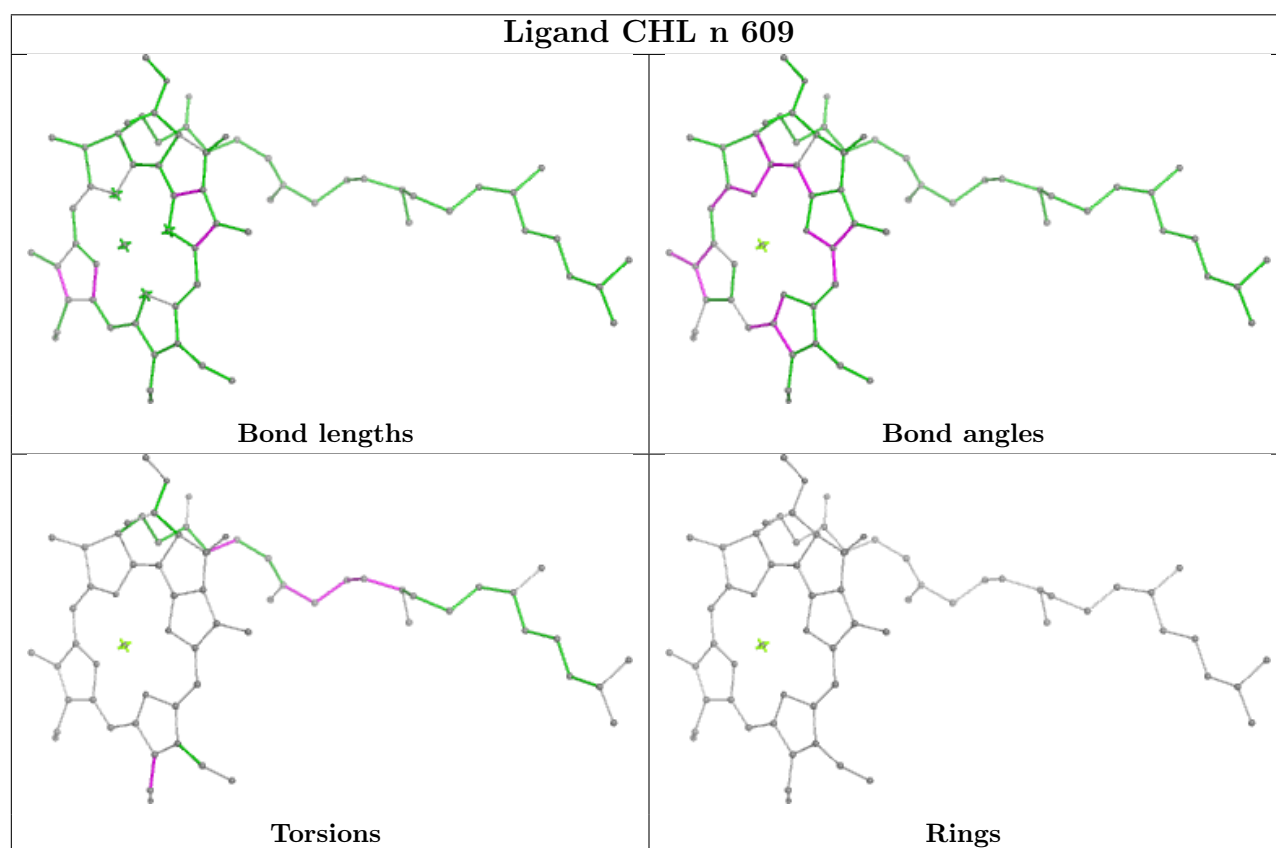
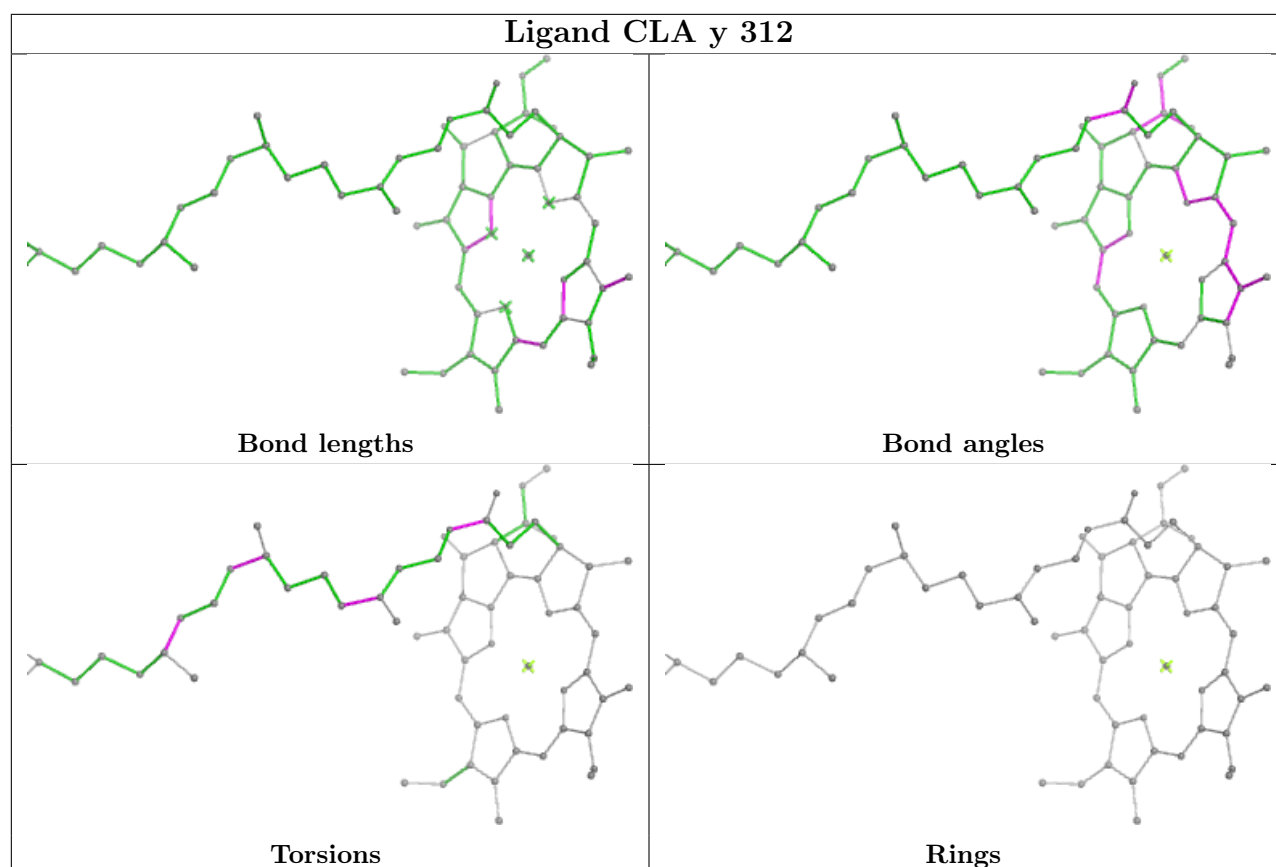


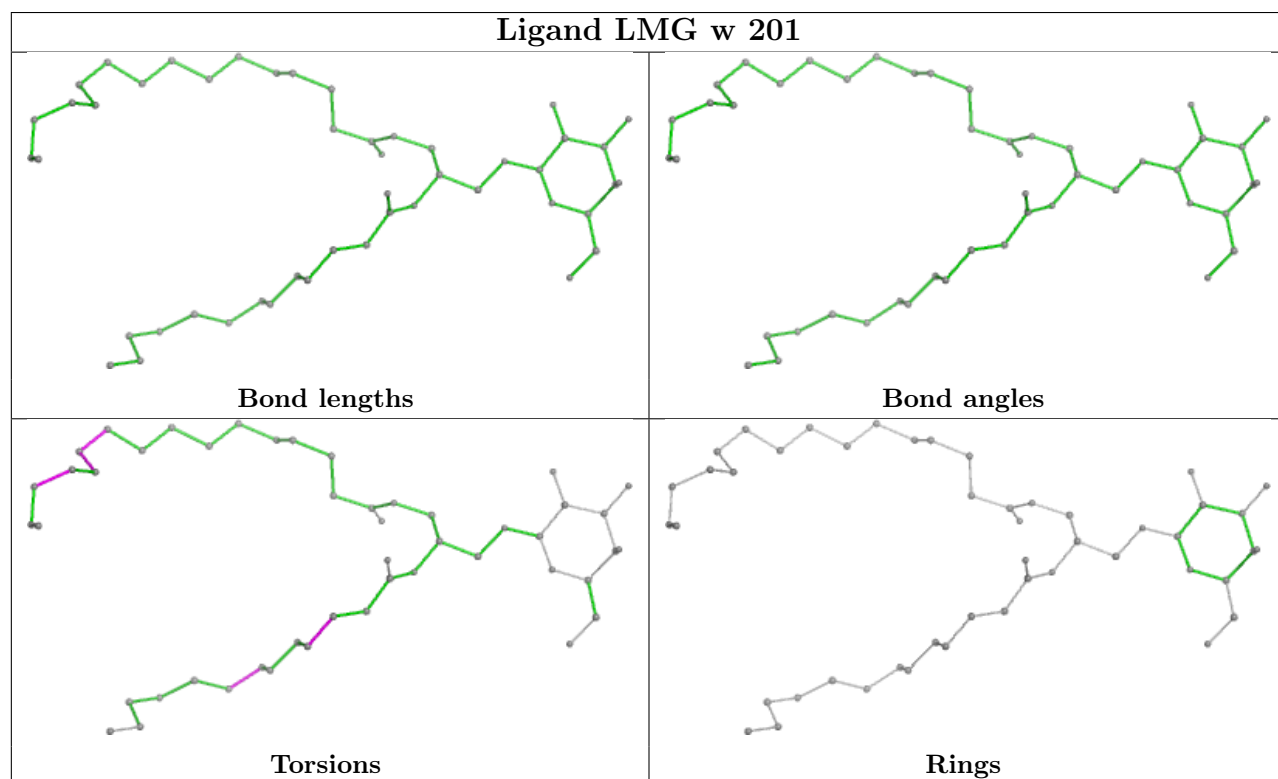
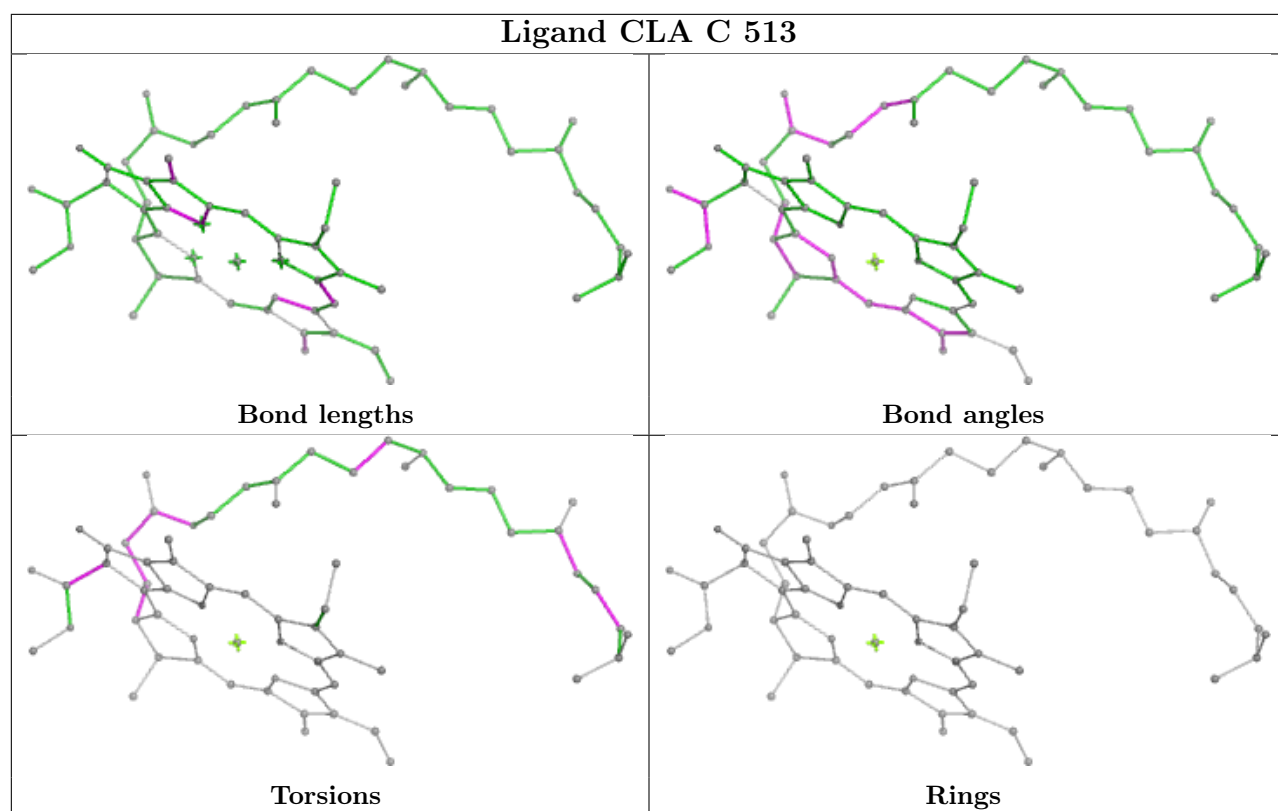




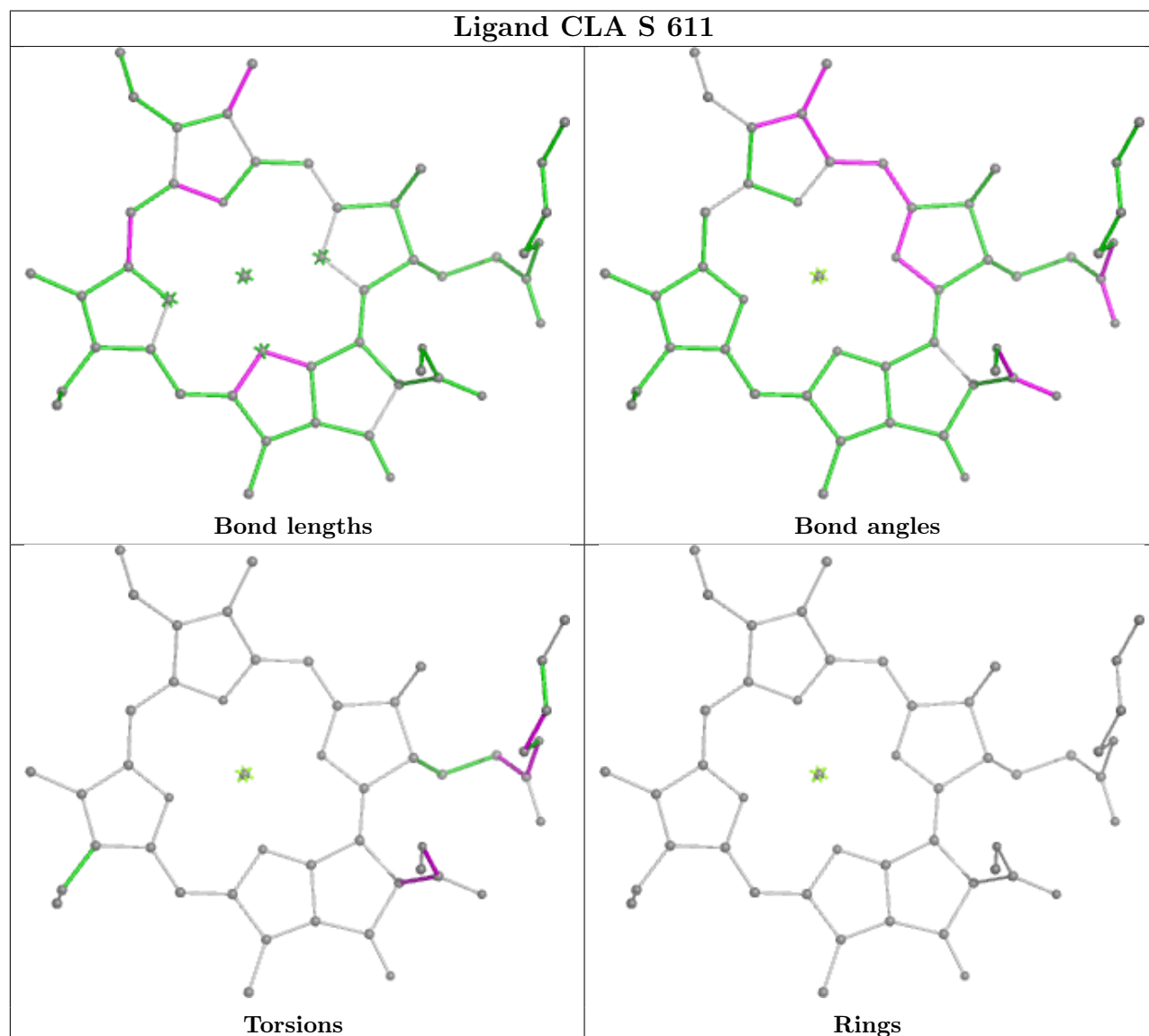
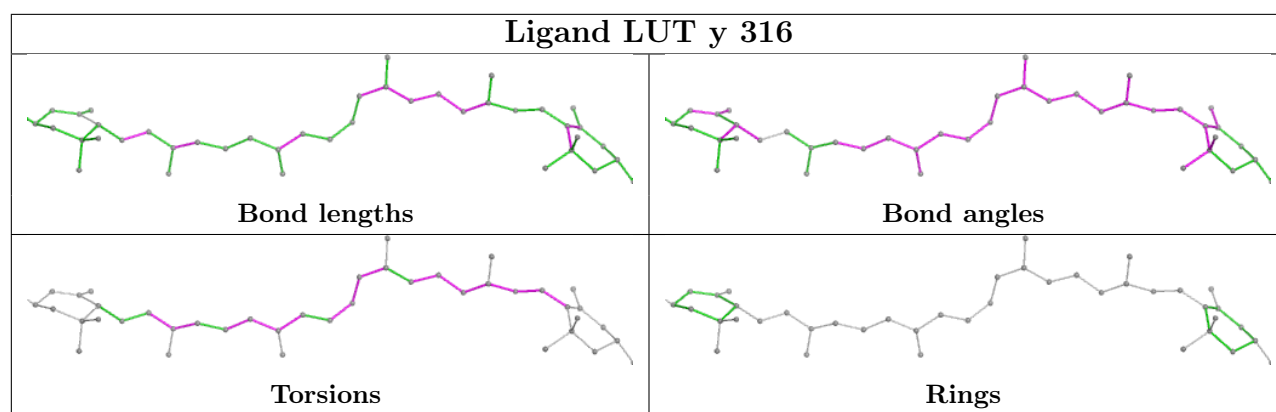


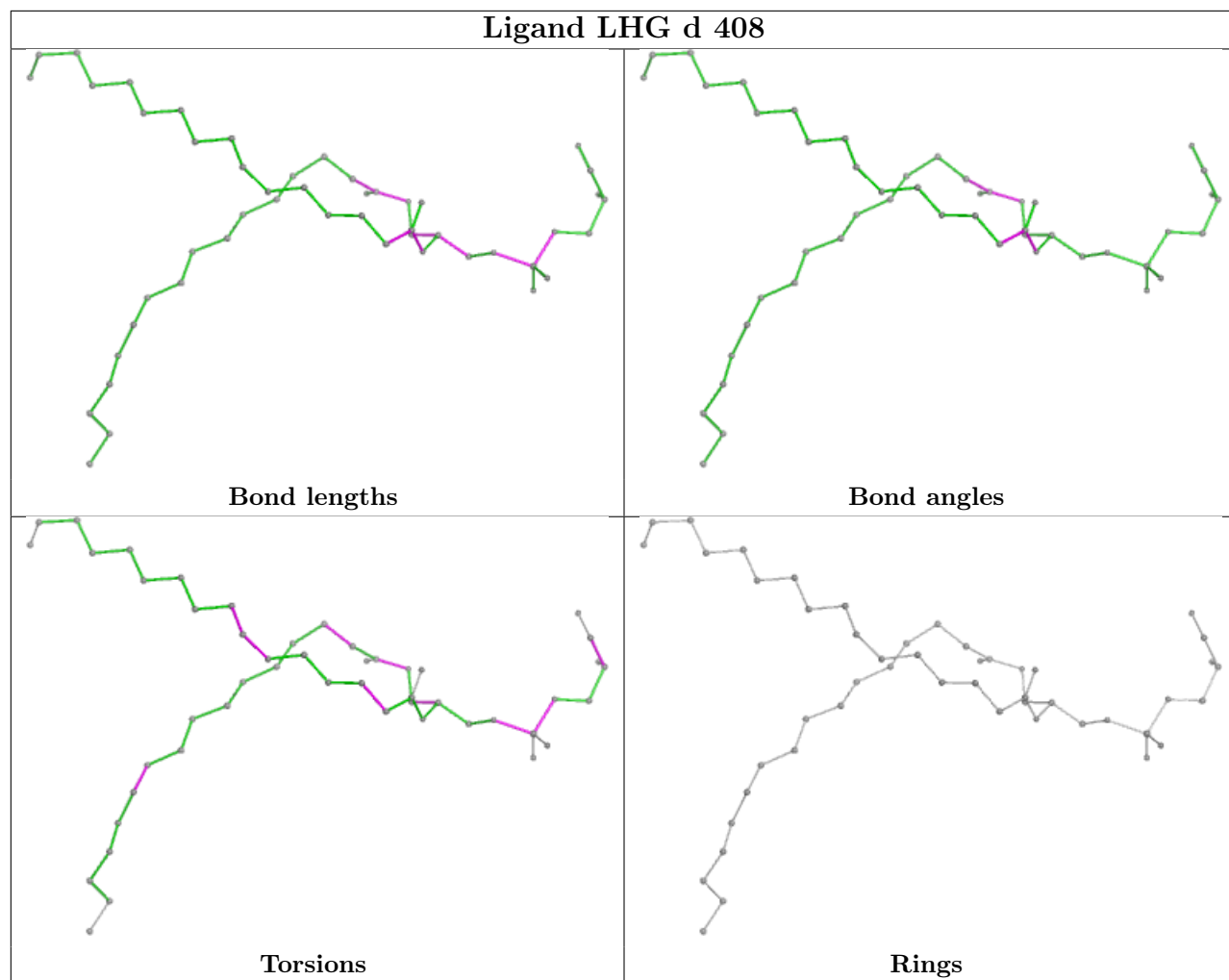


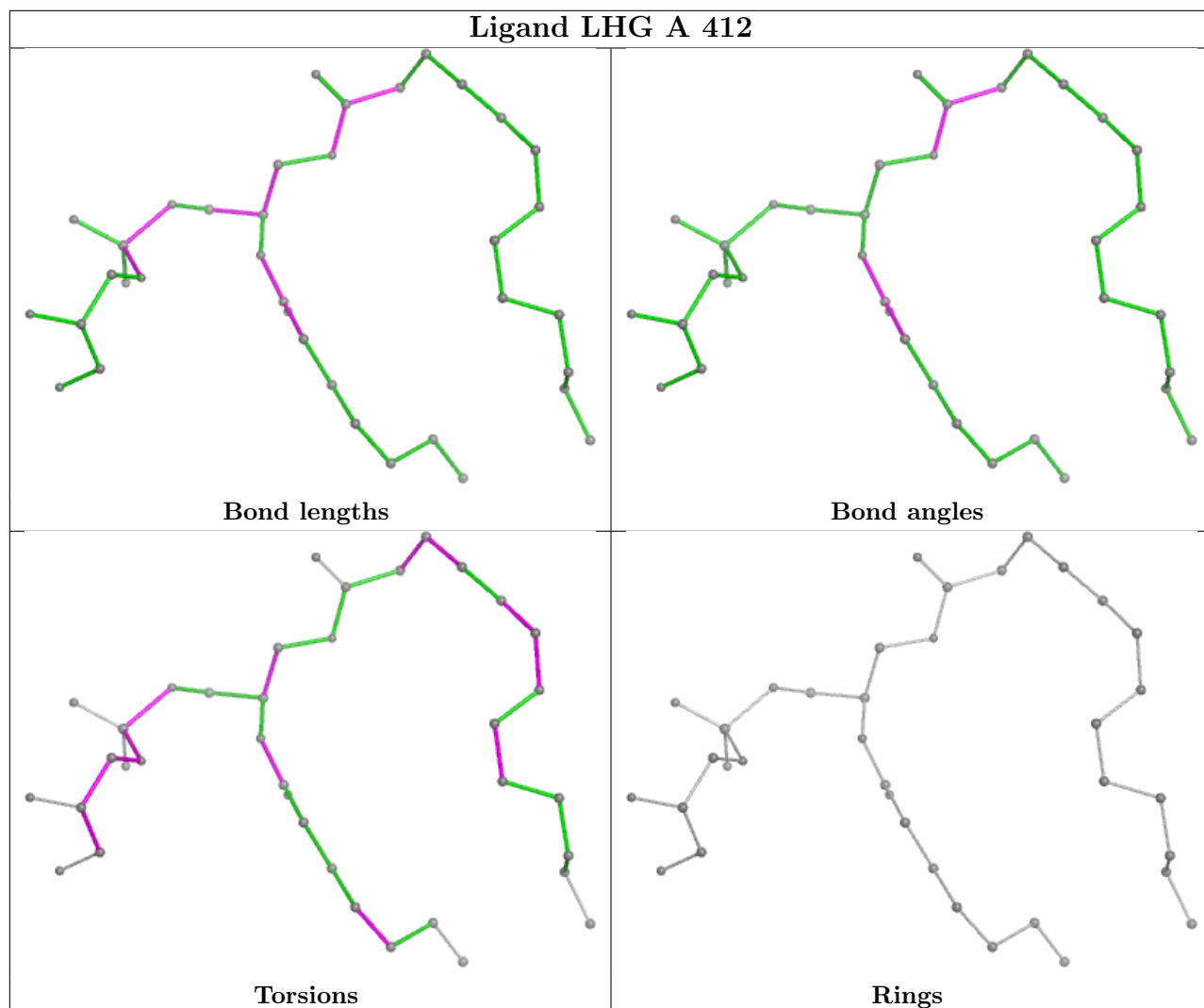


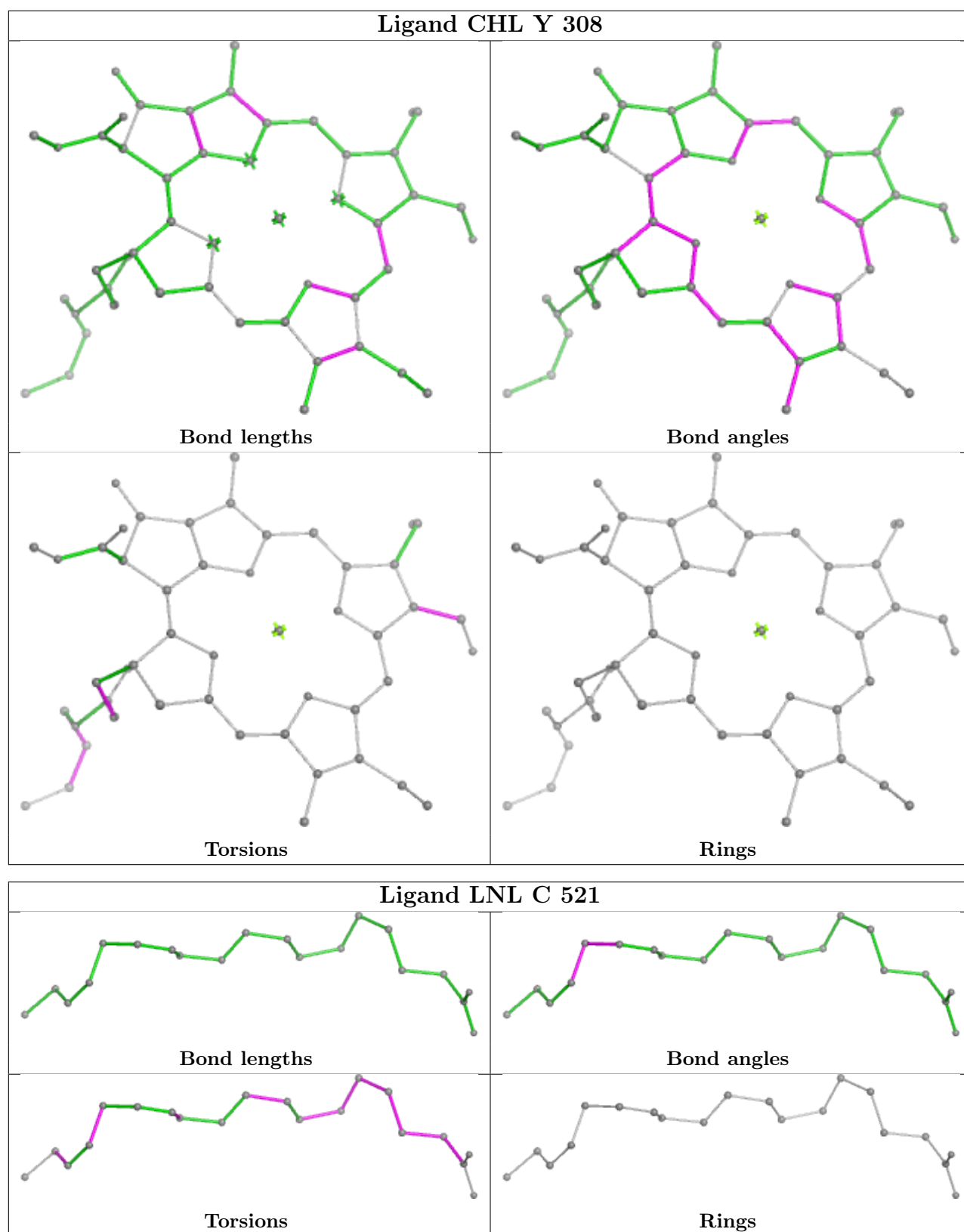


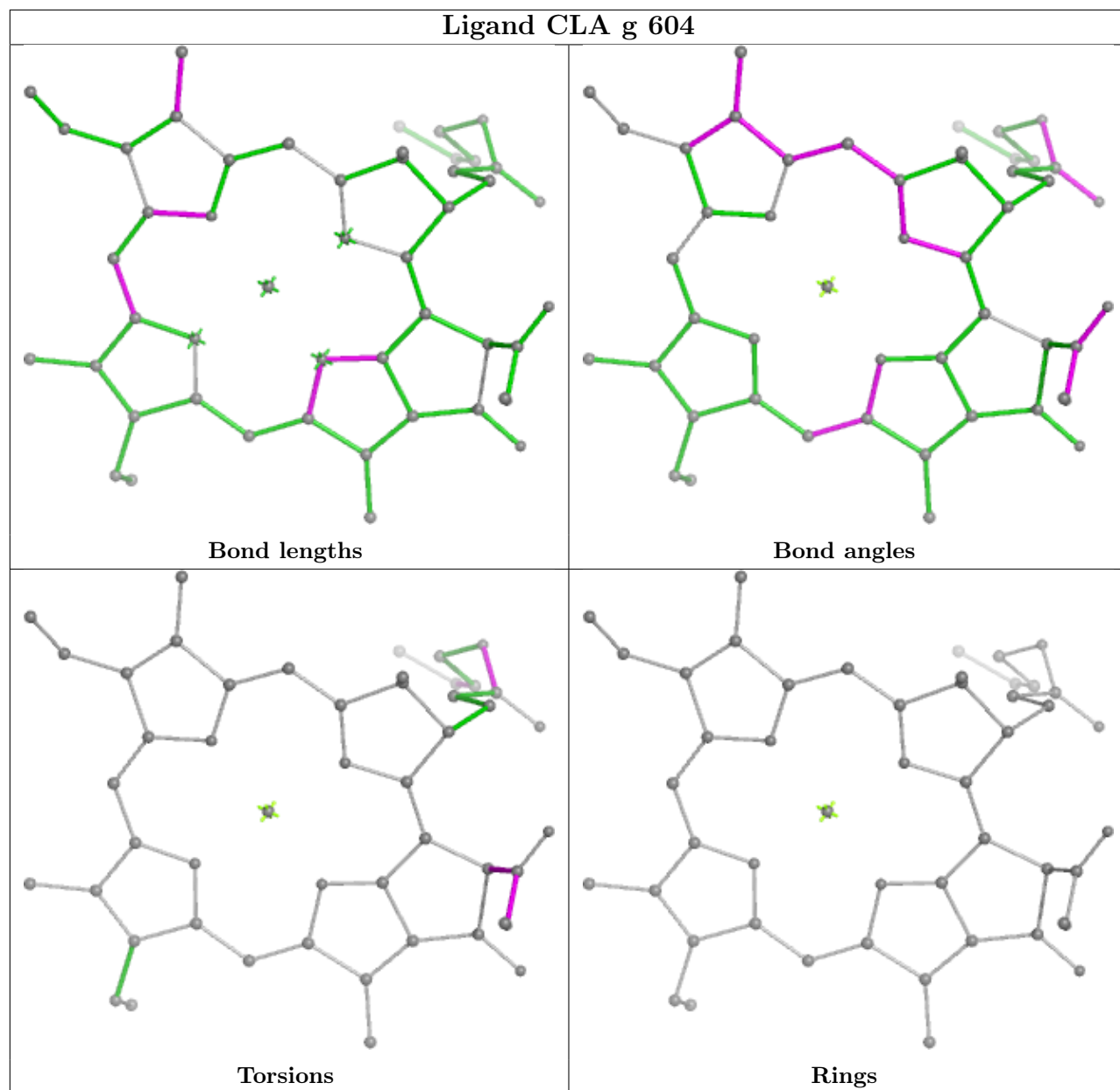


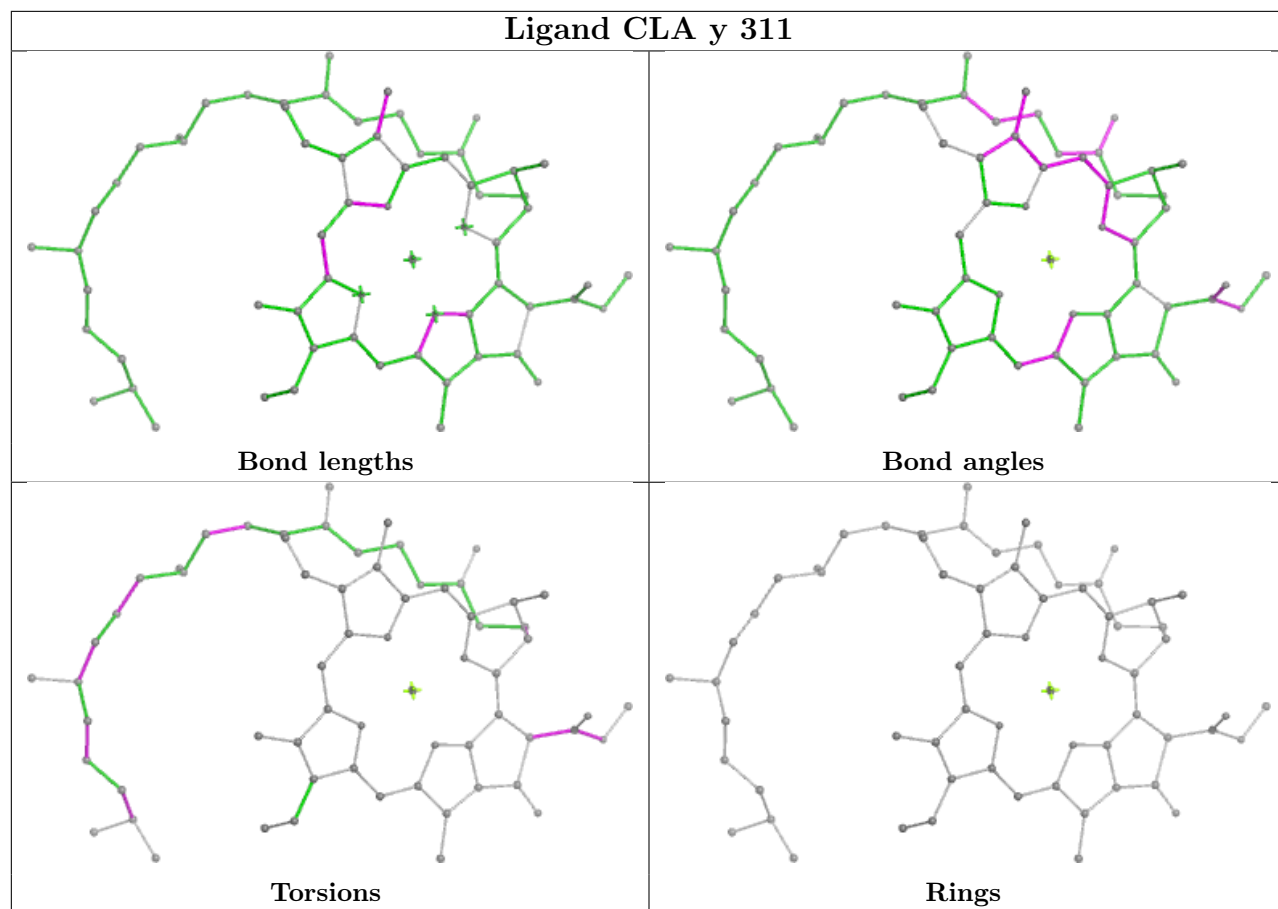


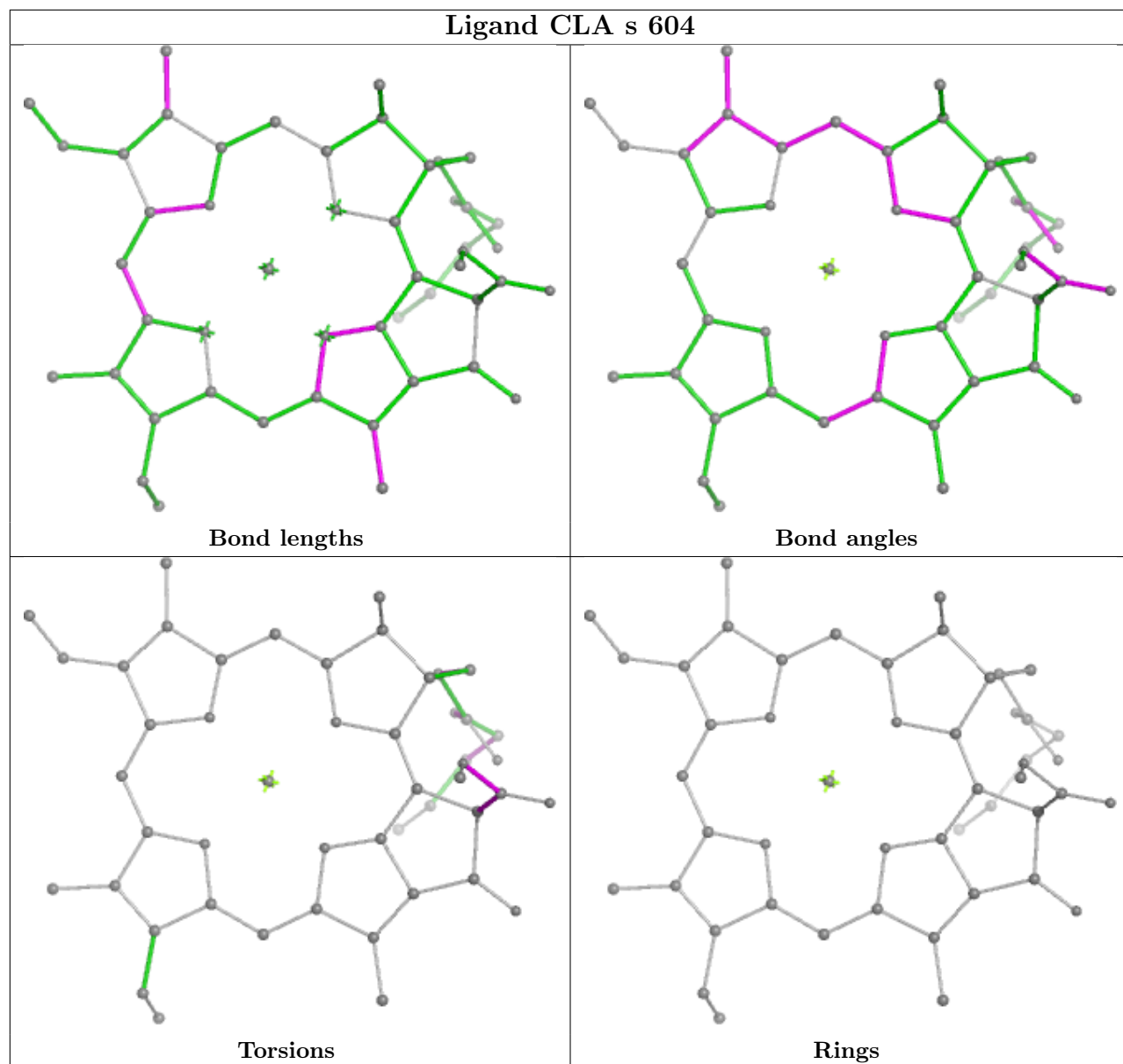


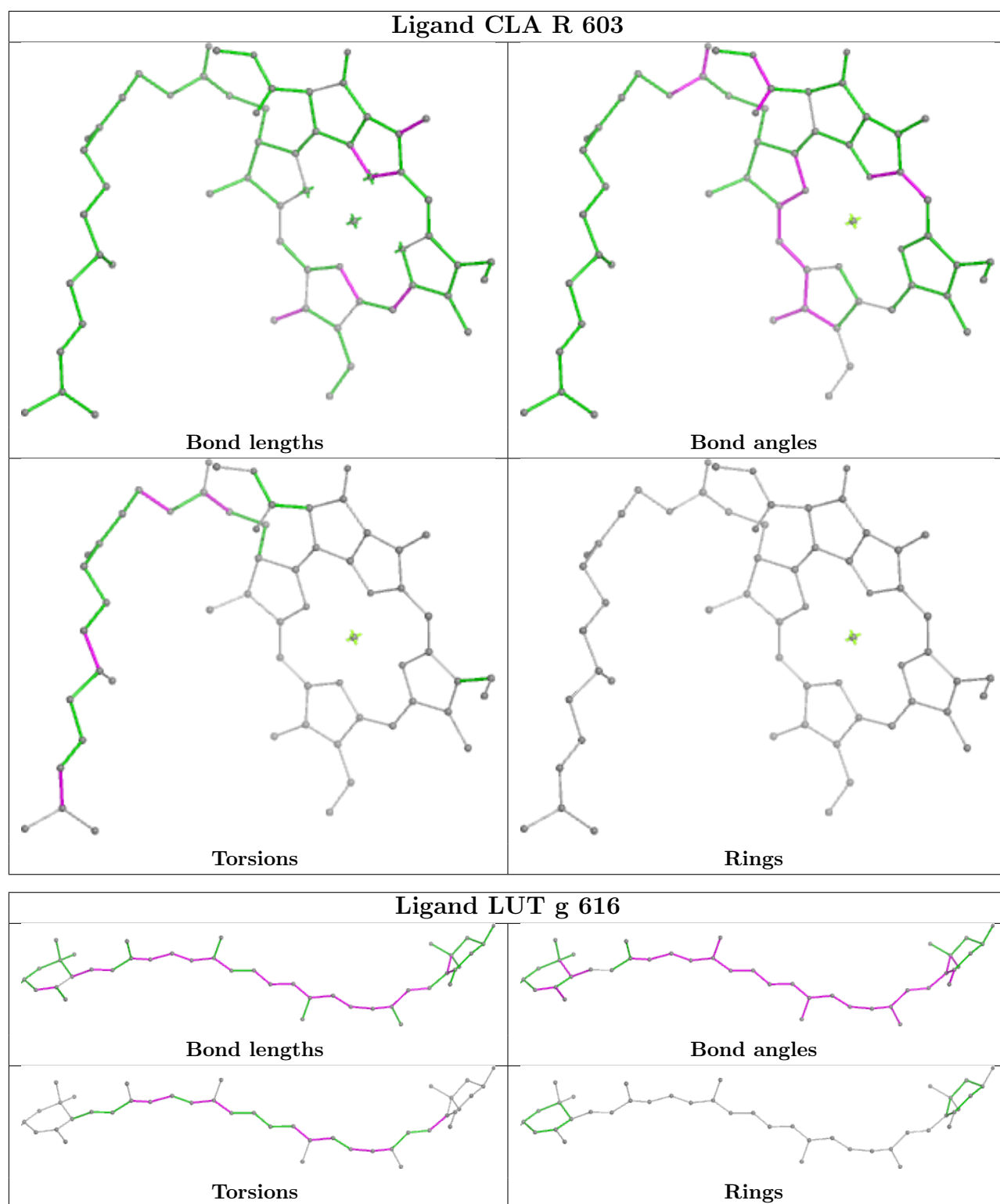




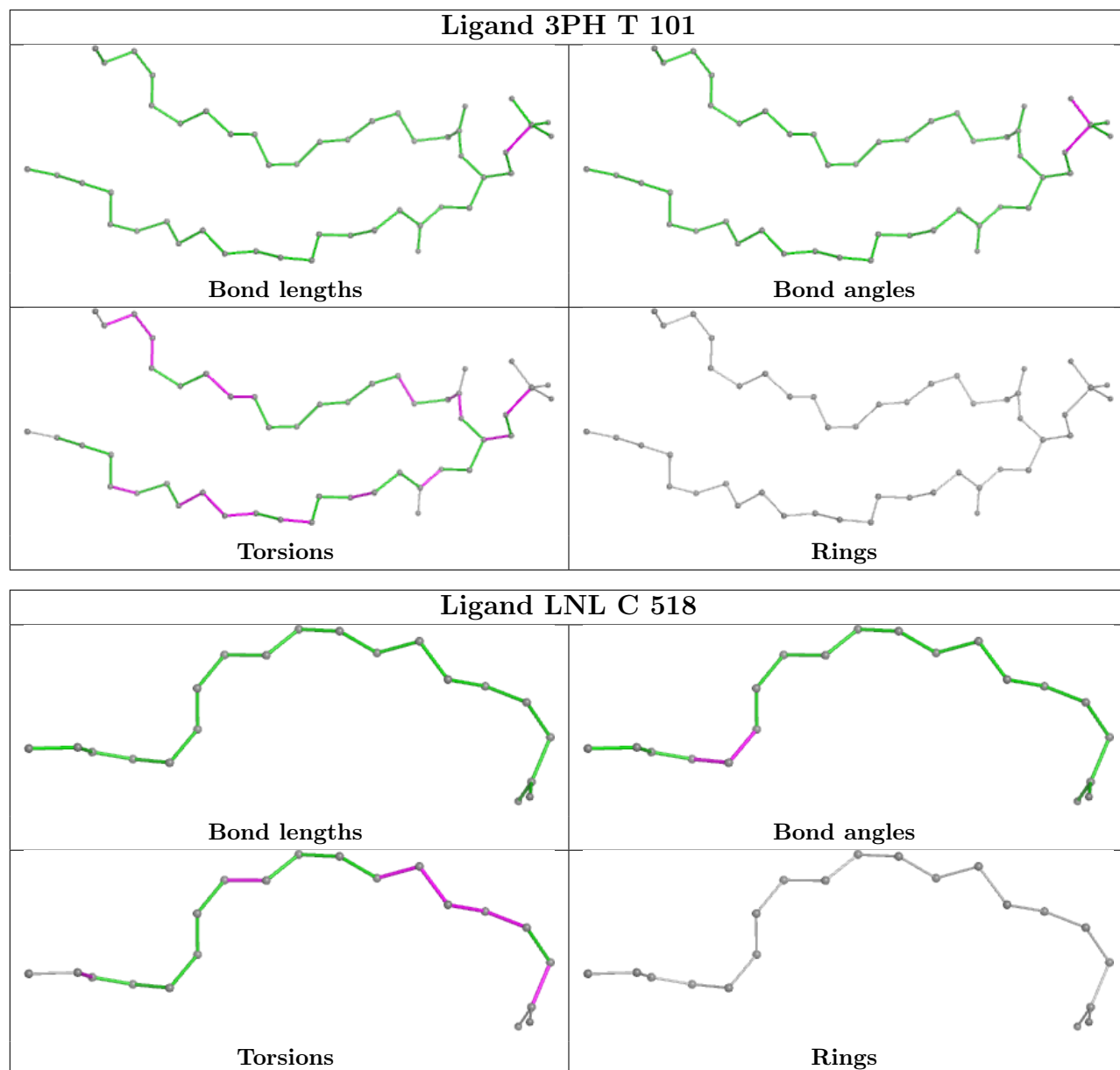


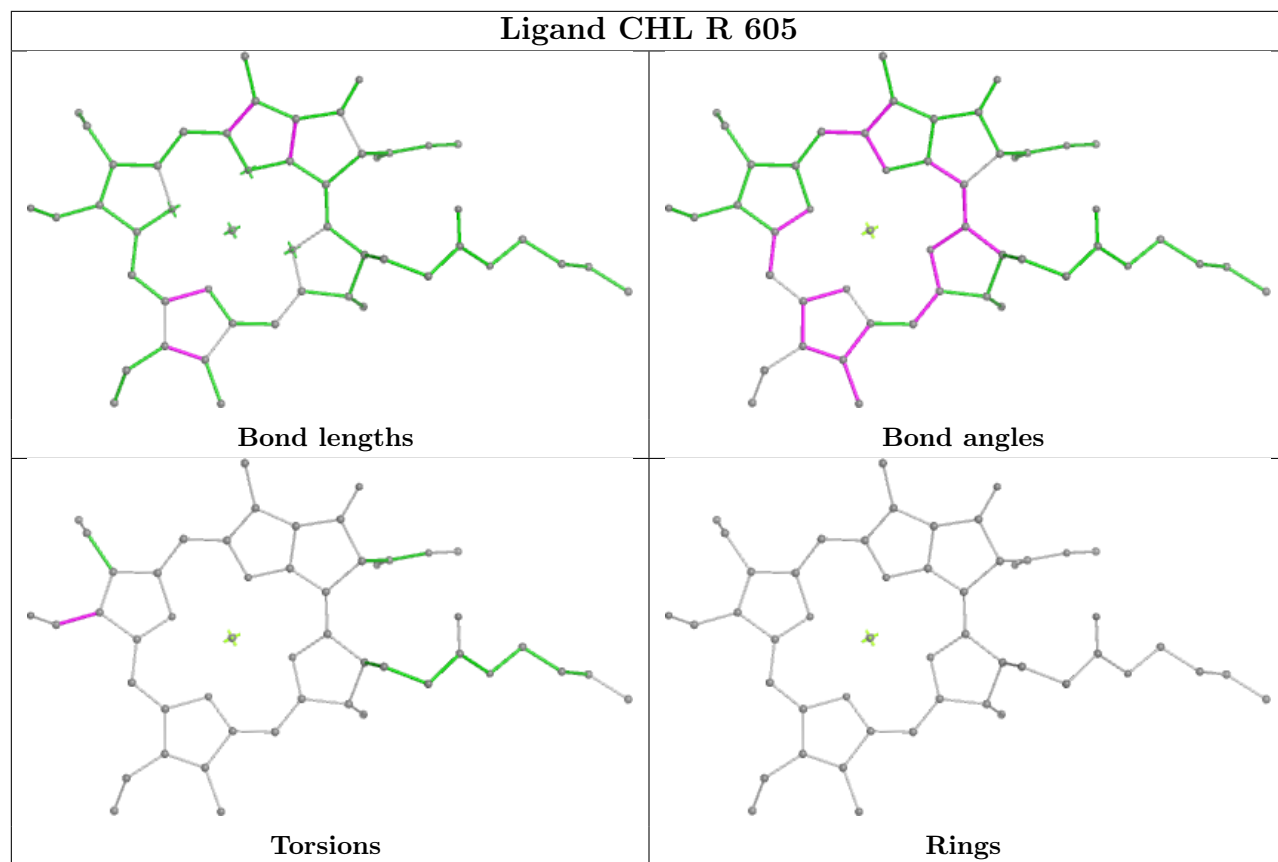


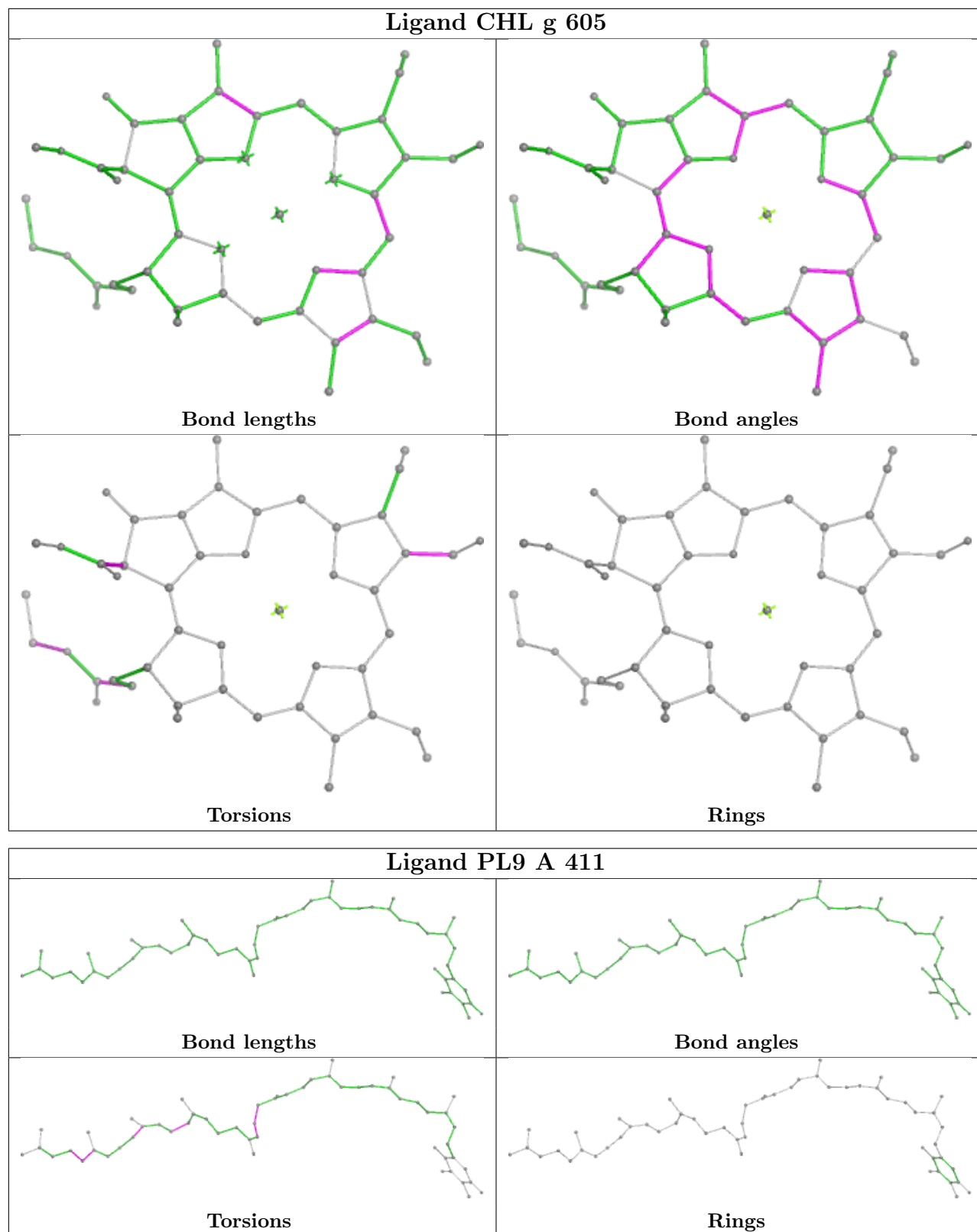


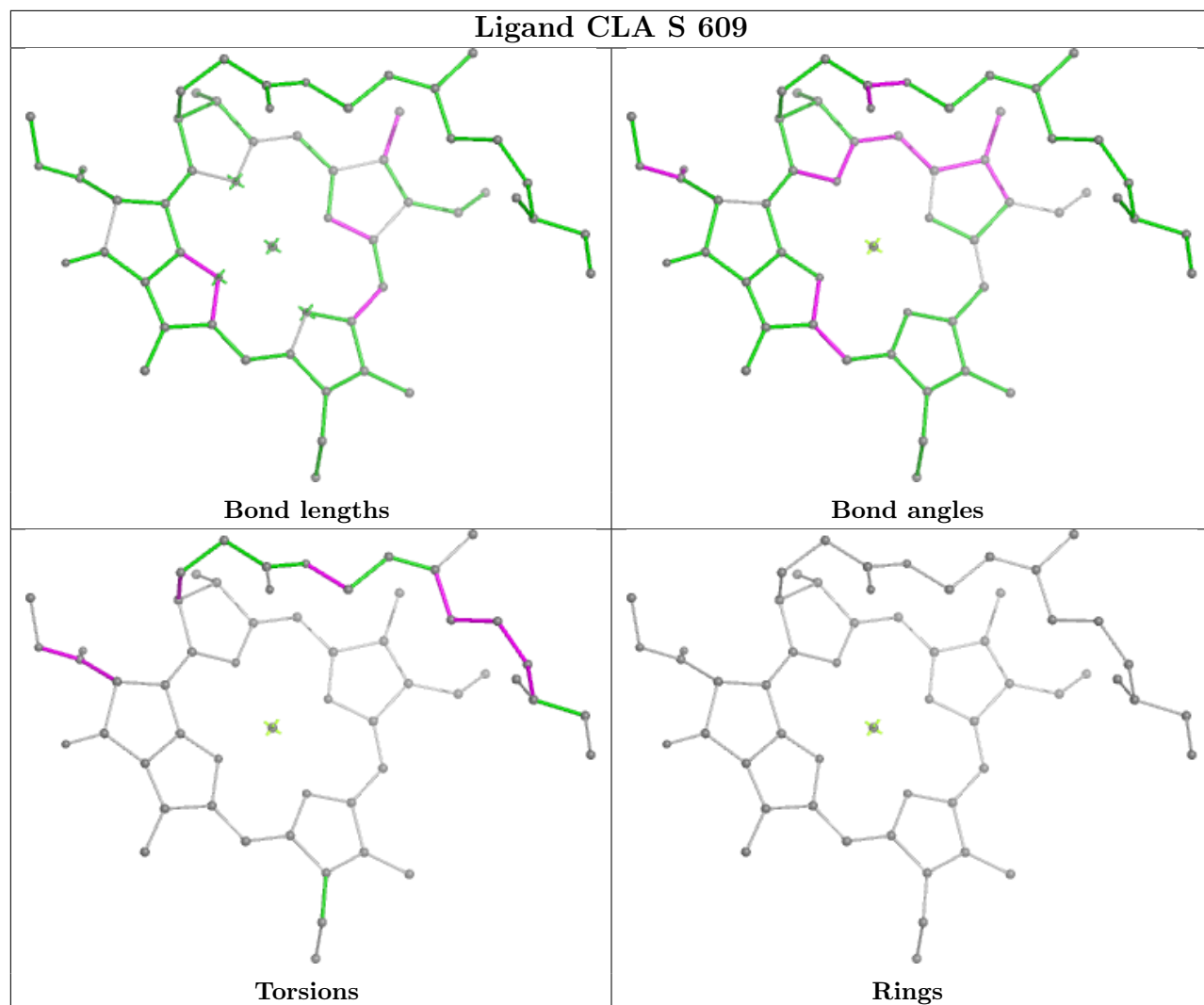


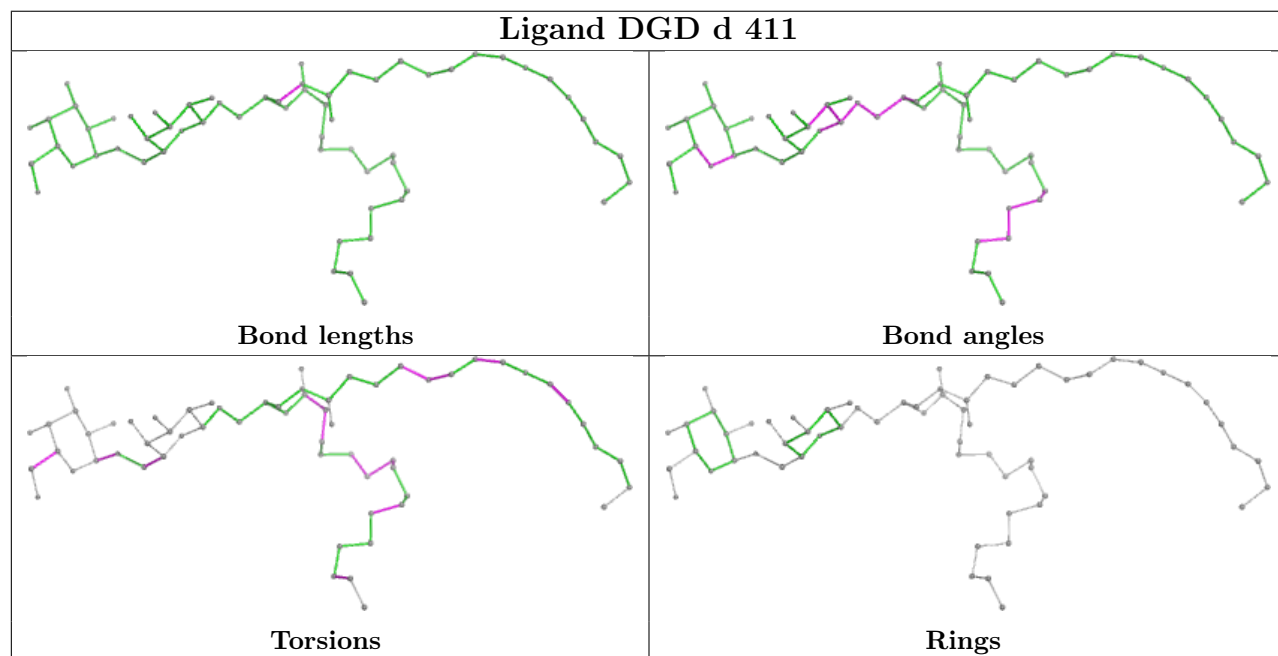
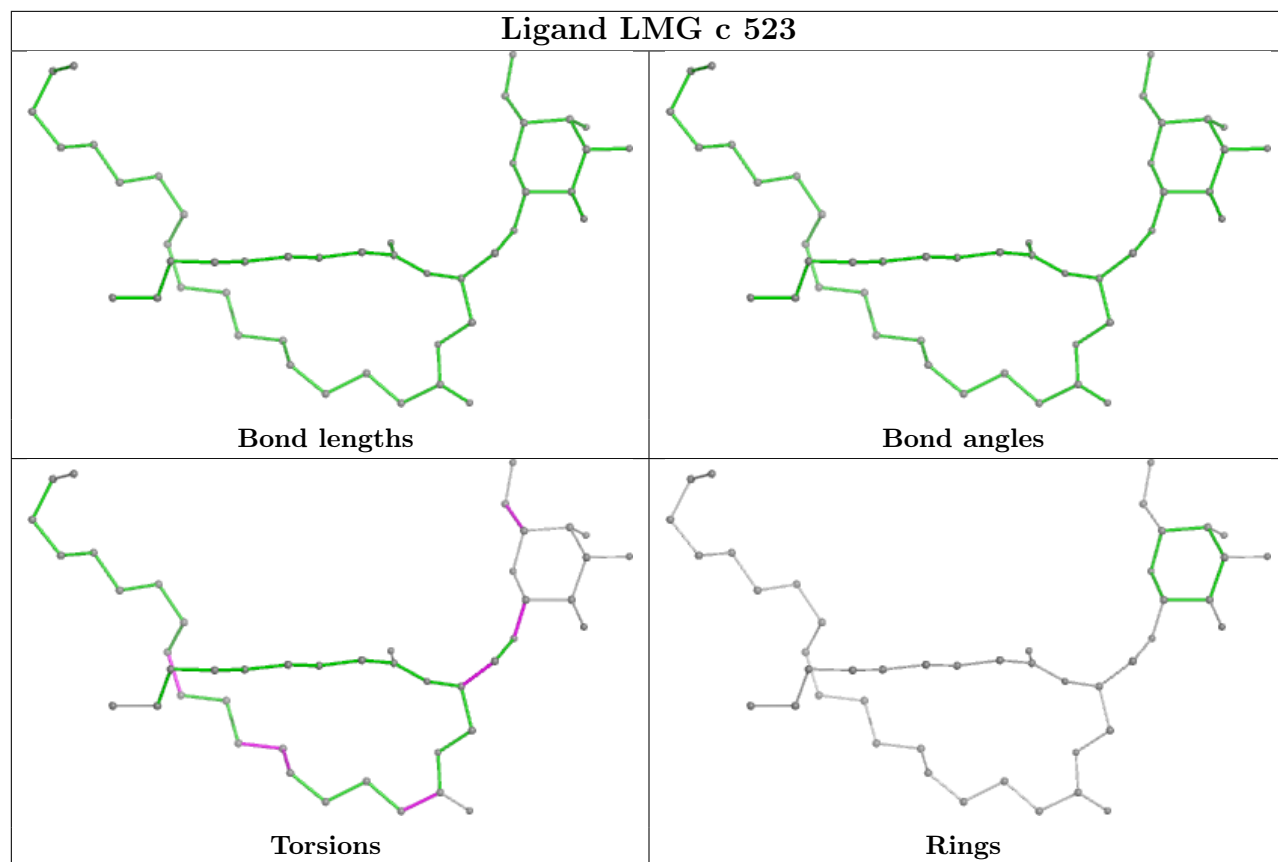


