



wwPDB EM Validation Summary Report ⓘ

Sep 20, 2026 – 06:32 pm BST

PDB ID : 7OUI / pdb_00007oui
EMDB ID : EMD-13078
Title : Structure of C2S2M2-type Photosystem supercomplex from *Arabidopsis thaliana* (digitonin-extracted)
Authors : Graca, A.T.; Hall, M.; Persson, K.; Schroder, W.P.
Deposited on : 2021-06-11
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:

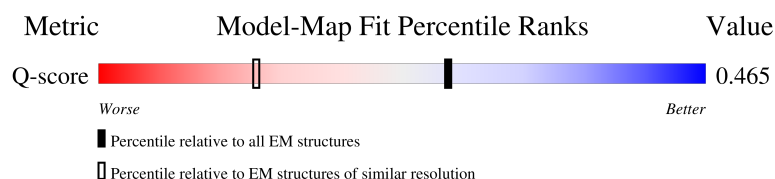
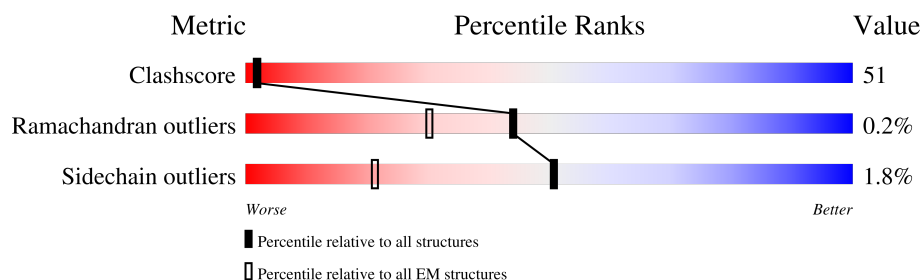
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	10811 (2.29 - 3.29)

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

Mol	Chain	Length	Quality of chain
1	1	266	76% 30% 43% 24%
1	3	266	76% 30% 43% 24%
1	5	266	76% 30% 43% 24%
1	7	266	76% 30% 43% 24%

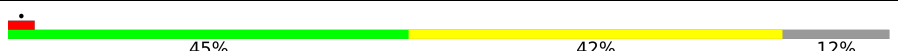
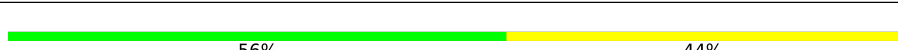
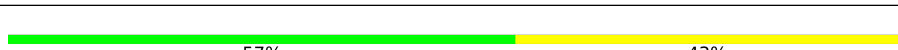
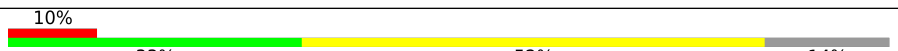
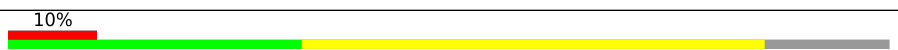
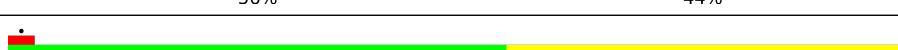
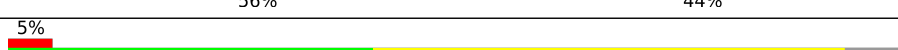
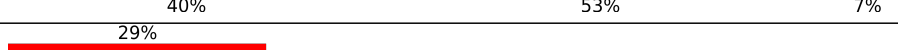
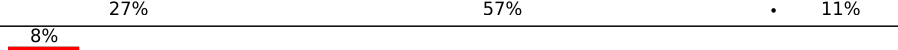
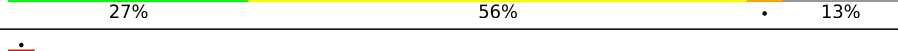
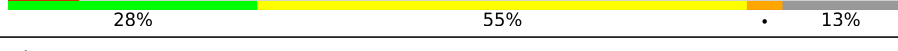
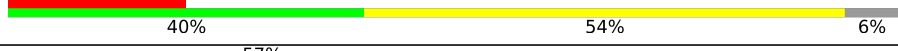
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Mol	Chain	Length	Quality of chain
2	2	243	
2	6	243	
3	4	212	
3	8	212	
4	A	352	
4	a	352	
5	B	508	
5	b	508	
6	C	459	
6	c	459	
7	D	352	
7	d	352	
8	E	83	
8	e	83	
9	F	39	
9	f	39	
10	H	72	
10	h	72	
11	I	36	
11	i	36	
12	K	37	
12	k	37	
13	L	38	
13	l	38	
14	M	34	

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Mol	Chain	Length	Quality of chain
14	m	34	
15	O	247	
15	o	247	
16	T	33	
16	t	33	
17	W	54	
17	w	54	
18	X	42	
18	x	42	
19	Z	62	
19	z	62	
20	S	232	
20	s	232	
21	G	232	
21	N	232	
21	Y	232	
21	g	232	
21	n	232	
21	y	232	
22	R	250	
22	r	250	
23	U	28	
23	u	28	

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
24	CHL	2	603	-	-	X	-
24	CHL	N	607	-	-	X	-
24	CHL	N	609	-	-	X	-
24	CHL	Y	302	-	-	X	-
24	CHL	n	607	-	-	X	-
24	CHL	n	609	-	-	X	-
24	CHL	y	302	-	-	X	-
25	CLA	C	510	-	-	X	-
25	CLA	G	610	-	-	X	-
25	CLA	N	602	-	-	X	-
25	CLA	N	603	-	-	X	-
25	CLA	N	610	-	-	X	-
25	CLA	N	613	-	-	X	-
25	CLA	Y	303	-	-	X	-
25	CLA	Y	304	-	-	X	-
25	CLA	Y	311	-	-	X	-
25	CLA	c	510	-	-	X	-
25	CLA	c	511	-	-	X	-
25	CLA	g	610	-	-	X	-
25	CLA	n	602	-	-	X	-
25	CLA	n	603	-	-	X	-
25	CLA	n	610	-	-	X	-
25	CLA	n	613	-	-	X	-
25	CLA	y	303	-	-	X	-
25	CLA	y	311	-	-	X	-
28	BCR	t	101	-	-	X	-
32	AJP	A	412	X	-	-	-
32	AJP	B	624	X	-	-	-
32	AJP	G	618	X	-	-	-
32	AJP	N	619	X	-	-	-
32	AJP	N	620	X	-	-	-
32	AJP	S	319	X	-	-	-
32	AJP	Y	320	X	-	-	-
32	AJP	Y	321	X	-	-	-
32	AJP	Y	322	X	-	-	-
32	AJP	Y	323	X	-	-	-
32	AJP	Y	324	X	-	-	-
32	AJP	a	413	X	-	-	-
32	AJP	b	624	X	-	-	-
32	AJP	g	618	X	-	-	-
32	AJP	n	619	X	-	-	-
32	AJP	n	620	X	-	-	-
32	AJP	s	319	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	AJP	y	320	X	-	-	-
32	AJP	y	321	X	-	-	-
32	AJP	y	322	X	-	-	-
32	AJP	y	323	X	-	-	-
32	AJP	y	324	X	-	-	-
33	BCT	A	413	-	-	X	-
39	LUT	s	316	-	-	X	-
41	XAT	r	616	-	-	X	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 85897 atoms, of which 1470 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	3	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	5	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	7	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		

- Molecule 2 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	205	Total	C	N	O	S	0	0
			1593	1040	258	290	5		
2	6	205	Total	C	N	O	S	0	0
			1593	1040	258	290	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		
3	8	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	326	Total	C	N	O	S	0	0
			2548	1664	419	452	13		
4	a	326	Total	C	N	O	S	0	0
			2548	1664	419	452	13		

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	487	Total	C	N	O	S	0	0
			3810	2495	644	659	12		
5	b	487	Total	C	N	O	S	0	0
			3810	2495	644	659	12		

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		
6	c	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	342	Total	C	N	O	S	0	0
			2722	1800	445	465	12		
7	d	342	Total	C	N	O	S	0	0
			2722	1800	445	465	12		

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	66	Total	C	N	O	0	0
			543	357	88	98		
8	e	66	Total	C	N	O	0	0
			543	357	88	98		

- Molecule 9 is a protein called Cytochrome b559 subunit beta (PsbF).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	29	Total	C	N	O	S	0	0
			224	147	40	36	1		
9	f	29	Total	C	N	O	S	0	0
			224	147	40	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	60	Total	C	N	O	S	0	0
			446	293	70	81	2		
10	h	60	Total	C	N	O	S	0	0
			446	293	70	81	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	35	Total	C	N	O	S	0	0
			286	195	44	46	1		
11	i	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	37	Total	C	N	O	S	0	0
			301	211	44	45	1		
12	k	37	Total	C	N	O	S	0	0
			301	211	44	45	1		

- Molecule 13 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	36	Total	C	N	O	S	0	0
			302	200	47	55			
13	l	36	Total	C	N	O	S	0	0
			302	200	47	55			

- Molecule 14 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	32	Total	C	N	O	S	0	0
			250	173	35	41	1		
14	m	32	Total	C	N	O	S	0	0
			250	173	35	41	1		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	197	Total	C	N	O	S	0	0
			1516	969	241	302	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	197	Total	C	N	O	S	0	0
			1516	969	241	302	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
16	t	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

- Molecule 17 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	54	Total	C	N	O	S	0	0
			427	282	61	83	1		
17	w	54	Total	C	N	O	S	0	0
			427	282	61	83	1		

- Molecule 18 is a protein called (thale cress) hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	36	Total	C	N	O		0	0
			248	162	39	47			
18	x	36	Total	C	N	O		0	0
			248	162	39	47			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0
			464	313	69	81	1		
19	z	62	Total	C	N	O	S	0	0
			464	313	69	81	1		

- Molecule 20 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	216	Total	C	N	O	S	0	0
			1670	1091	272	303	4		
20	s	216	Total	C	N	O	S	0	0
			1670	1091	272	303	4		

- Molecule 21 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
21	N	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
21	Y	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		
21	g	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
21	n	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
21	y	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		

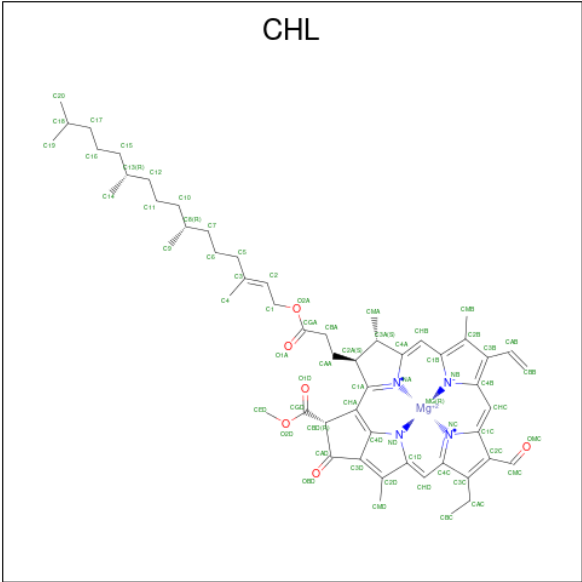
- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	235	Total	C	N	O	S	0	0
			1827	1183	298	343	3		
22	r	235	Total	C	N	O	S	0	0
			1827	1183	298	343	3		

- Molecule 23 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	25	Total	C	N	O	S	0	0
			194	122	36	33	3		
23	u	25	Total	C	N	O	S	0	0
			194	122	36	33	3		

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	2	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 61	C 50	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	N	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	N	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	Y	1	Total 58	C 47	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	R	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	R	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	6	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	s	1	Total 46	C 35	Mg 1	N 4	O 6	0

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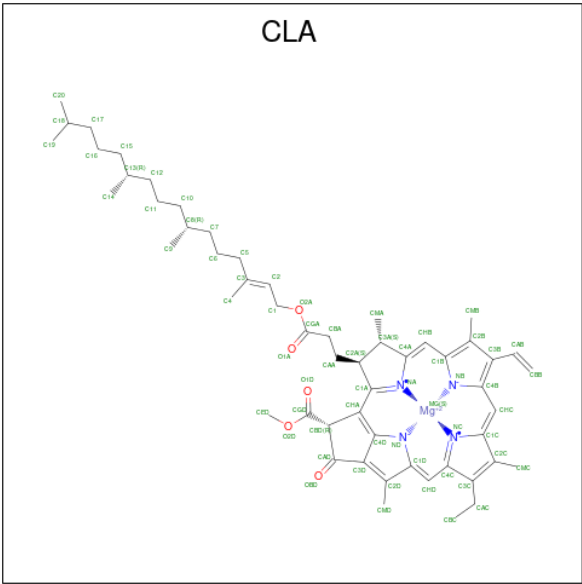
Mol	Chain	Residues	Atoms					AltConf
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	G	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	N	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	R	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	6	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	s	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	g	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0

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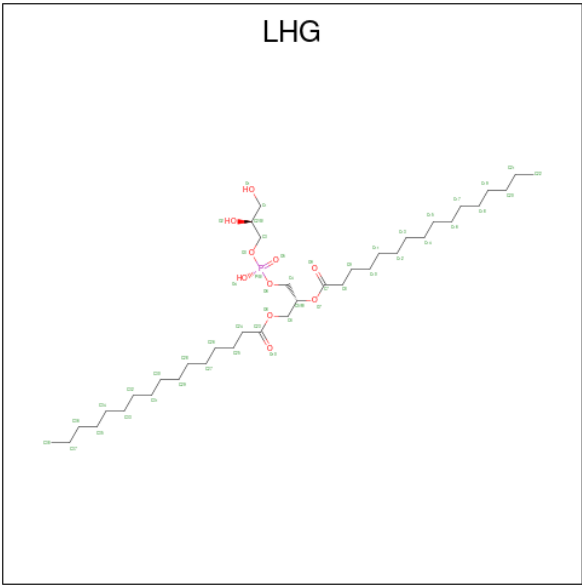
Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
26	2	1	Total	C	O	P	0
			47	36	10	1	
26	B	1	Total	C	O	P	0
			47	36	10	1	
26	B	1	Total	C	O	P	0
			49	38	10	1	

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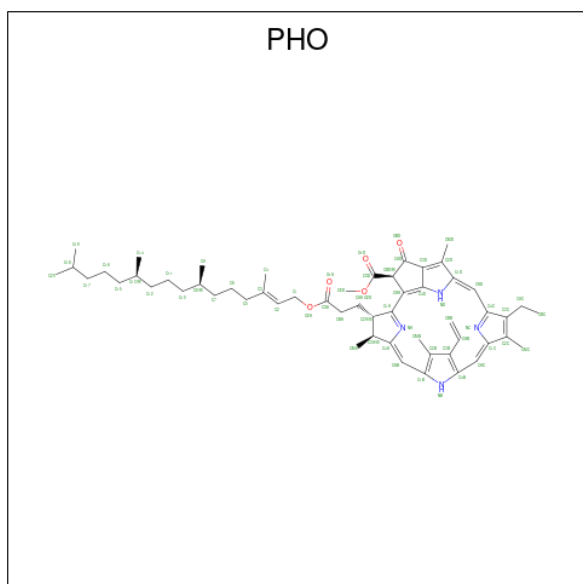
Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 46	C 35	O 10	P 1	0	
26	C	1	Total 49	C 38	O 10	P 1	0	
26	C	1	Total 49	C 38	O 10	P 1	0	
26	C	1	Total 123	C 38	H 74	O 10 P 1	0	
26	D	1	Total 49	C 38	O 10	P 1	0	
26	L	1	Total 49	C 38	O 10	P 1	0	
26	S	1	Total 49	C 38	O 10	P 1	0	
26	S	1	Total 49	C 38	O 10	P 1	0	
26	N	1	Total 49	C 38	O 10	P 1	0	
26	Y	1	Total 49	C 38	O 10	P 1	0	
26	Y	1	Total 49	C 38	O 10	P 1	0	
26	R	1	Total 42	C 31	O 10	P 1	0	
26	6	1	Total 47	C 36	O 10	P 1	0	
26	b	1	Total 47	C 36	O 10	P 1	0	
26	b	1	Total 49	C 38	O 10	P 1	0	
26	b	1	Total 46	C 35	O 10	P 1	0	
26	c	1	Total 49	C 38	O 10	P 1	0	
26	c	1	Total 49	C 38	O 10	P 1	0	
26	c	1	Total 123	C 38	H 74	O 10 P 1	0	
26	d	1	Total 49	C 38	O 10	P 1	0	
26	l	1	Total 49	C 38	O 10	P 1	0	

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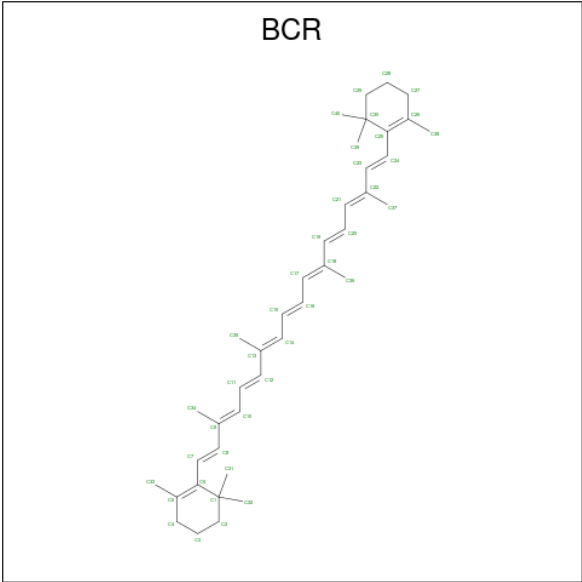
Mol	Chain	Residues	Atoms				AltConf
26	s	1	Total	C	O	P	0
			49	38	10	1	
26	s	1	Total	C	O	P	0
			49	38	10	1	
26	n	1	Total	C	O	P	0
			49	38	10	1	
26	y	1	Total	C	O	P	0
			49	38	10	1	
26	y	1	Total	C	O	P	0
			49	38	10	1	
26	r	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



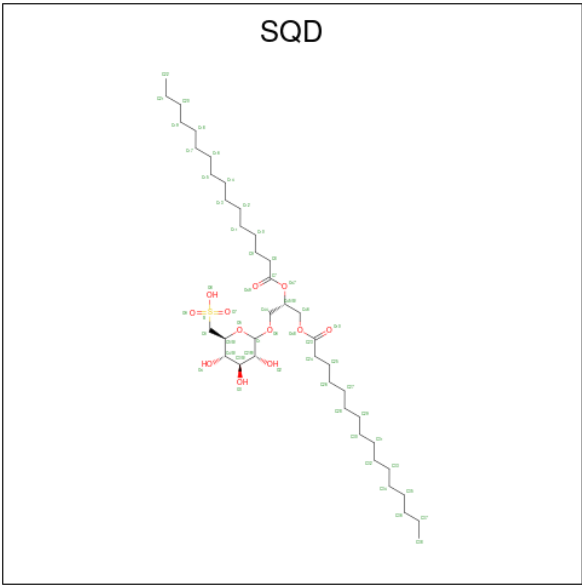
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	C	1	Total	C	0
			40	40	
28	D	1	Total	C	0
			40	40	
28	H	1	Total	C	0
			40	40	
28	I	1	Total	C	0
			40	40	
28	K	1	Total	C	0
			40	40	
28	T	1	Total	C	0
			40	40	
28	Z	1	Total	C	0
			40	40	
28	a	1	Total	C	0
			40	40	
28	b	1	Total	C	0
			40	40	
28	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
28	b	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	d	1	Total C 40 40	0
28	h	1	Total C 40 40	0
28	i	1	Total C 40 40	0
28	k	1	Total C 40 40	0
28	t	1	Total C 40 40	0
28	z	1	Total C 40 40	0

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



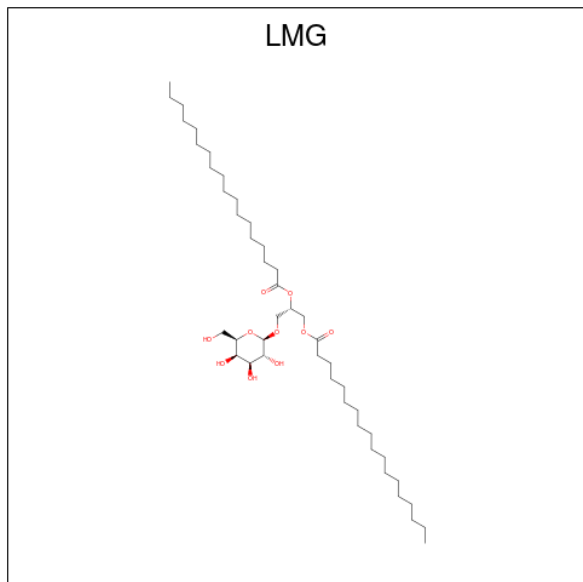
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C O S 50 37 12 1	0
29	A	1	Total C O S 54 41 12 1	0
29	L	1	Total C O S 42 29 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
29	L	1	Total	C	O	S	0
			54	41	12	1	
29	a	1	Total	C	O	S	0
			50	37	12	1	
29	a	1	Total	C	O	S	0
			54	41	12	1	
29	l	1	Total	C	O	S	0
			54	41	12	1	
29	l	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



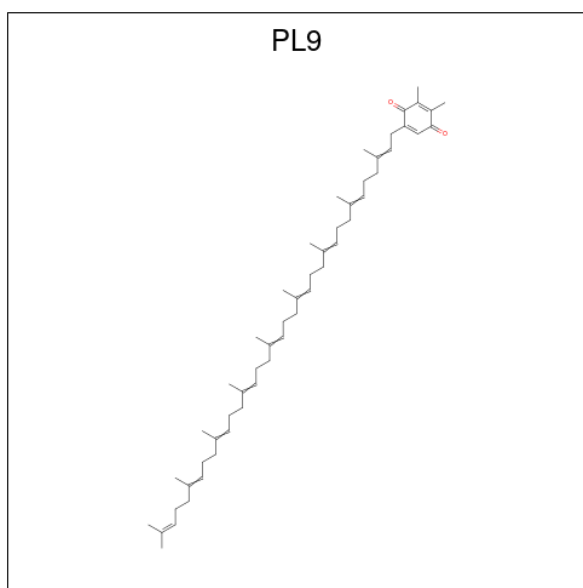
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O		0
			48	38	10		
30	A	1	Total	C	O		0
			40	30	10		
30	B	1	Total	C	O		0
			51	41	10		
30	B	1	Total	C	O		0
			55	45	10		
30	C	1	Total	C	O		0
			51	41	10		
30	D	1	Total	C	O		0
			46	36	10		

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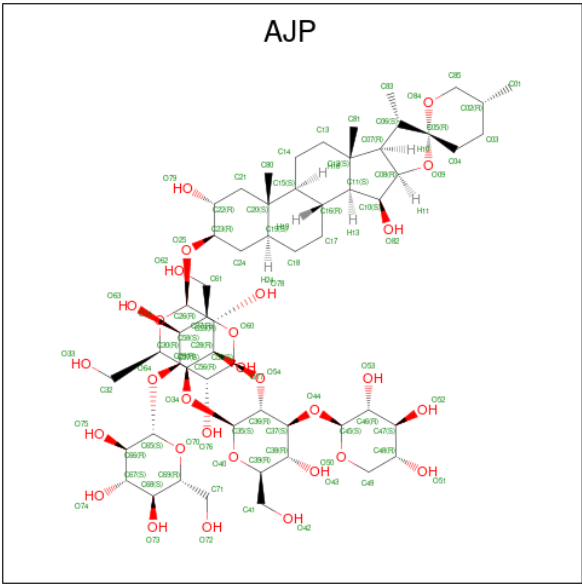
Mol	Chain	Residues	Atoms			AltConf
30	a	1	Total	C	O	0
			48	38	10	
30	a	1	Total	C	O	0
			40	30	10	
30	b	1	Total	C	O	0
			51	41	10	
30	b	1	Total	C	O	0
			55	45	10	
30	c	1	Total	C	O	0
			51	41	10	
30	d	1	Total	C	O	0
			46	36	10	

- Molecule 31 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
31	A	1	Total	C	O	0
			13	11	2	
31	D	1	Total	C	O	0
			55	53	2	
31	a	1	Total	C	O	0
			13	11	2	
31	d	1	Total	C	O	0
			55	53	2	

- Molecule 32 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉) (labeled as "Ligand of Interest" by depositor).



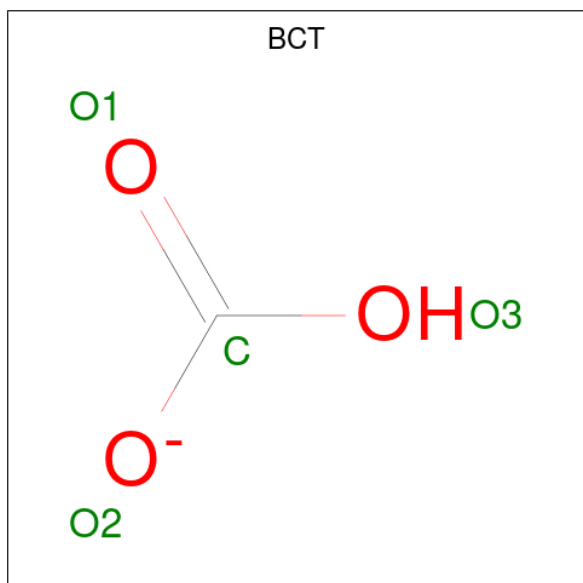
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	H	O	0
			177	56	92	29	
32	B	1	Total	C	H	O	0
			177	56	92	29	
32	S	1	Total	C	H	O	0
			95	33	53	9	
32	G	1	Total	C	H	O	0
			95	33	53	9	
32	N	1	Total	C	H	O	0
			95	33	53	9	
32	N	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	a	1	Total	C	H	O	0
			177	56	92	29	

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Mol	Chain	Residues	Atoms				AltConf
32	b	1	Total	C	H	O	0
			177	56	92	29	
32	s	1	Total	C	H	O	0
			95	33	53	9	
32	g	1	Total	C	H	O	0
			95	33	53	9	
32	n	1	Total	C	H	O	0
			95	33	53	9	
32	n	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			4	1	3	

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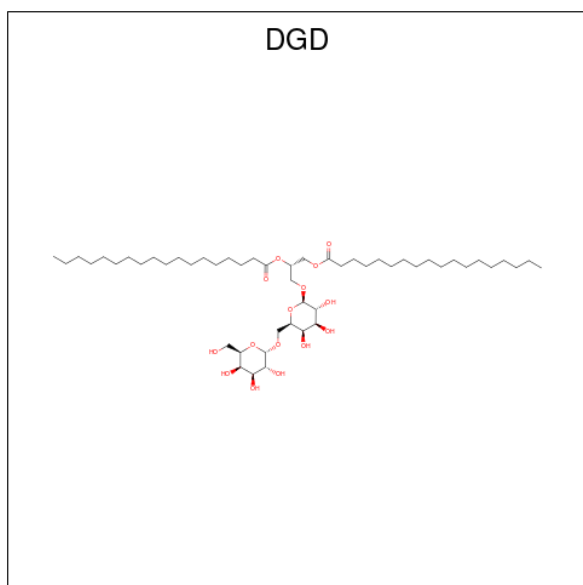
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Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total	C	O	0
			4	1	3	

- Molecule 34 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			59	44	15	
35	B	1	Total	C	O	0
			62	47	15	
35	C	1	Total	C	O	0
			55	40	15	
35	C	1	Total	C	O	0
			62	47	15	
35	a	1	Total	C	O	0
			59	44	15	
35	b	1	Total	C	O	0
			62	47	15	

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Mol	Chain	Residues	Atoms			AltConf
35	c	1	Total	C	O	0
			55	40	15	
35	c	1	Total	C	O	0
			62	47	15	

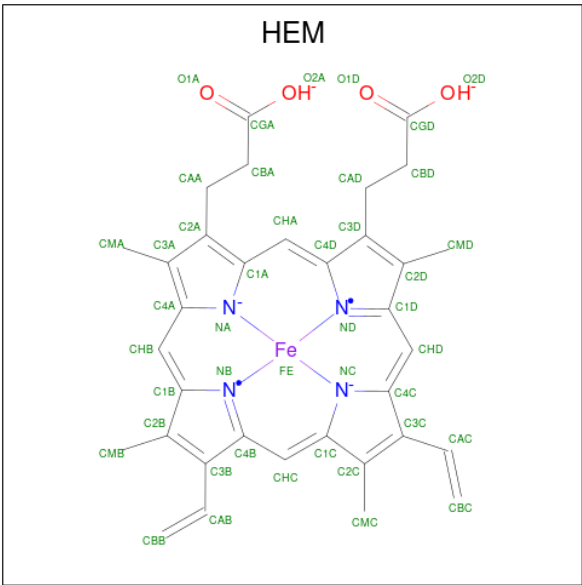
- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Ca	0
			1	1	
36	B	1	Total	Ca	0
			1	1	
36	a	1	Total	Ca	0
			1	1	
36	b	1	Total	Ca	0
			1	1	

- Molecule 37 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

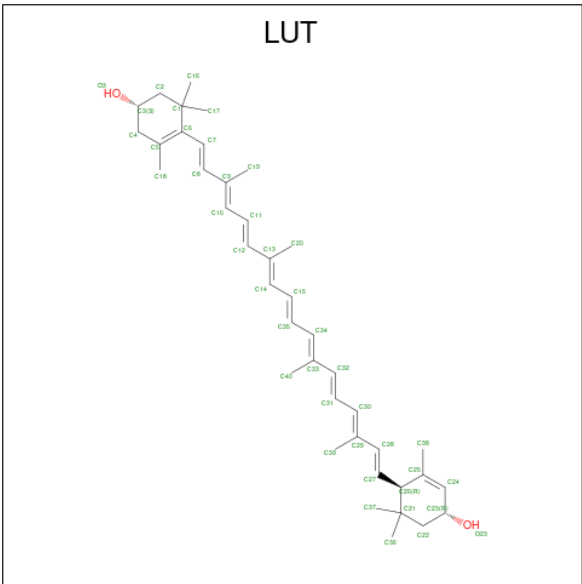
Mol	Chain	Residues	Atoms		AltConf
37	D	1	Total	Cl	0
			1	1	
37	d	1	Total	Cl	0
			1	1	

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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 (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



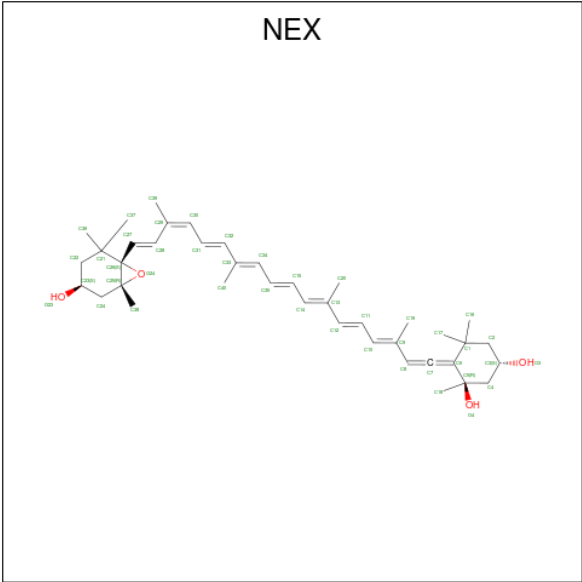
Mol	Chain	Residues	Atoms			AltConf
39	S	1	Total	C	O	0
			42	40	2	

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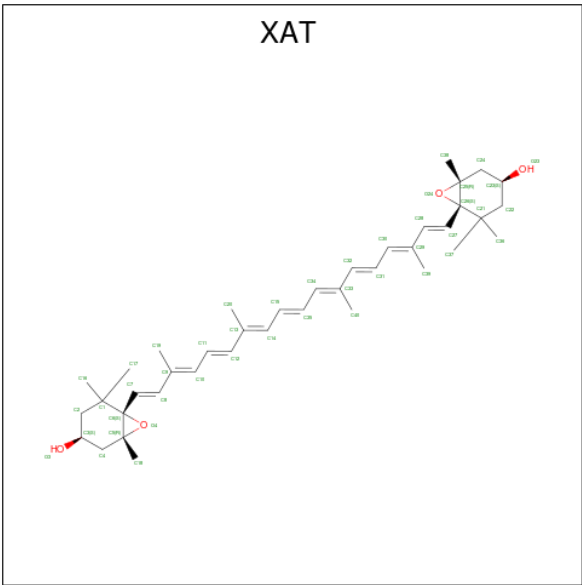
Mol	Chain	Residues	Atoms			AltConf
39	S	1	Total	C	O	0
			42	40	2	
39	G	1	Total	C	O	0
			42	40	2	
39	G	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	R	1	Total	C	O	0
			42	40	2	
39	s	1	Total	C	O	0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

- Molecule 40 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-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
40	S	1	Total	C	O	0
			44	40	4	
40	G	1	Total	C	O	0
			44	40	4	
40	N	1	Total	C	O	0
			44	40	4	
40	Y	1	Total	C	O	0
			44	40	4	
40	R	1	Total	C	O	0
			44	40	4	
40	s	1	Total	C	O	0
			44	40	4	
40	g	1	Total	C	O	0
			44	40	4	
40	n	1	Total	C	O	0
			44	40	4	
40	y	1	Total	C	O	0
			44	40	4	
40	r	1	Total	C	O	0
			44	40	4	

- Molecule 41 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
41	R	1	Total	C	O	0
			44	40	4	
41	r	1	Total	C	O	0
			44	40	4	

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	A	23	Total	O	0
			23	23	
42	B	10	Total	O	0
			10	10	
42	C	14	Total	O	0
			14	14	
42	D	14	Total	O	0
			14	14	
42	H	1	Total	O	0
			1	1	
42	I	1	Total	O	0
			1	1	
42	L	3	Total	O	0
			3	3	
42	M	1	Total	O	0
			1	1	
42	T	1	Total	O	0
			1	1	
42	W	1	Total	O	0
			1	1	

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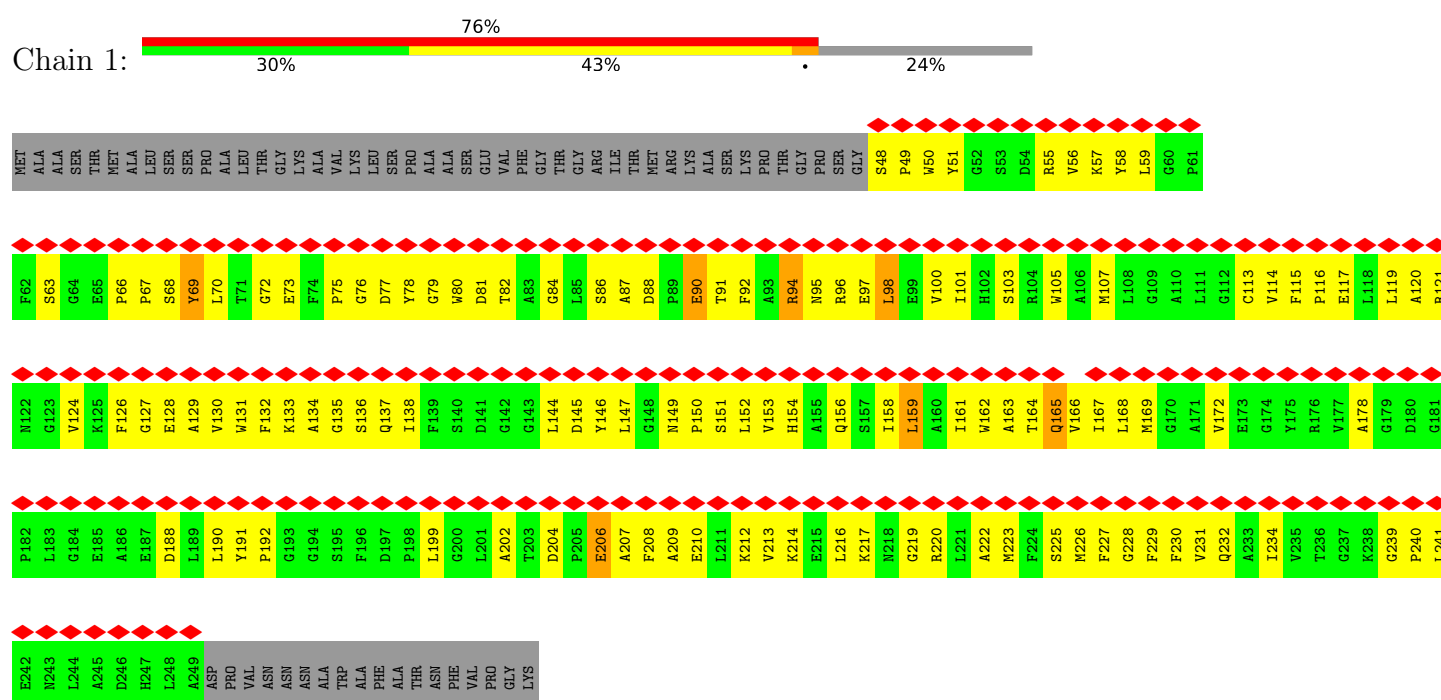
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Mol	Chain	Residues	Atoms		AltConf
42	a	23	Total 23	O 23	0
42	b	10	Total 10	O 10	0
42	c	14	Total 14	O 14	0
42	d	14	Total 14	O 14	0
42	h	1	Total 1	O 1	0
42	i	1	Total 1	O 1	0
42	l	3	Total 3	O 3	0
42	m	2	Total 2	O 2	0
42	t	1	Total 1	O 1	0
42	w	1	Total 1	O 1	0

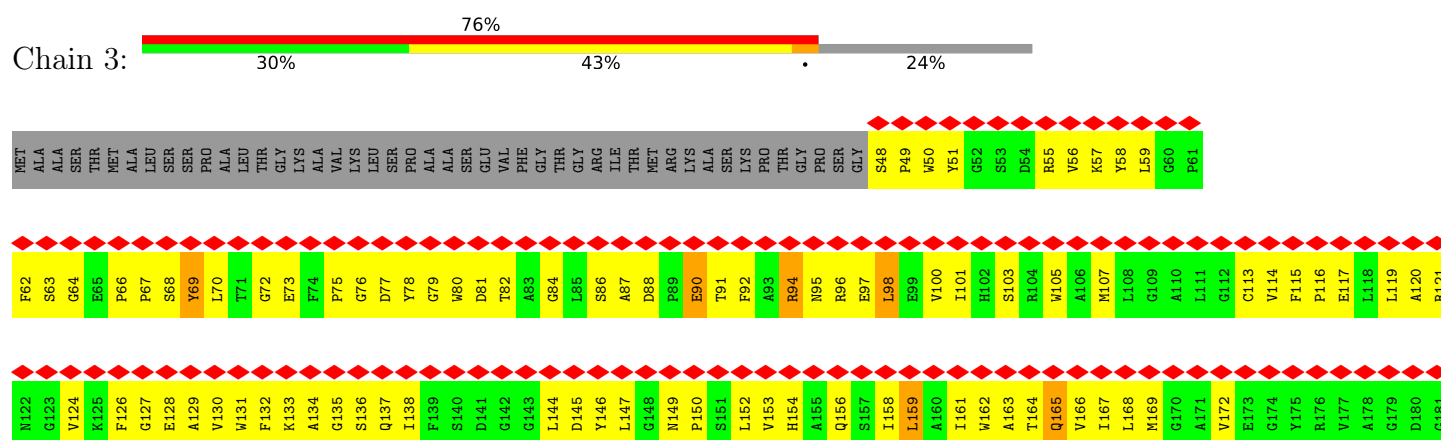
3 Residue-property plots [i](#)

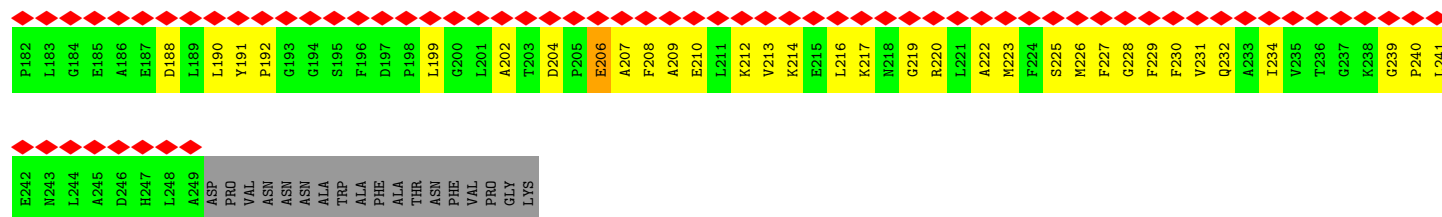
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

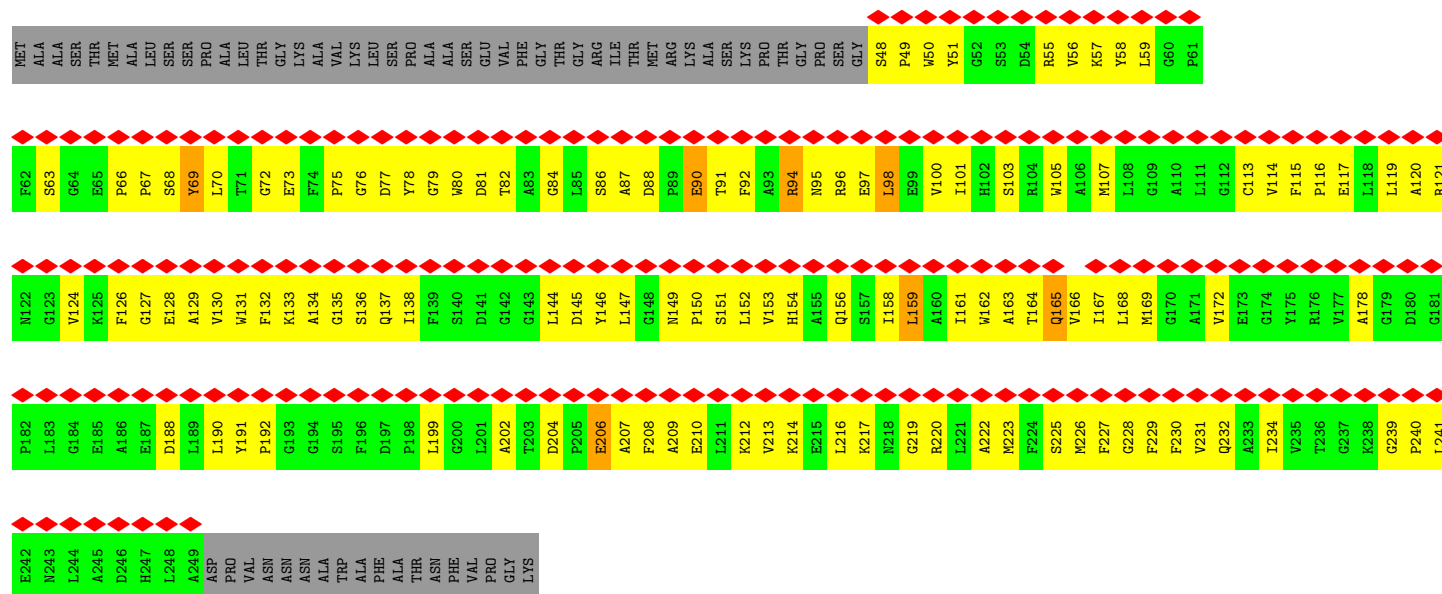
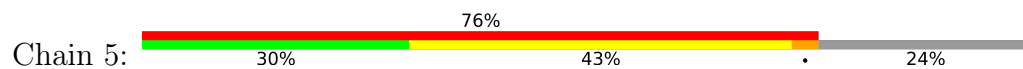


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

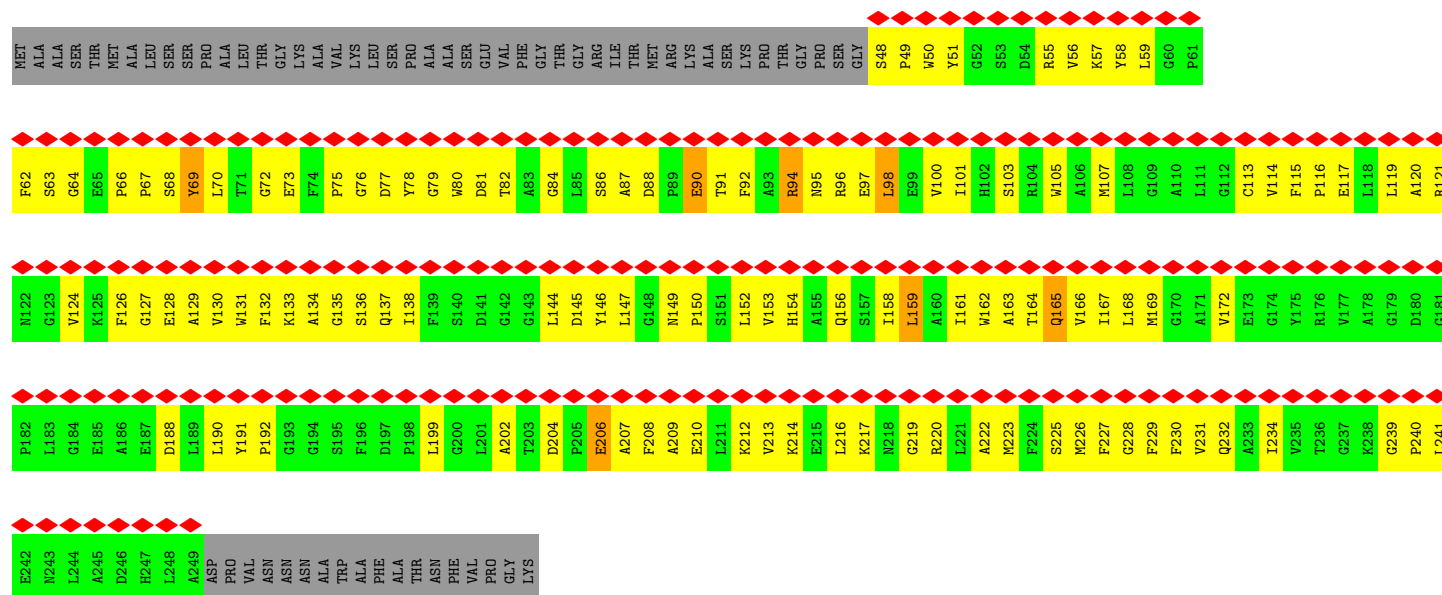
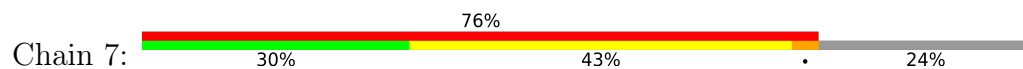




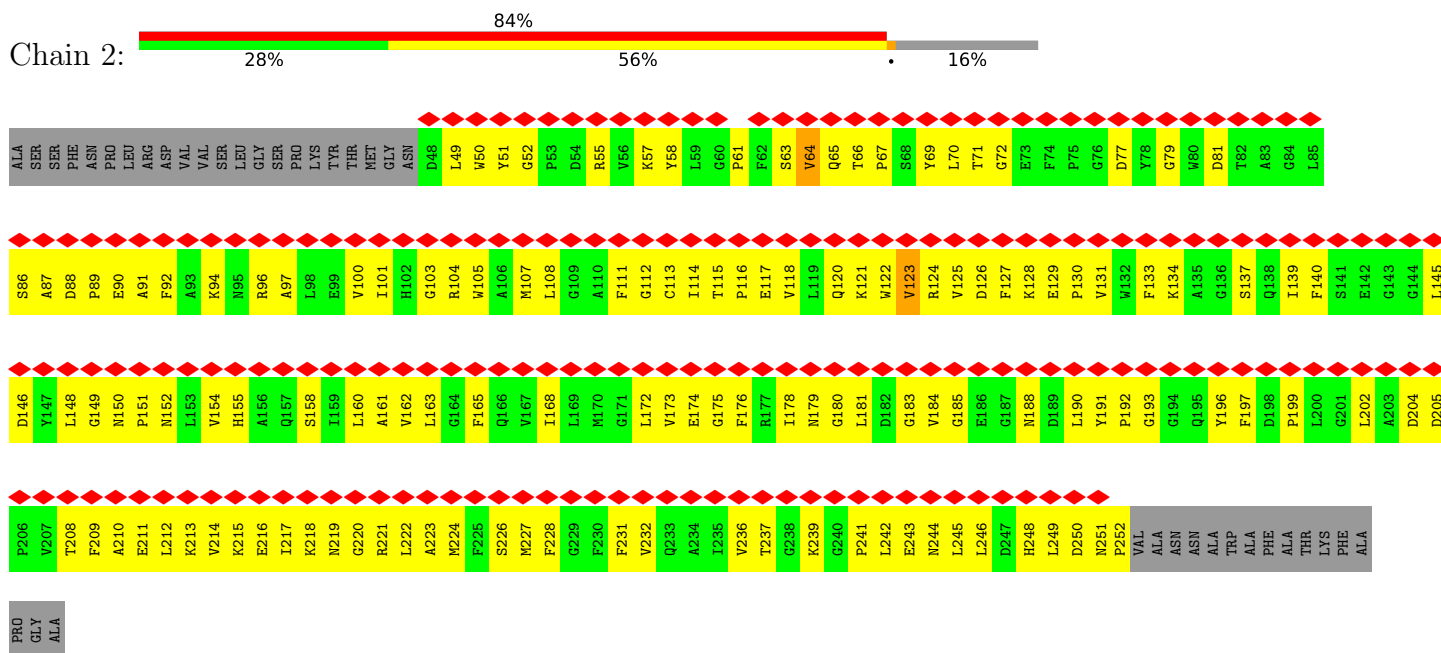
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



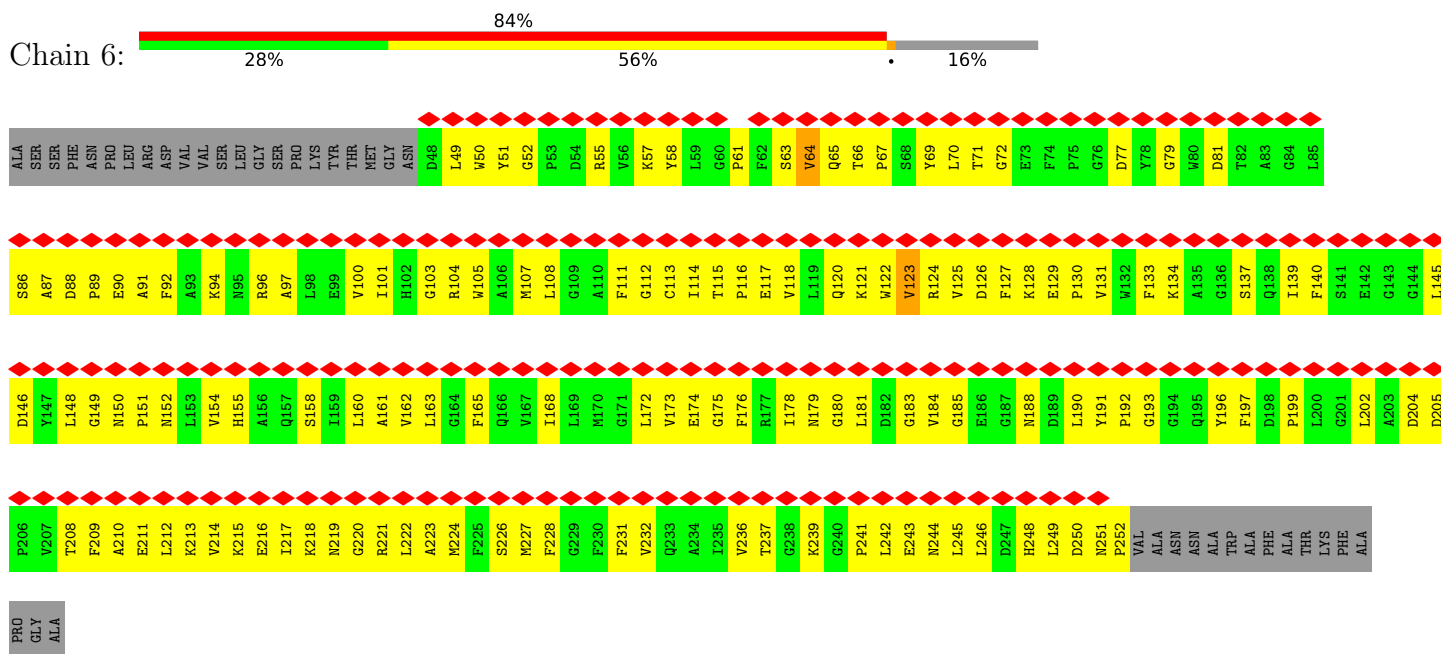
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



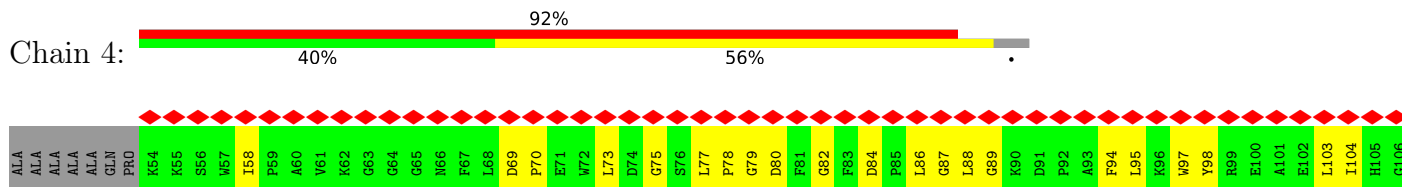
- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

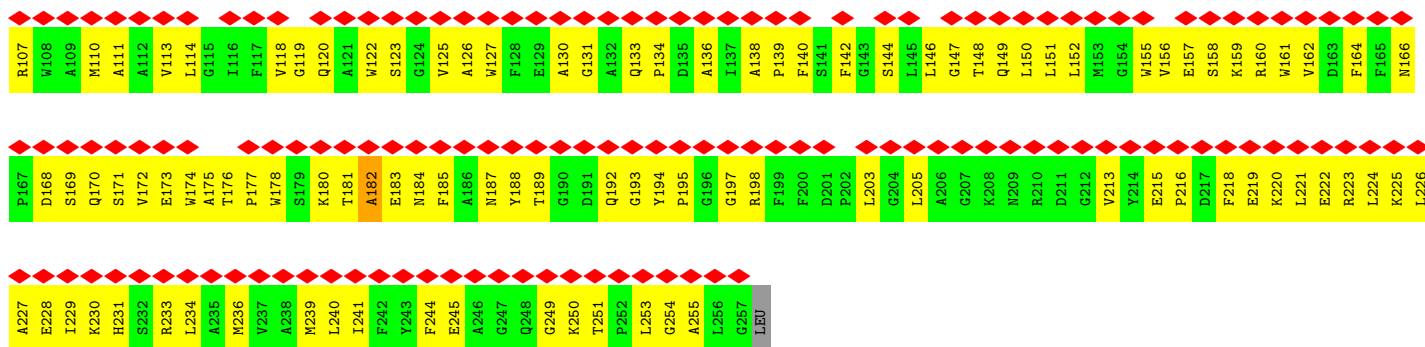


- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

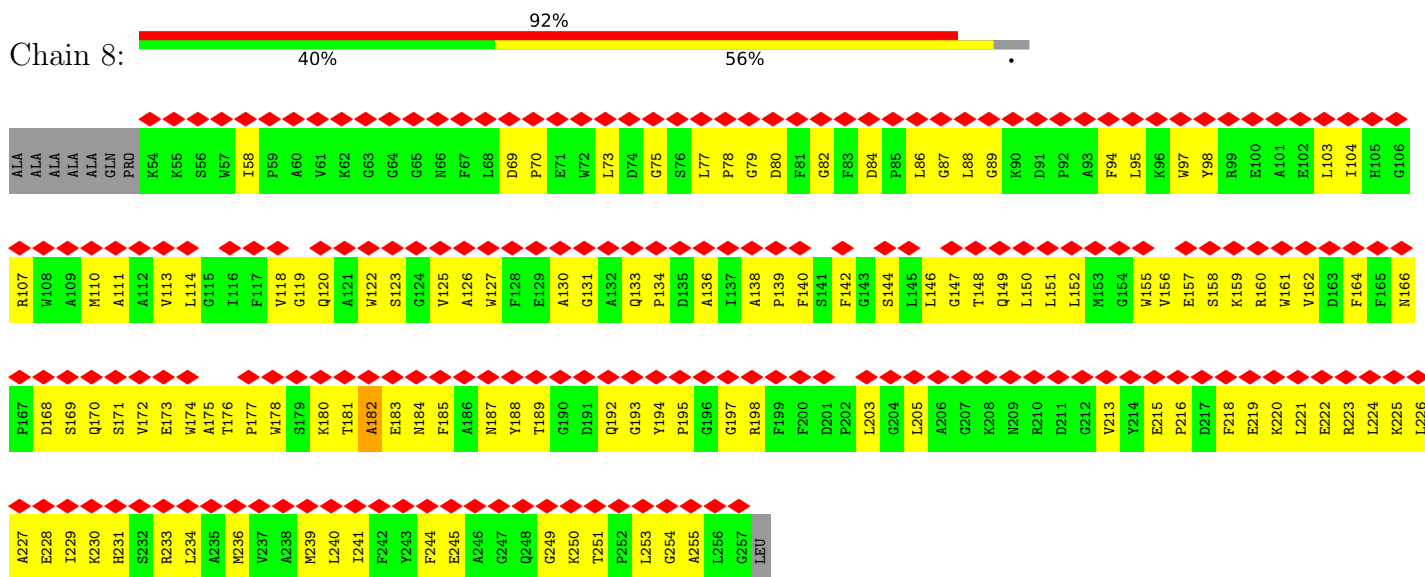


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

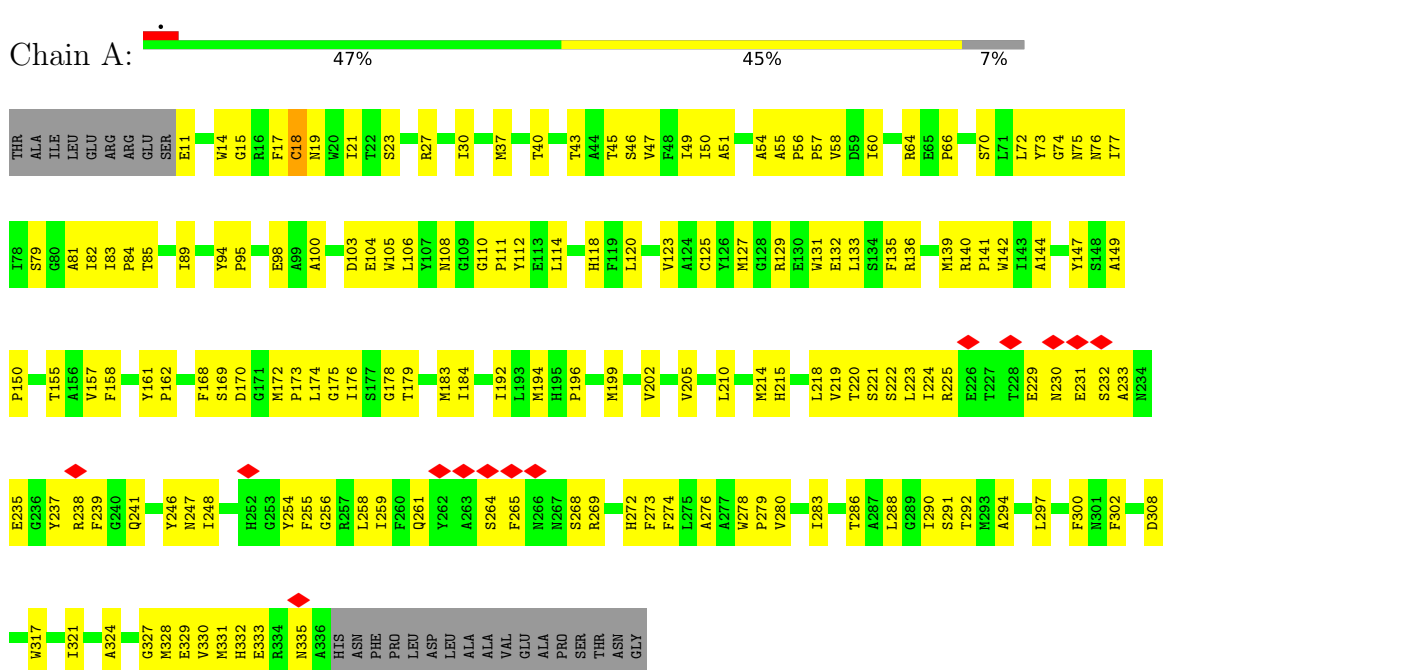




• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

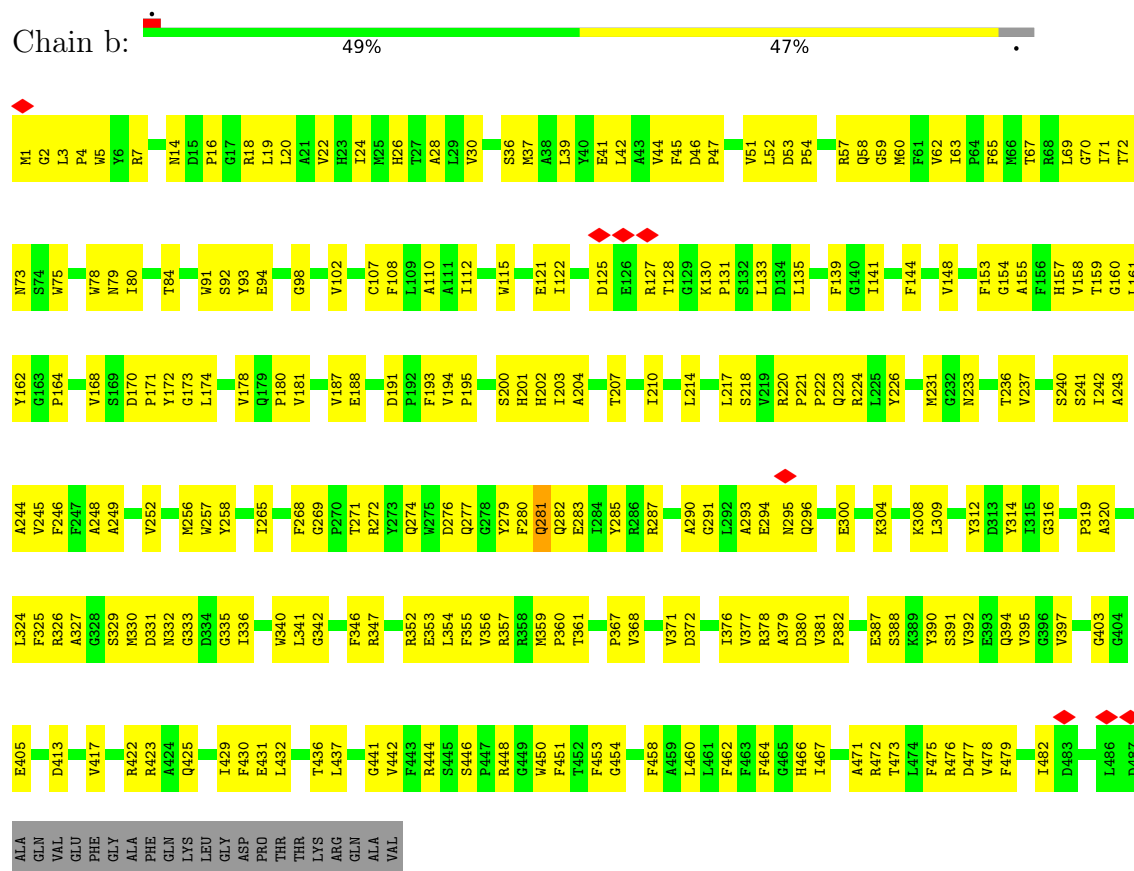


• Molecule 4: Photosystem II protein D1

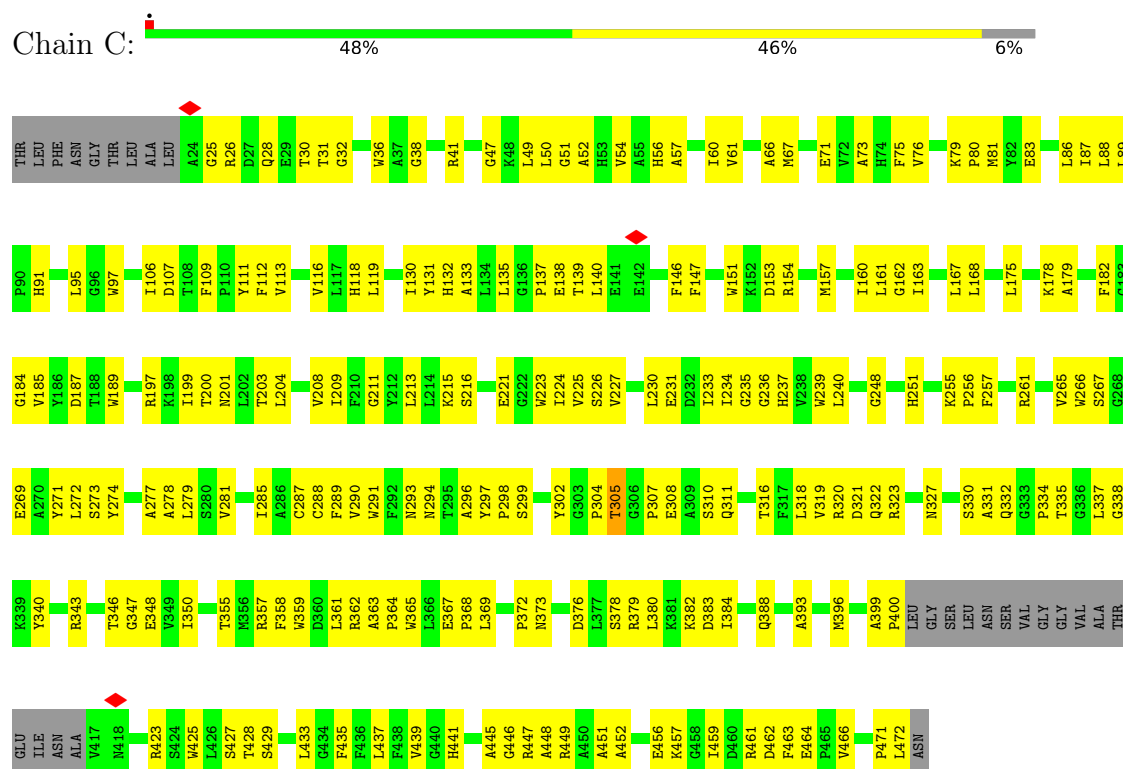


Chain a: 47% 45% 7%

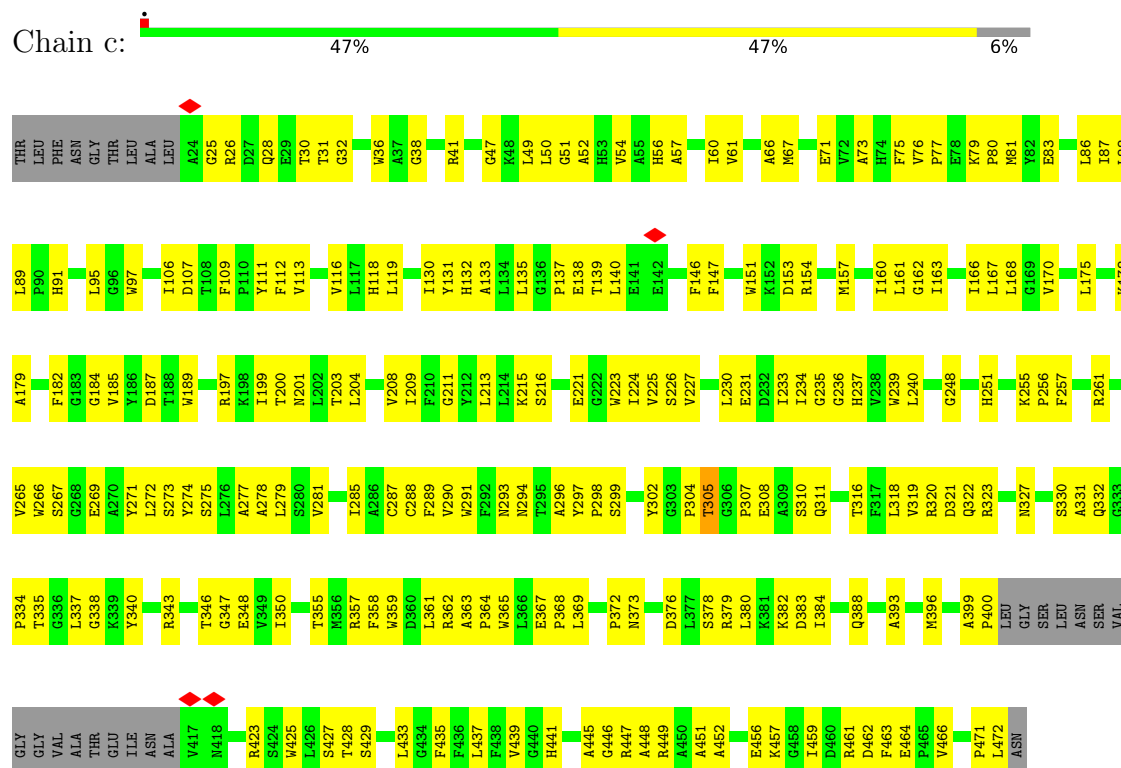




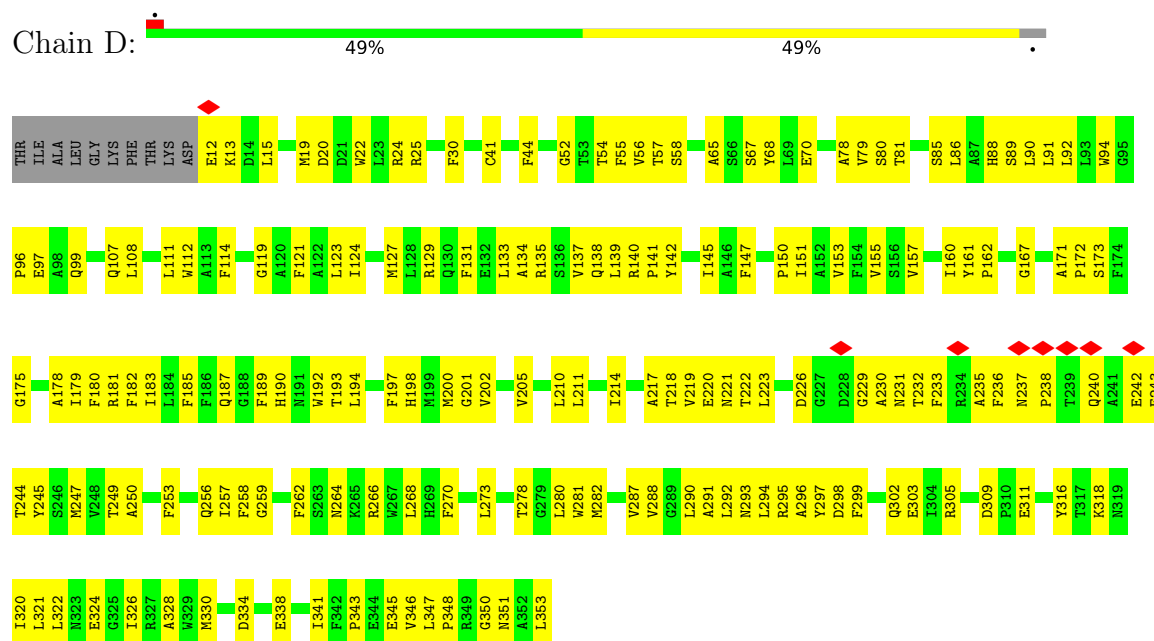
• Molecule 6: Photosystem II CP43 reaction center protein



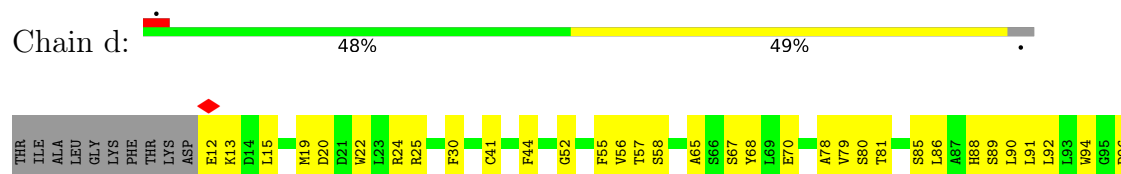
• Molecule 6: Photosystem II CP43 reaction center protein

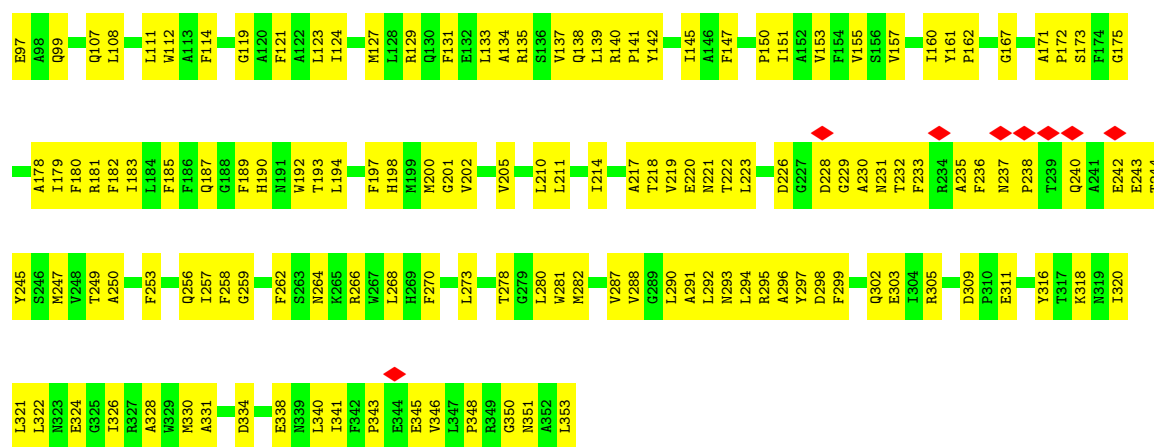


• Molecule 7: Photosystem II D2 protein

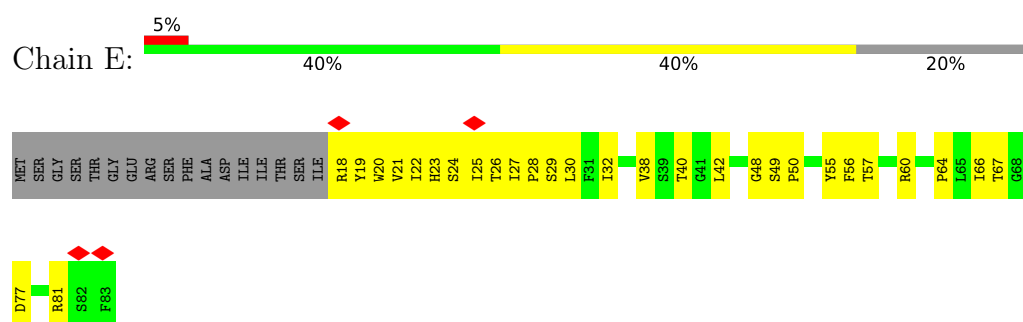


• Molecule 7: Photosystem II D2 protein

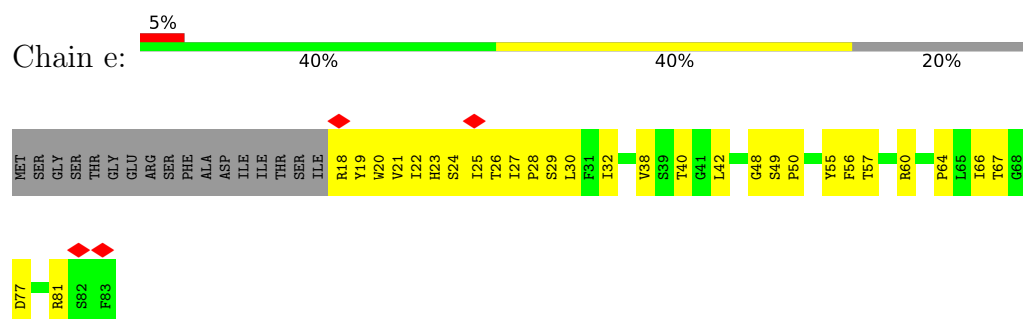




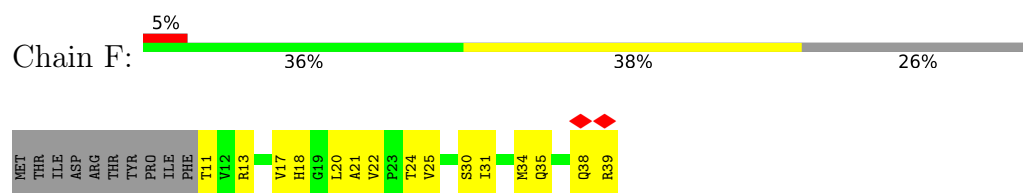
• Molecule 8: Cytochrome b559 subunit alpha



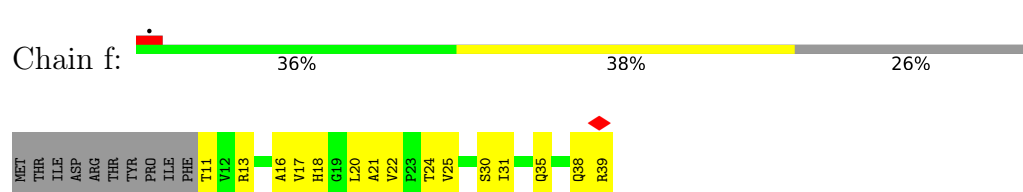
• Molecule 8: Cytochrome b559 subunit alpha



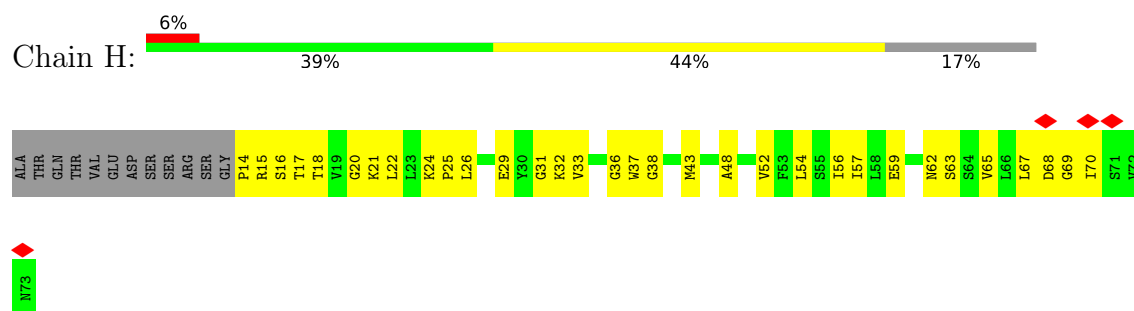
• Molecule 9: Cytochrome b559 subunit beta (PsbF)



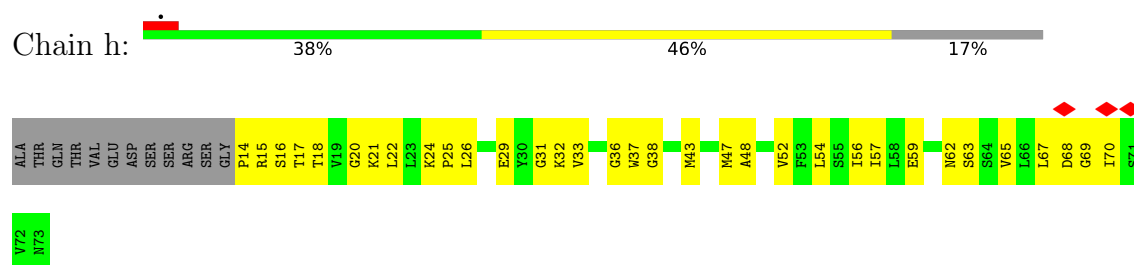
• Molecule 9: Cytochrome b559 subunit beta (PsbF)



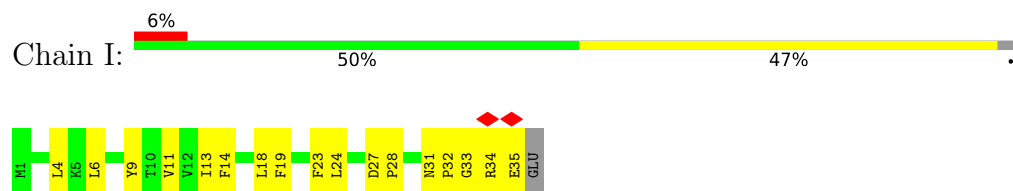
- Molecule 10: Photosystem II reaction center protein H



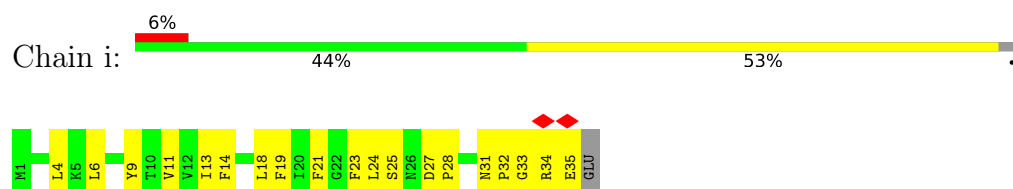
- Molecule 10: Photosystem II reaction center protein H



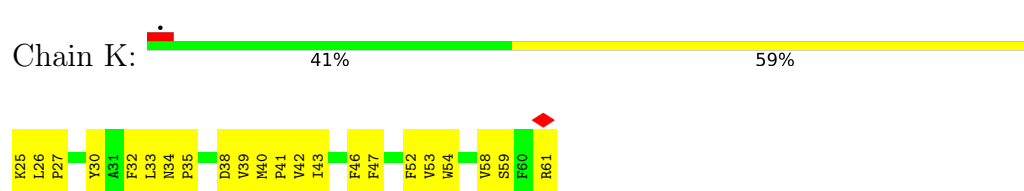
- Molecule 11: Photosystem II reaction center protein I



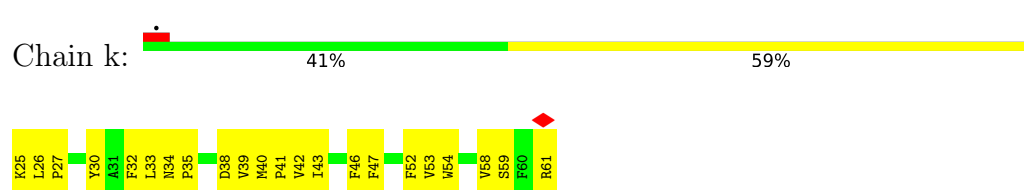
- Molecule 11: Photosystem II reaction center protein I



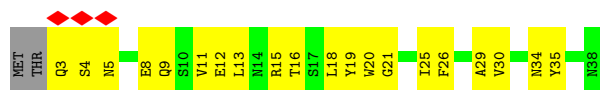
- Molecule 12: Photosystem II reaction center protein K



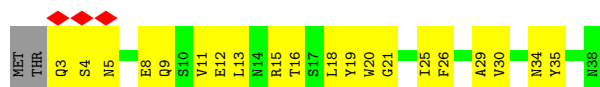
- Molecule 12: Photosystem II reaction center protein K



- Molecule 13: Photosystem II reaction center protein L



- Molecule 13: Photosystem II reaction center protein L



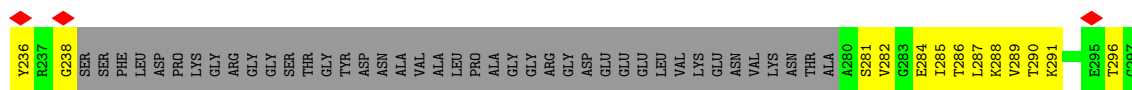
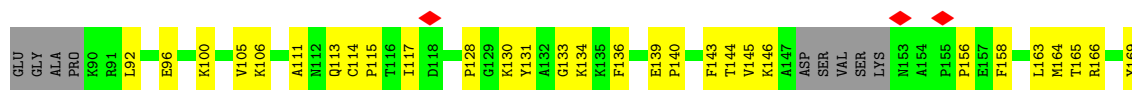
- Molecule 14: Photosystem II reaction center protein M



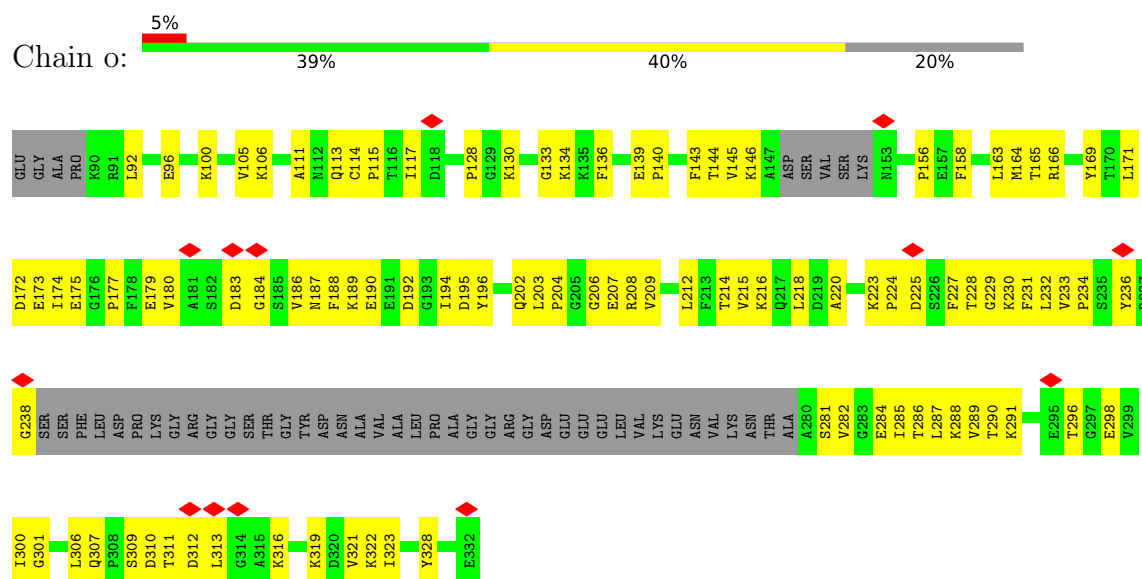
- Molecule 14: Photosystem II reaction center protein M



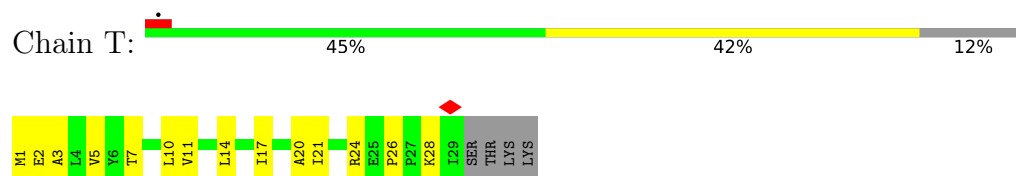
- Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic



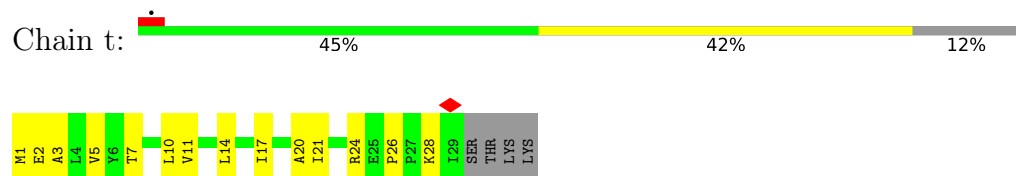
- Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic



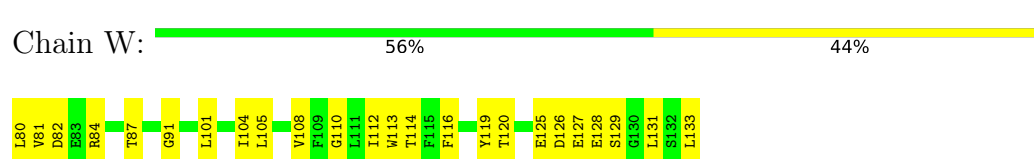
- Molecule 16: Photosystem II reaction center protein T



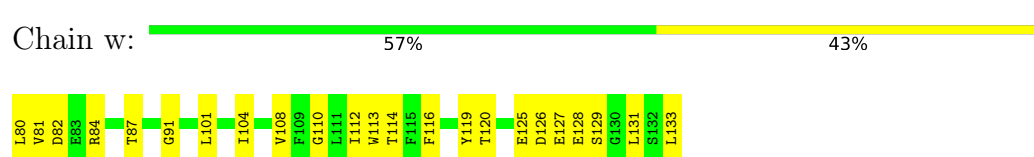
- Molecule 16: Photosystem II reaction center protein T



- Molecule 17: Photosystem II reaction center W protein, chloroplastic



- Molecule 17: Photosystem II reaction center W protein, chloroplastic

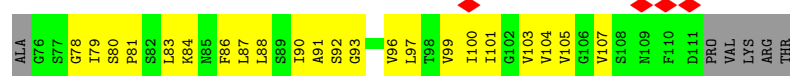


- Molecule 18: (thale cress) hypothetical protein

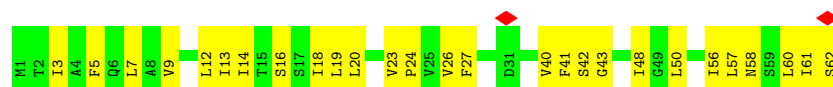




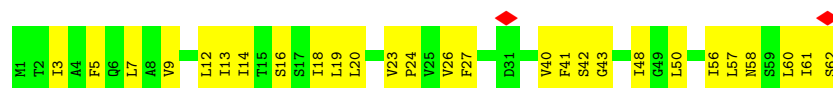
- Molecule 18: (thale cress) hypothetical protein



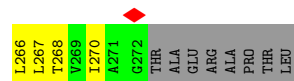
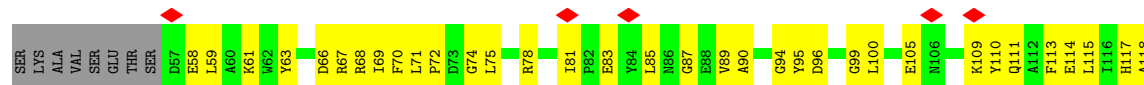
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z

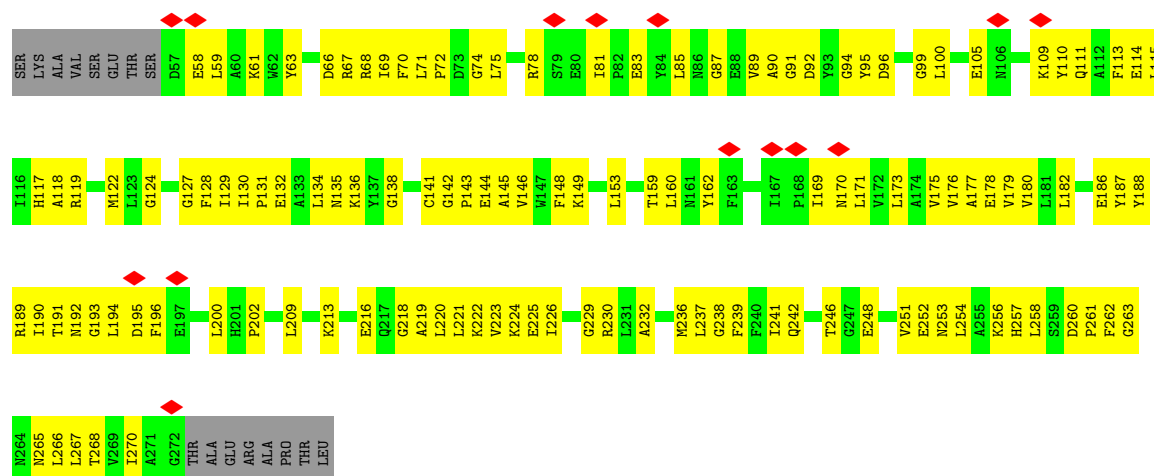


- Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic

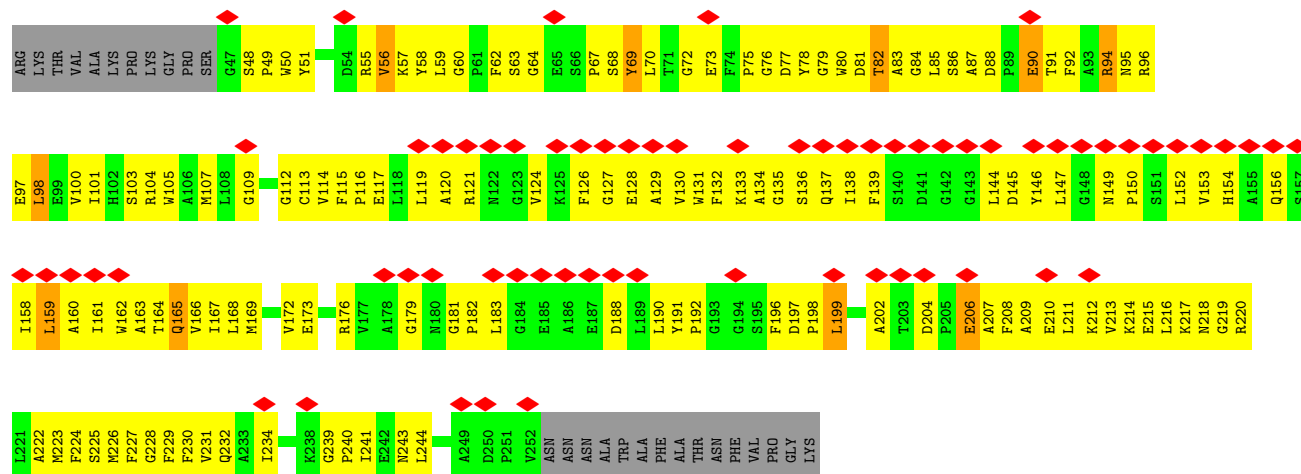


- Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic

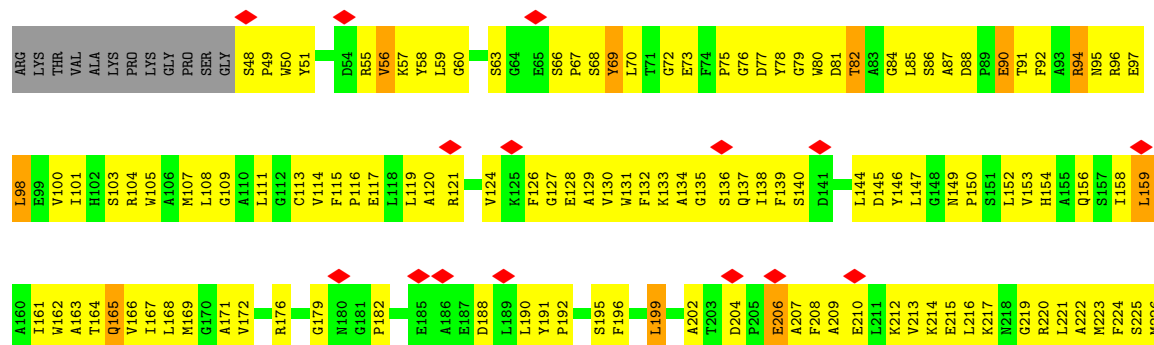


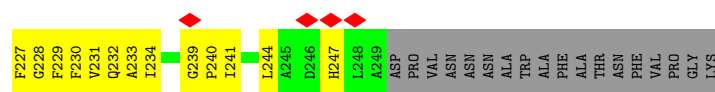


- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

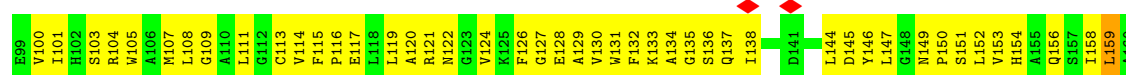
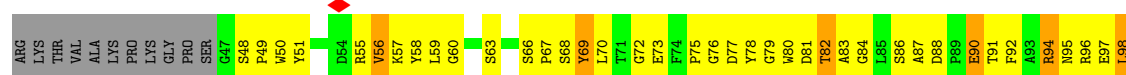
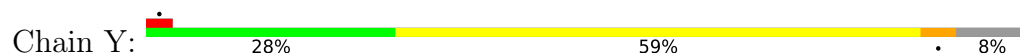


- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

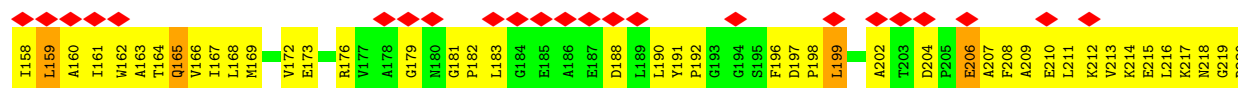
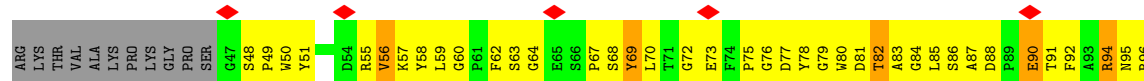




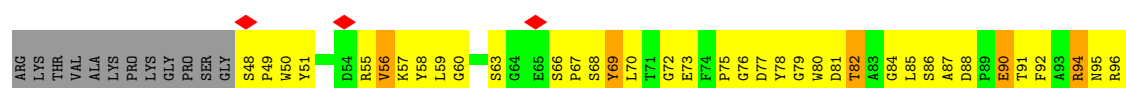
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

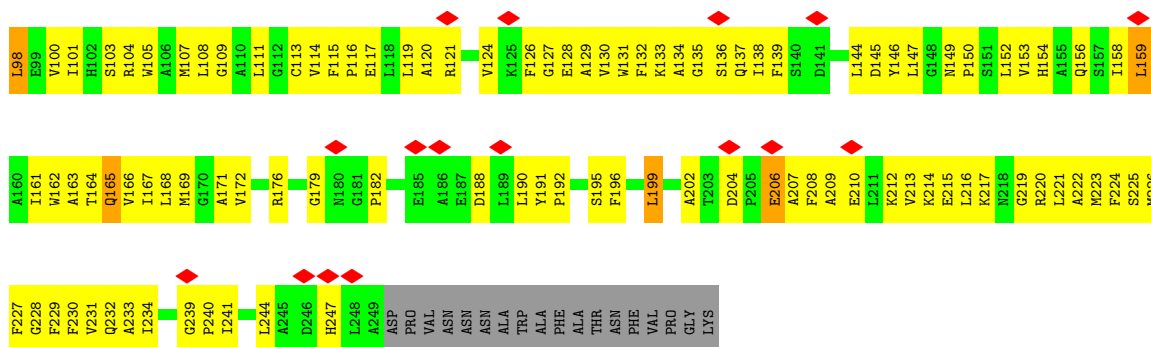


- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic



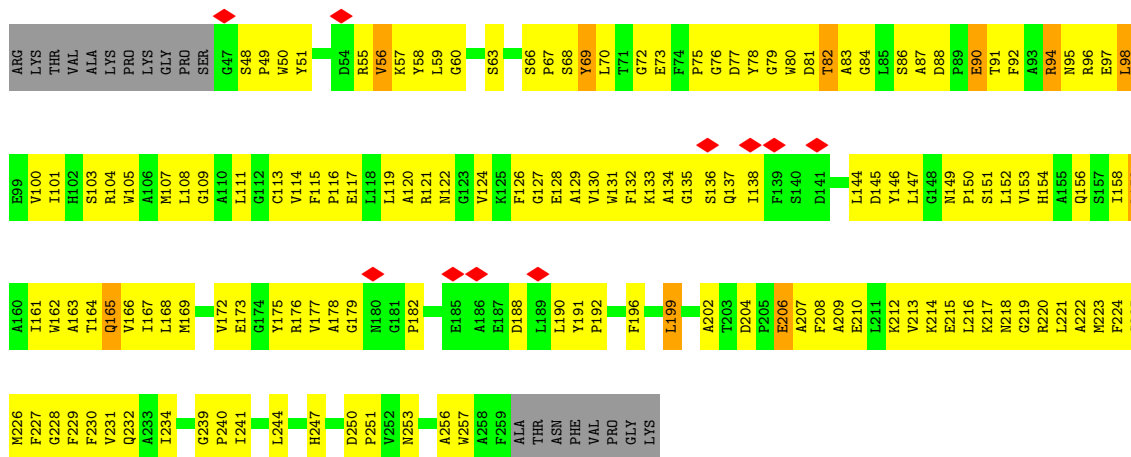
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic





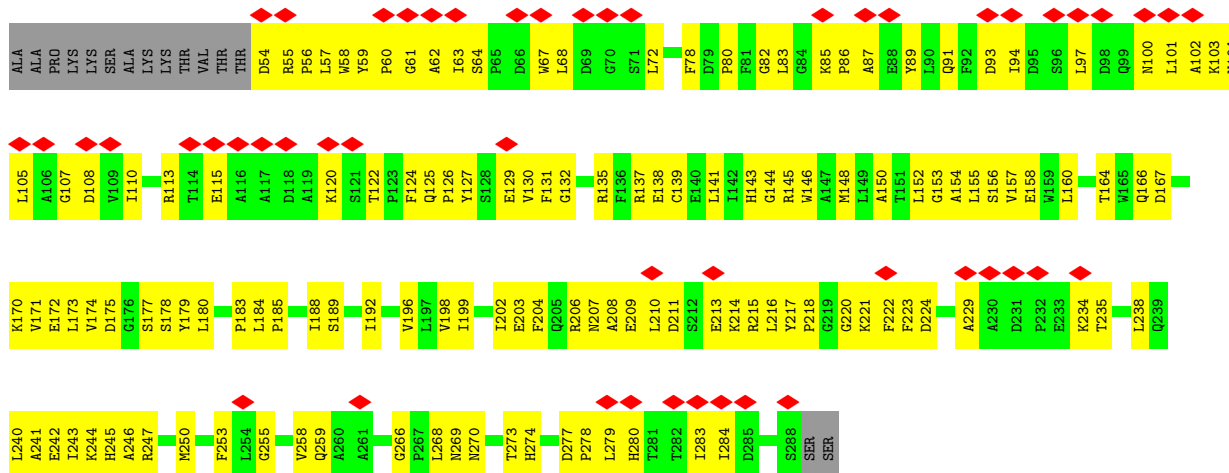
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

Chain y: 29% 59% 8%

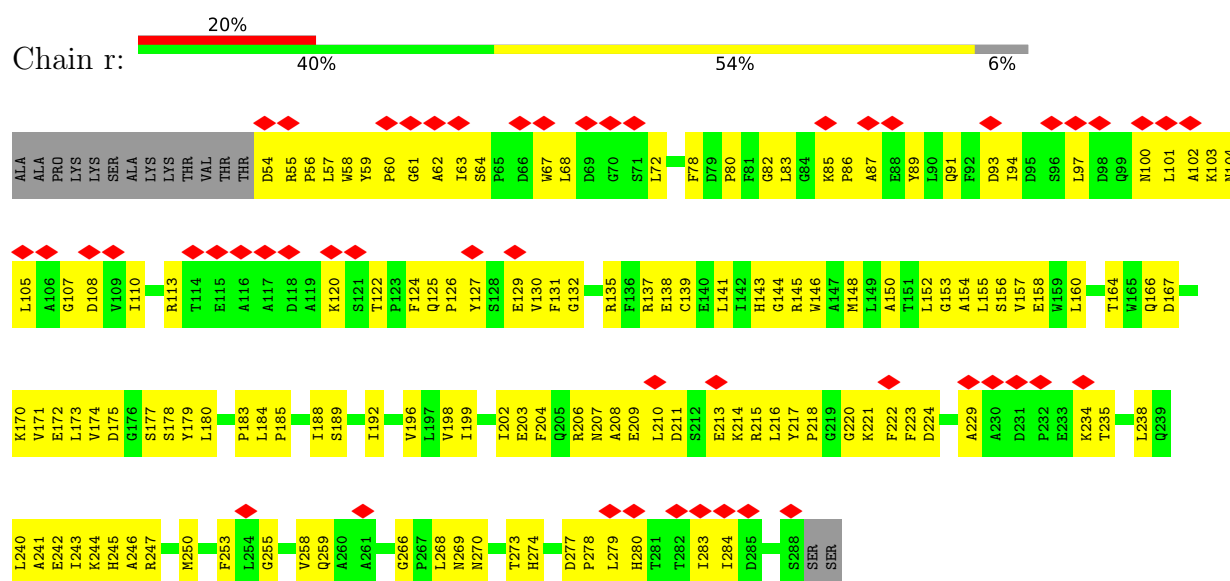


- Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic

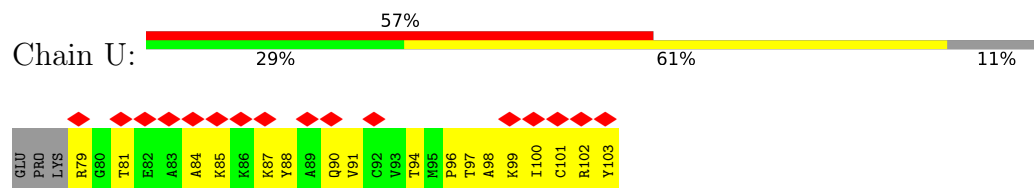
Chain R: 20% 39% 55% 6%



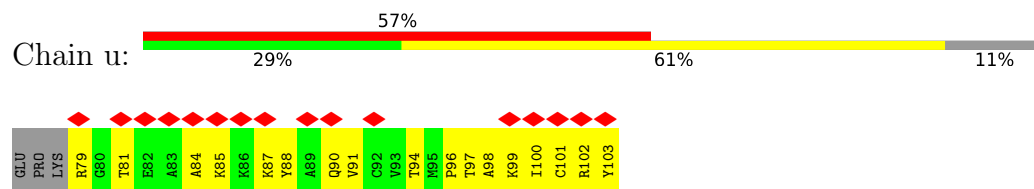
- Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic



- Molecule 23: Photosystem II 5 kDa protein, chloroplastic



- Molecule 23: Photosystem II 5 kDa protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.49	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	33.682	Depositor
Minimum map value	-19.496	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.976	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	410.0, 410.0, 410.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	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: FE2, LHG, DGD, CA, SQD, HEM, CL, PL9, NEX, XAT, BCT, LMG, BCR, AJP, PHO, LUT, CHL, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.19	0/1582	0.45	0/2150
1	3	0.19	0/1582	0.45	0/2150
1	5	0.19	0/1582	0.45	0/2150
1	7	0.19	0/1582	0.45	0/2150
2	2	0.17	0/1640	0.42	0/2229
2	6	0.17	0/1640	0.42	0/2229
3	4	0.17	0/1652	0.43	0/2242
3	8	0.17	0/1652	0.43	0/2242
4	A	0.12	0/2626	0.34	0/3580
4	a	0.12	0/2626	0.34	0/3580
5	B	0.12	0/3940	0.29	0/5368
5	b	0.12	0/3940	0.29	0/5368
6	C	0.11	0/3487	0.26	0/4750
6	c	0.11	0/3487	0.26	0/4750
7	D	0.12	0/2815	0.28	0/3837
7	d	0.12	0/2815	0.28	0/3837
8	E	0.10	0/561	0.29	0/763
8	e	0.10	0/561	0.29	0/763
9	F	0.09	0/229	0.24	0/311
9	f	0.09	0/229	0.24	0/311
10	H	0.10	0/455	0.36	0/619
10	h	0.10	0/455	0.35	0/619
11	I	0.13	0/294	0.38	0/397
11	i	0.12	0/294	0.38	0/397
12	K	0.10	0/312	0.27	0/428
12	k	0.10	0/312	0.27	0/428
13	L	0.09	0/310	0.20	0/421
13	l	0.09	0/310	0.20	0/421
14	M	0.11	0/254	0.28	0/347
14	m	0.11	0/254	0.28	0/347
15	O	0.10	0/1548	0.31	0/2091

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	o	0.10	0/1548	0.31	0/2091
16	T	0.09	0/246	0.22	0/333
16	t	0.09	0/246	0.22	0/333
17	W	0.10	0/438	0.26	0/594
17	w	0.10	0/438	0.26	0/594
18	X	0.09	0/250	0.23	0/339
18	x	0.10	0/250	0.23	0/339
19	Z	0.15	0/474	0.30	0/649
19	z	0.15	0/474	0.30	0/649
20	S	0.12	0/1715	0.29	0/2328
20	s	0.12	0/1715	0.30	0/2328
21	G	0.19	0/1607	0.44	0/2184
21	N	0.19	0/1580	0.44	0/2146
21	Y	0.19	0/1669	0.44	0/2270
21	g	0.19	0/1607	0.44	0/2184
21	n	0.19	0/1580	0.44	0/2146
21	y	0.19	0/1669	0.44	0/2270
22	R	0.15	0/1878	0.34	0/2561
22	r	0.15	0/1878	0.34	0/2561
23	U	0.08	0/196	0.27	0/261
23	u	0.09	0/196	0.27	0/261
All	All	0.14	0/66680	0.35	0/90696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1537	0	1480	181	0
1	3	1537	0	1480	182	0
1	5	1537	0	1480	179	0
1	7	1537	0	1480	183	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1593	0	1543	287	0
2	6	1593	0	1543	292	0
3	4	1597	0	1534	197	0
3	8	1597	0	1534	200	0
4	A	2548	0	2460	229	0
4	a	2548	0	2460	233	0
5	B	3810	0	3688	326	0
5	b	3810	0	3688	327	0
6	C	3373	0	3302	277	0
6	c	3373	0	3302	284	0
7	D	2722	0	2615	251	0
7	d	2722	0	2615	255	0
8	E	543	0	519	38	0
8	e	543	0	519	37	0
9	F	224	0	233	14	0
9	f	224	0	233	14	0
10	H	446	0	471	58	0
10	h	446	0	471	60	0
11	I	286	0	295	32	0
11	i	286	0	295	32	0
12	K	301	0	313	28	0
12	k	301	0	313	28	0
13	L	302	0	291	29	0
13	l	302	0	291	30	0
14	M	250	0	279	41	0
14	m	250	0	279	41	0
15	O	1516	0	1494	133	0
15	o	1516	0	1494	131	0
16	T	239	0	255	19	0
16	t	239	0	255	20	0
17	W	427	0	405	33	0
17	w	427	0	405	34	0
18	X	248	0	266	43	0
18	x	248	0	266	43	0
19	Z	464	0	495	38	0
19	z	464	0	495	40	0
20	S	1670	0	1647	186	0
20	s	1670	0	1647	188	0
21	G	1562	0	1501	302	0
21	N	1536	0	1478	293	0
21	Y	1621	0	1546	306	0
21	g	1562	0	1501	300	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	n	1536	0	1478	295	0
21	y	1621	0	1546	307	0
22	R	1827	0	1777	212	0
22	r	1827	0	1777	211	0
23	U	194	0	206	36	0
23	u	194	0	206	35	0
24	1	92	0	62	18	0
24	2	110	0	91	29	0
24	5	92	0	62	17	0
24	6	110	0	91	30	0
24	G	335	0	296	78	0
24	N	348	0	321	117	0
24	R	195	0	146	23	0
24	S	184	0	124	28	0
24	Y	344	0	308	94	0
24	g	335	0	296	77	0
24	n	348	0	321	116	0
24	r	195	0	146	24	0
24	s	184	0	124	33	0
24	y	344	0	308	93	0
25	2	163	0	142	33	0
25	6	163	0	142	37	0
25	A	190	0	203	39	0
25	B	1040	0	1150	147	0
25	C	840	0	923	145	0
25	D	180	0	183	41	0
25	G	472	0	464	110	0
25	N	473	0	468	139	0
25	R	543	0	490	113	0
25	S	465	0	393	90	0
25	Y	470	0	465	123	0
25	a	190	0	203	39	0
25	b	1040	0	1150	149	0
25	c	840	0	923	157	0
25	d	180	0	183	42	0
25	g	472	0	464	115	0
25	n	473	0	468	136	0
25	r	543	0	490	121	0
25	s	465	0	393	92	0
25	y	470	0	465	120	0
26	2	47	0	67	14	0
26	6	47	0	67	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	142	0	206	18	0
26	C	147	74	222	10	0
26	D	49	0	74	10	0
26	L	49	0	74	5	0
26	N	49	0	74	11	0
26	R	42	0	56	14	0
26	S	98	0	148	13	0
26	Y	98	0	146	20	0
26	b	142	0	206	18	0
26	c	147	74	222	10	0
26	d	49	0	74	10	0
26	l	49	0	74	5	0
26	n	49	0	74	10	0
26	r	42	0	56	16	0
26	s	98	0	148	15	0
26	y	98	0	146	20	0
27	A	128	0	148	27	0
27	a	128	0	148	28	0
28	A	40	0	56	4	0
28	B	120	0	168	18	0
28	C	40	0	56	7	0
28	D	40	0	56	3	0
28	H	40	0	56	6	0
28	I	40	0	56	20	0
28	K	40	0	56	7	0
28	T	40	0	54	20	0
28	Z	40	0	56	5	0
28	a	40	0	56	5	0
28	b	120	0	168	19	0
28	c	40	0	56	7	0
28	d	40	0	56	3	0
28	h	40	0	56	8	0
28	i	40	0	56	20	0
28	k	40	0	56	9	0
28	t	40	0	54	21	0
28	z	40	0	56	5	0
29	A	104	0	145	13	0
29	L	96	0	126	25	0
29	a	104	0	145	12	0
29	l	96	0	126	25	0
30	A	88	0	116	6	0
30	B	106	0	158	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	C	51	0	72	4	0
30	D	46	0	62	3	0
30	a	88	0	116	6	0
30	b	106	0	158	10	0
30	c	51	0	72	4	0
30	d	46	0	62	3	0
31	A	13	0	7	2	0
31	D	55	0	80	6	0
31	a	13	0	7	2	0
31	d	55	0	80	6	0
32	A	85	92	0	0	0
32	B	85	92	0	0	0
32	G	42	53	0	0	0
32	N	84	106	0	3	0
32	S	42	53	0	2	0
32	Y	210	265	0	7	0
32	a	85	92	0	0	0
32	b	85	92	0	0	0
32	g	42	53	0	0	0
32	n	84	106	0	3	0
32	s	42	53	0	2	0
32	y	210	265	0	7	0
33	A	4	0	1	2	0
33	a	4	0	1	1	0
34	A	1	0	0	0	0
34	a	1	0	0	0	0
35	A	59	0	76	3	0
35	B	62	0	82	5	0
35	C	117	0	150	18	0
35	a	59	0	76	3	0
35	b	62	0	82	6	0
35	c	117	0	150	17	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	a	1	0	0	0	0
36	b	1	0	0	0	0
37	D	1	0	0	1	0
37	d	1	0	0	1	0
38	F	43	0	30	7	0
38	f	43	0	30	8	0
39	G	84	0	112	30	0
39	N	84	0	112	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	R	42	0	56	6	0
39	S	84	0	112	27	0
39	Y	84	0	112	25	0
39	g	84	0	112	30	0
39	n	84	0	112	27	0
39	r	42	0	56	8	0
39	s	84	0	112	29	0
39	y	84	0	112	25	0
40	G	44	0	56	15	0
40	N	44	0	56	15	0
40	R	44	0	56	8	0
40	S	44	0	56	6	0
40	Y	44	0	56	7	0
40	g	44	0	56	15	0
40	n	44	0	56	13	0
40	r	44	0	56	10	0
40	s	44	0	56	5	0
40	y	44	0	56	10	0
41	R	44	0	56	20	0
41	r	44	0	56	22	0
42	A	23	0	0	0	0
42	B	10	0	0	3	0
42	C	14	0	0	1	0
42	D	14	0	0	0	0
42	H	1	0	0	0	0
42	I	1	0	0	0	0
42	L	3	0	0	2	0
42	M	1	0	0	0	0
42	T	1	0	0	0	0
42	W	1	0	0	0	0
42	a	23	0	0	1	0
42	b	10	0	0	3	0
42	c	14	0	0	1	0
42	d	14	0	0	0	0
42	h	1	0	0	0	0
42	i	1	0	0	0	0
42	l	3	0	0	2	0
42	m	2	0	0	0	0
42	t	1	0	0	0	0
42	w	1	0	0	0	0
All	All	84427	1470	83152	8481	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 51.

The worst 5 of 8481 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)
15:O:196:TYR:HB2	15:O:212:LEU:HD21	1.21	1.19
10:h:56:ILE:HD13	18:x:84:LYS:HE3	1.25	1.17
21:n:138:ILE:HG21	24:n:606:CHL:HBC1	1.23	1.17
22:r:144:GLY:HA3	22:r:246:ALA:HB1	1.28	1.16
22:R:144:GLY:HA3	22:R:246:ALA:HB1	1.28	1.14

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	1	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
1	3	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
1	5	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
1	7	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
2	2	203/243 (84%)	181 (89%)	20 (10%)	2 (1%)	12	38
2	6	203/243 (84%)	181 (89%)	20 (10%)	2 (1%)	12	38
3	4	202/212 (95%)	183 (91%)	18 (9%)	1 (0%)	24	55
3	8	202/212 (95%)	183 (91%)	18 (9%)	1 (0%)	24	55
4	A	324/352 (92%)	309 (95%)	14 (4%)	1 (0%)	36	66
4	a	324/352 (92%)	308 (95%)	15 (5%)	1 (0%)	36	66
5	B	485/508 (96%)	466 (96%)	18 (4%)	1 (0%)	43	72
5	b	485/508 (96%)	466 (96%)	18 (4%)	1 (0%)	43	72
6	C	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	c	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	43	72
7	D	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
7	d	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
8	E	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
8	e	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
9	F	27/39 (69%)	27 (100%)	0	0	100	100
9	f	27/39 (69%)	27 (100%)	0	0	100	100
10	H	58/72 (81%)	52 (90%)	6 (10%)	0	100	100
10	h	58/72 (81%)	52 (90%)	6 (10%)	0	100	100
11	I	33/36 (92%)	28 (85%)	5 (15%)	0	100	100
11	i	33/36 (92%)	28 (85%)	5 (15%)	0	100	100
12	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
13	L	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
13	l	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
14	M	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	11
14	m	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	11
15	O	191/247 (77%)	183 (96%)	8 (4%)	0	100	100
15	o	191/247 (77%)	183 (96%)	8 (4%)	0	100	100
16	T	27/33 (82%)	25 (93%)	2 (7%)	0	100	100
16	t	27/33 (82%)	25 (93%)	2 (7%)	0	100	100
17	W	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
17	w	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
18	X	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
18	x	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
20	S	214/232 (92%)	204 (95%)	10 (5%)	0	100	100
20	s	214/232 (92%)	203 (95%)	11 (5%)	0	100	100
21	G	204/232 (88%)	192 (94%)	12 (6%)	0	100	100
21	N	200/232 (86%)	189 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Y	211/232 (91%)	200 (95%)	11 (5%)	0	100	100
21	g	204/232 (88%)	192 (94%)	12 (6%)	0	100	100
21	n	200/232 (86%)	189 (94%)	11 (6%)	0	100	100
21	y	211/232 (91%)	200 (95%)	11 (5%)	0	100	100
22	R	233/250 (93%)	223 (96%)	10 (4%)	0	100	100
22	r	233/250 (93%)	223 (96%)	10 (4%)	0	100	100
23	U	23/28 (82%)	19 (83%)	4 (17%)	0	100	100
23	u	23/28 (82%)	19 (83%)	4 (17%)	0	100	100
All	All	8226/9282 (89%)	7790 (95%)	422 (5%)	14 (0%)	44	72

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	123	VAL
3	4	182	ALA
4	A	18	CYS
14	M	3	VAL
2	6	123	VAL

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	1	154/201 (77%)	142 (92%)	12 (8%)	11	35
1	3	154/201 (77%)	142 (92%)	12 (8%)	11	35
1	5	154/201 (77%)	142 (92%)	12 (8%)	11	35
1	7	154/201 (77%)	142 (92%)	12 (8%)	11	35
2	2	164/192 (85%)	164 (100%)	0	100	100
2	6	164/192 (85%)	164 (100%)	0	100	100
3	4	156/159 (98%)	156 (100%)	0	100	100
3	8	156/159 (98%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	263/284 (93%)	263 (100%)	0	100	100
4	a	263/284 (93%)	263 (100%)	0	100	100
5	B	384/402 (96%)	384 (100%)	0	100	100
5	b	384/402 (96%)	384 (100%)	0	100	100
6	C	340/359 (95%)	340 (100%)	0	100	100
6	c	340/359 (95%)	340 (100%)	0	100	100
7	D	274/282 (97%)	274 (100%)	0	100	100
7	d	274/282 (97%)	274 (100%)	0	100	100
8	E	59/73 (81%)	59 (100%)	0	100	100
8	e	59/73 (81%)	59 (100%)	0	100	100
9	F	24/34 (71%)	24 (100%)	0	100	100
9	f	24/34 (71%)	24 (100%)	0	100	100
10	H	50/60 (83%)	50 (100%)	0	100	100
10	h	50/60 (83%)	50 (100%)	0	100	100
11	I	32/33 (97%)	32 (100%)	0	100	100
11	i	32/33 (97%)	32 (100%)	0	100	100
12	K	32/32 (100%)	32 (100%)	0	100	100
12	k	32/32 (100%)	32 (100%)	0	100	100
13	L	34/36 (94%)	34 (100%)	0	100	100
13	l	34/36 (94%)	34 (100%)	0	100	100
14	M	28/30 (93%)	28 (100%)	0	100	100
14	m	28/30 (93%)	28 (100%)	0	100	100
15	O	167/204 (82%)	167 (100%)	0	100	100
15	o	167/204 (82%)	167 (100%)	0	100	100
16	T	26/30 (87%)	26 (100%)	0	100	100
16	t	26/30 (87%)	26 (100%)	0	100	100
17	W	47/47 (100%)	47 (100%)	0	100	100
17	w	47/47 (100%)	47 (100%)	0	100	100
18	X	29/34 (85%)	29 (100%)	0	100	100
18	x	29/34 (85%)	29 (100%)	0	100	100
19	Z	54/54 (100%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	z	54/54 (100%)	54 (100%)	0	100	100
20	S	167/180 (93%)	167 (100%)	0	100	100
20	s	167/180 (93%)	167 (100%)	0	100	100
21	G	157/177 (89%)	145 (92%)	12 (8%)	12	36
21	N	154/177 (87%)	142 (92%)	12 (8%)	11	35
21	Y	162/177 (92%)	150 (93%)	12 (7%)	13	37
21	g	157/177 (89%)	145 (92%)	12 (8%)	12	36
21	n	154/177 (87%)	142 (92%)	12 (8%)	11	35
21	y	162/177 (92%)	150 (93%)	12 (7%)	13	37
22	R	189/201 (94%)	189 (100%)	0	100	100
22	r	189/201 (94%)	189 (100%)	0	100	100
23	U	20/23 (87%)	20 (100%)	0	100	100
23	u	20/23 (87%)	20 (100%)	0	100	100
All	All	6640/7364 (90%)	6520 (98%)	120 (2%)	51	82

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	Y	165	GLN
21	y	68	SER
1	5	206	GLU
21	y	56	VAL
21	y	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	6	150	ASN
6	c	237	HIS
20	s	135	ASN
5	b	73	ASN
5	b	296	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 374 ligands modelled in this entry, 8 are monoatomic - leaving 366 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$
39	LUT	R	615	-	42,43,43	0.96	3 (7%)	51,60,60	1.67	9 (17%)
25	CLA	s	313	20	59,63,73	1.50	11 (18%)	71,101,113	2.36	18 (25%)
25	CLA	N	612	21	64,68,73	1.45	11 (17%)	77,107,113	1.84	16 (20%)
28	BCR	k	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.30	9 (16%)
28	BCR	a	407	-	41,41,41	1.15	2 (4%)	56,56,56	1.34	10 (17%)
24	CHL	G	606	-	54,58,74	1.46	6 (11%)	59,94,114	2.06	13 (22%)
32	AJP	N	620	-	48,48,95	0.72	0	71,78,149	4.20	32 (45%)
32	AJP	s	319	-	48,48,95	0.77	0	71,78,149	4.19	29 (40%)
32	AJP	n	619	-	48,48,95	0.71	0	71,78,149	4.14	33 (46%)
25	CLA	S	312	20	53,57,73	1.61	11 (20%)	62,93,113	1.82	15 (24%)
32	AJP	G	618	-	48,48,95	0.88	1 (2%)	71,78,149	5.33	38 (53%)
25	CLA	Y	303	21	69,73,73	1.36	12 (17%)	83,113,113	1.72	15 (18%)
24	CHL	G	608	-	70,74,74	1.34	8 (11%)	80,114,114	1.74	13 (16%)
39	LUT	N	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.53	6 (11%)
29	SQD	a	408	-	49,50,54	0.82	1 (2%)	58,61,65	0.95	3 (5%)
24	CHL	N	606	-	50,54,74	1.52	8 (16%)	56,90,114	2.04	14 (25%)
24	CHL	R	606	-	50,54,74	1.54	8 (16%)	56,90,114	1.92	10 (17%)
24	CHL	N	605	21	52,56,74	1.47	7 (13%)	58,92,114	1.99	14 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	b	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	10 (17%)
24	CHL	S	307	-	50,54,74	1.53	7 (14%)	56,90,114	2.04	11 (19%)
25	CLA	R	604	-	52,56,73	1.60	10 (19%)	62,92,113	2.07	20 (32%)
32	AJP	a	413	-	95,95,95	0.63	0	143,149,149	3.67	64 (44%)
25	CLA	S	304	-	49,53,73	1.61	12 (24%)	59,89,113	2.10	11 (18%)
24	CHL	g	601	21	70,74,74	1.32	8 (11%)	80,114,114	1.71	14 (17%)
24	CHL	Y	310	21	60,64,74	1.44	7 (11%)	68,102,114	1.80	13 (19%)
28	BCR	i	101	-	41,41,41	1.20	2 (4%)	56,56,56	1.27	9 (16%)
25	CLA	G	604	40	54,58,73	1.56	11 (20%)	65,95,113	1.94	15 (23%)
25	CLA	D	403	-	69,73,73	1.55	8 (11%)	83,113,113	2.82	24 (28%)
24	CHL	y	310	21	60,64,74	1.44	8 (13%)	68,102,114	1.81	13 (19%)
40	NEX	n	617	-	38,46,46	1.67	7 (18%)	50,70,70	2.43	18 (36%)
29	SQD	L	101	-	41,42,54	0.88	1 (2%)	50,53,65	1.11	3 (6%)
25	CLA	b	602	5	69,73,73	1.38	11 (15%)	83,113,113	1.71	16 (19%)
30	LMG	A	410	-	40,40,55	0.48	0	48,48,63	1.28	4 (8%)
26	LHG	B	621	-	46,46,48	0.45	0	49,52,54	1.18	4 (8%)
26	LHG	s	301	-	48,48,48	0.44	0	51,54,54	1.16	4 (7%)
40	NEX	s	317	-	38,46,46	1.62	8 (21%)	50,70,70	2.23	11 (22%)
24	CHL	s	306	-	50,54,74	1.53	8 (16%)	56,90,114	2.05	15 (26%)
24	CHL	n	601	21	60,64,74	1.44	8 (13%)	68,102,114	1.78	13 (19%)
25	CLA	B	606	5	69,73,73	1.36	11 (15%)	83,113,113	1.83	15 (18%)
32	AJP	N	619	-	48,48,95	0.70	0	71,78,149	4.14	33 (46%)
25	CLA	n	610	21	69,73,73	1.39	11 (15%)	83,113,113	1.71	16 (19%)
25	CLA	G	603	-	64,68,73	1.44	11 (17%)	77,107,113	1.82	15 (19%)
25	CLA	Y	313	21	64,68,73	1.46	12 (18%)	77,107,113	1.71	16 (20%)
25	CLA	g	612	21	64,68,73	1.44	10 (15%)	77,107,113	1.66	13 (16%)
26	LHG	L	102	-	48,48,48	0.44	0	51,54,54	1.17	4 (7%)
25	CLA	b	607	-	69,73,73	1.37	11 (15%)	83,113,113	1.78	15 (18%)
35	DGD	a	401	-	60,60,67	0.48	0	74,74,81	1.22	5 (6%)
25	CLA	y	303	21	69,73,73	1.36	12 (17%)	83,113,113	1.72	15 (18%)
25	CLA	g	613	21	69,73,73	1.42	10 (14%)	83,113,113	1.97	15 (18%)
32	AJP	n	620	-	48,48,95	0.72	0	71,78,149	4.20	32 (45%)
25	CLA	C	509	6	69,73,73	1.38	12 (17%)	83,113,113	1.78	13 (15%)
38	HEM	F	101	9	50,50,50	2.49	9 (18%)	66,82,82	1.75	13 (19%)
29	SQD	L	103	-	53,54,54	0.80	1 (1%)	62,65,65	1.01	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	n	613	21	64,68,73	1.45	10 (15%)	77,107,113	1.96	19 (24%)
24	CHL	Y	307	21	54,58,74	1.49	6 (11%)	59,94,114	1.79	13 (22%)
31	PL9	a	410	-	13,13,55	0.96	0	17,17,69	0.72	0
25	CLA	B	603	-	69,73,73	1.37	11 (15%)	83,113,113	1.70	16 (19%)
24	CHL	y	308	-	62,66,74	1.43	7 (11%)	70,104,114	1.86	14 (20%)
26	LHG	B	622	-	48,48,48	0.45	0	51,54,54	1.15	4 (7%)
29	SQD	A	407	-	49,50,54	0.82	1 (2%)	58,61,65	0.95	3 (5%)
24	CHL	s	307	-	50,54,74	1.54	8 (16%)	56,90,114	2.04	12 (21%)
39	LUT	y	316	-	42,43,43	0.83	2 (4%)	51,60,60	1.74	8 (15%)
27	PHO	A	403	-	58,69,69	0.49	0	56,99,99	1.66	8 (14%)
24	CHL	N	601	21	60,64,74	1.44	8 (13%)	68,102,114	1.79	13 (19%)
39	LUT	r	615	-	42,43,43	0.95	3 (7%)	51,60,60	1.68	9 (17%)
25	CLA	N	610	21	69,73,73	1.39	11 (15%)	83,113,113	1.70	16 (19%)
32	AJP	B	624	-	95,95,95	0.61	0	143,149,149	3.44	56 (39%)
24	CHL	5	302	1	50,54,74	1.57	8 (16%)	56,90,114	2.06	10 (17%)
32	AJP	b	624	-	95,95,95	0.61	0	143,149,149	3.44	56 (39%)
26	LHG	B	625	-	45,45,48	0.44	0	48,51,54	1.19	4 (8%)
25	CLA	g	610	-	68,72,73	1.44	9 (13%)	81,111,113	2.09	19 (23%)
28	BCR	B	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	10 (17%)
30	LMG	B	620	25	51,51,55	0.44	0	59,59,63	1.21	4 (6%)
25	CLA	r	603	22	64,68,73	1.60	7 (10%)	77,107,113	2.87	22 (28%)
25	CLA	r	602	22	64,68,73	1.43	11 (17%)	77,107,113	1.86	19 (24%)
25	CLA	A	405	4	64,68,73	1.43	12 (18%)	77,107,113	1.86	15 (19%)
25	CLA	r	601	-	53,57,73	1.77	9 (16%)	62,93,113	3.28	20 (32%)
25	CLA	n	611	26	64,68,73	1.44	12 (18%)	77,107,113	1.68	18 (23%)
25	CLA	b	608	5	69,73,73	1.37	12 (17%)	83,113,113	1.78	16 (19%)
25	CLA	Y	311	21	64,68,73	1.44	11 (17%)	77,107,113	1.76	16 (20%)
24	CHL	Y	308	-	62,66,74	1.43	7 (11%)	70,104,114	1.86	14 (20%)
24	CHL	r	606	-	50,54,74	1.54	7 (14%)	56,90,114	1.91	9 (16%)
24	CHL	s	302	20	50,54,74	1.53	8 (16%)	56,90,114	2.00	12 (21%)
24	CHL	n	607	-	70,74,74	1.34	7 (10%)	80,114,114	1.72	13 (16%)
25	CLA	S	305	-	54,58,73	1.75	7 (12%)	65,95,113	3.39	22 (33%)
25	CLA	R	611	-	53,57,73	1.88	9 (16%)	62,93,113	3.56	25 (40%)
26	LHG	S	318	25	48,48,48	0.42	0	51,54,54	1.19	4 (7%)
32	AJP	Y	322	-	48,48,95	0.72	0	71,78,149	4.09	30 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	s	308	-	50,54,74	1.54	8 (16%)	56,90,114	2.10	13 (23%)
38	HEM	f	101	9	50,50,50	2.49	9 (18%)	66,82,82	1.75	13 (19%)
24	CHL	2	603	2	50,54,74	1.67	10 (20%)	56,90,114	2.38	16 (28%)
24	CHL	5	301	1	50,54,74	1.54	8 (16%)	56,90,114	1.94	12 (21%)
25	CLA	g	611	-	64,68,73	1.50	11 (17%)	77,107,113	1.89	24 (31%)
30	LMG	b	623	-	55,55,55	0.43	0	63,63,63	1.23	4 (6%)
25	CLA	B	611	5	69,73,73	1.36	11 (15%)	83,113,113	1.83	17 (20%)
39	LUT	n	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.53	6 (11%)
25	CLA	G	612	21	64,68,73	1.43	11 (17%)	77,107,113	1.66	13 (16%)
26	LHG	C	518	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
28	BCR	T	101	16	41,41,41	1.15	3 (7%)	56,56,56	1.28	8 (14%)
25	CLA	s	314	20	53,57,73	1.57	12 (22%)	62,93,113	1.76	14 (22%)
24	CHL	R	613	22	46,50,74	1.49	6 (13%)	51,85,114	2.17	11 (21%)
27	PHO	a	405	-	58,69,69	0.49	0	56,99,99	1.64	9 (16%)
25	CLA	C	511	6	69,73,73	1.39	11 (15%)	83,113,113	2.18	19 (22%)
39	LUT	G	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.44	4 (7%)
24	CHL	g	607	-	50,54,74	1.53	7 (14%)	56,90,114	1.93	14 (25%)
24	CHL	G	601	21	70,74,74	1.32	8 (11%)	80,114,114	1.72	15 (18%)
28	BCR	c	514	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	7 (12%)
30	LMG	d	407	-	46,46,55	0.44	0	54,54,63	1.21	4 (7%)
25	CLA	g	604	40	54,58,73	1.56	11 (20%)	65,95,113	1.94	15 (23%)
24	CHL	R	607	-	65,69,74	1.39	8 (12%)	74,108,114	1.86	14 (18%)
26	LHG	y	301	21	48,48,48	0.44	0	51,54,54	1.18	4 (7%)
25	CLA	n	614	21	52,56,73	1.61	10 (19%)	62,92,113	2.14	16 (25%)
25	CLA	c	504	-	64,68,73	1.60	7 (10%)	77,107,113	2.83	24 (31%)
25	CLA	n	612	21	64,68,73	1.45	11 (17%)	77,107,113	1.85	16 (20%)
26	LHG	D	406	-	48,48,48	0.43	0	51,54,54	1.18	4 (7%)
25	CLA	y	314	21	69,73,73	1.37	11 (15%)	83,113,113	1.91	15 (18%)
29	SQD	l	102	-	41,42,54	0.88	1 (2%)	50,53,65	1.11	3 (6%)
25	CLA	N	611	26	64,68,73	1.44	12 (18%)	77,107,113	1.68	18 (23%)
24	CHL	2	601	2	68,72,74	1.36	8 (11%)	77,111,114	1.99	15 (19%)
25	CLA	C	503	6	69,73,73	1.36	11 (15%)	83,113,113	1.86	16 (19%)
35	DGD	C	515	-	56,56,67	0.48	0	70,70,81	1.23	6 (8%)
40	NEX	S	317	-	38,46,46	1.61	8 (21%)	50,70,70	2.23	11 (22%)
28	BCR	b	617	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	Z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
25	CLA	C	501	-	69,73,73	1.51	7 (10%)	83,113,113	2.63	24 (28%)
24	CHL	g	609	21	65,69,74	1.39	8 (12%)	74,108,114	1.89	13 (17%)
25	CLA	C	507	-	69,73,73	1.41	11 (15%)	83,113,113	1.68	15 (18%)
25	CLA	r	608	22	62,66,73	1.44	11 (17%)	74,104,113	1.81	16 (21%)
25	CLA	R	614	22	49,53,73	1.62	10 (20%)	59,89,113	1.74	15 (25%)
25	CLA	B	614	30,5	69,73,73	1.36	11 (15%)	83,113,113	1.82	14 (16%)
25	CLA	C	502	6	69,73,73	1.38	11 (15%)	83,113,113	1.81	17 (20%)
32	AJP	Y	320	-	48,48,95	0.80	1 (2%)	71,78,149	4.20	33 (46%)
26	LHG	d	406	-	48,48,48	0.43	0	51,54,54	1.18	4 (7%)
41	XAT	R	616	-	39,47,47	1.17	6 (15%)	54,74,74	2.41	16 (29%)
25	CLA	y	312	26	64,68,73	1.45	12 (18%)	77,107,113	1.68	17 (22%)
25	CLA	c	510	-	69,73,73	1.36	12 (17%)	83,113,113	1.79	16 (19%)
32	AJP	g	618	-	48,48,95	0.88	1 (2%)	71,78,149	5.33	38 (53%)
28	BCR	H	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	9 (16%)
25	CLA	c	502	6	69,73,73	1.38	11 (15%)	83,113,113	1.81	17 (20%)
25	CLA	s	311	26	60,64,73	1.47	11 (18%)	72,102,113	2.18	14 (19%)
26	LHG	r	618	25	41,41,48	0.46	0	44,47,54	1.22	4 (9%)
25	CLA	s	304	-	49,53,73	1.62	11 (22%)	59,89,113	2.11	11 (18%)
24	CHL	S	302	20	50,54,74	1.53	8 (16%)	56,90,114	2.00	12 (21%)
26	LHG	b	621	-	46,46,48	0.45	0	49,52,54	1.18	4 (8%)
28	BCR	B	619	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	8 (14%)
26	LHG	Y	301	21	48,48,48	0.44	0	51,54,54	1.19	4 (7%)
25	CLA	B	605	5	69,73,73	1.38	11 (15%)	83,113,113	1.93	14 (16%)
25	CLA	S	313	20	59,63,73	1.51	12 (20%)	71,101,113	2.36	18 (25%)
25	CLA	S	303	20	65,69,73	1.42	12 (18%)	78,108,113	1.72	15 (19%)
28	BCR	h	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.30	9 (16%)
25	CLA	2	605	2	52,56,73	1.58	11 (21%)	62,92,113	1.94	13 (20%)
25	CLA	6	605	2	52,56,73	1.58	11 (21%)	62,92,113	1.94	12 (19%)
28	BCR	t	101	16	41,41,41	1.15	3 (7%)	56,56,56	1.27	8 (14%)
25	CLA	y	305	-	54,58,73	1.55	11 (20%)	65,95,113	1.80	16 (24%)
32	AJP	Y	324	-	48,48,95	0.70	0	71,78,149	4.32	32 (45%)
40	NEX	G	617	25	38,46,46	1.52	8 (21%)	50,70,70	2.76	14 (28%)
25	CLA	D	401	42	54,58,73	1.55	12 (22%)	65,95,113	2.08	15 (23%)
35	DGD	c	515	-	56,56,67	0.48	0	70,70,81	1.23	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	6	603	2	50,54,74	1.67	10 (20%)	56,90,114	2.38	16 (28%)
25	CLA	d	401	42	54,58,73	1.55	12 (22%)	65,95,113	2.09	15 (23%)
26	LHG	C	519	6	48,48,48	0.45	0	51,54,54	1.18	4 (7%)
25	CLA	n	604	-	54,58,73	1.54	12 (22%)	65,95,113	2.10	16 (24%)
25	CLA	G	611	-	64,68,73	1.50	9 (14%)	77,107,113	1.88	24 (31%)
35	DGD	C	516	-	63,63,67	0.52	0	77,77,81	1.23	6 (7%)
25	CLA	b	614	30,5	69,73,73	1.36	11 (15%)	83,113,113	1.81	14 (16%)
25	CLA	b	612	5	69,73,73	1.38	12 (17%)	83,113,113	1.78	16 (19%)
25	CLA	G	610	-	68,72,73	1.44	9 (13%)	81,111,113	2.09	20 (24%)
26	LHG	b	622	-	48,48,48	0.45	0	51,54,54	1.15	4 (7%)
25	CLA	C	508	6	69,73,73	1.38	10 (14%)	83,113,113	1.92	18 (21%)
25	CLA	S	314	20	53,57,73	1.56	12 (22%)	62,93,113	1.76	14 (22%)
27	PHO	a	404	-	58,69,69	0.50	0	56,99,99	1.66	8 (14%)
39	LUT	S	316	-	42,43,43	0.89	4 (9%)	51,60,60	1.65	8 (15%)
32	AJP	Y	321	-	48,48,95	0.76	0	71,78,149	4.21	27 (38%)
25	CLA	c	503	6	69,73,73	1.37	11 (15%)	83,113,113	1.86	16 (19%)
25	CLA	c	512	-	69,73,73	1.37	12 (17%)	83,113,113	1.78	18 (21%)
30	LMG	a	409	-	48,48,55	0.44	0	56,56,63	1.19	5 (8%)
25	CLA	Y	305	-	54,58,73	1.55	11 (20%)	65,95,113	1.80	16 (24%)
24	CHL	G	607	-	50,54,74	1.53	7 (14%)	56,90,114	1.93	14 (25%)
24	CHL	Y	306	21	52,56,74	1.47	7 (13%)	58,92,114	1.98	12 (20%)
28	BCR	d	404	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	5 (8%)
29	SQD	a	412	-	53,54,54	0.80	1 (1%)	62,65,65	0.97	2 (3%)
39	LUT	N	615	-	42,43,43	0.89	2 (4%)	51,60,60	1.73	9 (17%)
25	CLA	B	602	5	69,73,73	1.37	11 (15%)	83,113,113	1.70	17 (20%)
32	AJP	A	412	-	95,95,95	0.63	0	143,149,149	3.67	64 (44%)
29	SQD	l	101	-	53,54,54	0.80	1 (1%)	62,65,65	1.01	3 (4%)
26	LHG	Y	319	25	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
25	CLA	s	305	-	54,58,73	1.75	7 (12%)	65,95,113	3.39	22 (33%)
25	CLA	c	511	6	69,73,73	1.39	10 (14%)	83,113,113	2.17	17 (20%)
25	CLA	c	507	-	69,73,73	1.40	11 (15%)	83,113,113	1.68	15 (18%)
25	CLA	g	603	-	64,68,73	1.44	11 (17%)	77,107,113	1.82	15 (19%)
24	CHL	N	608	-	70,74,74	1.33	7 (10%)	80,114,114	1.72	10 (12%)
30	LMG	A	408	-	48,48,55	0.44	0	56,56,63	1.20	5 (8%)
25	CLA	c	505	6	69,73,73	1.37	11 (15%)	83,113,113	1.74	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	y	307	21	54,58,74	1.50	7 (12%)	59,94,114	1.80	13 (22%)
25	CLA	s	312	20	53,57,73	1.61	11 (20%)	62,93,113	1.82	15 (24%)
25	CLA	y	313	21	64,68,73	1.46	12 (18%)	77,107,113	1.71	16 (20%)
28	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	9 (16%)
41	XAT	r	616	-	39,47,47	1.16	6 (15%)	54,74,74	2.42	16 (29%)
25	CLA	C	513	6	69,73,73	1.37	12 (17%)	83,113,113	1.80	18 (21%)
33	BCT	a	414	34	2,3,3	1.20	0	2,3,3	4.33	2 (100%)
25	CLA	R	610	26	53,57,73	1.80	7 (13%)	62,93,113	3.21	19 (30%)
25	CLA	B	610	-	69,73,73	1.41	11 (15%)	83,113,113	1.62	14 (16%)
25	CLA	N	604	-	54,58,73	1.54	11 (20%)	65,95,113	2.10	16 (24%)
25	CLA	C	510	-	69,73,73	1.36	12 (17%)	83,113,113	1.79	16 (19%)
31	PL9	A	409	-	13,13,55	0.96	0	17,17,69	0.72	0
25	CLA	N	603	-	69,73,73	1.38	12 (17%)	83,113,113	1.75	18 (21%)
25	CLA	N	602	21	69,73,73	1.36	12 (17%)	83,113,113	1.72	19 (22%)
24	CHL	R	605	-	50,54,74	1.54	8 (16%)	56,90,114	2.10	14 (25%)
25	CLA	r	614	22	49,53,73	1.63	10 (20%)	59,89,113	1.75	15 (25%)
25	CLA	y	311	21	64,68,73	1.44	11 (17%)	77,107,113	1.76	16 (20%)
25	CLA	b	609	5	69,73,73	1.38	11 (15%)	83,113,113	1.80	19 (22%)
24	CHL	r	613	22	46,50,74	1.48	6 (13%)	51,85,114	2.16	10 (19%)
25	CLA	D	402	7	69,73,73	1.41	12 (17%)	83,113,113	1.79	18 (21%)
25	CLA	G	613	21	69,73,73	1.42	10 (14%)	83,113,113	1.96	16 (19%)
25	CLA	b	606	5	69,73,73	1.36	11 (15%)	83,113,113	1.83	15 (18%)
25	CLA	C	504	-	64,68,73	1.60	7 (10%)	77,107,113	2.83	24 (31%)
35	DGD	A	415	-	60,60,67	0.49	0	74,74,81	1.22	5 (6%)
25	CLA	N	614	21	52,56,73	1.61	10 (19%)	62,92,113	2.15	16 (25%)
25	CLA	C	506	6	69,73,73	1.38	11 (15%)	83,113,113	1.65	17 (20%)
26	LHG	2	606	25	46,46,48	0.44	0	49,52,54	1.19	4 (8%)
25	CLA	2	604	26,2	59,63,73	1.61	8 (13%)	71,101,113	2.32	23 (32%)
39	LUT	g	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.44	4 (7%)
25	CLA	6	602	2	64,68,73	1.64	7 (10%)	77,107,113	2.77	29 (37%)
25	CLA	a	402	4	69,73,73	1.37	12 (17%)	83,113,113	1.78	17 (20%)
39	LUT	s	316	-	42,43,43	0.89	4 (9%)	51,60,60	1.65	8 (15%)
30	LMG	c	520	-	51,51,55	0.45	0	59,59,63	1.23	4 (6%)
25	CLA	R	608	22	62,66,73	1.44	11 (17%)	74,104,113	1.81	16 (21%)
32	AJP	S	319	-	48,48,95	0.77	0	71,78,149	4.19	29 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	608	5	69,73,73	1.37	12 (17%)	83,113,113	1.78	16 (19%)
25	CLA	S	309	20	49,53,73	1.67	11 (22%)	59,89,113	2.01	14 (23%)
25	CLA	A	402	-	69,73,73	1.39	12 (17%)	83,113,113	1.85	17 (20%)
31	PL9	d	405	-	55,55,55	0.50	0	68,69,69	0.78	0
24	CHL	n	609	21	70,74,74	1.34	8 (11%)	80,114,114	1.66	14 (17%)
25	CLA	R	602	22	64,68,73	1.44	11 (17%)	77,107,113	1.86	19 (24%)
25	CLA	r	604	-	52,56,73	1.59	9 (17%)	62,92,113	2.07	20 (32%)
39	LUT	n	615	-	42,43,43	0.88	2 (4%)	51,60,60	1.72	9 (17%)
24	CHL	6	601	2	68,72,74	1.37	8 (11%)	77,111,114	2.00	15 (19%)
30	LMG	b	620	25	51,51,55	0.44	0	59,59,63	1.20	4 (6%)
25	CLA	b	610	-	69,73,73	1.40	11 (15%)	83,113,113	1.62	14 (16%)
24	CHL	G	609	21	65,69,74	1.39	8 (12%)	74,108,114	1.87	14 (18%)
24	CHL	y	306	21	52,56,74	1.47	7 (13%)	58,92,114	1.98	12 (20%)
24	CHL	n	605	21	52,56,74	1.46	6 (11%)	58,92,114	1.98	14 (24%)
25	CLA	s	303	20	65,69,73	1.42	11 (16%)	78,108,113	1.71	16 (20%)
24	CHL	Y	309	-	70,74,74	1.33	7 (10%)	80,114,114	1.69	14 (17%)
25	CLA	n	603	-	69,73,73	1.38	12 (17%)	83,113,113	1.75	18 (21%)
40	NEX	r	617	-	38,46,46	1.68	8 (21%)	50,70,70	3.05	17 (34%)
25	CLA	b	616	5	69,73,73	1.37	11 (15%)	83,113,113	1.69	14 (16%)
25	CLA	Y	304	-	69,73,73	1.39	12 (17%)	83,113,113	1.75	17 (20%)
26	LHG	c	517	-	48,48,48	0.43	0	51,54,54	1.18	4 (7%)
30	LMG	a	411	-	40,40,55	0.48	0	48,48,63	1.28	4 (8%)
24	CHL	G	605	21	50,54,74	1.53	8 (16%)	56,90,114	1.96	10 (17%)
40	NEX	Y	318	-	38,46,46	1.73	8 (21%)	50,70,70	2.21	18 (36%)
39	LUT	g	615	-	42,43,43	0.86	2 (4%)	51,60,60	1.65	8 (15%)
24	CHL	y	302	21	70,74,74	1.32	8 (11%)	80,114,114	1.76	16 (20%)
25	CLA	r	609	22	69,73,73	1.40	11 (15%)	83,113,113	1.72	17 (20%)
25	CLA	c	513	6	69,73,73	1.37	12 (17%)	83,113,113	1.80	18 (21%)
32	AJP	y	320	-	48,48,95	0.80	1 (2%)	71,78,149	4.19	33 (46%)
25	CLA	r	610	26	53,57,73	1.80	7 (13%)	62,93,113	3.21	19 (30%)
24	CHL	g	608	-	70,74,74	1.34	8 (11%)	80,114,114	1.73	13 (16%)
24	CHL	r	605	-	50,54,74	1.54	8 (16%)	56,90,114	2.11	14 (25%)
25	CLA	B	601	-	69,73,73	1.39	10 (14%)	83,113,113	1.97	18 (21%)
39	LUT	S	315	-	42,43,43	0.92	3 (7%)	51,60,60	1.57	8 (15%)
28	BCR	z	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.29	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	c	519	6	48,48,48	0.45	0	51,54,54	1.18	4 (7%)
26	LHG	N	618	25	48,48,48	0.43	0	51,54,54	1.15	4 (7%)
32	AJP	y	323	-	48,48,95	0.74	0	71,78,149	4.38	30 (42%)
28	BCR	b	619	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	8 (14%)
25	CLA	R	601	-	53,57,73	1.77	9 (16%)	62,93,113	3.25	20 (32%)
24	CHL	n	608	-	70,74,74	1.33	7 (10%)	80,114,114	1.72	10 (12%)
26	LHG	c	518	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
25	CLA	b	604	5	69,73,73	1.38	11 (15%)	83,113,113	1.81	16 (19%)
25	CLA	n	602	21	69,73,73	1.36	12 (17%)	83,113,113	1.72	19 (22%)
24	CHL	N	607	-	70,74,74	1.34	7 (10%)	80,114,114	1.73	13 (16%)
24	CHL	l	302	1	50,54,74	1.57	8 (16%)	56,90,114	2.07	11 (19%)
25	CLA	c	508	6	69,73,73	1.38	10 (14%)	83,113,113	1.93	17 (20%)
25	CLA	d	403	-	69,73,73	1.55	8 (11%)	83,113,113	2.82	24 (28%)
25	CLA	B	616	5	69,73,73	1.37	11 (15%)	83,113,113	1.69	14 (16%)
25	CLA	C	512	-	69,73,73	1.37	12 (17%)	83,113,113	1.78	19 (22%)
39	LUT	Y	316	-	42,43,43	0.83	2 (4%)	51,60,60	1.73	9 (17%)
25	CLA	g	602	21	69,73,73	1.37	12 (17%)	83,113,113	1.76	17 (20%)
25	CLA	Y	315	21	49,53,73	1.63	11 (22%)	59,89,113	1.76	14 (23%)
25	CLA	G	602	21	69,73,73	1.37	12 (17%)	83,113,113	1.76	17 (20%)
31	PL9	D	405	-	55,55,55	0.50	0	68,69,69	0.79	0
24	CHL	r	607	-	65,69,74	1.39	8 (12%)	74,108,114	1.85	14 (18%)
25	CLA	y	304	-	69,73,73	1.39	12 (17%)	83,113,113	1.75	17 (20%)
25	CLA	b	603	-	69,73,73	1.38	11 (15%)	83,113,113	1.70	16 (19%)
25	CLA	b	615	5	69,73,73	1.41	9 (13%)	83,113,113	1.70	17 (20%)
25	CLA	c	509	6	69,73,73	1.39	12 (17%)	83,113,113	1.78	12 (14%)
40	NEX	y	318	-	38,46,46	1.73	9 (23%)	50,70,70	2.21	18 (36%)
24	CHL	N	609	21	70,74,74	1.34	7 (10%)	80,114,114	1.66	14 (17%)
25	CLA	b	613	5	69,73,73	1.38	11 (15%)	83,113,113	1.63	15 (18%)
25	CLA	G	614	21	52,56,73	1.56	11 (21%)	62,92,113	1.79	15 (24%)
27	PHO	A	404	-	58,69,69	0.49	0	56,99,99	1.64	9 (16%)
28	BCR	A	406	-	41,41,41	1.16	2 (4%)	56,56,56	1.34	10 (17%)
25	CLA	d	402	7	69,73,73	1.41	12 (17%)	83,113,113	1.79	18 (21%)
30	LMG	C	520	-	51,51,55	0.45	0	59,59,63	1.23	4 (6%)
25	CLA	r	611	-	53,57,73	1.88	9 (16%)	62,93,113	3.55	25 (40%)
25	CLA	B	604	5	69,73,73	1.38	12 (17%)	83,113,113	1.80	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	R	618	25	41,41,48	0.45	0	44,47,54	1.23	4 (9%)
32	AJP	y	321	-	48,48,95	0.76	0	71,78,149	4.21	27 (38%)
39	LUT	G	615	-	42,43,43	0.87	3 (7%)	51,60,60	1.65	8 (15%)
25	CLA	c	501	-	69,73,73	1.51	7 (10%)	83,113,113	2.63	24 (28%)
25	CLA	Y	314	21	69,73,73	1.36	10 (14%)	83,113,113	1.90	15 (18%)
25	CLA	a	403	-	69,73,73	1.39	12 (17%)	83,113,113	1.85	17 (20%)
24	CHL	y	309	-	70,74,74	1.33	7 (10%)	80,114,114	1.68	14 (17%)
25	CLA	Y	312	26	64,68,73	1.45	12 (18%)	77,107,113	1.68	17 (22%)
26	LHG	y	319	25	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
26	LHG	S	301	-	48,48,48	0.44	0	51,54,54	1.16	4 (7%)
25	CLA	B	615	5	69,73,73	1.41	9 (13%)	83,113,113	1.70	17 (20%)
24	CHL	S	306	-	50,54,74	1.53	8 (16%)	56,90,114	2.04	15 (26%)
25	CLA	B	613	5	69,73,73	1.38	11 (15%)	83,113,113	1.62	15 (18%)
25	CLA	S	311	26	60,64,73	1.48	11 (18%)	72,102,113	2.19	14 (19%)
28	BCR	B	617	-	41,41,41	1.18	2 (4%)	56,56,56	1.30	6 (10%)
25	CLA	g	614	21	52,56,73	1.56	11 (21%)	62,92,113	1.79	15 (24%)
25	CLA	b	605	5	69,73,73	1.37	11 (15%)	83,113,113	1.92	14 (16%)
25	CLA	a	406	4	64,68,73	1.43	12 (18%)	77,107,113	1.85	15 (19%)
25	CLA	B	607	-	69,73,73	1.36	11 (15%)	83,113,113	1.78	15 (18%)
40	NEX	N	617	-	38,46,46	1.67	7 (18%)	50,70,70	2.43	18 (36%)
25	CLA	S	310	20	59,63,73	1.51	11 (18%)	71,101,113	1.75	13 (18%)
26	LHG	b	625	-	45,45,48	0.44	0	48,51,54	1.19	4 (8%)
40	NEX	R	617	-	38,46,46	1.68	7 (18%)	50,70,70	3.06	17 (34%)
25	CLA	r	612	22	64,68,73	1.46	11 (17%)	77,107,113	2.12	20 (25%)
25	CLA	s	309	20	49,53,73	1.66	11 (22%)	59,89,113	2.00	14 (23%)
26	LHG	s	318	25	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
26	LHG	l	103	-	48,48,48	0.44	0	51,54,54	1.17	4 (7%)
32	AJP	y	324	-	48,48,95	0.71	0	71,78,149	4.32	32 (45%)
25	CLA	R	603	22	64,68,73	1.60	7 (10%)	77,107,113	2.87	22 (28%)
39	LUT	s	315	-	42,43,43	0.92	3 (7%)	51,60,60	1.57	8 (15%)
25	CLA	R	609	22	69,73,73	1.40	11 (15%)	83,113,113	1.72	17 (20%)
40	NEX	g	617	25	38,46,46	1.61	8 (21%)	50,70,70	2.77	15 (30%)
25	CLA	b	611	5	69,73,73	1.36	11 (15%)	83,113,113	1.82	17 (20%)
30	LMG	B	623	-	55,55,55	0.43	0	63,63,63	1.23	4 (6%)
24	CHL	1	301	1	50,54,74	1.54	8 (16%)	56,90,114	1.94	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	B	626	-	63,63,67	0.49	0	77,77,81	1.29	6 (7%)
26	LHG	n	618	25	48,48,48	0.43	0	51,54,54	1.15	4 (7%)
26	LHG	C	517	-	48,48,48	0.44	0	51,54,54	1.18	4 (7%)
25	CLA	N	613	21	64,68,73	1.45	10 (15%)	77,107,113	1.96	19 (24%)
33	BCT	A	413	34	2,3,3	1.20	0	2,3,3	4.33	2 (100%)
25	CLA	c	506	6	69,73,73	1.39	11 (15%)	83,113,113	1.66	17 (20%)
35	DGD	c	516	-	63,63,67	0.52	0	77,77,81	1.23	6 (7%)
39	LUT	Y	317	-	42,43,43	0.92	4 (9%)	51,60,60	1.50	6 (11%)
32	AJP	Y	323	-	48,48,95	0.74	0	71,78,149	4.38	30 (42%)
39	LUT	y	317	-	42,43,43	0.92	3 (7%)	51,60,60	1.50	6 (11%)
30	LMG	D	407	-	46,46,55	0.44	0	54,54,63	1.21	4 (7%)
28	BCR	D	404	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	5 (8%)
24	CHL	g	605	21	50,54,74	1.52	8 (16%)	56,90,114	1.97	11 (19%)
25	CLA	s	310	20	59,63,73	1.51	11 (18%)	71,101,113	1.75	12 (16%)
26	LHG	6	606	25	46,46,48	0.44	0	49,52,54	1.19	4 (8%)
25	CLA	C	505	6	69,73,73	1.37	11 (15%)	83,113,113	1.73	15 (18%)
25	CLA	A	401	4	69,73,73	1.37	12 (17%)	83,113,113	1.78	17 (20%)
25	CLA	2	602	2	64,68,73	1.64	7 (10%)	77,107,113	2.77	29 (37%)
24	CHL	n	606	-	50,54,74	1.52	8 (16%)	56,90,114	2.06	15 (26%)
25	CLA	y	315	21	49,53,73	1.64	11 (22%)	59,89,113	1.76	14 (23%)
25	CLA	R	612	22	64,68,73	1.46	11 (17%)	77,107,113	2.12	20 (25%)
28	BCR	I	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.28	9 (16%)
25	CLA	B	612	5	69,73,73	1.38	12 (17%)	83,113,113	1.78	16 (19%)
32	AJP	y	322	-	48,48,95	0.72	0	71,78,149	4.10	30 (42%)
24	CHL	S	308	-	50,54,74	1.54	8 (16%)	56,90,114	2.09	13 (23%)
25	CLA	B	609	5	69,73,73	1.38	11 (15%)	83,113,113	1.80	19 (22%)
28	BCR	C	514	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
25	CLA	b	601	-	69,73,73	1.39	9 (13%)	83,113,113	1.97	18 (21%)
24	CHL	Y	302	21	70,74,74	1.32	8 (11%)	80,114,114	1.76	16 (20%)
25	CLA	6	604	26,2	59,63,73	1.61	8 (13%)	71,101,113	2.32	23 (32%)
29	SQD	A	411	-	53,54,54	0.80	1 (1%)	62,65,65	0.97	2 (3%)
24	CHL	g	606	-	54,58,74	1.46	6 (11%)	59,94,114	2.06	12 (20%)
35	DGD	b	626	-	63,63,67	0.49	0	77,77,81	1.29	6 (7%)

