



wwPDB EM Validation Summary Report ⓘ

Sep 11, 2026 – 07:29 am BST

PDB ID : 8C29 / pdb_00008c29
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

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

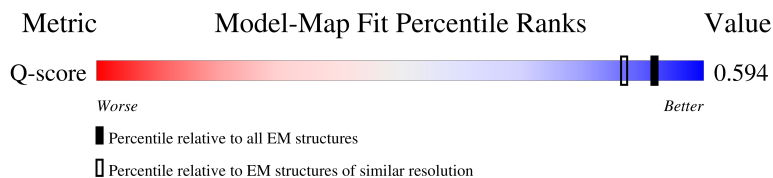
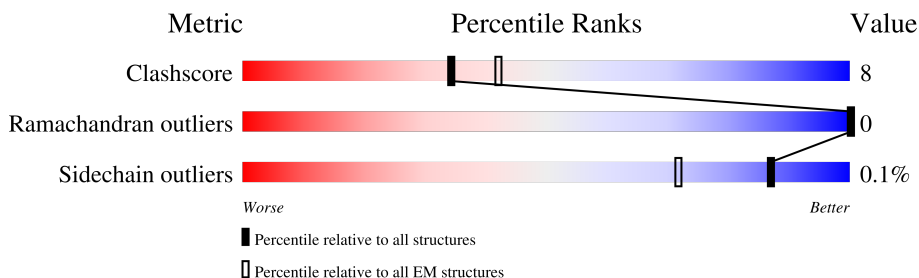
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

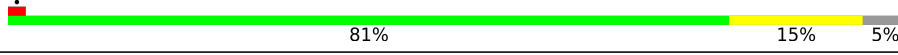
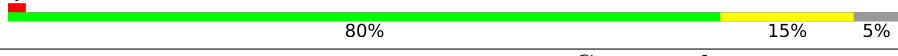
The reported resolution of this entry is 2.79 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10740 (2.29 - 3.28)

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

Mol	Chain	Length	Quality of chain
1	A	353	
1	a	353	
2	B	508	
2	b	508	

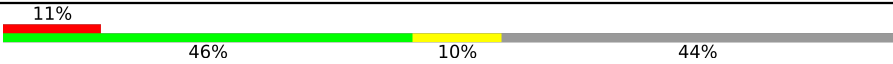
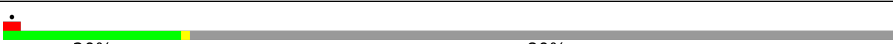
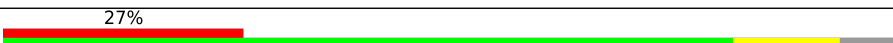
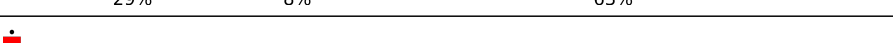
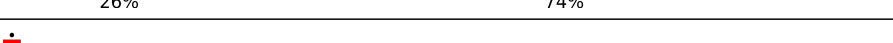
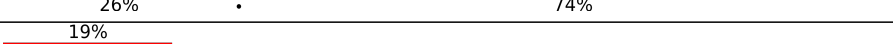
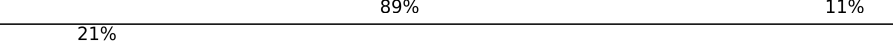
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Mol	Chain	Length	Quality of chain
3	C	473	
3	c	473	
4	D	353	
4	d	353	
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	G	275	
7	N	275	
7	Y	275	
7	g	275	
7	n	275	
7	y	275	
8	H	75	
8	h	75	
9	I	36	
9	i	36	
10	K	59	
10	k	59	
11	L	38	
11	l	38	
12	M	37	
12	m	37	
13	O	341	

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Mol	Chain	Length	Quality of chain
13	o	341	
14	R	300	
14	r	300	
15	S	303	
15	s	303	
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
36	BCT	D	401	-	-	X	-
36	BCT	d	401	-	-	X	-

2 Entry composition

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
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
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
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
4	D	337	Total	C	N	O	S	0	0
			2686	1781	439	455	11		
4	d	337	Total	C	N	O	S	0	0
			2685	1781	439	454	11		

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
5	E	65	Total	C	N	O	0	0
			537	353	84	100		
5	e	65	Total	C	N	O	0	0
			537	353	84	100		

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

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

- 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 A9NKKX0
R	56	ALA	-	insertion	UNP A9NKKX0
R	57	VAL	-	insertion	UNP A9NKKX0
R	58	ALA	-	insertion	UNP A9NKKX0
R	59	LYS	-	insertion	UNP A9NKKX0
R	60	PRO	-	insertion	UNP A9NKKX0
R	61	LYS	-	insertion	UNP A9NKKX0
R	62	THR	-	insertion	UNP A9NKKX0
R	63	LYS	-	insertion	UNP A9NKKX0
R	64	ALA	-	insertion	UNP A9NKKX0
R	65	VAL	-	insertion	UNP A9NKKX0
R	66	ALA	-	insertion	UNP A9NKKX0
R	67	LYS	-	insertion	UNP A9NKKX0
r	54	THR	PRO	conflict	UNP A9NKKX0
r	56	ALA	-	insertion	UNP A9NKKX0
r	57	VAL	-	insertion	UNP A9NKKX0
r	58	ALA	-	insertion	UNP A9NKKX0
r	59	LYS	-	insertion	UNP A9NKKX0
r	60	PRO	-	insertion	UNP A9NKKX0
r	61	LYS	-	insertion	UNP A9NKKX0
r	62	THR	-	insertion	UNP A9NKKX0

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Chain	Residue	Modelled	Actual	Comment	Reference
r	63	LYS	-	insertion	UNP A9NKKX0
r	64	ALA	-	insertion	UNP A9NKKX0
r	65	VAL	-	insertion	UNP A9NKKX0
r	66	ALA	-	insertion	UNP A9NKKX0
r	67	LYS	-	insertion	UNP A9NKKX0

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

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

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
16	T	31	Total	C	N	O	S	0	0
			254	177	36	40	1		
16	t	31	Total	C	N	O	S	0	0
			254	177	36	40	1		

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

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

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

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

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

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

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

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
20	X	34	Total	C	N	O	0	0
			226	146	37	43		
20	x	34	Total	C	N	O	0	0
			226	146	37	43		

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
21	Z	62	Total	C	N	O	S	0	0
			453	305	68	79	1		
21	z	62	Total	C	N	O	S	0	0
			453	305	68	79	1		

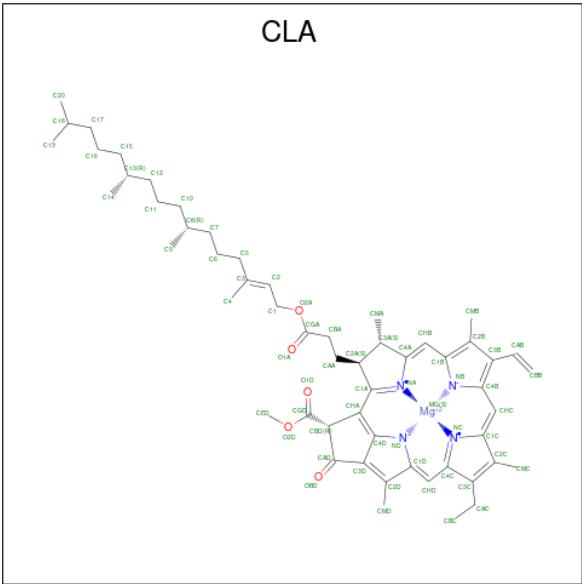
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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

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

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



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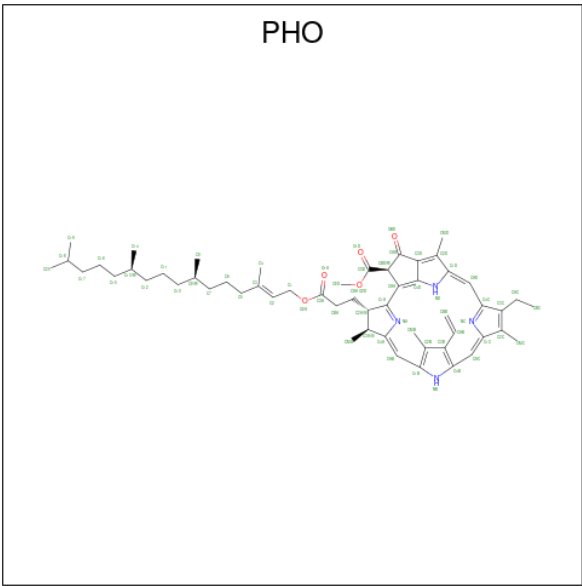
Mol	Chain	Residues	Atoms					AltConf
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total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

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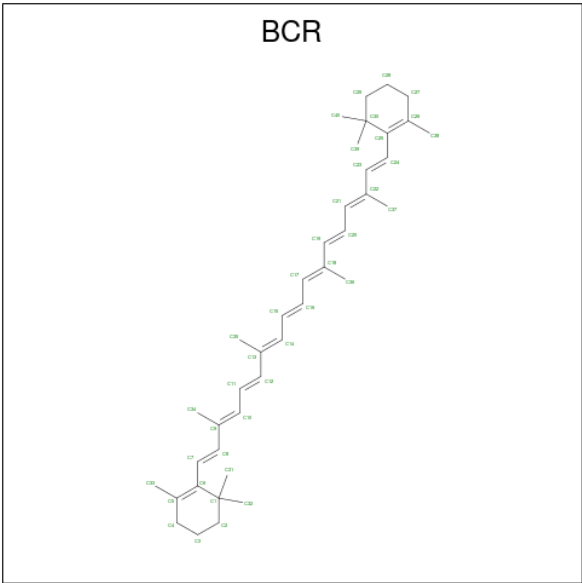
Mol	Chain	Residues	Atoms					AltConf
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 57	C 47	Mg 1	N 4	O 5	0
23	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total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

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



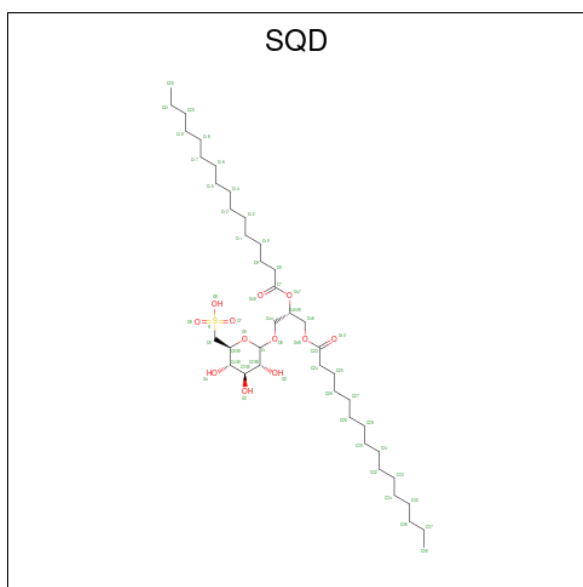
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



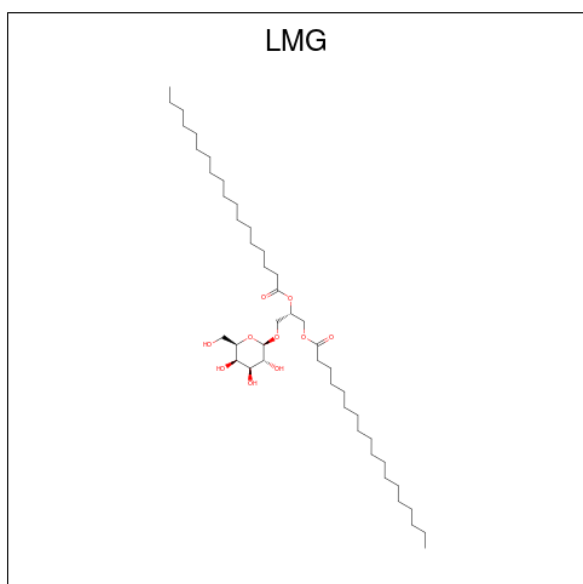
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 39 39	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	H	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	V	1	Total C 40 40	0
25	Z	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 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 (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



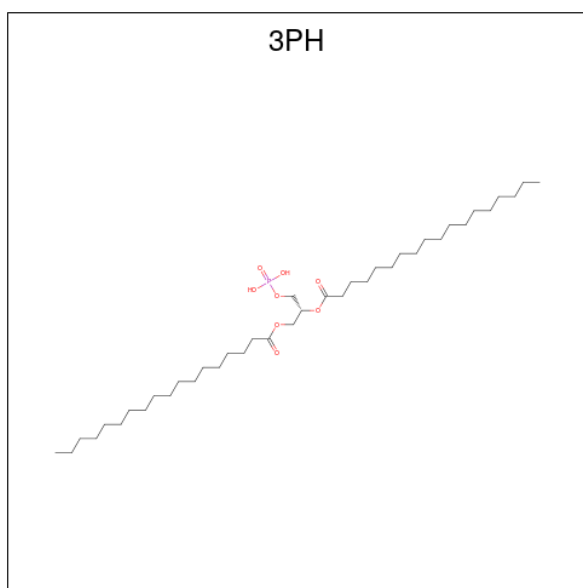
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			50	37	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	
26	M	1	Total	C	O	S	0
			50	37	12	1	
26	a	1	Total	C	O	S	0
			48	35	12	1	

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



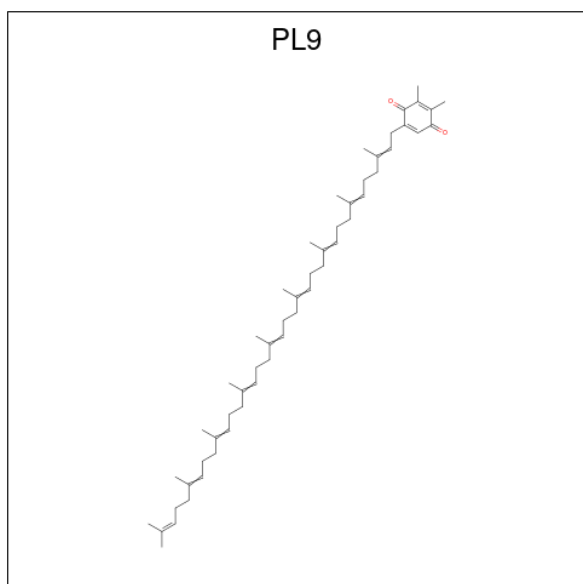
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			53	43	10	
27	B	1	Total	C	O	0
			48	38	10	
27	B	1	Total	C	O	0
			49	39	10	
27	C	1	Total	C	O	0
			45	35	10	
27	D	1	Total	C	O	0
			36	26	10	
27	R	1	Total	C	O	0
			51	41	10	
27	b	1	Total	C	O	0
			51	41	10	
27	b	1	Total	C	O	0
			50	40	10	
27	c	1	Total	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 (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



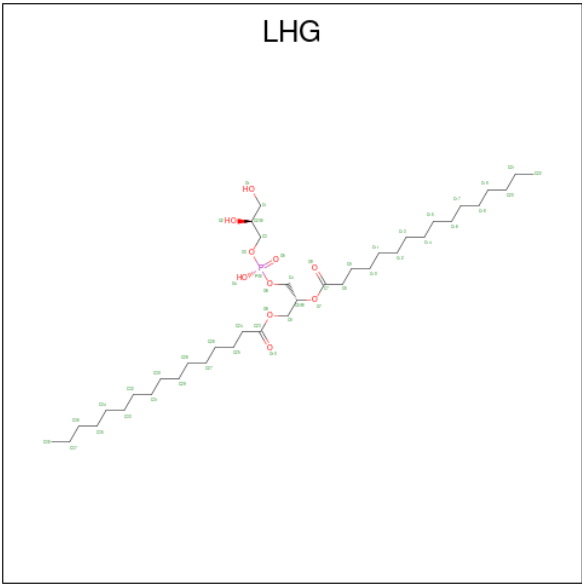
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			48	39	8	1	
28	C	1	Total	C	O	P	0
			48	39	8	1	
28	D	1	Total	C	O	P	0
			38	29	8	1	
28	L	1	Total	C	O	P	0
			41	32	8	1	
28	T	1	Total	C	O	P	0
			48	39	8	1	
28	W	1	Total	C	O	P	0
			46	37	8	1	
28	X	1	Total	C	O	P	0
			46	37	8	1	
28	a	1	Total	C	O	P	0
			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 (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



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

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



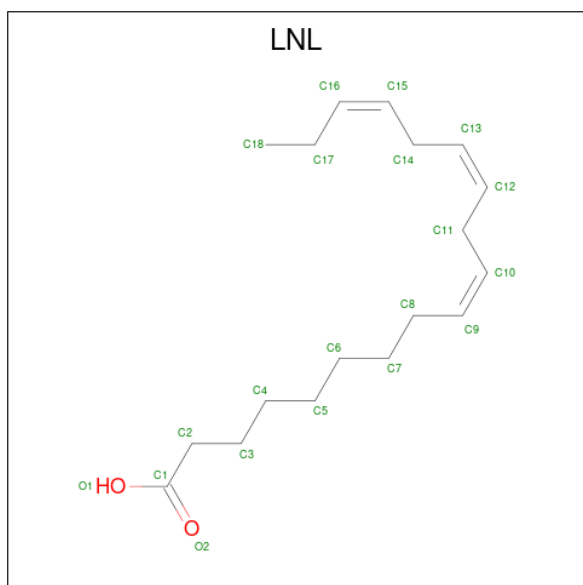
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			37	26	10	1	
30	D	1	Total	C	O	P	0
			43	32	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	G	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	R	1	Total	C	O	P	0
			38	27	10	1	

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Mol	Chain	Residues	Atoms				AltConf
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 (CCD ID: LNL) (formula: $C_{18}H_{30}O_2$).



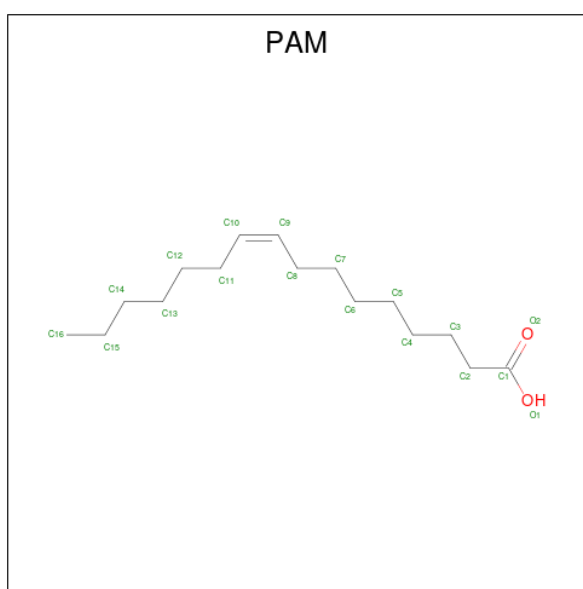
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			20	18	2	
31	A	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0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

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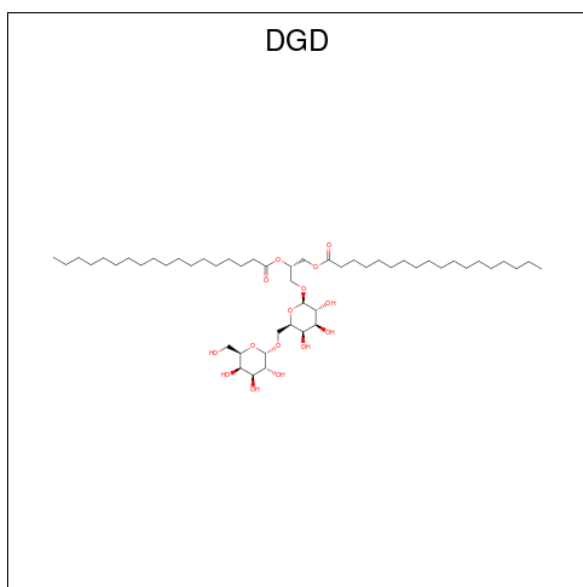
Mol	Chain	Residues	Atoms			AltConf
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	i	1	Total	C	O	0
			20	18	2	

- Molecule 32 is PALMITOLEIC ACID (CCD ID: 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) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

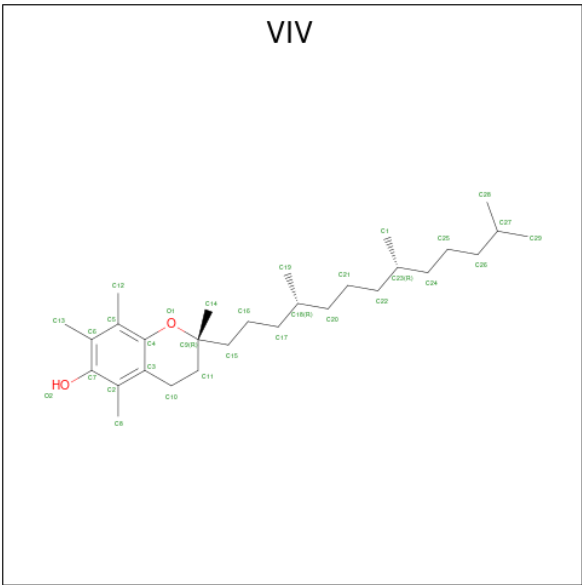


Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			66	51	15	
33	H	1	Total	C	O	0
			62	47	15	
33	c	1	Total	C	O	0
			55	40	15	
33	d	1	Total	C	O	0
			62	47	15	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

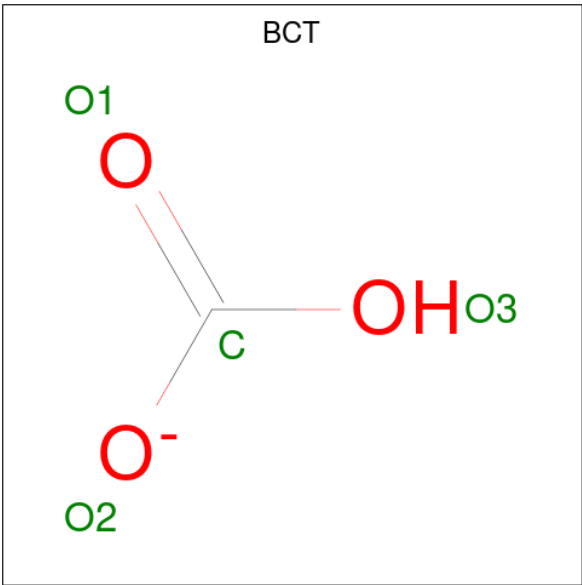
Mol	Chain	Residues	Atoms		AltConf
34	C	1	Total	Mg	0
			1	1	
34	c	1	Total	Mg	0
			1	1	

- Molecule 35 is (2R)-2,5,7,8-TETRAMETHYL-2-[(4R,8R)-4,8,12-TRIMETHYLTRIDECYL]CHROMAN-6-OL (CCD ID: VIV) (formula: C₂₉H₅₀O₂).



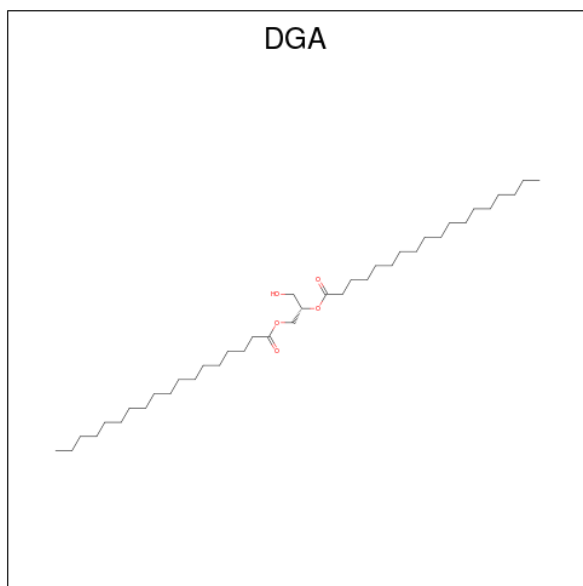
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			31	29	2	
35	y	1	Total	C	O	0
			31	29	2	

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



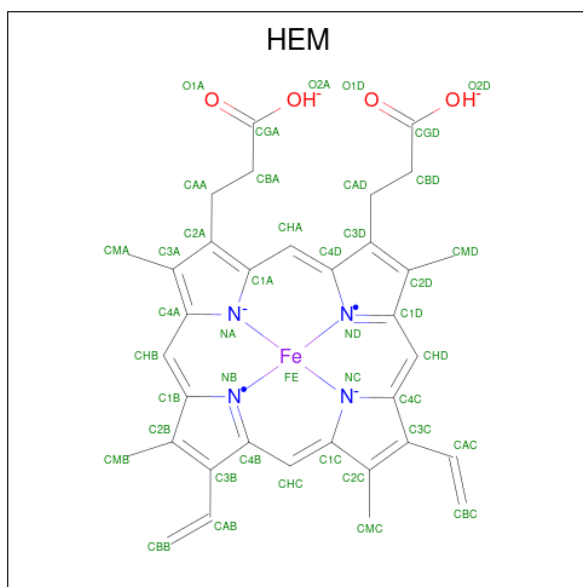
Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total	C	O	0
			4	1	3	
36	d	1	Total	C	O	0
			4	1	3	

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



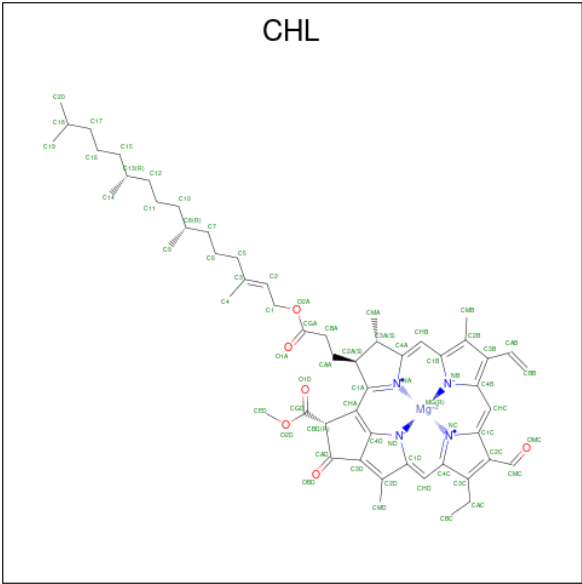
Mol	Chain	Residues	Atoms			AltConf
37	D	1	Total	C	O	0
			40	35	5	
37	b	1	Total	C	O	0
			44	39	5	

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



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

- Molecule 39 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



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

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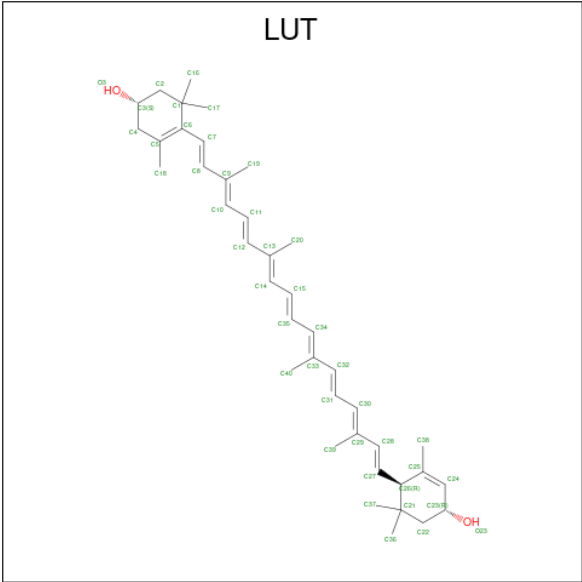
Mol	Chain	Residues	Atoms					AltConf
39	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
39	S	1	Total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

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Mol	Chain	Residues	Atoms					AltConf
39	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
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 (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



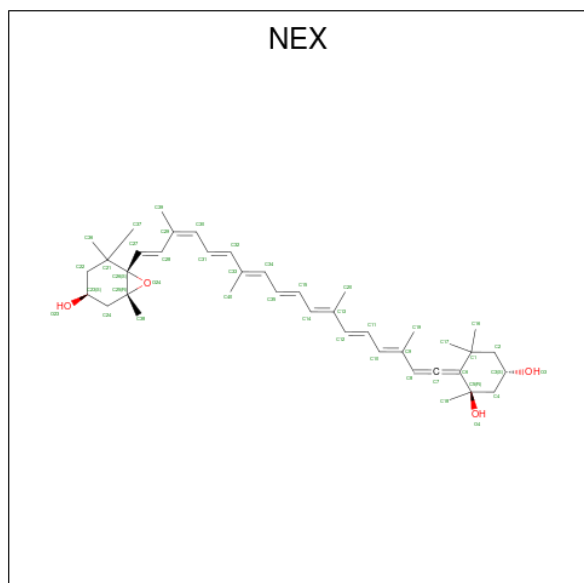
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40	G	1	Total	C	O	0
			42	40	2	
40	G	1	Total	C	O	0
			42	40	2	
40	N	1	Total	C	O	0
			42	40	2	
40	N	1	Total	C	O	0
			42	40	2	
40	R	1	Total	C	O	0
			42	40	2	
40	S	1	Total	C	O	0
			42	40	2	
40	S	1	Total	C	O	0
			42	40	2	
40	Y	1	Total	C	O	0
			42	40	2	
40	Y	1	Total	C	O	0
			42	40	2	
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
40	s	1	Total	C	O	0
			42	40	2	
40	s	1	Total	C	O	0
			42	40	2	
40	y	1	Total	C	O	0
			42	40	2	
40	y	1	Total	C	O	0
			42	40	2	

- 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 (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



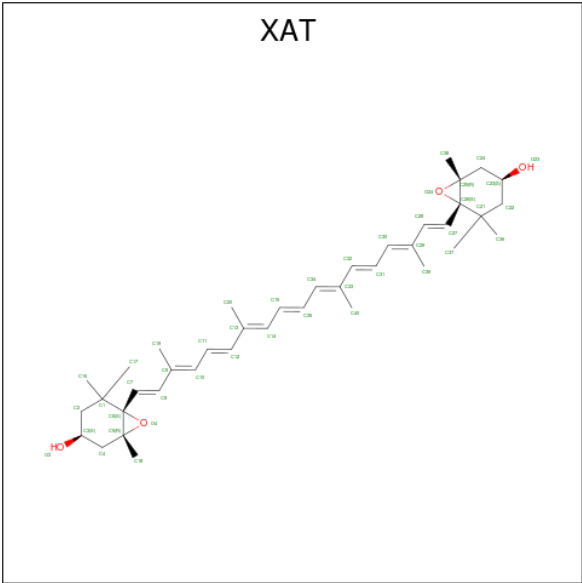
Mol	Chain	Residues	Atoms			AltConf
41	G	1	Total	C	O	0
			24	22	2	
41	N	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	S	1	Total	C	O	0
			23	21	2	
41	Y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
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 (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



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	

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Mol	Chain	Residues	Atoms			AltConf
42	y	1	Total	C	O	0
			44	40	4	

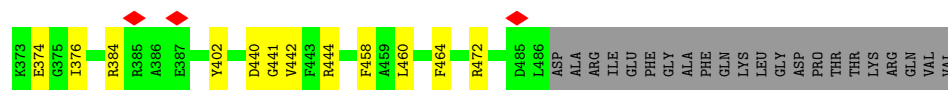
- Molecule 43 is water.

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		
43	E	4	Total	O		0
			4	4		
43	H	10	Total	O		0
			10	10		
43	I	1	Total	O		0
			1	1		
43	L	2	Total	O		0
			2	2		
43	N	4	Total	O		0
			4	4		
43	O	4	Total	O		0
			4	4		
43	R	8	Total	O		0
			8	8		
43	S	1	Total	O		0
			1	1		
43	T	5	Total	O		0
			5	5		
43	U	1	Total	O		0
			1	1		
43	V	1	Total	O		0
			1	1		
43	Y	8	Total	O		0
			8	8		
43	Z	1	Total	O		0
			1	1		
43	a	20	Total	O		0
			20	20		

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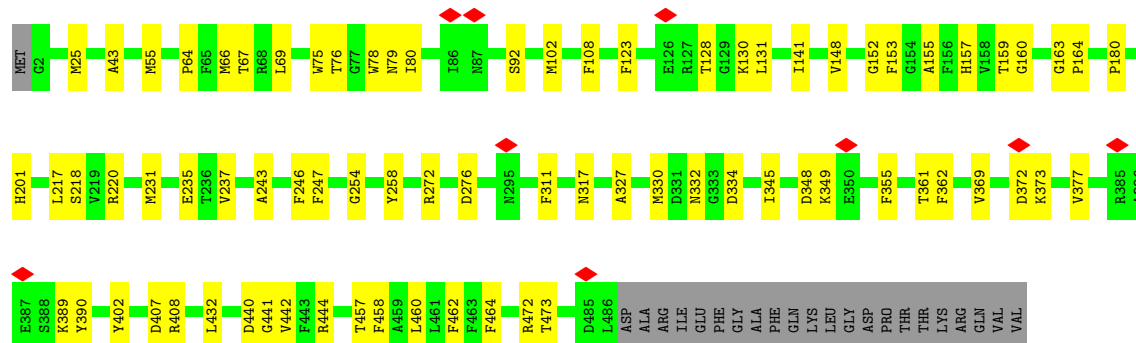
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Mol	Chain	Residues	Atoms		AltConf
43	b	31	Total 31	O 31	0
43	c	14	Total 14	O 14	0
43	d	25	Total 25	O 25	0
43	e	4	Total 4	O 4	0
43	f	1	Total 1	O 1	0
43	g	1	Total 1	O 1	0
43	h	11	Total 11	O 11	0
43	i	2	Total 2	O 2	0
43	l	4	Total 4	O 4	0
43	n	1	Total 1	O 1	0
43	o	2	Total 2	O 2	0
43	r	7	Total 7	O 7	0
43	t	4	Total 4	O 4	0
43	v	2	Total 2	O 2	0
43	x	1	Total 1	O 1	0
43	y	13	Total 13	O 13	0



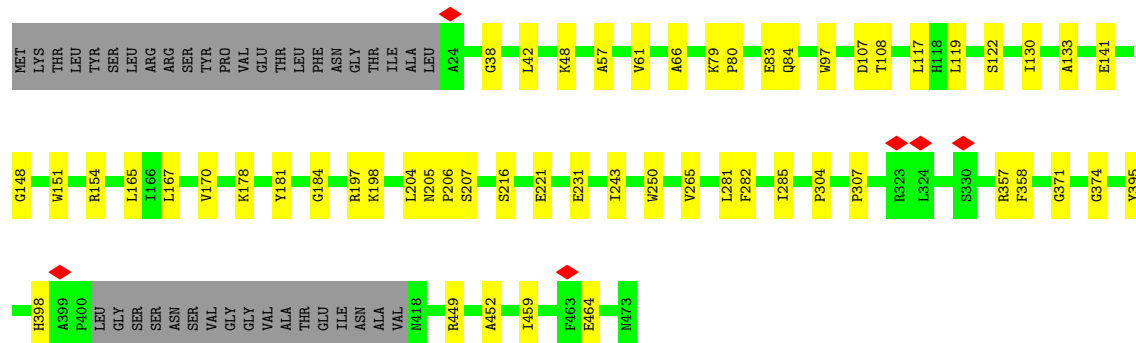
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 80% 15% 5%



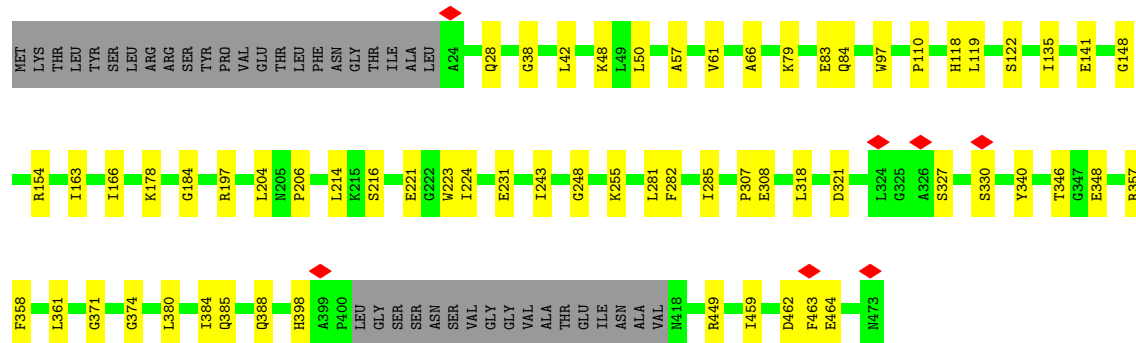
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 80% 12% 8%



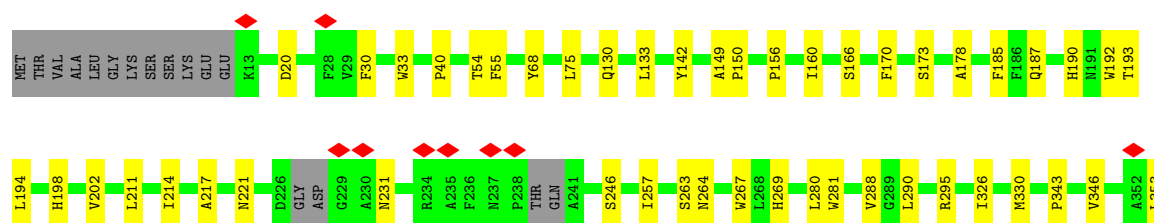
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 78% 13% 8%



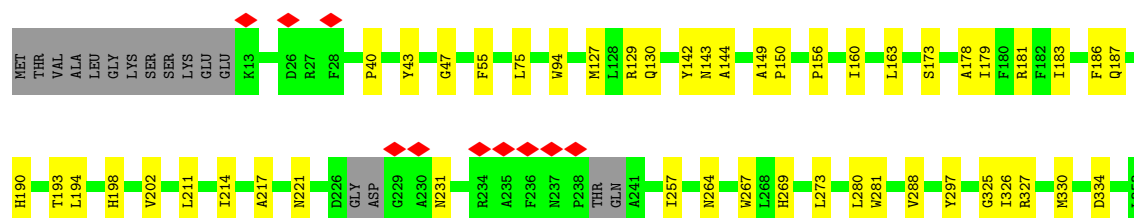
• Molecule 4: Photosystem II D2 protein

Chain D: 



• Molecule 4: Photosystem II D2 protein

Chain d: 



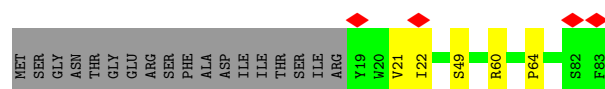
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 



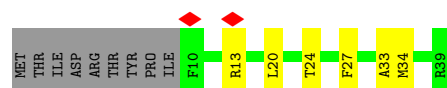
• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 



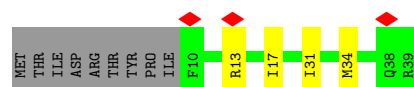
• Molecule 6: Cytochrome b559 subunit beta

Chain F: 

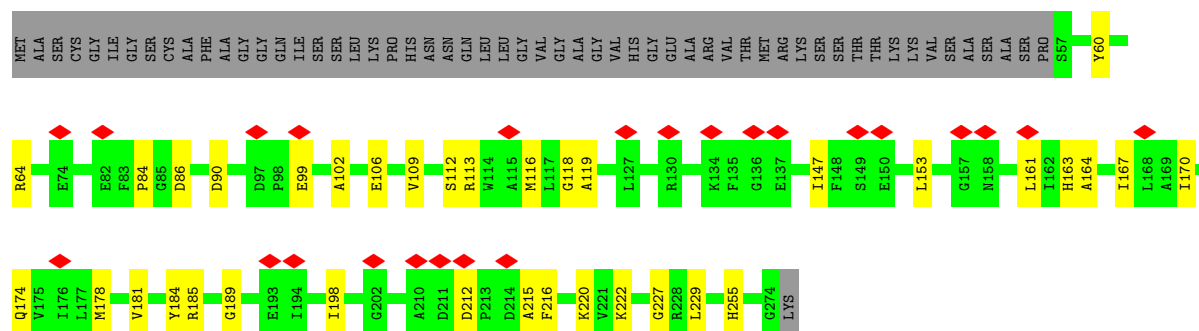


• Molecule 6: Cytochrome b559 subunit beta

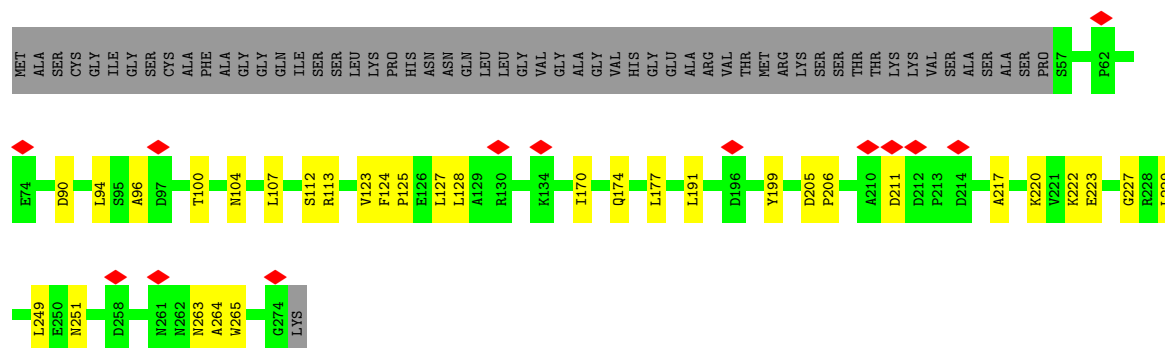
Chain f: 



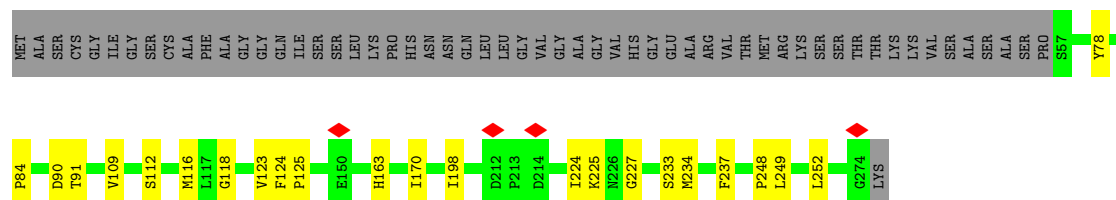
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



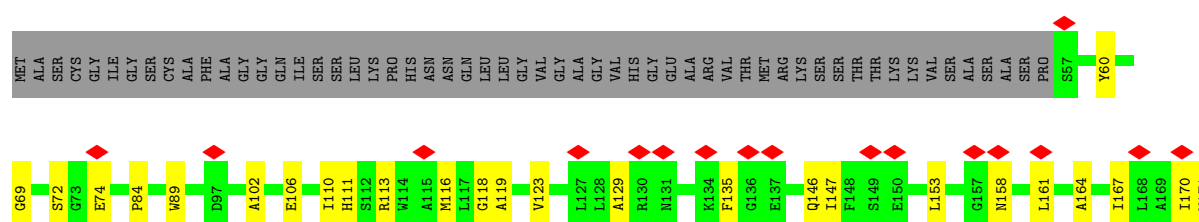
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

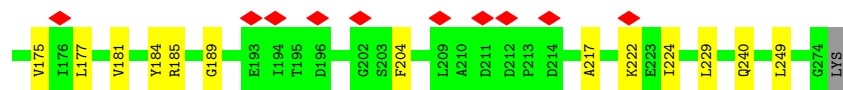


- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

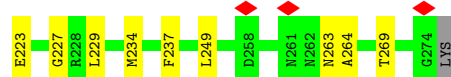
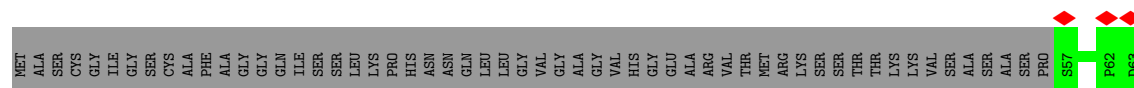


- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

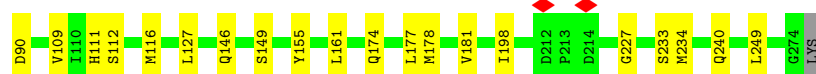
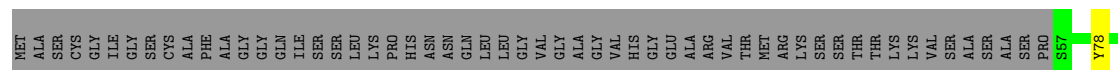




- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



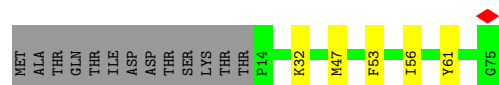
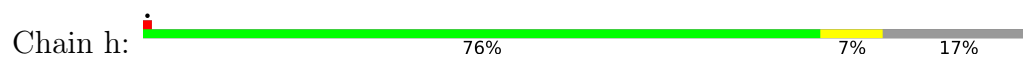
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



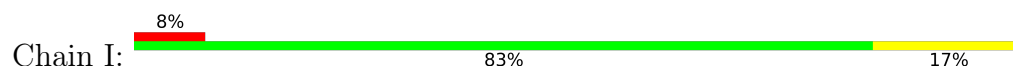
- Molecule 8: Photosystem II reaction center protein H

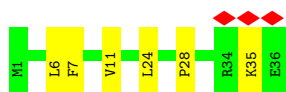


- Molecule 8: Photosystem II reaction center protein H

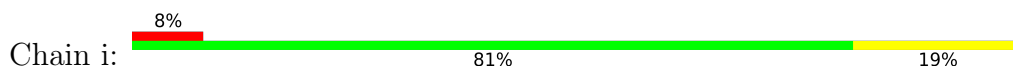


- Molecule 9: Photosystem II reaction center protein I

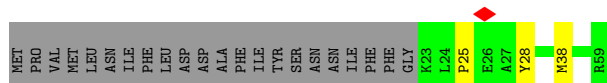




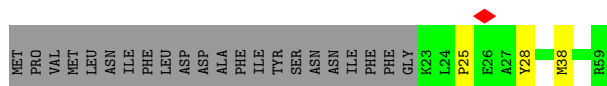
- Molecule 9: Photosystem II reaction center protein I



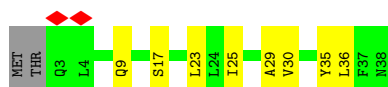
- Molecule 10: Photosystem II reaction center protein K



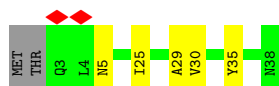
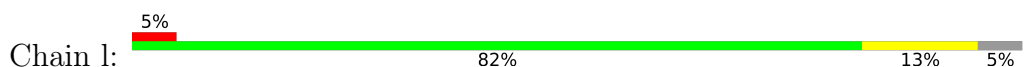
- Molecule 10: Photosystem II reaction center protein K



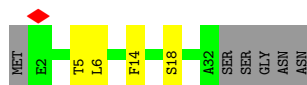
- Molecule 11: Photosystem II reaction center protein L



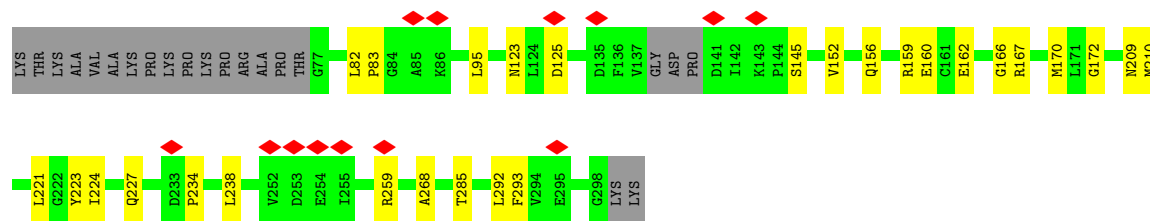
- Molecule 11: Photosystem II reaction center protein L



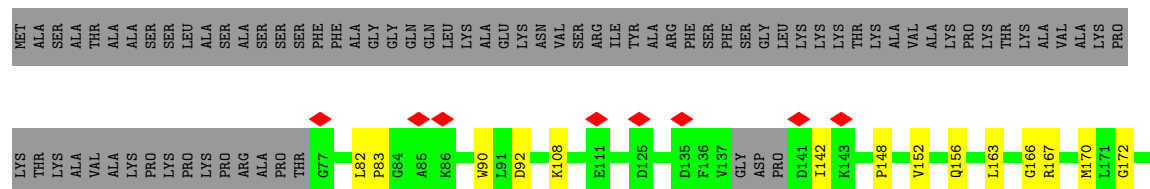
- Molecule 12: Photosystem II reaction center protein M



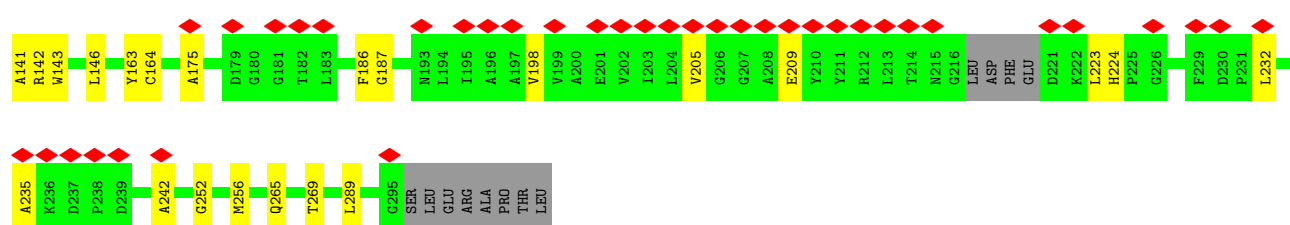
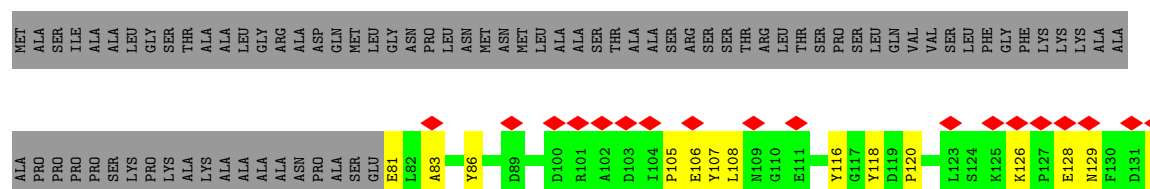
- Molecule 12: Photosystem II reaction center protein M



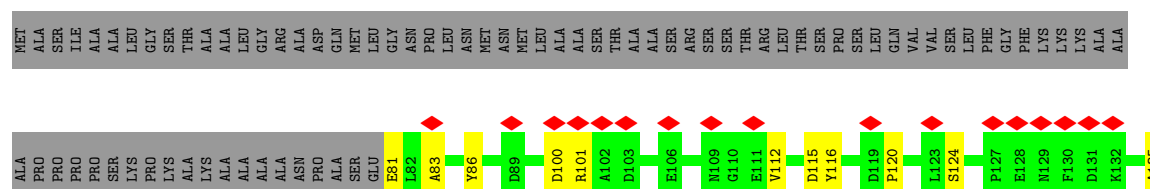
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

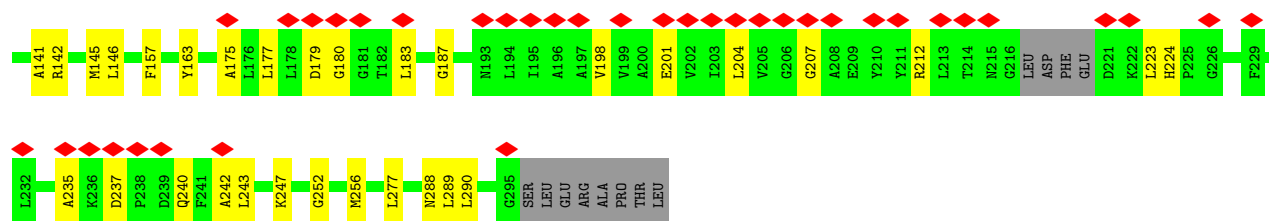


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

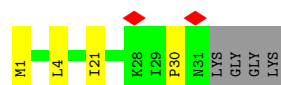
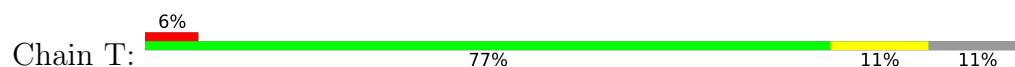


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

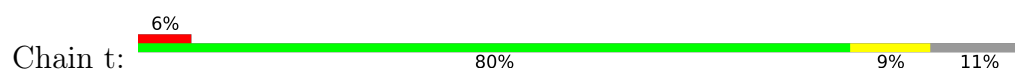




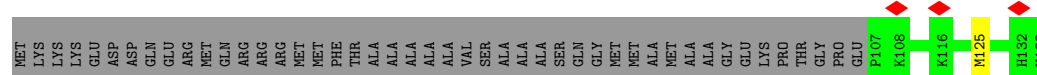
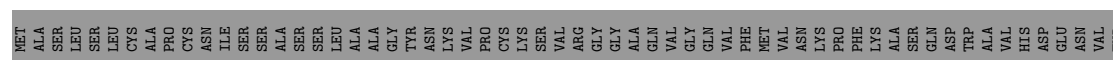
- Molecule 16: Photosystem II reaction center protein T



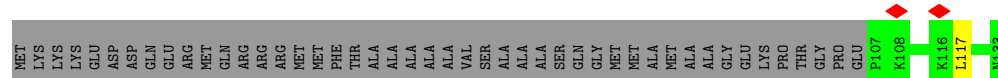
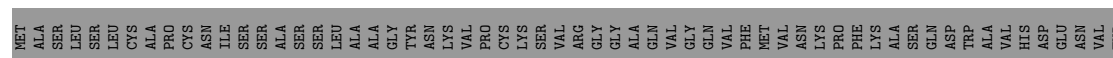
- Molecule 16: Photosystem II reaction center protein T



- Molecule 17: Photosystem II 5 kDa protein, chloroplastic



- Molecule 17: Photosystem II 5 kDa protein, chloroplastic

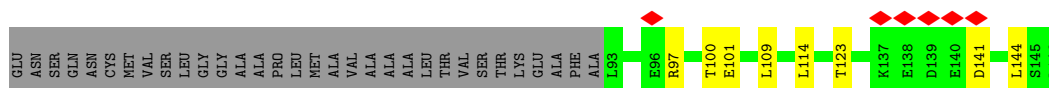


- Molecule 18: Photosystem II reaction center protein Ycf12

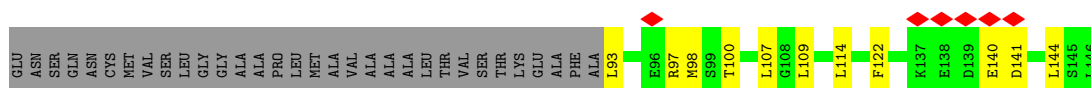


-
- Diagram illustrating the network topology for the L3-L33 segment. The nodes are arranged in a sequence: MET, ASN, L3, E4, V5, I6, A7, Q8, L9, T10, L14, L26, R29, N32, and L33. The nodes are color-coded: MET and ASN are grey, L3 through T10 are green, L14, L26, R29, and N32 are yellow, and L33 is green. Red diamonds are placed above the connections between MET-ASN, ASN-L3, L3-E4, E4-V5, V5-I6, I6-A7, A7-Q8, Q8-L9, L9-T10, T10-L14, L14-L26, L26-R29, R29-N32, and N32-L33.

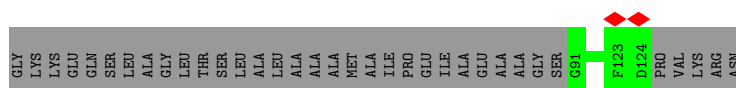
- | |
|-----|
| MET | ALA | ALA | THR | ALA | VAL | PHE | THR | THR | THR | SER | VAL | ALA | SER | ALA | PHE | LEU | LEU | ASN | ARG | SER | SER | LEU | LEU | GLY | SER | ALA | ALA | ALA | ALA | ARG | PRO | SER | SER | SER | SER | VAL | VAL | GLY | LEU | PRO | ALA | LEU | ASP | LYS | ARG | CYS | THR | THR | CYS | TYR | ALA | ALA | GLN | LYS | GLN | GLU | ILE | VAL | ARG | ALA | ALA |
|-----|



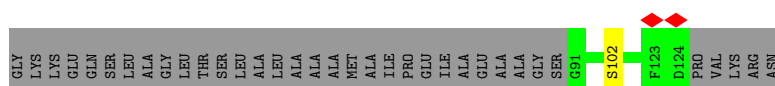
- | |
|-----|
| MET | ALA | ALA | ALA | ALA | ALA | THR | THR | VAL | PHE | SER | SER | THR | THR | THR | SER | VAL | VAL | SER | ALA | SER | PHE | LEU | LEU | ASN | ARG | SER | SER | GLY | SER | ALA | ALA | ALA | ALA | SER | ARG | ARG | PRO | PRO | SER | SER | SER | SER | LEU | LEU | VAL | VAL | VAL | ASP | LYS | ARG | ARG | CYS | THR | THR | VAL | VAL | CYS | TYR | ALA | ALA | GLN | GLN | LYS | GLN | GLU | ILE | GLU | VAL | VAL | ARG | ALA | ALA |
|-----|

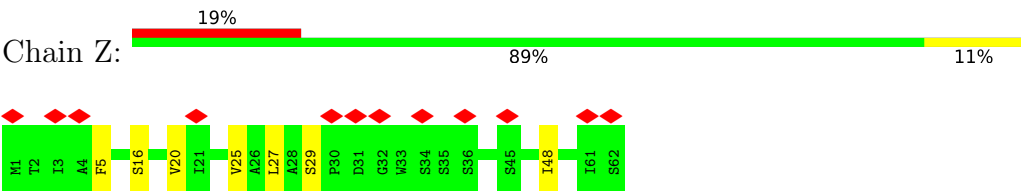


- | |
|-----|
| NET | ALA | SER | ALA | ALA | THR | ALA | ALA | ILE | SER | LEU | ALA | ALA | PRO | NET | ALA | THR | ALA | ALA | SER | SER | VAL | GLN | ARG | ASP | ALA | ALA | LEU | LYS | ALA | ALA | LYS | HIS | ALA | HIS | SER | SER | LEU | PHE | THR | THR | PRO | PRO | ASN | LYS | LEU | TYR | SER | SER | ASN | ARG | SER | ARG | VAL | VAL | NET | HIS | ALA | SER |
|-----|

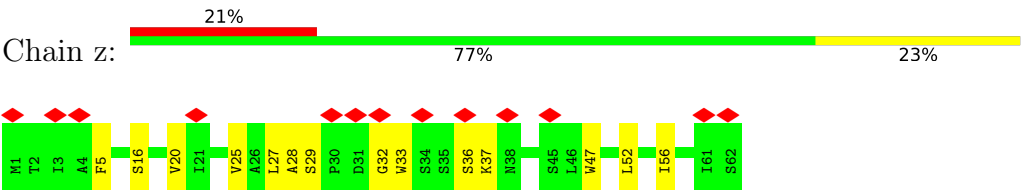


- | |
|-----|
| MET | ALA | SER | ALA | ALA | THR | ALA | ALA | ILE | SER | LEU | ALA | ALA | PRO | MET | ALA | THR | ALA | ALA | SER | SER | VAL | SER | GLN | ARG | ASP | ALA | LEU | LYS | ALA | ALA | LYS | HIS | HIS | GLY | SER | SER | LEU | PHE | THR | THR | PRO | PRO | ASN | LYS | LEU | TYR | SER | SER | ASN | ALA | VAL | VAL | MET | HIS | ALA | SER |
|-----|





• Molecule 21: Photosystem II reaction center protein Z



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: CLA, DGD, XAT, FE2, DGA, SQD, PHO, MG, 3PH, PAM, LMG, LUT, VIV, LNL, NEX, HEM, BCT, LHG, PL9, BCR, CHL

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	0.14	0/2578	0.29	0/3513
1	a	0.13	0/2578	0.33	0/3513
2	B	0.13	0/3940	0.29	0/5363
2	b	0.14	0/3940	0.31	0/5363
3	C	0.21	2/3493 (0.1%)	0.28	0/4757
3	c	0.19	1/3493 (0.0%)	0.30	0/4757
4	D	0.12	0/2778	0.28	0/3786
4	d	0.16	0/2777	0.30	0/3786
5	E	0.12	0/555	0.25	0/756
5	e	0.12	0/555	0.27	0/756
6	F	0.11	0/247	0.22	0/333
6	f	0.12	0/247	0.26	0/333
7	G	0.15	0/1712	0.36	0/2335
7	N	0.13	0/1712	0.28	0/2335
7	Y	0.24	2/1712 (0.1%)	0.31	0/2335
7	g	0.15	0/1712	0.34	0/2335
7	n	0.13	0/1712	0.29	0/2335
7	y	0.13	0/1712	0.28	0/2335
8	H	0.18	0/475	0.35	0/647
8	h	0.23	0/475	0.36	0/647
9	I	0.12	0/305	0.29	0/409
9	i	0.12	0/305	0.29	0/409
10	K	0.16	0/313	0.34	0/428
10	k	0.15	0/313	0.34	0/428
11	L	0.09	0/309	0.22	0/421
11	l	0.10	0/309	0.23	0/421
12	M	0.10	0/242	0.23	0/330
12	m	0.12	0/242	0.27	0/330
13	O	0.09	0/1497	0.26	0/2017
13	o	0.10	0/1497	0.27	0/2017
14	R	0.10	0/1767	0.23	0/2397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	r	0.11	0/1767	0.26	0/2397
15	S	0.18	0/1673	0.28	0/2272
15	s	0.16	0/1673	0.27	0/2272
16	T	0.09	0/262	0.23	0/356
16	t	0.09	0/262	0.21	0/356
17	U	0.07	0/209	0.20	0/280
17	u	0.08	0/209	0.19	0/280
18	V	0.09	0/228	0.21	0/311
18	v	0.07	0/228	0.20	0/311
19	W	0.11	0/423	0.28	0/574
19	w	0.09	0/423	0.24	0/574
20	X	0.09	0/228	0.21	0/310
20	x	0.09	0/228	0.20	0/310
21	Z	0.10	0/463	0.24	0/633
21	z	0.10	0/463	0.23	0/633
All	All	0.15	5/54241 (0.0%)	0.29	0/73796

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	97	TRP	C-O	-5.82	1.17	1.24
3	c	97	TRP	C-O	-5.75	1.17	1.24
7	Y	163	HIS	CA-C	-5.53	1.46	1.53
3	C	151	TRP	C-N	5.46	1.42	1.33
7	Y	163	HIS	C-O	-5.09	1.17	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2502	0	2425	45	0
1	a	2502	0	2425	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3812	0	3712	54	0
2	b	3812	0	3712	59	0
3	C	3377	0	3299	46	0
3	c	3377	0	3299	45	0
4	D	2686	0	2588	38	0
4	d	2685	0	2588	42	0
5	E	537	0	507	5	0
5	e	537	0	507	3	0
6	F	240	0	242	5	0
6	f	240	0	242	2	0
7	G	1659	0	1591	28	0
7	N	1659	0	1591	32	0
7	Y	1659	0	1591	17	0
7	g	1659	0	1591	32	0
7	n	1659	0	1591	29	0
7	y	1659	0	1591	15	0
8	H	462	0	471	7	0
8	h	462	0	471	5	0
9	I	297	0	310	5	0
9	i	297	0	310	8	0
10	K	302	0	311	3	0
10	k	302	0	311	3	0
11	L	302	0	300	8	0
11	l	302	0	300	5	0
12	M	238	0	256	4	0
12	m	238	0	256	5	0
13	O	1470	0	1468	21	0
13	o	1470	0	1468	21	0
14	R	1722	0	1708	21	0
14	r	1722	0	1708	24	0
15	S	1626	0	1593	29	0
15	s	1626	0	1593	34	0
16	T	254	0	268	4	0
16	t	254	0	268	3	0
17	U	205	0	213	1	0
17	u	205	0	213	1	0
18	V	228	0	267	7	0
18	v	228	0	267	3	0
19	W	415	0	413	9	0
19	w	415	0	413	13	0
20	X	226	0	236	0	0
20	x	226	0	236	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Z	453	0	480	8	0
21	z	453	0	480	12	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	239	0	242	7	0
23	B	1024	0	1119	48	0
23	C	835	0	913	20	0
23	D	130	0	144	6	0
23	G	451	0	431	20	0
23	N	472	0	477	24	0
23	R	522	0	513	7	0
23	S	494	0	453	21	0
23	Y	520	0	576	23	0
23	a	239	0	242	6	0
23	b	1025	0	1119	39	0
23	c	840	0	923	23	0
23	d	130	0	144	4	0
23	g	472	0	477	19	0
23	n	456	0	444	21	0
23	r	522	0	513	11	0
23	s	494	0	453	26	0
23	y	520	0	576	23	0
24	A	64	0	74	3	0
24	D	64	0	74	4	0
24	a	64	0	74	3	0
24	d	64	0	74	2	0
25	A	40	0	56	4	0
25	B	119	0	165	14	0
25	C	40	0	56	6	0
25	D	40	0	56	2	0
25	H	40	0	56	2	0
25	K	40	0	56	0	0
25	V	40	0	56	0	0
25	Z	40	0	56	3	0
25	a	40	0	56	4	0
25	b	120	0	168	6	0
25	c	40	0	56	3	0
25	d	40	0	56	3	0
25	h	40	0	56	0	0
25	k	40	0	56	1	0
25	v	40	0	56	1	0
25	z	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	50	0	67	2	0
26	L	54	0	78	4	0
26	M	50	0	67	2	0
26	a	48	0	63	3	0
27	A	53	0	79	5	0
27	B	97	0	137	7	0
27	C	45	0	63	3	0
27	D	36	0	42	1	0
27	R	51	0	75	3	0
27	b	101	0	145	9	0
27	c	46	0	65	2	0
27	d	46	0	62	2	0
27	r	51	0	75	3	0
27	w	48	0	66	1	0
28	A	48	0	75	4	0
28	C	48	0	75	4	0
28	D	38	0	49	2	0
28	L	41	0	58	2	0
28	T	48	0	75	0	0
28	W	46	0	68	2	0
28	X	46	0	68	0	0
28	a	48	0	75	9	0
28	d	38	0	49	3	0
28	s	38	0	52	1	0
28	w	48	0	75	4	0
28	x	46	0	68	3	0
29	A	55	0	80	9	0
29	D	55	0	80	2	0
29	a	55	0	80	7	0
29	d	55	0	80	3	0
30	A	37	0	44	1	0
30	D	92	0	133	6	0
30	G	49	0	74	3	0
30	L	49	0	74	2	0
30	N	49	0	74	3	0
30	R	38	0	49	0	0
30	S	49	0	74	3	0
30	Y	49	0	74	5	0
30	a	49	0	74	4	0
30	b	49	0	74	1	0
30	d	98	0	148	5	0
30	g	49	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	n	45	0	63	2	0
30	r	37	0	44	0	0
30	s	49	0	74	2	0
30	y	49	0	74	3	0
31	A	40	0	58	3	0
31	B	80	0	116	9	0
31	C	120	0	174	8	0
31	I	20	0	29	0	0
31	a	40	0	58	2	0
31	b	80	0	116	6	0
31	c	120	0	174	7	0
31	i	20	0	29	2	0
32	B	18	0	29	1	0
32	b	18	0	29	0	0
33	C	66	0	96	3	0
33	H	62	0	82	1	0
33	c	55	0	68	1	0
33	d	62	0	82	3	0
34	C	1	0	0	0	0
34	c	1	0	0	0	0
35	C	31	0	49	5	0
35	y	31	0	49	4	0
36	D	4	0	0	5	0
36	d	4	0	0	5	0
37	D	40	0	65	3	0
37	b	44	0	76	4	0
38	F	43	0	30	3	0
38	f	43	0	30	2	0
39	G	412	0	387	19	0
39	N	364	0	354	18	0
39	R	182	0	177	8	0
39	S	201	0	147	9	0
39	Y	296	0	280	11	0
39	g	412	0	387	7	0
39	n	362	0	350	17	0
39	r	182	0	177	9	0
39	s	201	0	147	4	0
39	y	280	0	247	5	0
40	G	84	0	112	12	0
40	N	84	0	112	10	0
40	R	42	0	56	2	0
40	S	84	0	112	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	Y	84	0	112	9	0
40	g	84	0	112	14	0
40	n	84	0	112	11	0
40	r	42	0	56	3	0
40	s	84	0	112	3	0
40	y	84	0	112	5	0
41	G	24	0	29	2	0
41	N	44	0	56	2	0
41	R	88	0	112	2	0
41	S	23	0	28	2	0
41	Y	44	0	56	1	0
41	g	44	0	56	4	0
41	n	44	0	56	4	0
41	r	44	0	56	2	0
41	s	27	0	33	2	0
42	G	44	0	56	4	0
42	N	44	0	56	6	0
42	R	44	0	56	2	0
42	Y	44	0	56	4	0
42	n	88	0	112	8	0
42	r	44	0	56	3	0
42	y	44	0	56	2	0
43	A	28	0	0	0	0
43	B	31	0	0	0	0
43	C	10	0	0	0	0
43	D	18	0	0	0	0
43	E	4	0	0	0	0
43	H	10	0	0	0	0
43	I	1	0	0	1	0
43	L	2	0	0	0	0
43	N	4	0	0	0	0
43	O	4	0	0	0	0
43	R	8	0	0	0	0
43	S	1	0	0	0	0
43	T	5	0	0	0	0
43	U	1	0	0	0	0
43	V	1	0	0	0	0
43	Y	8	0	0	0	0
43	Z	1	0	0	0	0
43	a	20	0	0	0	0
43	b	31	0	0	0	0
43	c	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	d	25	0	0	1	0
43	e	4	0	0	0	0
43	f	1	0	0	0	0
43	g	1	0	0	0	0
43	h	11	0	0	0	0
43	i	2	0	0	0	0
43	l	4	0	0	1	0
43	n	1	0	0	0	0
43	o	2	0	0	0	0
43	r	7	0	0	0	0
43	t	4	0	0	0	0
43	v	2	0	0	1	0
43	x	1	0	0	0	0
43	y	13	0	0	1	0
All	All	71174	0	72294	1166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1166 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:609:CLA:H2	23:b:610:CLA:HBB2	1.49	0.93
30:D:408:LHG:H262	11:L:23:LEU:HD22	1.60	0.83
3:c:216:SER:OG	3:c:221:GLU:OE2	1.96	0.83
2:b:372:ASP:OD1	2:b:373:LYS:N	2.16	0.79
30:G:618:LHG:H192	42:Y:301:XAT:H12	1.64	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
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 ⓘ

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%)	84	93
1	a	257/282 (91%)	256 (100%)	1 (0%)	84	93
2	B	387/406 (95%)	386 (100%)	1 (0%)	86	94
2	b	387/406 (95%)	386 (100%)	1 (0%)	86	94
3	C	338/371 (91%)	338 (100%)	0	100	100
3	c	338/371 (91%)	338 (100%)	0	100	100
4	D	271/284 (95%)	271 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	271/284 (95%)	271 (100%)	0	100	100
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%)	50 (100%)	0	100	100
8	h	50/62 (81%)	50 (100%)	0	100	100
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%)	180 (100%)	0	100	100
14	r	180/241 (75%)	180 (100%)	0	100	100
15	S	162/230 (70%)	162 (100%)	0	100	100
15	s	162/230 (70%)	162 (100%)	0	100	100
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%)	5422 (100%)	4 (0%)	87	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	HIS
2	B	362	PHE
1	a	332	HIS
2	b	362	PHE

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

Mol	Chain	Res	Type
4	d	231	ASN
14	r	147	GLN
4	d	335	GLN
13	o	189	GLN
15	s	224	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	n	610	7	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
31	LNL	C	521	-	19,19,19	0.45	0	18,19,19	0.93	1 (5%)
30	LHG	a	412	-	48,48,48	1.40	8 (16%)	51,54,54	0.73	2 (3%)
30	LHG	A	412	-	36,36,48	1.52	8 (22%)	39,42,54	0.89	2 (5%)
40	LUT	s	615	-	42,43,43	2.55	21 (50%)	51,60,60	3.15	24 (47%)
27	LMG	d	409	-	46,46,55	0.19	0	54,54,63	0.15	0
23	CLA	C	509	3	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
39	CHL	R	607	-	70,74,74	1.04	5 (7%)	80,114,114	1.68	13 (16%)
39	CHL	g	601	7	70,74,74	1.02	4 (5%)	80,114,114	1.65	10 (12%)
25	BCR	B	618	-	40,40,41	1.09	2 (5%)	52,54,56	1.25	6 (11%)
39	CHL	G	601	7	70,74,74	1.02	4 (5%)	80,114,114	1.66	10 (12%)
33	DGD	C	515	-	67,67,67	0.88	2 (2%)	81,81,81	1.46	10 (12%)
23	CLA	s	613	15	69,73,73	1.25	7 (10%)	83,113,113	1.27	7 (8%)
23	CLA	B	602	2	69,73,73	1.26	7 (10%)	83,113,113	1.29	9 (10%)
23	CLA	N	604	-	53,57,73	1.43	9 (16%)	62,93,113	1.42	8 (12%)
25	BCR	z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
31	LNL	C	519	-	19,19,19	0.43	0	18,19,19	0.95	1 (5%)
23	CLA	a	404	43	69,73,73	1.25	9 (13%)	83,113,113	1.32	7 (8%)
25	BCR	Z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
28	3PH	L	102	-	40,40,47	0.68	1 (2%)	44,45,52	0.64	1 (2%)
23	CLA	D	406	4	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
41	NEX	s	617	-	23,27,46	4.08	19 (82%)	28,38,70	3.76	14 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	507	43	69,73,73	1.26	8 (11%)	83,113,113	1.31	5 (6%)
31	LNL	A	413	-	19,19,19	0.44	0	18,19,19	0.89	1 (5%)
23	CLA	r	611	14	53,57,73	1.43	7 (13%)	62,93,113	1.42	5 (8%)
40	LUT	n	616	-	42,43,43	2.36	19 (45%)	51,60,60	3.07	21 (41%)
33	DGD	d	411	-	63,63,67	0.85	1 (1%)	77,77,81	1.35	7 (9%)
23	CLA	G	610	7	69,73,73	1.25	6 (8%)	83,113,113	1.30	8 (9%)
23	CLA	g	602	7	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
40	LUT	G	616	-	42,43,43	2.41	20 (47%)	51,60,60	3.11	21 (41%)
42	XAT	n	617	-	39,47,47	3.04	21 (53%)	54,74,74	4.50	30 (55%)
23	CLA	s	610	30	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
23	CLA	N	612	7	53,57,73	1.43	8 (15%)	62,93,113	1.41	5 (8%)
30	LHG	Y	318	23	48,48,48	1.39	8 (16%)	51,54,54	0.69	2 (3%)
23	CLA	R	612	14	53,57,73	1.44	7 (13%)	62,93,113	1.40	5 (8%)
23	CLA	r	602	14	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
39	CHL	s	601	-	56,60,74	1.15	3 (5%)	63,97,114	1.86	10 (15%)
23	CLA	c	504	43	69,73,73	1.26	7 (10%)	83,113,113	1.28	4 (4%)
23	CLA	y	314	7	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
27	LMG	D	409	-	36,36,55	0.20	0	44,44,63	0.14	0
23	CLA	n	613	7	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
28	3PH	W	201	-	45,45,47	0.64	1 (2%)	49,50,52	0.60	1 (2%)
23	CLA	c	501	3	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
23	CLA	y	305	7	69,73,73	1.25	6 (8%)	83,113,113	1.31	6 (7%)
23	CLA	Y	303	7	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
41	NEX	S	617	-	19,23,46	4.24	16 (84%)	23,33,70	4.24	11 (47%)
31	LNL	b	625	-	19,19,19	0.44	0	18,19,19	0.92	1 (5%)
39	CHL	g	608	-	54,58,74	1.19	4 (7%)	59,94,114	1.84	10 (16%)
31	LNL	C	522	-	19,19,19	0.44	0	18,19,19	0.91	1 (5%)
31	LNL	I	101	-	19,19,19	0.43	0	18,19,19	0.91	1 (5%)
23	CLA	c	505	3	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
26	SQD	a	409	-	47,48,54	1.61	7 (14%)	56,59,65	1.45	6 (10%)
28	3PH	C	524	-	47,47,47	0.63	1 (2%)	51,52,52	0.60	1 (1%)
28	3PH	X	201	-	45,45,47	0.65	1 (2%)	49,50,52	0.60	1 (2%)
31	LNL	A	414	-	19,19,19	0.43	0	18,19,19	0.92	1 (5%)
30	LHG	L	103	-	48,48,48	1.36	8 (16%)	51,54,54	0.71	2 (3%)
23	CLA	Y	313	-	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	G	606	-	54,58,74	1.21	3 (5%)	59,94,114	1.94	9 (15%)
23	CLA	Y	311	30	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
23	CLA	r	610	30	69,73,73	1.26	7 (10%)	83,113,113	1.33	7 (8%)
39	CHL	r	605	-	54,58,74	1.16	5 (9%)	59,94,114	1.91	11 (18%)
25	BCR	h	501	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	4 (7%)
23	CLA	a	405	43	53,57,73	1.42	6 (11%)	62,93,113	1.44	7 (11%)
23	CLA	d	406	4	69,73,73	1.25	7 (10%)	83,113,113	1.31	6 (7%)
39	CHL	S	606	-	54,58,74	1.18	4 (7%)	59,94,114	1.93	11 (18%)
23	CLA	b	608	2	69,73,73	1.25	7 (10%)	83,113,113	1.28	7 (8%)
39	CHL	s	606	-	54,58,74	1.17	4 (7%)	59,94,114	1.87	10 (16%)
39	CHL	n	608	-	54,58,74	1.18	4 (7%)	59,94,114	1.92	10 (16%)
23	CLA	a	407	1	64,68,73	1.30	7 (10%)	77,107,113	1.34	7 (9%)
23	CLA	Y	312	7	69,73,73	1.27	6 (8%)	83,113,113	1.26	6 (7%)
23	CLA	s	608	-	53,57,73	1.44	6 (11%)	62,93,113	1.36	5 (8%)
23	CLA	c	512	3	69,73,73	1.25	7 (10%)	83,113,113	1.28	8 (9%)
25	BCR	k	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	6 (10%)
23	CLA	g	603	7	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
23	CLA	c	513	3	64,68,73	1.29	8 (12%)	77,107,113	1.31	6 (7%)
23	CLA	g	611	-	69,73,73	1.25	7 (10%)	83,113,113	1.27	5 (6%)
41	NEX	g	617	-	38,46,46	4.18	33 (86%)	50,70,70	4.94	24 (48%)
35	VIV	C	523	-	32,32,32	0.93	2 (6%)	41,45,45	1.14	4 (9%)
41	NEX	n	618	-	38,46,46	4.08	32 (84%)	50,70,70	4.99	22 (44%)
23	CLA	R	603	14	64,68,73	1.30	8 (12%)	77,107,113	1.33	7 (9%)
23	CLA	G	604	-	53,57,73	1.43	8 (15%)	62,93,113	1.41	7 (11%)
23	CLA	A	404	43	53,57,73	1.42	7 (13%)	62,93,113	1.44	6 (9%)
23	CLA	B	601	-	53,57,73	1.42	6 (11%)	62,93,113	1.45	6 (9%)
23	CLA	a	403	1	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
23	CLA	B	616	2	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
23	CLA	n	604	-	53,57,73	1.43	9 (16%)	62,93,113	1.42	8 (12%)
39	CHL	g	619	43	70,74,74	1.03	4 (5%)	80,114,114	1.70	11 (13%)
39	CHL	G	609	7	70,74,74	1.08	4 (5%)	80,114,114	1.76	9 (11%)
23	CLA	s	604	-	53,57,73	1.42	9 (16%)	62,93,113	1.44	7 (11%)
40	LUT	R	613	-	42,43,43	2.53	21 (50%)	51,60,60	3.16	25 (49%)
23	CLA	N	613	7	69,73,73	1.26	6 (8%)	83,113,113	1.39	7 (8%)
30	LHG	N	618	23	48,48,48	1.45	8 (16%)	51,54,54	0.69	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LNL	b	624	-	19,19,19	0.43	0	18,19,19	0.88	1 (5%)
23	CLA	c	508	3	69,73,73	1.25	7 (10%)	83,113,113	1.30	8 (9%)
23	CLA	c	503	3	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
23	CLA	R	610	30	69,73,73	1.27	7 (10%)	83,113,113	1.27	6 (7%)
23	CLA	C	502	3	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
23	CLA	B	615	2	69,73,73	1.26	7 (10%)	83,113,113	1.28	5 (6%)
23	CLA	b	615	2	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
23	CLA	Y	304	7	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
39	CHL	R	605	-	54,58,74	1.17	4 (7%)	59,94,114	1.90	11 (18%)
32	PAM	B	621	-	17,17,17	0.61	0	17,17,17	0.78	0
23	CLA	y	311	7	69,73,73	1.25	8 (11%)	83,113,113	1.28	8 (9%)
39	CHL	R	606	-	70,74,74	1.03	4 (5%)	80,114,114	1.66	12 (15%)
36	BCT	D	401	22	2,3,3	1.16	0	2,3,3	4.53	2 (100%)
40	LUT	Y	315	-	42,43,43	1.78	10 (23%)	51,60,60	2.77	20 (39%)
30	LHG	d	408	-	48,48,48	1.36	8 (16%)	51,54,54	0.74	2 (3%)
23	CLA	C	513	3	69,73,73	1.24	7 (10%)	83,113,113	1.33	8 (9%)
23	CLA	G	613	7	69,73,73	1.26	7 (10%)	83,113,113	1.30	6 (7%)
27	LMG	b	628	-	50,50,55	0.19	0	58,58,63	0.18	0
23	CLA	r	603	14	64,68,73	1.30	8 (12%)	77,107,113	1.32	7 (9%)
23	CLA	B	610	43	69,73,73	1.26	7 (10%)	83,113,113	1.27	7 (8%)
23	CLA	b	610	43	69,73,73	1.27	7 (10%)	83,113,113	1.28	7 (8%)
24	PHO	A	405	-	58,69,69	2.04	10 (17%)	56,99,99	1.48	8 (14%)
25	BCR	C	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
23	CLA	c	506	3	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
30	LHG	r	616	23	36,36,48	1.60	8 (22%)	39,42,54	0.82	2 (5%)
23	CLA	y	312	30	69,73,73	1.25	7 (10%)	83,113,113	1.27	8 (9%)
23	CLA	C	508	3	69,73,73	1.25	7 (10%)	83,113,113	1.31	7 (8%)
40	LUT	y	317	-	42,43,43	2.38	20 (47%)	51,60,60	3.16	23 (45%)
26	SQD	L	101	-	53,54,54	1.53	8 (15%)	62,65,65	1.40	6 (9%)
32	PAM	b	621	-	17,17,17	0.63	0	17,17,17	0.78	0
39	CHL	N	608	-	54,58,74	1.17	4 (7%)	59,94,114	1.92	11 (18%)
40	LUT	g	616	-	42,43,43	2.40	19 (45%)	51,60,60	3.11	21 (41%)
27	LMG	A	409	-	53,53,55	0.19	0	61,61,63	0.19	0
42	XAT	R	615	-	39,47,47	3.21	20 (51%)	54,74,74	4.68	31 (57%)
25	BCR	b	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	n	603	7	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
27	LMG	b	620	-	51,51,55	0.19	0	59,59,63	0.22	0
23	CLA	R	604	43	59,63,73	1.35	9 (15%)	71,101,113	1.36	7 (9%)
24	PHO	d	402	-	58,69,69	2.06	10 (17%)	56,99,99	1.52	7 (12%)
23	CLA	A	402	1	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
25	BCR	A	407	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	5 (8%)
23	CLA	s	602	15	61,65,73	1.34	7 (11%)	73,103,113	1.33	5 (6%)
23	CLA	C	506	3	59,63,73	1.35	9 (15%)	71,101,113	1.33	7 (9%)
23	CLA	B	609	2	69,73,73	1.25	7 (10%)	83,113,113	1.26	7 (8%)
25	BCR	b	617	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	8 (14%)
39	CHL	y	309	-	54,58,74	1.18	4 (7%)	59,94,114	1.88	9 (15%)
25	BCR	D	411	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
23	CLA	G	614	7	53,57,73	1.44	6 (11%)	62,93,113	1.36	6 (9%)
42	XAT	N	619	-	39,47,47	3.16	23 (58%)	54,74,74	4.58	32 (59%)
26	SQD	M	101	-	49,50,54	1.59	8 (16%)	58,61,65	1.38	6 (10%)
39	CHL	S	607	-	53,57,74	1.20	5 (9%)	59,93,114	1.87	11 (18%)
41	NEX	R	614	-	38,46,46	4.09	32 (84%)	50,70,70	4.87	22 (44%)
31	LNL	C	517	-	19,19,19	0.43	0	18,19,19	0.92	1 (5%)
39	CHL	g	605	7	52,56,74	1.20	4 (7%)	58,92,114	2.09	11 (18%)
40	LUT	S	614	-	42,43,43	2.60	21 (50%)	51,60,60	3.23	25 (49%)
39	CHL	g	606	-	54,58,74	1.21	4 (7%)	59,94,114	1.95	11 (18%)
23	CLA	c	511	3	69,73,73	1.26	8 (11%)	83,113,113	1.31	7 (8%)
28	3PH	T	101	-	47,47,47	0.63	1 (2%)	51,52,52	0.61	1 (1%)
23	CLA	c	509	3	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
42	XAT	Y	301	-	39,47,47	3.30	24 (61%)	54,74,74	4.45	32 (59%)
35	VIV	y	301	-	32,32,32	0.88	1 (3%)	41,45,45	1.13	5 (12%)
25	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	8 (14%)
23	CLA	n	614	7	53,57,73	1.43	7 (13%)	62,93,113	1.40	6 (9%)
31	LNL	c	522	-	19,19,19	0.43	0	18,19,19	0.94	1 (5%)
28	3PH	w	202	-	47,47,47	0.63	1 (2%)	51,52,52	0.59	1 (1%)
40	LUT	g	615	-	42,43,43	1.88	10 (23%)	51,60,60	2.93	21 (41%)
40	LUT	G	615	-	42,43,43	1.97	12 (28%)	51,60,60	2.89	22 (43%)
23	CLA	S	608	-	53,57,73	1.43	6 (11%)	62,93,113	1.34	5 (8%)
23	CLA	A	403	43	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
23	CLA	G	612	7	53,57,73	1.43	7 (13%)	62,93,113	1.42	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	S	609	15	60,64,73	1.35	8 (13%)	72,102,113	1.30	8 (11%)
23	CLA	B	612	2	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
28	3PH	x	201	-	45,45,47	0.65	1 (2%)	49,50,52	0.60	1 (2%)
23	CLA	B	604	2	69,73,73	1.25	8 (11%)	83,113,113	1.36	6 (7%)
27	LMG	R	617	-	51,51,55	0.18	0	59,59,63	0.26	0
25	BCR	d	410	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	6 (10%)
36	BCT	d	401	22	2,3,3	1.15	0	2,3,3	4.51	2 (100%)
30	LHG	D	408	-	48,48,48	1.13	4 (8%)	51,54,54	0.93	3 (5%)
29	PL9	a	411	-	55,55,55	0.11	0	68,69,69	0.28	0
23	CLA	b	609	-	69,73,73	1.25	6 (8%)	83,113,113	1.28	7 (8%)
23	CLA	A	406	1	64,68,73	1.29	6 (9%)	77,107,113	1.33	7 (9%)
30	LHG	n	619	23	44,44,48	1.45	8 (18%)	47,50,54	0.75	2 (4%)
28	3PH	a	410	-	47,47,47	0.63	1 (2%)	51,52,52	0.56	1 (1%)
23	CLA	b	616	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
40	LUT	S	615	-	42,43,43	2.65	22 (52%)	51,60,60	3.22	24 (47%)
23	CLA	B	605	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
40	LUT	n	615	-	42,43,43	1.89	11 (26%)	51,60,60	2.97	19 (37%)
23	CLA	S	610	30	69,73,73	1.27	6 (8%)	83,113,113	1.28	6 (7%)
31	LNL	a	401	-	19,19,19	0.43	0	18,19,19	0.93	1 (5%)
30	LHG	b	627	-	48,48,48	1.36	8 (16%)	51,54,54	0.73	2 (3%)
23	CLA	C	511	3	69,73,73	1.26	7 (10%)	83,113,113	1.31	6 (7%)
39	CHL	Y	302	7	70,74,74	1.04	4 (5%)	80,114,114	1.64	11 (13%)
25	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
30	LHG	g	618	-	48,48,48	1.40	8 (16%)	51,54,54	0.77	2 (3%)
23	CLA	B	607	-	69,73,73	1.25	7 (10%)	83,113,113	1.30	6 (7%)
40	LUT	N	616	-	42,43,43	2.59	22 (52%)	51,60,60	3.21	22 (43%)
23	CLA	B	611	2	69,73,73	1.25	7 (10%)	83,113,113	1.28	7 (8%)
23	CLA	N	603	7	69,73,73	1.24	8 (11%)	83,113,113	1.31	6 (7%)
23	CLA	C	503	3	69,73,73	1.25	6 (8%)	83,113,113	1.29	5 (6%)
23	CLA	S	612	15	59,63,73	1.36	7 (11%)	71,101,113	1.37	5 (7%)
23	CLA	b	605	2	69,73,73	1.25	8 (11%)	83,113,113	1.25	5 (6%)
23	CLA	s	612	15	59,63,73	1.36	7 (11%)	71,101,113	1.36	5 (7%)
28	3PH	A	410	-	47,47,47	0.62	1 (2%)	51,52,52	0.60	1 (1%)
31	LNL	c	520	-	19,19,19	0.43	0	18,19,19	0.95	1 (5%)
23	CLA	b	604	2	69,73,73	1.25	8 (11%)	83,113,113	1.36	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	A	408	-	49,50,54	1.57	7 (14%)	58,61,65	1.45	7 (12%)
25	BCR	c	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
37	DGA	b	626	-	43,43,43	0.19	0	45,45,45	0.15	0
23	CLA	y	313	7	69,73,73	1.26	6 (8%)	83,113,113	1.26	6 (7%)
39	CHL	r	606	-	70,74,74	1.03	4 (5%)	80,114,114	1.65	11 (13%)
40	LUT	r	613	-	42,43,43	2.49	20 (47%)	51,60,60	3.11	24 (47%)
39	CHL	Y	306	7	52,56,74	1.19	4 (7%)	58,92,114	2.12	9 (15%)
23	CLA	G	602	7	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
23	CLA	N	614	7	53,57,73	1.42	6 (11%)	62,93,113	1.39	6 (9%)
42	XAT	r	615	-	39,47,47	3.22	20 (51%)	54,74,74	4.70	31 (57%)
23	CLA	r	601	14	53,57,73	1.44	6 (11%)	62,93,113	1.38	5 (8%)
23	CLA	C	504	43	69,73,73	1.25	7 (10%)	83,113,113	1.29	4 (4%)
23	CLA	S	602	15	61,65,73	1.35	7 (11%)	73,103,113	1.34	6 (8%)
24	PHO	D	402	-	58,69,69	2.05	10 (17%)	56,99,99	1.50	6 (10%)
39	CHL	G	620	-	70,74,74	1.04	4 (5%)	80,114,114	1.70	11 (13%)
23	CLA	C	512	3	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
40	LUT	Y	316	-	42,43,43	2.36	20 (47%)	51,60,60	3.15	23 (45%)
39	CHL	N	605	7	54,58,74	1.18	3 (5%)	59,94,114	2.15	9 (15%)
25	BCR	V	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	4 (7%)
31	LNL	c	517	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
23	CLA	d	405	4	69,73,73	1.25	8 (11%)	83,113,113	1.28	4 (4%)
41	NEX	N	617	-	38,46,46	4.10	32 (84%)	50,70,70	4.96	22 (44%)
23	CLA	B	614	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
33	DGD	H	502	-	63,63,67	0.87	1 (1%)	77,77,81	1.33	7 (9%)
23	CLA	b	613	2	69,73,73	1.26	7 (10%)	83,113,113	1.27	5 (6%)
23	CLA	c	510	3	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
39	CHL	n	606	-	70,74,74	1.03	4 (5%)	80,114,114	1.59	10 (12%)
39	CHL	g	607	-	70,74,74	1.03	5 (7%)	80,114,114	1.71	10 (12%)
23	CLA	n	612	7	53,57,73	1.43	7 (13%)	62,93,113	1.39	4 (6%)
23	CLA	b	607	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
30	LHG	s	616	23	48,48,48	1.39	8 (16%)	51,54,54	0.74	2 (3%)
40	LUT	N	615	-	42,43,43	2.58	21 (50%)	51,60,60	3.25	24 (47%)
41	NEX	R	618	-	38,46,46	3.93	31 (81%)	50,70,70	4.85	20 (40%)
23	CLA	n	611	30	53,57,73	1.43	7 (13%)	62,93,113	1.39	6 (9%)
42	XAT	y	302	-	39,47,47	3.39	24 (61%)	54,74,74	4.46	31 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	611	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	9 (10%)
31	LNL	a	413	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
23	CLA	B	606	2	69,73,73	1.27	9 (13%)	83,113,113	1.30	7 (8%)
23	CLA	C	501	3	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
39	CHL	s	607	-	53,57,74	1.19	4 (7%)	59,93,114	1.86	11 (18%)
23	CLA	y	306	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	9 (10%)
31	LNL	i	101	-	19,19,19	0.45	0	18,19,19	0.89	1 (5%)
23	CLA	B	603	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
23	CLA	G	611	30	53,57,73	1.43	8 (15%)	62,93,113	1.40	6 (9%)
39	CHL	Y	309	7	70,74,74	1.05	4 (5%)	80,114,114	1.61	10 (12%)
23	CLA	g	610	7	69,73,73	1.24	6 (8%)	83,113,113	1.30	8 (9%)
39	CHL	n	609	7	70,74,74	1.02	5 (7%)	80,114,114	1.61	11 (13%)
23	CLA	b	601	-	54,58,73	1.41	7 (12%)	65,95,113	1.42	7 (10%)
39	CHL	N	609	7	70,74,74	1.03	5 (7%)	80,114,114	1.62	11 (13%)
42	XAT	G	619	-	39,47,47	3.01	22 (56%)	54,74,74	4.57	30 (55%)
28	3PH	s	618	-	37,37,47	0.70	1 (2%)	41,42,52	0.64	1 (2%)
23	CLA	C	507	43	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
23	CLA	B	613	2	69,73,73	1.26	6 (8%)	83,113,113	1.27	5 (6%)
23	CLA	R	602	14	69,73,73	1.26	7 (10%)	83,113,113	1.28	4 (4%)
23	CLA	Y	314	7	69,73,73	1.26	9 (13%)	83,113,113	1.28	8 (9%)
23	CLA	g	612	7	53,57,73	1.43	7 (13%)	62,93,113	1.46	5 (8%)
39	CHL	Y	307	-	70,74,74	1.03	4 (5%)	80,114,114	1.64	9 (11%)
23	CLA	g	614	7	53,57,73	1.42	7 (13%)	62,93,113	1.38	6 (9%)
27	LMG	r	617	-	51,51,55	0.19	0	59,59,63	0.16	0
39	CHL	r	607	-	70,74,74	1.05	5 (7%)	80,114,114	1.68	12 (15%)
25	BCR	H	501	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	4 (7%)
23	CLA	S	611	15	53,57,73	1.43	7 (13%)	62,93,113	1.40	5 (8%)
31	LNL	B	623	-	19,19,19	0.45	0	18,19,19	0.86	1 (5%)
23	CLA	s	611	15	53,57,73	1.43	7 (13%)	62,93,113	1.40	4 (6%)
39	CHL	N	601	7	70,74,74	1.04	5 (7%)	80,114,114	1.69	11 (13%)
23	CLA	R	601	14	53,57,73	1.44	7 (13%)	62,93,113	1.40	6 (9%)
23	CLA	b	606	2	69,73,73	1.27	8 (11%)	83,113,113	1.29	8 (9%)
23	CLA	C	510	3	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
31	LNL	B	622	-	19,19,19	0.45	0	18,19,19	0.93	1 (5%)
23	CLA	D	405	4	69,73,73	1.24	8 (11%)	83,113,113	1.27	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	C	525	-	45,45,55	0.20	0	53,53,63	0.14	0
37	DGA	D	410	-	39,39,43	0.20	0	41,41,45	0.15	0
42	XAT	n	620	-	39,47,47	3.15	23 (58%)	54,74,74	4.56	31 (57%)
23	CLA	r	608	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
23	CLA	N	611	30	69,73,73	1.26	7 (10%)	83,113,113	1.25	6 (7%)
39	CHL	G	605	7	52,56,74	1.21	3 (5%)	58,92,114	2.07	12 (20%)
23	CLA	r	609	14	69,73,73	1.25	7 (10%)	83,113,113	1.26	7 (8%)
31	LNL	b	623	-	19,19,19	0.45	0	18,19,19	0.89	1 (5%)
30	LHG	d	404	-	48,48,48	1.36	8 (16%)	51,54,54	0.78	2 (3%)
39	CHL	G	607	-	70,74,74	1.04	4 (5%)	80,114,114	1.71	10 (12%)
23	CLA	b	612	2	69,73,73	1.25	7 (10%)	83,113,113	1.31	6 (7%)
31	LNL	c	518	-	19,19,19	0.44	0	18,19,19	0.92	1 (5%)
30	LHG	S	616	23	48,48,48	1.43	8 (16%)	51,54,54	0.73	2 (3%)
41	NEX	r	614	-	38,46,46	3.97	31 (81%)	50,70,70	4.87	22 (44%)
23	CLA	b	614	2	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
38	HEM	f	501	6,5	50,50,50	1.52	7 (14%)	66,82,82	1.21	7 (10%)
31	LNL	C	520	-	19,19,19	0.44	0	18,19,19	0.90	1 (5%)
41	NEX	Y	317	-	38,46,46	4.00	31 (81%)	50,70,70	4.95	22 (44%)
23	CLA	c	502	3	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
39	CHL	y	310	7	70,74,74	1.03	4 (5%)	80,114,114	1.59	11 (13%)
23	CLA	R	609	14	69,73,73	1.26	7 (10%)	83,113,113	1.26	5 (6%)
40	LUT	y	316	-	42,43,43	1.80	10 (23%)	51,60,60	2.77	19 (37%)
39	CHL	N	606	-	70,74,74	1.03	4 (5%)	80,114,114	1.60	10 (12%)
23	CLA	n	602	7	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
39	CHL	g	609	7	70,74,74	1.04	4 (5%)	80,114,114	1.68	11 (13%)
25	BCR	a	408	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	6 (10%)
39	CHL	n	605	7	52,56,74	1.19	4 (7%)	58,92,114	2.07	10 (17%)
24	PHO	a	406	-	58,69,69	2.03	10 (17%)	56,99,99	1.47	6 (10%)
23	CLA	g	604	-	53,57,73	1.43	8 (15%)	62,93,113	1.41	7 (11%)
39	CHL	n	607	-	70,74,74	1.04	4 (5%)	80,114,114	1.70	9 (11%)
31	LNL	B	625	-	19,19,19	0.45	0	18,19,19	0.91	1 (5%)
30	LHG	G	618	23	48,48,48	1.39	8 (16%)	51,54,54	0.75	2 (3%)
39	CHL	s	605	-	54,58,74	1.17	3 (5%)	59,94,114	1.91	11 (18%)
39	CHL	Y	308	-	54,58,74	1.17	4 (7%)	59,94,114	1.91	9 (15%)
27	LMG	c	523	-	46,46,55	0.19	0	54,54,63	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	y	318	23	48,48,48	1.39	8 (16%)	51,54,54	0.71	2 (3%)
23	CLA	g	613	7	69,73,73	1.26	6 (8%)	83,113,113	1.31	7 (8%)
23	CLA	r	612	14	53,57,73	1.43	7 (13%)	62,93,113	1.37	5 (8%)
23	CLA	y	315	7	69,73,73	1.27	8 (11%)	83,113,113	1.27	7 (8%)
23	CLA	Y	310	7	69,73,73	1.25	7 (10%)	83,113,113	1.28	8 (9%)
39	CHL	S	601	-	56,60,74	1.14	3 (5%)	63,97,114	1.86	10 (15%)
23	CLA	C	505	3	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
23	CLA	R	608	-	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
23	CLA	N	610	7	69,73,73	1.25	8 (11%)	83,113,113	1.26	8 (9%)
23	CLA	B	608	2	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
27	LMG	B	626	-	49,49,55	0.19	0	57,57,63	0.14	0
23	CLA	S	604	-	53,57,73	1.42	8 (15%)	62,93,113	1.44	6 (9%)
23	CLA	Y	305	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	8 (9%)
23	CLA	y	304	7	69,73,73	1.26	7 (10%)	83,113,113	1.29	7 (8%)
29	PL9	A	411	-	55,55,55	0.11	0	68,69,69	0.42	0
31	LNL	c	519	-	19,19,19	0.43	0	18,19,19	0.93	1 (5%)
23	CLA	G	603	7	64,68,73	1.30	8 (12%)	77,107,113	1.31	5 (6%)
23	CLA	s	609	15	60,64,73	1.36	8 (13%)	72,102,113	1.34	8 (11%)
23	CLA	R	611	14	53,57,73	1.43	7 (13%)	62,93,113	1.40	5 (8%)
29	PL9	D	407	-	55,55,55	0.08	0	68,69,69	0.21	0
39	CHL	G	608	-	54,58,74	1.19	5 (9%)	59,94,114	1.86	10 (16%)
23	CLA	S	613	15	69,73,73	1.26	6 (8%)	83,113,113	1.28	7 (8%)
31	LNL	C	518	-	19,19,19	0.44	0	18,19,19	0.97	1 (5%)
25	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
39	CHL	S	605	-	54,58,74	1.17	4 (7%)	59,94,114	1.94	10 (16%)
39	CHL	y	307	7	52,56,74	1.19	4 (7%)	58,92,114	2.09	9 (15%)
28	3PH	D	403	-	37,37,47	0.70	1 (2%)	41,42,52	0.65	1 (2%)
39	CHL	y	308	43	54,58,74	1.17	4 (7%)	59,94,114	1.90	9 (15%)
31	LNL	c	521	-	19,19,19	0.43	0	18,19,19	0.94	1 (5%)
30	LHG	D	404	-	42,42,48	1.43	8 (19%)	45,48,54	0.80	2 (4%)
40	LUT	s	614	-	42,43,43	2.74	23 (54%)	51,60,60	3.28	24 (47%)
25	BCR	v	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	4 (7%)
23	CLA	N	602	7	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
31	LNL	B	624	-	19,19,19	0.44	0	18,19,19	0.90	1 (5%)
30	LHG	R	616	23	37,37,48	1.56	8 (21%)	40,43,54	0.86	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	n	601	7	70,74,74	1.03	4 (5%)	80,114,114	1.68	9 (11%)
27	LMG	w	201	-	48,48,55	0.19	0	56,56,63	0.18	0
39	CHL	y	303	7	70,74,74	1.03	5 (7%)	80,114,114	1.67	11 (13%)
23	CLA	b	602	2	69,73,73	1.25	6 (8%)	83,113,113	1.29	6 (7%)
39	CHL	N	607	-	70,74,74	1.04	4 (5%)	80,114,114	1.68	9 (11%)
25	BCR	b	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
29	PL9	d	407	-	55,55,55	0.08	0	68,69,69	0.22	0
33	DGD	c	515	-	56,56,67	0.95	2 (3%)	70,70,81	1.45	9 (12%)
23	CLA	b	603	2	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
41	NEX	G	617	-	21,25,46	4.26	19 (90%)	28,38,70	5.44	11 (39%)
38	HEM	F	501	-	50,50,50	1.41	6 (12%)	66,82,82	1.22	6 (9%)
23	CLA	S	603	15	53,57,73	1.43	7 (13%)	62,93,113	1.42	5 (8%)
23	CLA	r	604	43	59,63,73	1.35	8 (13%)	71,101,113	1.37	8 (11%)
23	CLA	s	603	15	53,57,73	1.43	8 (15%)	62,93,113	1.41	6 (9%)
28	3PH	d	403	-	37,37,47	0.71	1 (2%)	41,42,52	0.66	1 (2%)
31	LNL	b	622	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
27	LMG	B	620	-	48,48,55	0.19	0	56,56,63	0.19	0

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	n	610	7	-	11/39/115/115	-
31	LNL	C	521	-	-	11/17/17/17	-
30	LHG	a	412	-	-	26/53/53/53	-
30	LHG	A	412	-	-	21/41/41/53	-
40	LUT	s	615	-	-	11/29/67/67	0/2/2/2
27	LMG	d	409	-	-	6/41/61/70	0/1/1/1
23	CLA	C	509	3	-	10/39/115/115	-
39	CHL	R	607	-	-	11/41/117/117	-
39	CHL	g	601	7	-	8/41/117/117	-
25	BCR	B	618	-	-	3/29/60/63	0/2/2/2
39	CHL	G	601	7	-	11/41/117/117	-
33	DGD	C	515	-	-	20/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	s	613	15	-	16/39/115/115	-
23	CLA	B	602	2	-	14/39/115/115	-
23	CLA	N	604	-	-	7/20/96/115	-
25	BCR	z	101	-	-	5/29/63/63	0/2/2/2
31	LNL	C	519	-	-	5/17/17/17	-
23	CLA	a	404	43	-	11/39/115/115	-
25	BCR	Z	101	-	-	5/29/63/63	0/2/2/2
28	3PH	L	102	-	-	14/42/42/49	-
23	CLA	D	406	4	-	17/39/115/115	-
41	NEX	s	617	-	-	8/15/40/83	0/1/1/3
23	CLA	c	507	43	-	8/39/115/115	-
31	LNL	A	413	-	-	10/17/17/17	-
23	CLA	r	611	14	-	6/20/96/115	-
40	LUT	n	616	-	-	14/29/67/67	0/2/2/2
33	DGD	d	411	-	-	18/51/91/95	0/2/2/2
23	CLA	G	610	7	-	10/39/115/115	-
23	CLA	g	602	7	-	5/39/115/115	-
40	LUT	G	616	-	-	9/29/67/67	0/2/2/2
42	XAT	n	617	-	-	6/31/93/93	0/4/4/4
23	CLA	s	610	30	-	16/39/115/115	-
23	CLA	N	612	7	-	9/20/96/115	-
30	LHG	Y	318	23	-	21/53/53/53	-
23	CLA	R	612	14	-	10/20/96/115	-
23	CLA	r	602	14	-	13/39/115/115	-
39	CHL	s	601	-	-	8/25/101/117	-
23	CLA	c	504	43	-	8/39/115/115	-
23	CLA	y	314	7	-	14/39/115/115	-
27	LMG	D	409	-	-	1/31/51/70	0/1/1/1
23	CLA	n	613	7	-	6/39/115/115	-
28	3PH	W	201	-	-	23/47/47/49	-
23	CLA	c	501	3	-	15/39/115/115	-
23	CLA	y	305	7	-	12/39/115/115	-
23	CLA	Y	303	7	-	13/39/115/115	-
41	NEX	S	617	-	-	6/11/36/83	0/1/1/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LNL	b	625	-	-	9/17/17/17	-
39	CHL	g	608	-	-	10/22/98/117	-
31	LNL	C	522	-	-	11/17/17/17	-
31	LNL	I	101	-	-	11/17/17/17	-
23	CLA	c	505	3	-	8/39/115/115	-
26	SQD	a	409	-	-	18/43/63/69	0/1/1/1
28	3PH	C	524	-	-	19/49/49/49	-
28	3PH	X	201	-	-	13/47/47/49	-
31	LNL	A	414	-	-	8/17/17/17	-
30	LHG	L	103	-	-	25/53/53/53	-
23	CLA	Y	313	-	-	10/39/115/115	-
39	CHL	G	606	-	-	4/22/98/117	-
23	CLA	Y	311	30	-	9/39/115/115	-
23	CLA	r	610	30	-	12/39/115/115	-
39	CHL	r	605	-	-	6/22/98/117	-
25	BCR	h	501	-	-	7/29/63/63	0/2/2/2
23	CLA	a	405	43	-	1/20/96/115	-
23	CLA	d	406	4	-	7/39/115/115	-
39	CHL	S	606	-	-	8/22/98/117	-
23	CLA	b	608	2	-	10/39/115/115	-
39	CHL	s	606	-	-	6/22/98/117	-
39	CHL	n	608	-	-	6/22/98/117	-
23	CLA	a	407	1	-	5/33/109/115	-
23	CLA	Y	312	7	-	9/39/115/115	-
23	CLA	s	608	-	-	9/20/96/115	-
23	CLA	c	512	3	-	21/39/115/115	-
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
23	CLA	g	603	7	-	10/39/115/115	-
23	CLA	c	513	3	-	8/33/109/115	-
23	CLA	g	611	-	-	11/39/115/115	-
41	NEX	g	617	-	-	14/27/83/83	0/3/3/3
35	VIV	C	523	-	-	12/19/30/30	0/2/2/2
41	NEX	n	618	-	-	14/27/83/83	0/3/3/3
23	CLA	R	603	14	-	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	G	604	-	-	6/20/96/115	-
23	CLA	A	404	43	-	5/20/96/115	-
23	CLA	B	601	-	-	12/20/96/115	-
23	CLA	a	403	1	-	10/39/115/115	-
23	CLA	B	616	2	-	11/39/115/115	-
23	CLA	n	604	-	-	7/20/96/115	-
39	CHL	g	619	43	-	10/41/117/117	-
39	CHL	G	609	7	-	12/41/117/117	-
23	CLA	s	604	-	-	8/20/96/115	-
40	LUT	R	613	-	-	16/29/67/67	0/2/2/2
23	CLA	N	613	7	-	12/39/115/115	-
30	LHG	N	618	23	-	25/53/53/53	-
31	LNL	b	624	-	-	9/17/17/17	-
23	CLA	c	508	3	-	3/39/115/115	-
23	CLA	c	503	3	-	7/39/115/115	-
23	CLA	R	610	30	-	11/39/115/115	-
23	CLA	C	502	3	-	12/39/115/115	-
23	CLA	B	615	2	-	9/39/115/115	-
23	CLA	b	615	2	-	6/39/115/115	-
23	CLA	Y	304	7	-	12/39/115/115	-
39	CHL	R	605	-	-	4/22/98/117	-
32	PAM	B	621	-	-	5/15/15/15	-
23	CLA	y	311	7	-	10/39/115/115	-
39	CHL	R	606	-	-	11/41/117/117	-
40	LUT	Y	315	-	-	17/29/67/67	0/2/2/2
30	LHG	d	408	-	-	15/53/53/53	-
23	CLA	C	513	3	-	12/39/115/115	-
23	CLA	G	613	7	-	12/39/115/115	-
27	LMG	b	628	-	-	11/45/65/70	0/1/1/1
23	CLA	r	603	14	-	5/33/109/115	-
23	CLA	B	610	43	-	8/39/115/115	-
23	CLA	b	610	43	-	10/39/115/115	-
24	PHO	A	405	-	-	10/37/103/103	0/5/6/6
25	BCR	C	514	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	3	-	15/39/115/115	-
30	LHG	r	616	23	-	19/41/41/53	-
23	CLA	y	312	30	-	8/39/115/115	-
23	CLA	C	508	3	-	7/39/115/115	-
40	LUT	y	317	-	-	15/29/67/67	0/2/2/2
26	SQD	L	101	-	-	24/49/69/69	0/1/1/1
32	PAM	b	621	-	-	3/15/15/15	-
39	CHL	N	608	-	-	8/22/98/117	-
40	LUT	g	616	-	-	10/29/67/67	0/2/2/2
27	LMG	A	409	-	-	11/48/68/70	0/1/1/1
42	XAT	R	615	-	-	14/31/93/93	0/4/4/4
25	BCR	b	618	-	-	5/29/63/63	0/2/2/2
23	CLA	n	603	7	-	11/39/115/115	-
27	LMG	b	620	-	-	8/46/66/70	0/1/1/1
23	CLA	R	604	43	-	9/27/103/115	-
24	PHO	d	402	-	-	5/37/103/103	0/5/6/6
23	CLA	A	402	1	-	10/39/115/115	-
25	BCR	A	407	-	-	4/29/63/63	0/2/2/2
23	CLA	s	602	15	-	9/30/106/115	-
23	CLA	C	506	3	-	9/27/103/115	-
23	CLA	B	609	2	-	8/39/115/115	-
25	BCR	b	617	-	-	11/29/63/63	0/2/2/2
39	CHL	y	309	-	-	5/22/98/117	-
25	BCR	D	411	-	-	5/29/63/63	0/2/2/2
23	CLA	G	614	7	-	8/20/96/115	-
42	XAT	N	619	-	-	13/31/93/93	0/4/4/4
26	SQD	M	101	-	-	24/45/65/69	0/1/1/1
39	CHL	S	607	-	-	7/21/97/117	-
41	NEX	R	614	-	-	13/27/83/83	0/3/3/3
31	LNL	C	517	-	-	12/17/17/17	-
39	CHL	g	605	7	-	7/20/96/117	-
40	LUT	S	614	-	-	15/29/67/67	0/2/2/2
39	CHL	g	606	-	-	4/22/98/117	-
23	CLA	c	511	3	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	3PH	T	101	-	-	22/49/49/49	-
23	CLA	c	509	3	-	10/39/115/115	-
42	XAT	Y	301	-	-	17/31/93/93	0/4/4/4
35	VIV	y	301	-	-	15/19/30/30	0/2/2/2
25	BCR	B	617	-	-	10/29/63/63	0/2/2/2
23	CLA	n	614	7	-	10/20/96/115	-
31	LNL	c	522	-	-	7/17/17/17	-
28	3PH	w	202	-	-	17/49/49/49	-
40	LUT	g	615	-	-	19/29/67/67	0/2/2/2
40	LUT	G	615	-	-	22/29/67/67	0/2/2/2
23	CLA	S	608	-	-	3/20/96/115	-
23	CLA	A	403	43	-	10/39/115/115	-
23	CLA	G	612	7	-	8/20/96/115	-
23	CLA	S	609	15	-	12/29/105/115	-
23	CLA	B	612	2	-	11/39/115/115	-
28	3PH	x	201	-	-	13/47/47/49	-
23	CLA	B	604	2	-	9/39/115/115	-
27	LMG	R	617	-	-	14/46/66/70	0/1/1/1
25	BCR	d	410	-	-	9/29/63/63	0/2/2/2
30	LHG	D	408	-	-	29/53/53/53	-
29	PL9	a	411	-	-	12/53/73/73	0/1/1/1
23	CLA	b	609	-	-	10/39/115/115	-
23	CLA	A	406	1	-	1/33/109/115	-
30	LHG	n	619	23	-	23/49/49/53	-
28	3PH	a	410	-	-	21/49/49/49	-
23	CLA	b	616	2	-	12/39/115/115	-
40	LUT	S	615	-	-	16/29/67/67	0/2/2/2
23	CLA	B	605	2	-	13/39/115/115	-
40	LUT	n	615	-	-	14/29/67/67	0/2/2/2
23	CLA	S	610	30	-	16/39/115/115	-
31	LNL	a	401	-	-	11/17/17/17	-
30	LHG	b	627	-	-	22/53/53/53	-
23	CLA	C	511	3	-	11/39/115/115	-
39	CHL	Y	302	7	-	13/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	619	-	-	4/29/63/63	0/2/2/2
30	LHG	g	618	-	-	15/53/53/53	-
23	CLA	B	607	-	-	21/39/115/115	-
40	LUT	N	616	-	-	20/29/67/67	0/2/2/2
23	CLA	B	611	2	-	10/39/115/115	-
23	CLA	N	603	7	-	10/39/115/115	-
23	CLA	C	503	3	-	8/39/115/115	-
23	CLA	S	612	15	-	9/27/103/115	-
23	CLA	b	605	2	-	15/39/115/115	-
23	CLA	s	612	15	-	7/27/103/115	-
28	3PH	A	410	-	-	18/49/49/49	-
31	LNL	c	520	-	-	6/17/17/17	-
23	CLA	b	604	2	-	6/39/115/115	-
26	SQD	A	408	-	-	29/45/65/69	0/1/1/1
25	BCR	c	514	-	-	7/29/63/63	0/2/2/2
37	DGA	b	626	-	-	14/45/45/45	-
23	CLA	y	313	7	-	9/39/115/115	-
39	CHL	r	606	-	-	12/41/117/117	-
40	LUT	r	613	-	-	11/29/67/67	0/2/2/2
39	CHL	Y	306	7	-	4/20/96/117	-
23	CLA	G	602	7	-	5/39/115/115	-
23	CLA	N	614	7	-	7/20/96/115	-
42	XAT	r	615	-	-	14/31/93/93	0/4/4/4
23	CLA	r	601	14	-	12/20/96/115	-
23	CLA	C	504	43	-	8/39/115/115	-
23	CLA	S	602	15	-	10/30/106/115	-
24	PHO	D	402	-	-	9/37/103/103	0/5/6/6
39	CHL	G	620	-	-	14/41/117/117	-
23	CLA	C	512	3	-	17/39/115/115	-
40	LUT	Y	316	-	-	15/29/67/67	0/2/2/2
39	CHL	N	605	7	-	7/22/98/117	-
25	BCR	V	101	-	-	11/29/63/63	0/2/2/2
31	LNL	c	517	-	-	5/17/17/17	-
23	CLA	d	405	4	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	NEX	N	617	-	-	12/27/83/83	0/3/3/3
23	CLA	B	614	2	-	13/39/115/115	-
33	DGD	H	502	-	-	24/51/91/95	0/2/2/2
23	CLA	b	613	2	-	13/39/115/115	-
23	CLA	c	510	3	-	14/39/115/115	-
39	CHL	n	606	-	-	8/41/117/117	-
39	CHL	g	607	-	-	15/41/117/117	-
23	CLA	n	612	7	-	5/20/96/115	-
23	CLA	b	607	-	-	16/39/115/115	-
30	LHG	s	616	23	-	19/53/53/53	-
40	LUT	N	615	-	-	13/29/67/67	0/2/2/2
41	NEX	R	618	-	-	12/27/83/83	0/3/3/3
23	CLA	n	611	30	-	7/20/96/115	-
42	XAT	y	302	-	-	18/31/93/93	0/4/4/4
23	CLA	b	611	2	-	6/39/115/115	-
31	LNL	a	413	-	-	9/17/17/17	-
23	CLA	B	606	2	-	9/39/115/115	-
23	CLA	C	501	3	-	13/39/115/115	-
39	CHL	s	607	-	-	8/21/97/117	-
23	CLA	y	306	-	-	20/39/115/115	-
31	LNL	i	101	-	-	9/17/17/17	-
23	CLA	B	603	2	-	10/39/115/115	-
23	CLA	G	611	30	-	10/20/96/115	-
39	CHL	Y	309	7	-	6/41/117/117	-
23	CLA	g	610	7	-	10/39/115/115	-
39	CHL	n	609	7	-	10/41/117/117	-
23	CLA	b	601	-	-	7/21/97/115	-
39	CHL	N	609	7	-	8/41/117/117	-
42	XAT	G	619	-	-	11/31/93/93	0/4/4/4
28	3PH	s	618	-	-	14/39/39/49	-
23	CLA	C	507	43	-	11/39/115/115	-
23	CLA	B	613	2	-	8/39/115/115	-
23	CLA	R	602	14	-	6/39/115/115	-
23	CLA	Y	314	7	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	g	612	7	-	6/20/96/115	-
39	CHL	Y	307	-	-	3/41/117/117	-
23	CLA	g	614	7	-	8/20/96/115	-
27	LMG	r	617	-	-	11/46/66/70	0/1/1/1
39	CHL	r	607	-	-	11/41/117/117	-
25	BCR	H	501	-	-	7/29/63/63	0/2/2/2
23	CLA	S	611	15	-	9/20/96/115	-
31	LNL	B	623	-	-	10/17/17/17	-
23	CLA	s	611	15	-	8/20/96/115	-
39	CHL	N	601	7	-	9/41/117/117	-
23	CLA	R	601	14	-	12/20/96/115	-
23	CLA	b	606	2	-	10/39/115/115	-
23	CLA	C	510	3	-	12/39/115/115	-
31	LNL	B	622	-	-	7/17/17/17	-
23	CLA	D	405	4	-	9/39/115/115	-
27	LMG	C	525	-	-	10/40/60/70	0/1/1/1
37	DGA	D	410	-	-	12/41/41/45	-
42	XAT	n	620	-	-	9/31/93/93	0/4/4/4
23	CLA	r	608	-	-	9/39/115/115	-
23	CLA	N	611	30	-	11/39/115/115	-
39	CHL	G	605	7	-	8/20/96/117	-
23	CLA	r	609	14	-	7/39/115/115	-
31	LNL	b	623	-	-	10/17/17/17	-
30	LHG	d	404	-	-	20/53/53/53	-
39	CHL	G	607	-	-	11/41/117/117	-
23	CLA	b	612	2	-	12/39/115/115	-
31	LNL	c	518	-	-	12/17/17/17	-
30	LHG	S	616	23	-	14/53/53/53	-
41	NEX	r	614	-	-	9/27/83/83	0/3/3/3
23	CLA	b	614	2	-	12/39/115/115	-
38	HEM	f	501	6,5	-	1/14/54/54	-
31	LNL	C	520	-	-	11/17/17/17	-
41	NEX	Y	317	-	-	14/27/83/83	0/3/3/3
23	CLA	c	502	3	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	y	310	7	-	10/41/117/117	-
23	CLA	R	609	14	-	6/39/115/115	-
40	LUT	y	316	-	-	17/29/67/67	0/2/2/2
39	CHL	N	606	-	-	9/41/117/117	-
23	CLA	n	602	7	-	11/39/115/115	-
39	CHL	g	609	7	-	13/41/117/117	-
25	BCR	a	408	-	-	4/29/63/63	0/2/2/2
39	CHL	n	605	7	-	6/20/96/117	-
24	PHO	a	406	-	-	10/37/103/103	0/5/6/6
23	CLA	g	604	-	-	8/20/96/115	-
39	CHL	n	607	-	-	10/41/117/117	-
31	LNL	B	625	-	-	7/17/17/17	-
30	LHG	G	618	23	-	19/53/53/53	-
39	CHL	s	605	-	-	5/22/98/117	-
39	CHL	Y	308	-	-	8/22/98/117	-
27	LMG	c	523	-	-	9/41/61/70	0/1/1/1
30	LHG	y	318	23	-	22/53/53/53	-
23	CLA	g	613	7	-	10/39/115/115	-
23	CLA	r	612	14	-	7/20/96/115	-
23	CLA	y	315	7	-	20/39/115/115	-
23	CLA	Y	310	7	-	13/39/115/115	-
39	CHL	S	601	-	-	6/25/101/117	-
23	CLA	C	505	3	-	6/39/115/115	-
23	CLA	R	608	-	-	7/39/115/115	-
23	CLA	N	610	7	-	10/39/115/115	-
23	CLA	B	608	2	-	10/39/115/115	-
27	LMG	B	626	-	-	8/44/64/70	0/1/1/1
23	CLA	S	604	-	-	7/20/96/115	-
23	CLA	Y	305	-	-	12/39/115/115	-
23	CLA	y	304	7	-	13/39/115/115	-
29	PL9	A	411	-	-	7/53/73/73	0/1/1/1
31	LNL	c	519	-	-	11/17/17/17	-
23	CLA	G	603	7	-	3/33/109/115	-
23	CLA	s	609	15	-	11/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	R	611	14	-	8/20/96/115	-
29	PL9	D	407	-	-	10/53/73/73	0/1/1/1
39	CHL	G	608	-	-	10/22/98/117	-
23	CLA	S	613	15	-	14/39/115/115	-
31	LNL	C	518	-	-	8/17/17/17	-
25	BCR	K	101	-	-	4/29/63/63	0/2/2/2
39	CHL	S	605	-	-	6/22/98/117	-
39	CHL	y	307	7	-	4/20/96/117	-
28	3PH	D	403	-	-	13/39/39/49	-
39	CHL	y	308	43	-	5/22/98/117	-
31	LNL	c	521	-	-	7/17/17/17	-
30	LHG	D	404	-	-	10/47/47/53	-
40	LUT	s	614	-	-	18/29/67/67	0/2/2/2
25	BCR	v	101	-	-	10/29/63/63	0/2/2/2
23	CLA	N	602	7	-	4/39/115/115	-
31	LNL	B	624	-	-	8/17/17/17	-
30	LHG	R	616	23	-	17/42/42/53	-
39	CHL	n	601	7	-	10/41/117/117	-
27	LMG	w	201	-	-	5/43/63/70	0/1/1/1
39	CHL	y	303	7	-	15/41/117/117	-
23	CLA	b	602	2	-	12/39/115/115	-
39	CHL	N	607	-	-	9/41/117/117	-
25	BCR	b	619	-	-	6/29/63/63	0/2/2/2
29	PL9	d	407	-	-	10/53/73/73	0/1/1/1
33	DGD	c	515	-	-	13/44/84/95	0/2/2/2
23	CLA	b	603	2	-	11/39/115/115	-
41	NEX	G	617	-	-	7/16/47/83	0/2/2/3
38	HEM	F	501	-	-	3/14/54/54	-
23	CLA	S	603	15	-	12/20/96/115	-
23	CLA	r	604	43	-	8/27/103/115	-
23	CLA	s	603	15	-	12/20/96/115	-
28	3PH	d	403	-	-	10/39/39/49	-
31	LNL	b	622	-	-	8/17/17/17	-
27	LMG	B	620	-	-	7/43/63/70	0/1/1/1

The worst 5 of 2393 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	PHO	C1B-C2B	9.46	1.50	1.39
24	d	402	PHO	C1B-C2B	9.39	1.50	1.39
24	D	402	PHO	C1B-C2B	9.37	1.50	1.39
24	a	406	PHO	C1B-C2B	9.33	1.49	1.39
42	y	302	XAT	C10-C9	8.32	1.46	1.35

The worst 5 of 2613 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

There are no chirality outliers.

5 of 3750 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.