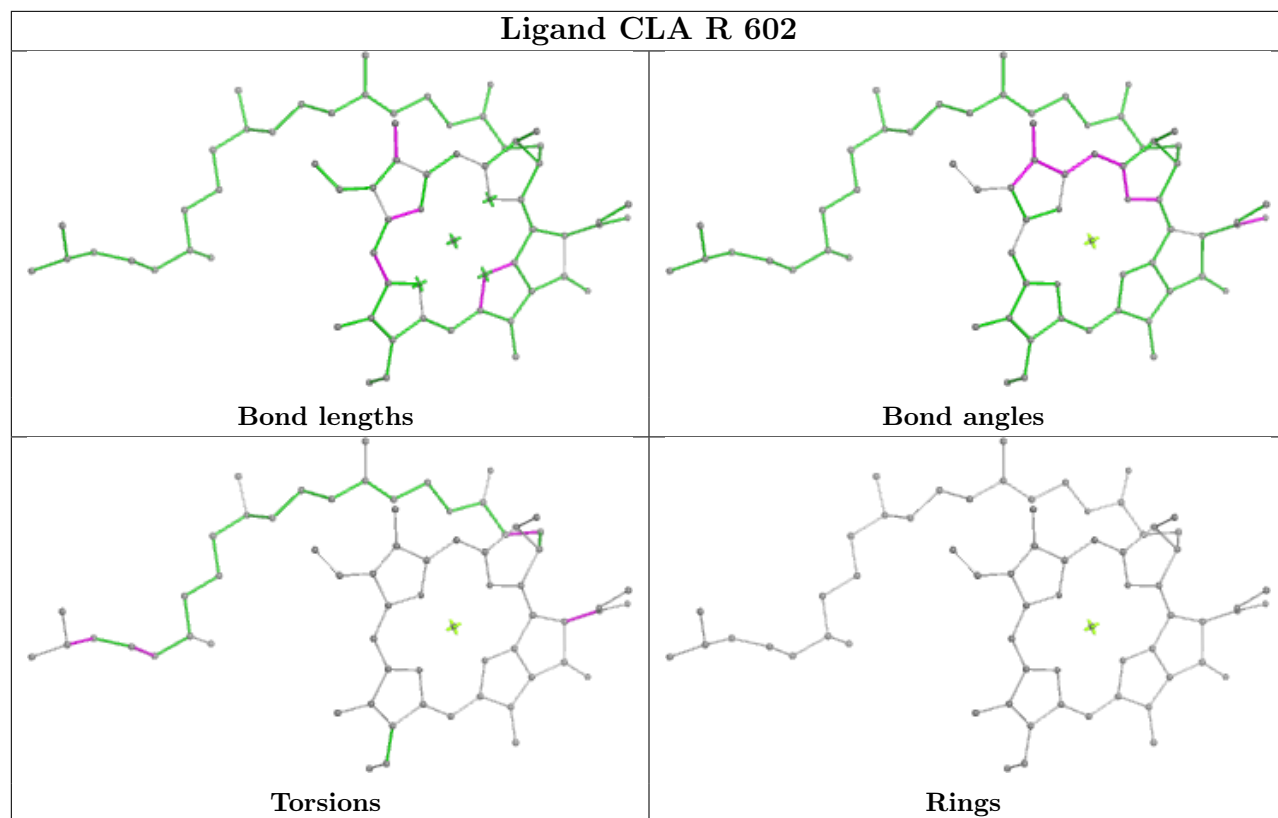


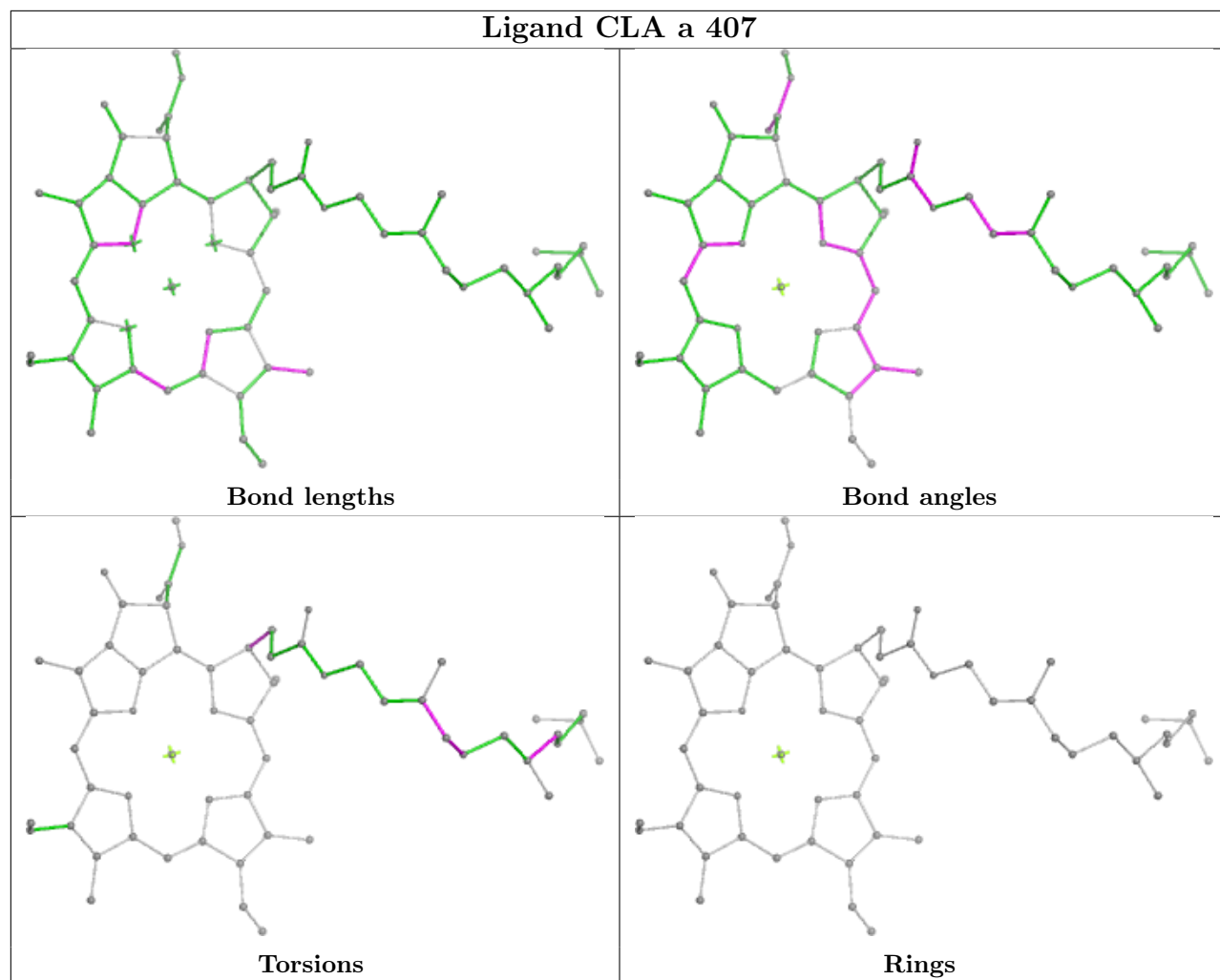


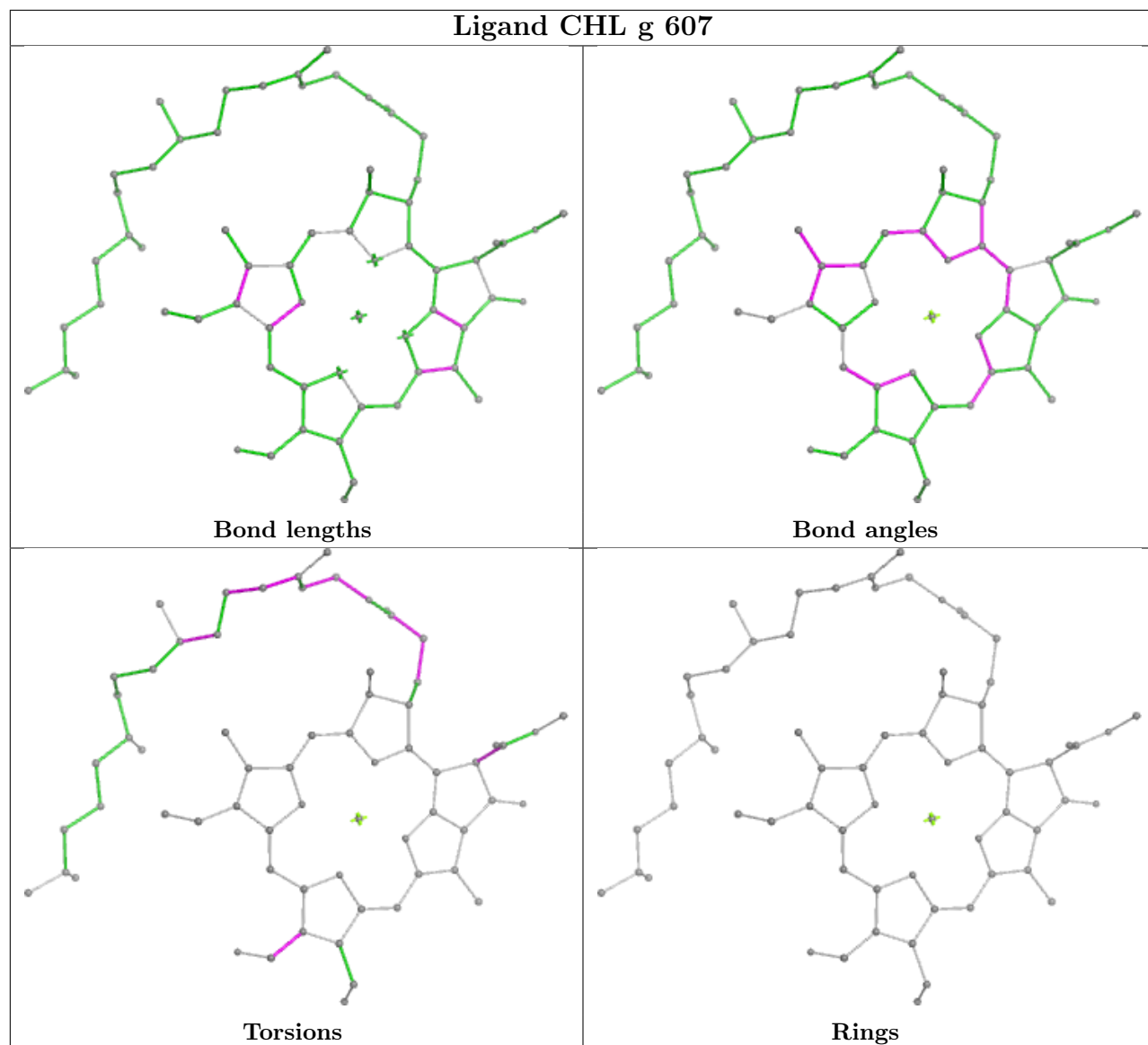




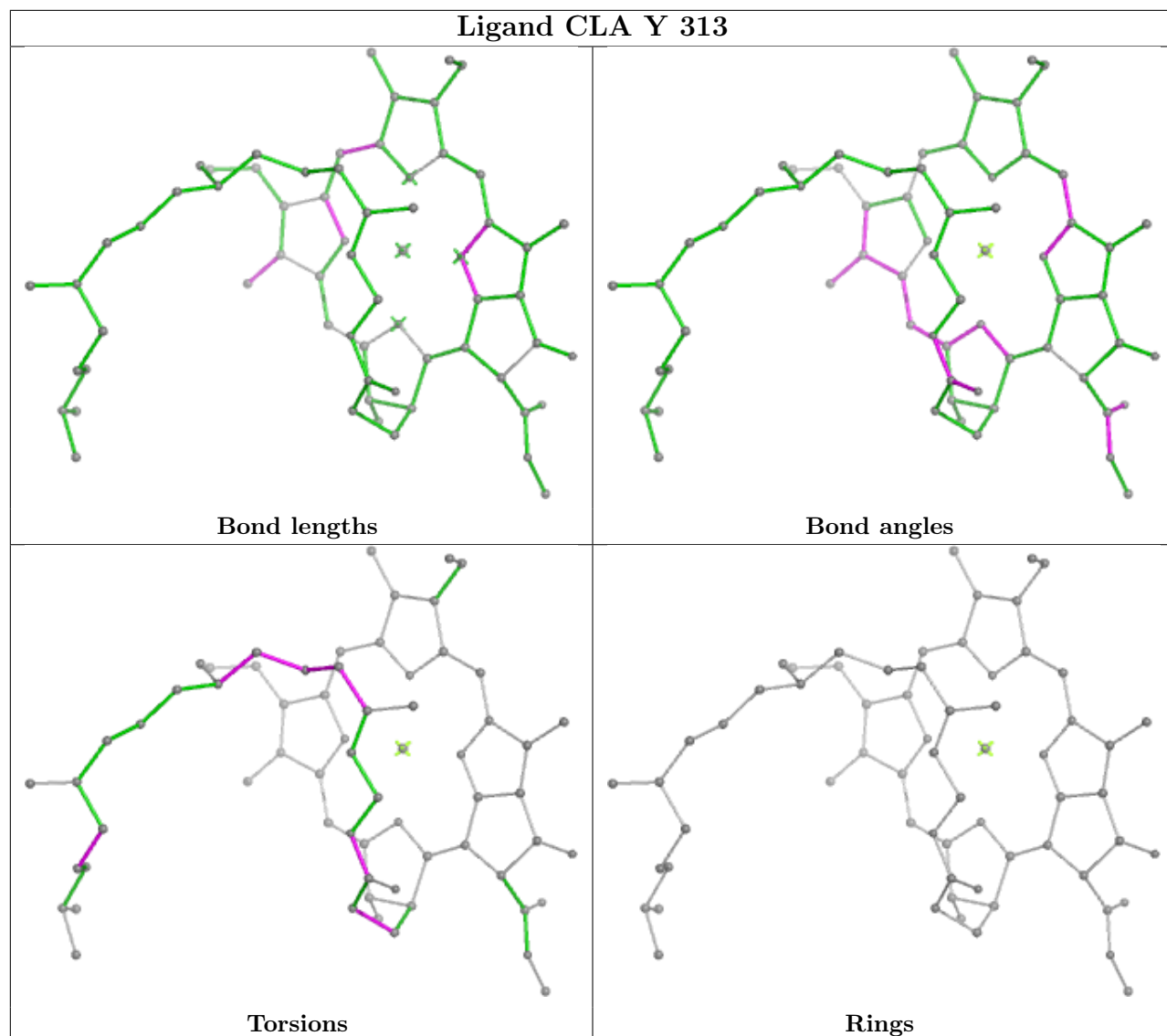


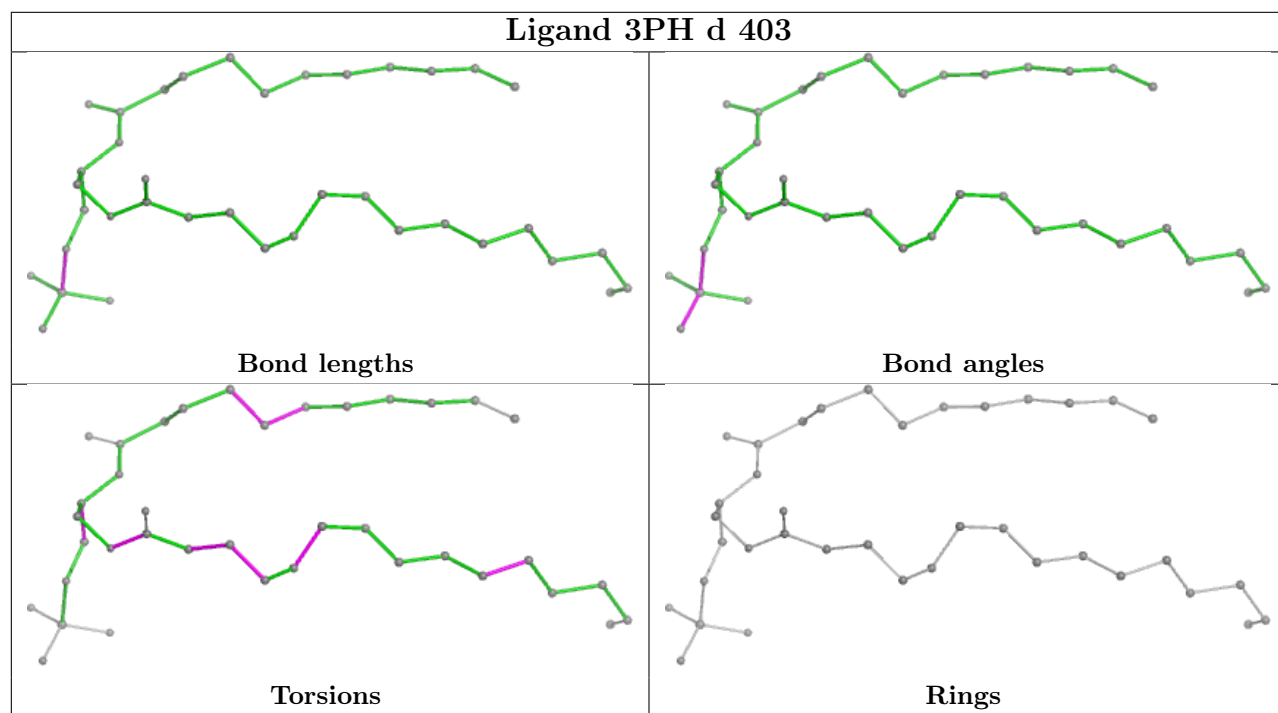
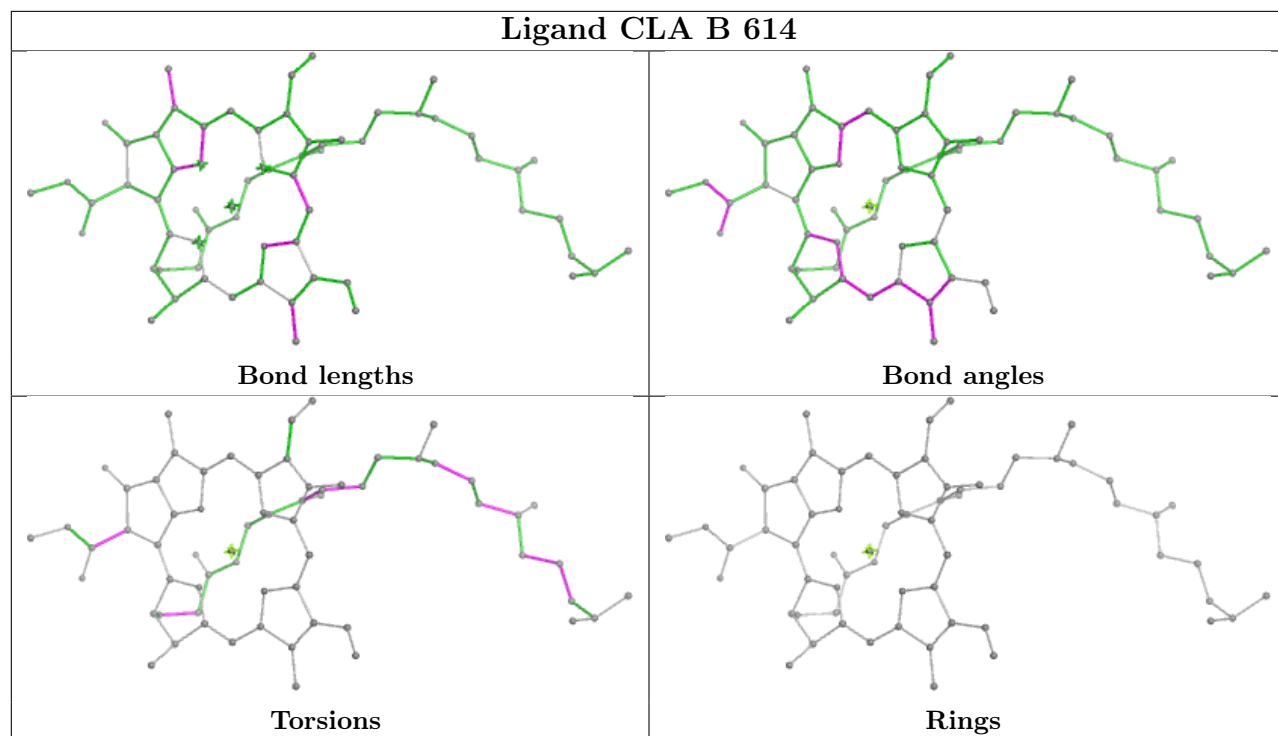


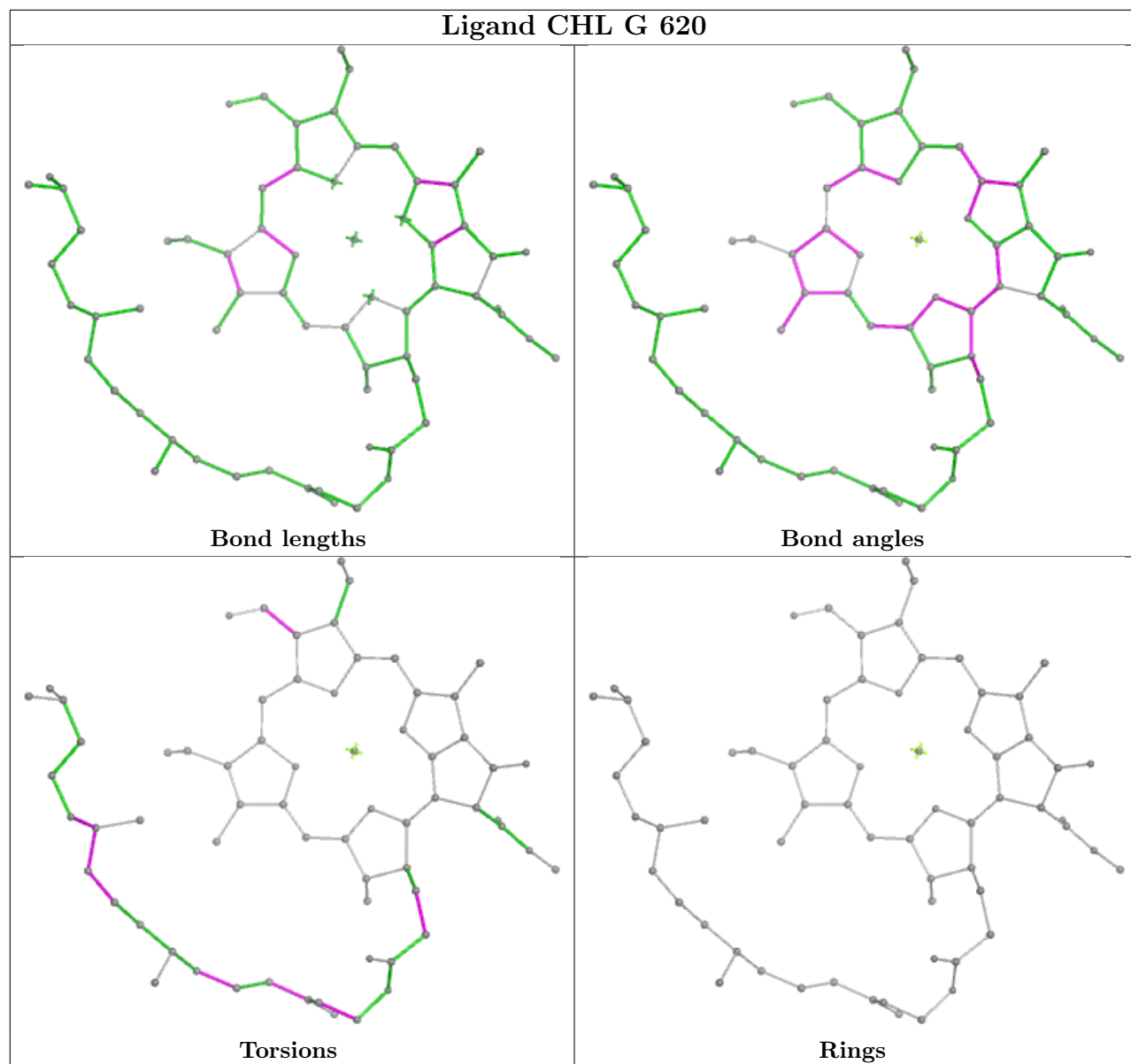


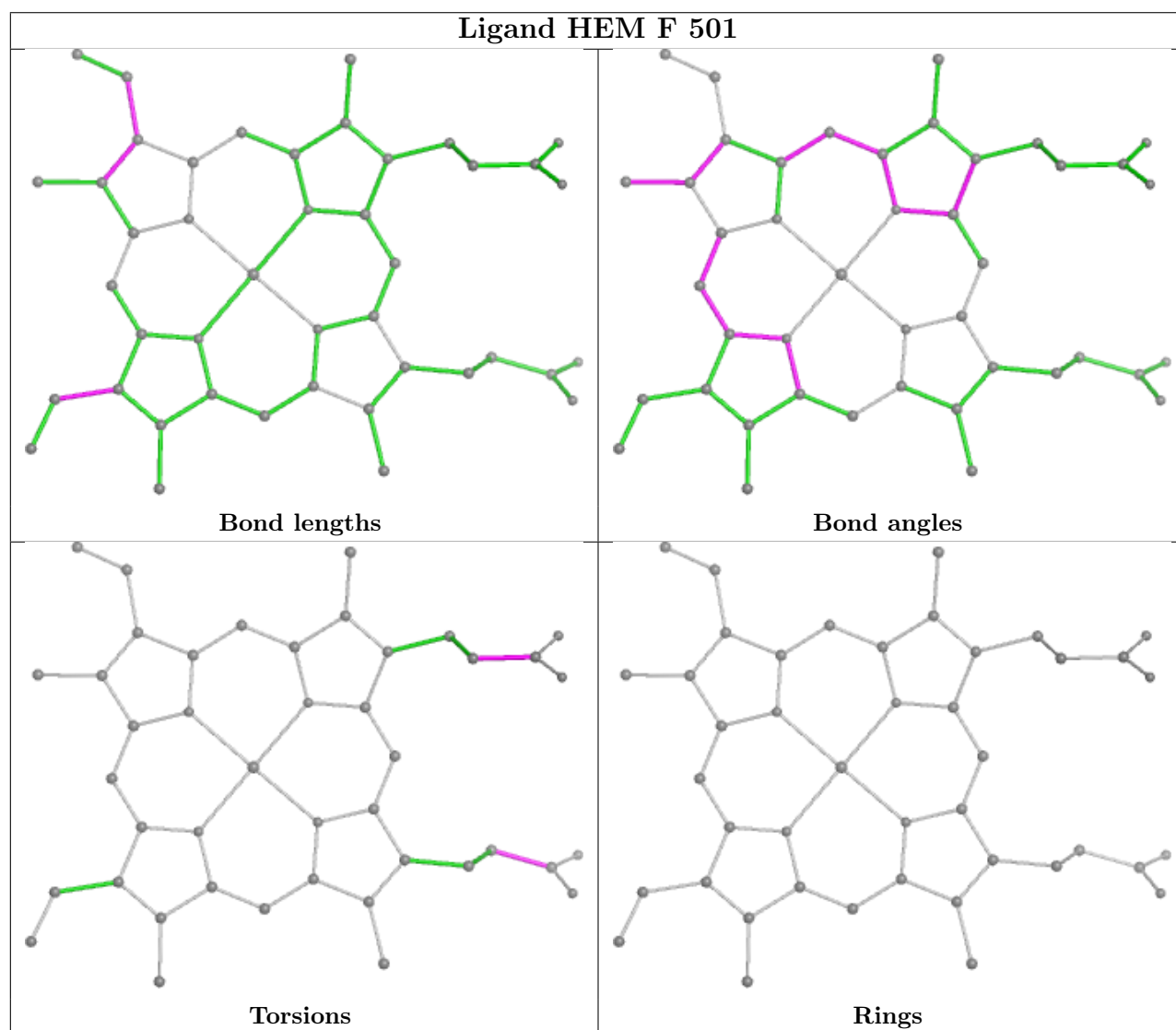
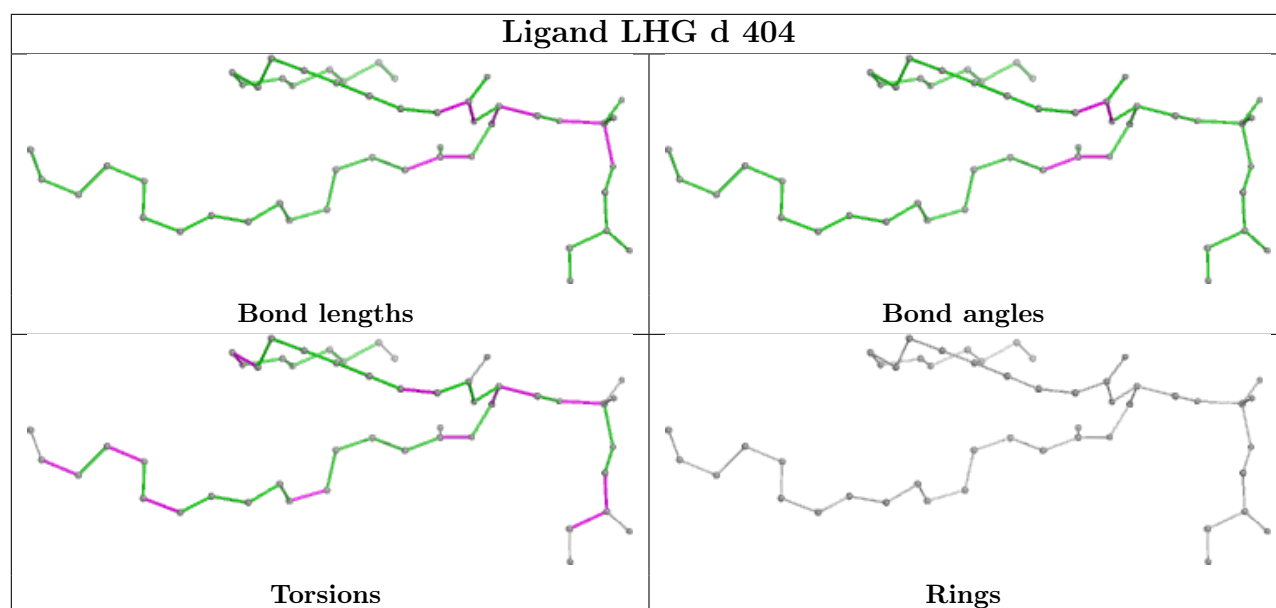


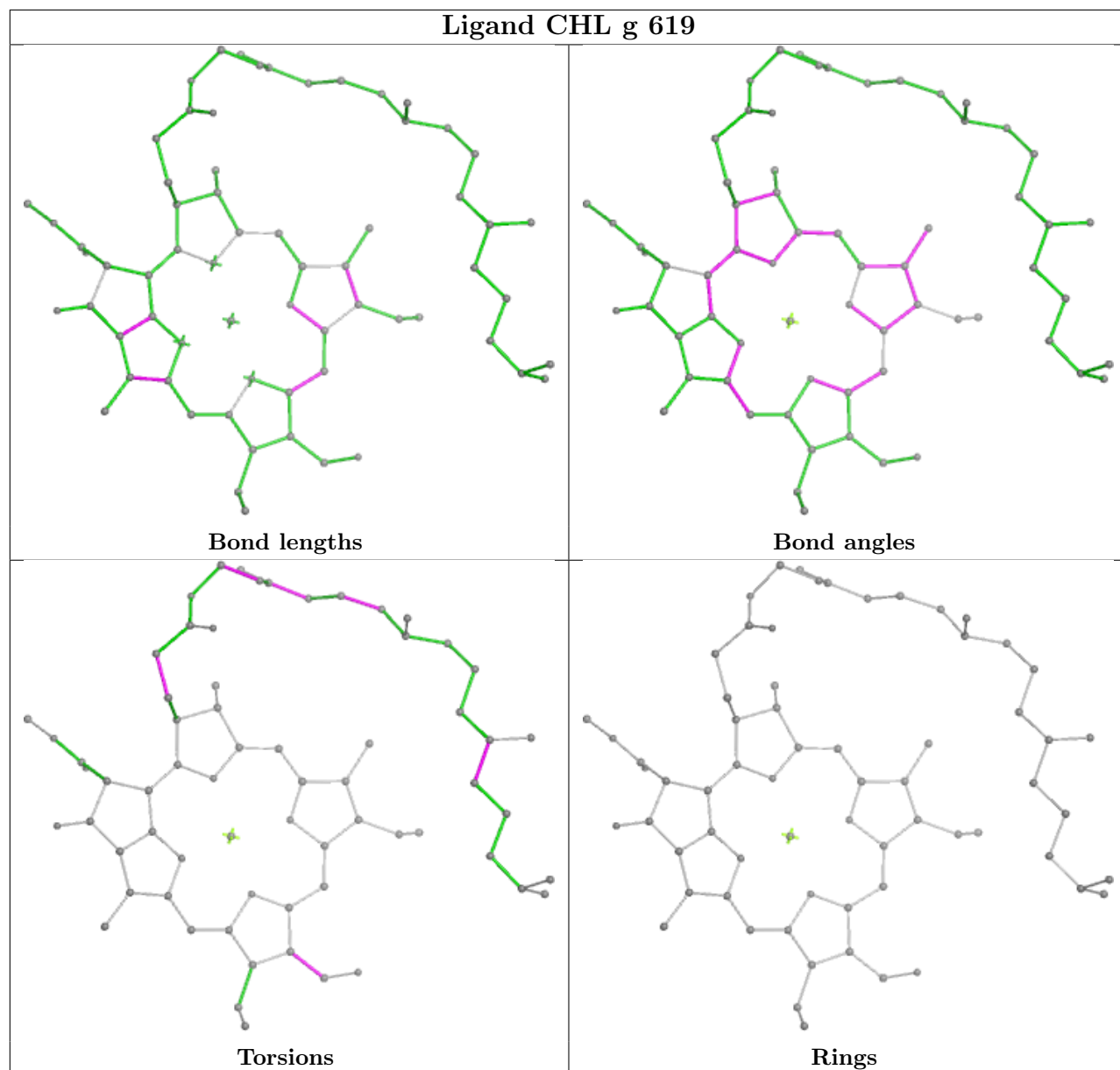


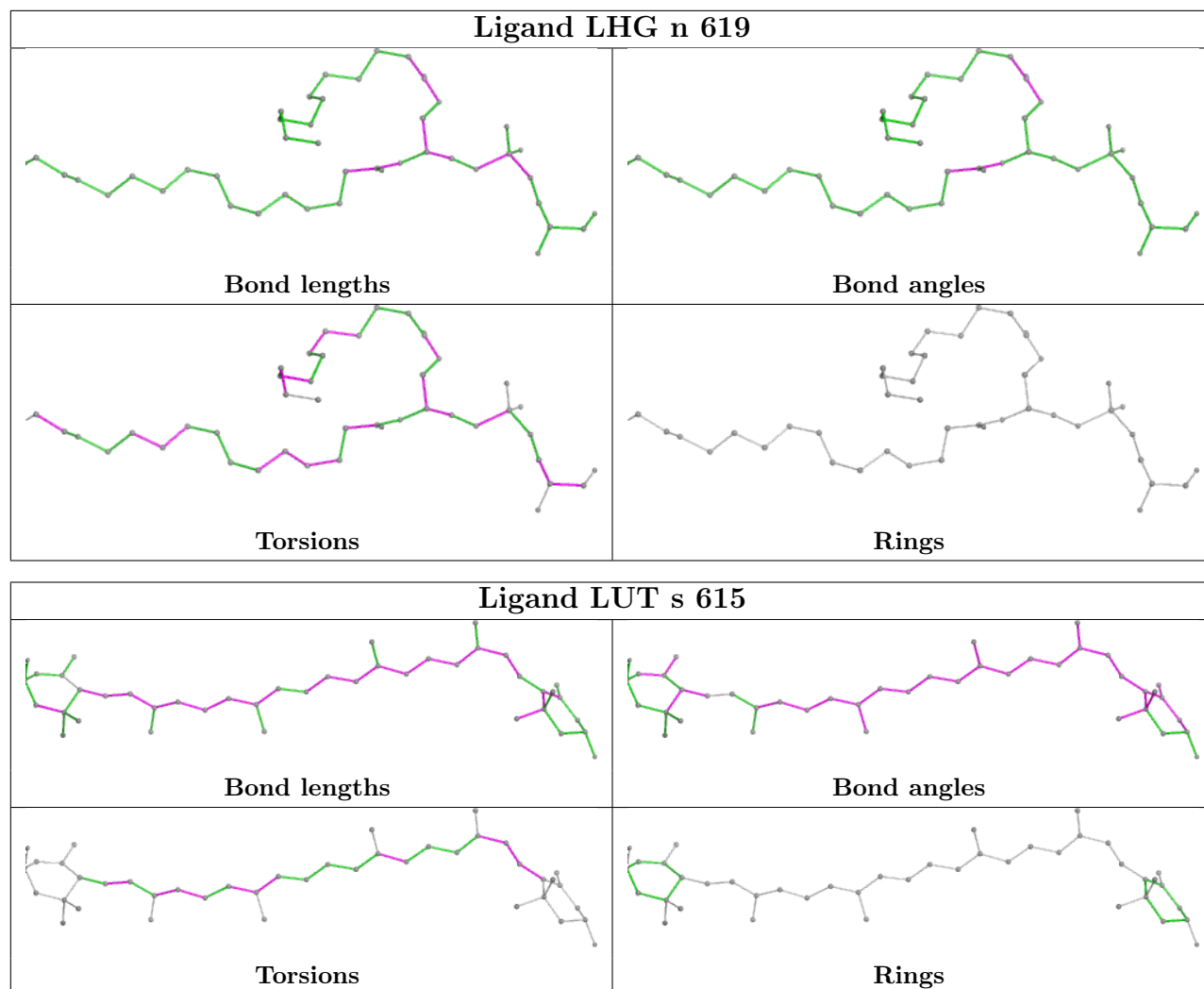


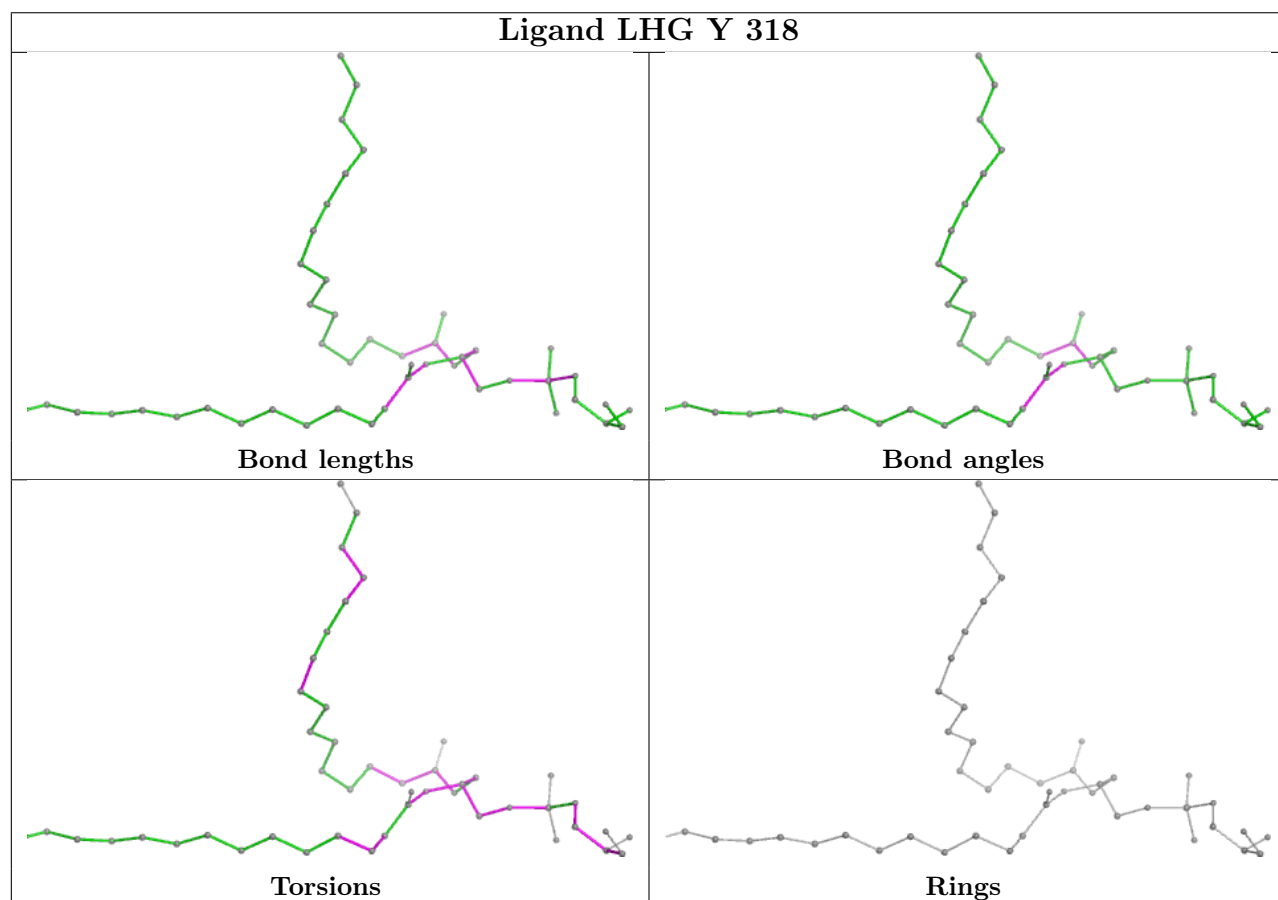
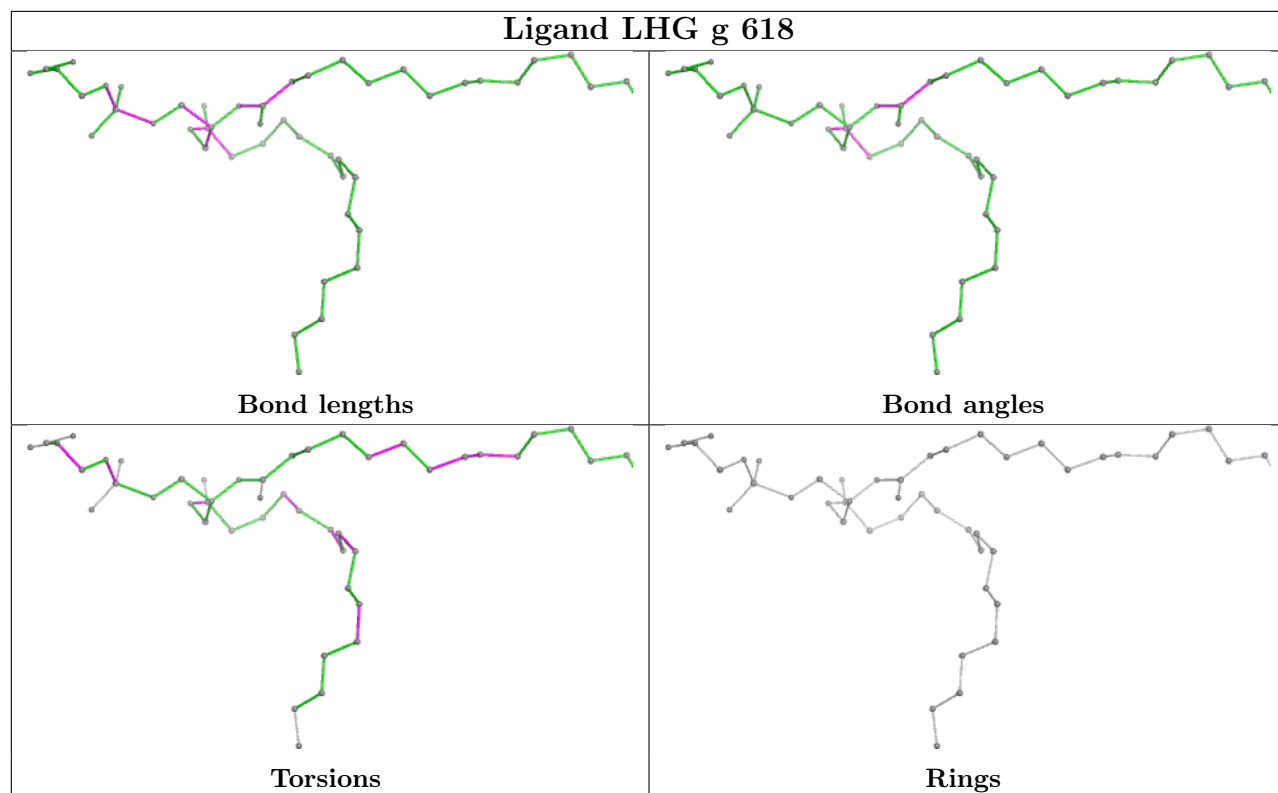


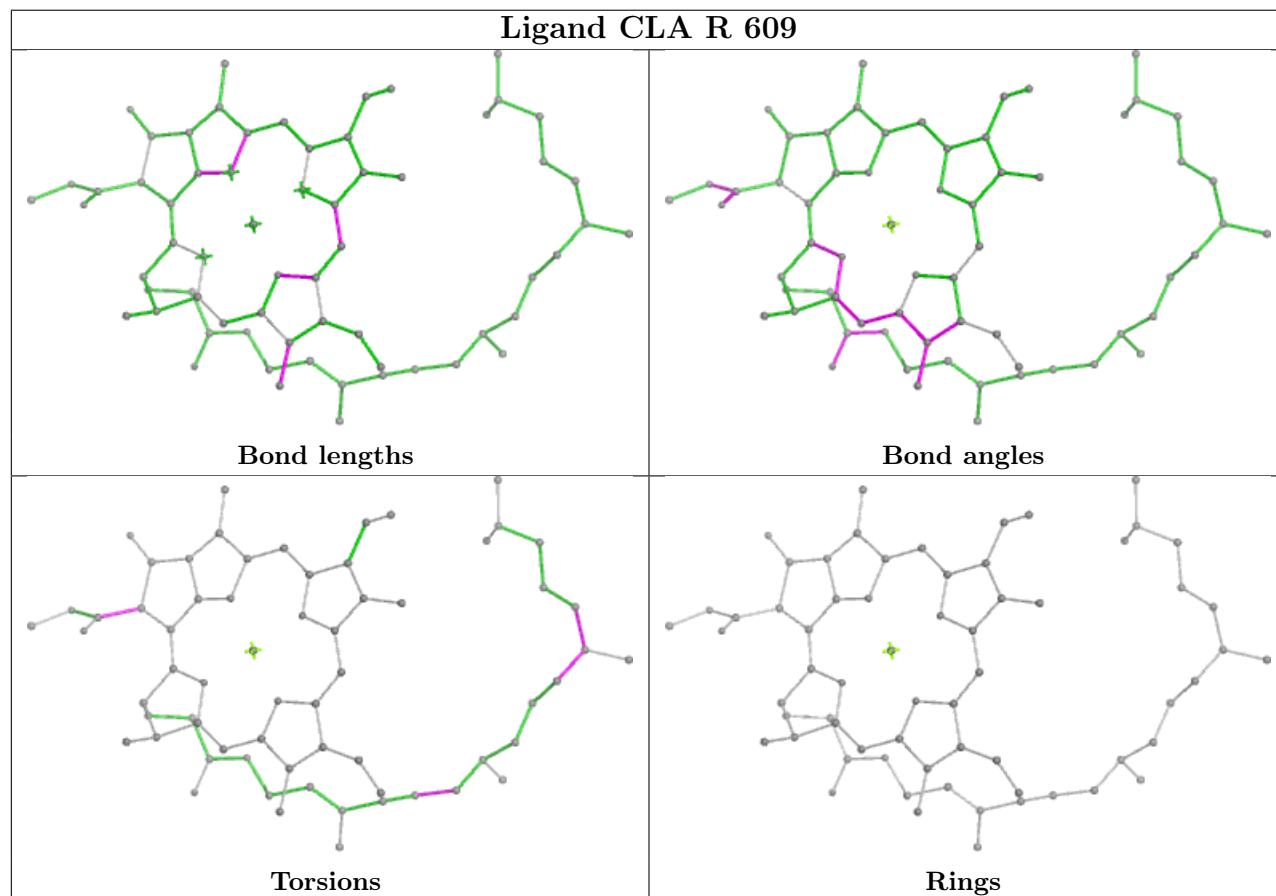
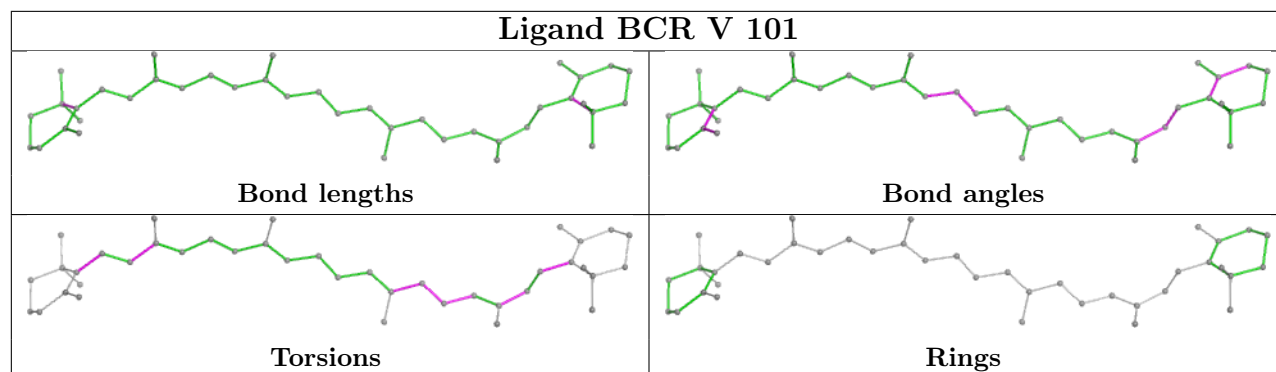