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
39	LUT	R	615	-	-	4/29/67/67	0/2/2/2
25	CLA	s	313	20	-	12/27/103/115	-
25	CLA	N	612	21	-	18/33/109/115	-
28	BCR	k	101	-	-	4/29/63/63	0/2/2/2
28	BCR	a	407	-	-	5/29/63/63	0/2/2/2
24	CHL	G	606	-	-	4/22/98/117	-
32	AJP	N	620	-	16/16/19/38	4/6/117/220	0/7/7/11
32	AJP	s	319	-	15/15/19/38	3/6/117/220	0/7/7/11
32	AJP	n	619	-	15/15/19/38	1/6/117/220	0/7/7/11
25	CLA	S	312	20	-	9/20/96/115	-
32	AJP	G	618	-	15/15/19/38	3/6/117/220	0/7/7/11
25	CLA	Y	303	21	-	12/39/115/115	-
24	CHL	G	608	-	-	22/41/117/117	-
39	LUT	N	616	-	-	4/29/67/67	0/2/2/2
29	SQD	a	408	-	-	21/45/65/69	0/1/1/1
24	CHL	N	606	-	-	4/17/93/117	-
24	CHL	R	606	-	-	13/17/93/117	-
24	CHL	N	605	21	-	7/20/96/117	-
28	BCR	b	618	-	-	3/29/63/63	0/2/2/2
24	CHL	S	307	-	-	9/17/93/117	-
25	CLA	R	604	-	-	6/19/95/115	-
32	AJP	a	413	-	34/34/38/38	9/28/220/220	0/11/11/11
25	CLA	S	304	-	-	4/15/91/115	-
24	CHL	g	601	21	-	24/41/117/117	-
24	CHL	Y	310	21	-	11/29/105/117	-
28	BCR	i	101	-	-	4/29/63/63	0/2/2/2
25	CLA	G	604	40	-	13/21/97/115	-
25	CLA	D	403	-	-	13/39/115/115	-
24	CHL	y	310	21	-	11/29/105/117	-
40	NEX	n	617	-	-	10/27/83/83	0/3/3/3
29	SQD	L	101	-	-	13/37/57/69	0/1/1/1
25	CLA	b	602	5	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMG	A	410	-	-	13/35/55/70	0/1/1/1
26	LHG	B	621	-	-	19/51/51/53	-
26	LHG	s	301	-	-	21/53/53/53	-
40	NEX	s	317	-	-	6/27/83/83	0/3/3/3
24	CHL	s	306	-	-	7/17/93/117	-
24	CHL	n	601	21	-	15/29/105/117	-
25	CLA	B	606	5	-	13/39/115/115	-
32	AJP	N	619	-	15/15/19/38	1/6/117/220	0/7/7/11
25	CLA	n	610	21	-	17/39/115/115	-
25	CLA	G	603	-	-	14/33/109/115	-
25	CLA	Y	313	21	-	11/33/109/115	-
25	CLA	g	612	21	-	11/33/109/115	-
26	LHG	L	102	-	-	29/53/53/53	-
25	CLA	b	607	-	-	16/39/115/115	-
35	DGD	a	401	-	-	27/48/88/95	0/2/2/2
25	CLA	y	303	21	-	12/39/115/115	-
32	AJP	n	620	-	16/16/19/38	4/6/117/220	0/7/7/11
25	CLA	g	613	21	-	16/39/115/115	-
25	CLA	C	509	6	-	9/39/115/115	-
38	HEM	F	101	9	-	3/14/54/54	-
29	SQD	L	103	-	-	27/49/69/69	0/1/1/1
25	CLA	n	613	21	-	23/33/109/115	-
24	CHL	Y	307	21	-	3/22/98/117	-
31	PL9	a	410	-	-	2/5/18/73	0/1/1/1
25	CLA	B	603	-	-	13/39/115/115	-
24	CHL	y	308	-	-	10/32/108/117	-
26	LHG	B	622	-	-	18/53/53/53	-
29	SQD	A	407	-	-	21/45/65/69	0/1/1/1
24	CHL	s	307	-	-	9/17/93/117	-
39	LUT	y	316	-	-	3/29/67/67	0/2/2/2
27	PHO	A	403	-	-	12/37/103/103	0/5/6/6
24	CHL	N	601	21	-	15/29/105/117	-
39	LUT	r	615	-	-	4/29/67/67	0/2/2/2
25	CLA	N	610	21	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	AJP	B	624	-	34/34/38/38	14/28/220/220	0/11/11/11
24	CHL	5	302	1	-	5/17/93/117	-
32	AJP	b	624	-	34/34/38/38	14/28/220/220	0/11/11/11
26	LHG	B	625	-	-	14/50/50/53	-
25	CLA	g	610	-	-	14/38/114/115	-
28	BCR	B	618	-	-	3/29/63/63	0/2/2/2
30	LMG	B	620	25	-	15/46/66/70	0/1/1/1
25	CLA	r	603	22	-	13/33/109/115	-
25	CLA	r	602	22	-	10/33/109/115	-
25	CLA	A	405	4	-	11/33/109/115	-
25	CLA	r	601	-	-	13/20/96/115	-
25	CLA	n	611	26	-	14/33/109/115	-
25	CLA	b	608	5	-	14/39/115/115	-
25	CLA	Y	311	21	-	11/33/109/115	-
24	CHL	Y	308	-	-	10/32/108/117	-
24	CHL	r	606	-	-	13/17/93/117	-
24	CHL	s	302	20	-	4/17/93/117	-
24	CHL	n	607	-	-	18/41/117/117	-
25	CLA	S	305	-	-	9/21/97/115	-
25	CLA	R	611	-	-	13/20/96/115	-
32	AJP	Y	322	-	15/15/19/38	3/6/117/220	0/7/7/11
26	LHG	S	318	25	-	20/53/53/53	-
24	CHL	s	308	-	-	2/17/93/117	-
38	HEM	f	101	9	-	3/14/54/54	-
24	CHL	2	603	2	-	10/17/93/117	-
24	CHL	5	301	1	-	4/17/93/117	-
25	CLA	g	611	-	-	16/33/109/115	-
30	LMG	b	623	-	-	28/50/70/70	0/1/1/1
25	CLA	B	611	5	-	12/39/115/115	-
39	LUT	n	616	-	-	4/29/67/67	0/2/2/2
25	CLA	G	612	21	-	11/33/109/115	-
26	LHG	C	518	-	-	12/53/53/53	-
28	BCR	T	101	16	-	17/29/63/63	0/2/2/2
25	CLA	s	314	20	-	3/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	R	613	22	-	6/12/88/117	-
27	PHO	a	405	-	-	1/37/103/103	0/5/6/6
25	CLA	C	511	6	-	9/39/115/115	-
39	LUT	G	616	-	-	0/29/67/67	0/2/2/2
24	CHL	g	607	-	-	6/17/93/117	-
24	CHL	G	601	21	-	24/41/117/117	-
28	BCR	c	514	-	-	2/29/63/63	0/2/2/2
30	LMG	d	407	-	-	16/41/61/70	0/1/1/1
25	CLA	g	604	40	-	13/21/97/115	-
24	CHL	R	607	-	-	15/35/111/117	-
26	LHG	y	301	21	-	16/53/53/53	-
25	CLA	n	614	21	-	4/19/95/115	-
25	CLA	c	504	-	-	14/33/109/115	-
25	CLA	n	612	21	-	18/33/109/115	-
26	LHG	D	406	-	-	18/53/53/53	-
25	CLA	y	314	21	-	16/39/115/115	-
29	SQD	l	102	-	-	13/37/57/69	0/1/1/1
25	CLA	N	611	26	-	14/33/109/115	-
24	CHL	2	601	2	-	16/39/115/117	-
25	CLA	C	503	6	-	11/39/115/115	-
35	DGD	C	515	-	-	17/44/84/95	0/2/2/2
40	NEX	S	317	-	-	6/27/83/83	0/3/3/3
28	BCR	b	617	-	-	3/29/63/63	0/2/2/2
28	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
25	CLA	C	501	-	-	7/39/115/115	-
24	CHL	g	609	21	-	10/35/111/117	-
25	CLA	C	507	-	-	17/39/115/115	-
25	CLA	r	608	22	-	17/31/107/115	-
25	CLA	R	614	22	-	8/15/91/115	-
32	AJP	Y	320	-	15/15/19/38	2/6/117/220	0/7/7/11
25	CLA	B	614	30,5	-	15/39/115/115	-
25	CLA	C	502	6	-	8/39/115/115	-
26	LHG	d	406	-	-	18/53/53/53	-
41	XAT	R	616	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	y	312	26	-	13/33/109/115	-
25	CLA	c	510	-	-	14/39/115/115	-
32	AJP	g	618	-	15/15/19/38	3/6/117/220	0/7/7/11
28	BCR	H	101	-	-	6/29/63/63	0/2/2/2
25	CLA	c	502	6	-	8/39/115/115	-
25	CLA	s	311	26	-	12/29/105/115	-
26	LHG	r	618	25	-	12/46/46/53	-
25	CLA	s	304	-	-	4/15/91/115	-
24	CHL	S	302	20	-	4/17/93/117	-
26	LHG	b	621	-	-	19/51/51/53	-
28	BCR	B	619	-	-	3/29/63/63	0/2/2/2
26	LHG	Y	301	21	-	16/53/53/53	-
25	CLA	B	605	5	-	9/39/115/115	-
25	CLA	S	313	20	-	12/27/103/115	-
25	CLA	S	303	20	-	18/35/111/115	-
28	BCR	h	101	-	-	6/29/63/63	0/2/2/2
25	CLA	2	605	2	-	10/19/95/115	-
25	CLA	6	605	2	-	10/19/95/115	-
28	BCR	t	101	16	-	17/29/63/63	0/2/2/2
25	CLA	y	305	-	-	7/21/97/115	-
32	AJP	Y	324	-	15/15/19/38	3/6/117/220	0/7/7/11
40	NEX	G	617	25	-	11/27/83/83	0/3/3/3
25	CLA	D	401	42	-	4/21/97/115	-
35	DGD	c	515	-	-	17/44/84/95	0/2/2/2
24	CHL	6	603	2	-	10/17/93/117	-
25	CLA	d	401	42	-	4/21/97/115	-
26	LHG	C	519	6	-	21/53/53/53	-
25	CLA	n	604	-	-	6/21/97/115	-
25	CLA	G	611	-	-	16/33/109/115	-
35	DGD	C	516	-	-	28/51/91/95	0/2/2/2
25	CLA	b	614	30,5	-	15/39/115/115	-
25	CLA	b	612	5	-	10/39/115/115	-
25	CLA	G	610	-	-	14/38/114/115	-
26	LHG	b	622	-	-	18/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	508	6	-	14/39/115/115	-
25	CLA	S	314	20	-	3/20/96/115	-
27	PHO	a	404	-	-	12/37/103/103	0/5/6/6
39	LUT	S	316	-	-	4/29/67/67	0/2/2/2
32	AJP	Y	321	-	16/16/19/38	4/6/117/220	0/7/7/11
25	CLA	c	503	6	-	11/39/115/115	-
25	CLA	c	512	-	-	14/39/115/115	-
30	LMG	a	409	-	-	18/43/63/70	0/1/1/1
25	CLA	Y	305	-	-	7/21/97/115	-
24	CHL	G	607	-	-	6/17/93/117	-
24	CHL	Y	306	21	-	9/20/96/117	-
28	BCR	d	404	-	-	5/29/63/63	0/2/2/2
29	SQD	a	412	-	-	22/49/69/69	0/1/1/1
39	LUT	N	615	-	-	8/29/67/67	0/2/2/2
25	CLA	B	602	5	-	14/39/115/115	-
32	AJP	A	412	-	34/34/38/38	9/28/220/220	0/11/11/11
29	SQD	l	101	-	-	27/49/69/69	0/1/1/1
26	LHG	Y	319	25	-	23/53/53/53	-
25	CLA	s	305	-	-	9/21/97/115	-
25	CLA	c	511	6	-	9/39/115/115	-
25	CLA	c	507	-	-	17/39/115/115	-
25	CLA	g	603	-	-	13/33/109/115	-
24	CHL	N	608	-	-	17/41/117/117	-
30	LMG	A	408	-	-	18/43/63/70	0/1/1/1
25	CLA	c	505	6	-	12/39/115/115	-
24	CHL	y	307	21	-	3/22/98/117	-
25	CLA	s	312	20	-	9/20/96/115	-
25	CLA	y	313	21	-	11/33/109/115	-
28	BCR	K	101	-	-	4/29/63/63	0/2/2/2
41	XAT	r	616	-	-	2/31/93/93	0/4/4/4
25	CLA	C	513	6	-	13/39/115/115	-
25	CLA	R	610	26	-	11/20/96/115	-
25	CLA	B	610	-	-	9/39/115/115	-
25	CLA	N	604	-	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	510	-	-	14/39/115/115	-
31	PL9	A	409	-	-	2/5/18/73	0/1/1/1
25	CLA	N	603	-	-	19/39/115/115	-
25	CLA	N	602	21	-	15/39/115/115	-
24	CHL	R	605	-	-	3/17/93/117	-
25	CLA	r	614	22	-	8/15/91/115	-
25	CLA	y	311	21	-	12/33/109/115	-
25	CLA	b	609	5	-	13/39/115/115	-
24	CHL	r	613	22	-	6/12/88/117	-
25	CLA	D	402	7	-	10/39/115/115	-
25	CLA	G	613	21	-	16/39/115/115	-
25	CLA	b	606	5	-	13/39/115/115	-
25	CLA	C	504	-	-	14/33/109/115	-
35	DGD	A	415	-	-	27/48/88/95	0/2/2/2
25	CLA	N	614	21	-	4/19/95/115	-
25	CLA	C	506	6	-	13/39/115/115	-
26	LHG	2	606	25	-	25/51/51/53	-
25	CLA	2	604	26,2	-	11/27/103/115	-
39	LUT	g	616	-	-	0/29/67/67	0/2/2/2
25	CLA	6	602	2	-	15/33/109/115	-
25	CLA	a	402	4	-	7/39/115/115	-
39	LUT	s	316	-	-	4/29/67/67	0/2/2/2
30	LMG	c	520	-	-	18/46/66/70	0/1/1/1
25	CLA	R	608	22	-	17/31/107/115	-
32	AJP	S	319	-	15/15/19/38	3/6/117/220	0/7/7/11
25	CLA	B	608	5	-	14/39/115/115	-
25	CLA	S	309	20	-	7/15/91/115	-
25	CLA	A	402	-	-	9/39/115/115	-
31	PL9	d	405	-	-	5/53/73/73	0/1/1/1
24	CHL	n	609	21	-	15/41/117/117	-
25	CLA	R	602	22	-	10/33/109/115	-
25	CLA	r	604	-	-	6/19/95/115	-
39	LUT	n	615	-	-	8/29/67/67	0/2/2/2
24	CHL	6	601	2	-	16/39/115/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMG	b	620	25	-	15/46/66/70	0/1/1/1
25	CLA	b	610	-	-	9/39/115/115	-
24	CHL	G	609	21	-	10/35/111/117	-
24	CHL	y	306	21	-	9/20/96/117	-
24	CHL	n	605	21	-	7/20/96/117	-
25	CLA	s	303	20	-	18/35/111/115	-
24	CHL	Y	309	-	-	22/41/117/117	-
25	CLA	n	603	-	-	19/39/115/115	-
40	NEX	r	617	-	-	6/27/83/83	0/3/3/3
25	CLA	b	616	5	-	19/39/115/115	-
25	CLA	Y	304	-	-	22/39/115/115	-
26	LHG	c	517	-	-	17/53/53/53	-
30	LMG	a	411	-	-	13/35/55/70	0/1/1/1
24	CHL	G	605	21	-	9/17/93/117	-
40	NEX	Y	318	-	-	7/27/83/83	1/3/3/3
39	LUT	g	615	-	-	5/29/67/67	0/2/2/2
24	CHL	y	302	21	-	23/41/117/117	-
25	CLA	r	609	22	-	16/39/115/115	-
25	CLA	c	513	6	-	13/39/115/115	-
32	AJP	y	320	-	15/15/19/38	2/6/117/220	0/7/7/11
25	CLA	r	610	26	-	11/20/96/115	-
24	CHL	g	608	-	-	22/41/117/117	-
24	CHL	r	605	-	-	3/17/93/117	-
25	CLA	B	601	-	-	18/39/115/115	-
39	LUT	S	315	-	-	4/29/67/67	0/2/2/2
28	BCR	z	101	-	-	8/29/63/63	0/2/2/2
26	LHG	c	519	6	-	21/53/53/53	-
26	LHG	N	618	25	-	29/53/53/53	-
32	AJP	y	323	-	15/15/19/38	3/6/117/220	0/7/7/11
28	BCR	b	619	-	-	3/29/63/63	0/2/2/2
25	CLA	R	601	-	-	13/20/96/115	-
24	CHL	n	608	-	-	17/41/117/117	-
26	LHG	c	518	-	-	12/53/53/53	-
25	CLA	b	604	5	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	n	602	21	-	15/39/115/115	-
24	CHL	N	607	-	-	18/41/117/117	-
24	CHL	1	302	1	-	5/17/93/117	-
25	CLA	c	508	6	-	14/39/115/115	-
25	CLA	d	403	-	-	13/39/115/115	-
25	CLA	B	616	5	-	19/39/115/115	-
25	CLA	C	512	-	-	14/39/115/115	-
39	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
25	CLA	g	602	21	-	17/39/115/115	-
25	CLA	Y	315	21	-	10/15/91/115	-
25	CLA	G	602	21	-	17/39/115/115	-
31	PL9	D	405	-	-	5/53/73/73	0/1/1/1
24	CHL	r	607	-	-	15/35/111/117	-
25	CLA	y	304	-	-	22/39/115/115	-
25	CLA	b	603	-	-	13/39/115/115	-
25	CLA	b	615	5	-	10/39/115/115	-
25	CLA	c	509	6	-	9/39/115/115	-
40	NEX	y	318	-	-	7/27/83/83	1/3/3/3
24	CHL	N	609	21	-	15/41/117/117	-
25	CLA	b	613	5	-	15/39/115/115	-
25	CLA	G	614	21	-	9/19/95/115	-
27	PHO	A	404	-	-	1/37/103/103	0/5/6/6
28	BCR	A	406	-	-	5/29/63/63	0/2/2/2
25	CLA	d	402	7	-	10/39/115/115	-
30	LMG	C	520	-	-	18/46/66/70	0/1/1/1
25	CLA	r	611	-	-	13/20/96/115	-
25	CLA	B	604	5	-	17/39/115/115	-
26	LHG	R	618	25	-	12/46/46/53	-
32	AJP	y	321	-	16/16/19/38	4/6/117/220	0/7/7/11
39	LUT	G	615	-	-	5/29/67/67	0/2/2/2
25	CLA	c	501	-	-	7/39/115/115	-
25	CLA	Y	314	21	-	16/39/115/115	-
25	CLA	a	403	-	-	9/39/115/115	-
24	CHL	y	309	-	-	22/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	Y	312	26	-	13/33/109/115	-
26	LHG	y	319	25	-	23/53/53/53	-
26	LHG	S	301	-	-	21/53/53/53	-
25	CLA	B	615	5	-	10/39/115/115	-
24	CHL	S	306	-	-	7/17/93/117	-
25	CLA	B	613	5	-	15/39/115/115	-
25	CLA	S	311	26	-	12/29/105/115	-
28	BCR	B	617	-	-	3/29/63/63	0/2/2/2
25	CLA	g	614	21	-	9/19/95/115	-
25	CLA	b	605	5	-	9/39/115/115	-
25	CLA	a	406	4	-	11/33/109/115	-
25	CLA	B	607	-	-	16/39/115/115	-
40	NEX	N	617	-	-	10/27/83/83	0/3/3/3
25	CLA	S	310	20	-	11/27/103/115	-
26	LHG	b	625	-	-	14/50/50/53	-
40	NEX	R	617	-	-	6/27/83/83	0/3/3/3
25	CLA	r	612	22	-	13/33/109/115	-
25	CLA	s	309	20	-	7/15/91/115	-
26	LHG	s	318	25	-	21/53/53/53	-
26	LHG	l	103	-	-	29/53/53/53	-
32	AJP	y	324	-	15/15/19/38	3/6/117/220	0/7/7/11
25	CLA	R	603	22	-	13/33/109/115	-
39	LUT	s	315	-	-	4/29/67/67	0/2/2/2
25	CLA	R	609	22	-	16/39/115/115	-
40	NEX	g	617	25	-	11/27/83/83	0/3/3/3
25	CLA	b	611	5	-	12/39/115/115	-
30	LMG	B	623	-	-	28/50/70/70	0/1/1/1
24	CHL	l	301	1	-	4/17/93/117	-
35	DGD	B	626	-	-	23/51/91/95	0/2/2/2
26	LHG	n	618	25	-	29/53/53/53	-
26	LHG	C	517	-	-	16/53/53/53	-
25	CLA	N	613	21	-	23/33/109/115	-
25	CLA	c	506	6	-	13/39/115/115	-
35	DGD	c	516	-	-	28/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LUT	Y	317	-	-	3/29/67/67	0/2/2/2
32	AJP	Y	323	-	15/15/19/38	3/6/117/220	0/7/7/11
39	LUT	y	317	-	-	3/29/67/67	0/2/2/2
30	LMG	D	407	-	-	16/41/61/70	0/1/1/1
28	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	CHL	g	605	21	-	9/17/93/117	-
25	CLA	s	310	20	-	11/27/103/115	-
26	LHG	6	606	25	-	25/51/51/53	-
25	CLA	C	505	6	-	12/39/115/115	-
25	CLA	A	401	4	-	7/39/115/115	-
25	CLA	2	602	2	-	15/33/109/115	-
24	CHL	n	606	-	-	4/17/93/117	-
25	CLA	y	315	21	-	10/15/91/115	-
25	CLA	R	612	22	-	13/33/109/115	-
28	BCR	I	101	-	-	5/29/63/63	0/2/2/2
25	CLA	B	612	5	-	10/39/115/115	-
32	AJP	y	322	-	15/15/19/38	3/6/117/220	0/7/7/11
24	CHL	S	308	-	-	2/17/93/117	-
25	CLA	B	609	5	-	13/39/115/115	-
28	BCR	C	514	-	-	2/29/63/63	0/2/2/2
25	CLA	b	601	-	-	18/39/115/115	-
24	CHL	Y	302	21	-	23/41/117/117	-
25	CLA	6	604	26,2	-	11/27/103/115	-
29	SQD	A	411	-	-	22/49/69/69	0/1/1/1
24	CHL	g	606	-	-	4/22/98/117	-
35	DGD	b	626	-	-	23/51/91/95	0/2/2/2

The worst 5 of 2402 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	F	101	HEM	FE-NB	14.44	2.39	1.94
38	f	101	HEM	FE-NB	14.44	2.39	1.94
25	R	611	CLA	MG-ND	-6.76	1.92	2.05
25	r	611	CLA	MG-ND	-6.71	1.92	2.05
25	R	611	CLA	MG-NB	-6.50	1.92	2.05

The worst 5 of 5149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	305	CLA	C4A-NA-C1A	-18.81	98.25	106.71
25	S	305	CLA	C4A-NA-C1A	-18.75	98.28	106.71
25	r	601	CLA	C4A-NA-C1A	-17.30	98.93	106.71
32	Y	320	AJP	O09-C08-C10	17.23	145.62	110.17
32	y	320	AJP	O09-C08-C10	17.23	145.62	110.17

5 of 410 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	A	412	AJP	C19
32	A	412	AJP	C02
32	A	412	AJP	C36
32	A	412	AJP	C15
32	A	412	AJP	C59

5 of 4215 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	302	CHL	C1A-C2A-CAA-CBA
24	1	302	CHL	C3A-C2A-CAA-CBA
24	2	601	CHL	C1C-C2C-CMC-OMC
24	2	601	CHL	C3C-C2C-CMC-OMC
24	2	601	CHL	CHA-CBD-CGD-O2D

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	Y	318	NEX	C1-C2-C3-C4-C5-C6
40	y	318	NEX	C1-C2-C3-C4-C5-C6

356 monomers are involved in 3261 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	R	615	LUT	6	0
25	s	313	CLA	9	0
25	N	612	CLA	10	0
28	k	101	BCR	9	0
28	a	407	BCR	5	0
24	G	606	CHL	19	0
32	N	620	AJP	1	0
32	s	319	AJP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	n	619	AJP	2	0
25	S	312	CLA	9	0
25	Y	303	CLA	26	0
24	G	608	CHL	19	0
39	N	616	LUT	15	0
29	a	408	SQD	6	0
24	N	606	CHL	18	0
24	R	606	CHL	2	0
24	N	605	CHL	5	0
28	b	618	BCR	8	0
24	S	307	CHL	6	0
25	R	604	CLA	8	0
25	S	304	CLA	12	0
24	g	601	CHL	15	0
24	Y	310	CHL	17	0
28	i	101	BCR	20	0
25	G	604	CLA	12	0
25	D	403	CLA	15	0
24	y	310	CHL	18	0
40	n	617	NEX	13	0
29	L	101	SQD	19	0
25	b	602	CLA	9	0
30	A	410	LMG	3	0
26	B	621	LHG	3	0
26	s	301	LHG	9	0
40	s	317	NEX	5	0
24	s	306	CHL	11	0
24	n	601	CHL	16	0
25	B	606	CLA	15	0
32	N	619	AJP	2	0
25	n	610	CLA	33	0
25	G	603	CLA	12	0
25	Y	313	CLA	9	0
25	g	612	CLA	9	0
26	L	102	LHG	5	0
25	b	607	CLA	14	0
35	a	401	DGD	3	0
25	y	303	CLA	24	0
25	g	613	CLA	17	0
32	n	620	AJP	1	0
25	C	509	CLA	7	0
38	F	101	HEM	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	L	103	SQD	6	0
25	n	613	CLA	28	0
24	Y	307	CHL	14	0
31	a	410	PL9	2	0
25	B	603	CLA	6	0
24	y	308	CHL	14	0
26	B	622	LHG	8	0
29	A	407	SQD	8	0
24	s	307	CHL	7	0
39	y	316	LUT	13	0
27	A	403	PHO	13	0
24	N	601	CHL	18	0
39	r	615	LUT	8	0
25	N	610	CLA	34	0
24	5	302	CHL	8	0
26	B	625	LHG	7	0
25	g	610	CLA	40	0
28	B	618	BCR	7	0
30	B	620	LMG	5	0
25	r	603	CLA	17	0
25	r	602	CLA	14	0
25	A	405	CLA	9	0
25	r	601	CLA	17	0
25	n	611	CLA	7	0
25	b	608	CLA	9	0
25	Y	311	CLA	25	0
24	Y	308	CHL	17	0
24	r	606	CHL	2	0
24	s	302	CHL	7	0
24	n	607	CHL	50	0
25	S	305	CLA	14	0
25	R	611	CLA	3	0
26	S	318	LHG	5	0
32	Y	322	AJP	2	0
24	s	308	CHL	9	0
38	f	101	HEM	8	0
24	2	603	CHL	21	0
24	5	301	CHL	9	0
25	g	611	CLA	14	0
30	b	623	LMG	5	0
25	B	611	CLA	7	0
39	n	616	LUT	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	G	612	CLA	8	0
26	C	518	LHG	3	0
28	T	101	BCR	20	0
25	s	314	CLA	10	0
24	R	613	CHL	4	0
27	a	405	PHO	14	0
25	C	511	CLA	20	0
39	G	616	LUT	15	0
24	g	607	CHL	11	0
24	G	601	CHL	17	0
28	c	514	BCR	7	0
30	d	407	LMG	3	0
25	g	604	CLA	12	0
24	R	607	CHL	9	0
26	y	301	LHG	12	0
25	n	614	CLA	6	0
25	c	504	CLA	15	0
25	n	612	CLA	10	0
26	D	406	LHG	10	0
25	y	314	CLA	17	0
29	l	102	SQD	20	0
25	N	611	CLA	7	0
24	2	601	CHL	8	0
25	C	503	CLA	4	0
35	C	515	DGD	8	0
40	S	317	NEX	6	0
28	b	617	BCR	7	0
28	Z	101	BCR	5	0
25	C	501	CLA	18	0
24	g	609	CHL	10	0
25	C	507	CLA	6	0
25	r	608	CLA	17	0
25	R	614	CLA	11	0
25	B	614	CLA	12	0
25	C	502	CLA	12	0
32	Y	320	AJP	3	0
26	d	406	LHG	10	0
41	R	616	XAT	20	0
25	y	312	CLA	11	0
25	c	510	CLA	24	0
28	H	101	BCR	6	0
25	c	502	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	s	311	CLA	9	0
26	r	618	LHG	16	0
25	s	304	CLA	12	0
24	S	302	CHL	4	0
26	b	621	LHG	3	0
28	B	619	BCR	4	0
26	Y	301	LHG	13	0
25	B	605	CLA	7	0
25	S	313	CLA	12	0
25	S	303	CLA	14	0
28	h	101	BCR	8	0
25	2	605	CLA	6	0
25	6	605	CLA	8	0
28	t	101	BCR	21	0
25	y	305	CLA	4	0
40	G	617	NEX	15	0
25	D	401	CLA	8	0
35	c	515	DGD	7	0
24	6	603	CHL	20	0
25	d	401	CLA	9	0
26	C	519	LHG	4	0
25	n	604	CLA	8	0
25	G	611	CLA	12	0
35	C	516	DGD	10	0
25	b	614	CLA	10	0
25	b	612	CLA	7	0
25	G	610	CLA	37	0
26	b	622	LHG	8	0
25	C	508	CLA	10	0
25	S	314	CLA	10	0
27	a	404	PHO	14	0
39	S	316	LUT	20	0
32	Y	321	AJP	2	0
25	c	503	CLA	5	0
25	c	512	CLA	12	0
30	a	409	LMG	3	0
25	Y	305	CLA	4	0
24	G	607	CHL	11	0
24	Y	306	CHL	6	0
28	d	404	BCR	3	0
29	a	412	SQD	6	0
39	N	615	LUT	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	602	CLA	8	0
29	l	101	SQD	5	0
26	Y	319	LHG	7	0
25	s	305	CLA	15	0
25	c	511	CLA	21	0
25	c	507	CLA	7	0
25	g	603	CLA	14	0
24	N	608	CHL	11	0
30	A	408	LMG	3	0
25	c	505	CLA	10	0
24	y	307	CHL	15	0
25	s	312	CLA	10	0
25	y	313	CLA	9	0
28	K	101	BCR	7	0
41	r	616	XAT	22	0
25	C	513	CLA	15	0
33	a	414	BCT	1	0
25	R	610	CLA	11	0
25	B	610	CLA	14	0
25	N	604	CLA	9	0
25	C	510	CLA	23	0
31	A	409	PL9	2	0
25	N	603	CLA	33	0
25	N	602	CLA	22	0
24	R	605	CHL	8	0
25	r	614	CLA	13	0
25	y	311	CLA	24	0
25	b	609	CLA	11	0
24	r	613	CHL	4	0
25	D	402	CLA	19	0
25	G	613	CLA	18	0
25	b	606	CLA	16	0
25	C	504	CLA	14	0
35	A	415	DGD	3	0
25	N	614	CLA	6	0
25	C	506	CLA	8	0
26	2	606	LHG	14	0
25	2	604	CLA	19	0
39	g	616	LUT	15	0
25	6	602	CLA	10	0
25	a	402	CLA	19	0
39	s	316	LUT	22	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	c	520	LMG	4	0
25	R	608	CLA	18	0
32	S	319	AJP	2	0
25	B	608	CLA	8	0
25	S	309	CLA	3	0
25	A	402	CLA	13	0
31	d	405	PL9	6	0
24	n	609	CHL	29	0
25	R	602	CLA	15	0
25	r	604	CLA	10	0
39	n	615	LUT	12	0
24	6	601	CHL	10	0
30	b	620	LMG	5	0
25	b	610	CLA	14	0
24	G	609	CHL	10	0
24	y	306	CHL	5	0
24	n	605	CHL	5	0
25	s	303	CLA	15	0
24	Y	309	CHL	14	0
25	n	603	CLA	33	0
40	r	617	NEX	10	0
25	b	616	CLA	15	0
25	Y	304	CLA	23	0
26	c	517	LHG	3	0
30	a	411	LMG	3	0
24	G	605	CHL	4	0
40	Y	318	NEX	7	0
39	g	615	LUT	15	0
24	y	302	CHL	31	0
25	r	609	CLA	7	0
25	c	513	CLA	17	0
32	y	320	AJP	3	0
25	r	610	CLA	11	0
24	g	608	CHL	20	0
24	r	605	CHL	9	0
25	B	601	CLA	10	0
39	S	315	LUT	7	0
28	z	101	BCR	5	0
26	c	519	LHG	4	0
26	N	618	LHG	11	0
28	b	619	BCR	4	0
25	R	601	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	n	608	CHL	9	0
26	c	518	LHG	3	0
25	b	604	CLA	14	0
25	n	602	CLA	23	0
24	N	607	CHL	48	0
24	l	302	CHL	9	0
25	c	508	CLA	12	0
25	d	403	CLA	15	0
25	B	616	CLA	14	0
25	C	512	CLA	12	0
39	Y	316	LUT	12	0
25	g	602	CLA	11	0
25	Y	315	CLA	17	0
25	G	602	CLA	12	0
31	D	405	PL9	6	0
24	r	607	CHL	9	0
25	y	304	CLA	20	0
25	b	603	CLA	6	0
25	b	615	CLA	16	0
25	c	509	CLA	9	0
40	y	318	NEX	10	0
24	N	609	CHL	26	0
25	b	613	CLA	14	0
25	G	614	CLA	5	0
27	A	404	PHO	14	0
28	A	406	BCR	4	0
25	d	402	CLA	19	0
30	C	520	LMG	4	0
25	r	611	CLA	4	0
25	B	604	CLA	14	0
26	R	618	LHG	14	0
32	y	321	AJP	2	0
39	G	615	LUT	15	0
25	c	501	CLA	19	0
25	Y	314	CLA	15	0
25	a	403	CLA	13	0
24	y	309	CHL	14	0
25	Y	312	CLA	10	0
26	y	319	LHG	8	0
26	S	301	LHG	8	0
25	B	615	CLA	15	0
24	S	306	CHL	10	0

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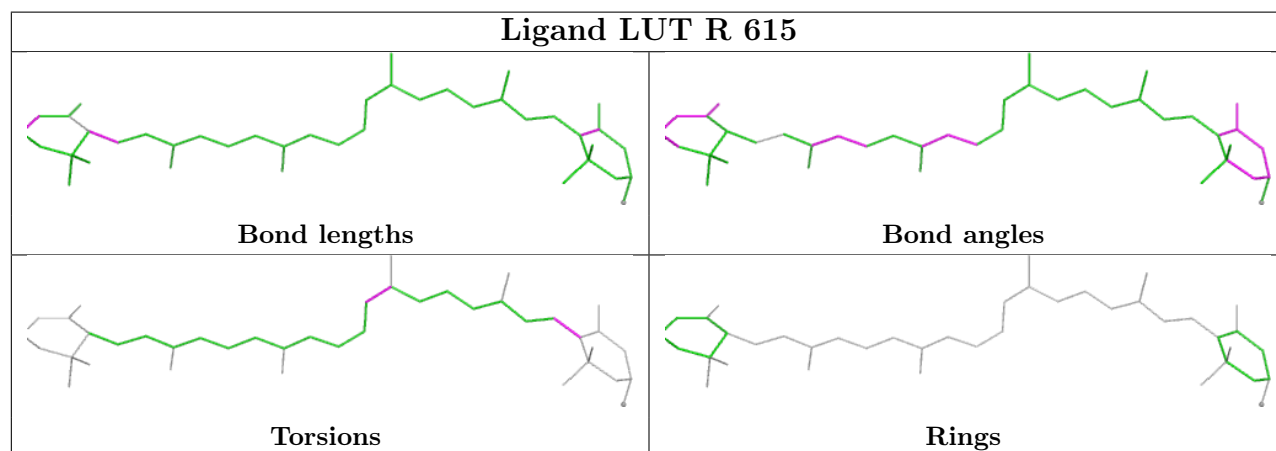
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	613	CLA	16	0
25	S	311	CLA	8	0
28	B	617	BCR	7	0
25	g	614	CLA	4	0
25	b	605	CLA	9	0
25	a	406	CLA	9	0
25	B	607	CLA	15	0
40	N	617	NEX	15	0
25	S	310	CLA	14	0
26	b	625	LHG	7	0
40	R	617	NEX	8	0
25	r	612	CLA	19	0
25	s	309	CLA	3	0
26	s	318	LHG	6	0
26	l	103	LHG	5	0
25	R	603	CLA	17	0
39	s	315	LUT	7	0
25	R	609	CLA	5	0
40	g	617	NEX	15	0
25	b	611	CLA	7	0
30	B	623	LMG	5	0
24	l	301	CHL	9	0
35	B	626	DGD	5	0
26	n	618	LHG	10	0
26	C	517	LHG	3	0
25	N	613	CLA	30	0
33	A	413	BCT	2	0
25	c	506	CLA	10	0
35	c	516	DGD	10	0
39	Y	317	LUT	13	0
39	y	317	LUT	12	0
30	D	407	LMG	3	0
28	D	404	BCR	3	0
24	g	605	CHL	4	0
25	s	310	CLA	15	0
26	6	606	LHG	14	0
25	C	505	CLA	10	0
25	A	401	CLA	19	0
25	2	602	CLA	8	0
24	n	606	CHL	17	0
25	y	315	CLA	17	0
25	R	612	CLA	19	0

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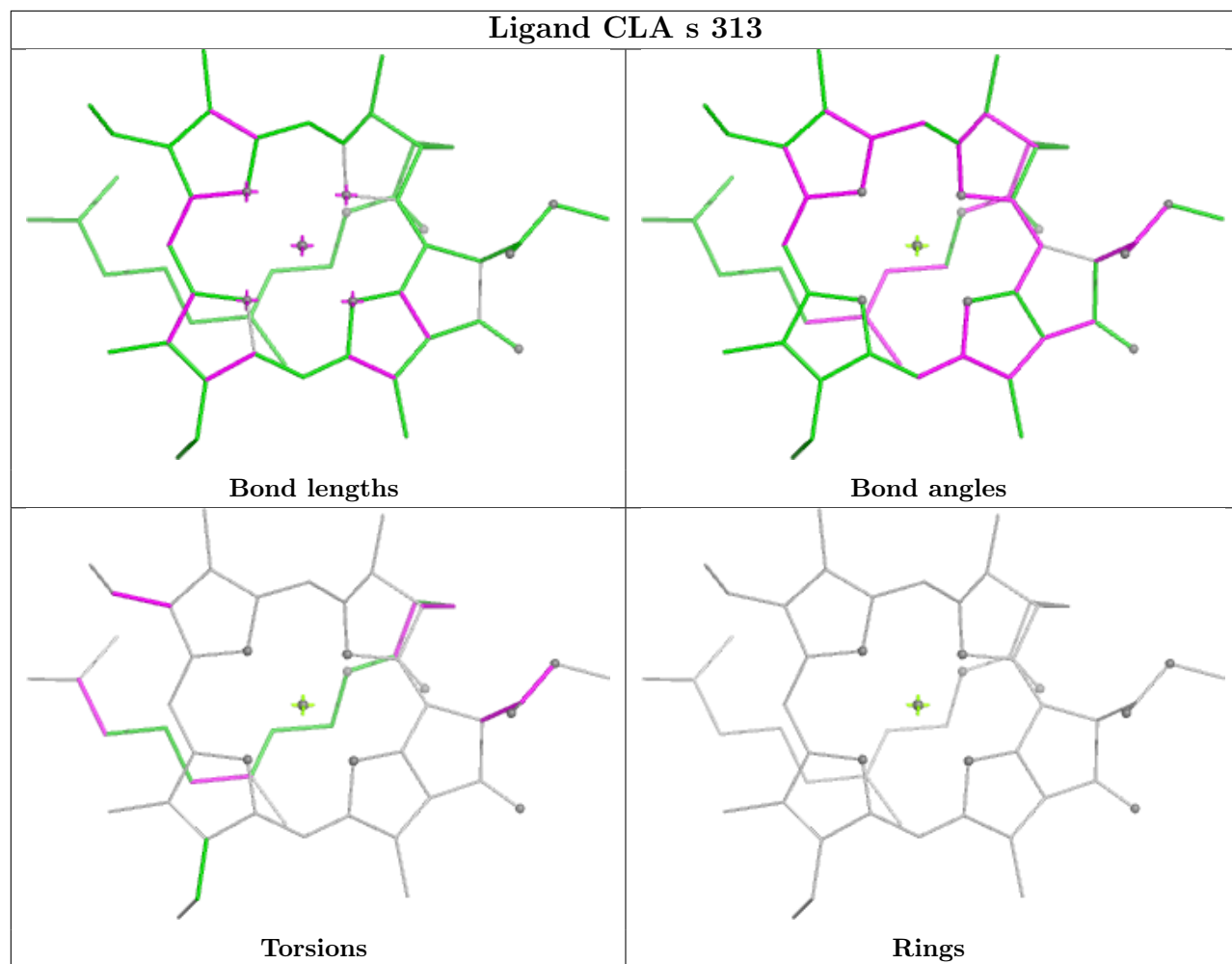
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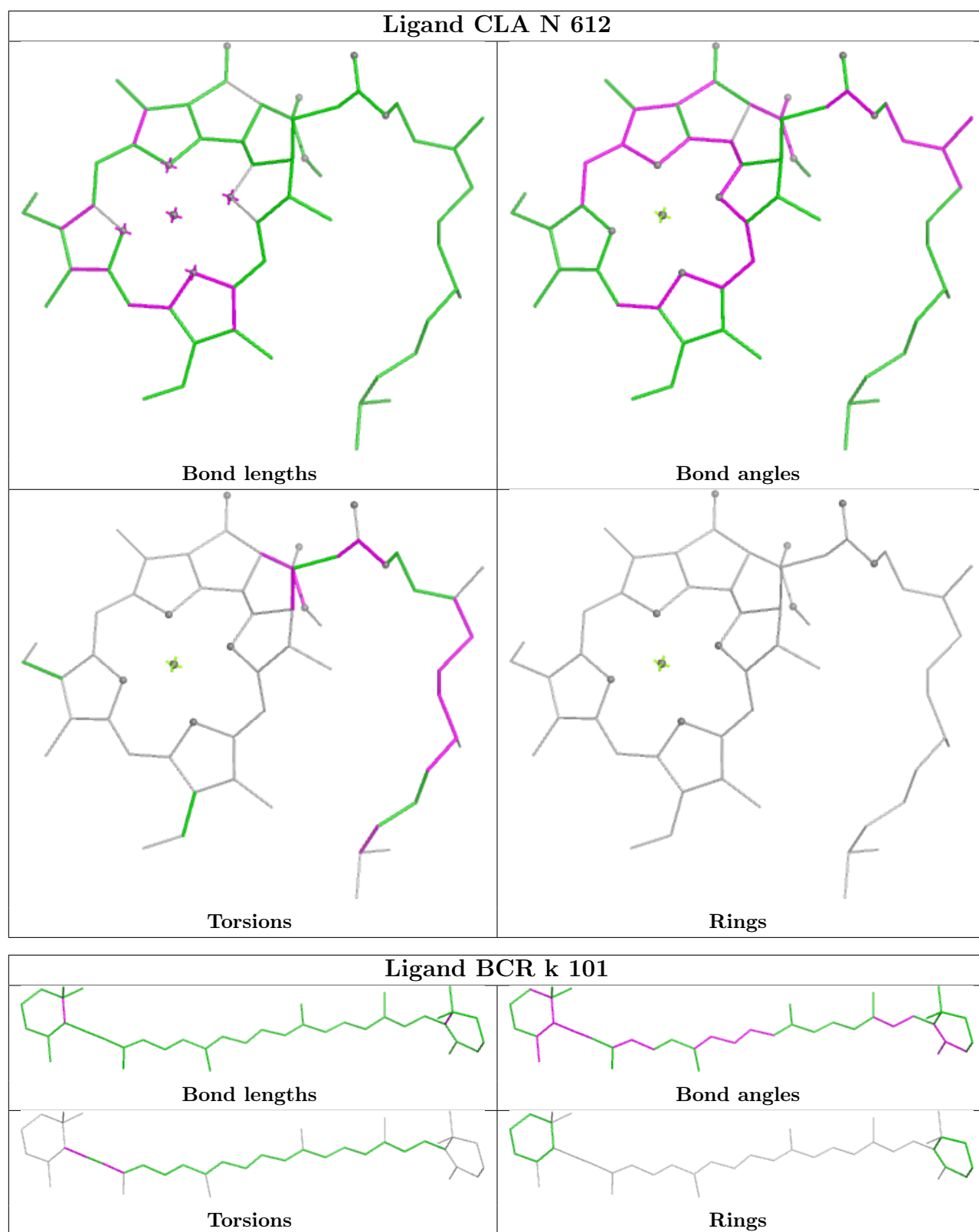
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	I	101	BCR	20	0
25	B	612	CLA	6	0
32	y	322	AJP	2	0
24	S	308	CHL	9	0
25	B	609	CLA	11	0
28	C	514	BCR	7	0
25	b	601	CLA	9	0
24	Y	302	CHL	30	0
25	6	604	CLA	19	0
29	A	411	SQD	5	0
24	g	606	CHL	19	0
35	b	626	DGD	6	0

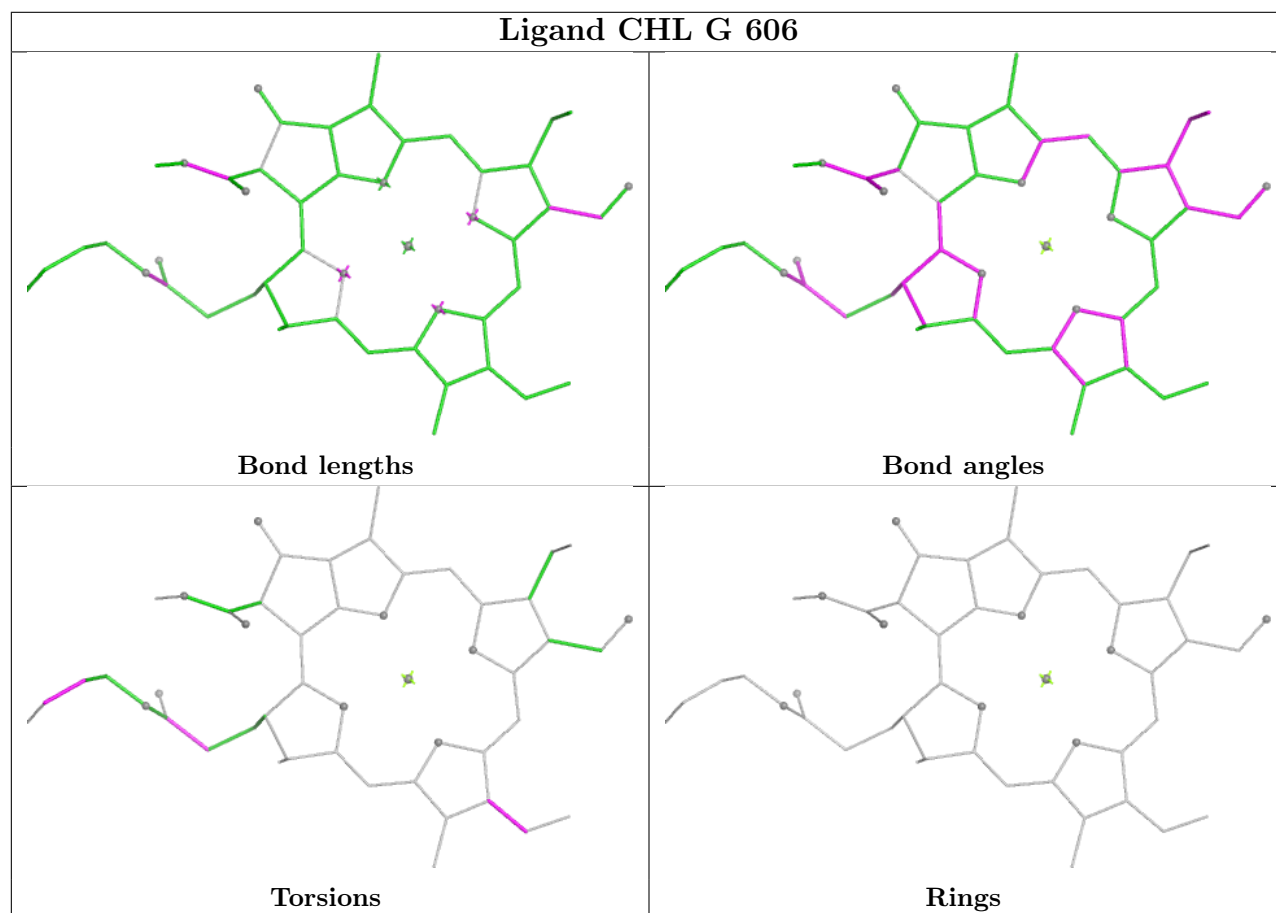
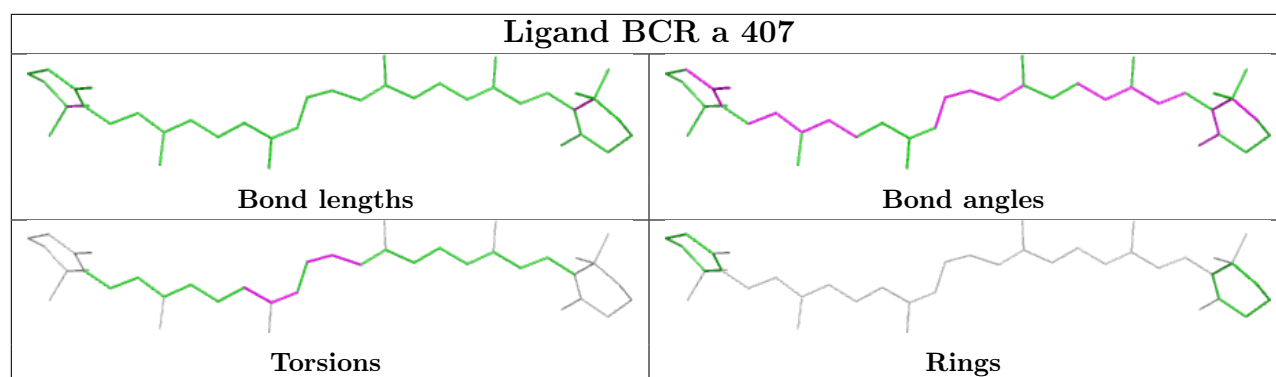
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

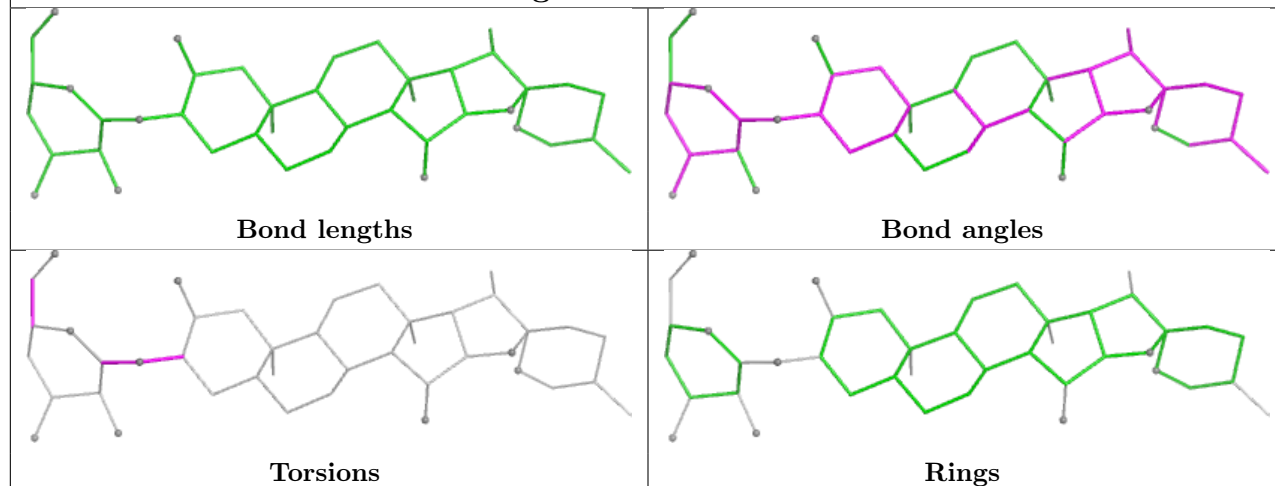
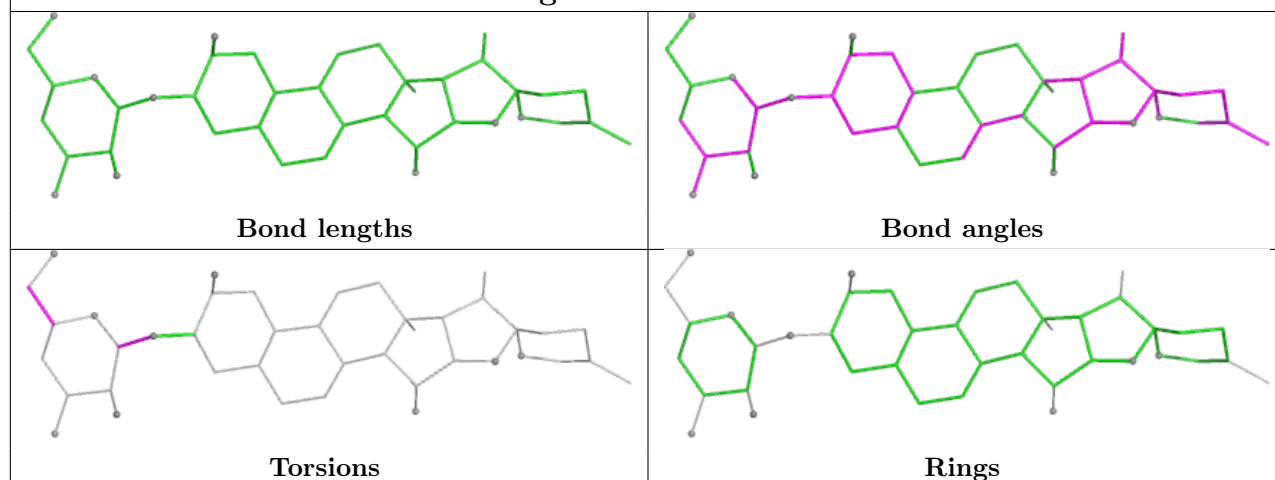
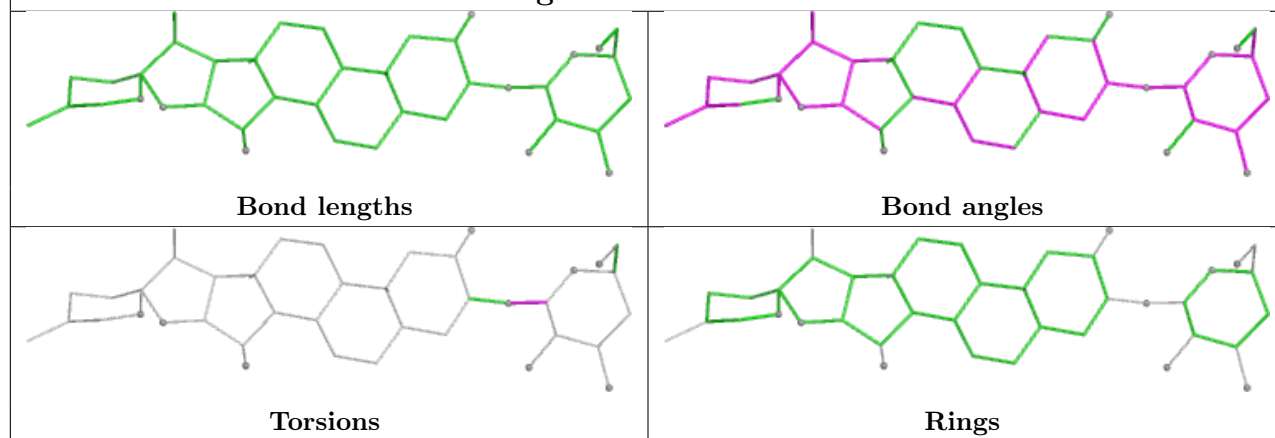


Ligand CLA s 313

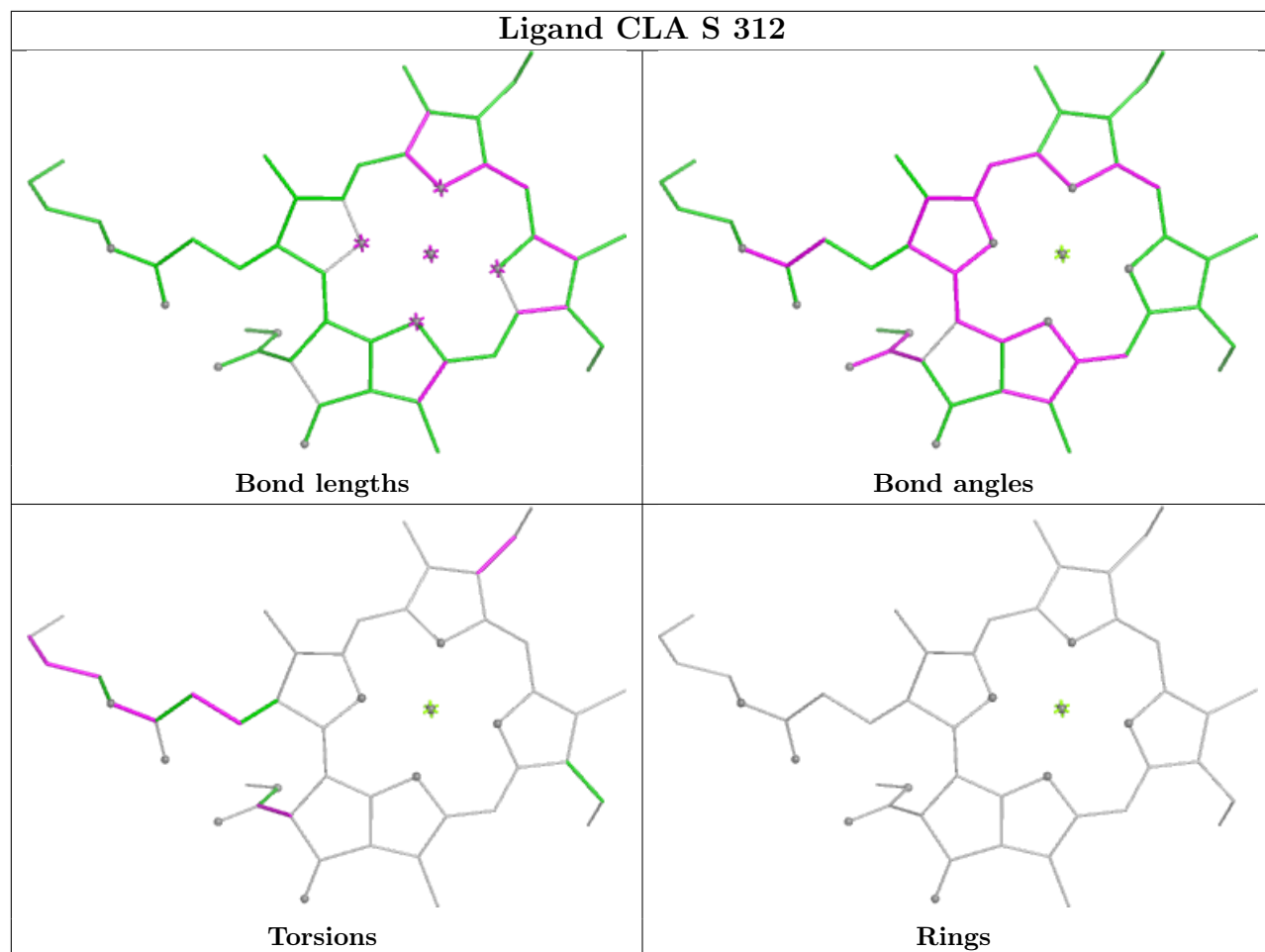




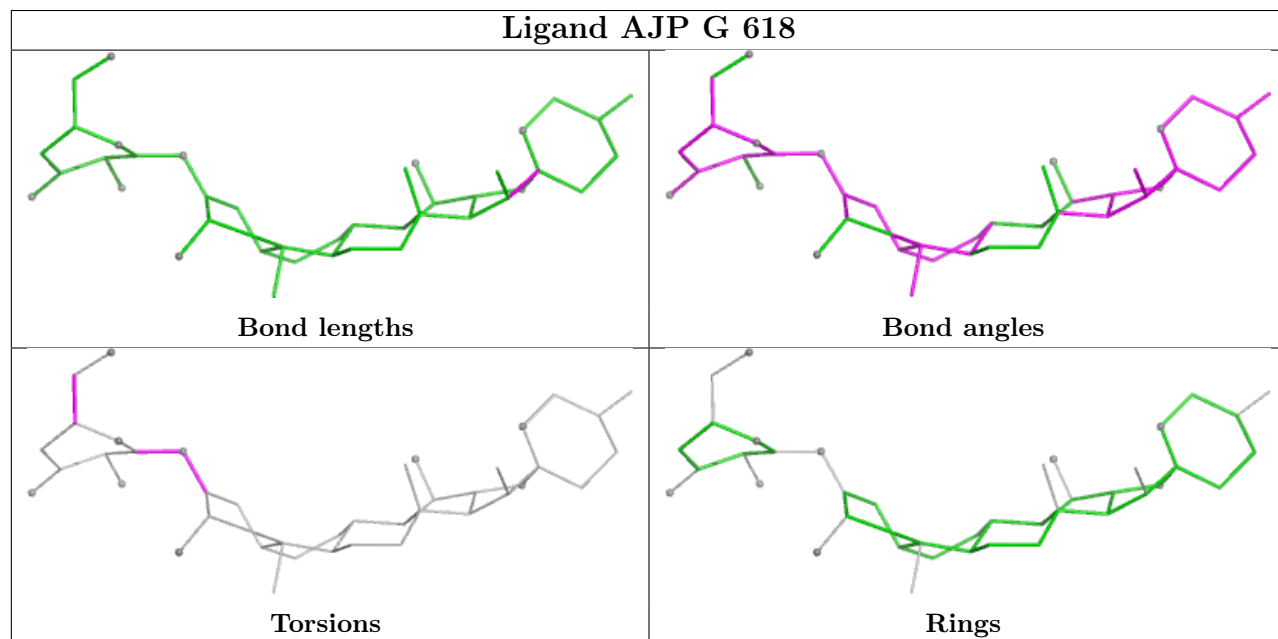


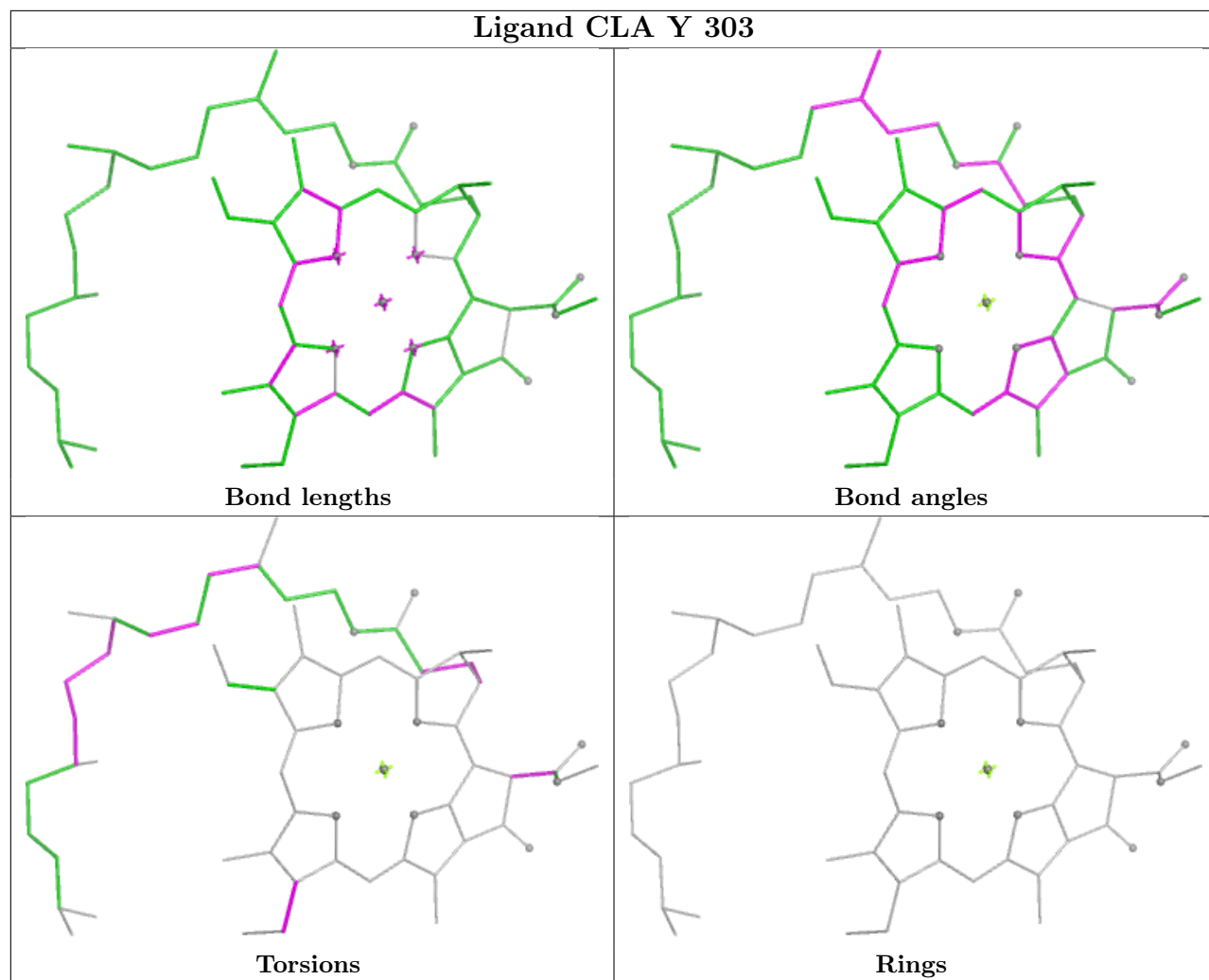
Ligand AJP N 620**Ligand AJP s 319****Ligand AJP n 619**

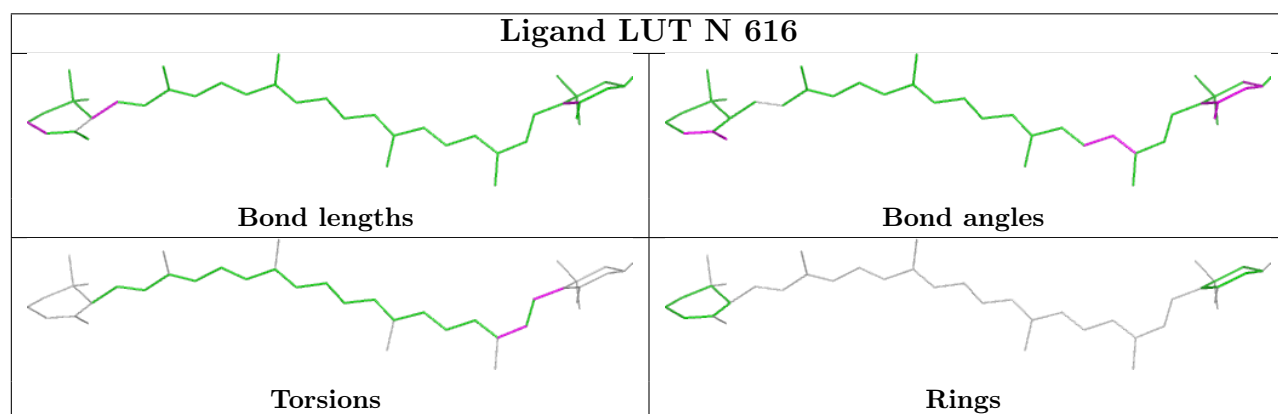
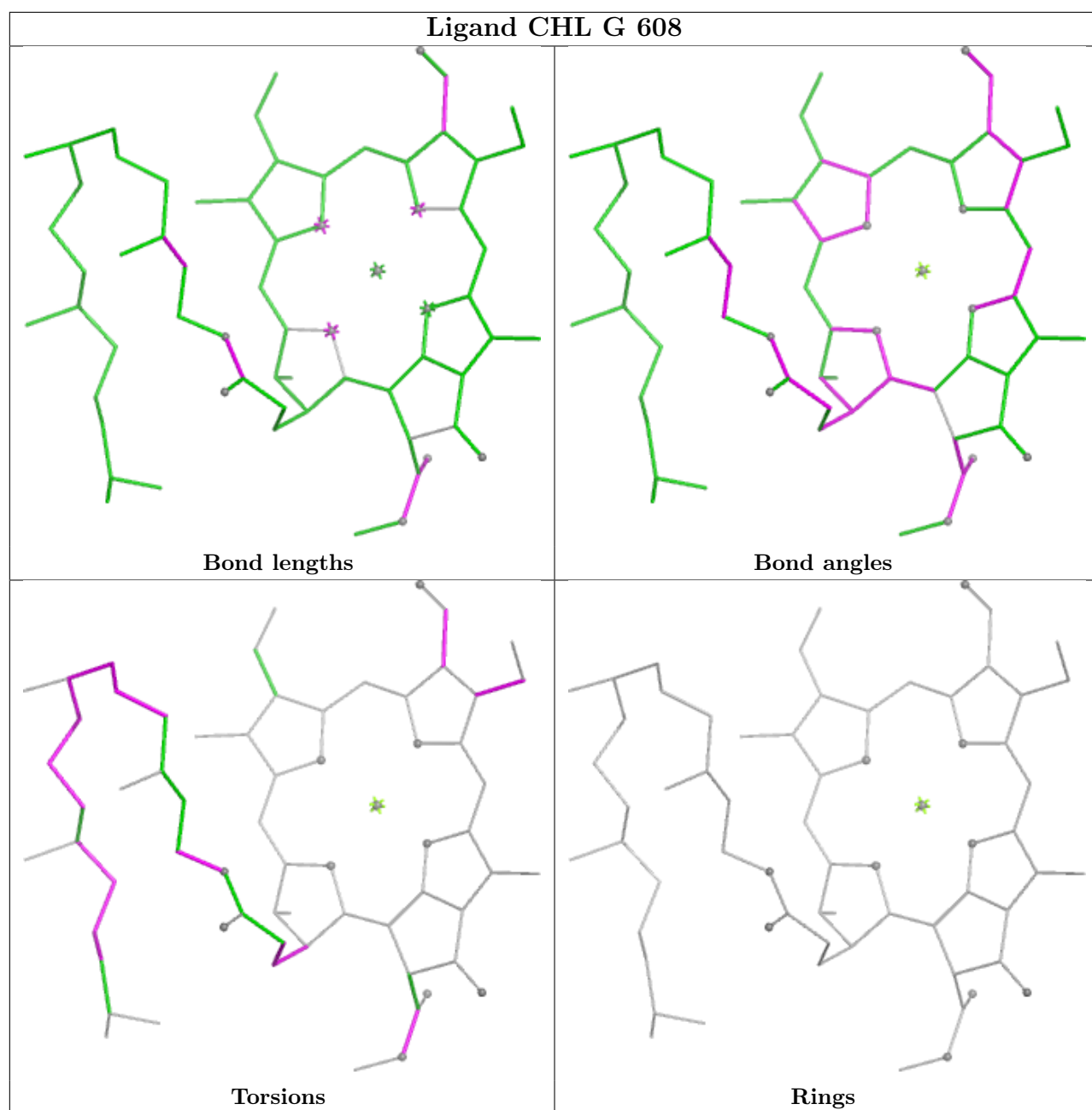
Ligand CLA S 312

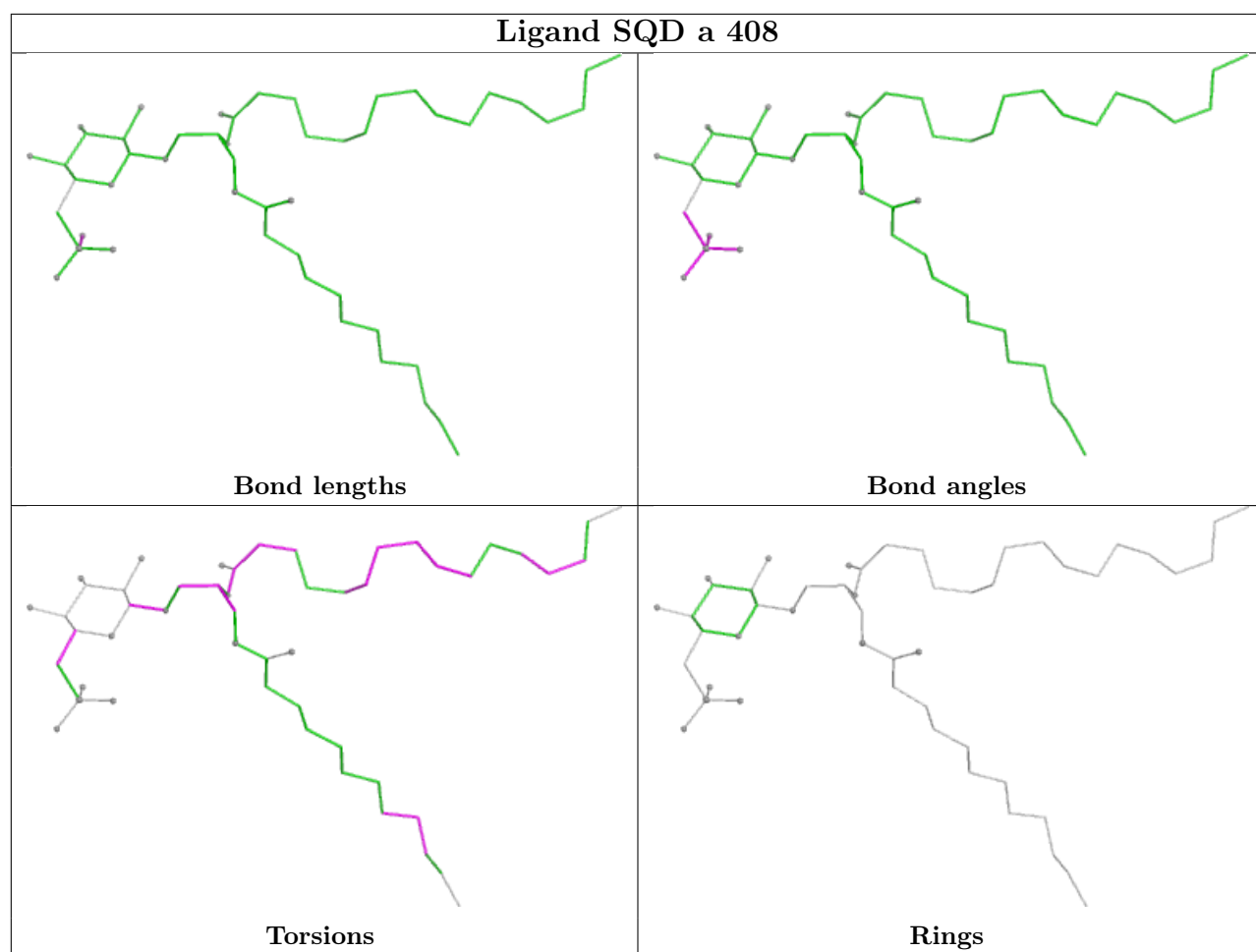


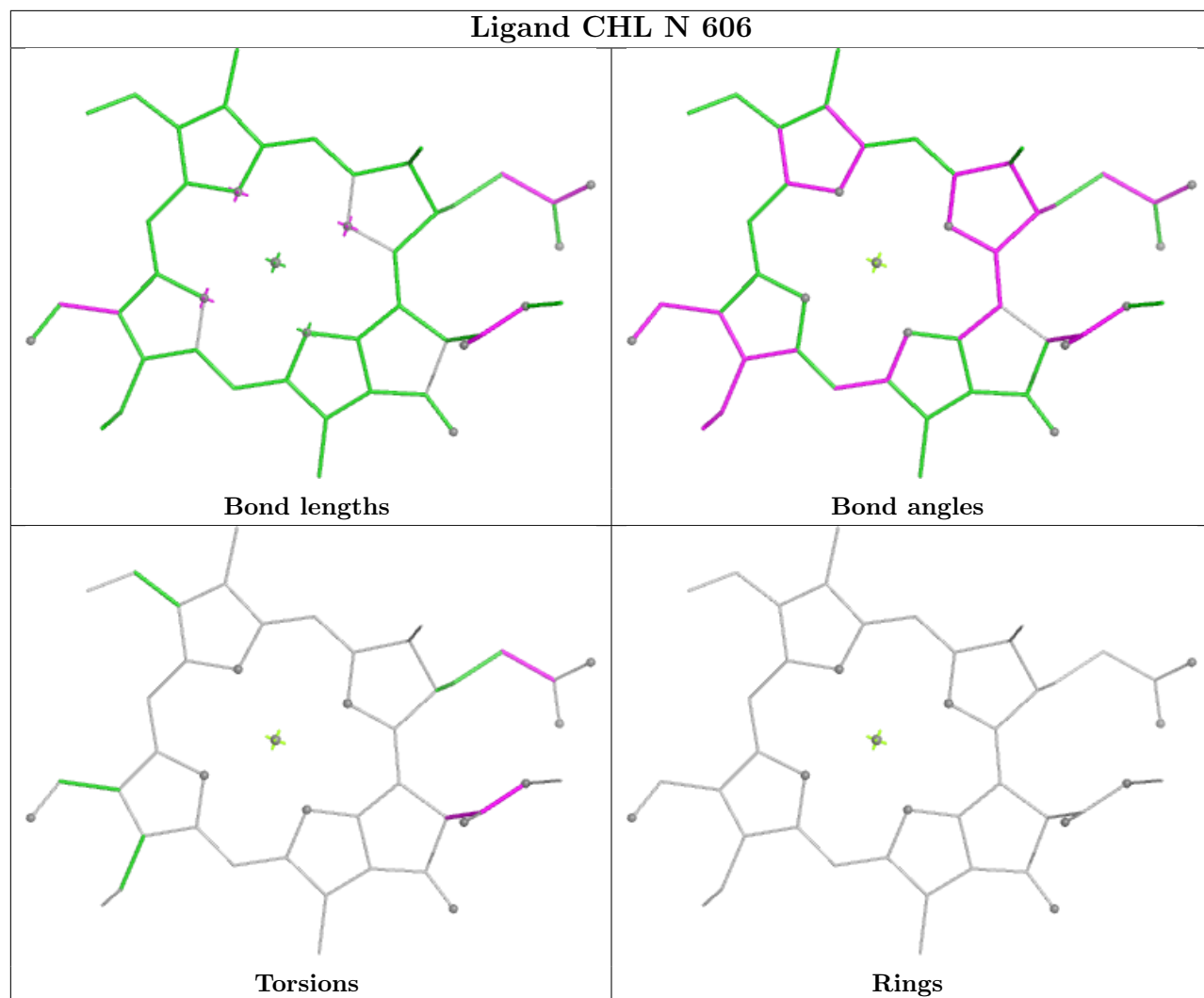
Ligand AJP G 618



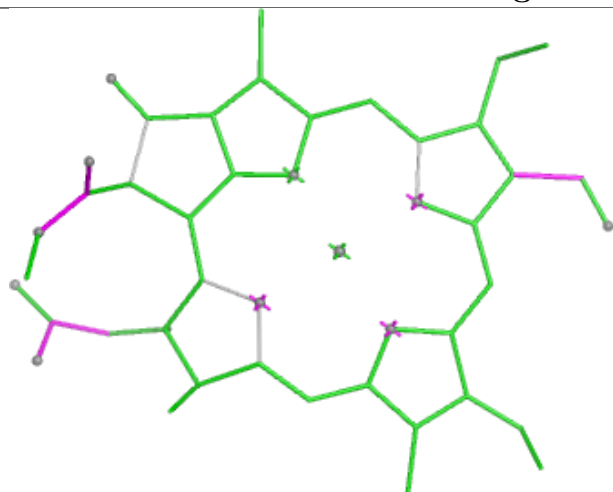
Ligand CLA Y 303



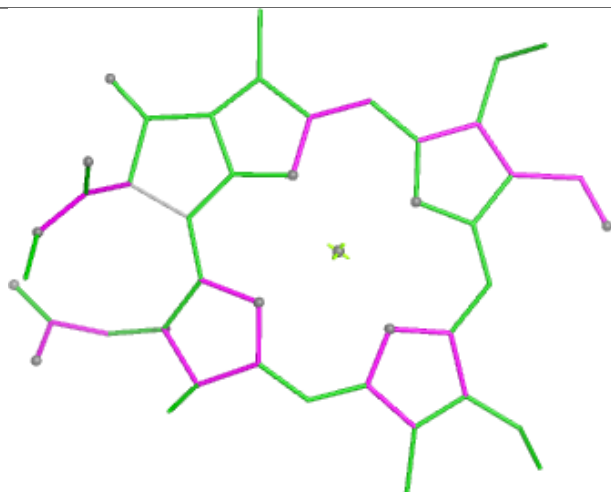




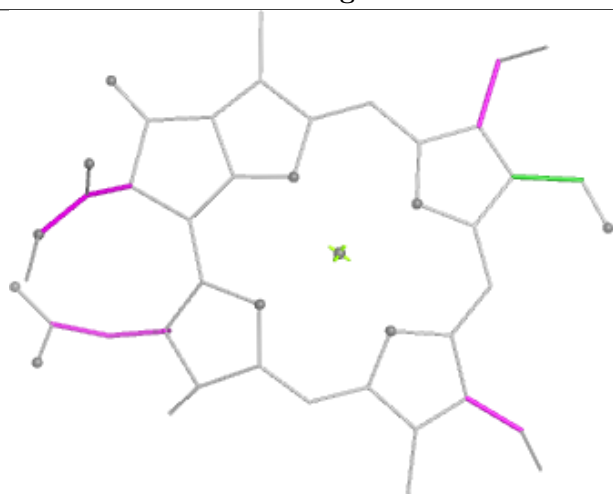
Ligand CHL R 606



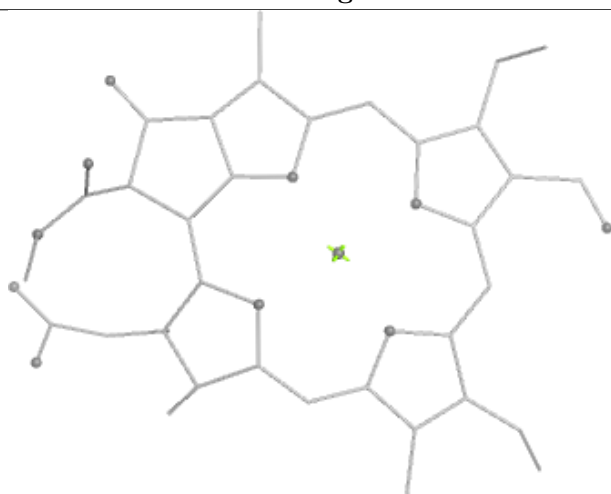
Bond lengths



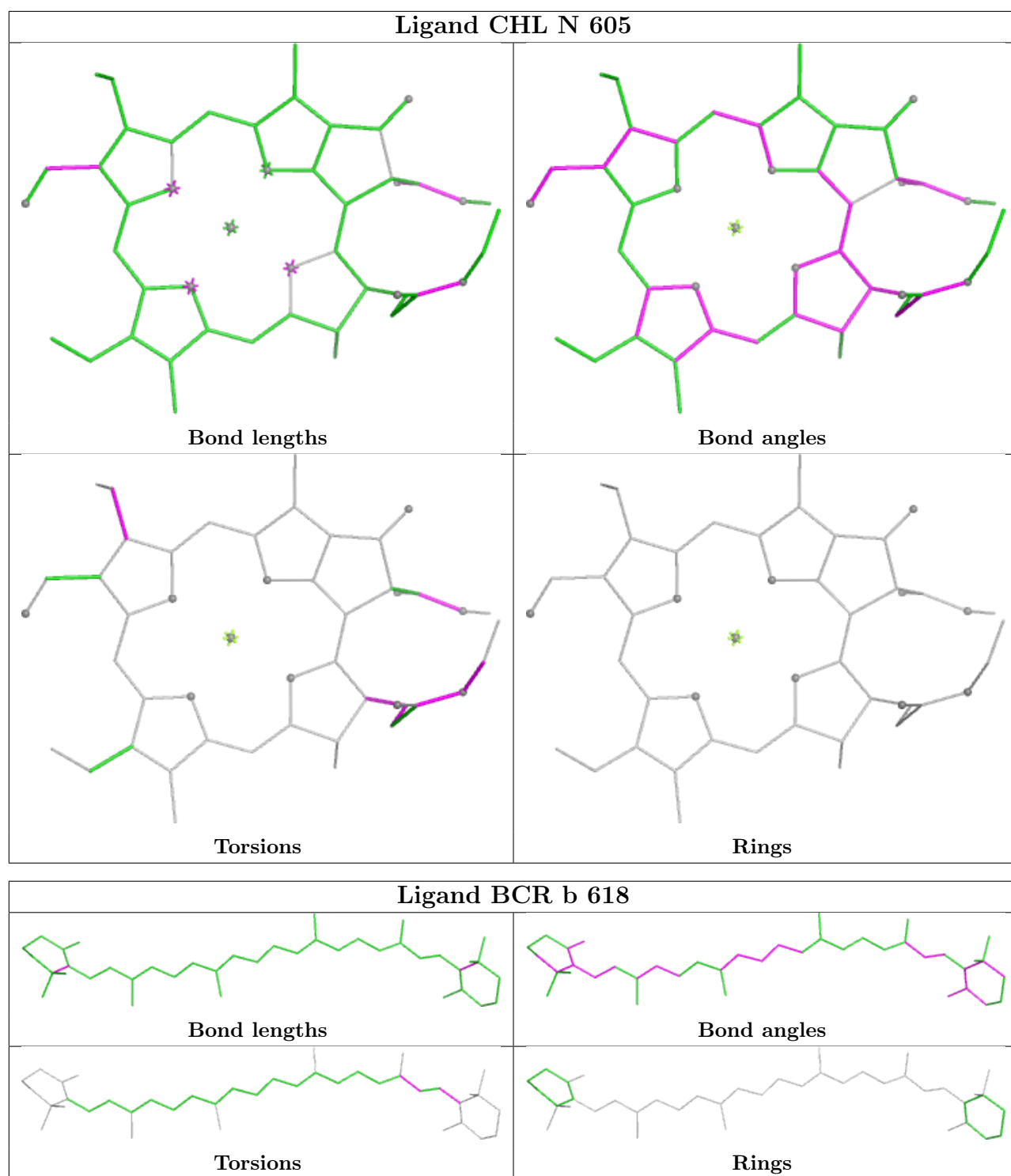
Bond angles



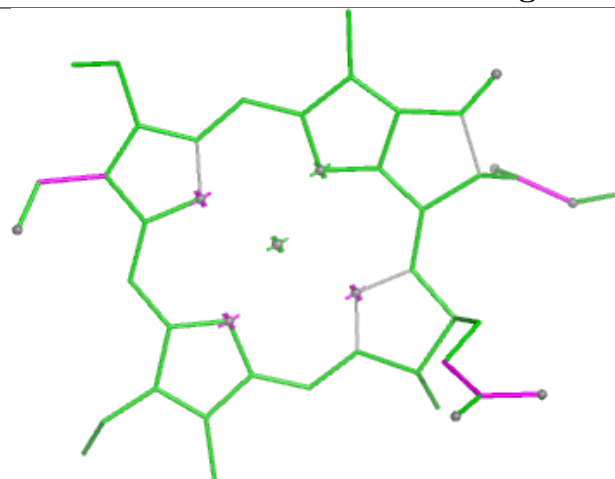
Torsions



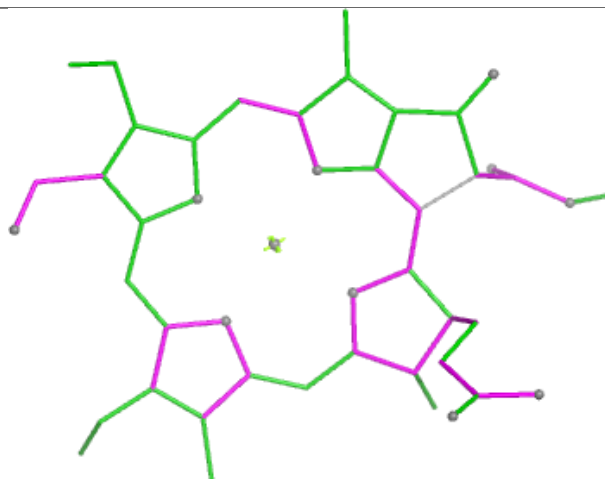
Rings



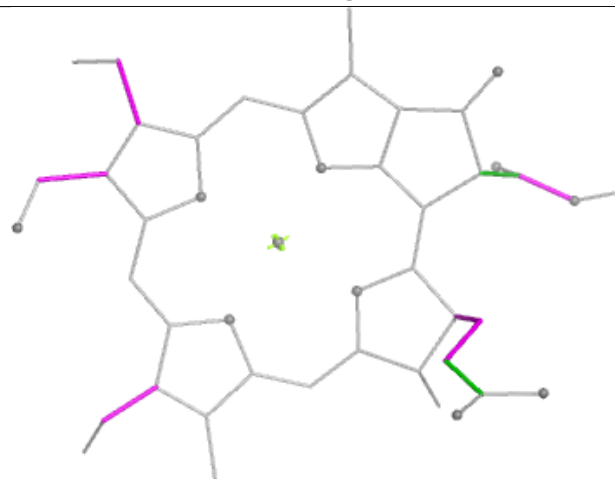
Ligand CHL S 307



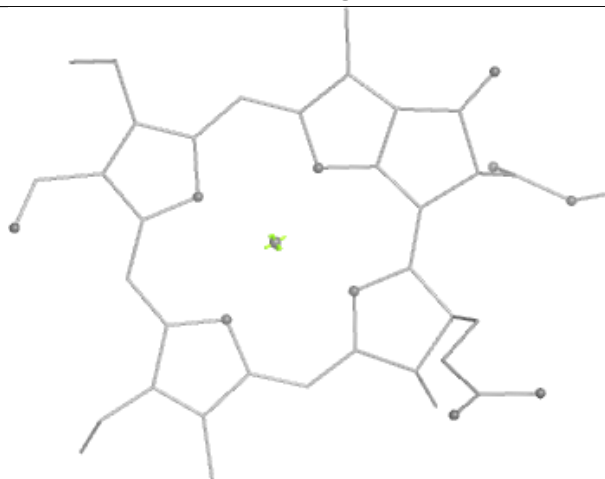
Bond lengths



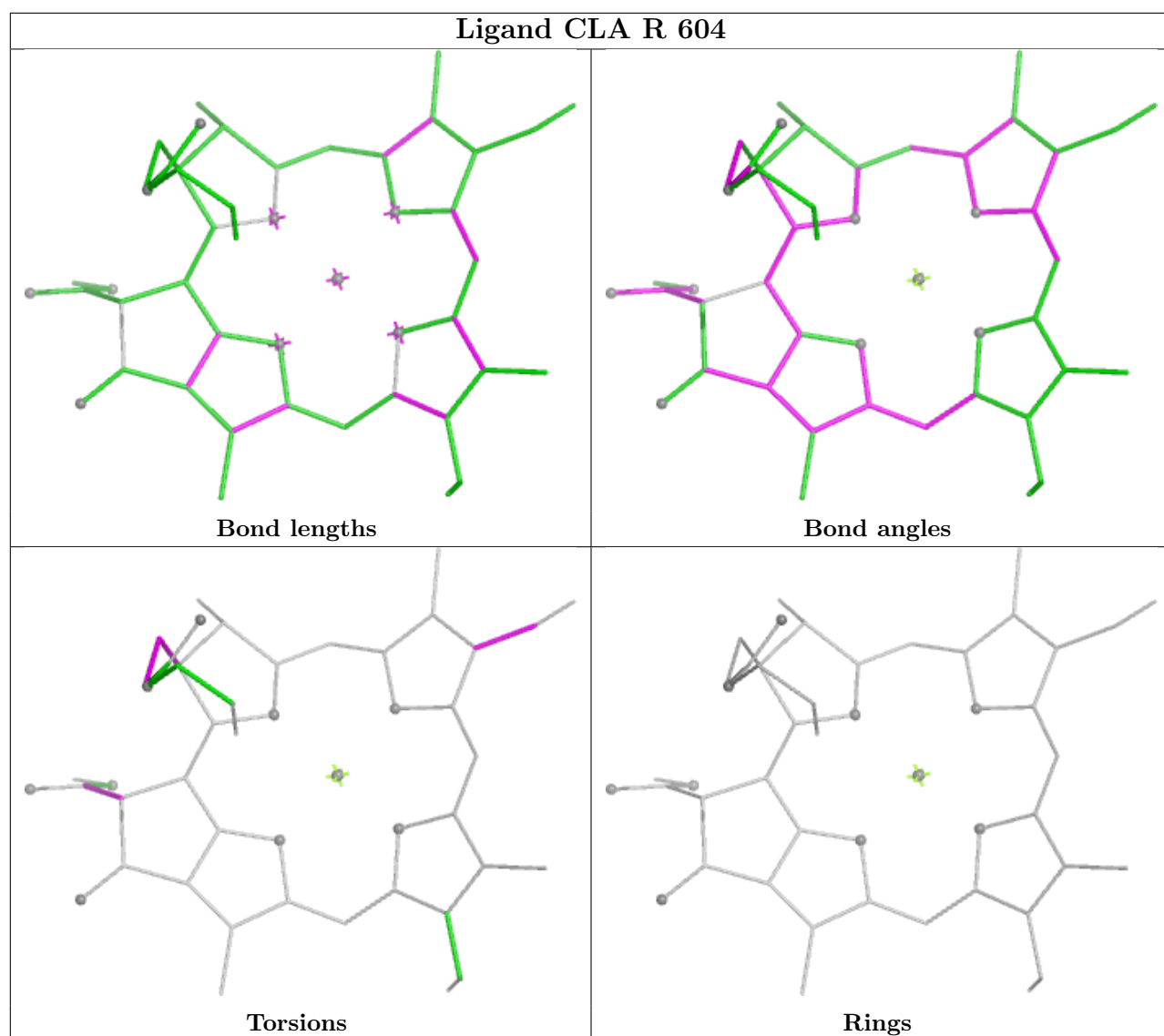
Bond angles

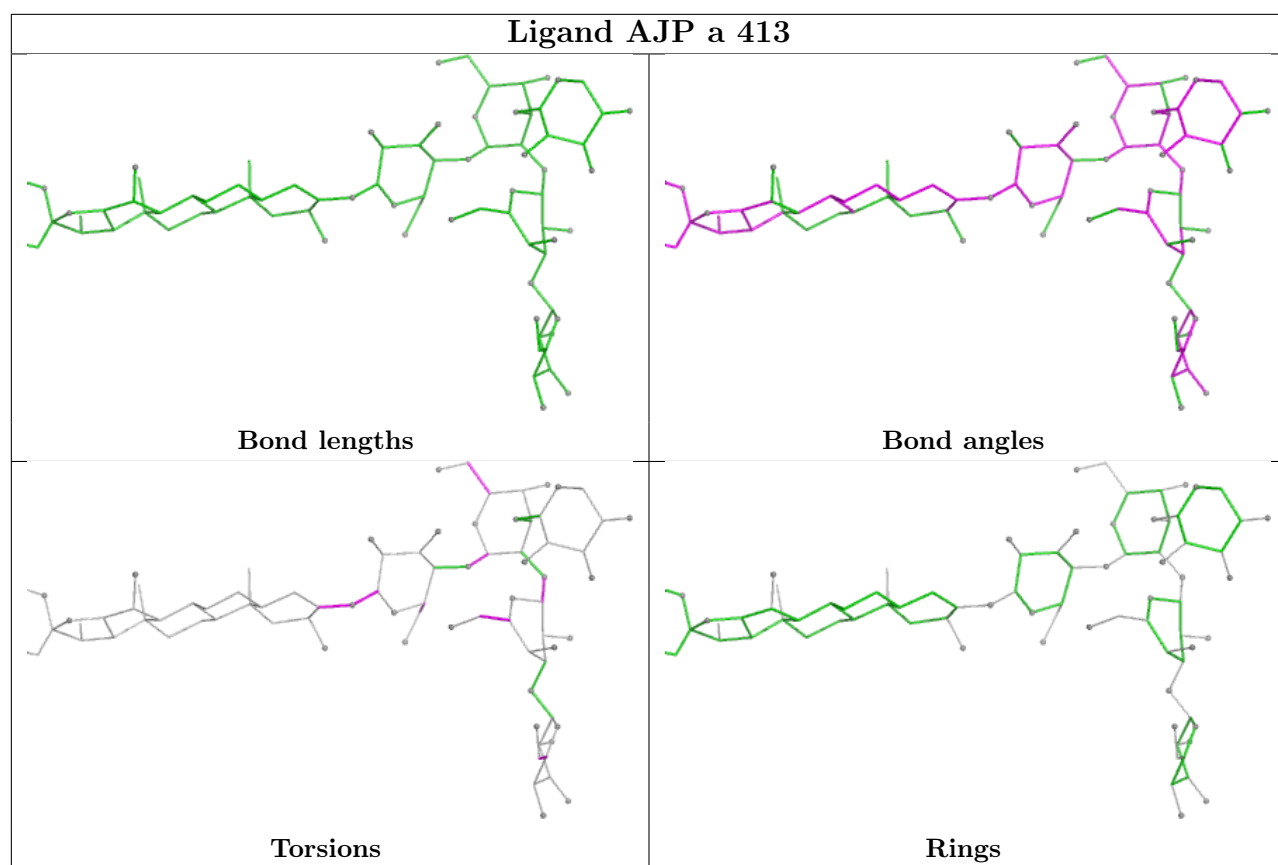


Torsions

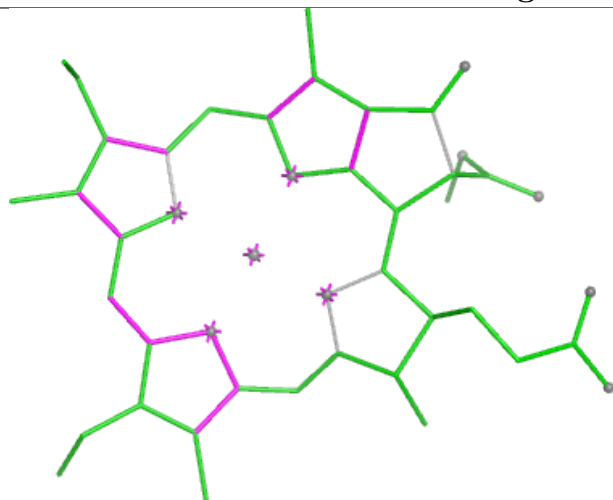


Rings

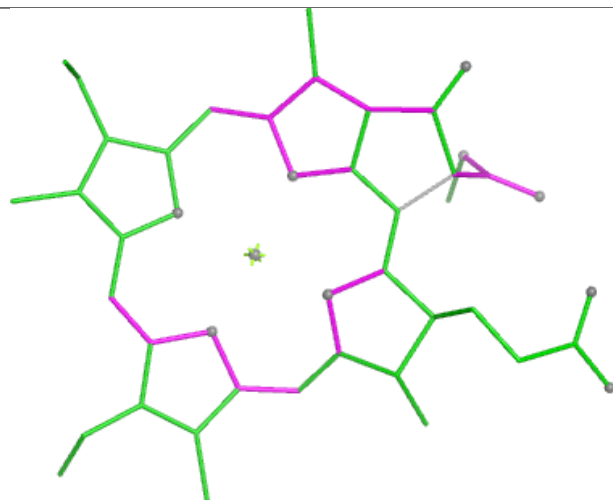




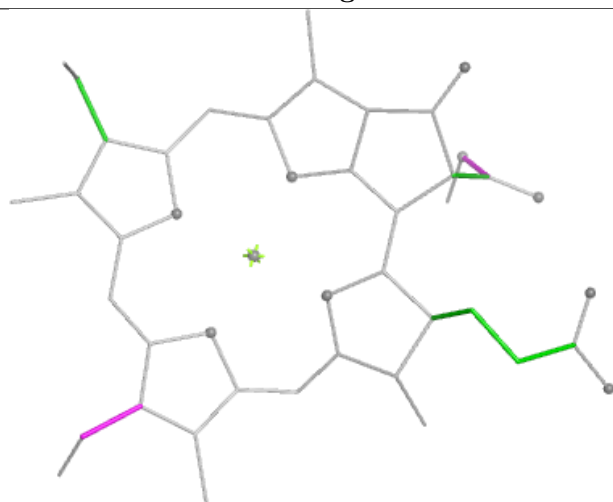
Ligand CLA S 304



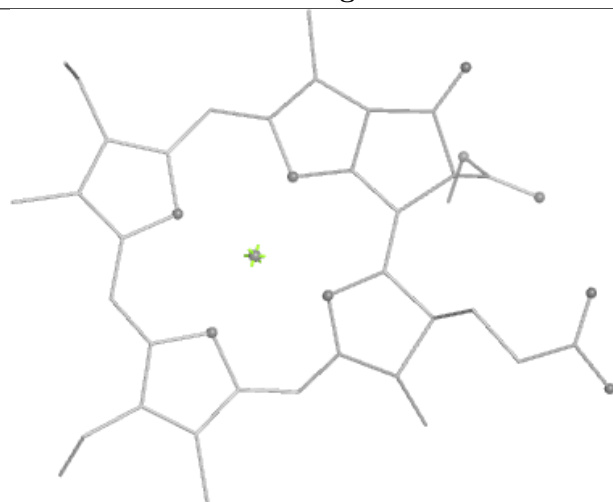
Bond lengths



Bond angles

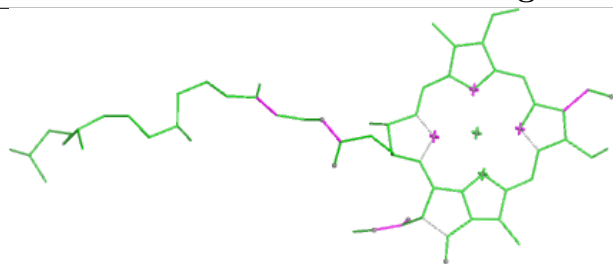


Torsions

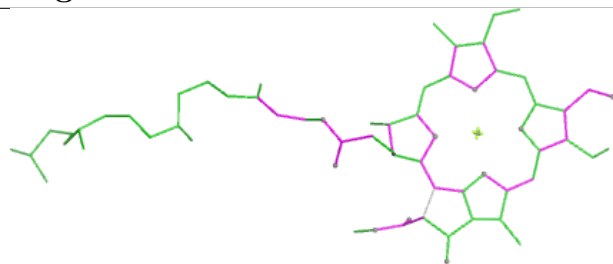


Rings

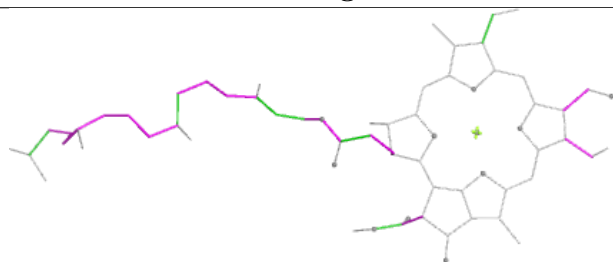
Ligand CHL g 601



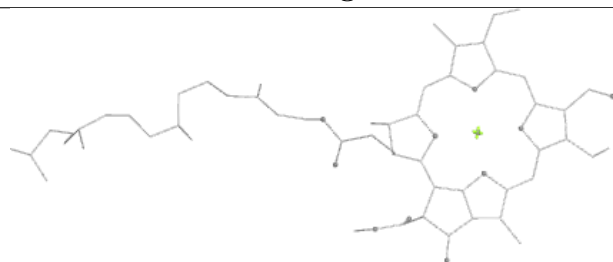
Bond lengths



Bond angles

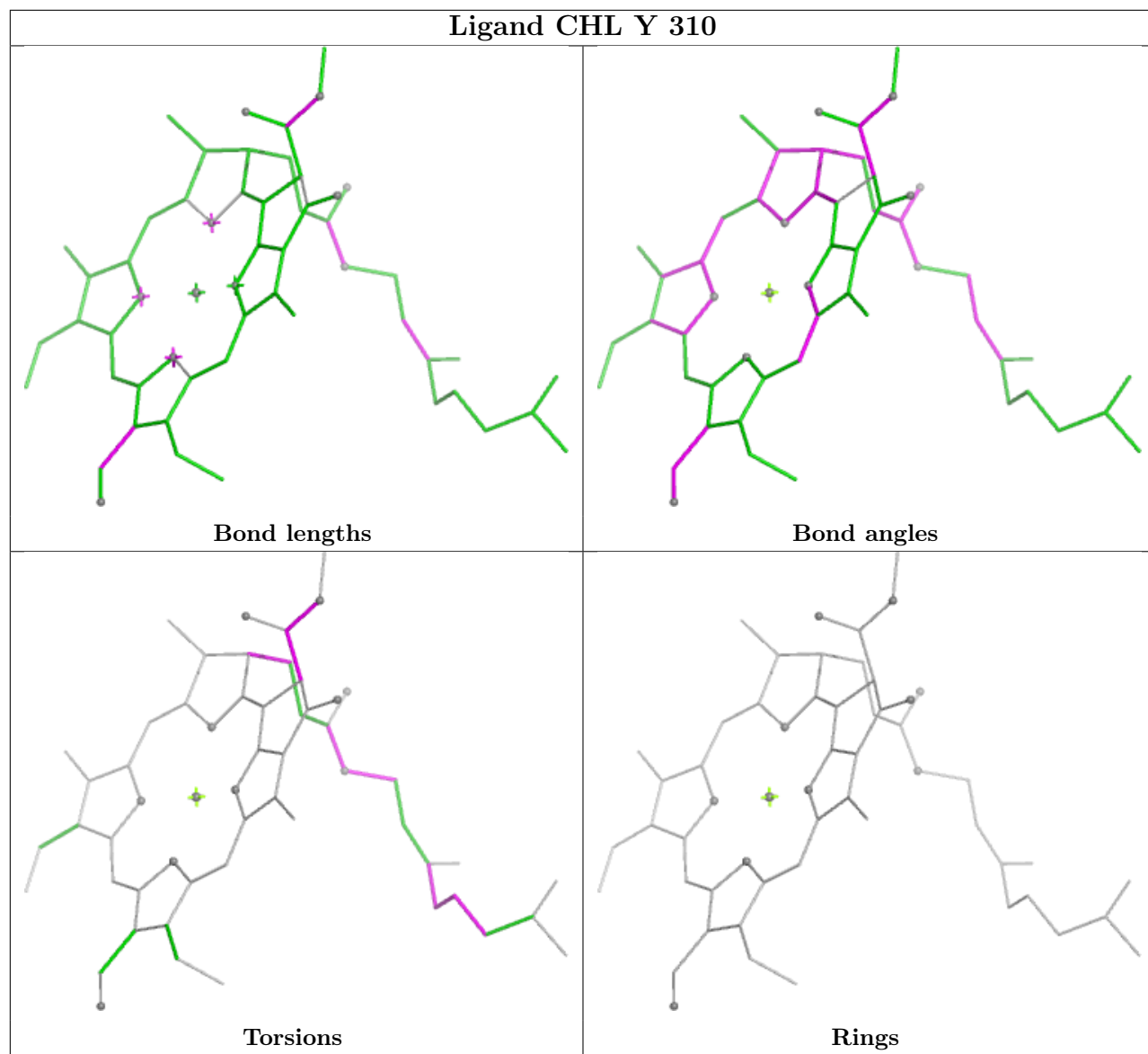


Torsions

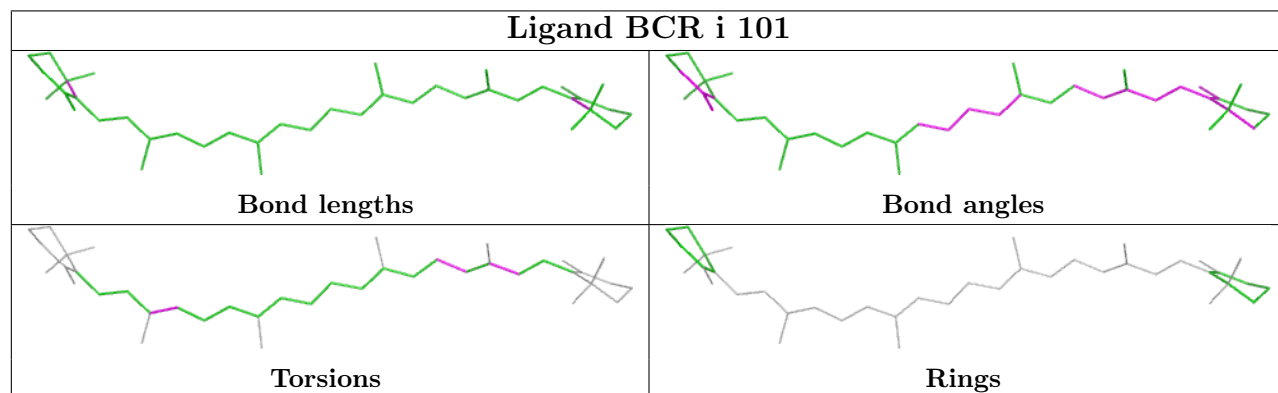


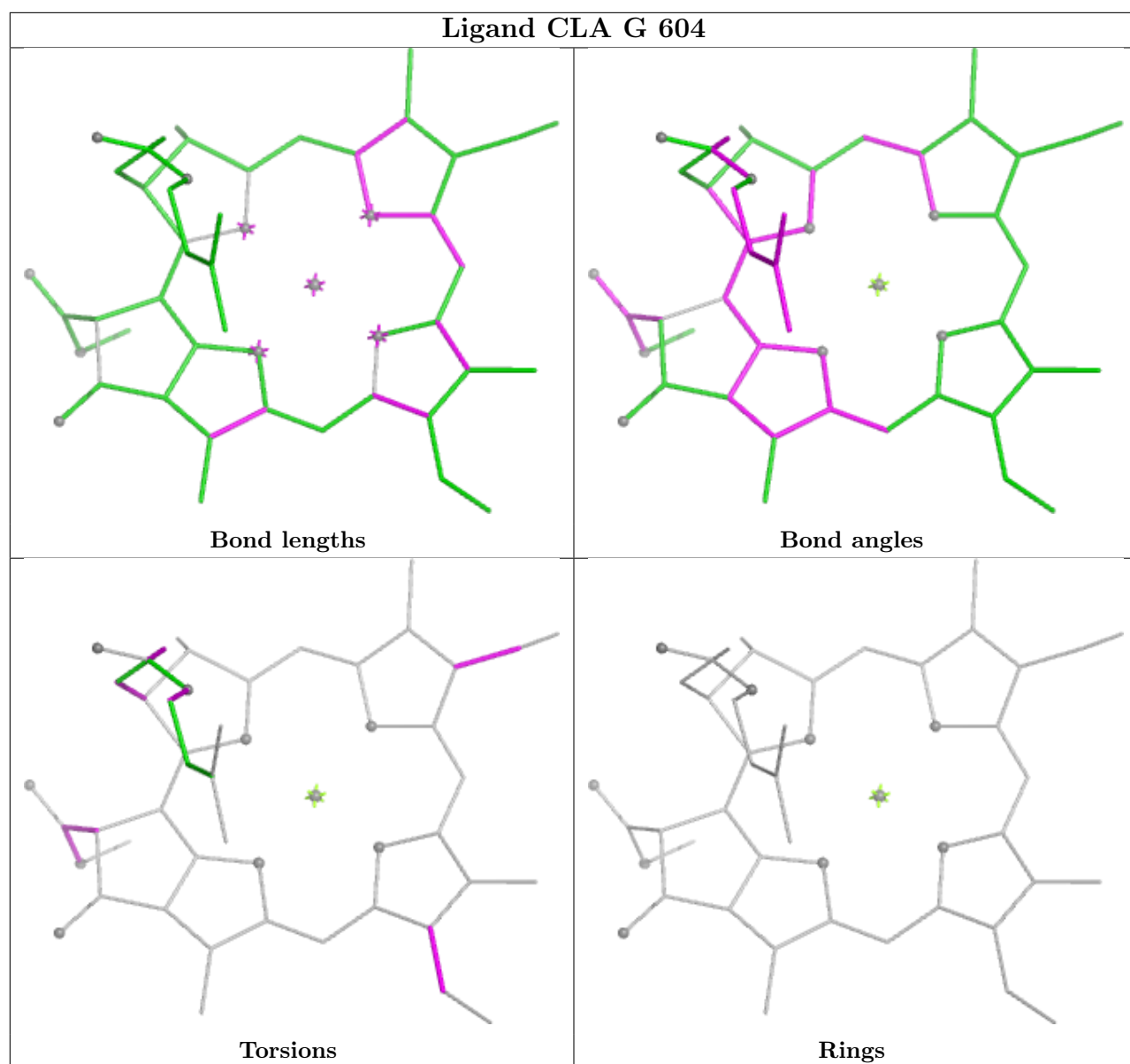
Rings

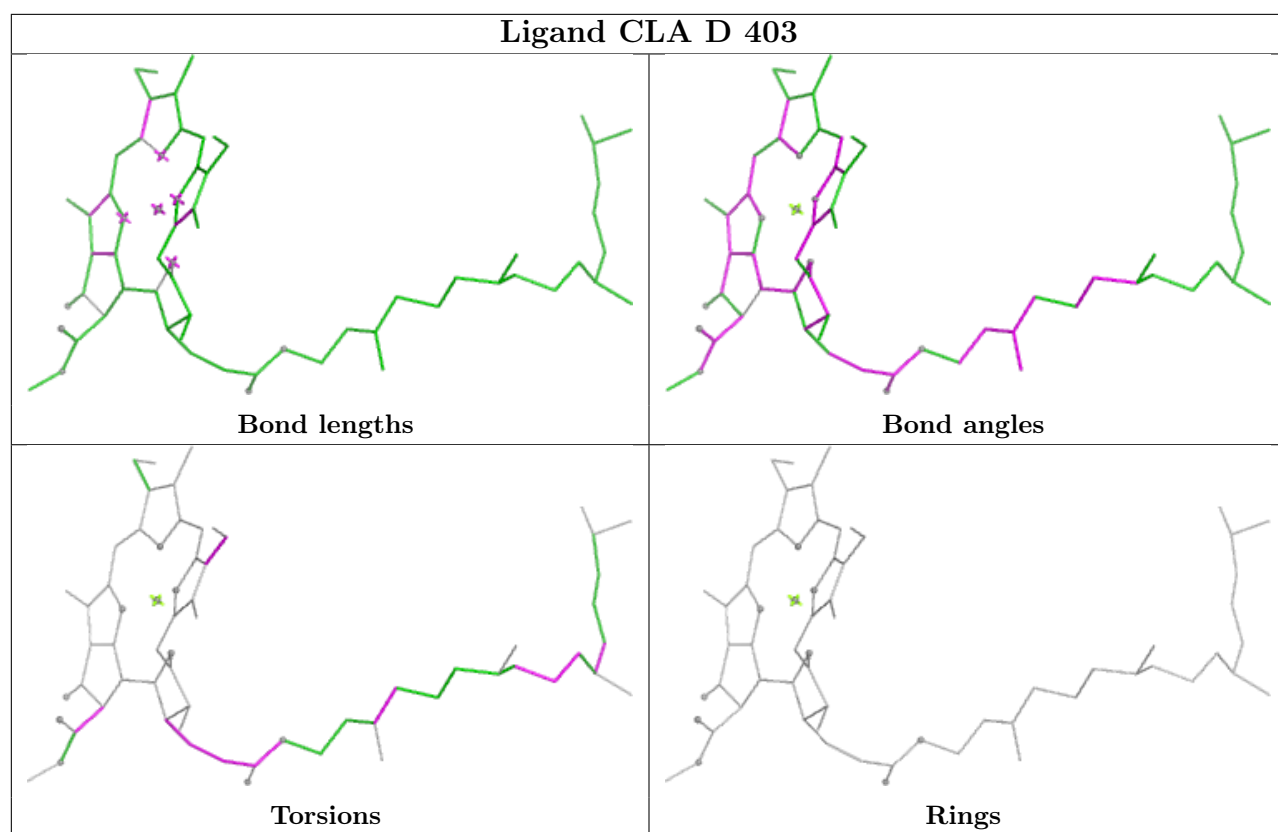
Ligand CHL Y 310

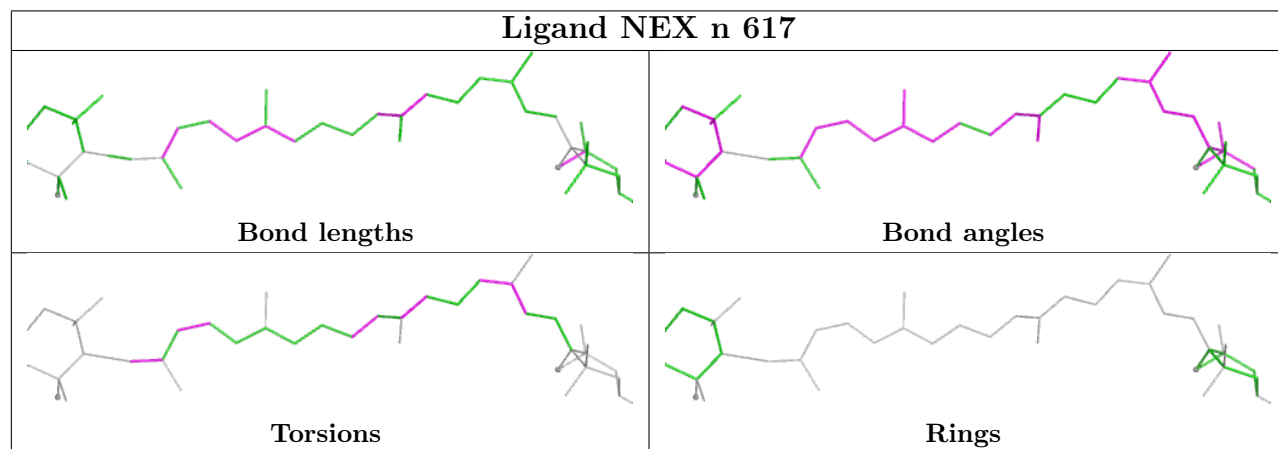
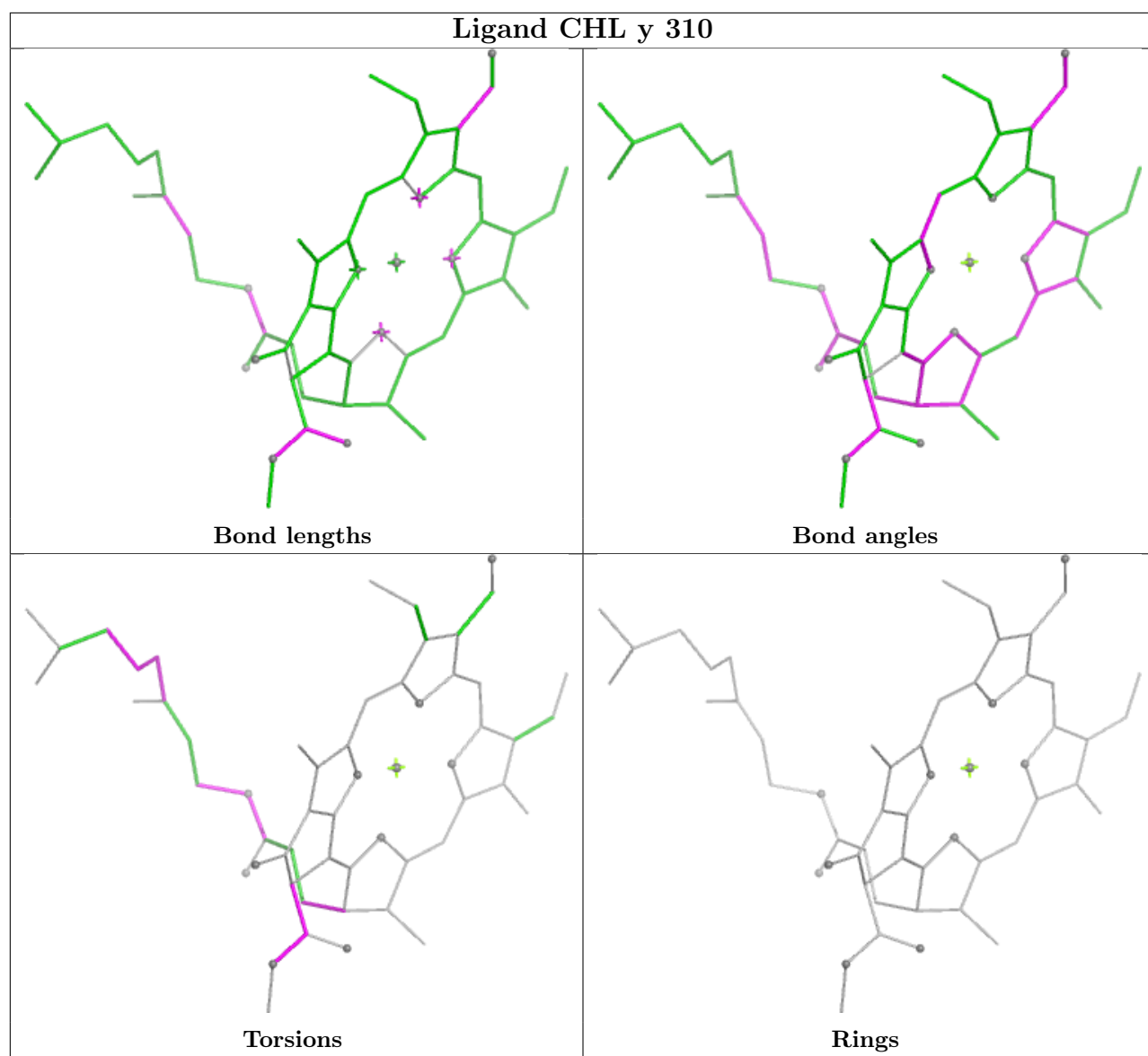


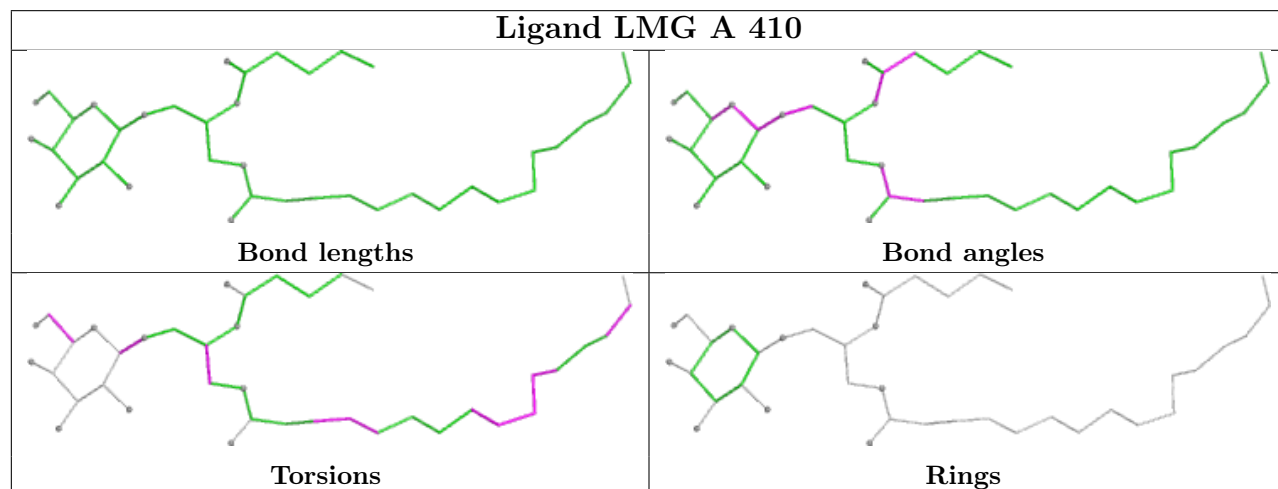
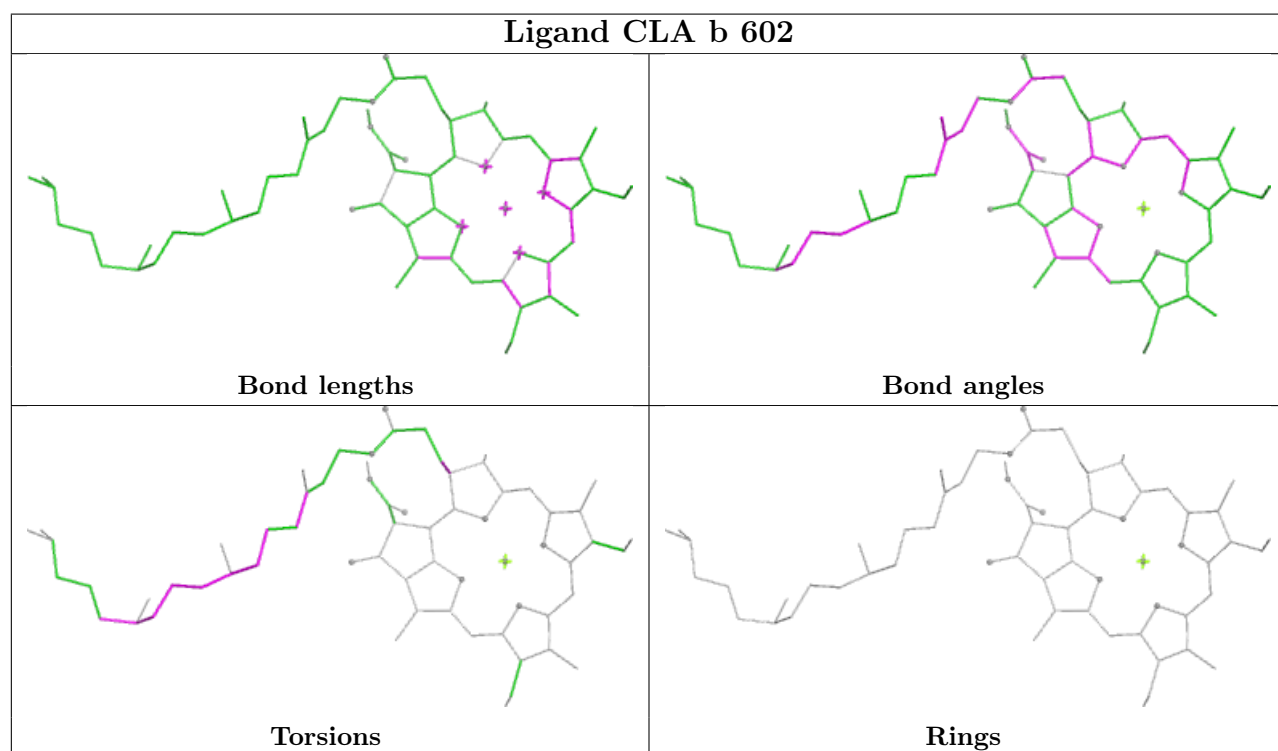
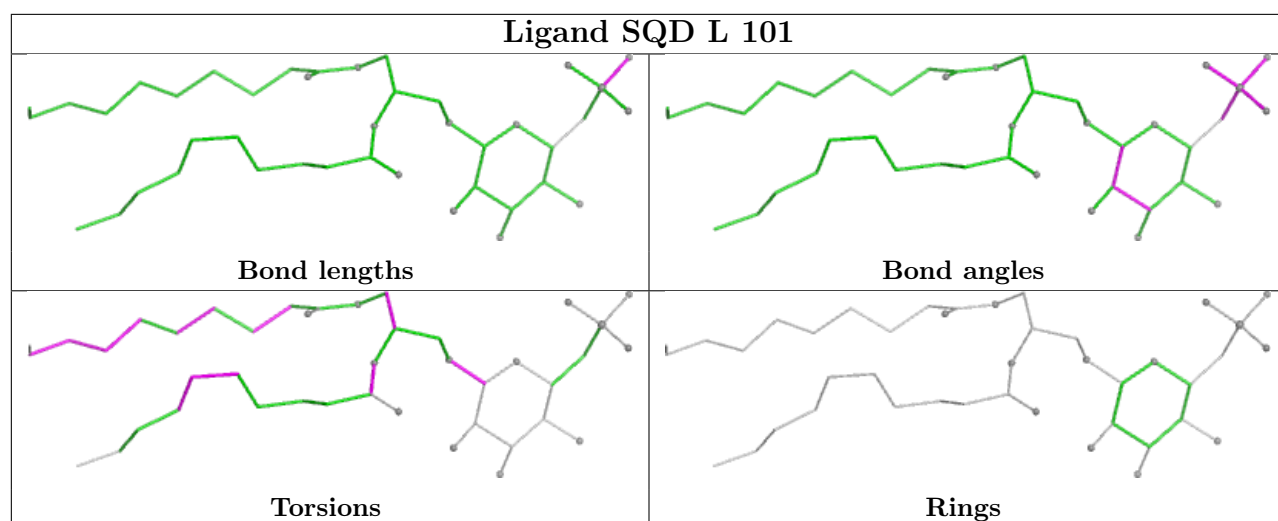
Ligand BCR i 101

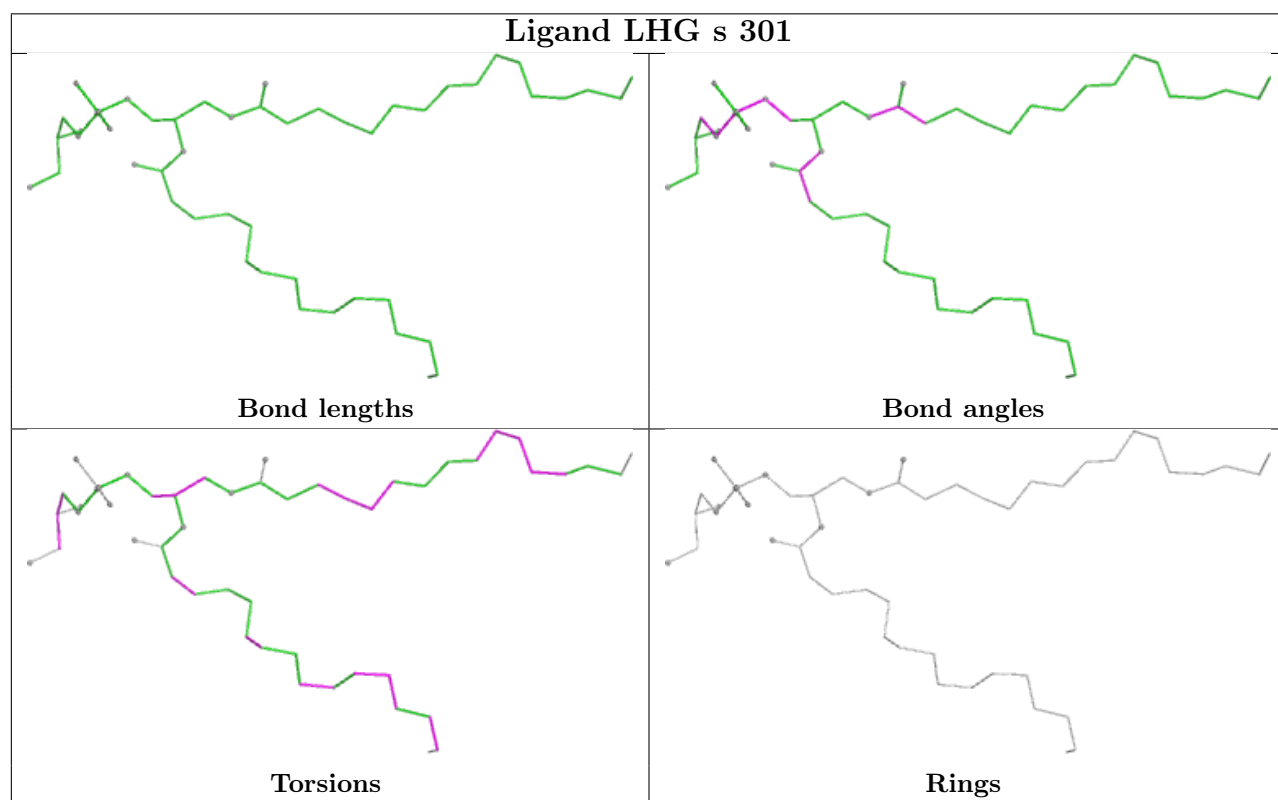
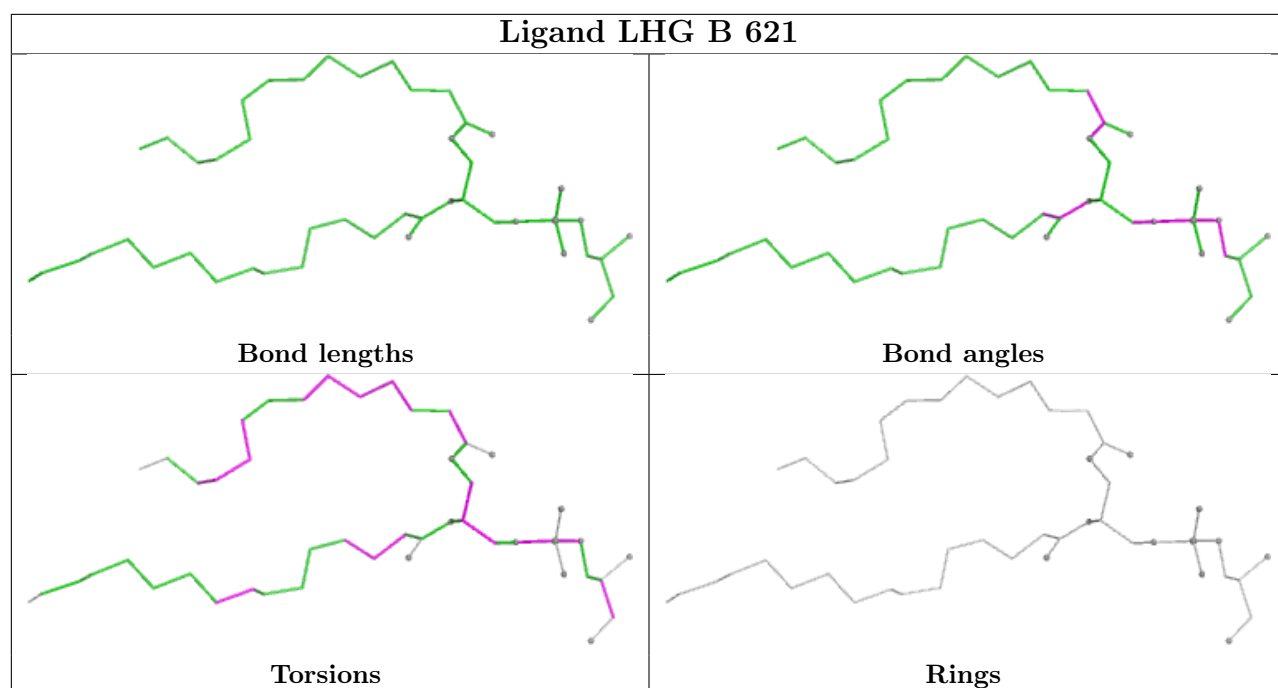




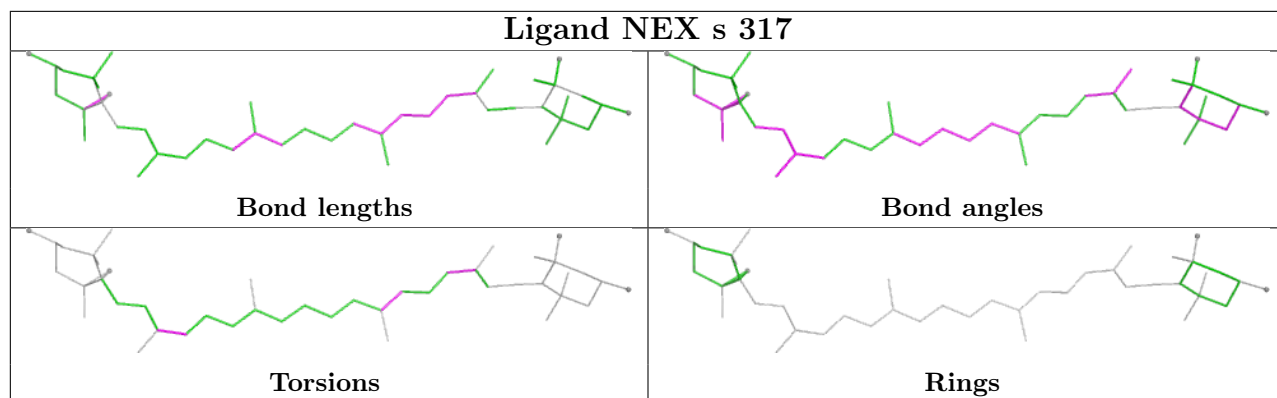




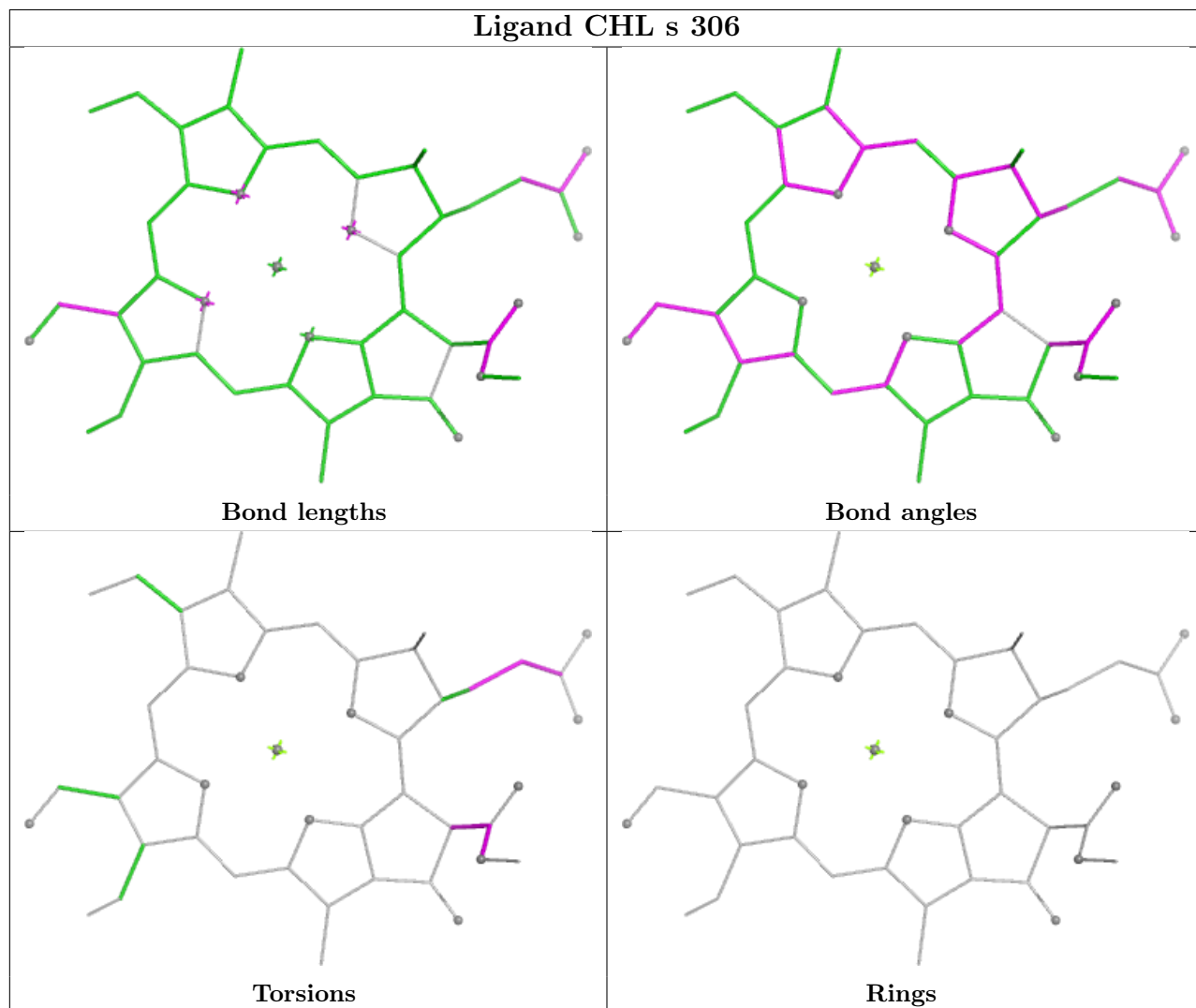


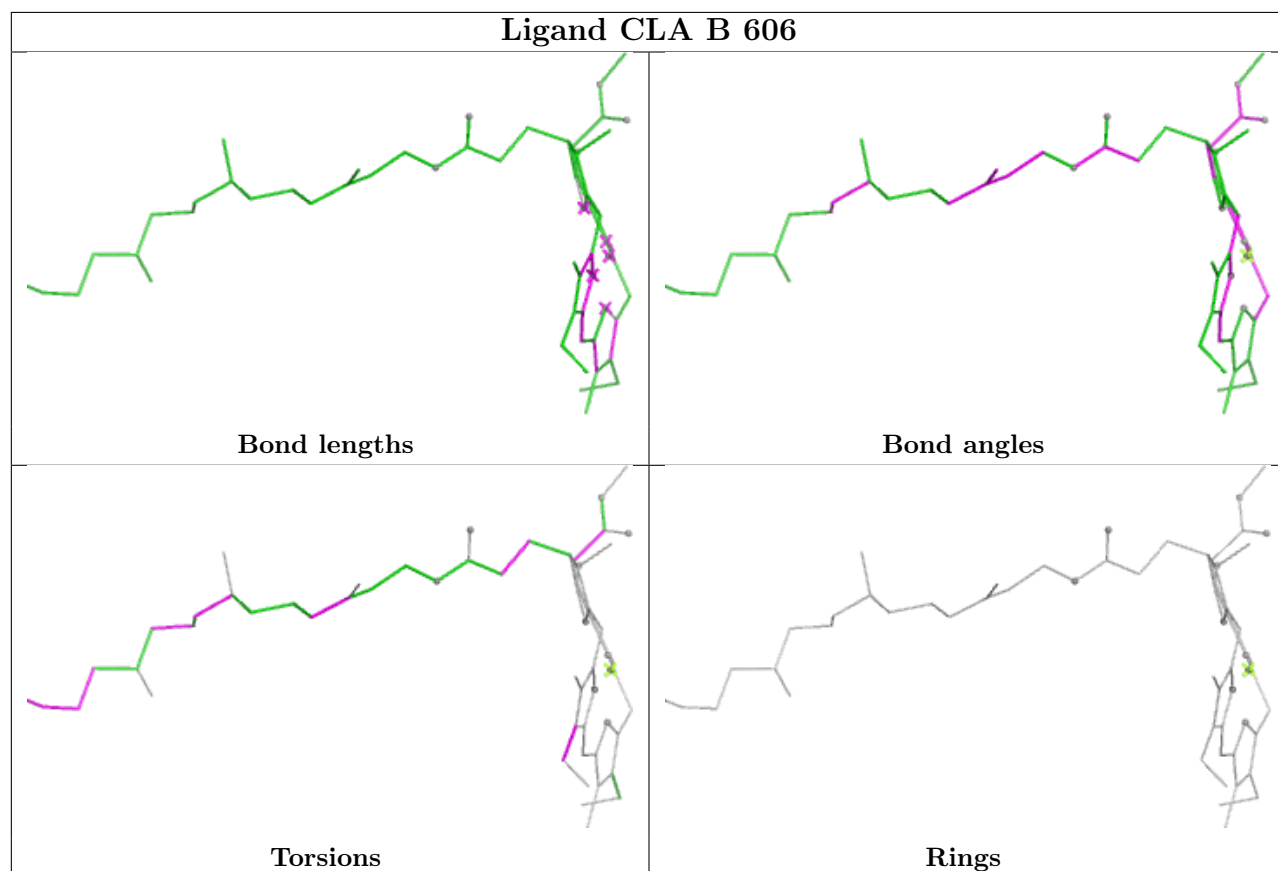
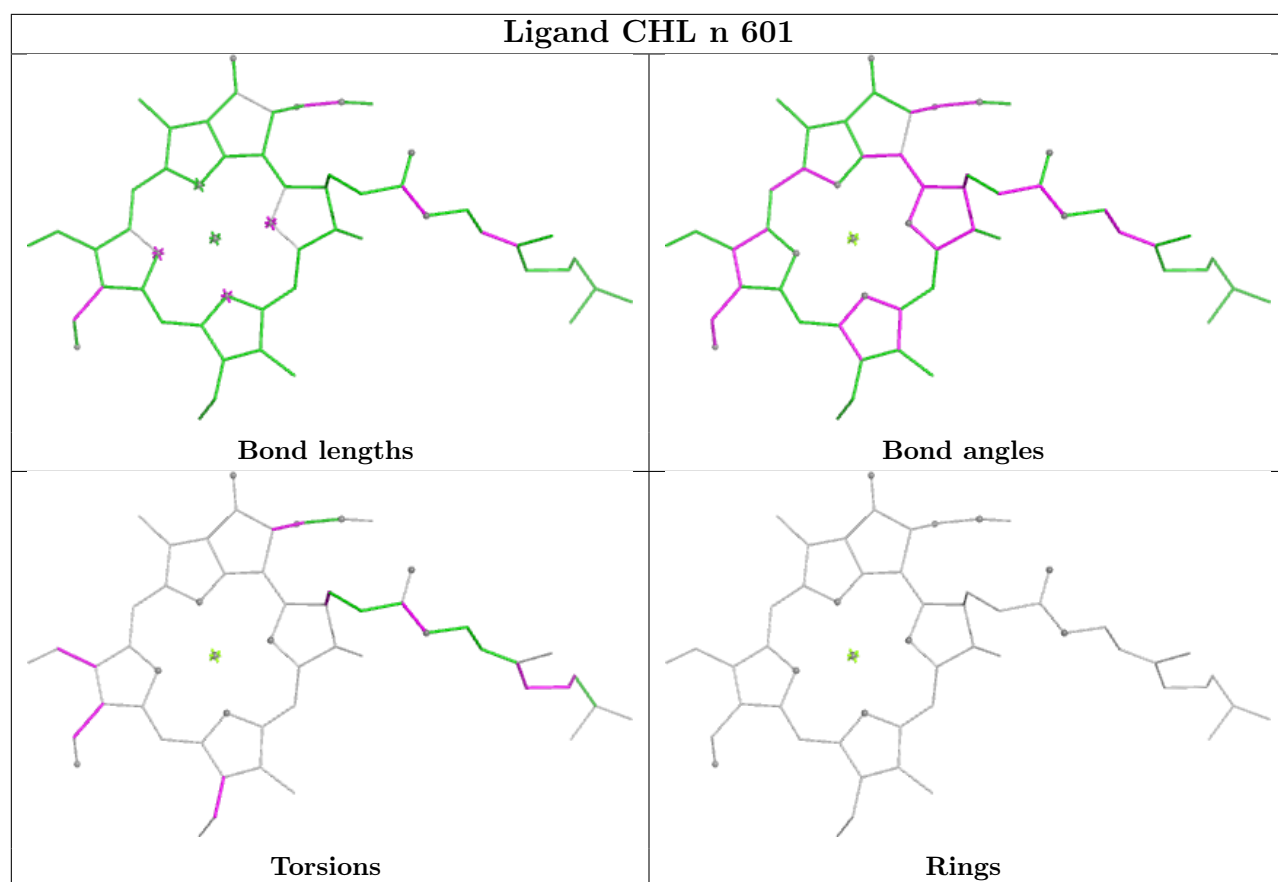


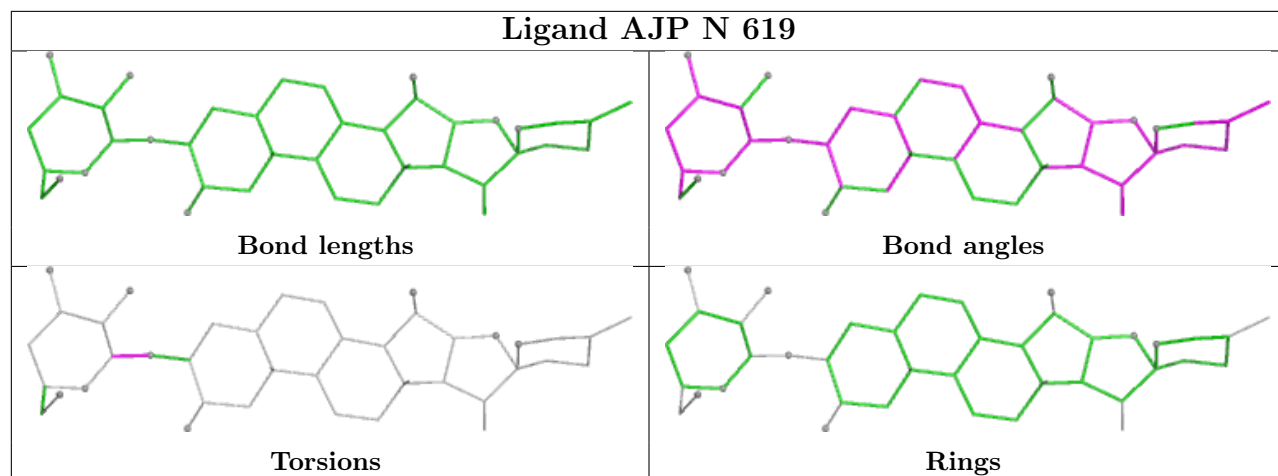
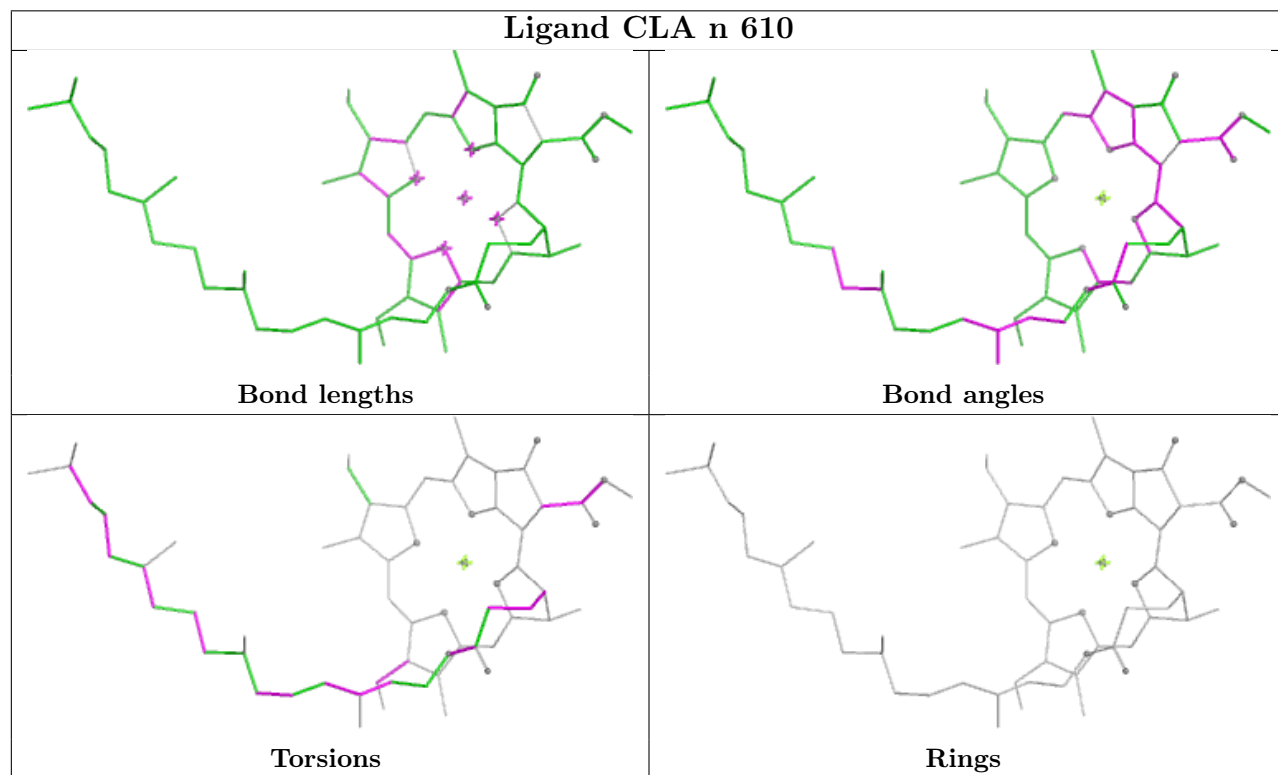
Ligand NEX s 317