310 monomers are involved in 716 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	n	610	CLA	7	0
31	C	521	LNL	4	0
30	a	412	LHG	4	0
30	A	412	LHG	1	0
40	s	615	LUT	3	0
27	d	409	LMG	2	0
23	C	509	CLA	2	0
39	R	607	CHL	3	0
25	B	618	BCR	2	0
39	G	601	CHL	2	0
33	C	515	DGD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	s	613	CLA	7	0
23	B	602	CLA	6	0
23	N	604	CLA	1	0
25	z	101	BCR	1	0
31	C	519	LNL	1	0
23	a	404	CLA	3	0
25	Z	101	BCR	3	0
28	L	102	3PH	2	0
23	D	406	CLA	1	0
41	s	617	NEX	2	0
23	c	507	CLA	1	0
31	A	413	LNL	1	0
23	r	611	CLA	1	0
40	n	616	LUT	5	0
33	d	411	DGD	3	0
23	G	610	CLA	6	0
23	g	602	CLA	3	0
40	G	616	LUT	5	0
42	n	617	XAT	3	0
23	s	610	CLA	2	0
23	N	612	CLA	4	0
30	Y	318	LHG	5	0
23	r	602	CLA	1	0
23	c	504	CLA	1	0
23	y	314	CLA	4	0
27	D	409	LMG	1	0
23	n	613	CLA	4	0
28	W	201	3PH	2	0
23	c	501	CLA	1	0
23	y	305	CLA	4	0
23	Y	303	CLA	5	0
41	S	617	NEX	2	0
31	b	625	LNL	1	0
39	g	608	CHL	3	0
31	C	522	LNL	2	0
23	c	505	CLA	4	0
26	a	409	SQD	3	0
28	C	524	3PH	4	0
31	A	414	LNL	2	0
30	L	103	LHG	2	0
23	Y	313	CLA	4	0
39	G	606	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Y	311	CLA	1	0
23	r	610	CLA	1	0
39	r	605	CHL	3	0
39	S	606	CHL	4	0
23	b	608	CLA	1	0
39	s	606	CHL	2	0
39	n	608	CHL	2	0
23	a	407	CLA	1	0
23	Y	312	CLA	1	0
23	s	608	CLA	1	0
23	c	512	CLA	3	0
25	k	101	BCR	1	0
23	g	603	CLA	3	0
23	c	513	CLA	3	0
23	g	611	CLA	1	0
41	g	617	NEX	4	0
35	C	523	VIV	5	0
41	n	618	NEX	4	0
23	G	604	CLA	2	0
23	a	403	CLA	2	0
23	B	616	CLA	6	0
23	n	604	CLA	1	0
39	G	609	CHL	8	0
23	s	604	CLA	2	0
40	R	613	LUT	2	0
23	N	613	CLA	3	0
30	N	618	LHG	3	0
31	b	624	LNL	1	0
23	c	503	CLA	2	0
23	R	610	CLA	2	0
23	B	615	CLA	7	0
23	b	615	CLA	3	0
23	Y	304	CLA	3	0
39	R	605	CHL	2	0
32	B	621	PAM	1	0
23	y	311	CLA	2	0
39	R	606	CHL	3	0
36	D	401	BCT	5	0
40	Y	315	LUT	4	0
30	d	408	LHG	4	0
23	C	513	CLA	1	0
23	G	613	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	628	LMG	1	0
23	r	603	CLA	2	0
23	B	610	CLA	5	0
23	b	610	CLA	5	0
24	A	405	PHO	3	0
25	C	514	BCR	6	0
23	c	506	CLA	4	0
23	y	312	CLA	2	0
23	C	508	CLA	3	0
40	y	317	LUT	2	0
26	L	101	SQD	4	0
39	N	608	CHL	2	0
40	g	616	LUT	6	0
27	A	409	LMG	5	0
42	R	615	XAT	2	0
25	b	618	BCR	2	0
23	n	603	CLA	5	0
27	b	620	LMG	8	0
23	R	604	CLA	2	0
24	d	402	PHO	2	0
23	A	402	CLA	2	0
25	A	407	BCR	4	0
23	s	602	CLA	5	0
23	C	506	CLA	1	0
23	B	609	CLA	2	0
25	b	617	BCR	1	0
25	D	411	BCR	2	0
42	N	619	XAT	6	0
26	M	101	SQD	2	0
39	S	607	CHL	4	0
31	C	517	LNL	1	0
40	S	614	LUT	3	0
39	g	606	CHL	2	0
23	c	511	CLA	3	0
42	Y	301	XAT	4	0
35	y	301	VIV	4	0
25	B	617	BCR	7	0
23	n	614	CLA	1	0
28	w	202	3PH	4	0
40	g	615	LUT	8	0
40	G	615	LUT	7	0
23	S	608	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	403	CLA	4	0
23	G	612	CLA	2	0
23	S	609	CLA	9	0
23	B	612	CLA	1	0
28	x	201	3PH	3	0
23	B	604	CLA	2	0
27	R	617	LMG	3	0
25	d	410	BCR	3	0
36	d	401	BCT	5	0
30	D	408	LHG	5	0
29	a	411	PL9	7	0
23	b	609	CLA	4	0
23	A	406	CLA	1	0
30	n	619	LHG	2	0
28	a	410	3PH	9	0
23	b	616	CLA	3	0
40	S	615	LUT	3	0
23	B	605	CLA	1	0
40	n	615	LUT	6	0
23	S	610	CLA	2	0
31	a	401	LNL	1	0
30	b	627	LHG	1	0
23	C	511	CLA	3	0
39	Y	302	CHL	3	0
25	B	619	BCR	5	0
30	g	618	LHG	3	0
23	B	607	CLA	7	0
40	N	616	LUT	6	0
23	B	611	CLA	1	0
23	N	603	CLA	5	0
23	S	612	CLA	1	0
23	b	605	CLA	2	0
23	s	612	CLA	3	0
28	A	410	3PH	4	0
31	c	520	LNL	1	0
23	b	604	CLA	2	0
26	A	408	SQD	2	0
25	c	514	BCR	3	0
37	b	626	DGA	4	0
23	y	313	CLA	3	0
39	r	606	CHL	4	0
40	r	613	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	Y	306	CHL	1	0
23	G	602	CLA	4	0
23	N	614	CLA	2	0
42	r	615	XAT	3	0
23	C	504	CLA	1	0
23	S	602	CLA	1	0
24	D	402	PHO	4	0
39	G	620	CHL	2	0
23	C	512	CLA	2	0
40	Y	316	LUT	5	0
39	N	605	CHL	1	0
31	c	517	LNL	3	0
23	d	405	CLA	4	0
41	N	617	NEX	2	0
23	B	614	CLA	6	0
33	H	502	DGD	1	0
23	b	613	CLA	1	0
23	c	510	CLA	3	0
39	n	606	CHL	3	0
39	g	607	CHL	1	0
23	n	612	CLA	3	0
23	b	607	CLA	4	0
30	s	616	LHG	2	0
40	N	615	LUT	4	0
41	R	618	NEX	2	0
42	y	302	XAT	2	0
23	b	611	CLA	2	0
31	a	413	LNL	1	0
23	B	606	CLA	3	0
23	C	501	CLA	1	0
39	s	607	CHL	1	0
23	y	306	CLA	3	0
31	i	101	LNL	2	0
23	B	603	CLA	1	0
39	Y	309	CHL	3	0
23	g	610	CLA	4	0
39	n	609	CHL	4	0
23	b	601	CLA	1	0
39	N	609	CHL	3	0
42	G	619	XAT	4	0
28	s	618	3PH	1	0
23	C	507	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	613	CLA	2	0
23	Y	314	CLA	5	0
23	g	612	CLA	4	0
39	Y	307	CHL	4	0
27	r	617	LMG	3	0
39	r	607	CHL	3	0
25	H	501	BCR	2	0
23	S	611	CLA	3	0
31	B	623	LNL	4	0
23	s	611	CLA	3	0
39	N	601	CHL	8	0
23	b	606	CLA	4	0
31	B	622	LNL	2	0
23	D	405	CLA	5	0
27	C	525	LMG	3	0
37	D	410	DGA	3	0
42	n	620	XAT	5	0
23	r	608	CLA	1	0
23	N	611	CLA	4	0
23	r	609	CLA	2	0
31	b	623	LNL	1	0
30	d	404	LHG	1	0
39	G	607	CHL	2	0
23	b	612	CLA	1	0
30	S	616	LHG	3	0
41	r	614	NEX	2	0
23	b	614	CLA	3	0
38	f	501	HEM	2	0
41	Y	317	NEX	1	0
39	y	310	CHL	1	0
23	R	609	CLA	1	0
40	y	316	LUT	3	0
39	N	606	CHL	3	0
23	n	602	CLA	2	0
39	g	609	CHL	1	0
25	a	408	BCR	4	0
39	n	605	CHL	3	0
24	a	406	PHO	3	0
23	g	604	CLA	2	0
39	n	607	CHL	4	0
31	B	625	LNL	3	0
30	G	618	LHG	3	0

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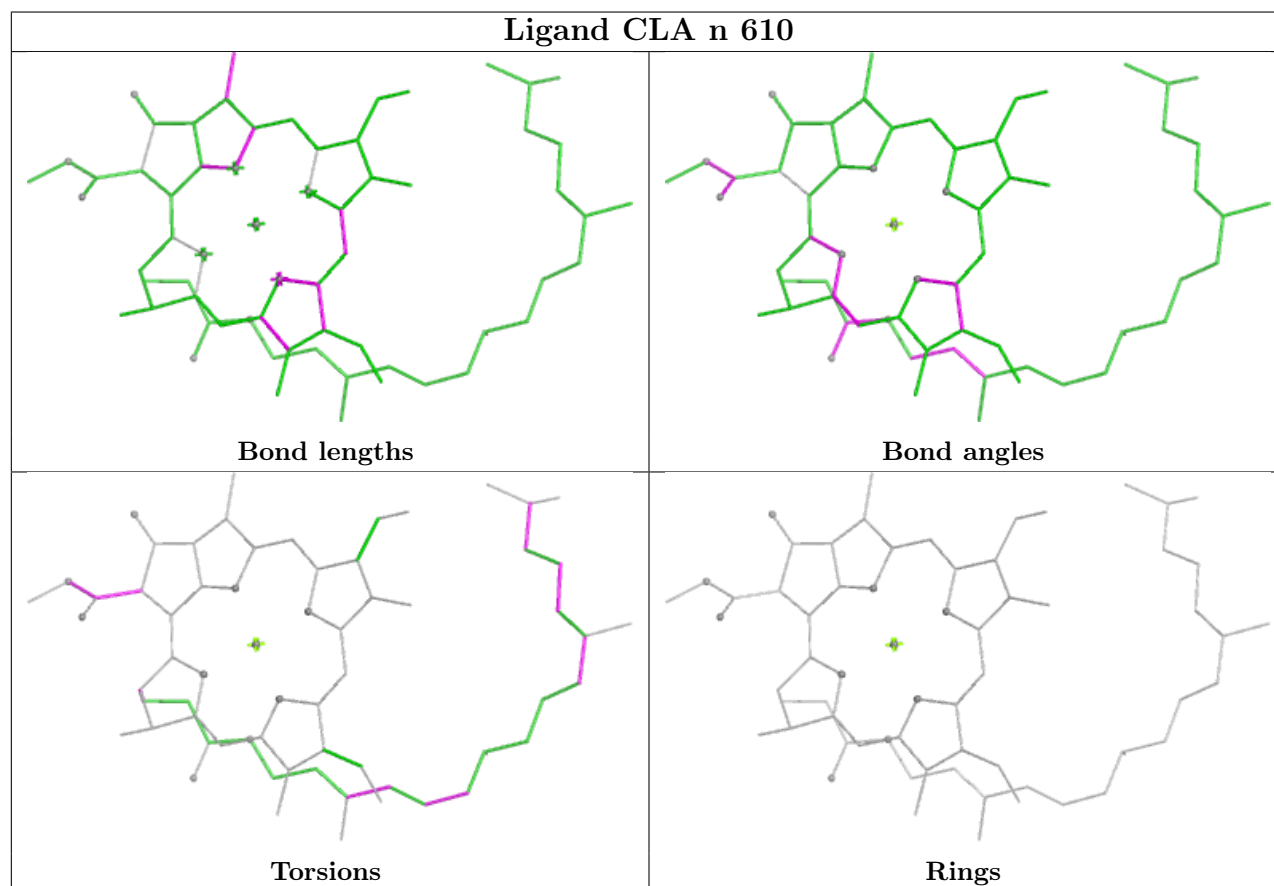
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39	s	605	CHL	1	0
39	Y	308	CHL	1	0
27	c	523	LMG	2	0
30	y	318	LHG	3	0
23	g	613	CLA	3	0
23	r	612	CLA	2	0
23	y	315	CLA	4	0
23	Y	310	CLA	2	0
39	S	601	CHL	1	0
23	C	505	CLA	3	0
23	R	608	CLA	2	0
23	N	610	CLA	5	0
23	B	608	CLA	3	0
23	S	604	CLA	3	0
23	Y	305	CLA	3	0
23	y	304	CLA	3	0
29	A	411	PL9	9	0
31	c	519	LNL	2	0
23	G	603	CLA	4	0
23	s	609	CLA	6	0
23	R	611	CLA	1	0
29	D	407	PL9	2	0
39	G	608	CHL	2	0
23	S	613	CLA	2	0
39	S	605	CHL	1	0
28	D	403	3PH	2	0
31	c	521	LNL	2	0
30	D	404	LHG	1	0
25	v	101	BCR	1	0
23	N	602	CLA	3	0
39	n	601	CHL	3	0
27	w	201	LMG	1	0
39	y	303	CHL	4	0
23	b	602	CLA	4	0
39	N	607	CHL	1	0
25	b	619	BCR	3	0
29	d	407	PL9	3	0
33	c	515	DGD	1	0
23	b	603	CLA	2	0
41	G	617	NEX	2	0
38	F	501	HEM	3	0
23	S	603	CLA	1	0

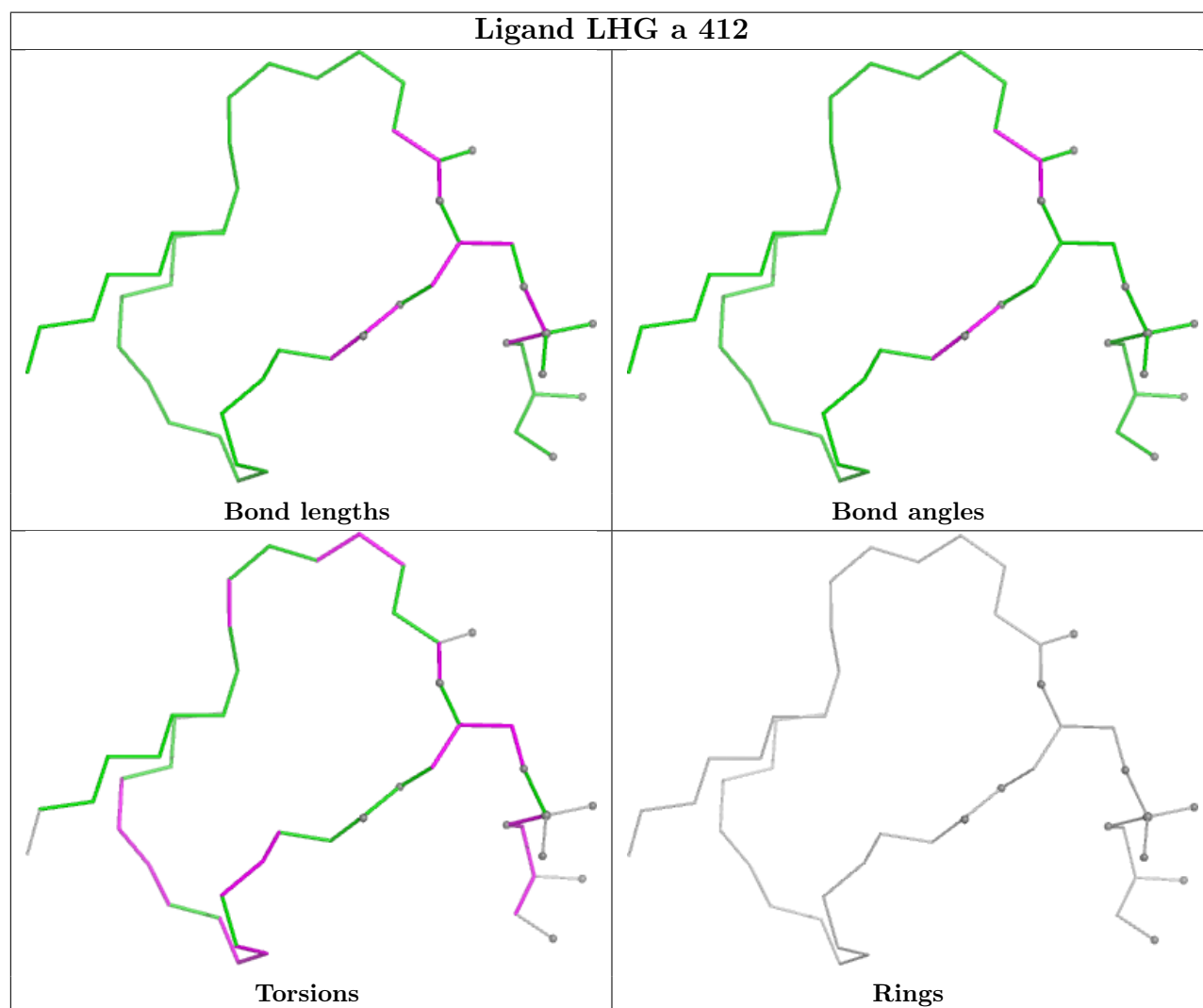
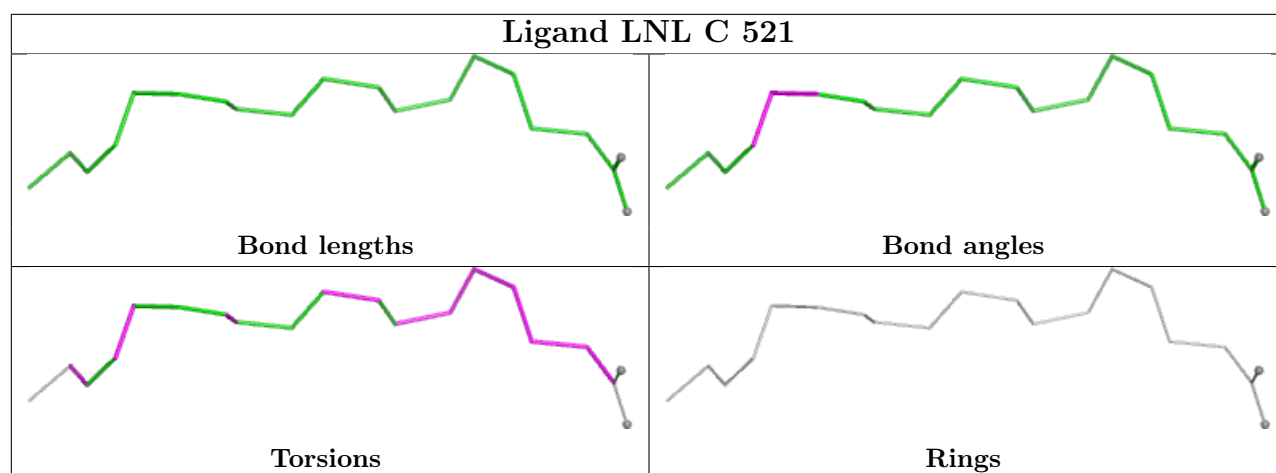
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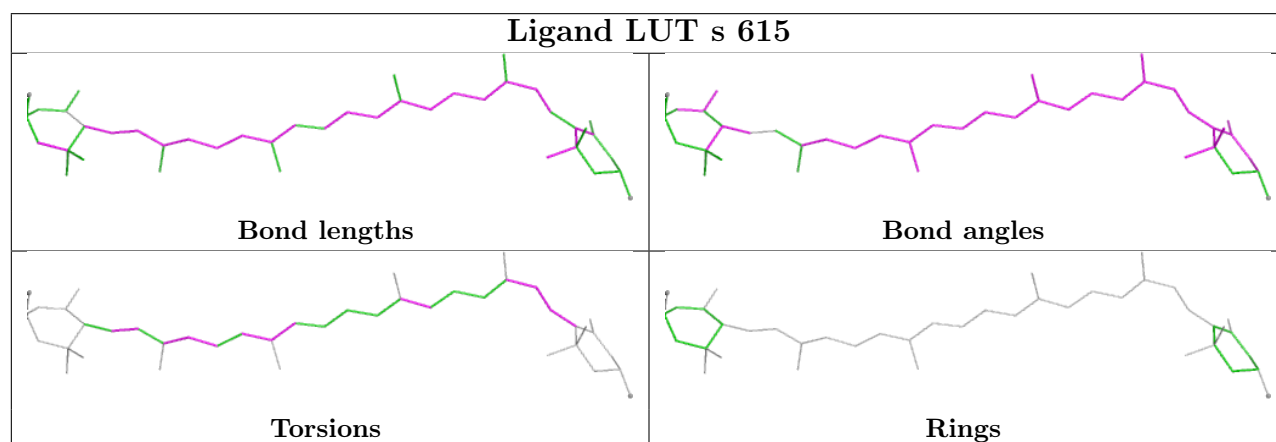
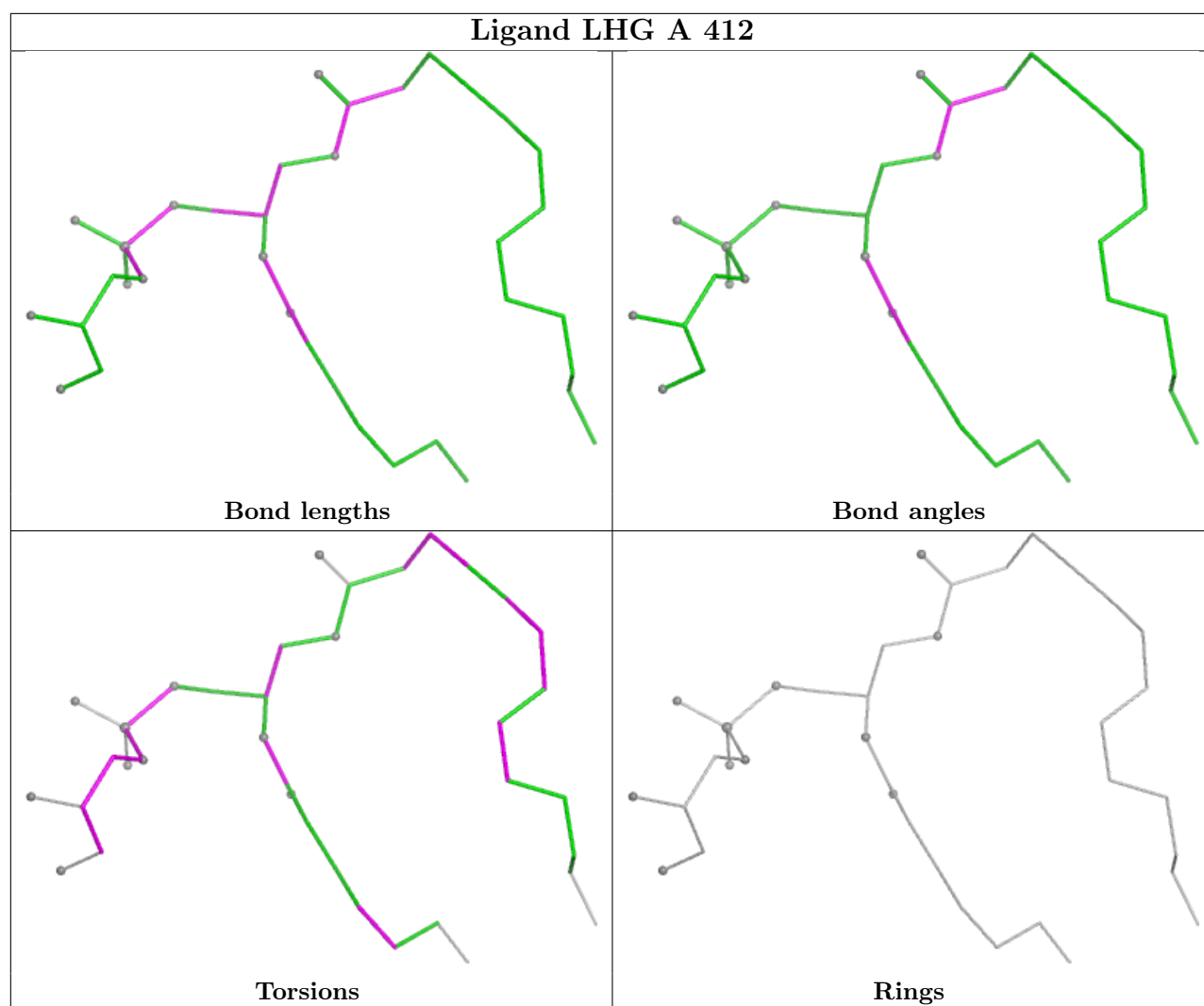
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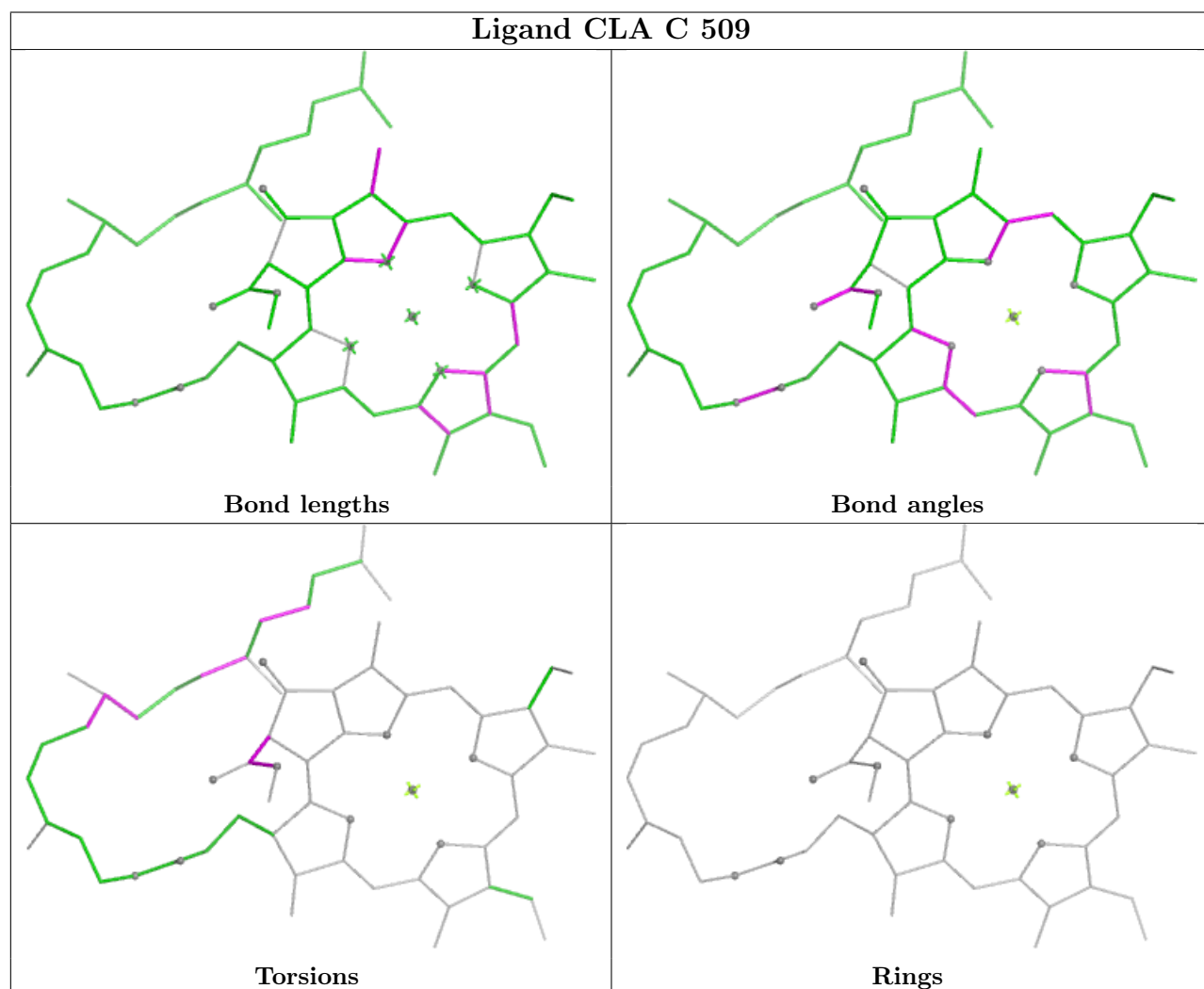
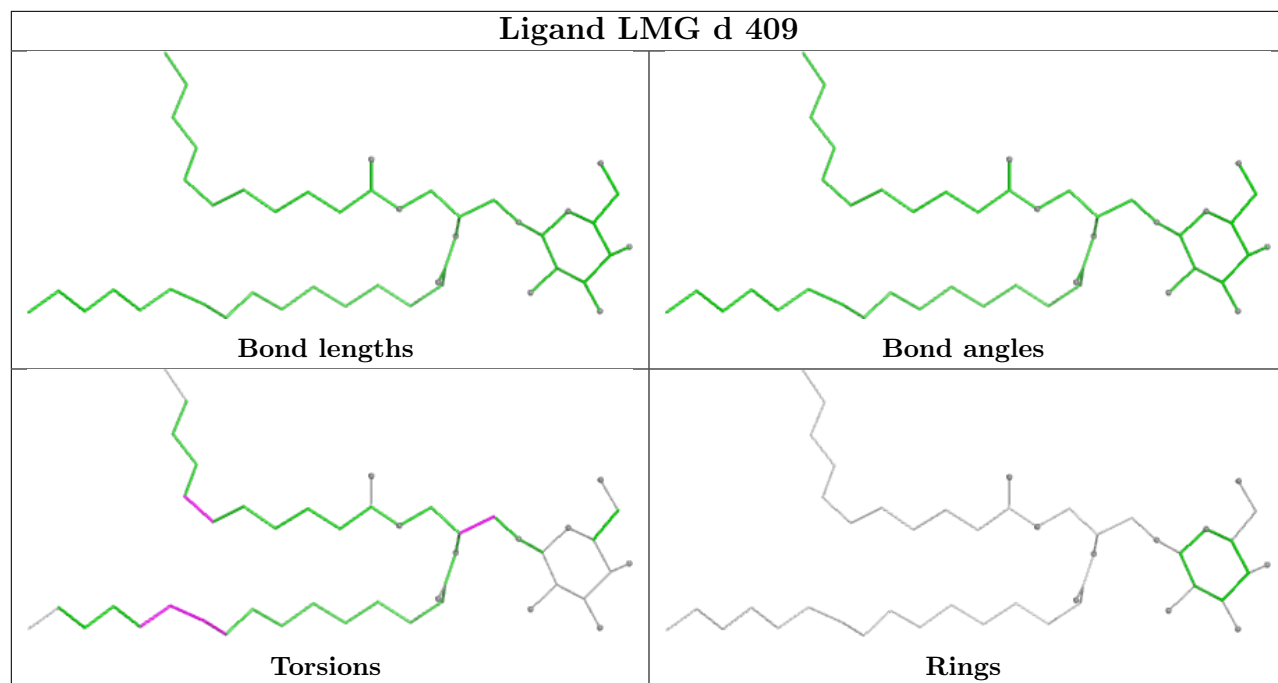
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	r	604	CLA	3	0
23	s	603	CLA	1	0
28	d	403	3PH	3	0
31	b	622	LNL	3	0
27	B	620	LMG	7	0

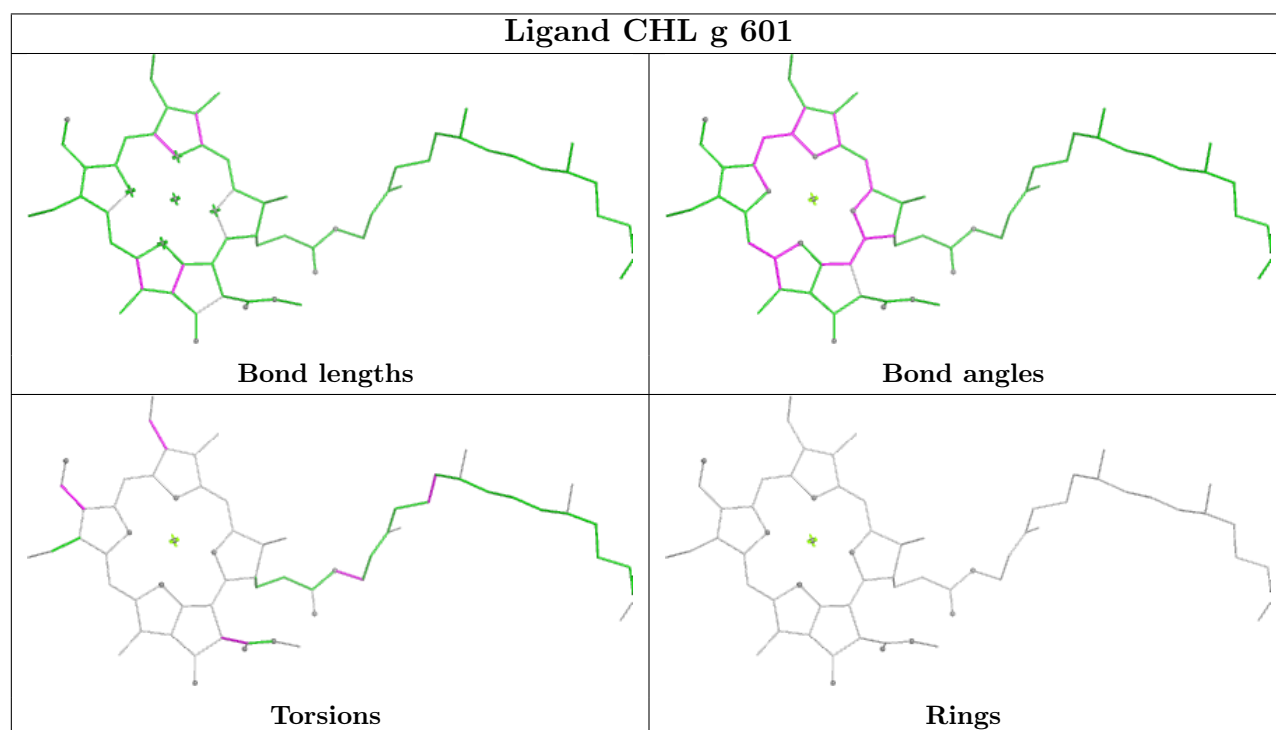
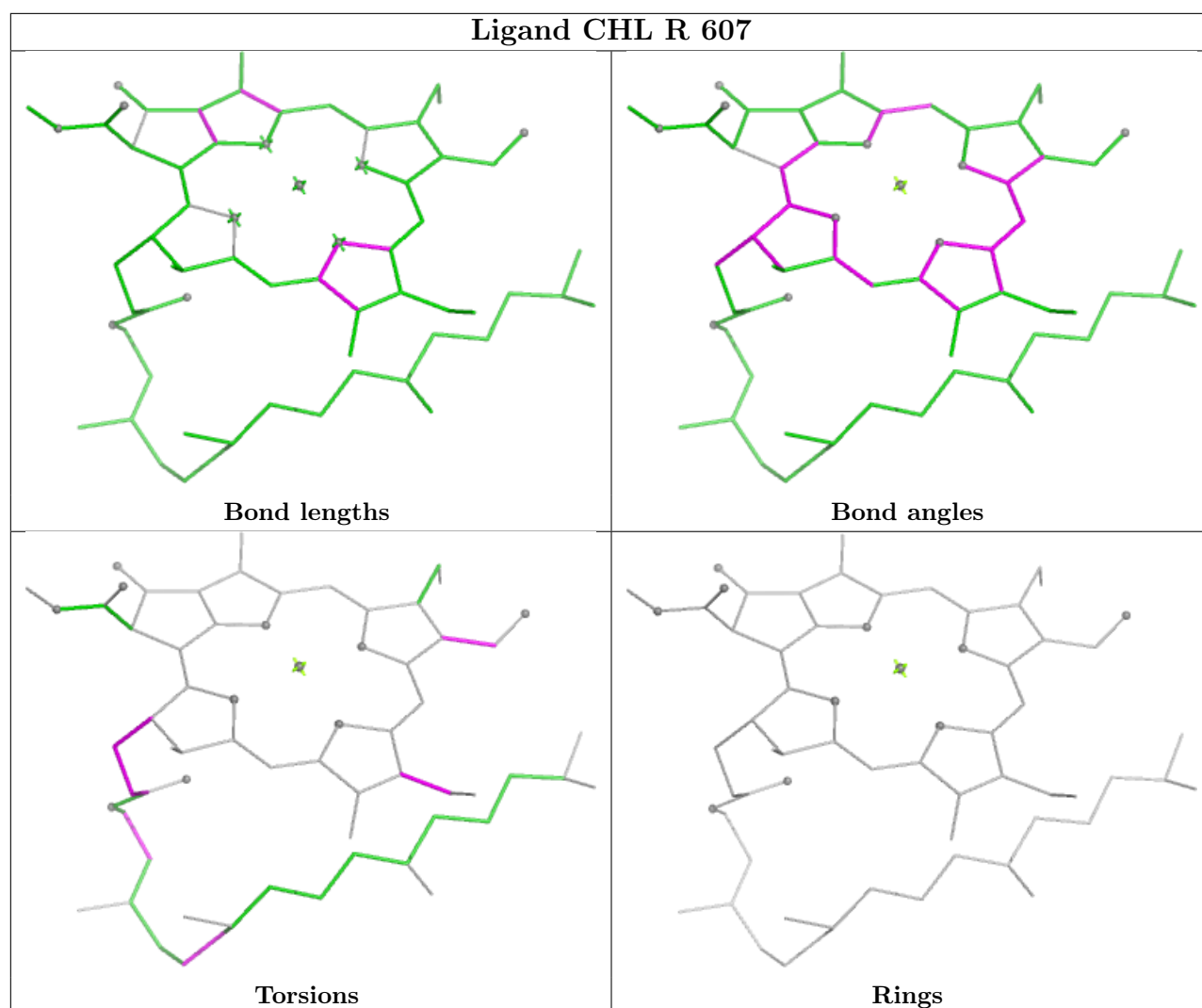
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

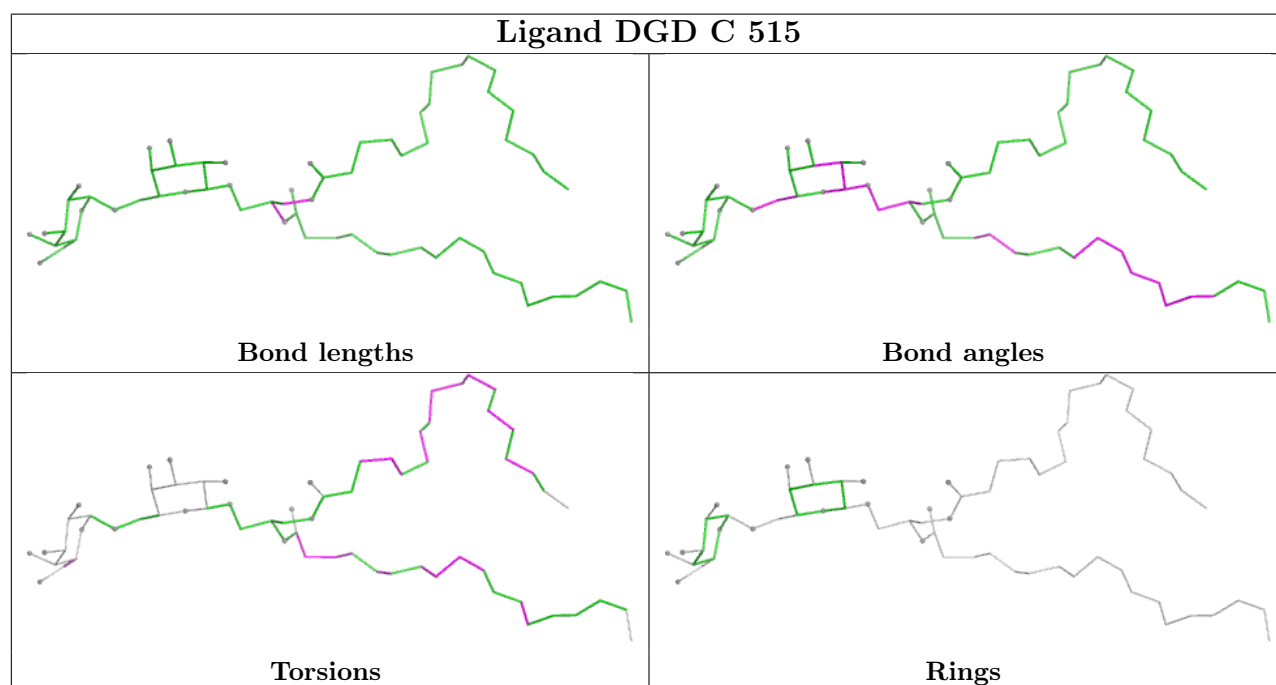
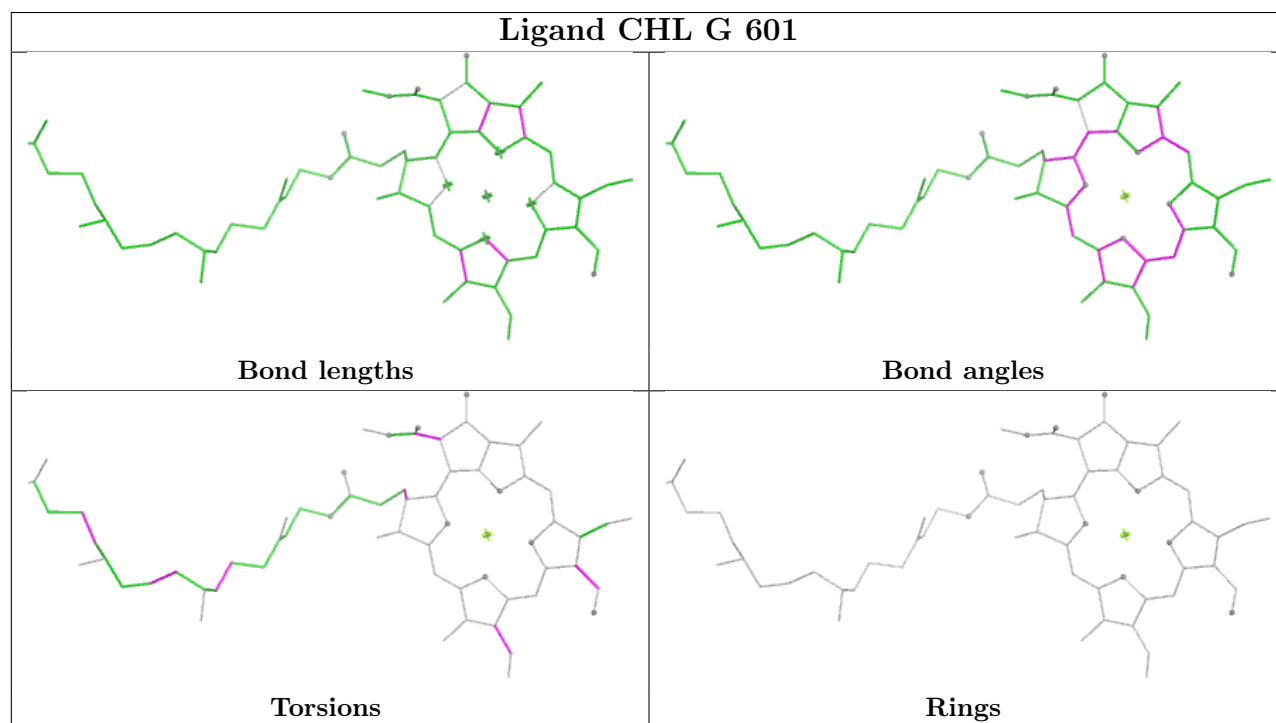
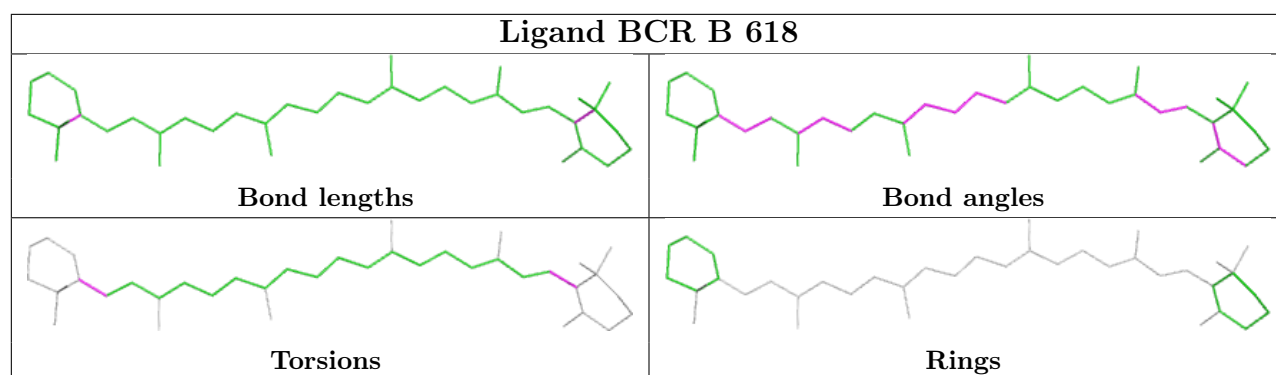


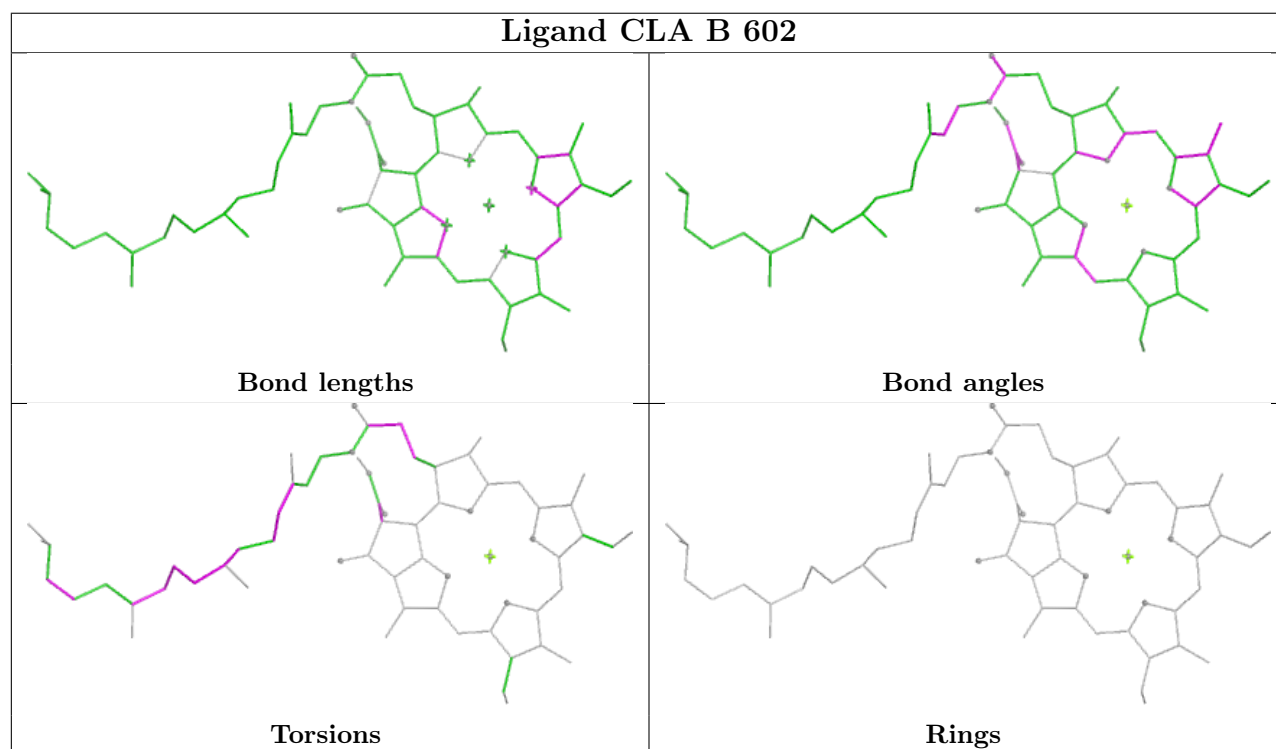
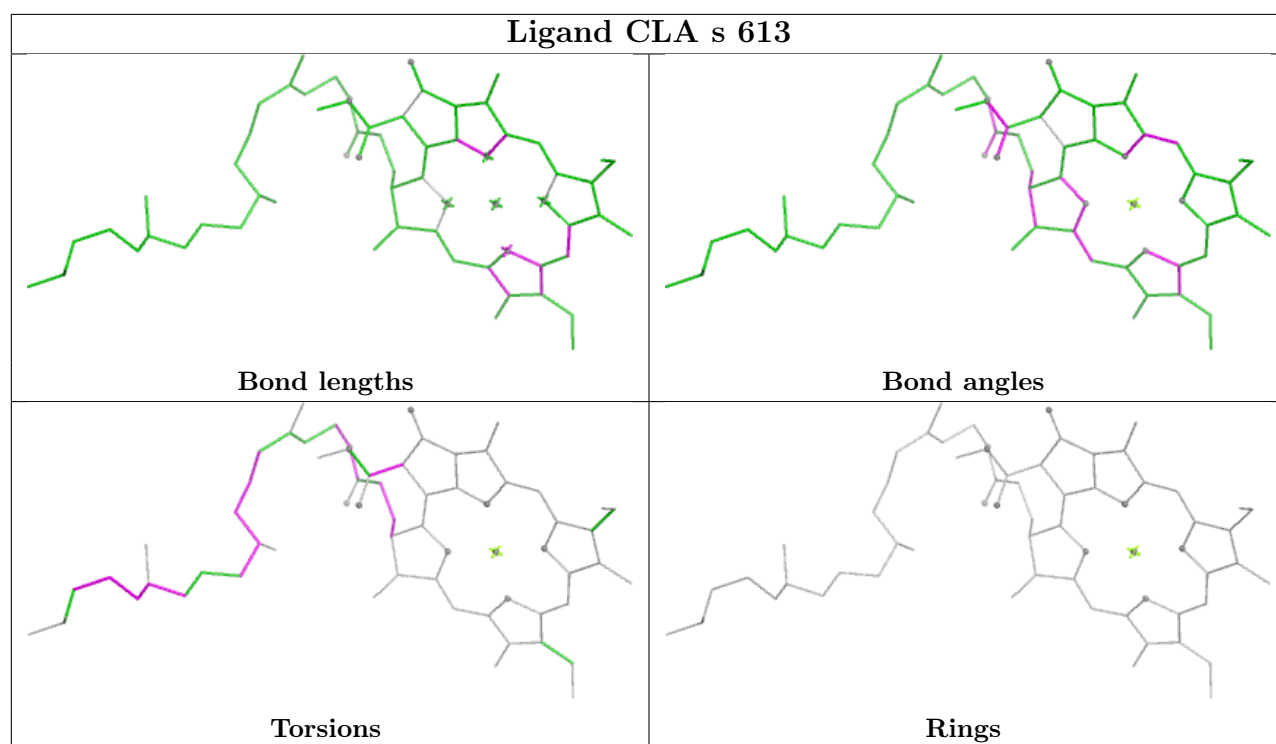




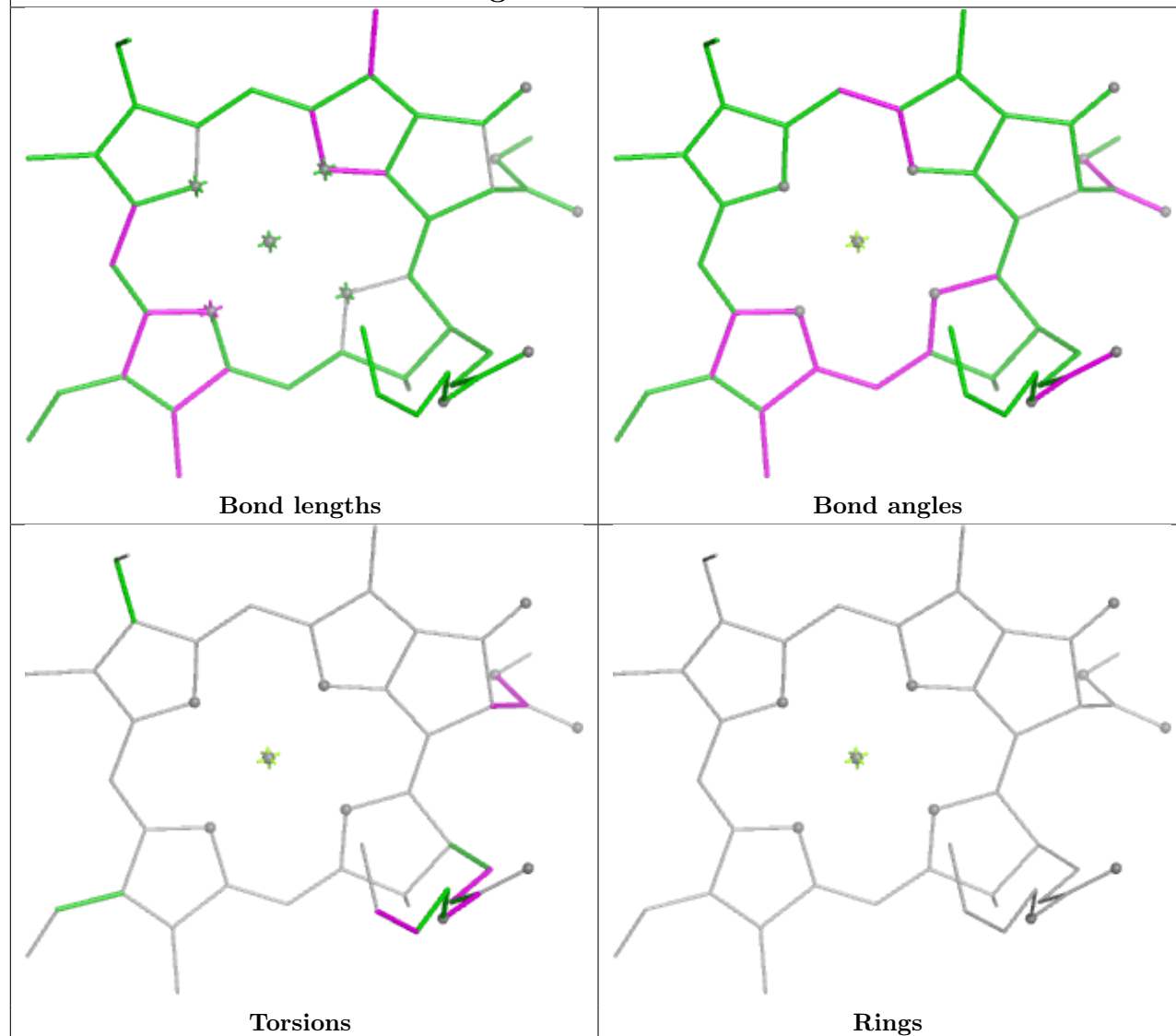




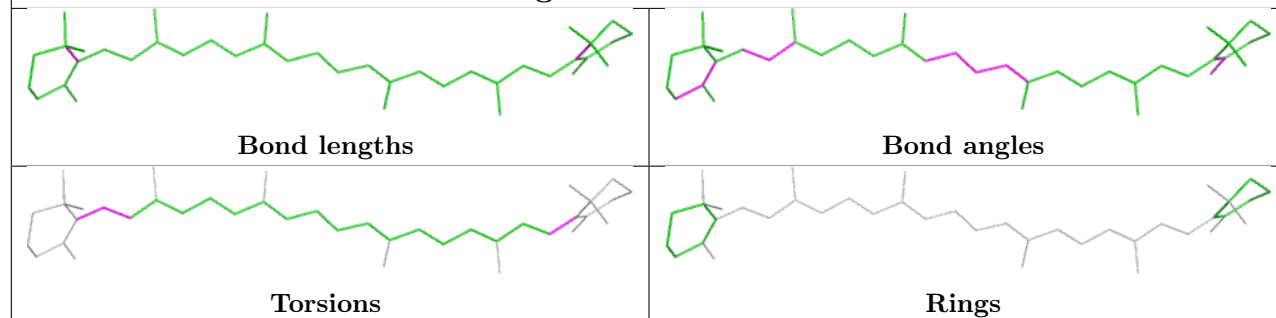


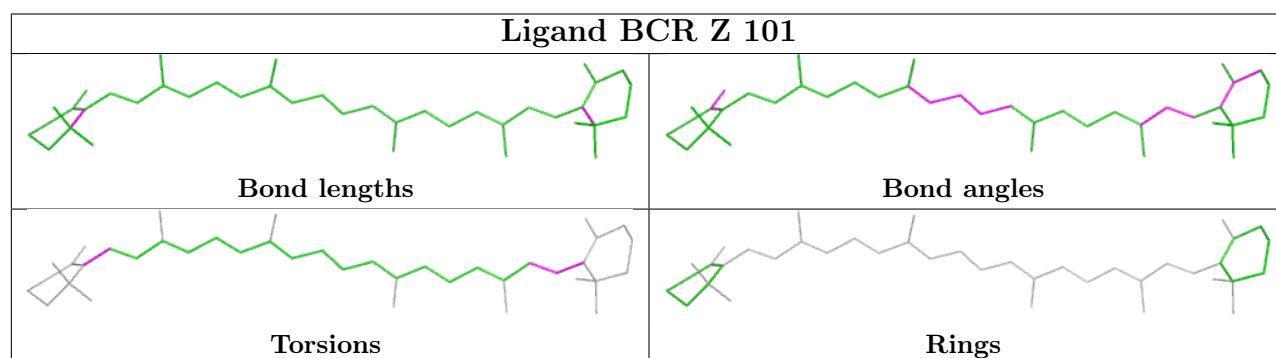
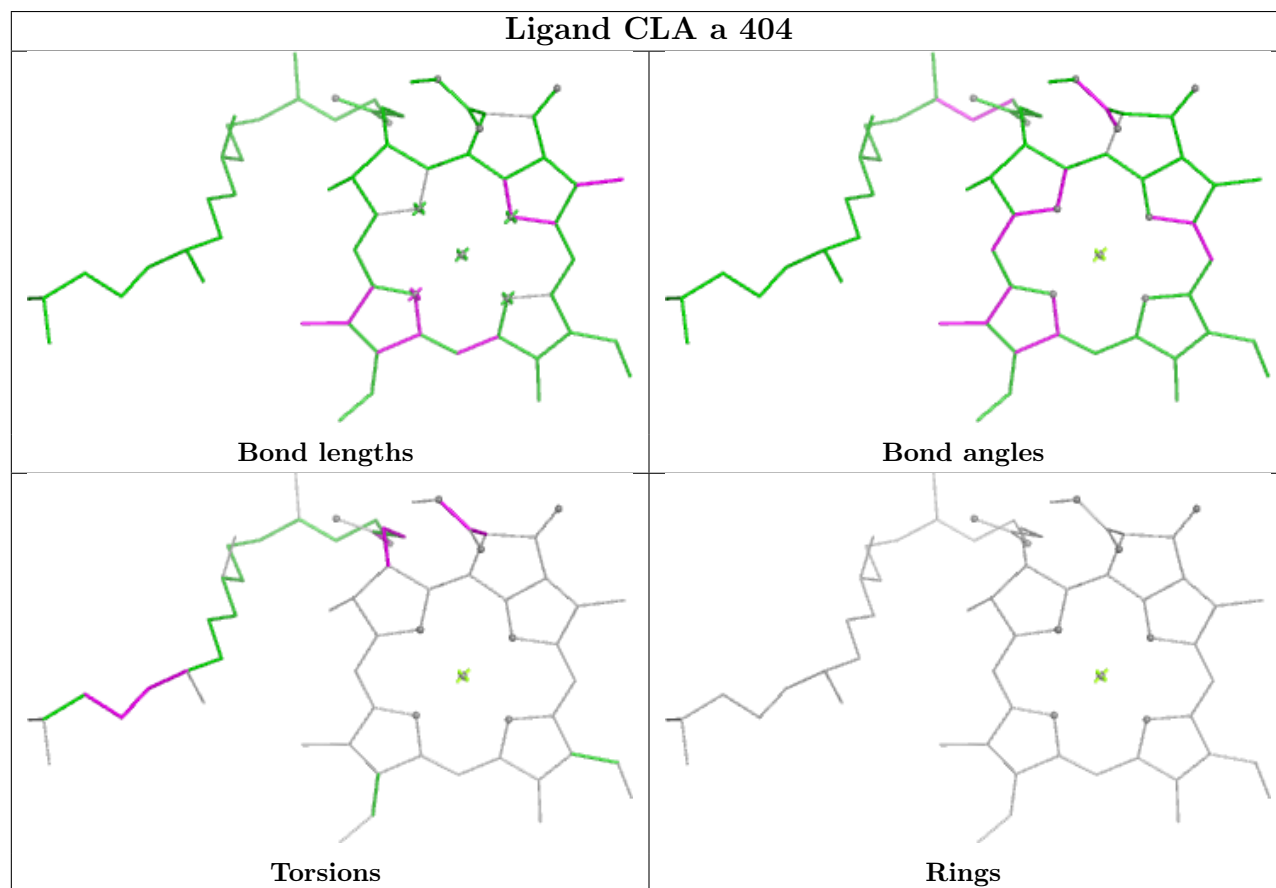
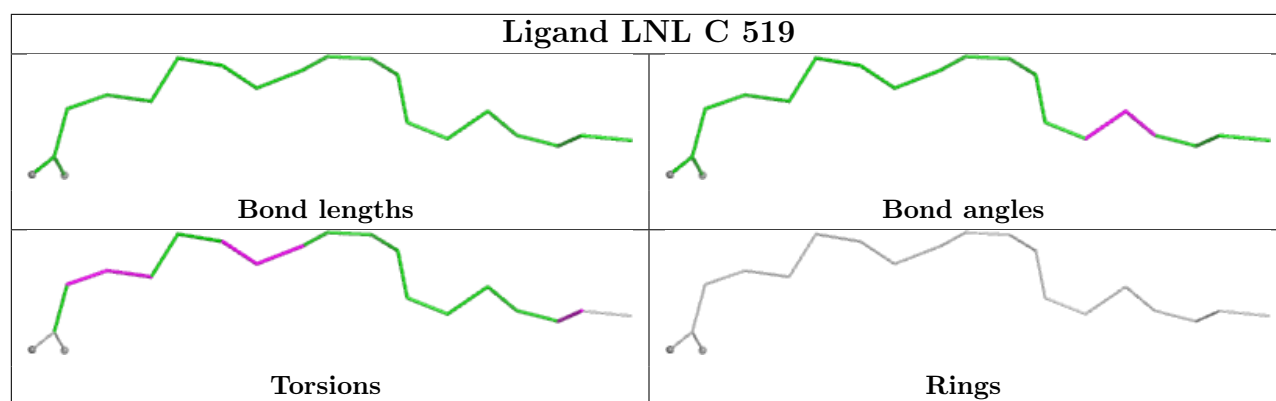


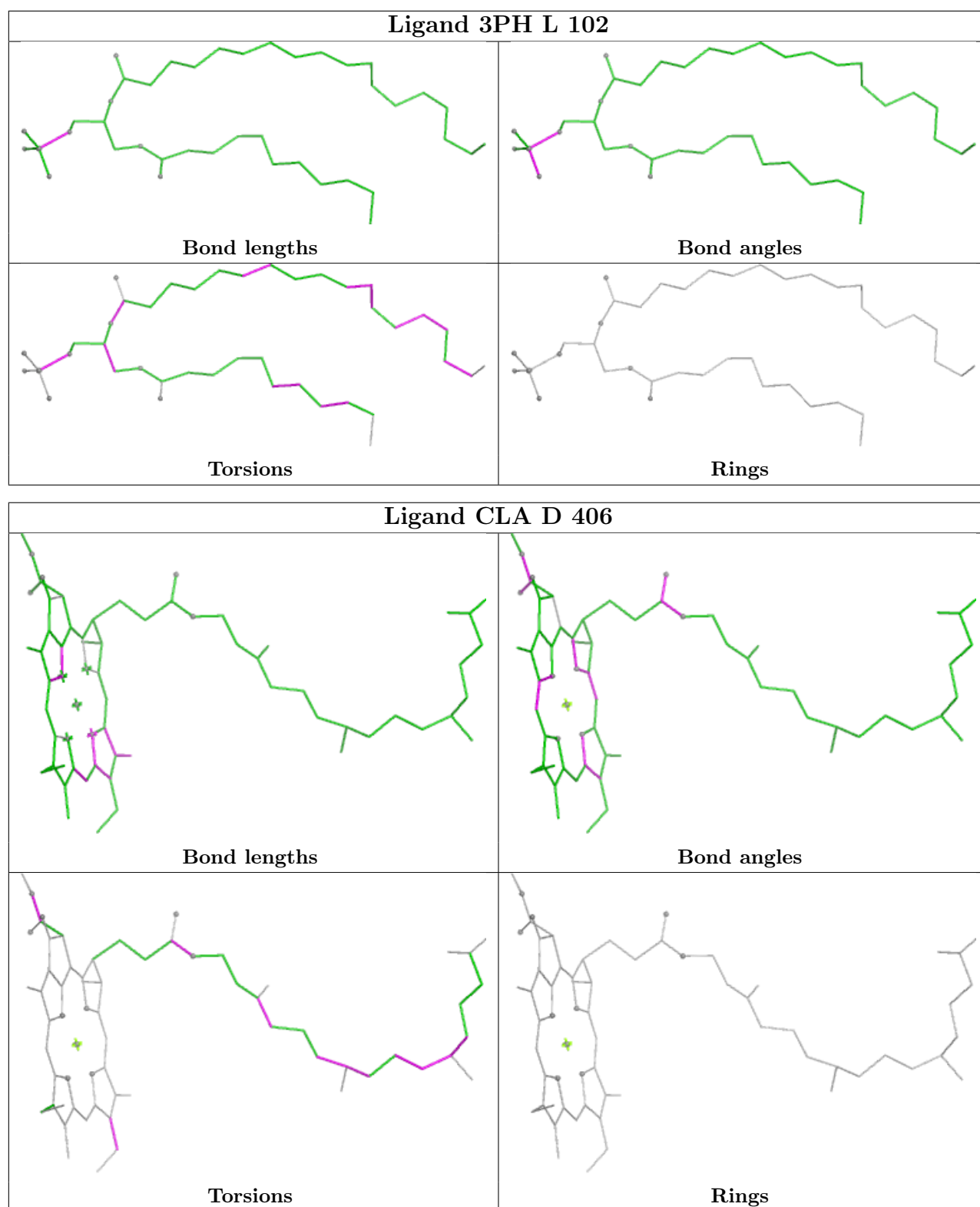
Ligand CLA N 604

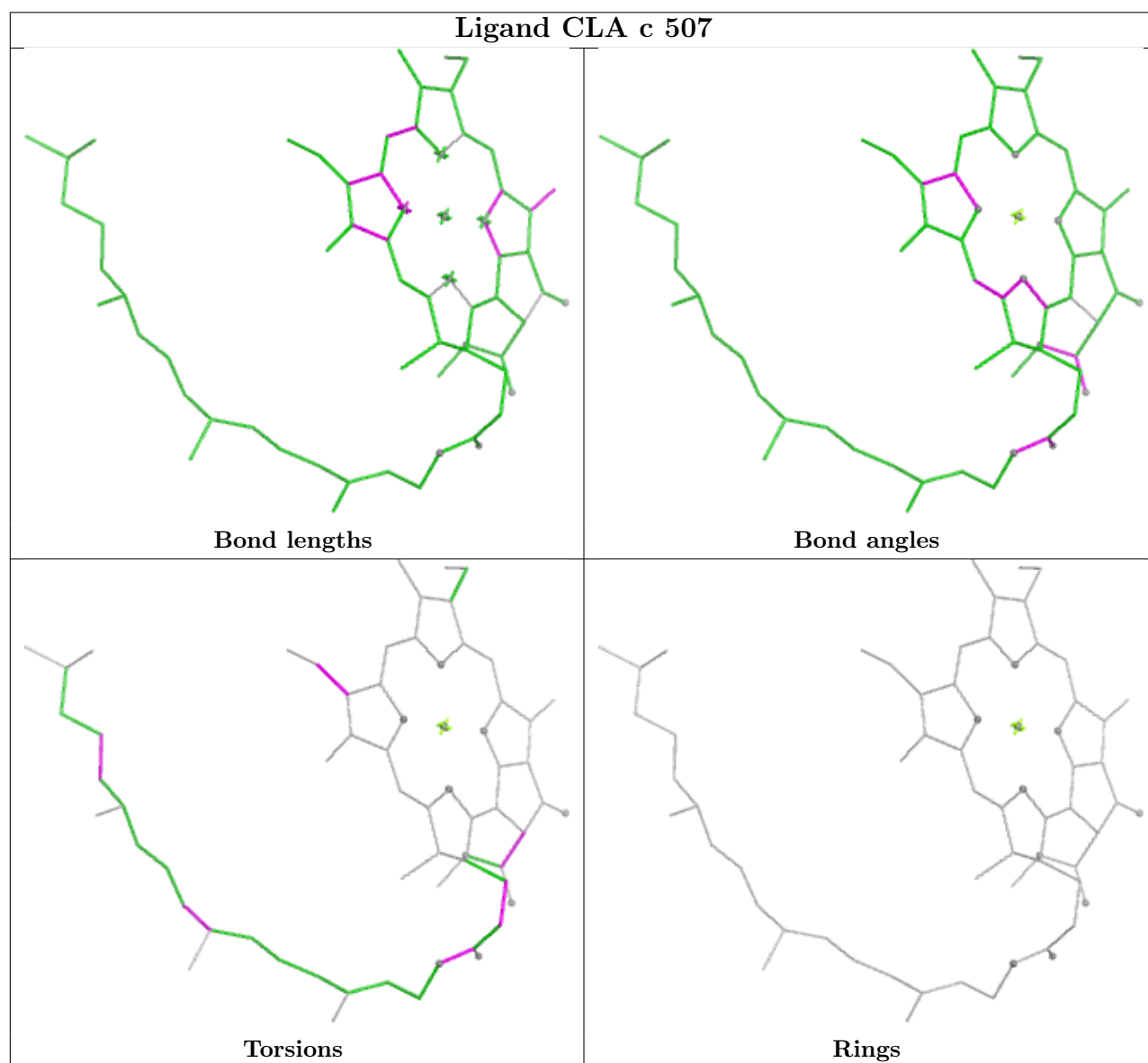
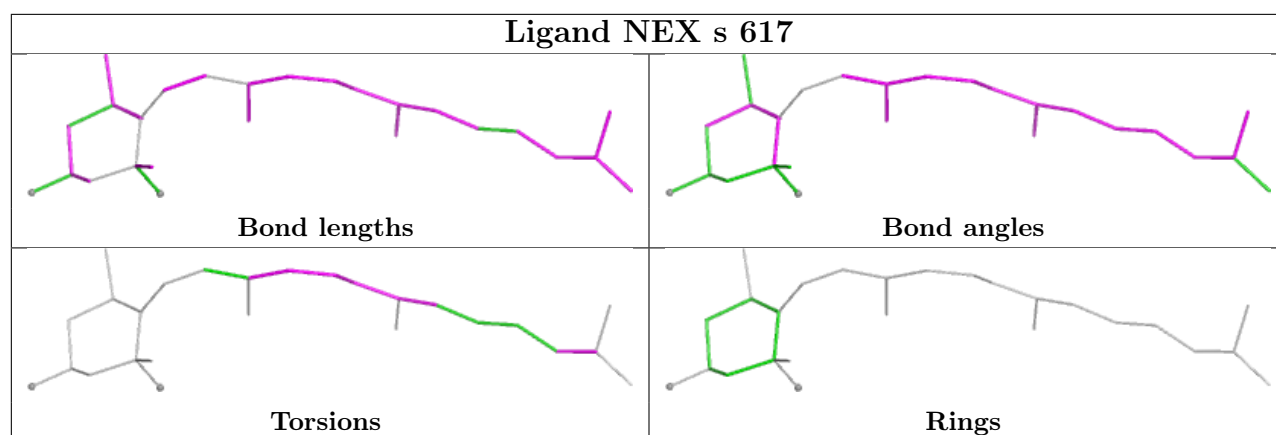


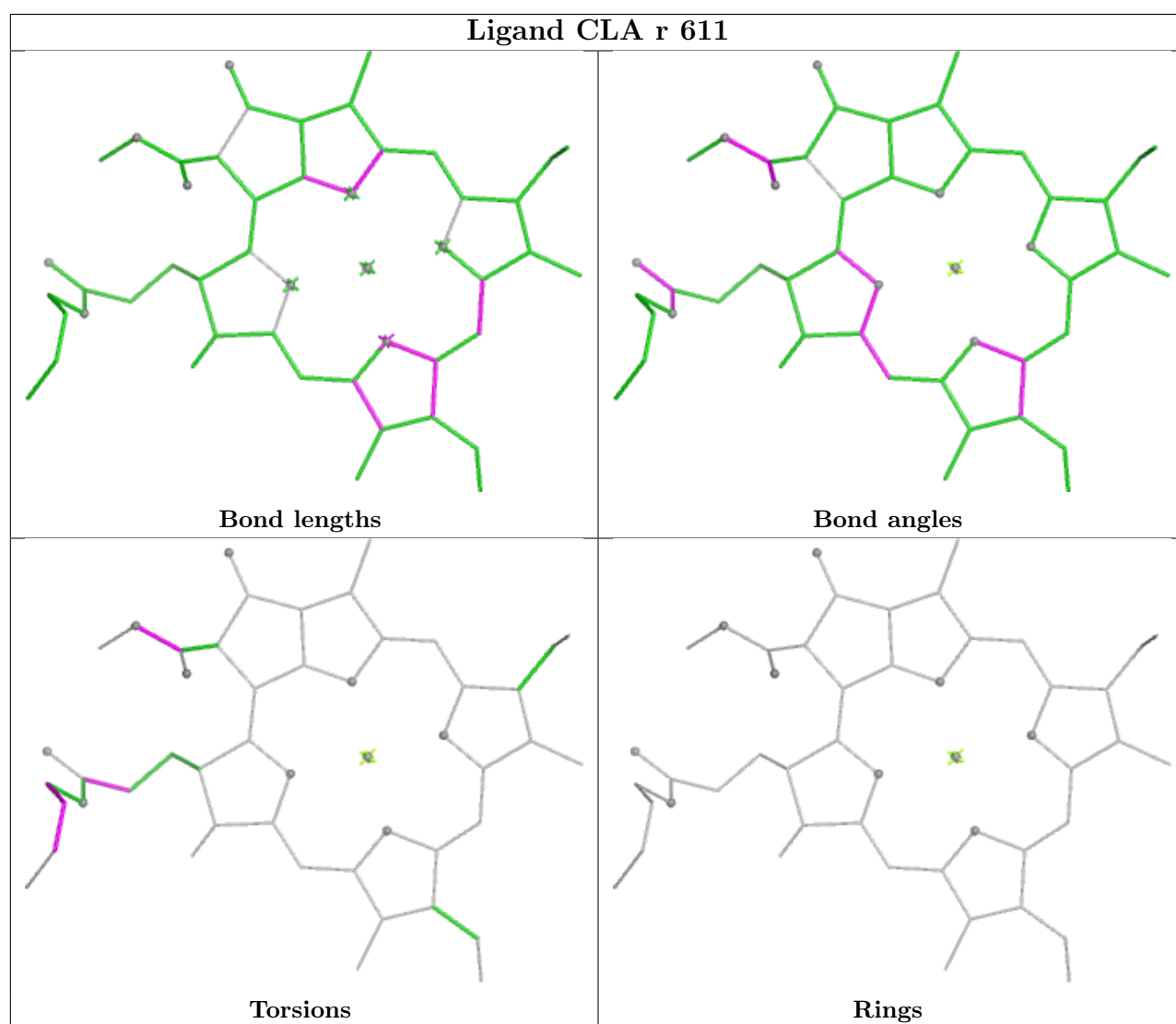
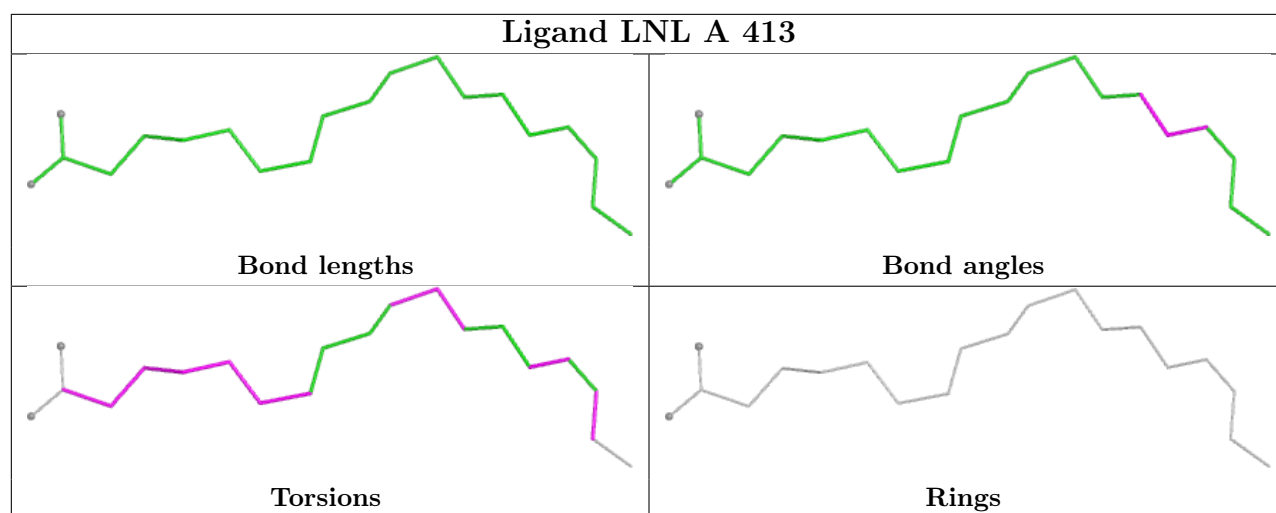
Ligand BCR z 101

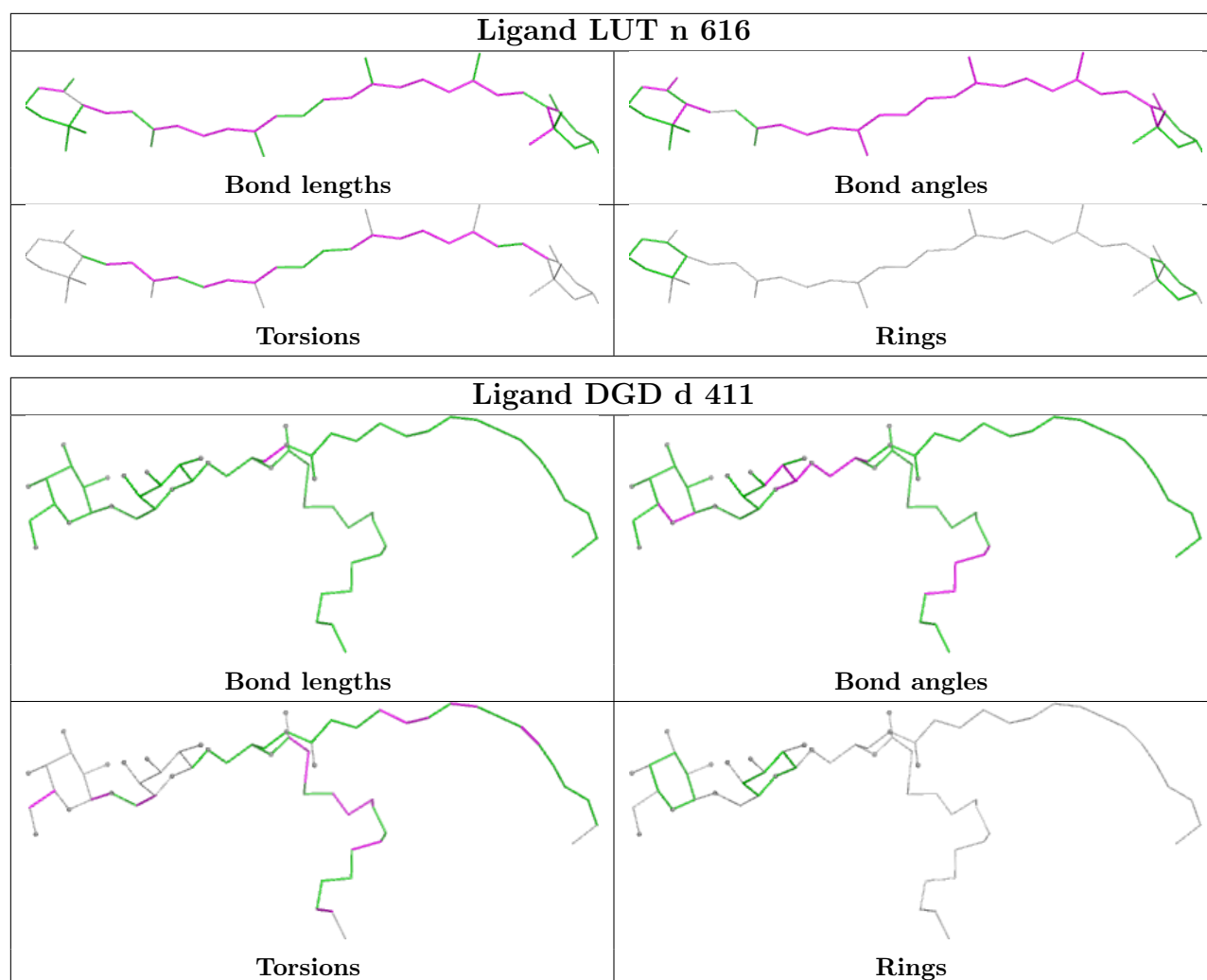


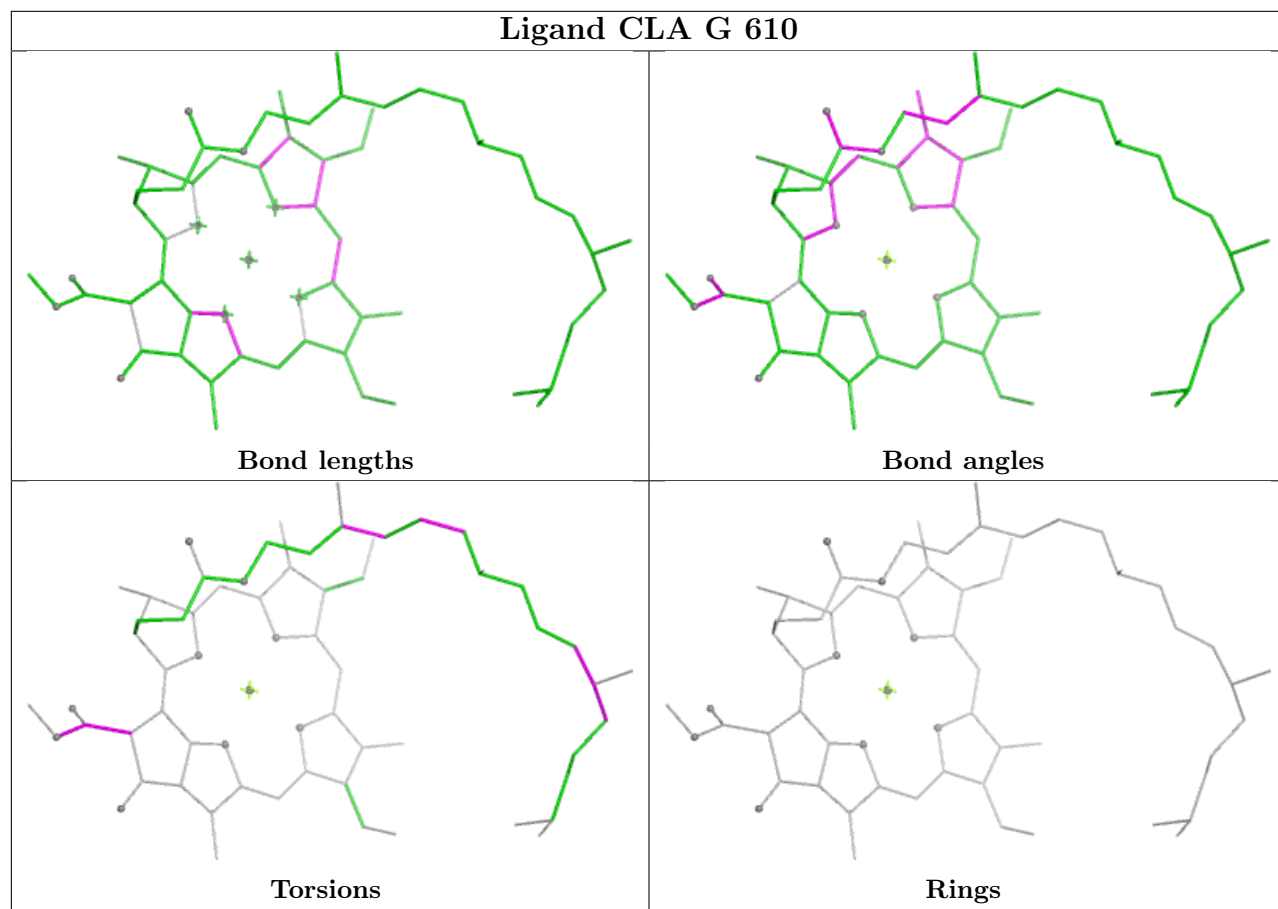


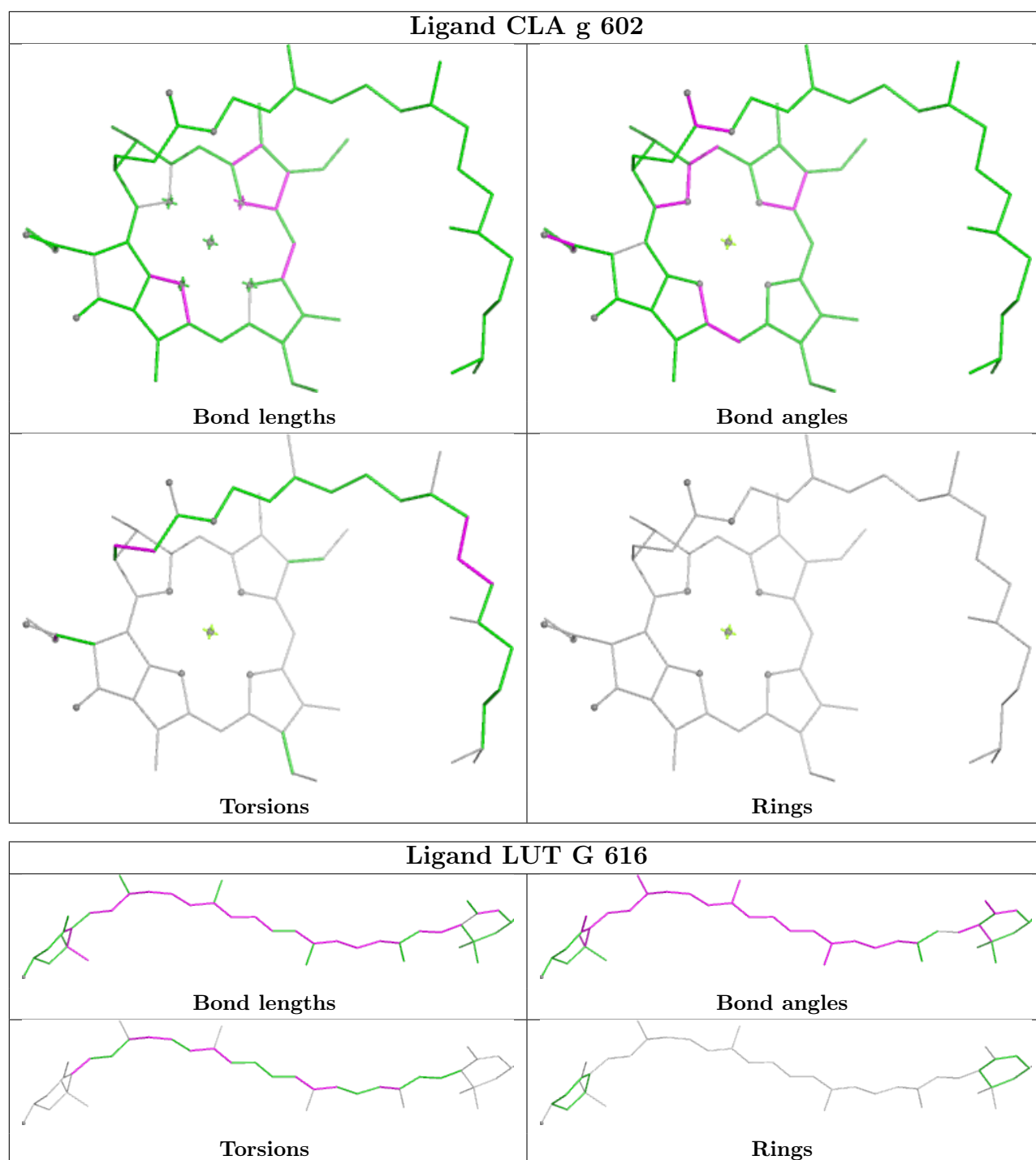


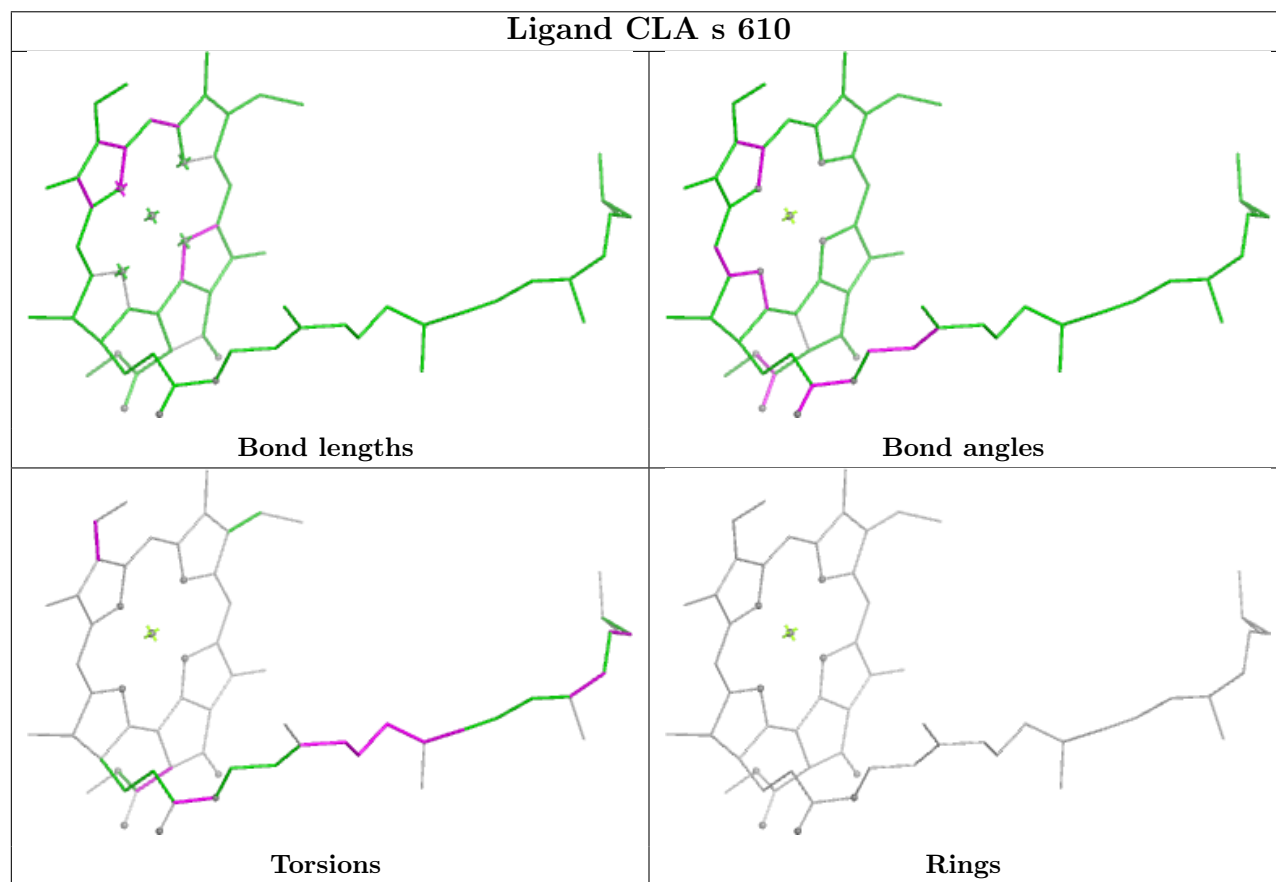
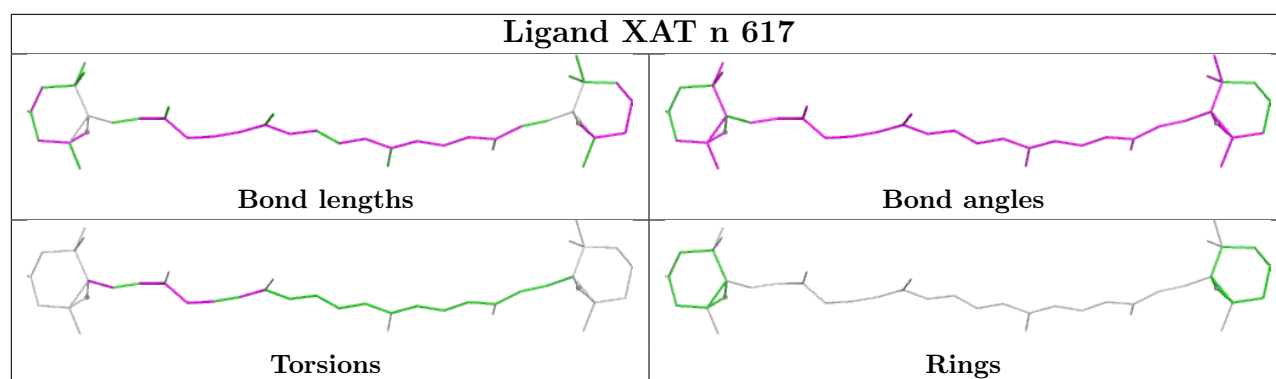


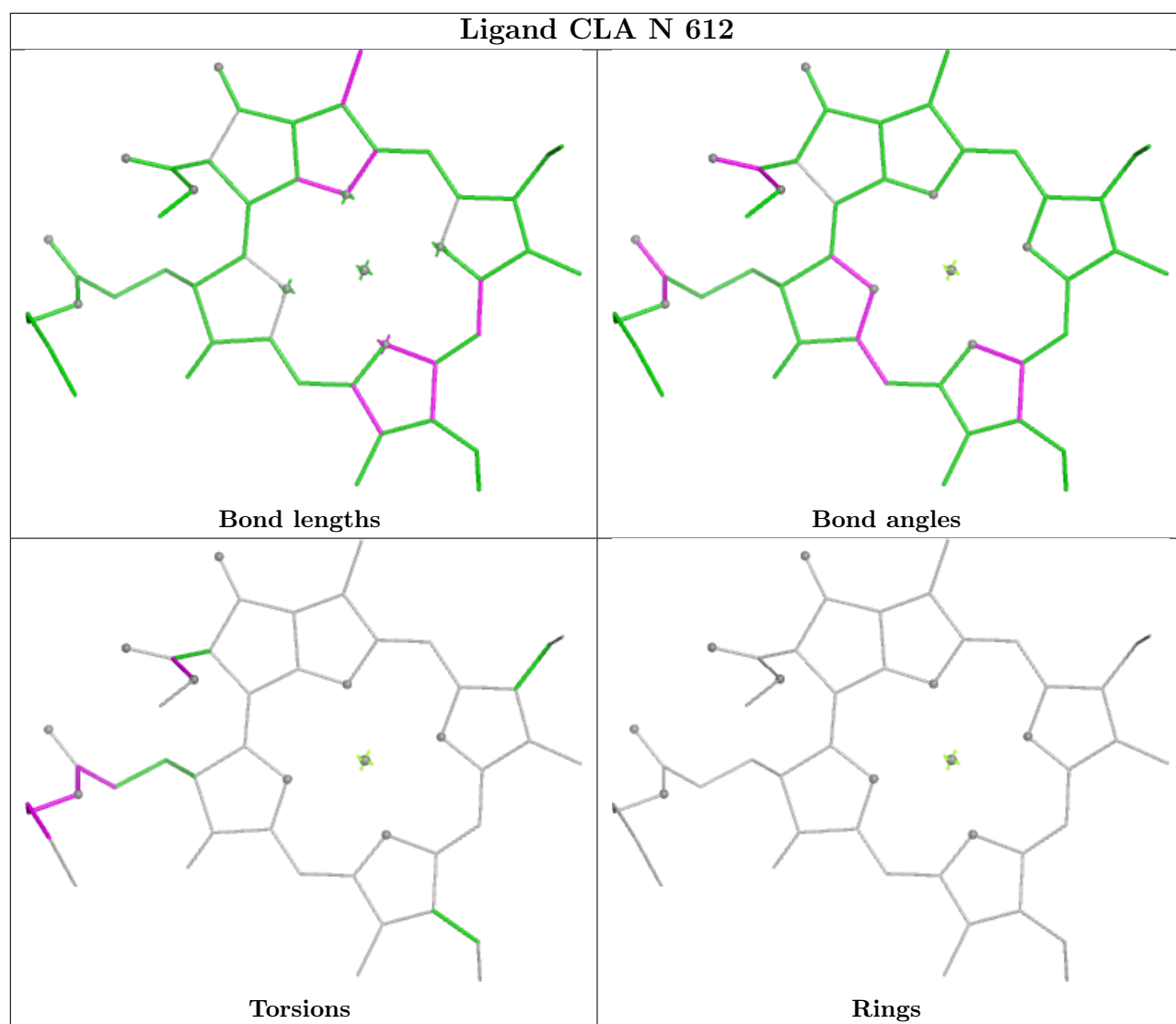


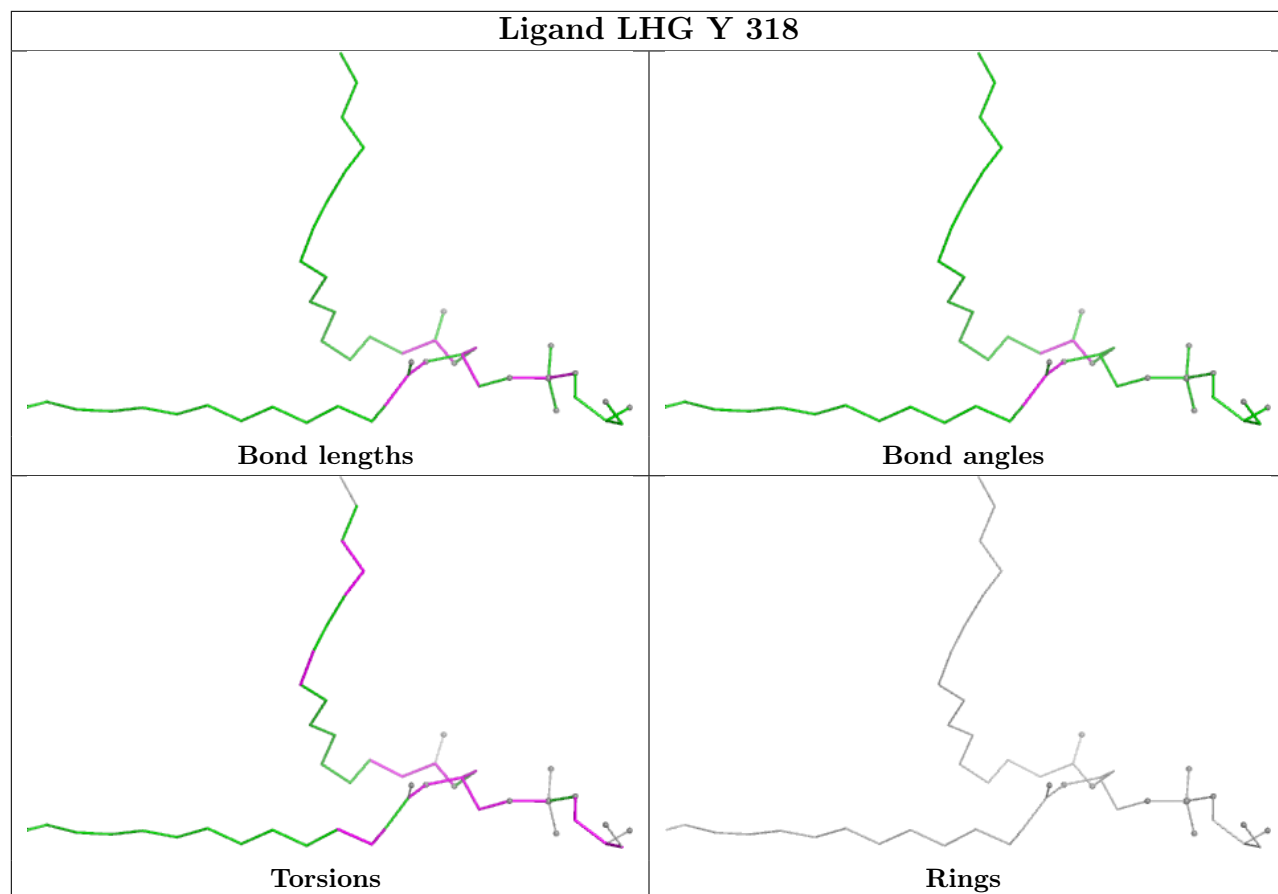


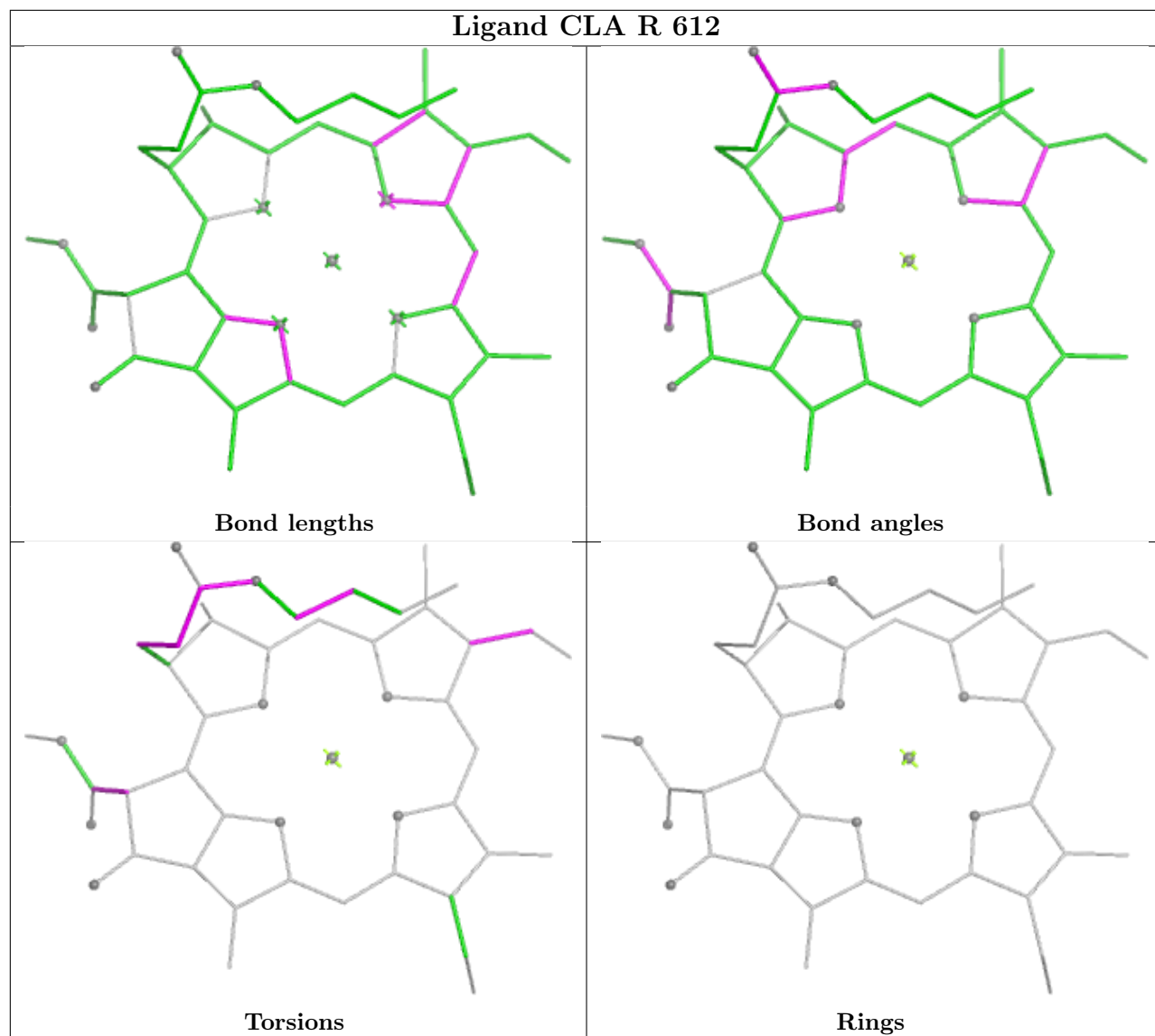


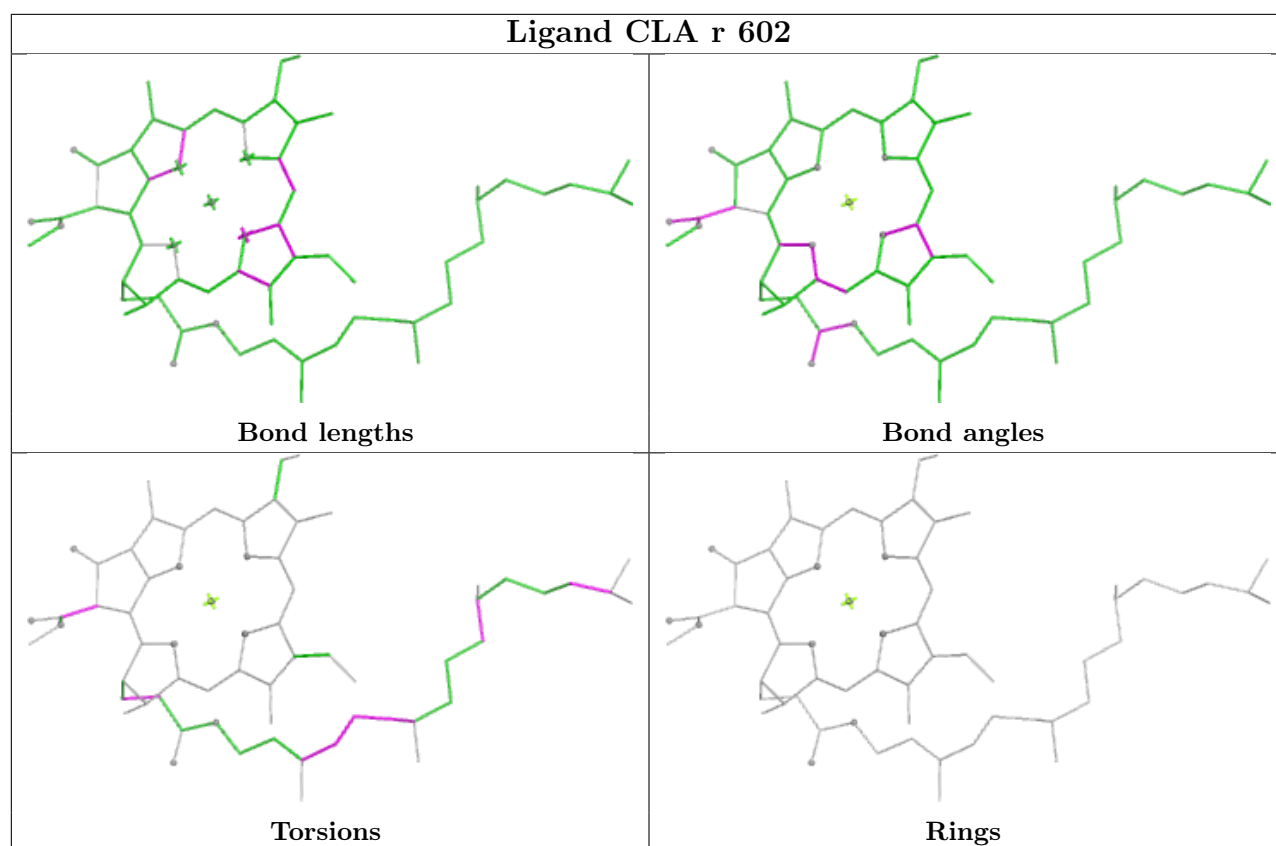




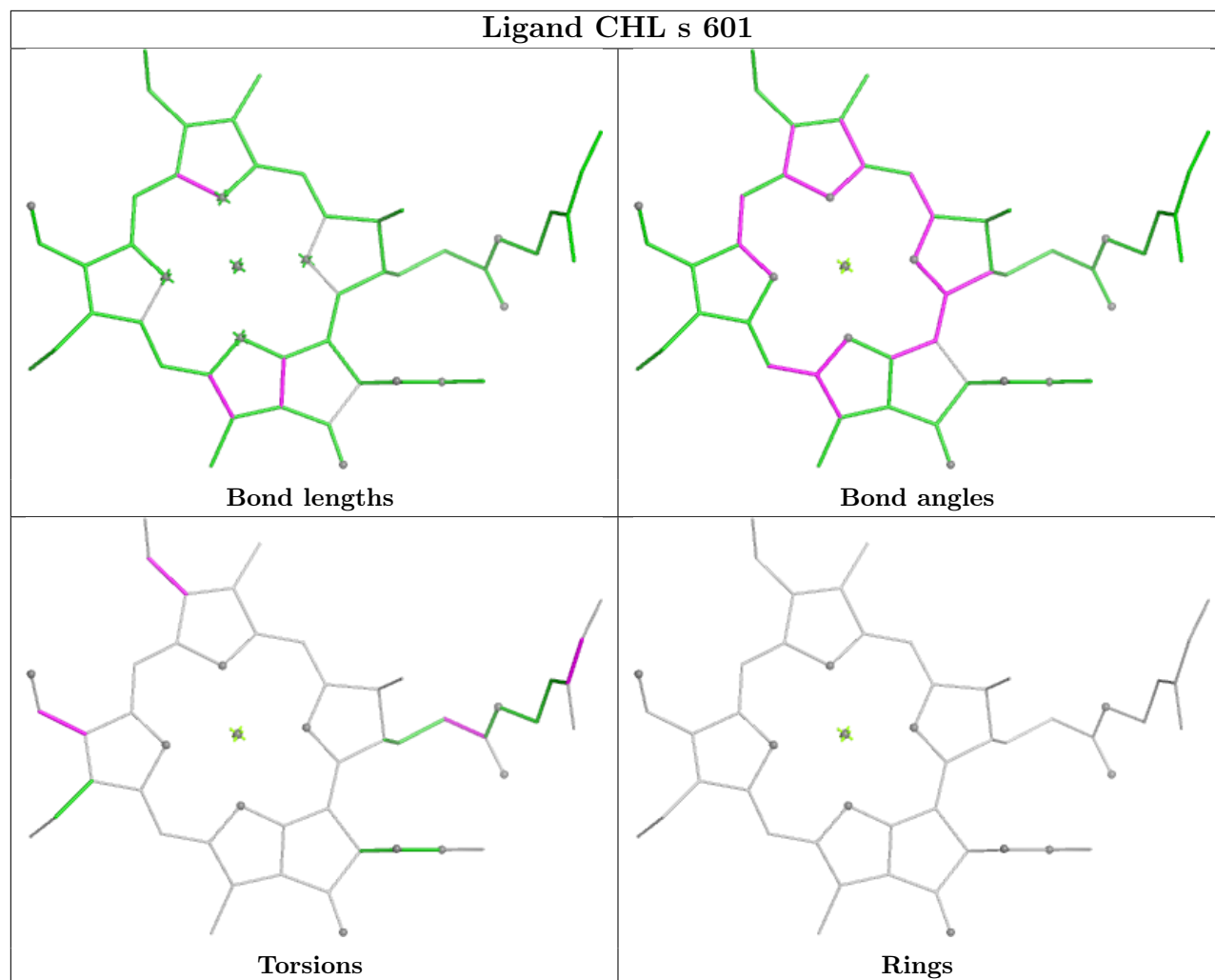




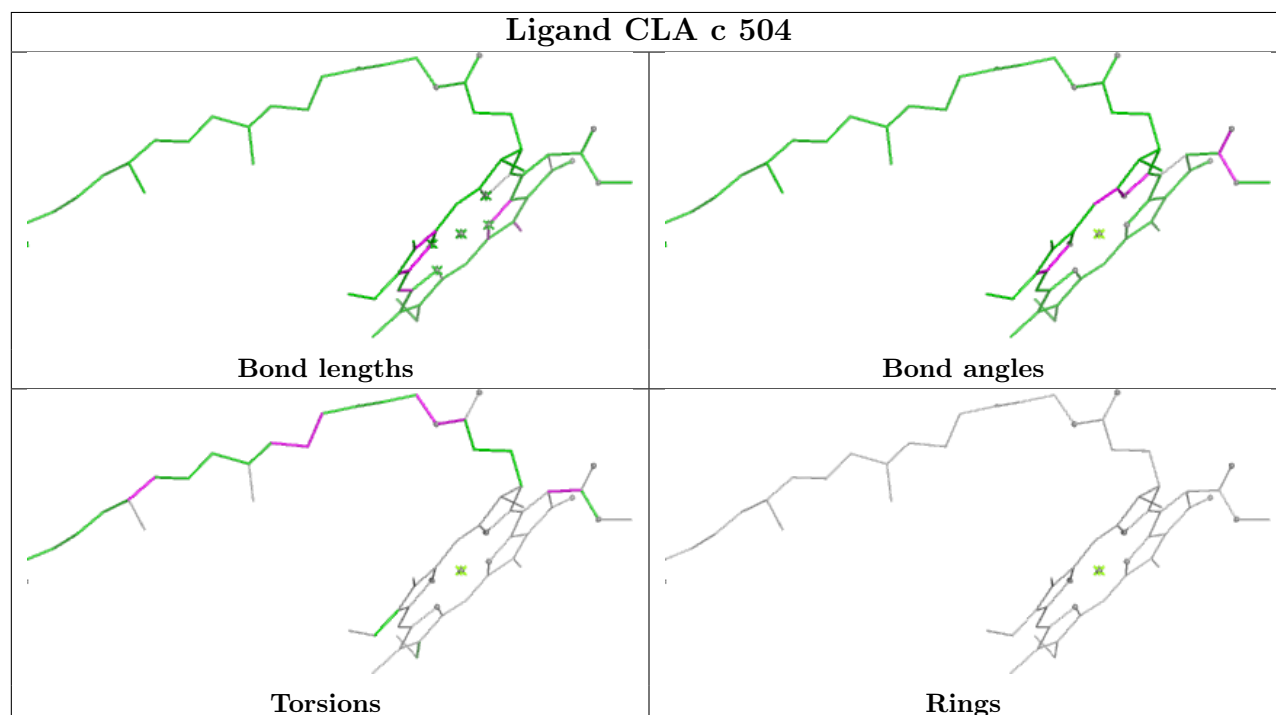


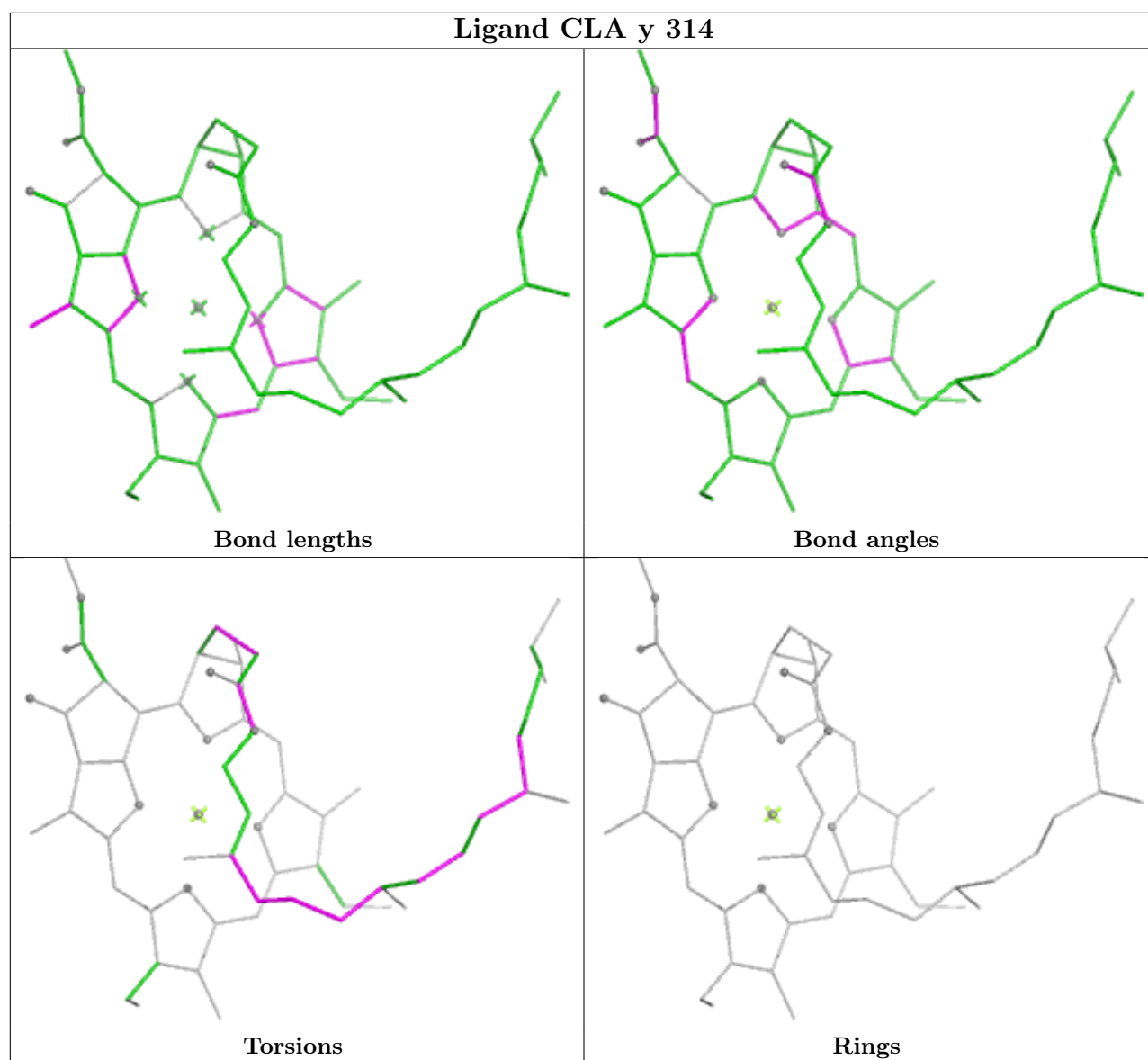


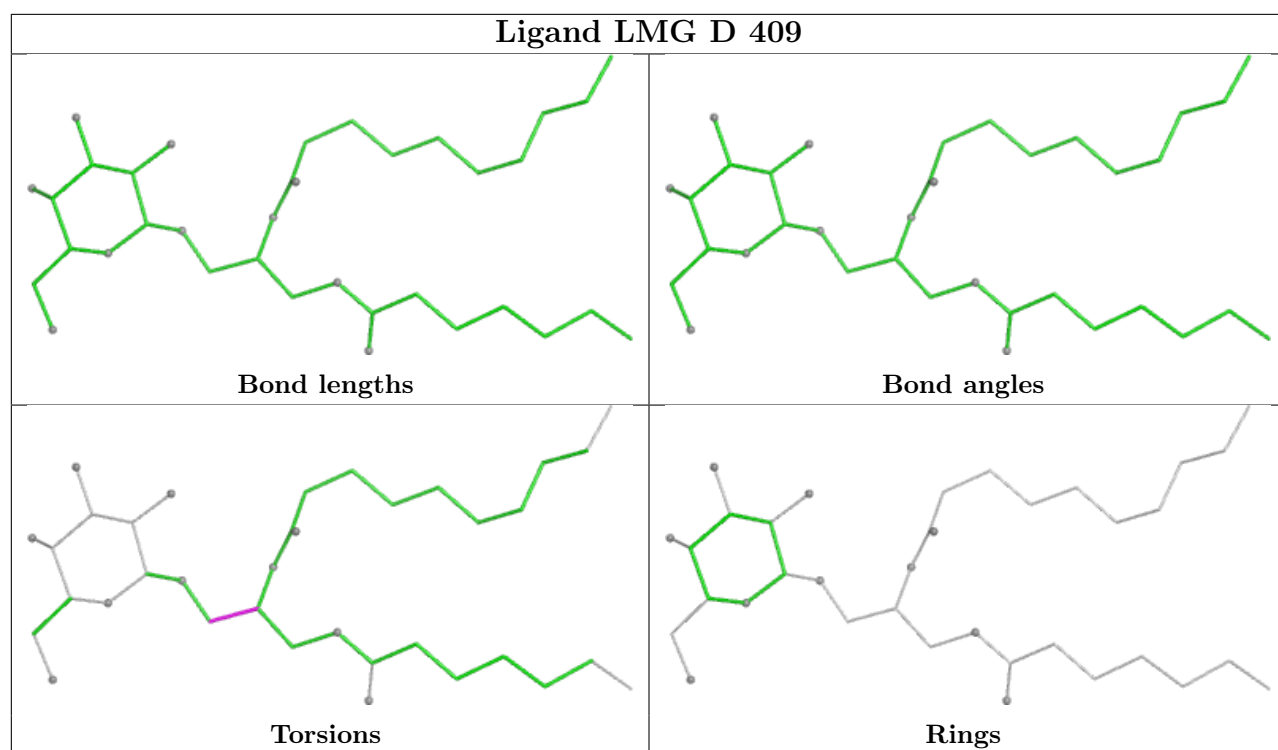
Ligand CHL s 601



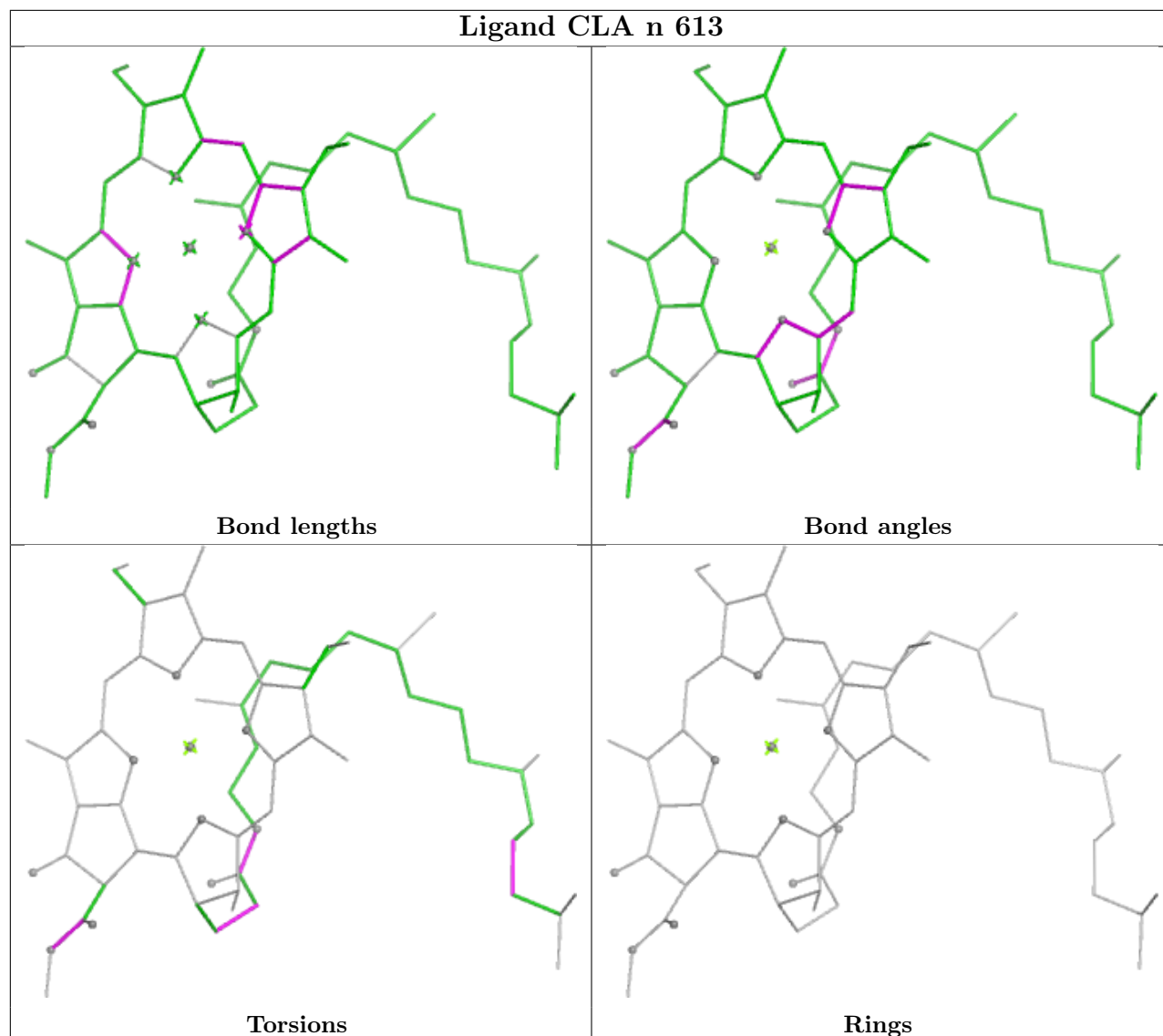
Ligand CLA c 504

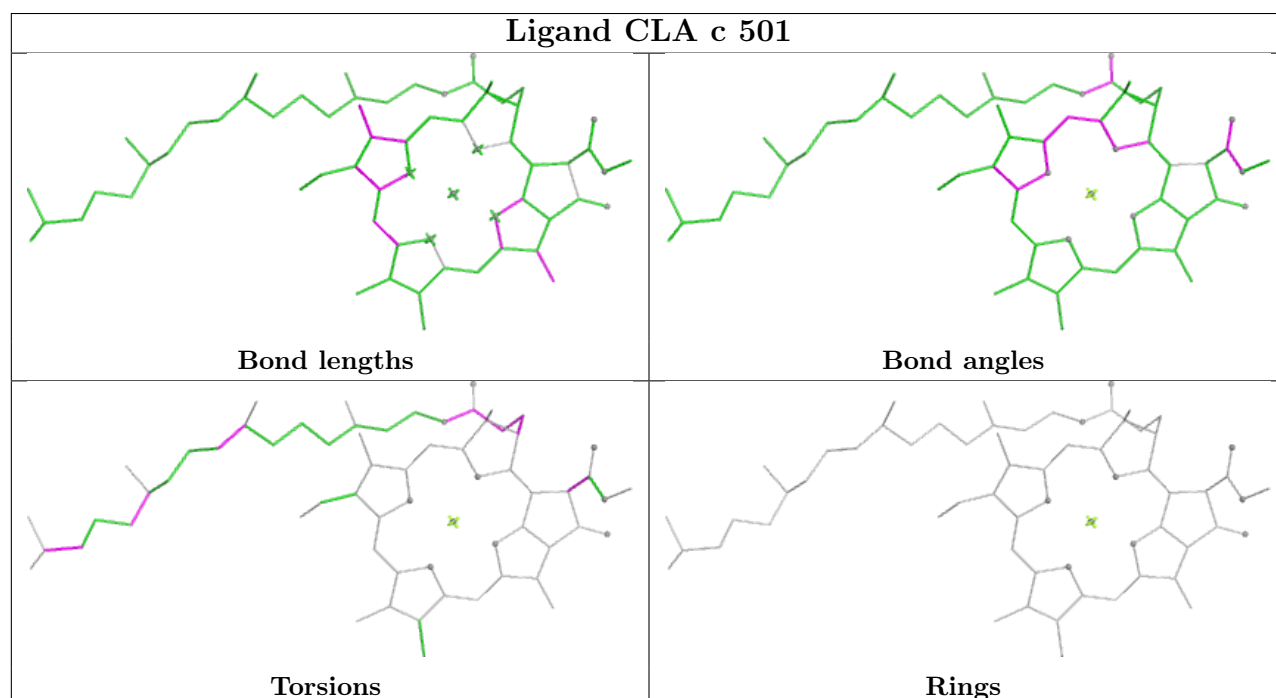
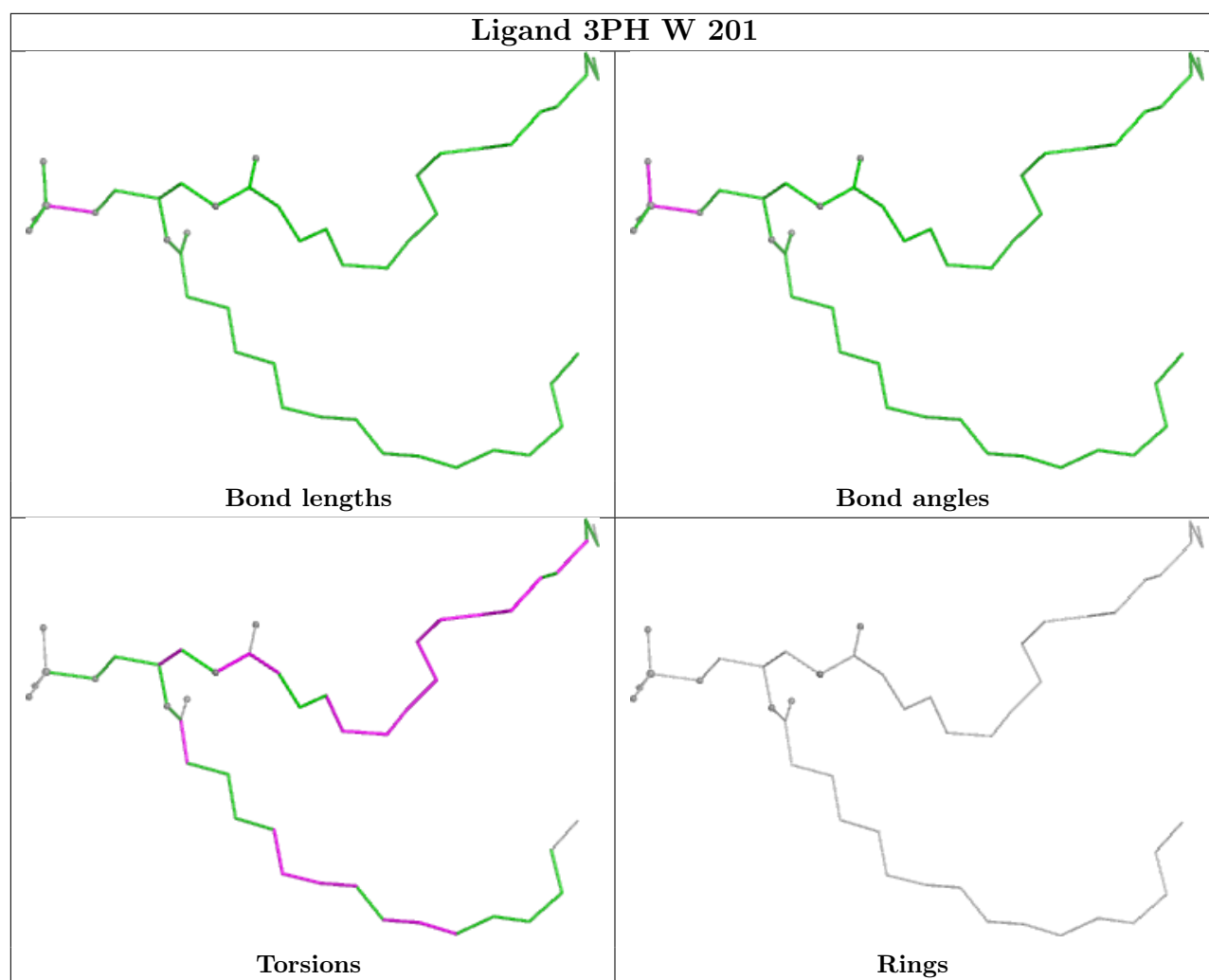


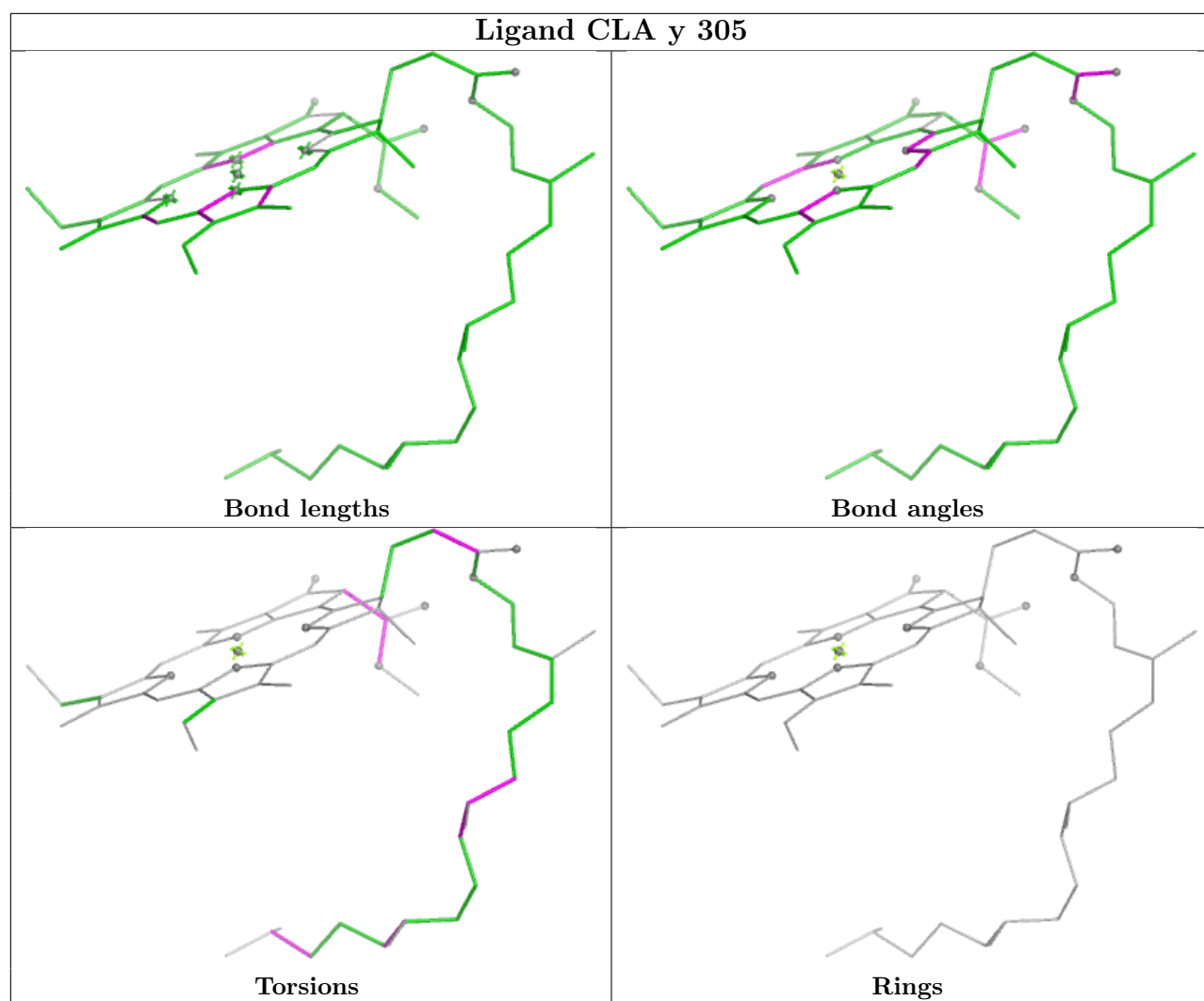




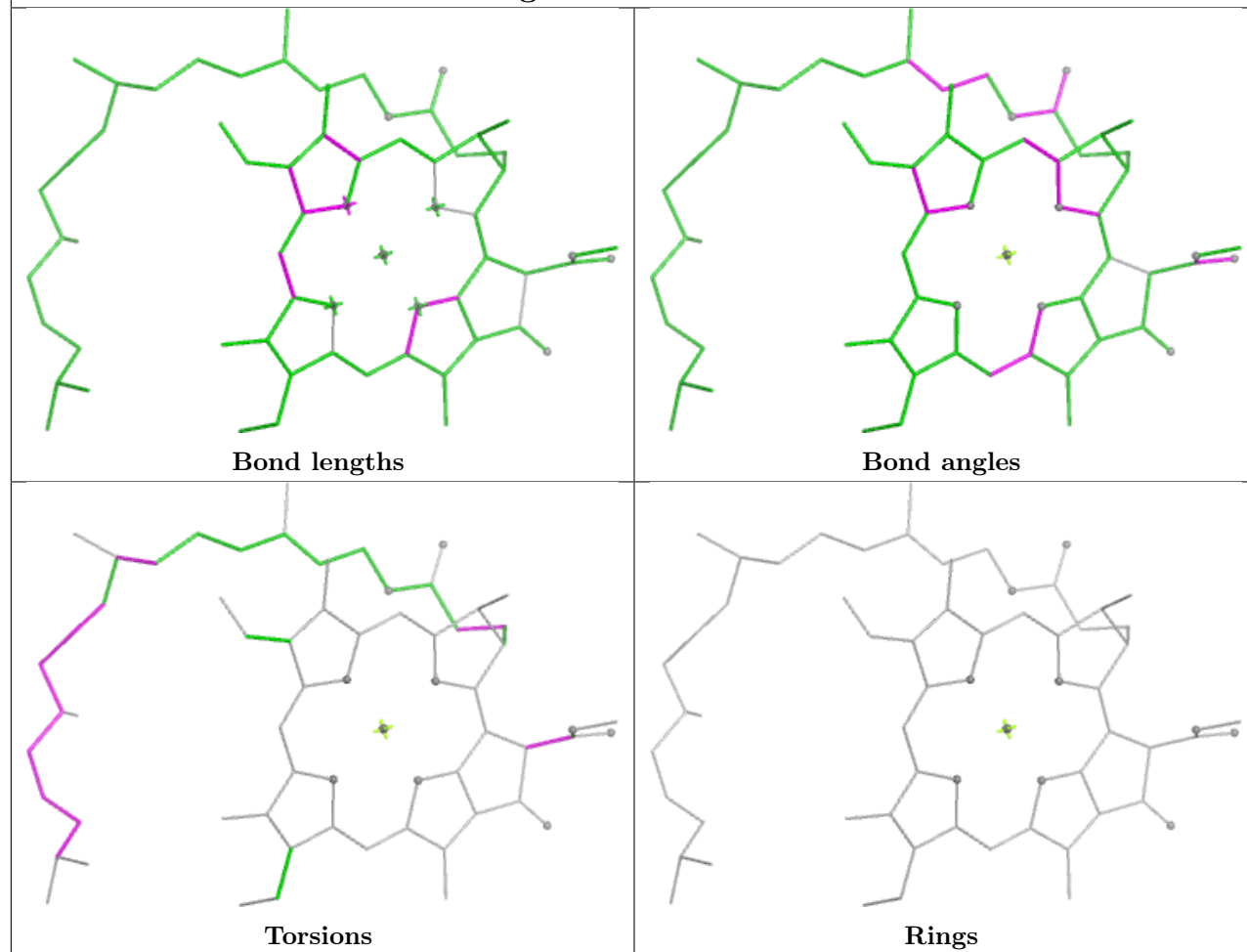
Ligand CLA n 613



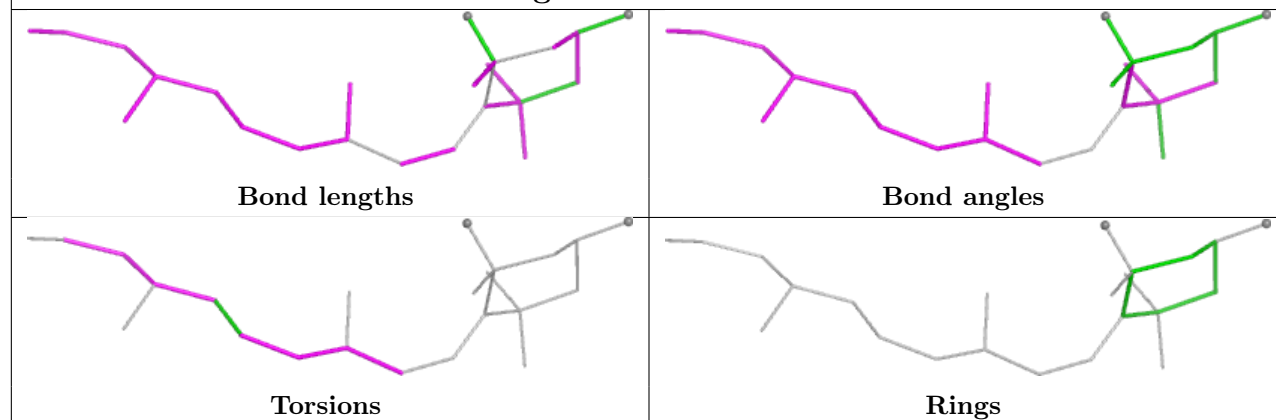


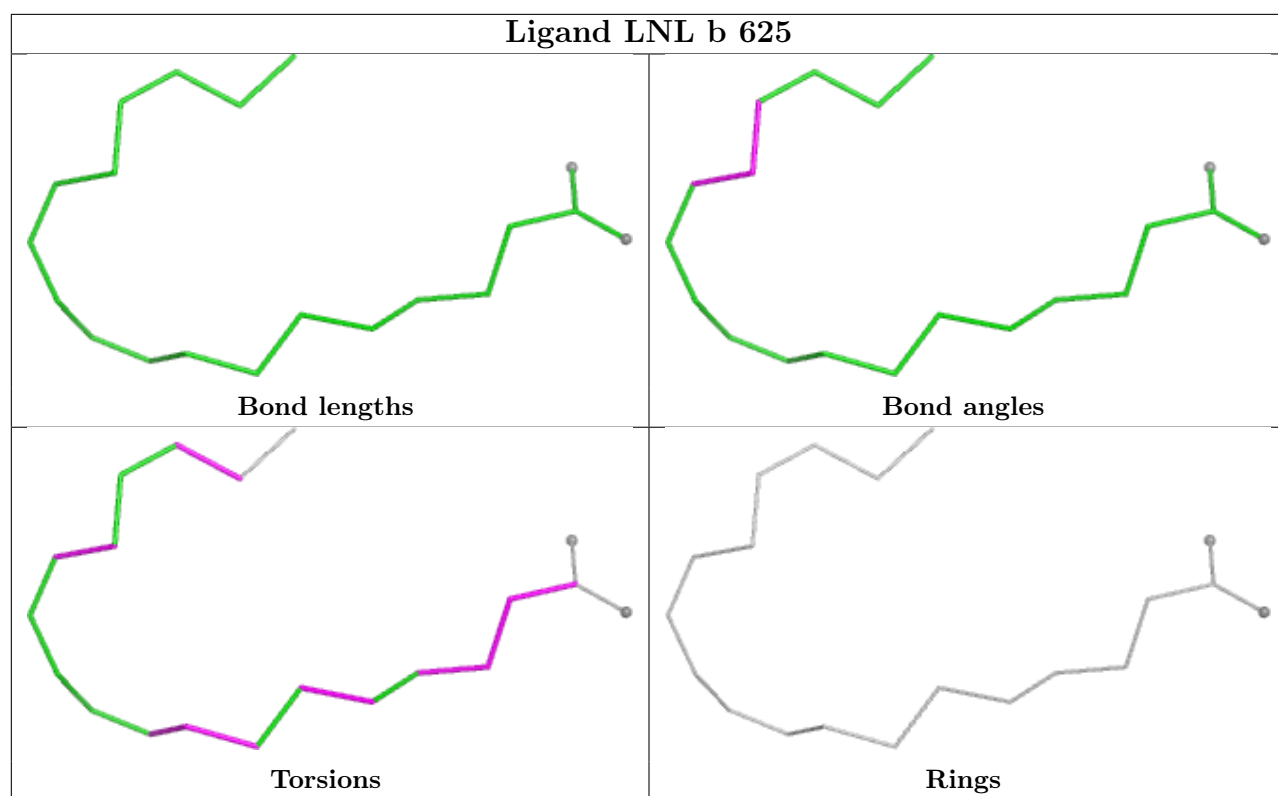


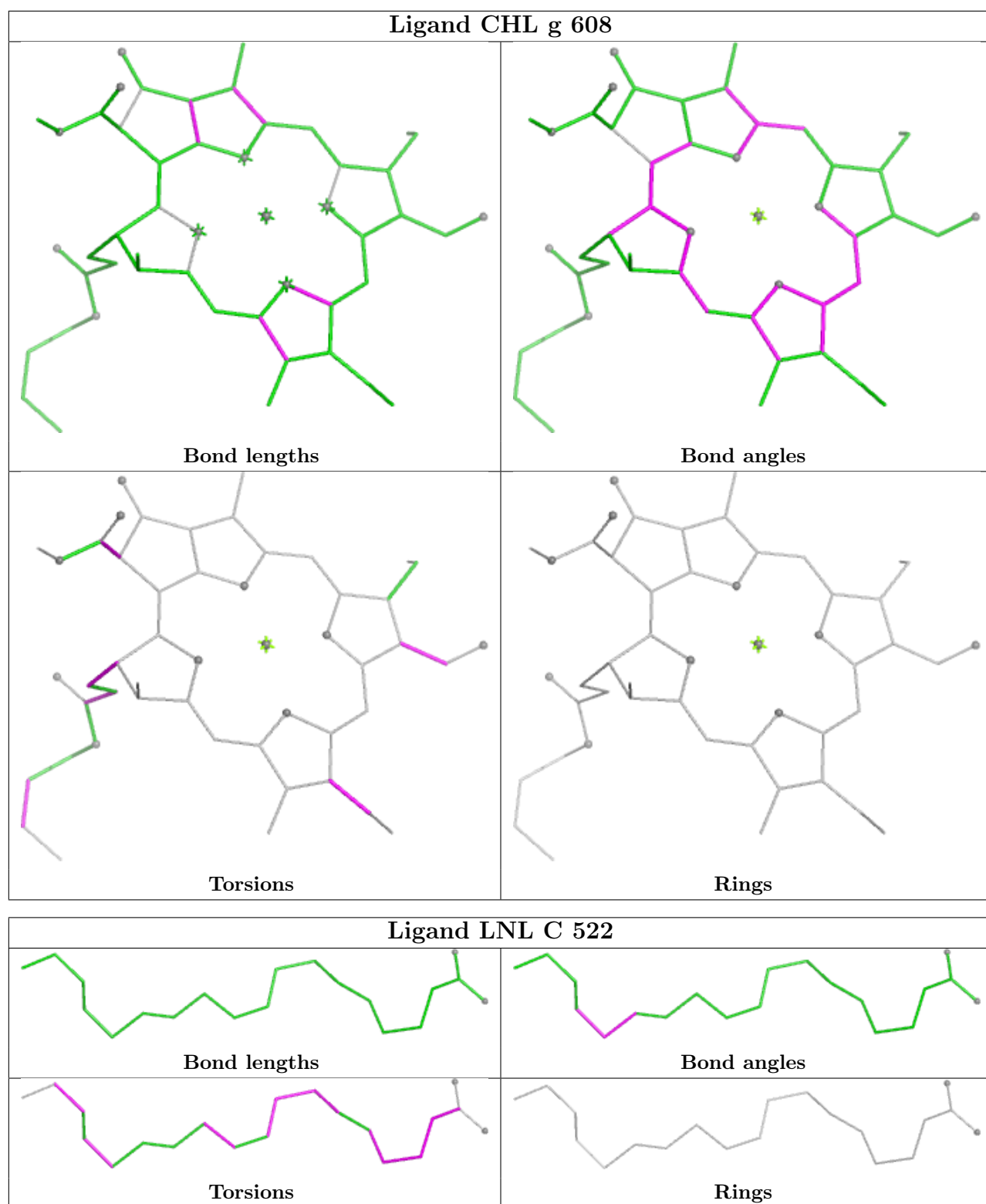
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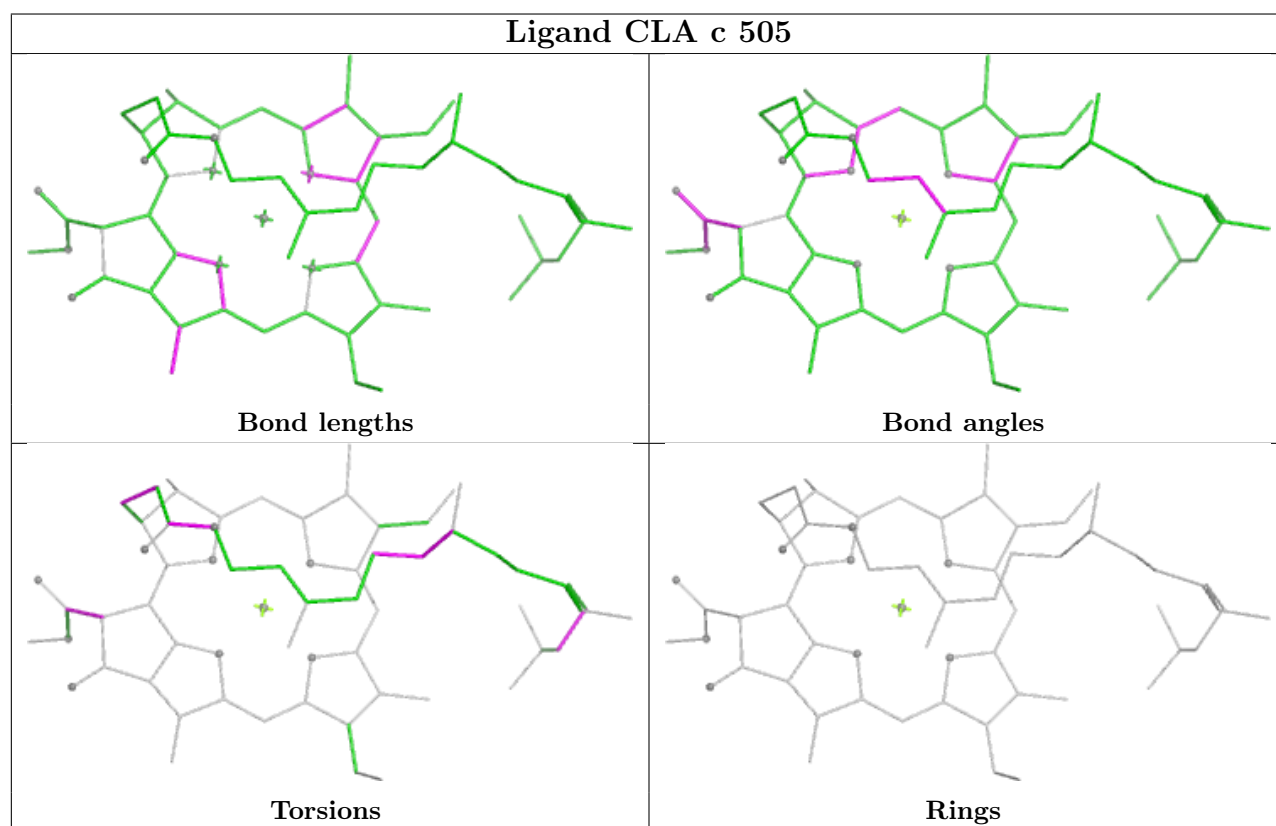
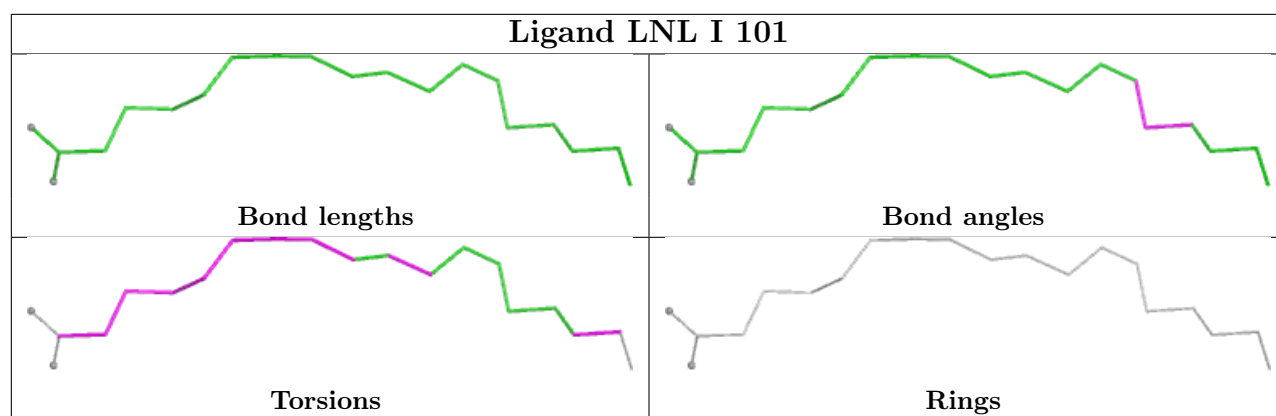


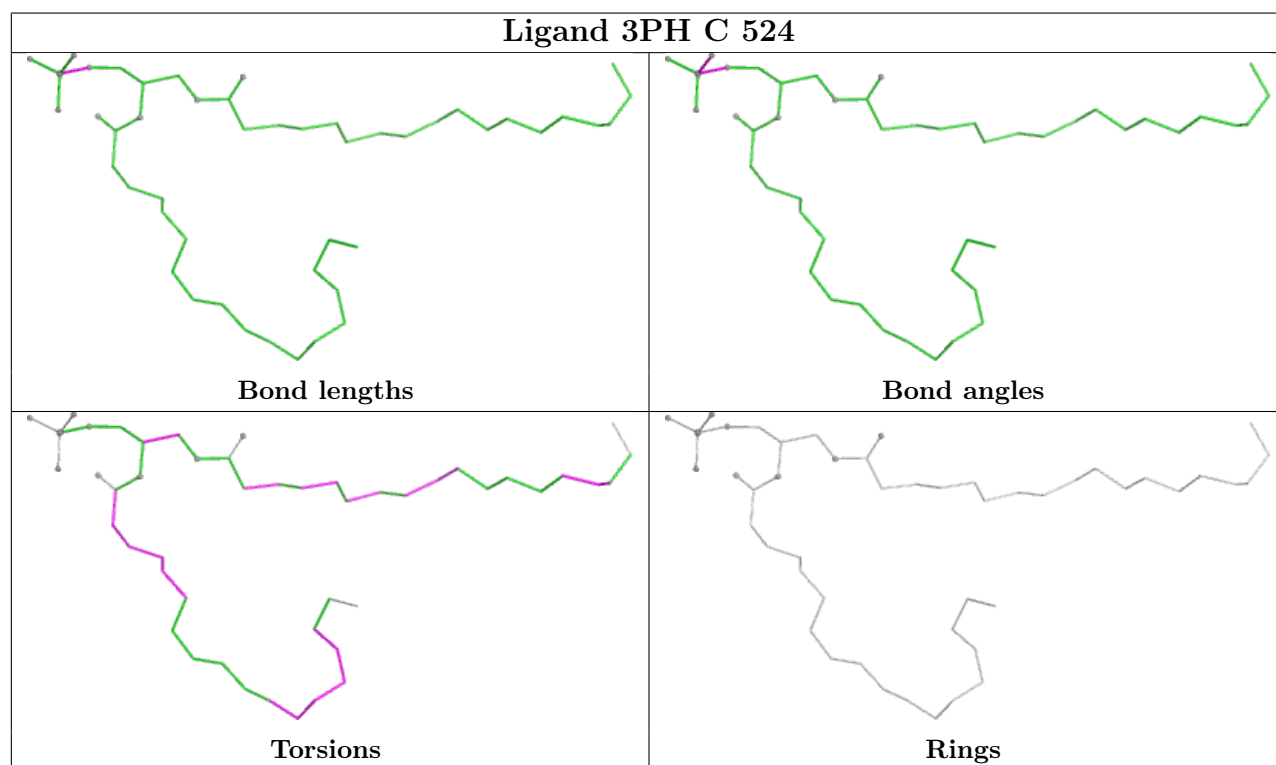
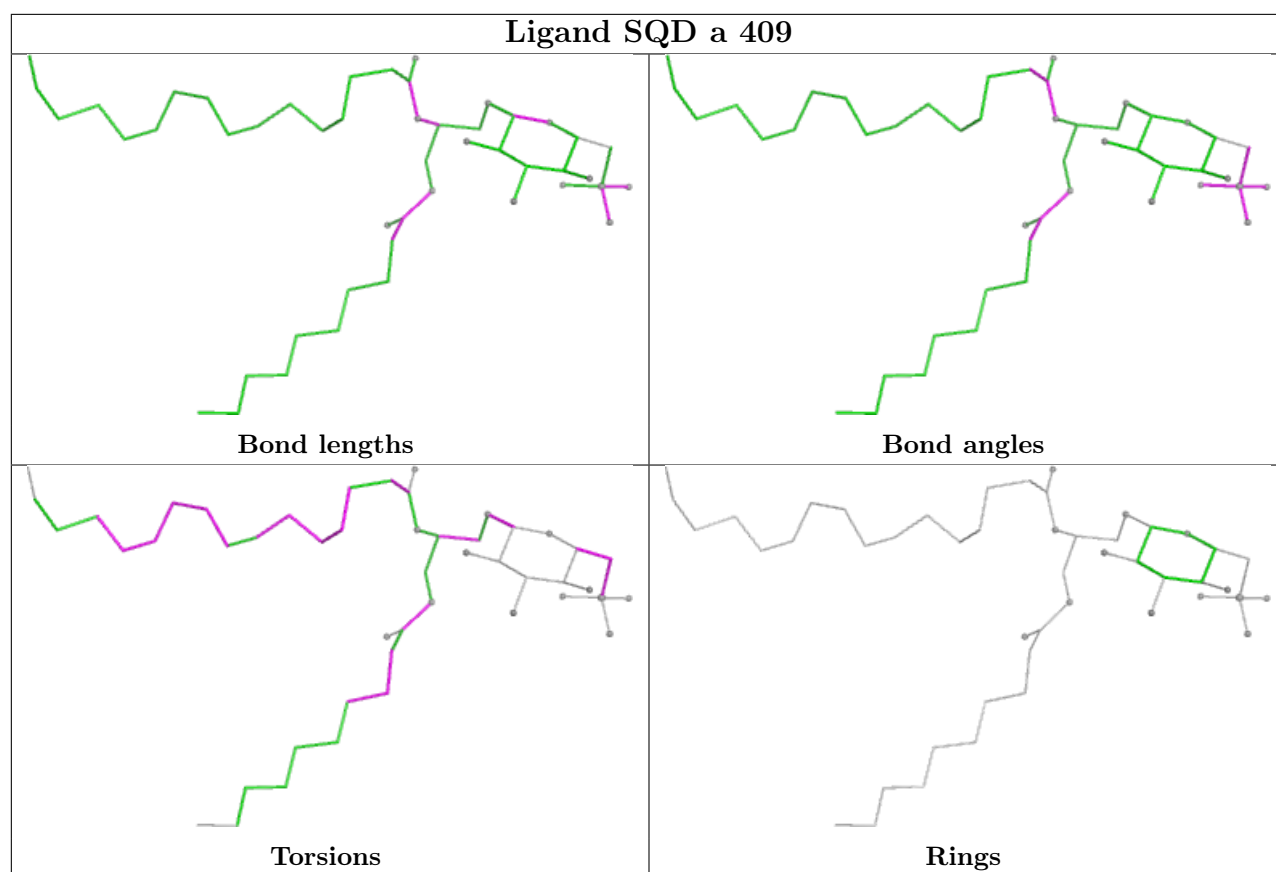
Ligand NEX S 617

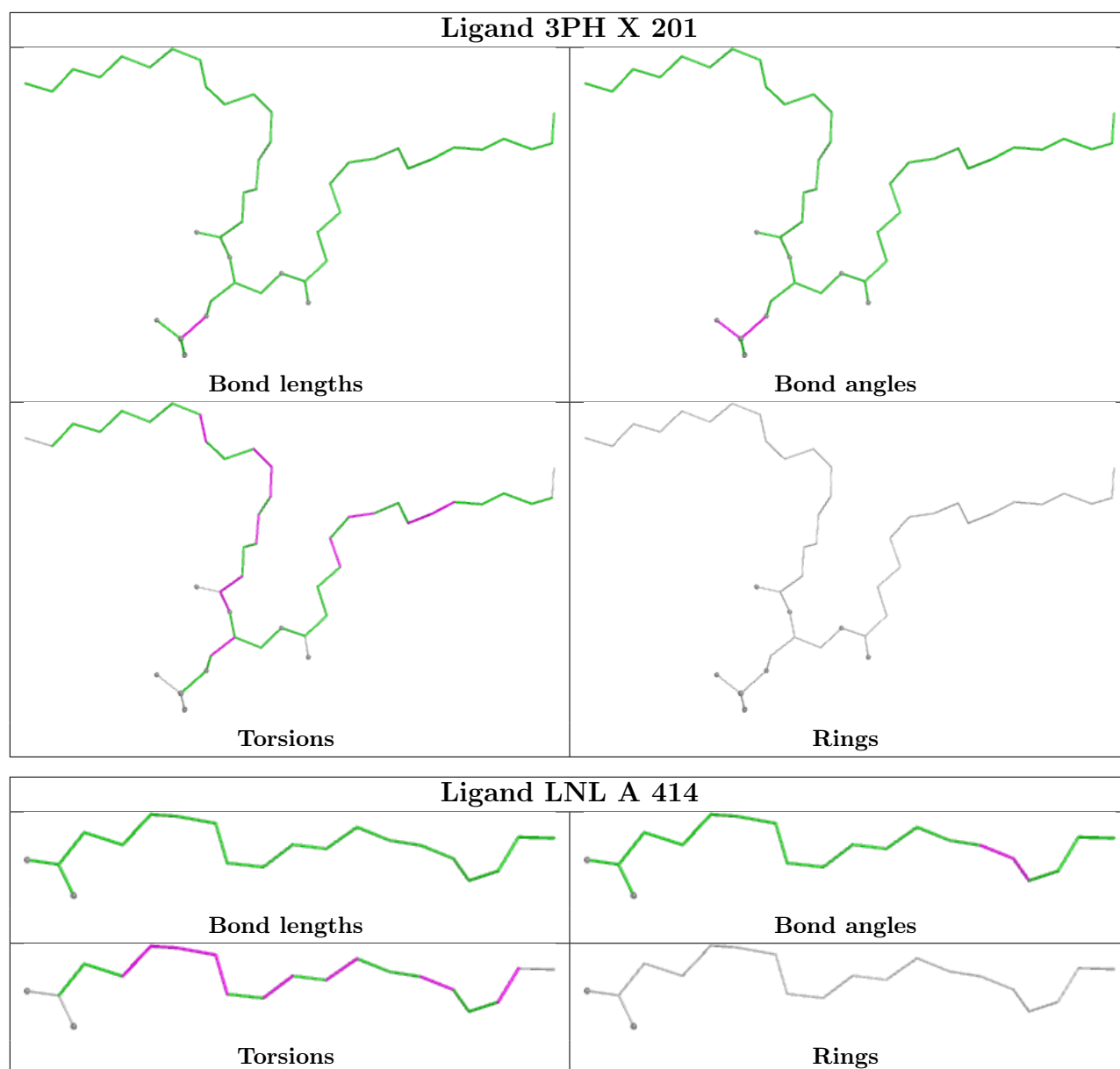


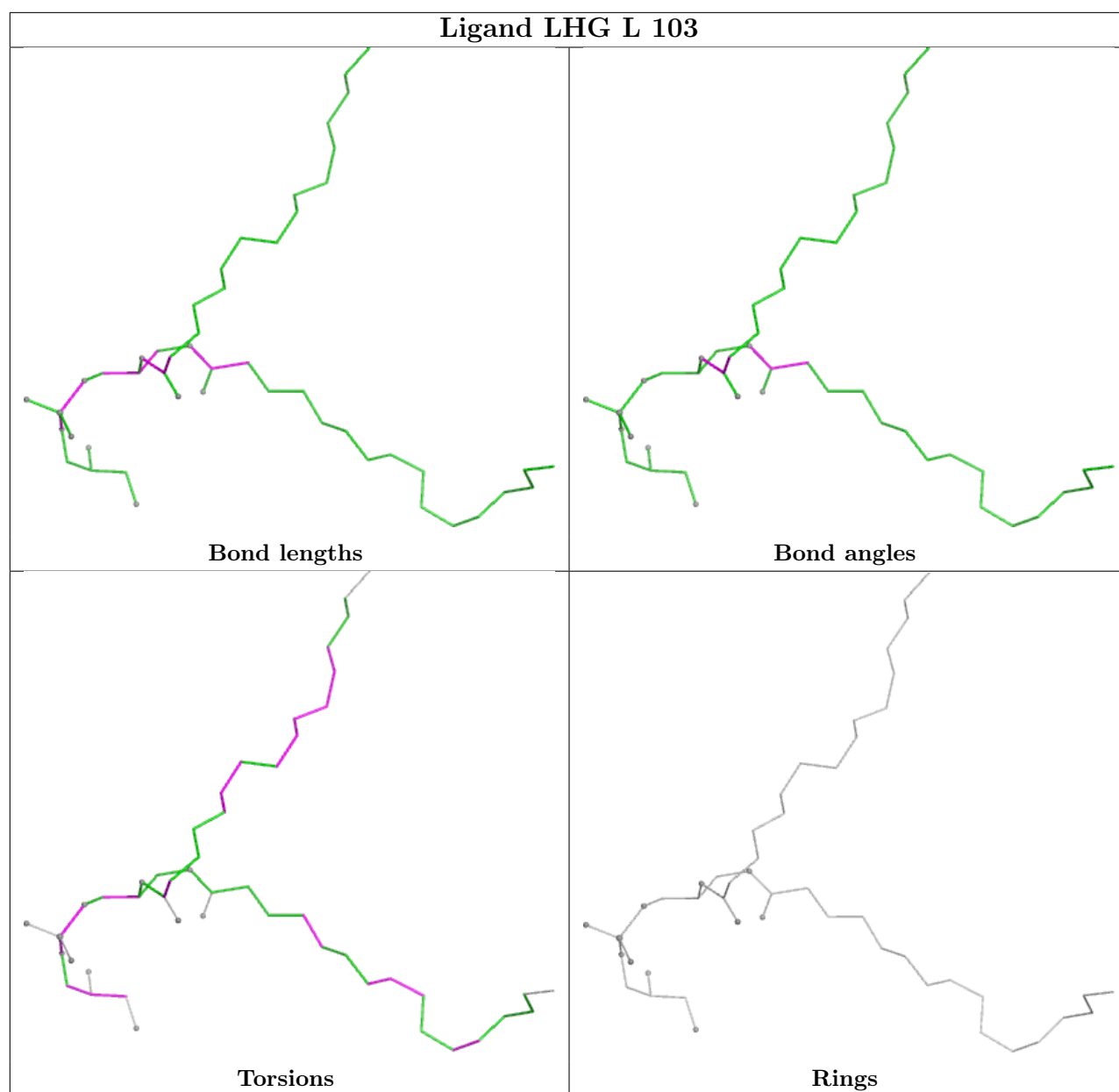


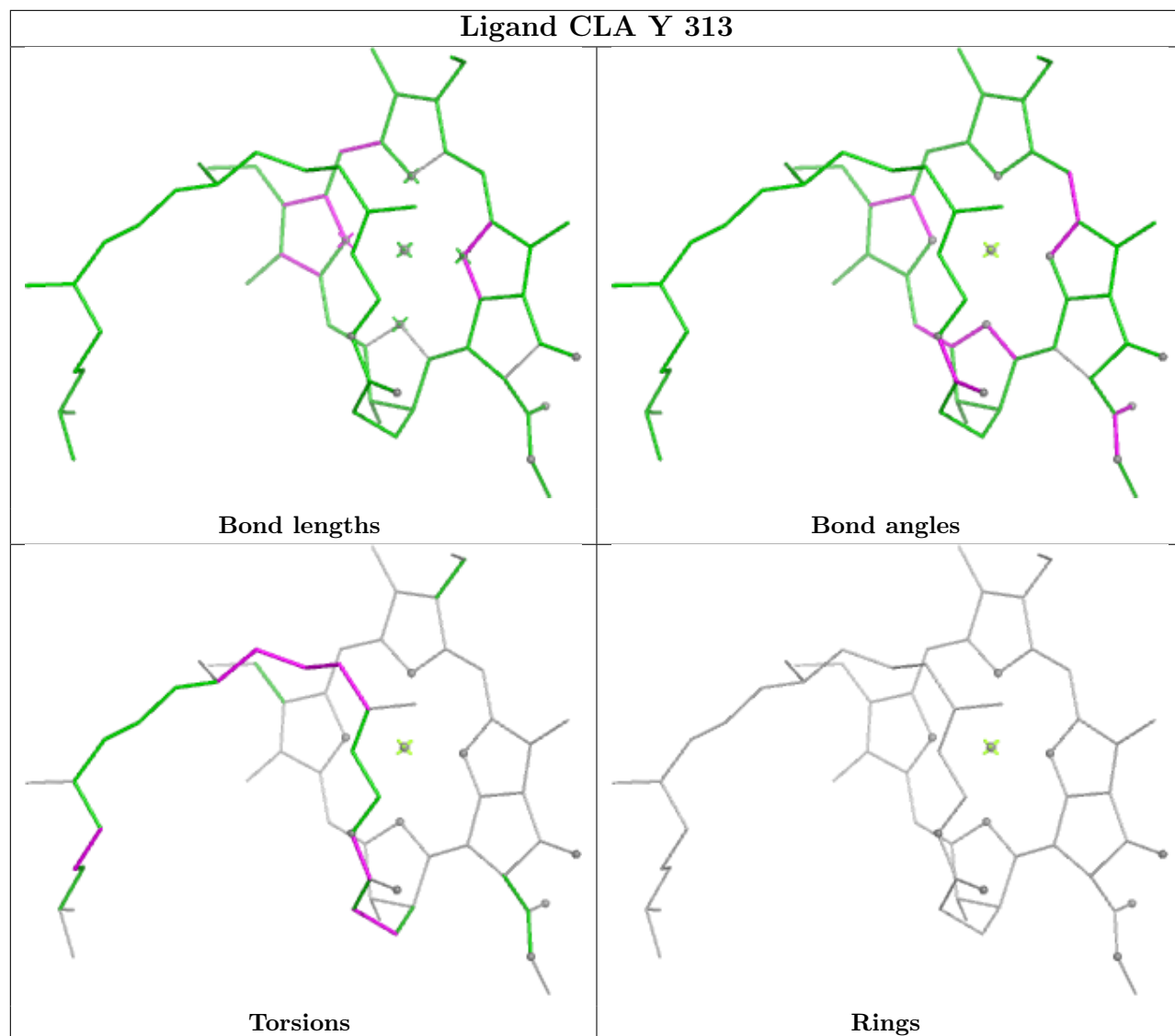


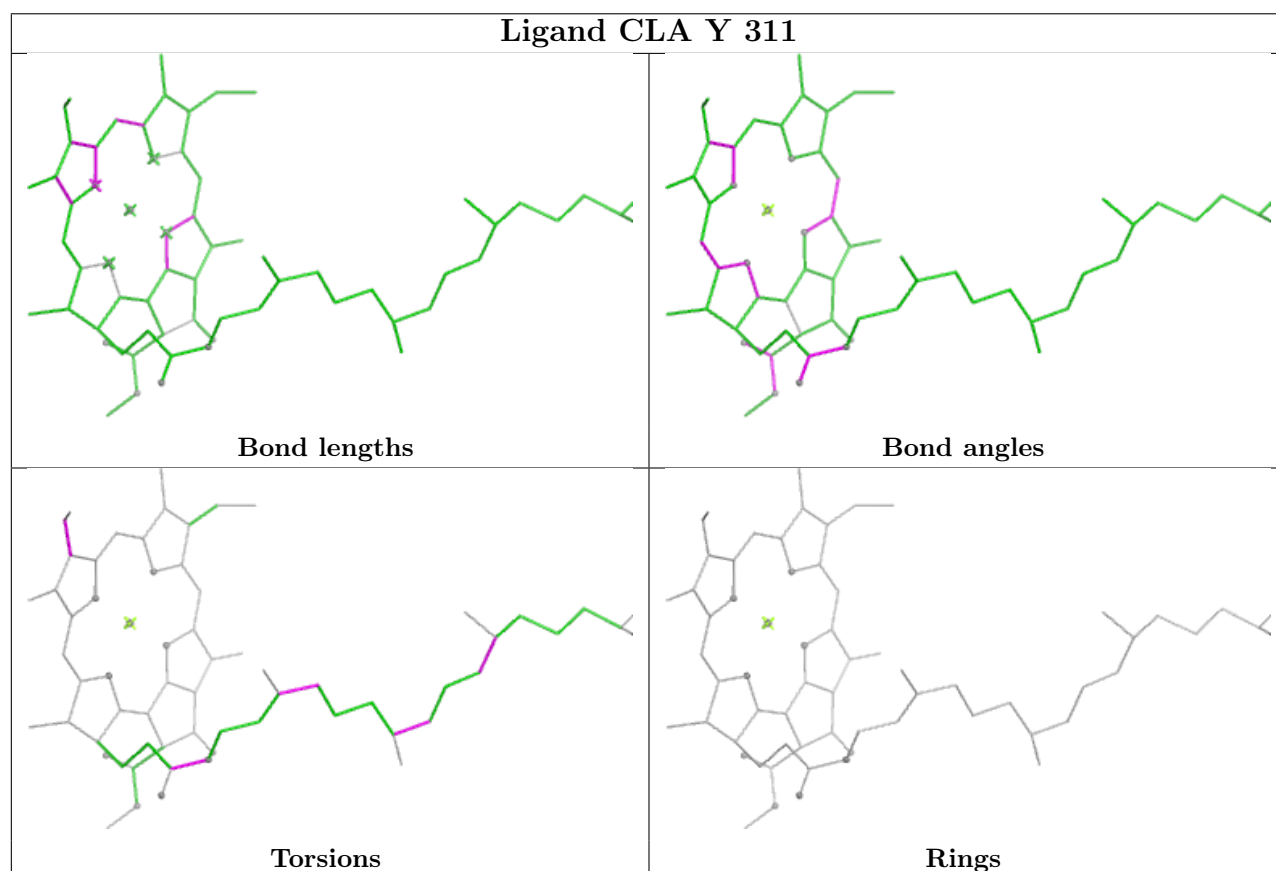
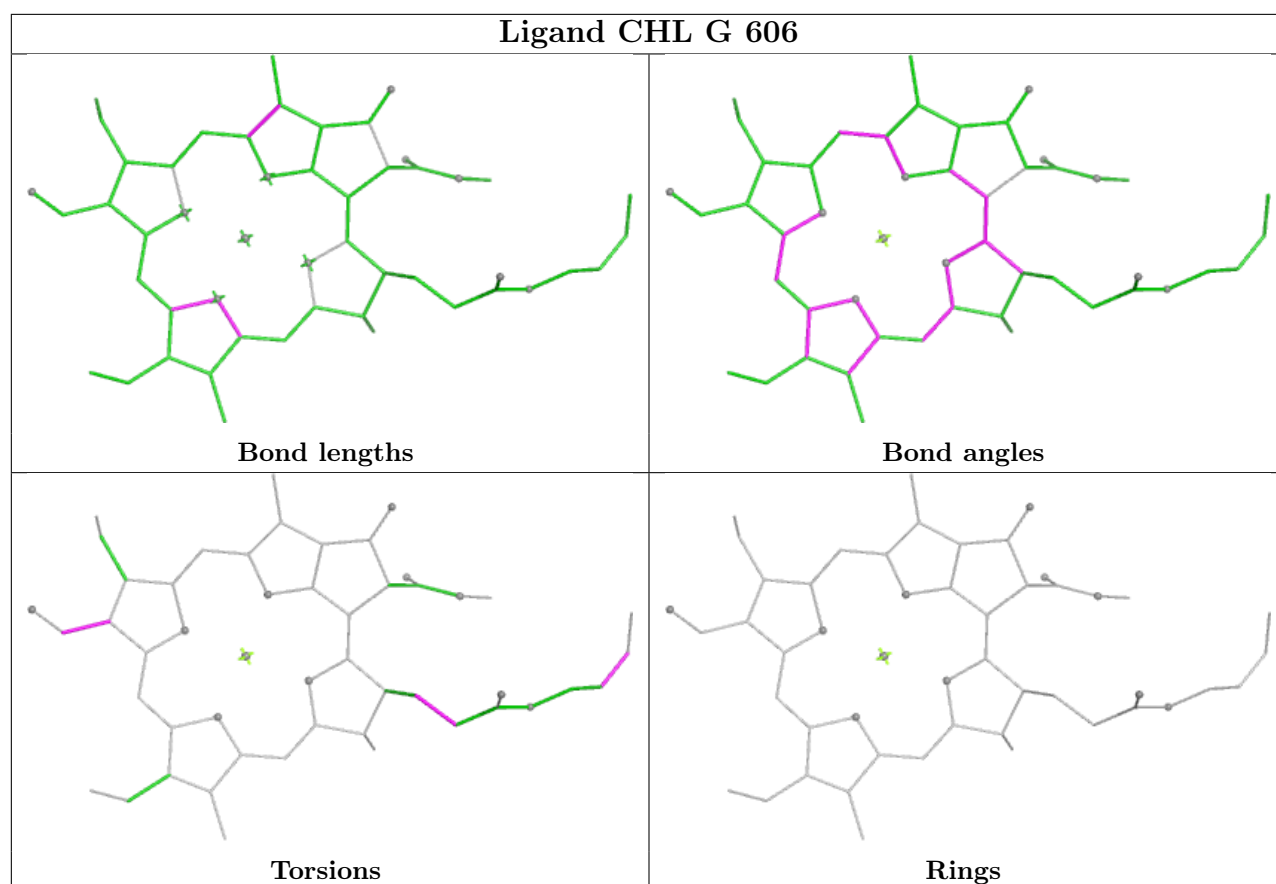