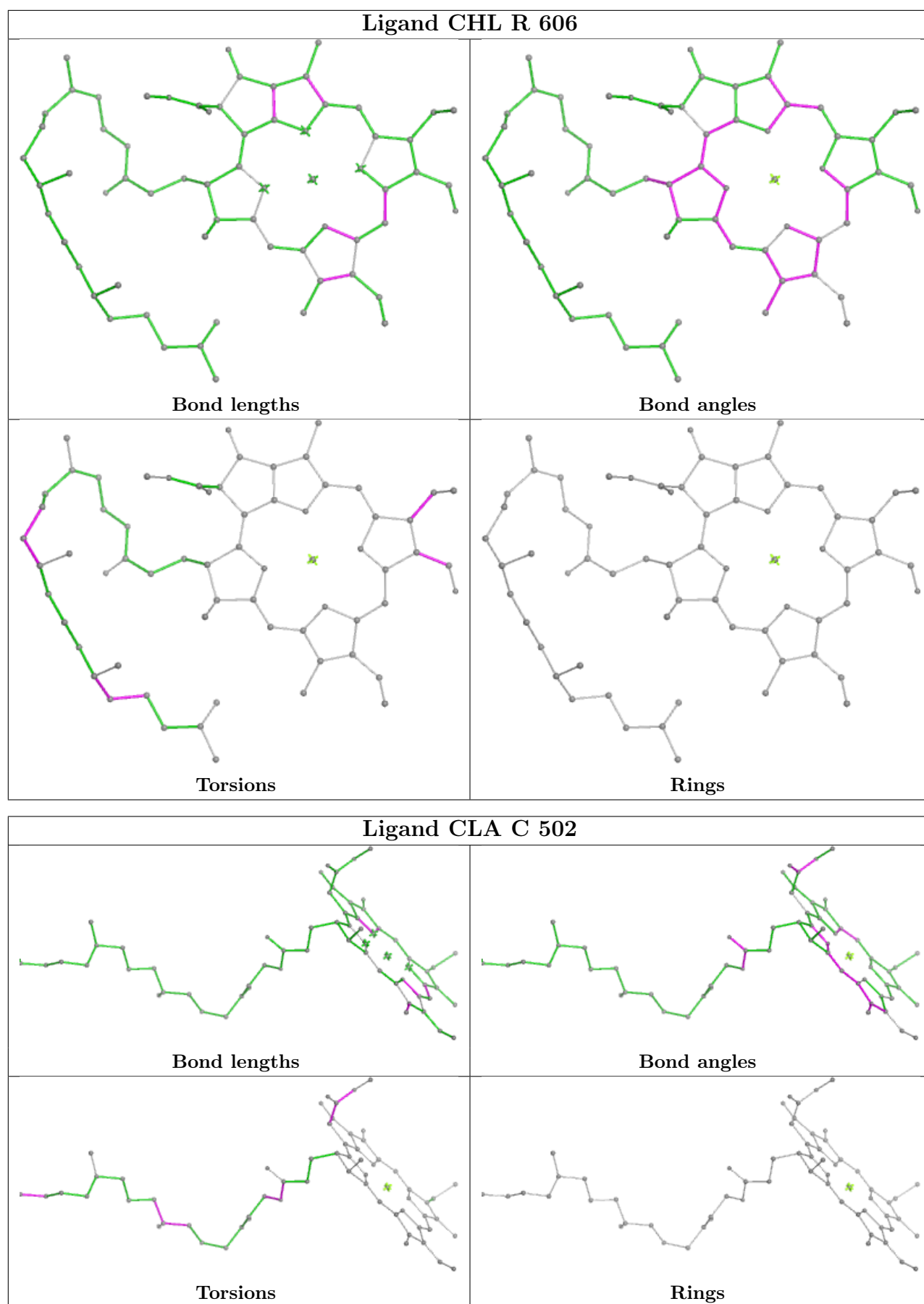


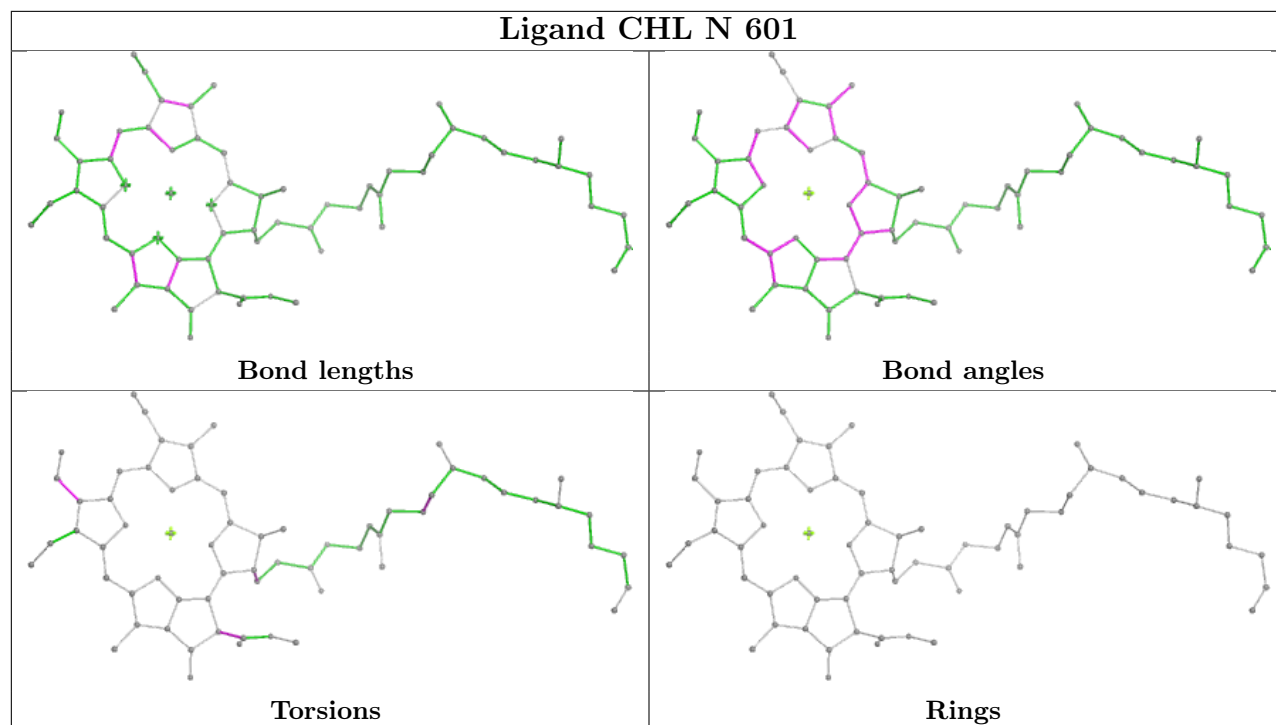


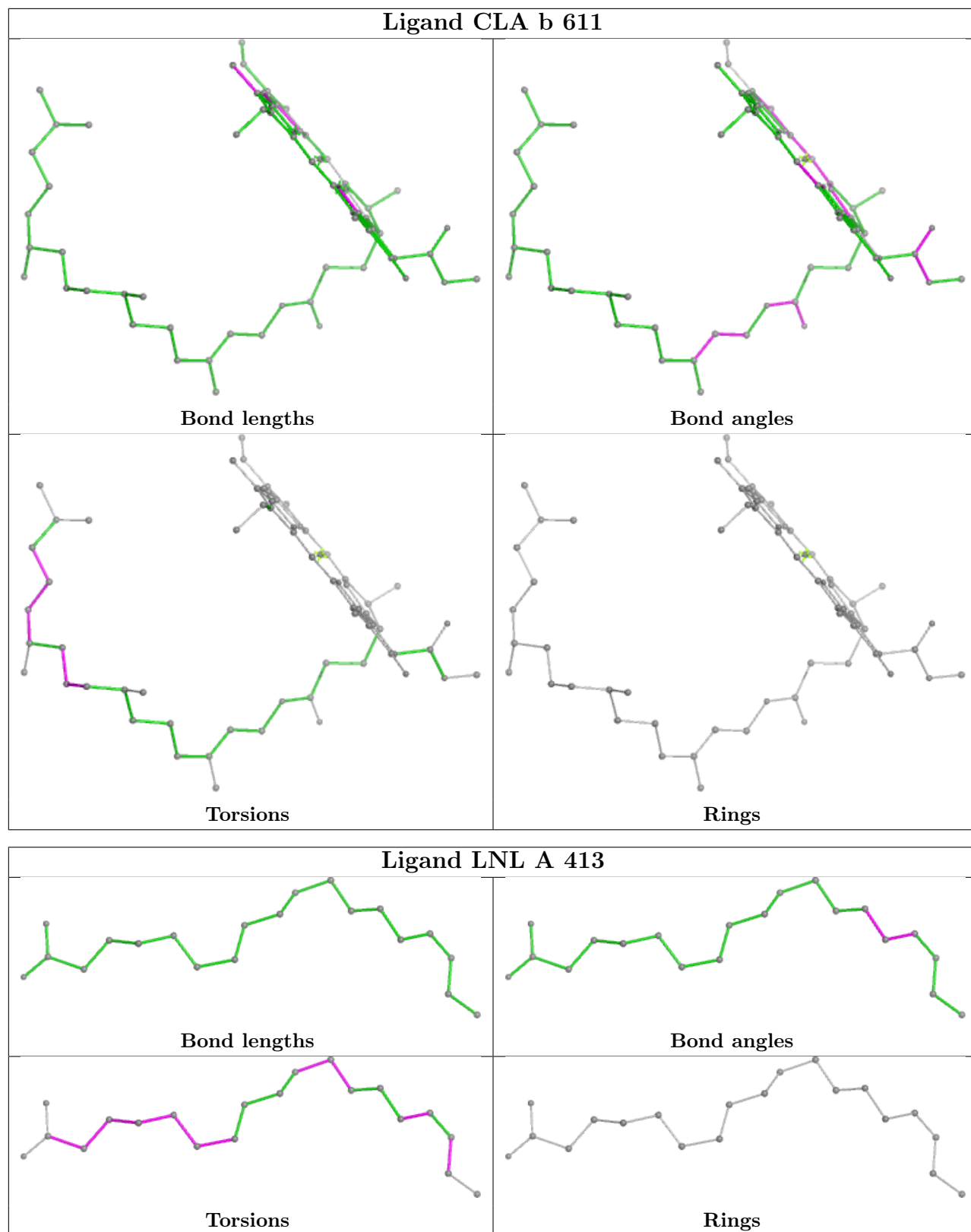


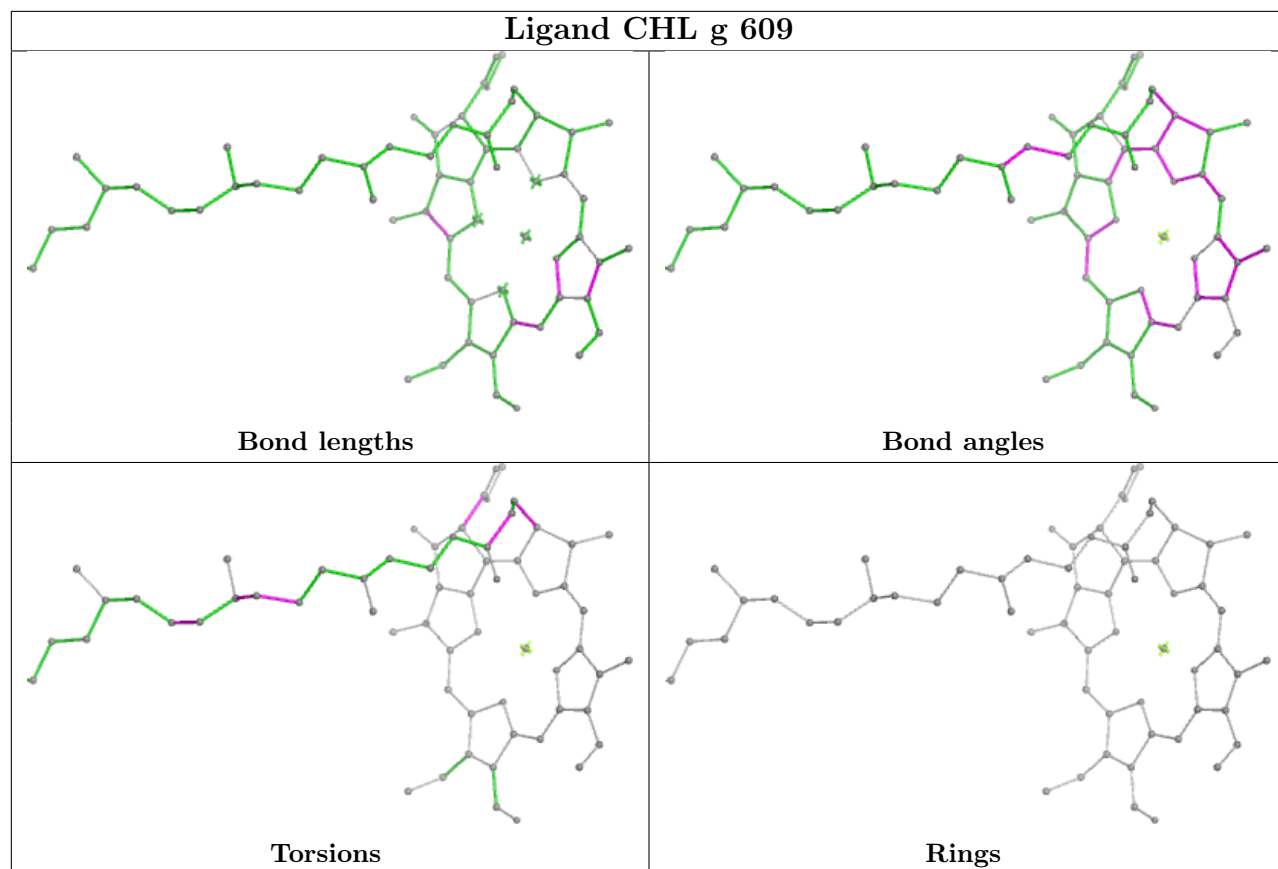


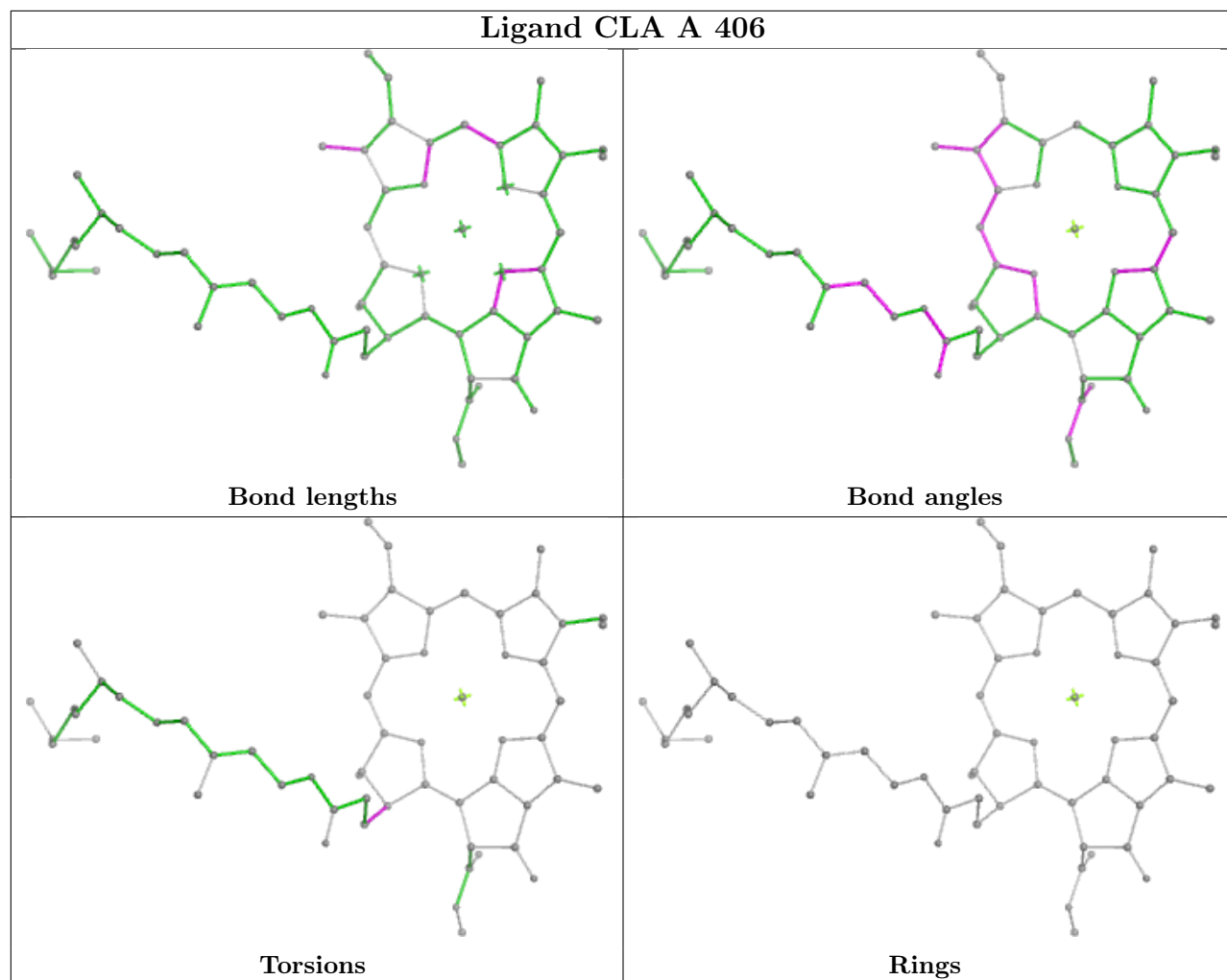


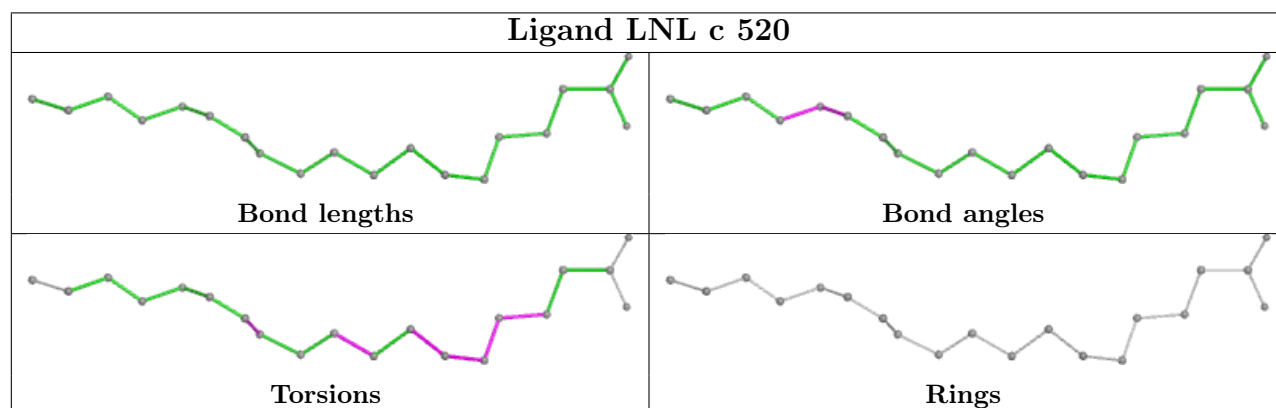
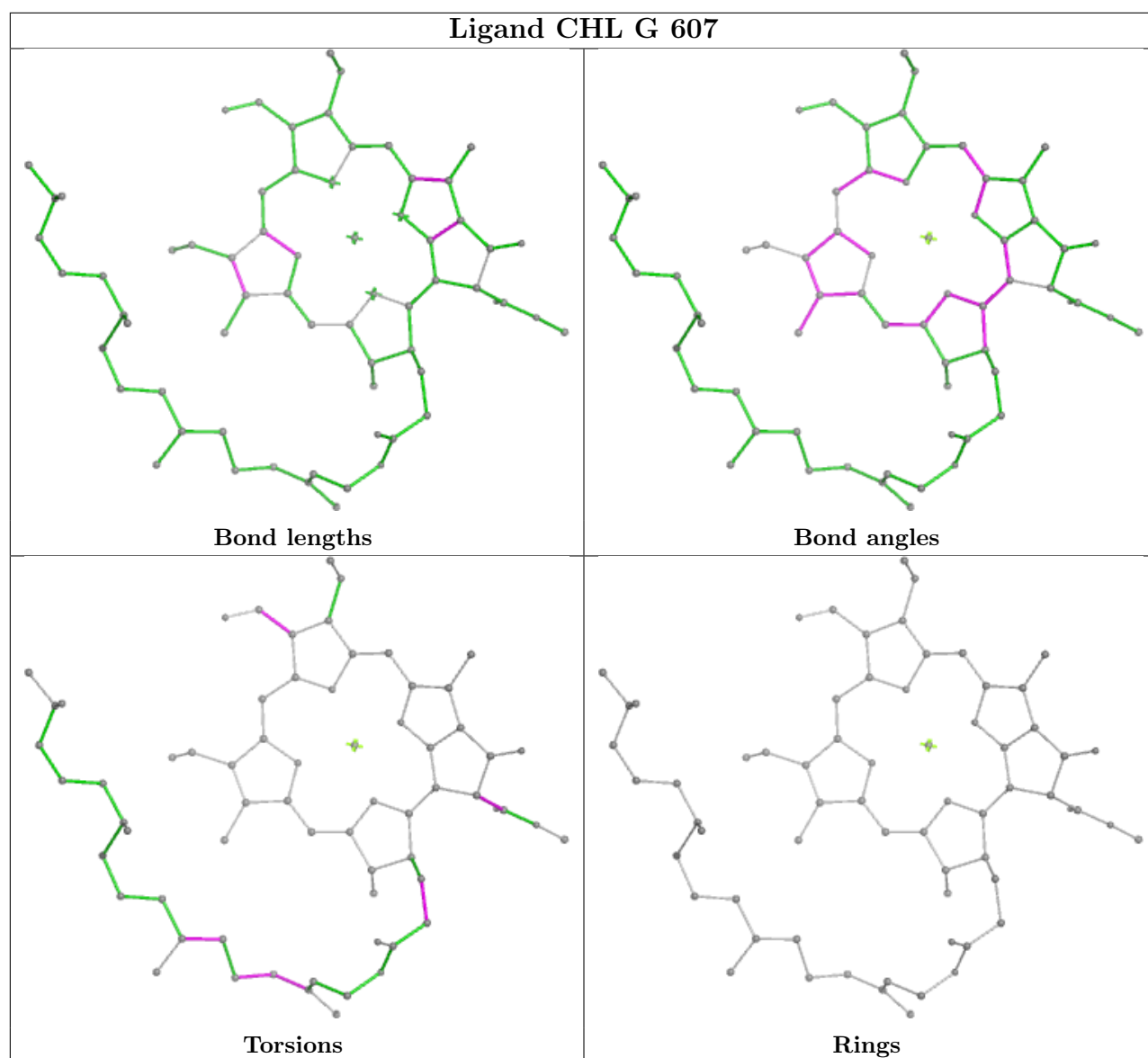


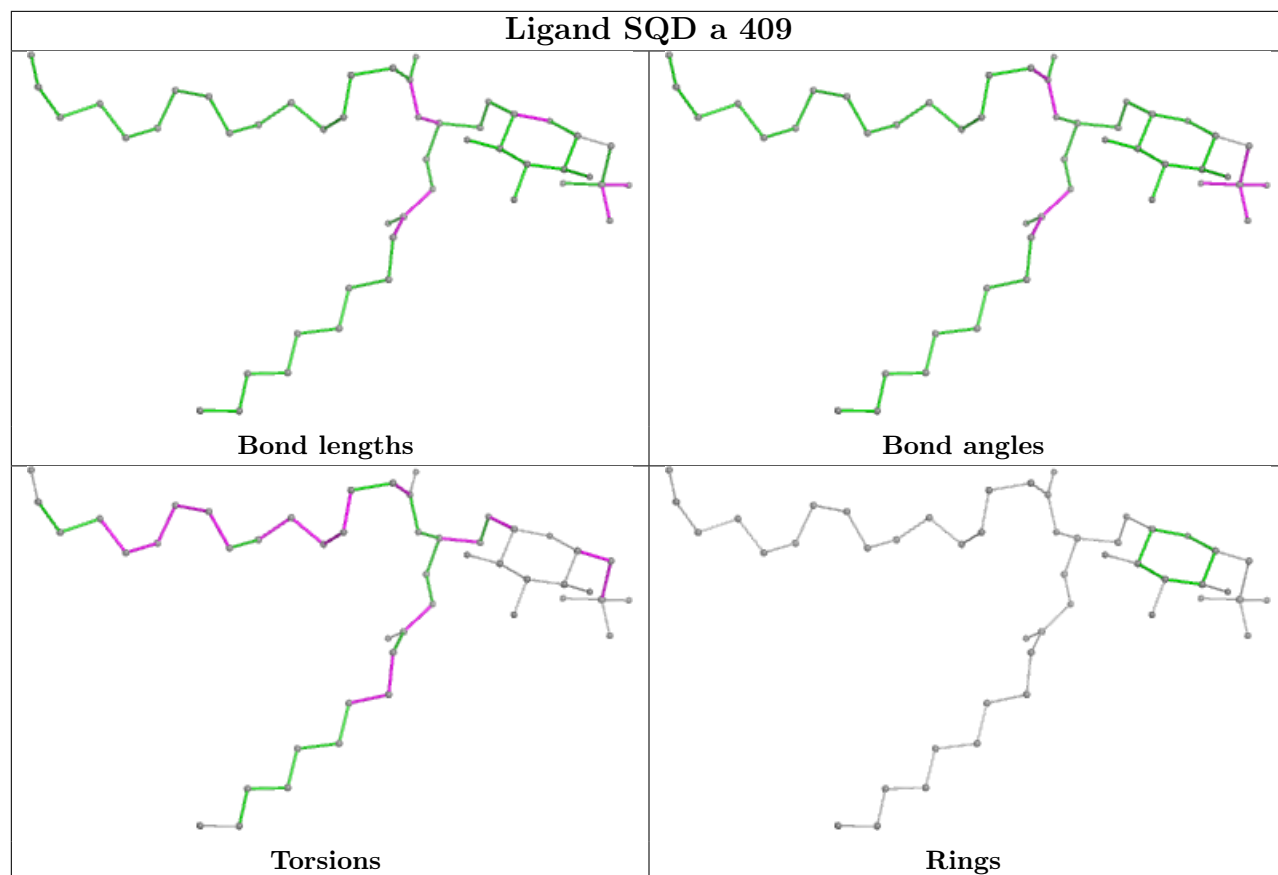


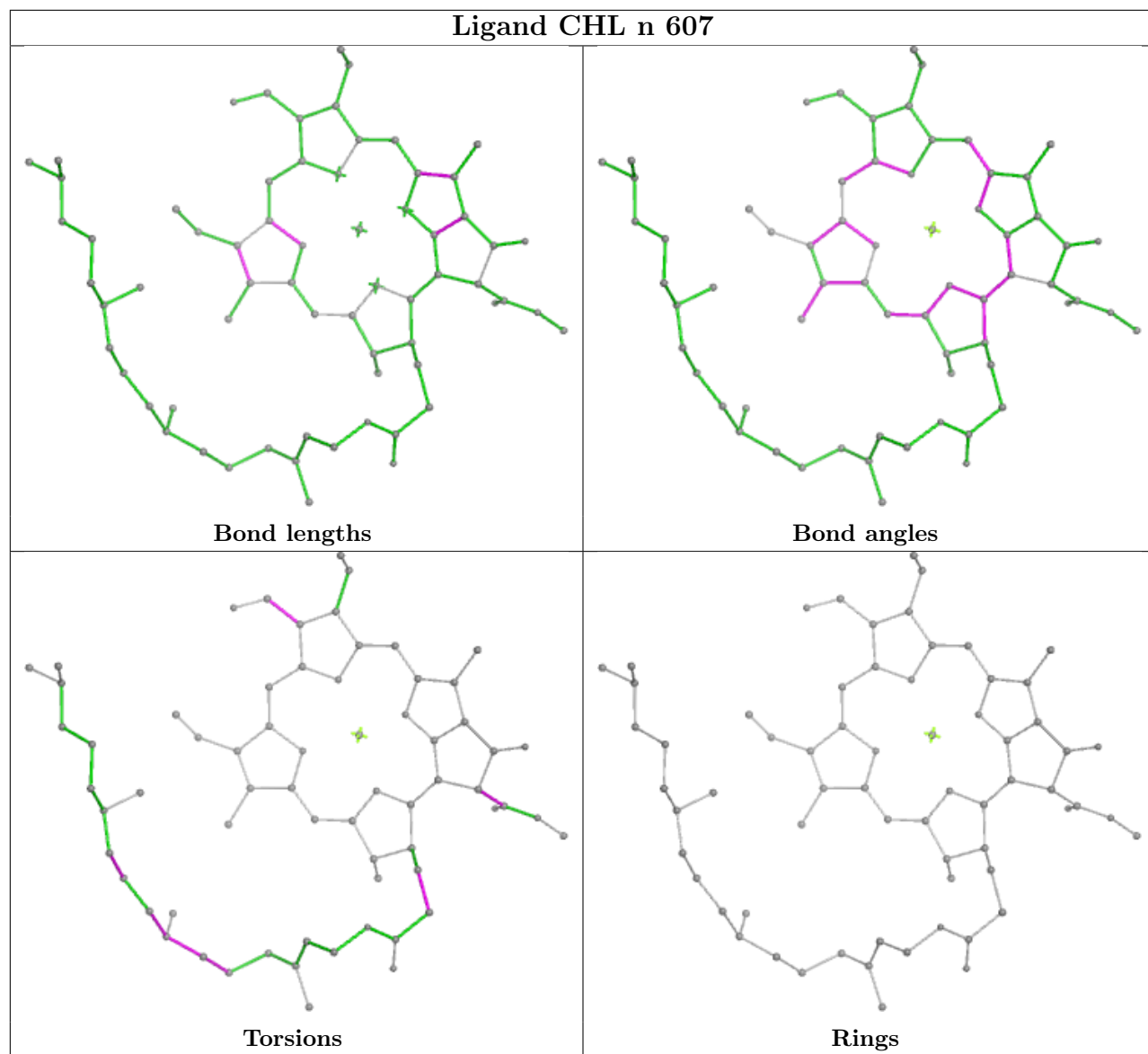




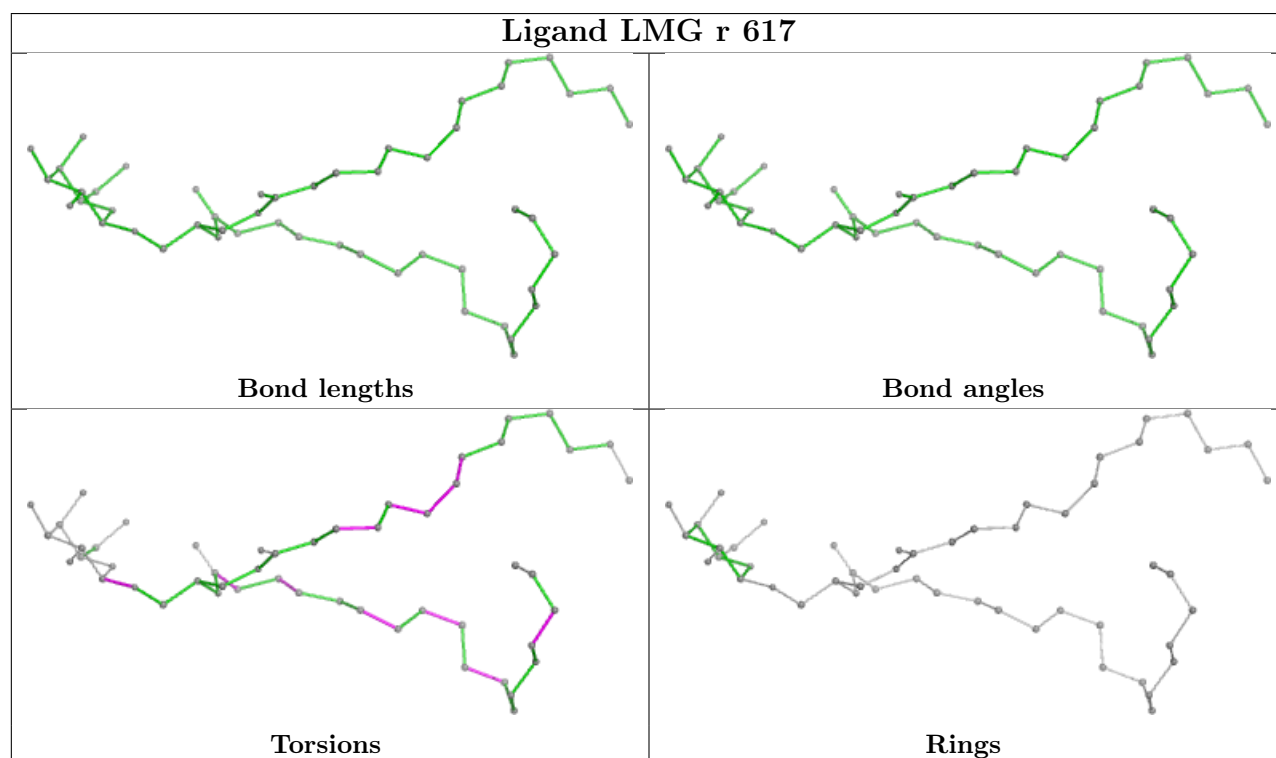
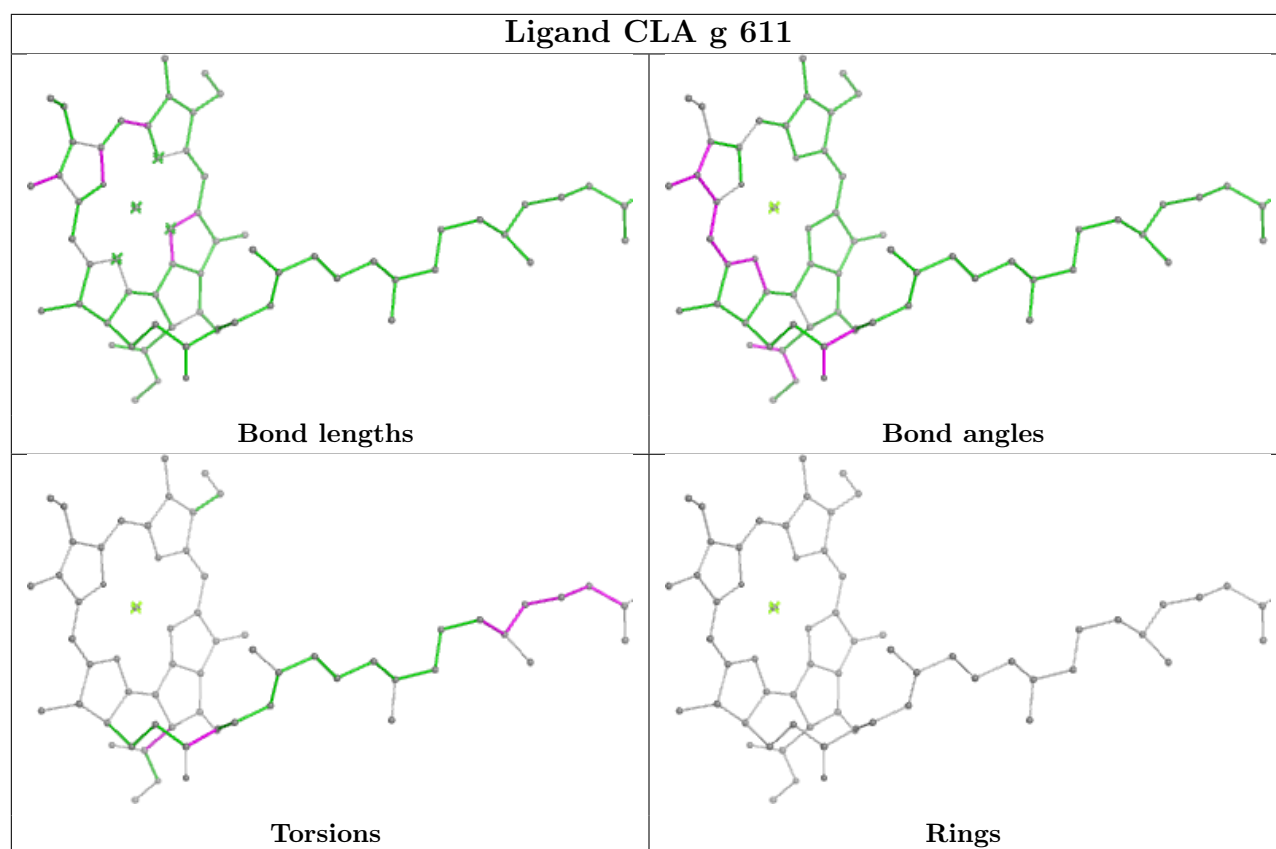


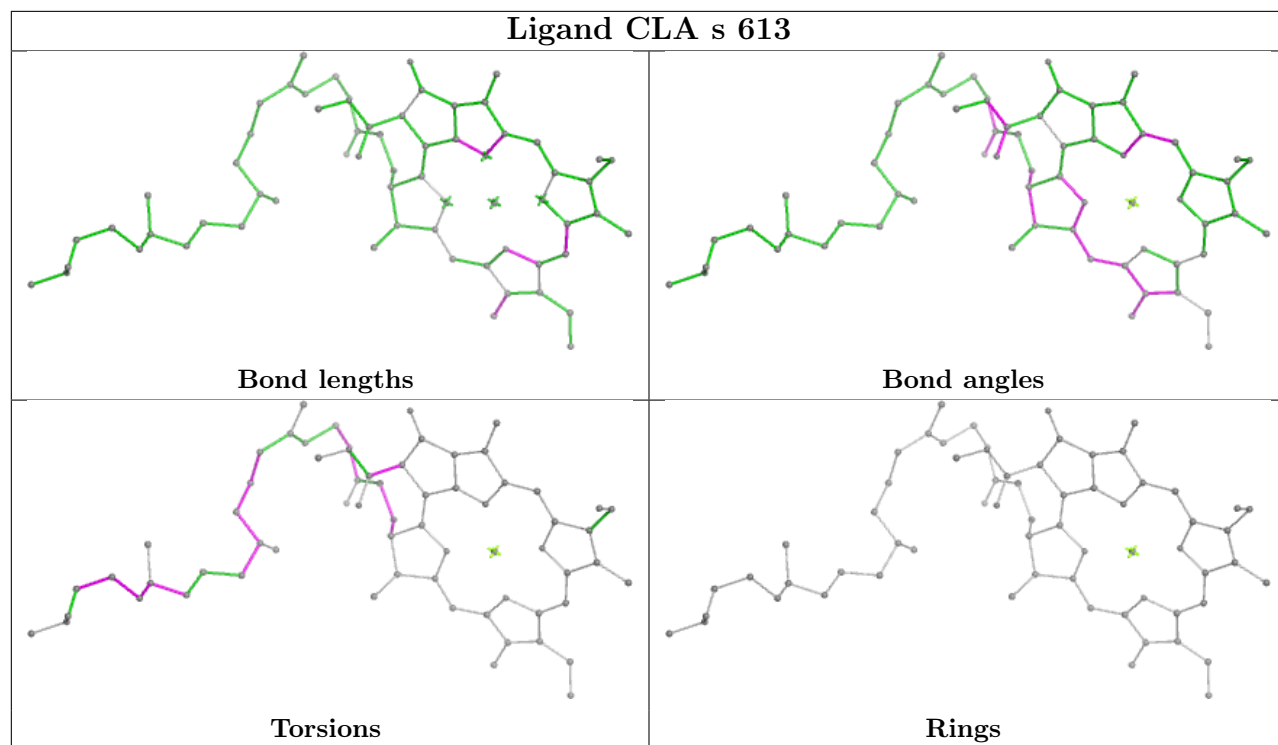


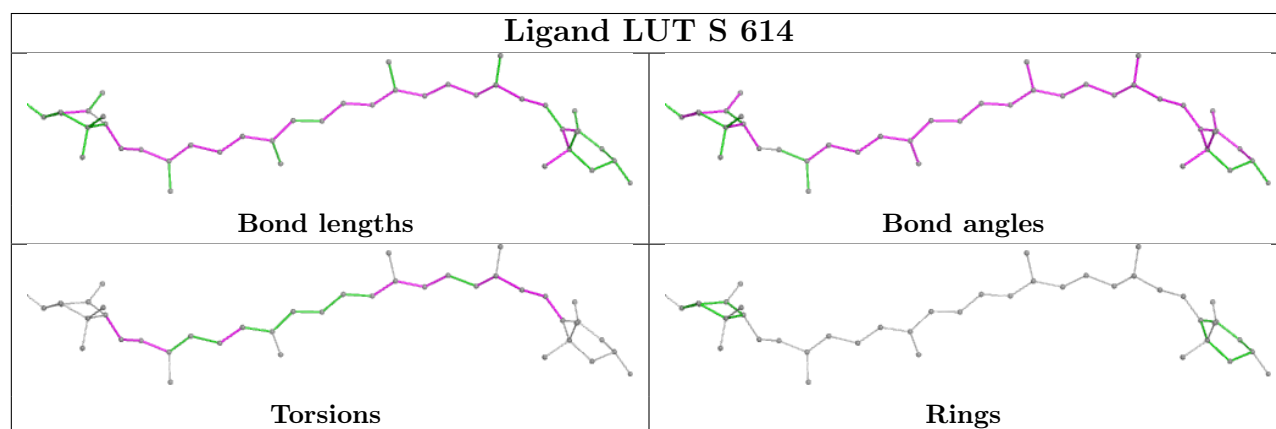
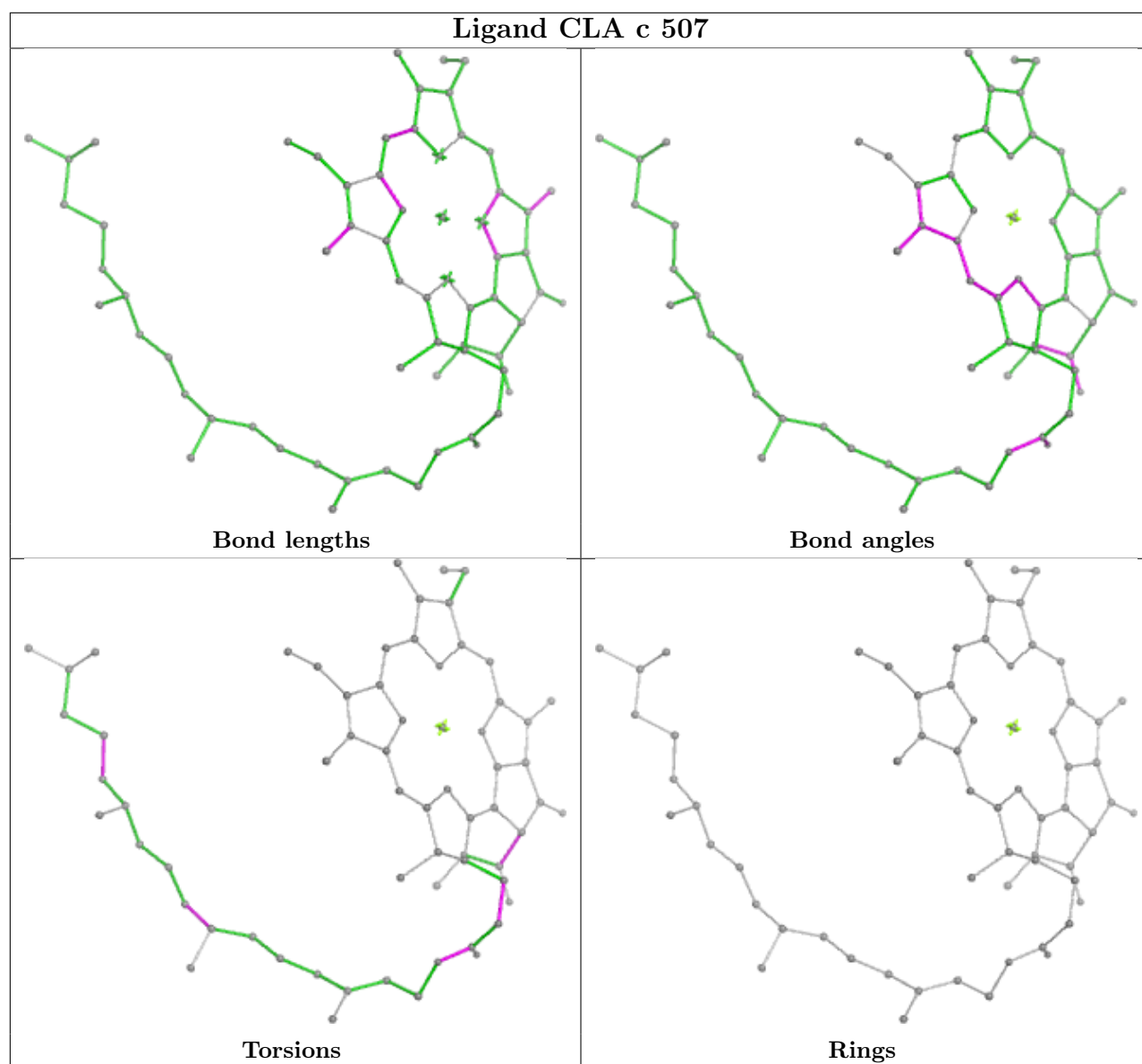


