



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 12:50 PM JST

PDB ID : 9LE8 / pdb_00009le8
EMDB ID : EMD-63018
Title : Coordinates of Cryo-EM structure of the Arabidopsis thaliana C2S2M2-type PSII supercomplex
Authors : Chen, S.J.B.; Wu, C.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2025-01-07
Resolution : 3.37 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 : 1.8.5 (274361), 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

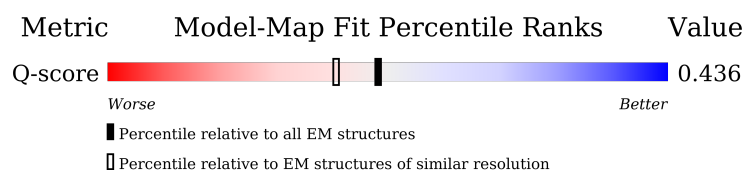
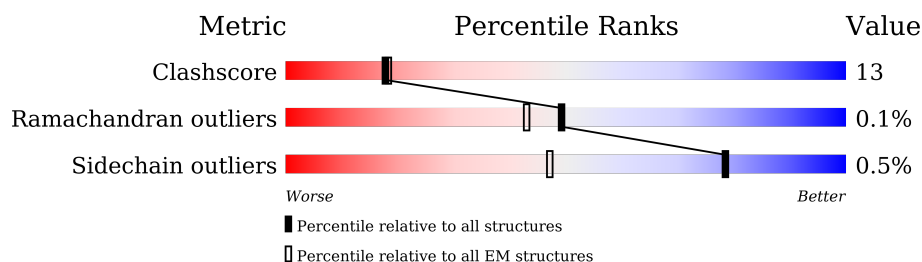
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.37 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	14287 (2.87 - 3.87)

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	9	266	
1	AA	266	
1	AC	266	
1	AE	266	

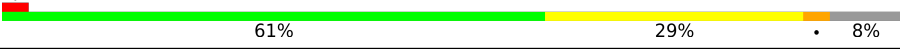
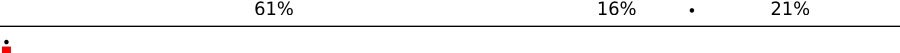
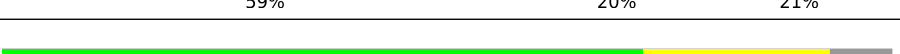
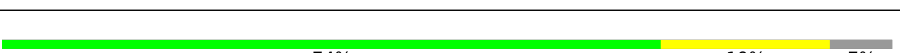
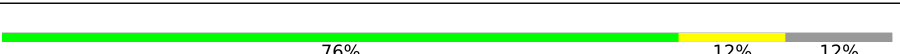
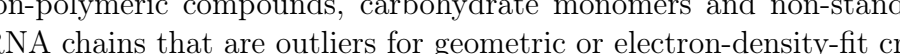
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Mol	Chain	Length	Quality of chain
2	0	243	
2	AD	243	
3	AB	212	
3	AF	212	
4	AJ	352	
4	J	352	
5	AK	508	
5	O	508	
6	AL	459	
6	P	459	
7	AM	352	
7	Q	352	
8	E	83	
8	e	83	
9	F	39	
9	f	39	
10	AH	232	
10	AN	232	
10	AQ	232	
10	AU	232	
10	V	232	
10	p	232	
11	AO	72	
11	j	72	
12	I	36	

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Mol	Chain	Length	Quality of chain
12	i	36	
13	K	37	
13	k	37	
14	AP	38	
14	o	38	
15	M	34	
15	m	34	
16	AR	250	
16	q	250	
17	AS	232	
17	v	232	
18	AG	33	
18	AT	33	
19	U	28	
19	u	28	
20	W	54	
20	w	54	
21	X	42	
21	x	42	
22	AI	62	
22	AV	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHL	AN	607	-	-	X	-

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 83915 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	9	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	AA	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	AC	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	AE	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	0	222	Total	C	N	O	S	0	0
			1716	1120	280	311	5		
2	AD	222	Total	C	N	O	S	0	0
			1716	1120	280	311	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	192	Total	C	N	O	S	0	0
			1512	993	245	270	4		
3	AF	192	Total	C	N	O	S	0	0
			1512	993	245	270	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	323	Total	C	N	O	S	0	0
			2525	1652	415	445	13		
4	AJ	323	Total	C	N	O	S	0	0
			2525	1652	415	445	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	479	Total	C	N	O	S	0	0
			3757	2462	636	647	12		
5	AK	479	Total	C	N	O	S	0	0
			3757	2462	636	647	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		
6	AL	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	Q	342	Total	C	N	O	S	0	0
			2723	1800	445	466	12		
7	AM	342	Total	C	N	O	S	0	0
			2723	1800	445	466	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	64	Total	C	N	O	0	0
			521	342	83	96		
8	e	64	Total	C	N	O	0	0
			521	342	83	96		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	29	Total	C	N	O	S	0	0
			225	147	40	37	1		
9	f	29	Total	C	N	O	S	0	0
			225	147	40	37	1		

- Molecule 10 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
10	p	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
10	AH	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		
10	AN	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
10	AQ	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
10	AU	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	j	60	Total	C	N	O	S	0	0
			447	293	70	82	2		
11	AO	60	Total	C	N	O	S	0	0
			447	293	70	82	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	37	Total	C	N	O	S	0	0
			302	211	44	46	1		
13	k	37	Total	C	N	O	S	0	0
			302	211	44	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	35	Total	C	N	O	S	0	0
			293	195	45	53			

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Mol	Chain	Residues	Atoms				AltConf	Trace
14	AP	35	Total	C	N	O	0	0
			293	195	45	53		

- Molecule 15 is a protein called Photosystem II reaction center protein M.

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

- Molecule 16 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	197	Total	C	N	O	S	0	0
			1539	1004	251	281	3		
16	AR	197	Total	C	N	O	S	0	0
			1539	1004	251	281	3		

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	v	216	Total	C	N	O	S	0	0
			1670	1091	272	303	4		
17	AS	216	Total	C	N	O	S	0	0
			1670	1091	272	303	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AG	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
18	AT	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

- Molecule 19 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	25	Total	C	N	O	S	0	0
			195	122	36	34	3		
19	u	25	Total	C	N	O	S	0	0
			195	122	36	34	3		

- Molecule 20 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	54	Total	C	N	O	S	0	0
			428	282	61	84	1		
20	w	54	Total	C	N	O	S	0	0
			428	282	61	84	1		

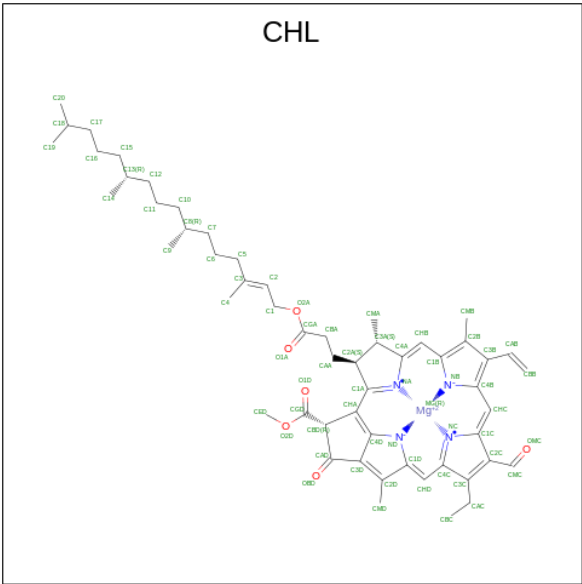
- Molecule 21 is a protein called (thale cress) hypothetical protein.

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

- Molecule 22 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AI	62	Total	C	N	O	S	0	0
			465	313	69	82	1		
22	AV	62	Total	C	N	O	S	0	0
			465	313	69	82	1		

- Molecule 23 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
23	9	1	Total 41	C 32	Mg 1	N 4	O 4	0
23	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	9	1	Total 63	C 52	Mg 1	N 4	O 6	0
23	9	1	Total 44	C 33	Mg 1	N 4	O 6	0
23	9	1	Total 62	C 51	Mg 1	N 4	O 6	0
23	0	1	Total 64	C 53	Mg 1	N 4	O 6	0
23	0	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	0	1	Total 53	C 42	Mg 1	N 4	O 6	0
23	0	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	0	1	Total 36	C 28	Mg 1	N 4	O 3	0
23	0	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 61	C 50	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AA	1	Total 59	C 48	Mg 1	N 4	O 6	0
23	AA	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AB	1	Total 45	C 34	Mg 1	N 4	O 6	0
23	AB	1	Total 40	C 32	Mg 1	N 4	O 3	0
23	AB	1	Total 44	C 33	Mg 1	N 4	O 6	0
23	AB	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
23	AB	1	Total 42	C 33	Mg 1	N 4	O 4	0
23	AC	1	Total 44	C 33	Mg 1	N 4	O 6	0
23	AC	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AC	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AC	1	Total 44	C 33	Mg 1	N 4	O 6	0
23	AC	1	Total 62	C 51	Mg 1	N 4	O 6	0
23	AD	1	Total 63	C 52	Mg 1	N 4	O 6	0
23	AD	1	Total 64	C 53	Mg 1	N 4	O 6	0
23	AD	1	Total 53	C 42	Mg 1	N 4	O 6	0
23	AD	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AD	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	AD	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AE	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AE	1	Total 61	C 50	Mg 1	N 4	O 6	0
23	AE	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AE	1	Total 61	C 50	Mg 1	N 4	O 6	0
23	AE	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AE	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AF	1	Total 45	C 34	Mg 1	N 4	O 6	0
23	AF	1	Total 33	C 27	Mg 1	N 4	O 1	0
23	AF	1	Total 35	C 26	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
23	AF	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	AF	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	V	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
23	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	V	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	V	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	p	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	p	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
23	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	p	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	q	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
23	q	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
23	q	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	q	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
23	v	1	Total	C	Mg	N	O	0
			44	33	1	4	6	
23	v	1	Total	C	Mg	N	O	0
			35	28	1	4	2	
23	v	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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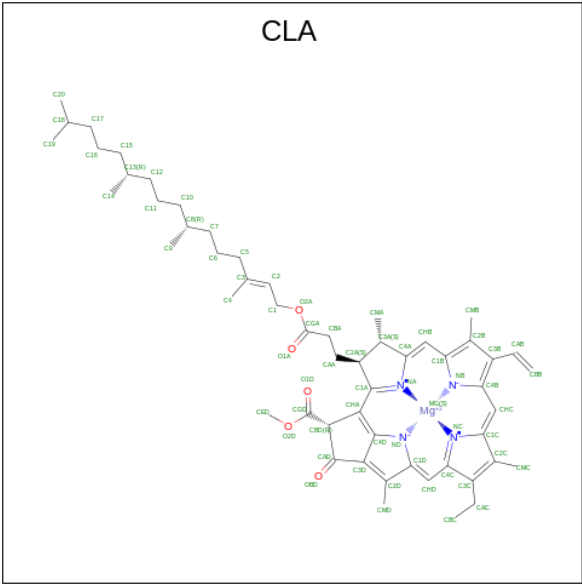
Mol	Chain	Residues	Atoms					AltConf
23	v	1	Total 38	C 30	Mg 1	N 4	O 3	0
23	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
23	AH	1	Total 48	C 37	Mg 1	N 4	O 6	0
23	AH	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
23	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0
23	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
23	AN	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
23	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
23	AN	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	AN	1	Total 46	C 35	Mg 1	N 4	O 6	0
23	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
23	AQ	1	Total 48	C 37	Mg 1	N 4	O 6	0
23	AQ	1	Total 50	C 39	Mg 1	N 4	O 6	0
23	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
23	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
23	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0
23	AR	1	Total 64	C 53	Mg 1	N 4	O 6	0
23	AR	1	Total 56	C 45	Mg 1	N 4	O 6	0
23	AR	1	Total 53	C 42	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
23	AR	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
23	AS	1	Total	C	Mg	N	O	0
			44	33	1	4	6	
23	AS	1	Total	C	Mg	N	O	0
			34	27	1	4	2	
23	AS	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
23	AS	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	AU	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	AU	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	AU	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
23	AU	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	AU	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
24	9	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	9	1	Total 54	C 45	Mg 1	N 4	O 4	0
24	9	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	9	1	Total 36	C 30	Mg 1	N 4	O 1	0
24	0	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	0	1	Total 58	C 49	Mg 1	N 4	O 4	0
24	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	0	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	0	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	AA	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	AA	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AA	1	Total 48	C 39	Mg 1	N 4	O 4	0
24	AA	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AB	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AB	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AB	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AB	1	Total 40	C 32	Mg 1	N 4	O 3	0
24	AB	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AB	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AC	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	AC	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	AC	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	AC	1	Total 54	C 45	Mg 1	N 4	O 4	0
24	AC	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	AC	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	AC	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	AC	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	AD	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	AD	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	AD	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AD	1	Total 58	C 49	Mg 1	N 4	O 4	0
24	AD	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	AD	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AD	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	AD	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	AE	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	AE	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	AE	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AE	1	Total 48	C 39	Mg 1	N 4	O 4	0
24	AE	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AE	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AE	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AE	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AE	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AF	1	Total 39	C 32	Mg 1	N 4	O 2	0
24	AF	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AF	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AF	1	Total 40	C 32	Mg 1	N 4	O 3	0
24	AF	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AF	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	J	1	Total 58	C 49	Mg 1	N 4	O 4	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 63	C 54	Mg 1	N 4	O 4	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	P	1	Total 61	C 52	Mg 1	N 4	O 4	0
24	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	V	1	Total 34	C 28	Mg 1	N 4	O 1	0
24	V	1	Total 62	C 53	Mg 1	N 4	O 4	0
24	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	V	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	V	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	p	1	Total 63	C 53	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	p	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
24	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	p	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
24	p	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	q	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
24	q	1	Total	C	Mg	N	O	0
			58	49	1	4	4	
24	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	q	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	q	1	Total	C	Mg	N	O	0
			63	54	1	4	4	
24	q	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
24	q	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
24	q	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	v	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	v	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	v	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	v	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
24	v	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	v	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	v	1	Total 53	C 44	Mg 1	N 4	O 4	0
24	v	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	AH	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AH	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AH	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	AH	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	AH	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	AH	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	AH	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AH	1	Total 46	C 37	Mg 1	N 4	O 4	0
24	AJ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AJ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AJ	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	AJ	1	Total 58	C 49	Mg 1	N 4	O 4	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 63	C 54	Mg 1	N 4	O 4	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AK	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AL	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	AL	1	Total 61	C 52	Mg 1	N 4	O 4	0
24	AM	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AM	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AN	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AN	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AN	1	Total 37	C 31	Mg 1	N 4	O 1	0
24	AN	1	Total 62	C 53	Mg 1	N 4	O 4	0
24	AN	1	Total 39	C 32	Mg 1	N 4	O 2	0
24	AN	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	AN	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AN	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	AQ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AQ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AQ	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	AQ	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AQ	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	AQ	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	AQ	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	AQ	1	Total 40	C 32	Mg 1	N 4	O 3	0
24	AR	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	AR	1	Total 58	C 49	Mg 1	N 4	O 4	0

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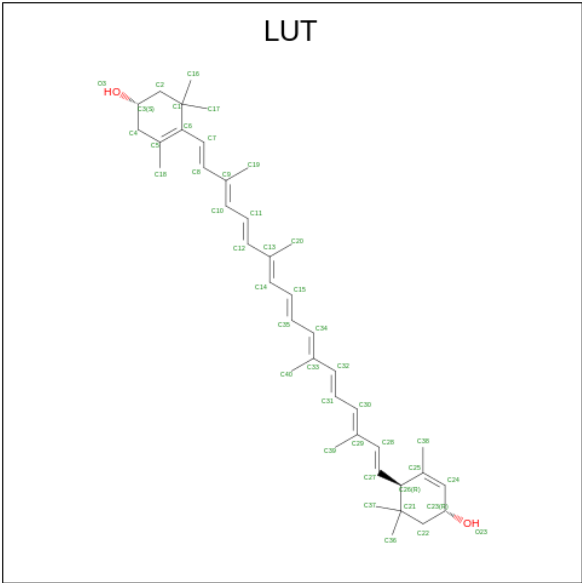
Mol	Chain	Residues	Atoms					AltConf
24	AR	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	AR	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	AR	1	Total 39	C 32	Mg 1	N 4	O 2	0
24	AR	1	Total 63	C 54	Mg 1	N 4	O 4	0
24	AR	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	AR	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	AR	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	AR	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	AS	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	AS	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	AS	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	AS	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	AS	1	Total 53	C 44	Mg 1	N 4	O 4	0
24	AS	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	AS	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	AS	1	Total 53	C 44	Mg 1	N 4	O 4	0
24	AS	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	AU	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AU	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	AU	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	AU	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	AU	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	AU	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	AU	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	AU	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

- Molecule 25 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
25	9	1	Total	C	O	0
			42	40	2	
25	9	1	Total	C	O	0
			42	40	2	
25	0	1	Total	C	O	0
			42	40	2	
25	0	1	Total	C	O	0
			42	40	2	
25	AA	1	Total	C	O	0
			42	40	2	
25	AA	1	Total	C	O	0
			42	40	2	
25	AC	1	Total	C	O	0
			42	40	2	

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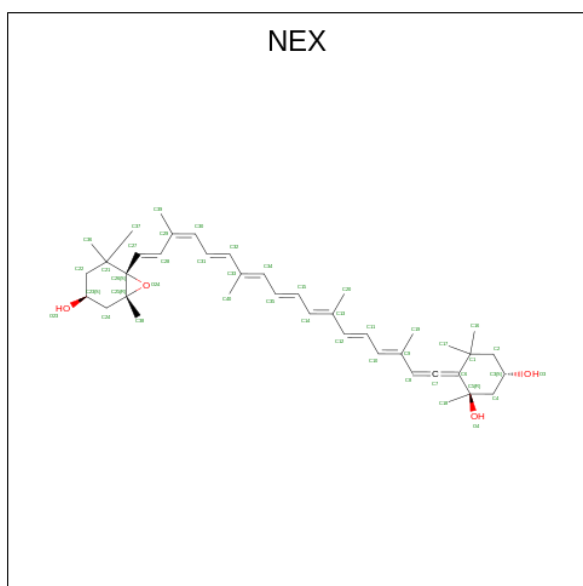
Mol	Chain	Residues	Atoms			AltConf
25	AC	1	Total 42	C 40	O 2	0
25	AD	1	Total 42	C 40	O 2	0
25	AD	1	Total 42	C 40	O 2	0
25	AE	1	Total 42	C 40	O 2	0
25	AE	1	Total 42	C 40	O 2	0
25	AF	1	Total 42	C 40	O 2	0
25	V	1	Total 42	C 40	O 2	0
25	V	1	Total 42	C 40	O 2	0
25	p	1	Total 42	C 40	O 2	0
25	p	1	Total 42	C 40	O 2	0
25	q	1	Total 42	C 40	O 2	0
25	v	1	Total 42	C 40	O 2	0
25	v	1	Total 42	C 40	O 2	0
25	AH	1	Total 42	C 40	O 2	0
25	AH	1	Total 42	C 40	O 2	0
25	AN	1	Total 42	C 40	O 2	0
25	AN	1	Total 42	C 40	O 2	0
25	AQ	1	Total 42	C 40	O 2	0
25	AQ	1	Total 42	C 40	O 2	0
25	AR	1	Total 42	C 40	O 2	0
25	AS	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
25	AS	1	Total	C	O	0
			42	40	2	
25	AU	1	Total	C	O	0
			42	40	2	
25	AU	1	Total	C	O	0
			42	40	2	

- Molecule 26 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



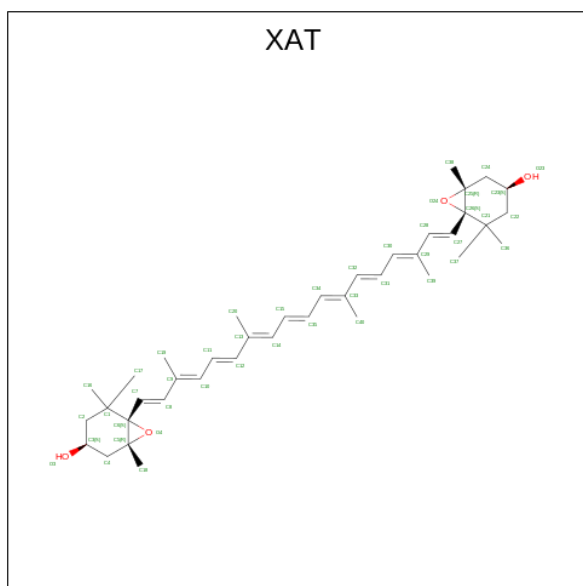
Mol	Chain	Residues	Atoms			AltConf
26	9	1	Total	C	O	0
			44	40	4	
26	AA	1	Total	C	O	0
			44	40	4	
26	AC	1	Total	C	O	0
			44	40	4	
26	AE	1	Total	C	O	0
			44	40	4	
26	p	1	Total	C	O	0
			44	40	4	
26	q	1	Total	C	O	0
			44	40	4	
26	v	1	Total	C	O	0
			44	40	4	

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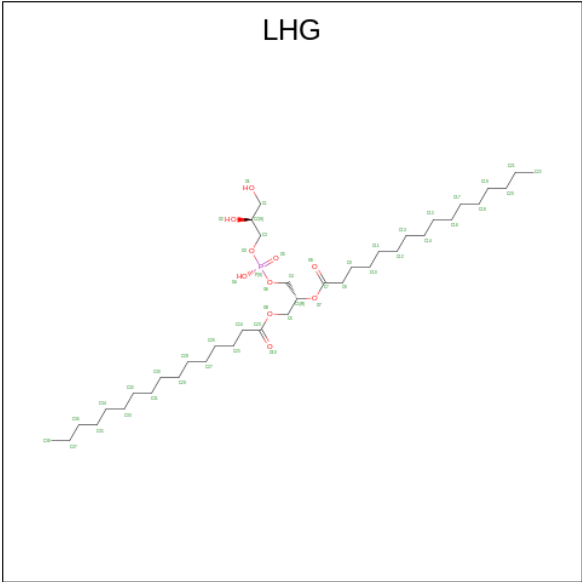
Mol	Chain	Residues	Atoms			AltConf
26	AQ	1	Total	C	O	0
			44	40	4	
26	AR	1	Total	C	O	0
			44	40	4	
26	AS	1	Total	C	O	0
			44	40	4	
26	AU	1	Total	C	O	0
			44	40	4	

- Molecule 27 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
27	9	1	Total	C	O	0
			44	40	4	
27	AB	1	Total	C	O	0
			44	40	4	
27	AF	1	Total	C	O	0
			44	40	4	
27	q	1	Total	C	O	0
			44	40	4	
27	AR	1	Total	C	O	0
			44	40	4	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



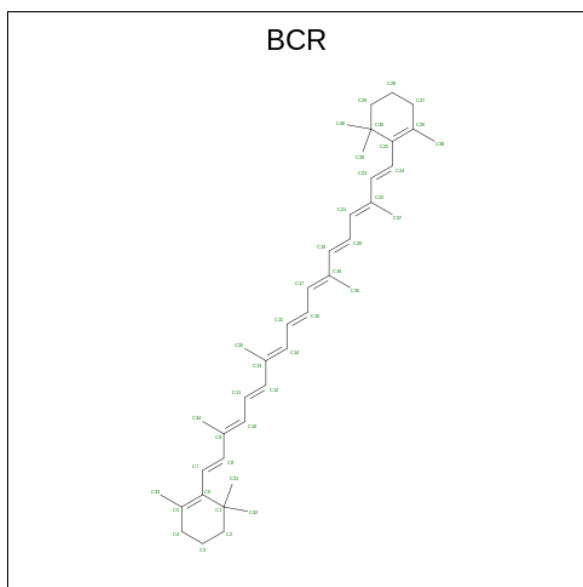
Mol	Chain	Residues	Atoms				AltConf
28	0	1	Total	C	O	P	0
			47	36	10	1	
28	AD	1	Total	C	O	P	0
			47	36	10	1	
28	O	1	Total	C	O	P	0
			49	38	10	1	
28	O	1	Total	C	O	P	0
			46	35	10	1	
28	O	1	Total	C	O	P	0
			49	38	10	1	
28	P	1	Total	C	O	P	0
			49	38	10	1	
28	Q	1	Total	C	O	P	0
			49	38	10	1	
28	V	1	Total	C	O	P	0
			49	38	10	1	
28	p	1	Total	C	O		0
			40	35	5		
28	q	1	Total	C	O	P	0
			42	31	10	1	
28	v	1	Total	C	O	P	0
			49	38	10	1	
28	W	1	Total	C	O	P	0
			49	38	10	1	
28	AH	1	Total	C	O	P	0
			49	38	10	1	
28	AK	1	Total	C	O	P	0
			46	35	10	1	

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Mol	Chain	Residues	Atoms				AltConf
28	AK	1	Total	C	O	P	0
			49	38	10	1	
28	AL	1	Total	C	O	P	0
			49	38	10	1	
28	AM	1	Total	C	O	P	0
			49	38	10	1	
28	AN	1	Total	C	O	P	0
			49	38	10	1	
28	AQ	1	Total	C	O	P	0
			49	38	10	1	
28	AS	1	Total	C	O	P	0
			49	38	10	1	
28	w	1	Total	C	O	P	0
			49	38	10	1	
28	AU	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



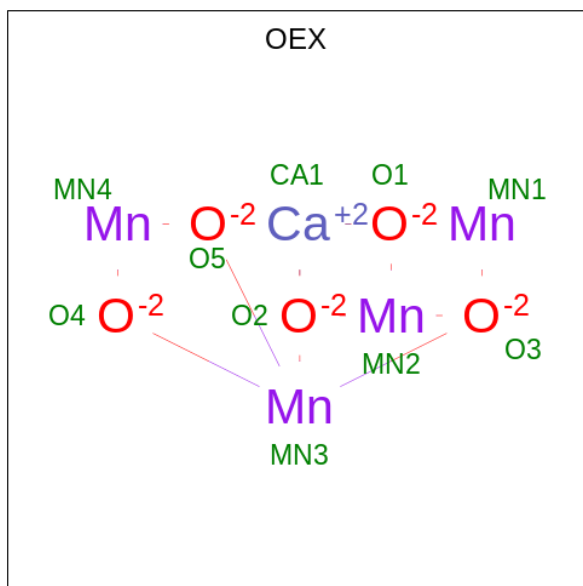
Mol	Chain	Residues	Atoms		AltConf
29	AB	1	Total	C	0
			40	40	
29	AF	1	Total	C	0
			40	40	
29	J	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
29	O	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	P	1	Total C 40 40	0
29	P	1	Total C 40 40	0
29	P	1	Total C 40 40	0
29	F	1	Total C 40 40	0
29	j	1	Total C 40 40	0
29	AI	1	Total C 40 40	0
29	AJ	1	Total C 40 40	0
29	AK	1	Total C 40 40	0
29	AK	1	Total C 40 40	0
29	AK	1	Total C 40 40	0
29	AK	1	Total C 40 40	0
29	AL	1	Total C 40 40	0
29	AL	1	Total C 40 40	0
29	f	1	Total C 40 40	0
29	AO	1	Total C 40 40	0
29	k	1	Total C 40 40	0
29	AV	1	Total C 40 40	0

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

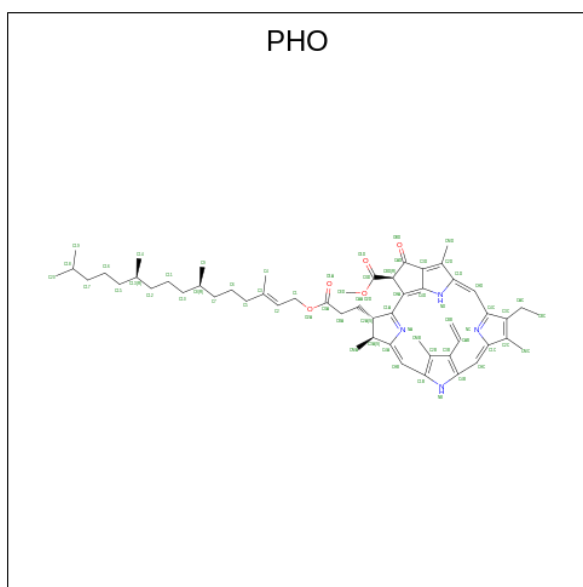


Mol	Chain	Residues	Atoms				AltConf
30	J	1	Total	Ca	Mn	O	0
			10	1	4	5	
30	AJ	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 31 is FE (II) ION (CCD ID: FE2) (formula: Fe).

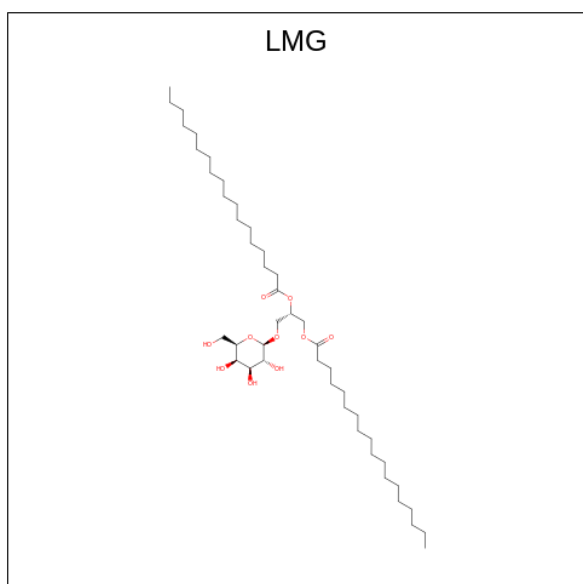
Mol	Chain	Residues	Atoms		AltConf
31	J	1	Total	Fe	0
			1	1	
31	AJ	1	Total	Fe	0
			1	1	

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$).



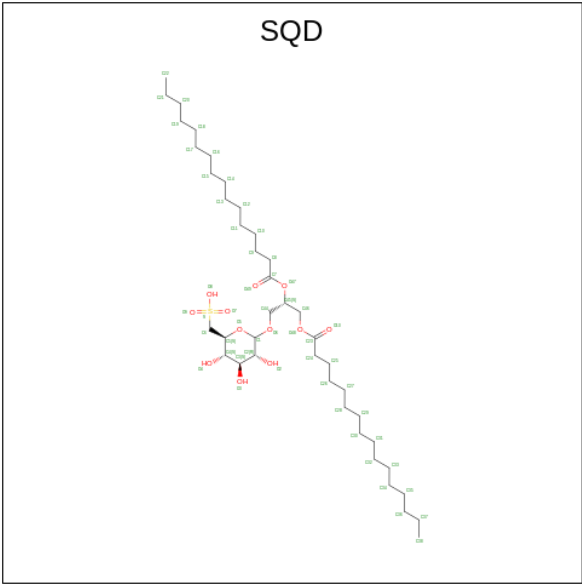
Mol	Chain	Residues	Atoms				AltConf
32	J	1	Total	C	N	O	0
			64	55	4	5	
32	J	1	Total	C	N	O	0
			64	55	4	5	
32	AJ	1	Total	C	N	O	0
			64	55	4	5	
32	AJ	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
33	J	1	Total	C	O	0
			48	38	10	
33	O	1	Total	C	O	0
			51	41	10	
33	O	1	Total	C	O	0
			40	30	10	
33	P	1	Total	C	O	0
			51	41	10	
33	Q	1	Total	C	O	0
			46	36	10	
33	AK	1	Total	C	O	0
			40	30	10	
33	AK	1	Total	C	O	0
			51	41	10	
33	AL	1	Total	C	O	0
			48	38	10	
33	AL	1	Total	C	O	0
			51	41	10	
33	AM	1	Total	C	O	0
			46	36	10	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



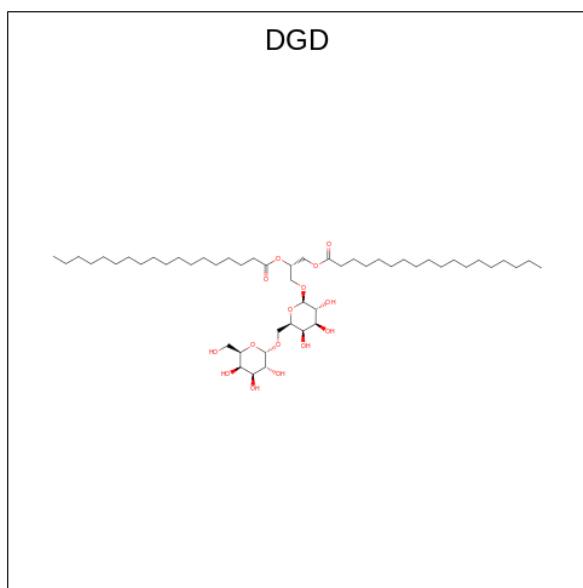
Mol	Chain	Residues	Atoms				AltConf
34	J	1	Total	C	O	S	0
			54	41	12	1	

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Mol	Chain	Residues	Atoms				AltConf
34	Q	1	Total	C	O	S	0
			50	37	12	1	
34	o	1	Total	C	O	S	0
			42	29	12	1	
34	M	1	Total	C	O	S	0
			54	41	12	1	
34	AJ	1	Total	C	O	S	0
			54	41	12	1	
34	AM	1	Total	C	O	S	0
			50	37	12	1	
34	AP	1	Total	C	O	S	0
			42	29	12	1	
34	m	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



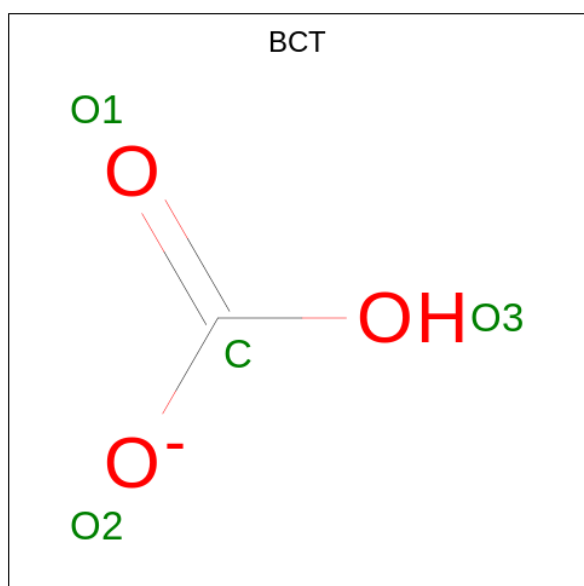
Mol	Chain	Residues	Atoms			AltConf
35	J	1	Total	C	O	0
			60	45	15	
35	J	1	Total	C	O	0
			59	44	15	
35	P	1	Total	C	O	0
			55	40	15	
35	j	1	Total	C	O	0
			62	47	15	

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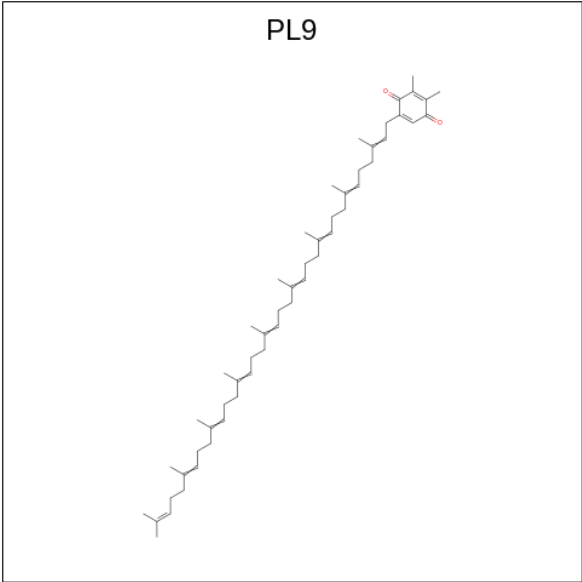
Mol	Chain	Residues	Atoms			AltConf
35	AJ	1	Total	C	O	0
			59	44	15	
35	AJ	1	Total	C	O	0
			60	45	15	
35	AL	1	Total	C	O	0
			55	40	15	
35	AL	1	Total	C	O	0
			62	47	15	
35	AO	1	Total	C	O	0
			62	47	15	

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



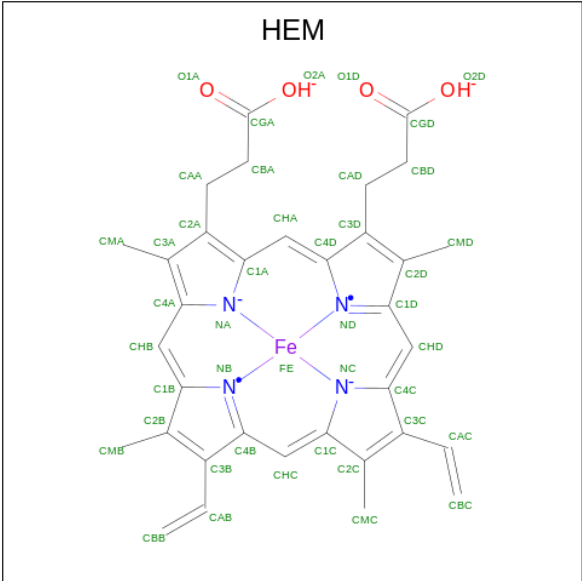
Mol	Chain	Residues	Atoms			AltConf
36	J	1	Total	C	O	0
			4	1	3	
36	AM	1	Total	C	O	0
			4	1	3	

- Molecule 37 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



Mol	Chain	Residues	Atoms			AltConf
37	Q	1	Total	C	O	0
			52	50	2	
37	AM	1	Total	C	O	0
			52	50	2	

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



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

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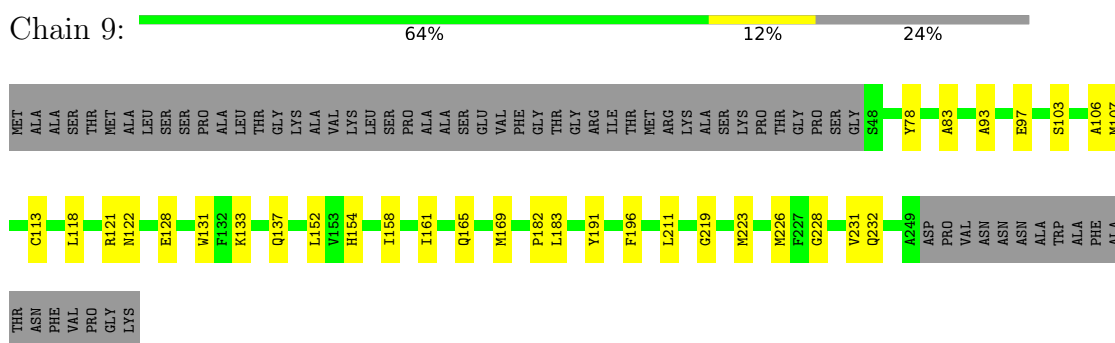
Continued from previous page...

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

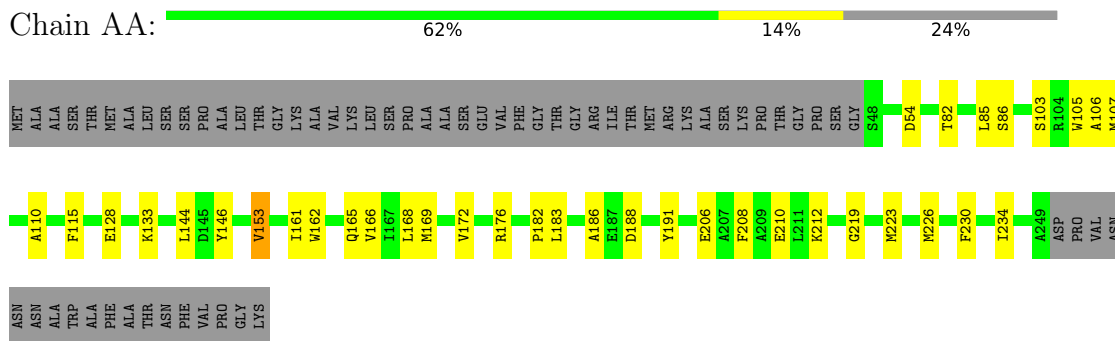
3 Residue-property plots

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.

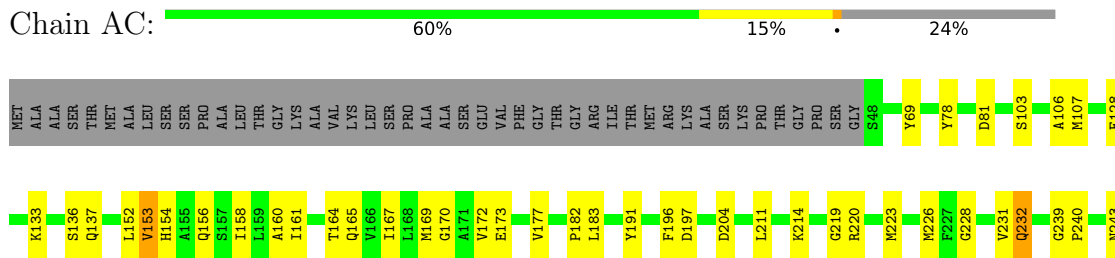
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

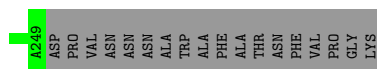


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



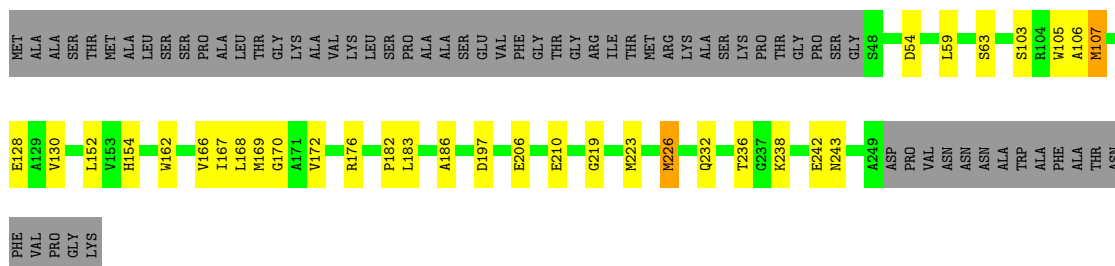
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic





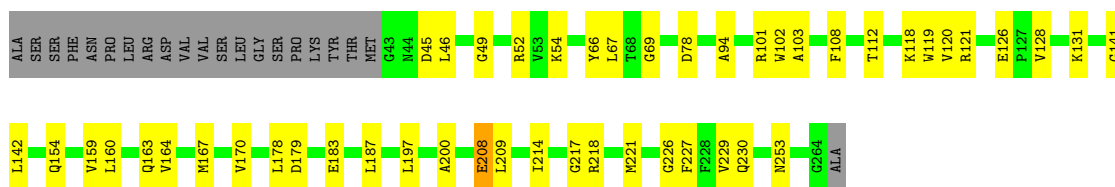
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain AE:  64% 12% 24%



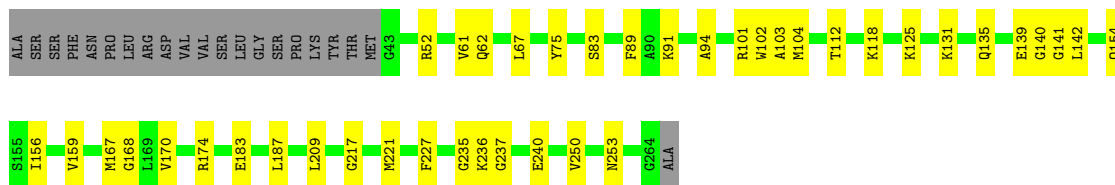
- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

Chain 0:  72% 19% 9%



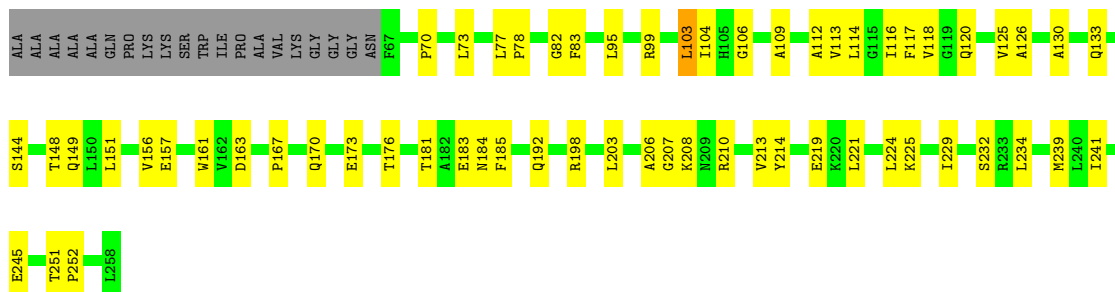
- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

Chain AD:  74% 17% 9%



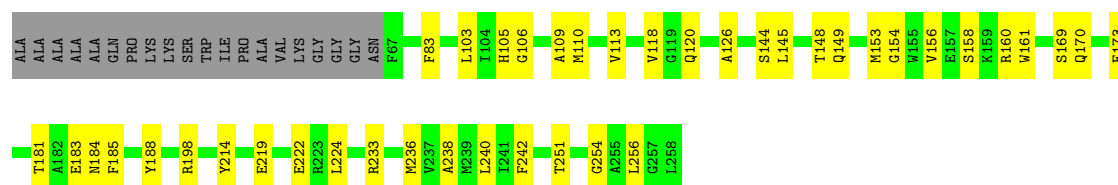
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain AB:  62% 28% 9%



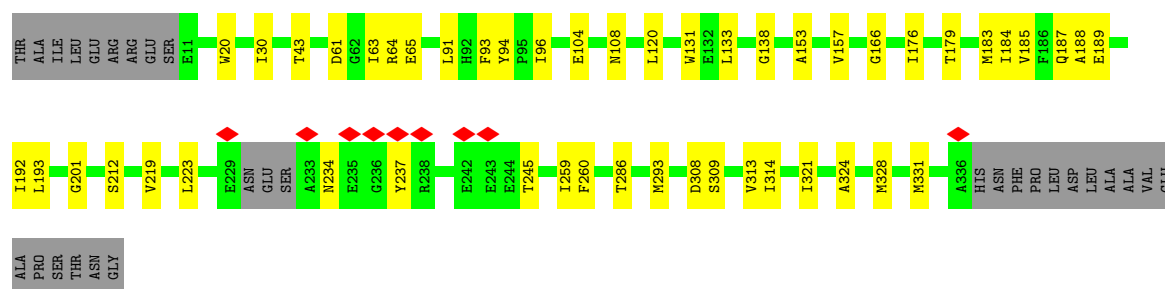
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain AF: 



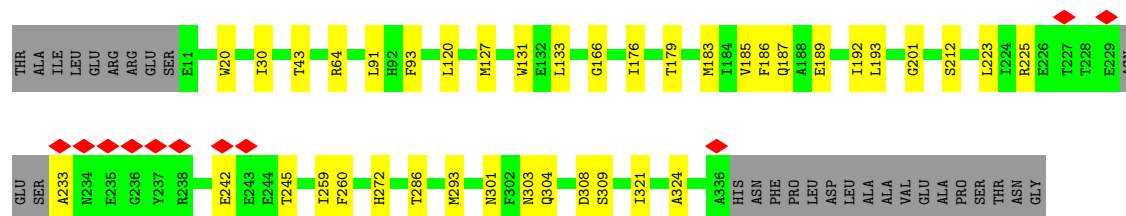
• Molecule 4: Photosystem II protein D1

Chain J: 



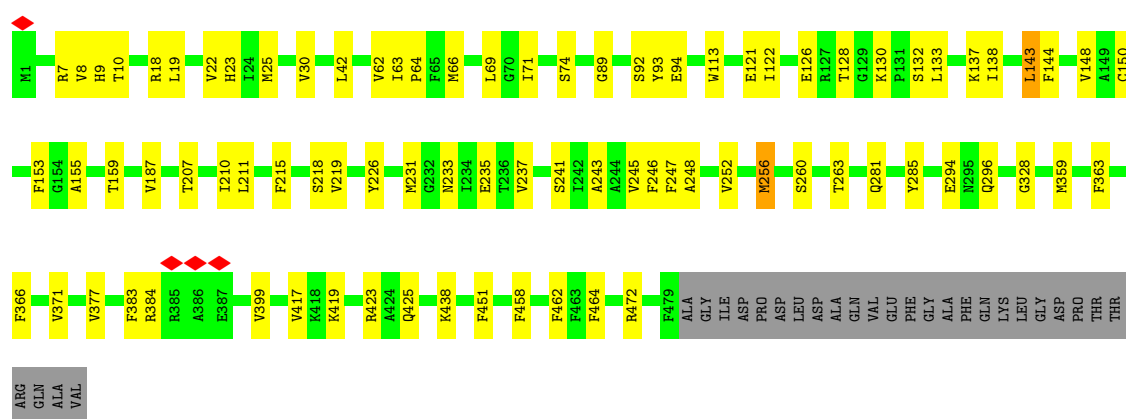
• Molecule 4: Photosystem II protein D1

Chain AJ: 

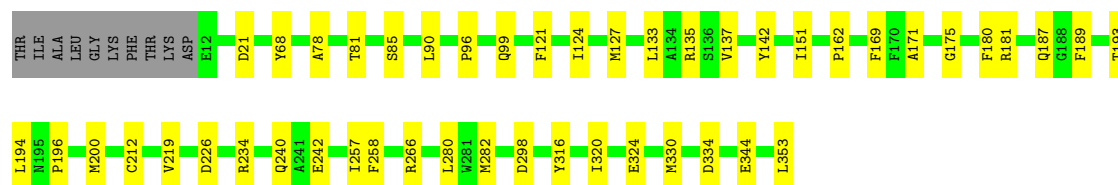


• Molecule 5: Photosystem II CP47 reaction center protein

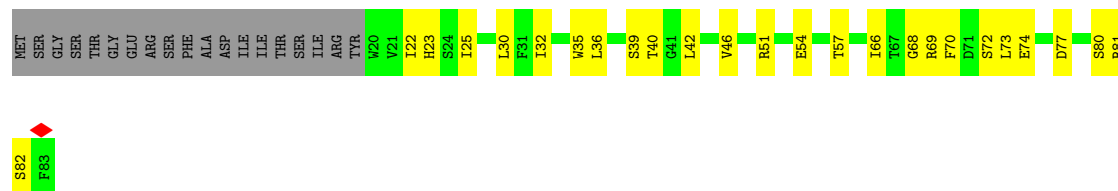
Chain O: 



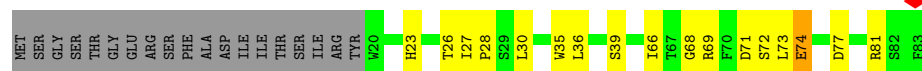
• Molecule 5: Photosystem II CP47 reaction center protein



- Molecule 8: Cytochrome b559 subunit alpha



- Molecule 8: Cytochrome b559 subunit alpha



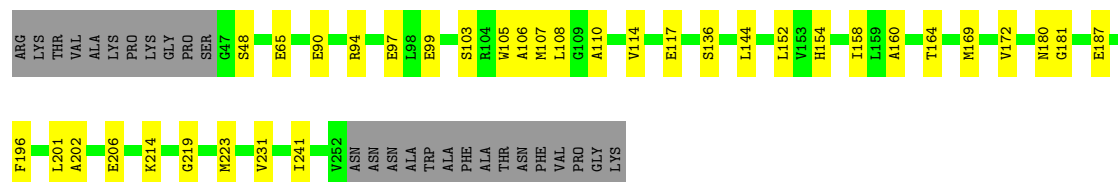
- Molecule 9: Cytochrome b559 subunit beta



- Molecule 9: Cytochrome b559 subunit beta

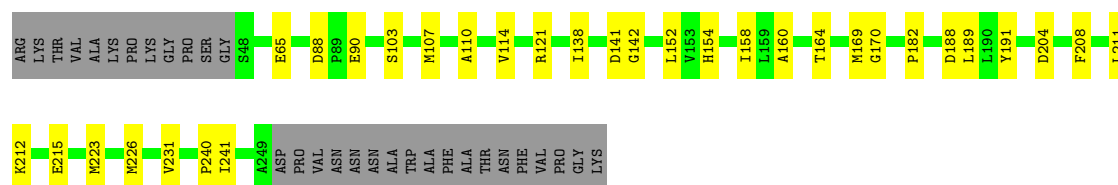


- Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic



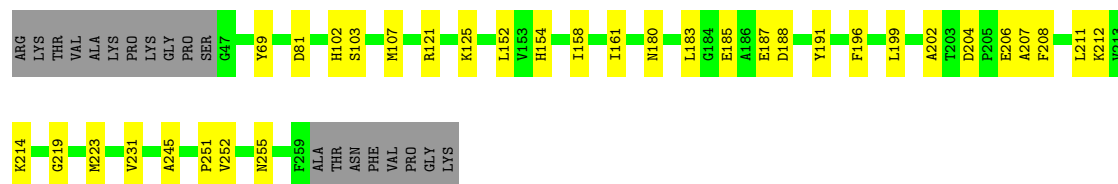
- Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