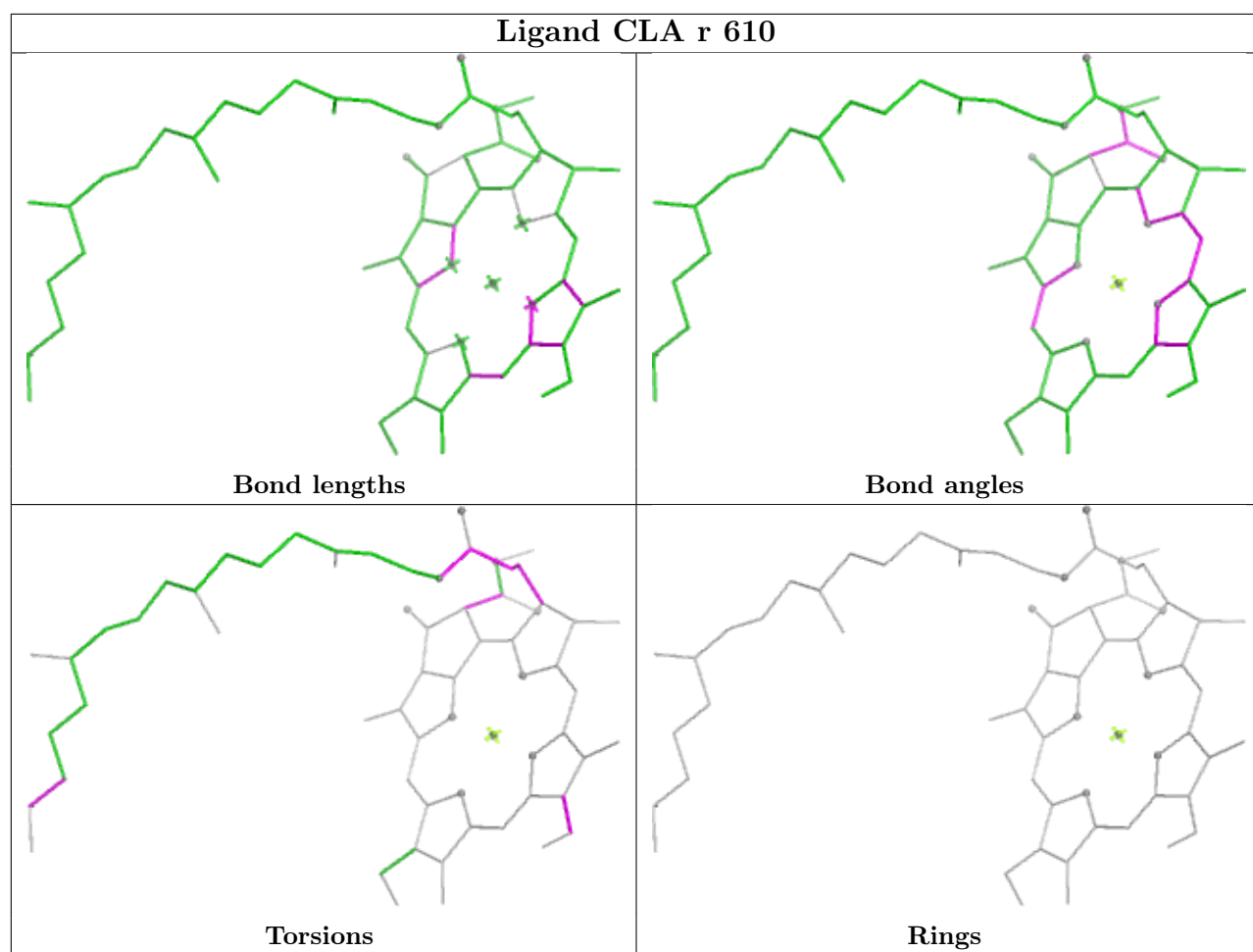


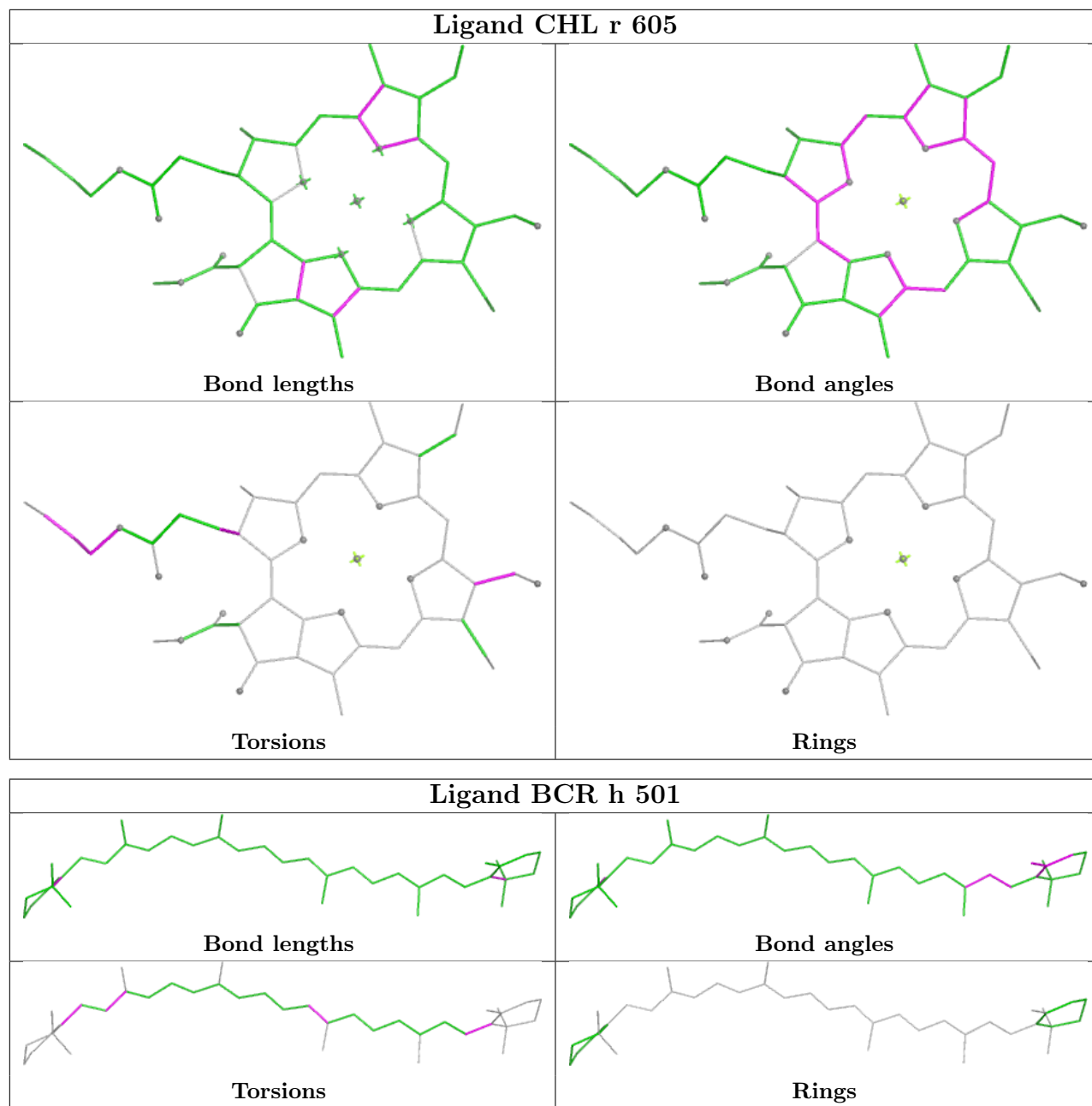


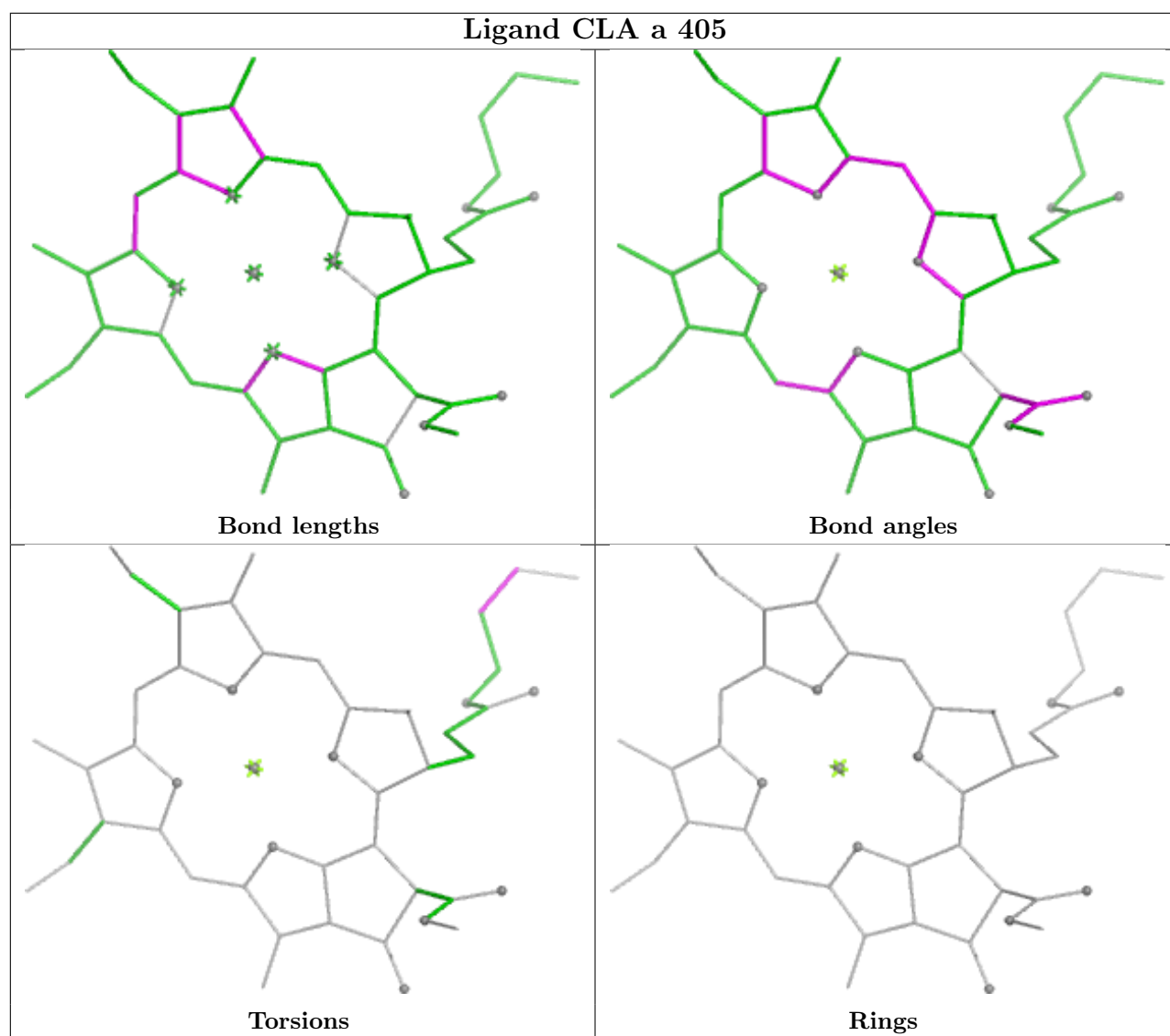


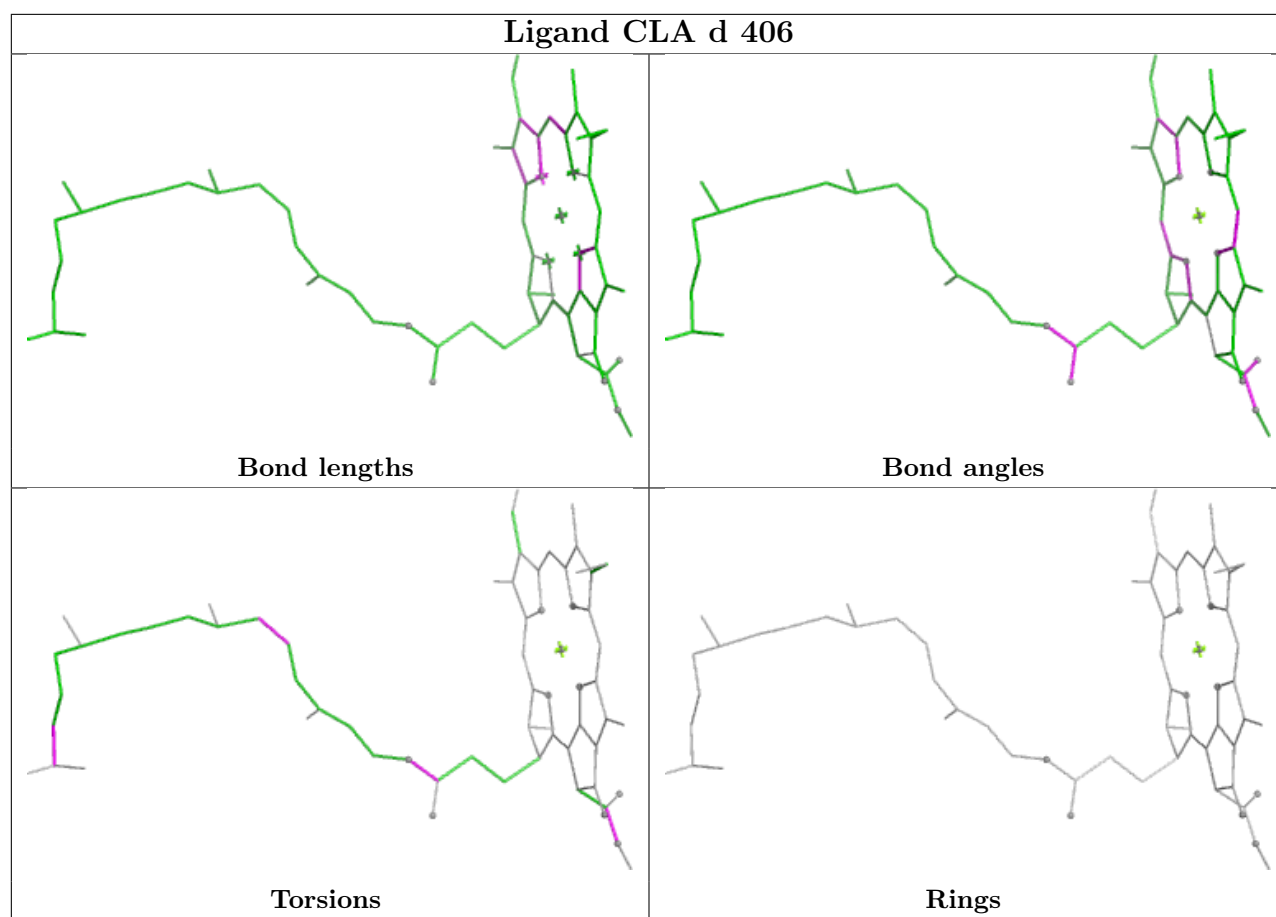




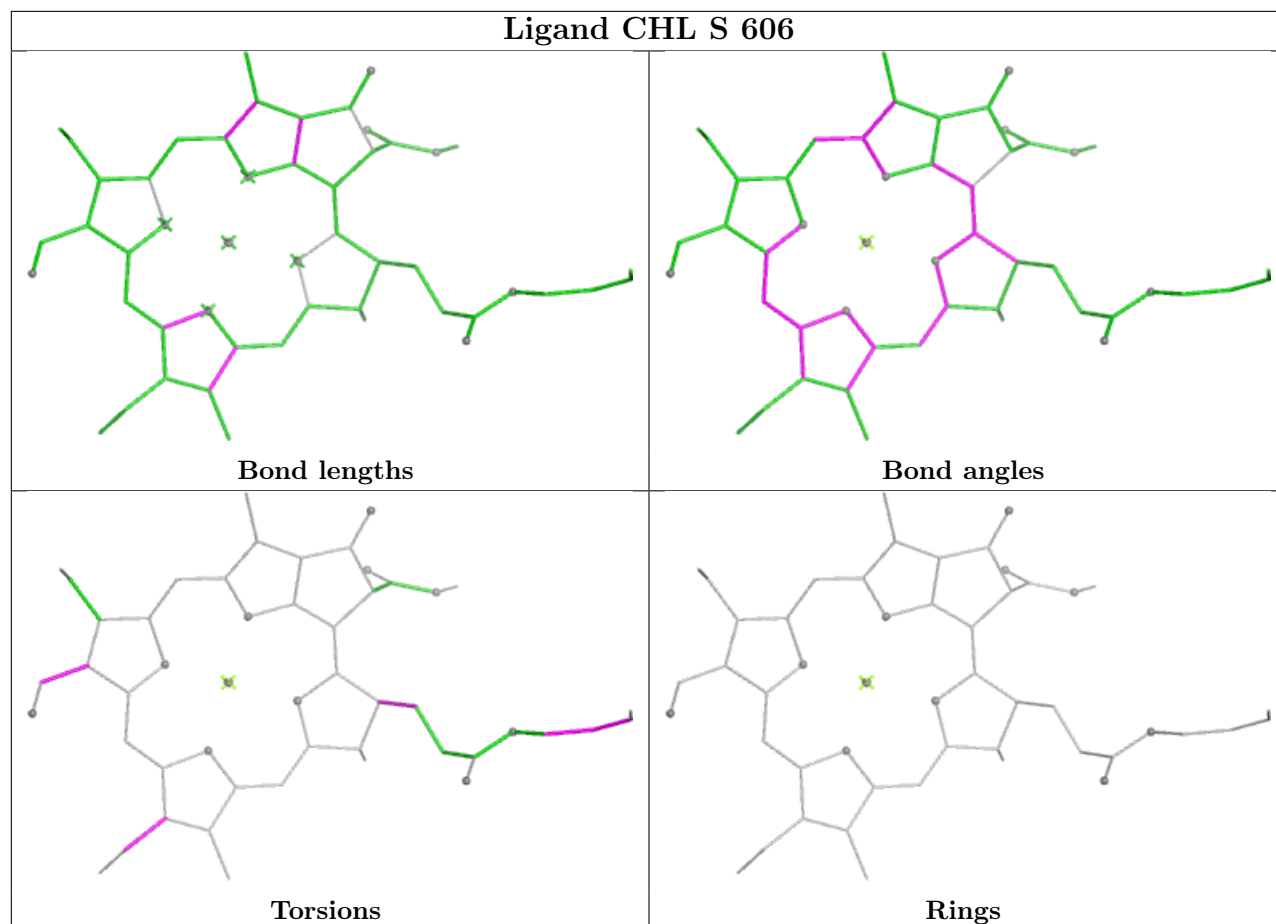




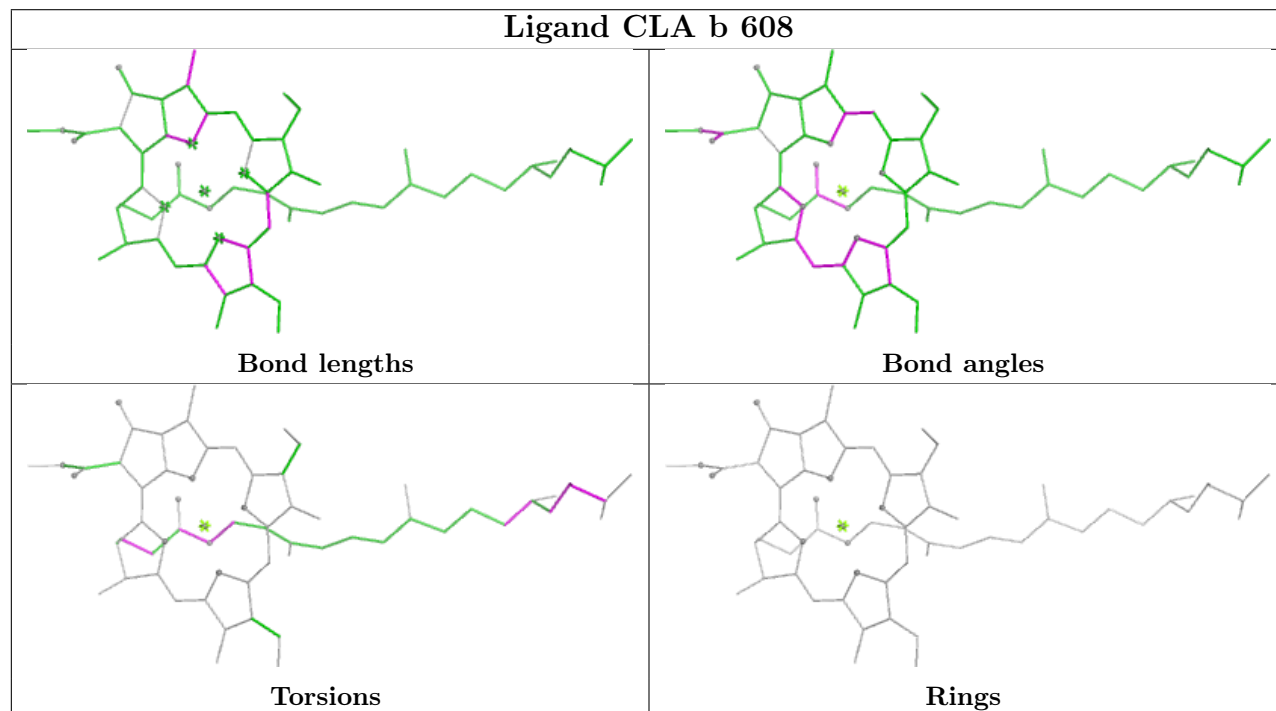


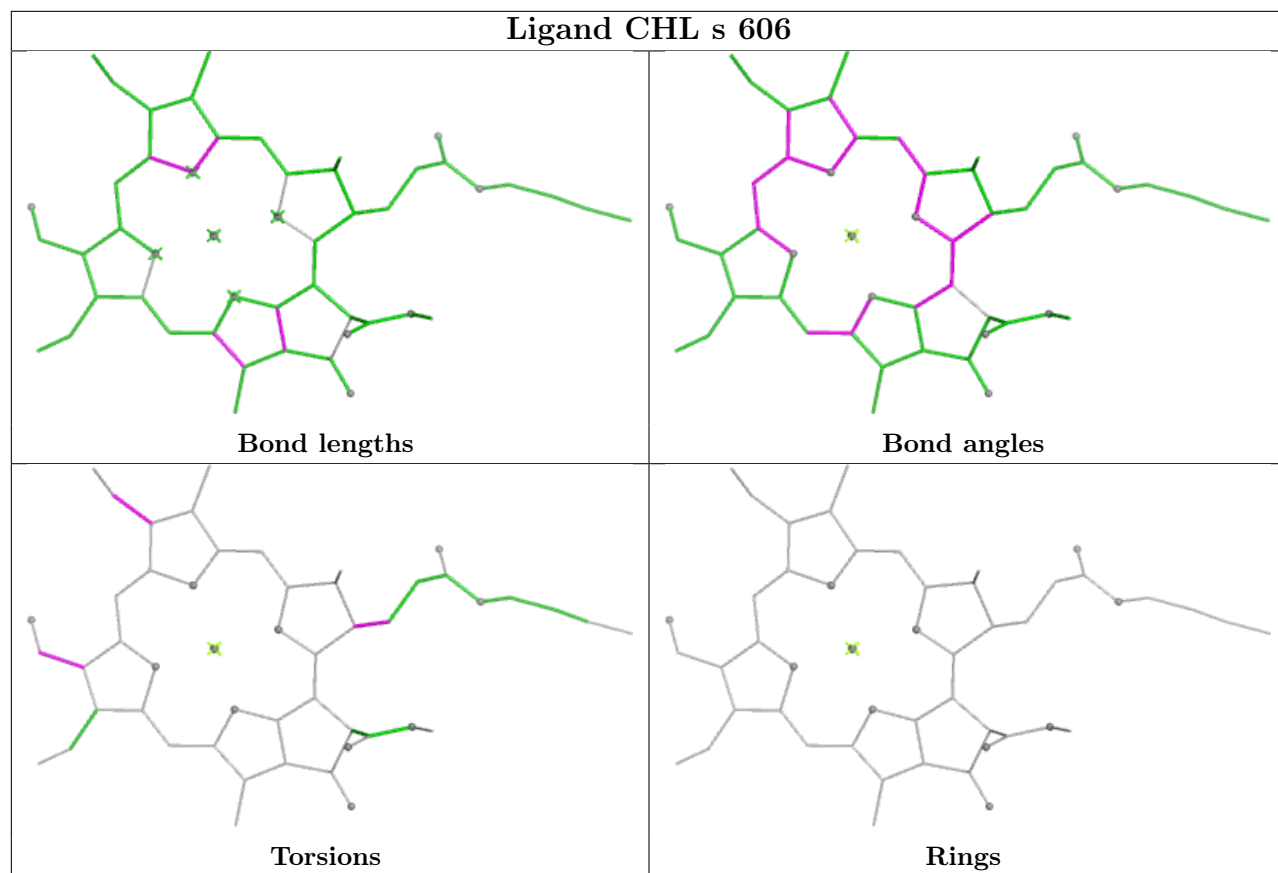


Ligand CHL S 606

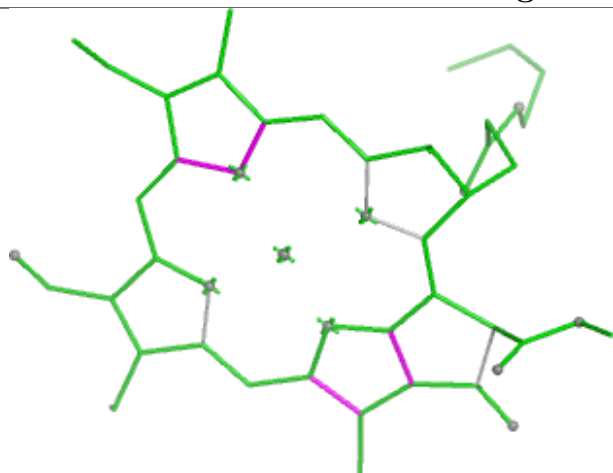


Ligand CLA b 608

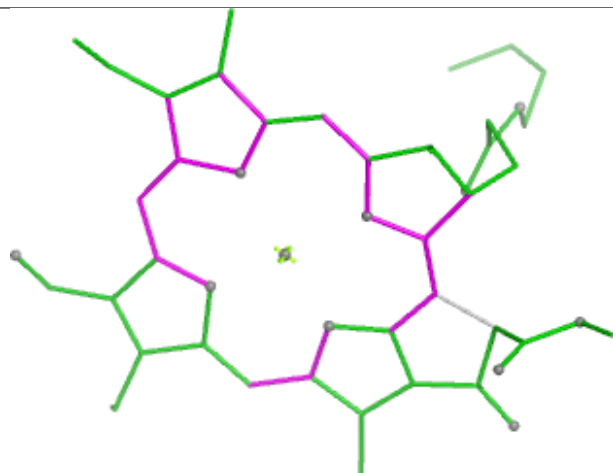




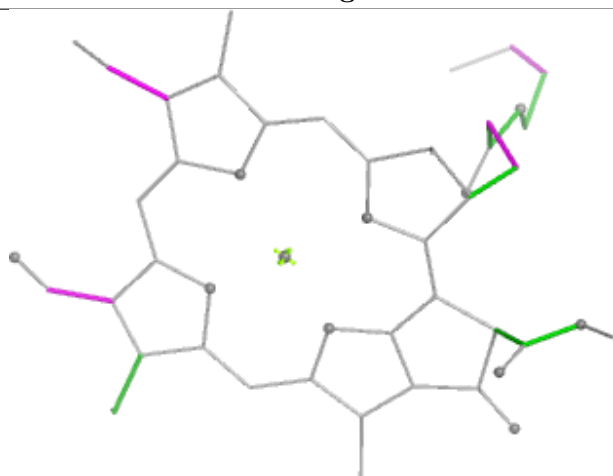
Ligand CHL n 608



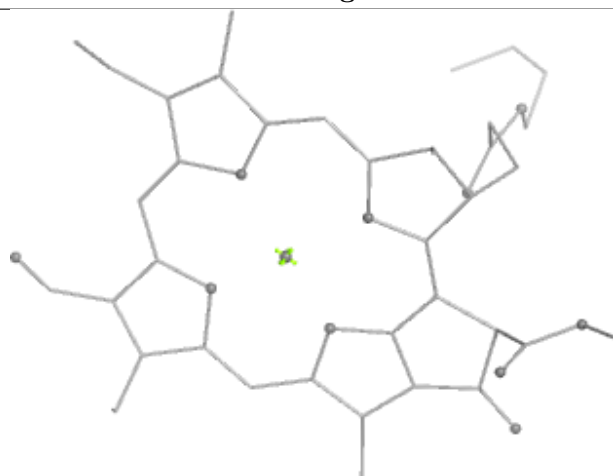
Bond lengths



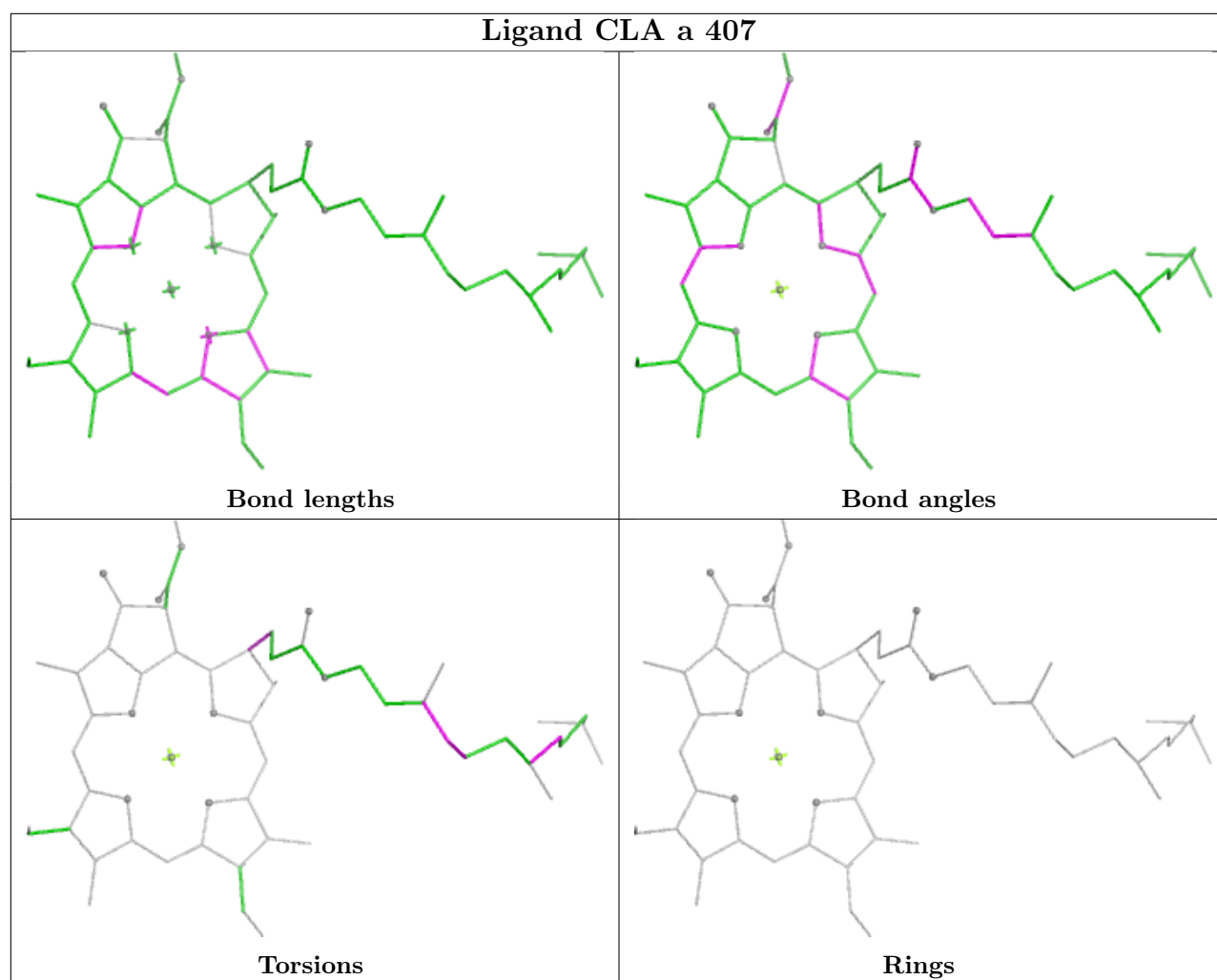
Bond angles

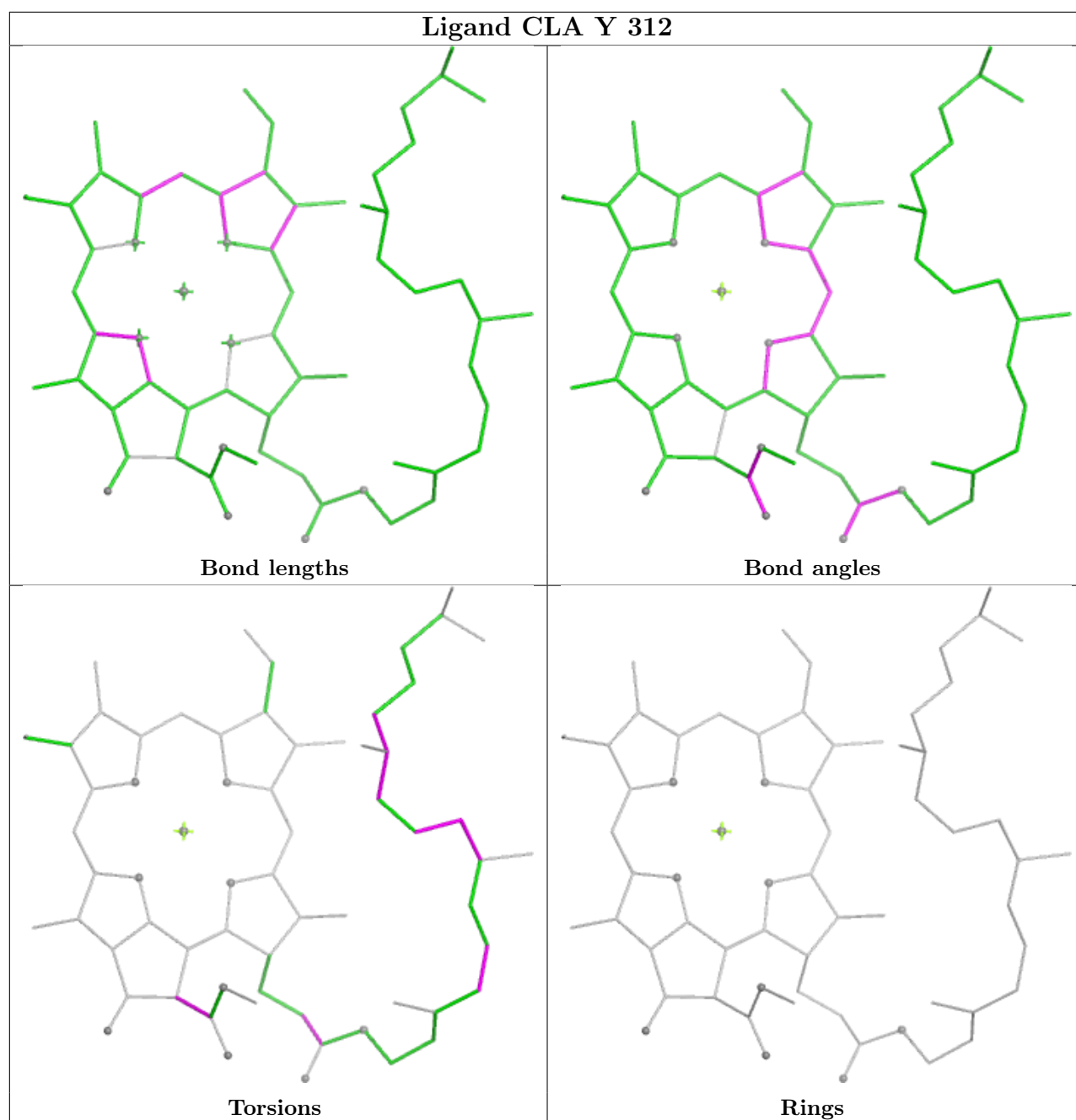


Torsions

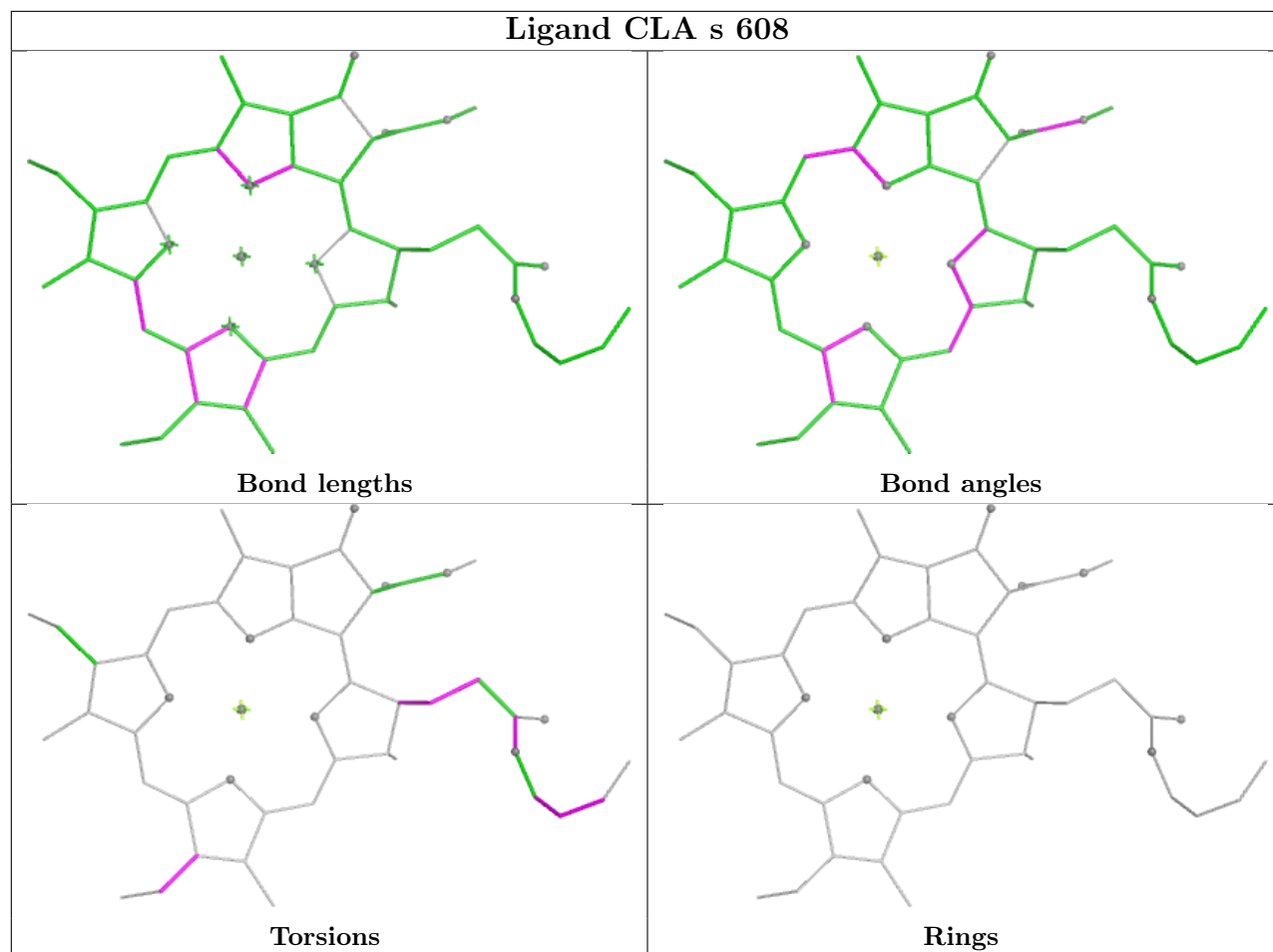


Rings

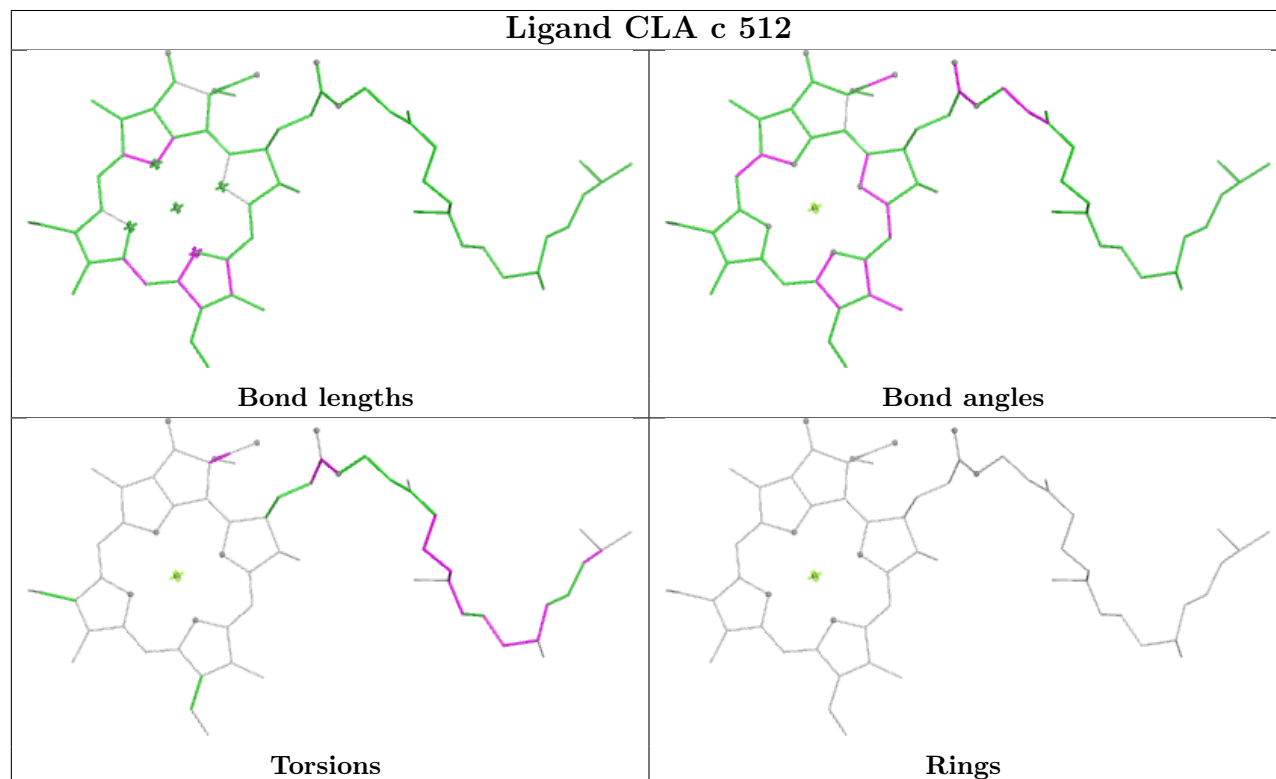


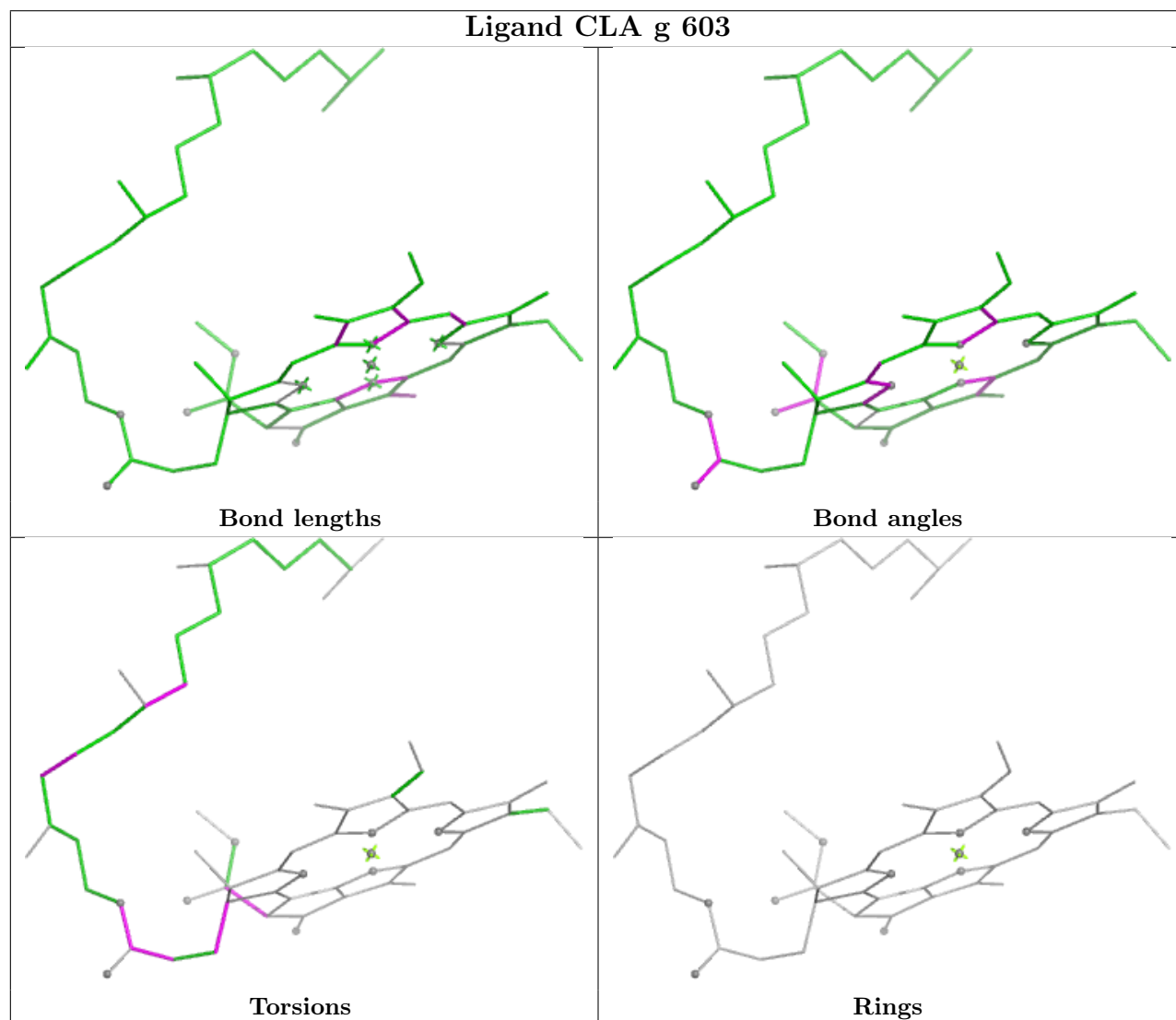
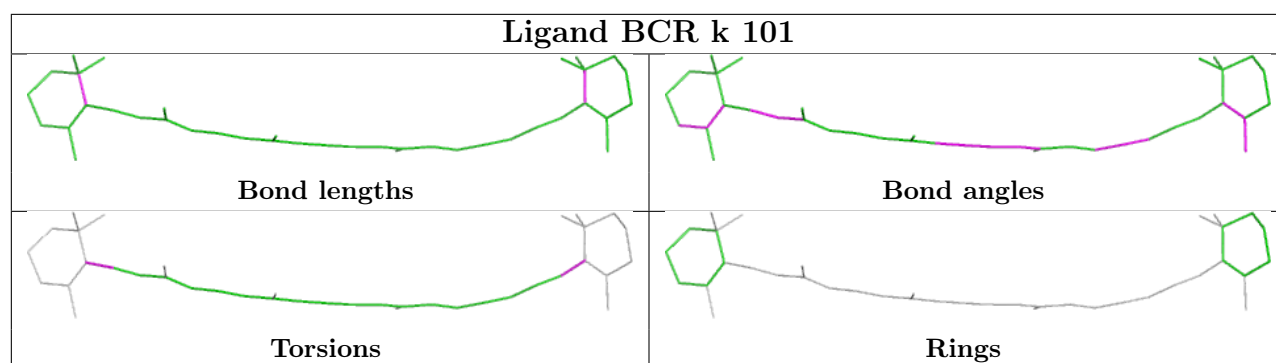


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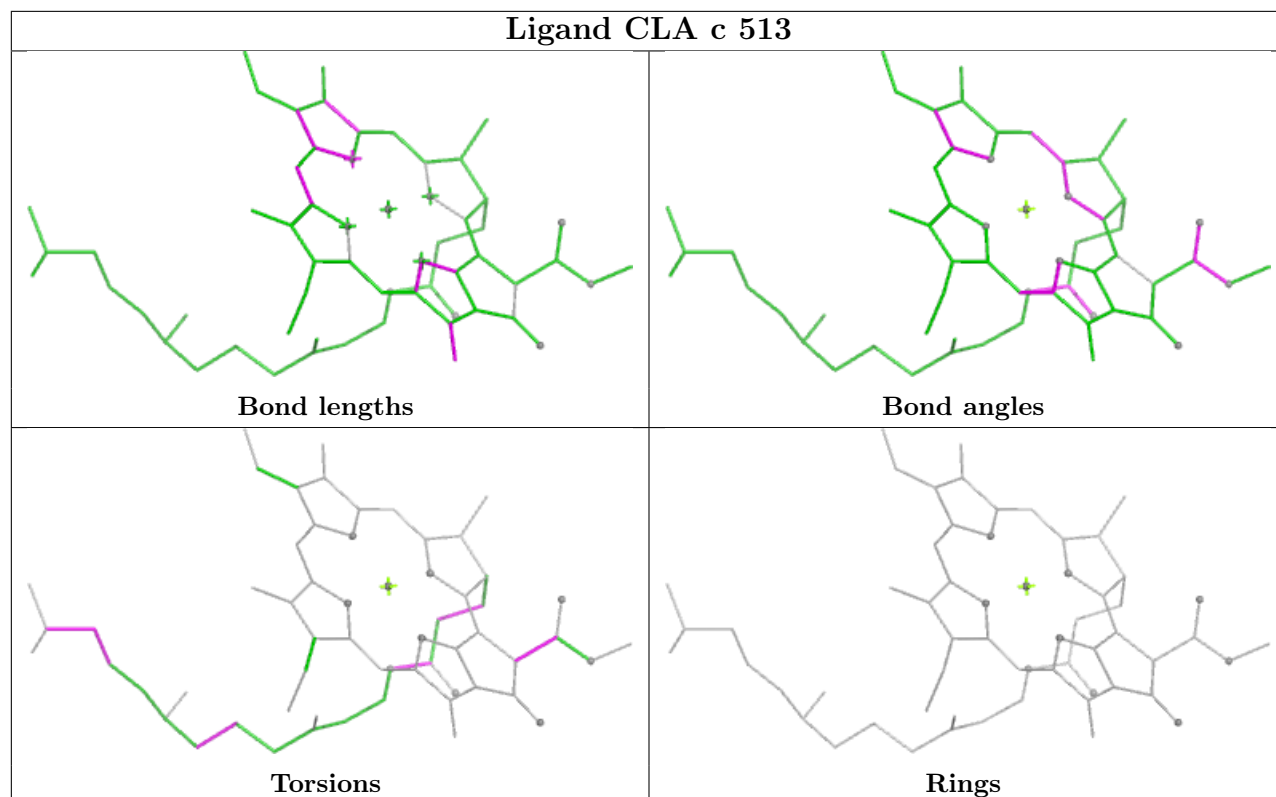


Ligand CLA c 512

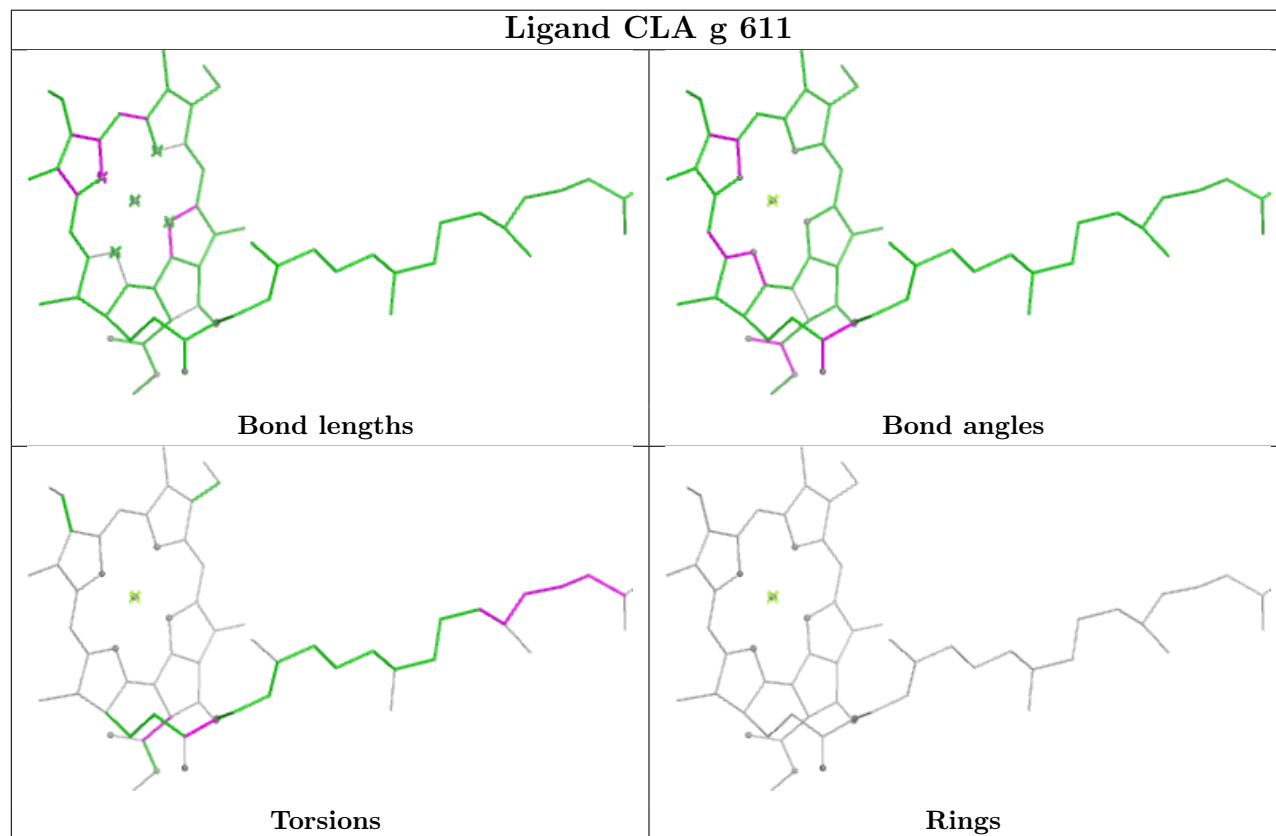


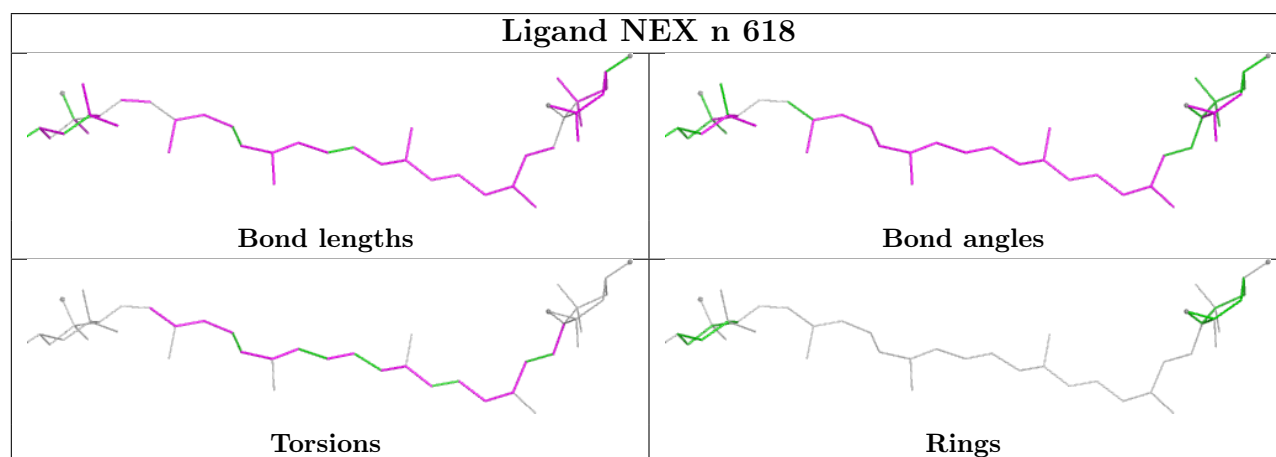
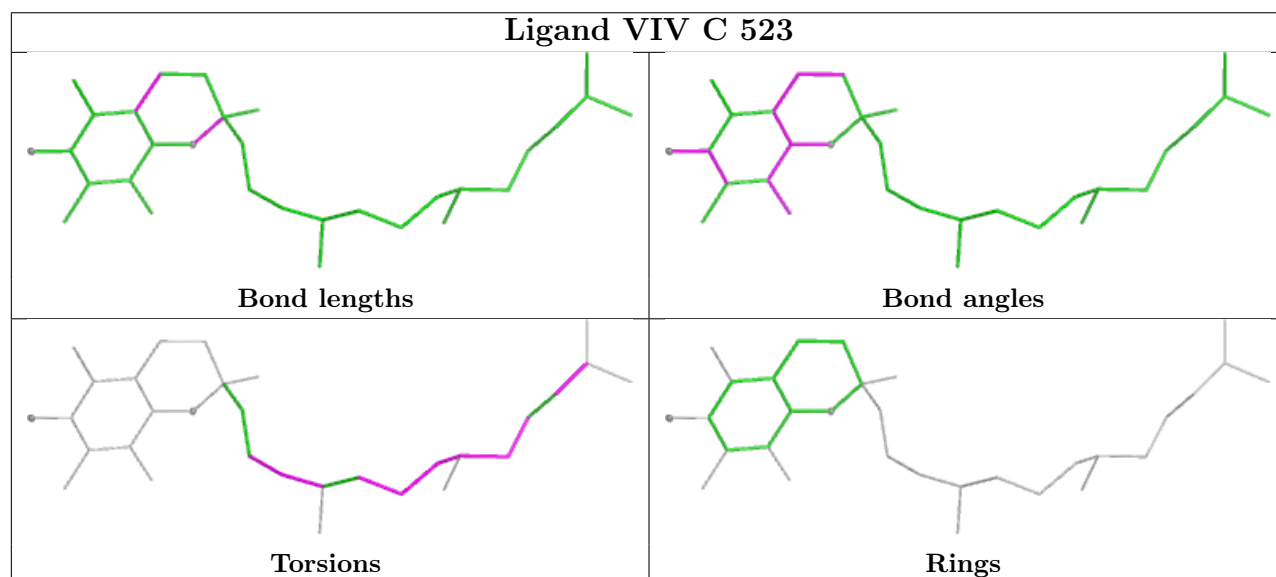
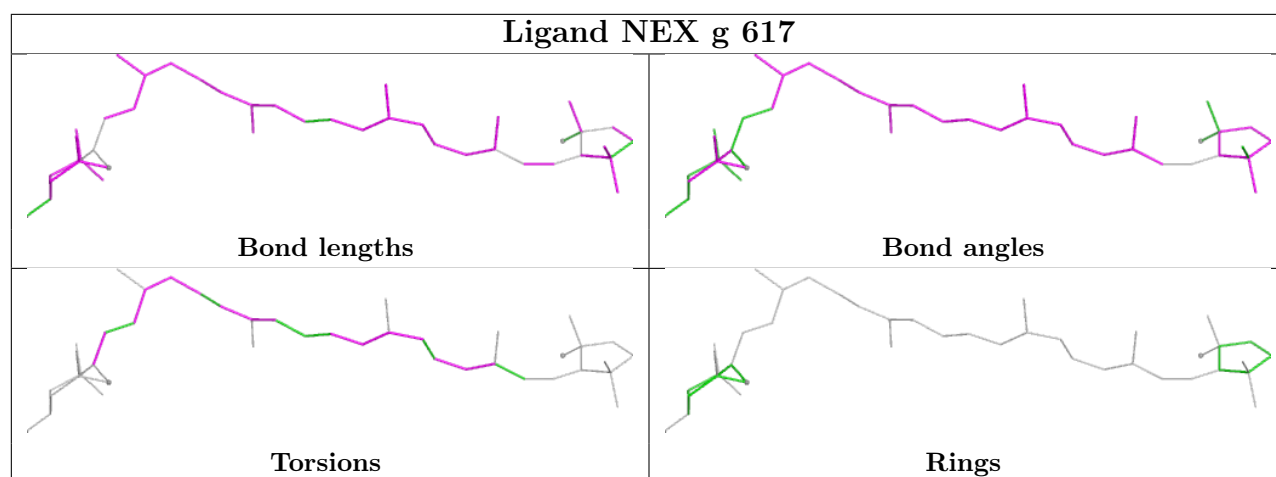


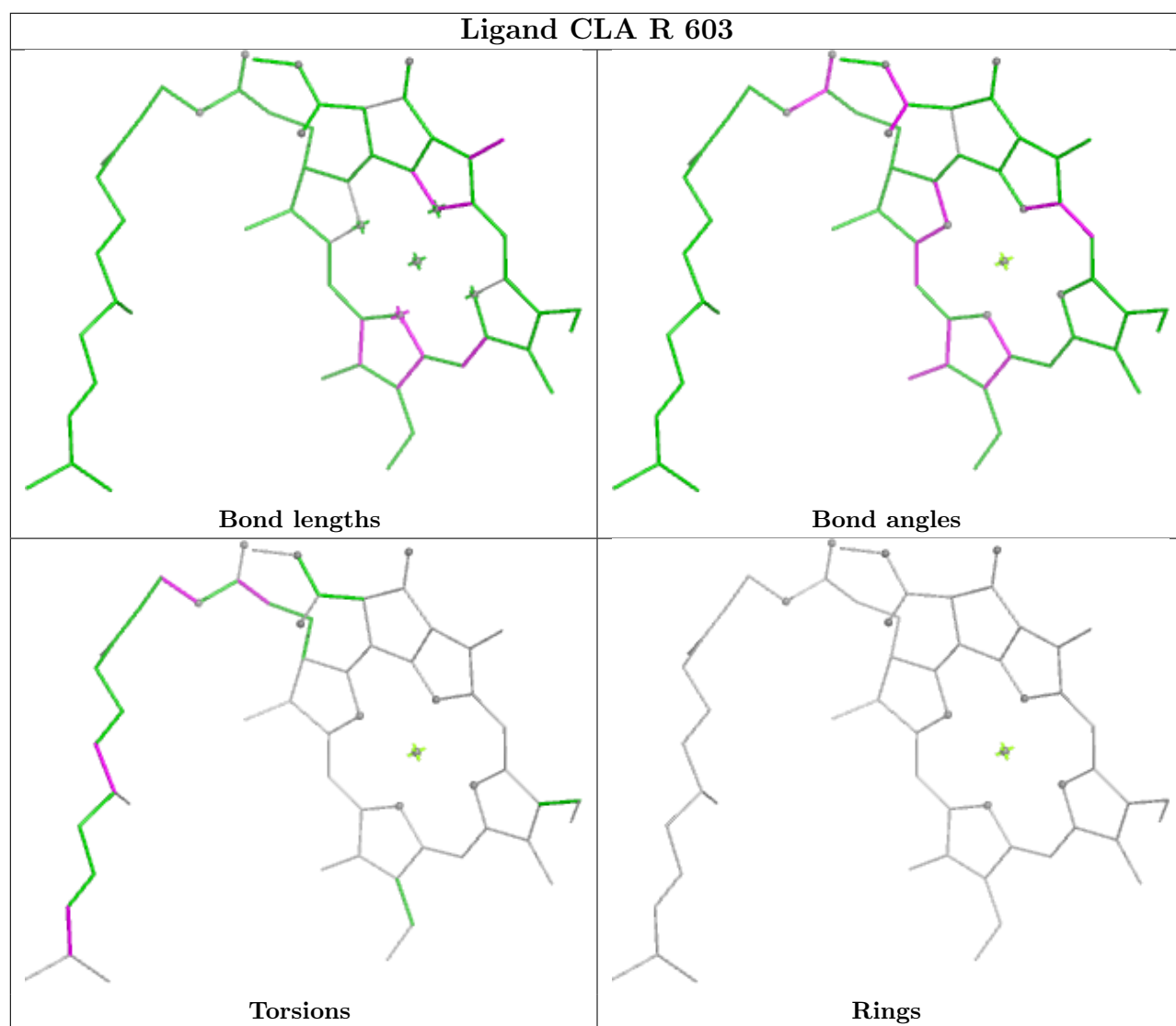
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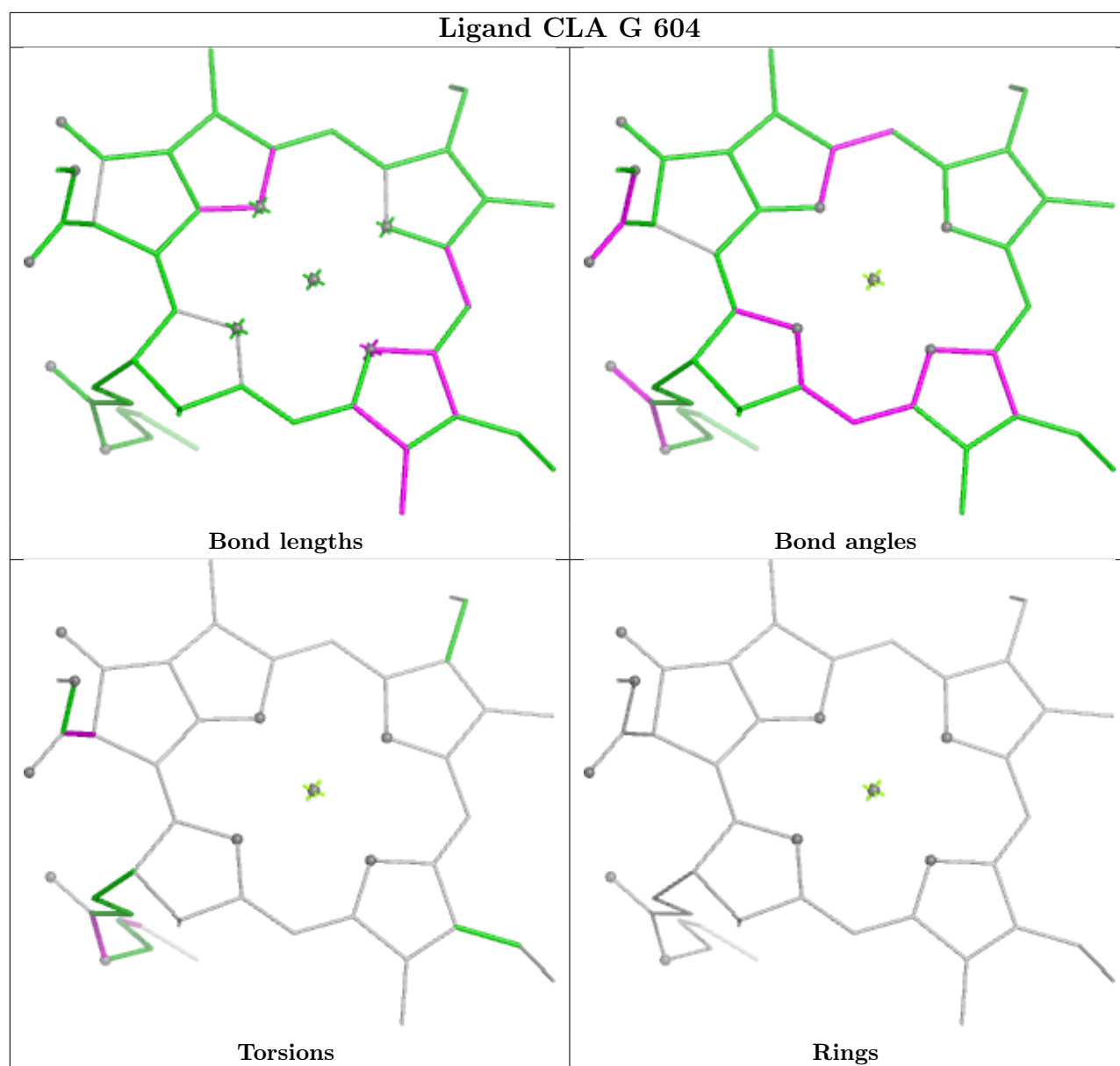


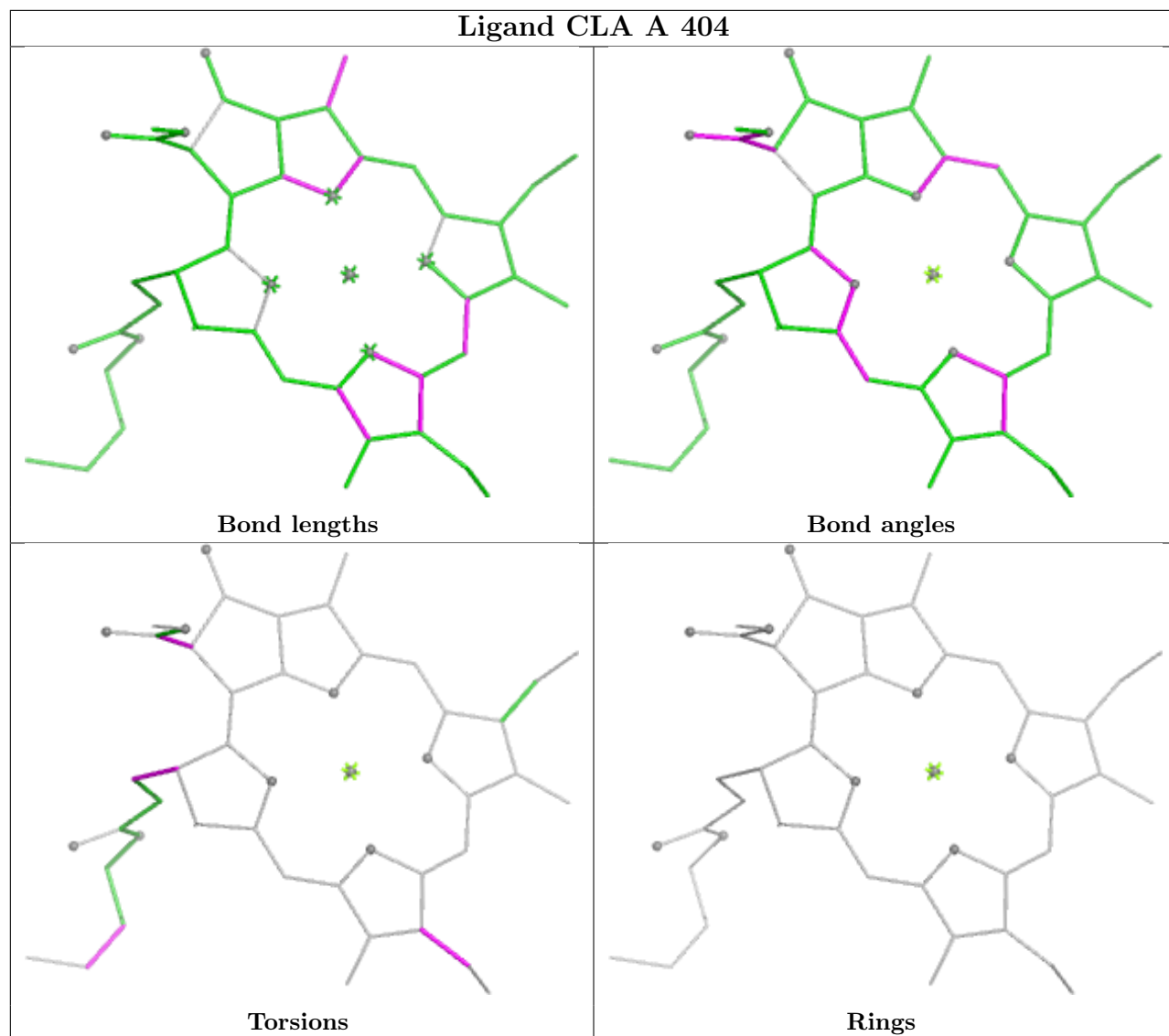
Ligand CLA g 611

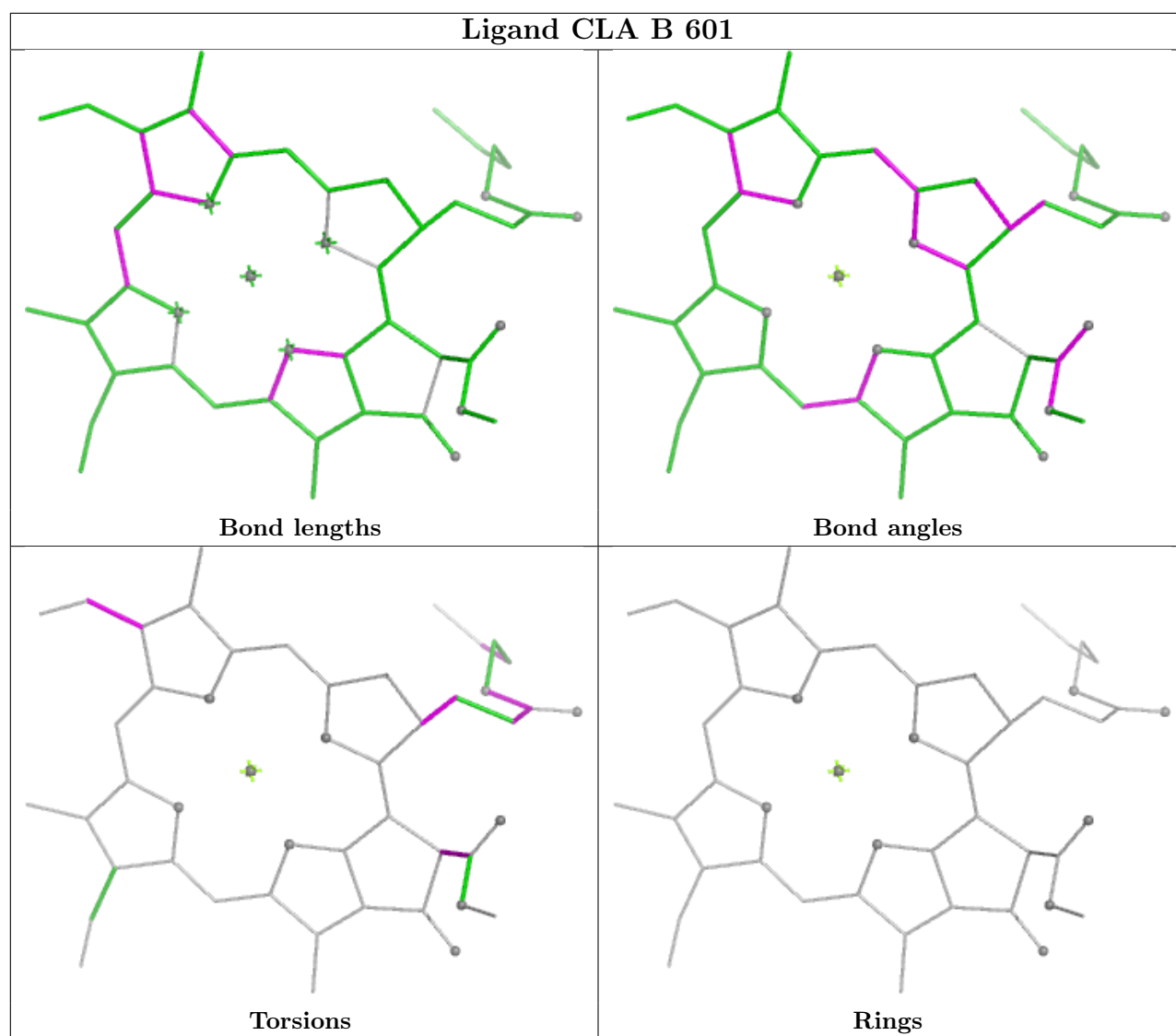


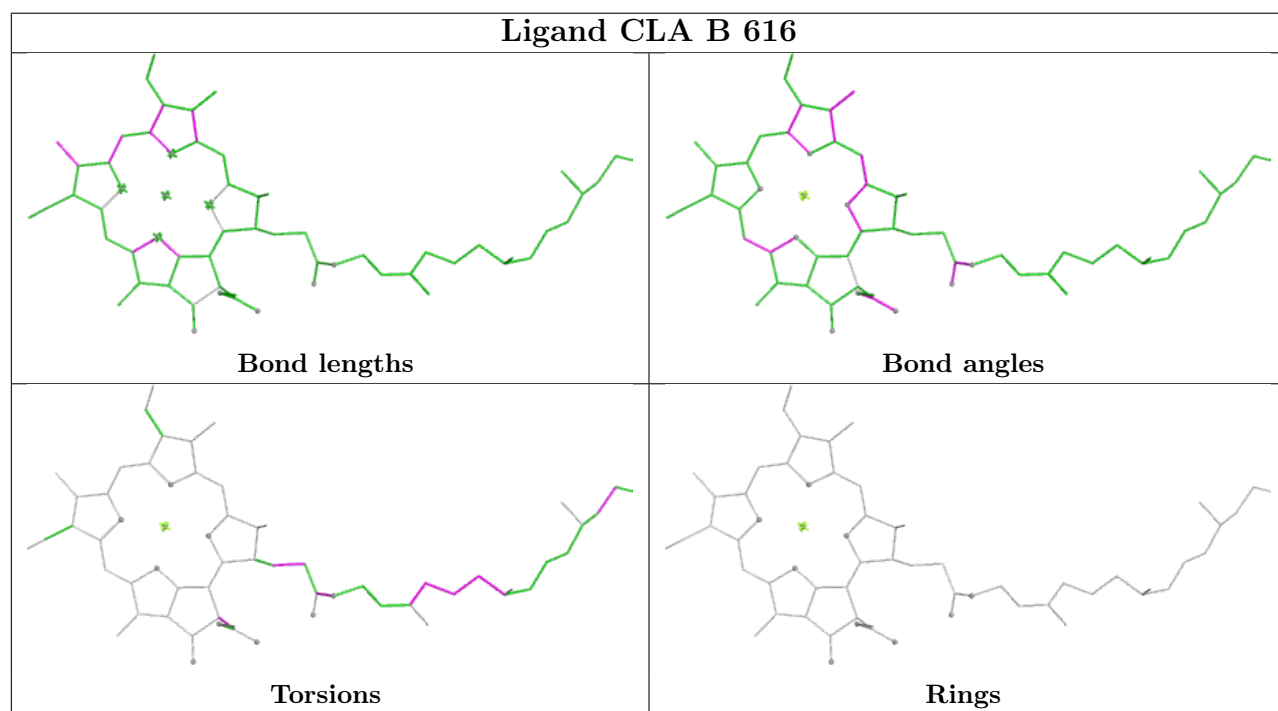
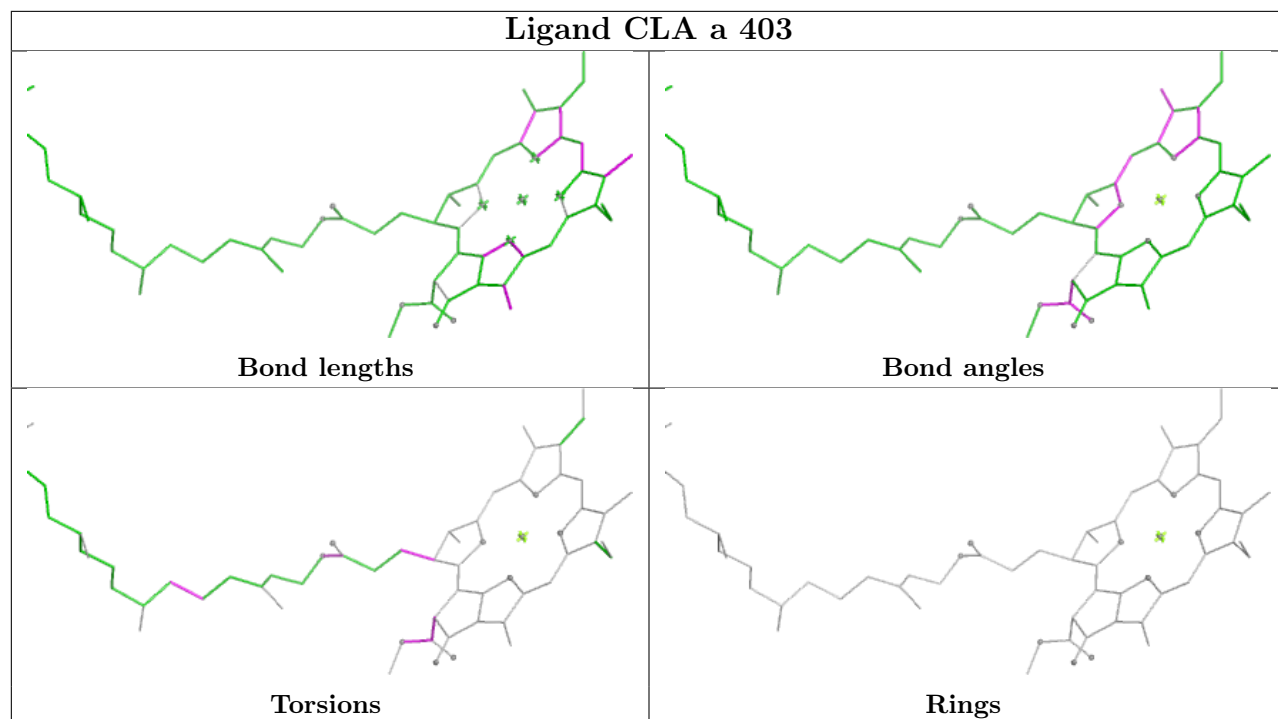




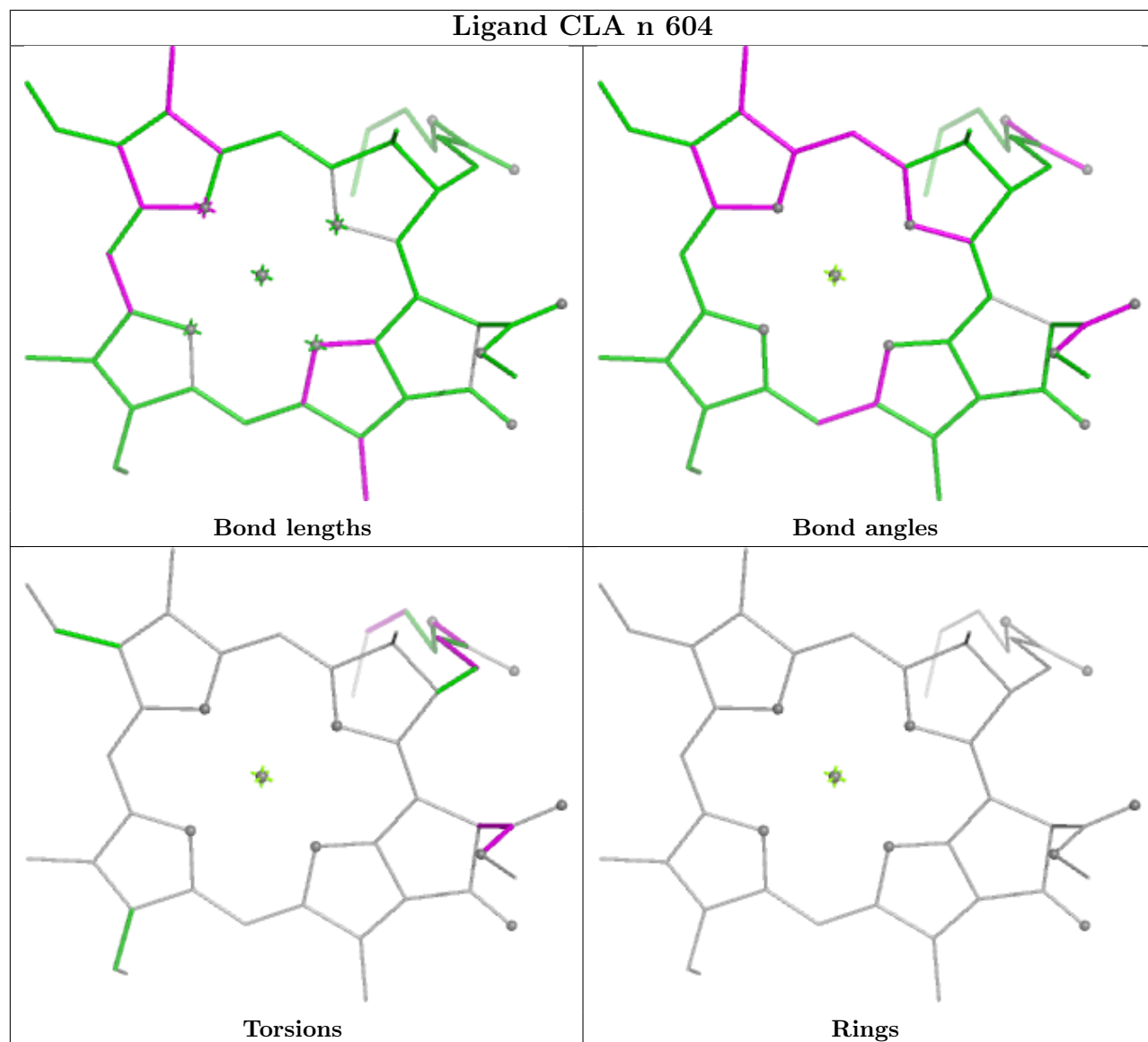


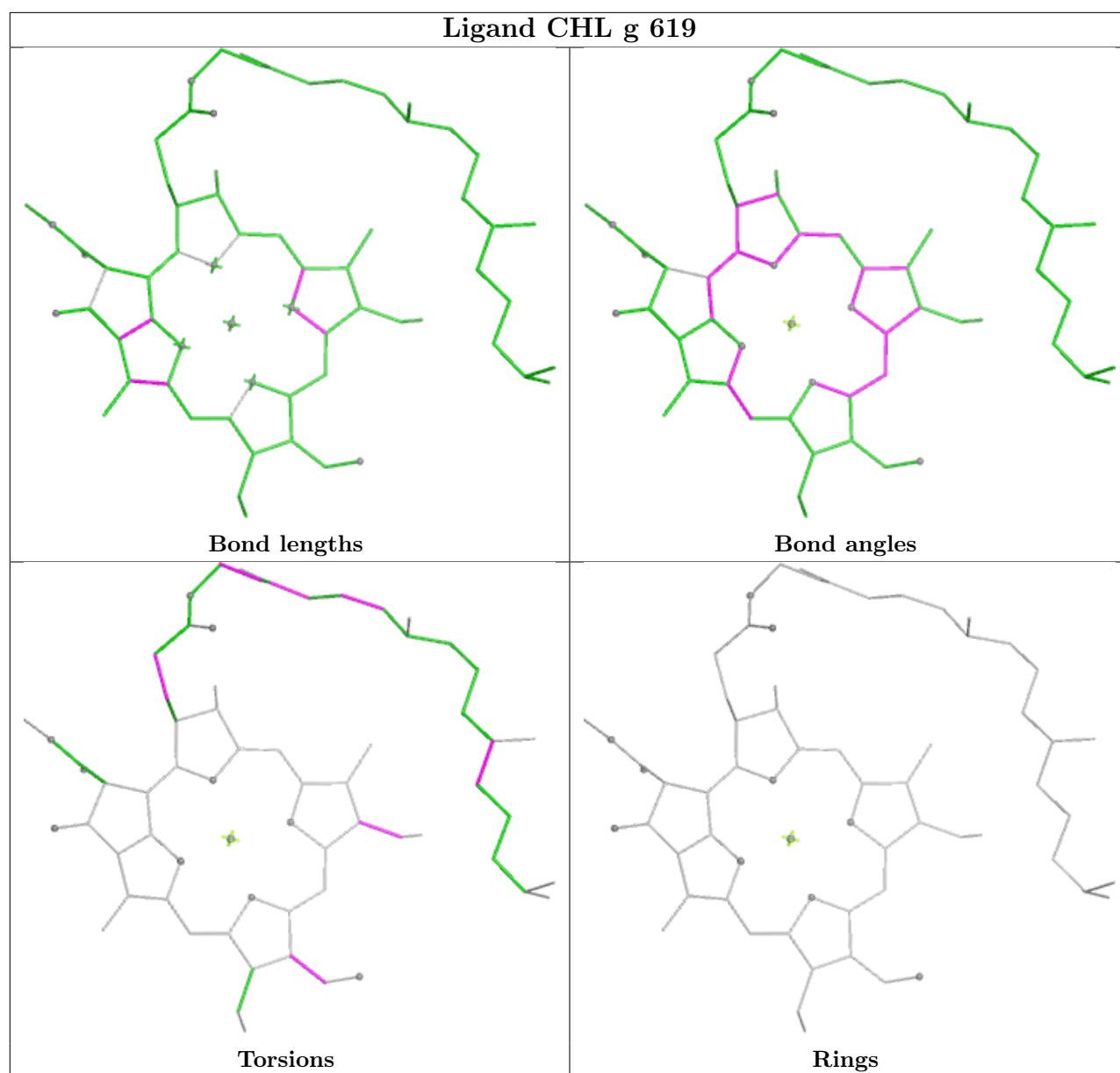


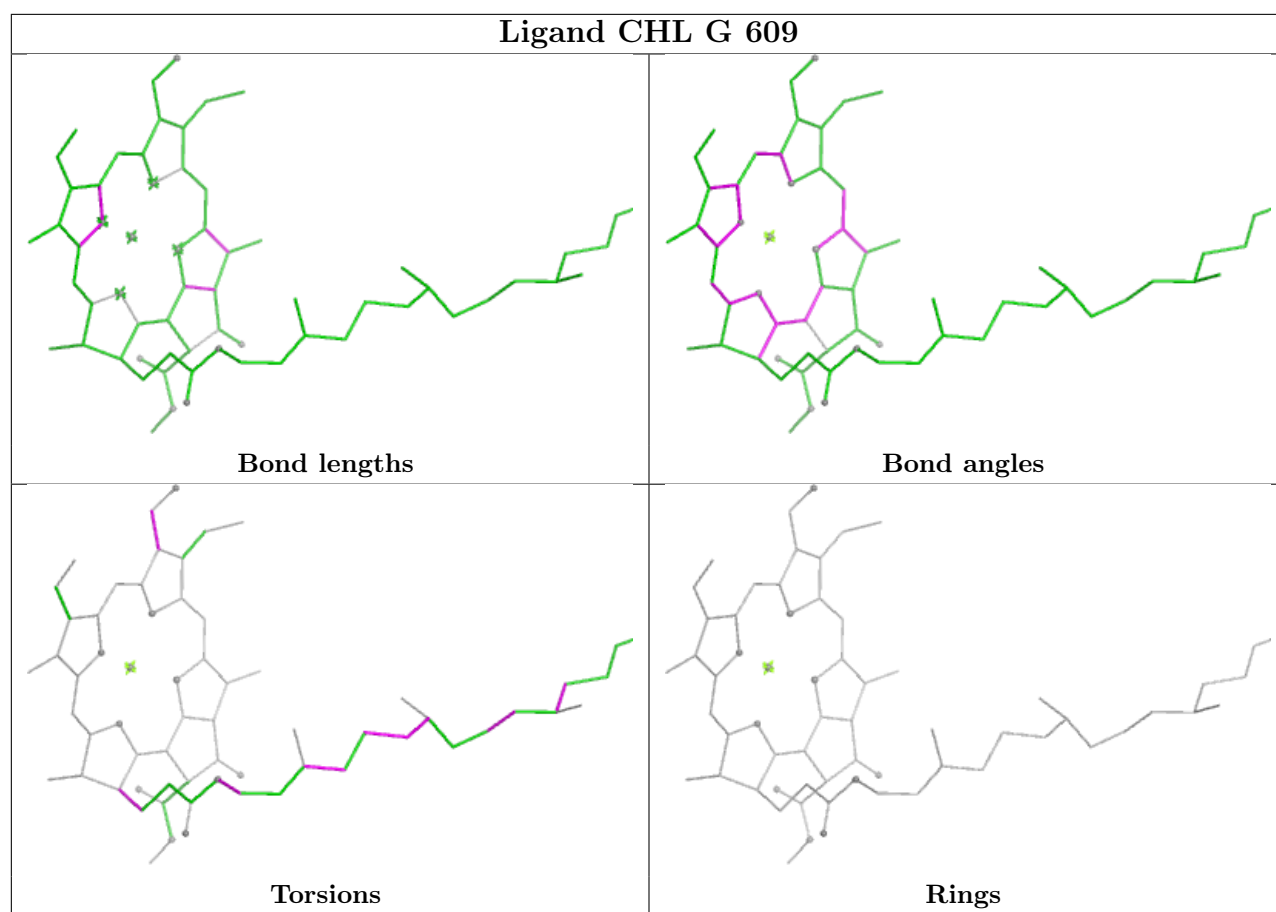




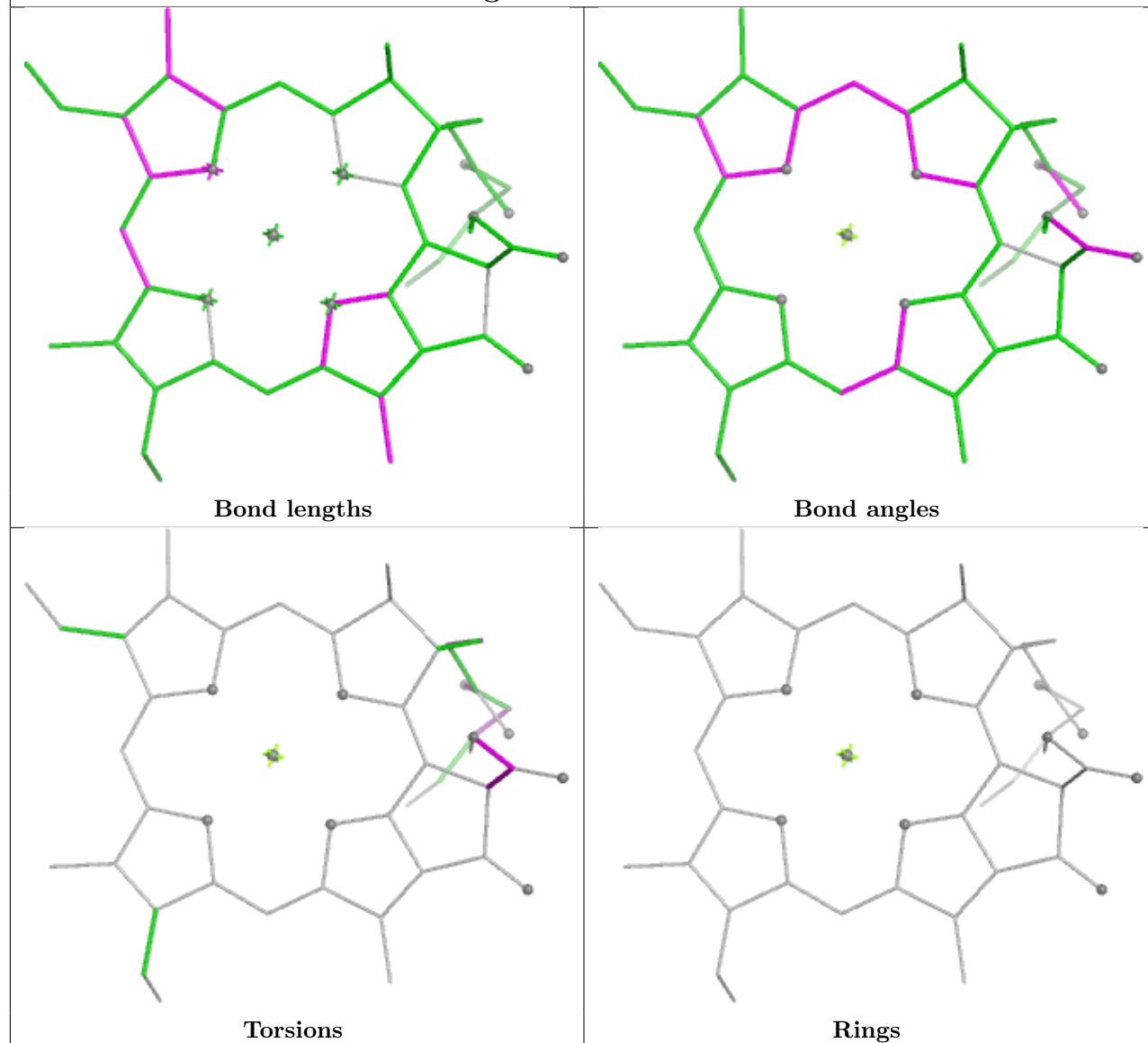
Ligand CLA n 604



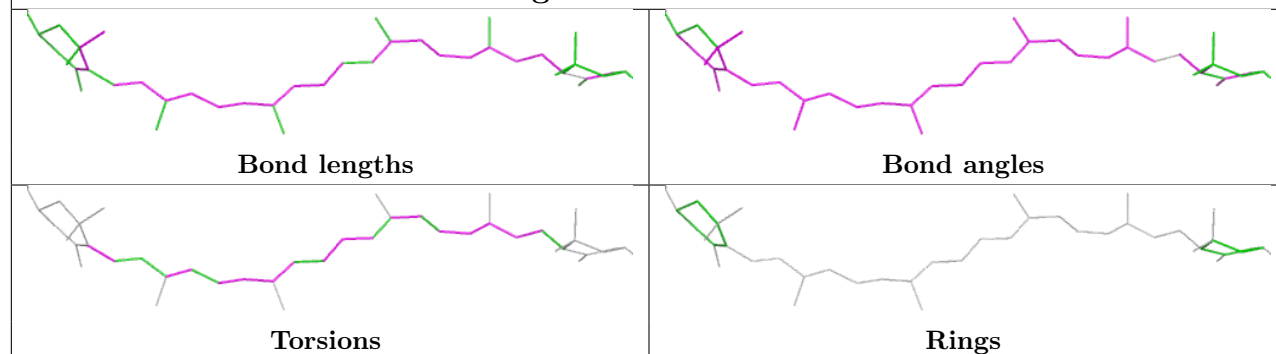


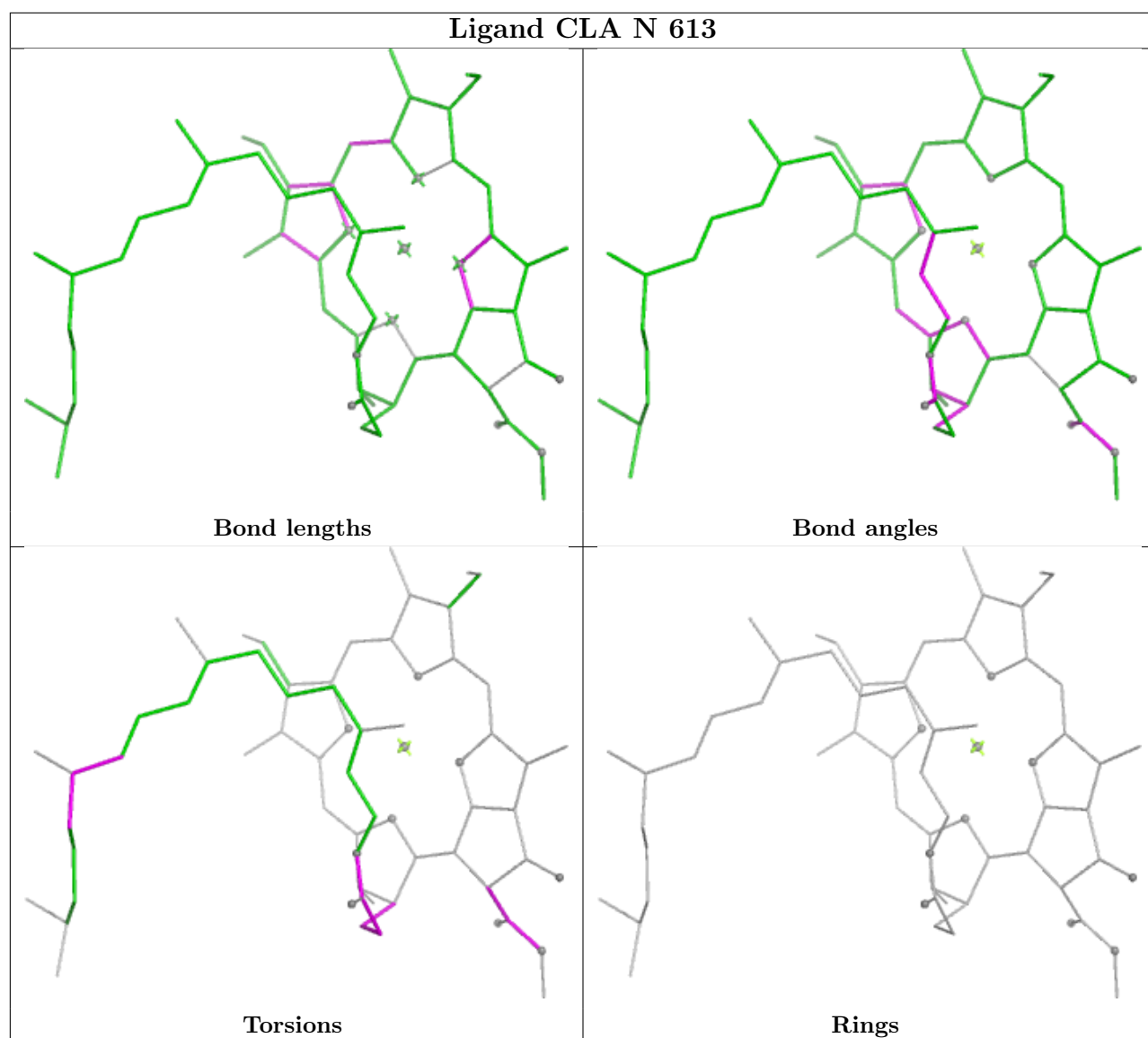


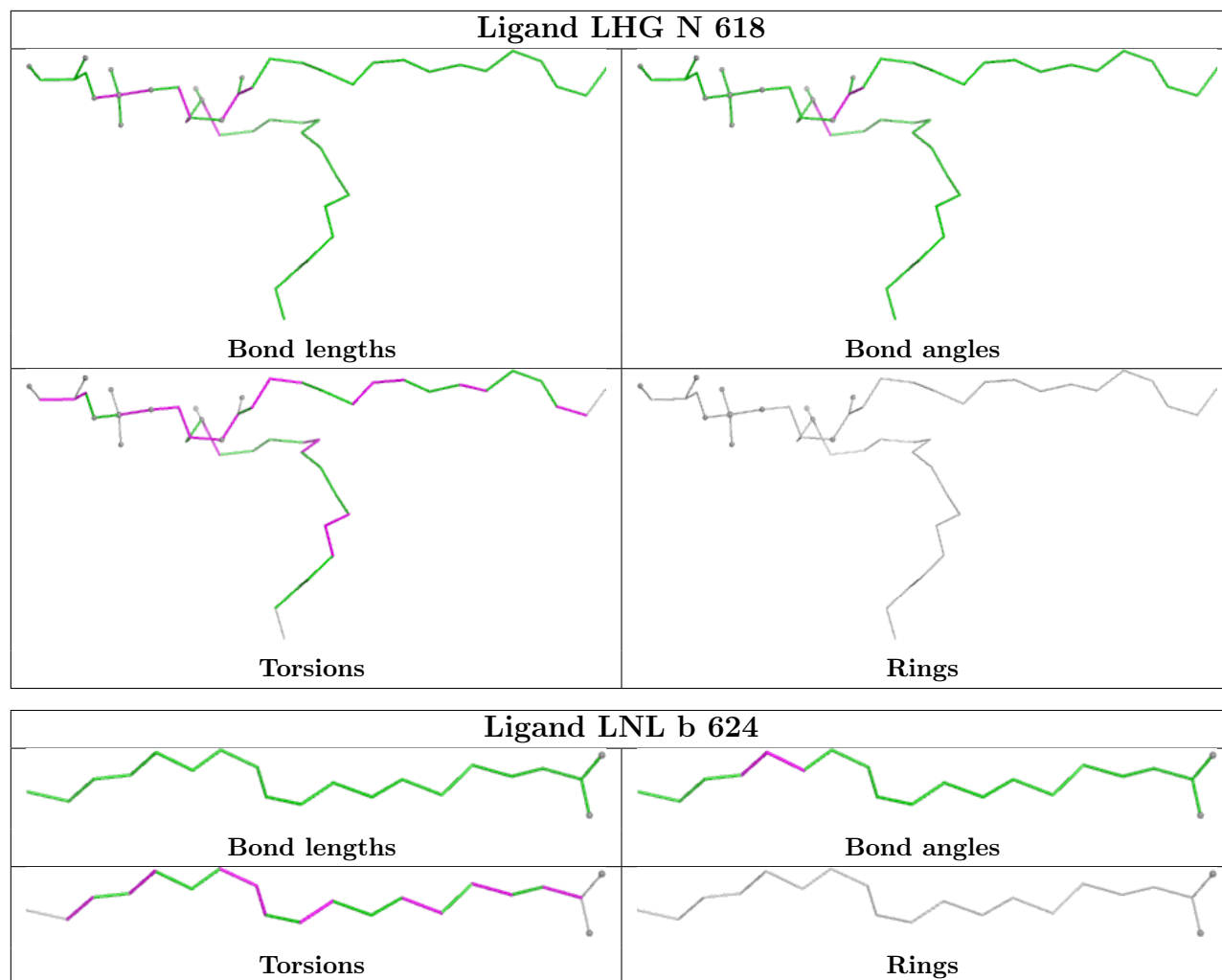
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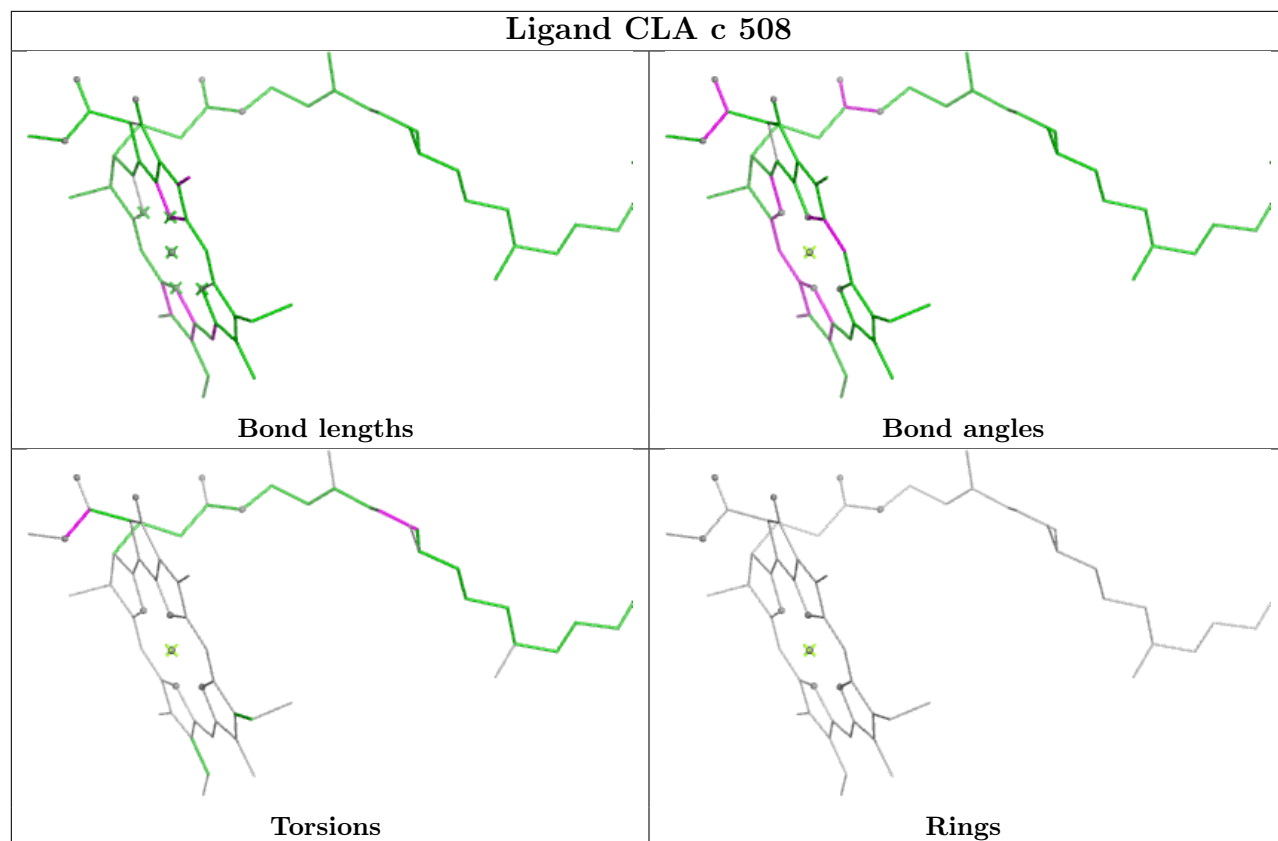


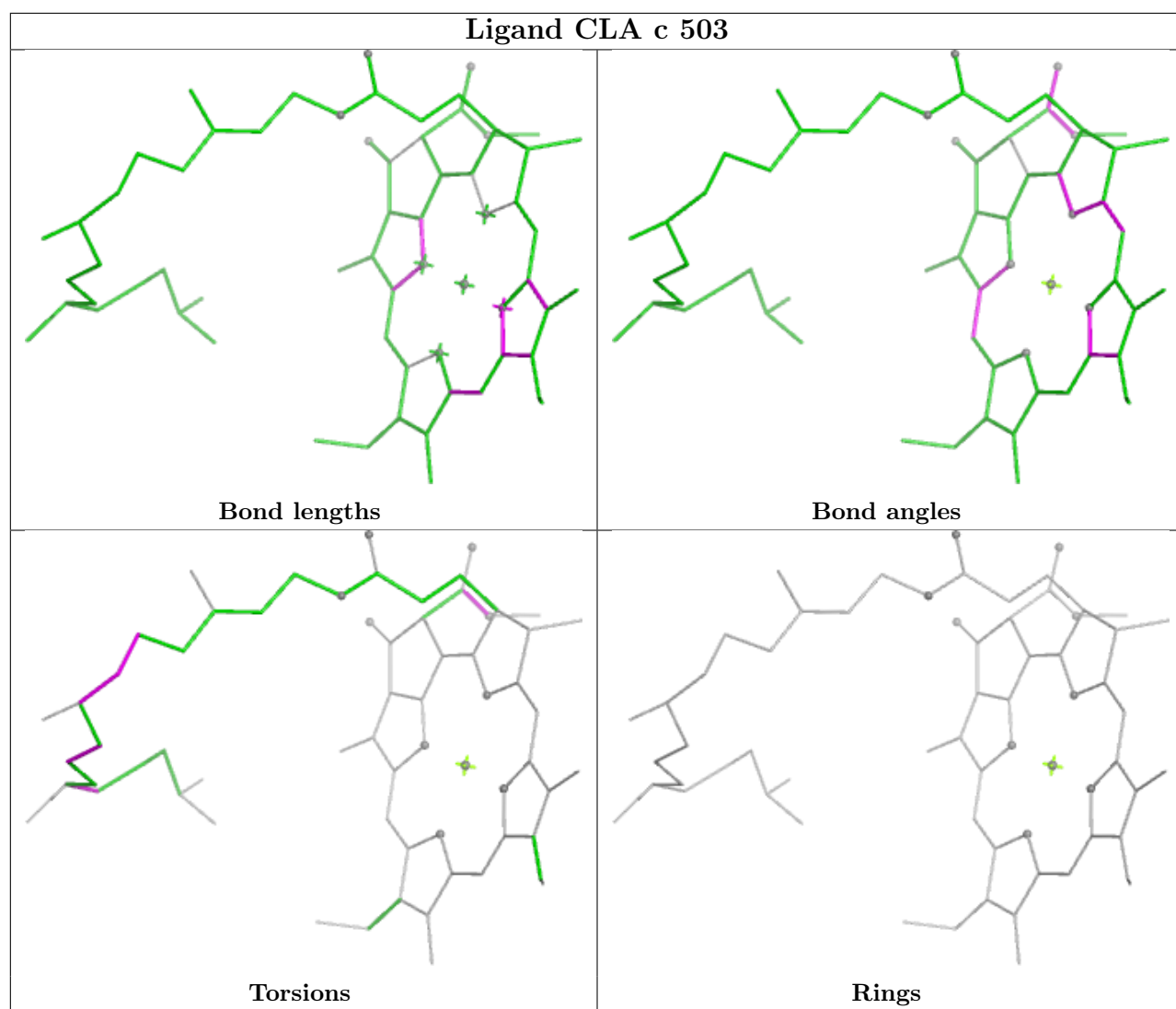
Ligand LUT R 613

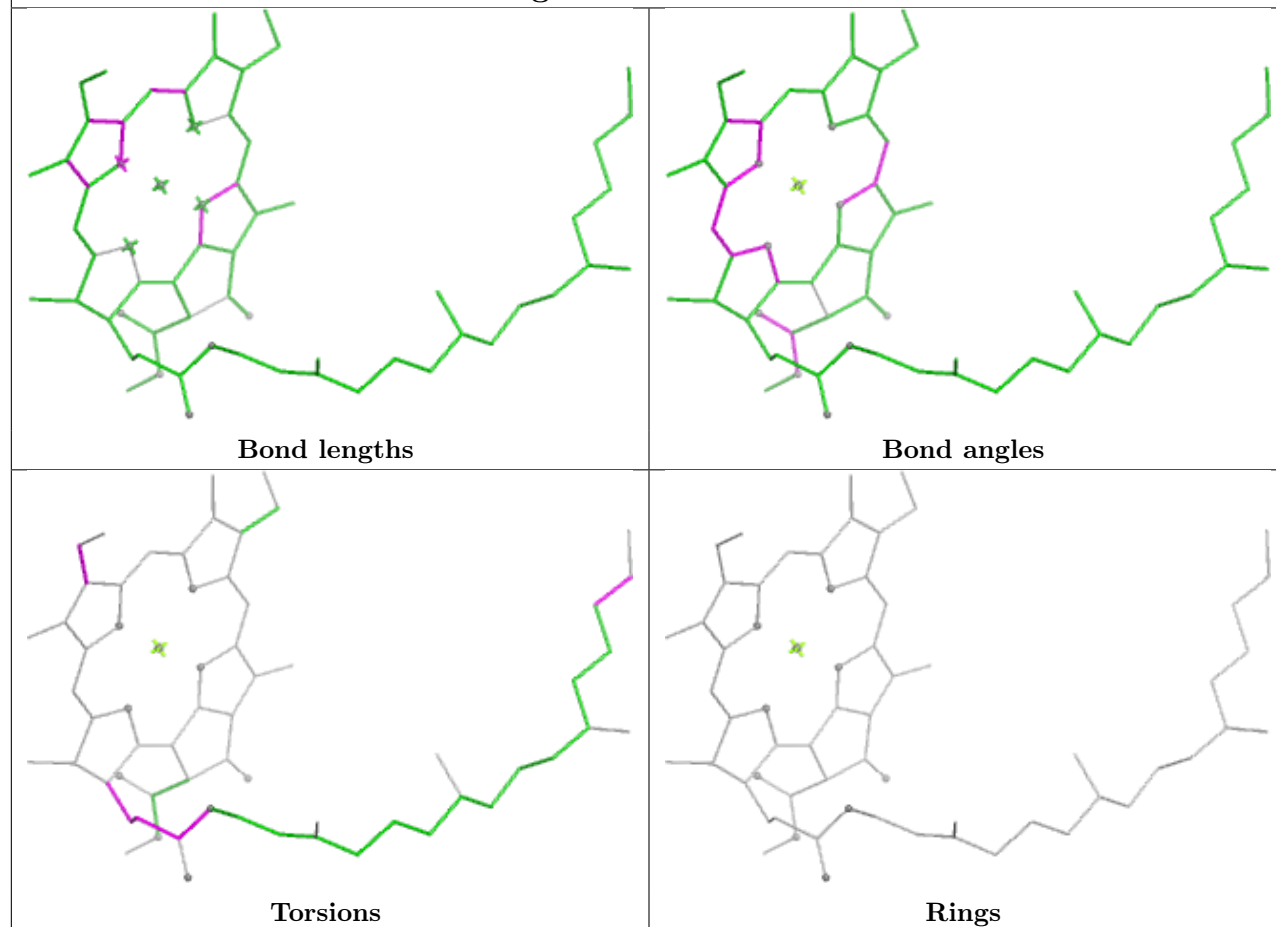
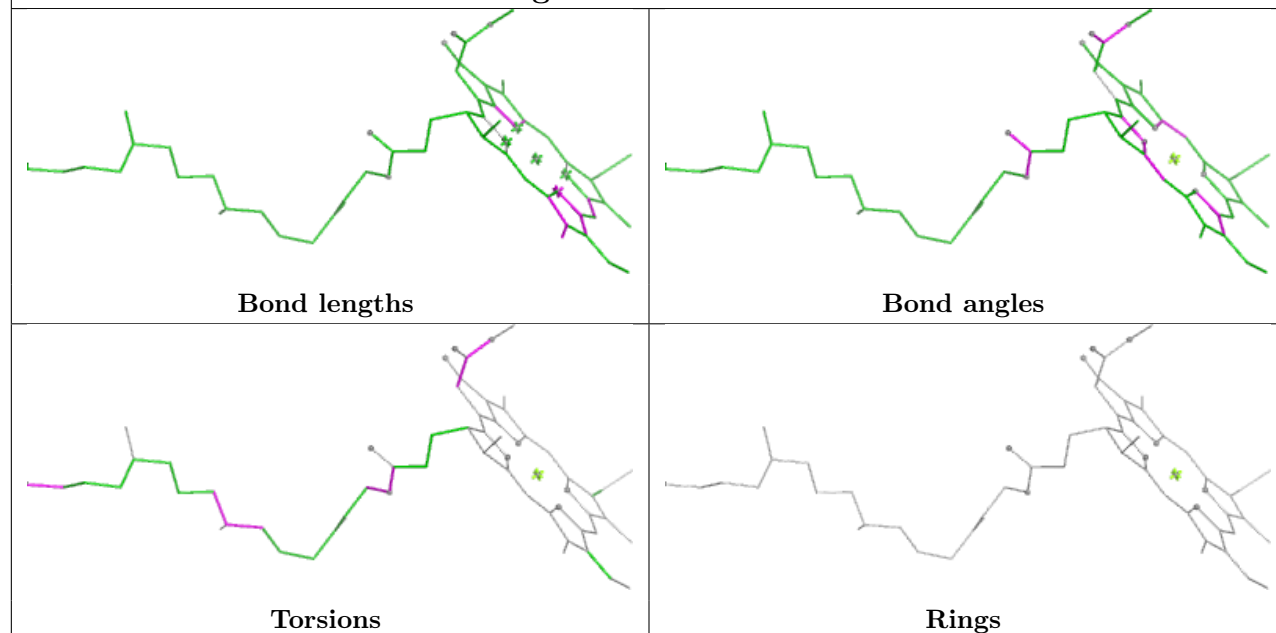


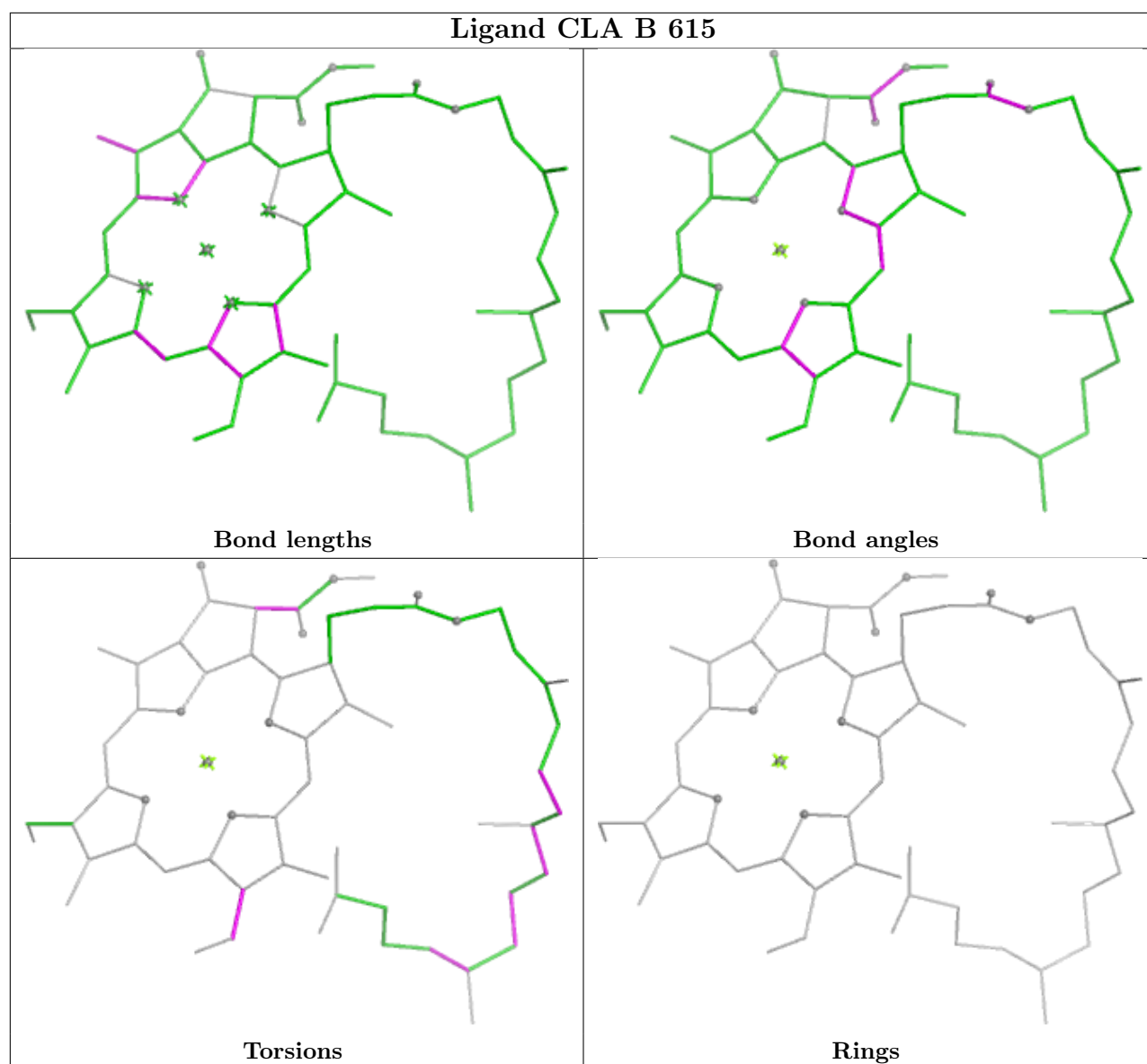




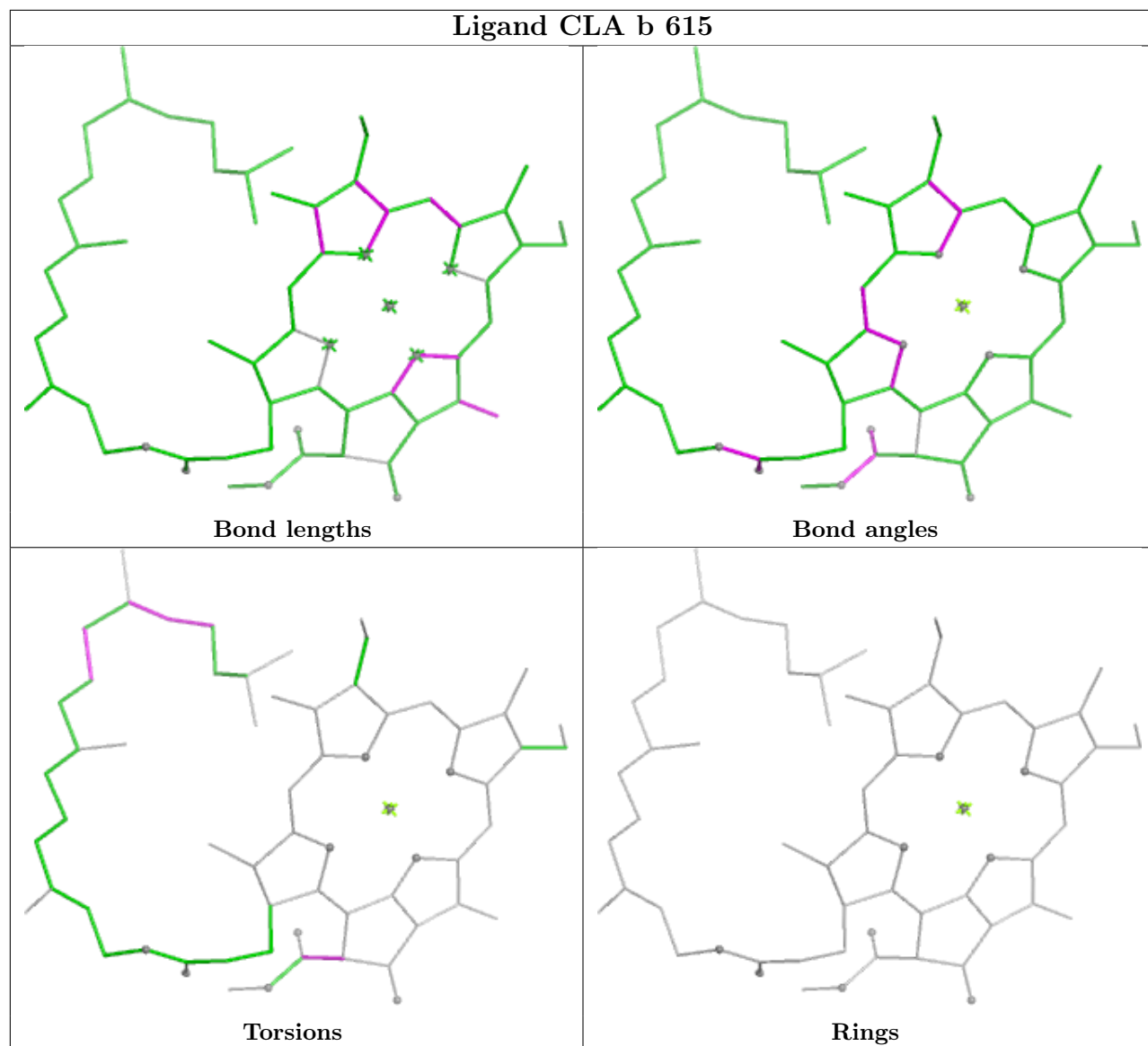


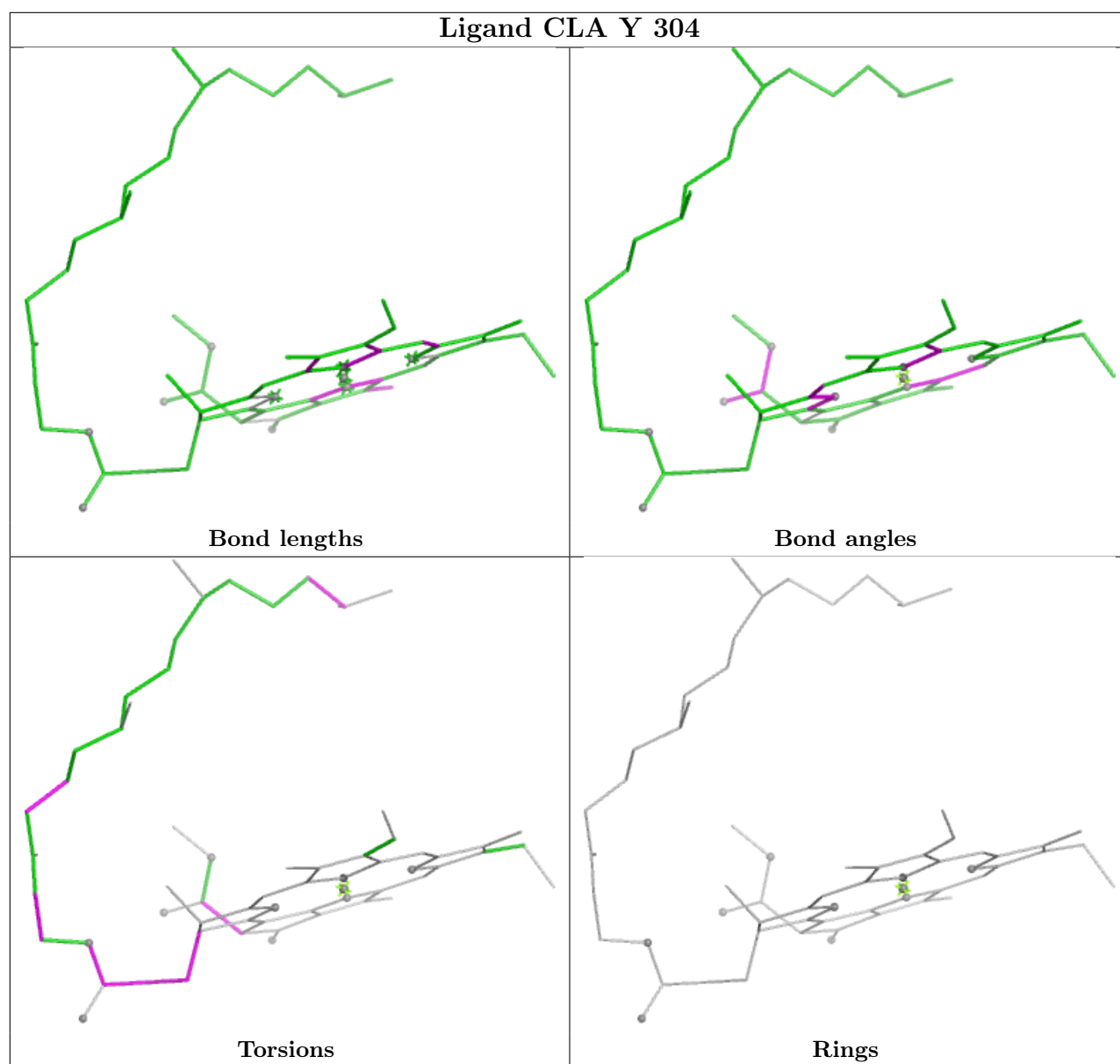


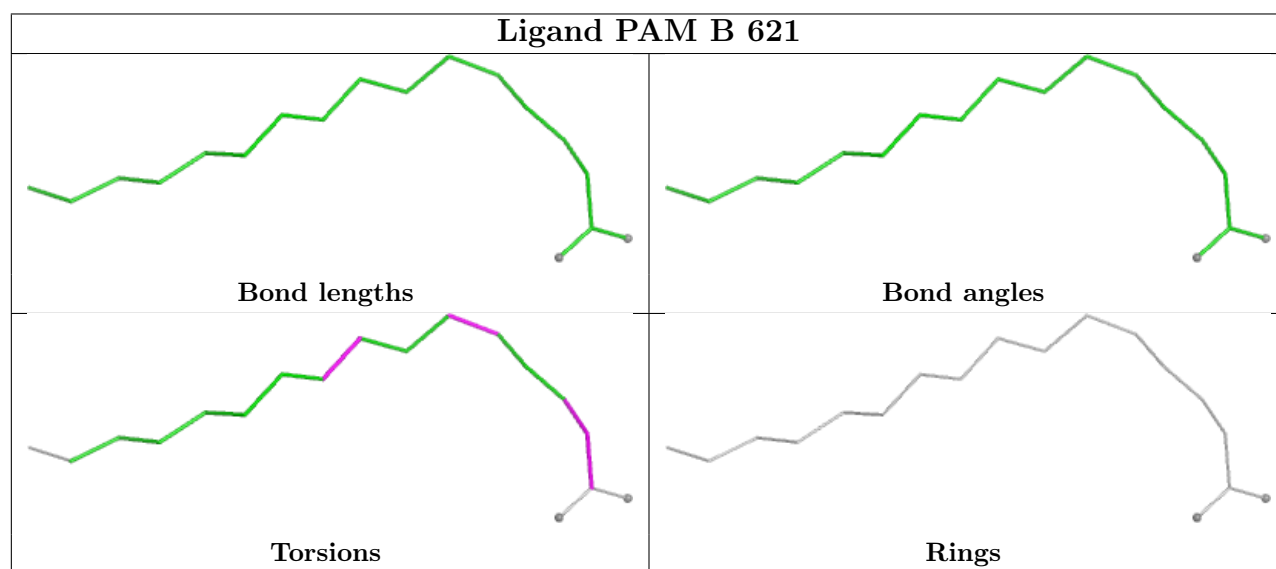
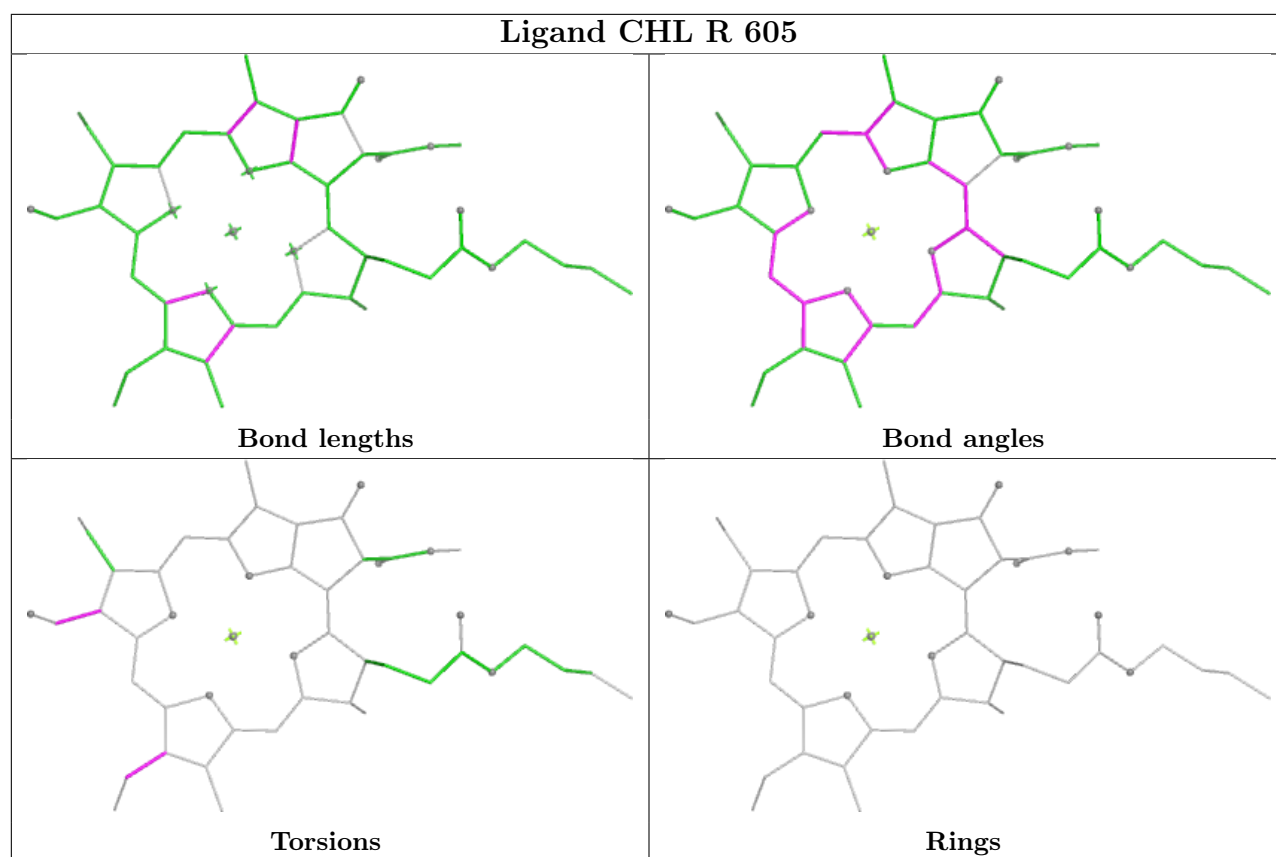
Ligand CLA R 610**Ligand CLA C 502**