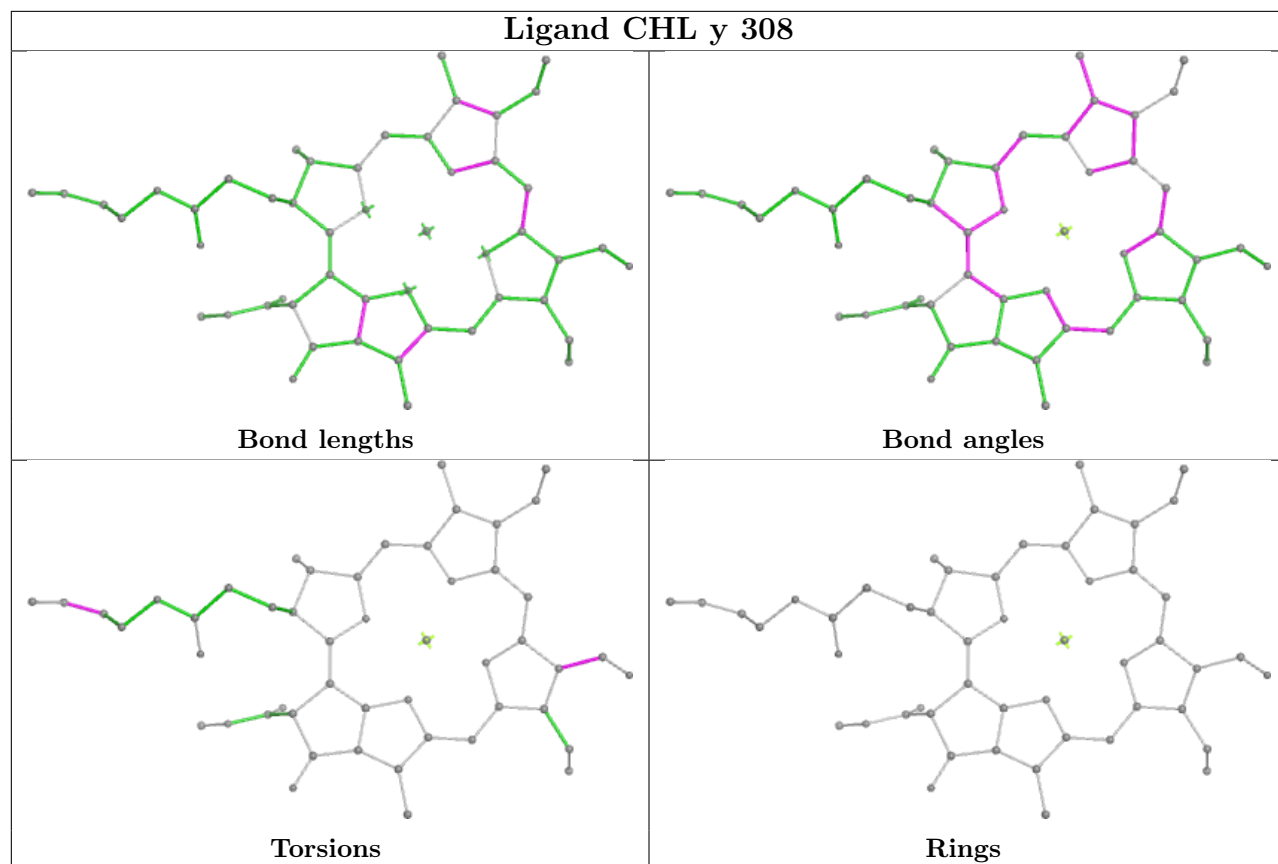


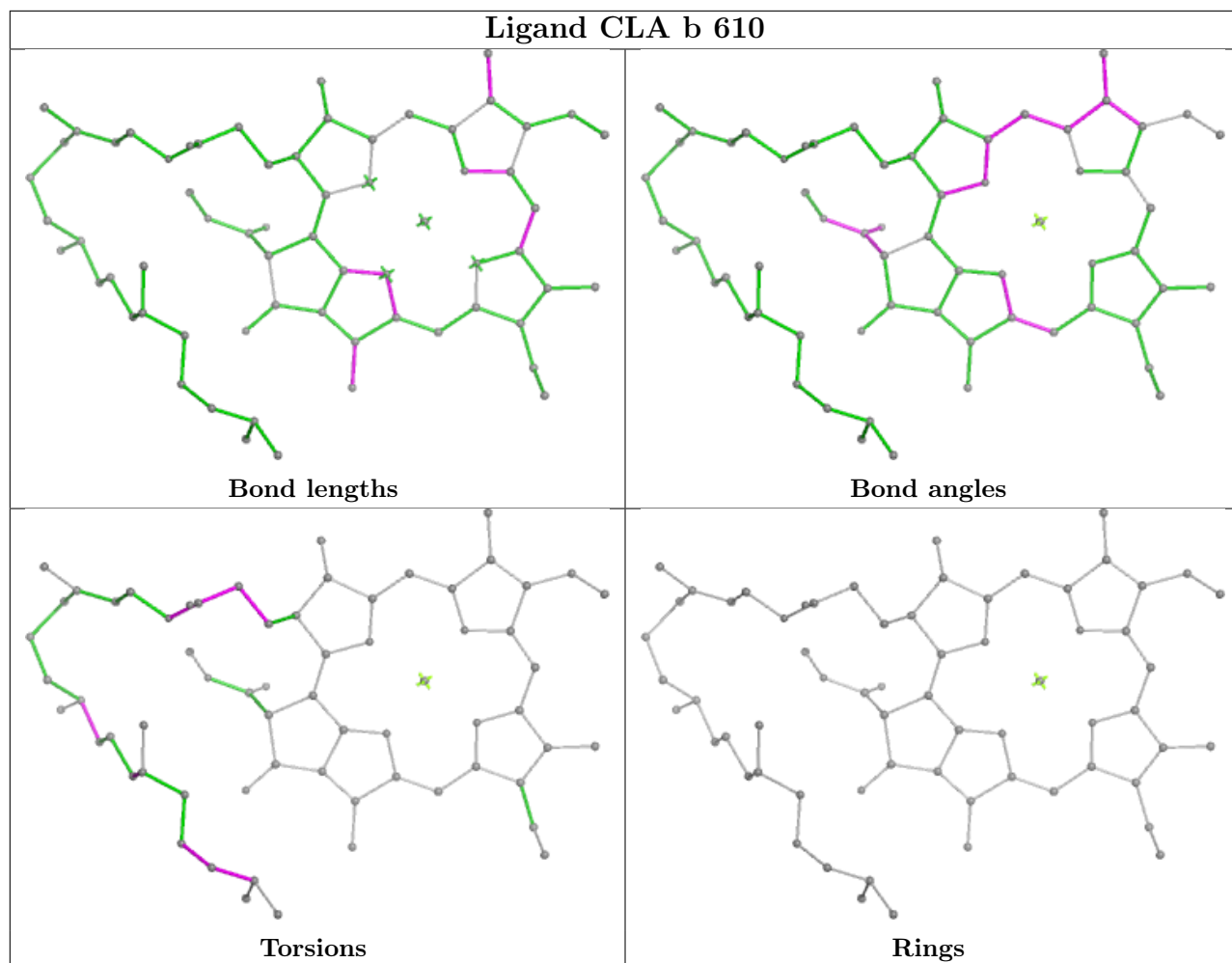


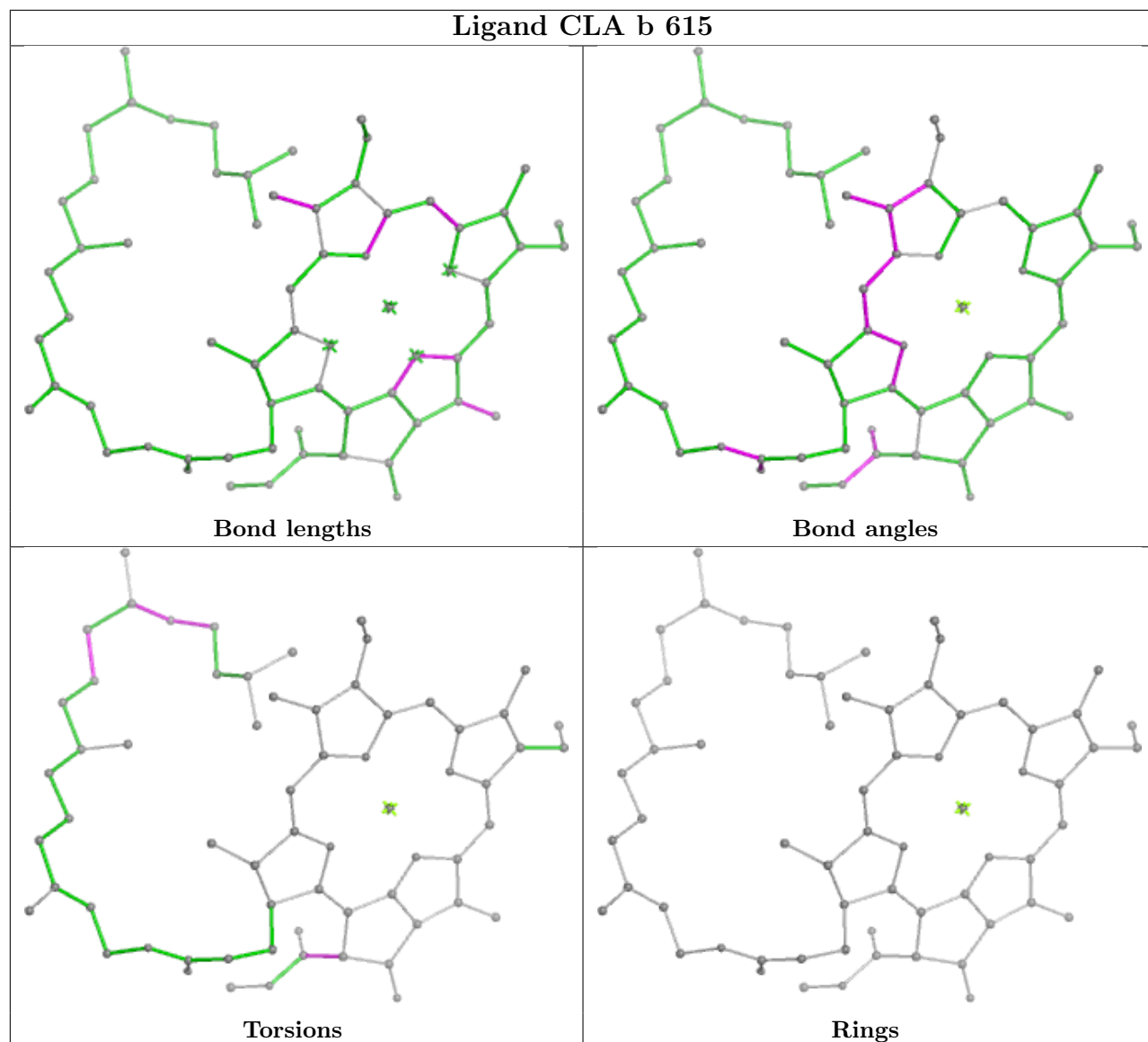


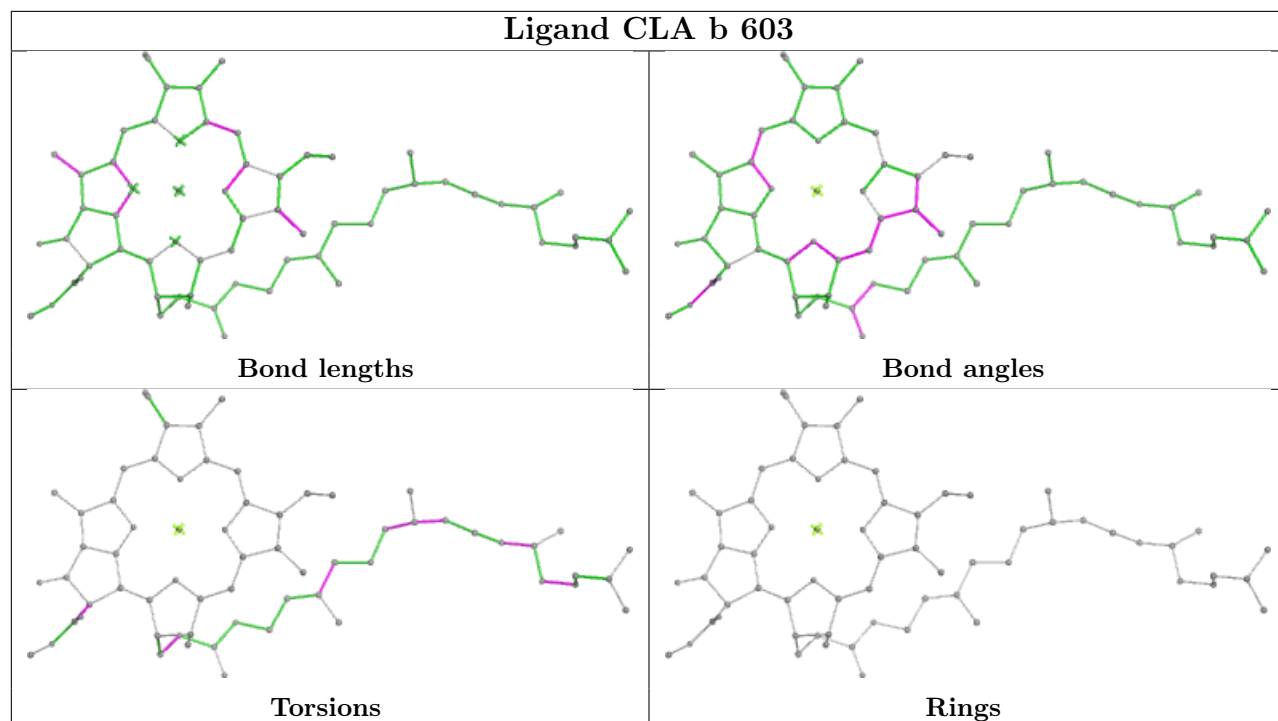


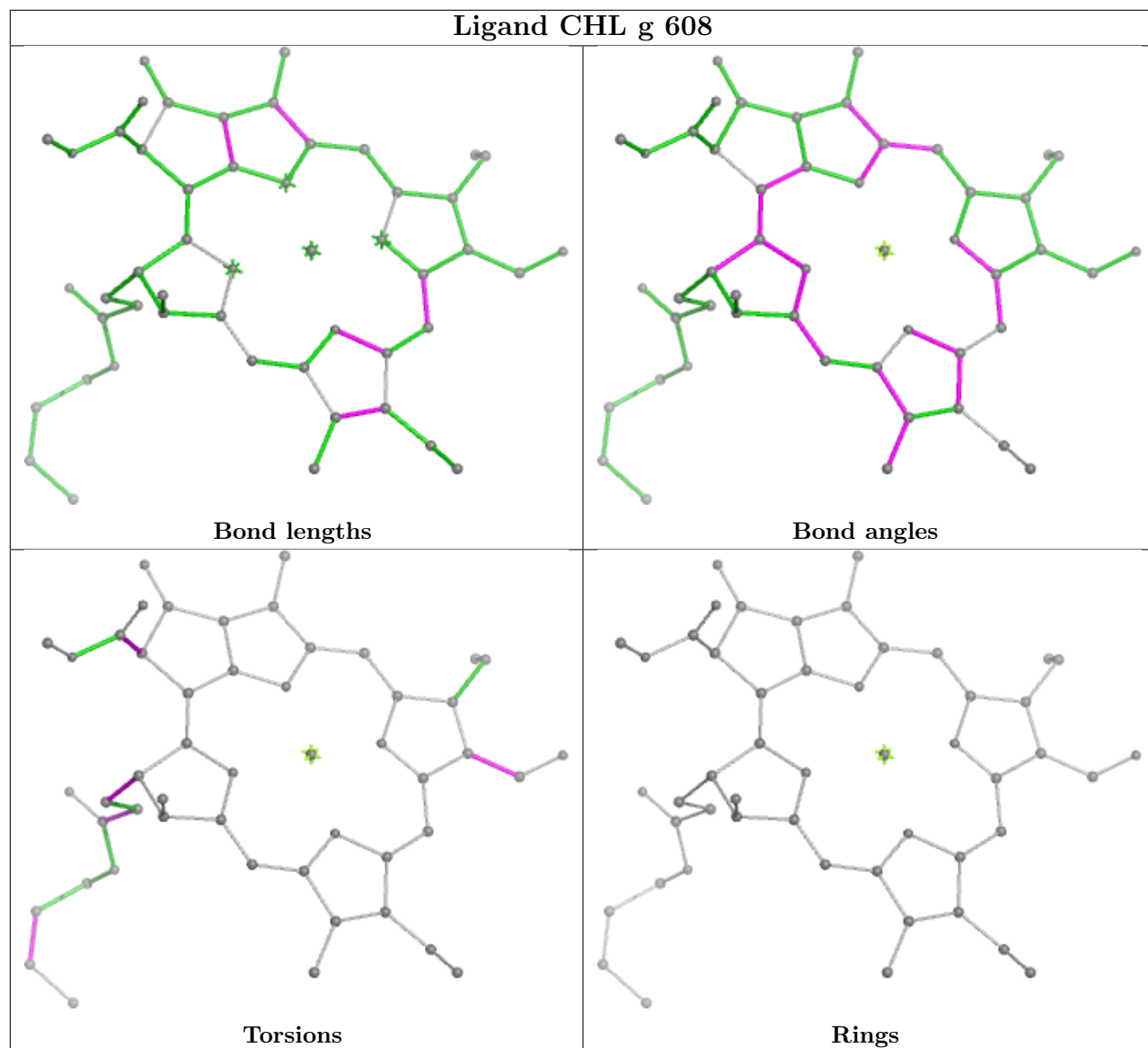




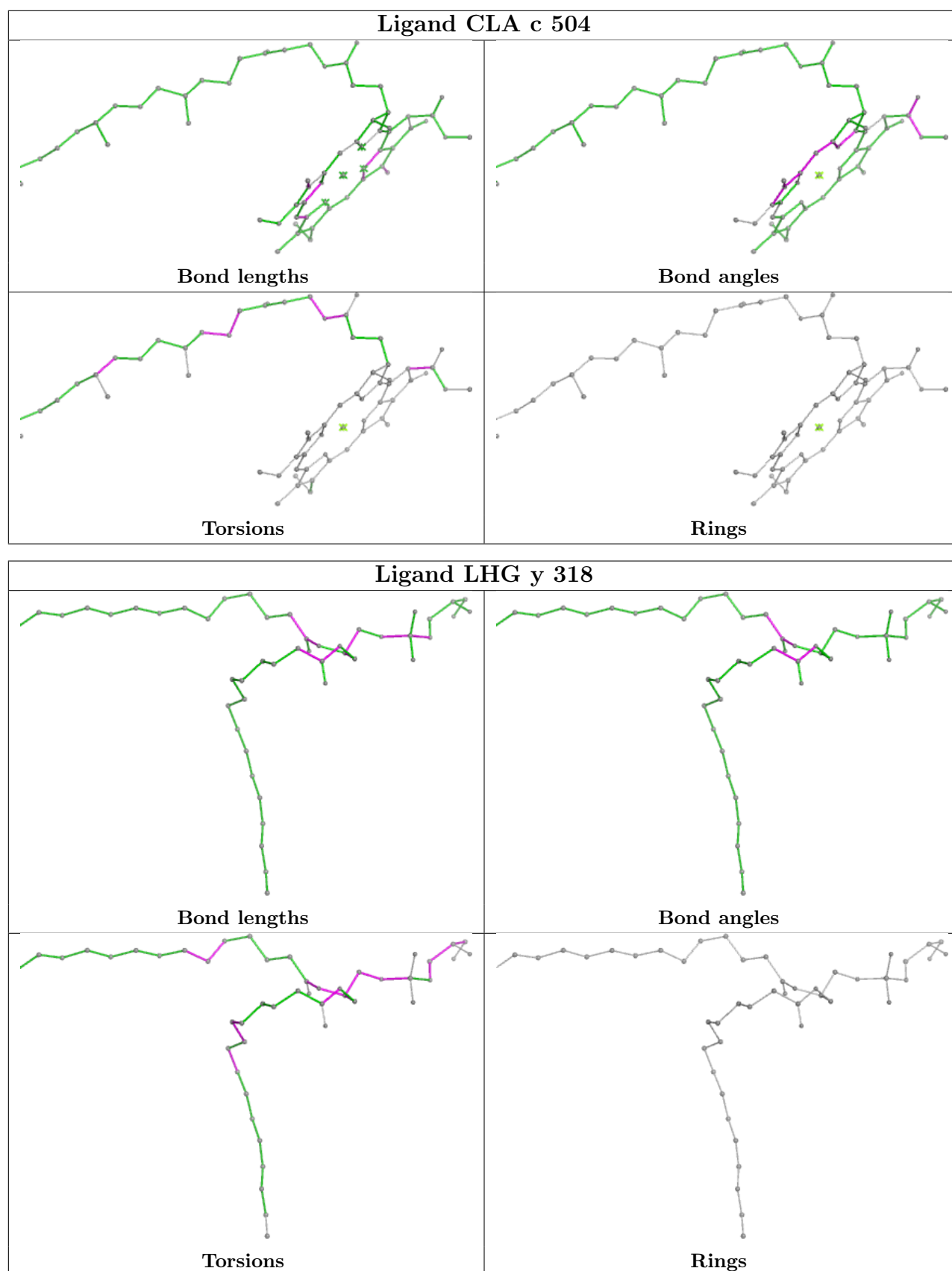


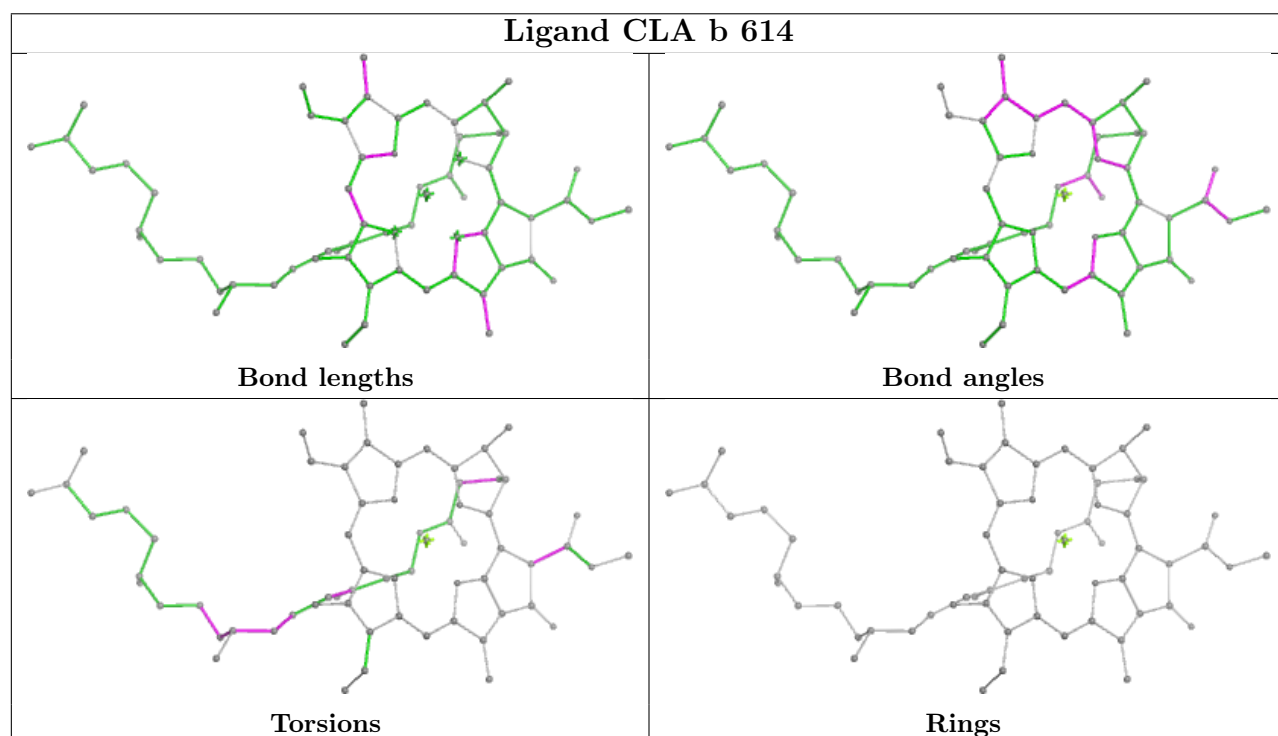
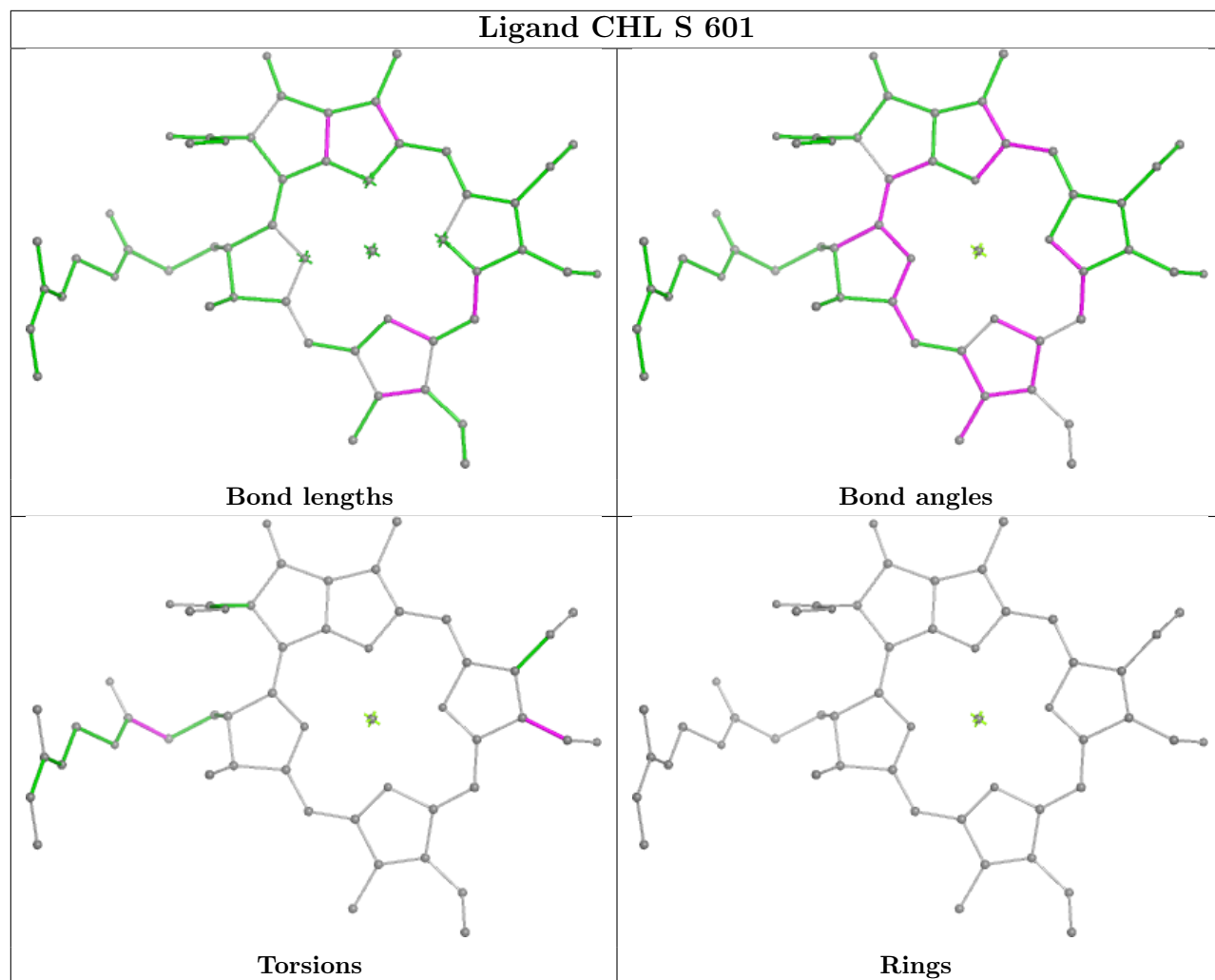


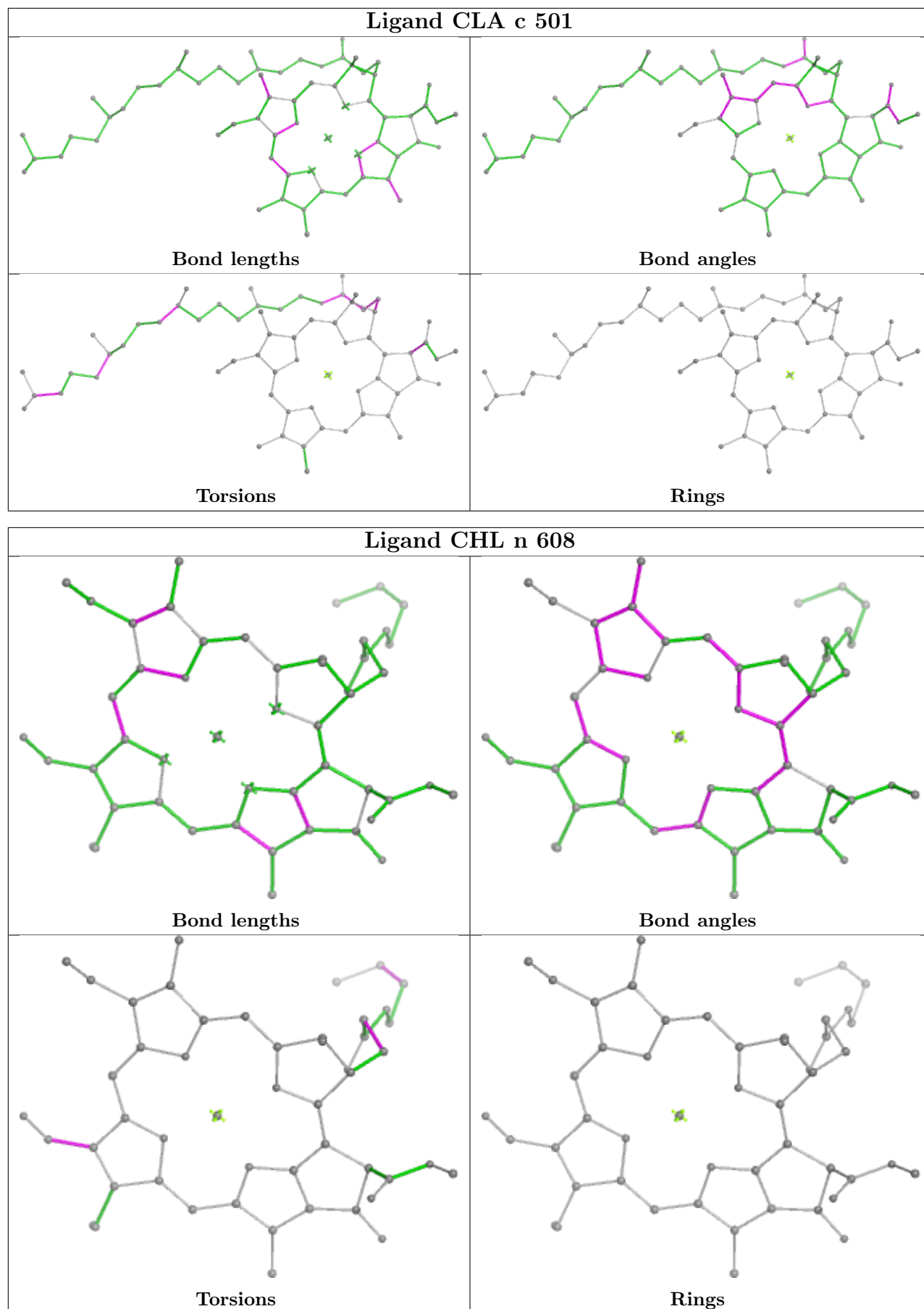


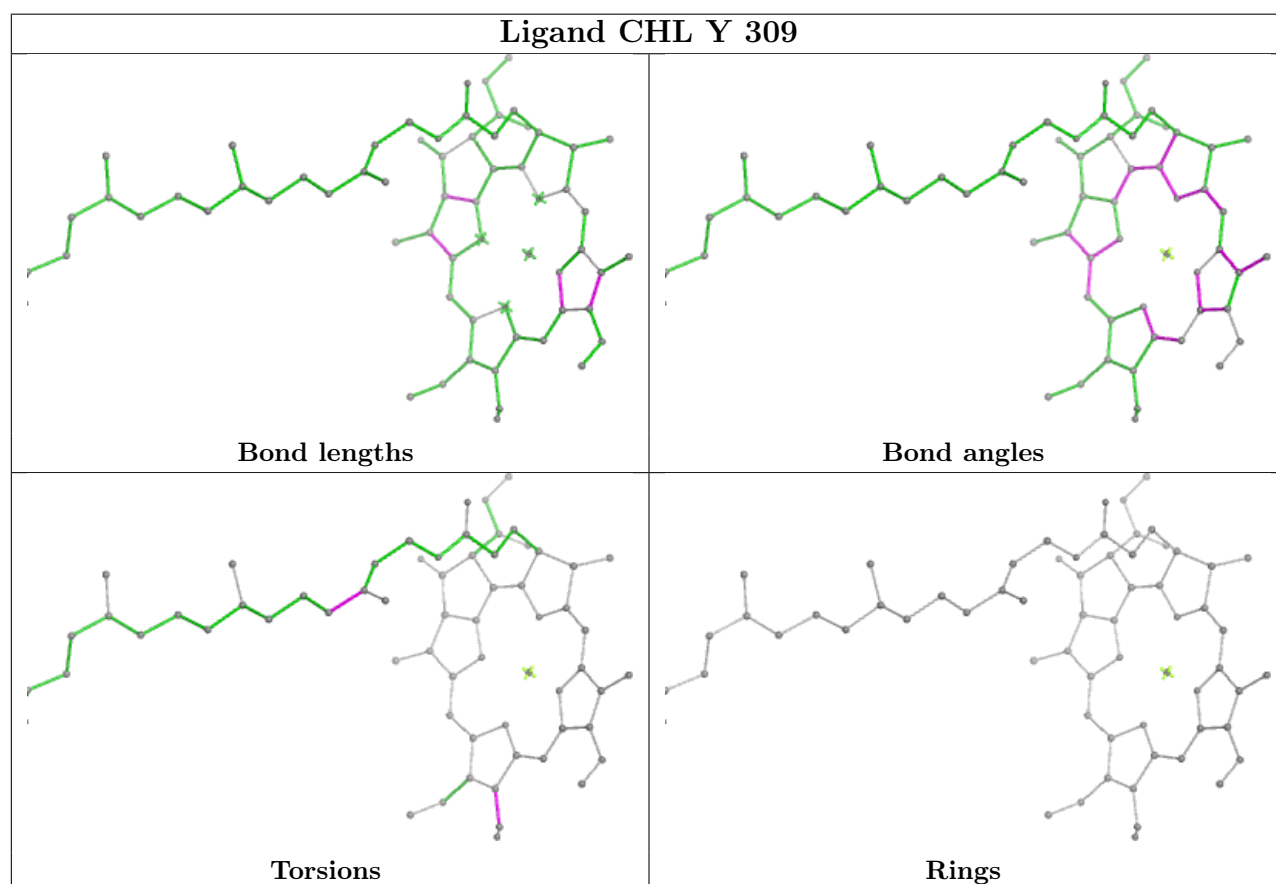
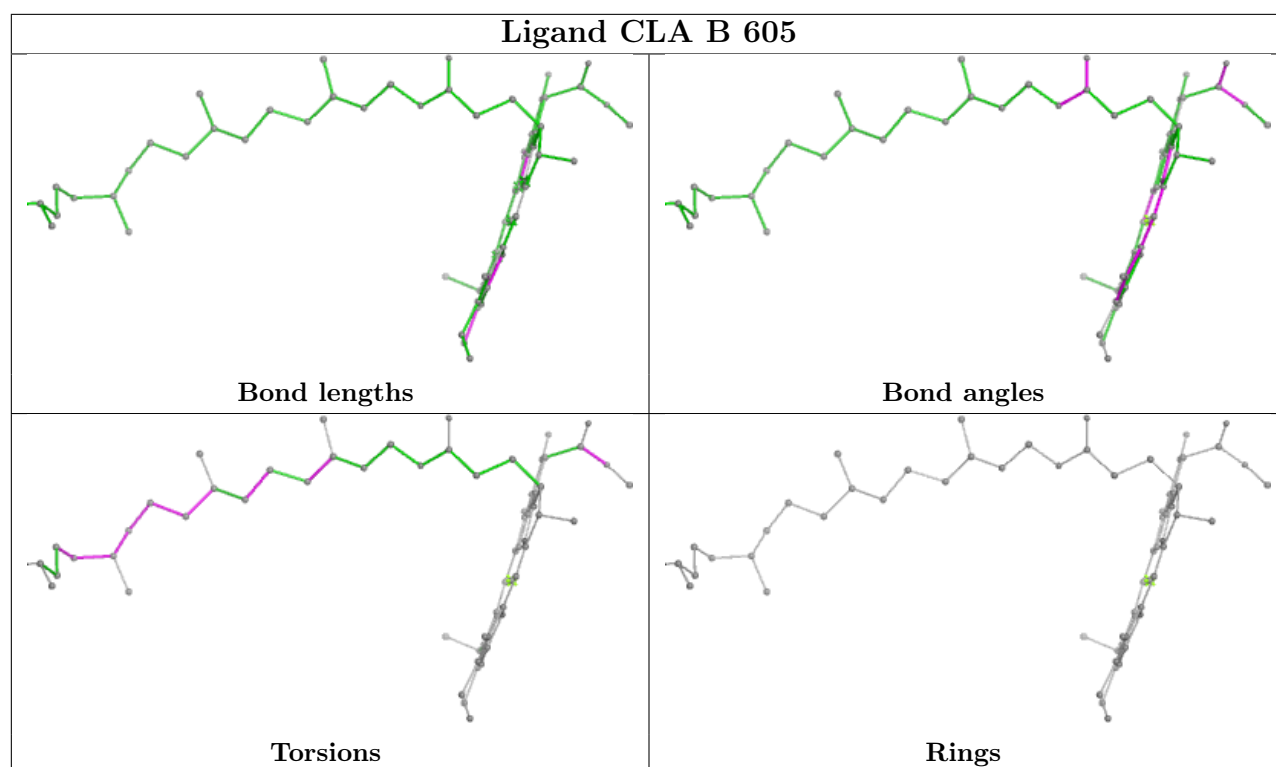


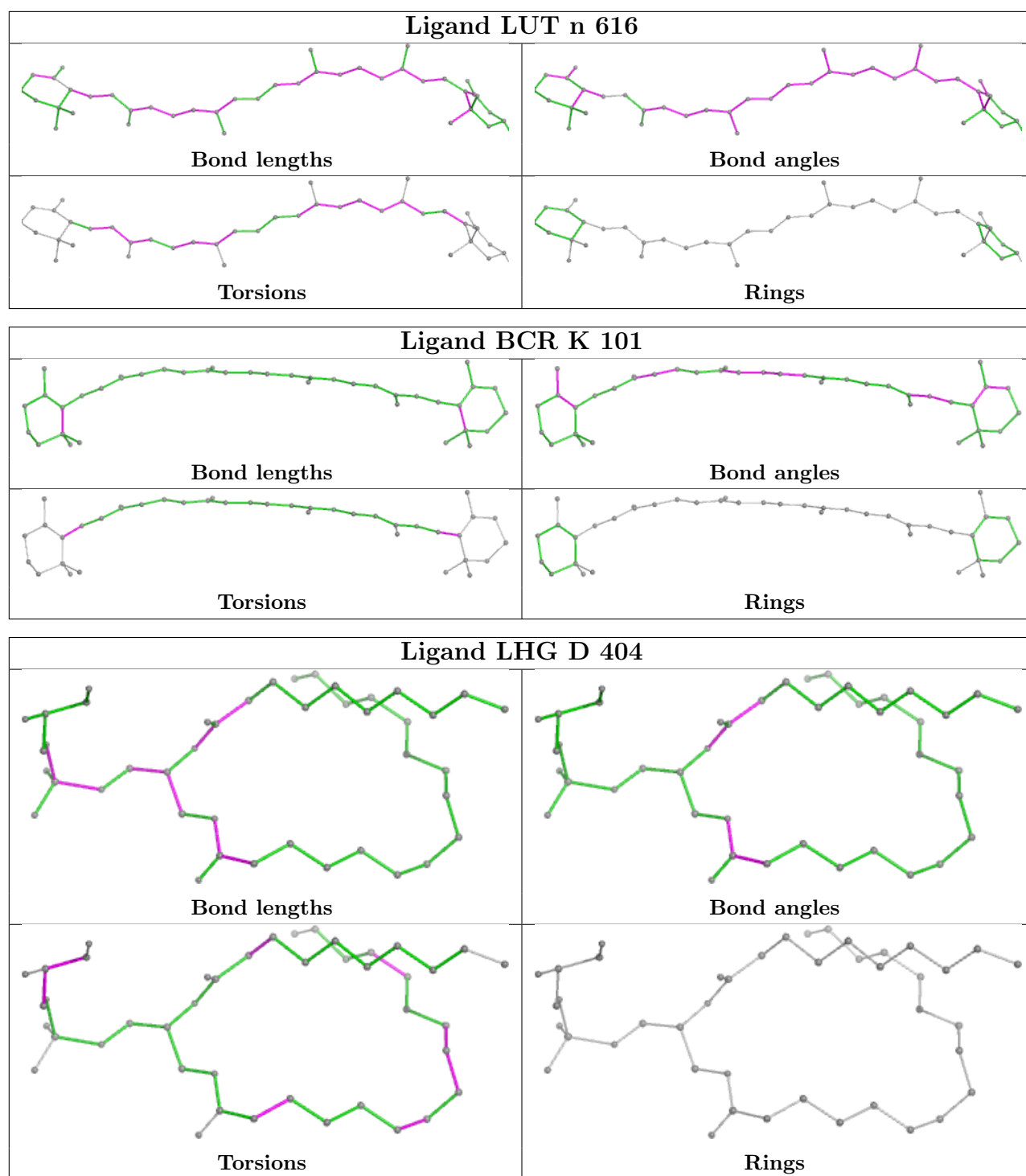


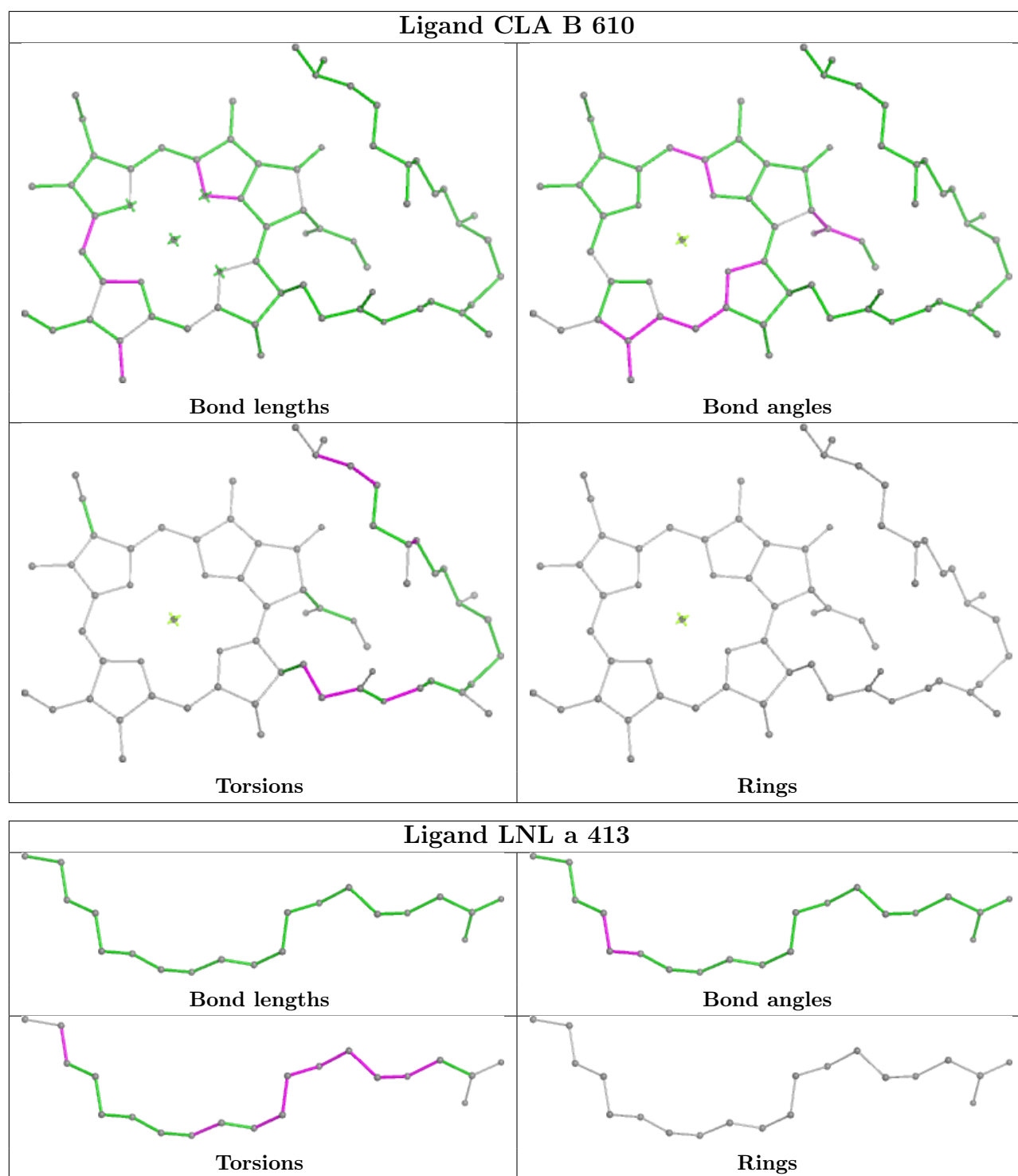


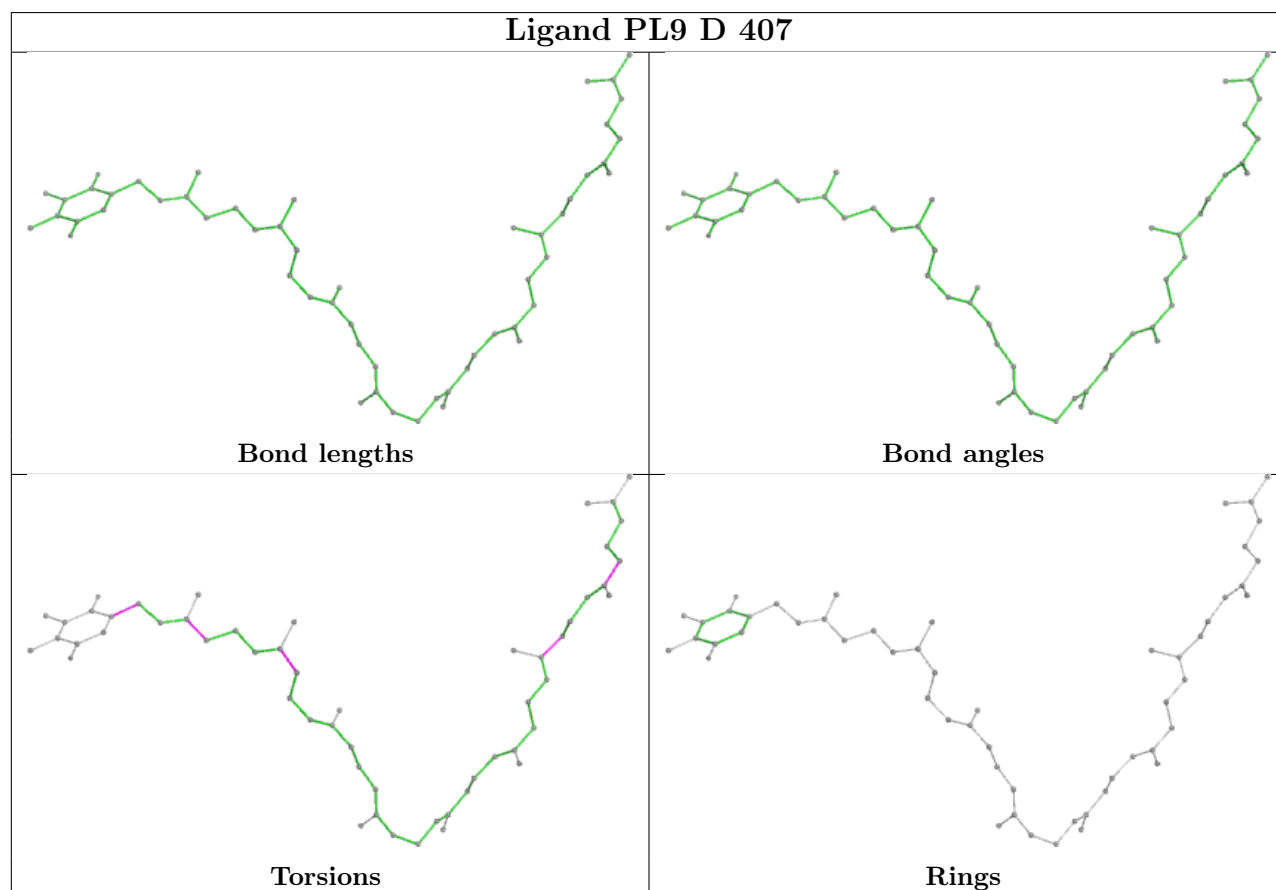
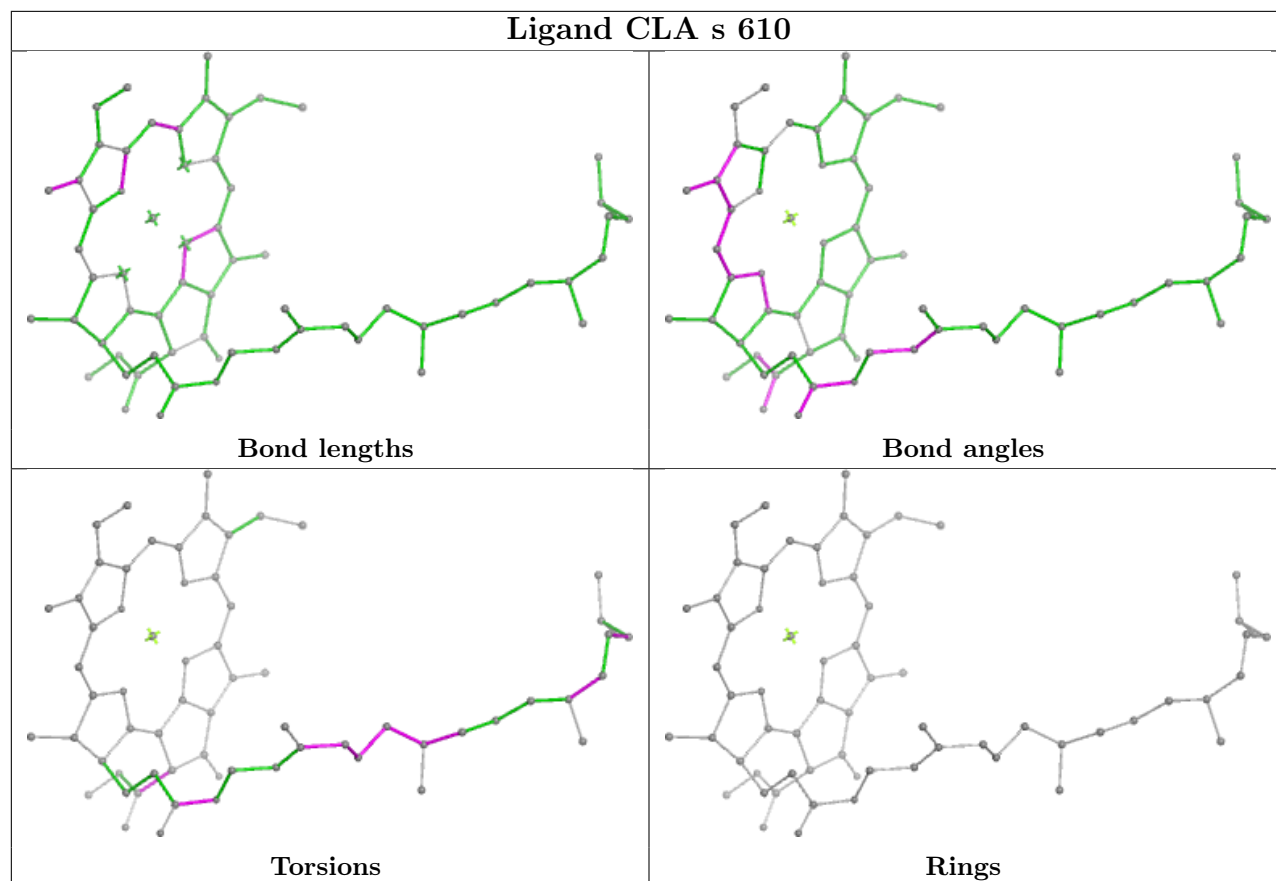


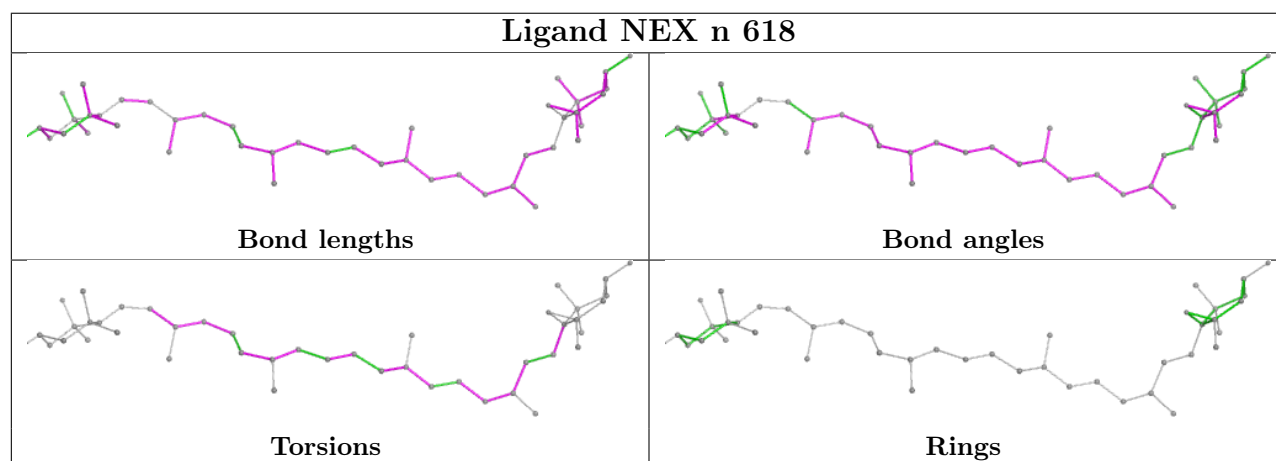
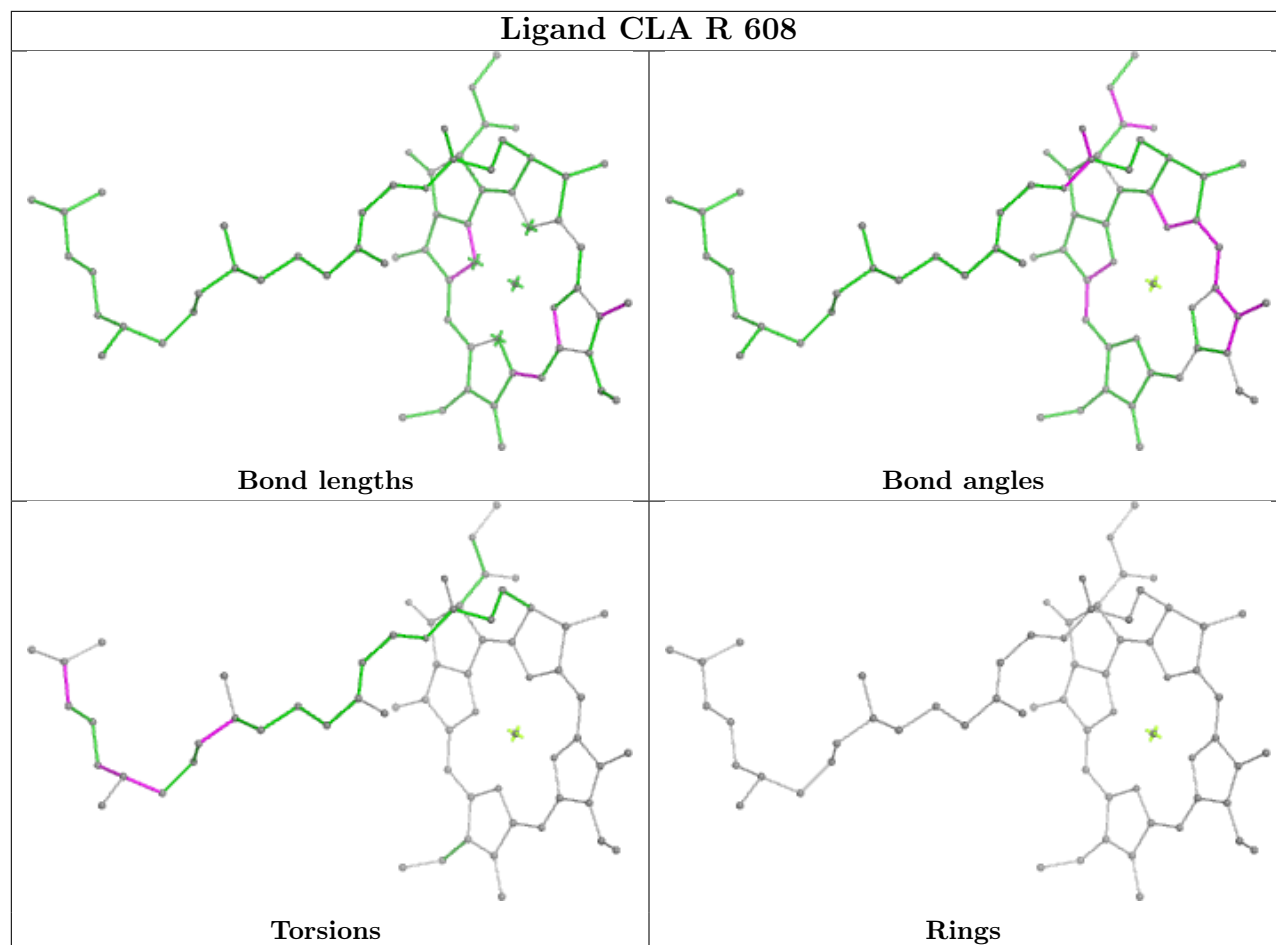




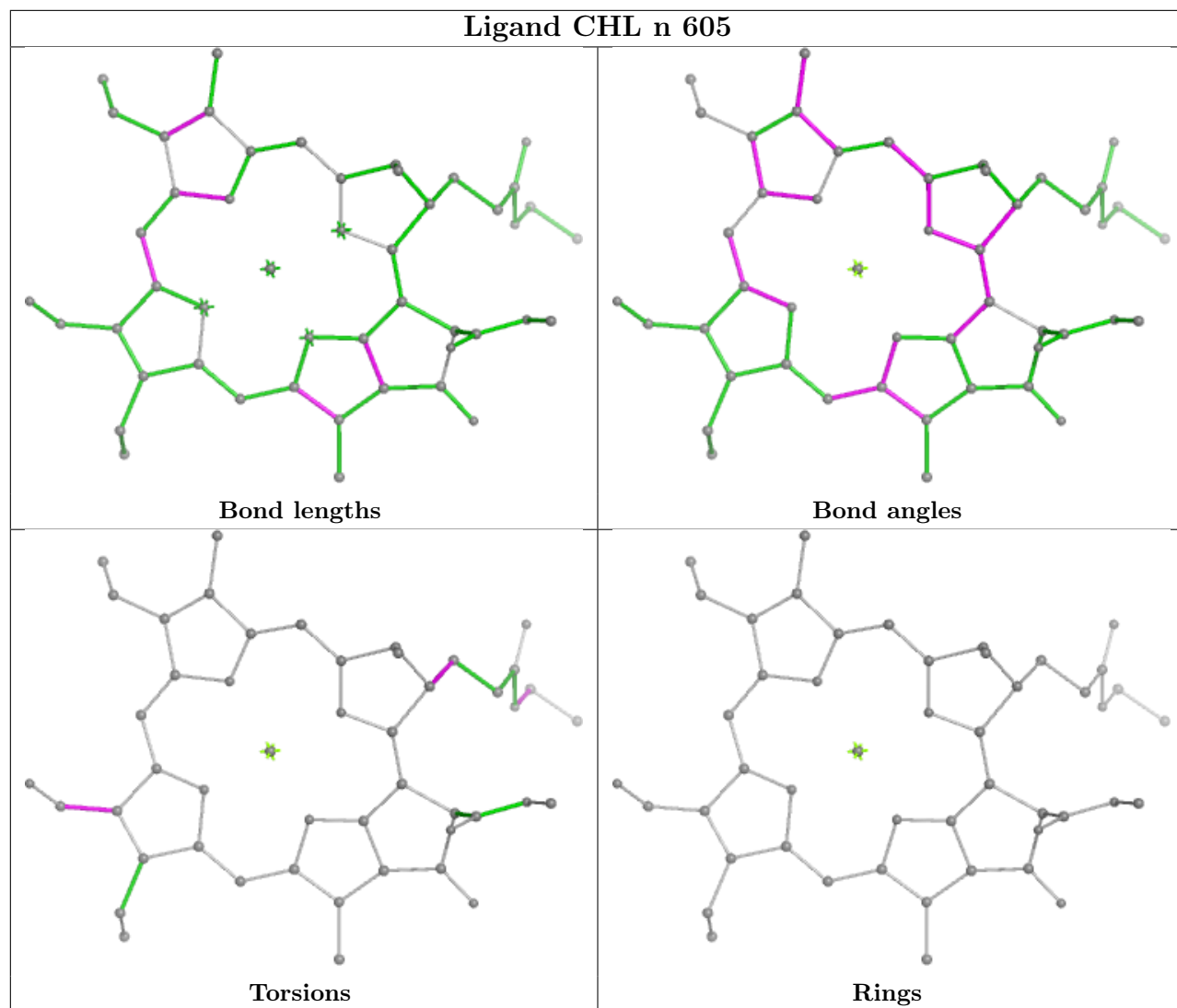


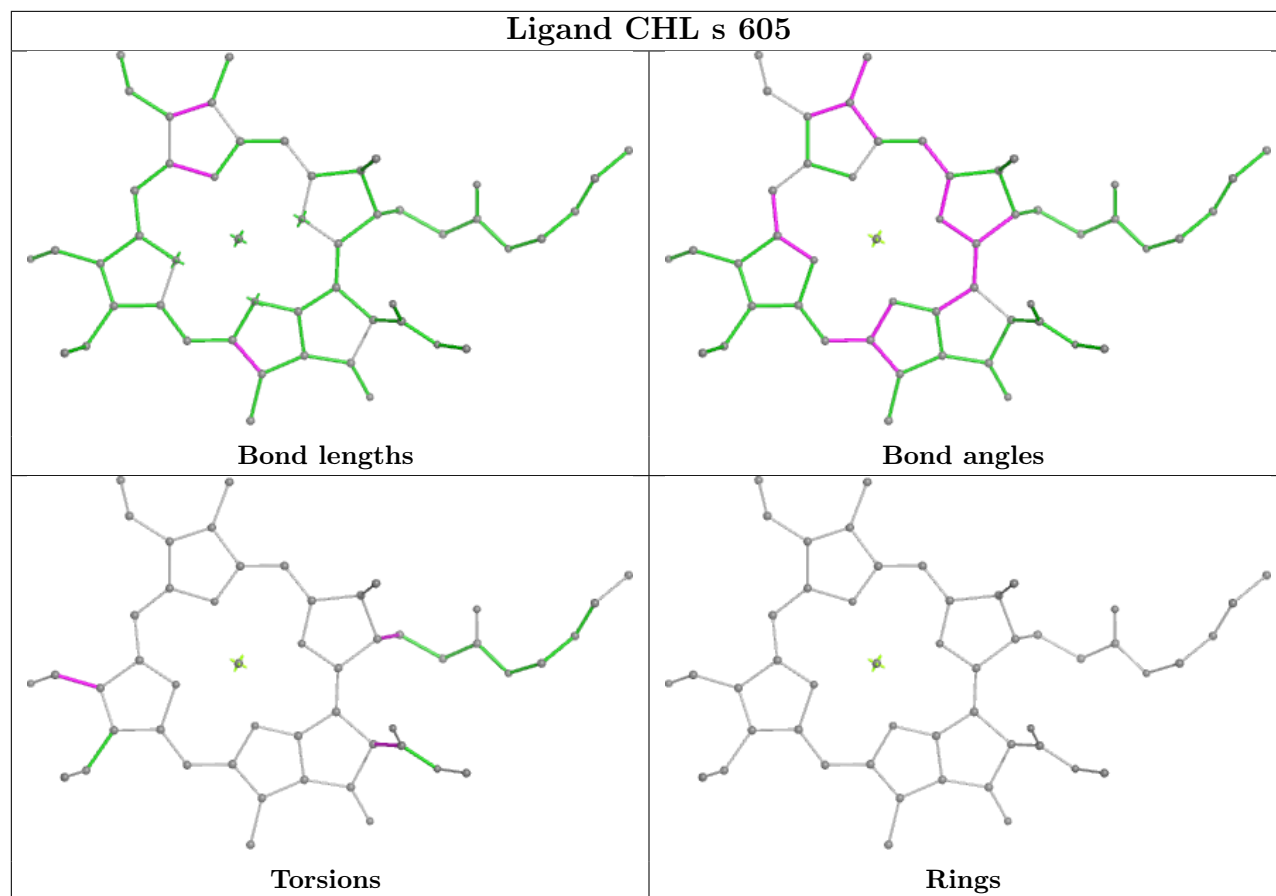


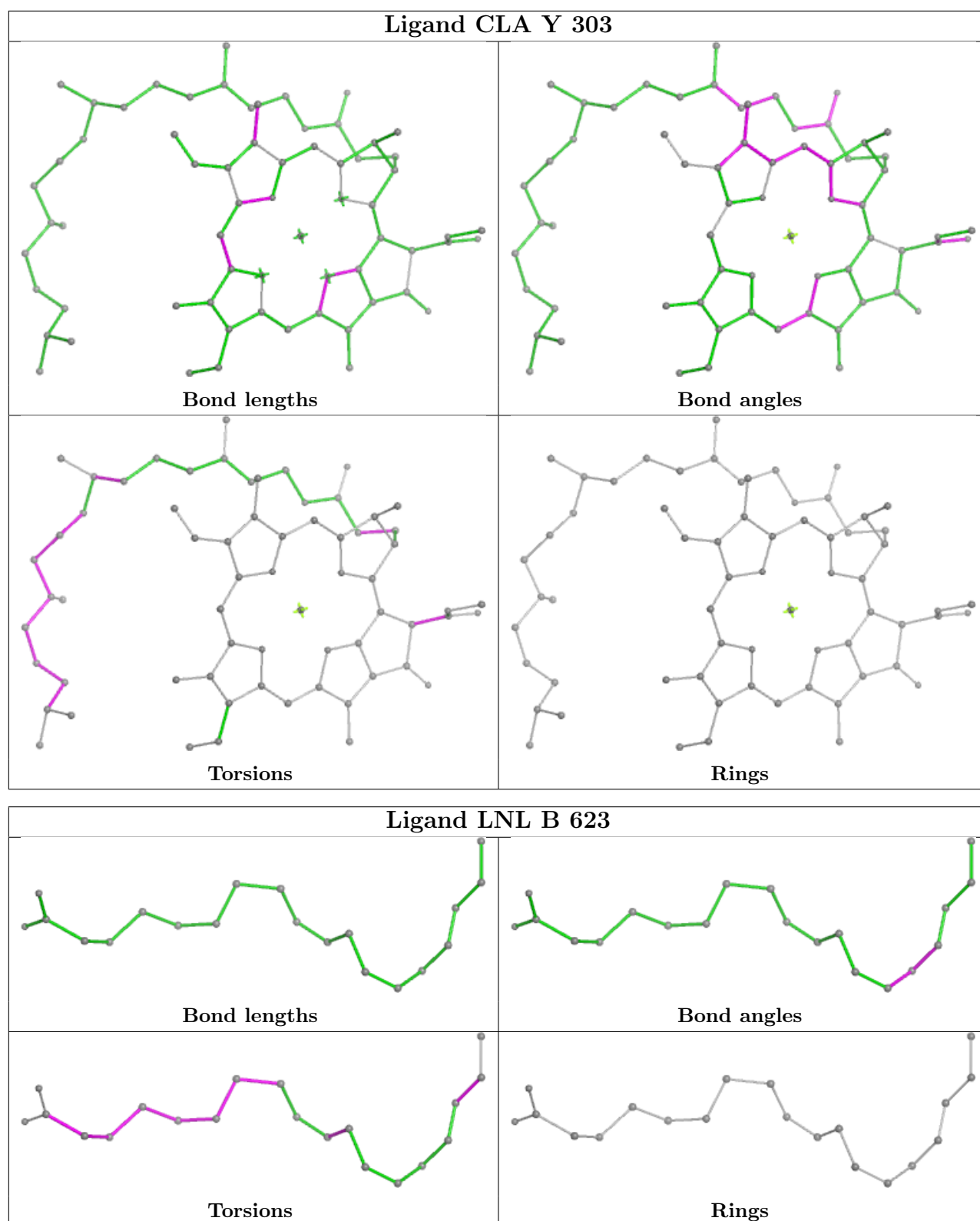


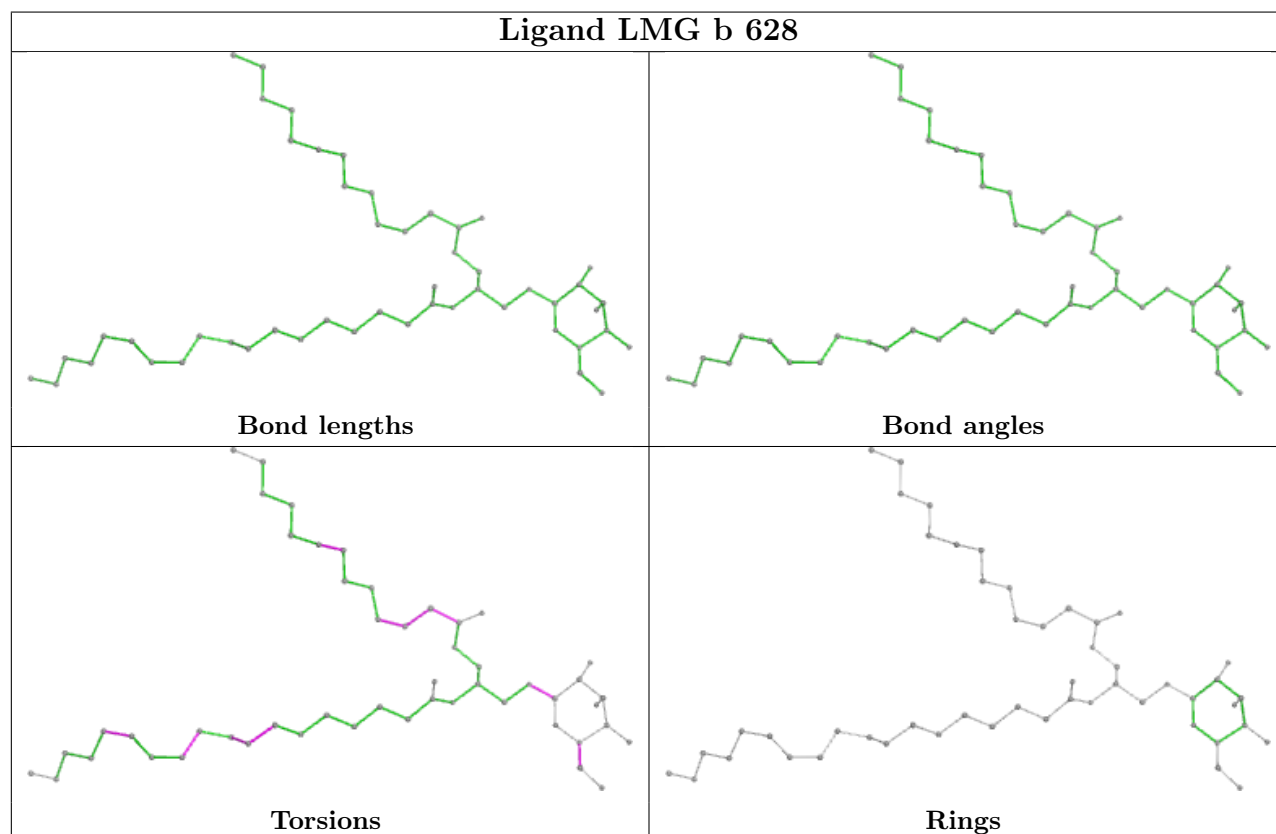
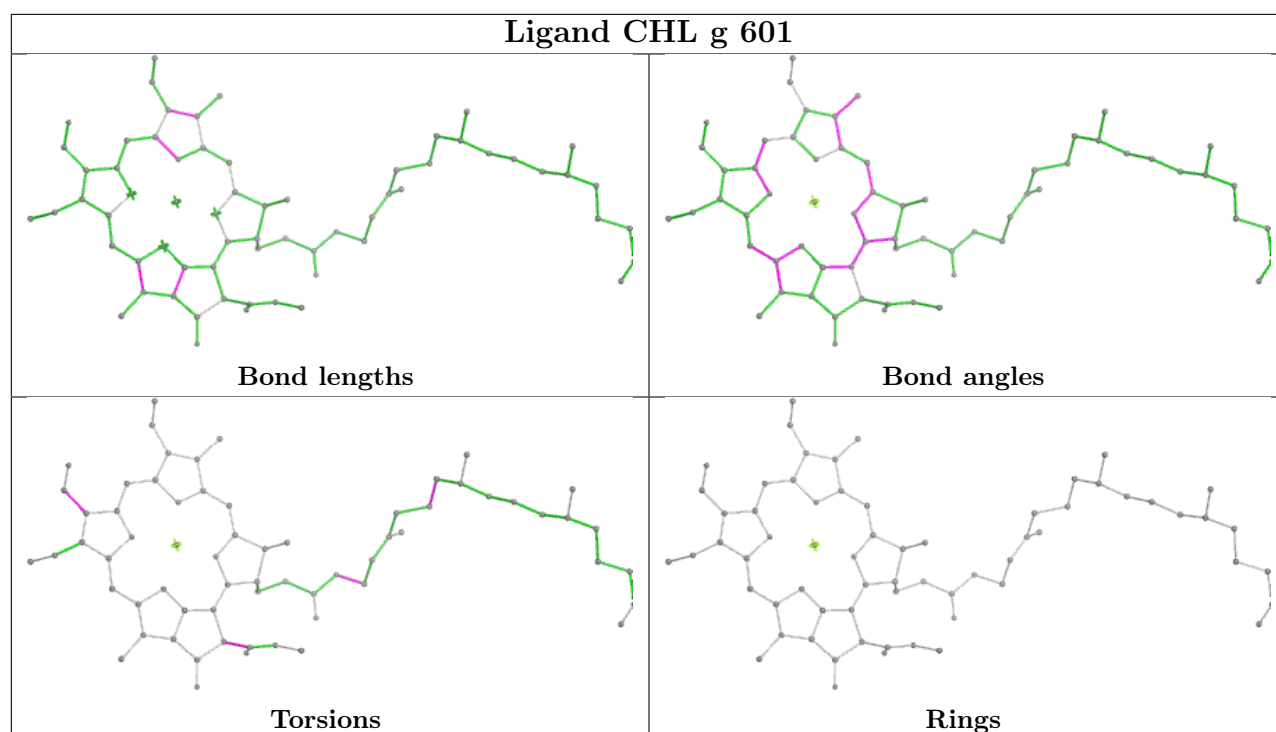