Chain p: 



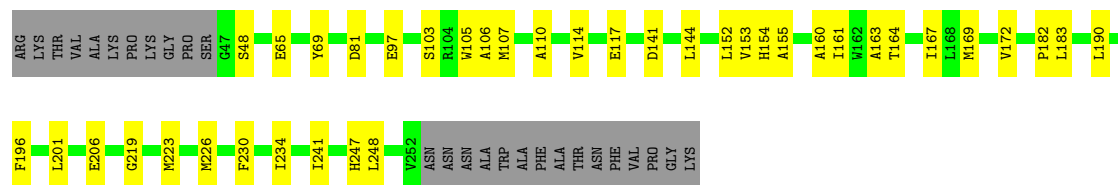
- Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

Chain AH: 



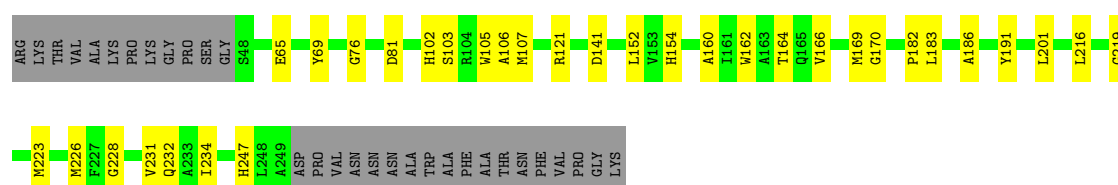
- Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

Chain AN: 



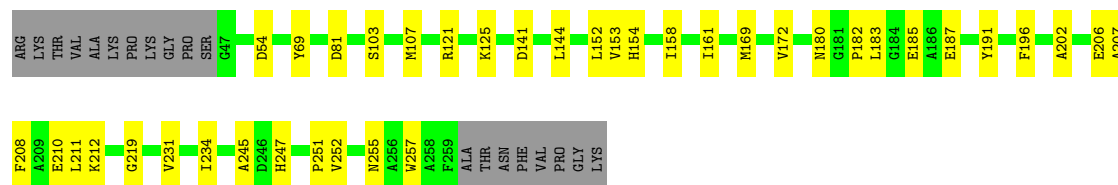
- Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

Chain AQ: 



- Molecule 10: Chlorophyll a-b binding protein 1, chloroplastic

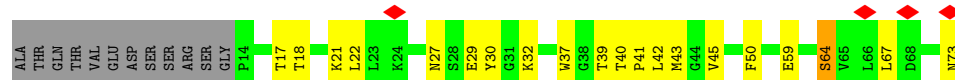
Chain AU: 



- Molecule 11: Photosystem II reaction center protein H



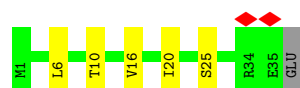
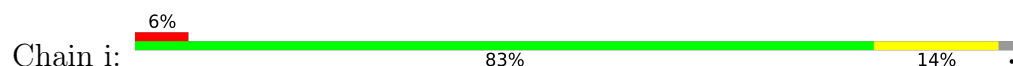
- Molecule 11: Photosystem II reaction center protein H



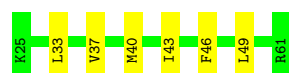
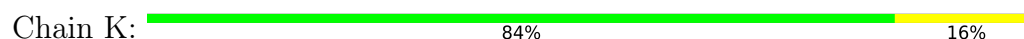
- Molecule 12: Photosystem II reaction center protein I



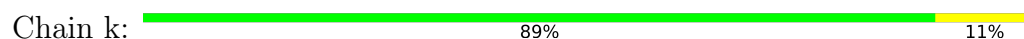
- Molecule 12: Photosystem II reaction center protein I



- Molecule 13: Photosystem II reaction center protein K



- Molecule 13: Photosystem II reaction center protein K

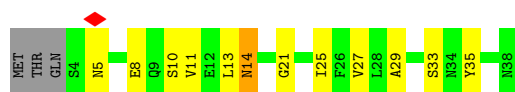


- Molecule 14: Photosystem II reaction center protein L



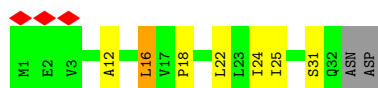
- Molecule 14: Photosystem II reaction center protein L

Chain AP:  61% 29% 8%



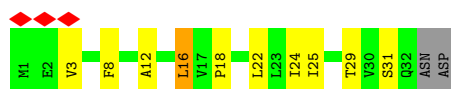
- Molecule 15: Photosystem II reaction center protein M

Chain M:  9% 74% 18% 6%



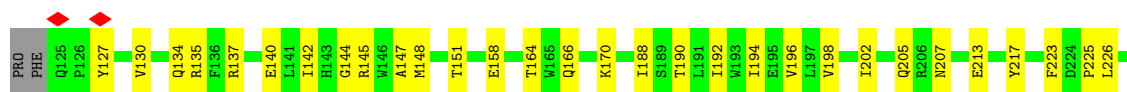
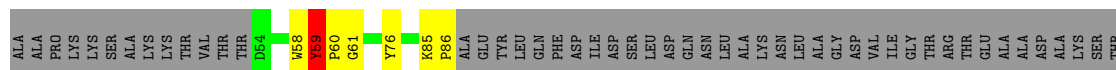
- Molecule 15: Photosystem II reaction center protein M

Chain m:  9% 65% 26% 6%



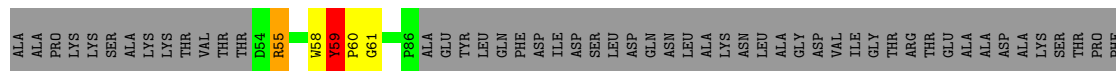
- Molecule 16: Chlorophyll a-b binding protein CP29.1, chloroplastic

Chain q:  59% 20% 21%



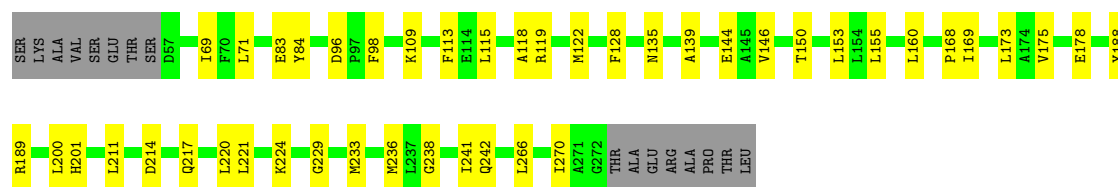
- Molecule 16: Chlorophyll a-b binding protein CP29.1, chloroplastic

Chain AR:  61% 16% 21%



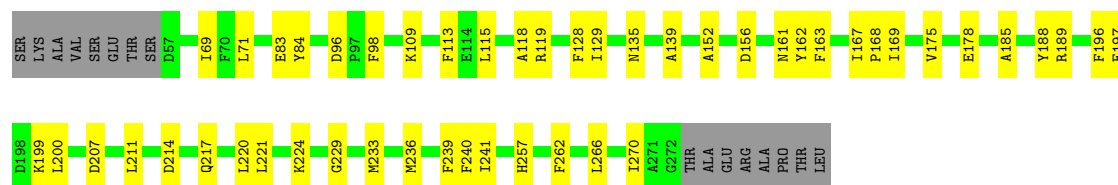
- Molecule 17: Chlorophyll a-b binding protein CP26, chloroplastic

Chain v: 



- Molecule 17: Chlorophyll a-b binding protein CP26, chloroplastic

Chain AS: 



- Molecule 18: Photosystem II reaction center protein T

Chain AG: 



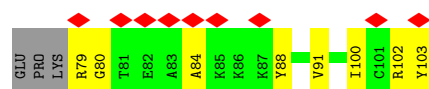
- Molecule 18: Photosystem II reaction center protein T

Chain AT: 



- Molecule 19: Photosystem II 5 kDa protein, chloroplastic

Chain U: 

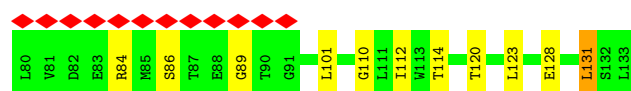
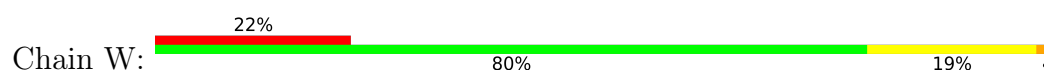


- Molecule 19: Photosystem II 5 kDa protein, chloroplastic

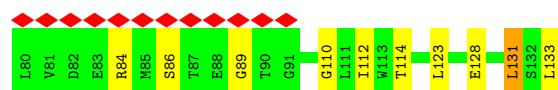
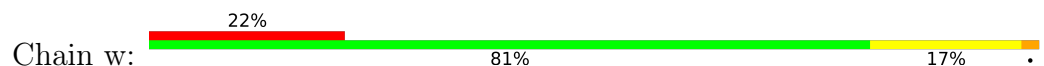
Chain u: 



- Molecule 20: Photosystem II reaction center W protein, chloroplastic



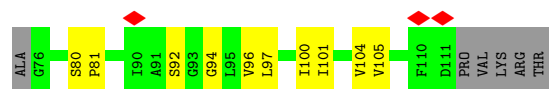
- Molecule 20: Photosystem II reaction center W protein, chloroplastic



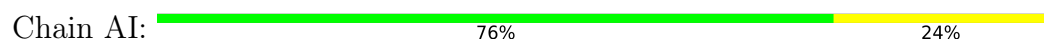
- Molecule 21: (thale cress) hypothetical protein



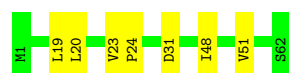
- Molecule 21: (thale cress) hypothetical protein



- Molecule 22: Photosystem II reaction center protein Z



- Molecule 22: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38544	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	57.686	Depositor
Minimum map value	-23.601	Depositor
Average map value	0.027	Depositor
Map value standard deviation	1.343	Depositor
Recommended contour level	4.62	Depositor
Map size ($\text{\AA}$)	583.2, 583.2, 583.2	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	9	0.15	0/1582	0.35	0/2150
1	AA	0.17	0/1582	0.41	0/2150
1	AC	0.15	0/1582	0.38	0/2150
1	AE	0.16	0/1582	0.39	0/2150
2	0	0.18	0/1768	0.45	0/2405
2	AD	0.19	0/1768	0.42	0/2405
3	AB	0.18	0/1564	0.46	0/2123
3	AF	0.22	0/1564	0.54	0/2123
4	AJ	0.14	0/2602	0.35	0/3546
4	J	0.15	0/2602	0.36	0/3546
5	AK	0.15	0/3886	0.36	1/5293 (0.0%)
5	O	0.16	0/3886	0.38	1/5293 (0.0%)
6	AL	0.14	0/3487	0.34	0/4750
6	P	0.13	0/3487	0.33	0/4750
7	AM	0.15	0/2816	0.39	0/3837
7	Q	0.16	0/2816	0.40	0/3837
8	E	0.19	0/538	0.48	0/731
8	e	0.21	0/538	0.56	1/731 (0.1%)
9	F	0.18	0/230	0.41	0/311
9	f	0.19	0/230	0.39	0/311
10	AH	0.17	0/1669	0.40	0/2270
10	AN	0.17	0/1607	0.40	0/2184
10	AQ	0.15	0/1580	0.35	0/2146
10	AU	0.15	0/1669	0.39	0/2270
10	V	0.16	0/1607	0.38	0/2184
10	p	0.16	0/1580	0.38	0/2146
11	AO	0.19	0/456	0.52	0/619
11	j	0.22	0/456	0.54	0/619
12	I	0.21	0/294	0.55	0/397
12	i	0.19	0/294	0.45	0/397
13	K	0.18	0/313	0.46	0/428
13	k	0.20	0/313	0.41	0/428

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	AP	0.19	0/301	0.36	0/409
14	o	0.16	0/301	0.34	0/409
15	M	0.25	0/254	0.52	0/347
15	m	0.27	0/254	0.52	0/347
16	AR	0.22	0/1585	0.51	0/2161
16	q	0.20	0/1585	0.48	0/2161
17	AS	0.16	0/1715	0.39	0/2328
17	v	0.15	0/1715	0.35	0/2328
18	AG	0.18	0/246	0.43	0/333
18	AT	0.14	0/246	0.27	0/333
19	U	0.26	0/197	0.59	0/261
19	u	0.24	0/197	0.50	0/261
20	W	0.16	0/439	0.42	0/594
20	w	0.15	0/439	0.36	0/594
21	X	0.20	0/250	0.40	0/339
21	x	0.17	0/250	0.39	0/339
22	AI	0.21	0/475	0.47	0/649
22	AV	0.18	0/475	0.42	0/649
All	All	0.17	0/62872	0.40	3/85522 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	AO	0	1
16	AR	0	2
16	q	0	2
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	74	GLU	CA-CB-CG	5.70	125.50	114.10
5	O	256	MET	CB-CG-SD	5.45	129.05	112.70
5	AK	256	MET	CB-CG-SD	5.39	128.87	112.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AO	64	SER	Peptide
16	AR	58	TRP	Peptide
16	AR	59	TYR	Peptide
16	q	58	TRP	Peptide
16	q	59	TYR	Peptide

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	9	1537	0	1480	28	0
1	AA	1537	0	1480	36	0
1	AC	1537	0	1480	37	0
1	AE	1537	0	1480	32	0
2	0	1716	0	1658	49	0
2	AD	1716	0	1658	33	0
3	AB	1512	0	1444	49	0
3	AF	1512	0	1444	48	0
4	AJ	2525	0	2443	35	0
4	J	2525	0	2443	39	0
5	AK	3757	0	3641	76	0
5	O	3757	0	3641	81	0
6	AL	3373	0	3302	30	0
6	P	3373	0	3302	37	0
7	AM	2723	0	2615	42	0
7	Q	2723	0	2615	55	0
8	E	521	0	497	23	0
8	e	521	0	497	12	0
9	F	225	0	233	15	0
9	f	225	0	233	14	0
10	AH	1621	0	1550	31	0
10	AN	1562	0	1503	33	0
10	AQ	1536	0	1480	36	0
10	AU	1621	0	1550	34	0
10	V	1562	0	1503	29	0
10	p	1536	0	1480	33	0
11	AO	447	0	471	21	0
11	j	447	0	471	25	0
12	I	286	0	295	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	i	286	0	295	3	0
13	K	302	0	313	4	0
13	k	302	0	313	3	0
14	AP	293	0	283	11	0
14	o	293	0	283	12	0
15	M	250	0	279	10	0
15	m	250	0	279	11	0
16	AR	1539	0	1502	45	0
16	q	1539	0	1502	48	0
17	AS	1670	0	1649	42	0
17	v	1670	0	1649	43	0
18	AG	239	0	255	4	0
18	AT	239	0	255	3	0
19	U	195	0	206	14	0
19	u	195	0	206	14	0
20	W	428	0	405	9	0
20	w	428	0	405	8	0
21	X	248	0	266	14	0
21	x	248	0	266	7	0
22	AI	465	0	495	12	0
22	AV	465	0	495	5	0
23	0	289	0	216	33	0
23	9	302	0	234	30	0
23	AA	304	0	233	27	0
23	AB	217	0	138	15	0
23	AC	242	0	175	20	0
23	AD	331	0	281	42	0
23	AE	306	0	238	35	0
23	AF	203	0	118	14	0
23	AH	296	0	280	47	0
23	AN	353	0	332	59	0
23	AQ	362	0	350	51	0
23	AR	215	0	180	16	0
23	AS	180	0	126	17	0
23	AU	296	0	280	47	0
23	V	349	0	328	55	0
23	p	360	0	347	52	0
23	q	211	0	169	17	0
23	v	163	0	97	14	0
24	0	424	0	369	15	0
24	9	399	0	333	23	0
24	AA	387	0	308	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	AB	265	0	192	11	0
24	AC	388	0	315	30	0
24	AD	424	0	370	20	0
24	AE	370	0	281	13	0
24	AF	259	0	186	18	0
24	AH	471	0	465	30	0
24	AJ	238	0	239	13	0
24	AK	1038	0	1149	79	0
24	AL	841	0	930	33	0
24	AM	130	0	144	5	0
24	AN	441	0	427	23	0
24	AQ	465	0	460	27	0
24	AR	518	0	451	29	0
24	AS	459	0	384	19	0
24	AU	473	0	468	29	0
24	J	188	0	200	12	0
24	K	65	0	72	2	0
24	O	1038	0	1149	77	0
24	P	776	0	858	29	0
24	Q	180	0	183	9	0
24	V	375	0	353	24	0
24	p	427	0	396	22	0
24	q	524	0	458	34	0
24	v	459	0	384	21	0
25	0	84	0	112	4	0
25	9	84	0	112	13	0
25	AA	84	0	112	8	0
25	AC	84	0	112	14	0
25	AD	84	0	112	6	0
25	AE	84	0	112	16	0
25	AF	42	0	56	7	0
25	AH	84	0	112	11	0
25	AN	84	0	112	16	0
25	AQ	84	0	112	6	0
25	AR	42	0	56	12	0
25	AS	84	0	112	8	0
25	AU	84	0	112	12	0
25	V	84	0	112	13	0
25	p	84	0	112	7	0
25	q	42	0	56	10	0
25	v	84	0	112	10	0
26	9	44	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	AA	44	0	56	1	0
26	AC	44	0	56	4	0
26	AE	44	0	56	1	0
26	AQ	44	0	56	2	0
26	AR	44	0	56	6	0
26	AS	44	0	56	1	0
26	AU	44	0	56	1	0
26	p	44	0	56	2	0
26	q	44	0	56	3	0
26	v	44	0	56	1	0
27	9	44	0	56	2	0
27	AB	44	0	56	7	0
27	AF	44	0	56	7	0
27	AR	44	0	56	0	0
27	q	44	0	56	1	0
28	0	47	0	67	3	0
28	AD	47	0	67	0	0
28	AH	49	0	74	0	0
28	AK	95	0	139	3	0
28	AL	49	0	74	2	0
28	AM	49	0	74	2	0
28	AN	49	0	74	2	0
28	AQ	49	0	74	1	0
28	AS	49	0	74	1	0
28	AU	49	0	74	0	0
28	O	144	0	213	7	0
28	P	49	0	74	2	0
28	Q	49	0	74	2	0
28	V	49	0	74	2	0
28	W	49	0	74	2	0
28	p	40	0	67	1	0
28	q	42	0	57	2	0
28	v	49	0	74	1	0
28	w	49	0	74	2	0
29	AB	40	0	56	4	0
29	AF	40	0	56	2	0
29	AI	40	0	56	2	0
29	AJ	40	0	56	4	0
29	AK	160	0	224	11	0
29	AL	80	0	112	5	0
29	AO	40	0	56	3	0
29	AV	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	F	40	0	56	2	0
29	J	40	0	56	4	0
29	O	160	0	224	15	0
29	P	120	0	168	10	0
29	f	40	0	56	3	0
29	j	40	0	56	5	0
29	k	40	0	56	4	0
30	AJ	10	0	0	0	0
30	J	10	0	0	0	0
31	AJ	1	0	0	0	0
31	J	1	0	0	0	0
32	AJ	128	0	148	8	0
32	J	128	0	148	7	0
33	AK	91	0	122	2	0
33	AL	99	0	138	2	0
33	AM	46	0	62	0	0
33	J	48	0	66	0	0
33	O	91	0	122	2	0
33	P	51	0	72	2	0
33	Q	46	0	62	0	0
34	AJ	54	0	78	6	0
34	AM	50	0	67	2	0
34	AP	42	0	48	5	0
34	J	54	0	78	7	0
34	M	54	0	78	3	0
34	Q	50	0	67	2	0
34	m	54	0	78	3	0
34	o	42	0	48	5	0
35	AJ	119	0	154	3	0
35	AL	117	0	150	2	0
35	AO	62	0	82	3	0
35	J	119	0	154	3	0
35	P	55	0	68	1	0
35	j	62	0	82	2	0
36	AM	4	0	1	0	0
36	J	4	0	1	0	0
37	AM	52	0	73	0	0
37	Q	52	0	73	0	0
38	F	43	0	30	4	0
38	f	43	0	30	3	0
All	All	83915	0	83064	2237	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 13.

The worst 5 of 2237 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:607:CHL:H121	23:V:607:CHL:C9	1.34	1.49
23:AU:608:CHL:H121	23:AU:608:CHL:C9	1.38	1.46
23:AH:601:CHL:H52	23:AH:601:CHL:C9	1.36	1.46
23:AH:608:CHL:H121	23:AH:608:CHL:C9	1.37	1.43
23:AN:607:CHL:C9	23:AN:607:CHL:H121	1.37	1.40

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	9	200/266 (75%)	198 (99%)	2 (1%)	0	100	100
1	AA	200/266 (75%)	196 (98%)	3 (2%)	1 (0%)	24	53
1	AC	200/266 (75%)	198 (99%)	1 (0%)	1 (0%)	24	53
1	AE	200/266 (75%)	197 (98%)	3 (2%)	0	100	100
2	0	220/243 (90%)	216 (98%)	4 (2%)	0	100	100
2	AD	220/243 (90%)	218 (99%)	2 (1%)	0	100	100
3	AB	190/212 (90%)	187 (98%)	3 (2%)	0	100	100
3	AF	190/212 (90%)	186 (98%)	4 (2%)	0	100	100
4	AJ	319/352 (91%)	311 (98%)	8 (2%)	0	100	100
4	J	319/352 (91%)	314 (98%)	5 (2%)	0	100	100
5	AK	477/508 (94%)	474 (99%)	3 (1%)	0	100	100
5	O	477/508 (94%)	471 (99%)	6 (1%)	0	100	100
6	AL	429/459 (94%)	427 (100%)	2 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	P	429/459 (94%)	425 (99%)	4 (1%)	0	100	100
7	AM	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
7	Q	340/352 (97%)	328 (96%)	12 (4%)	0	100	100
8	E	62/83 (75%)	61 (98%)	1 (2%)	0	100	100
8	e	62/83 (75%)	60 (97%)	2 (3%)	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	AH	211/232 (91%)	208 (99%)	3 (1%)	0	100	100
10	AN	204/232 (88%)	201 (98%)	2 (1%)	1 (0%)	24	53
10	AQ	200/232 (86%)	199 (100%)	1 (0%)	0	100	100
10	AU	211/232 (91%)	206 (98%)	5 (2%)	0	100	100
10	V	204/232 (88%)	202 (99%)	1 (0%)	1 (0%)	24	53
10	p	200/232 (86%)	196 (98%)	4 (2%)	0	100	100
11	AO	58/72 (81%)	57 (98%)	1 (2%)	0	100	100
11	j	58/72 (81%)	56 (97%)	2 (3%)	0	100	100
12	I	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	i	33/36 (92%)	33 (100%)	0	0	100	100
13	K	35/37 (95%)	35 (100%)	0	0	100	100
13	k	35/37 (95%)	35 (100%)	0	0	100	100
14	AP	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
14	o	33/38 (87%)	33 (100%)	0	0	100	100
15	M	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
15	m	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
16	AR	193/250 (77%)	187 (97%)	4 (2%)	2 (1%)	12	39
16	q	193/250 (77%)	191 (99%)	0	2 (1%)	12	39
17	AS	214/232 (92%)	204 (95%)	10 (5%)	0	100	100
17	v	214/232 (92%)	213 (100%)	1 (0%)	0	100	100
18	AG	27/33 (82%)	27 (100%)	0	0	100	100
18	AT	27/33 (82%)	27 (100%)	0	0	100	100
19	U	23/28 (82%)	22 (96%)	1 (4%)	0	100	100
19	u	23/28 (82%)	20 (87%)	3 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	W	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
20	w	52/54 (96%)	52 (100%)	0	0	100	100
21	X	34/42 (81%)	34 (100%)	0	0	100	100
21	x	34/42 (81%)	34 (100%)	0	0	100	100
22	AI	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
22	AV	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
All	All	7742/8788 (88%)	7614 (98%)	120 (2%)	8 (0%)	49	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	q	59	TYR
16	AR	59	TYR
16	AR	60	PRO
10	V	48	SER
16	q	60	PRO

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	9	154/201 (77%)	154 (100%)	0	100	100
1	AA	154/201 (77%)	154 (100%)	0	100	100
1	AC	154/201 (77%)	151 (98%)	3 (2%)	50	66
1	AE	154/201 (77%)	151 (98%)	3 (2%)	50	66
2	0	174/192 (91%)	173 (99%)	1 (1%)	78	80
2	AD	174/192 (91%)	173 (99%)	1 (1%)	78	80
3	AB	148/159 (93%)	146 (99%)	2 (1%)	59	70
3	AF	148/159 (93%)	148 (100%)	0	100	100
4	AJ	260/284 (92%)	259 (100%)	1 (0%)	84	82
4	J	260/284 (92%)	260 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AK	379/402 (94%)	378 (100%)	1 (0%)	86	84
5	O	379/402 (94%)	378 (100%)	1 (0%)	86	84
6	AL	340/359 (95%)	339 (100%)	1 (0%)	86	84
6	P	340/359 (95%)	339 (100%)	1 (0%)	86	84
7	AM	274/282 (97%)	274 (100%)	0	100	100
7	Q	274/282 (97%)	273 (100%)	1 (0%)	84	82
8	E	57/73 (78%)	57 (100%)	0	100	100
8	e	57/73 (78%)	57 (100%)	0	100	100
9	F	24/34 (71%)	24 (100%)	0	100	100
9	f	24/34 (71%)	23 (96%)	1 (4%)	26	52
10	AH	162/177 (92%)	162 (100%)	0	100	100
10	AN	157/177 (89%)	157 (100%)	0	100	100
10	AQ	154/177 (87%)	154 (100%)	0	100	100
10	AU	162/177 (92%)	162 (100%)	0	100	100
10	V	157/177 (89%)	156 (99%)	1 (1%)	78	80
10	p	154/177 (87%)	154 (100%)	0	100	100
11	AO	50/60 (83%)	50 (100%)	0	100	100
11	j	50/60 (83%)	50 (100%)	0	100	100
12	I	32/33 (97%)	32 (100%)	0	100	100
12	i	32/33 (97%)	32 (100%)	0	100	100
13	K	32/32 (100%)	31 (97%)	1 (3%)	35	59
13	k	32/32 (100%)	32 (100%)	0	100	100
14	AP	33/36 (92%)	32 (97%)	1 (3%)	36	60
14	o	33/36 (92%)	32 (97%)	1 (3%)	36	60
15	M	28/30 (93%)	27 (96%)	1 (4%)	31	56
15	m	28/30 (93%)	27 (96%)	1 (4%)	31	56
16	AR	159/201 (79%)	157 (99%)	2 (1%)	61	71
16	q	159/201 (79%)	159 (100%)	0	100	100
17	AS	167/180 (93%)	166 (99%)	1 (1%)	78	80
17	v	167/180 (93%)	166 (99%)	1 (1%)	78	80
18	AG	26/30 (87%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AT	26/30 (87%)	26 (100%)	0	100	100
19	U	20/23 (87%)	20 (100%)	0	100	100
19	u	20/23 (87%)	20 (100%)	0	100	100
20	W	47/47 (100%)	46 (98%)	1 (2%)	47	64
20	w	47/47 (100%)	45 (96%)	2 (4%)	26	51
21	X	29/34 (85%)	29 (100%)	0	100	100
21	x	29/34 (85%)	29 (100%)	0	100	100
22	AI	54/54 (100%)	54 (100%)	0	100	100
22	AV	54/54 (100%)	54 (100%)	0	100	100
All	All	6228/6956 (90%)	6198 (100%)	30 (0%)	78	80