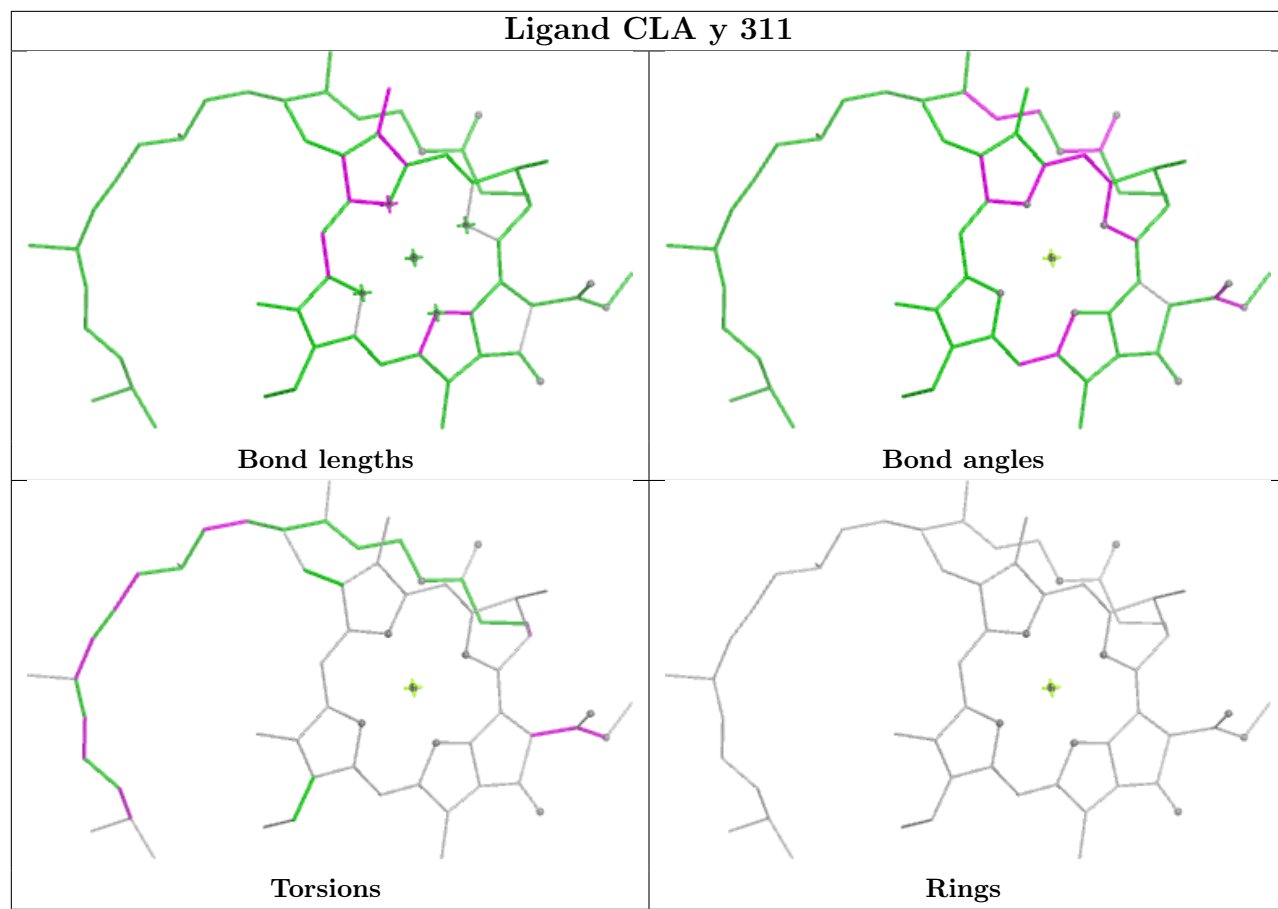


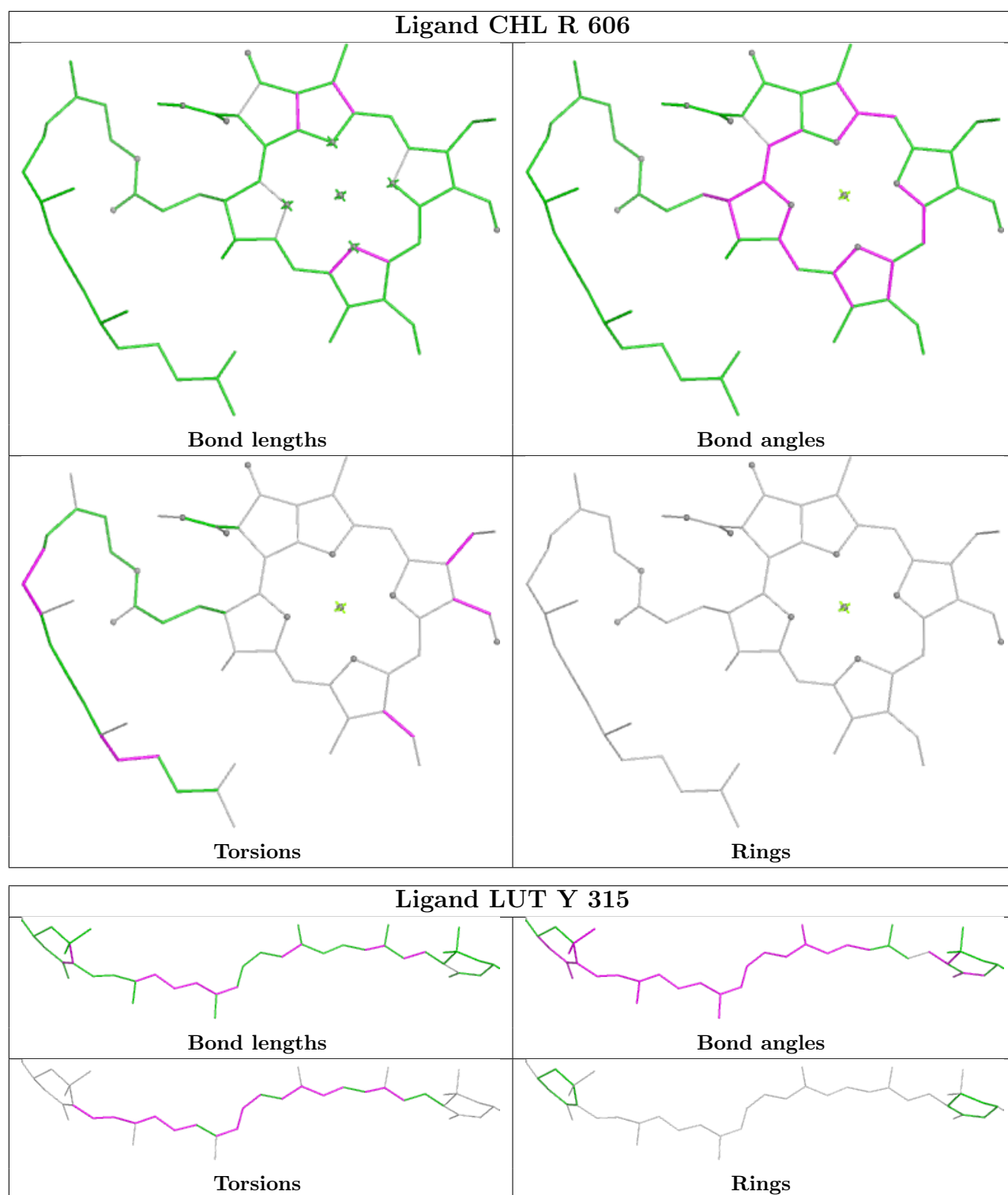
Ligand CLA b 615

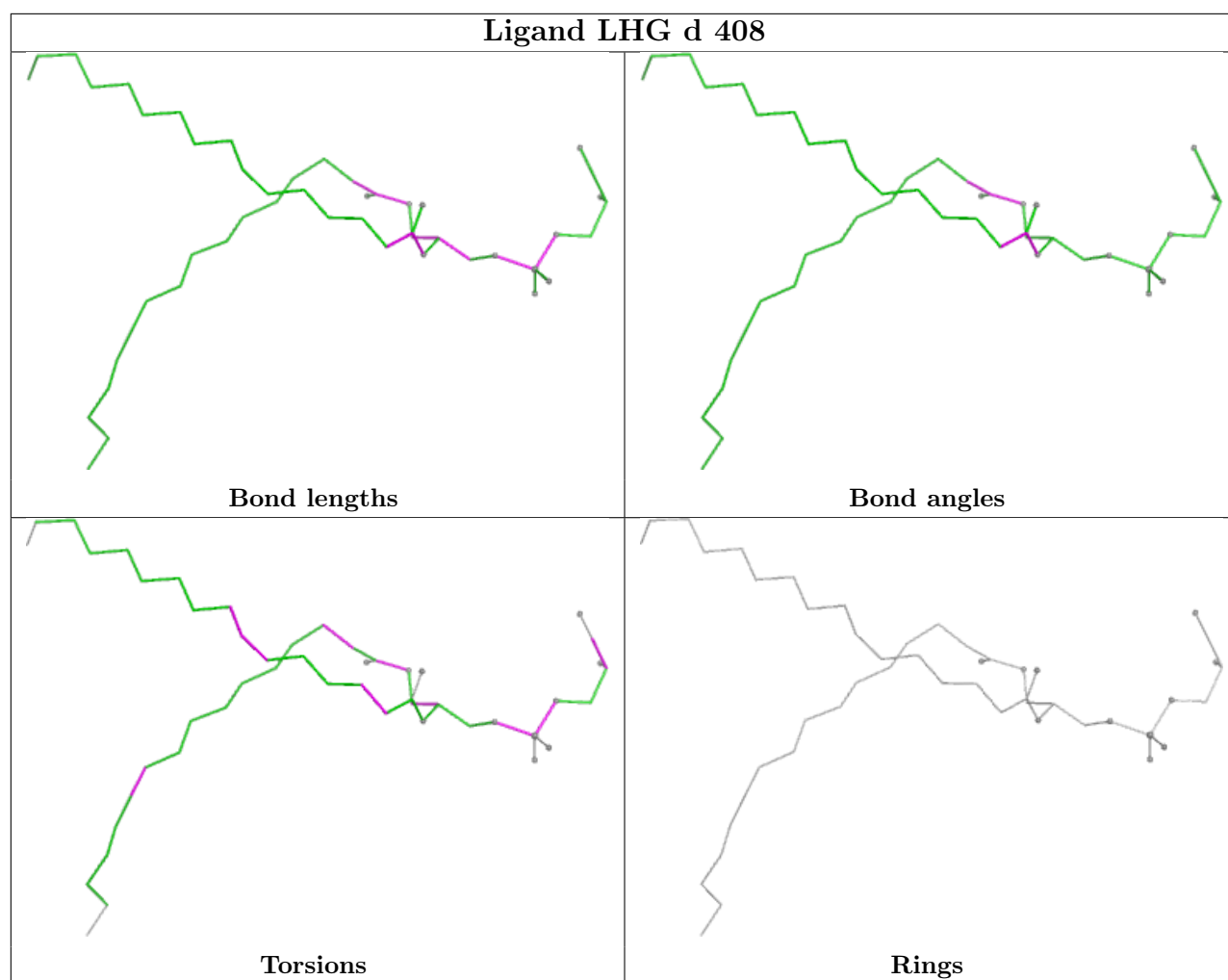


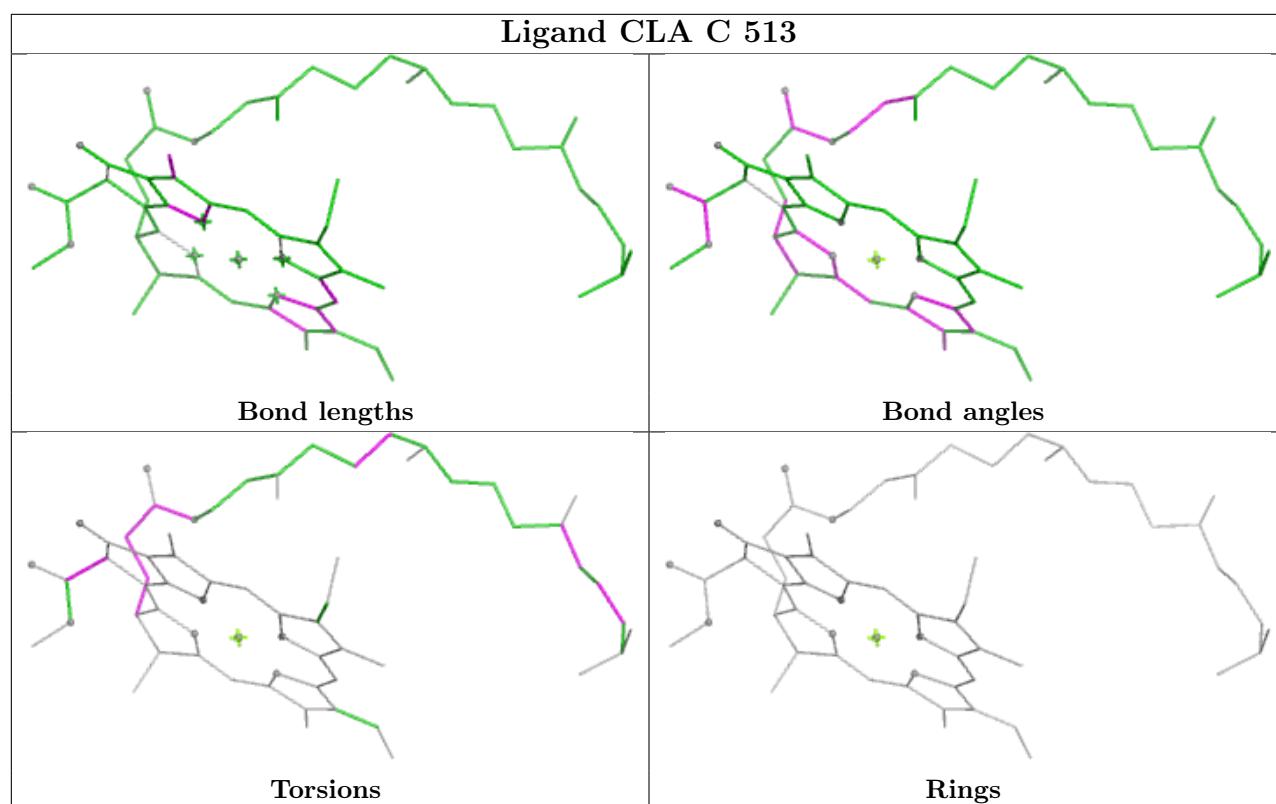


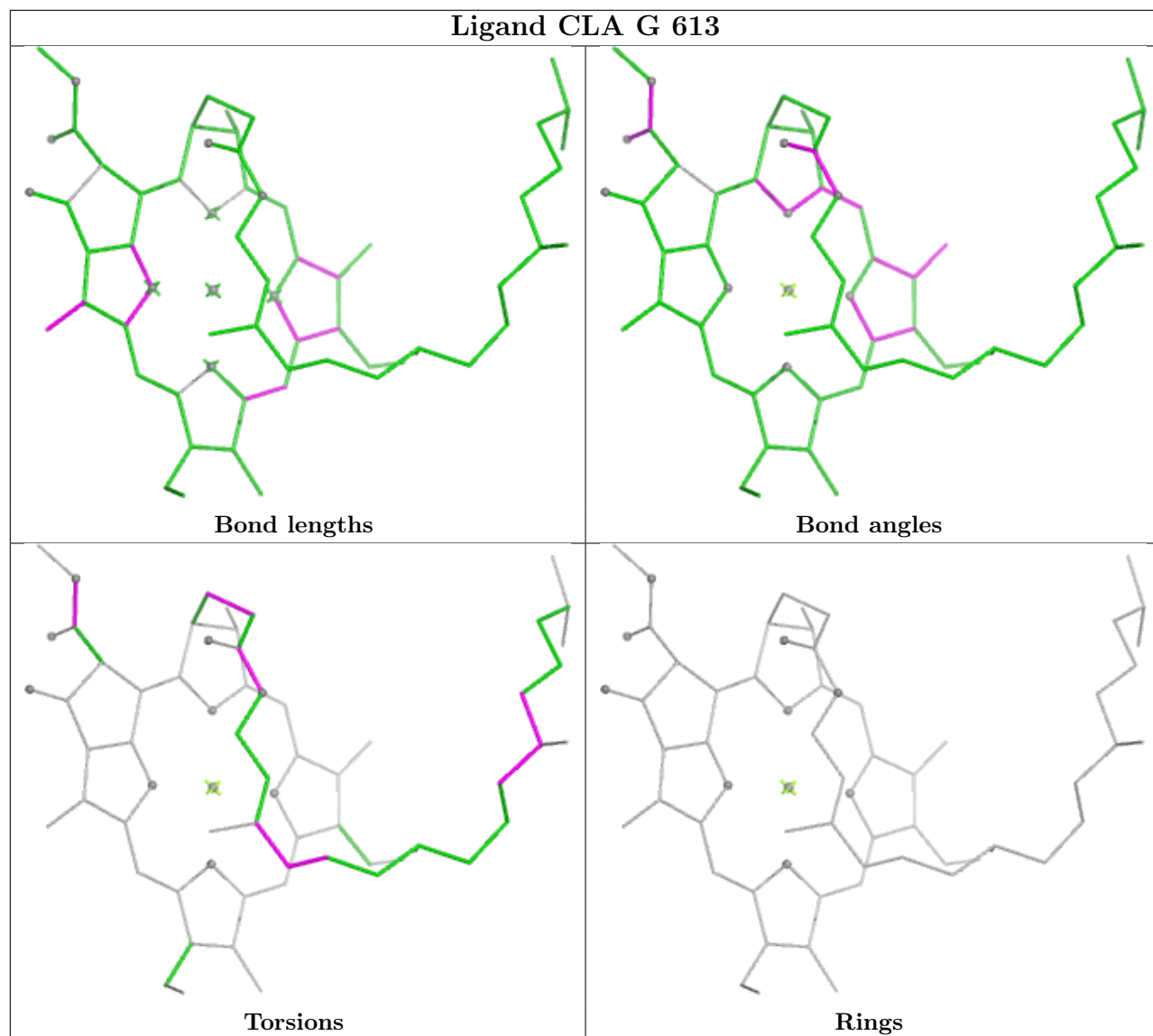


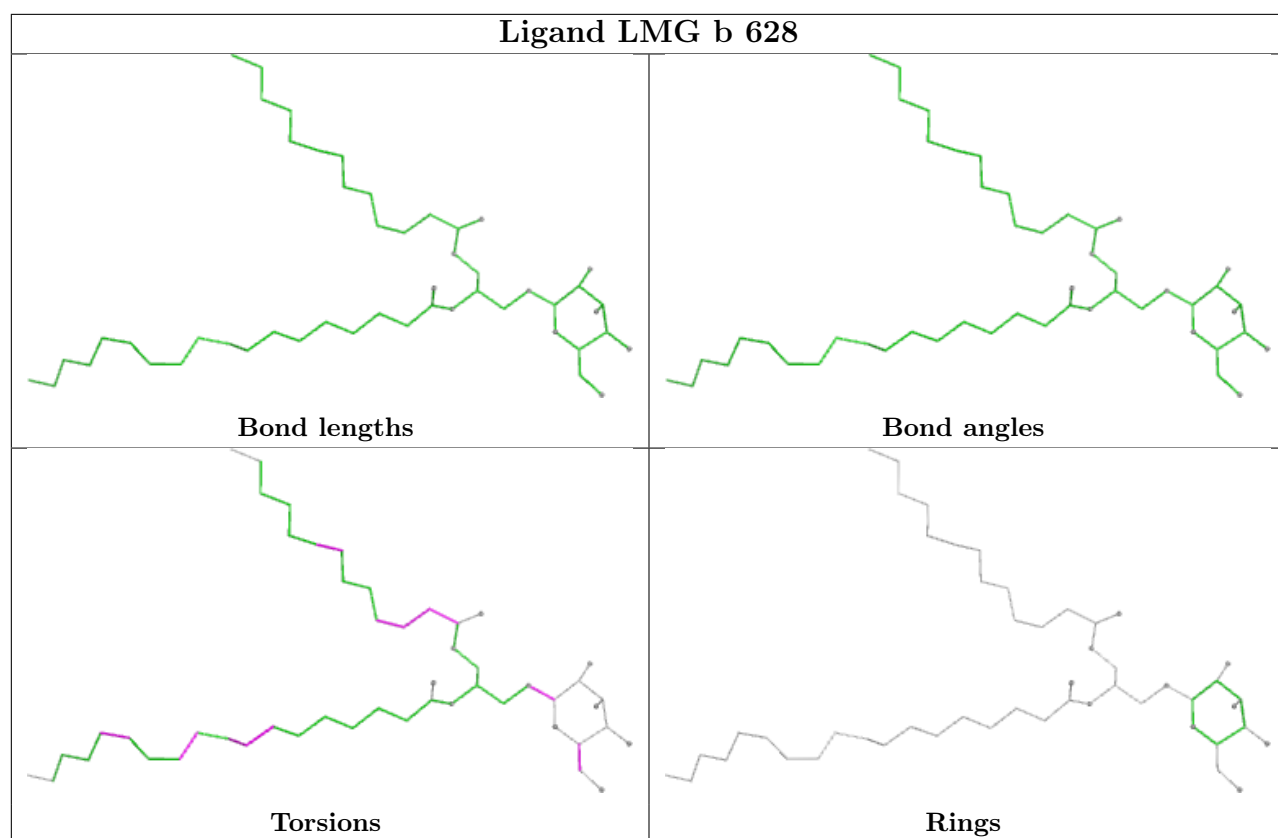




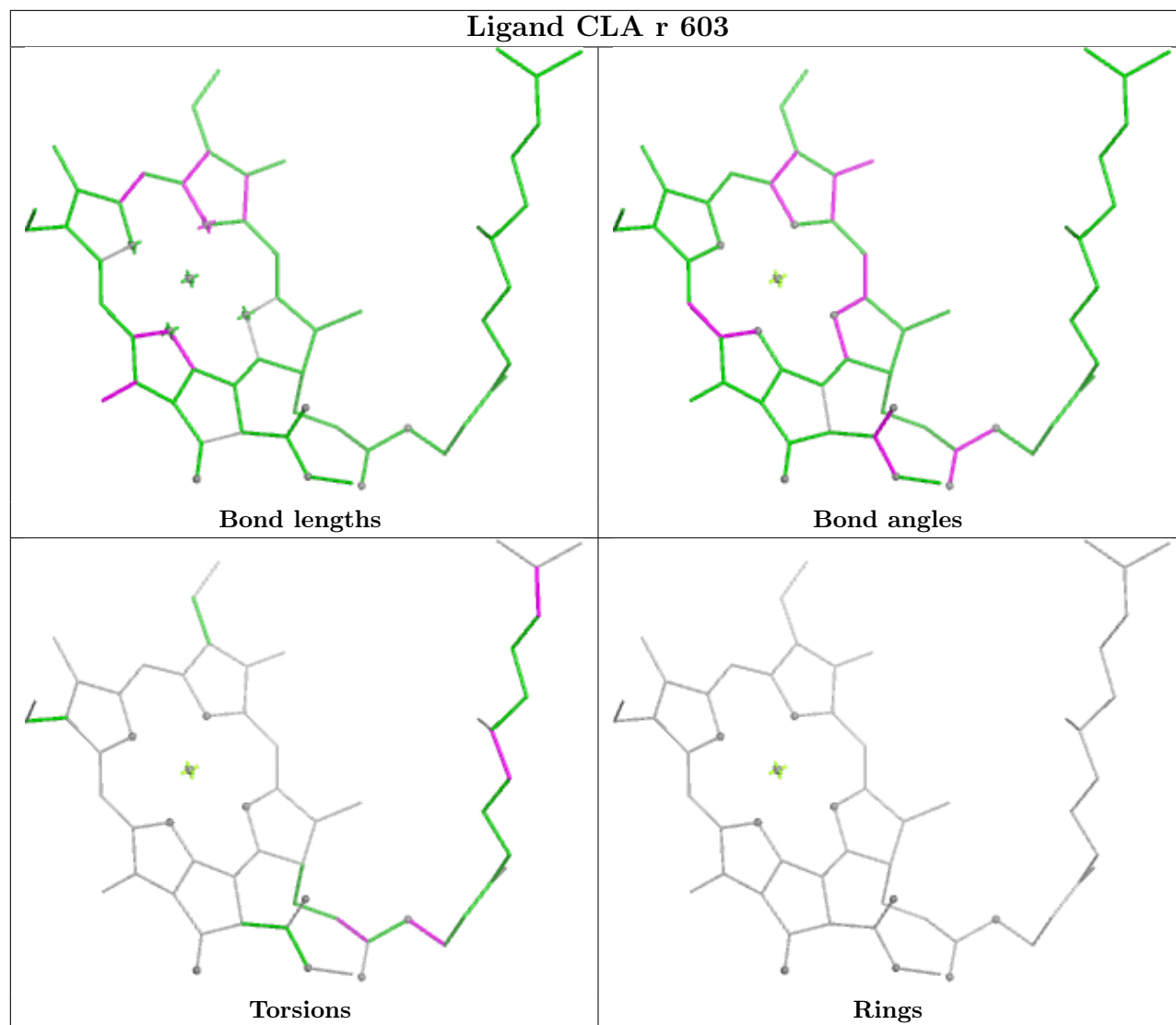




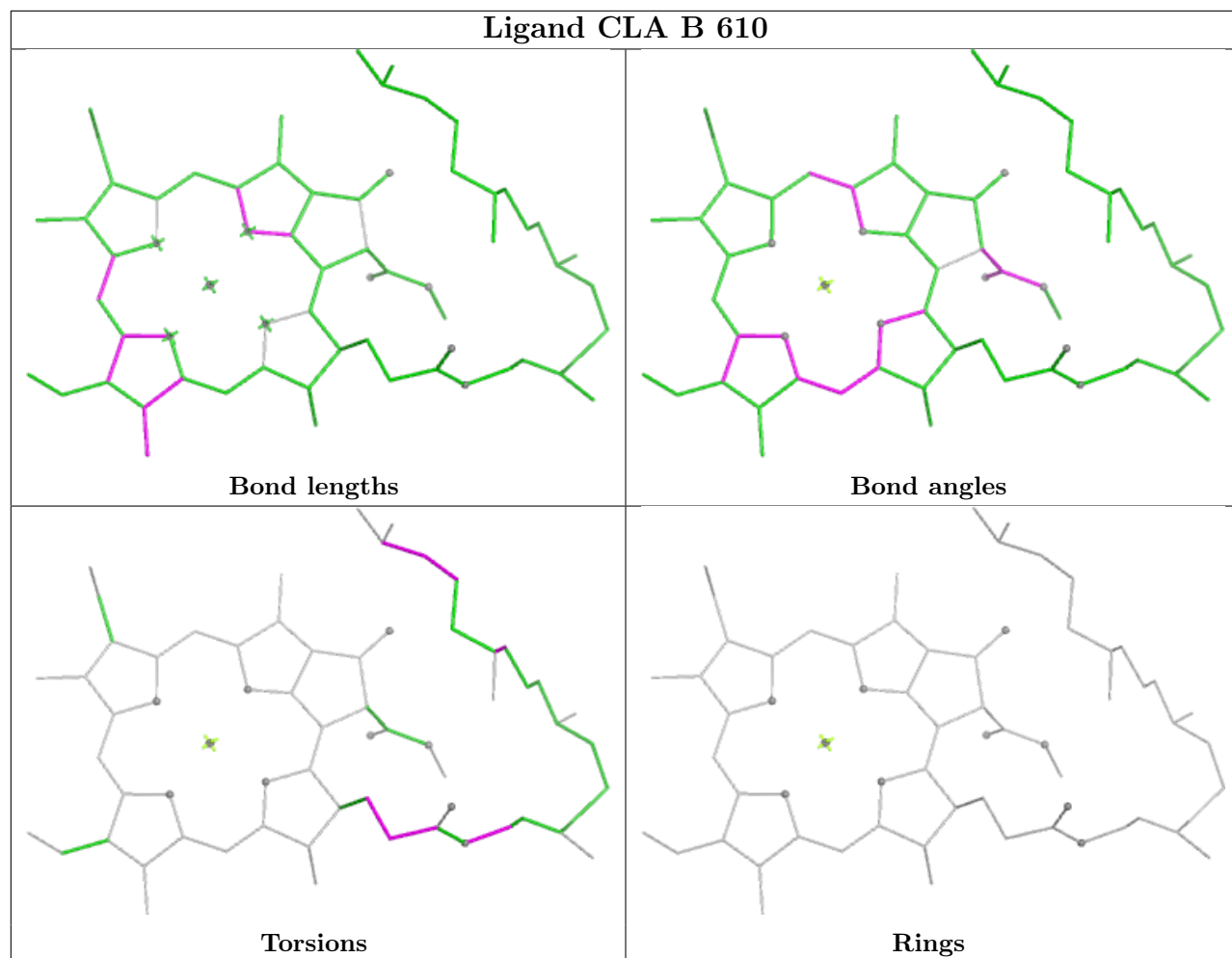


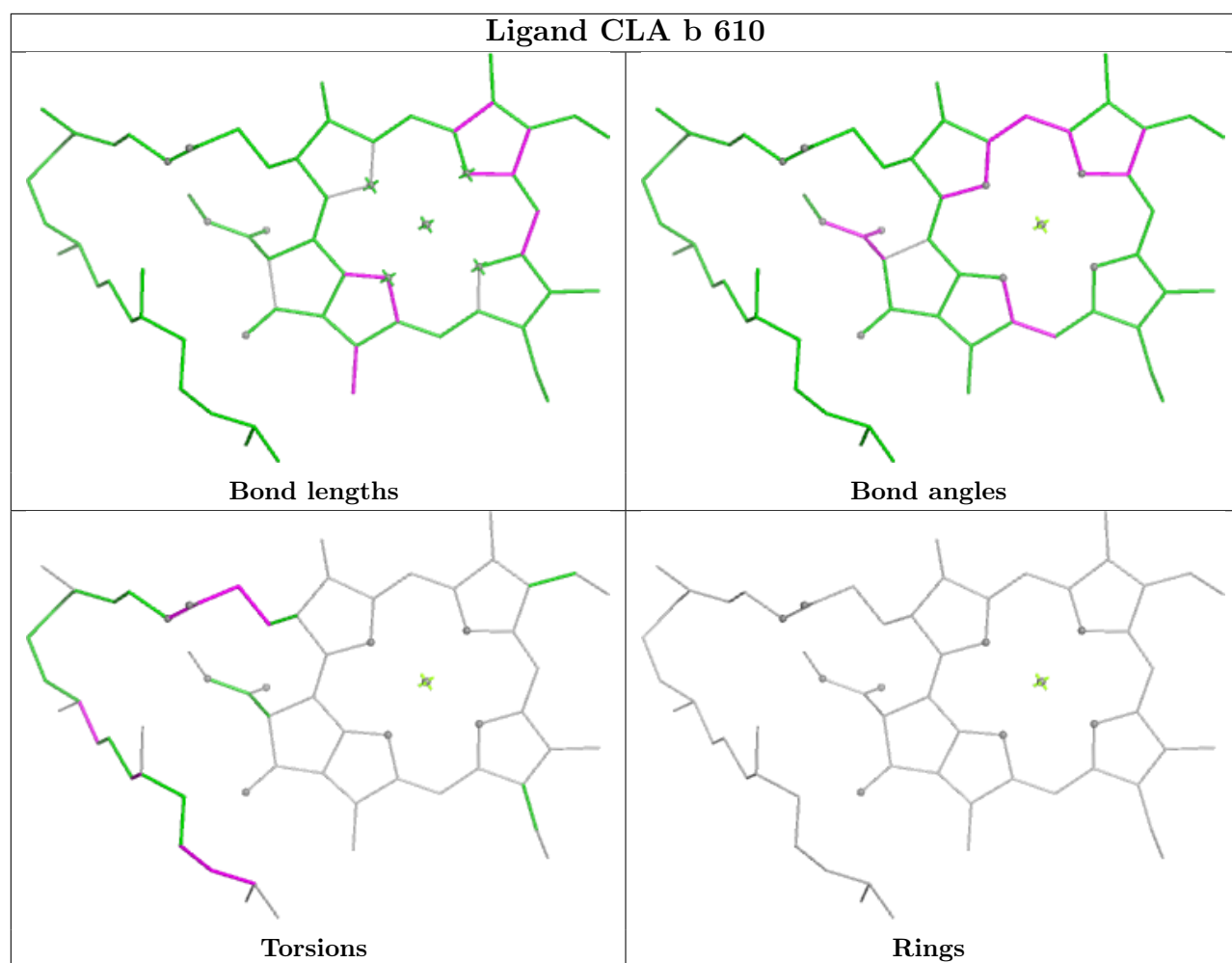


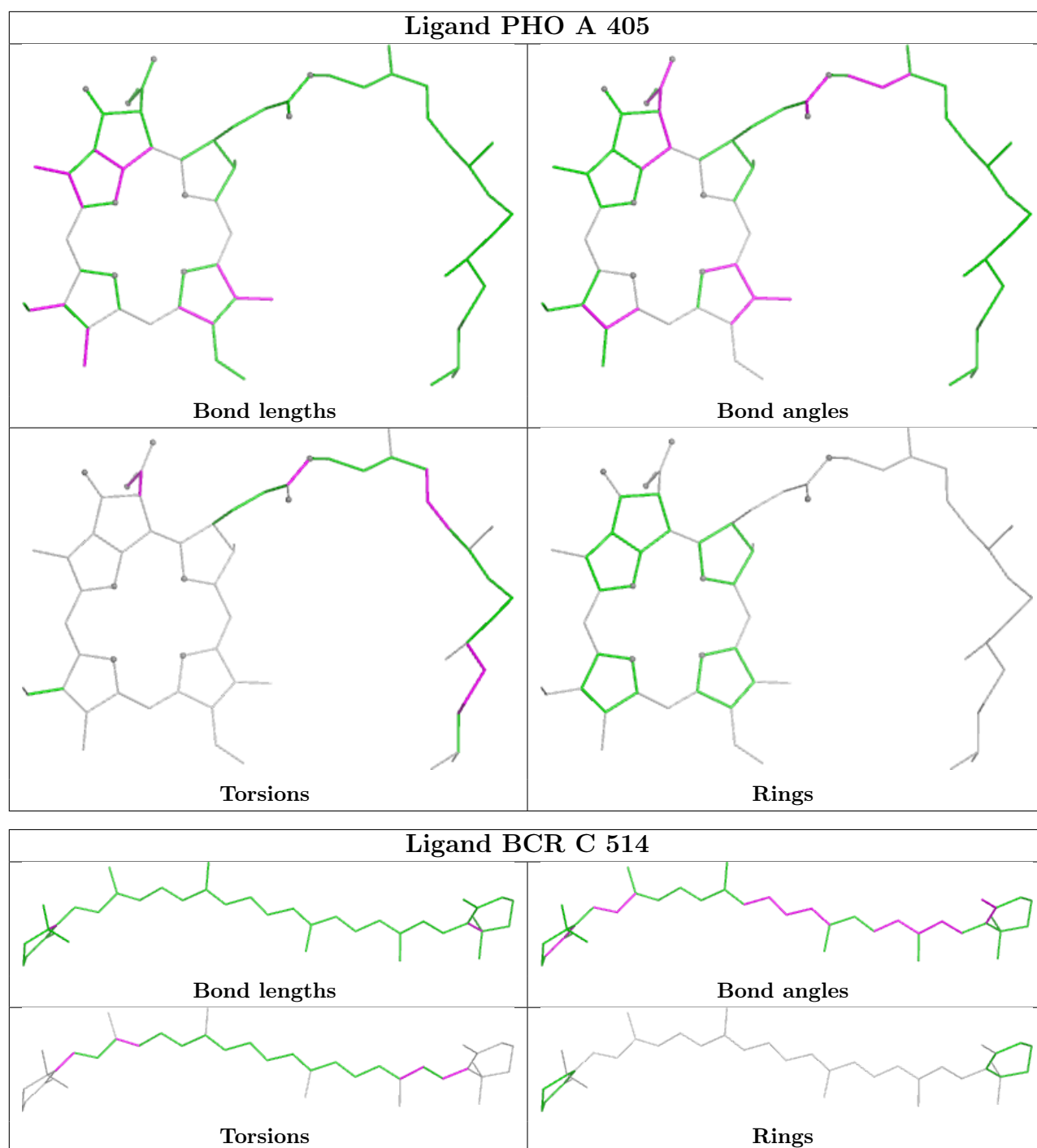
Ligand CLA r 603



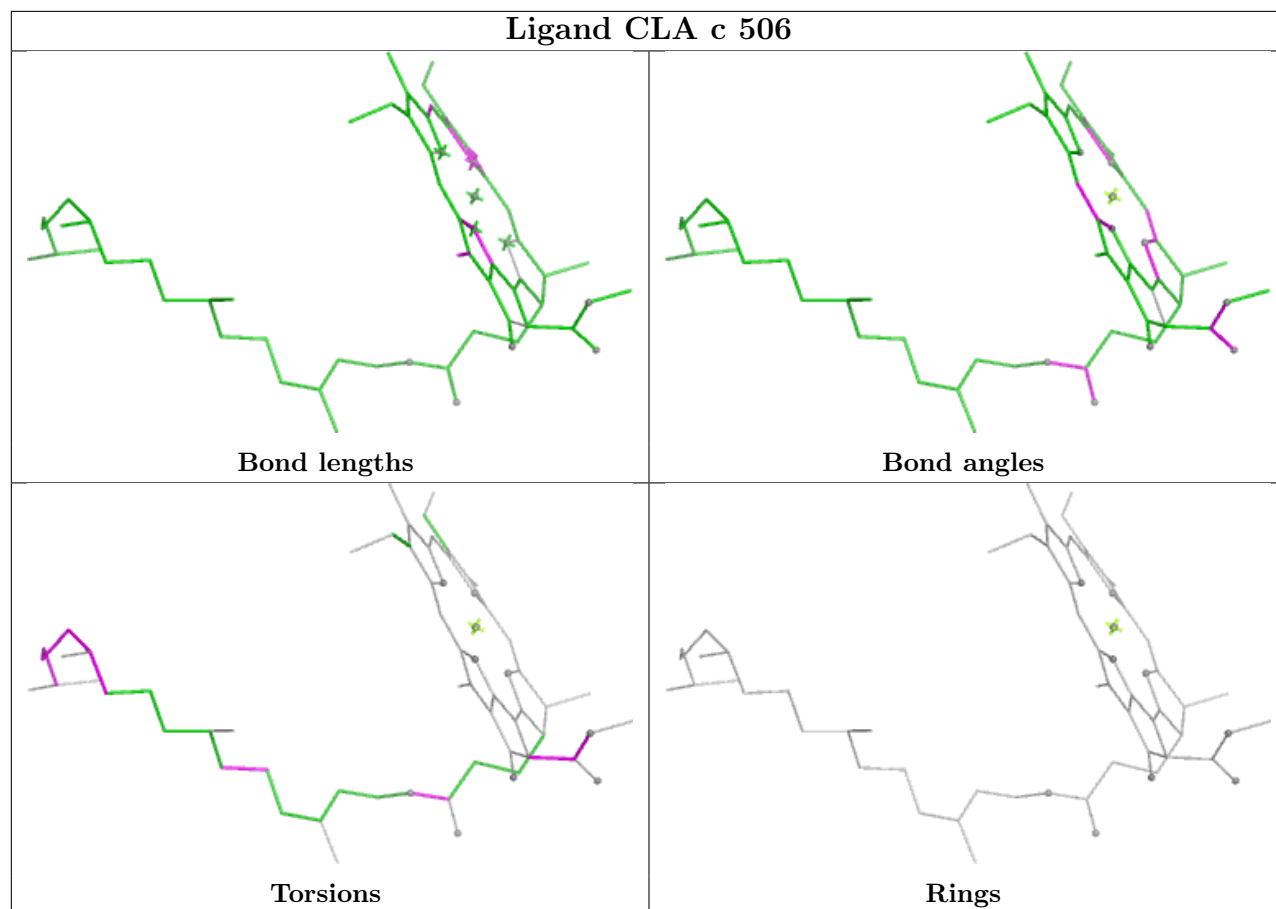
Ligand CLA B 610



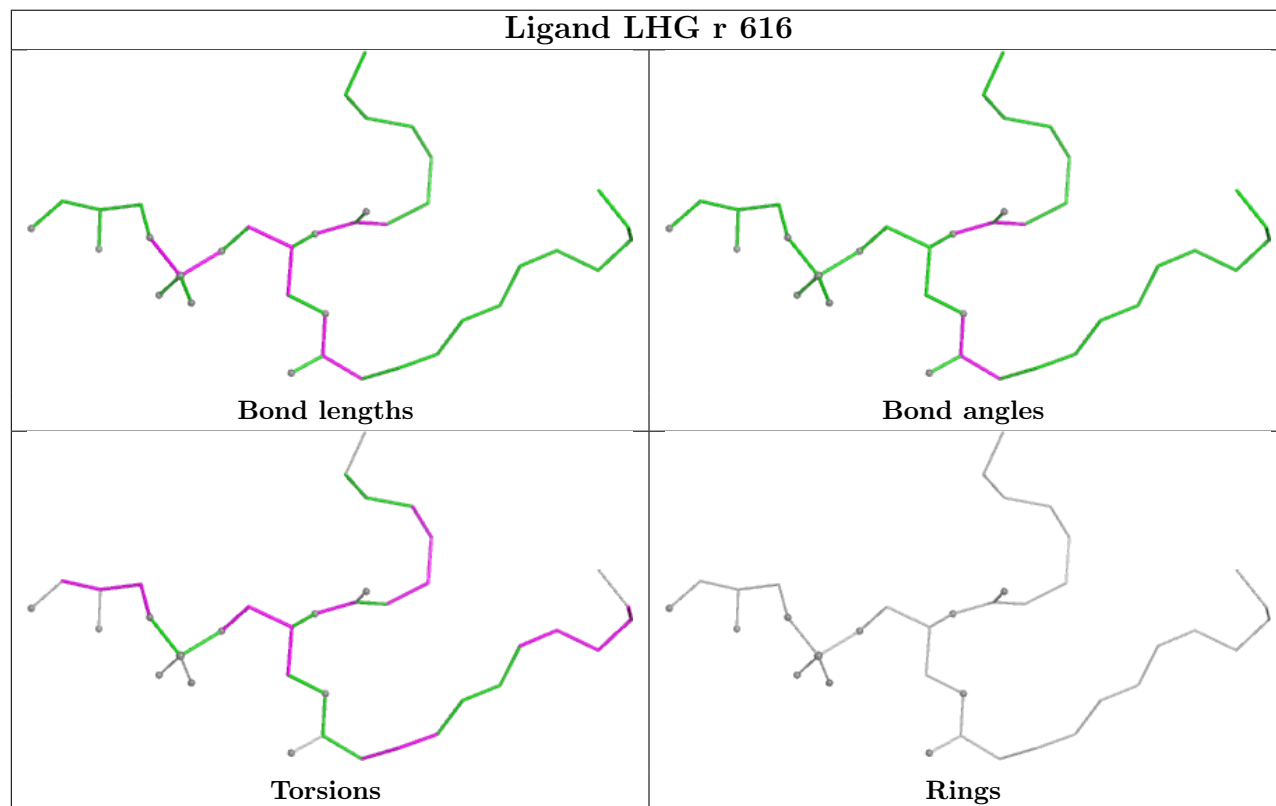


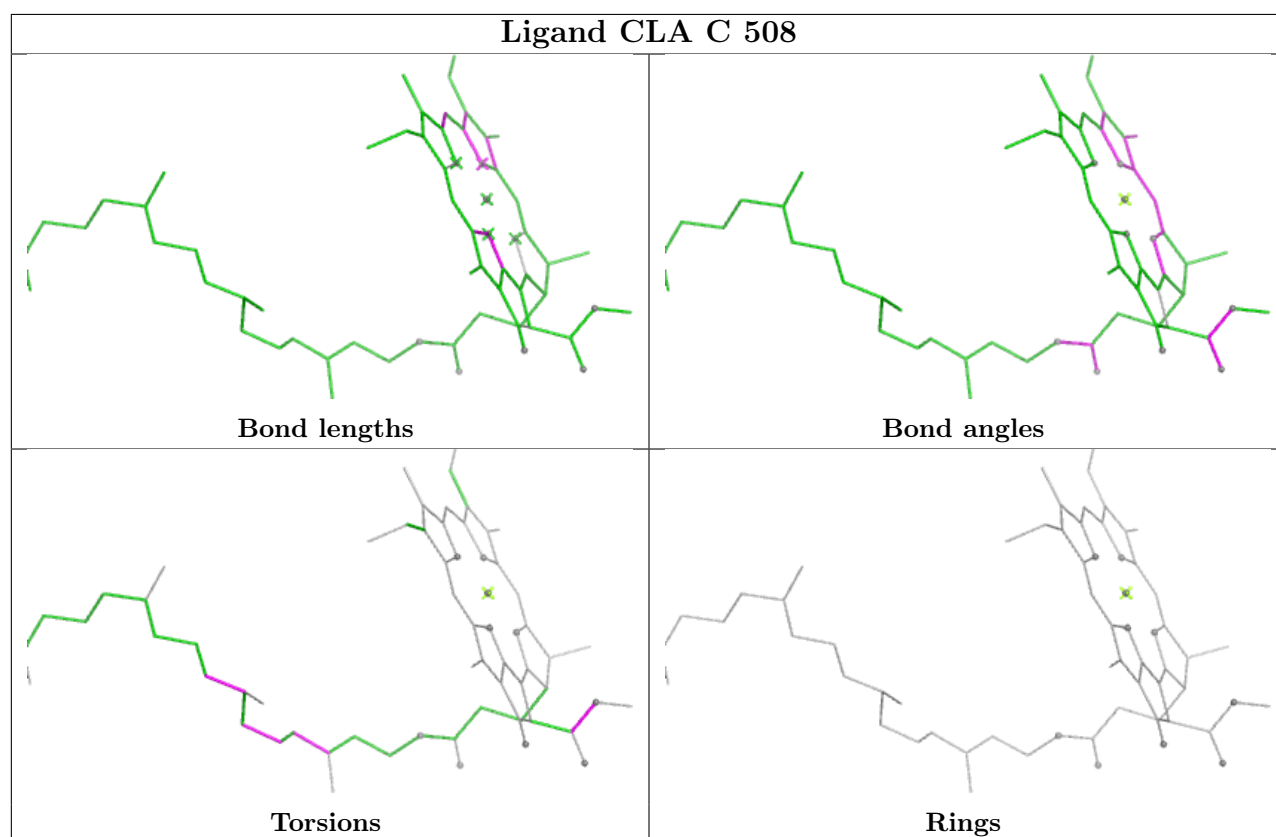
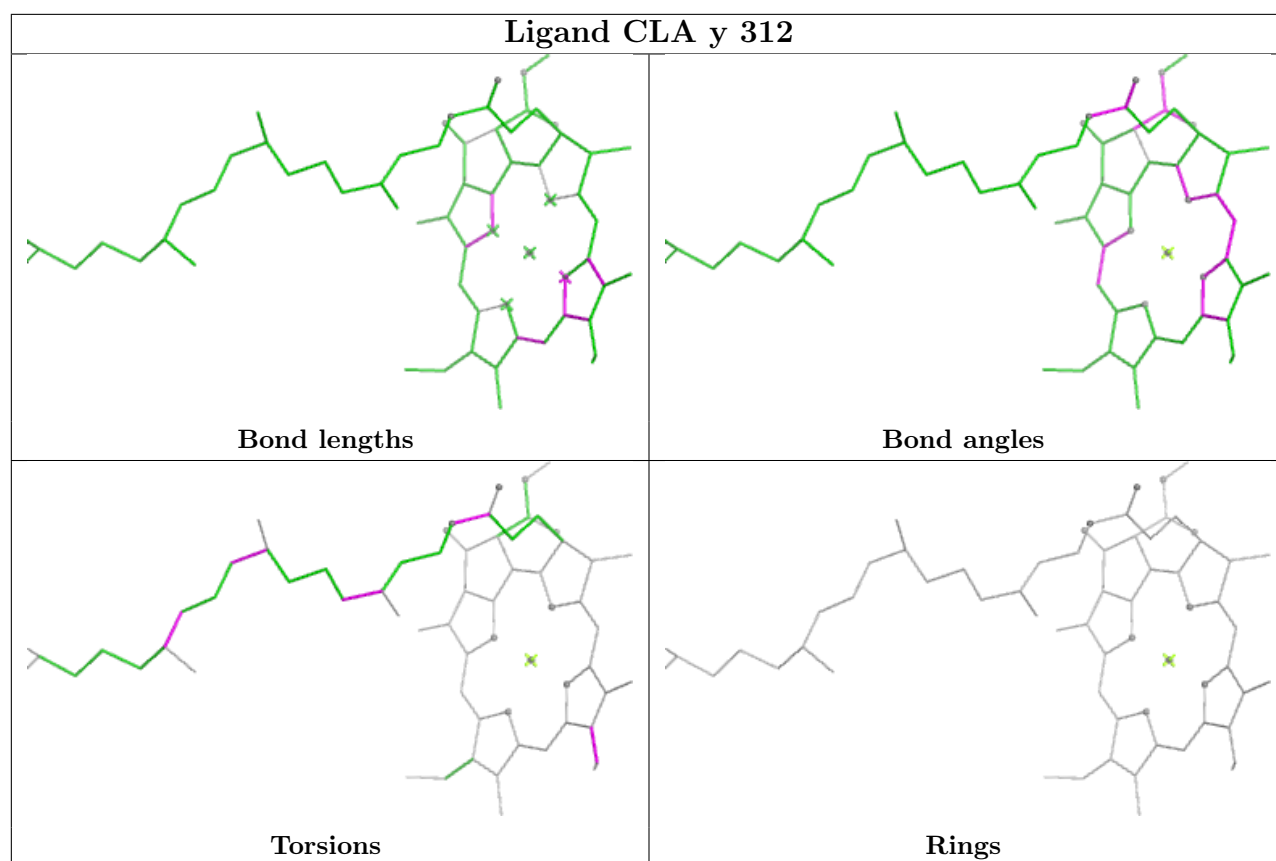


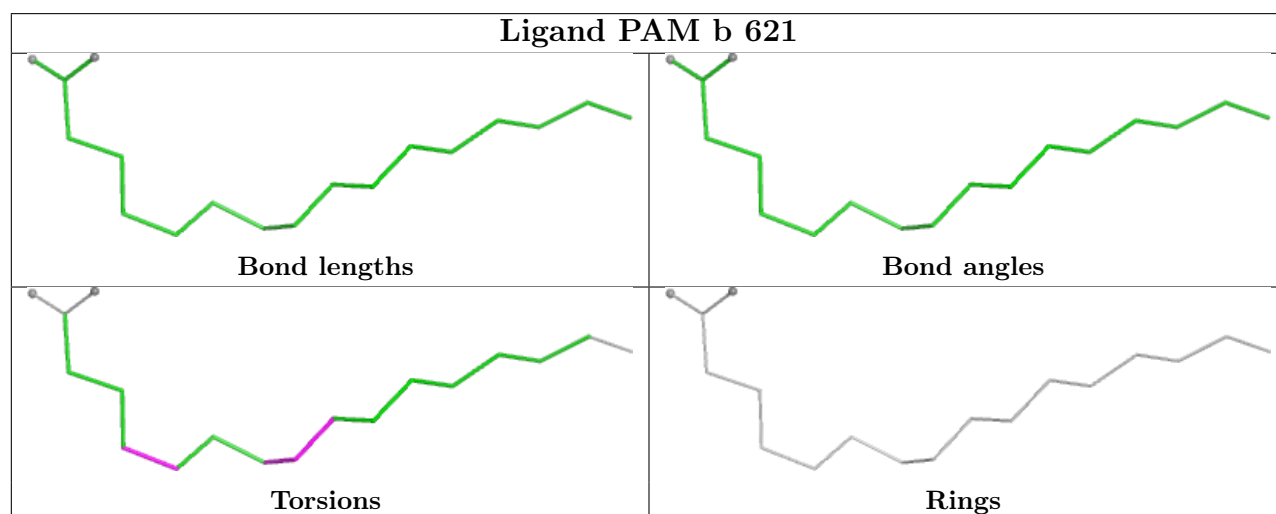
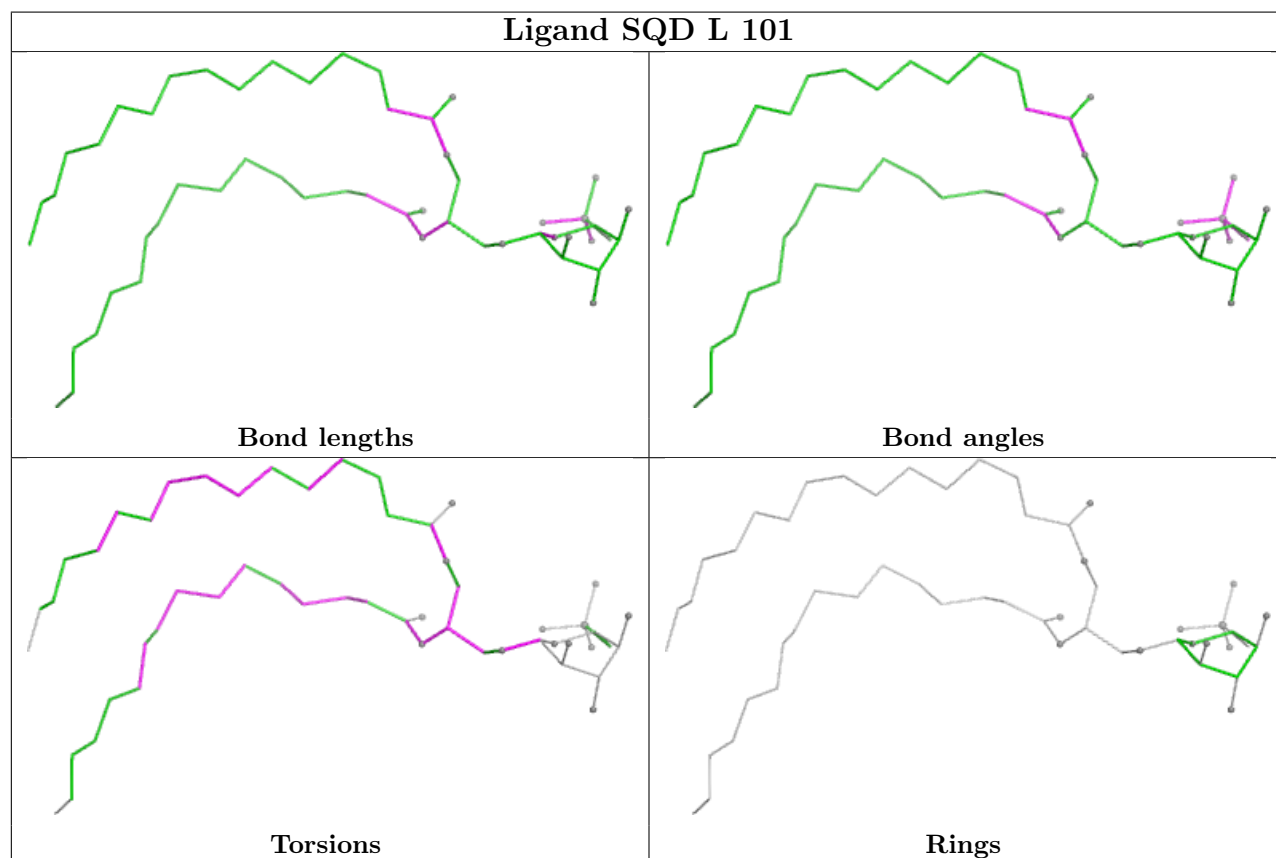
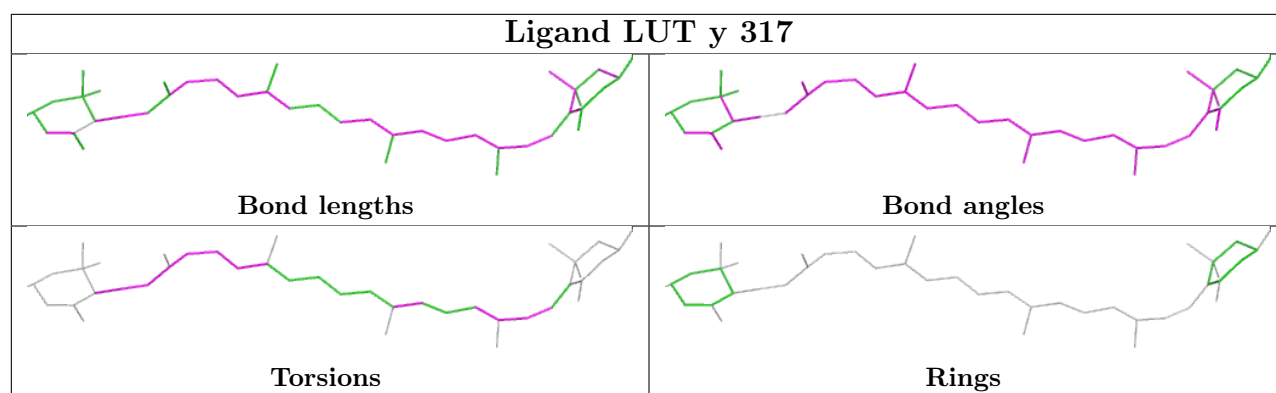
Ligand CLA c 506

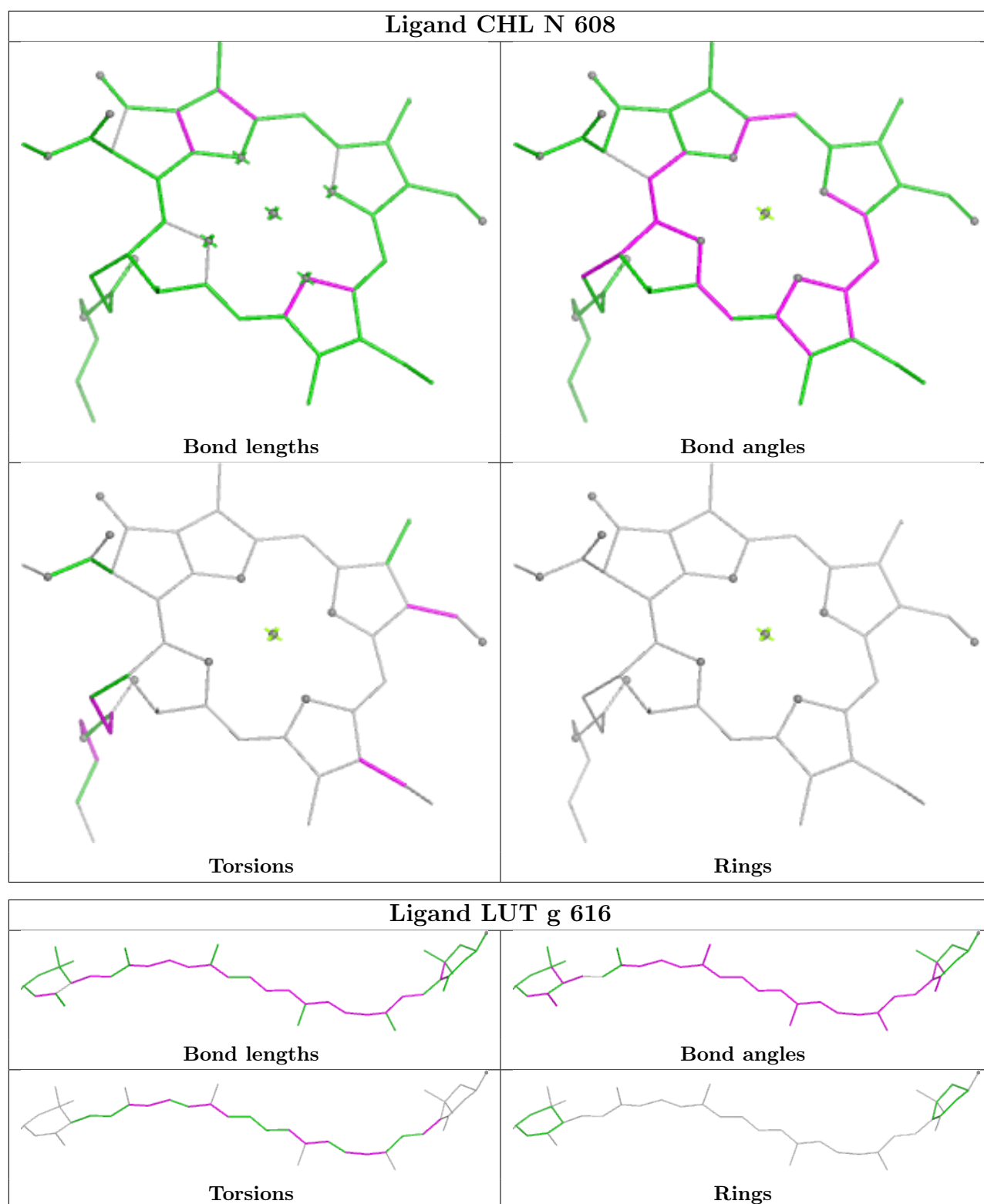


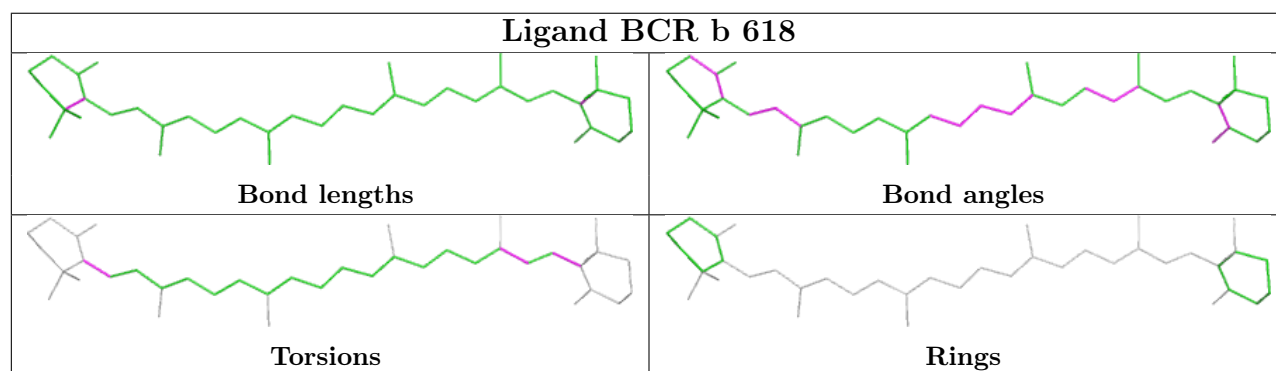
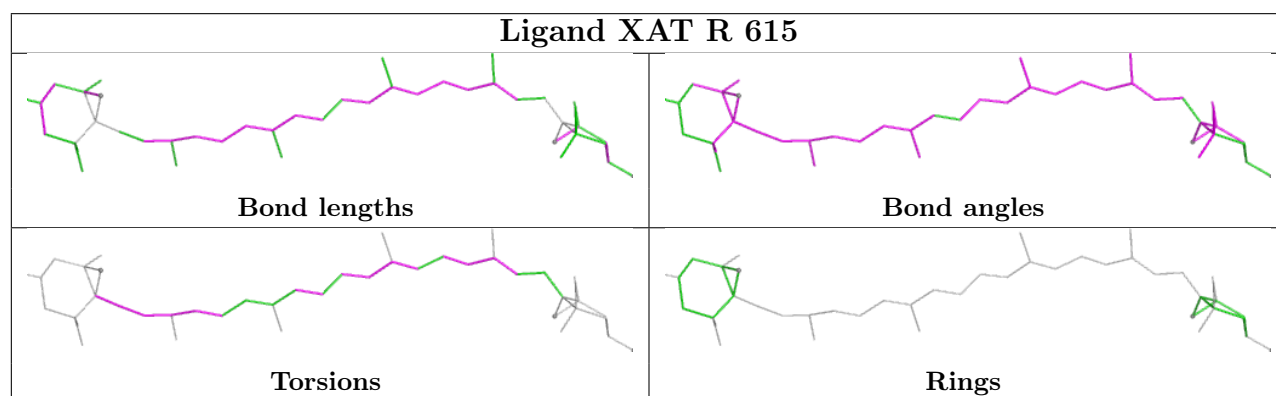
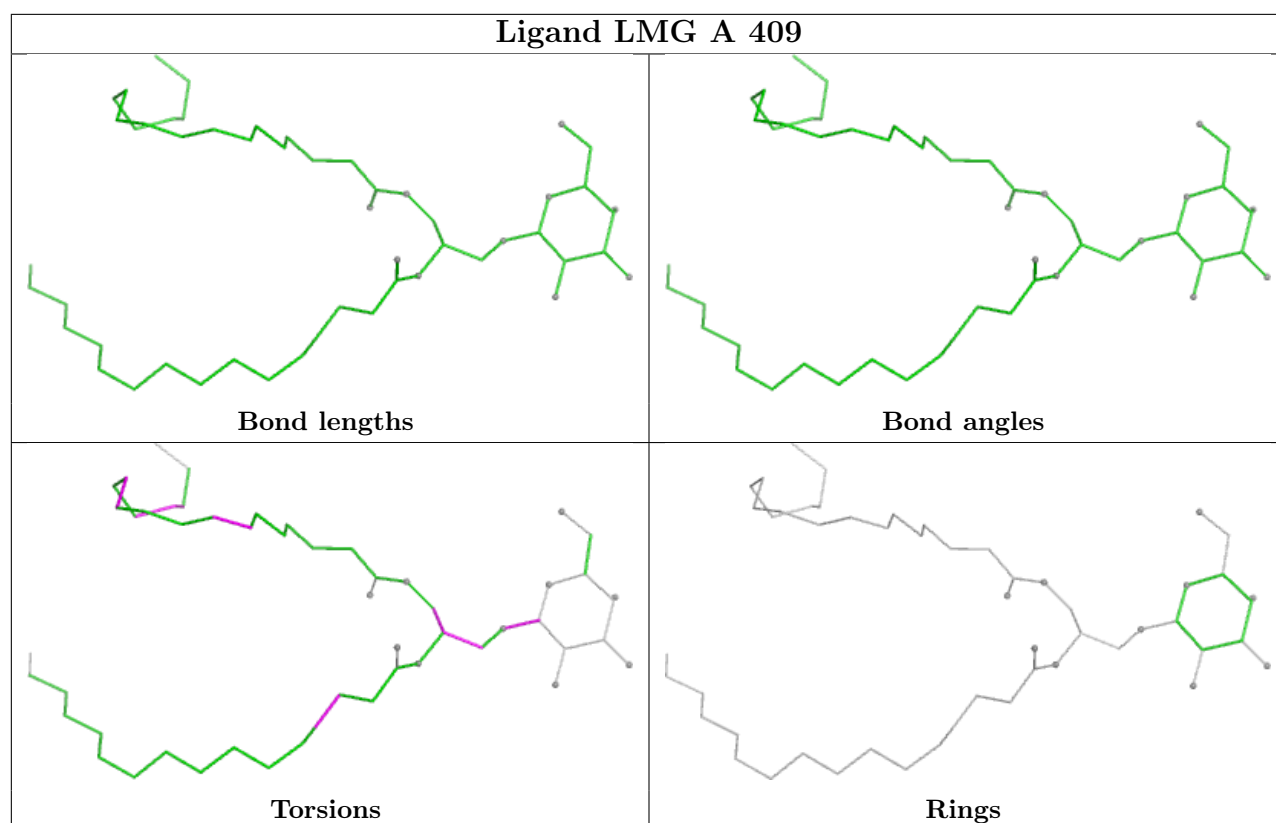
Ligand LHG r 616

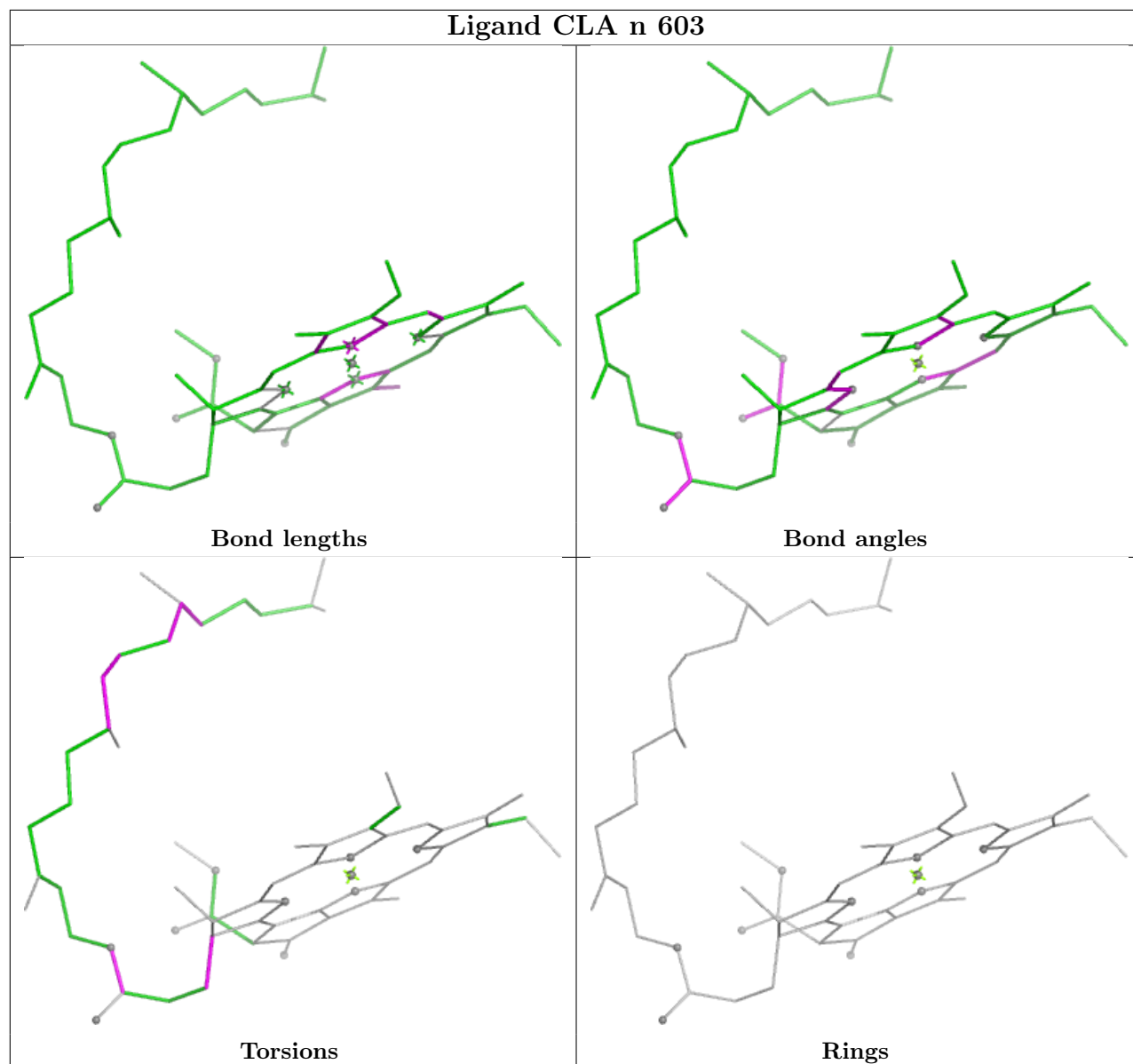


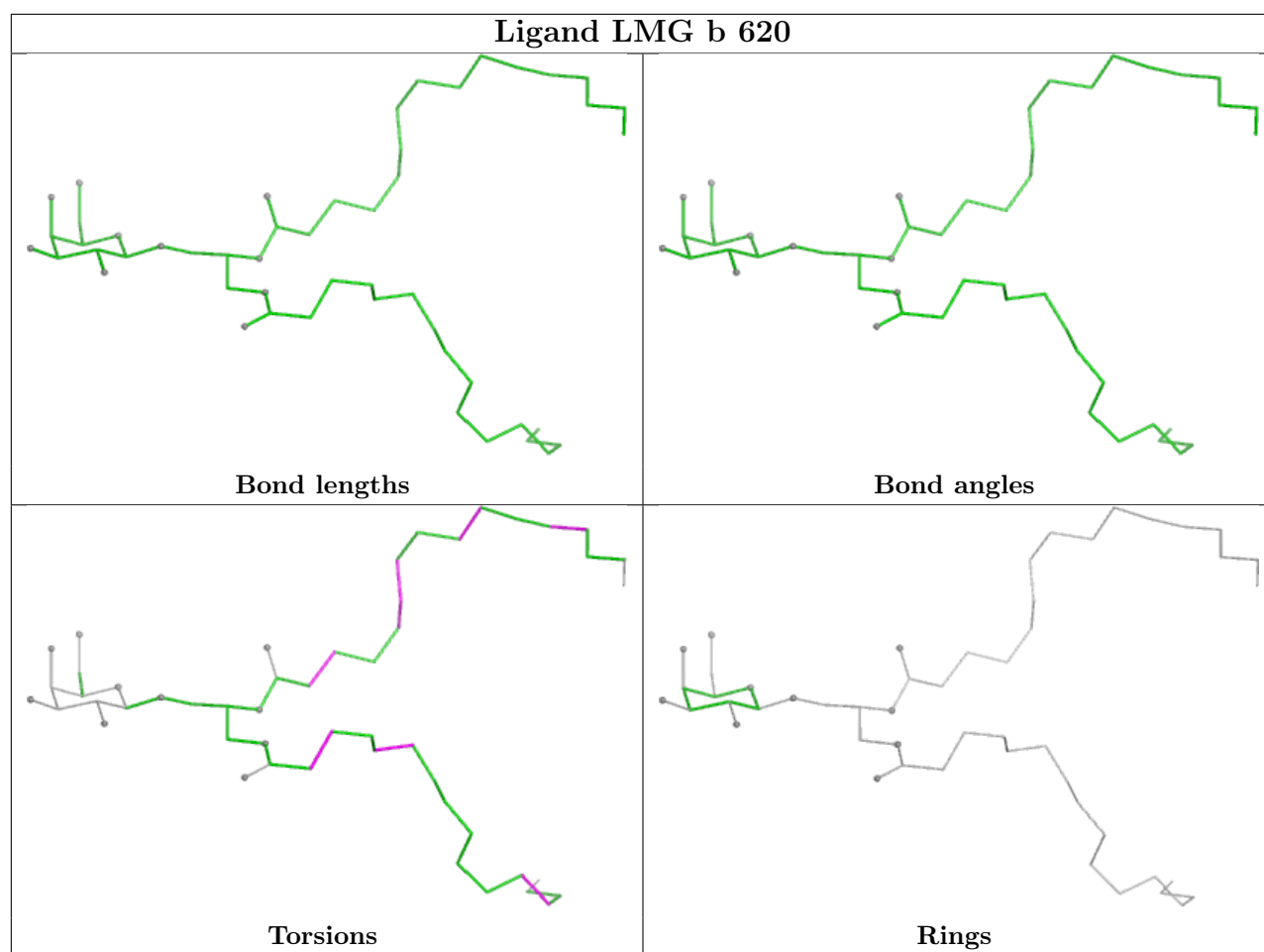


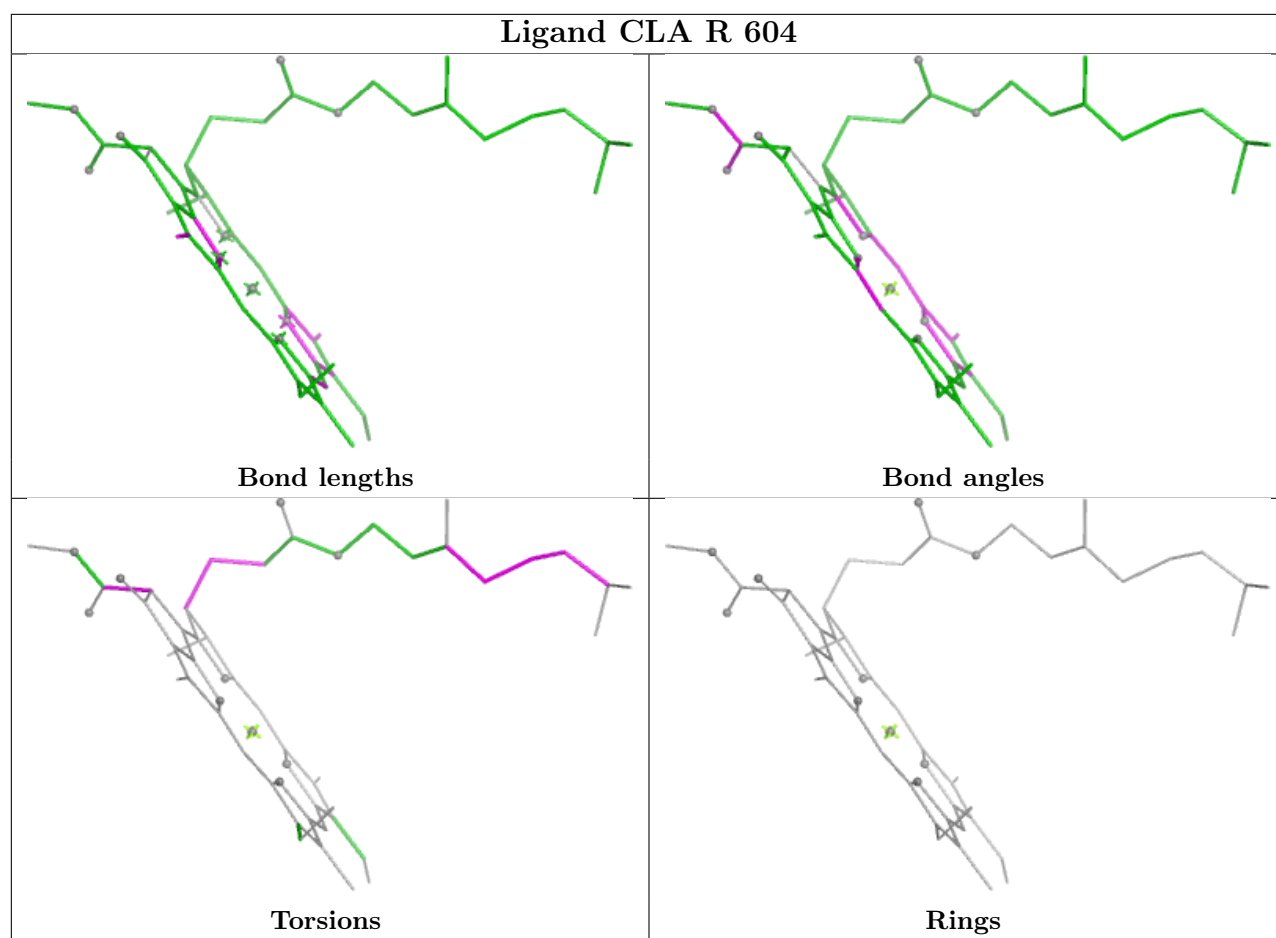


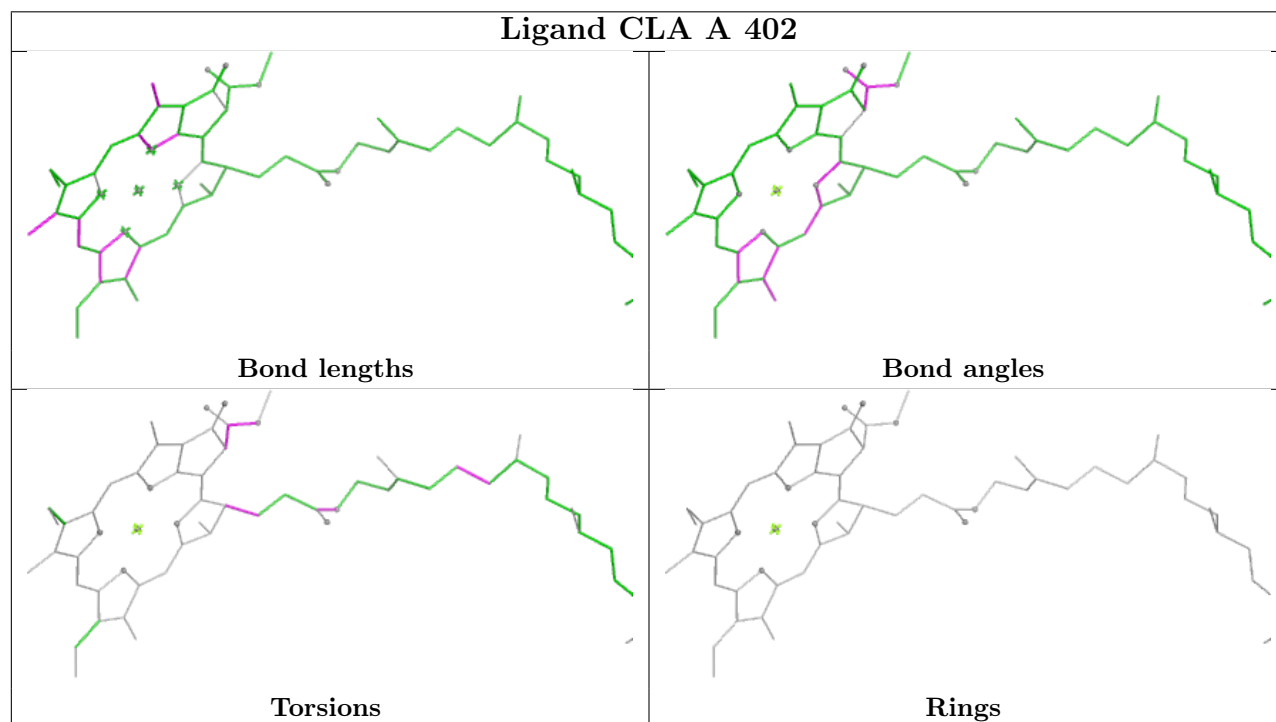
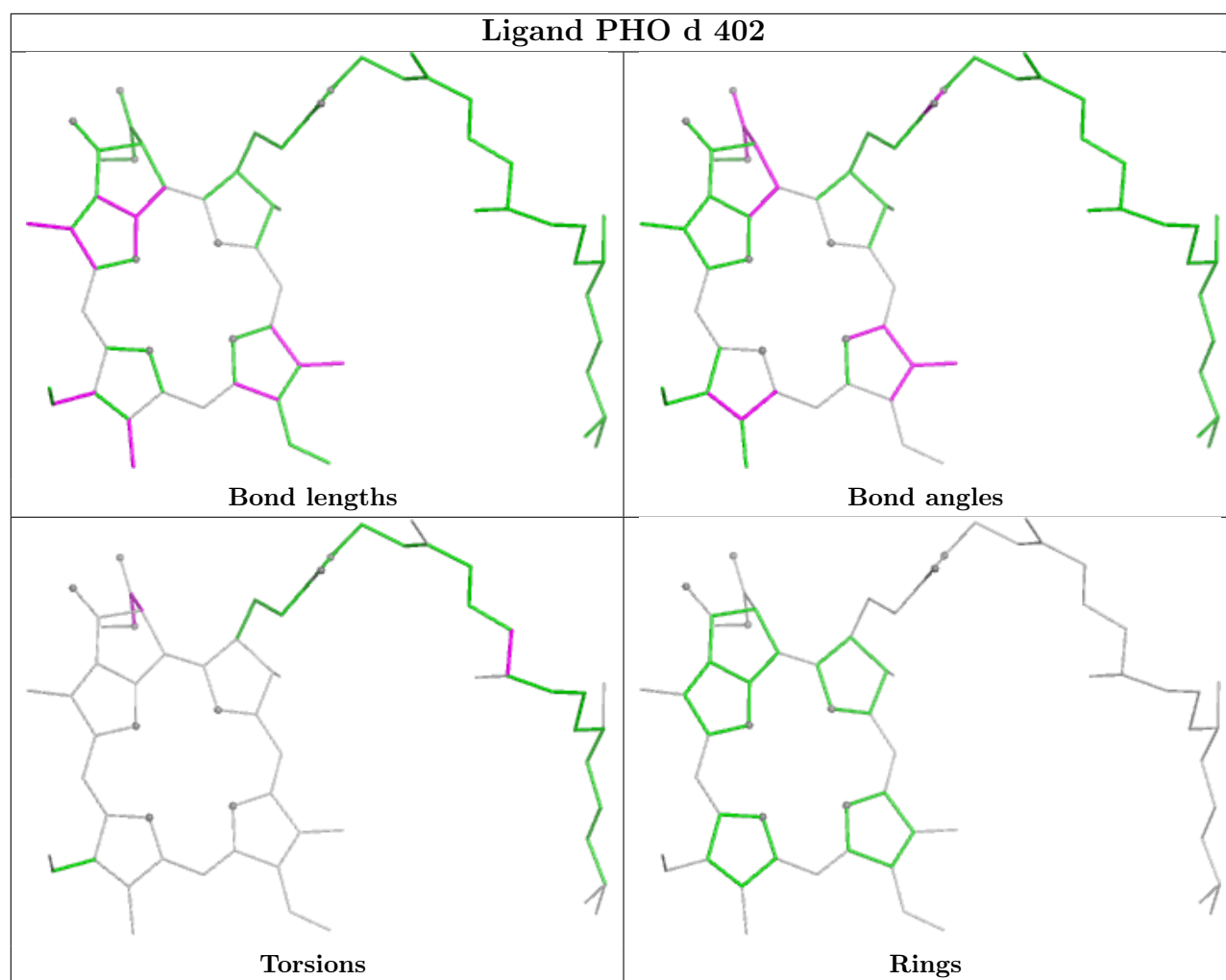


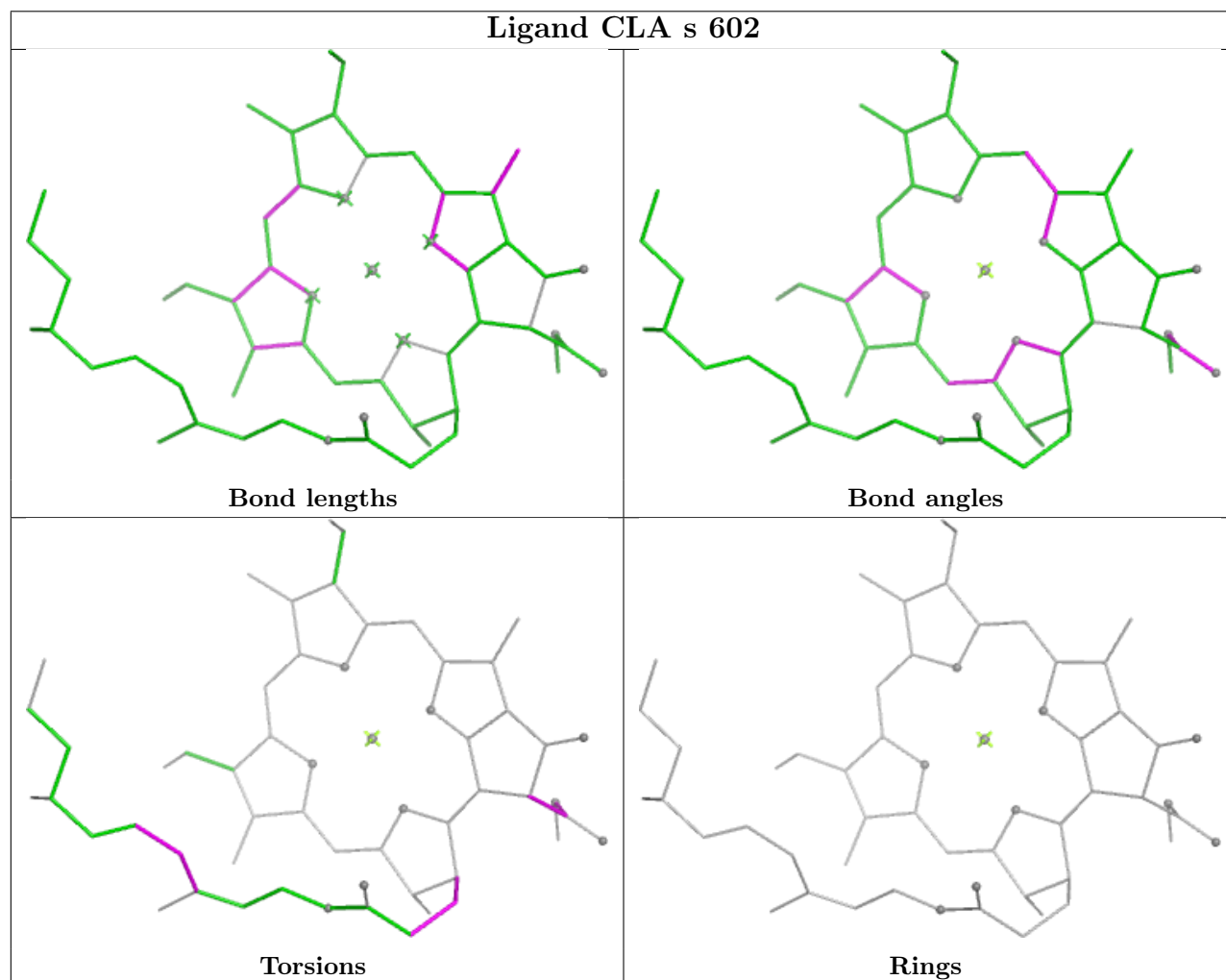
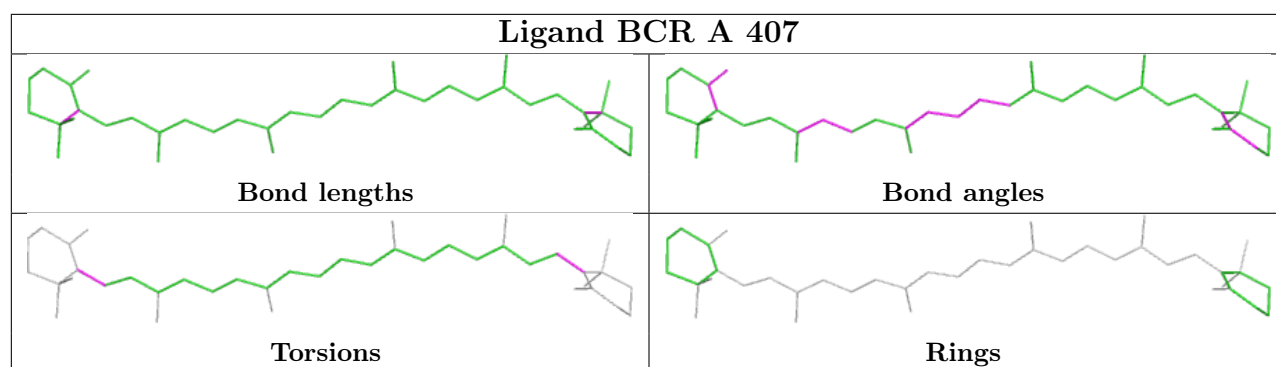


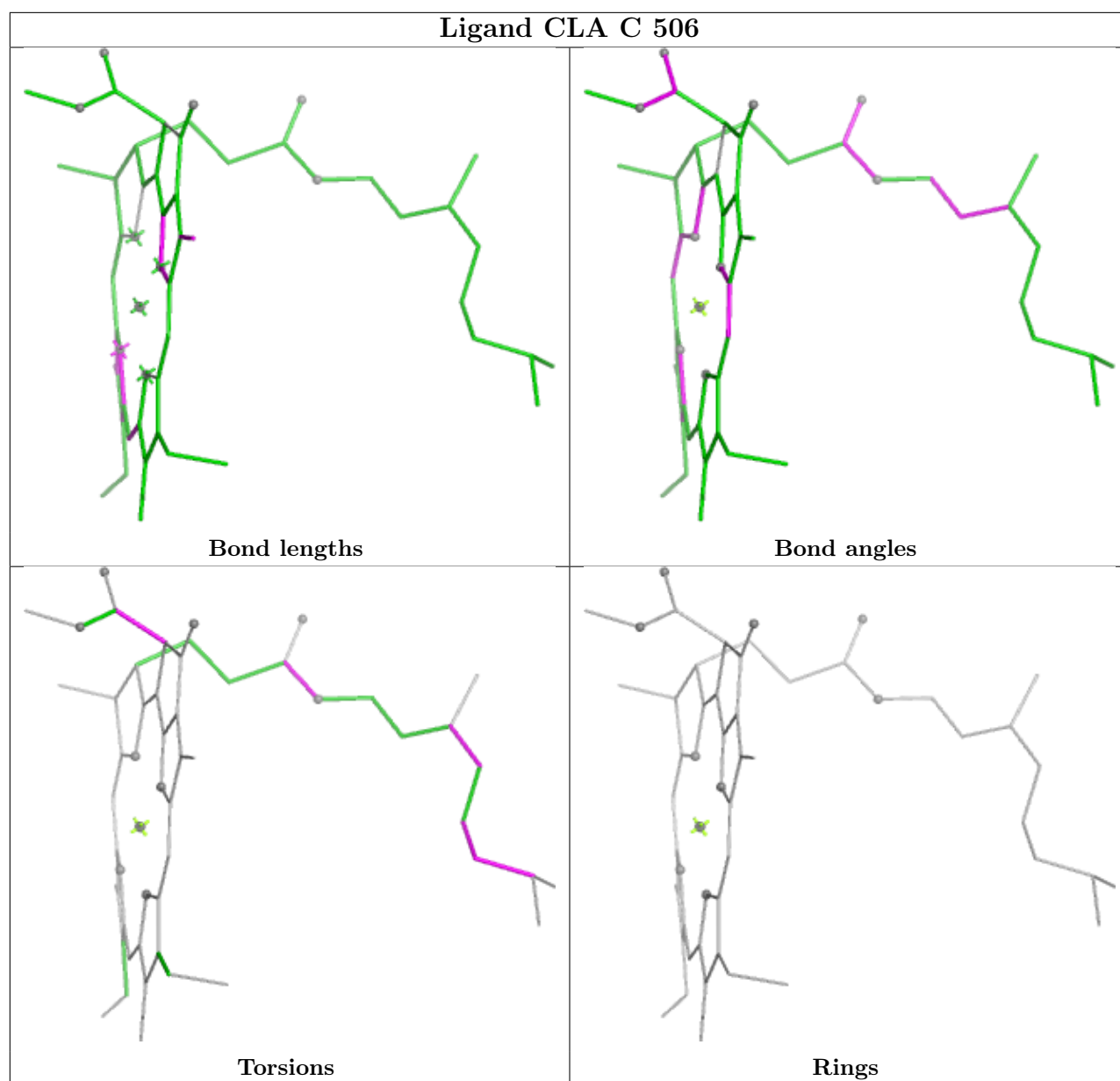


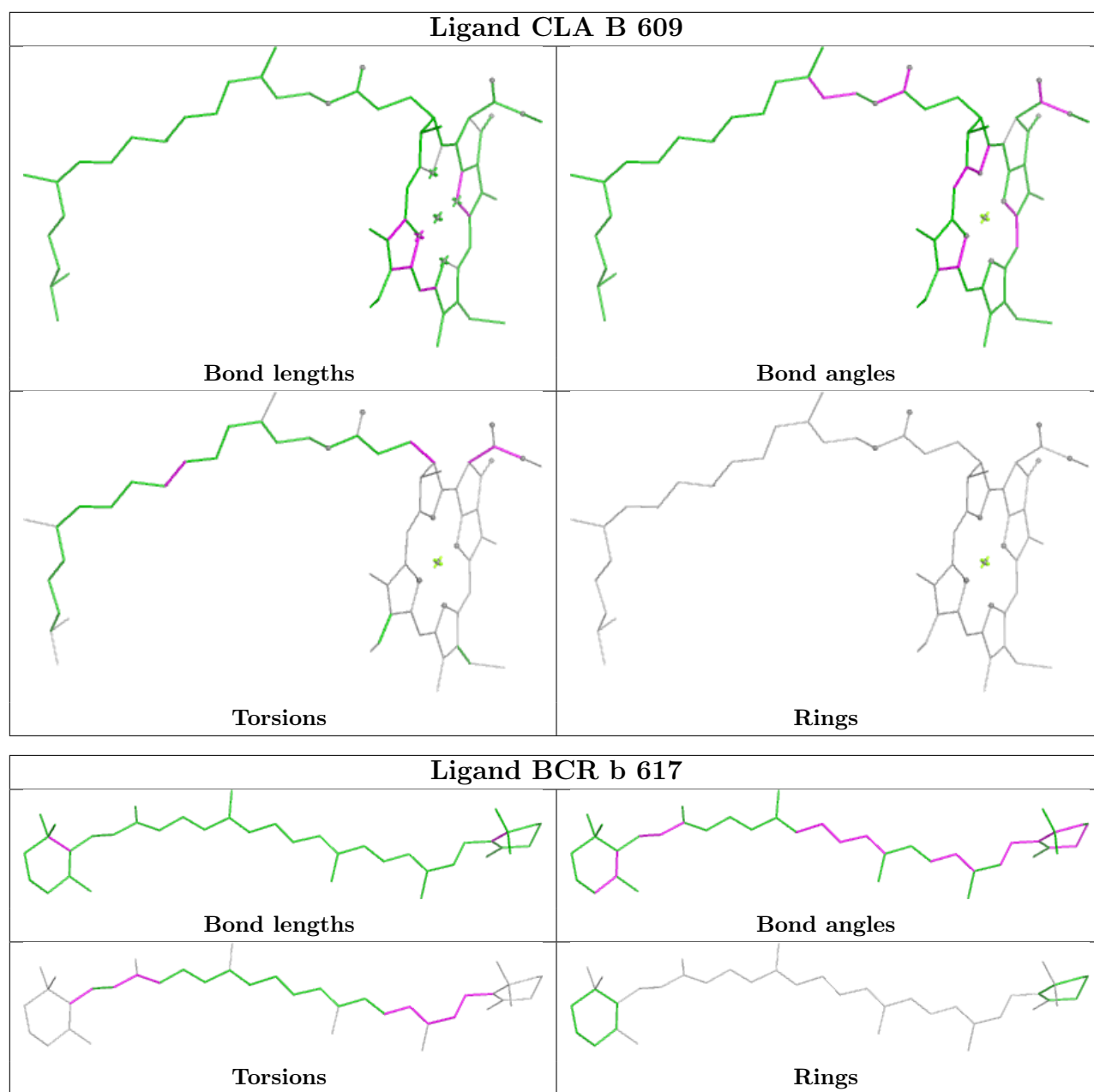




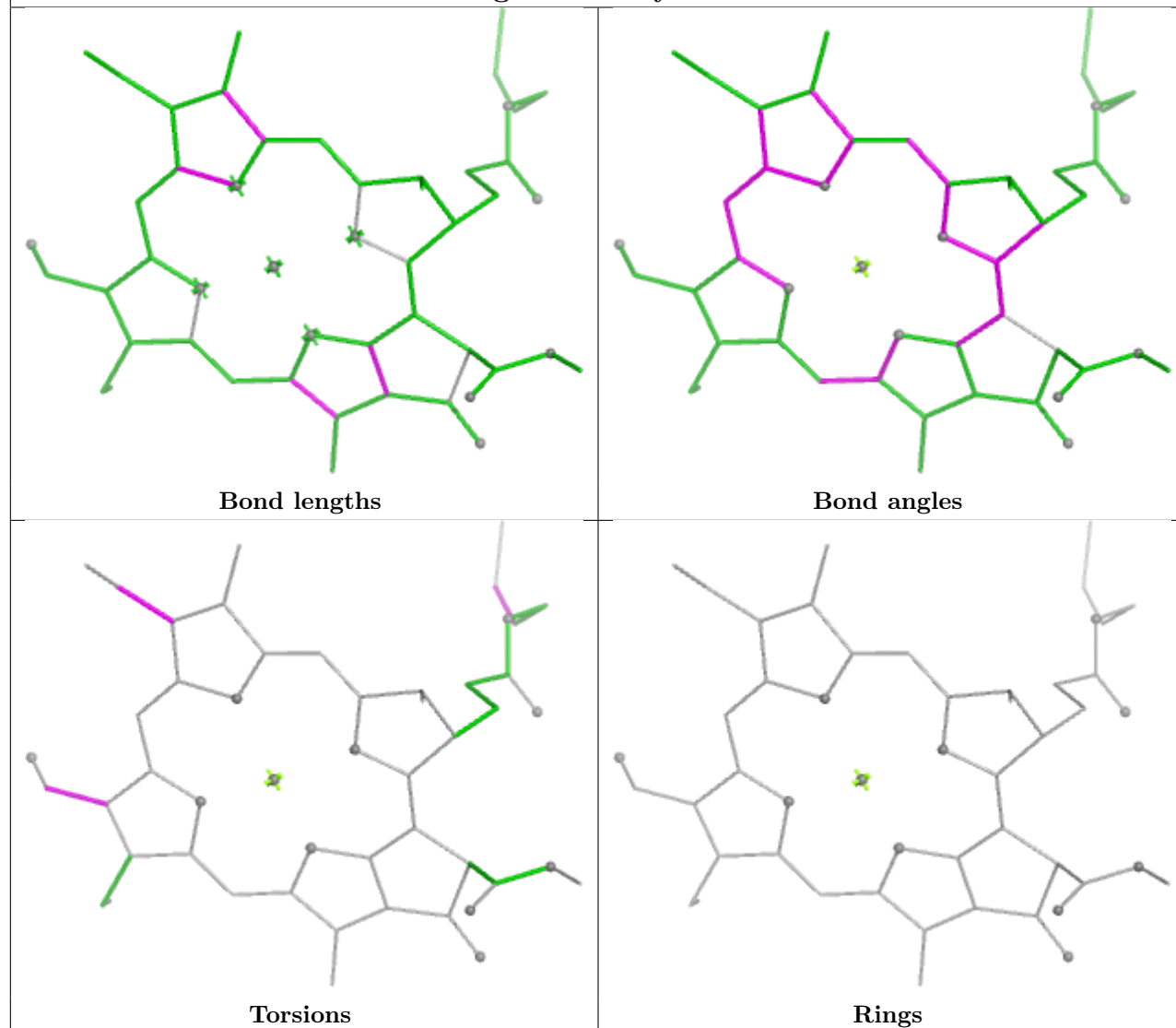




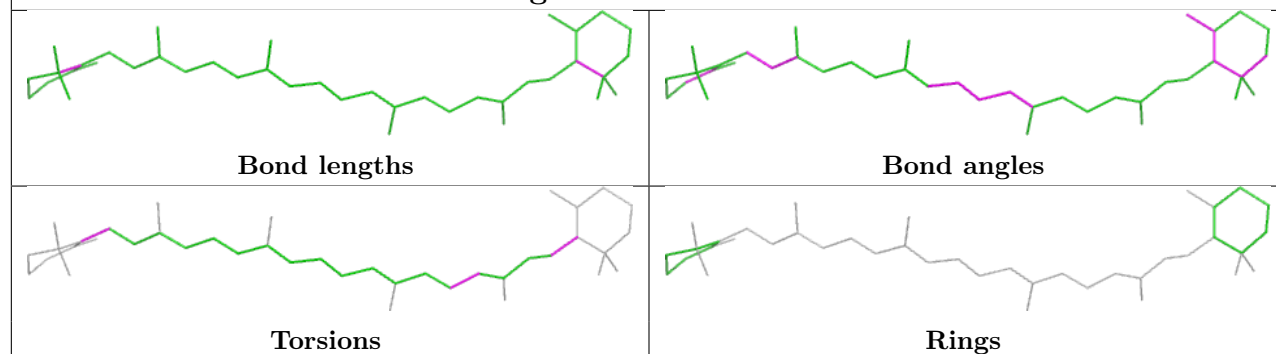




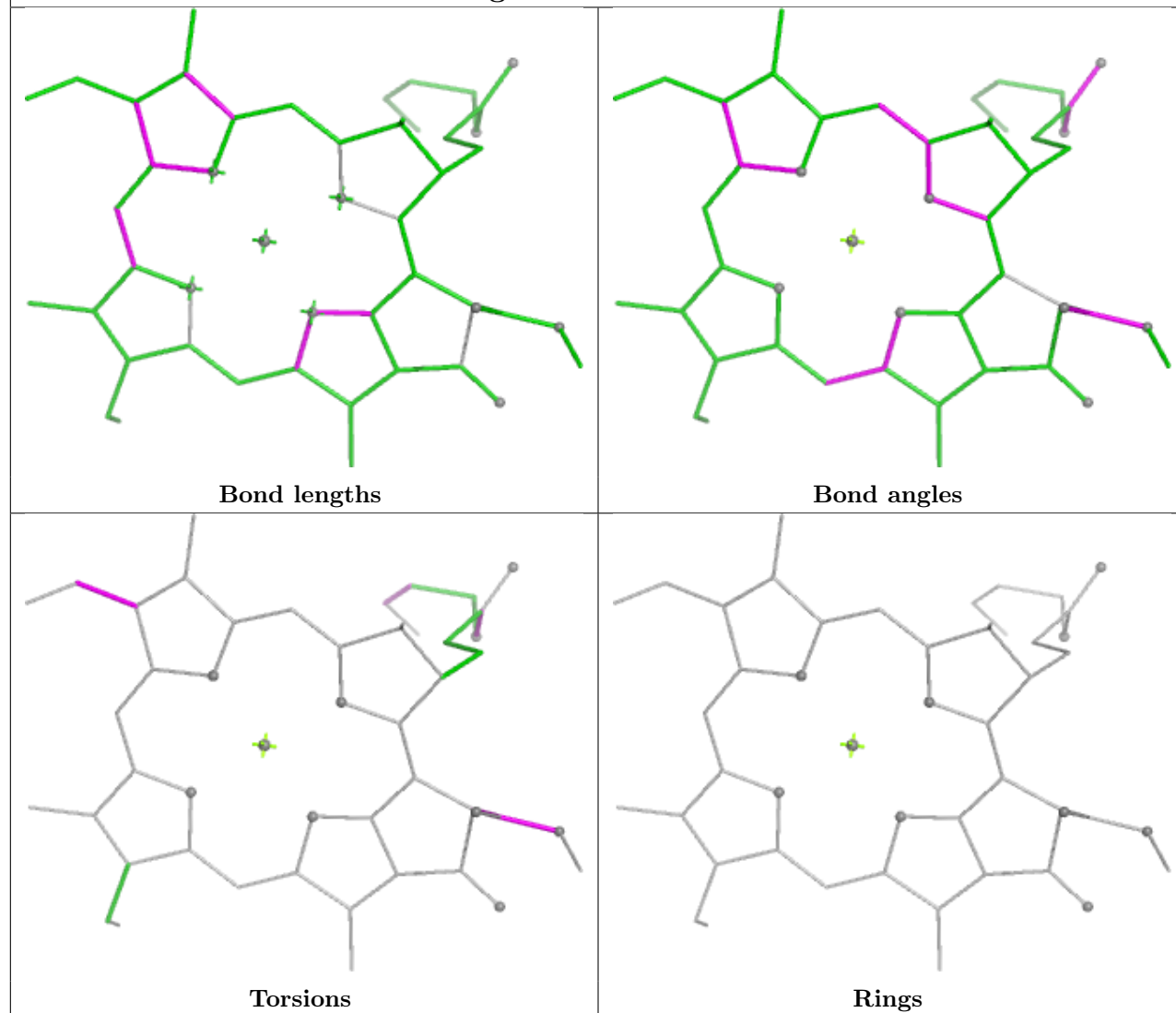
Ligand CHL y 309



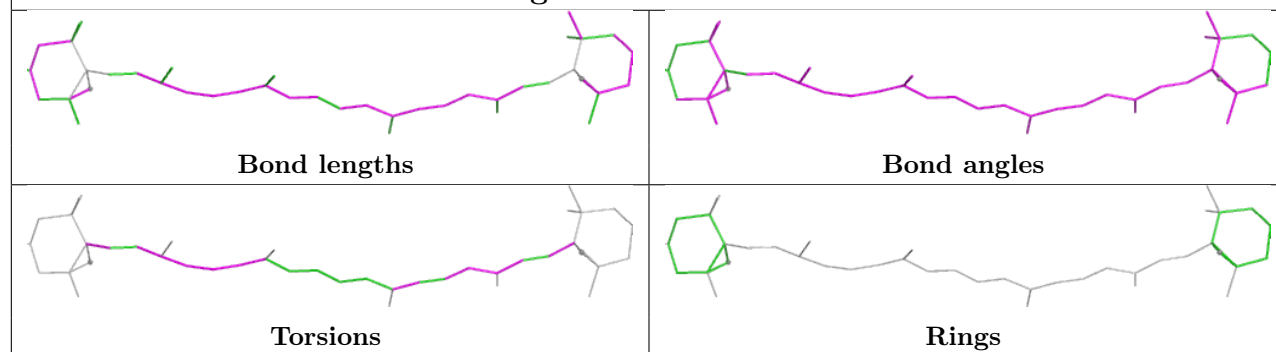
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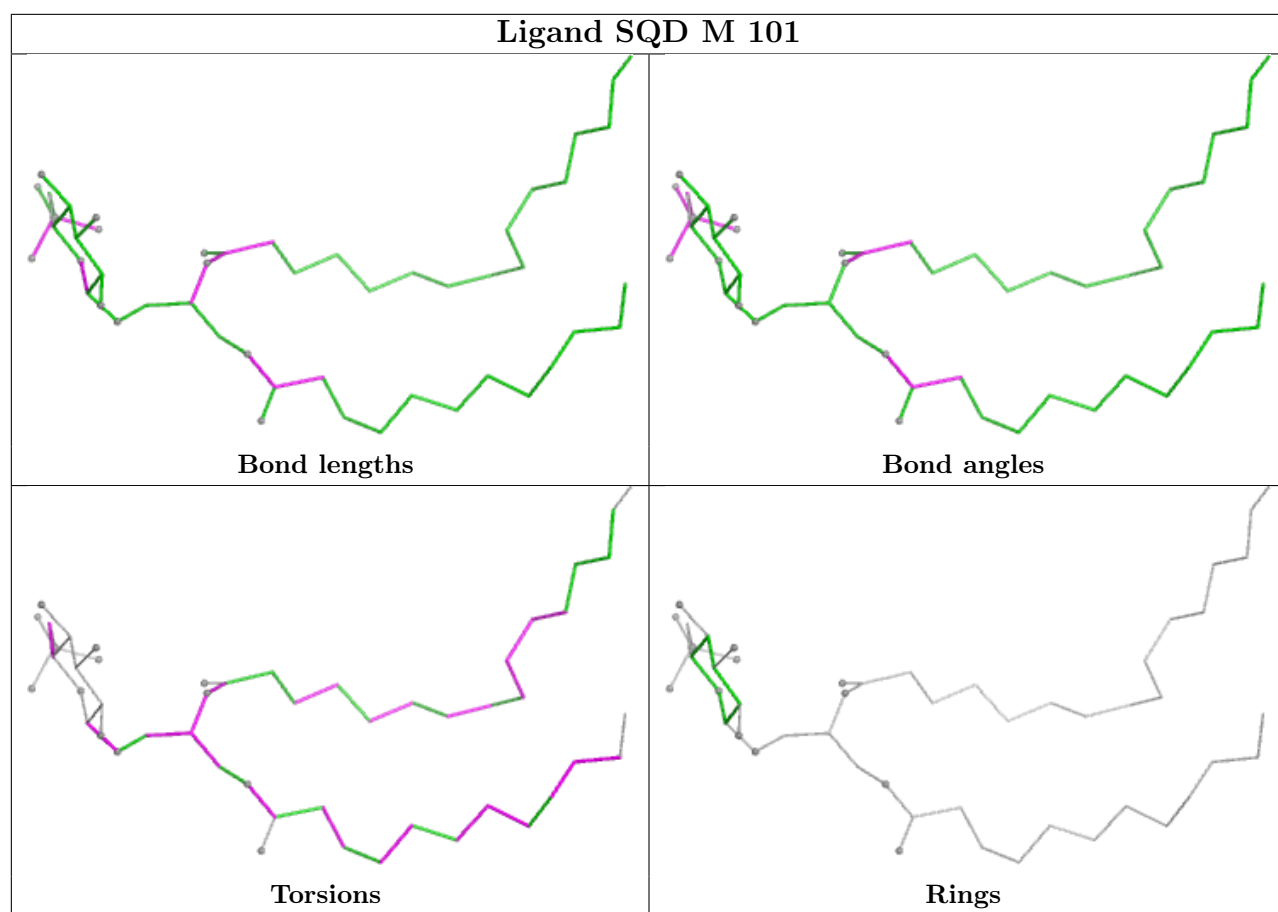


Ligand CLA G 614

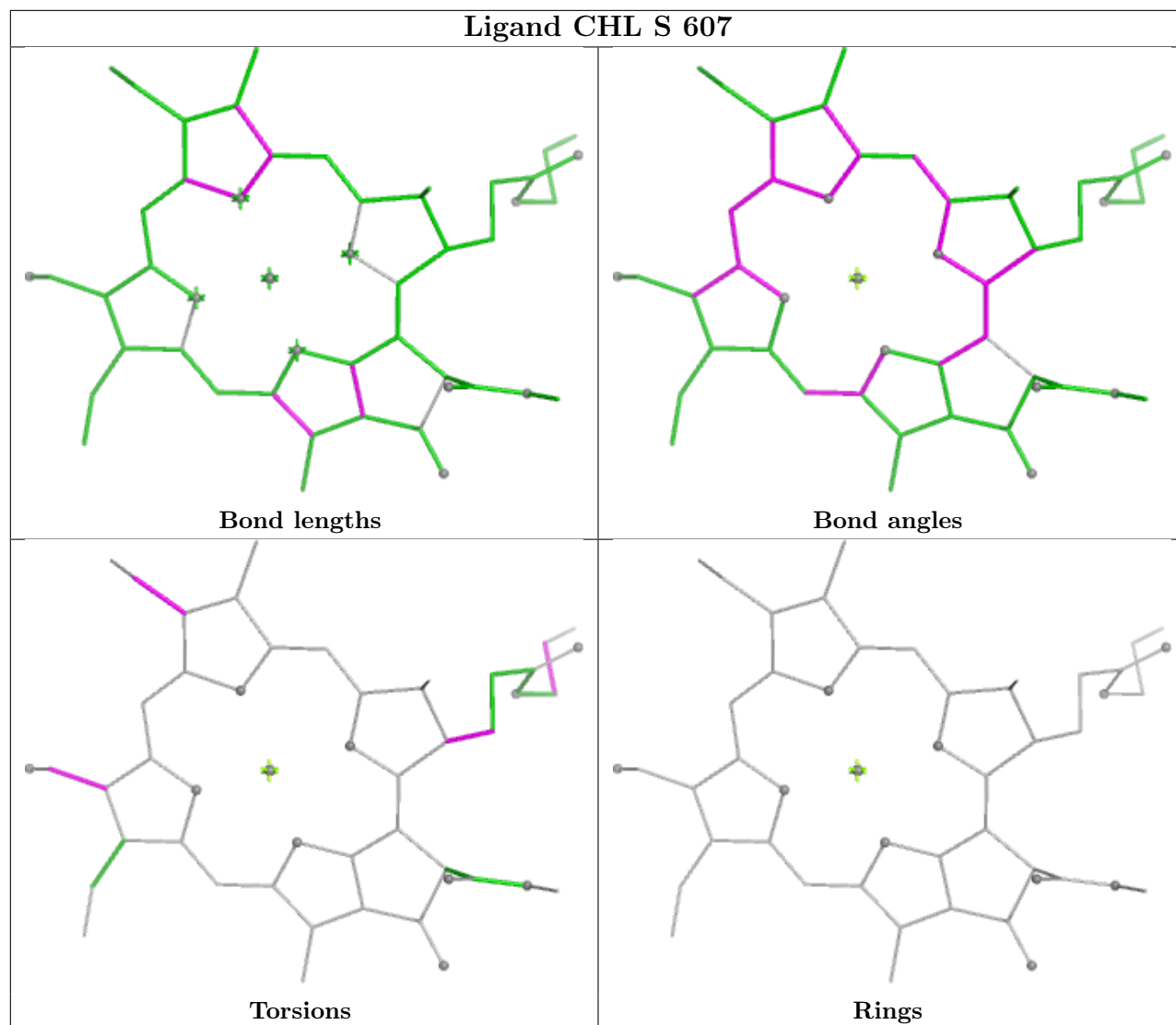


Ligand XAT N 619

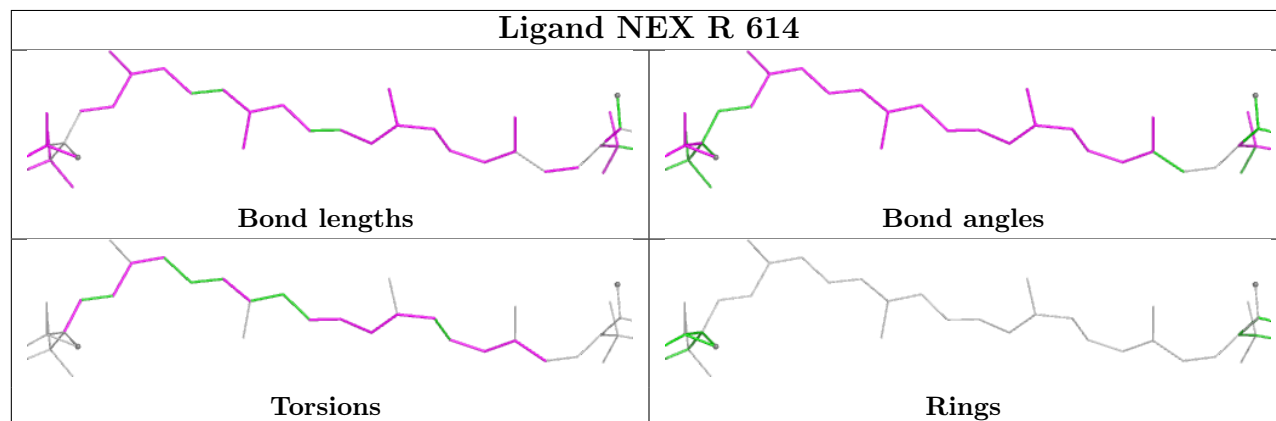


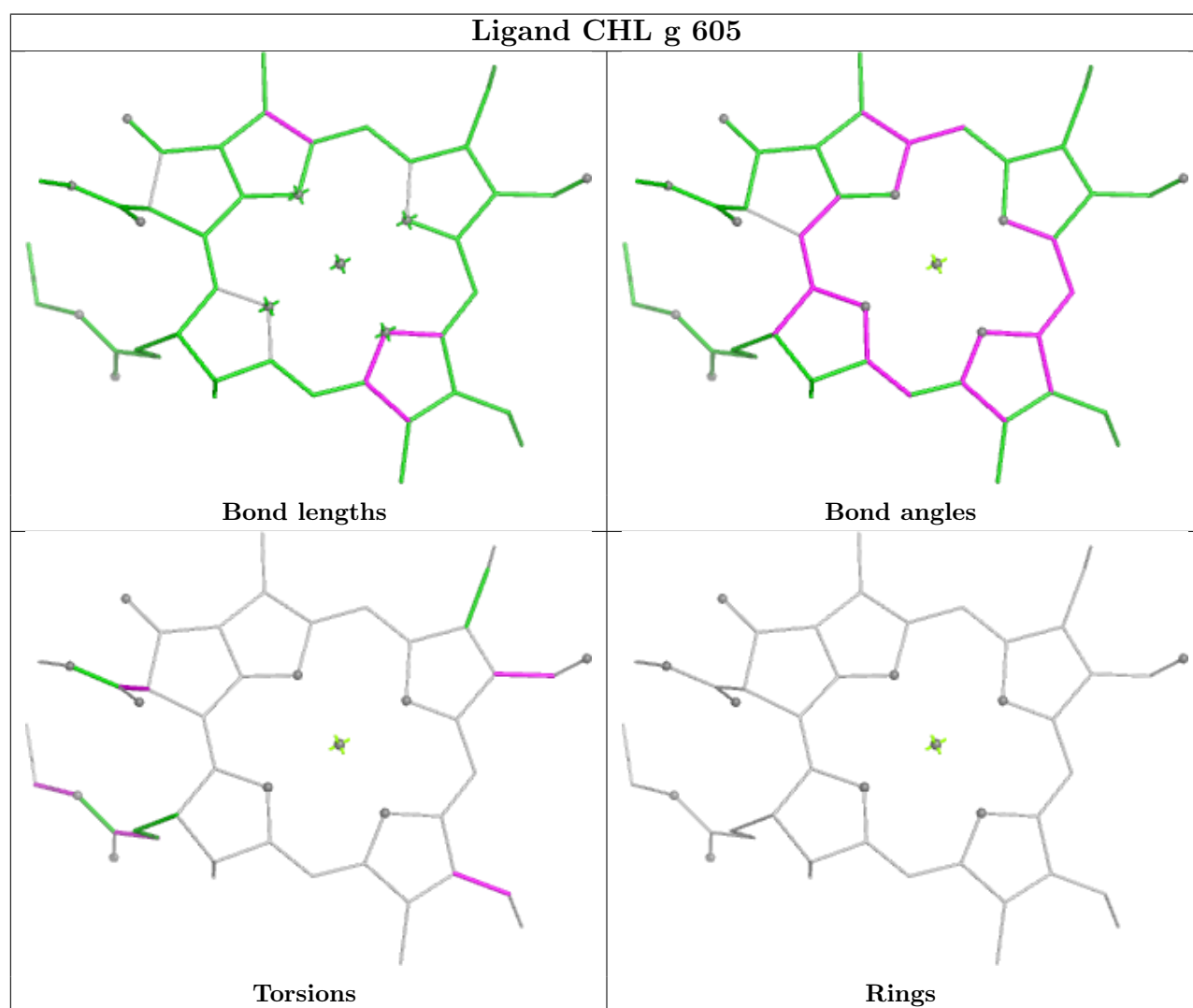
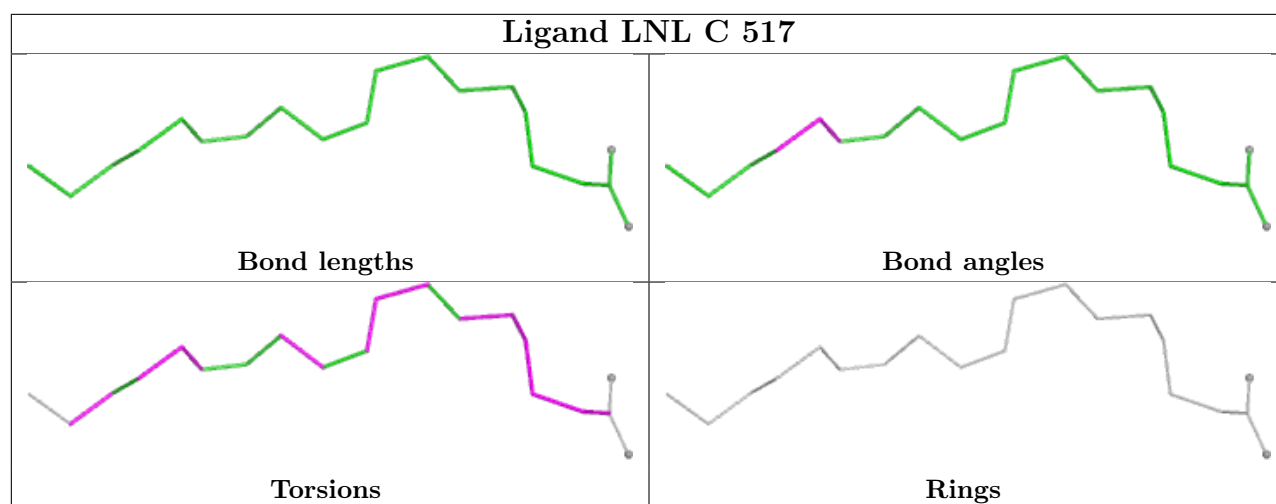


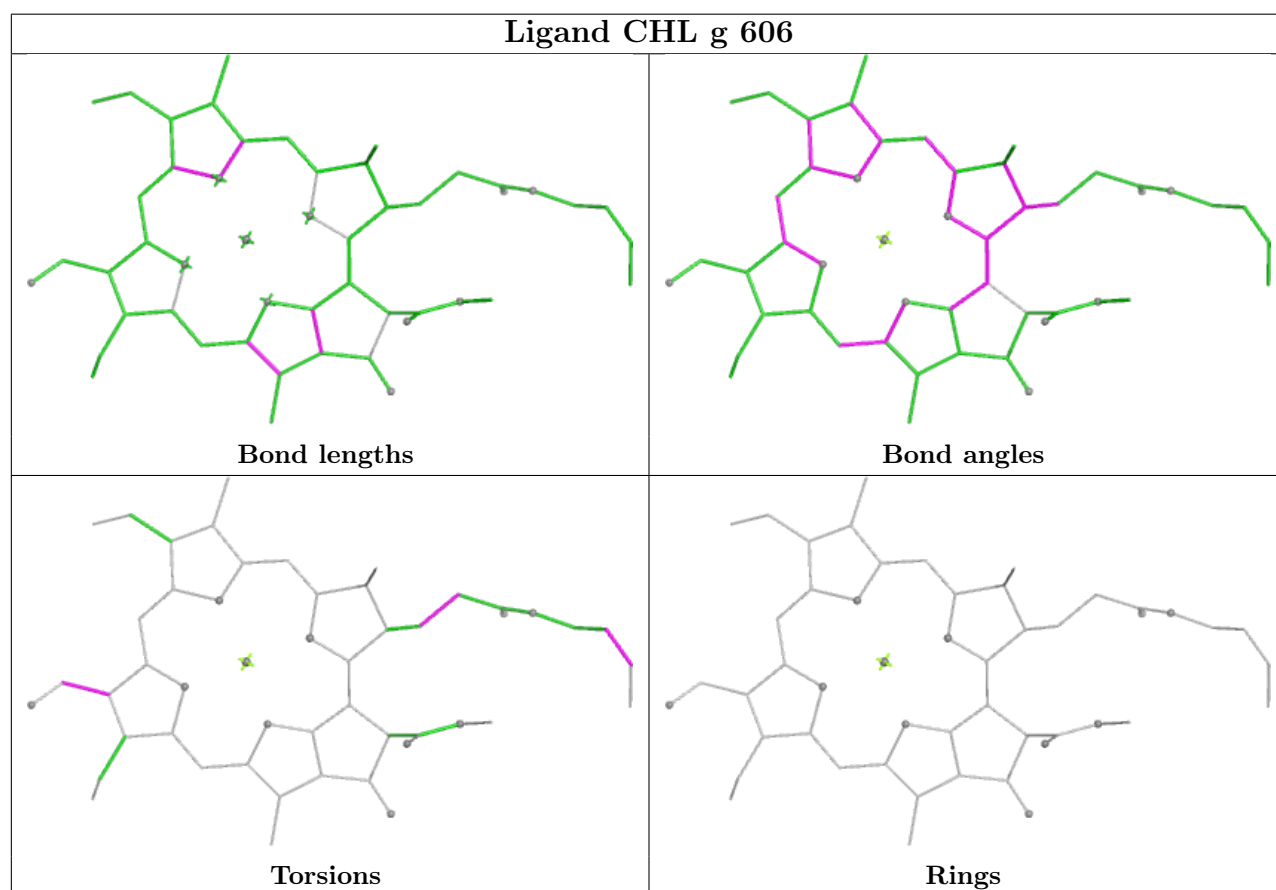
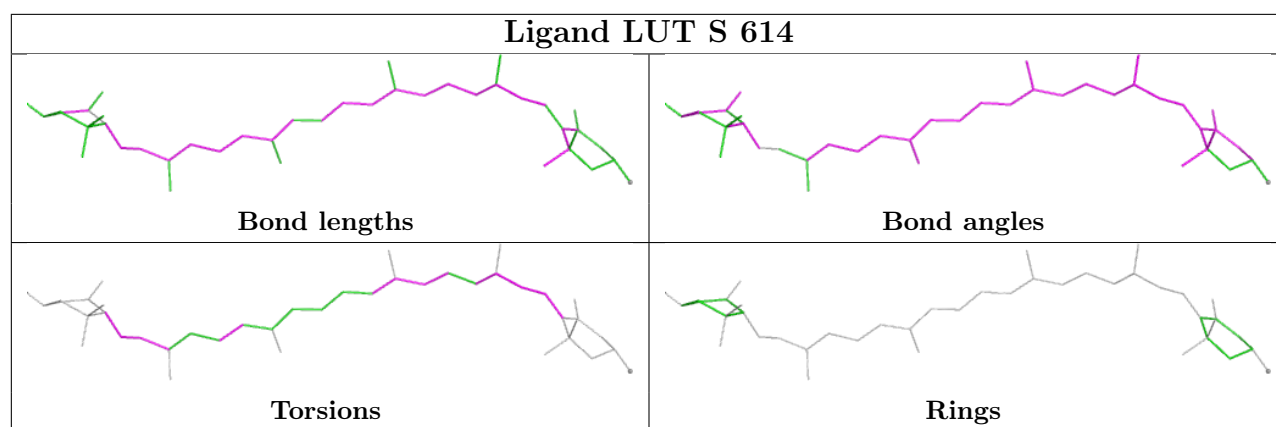
Ligand CHL S 607

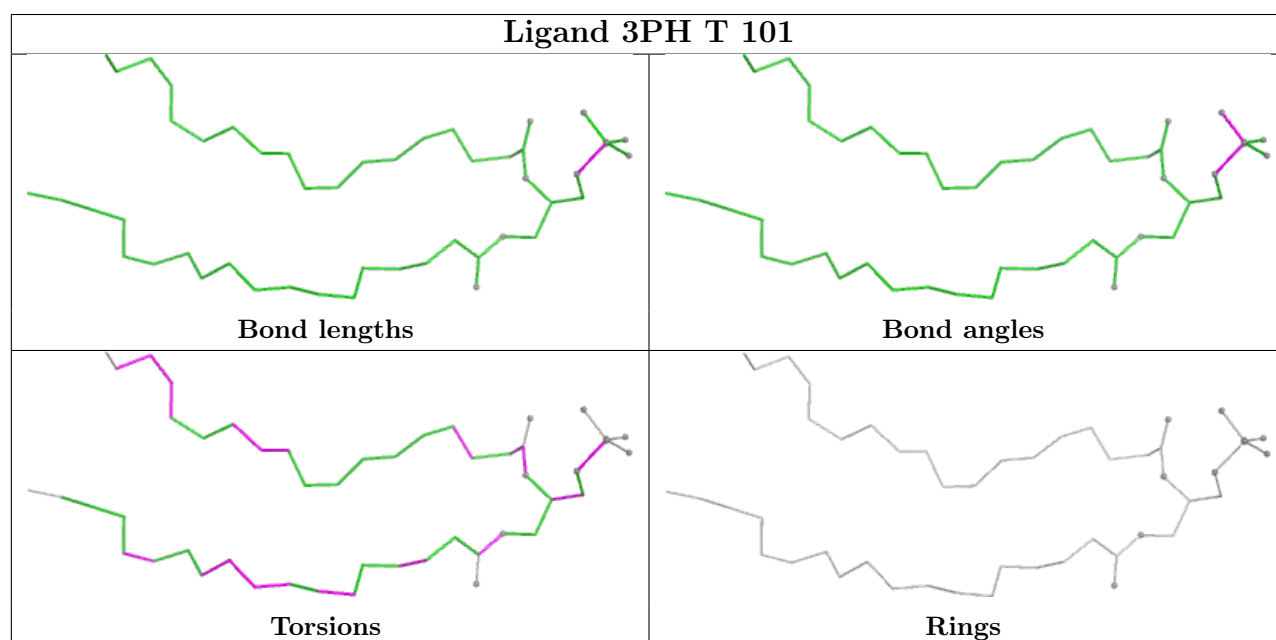
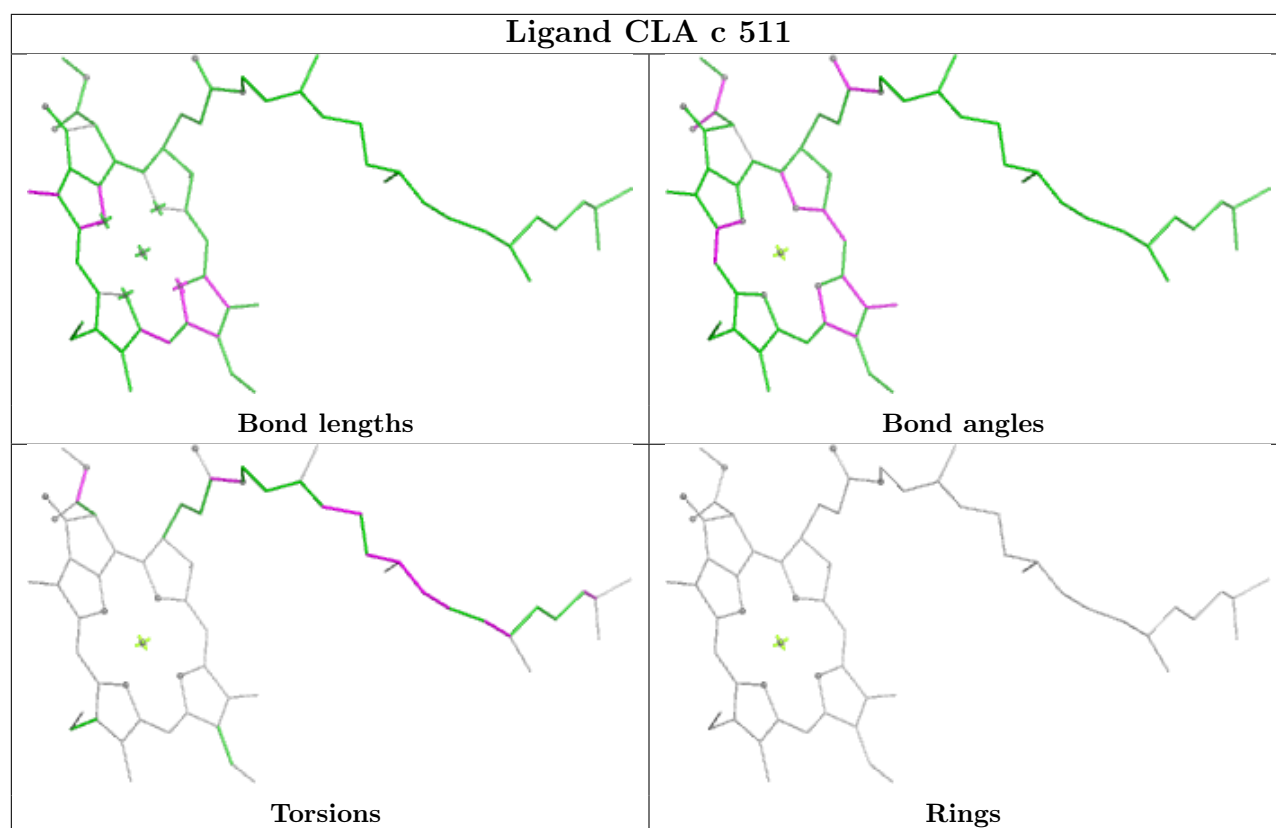