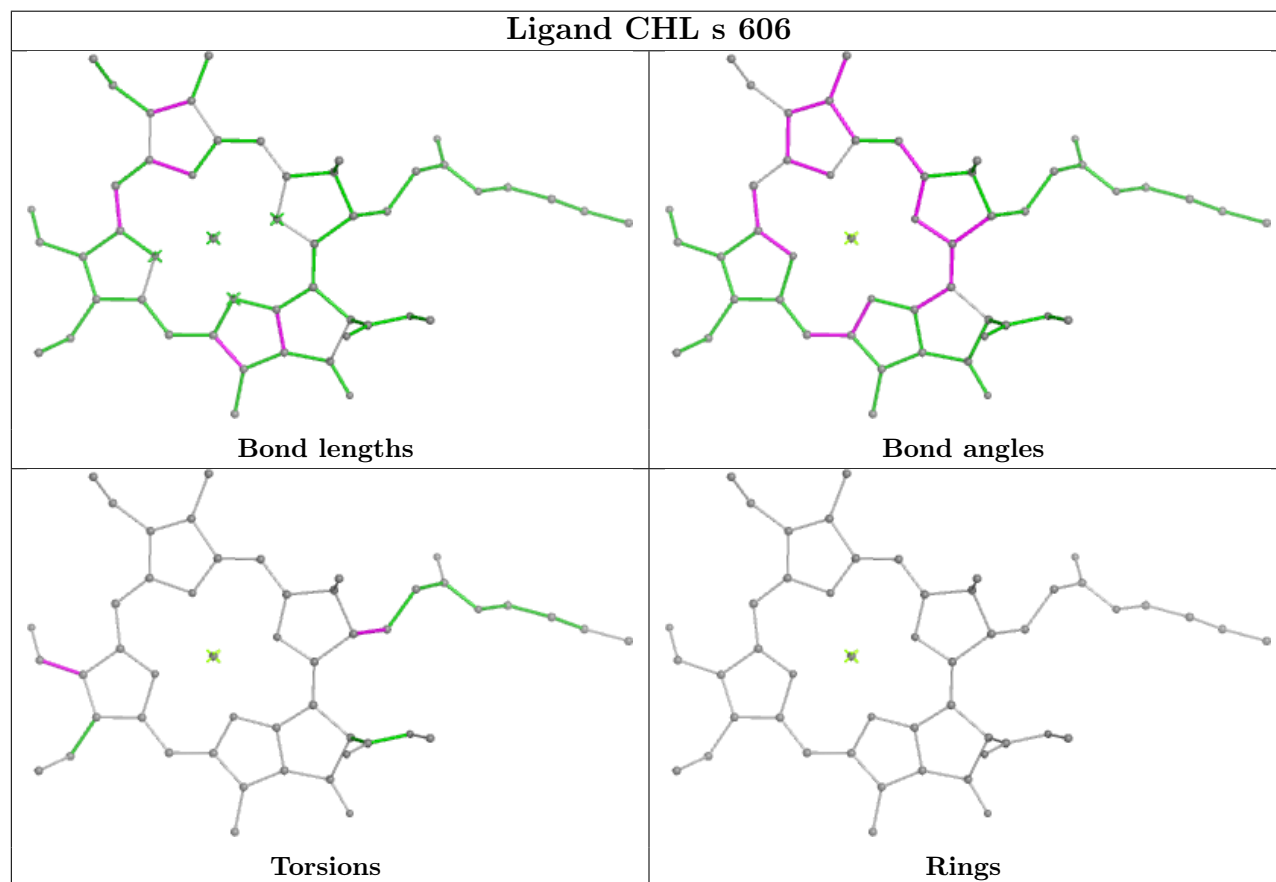
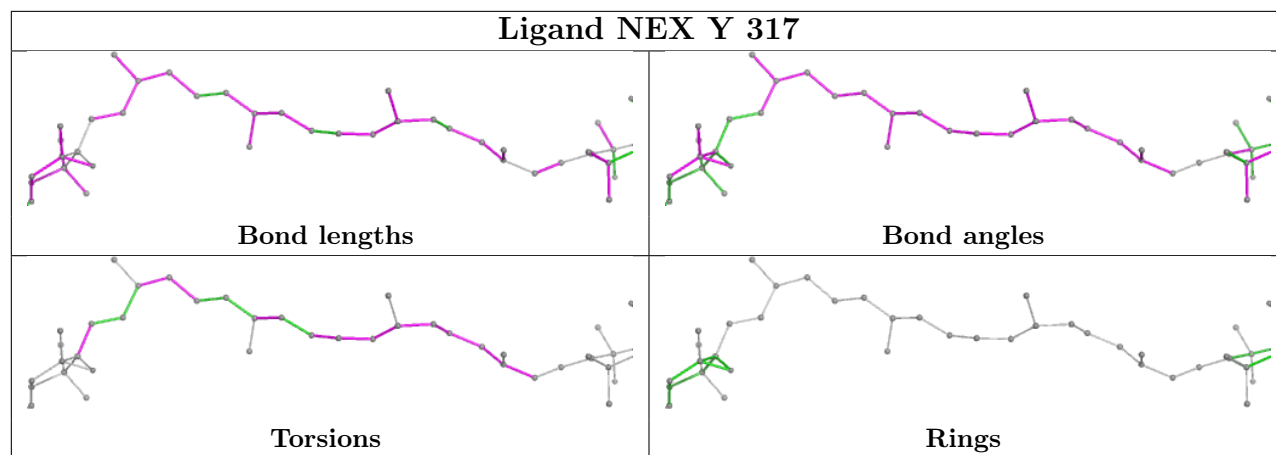


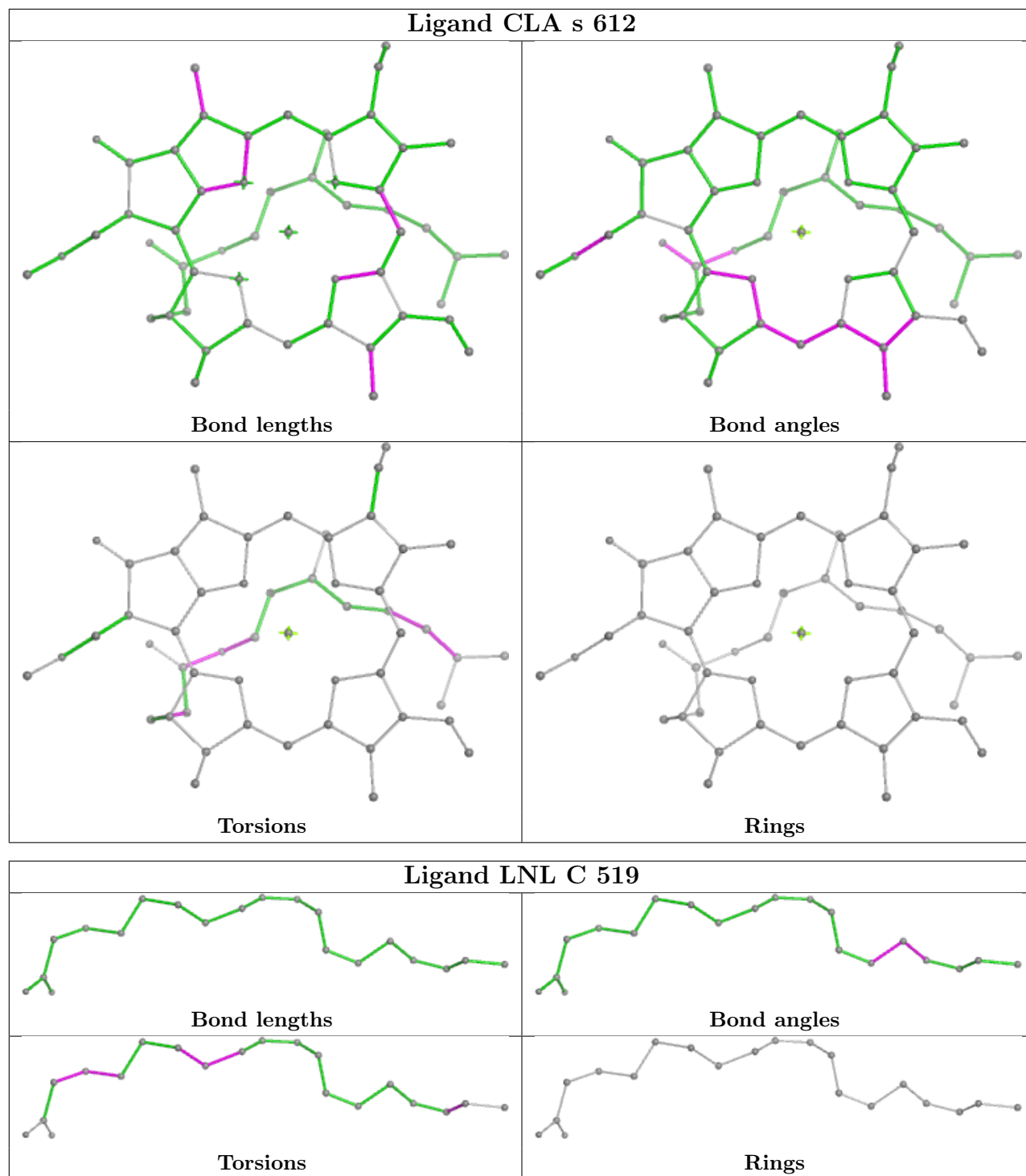


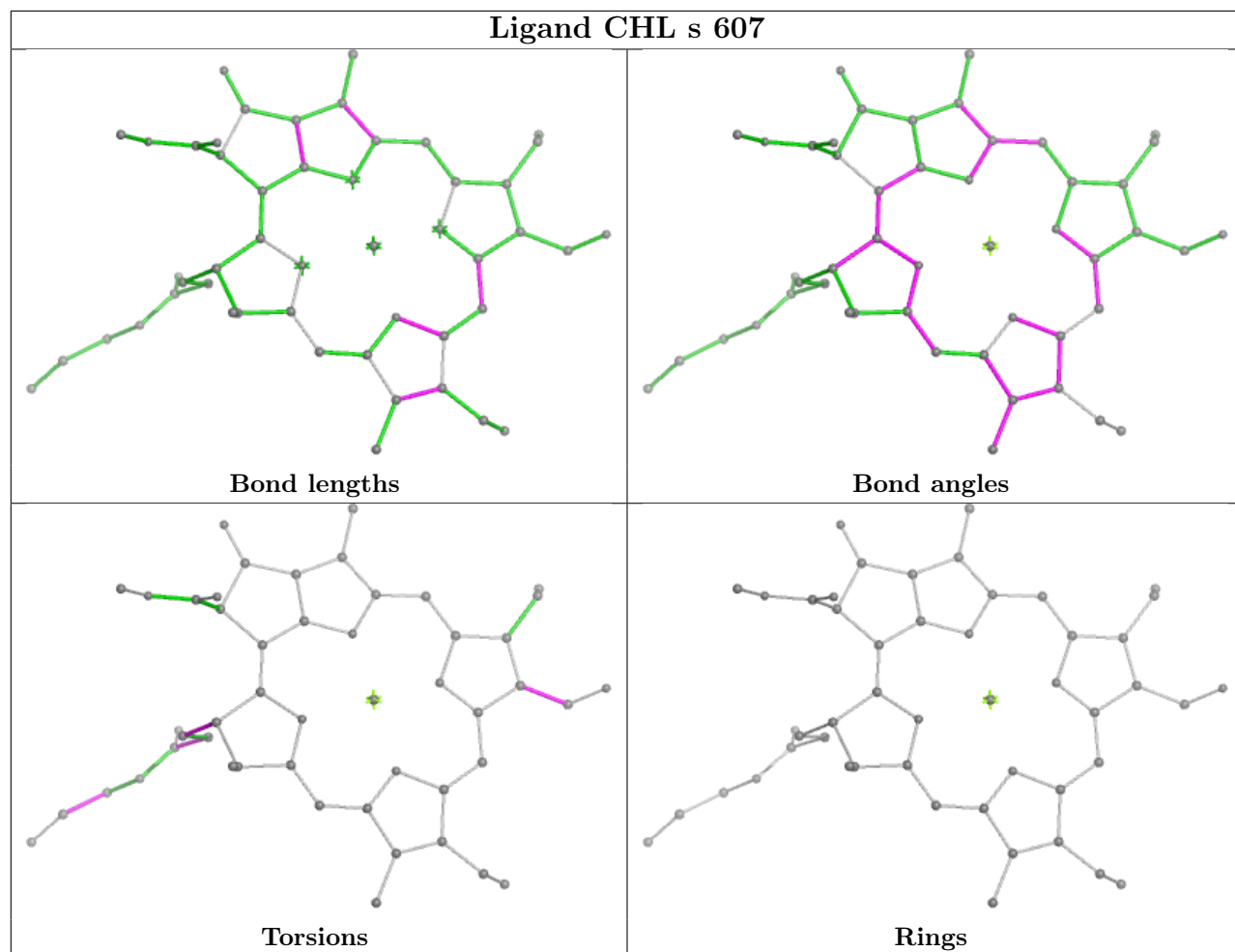


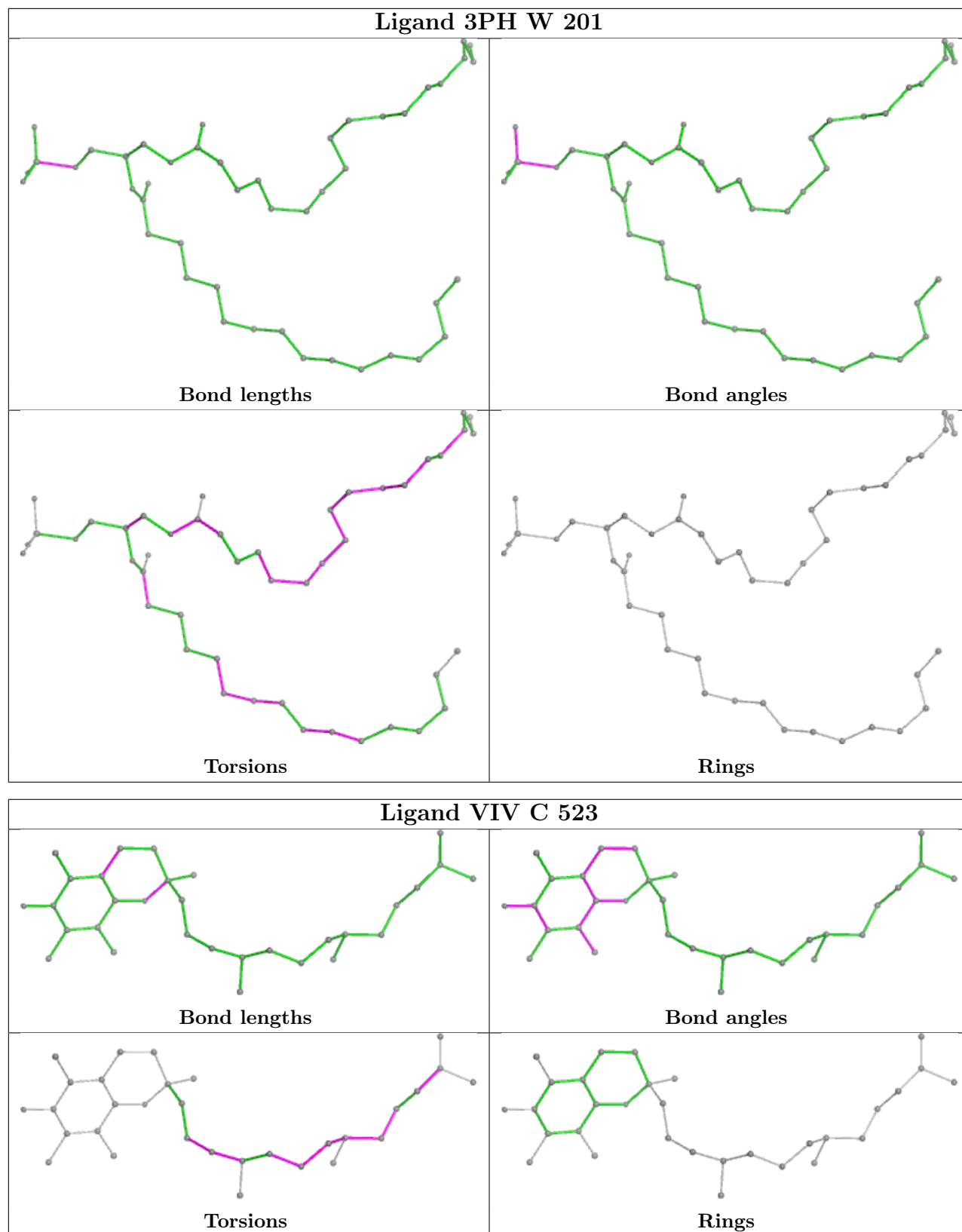




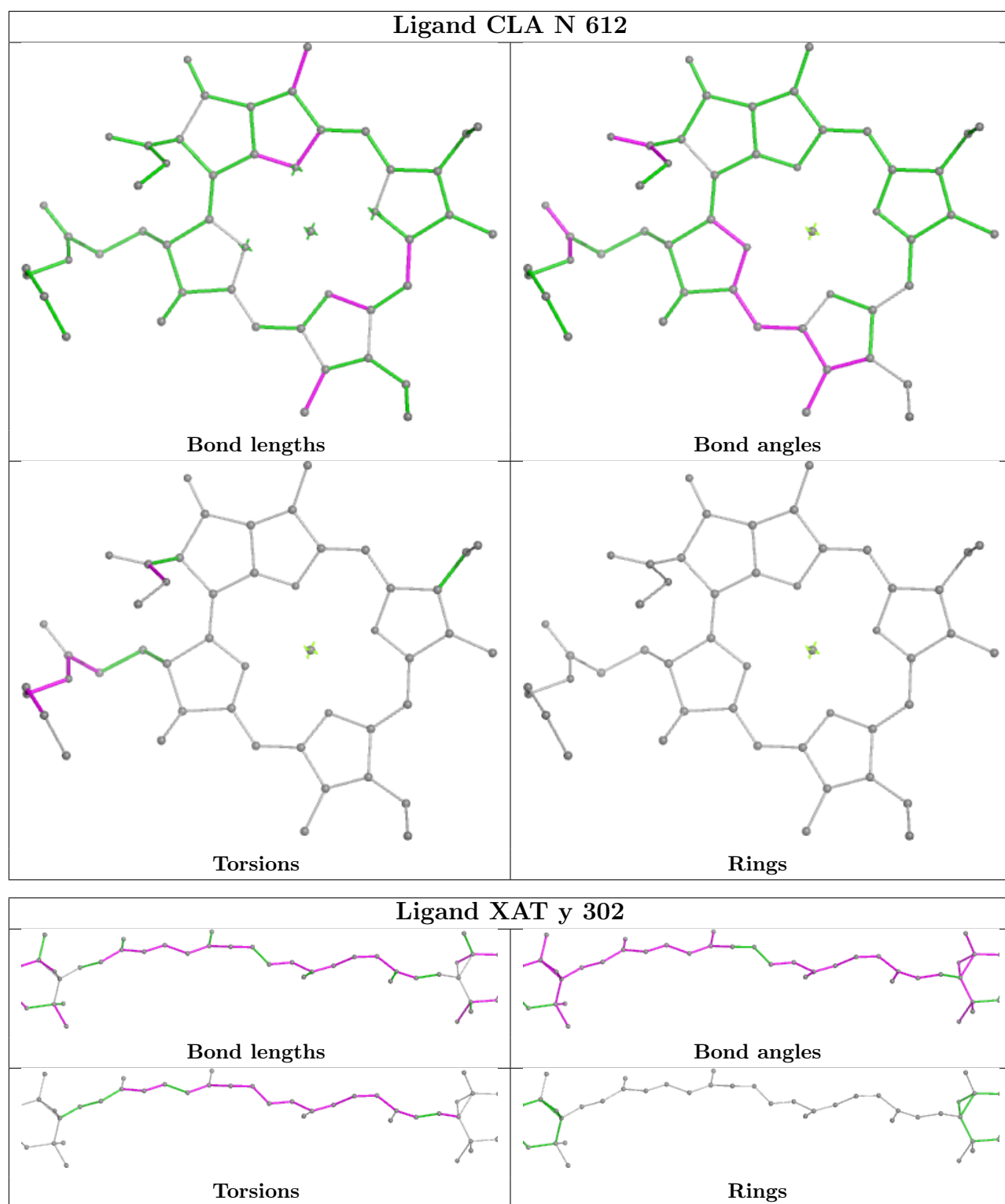


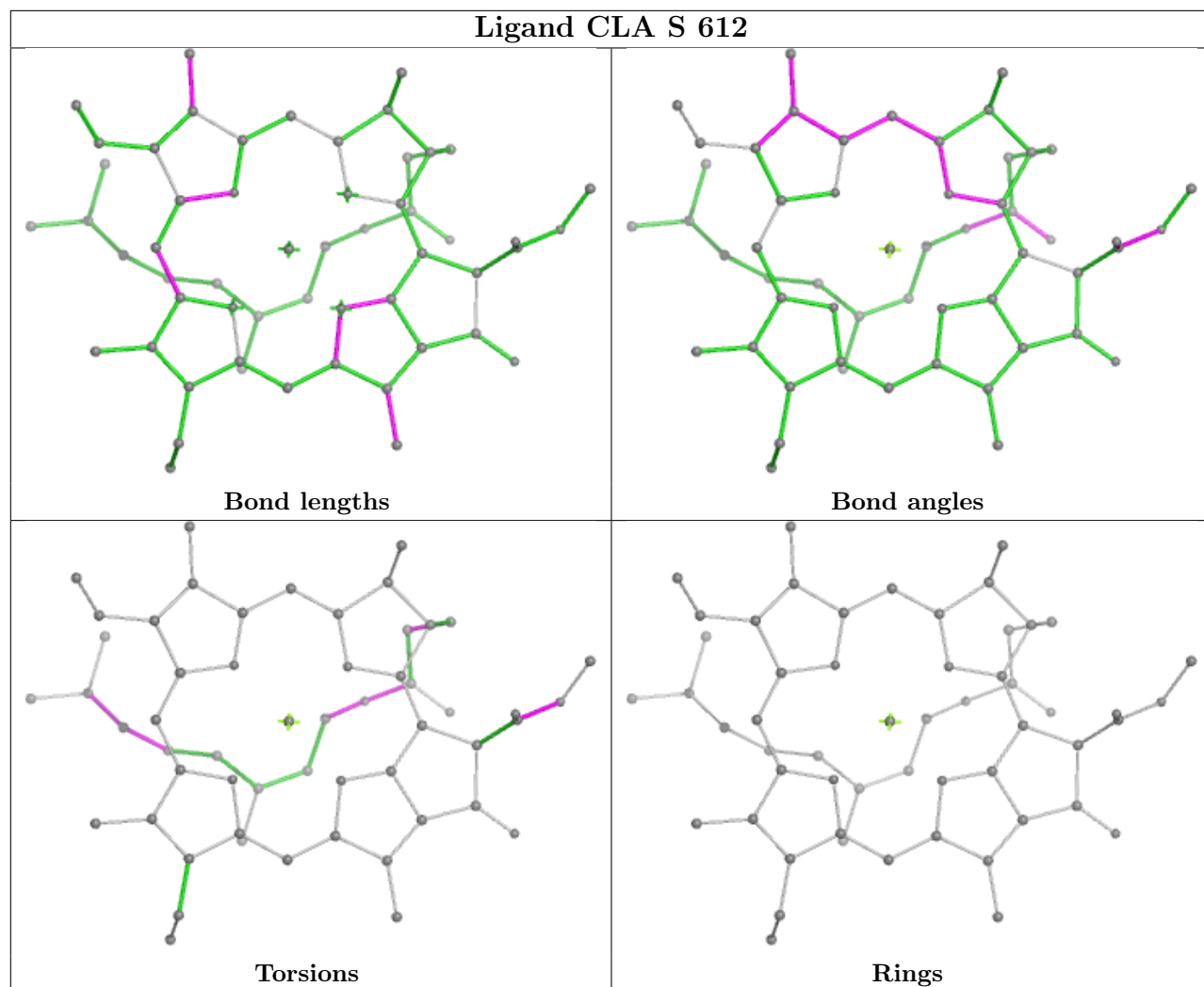


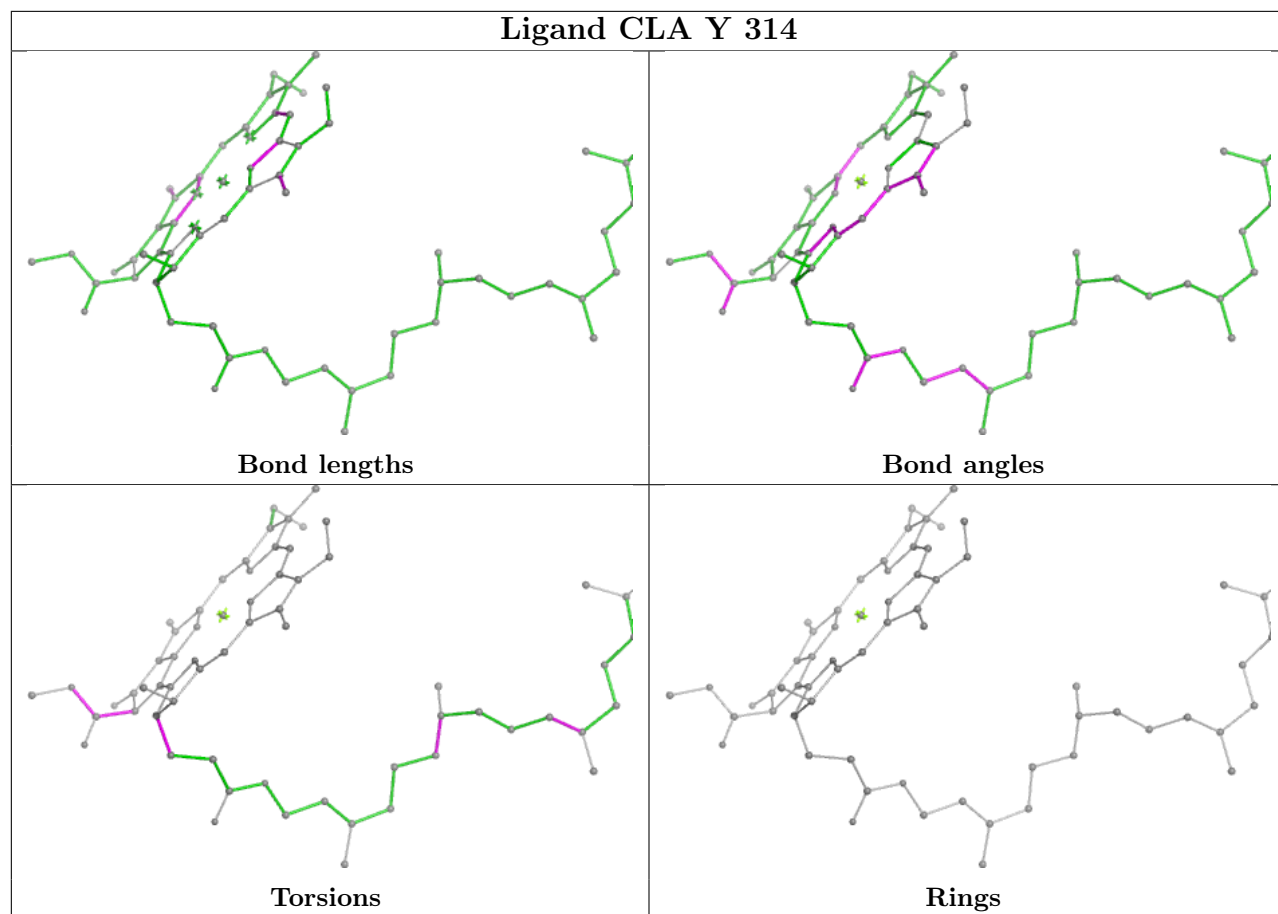


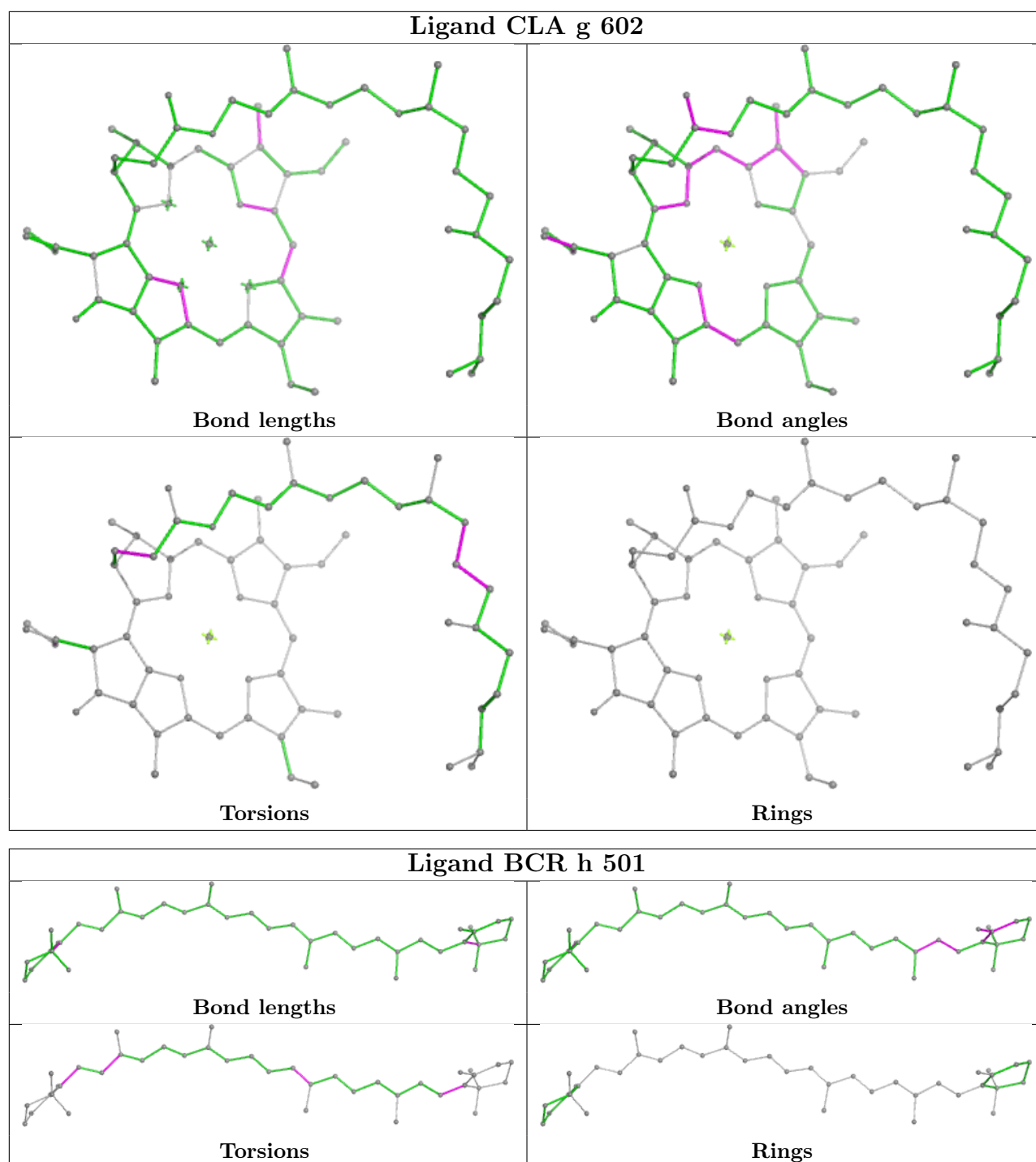


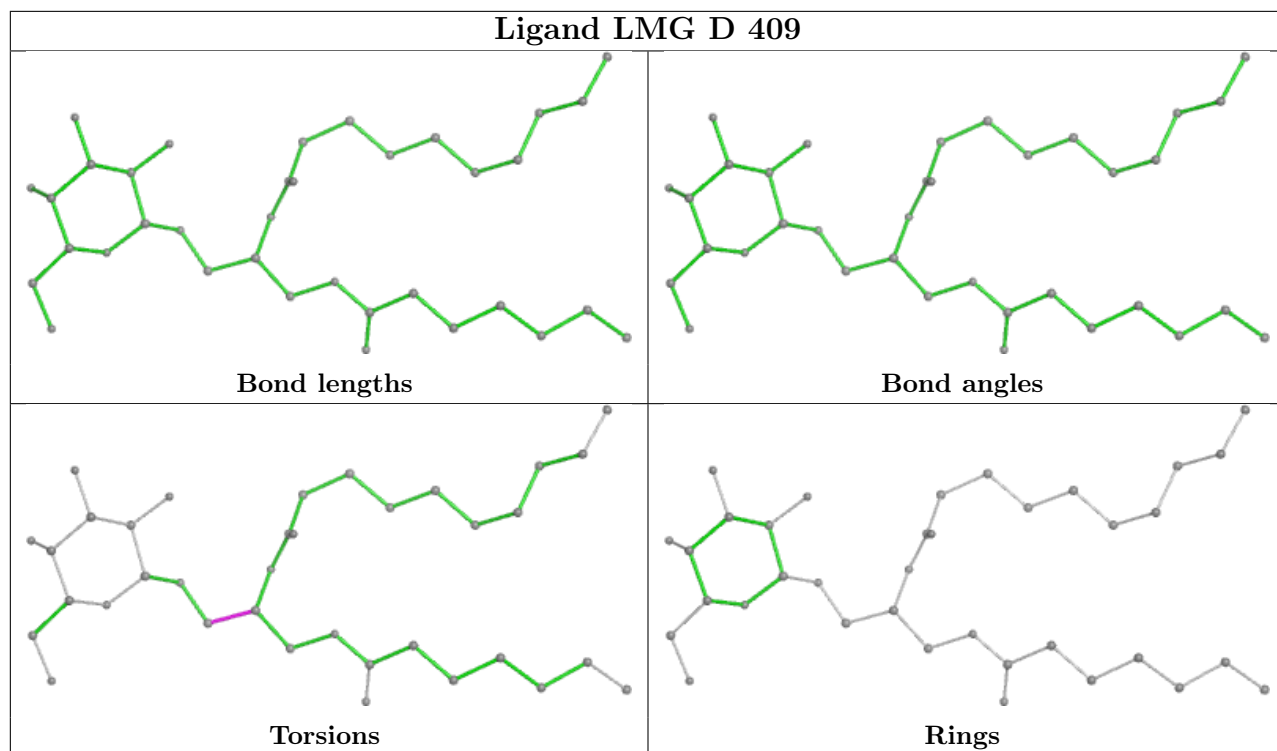


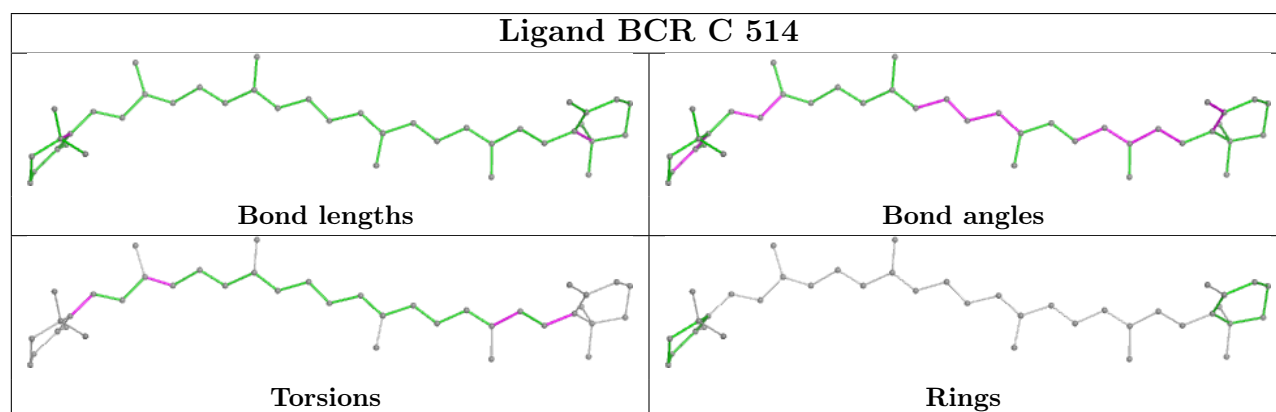
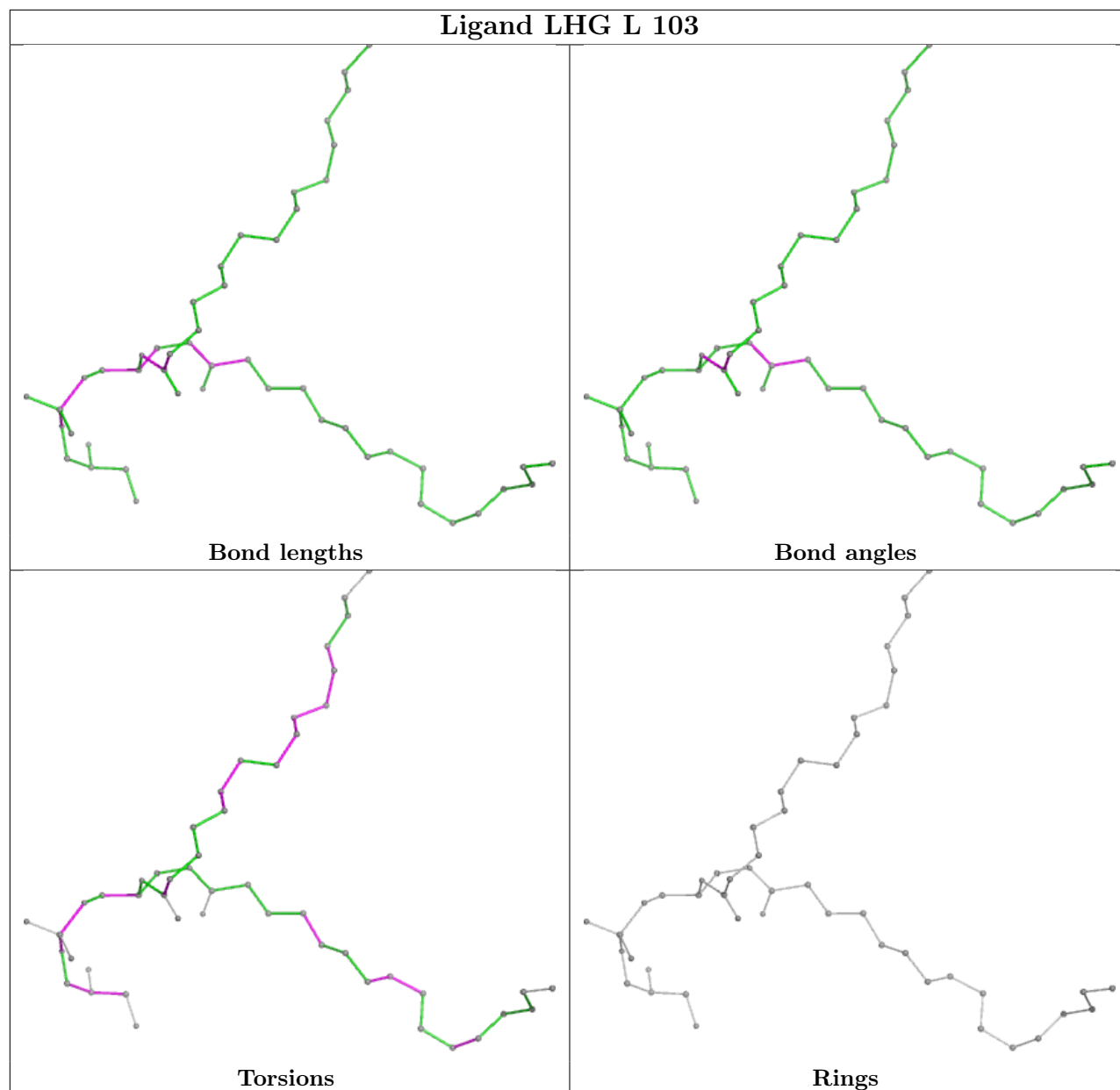


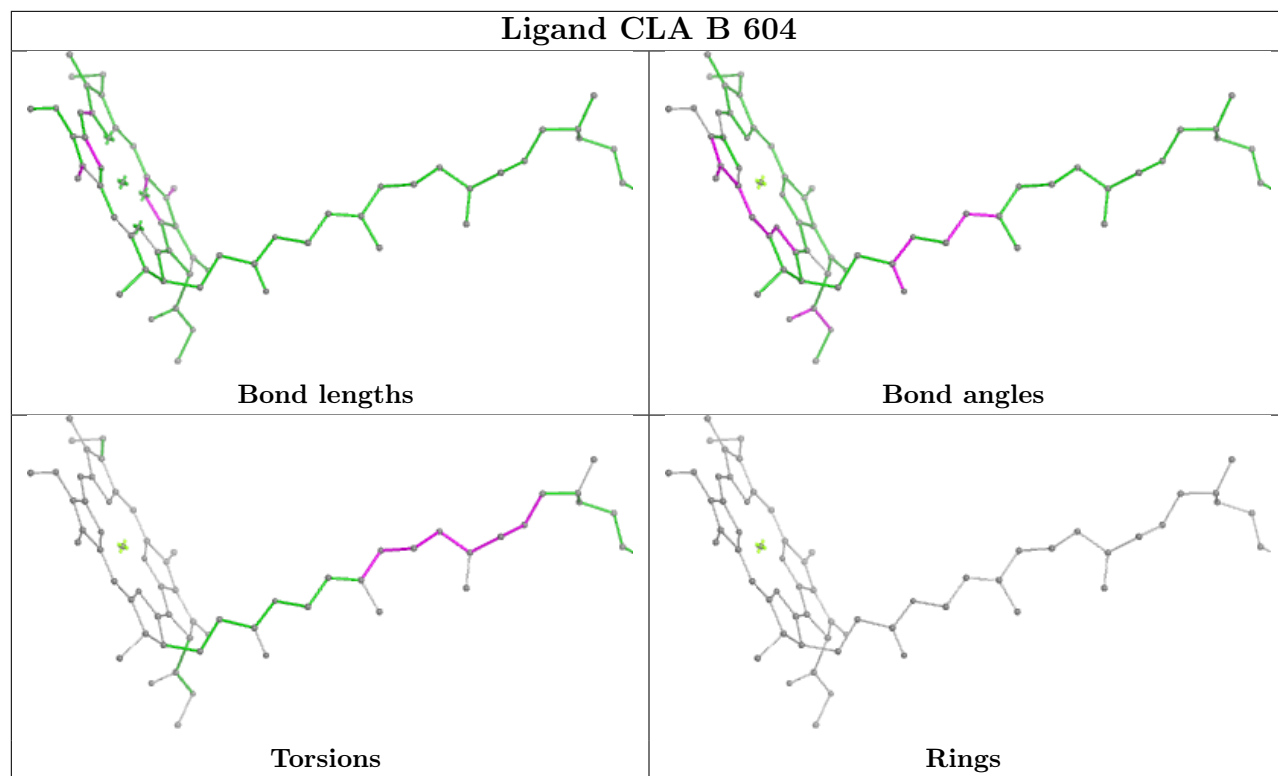


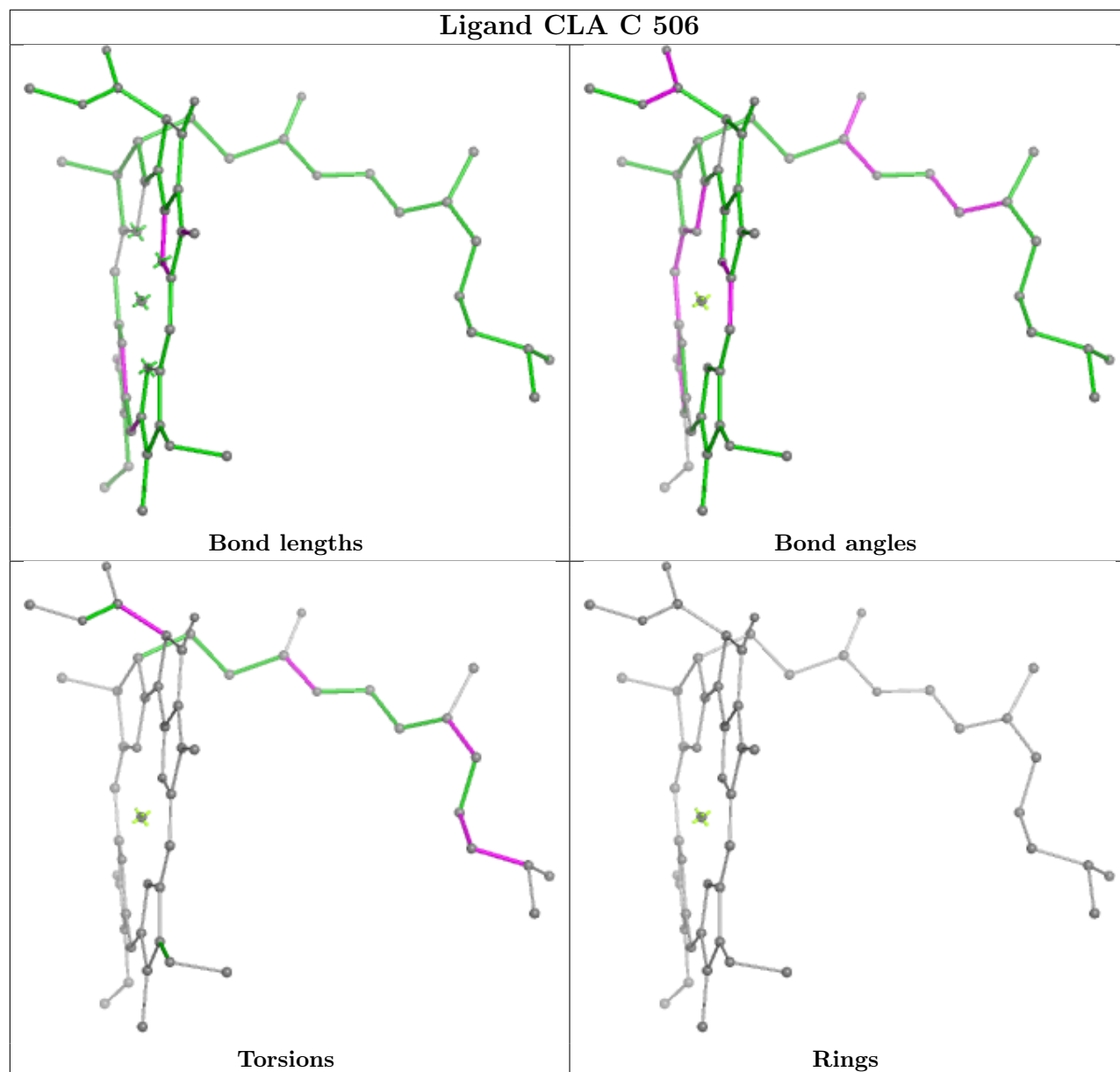




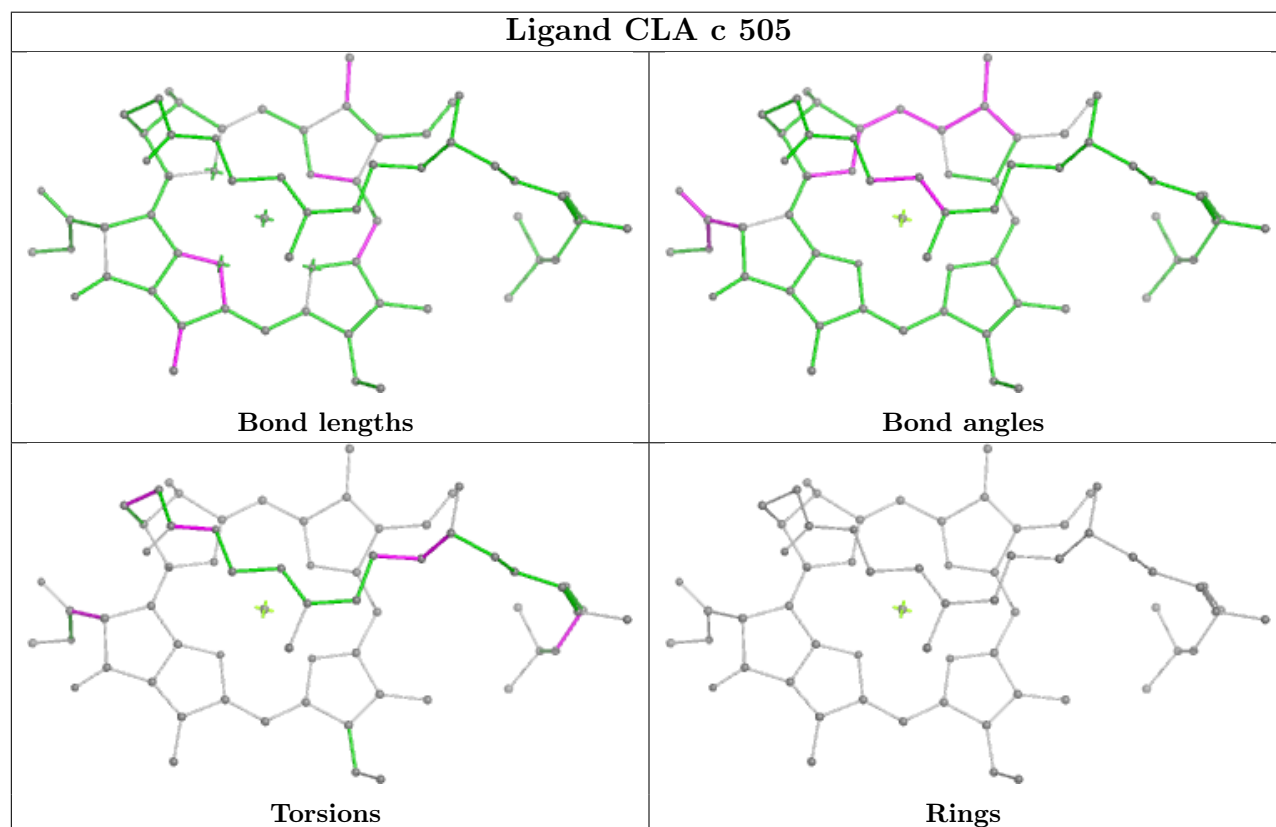
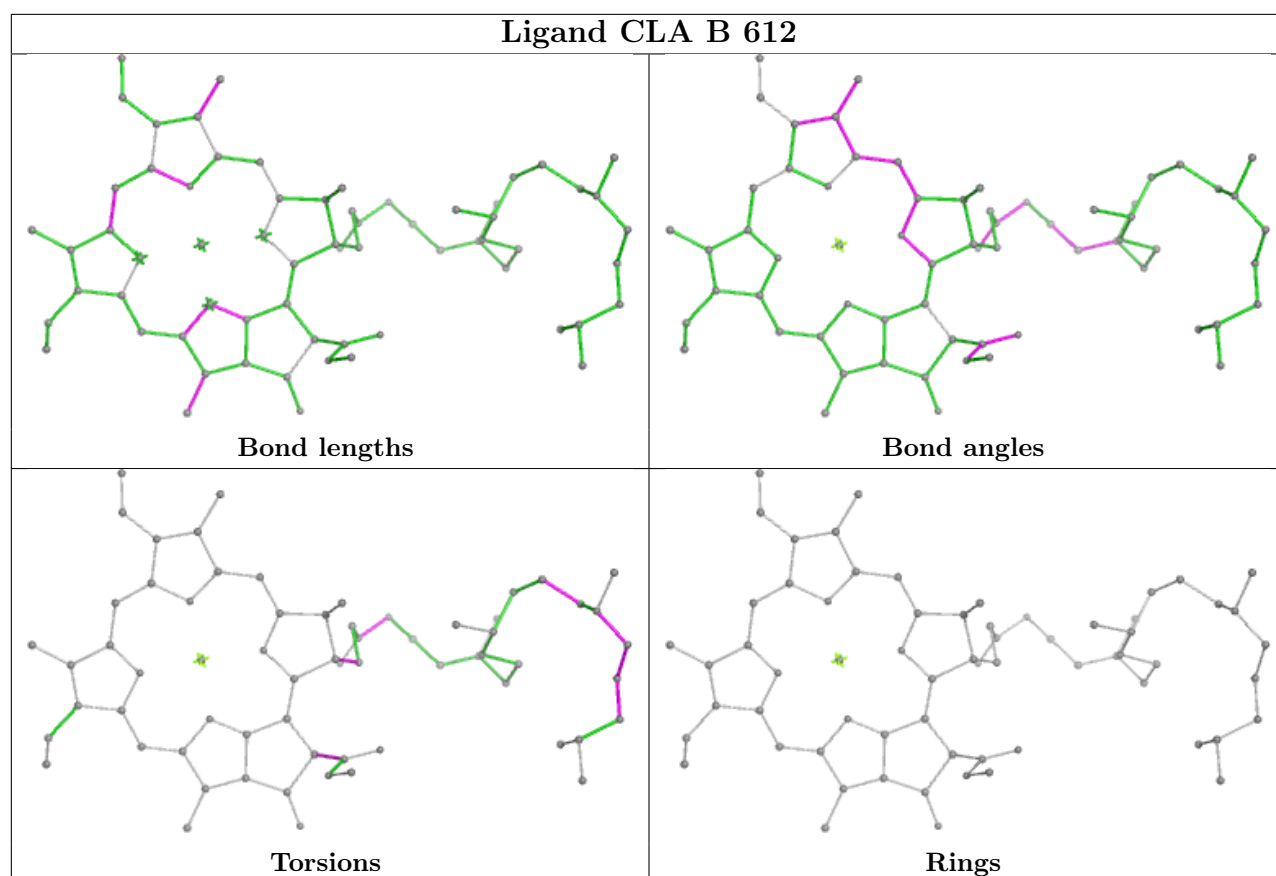