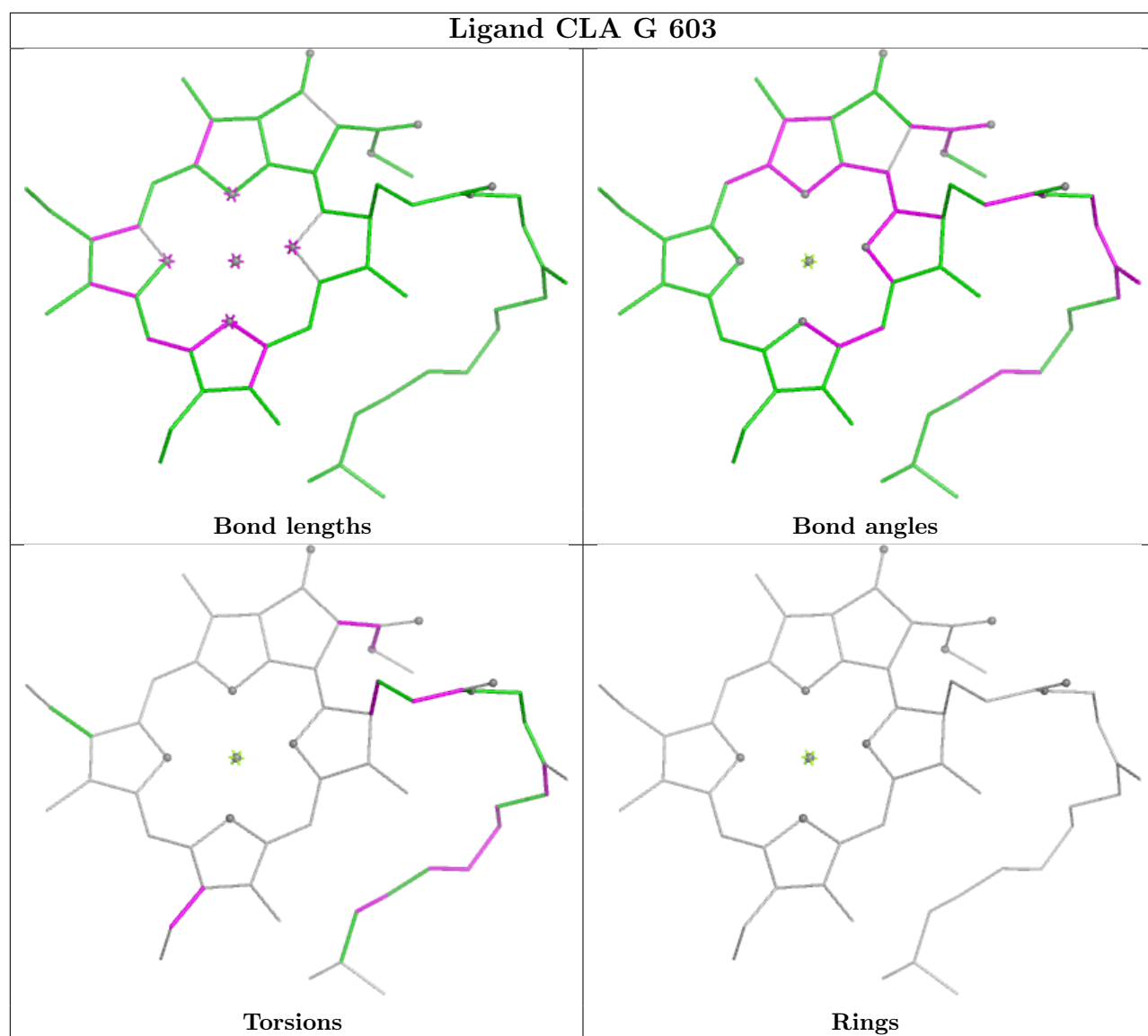


Ligand CHL s 306

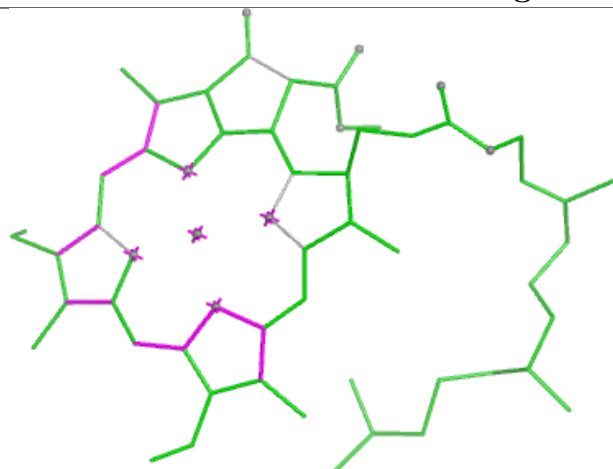




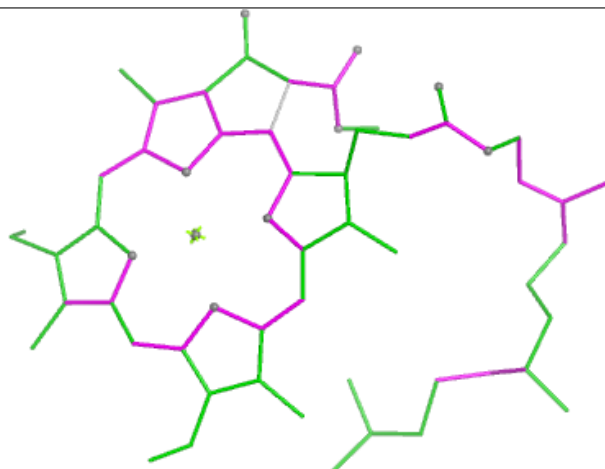
Ligand AJP N 619**Ligand CLA n 610**



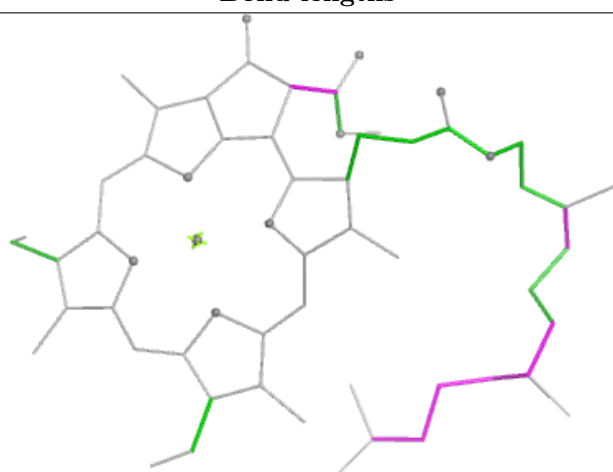
Ligand CLA Y 313



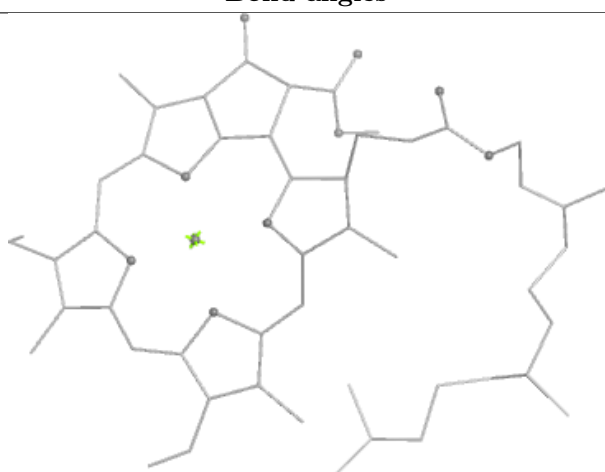
Bond lengths



Bond angles

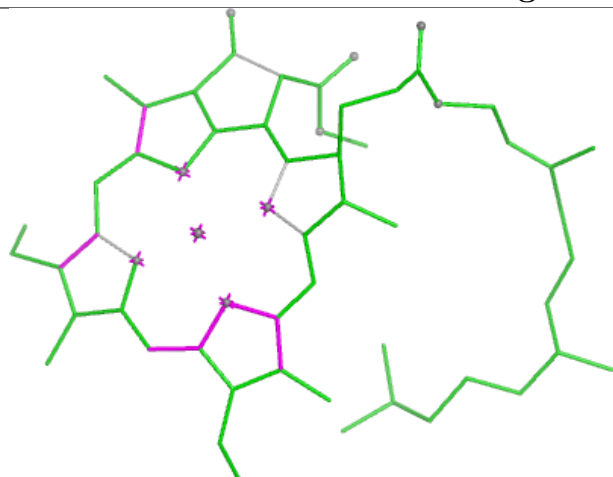


Torsions

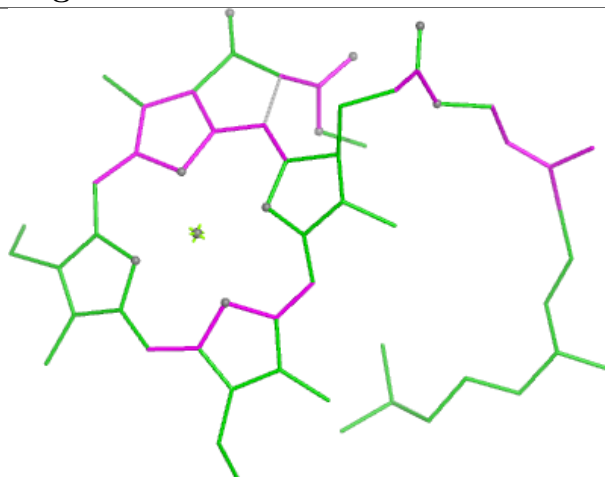


Rings

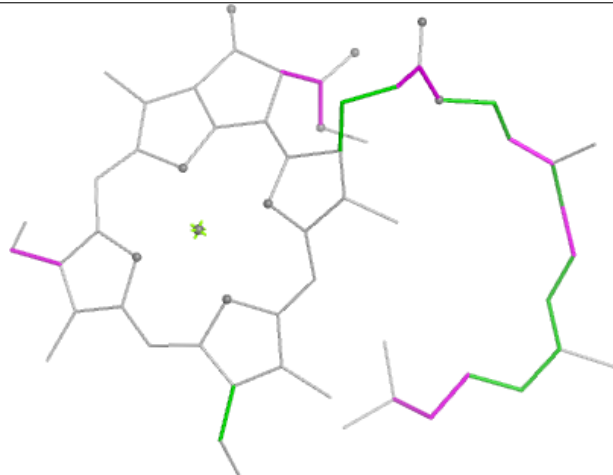
Ligand CLA g 612



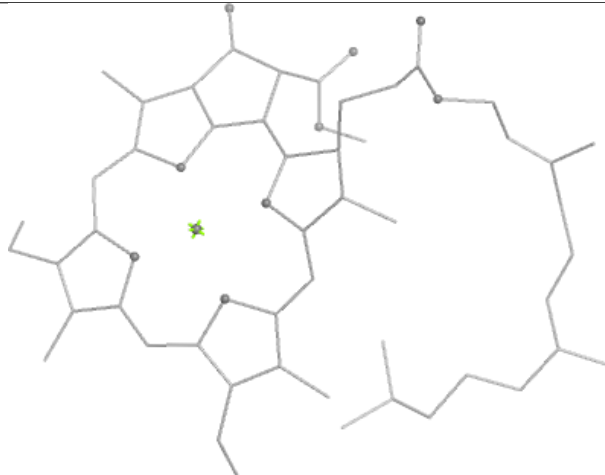
Bond lengths



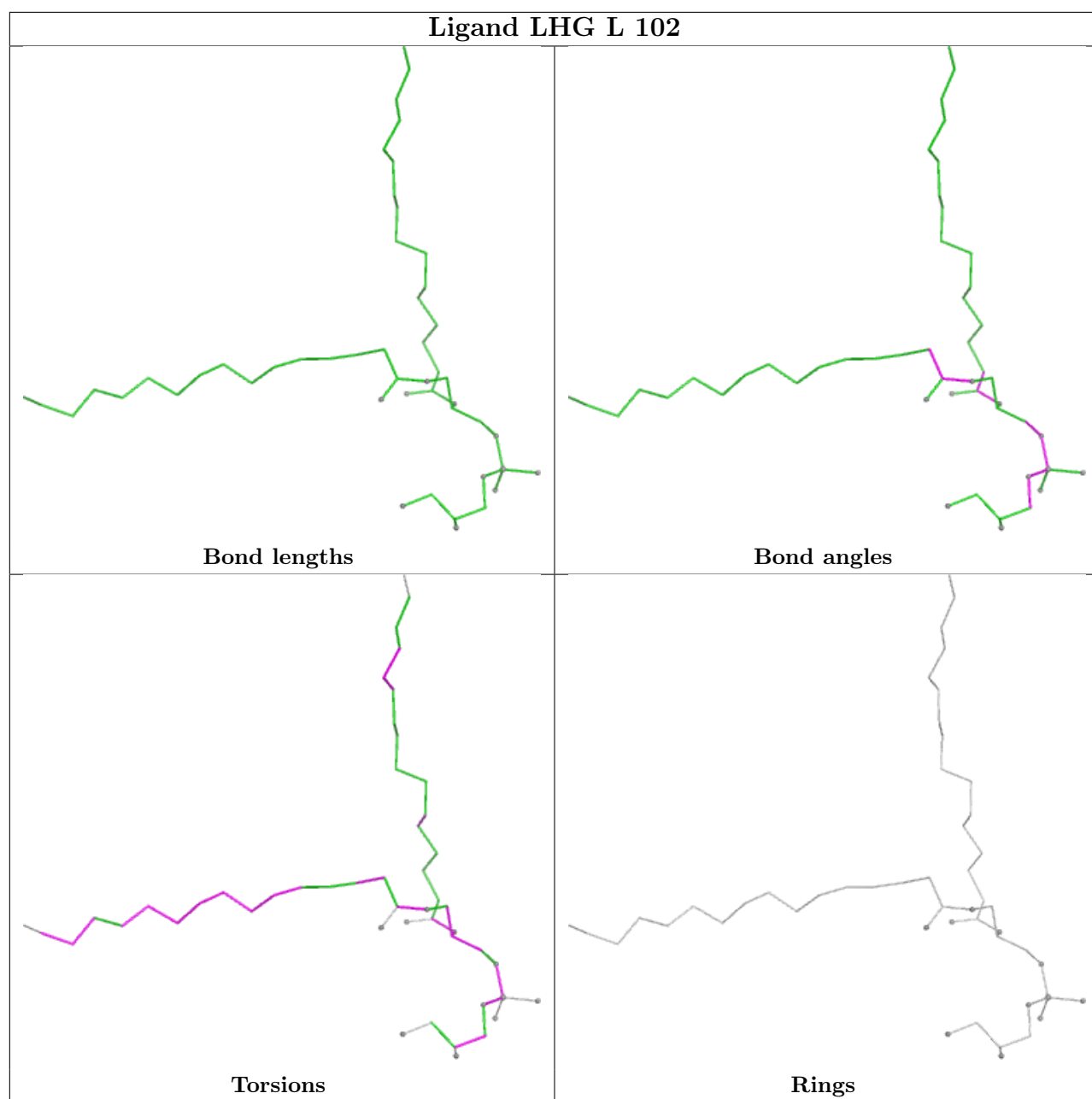
Bond angles



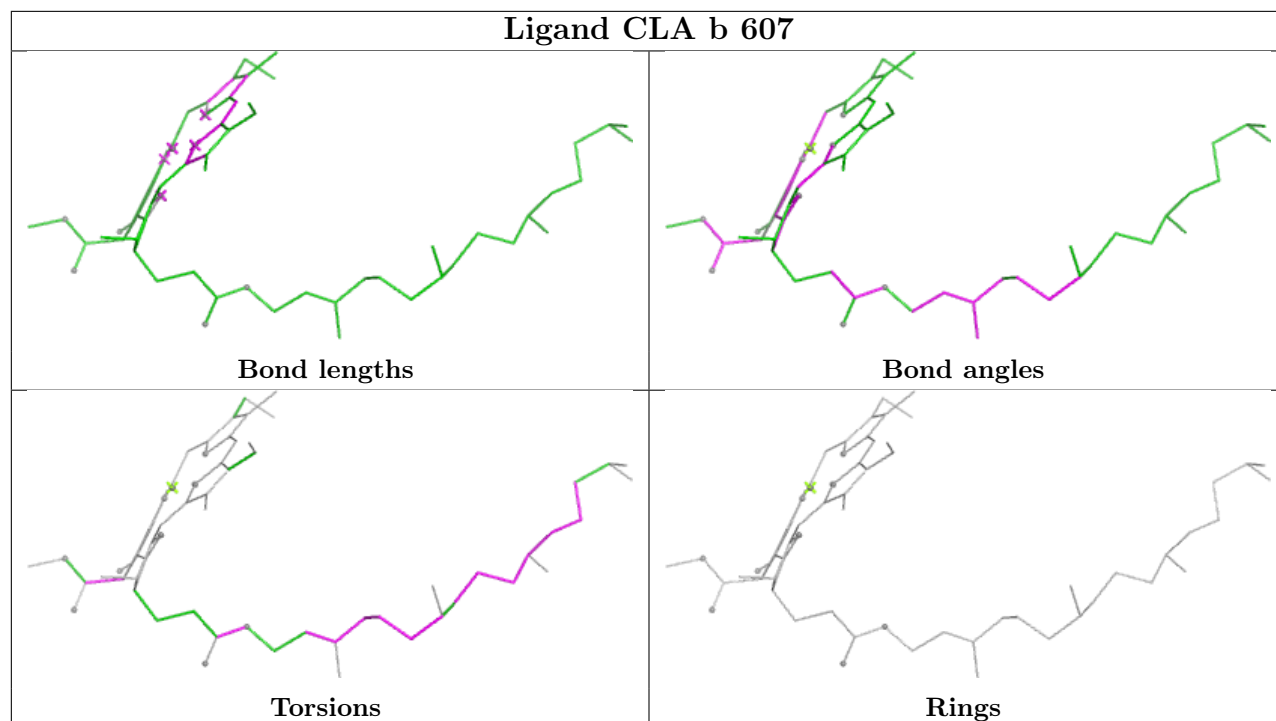
Torsions



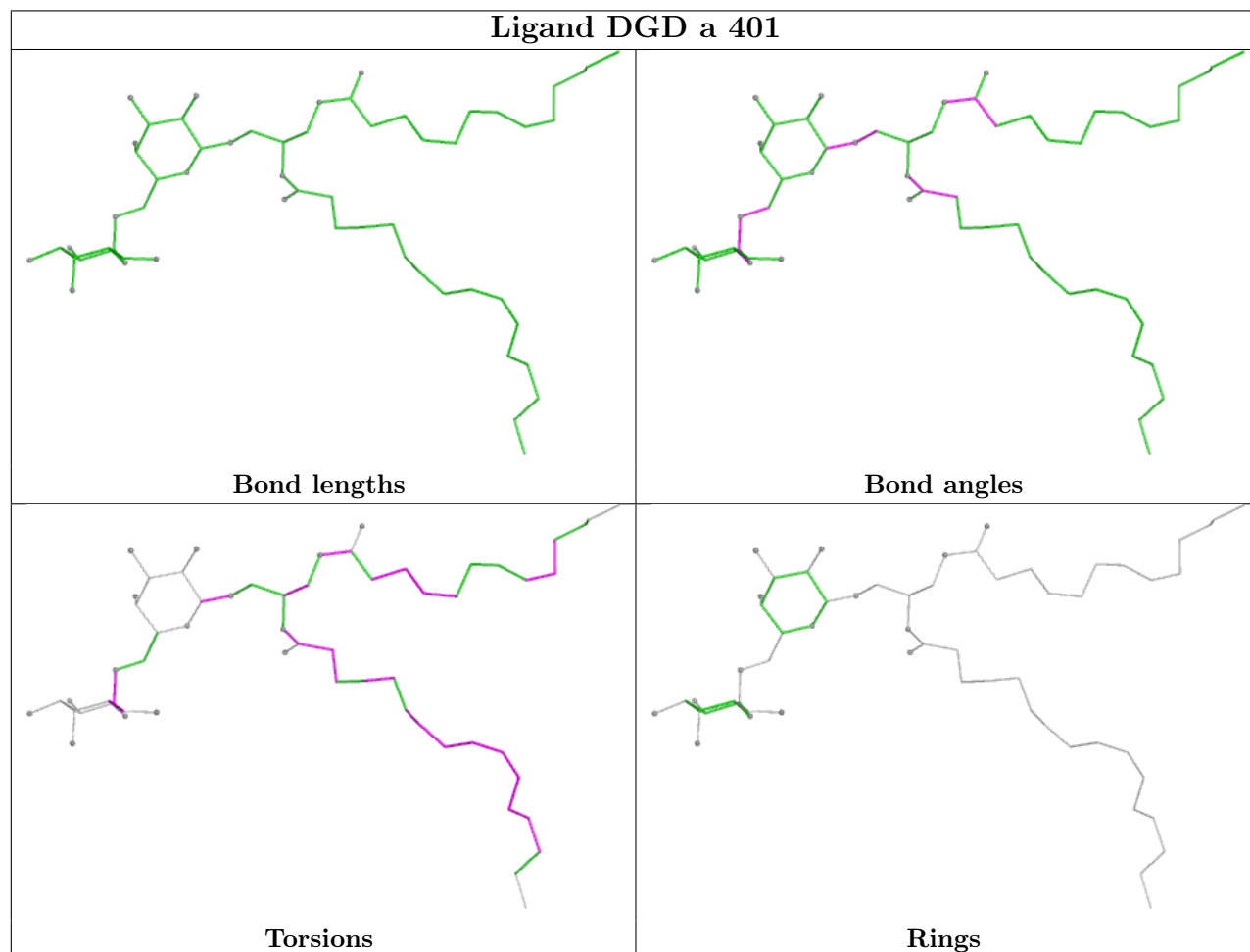
Rings

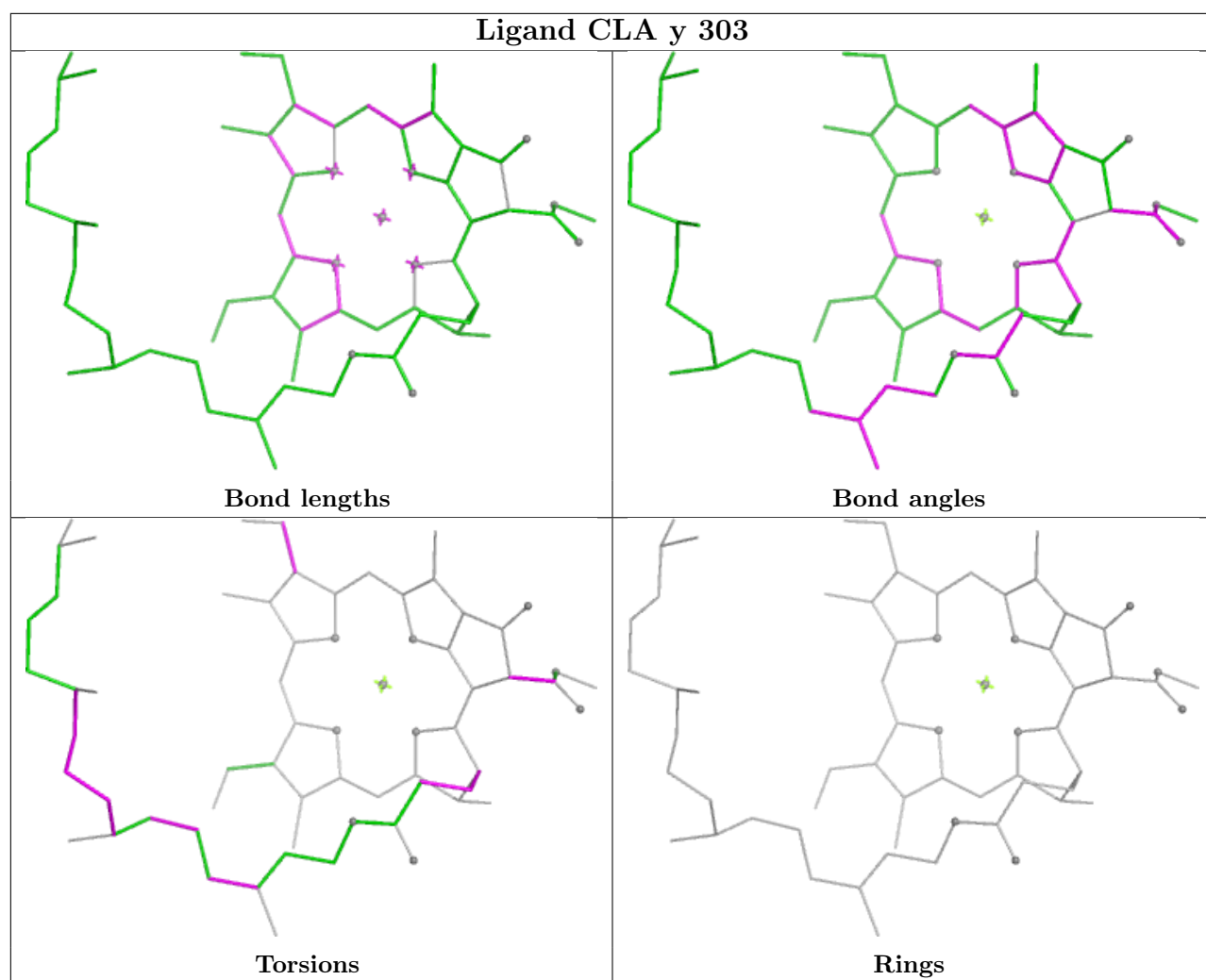


Ligand CLA b 607

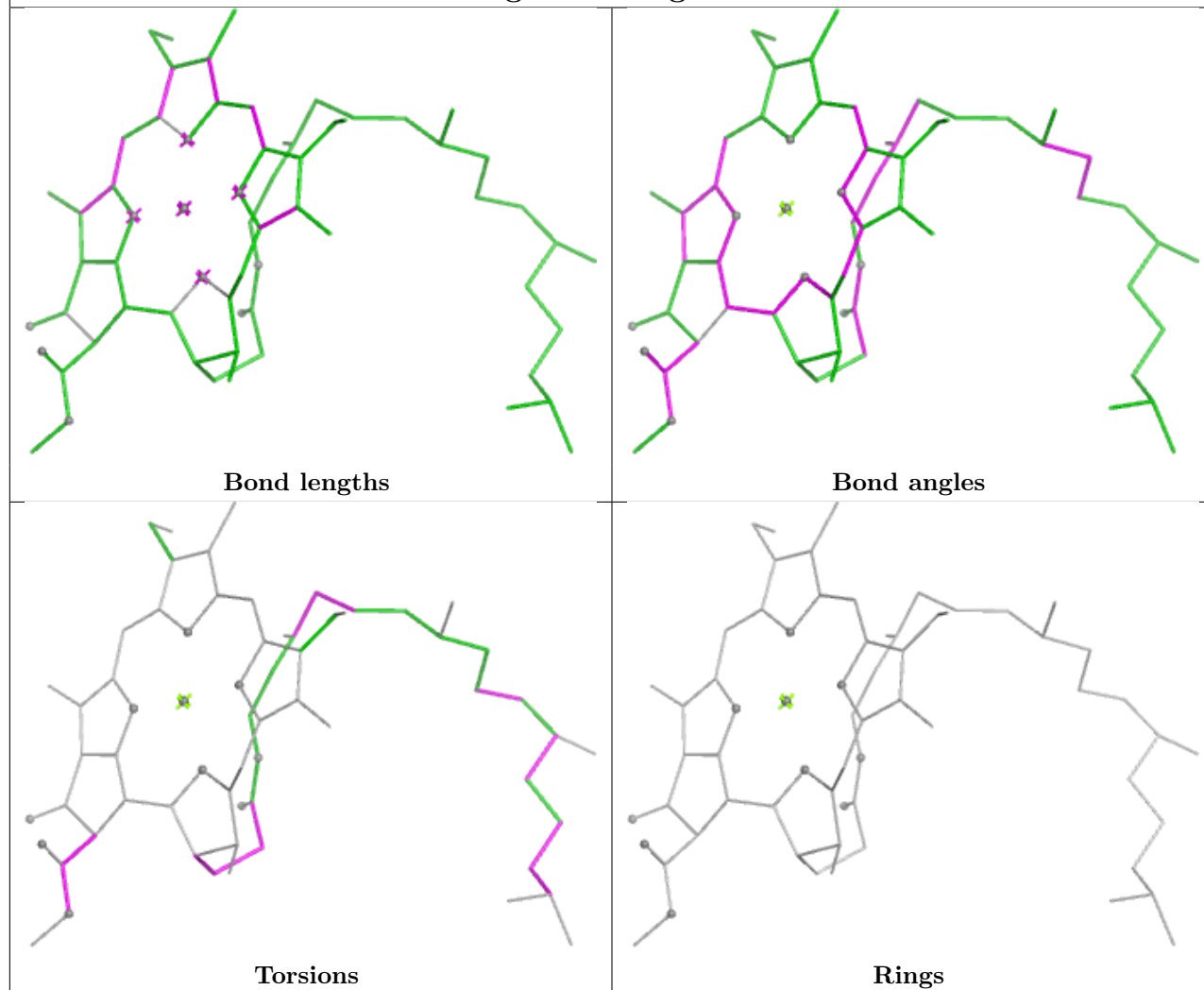


Ligand DGD a 401

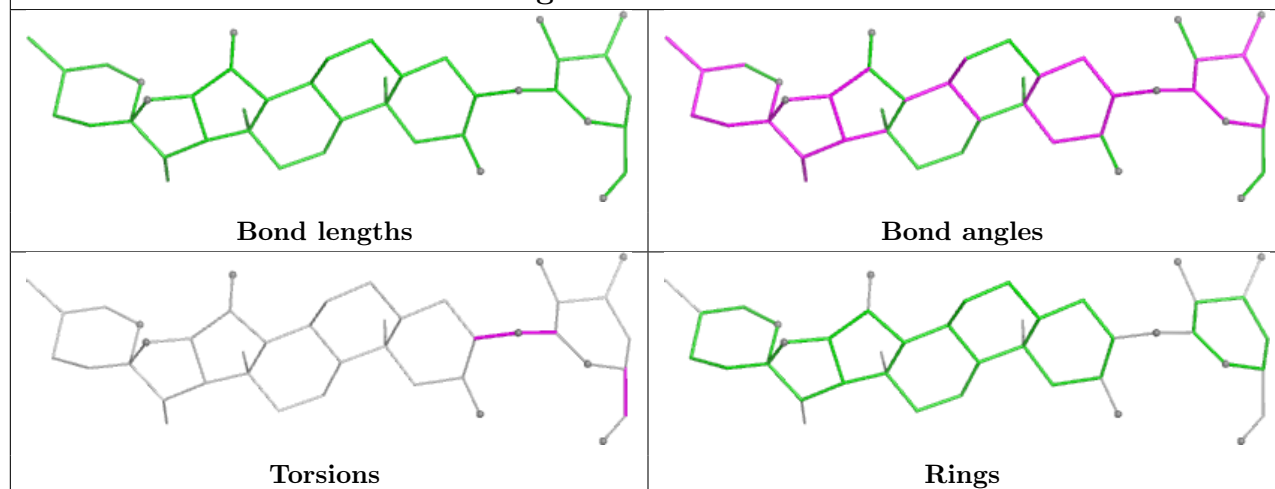




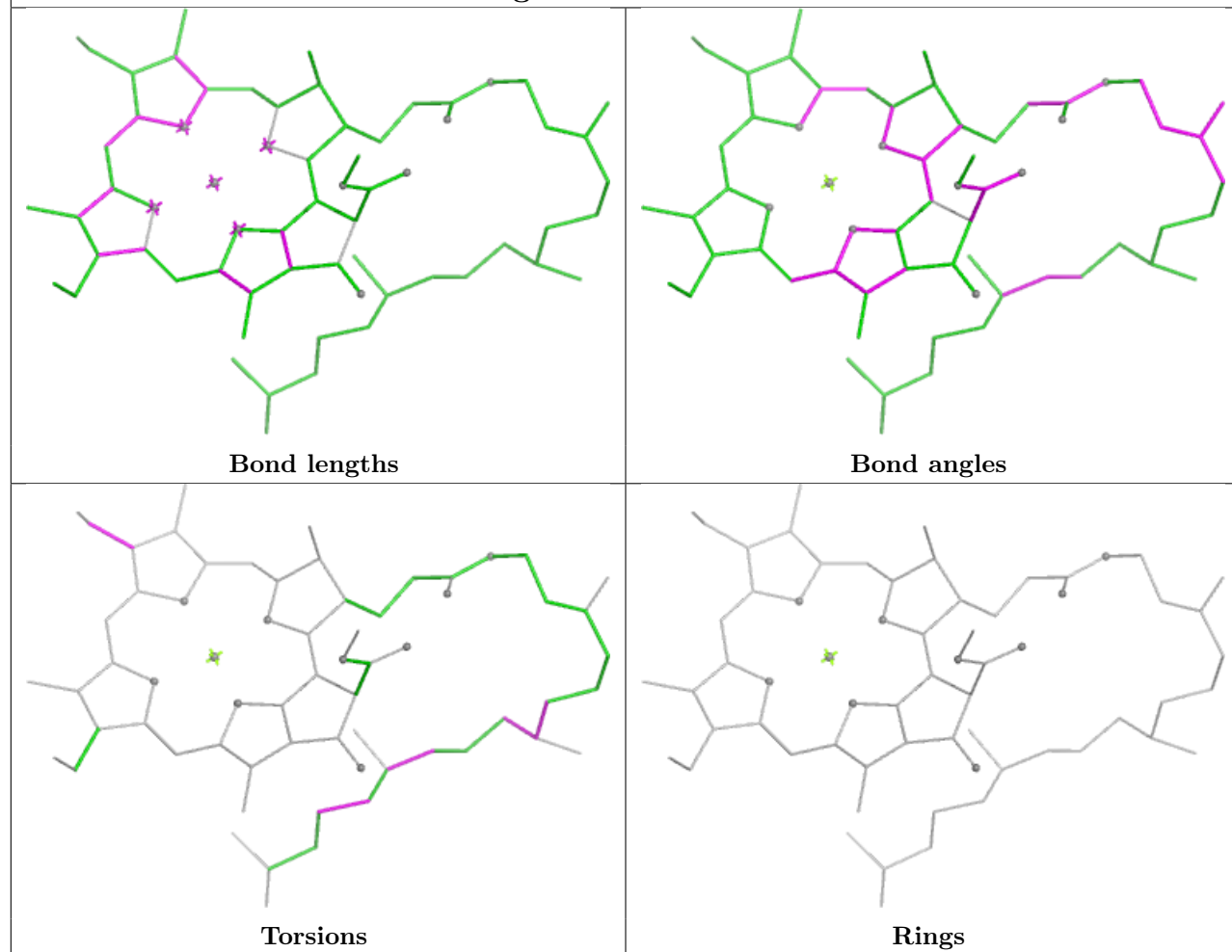
Ligand CLA g 613

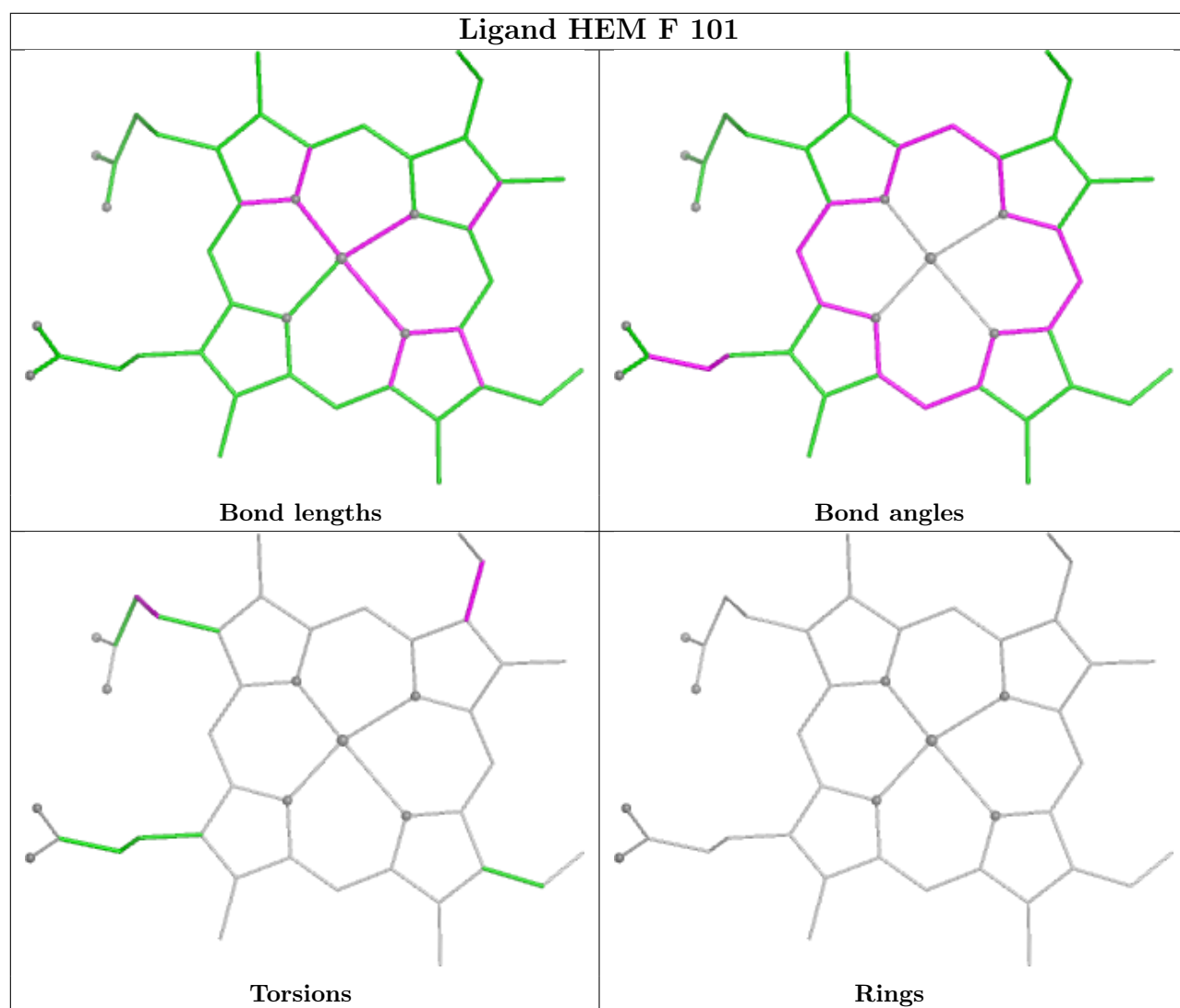


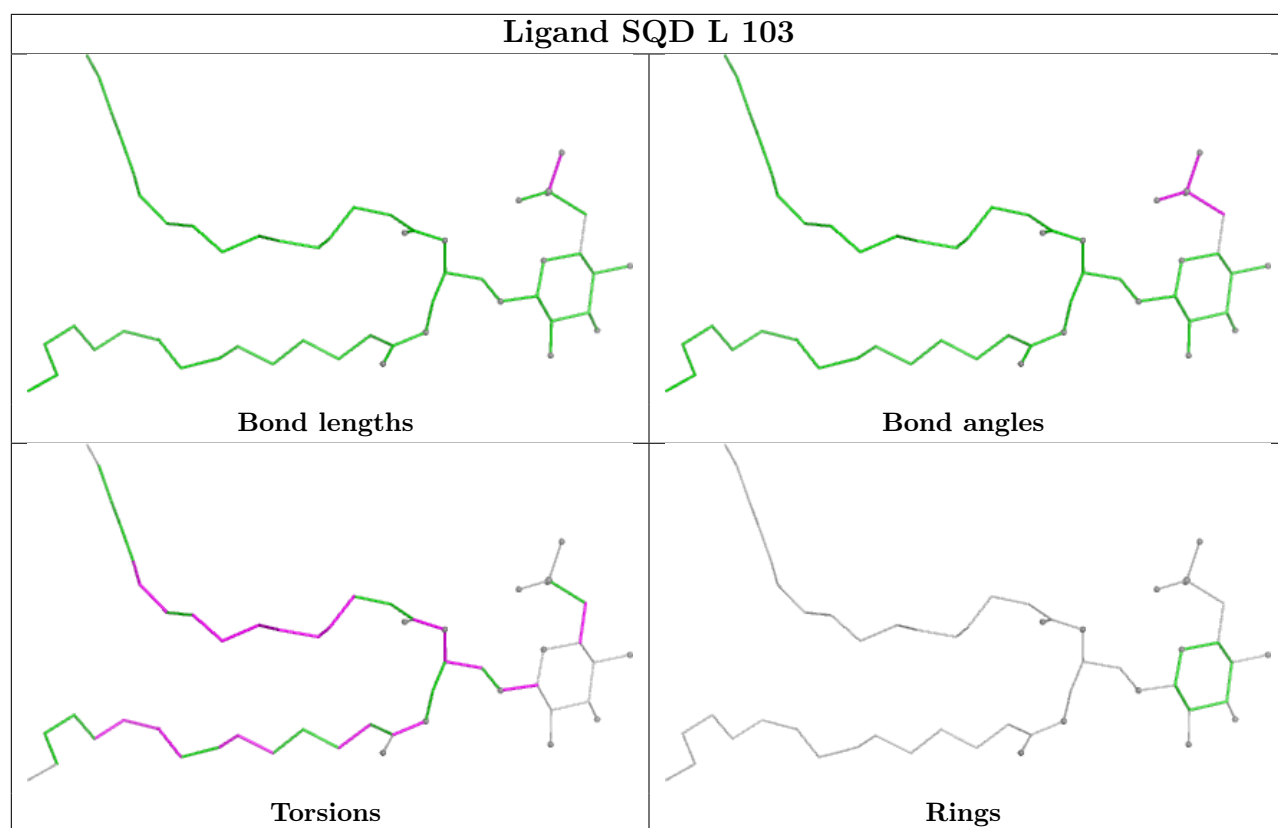
Ligand AJP n 620



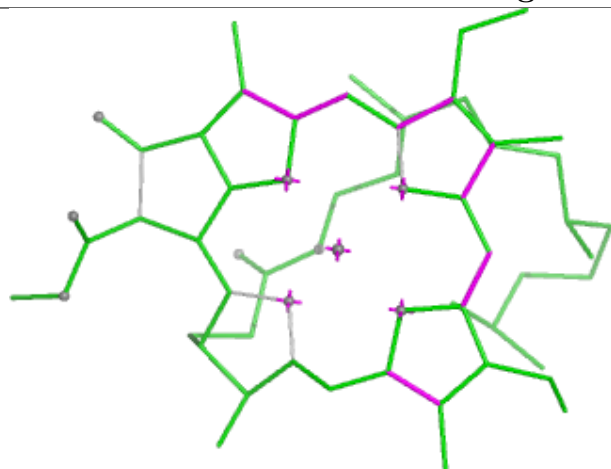
Ligand CLA C 509



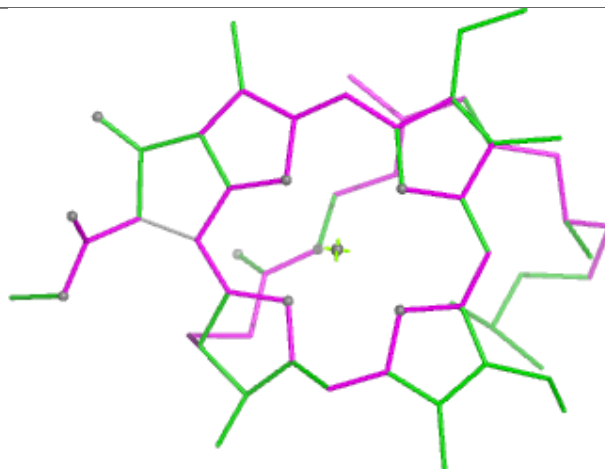




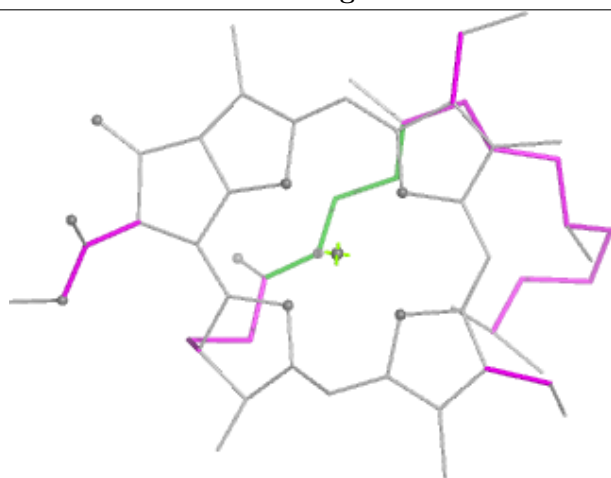
Ligand CLA n 613



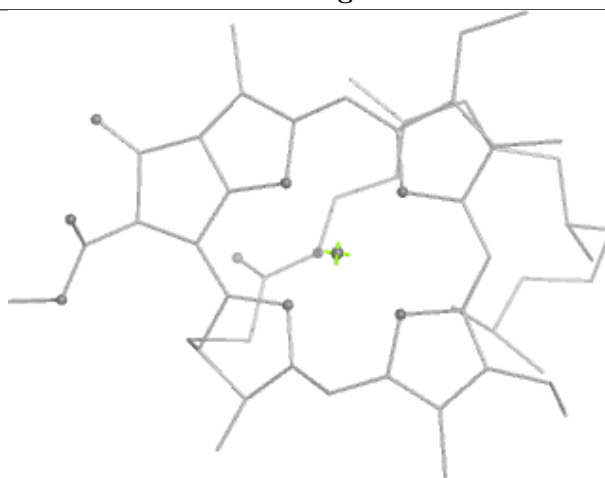
Bond lengths



Bond angles

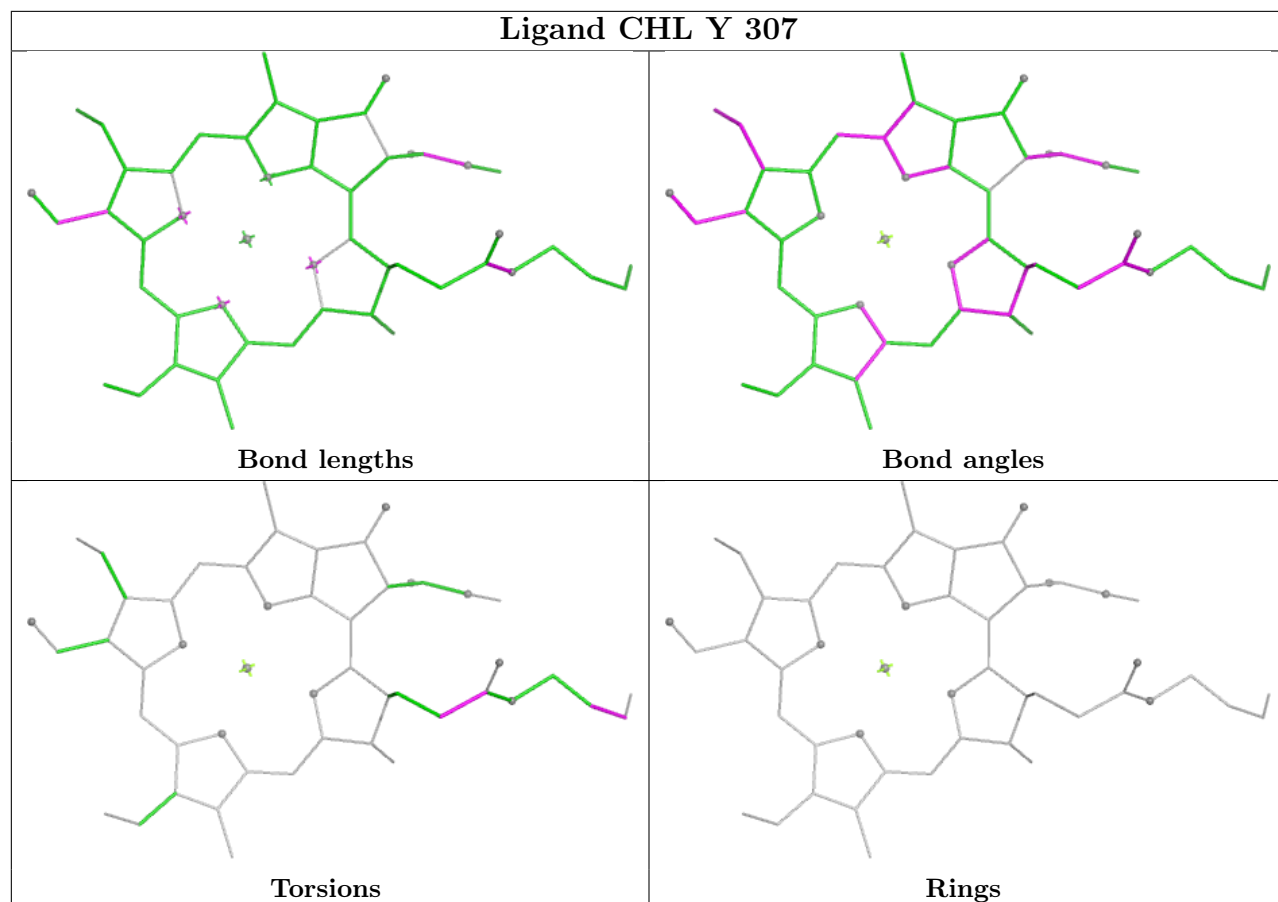


Torsions

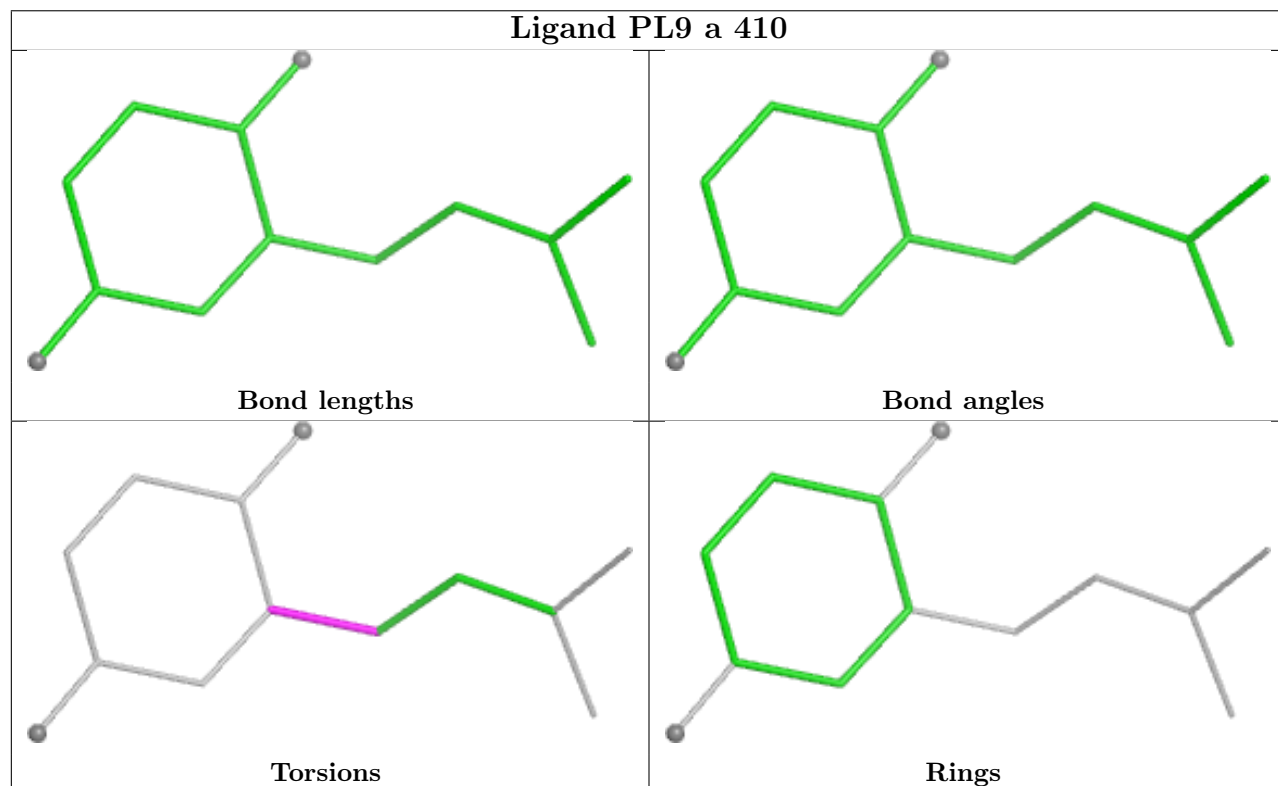


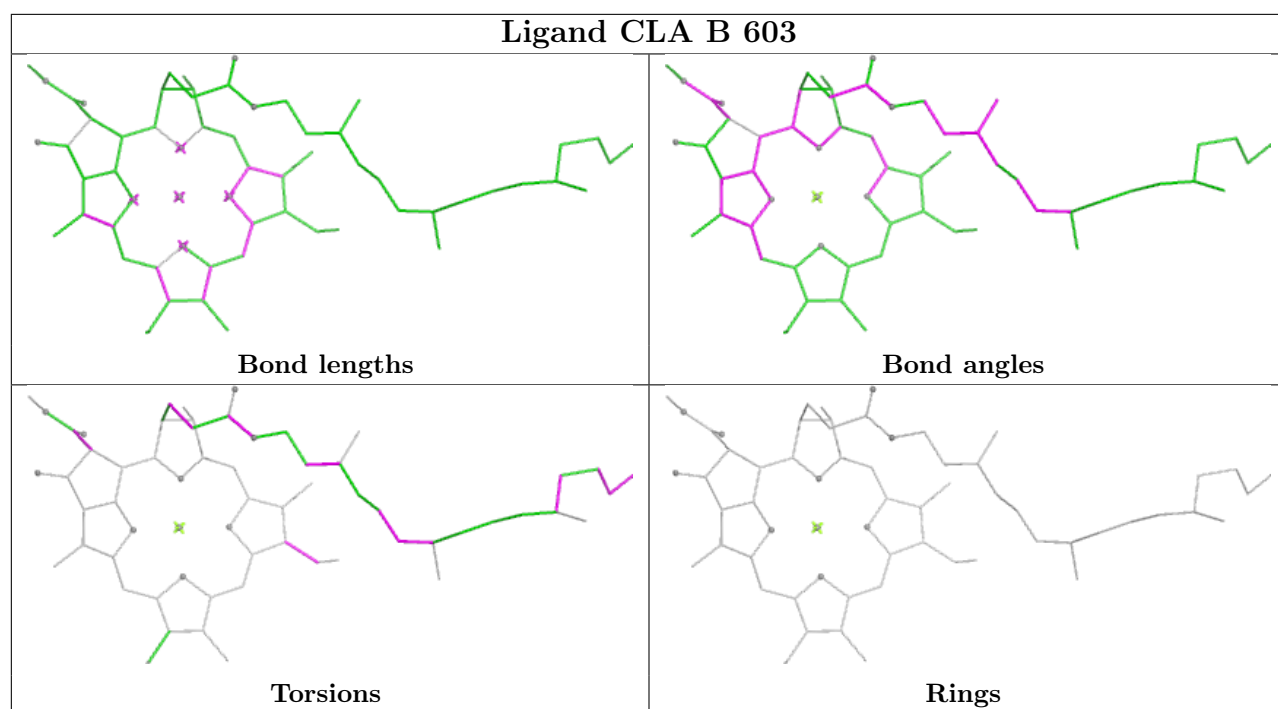
Rings

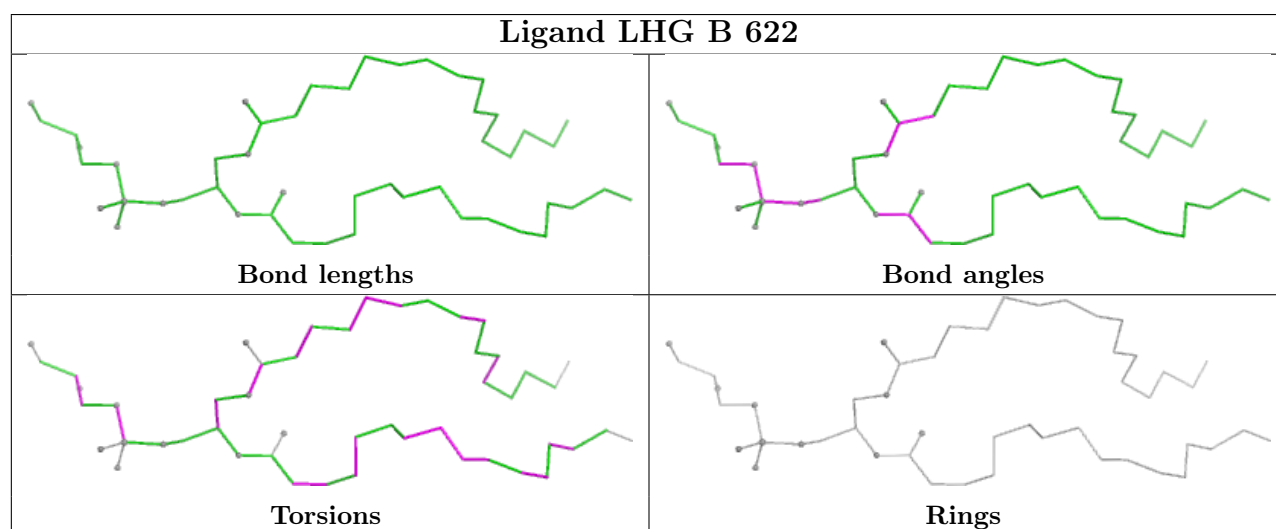
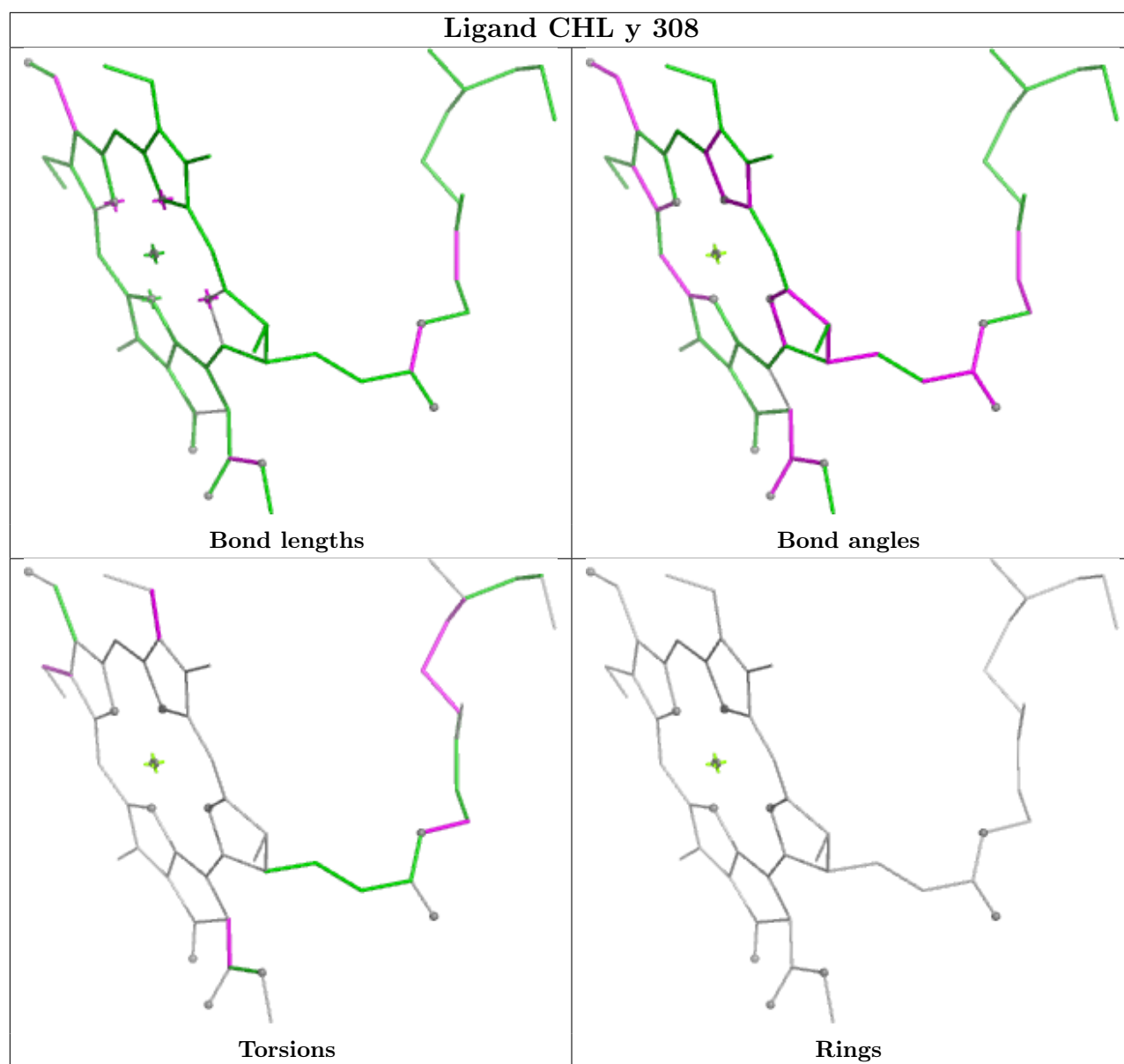
Ligand CHL Y 307

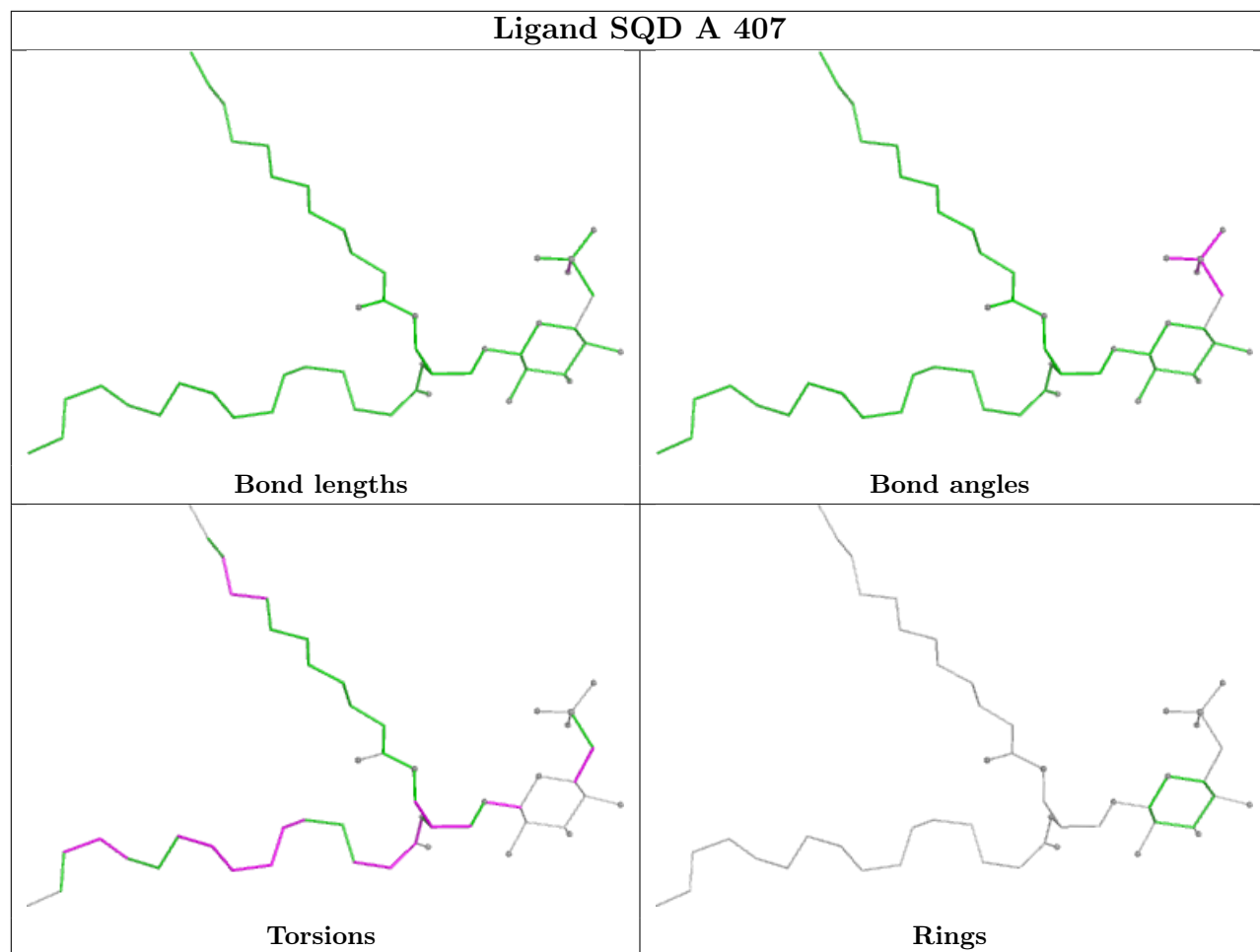


Ligand PL9 a 410

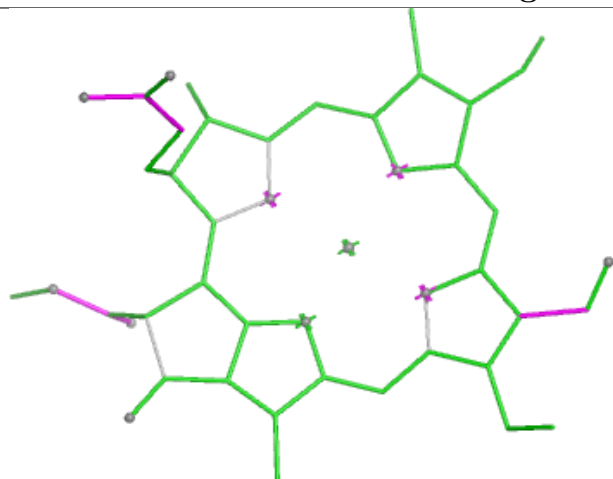




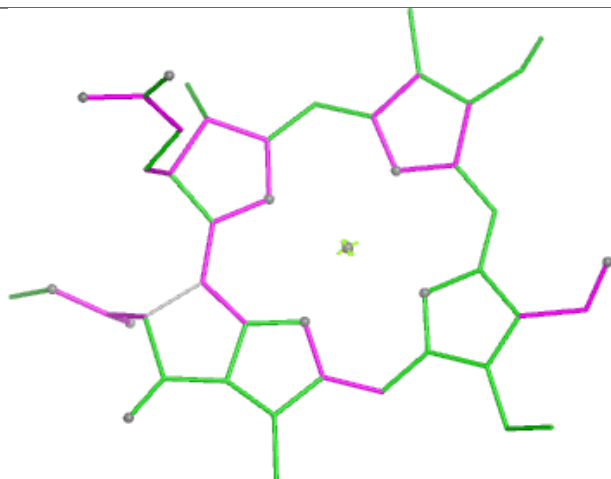




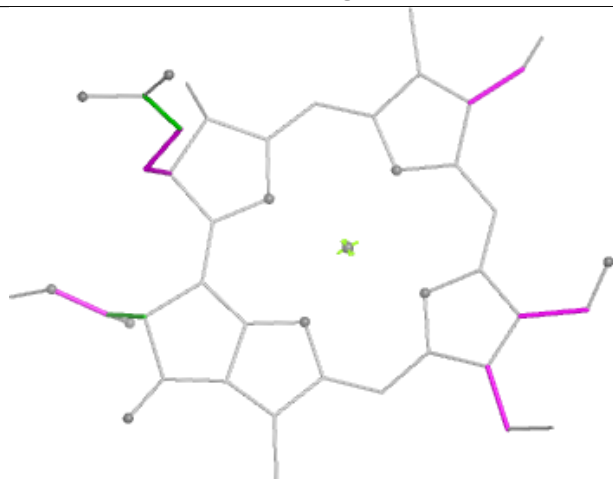
Ligand CHL s 307



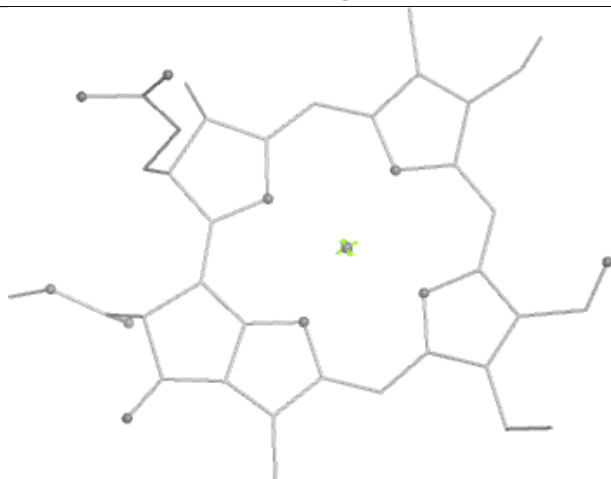
Bond lengths



Bond angles



Torsions



Rings

Ligand LUT y 316



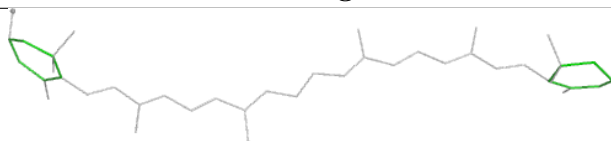
Bond lengths



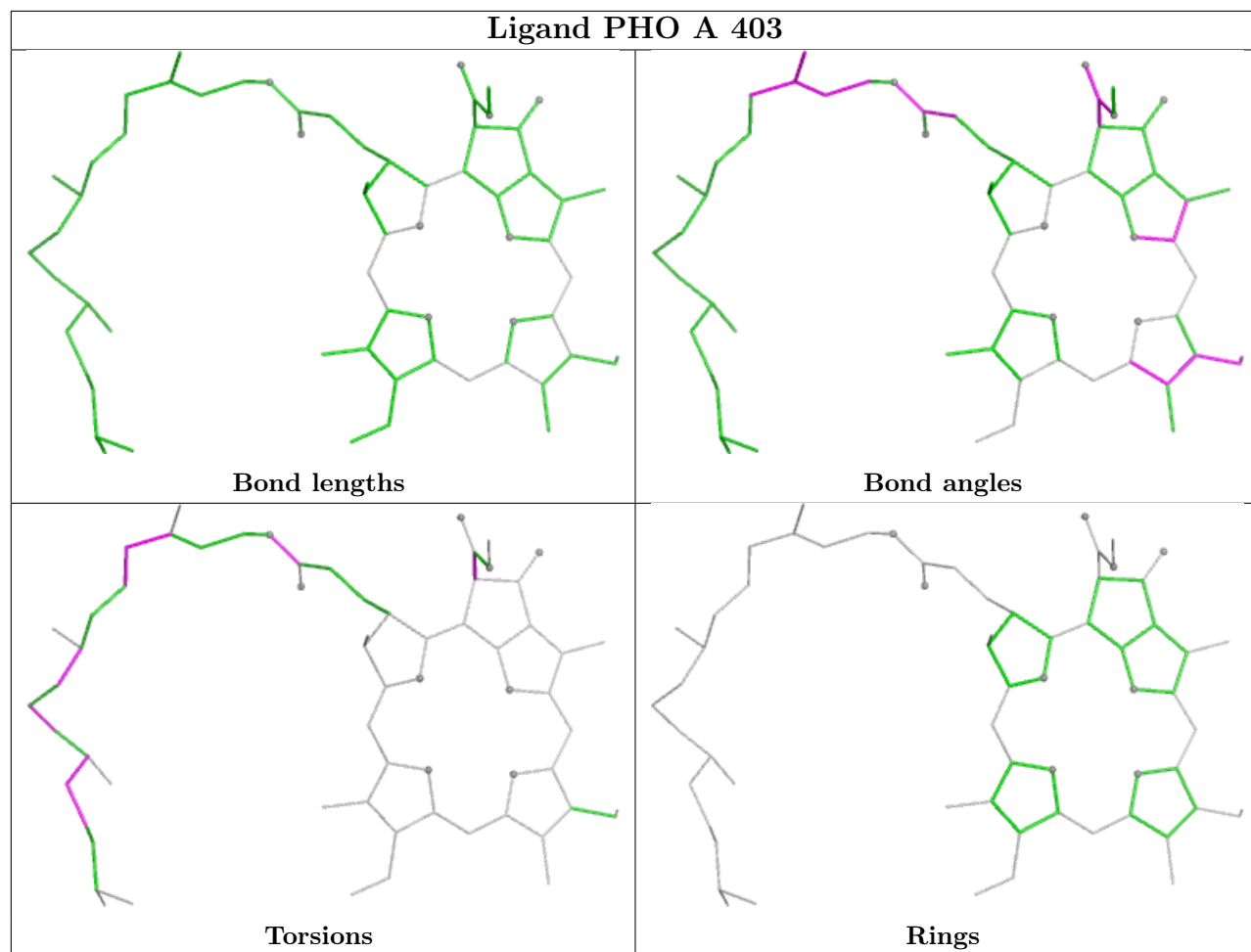
Bond angles

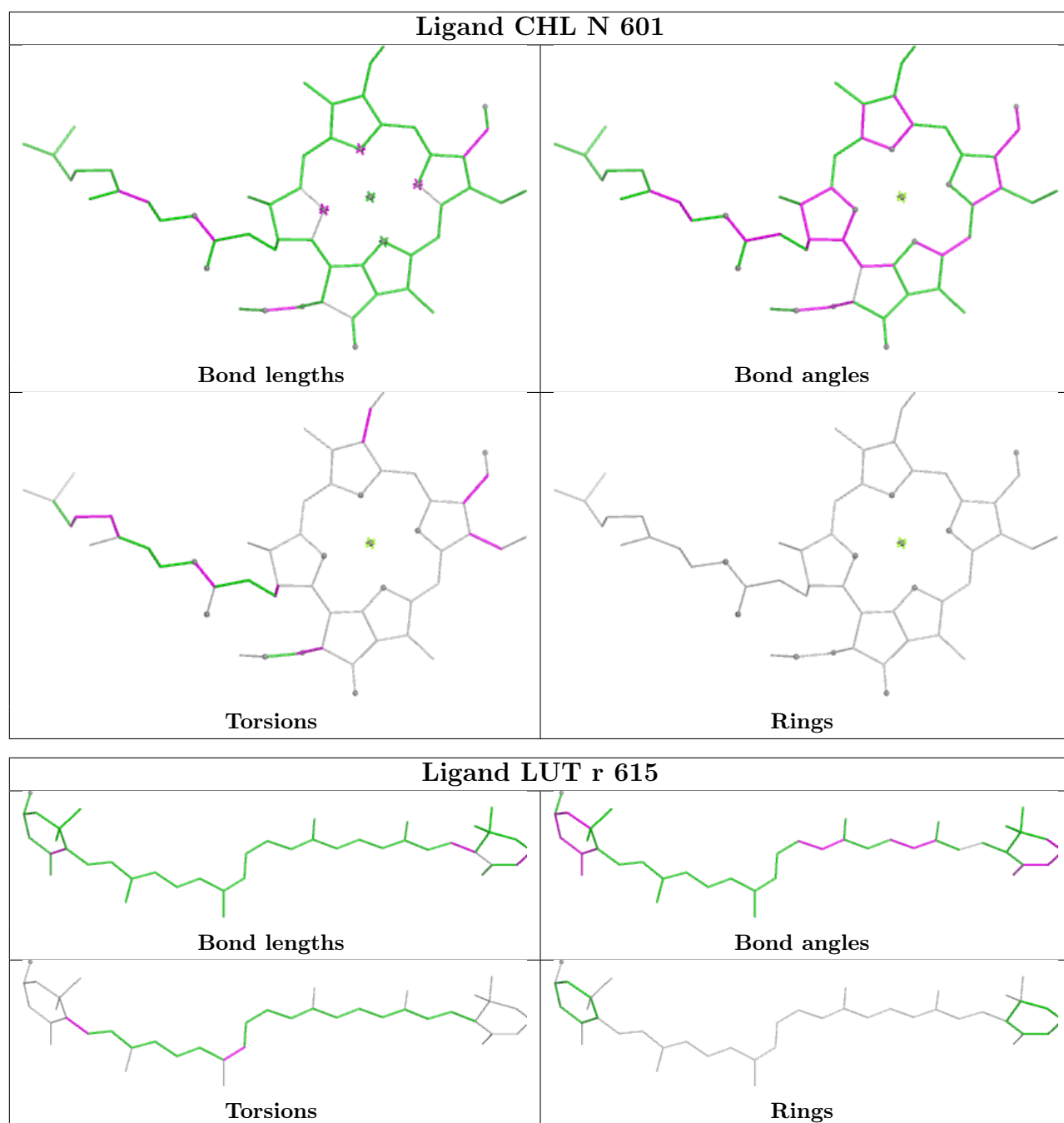


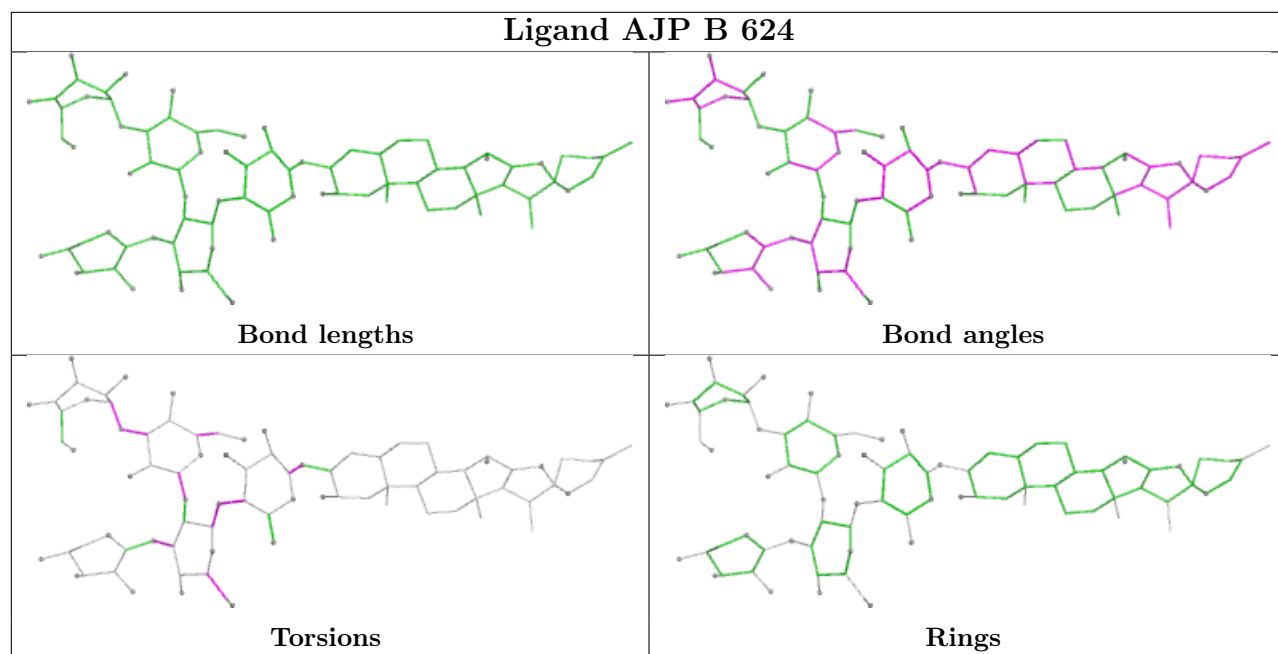
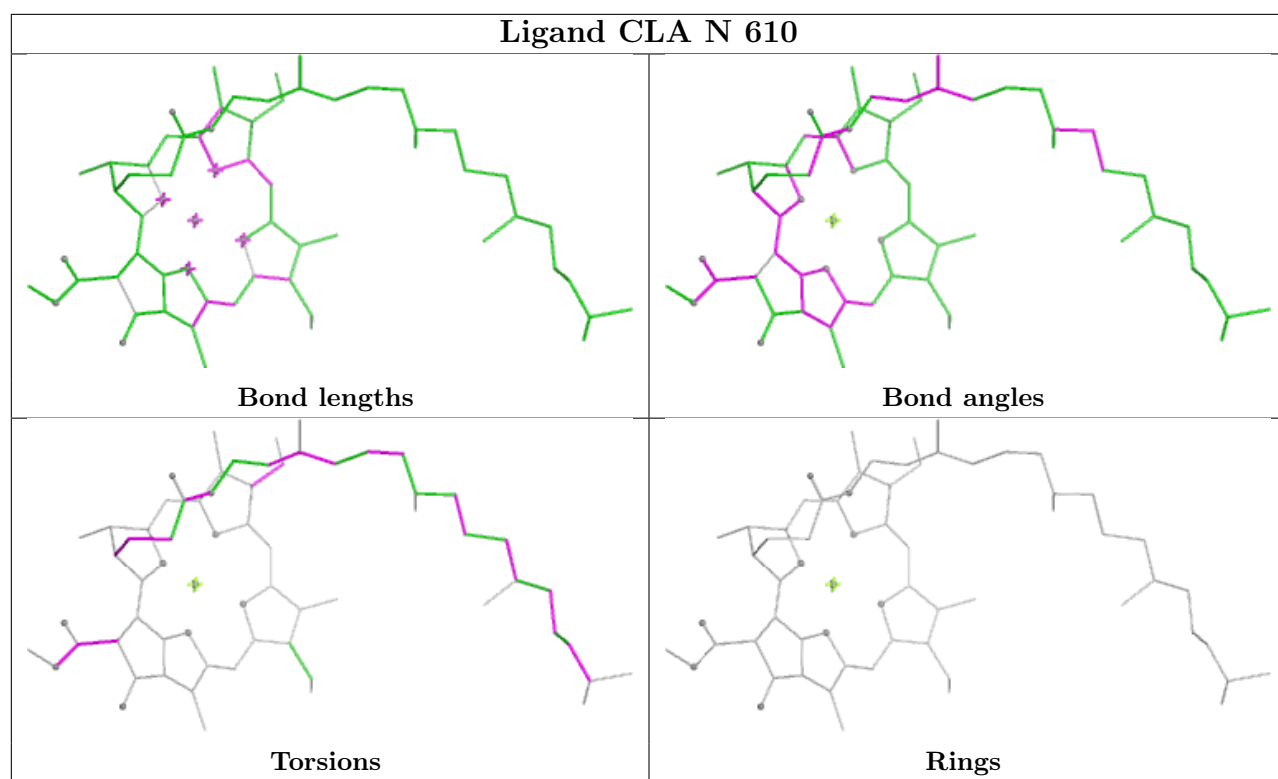
Torsions



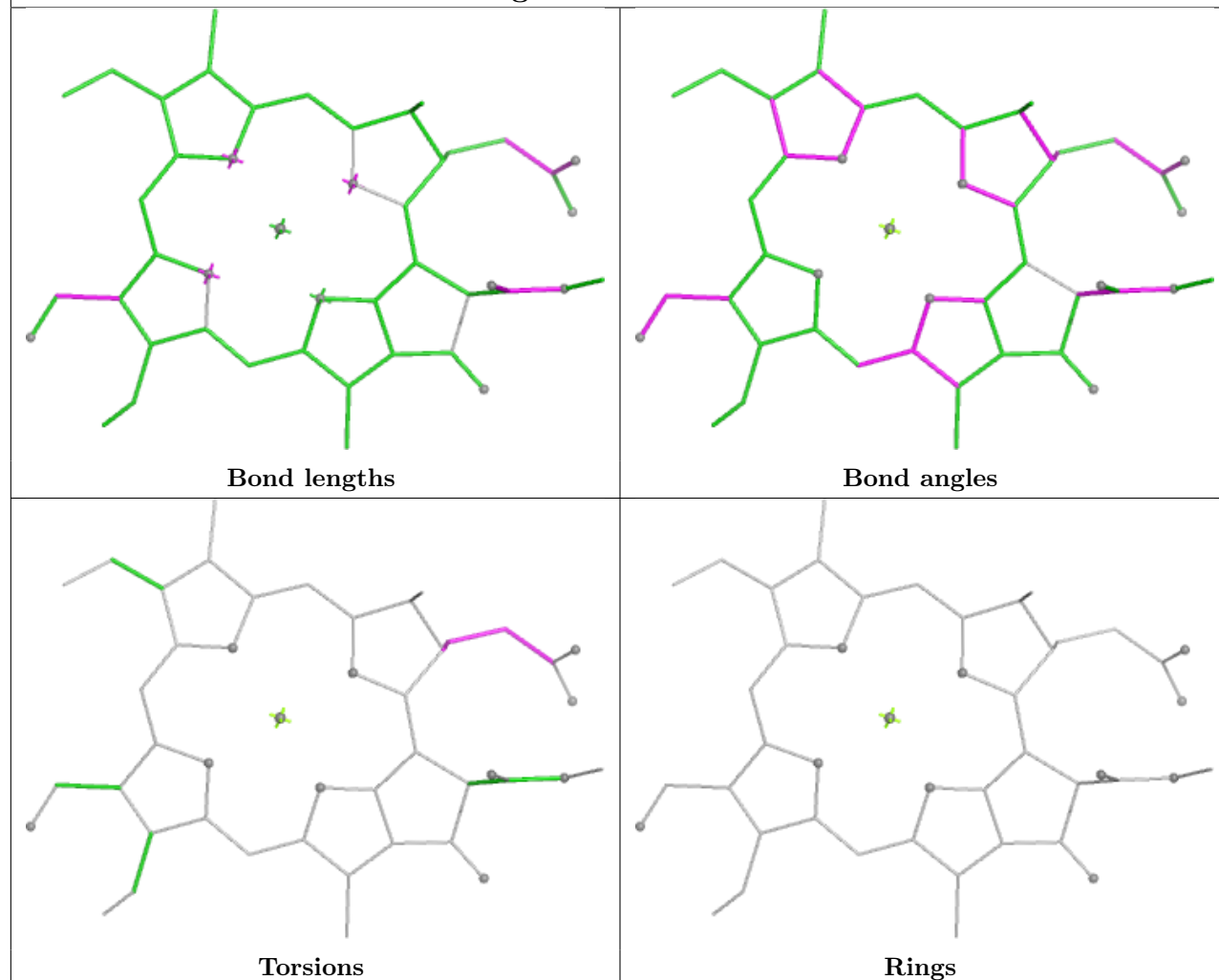
Rings



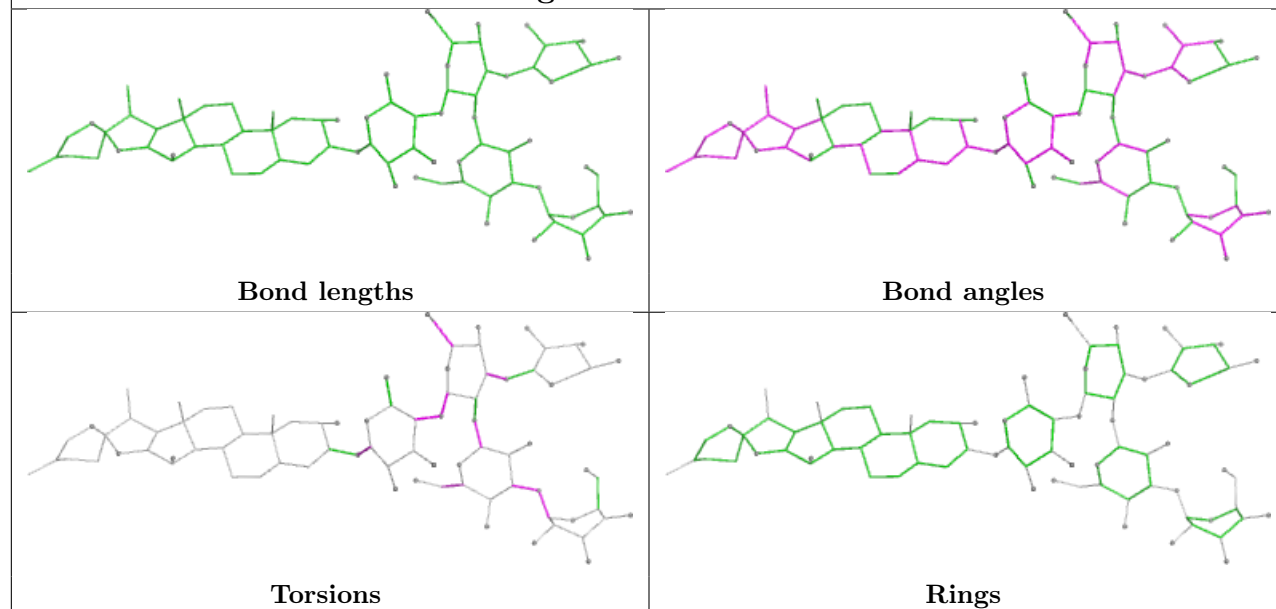


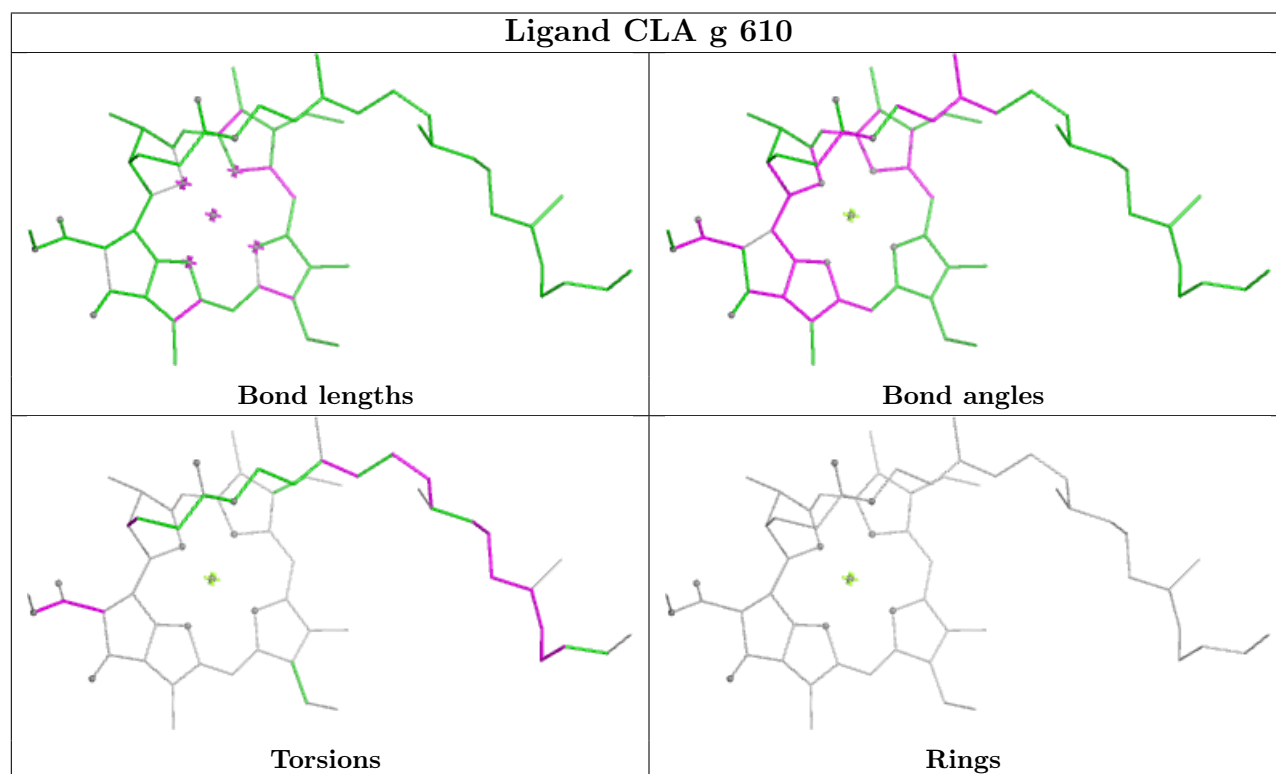
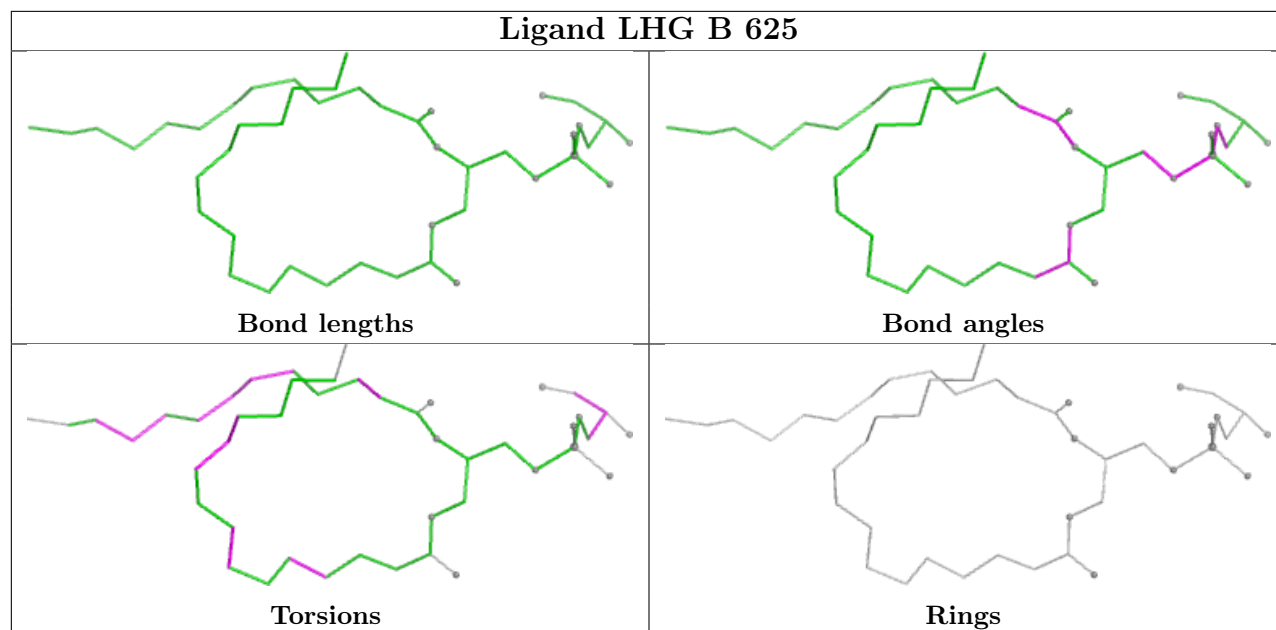


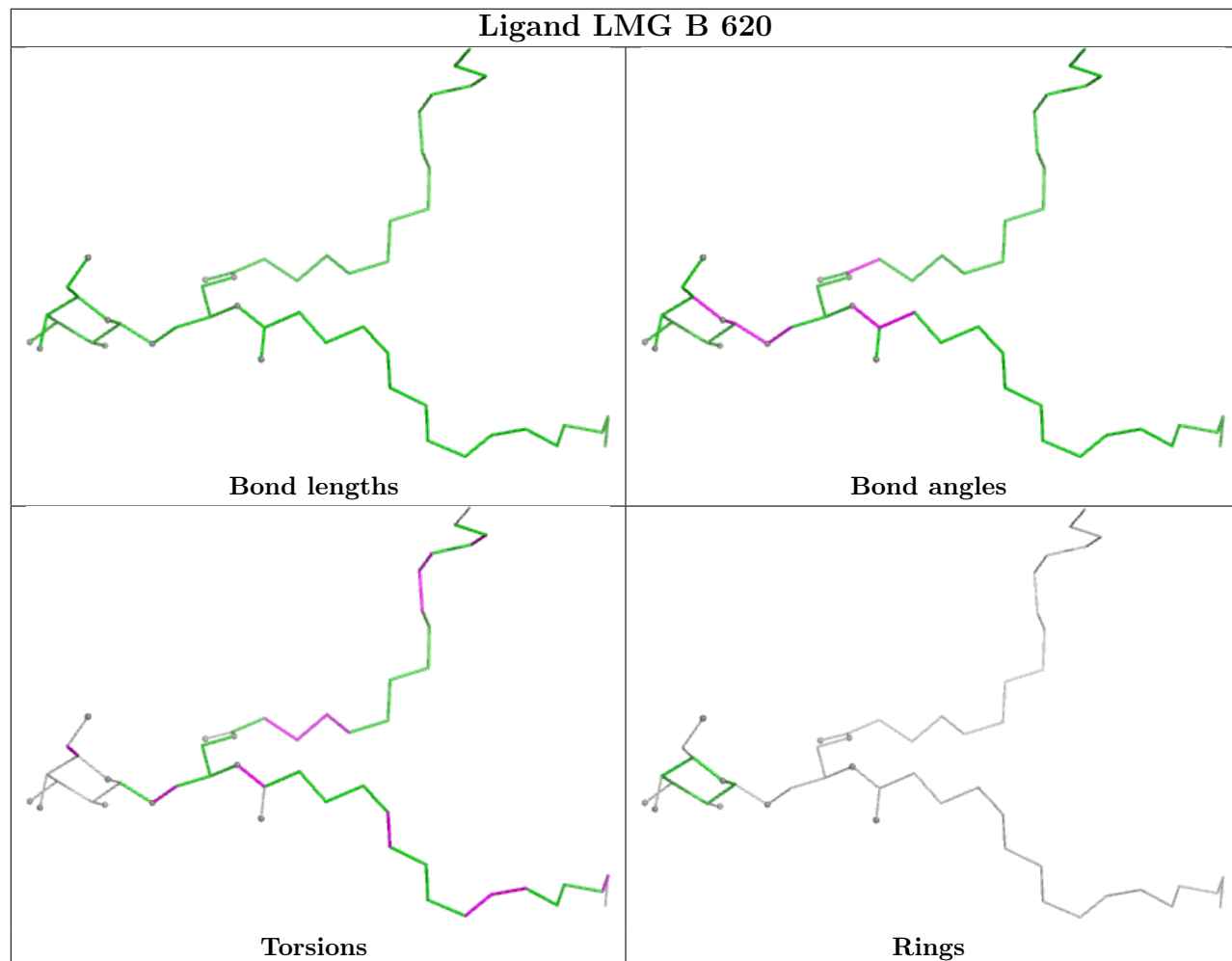
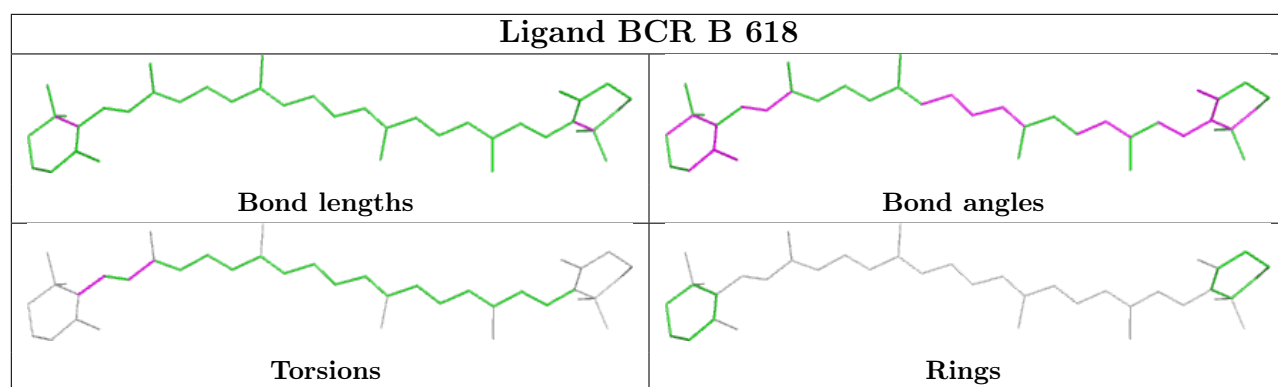
Ligand CHL 5 302

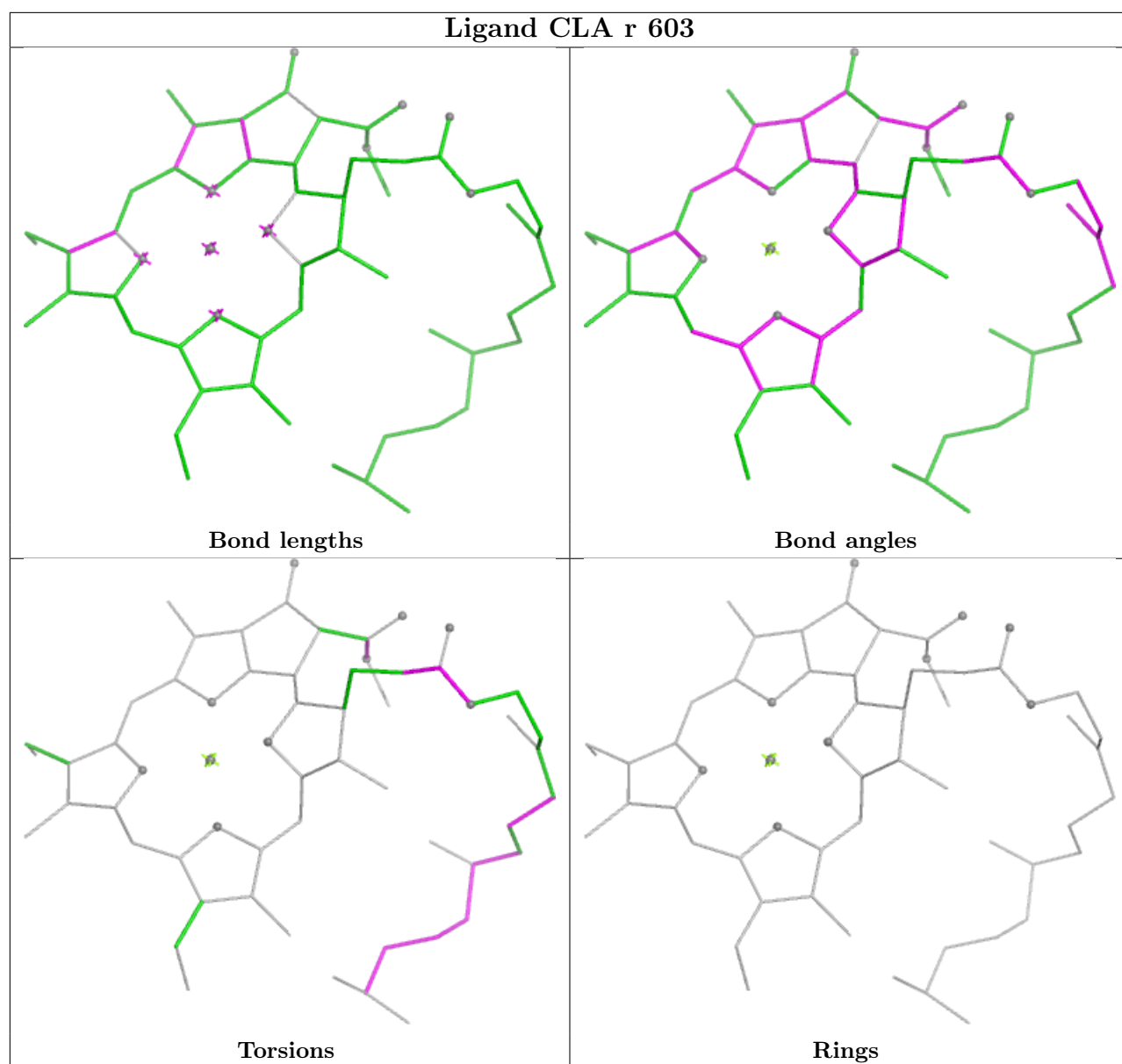


Ligand AJP b 624

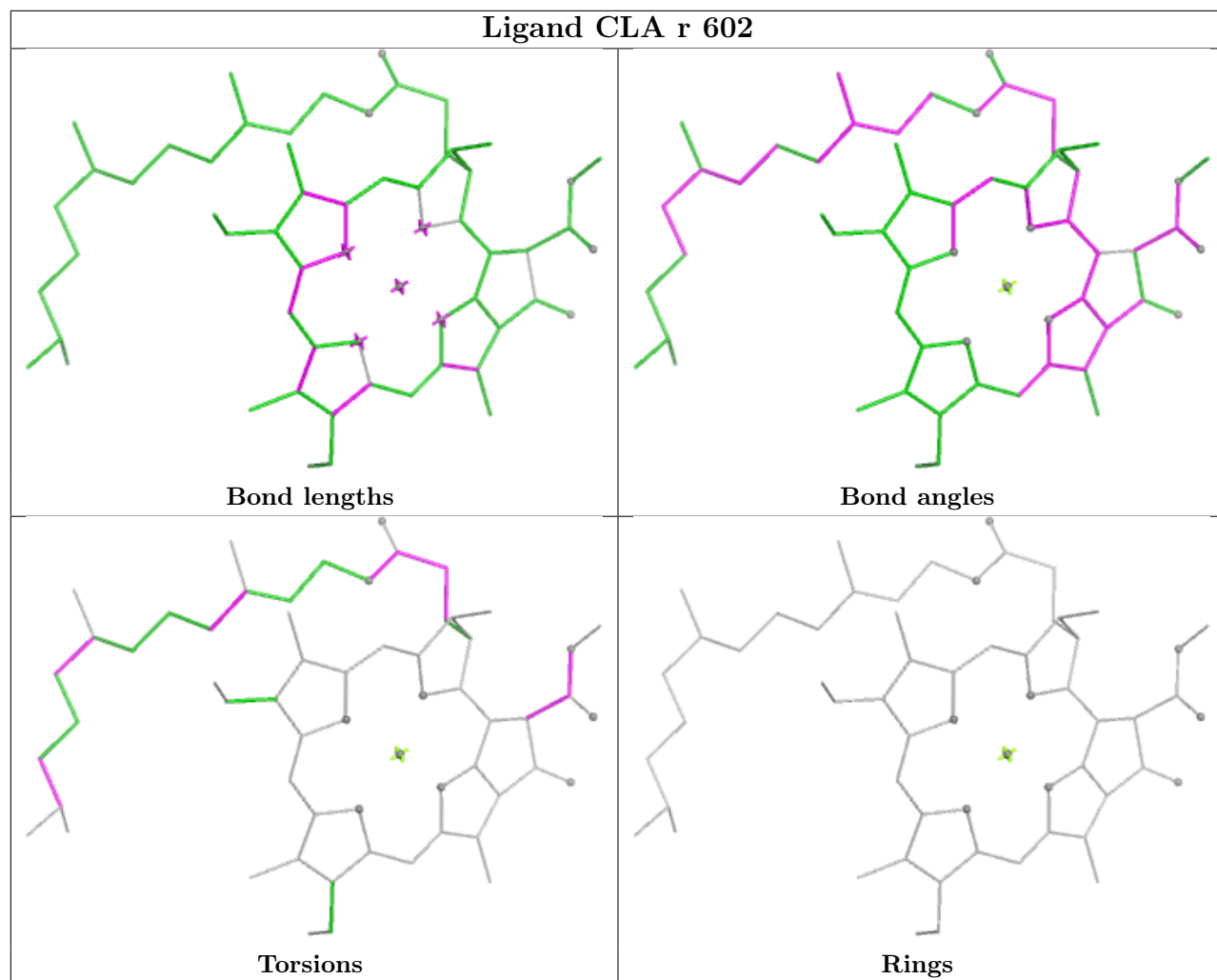


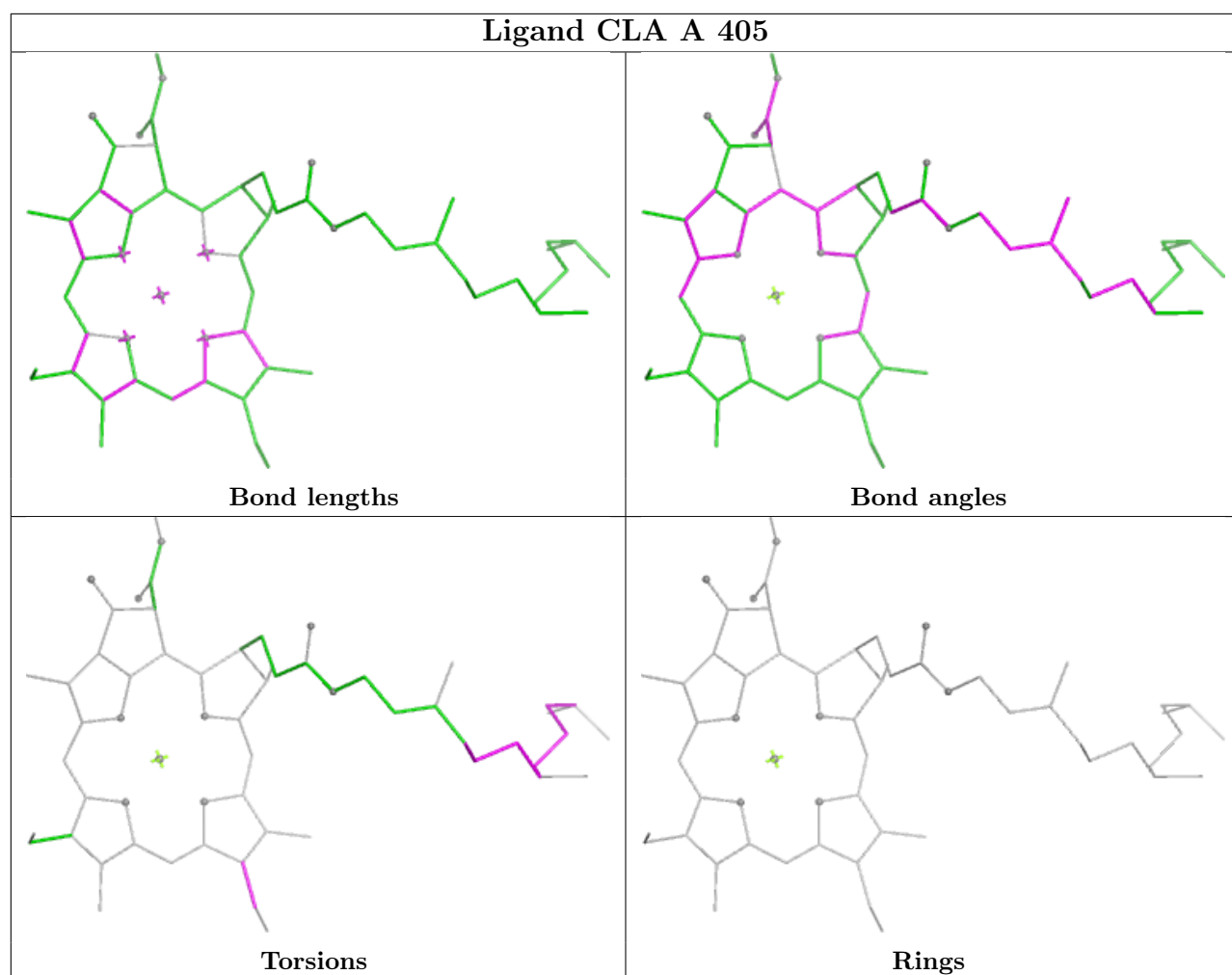


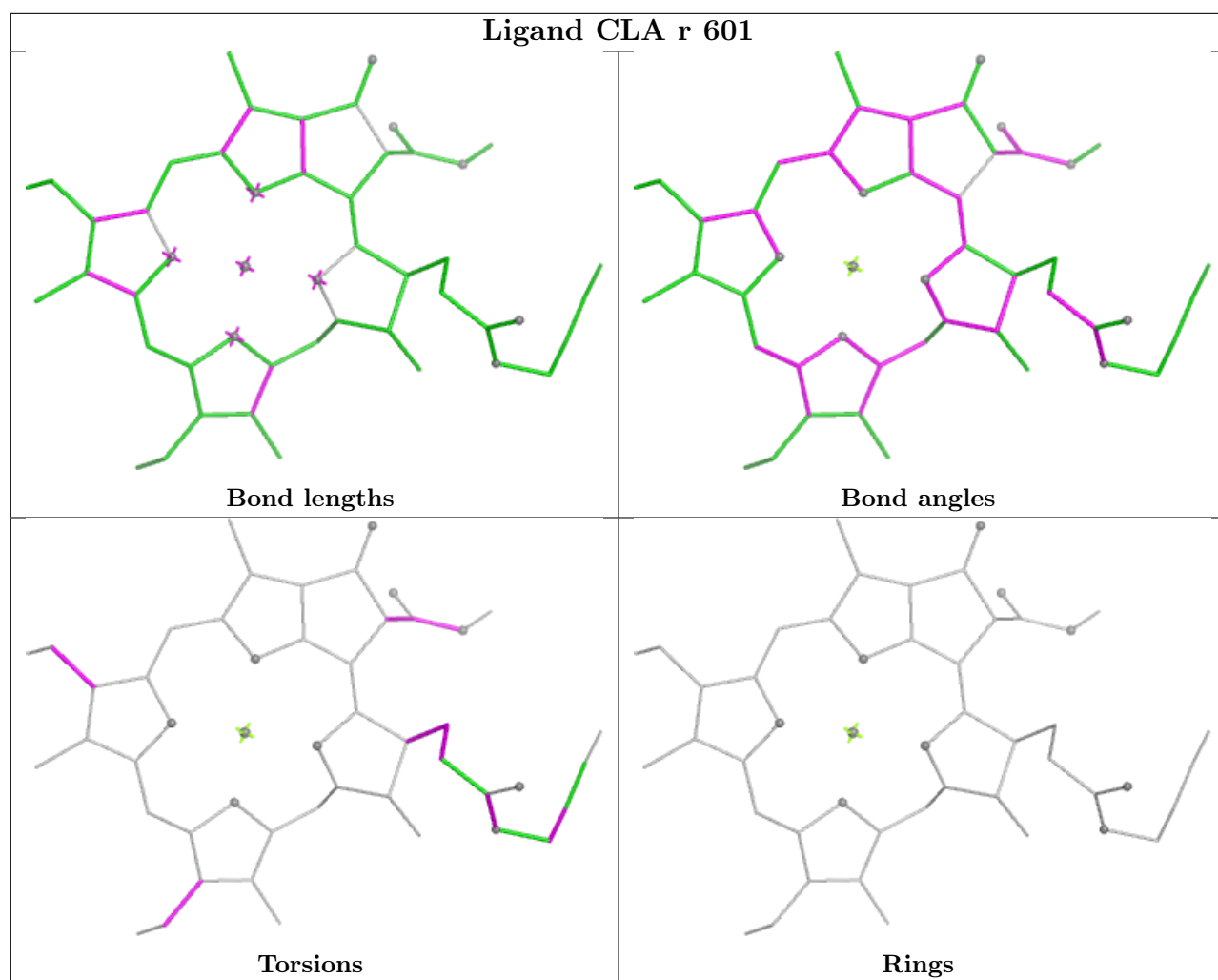


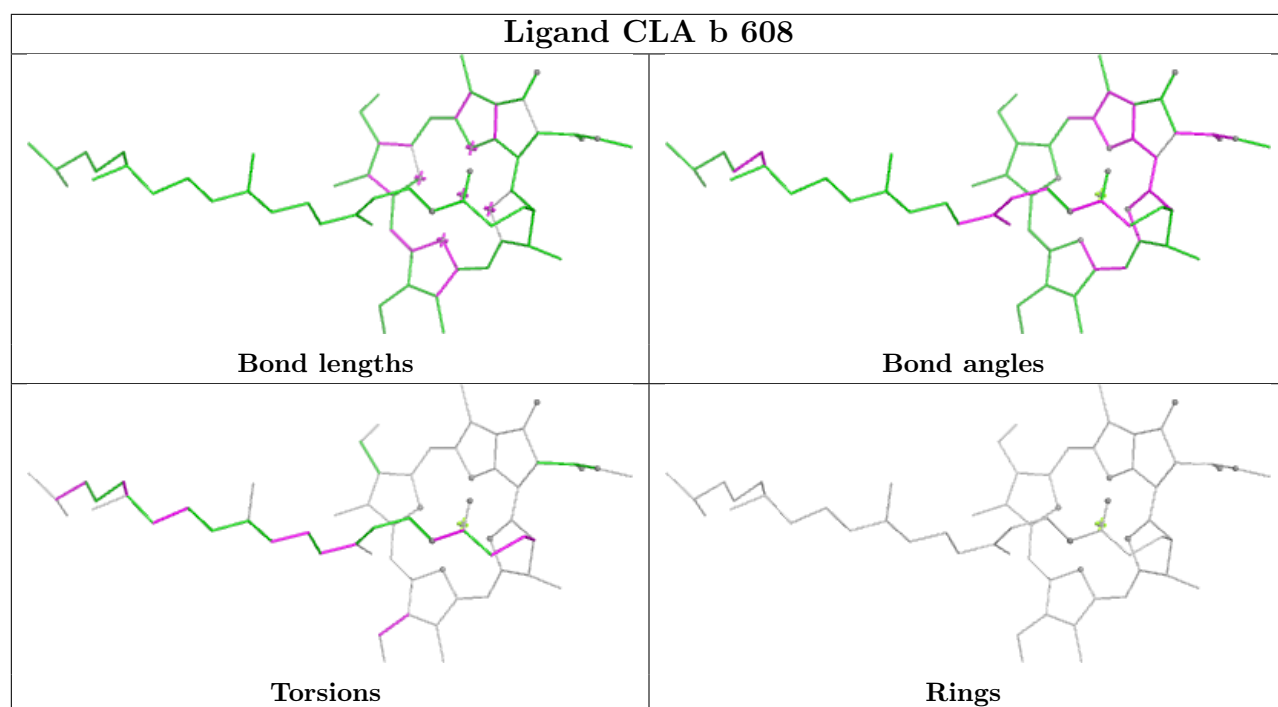
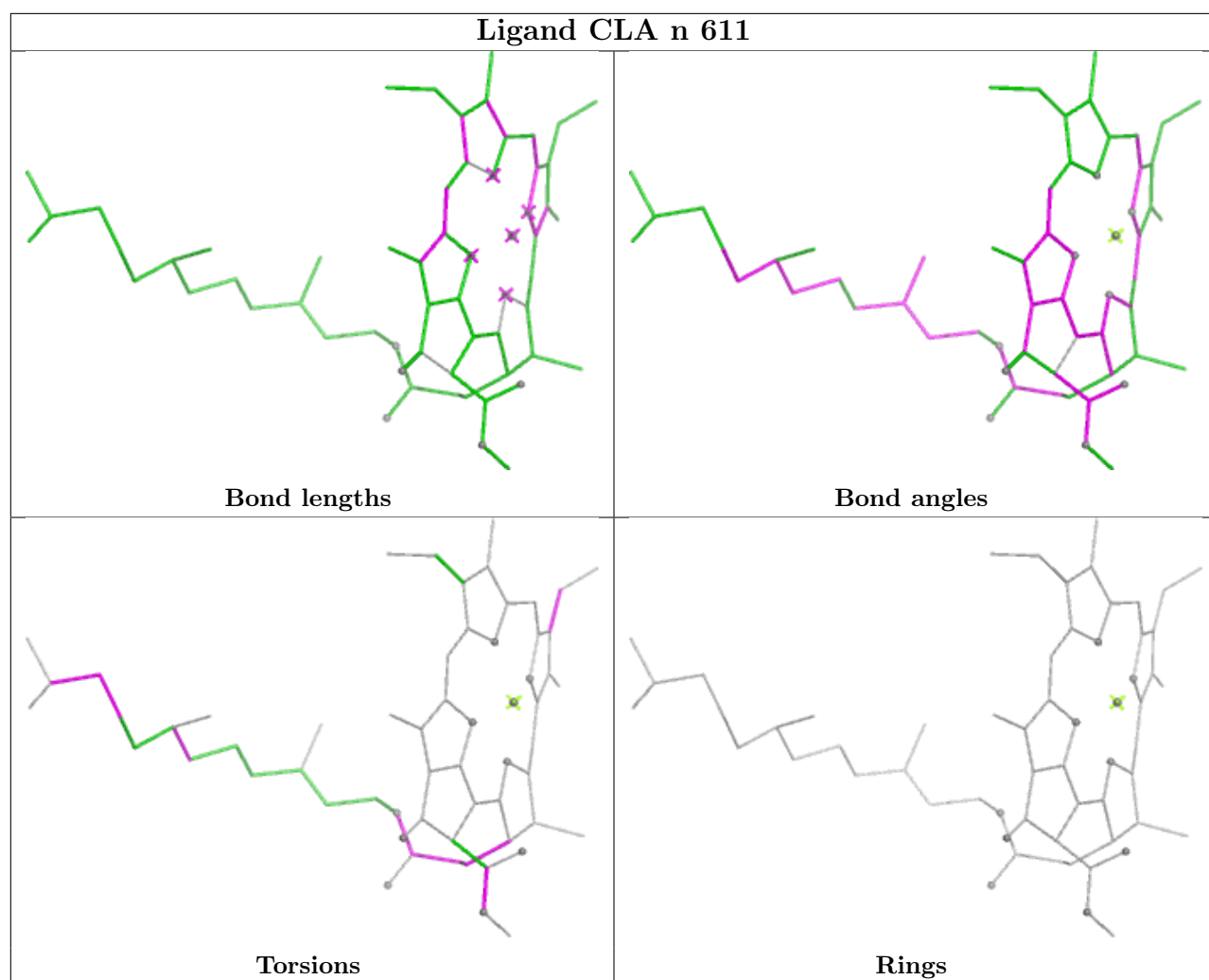


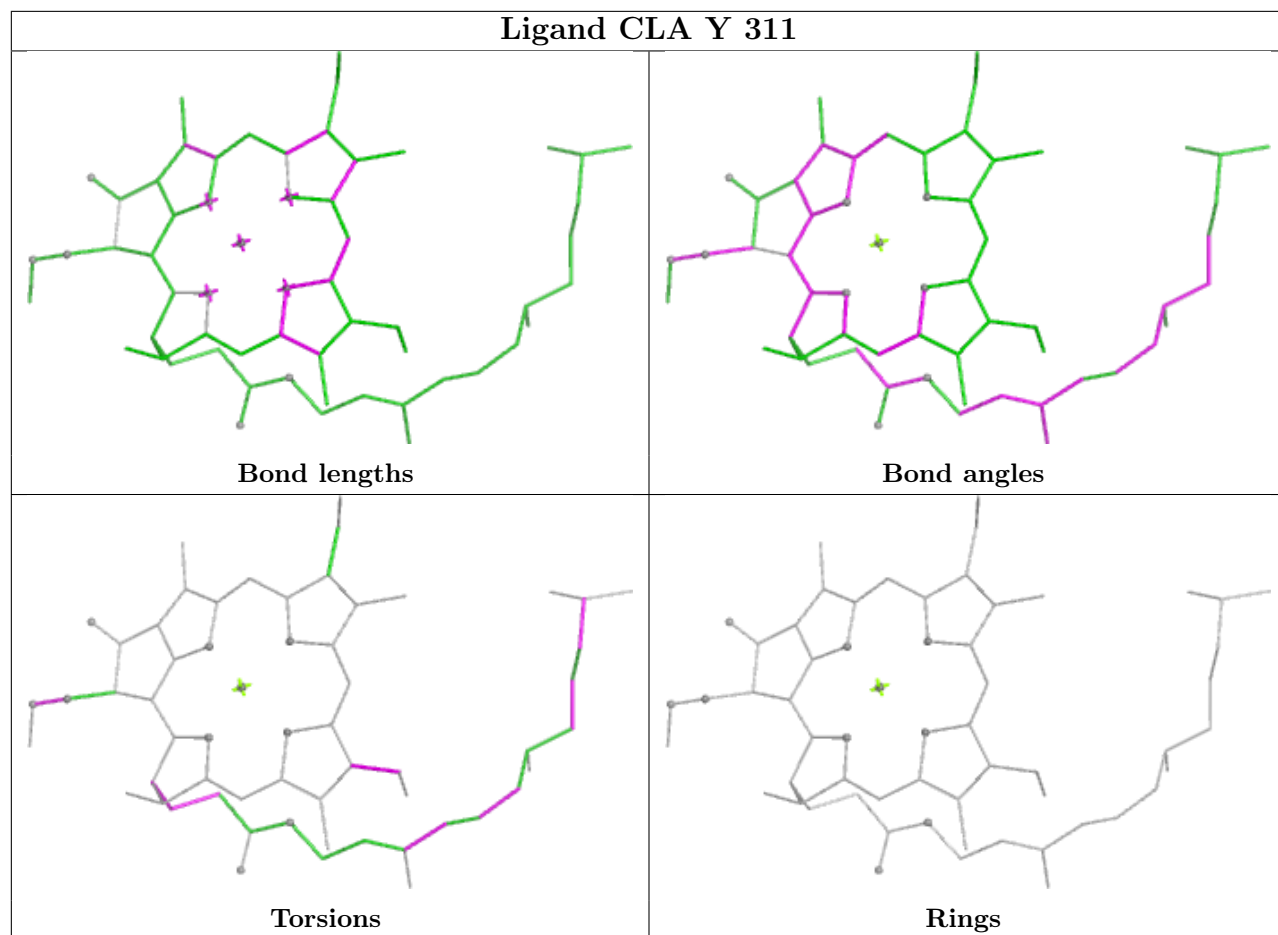
Ligand CLA r 602

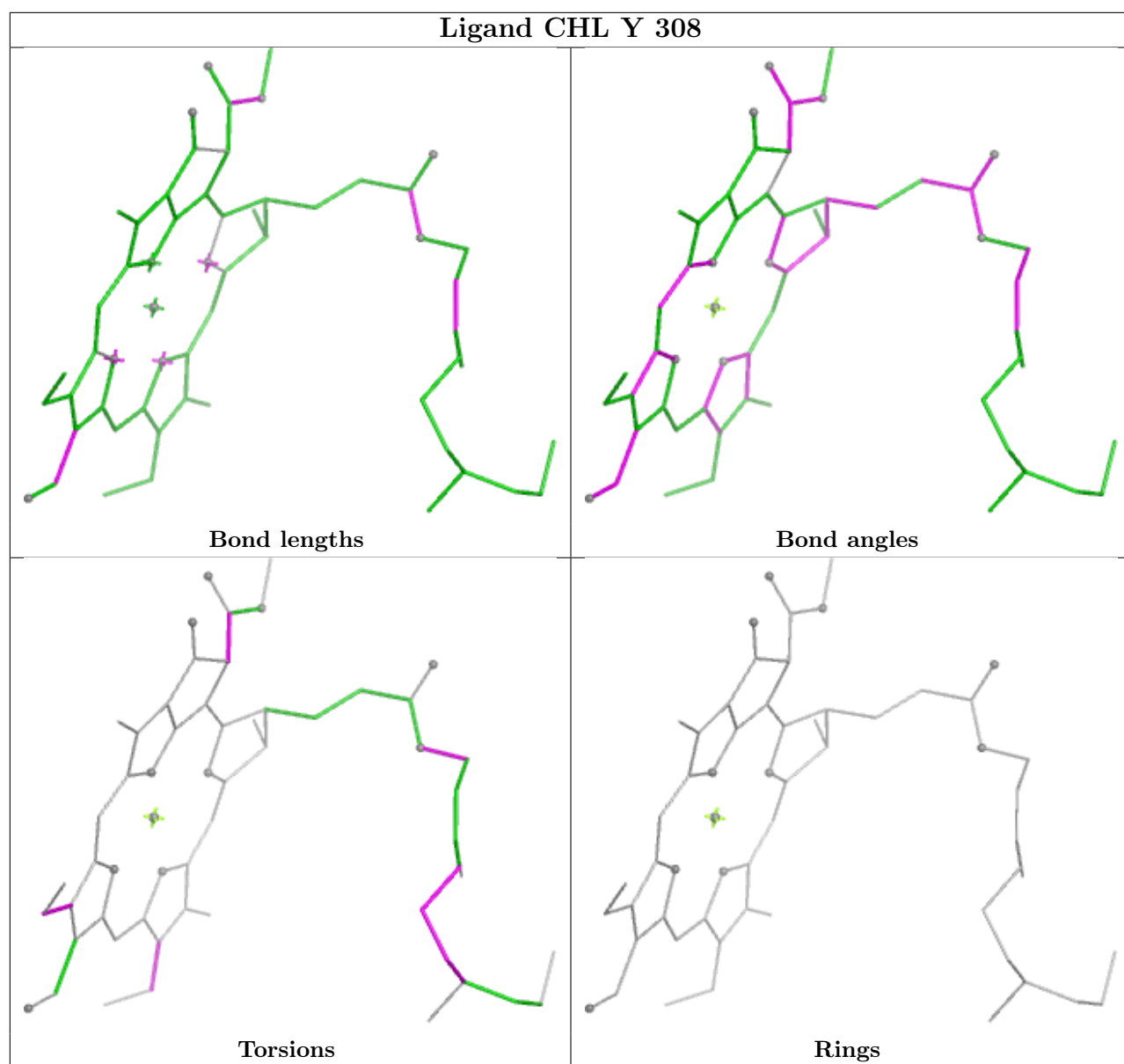




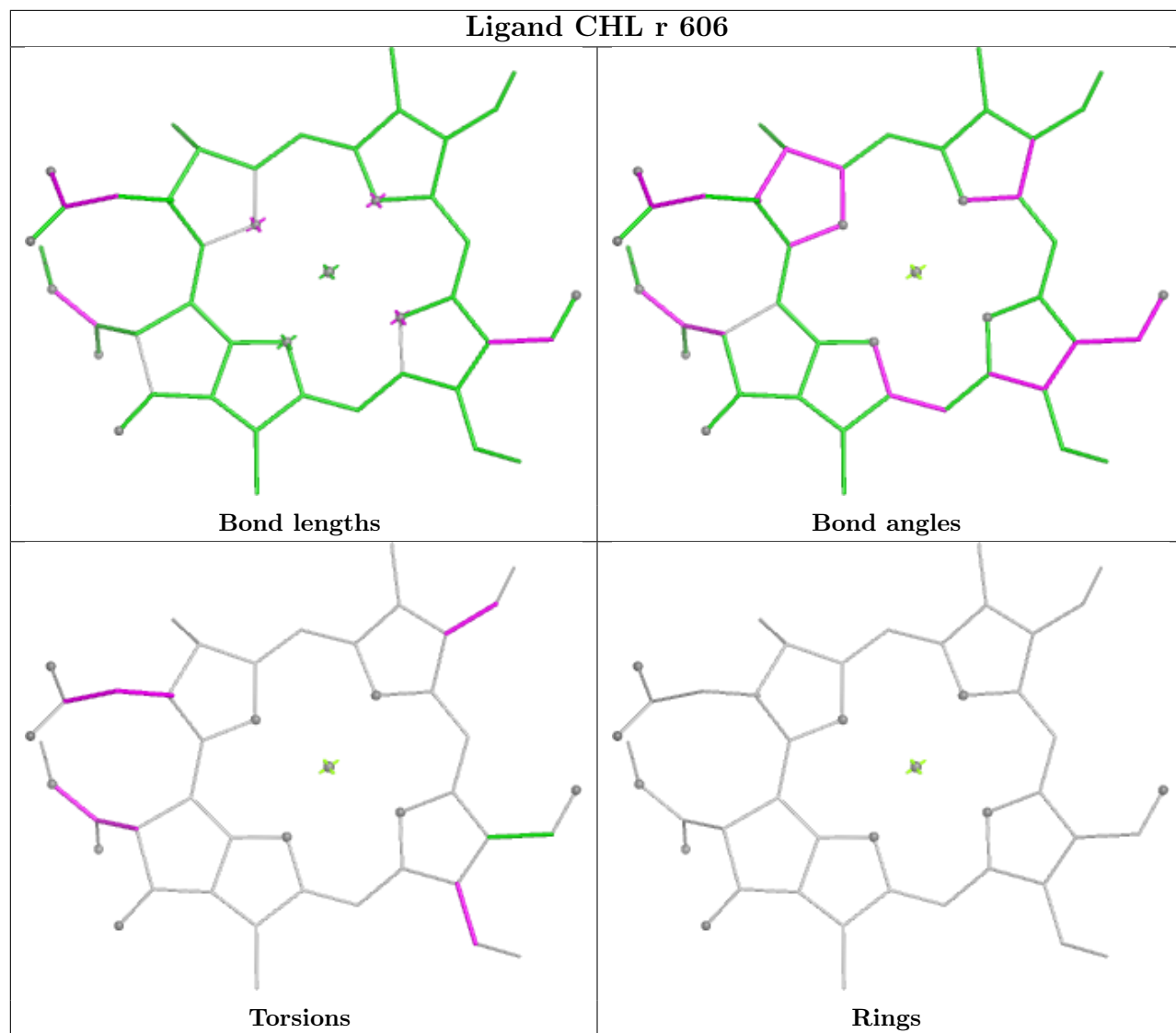


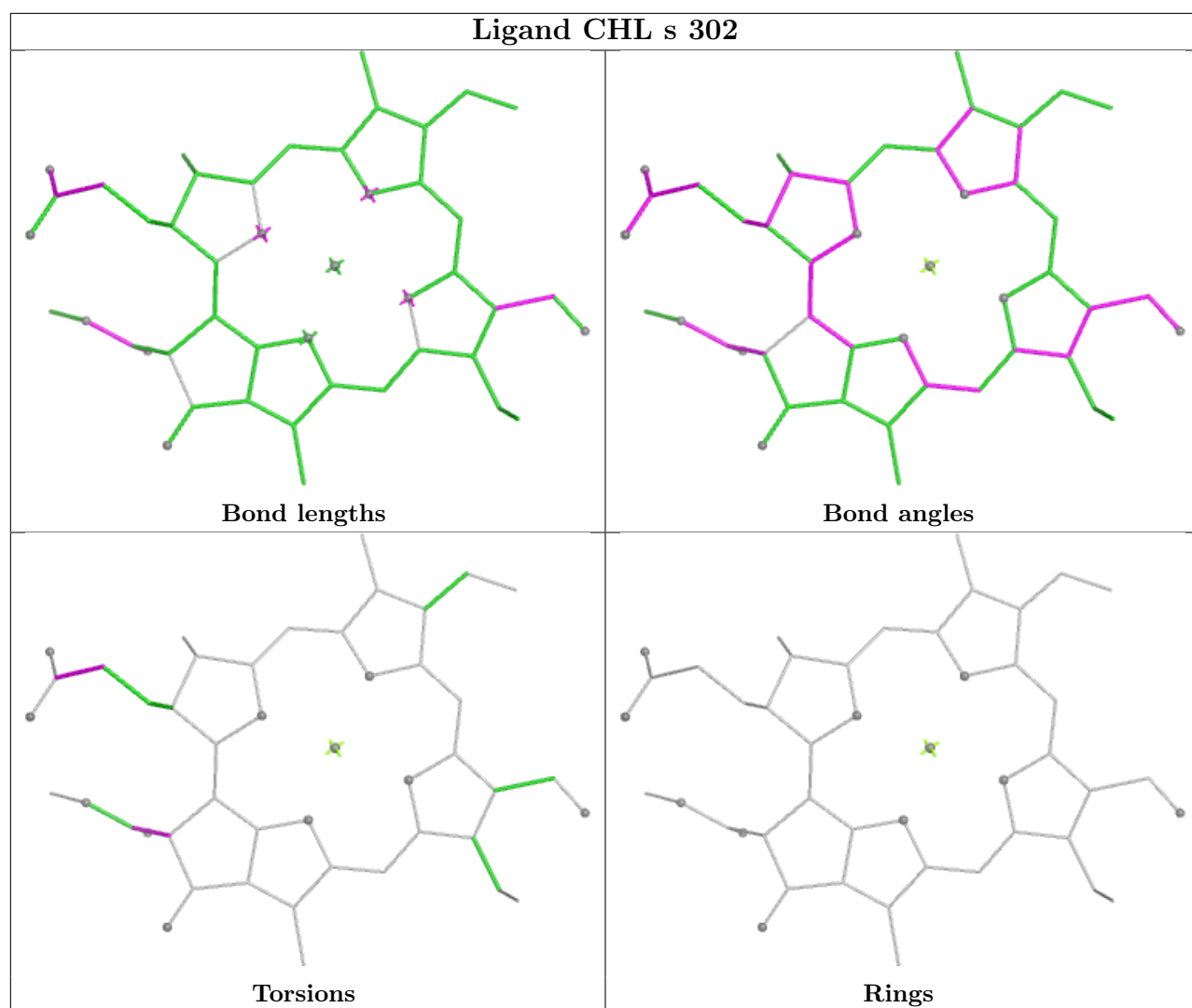


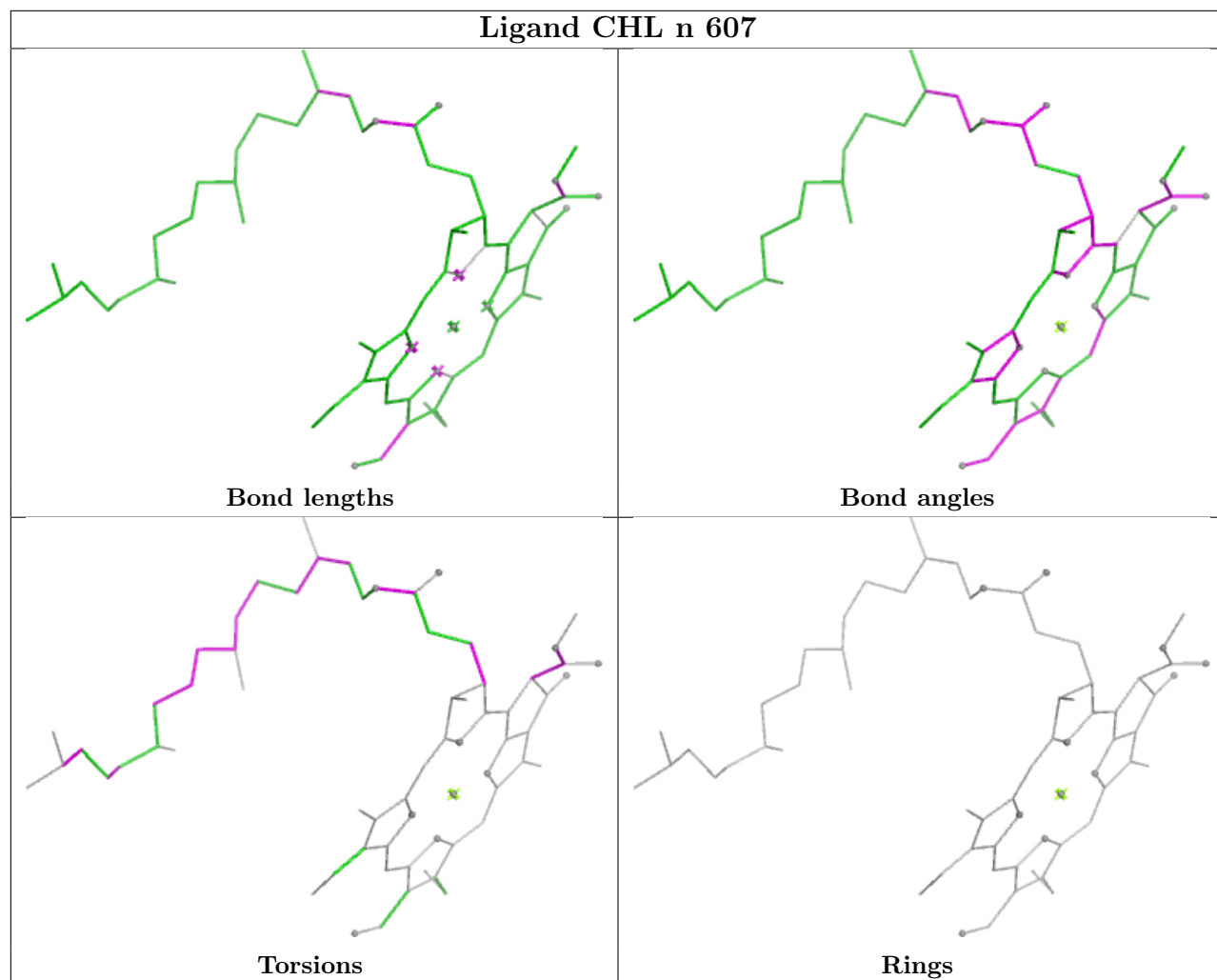




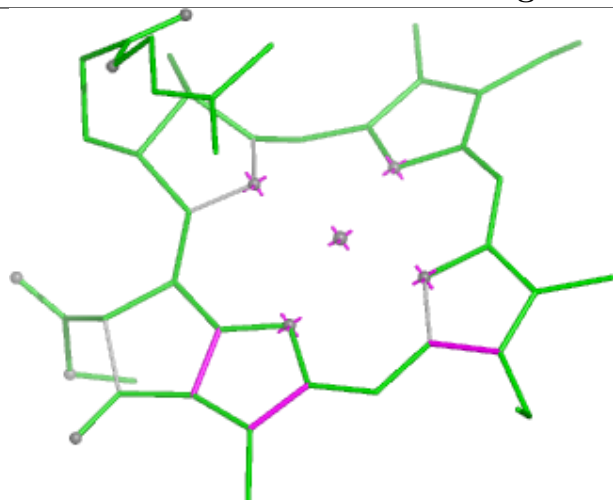
Ligand CHL r 606



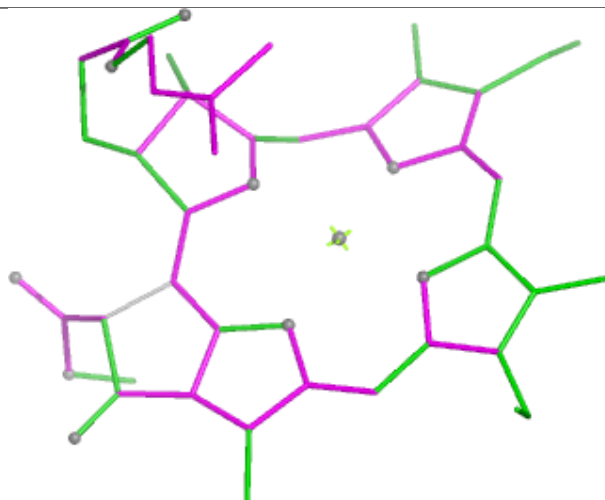




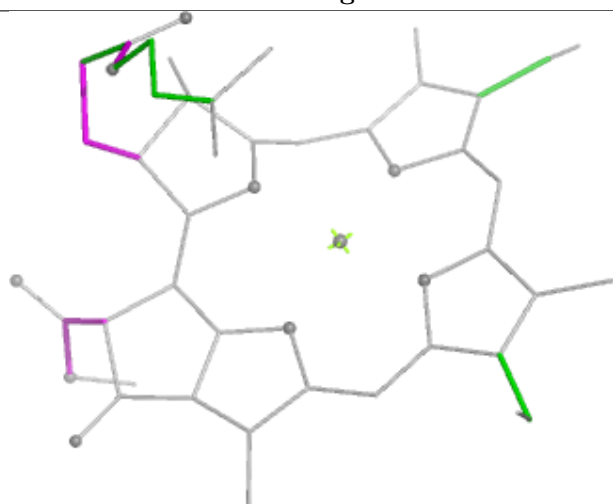
Ligand CLA S 305



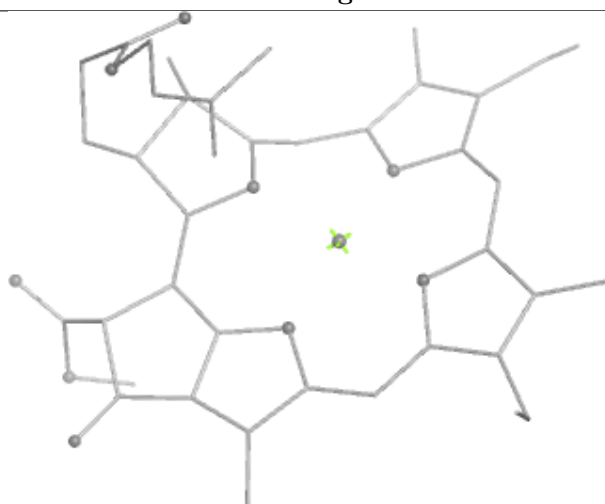
Bond lengths



Bond angles

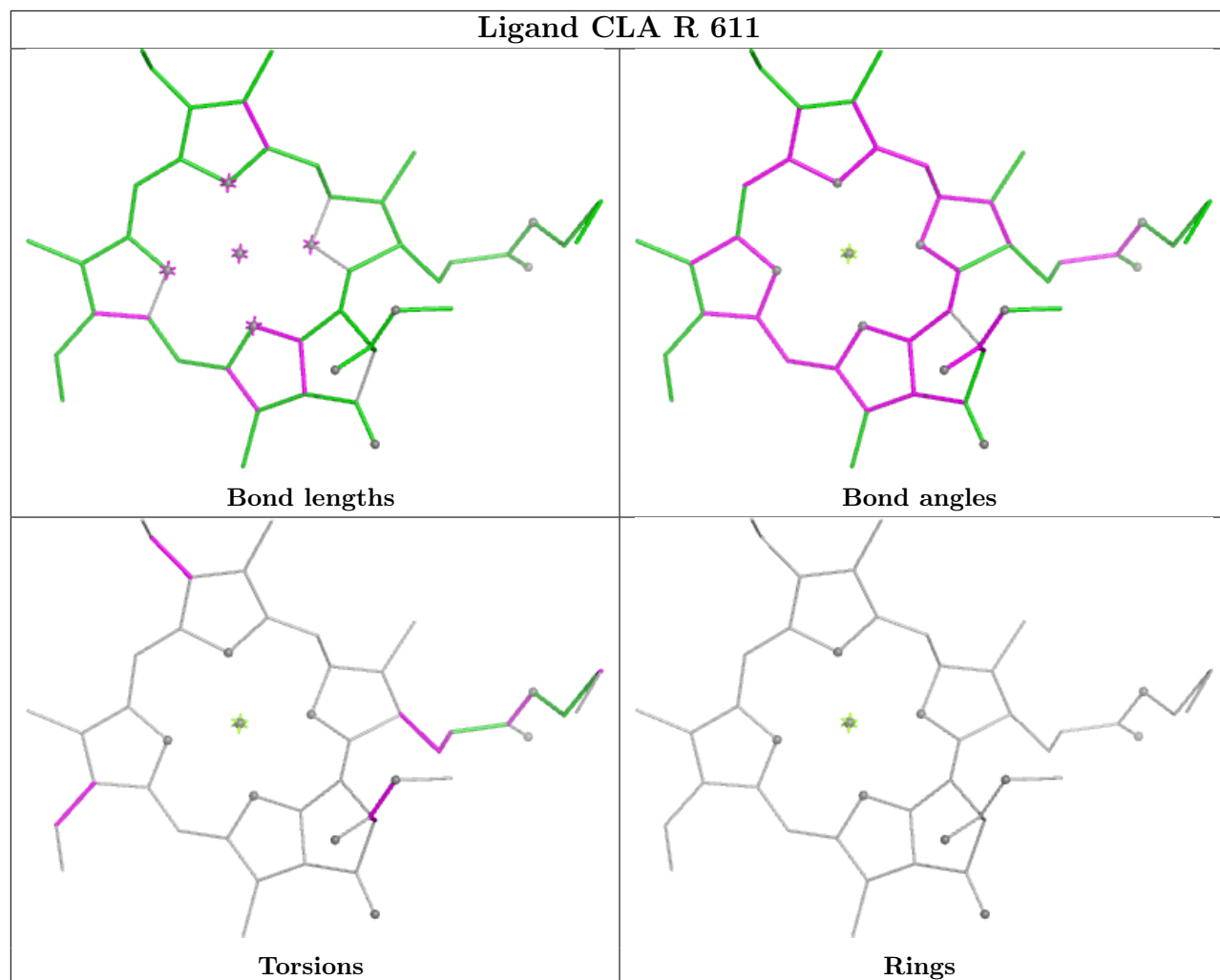


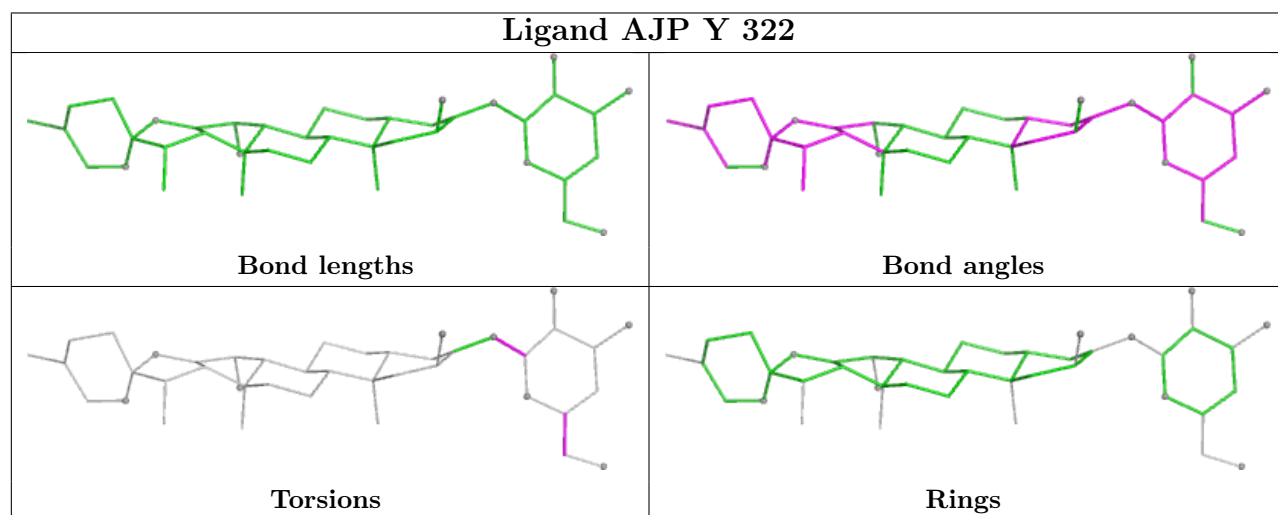
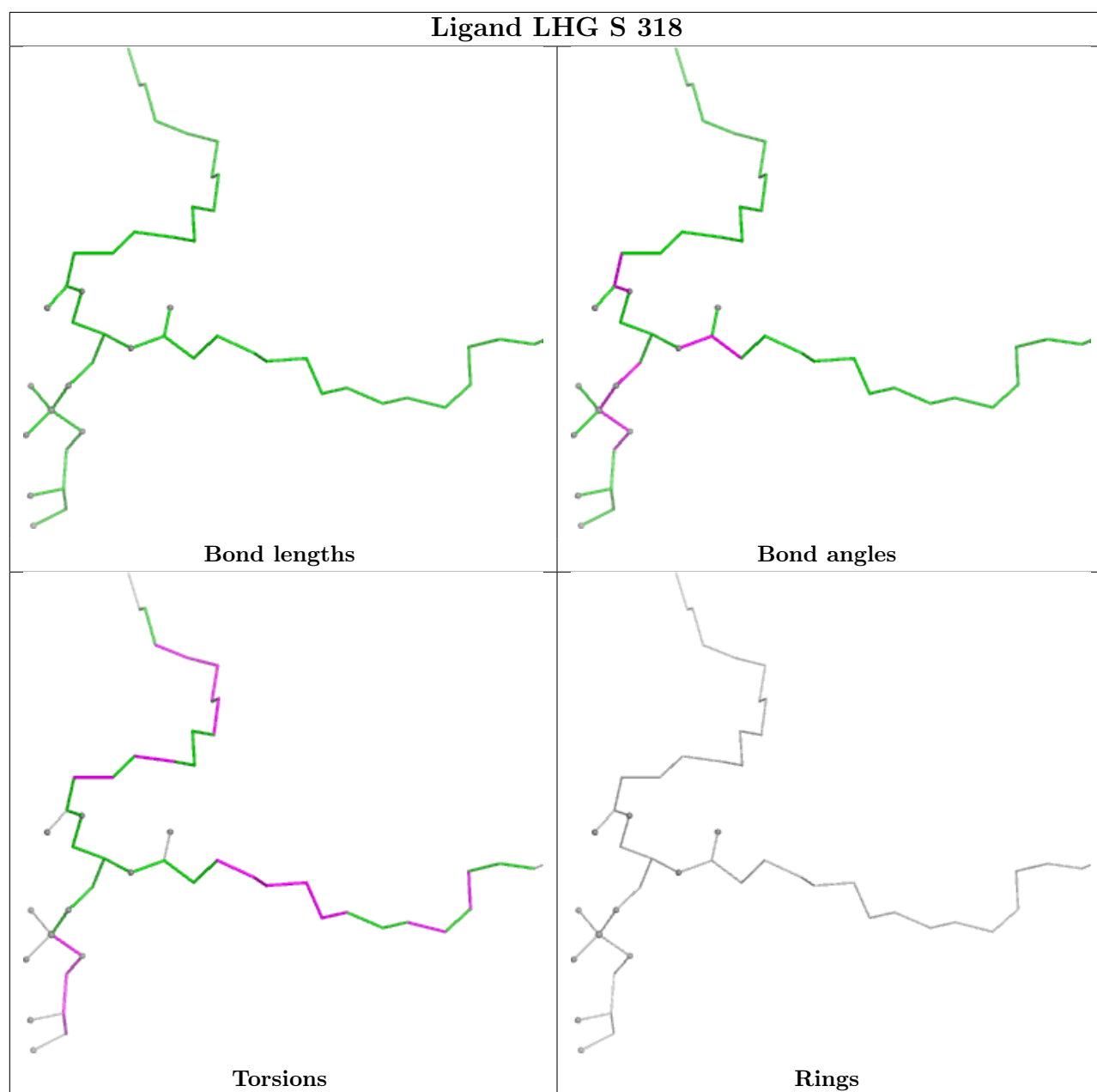
Torsions