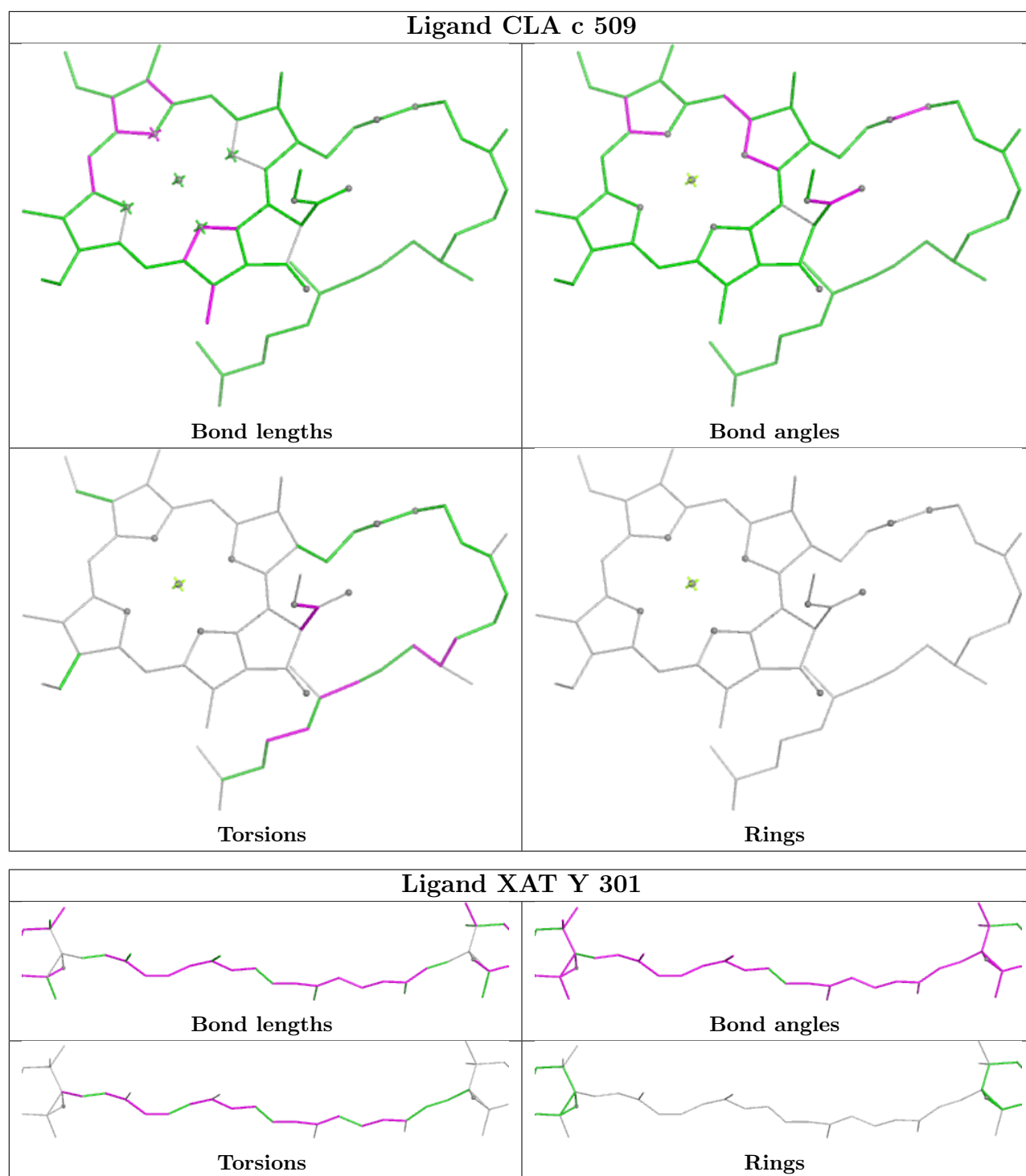
Ligand NEX R 614

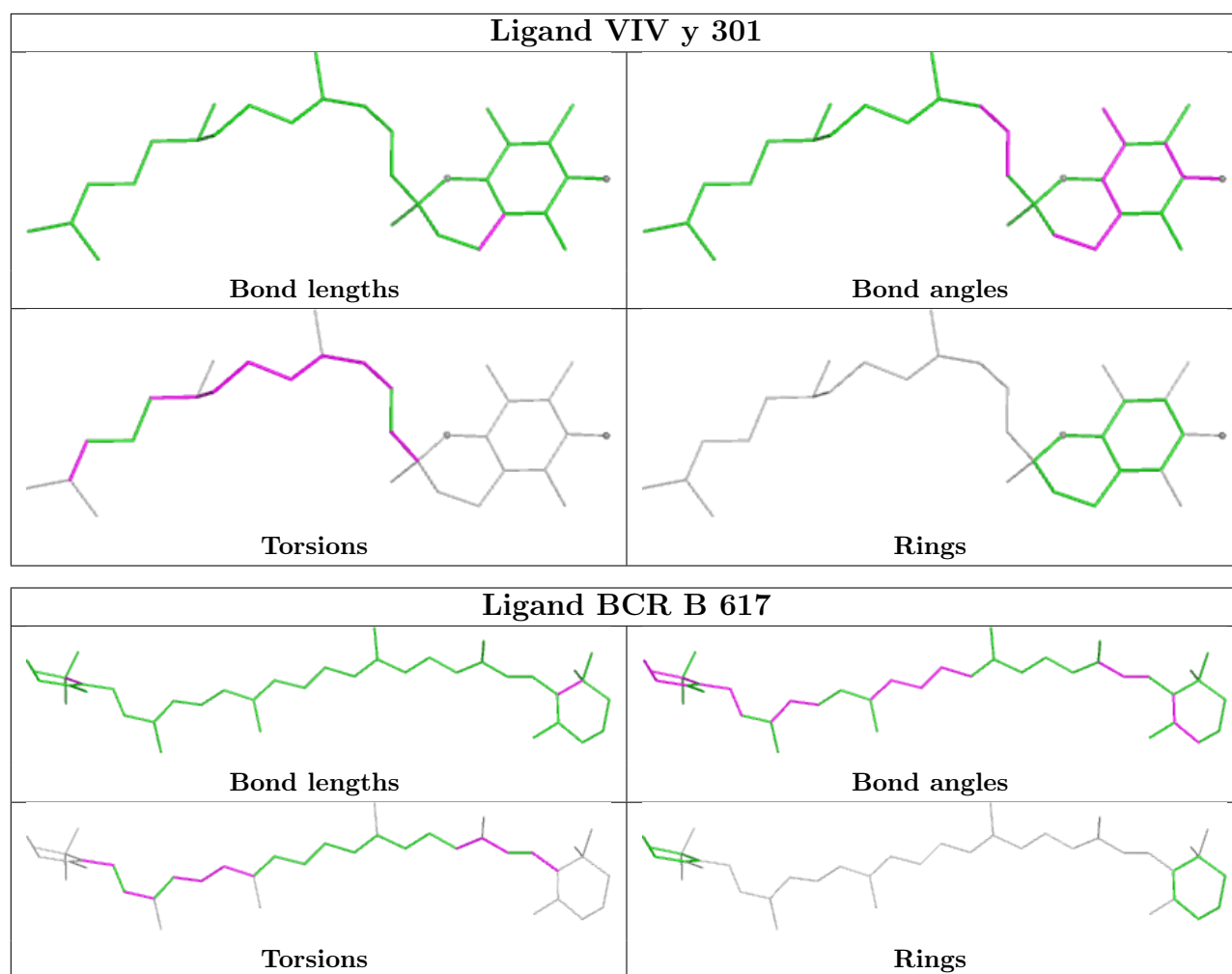


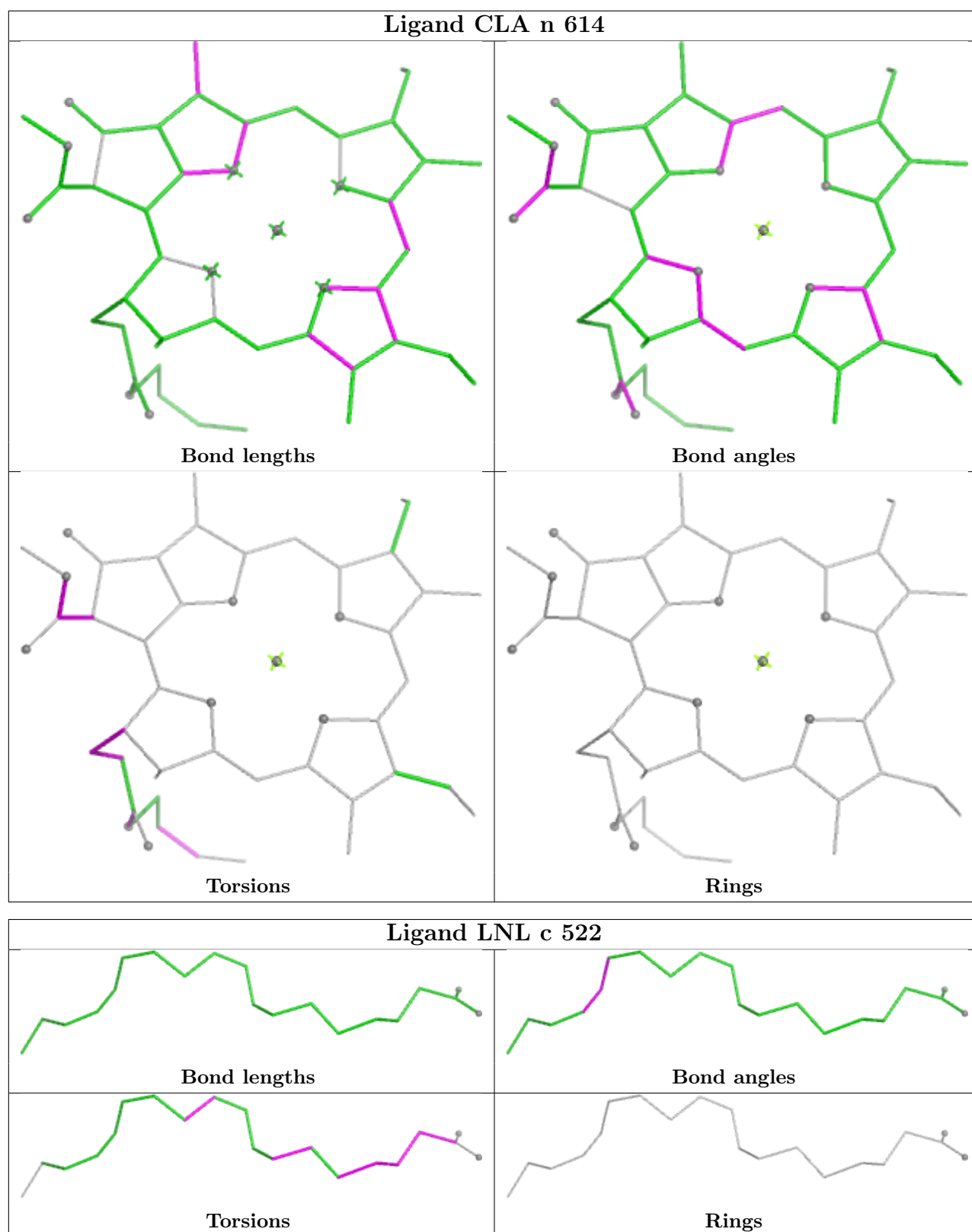


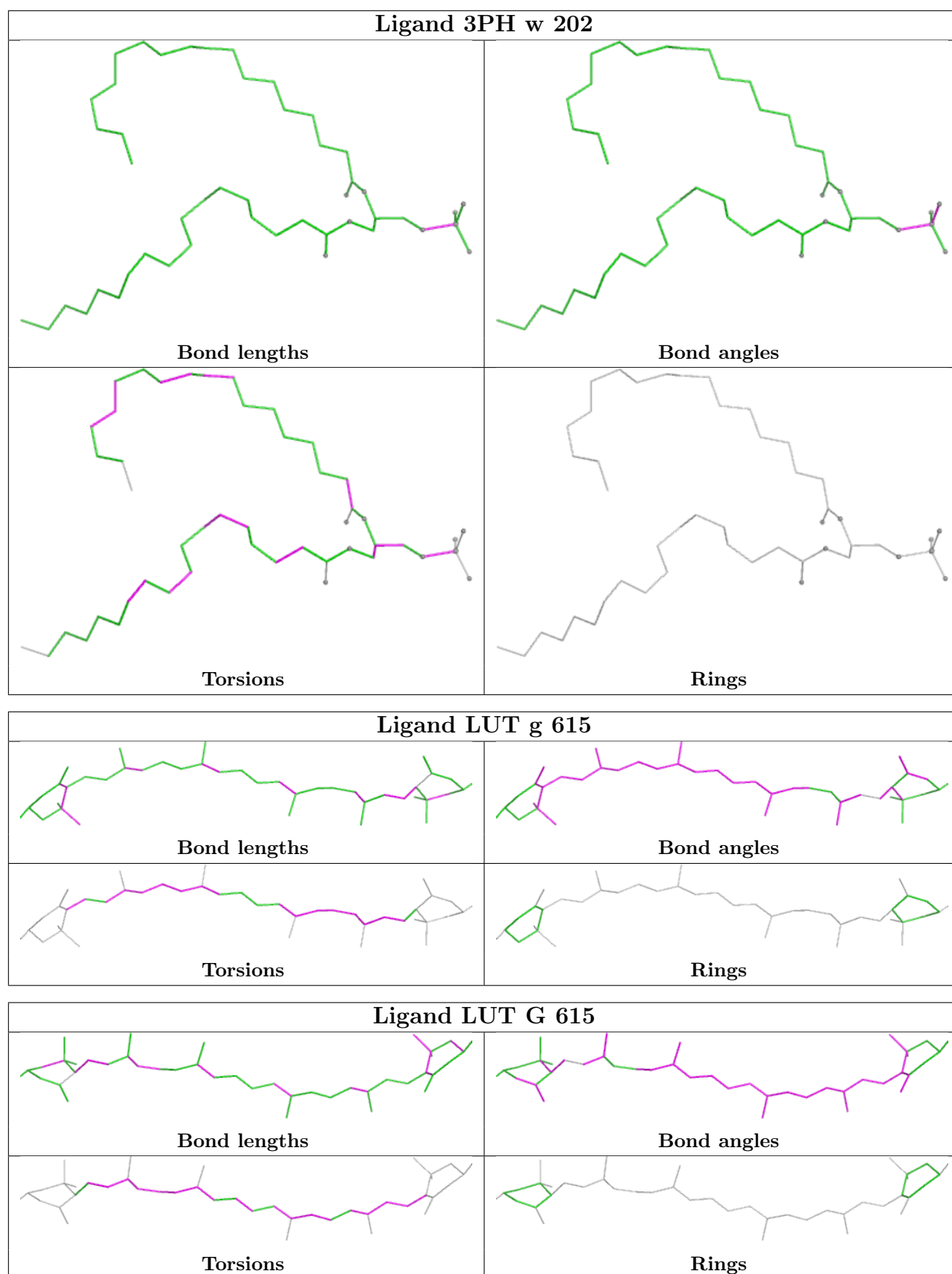


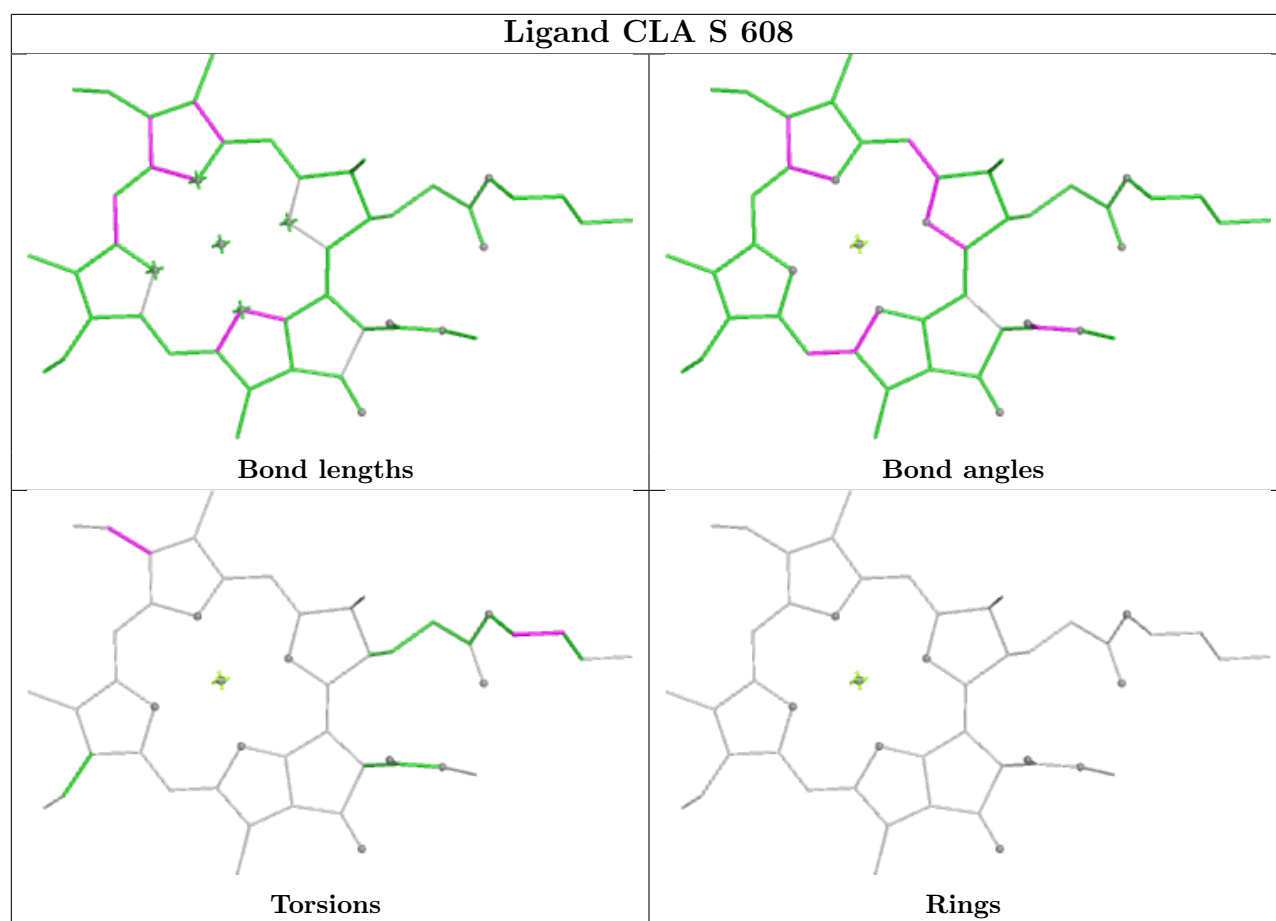


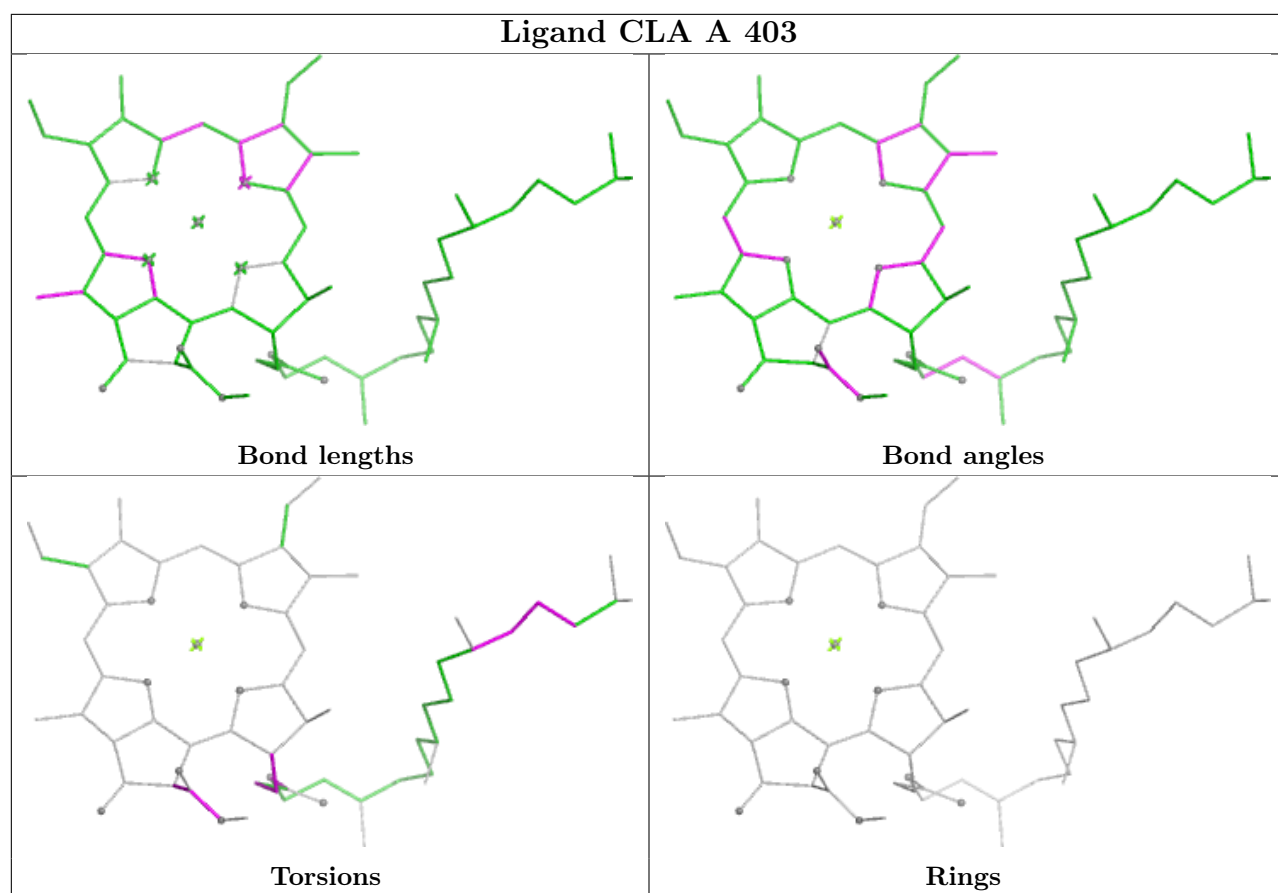


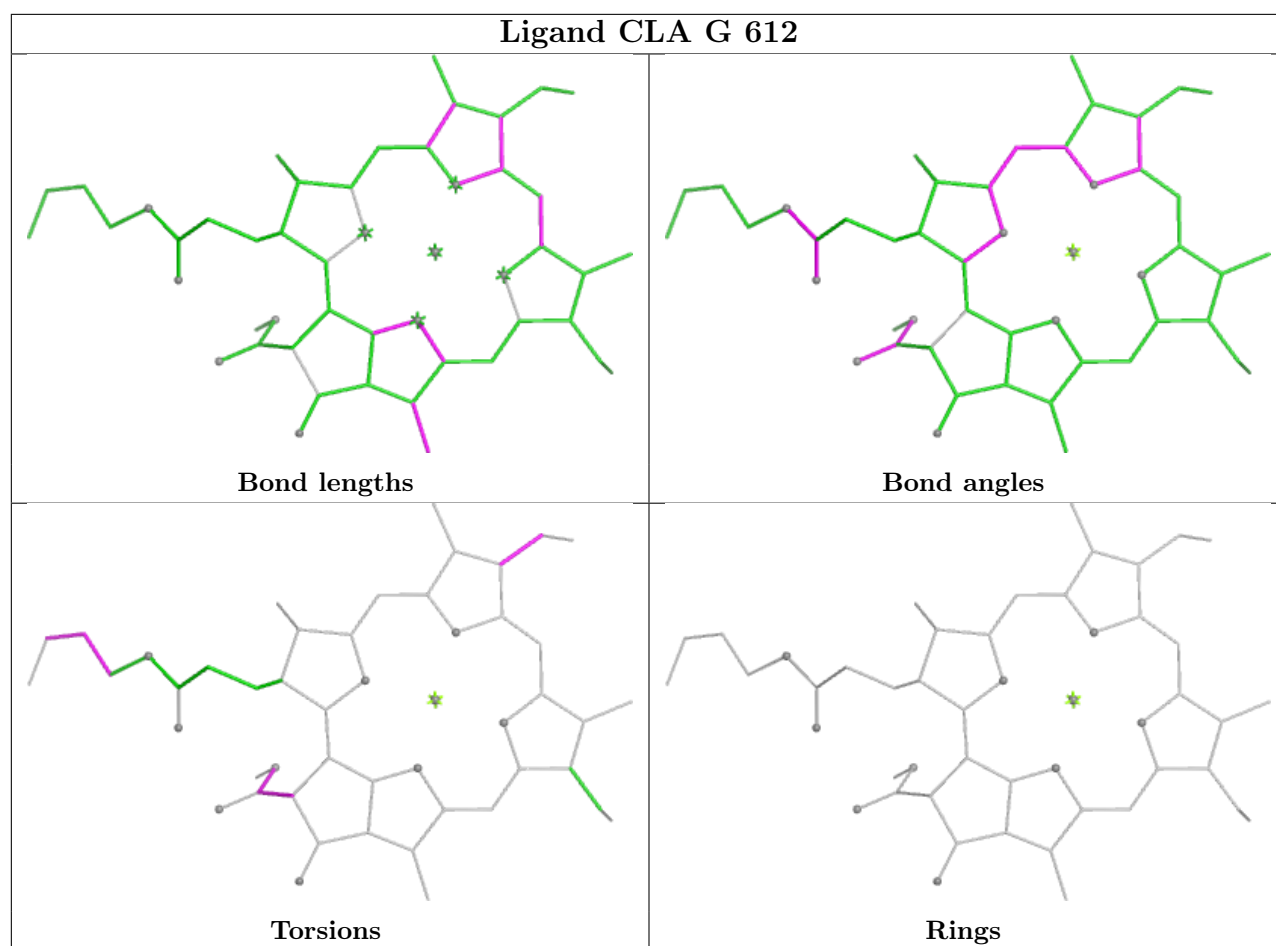


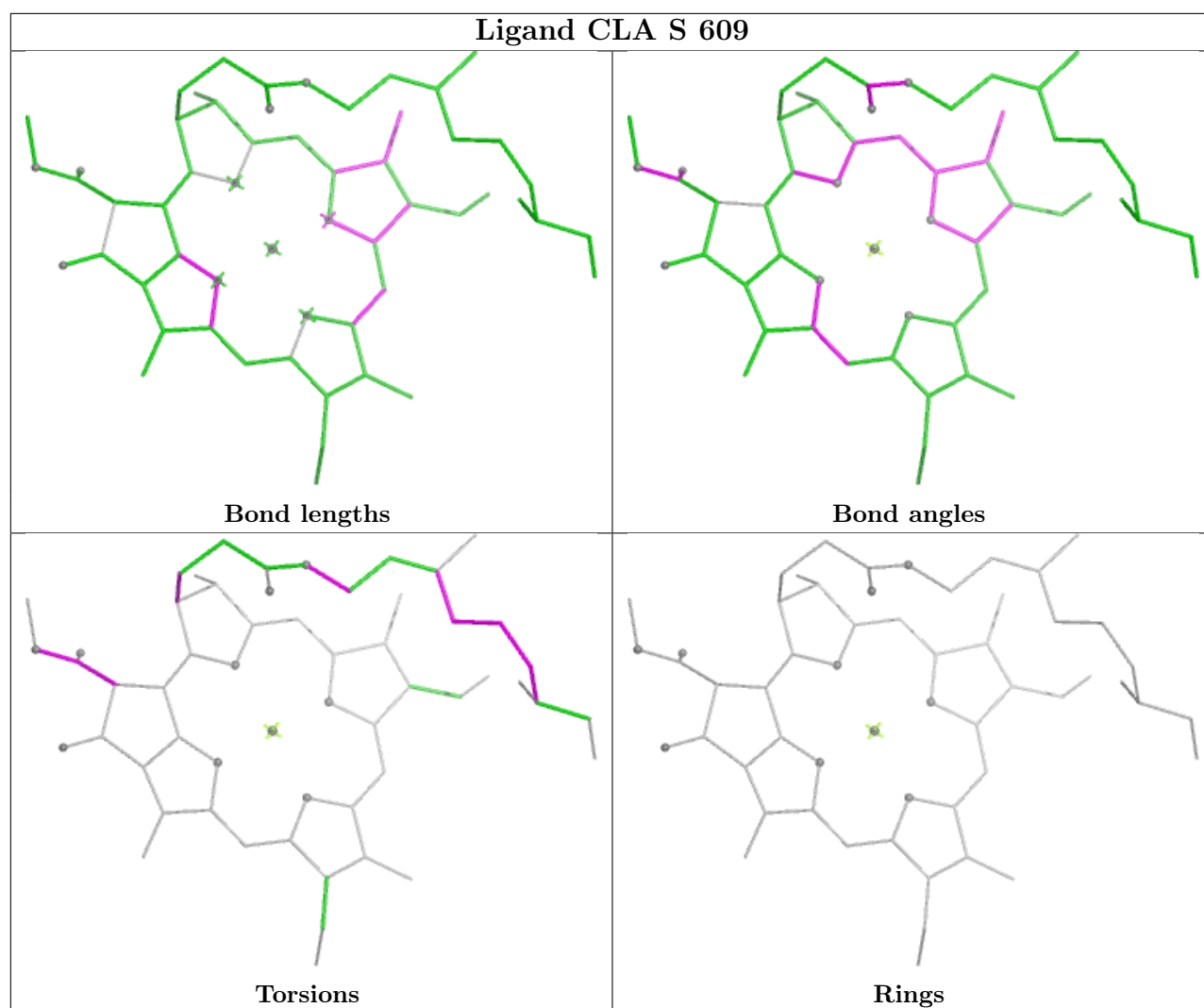


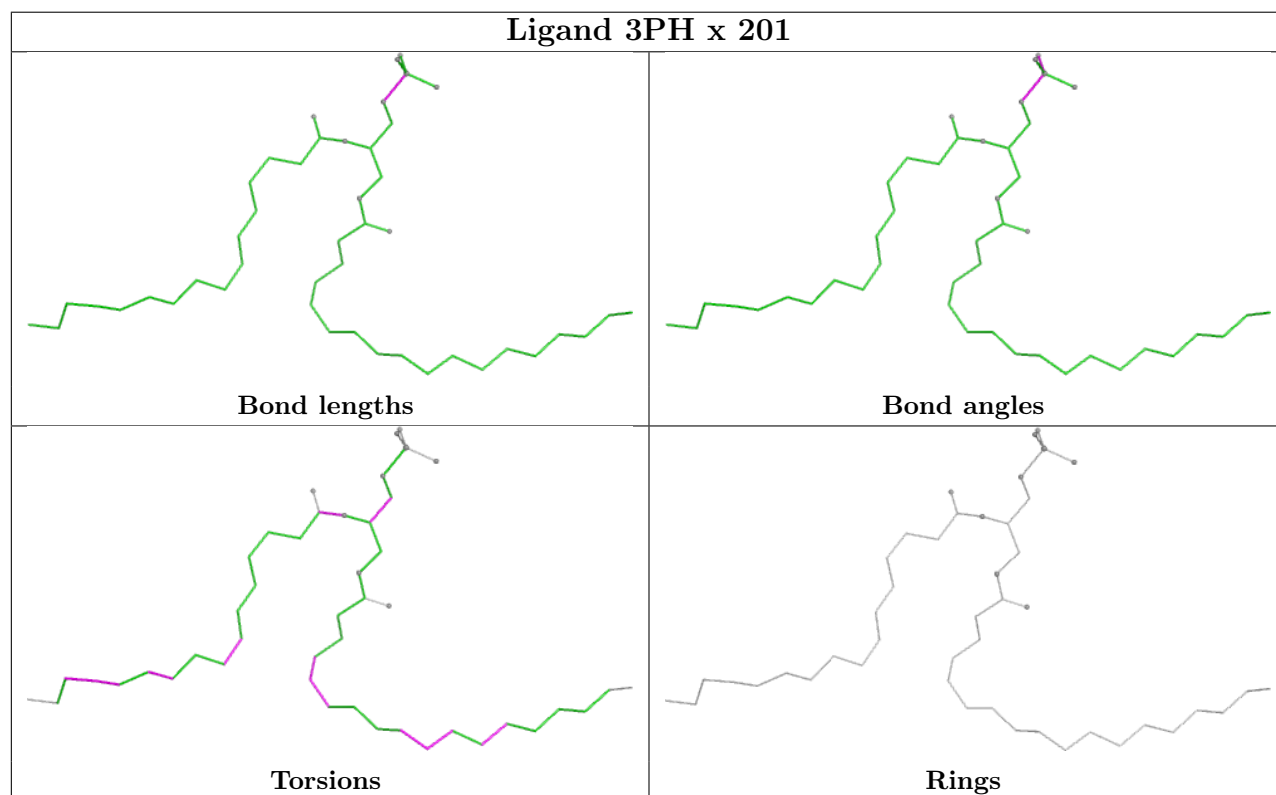
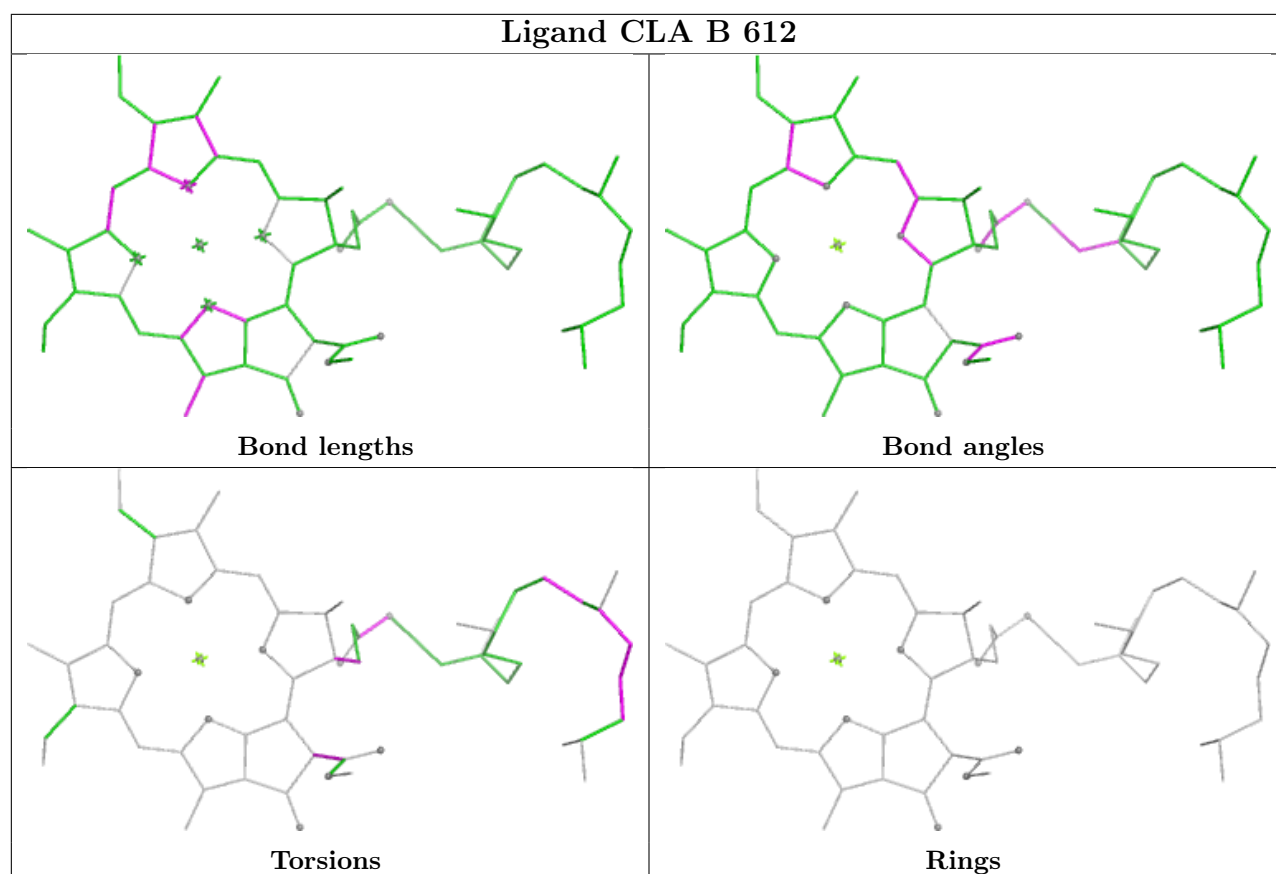


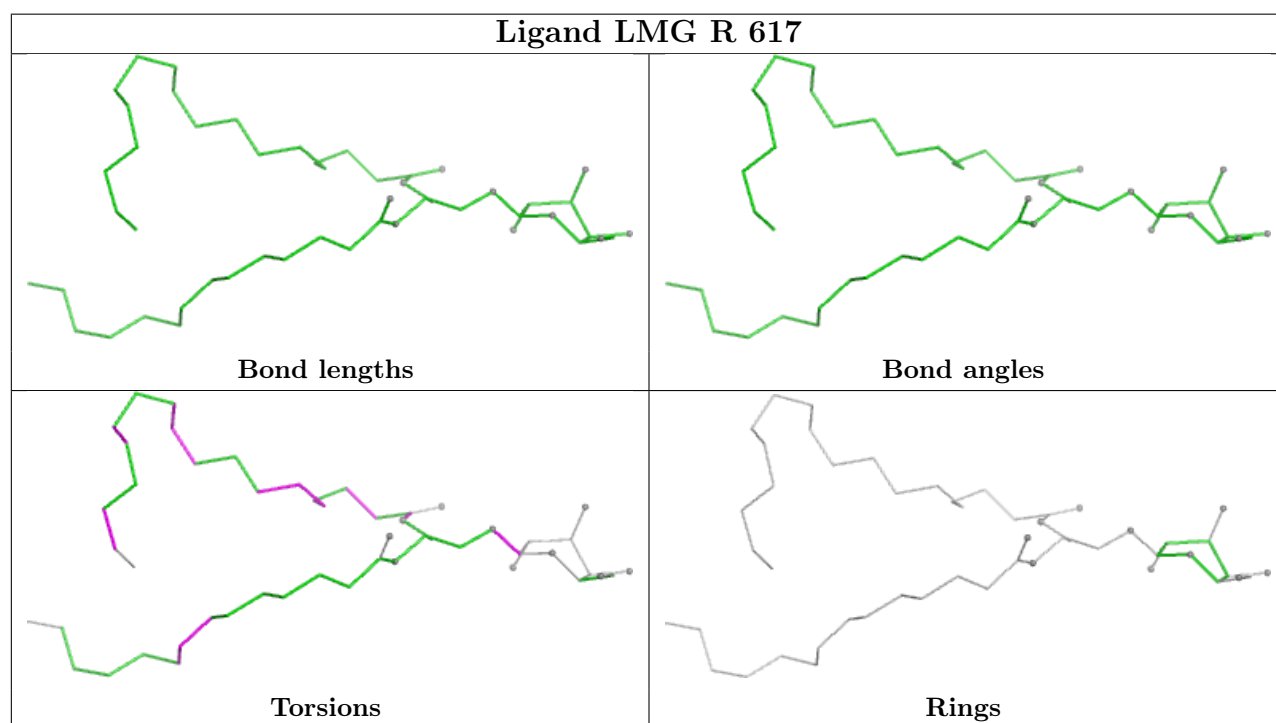
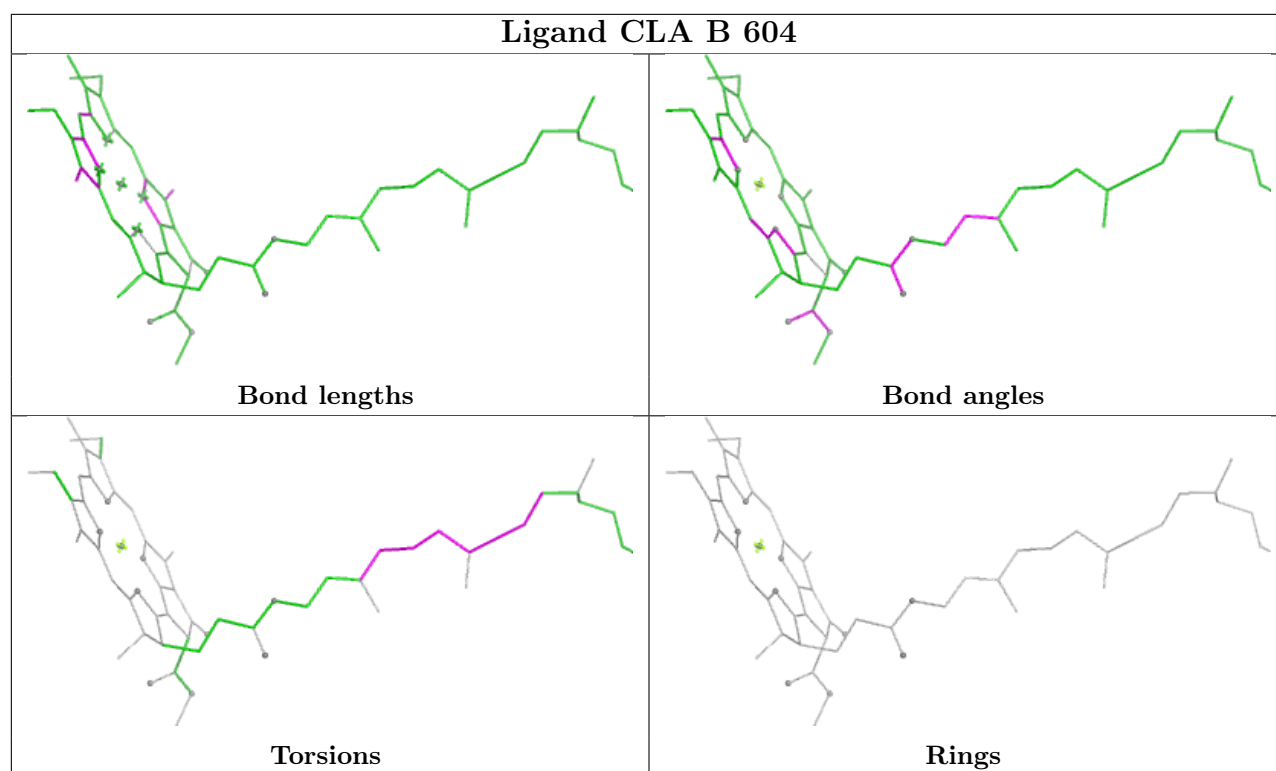


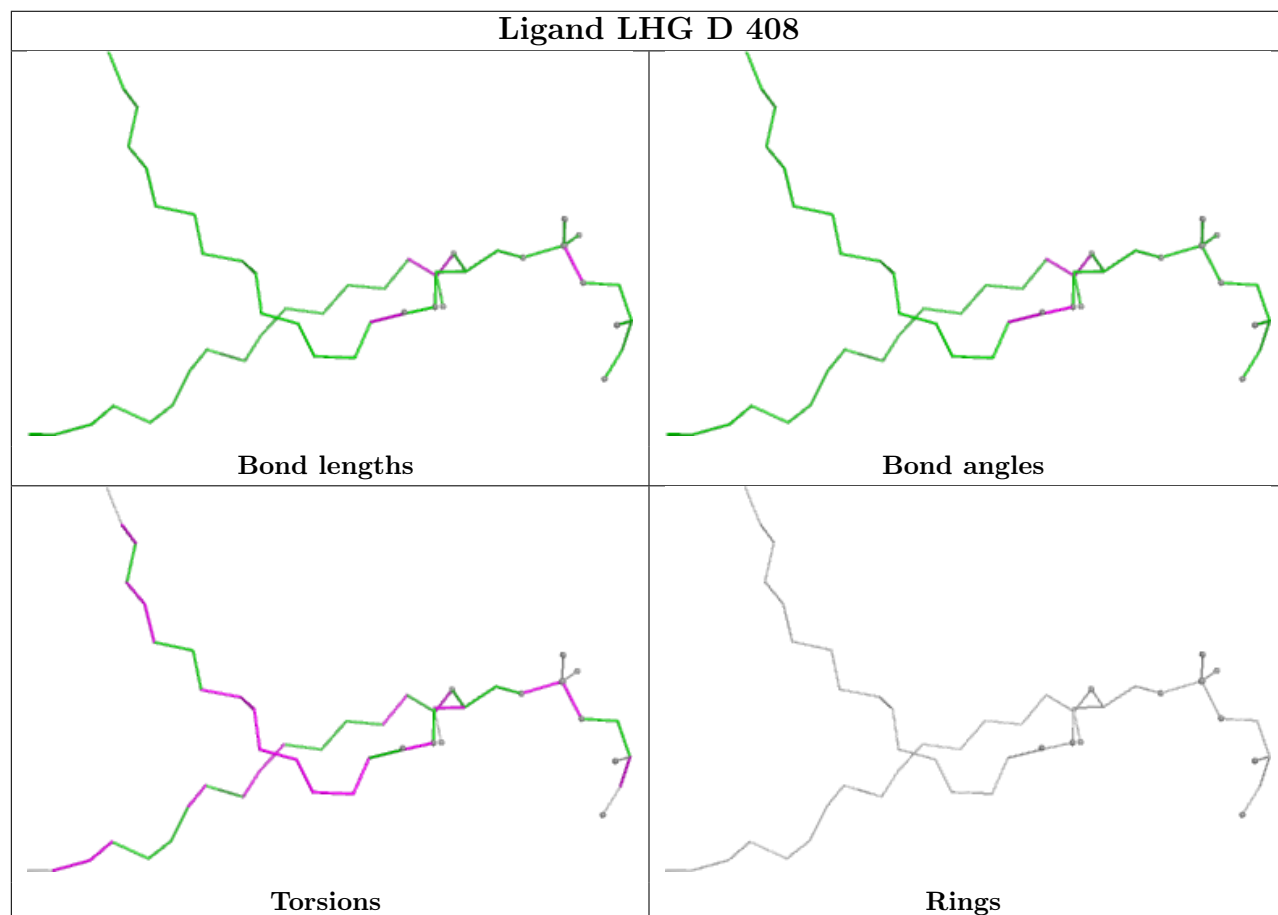
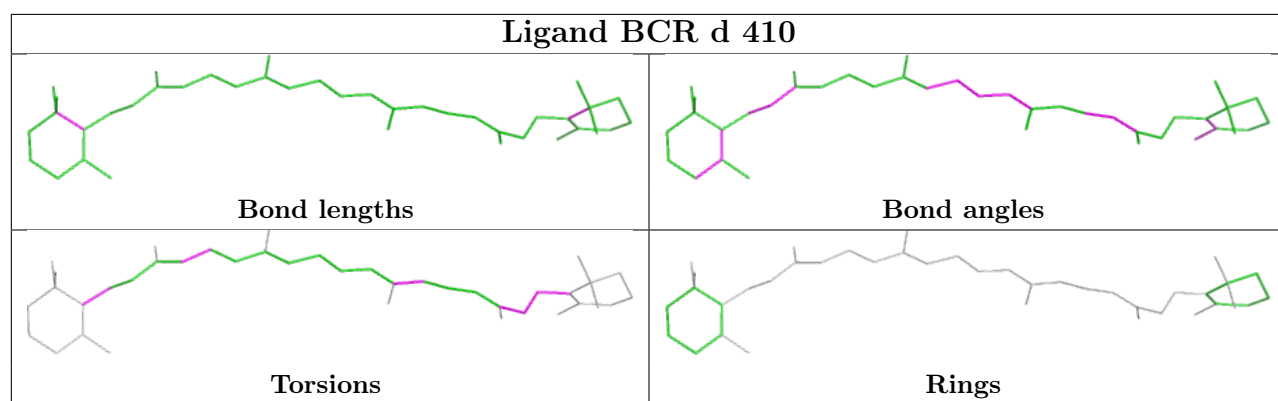


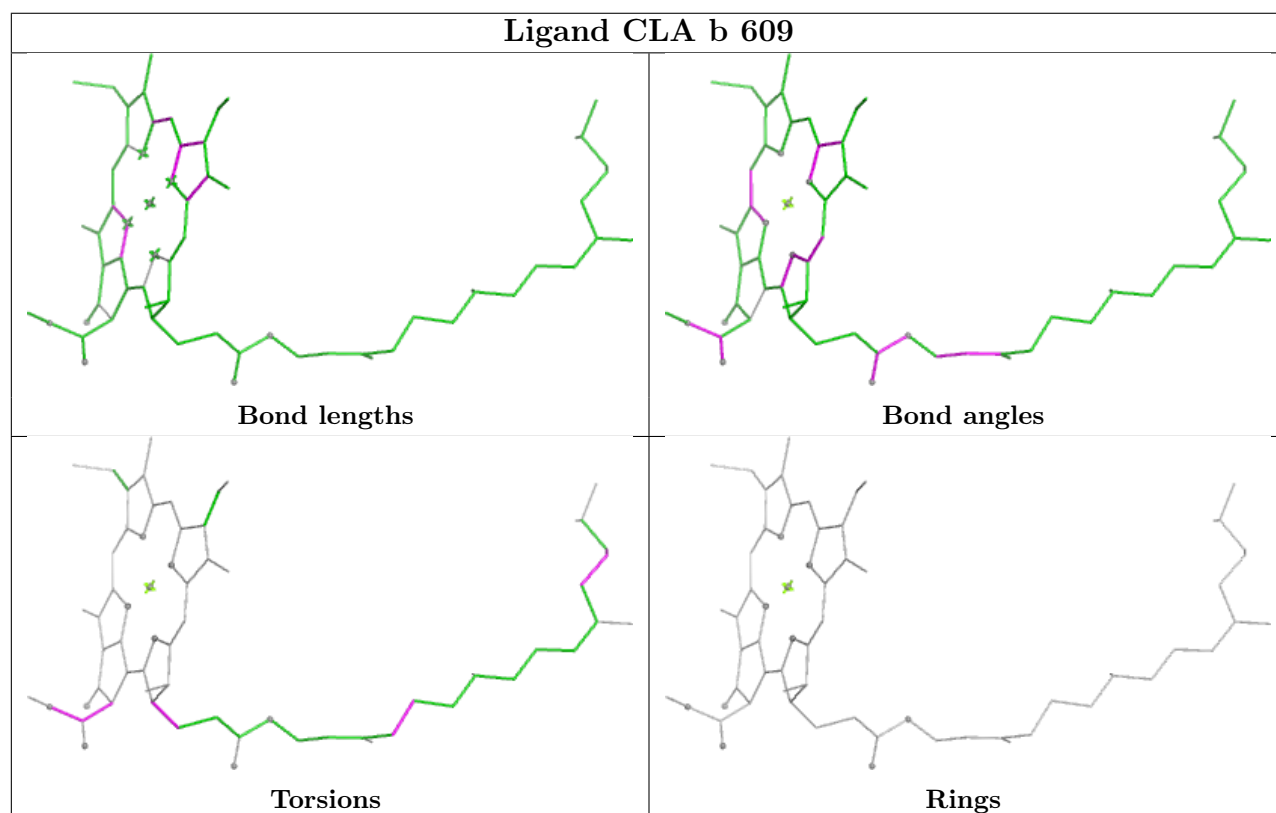
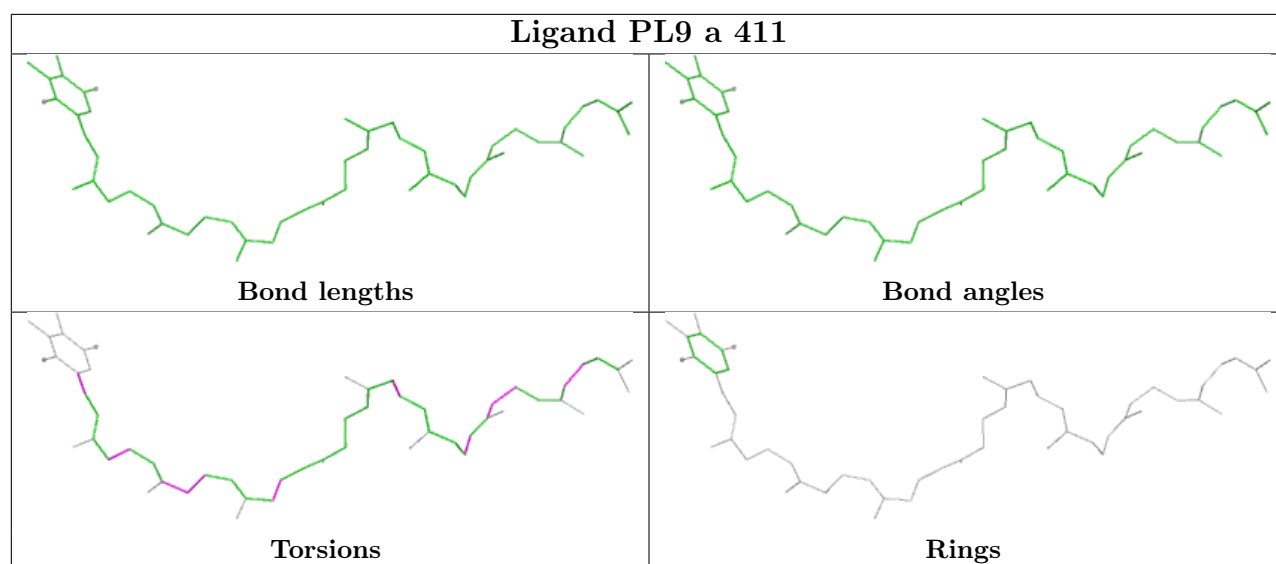


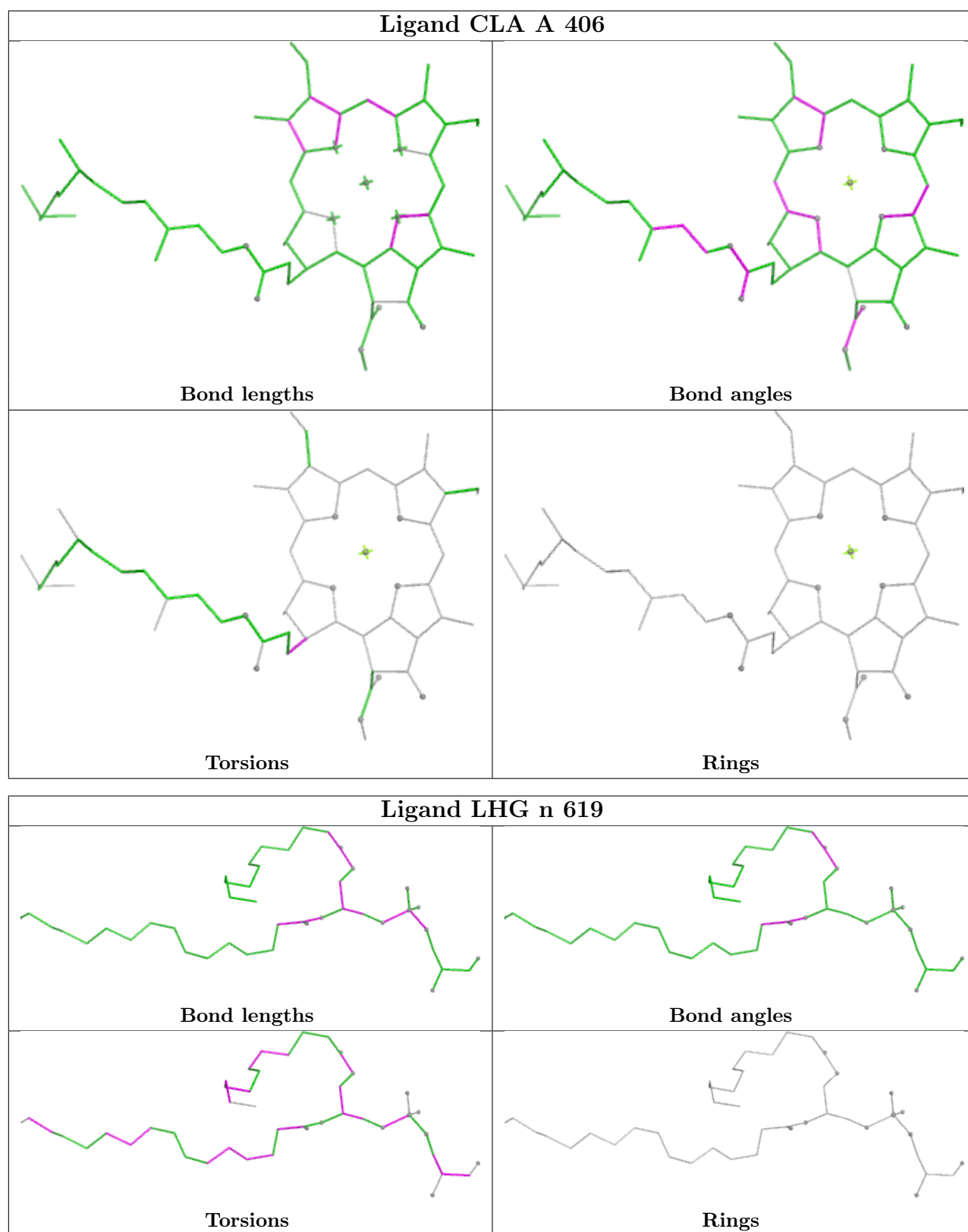


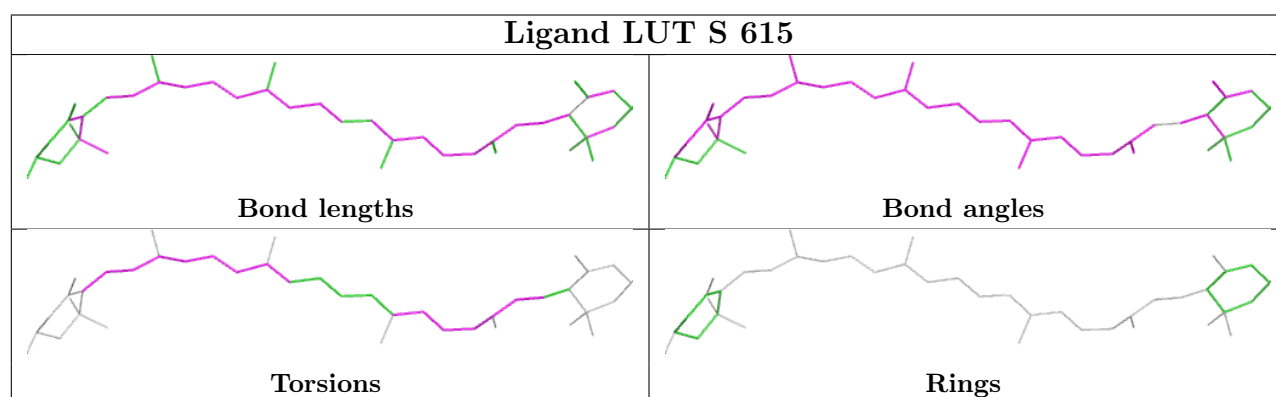
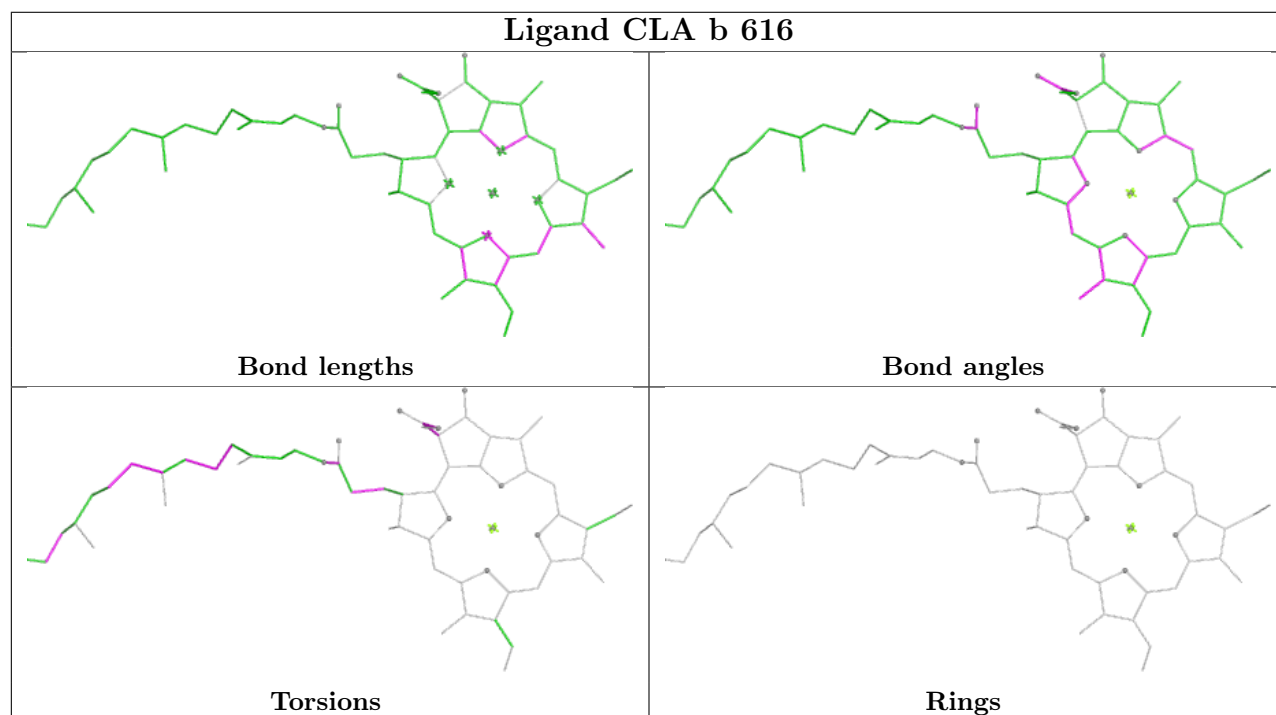
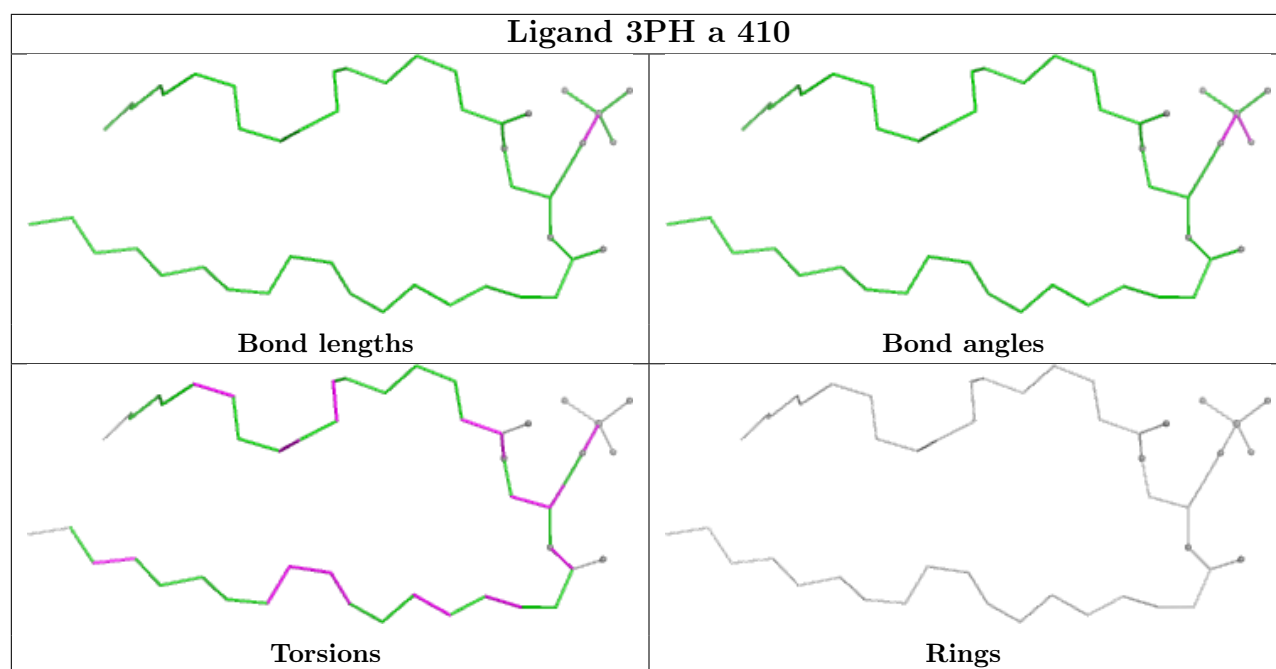


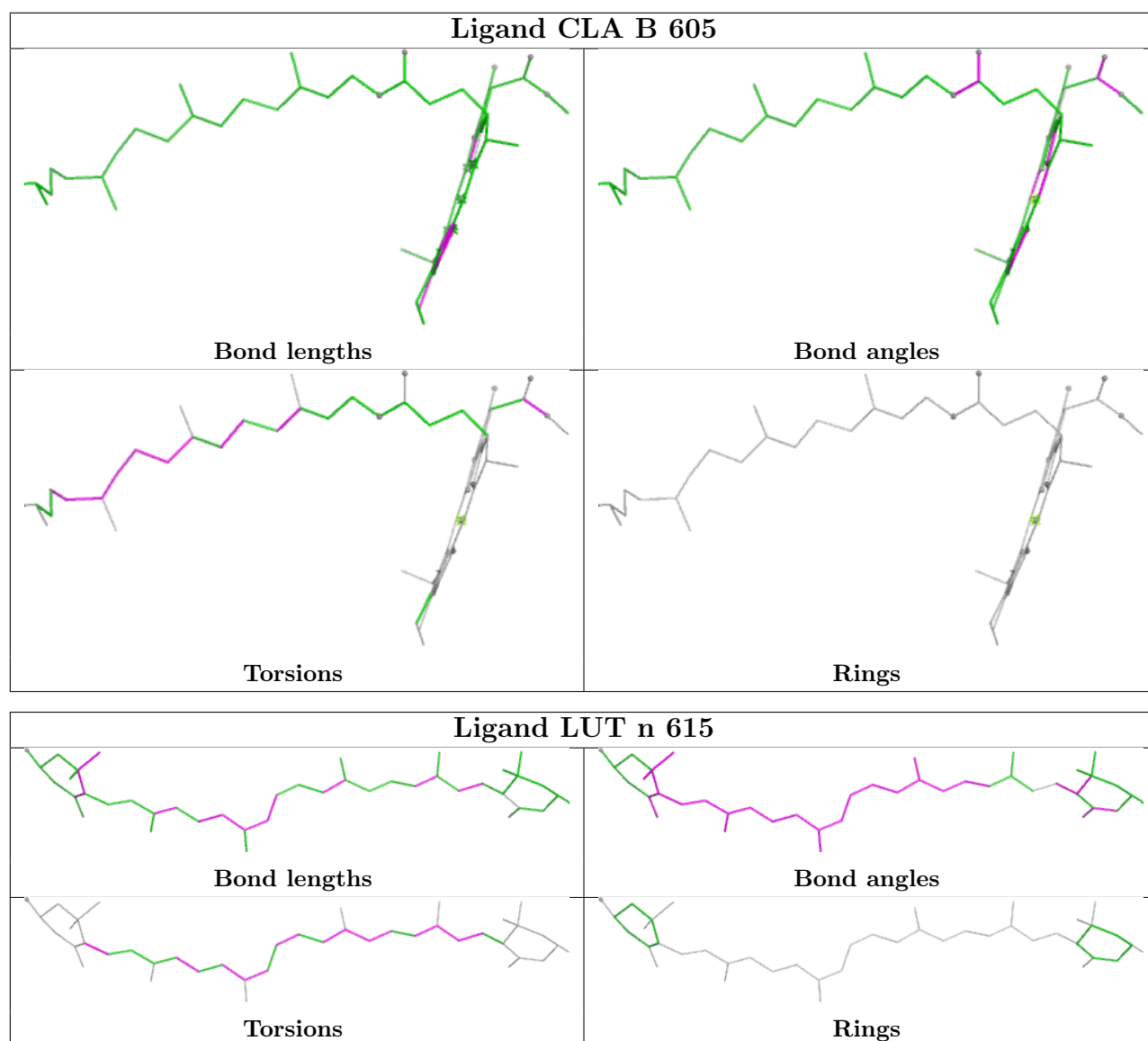


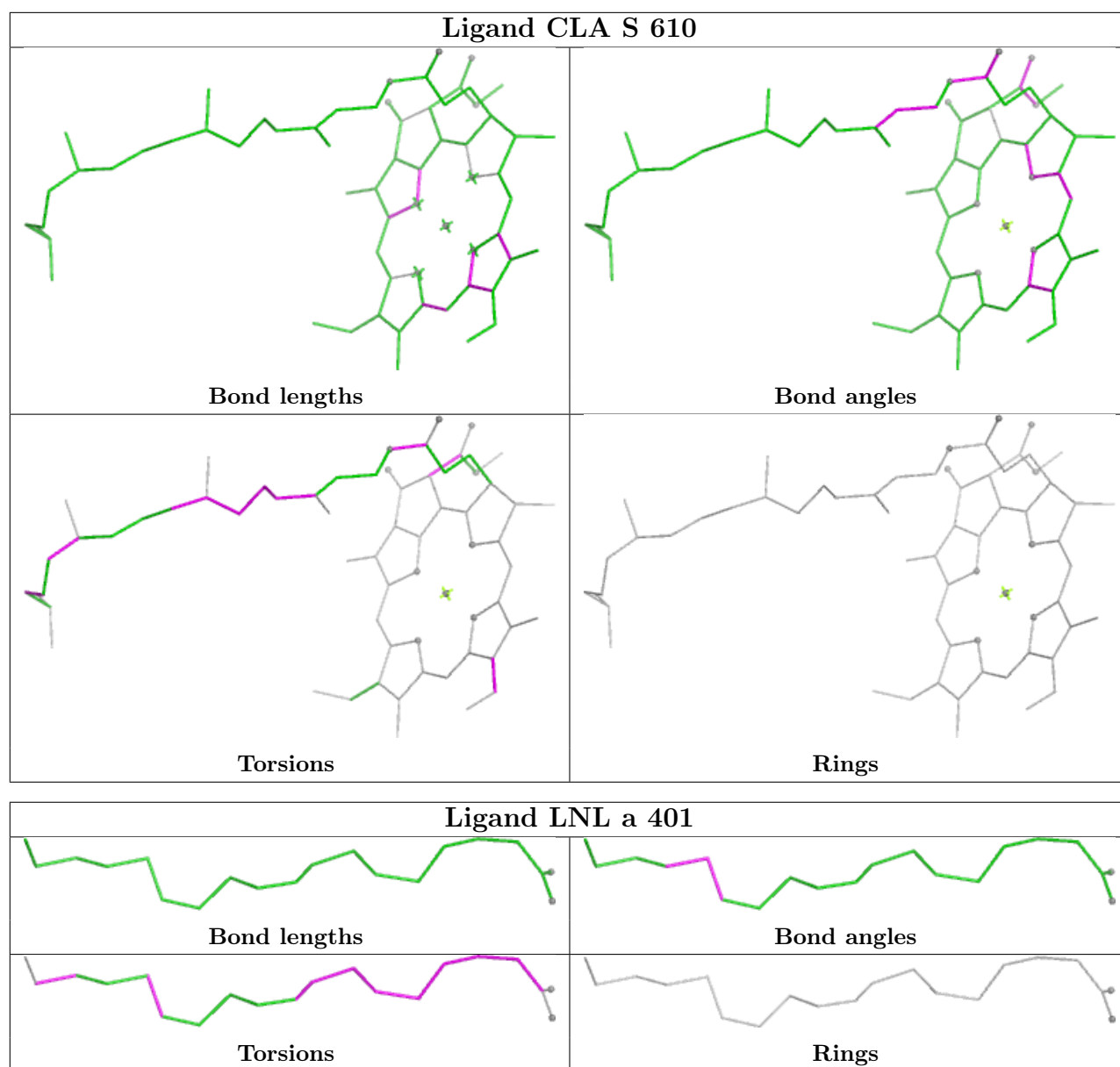


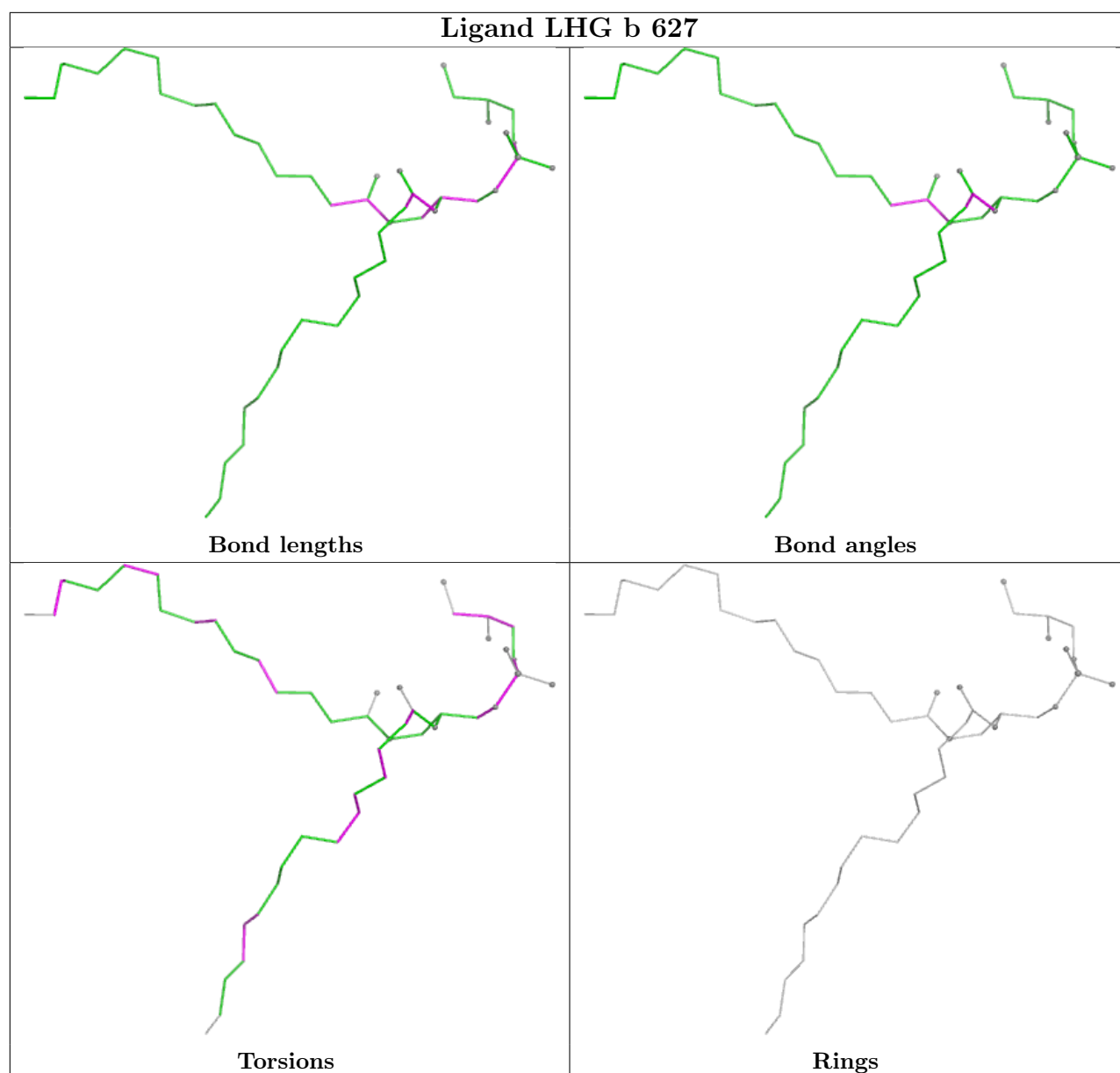


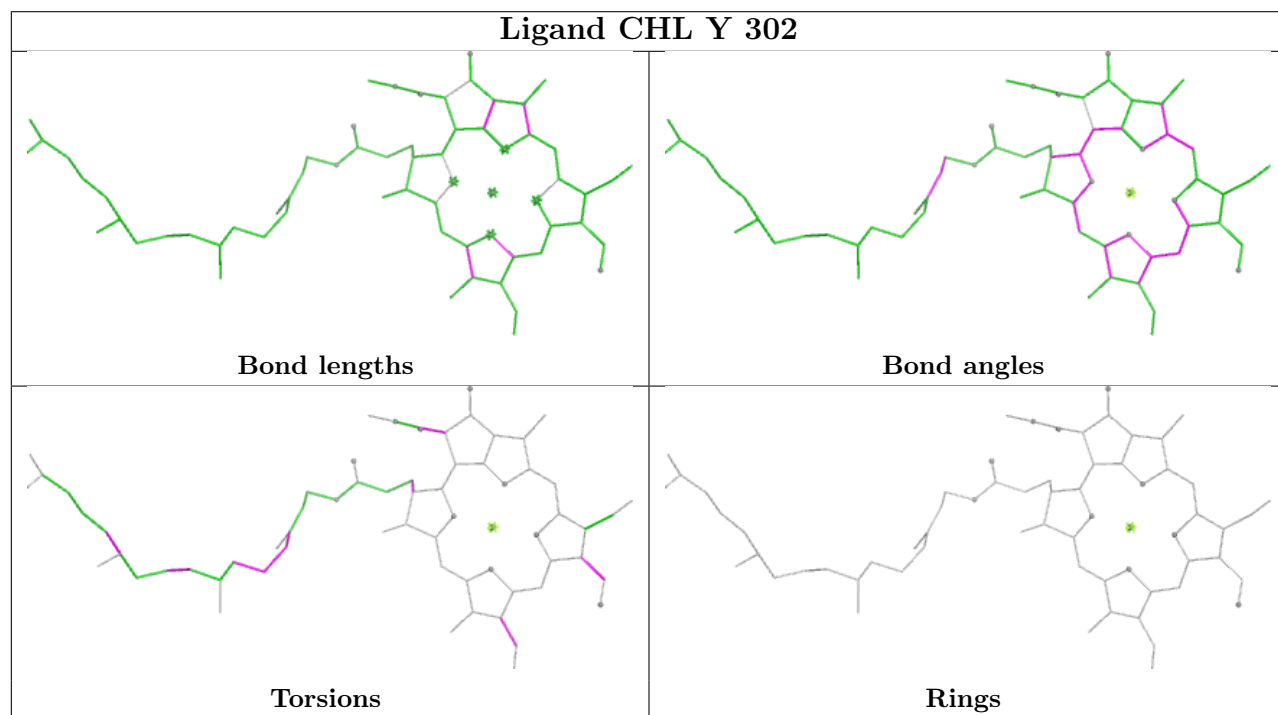
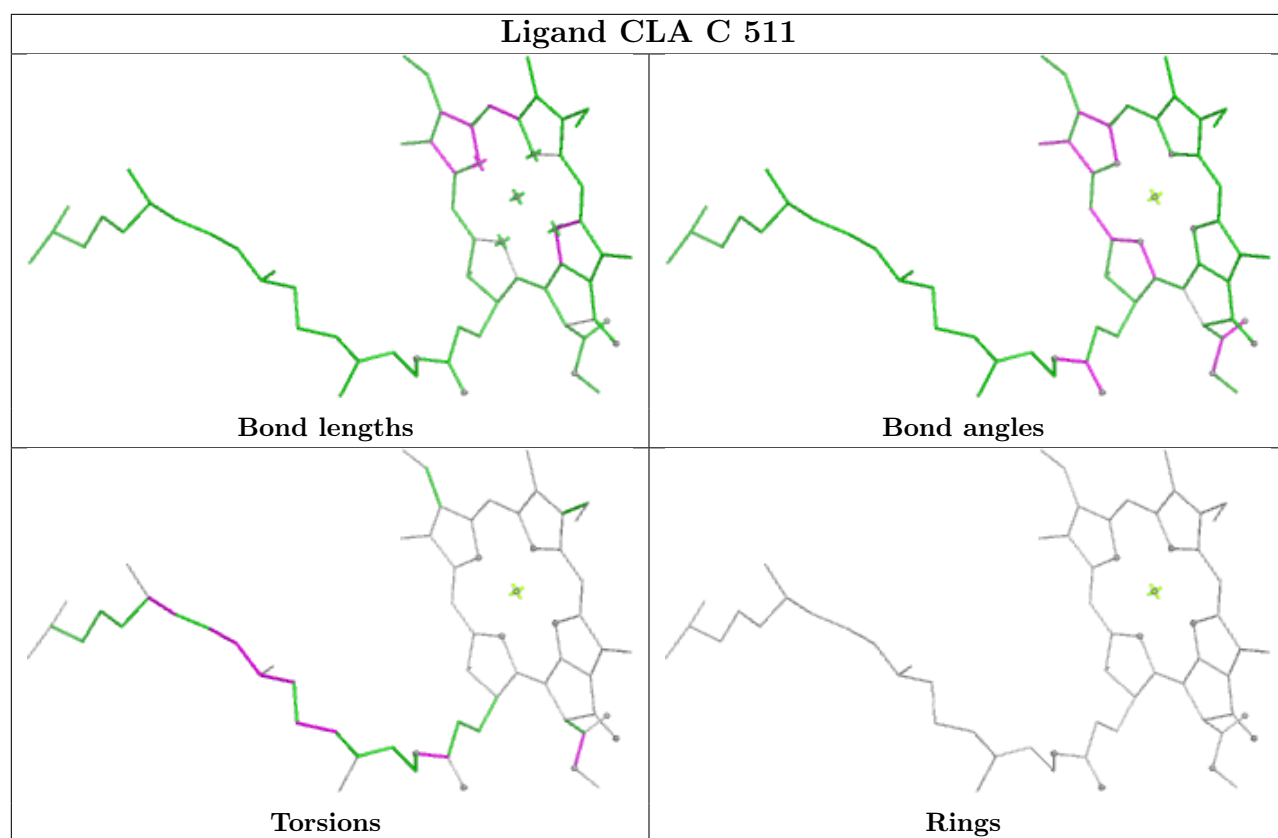


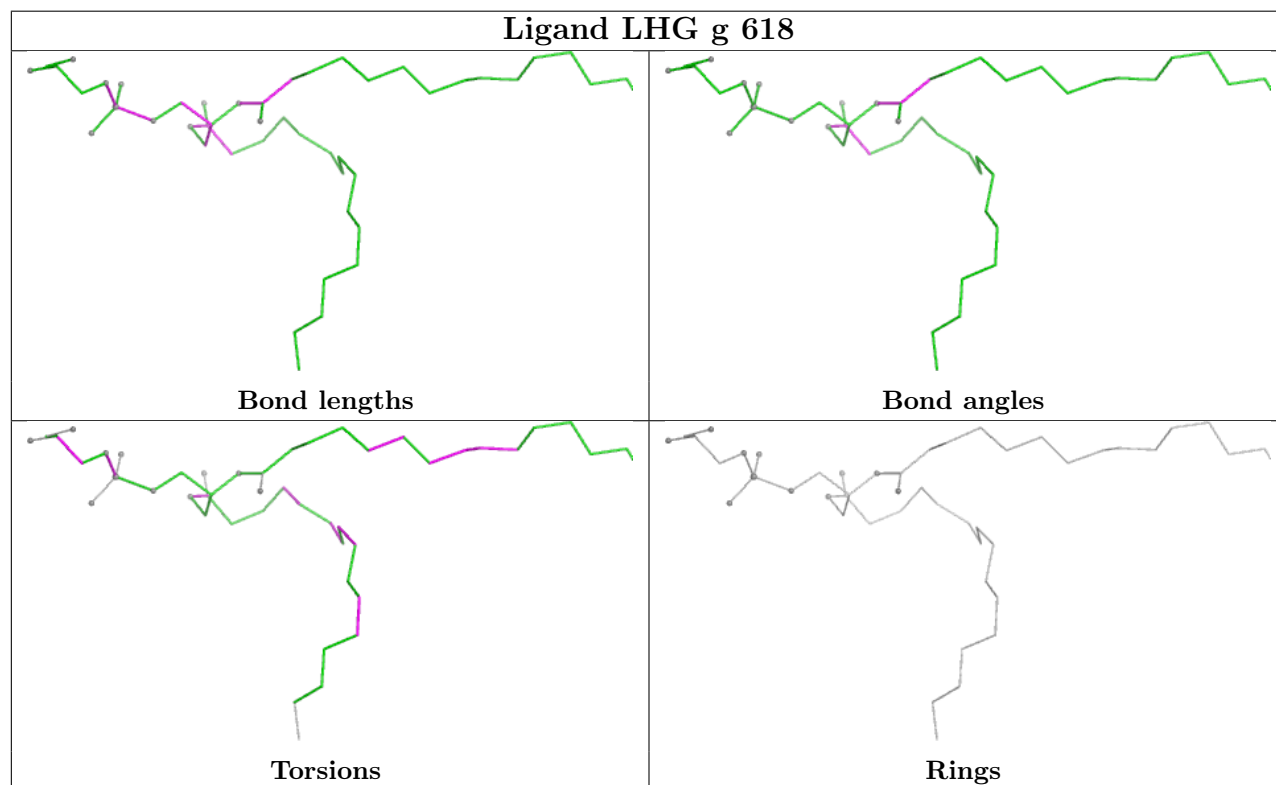
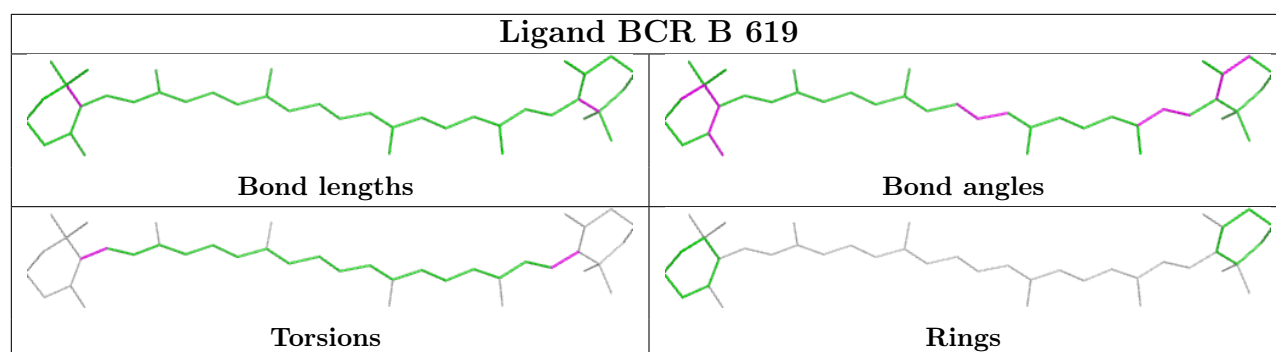


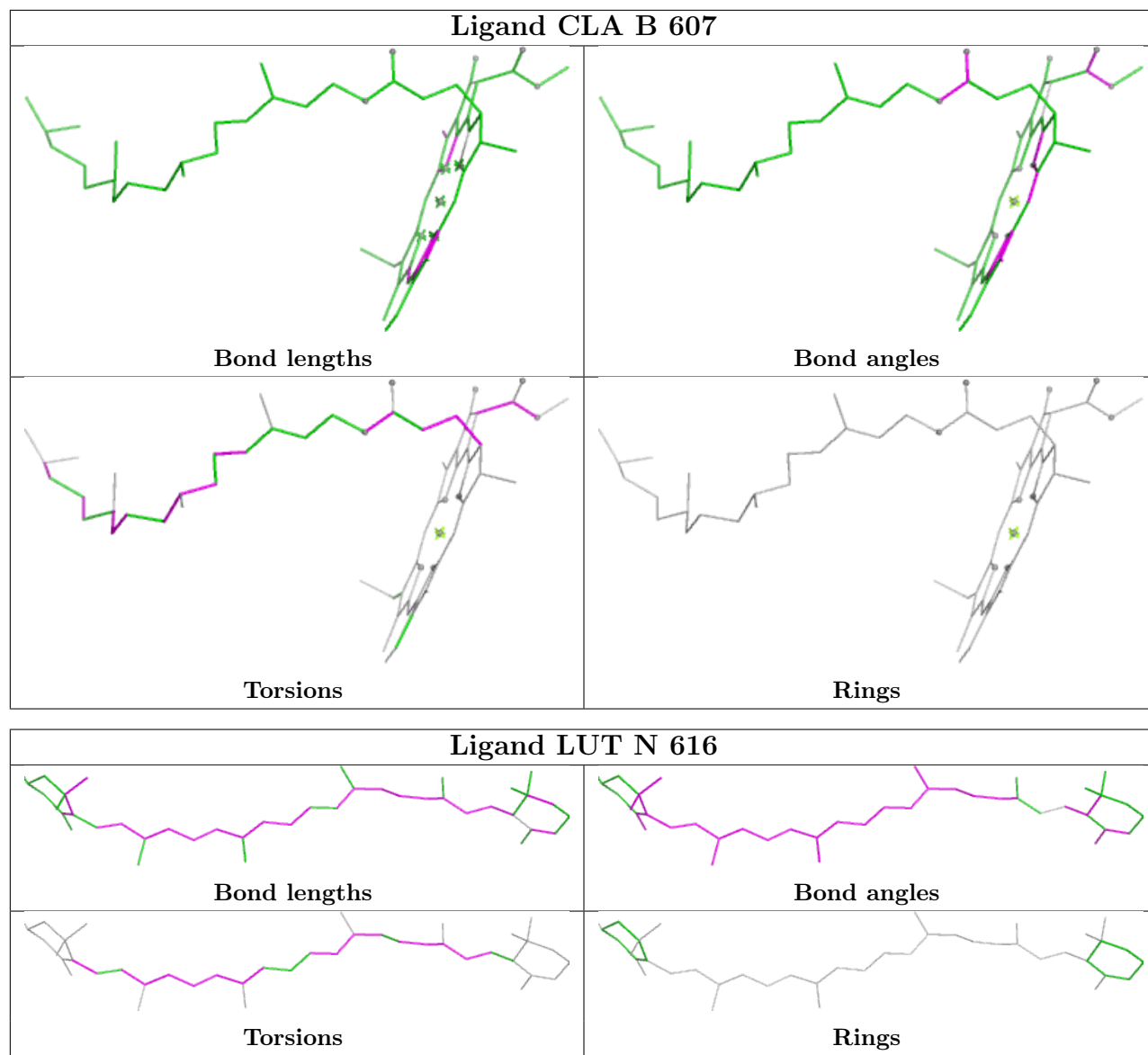


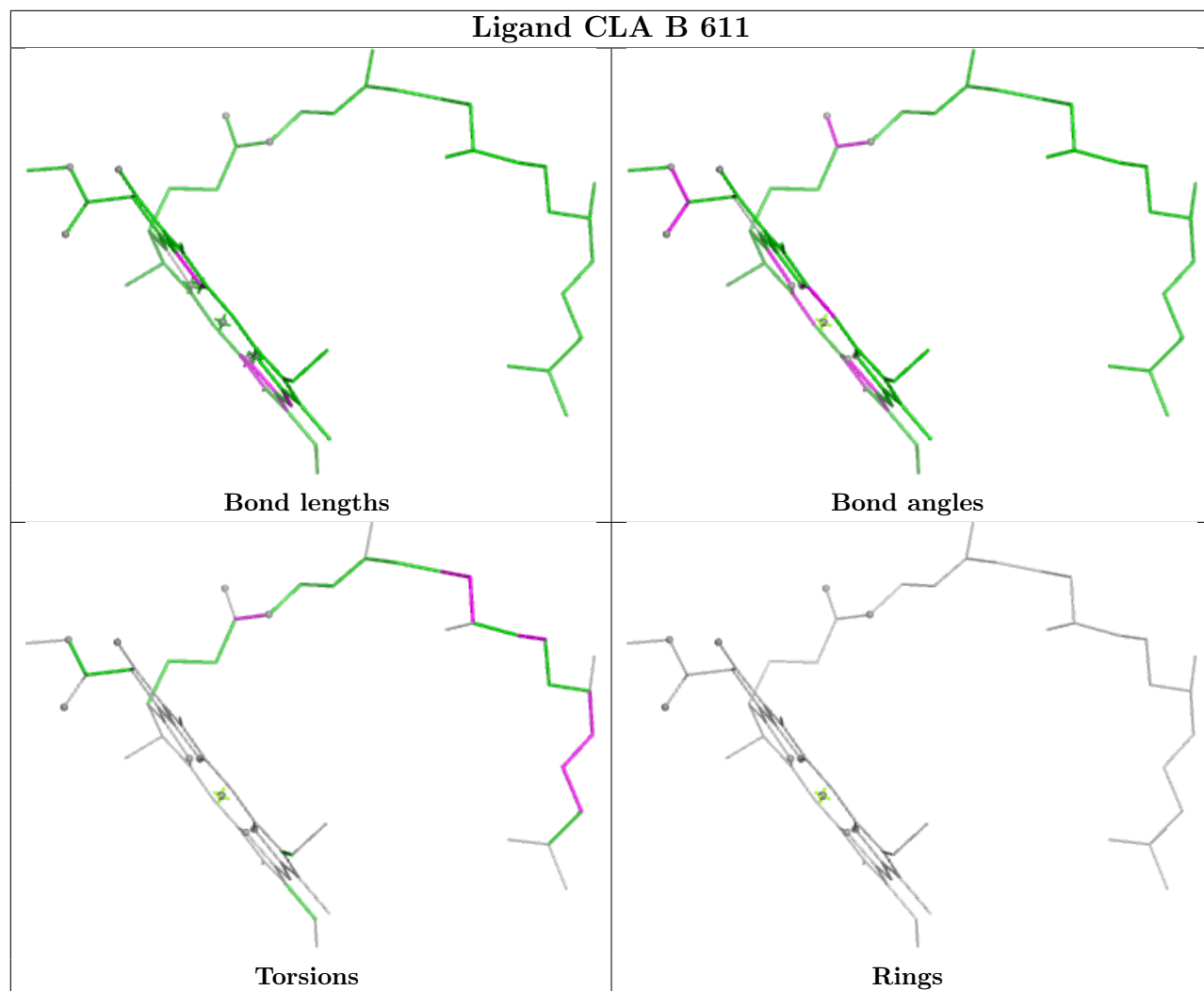


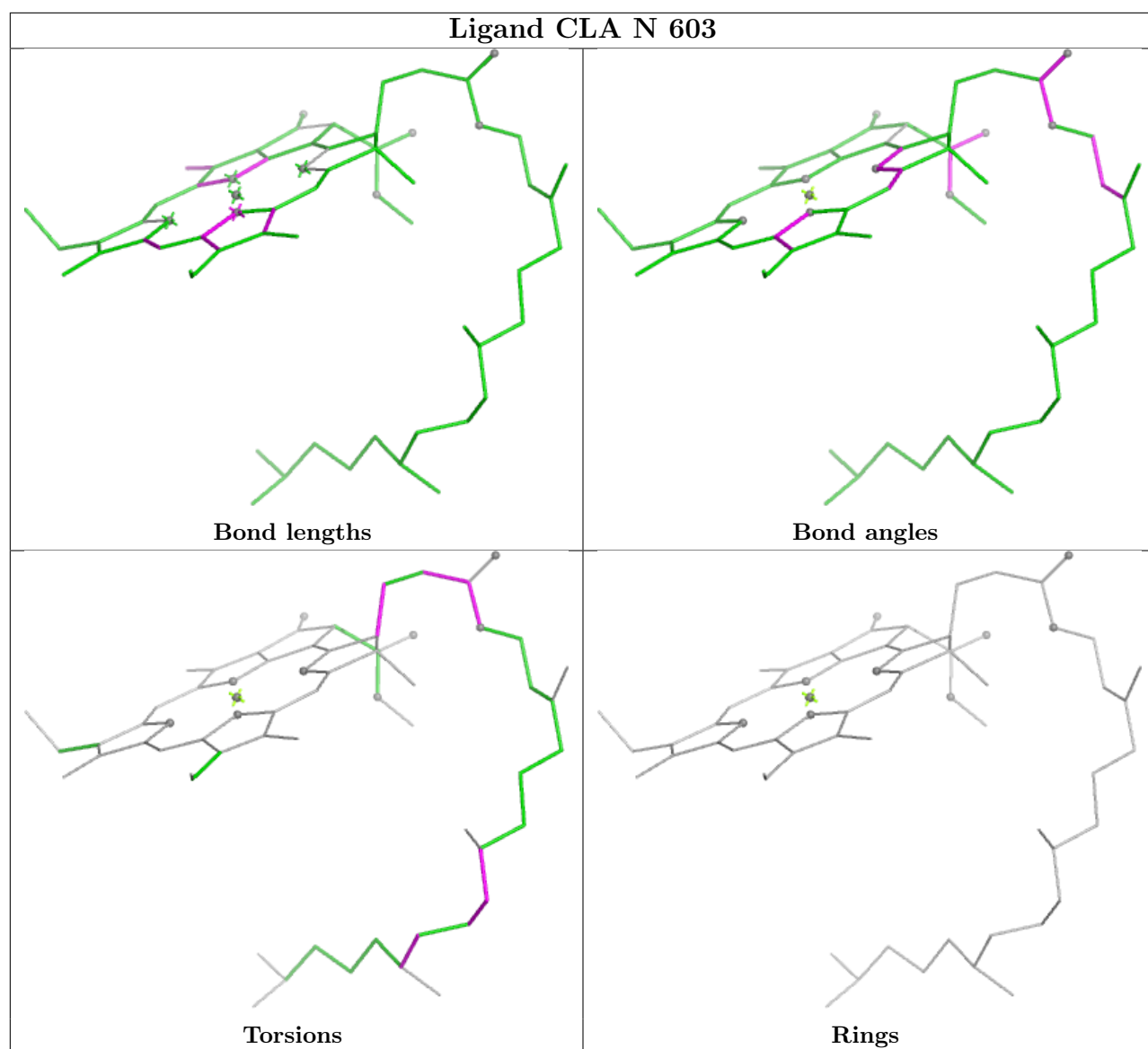


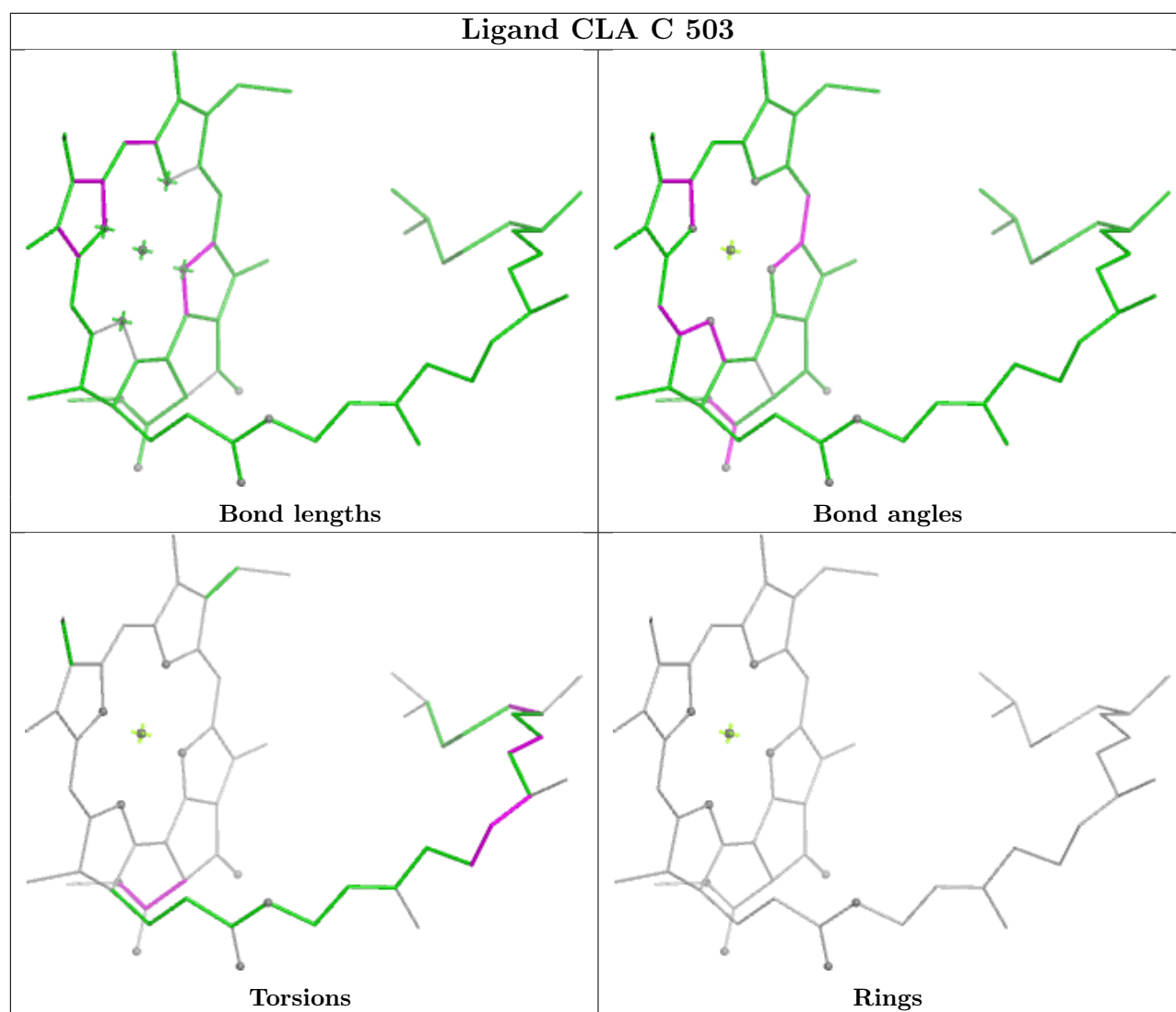




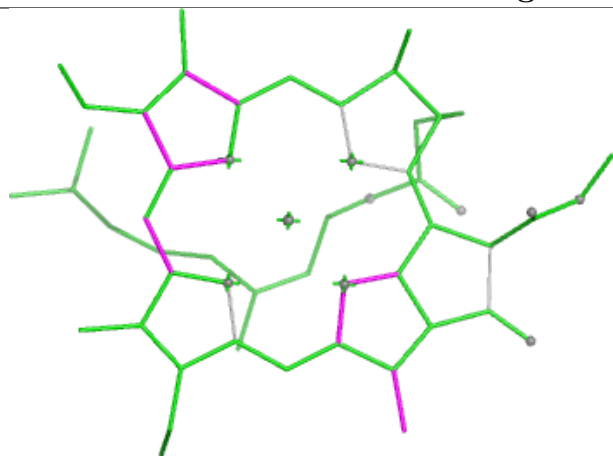




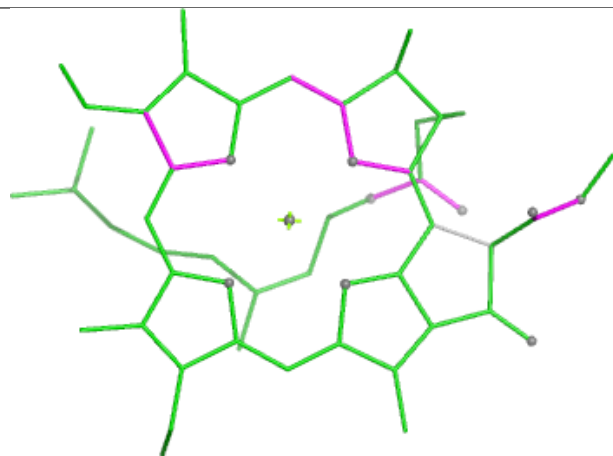




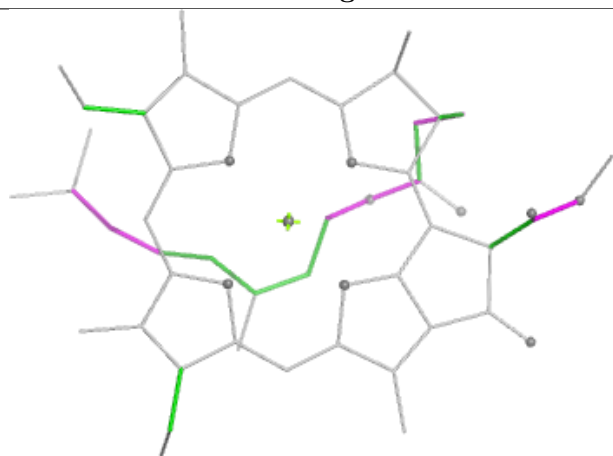
Ligand CLA S 612



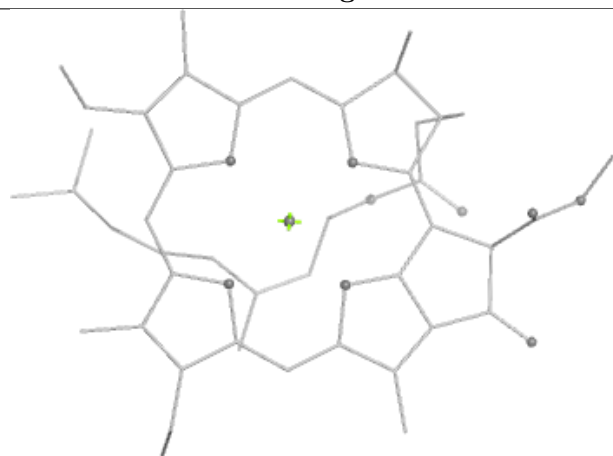
Bond lengths



Bond angles

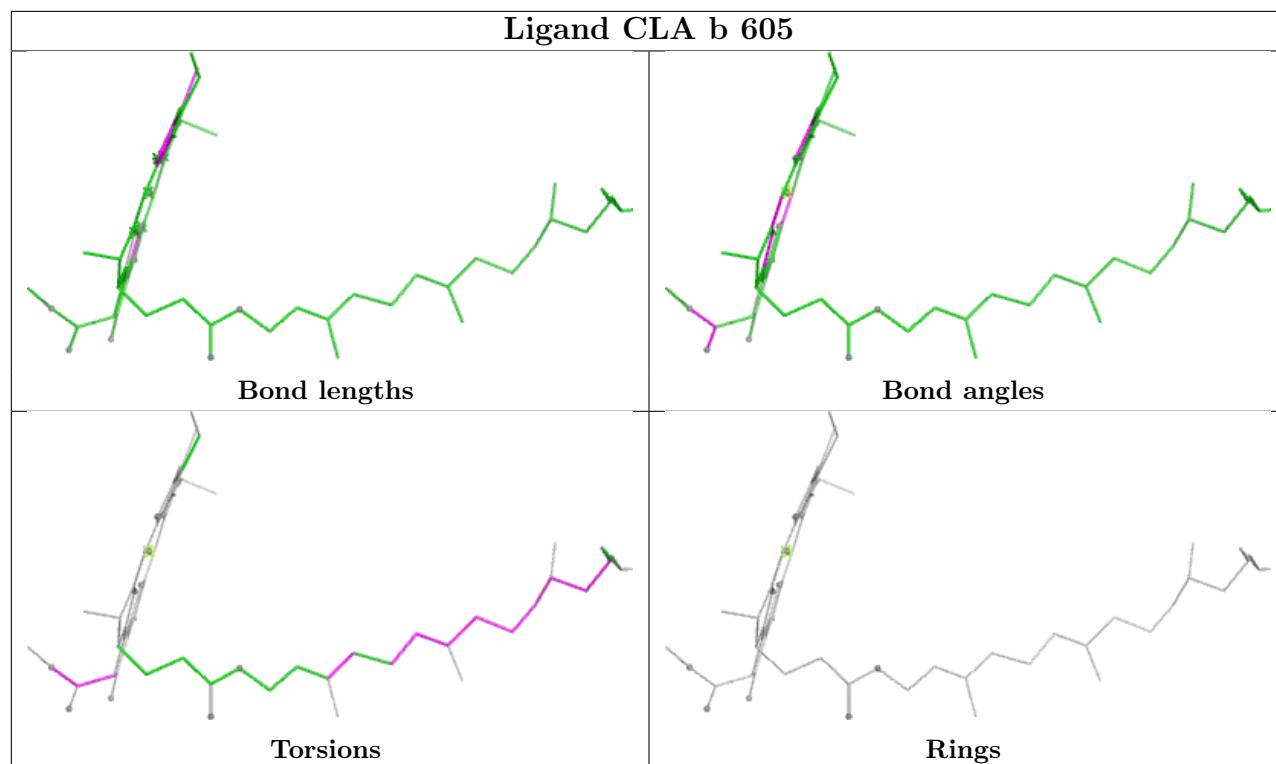


Torsions

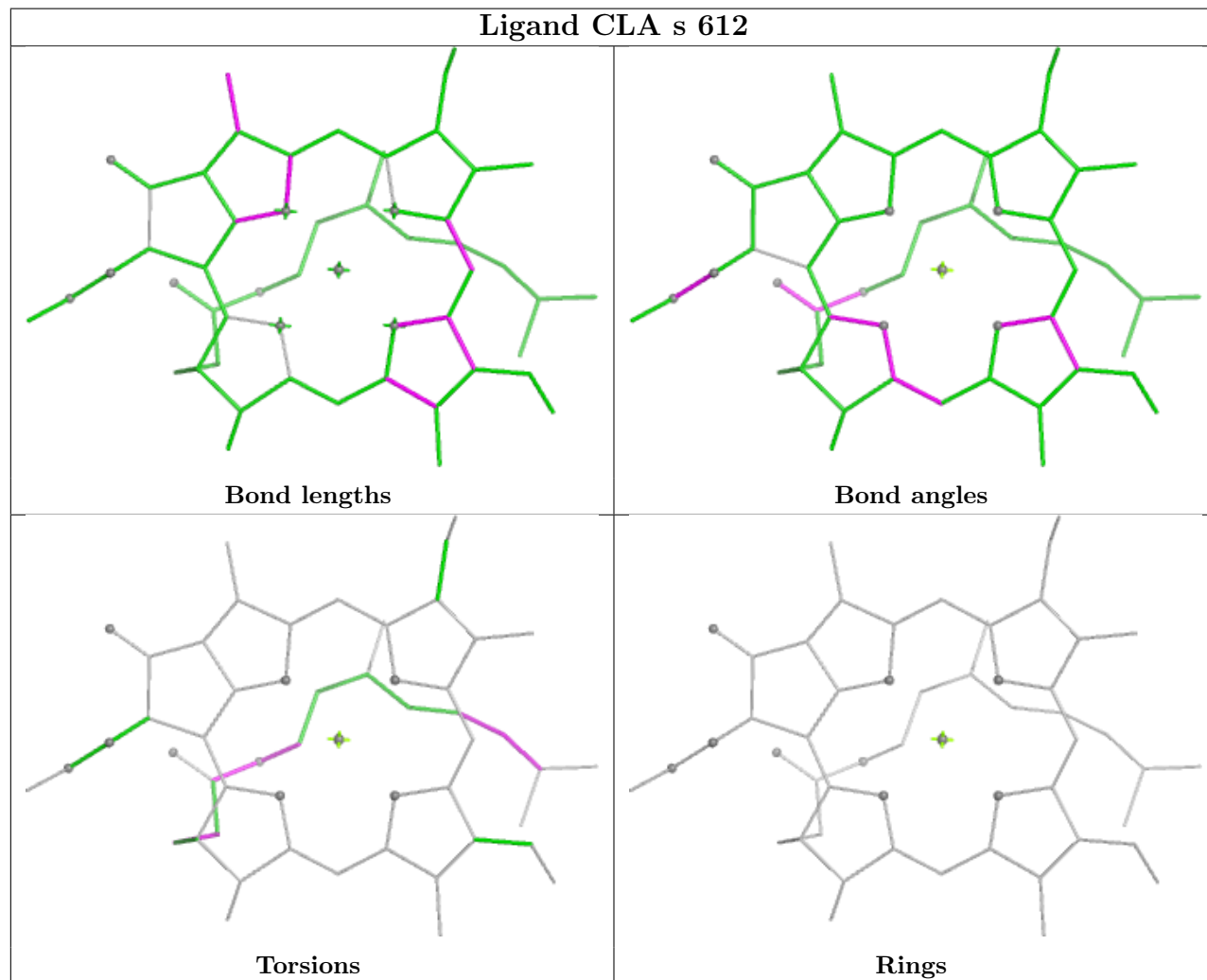


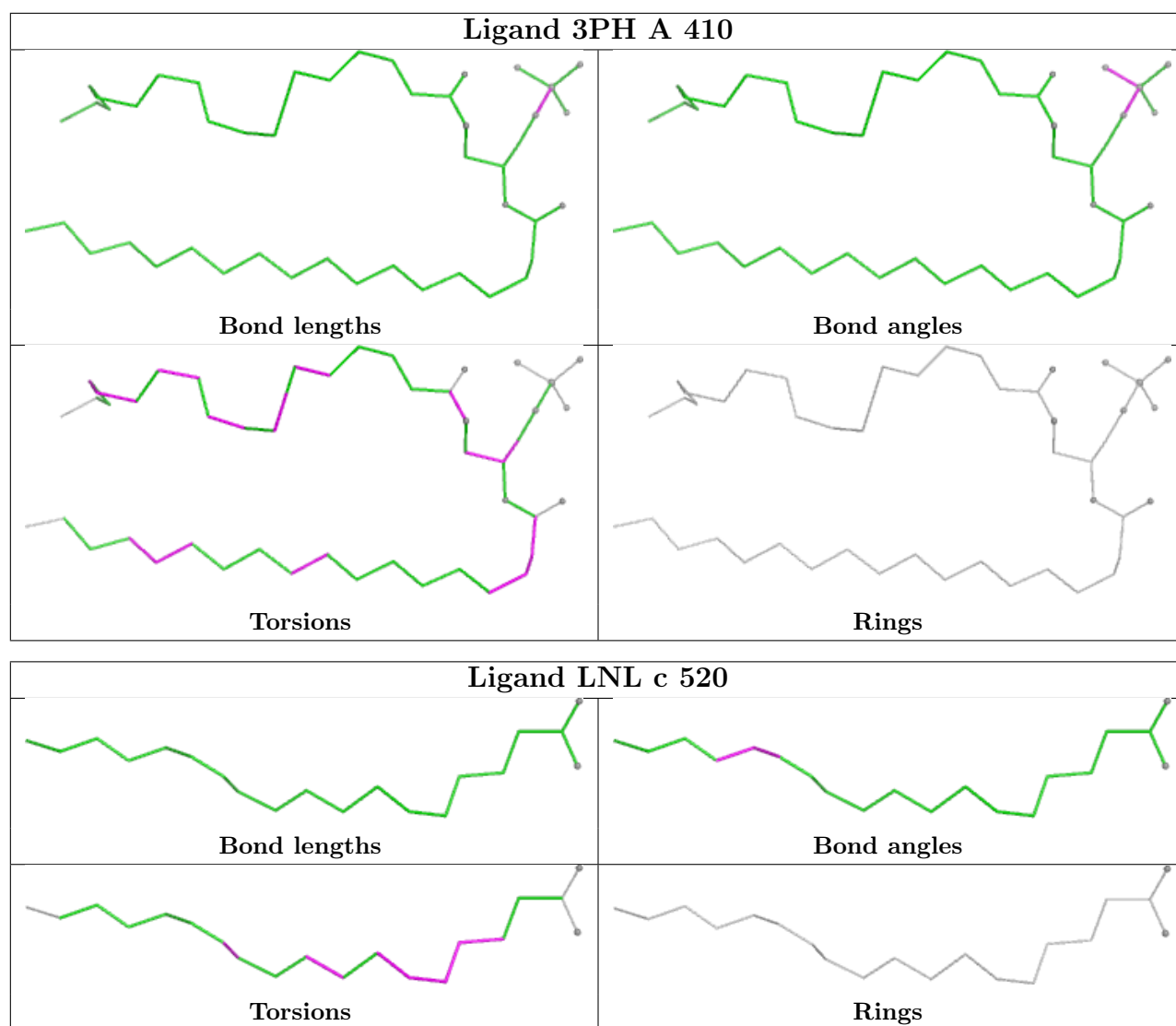
Rings

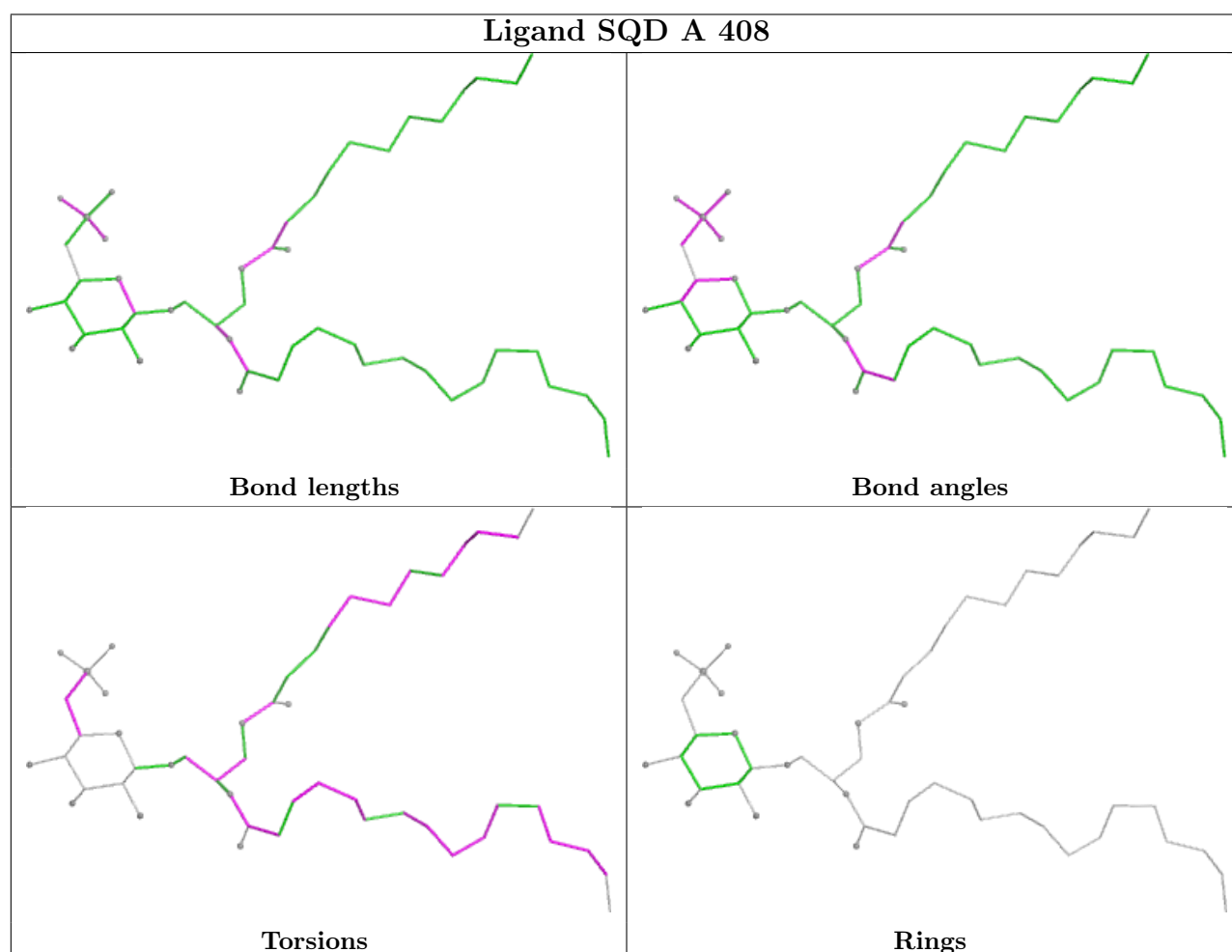
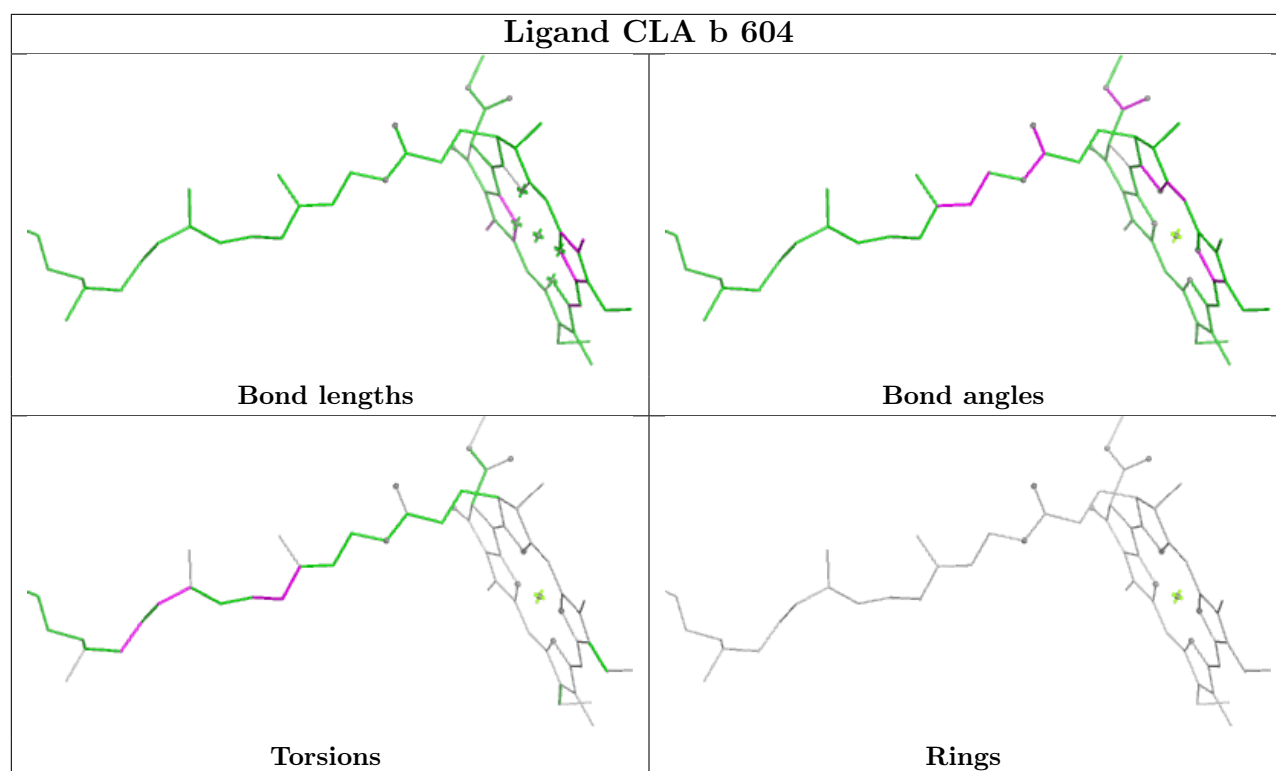
Ligand CLA b 605

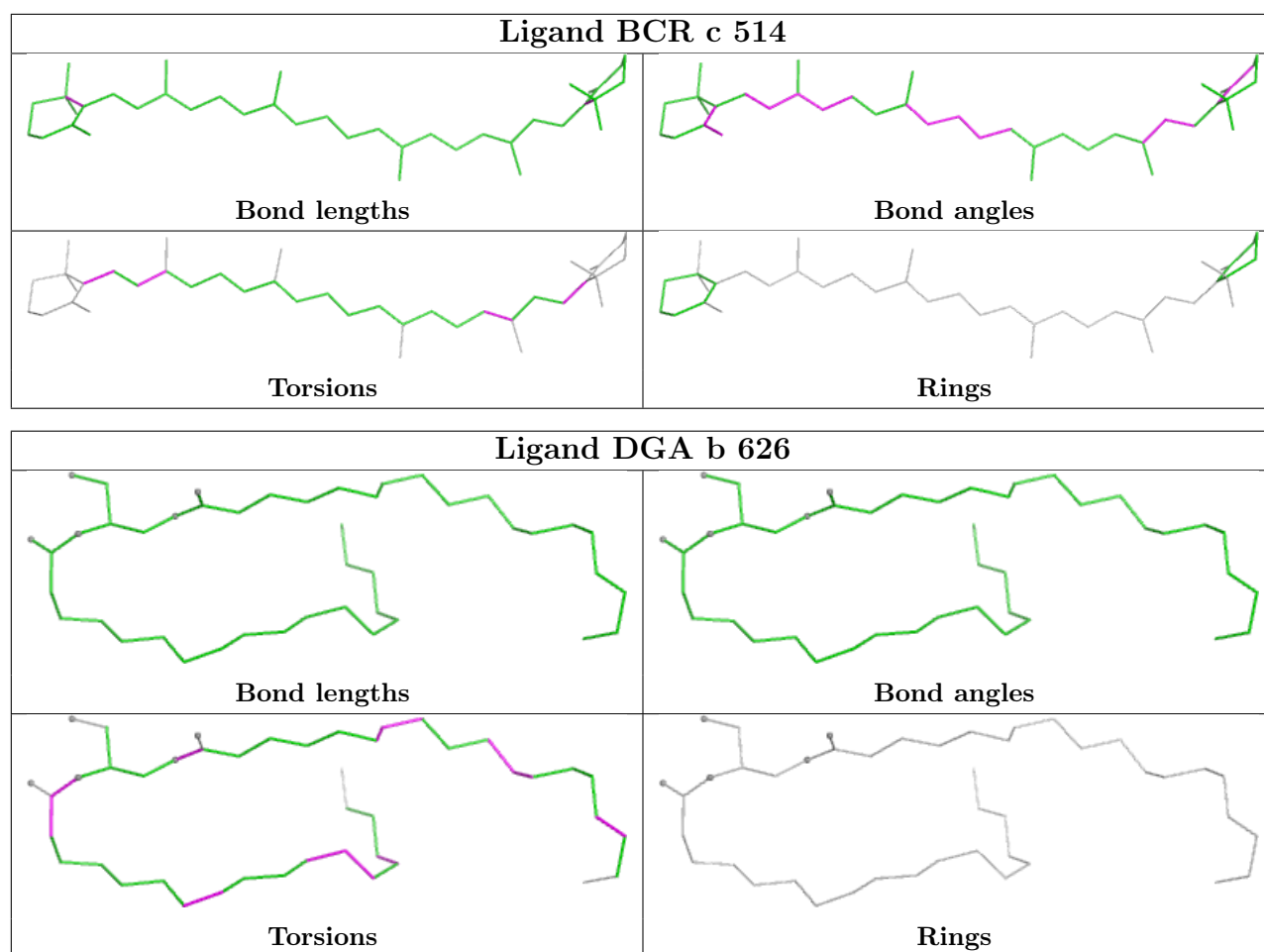


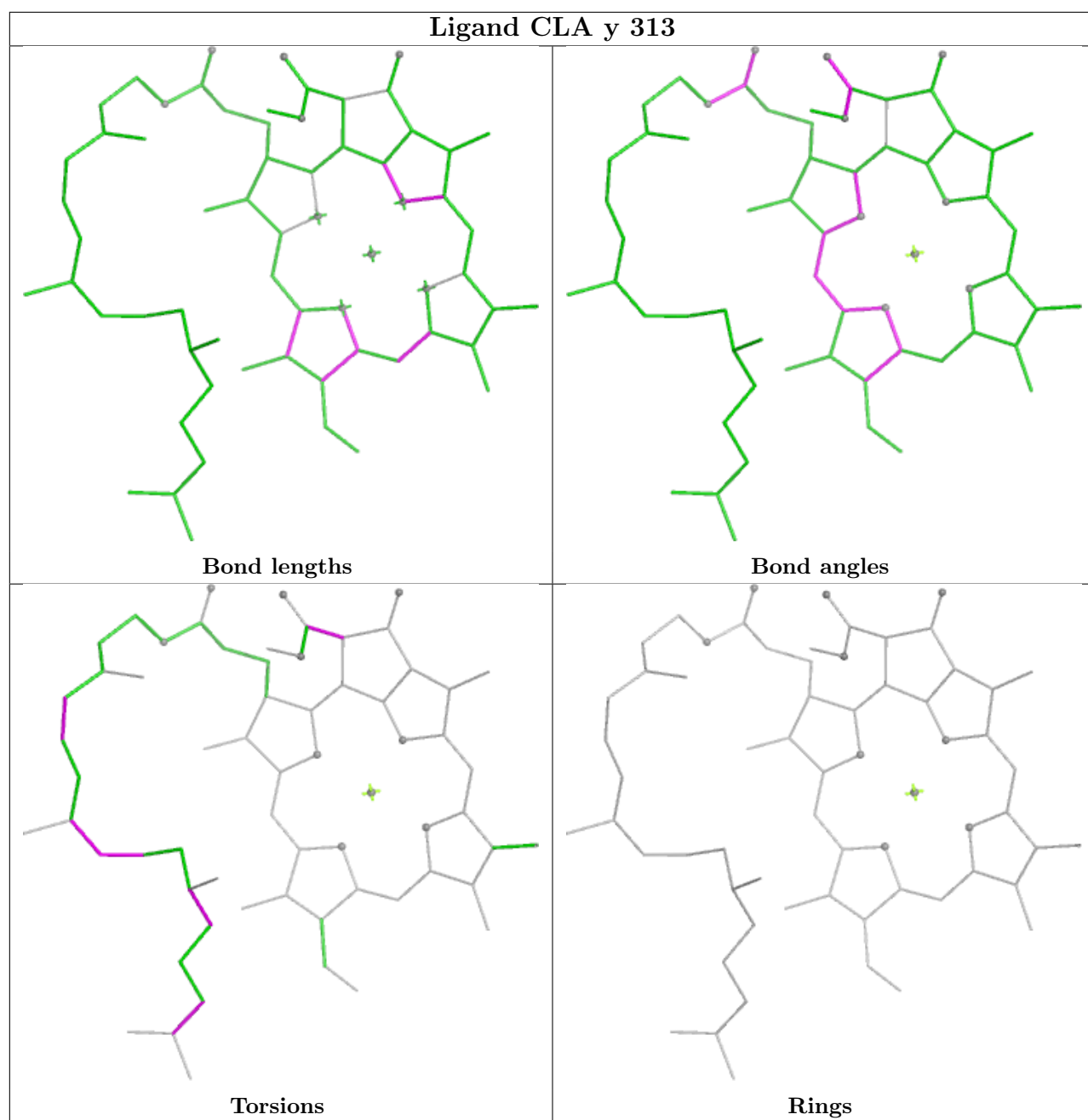
Ligand CLA s 612

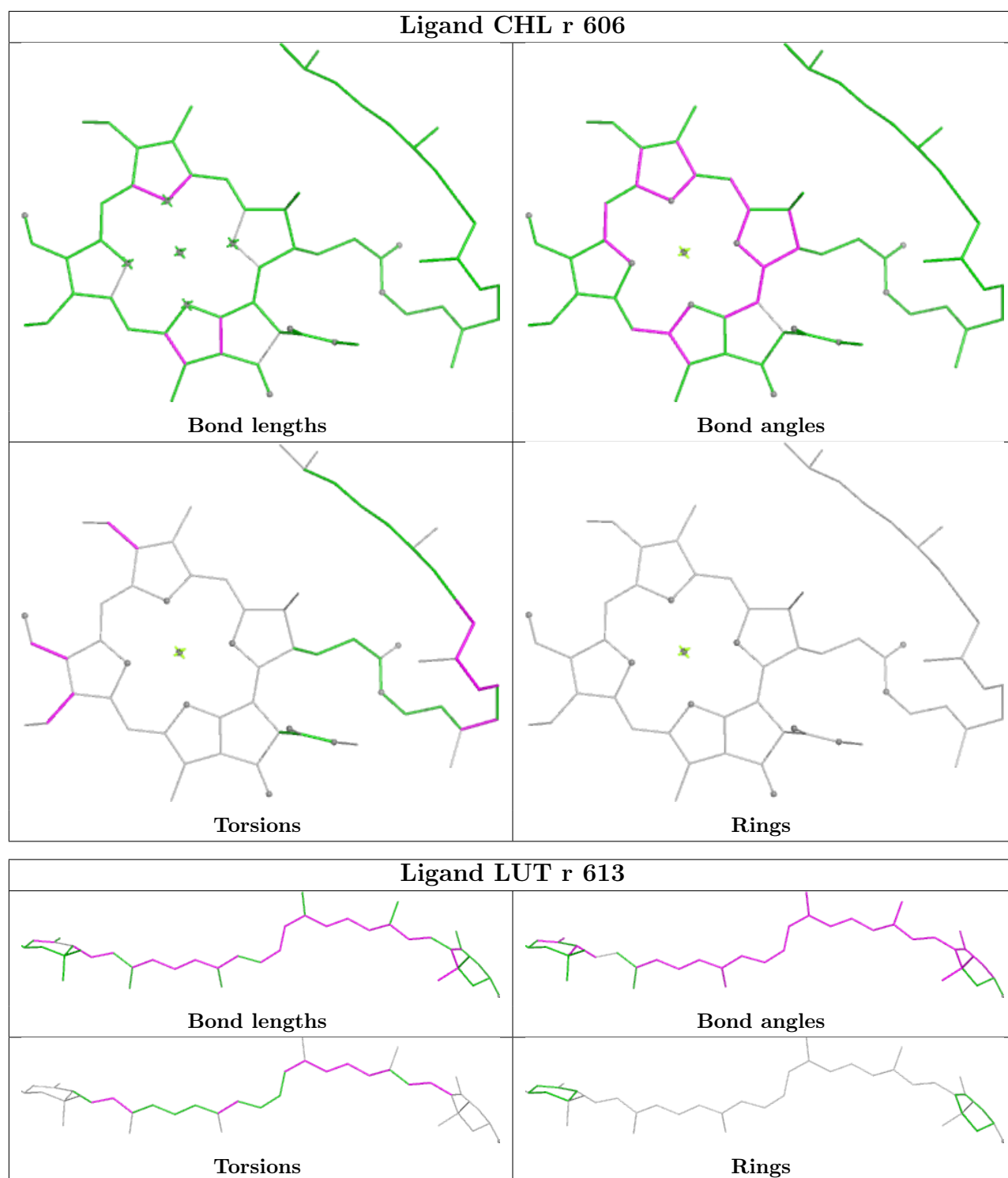




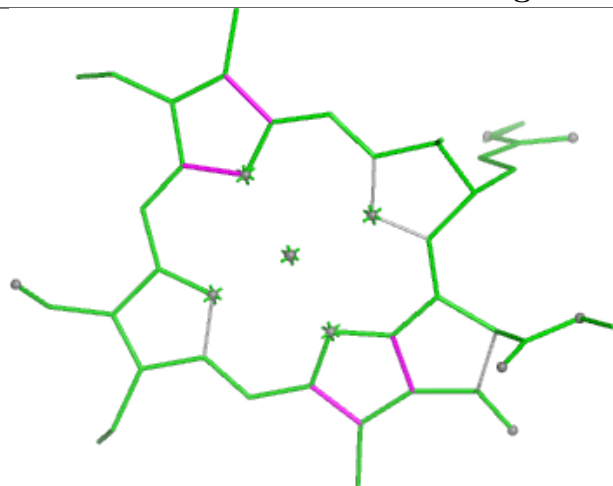




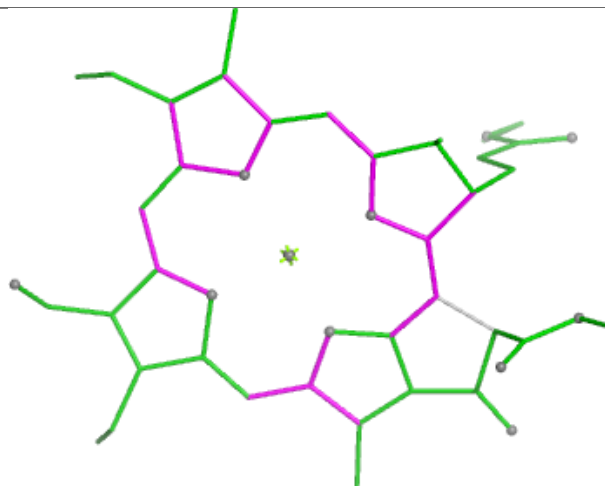




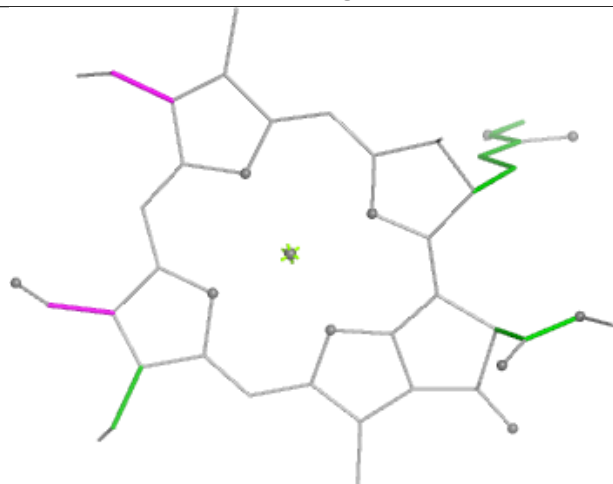
Ligand CHL Y 306



Bond lengths



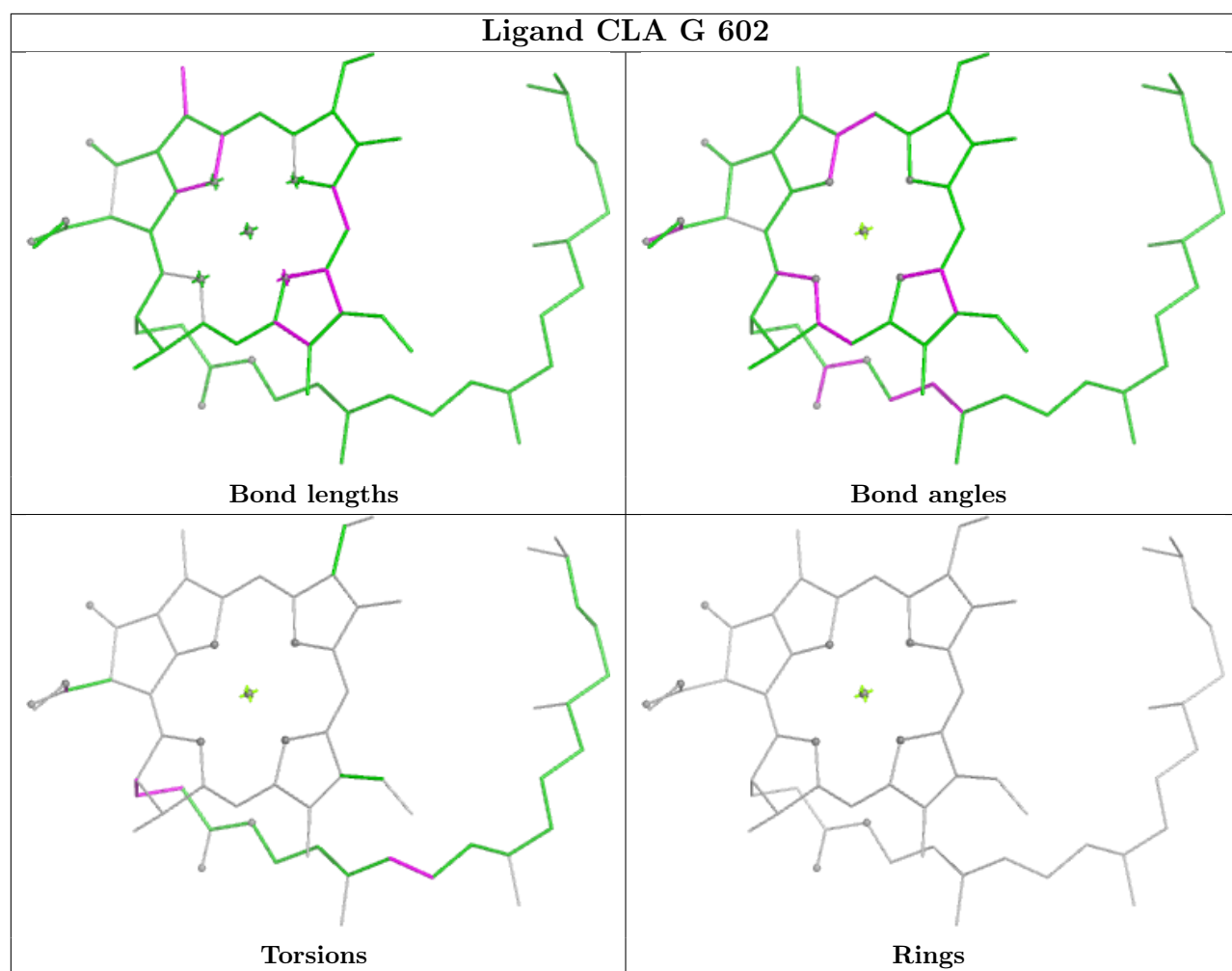
Bond angles

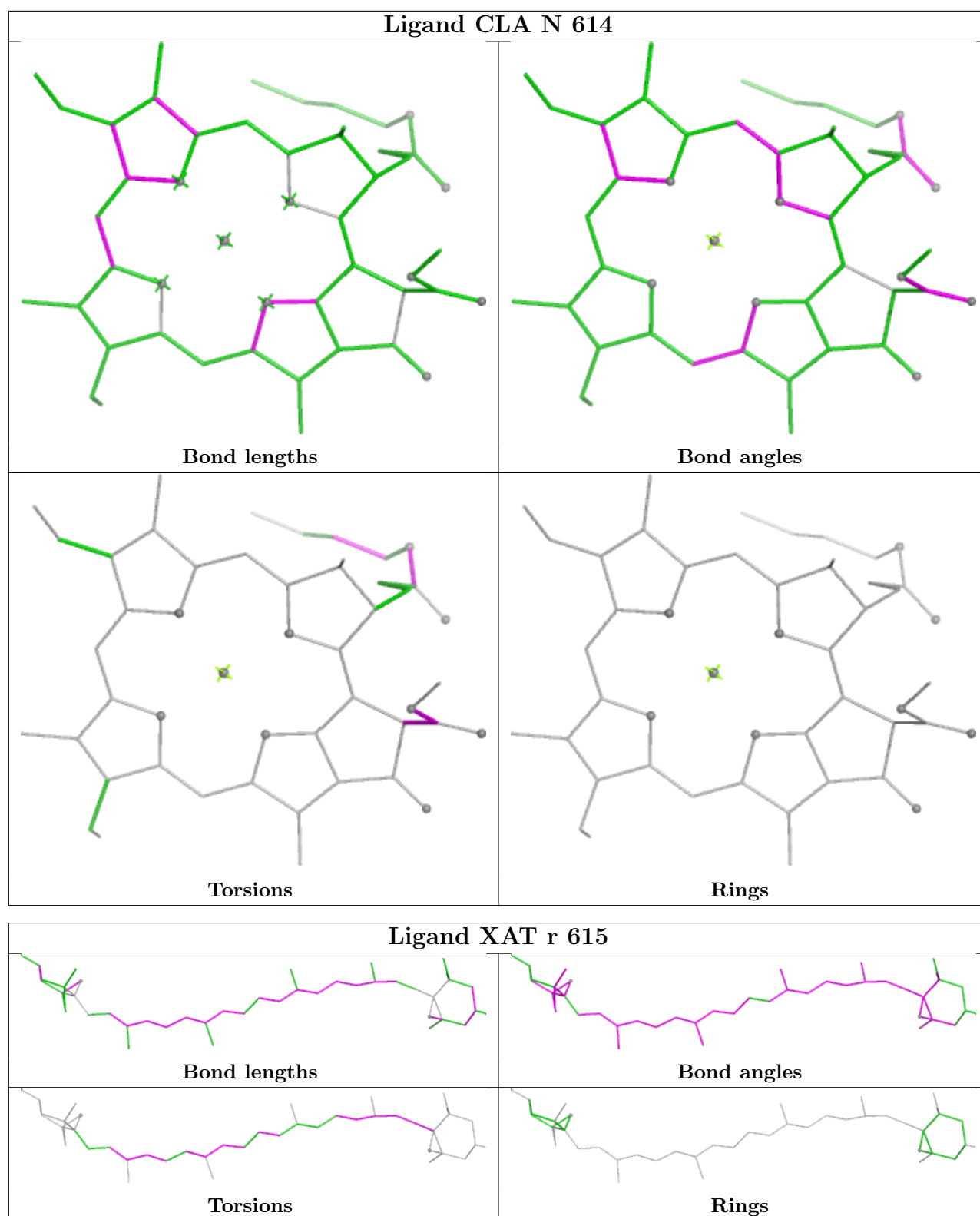


Torsions

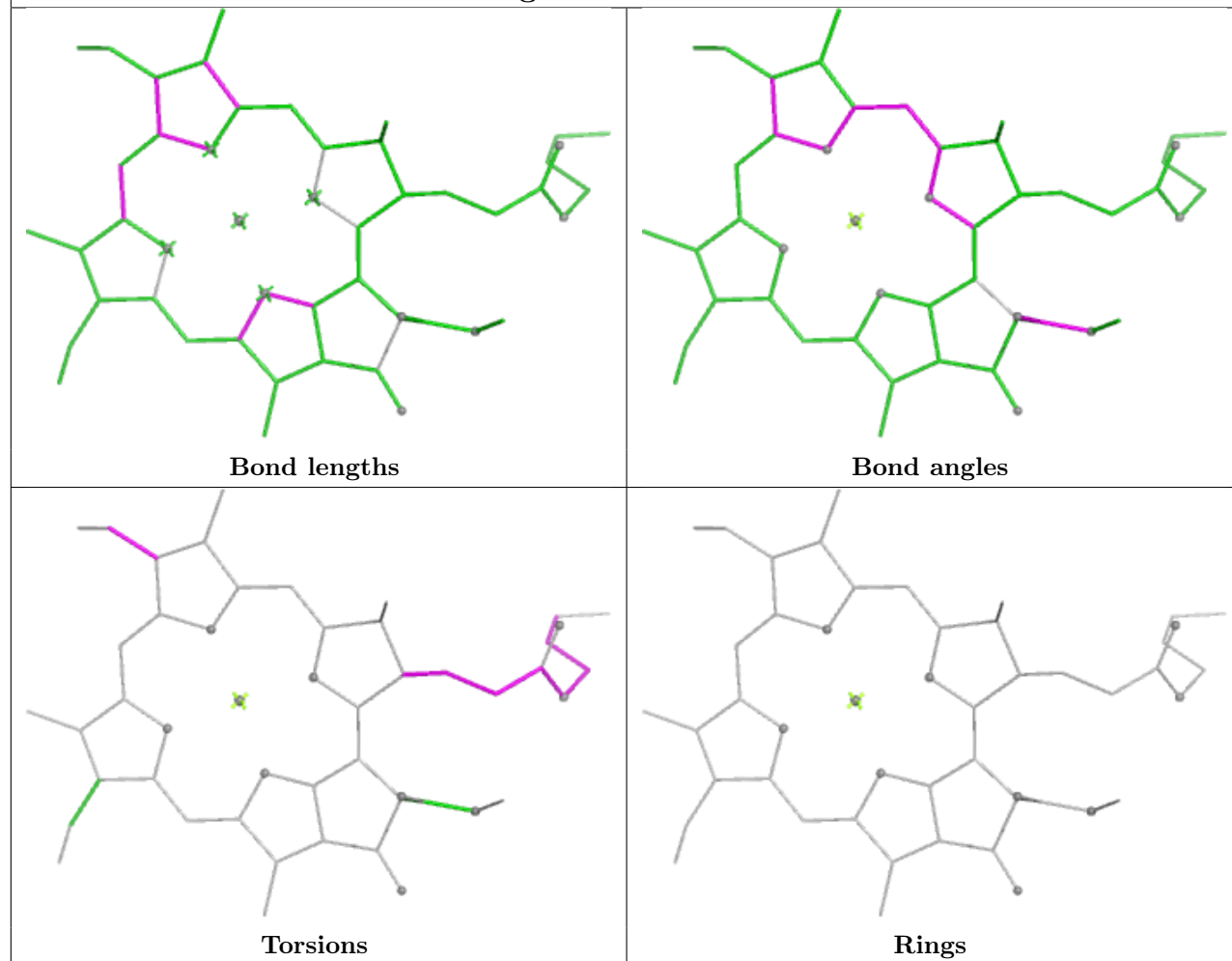


Rings

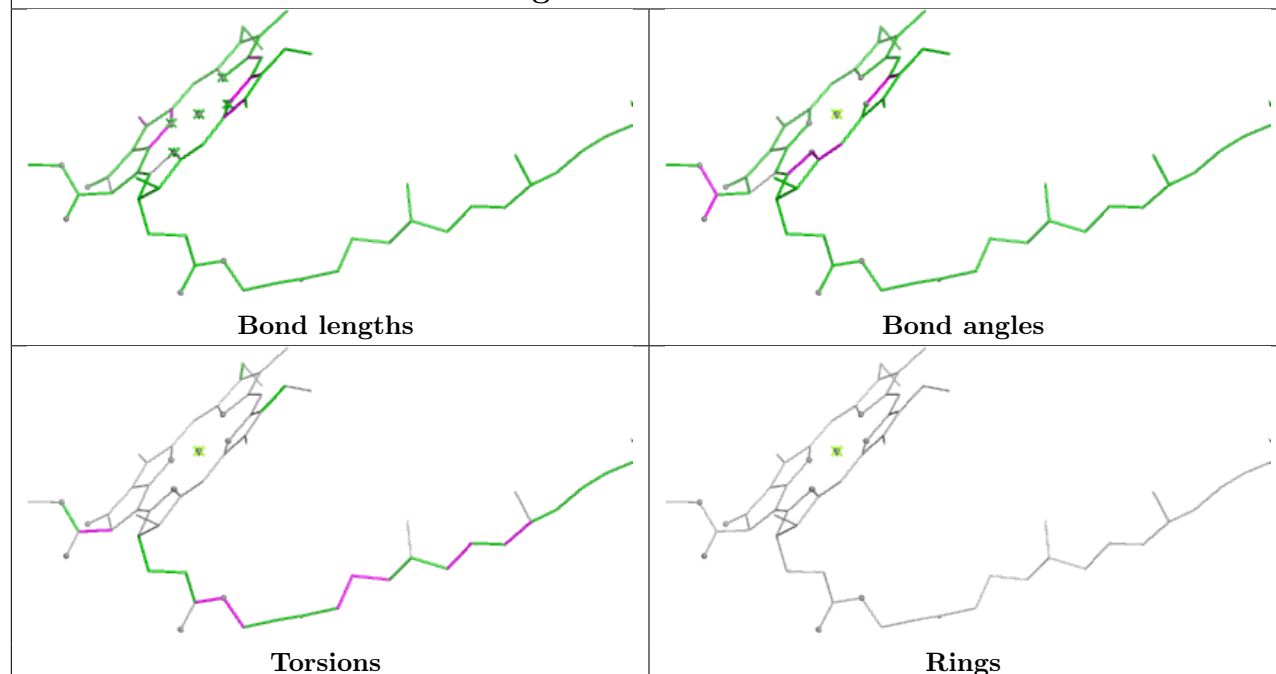




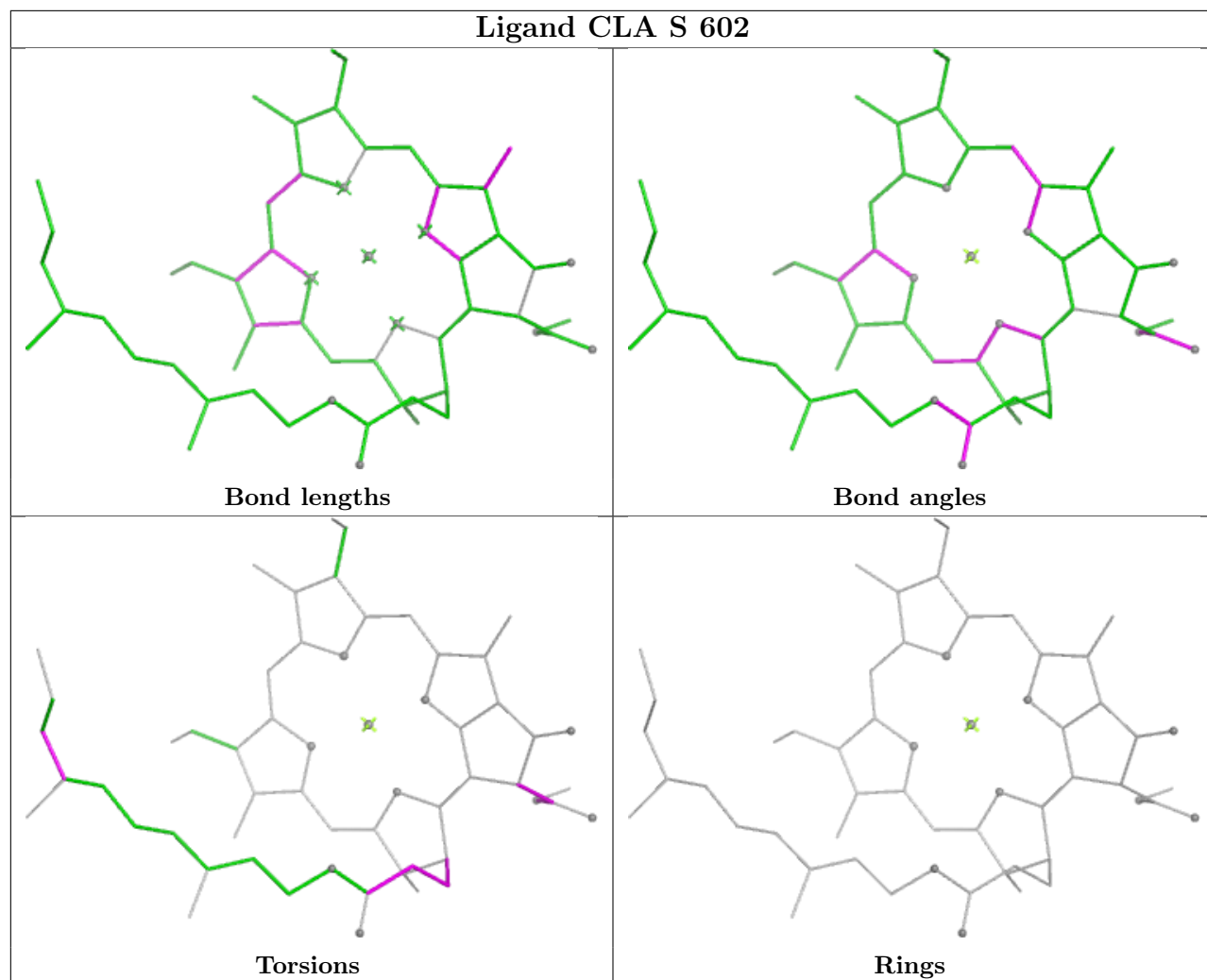
Ligand CLA r 601

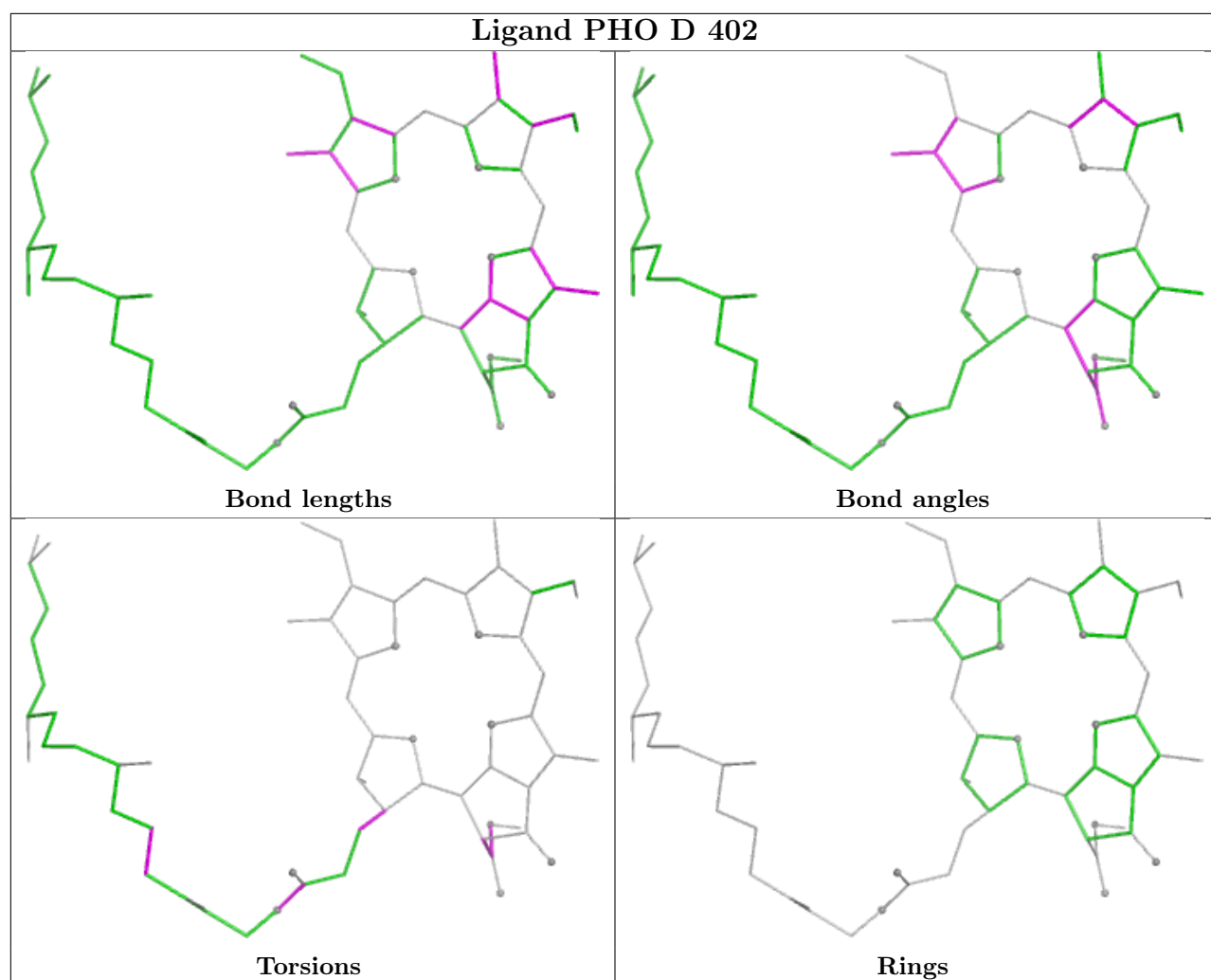


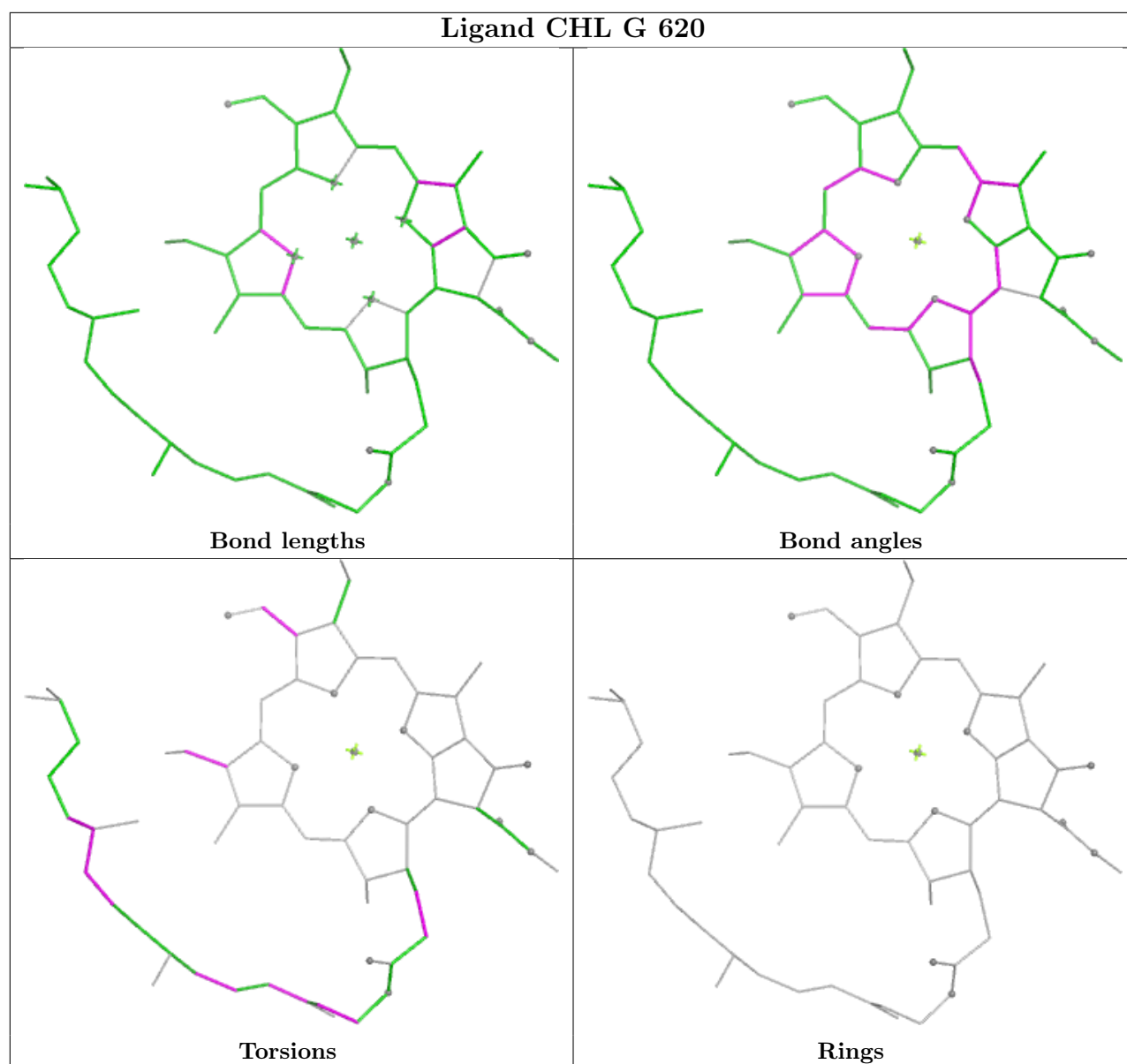
Ligand CLA C 504

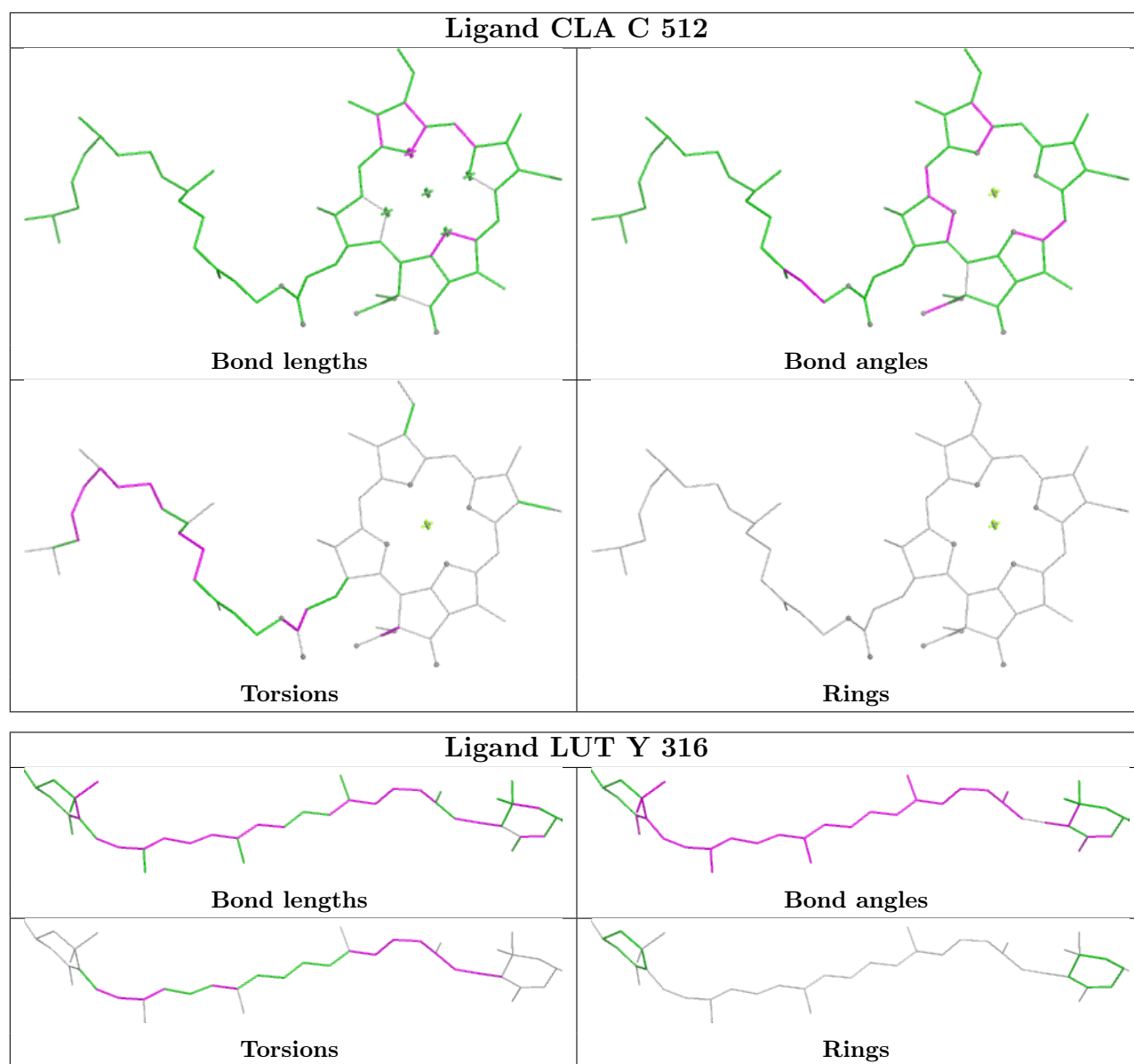


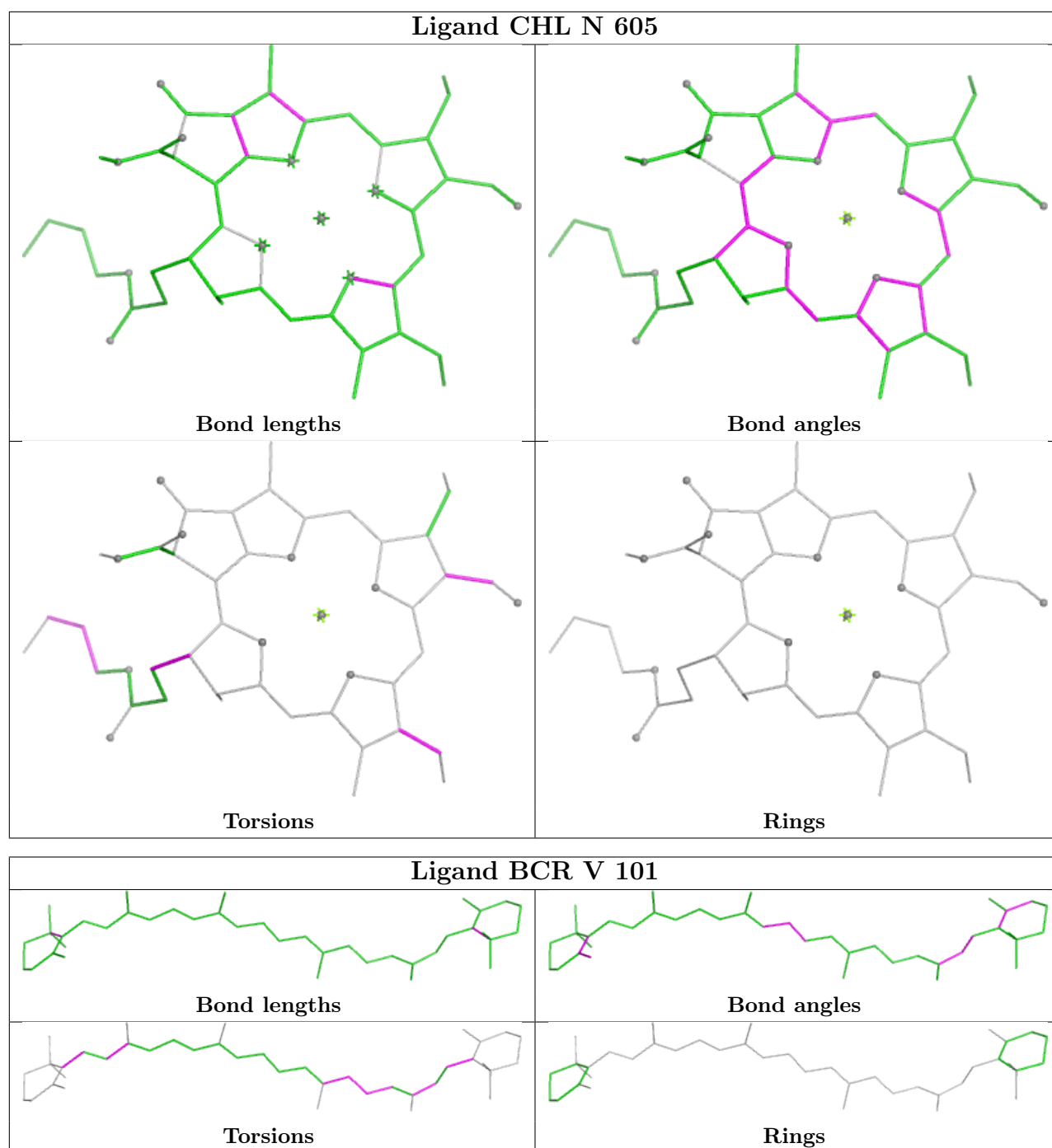
Ligand CLA S 602

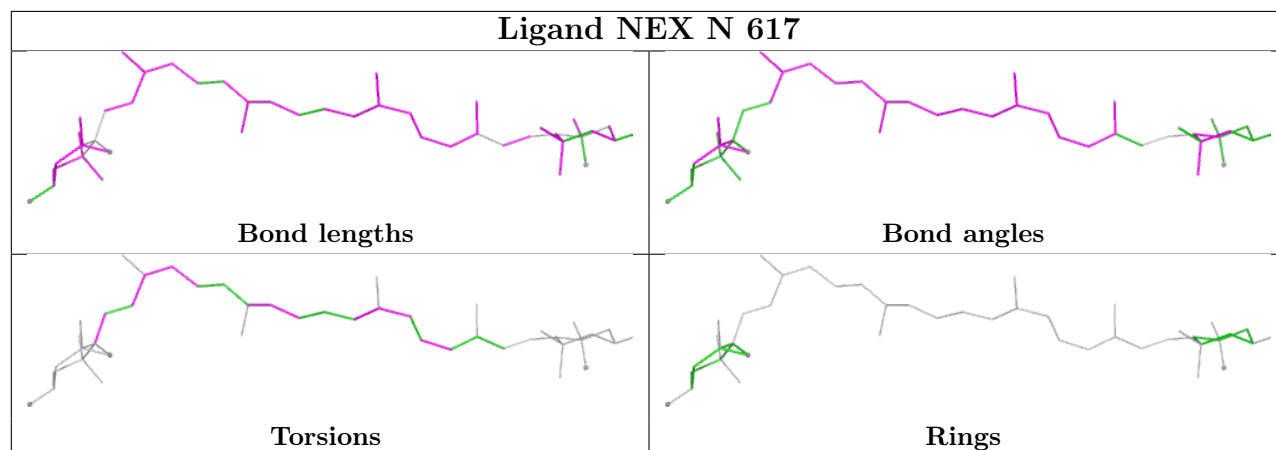
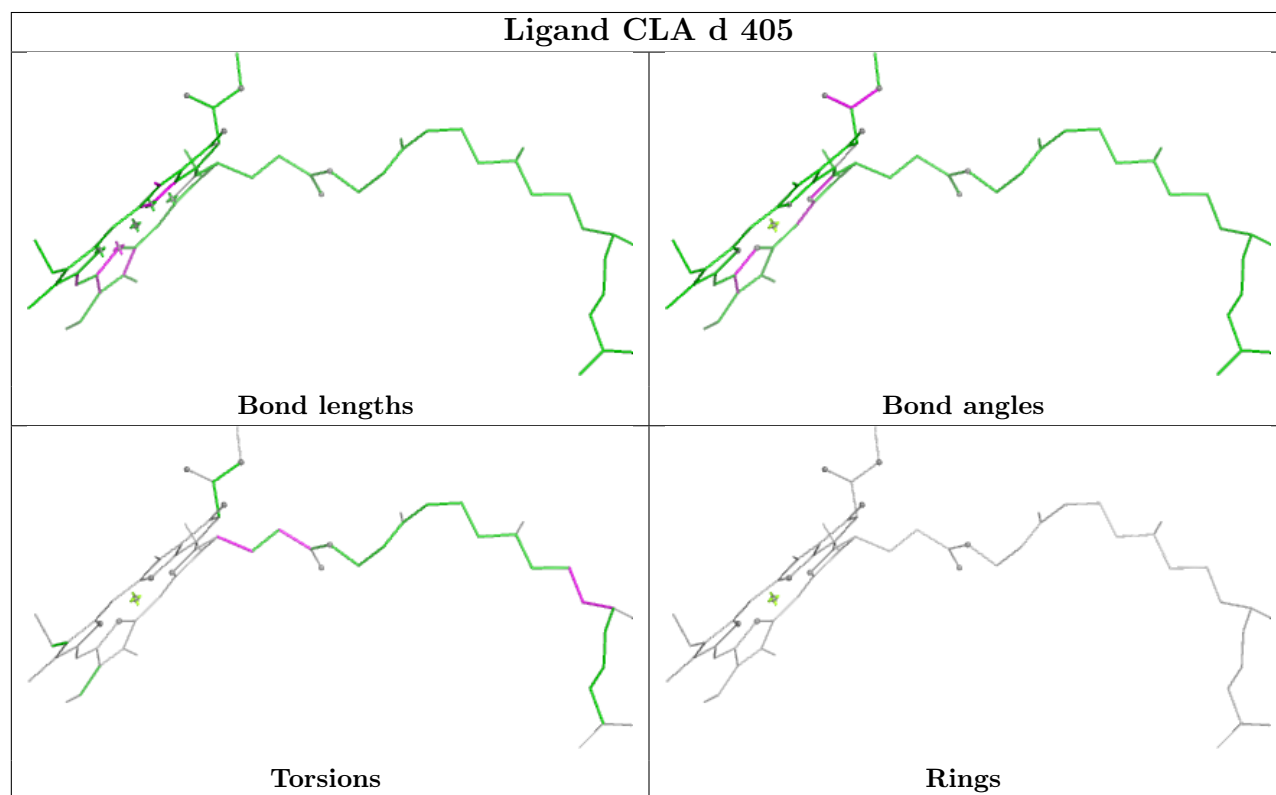
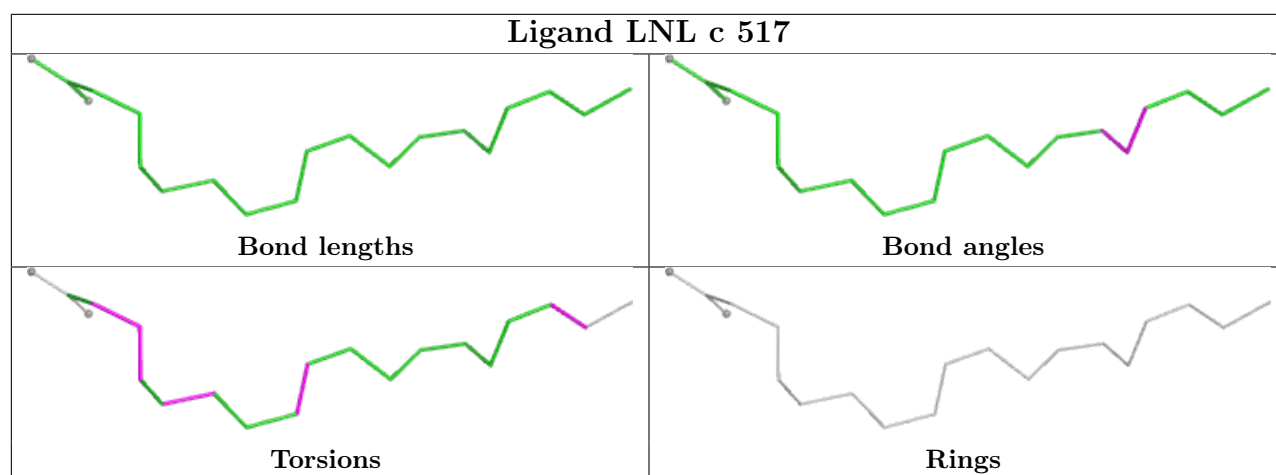