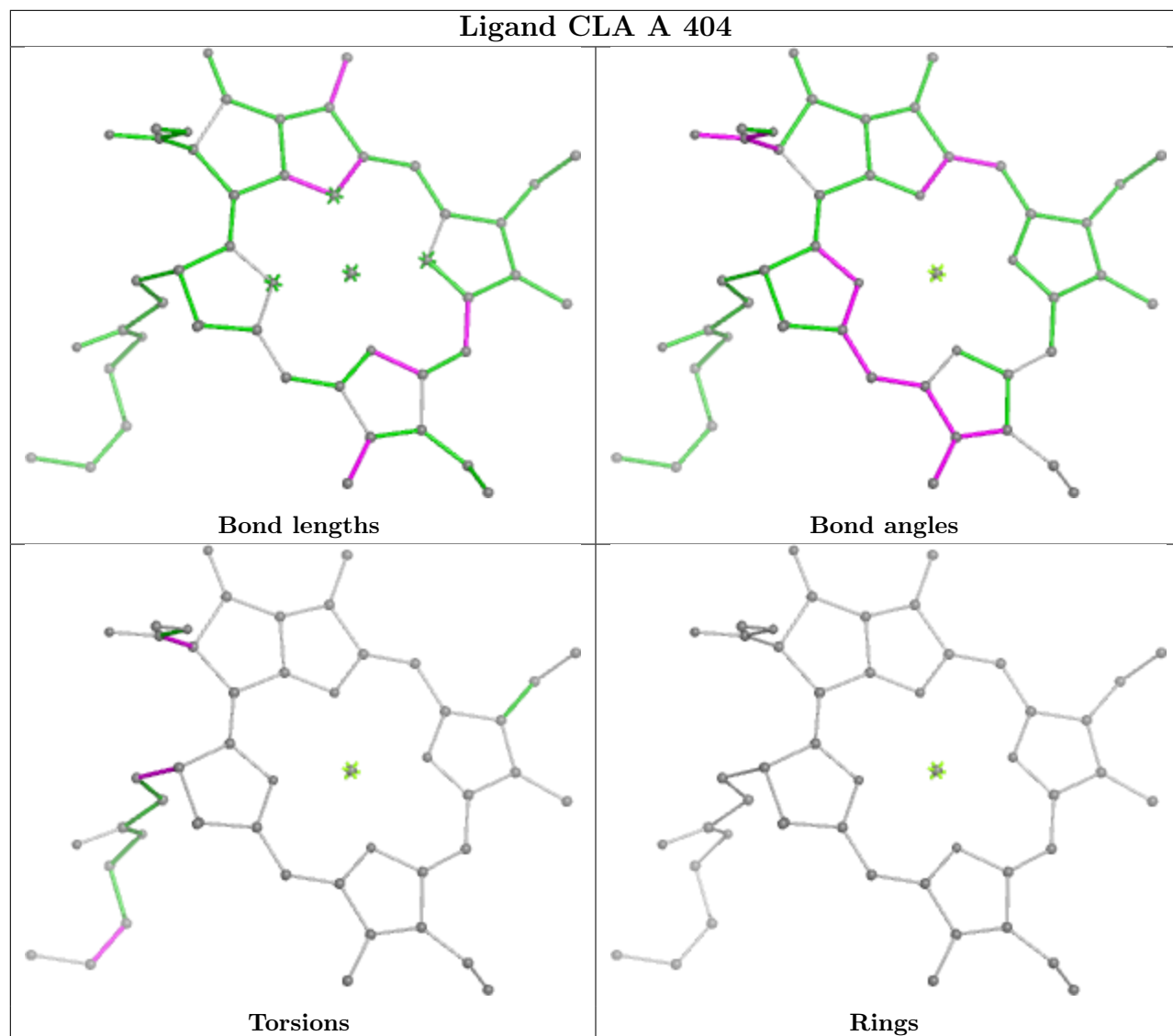


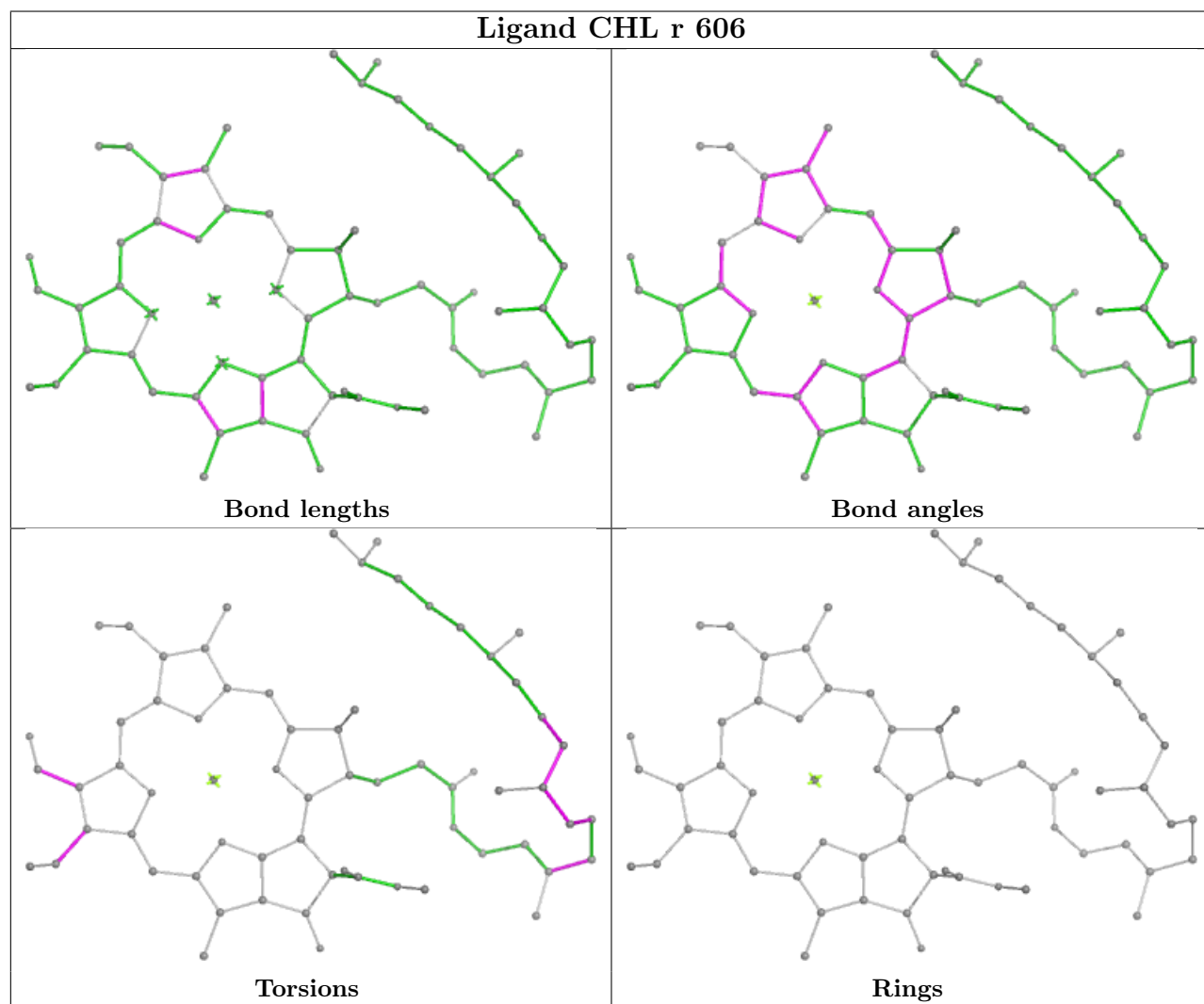
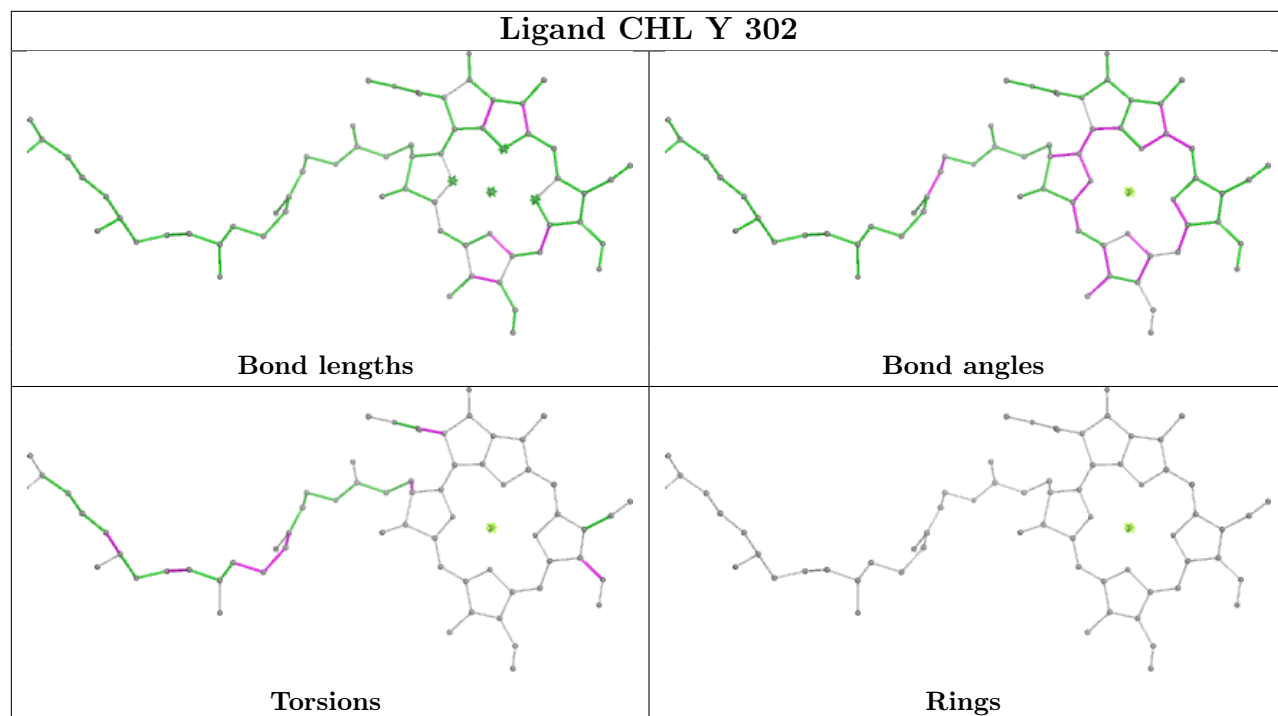


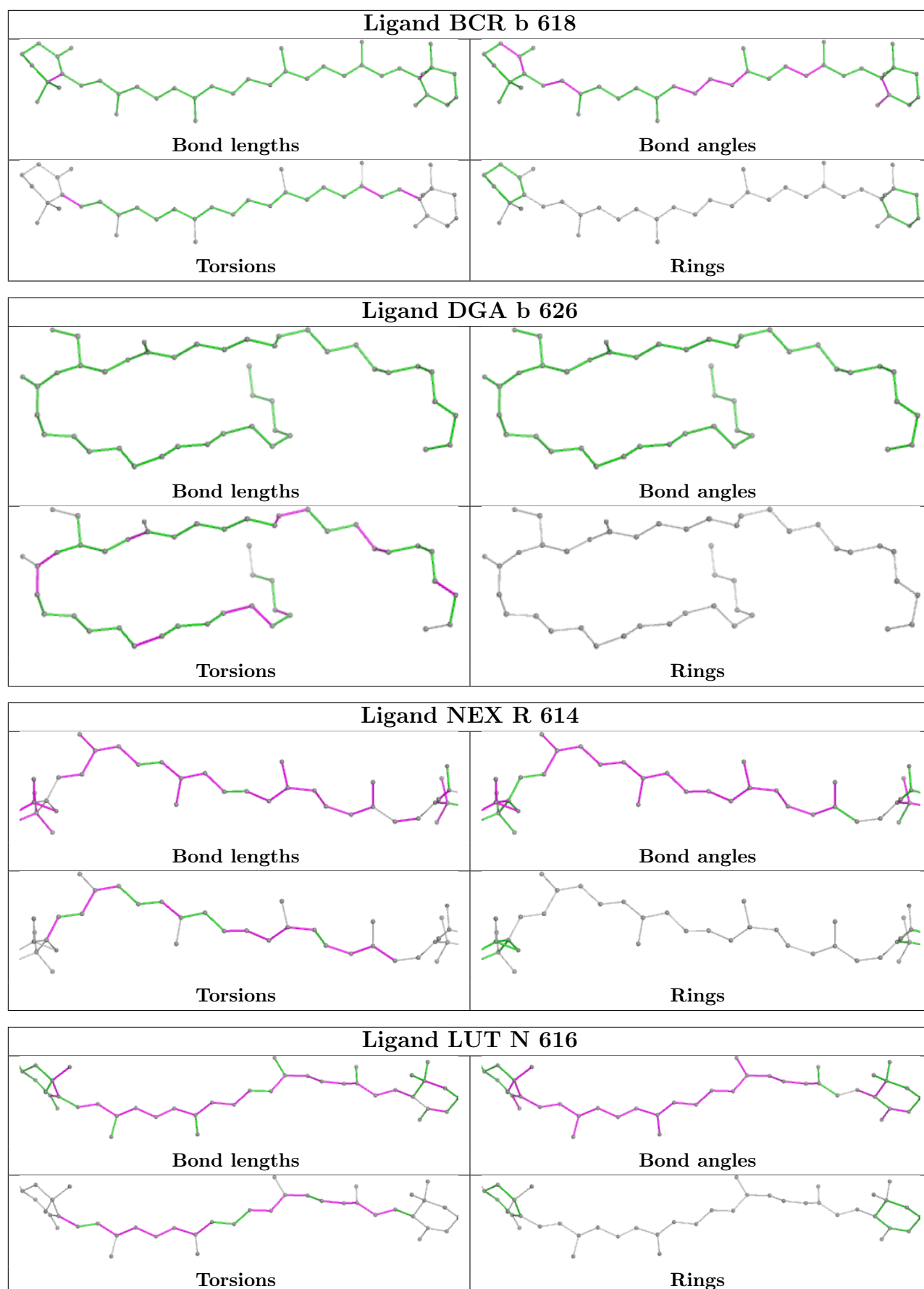


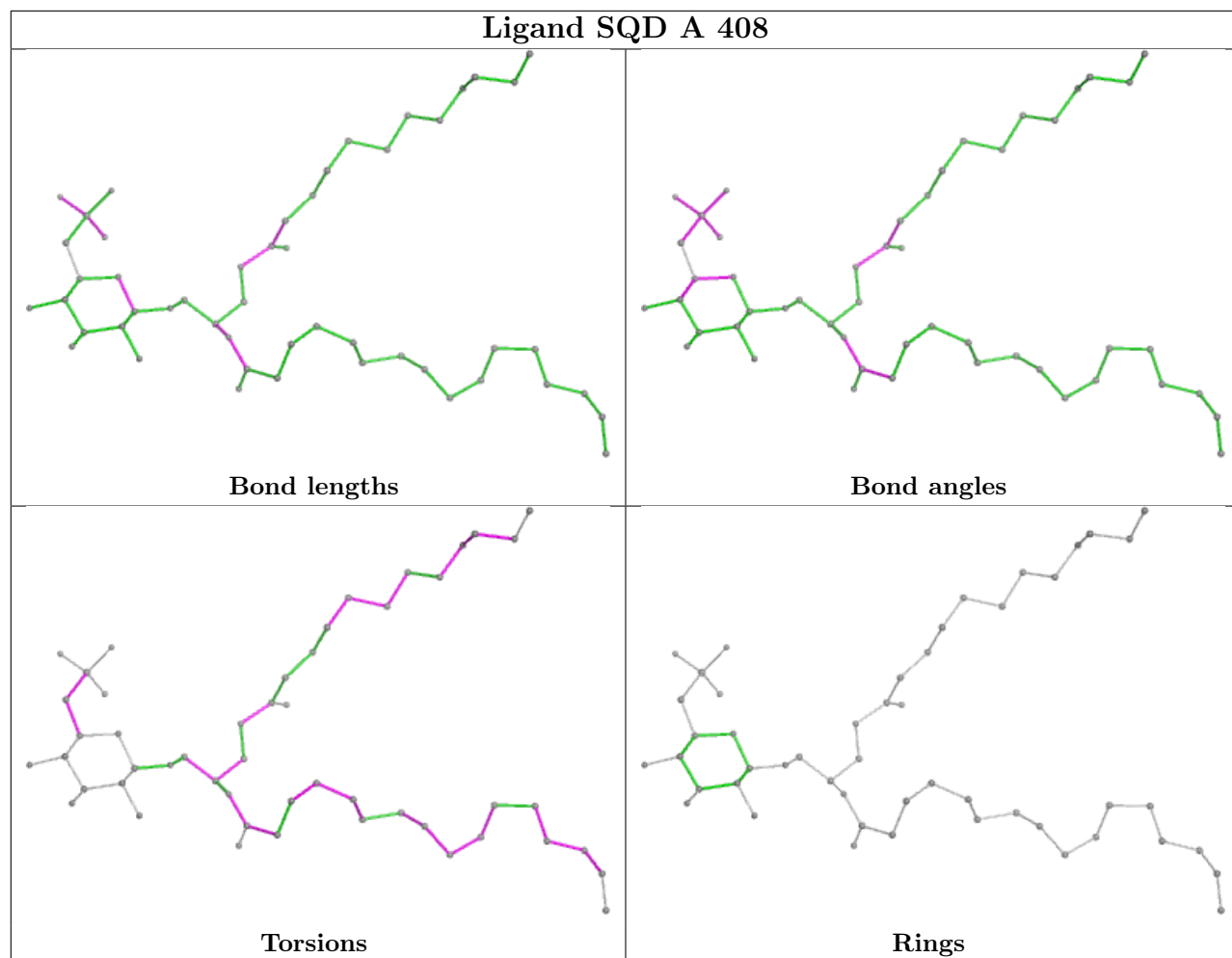


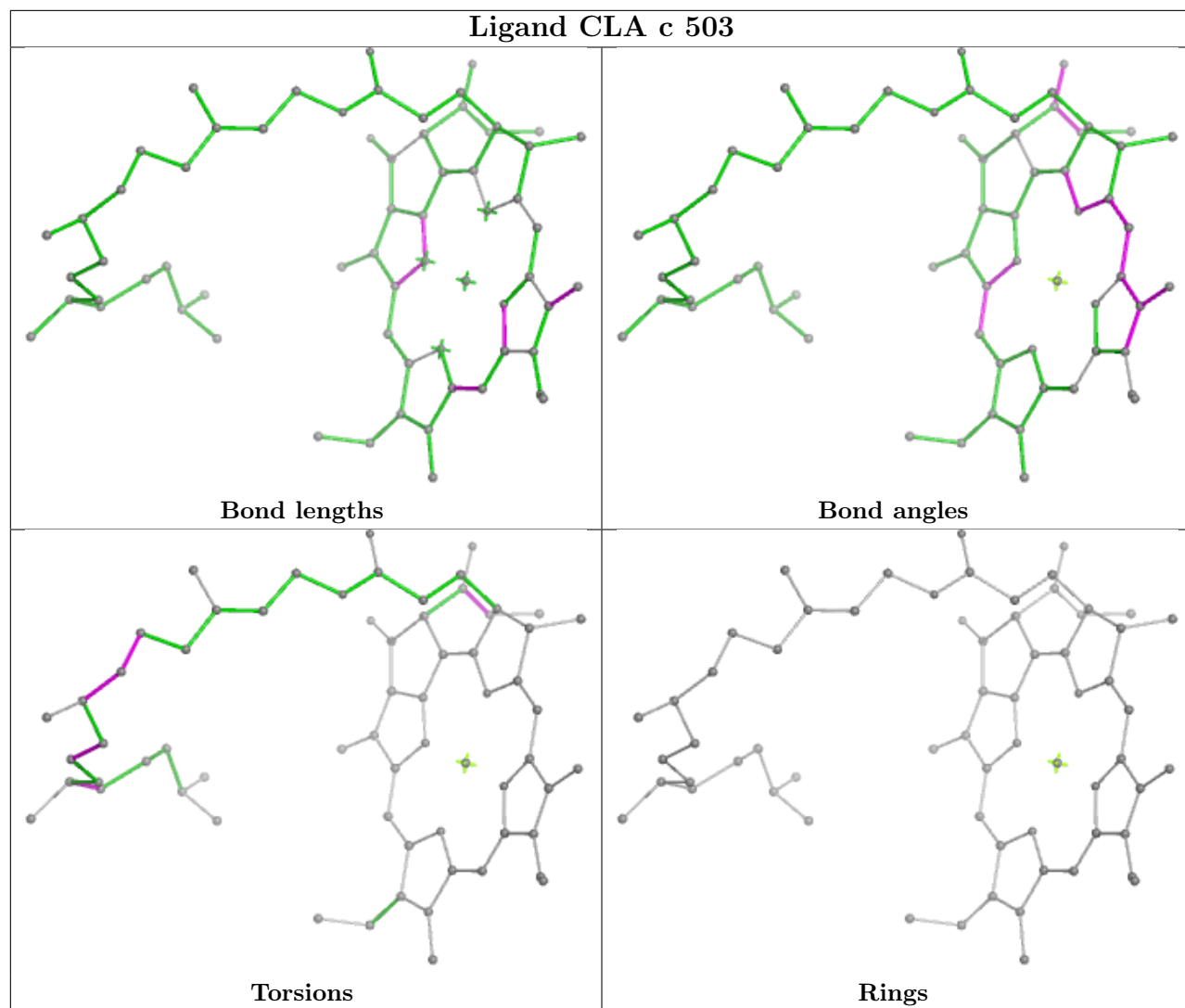


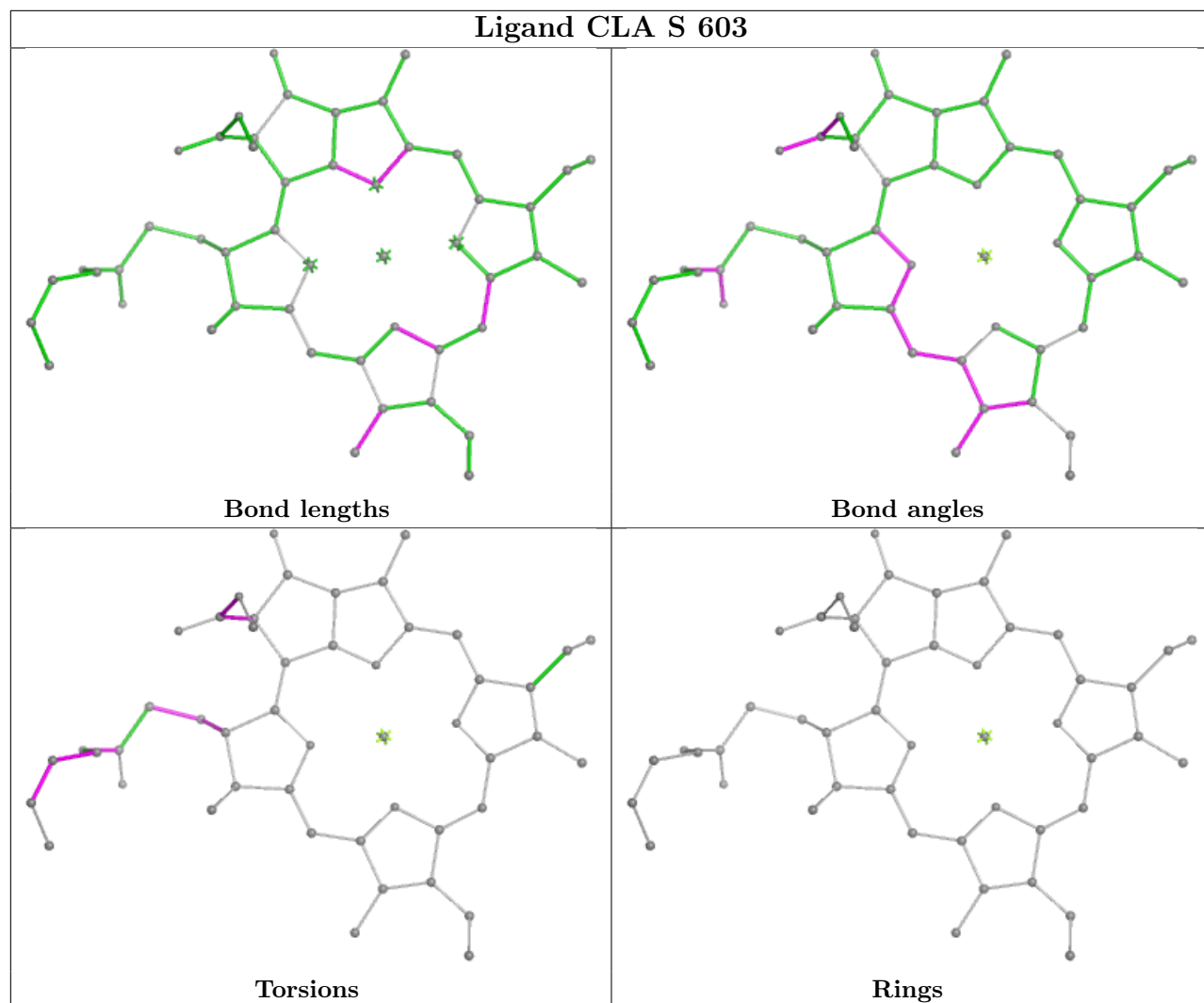


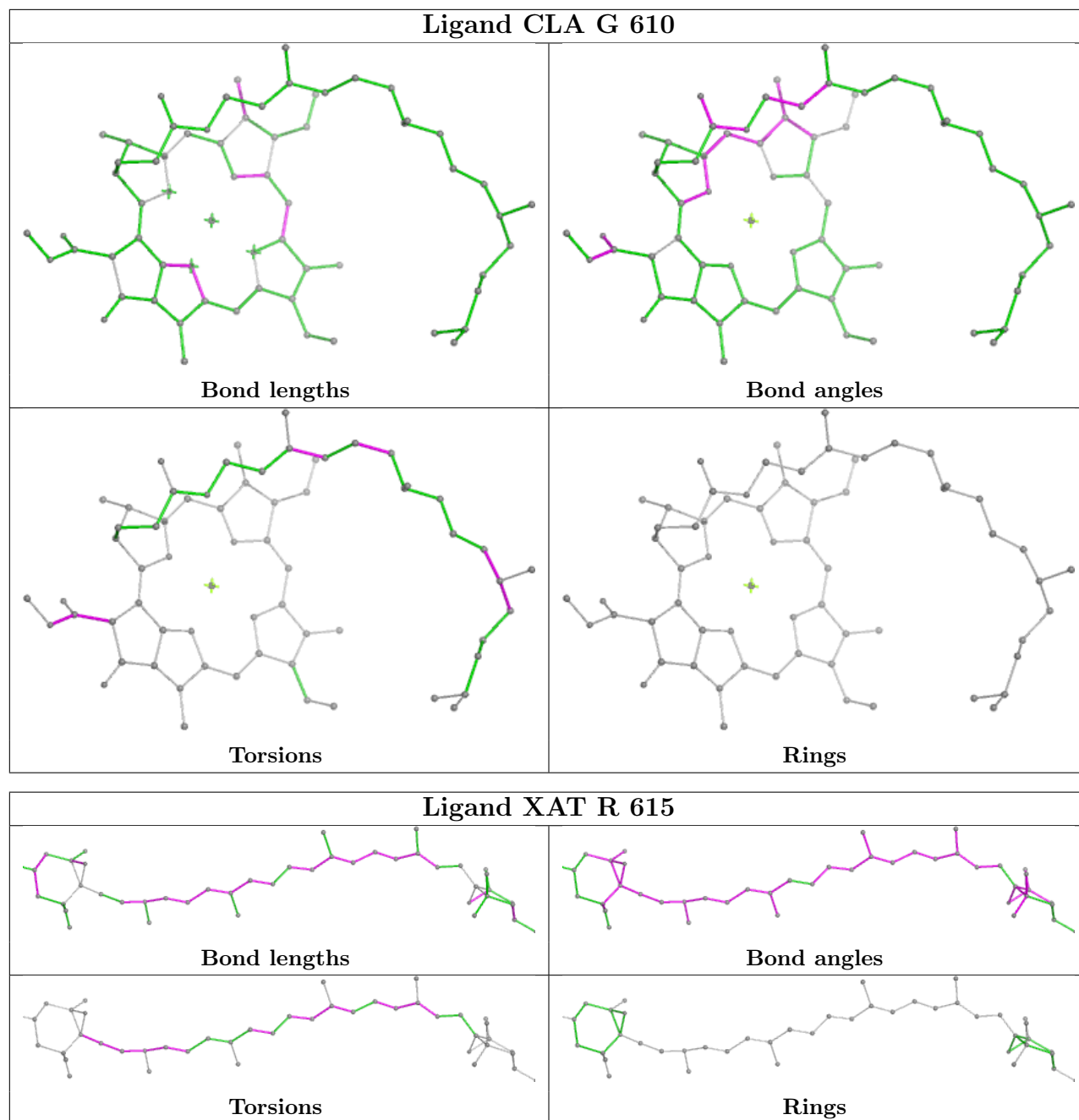




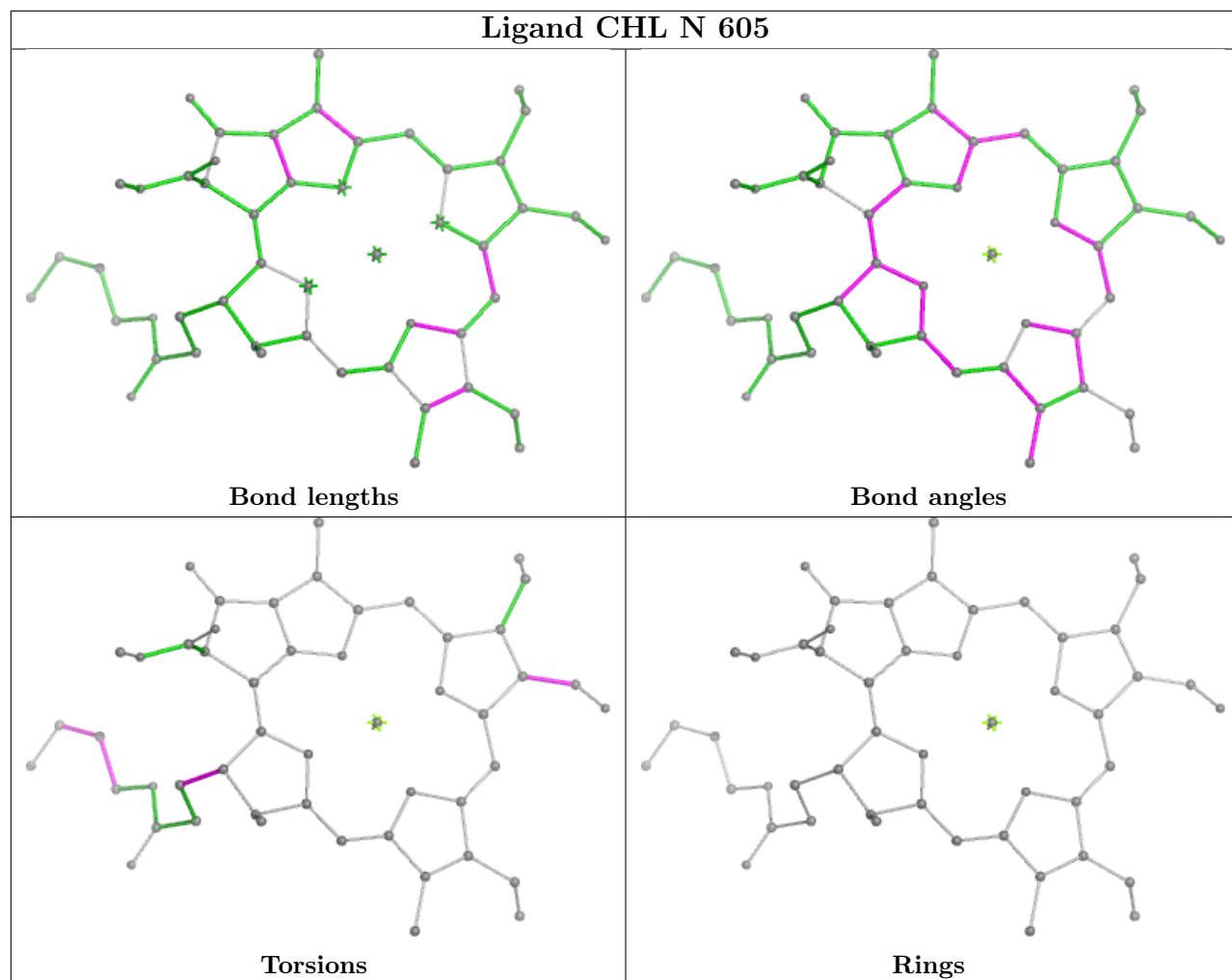


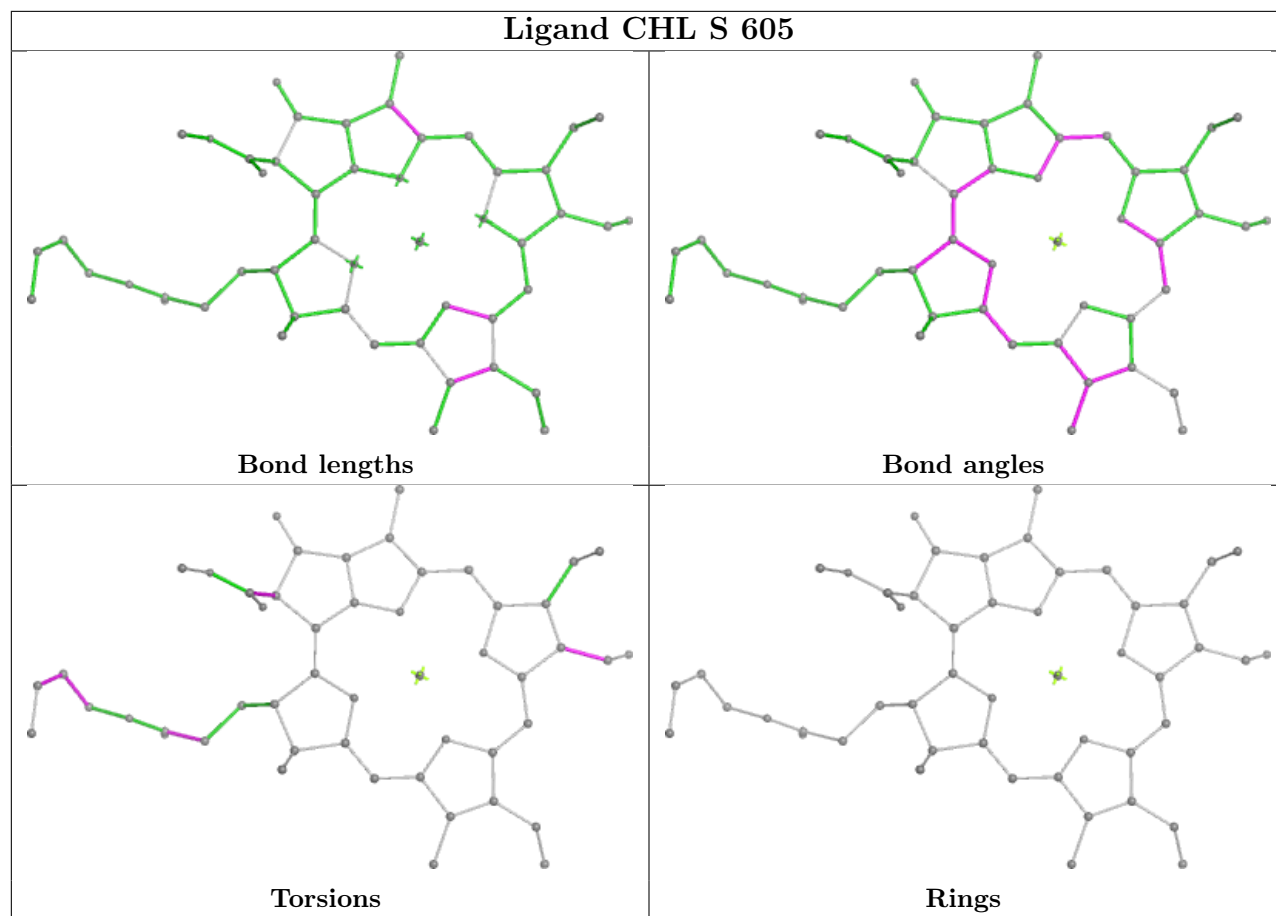


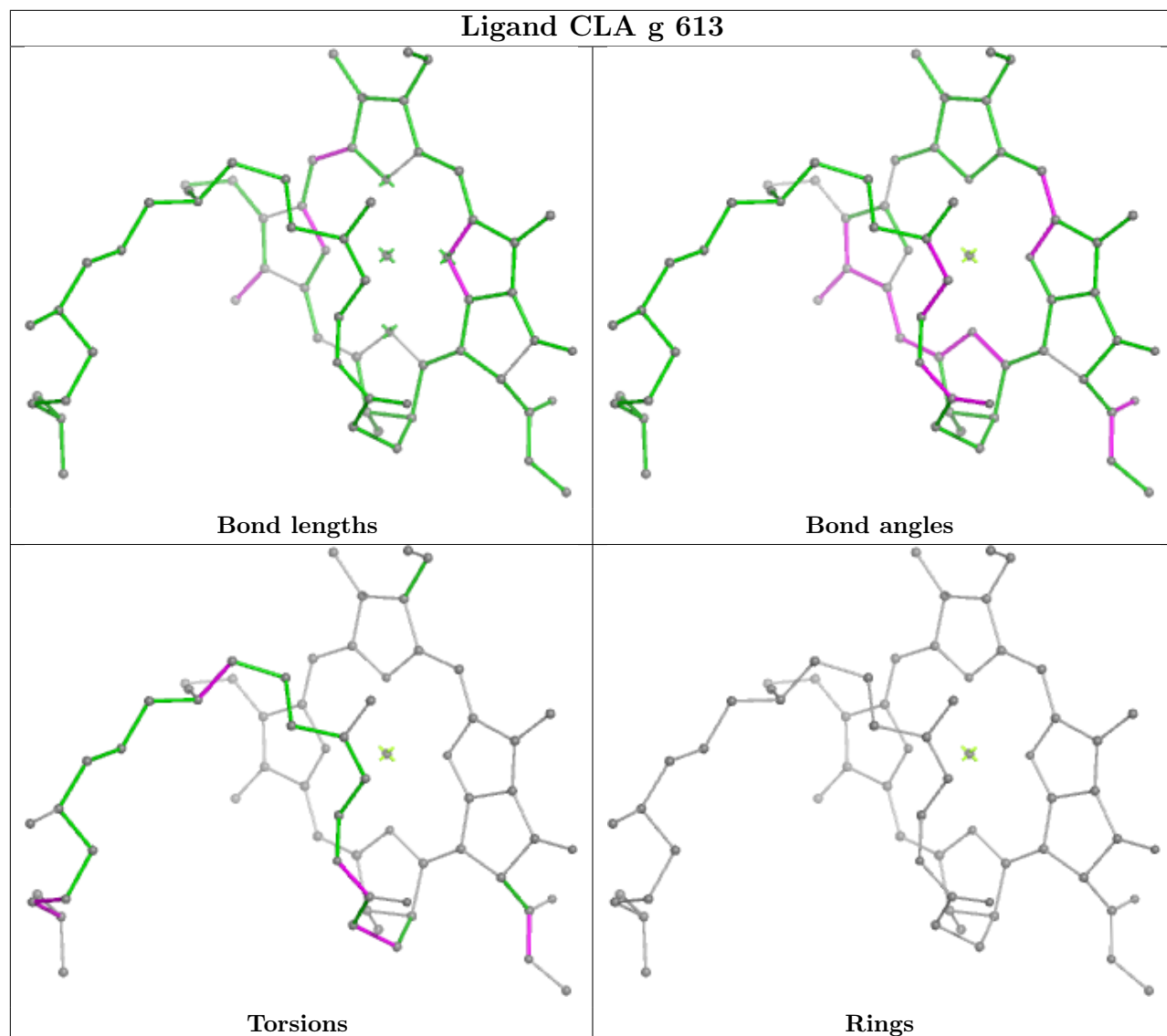


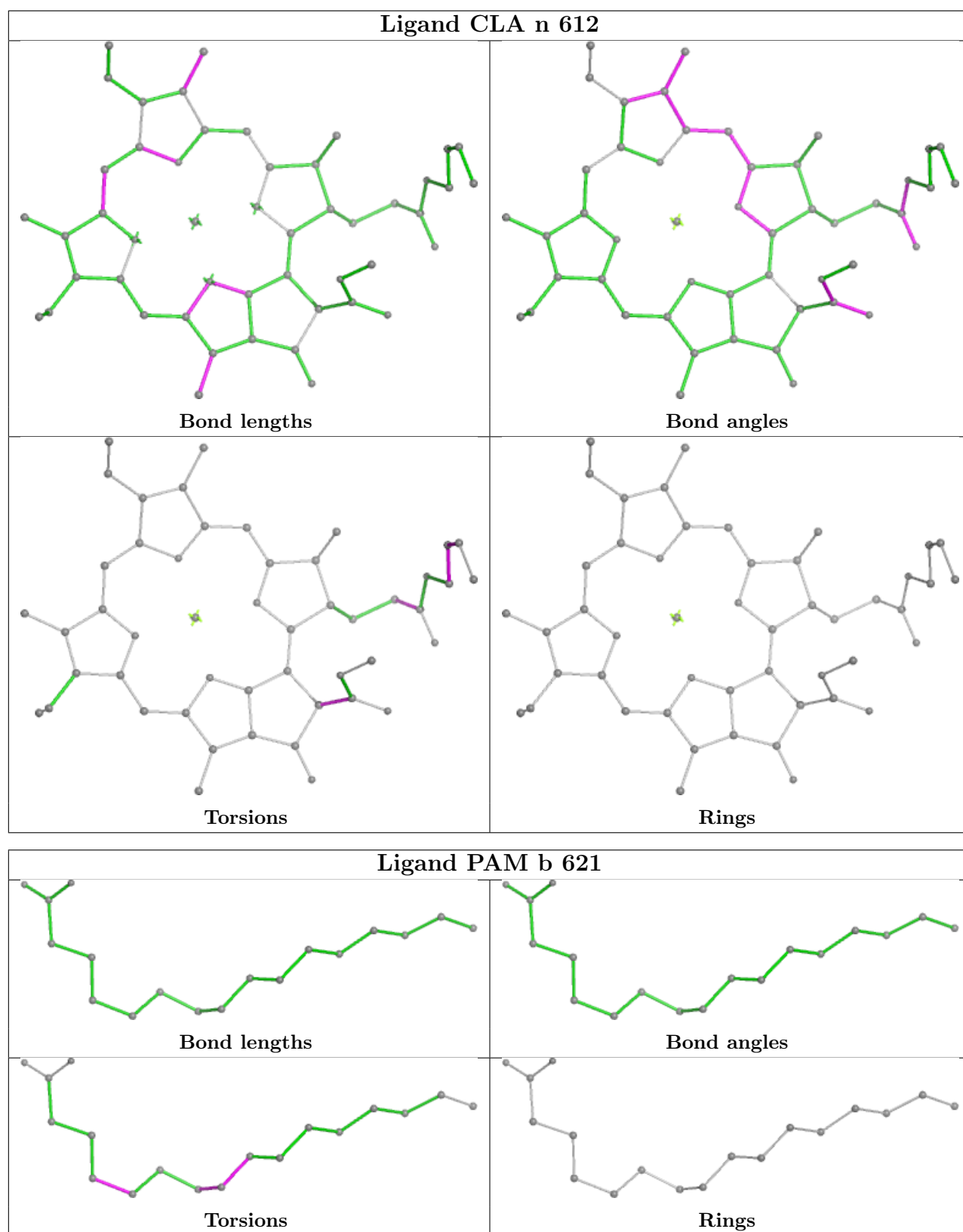


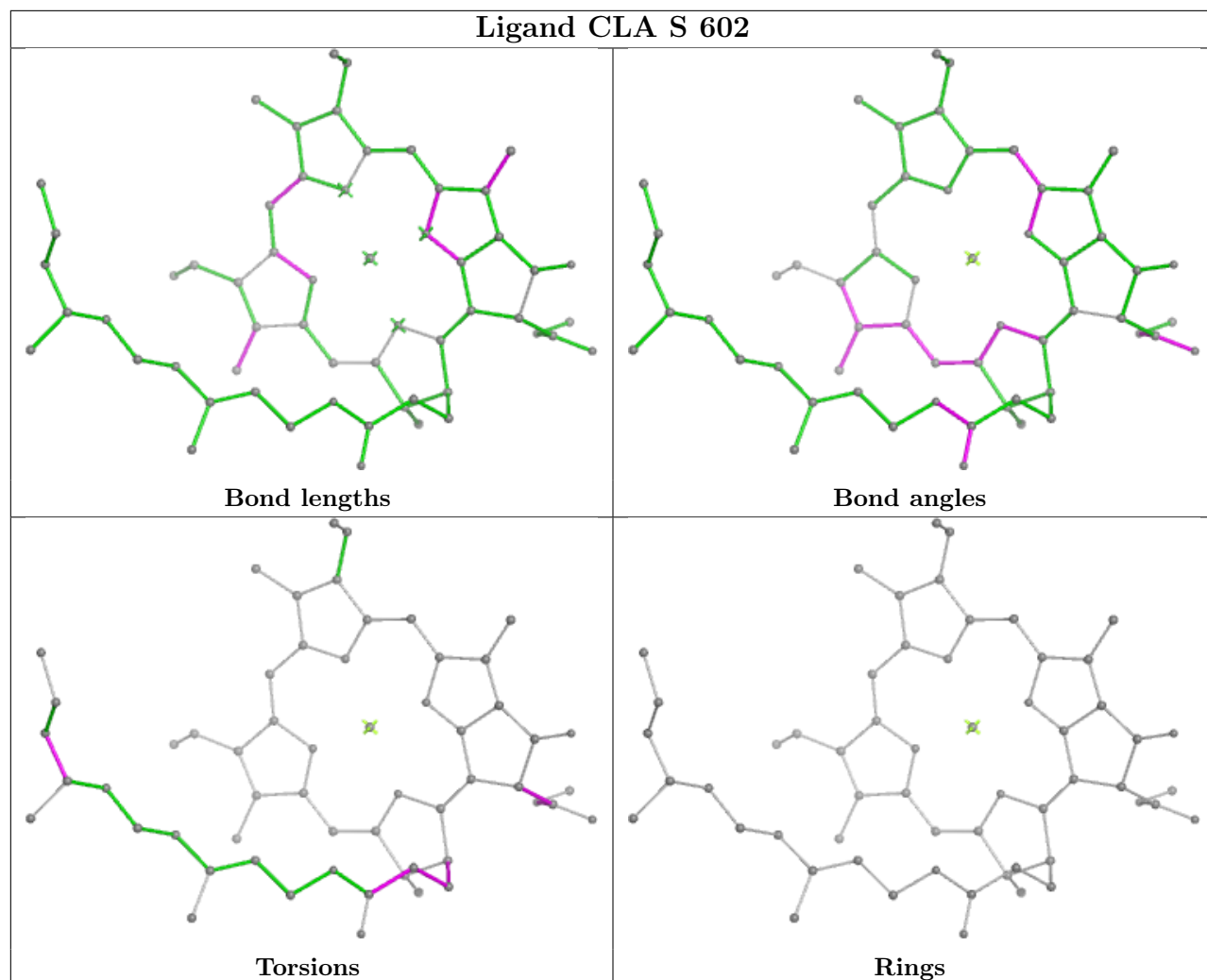


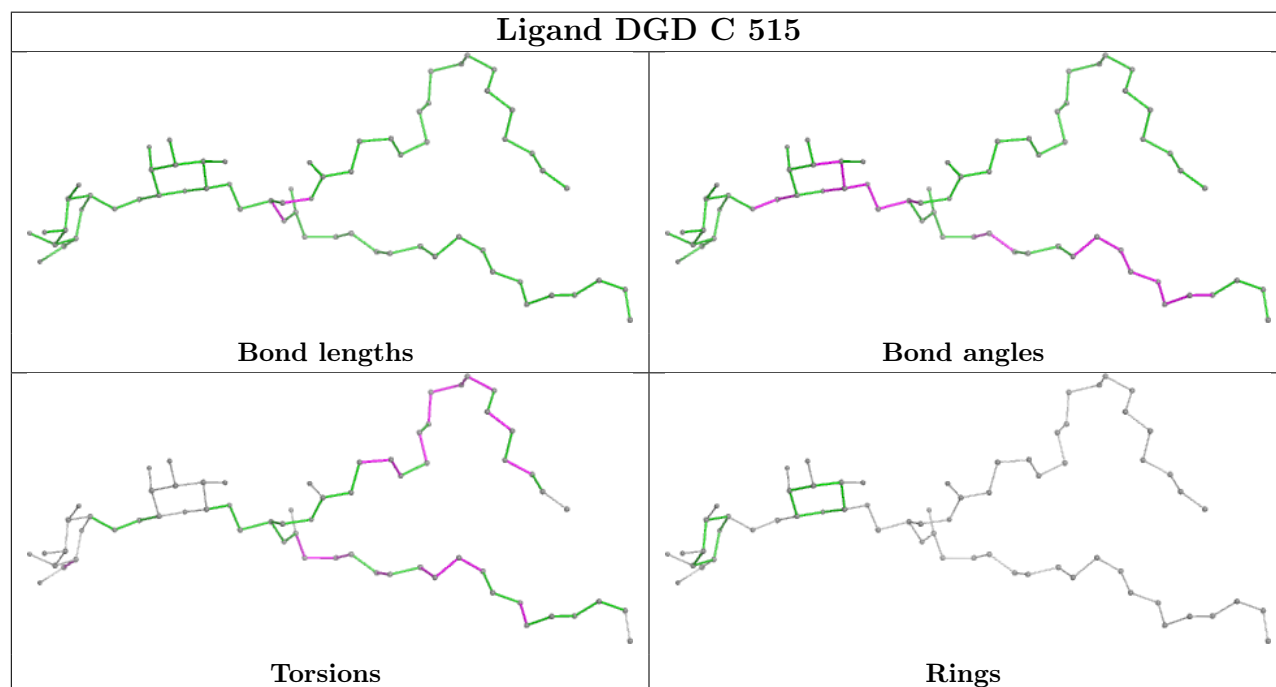
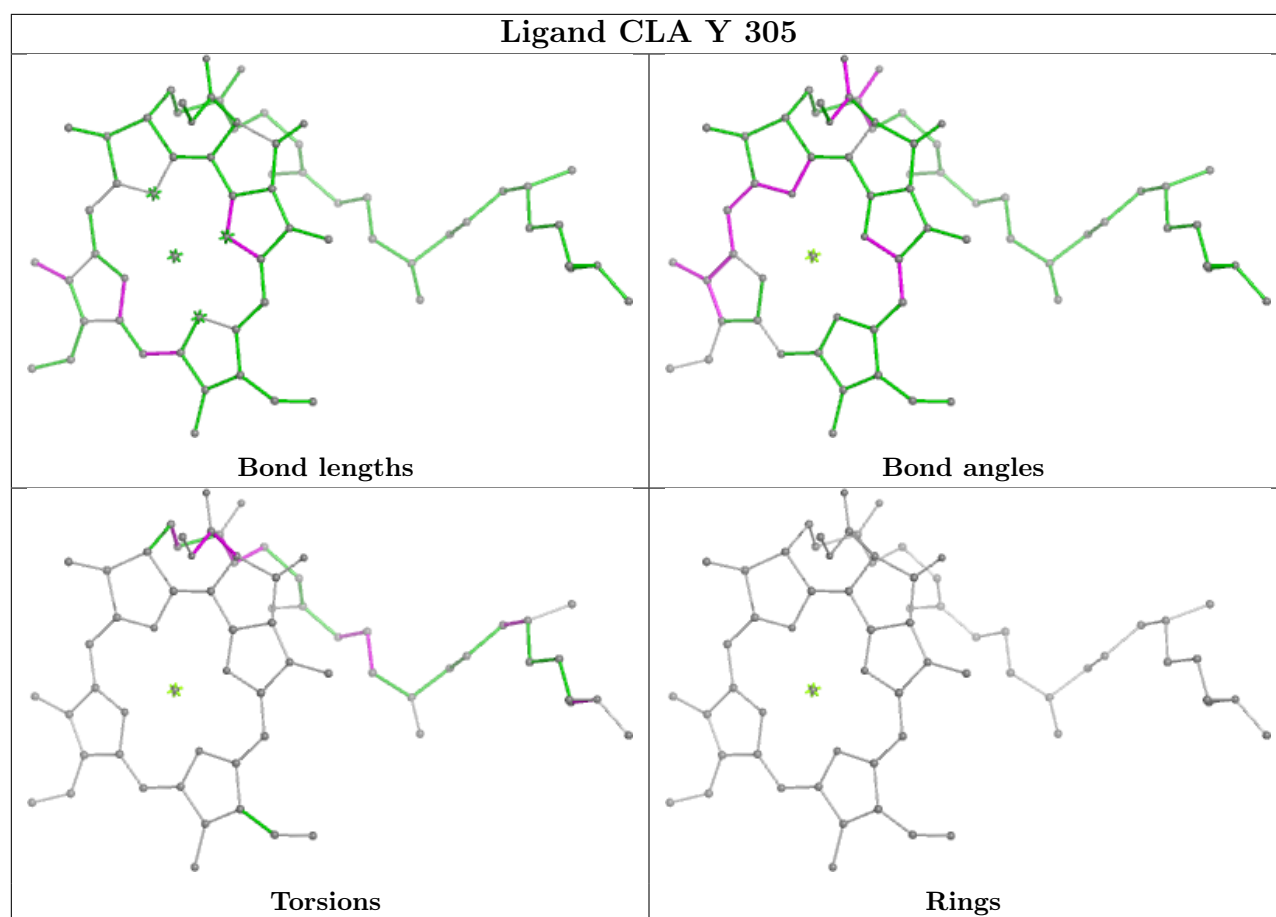