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	K	33	LEU
17	AS	156	ASP
17	v	155	LEU
20	w	133	LEU
15	m	16	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
14	o	9	GLN
4	AJ	181	ASN
10	AU	137	GLN
10	AQ	137	GLN
14	o	38	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 444 ligands modelled in this entry, 2 are monoatomic - leaving 442 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	$\# Z > 2$
24	CLA	v	312	-	53,57,73	1.45	9 (16%)	62,93,113	1.38	6 (9%)
24	CLA	AQ	602	-	69,73,73	1.25	8 (11%)	83,113,113	1.33	5 (6%)
30	OEX	J	401	4	0,14,14	-	-	-	-	-
35	DGD	AL	517	-	56,56,67	0.92	2 (3%)	70,70,81	1.44	8 (11%)
24	CLA	O	601	-	69,73,73	1.27	7 (10%)	83,113,113	1.49	11 (13%)
24	CLA	AQ	614	-	43,48,73	1.58	6 (13%)	52,82,113	1.61	8 (15%)
23	CHL	9	601	1	44,49,74	2.41	16 (36%)	52,83,114	3.33	23 (44%)
23	CHL	AC	607	-	49,52,74	2.32	17 (34%)	56,87,114	3.44	21 (37%)
26	NEX	AR	615	-	38,46,46	1.68	6 (15%)	50,70,70	1.70	10 (20%)
29	BCR	AK	602	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	8 (14%)
23	CHL	p	606	-	54,58,74	2.13	16 (29%)	59,94,114	3.02	24 (40%)
24	CLA	O	603	-	69,73,73	1.27	7 (10%)	83,113,113	1.30	4 (4%)
24	CLA	AC	604	-	54,58,73	1.42	9 (16%)	65,95,113	1.50	6 (9%)
25	LUT	0	614	-	42,43,43	1.69	8 (19%)	51,60,60	1.55	11 (21%)
25	LUT	AC	614	-	42,43,43	1.68	8 (19%)	51,60,60	1.59	10 (19%)
27	XAT	AR	616	-	39,47,47	6.17	21 (53%)	54,74,74	7.62	35 (64%)
23	CHL	AF	606	-	37,42,74	3.37	19 (51%)	37,70,114	3.52	18 (48%)
23	CHL	AD	302	2	68,72,74	1.92	16 (23%)	77,111,114	2.78	26 (33%)
24	CLA	AL	503	-	69,73,73	1.26	7 (10%)	83,113,113	1.36	6 (7%)
23	CHL	AN	617	10	50,54,74	2.25	19 (38%)	56,90,114	2.84	22 (39%)
23	CHL	AC	608	-	66,70,74	1.94	16 (24%)	75,109,114	2.87	29 (38%)
24	CLA	AK	618	5	69,73,73	1.27	8 (11%)	83,113,113	1.23	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AJ	406	-	54,58,73	1.43	9 (16%)	65,95,113	1.58	7 (10%)
23	CHL	AR	605	16	69,72,74	2.00	18 (26%)	80,111,114	2.83	23 (28%)
24	CLA	q	608	16	49,53,73	1.53	9 (18%)	59,89,113	1.50	9 (15%)
38	HEM	F	102	9,8	50,50,50	1.43	7 (14%)	66,82,82	1.21	8 (12%)
24	CLA	AU	613	-	52,56,73	1.47	9 (17%)	62,92,113	1.46	6 (9%)
24	CLA	Q	401	-	54,58,73	1.43	9 (16%)	65,95,113	1.55	6 (9%)
26	NEX	p	616	-	38,46,46	1.65	7 (18%)	50,70,70	1.83	11 (22%)
23	CHL	0	617	2	50,54,74	2.27	17 (34%)	56,90,114	2.95	23 (41%)
23	CHL	AD	306	-	57,61,74	2.07	16 (28%)	64,98,114	2.93	24 (37%)
23	CHL	AD	317	2	50,54,74	2.26	17 (34%)	56,90,114	2.94	24 (42%)
24	CLA	AN	612	10	69,73,73	1.27	8 (11%)	83,113,113	1.38	9 (10%)
24	CLA	AE	603	-	59,63,73	1.38	9 (15%)	71,101,113	1.32	7 (9%)
24	CLA	O	611	5	69,73,73	1.26	8 (11%)	83,113,113	1.45	9 (10%)
25	LUT	9	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.56	11 (21%)
25	LUT	AN	614	-	42,43,43	1.61	8 (19%)	51,60,60	1.50	11 (21%)
25	LUT	AU	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.51	9 (17%)
23	CHL	AF	605	-	38,41,74	2.40	18 (47%)	43,71,114	3.37	22 (51%)
23	CHL	0	608	-	35,43,74	2.16	10 (28%)	36,72,114	3.84	16 (44%)
34	SQD	J	410	-	53,54,54	1.54	7 (13%)	62,65,65	1.32	6 (9%)
27	XAT	9	618	-	39,47,47	6.14	21 (53%)	54,74,74	7.87	34 (62%)
24	CLA	V	611	10	45,49,73	1.53	8 (17%)	54,84,113	1.52	6 (11%)
25	LUT	0	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.54	8 (15%)
25	LUT	AC	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.54	10 (19%)
24	CLA	AF	614	-	49,53,73	1.45	8 (16%)	59,89,113	1.75	10 (16%)
33	LMG	J	409	-	48,48,55	0.76	0	56,56,63	1.29	4 (7%)
23	CHL	0	607	-	48,52,74	2.34	18 (37%)	58,87,114	3.47	29 (50%)
26	NEX	9	617	-	38,46,46	1.67	7 (18%)	50,70,70	1.63	9 (18%)
23	CHL	AE	601	1	50,54,74	2.21	17 (34%)	56,90,114	3.19	23 (41%)
23	CHL	p	605	10	52,56,74	2.17	17 (32%)	58,92,114	3.06	20 (34%)
24	CLA	9	611	-	47,51,73	1.53	8 (17%)	54,86,113	1.41	5 (9%)
23	CHL	p	601	10	70,74,74	1.90	16 (22%)	80,114,114	2.69	27 (33%)
24	CLA	O	606	-	67,71,73	1.27	7 (10%)	78,110,113	1.36	8 (10%)
24	CLA	AD	310	28	59,63,73	1.35	8 (13%)	71,101,113	1.42	6 (8%)
24	CLA	O	609	-	69,73,73	1.26	8 (11%)	83,113,113	1.33	5 (6%)
25	LUT	AS	316	-	42,43,43	1.64	8 (19%)	51,60,60	1.82	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AM	403	7	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
24	CLA	AD	303	-	64,68,73	1.31	8 (12%)	77,107,113	1.37	6 (7%)
23	CHL	AQ	608	-	70,74,74	1.86	17 (24%)	80,114,114	2.74	27 (33%)
28	LHG	O	621	-	48,48,48	0.66	1 (2%)	51,54,54	1.22	6 (11%)
29	BCR	AO	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	8 (14%)
29	BCR	AV	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	6 (10%)
24	CLA	AS	303	17	65,69,73	1.31	8 (12%)	78,108,113	1.36	7 (8%)
24	CLA	AH	603	-	69,73,73	1.29	8 (11%)	83,113,113	1.28	7 (8%)
24	CLA	AJ	409	4	62,66,73	1.31	6 (9%)	72,104,113	1.34	6 (8%)
32	PHO	J	405	-	58,69,69	2.07	10 (17%)	56,99,99	1.51	7 (12%)
23	CHL	AH	608	-	70,74,74	1.86	17 (24%)	80,114,114	2.79	27 (33%)
28	LHG	AK	623	-	45,45,48	0.64	1 (2%)	48,51,54	1.22	4 (8%)
23	CHL	V	606	-	70,74,74	1.90	17 (24%)	80,114,114	2.71	28 (35%)
24	CLA	AA	609	-	52,56,73	1.43	7 (13%)	60,92,113	1.41	4 (6%)
24	CLA	K	101	6	69,73,73	1.27	8 (11%)	83,113,113	1.44	7 (8%)
23	CHL	AQ	607	-	70,74,74	1.89	17 (24%)	80,114,114	2.75	25 (31%)
24	CLA	AE	602	1	46,50,73	1.52	8 (17%)	55,85,113	1.50	5 (9%)
24	CLA	AN	611	-	64,68,73	1.33	9 (14%)	77,107,113	1.25	6 (7%)
33	LMG	P	518	-	51,51,55	0.73	0	59,59,63	1.34	5 (8%)
24	CLA	AK	617	-	69,73,73	1.28	8 (11%)	83,113,113	1.27	7 (8%)
24	CLA	p	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.45	5 (7%)
28	LHG	W	201	-	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
24	CLA	0	610	28	59,63,73	1.36	6 (10%)	71,101,113	1.45	5 (7%)
28	LHG	p	617	-	39,39,48	0.50	1 (2%)	41,41,54	1.29	6 (14%)
24	CLA	Q	404	-	69,73,73	1.27	7 (10%)	83,113,113	1.29	5 (6%)
29	BCR	AI	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
24	CLA	AR	611	16	53,57,73	1.44	8 (15%)	62,93,113	1.36	6 (9%)
36	BCT	AM	402	-	2,3,3	1.24	0	2,3,3	4.20	1 (50%)
25	LUT	AR	614	-	42,43,43	1.62	8 (19%)	51,60,60	1.52	11 (21%)
33	LMG	Q	407	-	46,46,55	0.76	1 (2%)	54,54,63	1.32	5 (9%)
24	CLA	V	604	-	40,41,73	2.09	11 (27%)	42,70,113	1.70	5 (11%)
25	LUT	V	614	-	42,43,43	1.64	8 (19%)	51,60,60	1.53	10 (19%)
24	CLA	V	610	-	64,68,73	1.33	8 (12%)	77,107,113	1.25	6 (7%)
24	CLA	AU	611	-	64,68,73	1.32	10 (15%)	77,107,113	1.29	6 (7%)
23	CHL	AU	605	10	52,56,74	2.15	17 (32%)	58,92,114	3.06	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	9	603	-	59,63,73	1.38	9 (15%)	71,101,113	1.30	7 (9%)
35	DGD	AJ	412	-	61,61,67	0.90	2 (3%)	75,75,81	1.41	8 (10%)
24	CLA	AK	608	-	67,71,73	1.30	8 (11%)	78,110,113	1.25	6 (7%)
24	CLA	AK	604	5	69,73,73	1.24	7 (10%)	83,113,113	1.42	12 (14%)
29	BCR	O	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
25	LUT	AF	611	-	42,43,43	1.56	9 (21%)	51,60,60	1.51	8 (15%)
24	CLA	AA	603	-	59,63,73	1.38	9 (15%)	71,101,113	1.33	7 (9%)
24	CLA	q	609	16	67,71,73	1.28	8 (11%)	78,110,113	1.24	3 (3%)
24	CLA	0	604	-	49,53,73	1.49	7 (14%)	59,89,113	1.80	6 (10%)
23	CHL	p	609	10	68,72,74	1.81	15 (22%)	75,111,114	2.65	24 (32%)
24	CLA	AA	613	-	49,53,73	1.50	6 (12%)	59,89,113	1.48	6 (10%)
24	CLA	P	506	6	69,73,73	1.27	9 (13%)	83,113,113	1.29	7 (8%)
24	CLA	AL	509	6	69,73,73	1.26	8 (11%)	83,113,113	1.32	7 (8%)
23	CHL	q	605	16	67,71,74	1.93	18 (26%)	76,110,114	2.67	23 (30%)
23	CHL	AN	607	-	70,74,74	1.88	17 (24%)	80,114,114	2.80	29 (36%)
24	CLA	AN	604	-	42,45,73	1.56	8 (19%)	50,78,113	1.47	4 (8%)
24	CLA	O	613	-	69,73,73	1.27	9 (13%)	83,113,113	1.29	8 (9%)
23	CHL	AQ	605	10	52,56,74	2.16	17 (32%)	58,92,114	3.06	20 (34%)
24	CLA	AM	404	-	69,73,73	1.27	7 (10%)	83,113,113	1.28	8 (9%)
24	CLA	AN	603	10	69,73,73	1.27	8 (11%)	83,113,113	1.33	8 (9%)
29	BCR	O	617	-	41,41,41	1.13	2 (4%)	56,56,56	1.26	7 (12%)
23	CHL	AF	607	-	50,54,74	2.31	17 (34%)	56,90,114	2.96	21 (37%)
32	PHO	J	406	-	58,69,69	2.07	10 (17%)	56,99,99	1.63	7 (12%)
23	CHL	9	607	-	67,71,74	1.90	17 (25%)	76,110,114	2.85	26 (34%)
25	LUT	9	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.61	10 (19%)
24	CLA	AR	612	16	64,68,73	1.29	10 (15%)	77,107,113	1.61	9 (11%)
23	CHL	p	608	-	70,74,74	1.86	18 (25%)	80,114,114	2.74	28 (35%)
29	BCR	k	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	7 (12%)
29	BCR	P	515	-	41,41,41	1.15	2 (4%)	56,56,56	1.28	7 (12%)
33	LMG	AK	601	-	40,40,55	0.81	0	48,48,63	1.34	7 (14%)
23	CHL	V	601	10	70,74,74	1.88	16 (22%)	80,114,114	2.76	25 (31%)
23	CHL	AU	606	-	54,58,74	2.16	16 (29%)	59,94,114	3.13	21 (35%)
26	NEX	q	615	-	38,46,46	1.67	7 (18%)	50,70,70	1.69	10 (20%)
29	BCR	AJ	410	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
25	LUT	v	316	-	42,43,43	1.66	8 (19%)	51,60,60	1.54	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	9	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.50	6 (9%)
23	CHL	AS	306	-	39,41,74	2.69	20 (51%)	39,69,114	3.94	19 (48%)
23	CHL	AB	605	-	45,48,74	2.39	19 (42%)	54,81,114	3.06	21 (38%)
24	CLA	O	608	5	69,73,73	1.34	7 (10%)	83,113,113	1.54	6 (7%)
23	CHL	AR	606	-	60,64,74	2.09	18 (30%)	68,102,114	2.81	22 (32%)
23	CHL	AD	307	-	50,54,74	2.16	16 (32%)	56,90,114	3.23	25 (44%)
23	CHL	AU	601	10	70,74,74	1.93	16 (22%)	80,114,114	2.72	29 (36%)
24	CLA	AR	609	16	67,71,73	1.26	9 (13%)	78,110,113	1.30	3 (3%)
29	BCR	AK	621	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	5 (8%)
24	CLA	AB	602	-	49,53,73	1.49	5 (10%)	59,89,113	1.76	8 (13%)
25	LUT	AE	613	-	42,43,43	1.59	8 (19%)	51,60,60	1.48	9 (17%)
24	CLA	J	403	-	69,73,73	1.24	6 (8%)	83,113,113	1.46	9 (10%)
28	LHG	P	517	-	48,48,48	0.57	0	51,54,54	1.24	6 (11%)
25	LUT	AN	615	-	42,43,43	1.63	8 (19%)	51,60,60	1.51	9 (17%)
24	CLA	AH	609	-	64,68,73	1.31	8 (12%)	77,107,113	1.33	9 (11%)
24	CLA	0	602	-	64,68,73	1.30	8 (12%)	77,107,113	1.35	6 (7%)
24	CLA	AE	611	1	49,53,73	1.51	8 (16%)	59,89,113	1.54	7 (11%)
24	CLA	P	507	-	69,73,73	1.25	8 (11%)	83,113,113	1.25	5 (6%)
24	CLA	AL	508	-	69,73,73	1.25	8 (11%)	83,113,113	1.25	6 (7%)
24	CLA	AS	311	-	60,64,73	1.37	8 (13%)	72,102,113	1.34	8 (11%)
29	BCR	AL	515	-	41,41,41	1.14	2 (4%)	56,56,56	1.16	4 (7%)
35	DGD	AJ	401	-	60,60,67	0.92	2 (3%)	74,74,81	1.34	6 (8%)
37	PL9	AM	405	-	52,52,55	1.08	4 (7%)	64,65,69	1.55	14 (21%)
23	CHL	AB	601	-	48,53,74	2.25	16 (33%)	53,89,114	3.10	20 (37%)
23	CHL	AB	607	-	50,54,74	2.32	19 (38%)	56,90,114	2.92	22 (39%)
24	CLA	AR	610	-	53,57,73	1.43	8 (15%)	62,93,113	1.40	5 (8%)
24	CLA	P	510	6	69,73,73	1.27	8 (11%)	83,113,113	1.26	5 (6%)
24	CLA	AK	607	-	69,73,73	1.28	8 (11%)	83,113,113	1.35	6 (7%)
23	CHL	AE	617	-	50,54,74	2.20	18 (36%)	56,90,114	3.02	21 (37%)
24	CLA	AS	312	-	53,57,73	1.45	10 (18%)	62,93,113	1.38	5 (8%)
24	CLA	O	610	-	69,73,73	1.28	8 (11%)	83,113,113	1.30	7 (8%)
34	SQD	AM	401	-	49,50,54	1.59	7 (14%)	58,61,65	1.39	6 (10%)
23	CHL	v	306	-	40,43,74	2.34	15 (37%)	44,74,114	3.67	22 (50%)
24	CLA	0	609	2	62,66,73	1.31	8 (12%)	72,104,113	1.30	4 (5%)
24	CLA	AC	602	1	65,69,73	1.32	9 (13%)	78,108,113	1.59	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	XAT	AB	613	-	39,47,47	6.23	22 (56%)	54,74,74	7.62	35 (64%)
24	CLA	P	505	-	69,73,73	1.25	8 (11%)	83,113,113	1.36	6 (7%)
24	CLA	AK	603	-	69,73,73	1.27	7 (10%)	83,113,113	1.47	11 (13%)
24	CLA	AL	510	6	69,73,73	1.27	9 (13%)	83,113,113	1.24	4 (4%)
28	LHG	AM	406	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
29	BCR	O	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	5 (8%)
24	CLA	AF	603	-	49,53,73	1.54	8 (16%)	59,89,113	1.37	7 (11%)
24	CLA	AL	502	-	69,73,73	1.27	8 (11%)	83,113,113	1.33	7 (8%)
23	CHL	AA	617	1	50,54,74	2.29	20 (40%)	56,90,114	2.90	23 (41%)
23	CHL	AF	608	3	48,52,74	2.35	16 (33%)	51,87,114	3.08	19 (37%)
24	CLA	P	508	6	69,73,73	1.26	8 (11%)	83,113,113	1.32	7 (8%)
24	CLA	AH	602	10	69,73,73	1.25	8 (11%)	83,113,113	1.39	6 (7%)
24	CLA	9	610	1	58,62,73	1.39	7 (12%)	67,99,113	1.36	5 (7%)
24	CLA	AQ	613	10	64,68,73	1.31	8 (12%)	77,107,113	1.36	6 (7%)
24	CLA	AK	614	-	69,73,73	1.25	10 (14%)	83,113,113	1.36	9 (10%)
23	CHL	AE	606	-	50,54,74	2.19	16 (32%)	56,90,114	3.15	21 (37%)
24	CLA	AS	309	-	47,51,73	1.52	7 (14%)	54,86,113	1.44	3 (5%)
24	CLA	AL	507	6	69,73,73	1.27	8 (11%)	83,113,113	1.29	7 (8%)
24	CLA	AD	304	-	59,63,73	1.37	7 (11%)	71,101,113	1.35	8 (11%)
24	CLA	O	614	-	69,73,73	1.25	8 (11%)	83,113,113	1.48	8 (9%)
24	CLA	AQ	612	-	64,68,73	1.34	8 (12%)	77,107,113	1.31	9 (11%)
24	CLA	AC	603	-	59,63,73	1.38	9 (15%)	71,101,113	1.31	7 (9%)
34	SQD	AJ	411	-	53,54,54	1.54	8 (15%)	62,65,65	1.33	6 (9%)
29	BCR	O	625	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	7 (12%)
33	LMG	AK	622	-	51,51,55	0.72	0	59,59,63	1.35	7 (11%)
35	DGD	AO	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.37	7 (9%)
24	CLA	0	613	-	52,56,73	1.45	7 (13%)	62,92,113	1.54	6 (9%)
24	CLA	AC	613	-	47,51,73	1.54	7 (14%)	54,86,113	1.54	10 (18%)
24	CLA	AK	605	-	69,73,73	1.26	7 (10%)	83,113,113	1.29	4 (4%)
25	LUT	p	614	-	42,43,43	1.65	8 (19%)	51,60,60	1.49	9 (17%)
23	CHL	AB	606	-	49,52,74	2.35	17 (34%)	56,87,114	3.35	21 (37%)
25	LUT	V	613	-	42,43,43	1.63	8 (19%)	51,60,60	1.50	11 (21%)
23	CHL	V	605	-	54,58,74	2.13	16 (29%)	59,94,114	3.08	24 (40%)
28	LHG	O	622	-	45,45,48	0.64	1 (2%)	48,51,54	1.22	4 (8%)
33	LMG	AL	501	-	48,48,55	0.76	0	56,56,63	1.29	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LUT	AS	315	-	42,43,43	1.65	8 (19%)	51,60,60	1.48	10 (19%)
28	LHG	AQ	618	24	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
24	CLA	p	603	-	69,73,73	1.28	9 (13%)	83,113,113	1.22	6 (7%)
24	CLA	AN	609	-	66,70,73	1.27	9 (13%)	76,108,113	1.25	4 (5%)
23	CHL	9	608	-	49,52,74	2.32	17 (34%)	56,87,114	3.42	21 (37%)
24	CLA	AA	602	1	65,69,73	1.31	8 (12%)	78,108,113	1.38	8 (10%)
24	CLA	AR	603	-	64,68,73	1.33	8 (12%)	77,107,113	1.30	7 (9%)
24	CLA	O	604	5	69,73,73	1.25	9 (13%)	83,113,113	1.51	7 (8%)
24	CLA	9	602	1	65,69,73	1.28	5 (7%)	78,108,113	1.46	7 (8%)
24	CLA	0	603	-	59,63,73	1.37	6 (10%)	71,101,113	1.42	7 (9%)
24	CLA	AR	602	16	62,66,73	1.34	8 (12%)	72,104,113	1.32	5 (6%)
24	CLA	AH	610	-	64,68,73	1.32	8 (12%)	77,107,113	1.38	7 (9%)
24	CLA	O	612	-	69,73,73	1.26	10 (14%)	83,113,113	1.36	8 (9%)
25	LUT	AD	314	-	42,43,43	1.73	8 (19%)	51,60,60	1.58	11 (21%)
23	CHL	AA	606	-	65,69,74	1.94	16 (24%)	74,108,114	2.75	23 (31%)
24	CLA	AU	603	-	69,73,73	1.29	9 (13%)	83,113,113	1.27	7 (8%)
24	CLA	v	311	-	60,64,73	1.36	7 (11%)	72,102,113	1.39	8 (11%)
38	HEM	f	102	9,8	50,50,50	1.52	6 (12%)	66,82,82	1.19	7 (10%)
24	CLA	AH	613	-	50,54,73	1.48	8 (16%)	57,89,113	1.46	4 (7%)
24	CLA	AB	610	-	49,53,73	1.51	7 (14%)	59,89,113	1.49	5 (8%)
23	CHL	AQ	609	-	70,74,74	1.89	16 (22%)	80,114,114	2.63	25 (31%)
33	LMG	O	620	-	51,51,55	0.72	0	59,59,63	1.35	7 (11%)
28	LHG	AU	617	-	48,48,48	0.62	2 (4%)	51,54,54	1.24	6 (11%)
24	CLA	9	614	-	40,44,73	1.62	8 (20%)	47,76,113	1.44	5 (10%)
23	CHL	AA	605	1	50,54,74	2.19	16 (32%)	56,90,114	3.10	23 (41%)
24	CLA	AB	611	-	49,53,73	1.51	6 (12%)	59,89,113	1.85	12 (20%)
24	CLA	AH	611	-	64,68,73	1.32	10 (15%)	77,107,113	1.30	6 (7%)
29	BCR	AL	516	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	7 (12%)
25	LUT	p	615	-	42,43,43	1.60	8 (19%)	51,60,60	1.47	9 (17%)
24	CLA	AJ	404	-	69,73,73	1.24	6 (8%)	83,113,113	1.45	11 (13%)
29	BCR	AK	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.26	6 (10%)
29	BCR	P	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	6 (10%)
24	CLA	AL	505	-	69,73,73	1.26	6 (8%)	83,113,113	1.39	7 (8%)
26	NEX	AA	616	-	38,46,46	1.71	7 (18%)	50,70,70	1.74	10 (20%)
24	CLA	AE	612	-	49,53,73	1.50	6 (12%)	59,89,113	1.47	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	q	603	-	64,68,73	1.32	8 (12%)	77,107,113	1.33	7 (9%)
29	BCR	P	513	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	4 (7%)
24	CLA	AA	610	-	47,51,73	1.51	8 (17%)	54,86,113	1.41	5 (9%)
23	CHL	p	607	-	70,74,74	1.90	18 (25%)	80,114,114	2.74	26 (32%)
24	CLA	q	602	16	62,66,73	1.32	8 (12%)	72,104,113	1.32	6 (8%)
29	BCR	f	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	5 (8%)
23	CHL	AD	301	-	67,71,74	1.91	16 (23%)	76,110,114	2.82	26 (34%)
24	CLA	9	612	-	49,53,73	1.48	9 (18%)	59,89,113	1.48	5 (8%)
24	CLA	AK	606	5	69,73,73	1.25	9 (13%)	83,113,113	1.54	8 (9%)
35	DGD	J	413	-	60,60,67	0.92	2 (3%)	74,74,81	1.34	6 (8%)
29	BCR	AF	612	-	41,41,41	1.16	2 (4%)	56,56,56	1.27	5 (8%)
24	CLA	P	501	-	69,73,73	1.28	8 (11%)	83,113,113	1.35	6 (7%)
24	CLA	AH	612	10	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
28	LHG	q	616	24	41,41,48	0.67	1 (2%)	44,47,54	1.29	6 (13%)
28	LHG	AS	301	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
25	LUT	v	315	-	42,43,43	1.66	8 (19%)	51,60,60	1.49	10 (19%)
34	SQD	M	101	-	53,54,54	1.55	7 (13%)	62,65,65	1.35	6 (9%)
23	CHL	AE	607	-	65,69,74	1.94	18 (27%)	74,108,114	2.95	29 (39%)
24	CLA	AS	310	-	57,61,73	1.37	8 (14%)	66,98,113	1.37	5 (7%)
28	LHG	AL	519	-	48,48,48	0.58	0	51,54,54	1.25	6 (11%)
24	CLA	AC	612	1	45,49,73	1.52	6 (13%)	54,84,113	1.54	7 (12%)
28	LHG	w	201	-	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
24	CLA	AB	609	-	43,48,73	1.55	7 (16%)	52,82,113	1.54	7 (13%)
24	CLA	O	615	-	69,73,73	1.27	7 (10%)	83,113,113	1.30	7 (8%)
23	CHL	AH	607	-	70,74,74	1.90	16 (22%)	80,114,114	2.68	26 (32%)
25	LUT	AQ	615	-	42,43,43	1.65	8 (19%)	51,60,60	1.49	9 (17%)
23	CHL	AD	308	-	63,67,74	1.91	16 (25%)	69,105,114	2.80	23 (33%)
33	LMG	AM	407	-	46,46,55	0.76	0	54,54,63	1.32	5 (9%)
23	CHL	0	606	-	57,61,74	2.14	19 (33%)	64,98,114	2.83	25 (39%)
24	CLA	v	309	-	47,51,73	1.50	6 (12%)	54,86,113	1.44	3 (5%)
23	CHL	AH	606	-	54,58,74	2.19	17 (31%)	59,94,114	3.14	25 (42%)
24	CLA	AL	504	-	69,73,73	1.27	7 (10%)	83,113,113	1.35	8 (9%)
23	CHL	AN	608	-	63,67,74	1.94	19 (30%)	69,105,114	3.00	23 (33%)
24	CLA	AD	309	-	62,66,73	1.31	9 (14%)	72,104,113	1.30	5 (6%)
24	CLA	AR	604	-	52,56,73	1.44	8 (15%)	62,92,113	1.52	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	q	613	16	46,50,74	2.37	19 (41%)	51,85,114	3.02	22 (43%)
24	CLA	AC	611	-	46,49,73	1.52	8 (17%)	55,83,113	1.40	3 (5%)
24	CLA	p	610	-	67,70,73	1.67	9 (13%)	76,106,113	1.44	6 (7%)
24	CLA	AN	602	10	69,73,73	1.26	8 (11%)	83,113,113	1.33	7 (8%)
34	SQD	m	101	-	53,54,54	1.55	7 (13%)	62,65,65	1.35	6 (9%)
36	BCT	J	412	-	2,3,3	1.24	0	2,3,3	4.13	2 (100%)
24	CLA	AS	304	17	49,53,73	1.49	8 (16%)	59,89,113	1.43	5 (8%)
29	BCR	AK	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	4 (7%)
24	CLA	AD	312	2	62,66,73	1.33	7 (11%)	74,104,113	1.37	6 (8%)
24	CLA	AU	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.49	6 (9%)
23	CHL	q	606	-	59,62,74	2.17	18 (30%)	68,99,114	3.11	25 (36%)
23	CHL	AS	307	-	62,66,74	1.97	16 (25%)	70,104,114	2.97	30 (42%)
24	CLA	AB	604	-	49,53,73	1.50	8 (16%)	59,89,113	1.44	4 (6%)
26	NEX	AQ	617	-	38,46,46	1.65	7 (18%)	50,70,70	1.63	9 (18%)
24	CLA	P	502	-	69,73,73	1.27	7 (10%)	83,113,113	1.43	6 (7%)
24	CLA	p	613	10	43,48,73	1.57	7 (16%)	52,82,113	1.63	6 (11%)
24	CLA	AL	511	6	69,73,73	1.26	9 (13%)	83,113,113	1.25	5 (6%)
28	LHG	AH	616	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
24	CLA	AK	611	-	69,73,73	1.26	7 (10%)	83,113,113	1.30	7 (8%)
24	CLA	O	607	-	69,73,73	1.26	8 (11%)	83,113,113	1.40	7 (8%)
23	CHL	AR	607	-	57,61,74	2.16	19 (33%)	64,98,114	2.86	27 (42%)
27	XAT	AF	613	-	39,47,47	6.17	20 (51%)	54,74,74	7.61	35 (64%)
24	CLA	AL	512	6	69,73,73	1.27	6 (8%)	83,113,113	1.46	7 (8%)
24	CLA	v	310	-	57,61,73	1.39	9 (15%)	66,98,113	1.38	6 (9%)
24	CLA	AL	514	6	64,69,73	1.38	5 (7%)	78,107,113	1.47	9 (11%)
23	CHL	AE	605	-	65,69,74	1.97	18 (27%)	74,108,114	2.76	25 (33%)
24	CLA	AA	612	-	49,53,73	1.50	7 (14%)	59,89,113	1.54	5 (8%)
23	CHL	V	608	-	63,67,74	1.91	16 (25%)	69,105,114	2.76	22 (31%)
33	LMG	AL	520	-	51,51,55	0.74	0	59,59,63	1.33	5 (8%)
24	CLA	AS	313	-	57,61,73	1.38	8 (14%)	66,98,113	1.45	7 (10%)
23	CHL	AC	606	-	50,54,74	2.26	16 (32%)	56,90,114	3.23	25 (44%)
25	LUT	AH	615	-	42,43,43	1.63	8 (19%)	51,60,60	1.50	9 (17%)
24	CLA	AC	609	1	58,62,73	1.40	9 (15%)	67,99,113	1.39	4 (5%)
24	CLA	q	610	28	53,57,73	1.43	7 (13%)	62,93,113	1.42	5 (8%)
24	CLA	AN	613	10	52,56,73	1.45	7 (13%)	62,92,113	1.56	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	AE	616	1	50,54,74	2.27	19 (38%)	56,90,114	2.96	24 (42%)
24	CLA	J	407	4	62,66,73	1.31	6 (9%)	72,104,113	1.34	5 (6%)
35	DGD	P	516	-	56,56,67	0.92	2 (3%)	70,70,81	1.44	9 (12%)
23	CHL	AH	605	10	52,56,74	2.15	17 (32%)	58,92,114	3.07	22 (37%)
24	CLA	O	602	5	69,73,73	1.26	8 (11%)	83,113,113	1.32	6 (7%)
24	CLA	J	404	-	69,73,73	1.26	8 (11%)	83,113,113	1.44	6 (7%)
24	CLA	AE	609	-	49,53,73	1.49	9 (18%)	59,89,113	1.51	7 (11%)
24	CLA	AK	616	-	69,73,73	1.26	8 (11%)	83,113,113	1.44	6 (7%)
24	CLA	AS	314	17	53,57,73	1.43	8 (15%)	62,93,113	1.47	5 (8%)
23	CHL	V	607	-	65,70,74	2.16	19 (29%)	82,108,114	3.03	39 (47%)
23	CHL	AC	601	1	47,52,74	2.45	18 (38%)	56,87,114	3.29	21 (37%)
28	LHG	0	616	24	46,46,48	0.63	1 (2%)	49,52,54	1.26	4 (8%)
24	CLA	p	611	-	40,44,73	1.61	8 (20%)	47,76,113	1.45	5 (10%)
24	CLA	v	304	17	49,53,73	1.50	8 (16%)	59,89,113	1.43	5 (8%)
24	CLA	AB	603	-	49,53,73	1.51	9 (18%)	59,89,113	1.39	6 (10%)
28	LHG	AK	624	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
27	XAT	q	617	-	39,47,47	6.17	22 (56%)	54,74,74	7.62	35 (64%)
23	CHL	AB	608	-	47,50,74	2.22	18 (38%)	52,84,114	2.92	20 (38%)
26	NEX	AC	616	-	38,46,46	1.74	7 (18%)	50,70,70	1.62	9 (18%)
24	CLA	AS	305	-	54,58,73	1.42	7 (12%)	65,95,113	1.49	7 (10%)
24	CLA	p	618	-	52,56,73	1.49	6 (11%)	62,92,113	1.77	10 (16%)
24	CLA	AQ	603	-	69,73,73	1.28	8 (11%)	83,113,113	1.24	7 (8%)
28	LHG	v	301	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
33	LMG	O	624	-	40,40,55	0.82	0	48,48,63	1.35	7 (14%)
29	BCR	F	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	5 (8%)
23	CHL	AS	302	17	47,52,74	2.45	18 (38%)	56,87,114	3.30	28 (50%)
24	CLA	AF	609	-	43,48,73	1.54	9 (20%)	52,82,113	1.75	13 (25%)
24	CLA	AQ	610	10	69,73,73	1.26	7 (10%)	83,113,113	1.36	10 (12%)
30	OEX	AJ	402	4	0,14,14	-	-	-	-	-
24	CLA	p	612	-	64,68,73	1.32	8 (12%)	77,107,113	1.28	8 (10%)
24	CLA	AR	601	16	53,57,73	1.45	8 (15%)	62,93,113	1.48	7 (11%)
37	PL9	Q	405	-	52,52,55	1.08	4 (7%)	64,65,69	1.54	14 (21%)
24	CLA	AE	610	-	49,53,73	1.51	7 (14%)	59,89,113	1.41	6 (10%)
24	CLA	v	313	17	57,61,73	1.38	8 (14%)	66,98,113	1.38	5 (7%)
24	CLA	O	605	-	69,73,73	1.28	7 (10%)	83,113,113	1.33	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AR	608	-	43,47,73	1.55	6 (13%)	49,81,113	1.62	7 (14%)
23	CHL	9	605	1	50,54,74	2.22	17 (34%)	56,90,114	3.09	22 (39%)
24	CLA	AE	604	-	49,53,73	1.48	9 (18%)	59,89,113	1.51	8 (13%)
24	CLA	V	602	-	69,73,73	1.25	7 (10%)	83,113,113	1.37	7 (8%)
23	CHL	AS	308	-	48,52,74	2.40	17 (35%)	58,87,114	3.24	23 (39%)
23	CHL	0	605	-	50,54,74	2.20	17 (34%)	56,90,114	3.13	22 (39%)
24	CLA	AH	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.47	5 (7%)
24	CLA	AK	610	5	69,73,73	1.31	6 (8%)	83,113,113	1.44	6 (7%)
24	CLA	p	602	10	69,73,73	1.26	7 (10%)	83,113,113	1.35	6 (7%)
23	CHL	AH	601	10	70,74,74	1.93	16 (22%)	80,114,114	2.73	29 (36%)
35	DGD	J	411	-	61,61,67	0.90	2 (3%)	75,75,81	1.41	9 (12%)
23	CHL	9	606	-	50,54,74	2.31	16 (32%)	56,90,114	3.29	23 (41%)
29	BCR	j	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	7 (12%)
25	LUT	AD	315	-	42,43,43	1.66	8 (19%)	51,60,60	1.57	8 (15%)
29	BCR	AB	612	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	7 (12%)
24	CLA	AF	610	-	49,53,73	1.53	7 (14%)	59,89,113	1.56	9 (15%)
24	CLA	Q	403	7	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
24	CLA	AC	610	-	47,51,73	1.54	9 (19%)	54,86,113	1.39	5 (9%)
24	CLA	AA	611	-	49,53,73	1.51	7 (14%)	59,89,113	1.42	6 (10%)
26	NEX	v	317	-	38,46,46	1.71	8 (21%)	50,70,70	1.79	10 (20%)
24	CLA	v	314	17	53,57,73	1.44	8 (15%)	62,93,113	1.46	6 (9%)
24	CLA	AU	602	10	69,73,73	1.25	7 (10%)	83,113,113	1.40	8 (9%)
24	CLA	q	612	-	61,65,73	1.45	7 (11%)	65,100,113	1.77	12 (18%)
23	CHL	AN	605	10	54,58,74	2.15	16 (29%)	59,94,114	3.00	26 (44%)
35	DGD	AL	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.41	8 (10%)
25	LUT	AE	614	-	42,43,43	1.65	8 (19%)	51,60,60	1.53	10 (19%)
25	LUT	AA	614	-	42,43,43	1.58	8 (19%)	51,60,60	1.54	9 (17%)
24	CLA	V	612	10	52,56,73	1.46	8 (15%)	62,92,113	1.47	5 (8%)
25	LUT	AU	615	-	42,43,43	1.63	8 (19%)	51,60,60	1.50	9 (17%)
24	CLA	P	504	-	69,73,73	1.27	7 (10%)	83,113,113	1.47	8 (9%)
28	LHG	AN	616	24	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
23	CHL	0	601	2	68,72,74	1.96	17 (25%)	77,111,114	2.77	26 (33%)
23	CHL	AR	613	-	46,50,74	2.37	20 (43%)	51,85,114	3.13	21 (41%)
34	SQD	Q	402	-	49,50,54	1.59	7 (14%)	58,61,65	1.38	6 (10%)
23	CHL	AQ	606	-	54,58,74	2.12	16 (29%)	59,94,114	3.11	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LHG	V	615	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
23	CHL	V	616	10	50,54,74	2.26	18 (36%)	56,90,114	2.95	23 (41%)
24	CLA	AF	602	-	43,47,73	1.64	9 (20%)	49,81,113	2.02	14 (28%)
23	CHL	v	307	-	50,54,74	2.17	17 (34%)	56,90,114	3.20	24 (42%)
24	CLA	q	601	16	53,57,73	1.45	9 (16%)	62,93,113	1.57	10 (16%)
24	CLA	V	609	10	66,70,73	1.27	8 (12%)	76,108,113	1.29	4 (5%)
24	CLA	AQ	604	-	54,58,73	1.42	9 (16%)	65,95,113	1.43	7 (10%)
23	CHL	AQ	601	10	70,74,74	1.89	16 (22%)	80,114,114	2.70	26 (32%)
28	LHG	Q	406	-	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
24	CLA	AK	609	-	69,73,73	1.26	8 (11%)	83,113,113	1.39	7 (8%)
23	CHL	AA	601	1	50,54,74	2.22	17 (34%)	56,90,114	3.12	26 (46%)
25	LUT	q	614	-	42,43,43	1.63	8 (19%)	51,60,60	1.50	10 (19%)
24	CLA	P	512	6	64,69,73	1.38	5 (7%)	78,107,113	1.47	9 (11%)
24	CLA	AK	612	-	69,73,73	1.28	7 (10%)	83,113,113	1.31	6 (7%)
24	CLA	v	305	-	54,58,73	1.42	6 (11%)	65,95,113	1.48	5 (7%)
24	CLA	AU	609	-	64,68,73	1.30	7 (10%)	77,107,113	1.33	9 (11%)
24	CLA	0	611	-	49,53,73	1.51	10 (20%)	59,89,113	1.39	5 (8%)
24	CLA	AE	608	-	52,56,73	1.44	8 (15%)	60,92,113	1.42	5 (8%)
23	CHL	v	302	17	47,52,74	2.45	18 (38%)	56,87,114	3.30	29 (51%)
24	CLA	V	603	-	69,73,73	1.27	8 (11%)	83,113,113	1.30	8 (9%)
24	CLA	AF	604	-	49,53,73	1.50	6 (12%)	59,89,113	1.49	6 (10%)
23	CHL	AN	606	-	70,74,74	1.90	16 (22%)	80,114,114	2.72	29 (36%)
34	SQD	o	101	-	41,42,54	1.67	7 (17%)	50,53,65	1.45	6 (12%)
28	LHG	O	623	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
23	CHL	v	308	-	43,46,74	2.39	17 (39%)	50,79,114	3.55	24 (48%)
26	NEX	AE	615	-	38,46,46	1.71	7 (18%)	50,70,70	1.76	11 (22%)
24	CLA	AD	313	-	52,56,73	1.45	7 (13%)	62,92,113	1.56	6 (9%)
23	CHL	AN	601	10	70,74,74	1.88	16 (22%)	80,114,114	2.75	25 (31%)
24	CLA	AR	617	-	47,51,73	1.56	7 (14%)	54,86,113	1.56	9 (16%)
24	CLA	v	303	17	65,69,73	1.30	8 (12%)	78,108,113	1.35	7 (8%)
24	CLA	9	613	-	59,63,73	1.37	7 (11%)	71,101,113	1.42	8 (11%)
35	DGD	j	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.39	8 (10%)
24	CLA	AL	513	-	69,73,73	1.25	8 (11%)	83,113,113	1.33	6 (7%)
24	CLA	q	618	-	49,53,73	1.51	8 (16%)	59,89,113	1.66	6 (10%)
28	LHG	AD	316	24	46,46,48	0.62	1 (2%)	49,52,54	1.25	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AJ	405	-	69,73,73	1.26	8 (11%)	83,113,113	1.46	6 (7%)
23	CHL	9	609	-	66,70,74	1.96	17 (25%)	75,109,114	2.84	28 (37%)
24	CLA	q	604	-	52,56,73	1.45	9 (17%)	62,92,113	1.53	5 (8%)
24	CLA	AN	610	28	43,47,73	1.56	8 (18%)	49,81,113	1.49	4 (8%)
23	CHL	AU	607	-	70,74,74	1.91	16 (22%)	80,114,114	2.68	27 (33%)
25	LUT	AH	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.50	9 (17%)
29	BCR	J	408	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
25	LUT	AA	615	-	42,43,43	1.68	8 (19%)	51,60,60	1.53	11 (21%)
24	CLA	AL	506	-	69,73,73	1.26	9 (13%)	83,113,113	1.35	6 (7%)
26	NEX	AS	317	-	38,46,46	1.59	6 (15%)	50,70,70	1.70	11 (22%)
23	CHL	AF	601	-	48,53,74	2.25	17 (35%)	53,89,114	3.09	20 (37%)
24	CLA	AQ	611	28	64,68,73	1.32	7 (10%)	77,107,113	1.34	7 (9%)
32	PHO	AJ	407	-	58,69,69	2.06	10 (17%)	56,99,99	1.50	8 (14%)
24	CLA	AD	305	-	49,53,73	1.48	9 (18%)	59,89,113	1.54	5 (8%)
24	CLA	0	612	-	62,66,73	1.33	8 (12%)	74,104,113	1.38	7 (9%)
23	CHL	AA	607	-	50,54,74	2.19	16 (32%)	56,90,114	3.15	21 (37%)
24	CLA	AU	612	-	69,73,73	1.26	9 (13%)	83,113,113	1.31	4 (4%)
24	CLA	AK	615	-	69,73,73	1.27	9 (13%)	83,113,113	1.28	8 (9%)
34	SQD	AP	101	-	41,42,54	1.66	7 (17%)	50,53,65	1.45	6 (12%)
23	CHL	AC	605	1	50,54,74	2.22	17 (34%)	56,90,114	3.12	24 (42%)
24	CLA	AD	311	-	49,53,73	1.50	10 (20%)	59,89,113	1.40	4 (6%)
26	NEX	AU	616	-	38,46,46	1.68	7 (18%)	50,70,70	1.64	9 (18%)
24	CLA	P	509	6	69,73,73	1.26	8 (11%)	83,113,113	1.24	4 (4%)
24	CLA	O	616	5	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
24	CLA	P	511	-	69,73,73	1.25	8 (11%)	83,113,113	1.33	7 (8%)
23	CHL	AU	608	-	70,74,74	1.85	17 (24%)	80,114,114	2.78	27 (33%)
24	CLA	AA	604	-	49,53,73	1.48	9 (18%)	59,89,113	1.50	5 (8%)
24	CLA	AK	613	5	69,73,73	1.27	8 (11%)	83,113,113	1.50	8 (9%)
32	PHO	AJ	408	-	58,69,69	2.07	9 (15%)	56,99,99	1.63	7 (12%)
24	CLA	AU	610	-	64,68,73	1.34	8 (12%)	77,107,113	1.41	9 (11%)
23	CHL	q	607	-	56,60,74	2.16	19 (33%)	63,97,114	2.90	26 (41%)
25	LUT	AQ	616	-	42,43,43	1.60	8 (19%)	51,60,60	1.51	11 (21%)
24	CLA	q	611	16	53,57,73	1.44	8 (15%)	62,93,113	1.36	6 (9%)
23	CHL	AA	608	-	63,66,74	2.36	20 (31%)	67,101,114	2.80	28 (41%)
24	CLA	P	503	-	69,73,73	1.27	7 (10%)	83,113,113	1.48	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	v	312	-	-	7/20/96/115	-
24	CLA	AQ	602	-	-	17/39/115/115	-
35	DGD	AL	517	-	-	11/44/84/95	0/2/2/2
24	CLA	O	601	-	-	17/39/115/115	-
24	CLA	AQ	614	-	-	2/10/82/115	-
23	CHL	9	601	1	-	5/12/88/117	-
23	CHL	AC	607	-	-	9/15/91/117	-
26	NEX	AR	615	-	-	16/27/83/83	0/3/3/3
29	BCR	AK	602	-	-	15/29/63/63	0/2/2/2
23	CHL	p	606	-	-	11/22/98/117	-
24	CLA	O	603	-	-	9/39/115/115	-
24	CLA	AC	604	-	-	6/21/97/115	-
25	LUT	0	614	-	-	0/29/67/67	0/2/2/2
25	LUT	AC	614	-	-	3/29/67/67	0/2/2/2
27	XAT	AR	616	-	-	19/31/93/93	0/4/4/4
23	CHL	AF	606	-	-	2/8/77/117	-
23	CHL	AD	302	2	-	18/39/115/117	-
24	CLA	AL	503	-	-	17/39/115/115	-
23	CHL	AN	617	10	-	7/17/93/117	-
23	CHL	AC	608	-	-	18/37/113/117	-
24	CLA	AK	618	5	-	15/39/115/115	-
24	CLA	AJ	406	-	-	6/21/97/115	-
23	CHL	AR	605	16	-	23/39/115/117	-
24	CLA	q	608	16	-	6/15/91/115	-
38	HEM	F	102	9,8	-	5/14/54/54	-
24	CLA	AU	613	-	-	7/19/95/115	-
24	CLA	Q	401	-	-	6/21/97/115	-
26	NEX	p	616	-	-	14/27/83/83	0/3/3/3
23	CHL	0	617	2	-	3/17/93/117	-
23	CHL	AD	306	-	-	10/26/102/117	-
23	CHL	AD	317	2	-	3/17/93/117	-
24	CLA	AN	612	10	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AE	603	-	-	11/27/103/115	-
24	CLA	O	611	5	-	11/39/115/115	-
25	LUT	9	616	-	-	3/29/67/67	0/2/2/2
25	LUT	AN	614	-	-	3/29/67/67	0/2/2/2
25	LUT	AU	614	-	-	2/29/67/67	0/2/2/2
23	CHL	AF	605	-	-	0/2/70/117	-
23	CHL	0	608	-	-	0/6/82/117	-
34	SQD	J	410	-	-	27/49/69/69	0/1/1/1
27	XAT	9	618	-	-	16/31/93/93	0/4/4/4
24	CLA	V	611	10	-	0/10/86/115	-
25	LUT	0	615	-	-	1/29/67/67	0/2/2/2
25	LUT	AC	615	-	-	2/29/67/67	0/2/2/2
24	CLA	AF	614	-	-	10/15/91/115	-
33	LMG	J	409	-	-	17/43/63/70	0/1/1/1
23	CHL	0	607	-	-	9/15/91/117	-
26	NEX	9	617	-	-	13/27/83/83	0/3/3/3
23	CHL	AE	601	1	-	5/17/93/117	-
23	CHL	p	605	10	-	9/20/96/117	-
24	CLA	9	611	-	-	5/9/87/115	-
23	CHL	p	601	10	-	25/41/117/117	-
24	CLA	O	606	-	-	11/33/111/115	-
24	CLA	AD	310	28	-	12/27/103/115	-
24	CLA	O	609	-	-	13/39/115/115	-
25	LUT	AS	316	-	-	3/29/67/67	0/2/2/2
24	CLA	AM	403	7	-	17/39/115/115	-
24	CLA	AD	303	-	-	16/33/109/115	-
23	CHL	AQ	608	-	-	15/41/117/117	-
28	LHG	O	621	-	-	27/53/53/53	-
29	BCR	AO	101	-	-	5/29/63/63	0/2/2/2
29	BCR	AV	101	-	-	9/29/63/63	0/2/2/2
24	CLA	AS	303	17	-	17/35/111/115	-
24	CLA	AH	603	-	-	9/39/115/115	-
24	CLA	AJ	409	4	-	7/27/105/115	-
32	PHO	J	405	-	-	6/37/103/103	0/5/6/6
23	CHL	AH	608	-	-	20/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	AK	623	-	-	15/50/50/53	-
23	CHL	V	606	-	-	18/41/117/117	-
24	CLA	AA	609	-	-	6/15/93/115	-
24	CLA	K	101	6	-	11/39/115/115	-
23	CHL	AQ	607	-	-	22/41/117/117	-
24	CLA	AE	602	1	-	5/12/88/115	-
24	CLA	AN	611	-	-	8/33/109/115	-
33	LMG	P	518	-	-	19/46/66/70	0/1/1/1
24	CLA	AK	617	-	-	14/39/115/115	-
24	CLA	p	604	-	-	10/21/97/115	-
28	LHG	W	201	-	-	14/53/53/53	-
24	CLA	0	610	28	-	11/27/103/115	-
28	LHG	p	617	-	-	15/41/41/53	-
24	CLA	Q	404	-	-	15/39/115/115	-
29	BCR	AI	101	-	-	10/29/63/63	0/2/2/2
24	CLA	AR	611	16	-	8/20/96/115	-
25	LUT	AR	614	-	-	1/29/67/67	0/2/2/2
33	LMG	Q	407	-	-	16/41/61/70	0/1/1/1
24	CLA	V	604	-	-	0/4/61/115	-
25	LUT	V	614	-	-	2/29/67/67	0/2/2/2
24	CLA	V	610	-	-	8/33/109/115	-
24	CLA	AU	611	-	-	11/33/109/115	-
23	CHL	AU	605	10	-	9/20/96/117	-
24	CLA	9	603	-	-	9/27/103/115	-
35	DGD	AJ	412	-	-	26/49/89/95	0/2/2/2
24	CLA	AK	608	-	-	11/33/111/115	-
24	CLA	AK	604	5	-	13/39/115/115	-
29	BCR	O	619	-	-	4/29/63/63	0/2/2/2
25	LUT	AF	611	-	-	2/29/67/67	0/2/2/2
24	CLA	AA	603	-	-	10/27/103/115	-
24	CLA	q	609	16	-	13/33/111/115	-
24	CLA	0	604	-	-	7/15/91/115	-
23	CHL	p	609	10	-	18/35/113/117	-
24	CLA	AA	613	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	P	506	6	-	15/39/115/115	-
24	CLA	AL	509	6	-	18/39/115/115	-
23	CHL	q	605	16	-	22/38/114/117	-
23	CHL	AN	607	-	-	26/41/117/117	-
24	CLA	AN	604	-	-	0/4/76/115	-
24	CLA	O	613	-	-	12/39/115/115	-
23	CHL	AQ	605	10	-	7/20/96/117	-
24	CLA	AM	404	-	-	15/39/115/115	-
24	CLA	AN	603	10	-	16/39/115/115	-
29	BCR	O	617	-	-	5/29/63/63	0/2/2/2
23	CHL	AF	607	-	-	6/17/93/117	-
32	PHO	J	406	-	-	18/37/103/103	0/5/6/6
23	CHL	9	607	-	-	17/38/114/117	-
25	LUT	9	615	-	-	3/29/67/67	0/2/2/2
24	CLA	AR	612	16	-	12/33/109/115	-
23	CHL	p	608	-	-	11/41/117/117	-
29	BCR	k	101	-	-	6/29/63/63	0/2/2/2
29	BCR	P	515	-	-	7/29/63/63	0/2/2/2
33	LMG	AK	601	-	-	14/35/55/70	0/1/1/1
23	CHL	V	601	10	-	25/41/117/117	-
23	CHL	AU	606	-	-	8/22/98/117	-
26	NEX	q	615	-	-	20/27/83/83	0/3/3/3
29	BCR	AJ	410	-	-	4/29/63/63	0/2/2/2
25	LUT	v	316	-	-	2/29/67/67	0/2/2/2
24	CLA	9	604	-	-	5/21/97/115	-
23	CHL	AS	306	-	-	2/6/62/117	-
23	CHL	AB	605	-	-	5/9/81/117	-
24	CLA	O	608	5	-	12/39/115/115	-
23	CHL	AR	606	-	-	9/29/105/117	-
23	CHL	AD	307	-	-	8/17/93/117	-
23	CHL	AU	601	10	-	24/41/117/117	-
24	CLA	AR	609	16	-	13/33/111/115	-
29	BCR	AK	621	-	-	4/29/63/63	0/2/2/2
24	CLA	AB	602	-	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LUT	AE	613	-	-	2/29/67/67	0/2/2/2
24	CLA	J	403	-	-	12/39/115/115	-
28	LHG	P	517	-	-	24/53/53/53	-
25	LUT	AN	615	-	-	2/29/67/67	0/2/2/2
24	CLA	AH	609	-	-	14/33/109/115	-
24	CLA	O	602	-	-	18/33/109/115	-
24	CLA	AE	611	1	-	7/15/91/115	-
24	CLA	P	507	-	-	17/39/115/115	-
24	CLA	AL	508	-	-	17/39/115/115	-
24	CLA	AS	311	-	-	13/29/105/115	-
29	BCR	AL	515	-	-	3/29/63/63	0/2/2/2
35	DGD	AJ	401	-	-	18/48/88/95	0/2/2/2
37	PL9	AM	405	-	-	3/50/70/73	0/1/1/1
23	CHL	AB	601	-	-	0/15/91/117	-
23	CHL	AB	607	-	-	7/17/93/117	-
24	CLA	AR	610	-	-	11/20/96/115	-
24	CLA	P	510	6	-	17/39/115/115	-
24	CLA	AK	607	-	-	18/39/115/115	-
23	CHL	AE	617	-	-	7/17/93/117	-
24	CLA	AS	312	-	-	8/20/96/115	-
24	CLA	O	610	-	-	12/39/115/115	-
34	SQD	AM	401	-	-	20/45/65/69	0/1/1/1
23	CHL	v	306	-	-	2/4/72/117	-
24	CLA	O	609	2	-	11/27/105/115	-
24	CLA	AC	602	1	-	20/35/111/115	-
27	XAT	AB	613	-	-	19/31/93/93	0/4/4/4
24	CLA	P	505	-	-	22/39/115/115	-
24	CLA	AK	603	-	-	16/39/115/115	-
24	CLA	AL	510	6	-	10/39/115/115	-
28	LHG	AM	406	-	-	17/53/53/53	-
29	BCR	O	618	-	-	6/29/63/63	0/2/2/2
24	CLA	AF	603	-	-	5/15/91/115	-
24	CLA	AL	502	-	-	17/39/115/115	-
23	CHL	AA	617	1	-	7/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	AF	608	3	-	4/11/89/117	-
24	CLA	P	508	6	-	18/39/115/115	-
24	CLA	AH	602	10	-	18/39/115/115	-
24	CLA	9	610	1	-	8/23/101/115	-
24	CLA	AQ	613	10	-	8/33/109/115	-
24	CLA	AK	614	-	-	15/39/115/115	-
23	CHL	AE	606	-	-	12/17/93/117	-
24	CLA	AS	309	-	-	2/9/87/115	-
24	CLA	AL	507	6	-	15/39/115/115	-
24	CLA	AD	304	-	-	11/27/103/115	-
24	CLA	O	614	-	-	18/39/115/115	-
24	CLA	AQ	612	-	-	2/33/109/115	-
24	CLA	AC	603	-	-	9/27/103/115	-
34	SQD	AJ	411	-	-	27/49/69/69	0/1/1/1
29	BCR	O	625	-	-	17/29/63/63	0/2/2/2
33	LMG	AK	622	-	-	18/46/66/70	0/1/1/1
35	DGD	AO	102	-	-	19/51/91/95	0/2/2/2
24	CLA	0	613	-	-	12/19/95/115	-
24	CLA	AC	613	-	-	5/9/87/115	-
24	CLA	AK	605	-	-	8/39/115/115	-
25	LUT	p	614	-	-	1/29/67/67	0/2/2/2
23	CHL	AB	606	-	-	7/15/91/117	-
25	LUT	V	613	-	-	2/29/67/67	0/2/2/2
23	CHL	V	605	-	-	12/22/98/117	-
28	LHG	O	622	-	-	15/50/50/53	-
33	LMG	AL	501	-	-	17/43/63/70	0/1/1/1
25	LUT	AS	315	-	-	2/29/67/67	0/2/2/2
28	LHG	AQ	618	24	-	16/53/53/53	-
24	CLA	p	603	-	-	16/39/115/115	-
24	CLA	AN	609	-	-	18/32/110/115	-
23	CHL	9	608	-	-	9/15/91/117	-
24	CLA	AA	602	1	-	9/35/111/115	-
24	CLA	AR	603	-	-	7/33/109/115	-
24	CLA	O	604	5	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	9	602	1	-	17/35/111/115	-
24	CLA	0	603	-	-	13/27/103/115	-
24	CLA	AR	602	16	-	11/27/105/115	-
24	CLA	AH	610	-	-	12/33/109/115	-
24	CLA	O	612	-	-	14/39/115/115	-
25	LUT	AD	314	-	-	0/29/67/67	0/2/2/2
23	CHL	AA	606	-	-	16/35/111/117	-
24	CLA	AU	603	-	-	10/39/115/115	-
24	CLA	v	311	-	-	10/29/105/115	-
38	HEM	f	102	9,8	-	5/14/54/54	-
24	CLA	AH	613	-	-	6/13/91/115	-
24	CLA	AB	610	-	-	7/15/91/115	-
23	CHL	AQ	609	-	-	21/41/117/117	-
33	LMG	O	620	-	-	18/46/66/70	0/1/1/1
28	LHG	AU	617	-	-	12/53/53/53	-
24	CLA	9	614	-	-	0/4/72/115	-
23	CHL	AA	605	1	-	9/17/93/117	-
24	CLA	AB	611	-	-	7/15/91/115	-
24	CLA	AH	611	-	-	11/33/109/115	-
29	BCR	AL	516	-	-	6/29/63/63	0/2/2/2
25	LUT	p	615	-	-	1/29/67/67	0/2/2/2
24	CLA	AJ	404	-	-	13/39/115/115	-
29	BCR	AK	619	-	-	5/29/63/63	0/2/2/2
29	BCR	P	514	-	-	6/29/63/63	0/2/2/2
24	CLA	AL	505	-	-	16/39/115/115	-
26	NEX	AA	616	-	-	18/27/83/83	0/3/3/3
24	CLA	AE	612	-	-	5/15/91/115	-
24	CLA	q	603	-	-	6/33/109/115	-
29	BCR	P	513	-	-	3/29/63/63	0/2/2/2
24	CLA	AA	610	-	-	6/9/87/115	-
23	CHL	p	607	-	-	22/41/117/117	-
24	CLA	q	602	16	-	11/27/105/115	-
29	BCR	f	101	-	-	11/29/63/63	0/2/2/2
23	CHL	AD	301	-	-	13/38/114/117	-
24	CLA	9	612	-	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AK	606	5	-	17/39/115/115	-
35	DGD	J	413	-	-	18/48/88/95	0/2/2/2
29	BCR	AF	612	-	-	13/29/63/63	0/2/2/2
24	CLA	P	501	-	-	16/39/115/115	-
24	CLA	AH	612	10	-	15/39/115/115	-
28	LHG	q	616	24	-	14/46/46/53	-
28	LHG	AS	301	-	-	22/53/53/53	-
25	LUT	v	315	-	-	2/29/67/67	0/2/2/2
34	SQD	M	101	-	-	19/49/69/69	0/1/1/1
23	CHL	AE	607	-	-	13/35/111/117	-
24	CLA	AS	310	-	-	5/21/99/115	-
28	LHG	AL	519	-	-	25/53/53/53	-
24	CLA	AC	612	1	-	3/10/86/115	-
28	LHG	w	201	-	-	14/53/53/53	-
24	CLA	AB	609	-	-	4/10/82/115	-
24	CLA	O	615	-	-	12/39/115/115	-
23	CHL	AH	607	-	-	18/41/117/117	-
25	LUT	AQ	615	-	-	1/29/67/67	0/2/2/2
23	CHL	AD	308	-	-	12/29/107/117	-
33	LMG	AM	407	-	-	16/41/61/70	0/1/1/1
23	CHL	0	606	-	-	10/26/102/117	-
24	CLA	v	309	-	-	2/9/87/115	-
23	CHL	AH	606	-	-	8/22/98/117	-
24	CLA	AL	504	-	-	21/39/115/115	-
23	CHL	AN	608	-	-	15/29/107/117	-
24	CLA	AD	309	-	-	9/27/105/115	-
24	CLA	AR	604	-	-	5/19/95/115	-
23	CHL	q	613	16	-	4/12/88/117	-
24	CLA	AC	611	-	-	5/9/81/115	-
24	CLA	p	610	-	-	21/40/101/115	-
24	CLA	AN	602	10	-	15/39/115/115	-
34	SQD	m	101	-	-	18/49/69/69	0/1/1/1
24	CLA	AS	304	17	-	2/15/91/115	-
29	BCR	AK	620	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AD	312	2	-	8/31/107/115	-
24	CLA	AU	604	-	-	7/21/97/115	-
23	CHL	q	606	-	-	9/27/103/117	-
23	CHL	AS	307	-	-	10/32/108/117	-
24	CLA	AB	604	-	-	5/15/91/115	-
26	NEX	AQ	617	-	-	17/27/83/83	0/3/3/3
24	CLA	P	502	-	-	17/39/115/115	-
24	CLA	p	613	10	-	2/10/82/115	-
24	CLA	AL	511	6	-	17/39/115/115	-
28	LHG	AH	616	-	-	12/53/53/53	-
24	CLA	AK	611	-	-	13/39/115/115	-
24	CLA	O	607	-	-	17/39/115/115	-
23	CHL	AR	607	-	-	11/26/102/117	-
27	XAT	AF	613	-	-	19/31/93/93	0/4/4/4
24	CLA	AL	512	6	-	13/39/115/115	-
24	CLA	v	310	-	-	5/21/99/115	-
24	CLA	AL	514	6	-	14/31/109/115	-
23	CHL	AE	605	-	-	16/35/111/117	-
24	CLA	AA	612	-	-	9/15/91/115	-
23	CHL	V	608	-	-	13/29/107/117	-
33	LMG	AL	520	-	-	20/46/66/70	0/1/1/1
24	CLA	AS	313	-	-	12/21/99/115	-
23	CHL	AC	606	-	-	5/17/93/117	-
25	LUT	AH	615	-	-	1/29/67/67	0/2/2/2
24	CLA	AC	609	1	-	6/23/101/115	-
24	CLA	q	610	28	-	11/20/96/115	-
24	CLA	AN	613	10	-	12/19/95/115	-
23	CHL	AE	616	1	-	9/17/93/117	-
24	CLA	J	407	4	-	7/27/105/115	-
35	DGD	P	516	-	-	11/44/84/95	0/2/2/2
23	CHL	AH	605	10	-	9/20/96/117	-
24	CLA	O	602	5	-	12/39/115/115	-
24	CLA	J	404	-	-	7/39/115/115	-
24	CLA	AE	609	-	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AK	616	-	-	18/39/115/115	-
24	CLA	AS	314	17	-	11/20/96/115	-
23	CHL	V	607	-	-	24/37/113/117	-
23	CHL	AC	601	1	-	9/15/91/117	-
28	LHG	0	616	24	-	8/51/51/53	-
24	CLA	p	611	-	-	2/4/72/115	-
24	CLA	v	304	17	-	2/15/91/115	-
24	CLA	AB	603	-	-	4/15/91/115	-
28	LHG	AK	624	-	-	21/53/53/53	-
27	XAT	q	617	-	-	20/31/93/93	0/4/4/4
23	CHL	AB	608	-	-	5/11/83/117	-
26	NEX	AC	616	-	-	15/27/83/83	0/3/3/3
24	CLA	AS	305	-	-	11/21/97/115	-
24	CLA	p	618	-	-	9/19/95/115	-
24	CLA	AQ	603	-	-	16/39/115/115	-
28	LHG	v	301	-	-	22/53/53/53	-
33	LMG	O	624	-	-	14/35/55/70	0/1/1/1
29	BCR	F	101	-	-	11/29/63/63	0/2/2/2
23	CHL	AS	302	17	-	3/15/91/117	-
24	CLA	AF	609	-	-	4/10/82/115	-
24	CLA	AQ	610	10	-	18/39/115/115	-
24	CLA	p	612	-	-	10/33/109/115	-
24	CLA	AR	601	16	-	10/20/96/115	-
37	PL9	Q	405	-	-	3/50/70/73	0/1/1/1
24	CLA	AE	610	-	-	6/15/91/115	-
24	CLA	v	313	17	-	11/21/99/115	-
24	CLA	O	605	-	-	19/39/115/115	-
24	CLA	AR	608	-	-	0/4/82/115	-
23	CHL	9	605	1	-	8/17/93/117	-
24	CLA	AE	604	-	-	8/15/91/115	-
24	CLA	V	602	-	-	16/39/115/115	-
23	CHL	AS	308	-	-	5/15/91/117	-
23	CHL	0	605	-	-	5/17/93/117	-
24	CLA	AH	604	-	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AK	610	5	-	13/39/115/115	-
24	CLA	p	602	10	-	15/39/115/115	-
23	CHL	AH	601	10	-	24/41/117/117	-
35	DGD	J	411	-	-	26/49/89/95	0/2/2/2
23	CHL	9	606	-	-	8/17/93/117	-
29	BCR	j	101	-	-	6/29/63/63	0/2/2/2
25	LUT	AD	315	-	-	1/29/67/67	0/2/2/2
29	BCR	AB	612	-	-	13/29/63/63	0/2/2/2
24	CLA	AF	610	-	-	5/15/91/115	-
24	CLA	Q	403	7	-	17/39/115/115	-
24	CLA	AC	610	-	-	5/9/87/115	-
24	CLA	AA	611	-	-	6/15/91/115	-
26	NEX	v	317	-	-	16/27/83/83	0/3/3/3
24	CLA	v	314	17	-	11/20/96/115	-
24	CLA	AU	602	10	-	18/39/115/115	-
24	CLA	q	612	-	-	12/33/106/115	-
23	CHL	AN	605	10	-	12/22/98/117	-
35	DGD	AL	518	-	-	21/51/91/95	0/2/2/2
25	LUT	AE	614	-	-	1/29/67/67	0/2/2/2
25	LUT	AA	614	-	-	2/29/67/67	0/2/2/2
24	CLA	V	612	10	-	11/19/95/115	-
25	LUT	AU	615	-	-	1/29/67/67	0/2/2/2
24	CLA	P	504	-	-	11/39/115/115	-
28	LHG	AN	616	24	-	16/53/53/53	-
23	CHL	0	601	2	-	19/39/115/117	-
23	CHL	AR	613	-	-	5/12/88/117	-
34	SQD	Q	402	-	-	19/45/65/69	0/1/1/1
23	CHL	AQ	606	-	-	11/22/98/117	-
28	LHG	V	615	-	-	18/53/53/53	-
23	CHL	V	616	10	-	9/17/93/117	-
24	CLA	AF	602	-	-	1/4/82/115	-
23	CHL	v	307	-	-	9/17/93/117	-
24	CLA	q	601	16	-	8/20/96/115	-
24	CLA	V	609	10	-	19/32/110/115	-
24	CLA	AQ	604	-	-	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	AQ	601	10	-	23/41/117/117	-
28	LHG	Q	406	-	-	17/53/53/53	-
24	CLA	AK	609	-	-	17/39/115/115	-
23	CHL	AA	601	1	-	6/17/93/117	-
25	LUT	q	614	-	-	1/29/67/67	0/2/2/2
24	CLA	P	512	6	-	13/31/109/115	-
24	CLA	AK	612	-	-	10/39/115/115	-
24	CLA	v	305	-	-	6/21/97/115	-
24	CLA	AU	609	-	-	12/33/109/115	-
24	CLA	0	611	-	-	8/15/91/115	-
24	CLA	AE	608	-	-	6/15/93/115	-
23	CHL	v	302	17	-	4/15/91/117	-
24	CLA	V	603	-	-	15/39/115/115	-
24	CLA	AF	604	-	-	3/15/91/115	-
23	CHL	AN	606	-	-	18/41/117/117	-
34	SQD	o	101	-	-	20/37/57/69	0/1/1/1
28	LHG	O	623	-	-	23/53/53/53	-
23	CHL	v	308	-	-	1/8/84/117	-
26	NEX	AE	615	-	-	17/27/83/83	0/3/3/3
24	CLA	AD	313	-	-	14/19/95/115	-
23	CHL	AN	601	10	-	24/41/117/117	-
24	CLA	AR	617	-	-	5/9/87/115	-
24	CLA	v	303	17	-	16/35/111/115	-
24	CLA	9	613	-	-	11/27/103/115	-
35	DGD	j	102	-	-	16/51/91/95	0/2/2/2
24	CLA	AL	513	-	-	13/39/115/115	-
24	CLA	q	618	-	-	7/15/91/115	-
28	LHG	AD	316	24	-	11/51/51/53	-
24	CLA	AJ	405	-	-	8/39/115/115	-
23	CHL	9	609	-	-	15/37/113/117	-
24	CLA	q	604	-	-	8/19/95/115	-
24	CLA	AN	610	28	-	2/4/82/115	-
23	CHL	AU	607	-	-	18/41/117/117	-
25	LUT	AH	614	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	J	408	-	-	4/29/63/63	0/2/2/2
25	LUT	AA	615	-	-	1/29/67/67	0/2/2/2
24	CLA	AL	506	-	-	23/39/115/115	-
26	NEX	AS	317	-	-	15/27/83/83	0/3/3/3
23	CHL	AF	601	-	-	1/15/91/117	-
24	CLA	AQ	611	28	-	18/33/109/115	-
32	PHO	AJ	407	-	-	6/37/103/103	0/5/6/6
24	CLA	AD	305	-	-	9/15/91/115	-
24	CLA	0	612	-	-	7/31/107/115	-
23	CHL	AA	607	-	-	12/17/93/117	-
24	CLA	AU	612	-	-	17/39/115/115	-
24	CLA	AK	615	-	-	12/39/115/115	-
34	SQD	AP	101	-	-	19/37/57/69	0/1/1/1
23	CHL	AC	605	1	-	9/17/93/117	-
24	CLA	AD	311	-	-	8/15/91/115	-
26	NEX	AU	616	-	-	14/27/83/83	0/3/3/3
24	CLA	P	509	6	-	9/39/115/115	-
24	CLA	O	616	5	-	16/39/115/115	-
24	CLA	P	511	-	-	12/39/115/115	-
23	CHL	AU	608	-	-	21/41/117/117	-
24	CLA	AA	604	-	-	9/15/91/115	-
24	CLA	AK	613	5	-	11/39/115/115	-
32	PHO	AJ	408	-	-	19/37/103/103	0/5/6/6
24	CLA	AU	610	-	-	13/33/109/115	-
23	CHL	q	607	-	-	13/25/101/117	-
25	LUT	AQ	616	-	-	1/29/67/67	0/2/2/2
24	CLA	q	611	16	-	8/20/96/115	-
23	CHL	AA	608	-	-	18/36/97/117	-
24	CLA	P	503	-	-	21/39/115/115	-

The worst 5 of 3944 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AF	613	XAT	C14-C13	15.14	1.55	1.35
27	AB	613	XAT	C34-C33	15.10	1.55	1.35
27	AB	613	XAT	C14-C13	15.03	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AB	613	XAT	C30-C29	14.94	1.55	1.35
27	q	617	XAT	C30-C29	14.93	1.55	1.35

The worst 5 of 4822 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	9	618	XAT	O4-C5-C4	32.84	138.05	113.38
27	9	618	XAT	O24-C25-C24	32.41	137.73	113.38
27	AB	613	XAT	O4-C5-C4	32.27	137.62	113.38
27	q	617	XAT	O4-C5-C4	32.17	137.55	113.38
27	AR	616	XAT	O4-C5-C4	32.12	137.51	113.38

There are no chirality outliers.

5 of 4813 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	9	601	CHL	C3A-C2A-CAA-CBA
23	9	605	CHL	C1A-C2A-CAA-CBA
23	9	605	CHL	C3A-C2A-CAA-CBA
23	9	605	CHL	CBD-CGD-O2D-CED
23	9	606	CHL	C2B-C3B-CAB-CBB

There are no ring outliers.