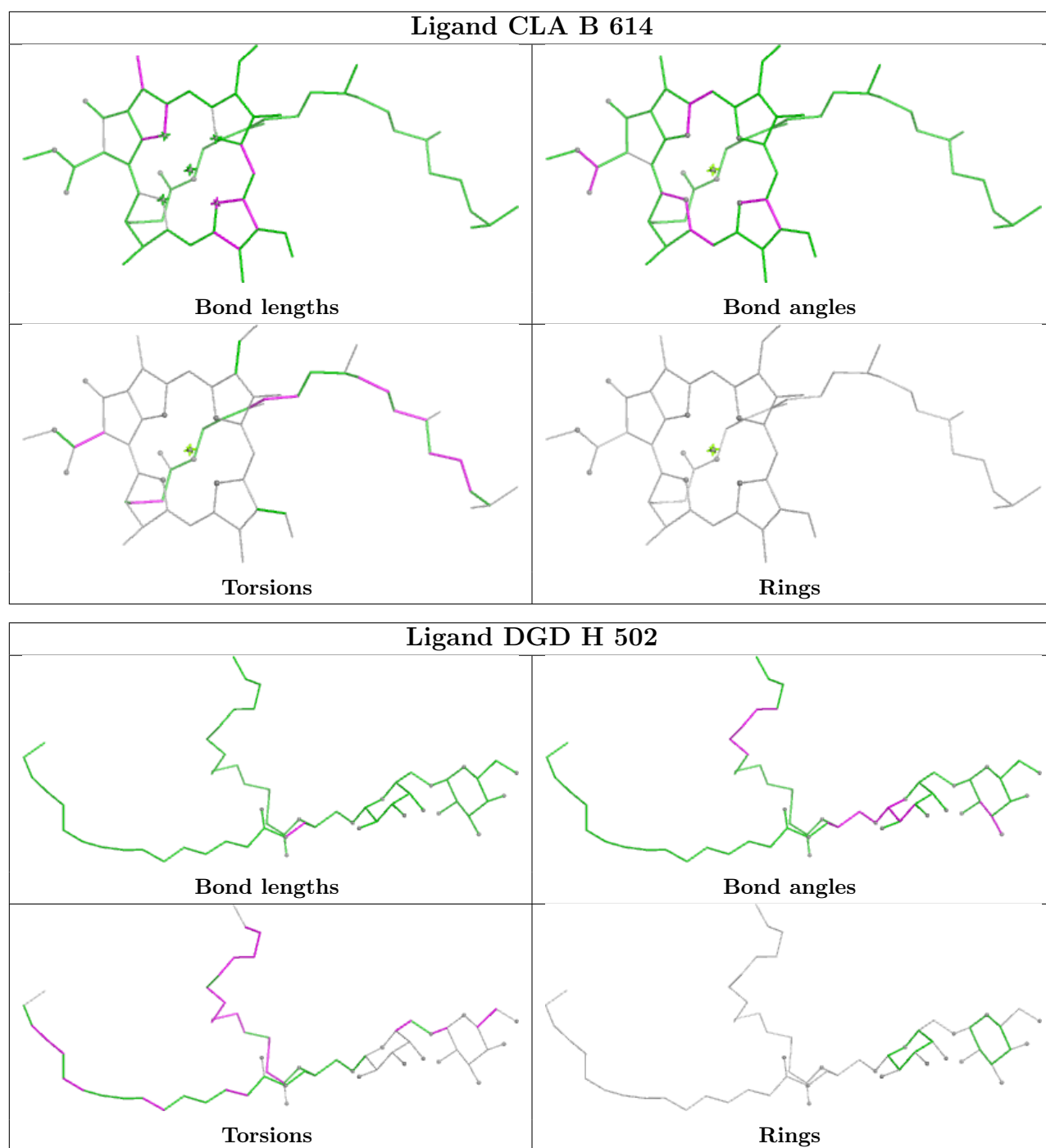


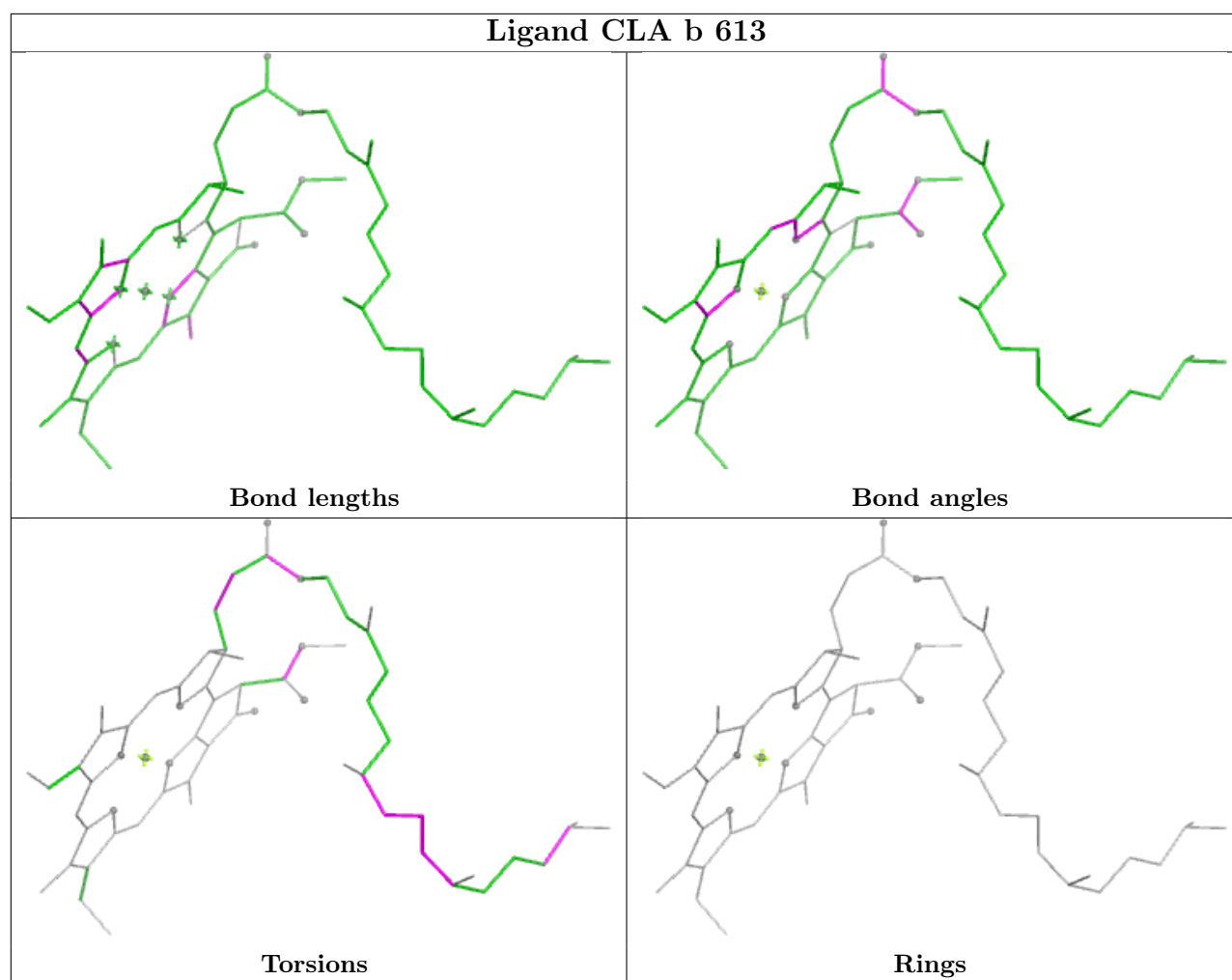


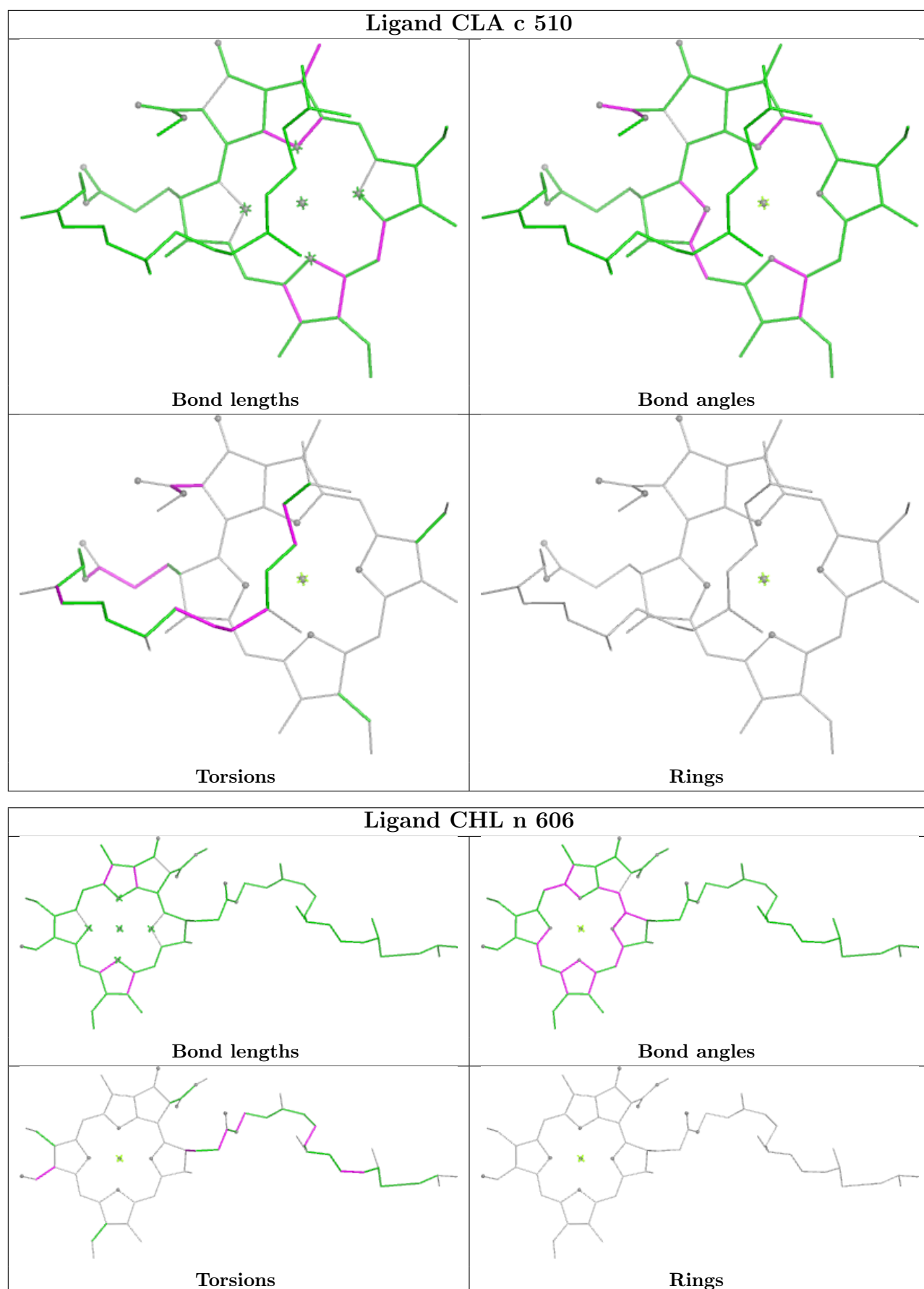




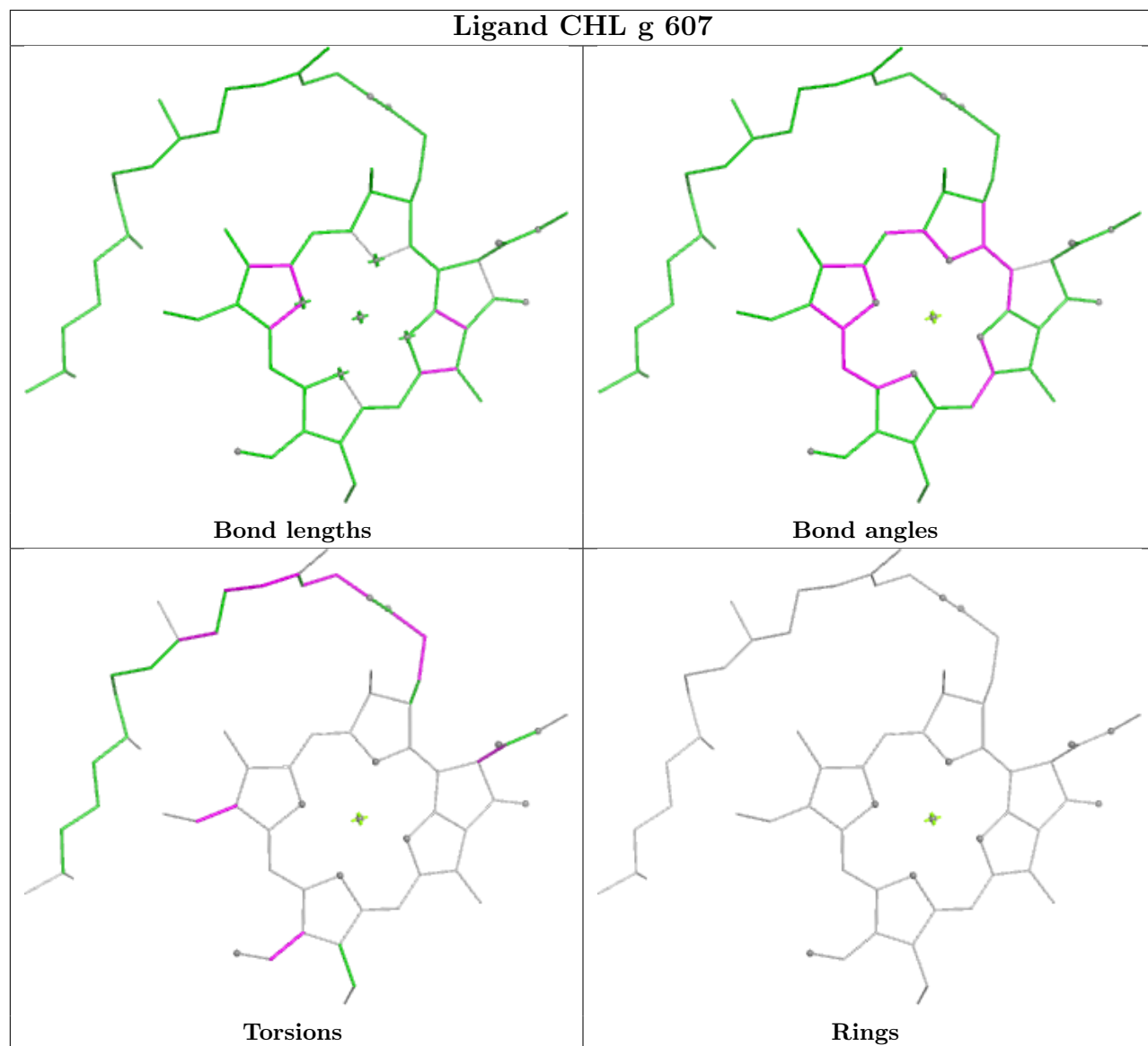




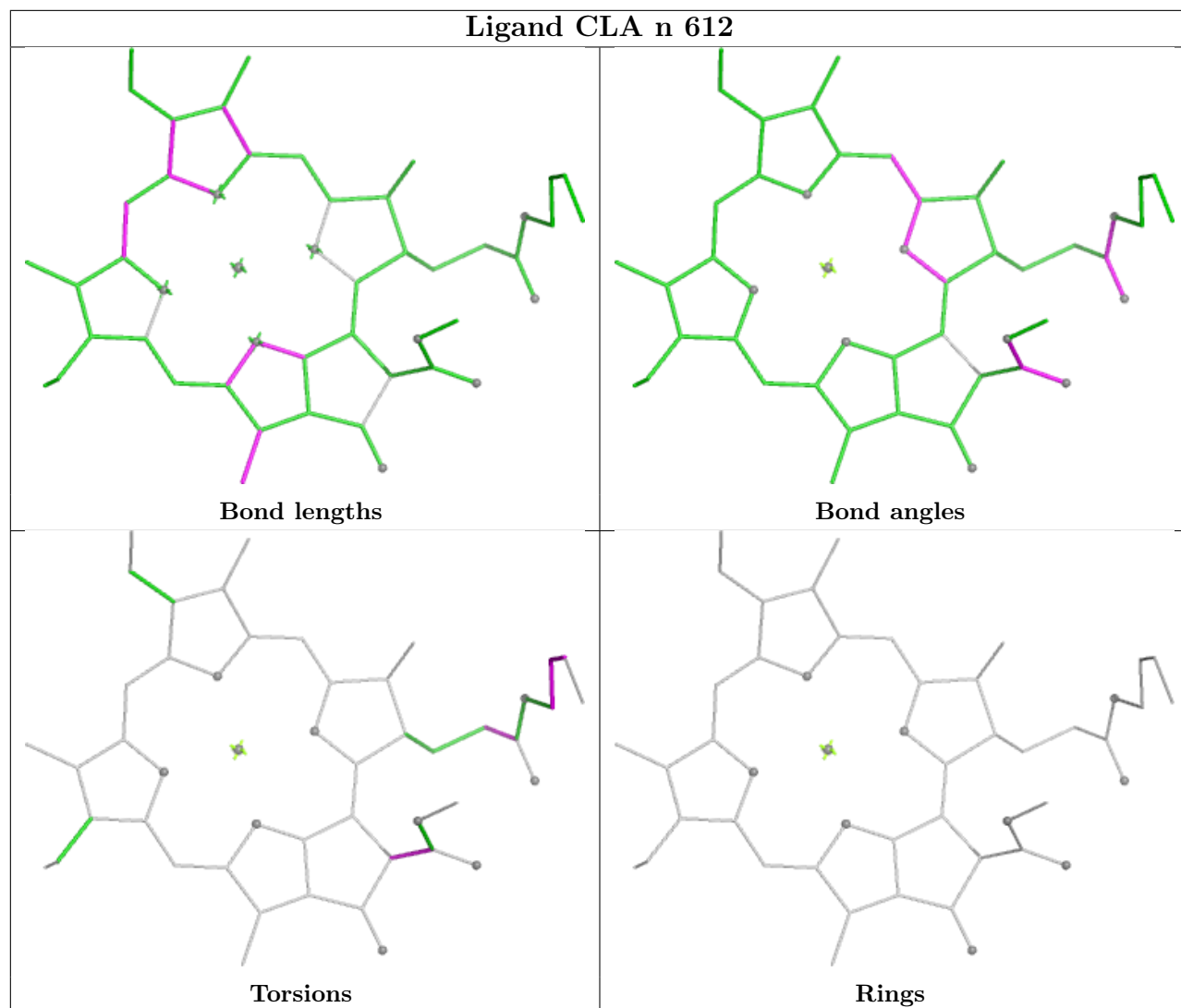


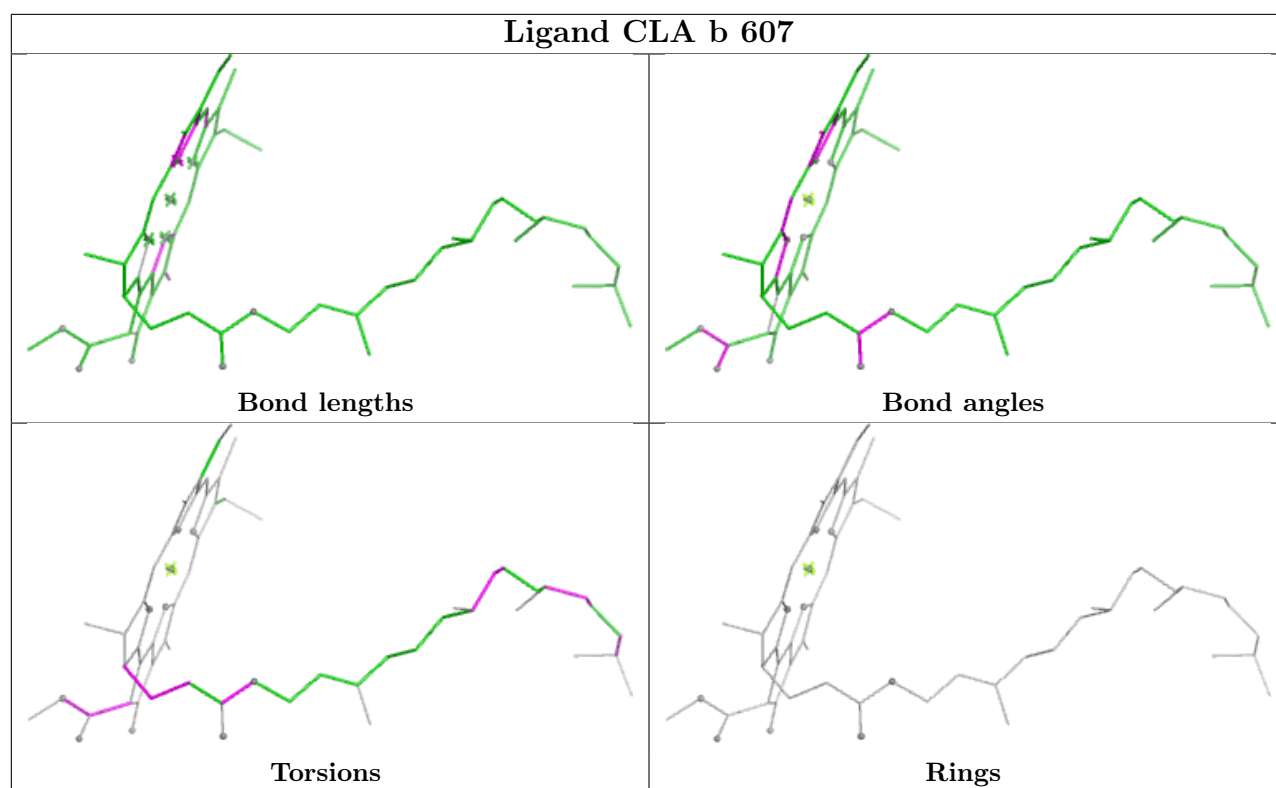


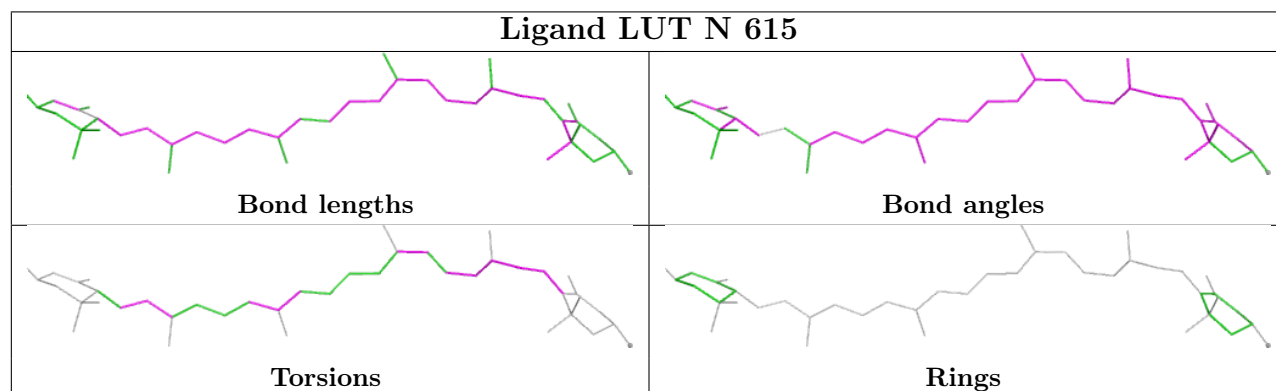
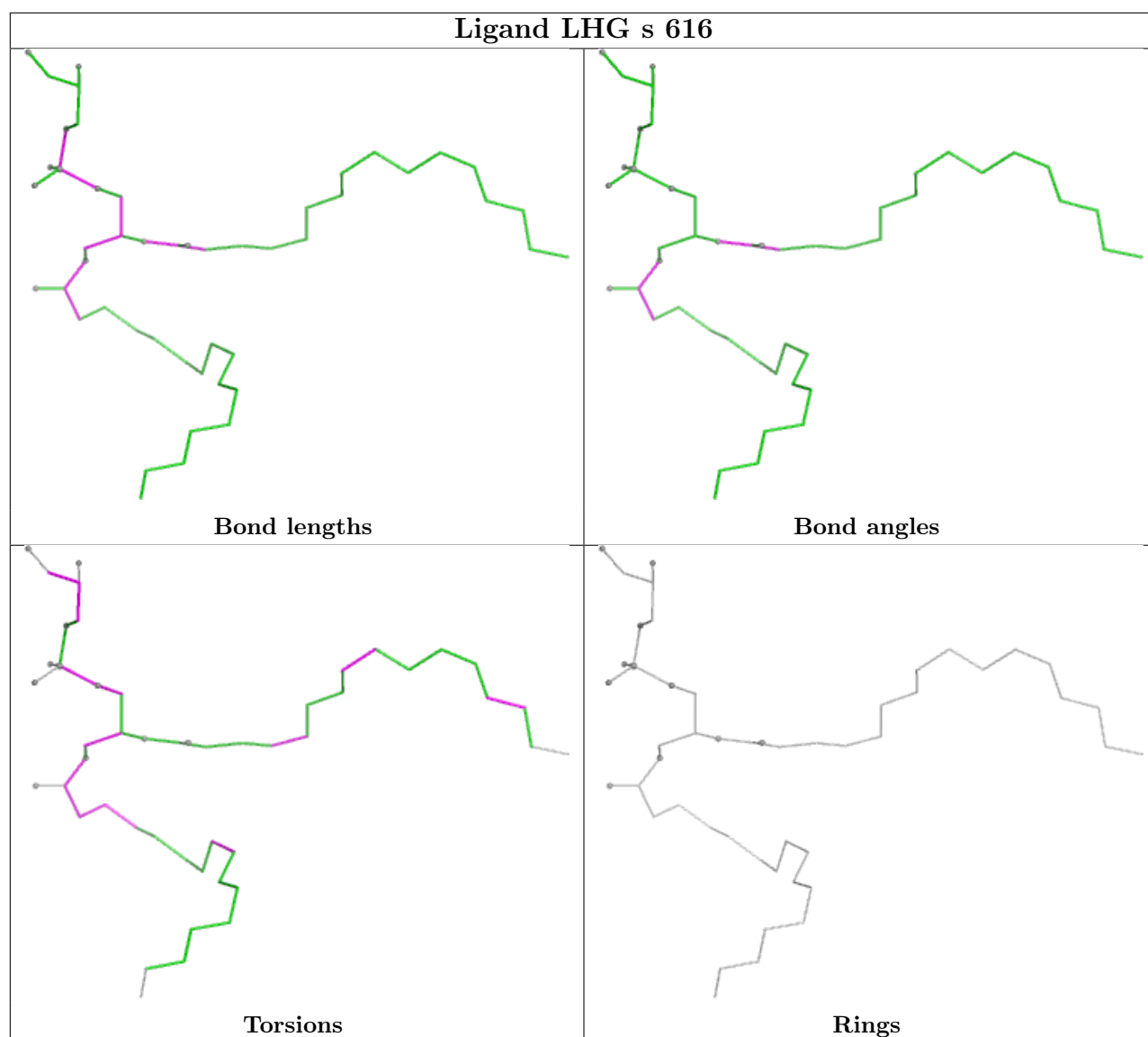
Ligand CHL g 607

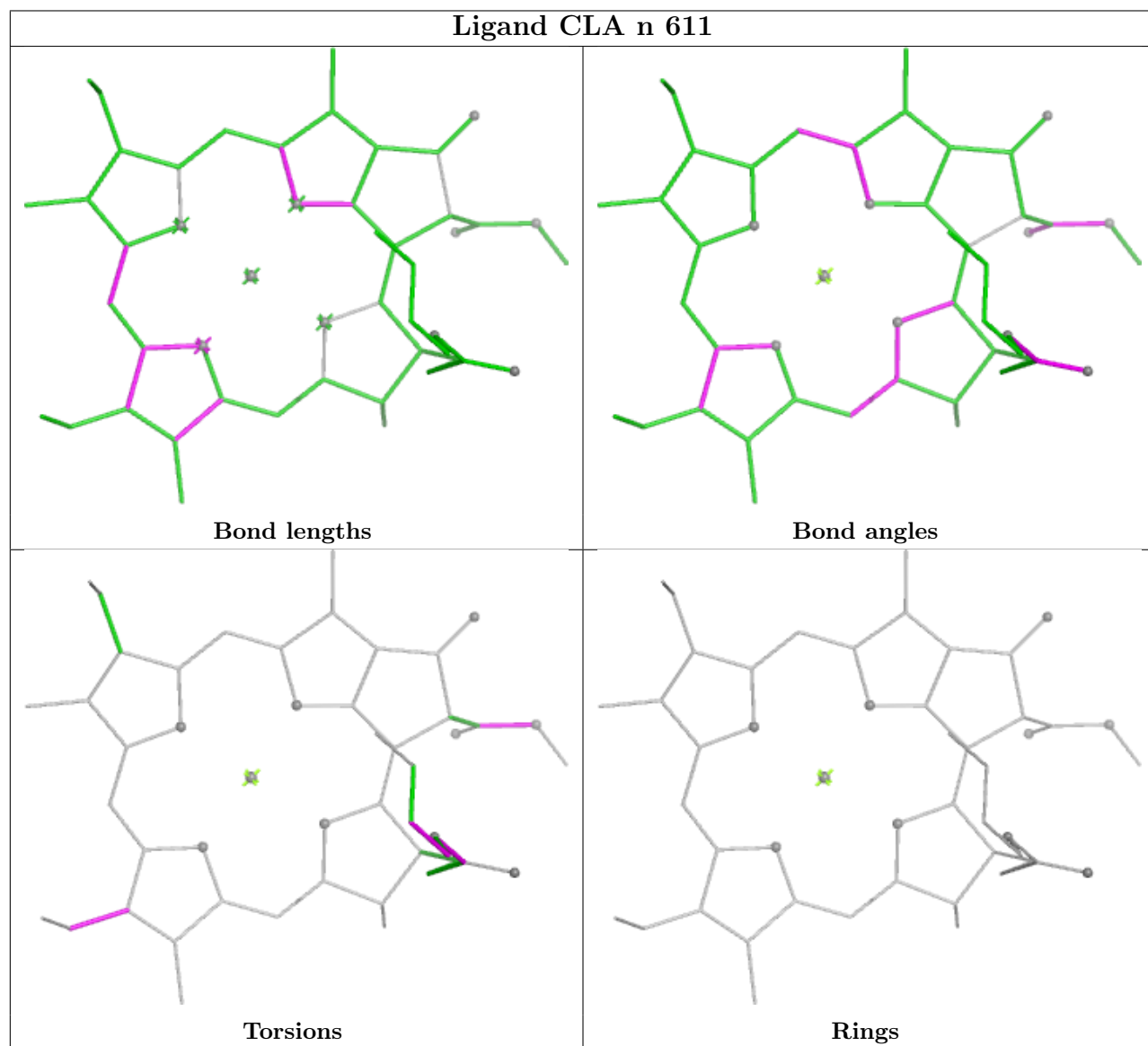
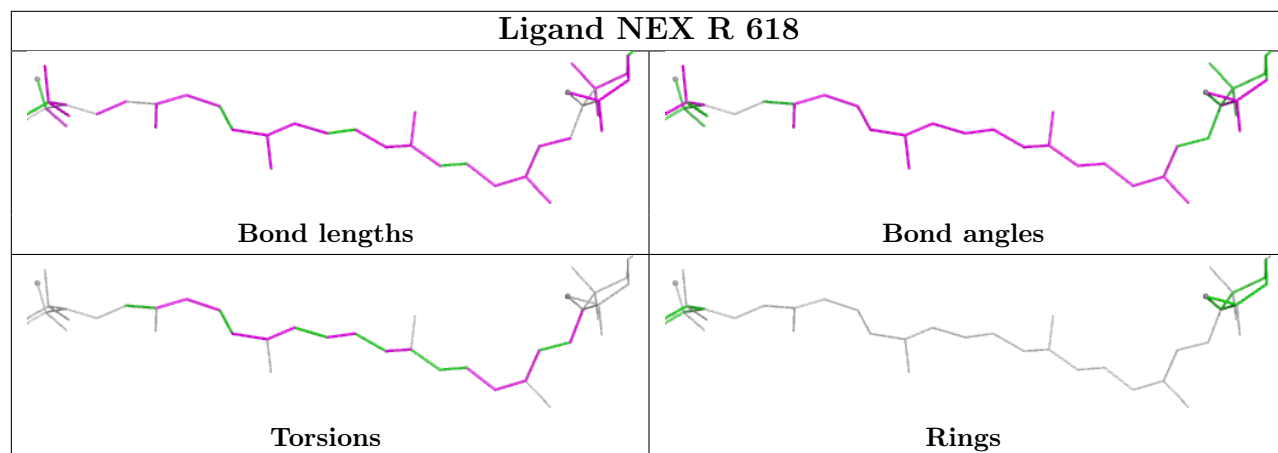


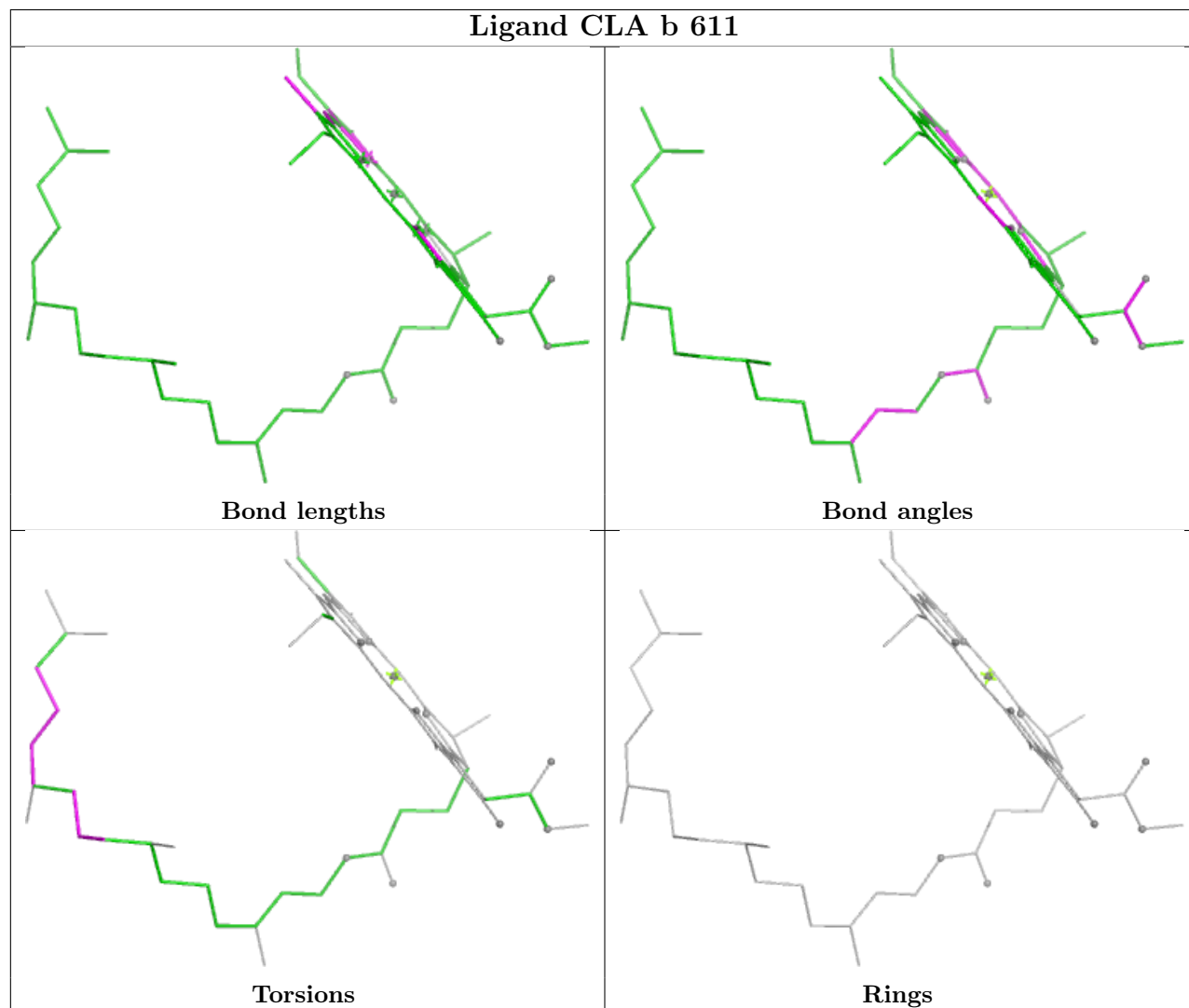
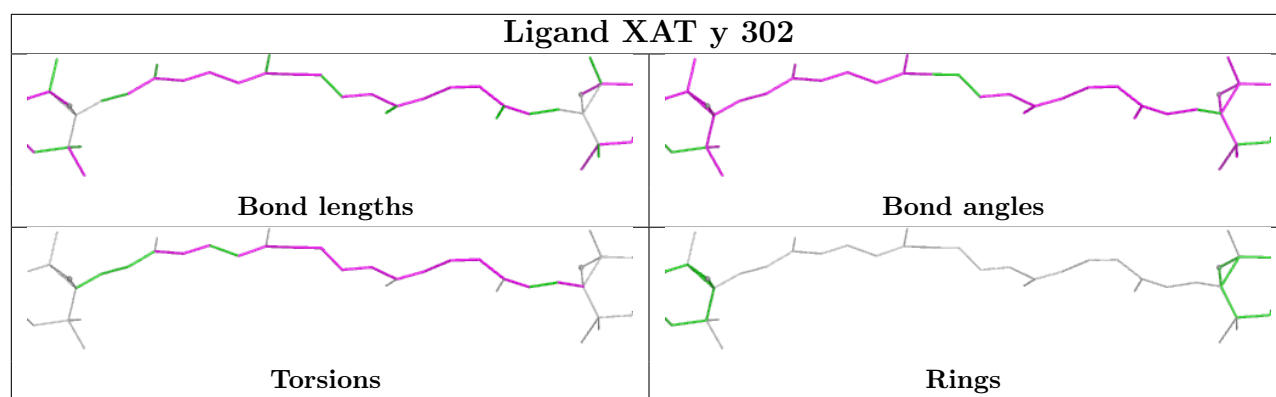
Ligand CLA n 612

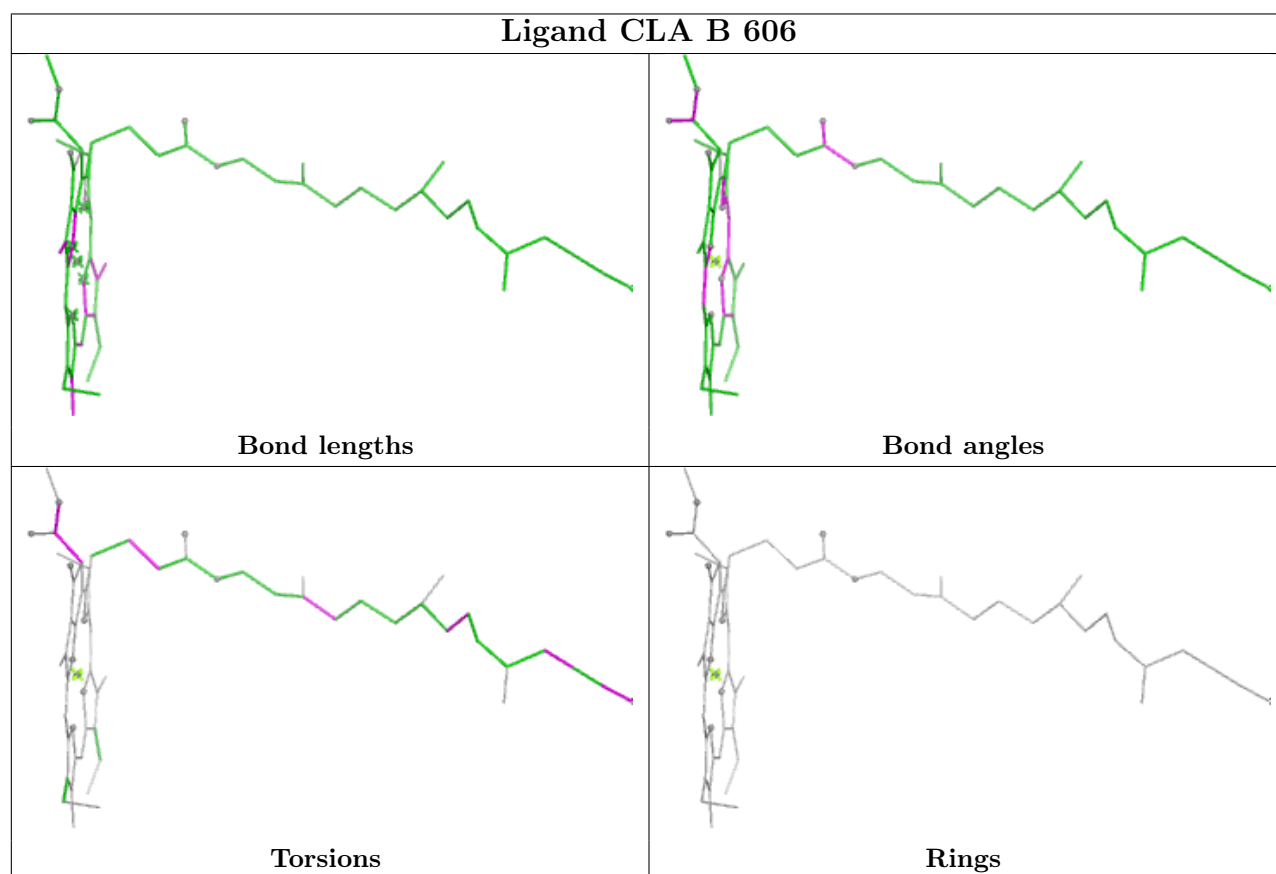
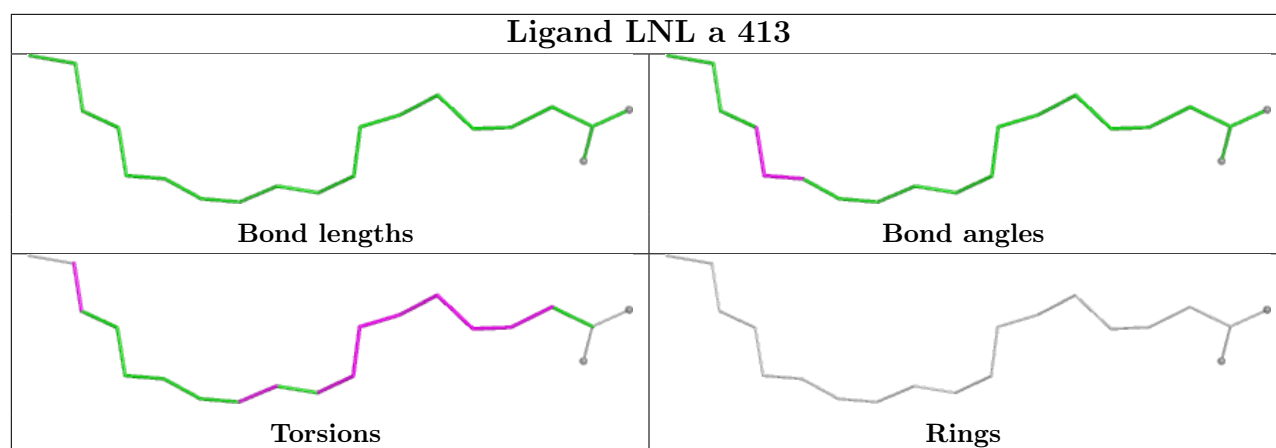


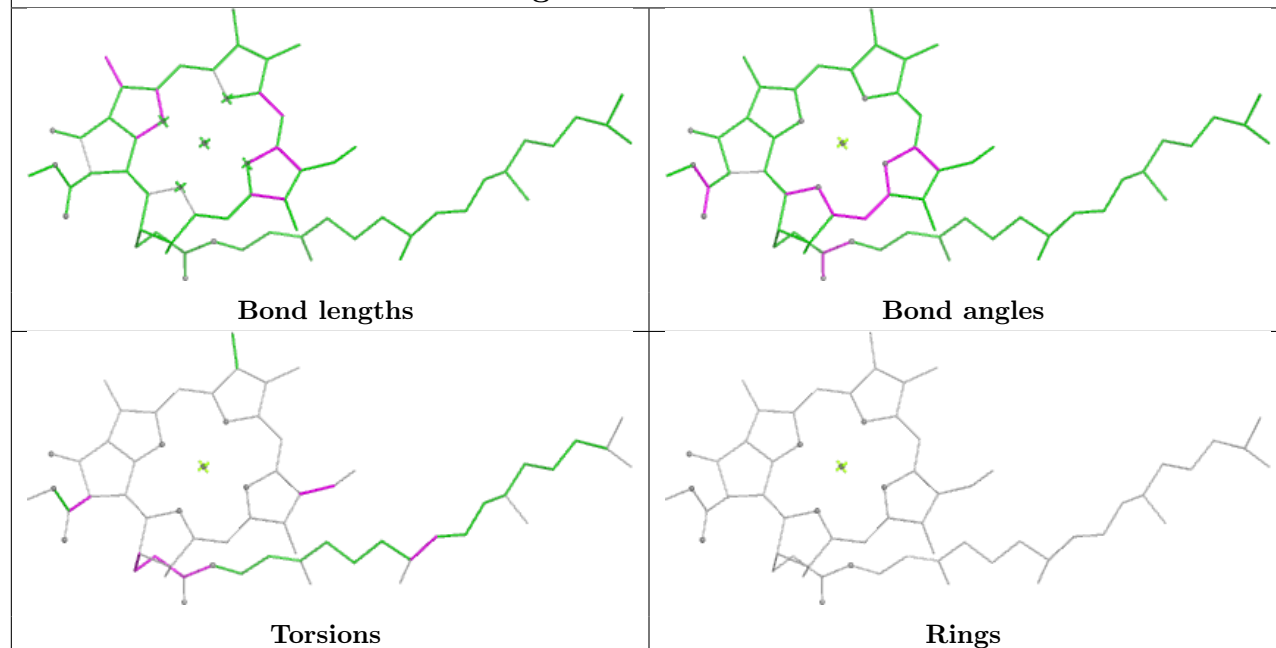
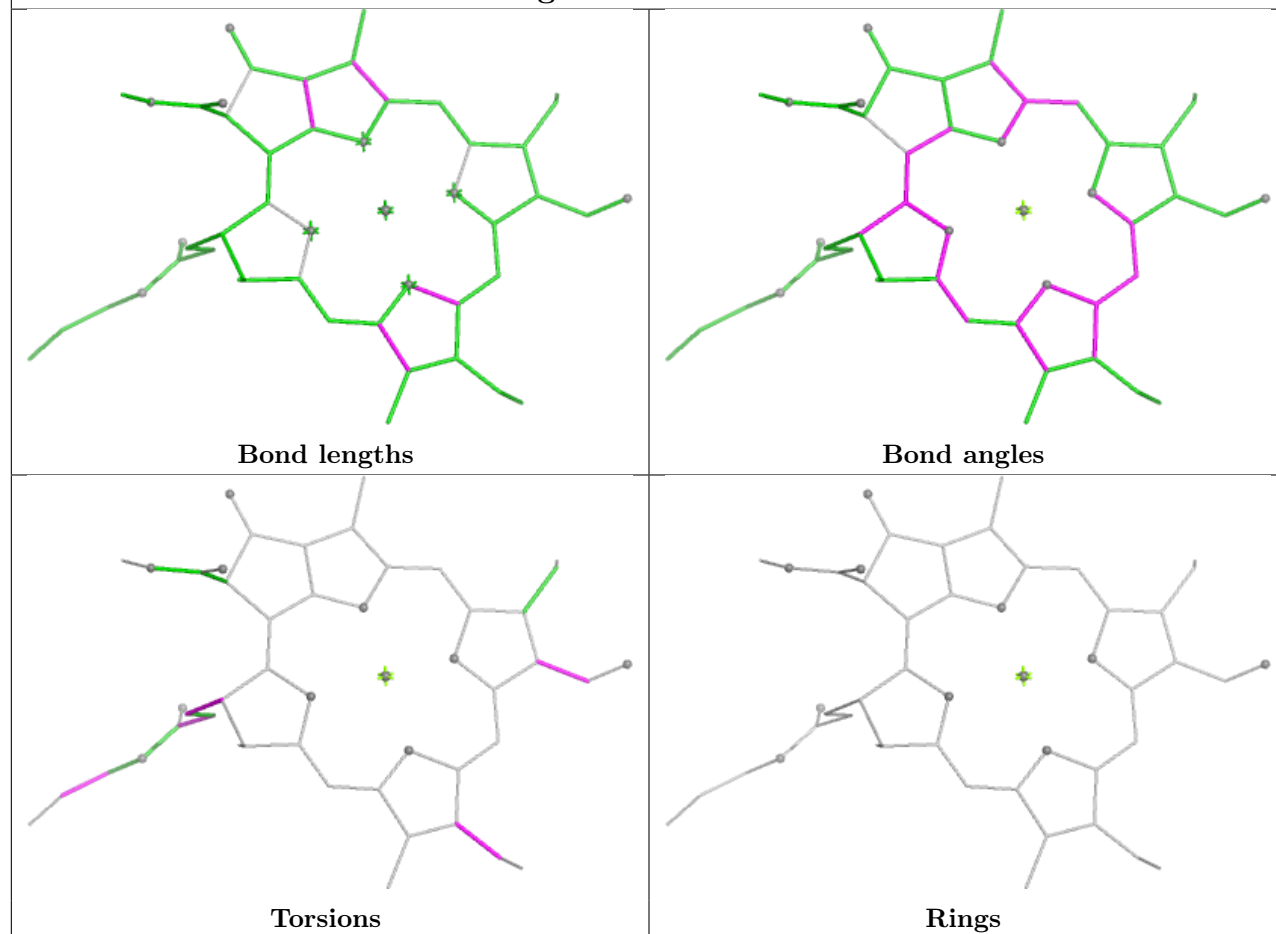


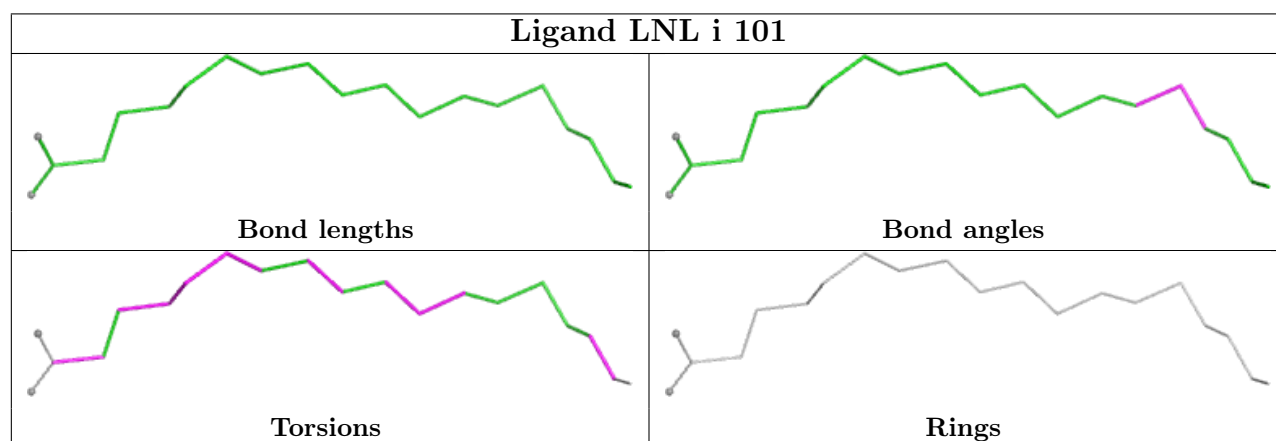
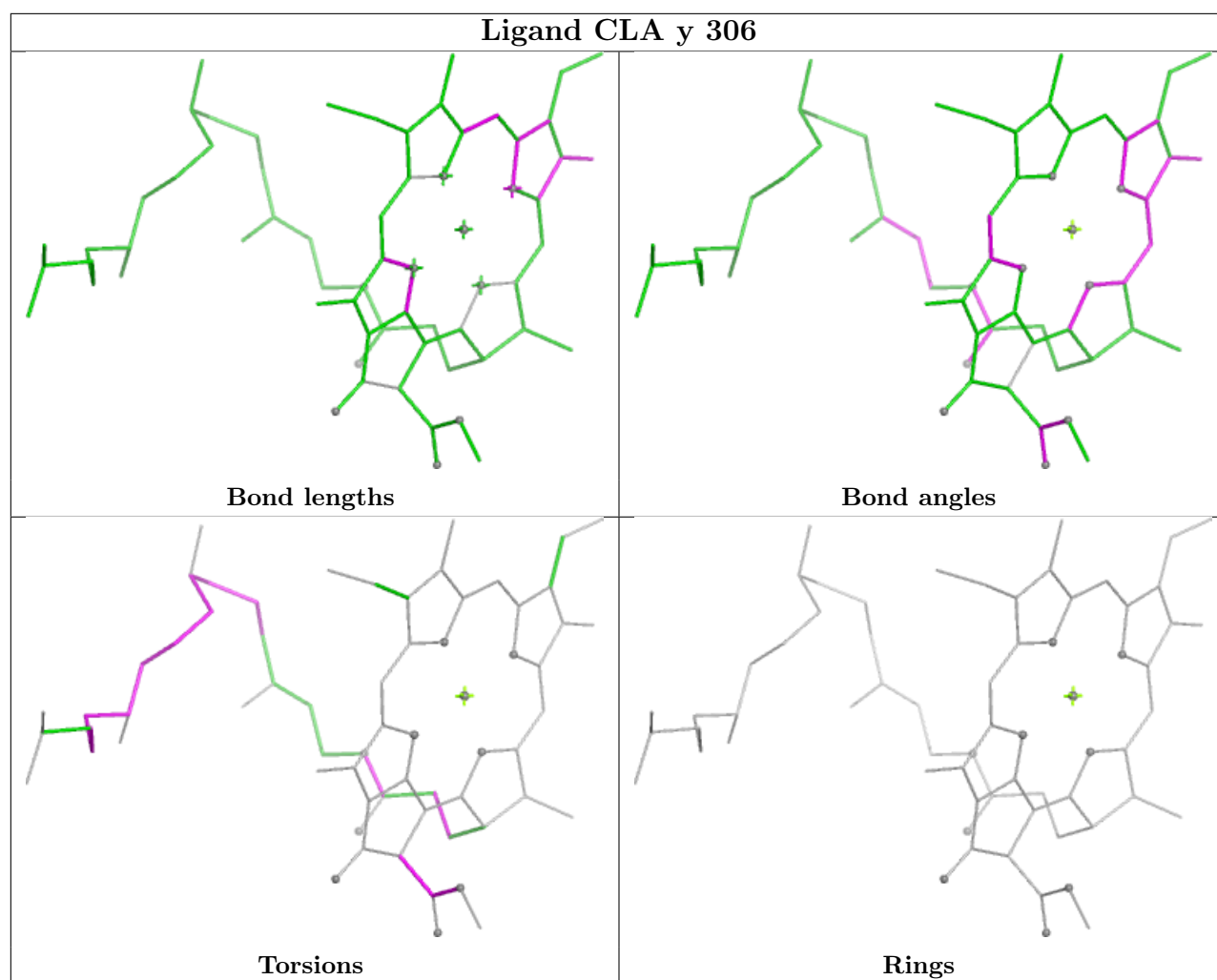


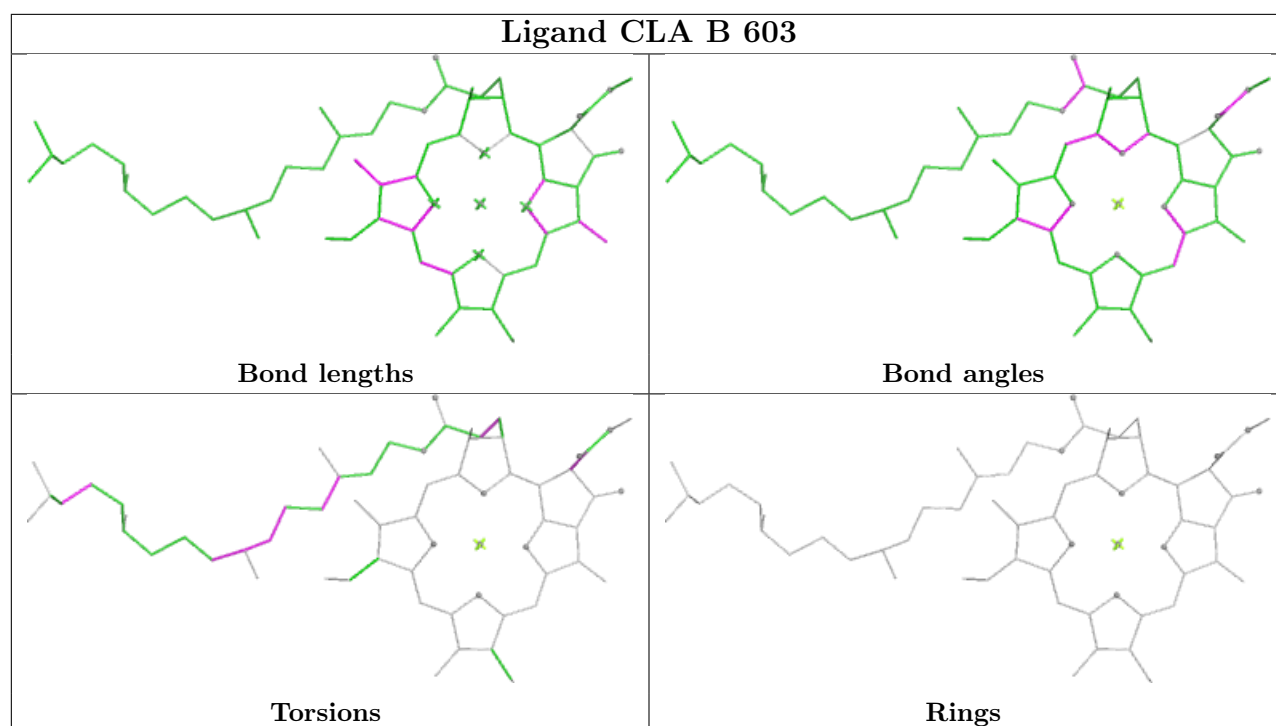


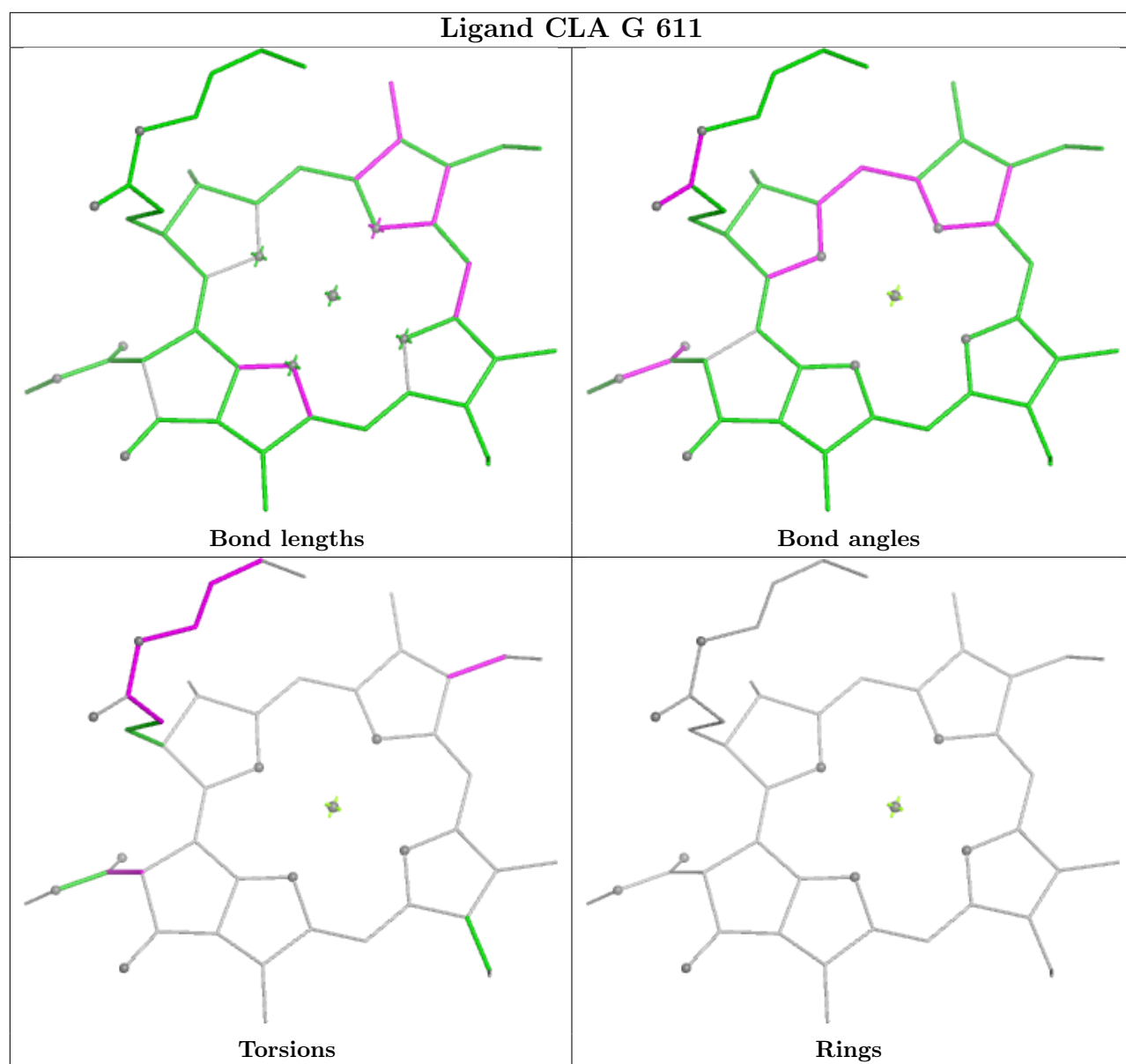


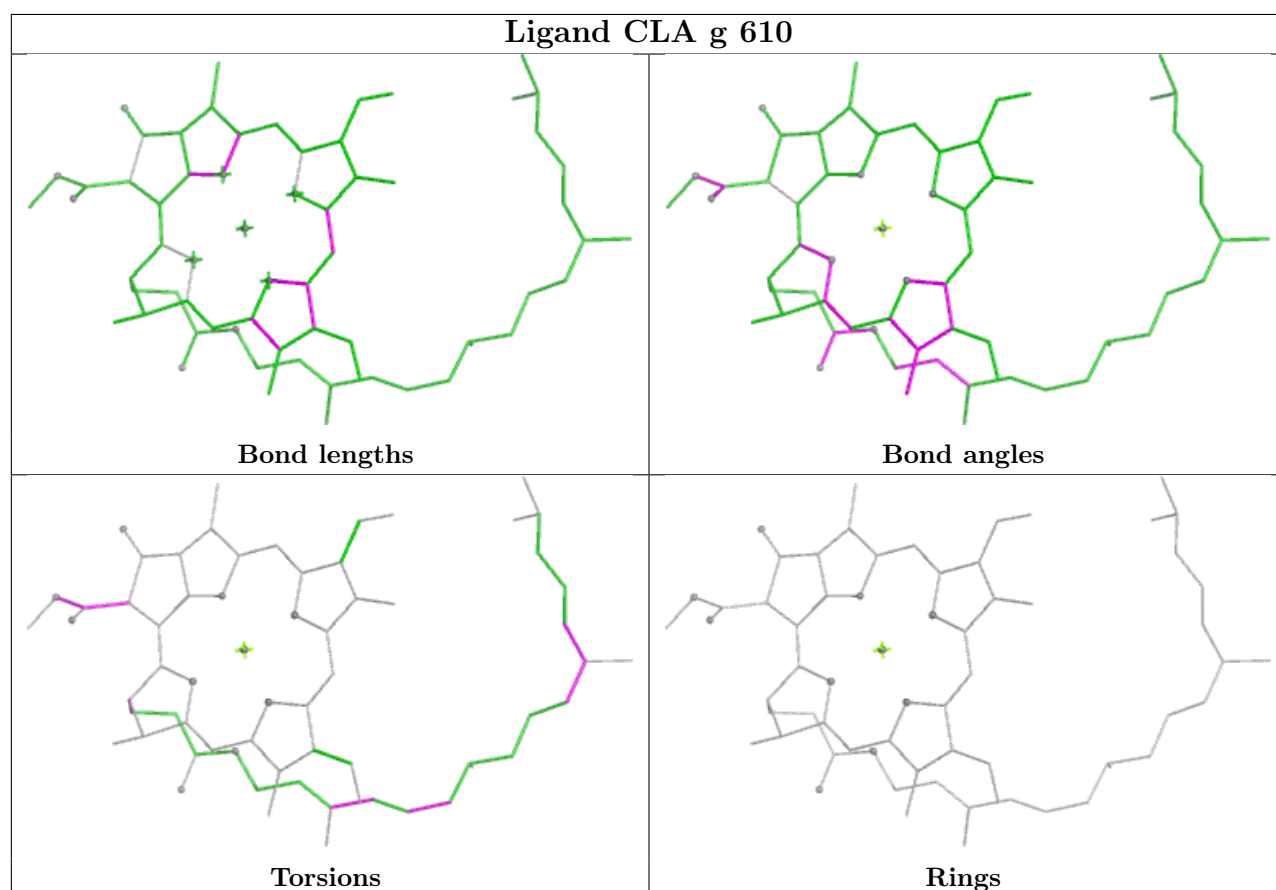
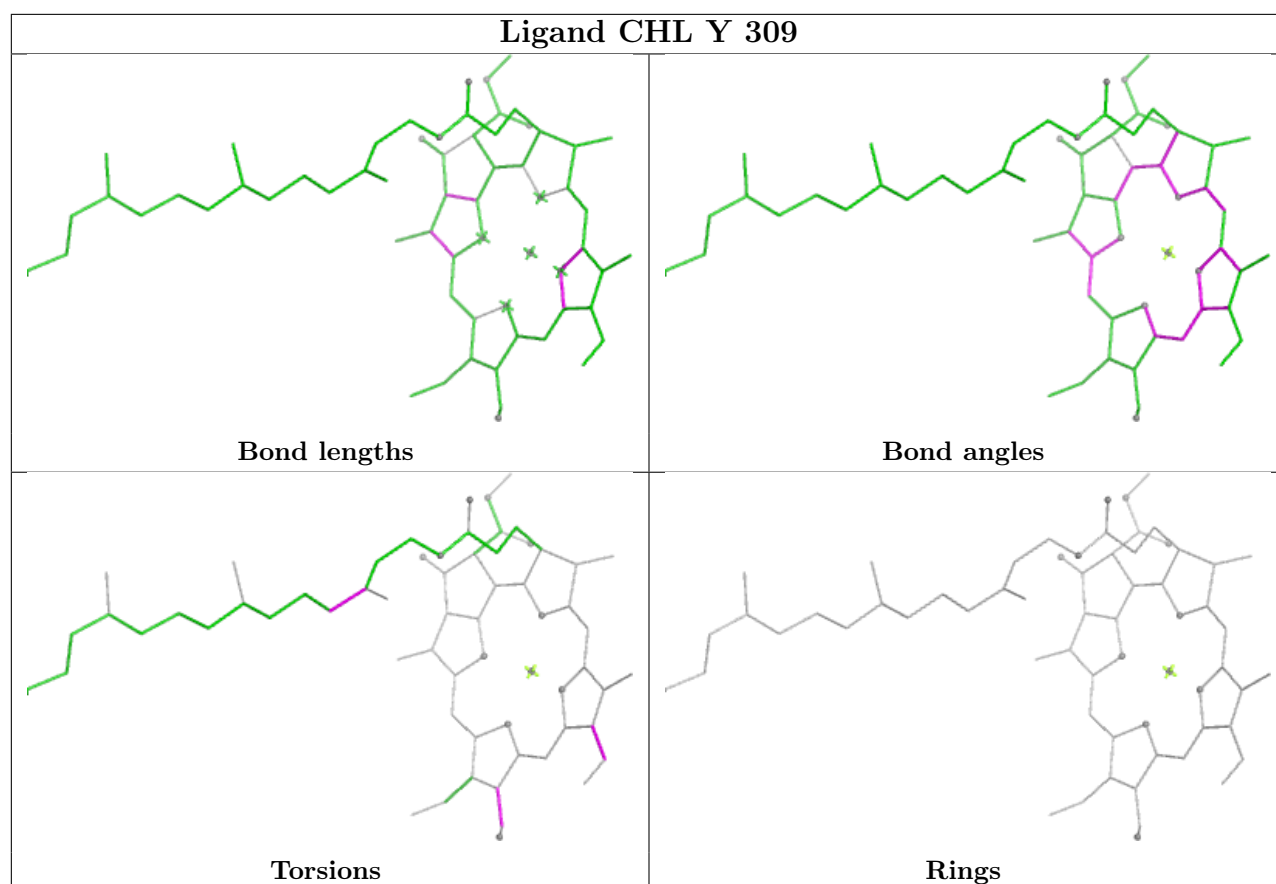


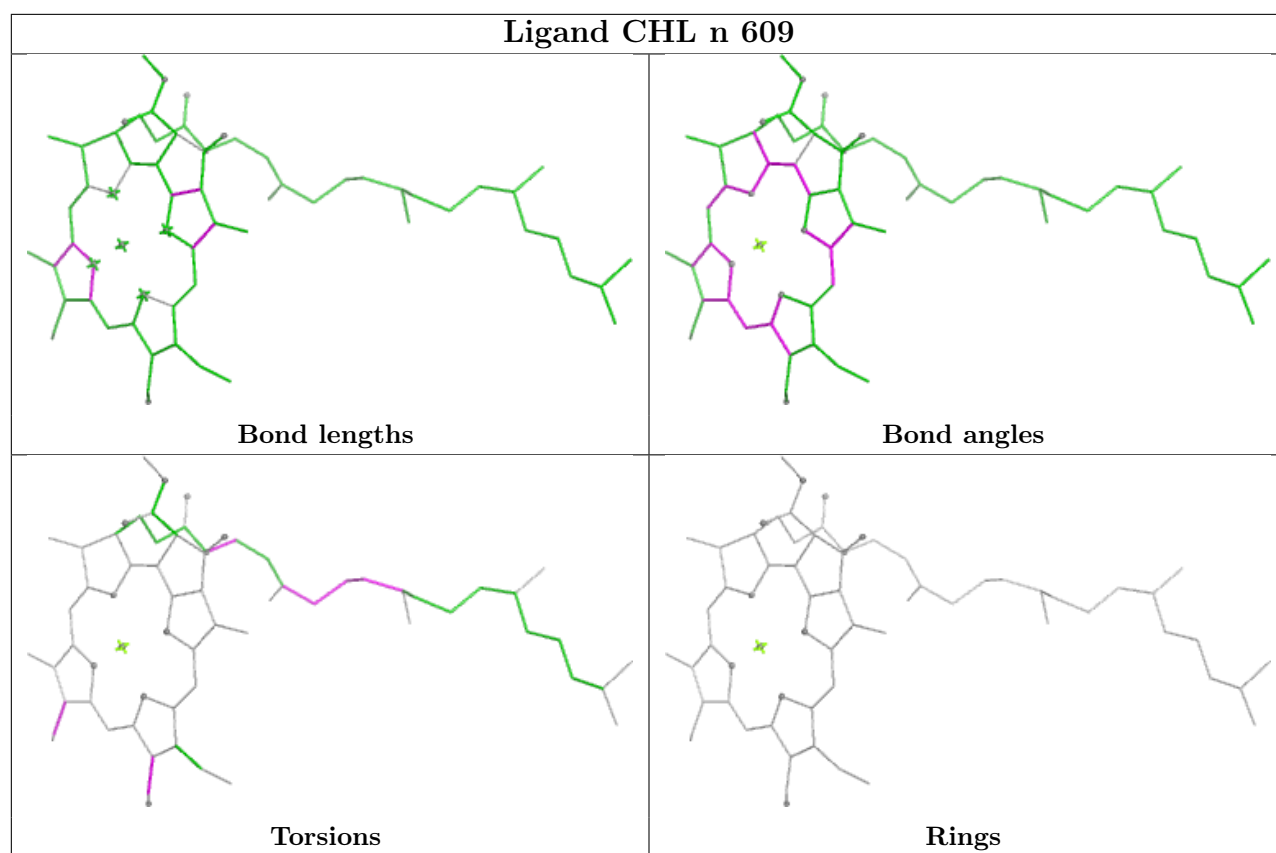
Ligand CLA C 501**Ligand CHL s 607**



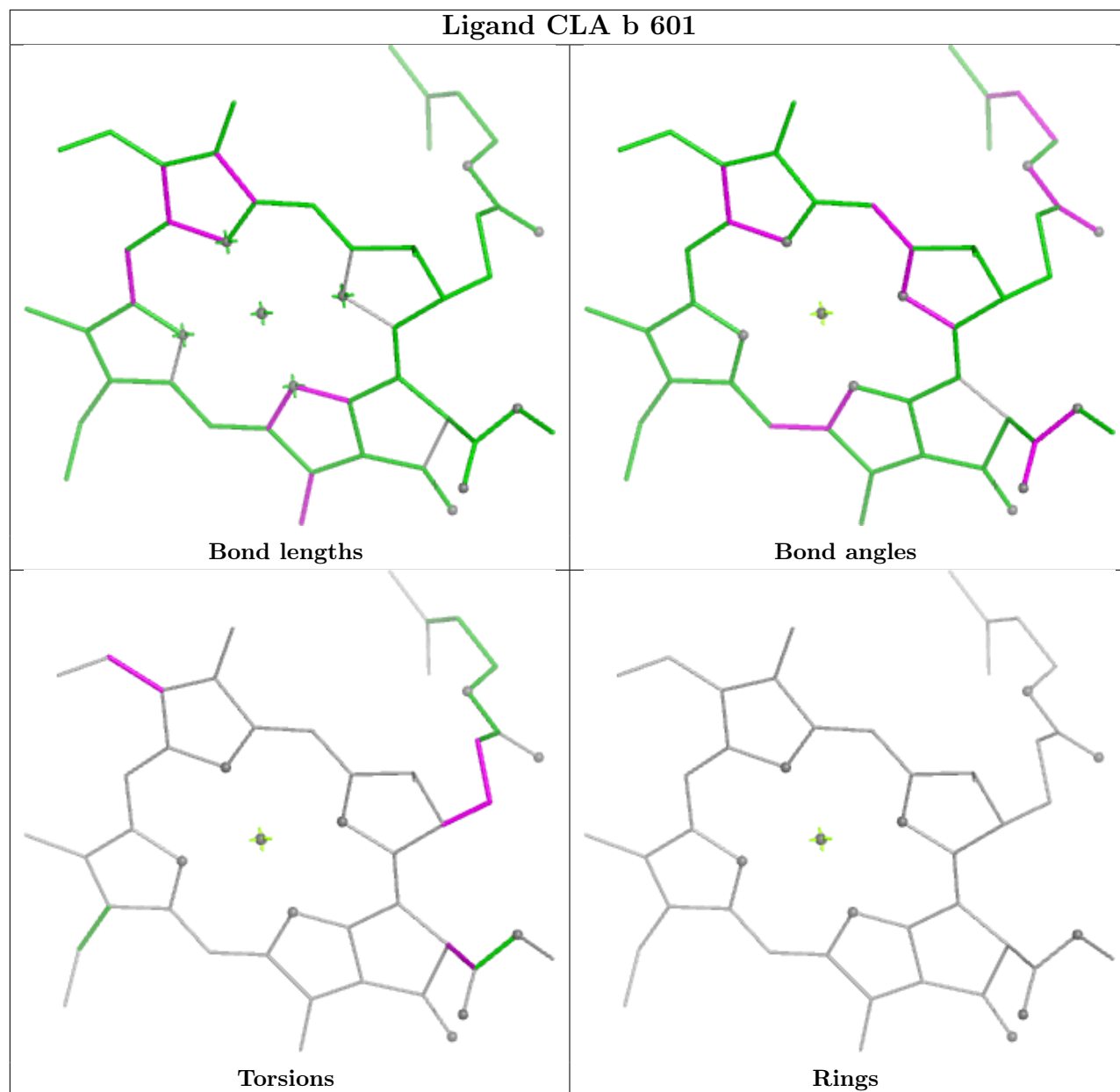


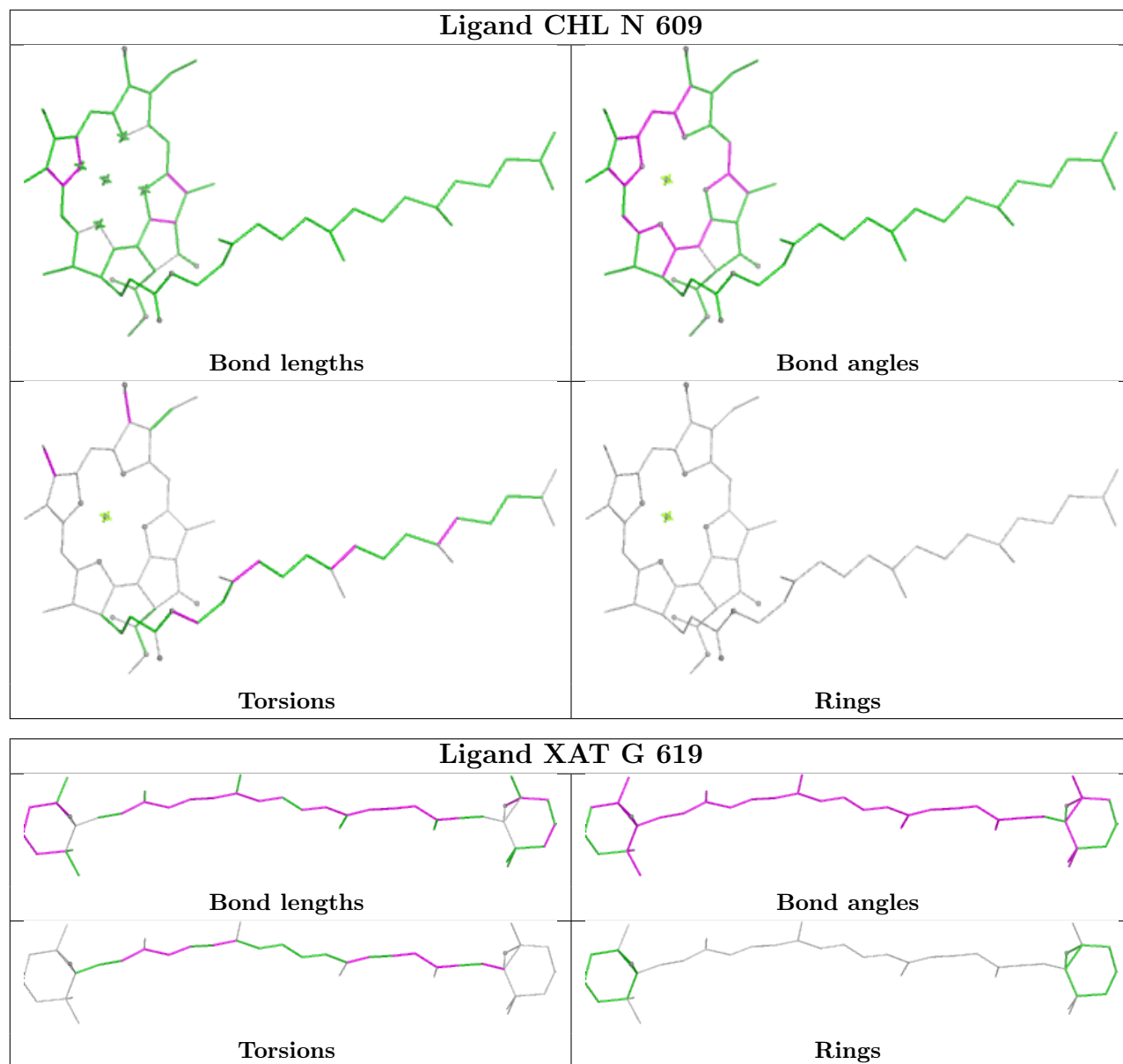


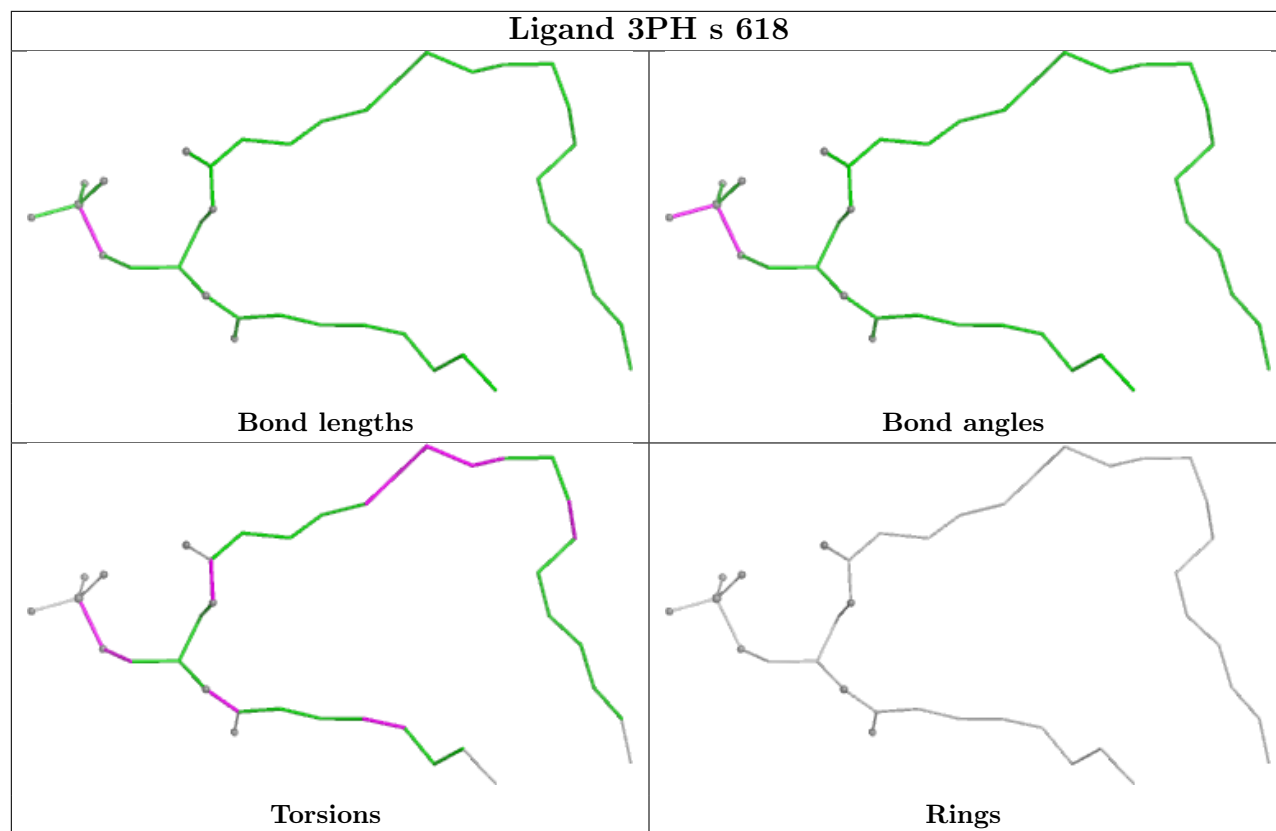


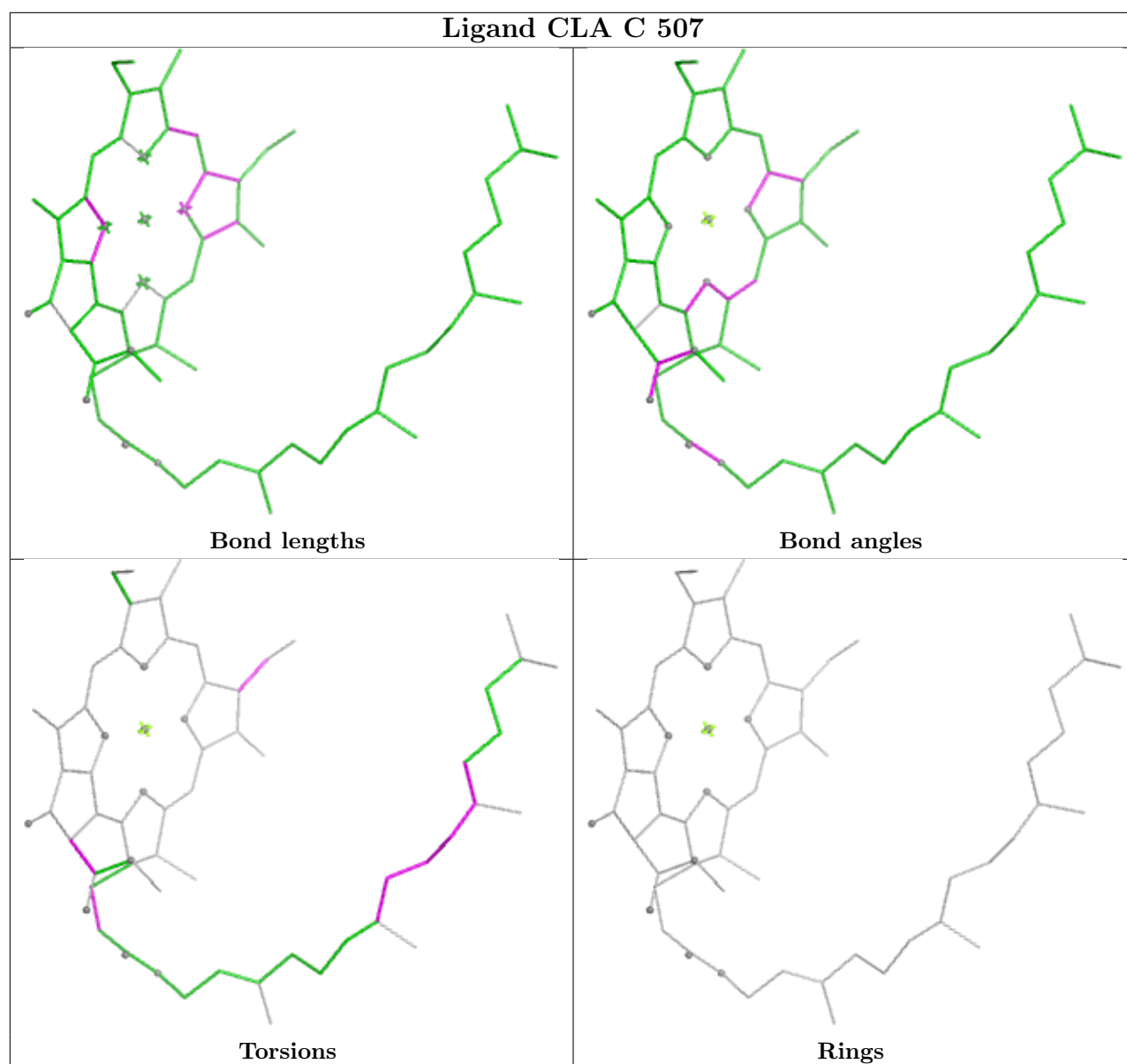


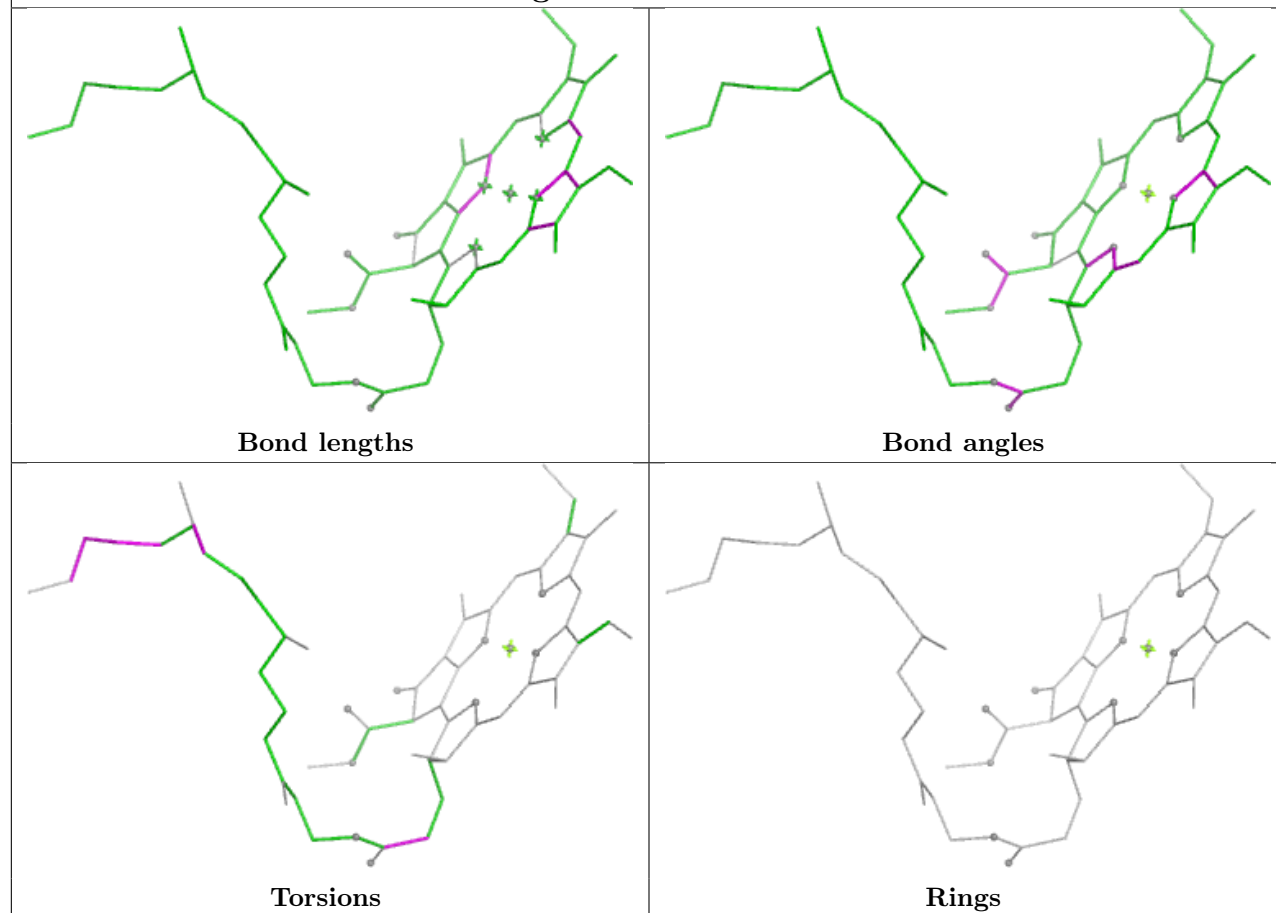
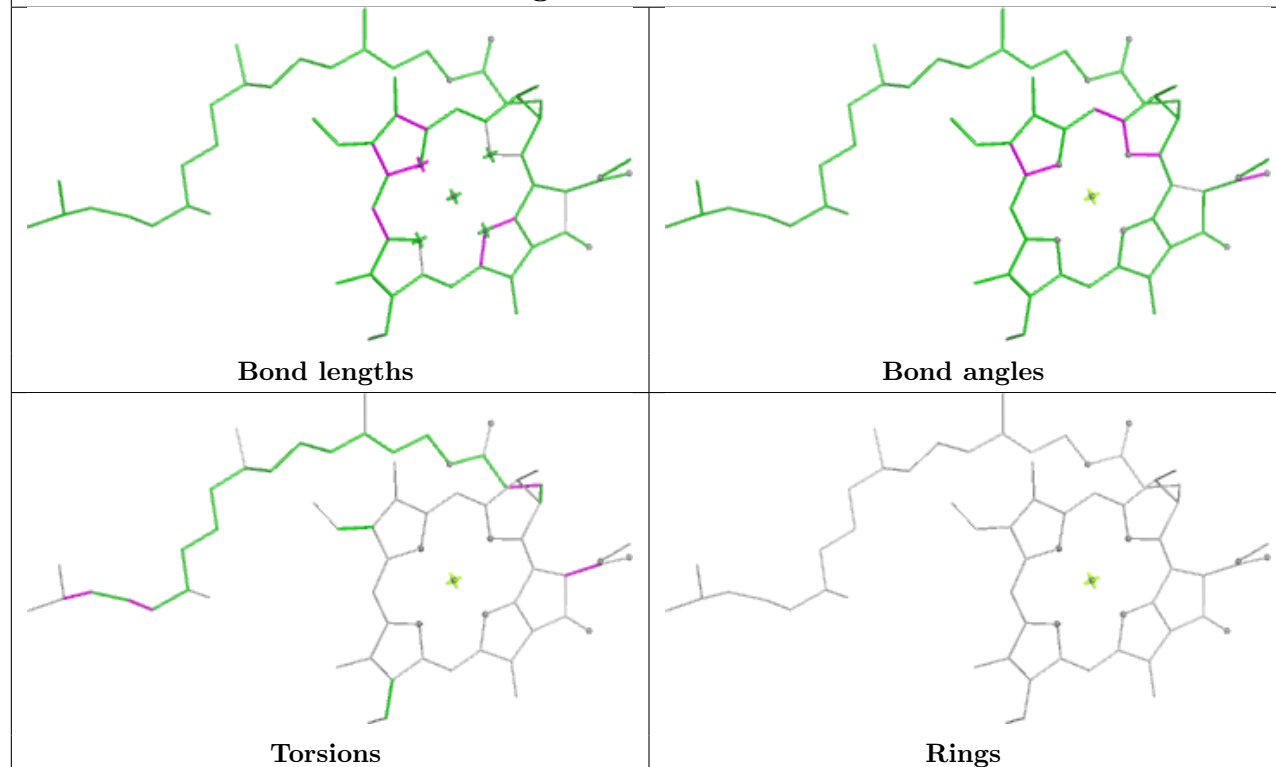
Ligand CLA b 601

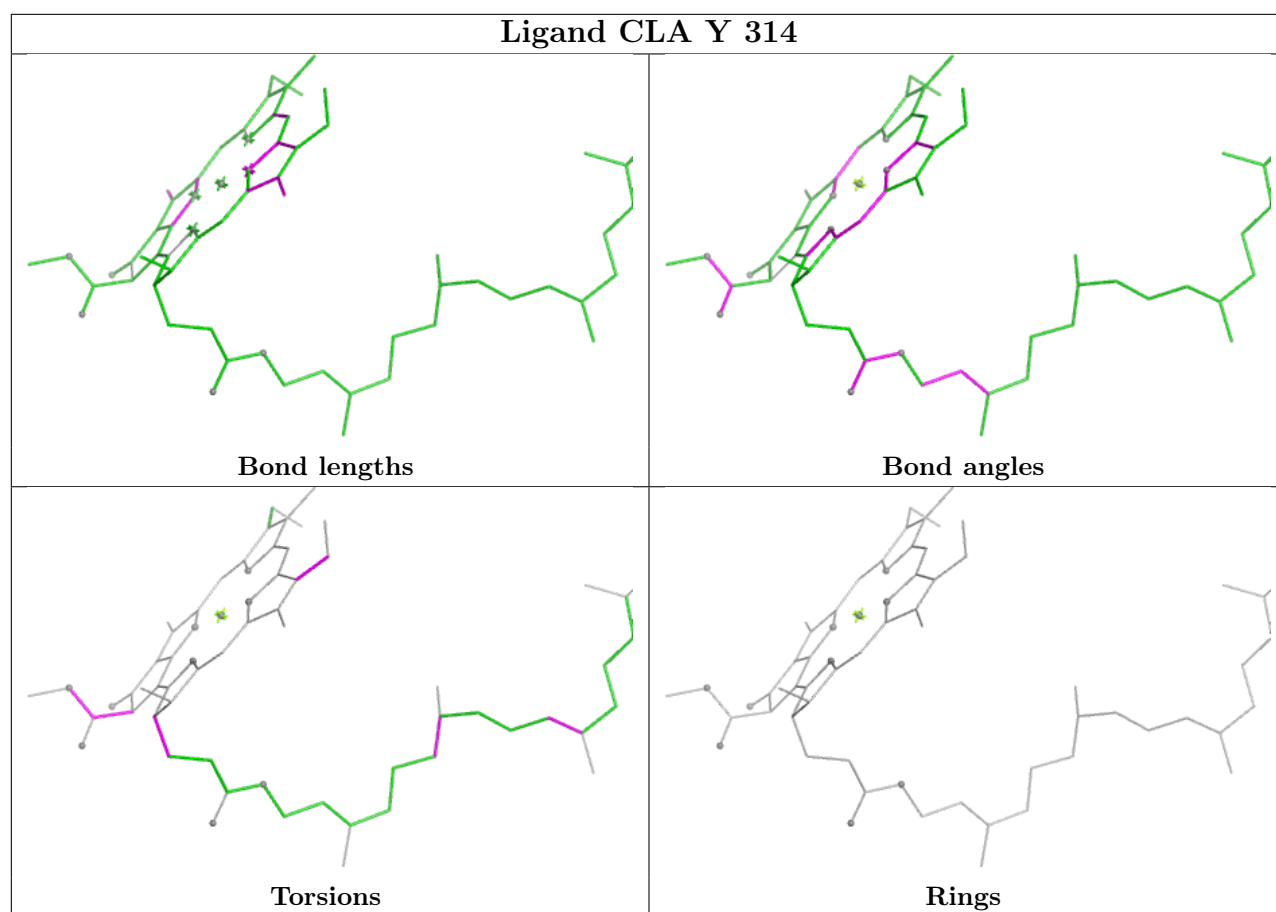




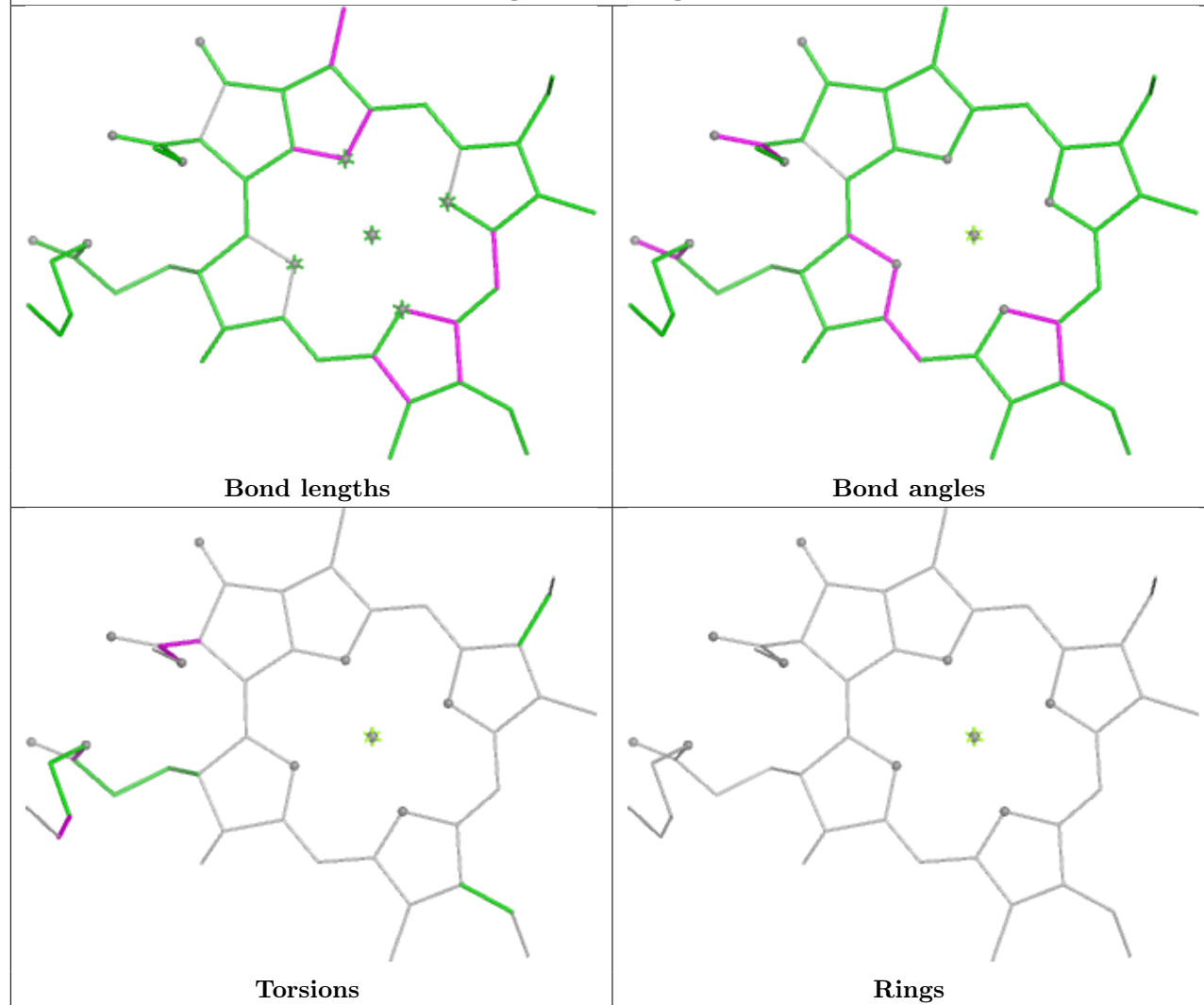




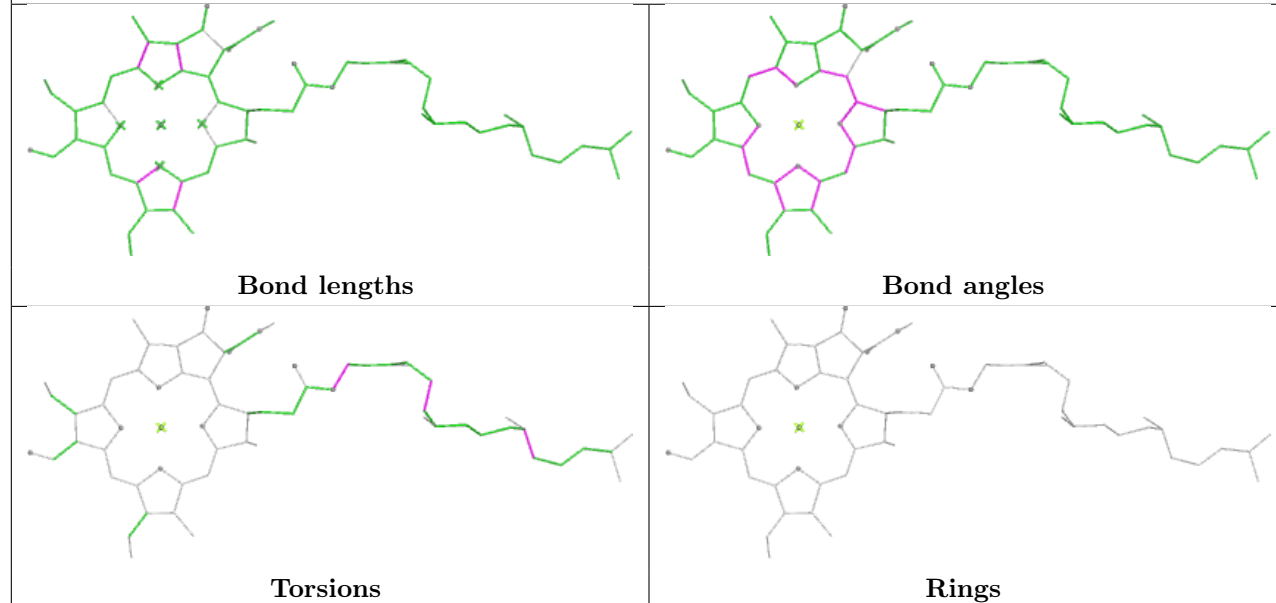
Ligand CLA B 613**Ligand CLA R 602**



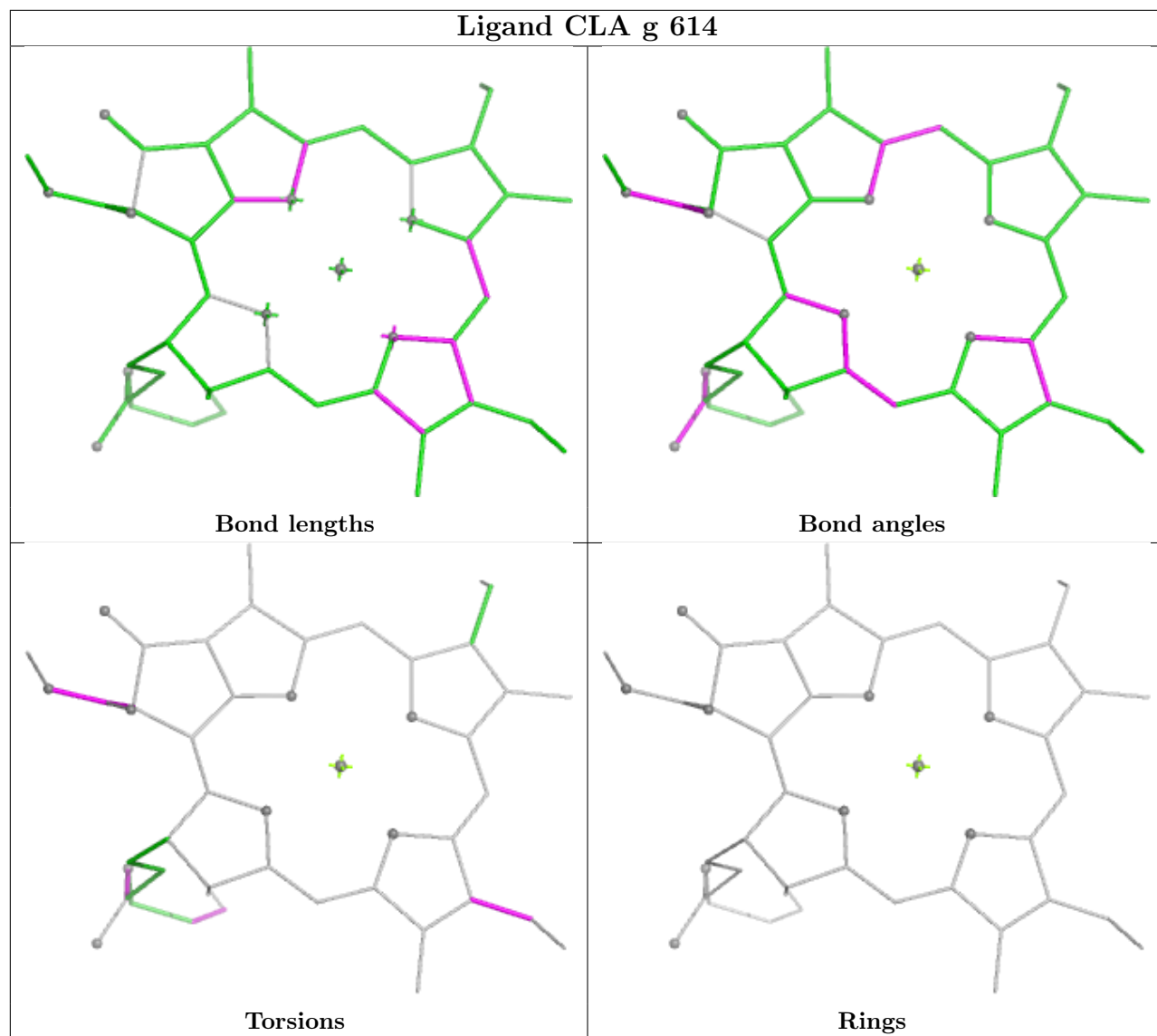
Ligand CLA g 612

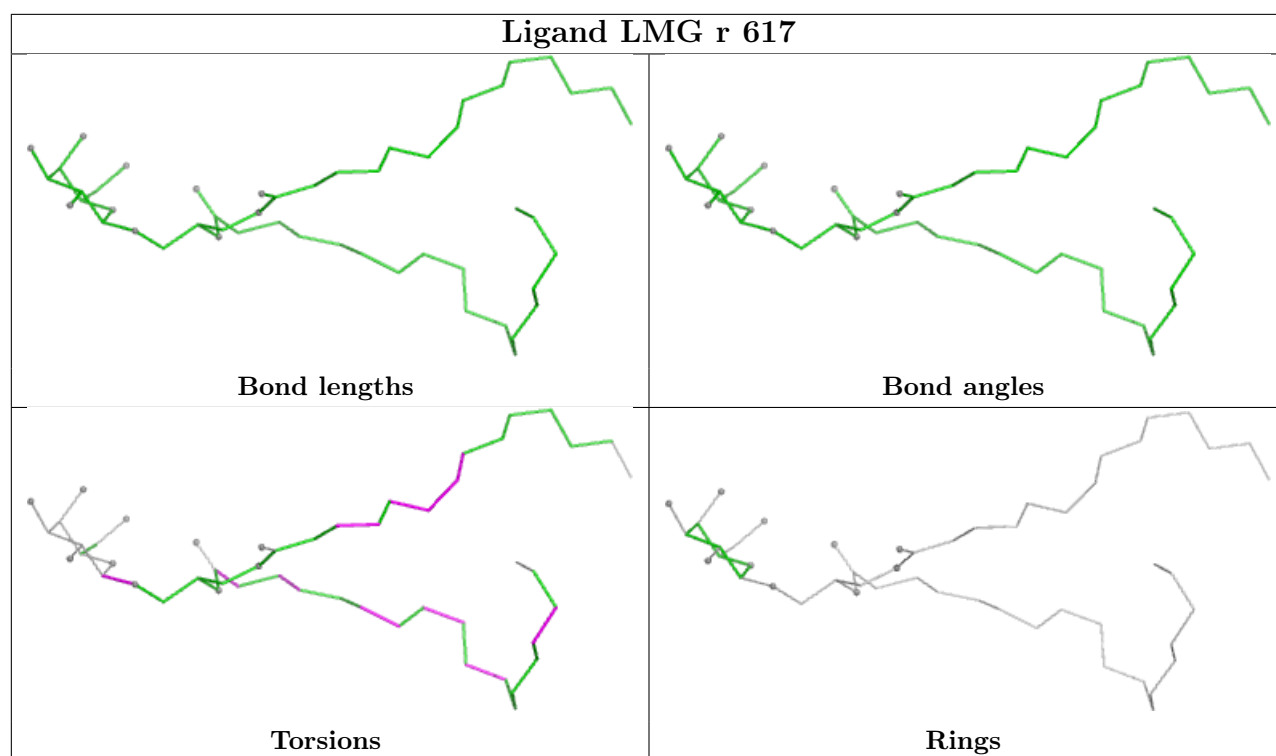


Ligand CHL Y 307

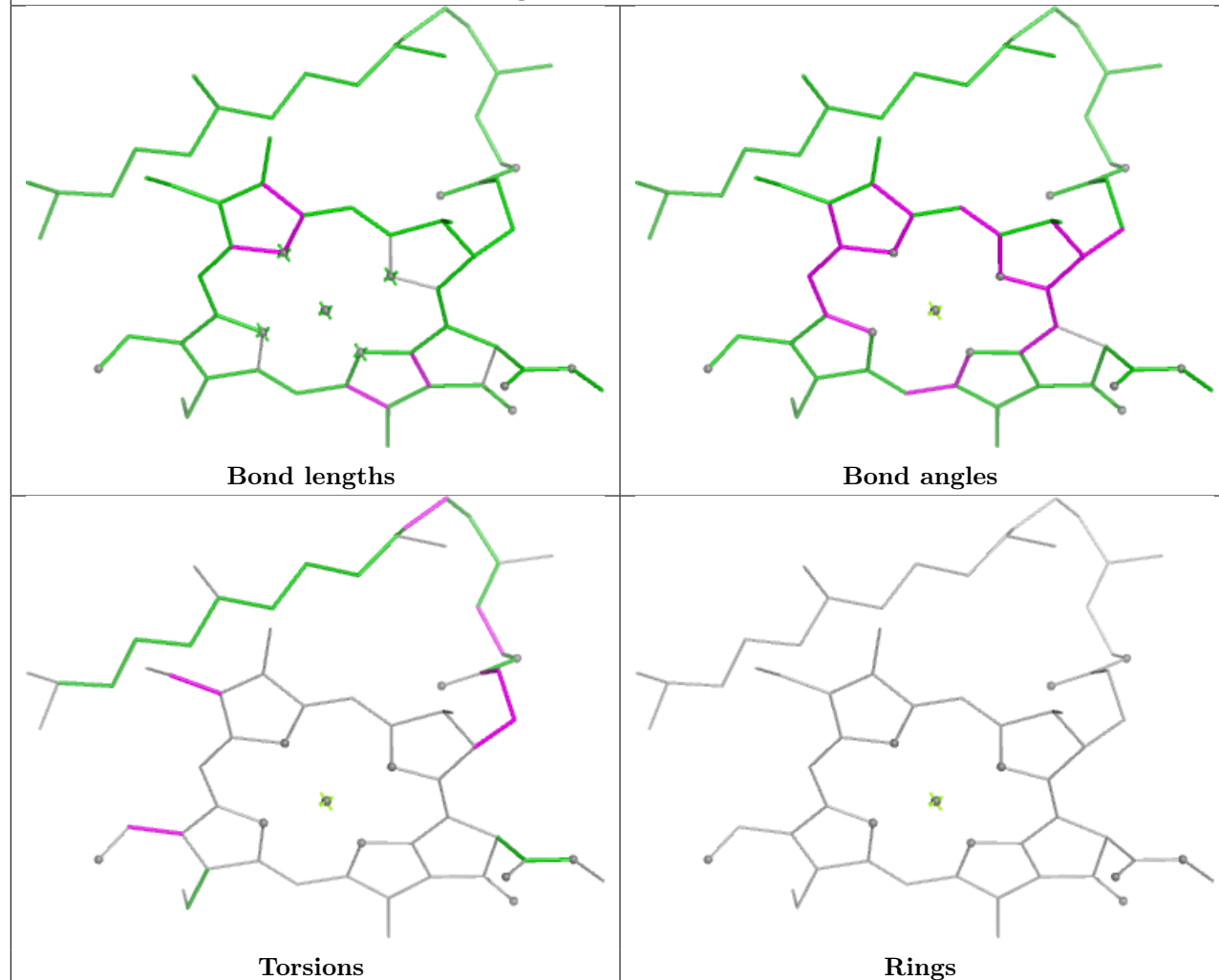


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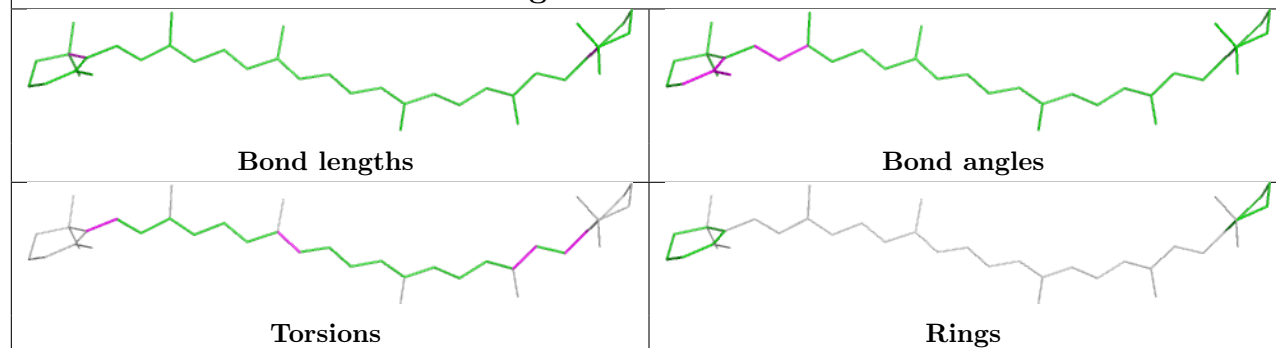




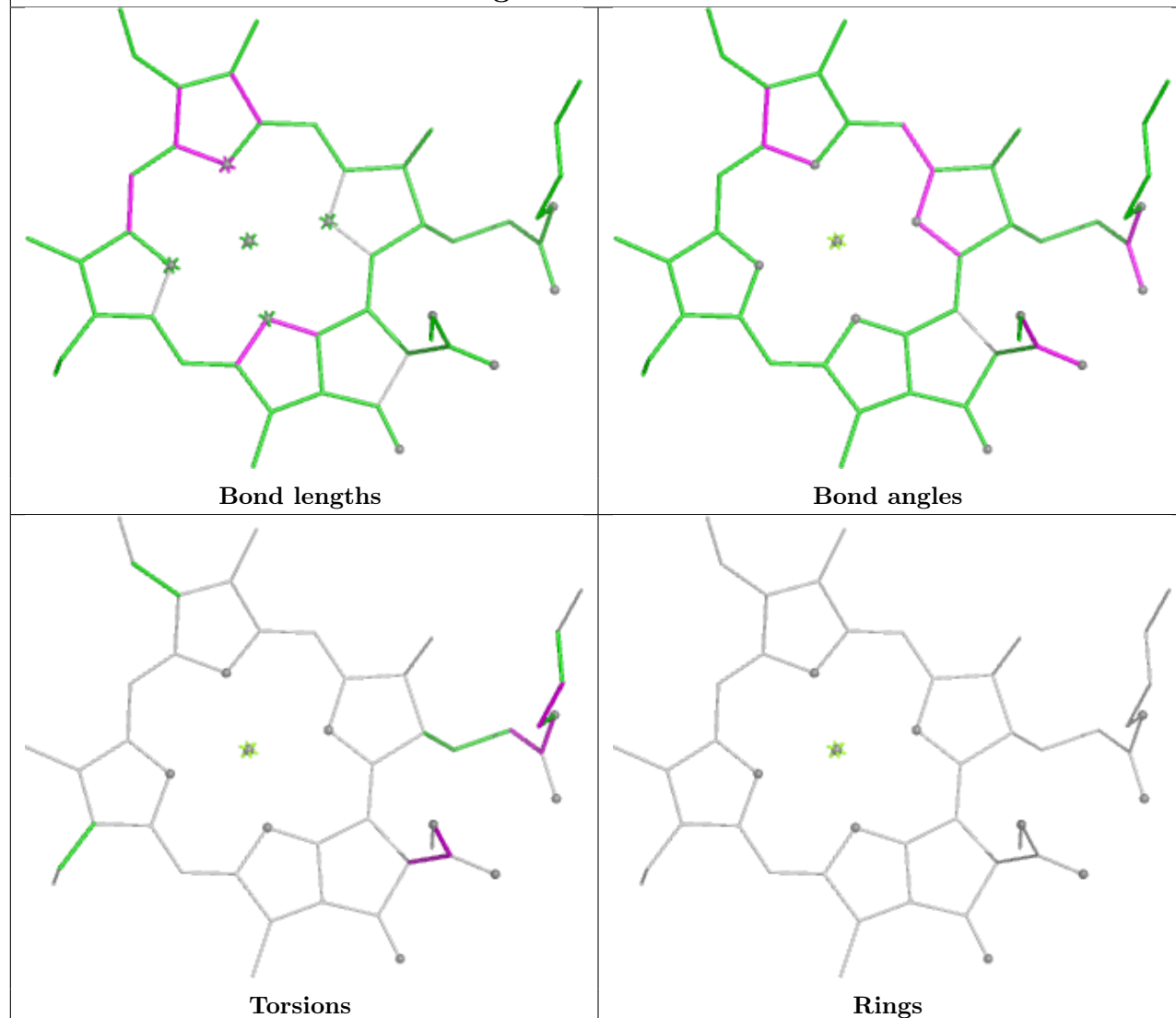
Ligand CHL r 607



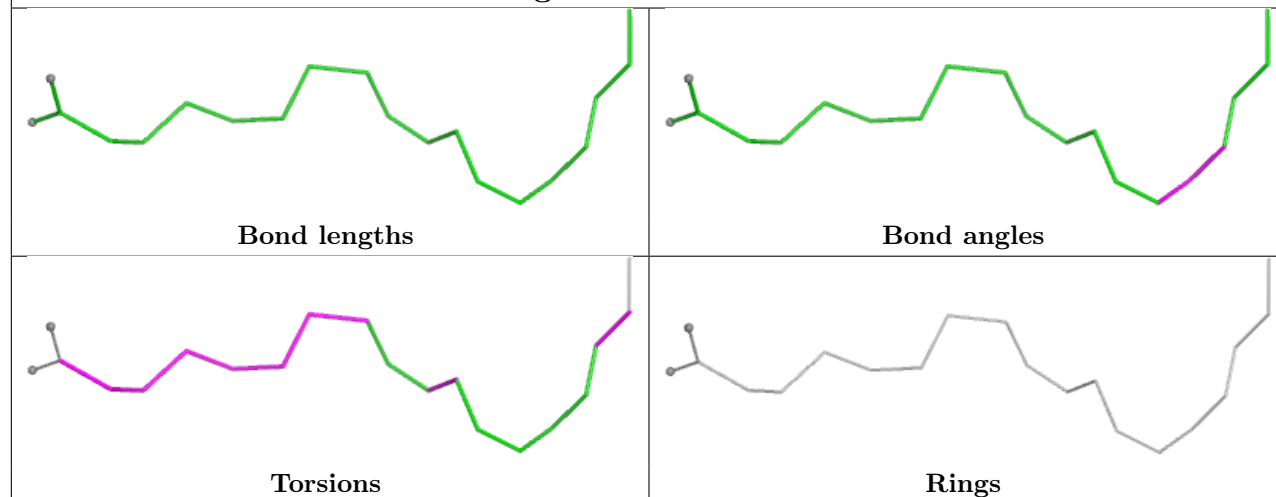
Ligand BCR H 501



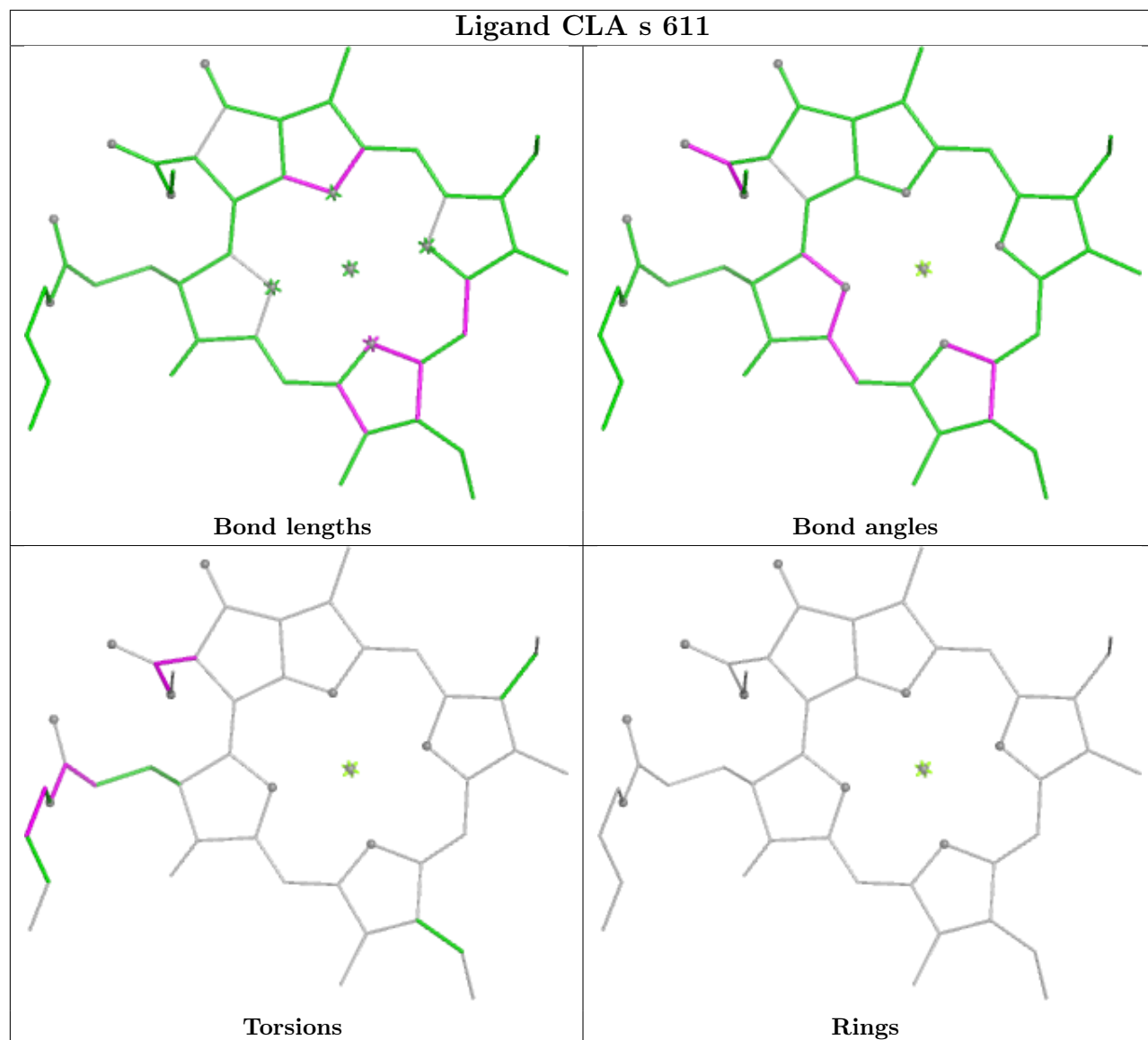
Ligand CLA S 611

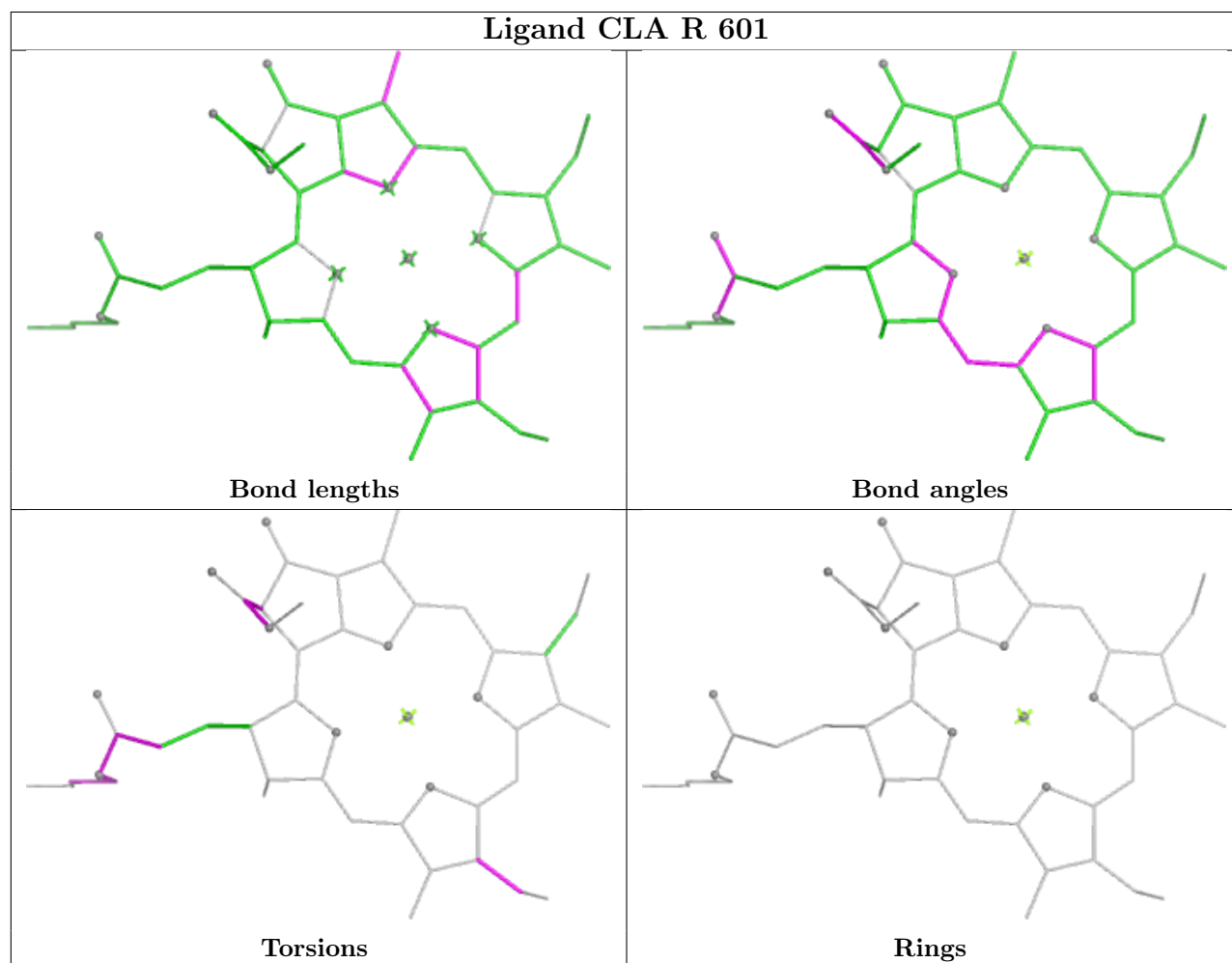
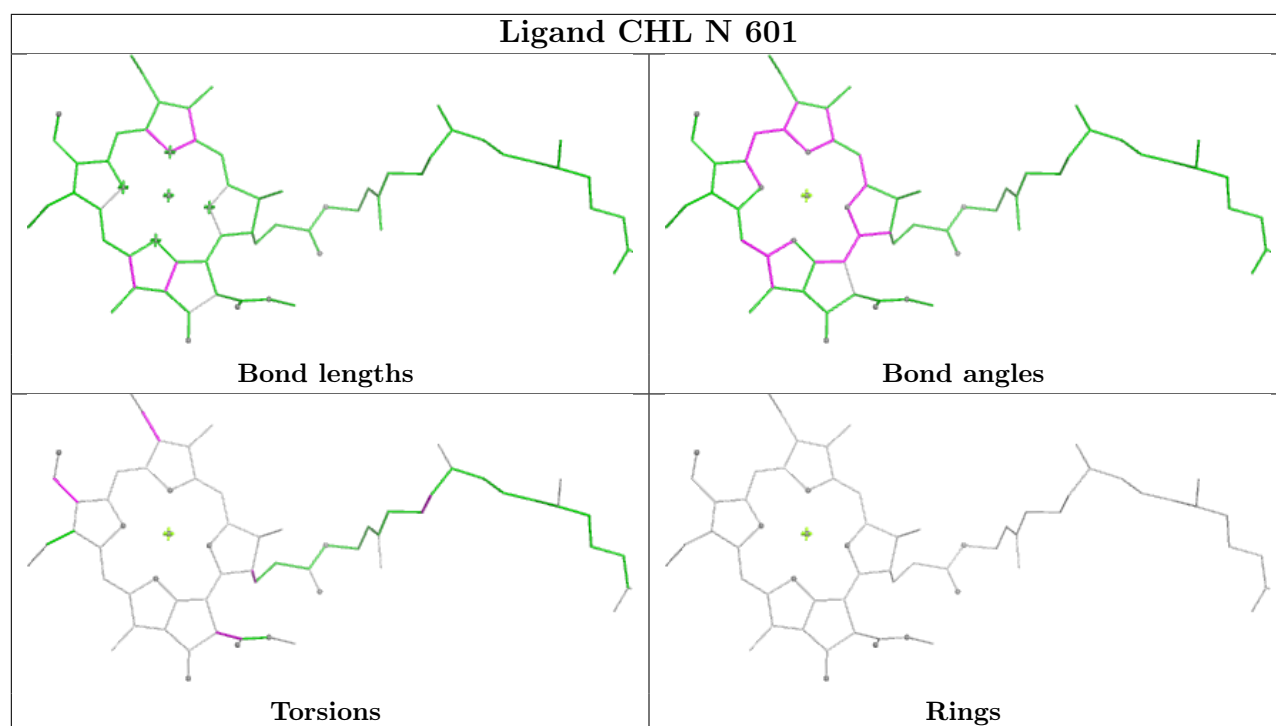