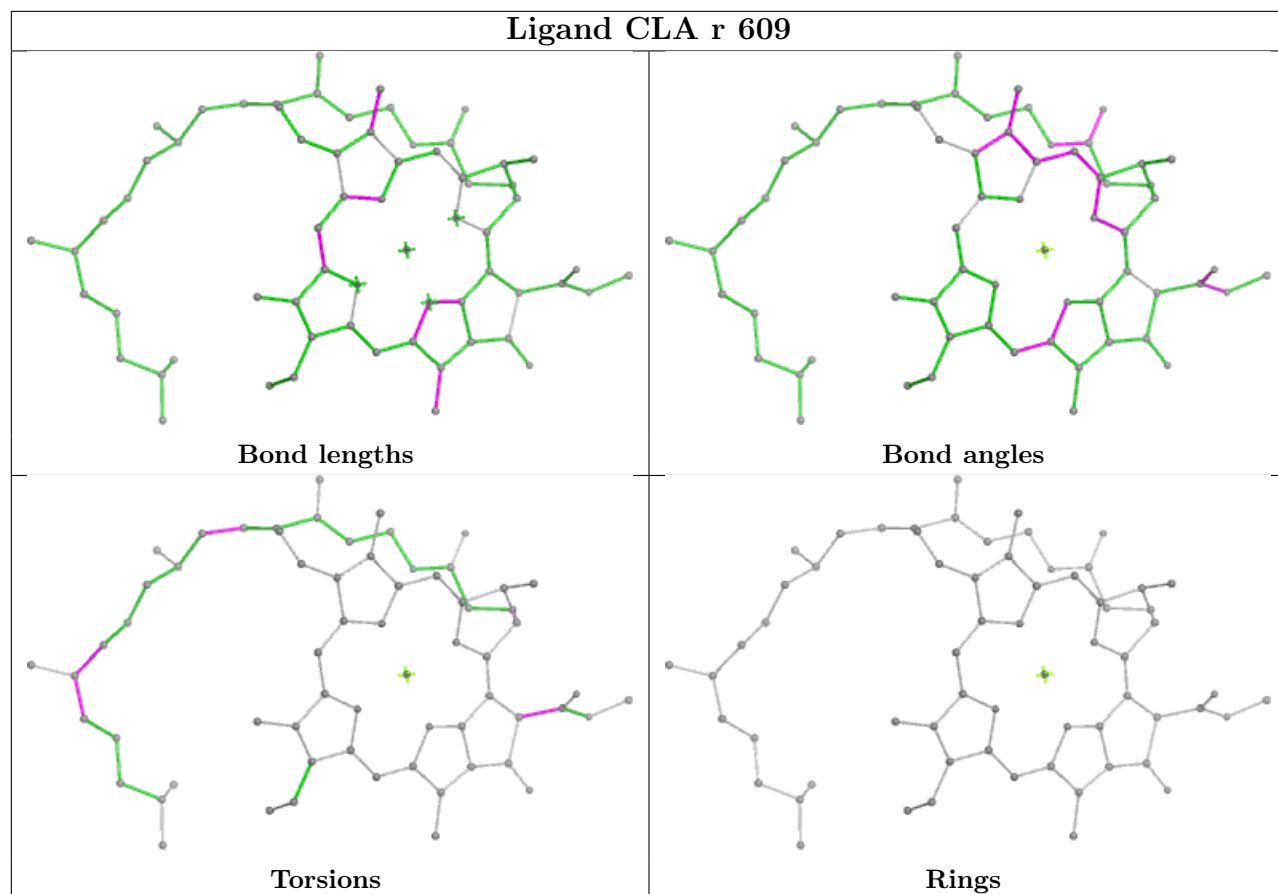


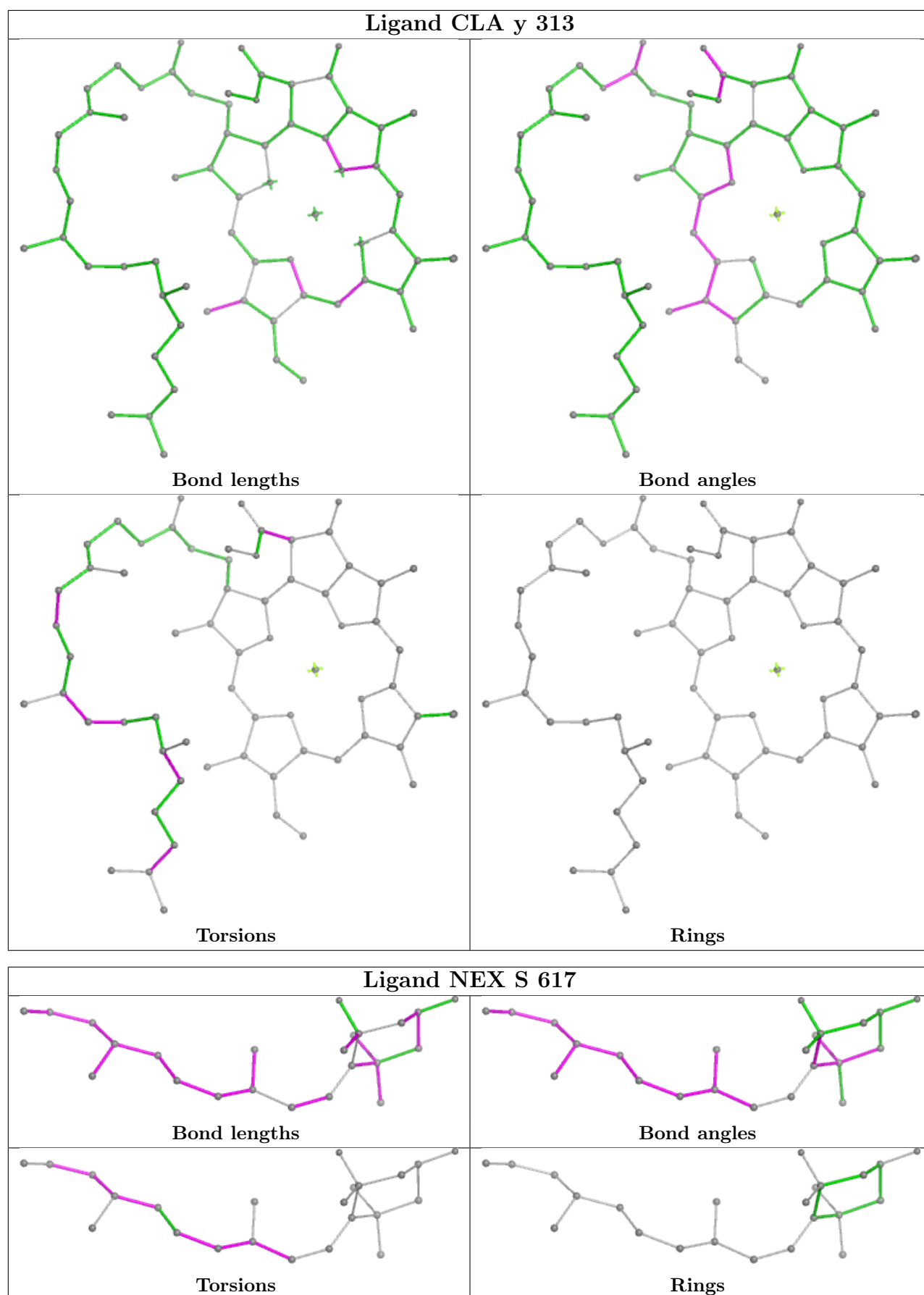




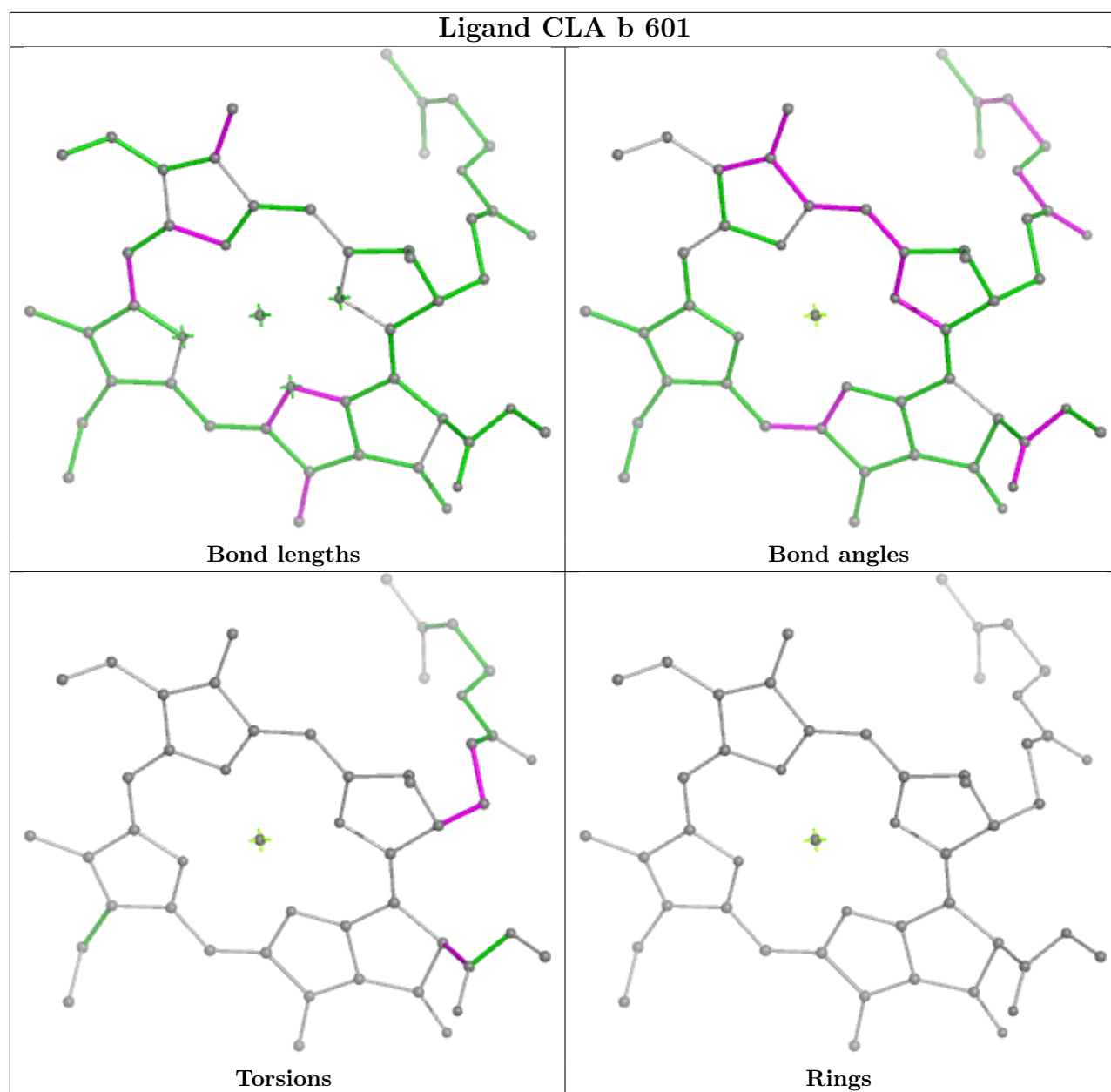


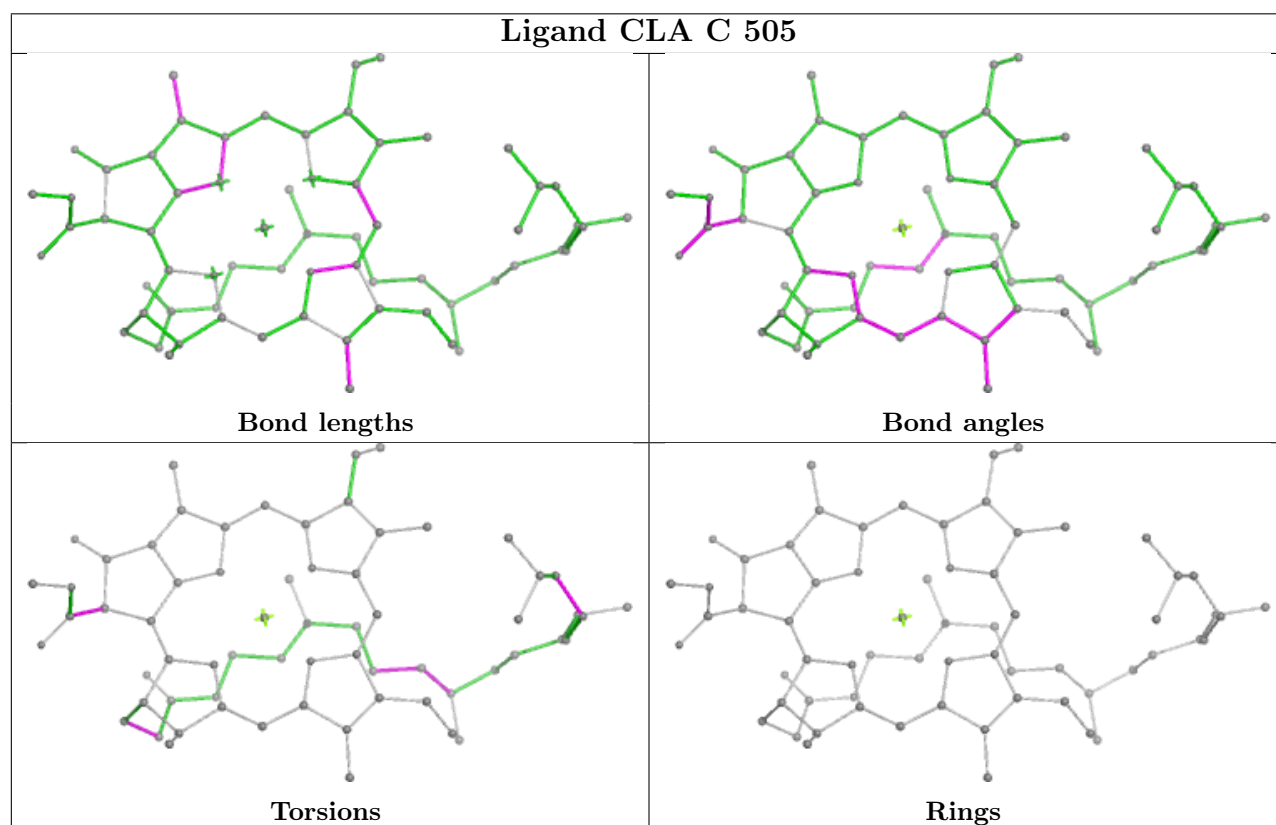
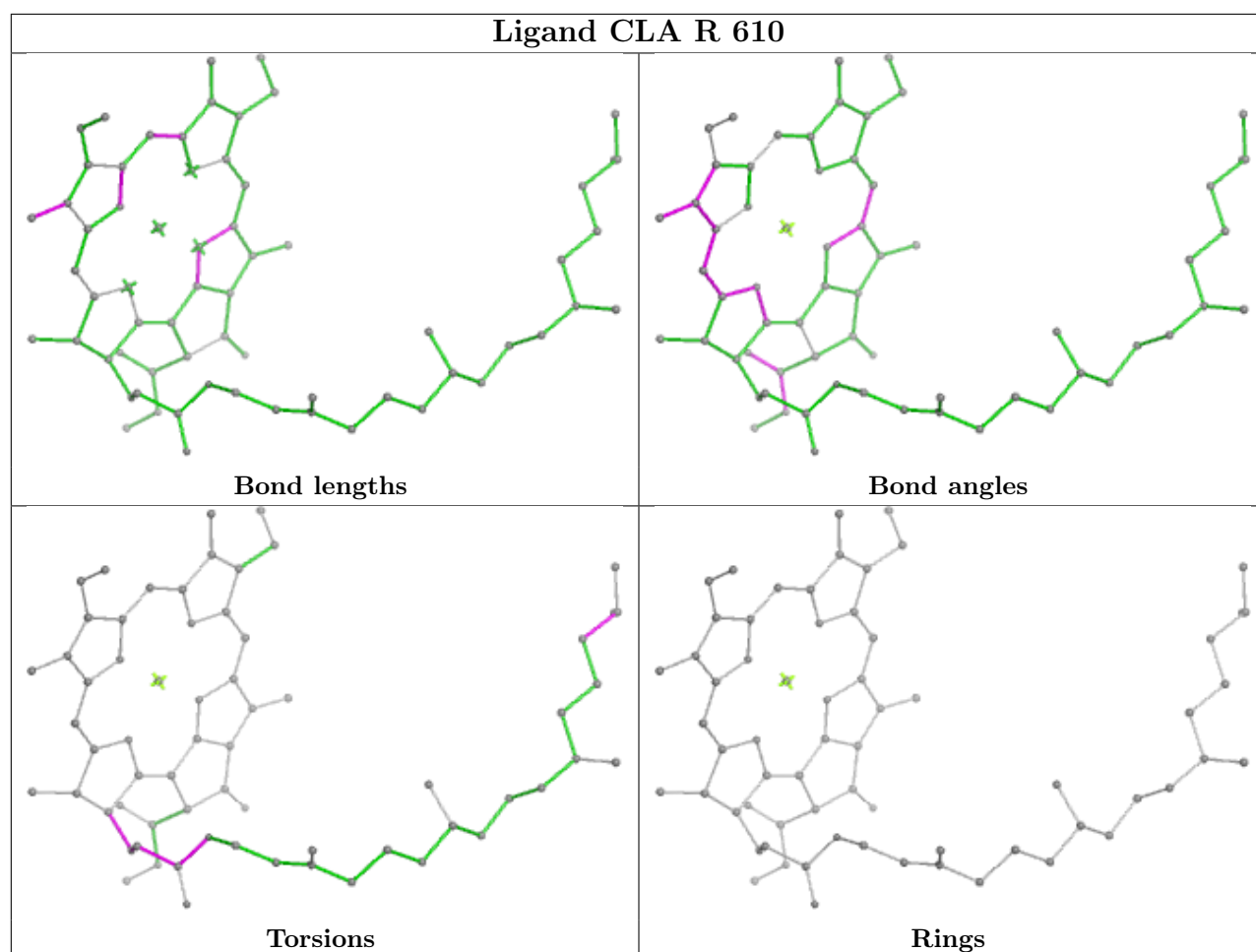


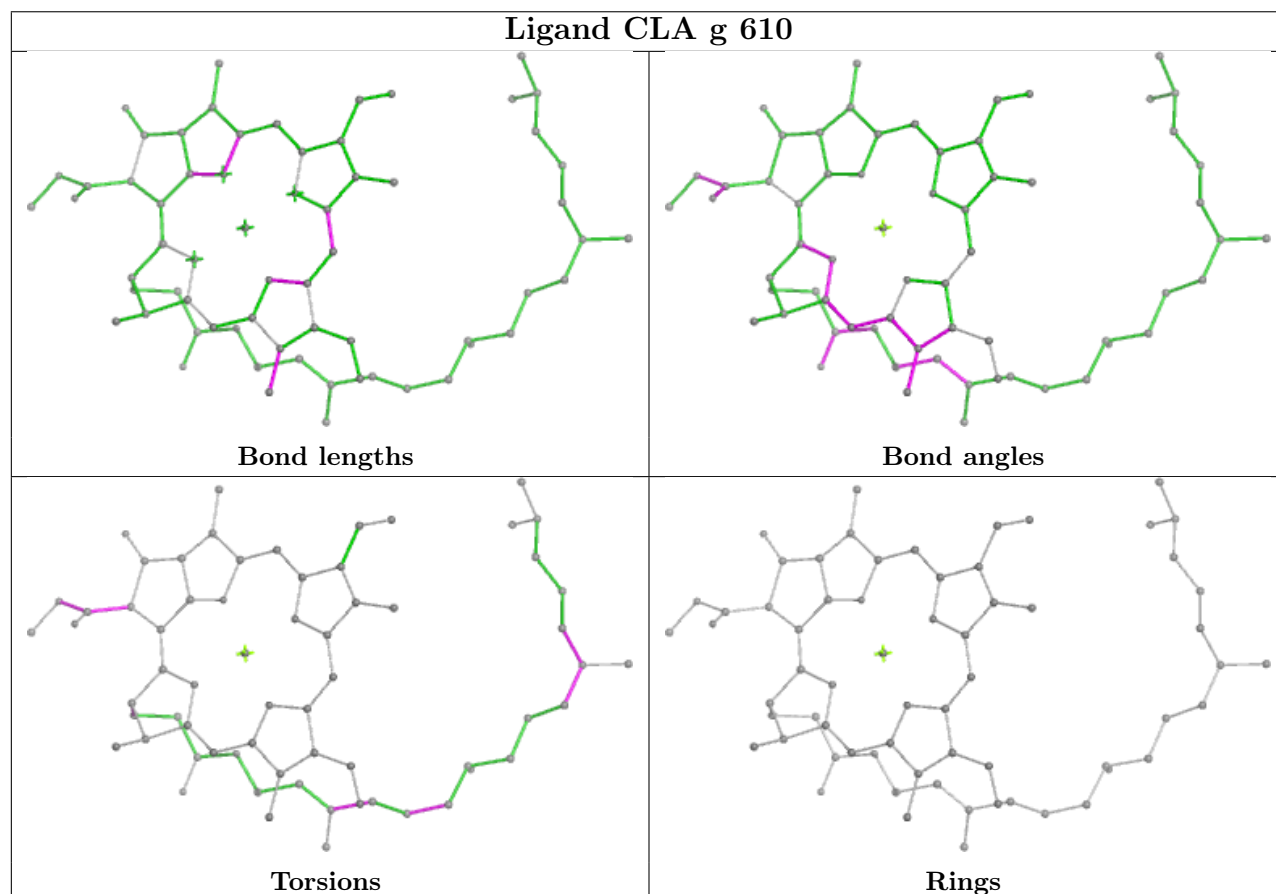
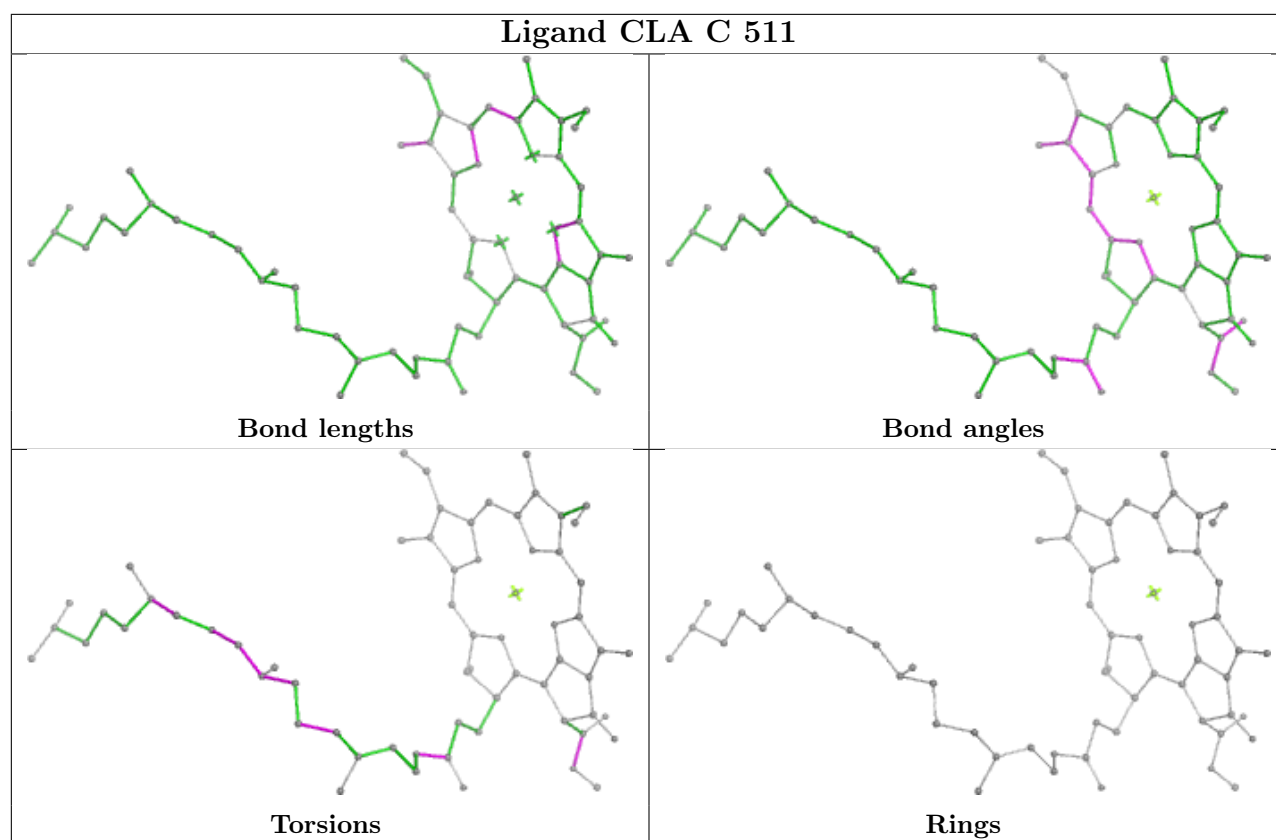


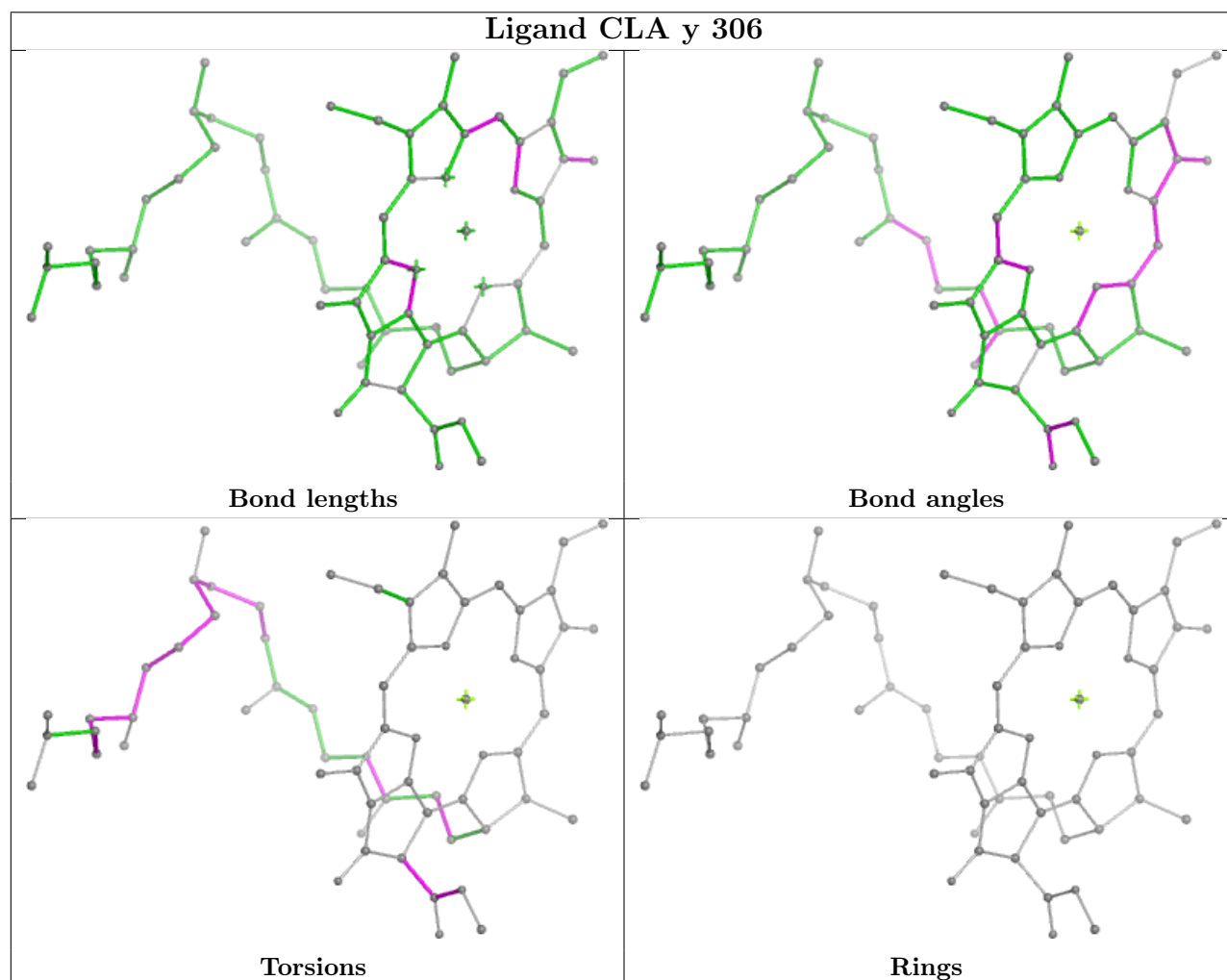
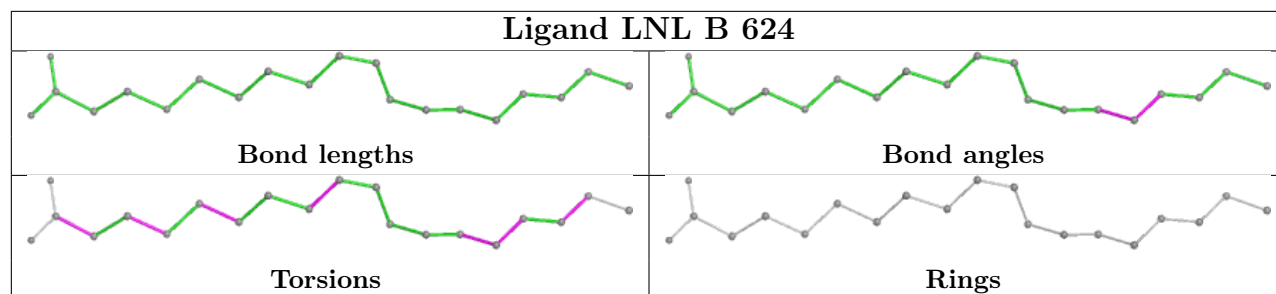


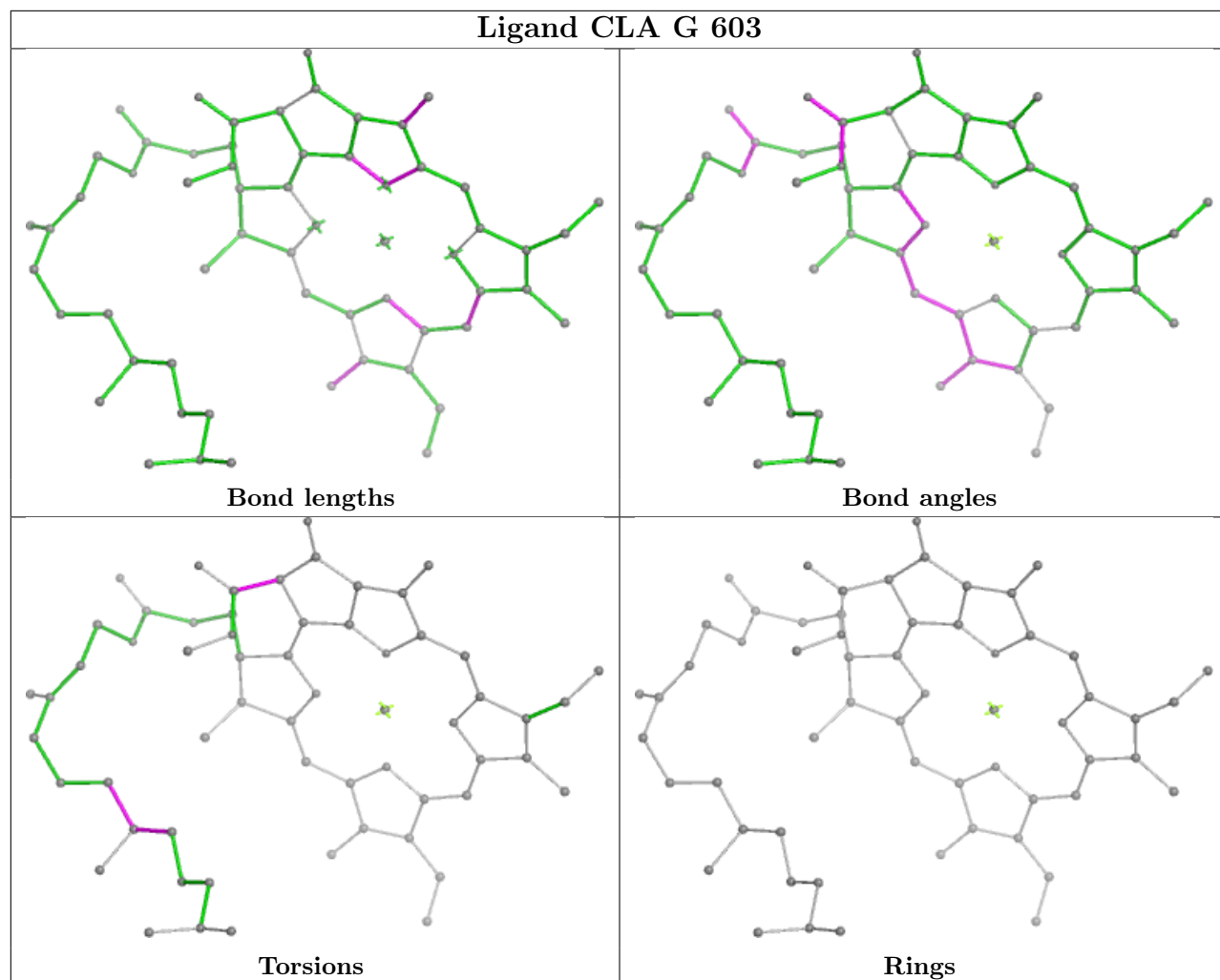


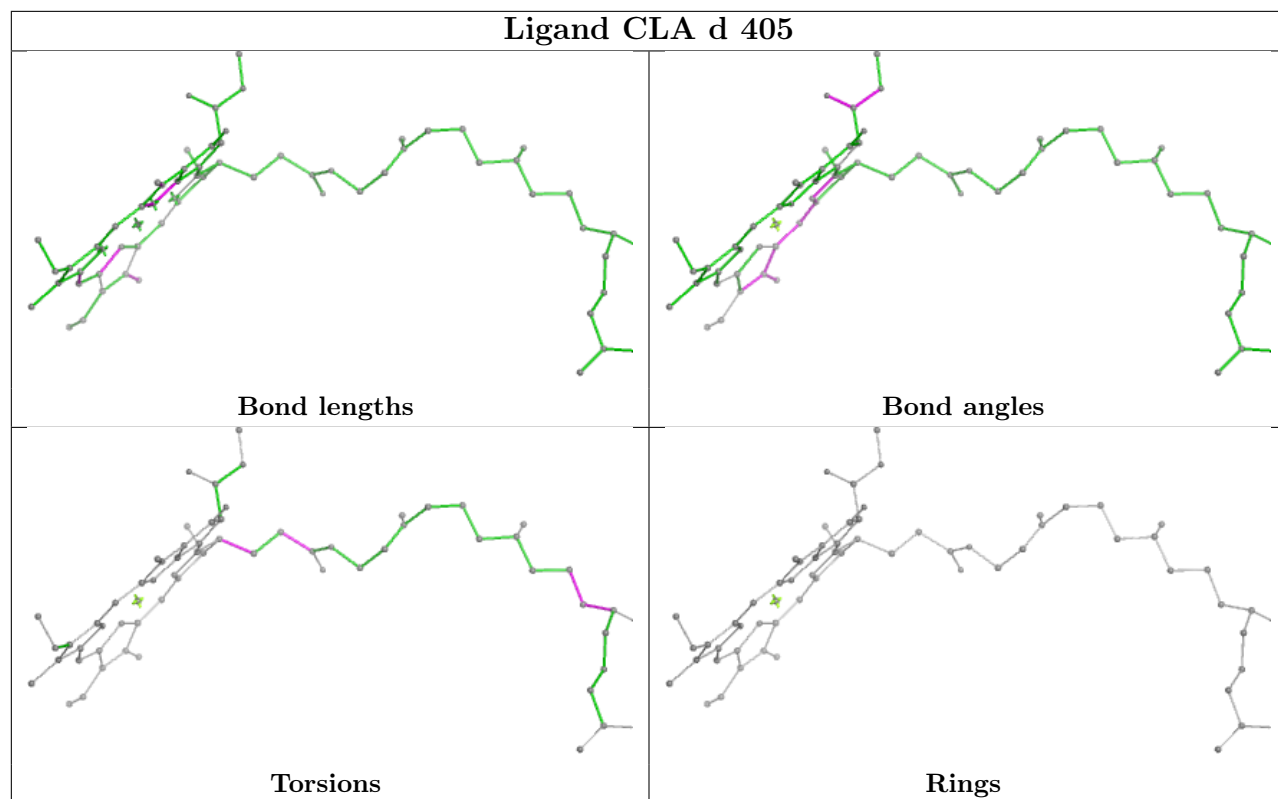


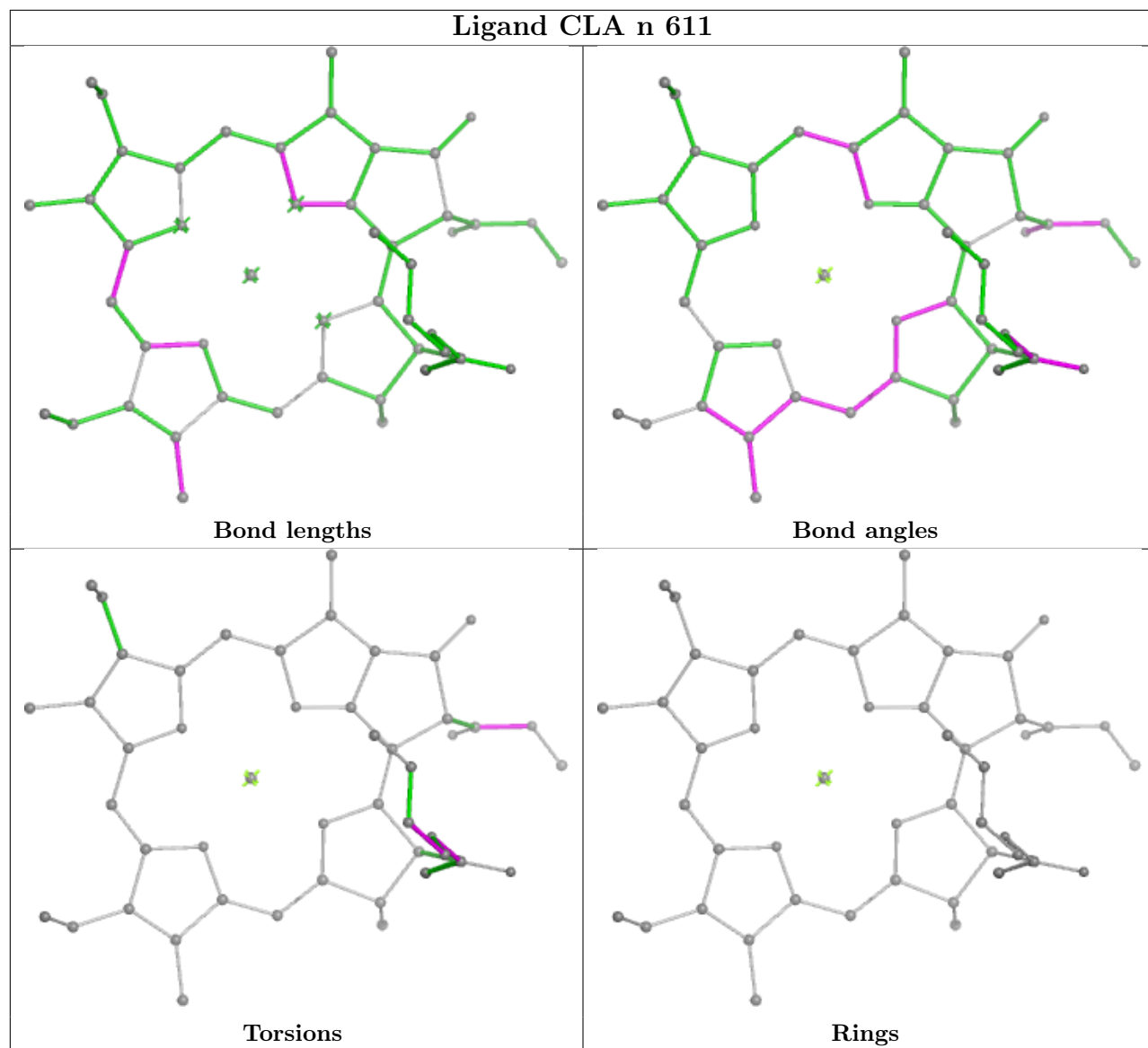


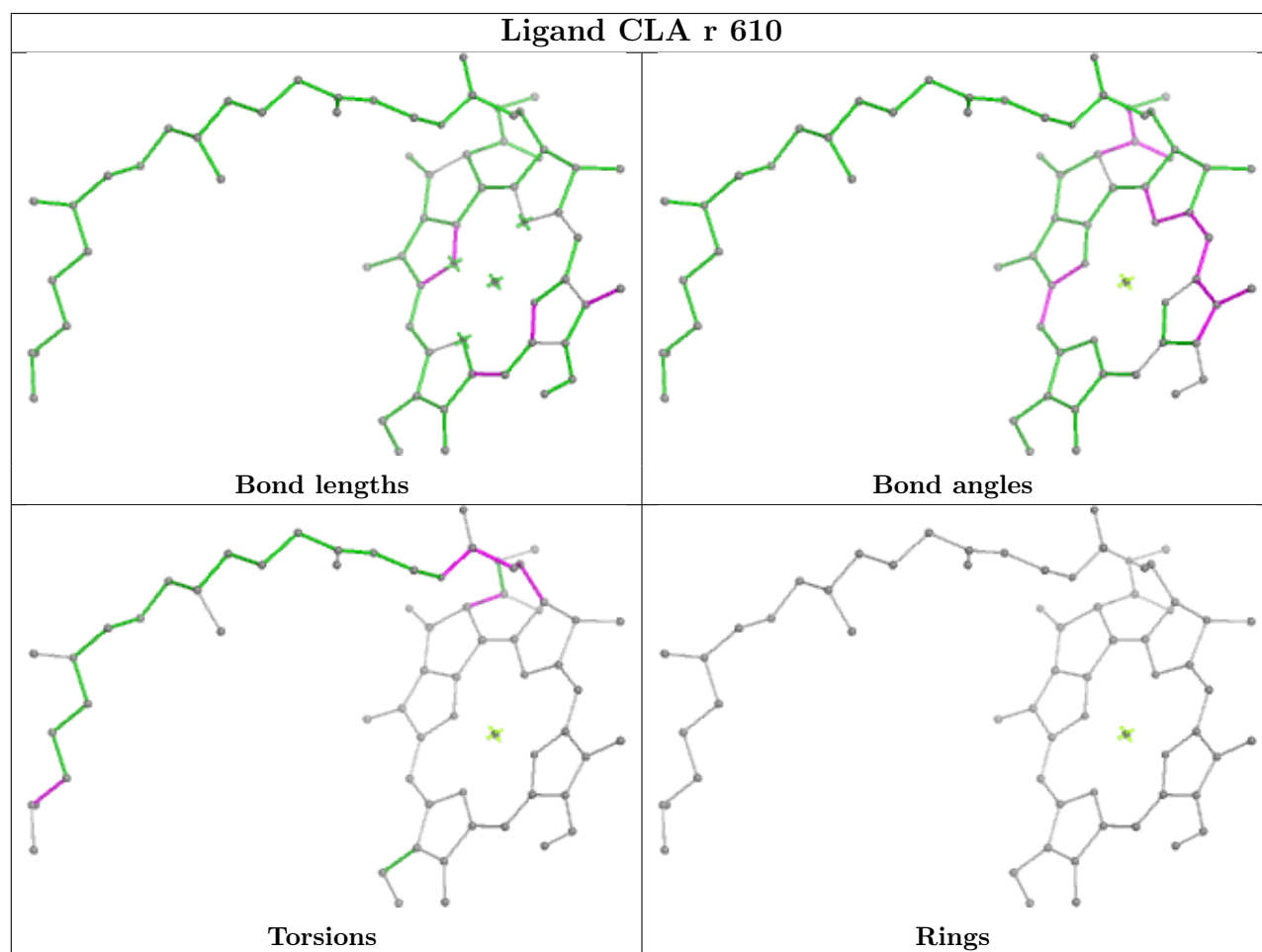
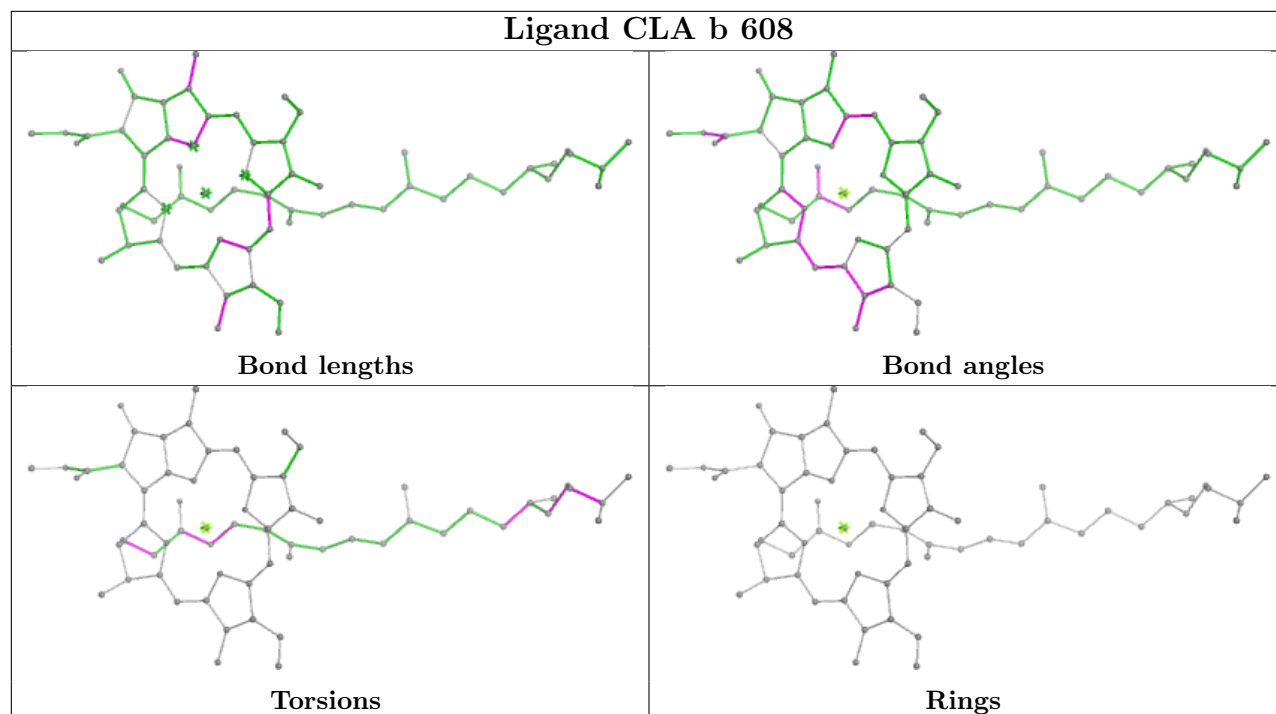