404 monomers are involved in 1453 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	v	312	CLA	1	0
24	AQ	602	CLA	3	0
35	AL	517	DGD	1	0
24	O	601	CLA	10	0
23	9	601	CHL	4	0
23	AC	607	CHL	4	0
26	AR	615	NEX	6	0
29	AK	602	BCR	2	0
23	p	606	CHL	7	0
24	O	603	CLA	4	0
24	AC	604	CLA	9	0
25	0	614	LUT	2	0
25	AC	614	LUT	7	0
23	AF	606	CHL	1	0
23	AD	302	CHL	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AL	503	CLA	1	0
23	AN	617	CHL	5	0
23	AC	608	CHL	5	0
24	AK	618	CLA	3	0
23	AR	605	CHL	9	0
24	q	608	CLA	2	0
38	F	102	HEM	4	0
24	AU	613	CLA	3	0
24	Q	401	CLA	1	0
26	p	616	NEX	2	0
23	0	617	CHL	3	0
23	AD	306	CHL	3	0
23	AD	317	CHL	4	0
24	AN	612	CLA	4	0
24	AE	603	CLA	4	0
24	O	611	CLA	6	0
25	9	616	LUT	6	0
25	AN	614	LUT	10	0
25	AU	614	LUT	4	0
23	AF	605	CHL	3	0
23	0	608	CHL	7	0
34	J	410	SQD	7	0
27	9	618	XAT	2	0
24	V	611	CLA	2	0
25	0	615	LUT	2	0
25	AC	615	LUT	7	0
24	AF	614	CLA	1	0
23	0	607	CHL	3	0
26	9	617	NEX	4	0
23	AE	601	CHL	4	0
23	p	605	CHL	1	0
24	9	611	CLA	1	0
23	p	601	CHL	9	0
24	O	606	CLA	4	0
24	AD	310	CLA	1	0
24	O	609	CLA	7	0
25	AS	316	LUT	5	0
24	AM	403	CLA	4	0
24	AD	303	CLA	4	0
23	AQ	608	CHL	19	0
28	O	621	LHG	3	0
29	AO	101	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	AV	101	BCR	3	0
24	AS	303	CLA	2	0
24	AH	603	CLA	1	0
24	AJ	409	CLA	1	0
32	J	405	PHO	4	0
23	AH	608	CHL	17	0
28	AK	623	LHG	1	0
23	V	606	CHL	12	0
24	AA	609	CLA	1	0
24	K	101	CLA	2	0
23	AQ	607	CHL	12	0
24	AE	602	CLA	2	0
24	AN	611	CLA	3	0
33	P	518	LMG	2	0
24	AK	617	CLA	3	0
24	p	604	CLA	2	0
28	W	201	LHG	2	0
24	0	610	CLA	2	0
28	p	617	LHG	1	0
24	Q	404	CLA	4	0
29	AI	101	BCR	2	0
25	AR	614	LUT	12	0
24	V	604	CLA	1	0
25	V	614	LUT	6	0
24	V	610	CLA	4	0
24	AU	611	CLA	4	0
23	AU	605	CHL	3	0
35	AJ	412	DGD	1	0
24	AK	608	CLA	4	0
24	AK	604	CLA	2	0
29	O	619	BCR	5	0
25	AF	611	LUT	7	0
24	AA	603	CLA	2	0
24	q	609	CLA	10	0
24	0	604	CLA	3	0
23	p	609	CHL	7	0
24	AA	613	CLA	1	0
24	P	506	CLA	2	0
24	AL	509	CLA	9	0
23	q	605	CHL	8	0
23	AN	607	CHL	24	0
24	O	613	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AQ	605	CHL	1	0
24	AM	404	CLA	1	0
24	AN	603	CLA	4	0
29	O	617	BCR	5	0
23	AF	607	CHL	7	0
32	J	406	PHO	3	0
23	9	607	CHL	12	0
25	9	615	LUT	7	0
24	AR	612	CLA	7	0
23	p	608	CHL	17	0
29	k	101	BCR	4	0
29	P	515	BCR	5	0
33	AK	601	LMG	1	0
23	V	601	CHL	10	0
23	AU	606	CHL	4	0
26	q	615	NEX	3	0
29	AJ	410	BCR	4	0
25	v	316	LUT	6	0
24	9	604	CLA	6	0
23	AS	306	CHL	2	0
23	AB	605	CHL	3	0
24	O	608	CLA	5	0
23	AR	606	CHL	5	0
23	AD	307	CHL	3	0
23	AU	601	CHL	15	0
24	AR	609	CLA	5	0
29	AK	621	BCR	2	0
24	AB	602	CLA	2	0
25	AE	613	LUT	8	0
24	J	403	CLA	7	0
28	P	517	LHG	2	0
25	AN	615	LUT	6	0
24	AH	609	CLA	10	0
24	0	602	CLA	2	0
24	AE	611	CLA	2	0
24	P	507	CLA	3	0
24	AL	508	CLA	4	0
24	AS	311	CLA	6	0
29	AL	515	BCR	2	0
35	AJ	401	DGD	2	0
23	AB	607	CHL	5	0
24	AR	610	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	P	510	CLA	2	0
24	AK	607	CLA	8	0
23	AE	617	CHL	6	0
24	AS	312	CLA	1	0
24	O	610	CLA	9	0
34	AM	401	SQD	2	0
23	v	306	CHL	3	0
24	0	609	CLA	3	0
24	AC	602	CLA	5	0
27	AB	613	XAT	7	0
24	P	505	CLA	2	0
24	AK	603	CLA	9	0
28	AM	406	LHG	2	0
29	O	618	BCR	4	0
24	AF	603	CLA	2	0
24	AL	502	CLA	2	0
23	AA	617	CHL	4	0
23	AF	608	CHL	3	0
24	P	508	CLA	8	0
24	AH	602	CLA	5	0
24	9	610	CLA	7	0
24	AQ	613	CLA	5	0
24	AK	614	CLA	4	0
23	AE	606	CHL	7	0
24	AS	309	CLA	1	0
24	AL	507	CLA	3	0
24	AD	304	CLA	5	0
24	O	614	CLA	9	0
24	AQ	612	CLA	4	0
34	AJ	411	SQD	6	0
29	O	625	BCR	1	0
33	AK	622	LMG	1	0
35	AO	102	DGD	3	0
24	0	613	CLA	2	0
24	AC	613	CLA	3	0
24	AK	605	CLA	6	0
25	p	614	LUT	3	0
23	AB	606	CHL	3	0
25	V	613	LUT	7	0
23	V	605	CHL	7	0
28	O	622	LHG	1	0
33	AL	501	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	AS	315	LUT	3	0
28	AQ	618	LHG	1	0
24	p	603	CLA	3	0
24	AN	609	CLA	5	0
23	9	608	CHL	4	0
24	AA	602	CLA	5	0
24	O	604	CLA	6	0
24	9	602	CLA	5	0
24	0	603	CLA	2	0
24	AR	602	CLA	1	0
24	AH	610	CLA	5	0
24	O	612	CLA	6	0
25	AD	314	LUT	2	0
23	AA	606	CHL	9	0
24	AU	603	CLA	1	0
24	v	311	CLA	5	0
38	f	102	HEM	3	0
24	AH	613	CLA	1	0
24	AB	610	CLA	2	0
23	AQ	609	CHL	8	0
33	O	620	LMG	1	0
23	AA	605	CHL	4	0
24	AB	611	CLA	2	0
24	AH	611	CLA	5	0
29	AL	516	BCR	3	0
25	p	615	LUT	4	0
24	AJ	404	CLA	9	0
29	AK	619	BCR	5	0
29	P	514	BCR	3	0
24	AL	505	CLA	2	0
26	AA	616	NEX	1	0
24	q	603	CLA	1	0
29	P	513	BCR	2	0
24	AA	610	CLA	1	0
23	p	607	CHL	14	0
24	q	602	CLA	3	0
29	f	101	BCR	3	0
23	AD	301	CHL	8	0
24	AK	606	CLA	4	0
35	J	413	DGD	2	0
29	AF	612	BCR	2	0
24	P	501	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AH	612	CLA	2	0
28	q	616	LHG	2	0
28	AS	301	LHG	1	0
25	v	315	LUT	4	0
34	M	101	SQD	3	0
23	AE	607	CHL	8	0
24	AS	310	CLA	3	0
28	AL	519	LHG	2	0
24	AC	612	CLA	3	0
28	w	201	LHG	2	0
24	AB	609	CLA	2	0
24	O	615	CLA	5	0
23	AH	607	CHL	9	0
25	AQ	615	LUT	3	0
23	AD	308	CHL	9	0
23	0	606	CHL	2	0
24	v	309	CLA	1	0
23	AH	606	CHL	4	0
23	AN	608	CHL	8	0
24	AD	309	CLA	5	0
24	AR	604	CLA	4	0
23	q	613	CHL	1	0
24	AC	611	CLA	1	0
24	p	610	CLA	10	0
24	AN	602	CLA	5	0
34	m	101	SQD	3	0
24	AS	304	CLA	1	0
29	AK	620	BCR	2	0
24	AU	604	CLA	3	0
23	q	606	CHL	6	0
23	AS	307	CHL	5	0
24	AB	604	CLA	1	0
26	AQ	617	NEX	2	0
24	P	502	CLA	1	0
24	p	613	CLA	2	0
24	AL	511	CLA	2	0
24	AK	611	CLA	10	0
24	O	607	CLA	3	0
23	AR	607	CHL	7	0
27	AF	613	XAT	7	0
24	AL	512	CLA	3	0
24	v	310	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AL	514	CLA	4	0
23	AE	605	CHL	6	0
24	AA	612	CLA	2	0
23	V	608	CHL	4	0
33	AL	520	LMG	1	0
24	AS	313	CLA	4	0
23	AC	606	CHL	5	0
25	AH	615	LUT	6	0
24	AC	609	CLA	8	0
24	q	610	CLA	2	0
24	AN	613	CLA	2	0
23	AE	616	CHL	5	0
24	J	407	CLA	3	0
35	P	516	DGD	1	0
23	AH	605	CHL	2	0
24	O	602	CLA	1	0
24	J	404	CLA	3	0
24	AE	609	CLA	1	0
24	AK	616	CLA	8	0
23	V	607	CHL	20	0
23	AC	601	CHL	3	0
28	0	616	LHG	3	0
24	AB	603	CLA	3	0
28	AK	624	LHG	2	0
27	q	617	XAT	1	0
23	AB	608	CHL	4	0
26	AC	616	NEX	4	0
24	AS	305	CLA	1	0
24	p	618	CLA	2	0
24	AQ	603	CLA	3	0
28	v	301	LHG	1	0
33	O	624	LMG	1	0
29	F	101	BCR	2	0
23	AS	302	CHL	3	0
24	AF	609	CLA	3	0
24	AQ	610	CLA	10	0
24	AR	601	CLA	1	0
24	v	313	CLA	6	0
24	O	605	CLA	6	0
24	AR	608	CLA	4	0
23	9	605	CHL	2	0
24	AE	604	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	V	602	CLA	6	0
23	AS	308	CHL	7	0
23	0	605	CHL	2	0
24	AH	604	CLA	2	0
24	AK	610	CLA	6	0
24	p	602	CLA	3	0
23	AH	601	CHL	15	0
35	J	411	DGD	1	0
23	9	606	CHL	4	0
29	j	101	BCR	5	0
25	AD	315	LUT	4	0
29	AB	612	BCR	4	0
24	AF	610	CLA	3	0
24	Q	403	CLA	4	0
24	AC	610	CLA	2	0
24	AA	611	CLA	1	0
26	v	317	NEX	1	0
24	v	314	CLA	1	0
24	AU	602	CLA	3	0
24	q	612	CLA	5	0
23	AN	605	CHL	5	0
35	AL	518	DGD	1	0
25	AE	614	LUT	8	0
25	AA	614	LUT	5	0
25	AU	615	LUT	8	0
24	P	504	CLA	3	0
28	AN	616	LHG	2	0
23	0	601	CHL	16	0
23	AR	613	CHL	1	0
34	Q	402	SQD	2	0
23	AQ	606	CHL	5	0
28	V	615	LHG	2	0
23	V	616	CHL	4	0
24	AF	602	CLA	7	0
23	v	307	CHL	7	0
24	q	601	CLA	2	0
24	V	609	CLA	7	0
24	AQ	604	CLA	1	0
23	AQ	601	CHL	9	0
28	Q	406	LHG	2	0
24	AK	609	CLA	5	0
23	AA	601	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	q	614	LUT	10	0
24	P	512	CLA	4	0
24	AK	612	CLA	3	0
24	AU	609	CLA	8	0
24	0	611	CLA	1	0
24	AE	608	CLA	2	0
23	v	302	CHL	3	0
24	V	603	CLA	4	0
24	AF	604	CLA	2	0
23	AN	606	CHL	12	0
34	o	101	SQD	5	0
28	O	623	LHG	3	0
23	v	308	CHL	3	0
26	AE	615	NEX	1	0
24	AD	313	CLA	2	0
23	AN	601	CHL	8	0
24	AR	617	CLA	7	0
24	v	303	CLA	3	0
24	9	613	CLA	4	0
35	j	102	DGD	2	0
24	AL	513	CLA	2	0
24	q	618	CLA	6	0
24	AJ	405	CLA	4	0
23	9	609	CHL	8	0
24	q	604	CLA	3	0
23	AU	607	CHL	7	0
25	AH	614	LUT	5	0
29	J	408	BCR	4	0
25	AA	615	LUT	3	0
24	AL	506	CLA	3	0
26	AS	317	NEX	1	0
24	AQ	611	CLA	2	0
32	AJ	407	PHO	5	0
24	AD	305	CLA	3	0
24	0	612	CLA	1	0
23	AA	607	CHL	4	0
24	AU	612	CLA	3	0
24	AK	615	CLA	2	0
34	AP	101	SQD	5	0
23	AC	605	CHL	3	0
24	AD	311	CLA	2	0
26	AU	616	NEX	1	0

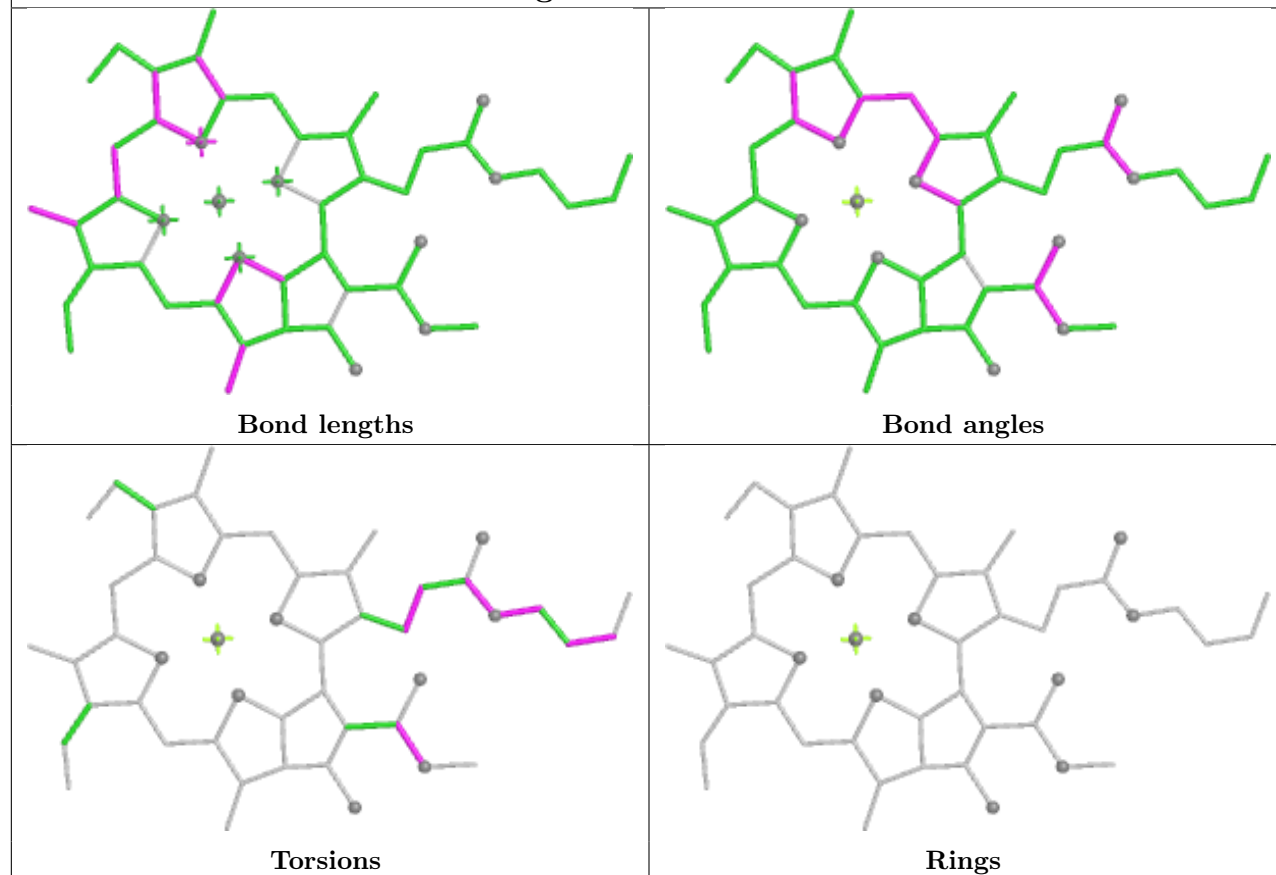
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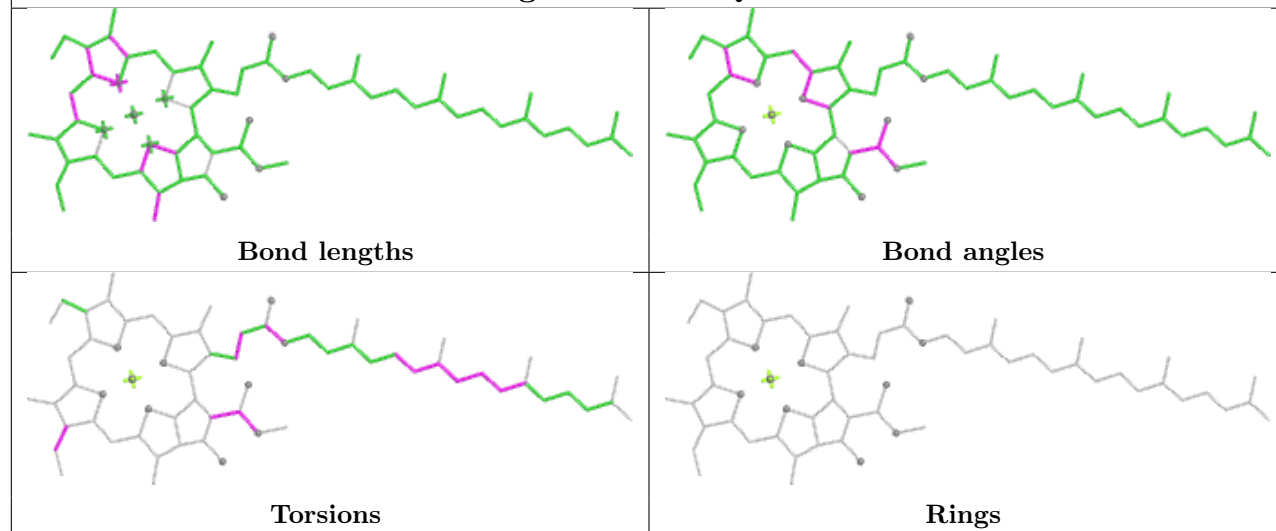
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	O	616	CLA	2	0
24	P	511	CLA	2	0
23	AU	608	CHL	18	0
24	AA	604	CLA	4	0
24	AK	613	CLA	8	0
32	AJ	408	PHO	3	0
24	AU	610	CLA	5	0
23	q	607	CHL	7	0
25	AQ	616	LUT	3	0
23	AA	608	CHL	5	0
24	P	503	CLA	1	0

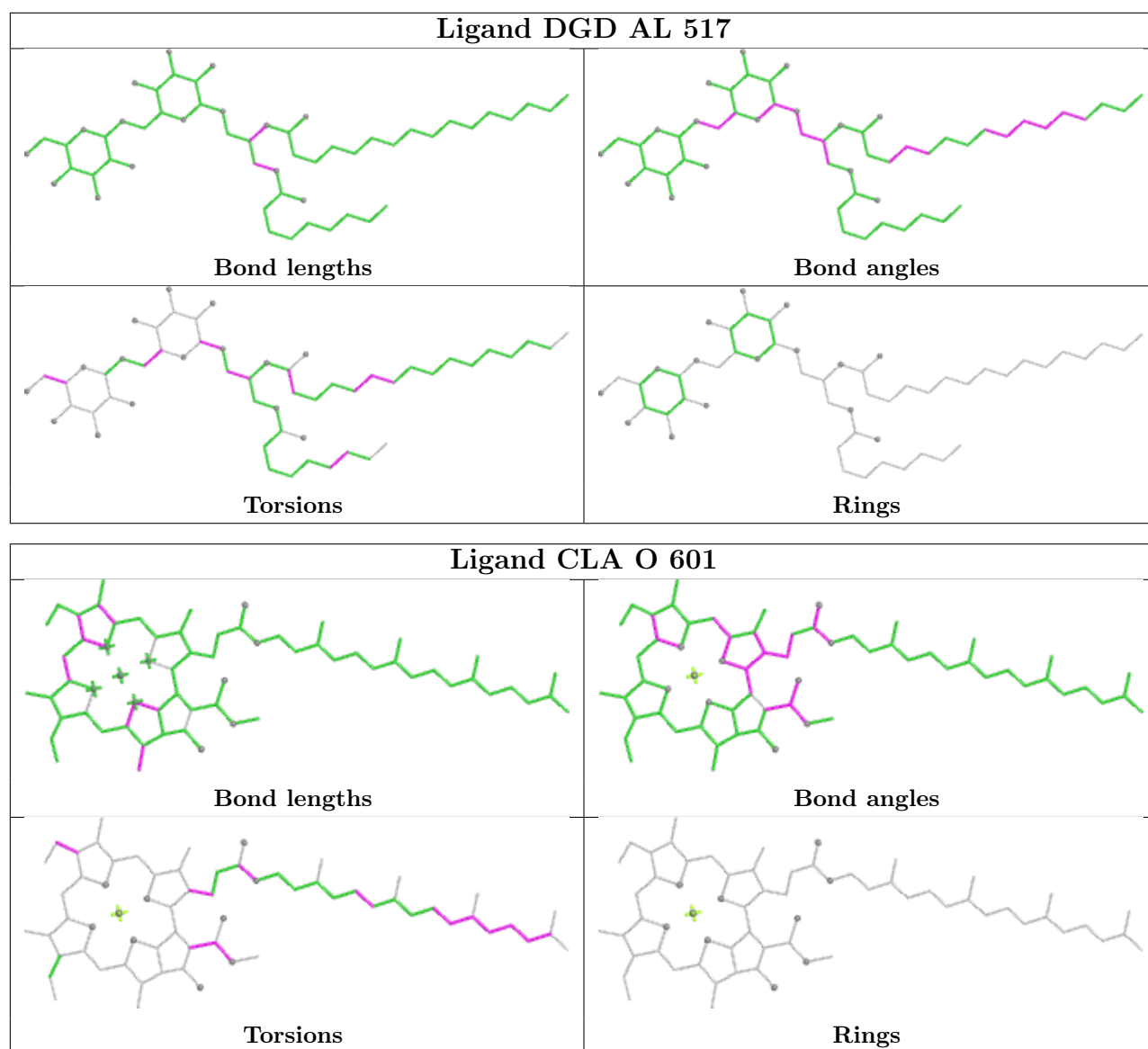
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA v 312

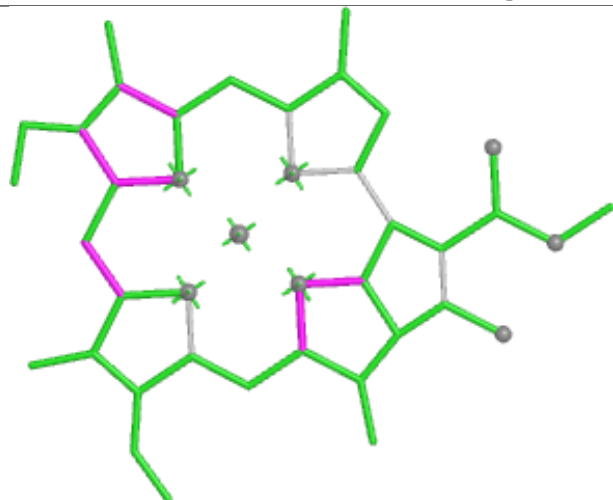


Ligand CLA AQ 602

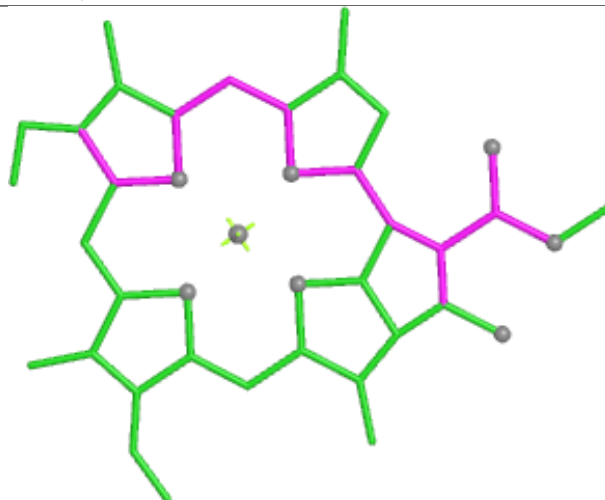




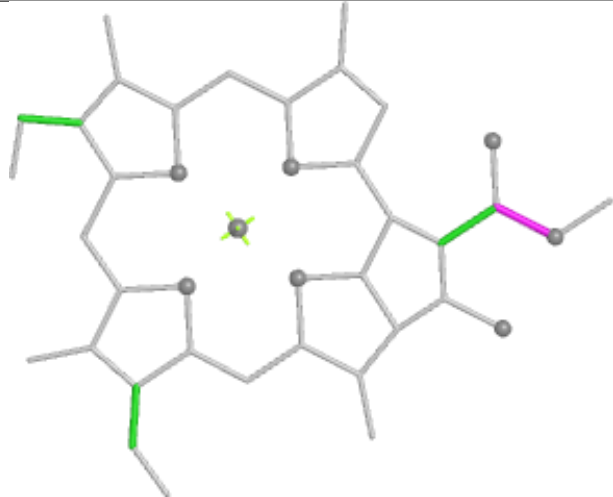
Ligand CLA AQ 614



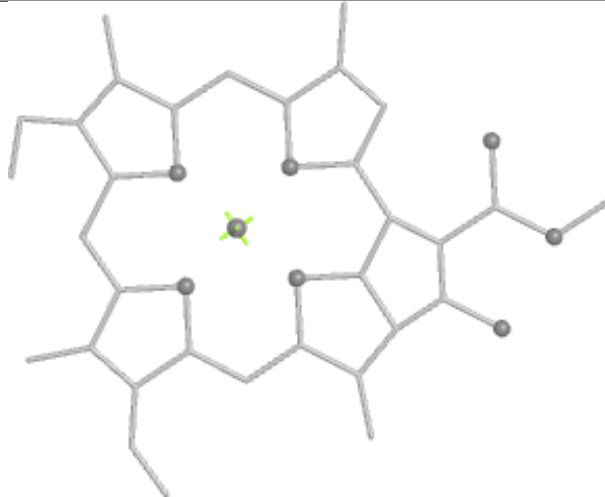
Bond lengths



Bond angles

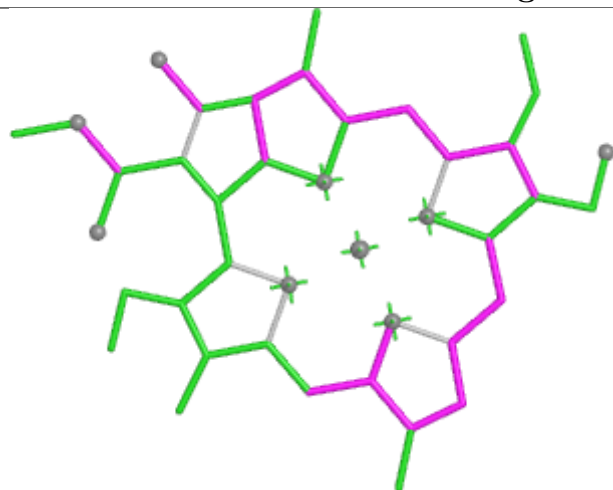


Torsions

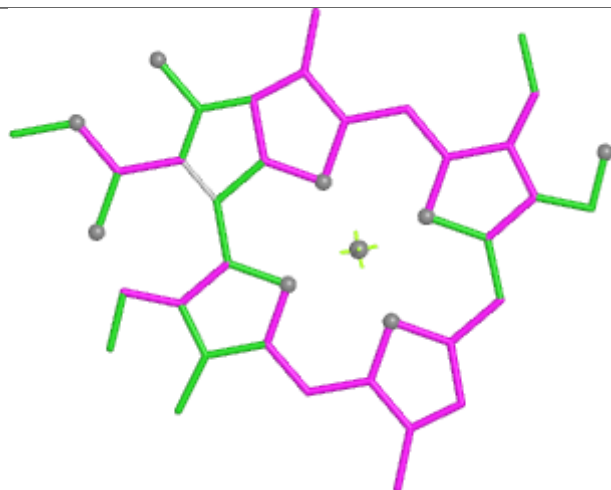


Rings

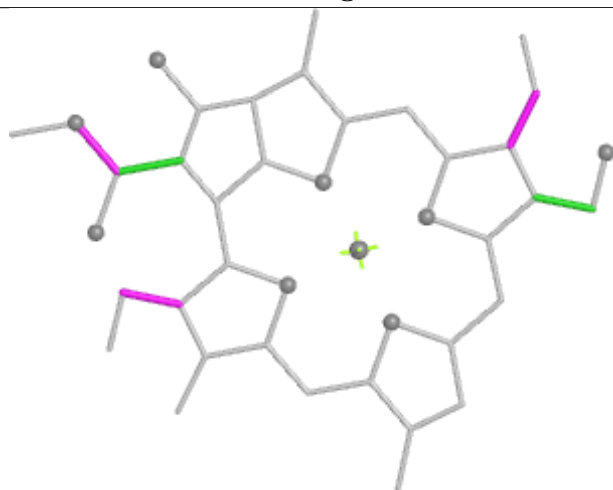
Ligand CHL 9 601



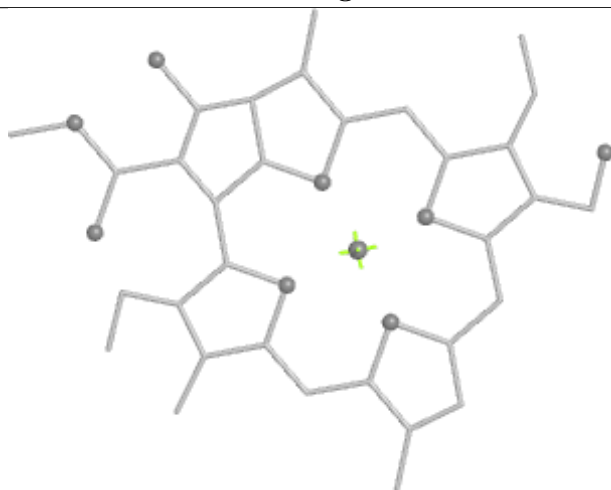
Bond lengths



Bond angles

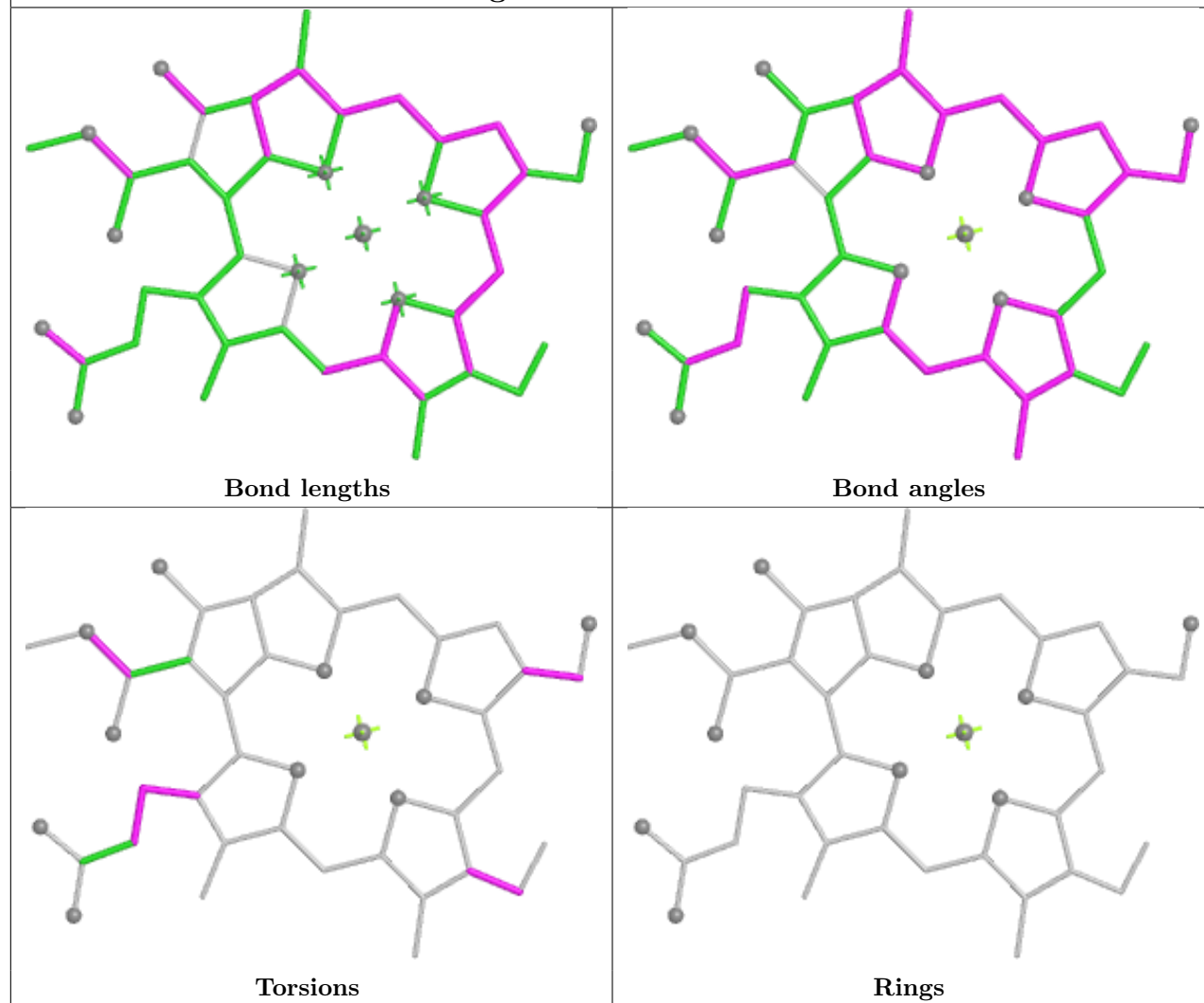


Torsions

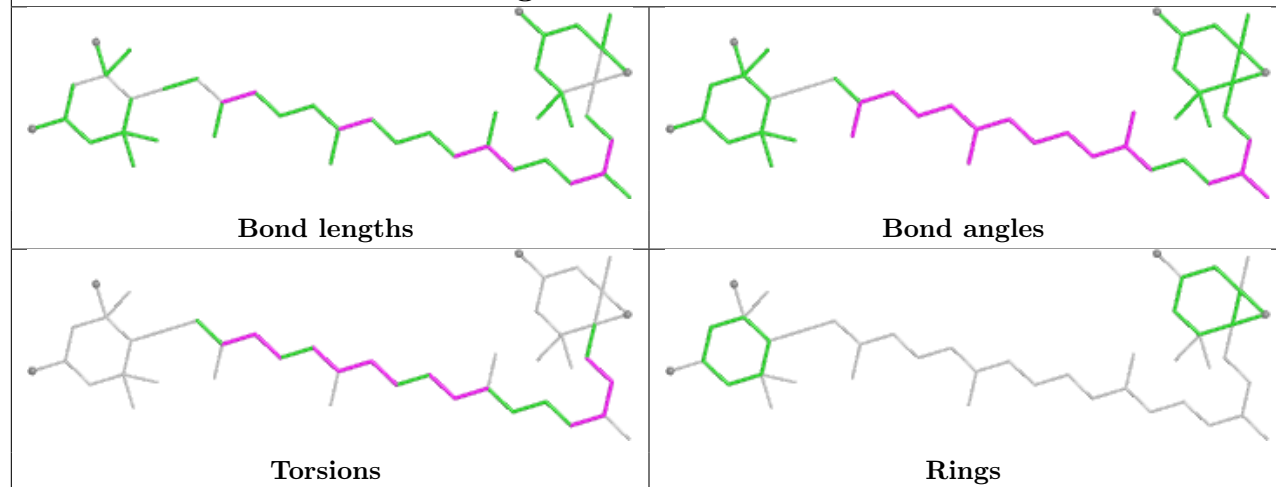


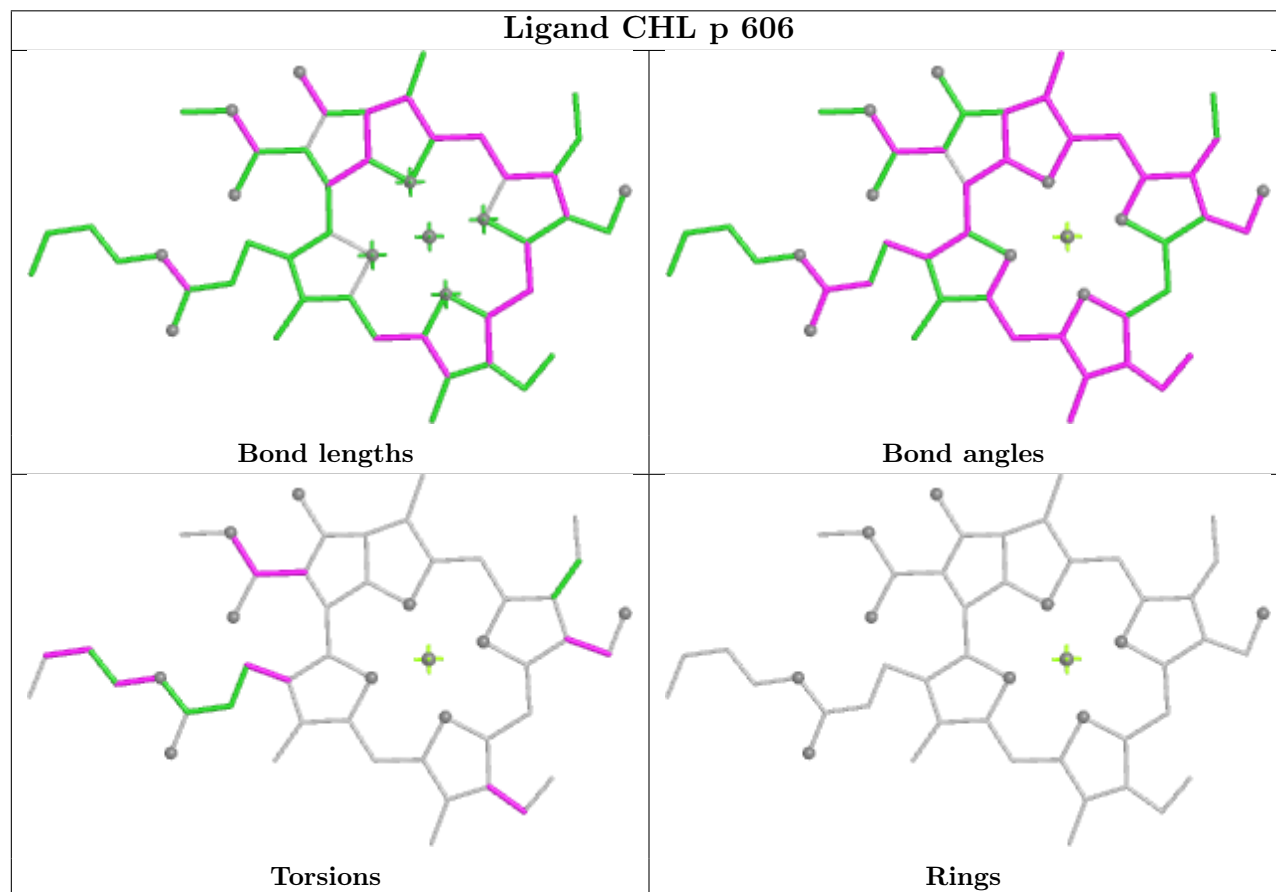
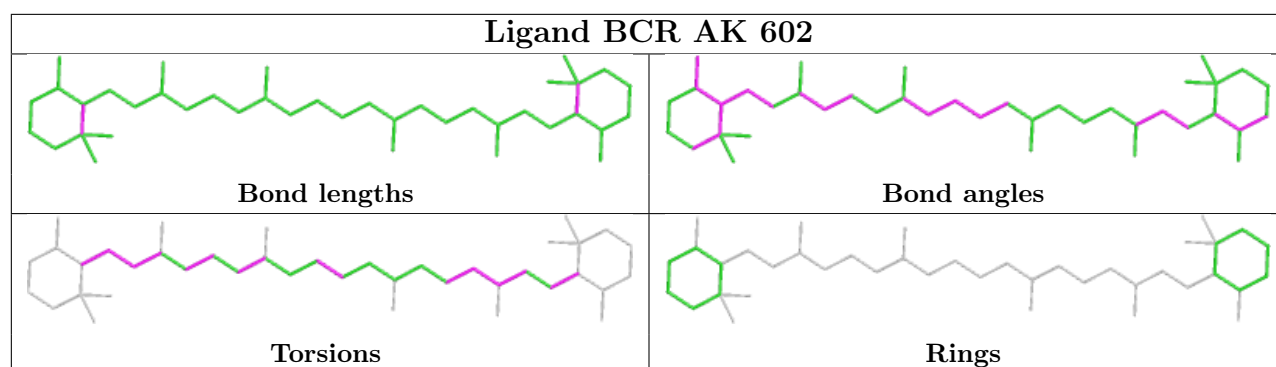
Rings

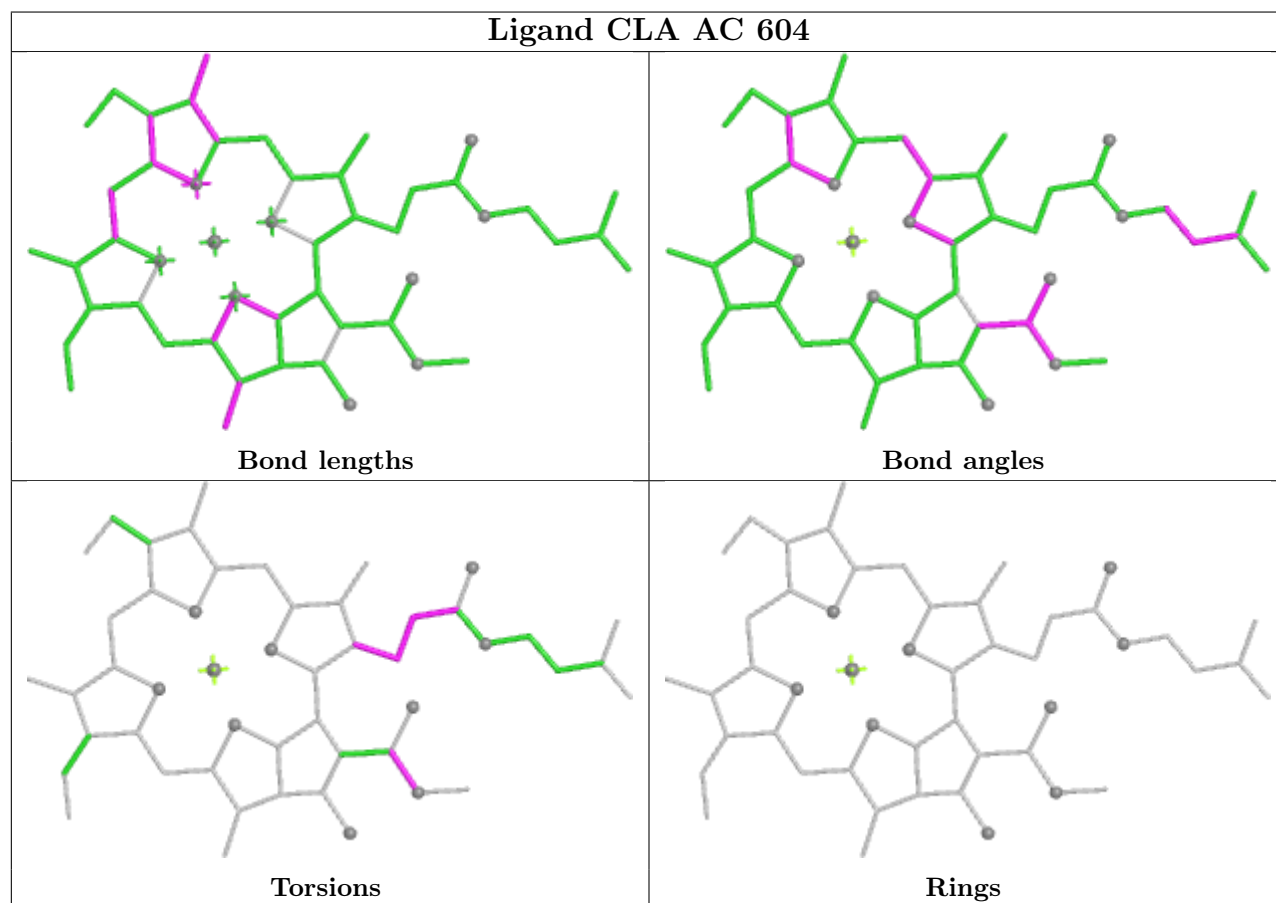
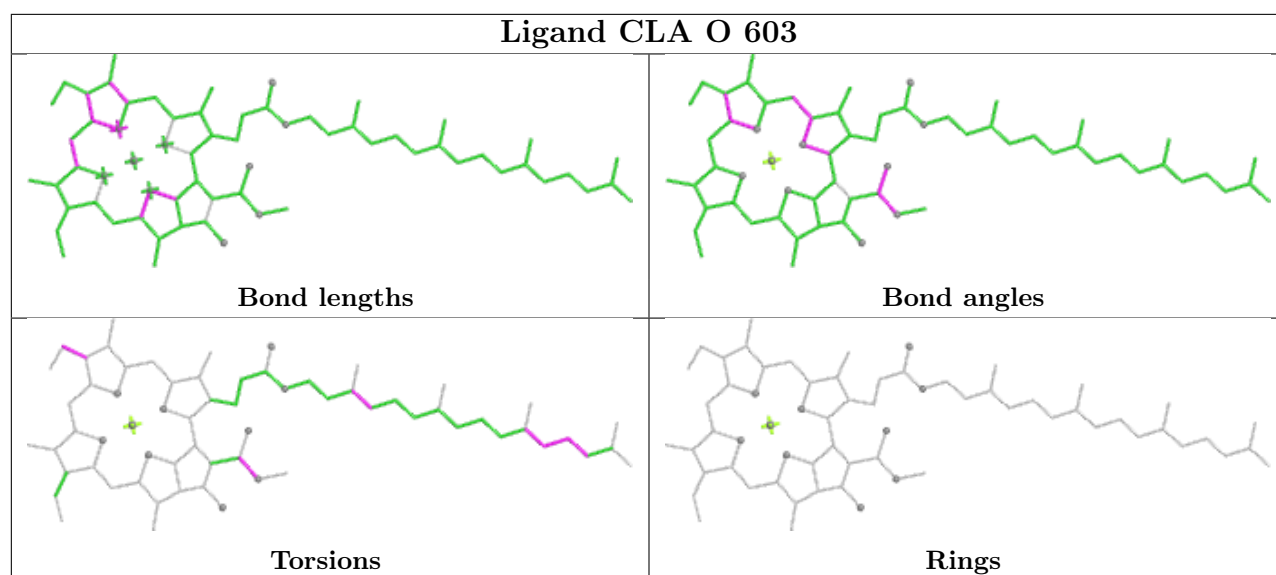
Ligand CHL AC 607

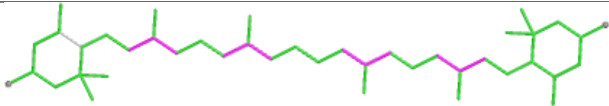
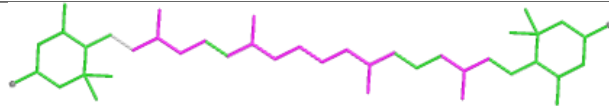
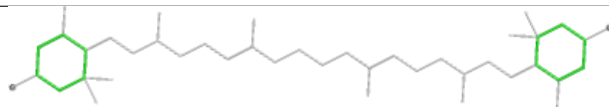


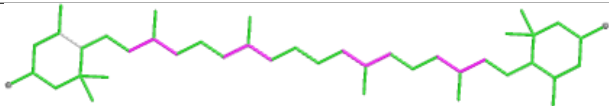
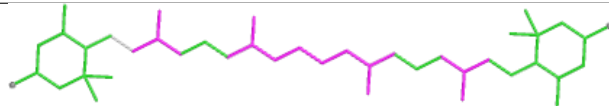
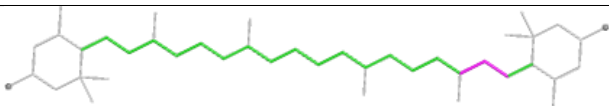
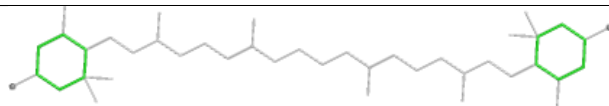
Ligand NEX AR 615

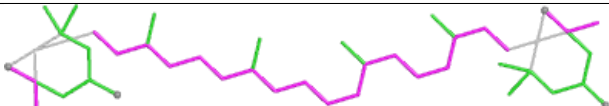
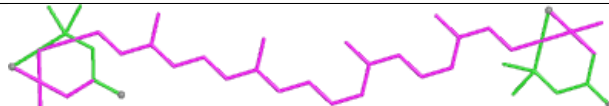
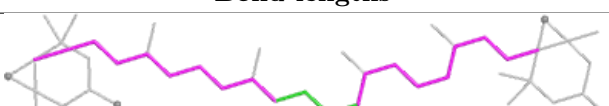
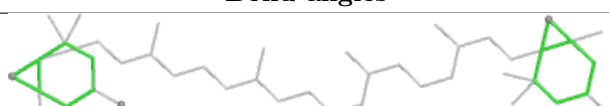


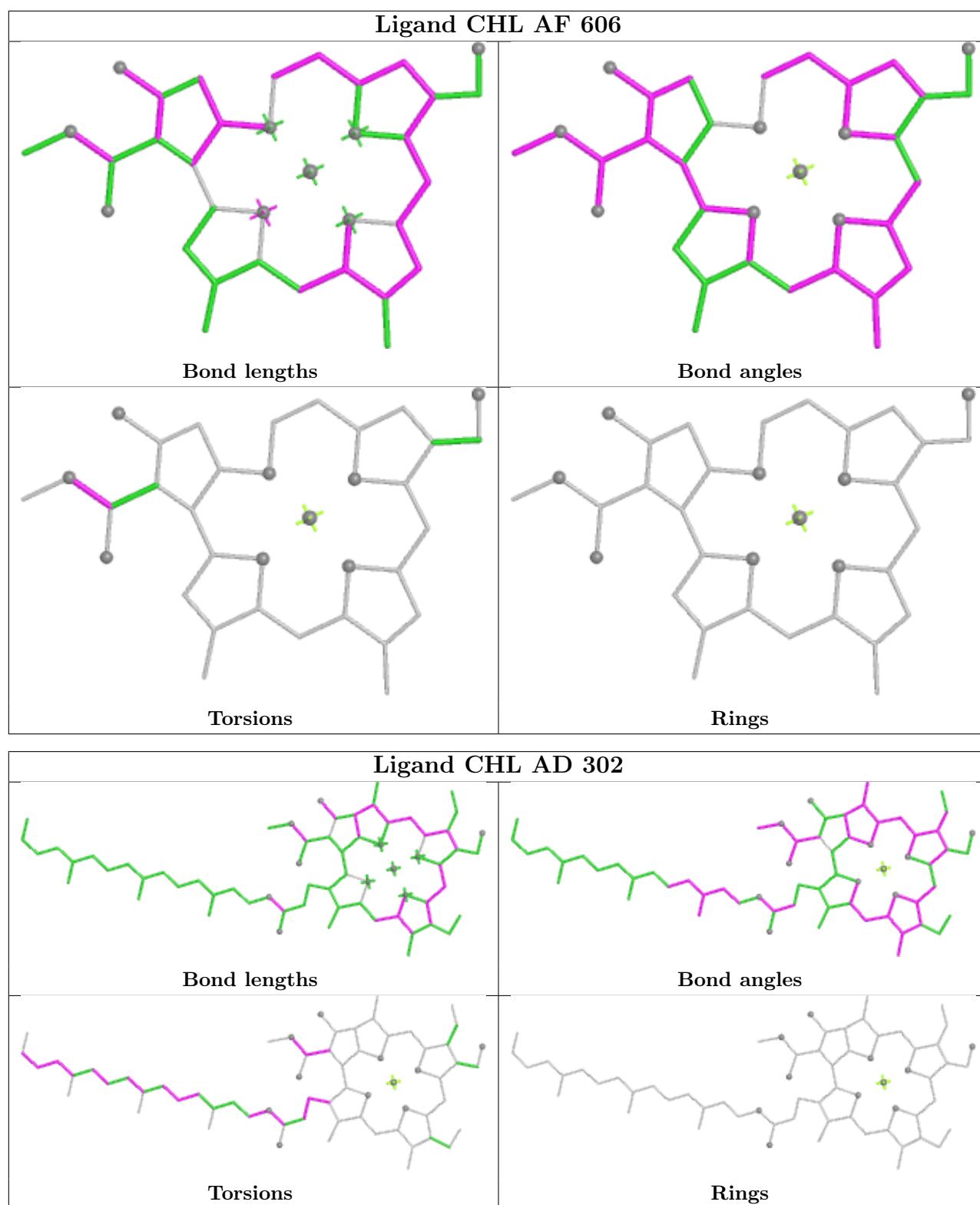




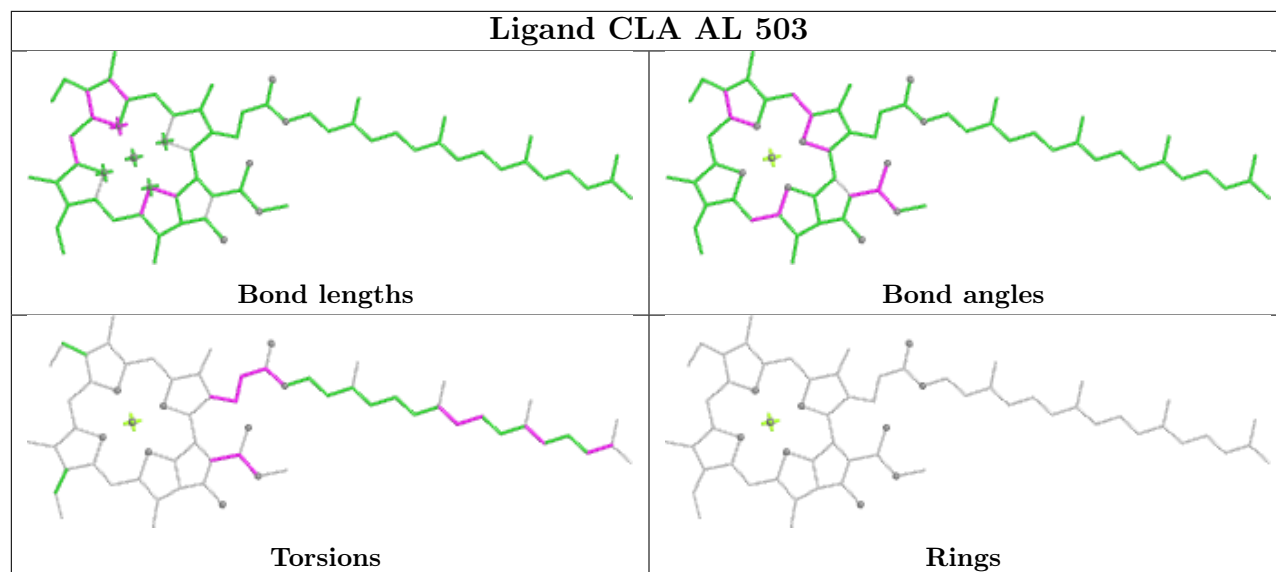
Ligand LUT 0 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT AC 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