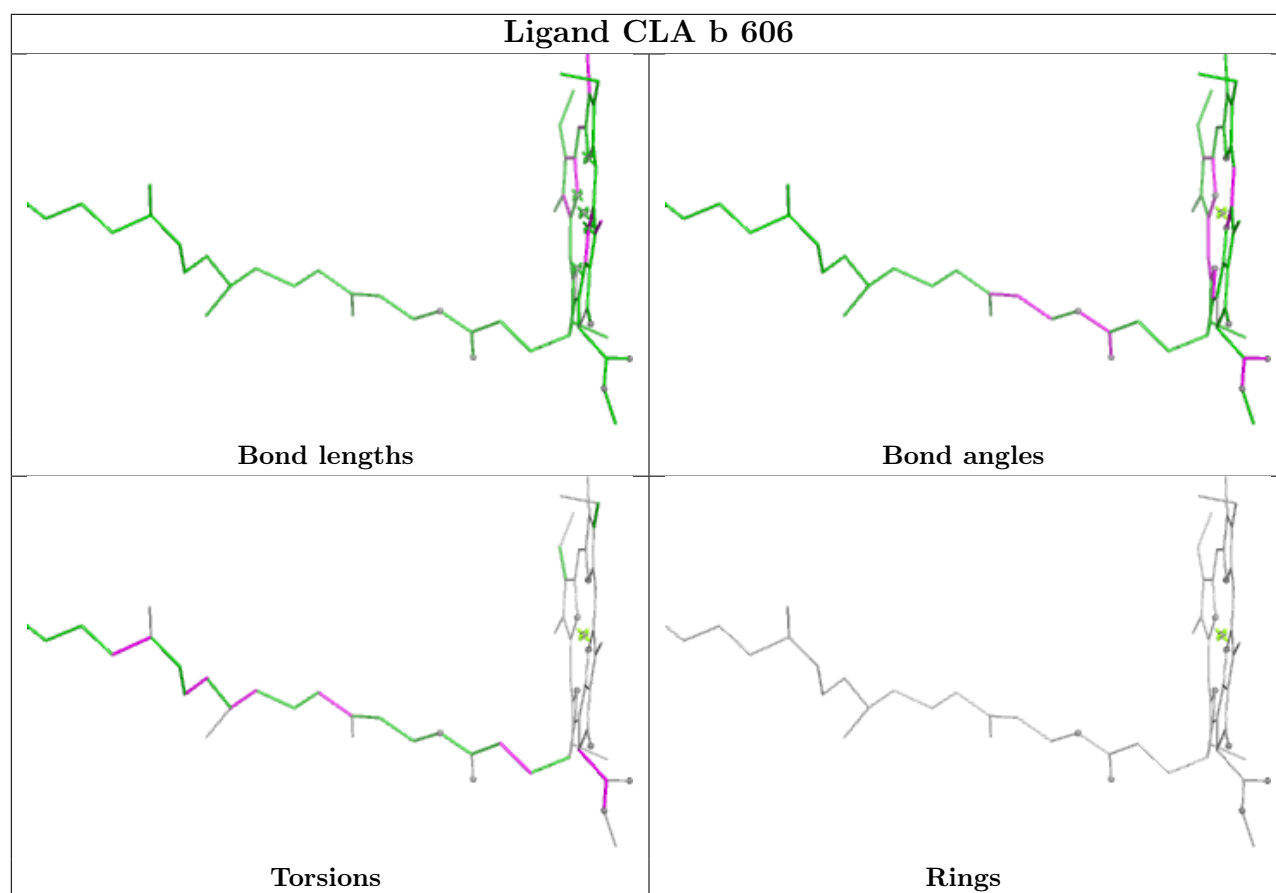
Ligand LNL B 623



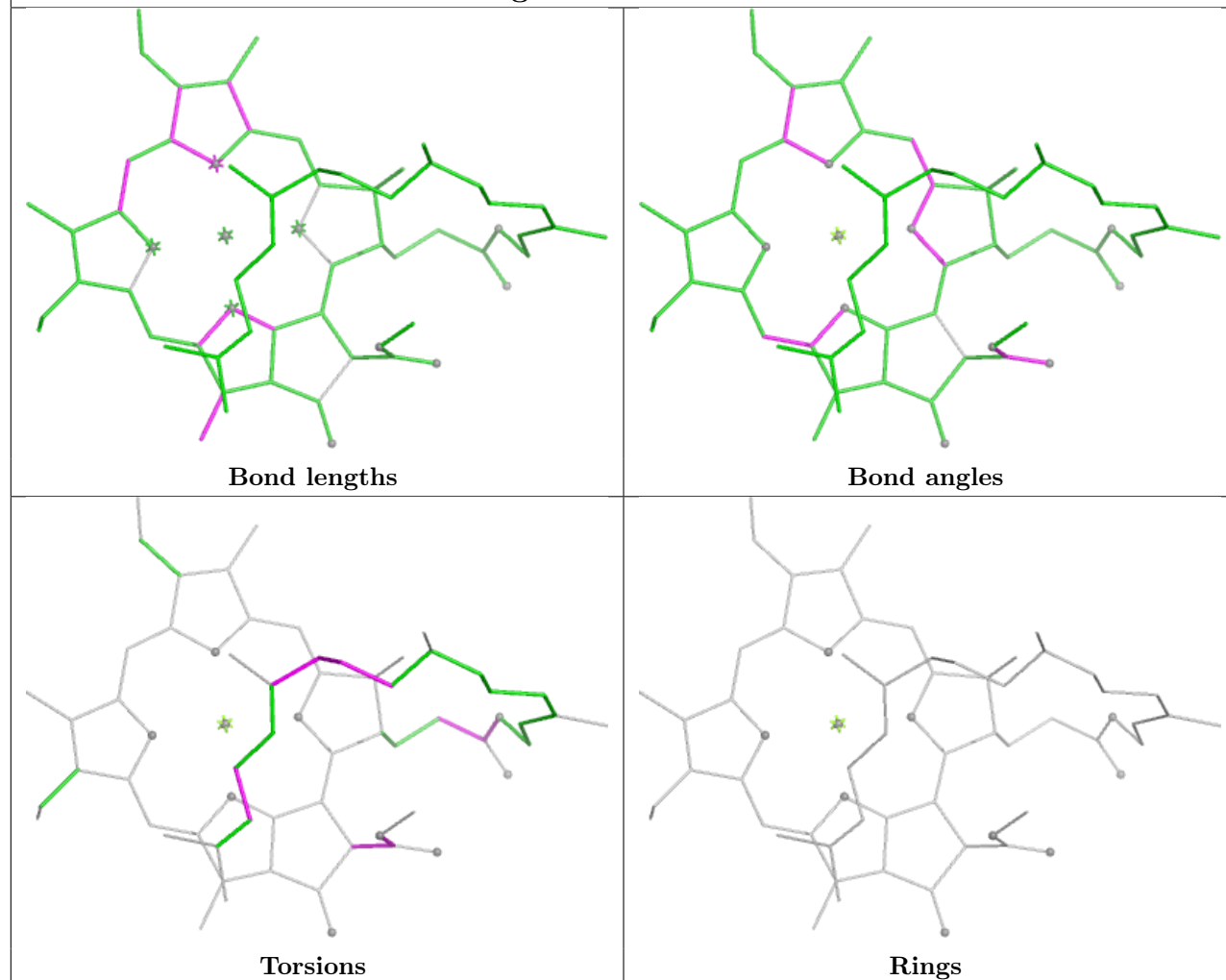
Ligand CLA s 611



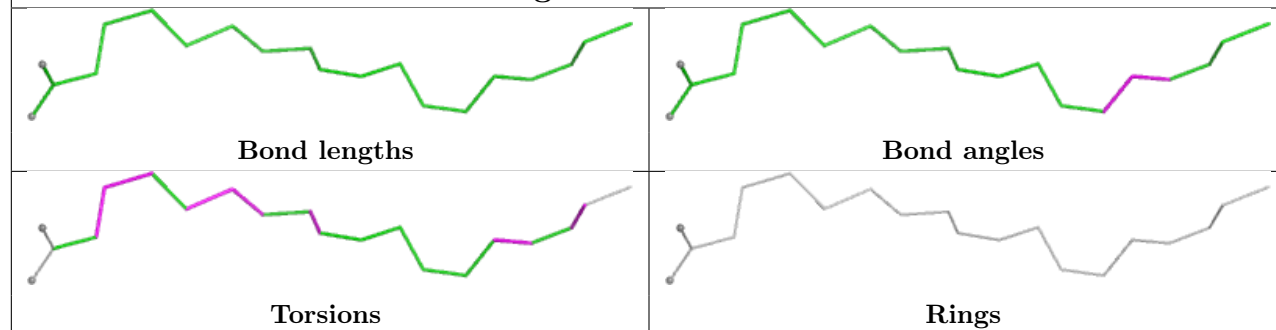


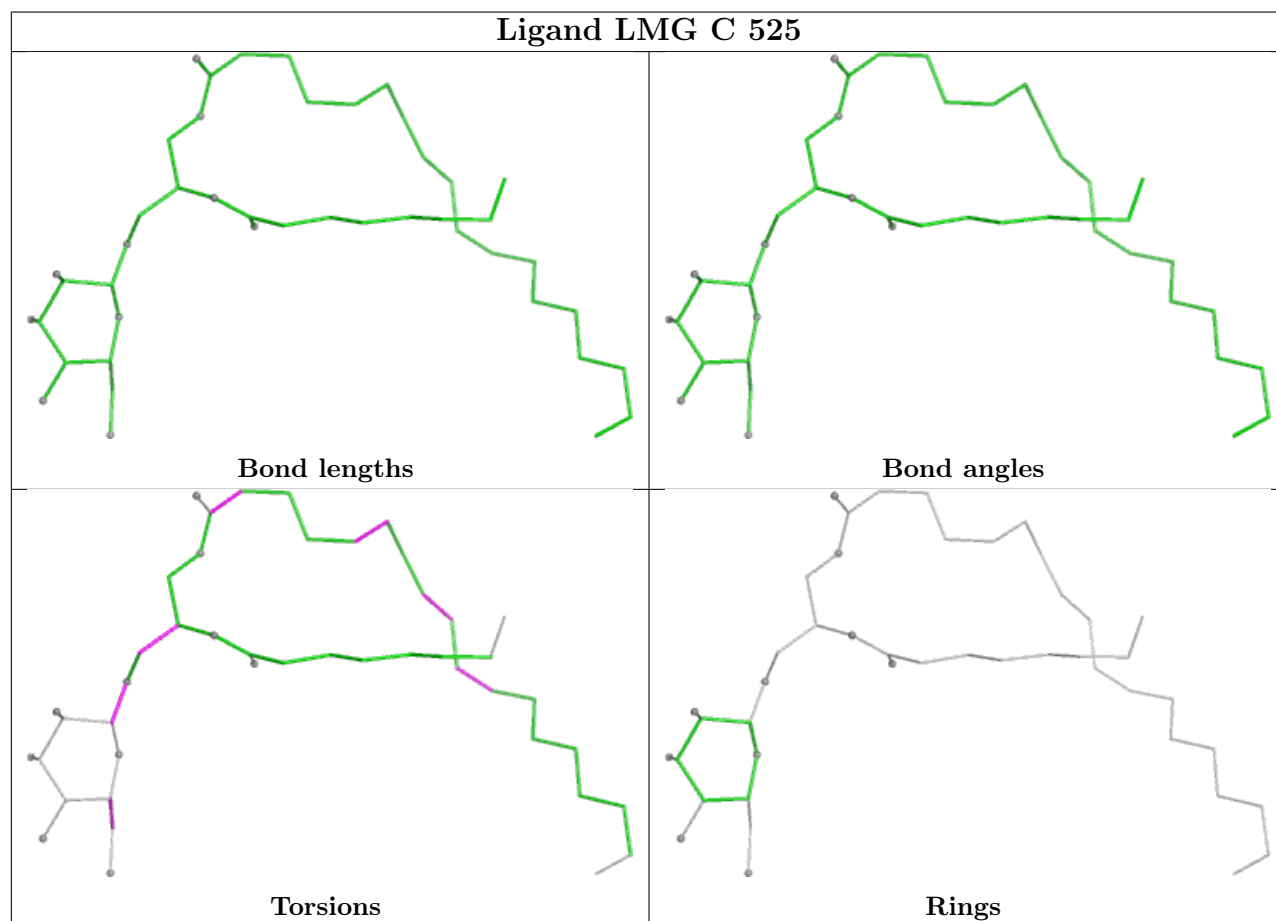
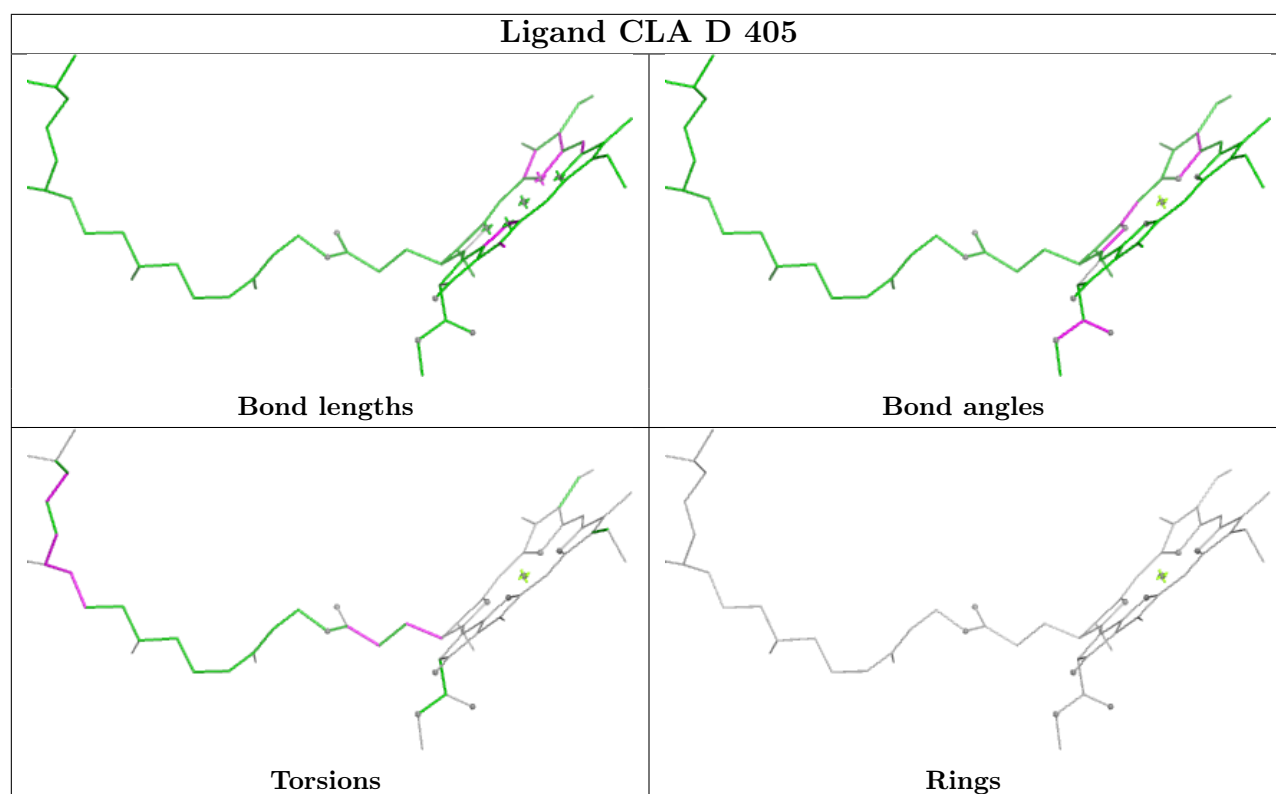


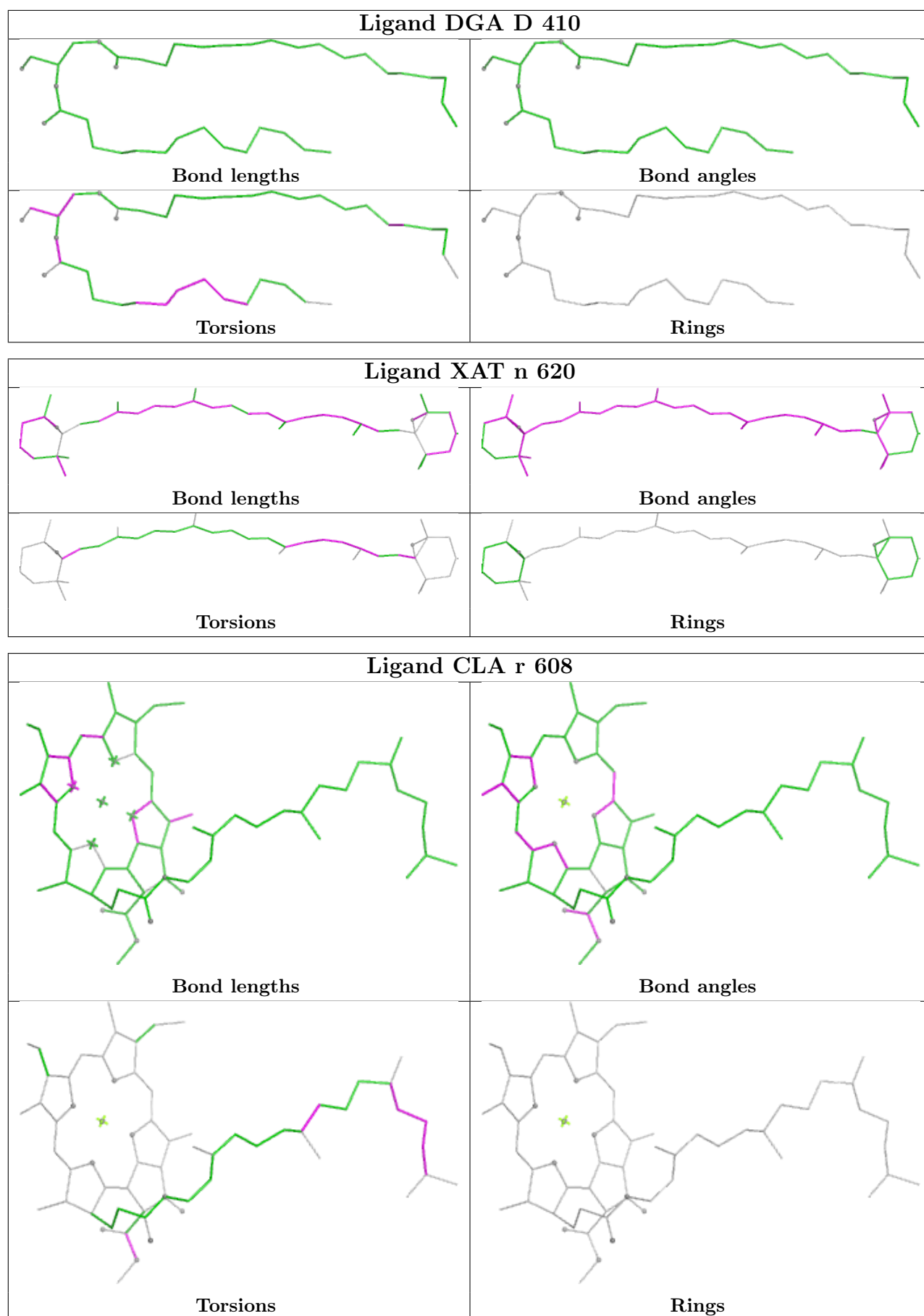
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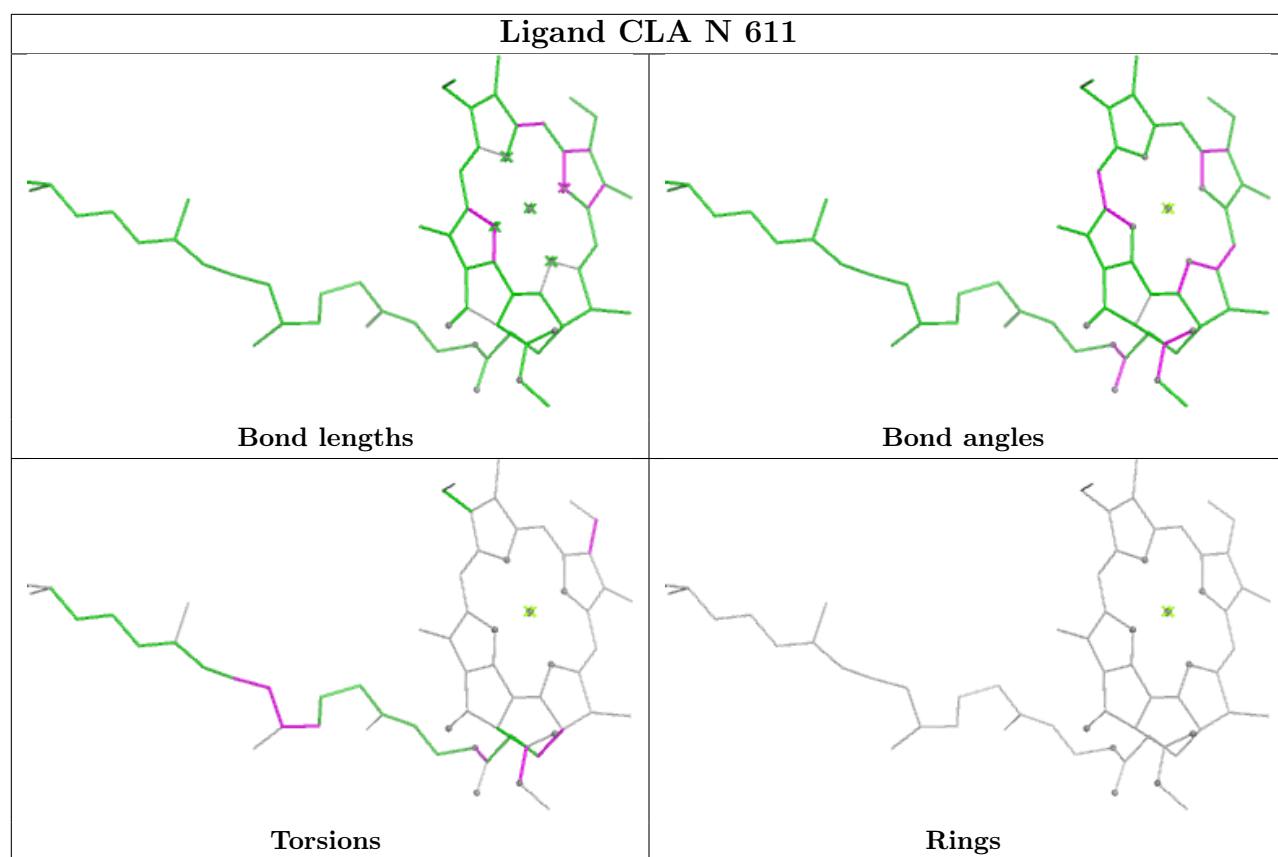


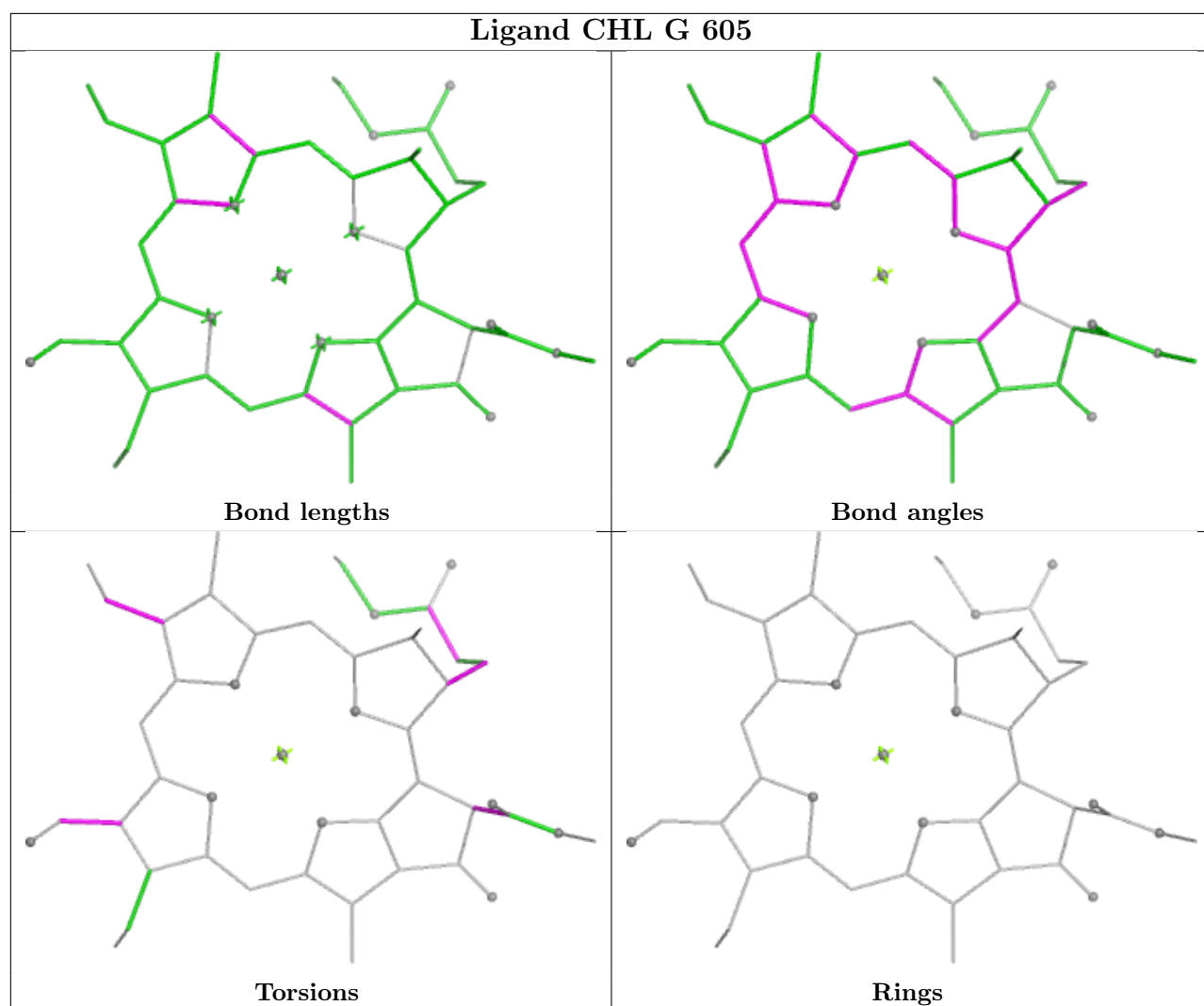
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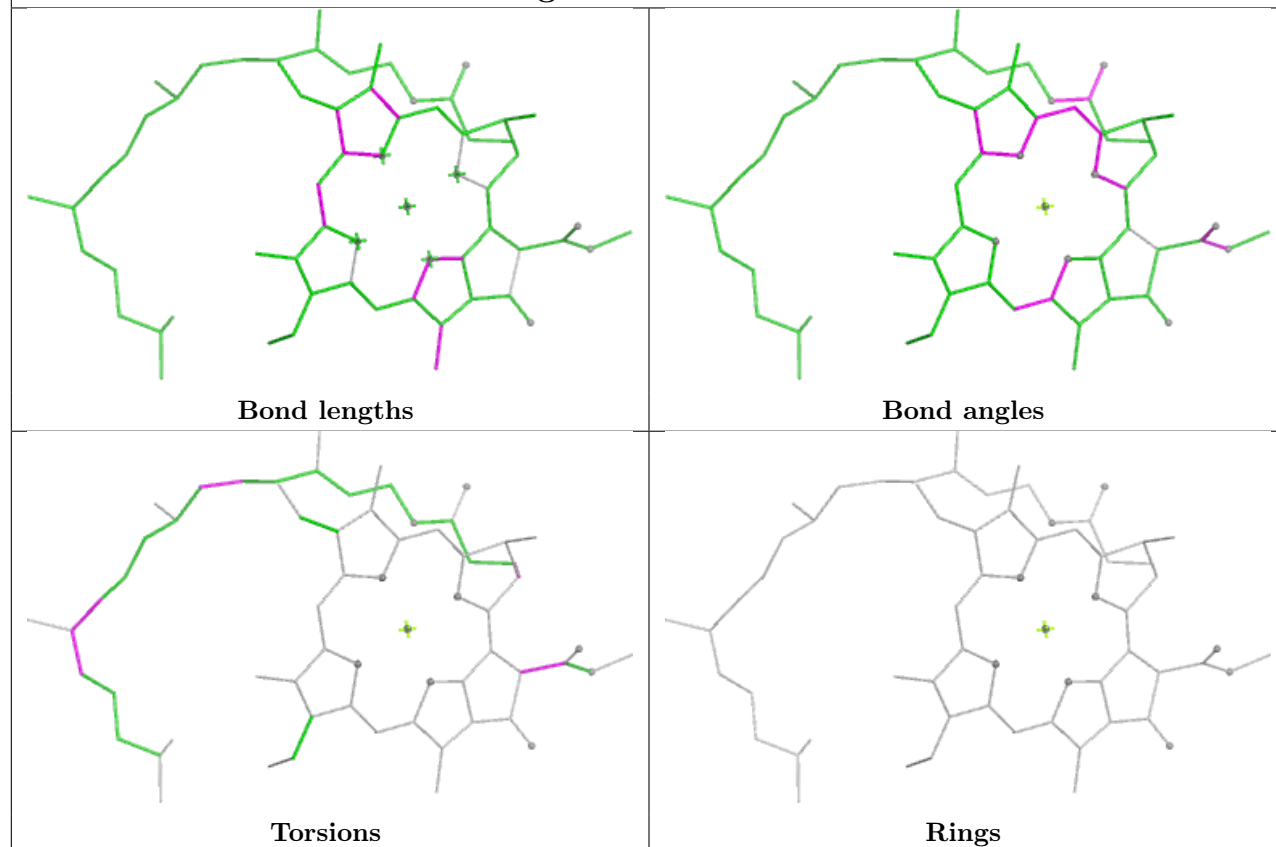




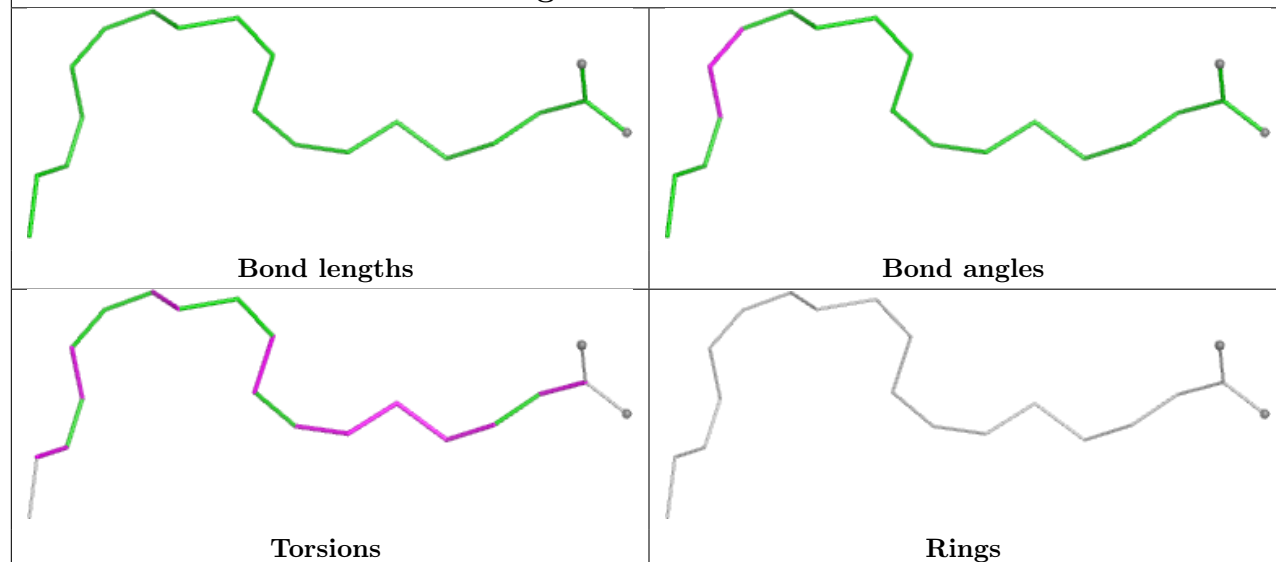


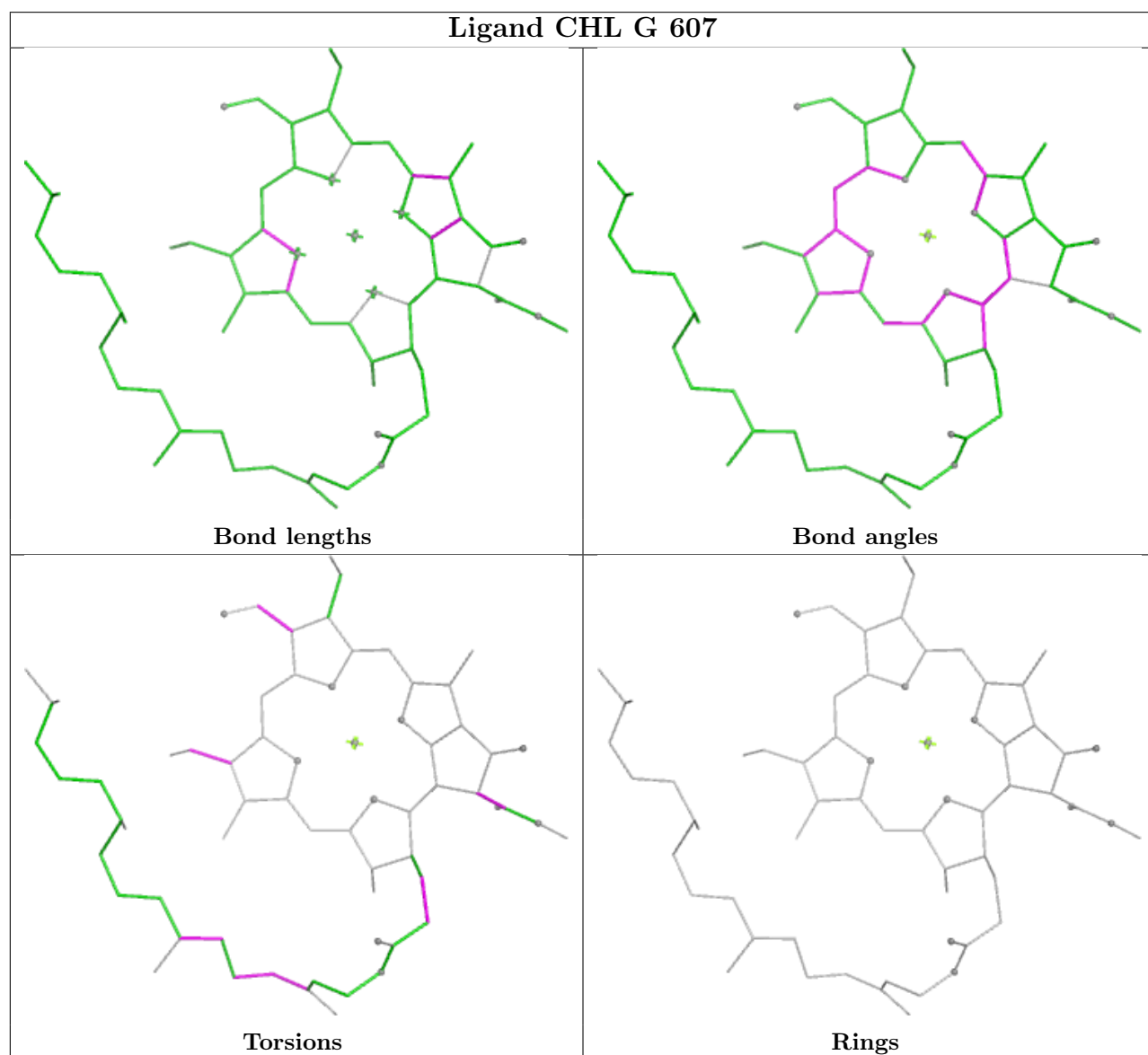
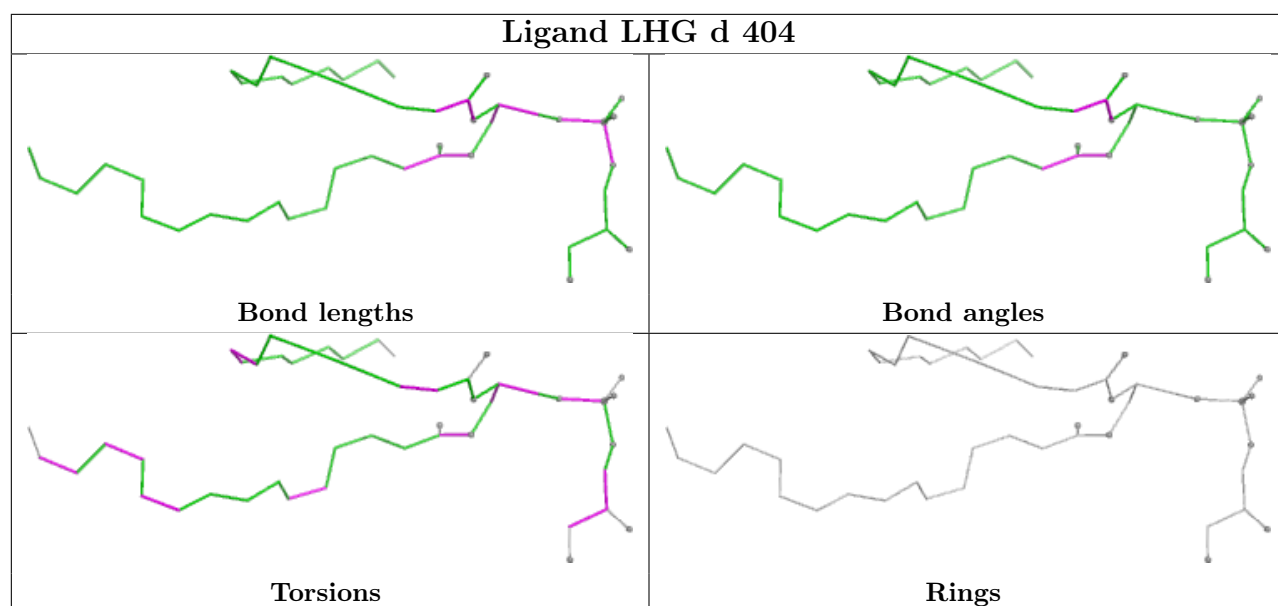


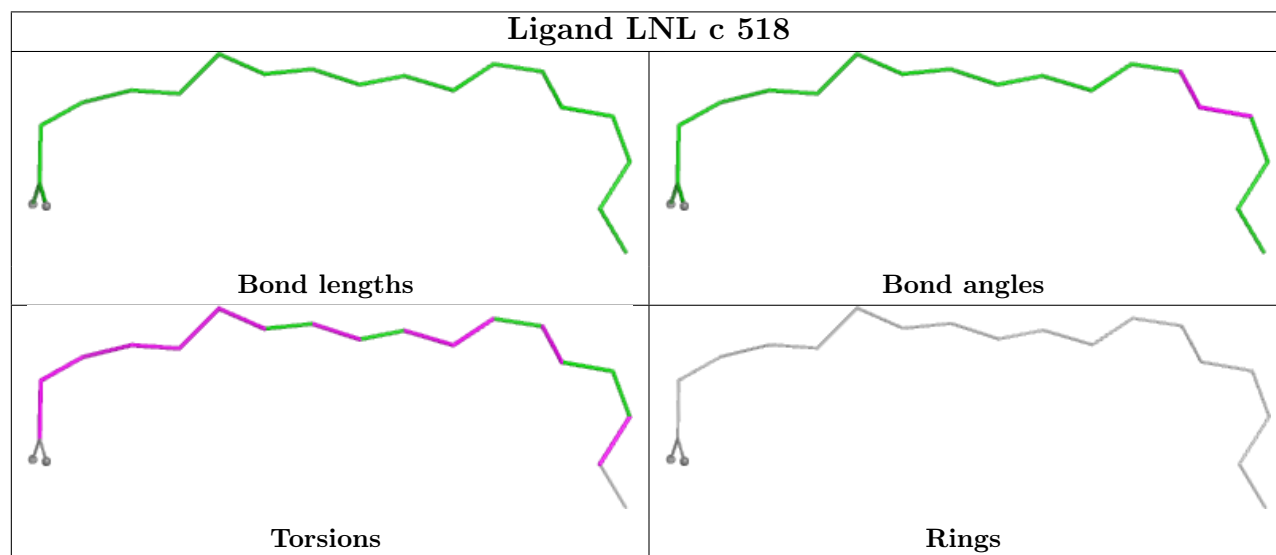
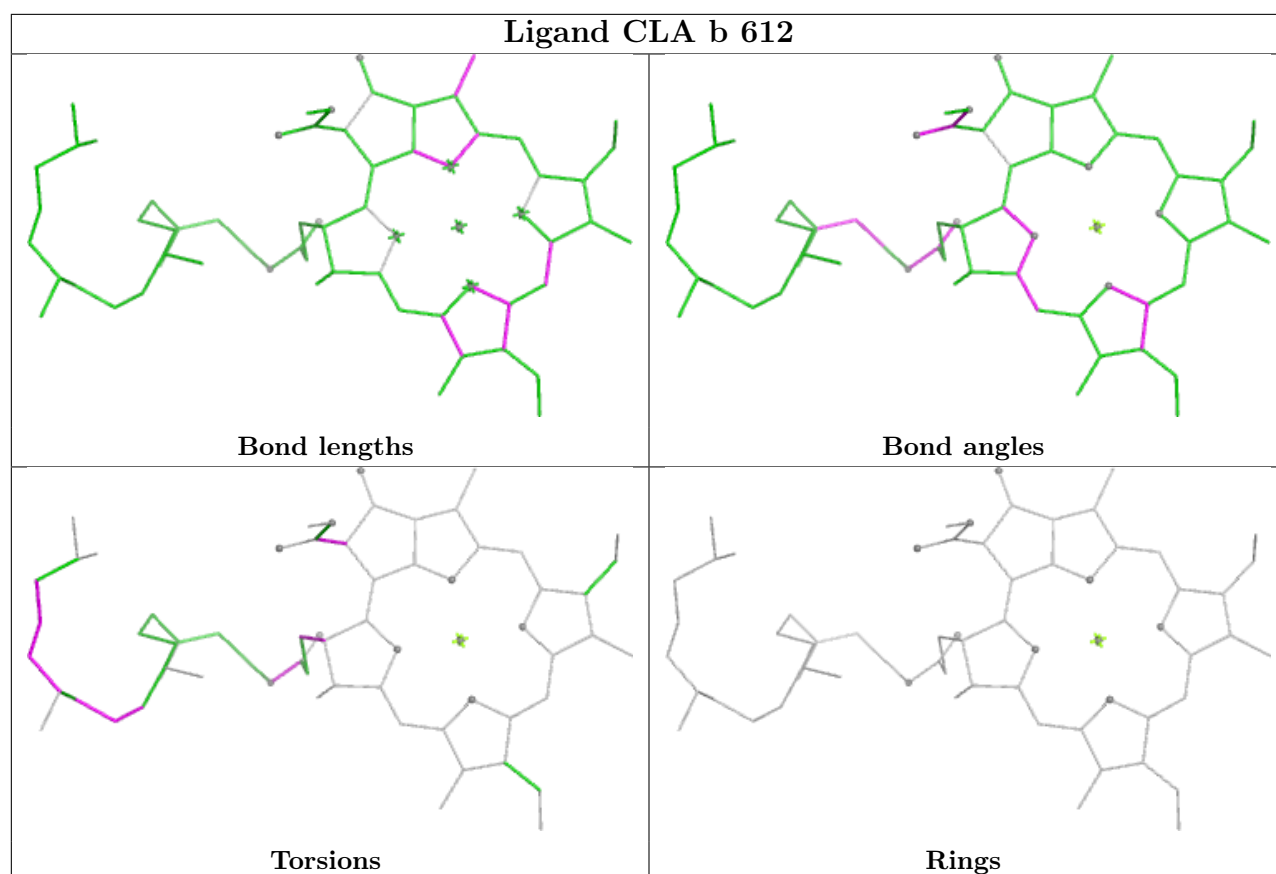
Ligand CLA r 609

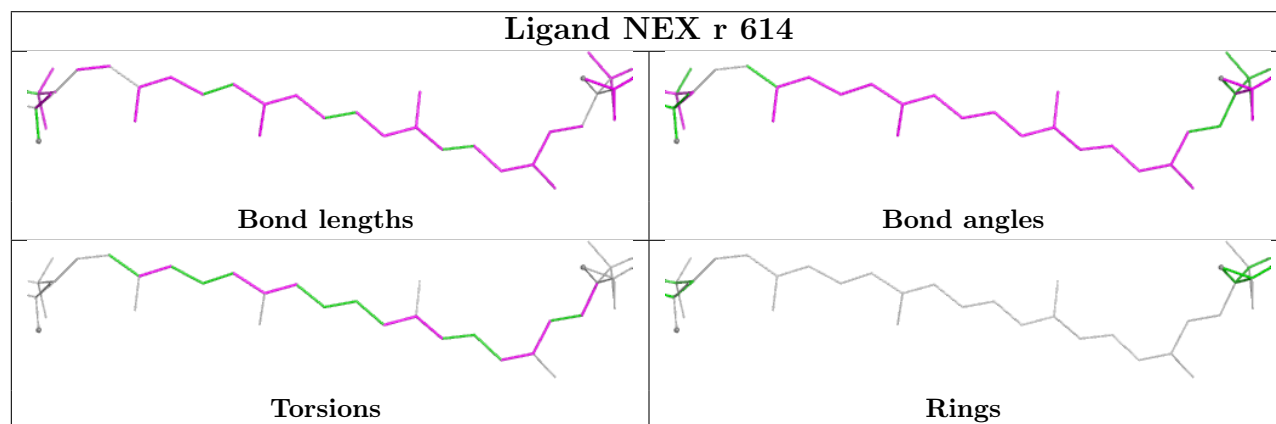
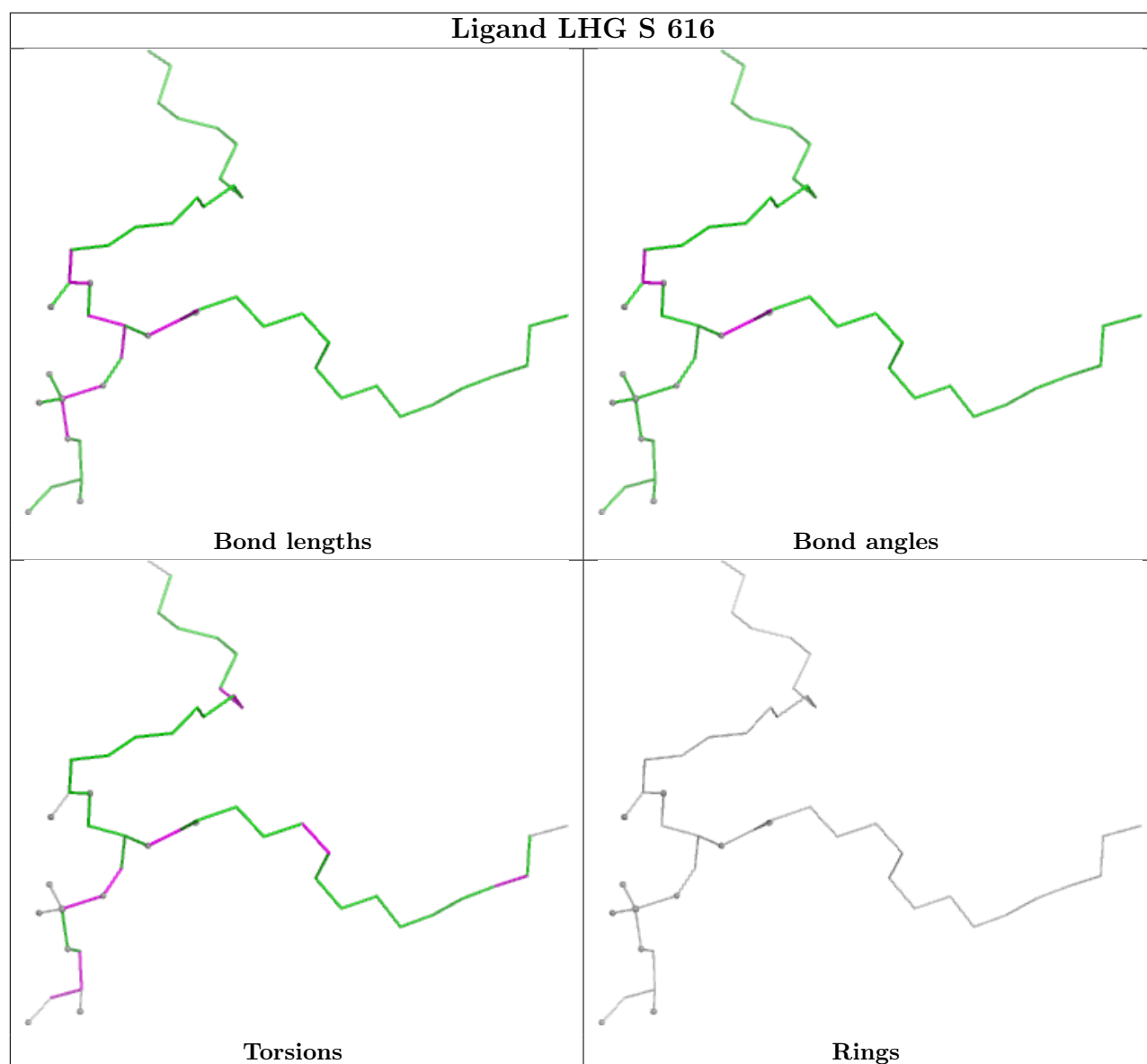


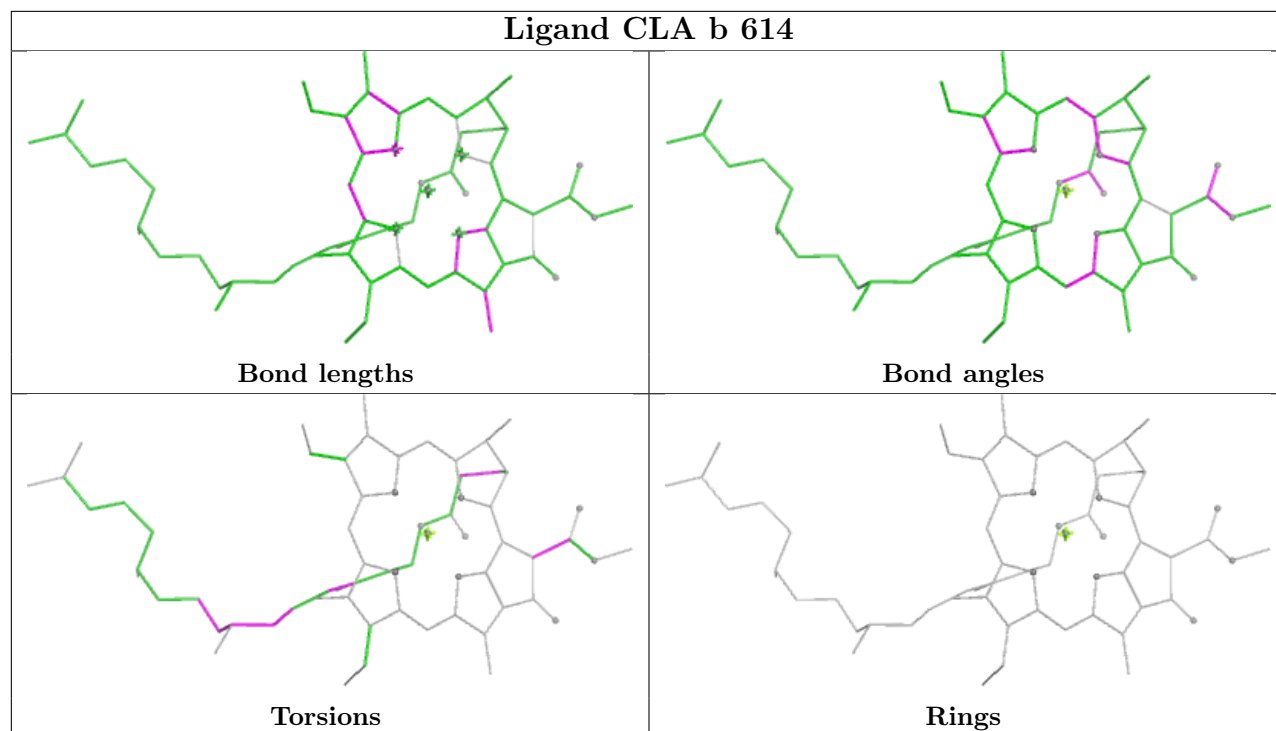
Ligand LNL b 623

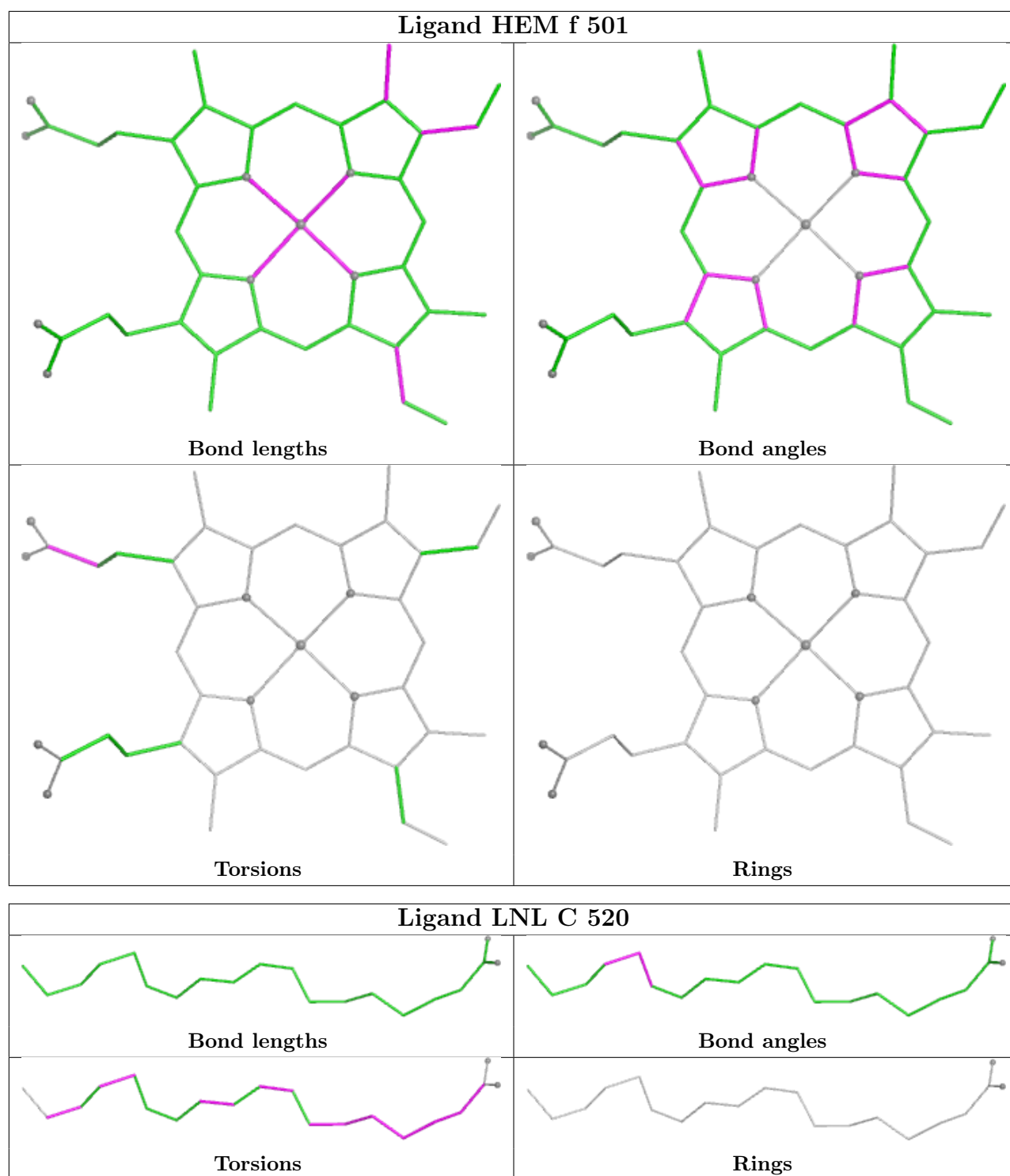


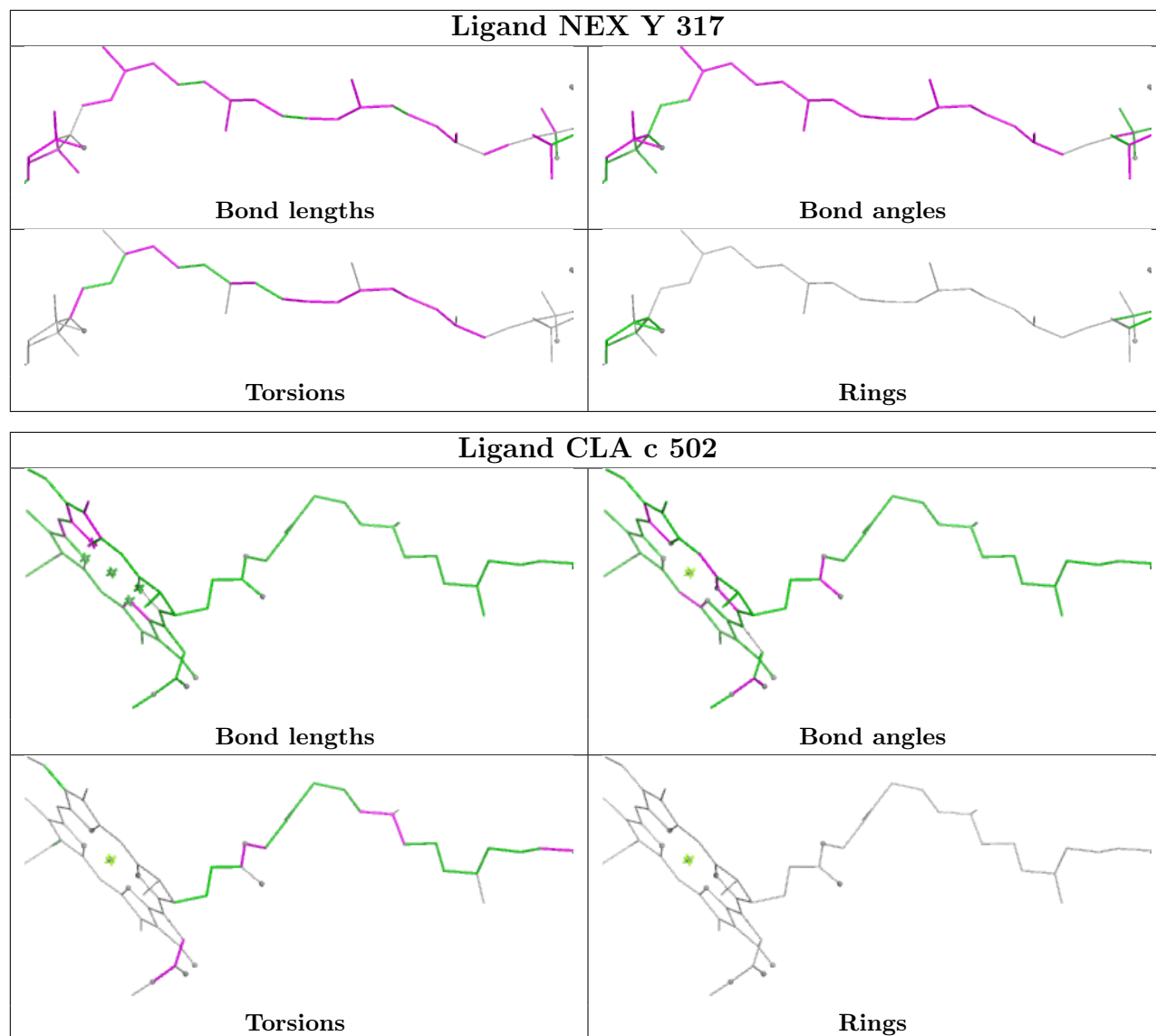


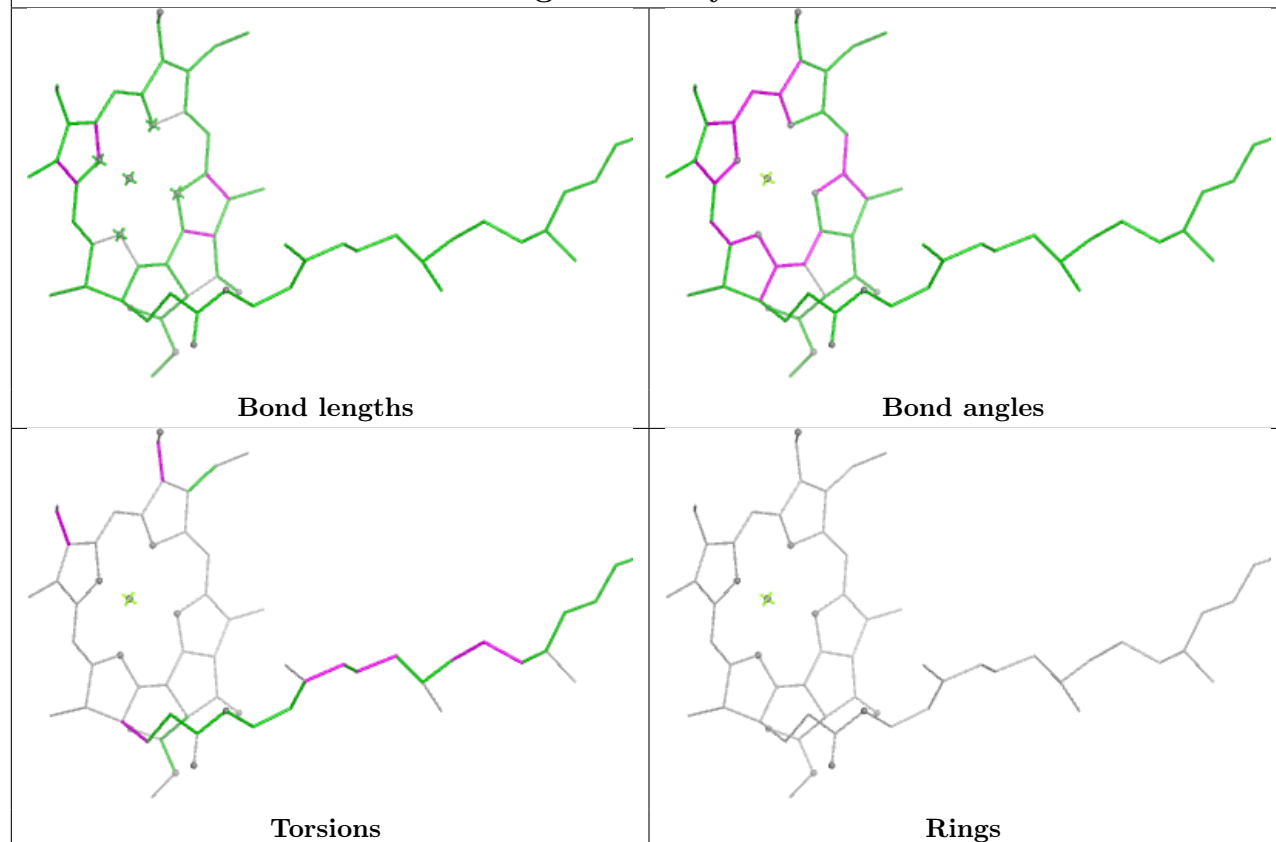
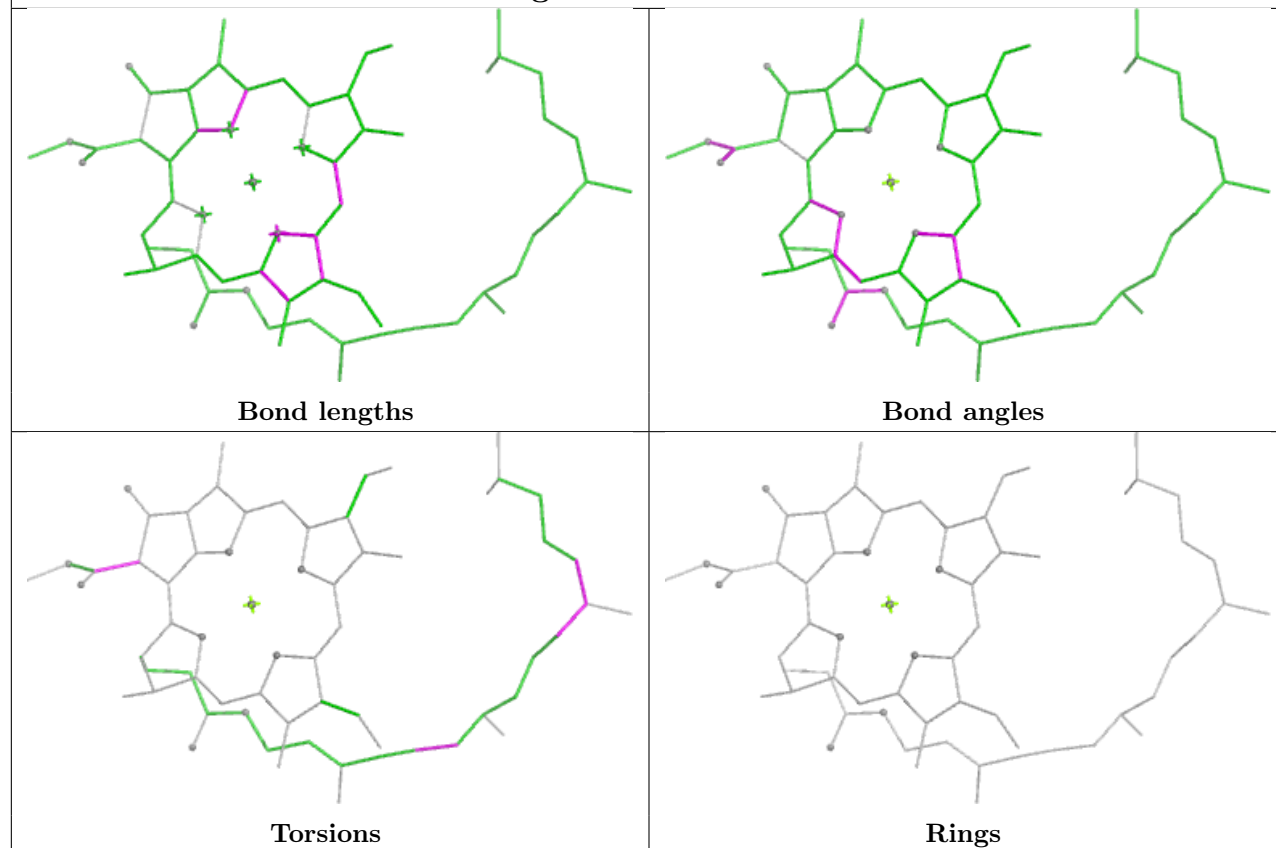


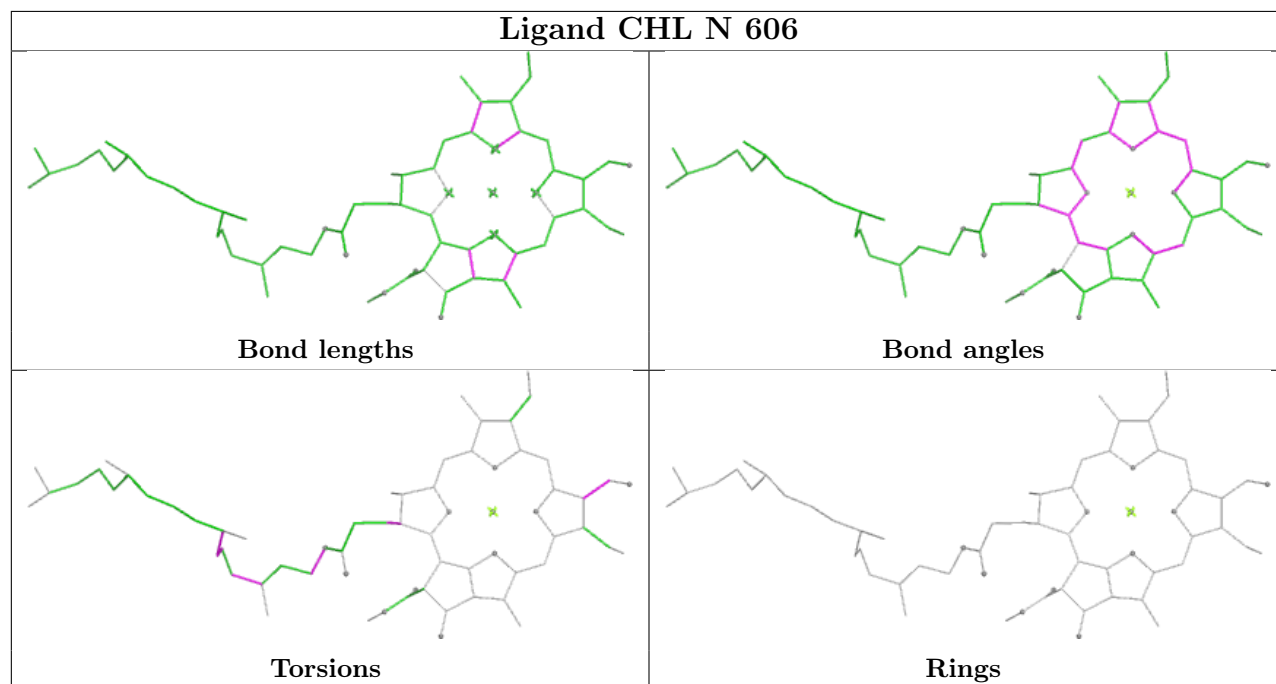
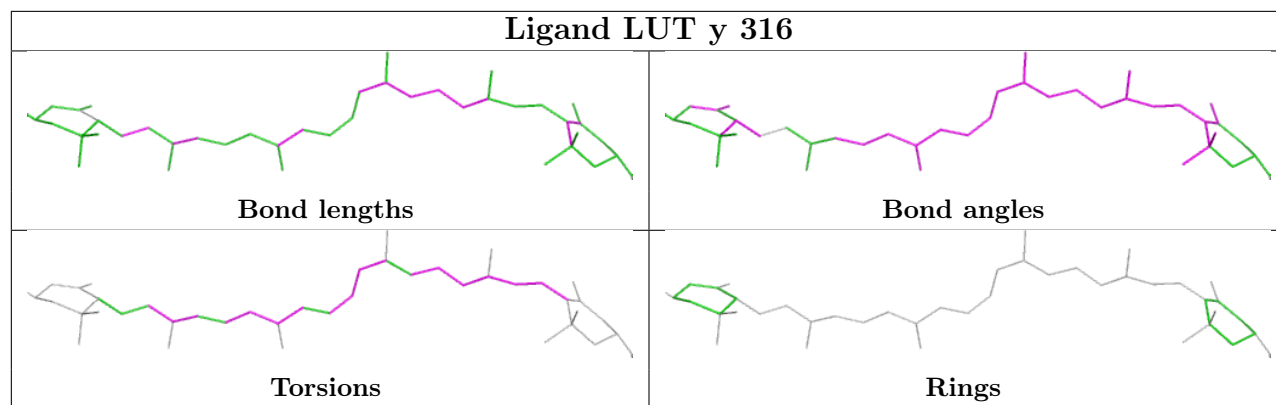




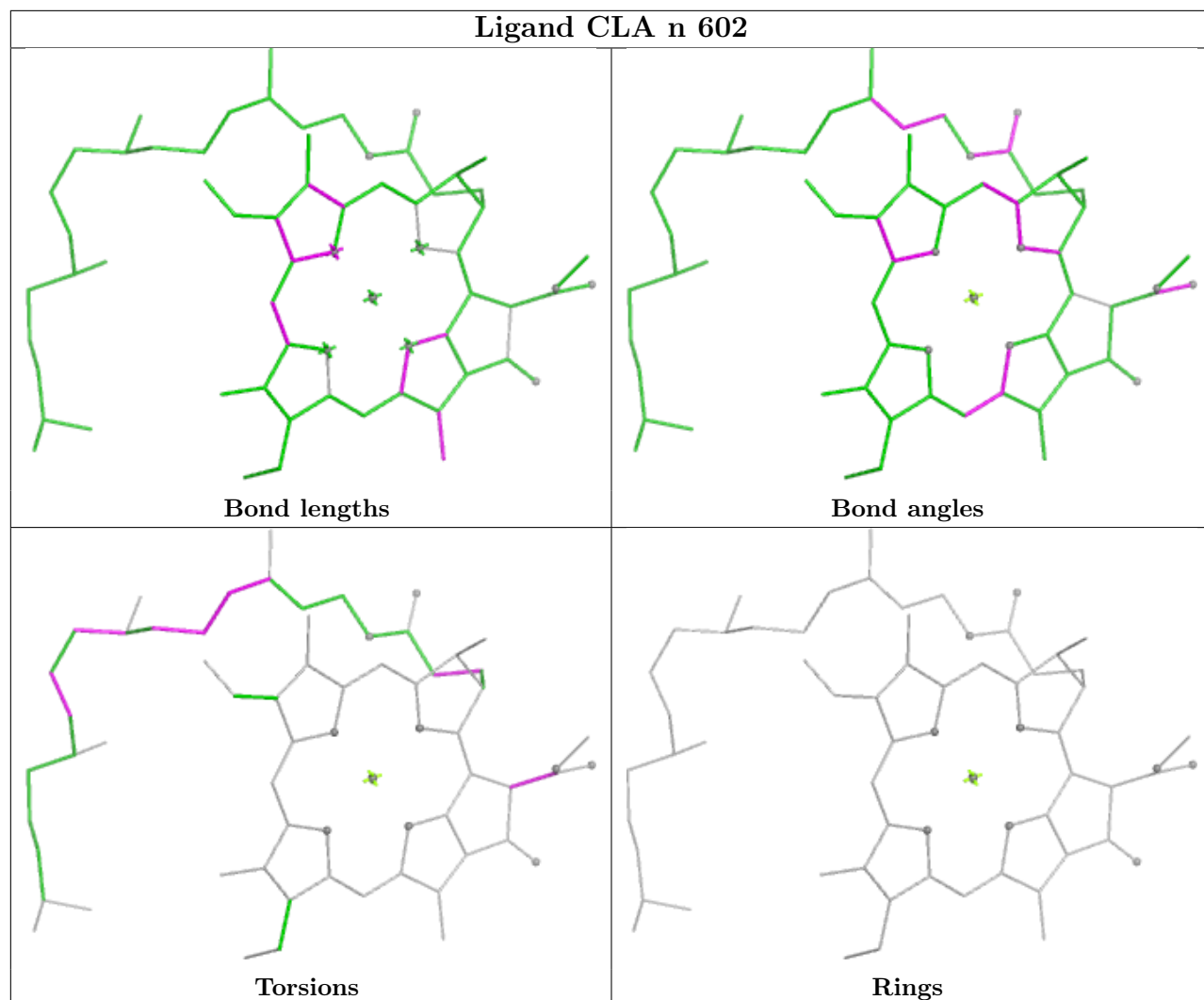


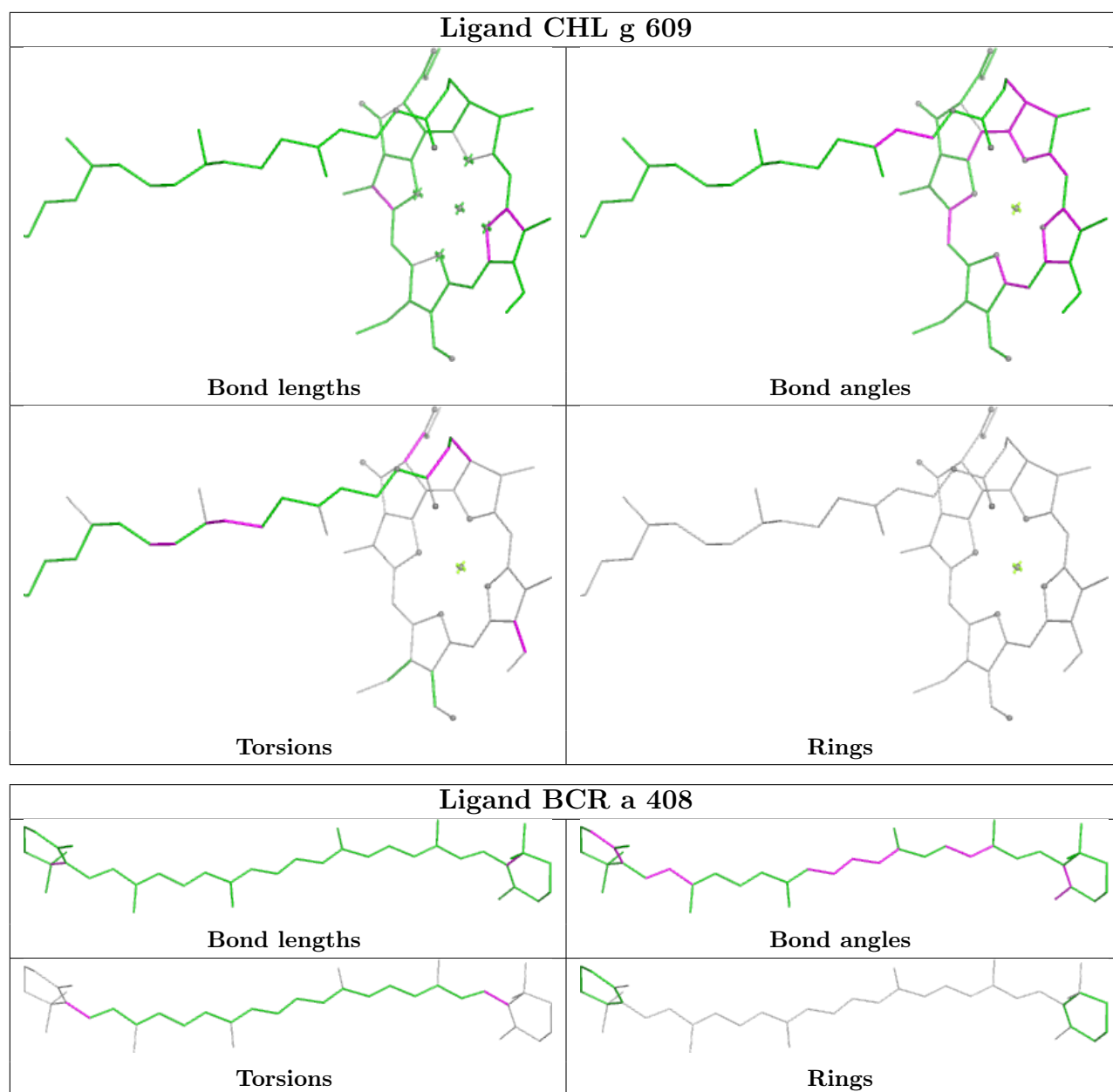


Ligand CHL y 310**Ligand CLA R 609**

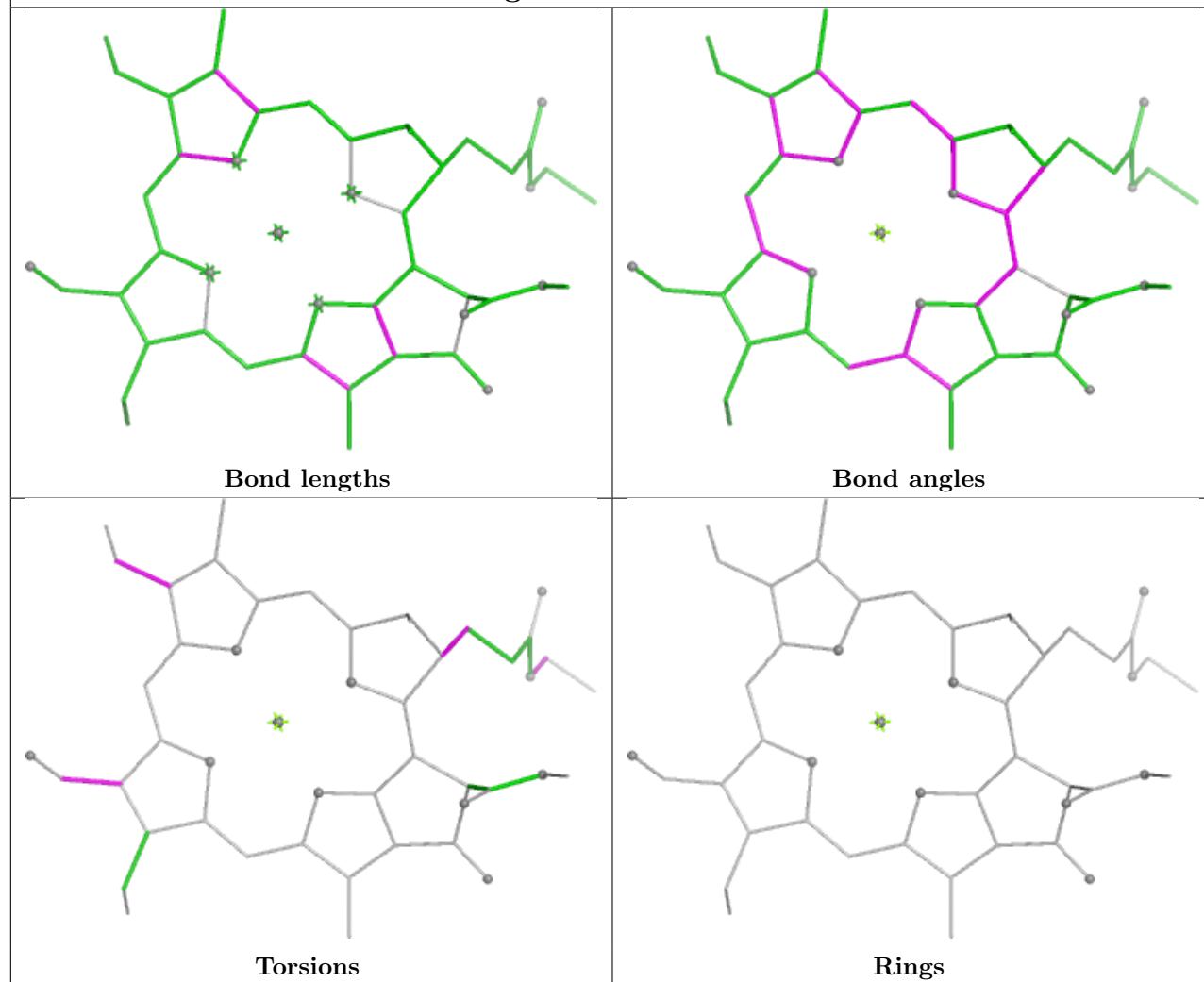


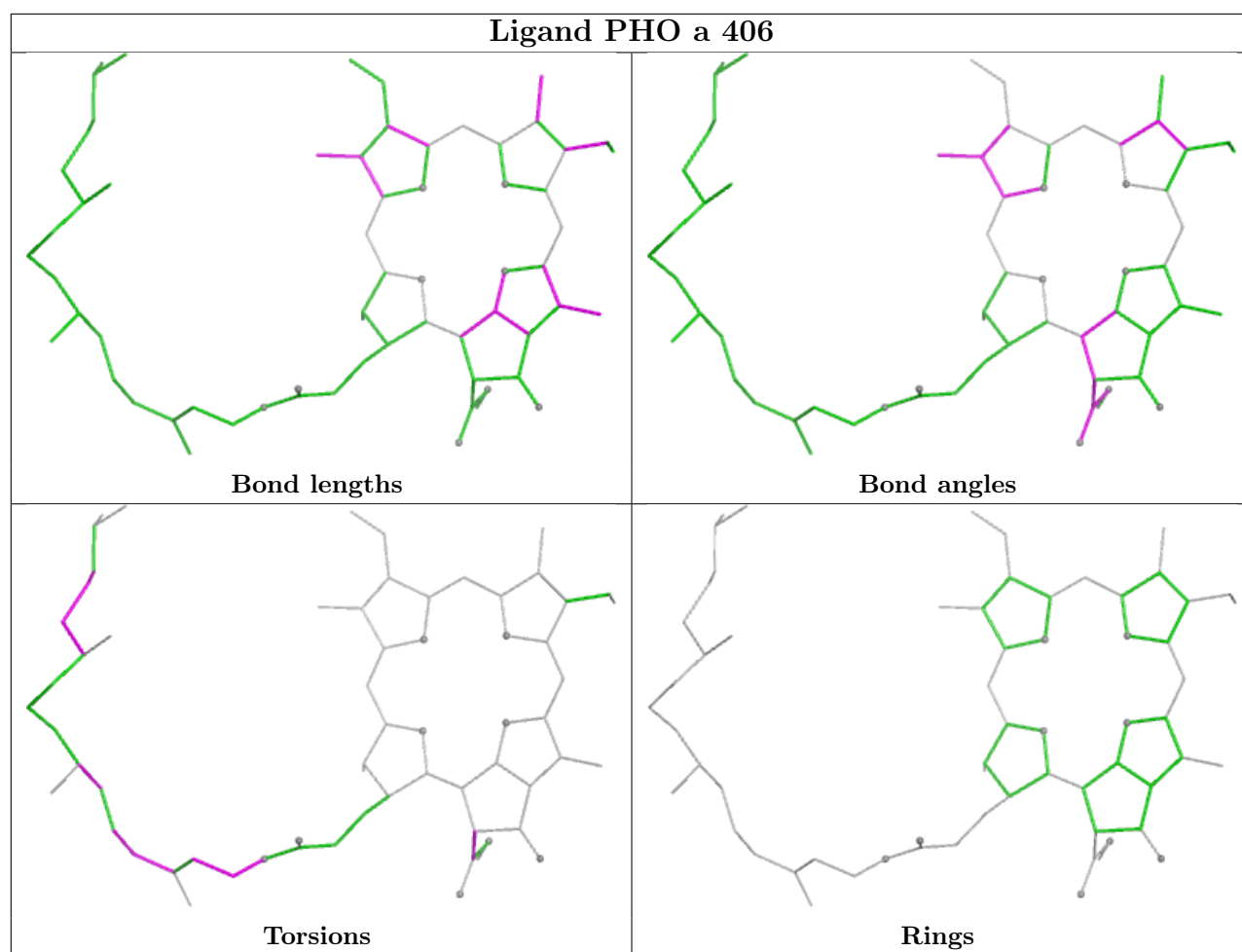
Ligand CLA n 602



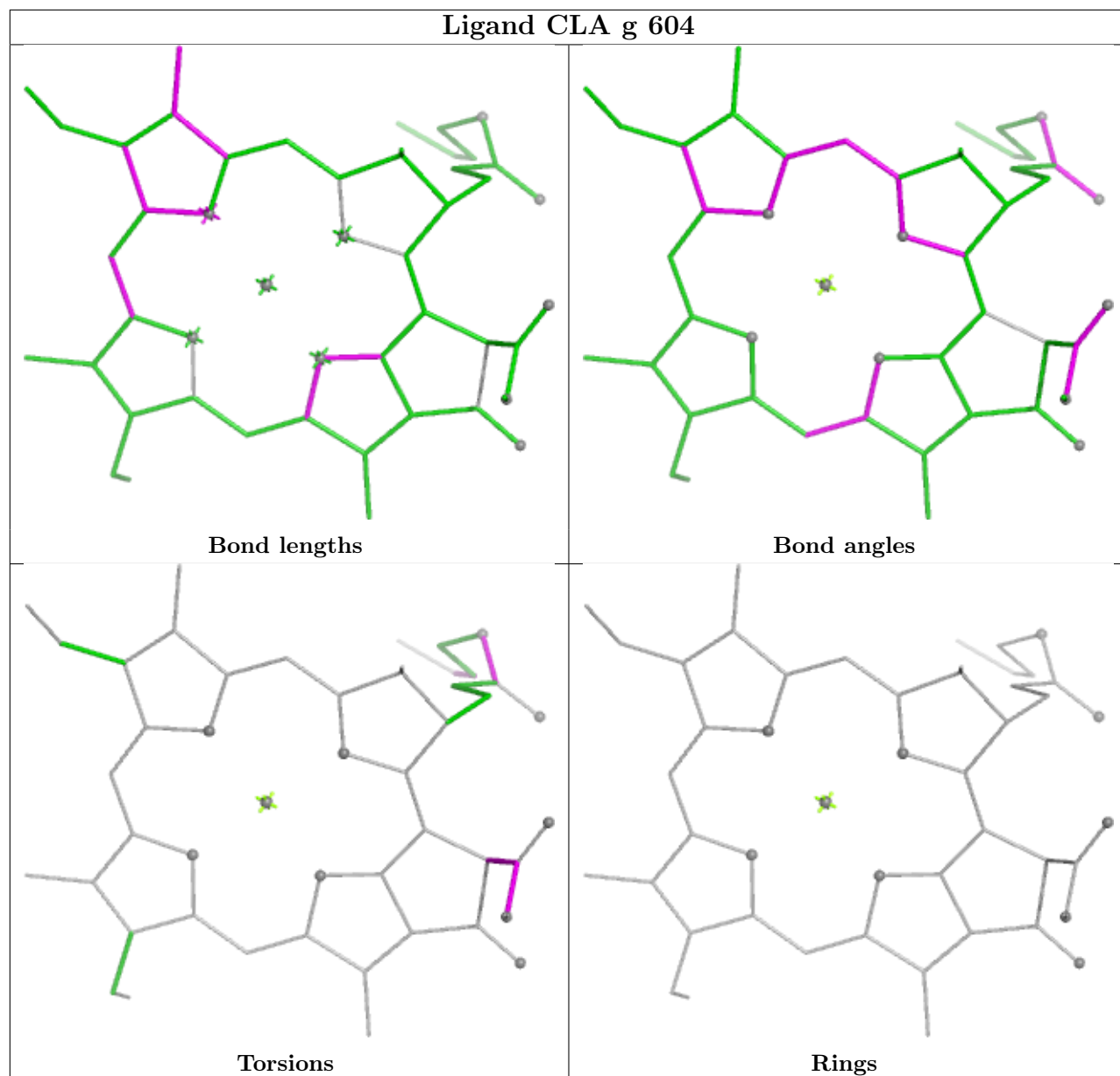


Ligand CHL n 605

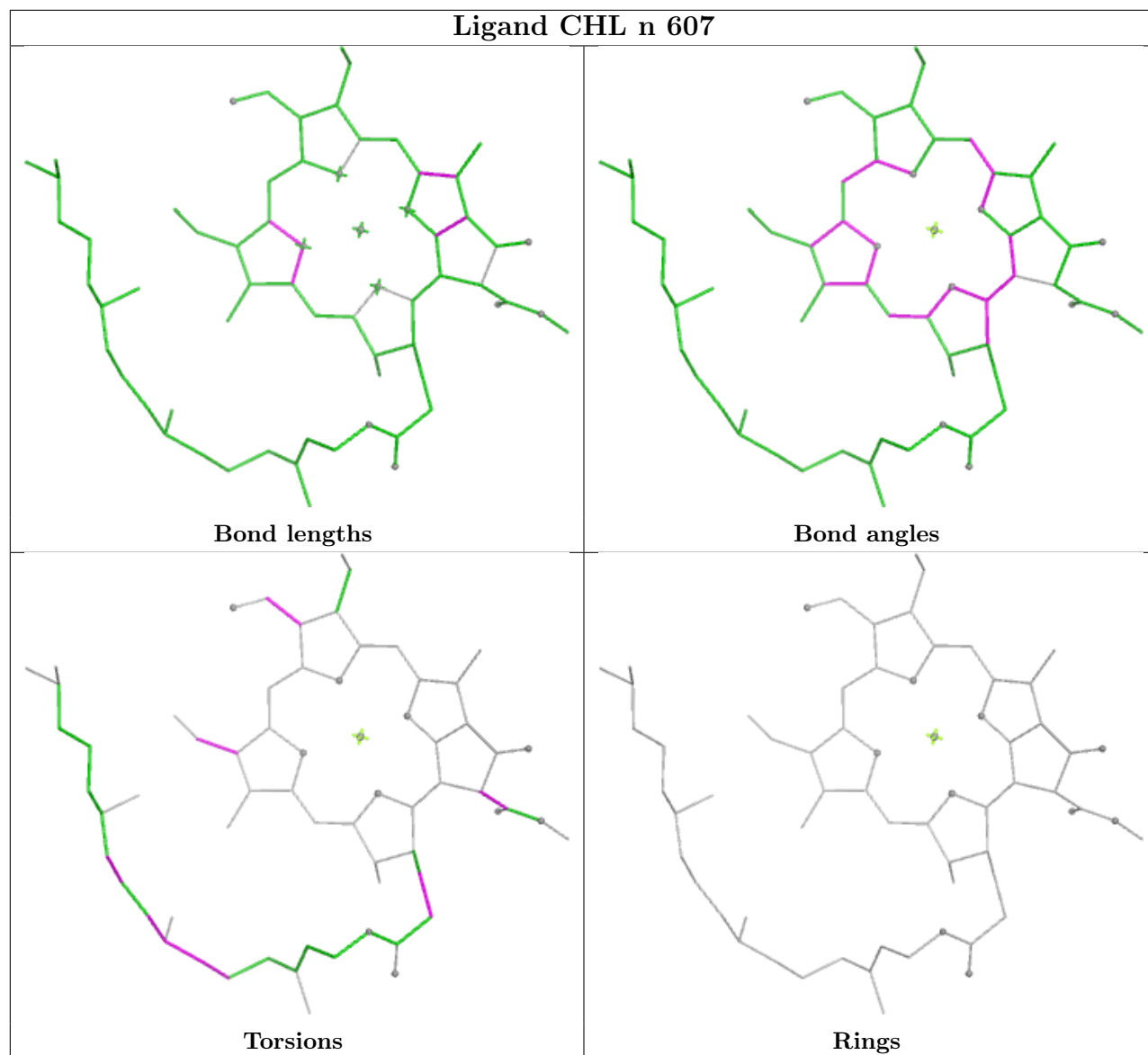


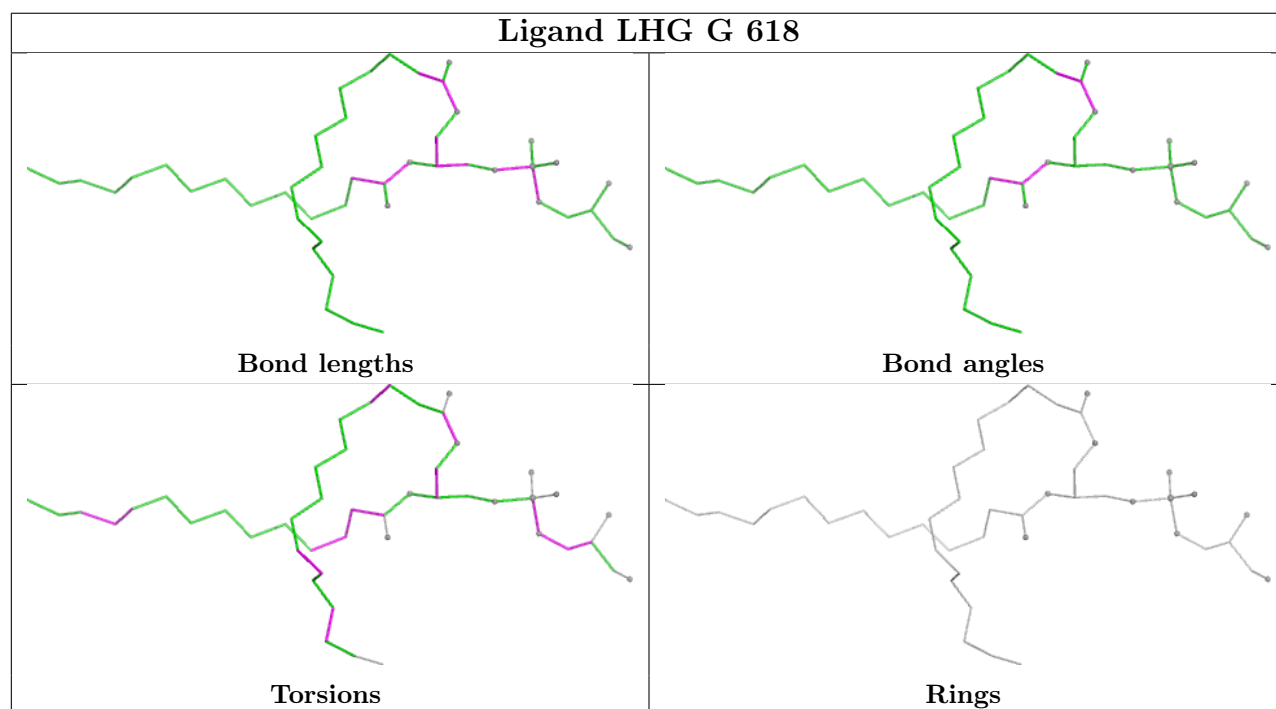
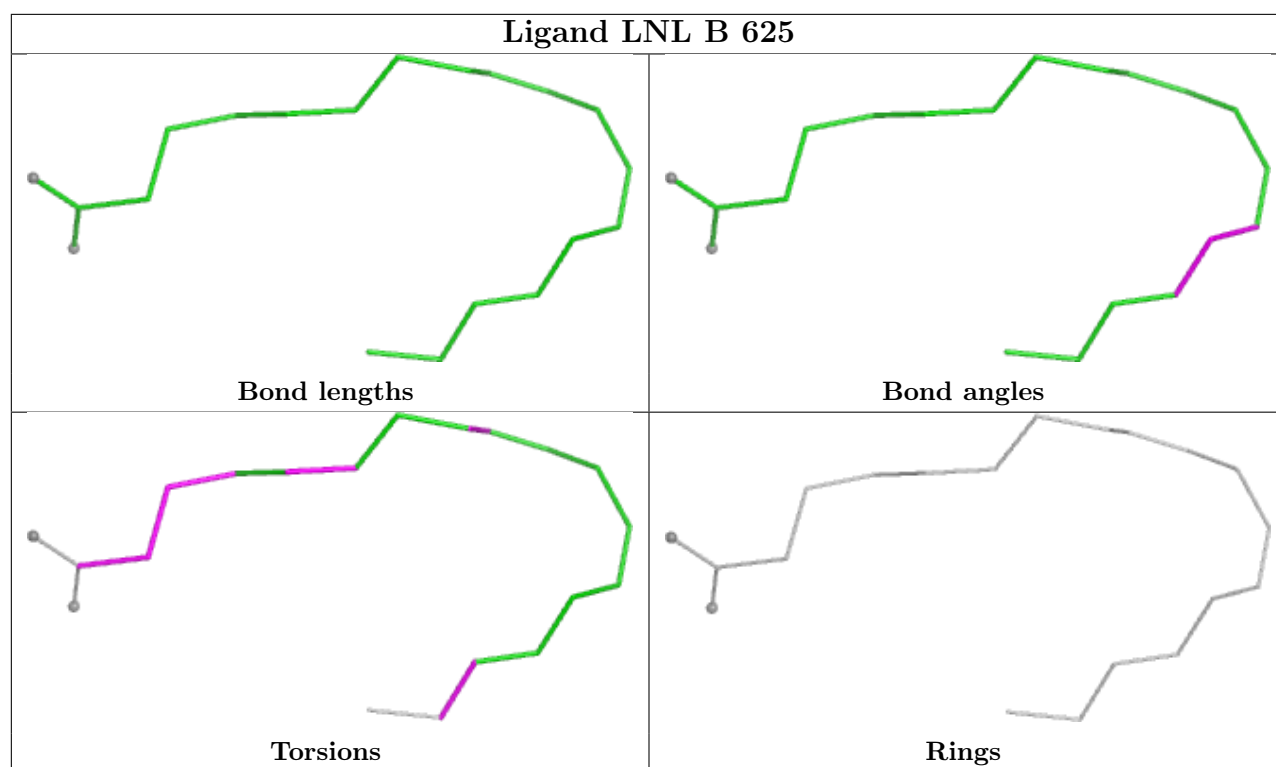


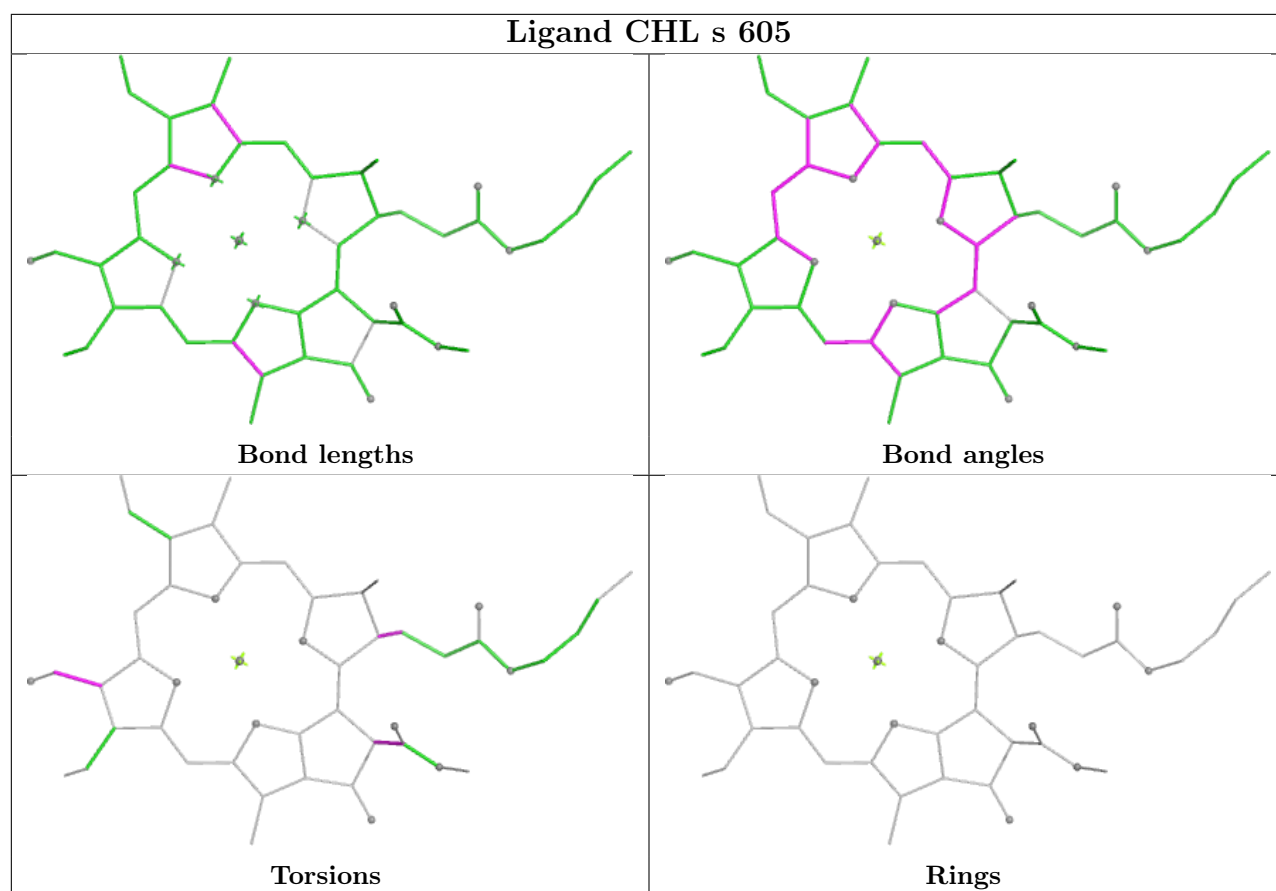
Ligand CLA g 604



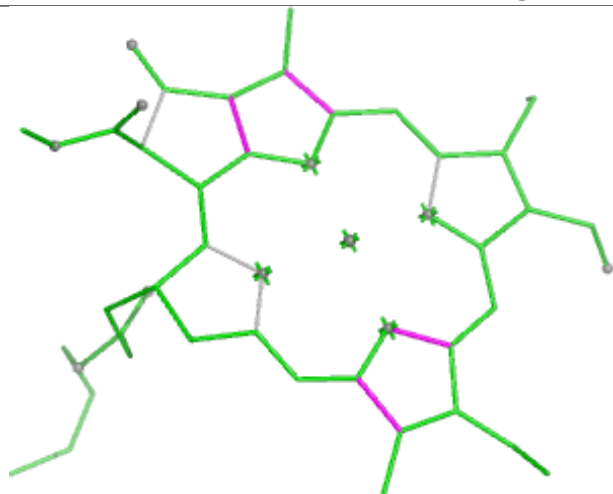
Ligand CHL n 607



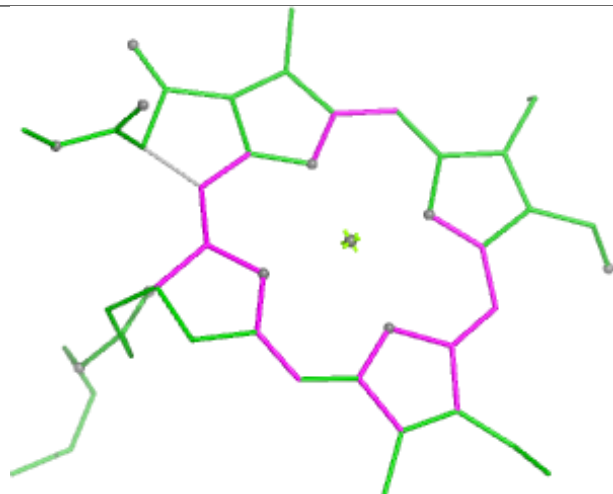




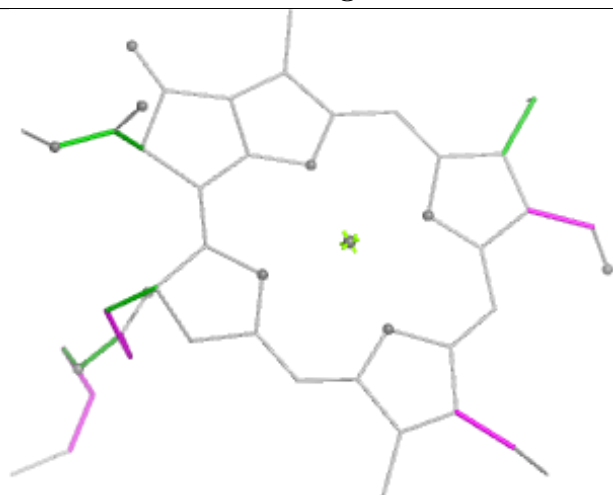
Ligand CHL Y 308



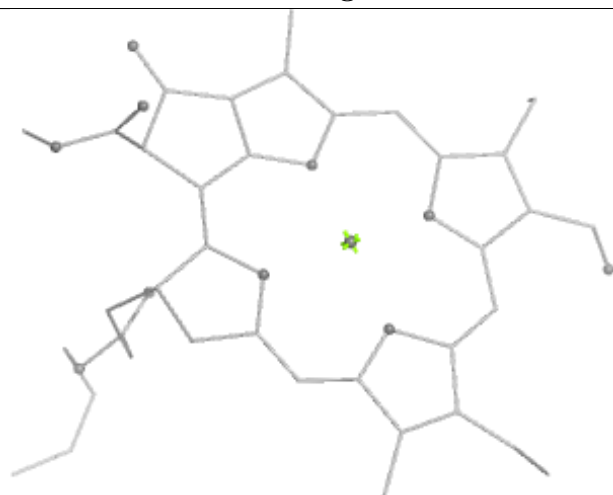
Bond lengths



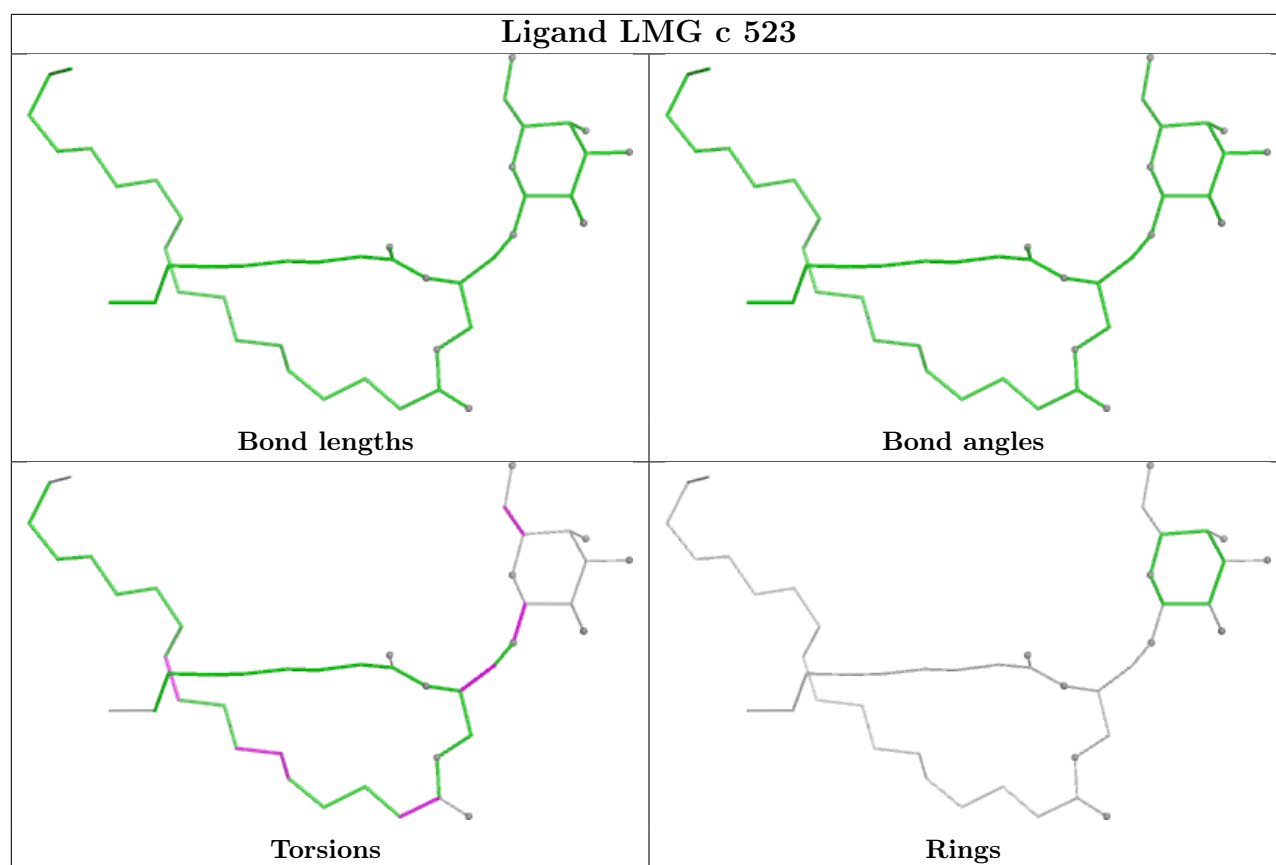
Bond angles

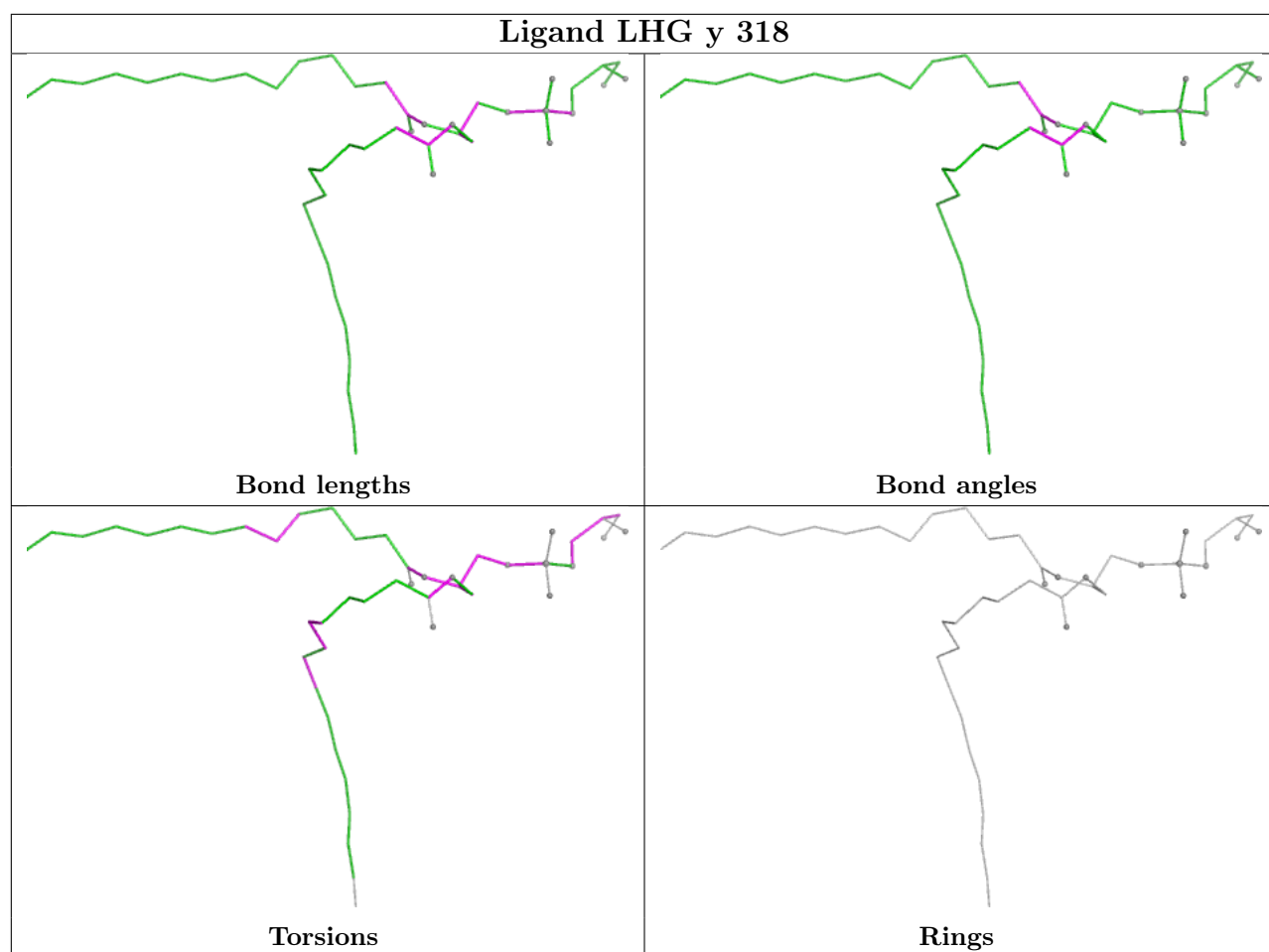


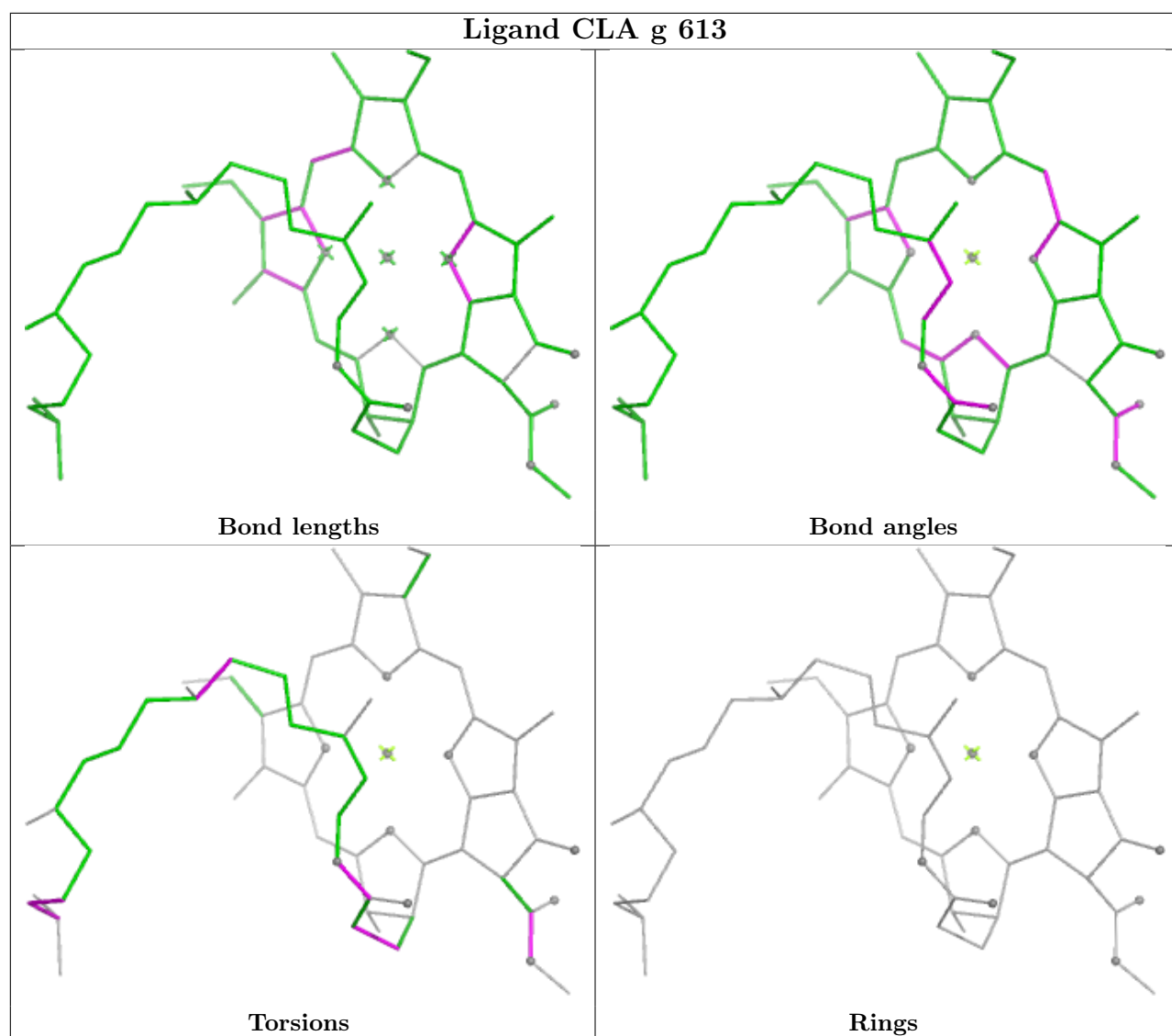
Torsions



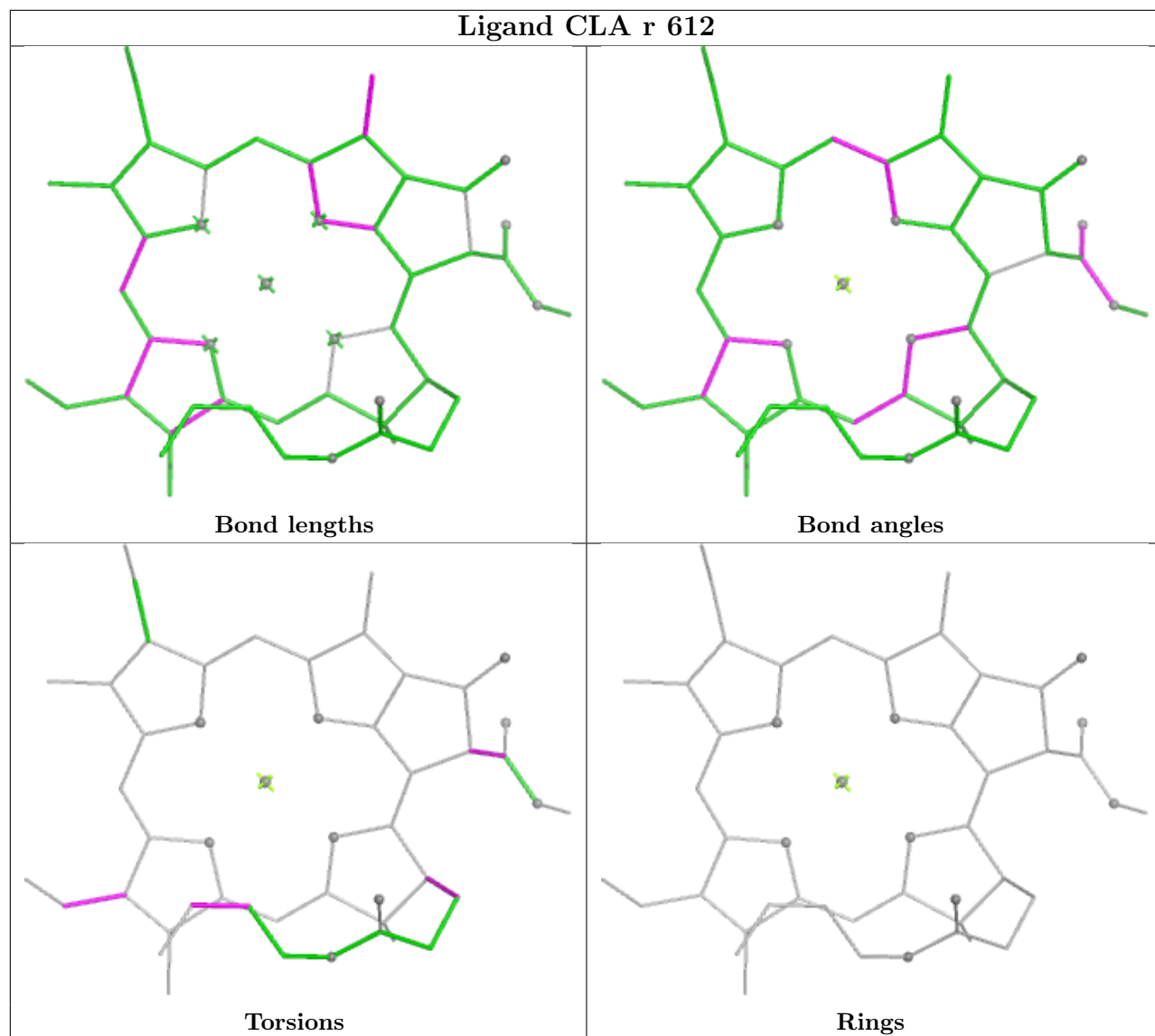
Rings

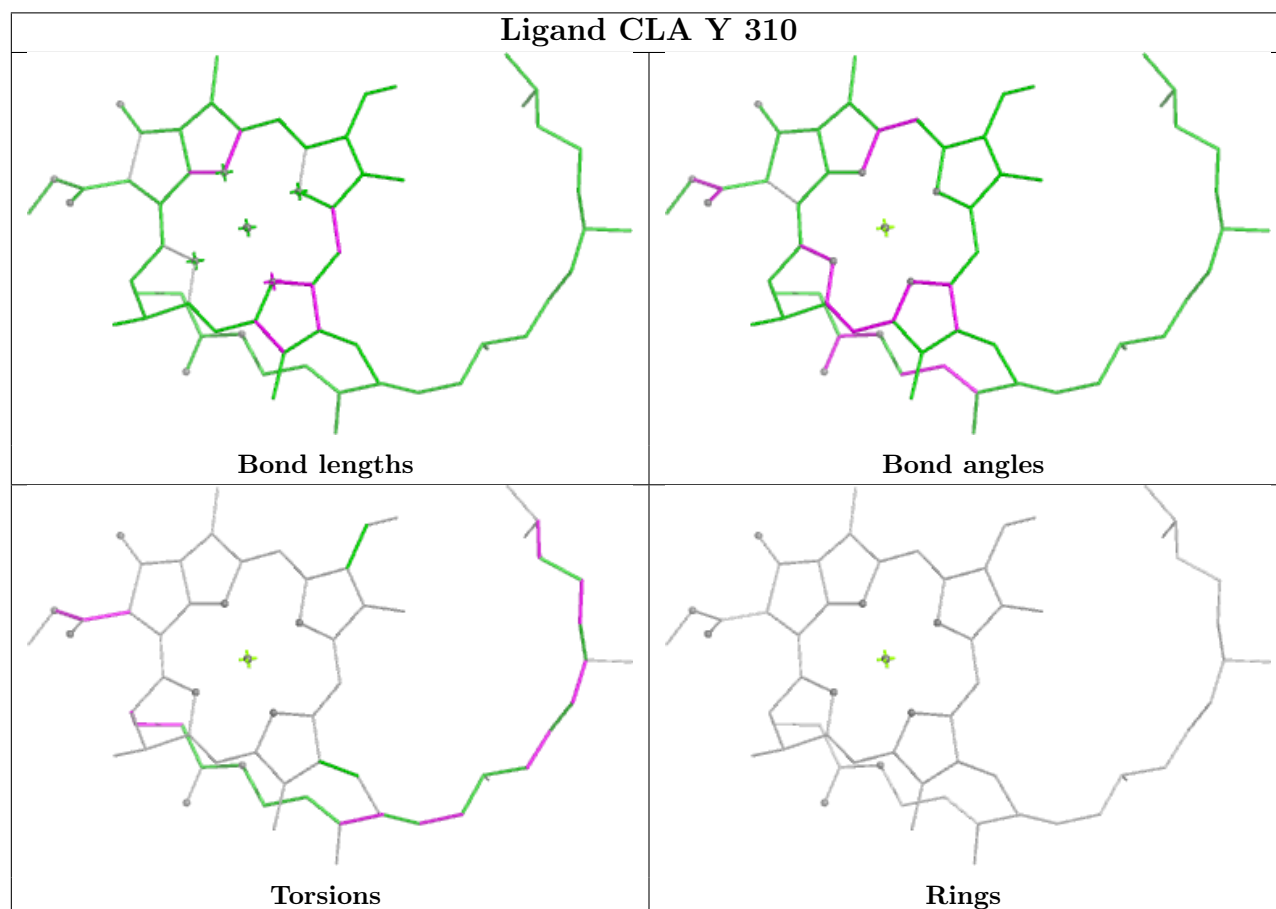
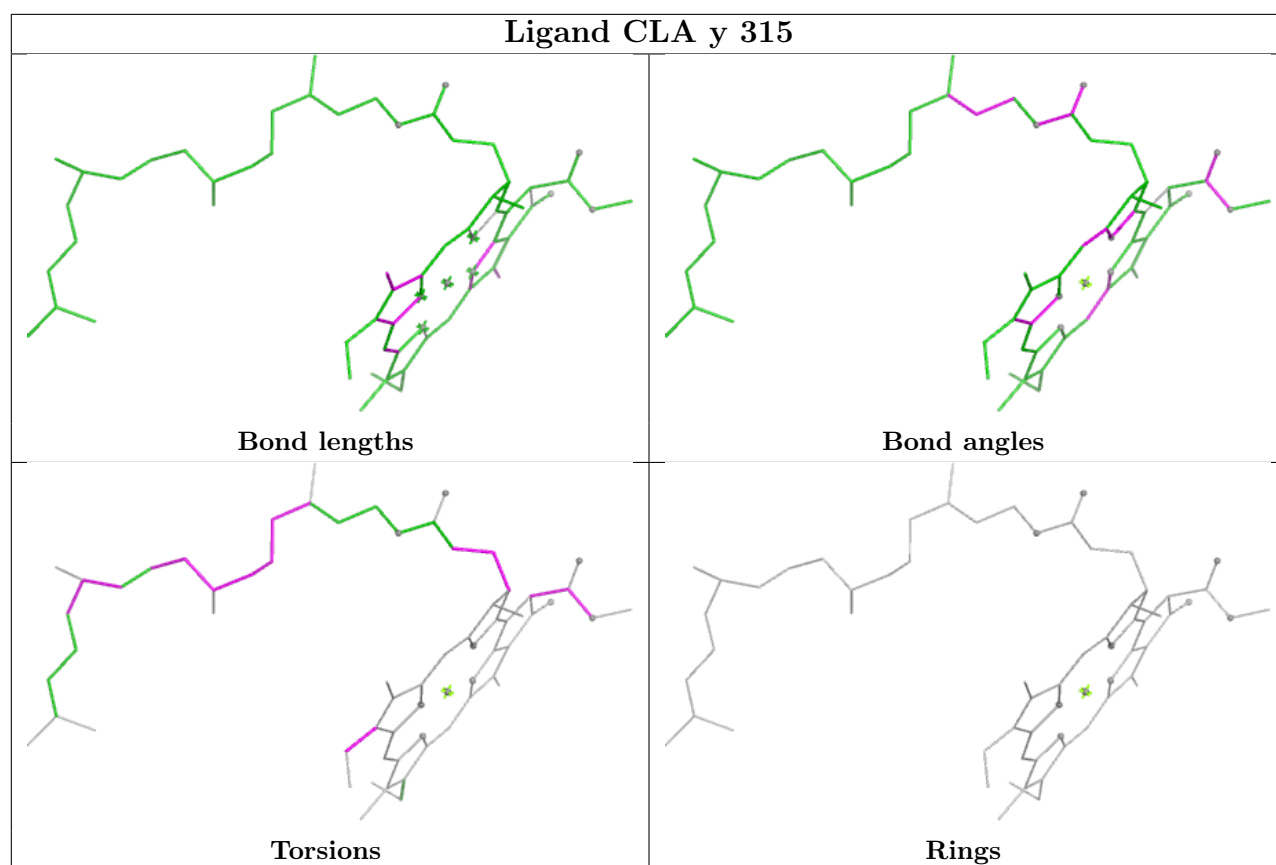


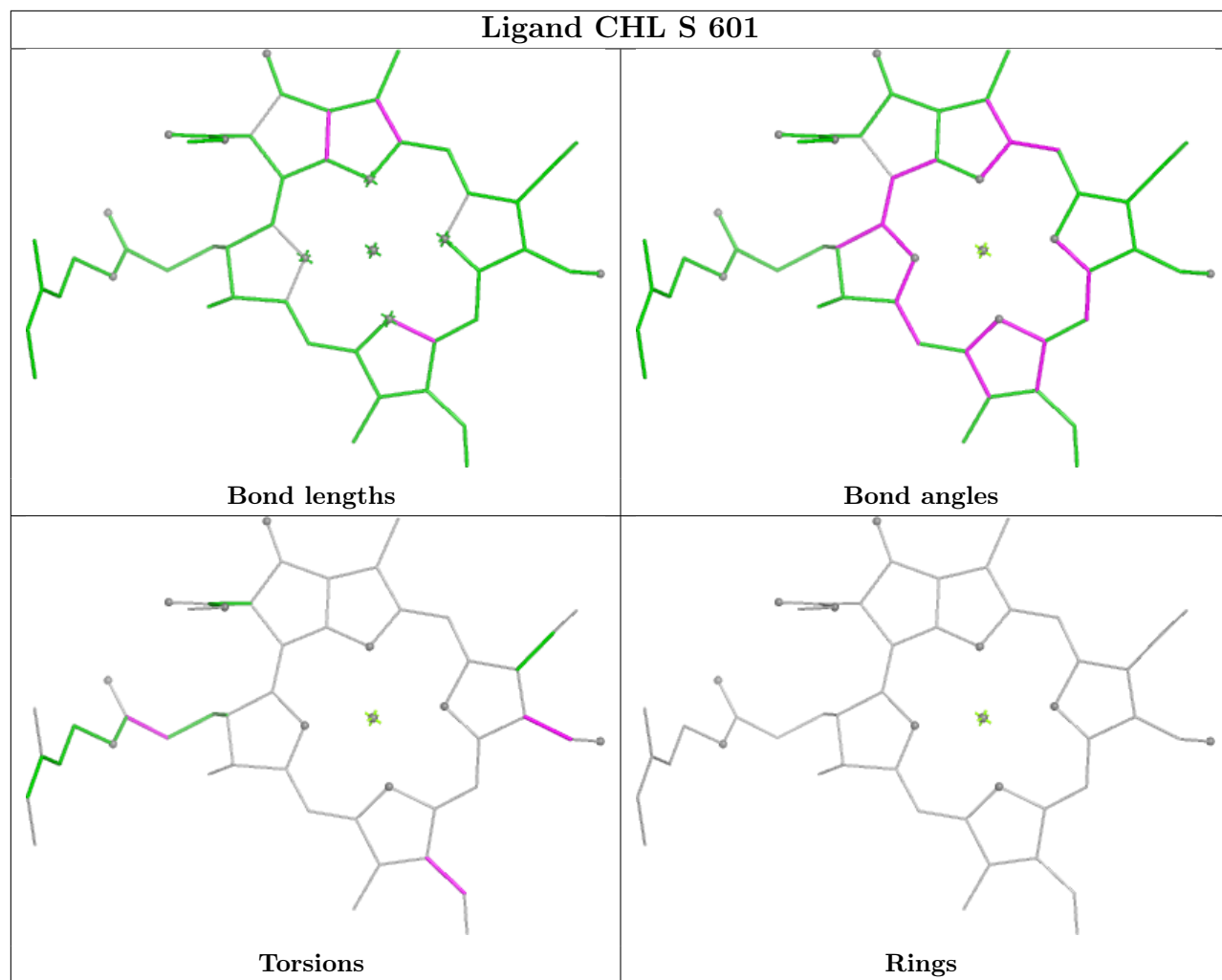


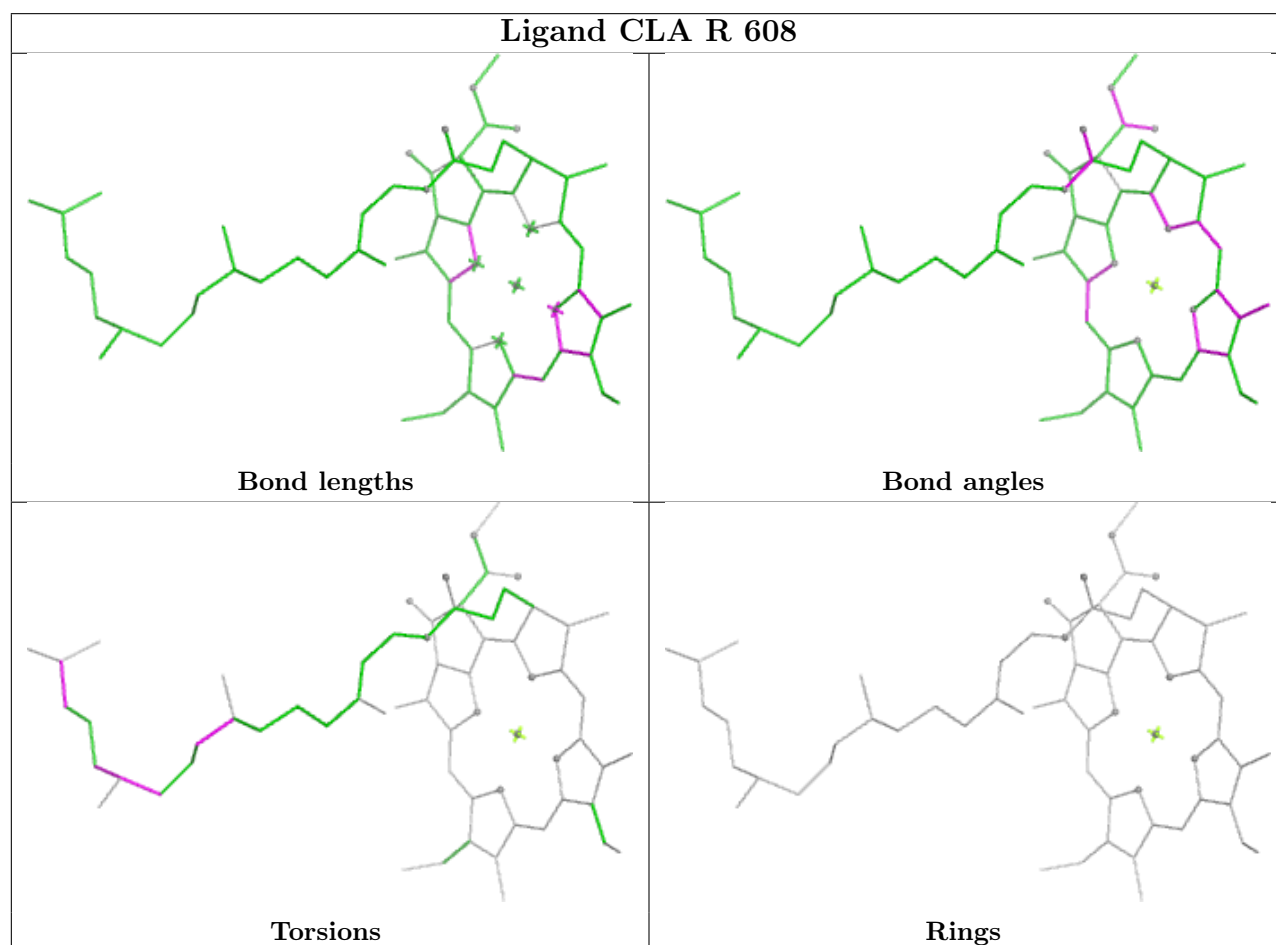
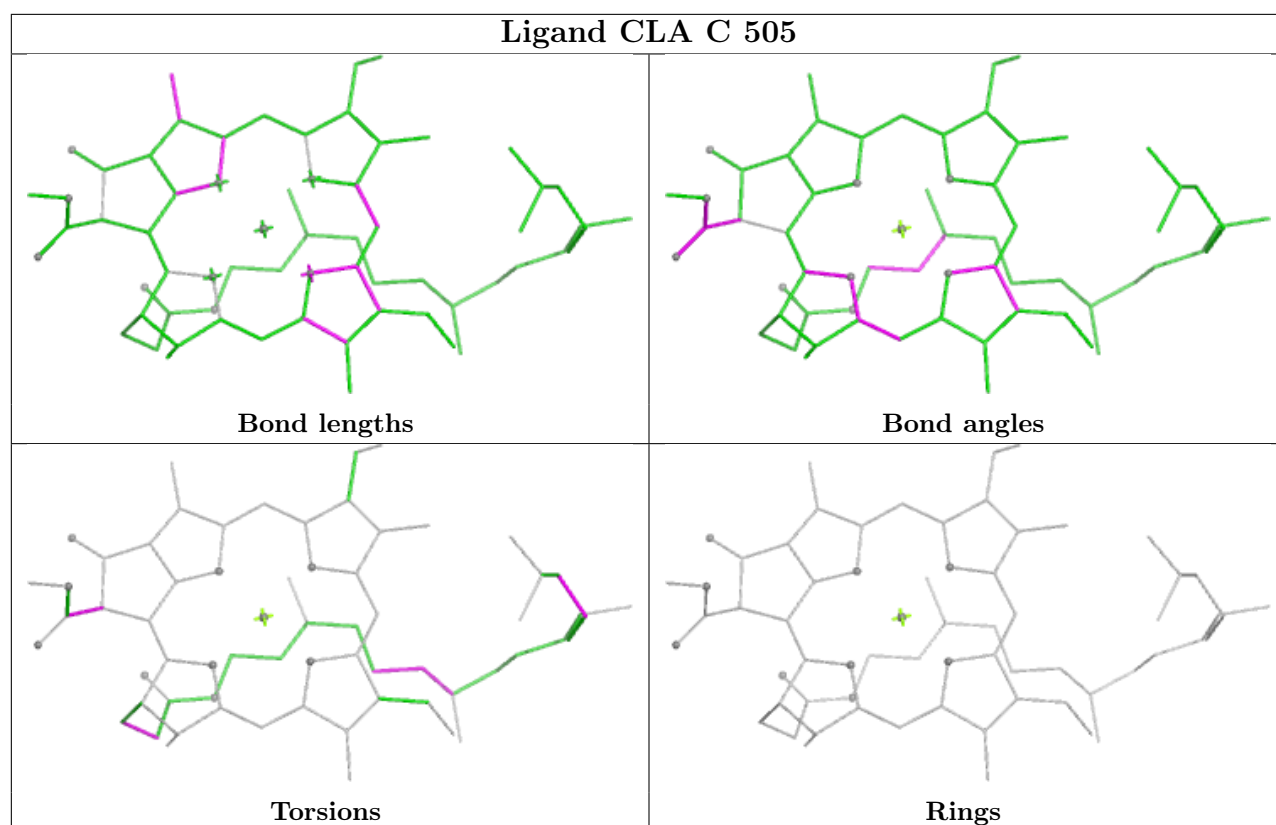


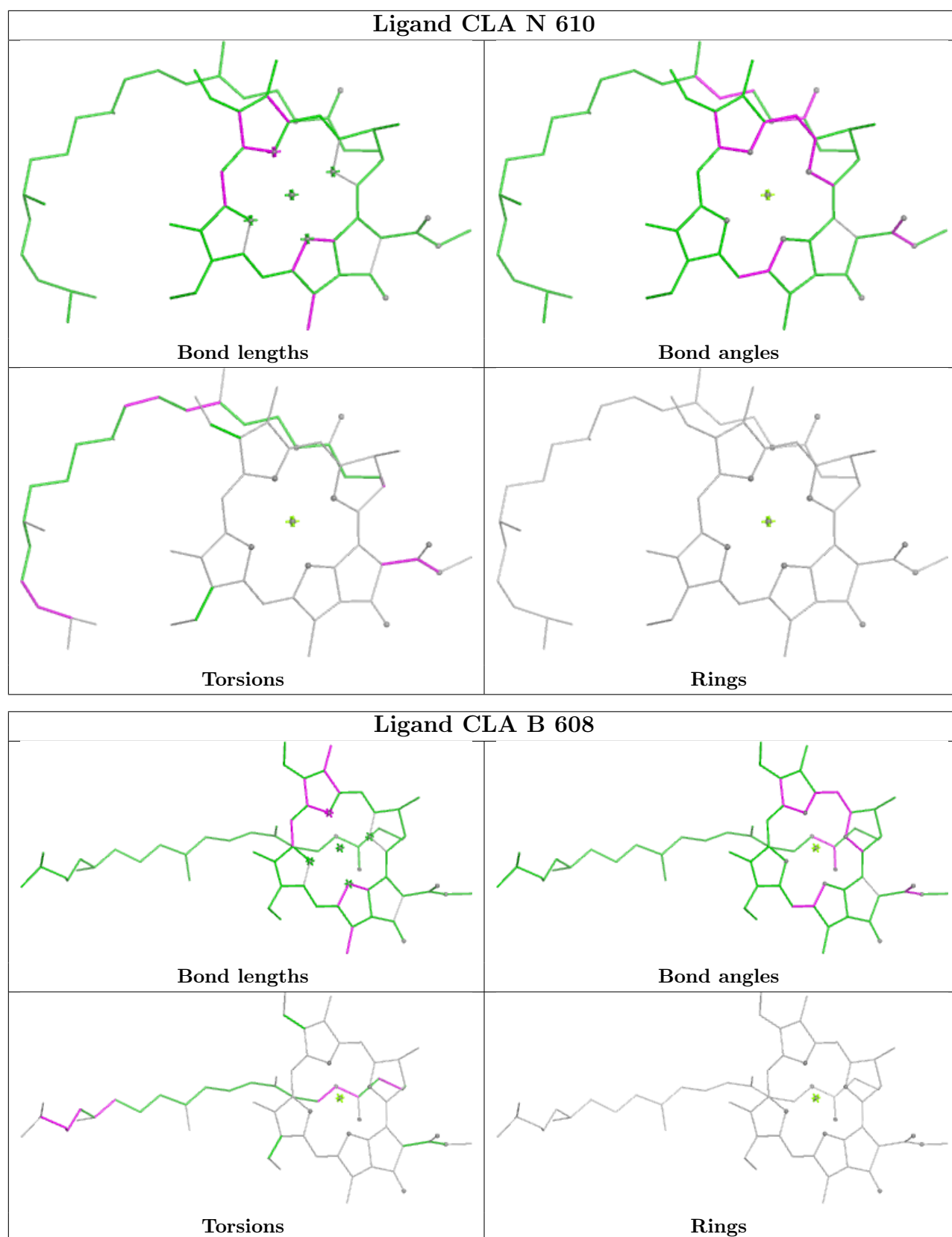
Ligand CLA r 612

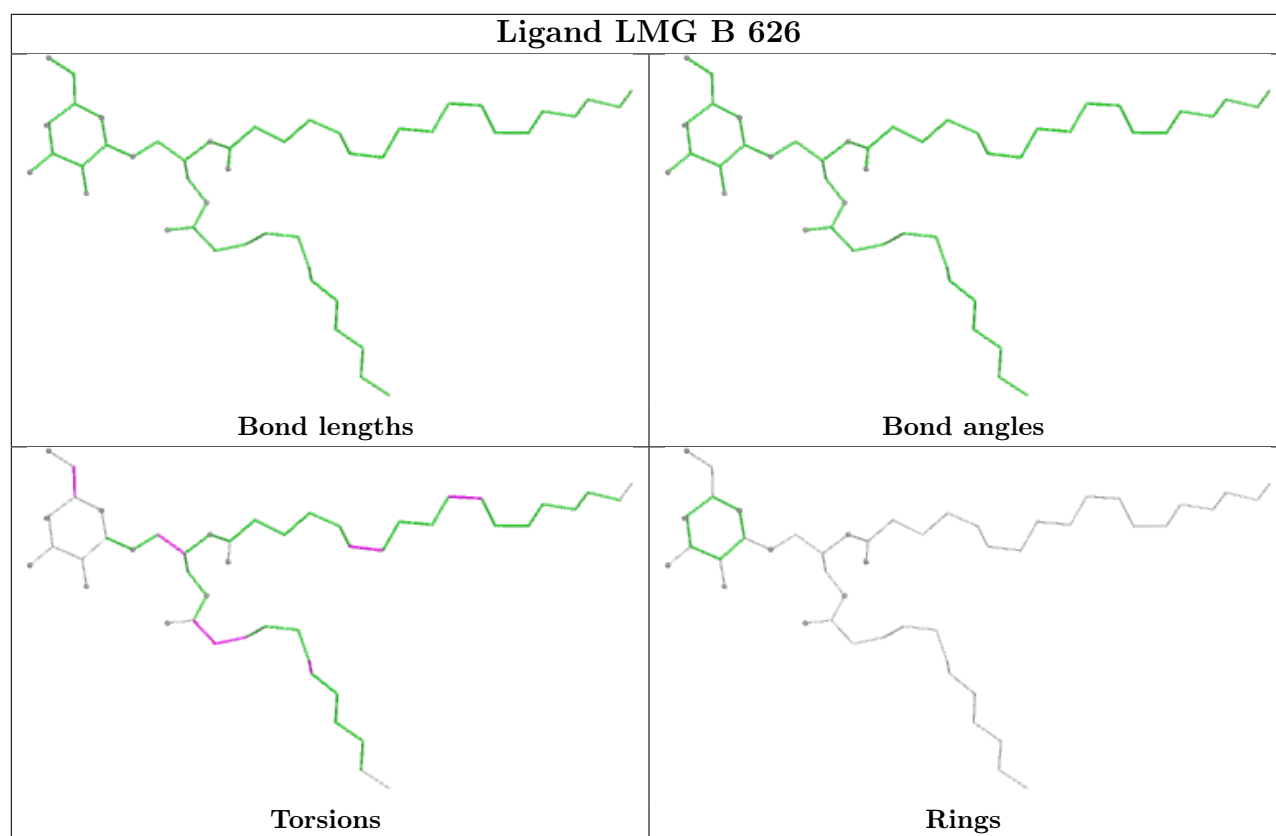




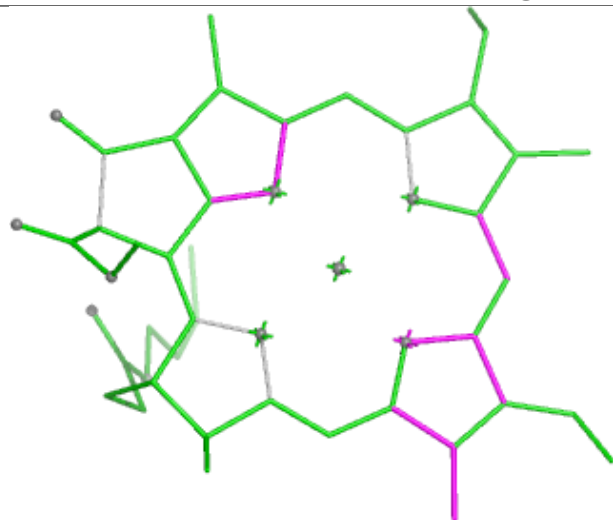




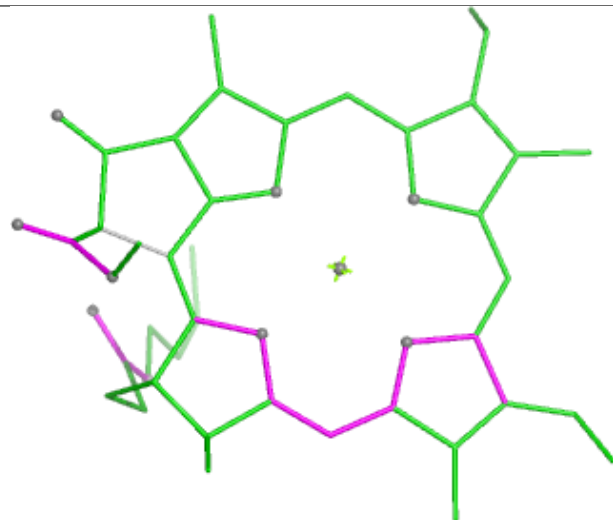




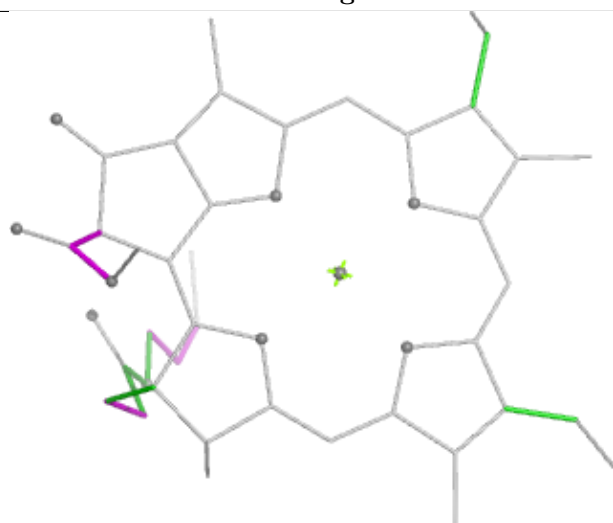
Ligand CLA S 604



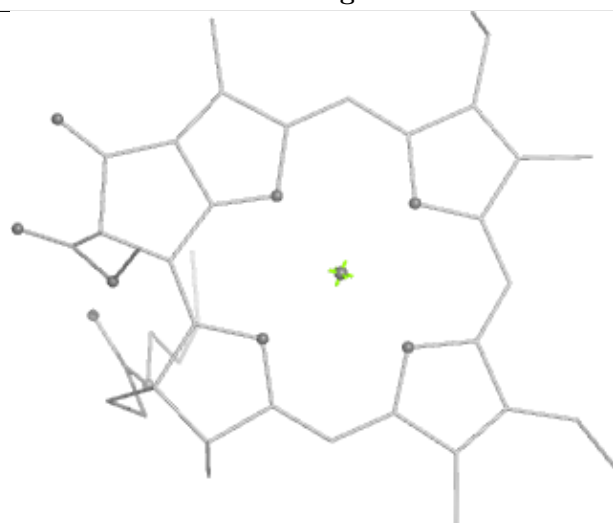
Bond lengths



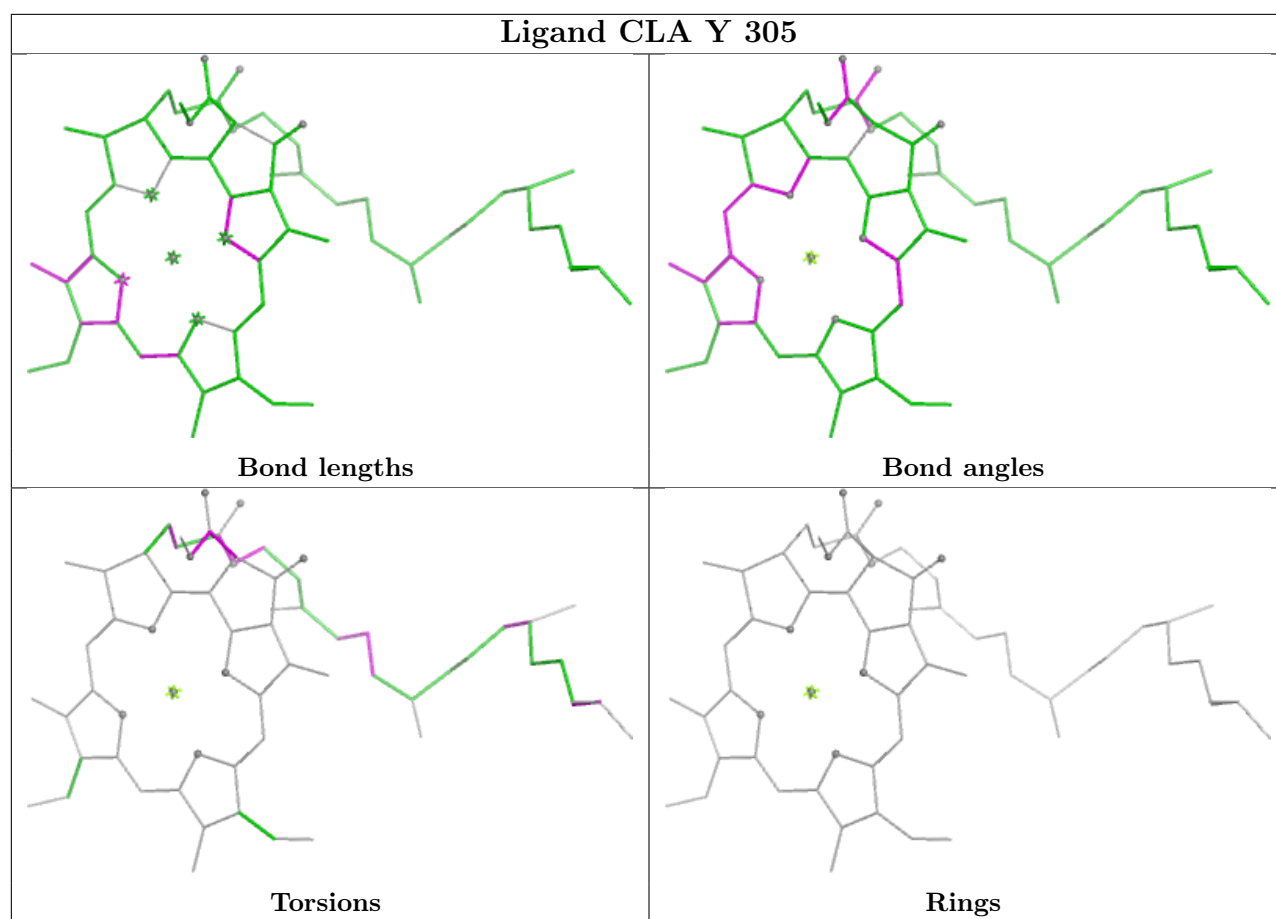
Bond angles

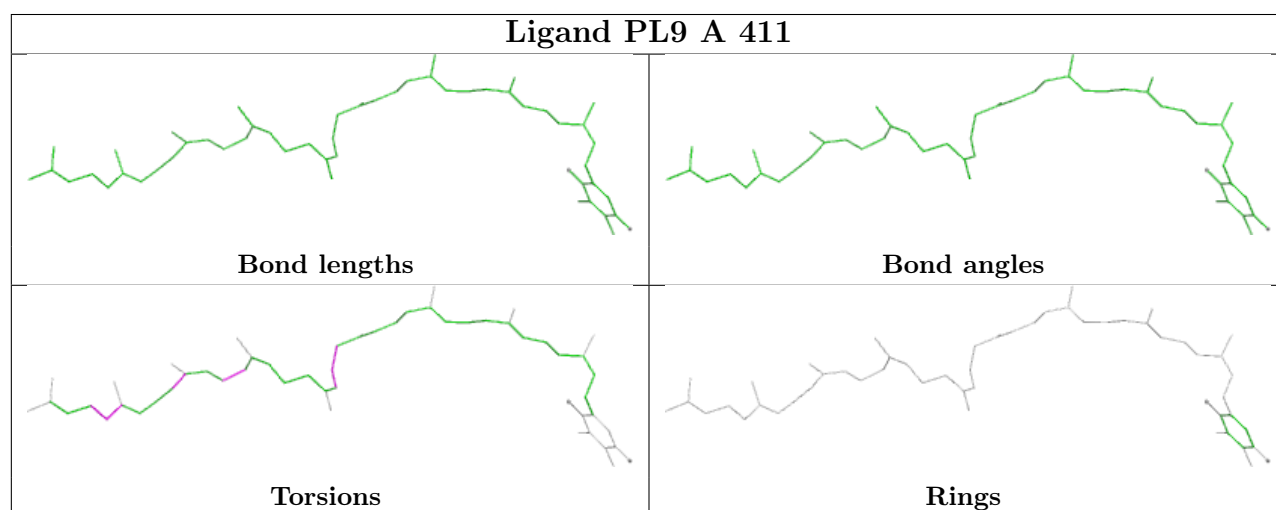
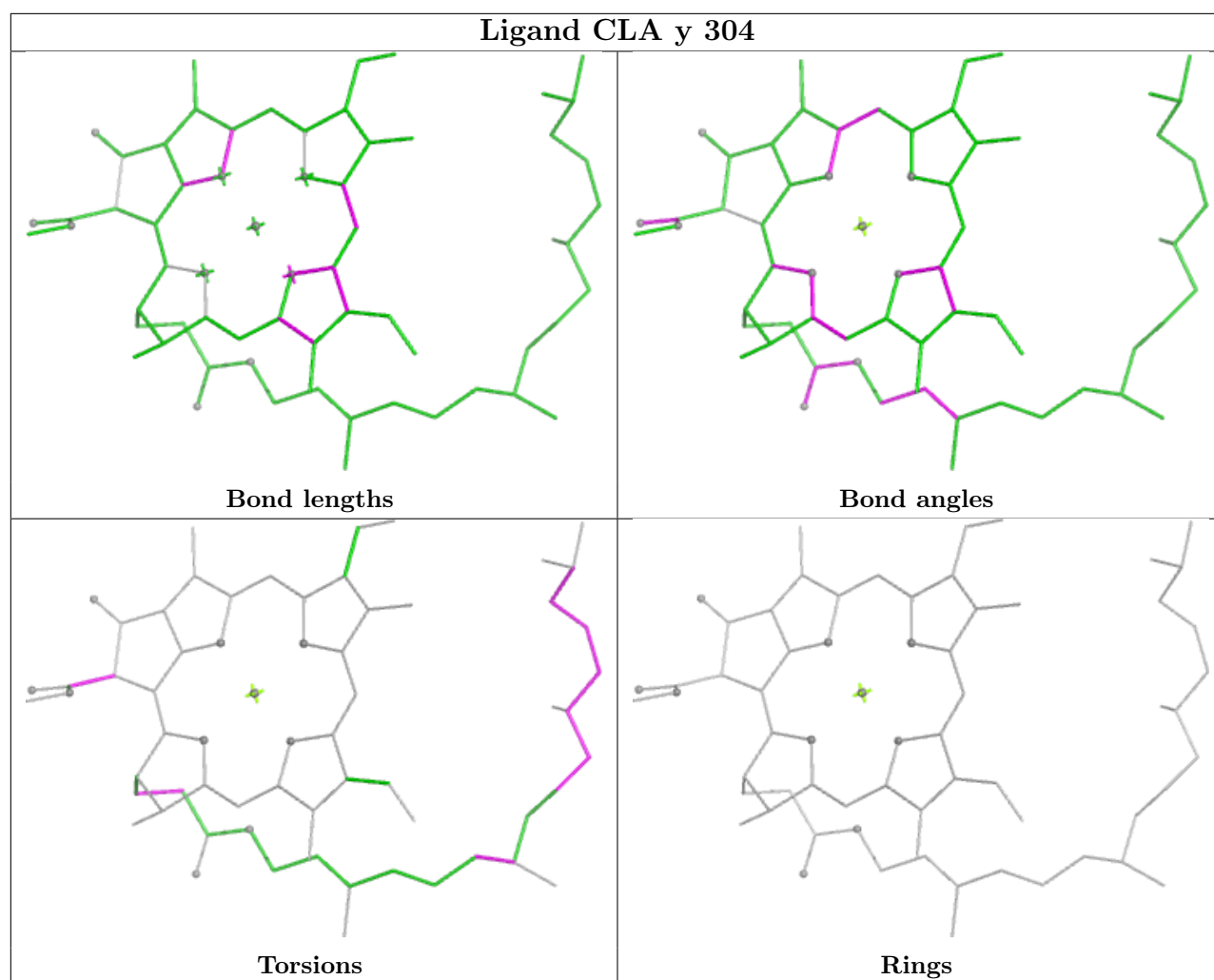