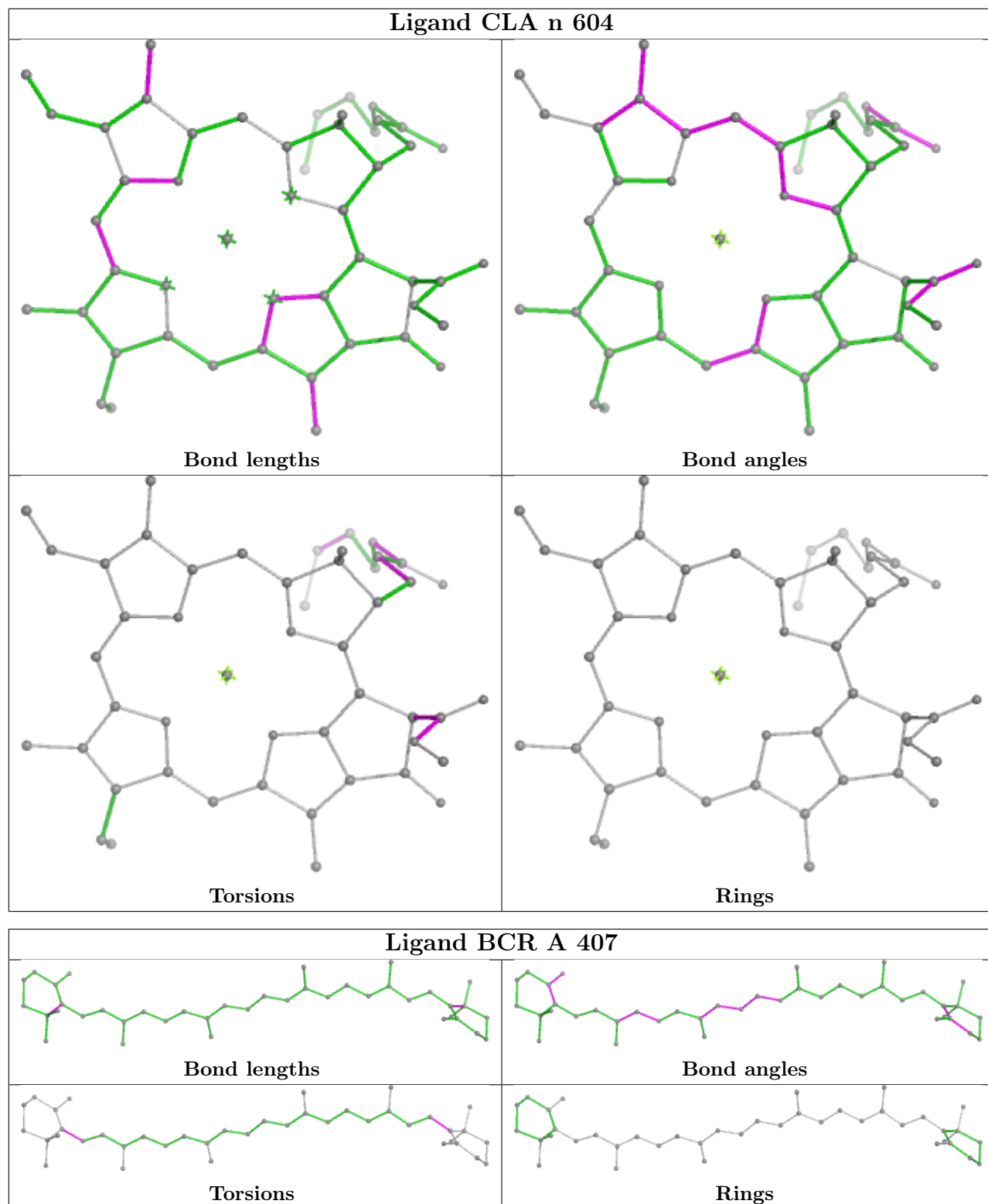


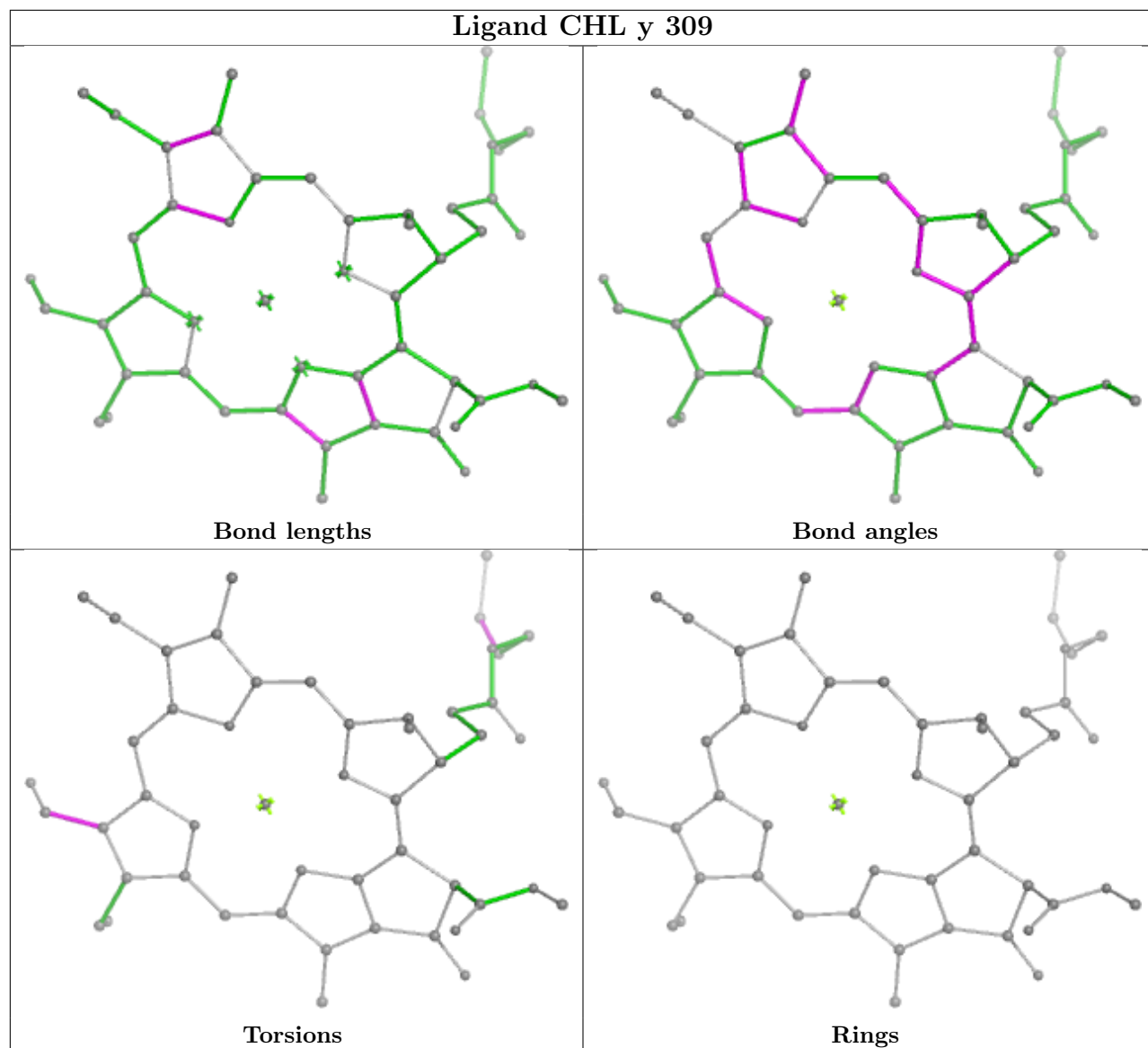


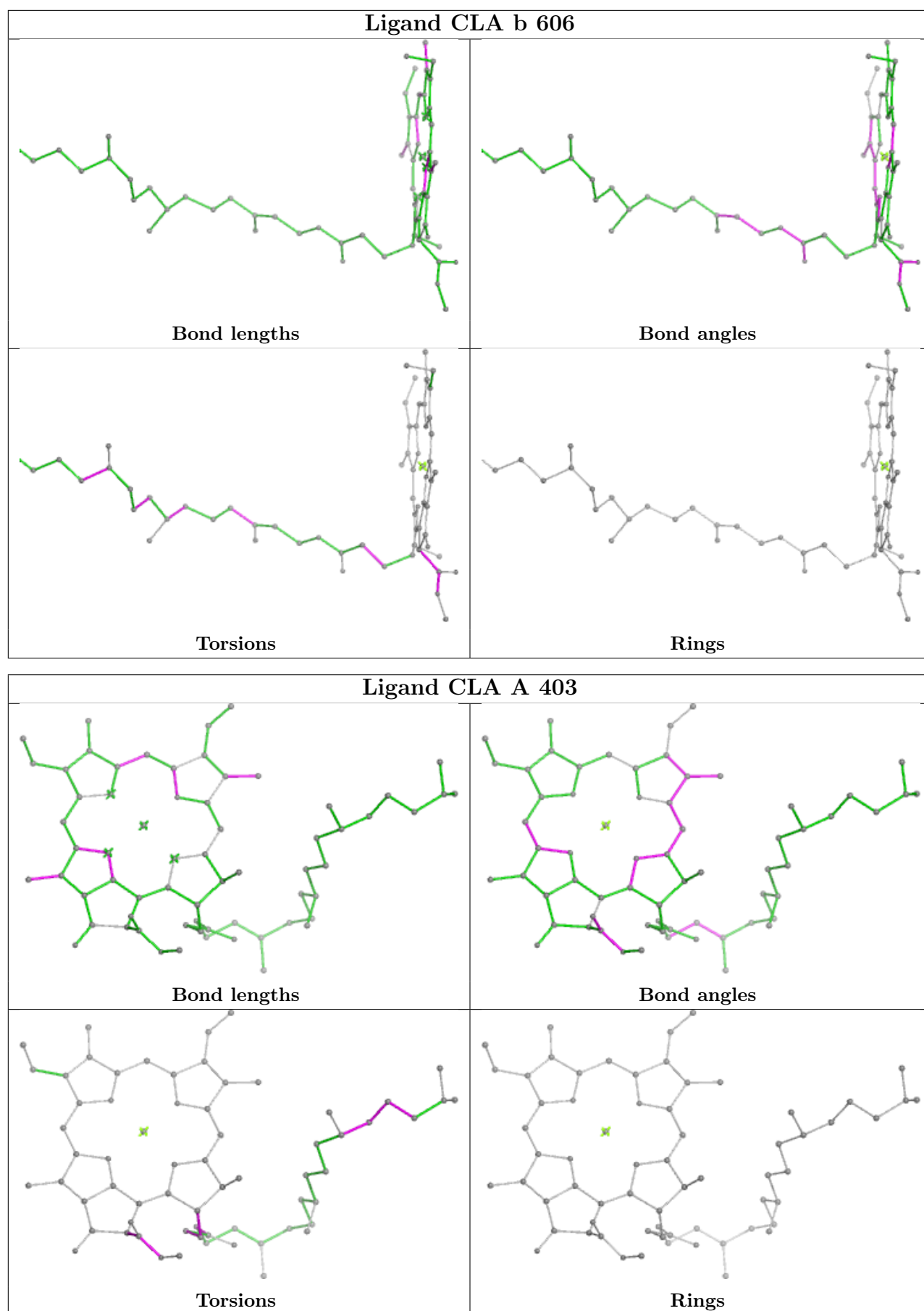


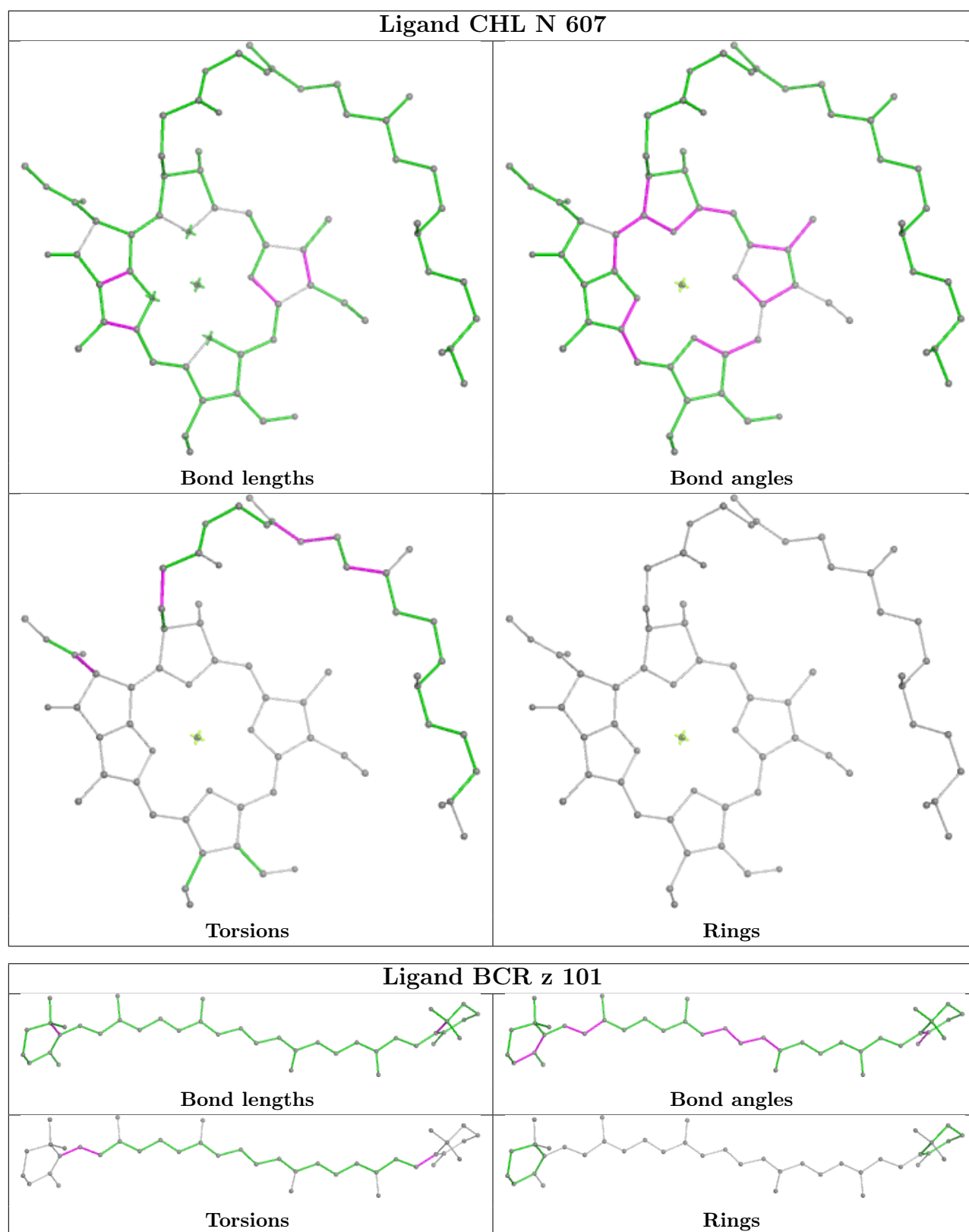


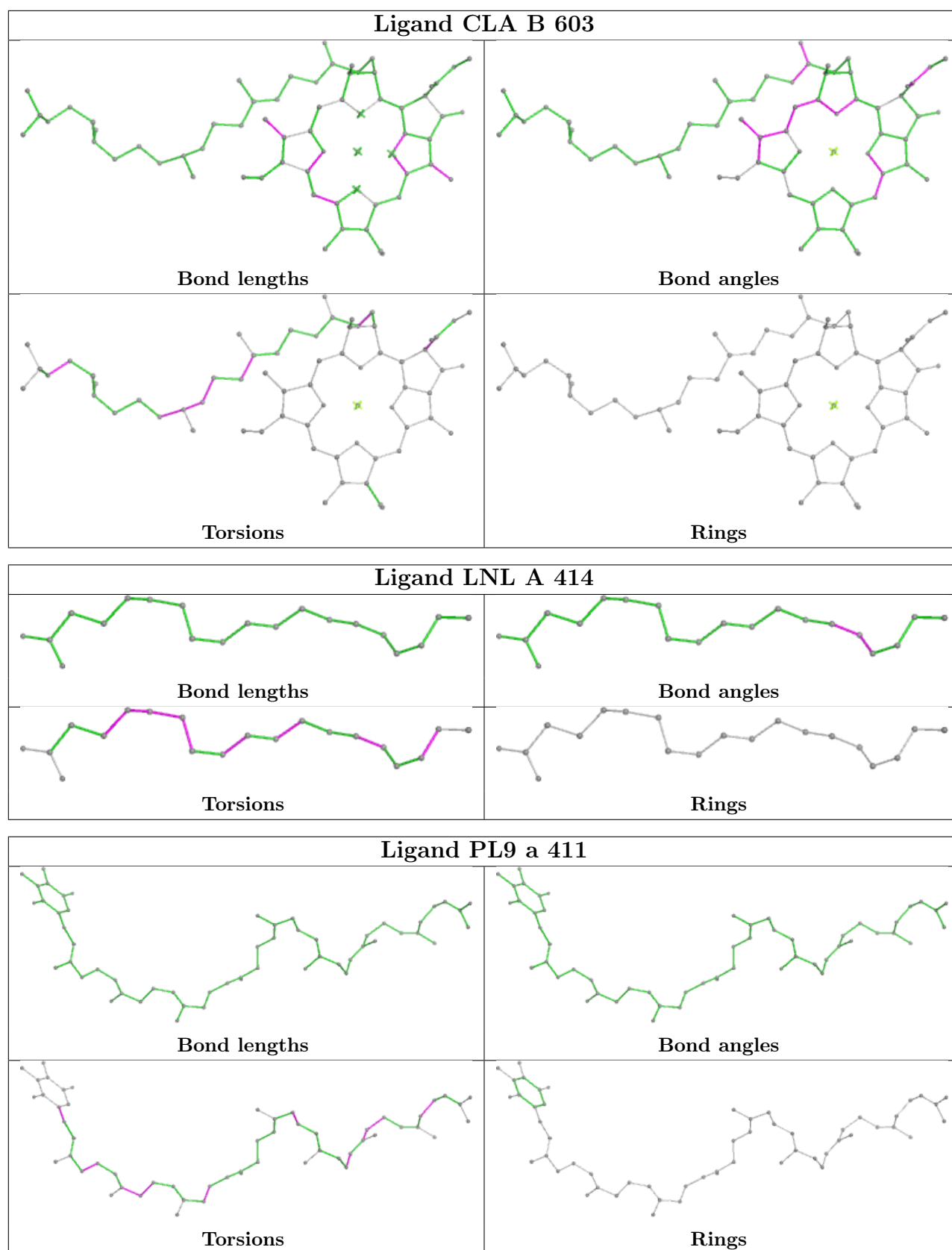


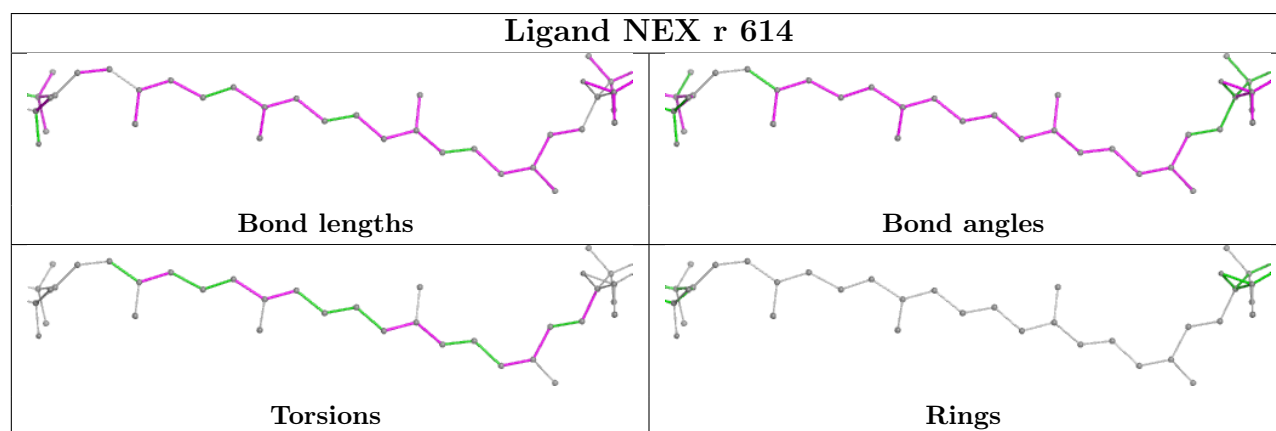
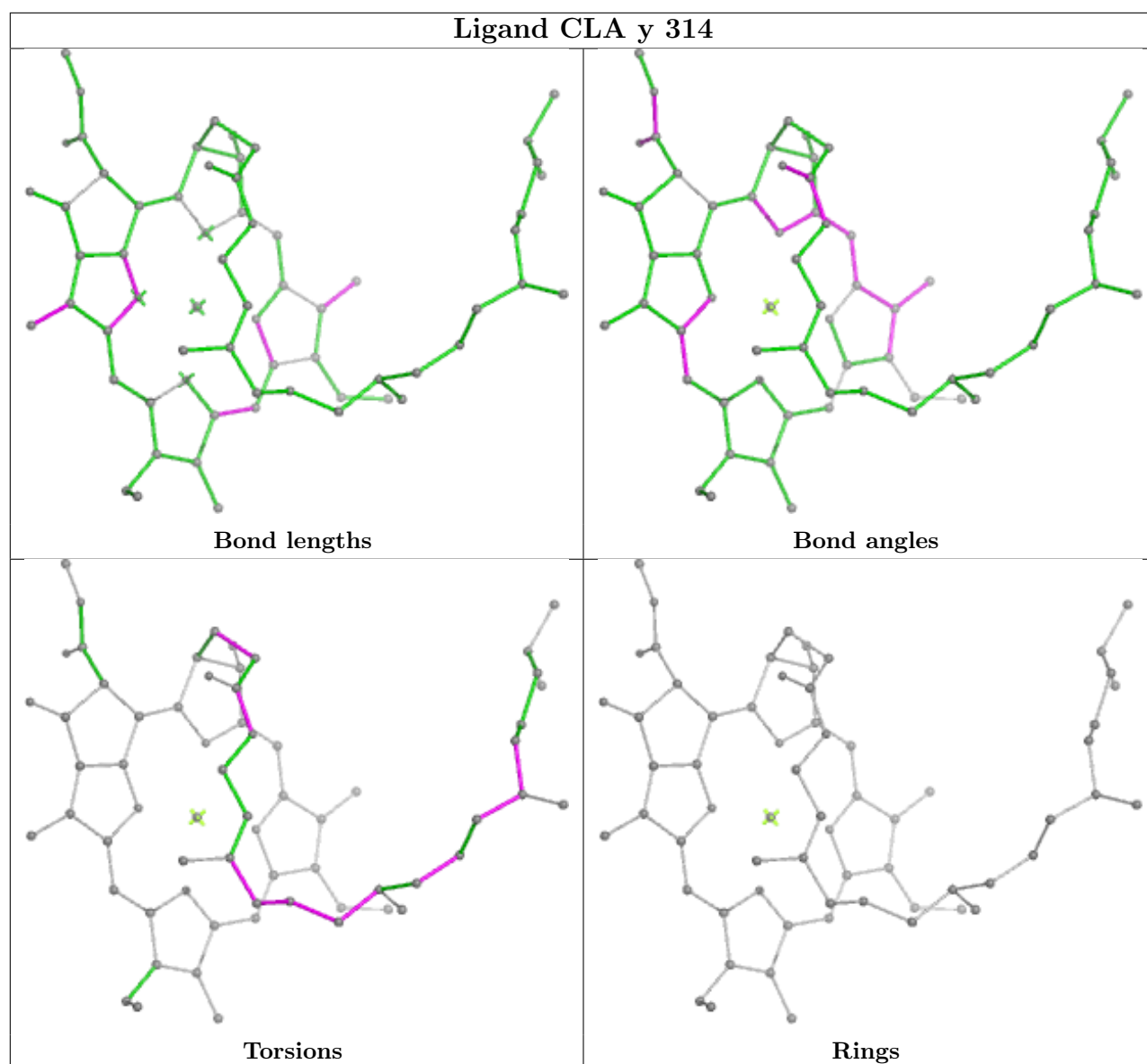


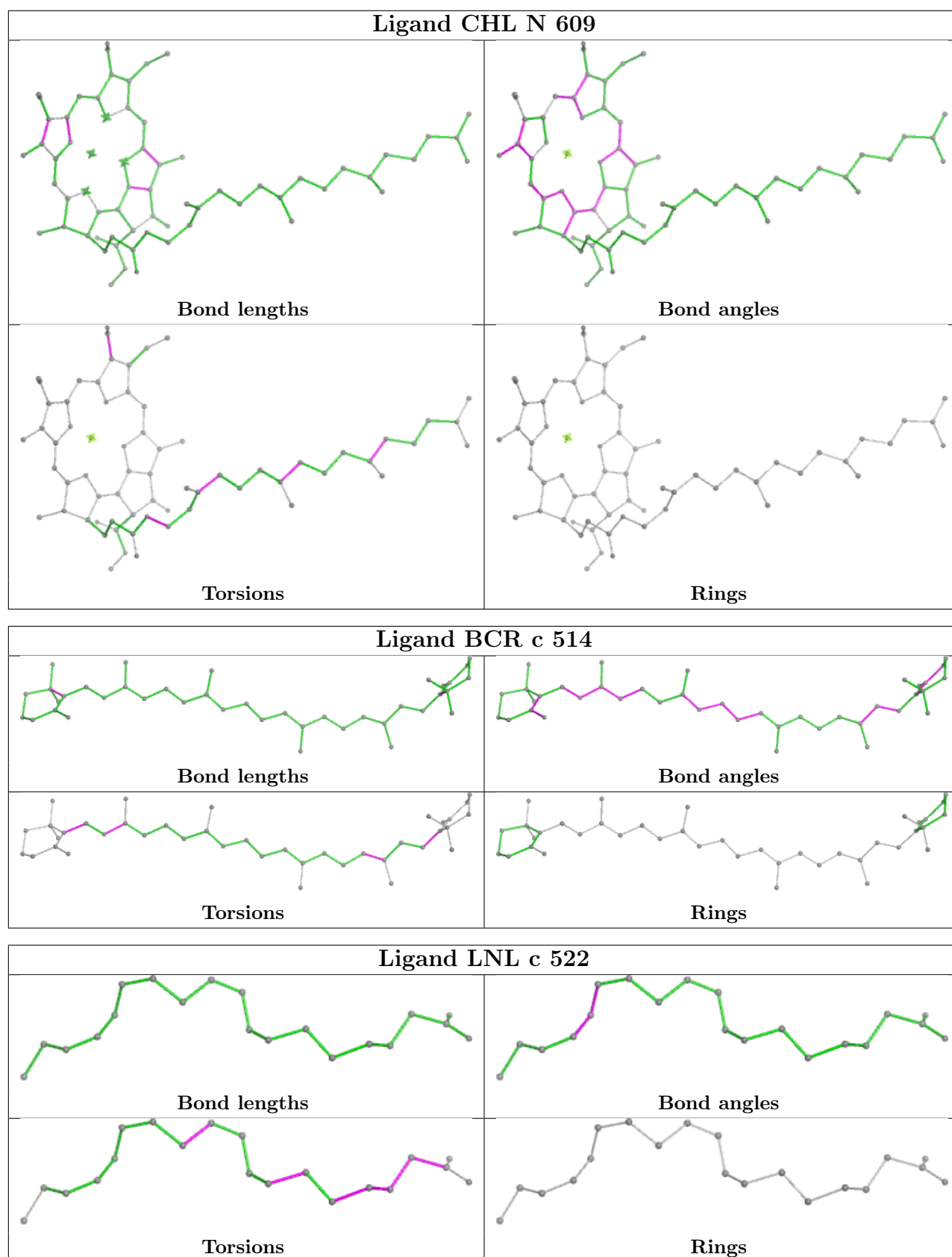












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



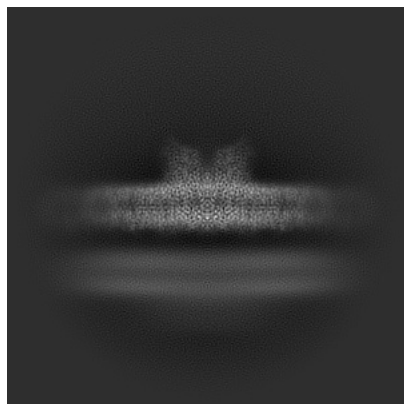
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16389. These allow visual inspection of the internal detail of the map and identification of artifacts.

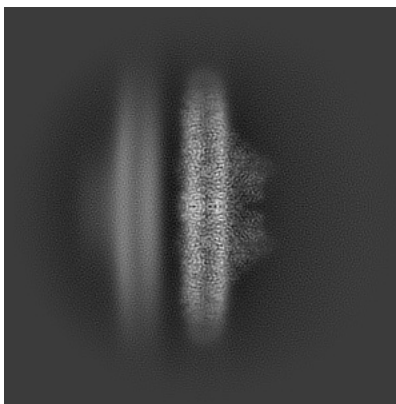
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

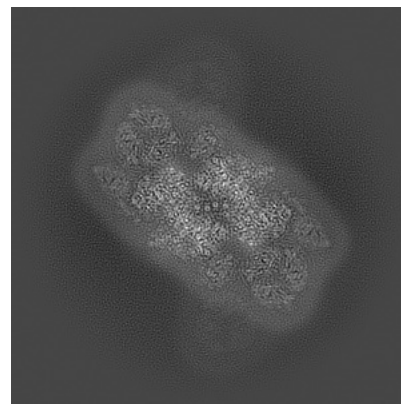
#### 6.1.1 Primary map



X

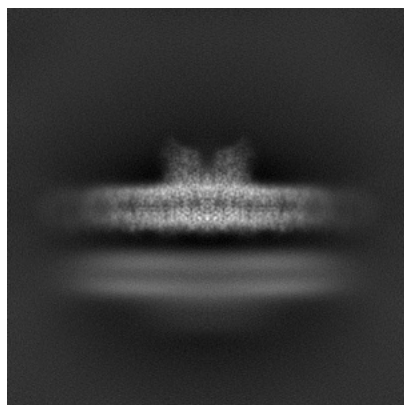


Y

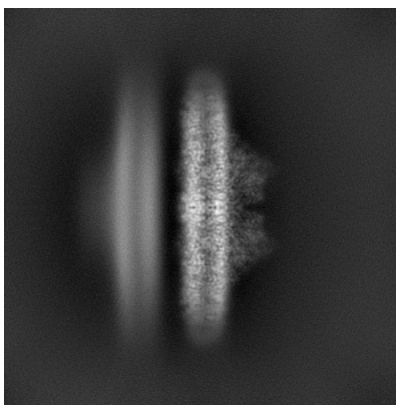


Z

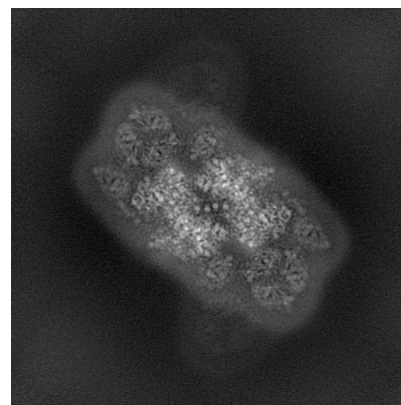
#### 6.1.2 Raw map



X



Y

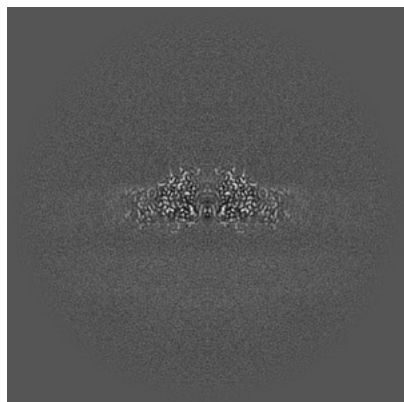


Z

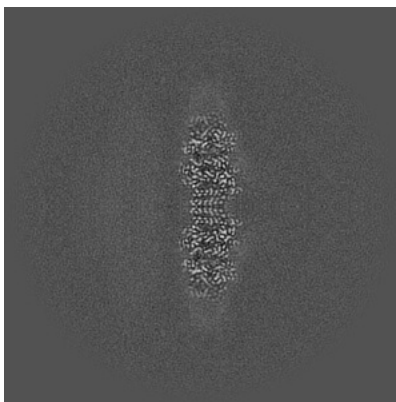
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

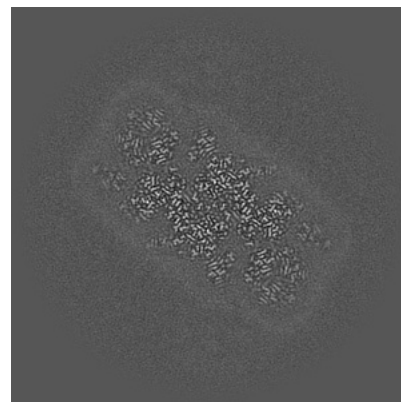
### 6.2.1 Primary map



X Index: 224

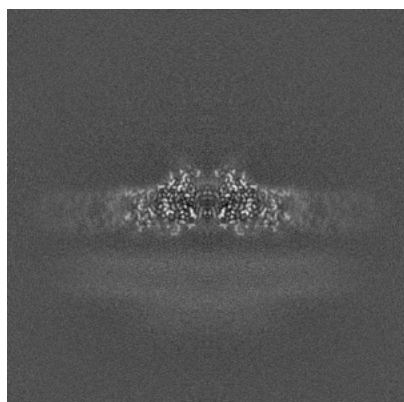


Y Index: 224

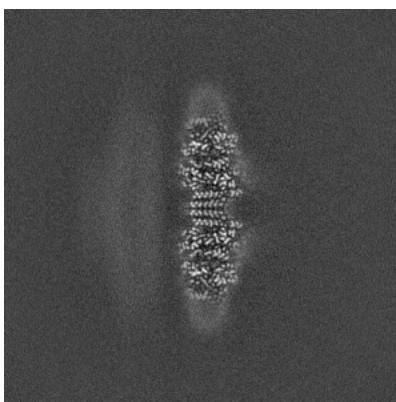


Z Index: 224

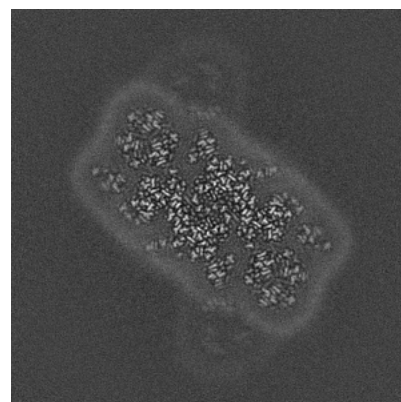
### 6.2.2 Raw map



X Index: 224



Y Index: 224

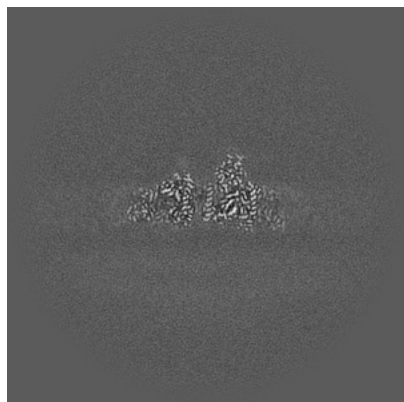


Z Index: 224

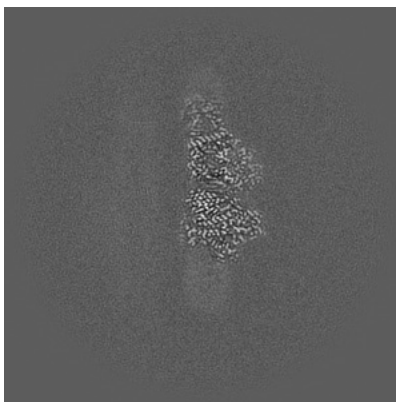
The images above show central slices of the map in three orthogonal directions.

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

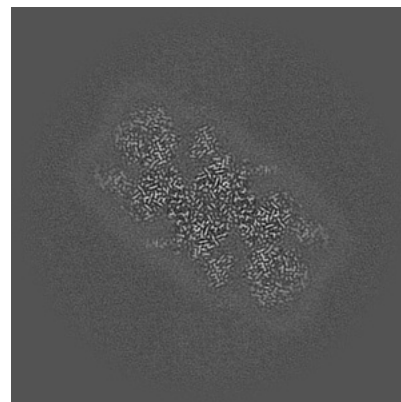
### 6.3.1 Primary map



X Index: 230

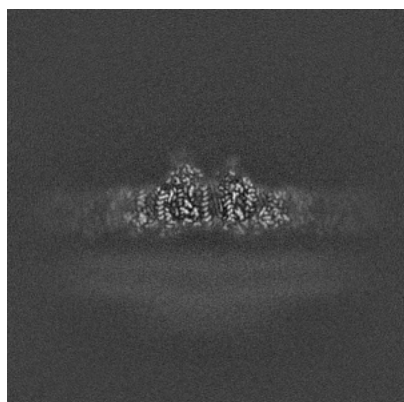


Y Index: 200

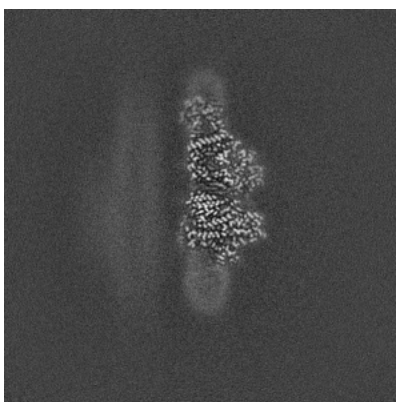


Z Index: 218

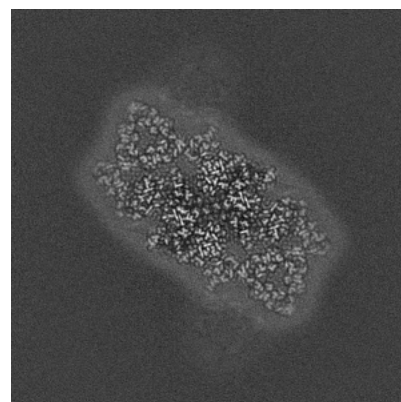
### 6.3.2 Raw map



X Index: 221



Y Index: 200

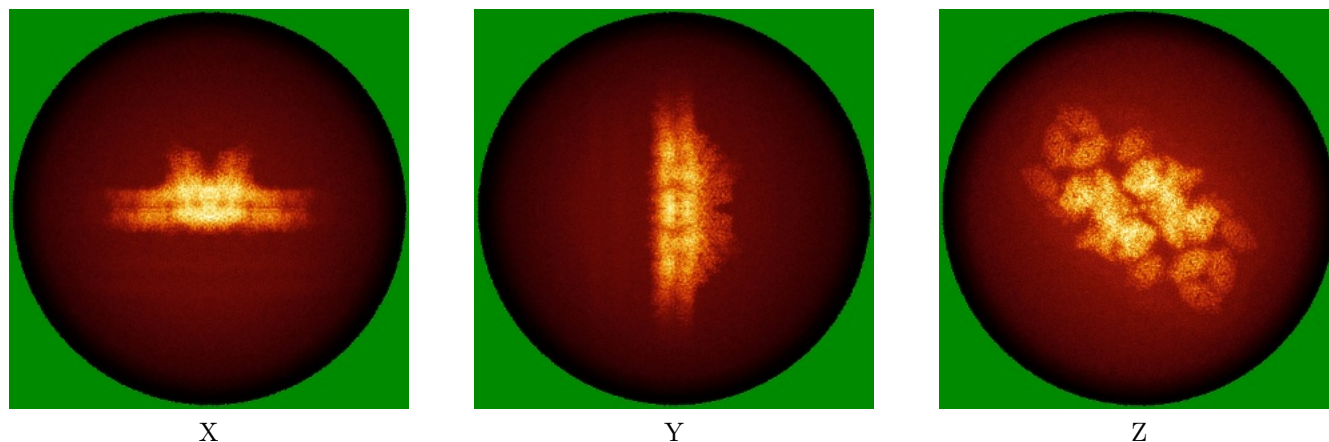


Z Index: 239

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

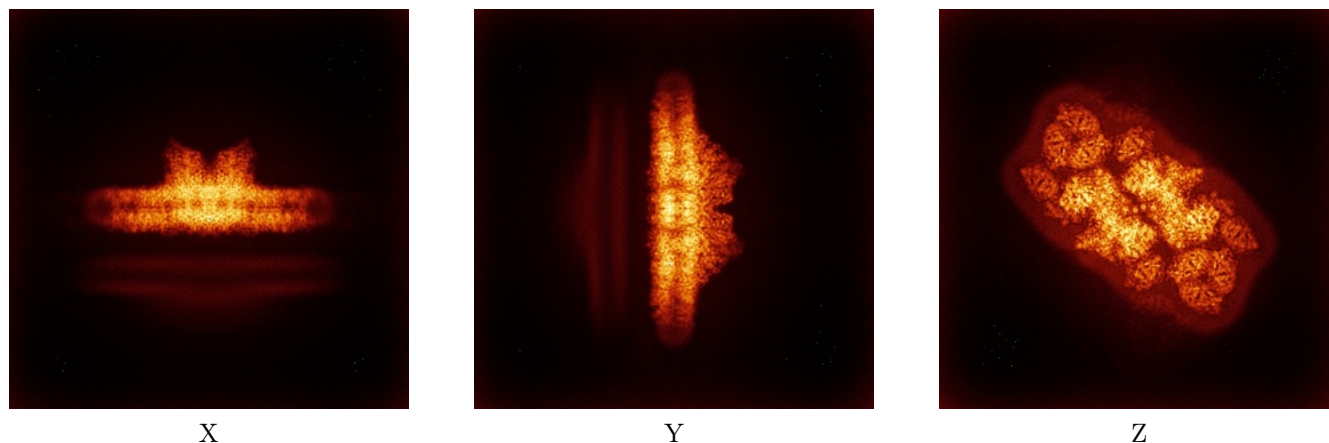


X

Y

Z

### 6.4.2 Raw map



X

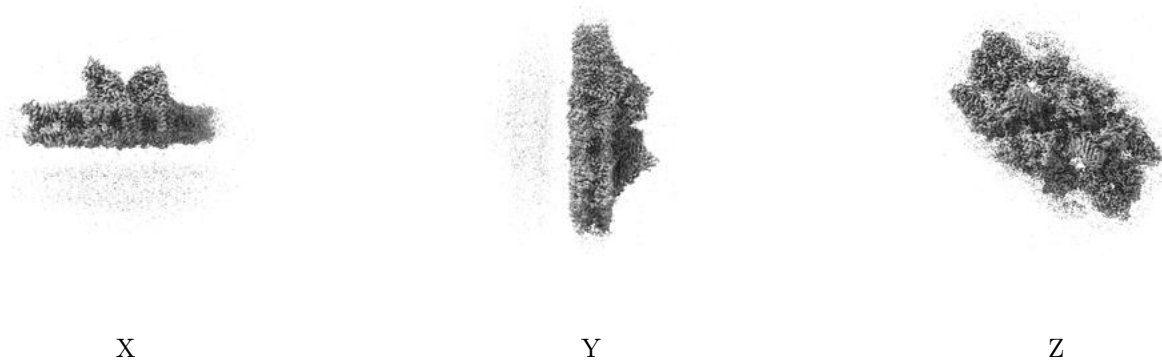
Y

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 0.886. 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.

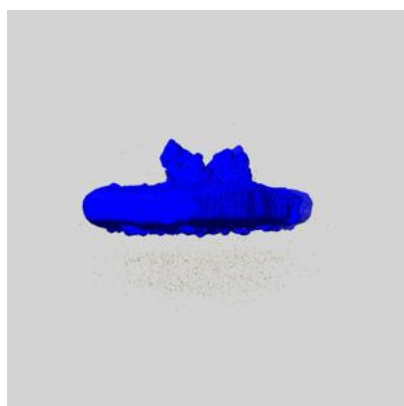
## 6.6 Mask visualisation [i](#)

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

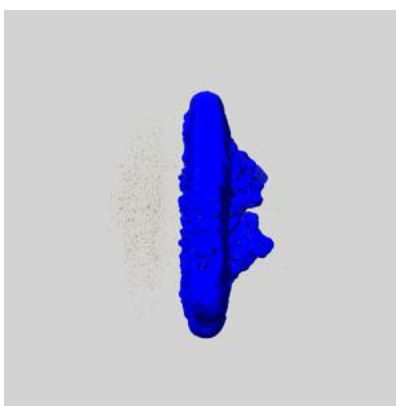
A mask typically either:

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

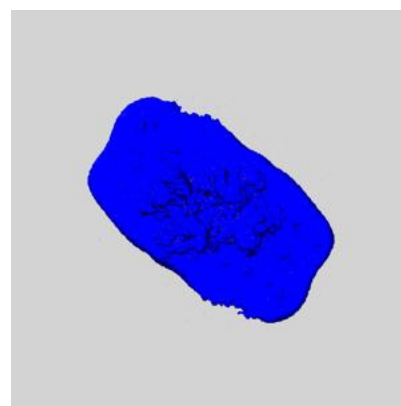
### 6.6.1 emd\_16389\_msk\_1.map [i](#)



X



Y

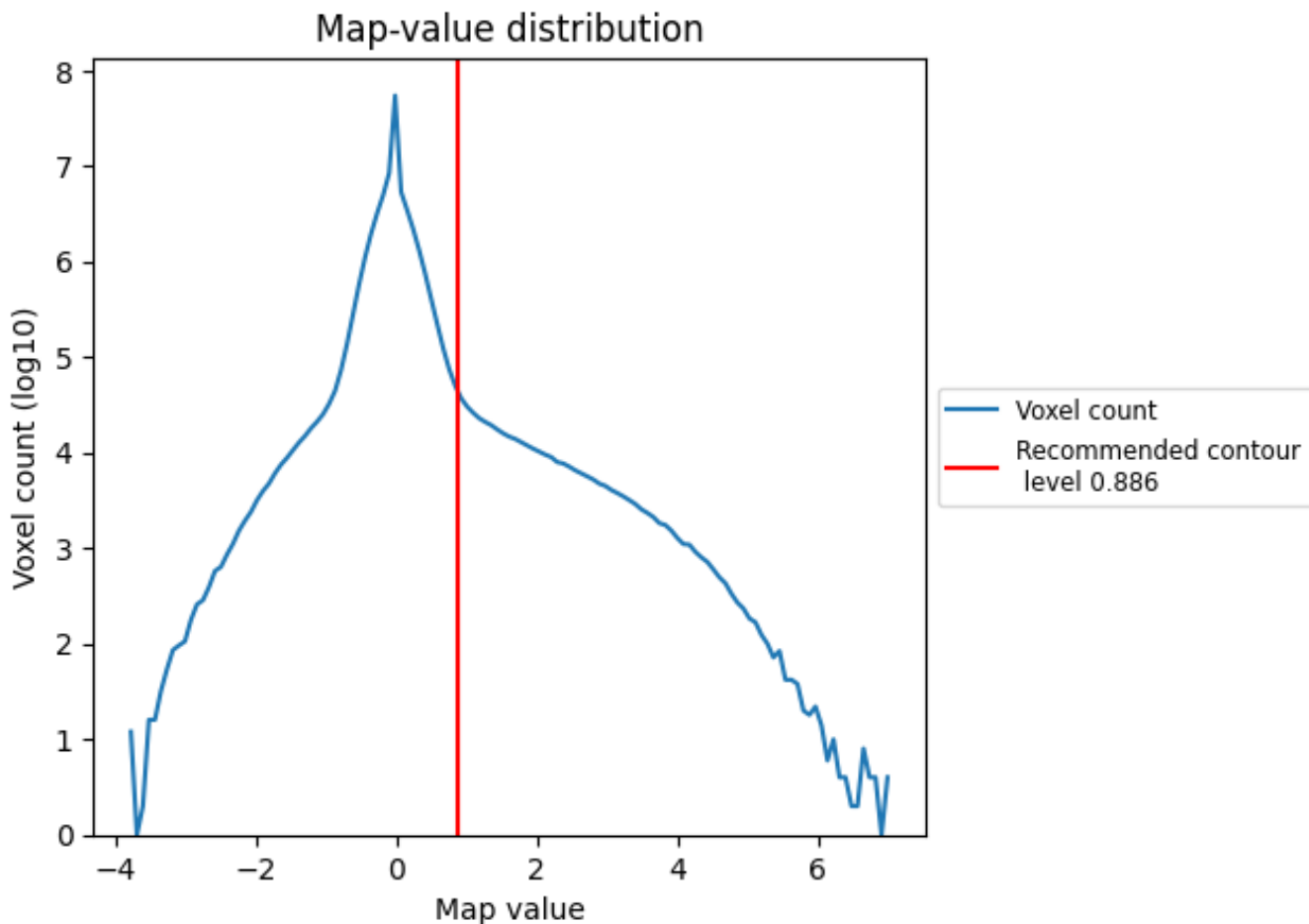


Z

## 7 Map analysis [i](#)

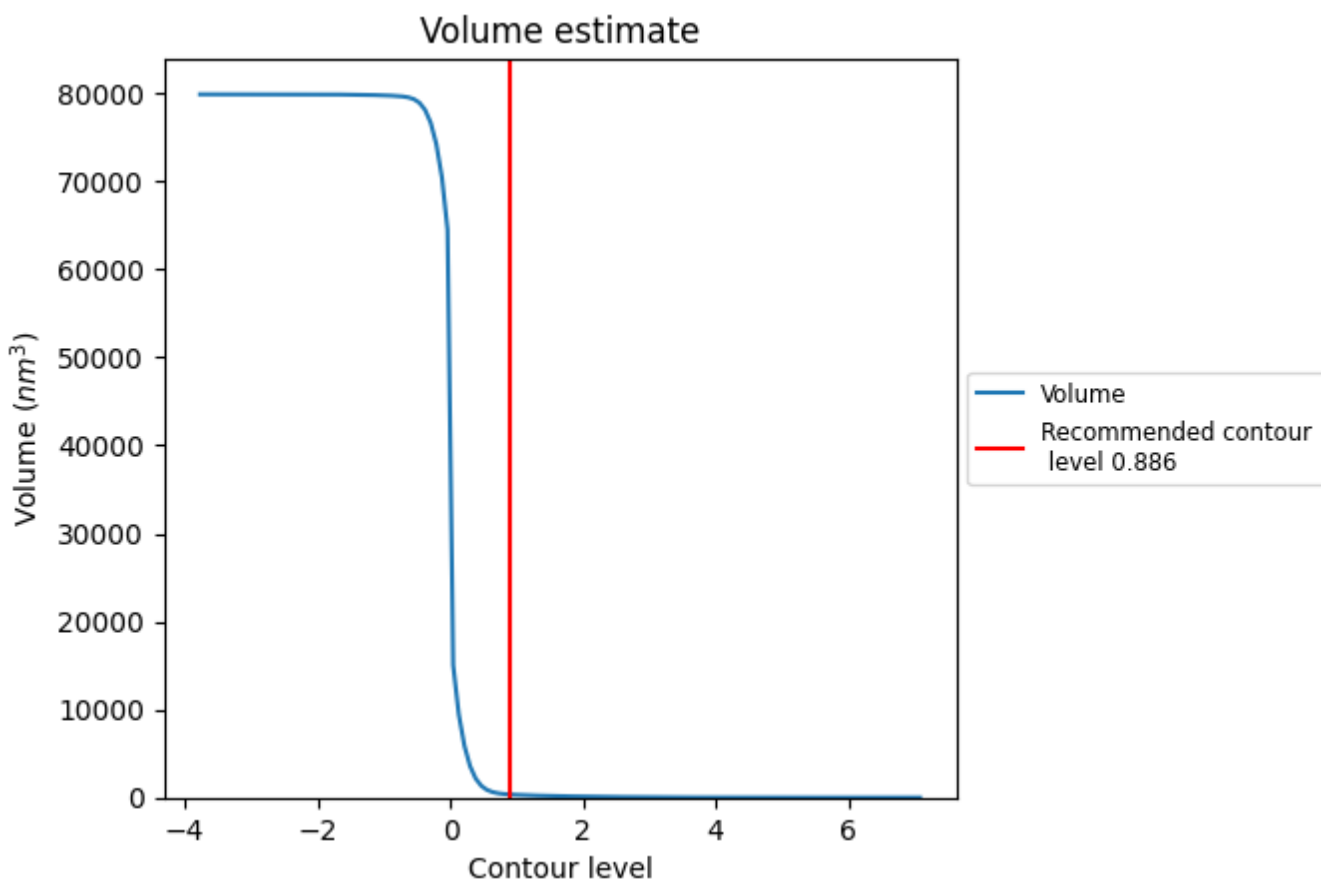
This section contains the results of statistical analysis of the map.

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



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

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

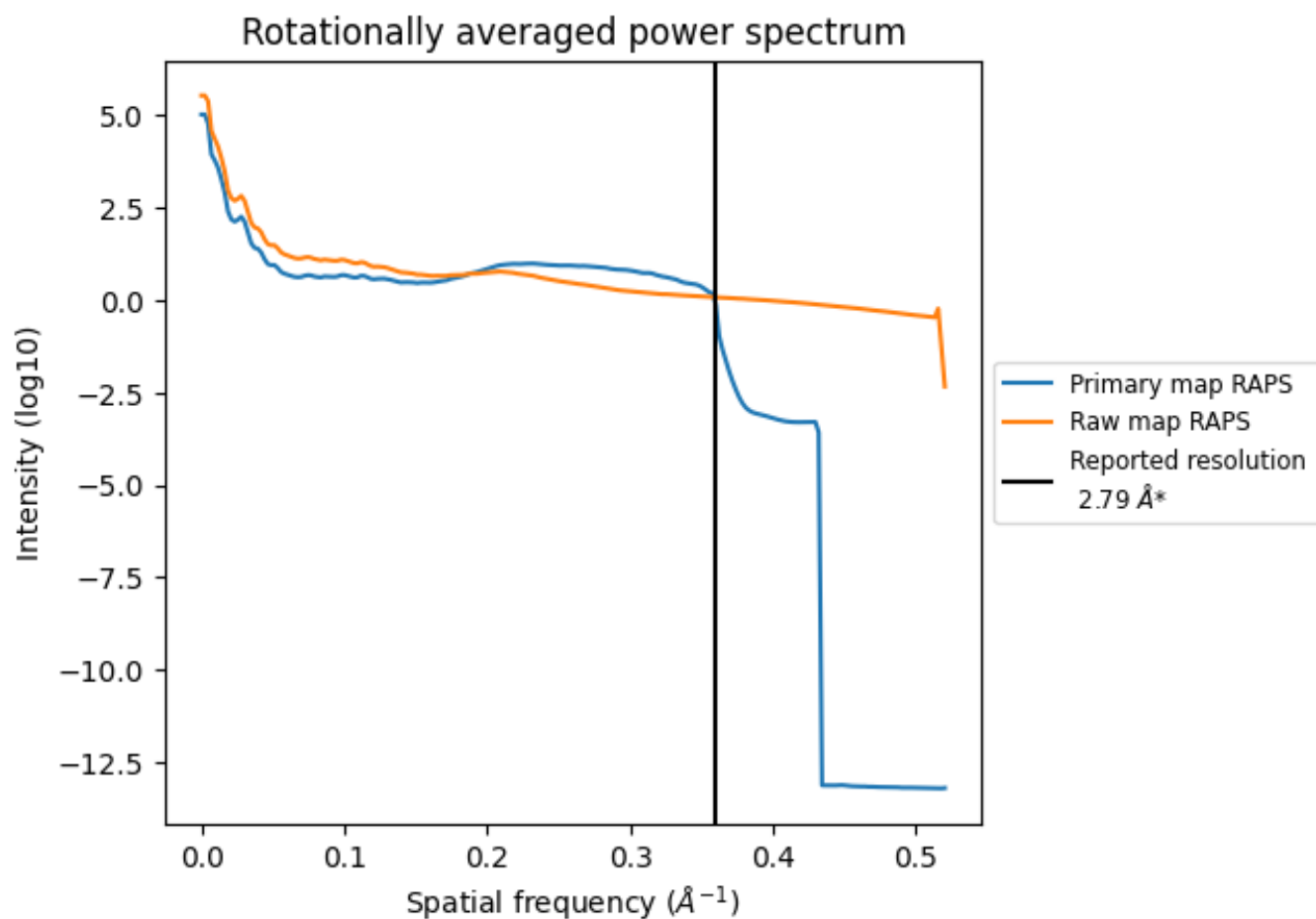


The volume at the recommended contour level is 356 nm<sup>3</sup>; this corresponds to an approximate mass of 322 kDa.

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](#)

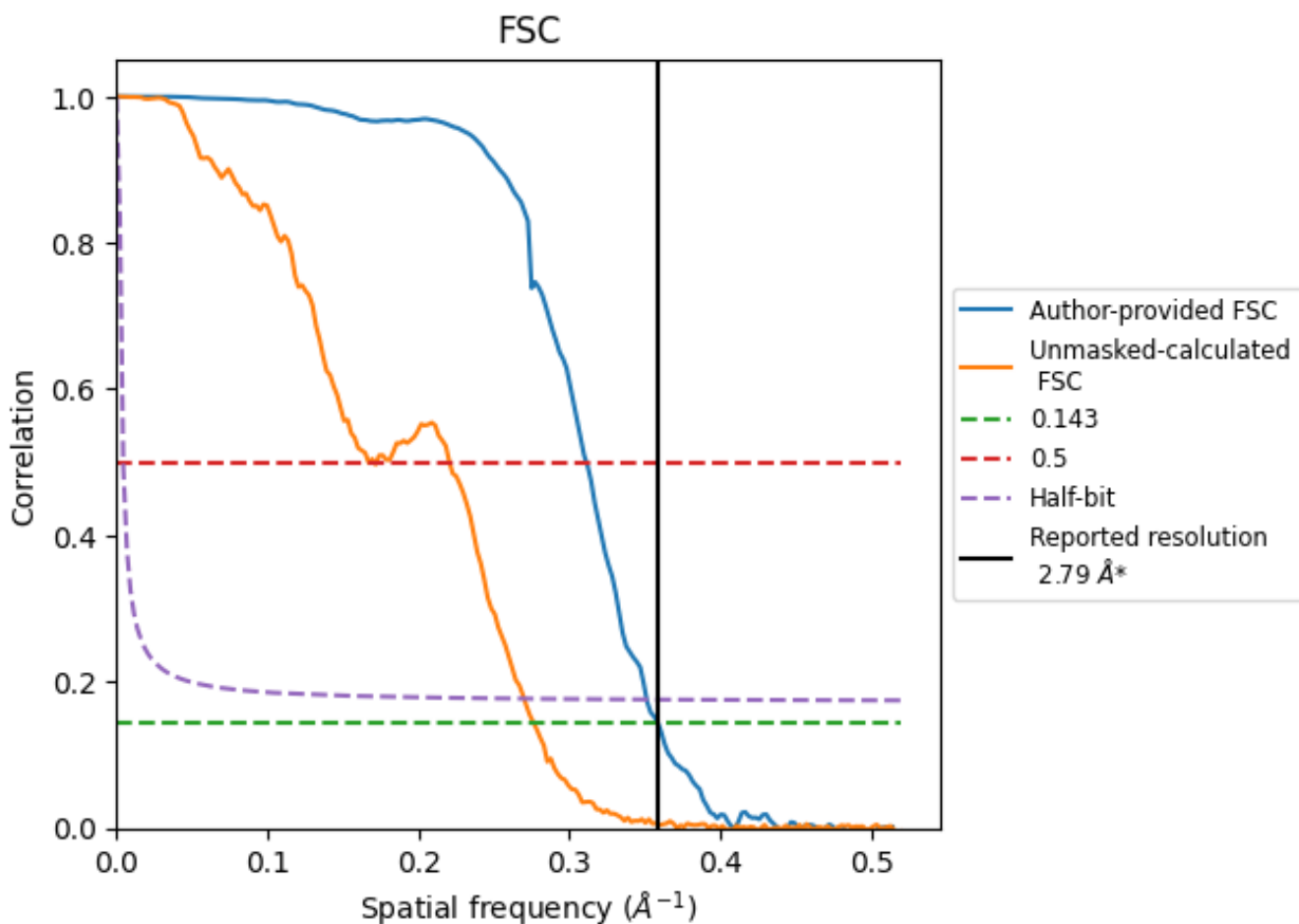


\*Reported resolution corresponds to spatial frequency of 0.359 Å<sup>-1</sup>

## 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 0.359 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

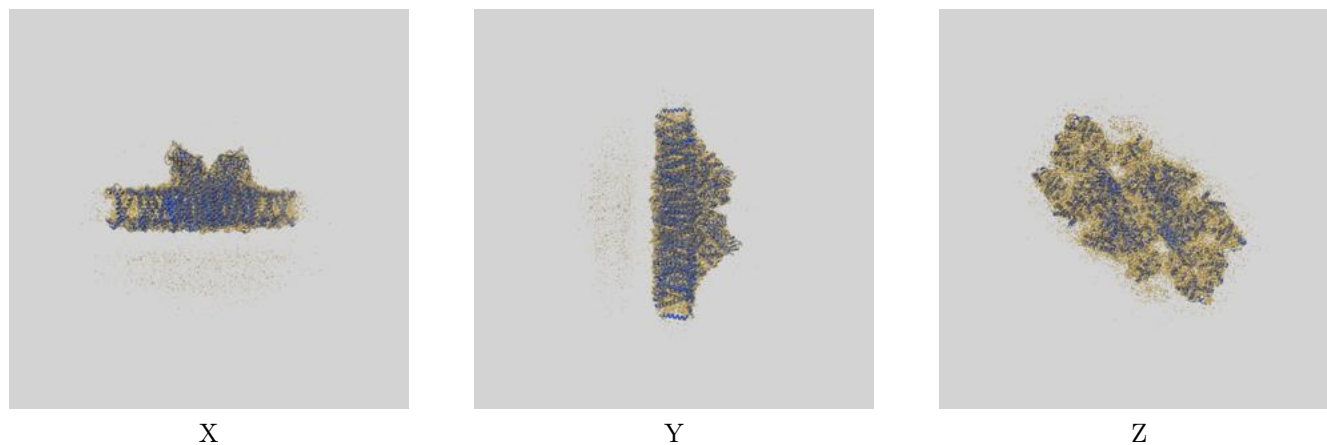
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.21	2.84
Unmasked-calculated*	3.62	5.99	3.70

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.62 differs from the reported value 2.785 by more than 10 %

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

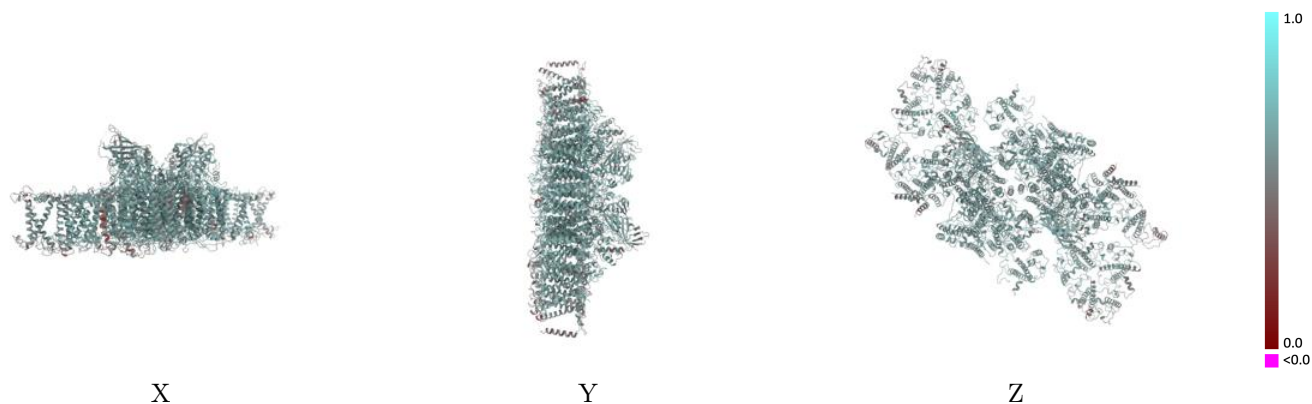
This section contains information regarding the fit between EMDB map EMD-16389 and PDB model 8C29. Per-residue inclusion information can be found in section [3](#) on page [46](#).

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



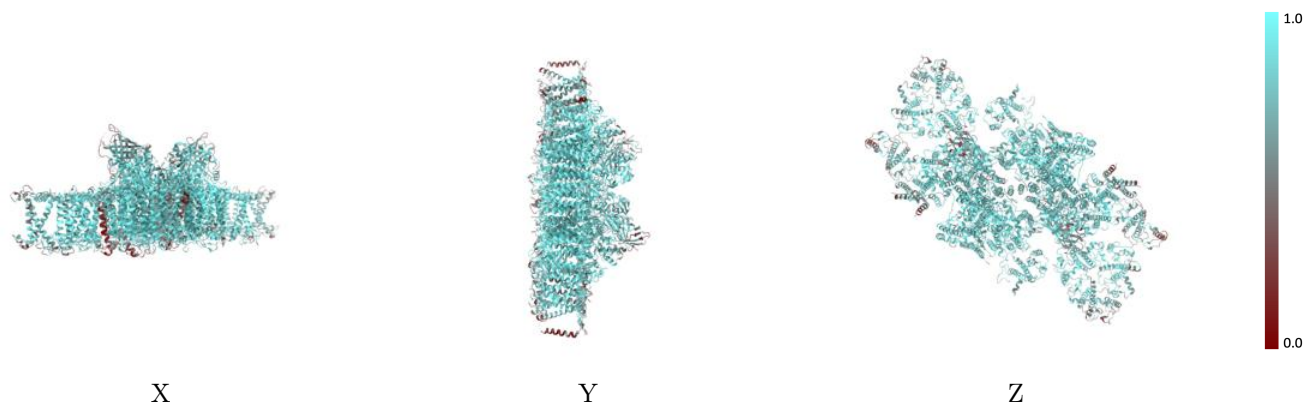
The images above show the 3D surface view of the map at the recommended contour level 0.886 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



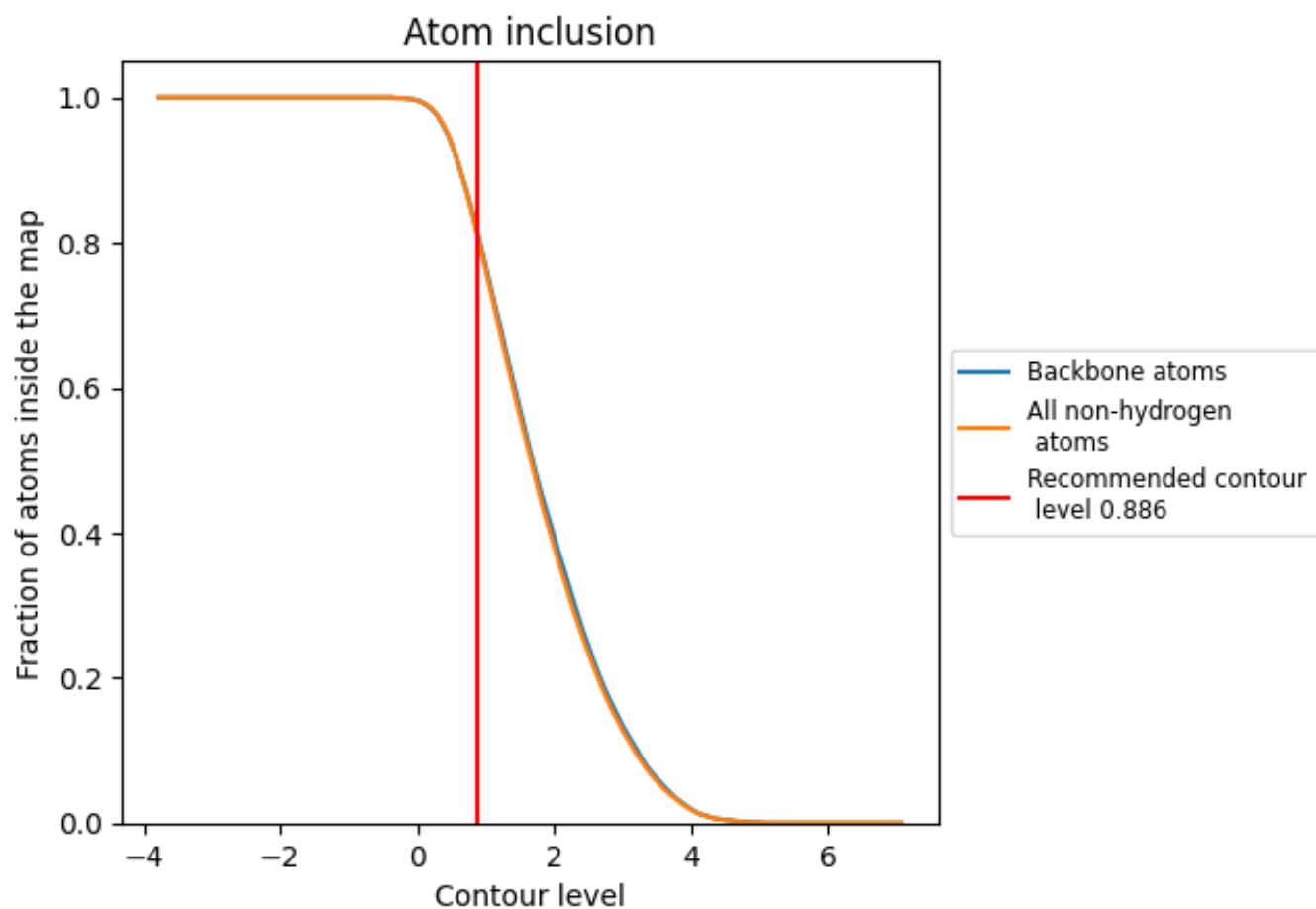
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.886).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.886) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.5940
A	 0.8960	 0.6280
B	 0.9040	 0.6220
C	 0.8840	 0.6170
D	 0.8970	 0.6250
E	 0.7820	 0.5800
F	 0.7590	 0.5570
G	 0.6900	 0.5490
H	 0.8960	 0.6190
I	 0.8810	 0.6120
K	 0.8250	 0.5820
L	 0.8480	 0.6220
M	 0.8080	 0.5920
N	 0.7500	 0.5650
O	 0.6380	 0.5610
R	 0.7710	 0.5880
S	 0.6040	 0.5240
T	 0.7910	 0.6000
U	 0.6850	 0.5800
V	 0.4960	 0.5000
W	 0.7230	 0.5730
X	 0.7600	 0.5730
Y	 0.8680	 0.6120
Z	 0.6150	 0.5390
a	 0.8970	 0.6240
b	 0.9010	 0.6240
c	 0.8870	 0.6170
d	 0.8980	 0.6270
e	 0.7940	 0.5770
f	 0.7550	 0.5620
g	 0.6830	 0.5500
h	 0.8930	 0.6200
i	 0.8720	 0.6050
k	 0.8250	 0.5830
l	 0.8920	 0.6190



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
m	 0.8140	 0.6030
n	 0.7440	 0.5620
o	 0.6360	 0.5600
r	 0.7680	 0.5870
s	 0.6030	 0.5240
t	 0.8170	 0.6110
u	 0.7050	 0.5920
v	 0.5000	 0.5000
w	 0.7360	 0.5810
x	 0.7750	 0.5860
y	 0.8750	 0.6120
z	 0.6050	 0.5330