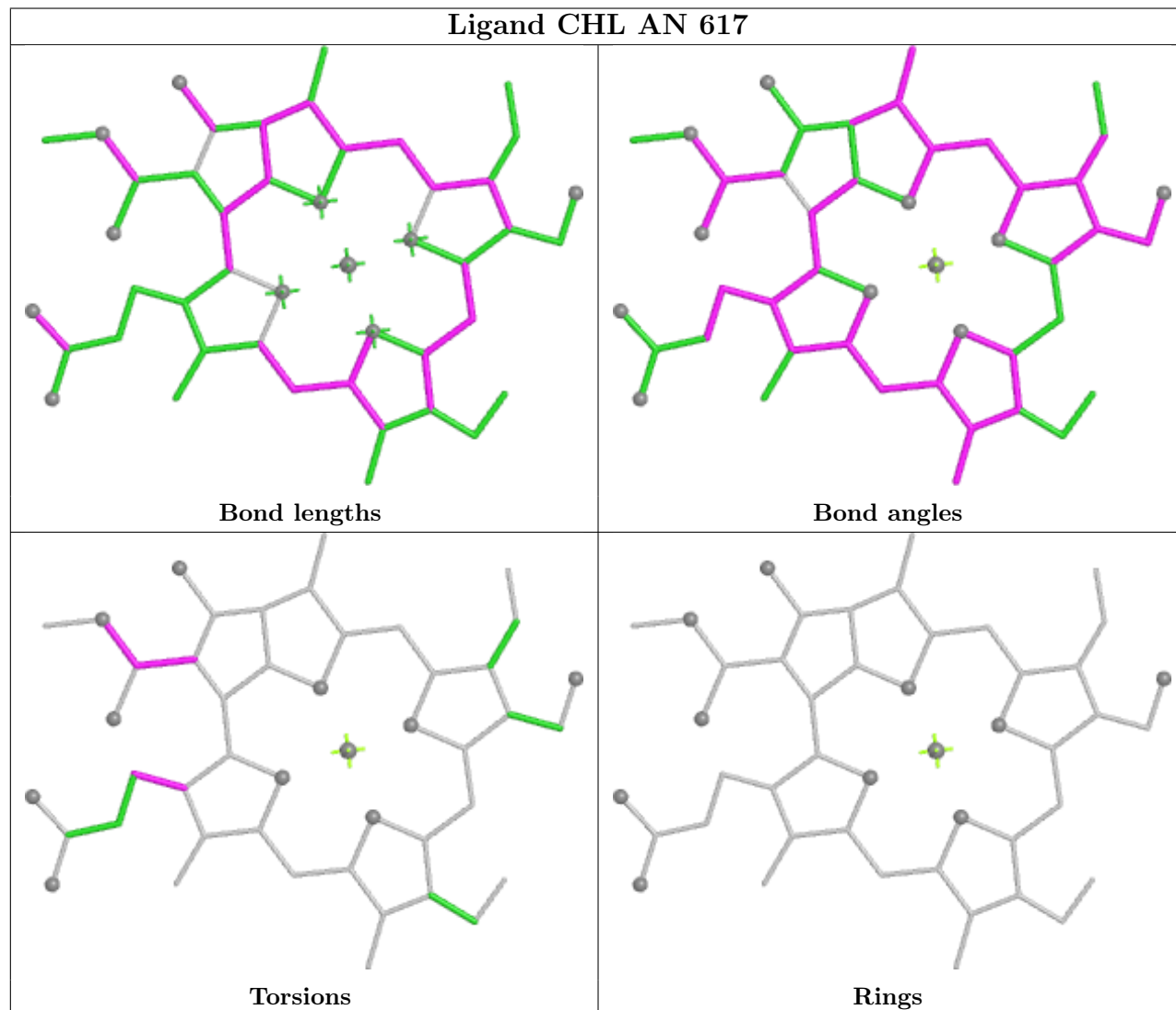
Ligand XAT AR 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

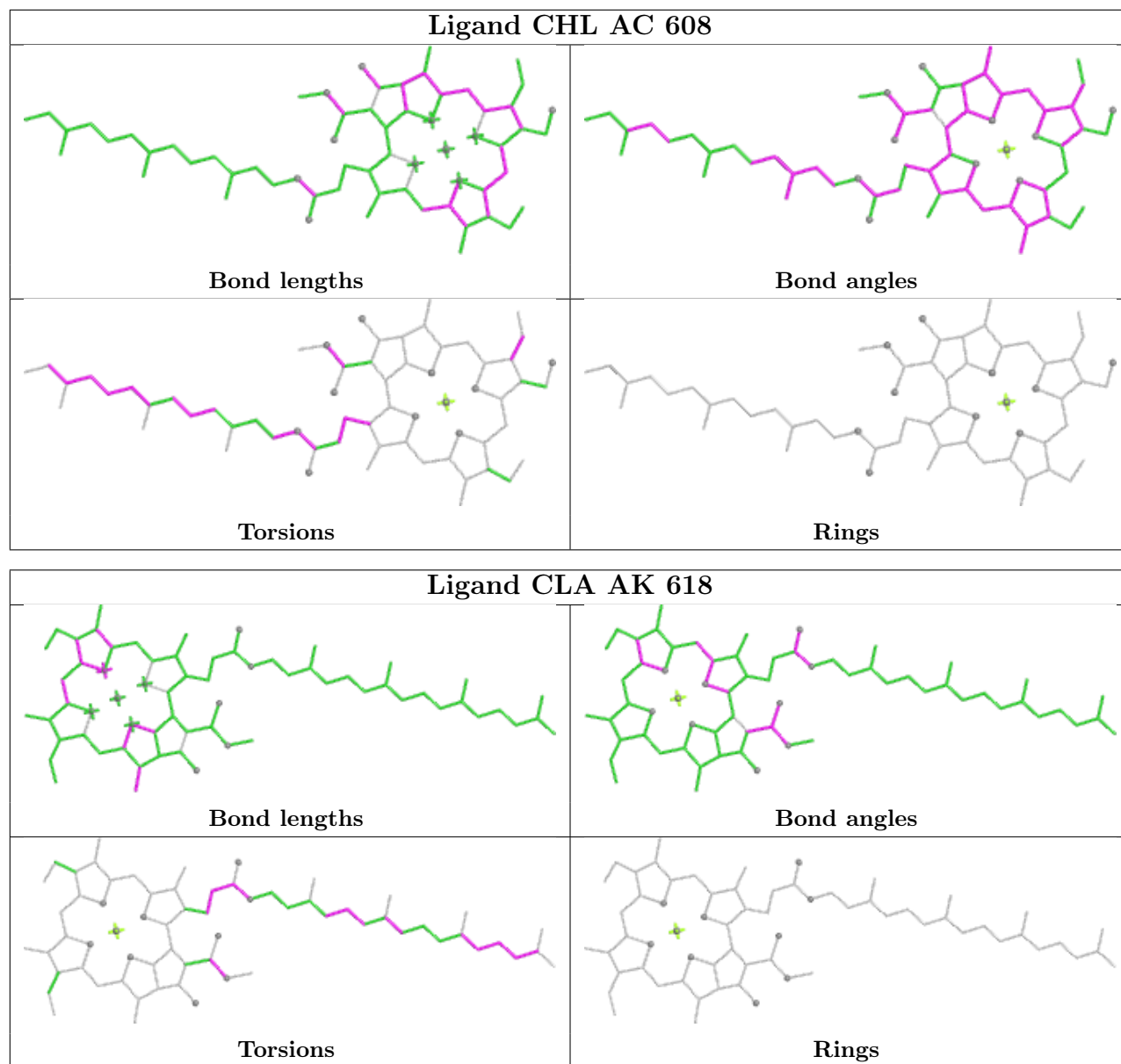


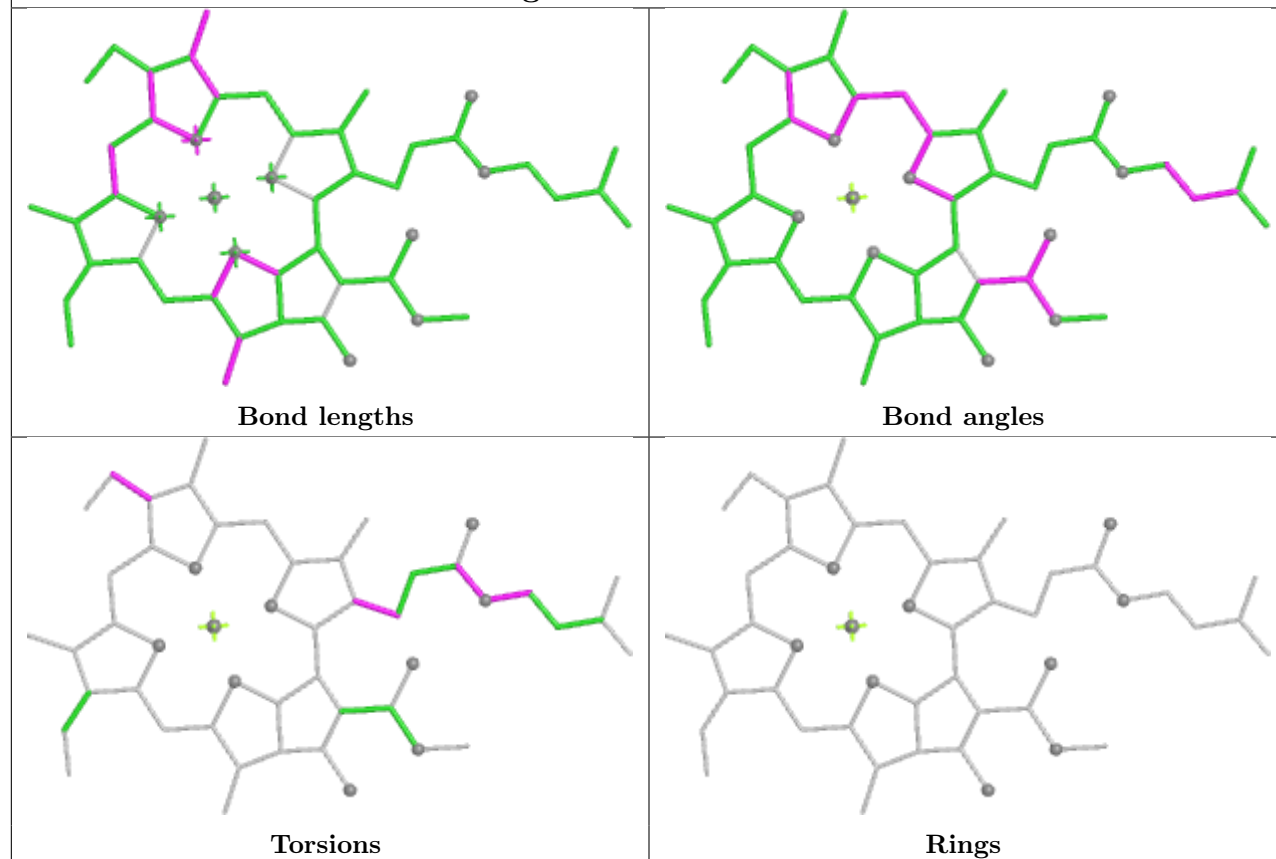
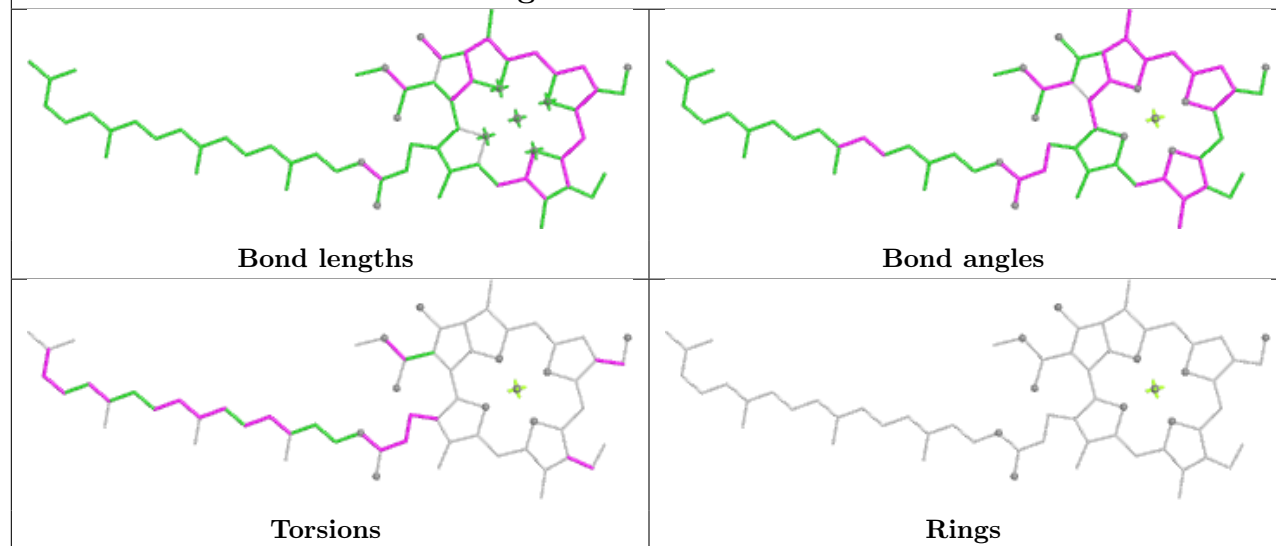
Ligand CLA AL 503

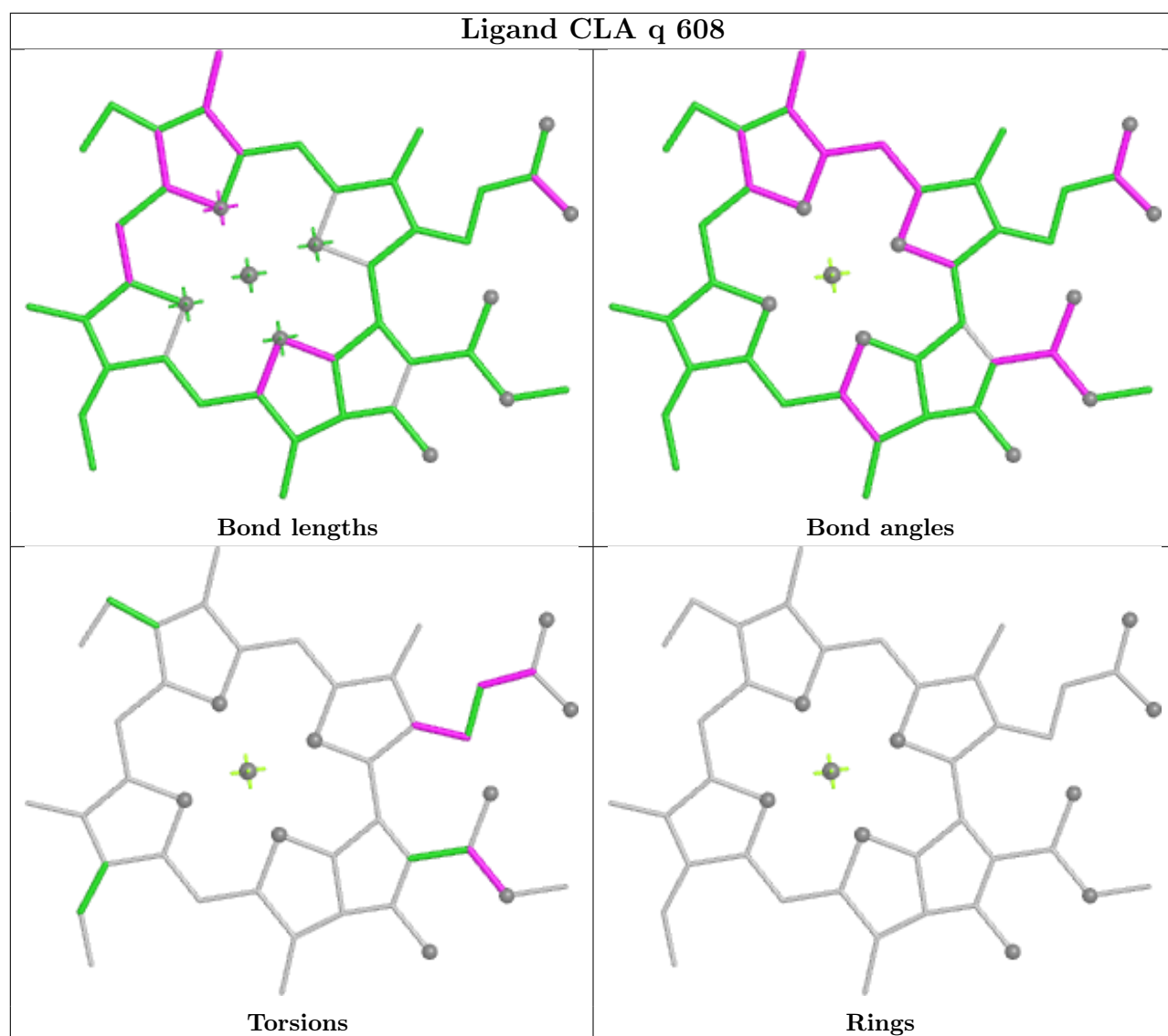


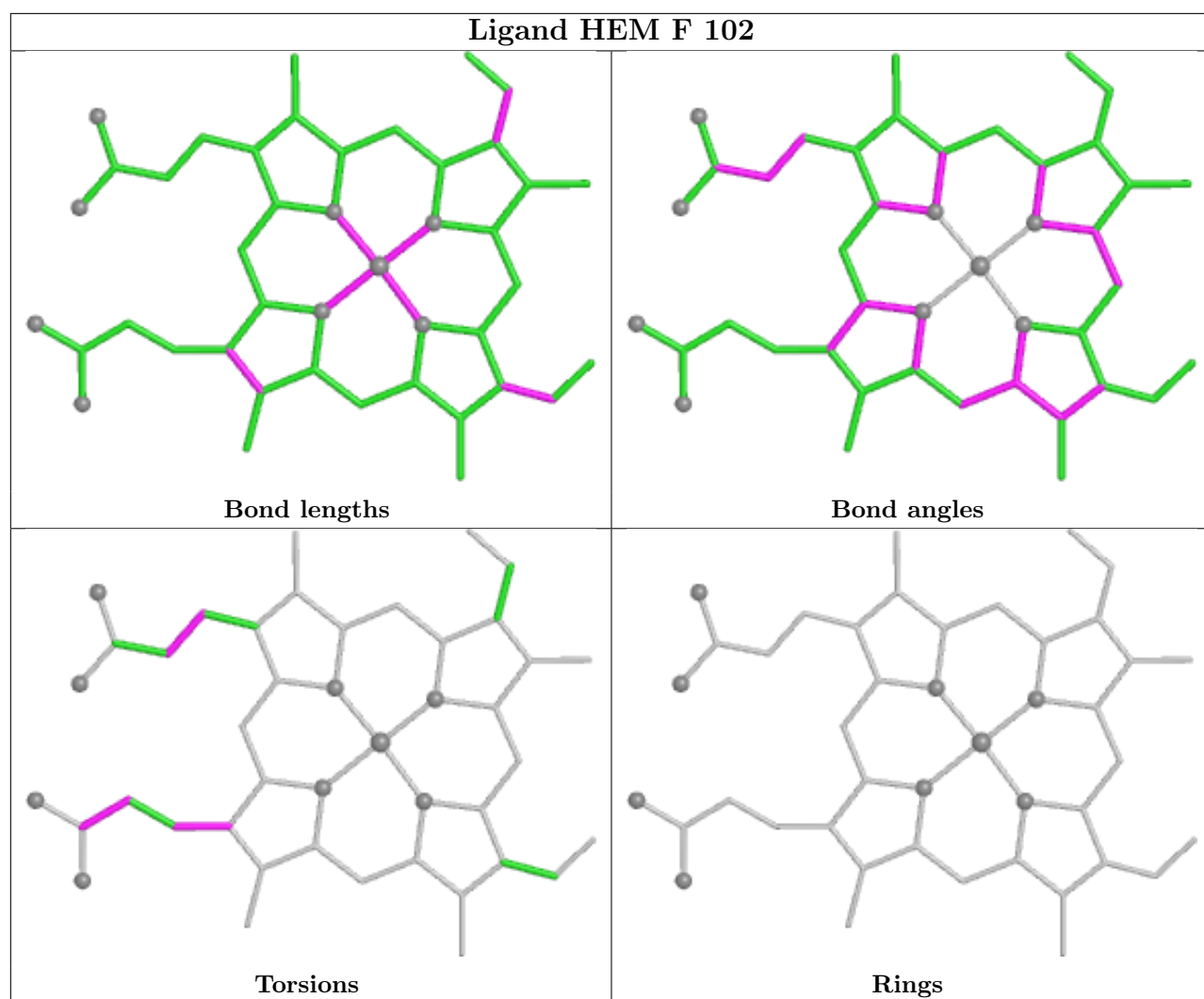
Ligand CHL AN 617



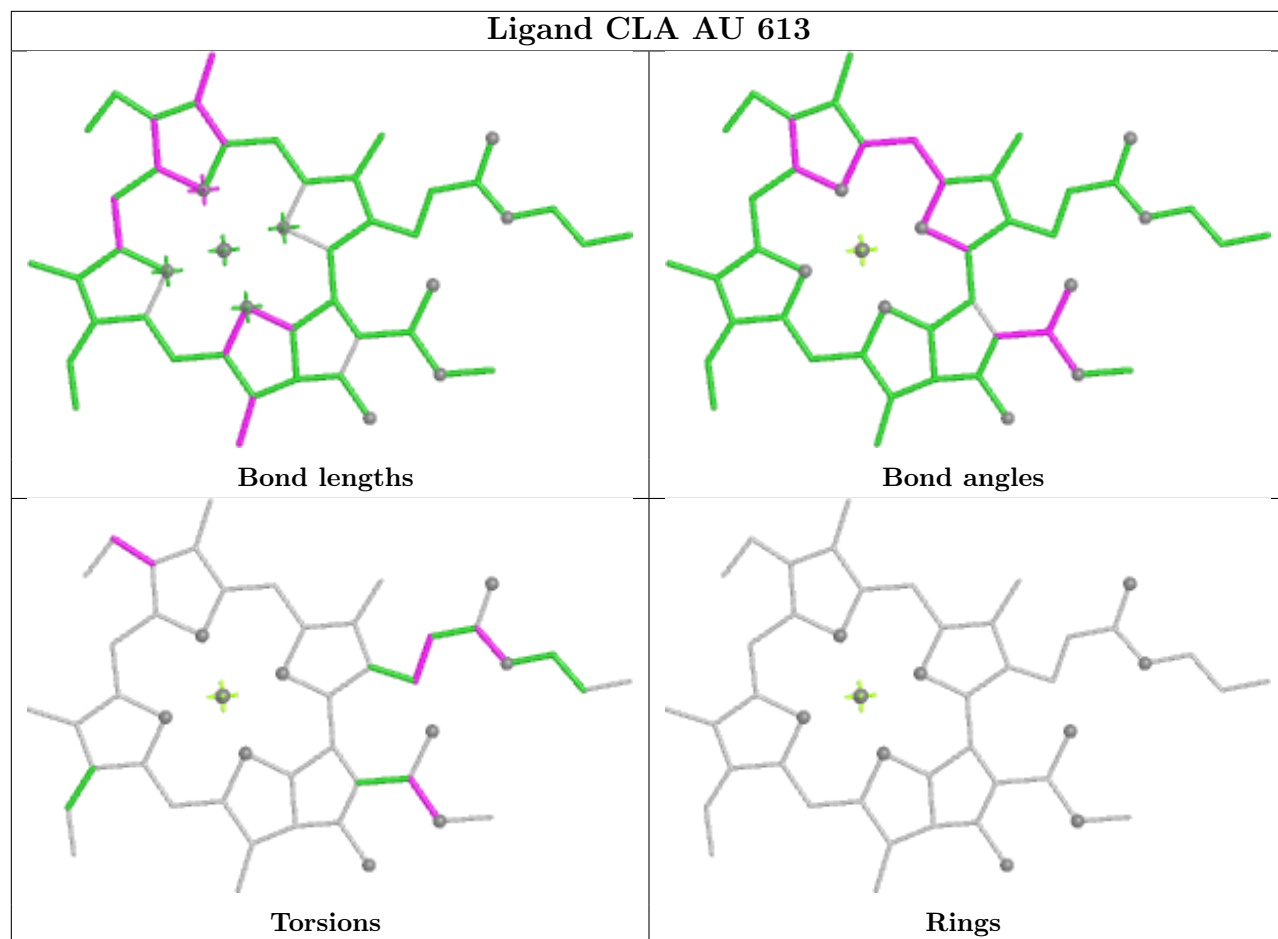


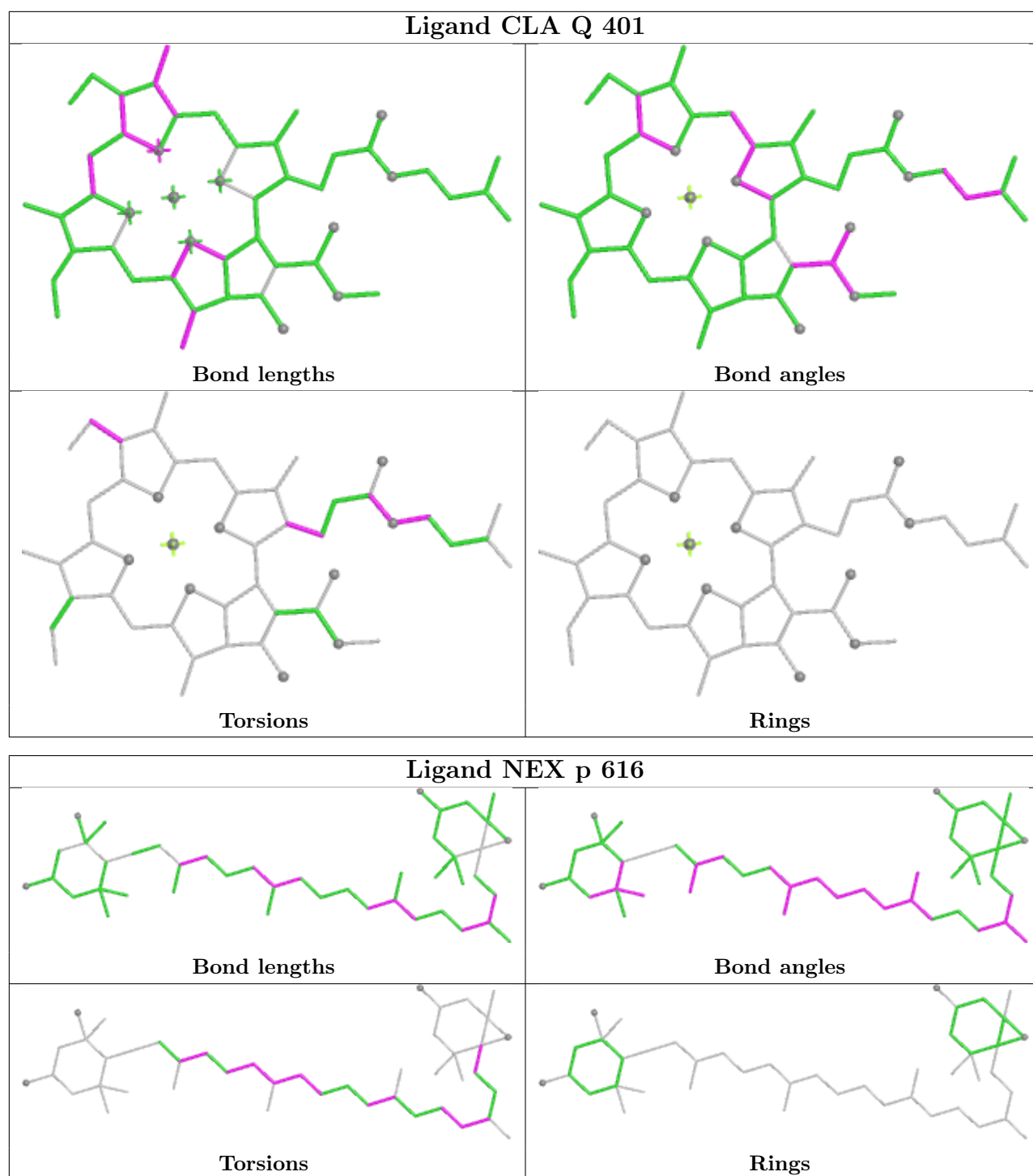
Ligand CLA AJ 406**Ligand CHL AR 605**



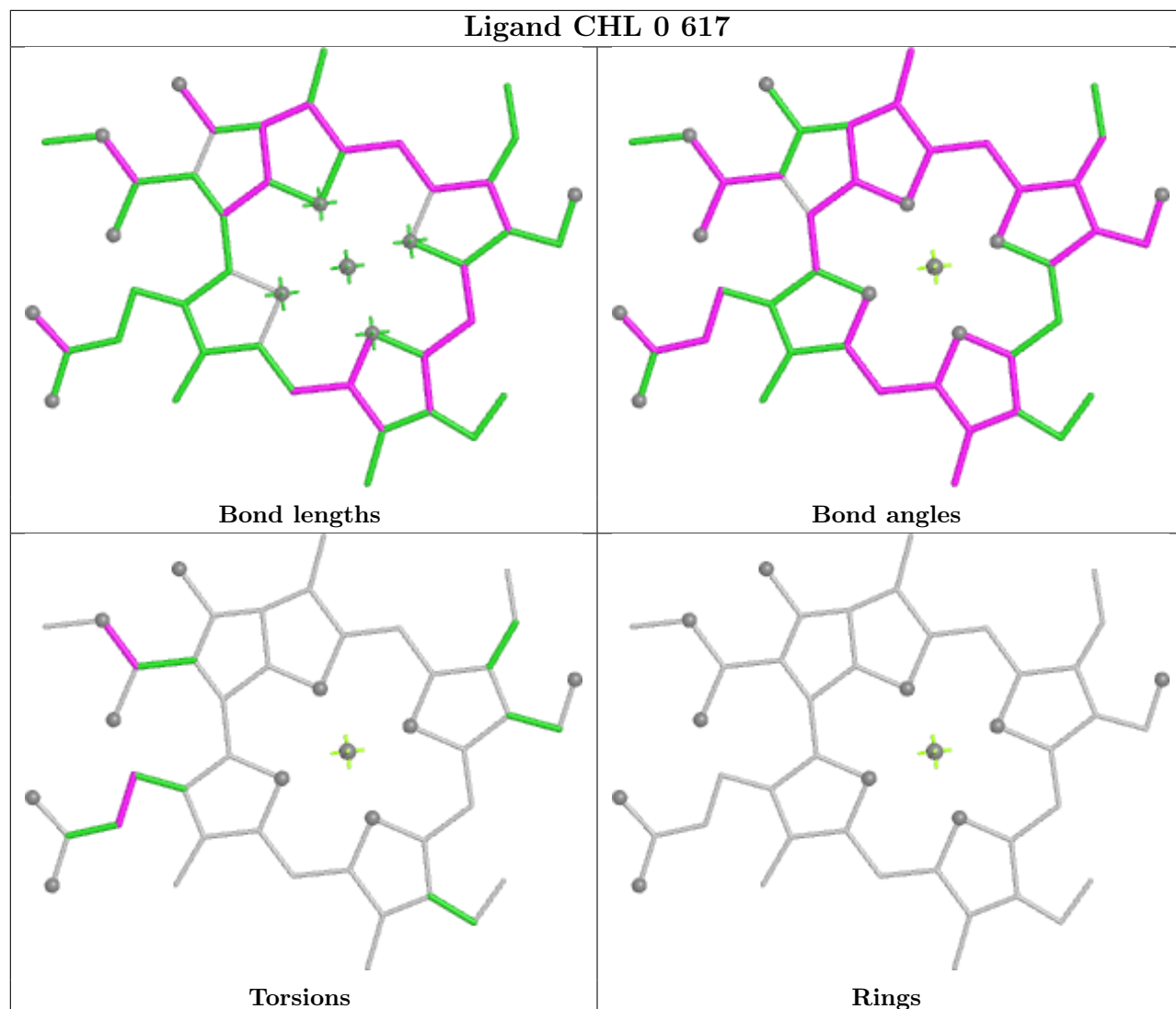


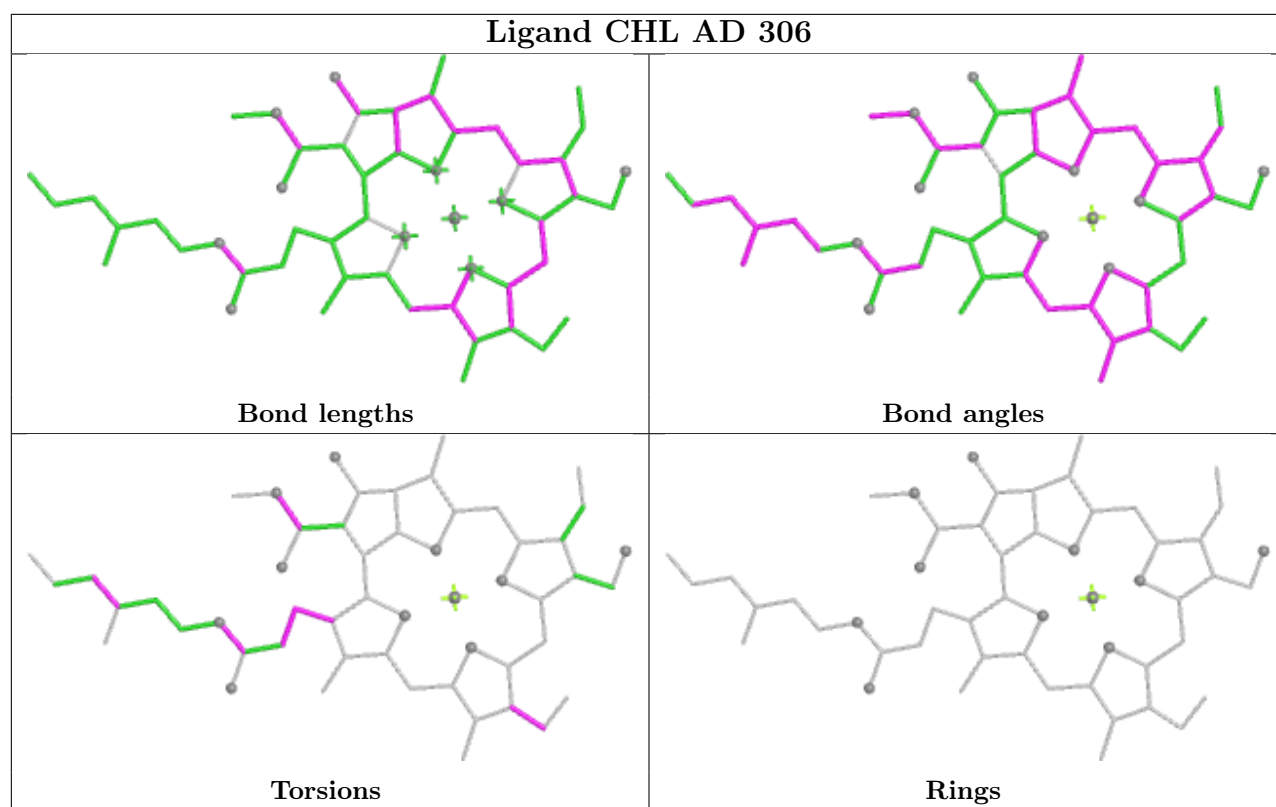
Ligand CLA AU 613



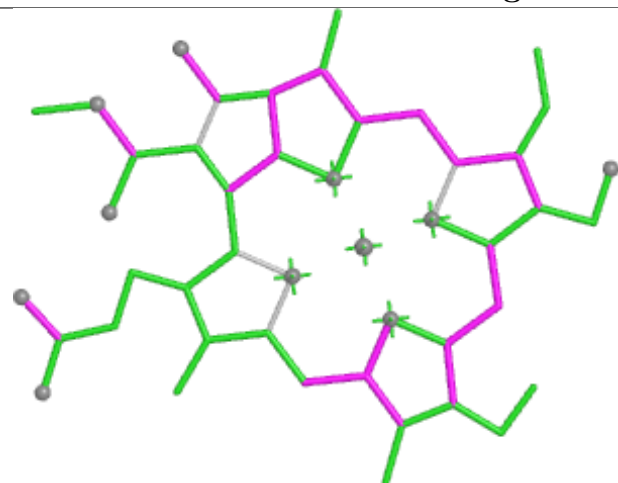


Ligand CHL 0 617

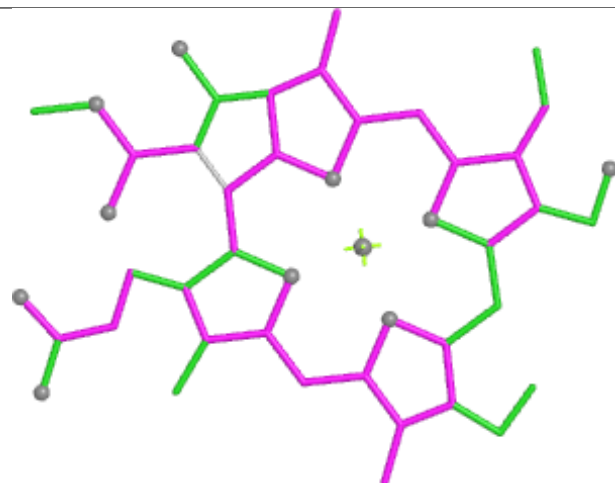




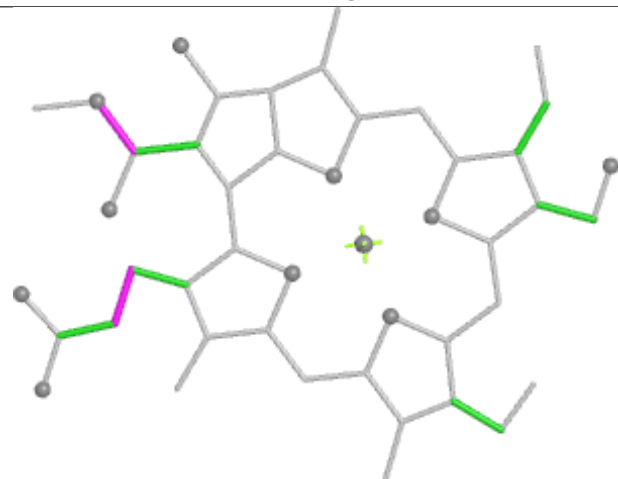
Ligand CHL AD 317



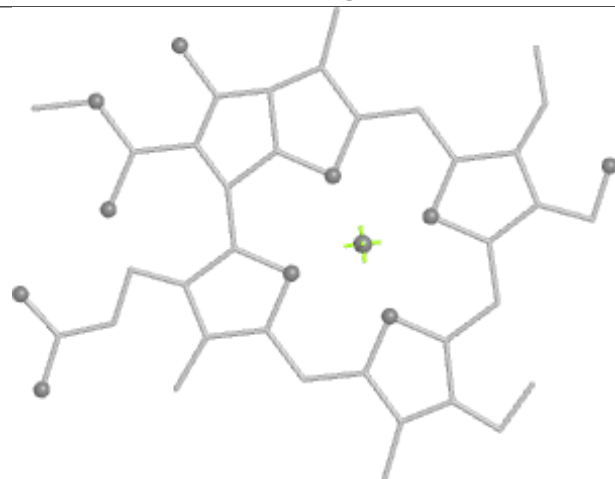
Bond lengths



Bond angles

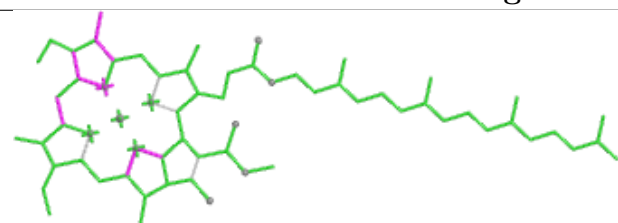


Torsions

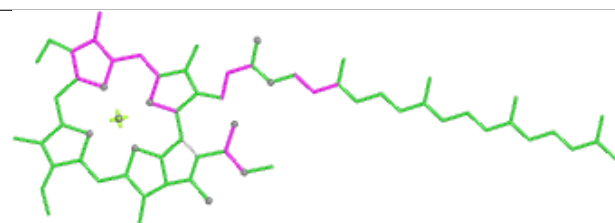


Rings

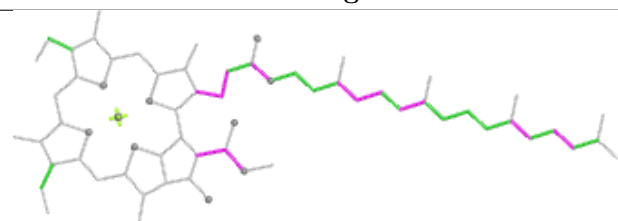
Ligand CLA AN 612



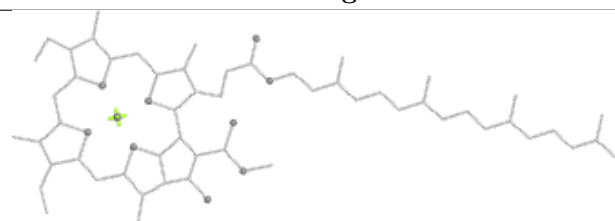
Bond lengths



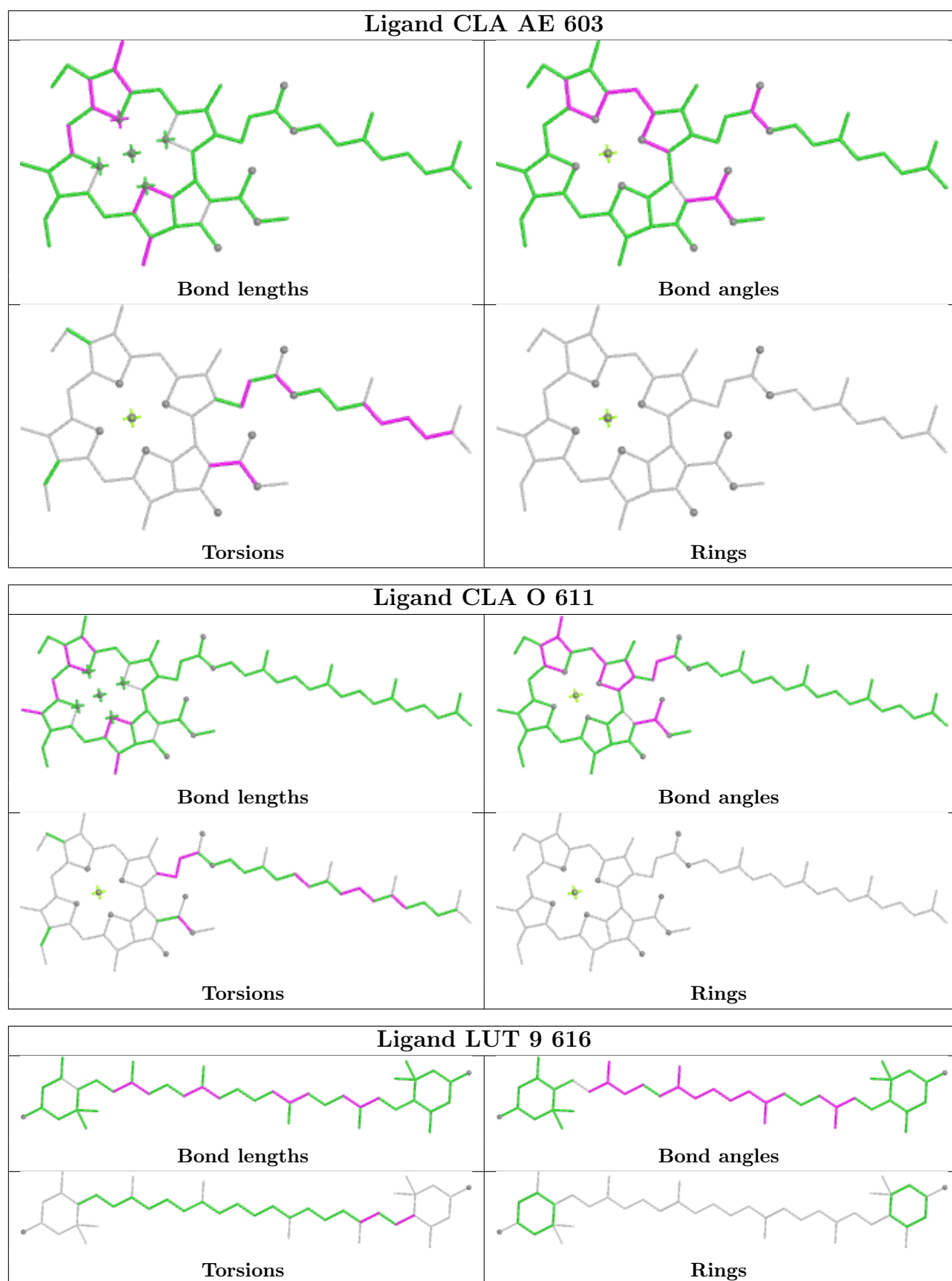
Bond angles

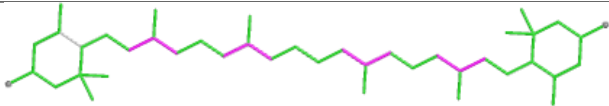
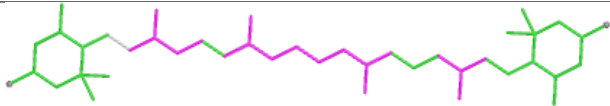
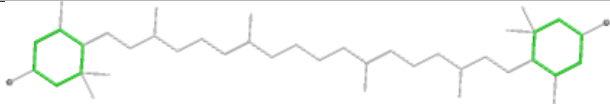


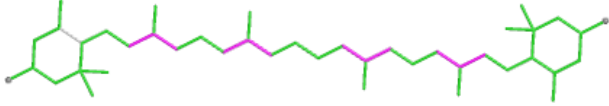
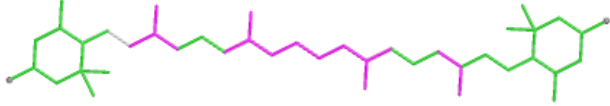
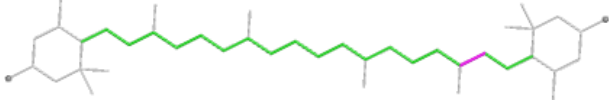
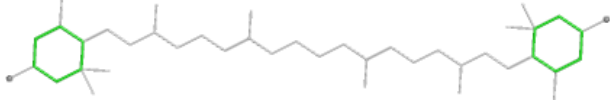
Torsions