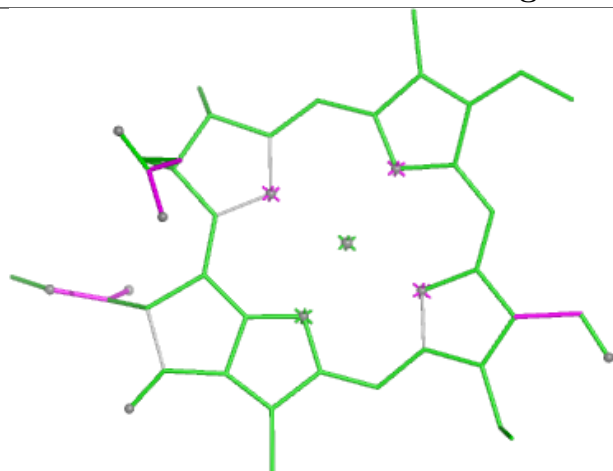
Rings

Ligand CLA R 611

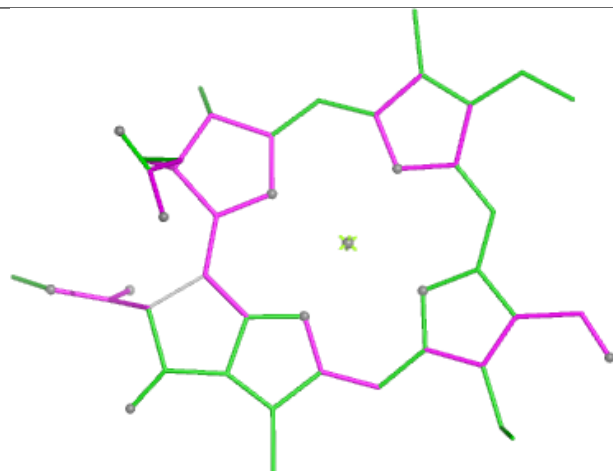




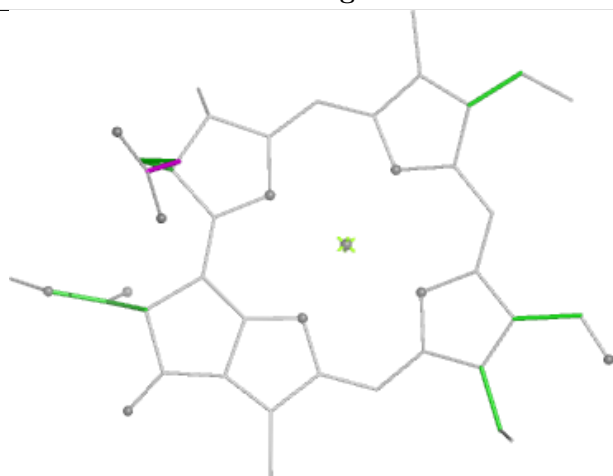
Ligand CHL s 308



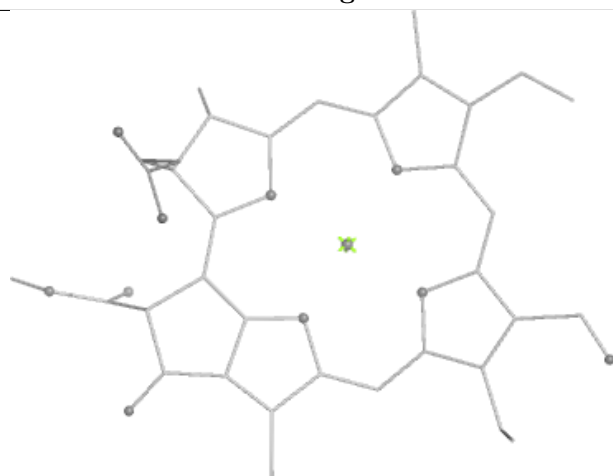
Bond lengths



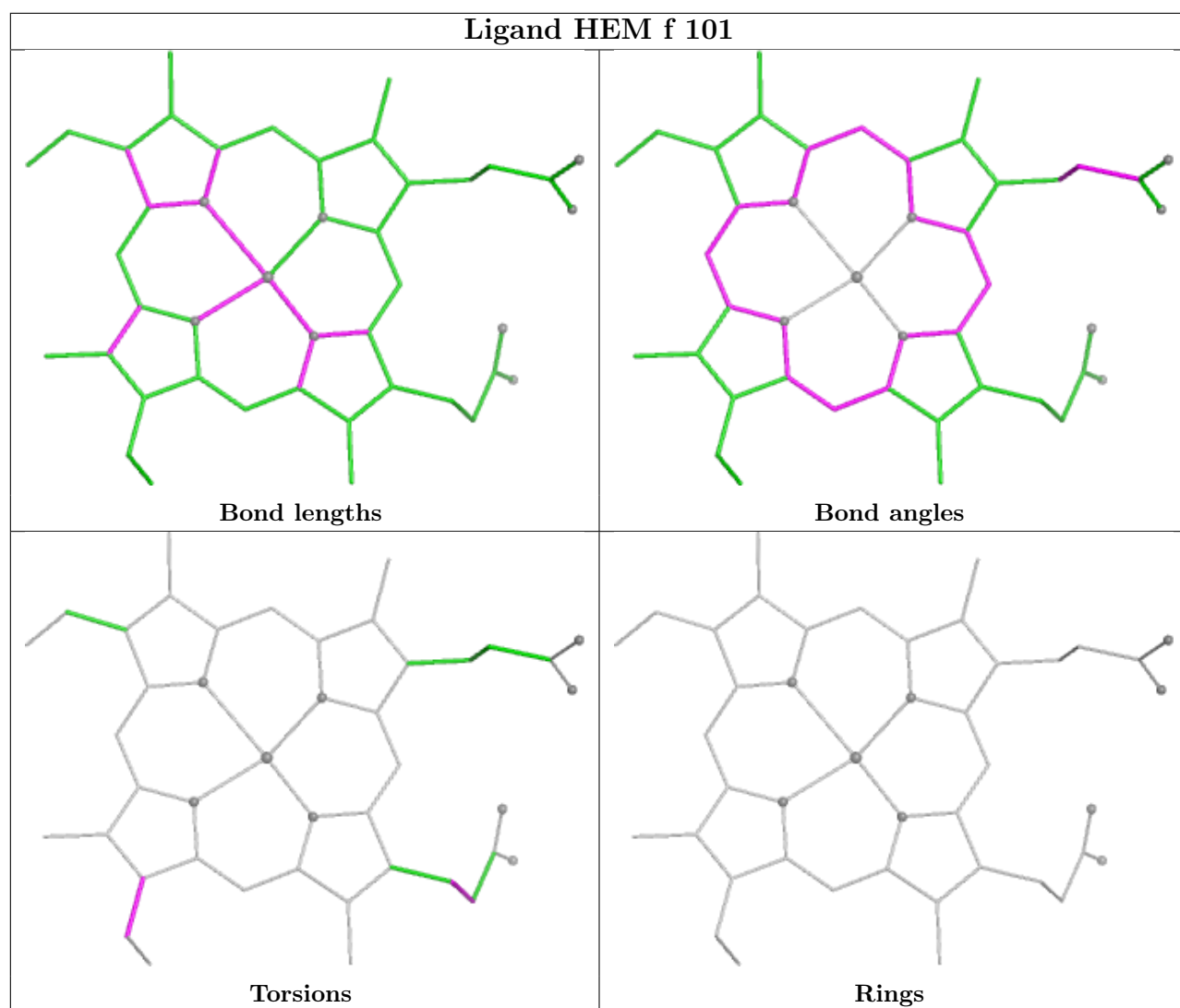
Bond angles



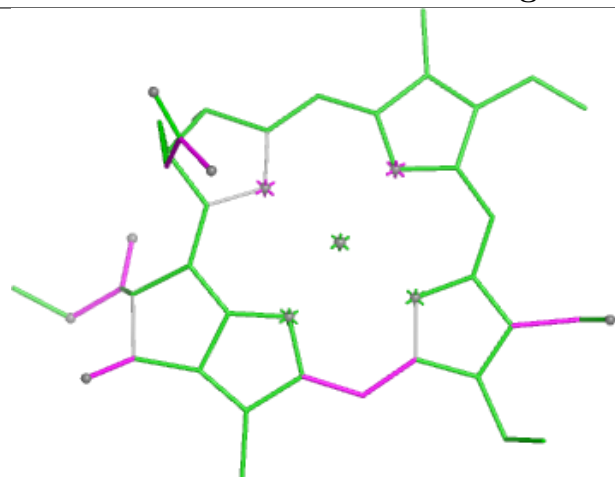
Torsions



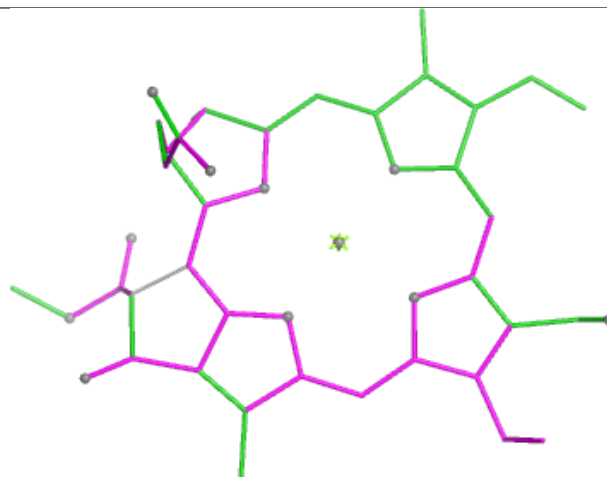
Rings



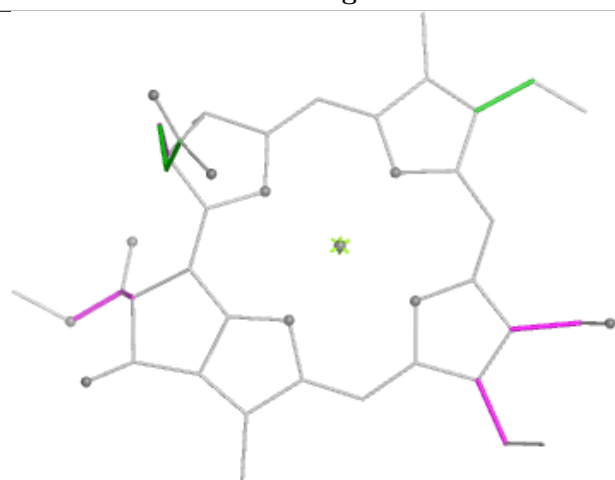
Ligand CHL 2 603



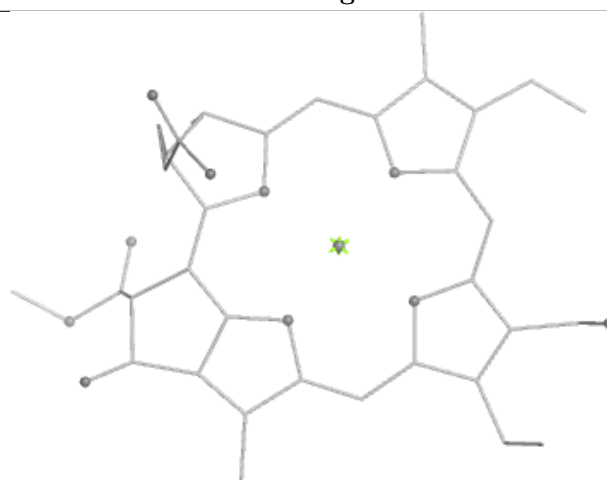
Bond lengths



Bond angles

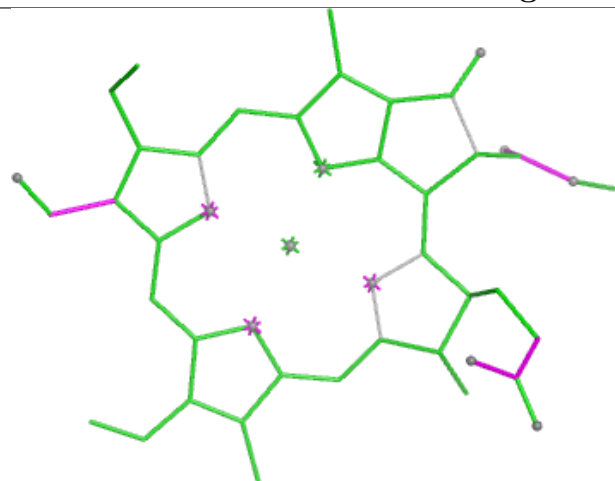


Torsions

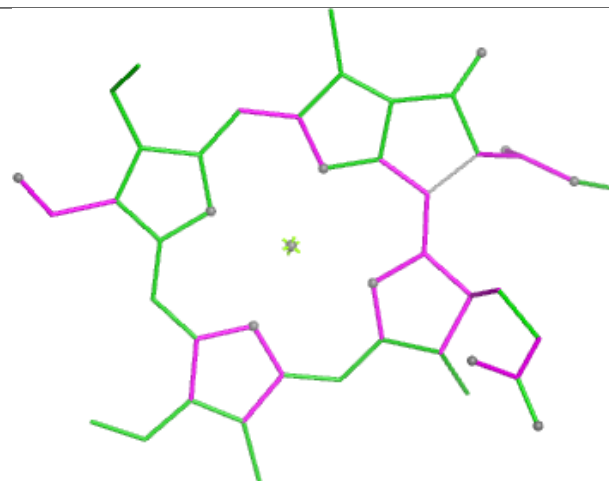


Rings

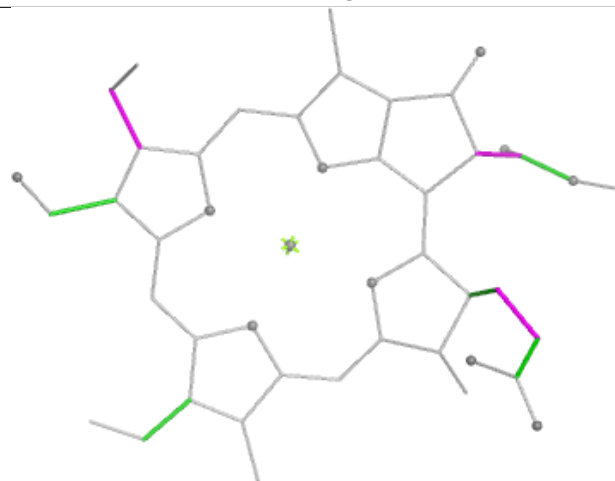
Ligand CHL 5 301



Bond lengths



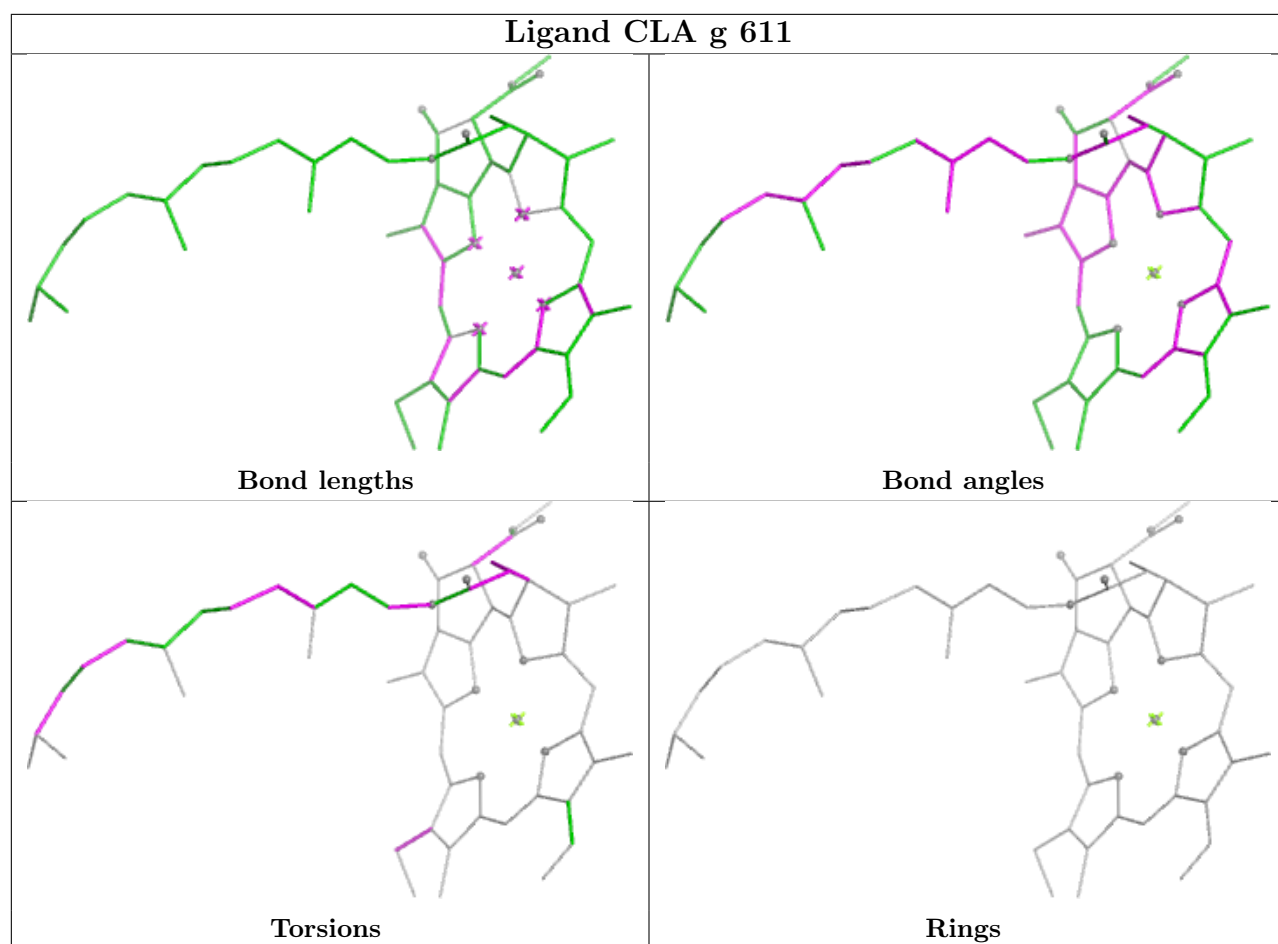
Bond angles

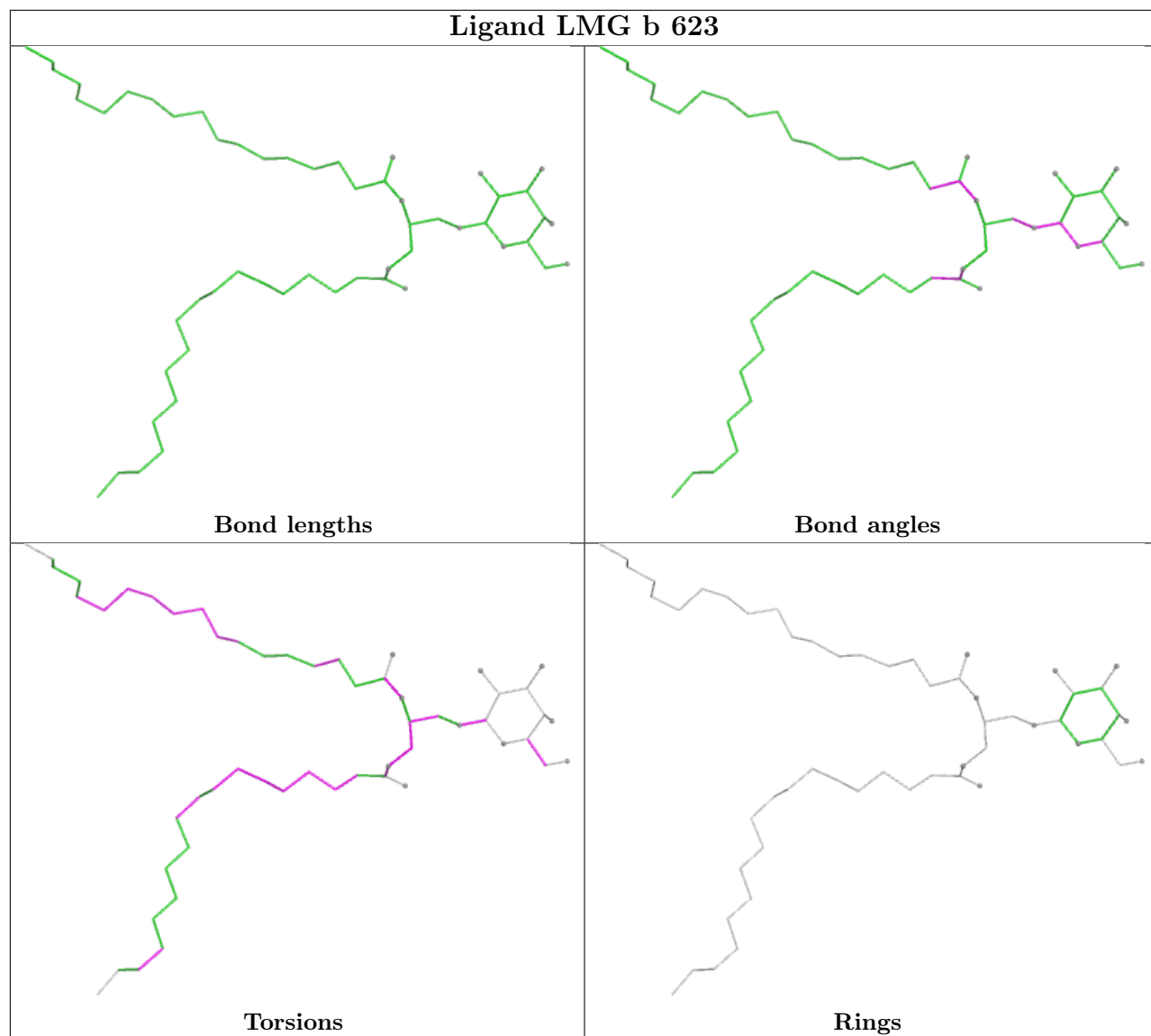


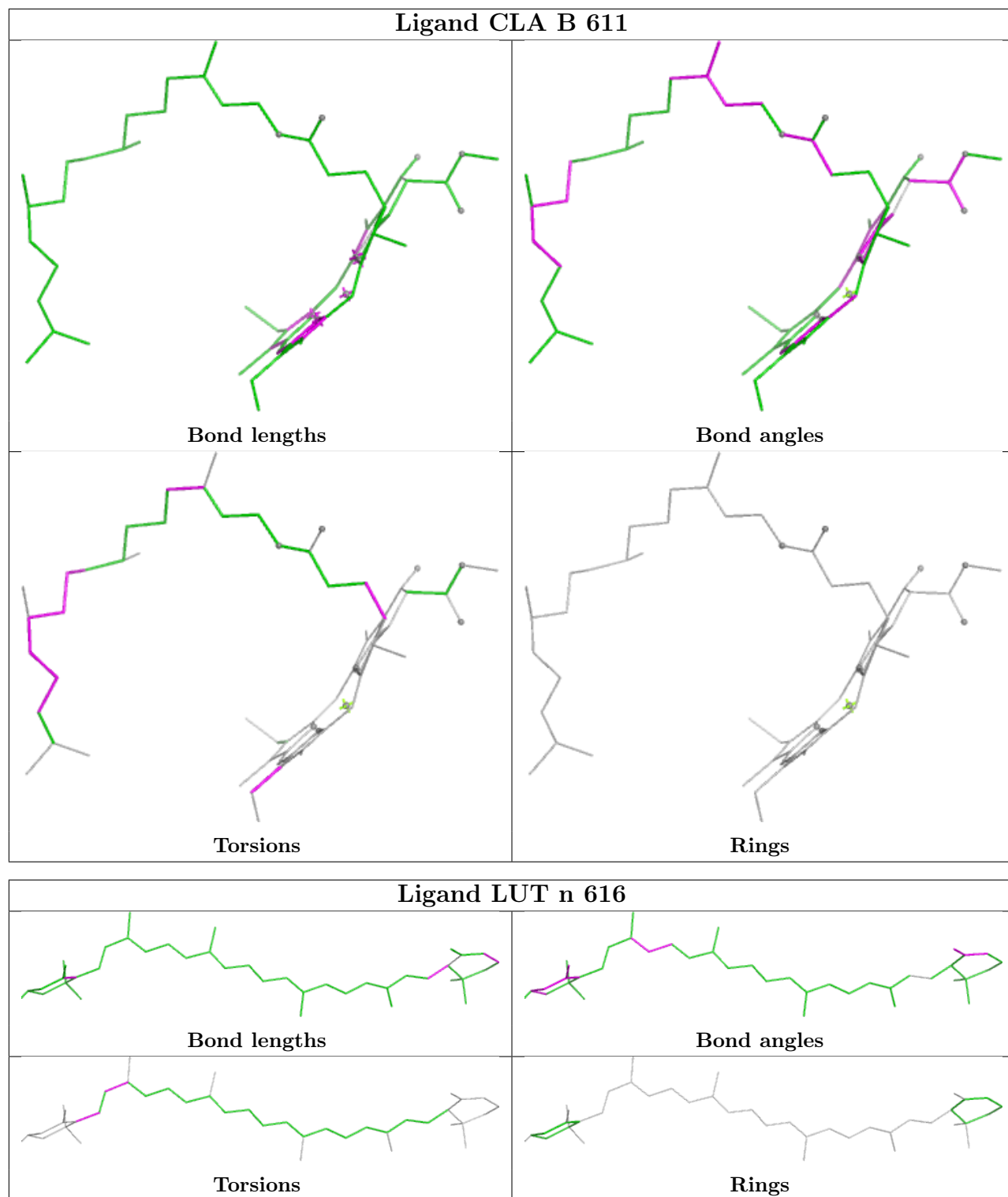
Torsions



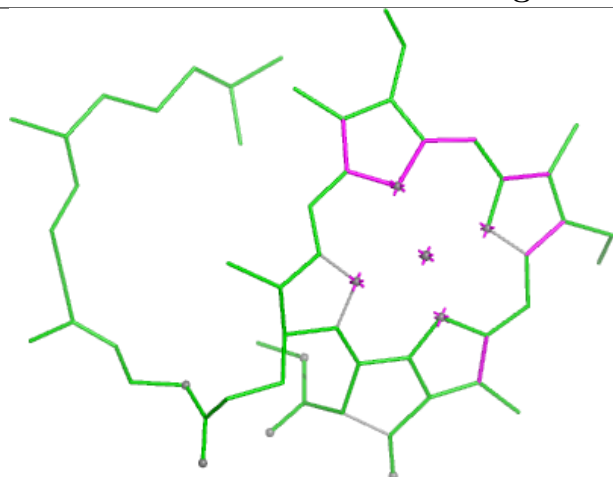
Rings



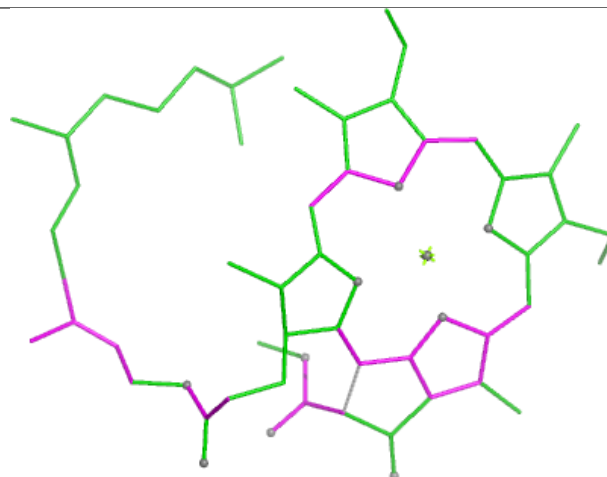




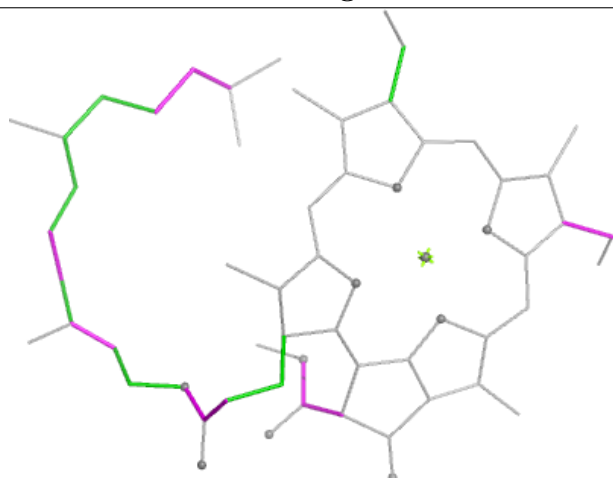
Ligand CLA G 612



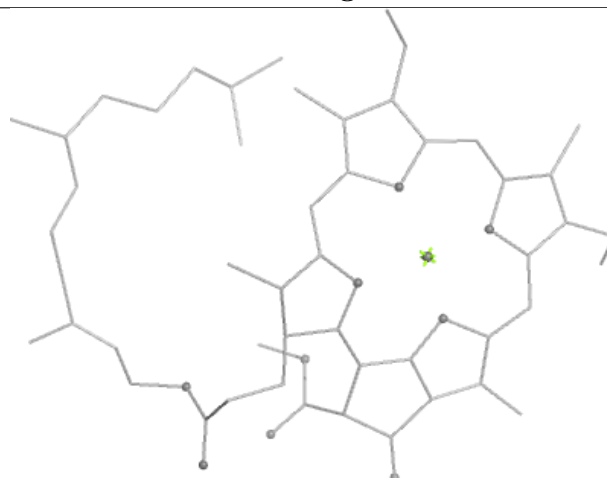
Bond lengths



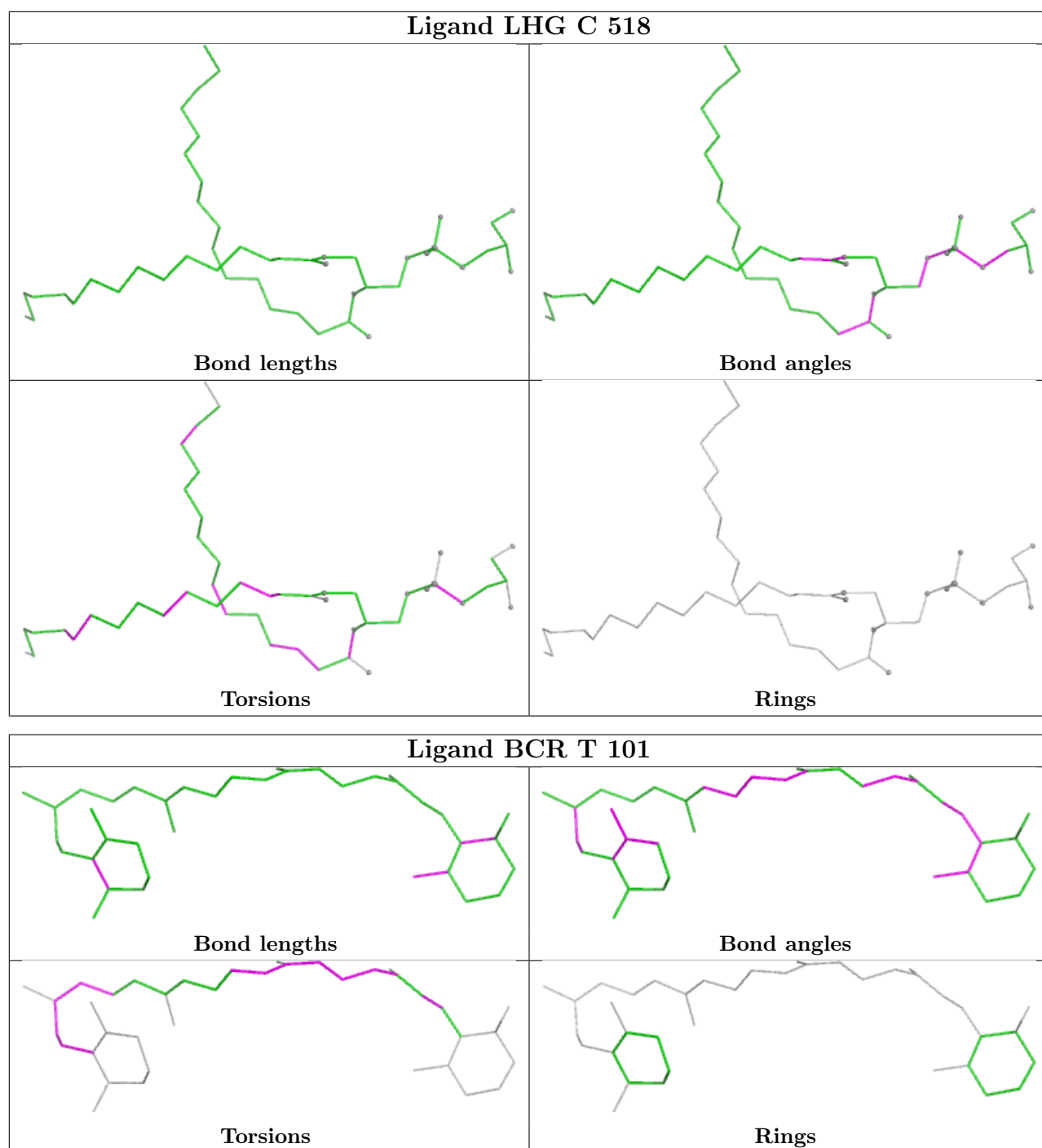
Bond angles



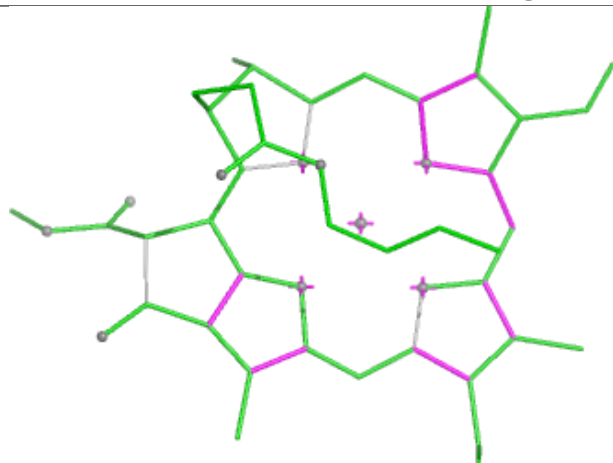
Torsions



Rings



Ligand CLA s 314



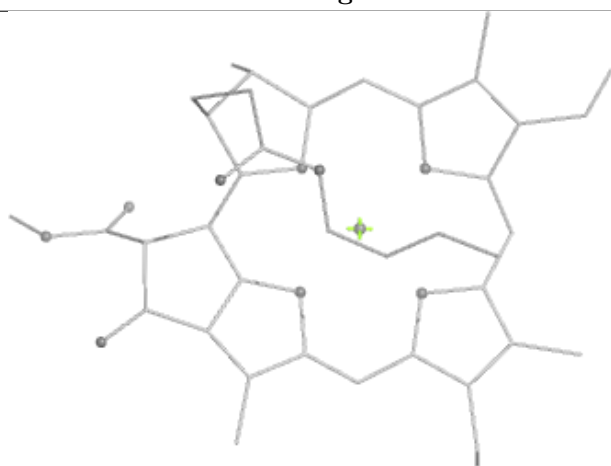
Bond lengths



Bond angles

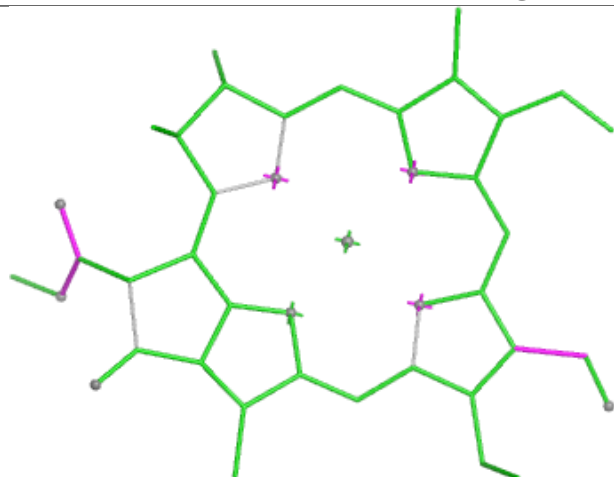


Torsions

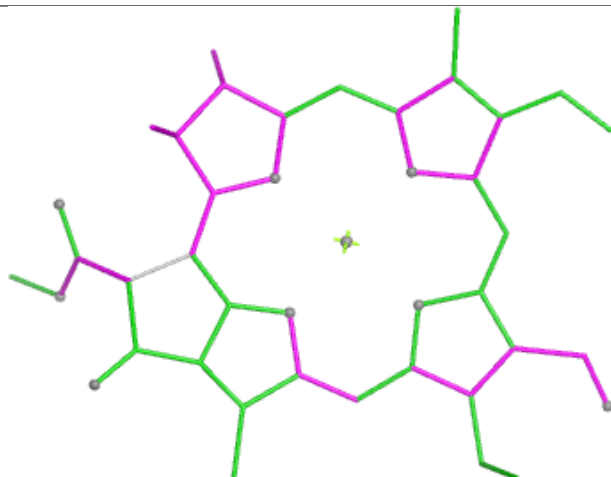


Rings

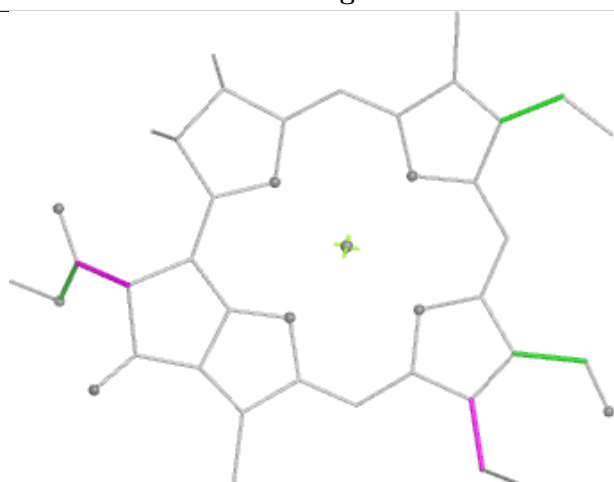
Ligand CHL R 613



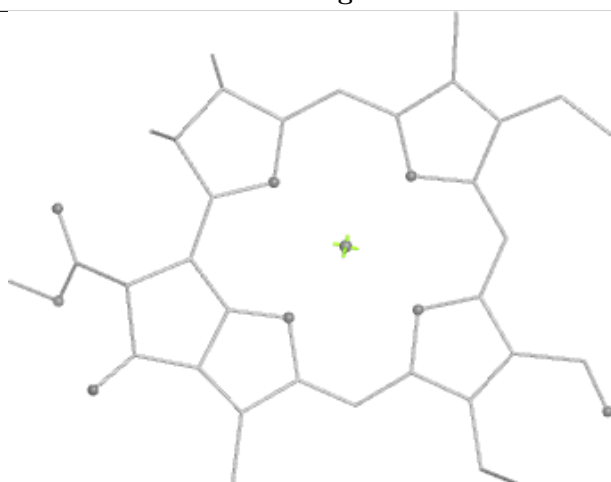
Bond lengths



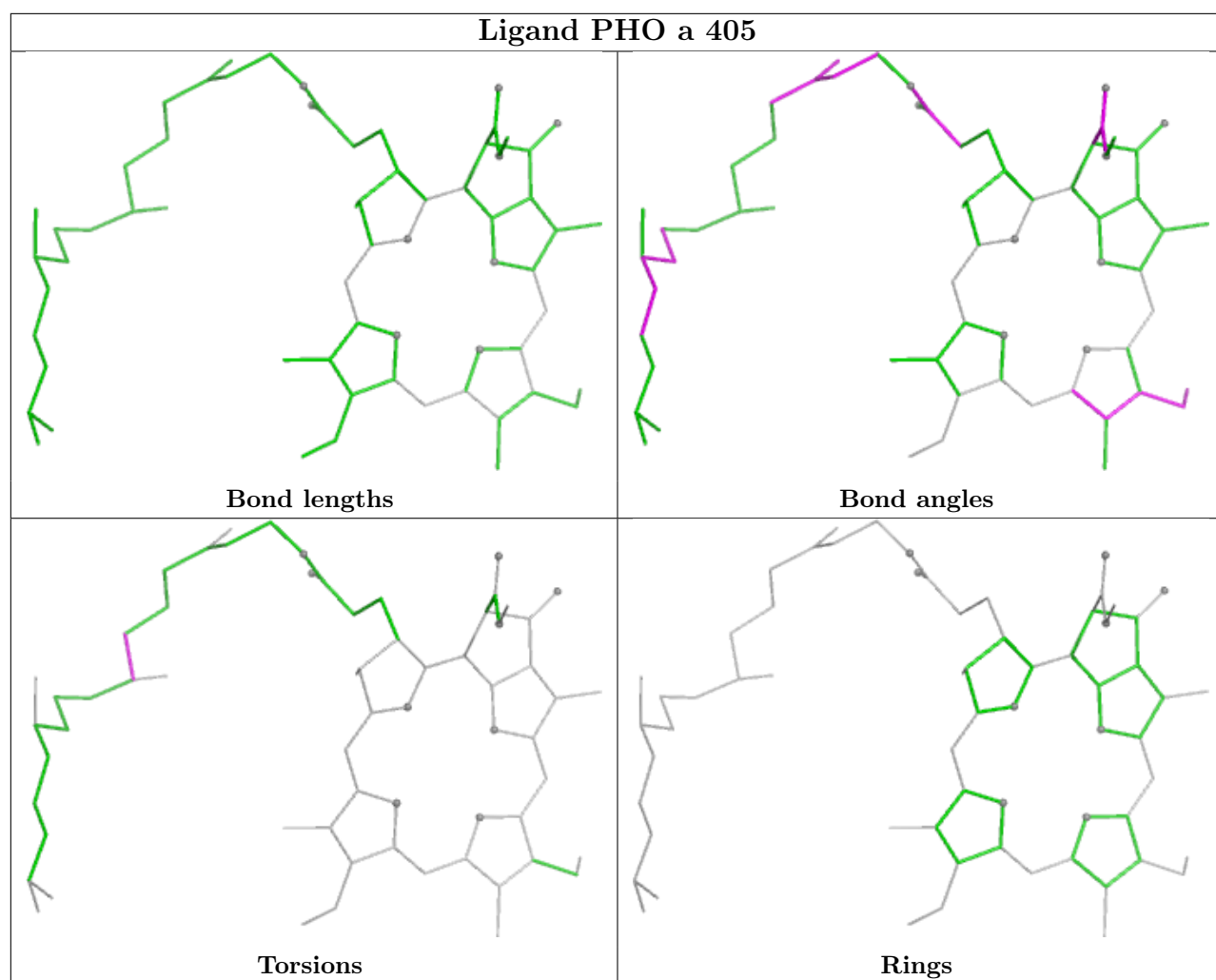
Bond angles

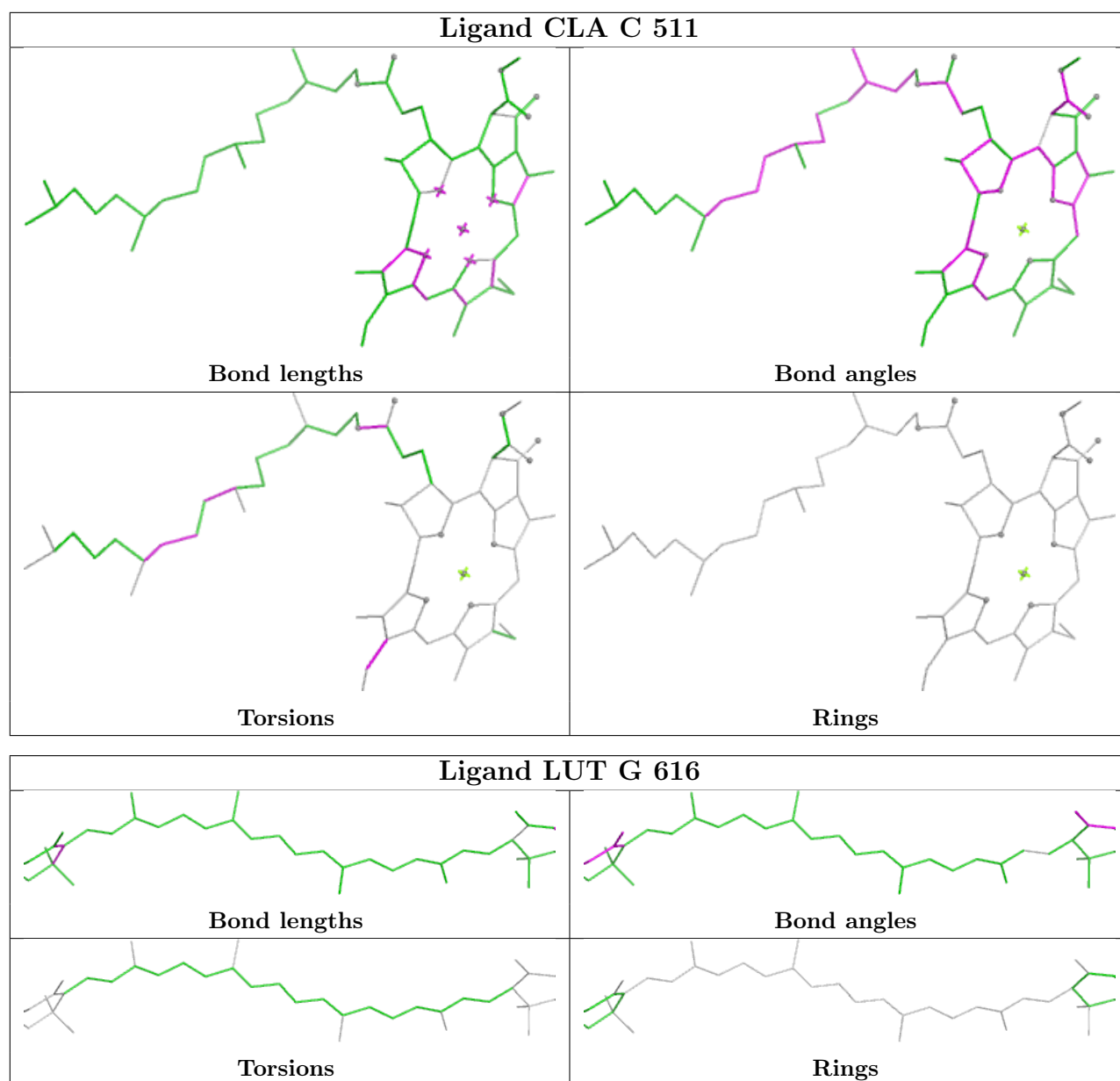


Torsions

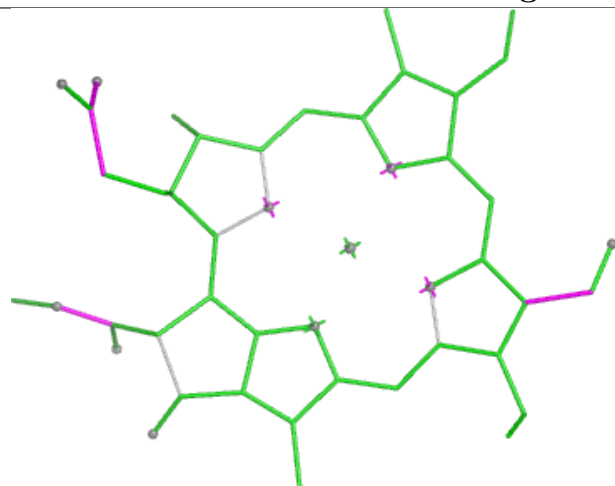


Rings

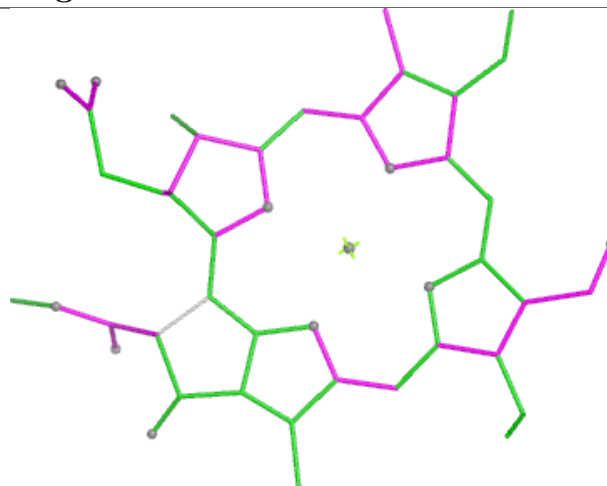




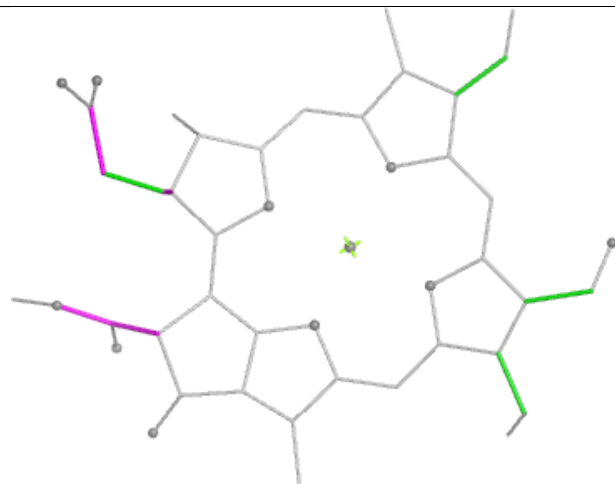
Ligand CHL g 607



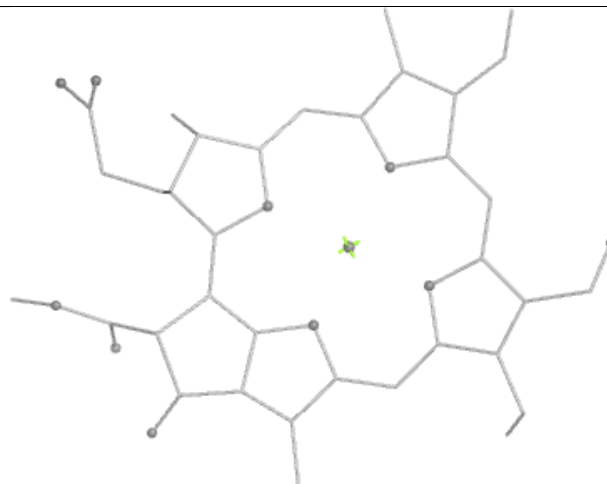
Bond lengths



Bond angles

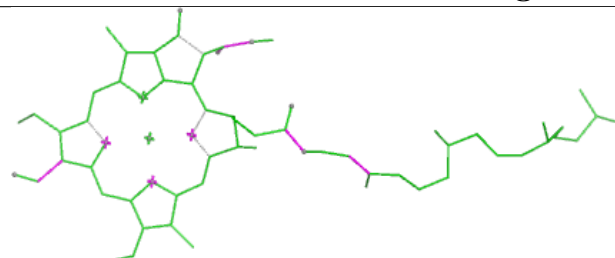


Torsions

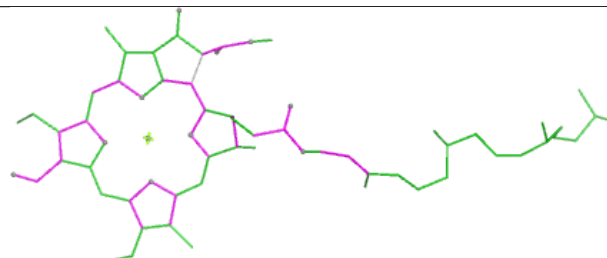


Rings

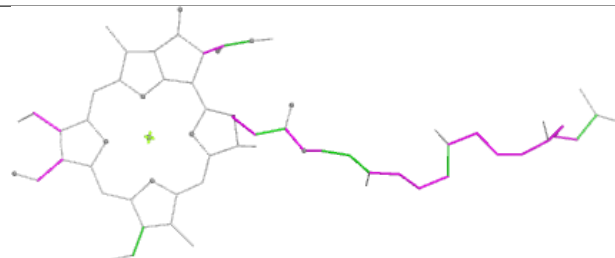
Ligand CHL G 601



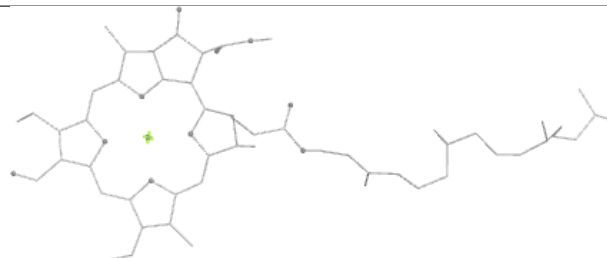
Bond lengths



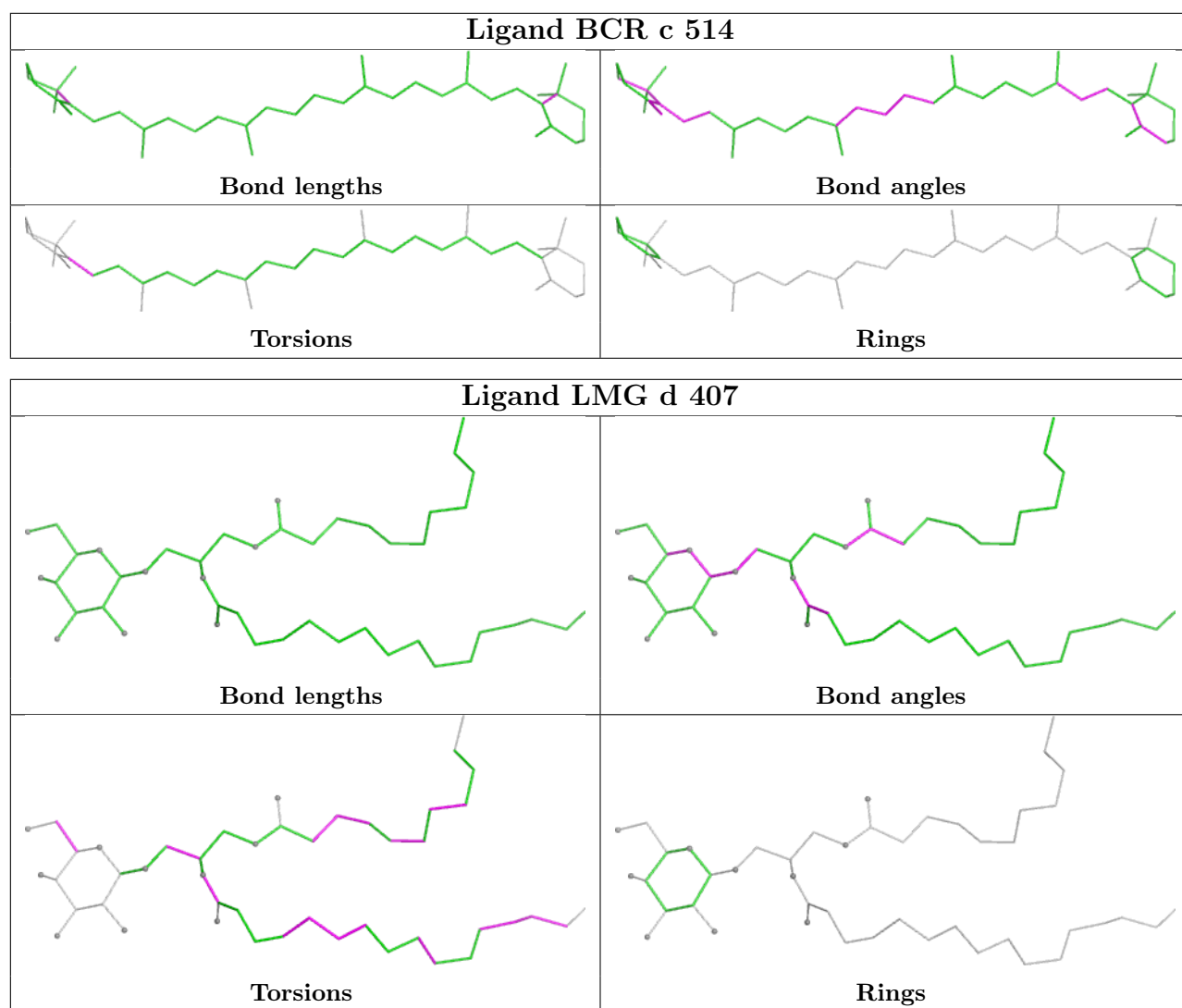
Bond angles

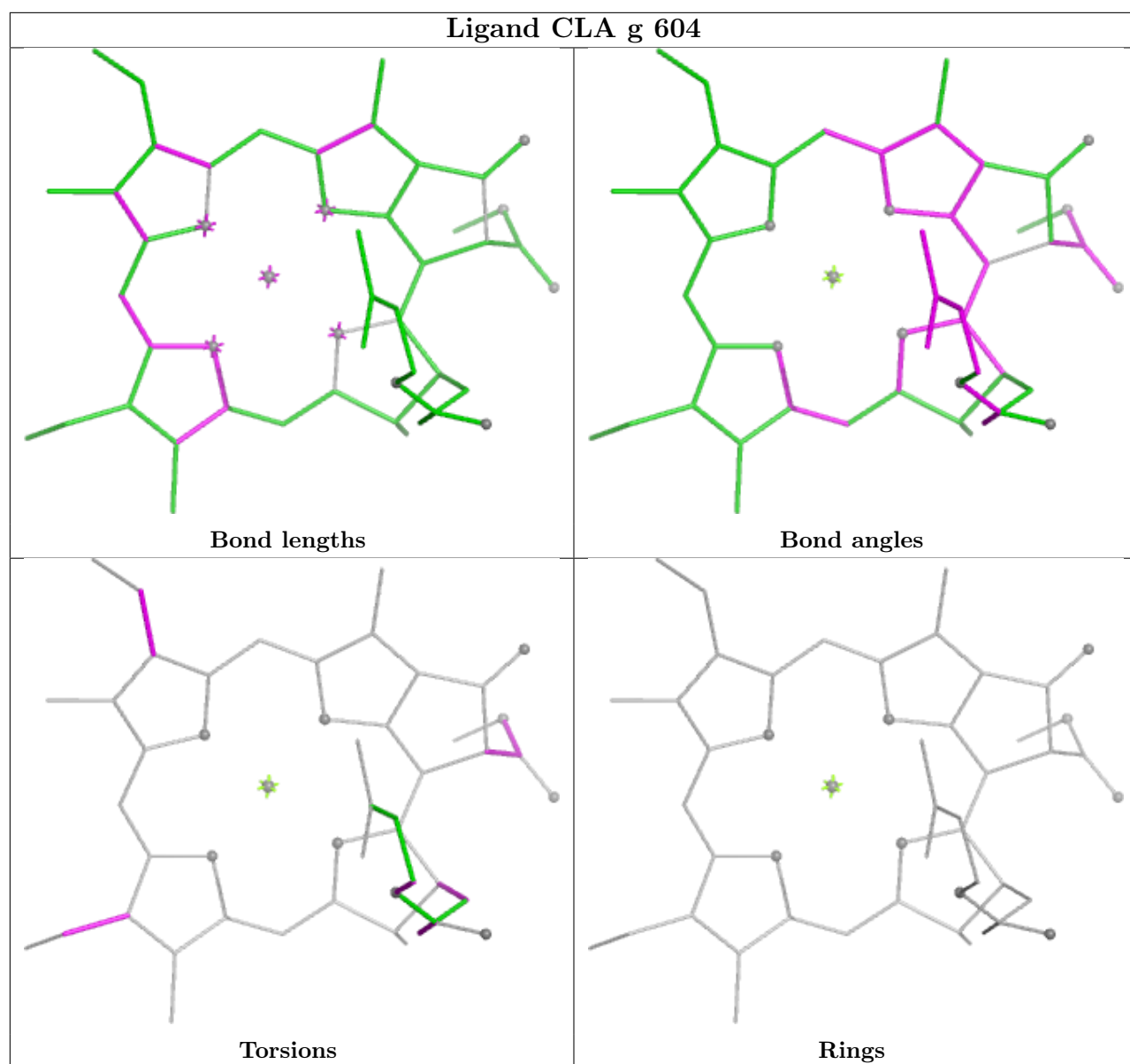


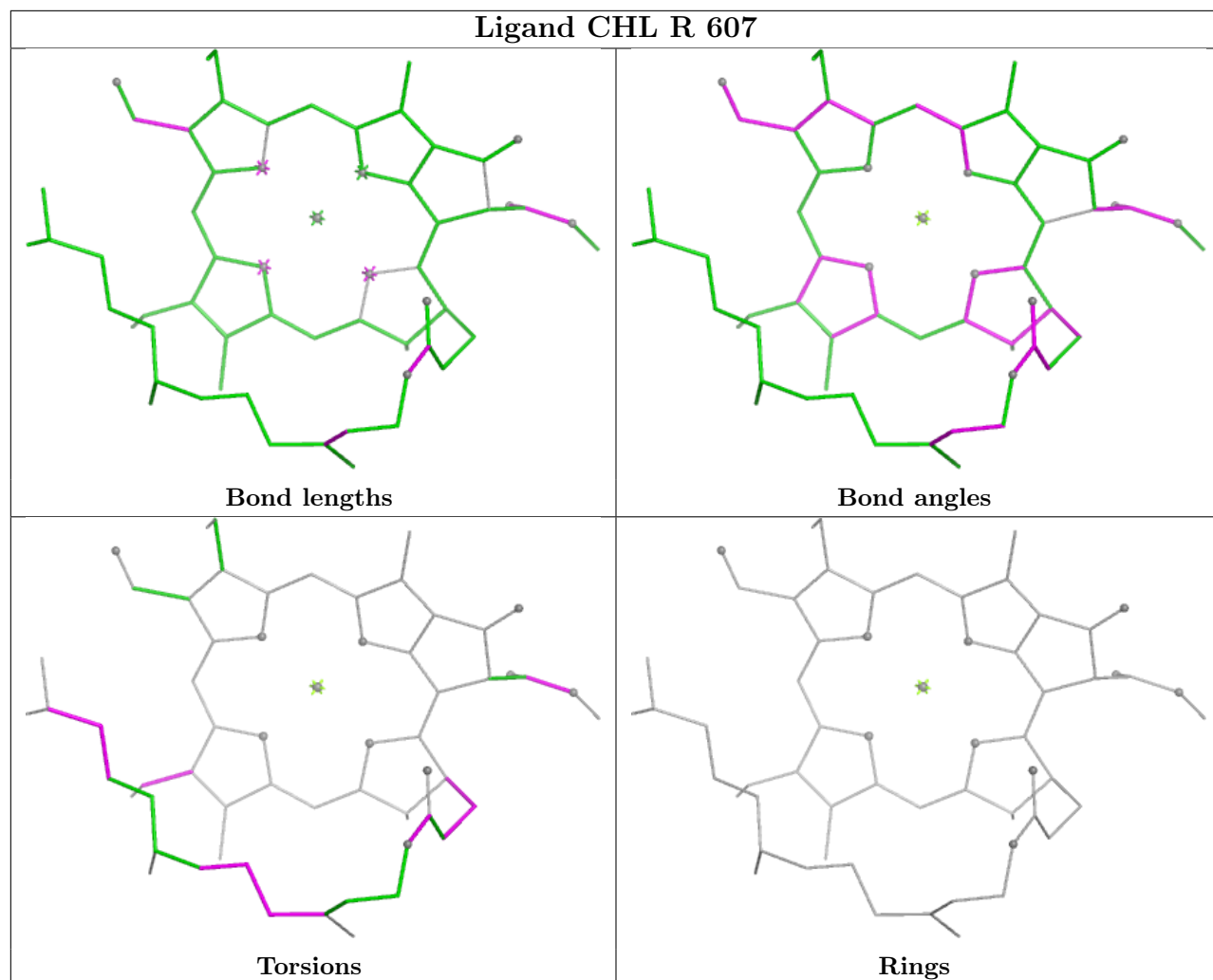
Torsions

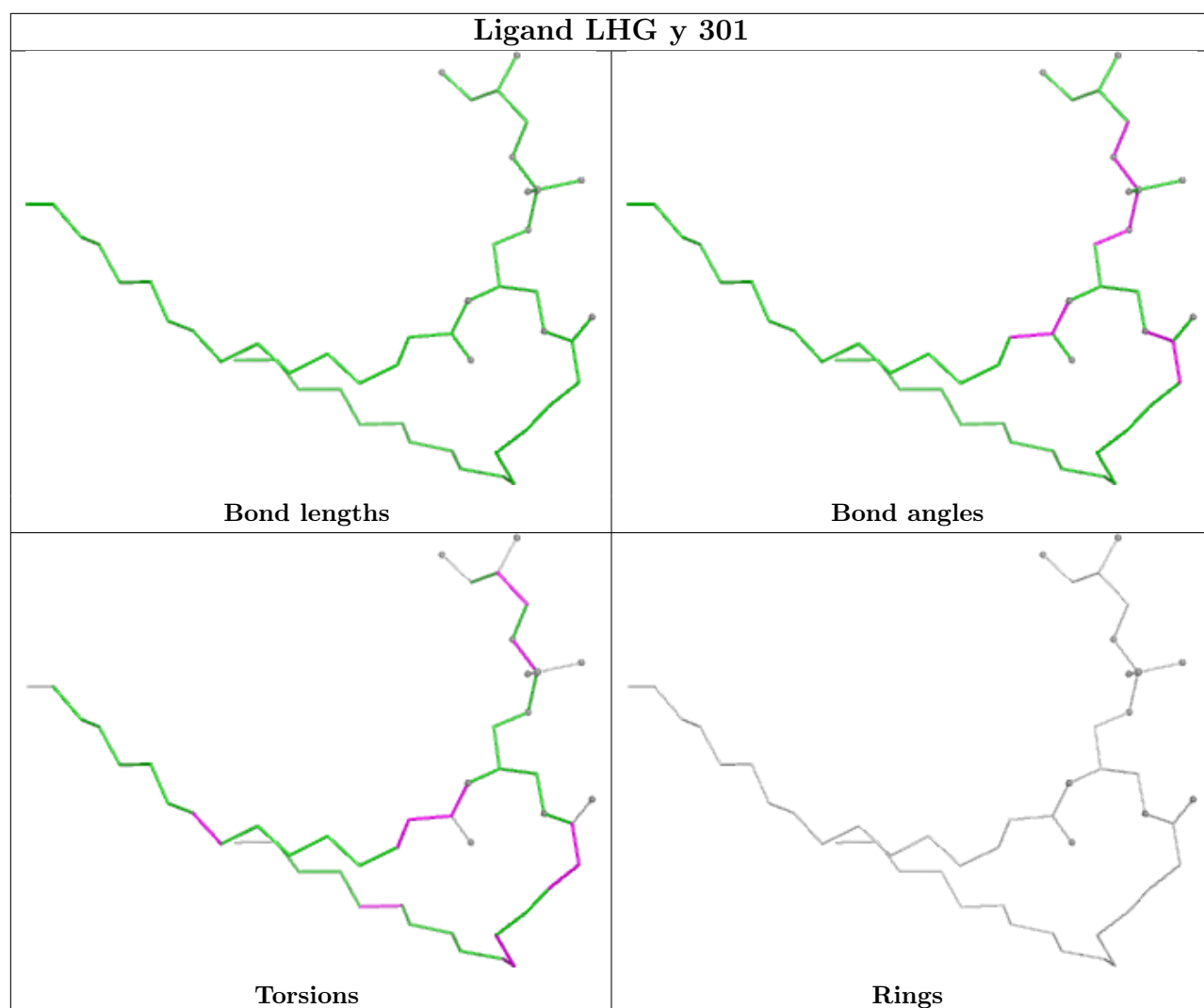


Rings

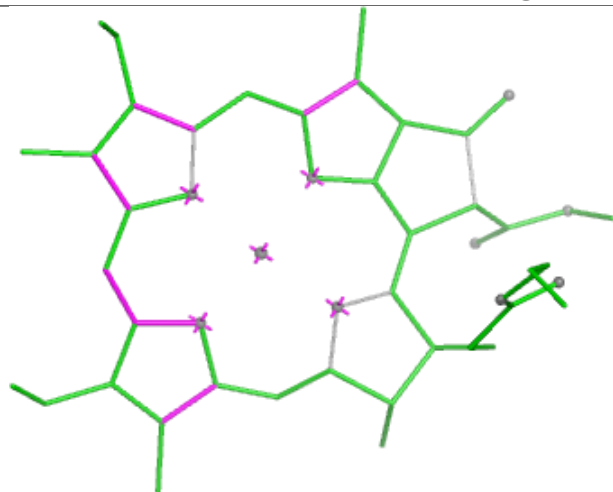




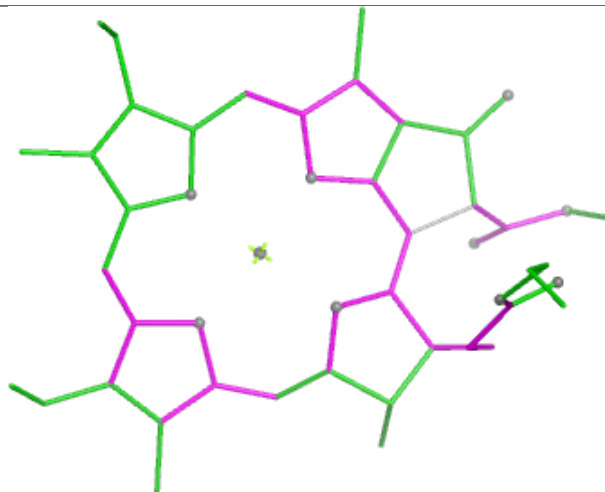




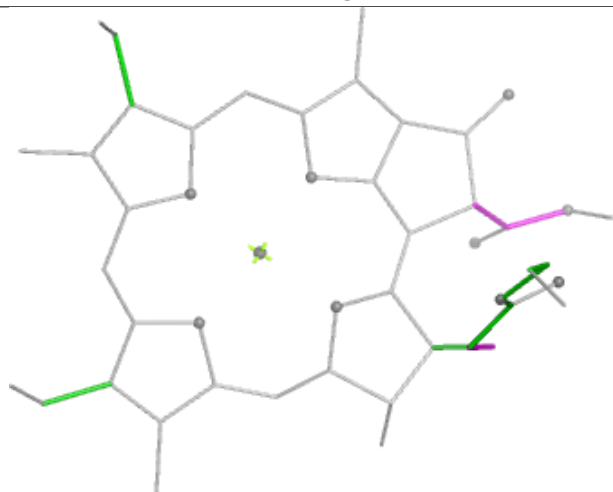
Ligand CLA n 614



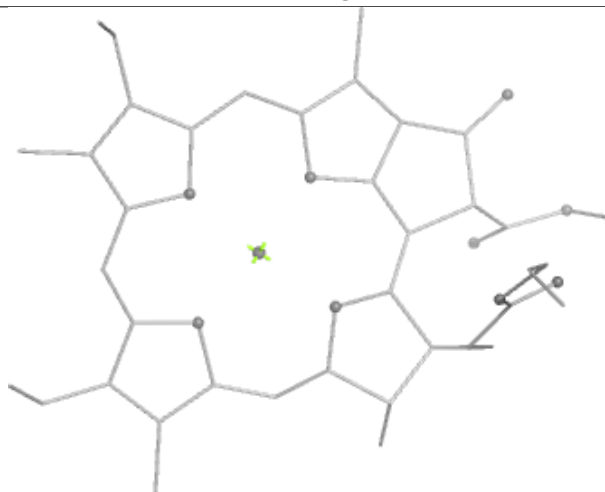
Bond lengths



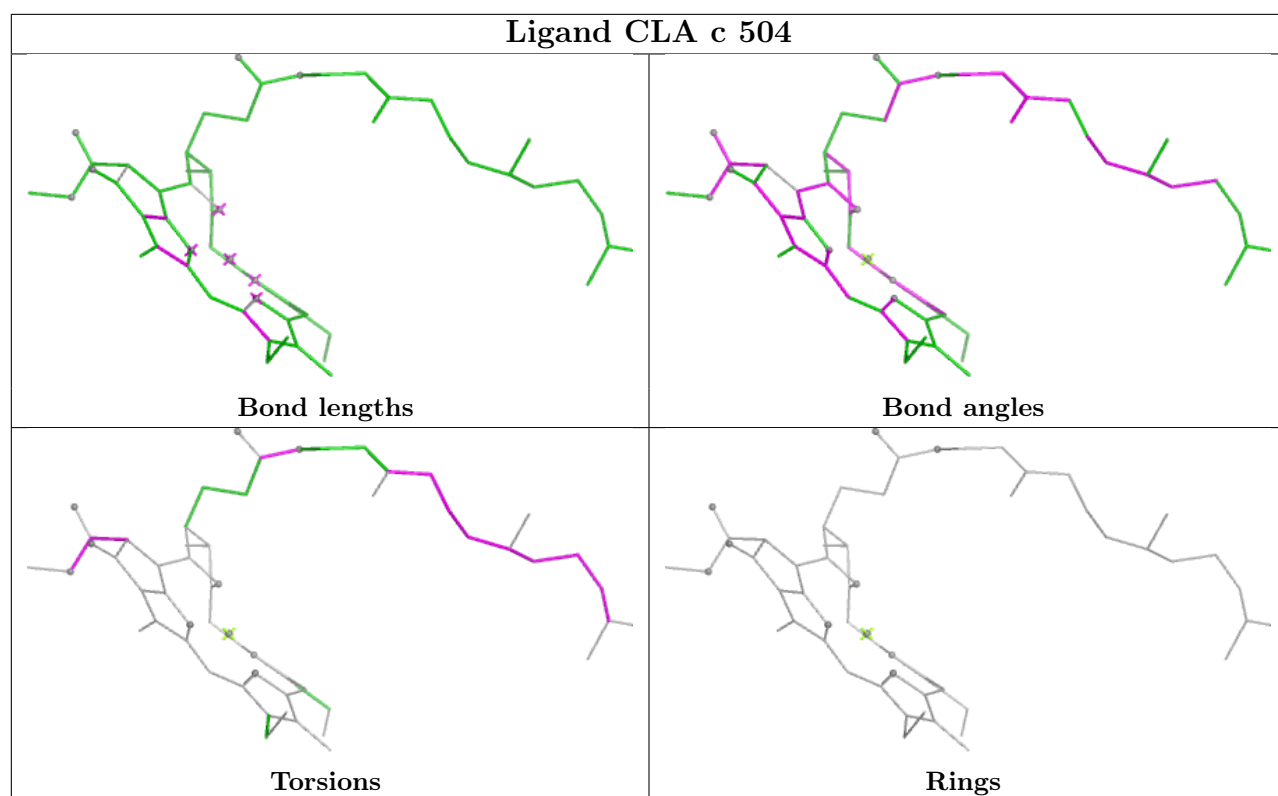
Bond angles

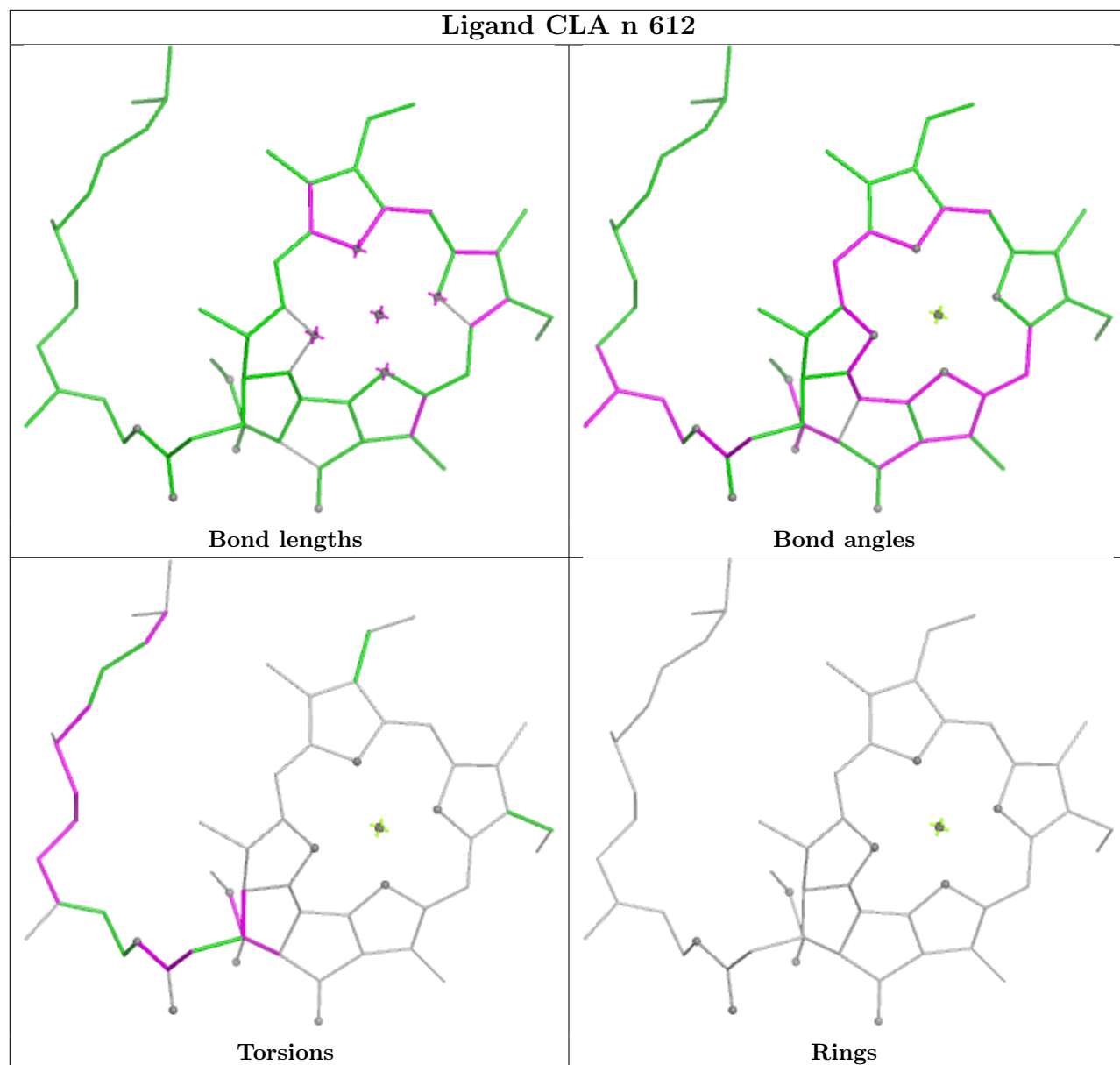


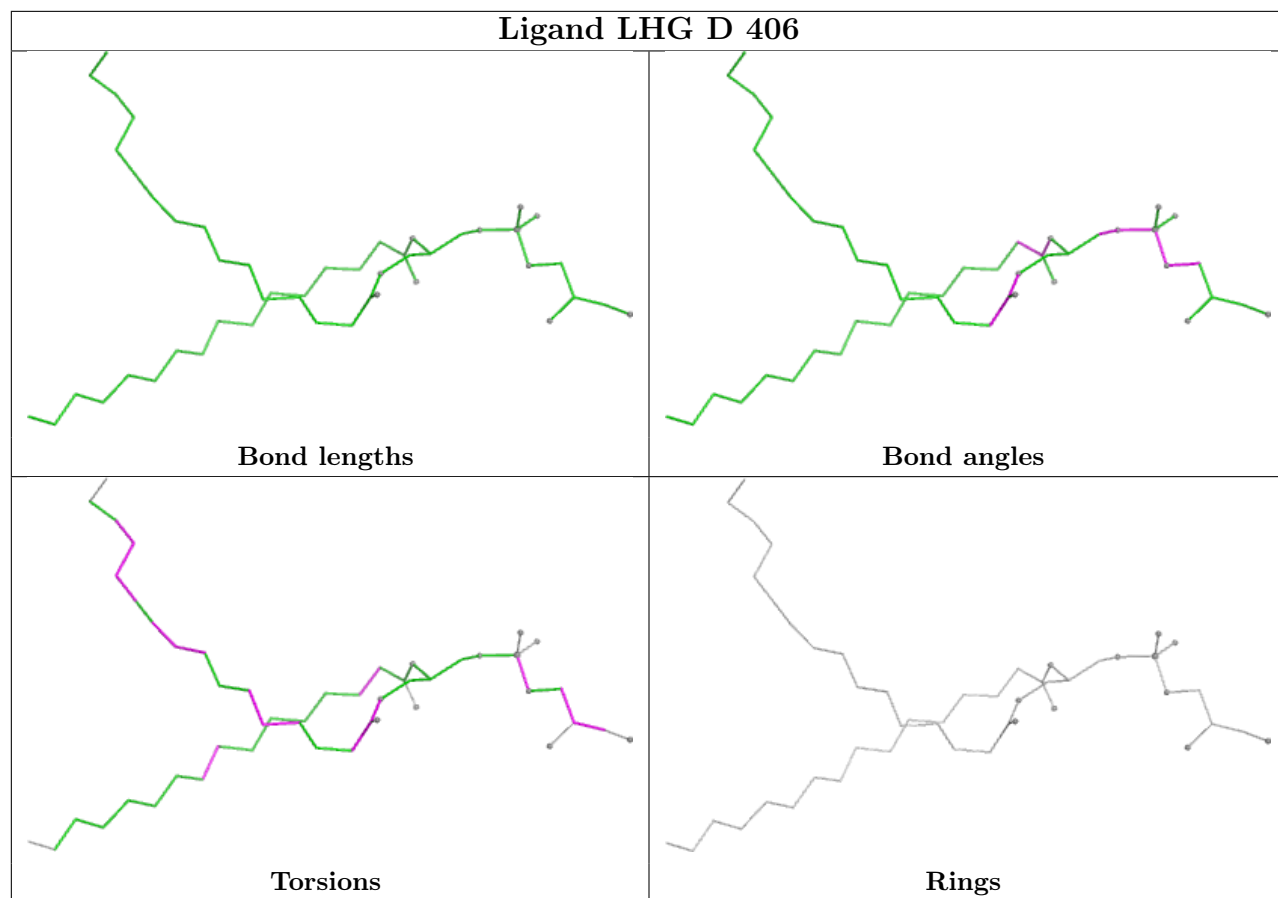
Torsions

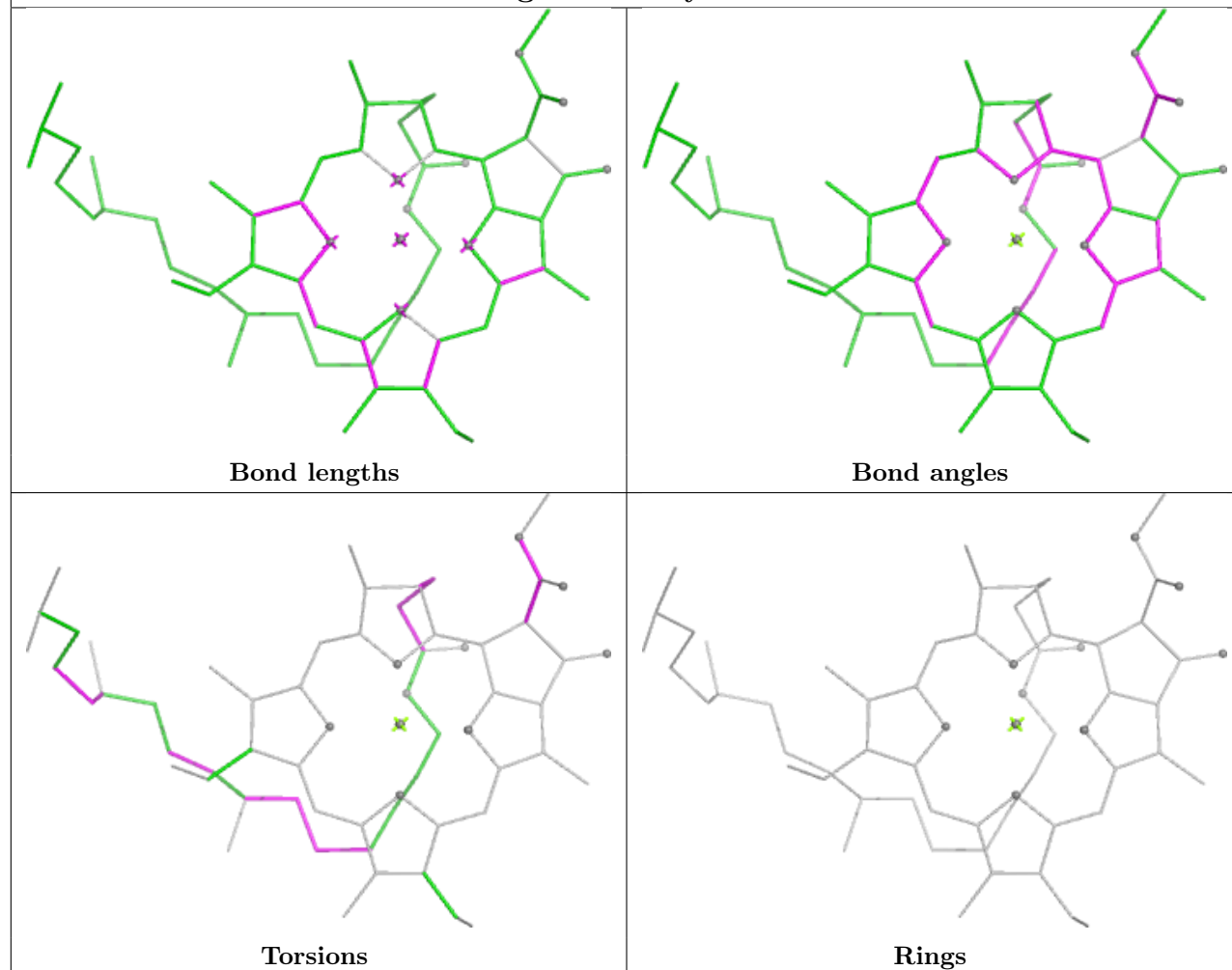
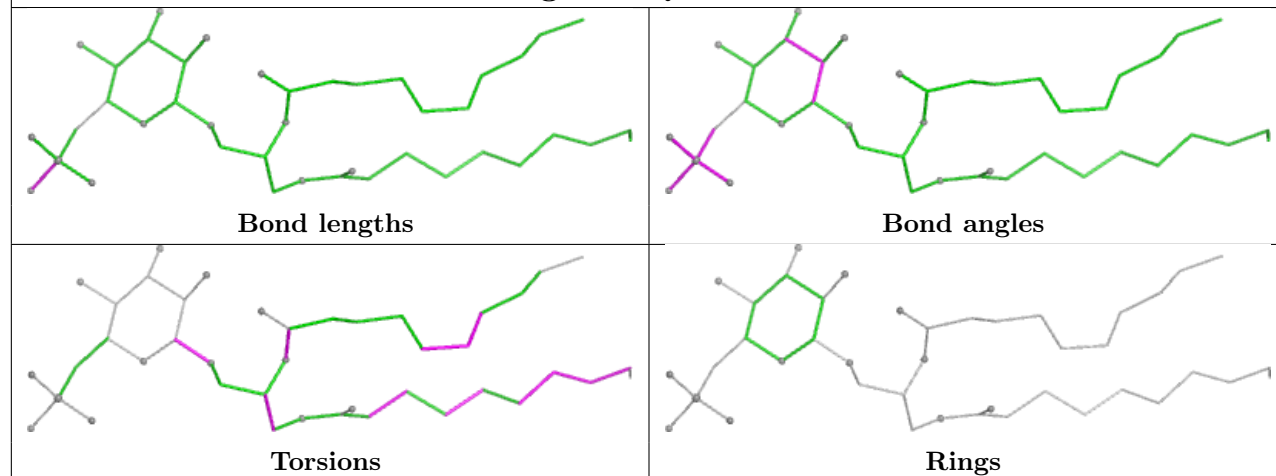


Rings

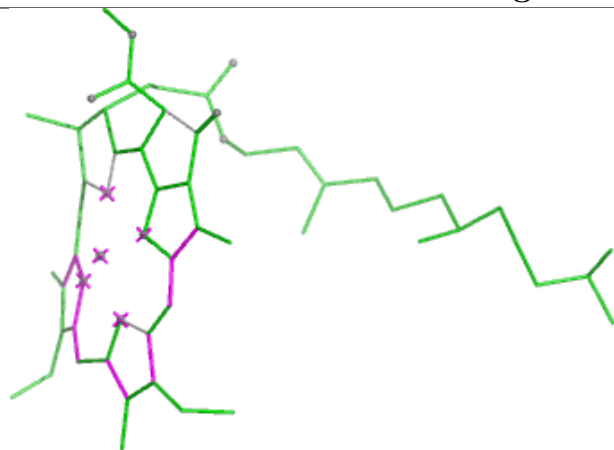




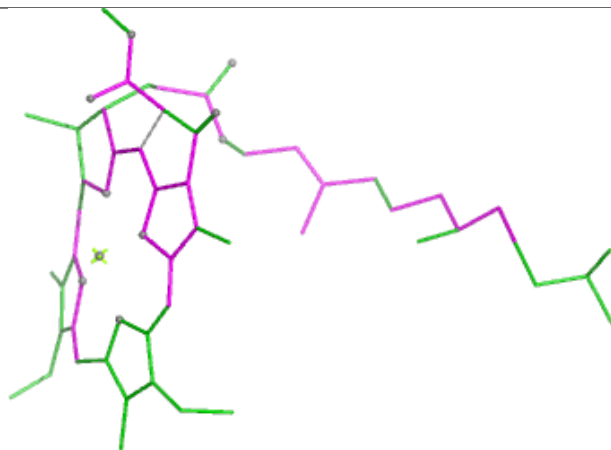


Ligand CLA y 314**Ligand SQD 1 102**

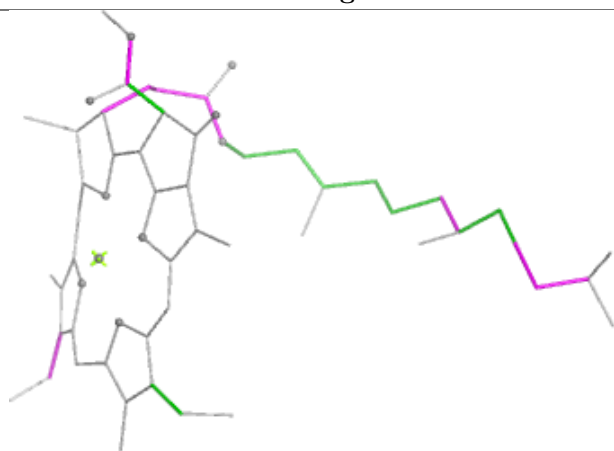
Ligand CLA N 611



Bond lengths



Bond angles

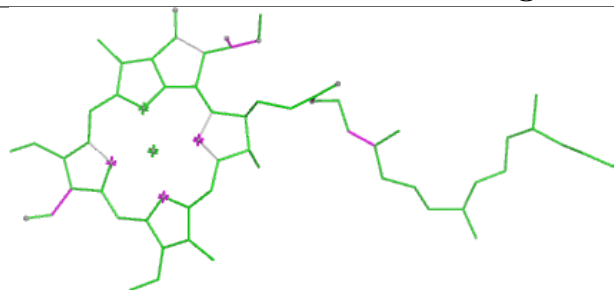


Torsions

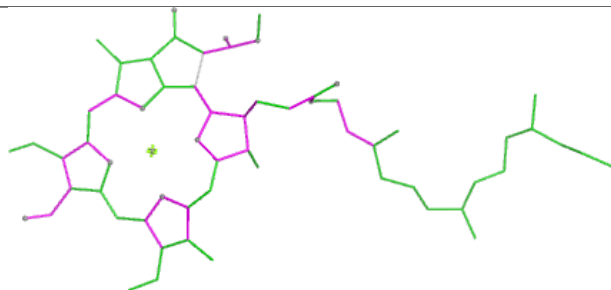


Rings

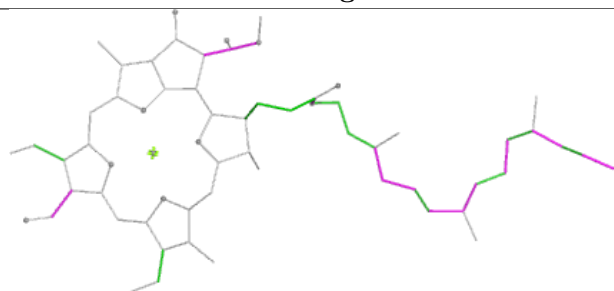
Ligand CHL 2 601



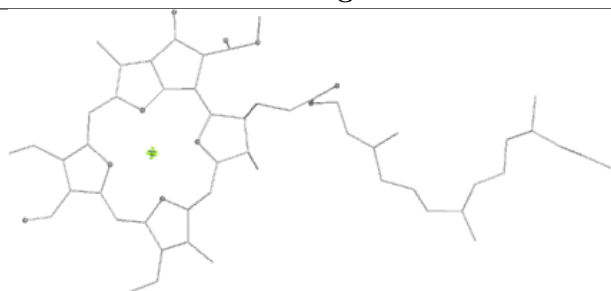
Bond lengths



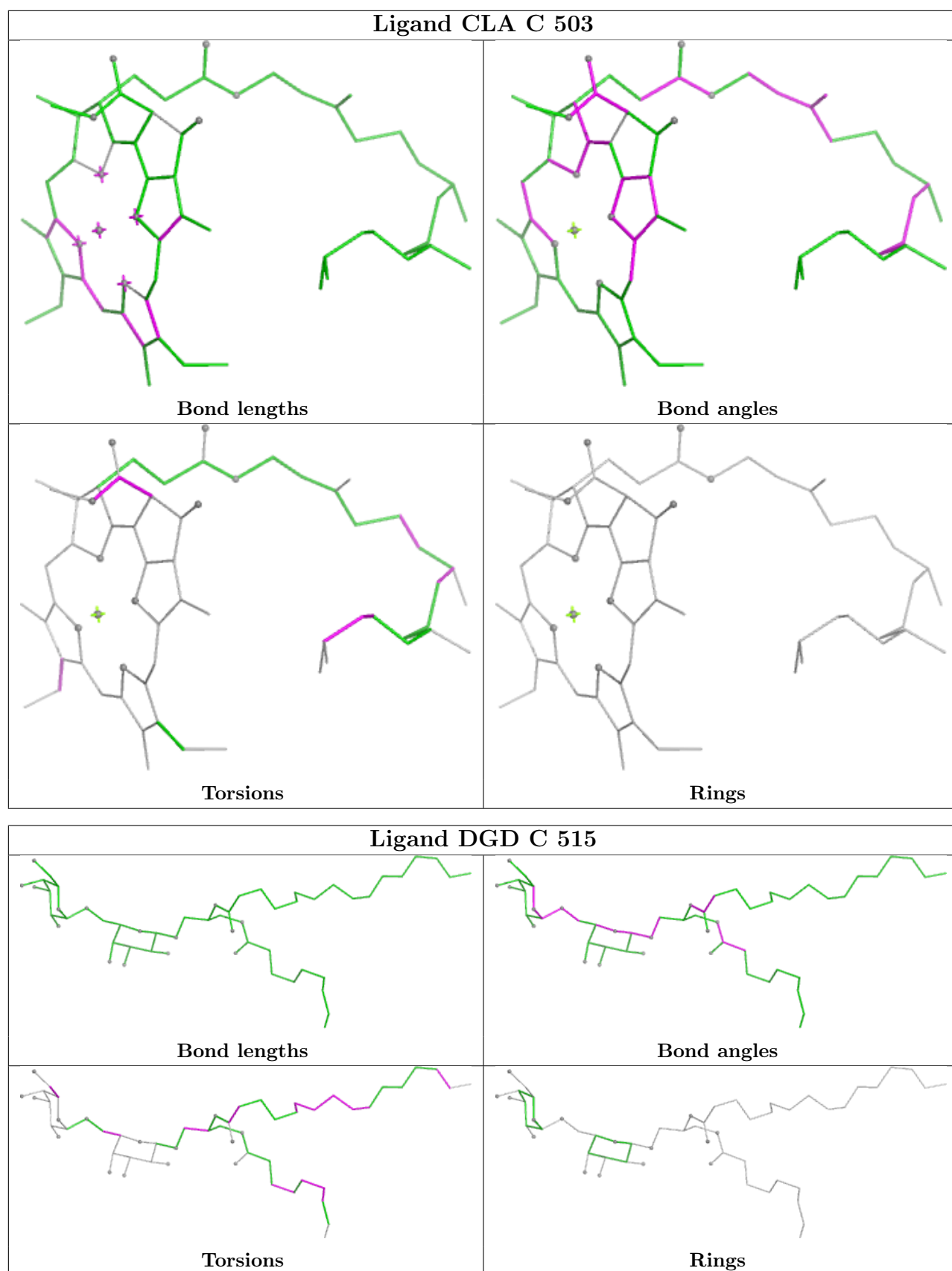
Bond angles

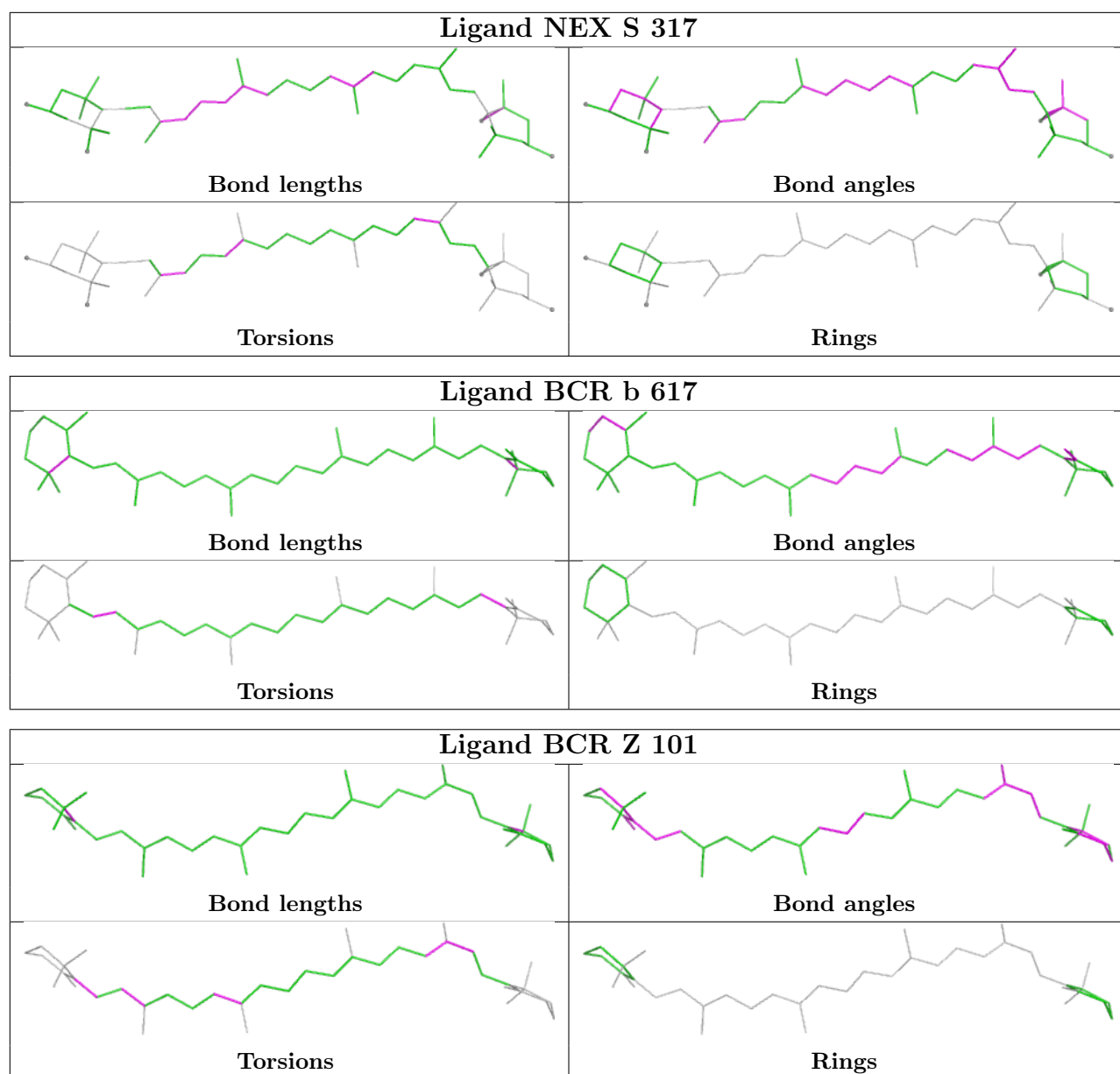


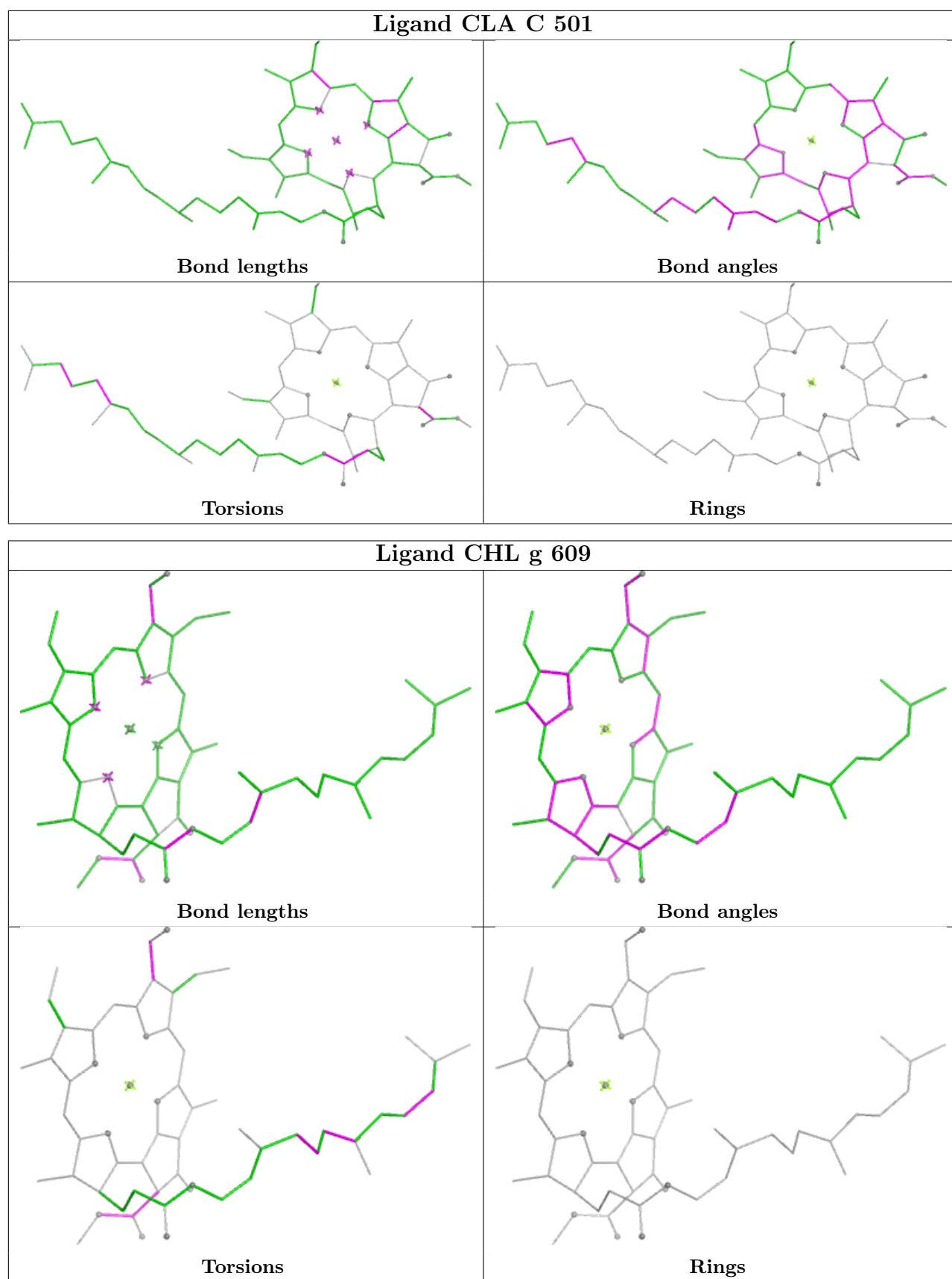
Torsions

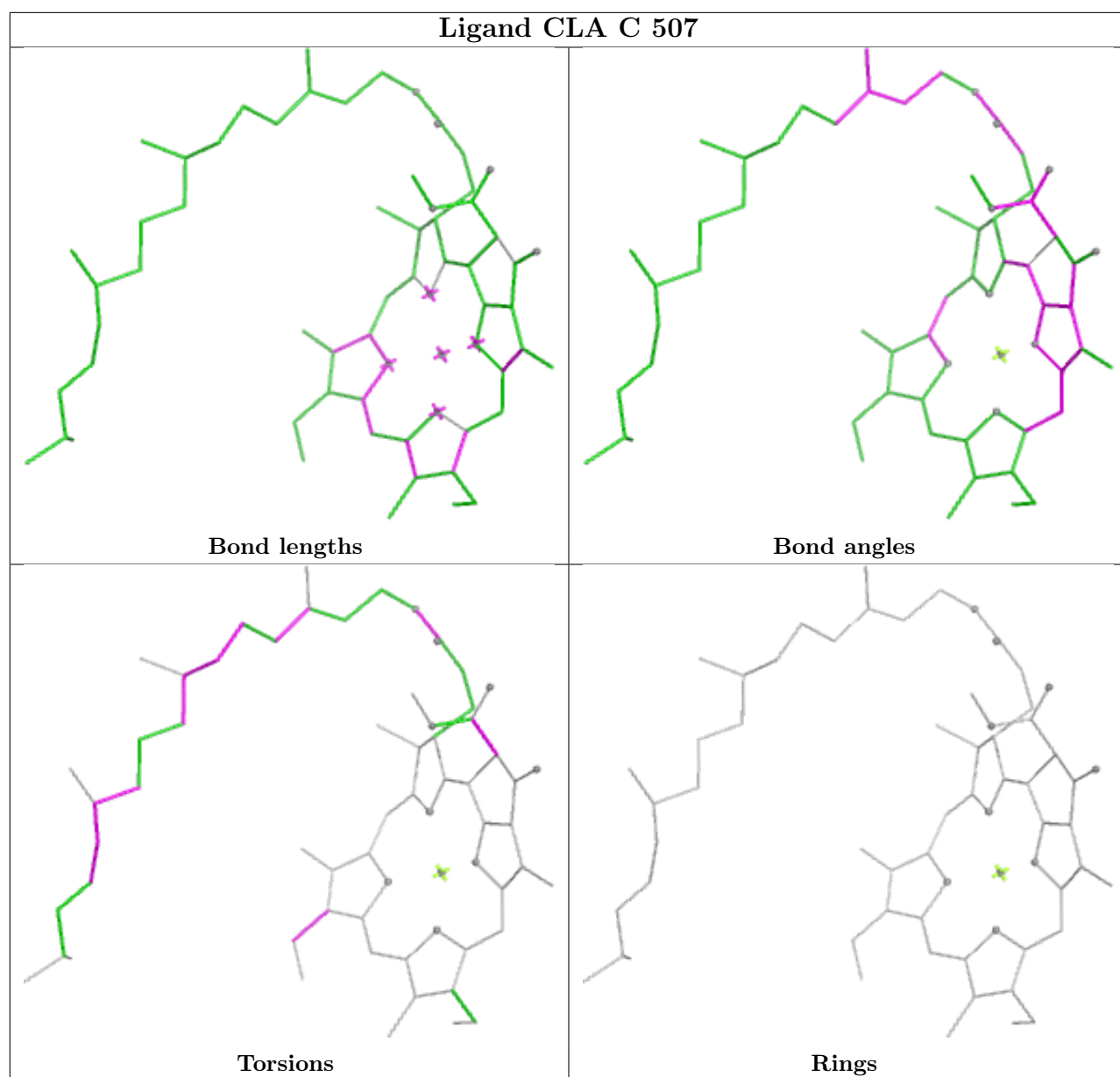


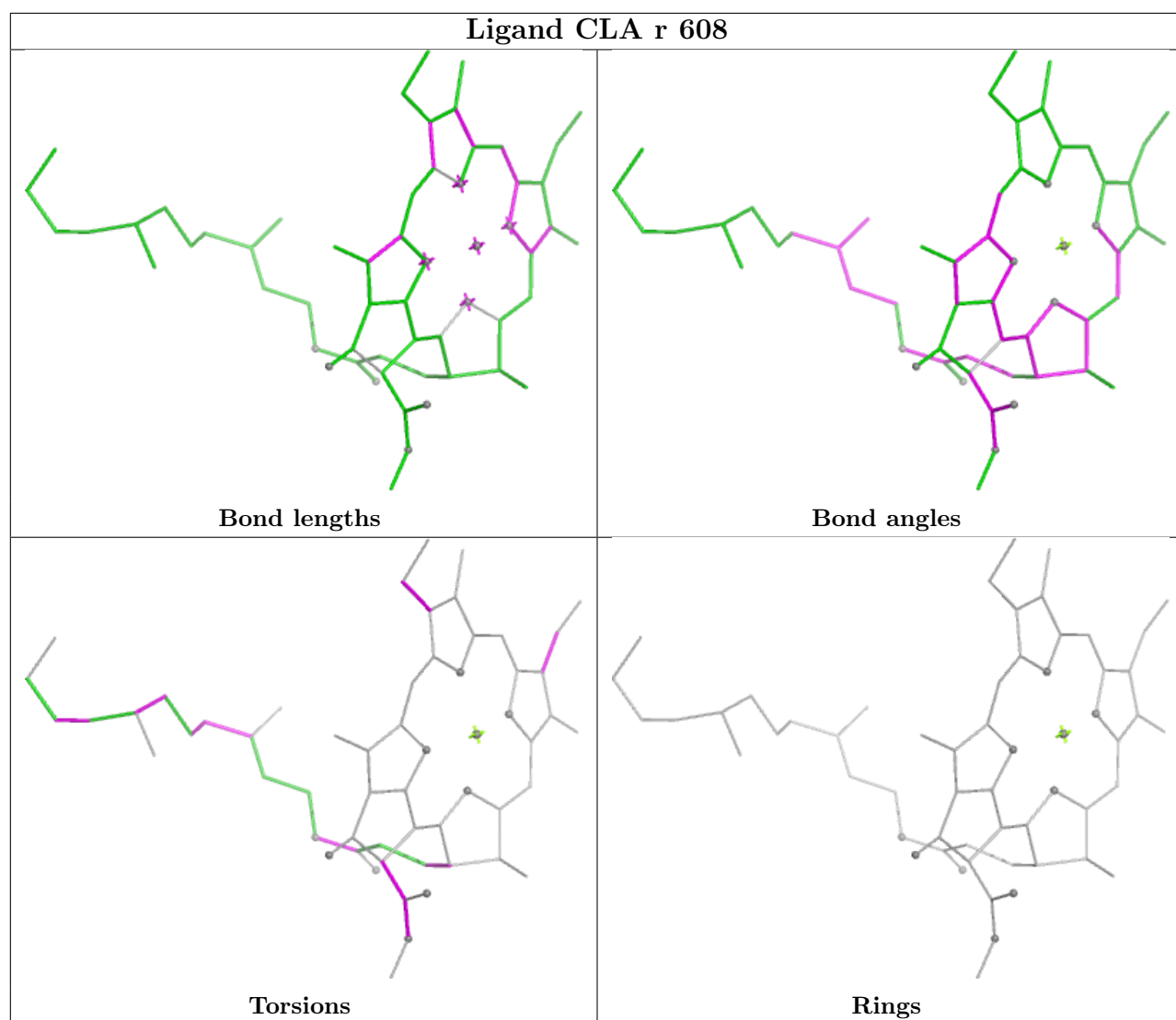
Rings



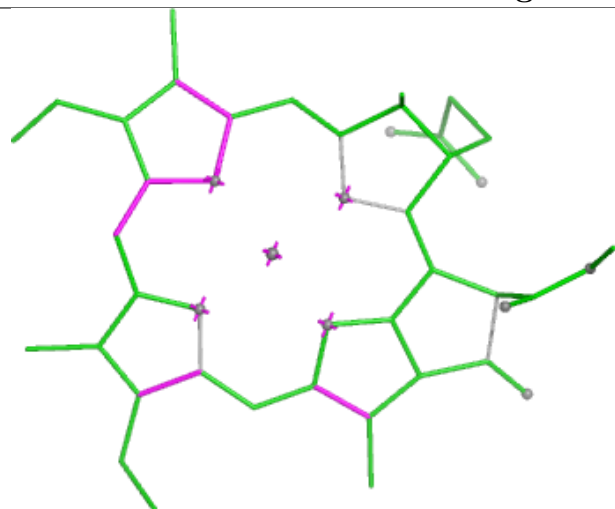




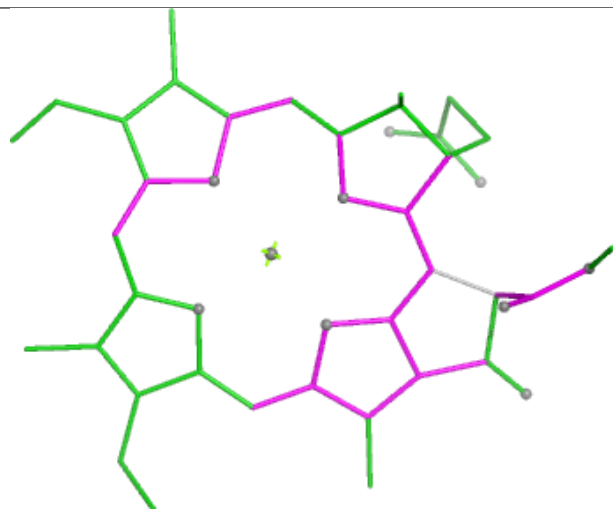




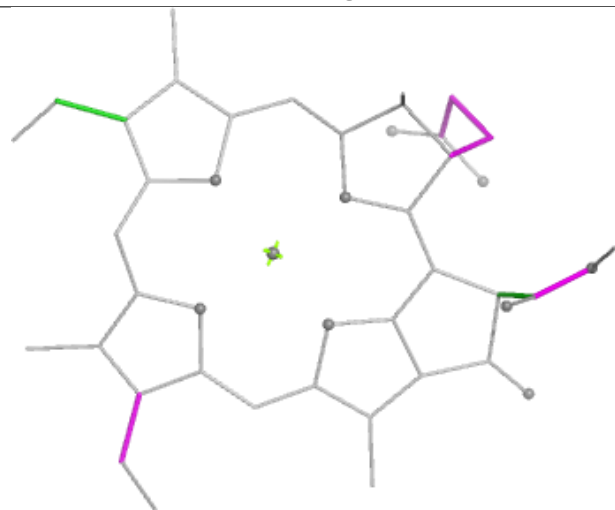
Ligand CLA R 614



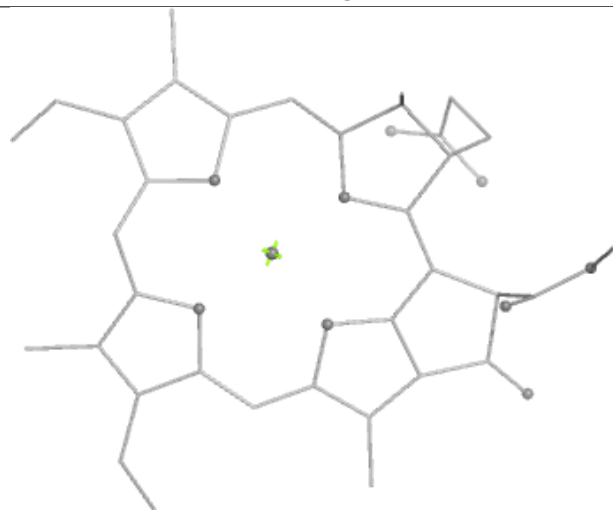
Bond lengths



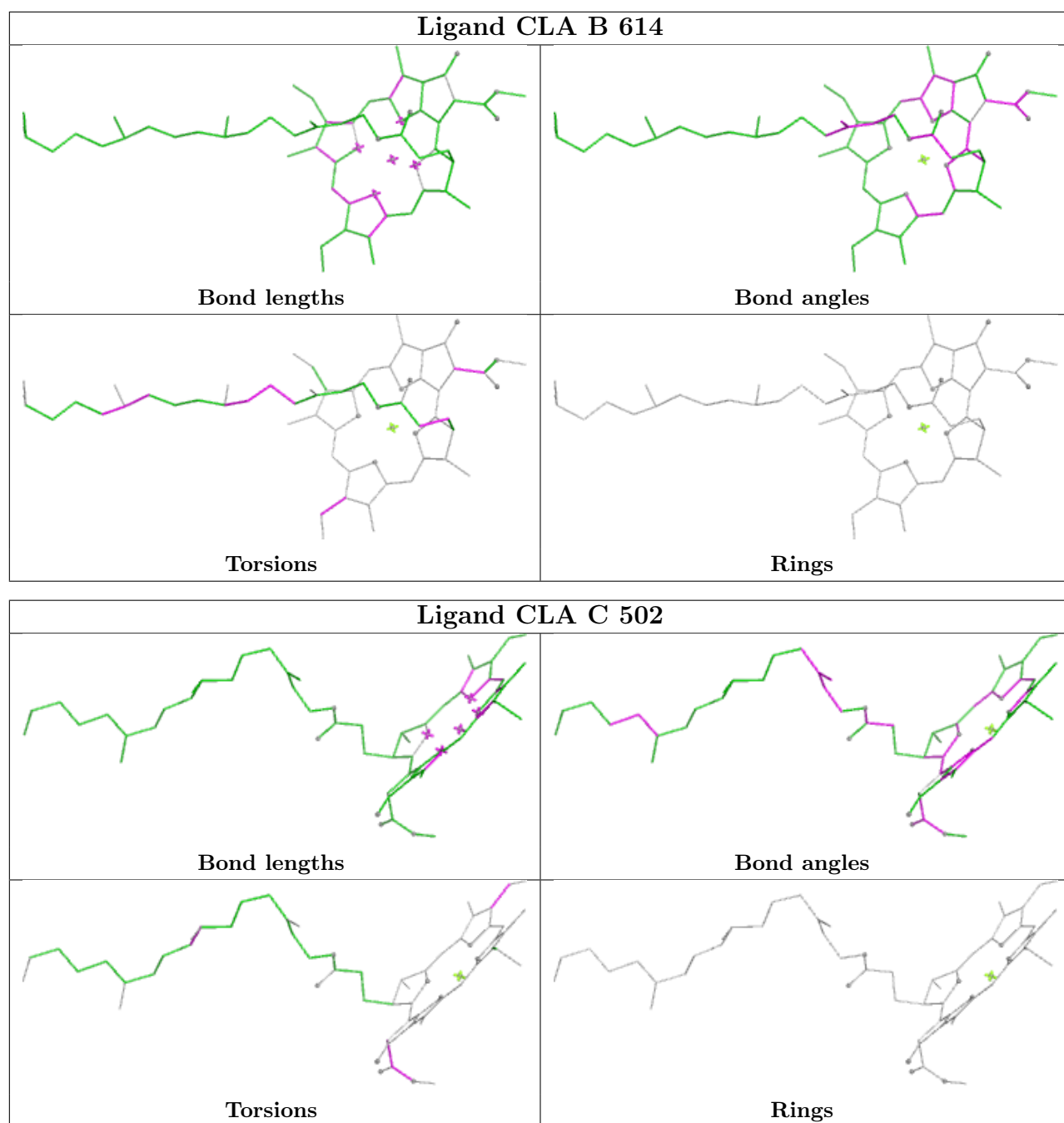
Bond angles

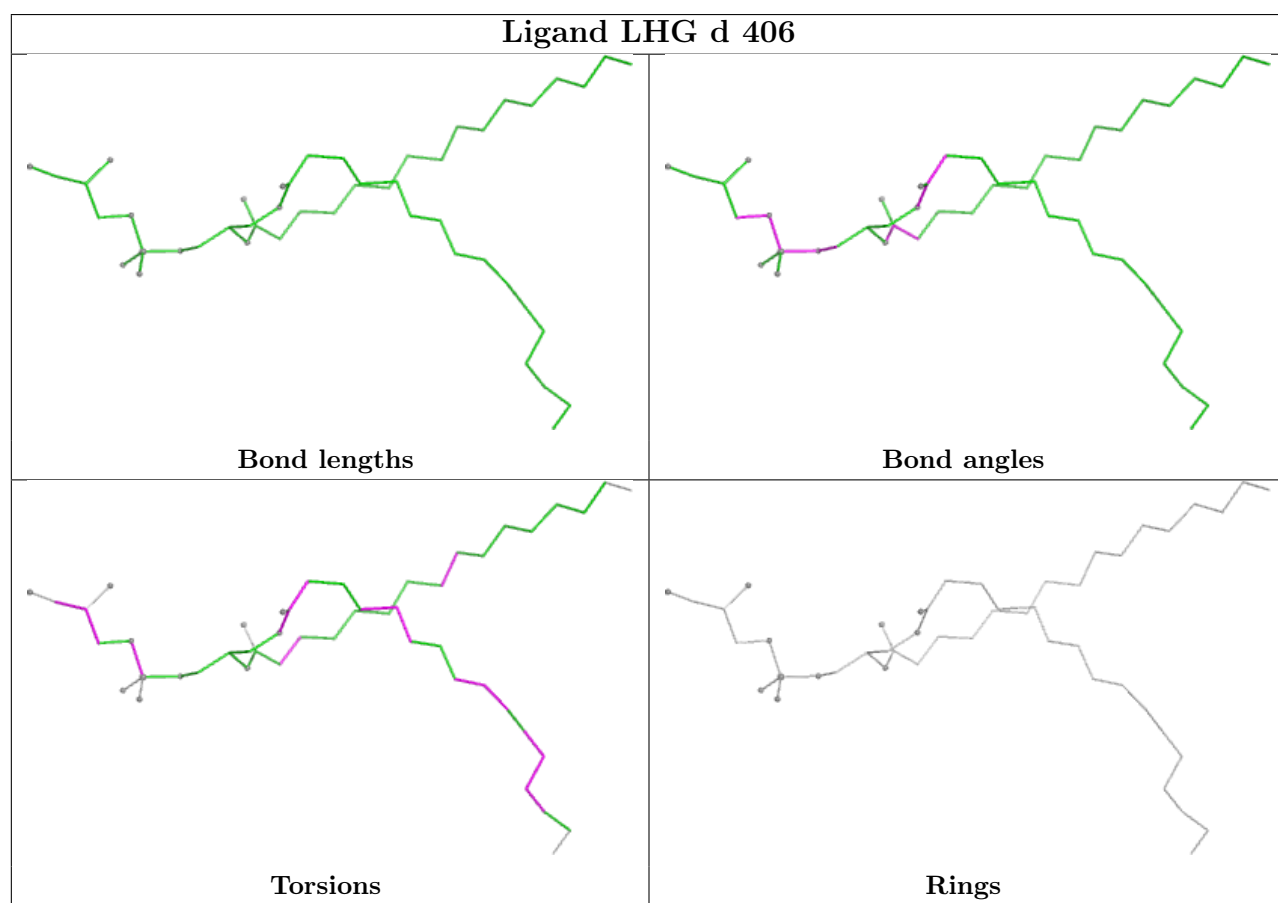
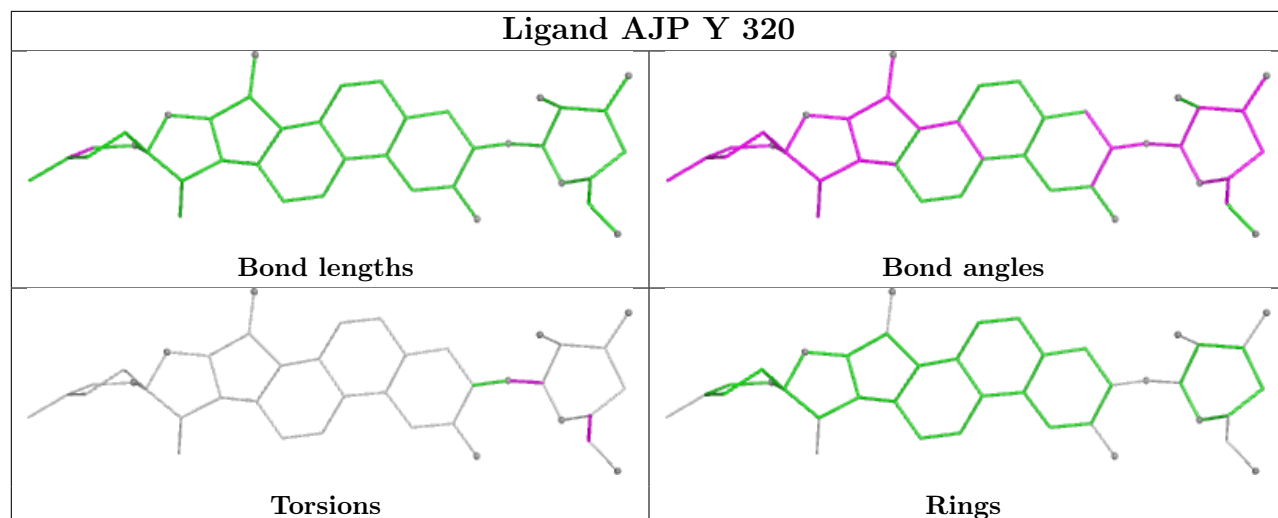


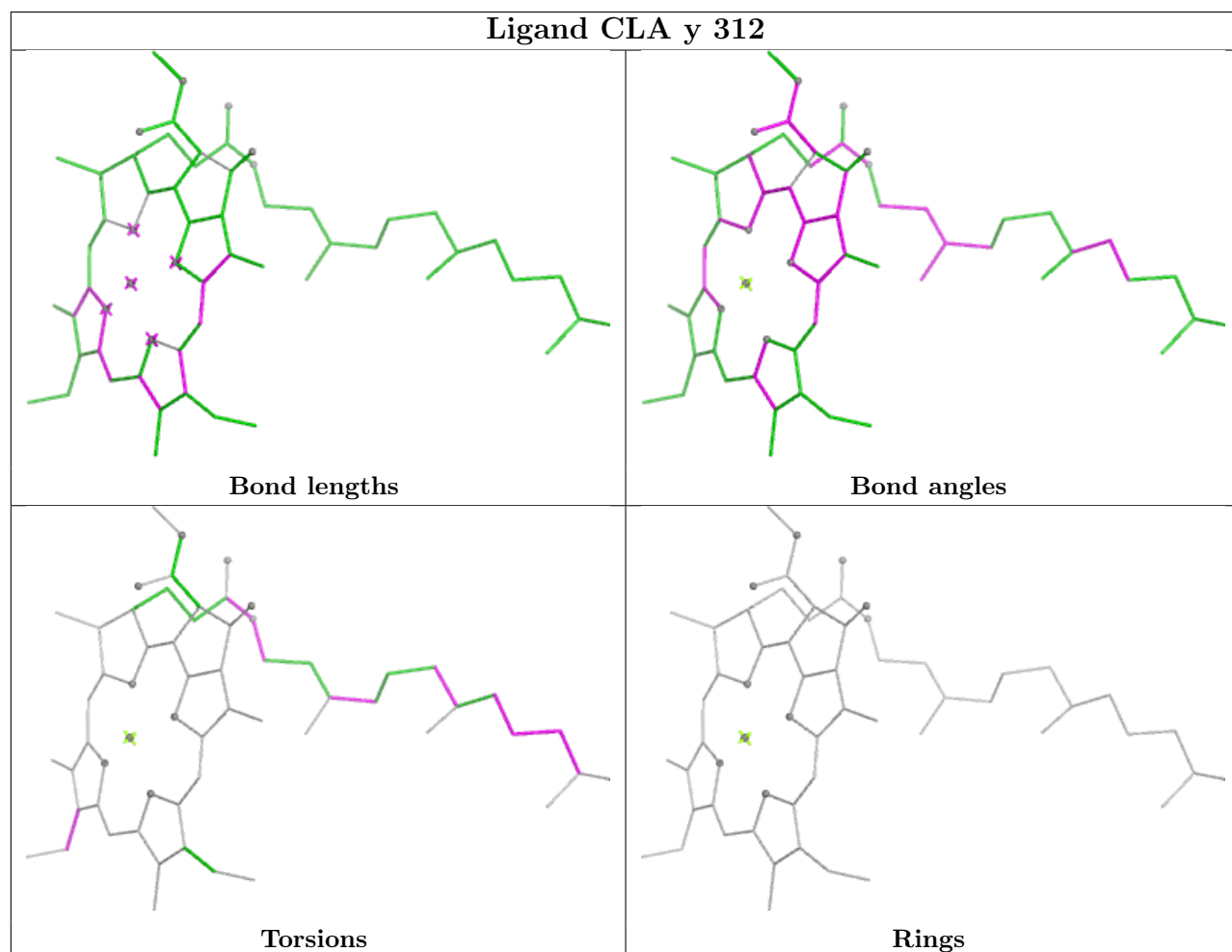
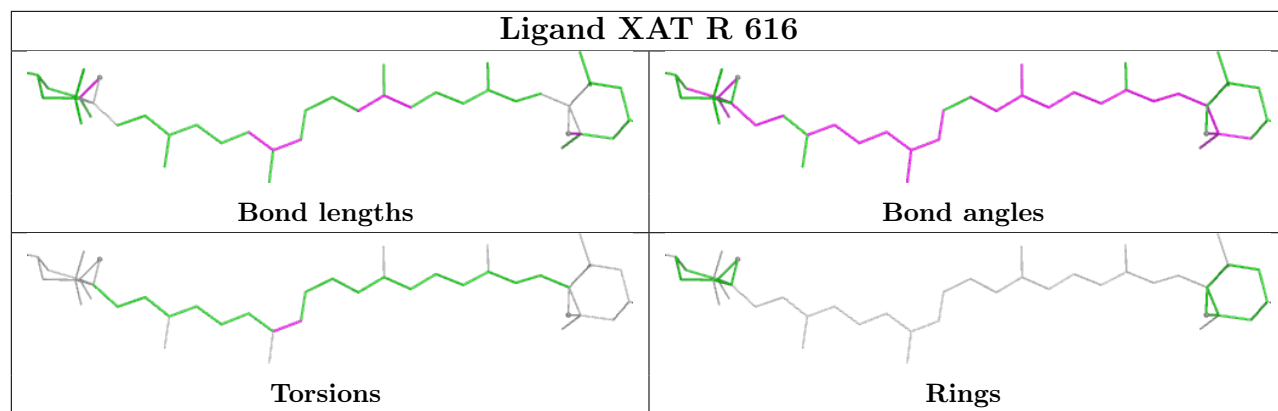
Torsions

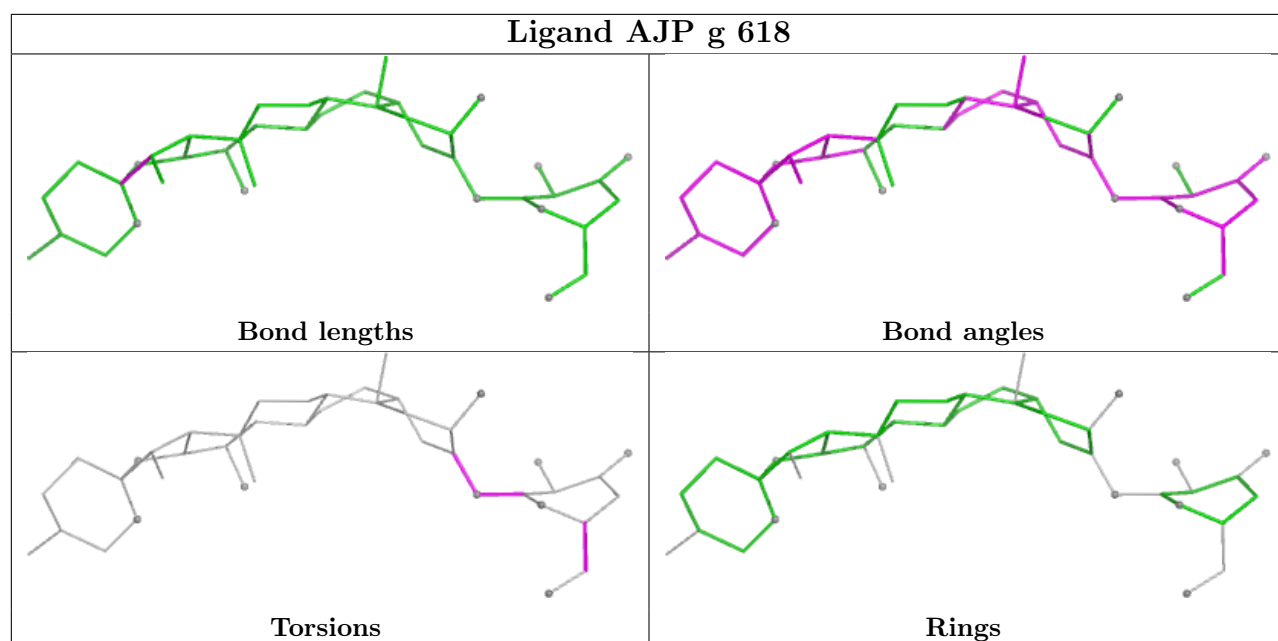
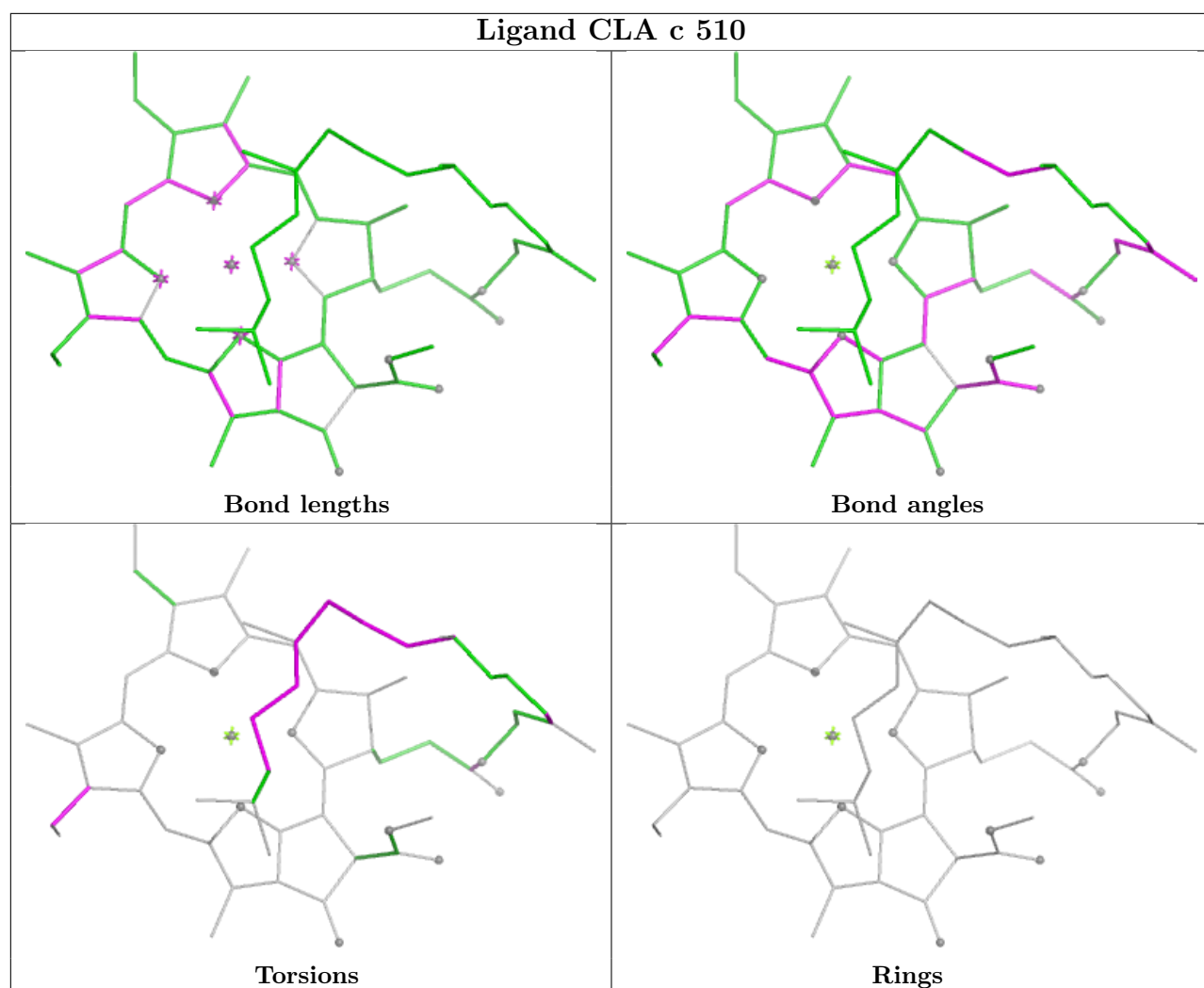


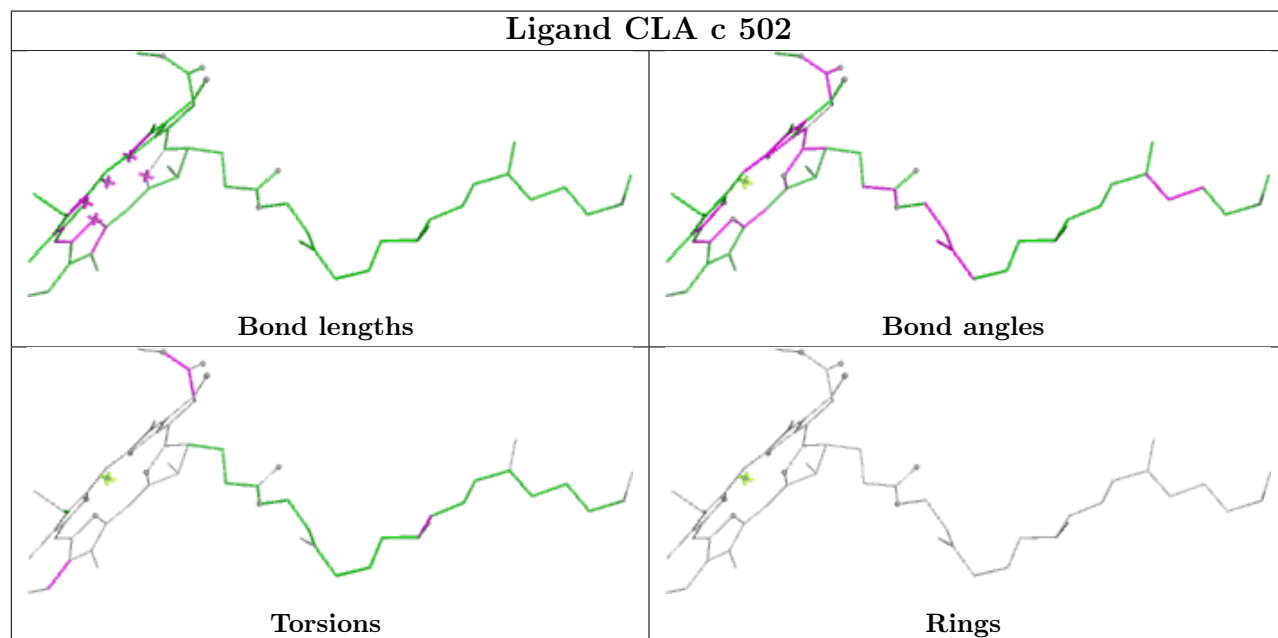
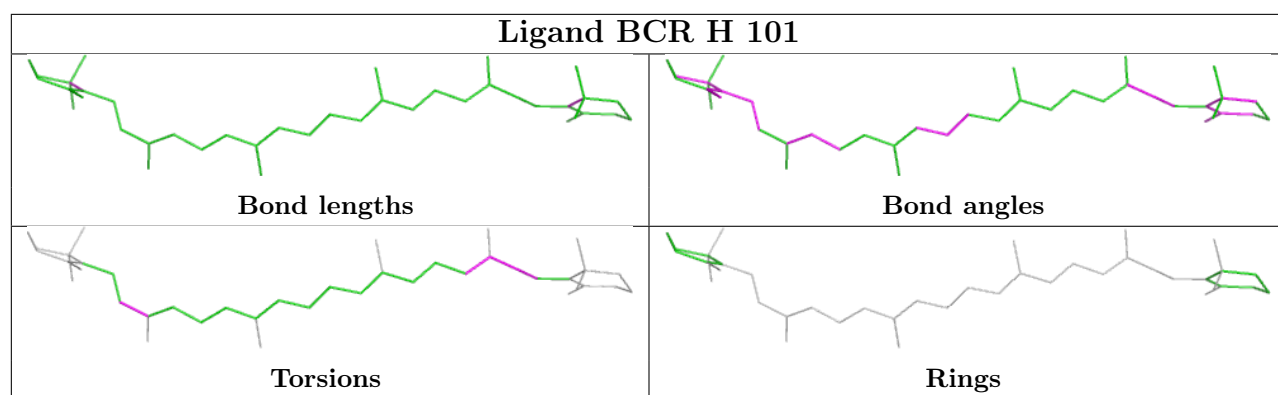
Rings

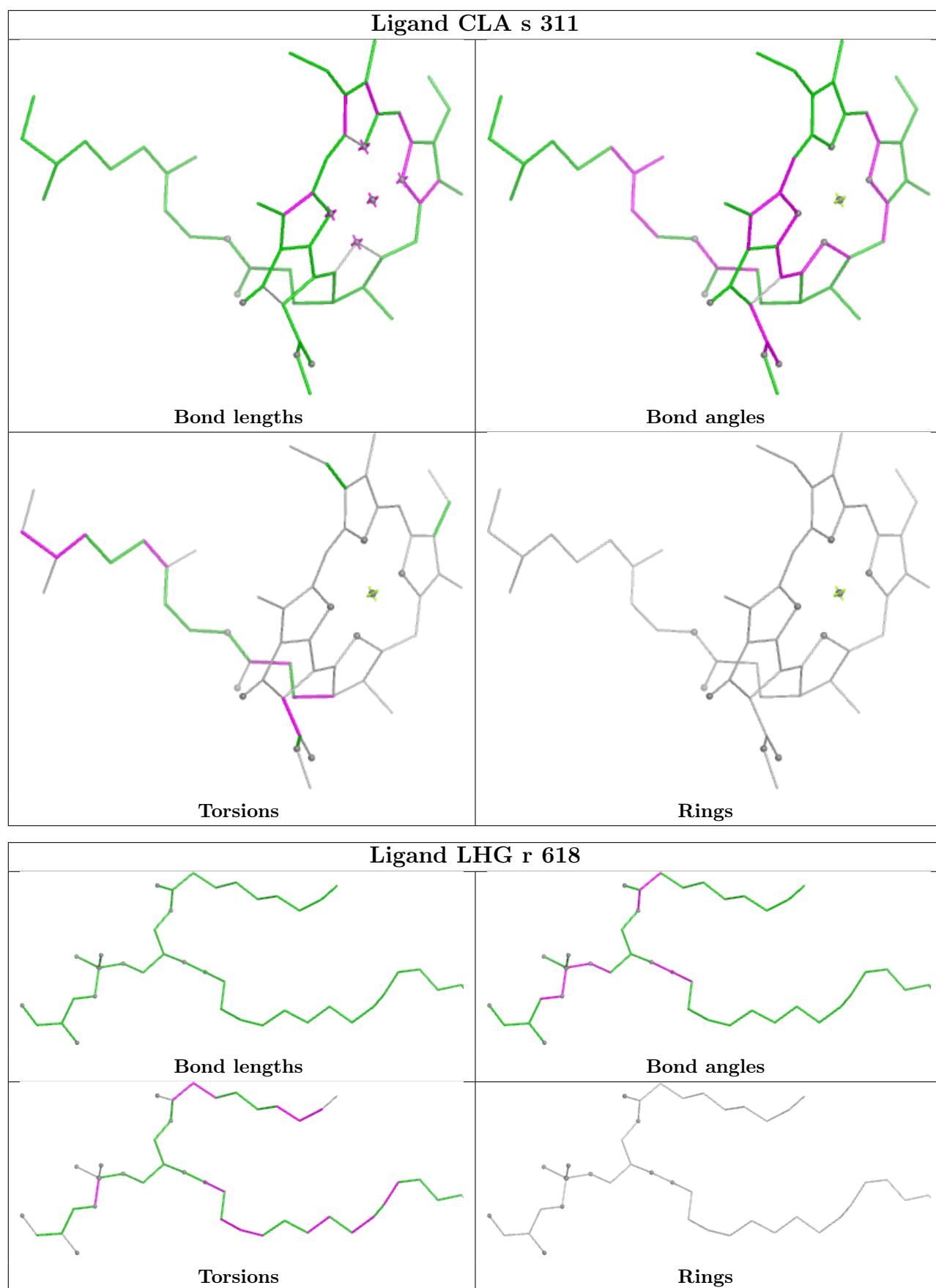




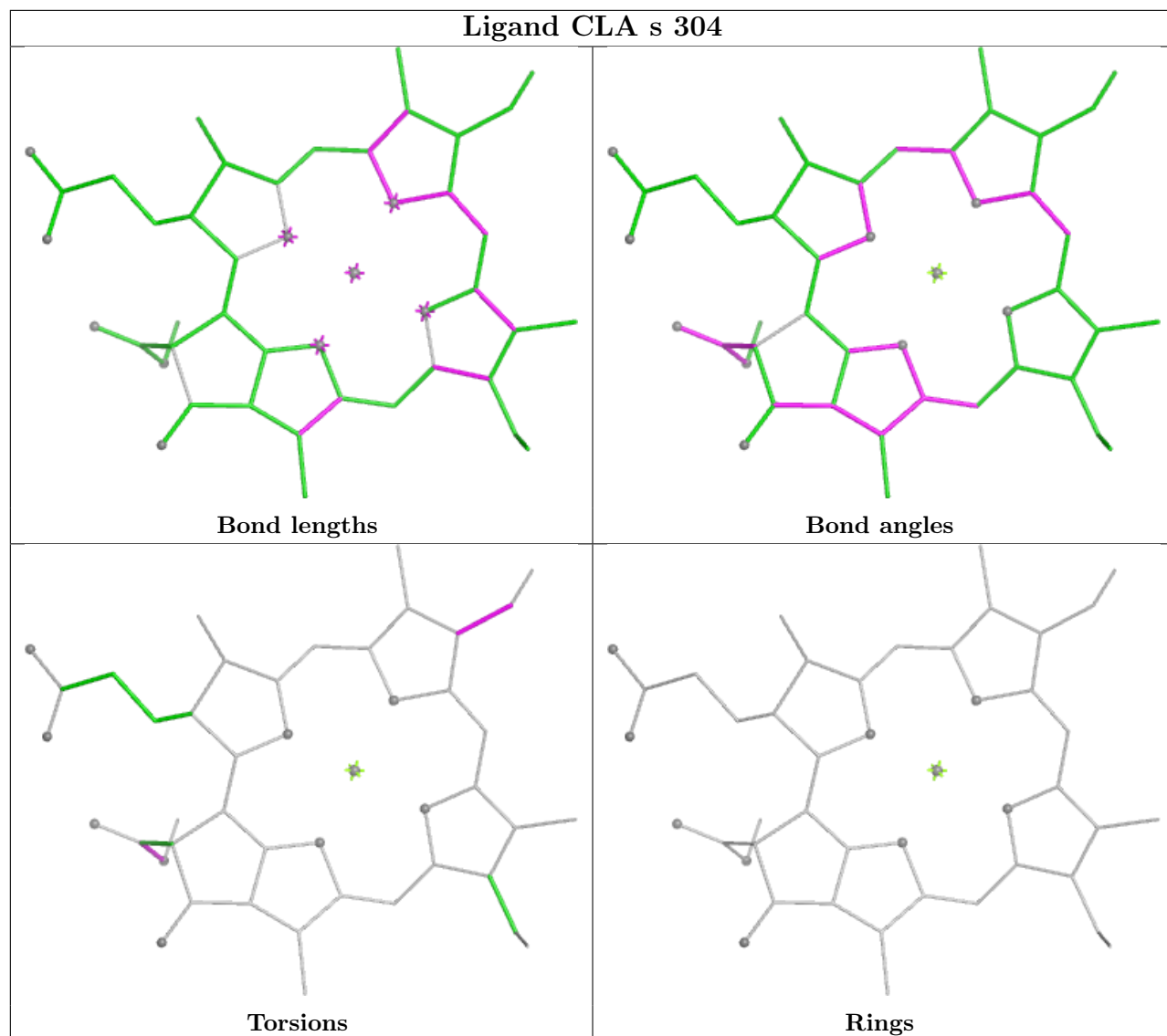


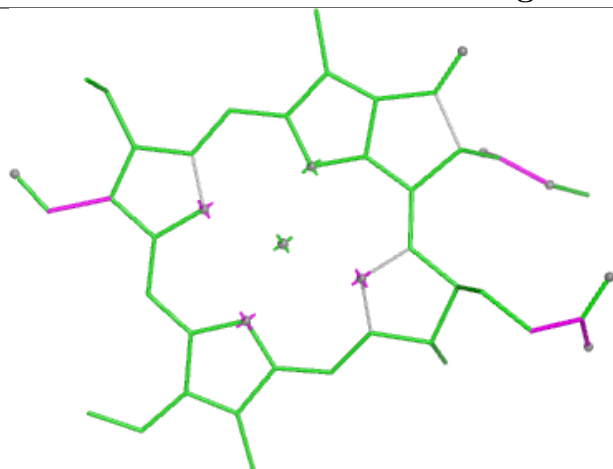




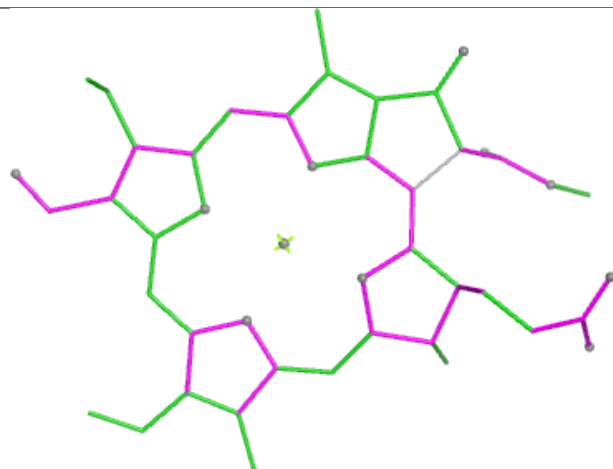


Ligand CLA s 304

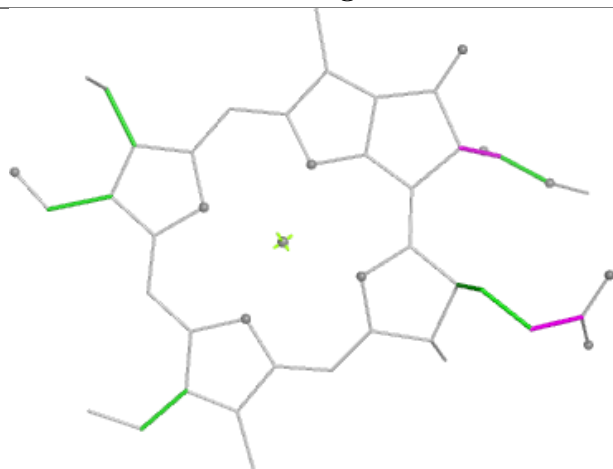


Ligand CHL S 302

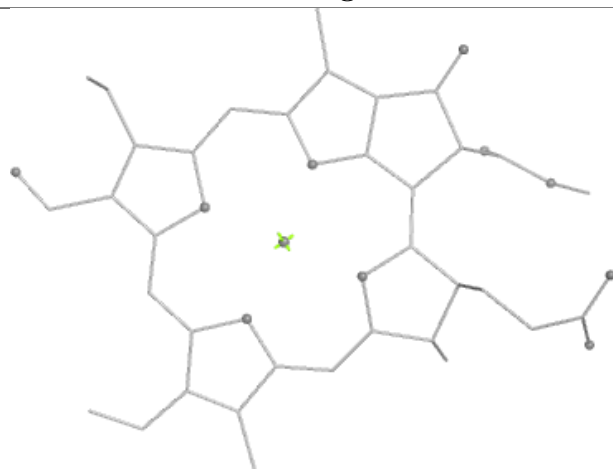
Bond lengths



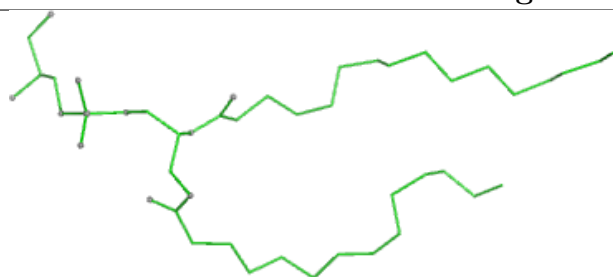
Bond angles



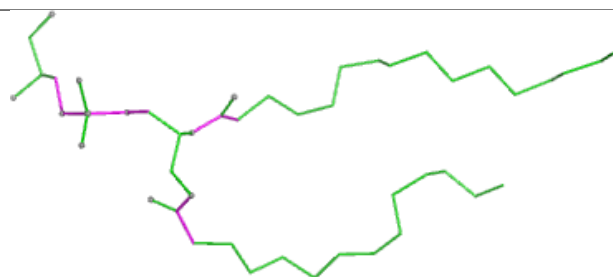
Torsions



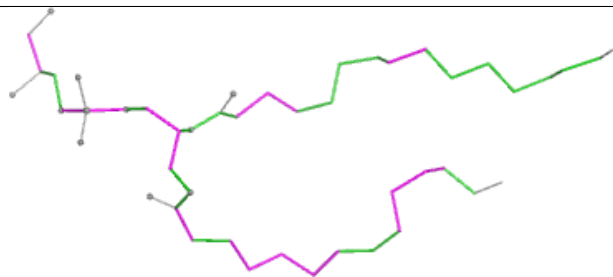
Rings

Ligand LHG b 621

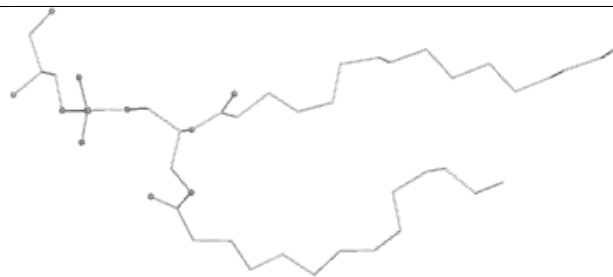
Bond lengths



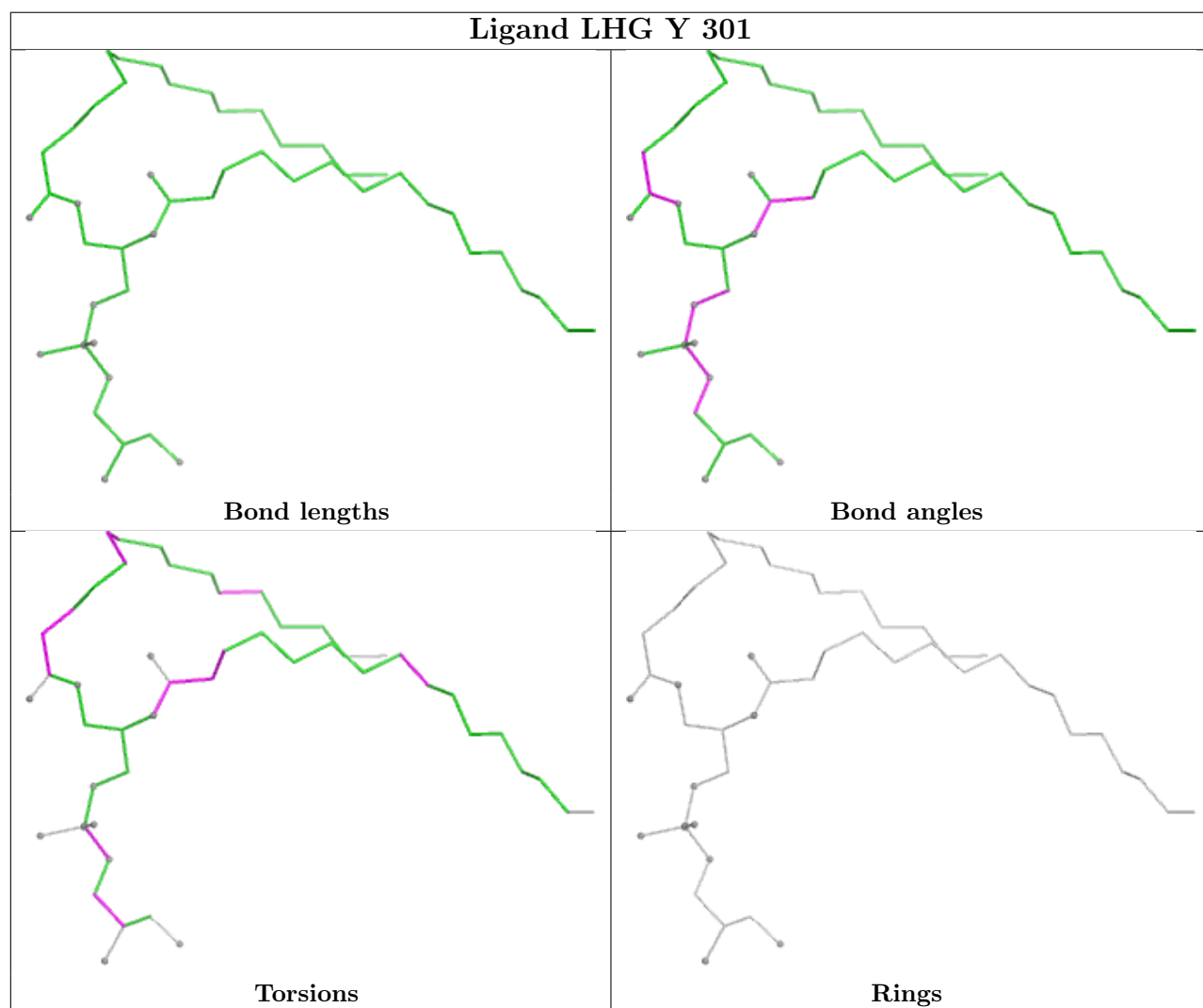
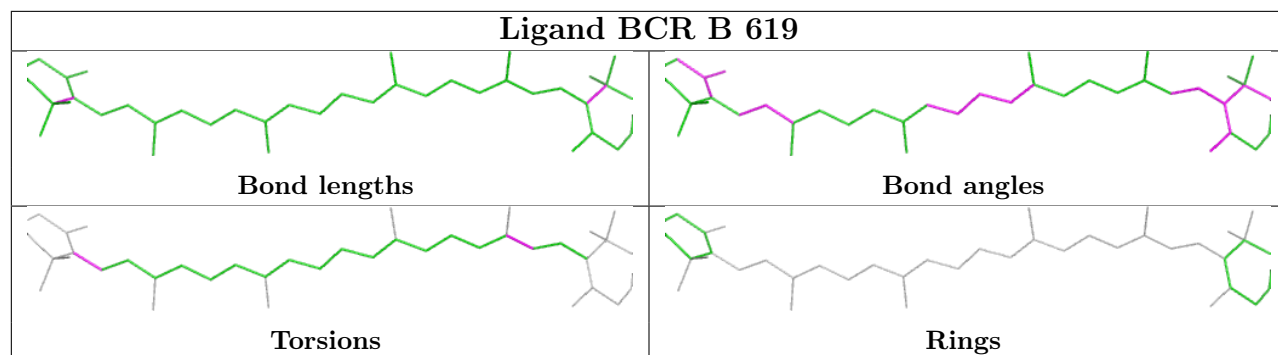
Bond angles



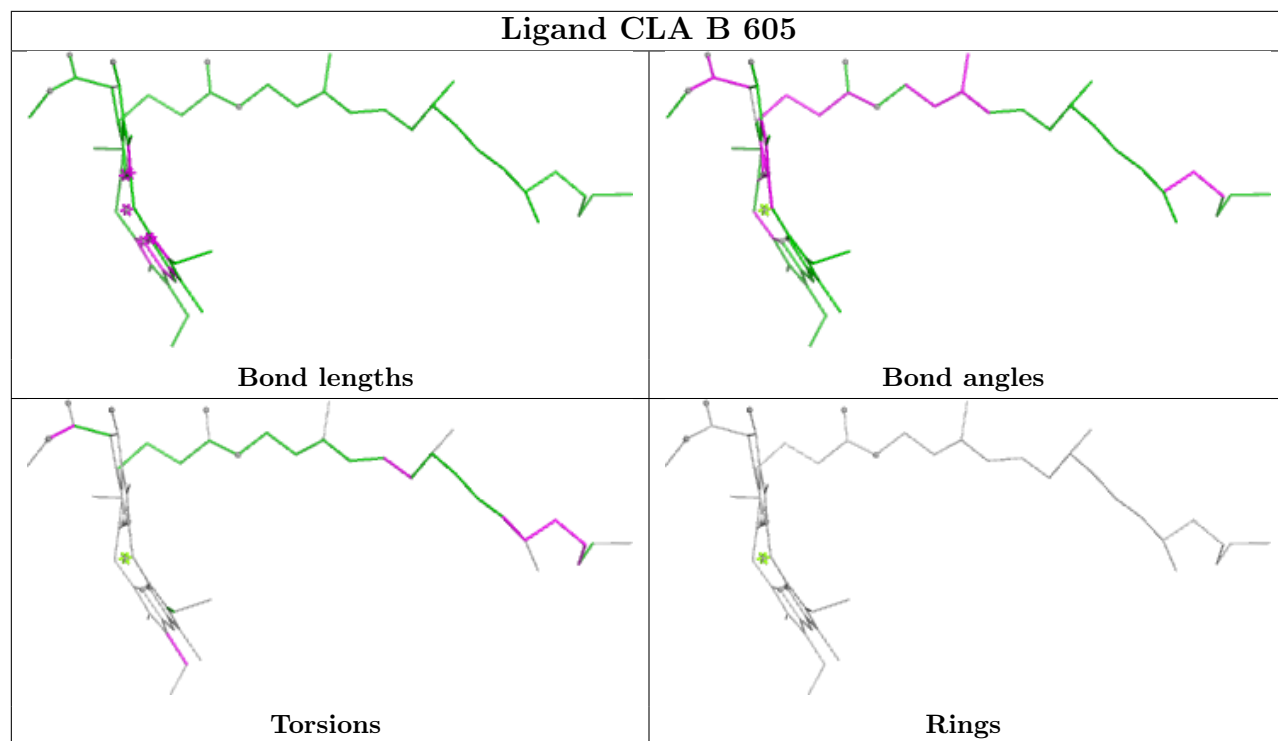
Torsions



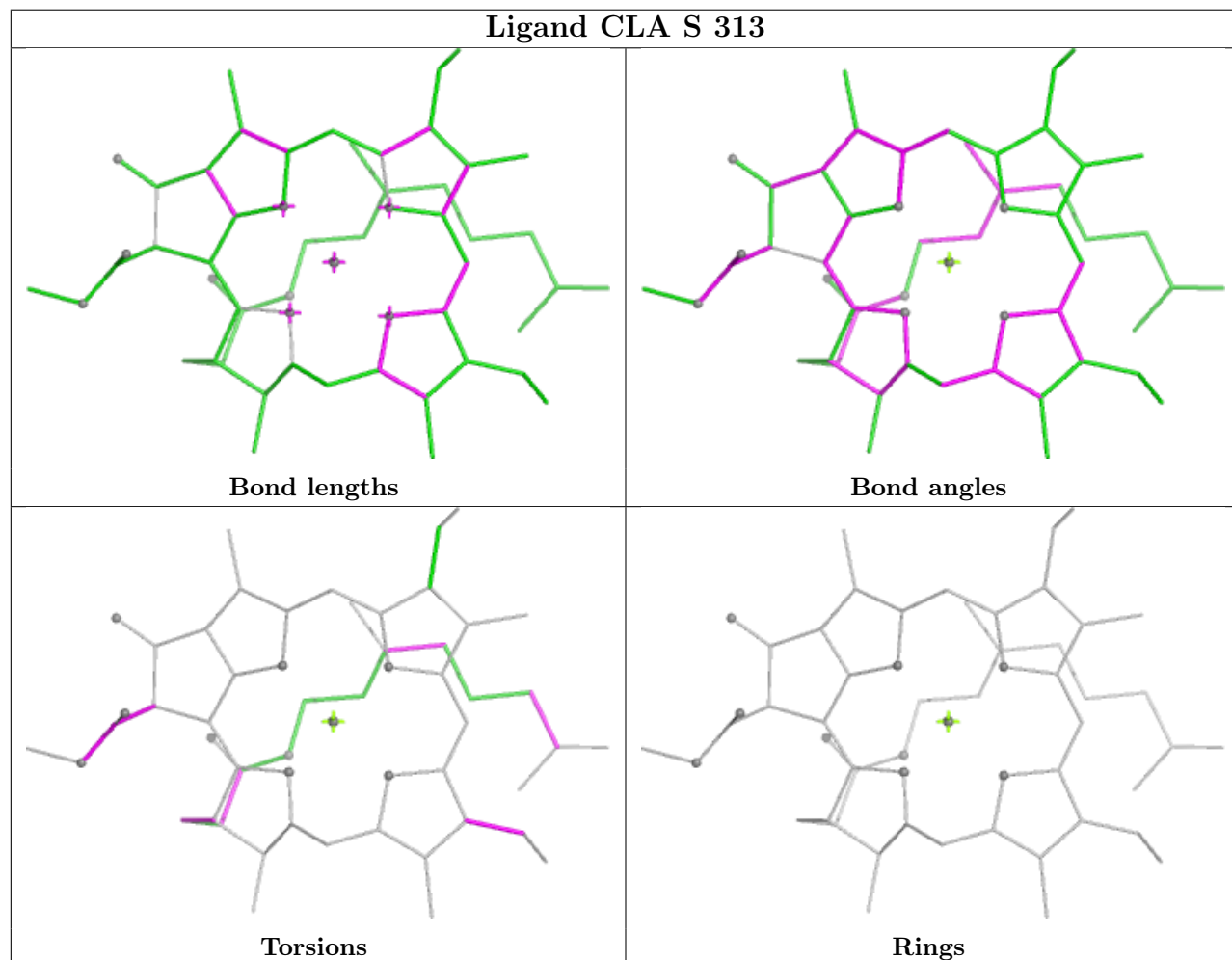
Rings

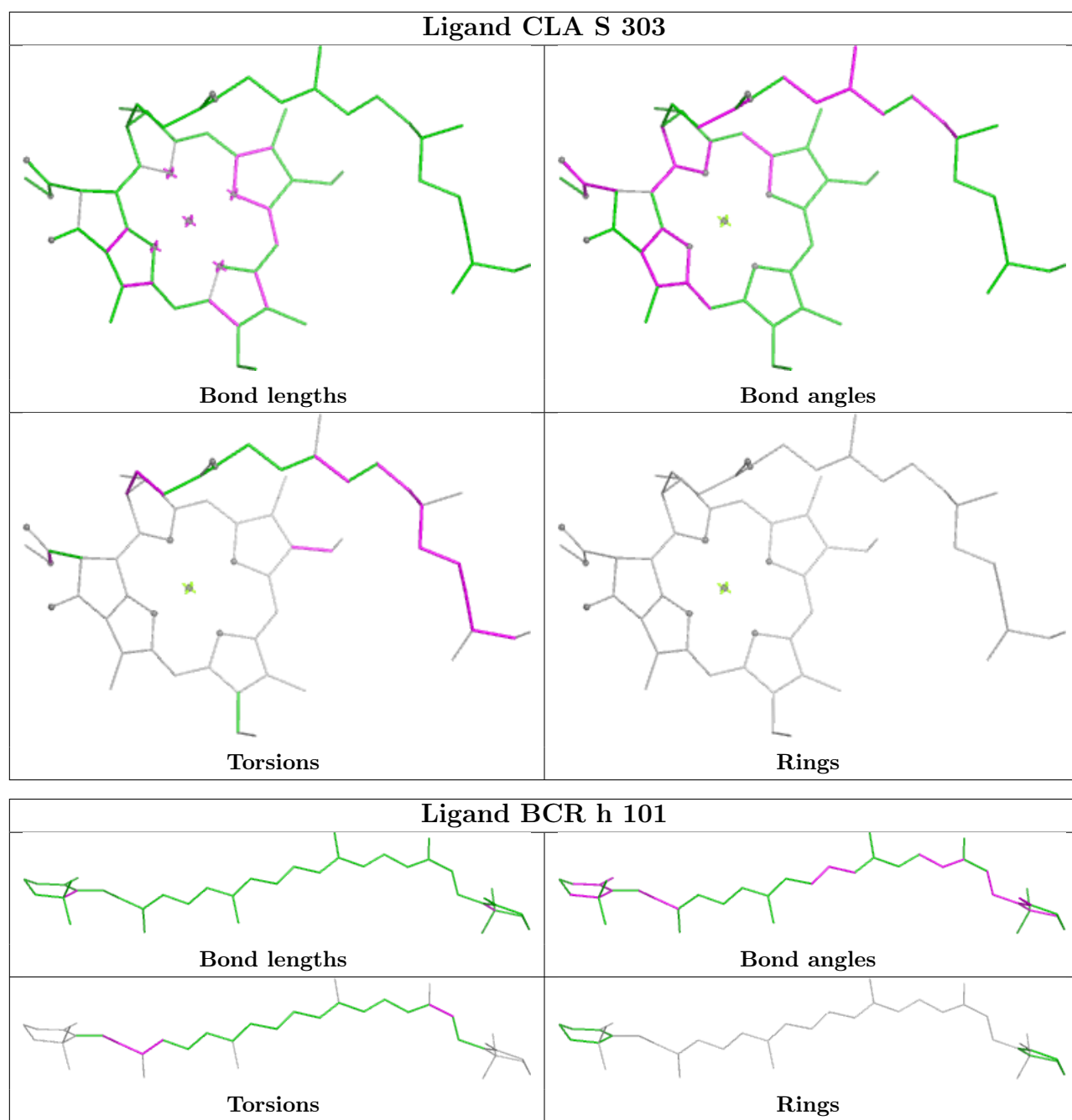


Ligand CLA B 605

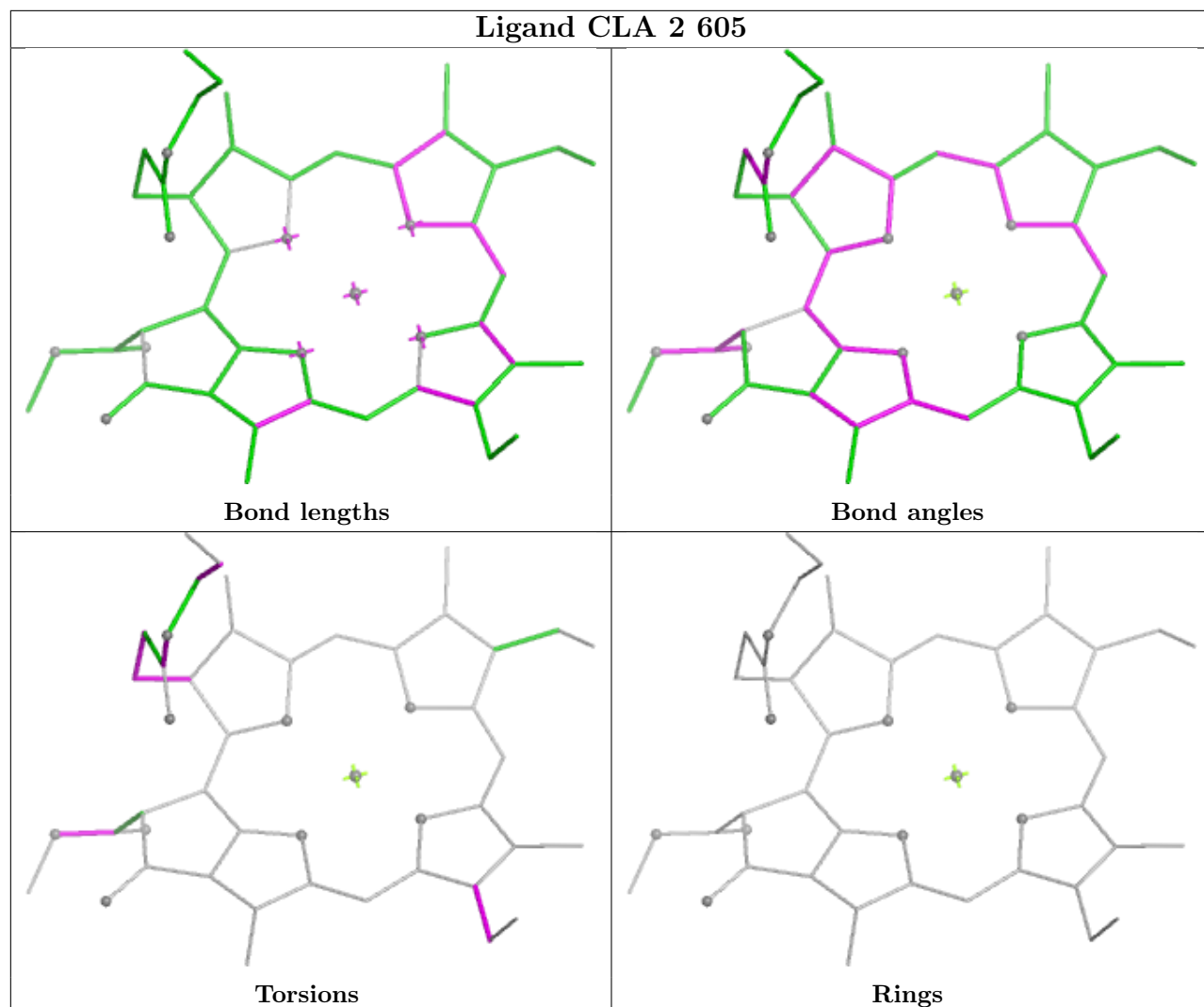


Ligand CLA S 313

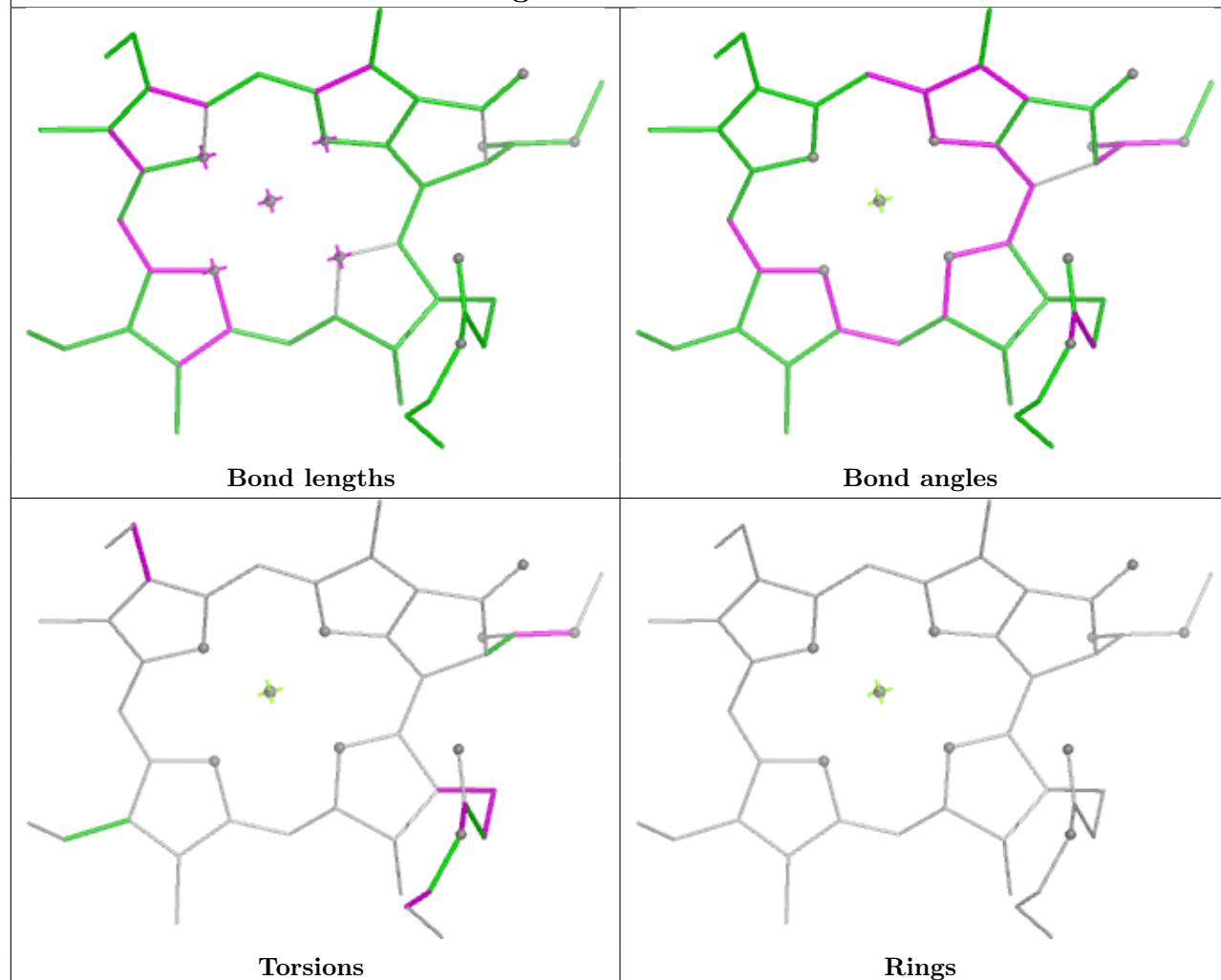




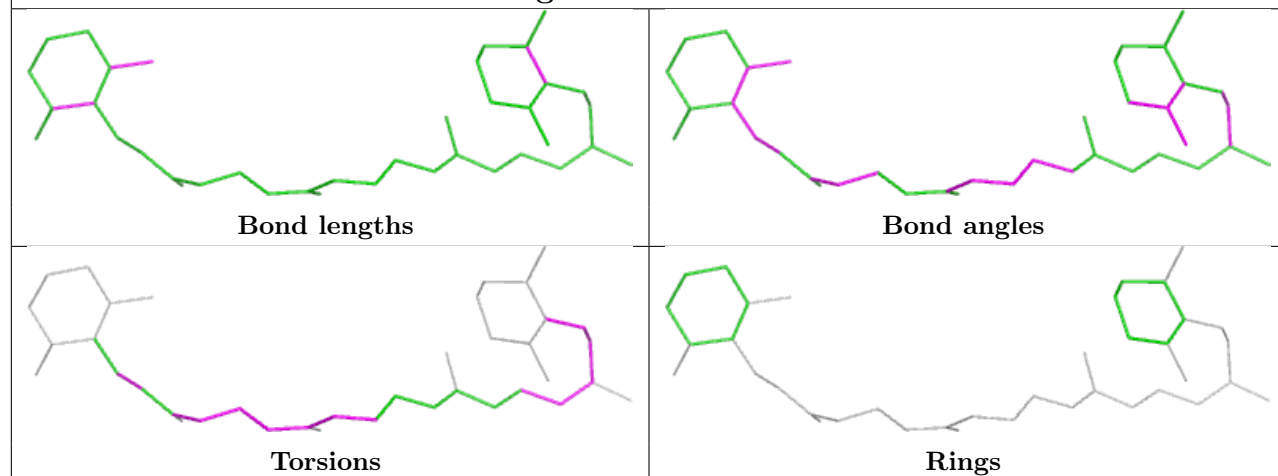
Ligand CLA 2 605



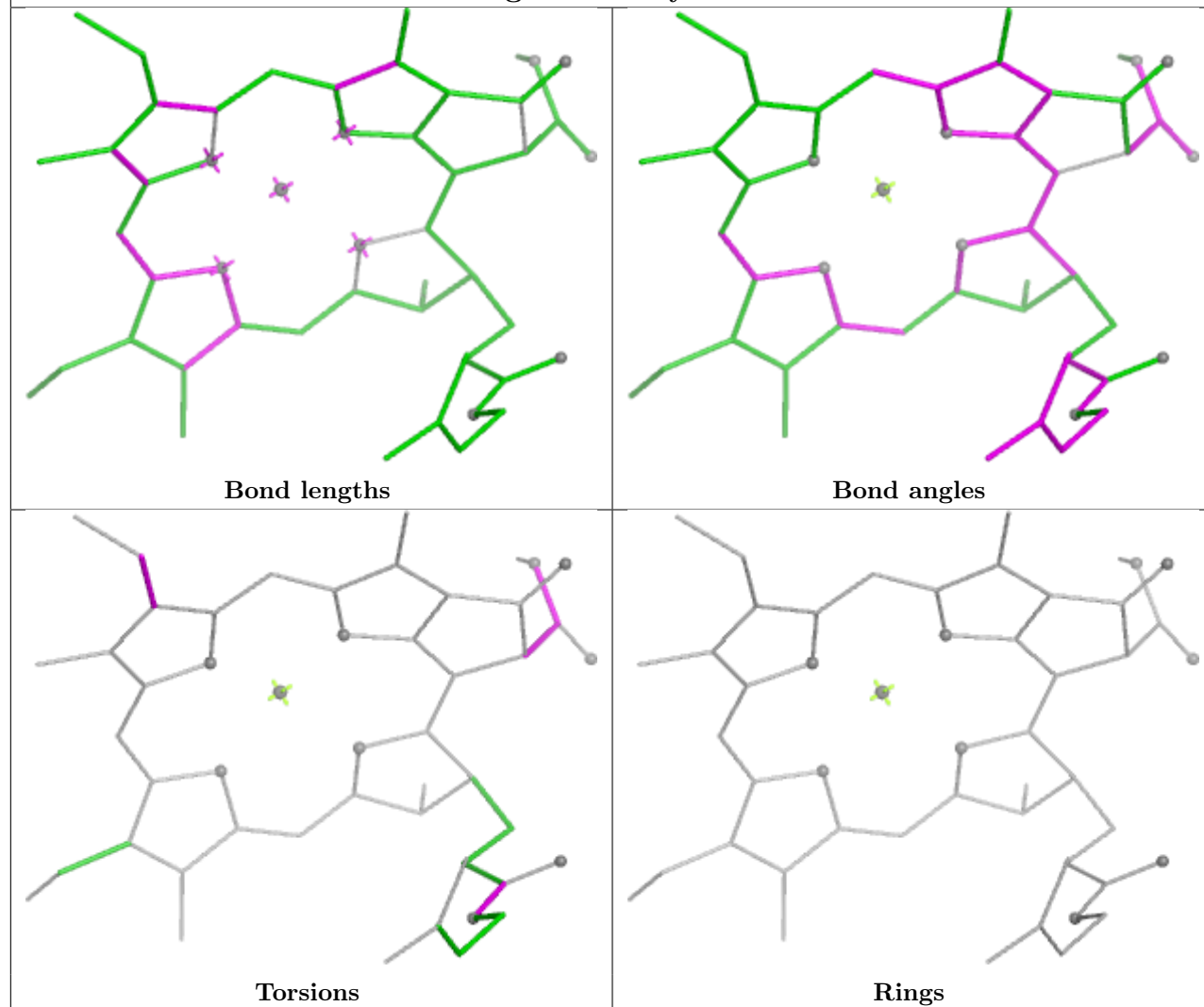
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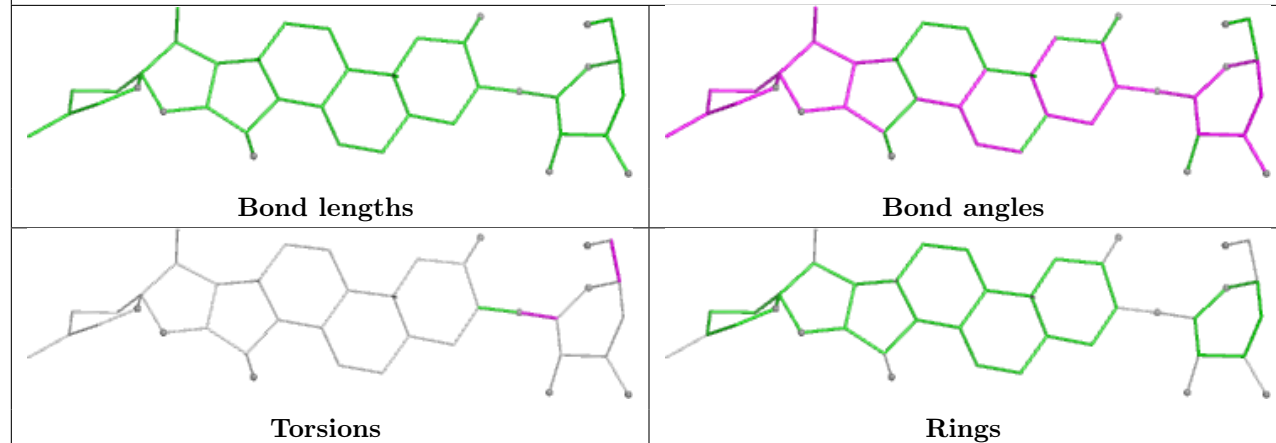
Ligand BCR t 101

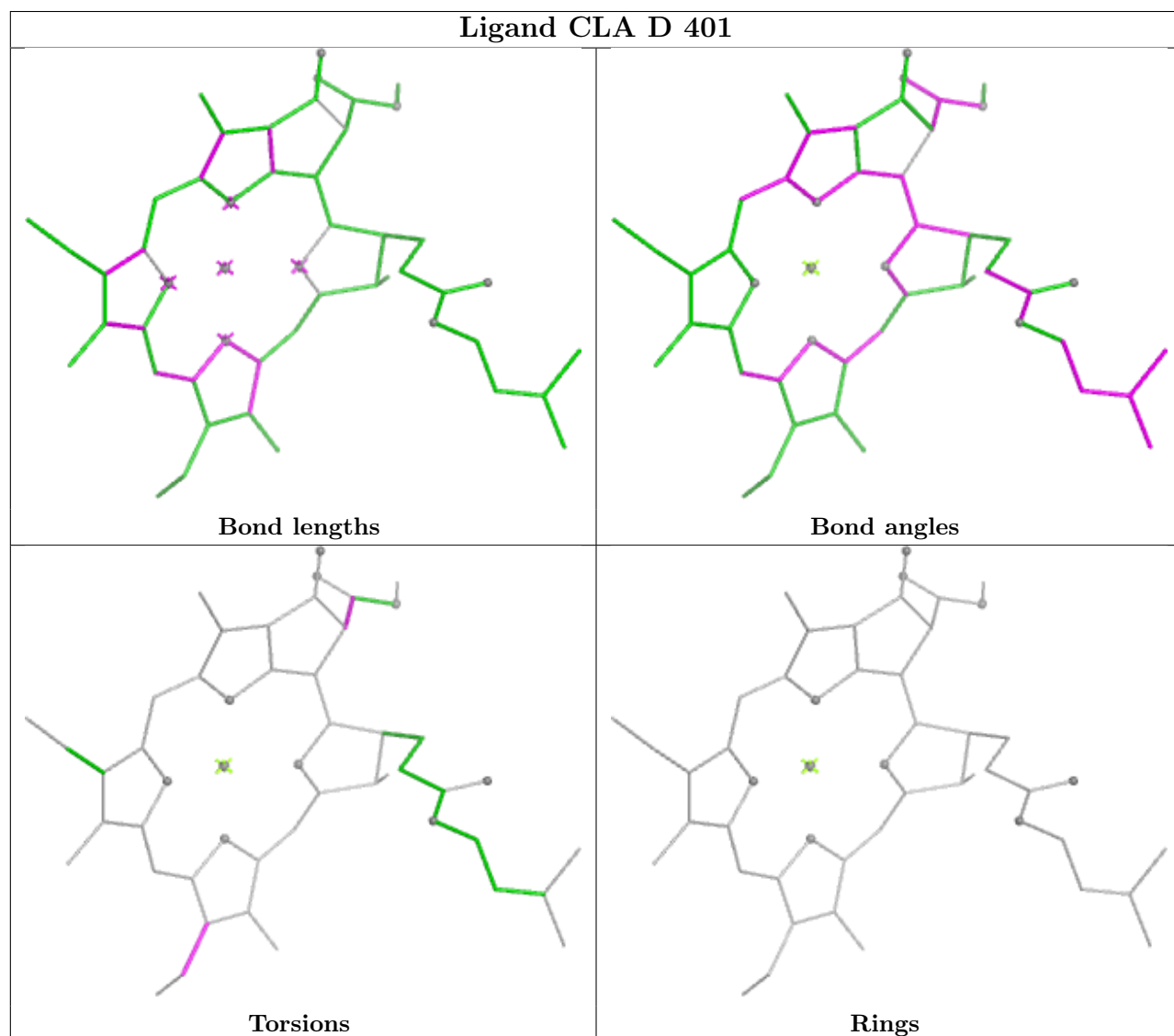
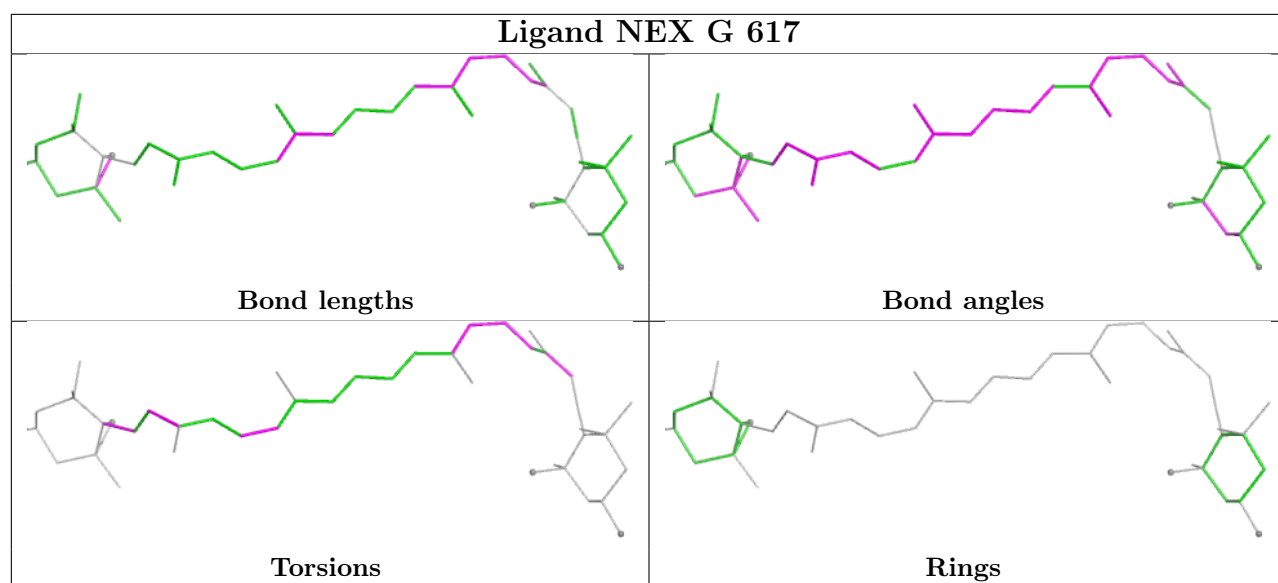