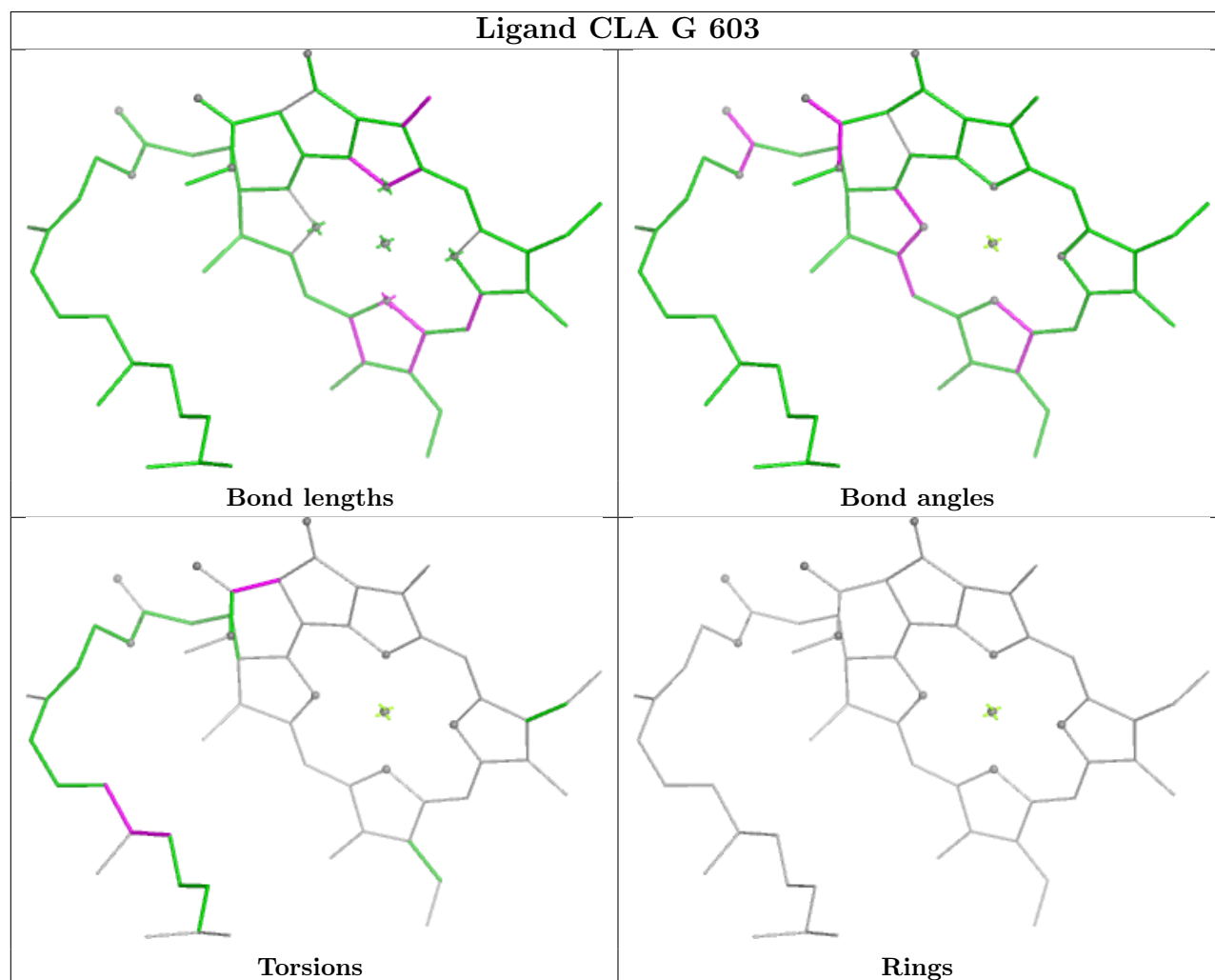
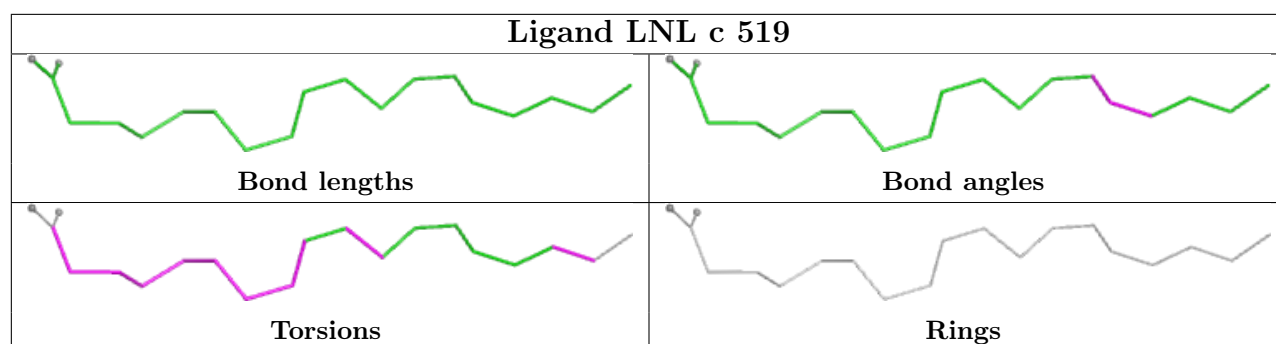
Torsions



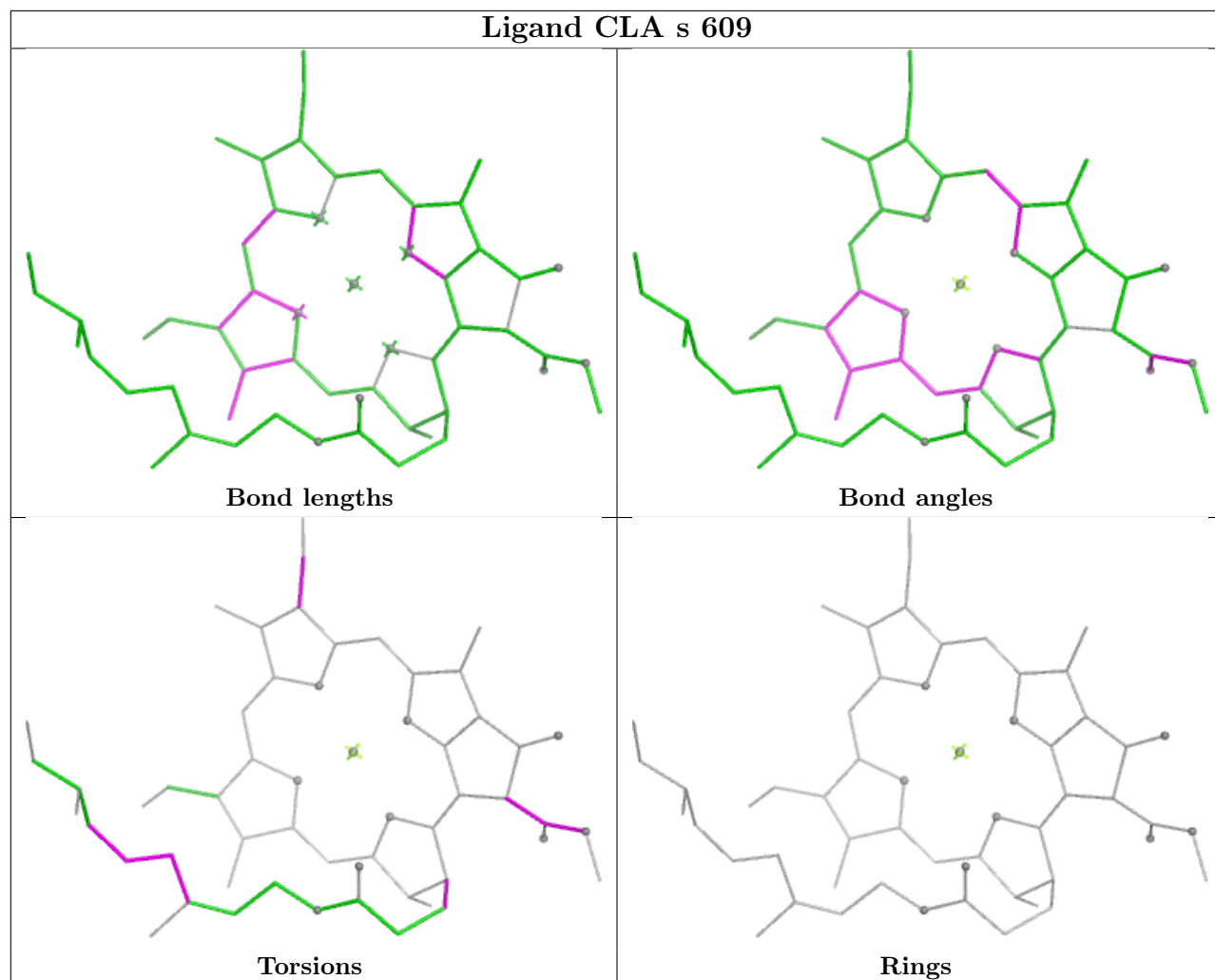
Rings



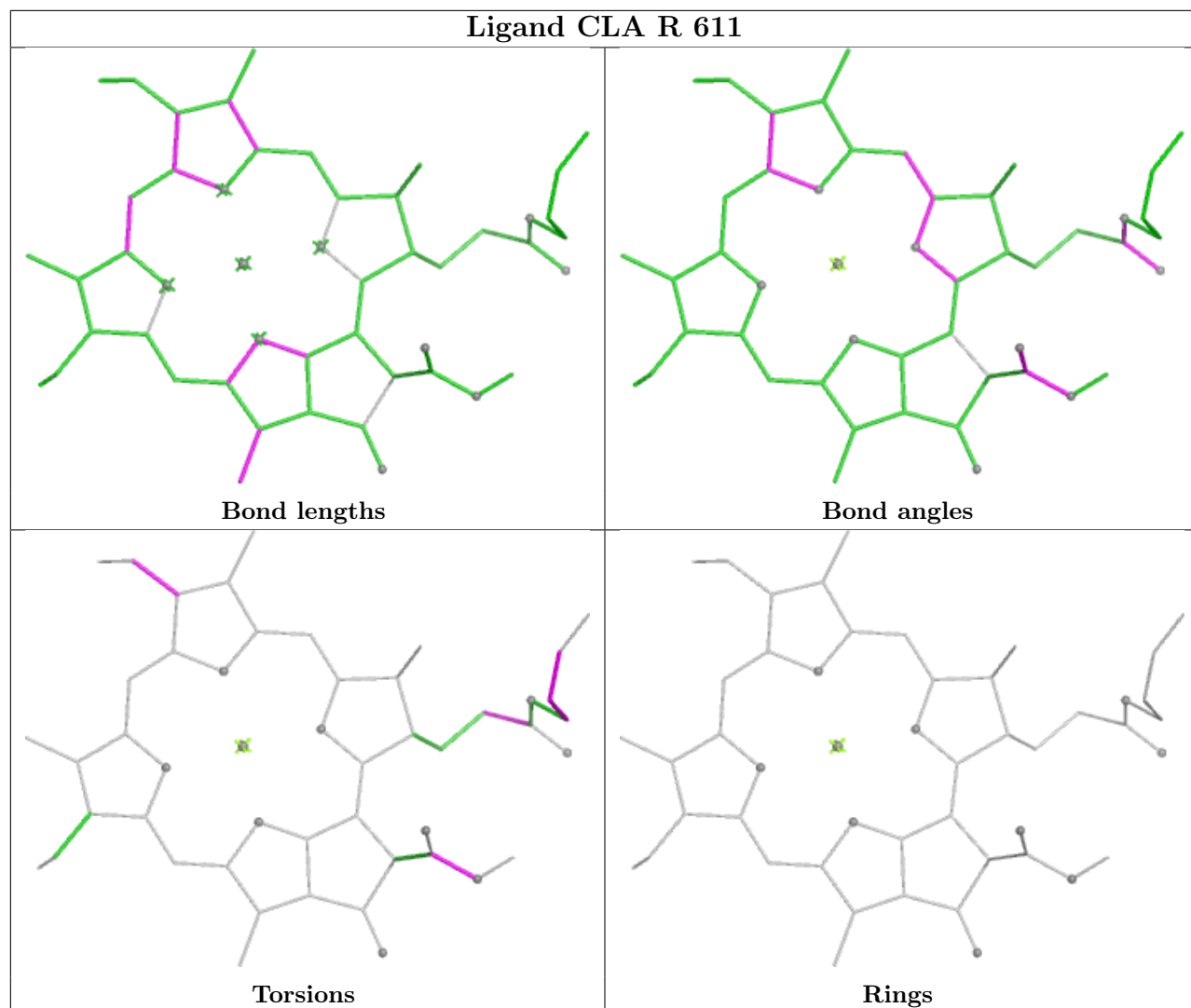


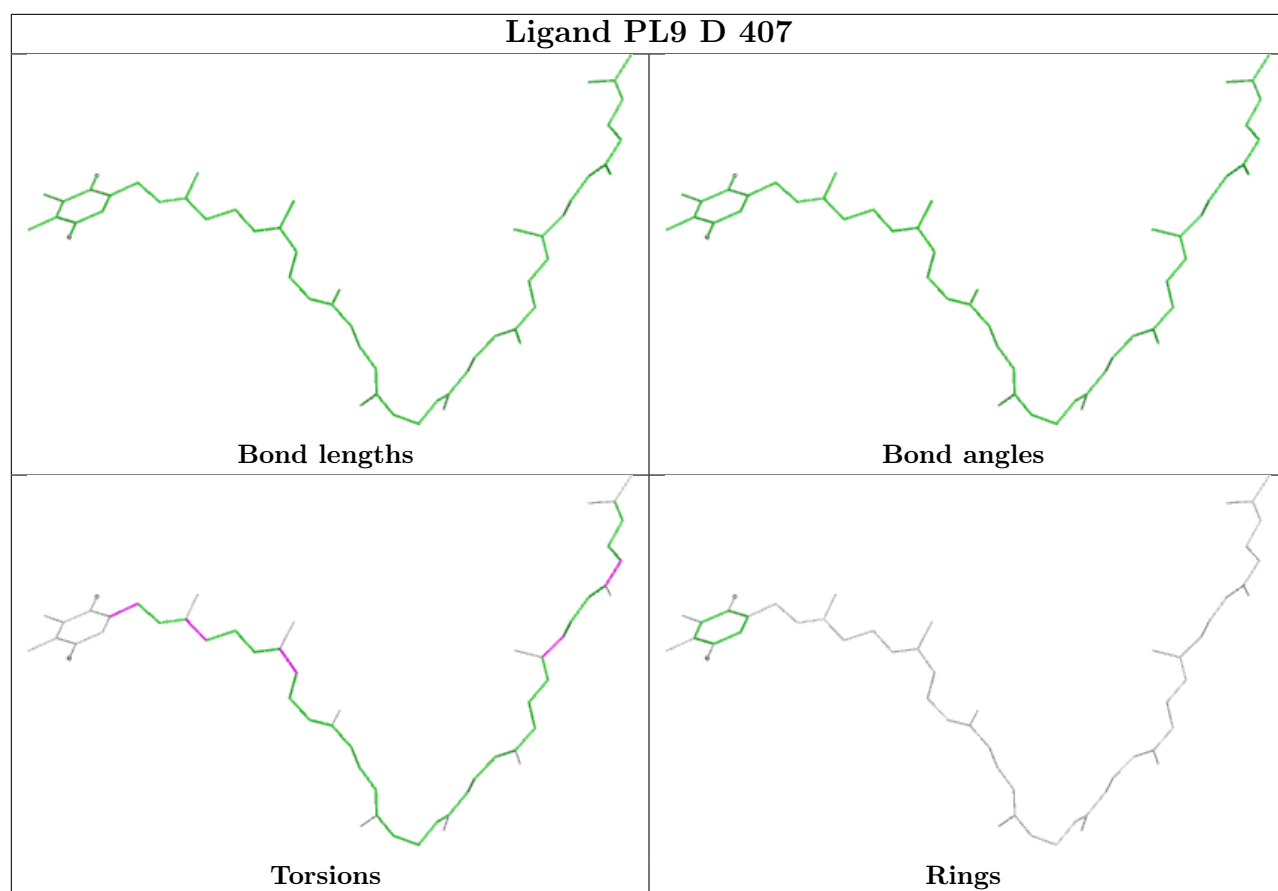


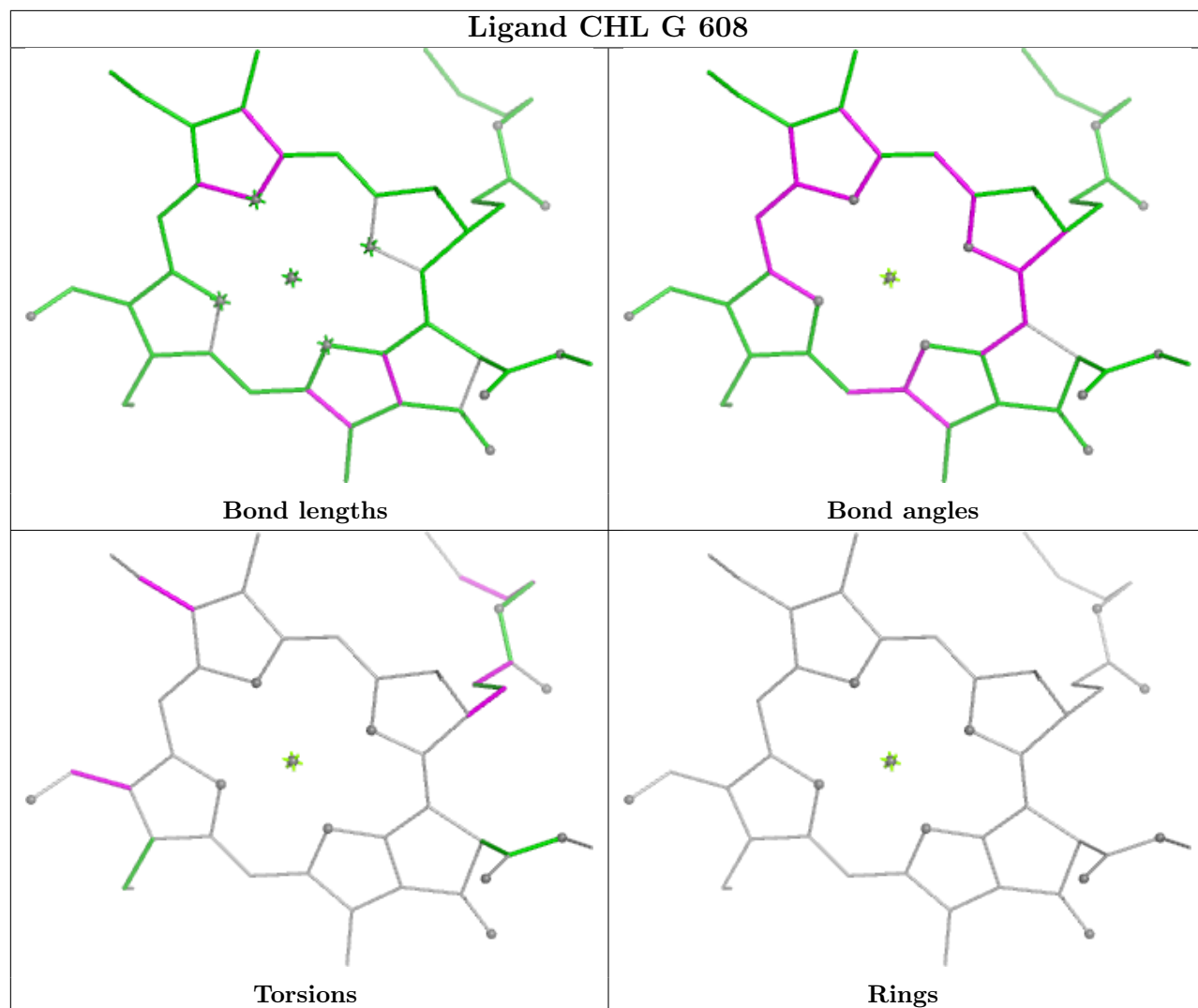
Ligand CLA s 609

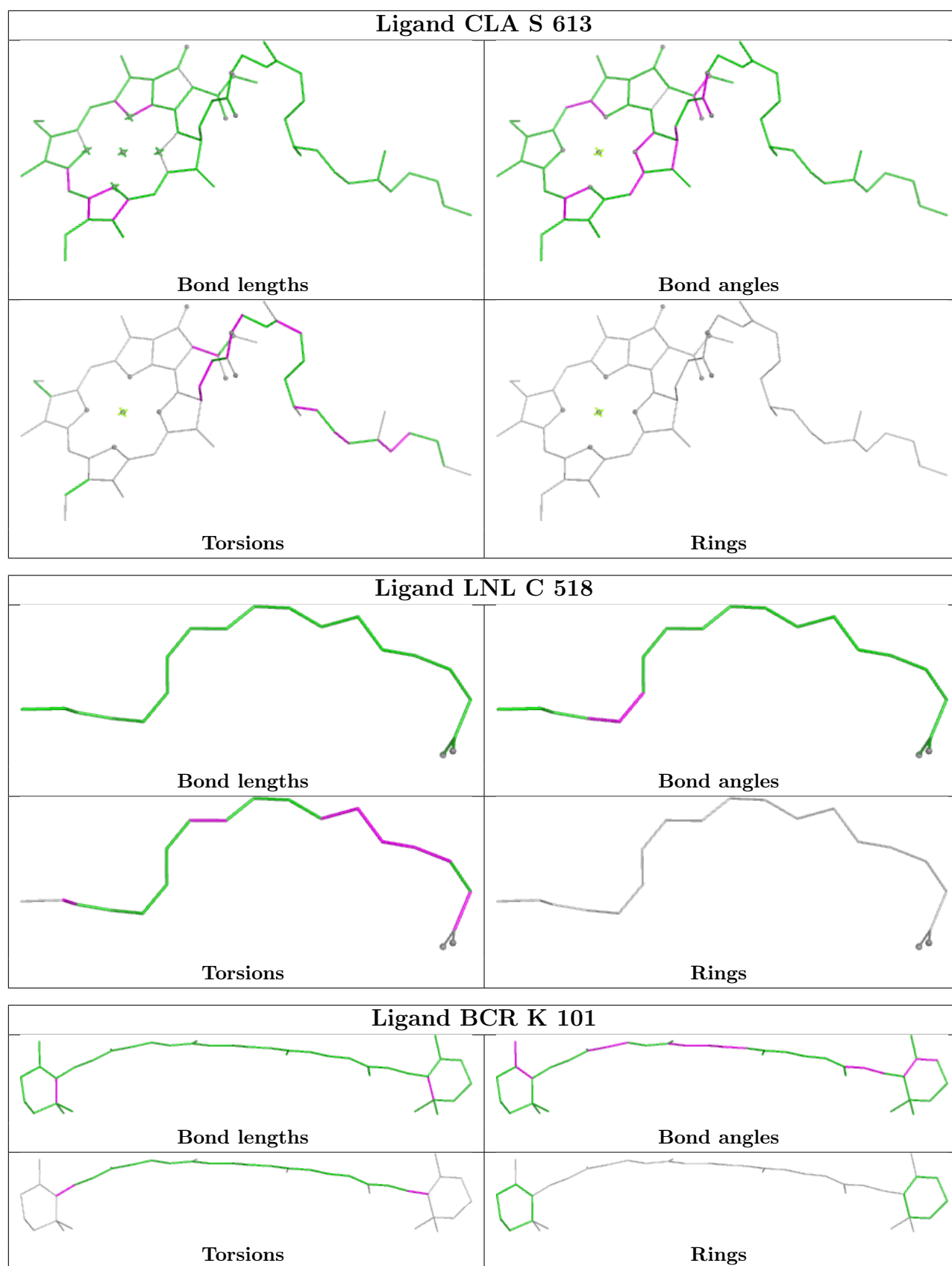


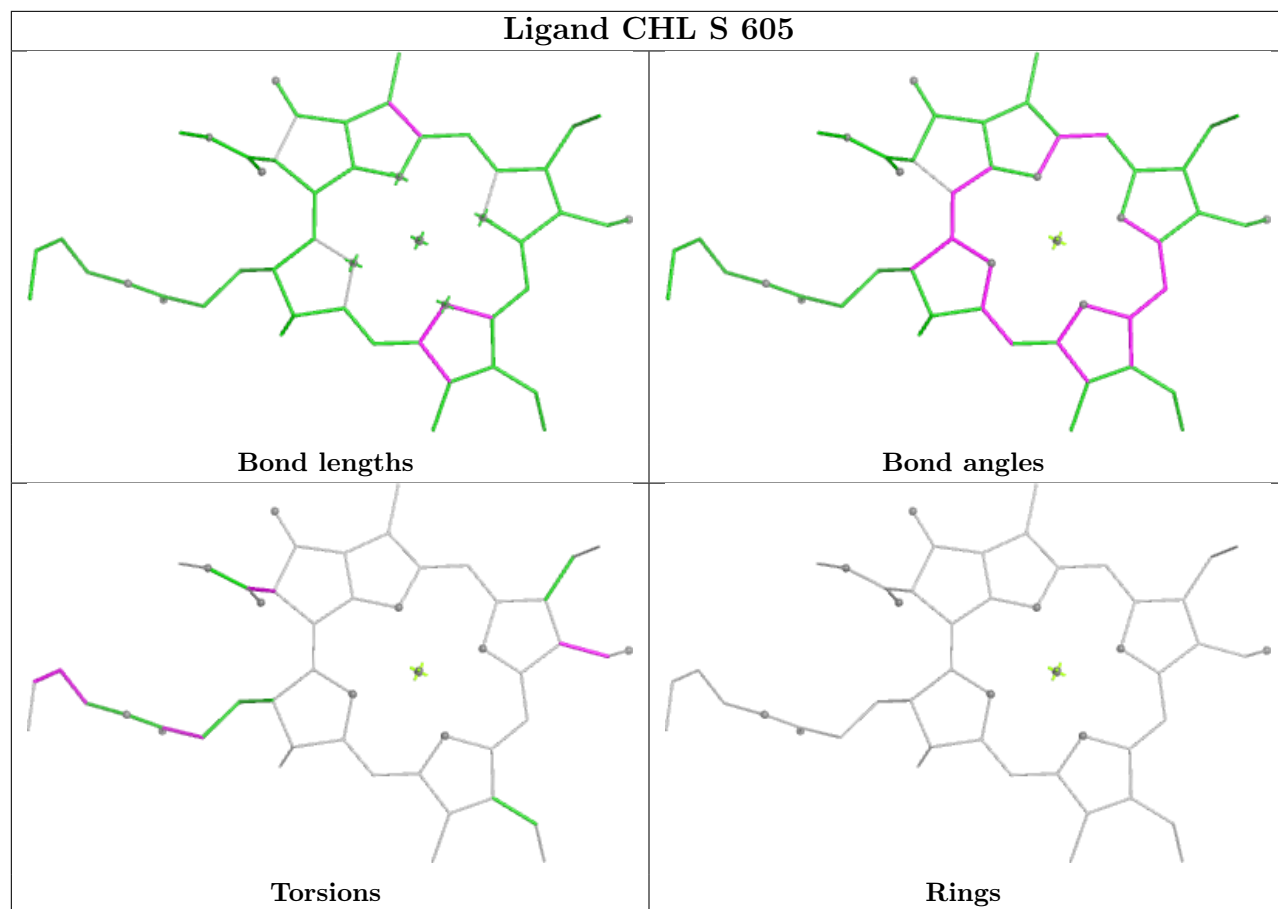
Ligand CLA R 611



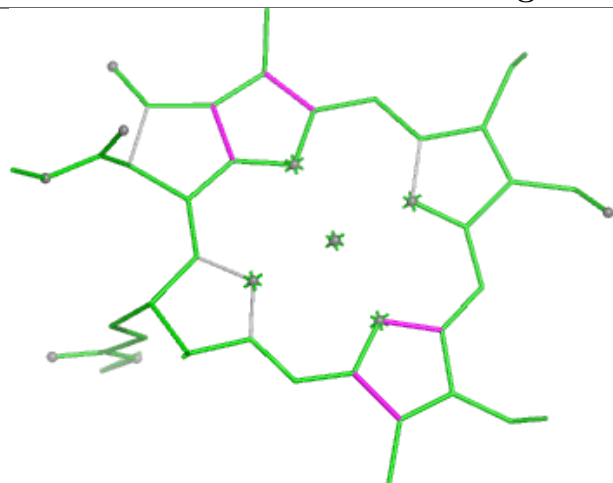




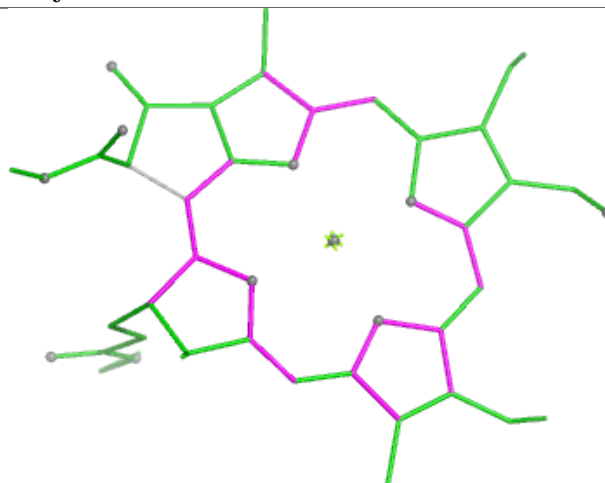




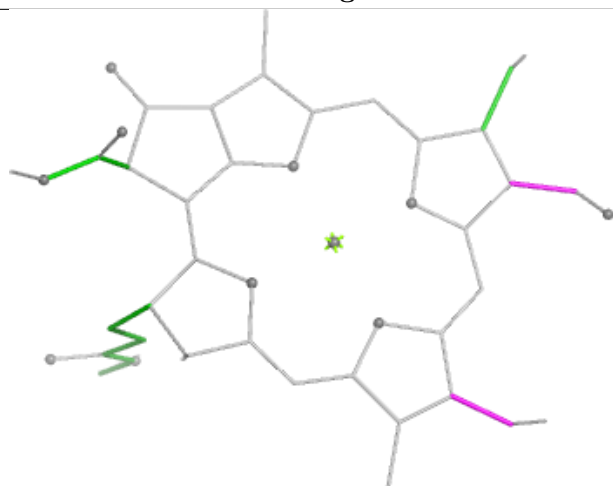
Ligand CHL y 307



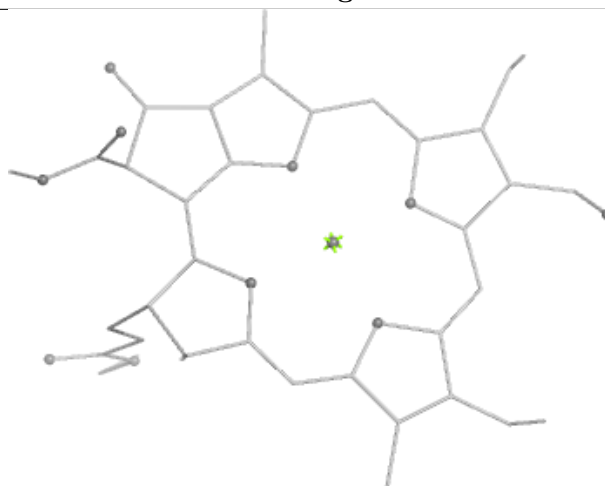
Bond lengths



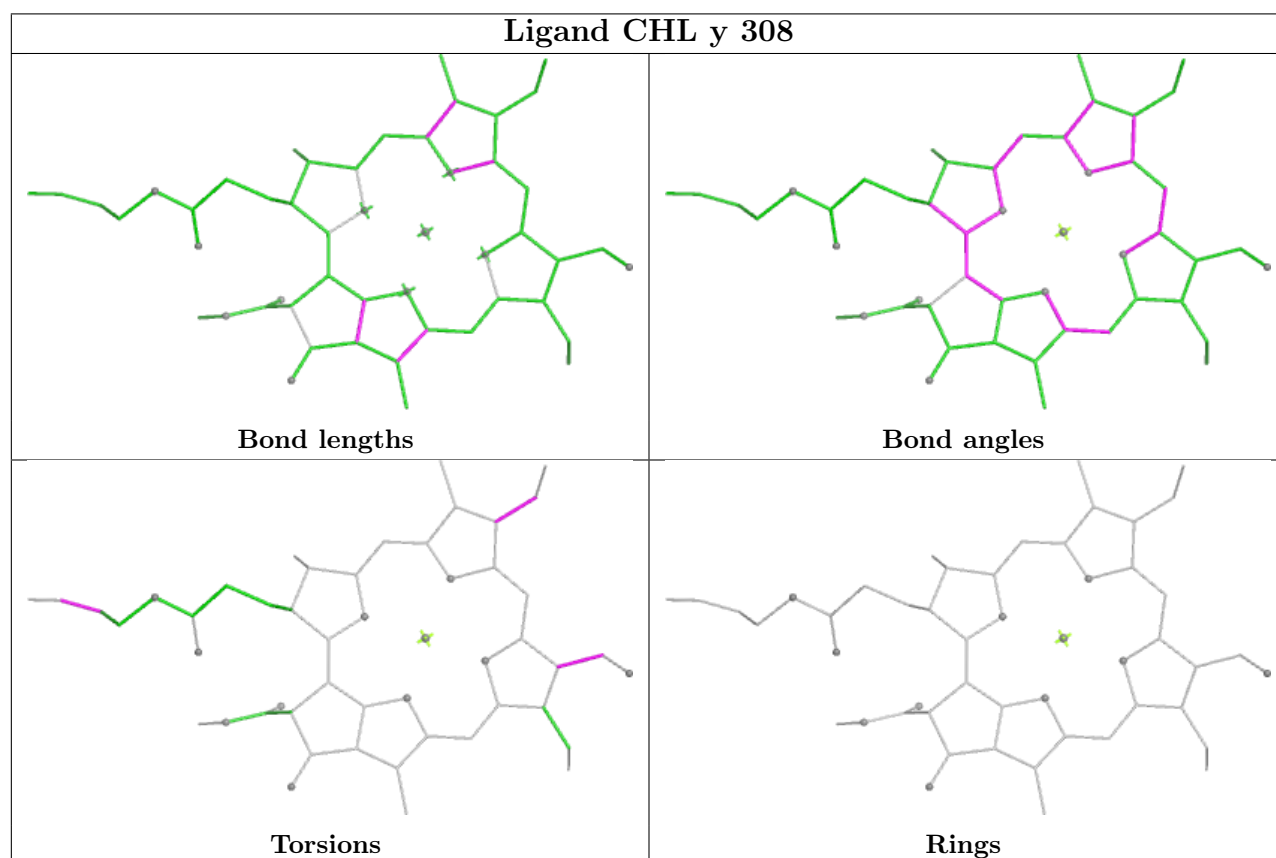
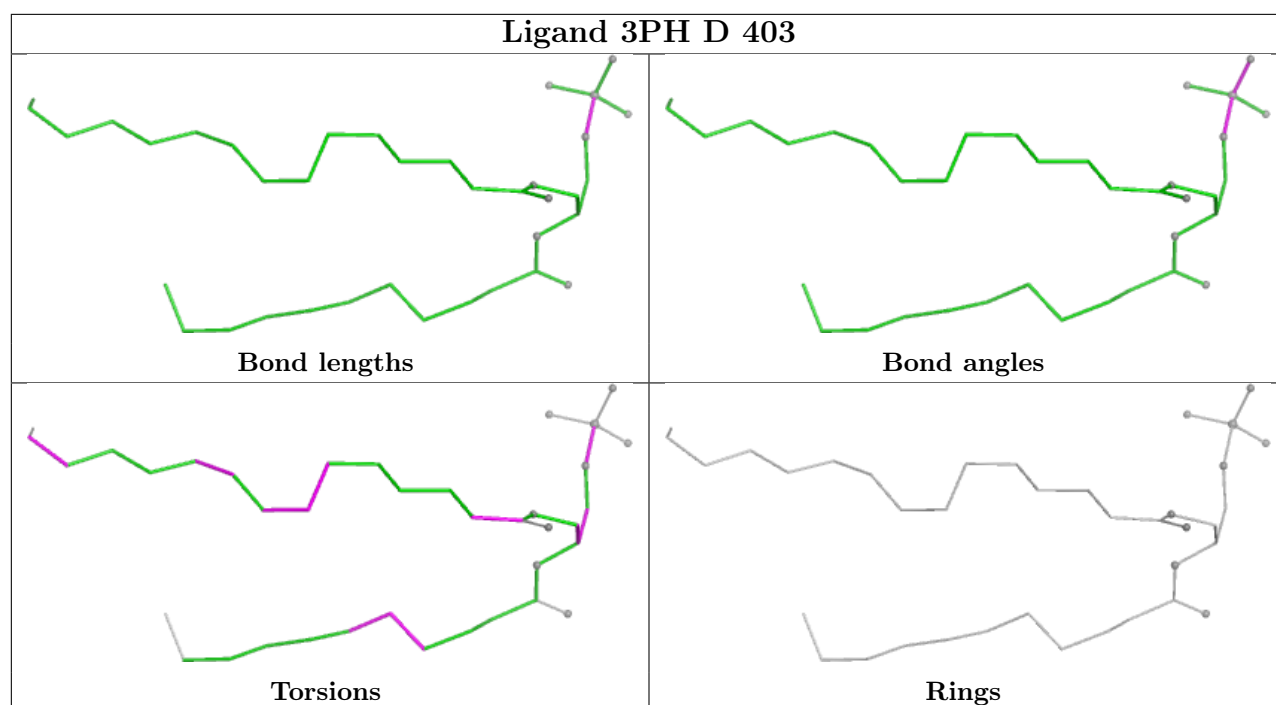
Bond angles

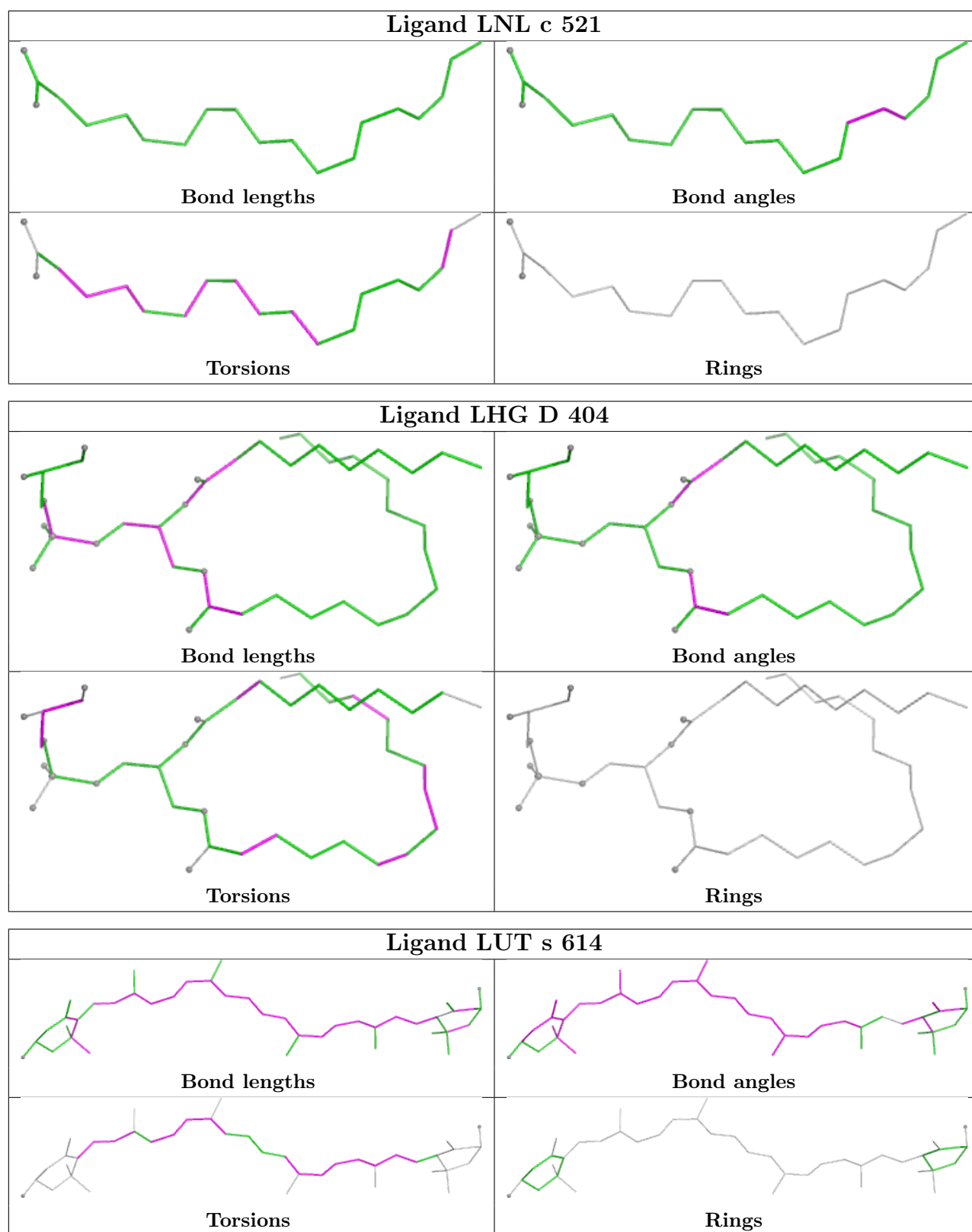


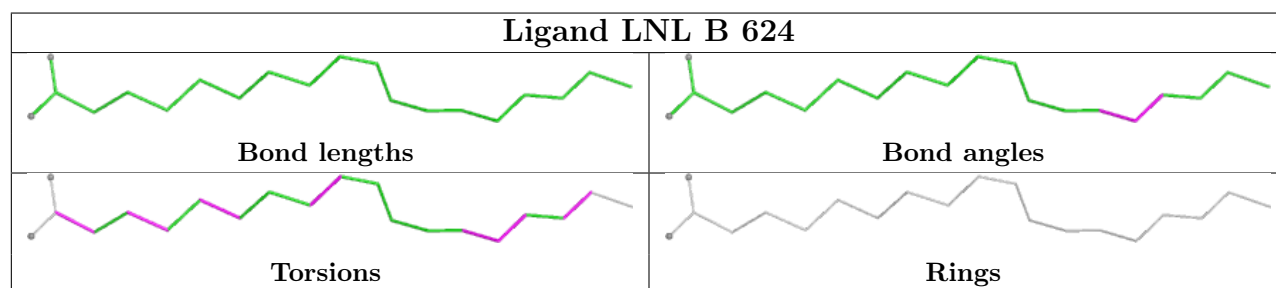
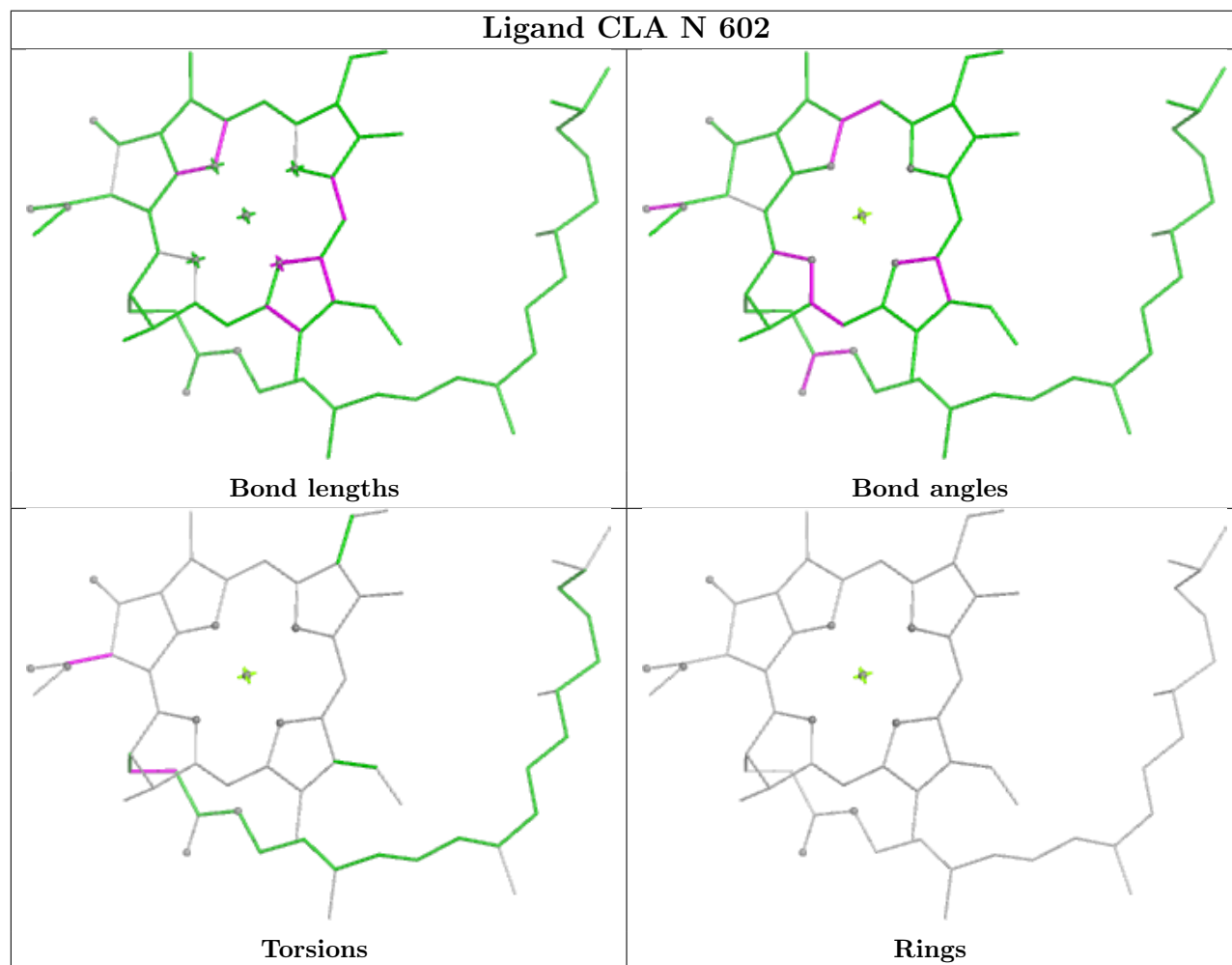
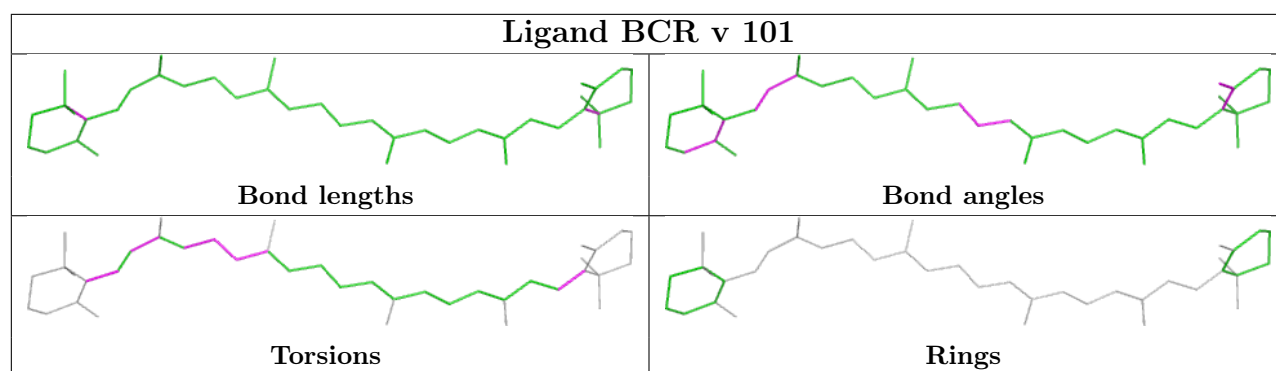
Torsions

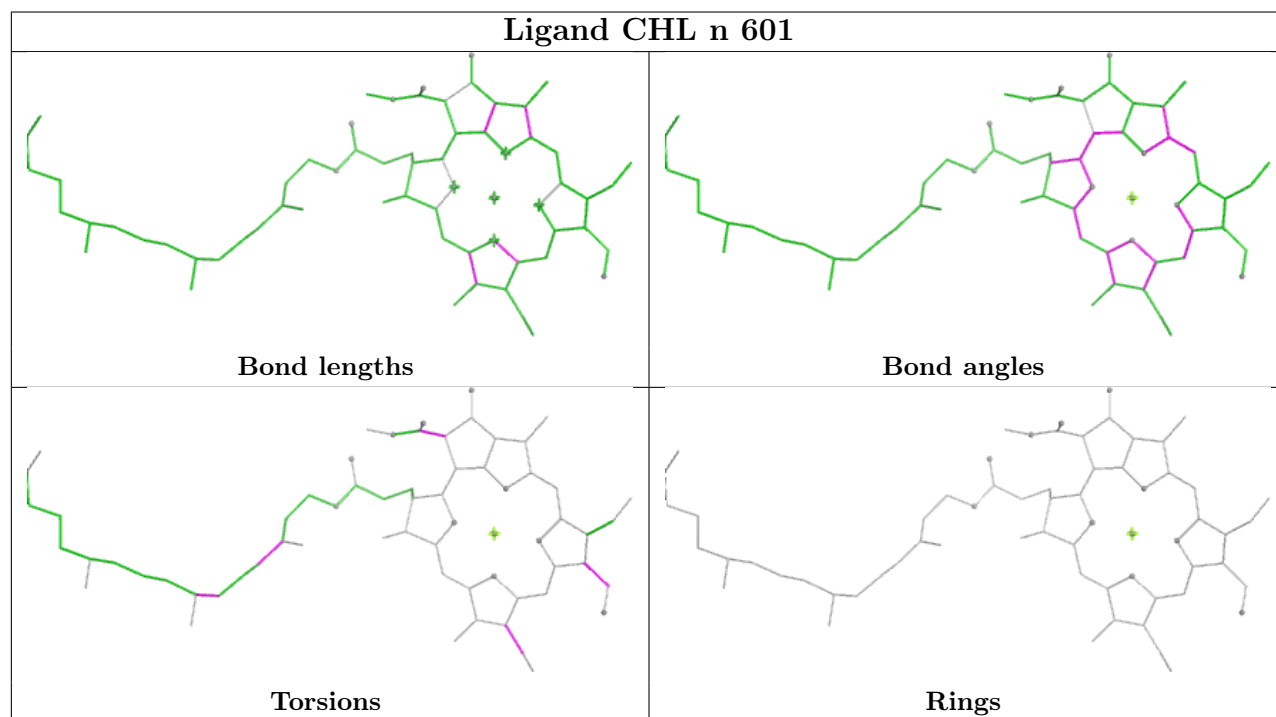
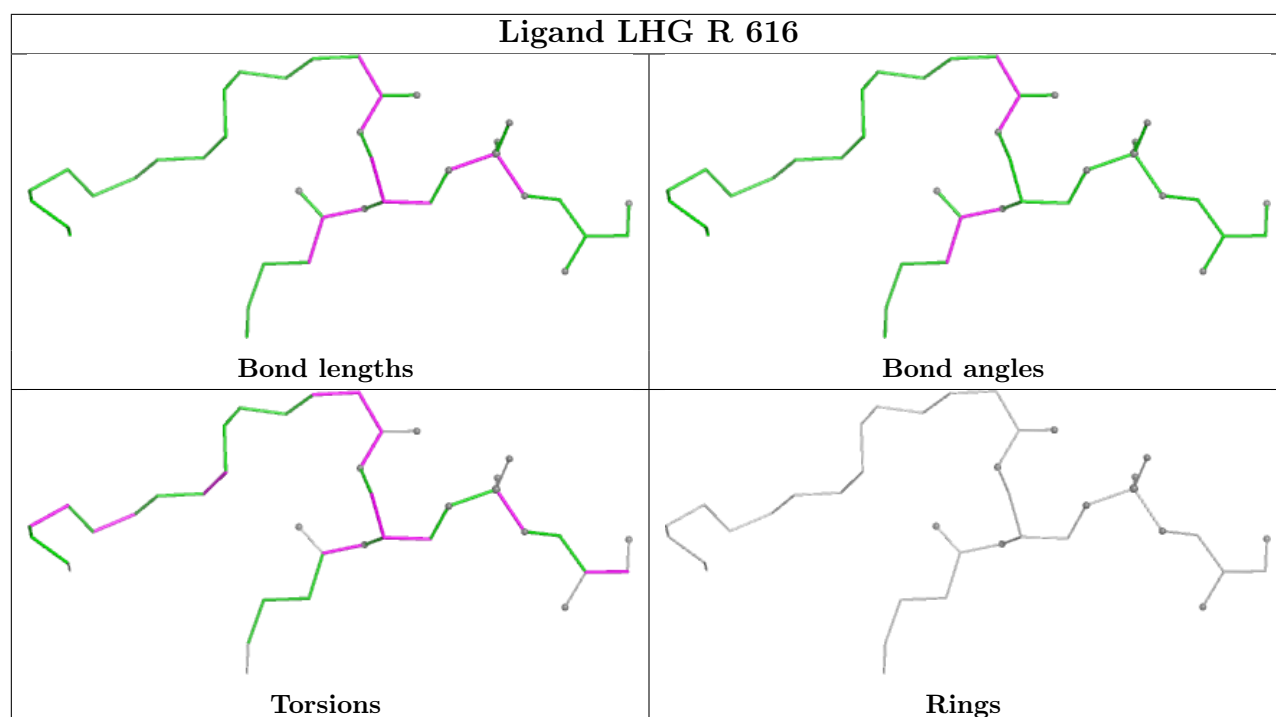


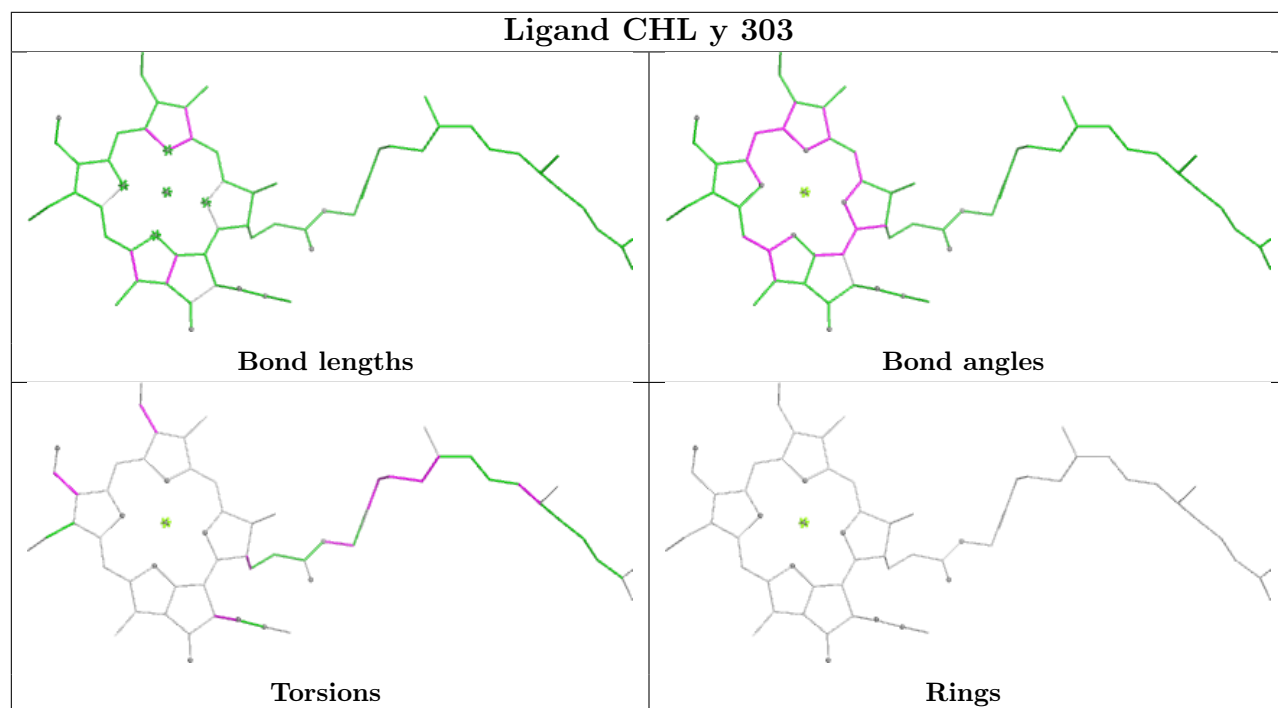
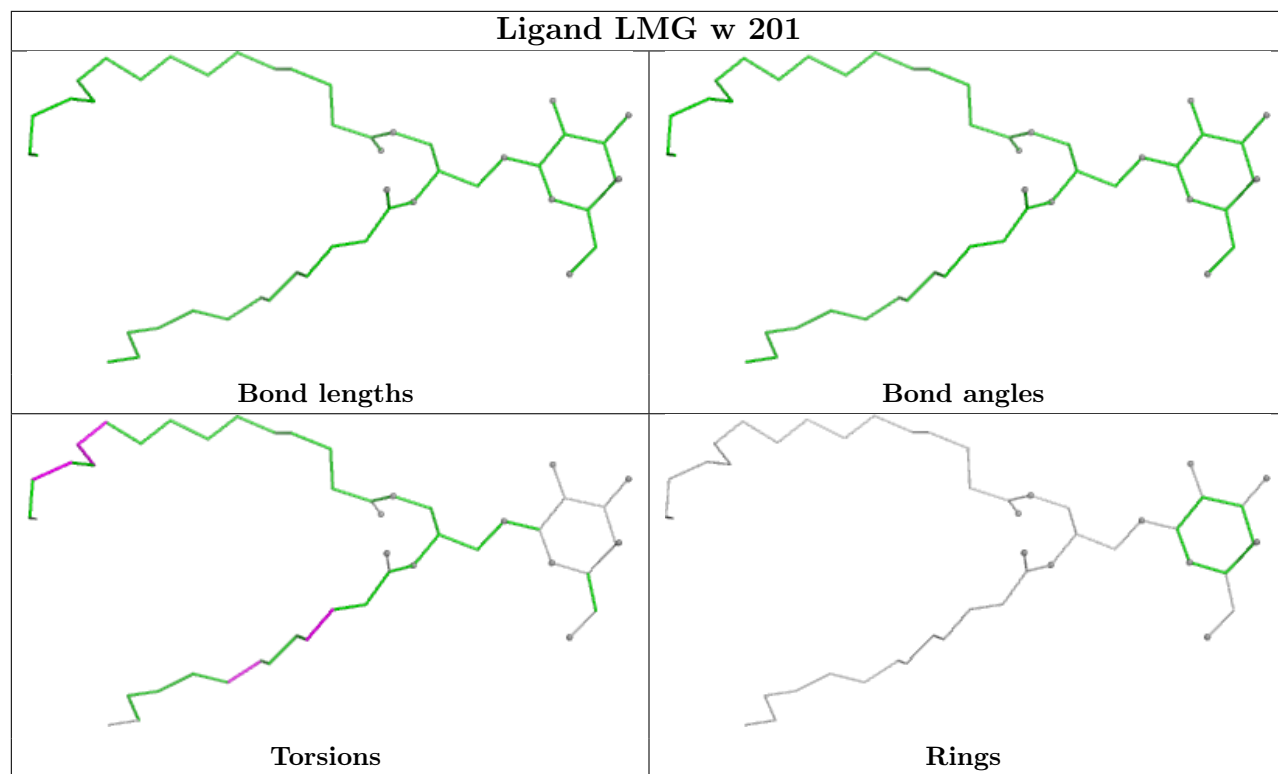
Rings

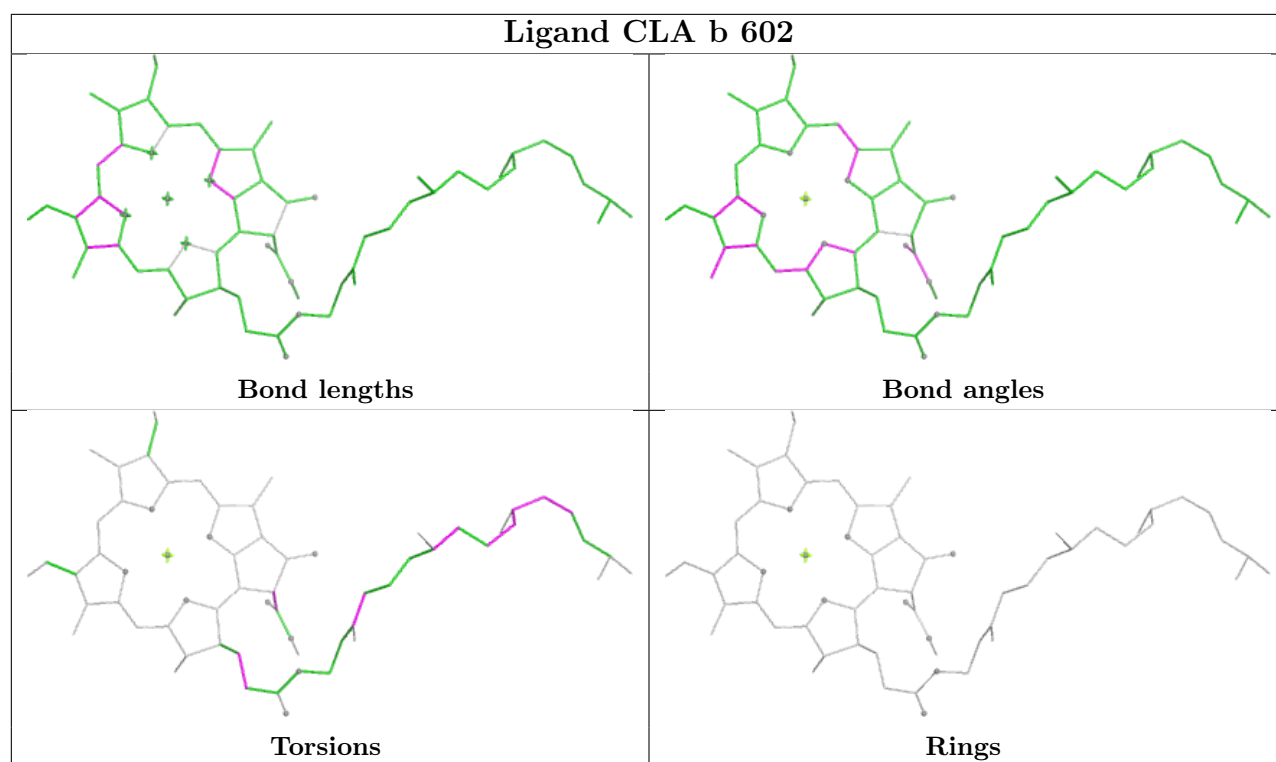


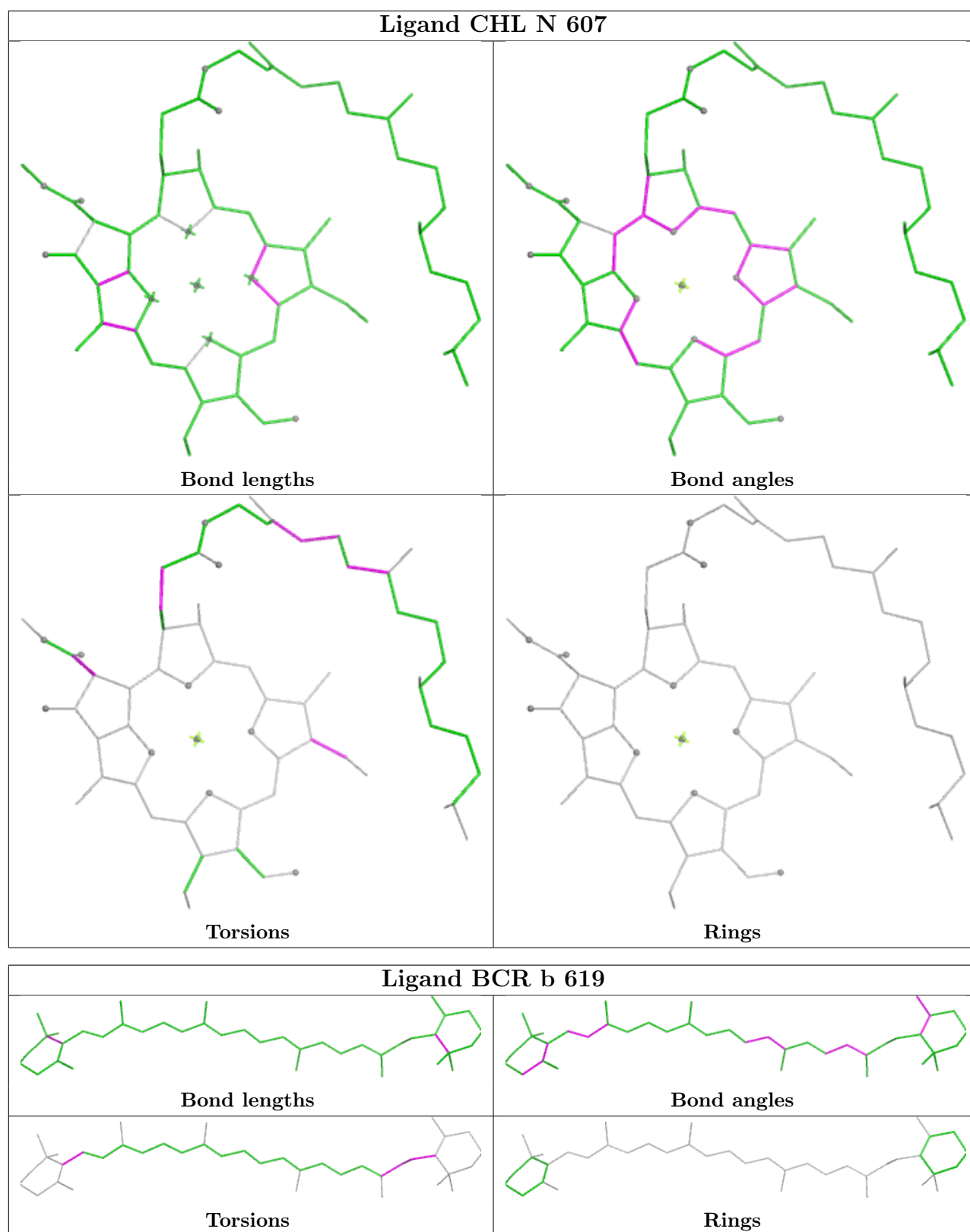


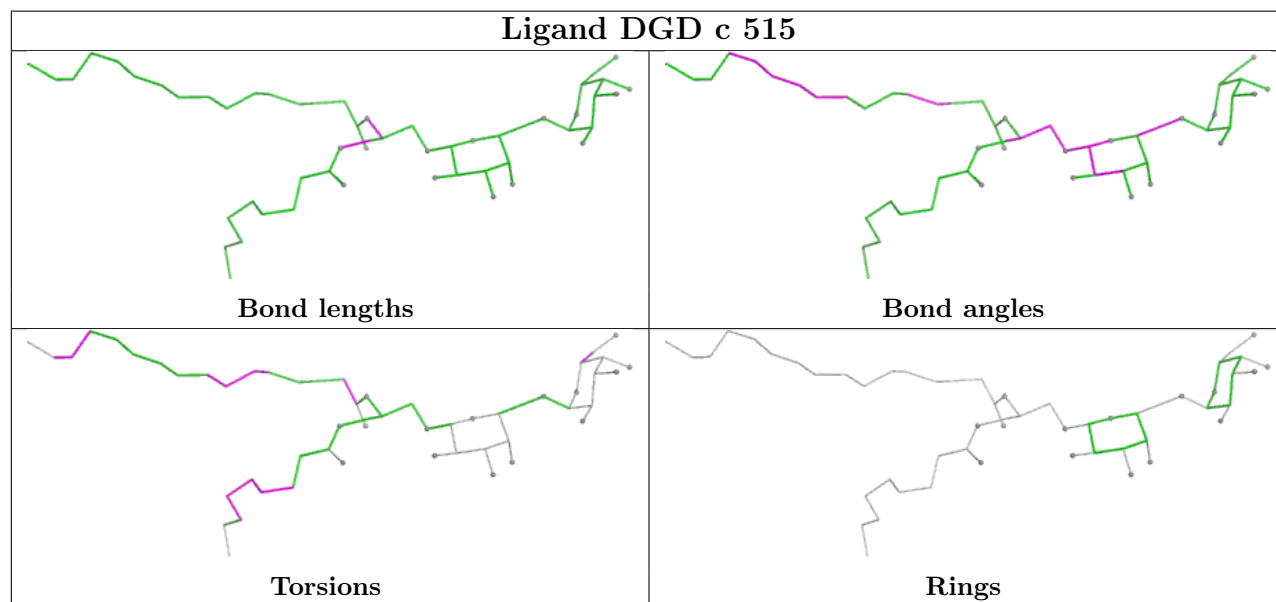
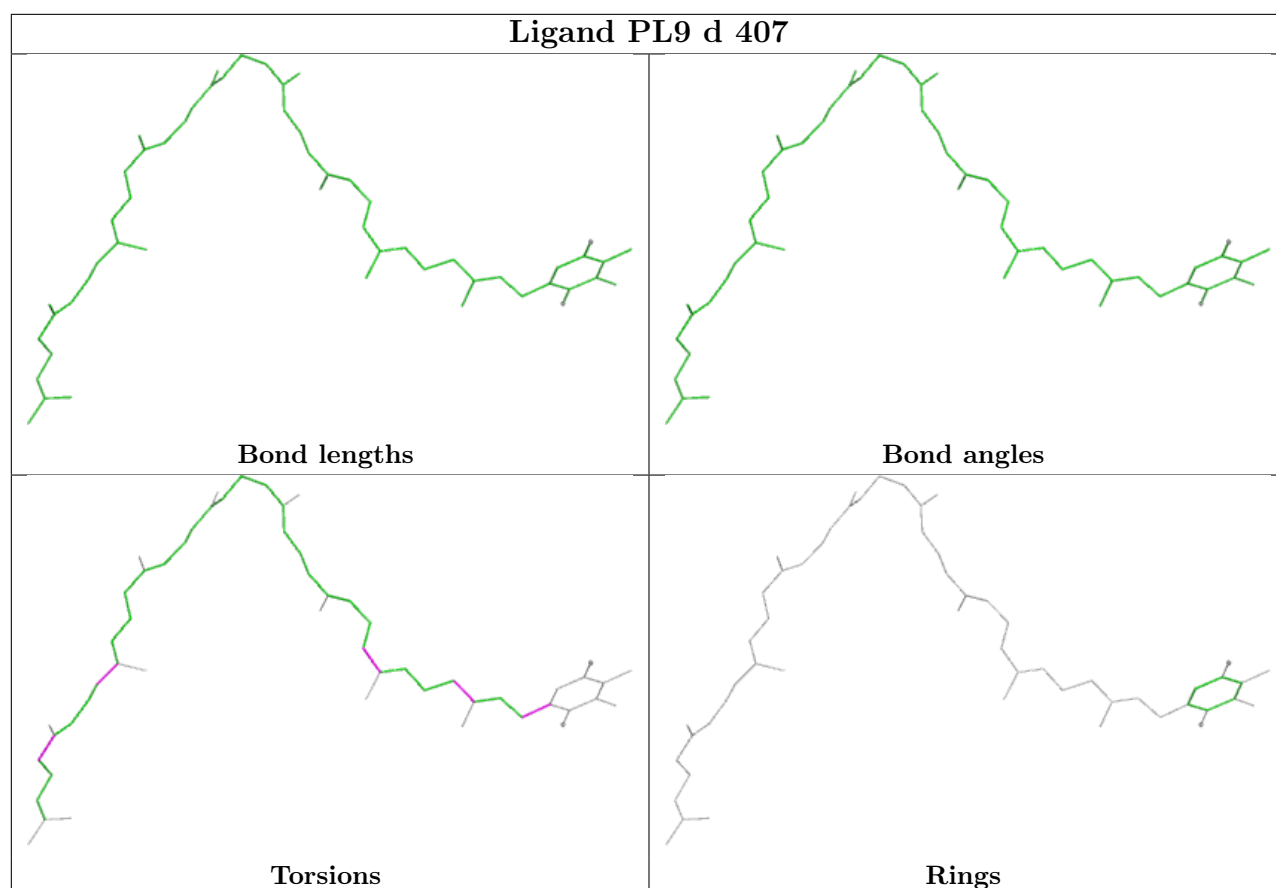


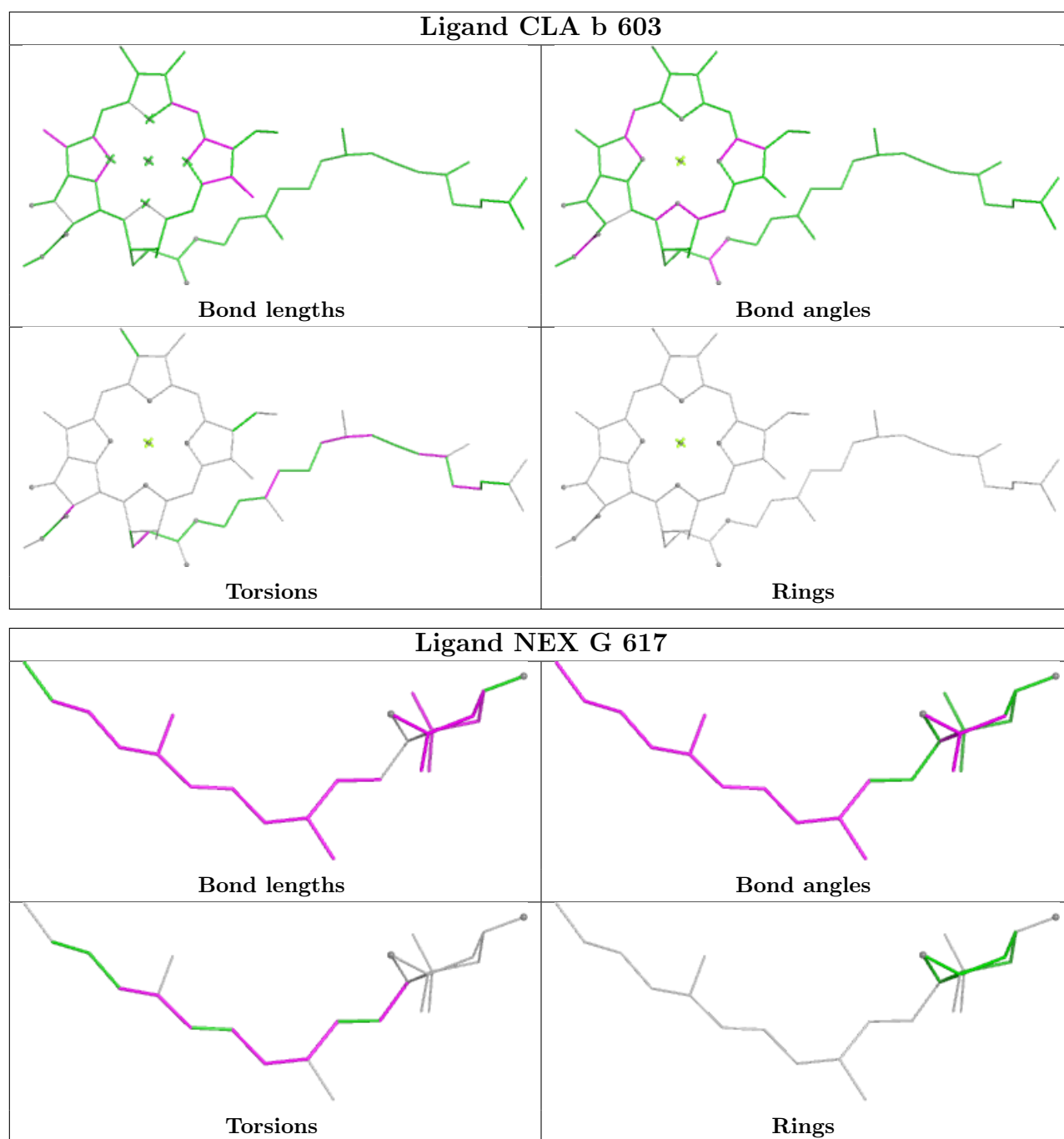


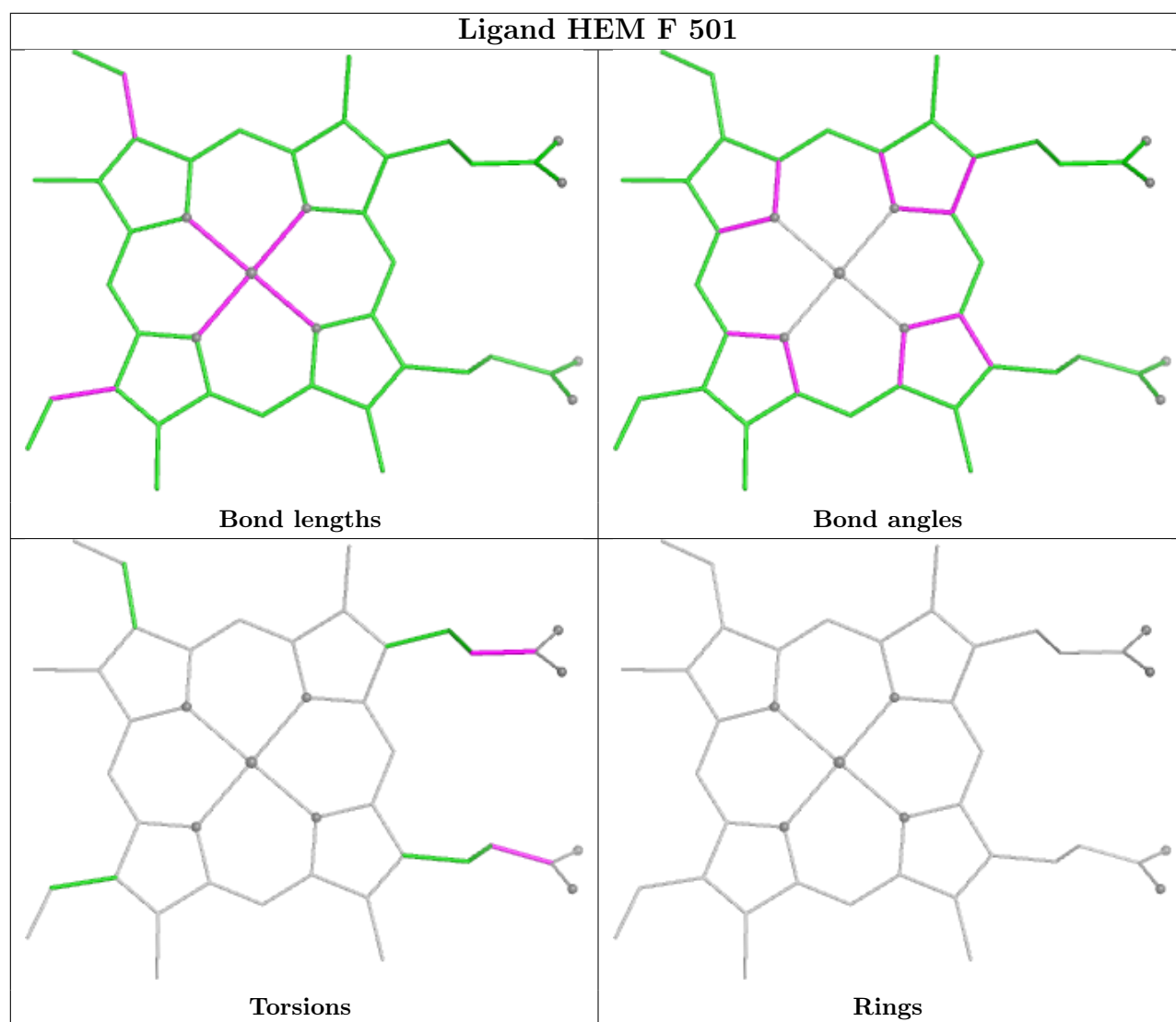


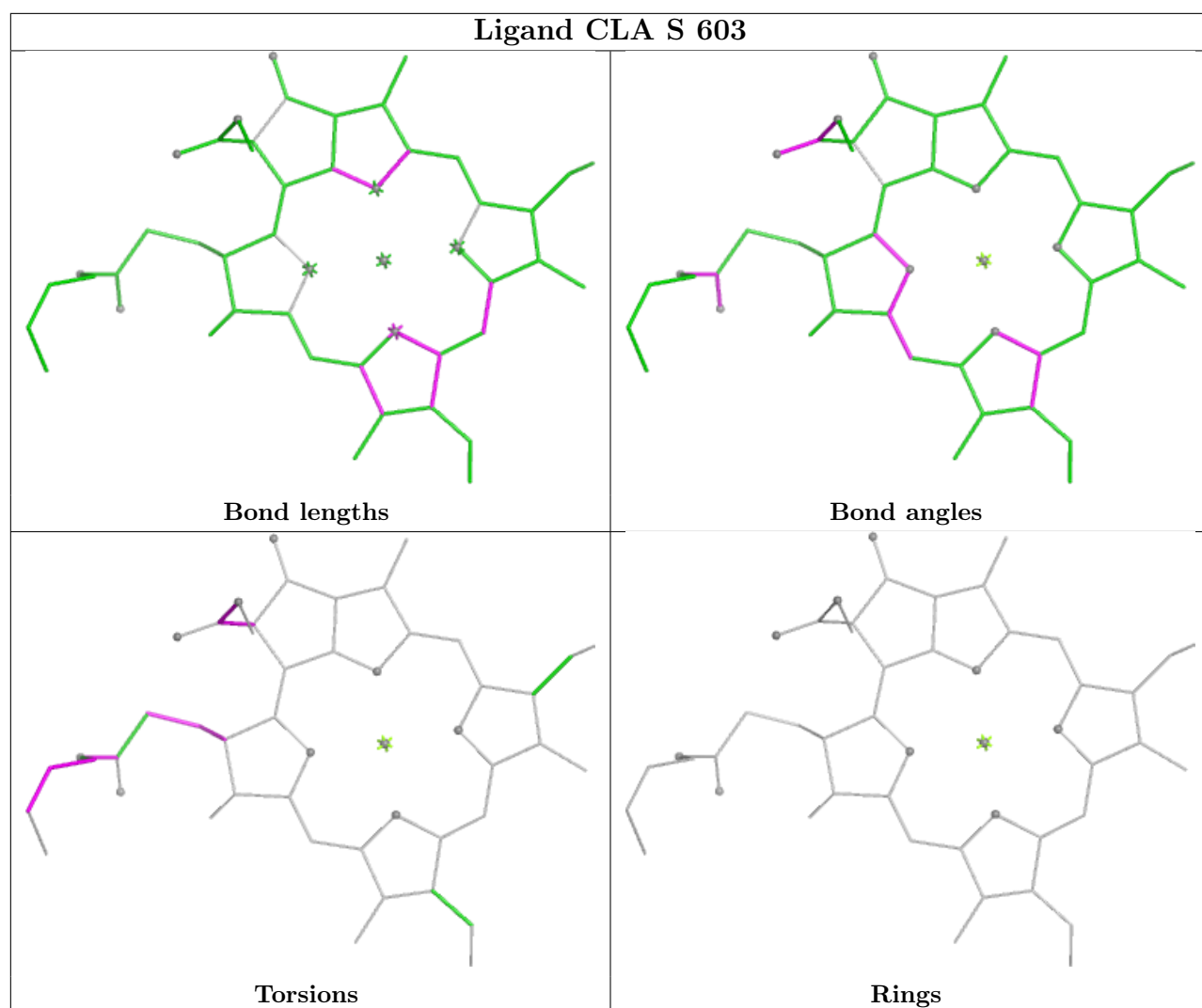


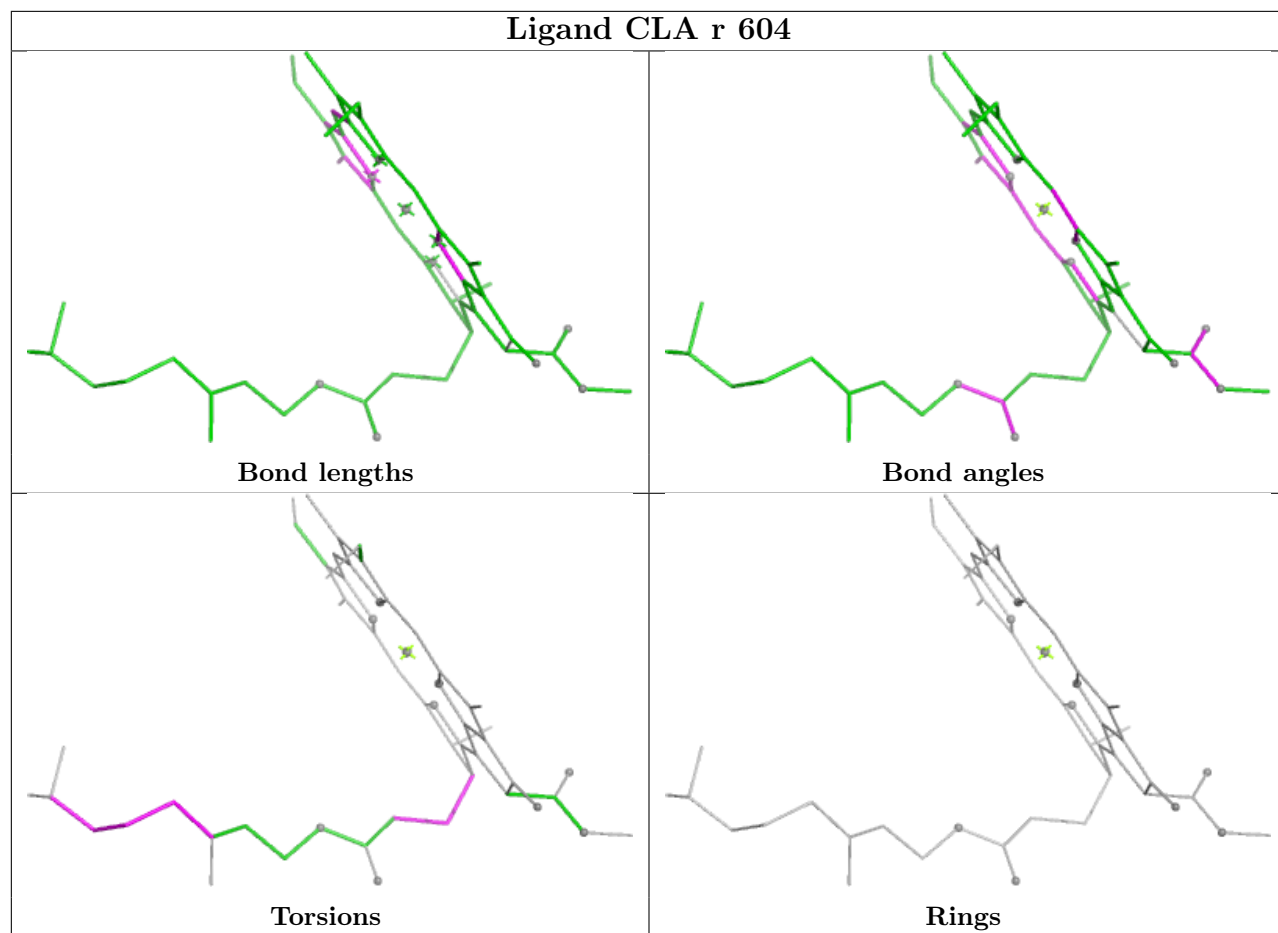




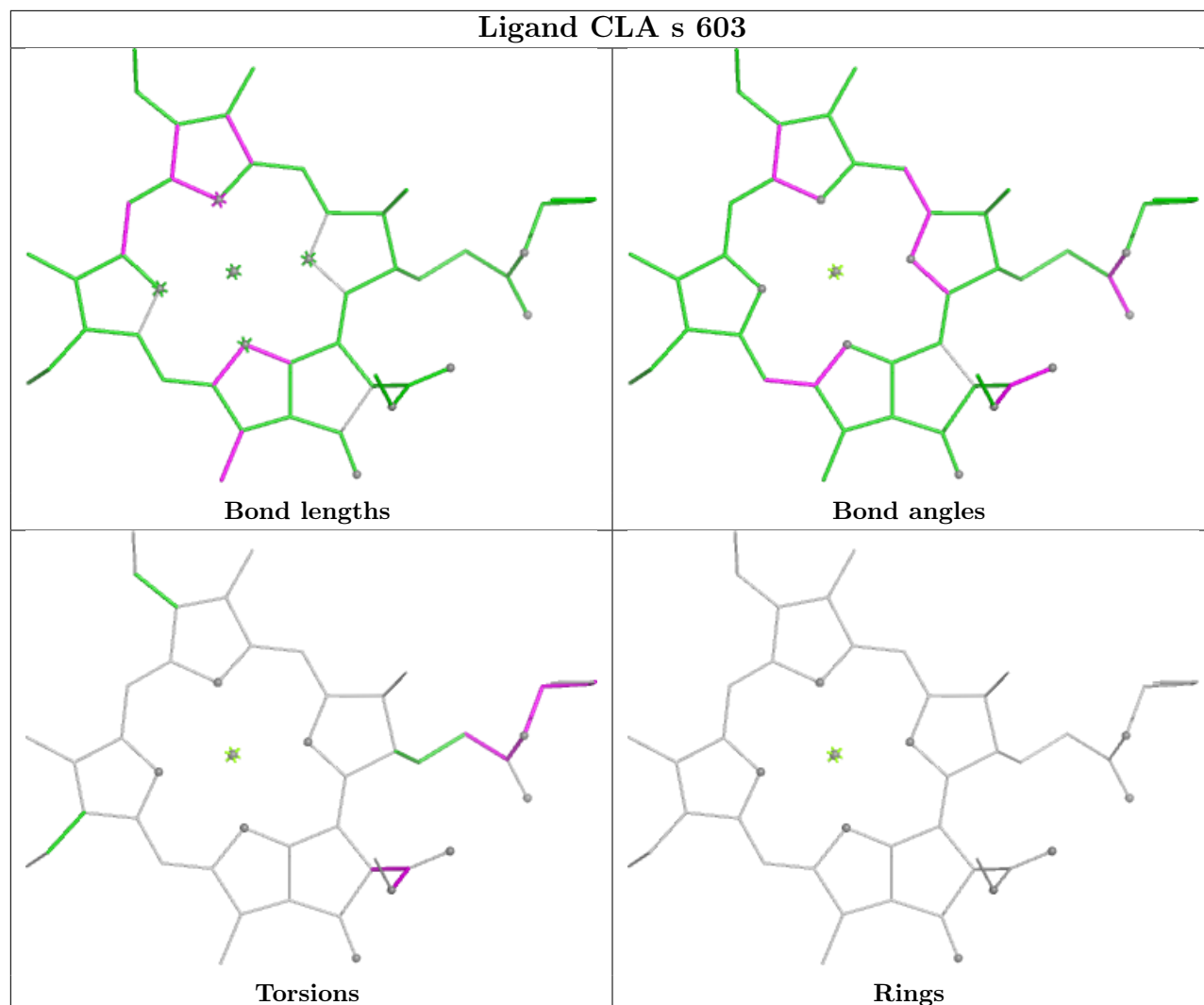




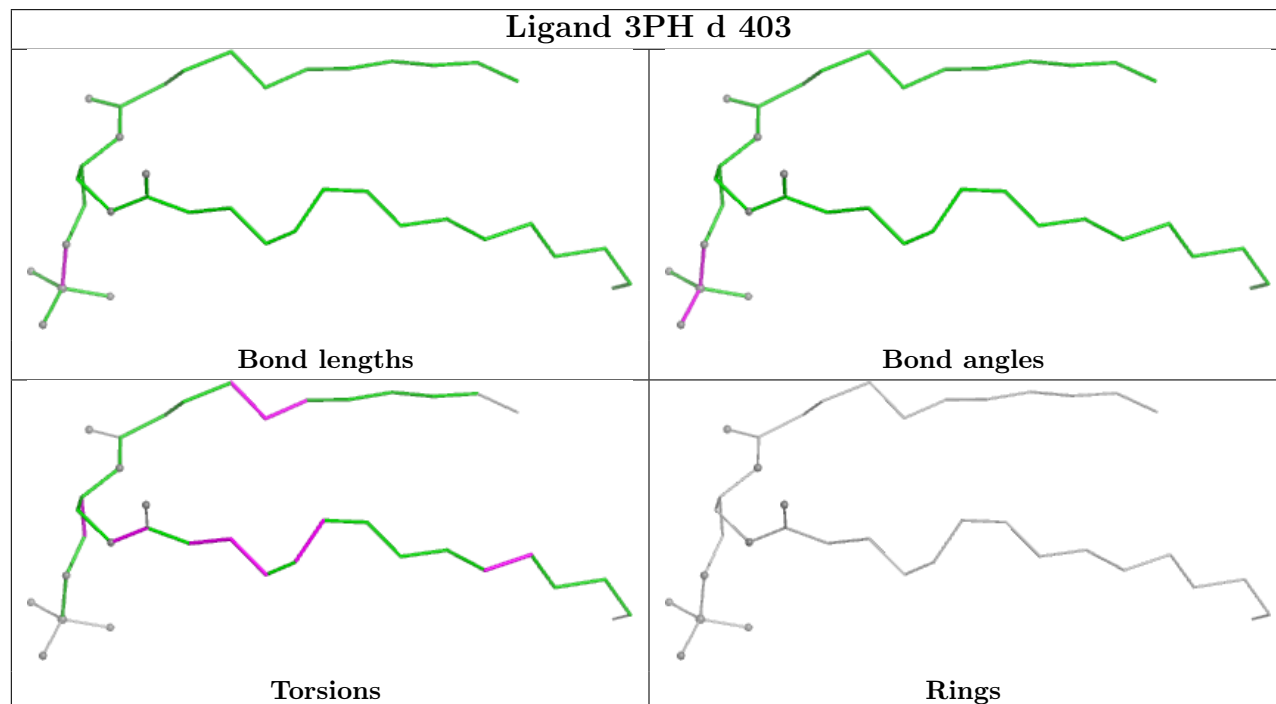


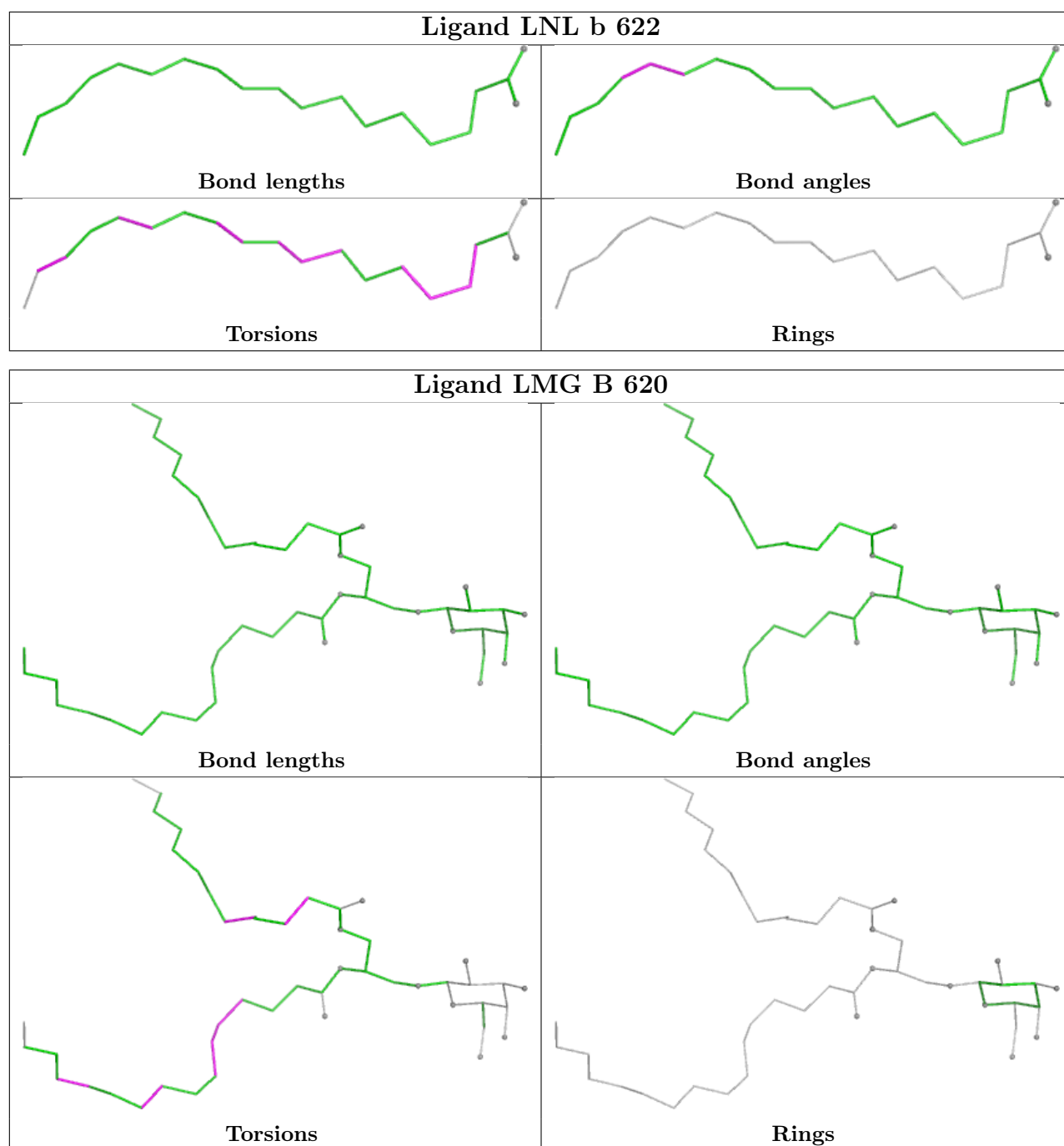


Ligand CLA s 603



Ligand 3PH d 403





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.

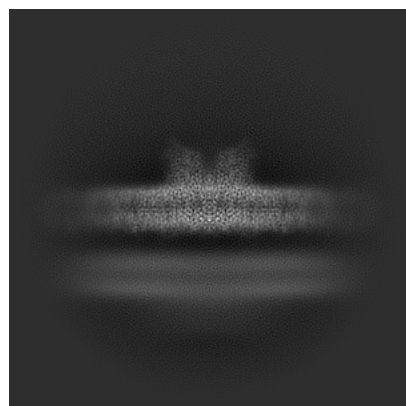
6 Map visualisation [i](#)

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.

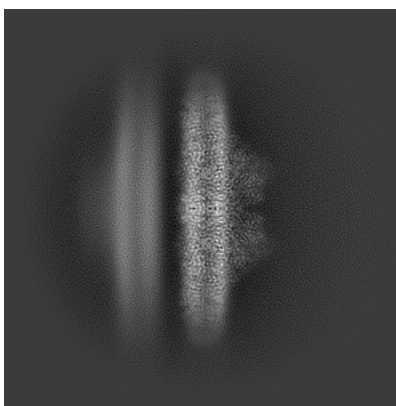
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

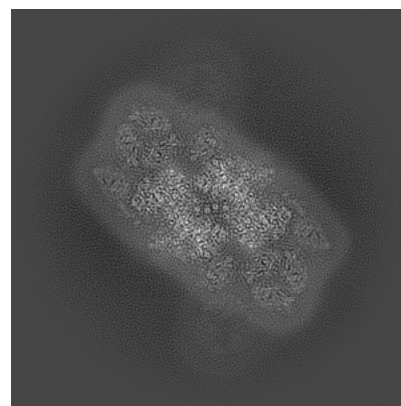
6.1.1 Primary map



X

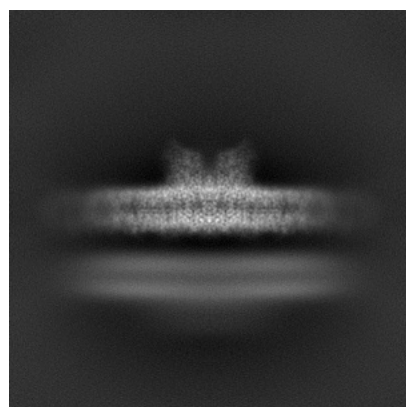


Y

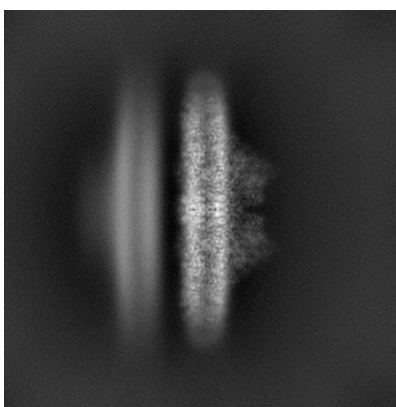


Z

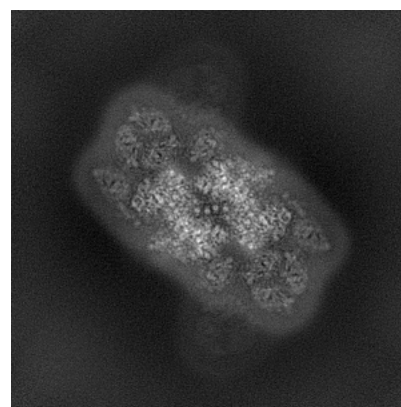
6.1.2 Raw map



X



Y

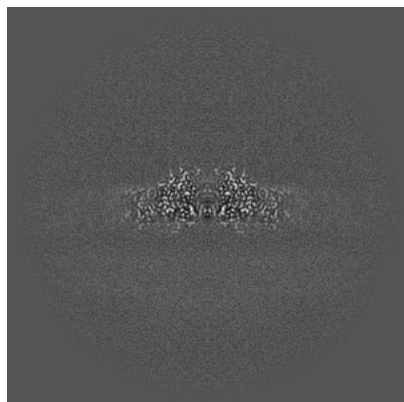


Z

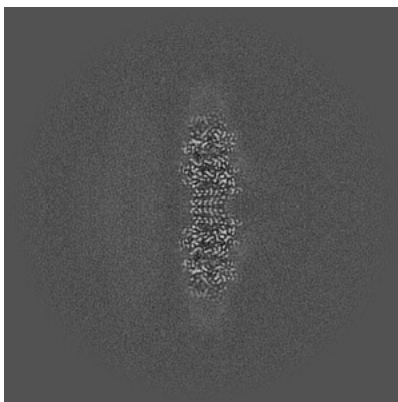
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

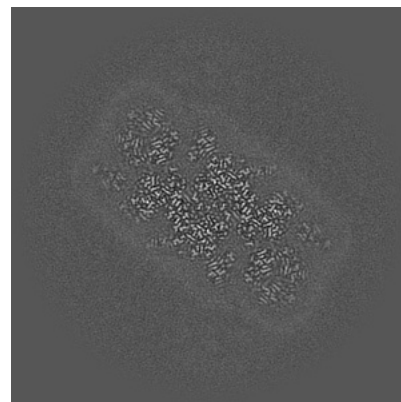
6.2.1 Primary map



X Index: 224

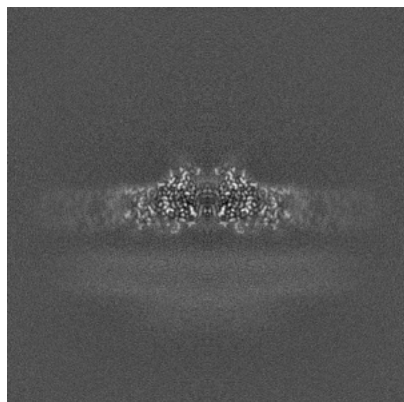


Y Index: 224

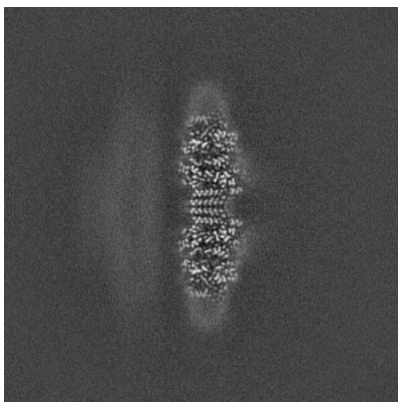


Z Index: 224

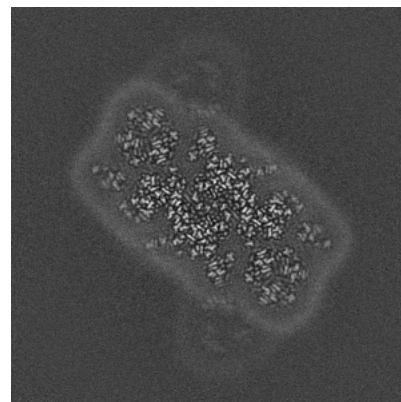
6.2.2 Raw map



X Index: 224



Y Index: 224

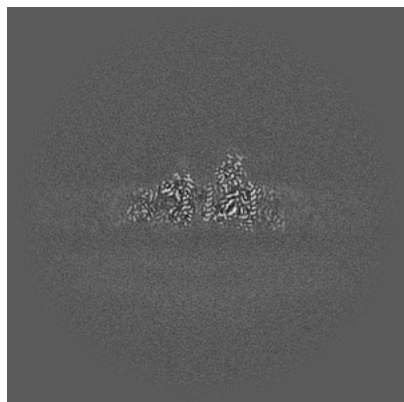


Z Index: 224

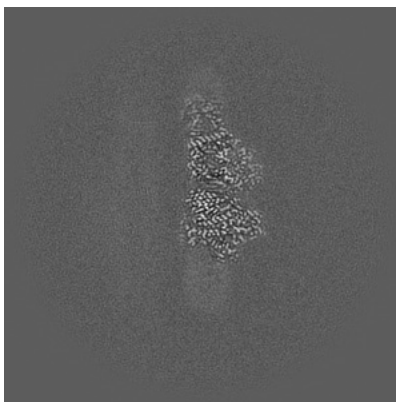
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

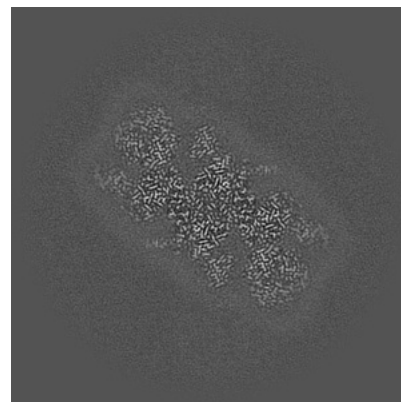
6.3.1 Primary map



X Index: 230

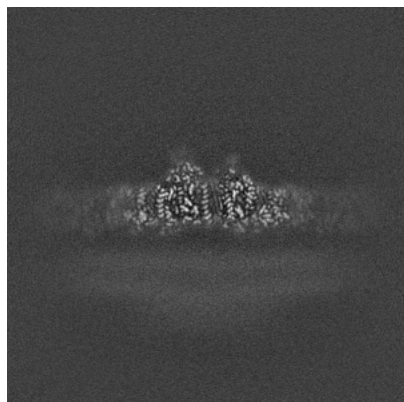


Y Index: 200

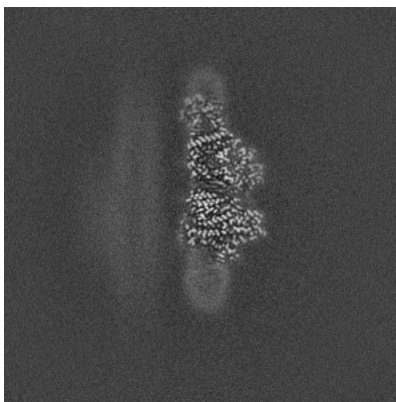


Z Index: 218

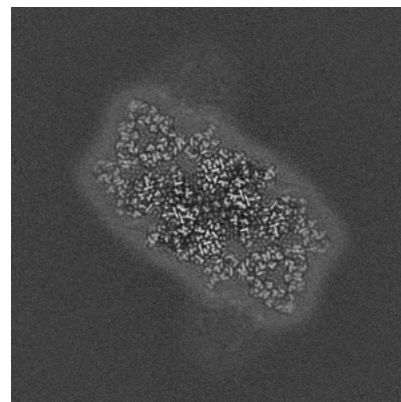
6.3.2 Raw map



X Index: 221



Y Index: 200

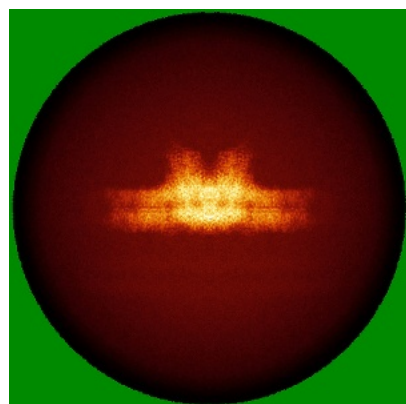


Z Index: 239

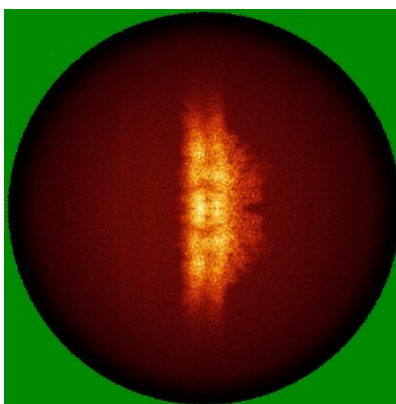
The images above show the largest variance slices of the map in three orthogonal directions.

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

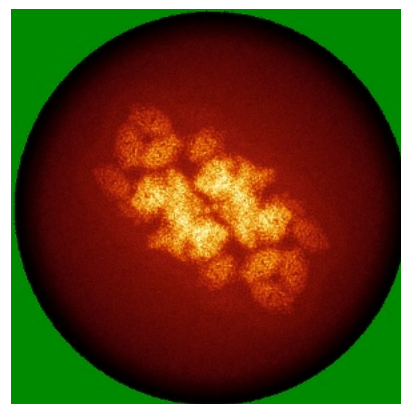
6.4.1 Primary map



X

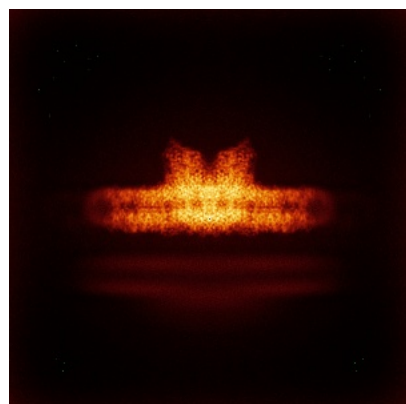


Y

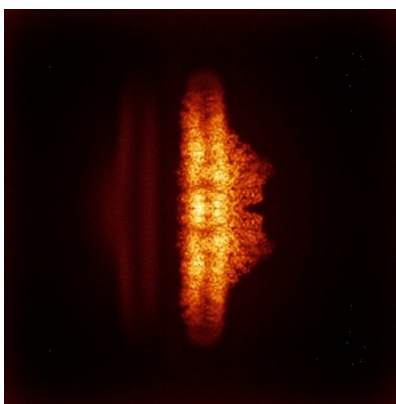


Z

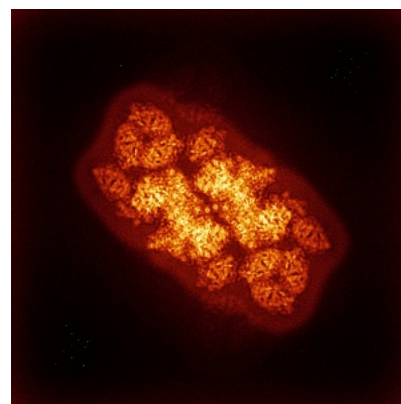
6.4.2 Raw map



X



Y

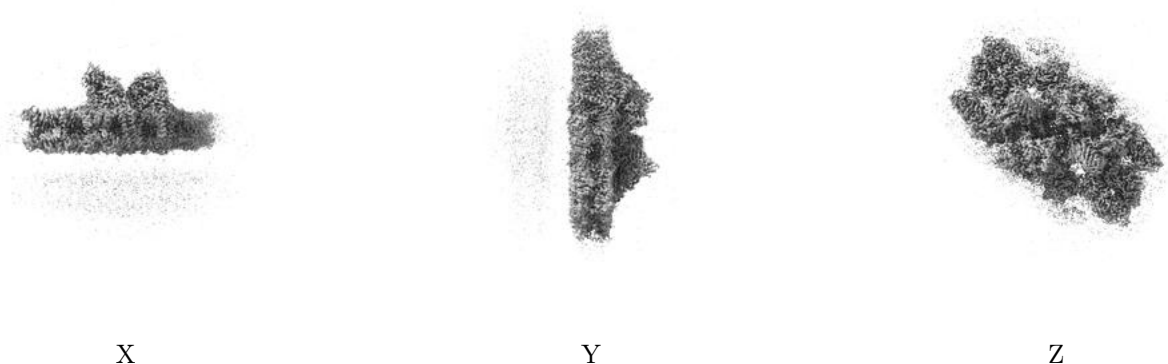


Z

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.

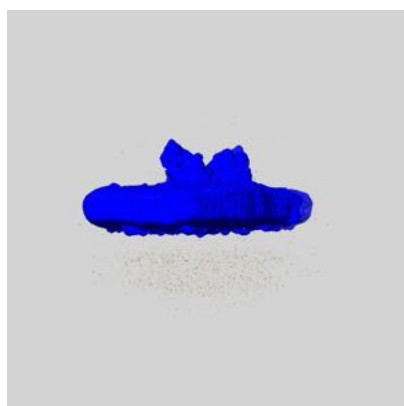
6.6 Mask visualisation [i](#)

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

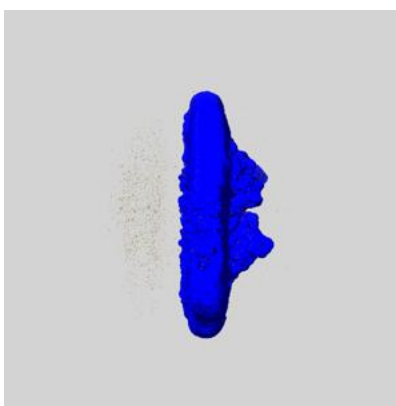
A mask typically either:

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

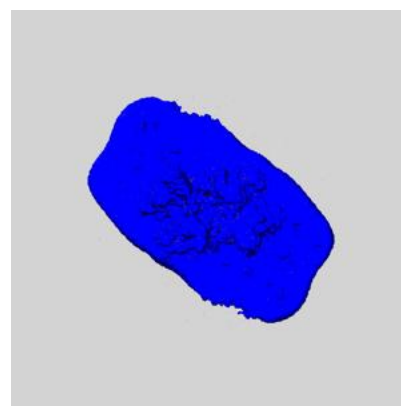
6.6.1 emd_16389_msk_1.map [i](#)



X



Y

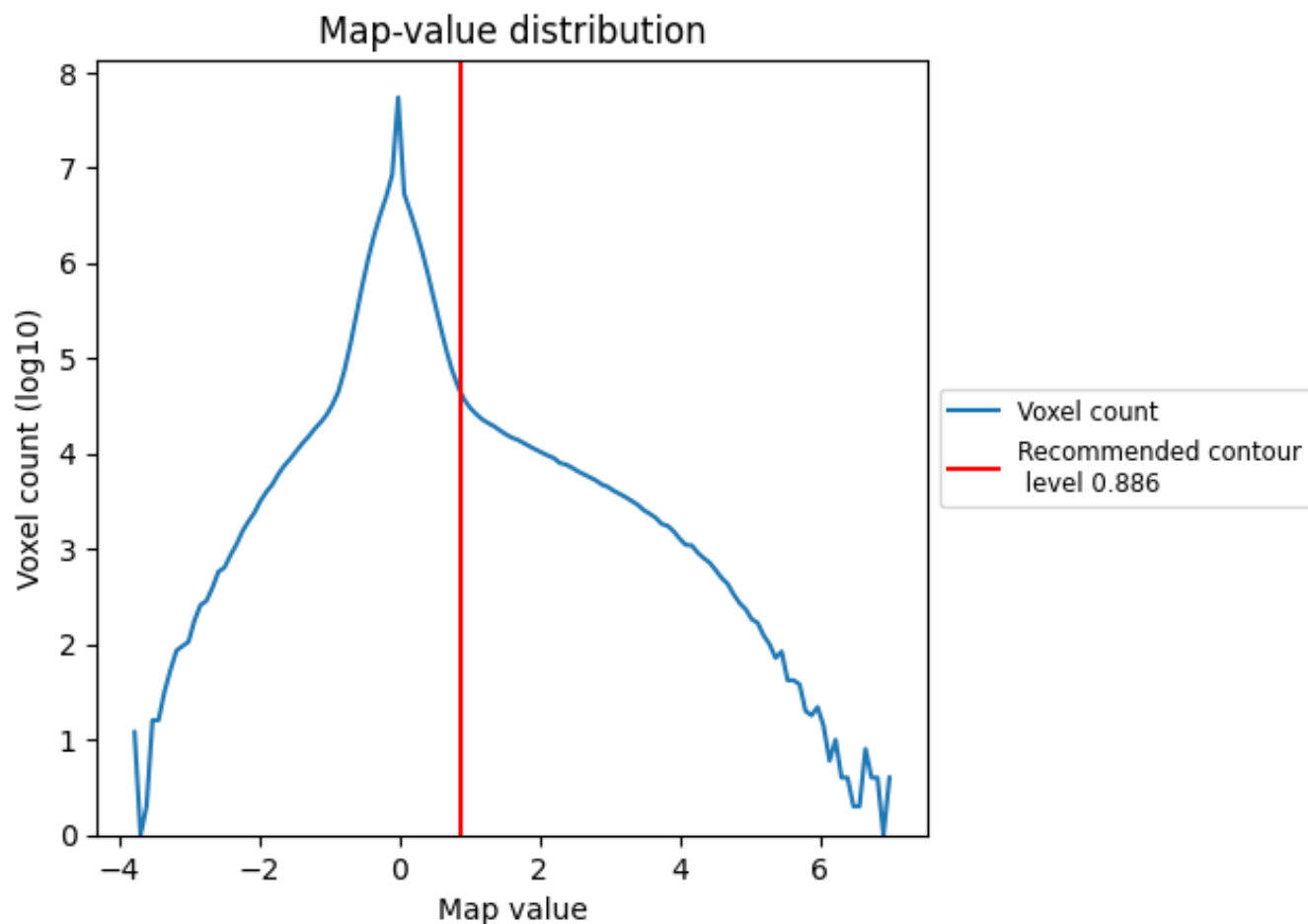


Z

7 Map analysis [i](#)

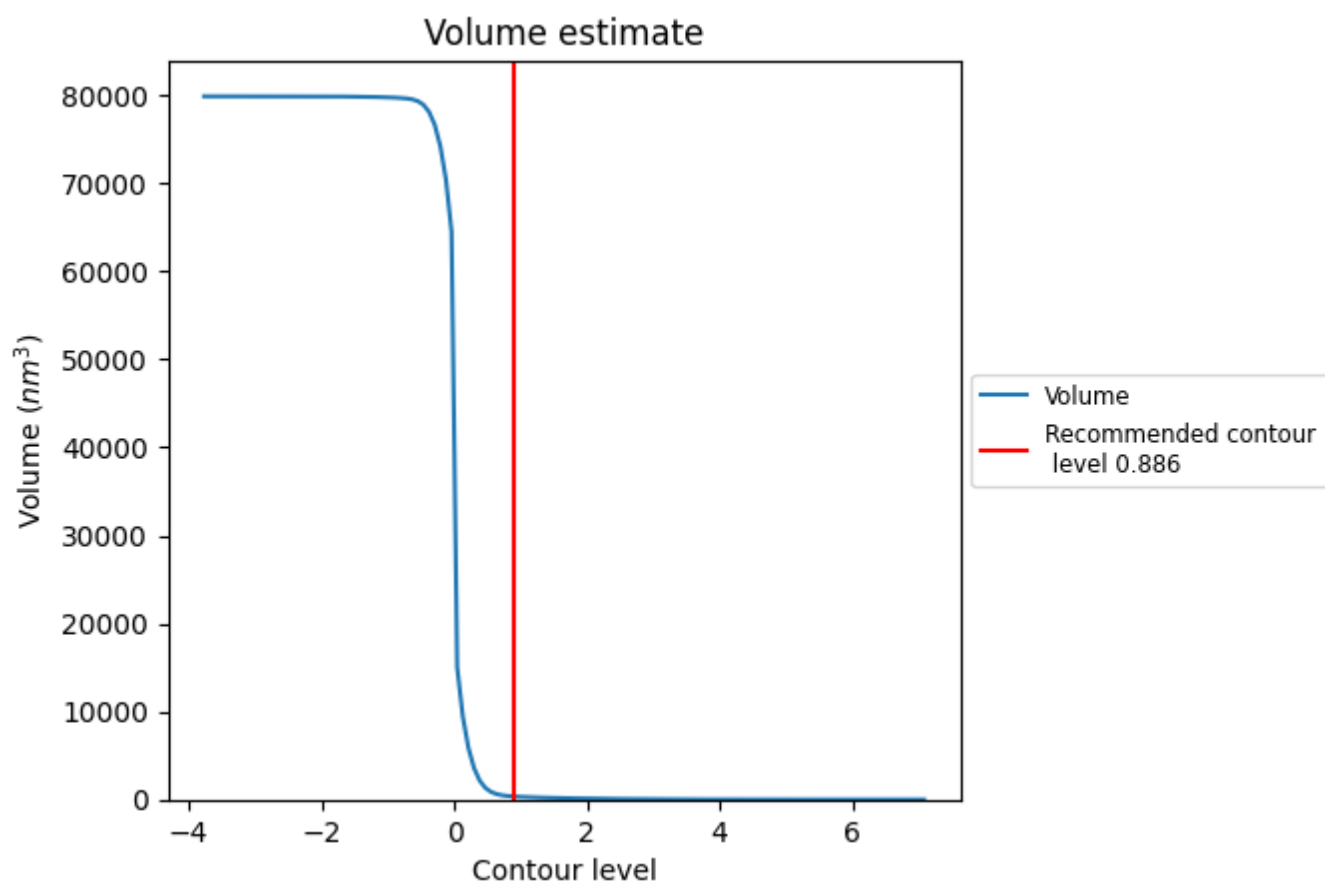
This section contains the results of statistical analysis of the map.

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.

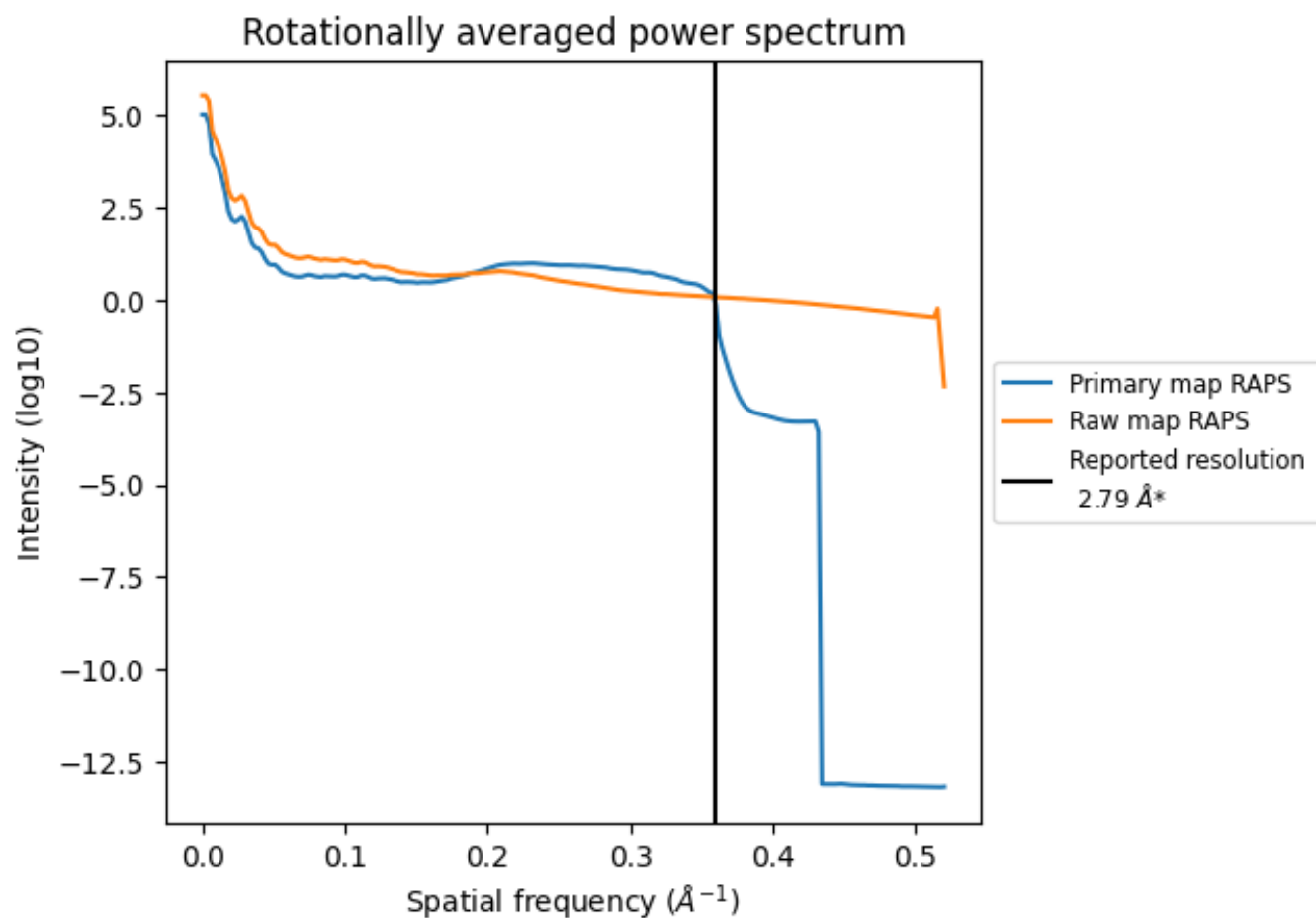
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; 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 ⓘ

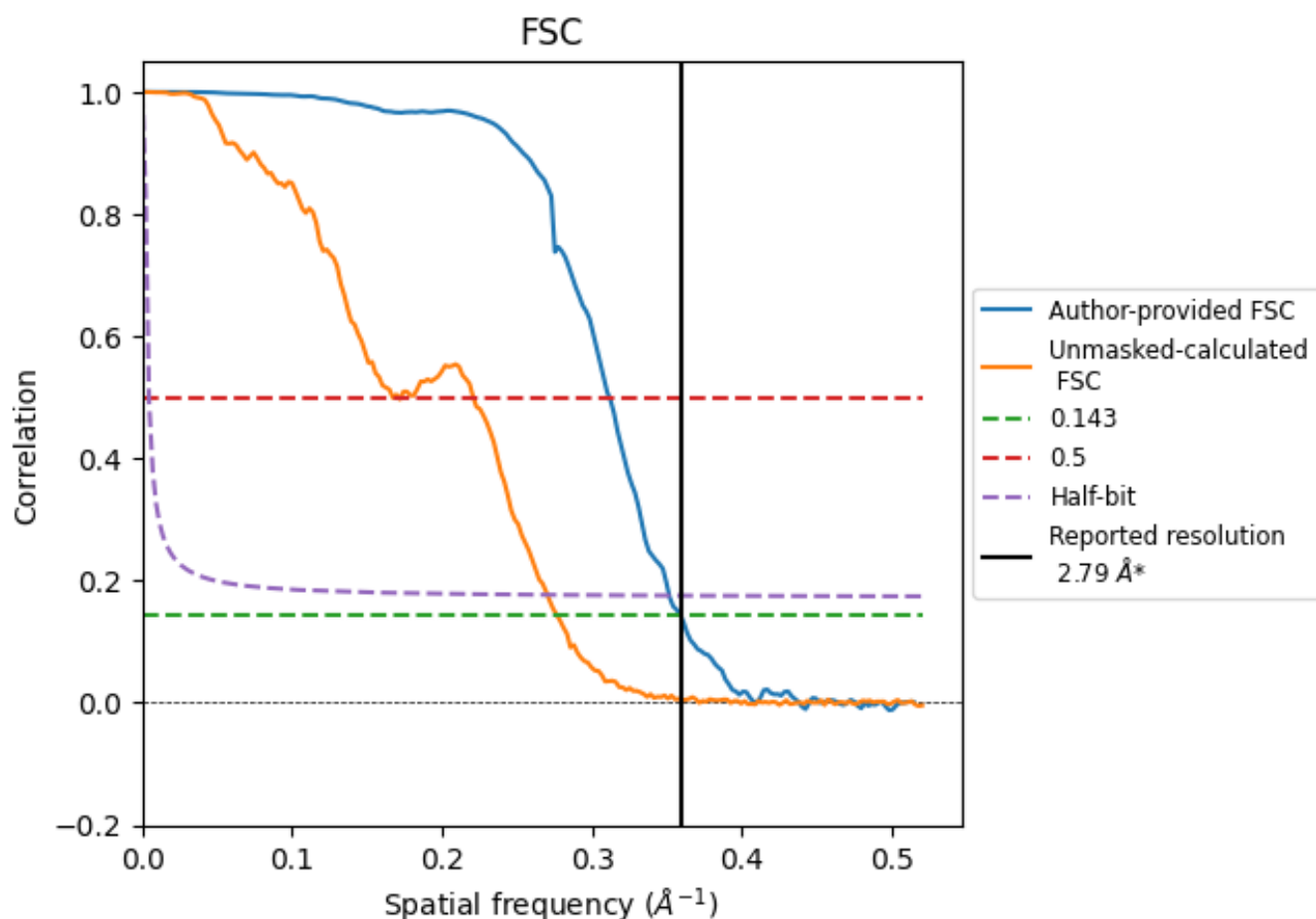


*Reported resolution corresponds to spatial frequency of 0.359 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.359 Å⁻¹

8.2 Resolution estimates [i](#)

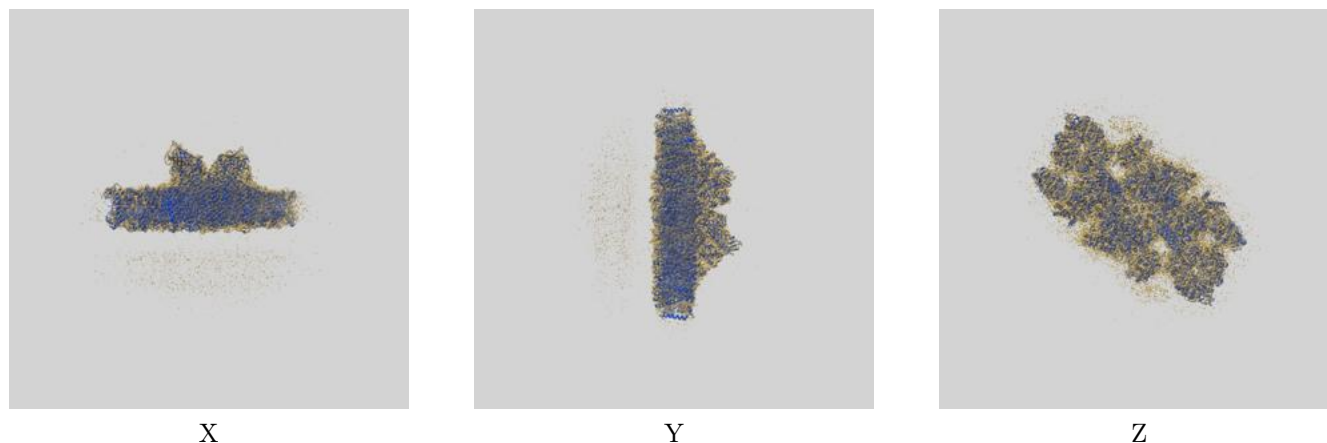
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.21	2.84
Unmasked-calculated*	3.62	5.99	3.70

*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](#)

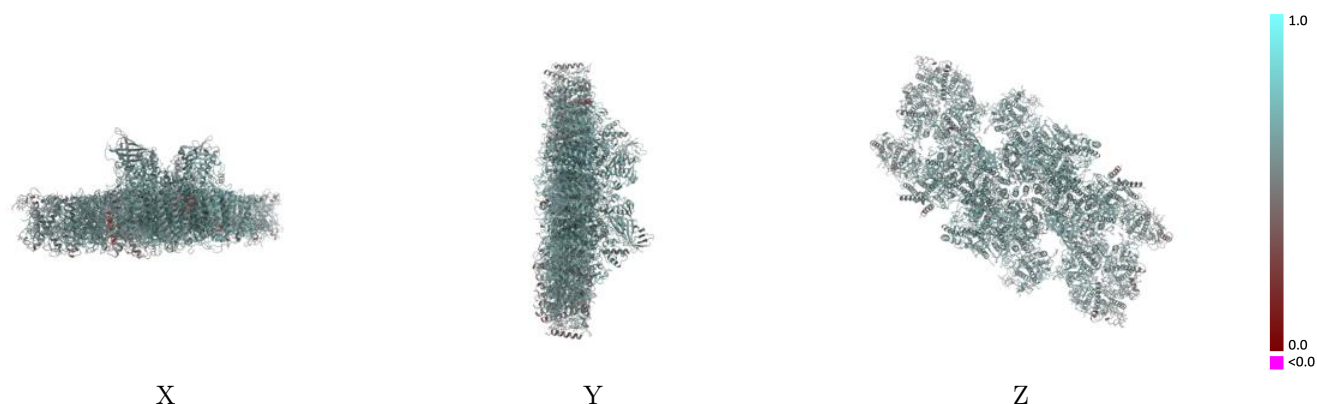
This section contains information regarding the fit between EMDB map EMD-16389 and PDB model 8C29. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

9.1 Map-model overlay [i](#)



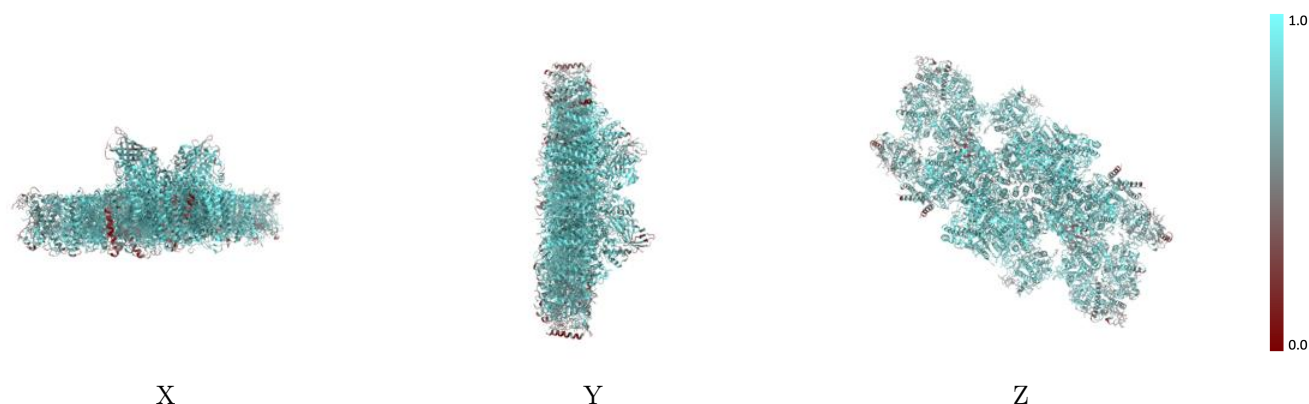
The images above show the 3D surface view of the map at the recommended contour level 0.886 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



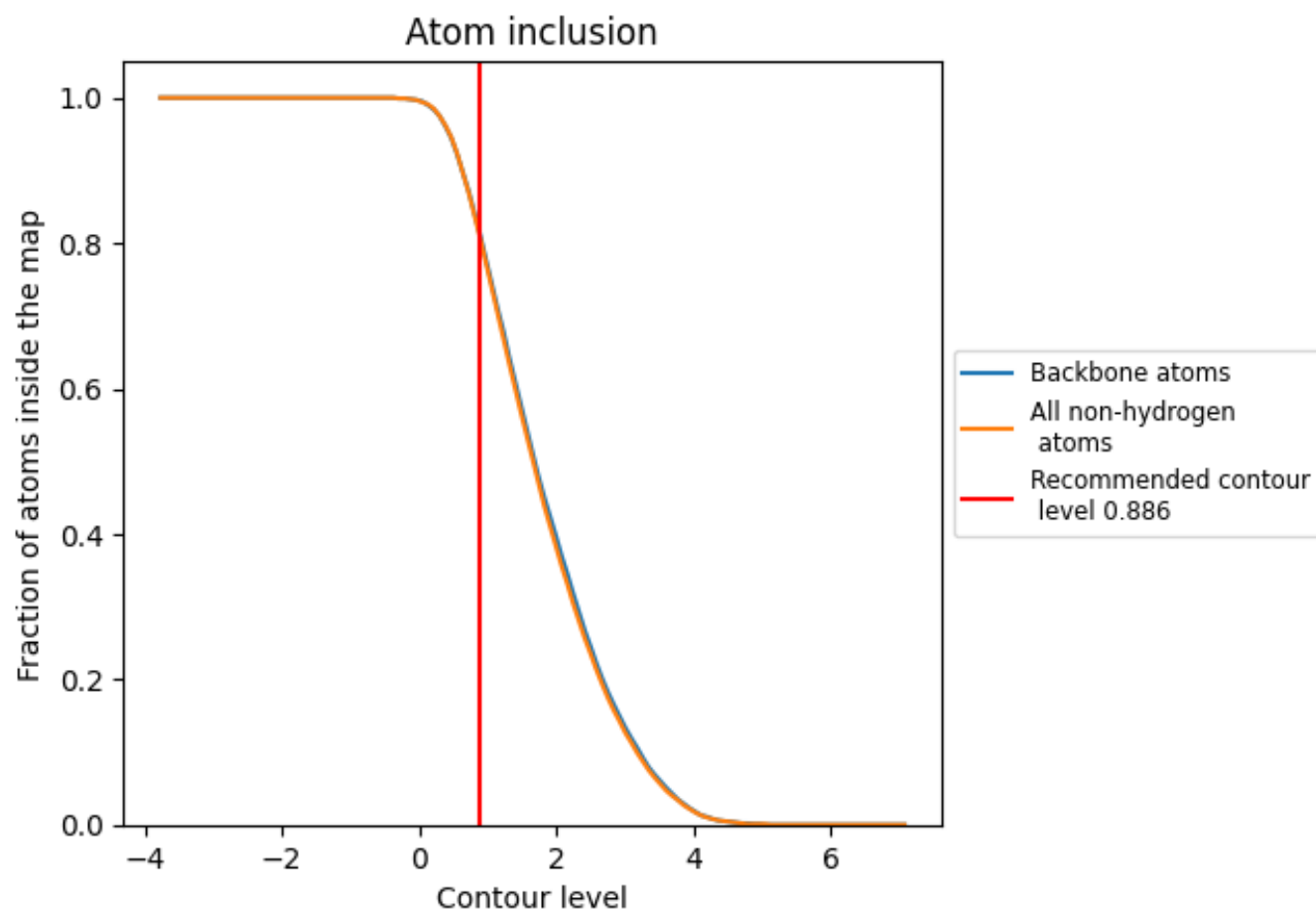
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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