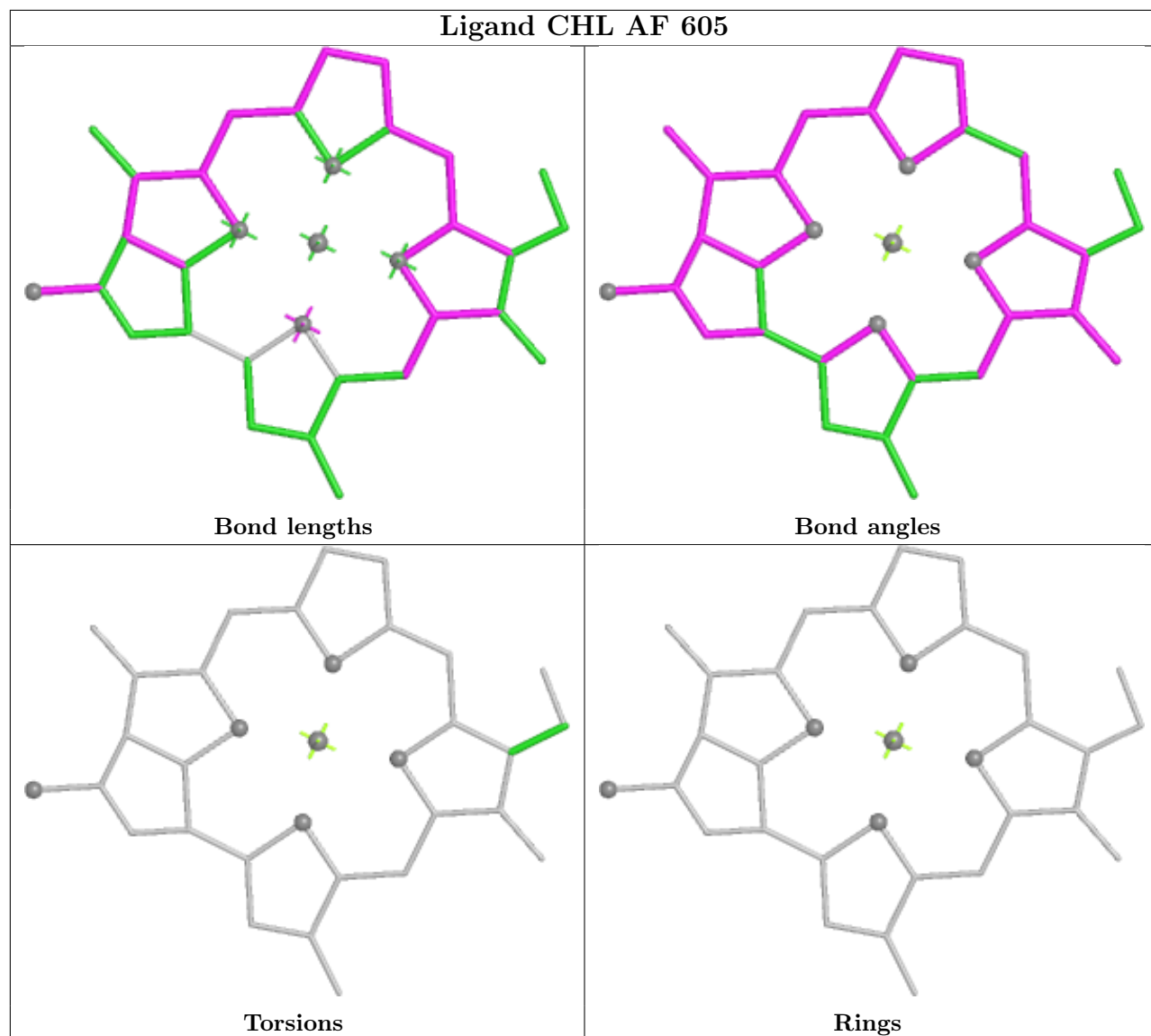
Rings

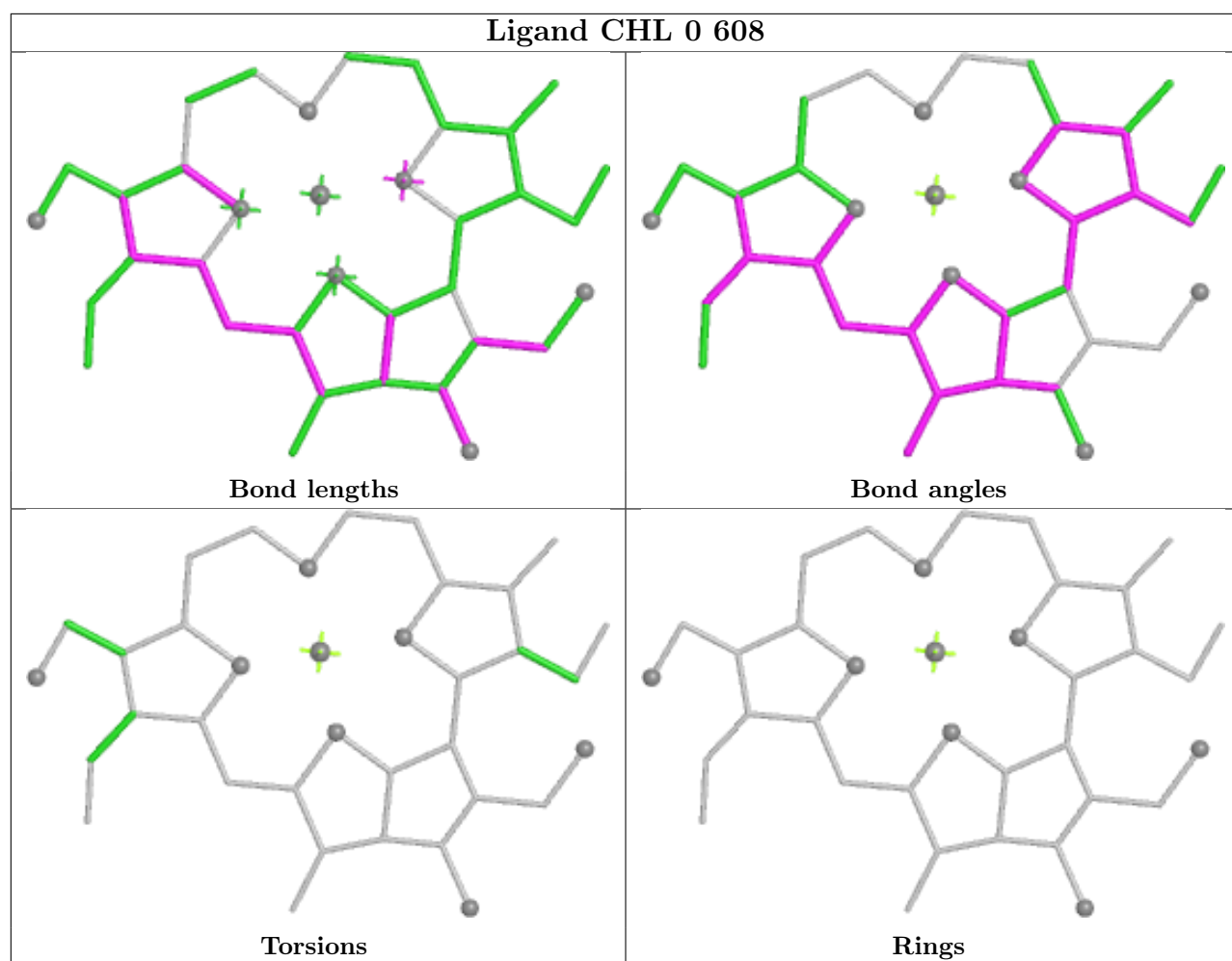


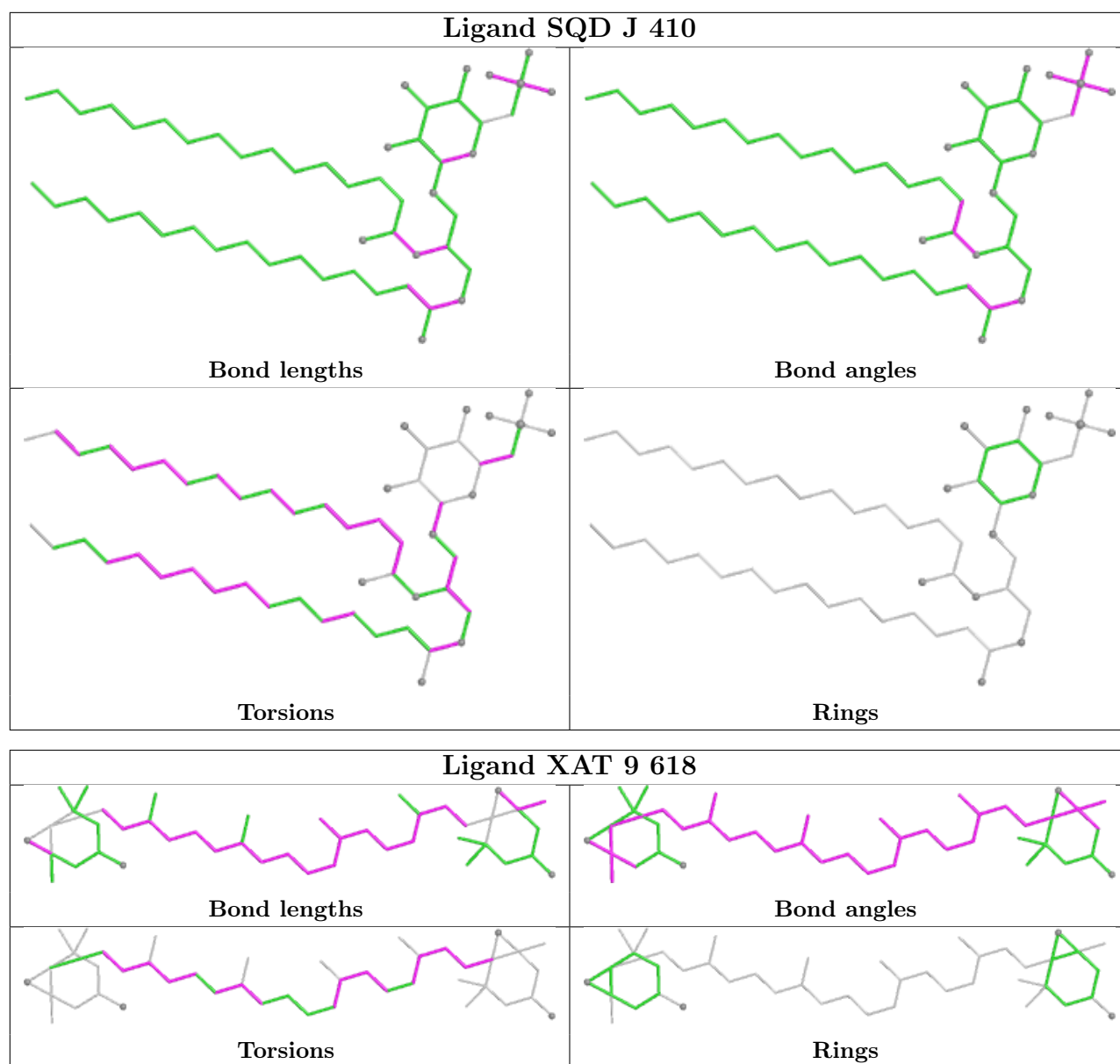
Ligand LUT AN 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT AU 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

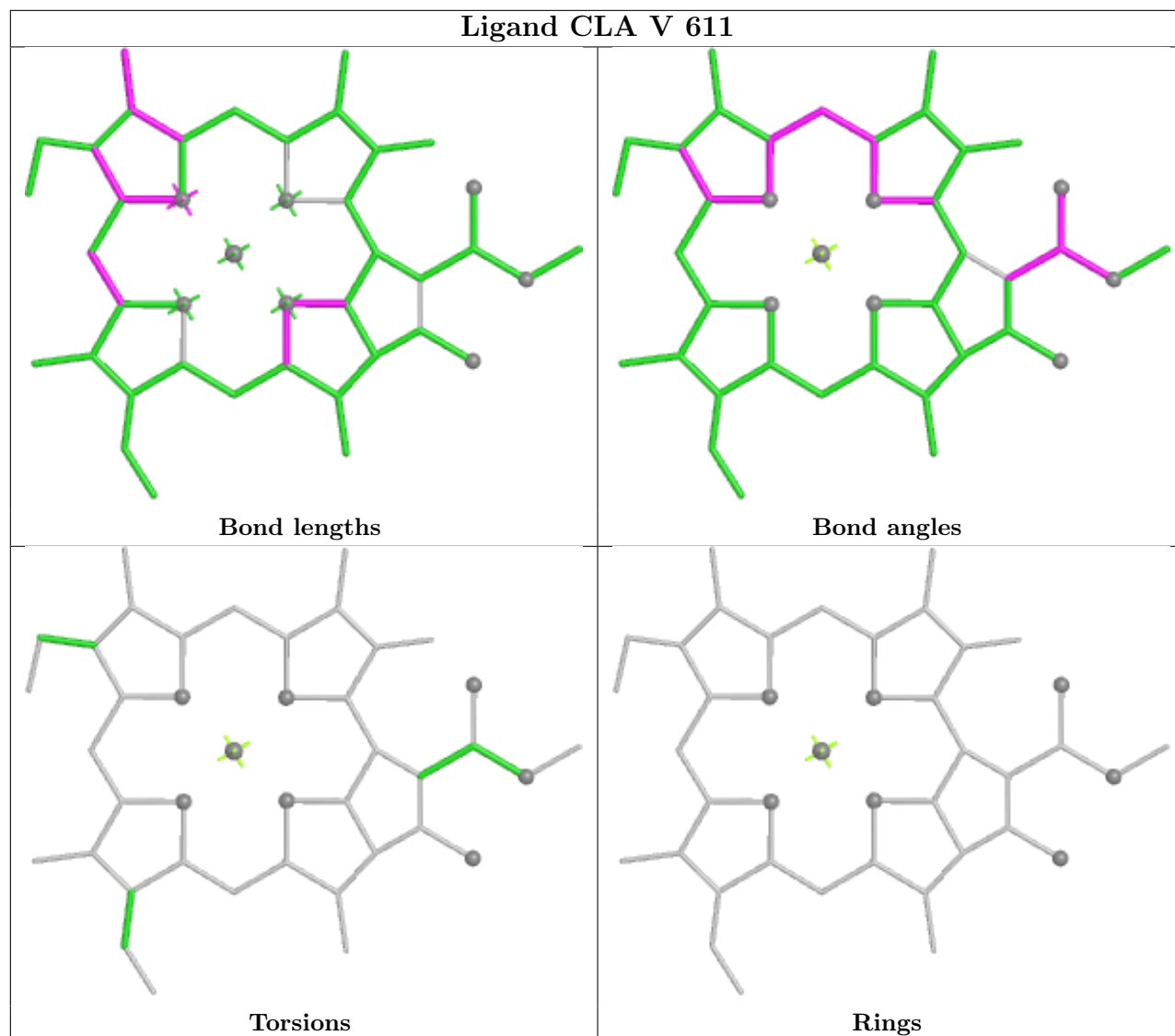
Ligand CHL AF 605



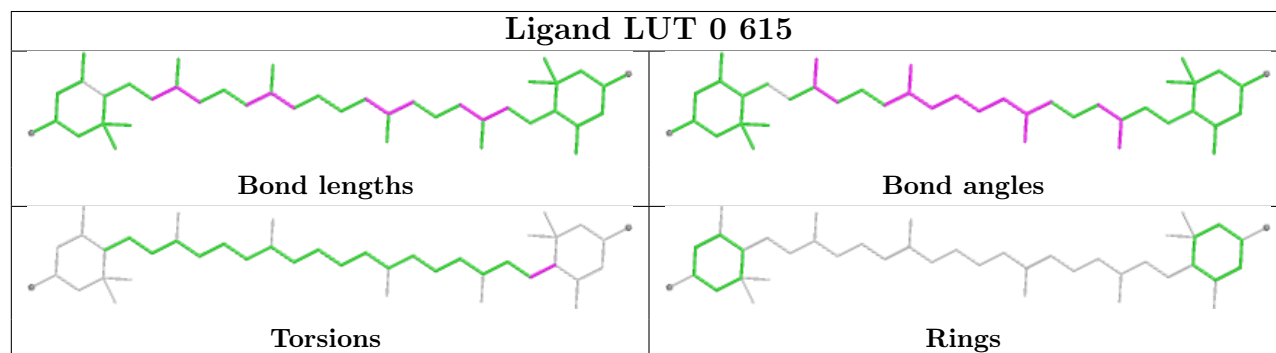


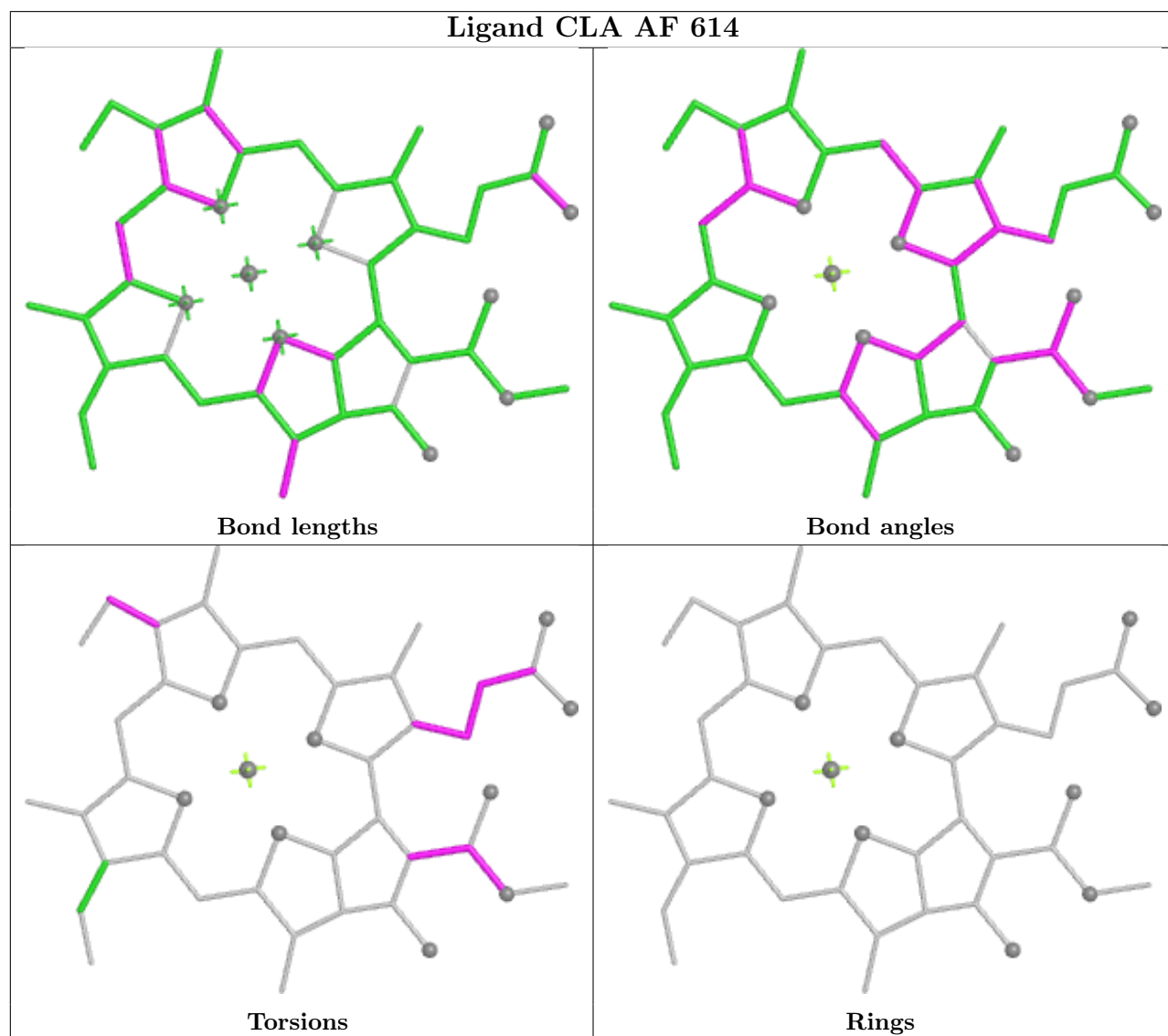
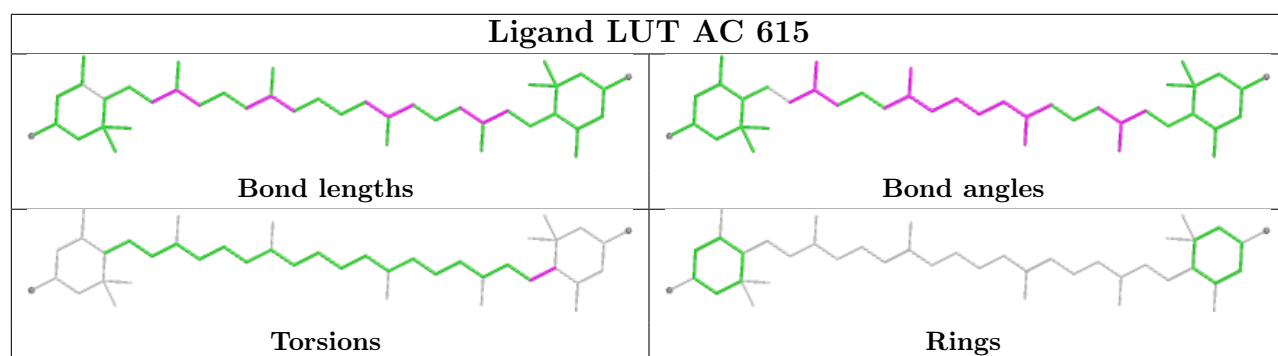


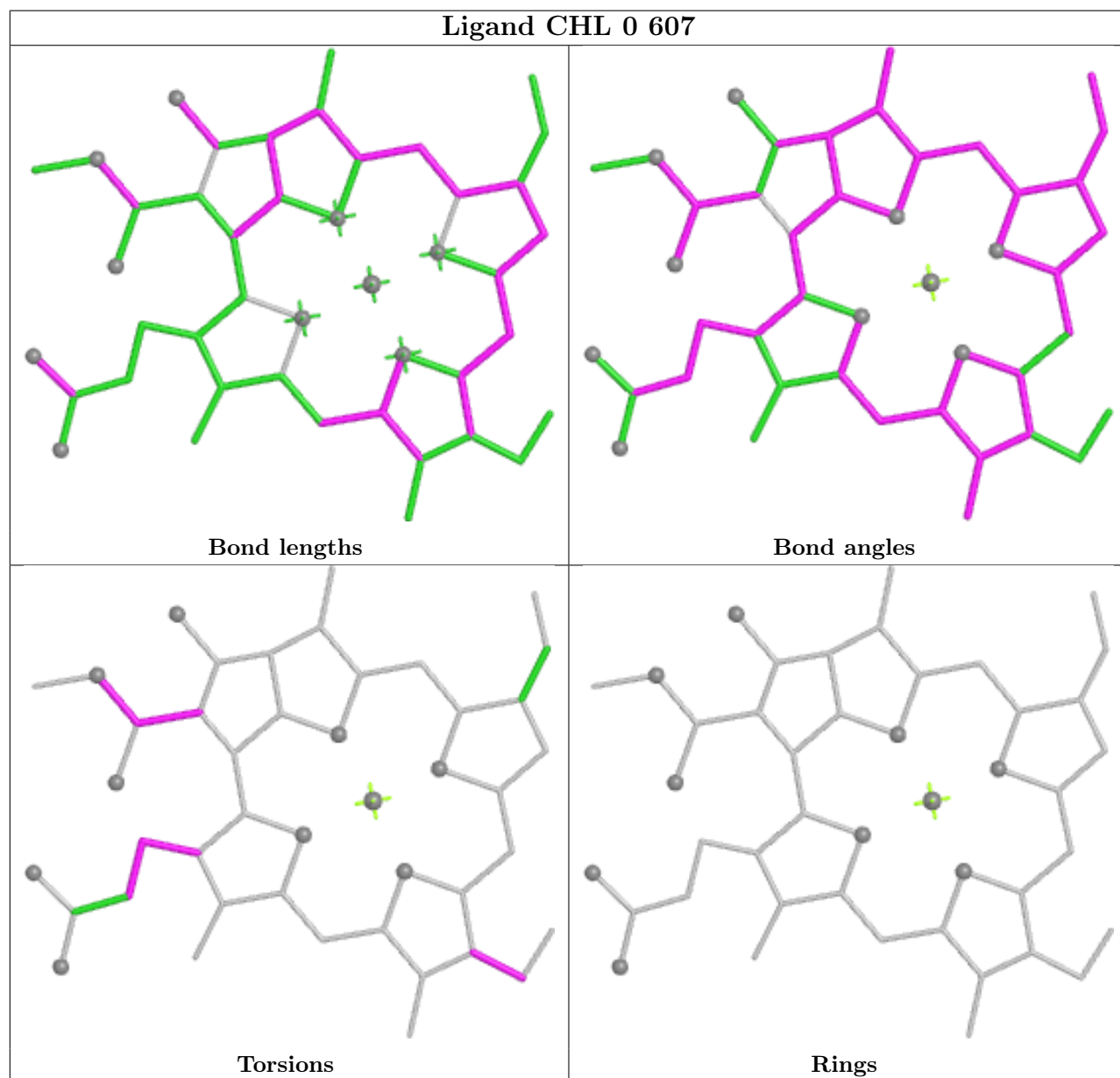
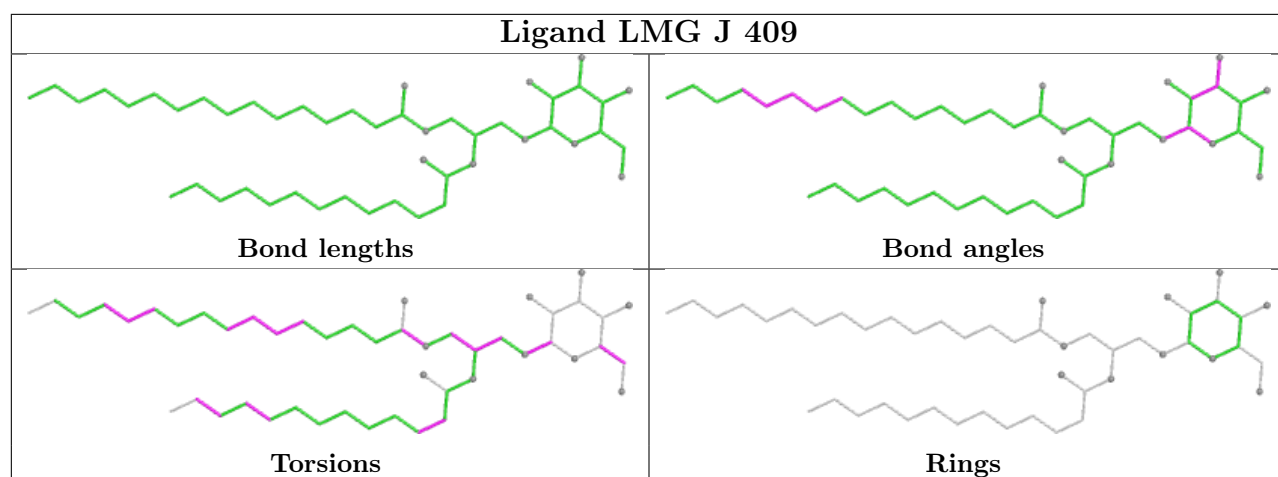
Ligand CLA V 611

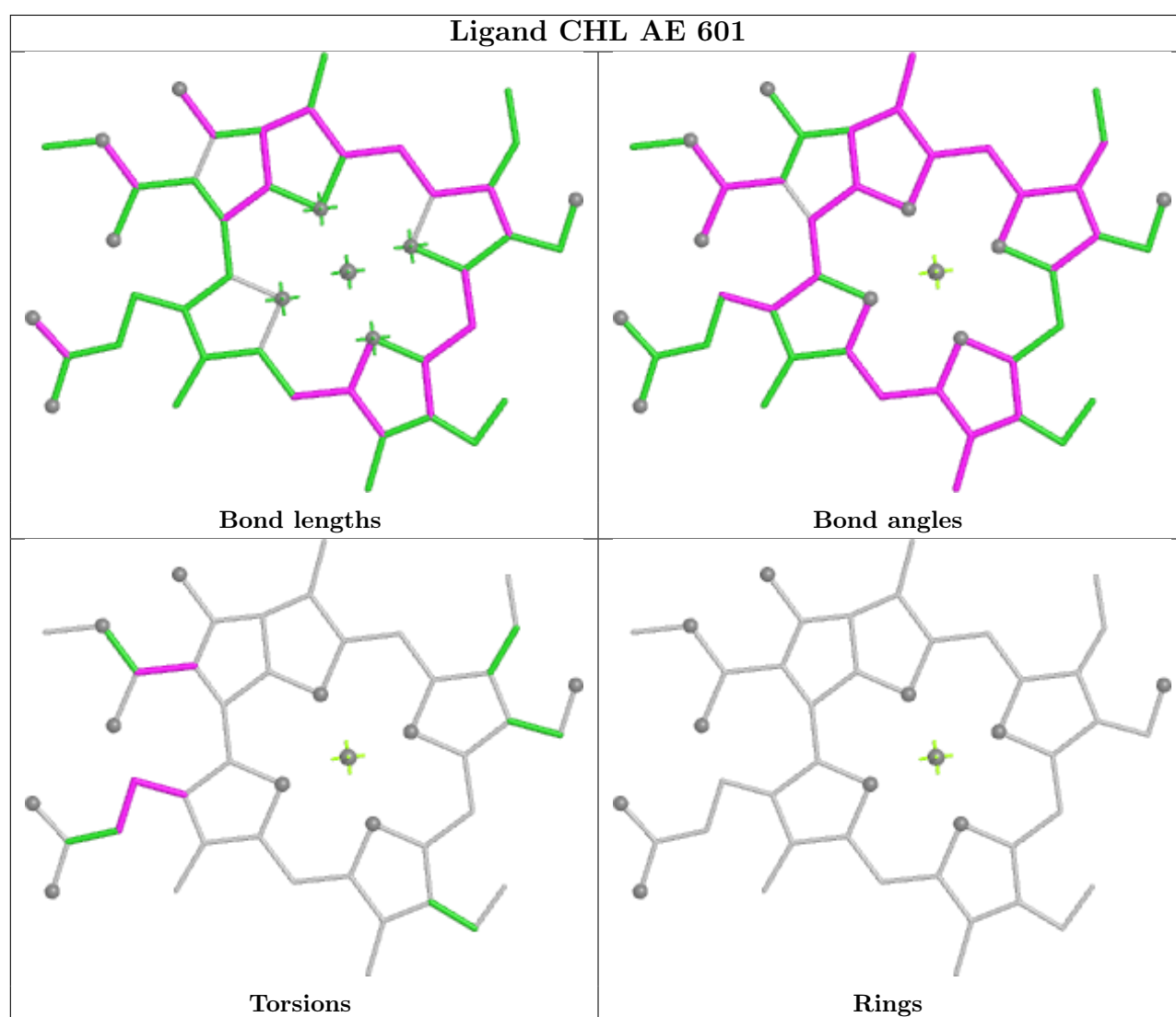
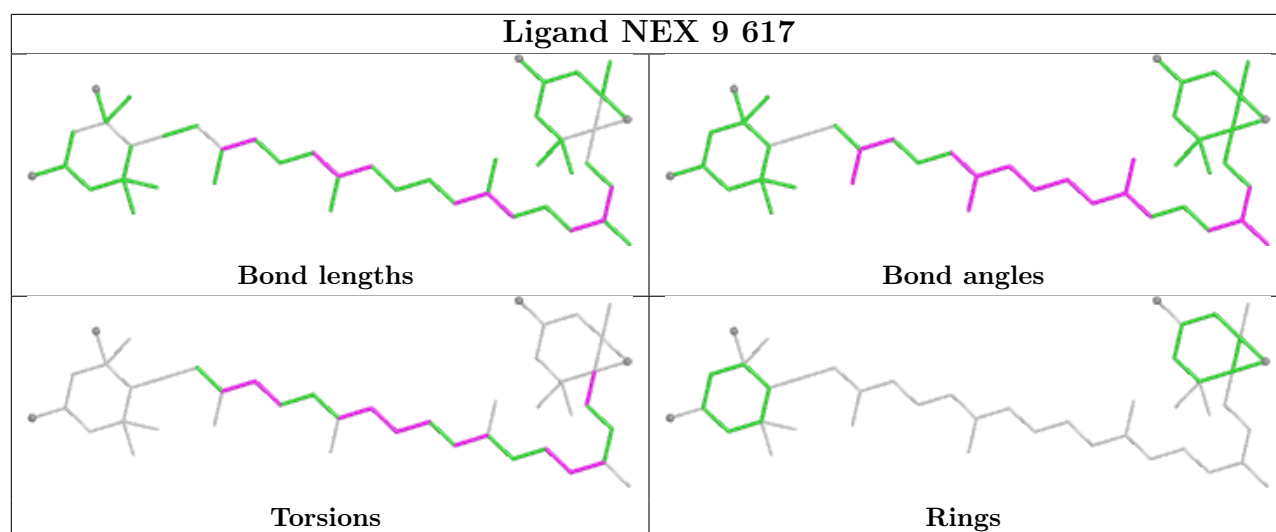


Ligand LUT 0 615

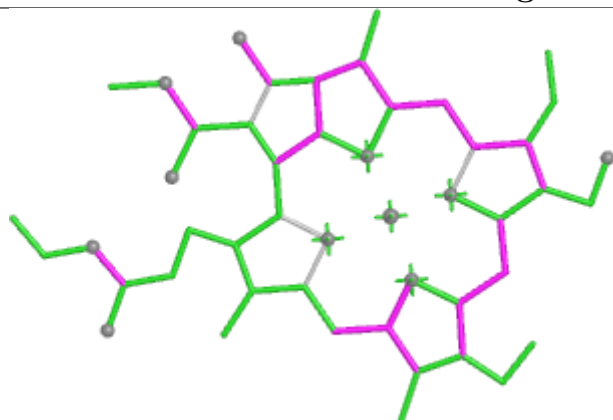




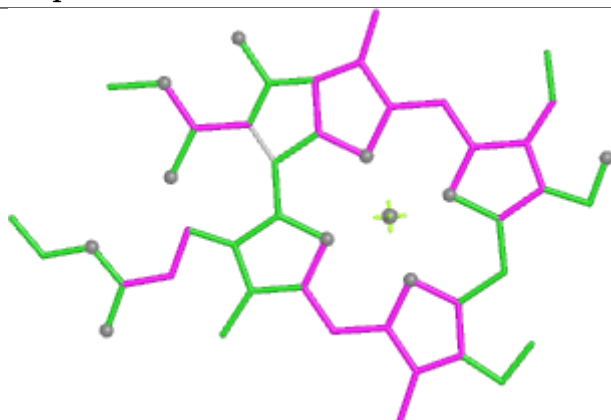




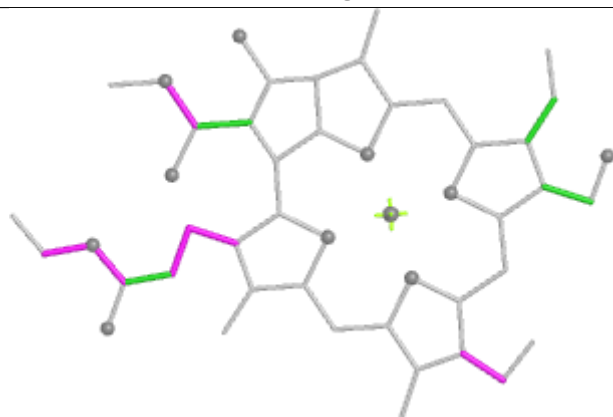
Ligand CHL p 605



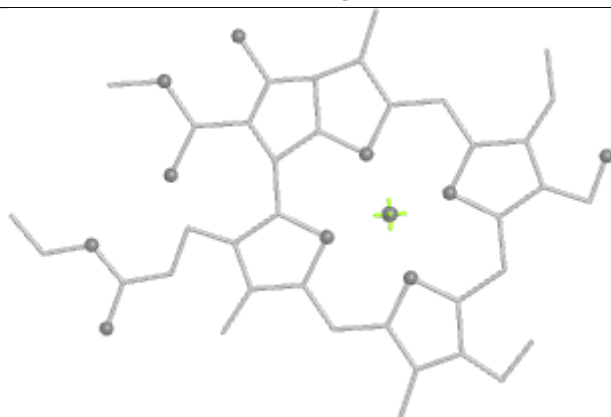
Bond lengths



Bond angles

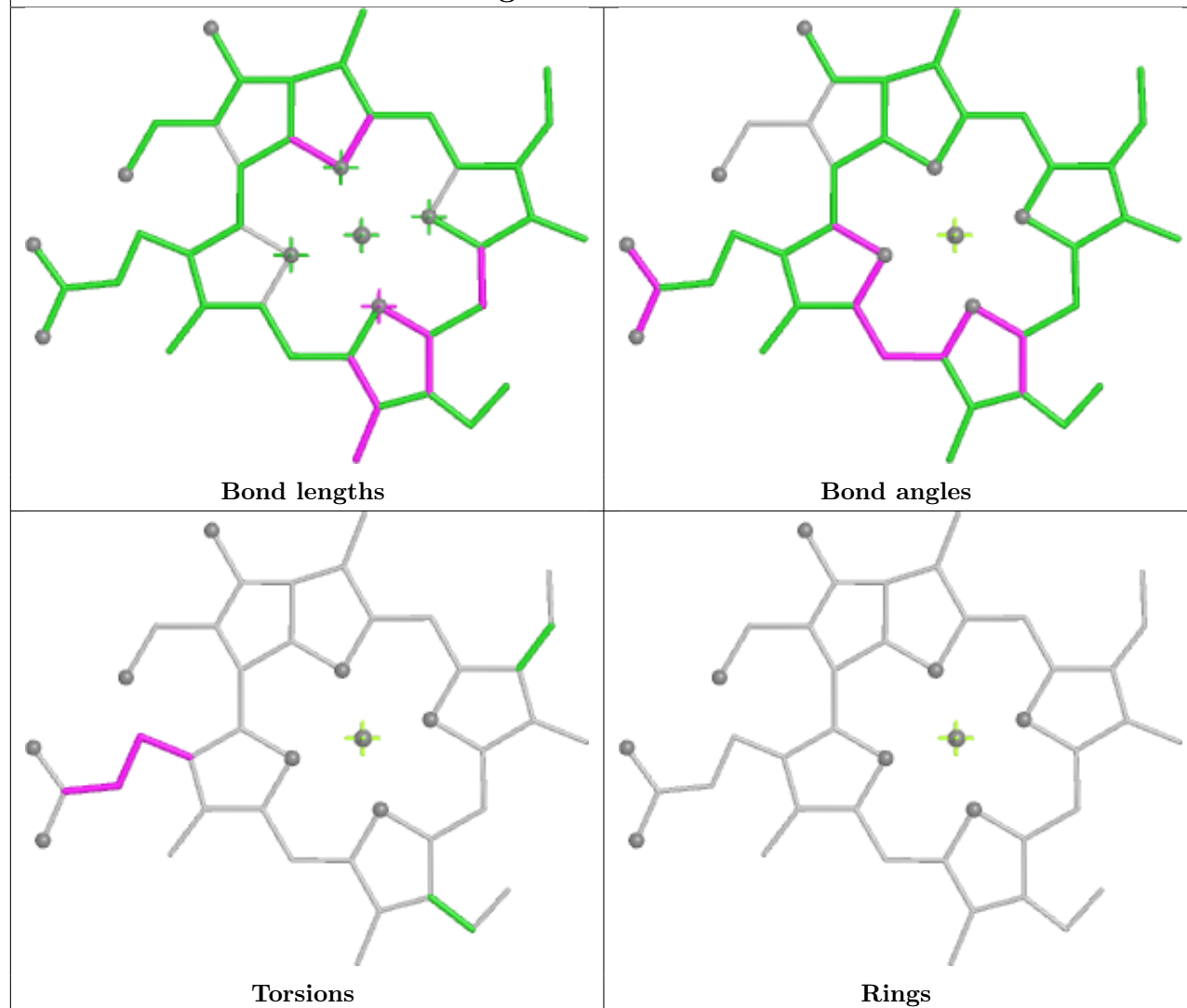


Torsions

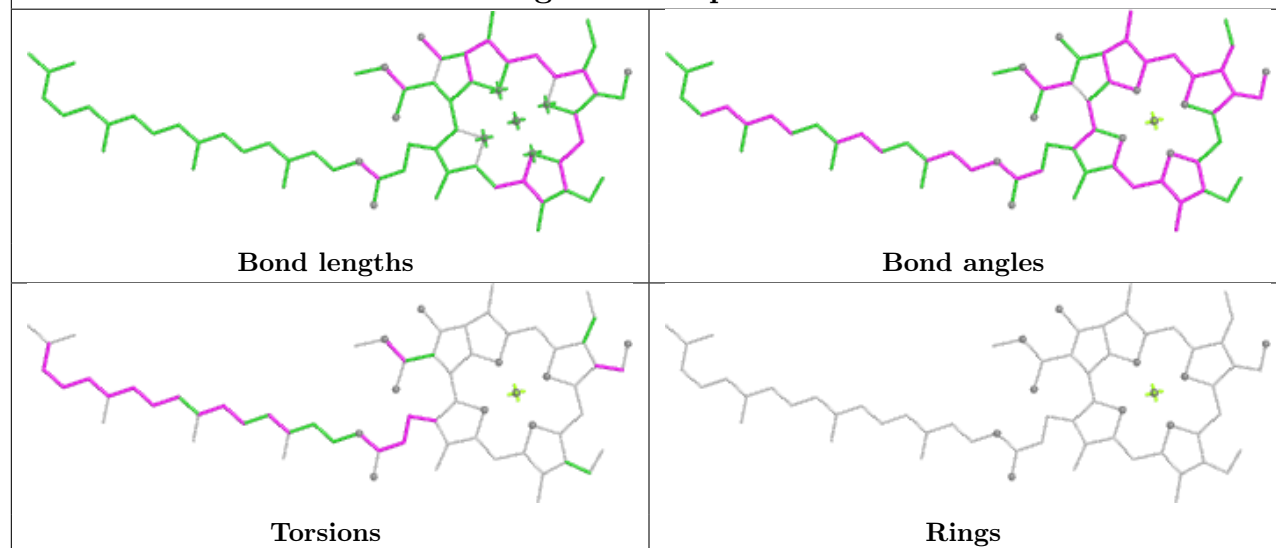


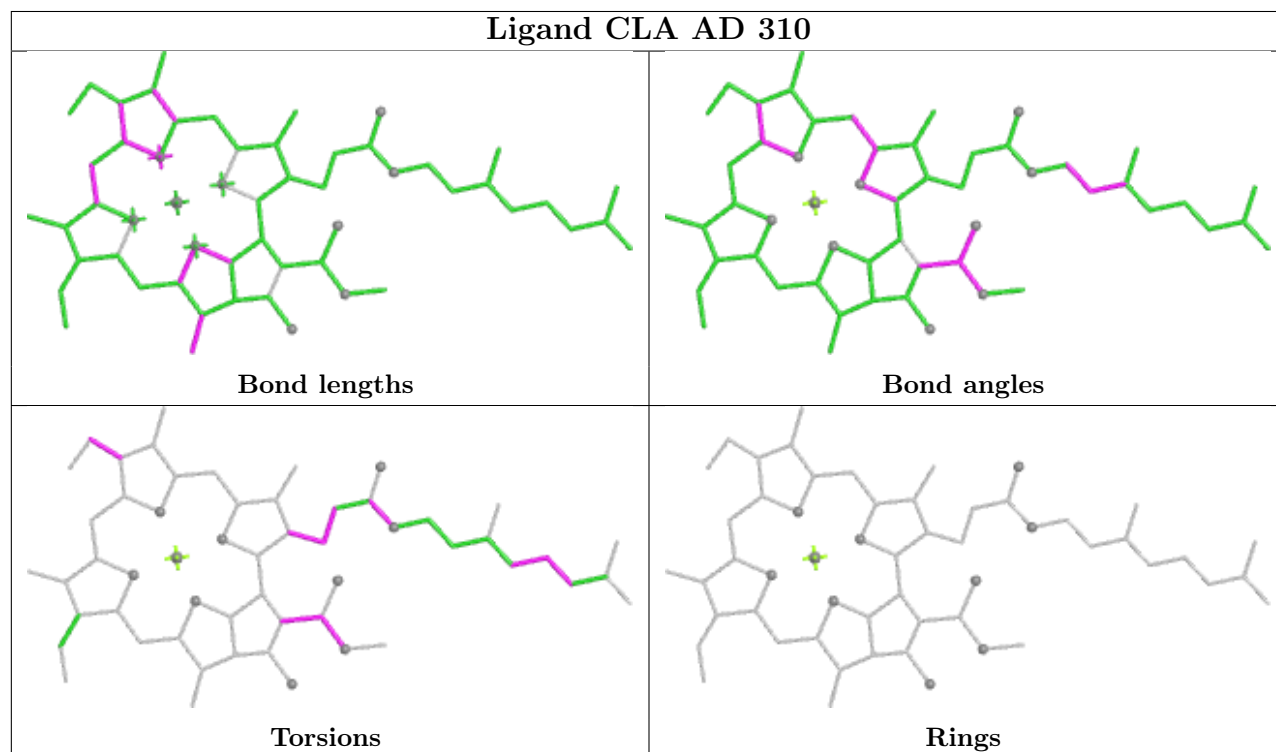
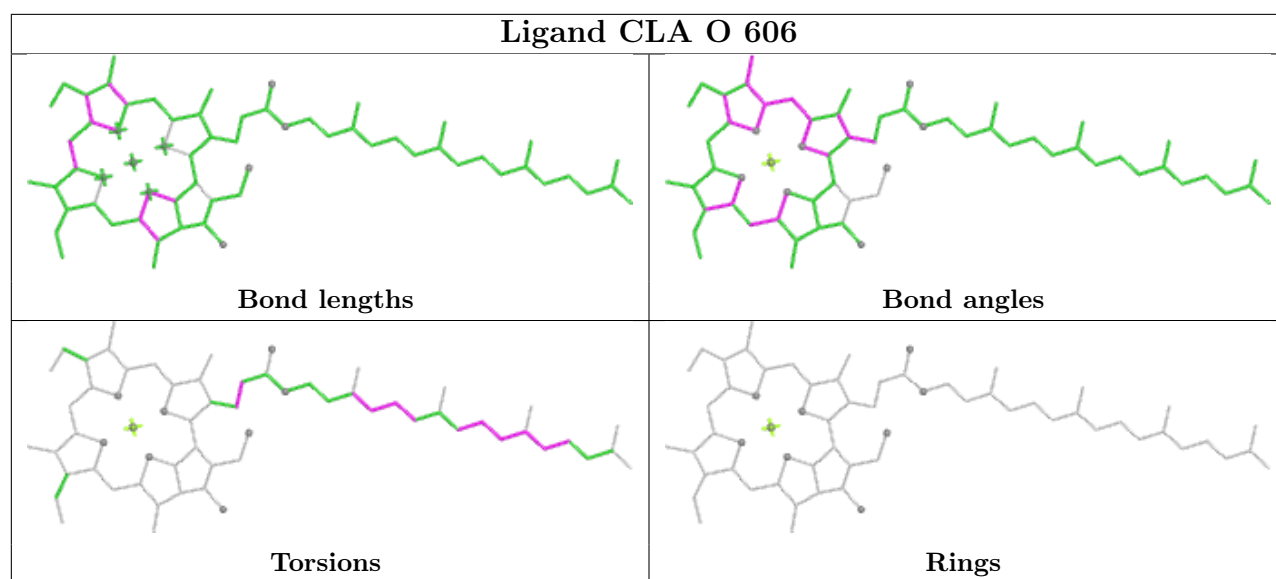
Rings

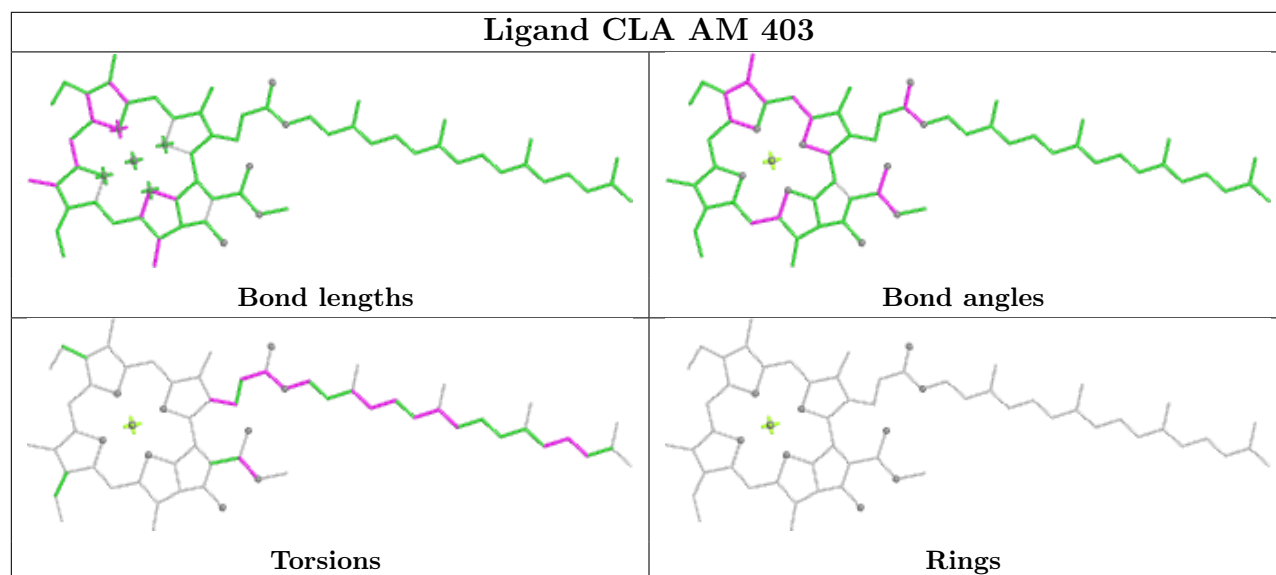
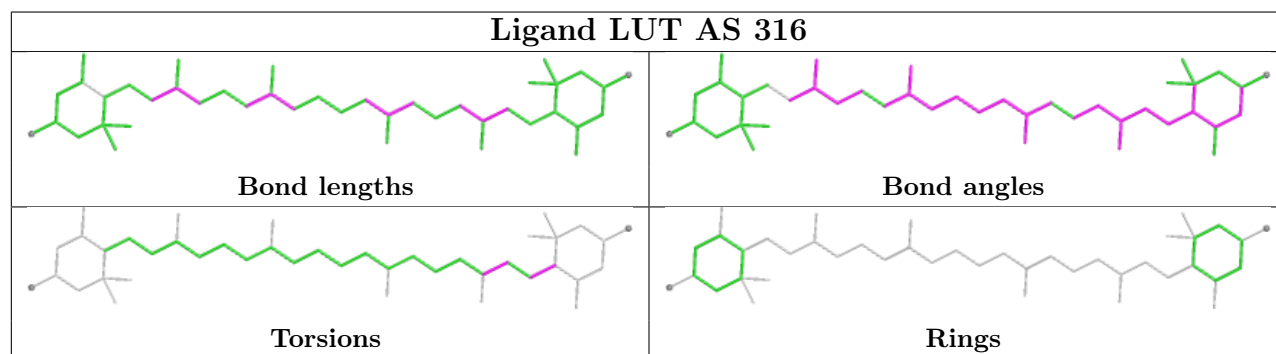
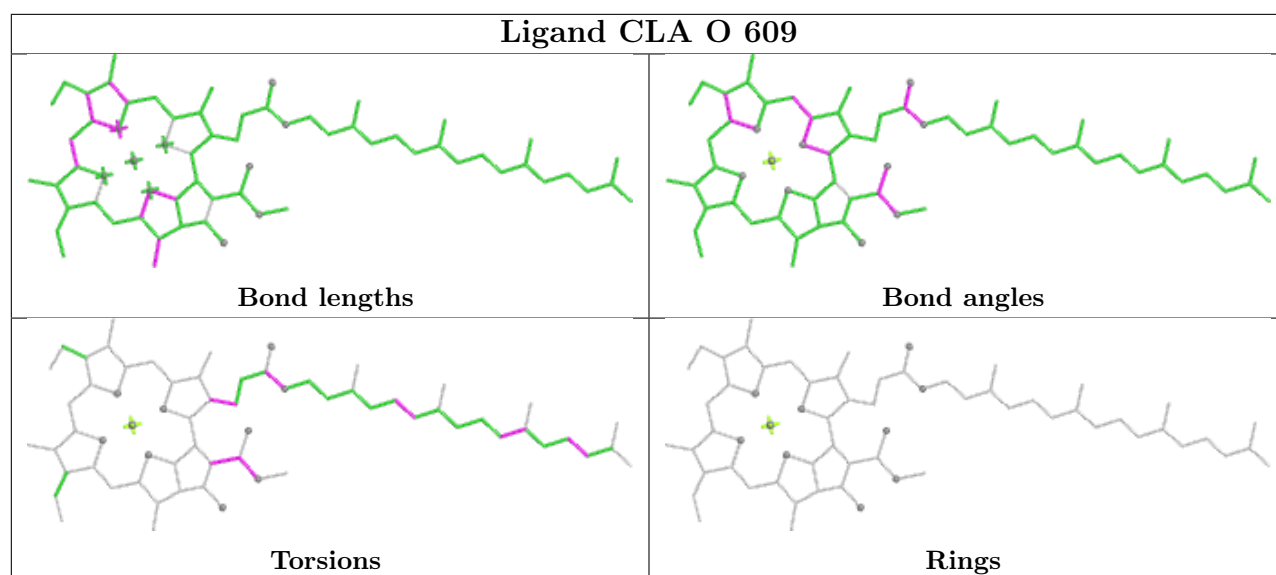
Ligand CLA 9 611

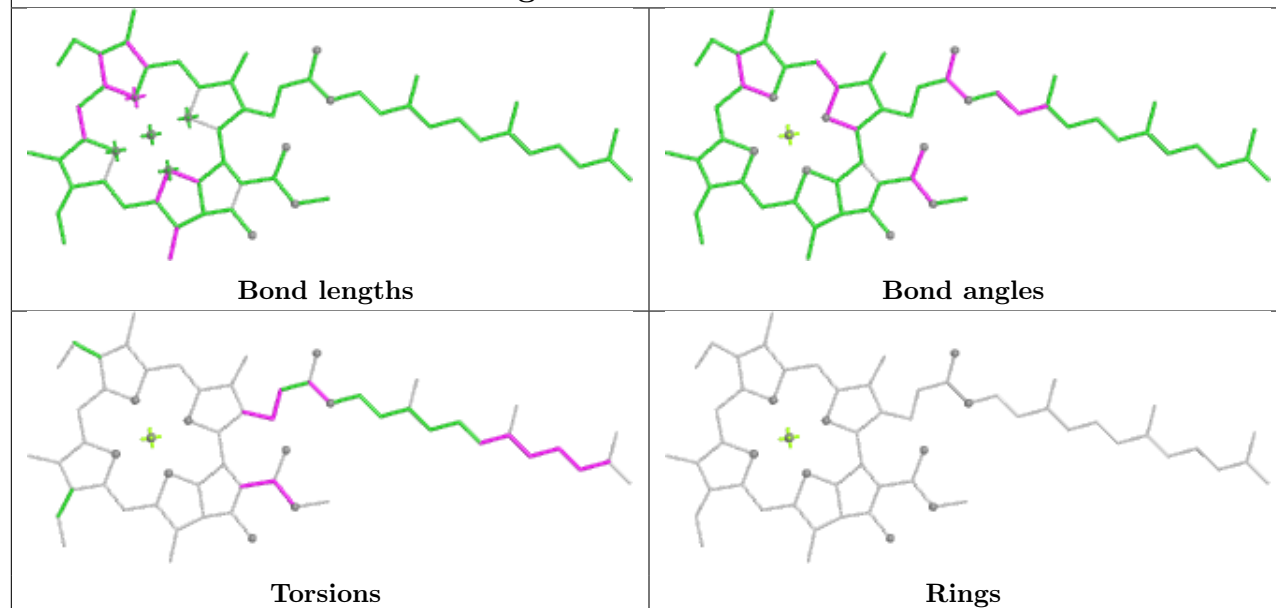
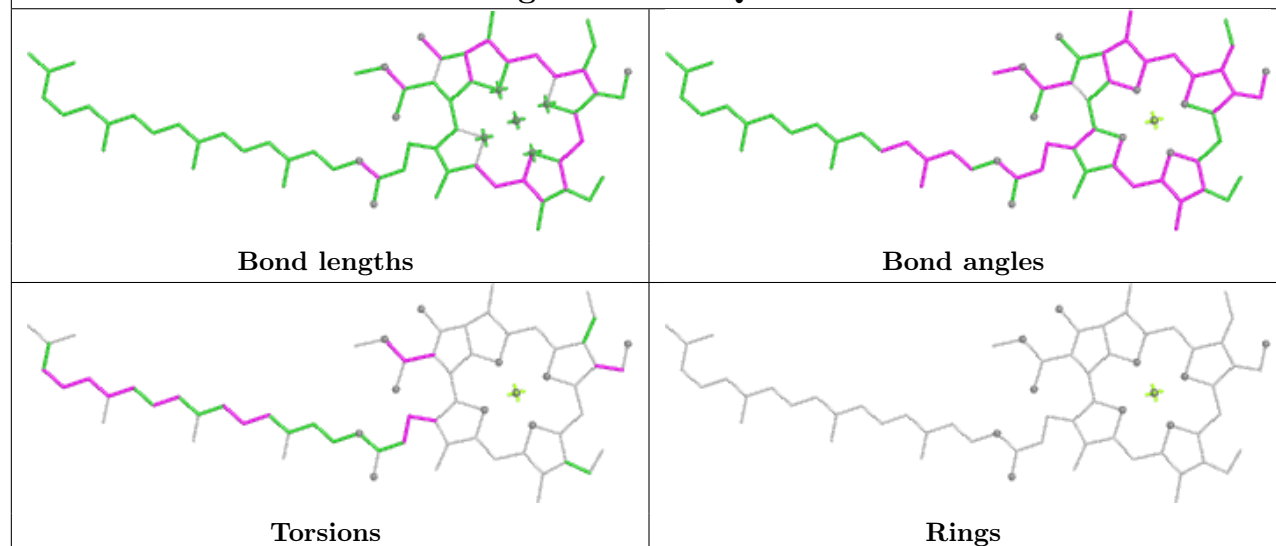