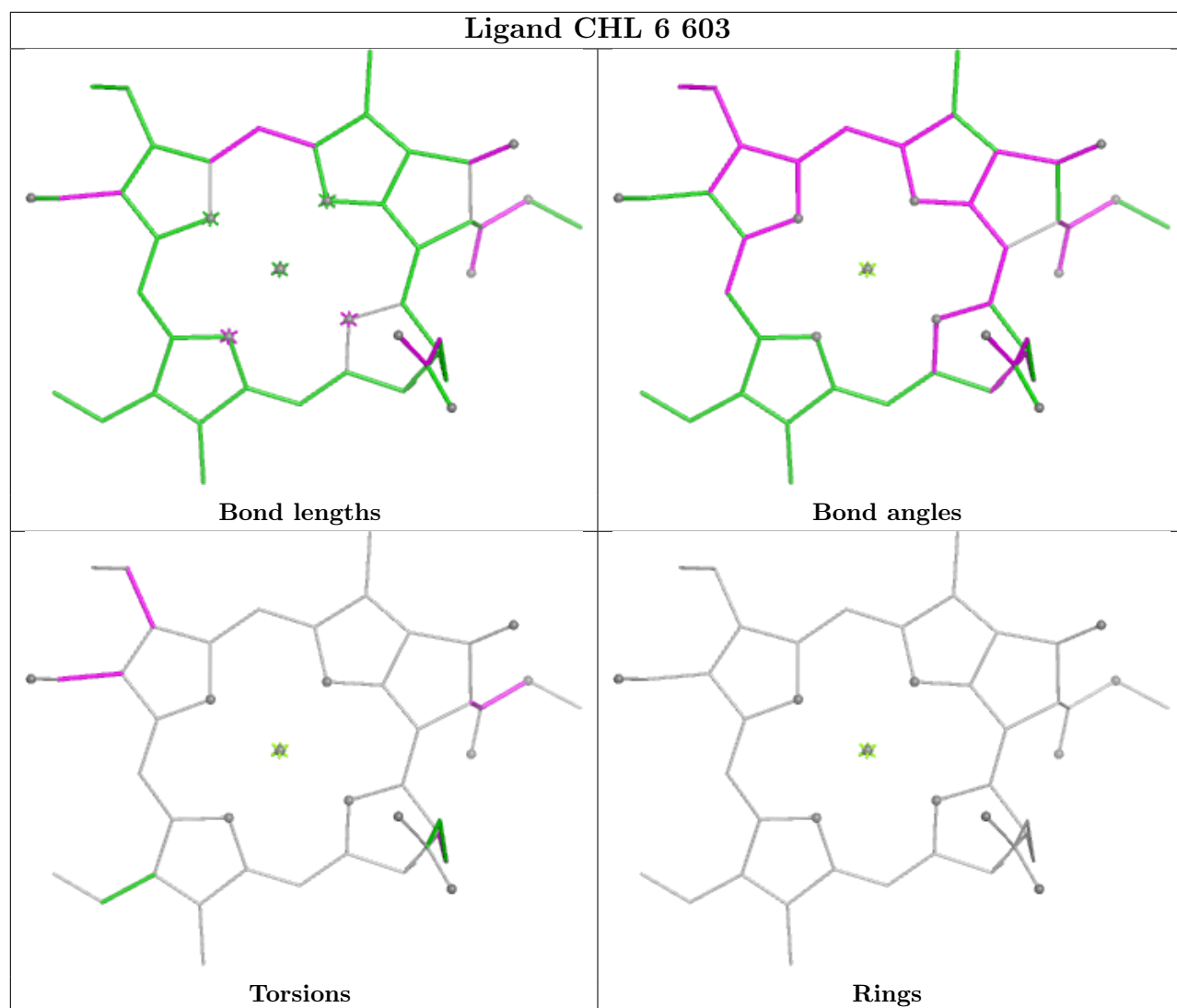
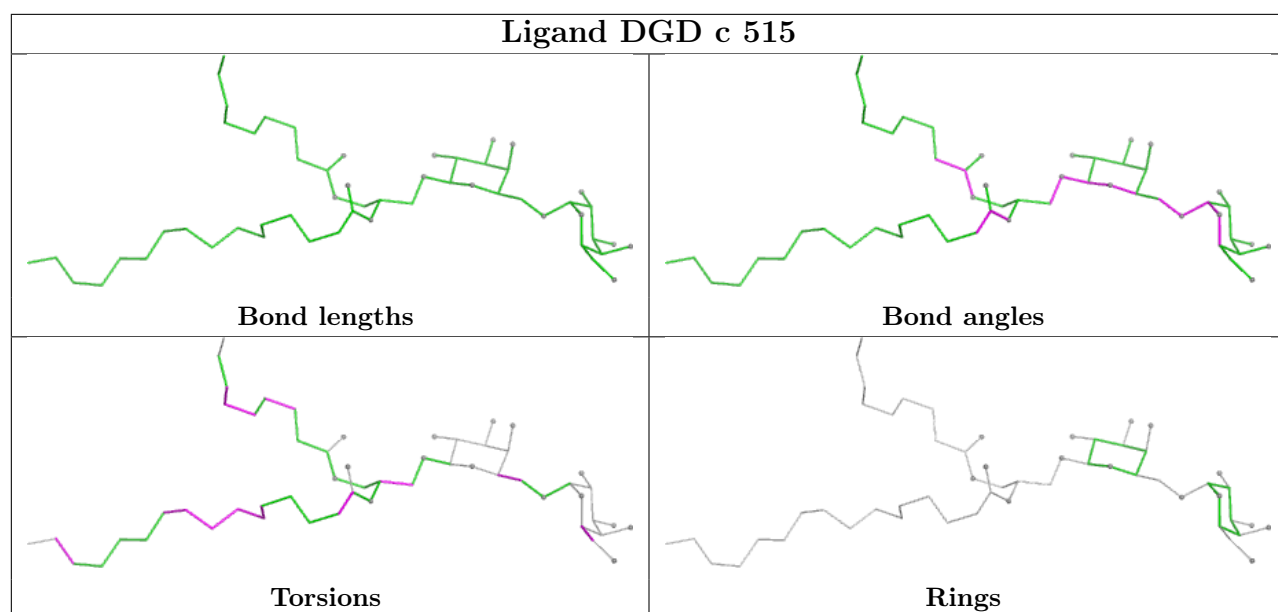
Ligand CLA y 305

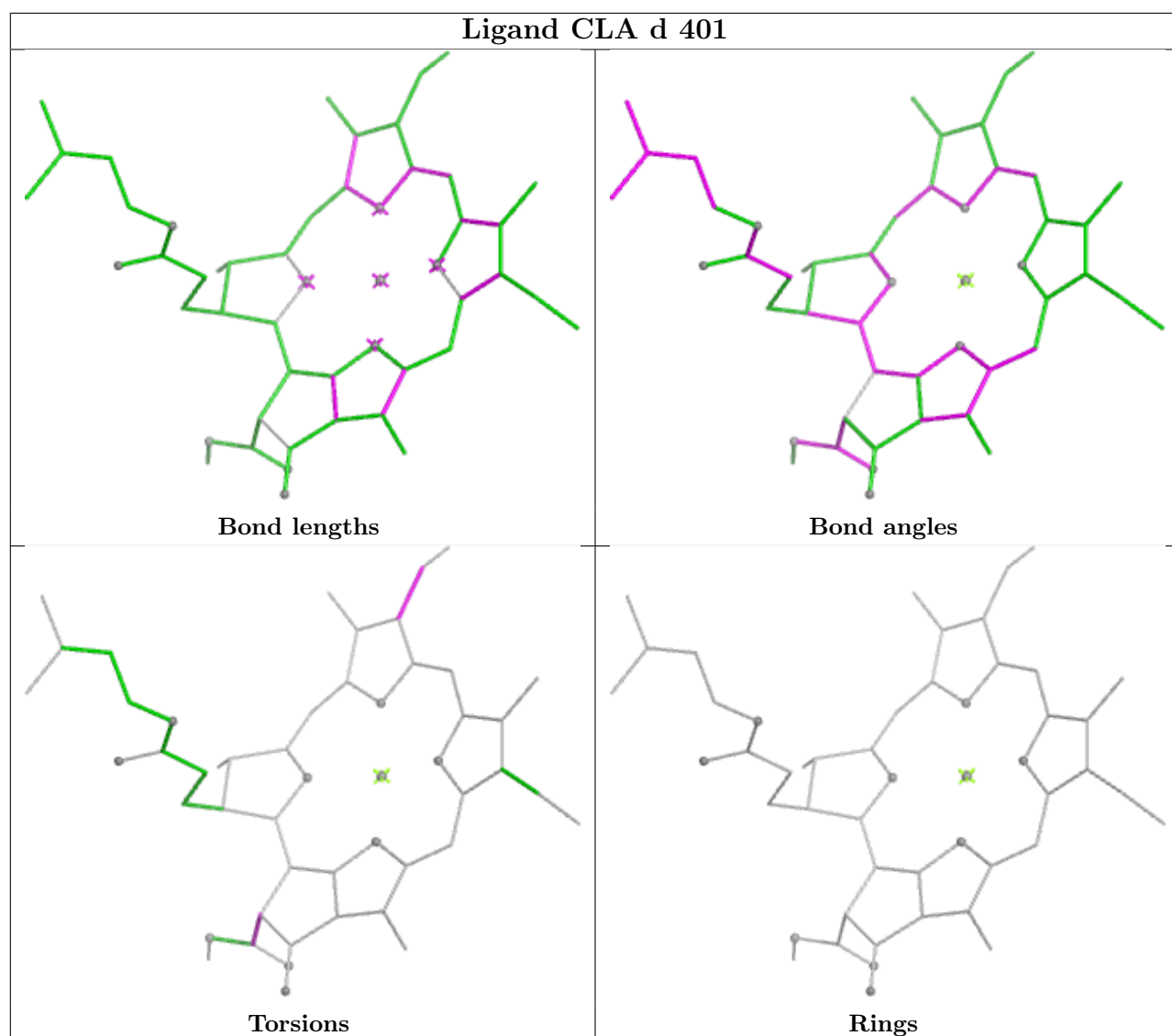


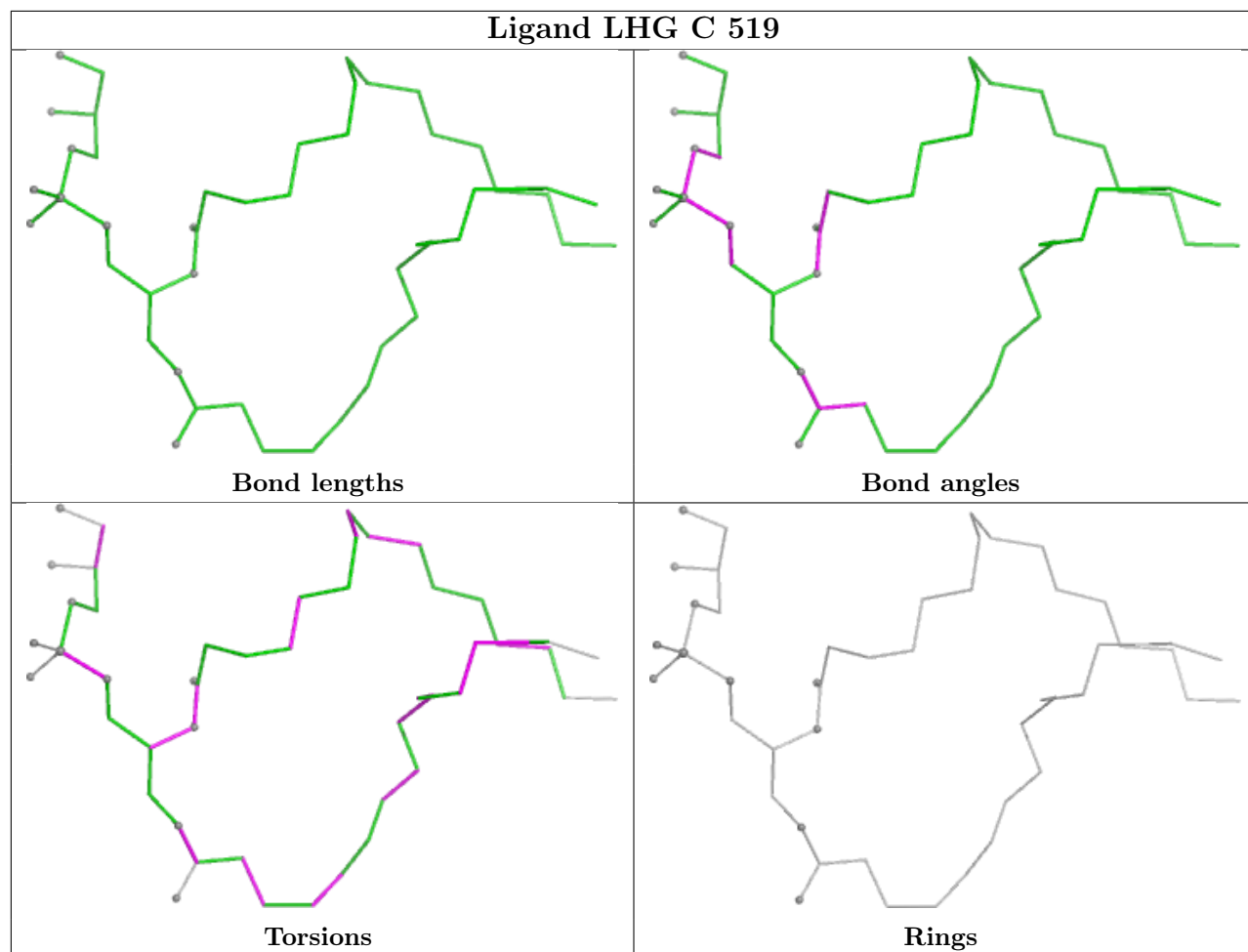
Ligand AJP Y 324

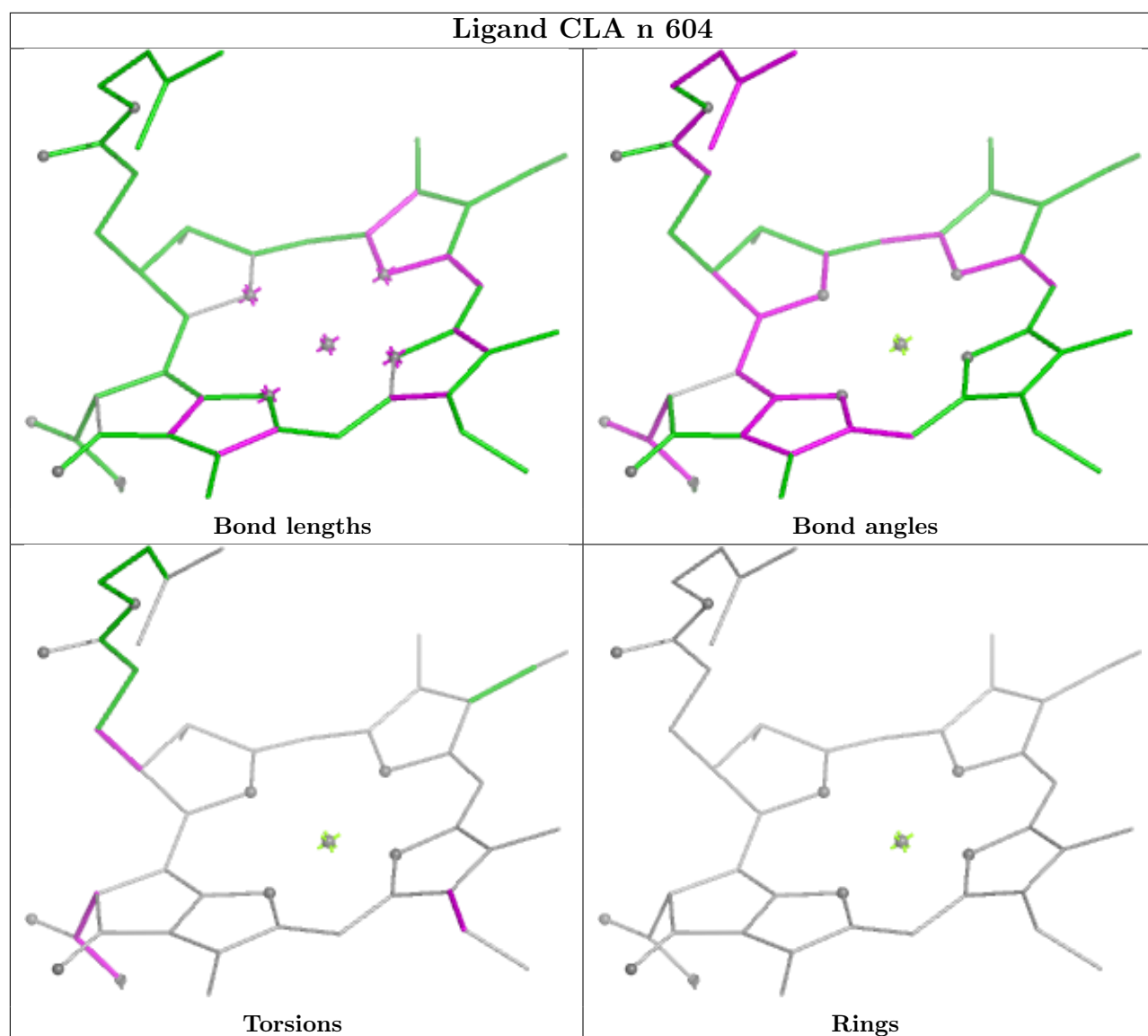


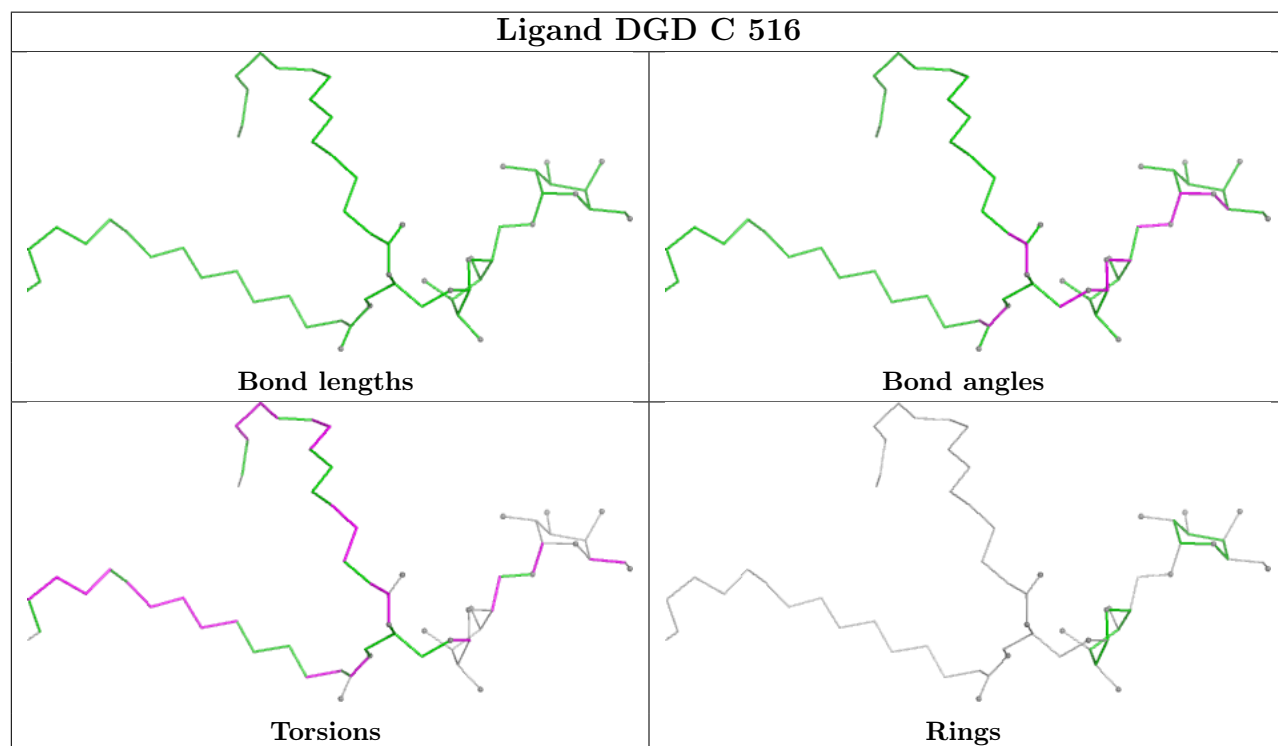
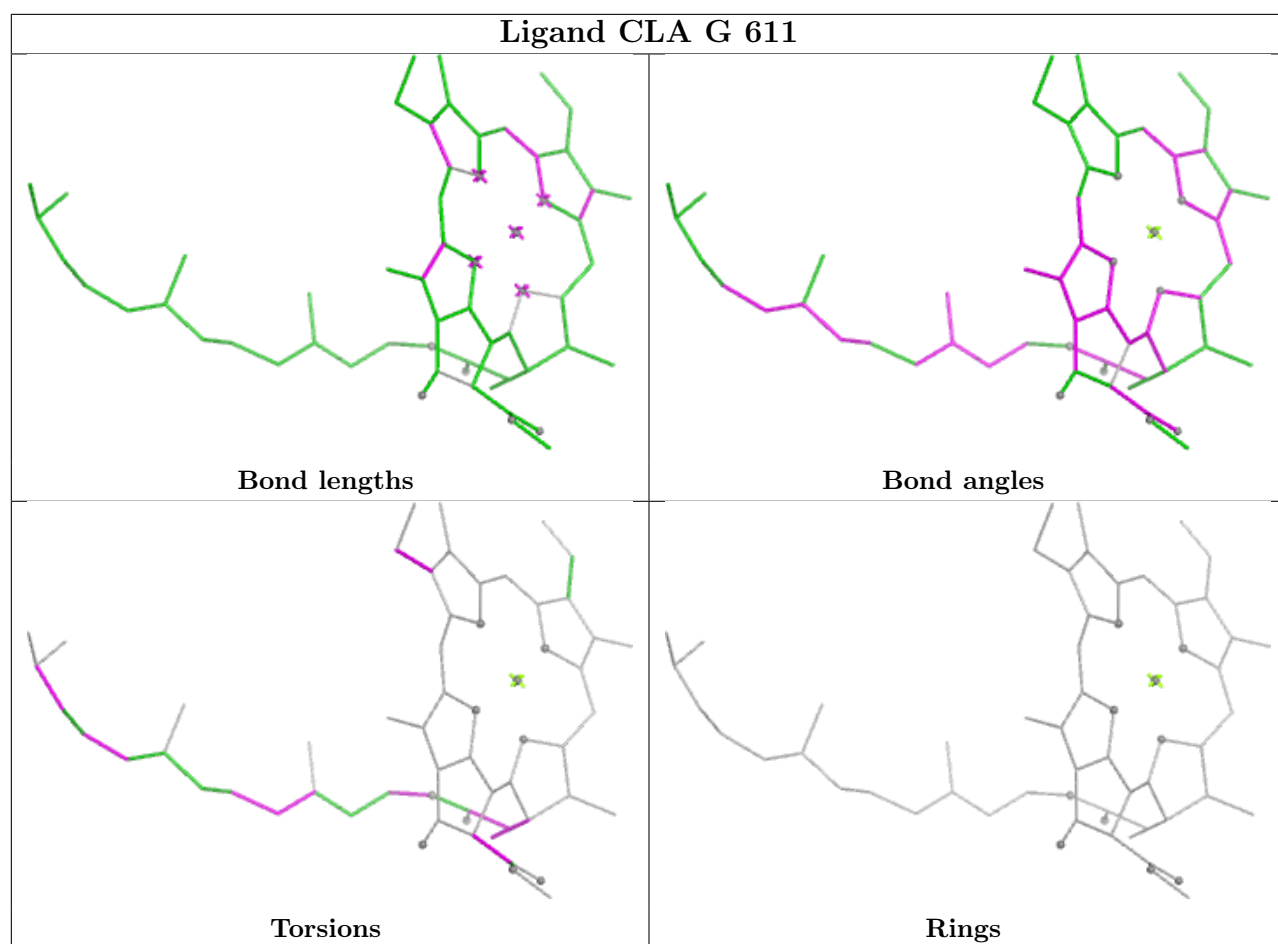


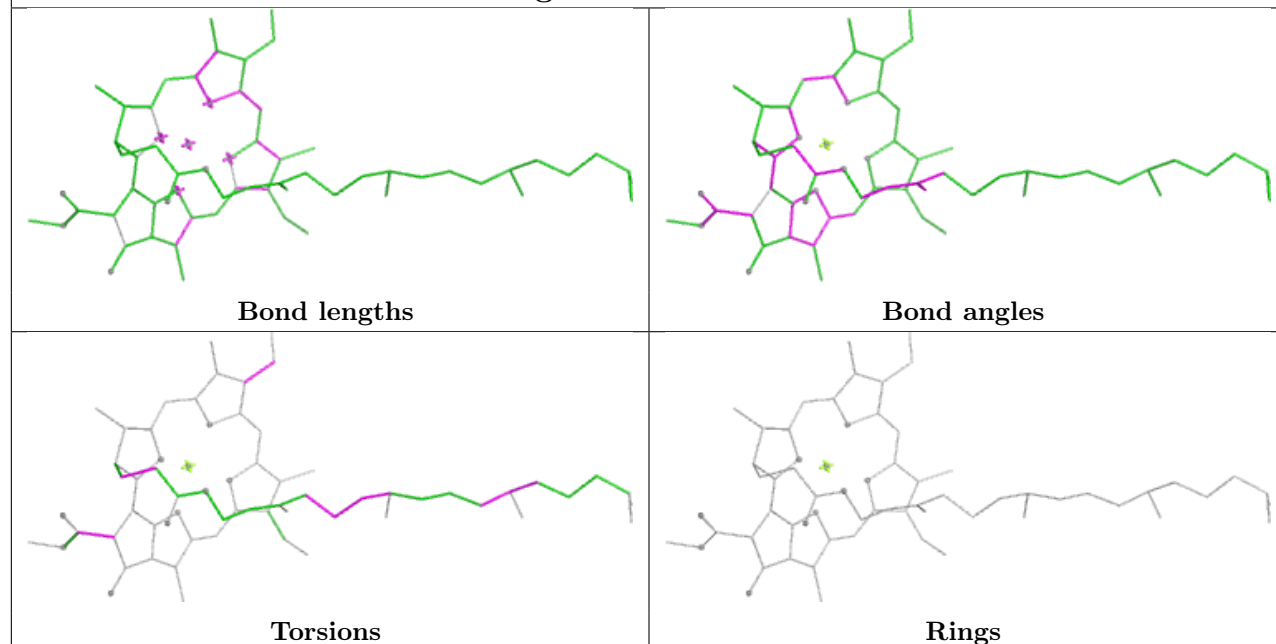
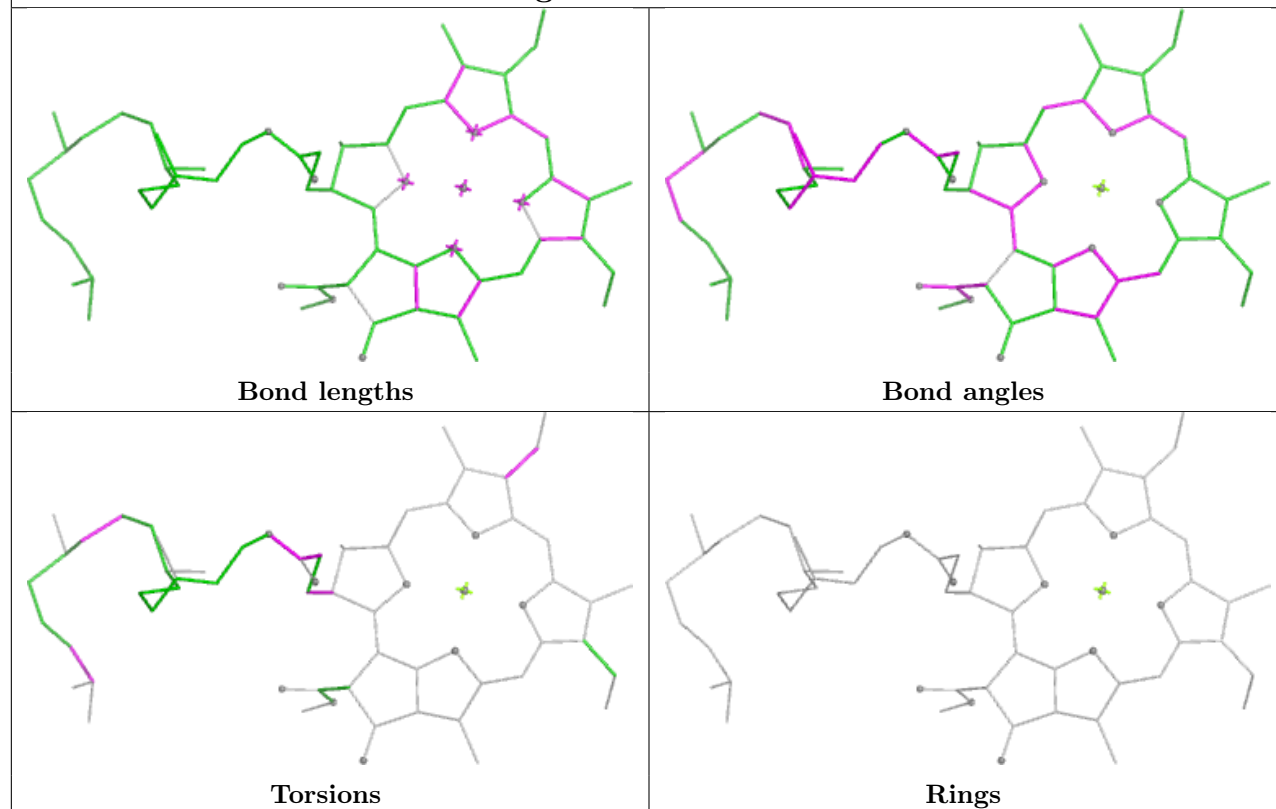


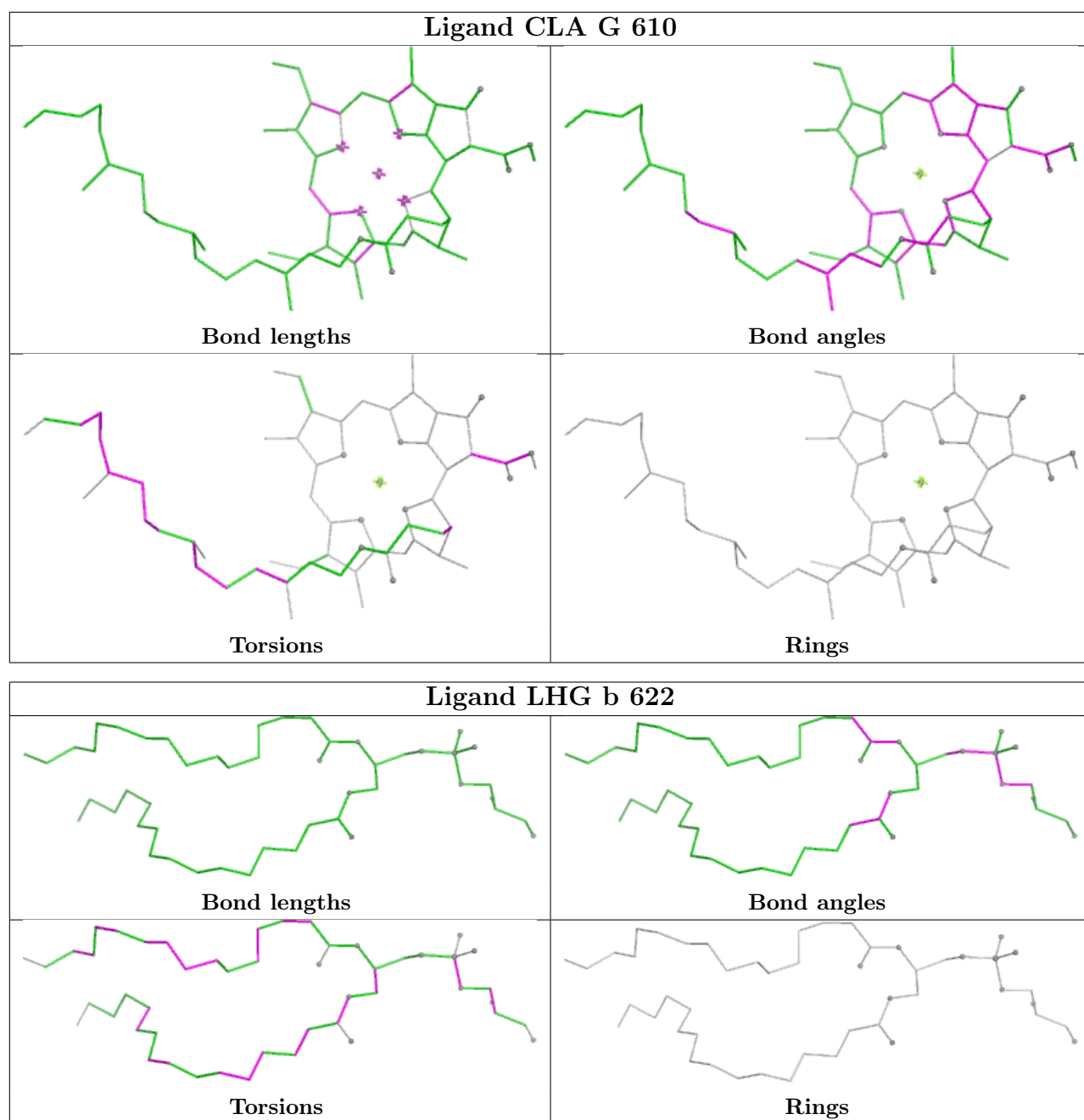


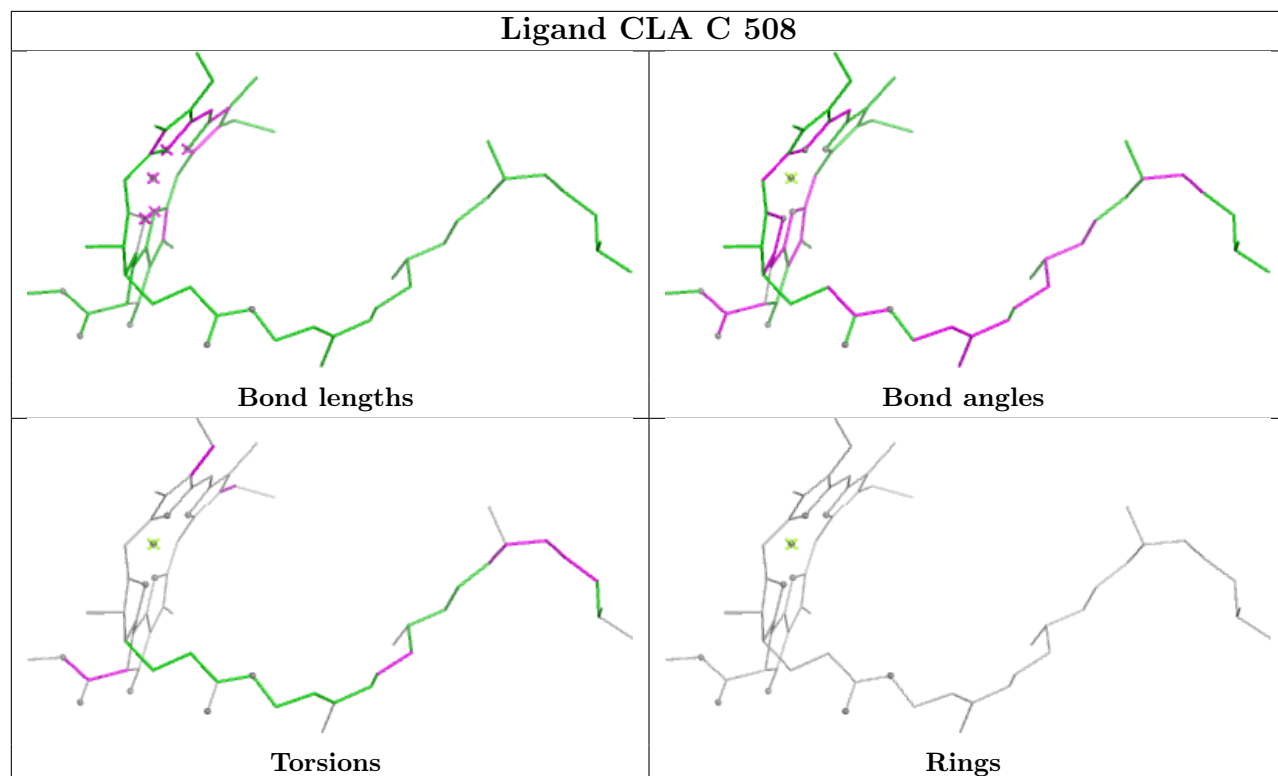




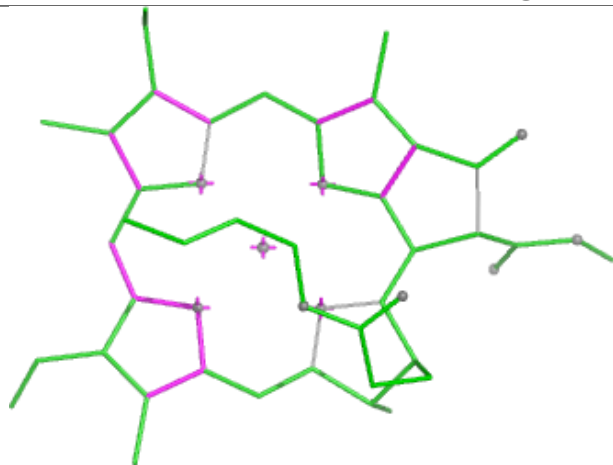


Ligand CLA b 614**Ligand CLA b 612**

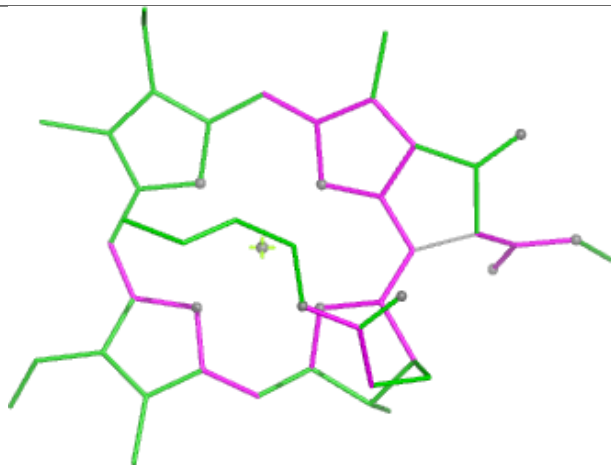




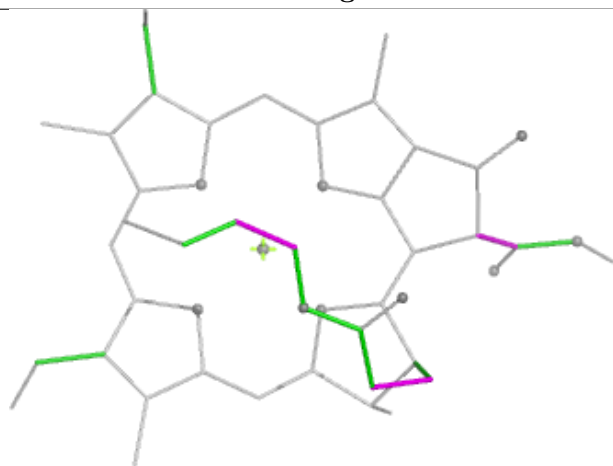
Ligand CLA S 314



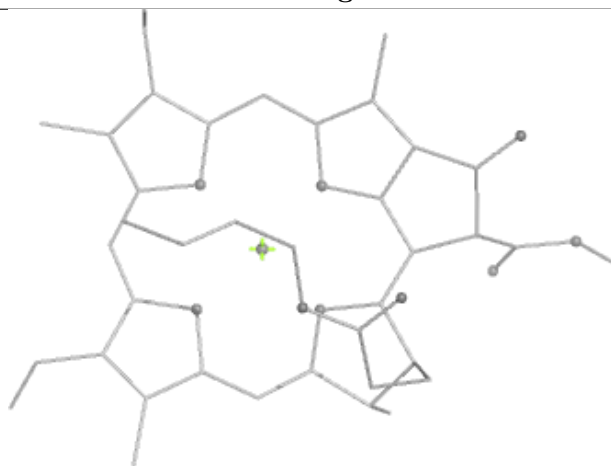
Bond lengths



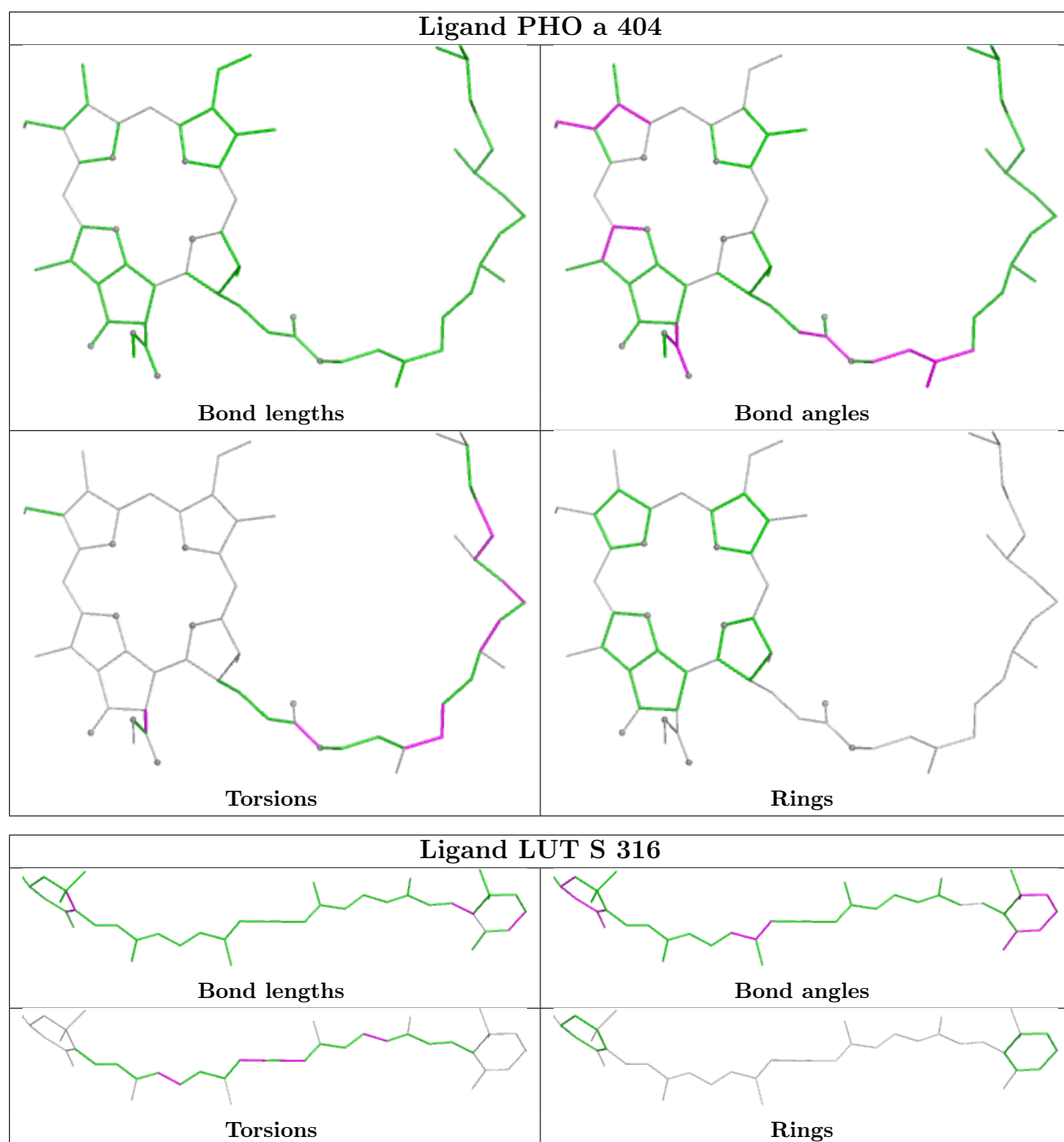
Bond angles

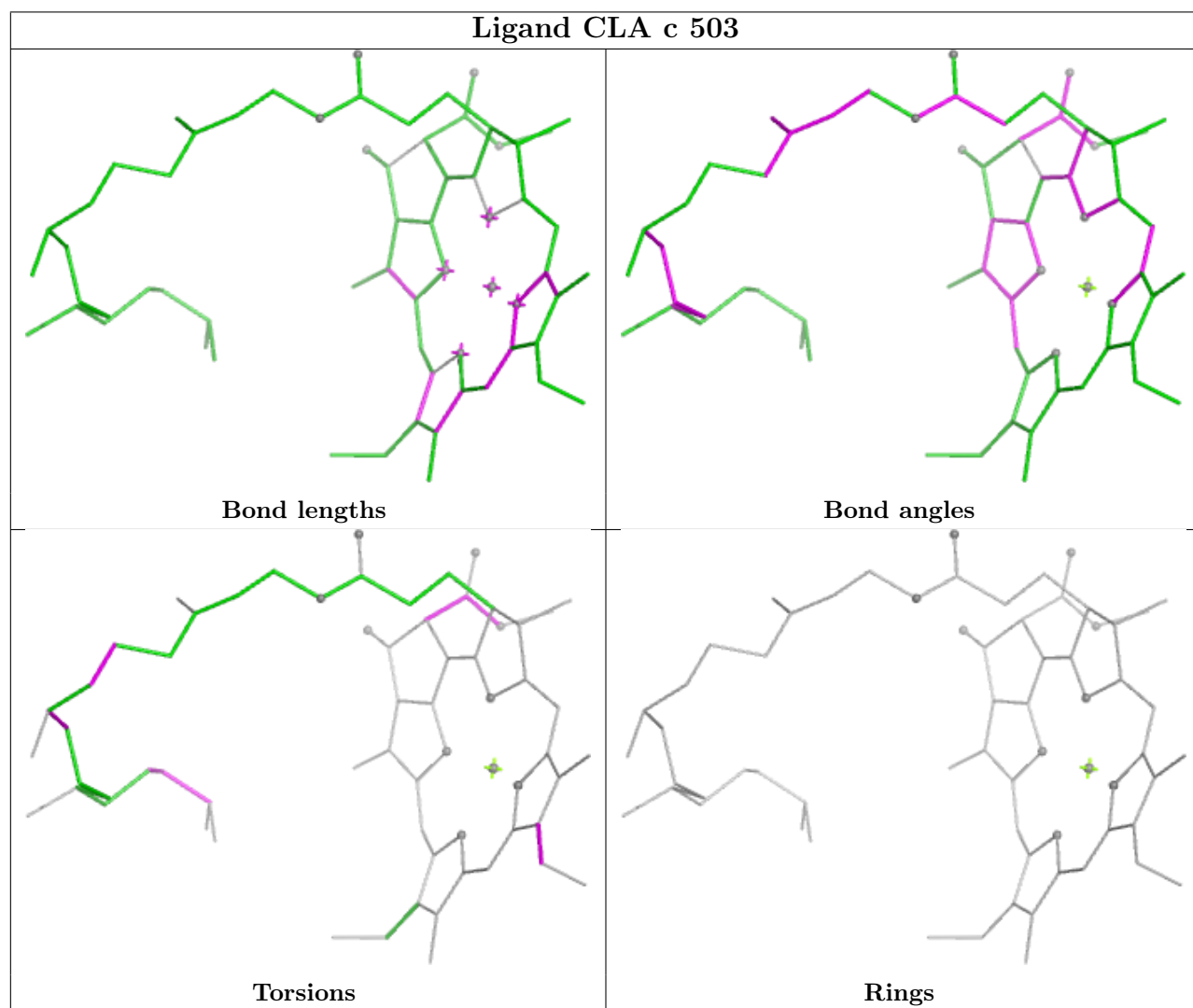
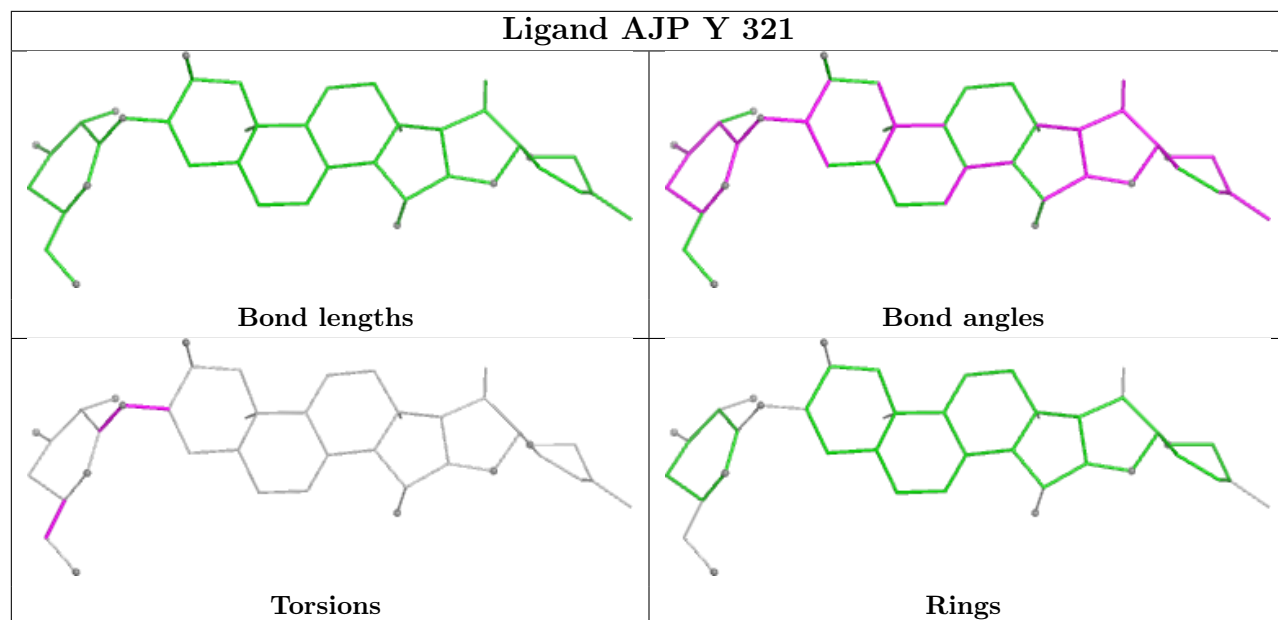


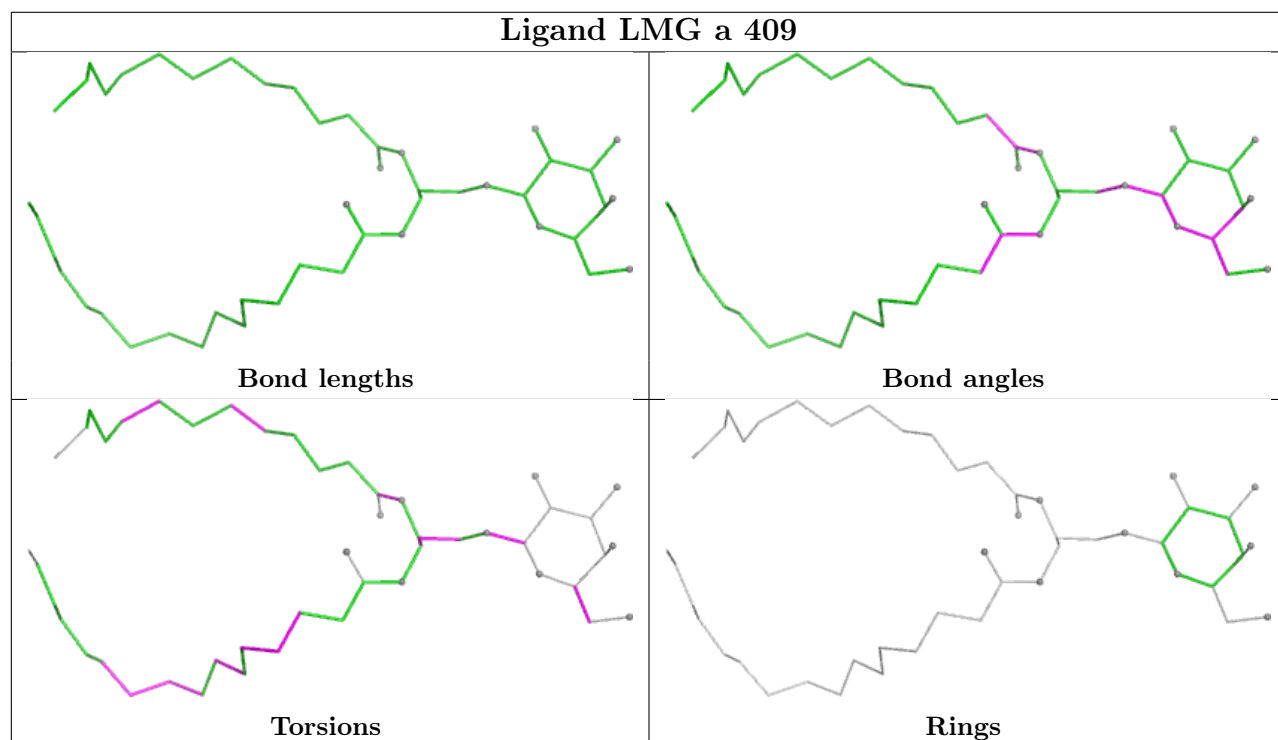
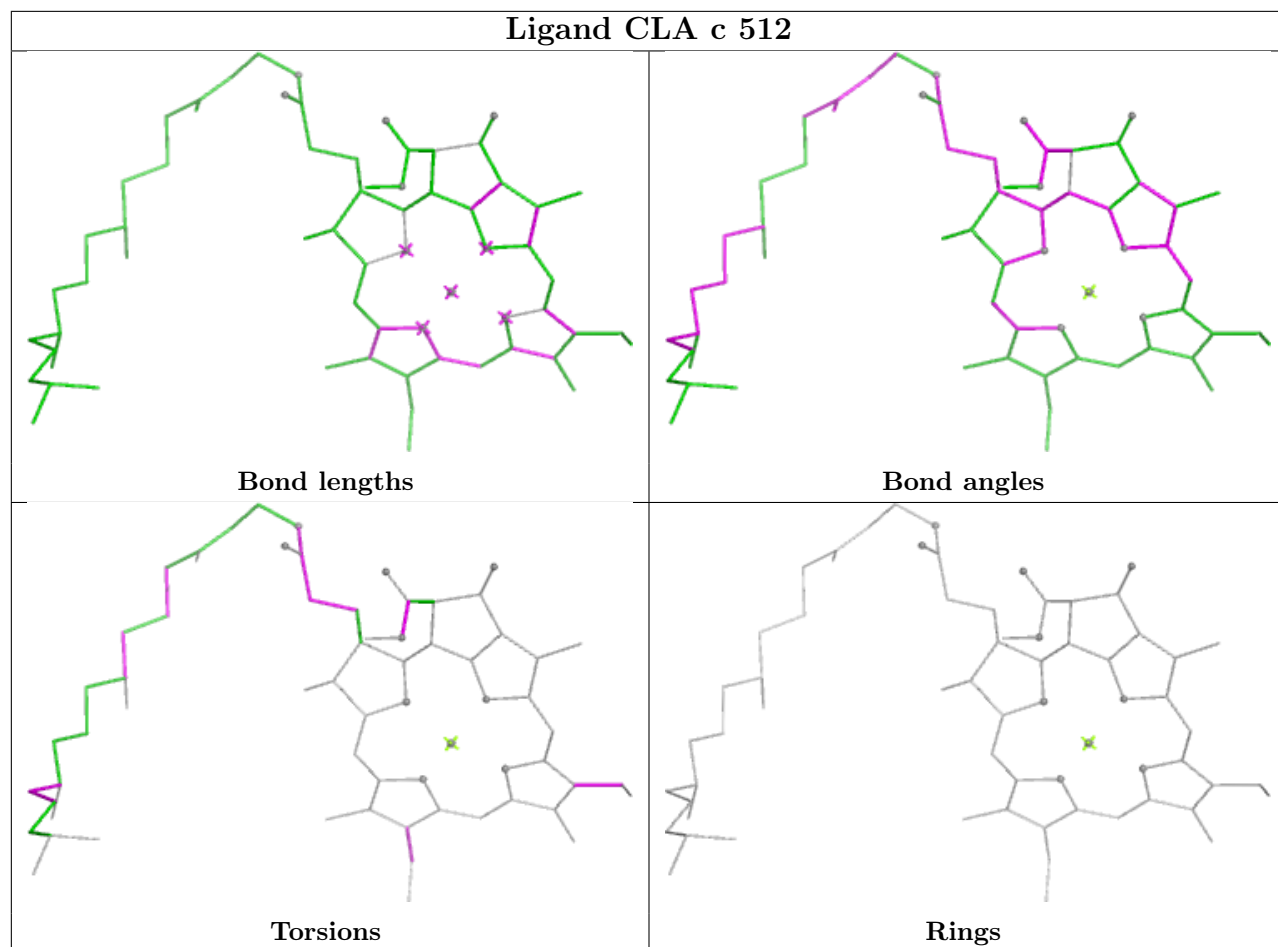
Torsions

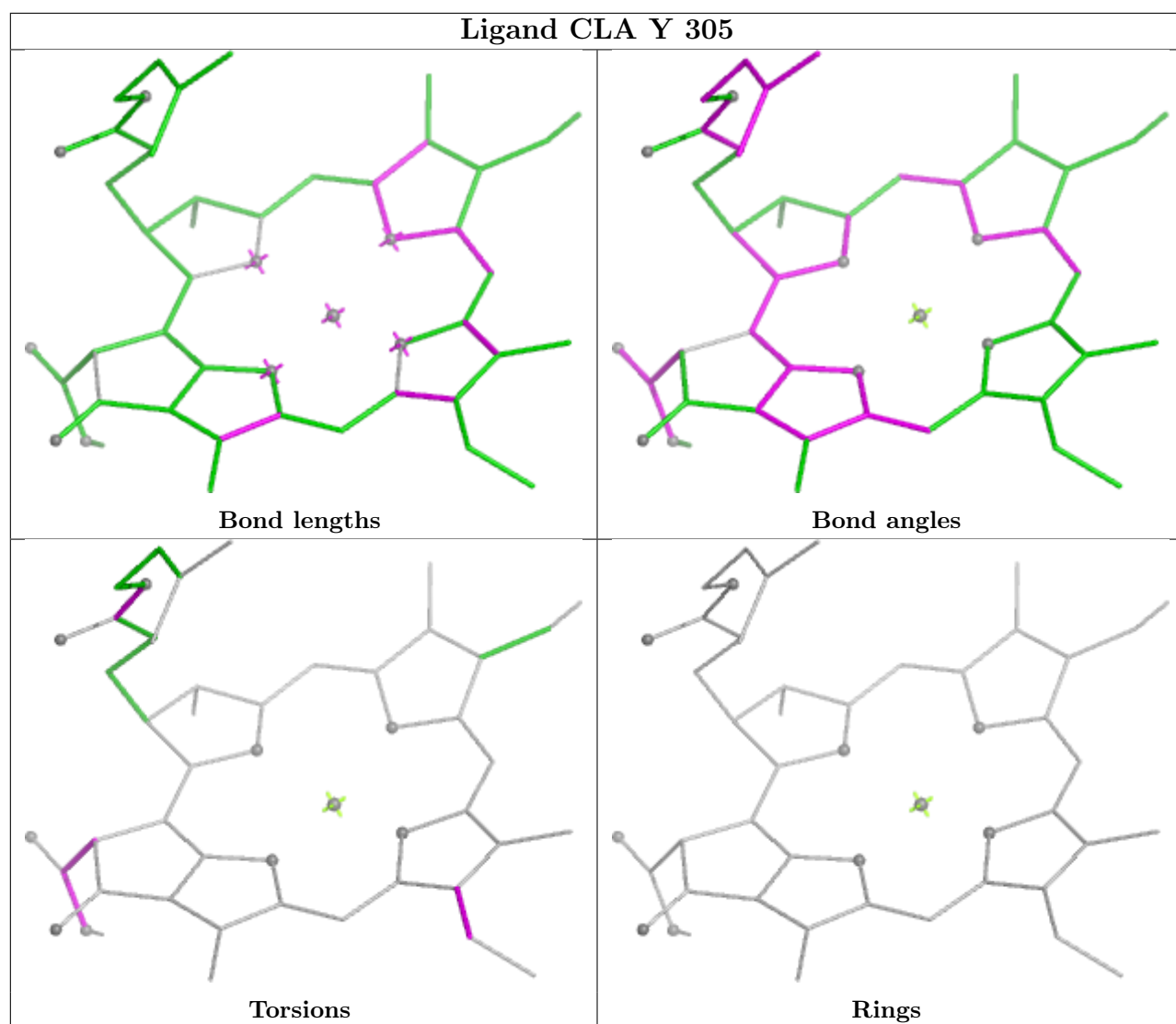


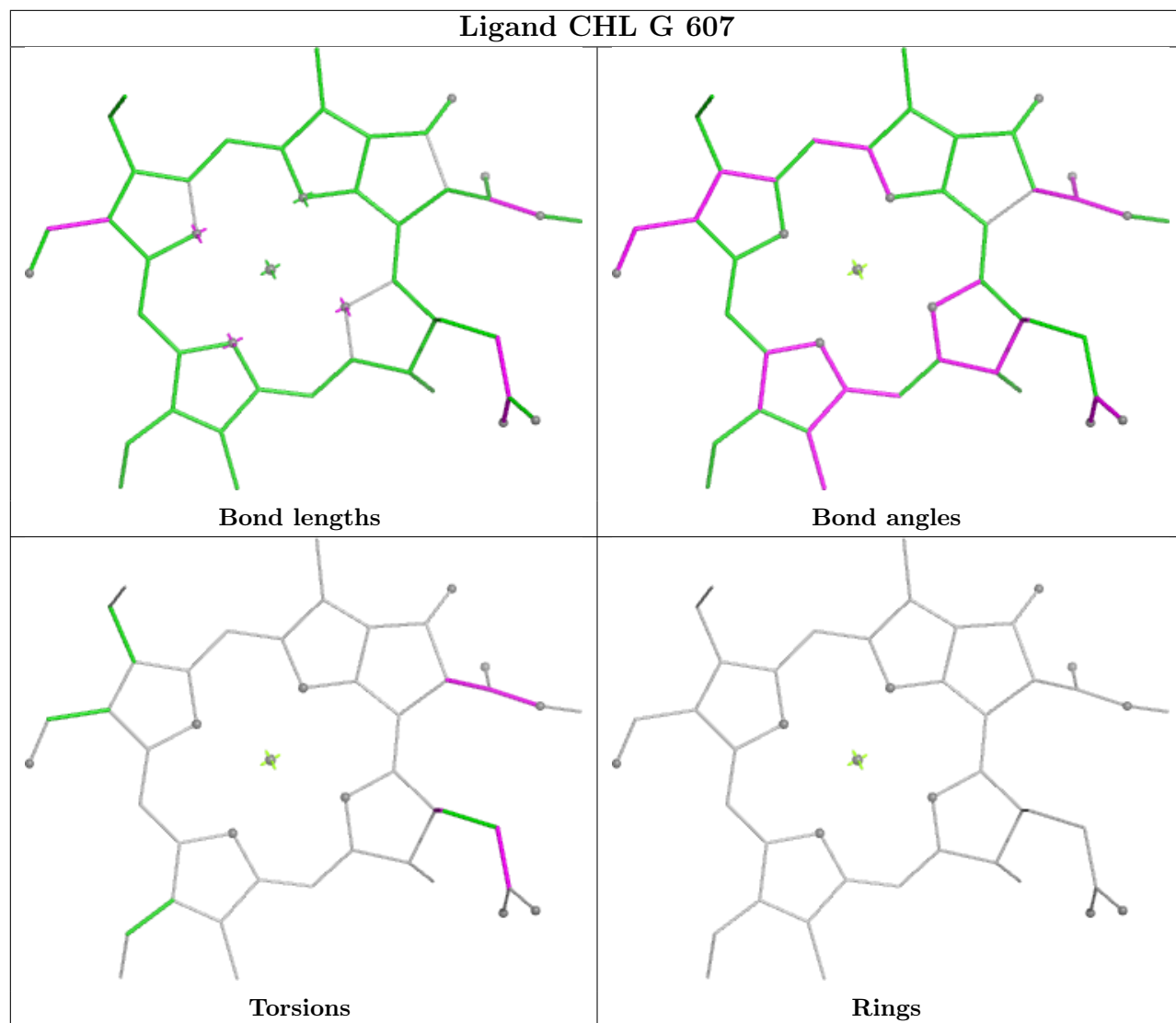
Rings



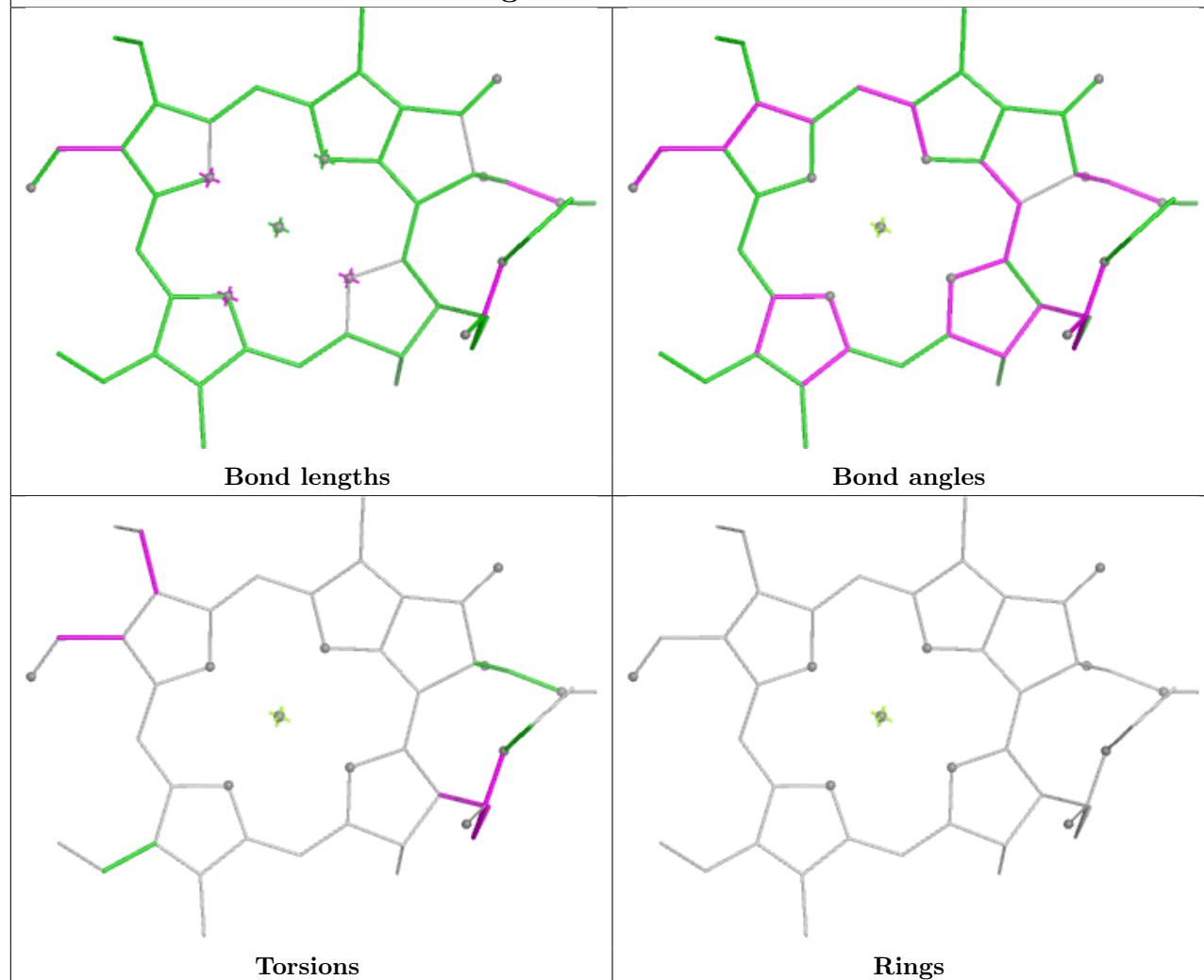




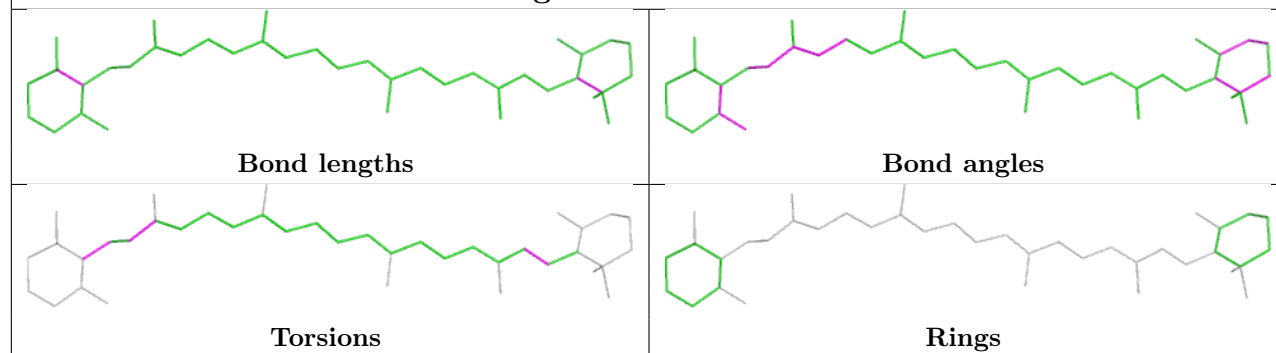


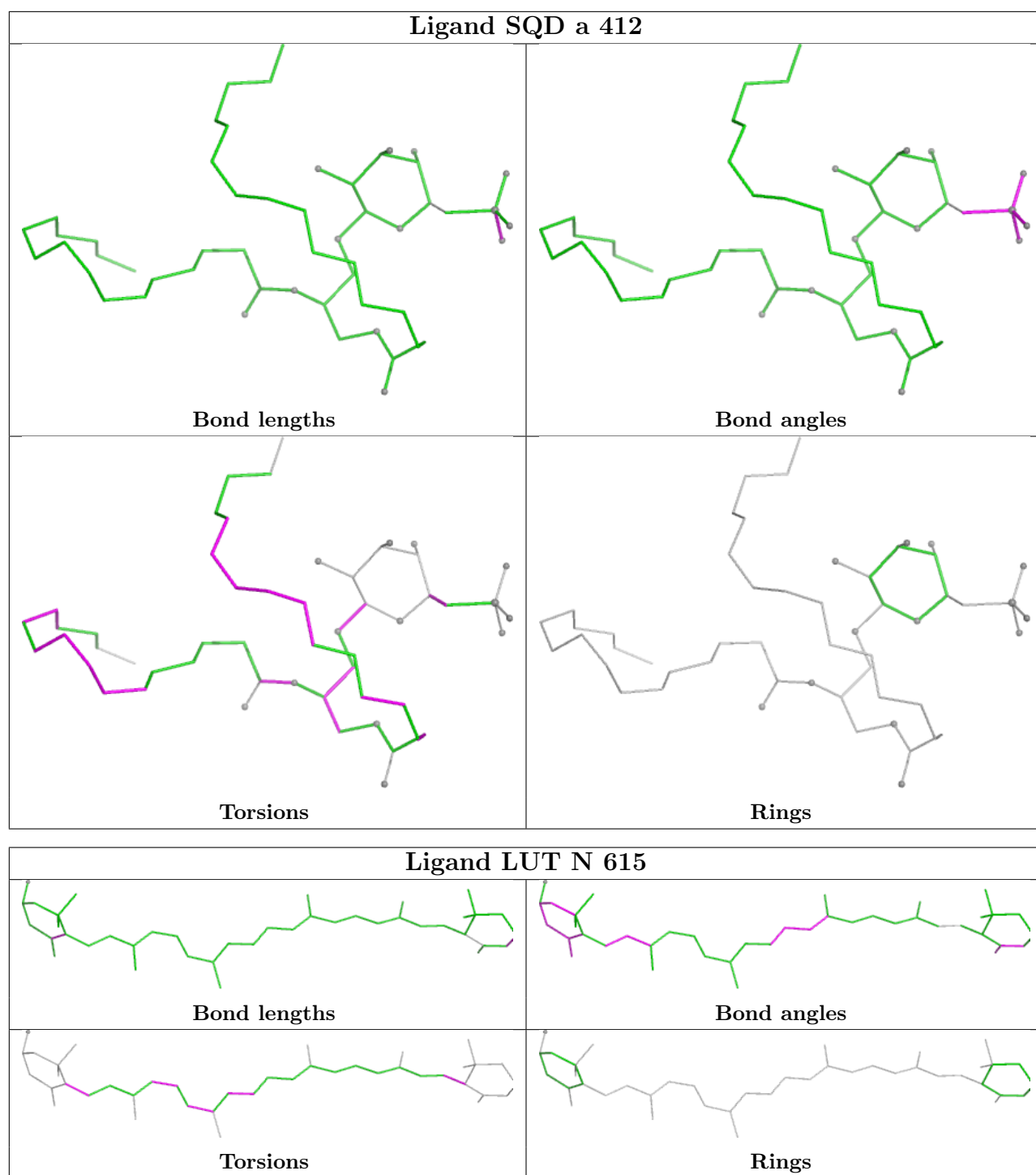


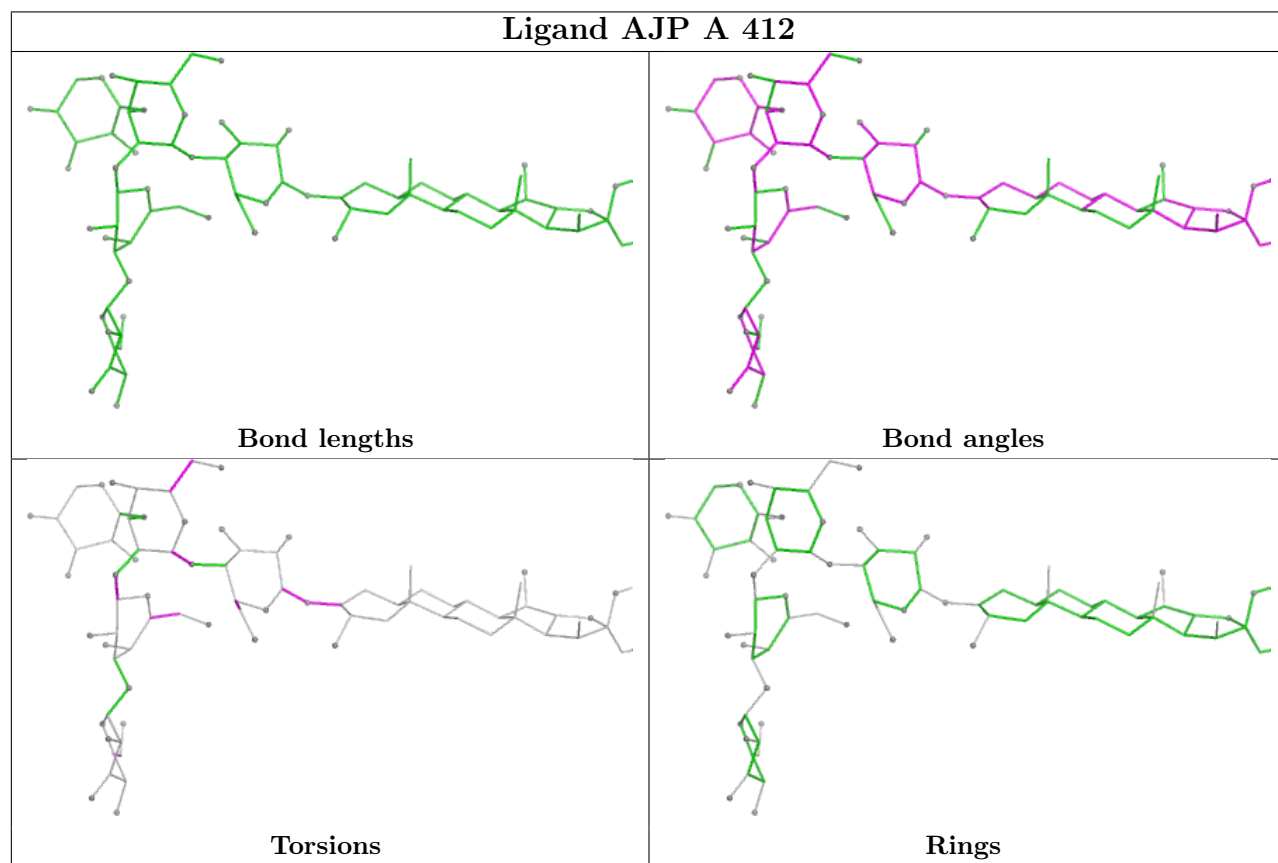
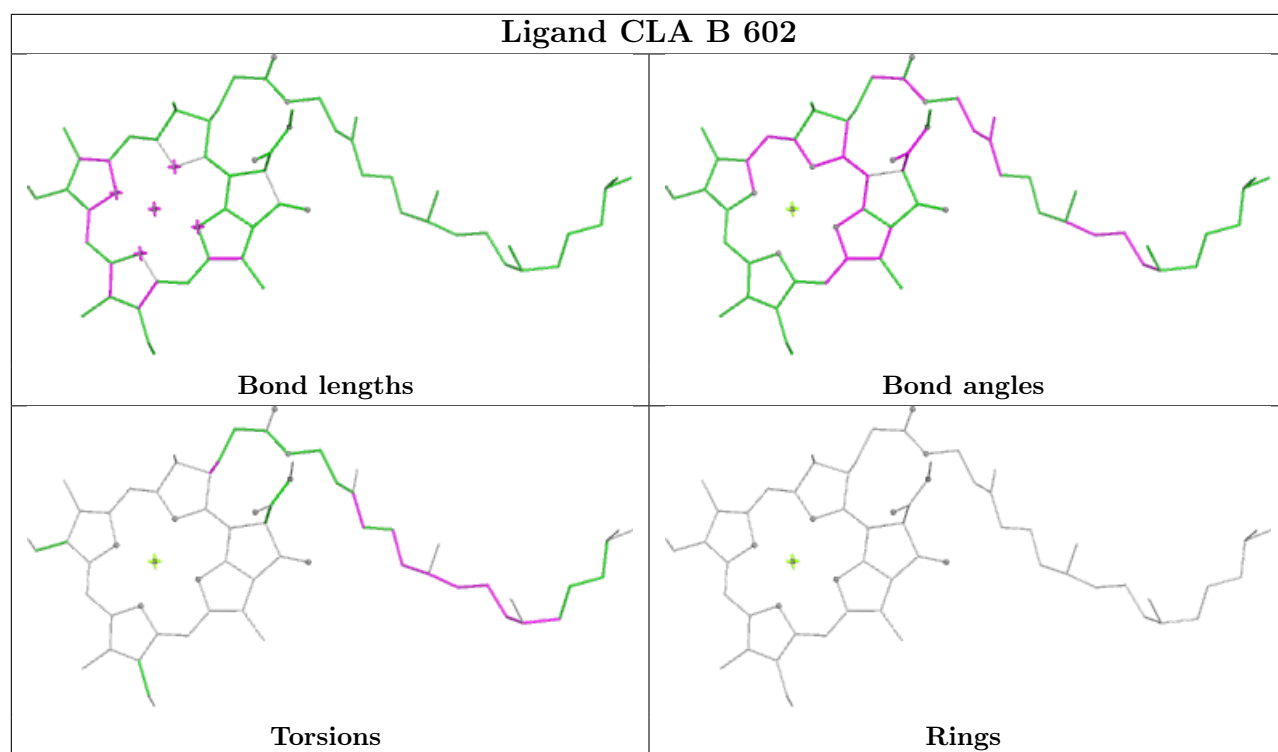
Ligand CHL Y 306

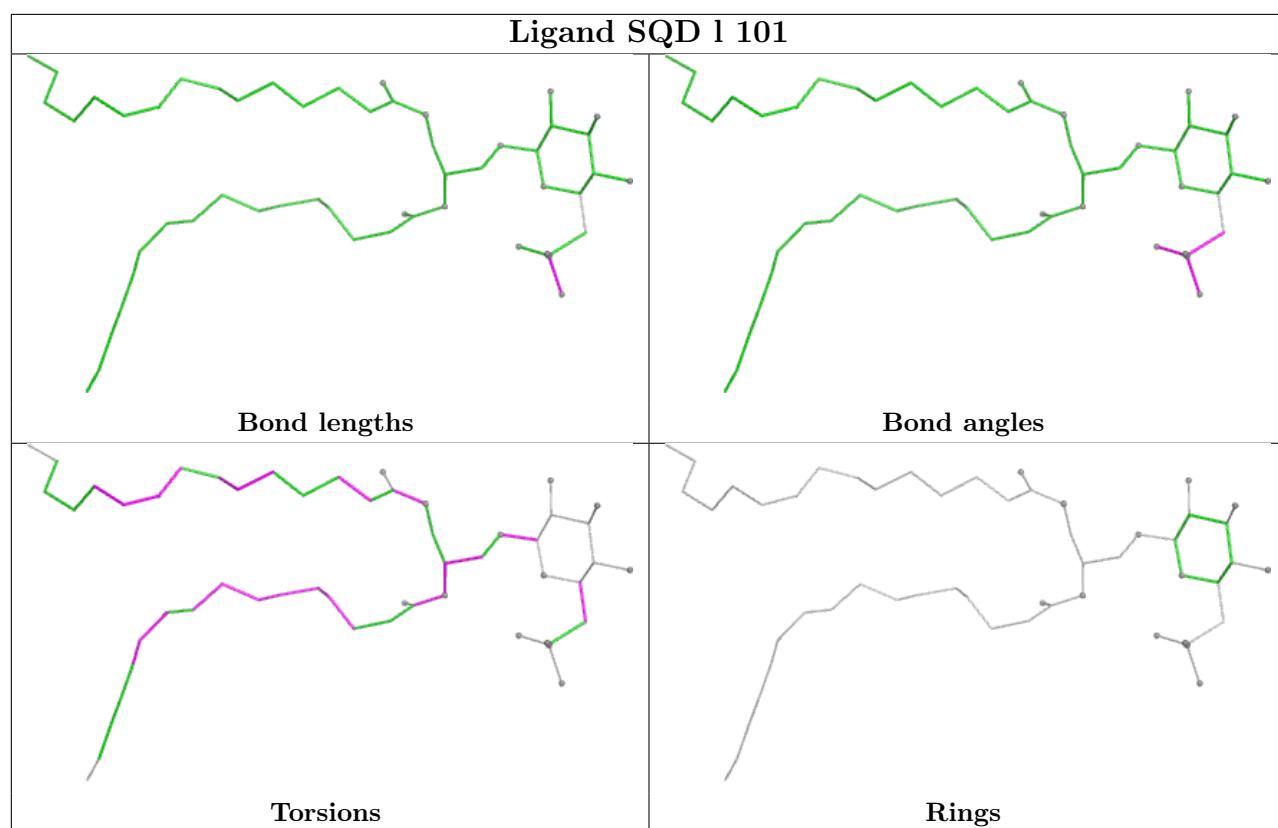


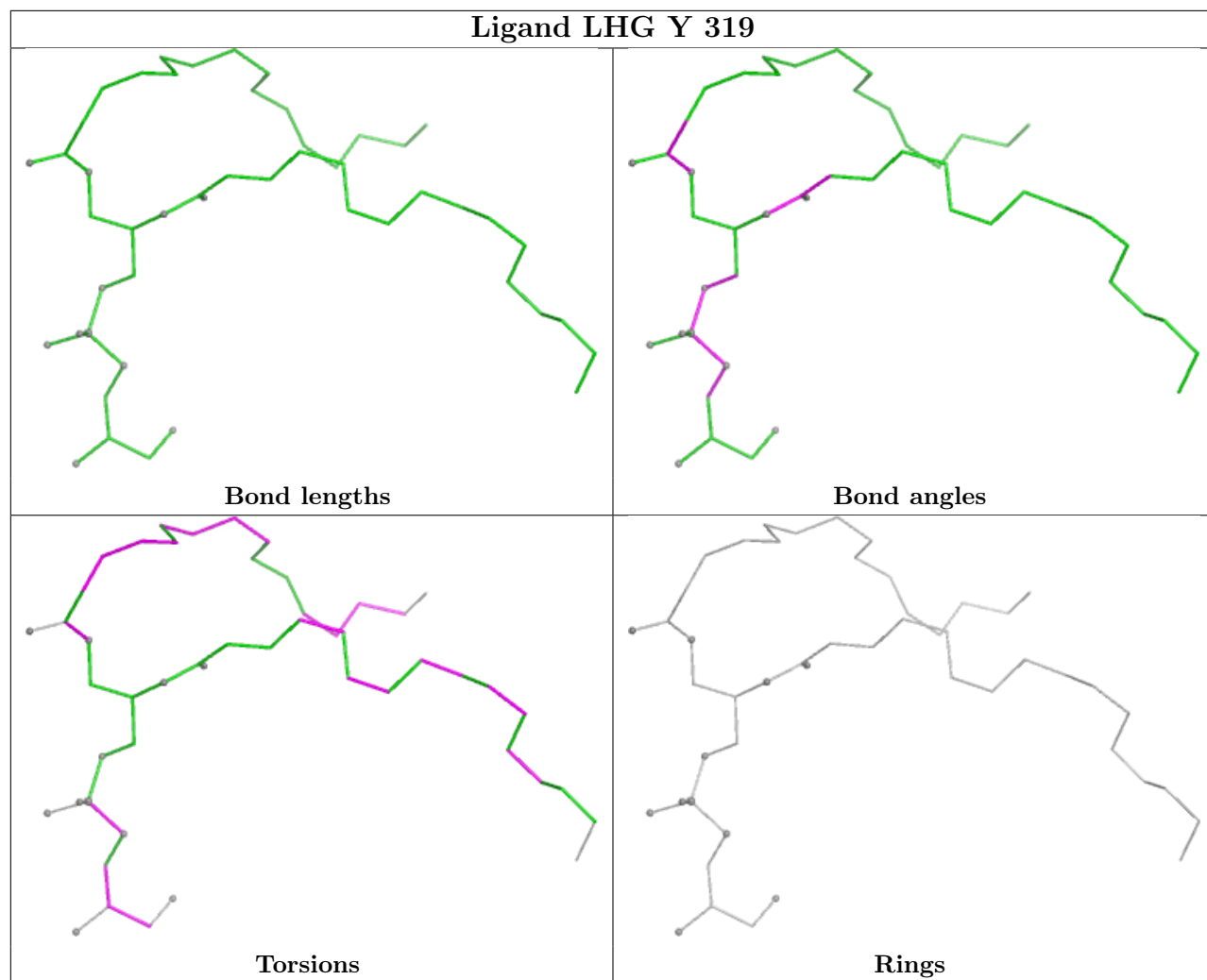
Ligand BCR d 404



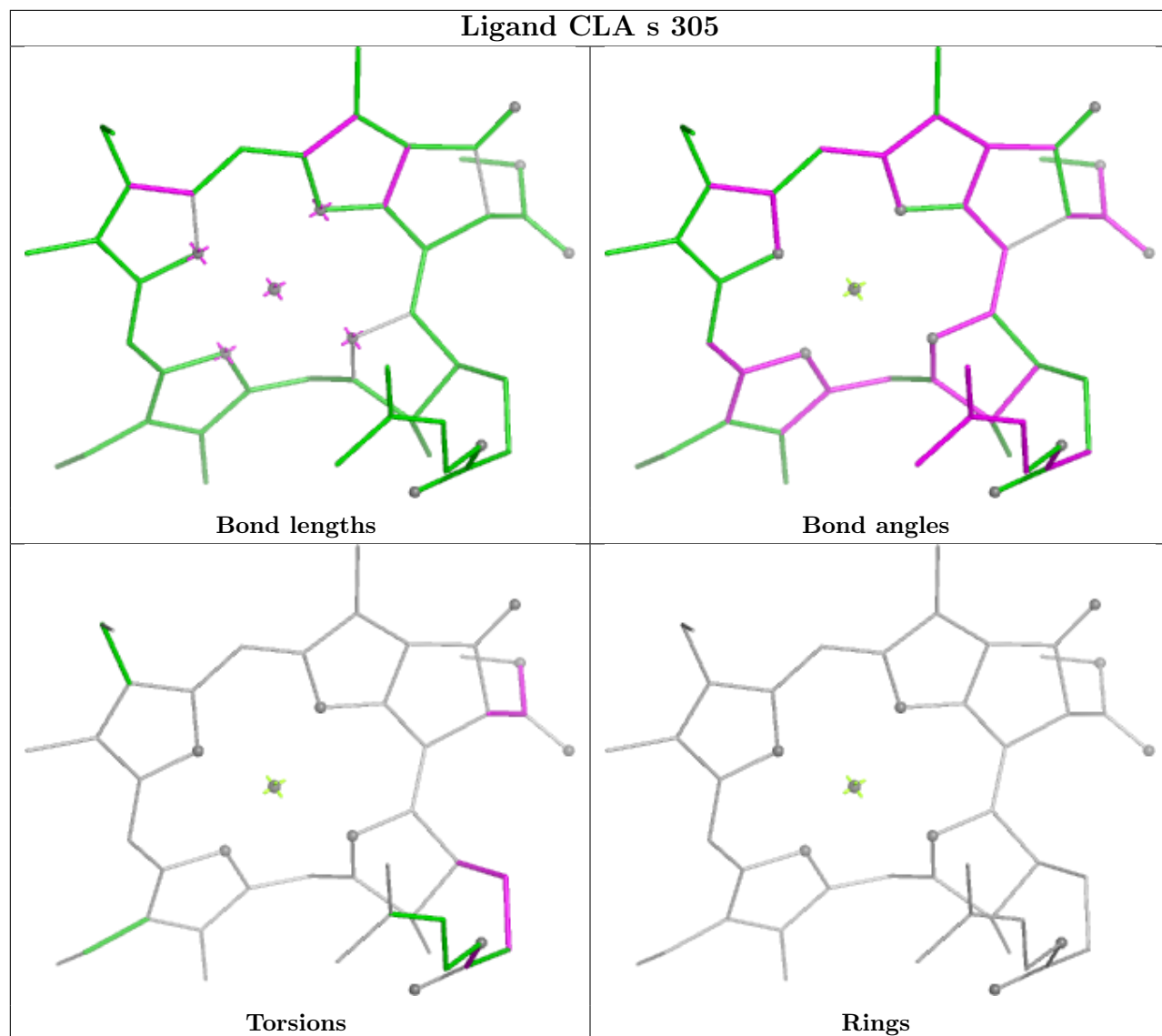


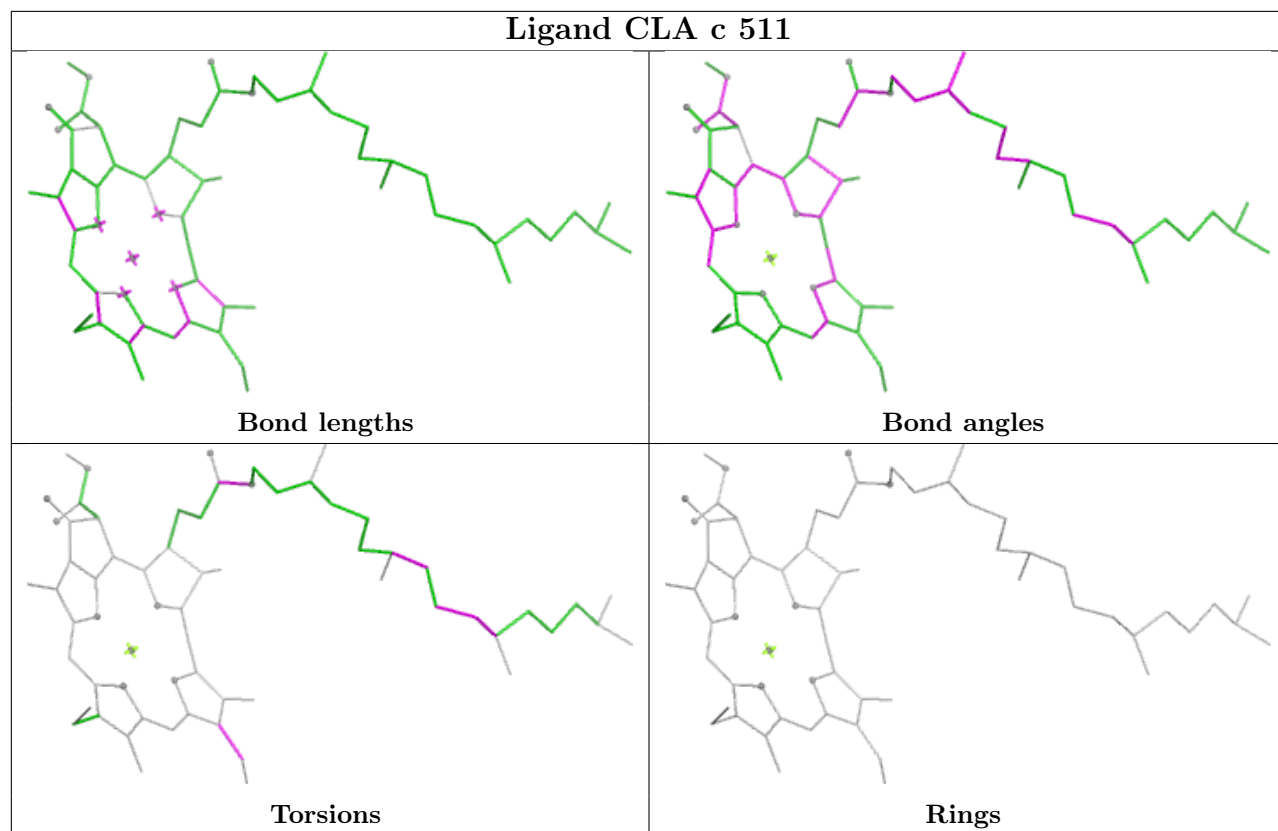




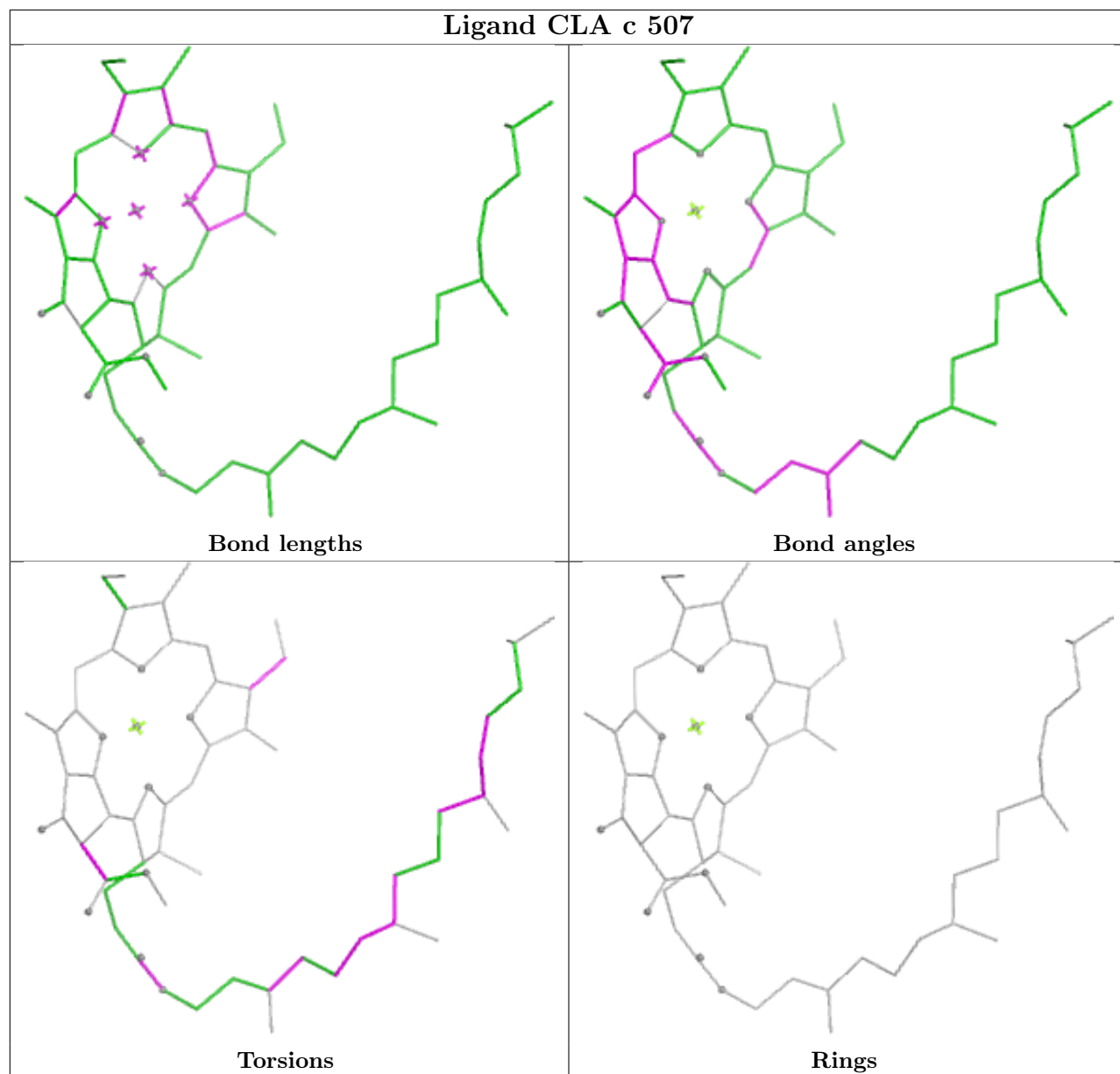


Ligand CLA s 305

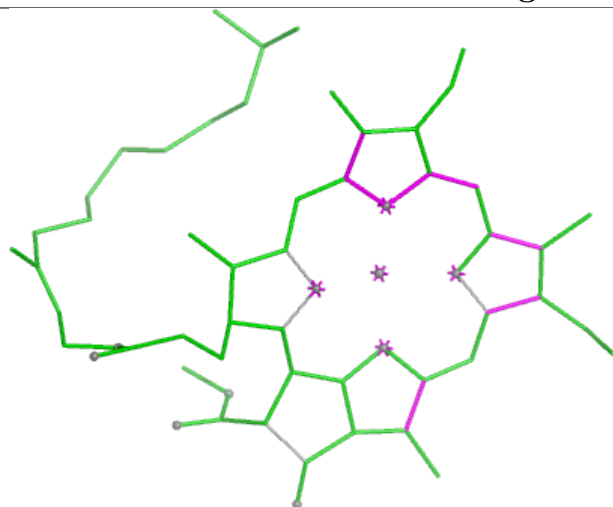




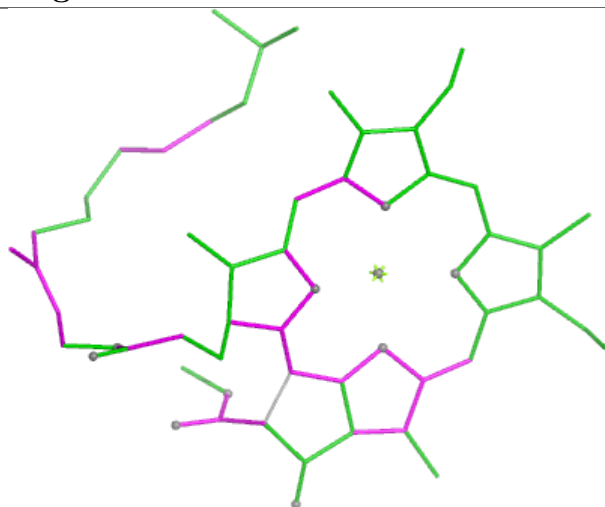
Ligand CLA c 507



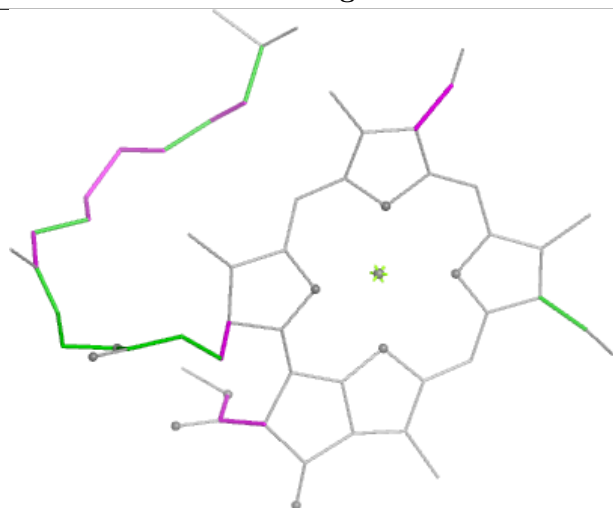
Ligand CLA g 603



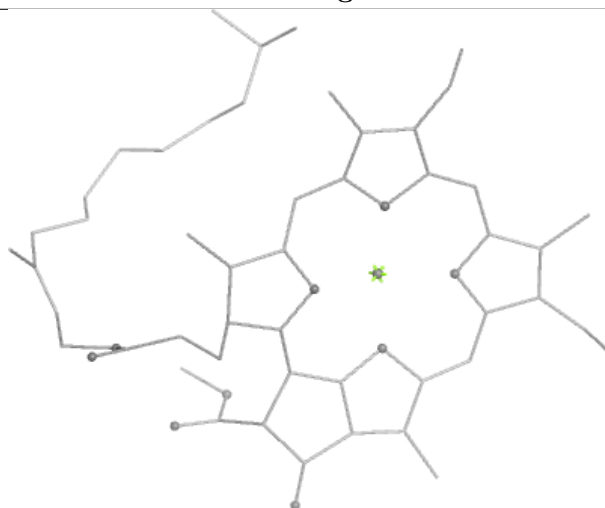
Bond lengths



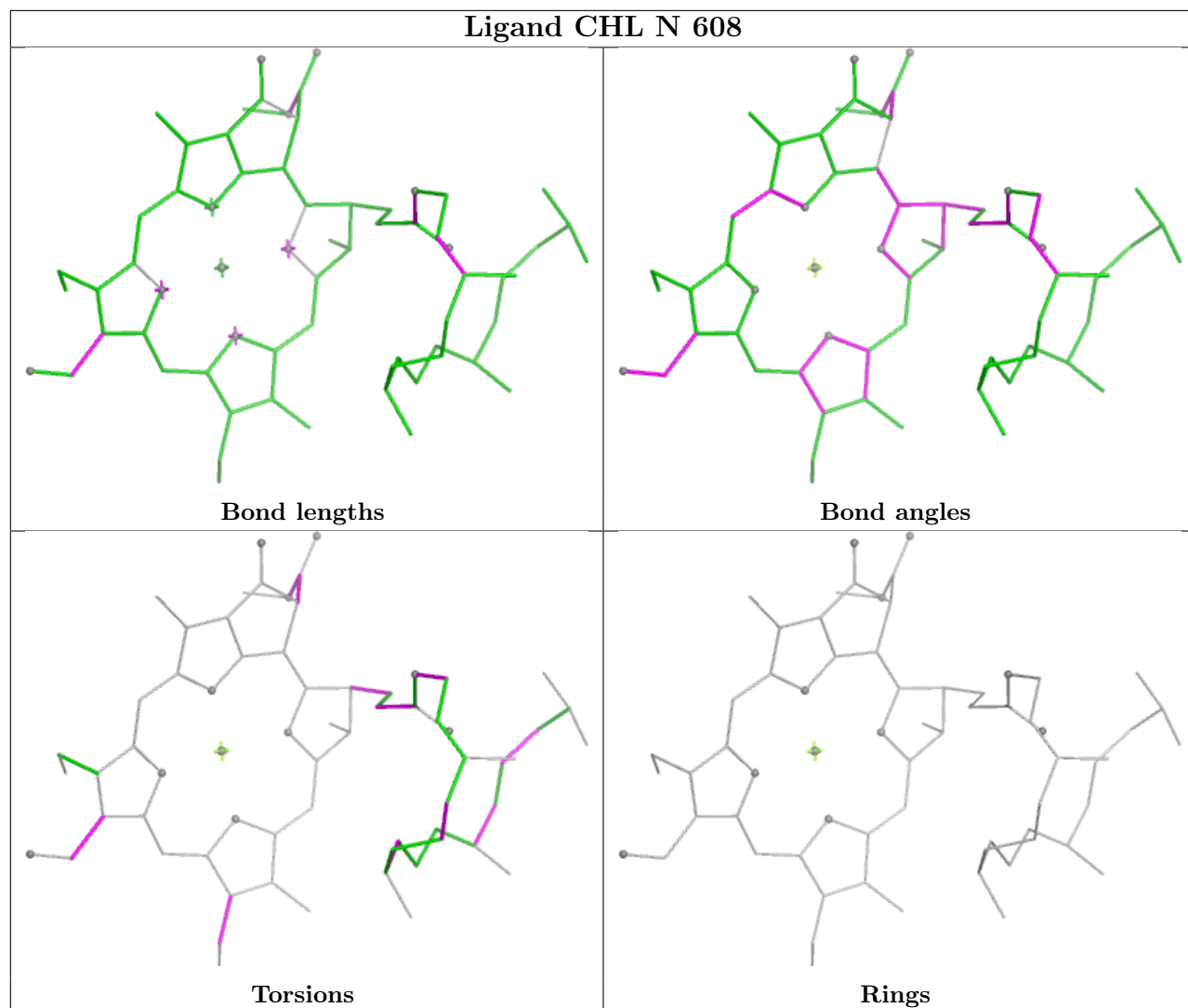
Bond angles

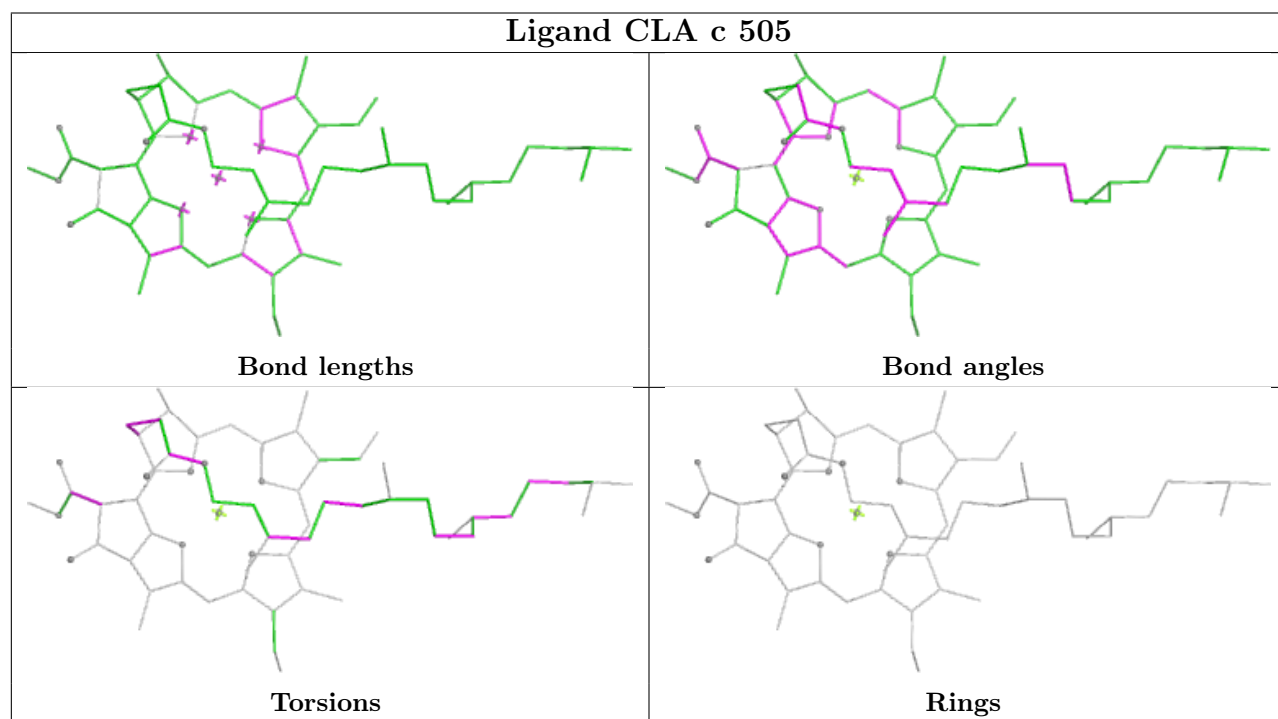
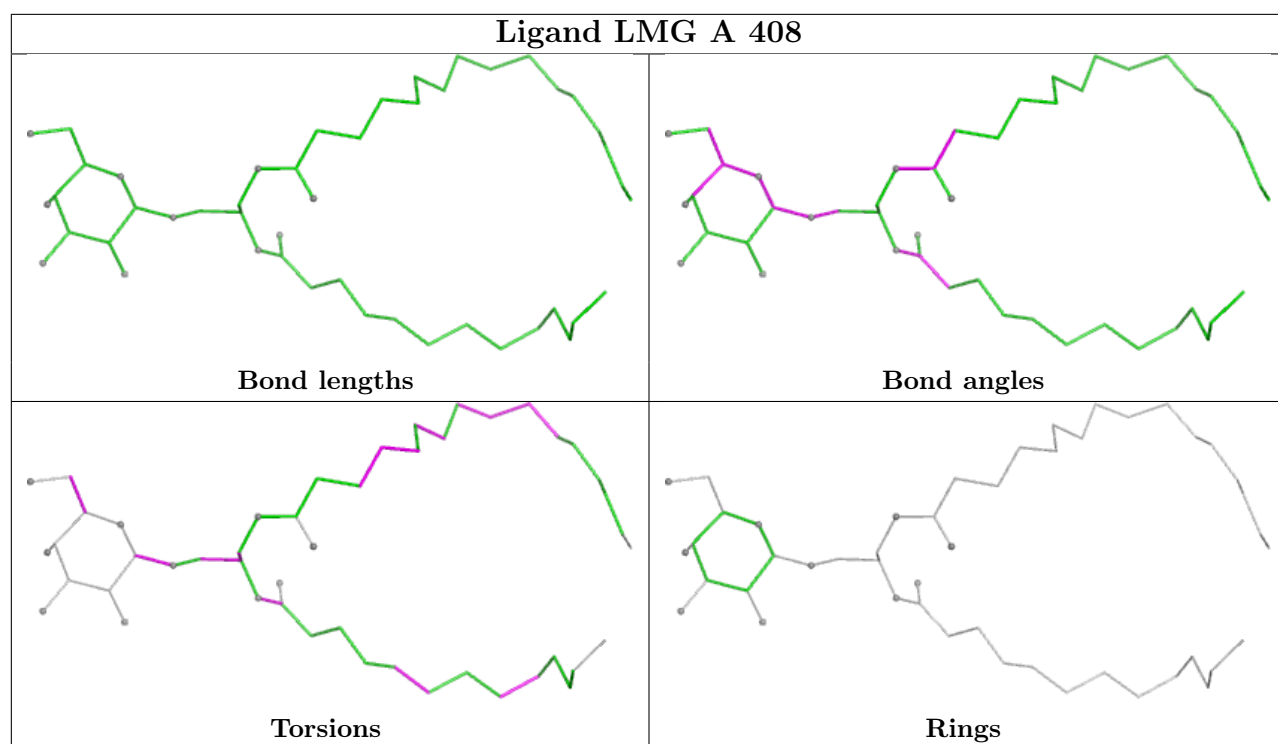


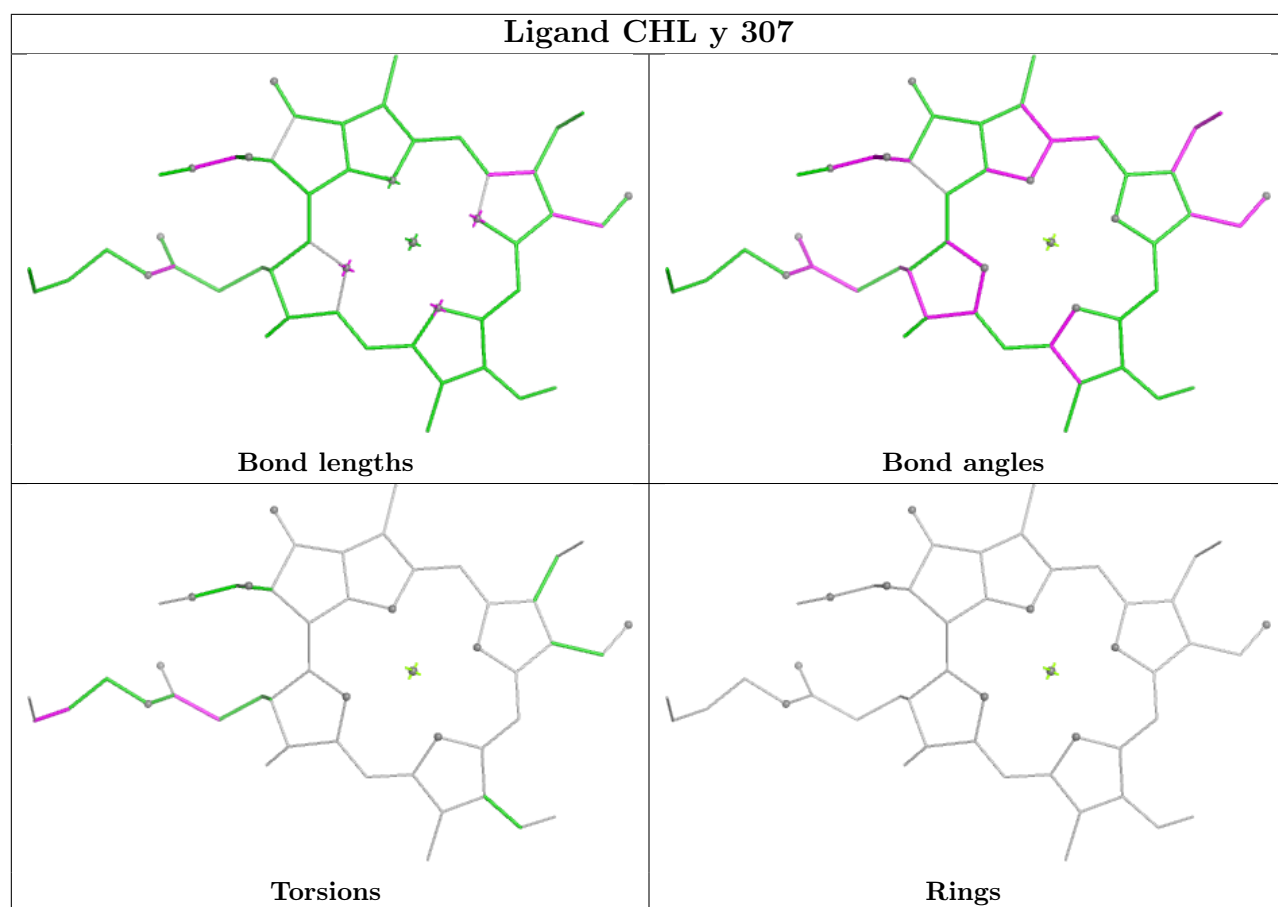
Torsions



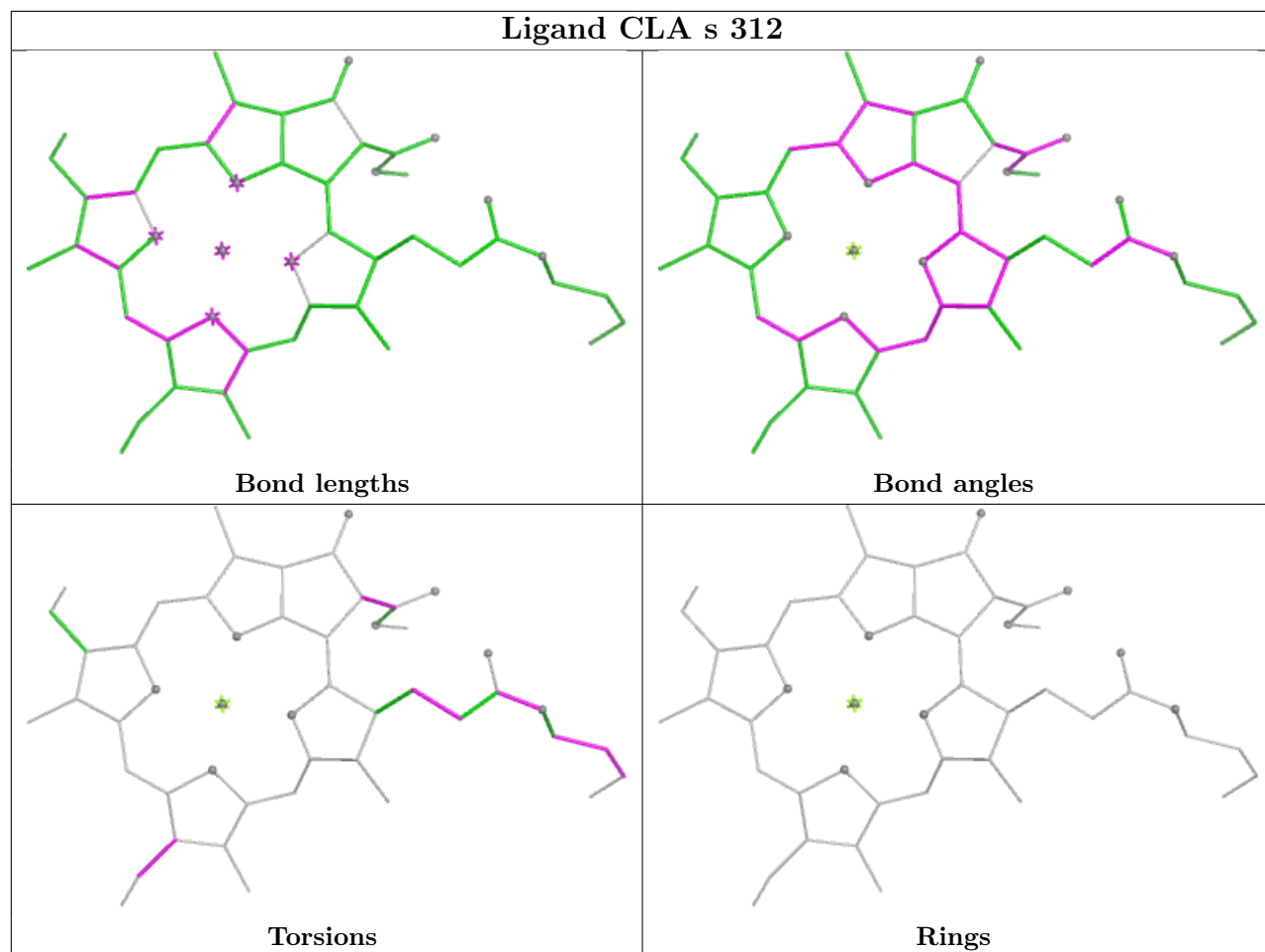
Rings

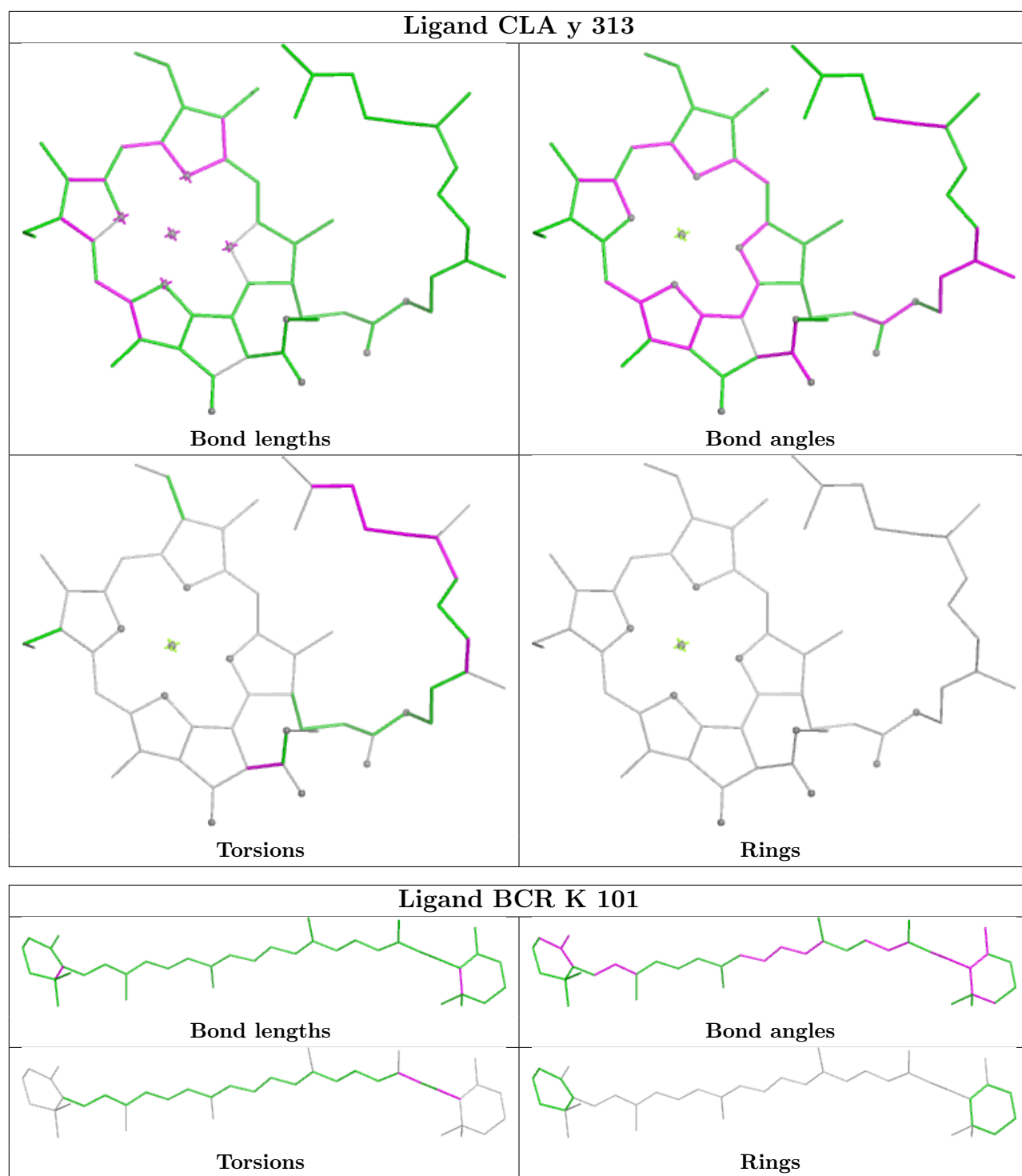


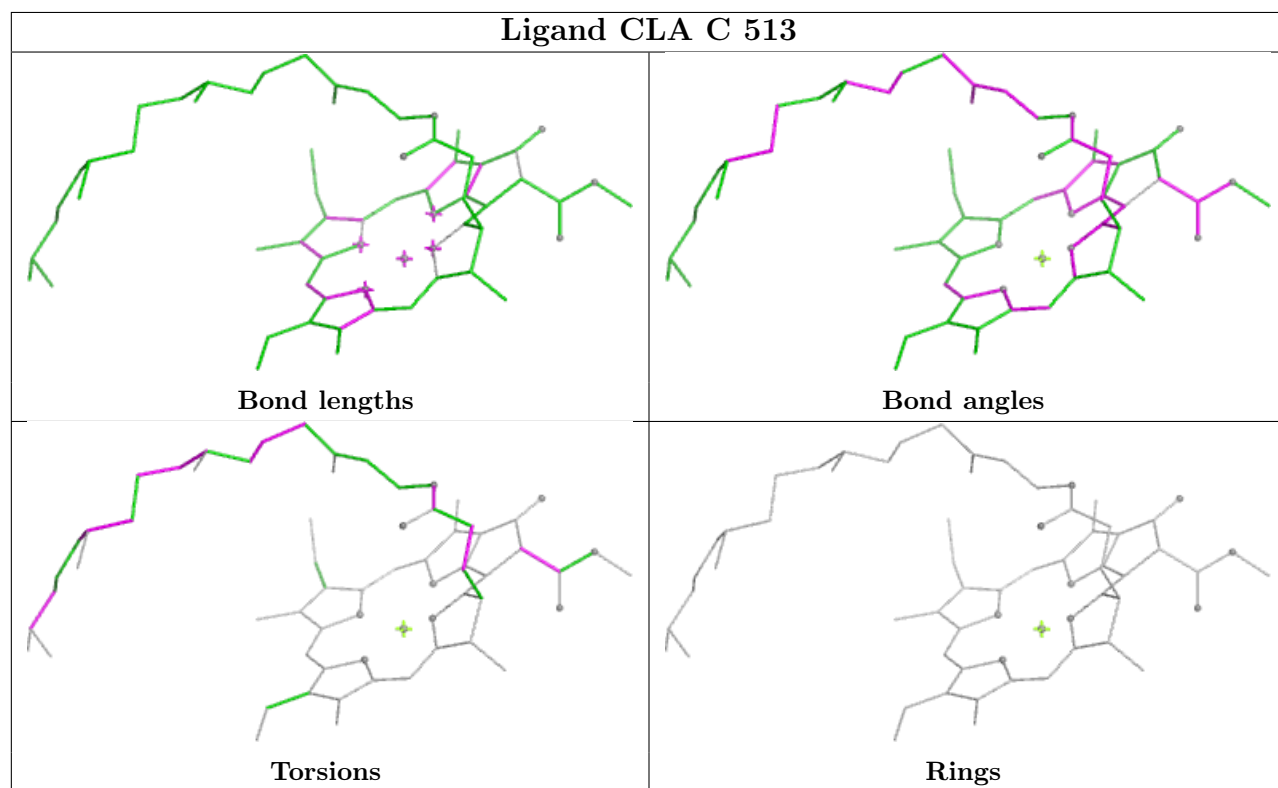
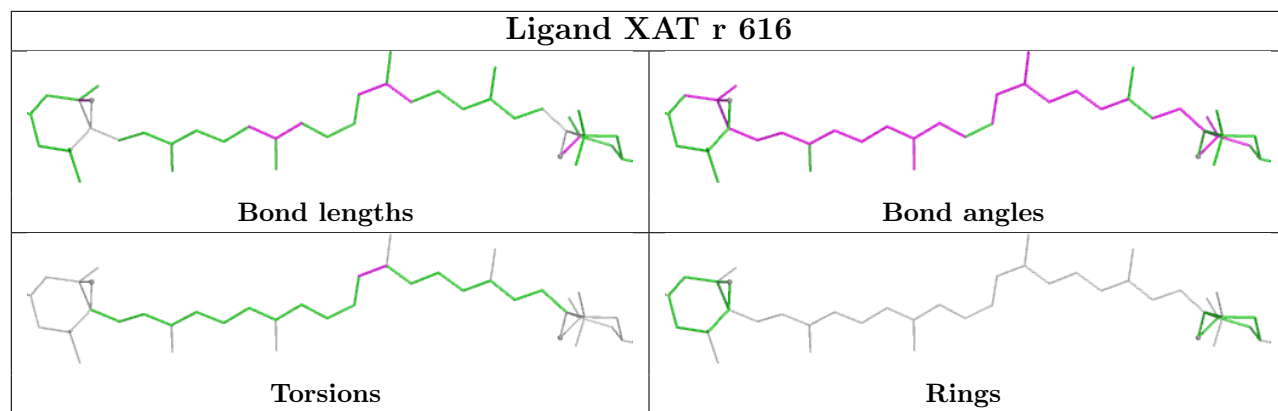




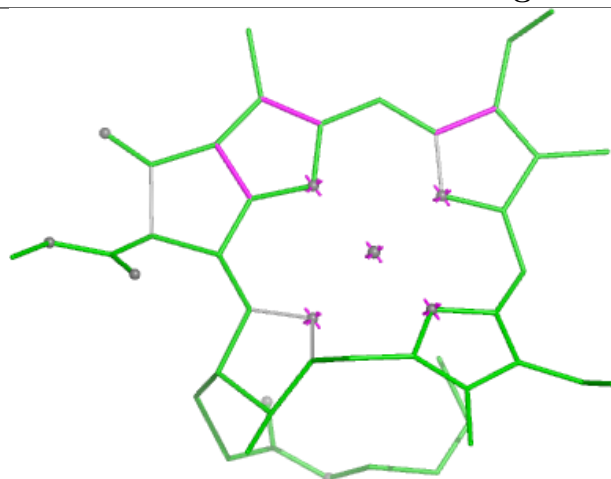
Ligand CLA s 312



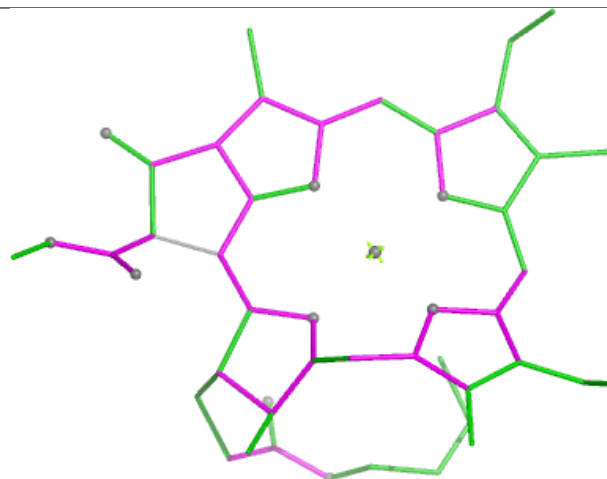




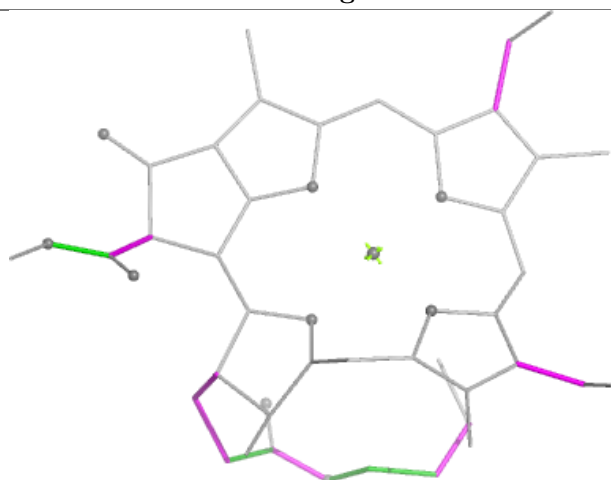
Ligand CLA R 610



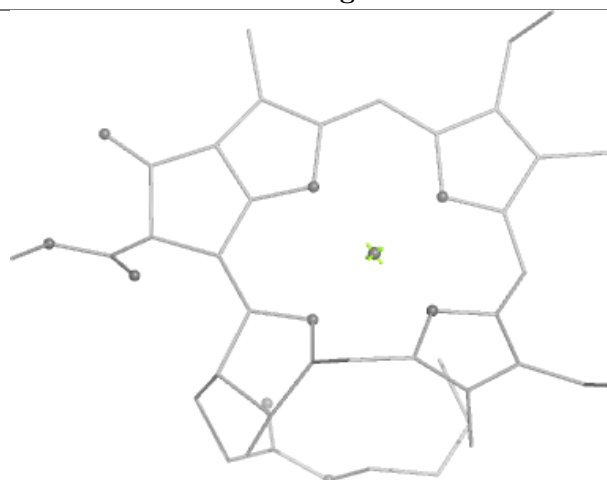
Bond lengths



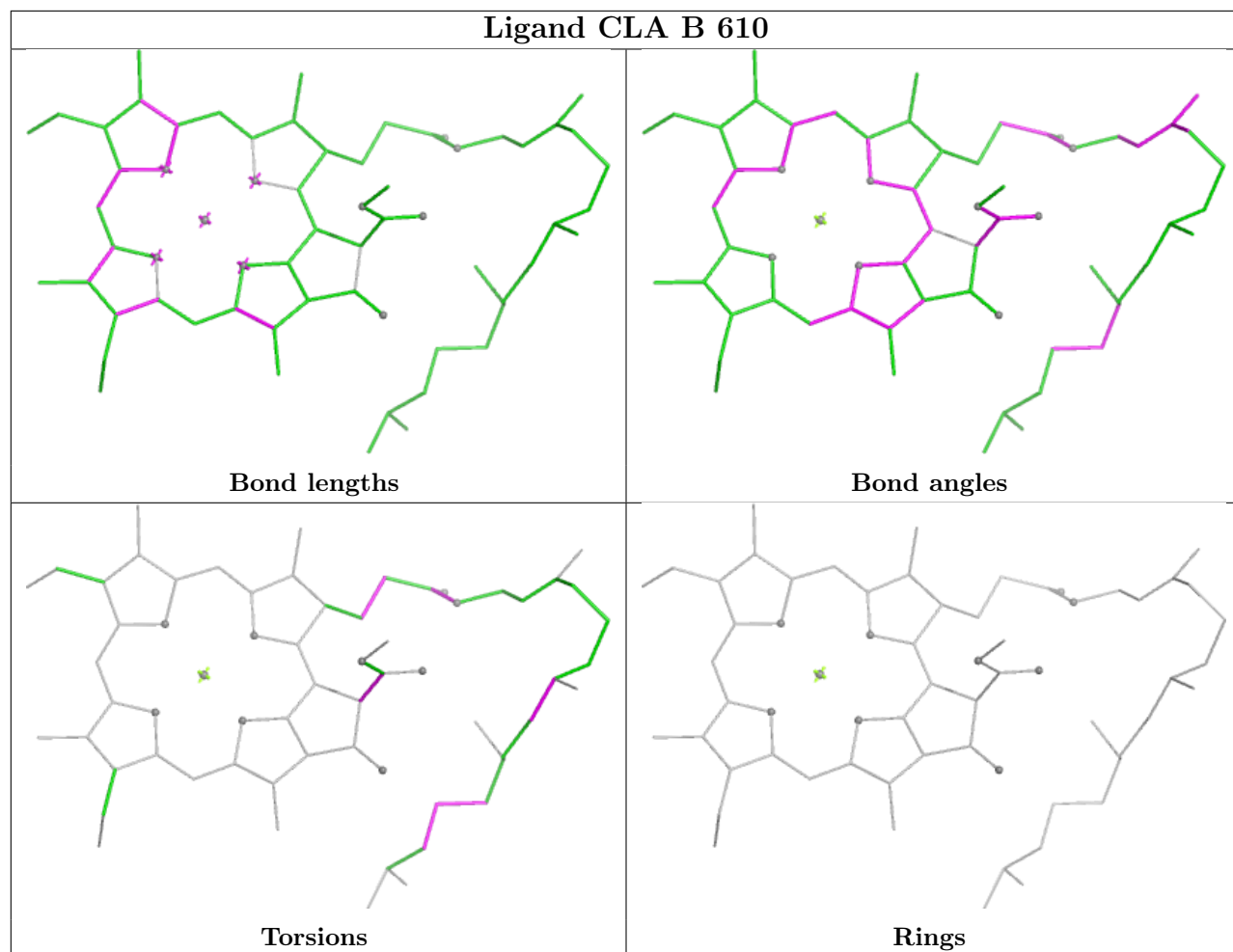
Bond angles

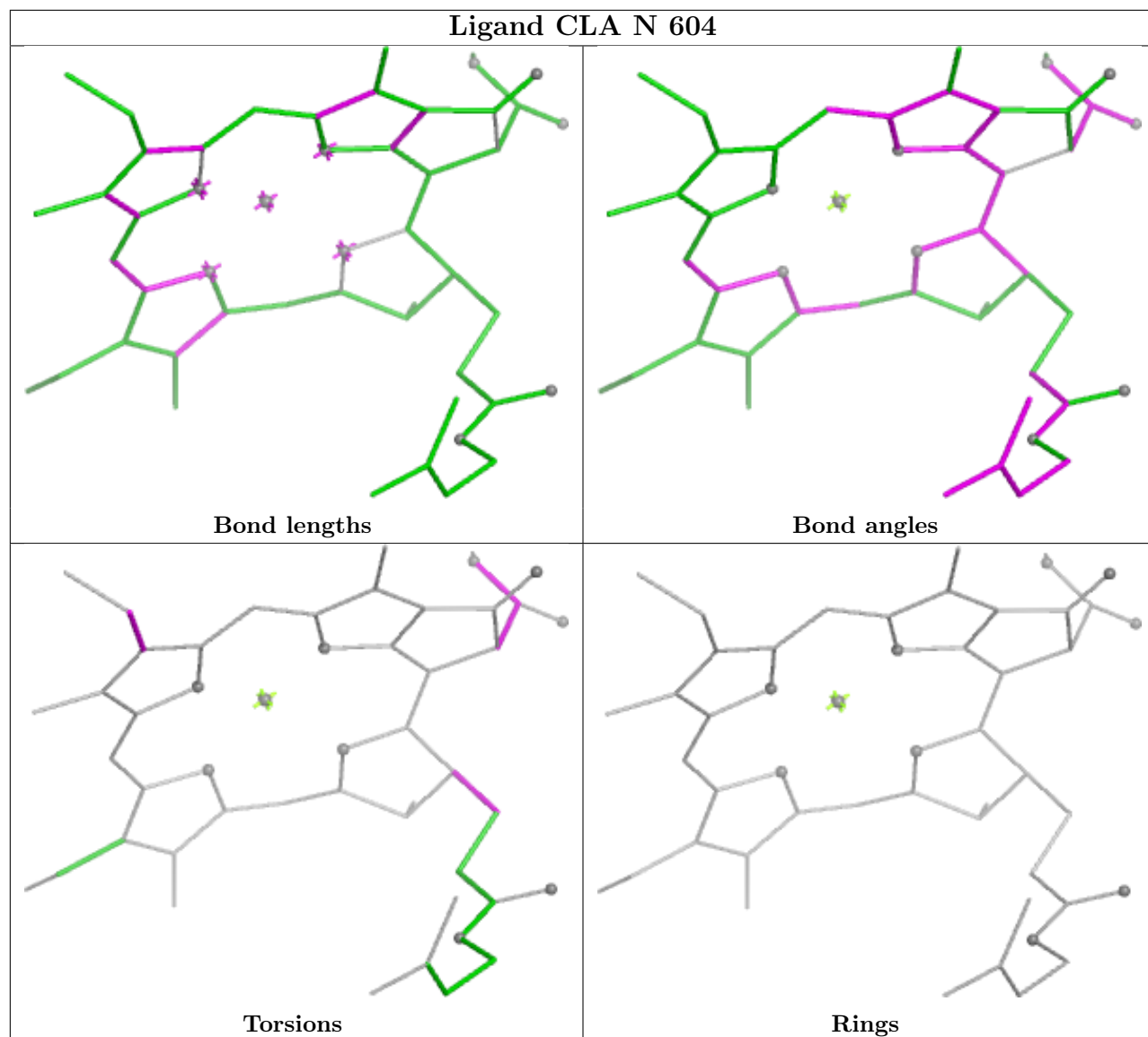


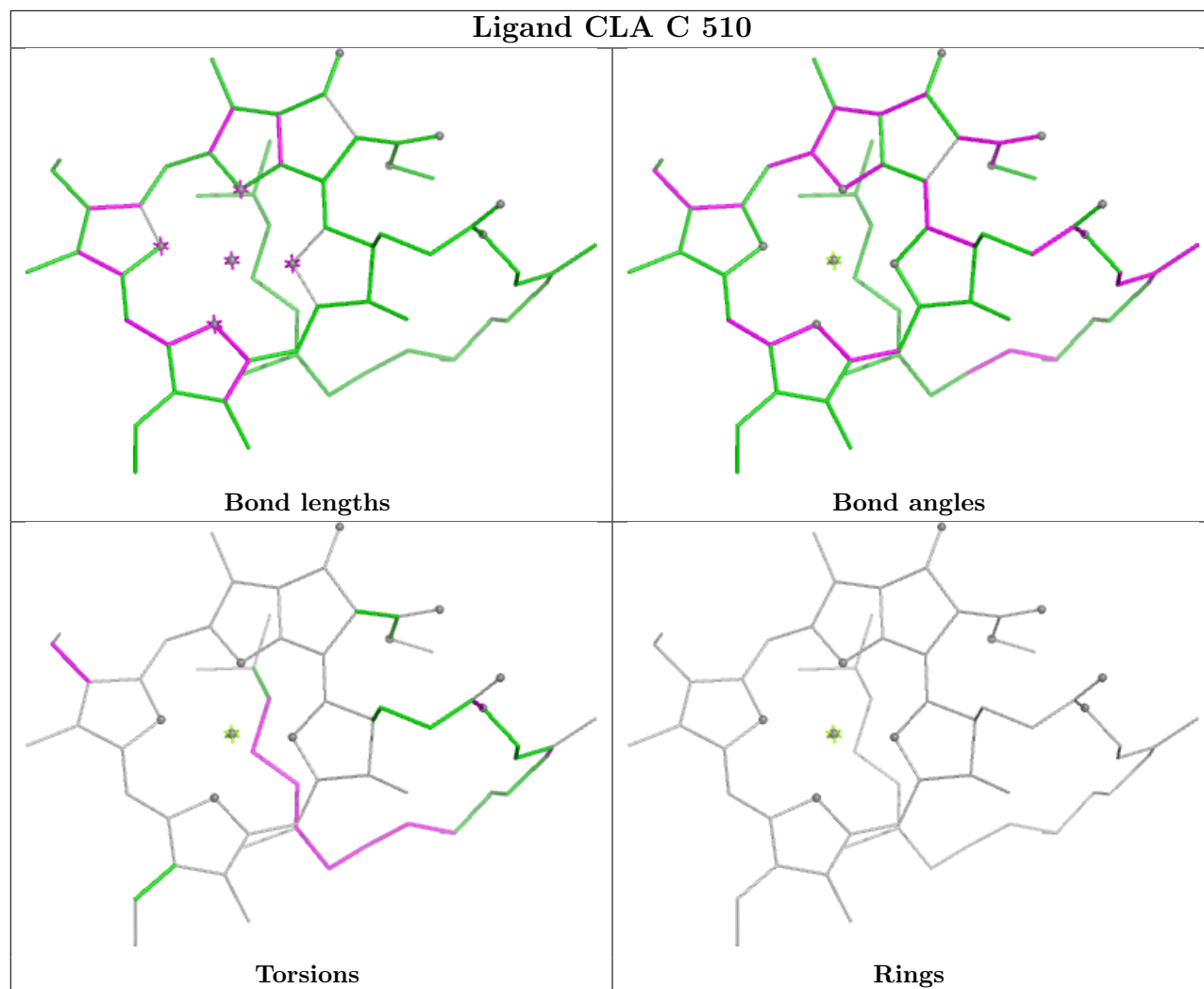
Torsions

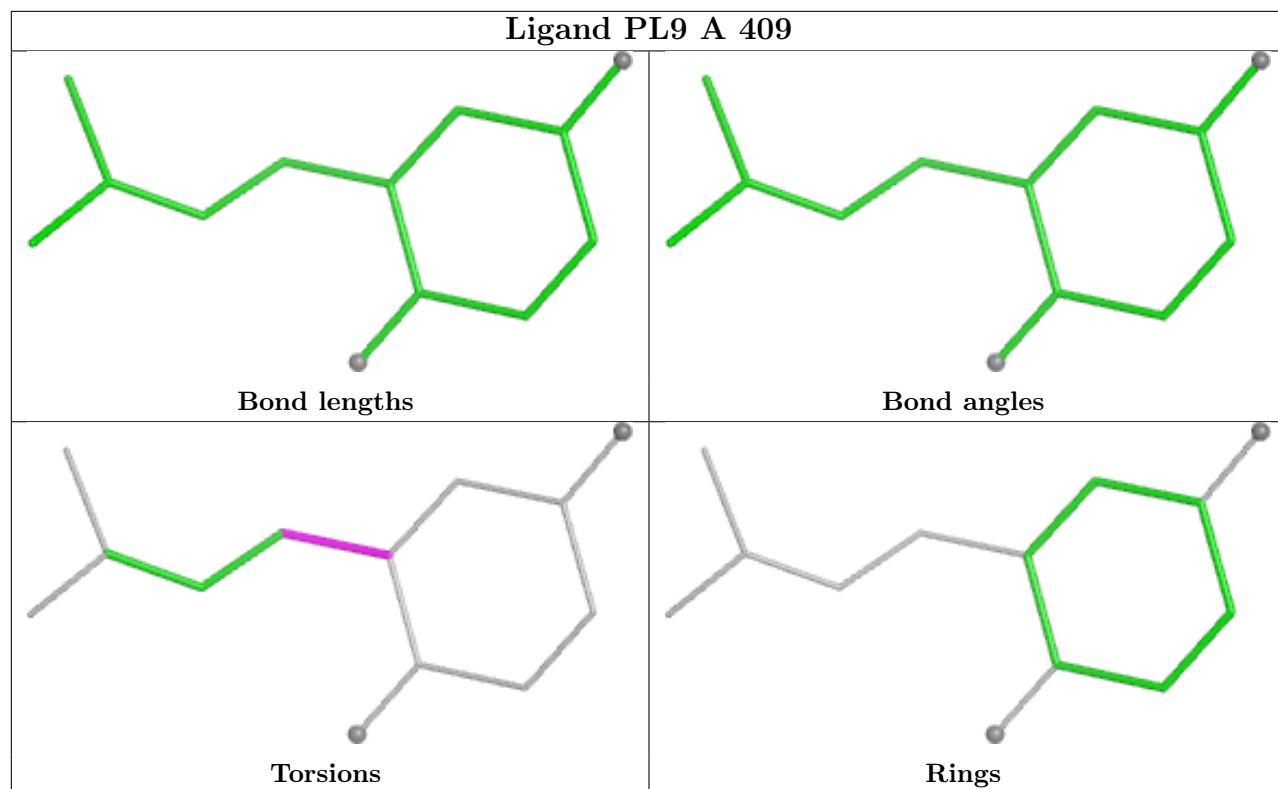


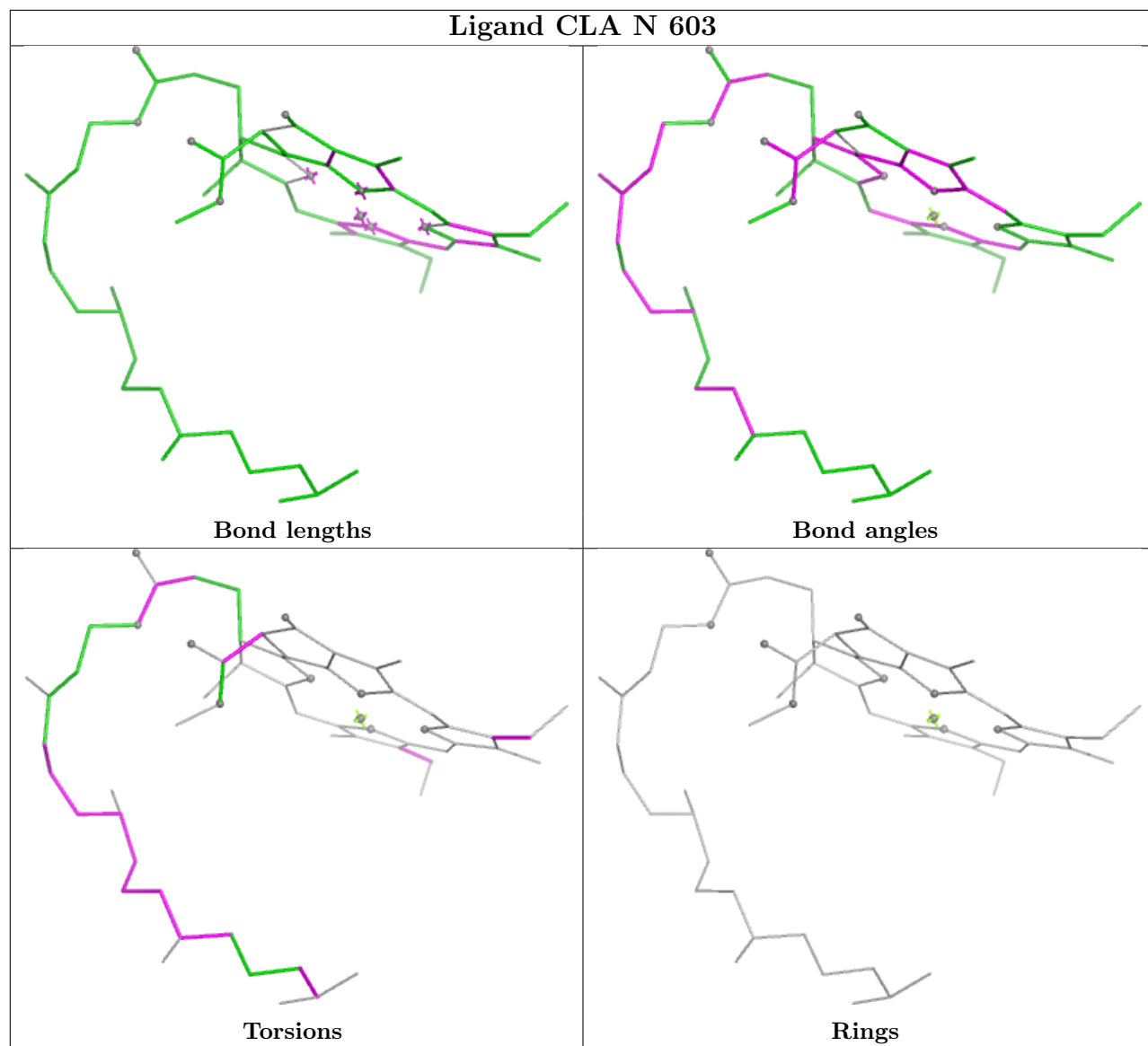
Rings

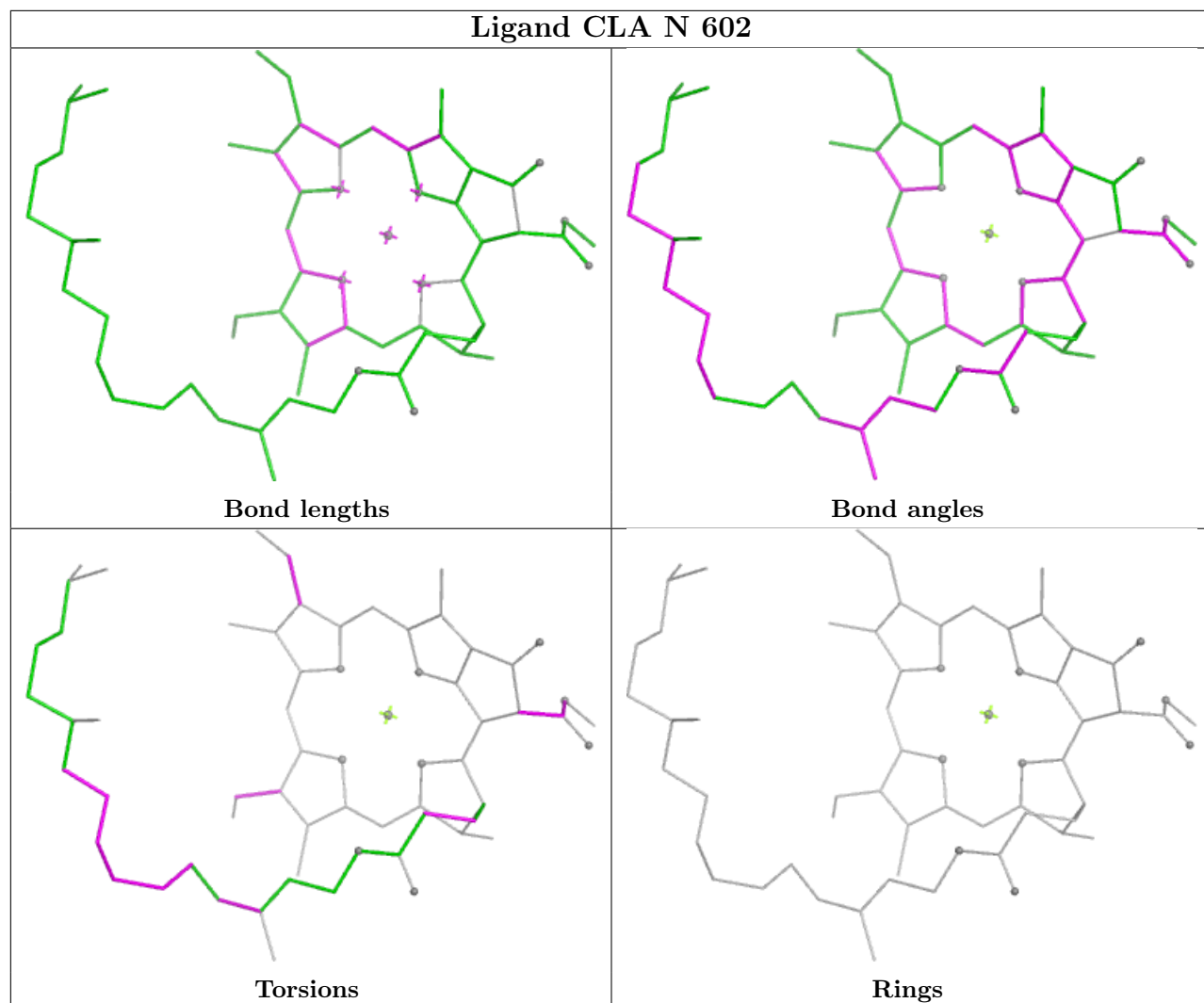




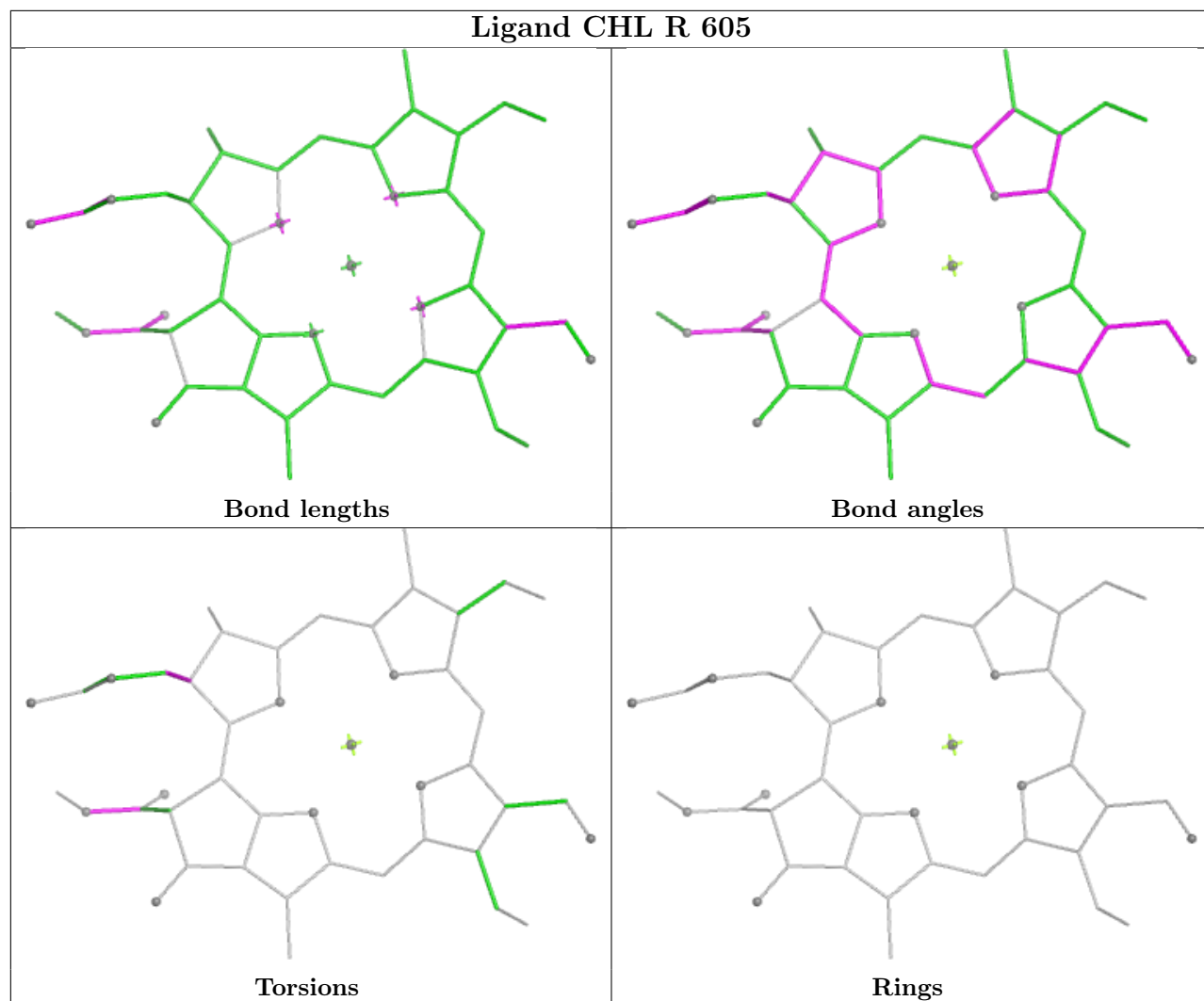




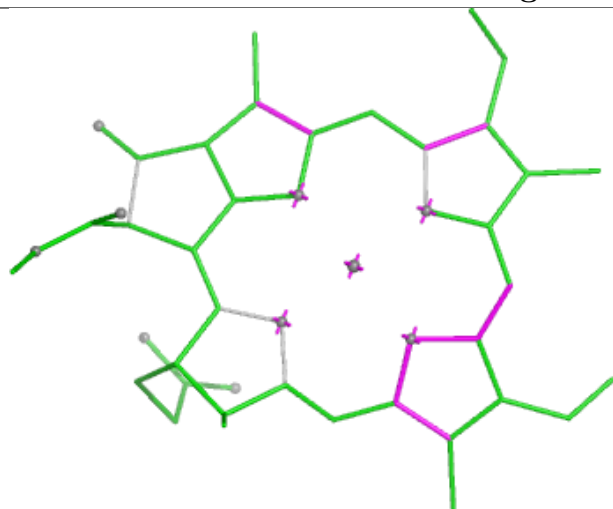




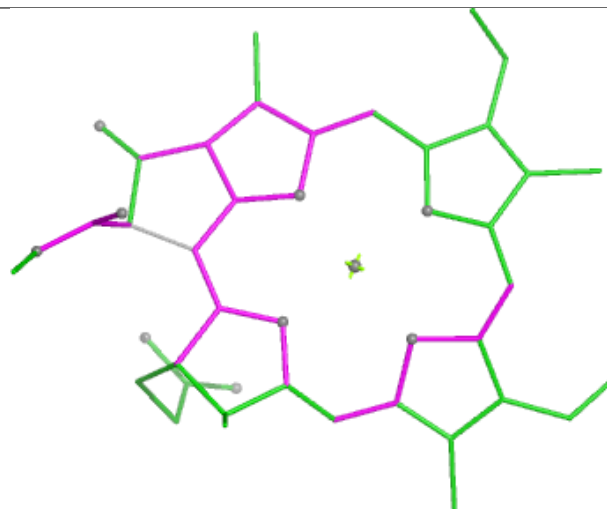
Ligand CHL R 605



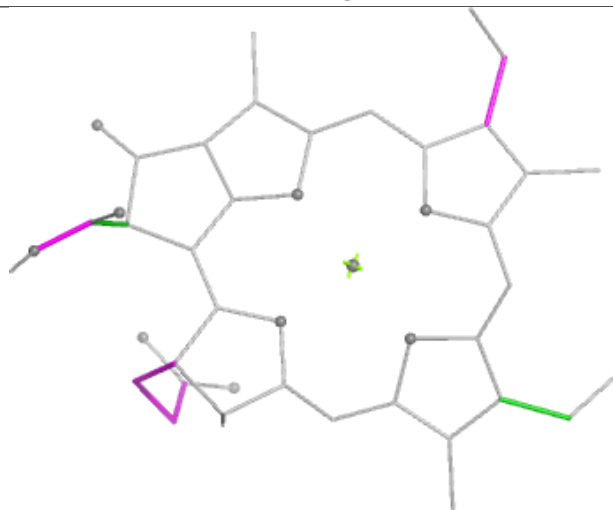
Ligand CLA r 614



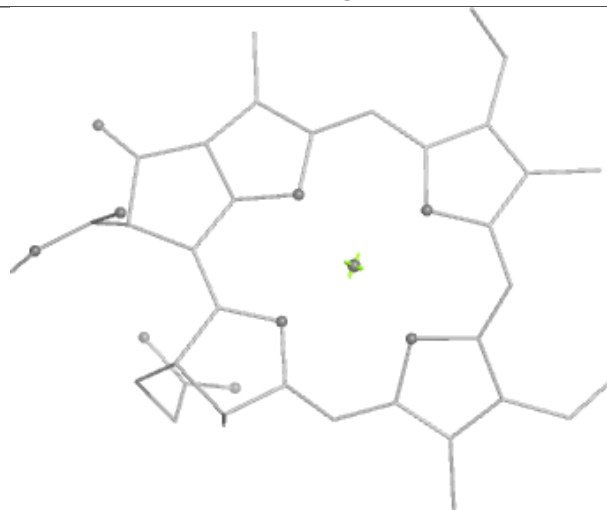
Bond lengths



Bond angles

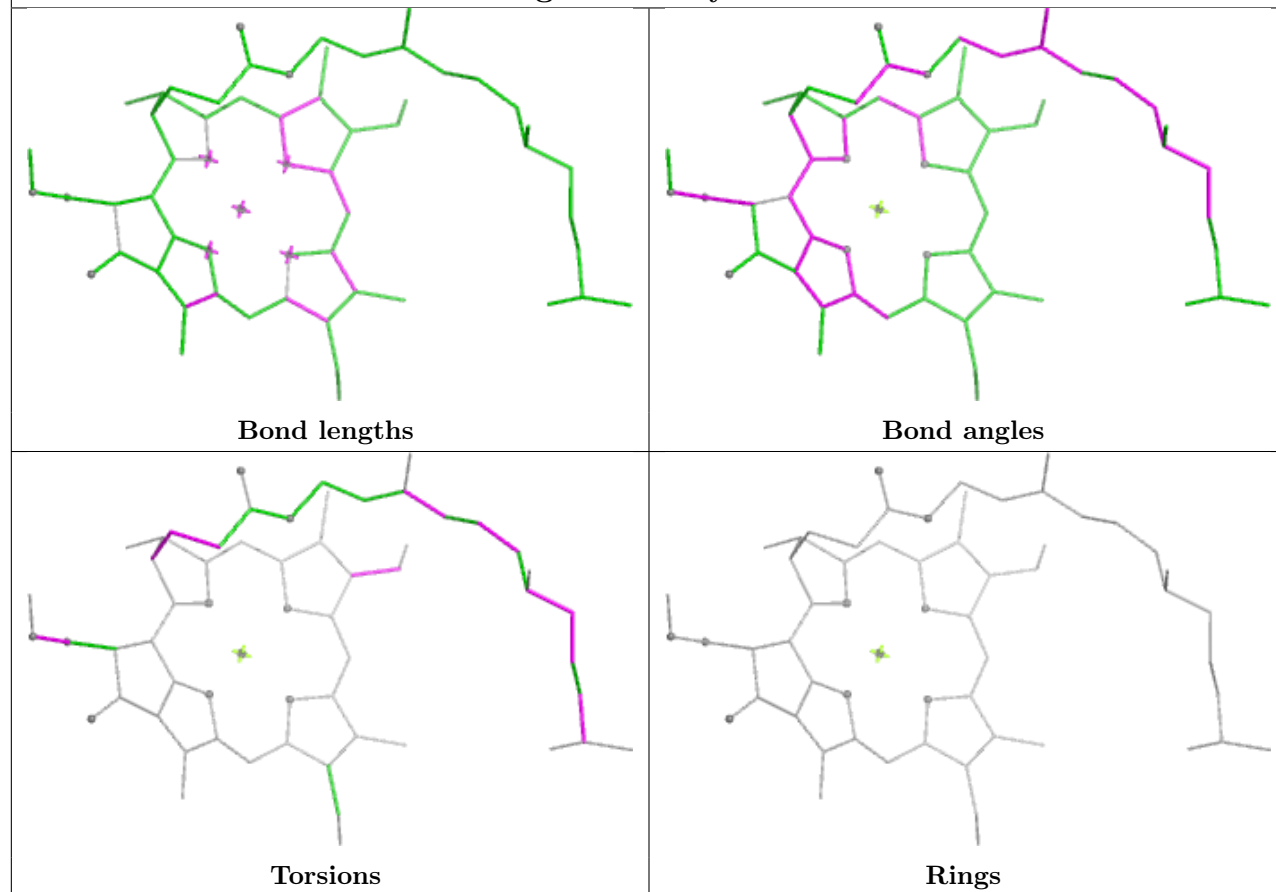


Torsions

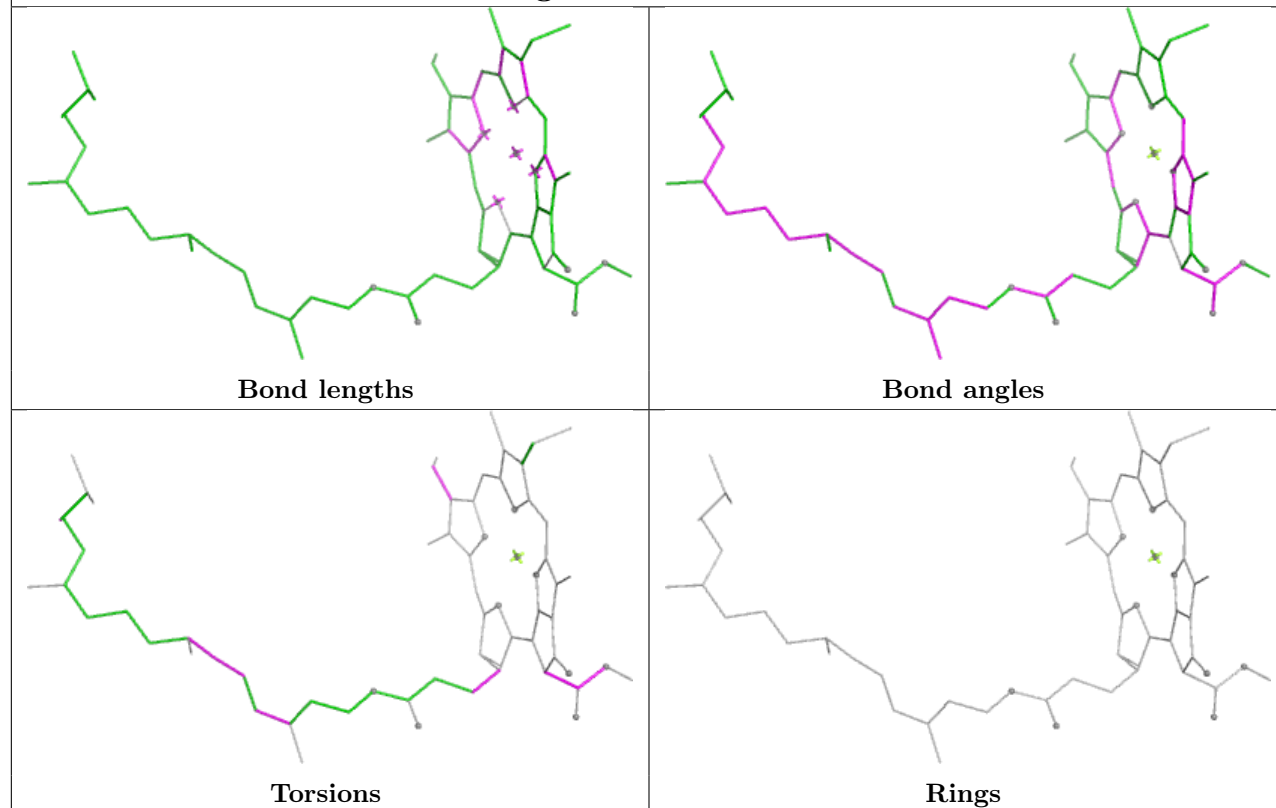


Rings

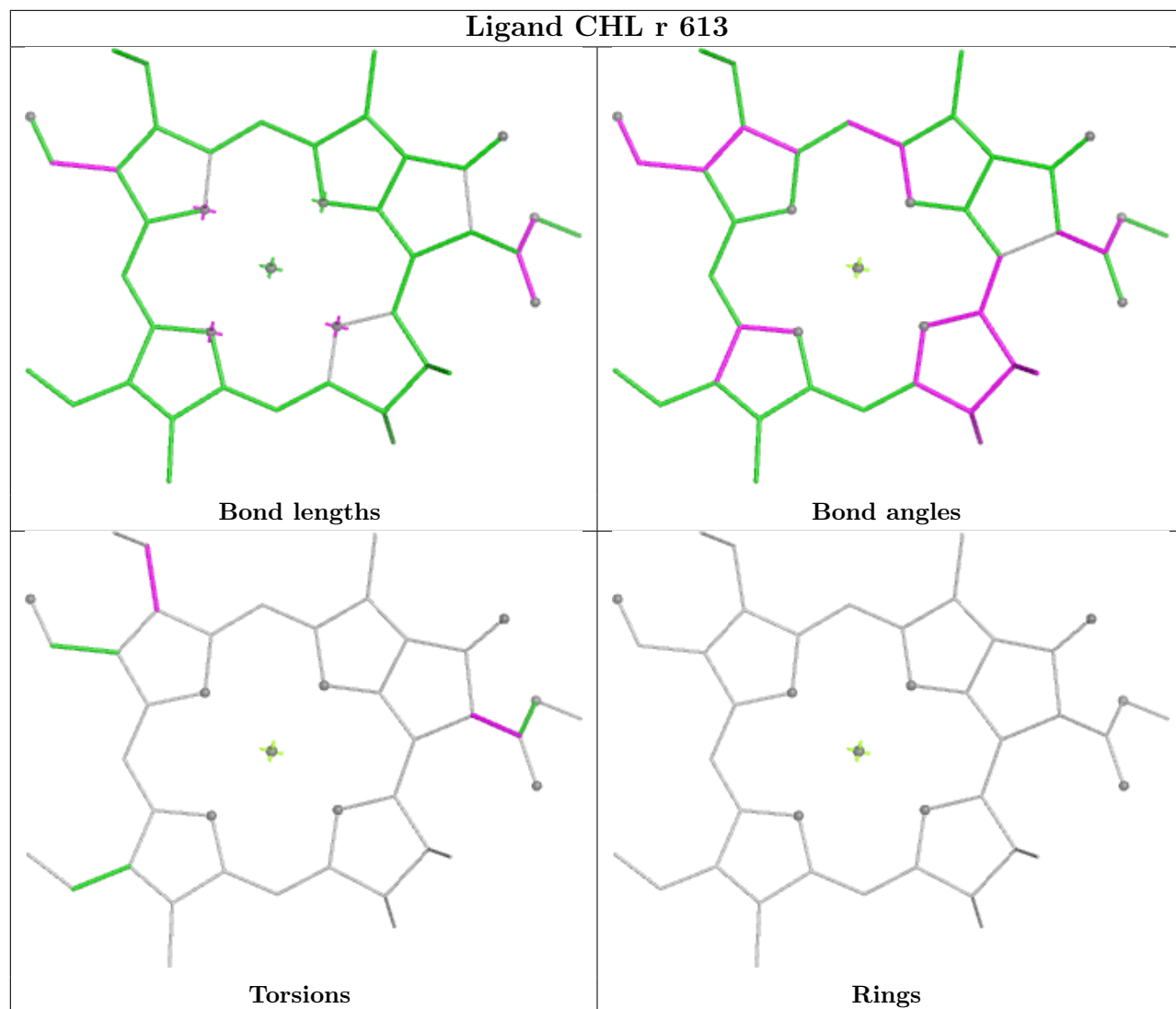
Ligand CLA y 311

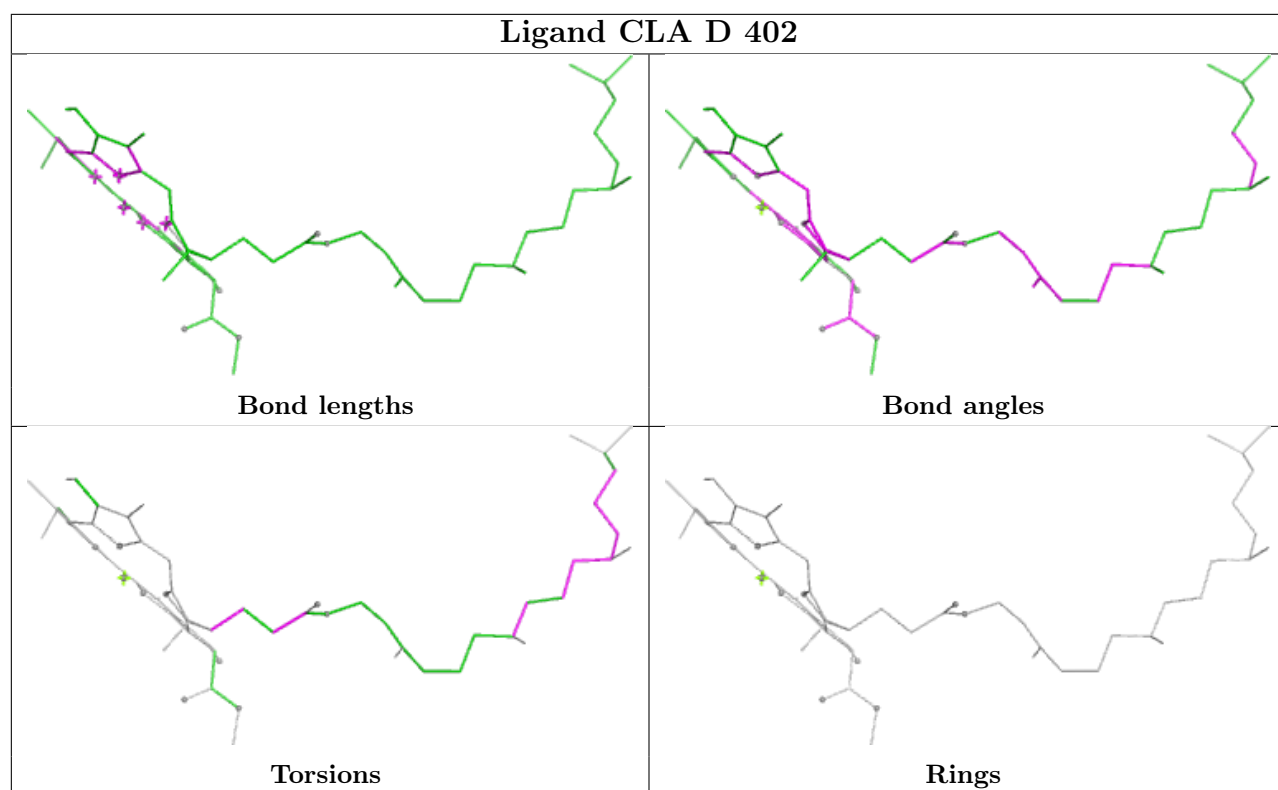


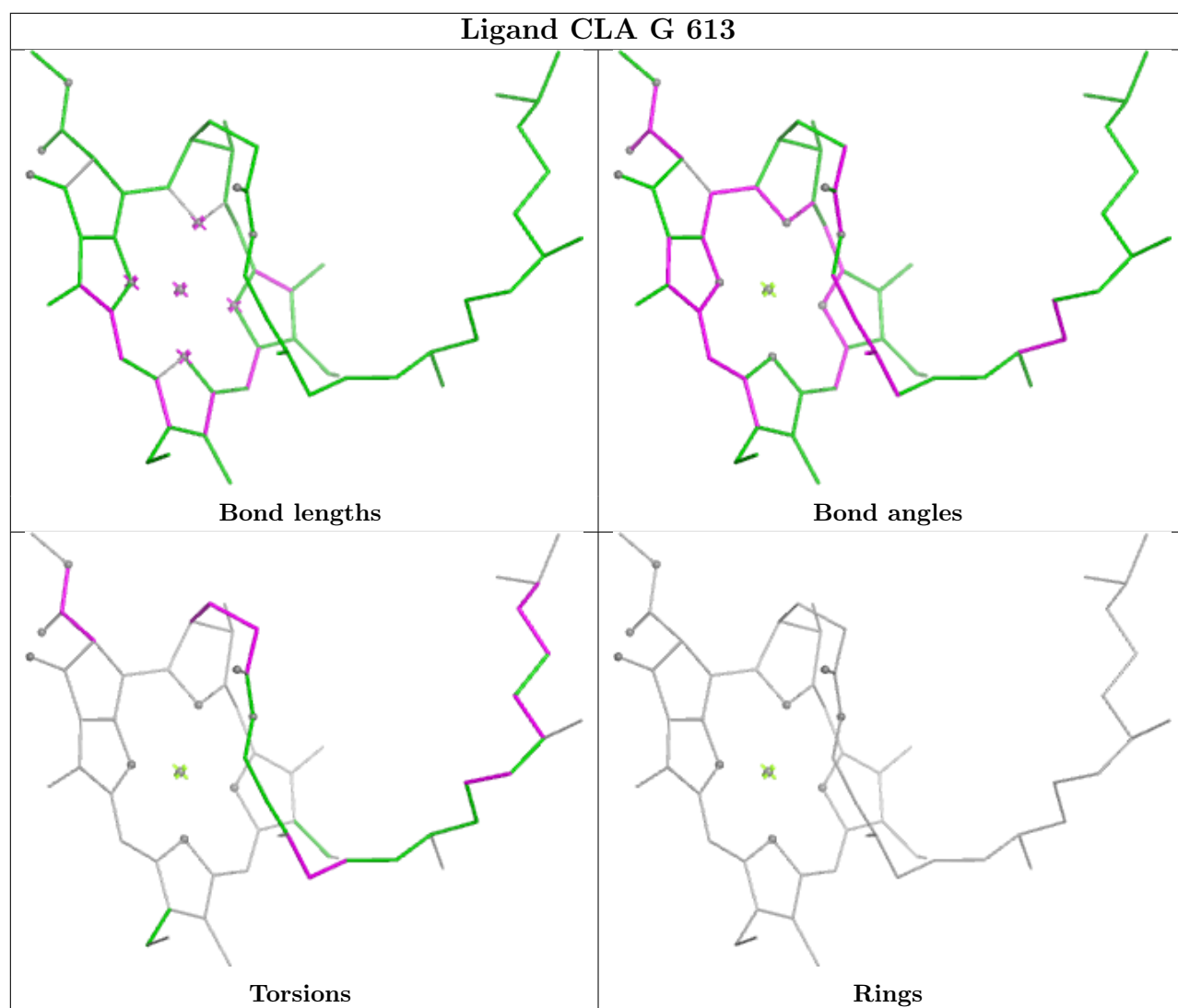
Ligand CLA b 609

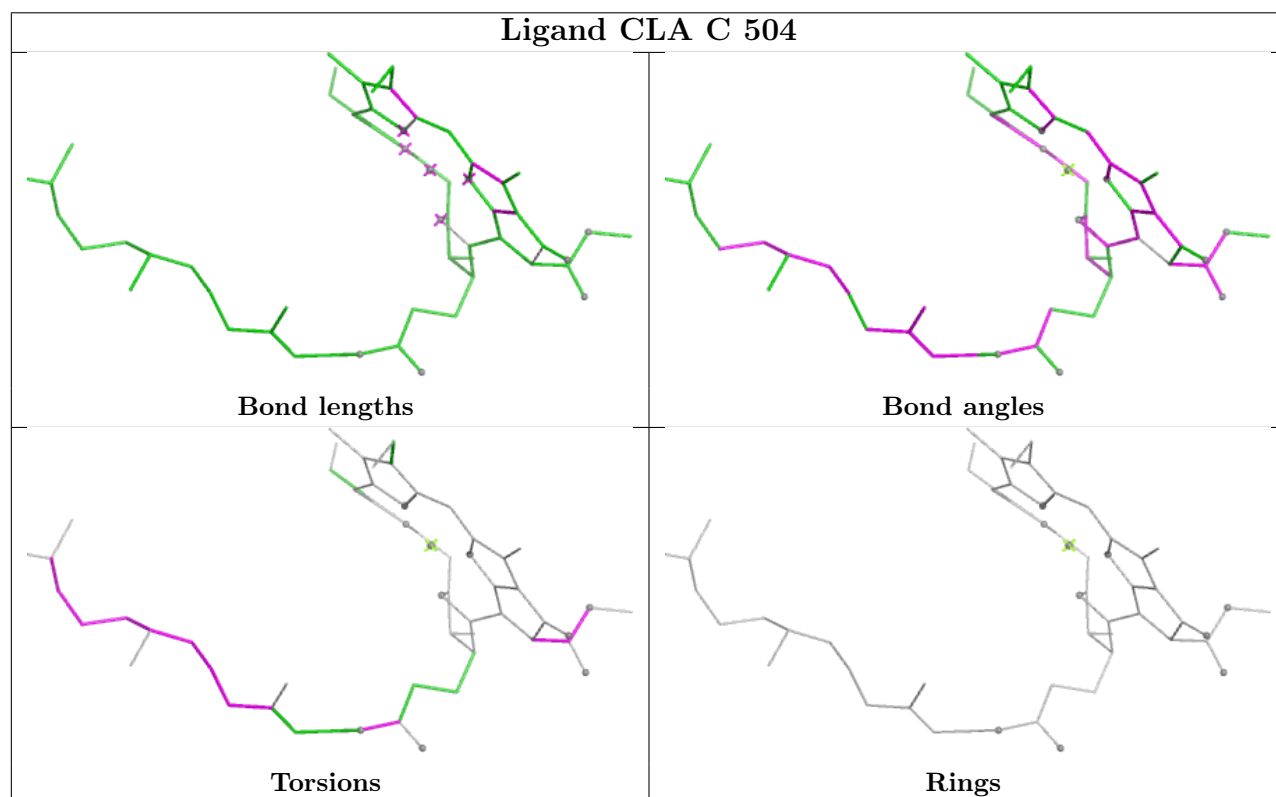
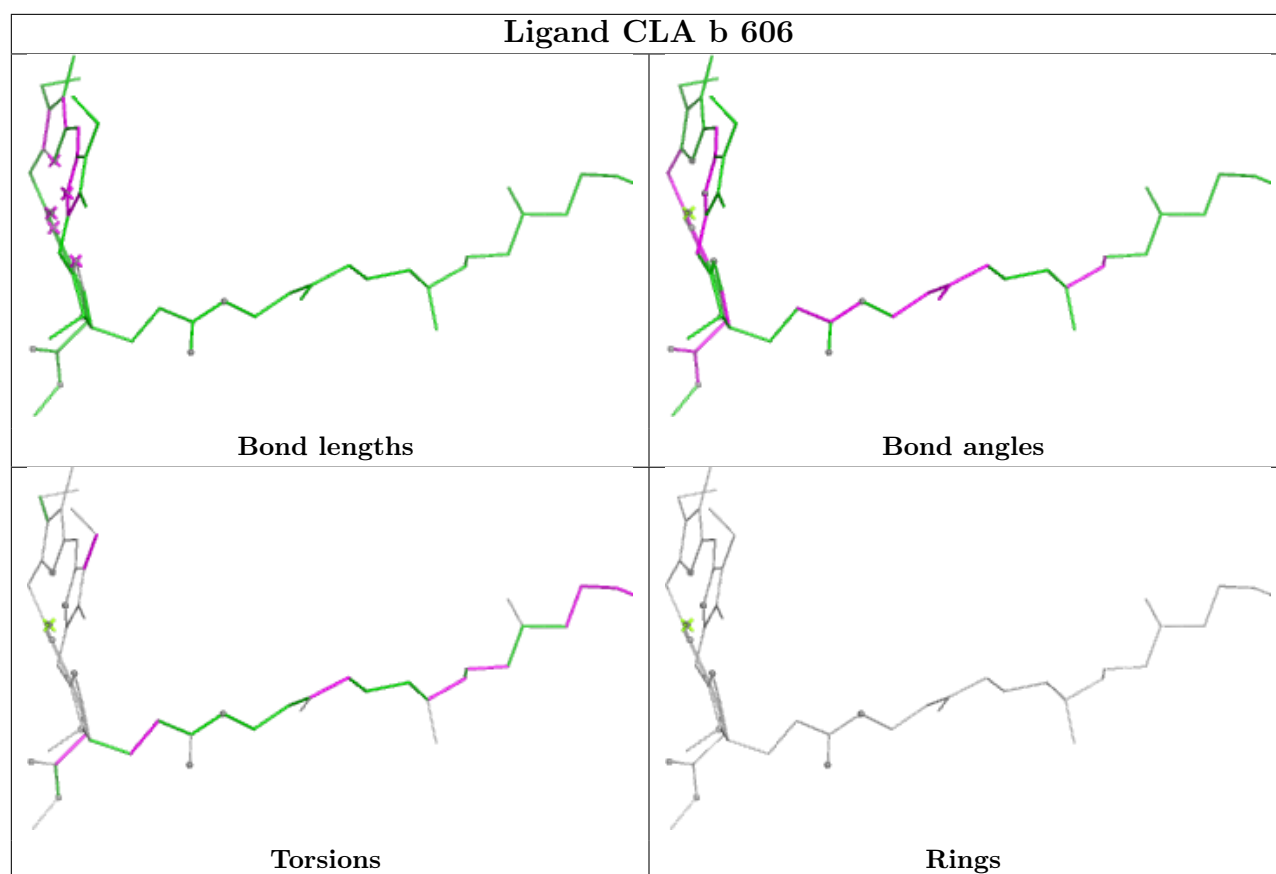