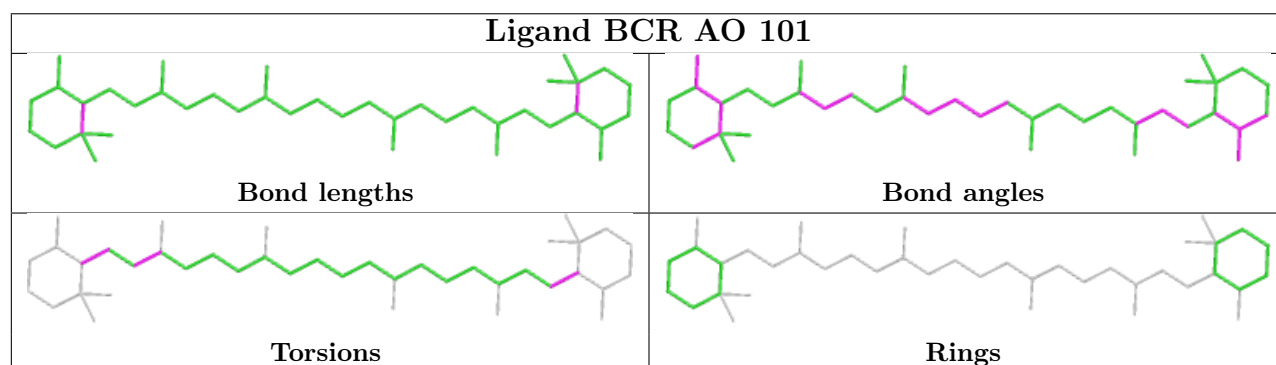
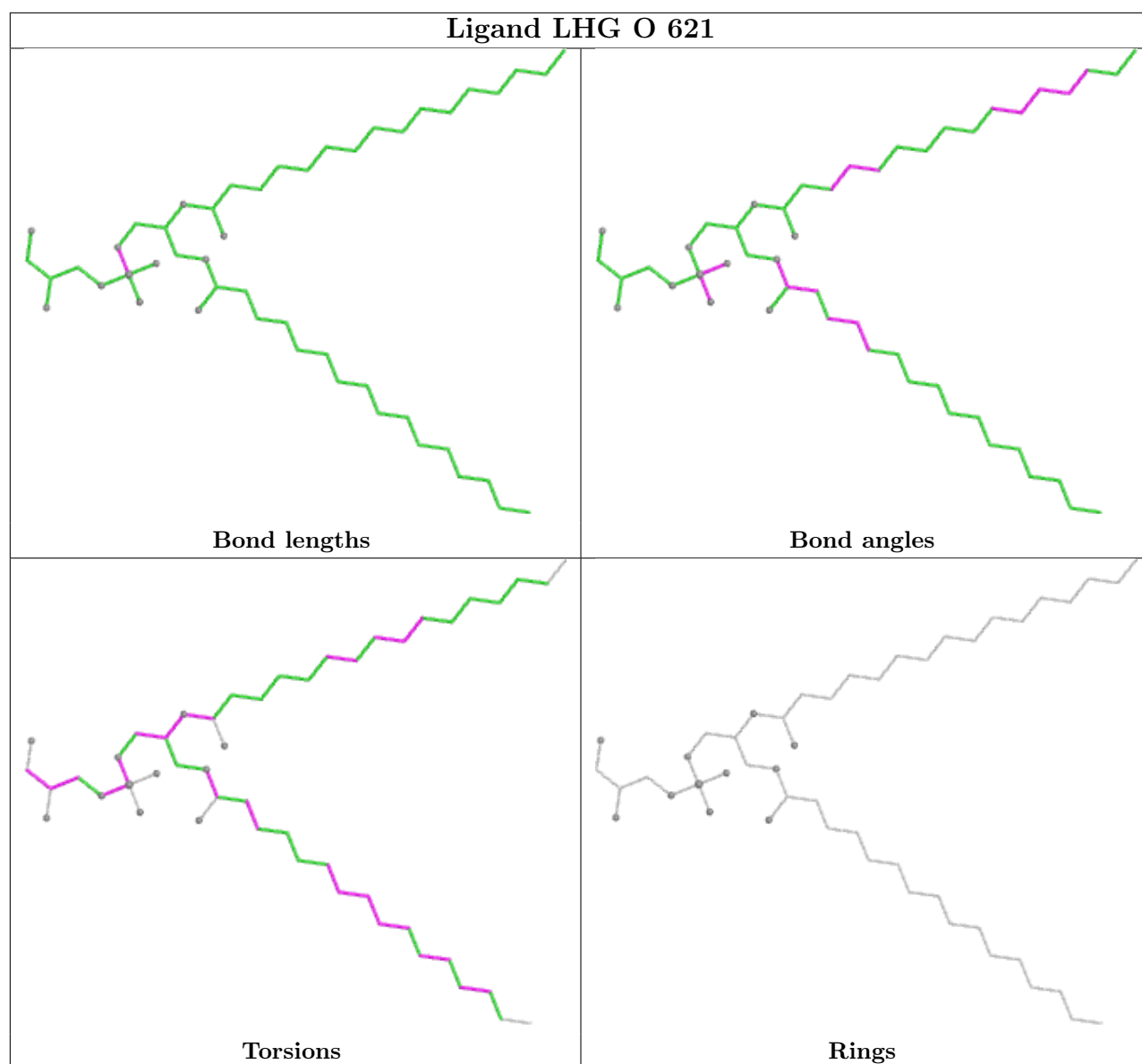
Ligand CHL p 601

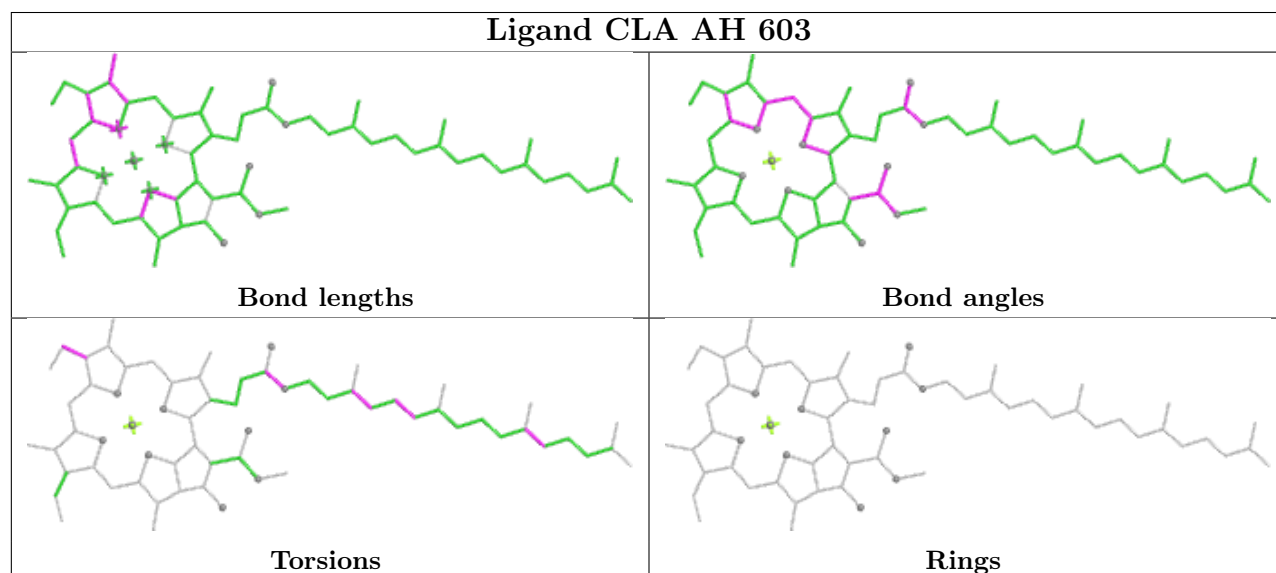
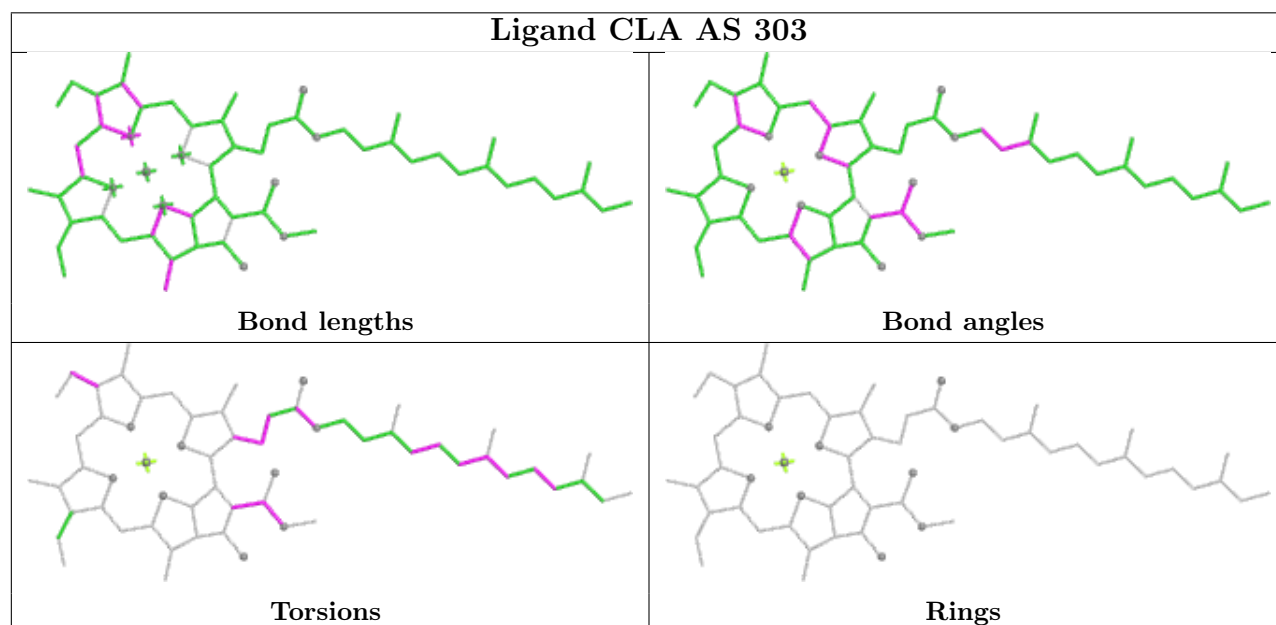
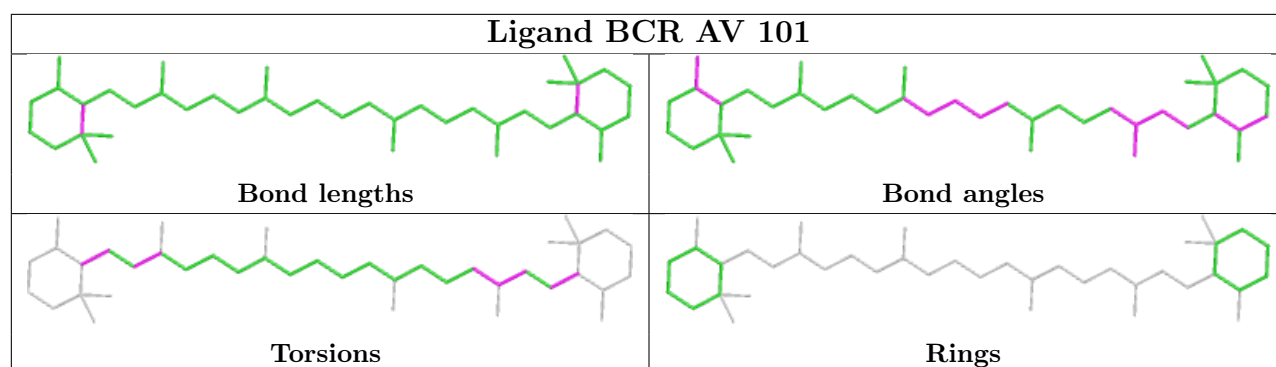


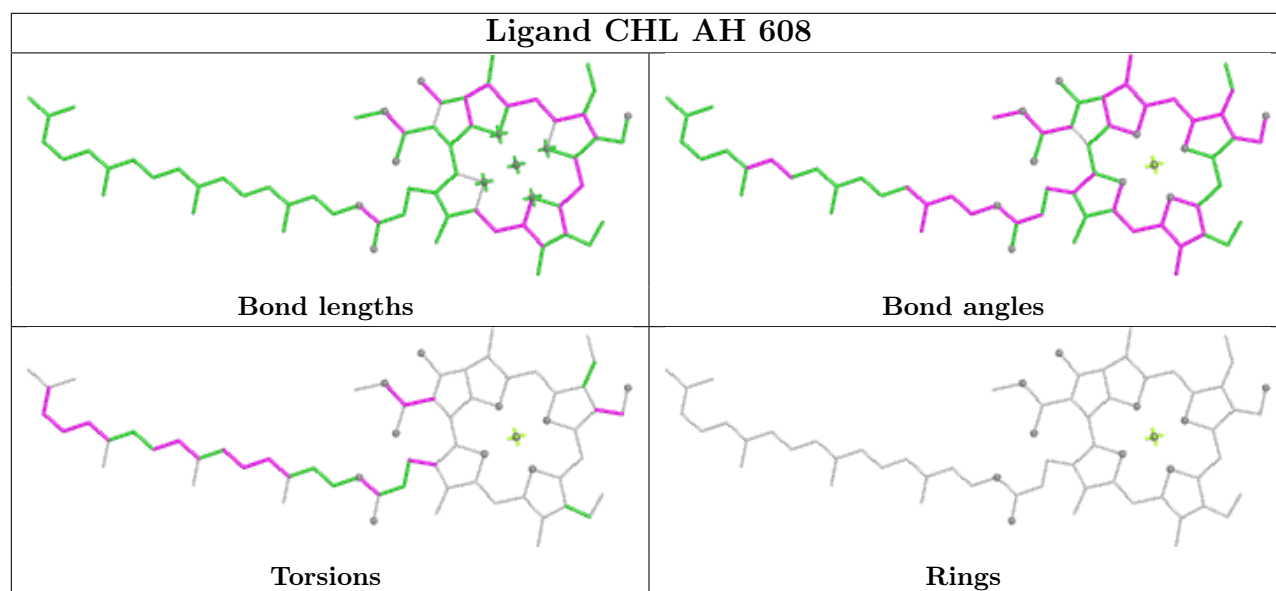
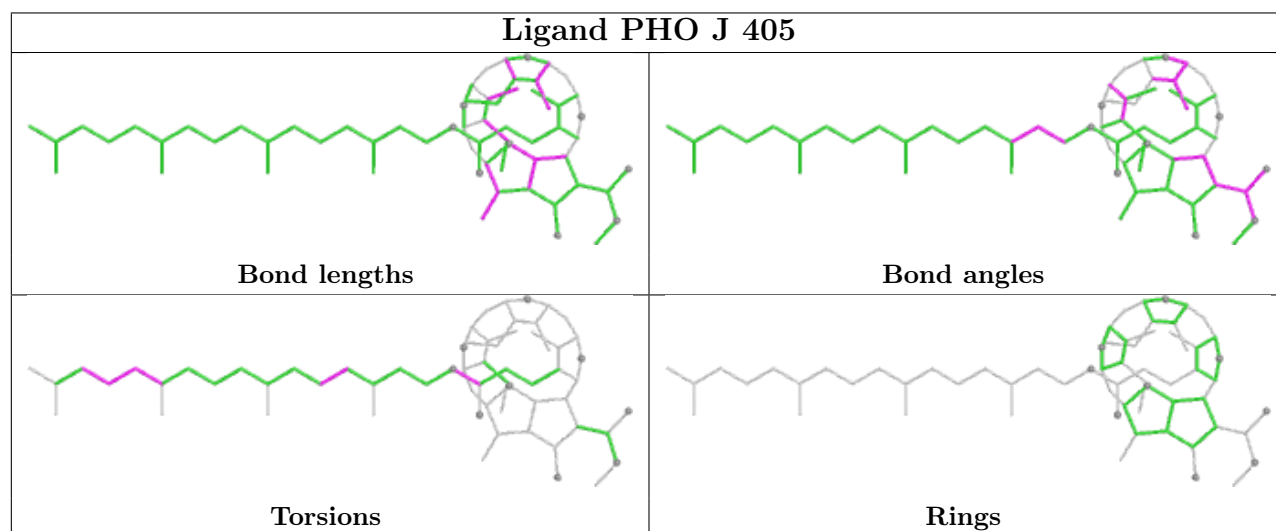
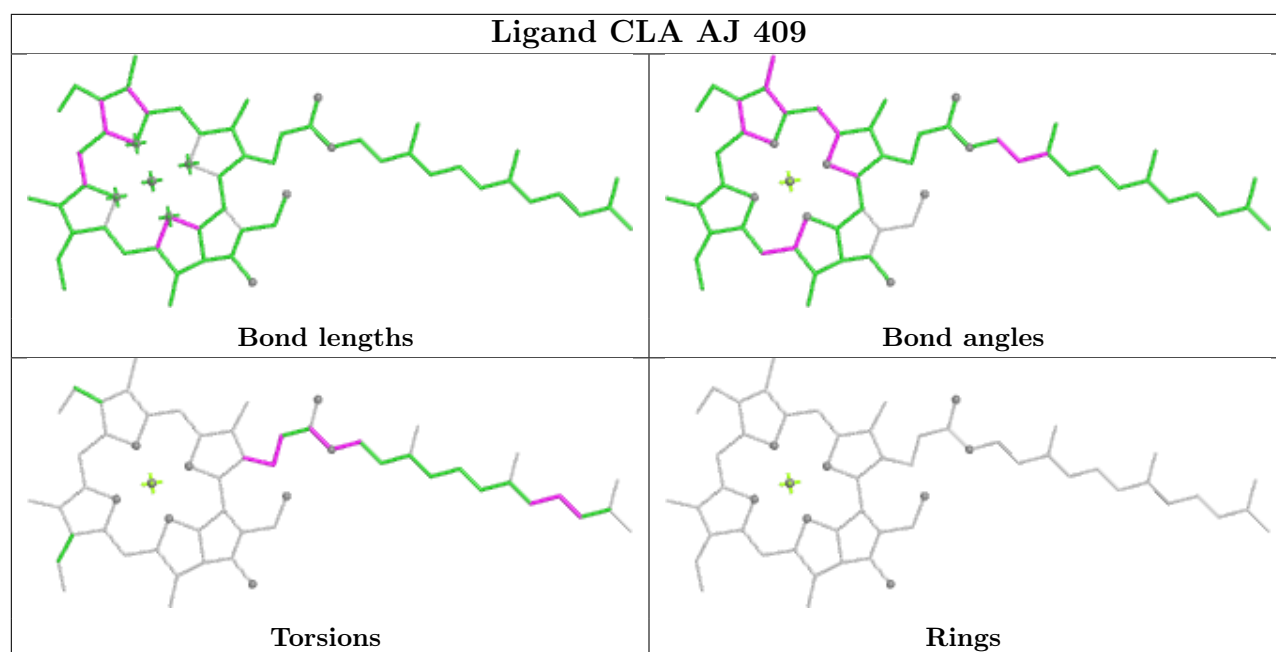




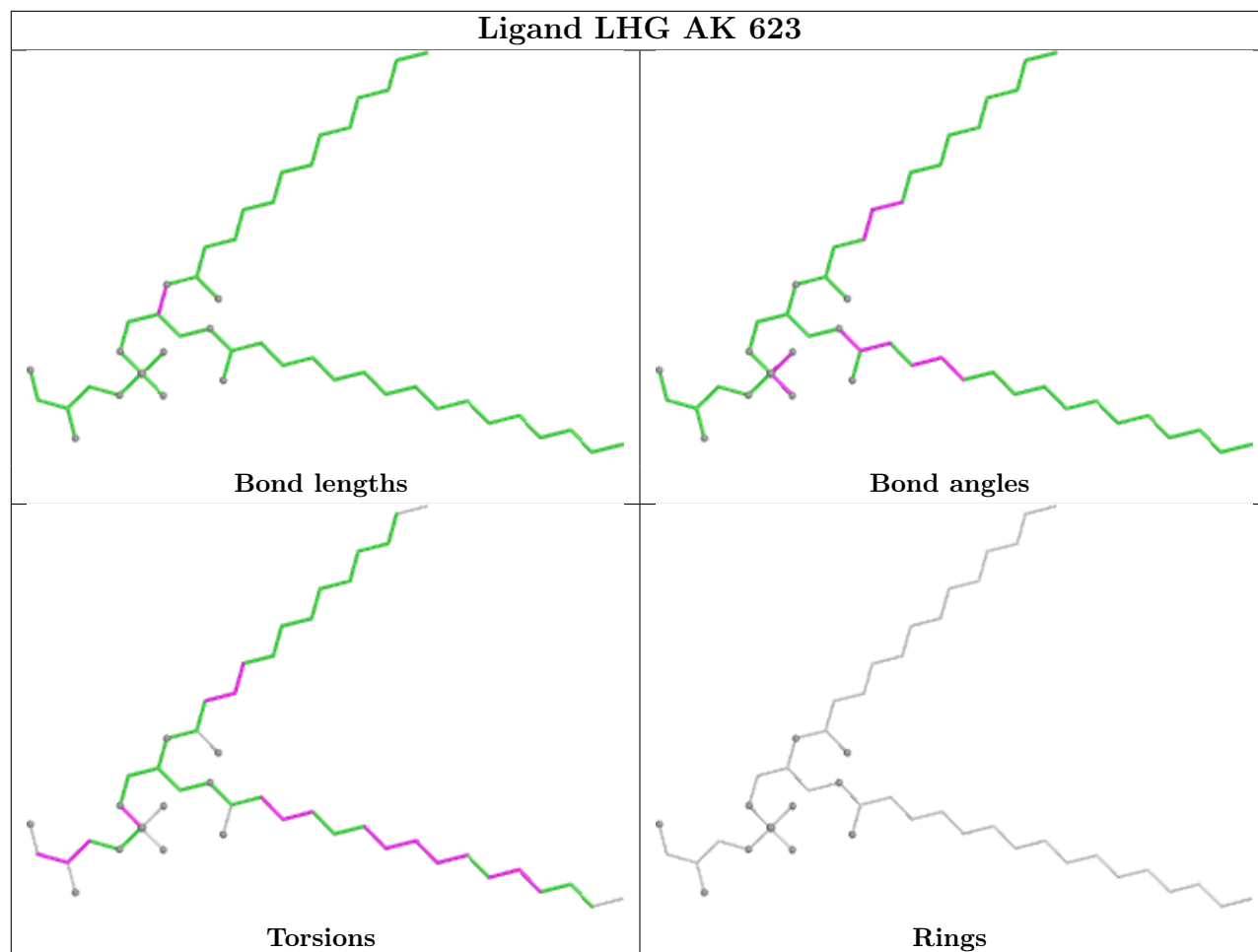
Ligand CLA AD 303**Ligand CHL AQ 608**



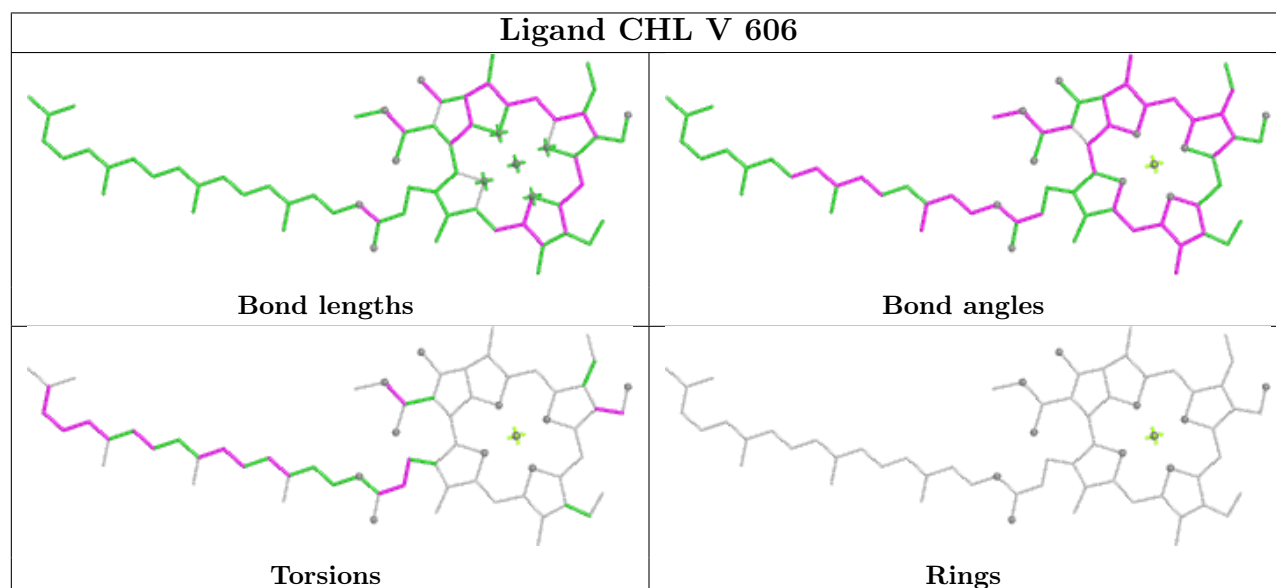




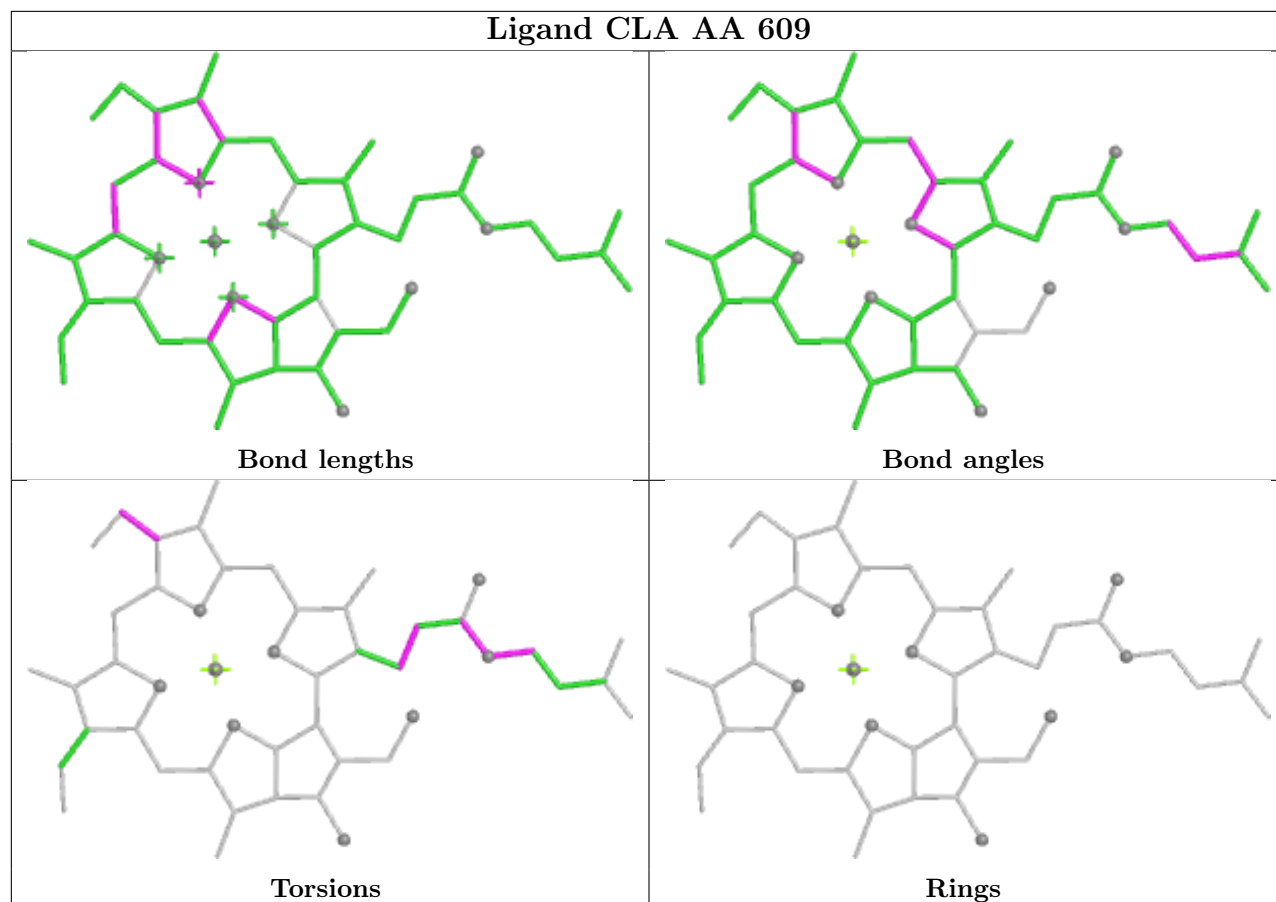
Ligand LHG AK 623



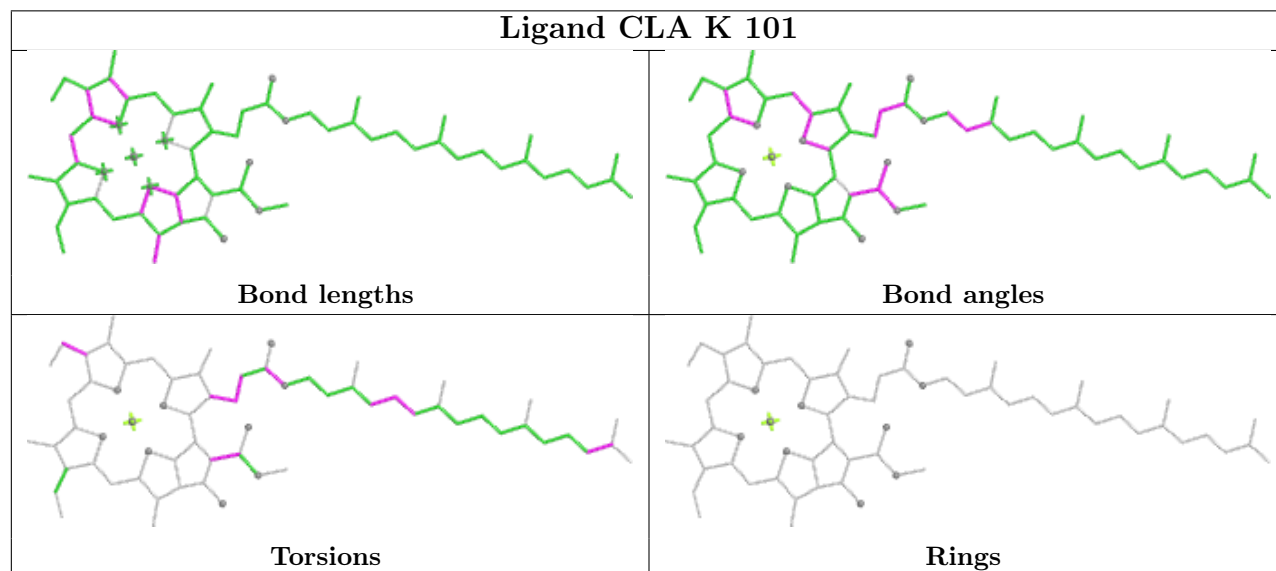
Ligand CHL V 606

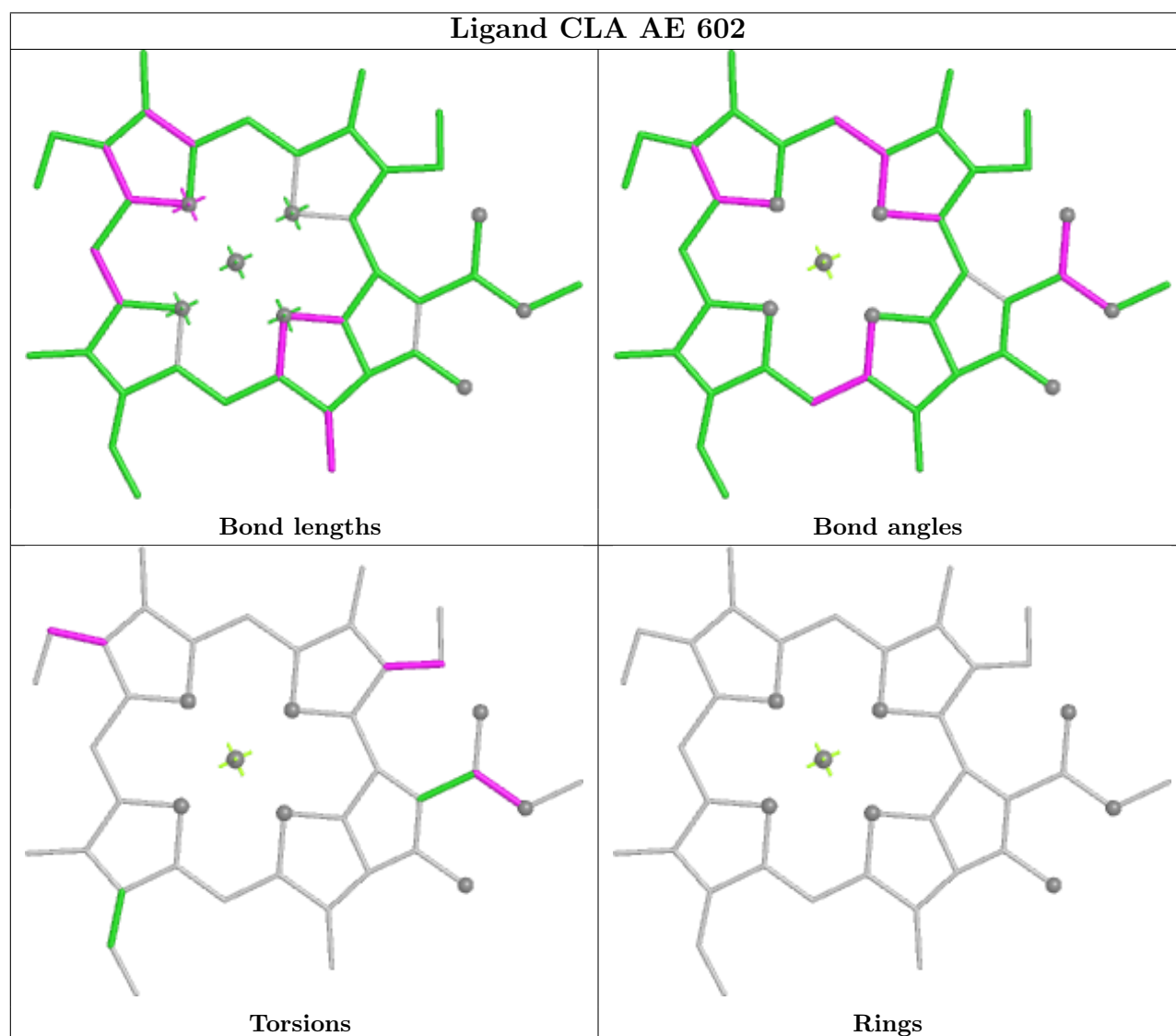
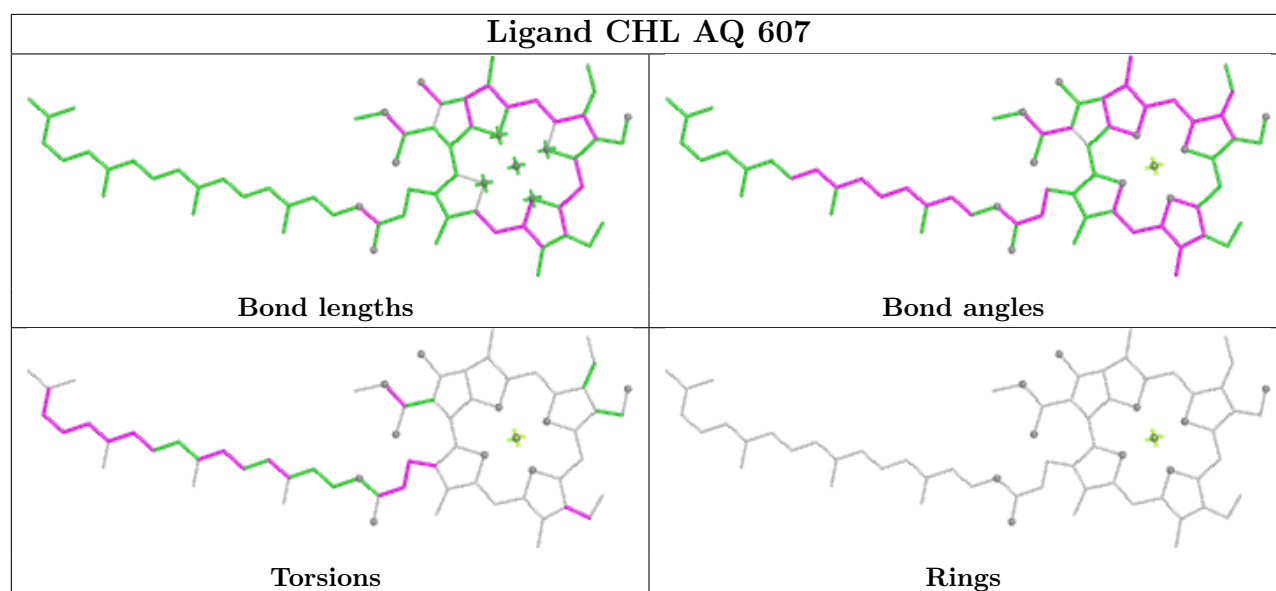


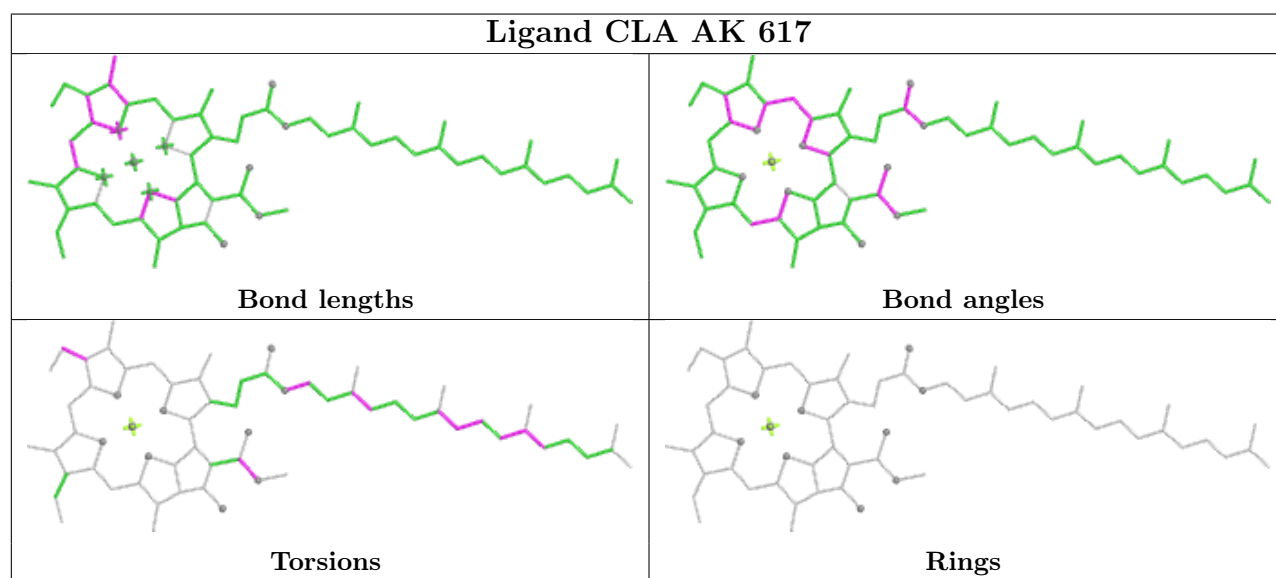
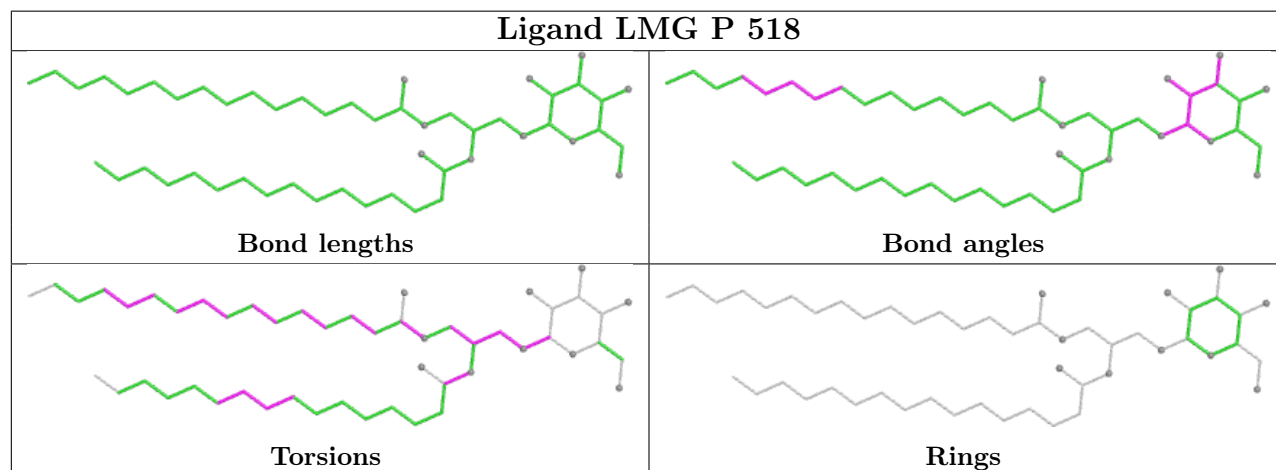
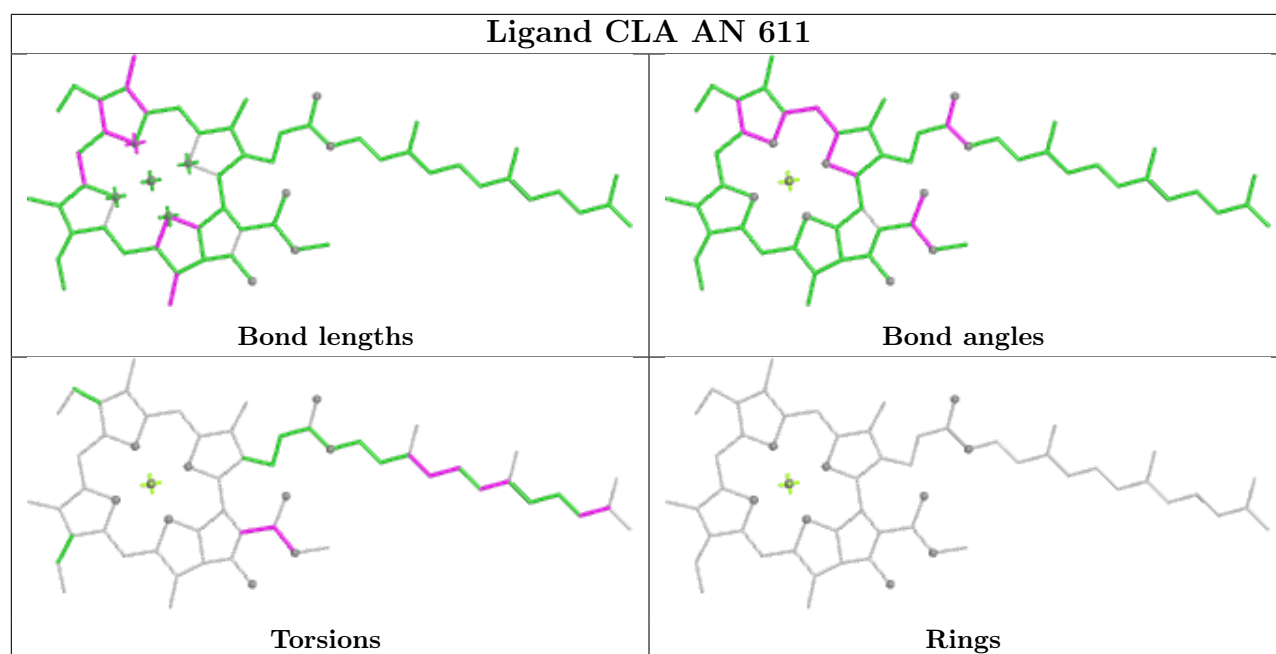
Ligand CLA AA 609