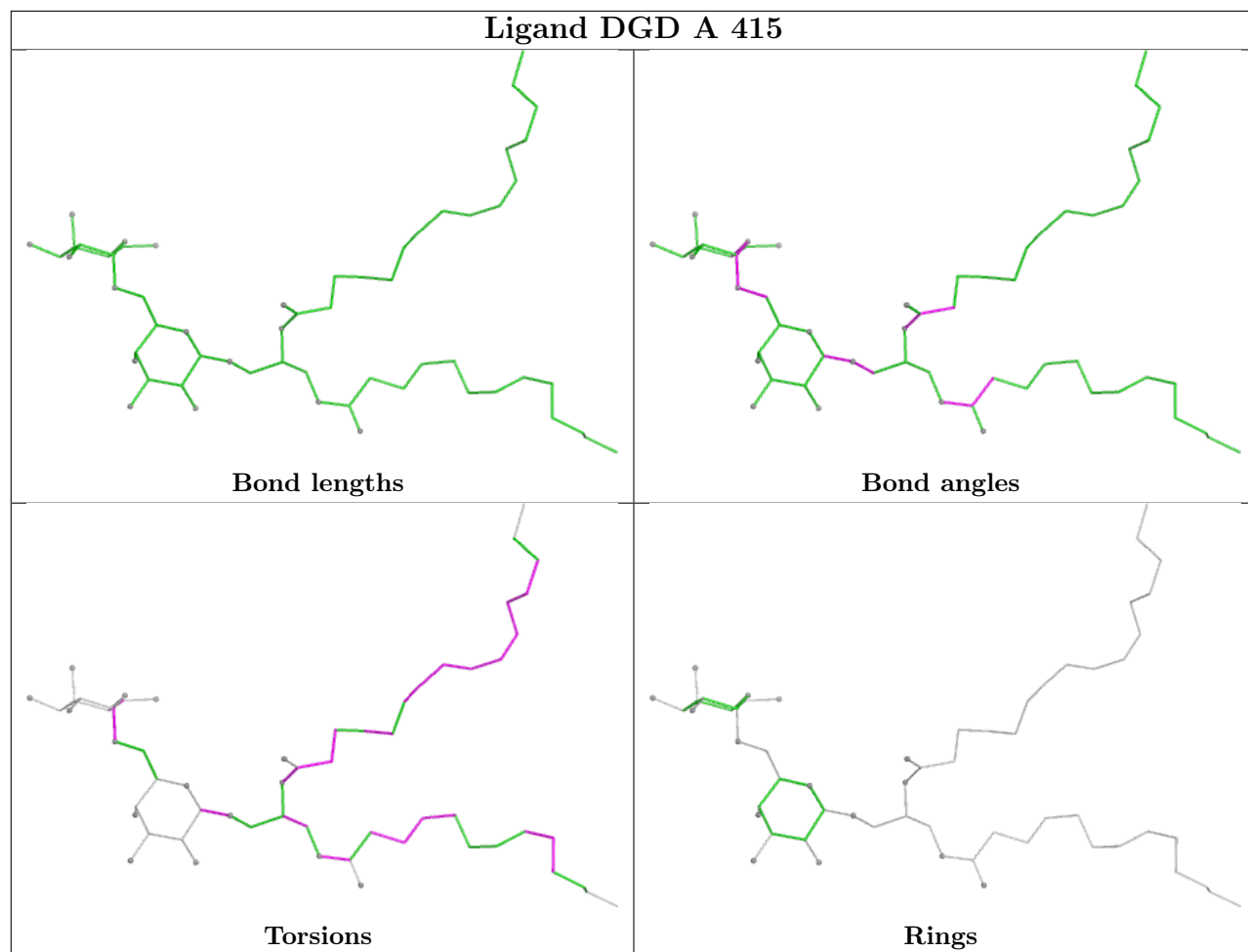
Ligand CHL r 613



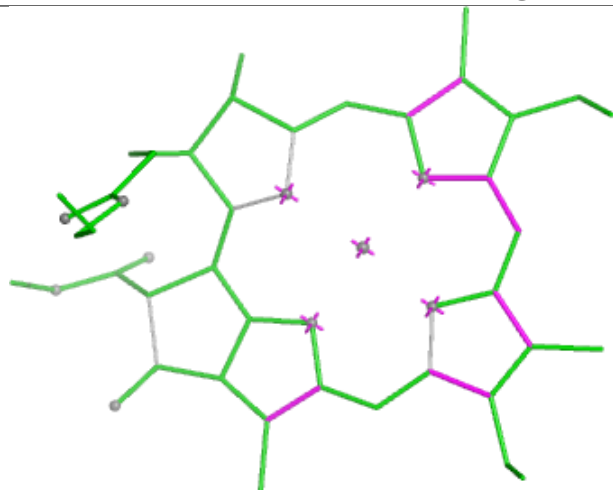




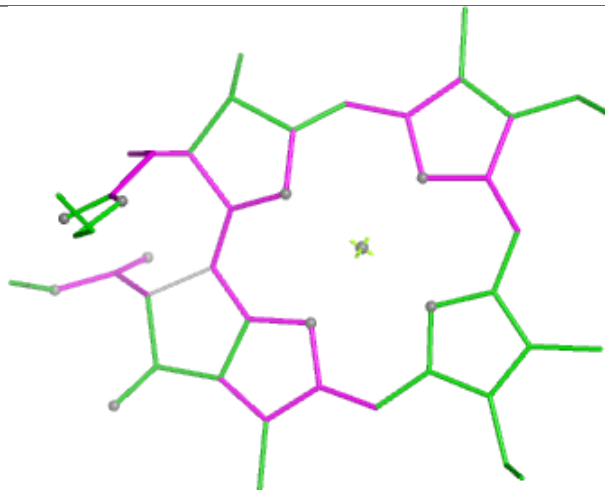




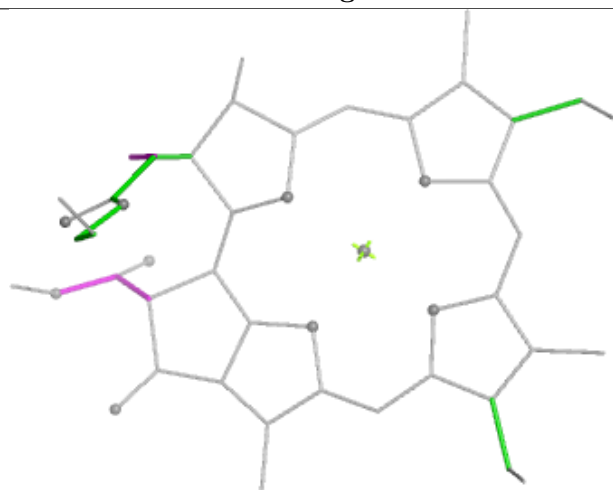
Ligand CLA N 614



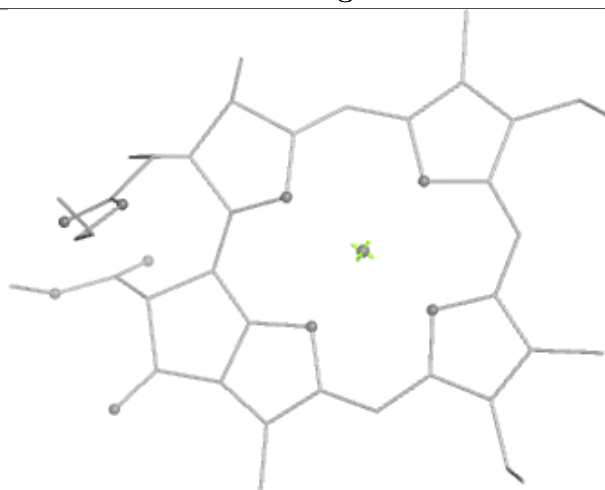
Bond lengths



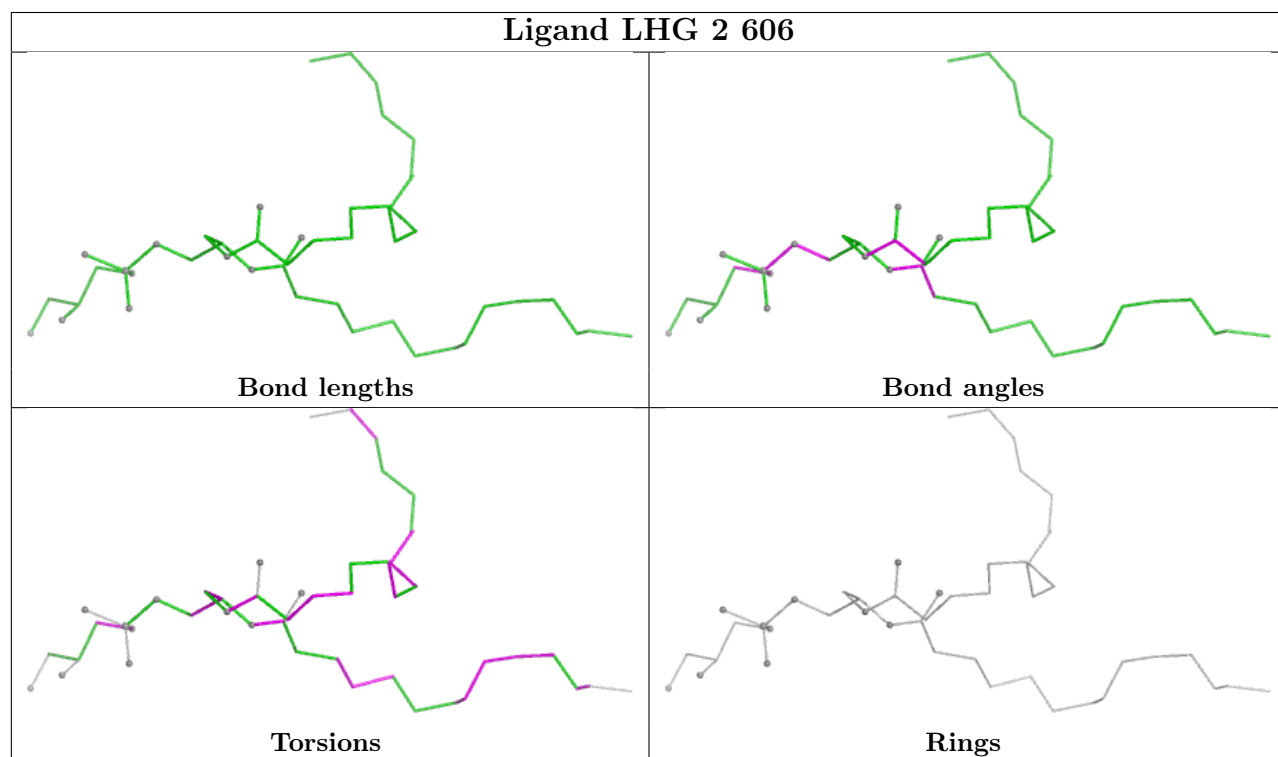
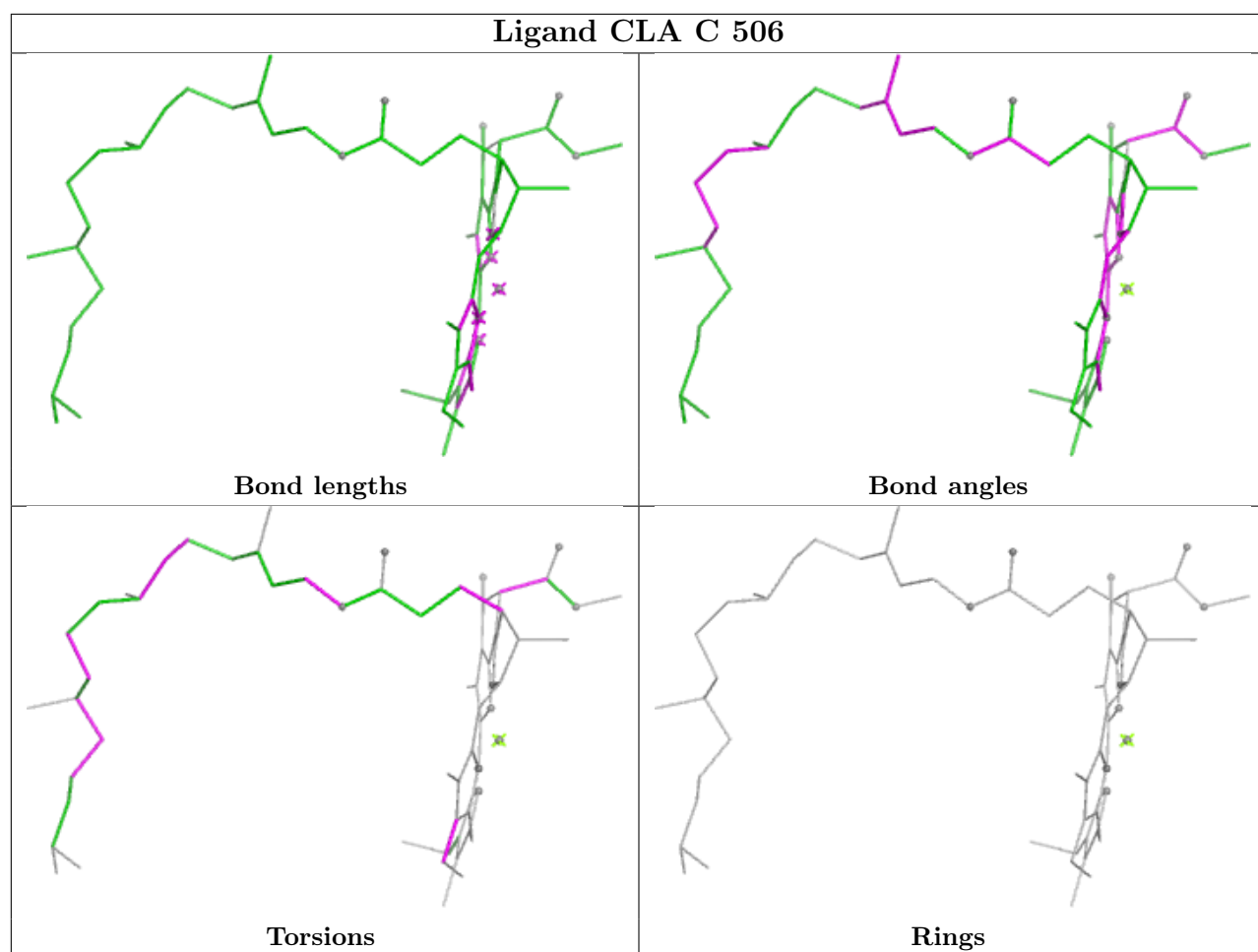
Bond angles



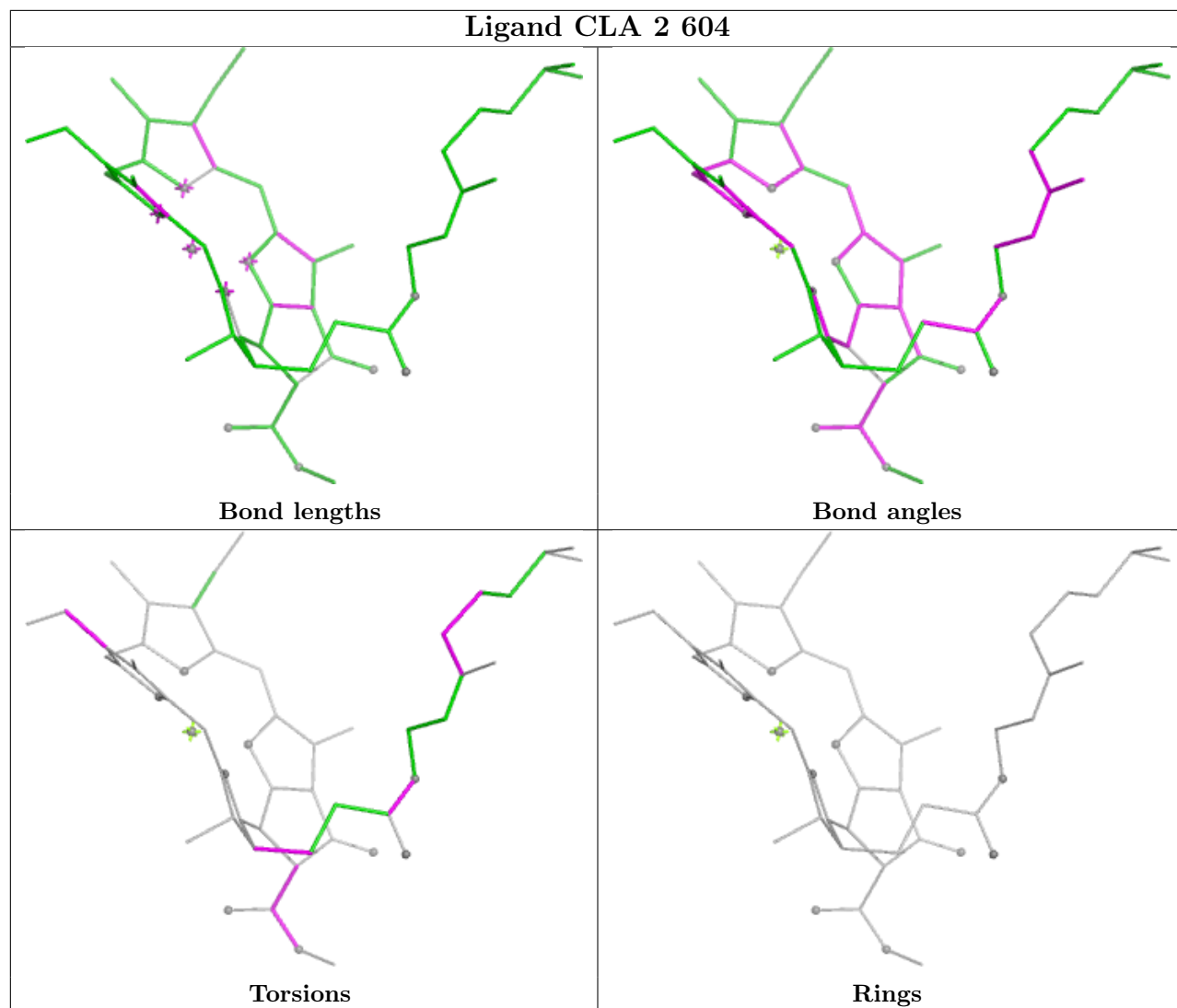
Torsions



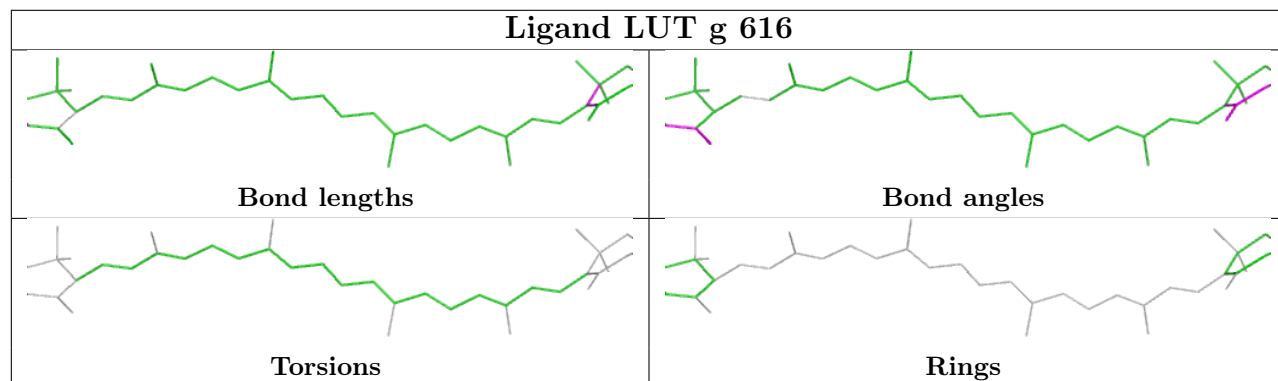
Rings

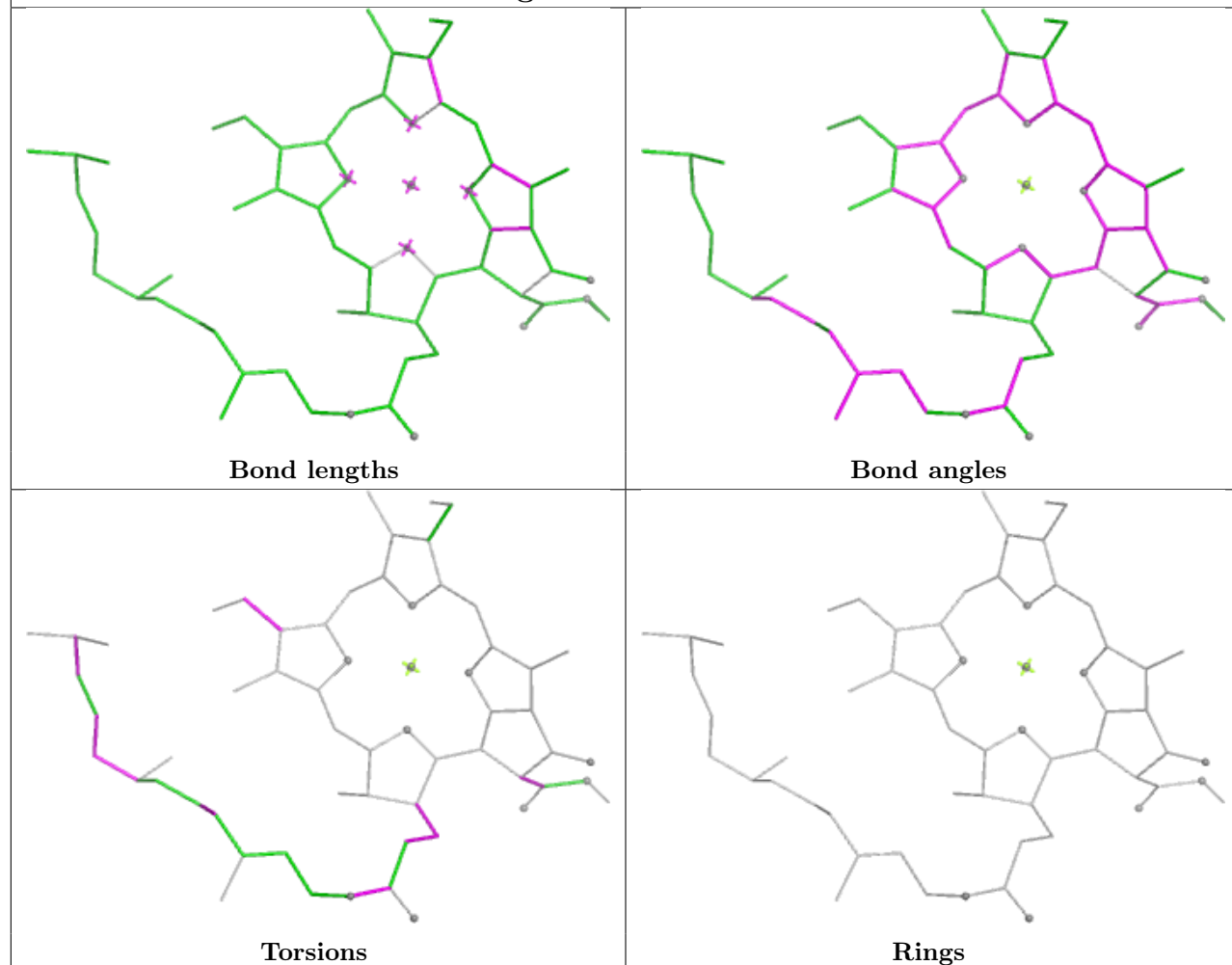
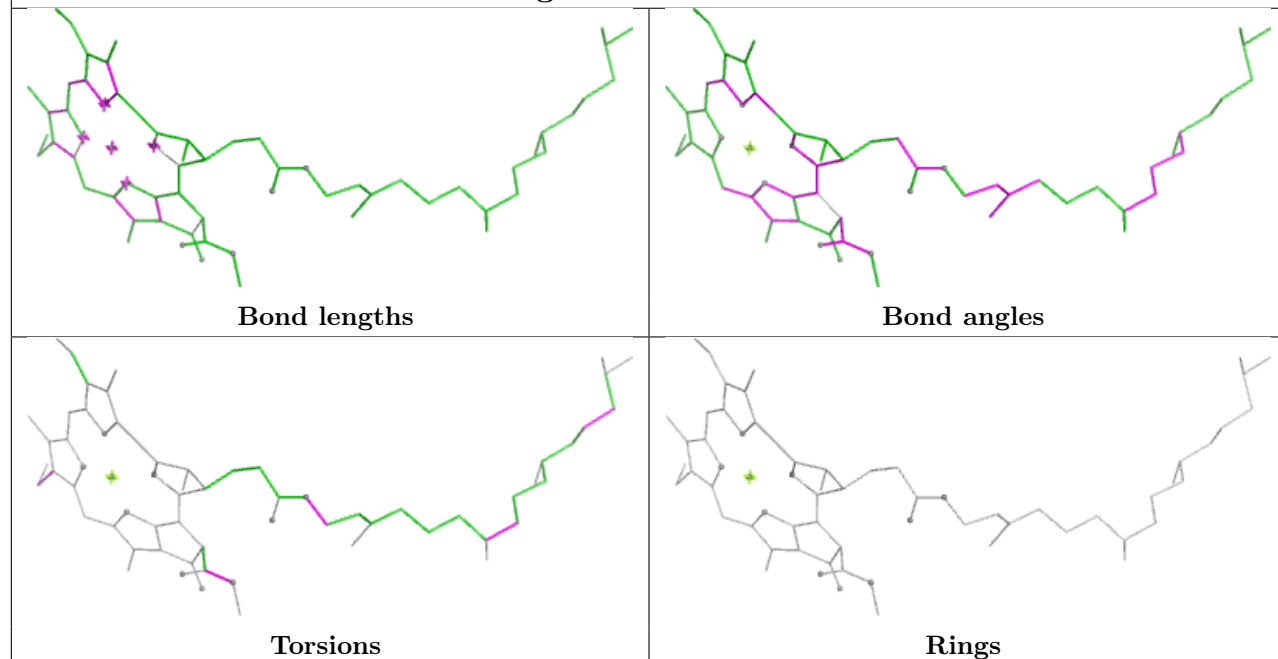


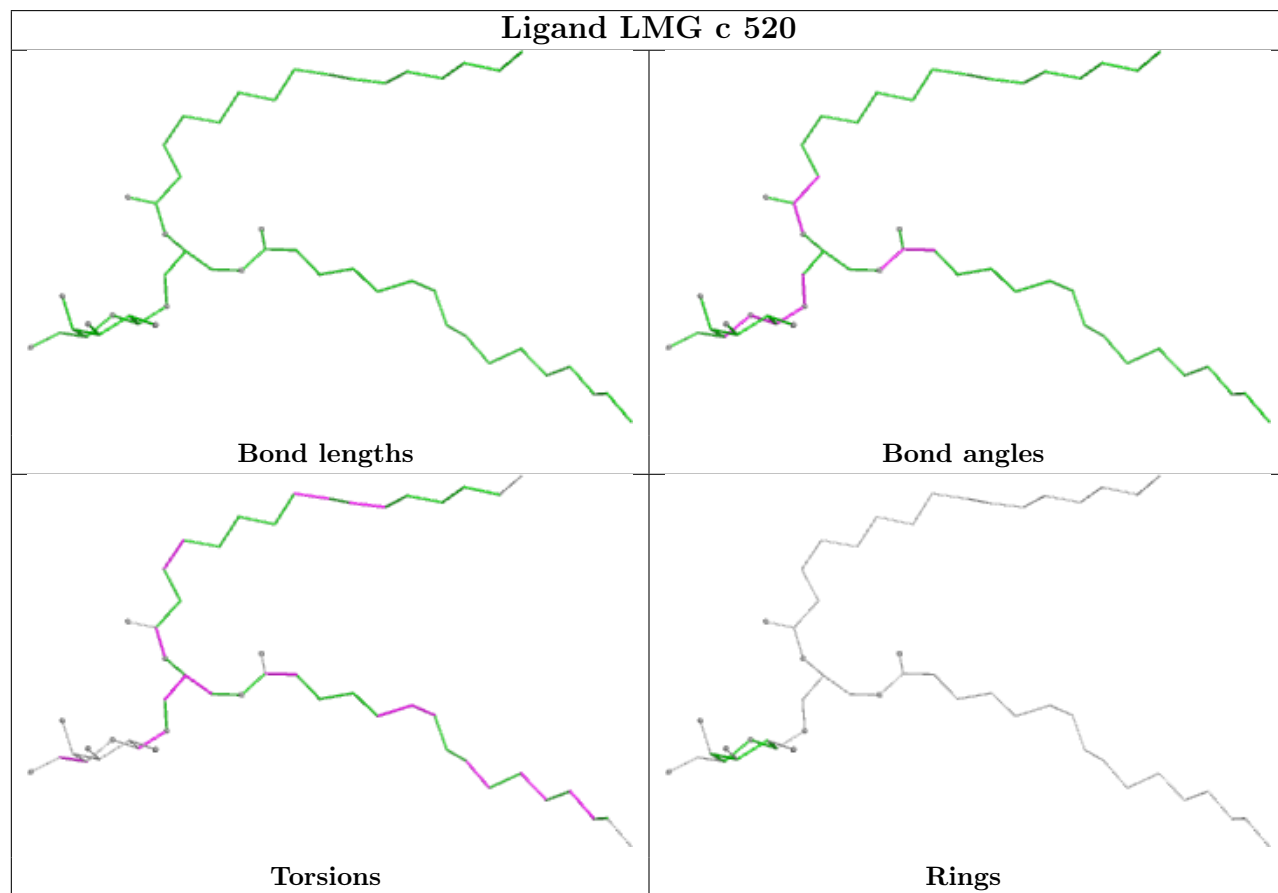
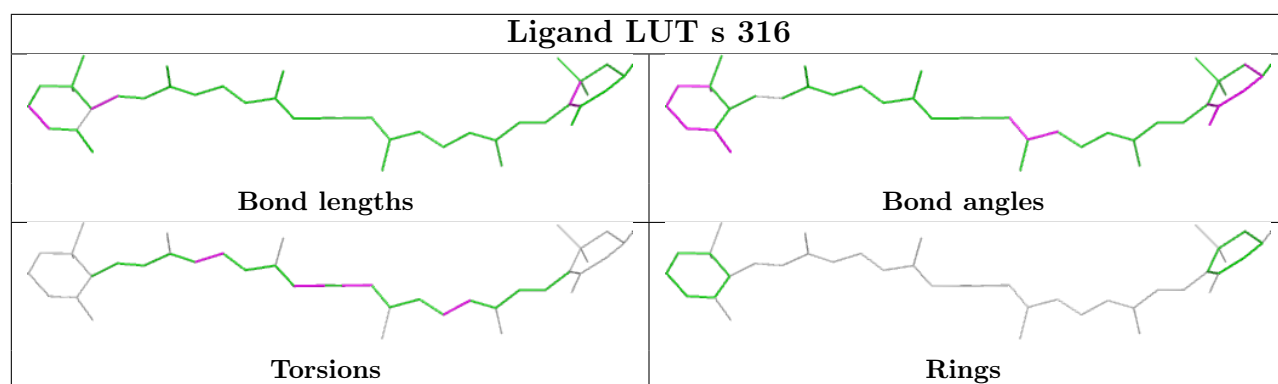
Ligand CLA 2 604

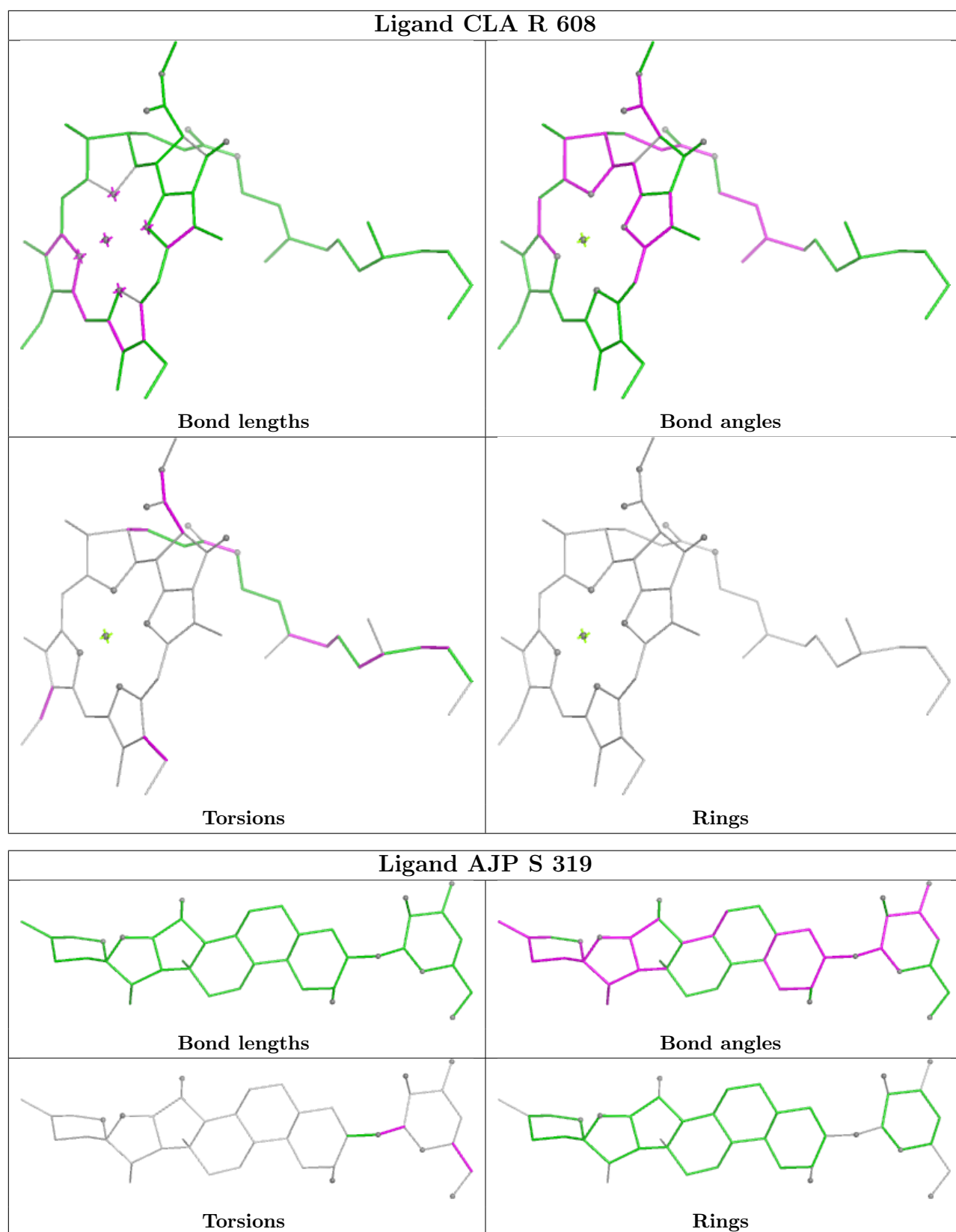


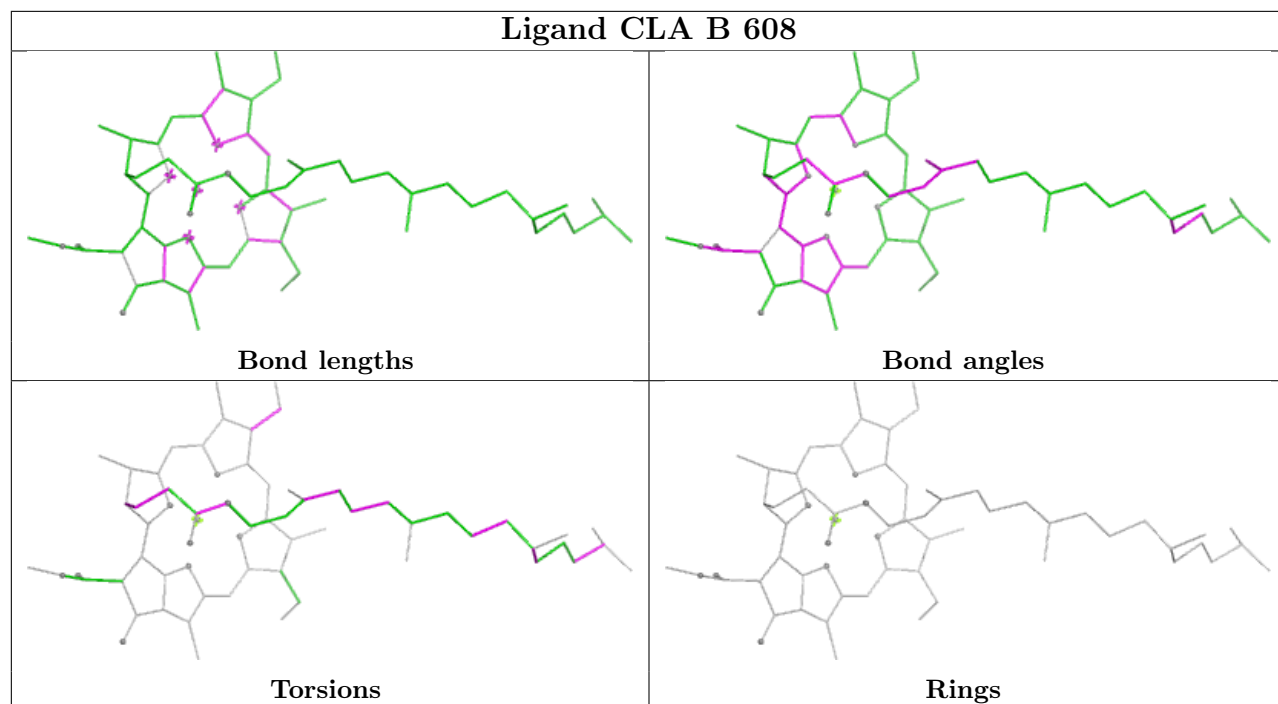
Ligand LUT g 616



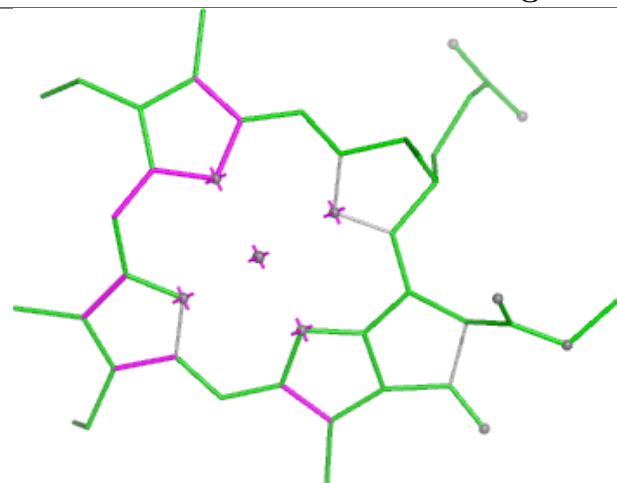
Ligand CLA 6 602**Ligand CLA a 402**



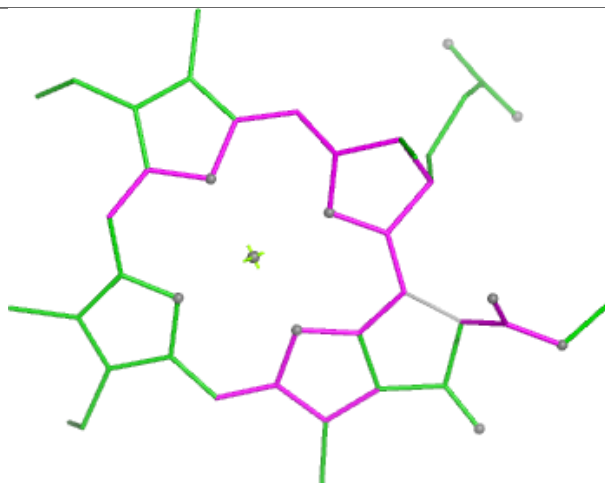




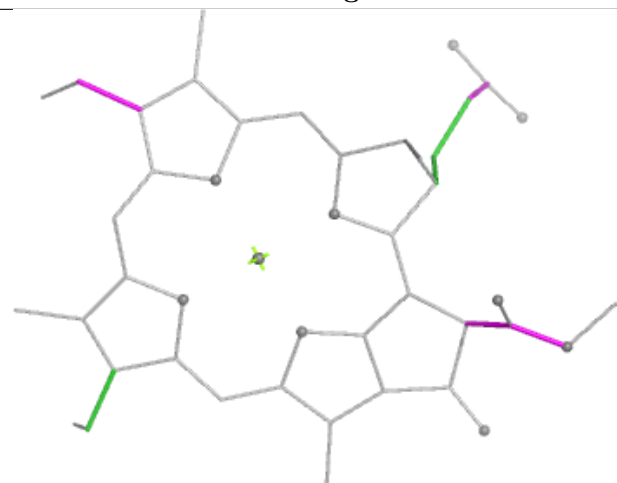
Ligand CLA S 309



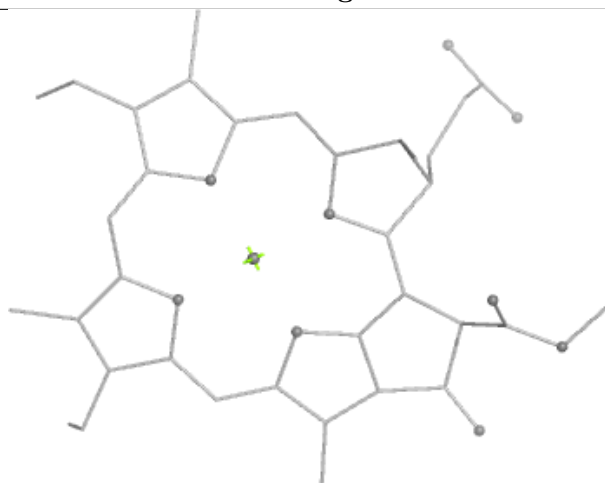
Bond lengths



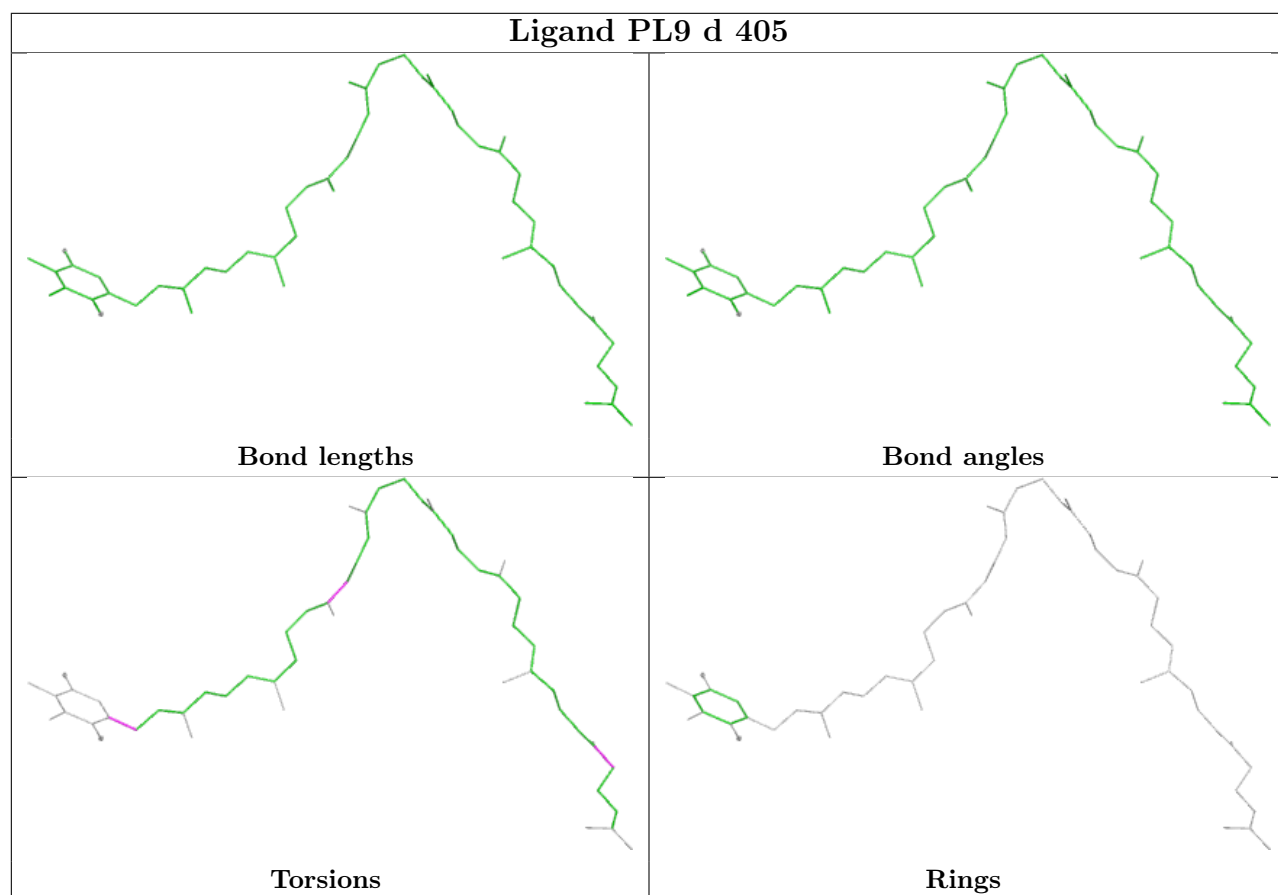
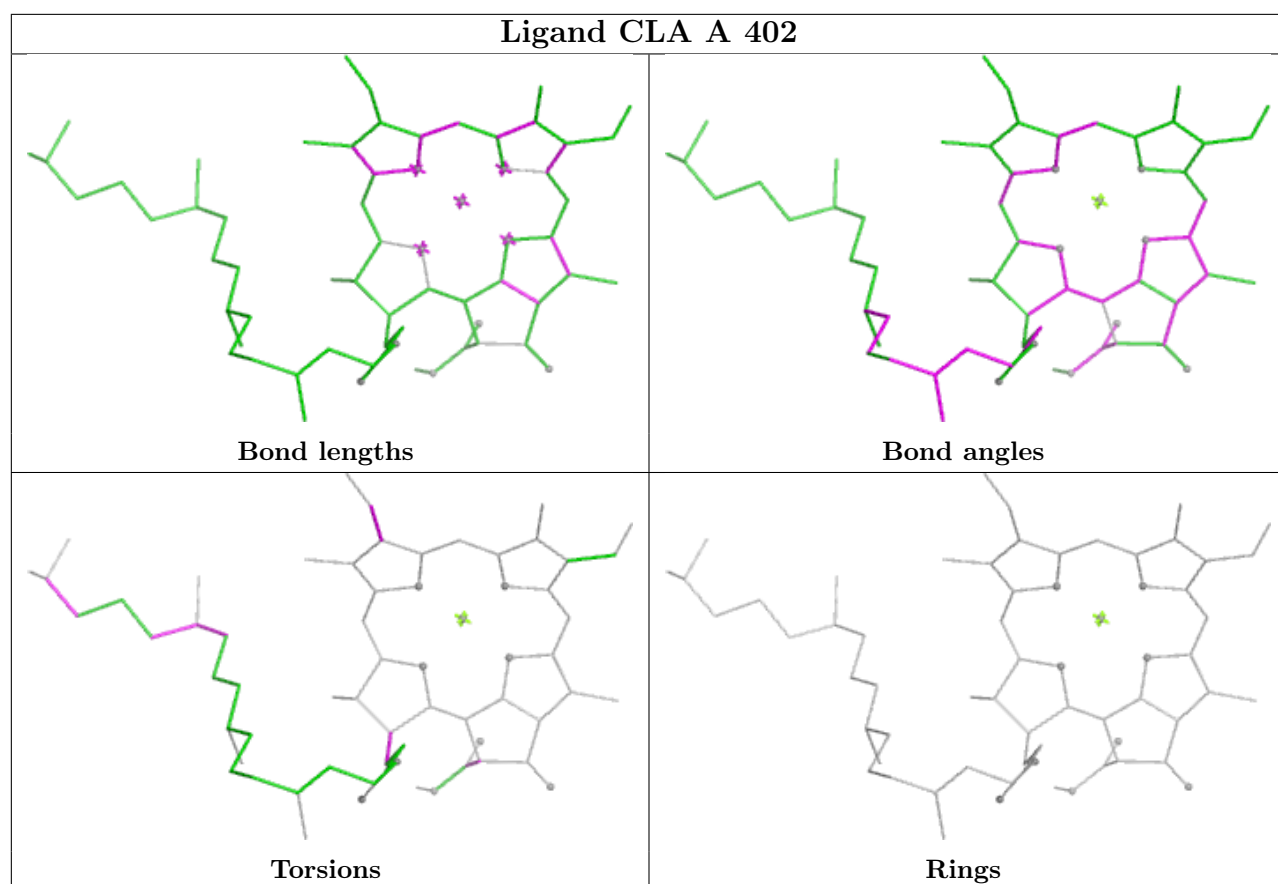
Bond angles

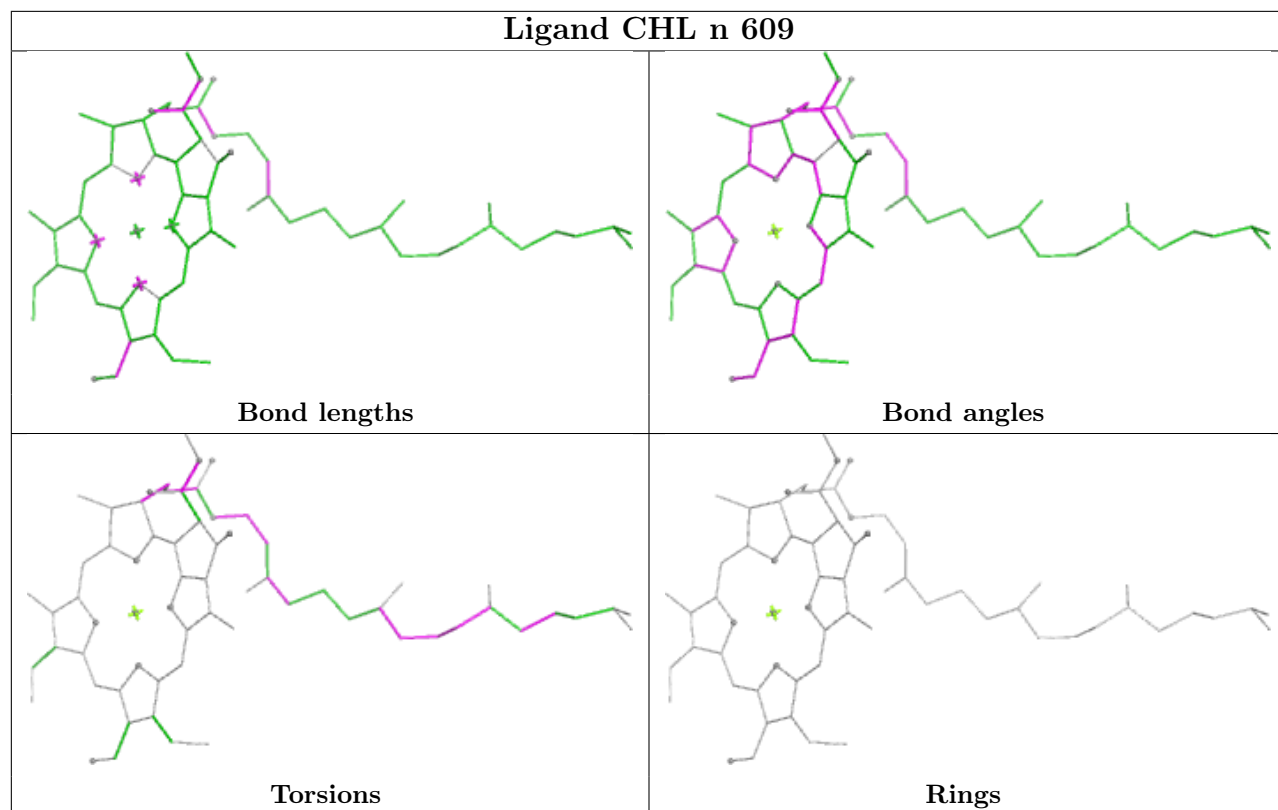


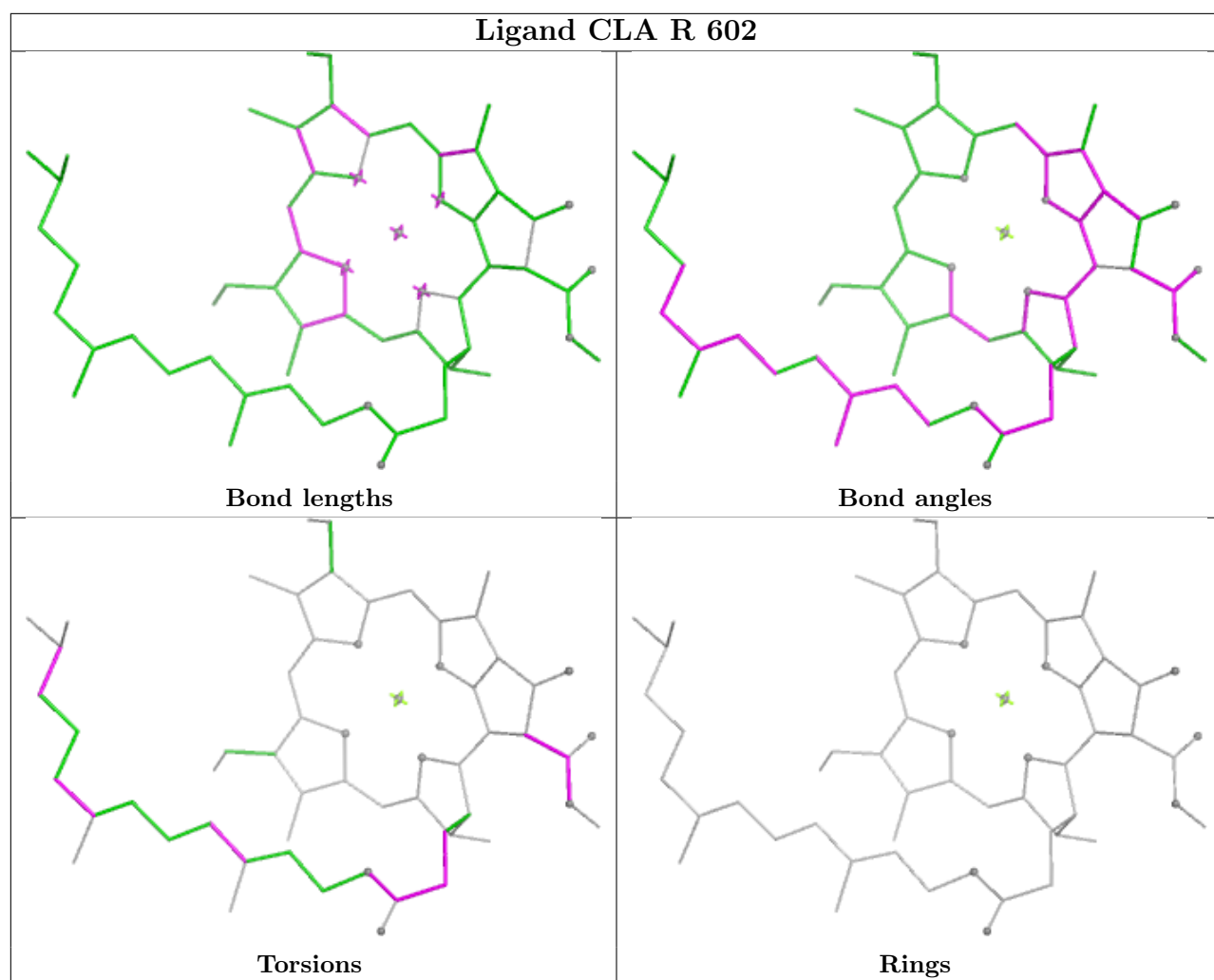
Torsions

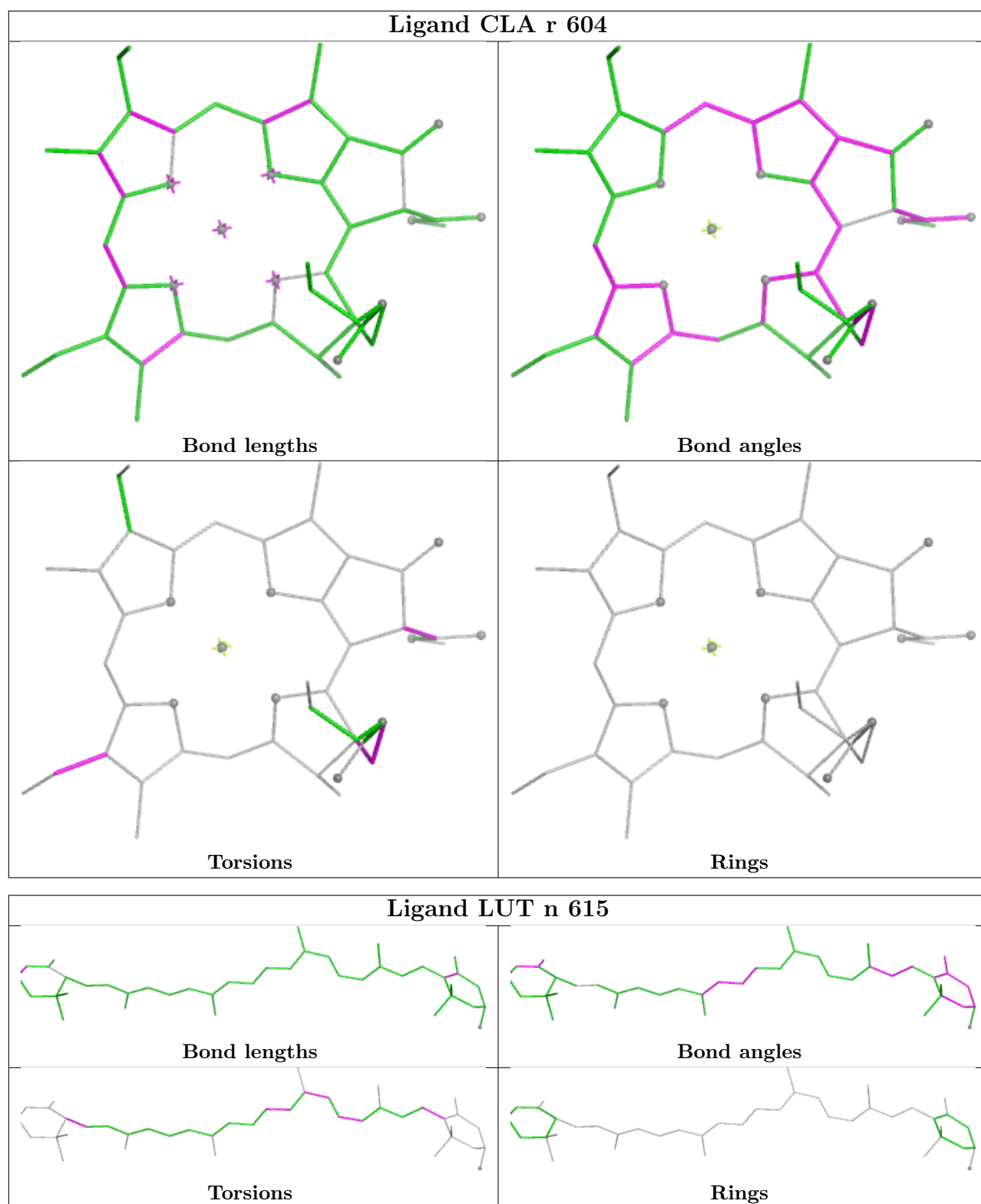


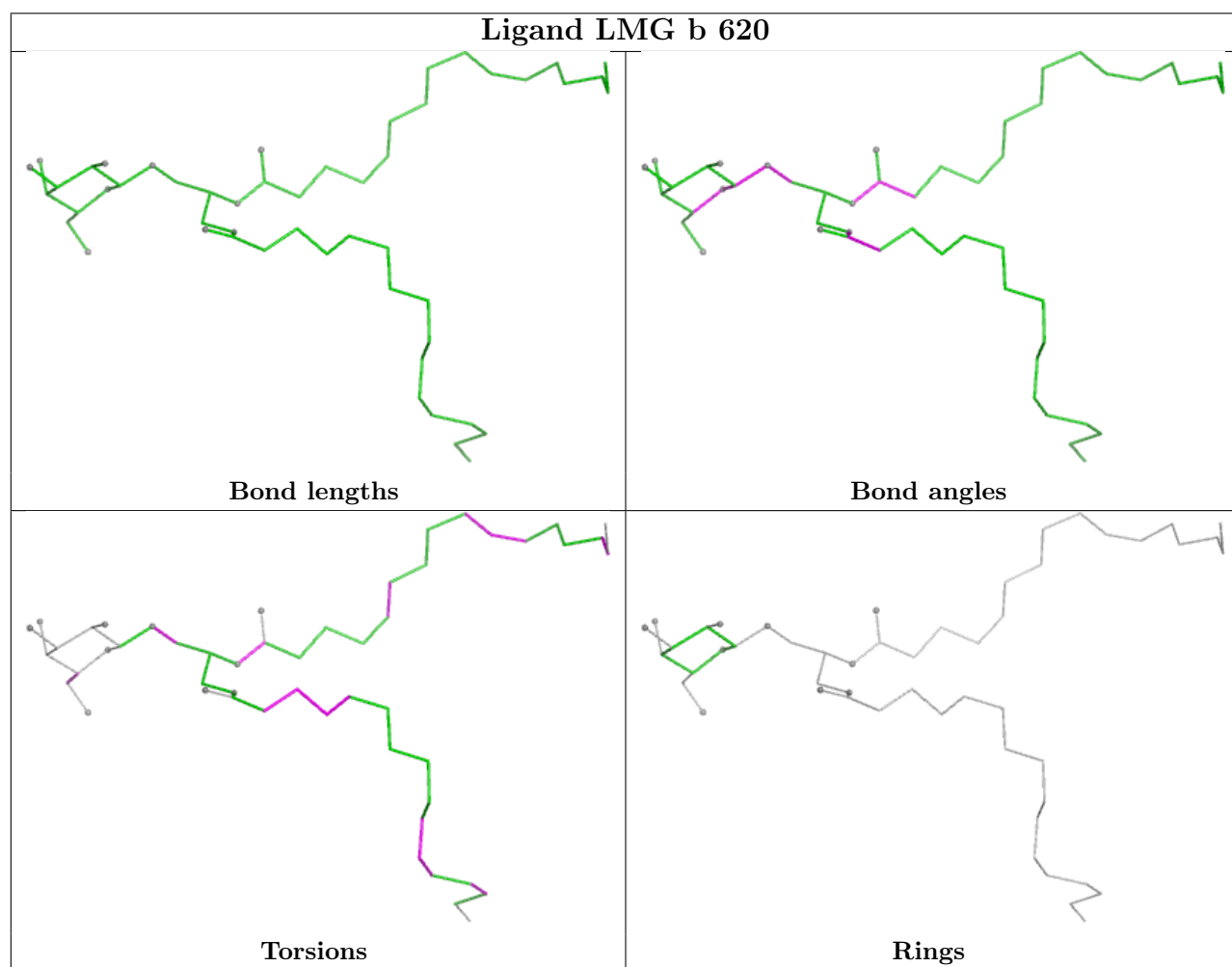
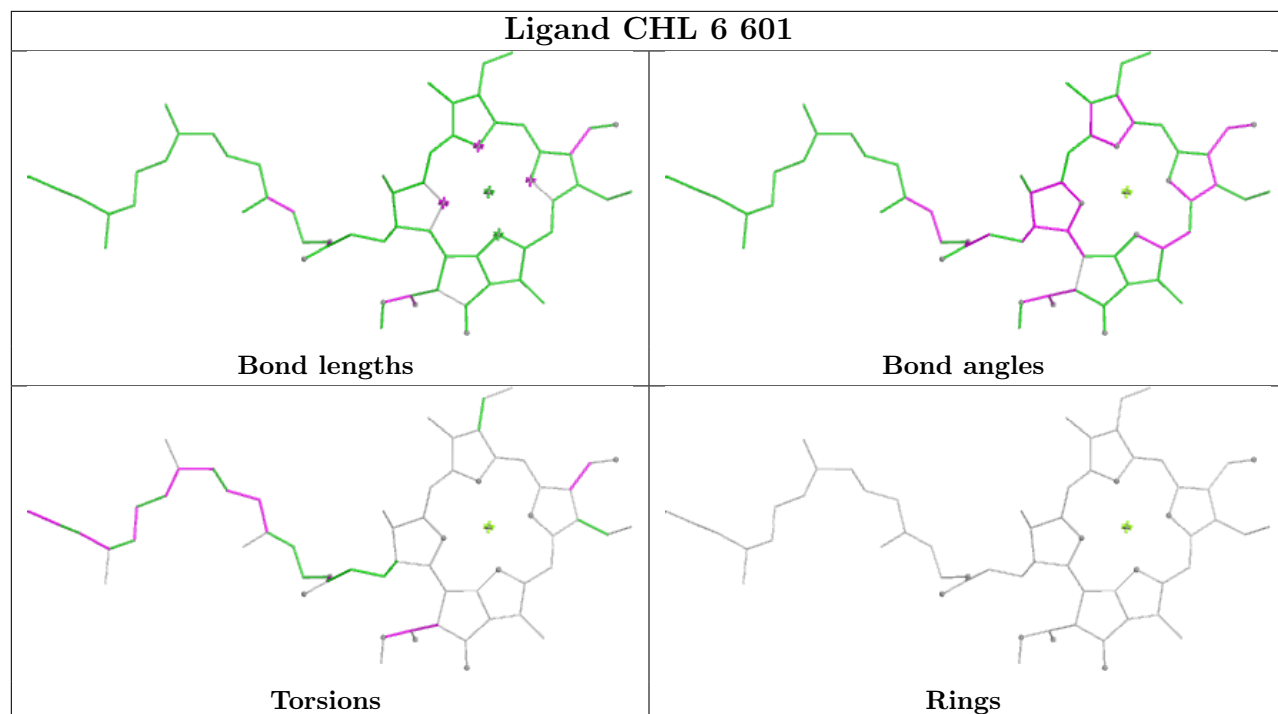
Rings

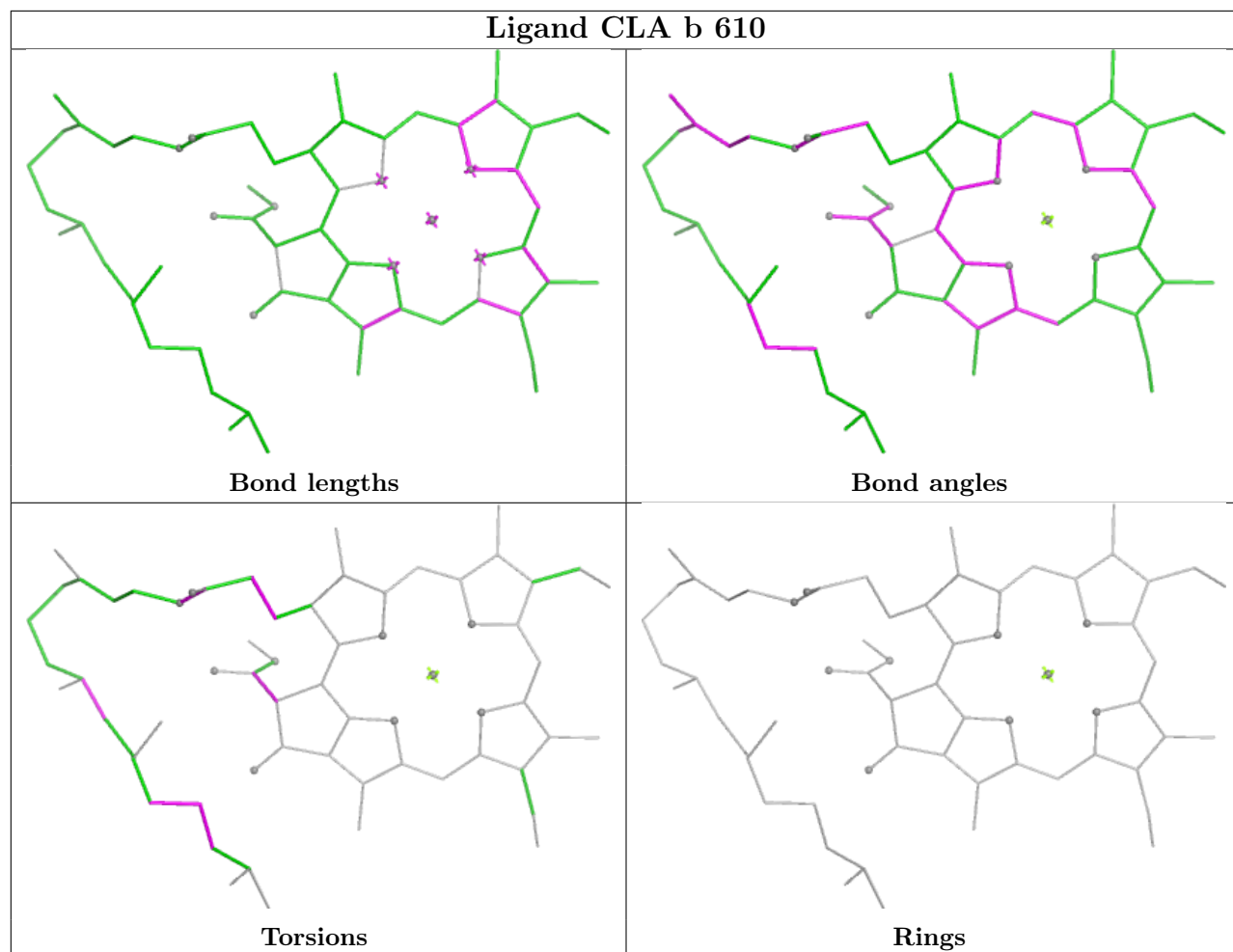


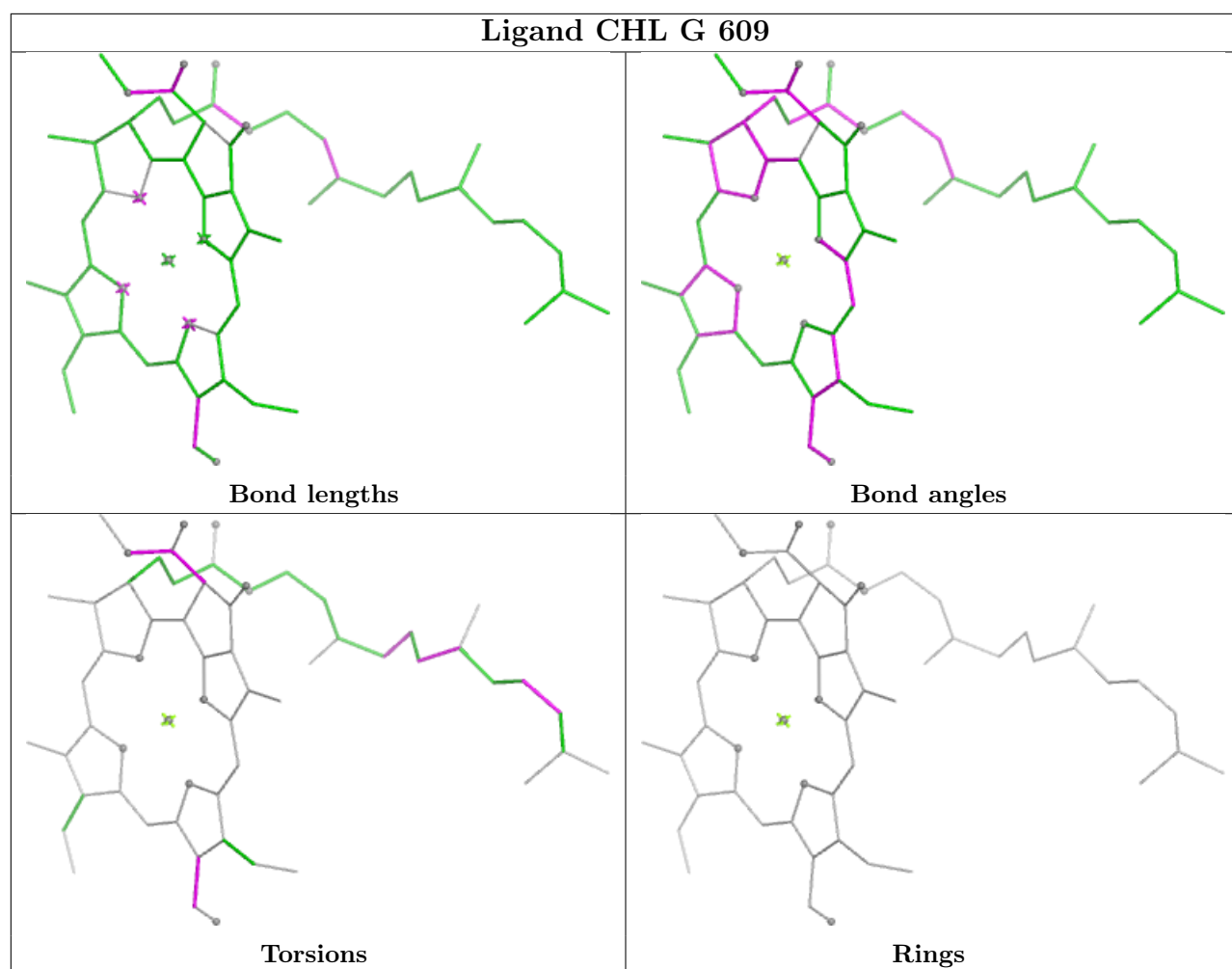




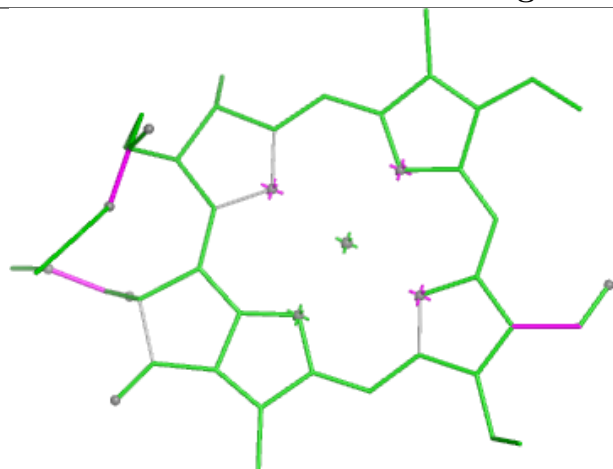




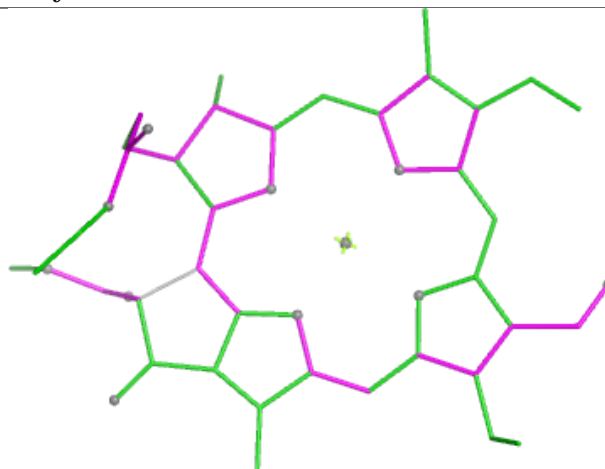




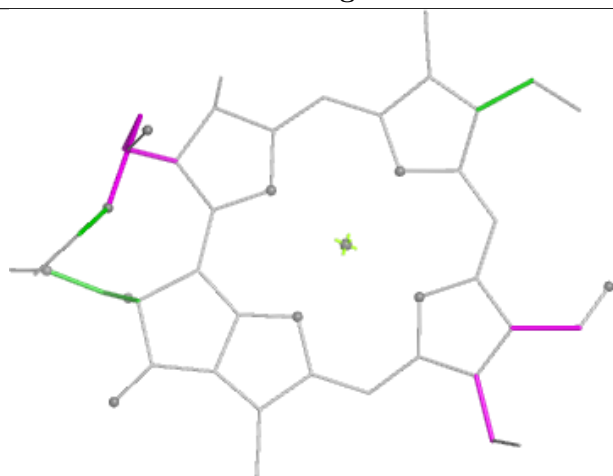
Ligand CHL y 306



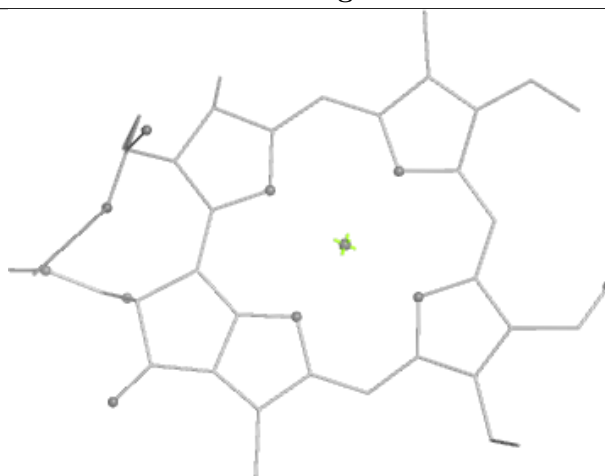
Bond lengths



Bond angles

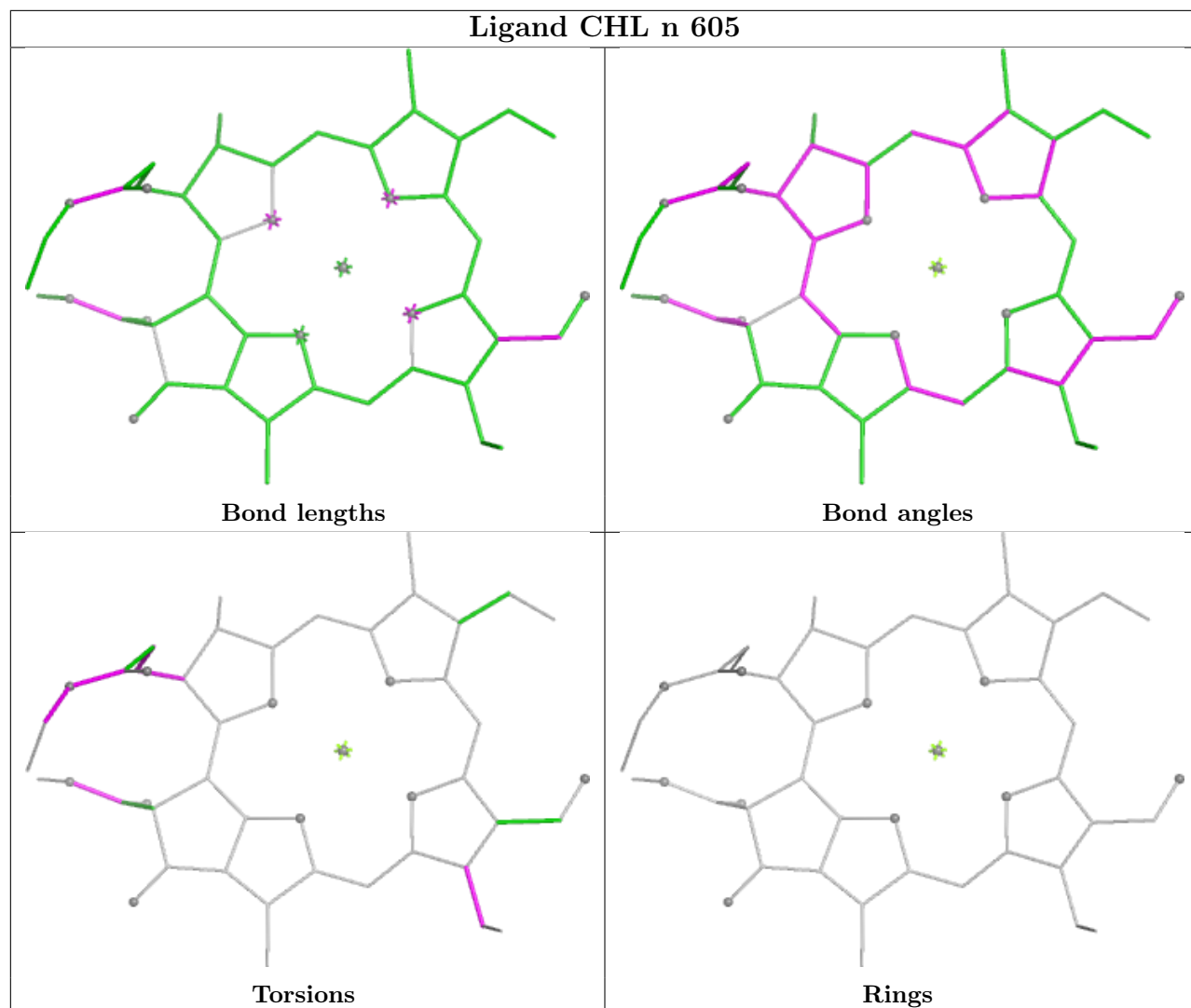


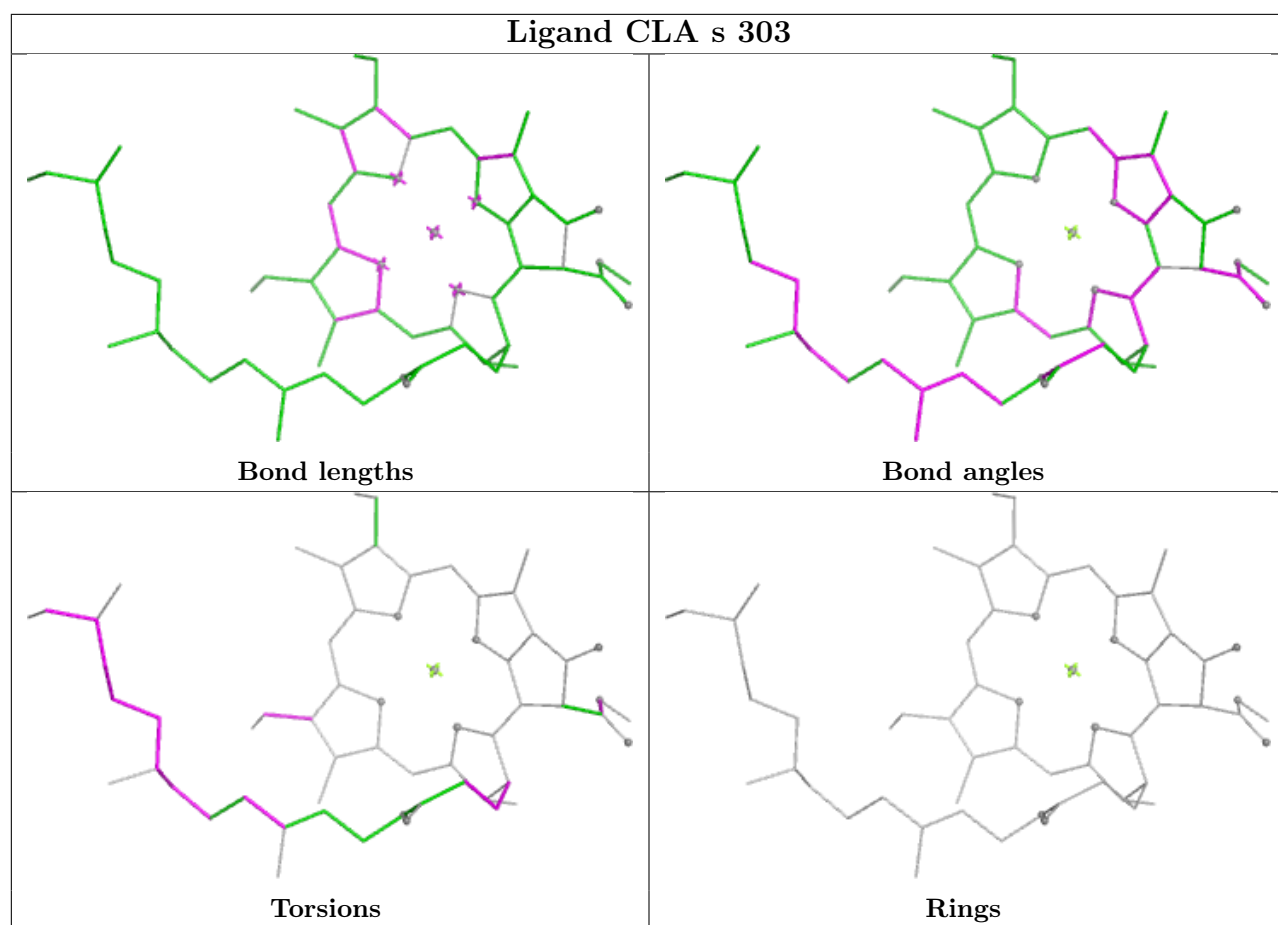
Torsions

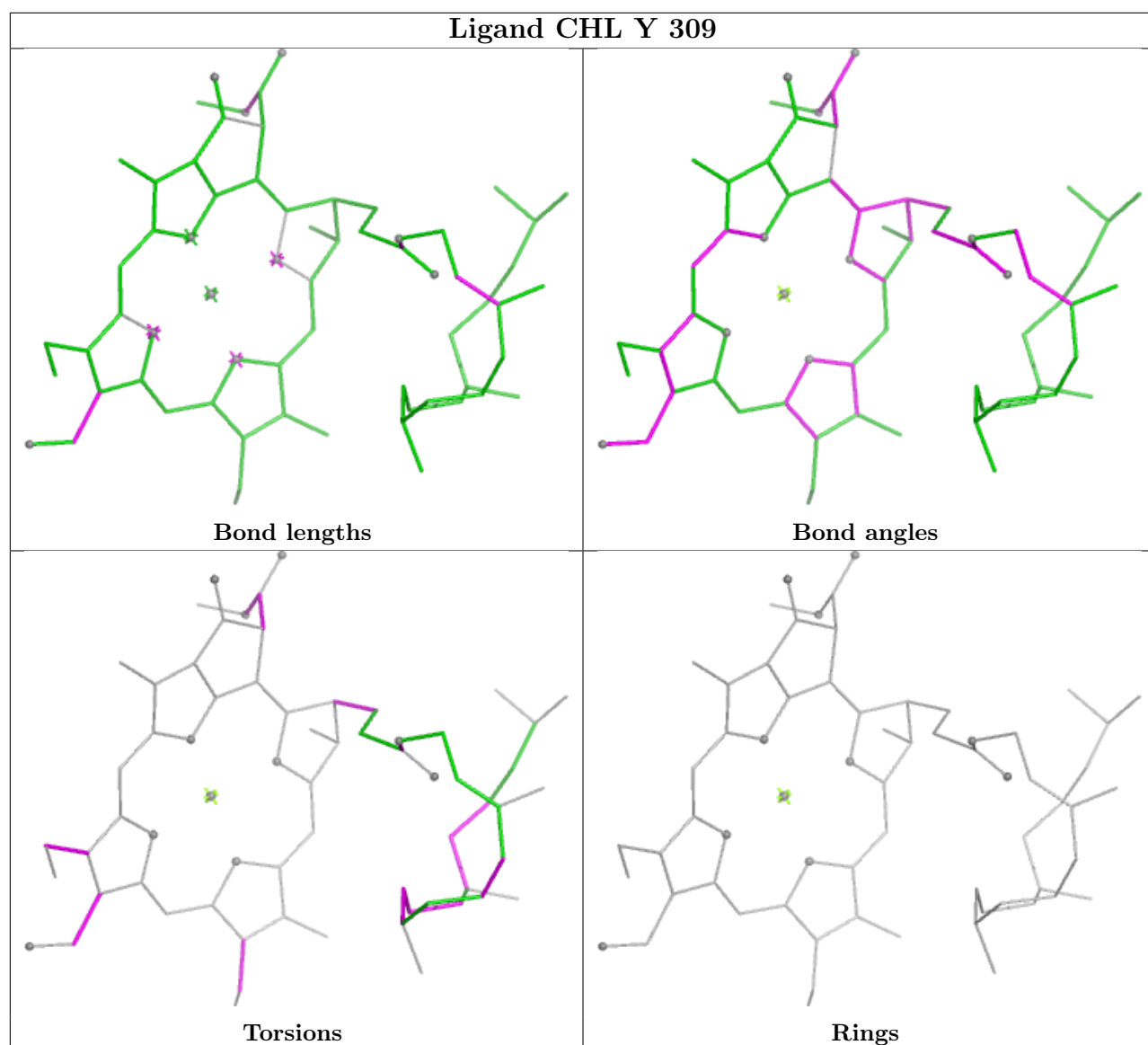


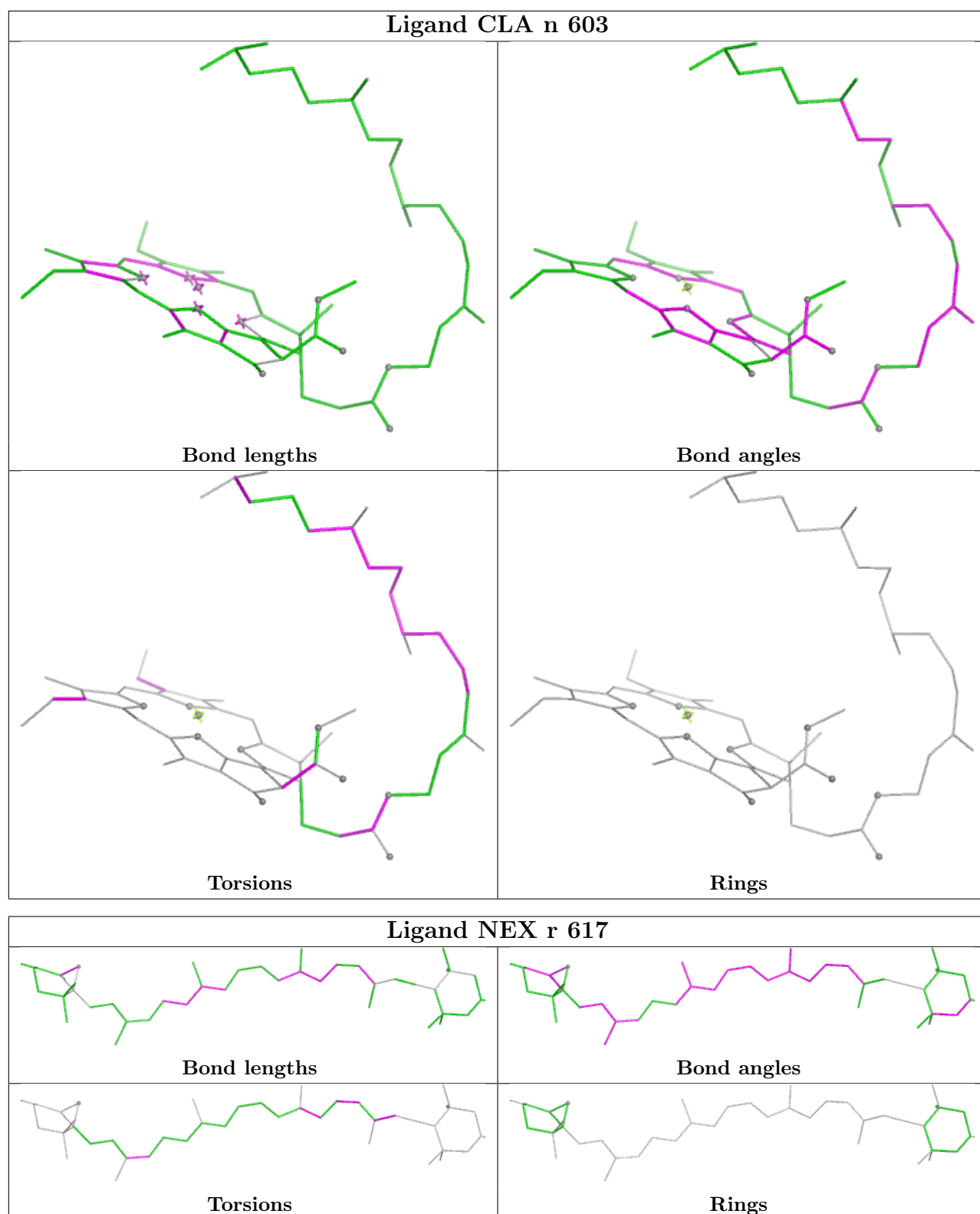
Rings

Ligand CHL n 605

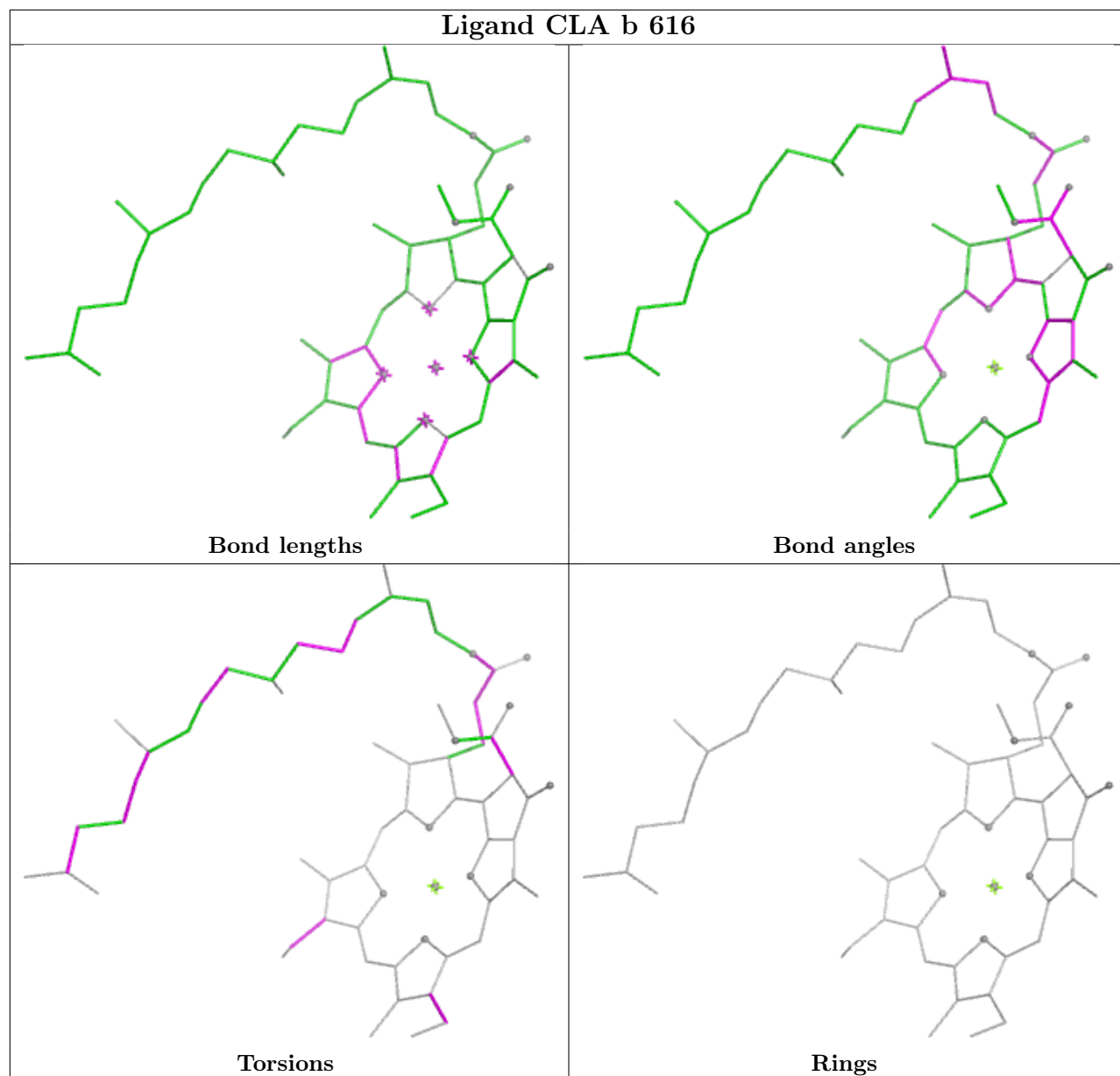




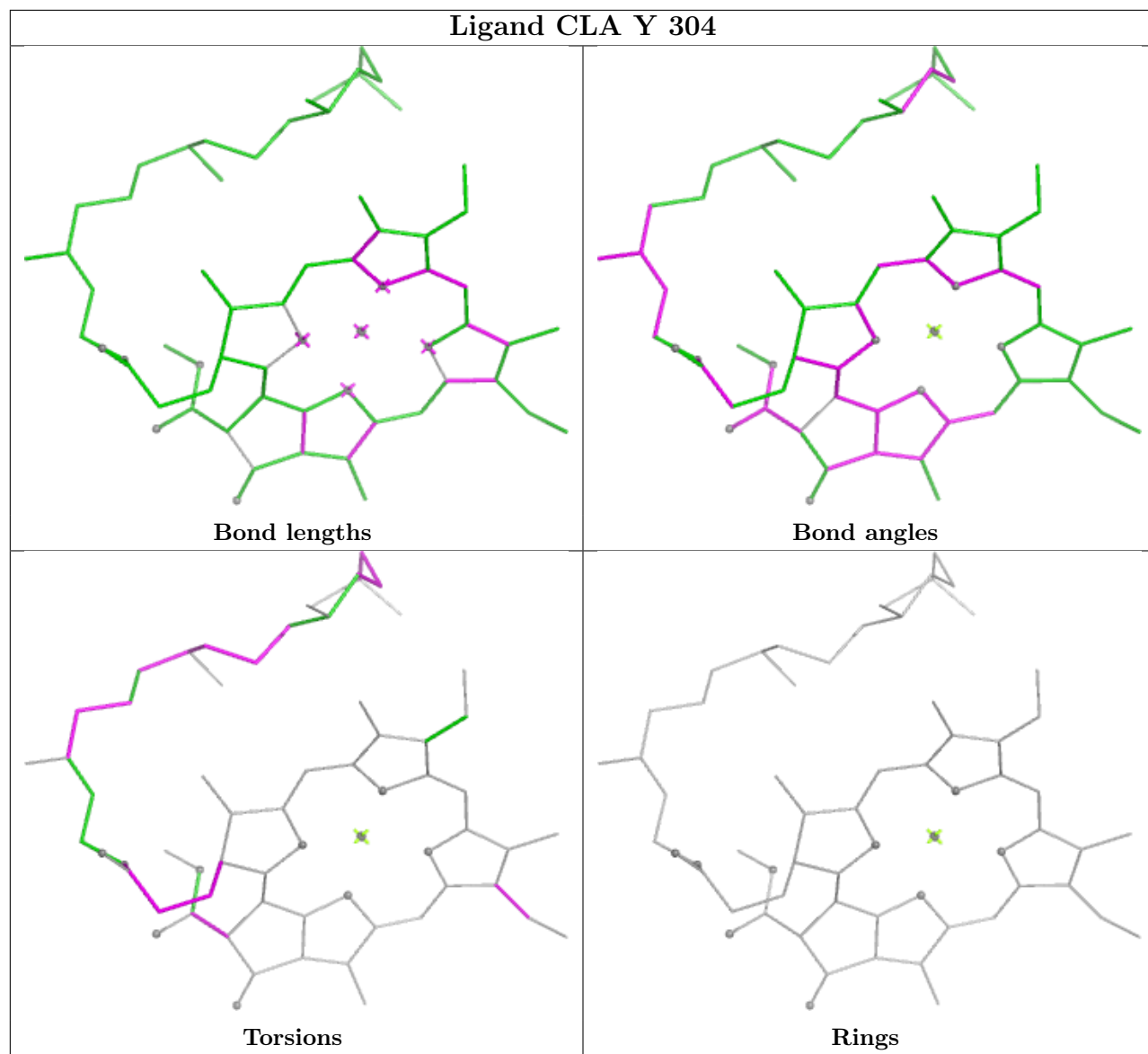


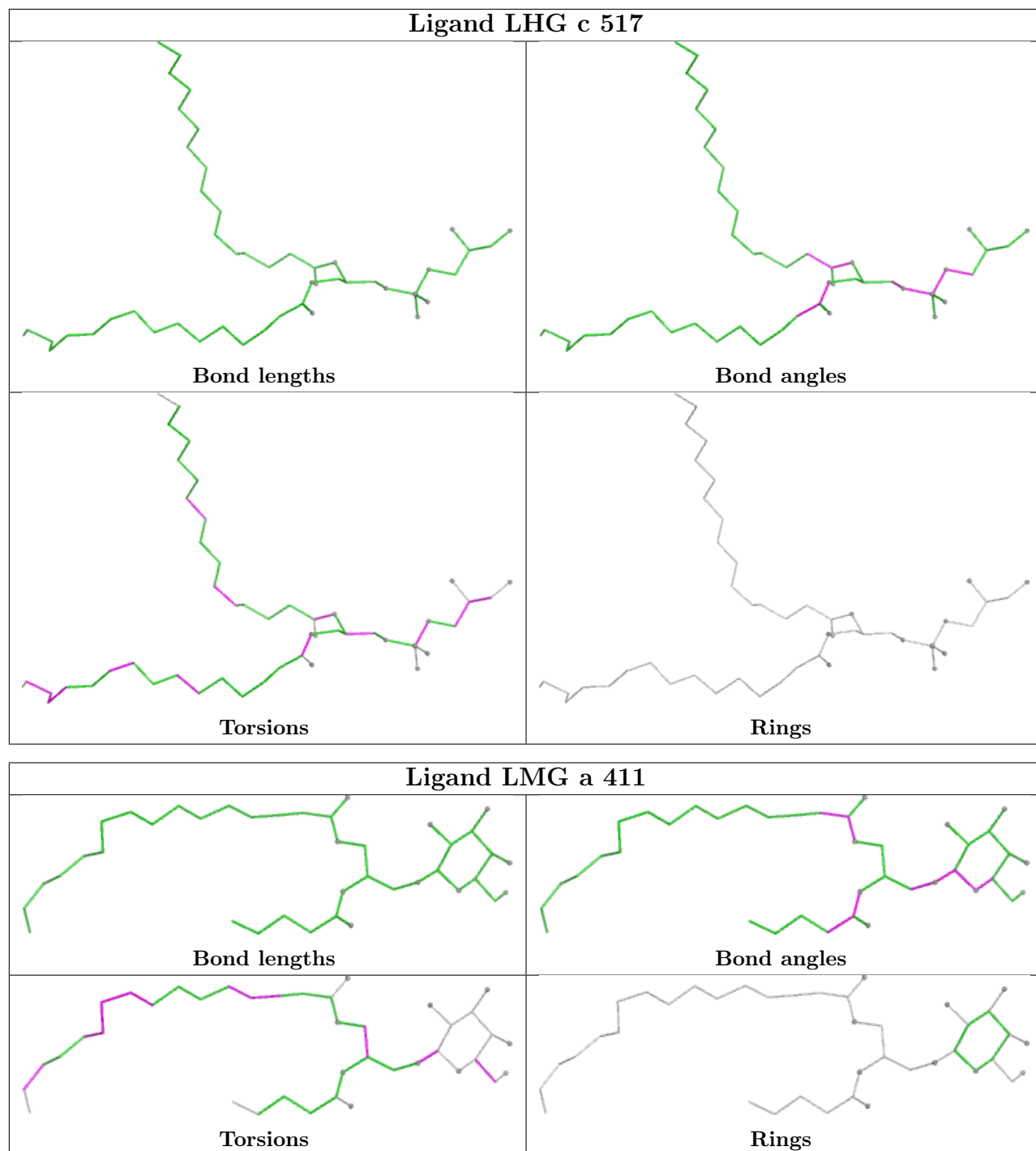


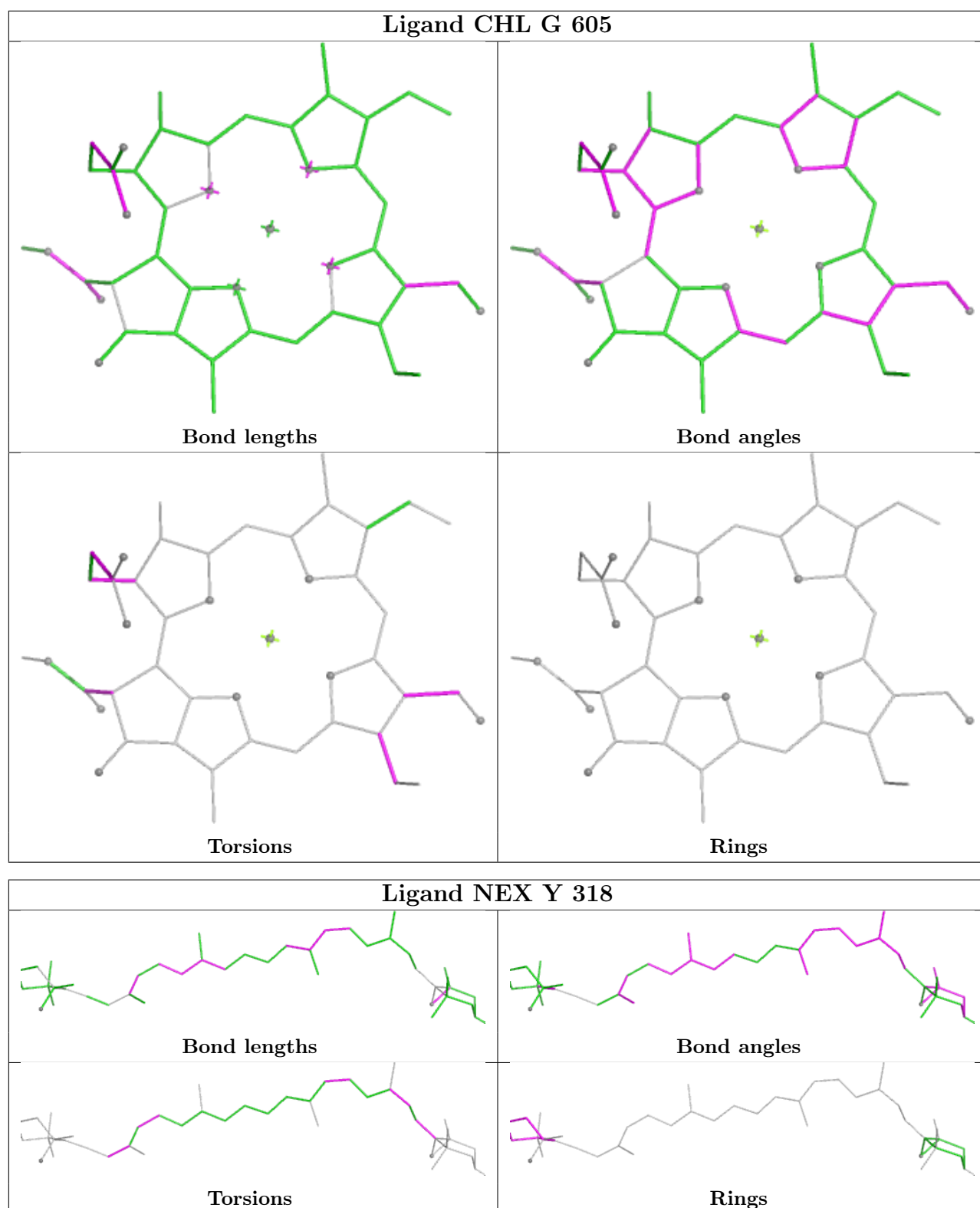
Ligand CLA b 616

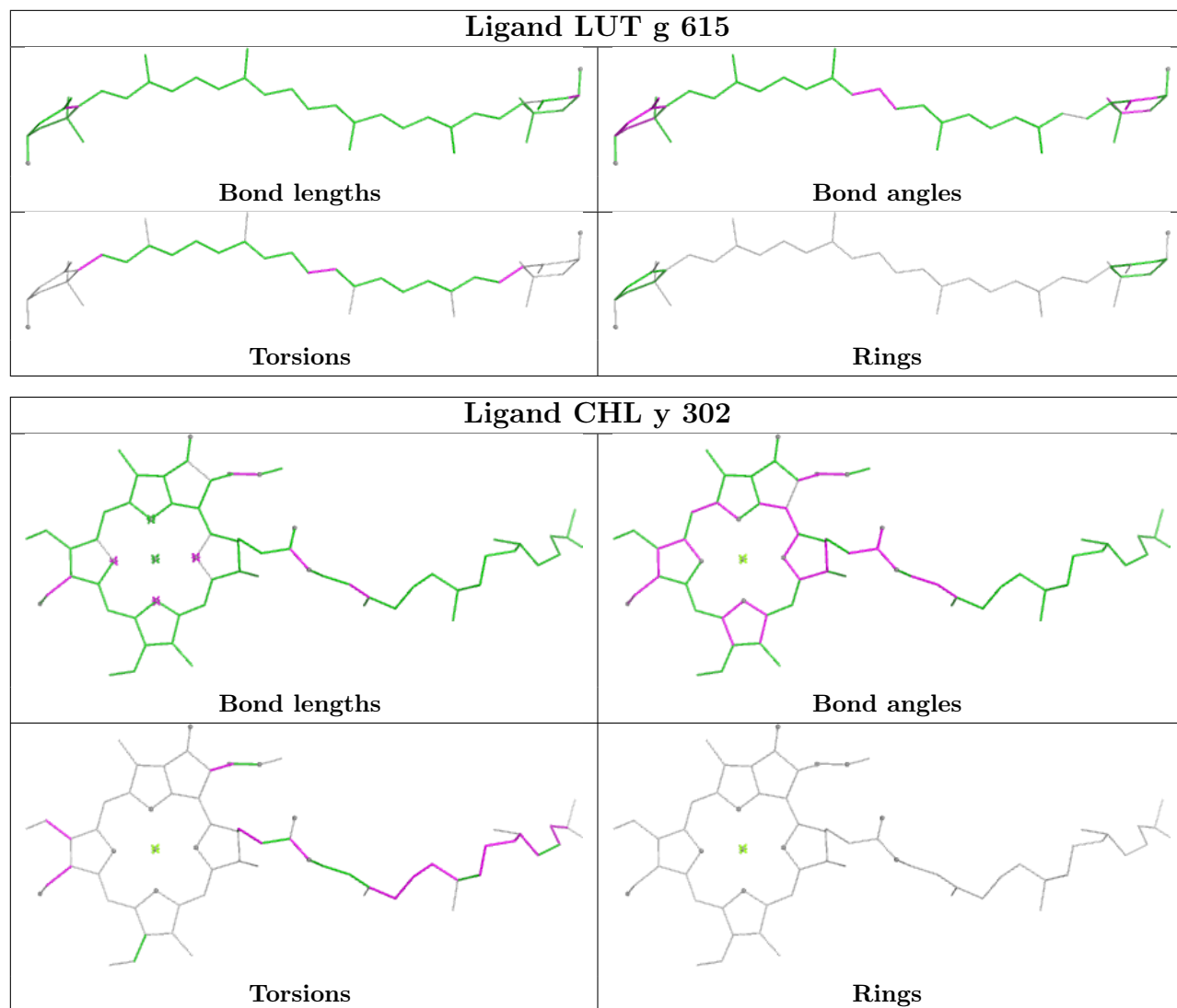


Ligand CLA Y 304

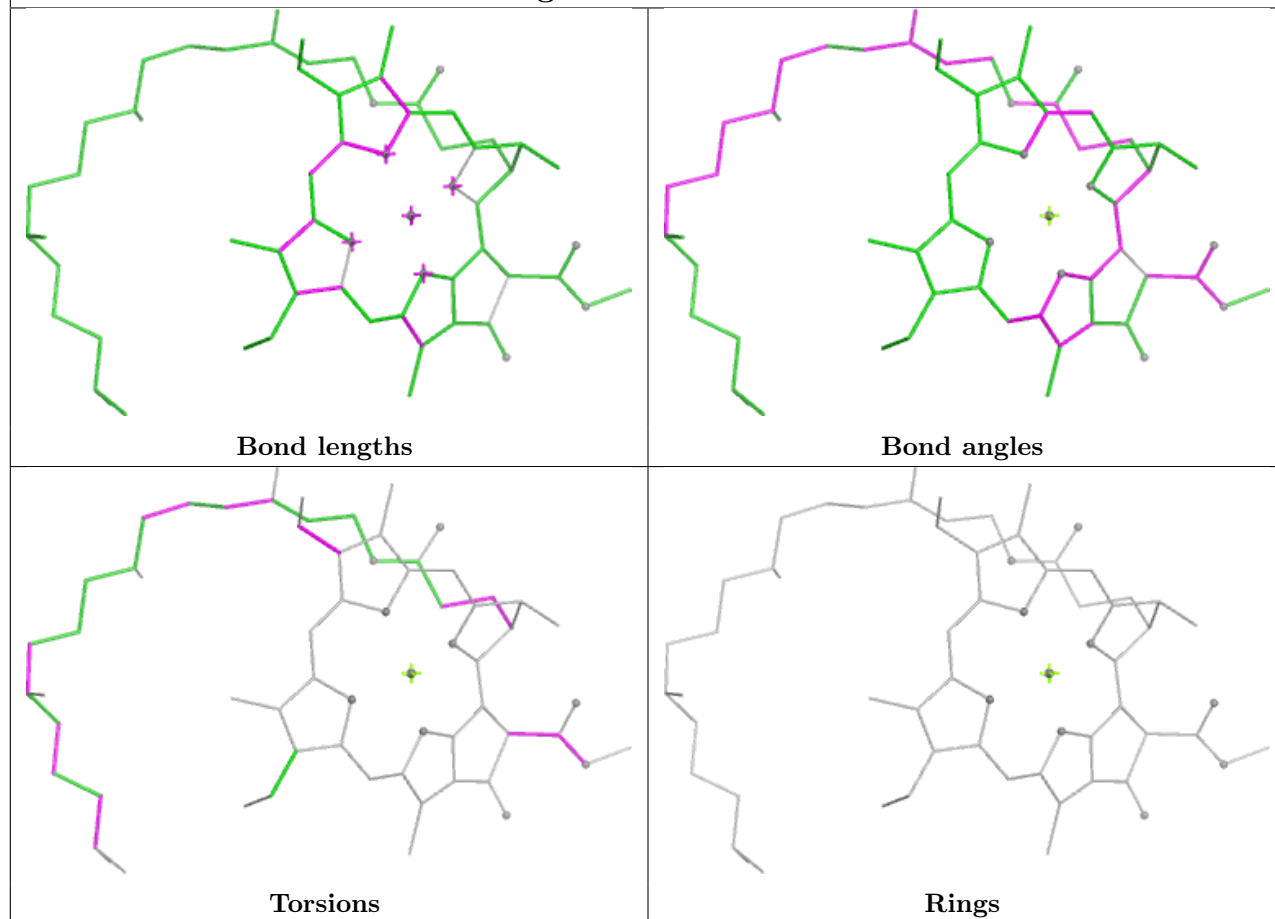




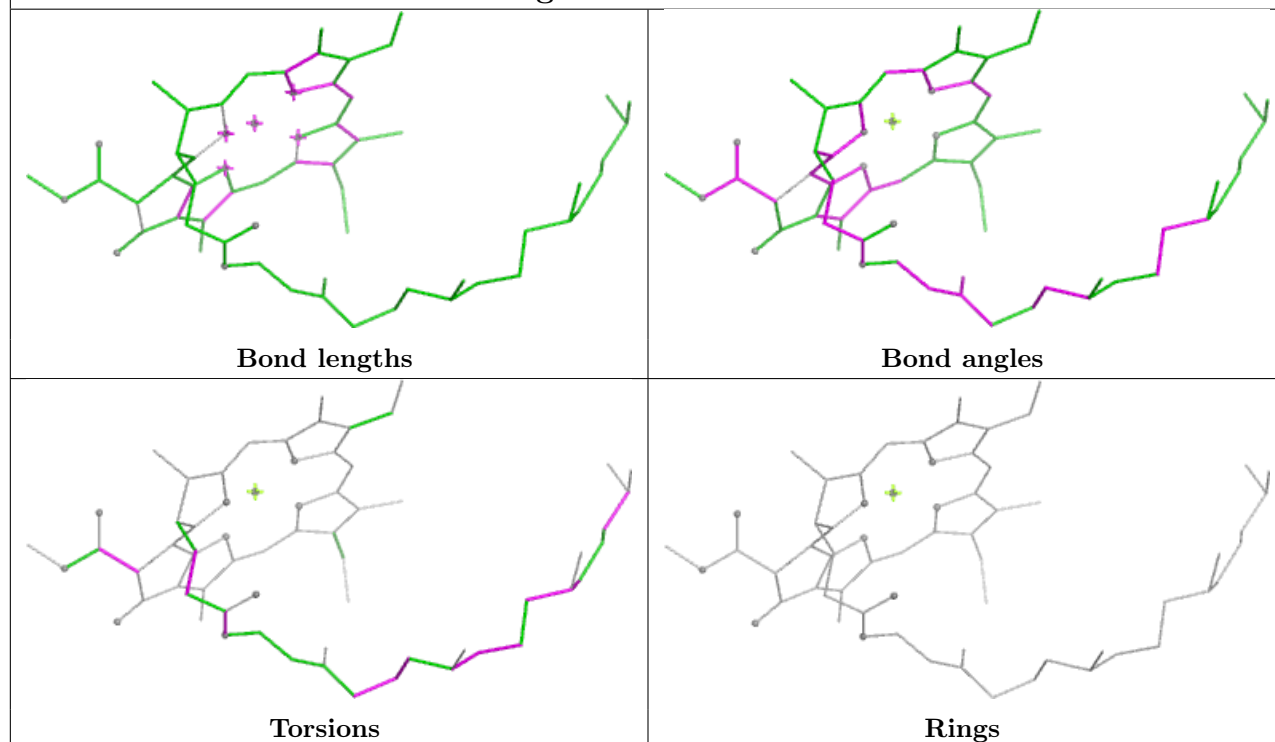


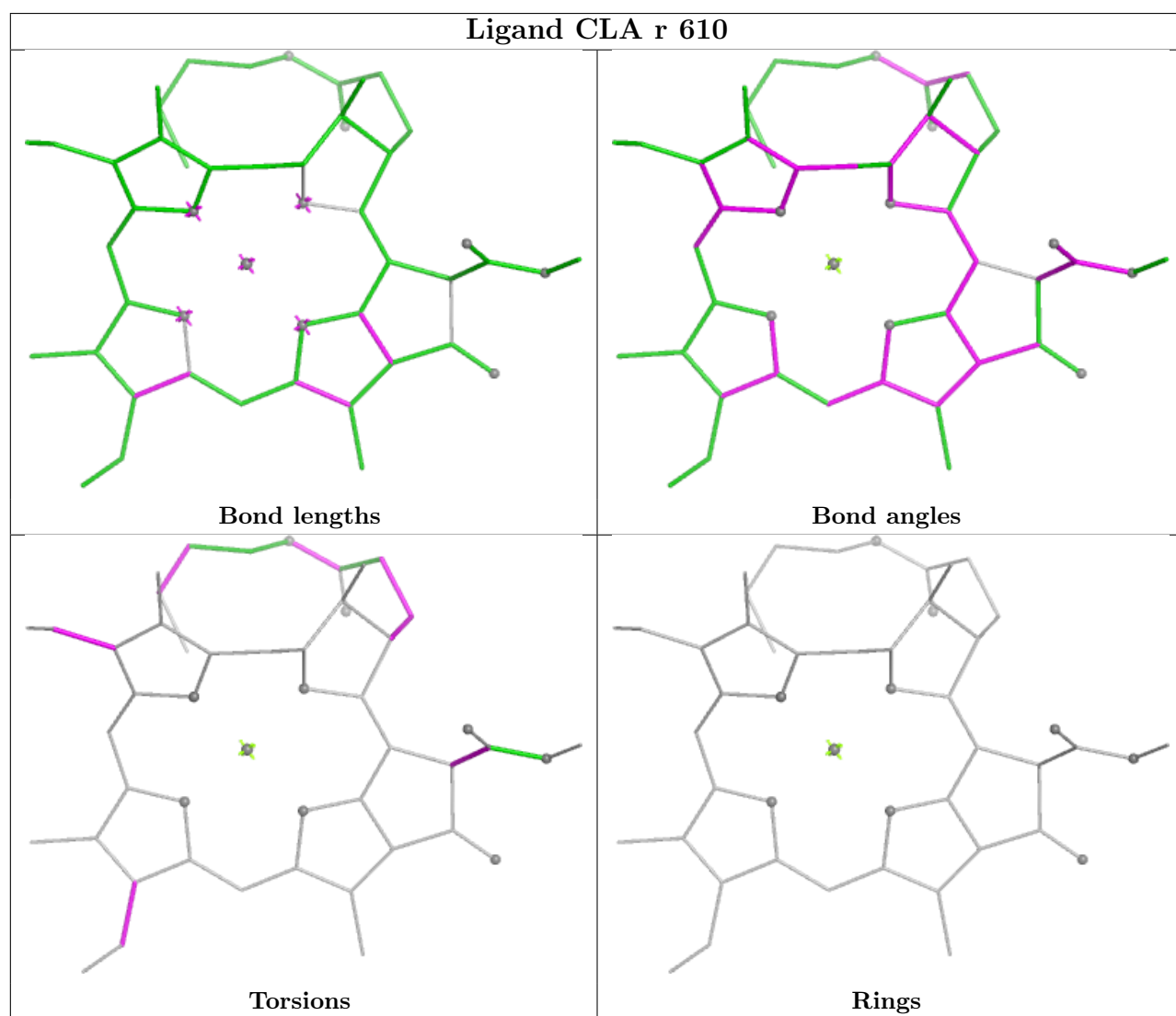
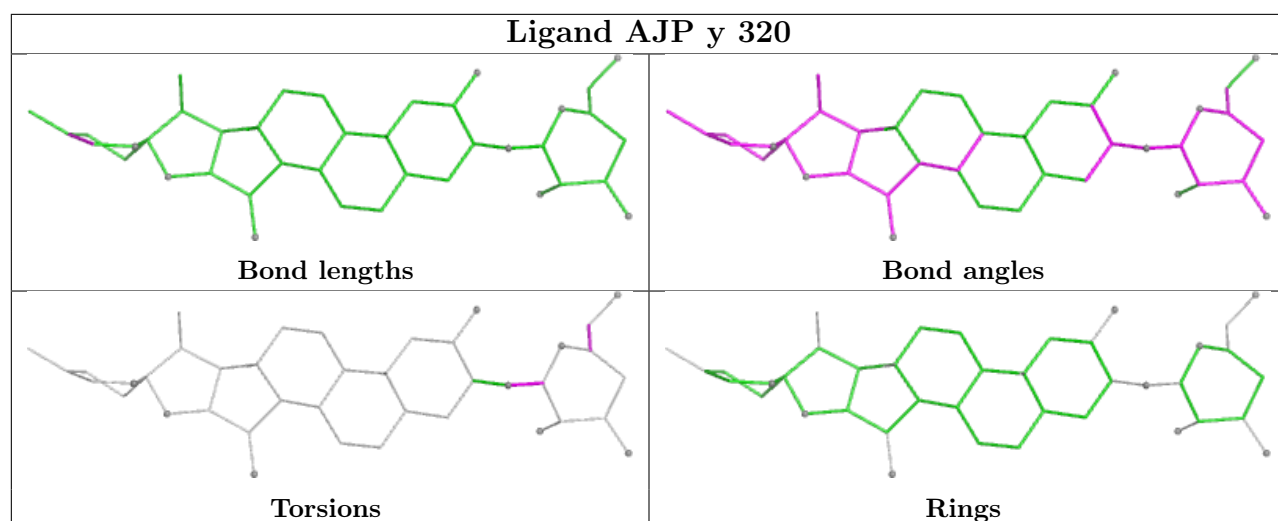


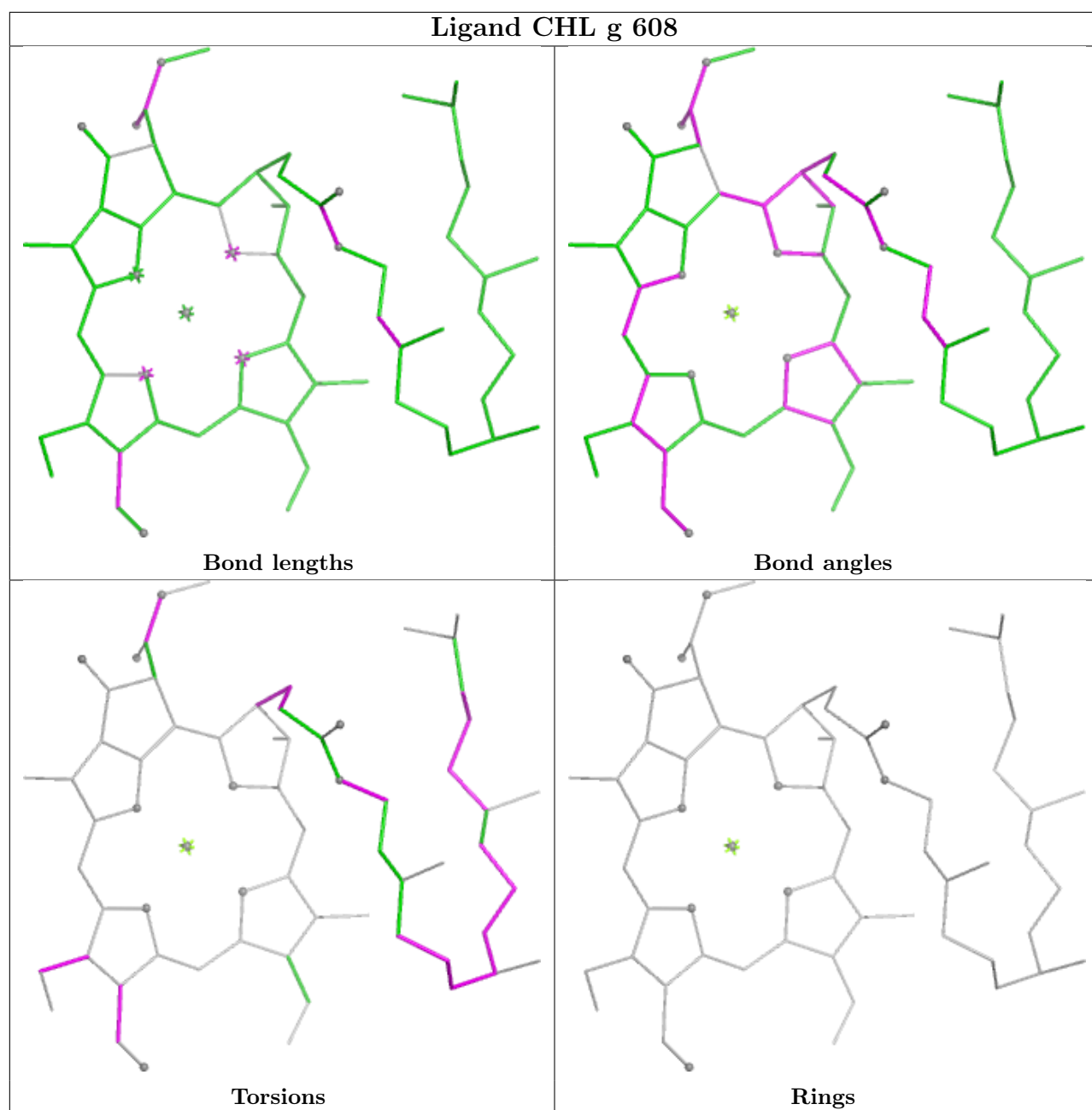
Ligand CLA r 609



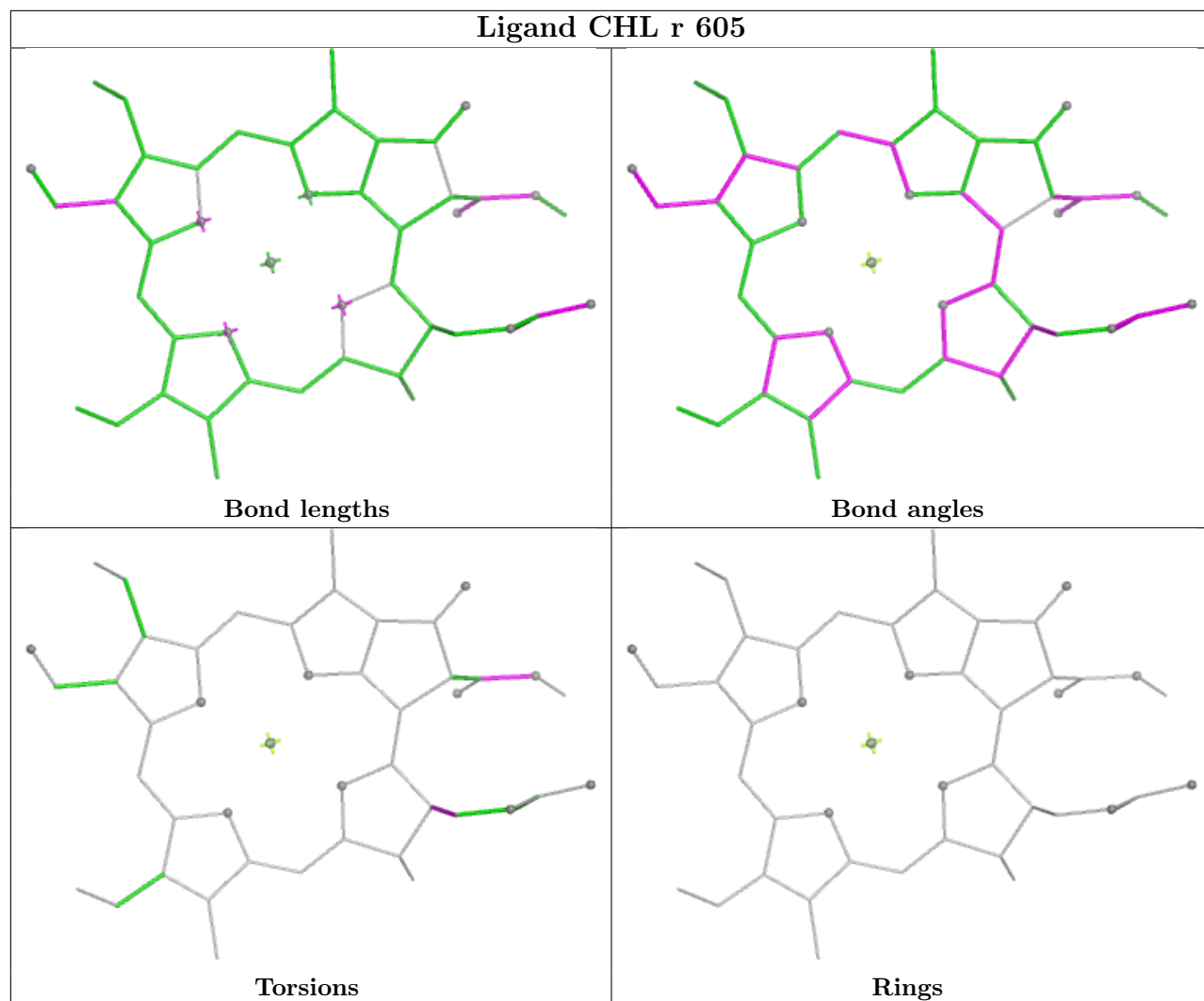
Ligand CLA c 513



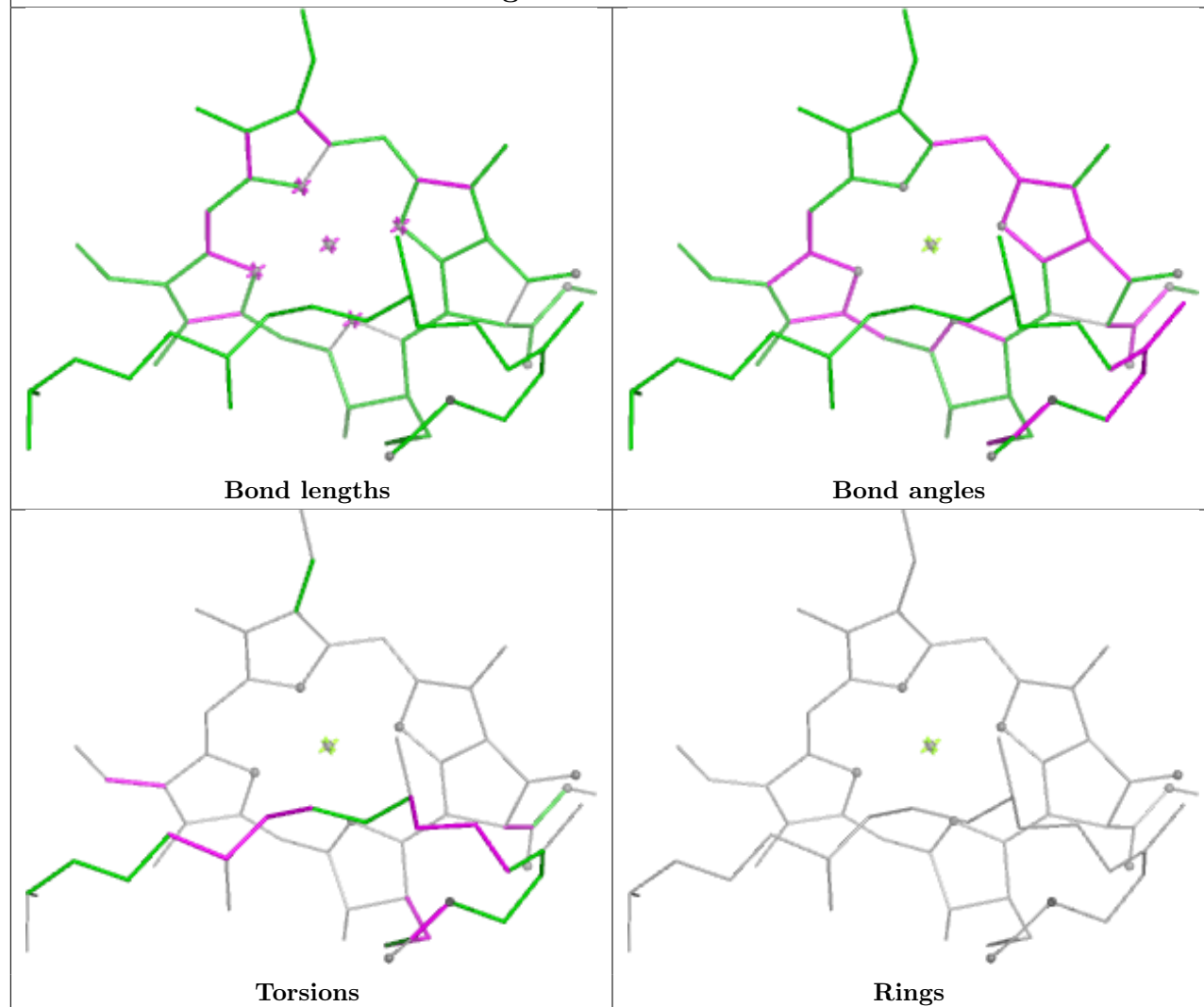




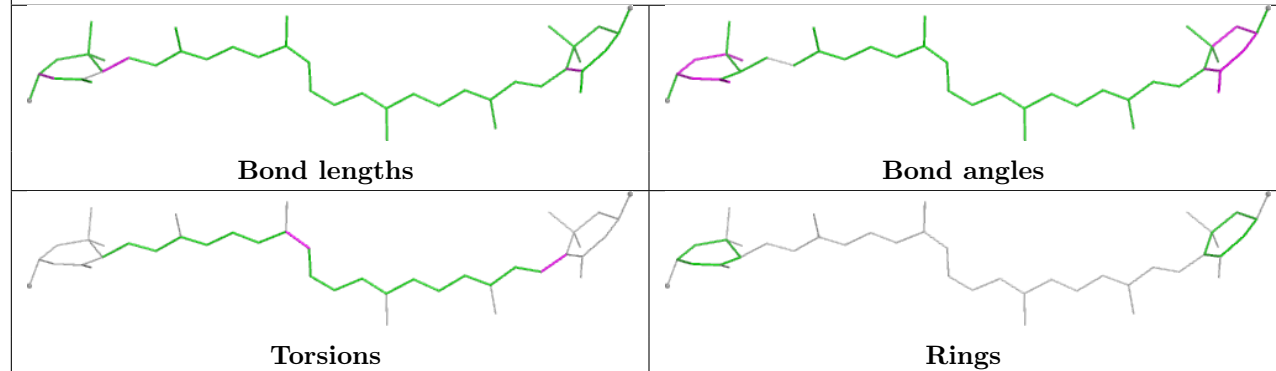
Ligand CHL r 605

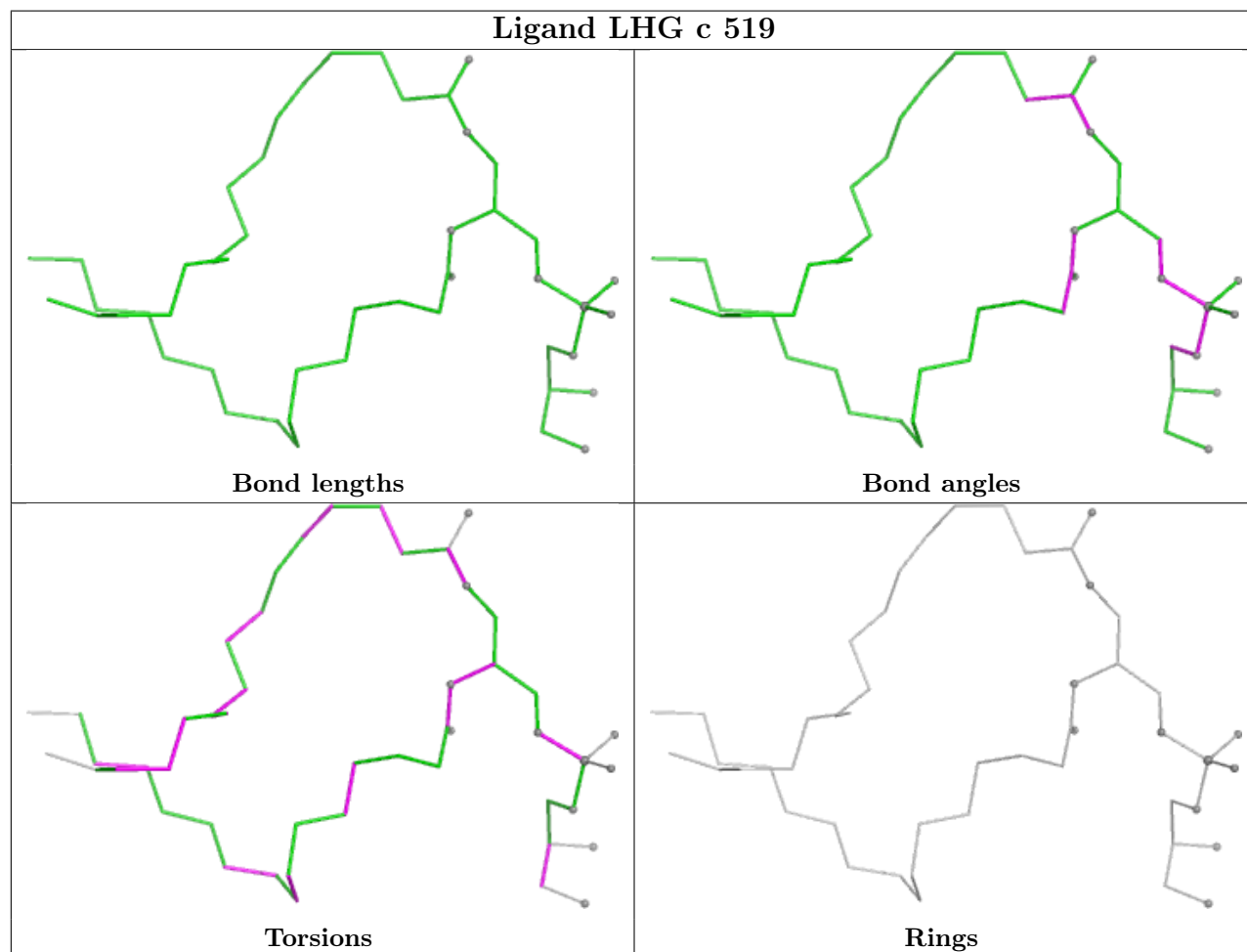
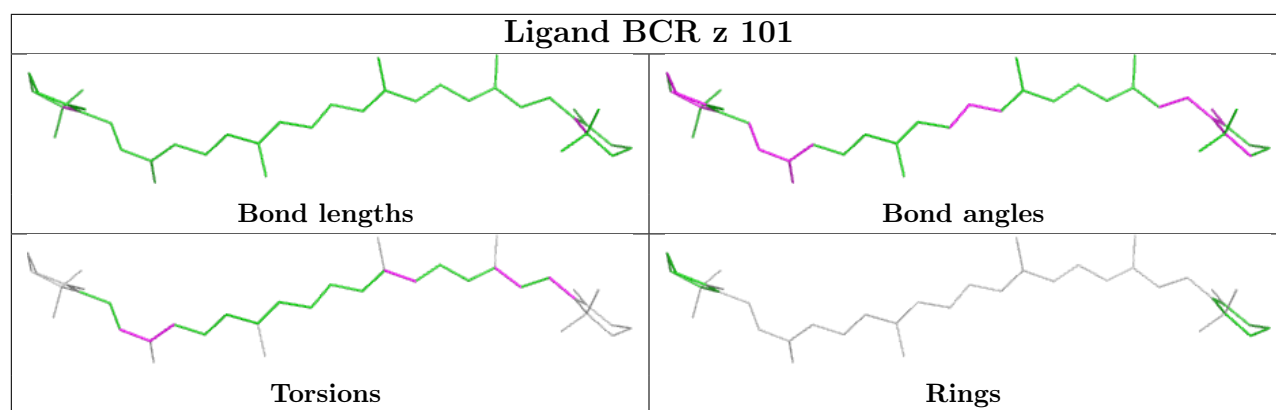


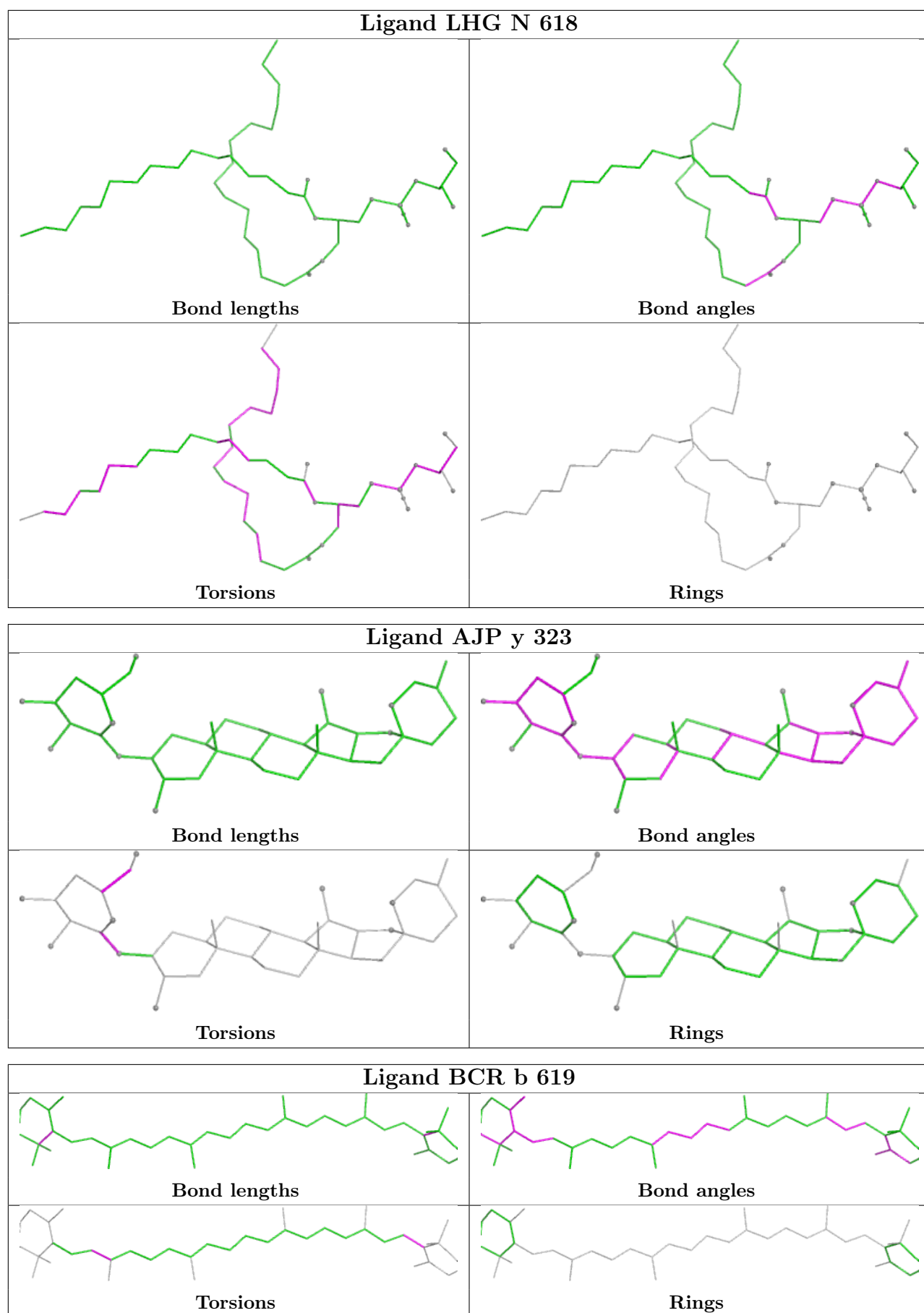
Ligand CLA B 601

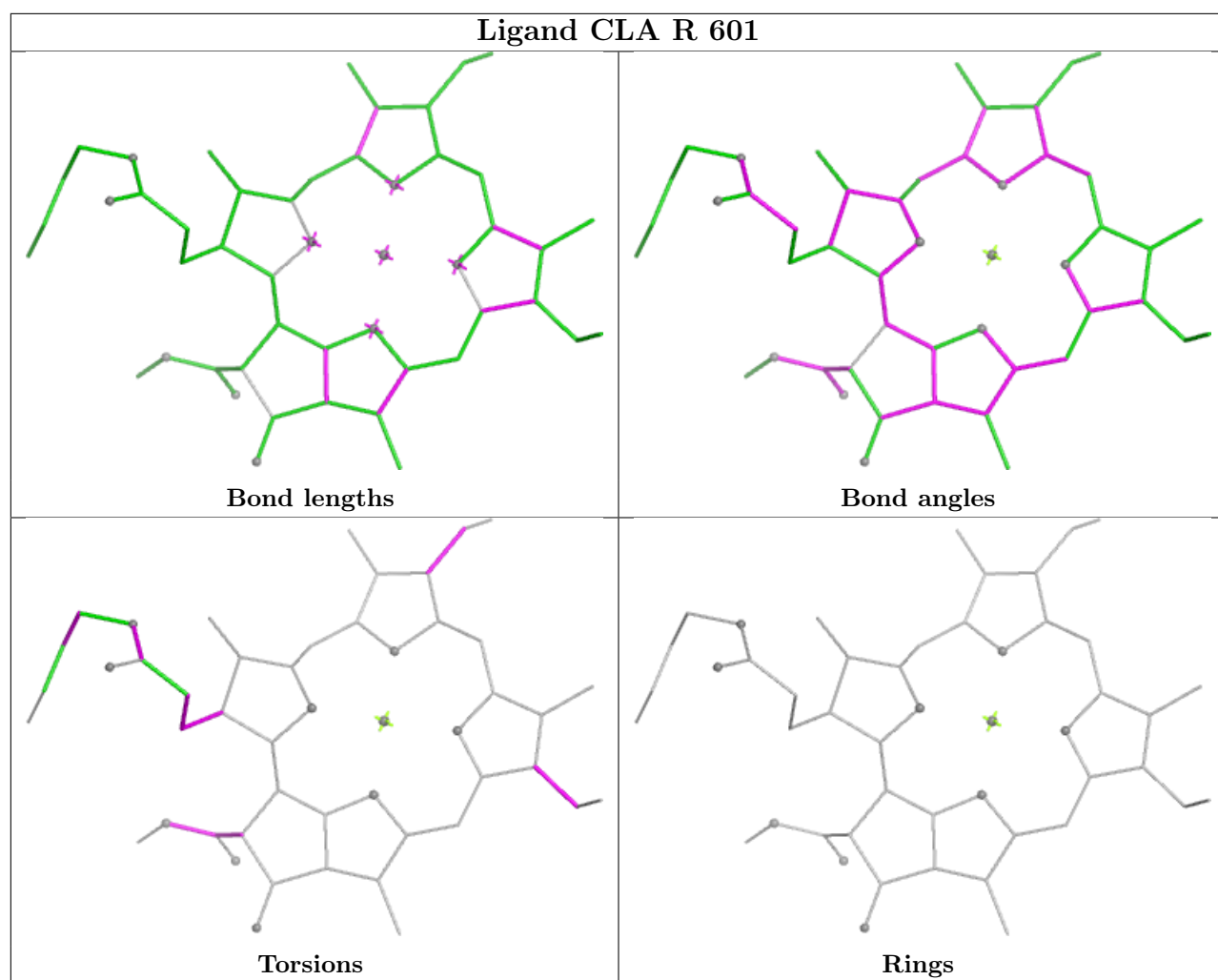


Ligand LUT S 315

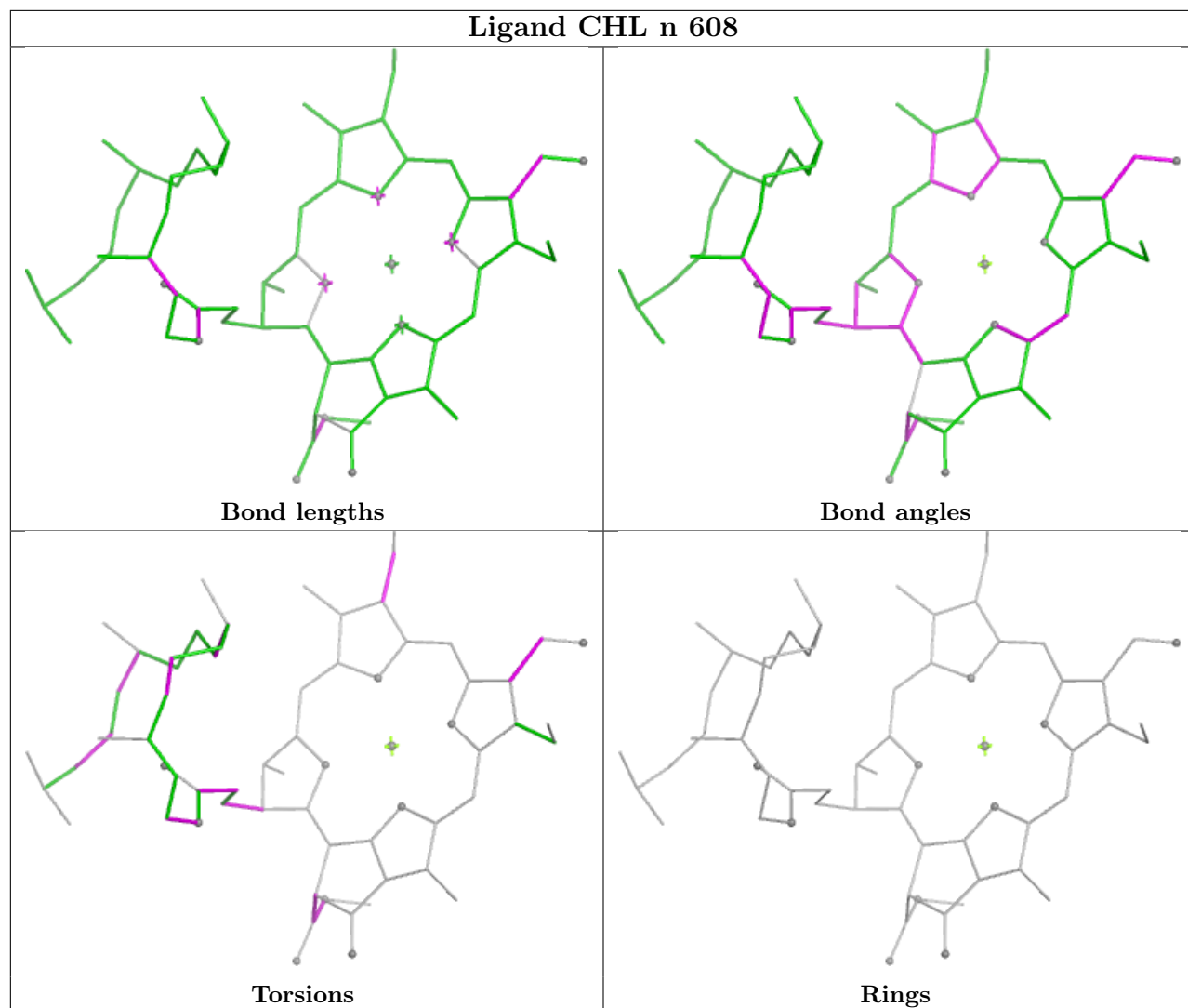


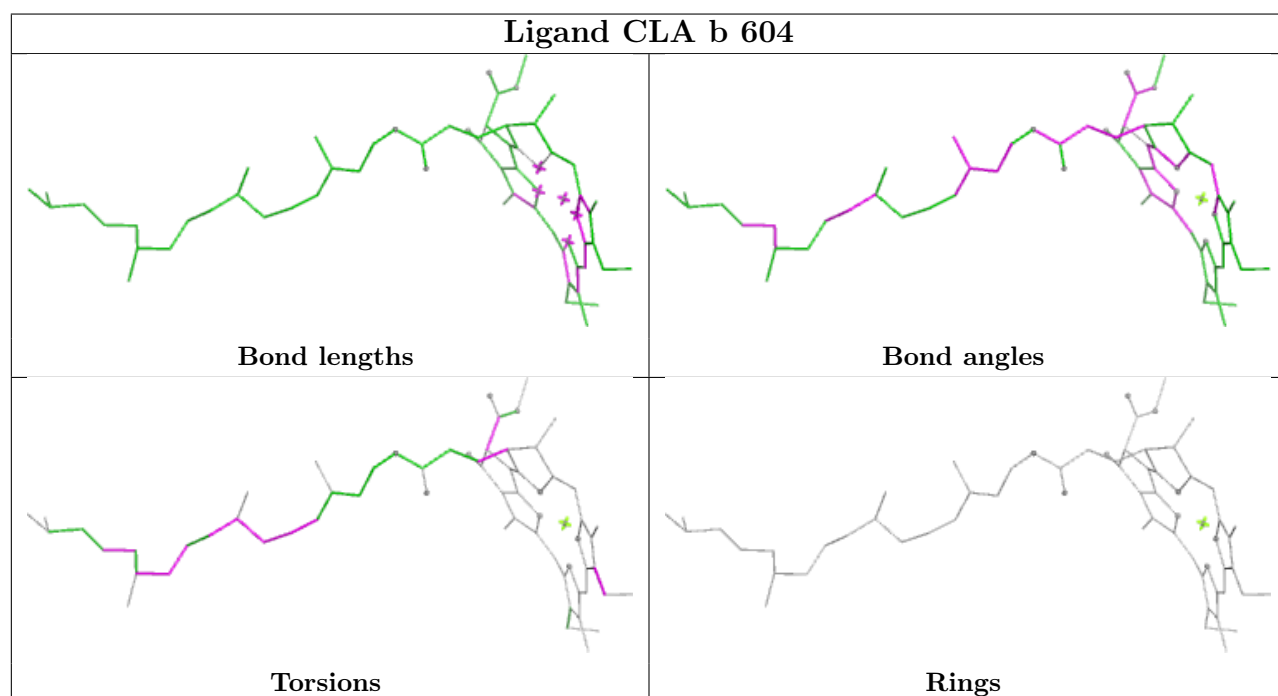
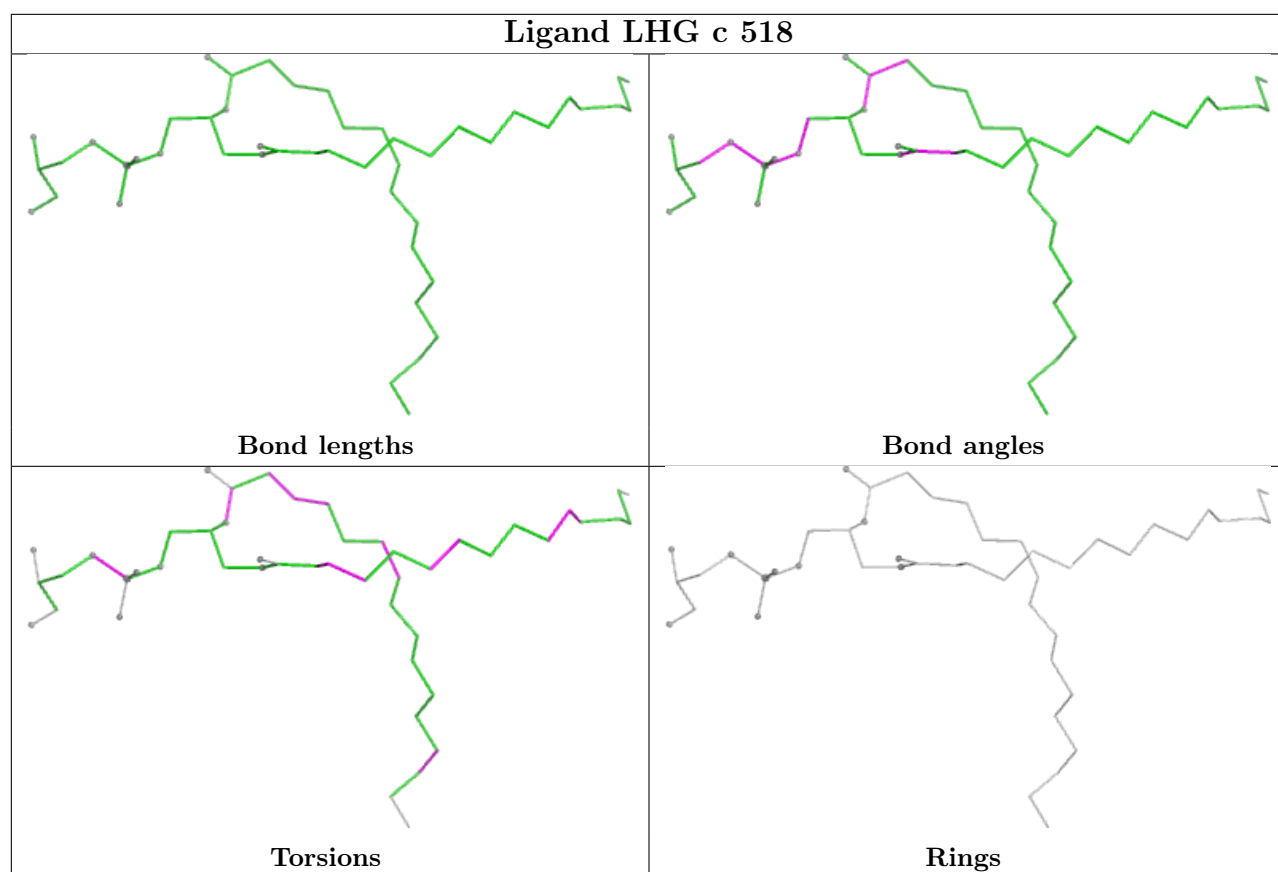




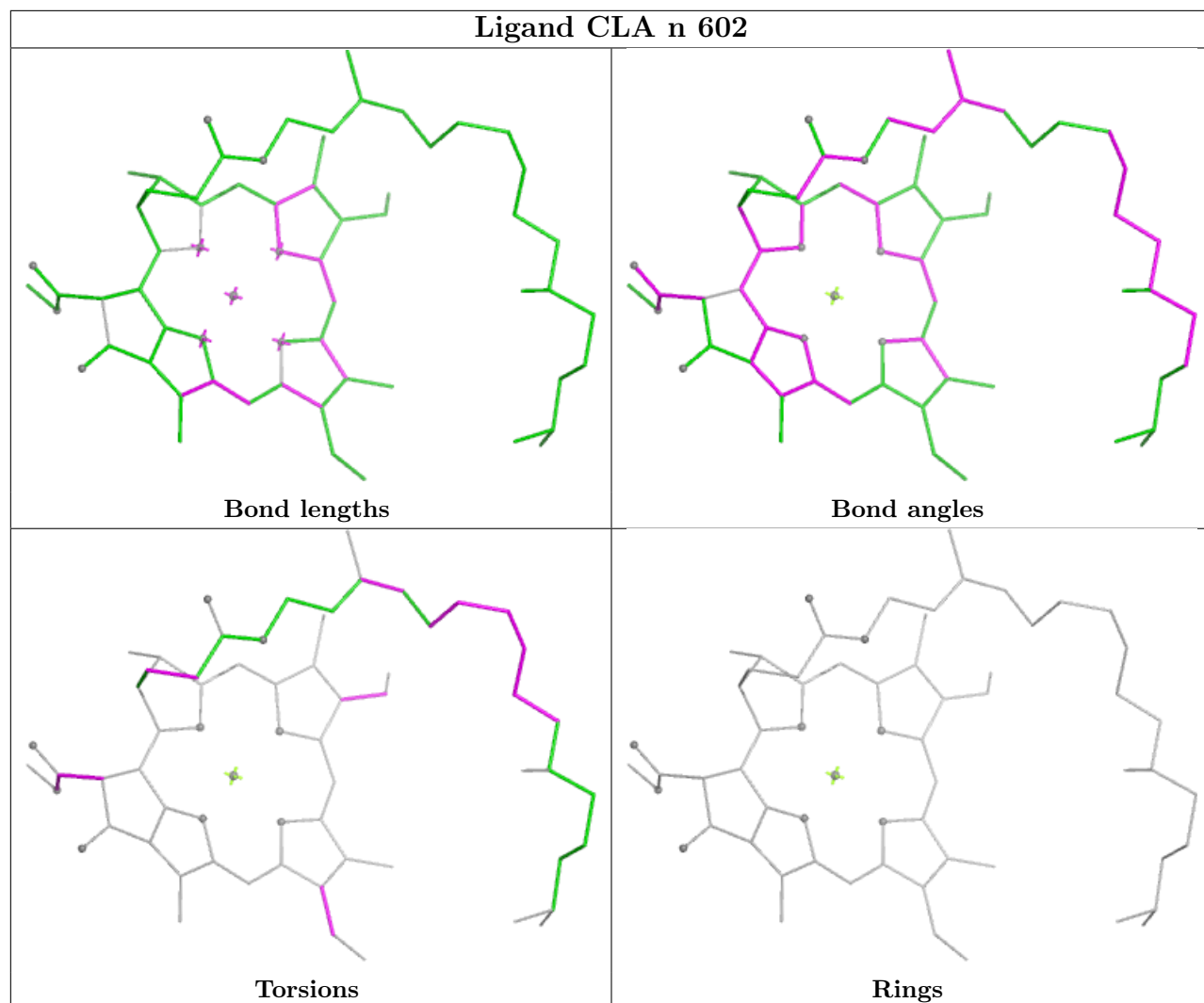


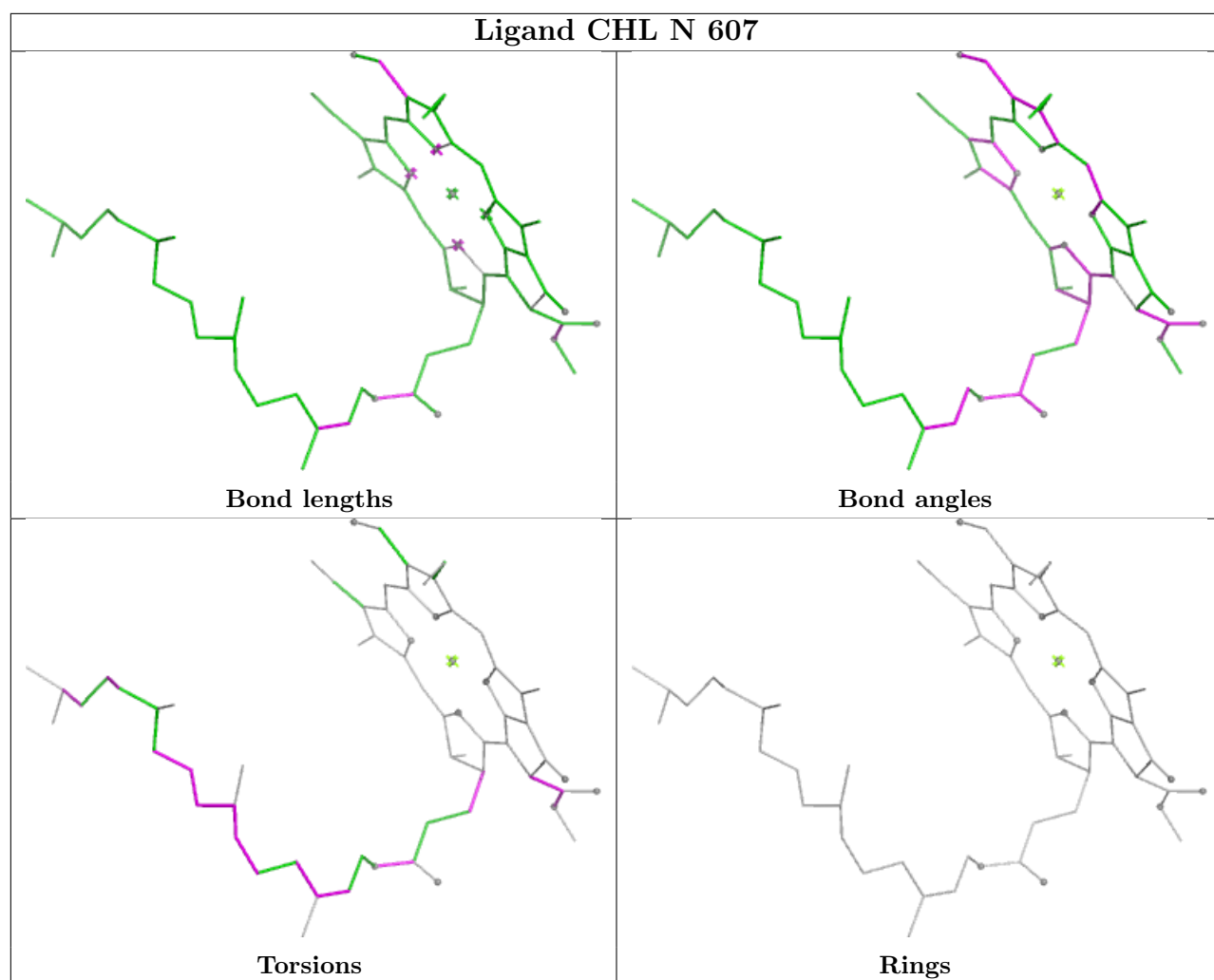
Ligand CHL n 608



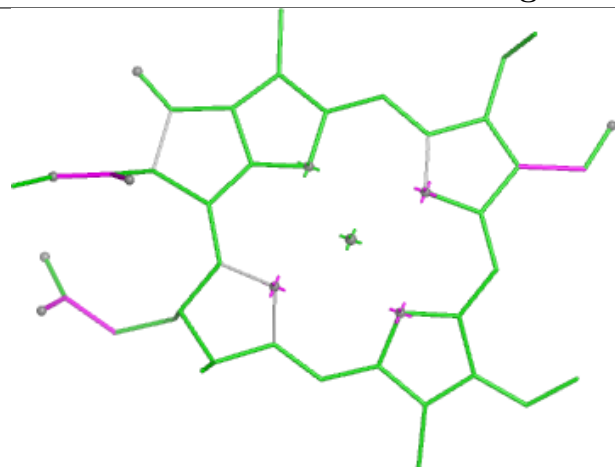


Ligand CLA n 602

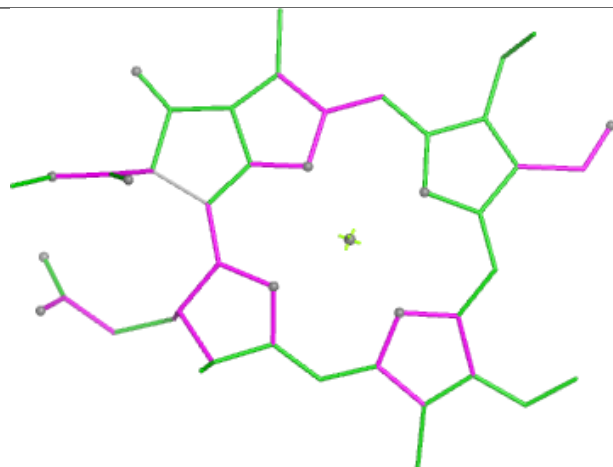




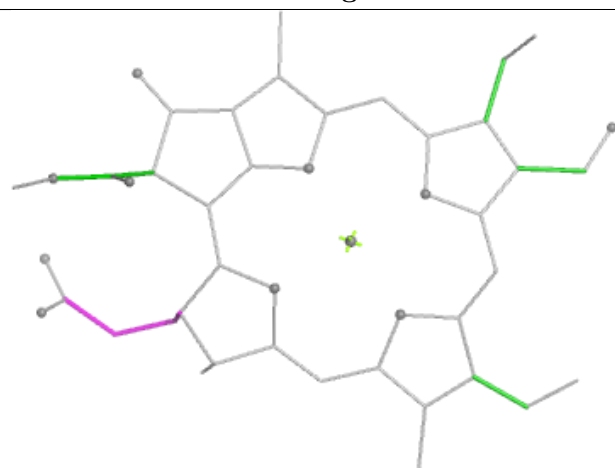
Ligand CHL 1 302



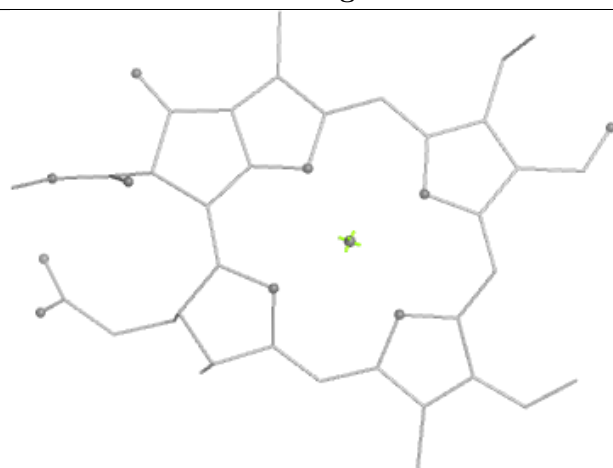
Bond lengths



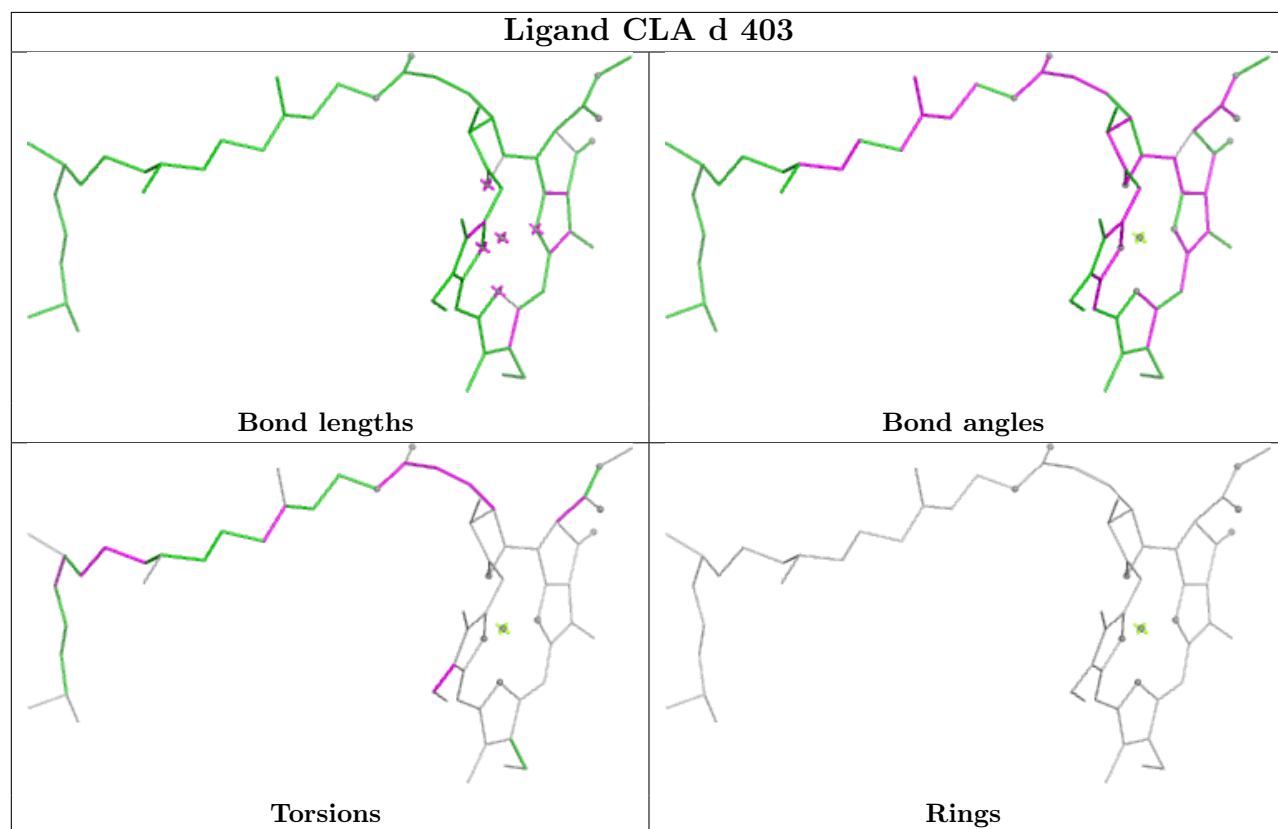
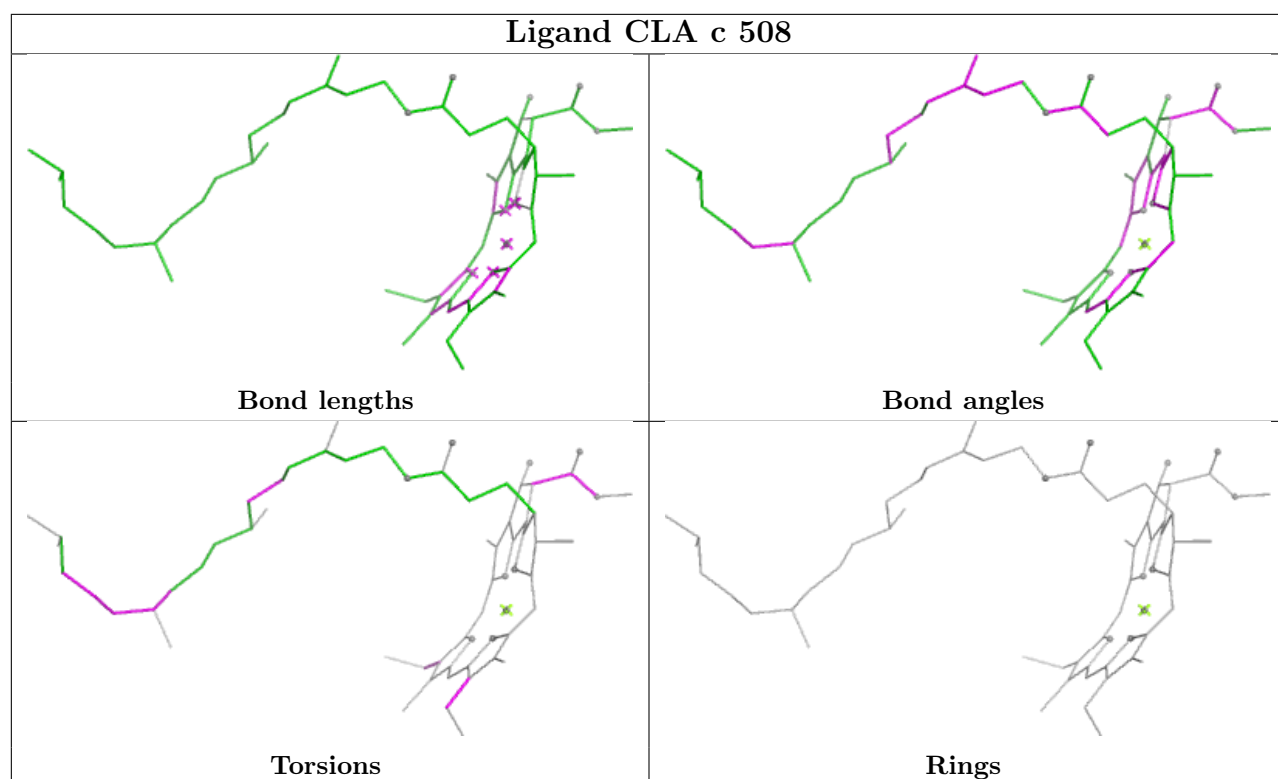
Bond angles

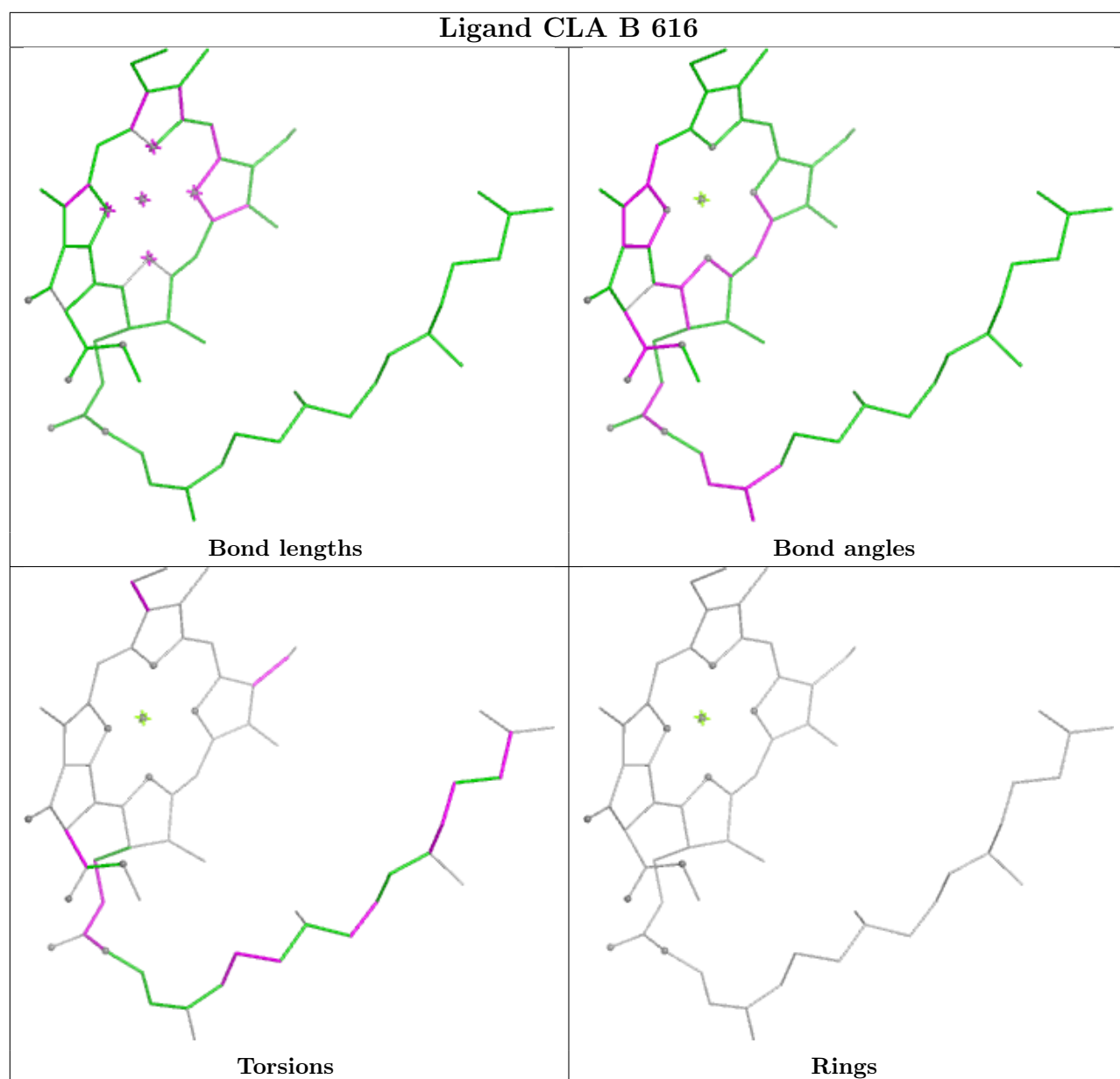


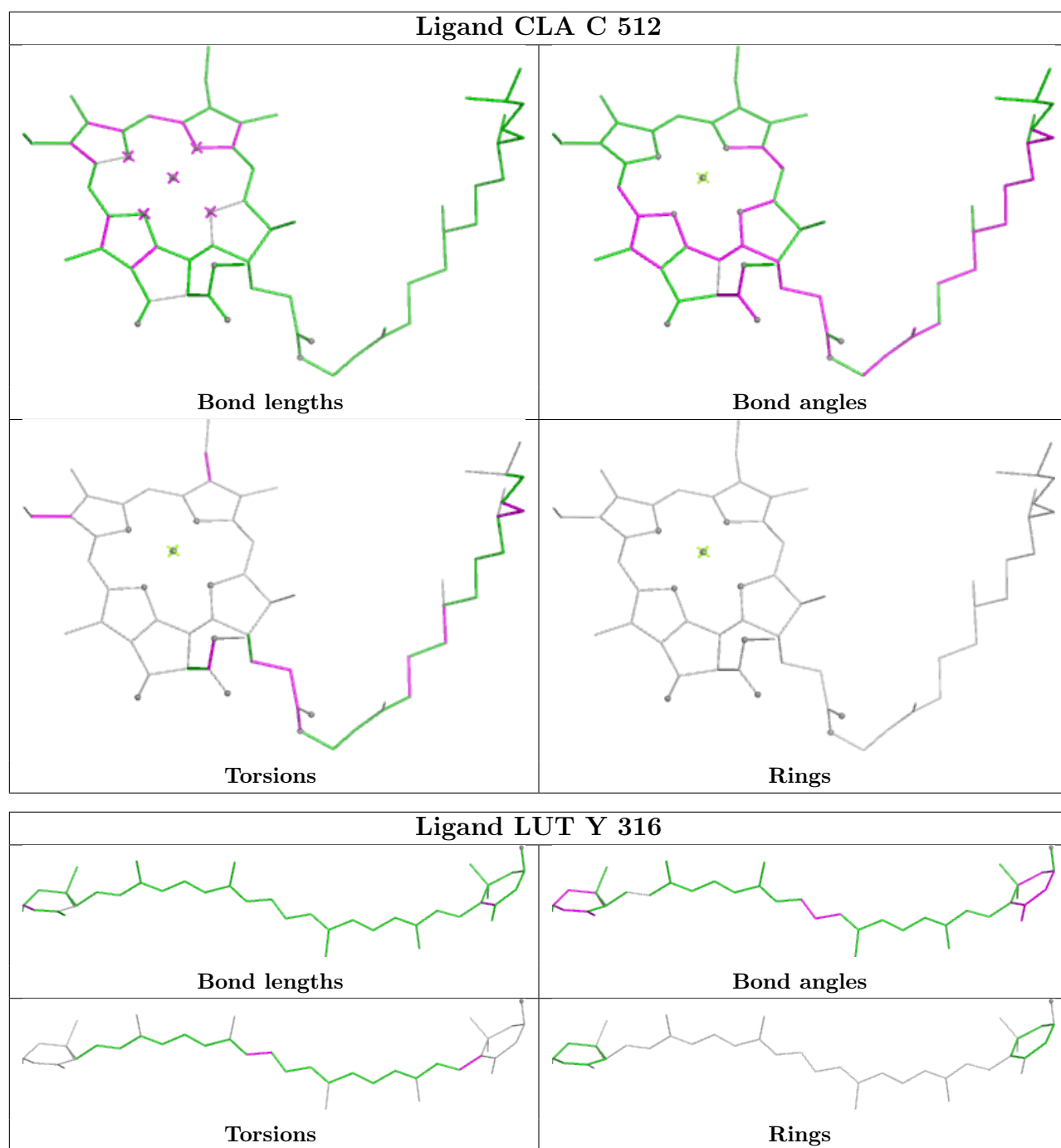
Torsions

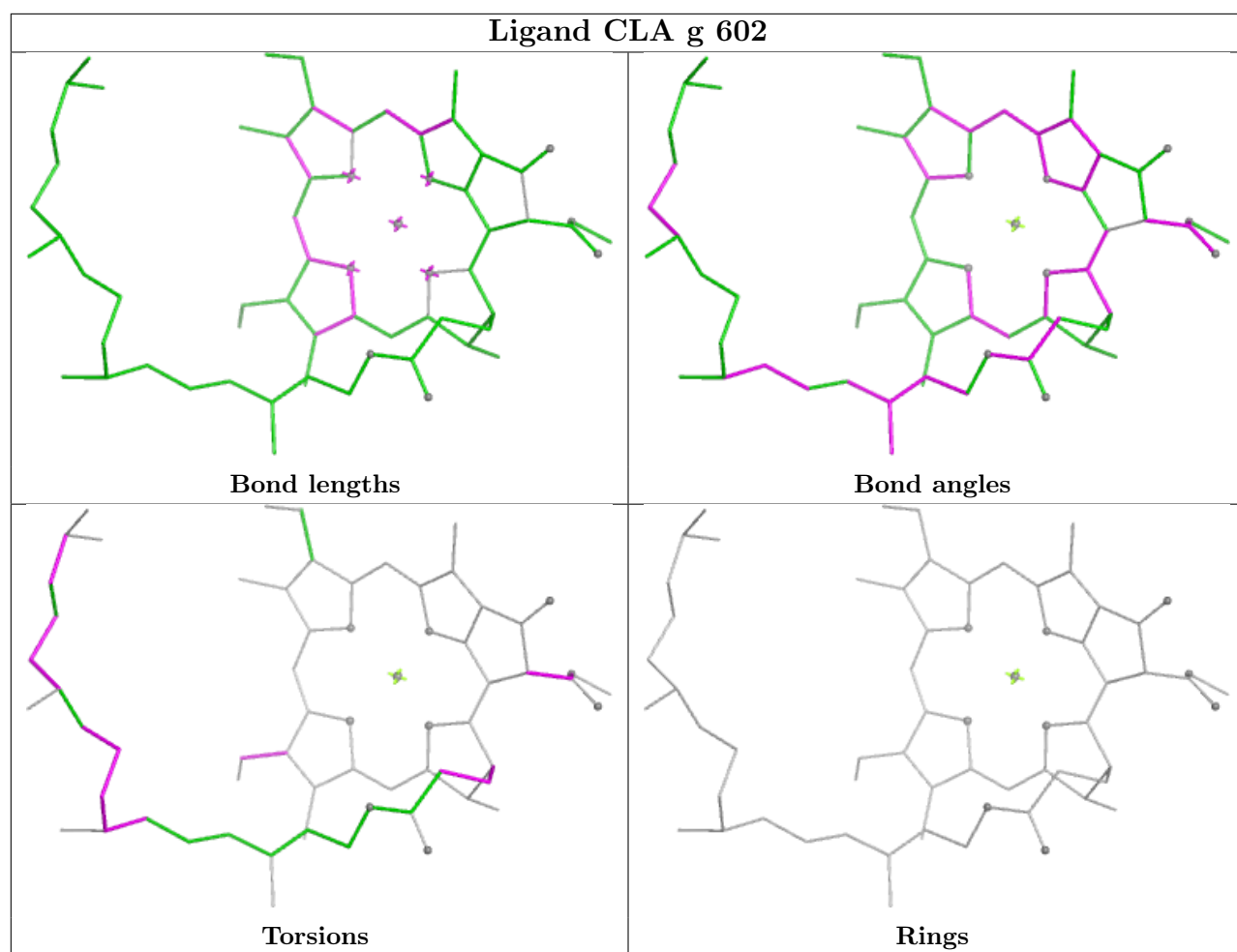


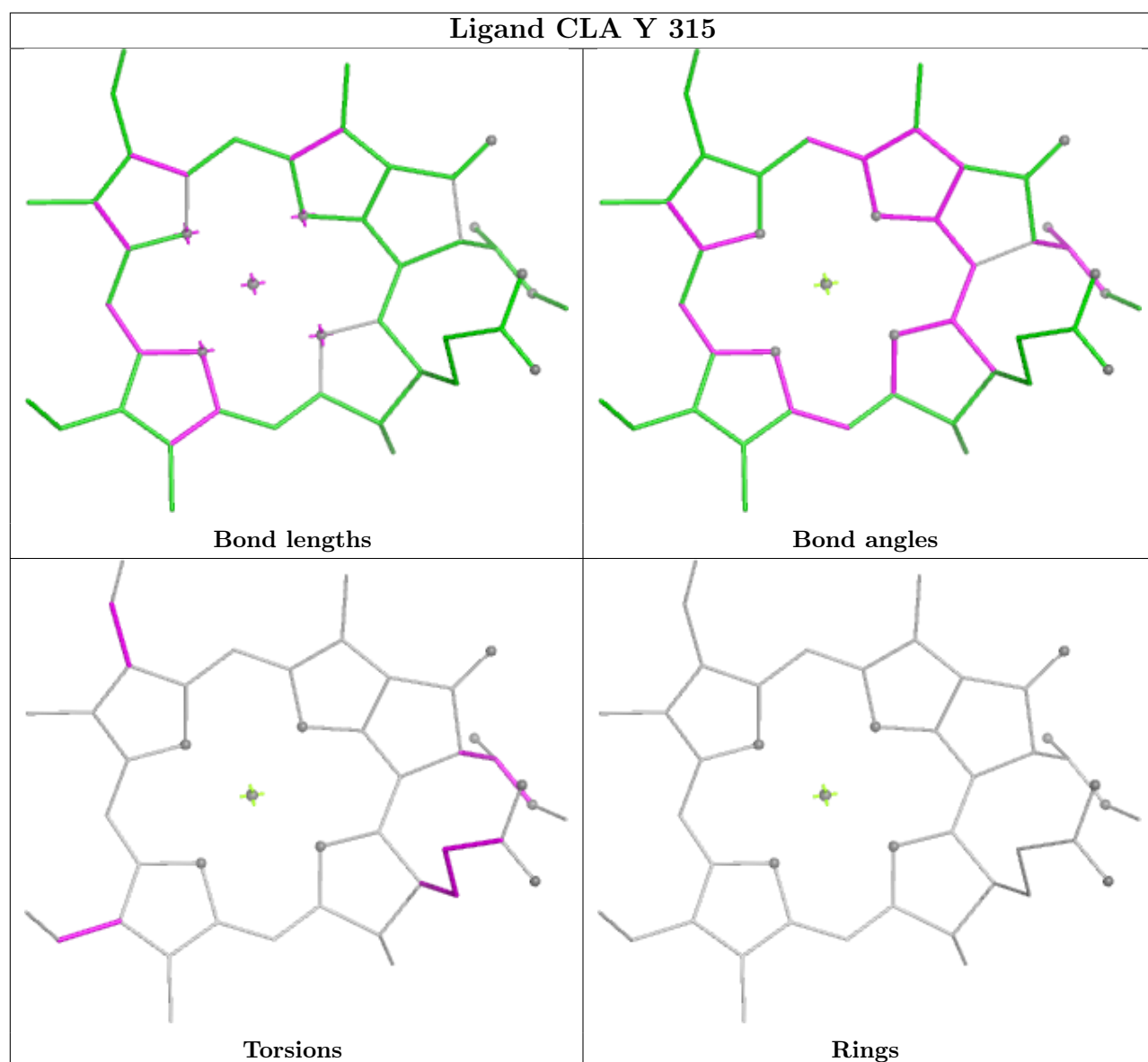
Rings

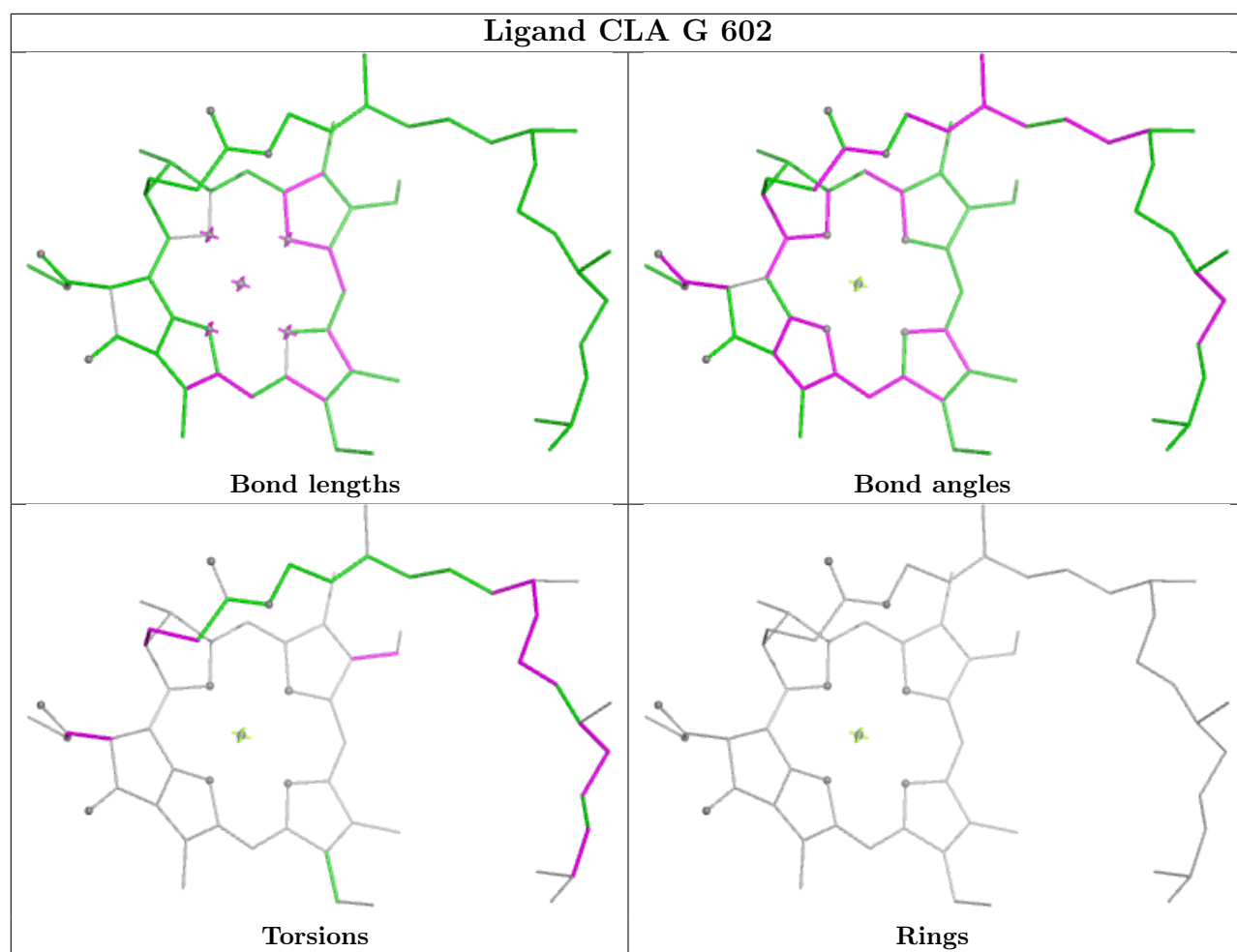


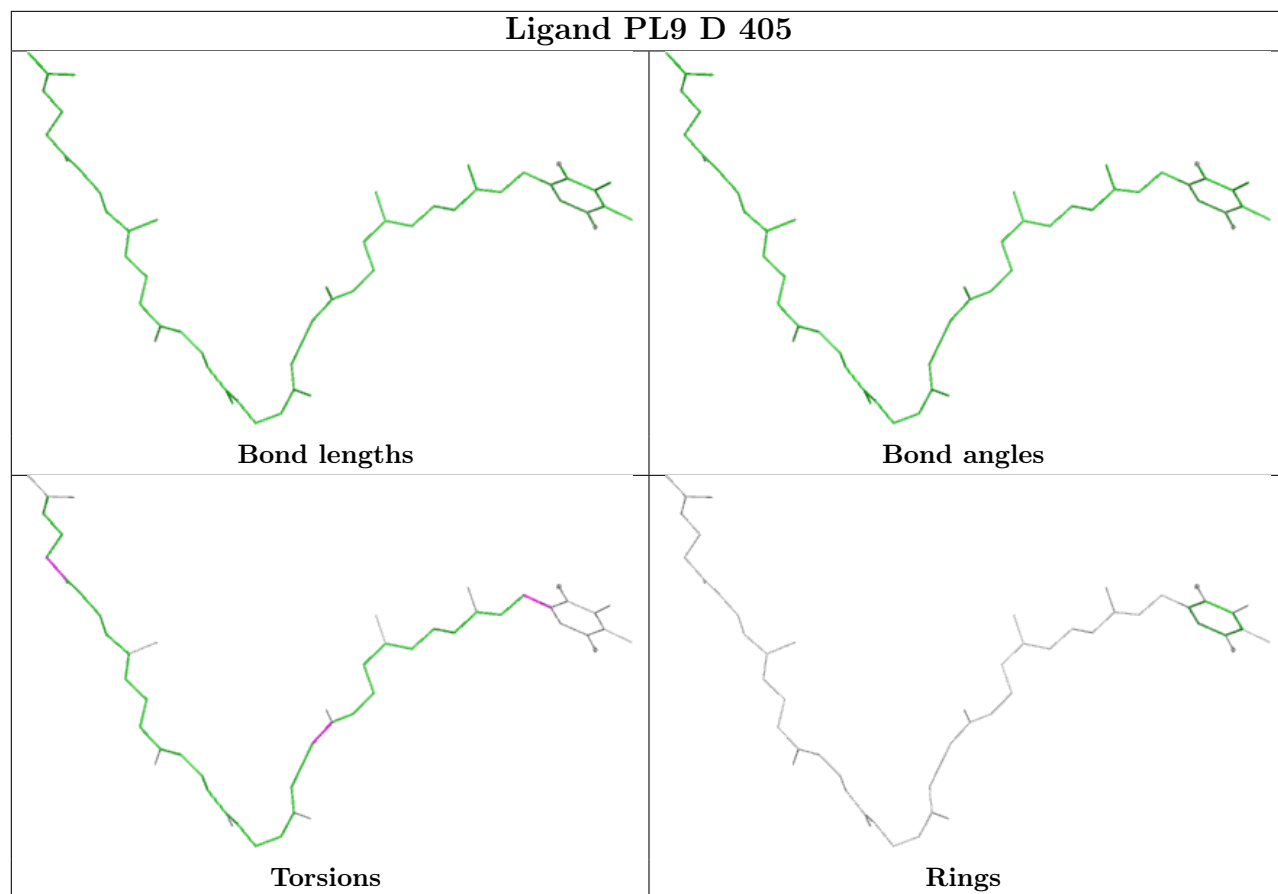




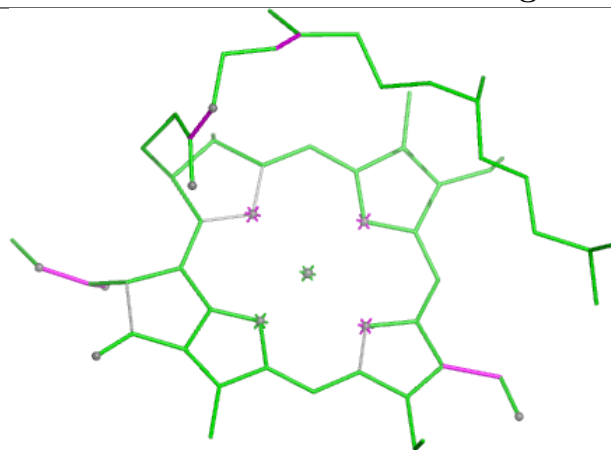




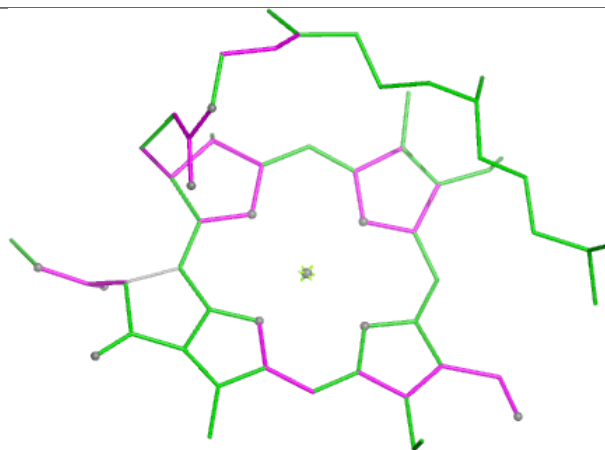




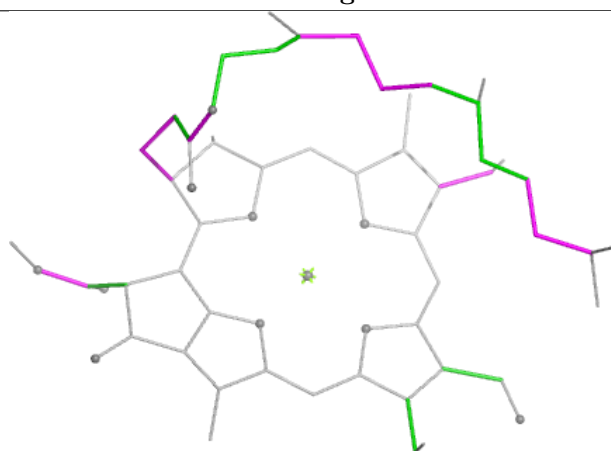
Ligand CHL r 607



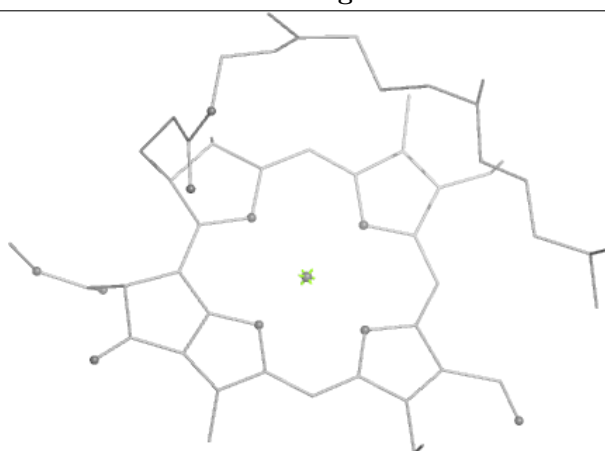
Bond lengths



Bond angles

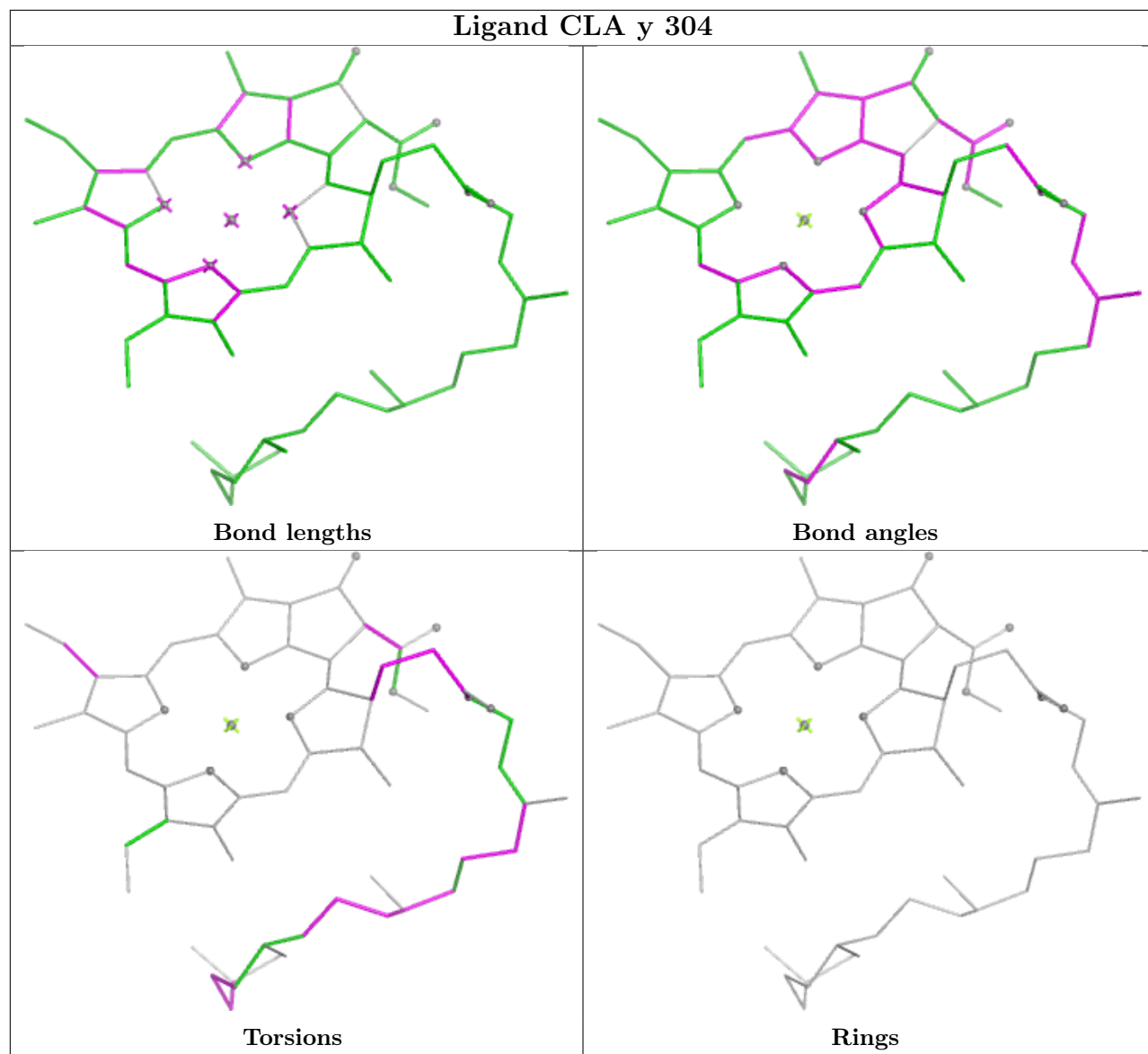


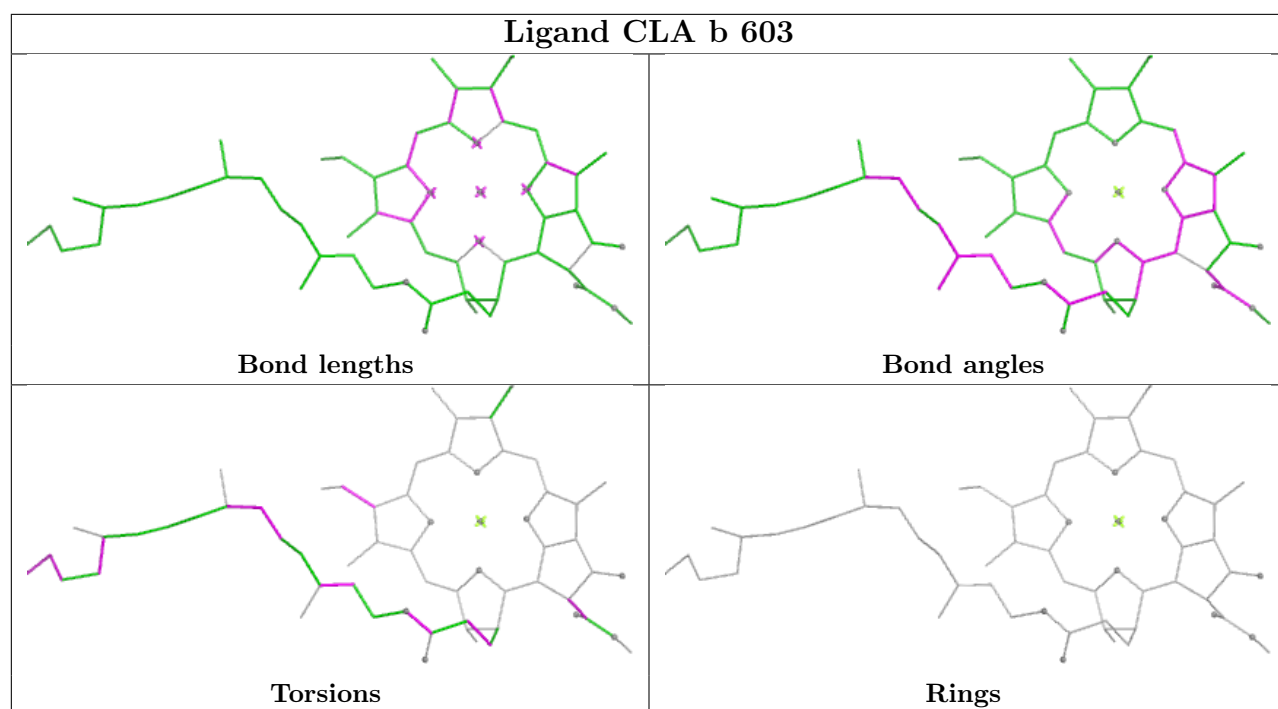
Torsions



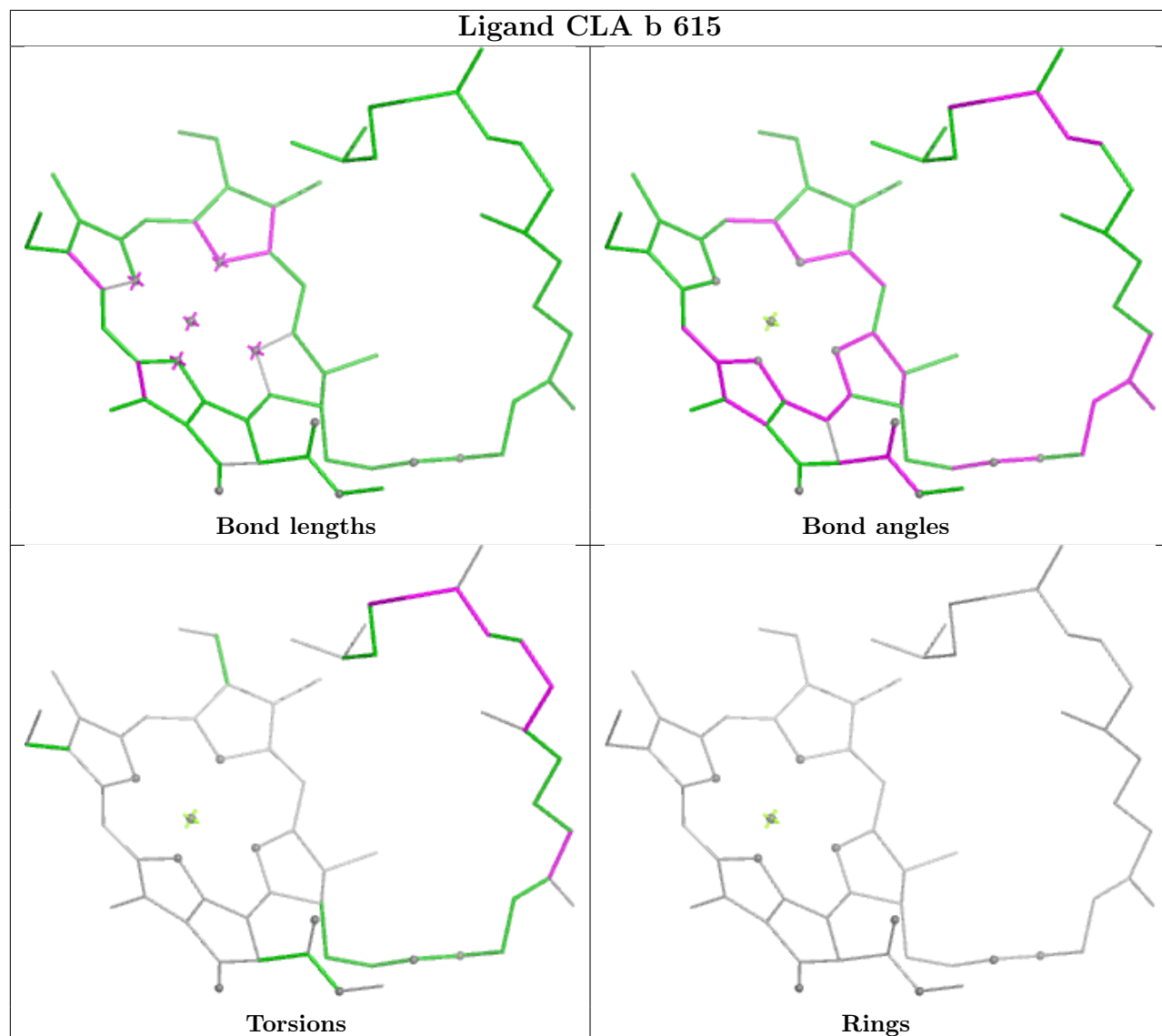
Rings

Ligand CLA y 304

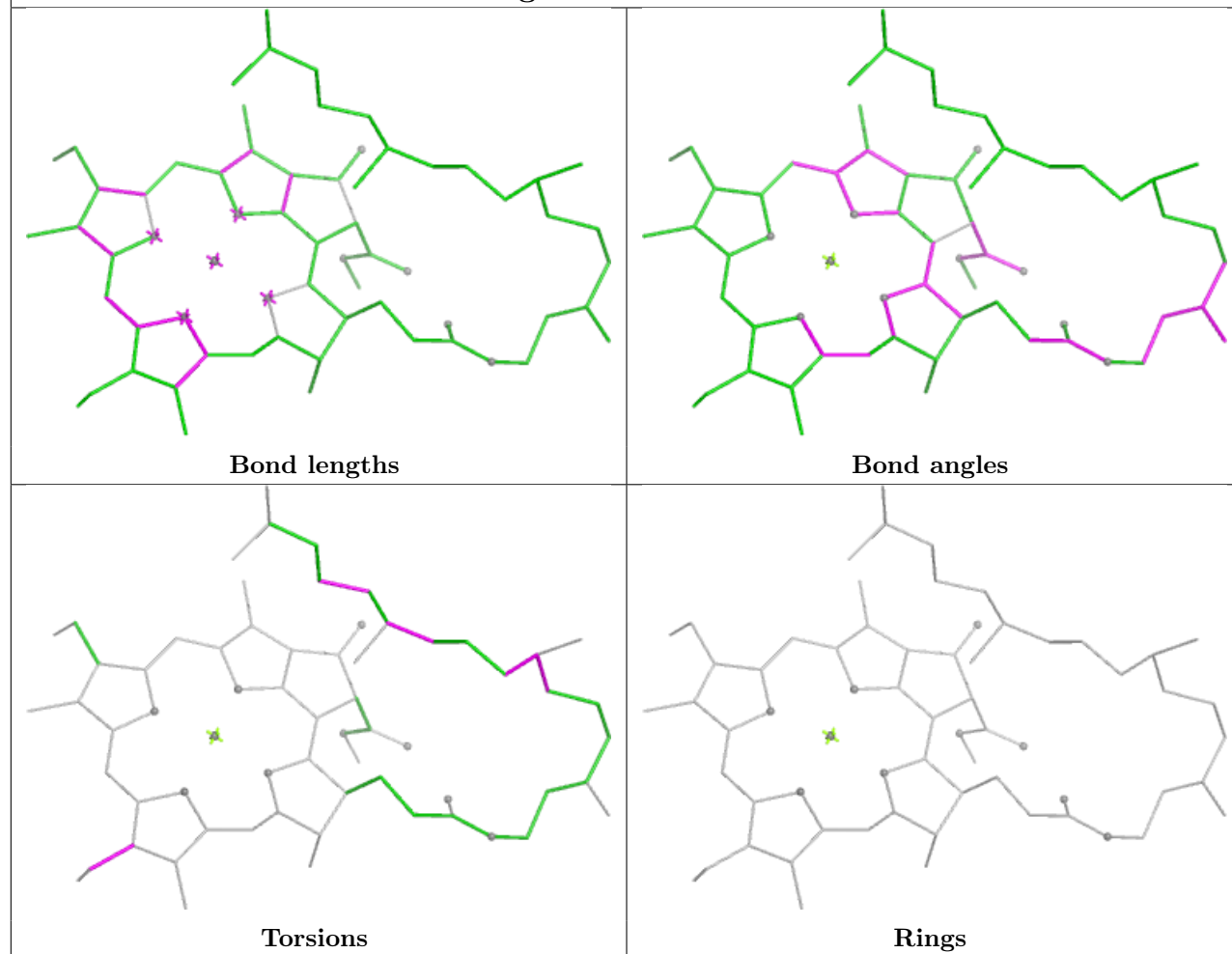




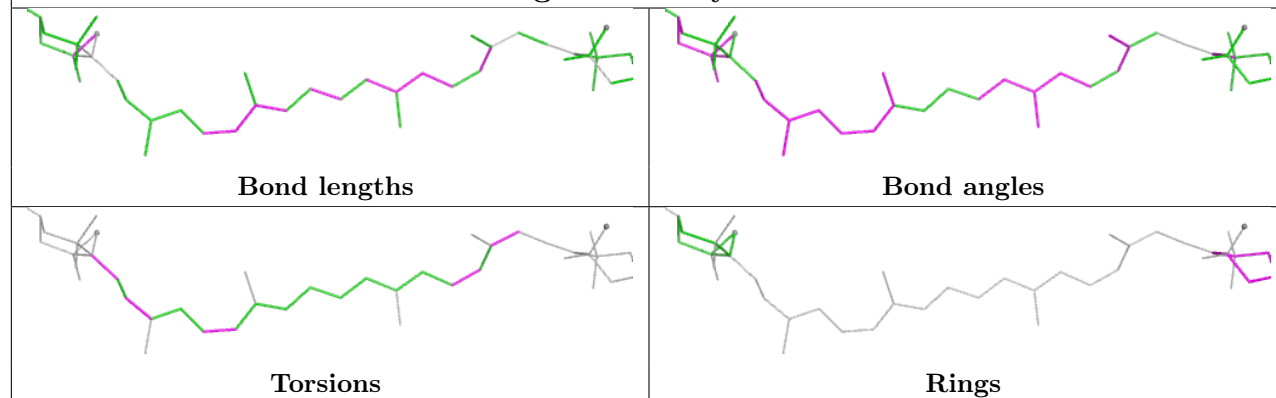
Ligand CLA b 615

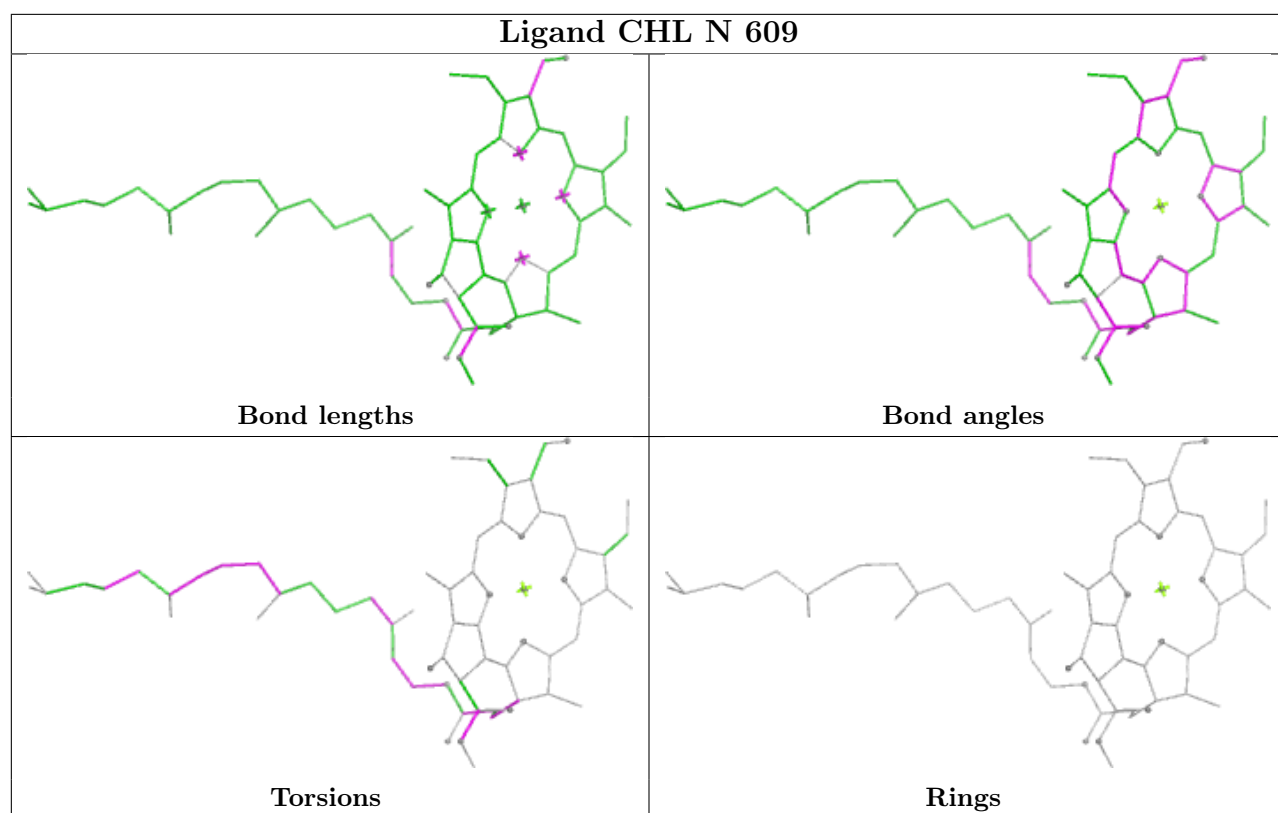


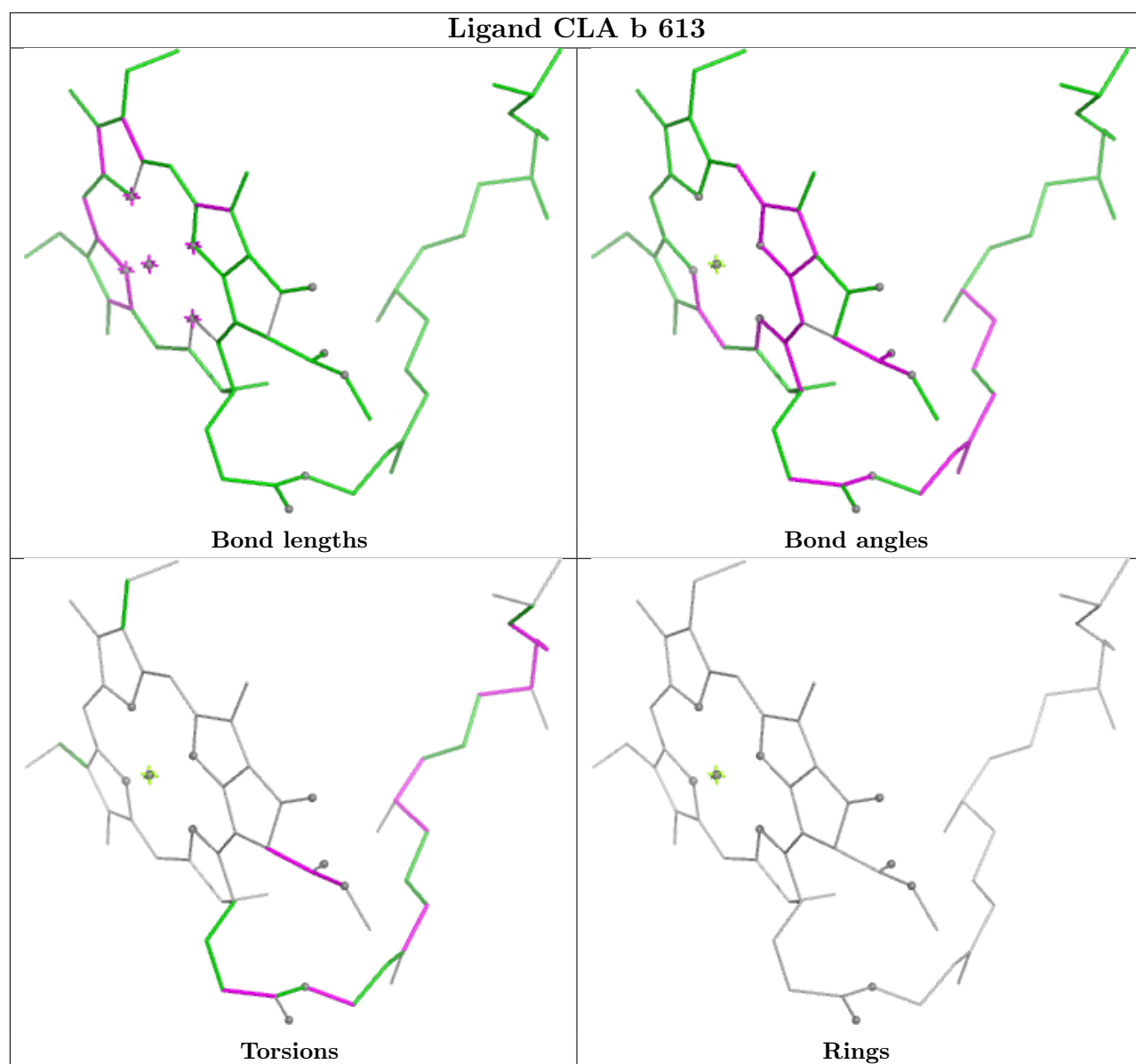
Ligand CLA c 509

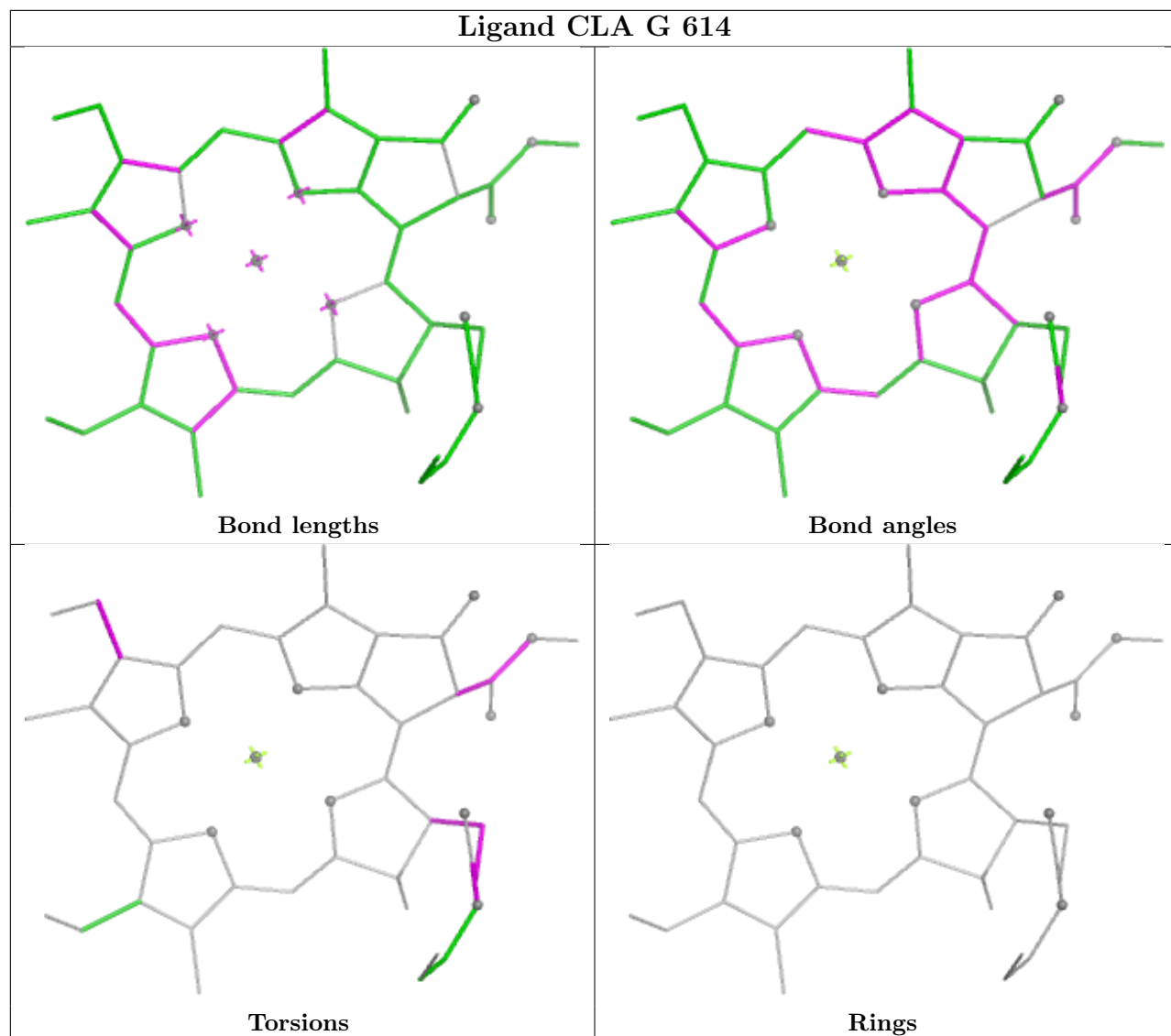


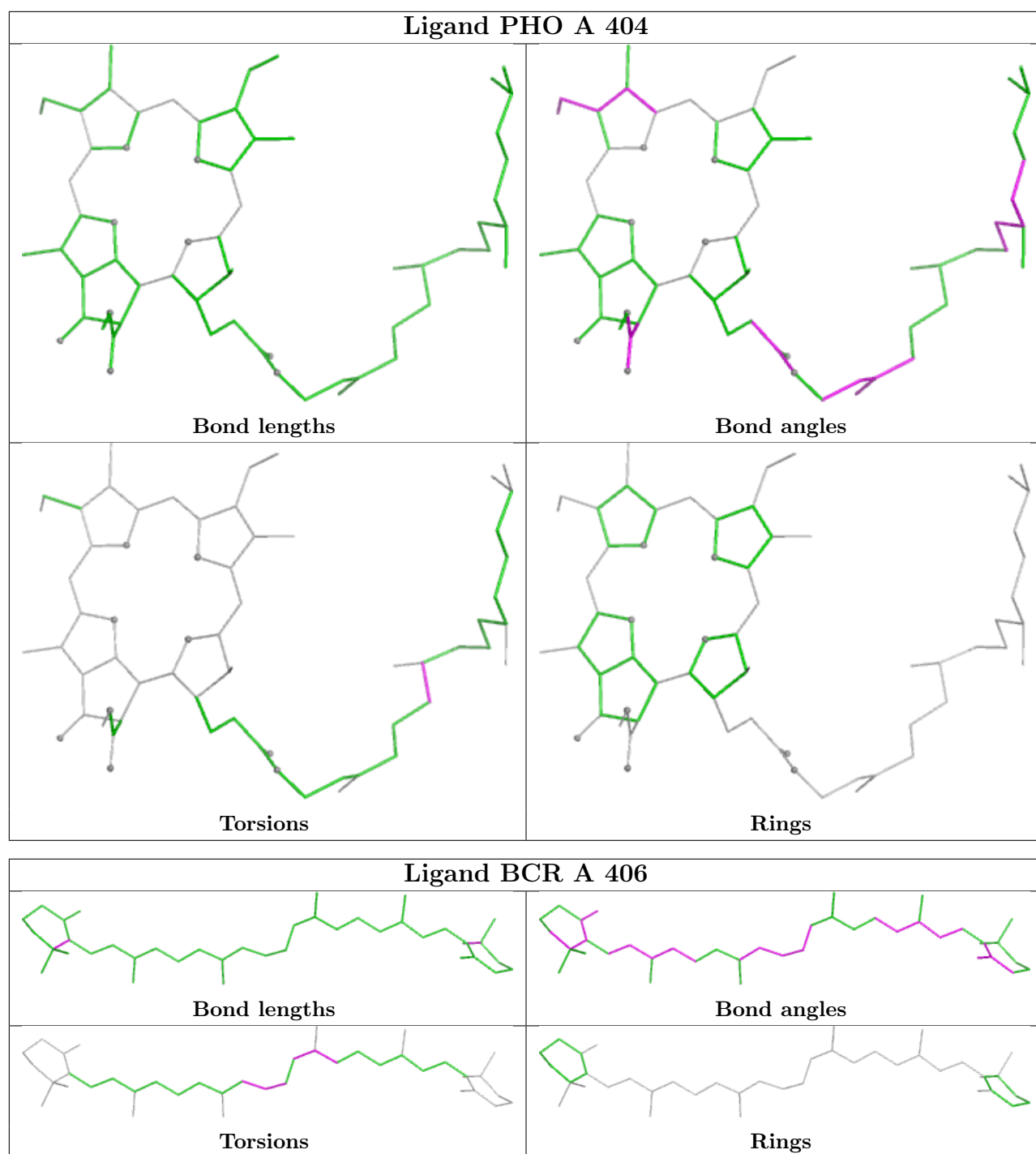
Ligand NEX y 318

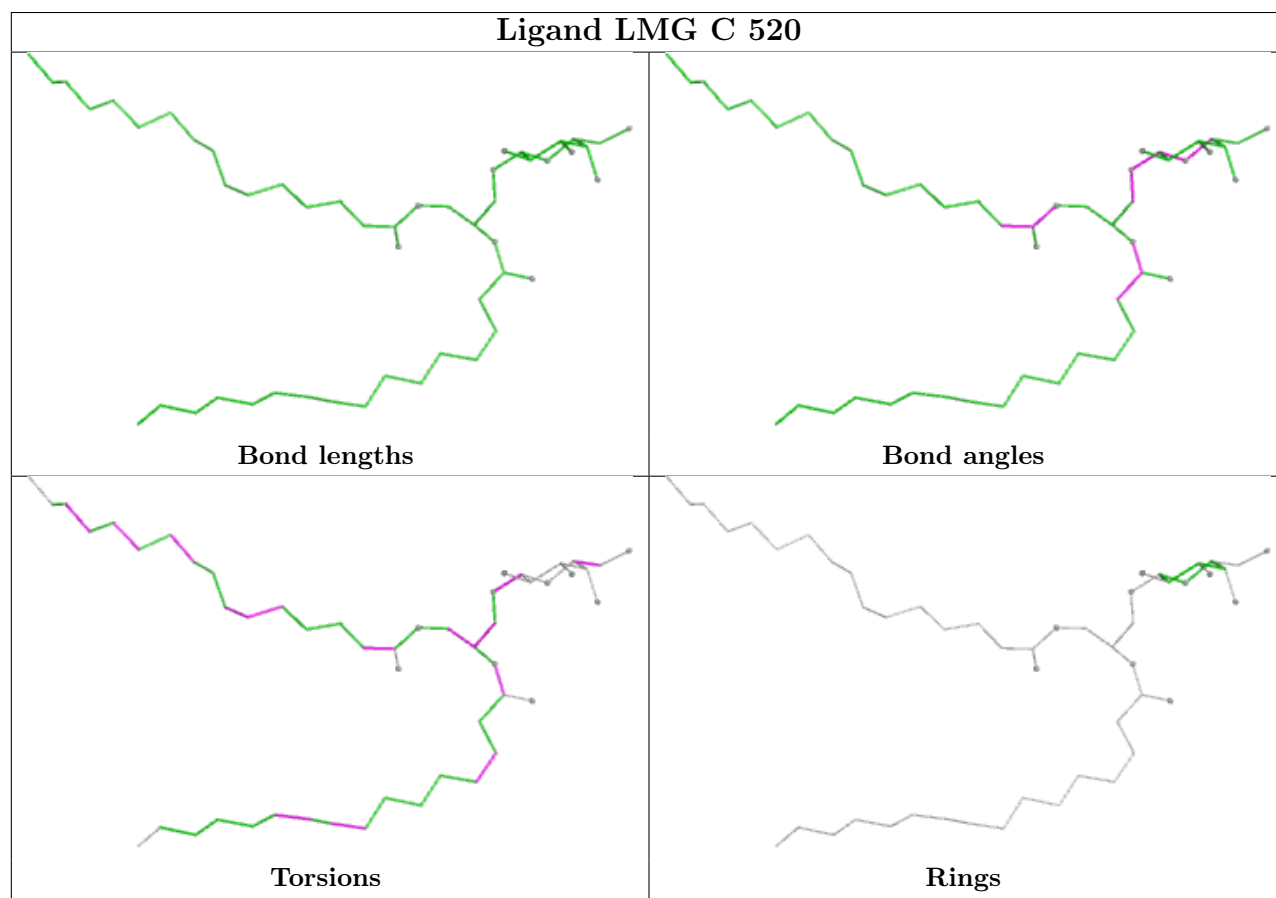
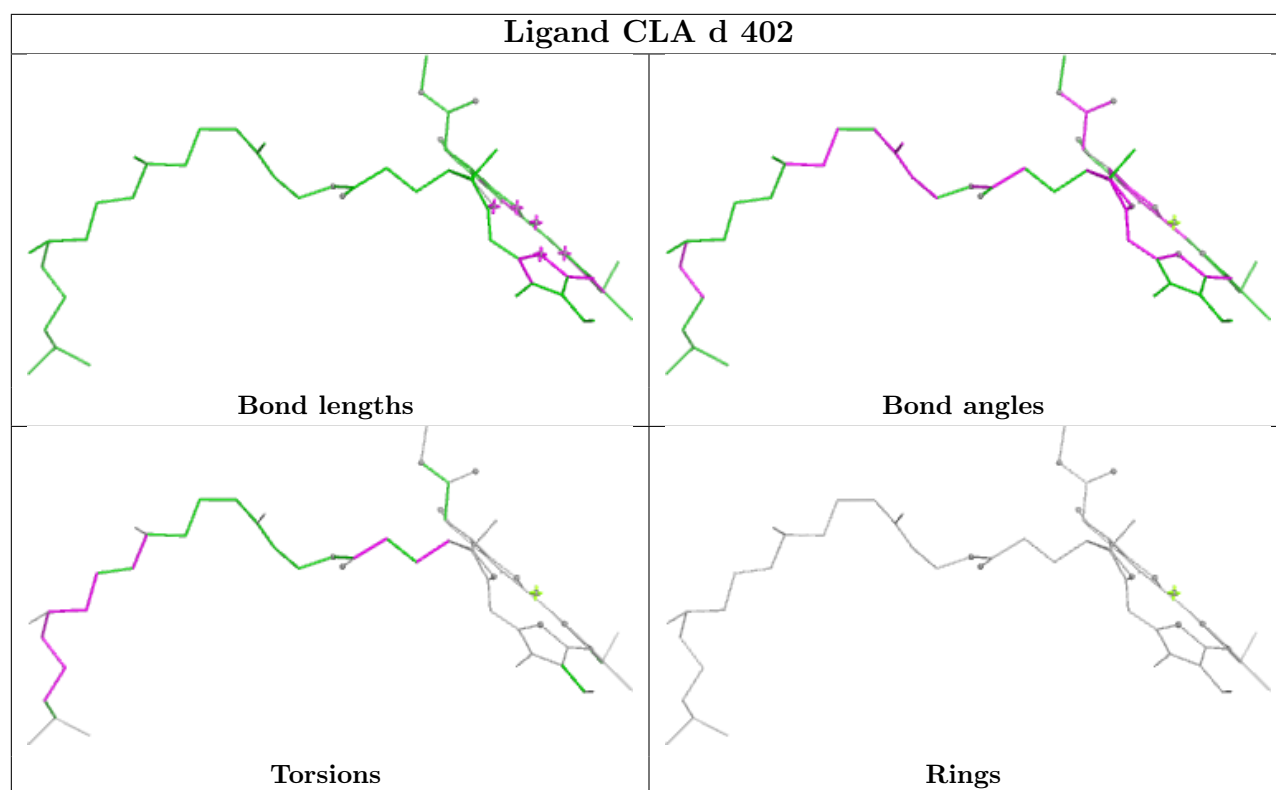




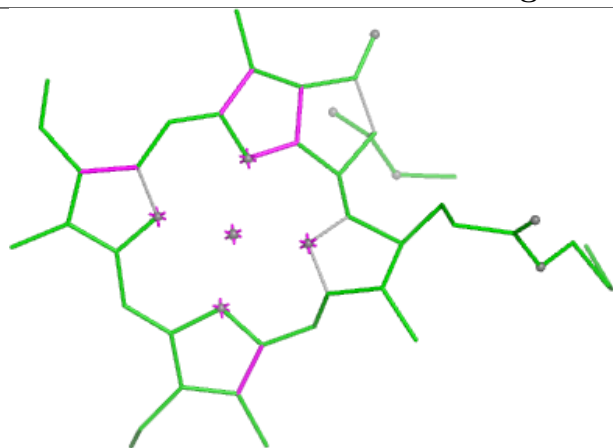




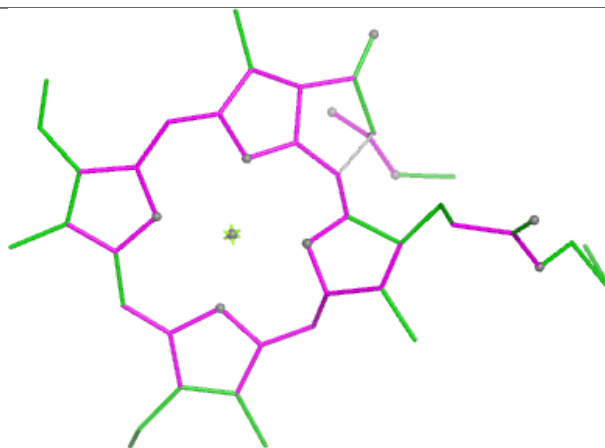




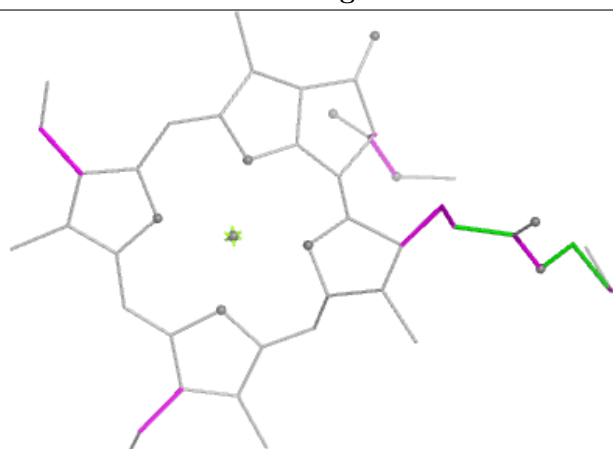
Ligand CLA r 611



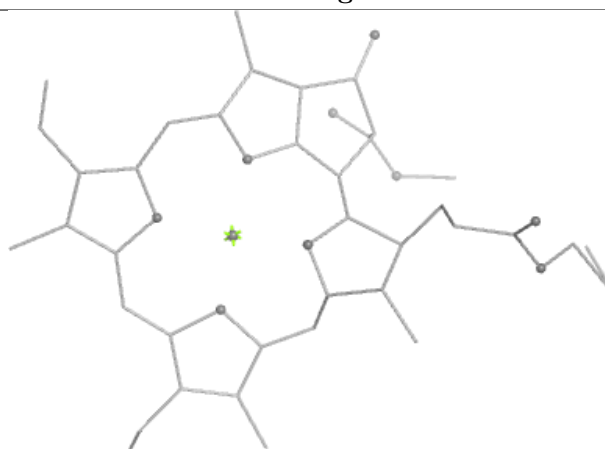
Bond lengths



Bond angles

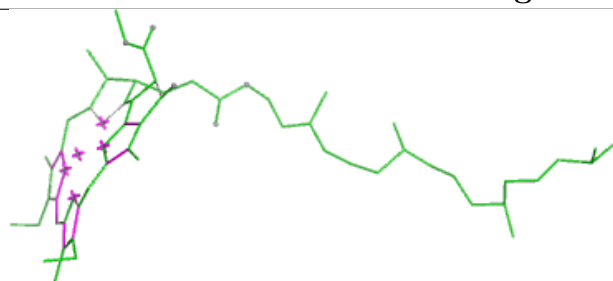


Torsions

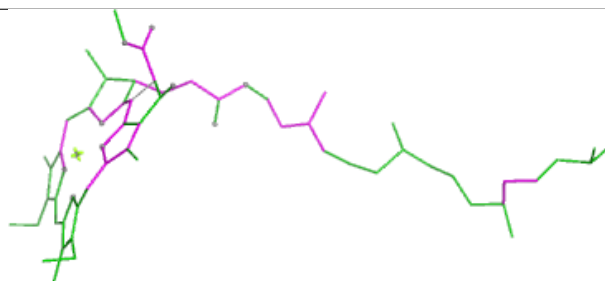


Rings

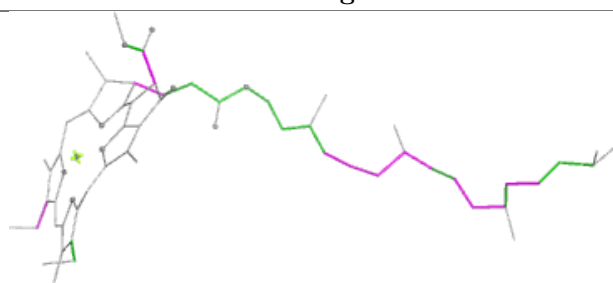
Ligand CLA B 604



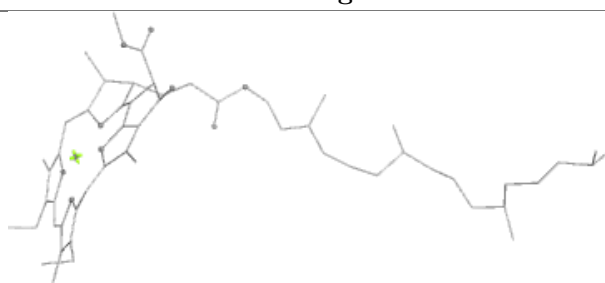
Bond lengths



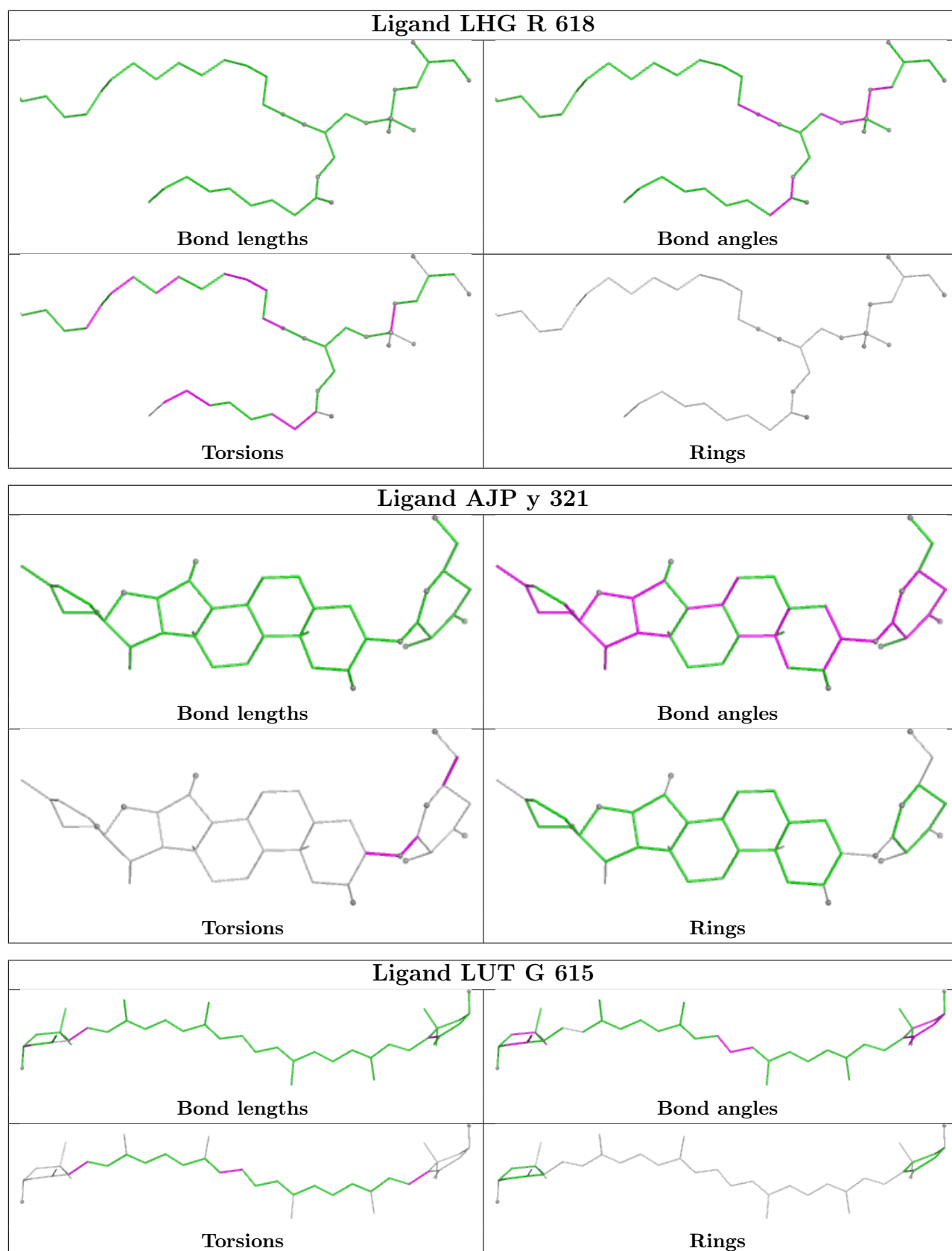
Bond angles



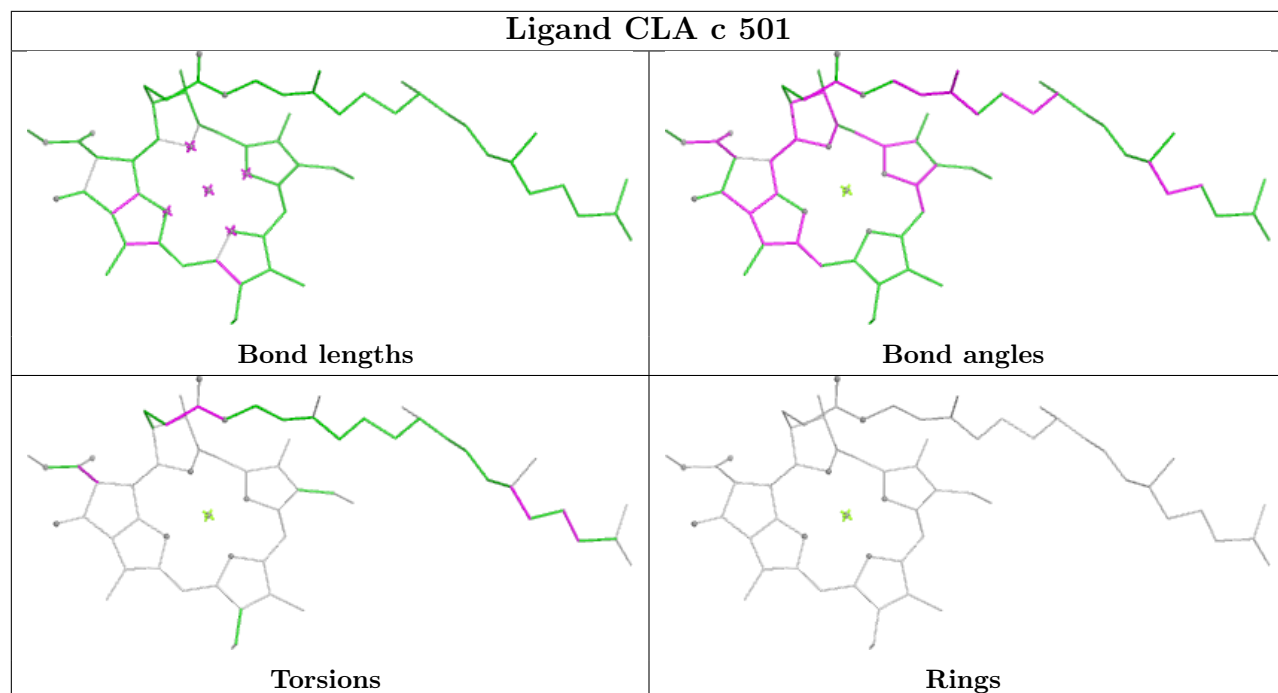
Torsions



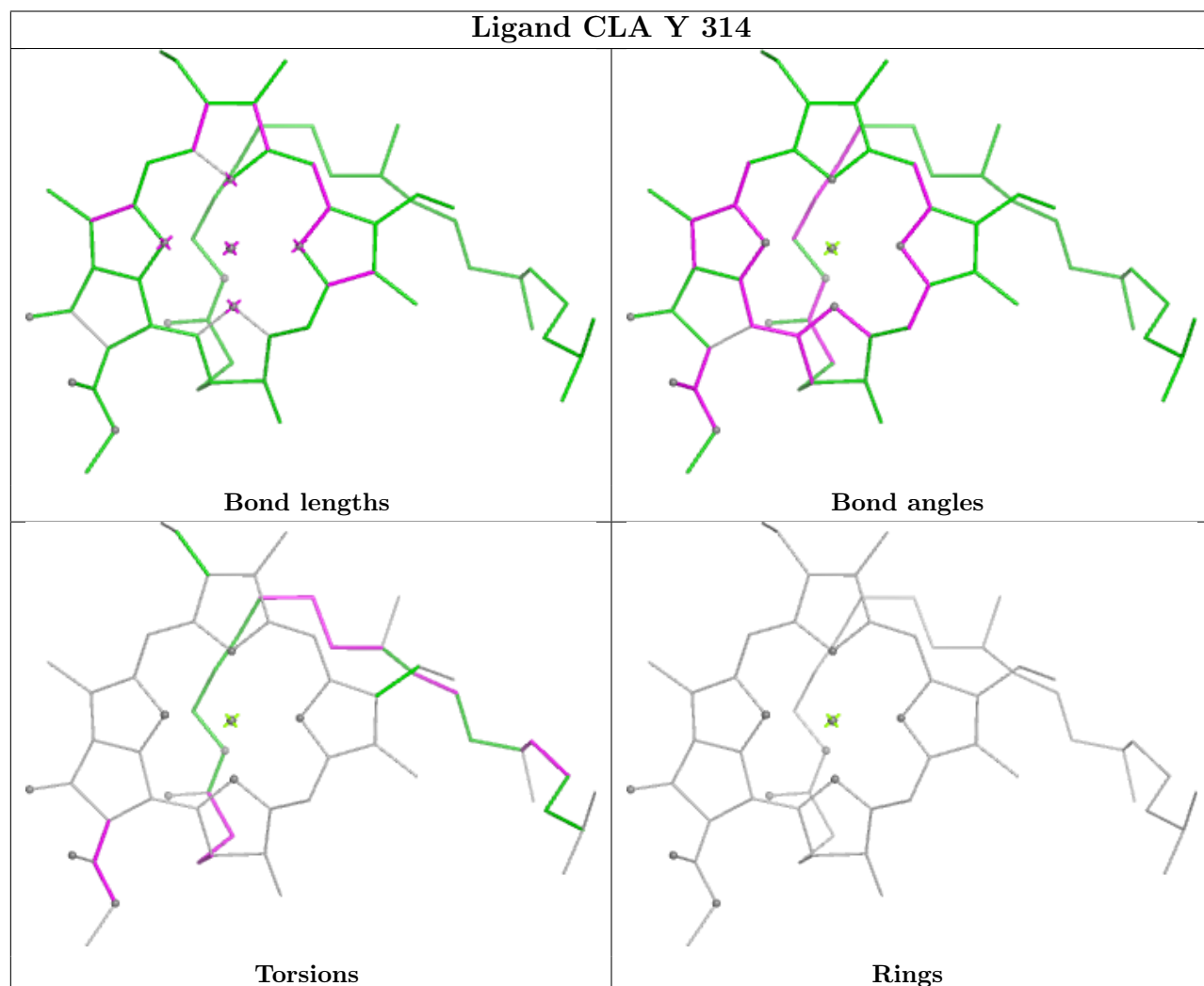
Rings

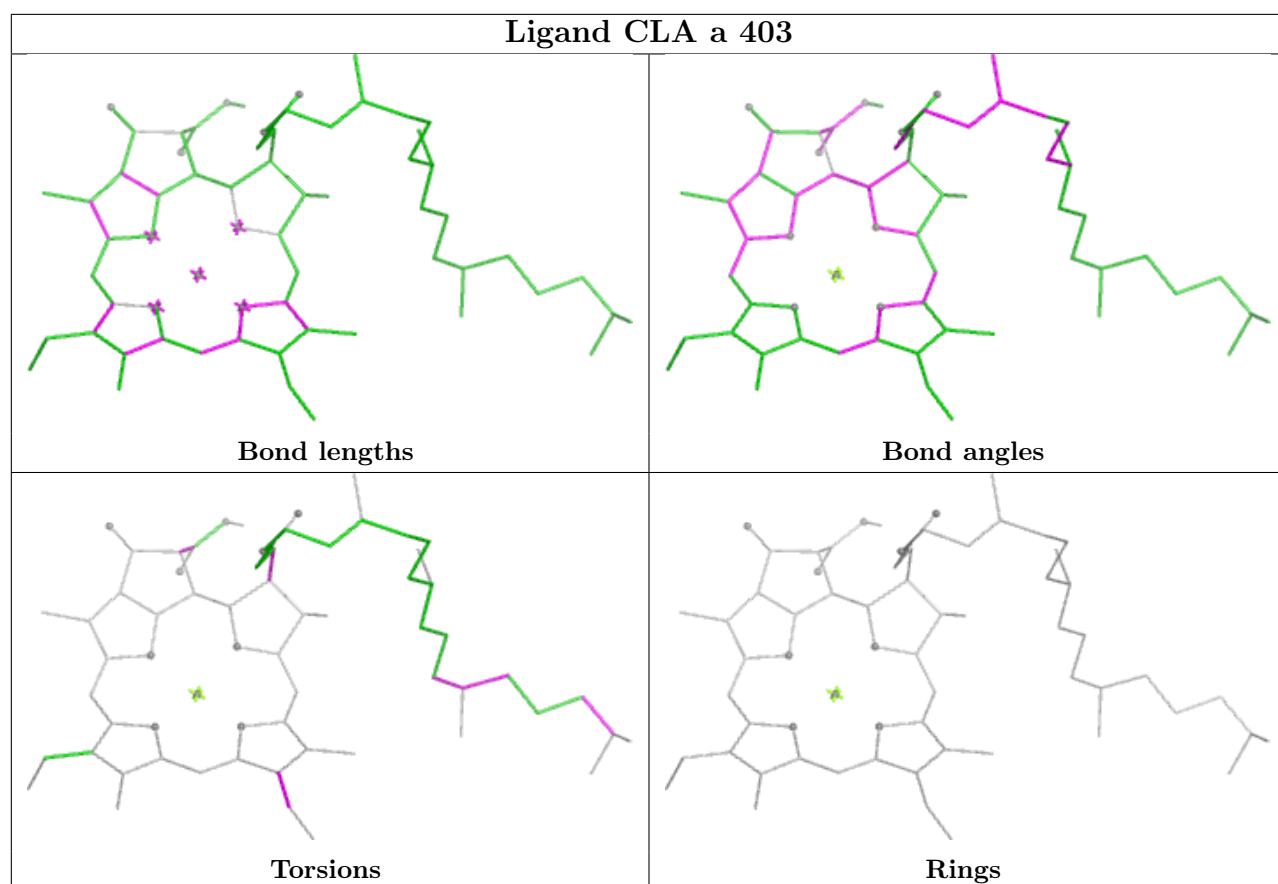


Ligand CLA c 501

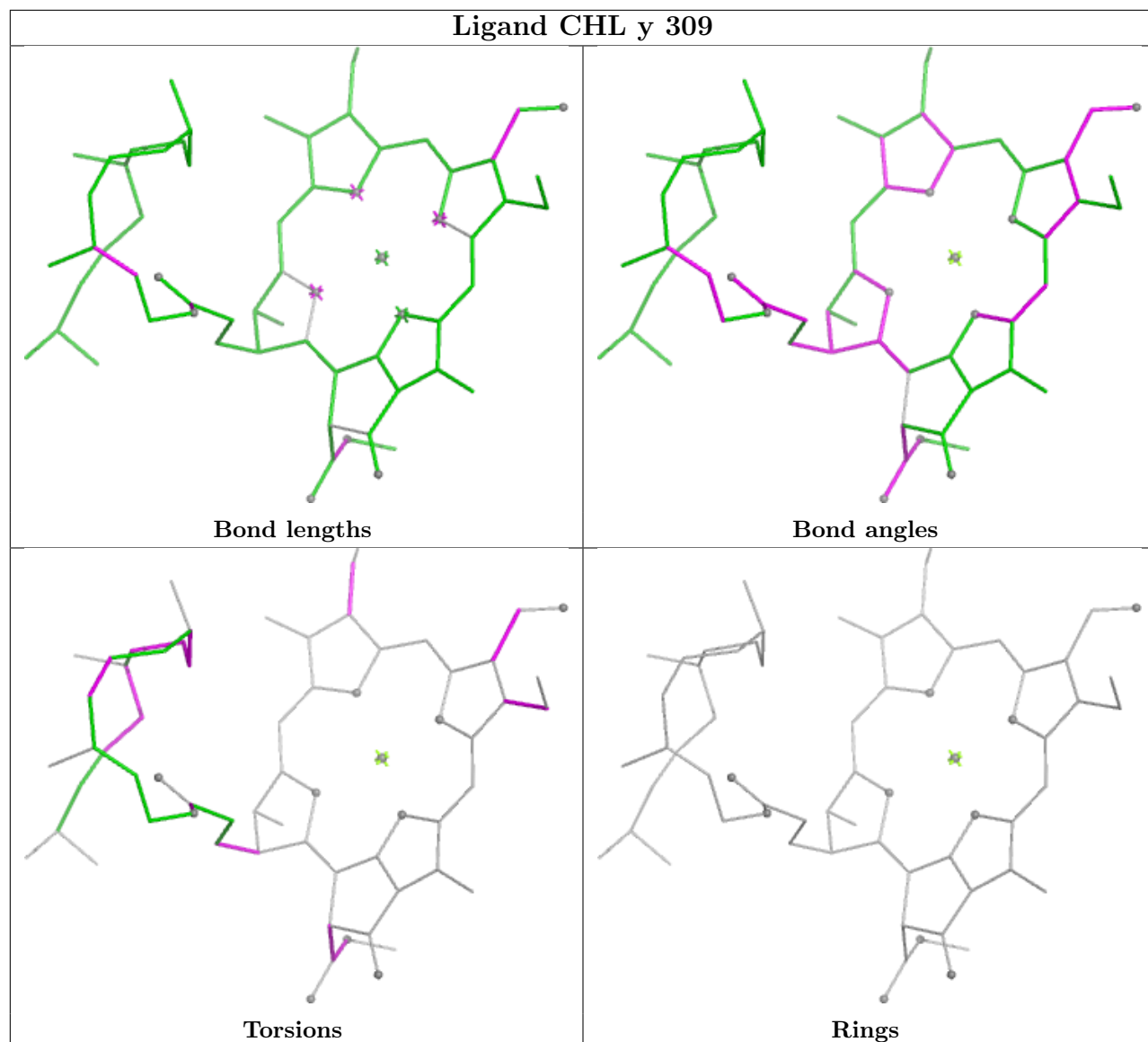


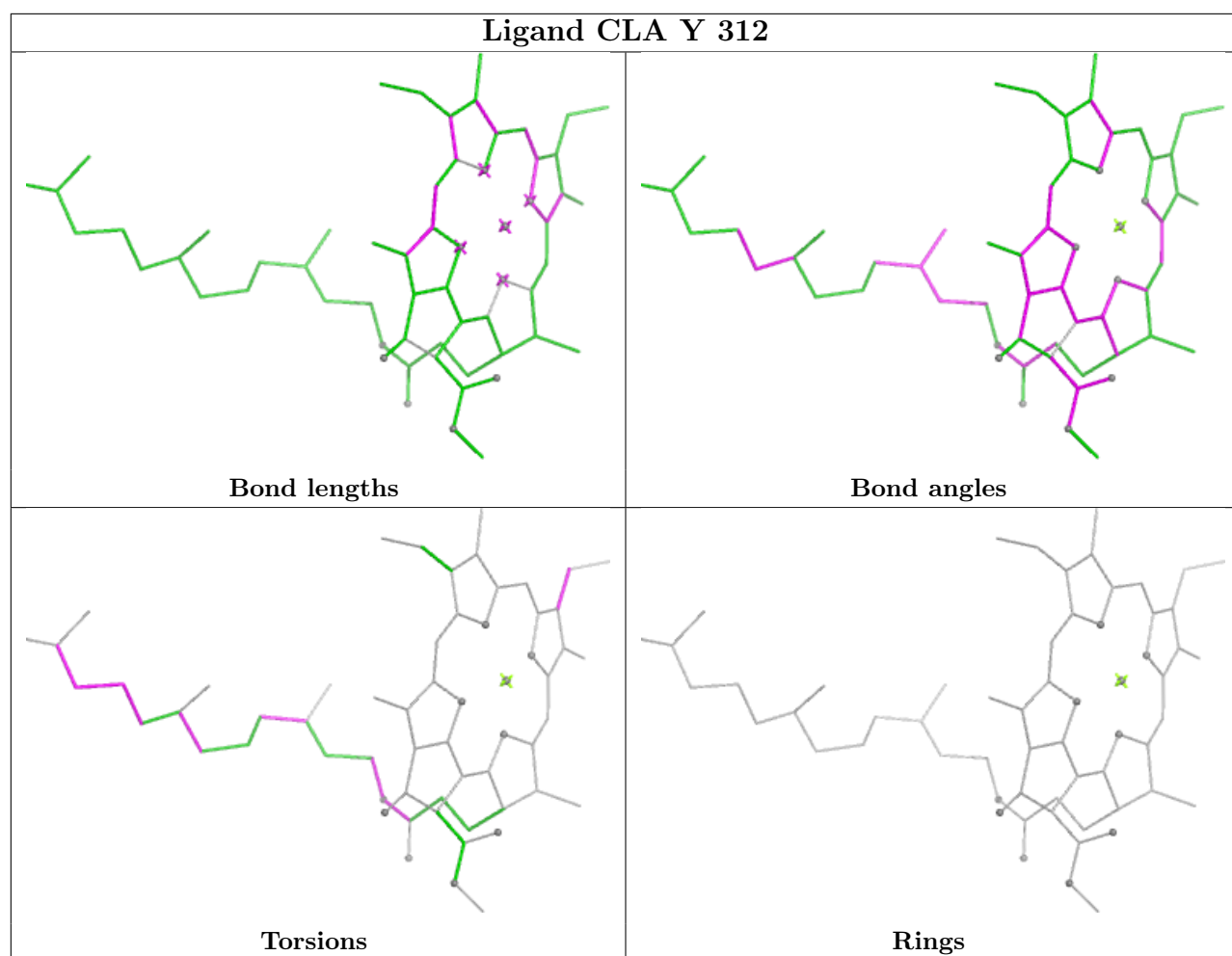
Ligand CLA Y 314

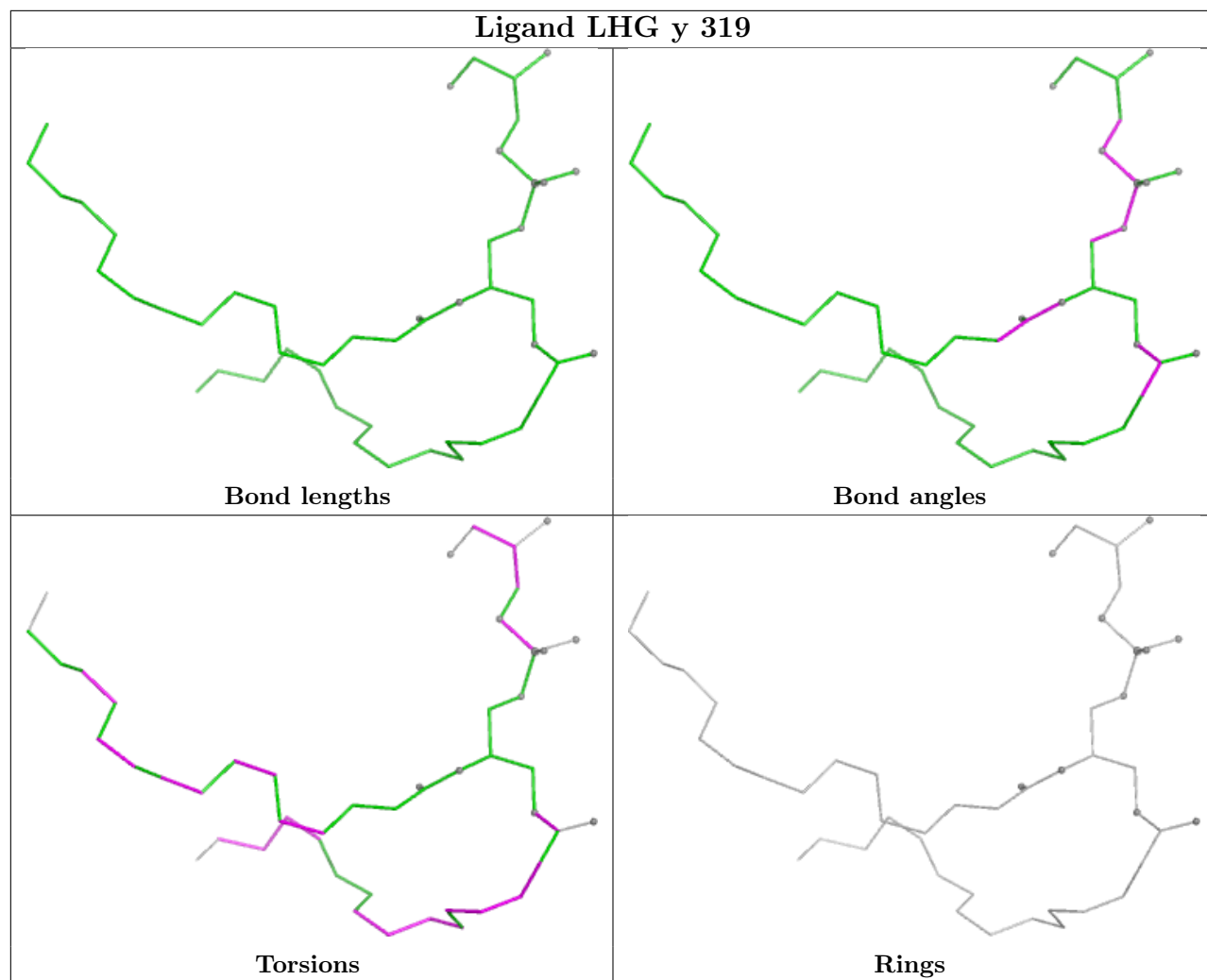


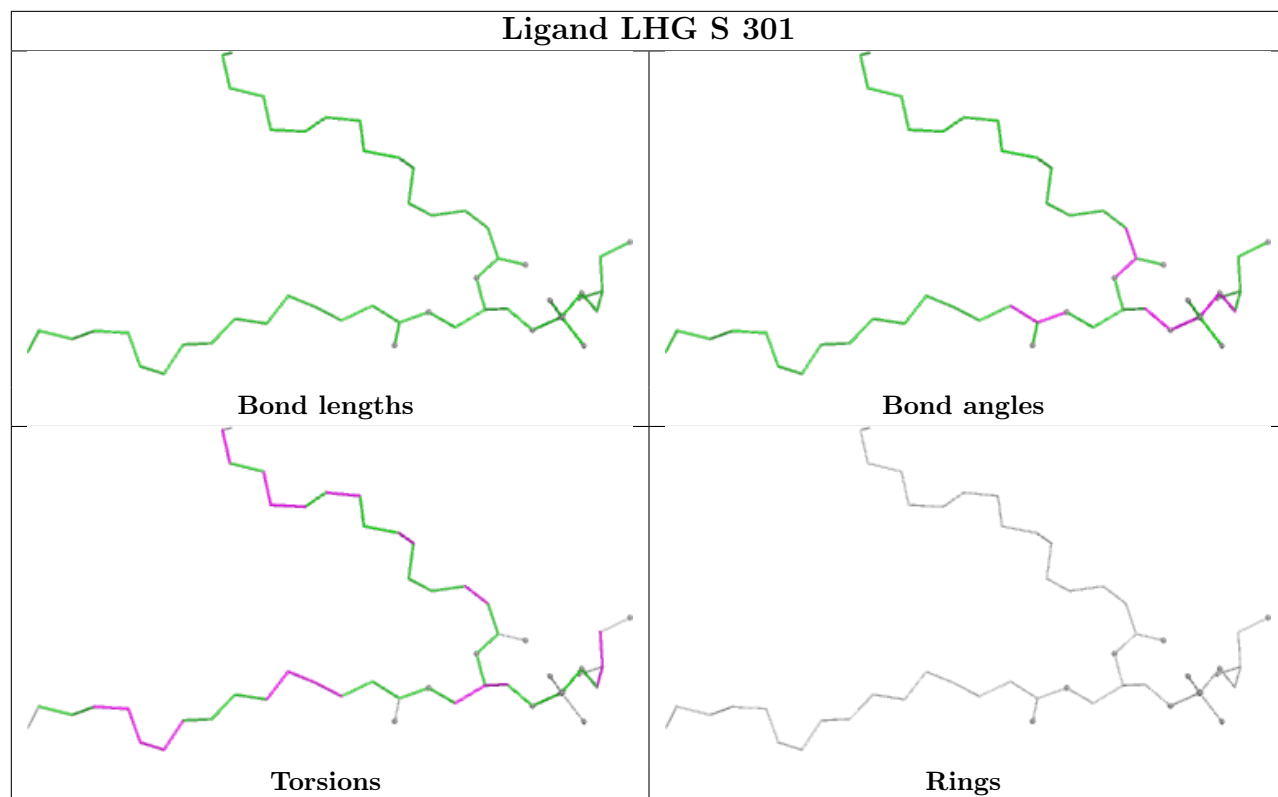


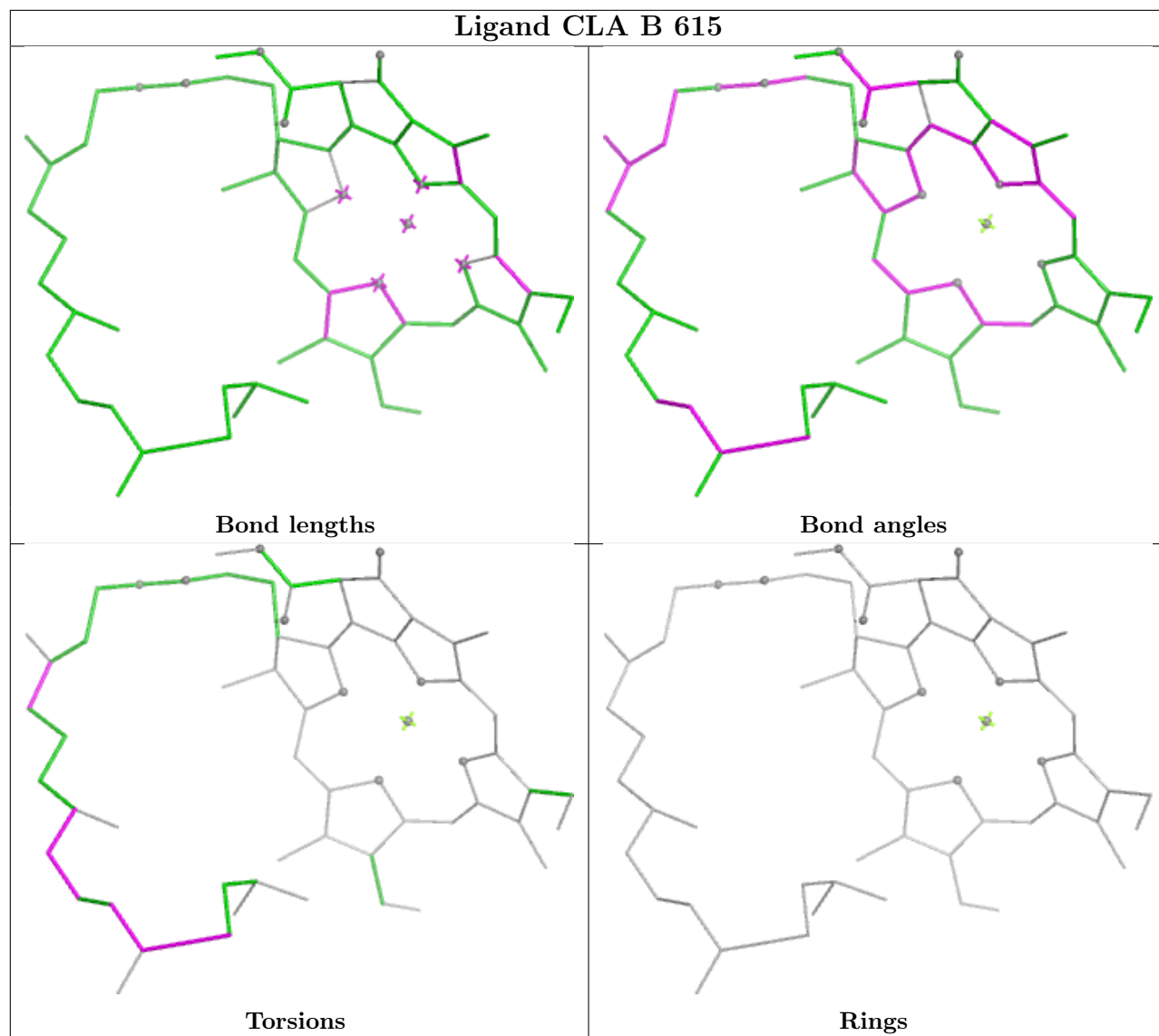
Ligand CHL y 309



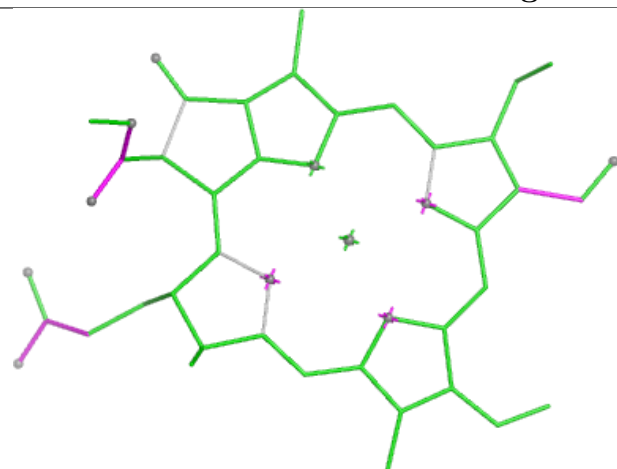




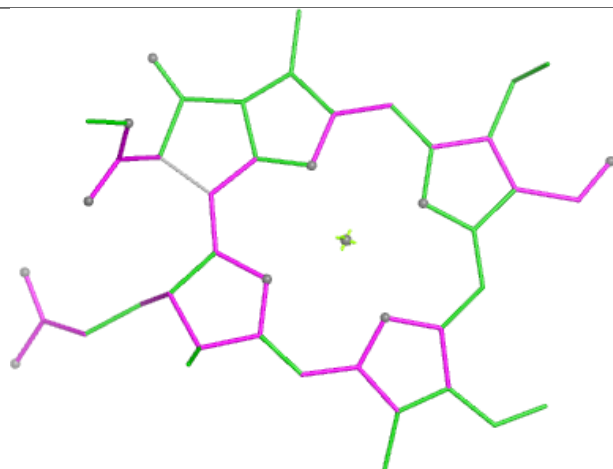




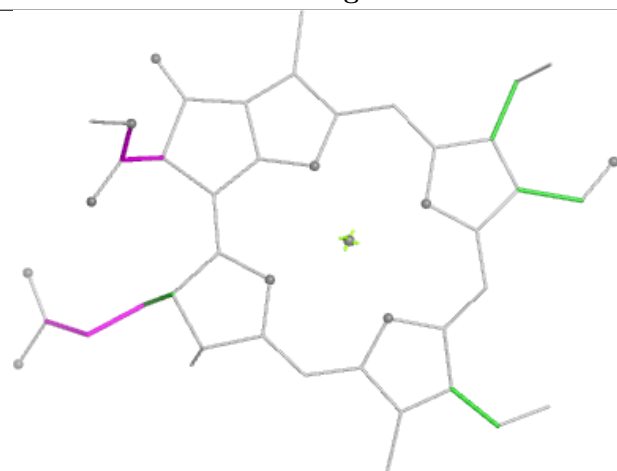
Ligand CHL S 306



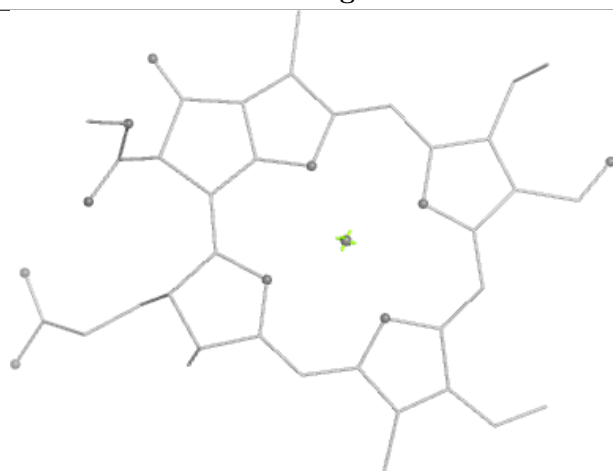
Bond lengths



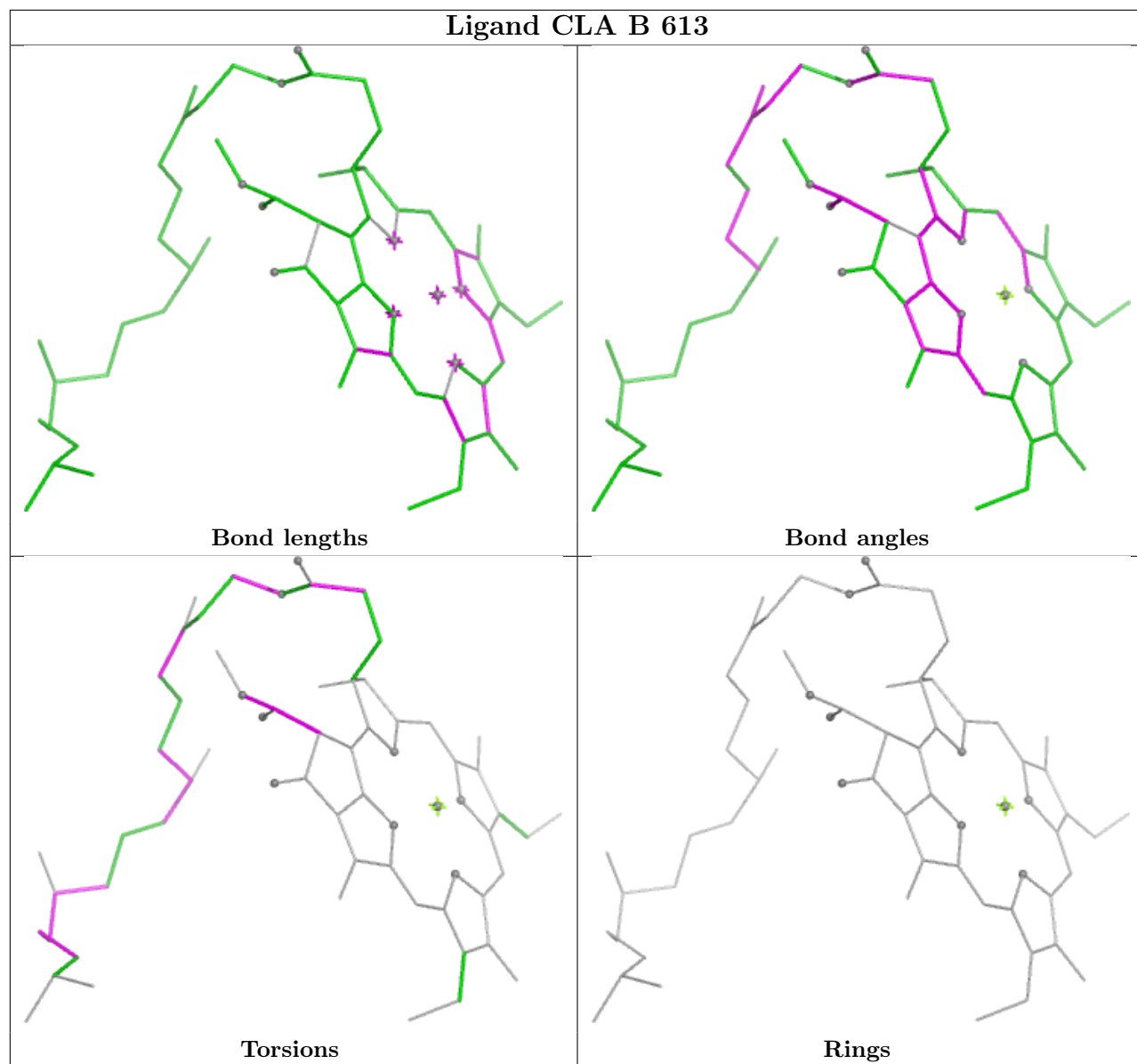
Bond angles



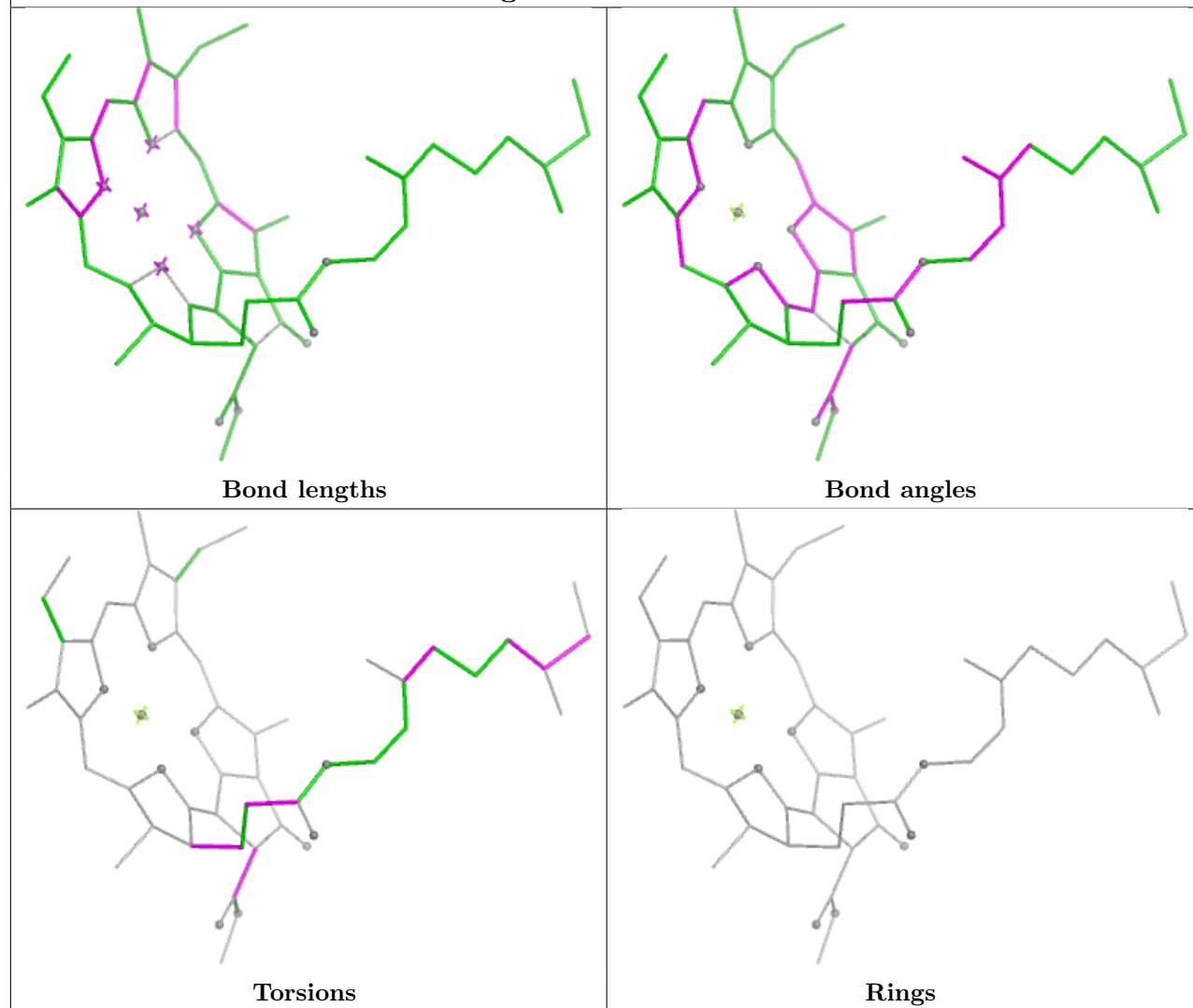
Torsions



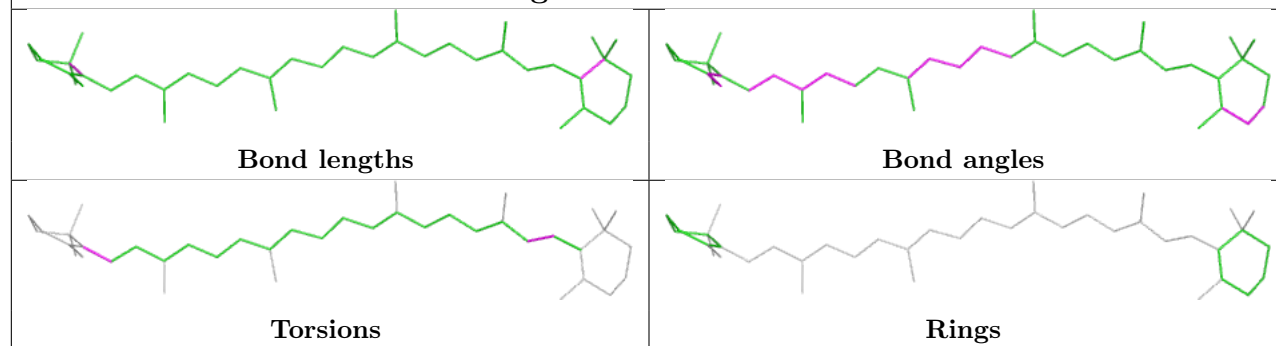
Rings



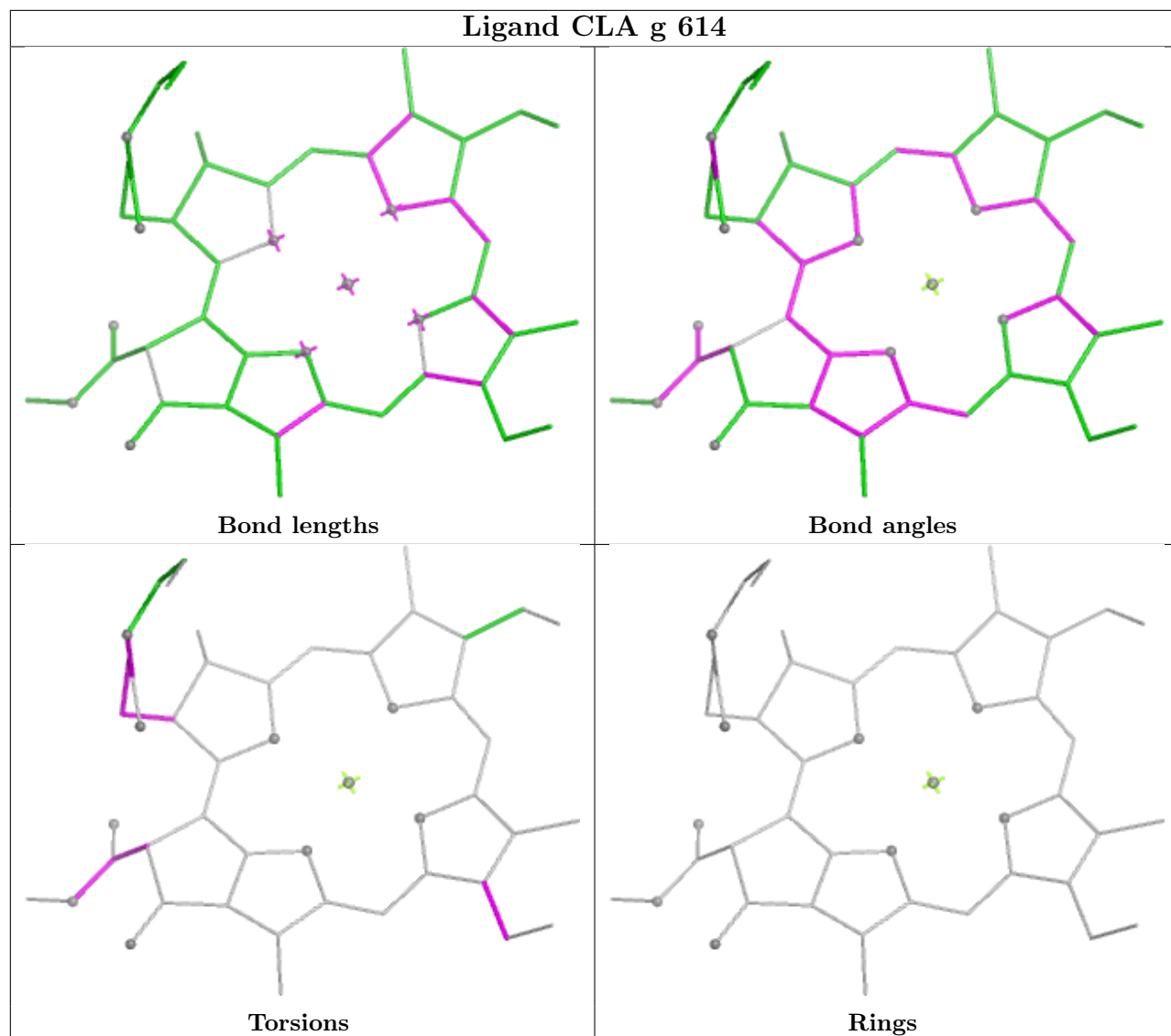
Ligand CLA S 311

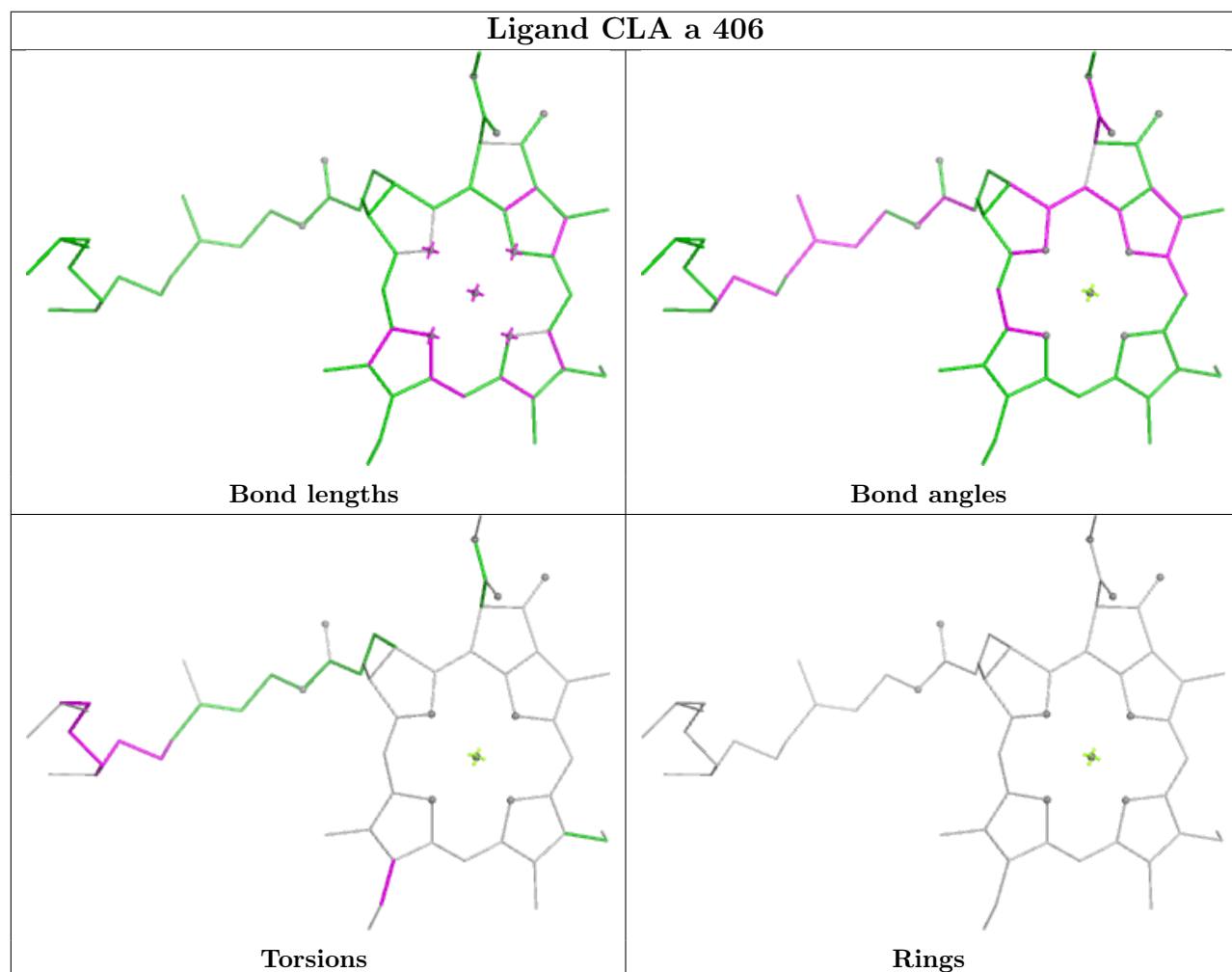
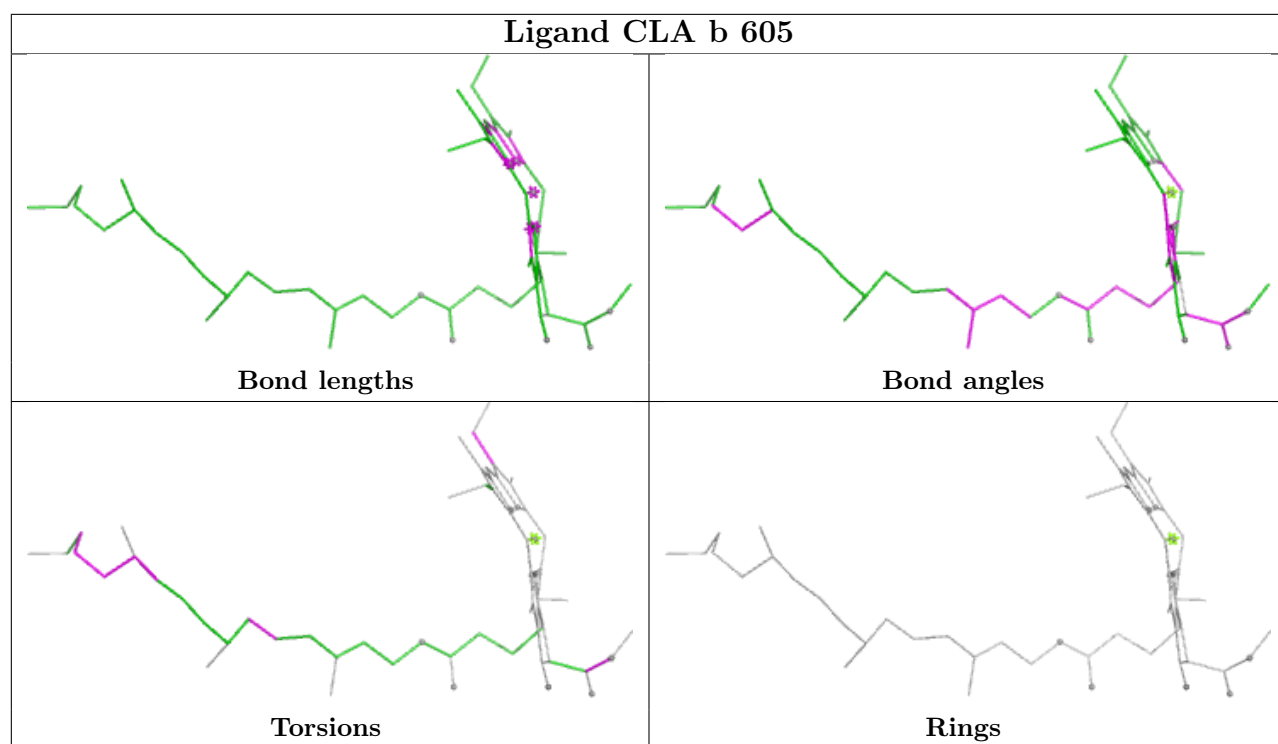


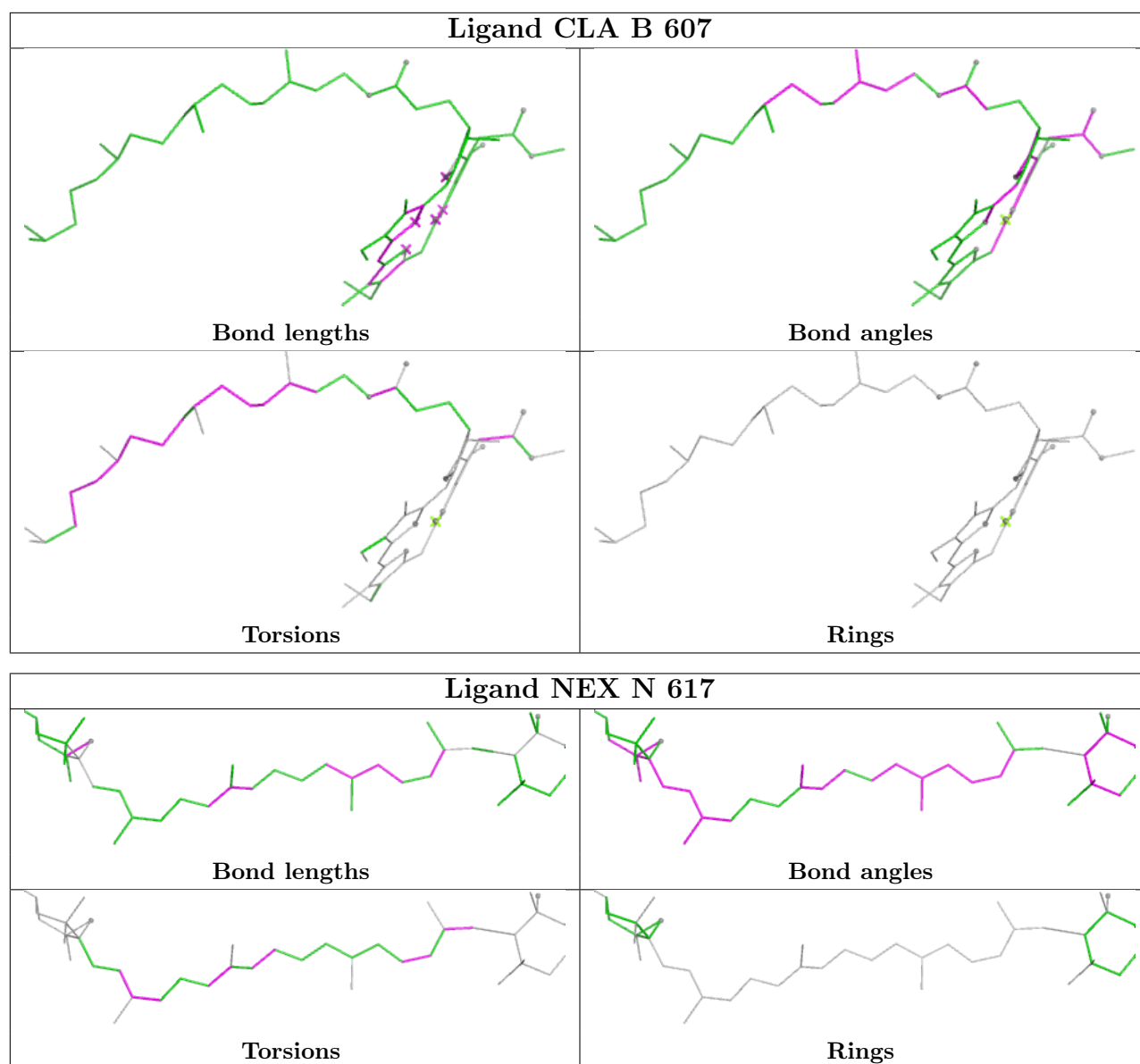
Ligand BCR B 617

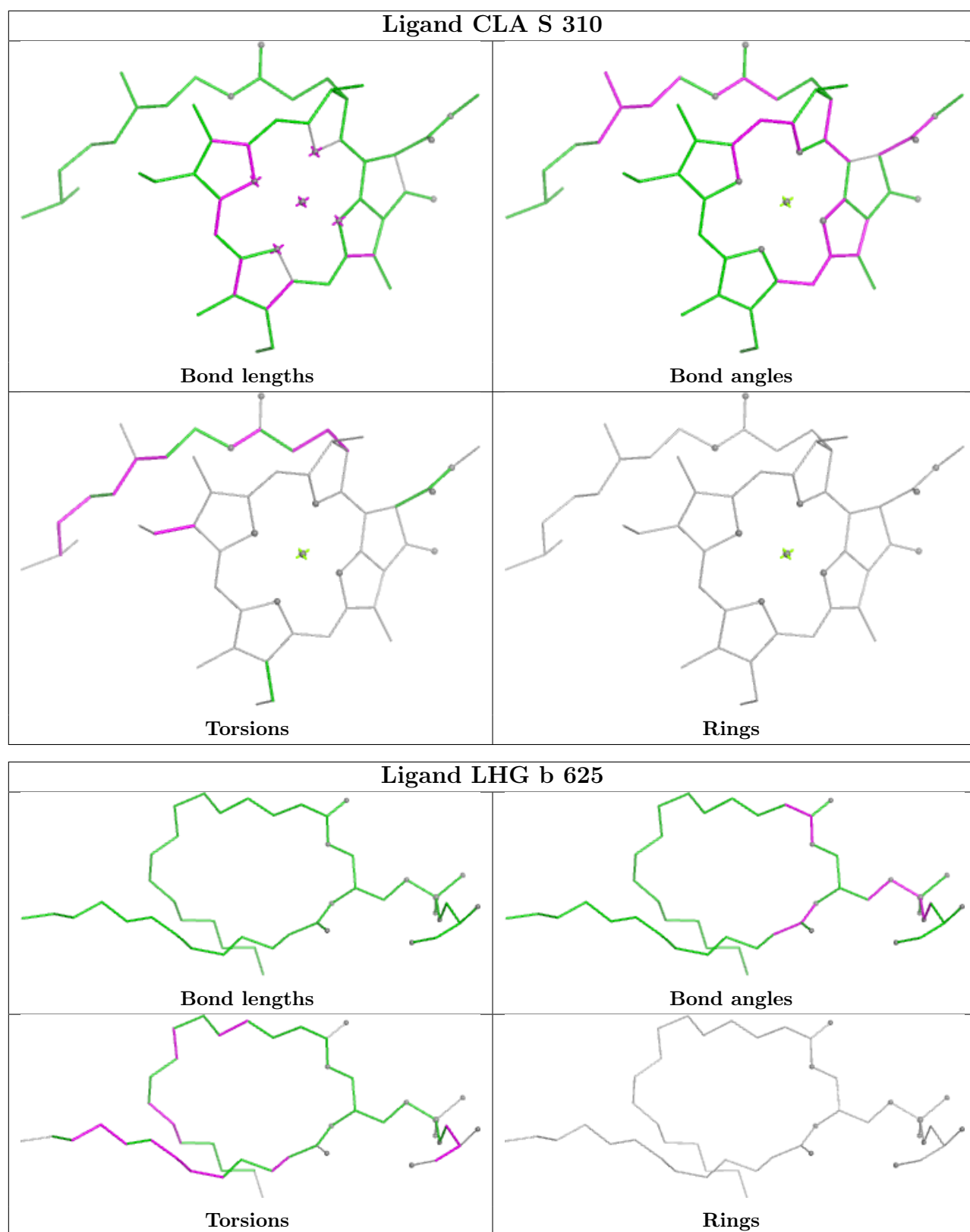


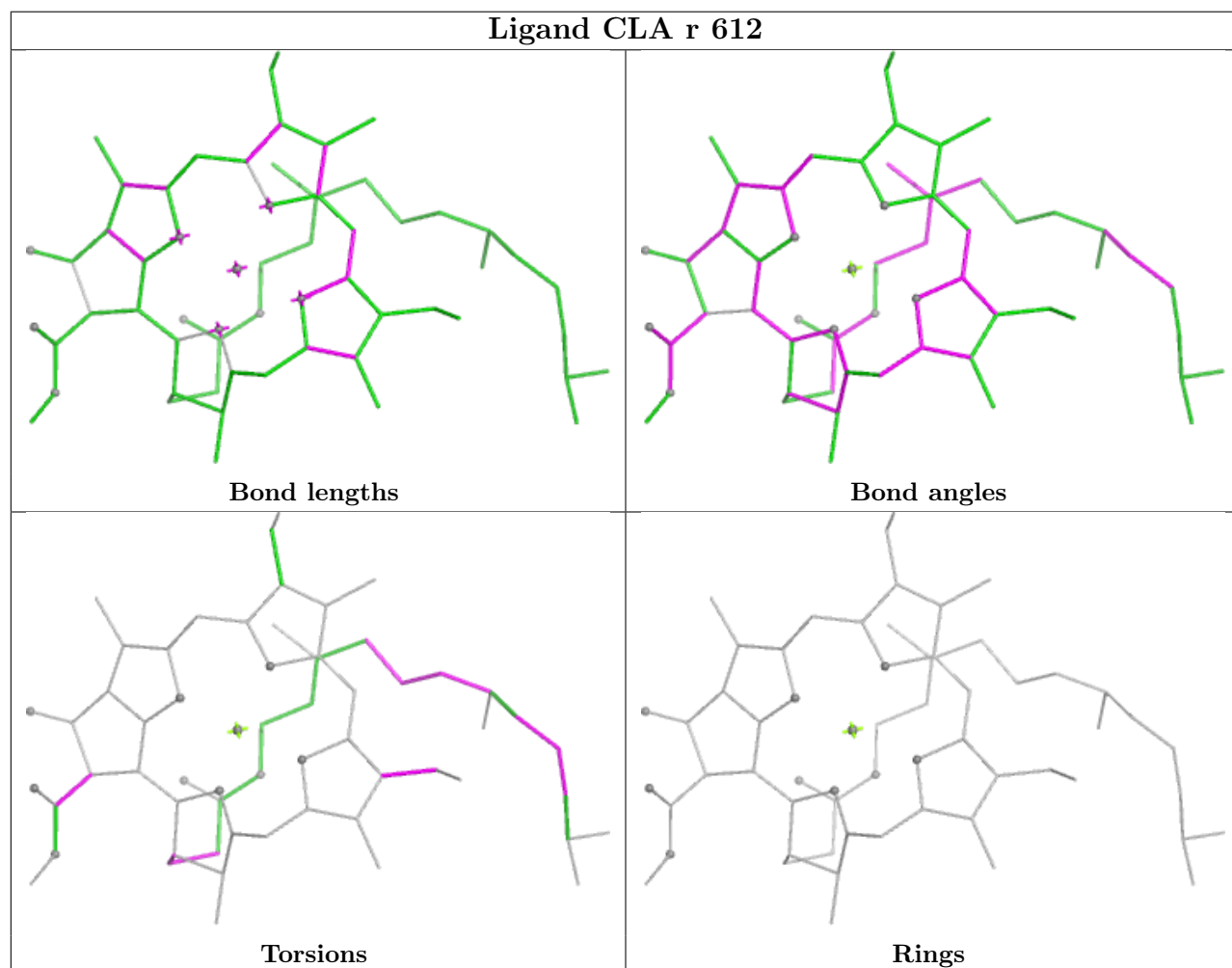
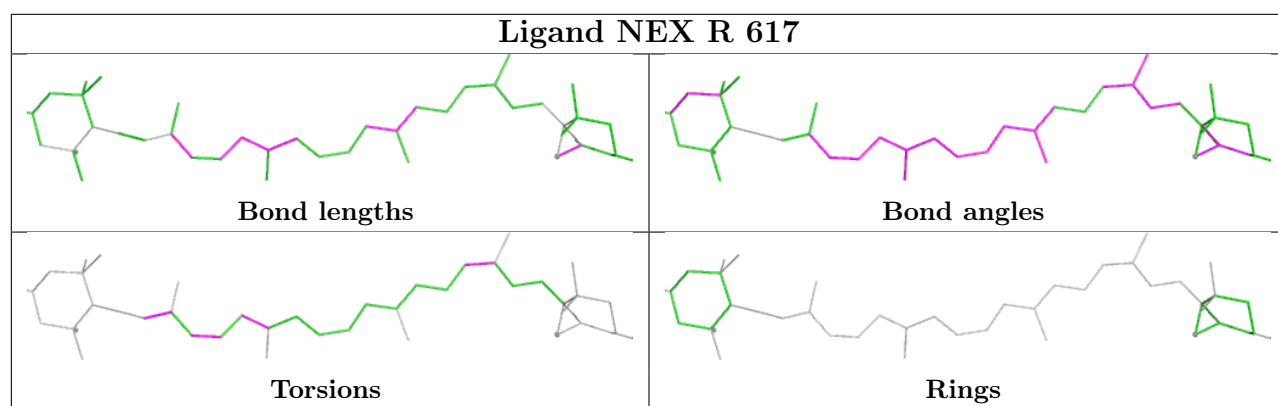
Ligand CLA g 614



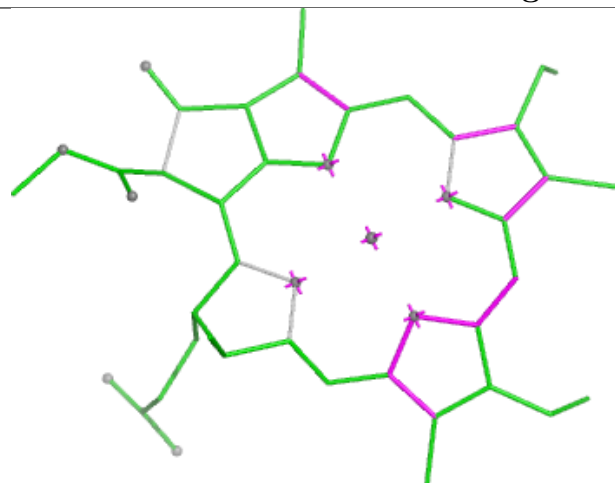




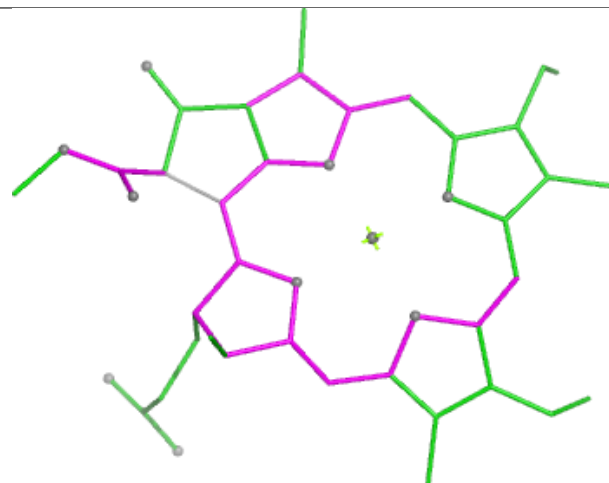




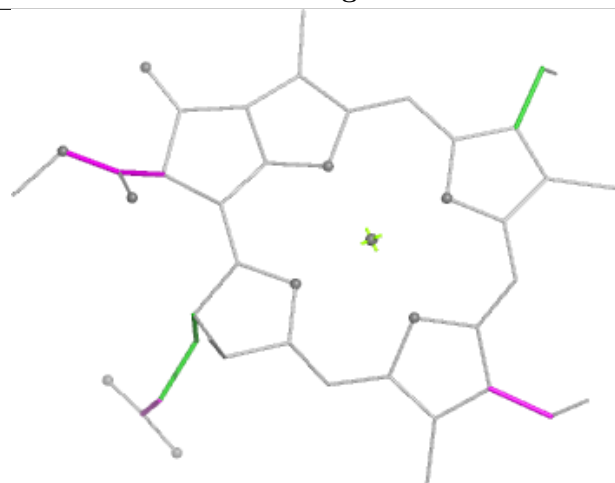
Ligand CLA s 309



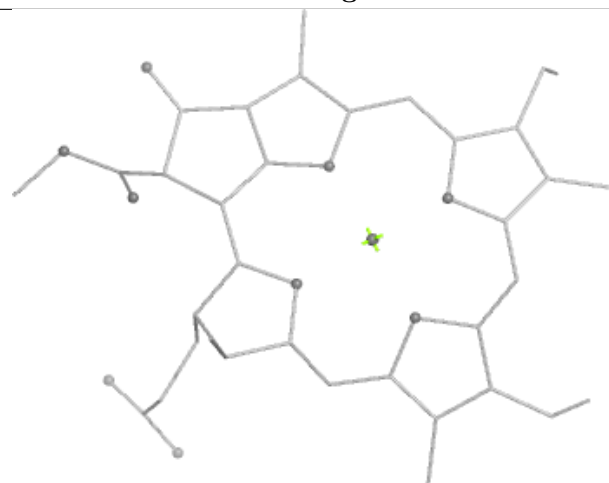
Bond lengths



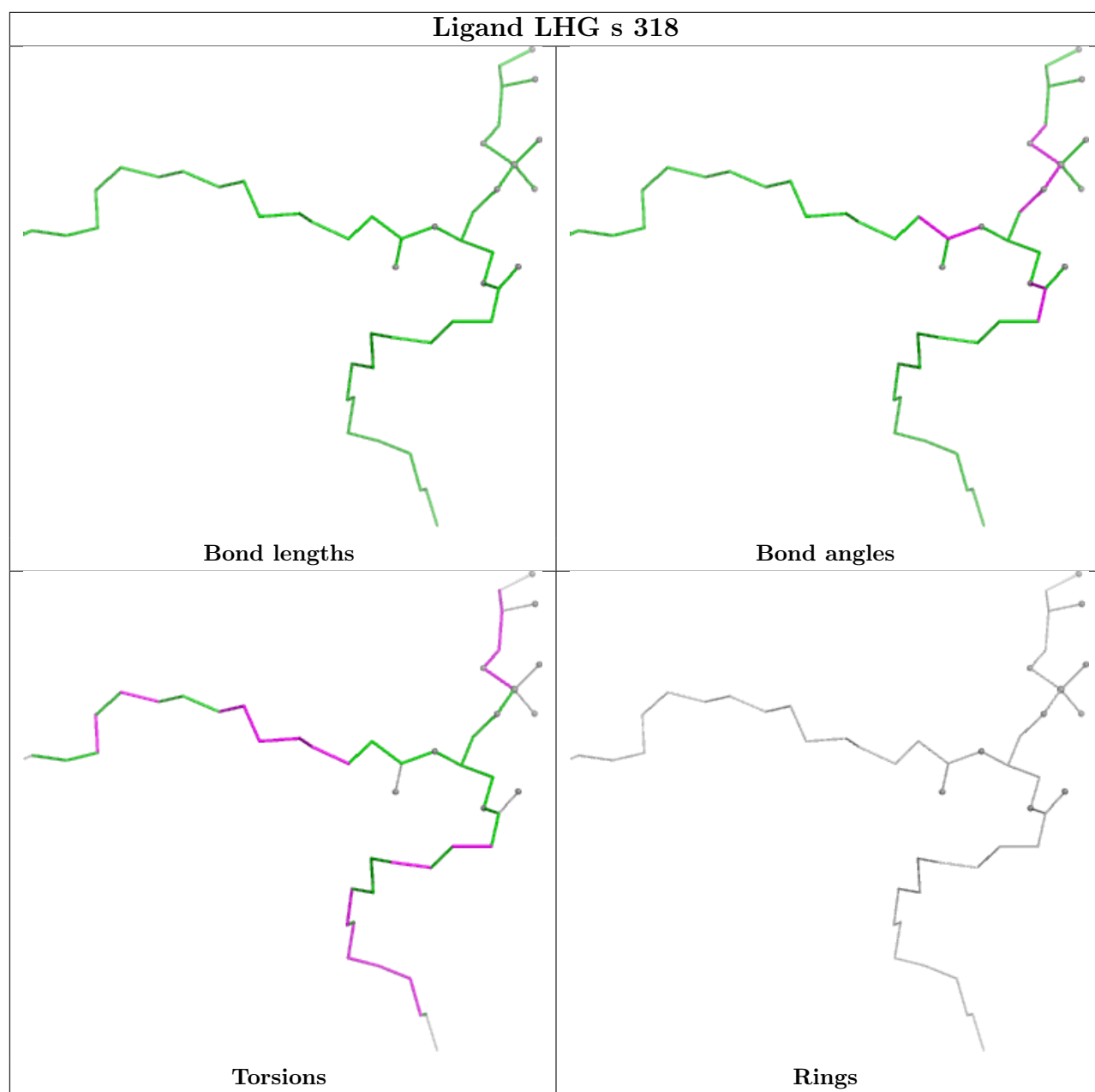
Bond angles

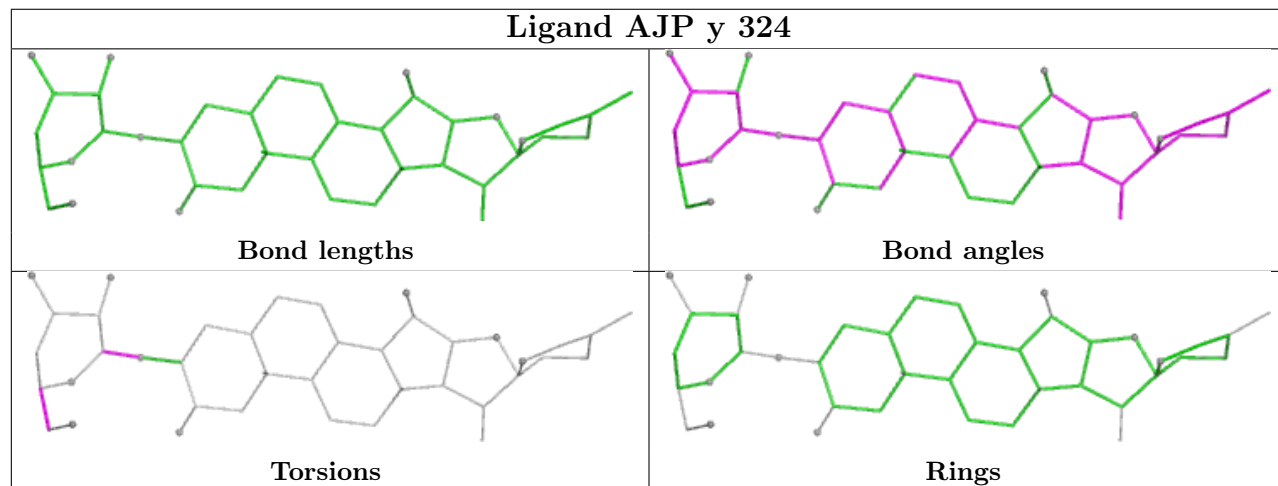
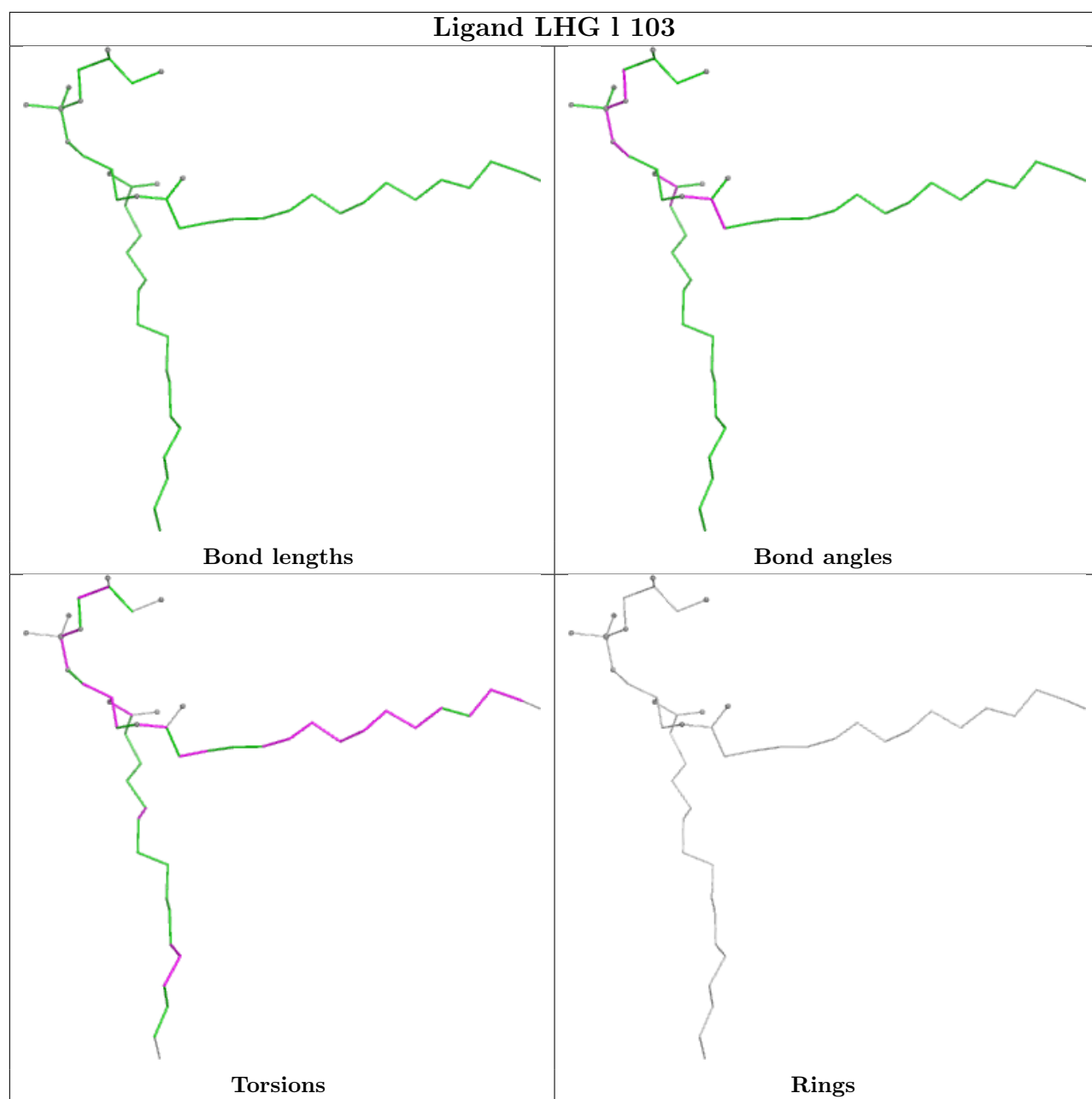


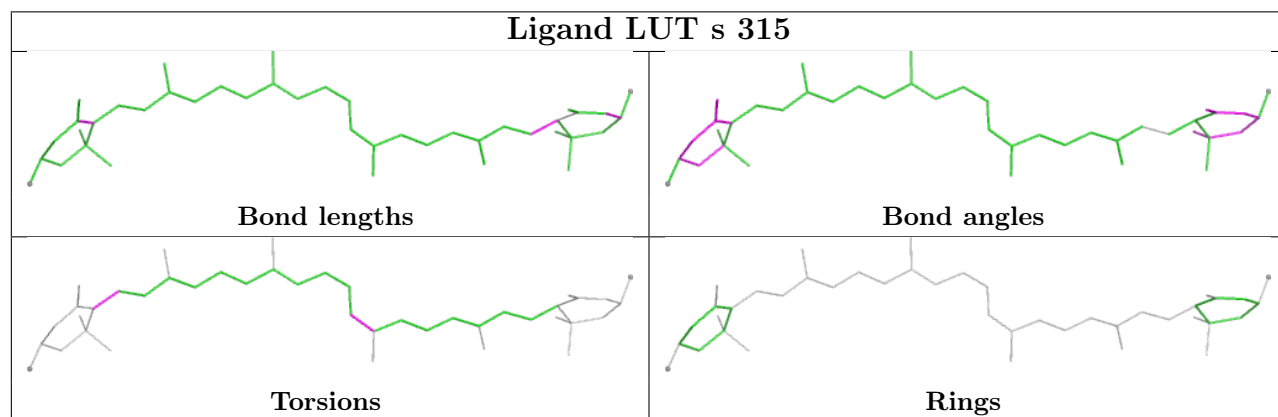
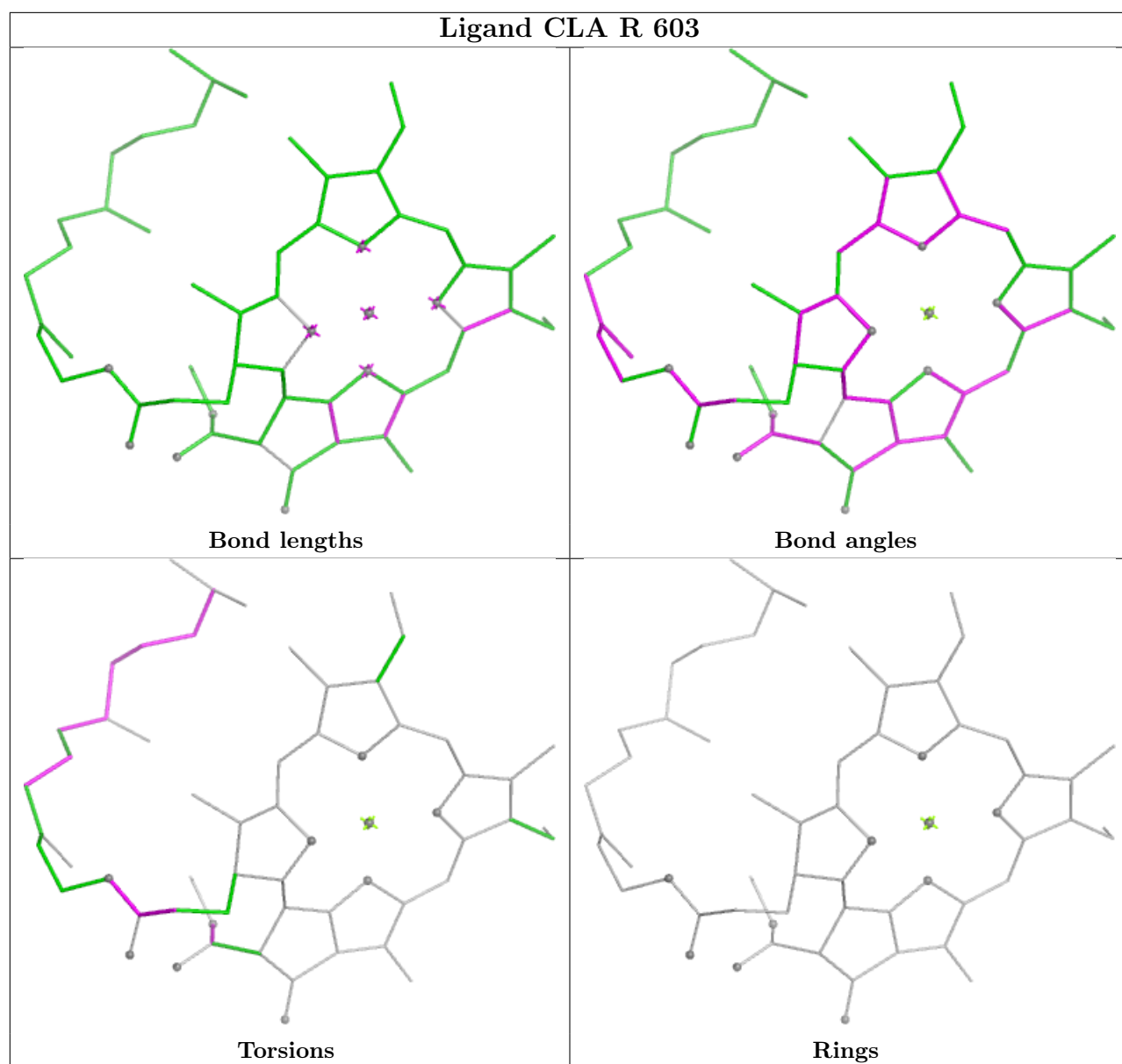
Torsions

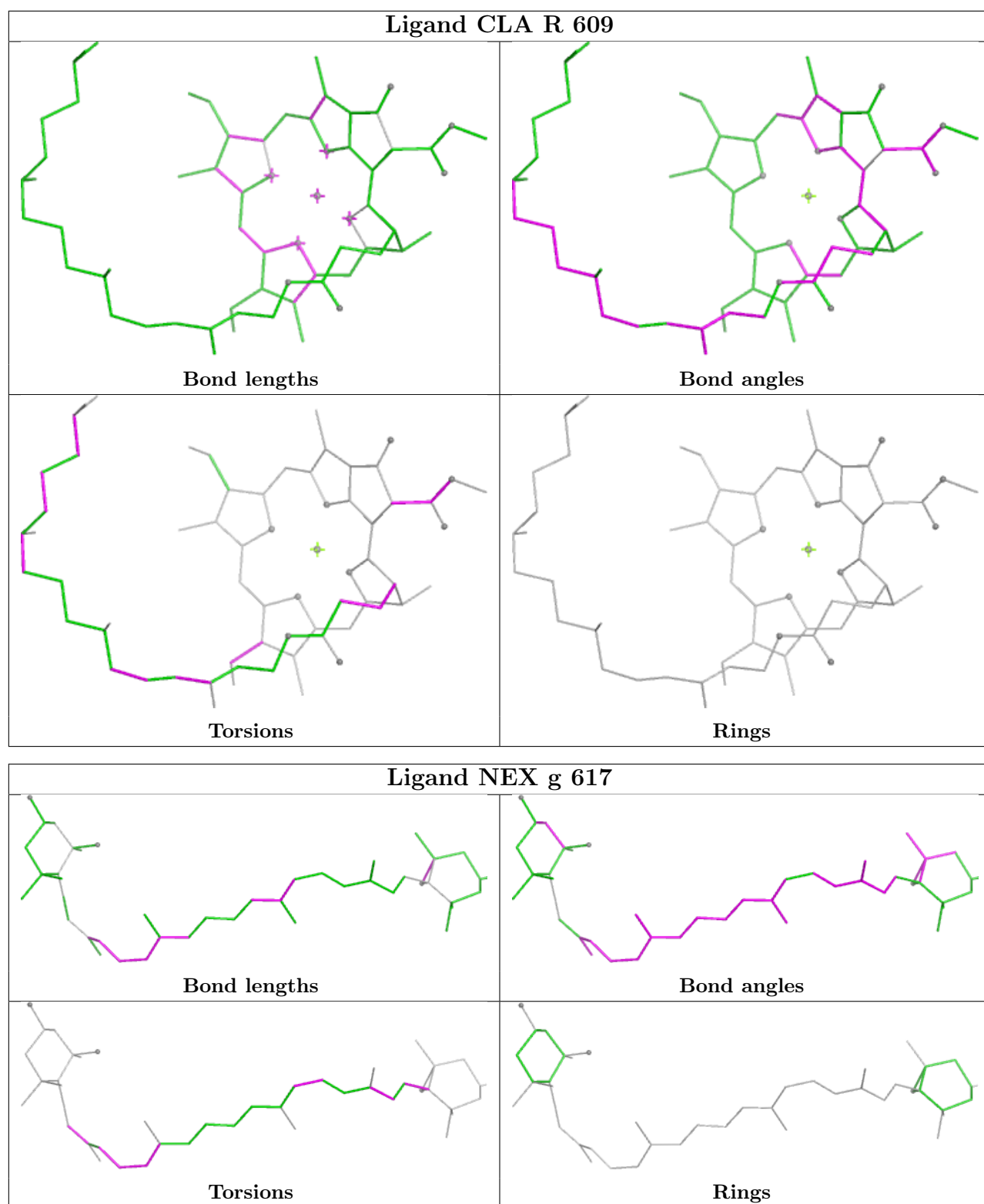


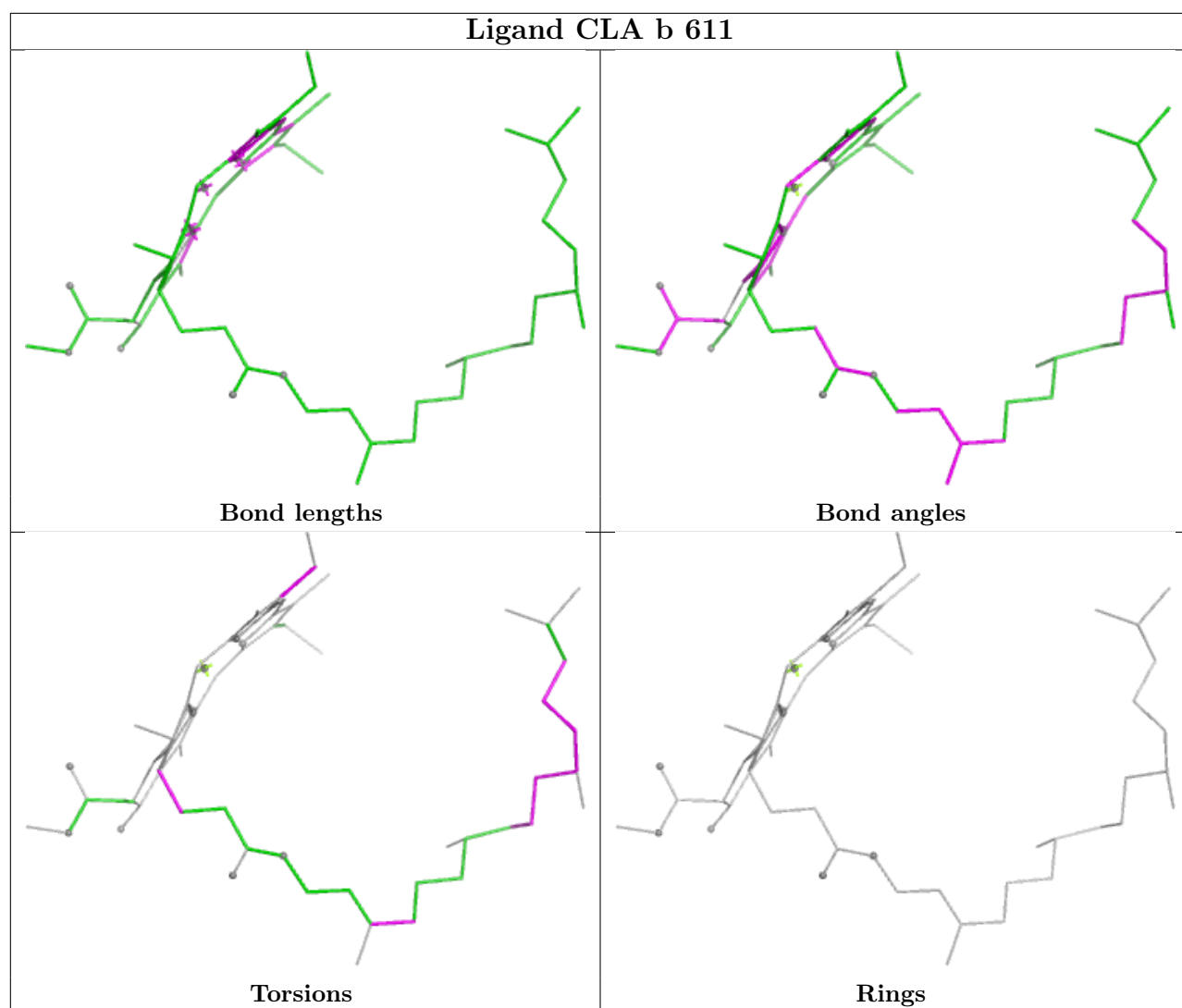
Rings

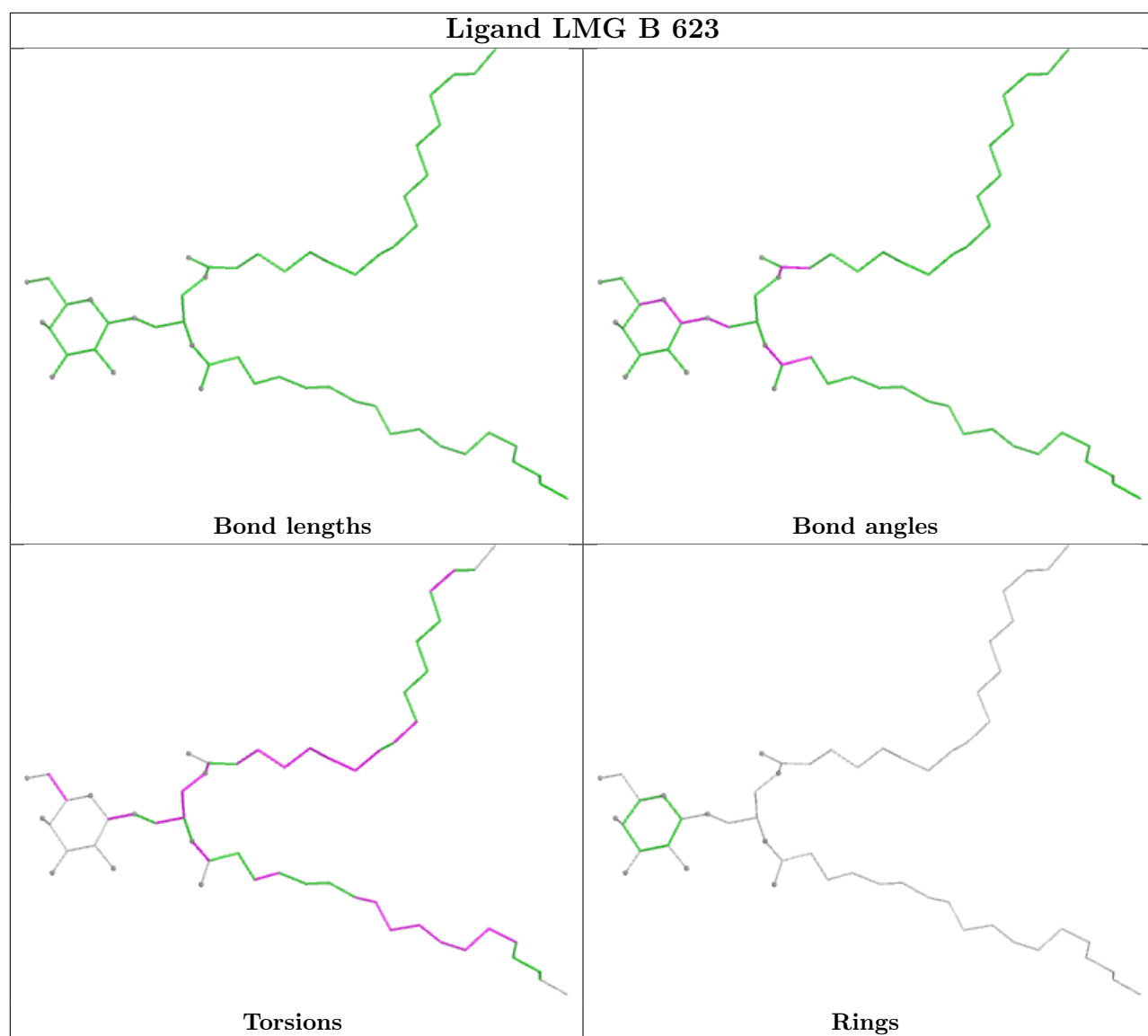




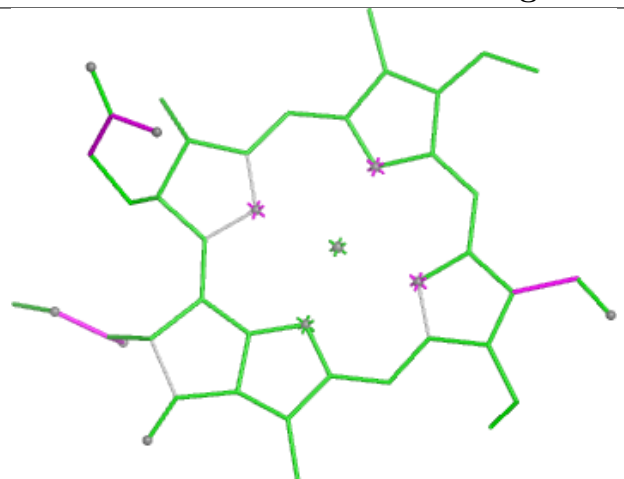




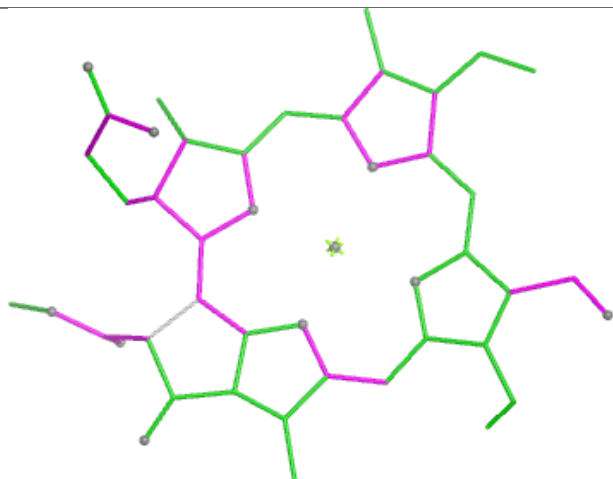




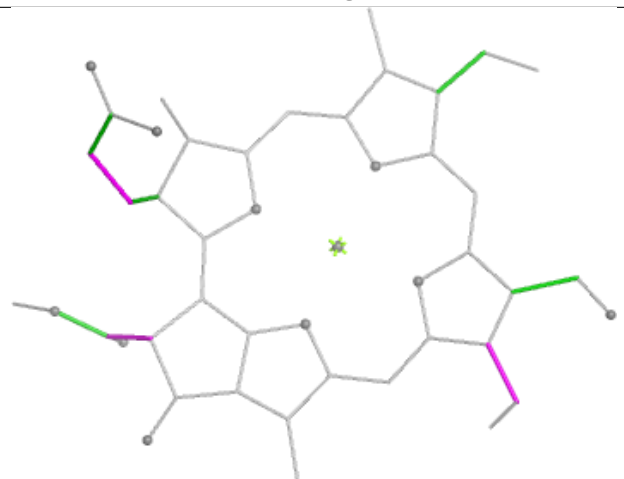
Ligand CHL 1 301



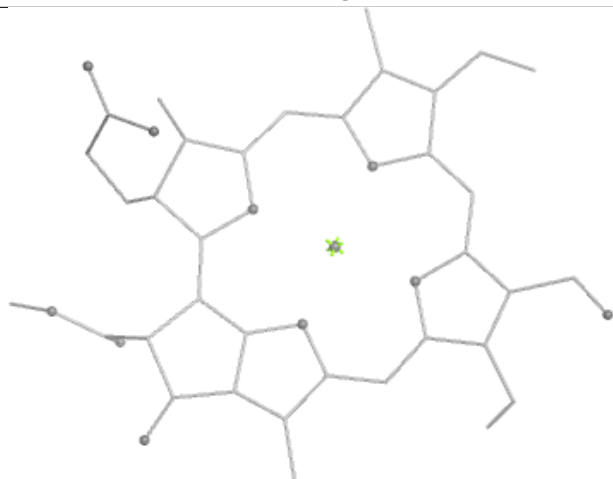
Bond lengths



Bond angles



Torsions

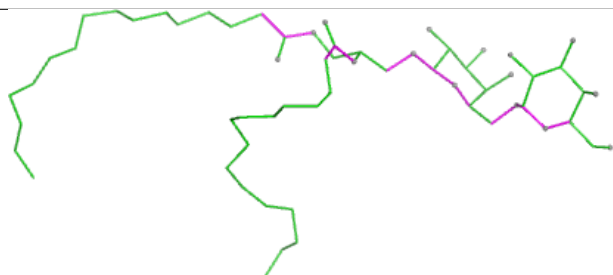


Rings

Ligand DGD B 626



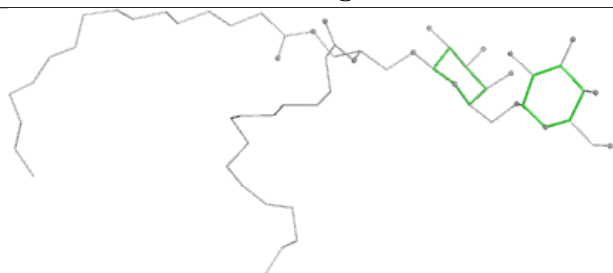
Bond lengths



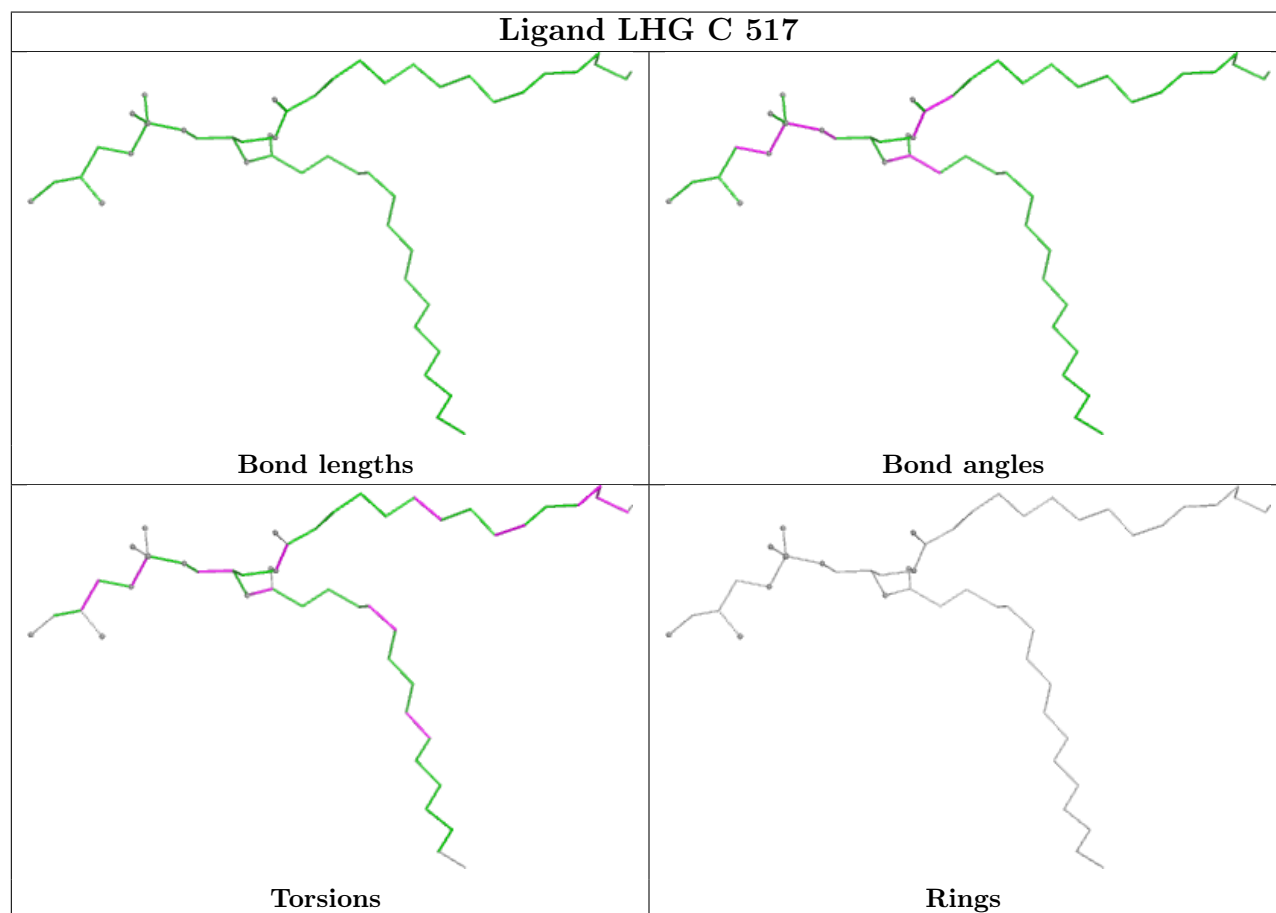
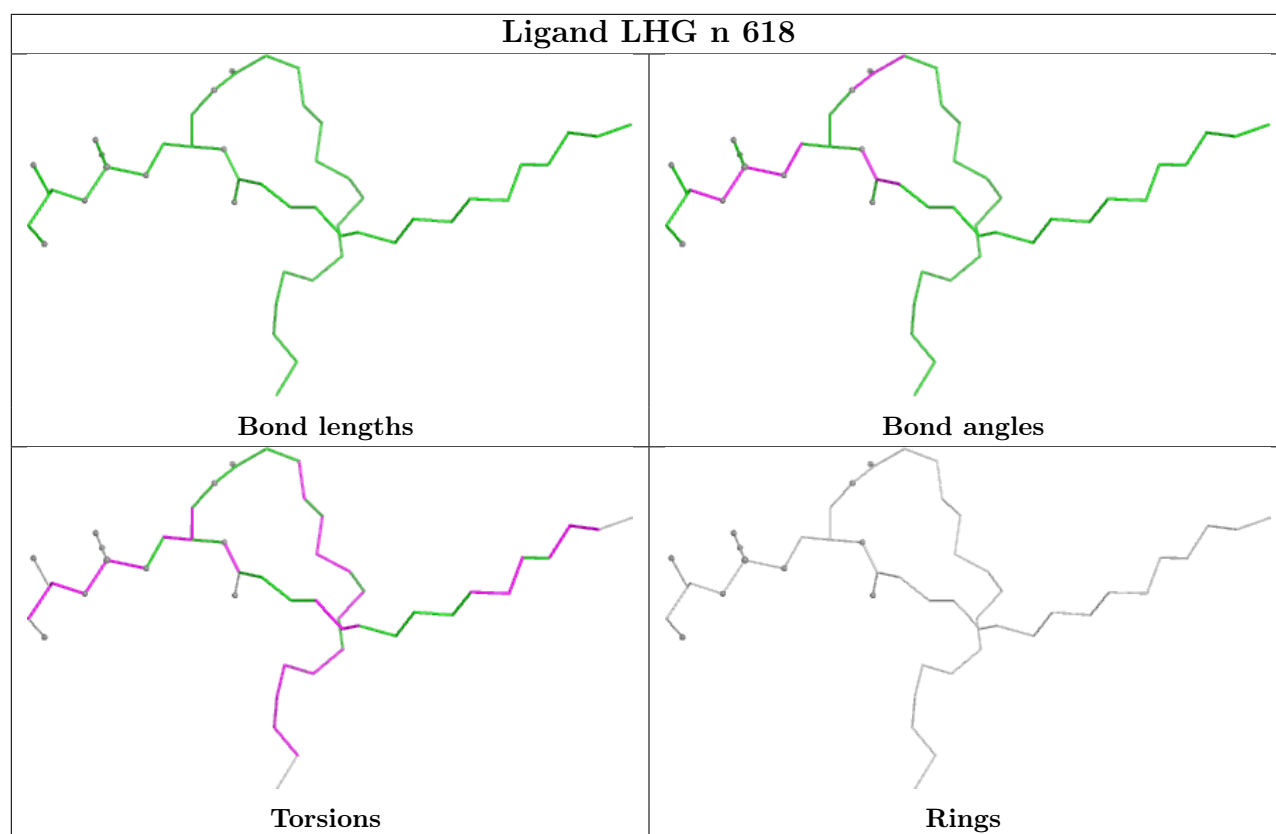
Bond angles



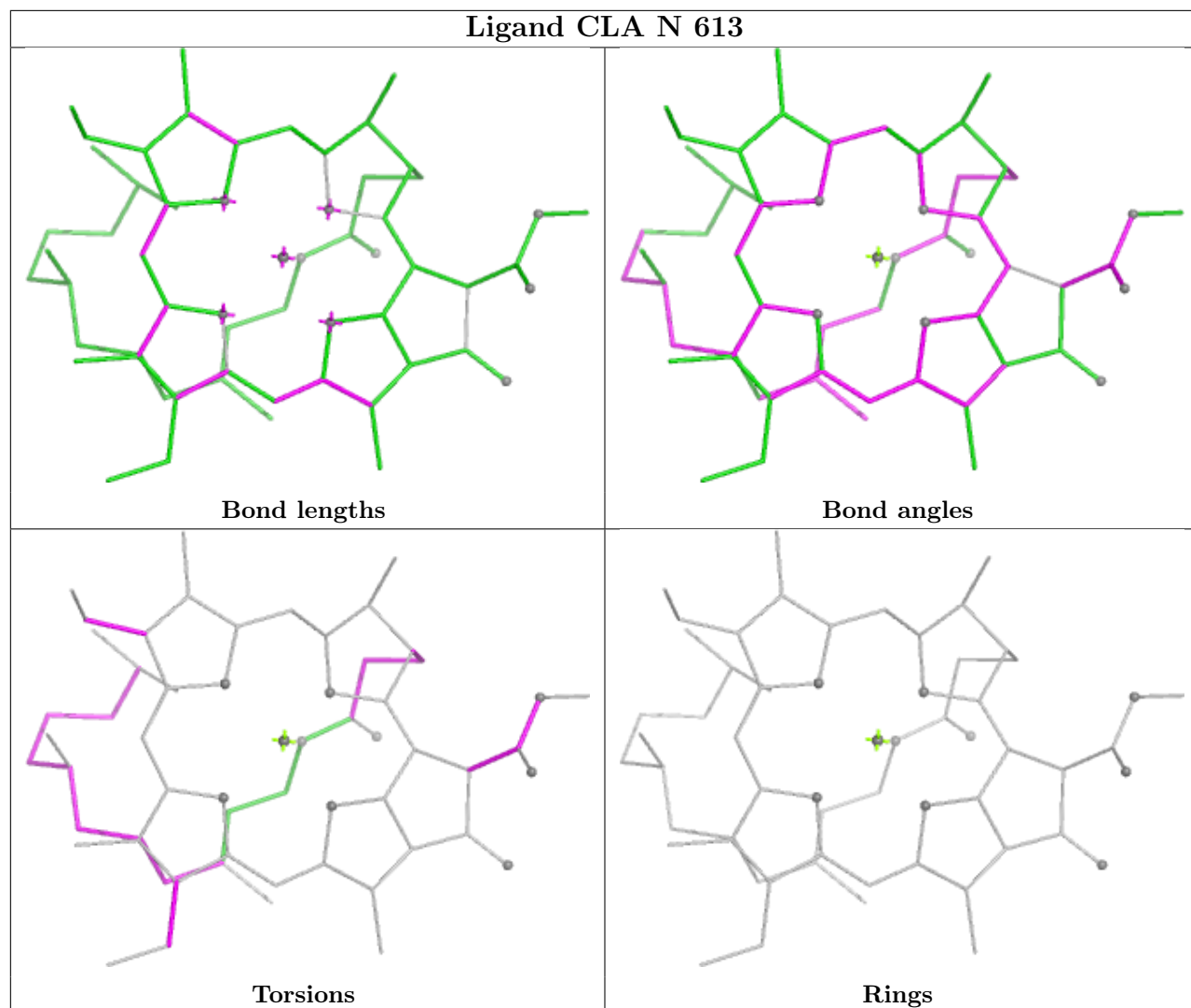
Torsions

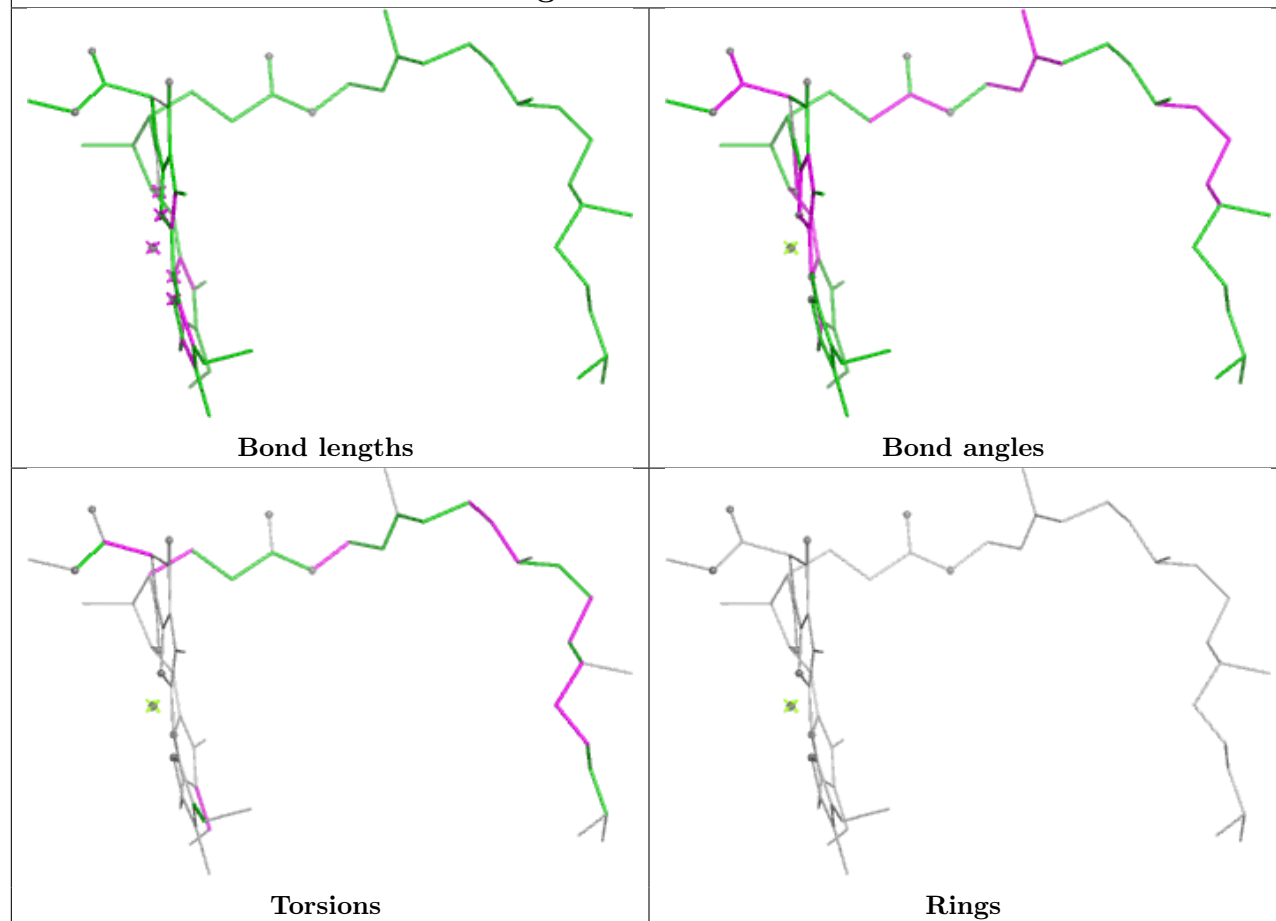
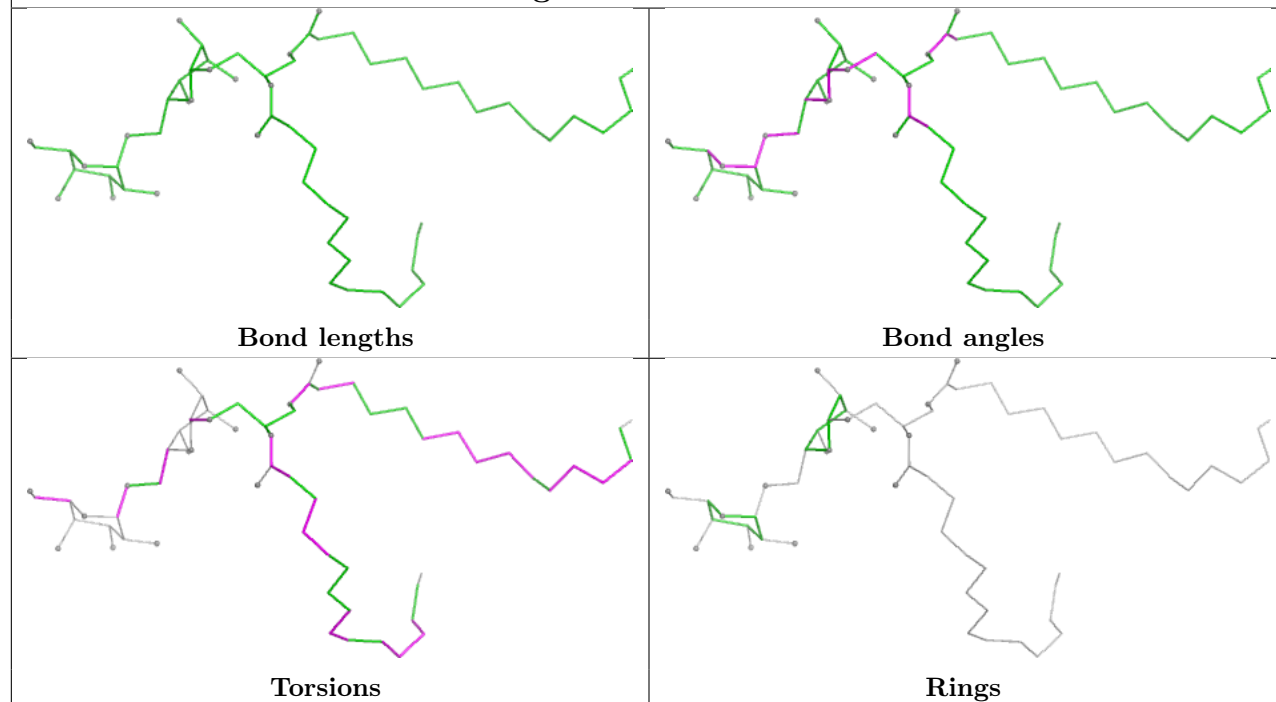


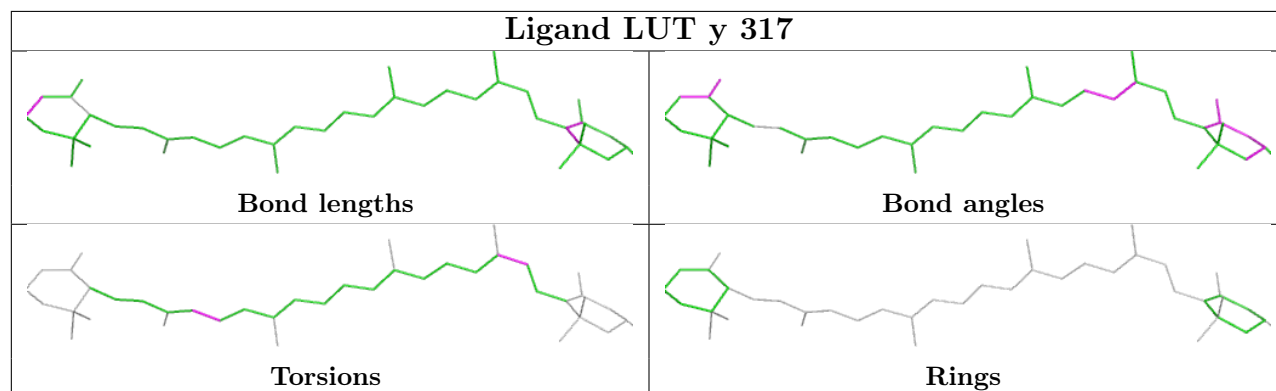
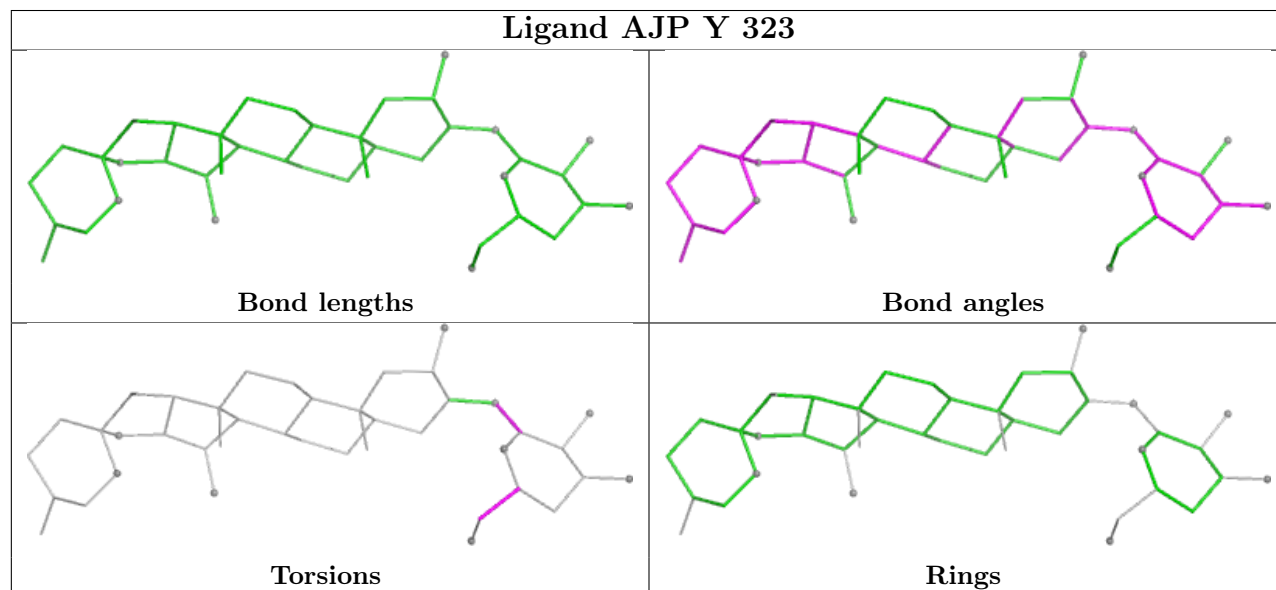
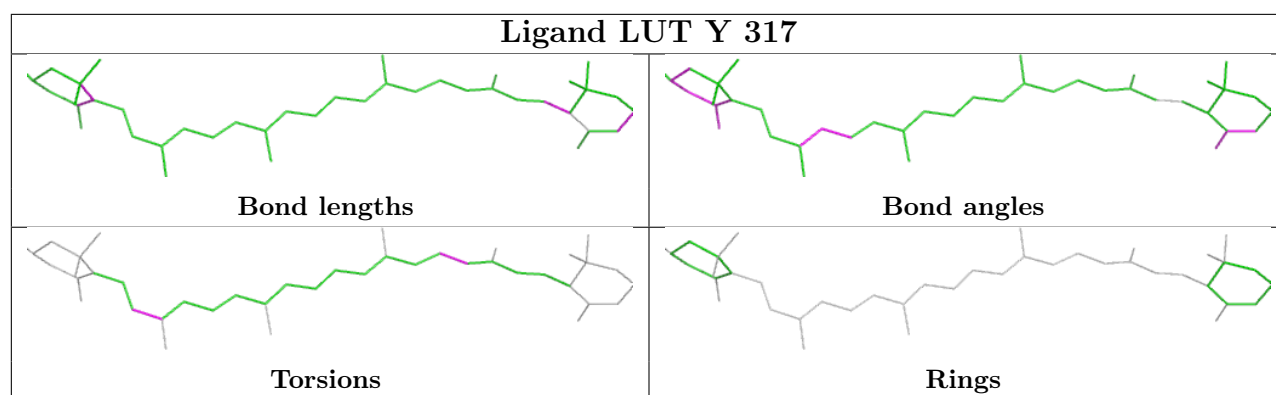
Rings

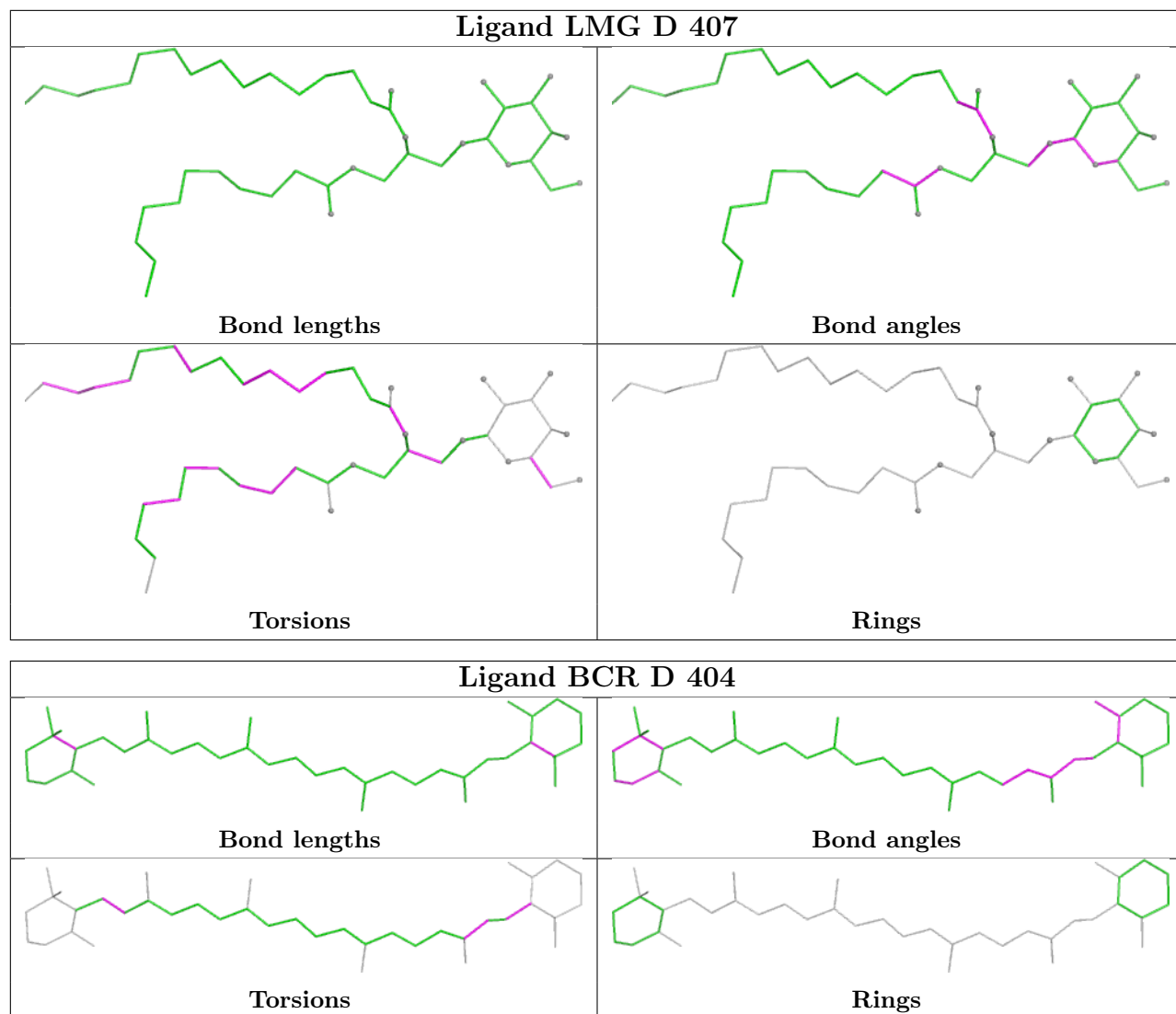


Ligand CLA N 613

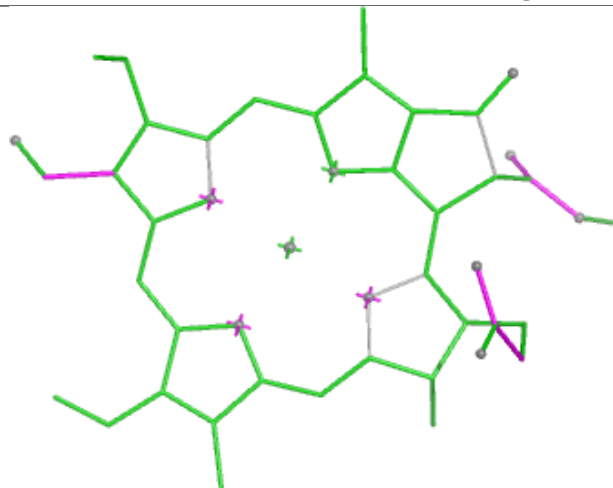


Ligand CLA c 506**Ligand DGD c 516**

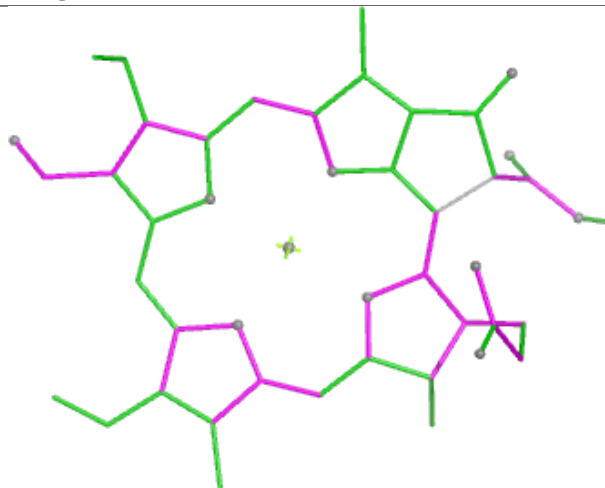




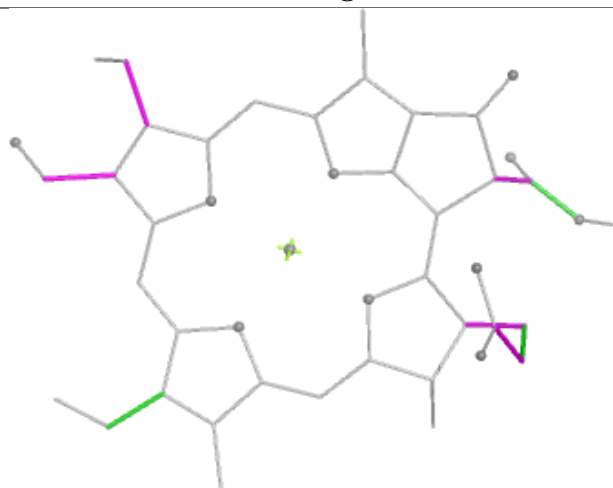
Ligand CHL g 605



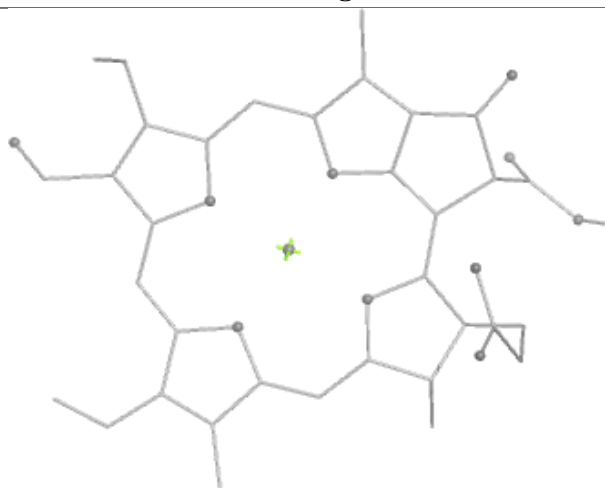
Bond lengths



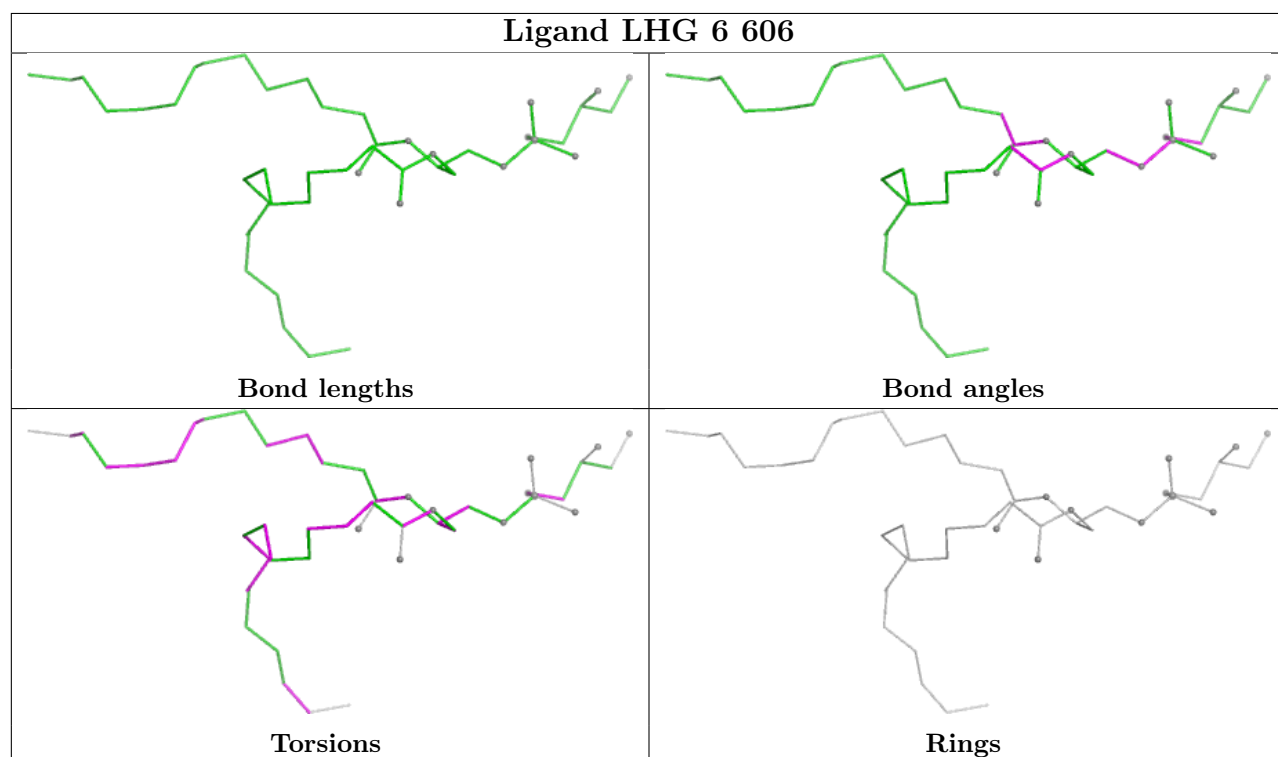
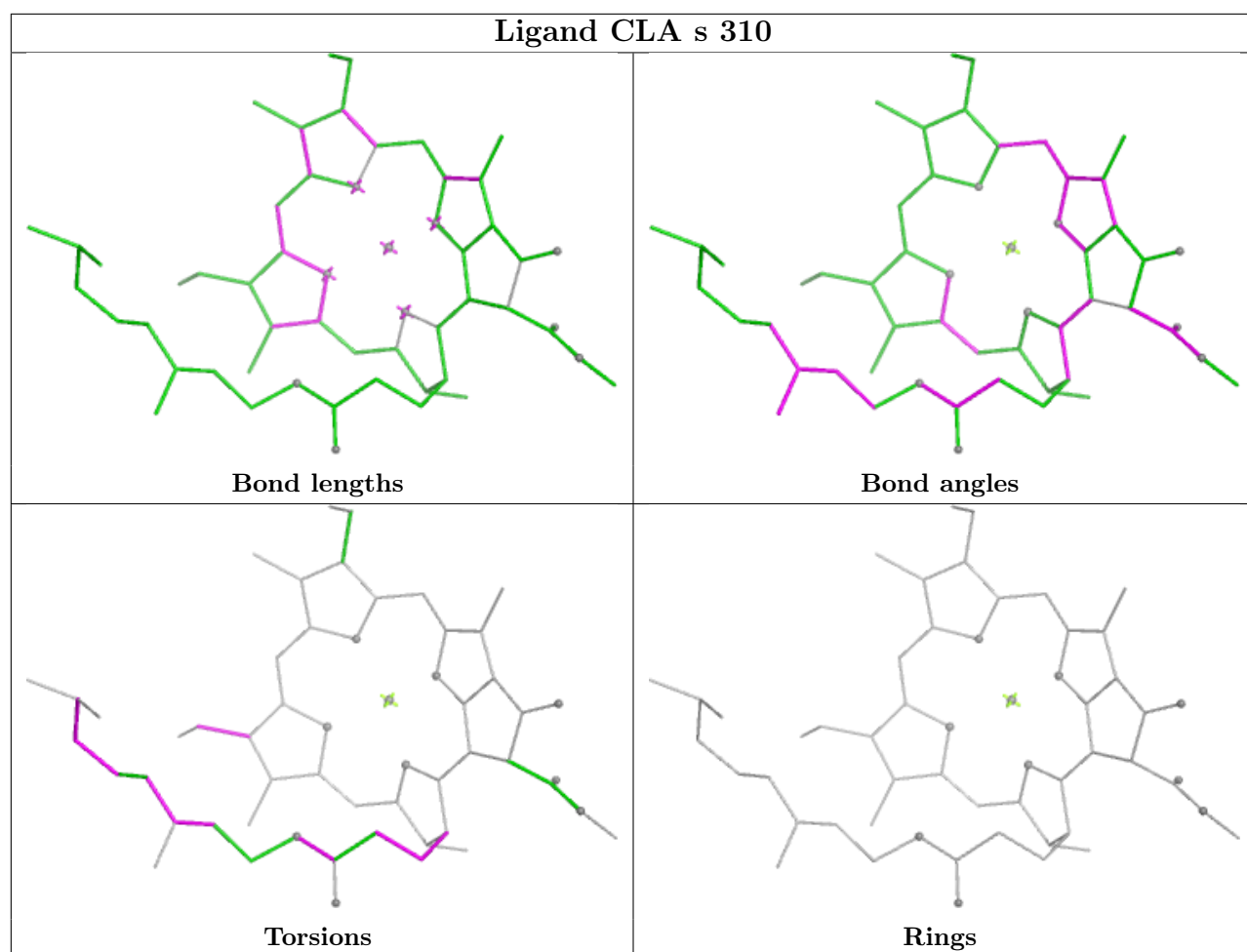
Bond angles

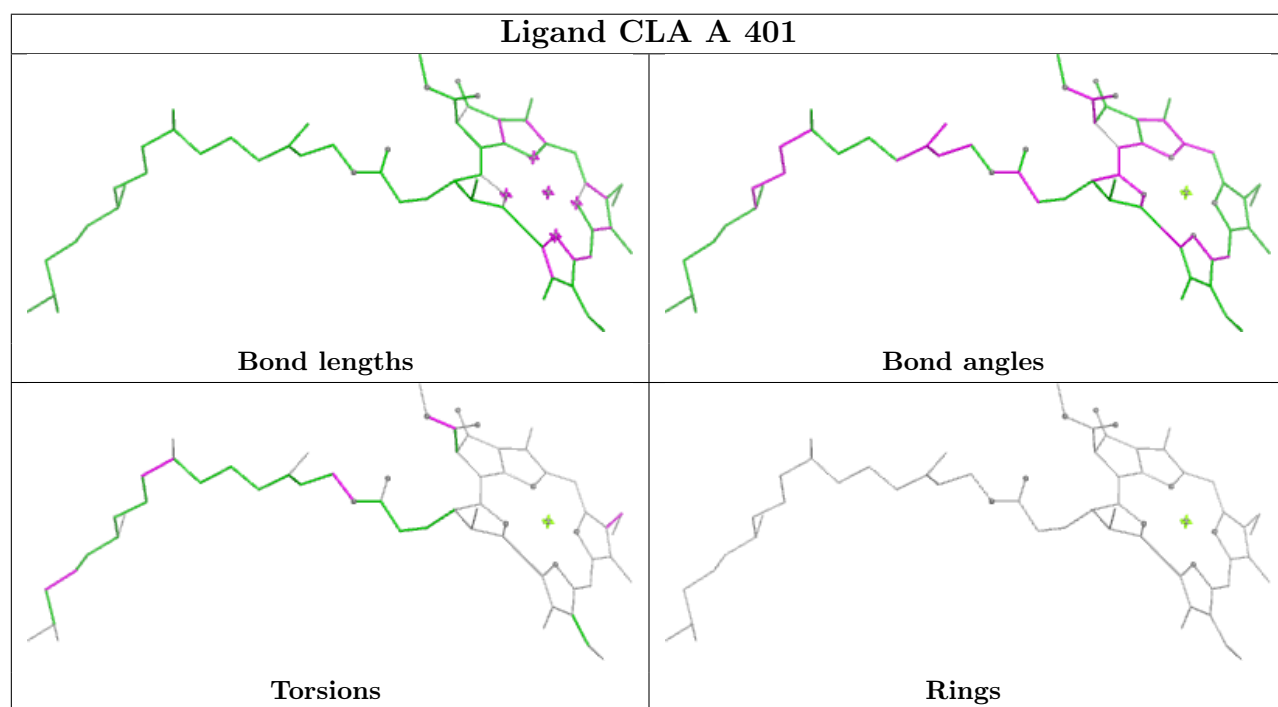
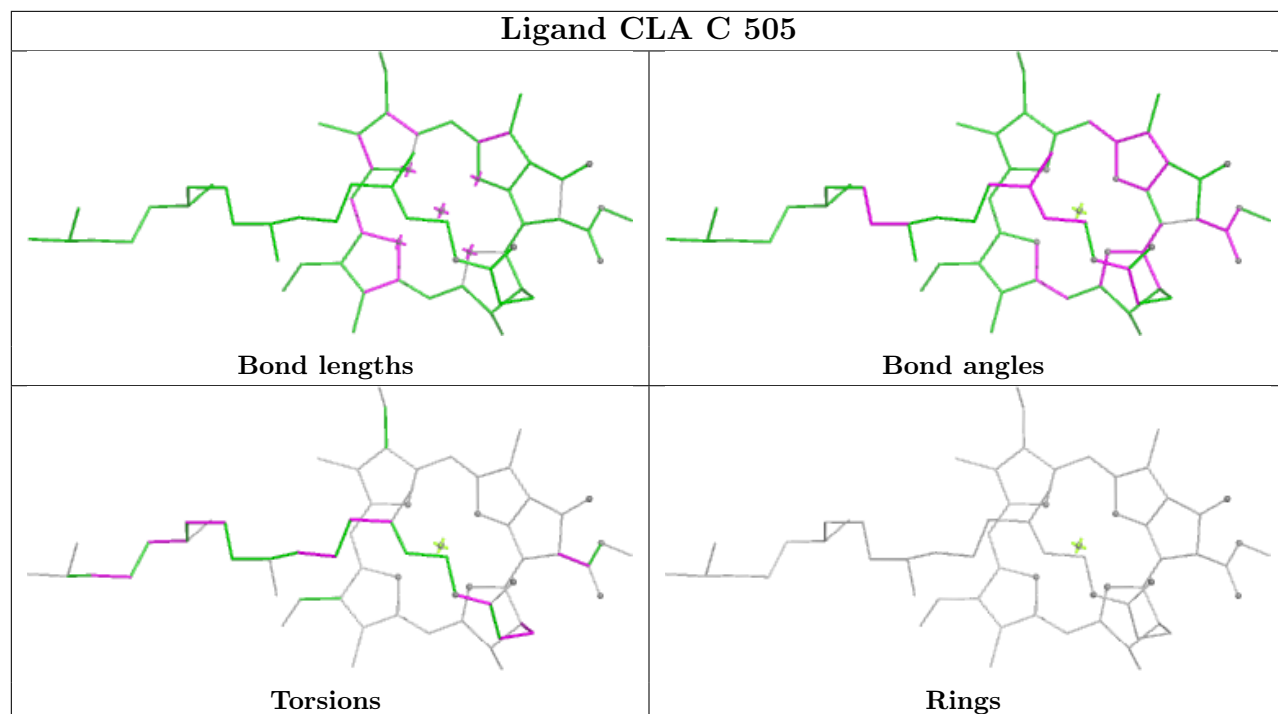


Torsions

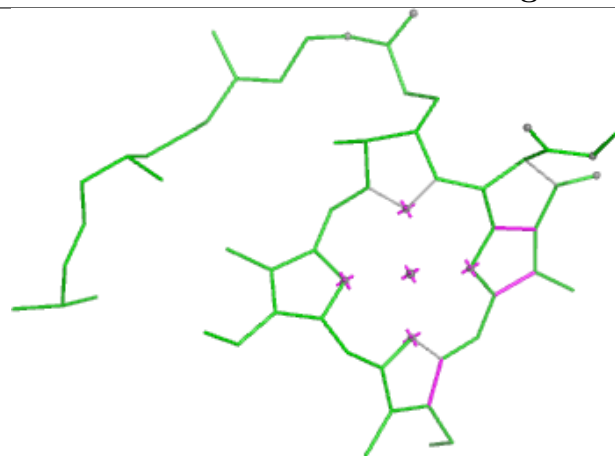


Rings

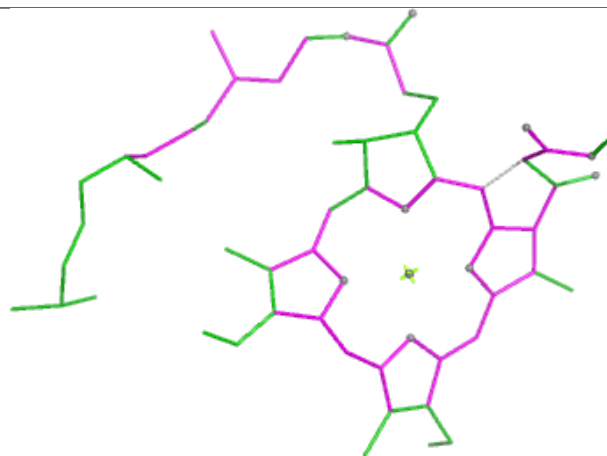




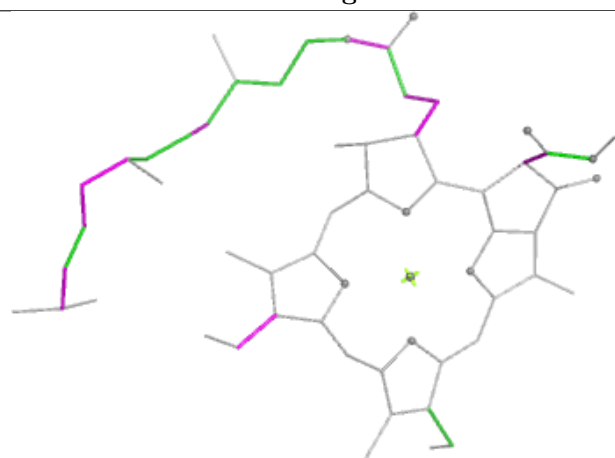
Ligand CLA 2 602



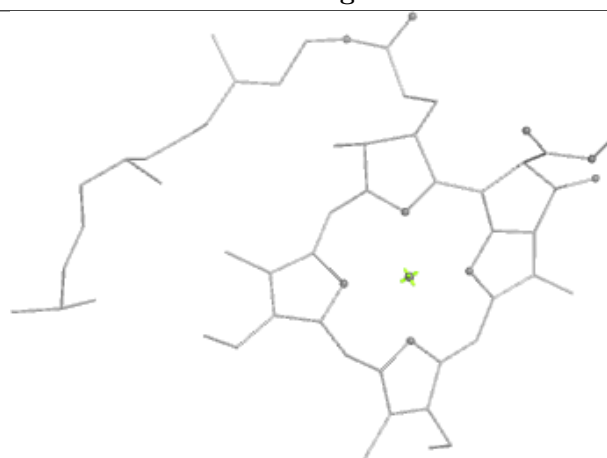
Bond lengths



Bond angles

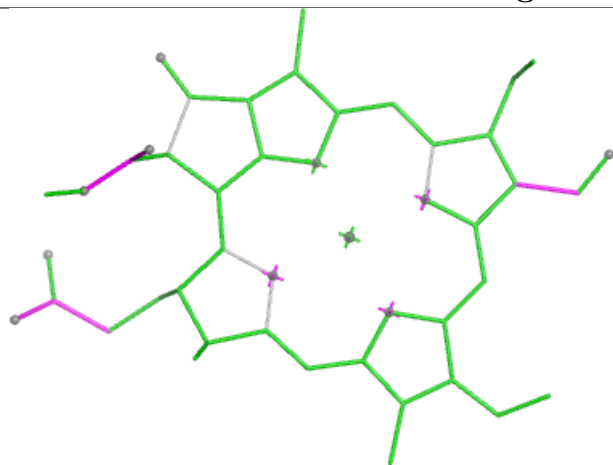


Torsions

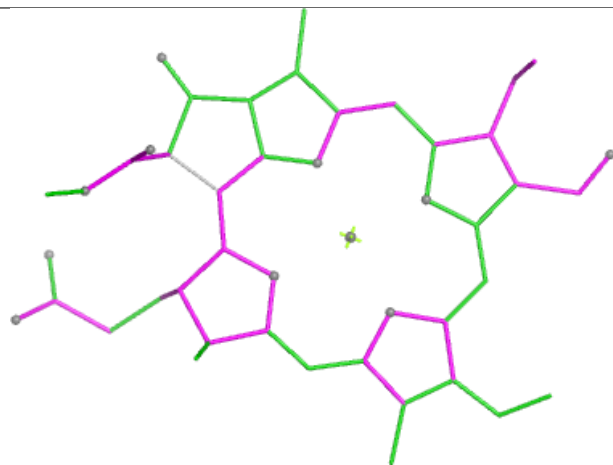


Rings

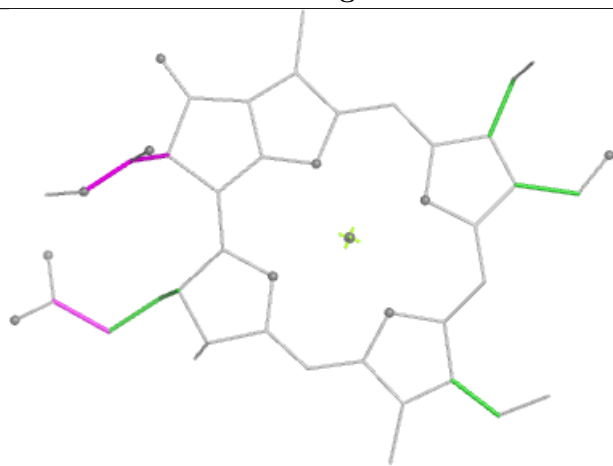
Ligand CHL n 606



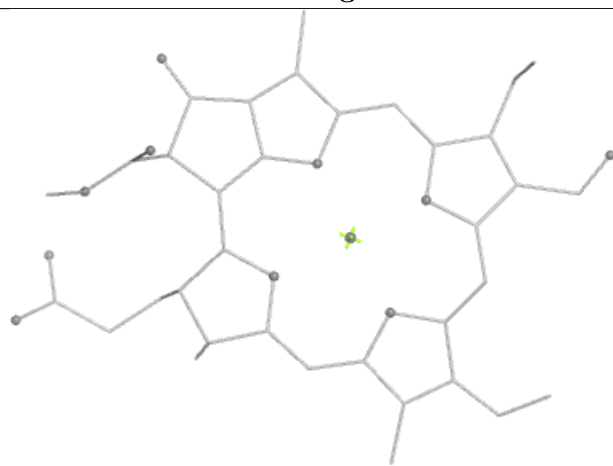
Bond lengths



Bond angles

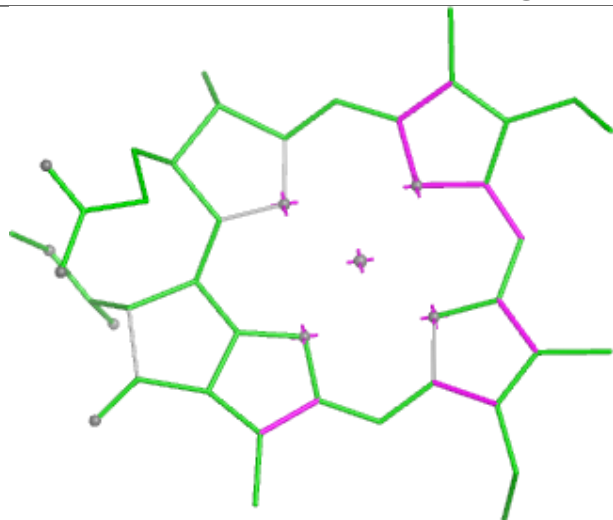


Torsions

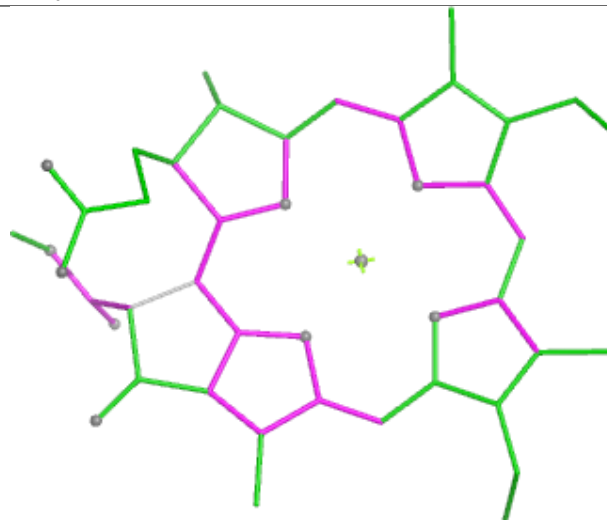


Rings

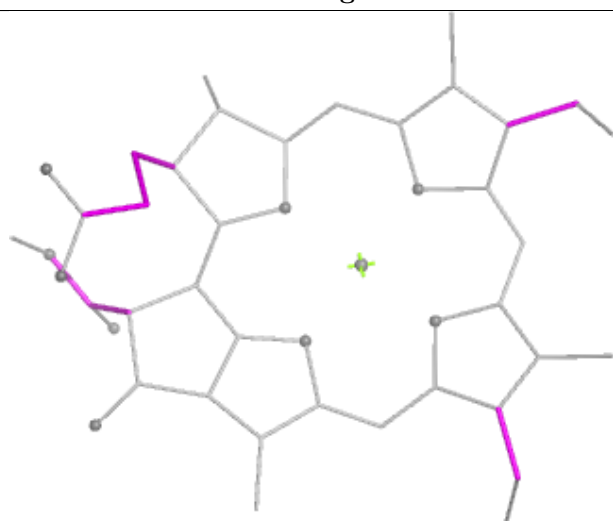
Ligand CLA y 315



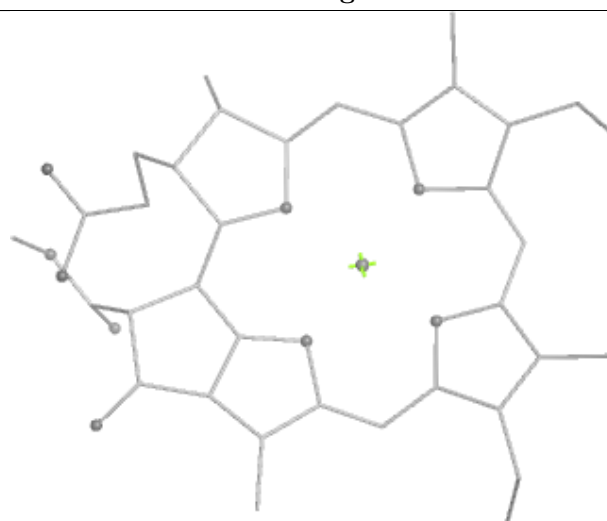
Bond lengths



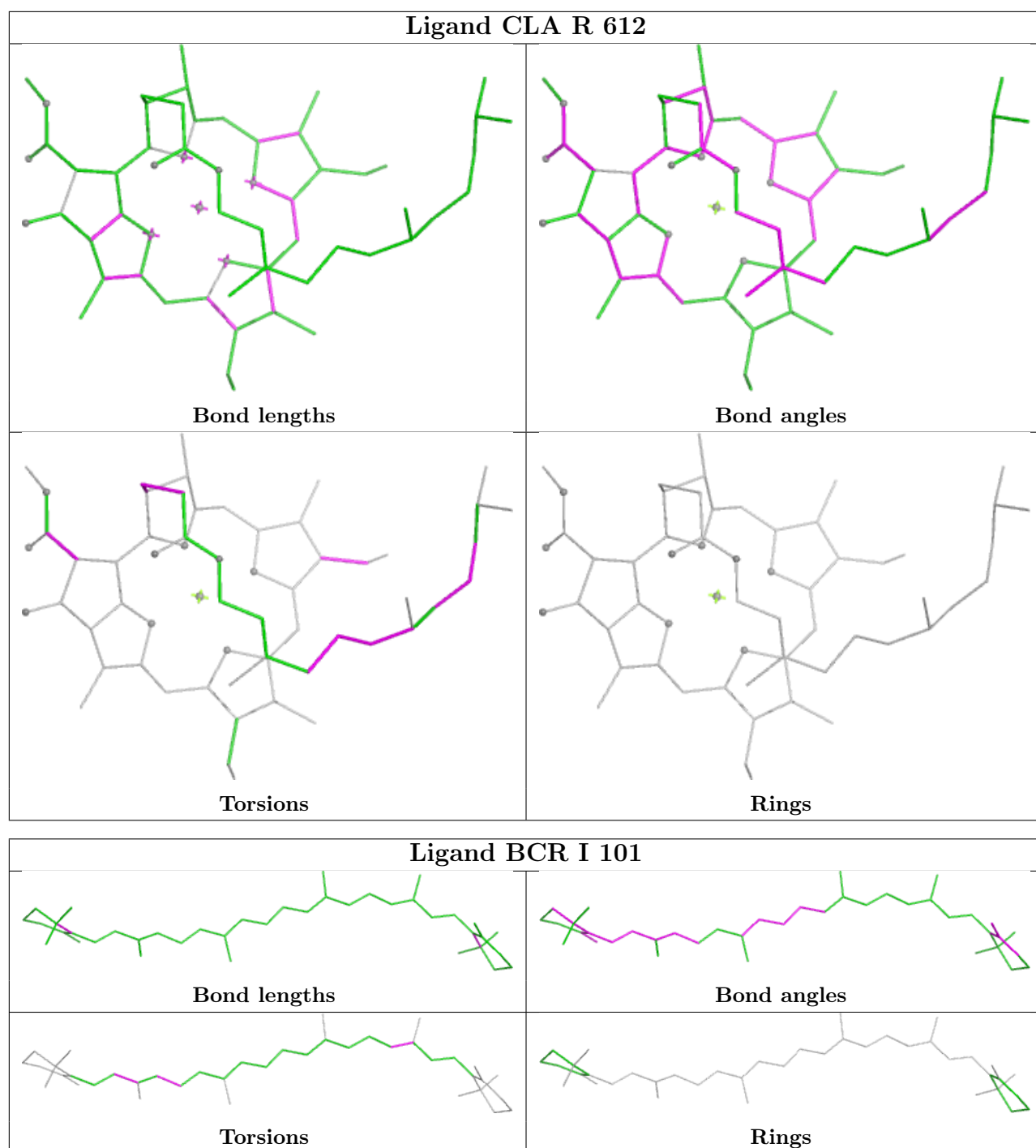
Bond angles

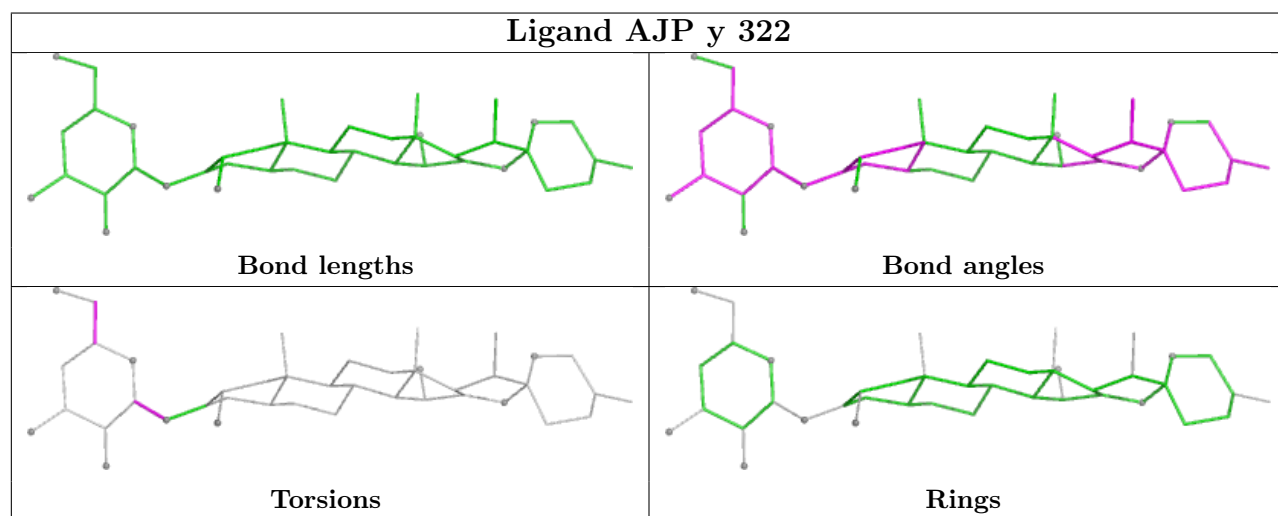
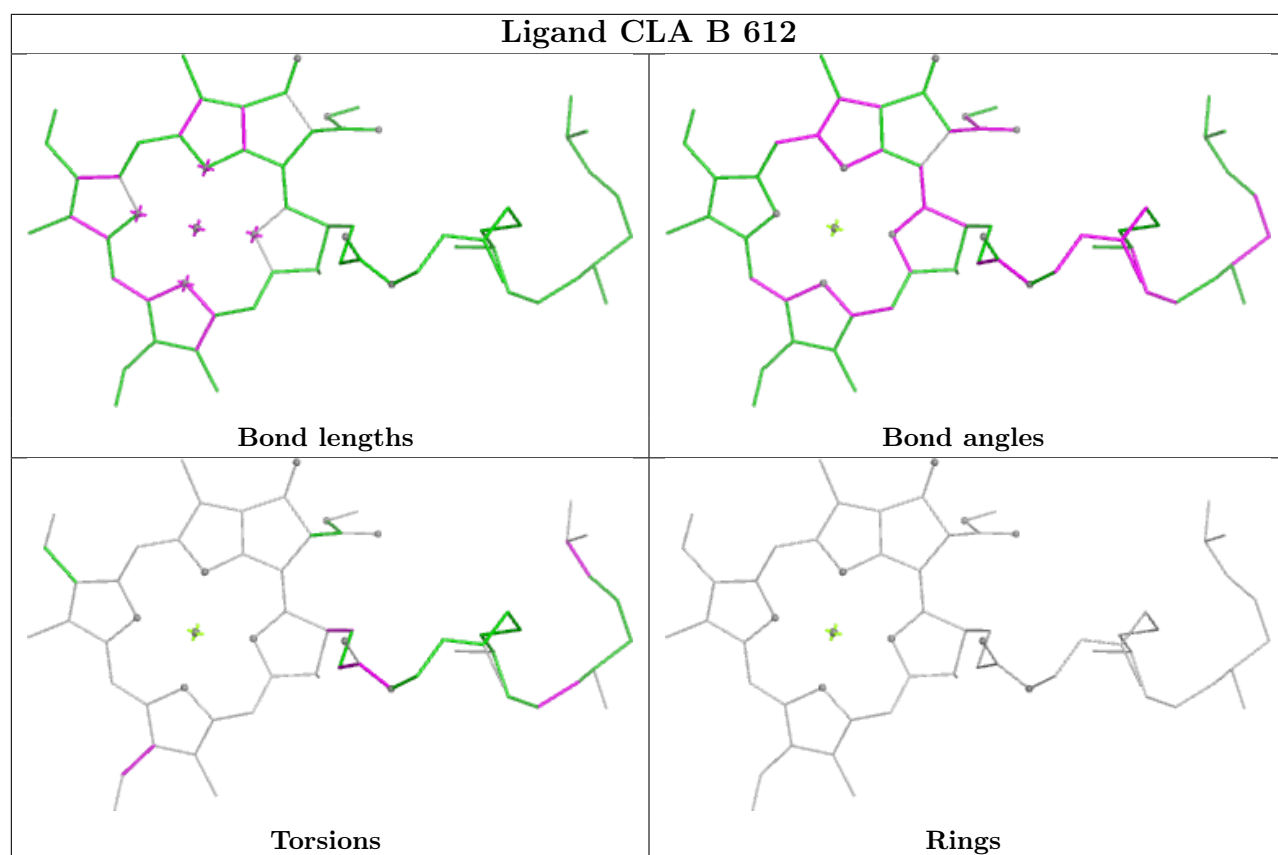


Torsions

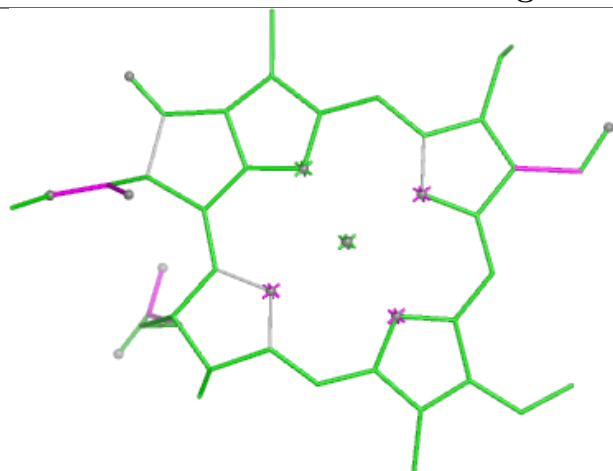


Rings

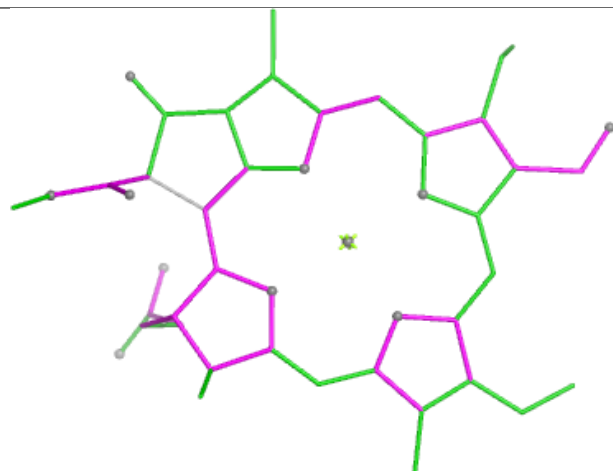




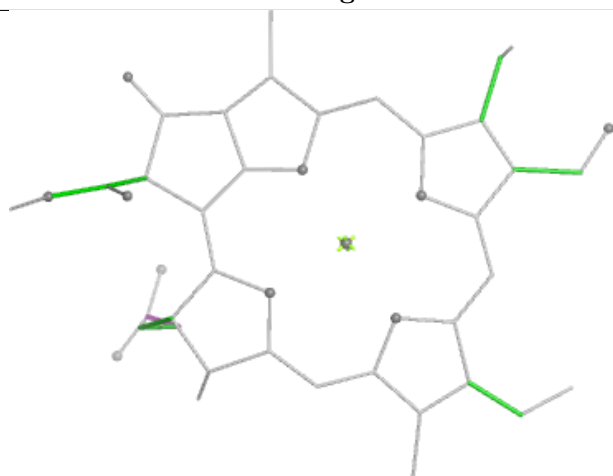
Ligand CHL S 308



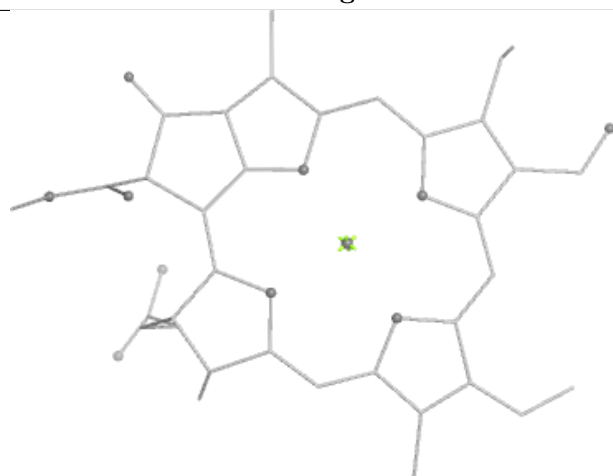
Bond lengths



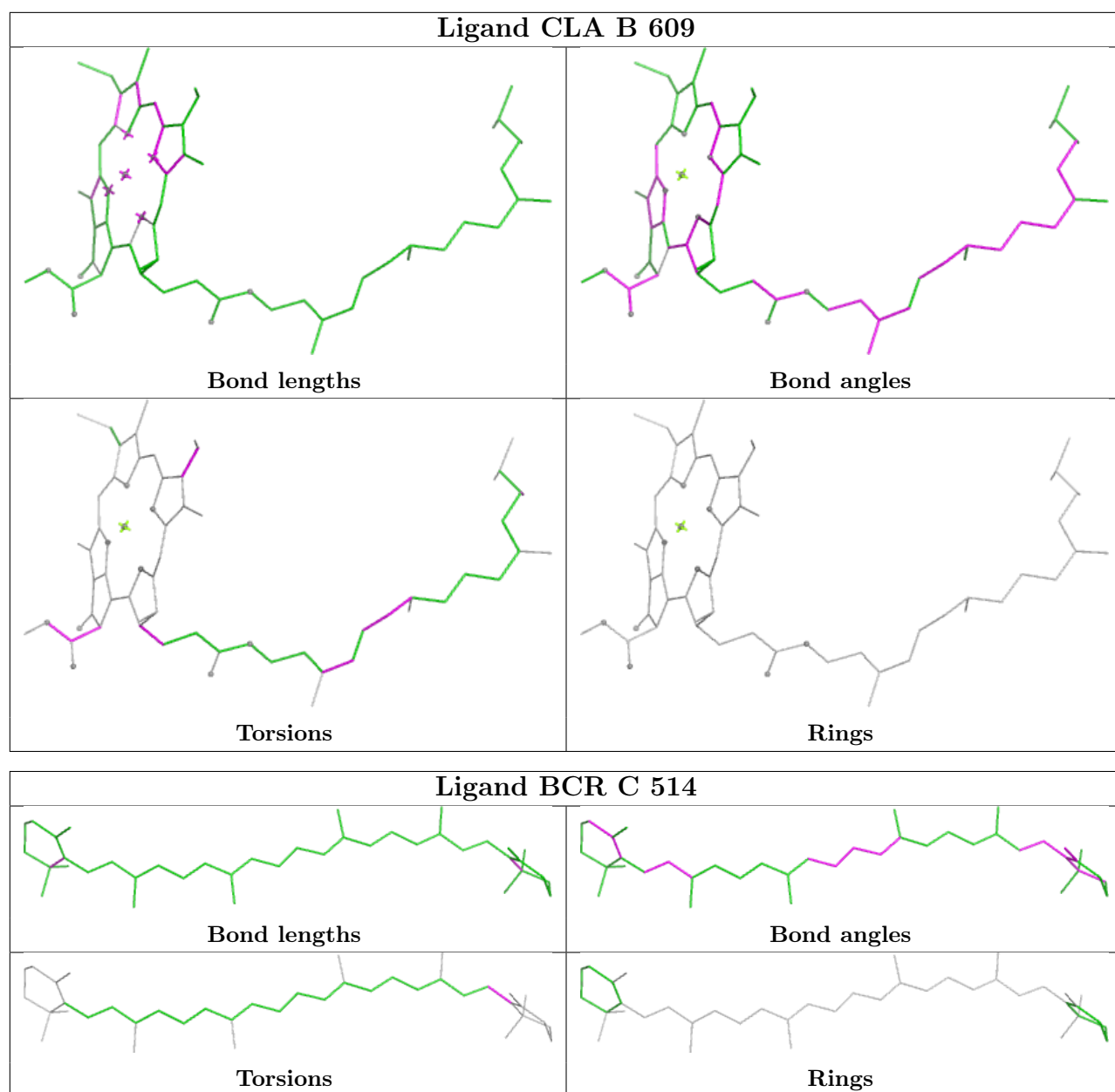
Bond angles



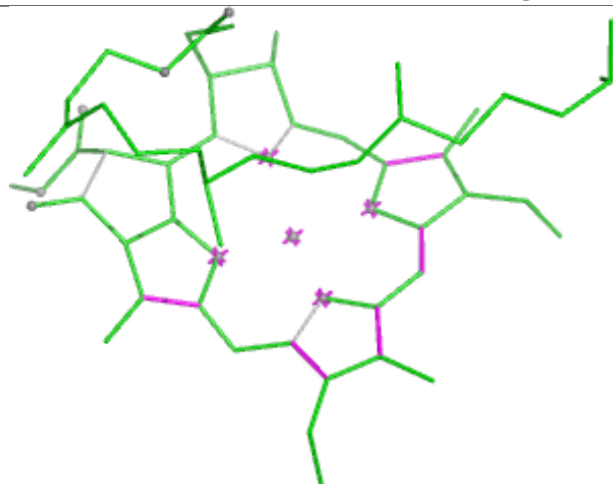
Torsions



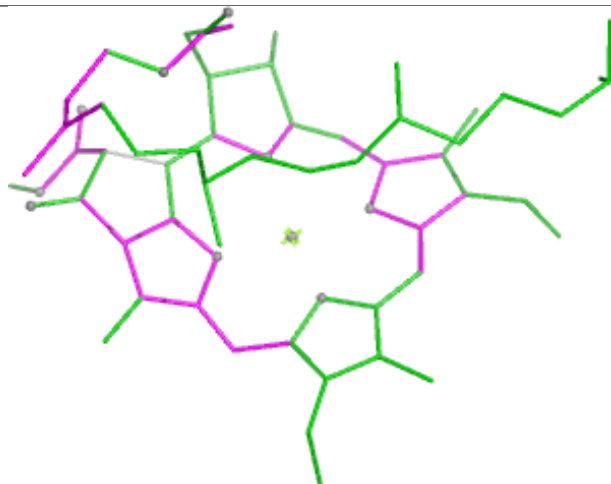
Rings



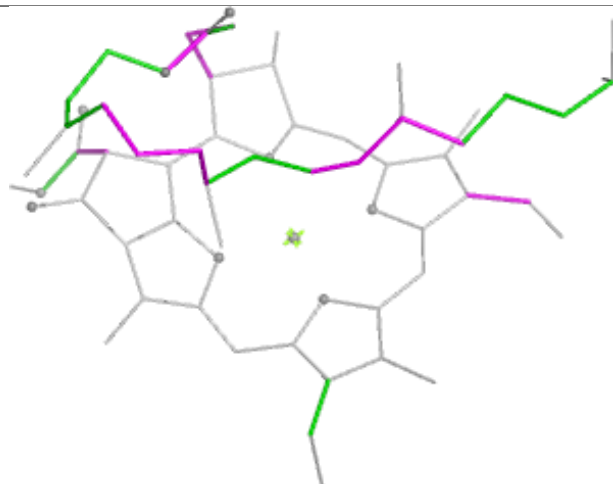
Ligand CLA b 601



Bond lengths



Bond angles

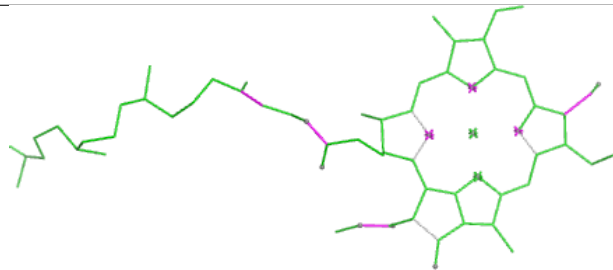


Torsions

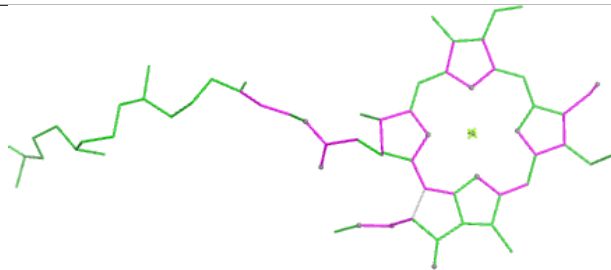


Rings

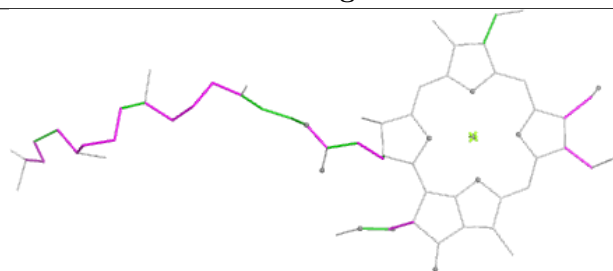
Ligand CHL Y 302



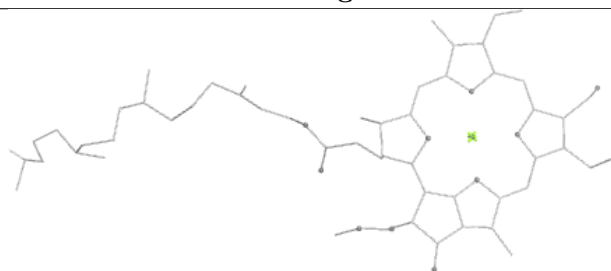
Bond lengths



Bond angles

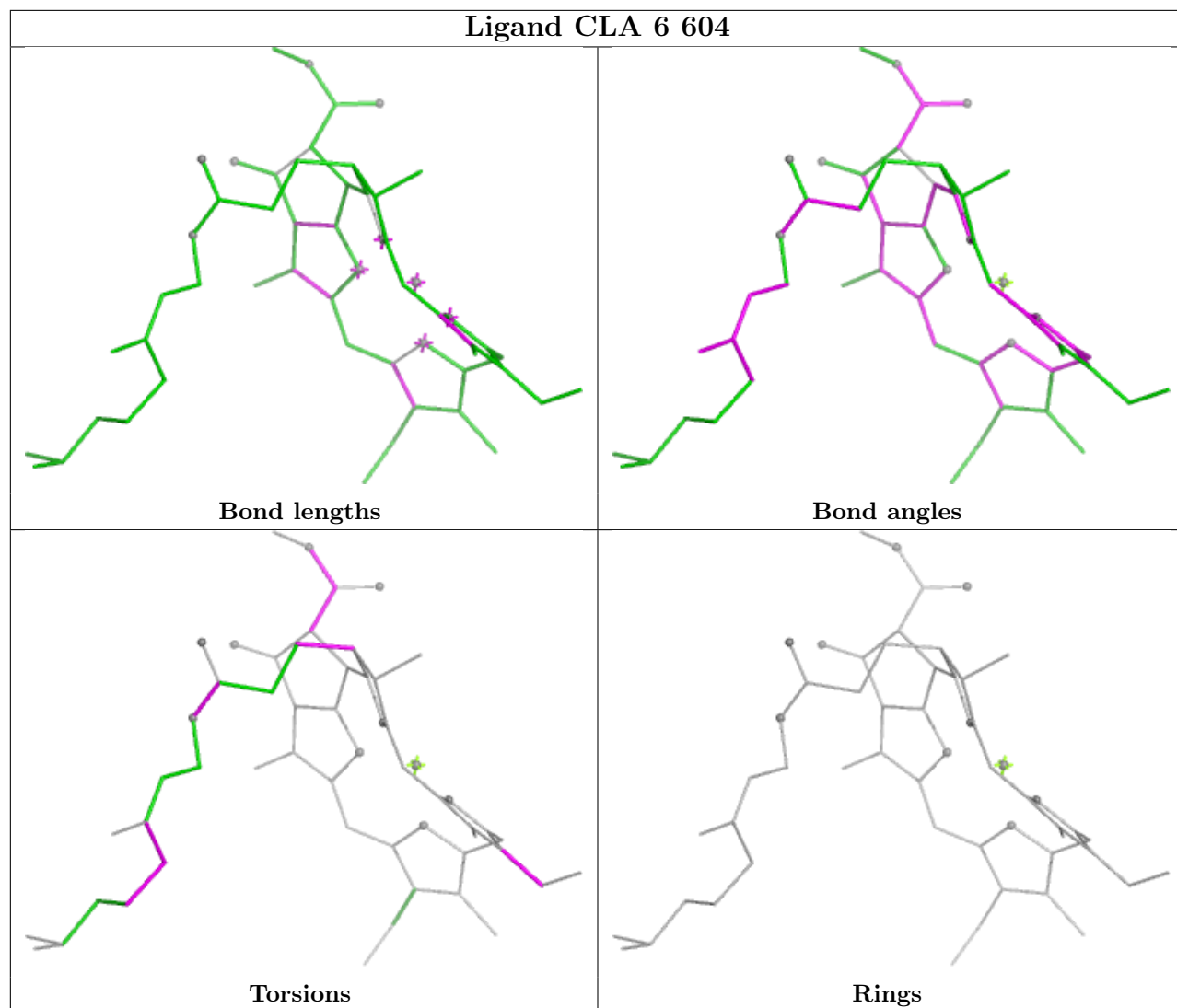


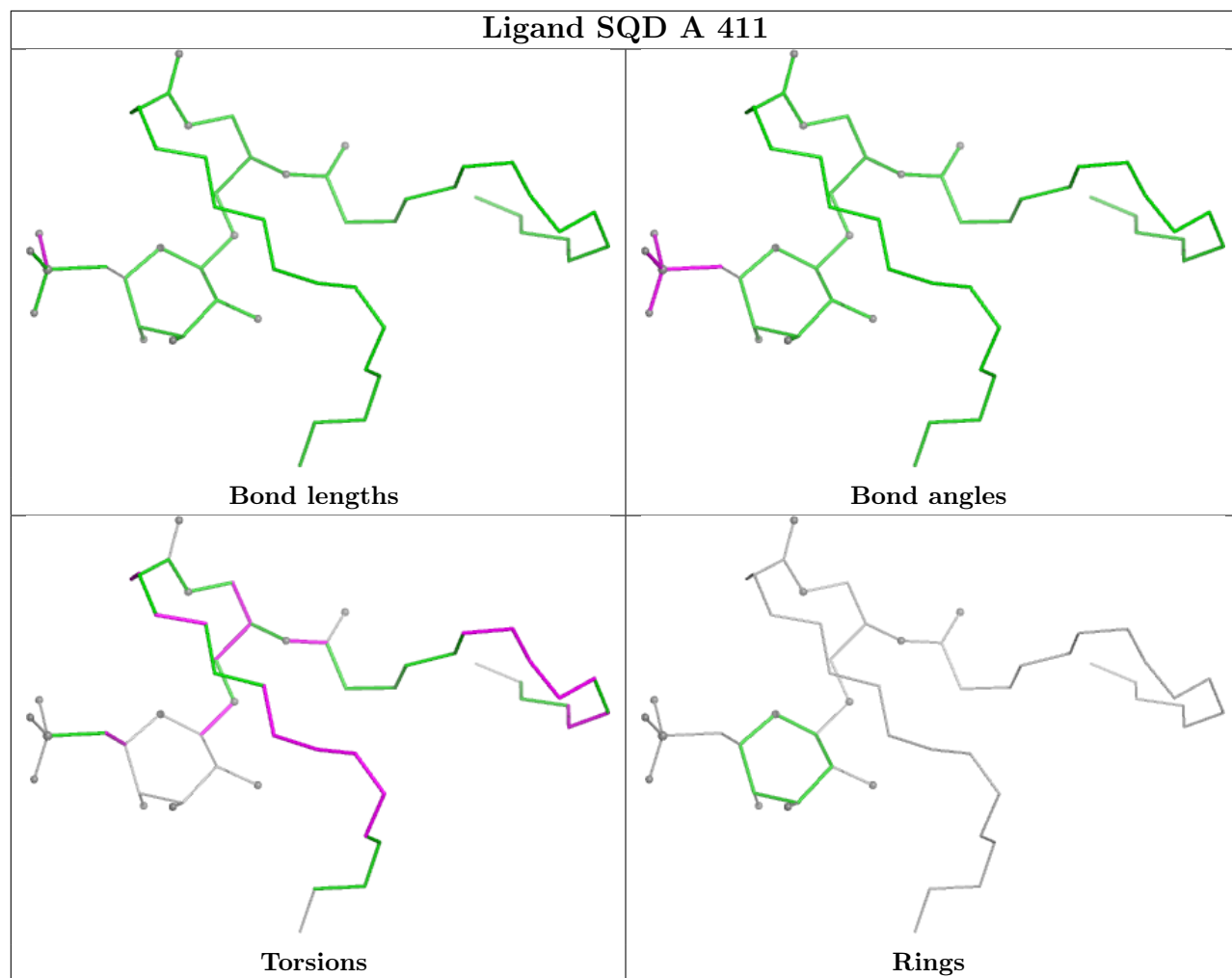
Torsions

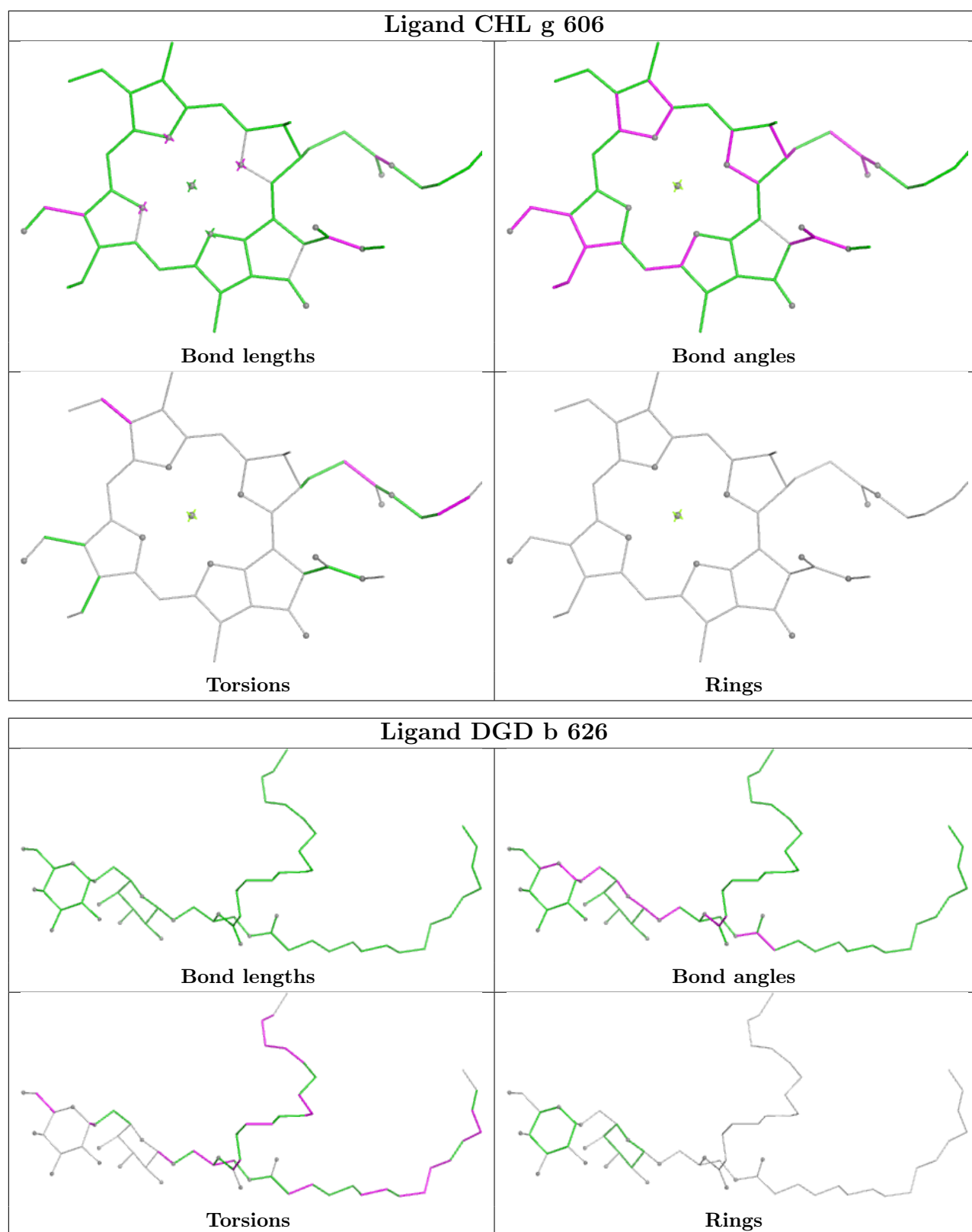


Rings

Ligand CLA 6 604







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

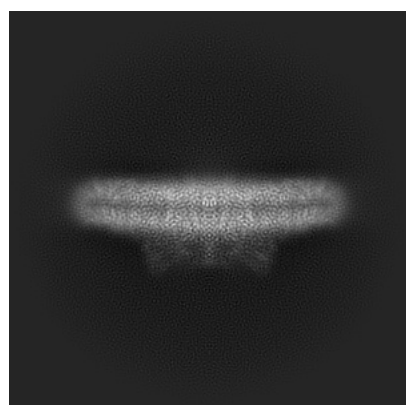
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13078. These allow visual inspection of the internal detail of the map and identification of artifacts.

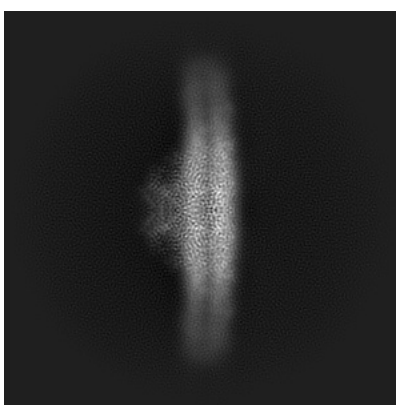
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

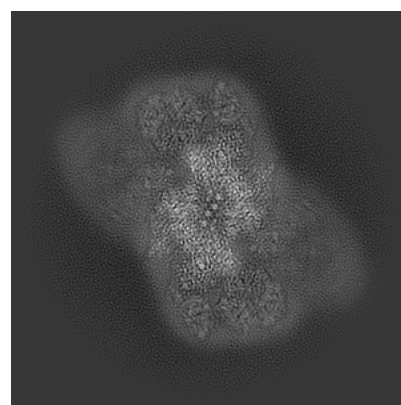
6.1.1 Primary map



X



Y

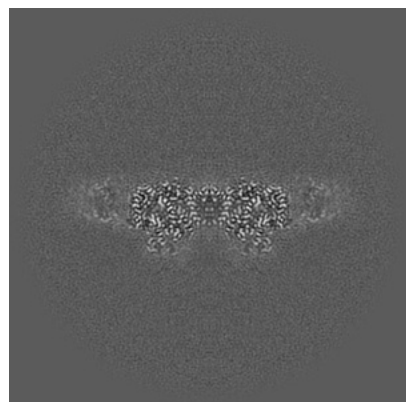


Z

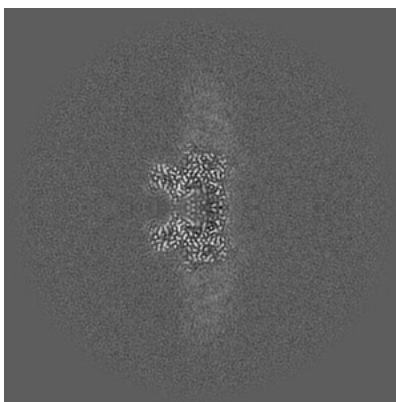
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

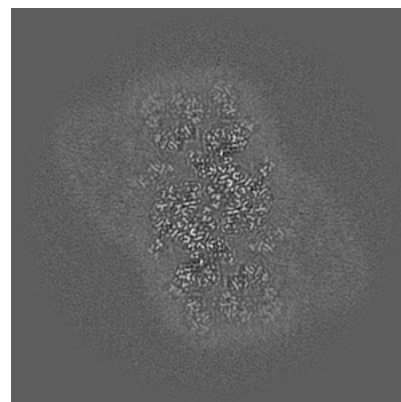
6.2.1 Primary map



X Index: 250



Y Index: 250

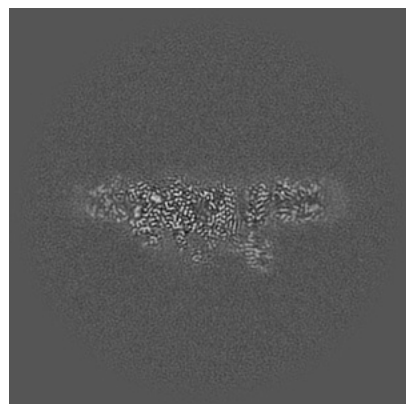


Z Index: 250

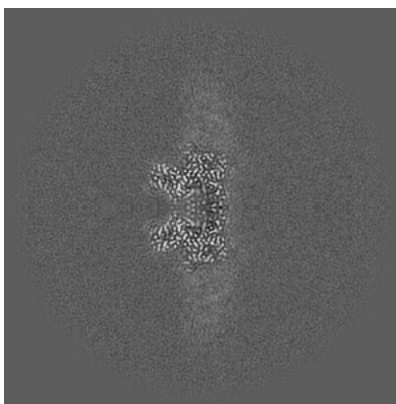
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

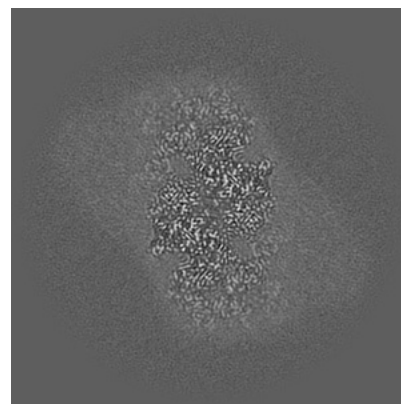
6.3.1 Primary map



X Index: 228



Y Index: 250

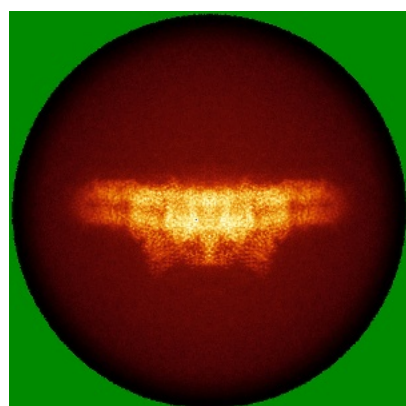


Z Index: 239

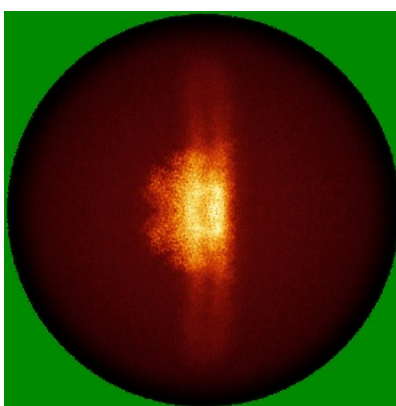
The images above show the largest variance slices of the map in three orthogonal directions.

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

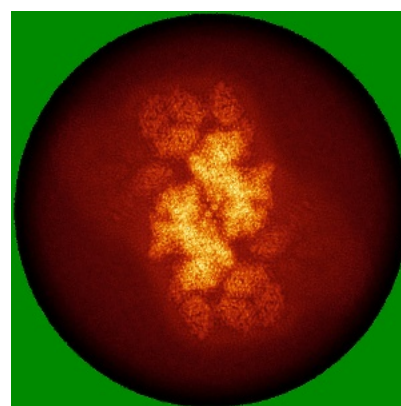
6.4.1 Primary map



X



Y

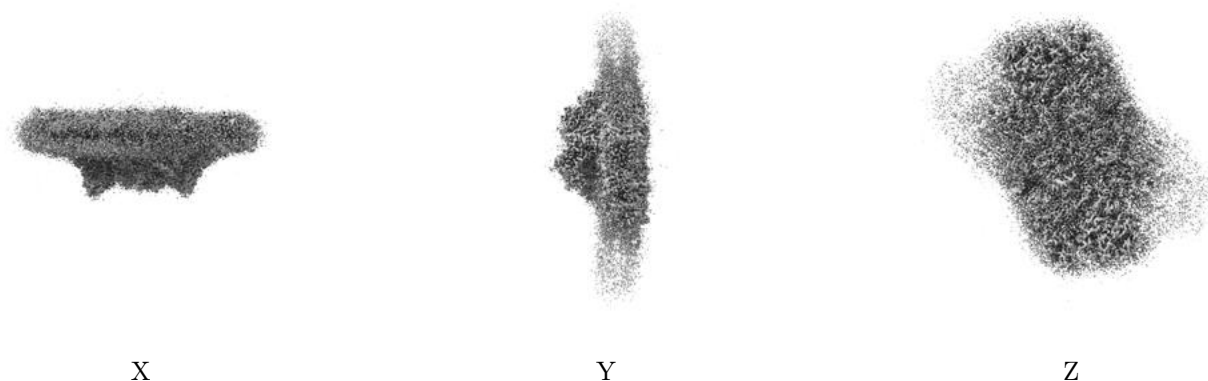


Z

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 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

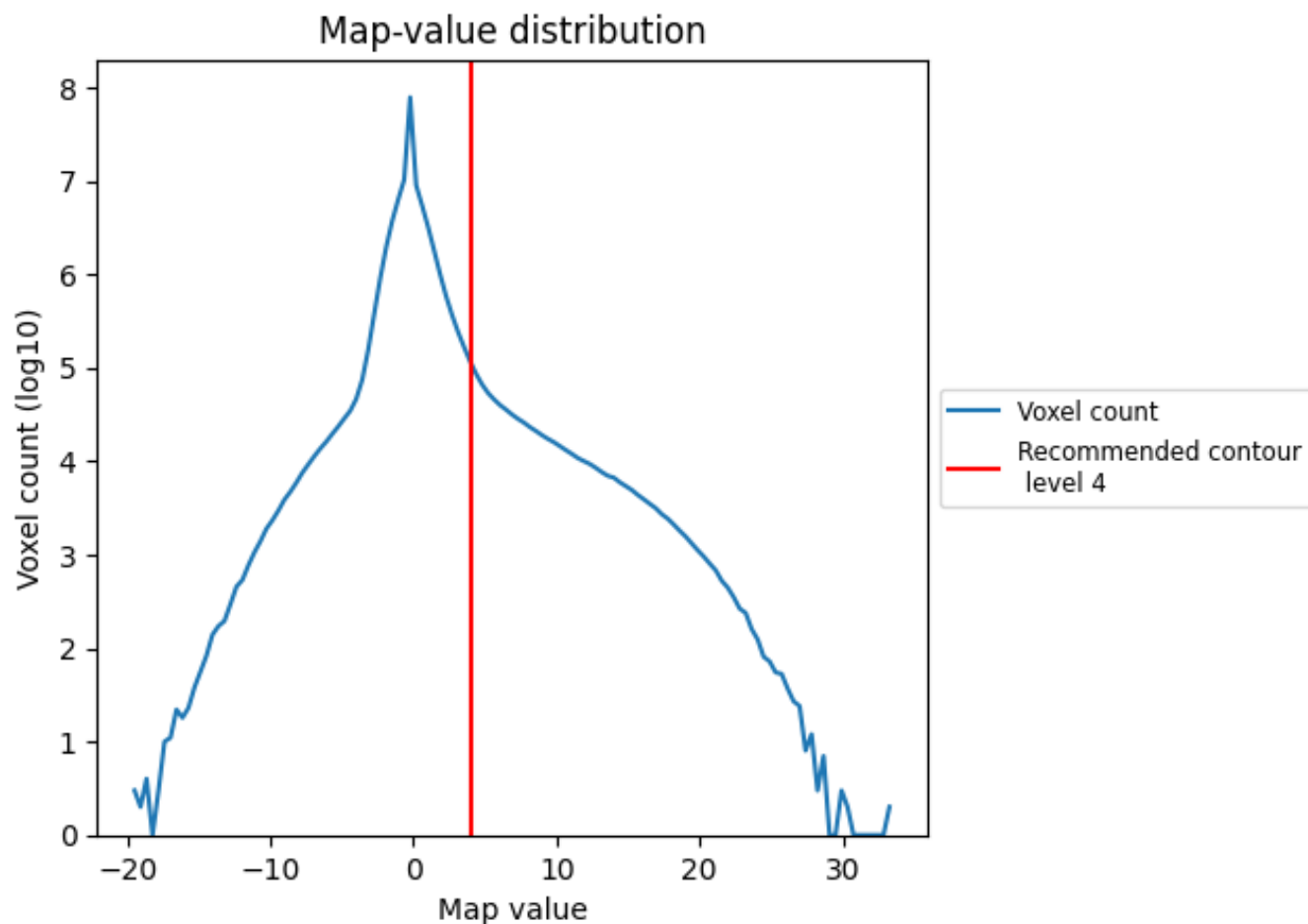
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

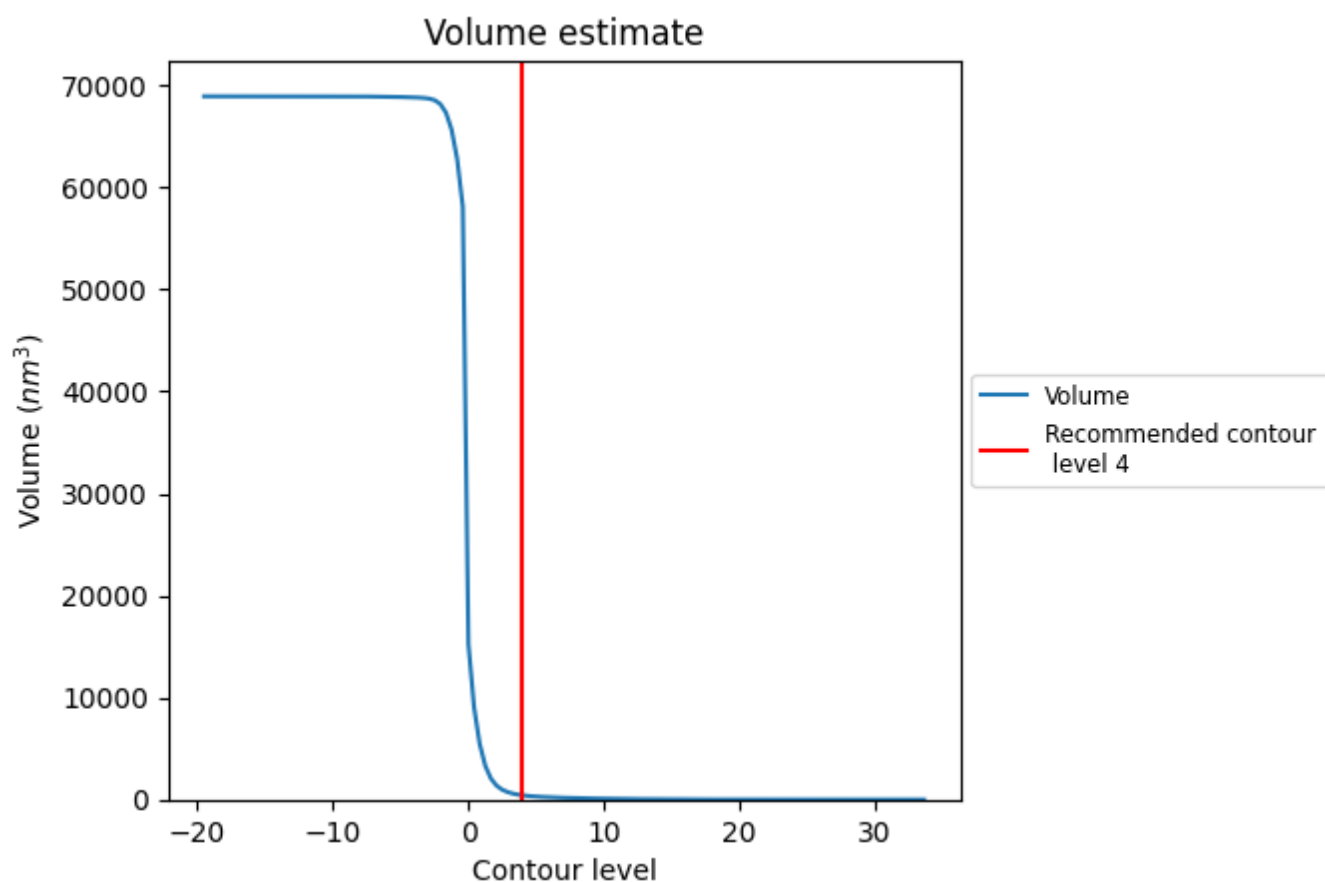
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

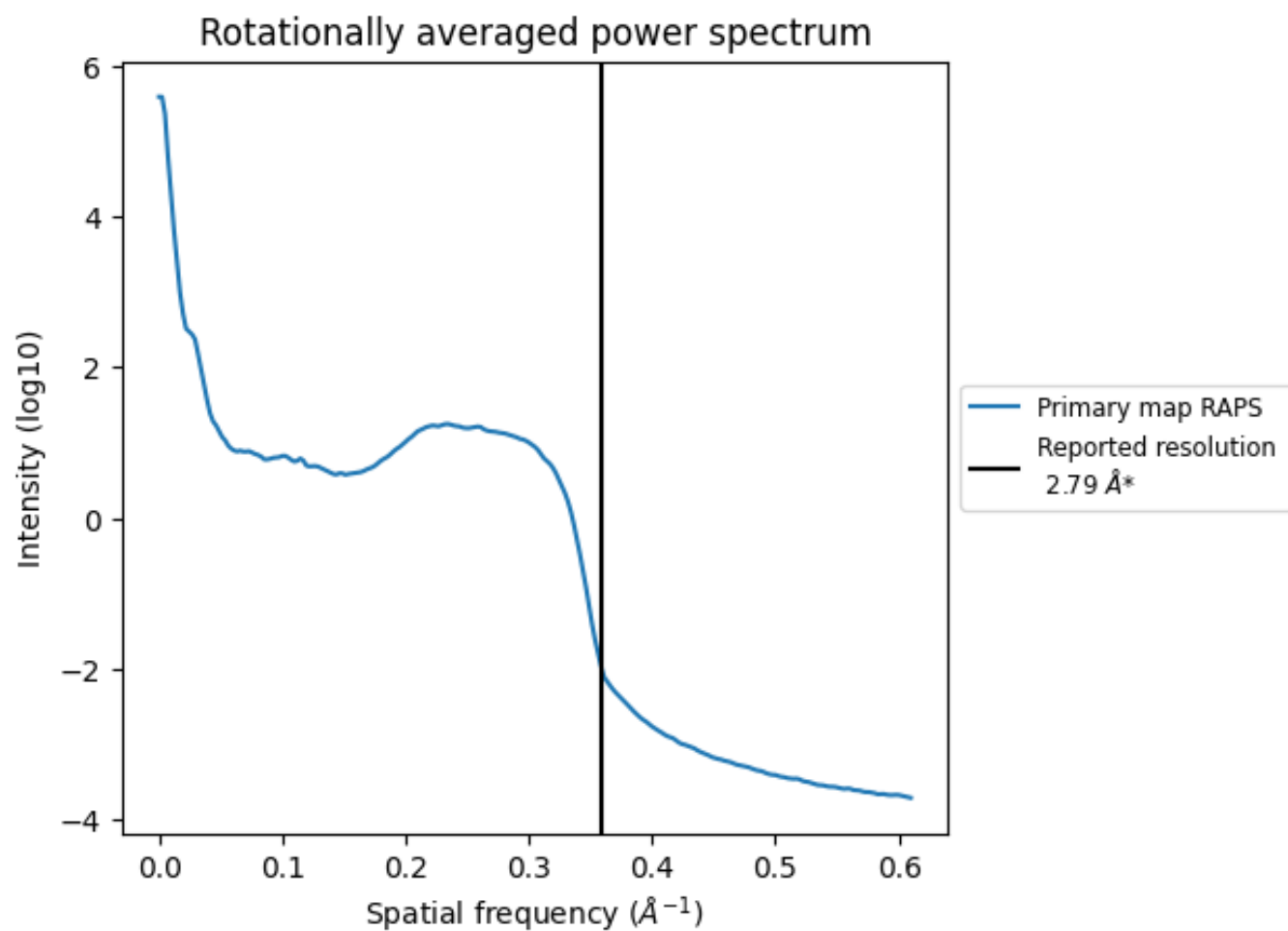
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 423 nm³; this corresponds to an approximate mass of 382 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 0.358 Å⁻¹

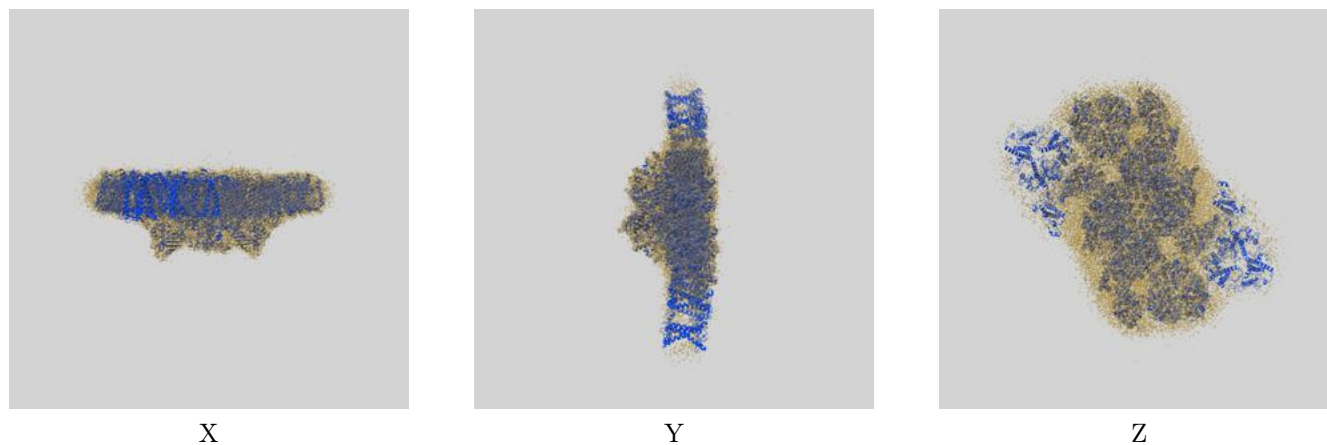
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

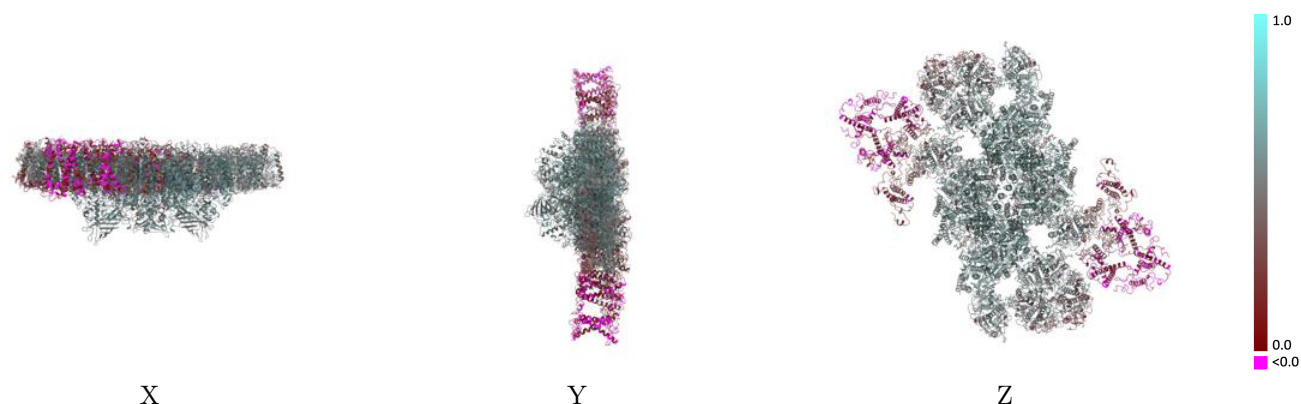
This section contains information regarding the fit between EMDB map EMD-13078 and PDB model 7OUI. Per-residue inclusion information can be found in section [3](#) on page [39](#).

9.1 Map-model overlay [i](#)



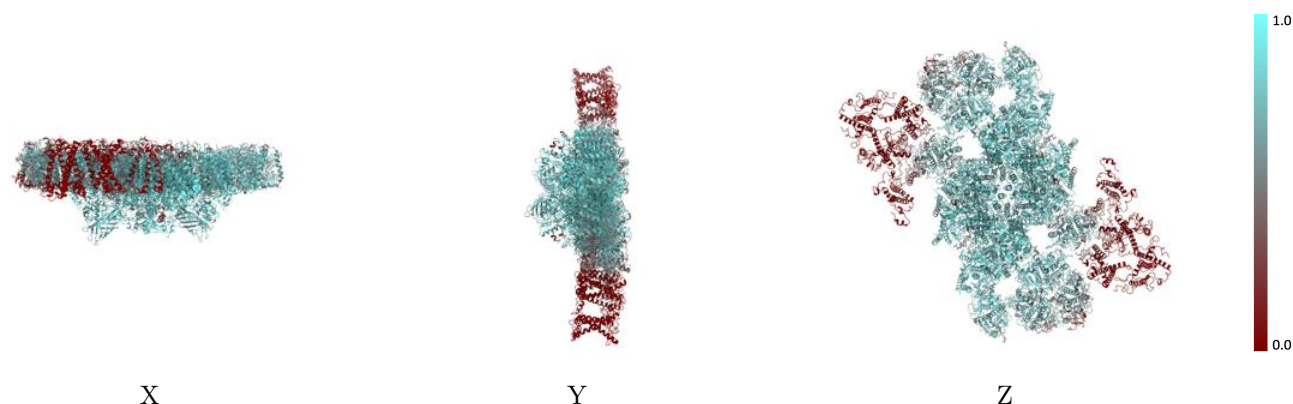
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



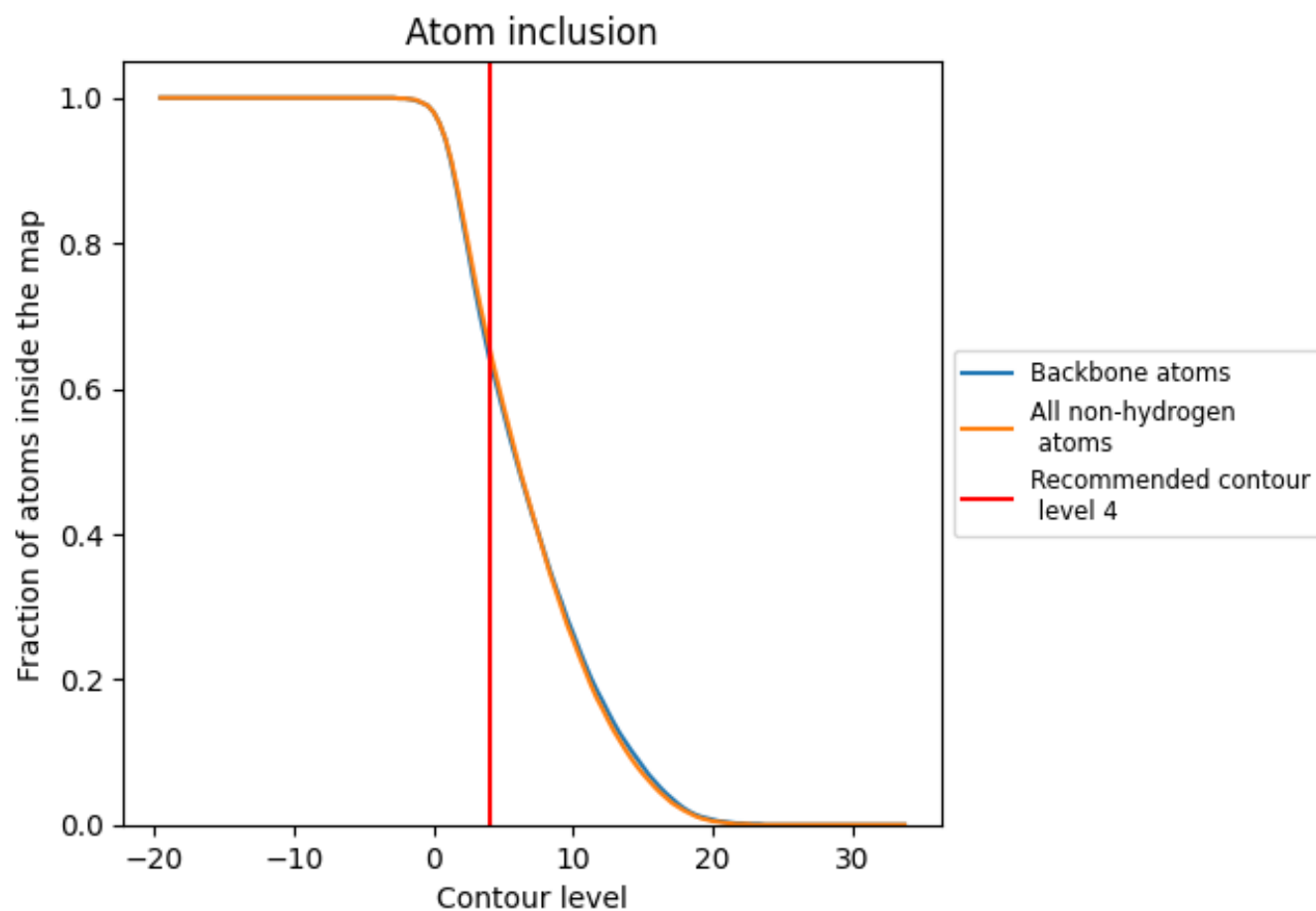
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 66% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6570	 0.4650
1	 0.0340	 0.0670
2	 0.0320	 0.1050
3	 0.0060	 0.0400
4	 0.0870	 0.2440
5	 0.0340	 0.0680
6	 0.0320	 0.1040
7	 0.0060	 0.0410
8	 0.0870	 0.2450
A	 0.8540	 0.5740
B	 0.8690	 0.5810
C	 0.8730	 0.5820
D	 0.8800	 0.5890
E	 0.7940	 0.5260
F	 0.7710	 0.5100
G	 0.5250	 0.3940
H	 0.7940	 0.5510
I	 0.8820	 0.6010
K	 0.8250	 0.5570
L	 0.8350	 0.5430
M	 0.8310	 0.5620
N	 0.6500	 0.4540
O	 0.7370	 0.5090
R	 0.6280	 0.4770
S	 0.7300	 0.5110
T	 0.8010	 0.5660
U	 0.2770	 0.4110
W	 0.8340	 0.5810
X	 0.6210	 0.4490
Y	 0.7790	 0.5100
Z	 0.7270	 0.5140
a	 0.8550	 0.5750
b	 0.8680	 0.5800
c	 0.8700	 0.5820
d	 0.8760	 0.5900



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Chain	Atom inclusion	Q-score
e	 0.7920	 0.5240
f	 0.7750	 0.5080
g	 0.5270	 0.3930
h	 0.7920	 0.5510
i	 0.8940	 0.5980
k	 0.8400	 0.5590
l	 0.8350	 0.5420
m	 0.8230	 0.5660
n	 0.6500	 0.4530
o	 0.7360	 0.5130
r	 0.6250	 0.4760
s	 0.7260	 0.5110
t	 0.8080	 0.5700
u	 0.2820	 0.4040
w	 0.8340	 0.5760
x	 0.6250	 0.4400
y	 0.7770	 0.5080
z	 0.7150	 0.5110