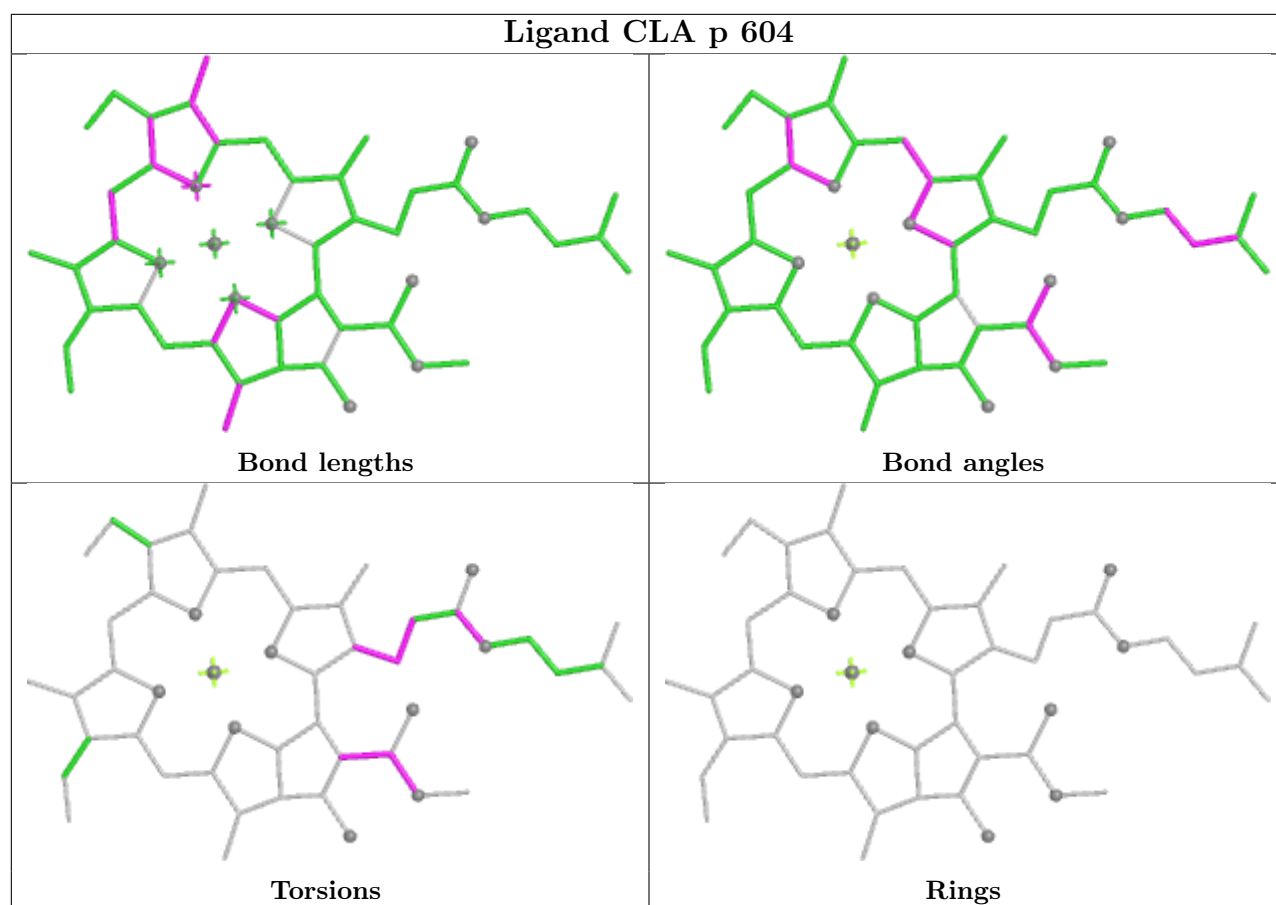


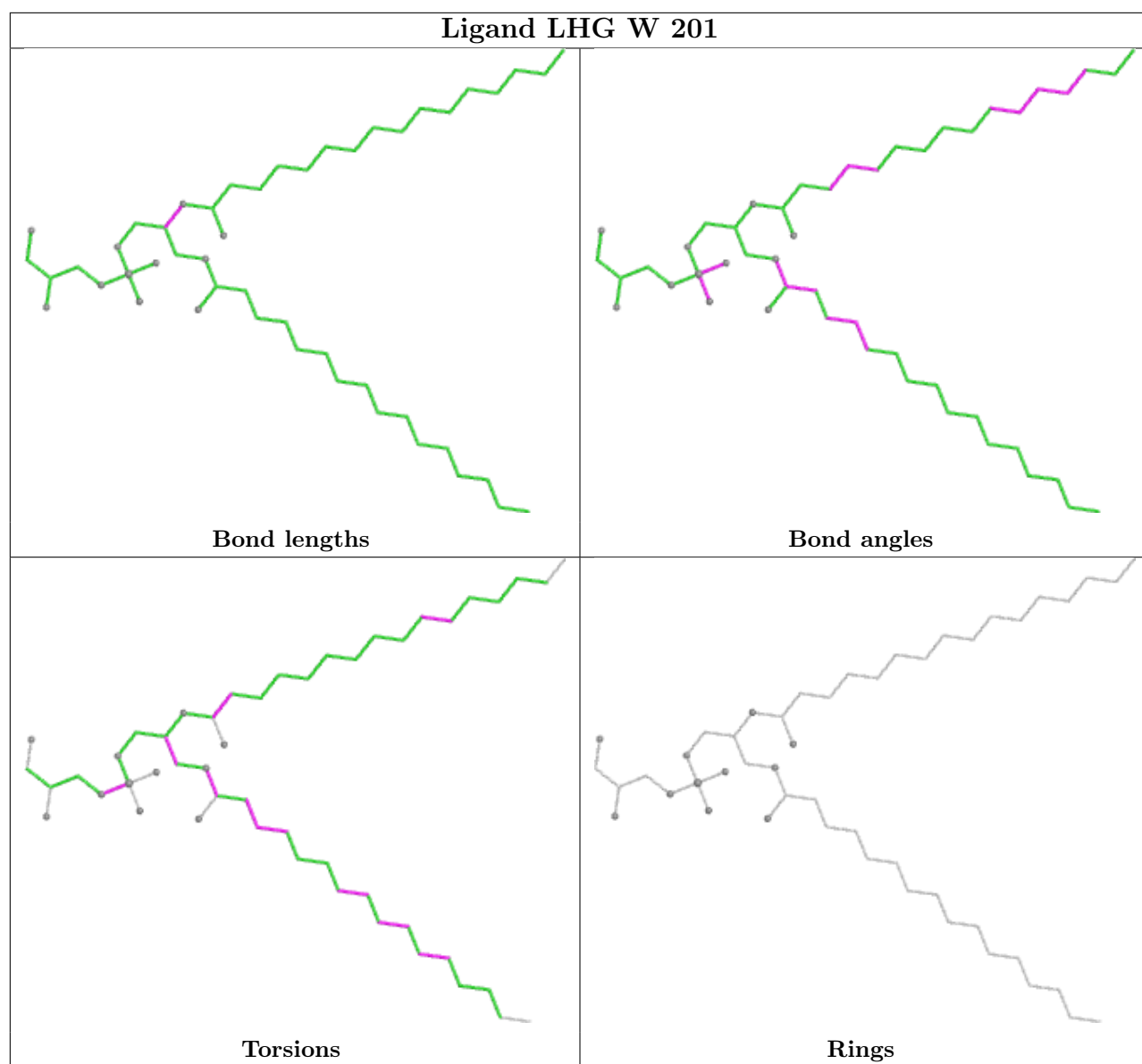
Ligand CLA K 101

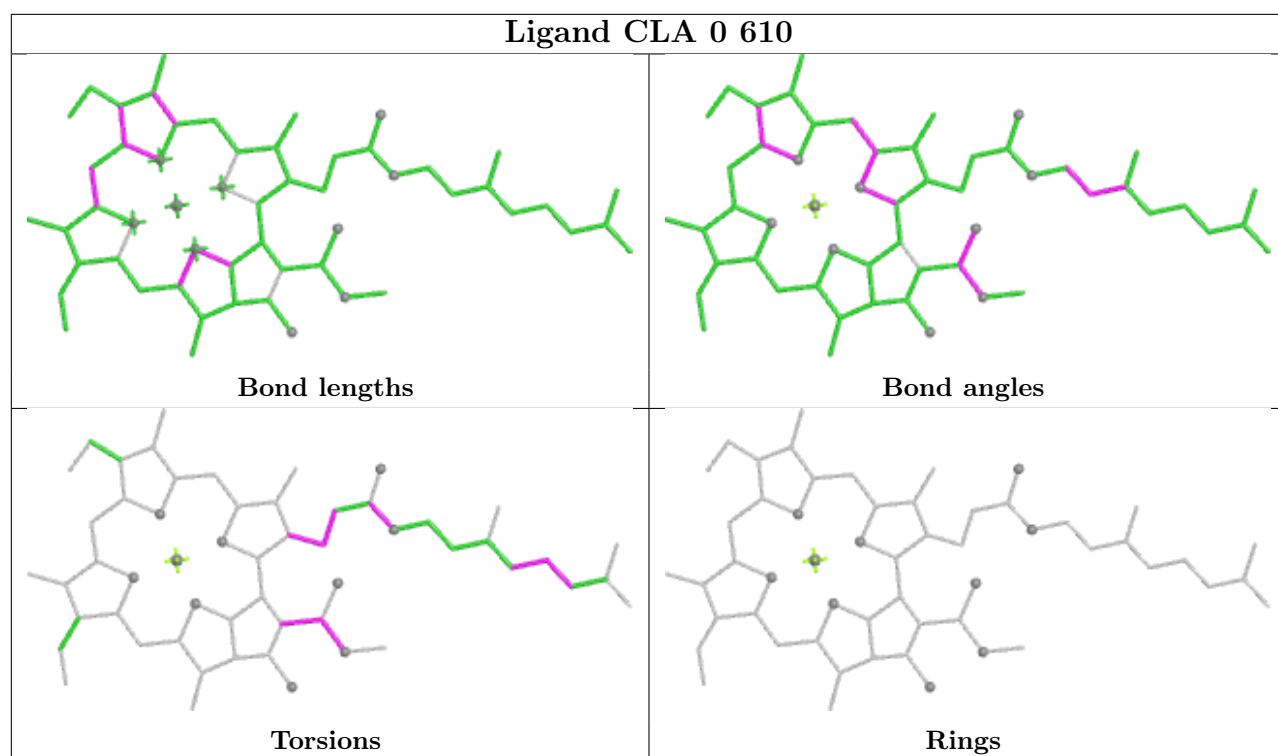


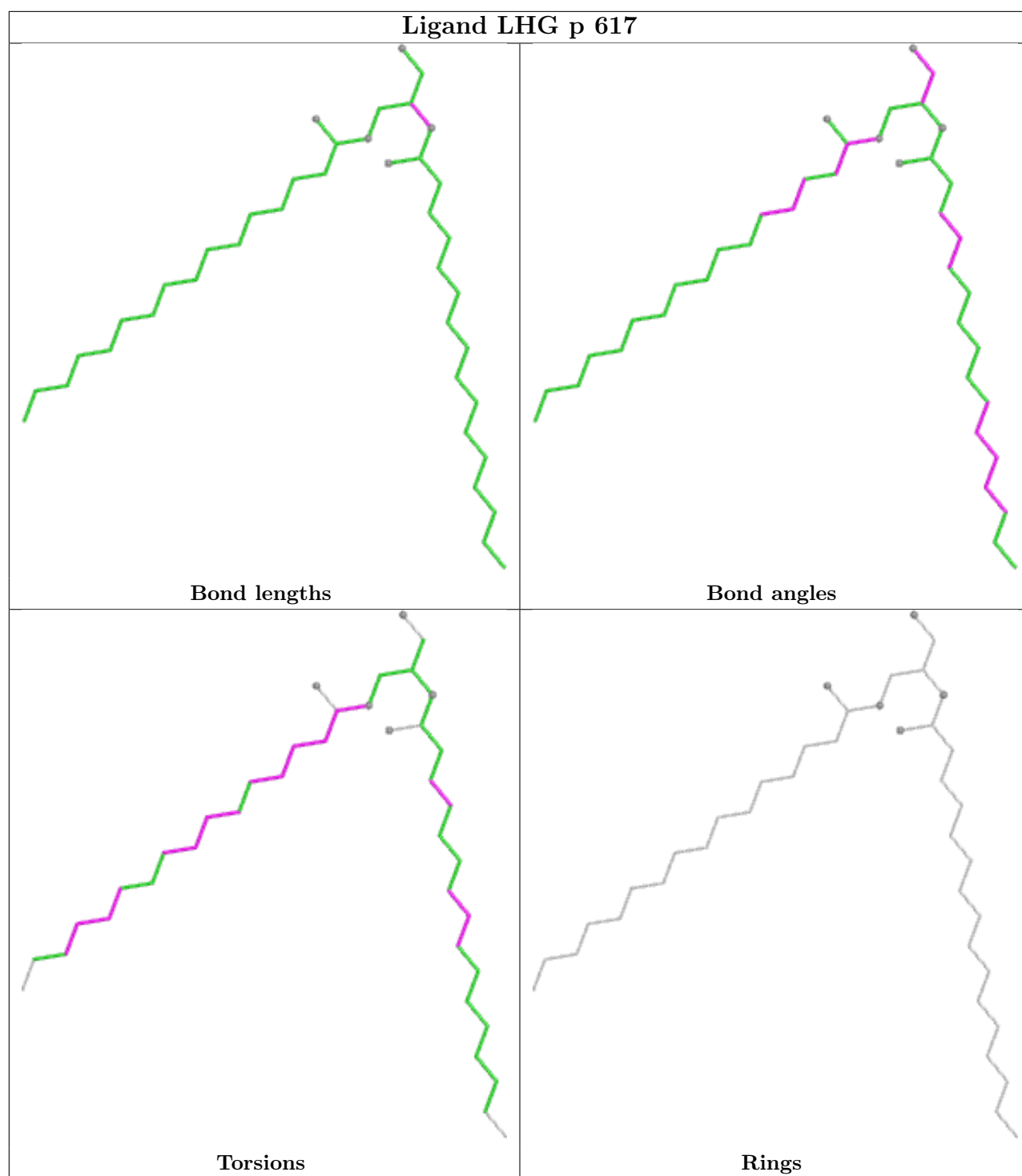


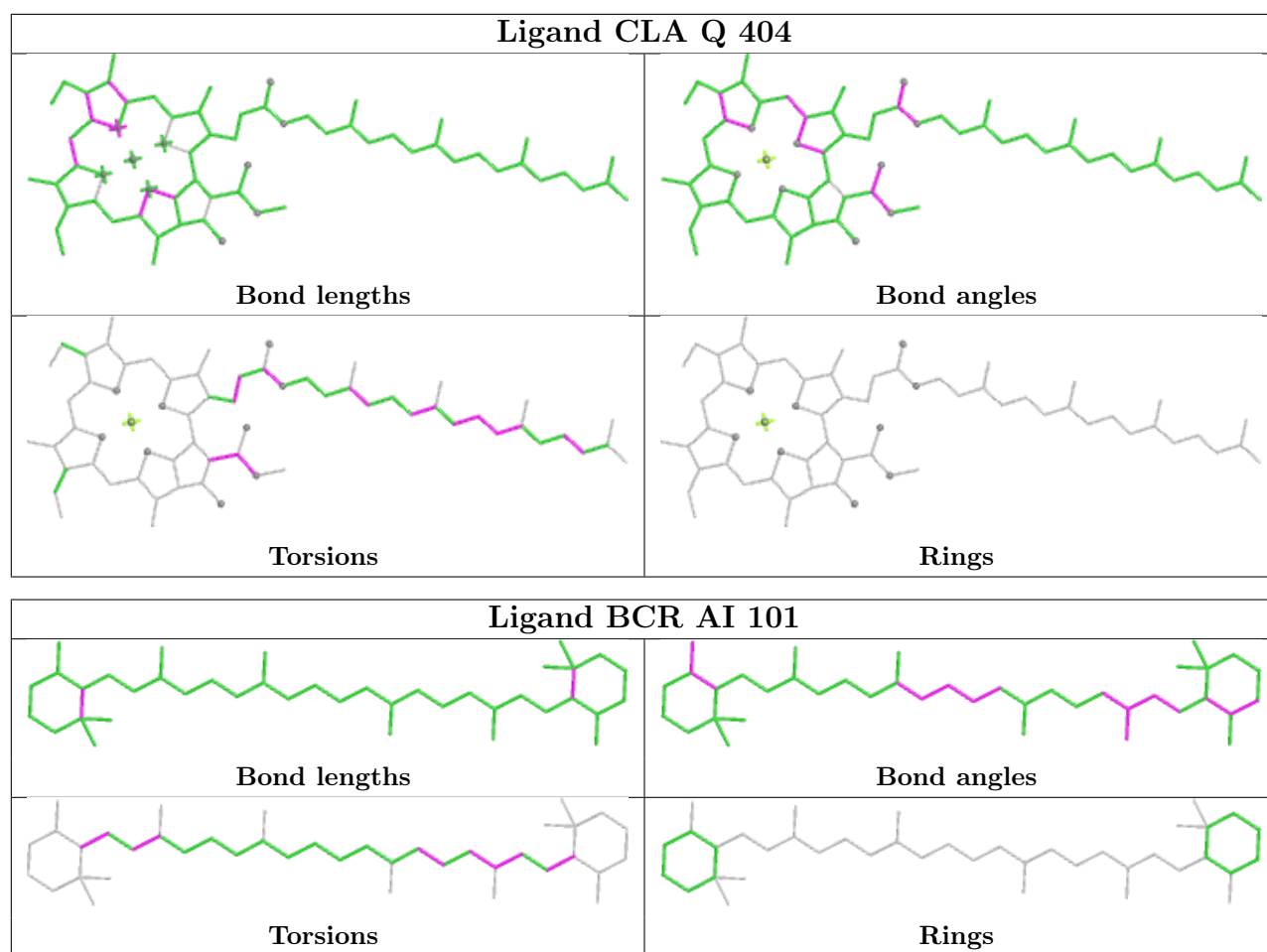




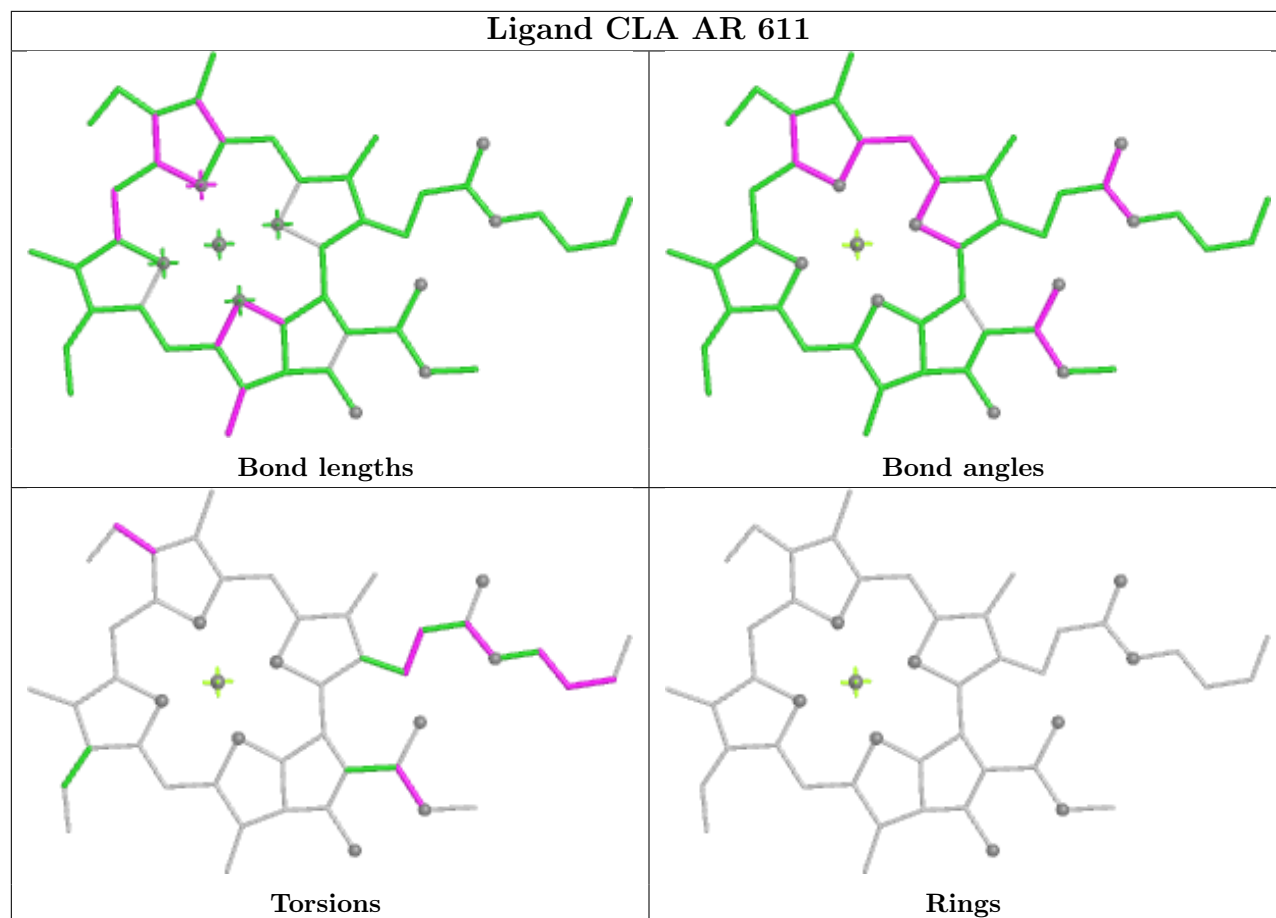




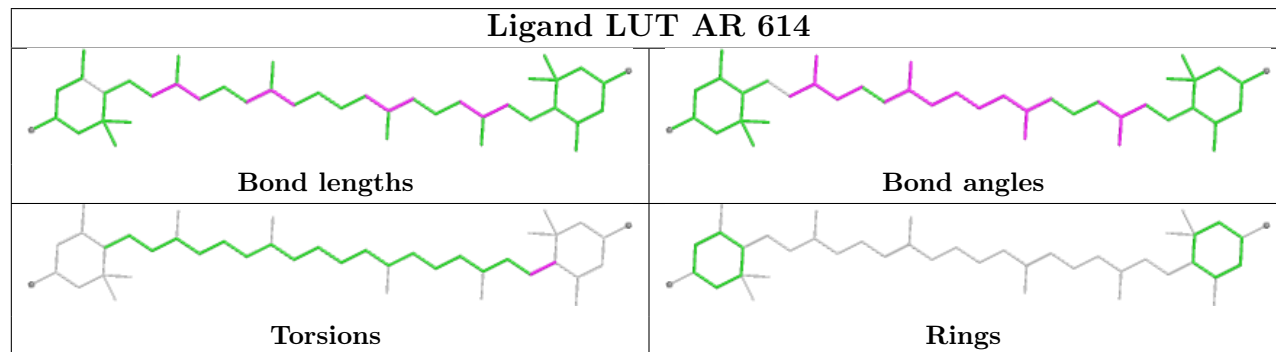




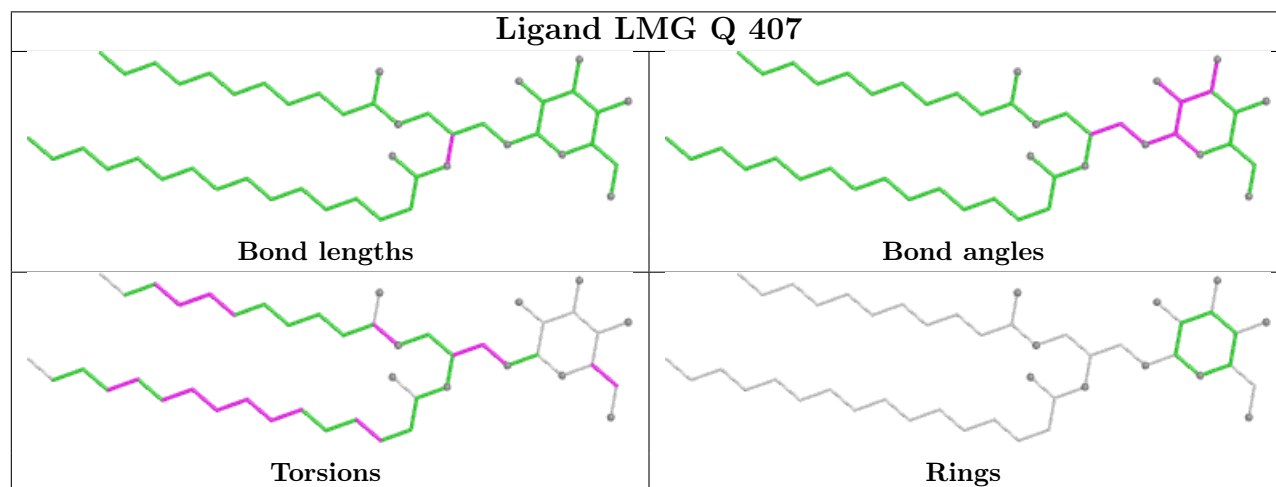
Ligand CLA AR 611



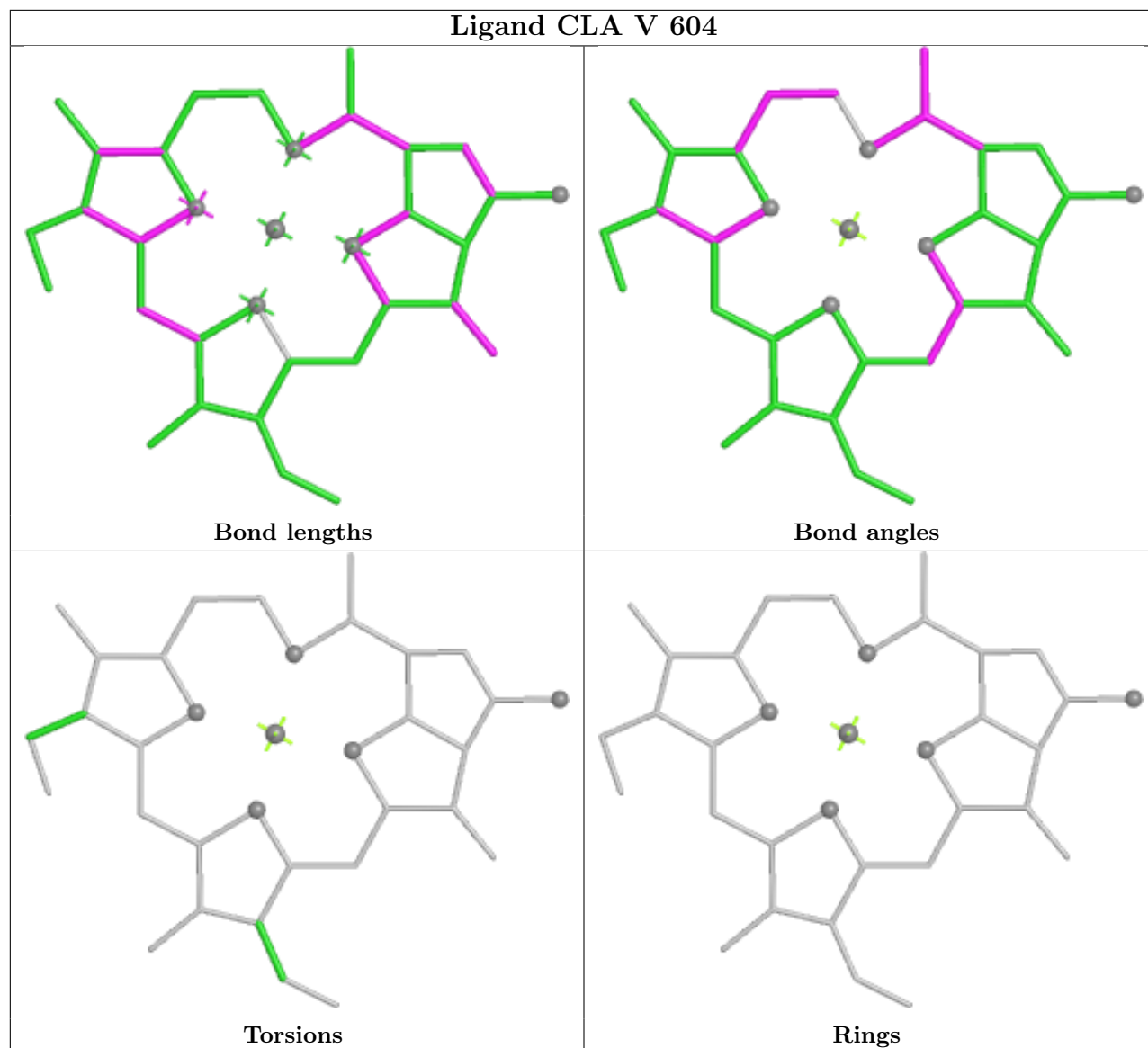
Ligand LUT AR 614



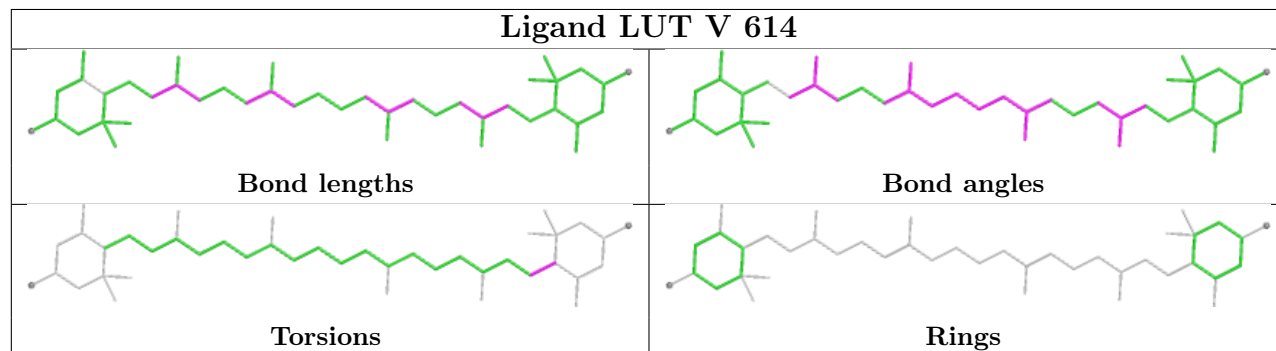
Ligand LMG Q 407

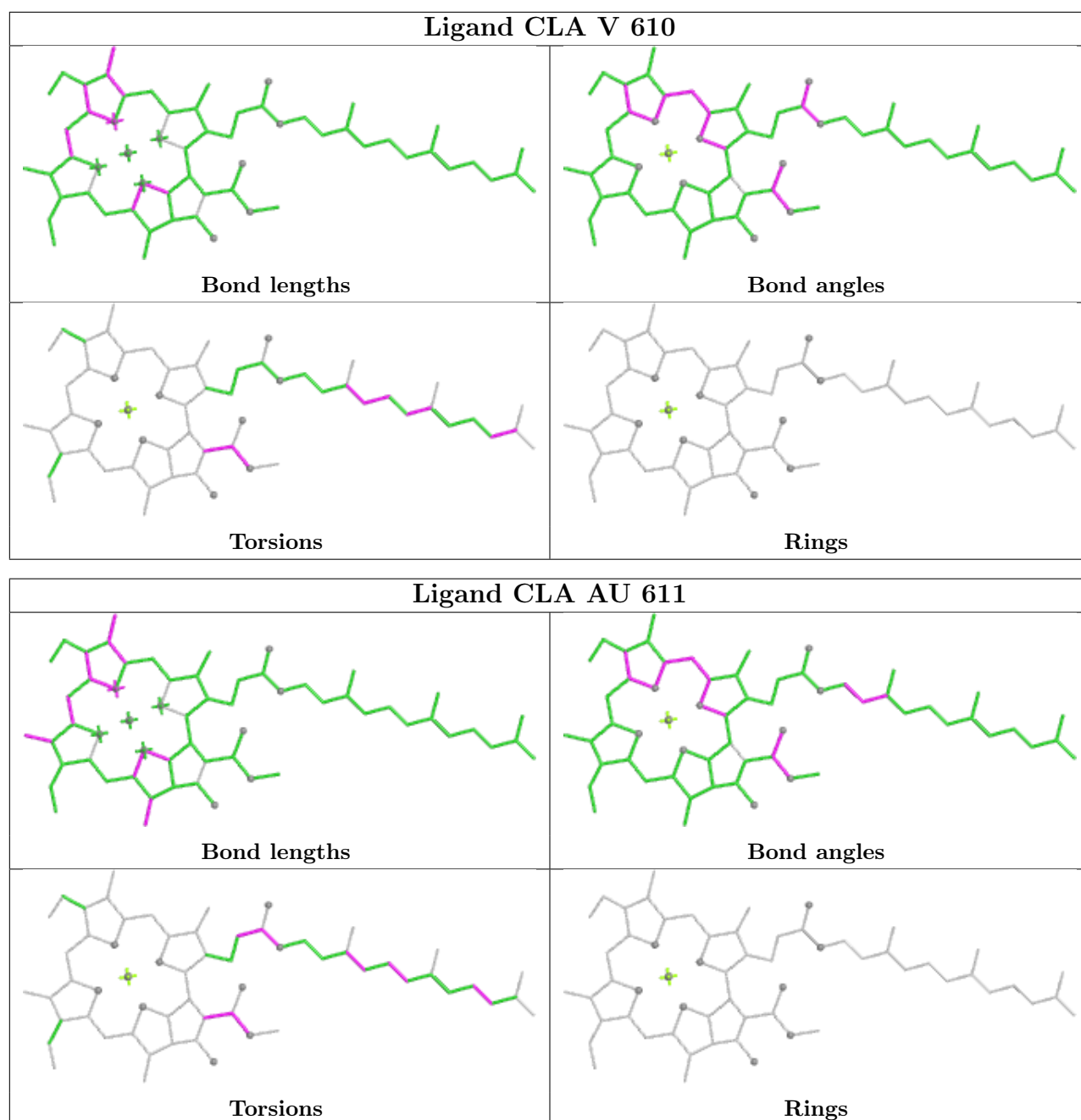


Ligand CLA V 604

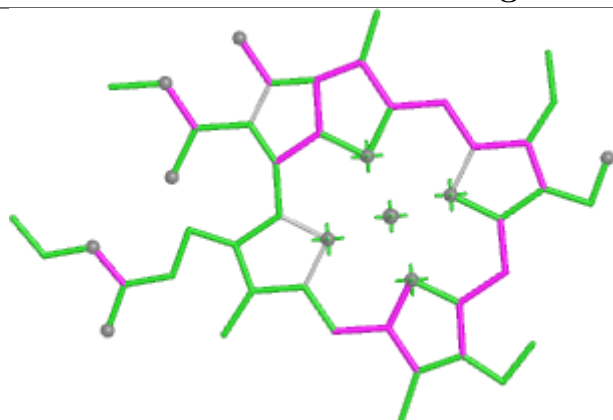


Ligand LUT V 614

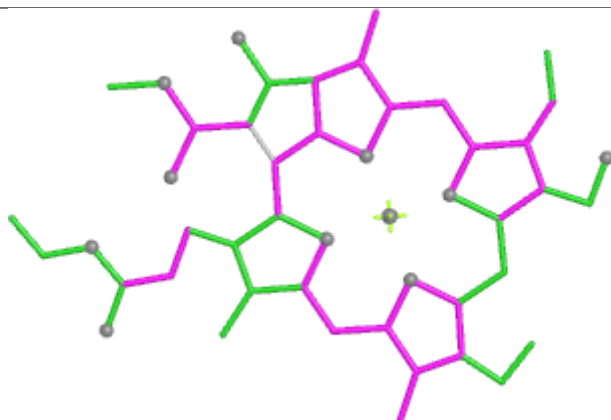




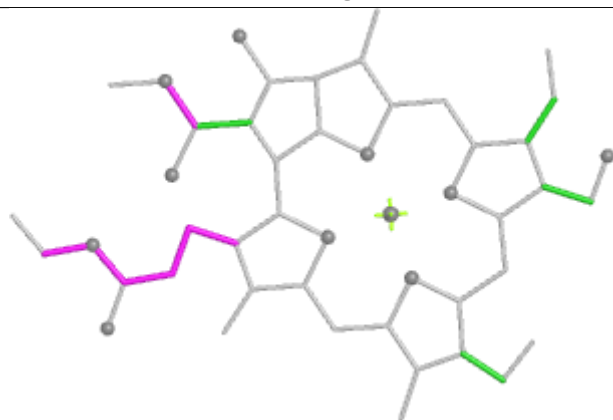
Ligand CHL AU 605



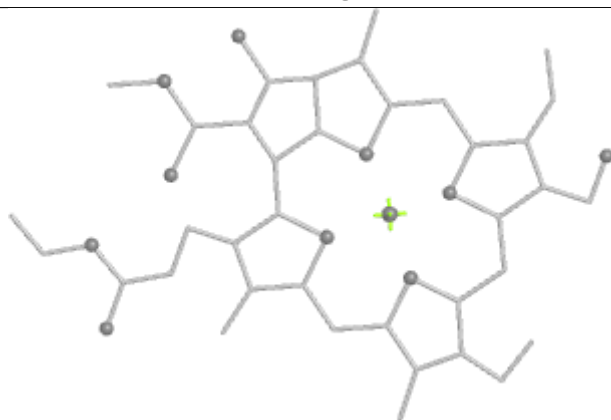
Bond lengths



Bond angles

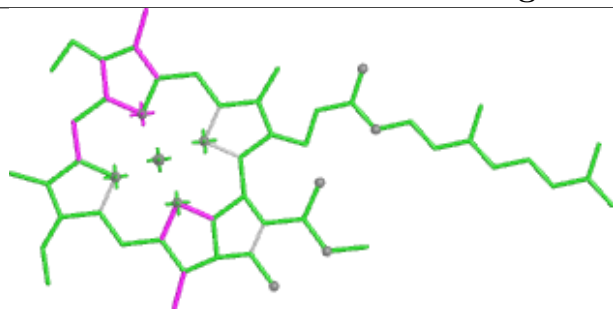


Torsions

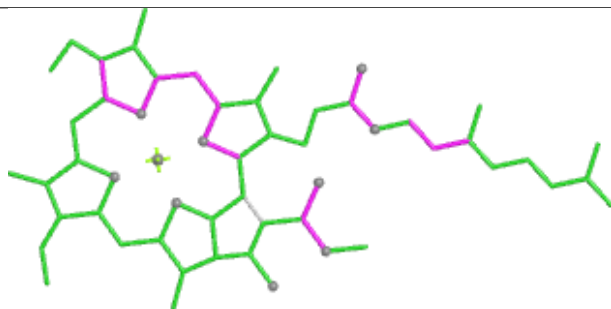


Rings

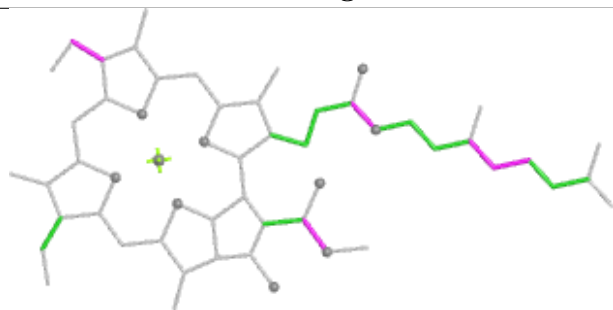
Ligand CLA 9 603



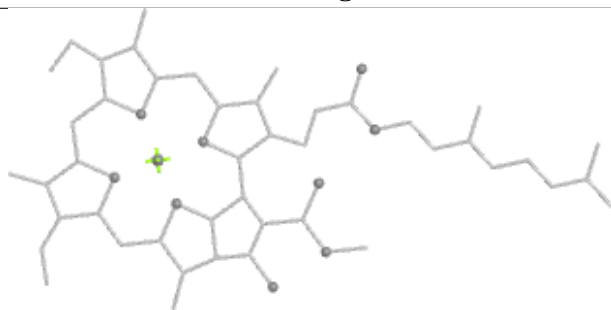
Bond lengths



Bond angles

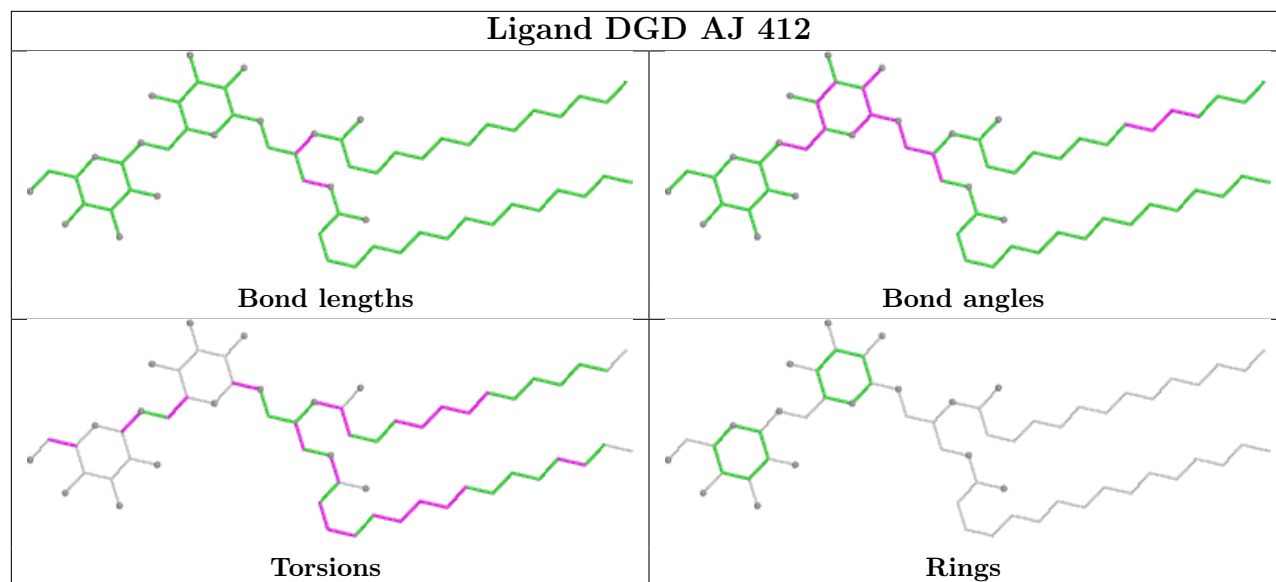


Torsions

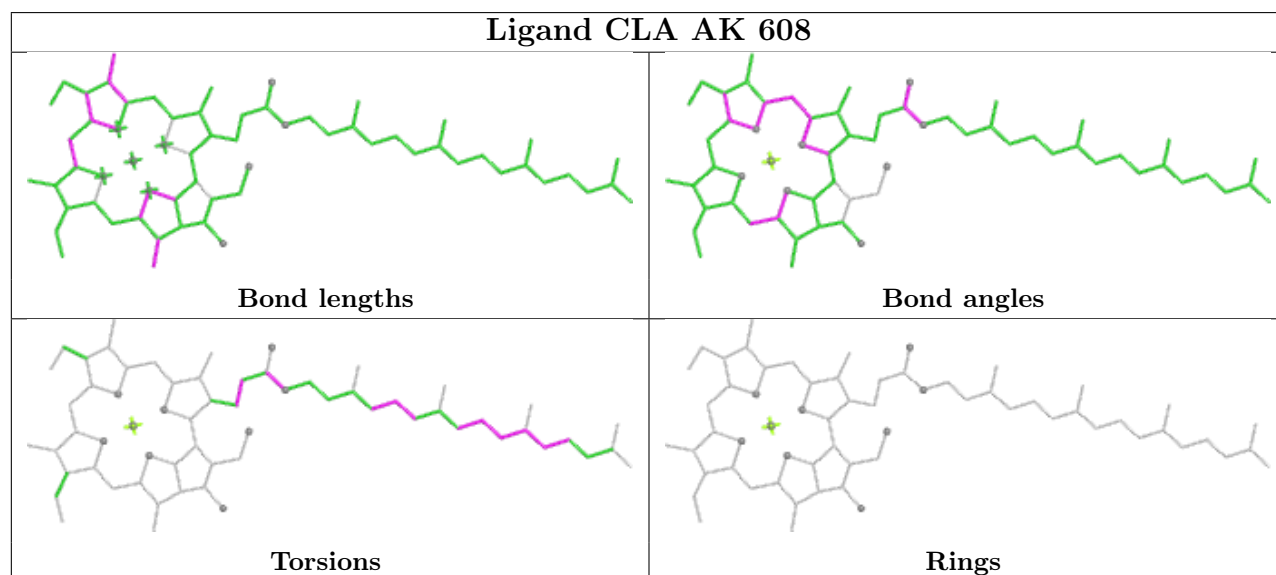


Rings

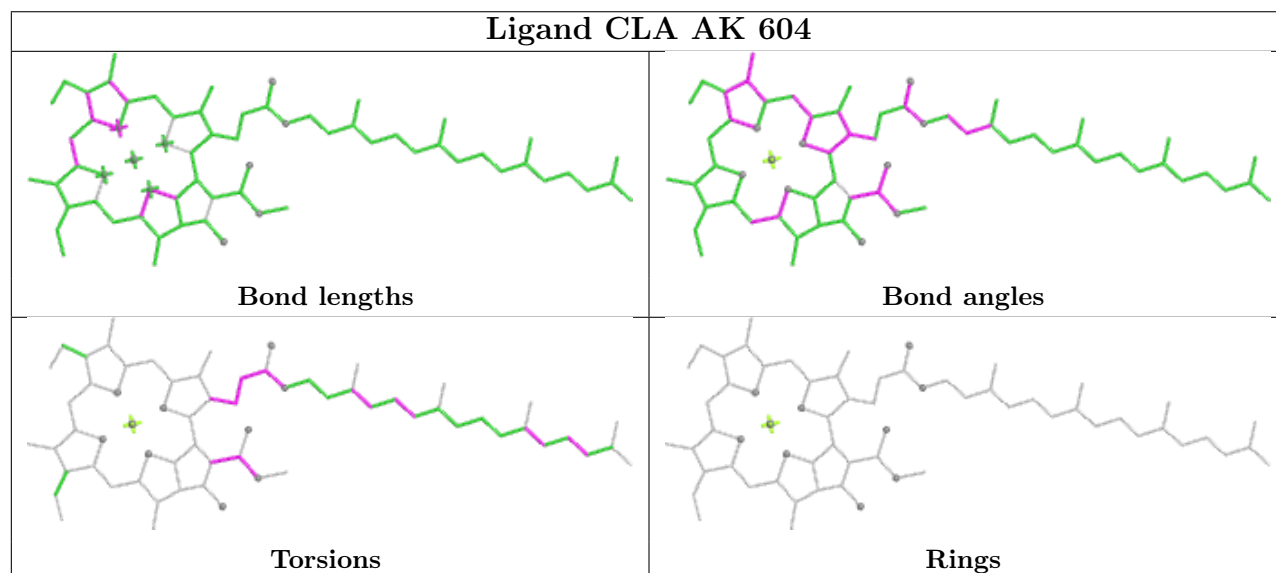
Ligand DGD AJ 412

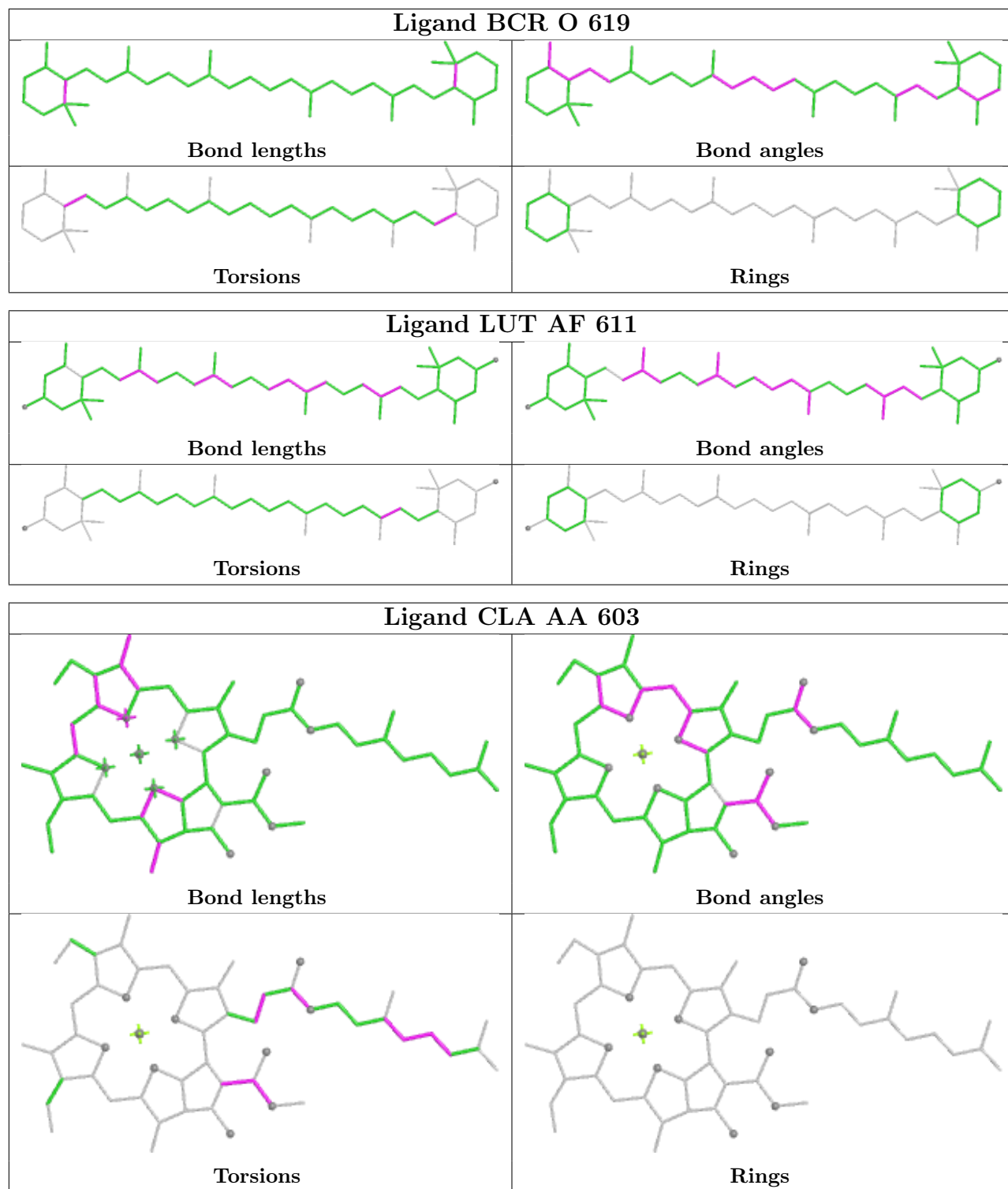


Ligand CLA AK 608

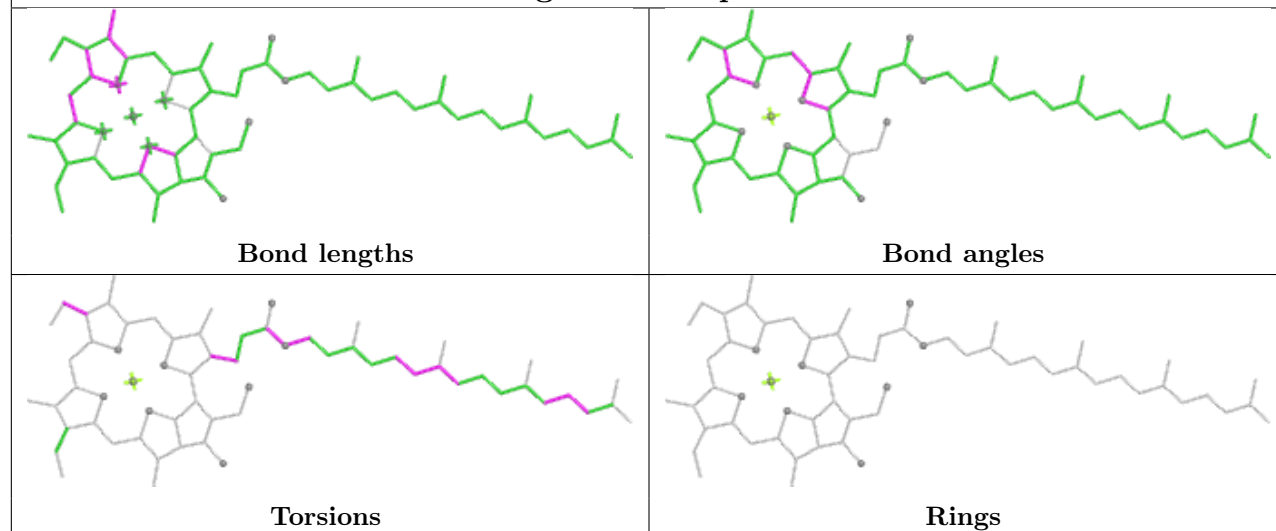


Ligand CLA AK 604

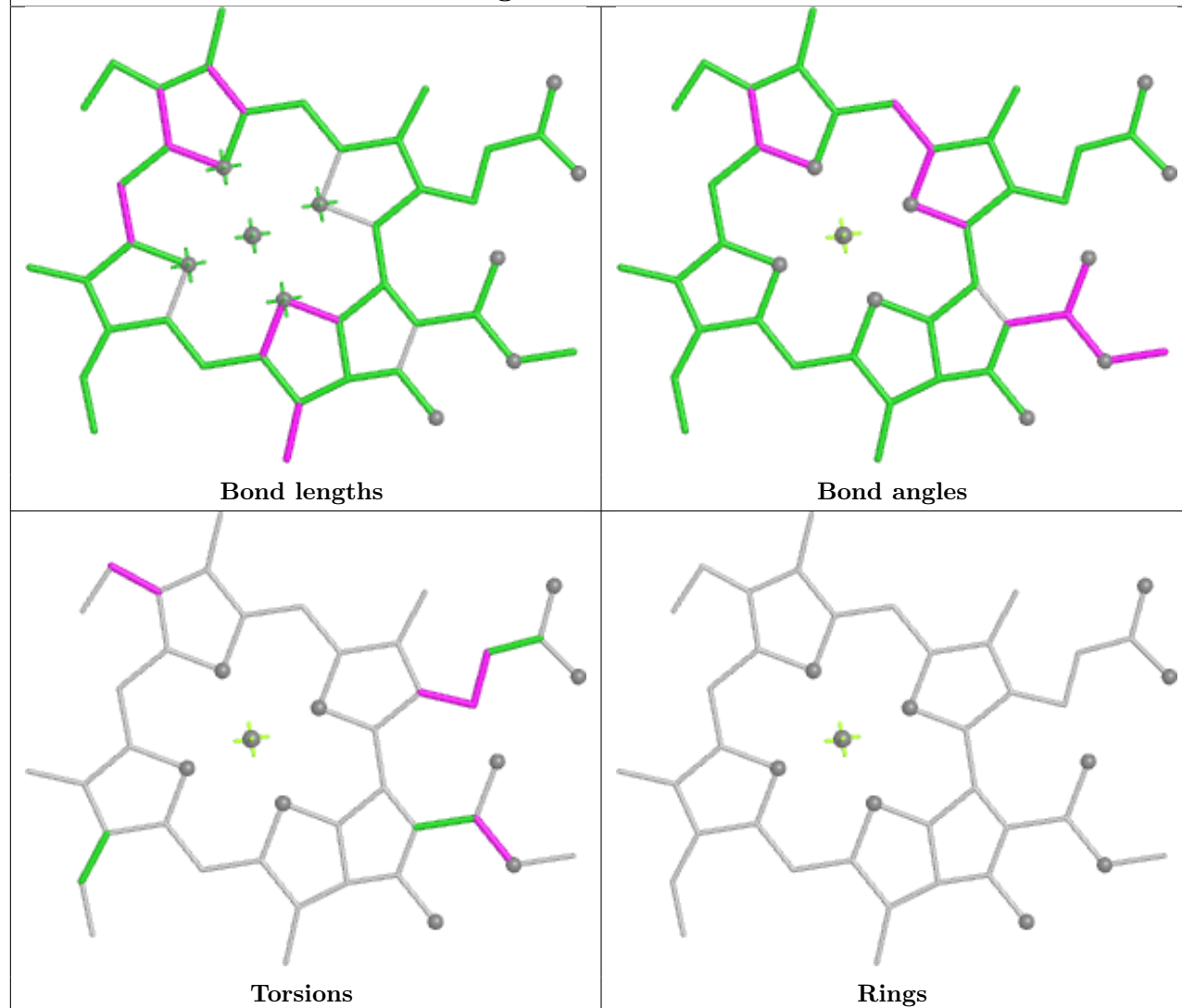


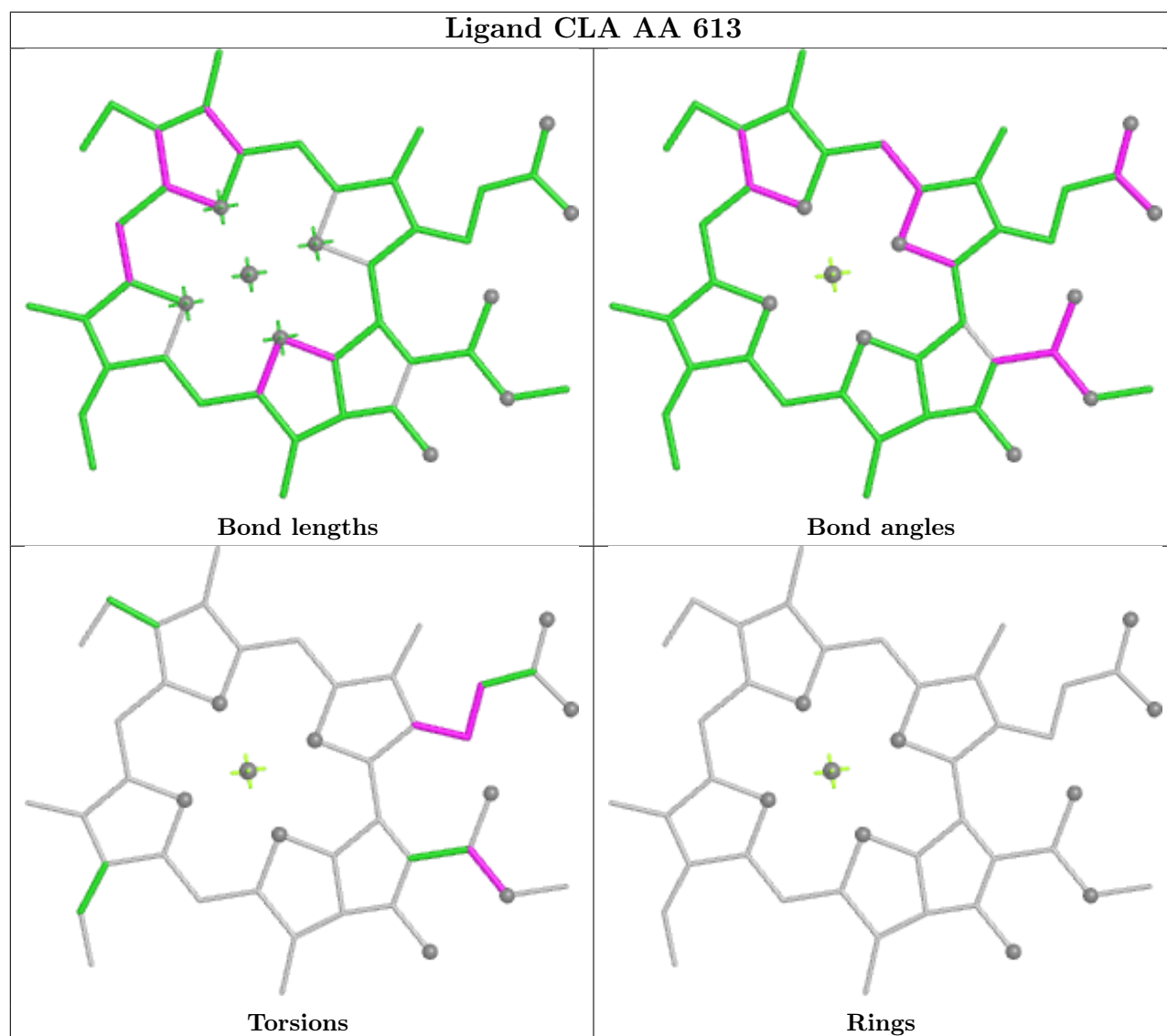
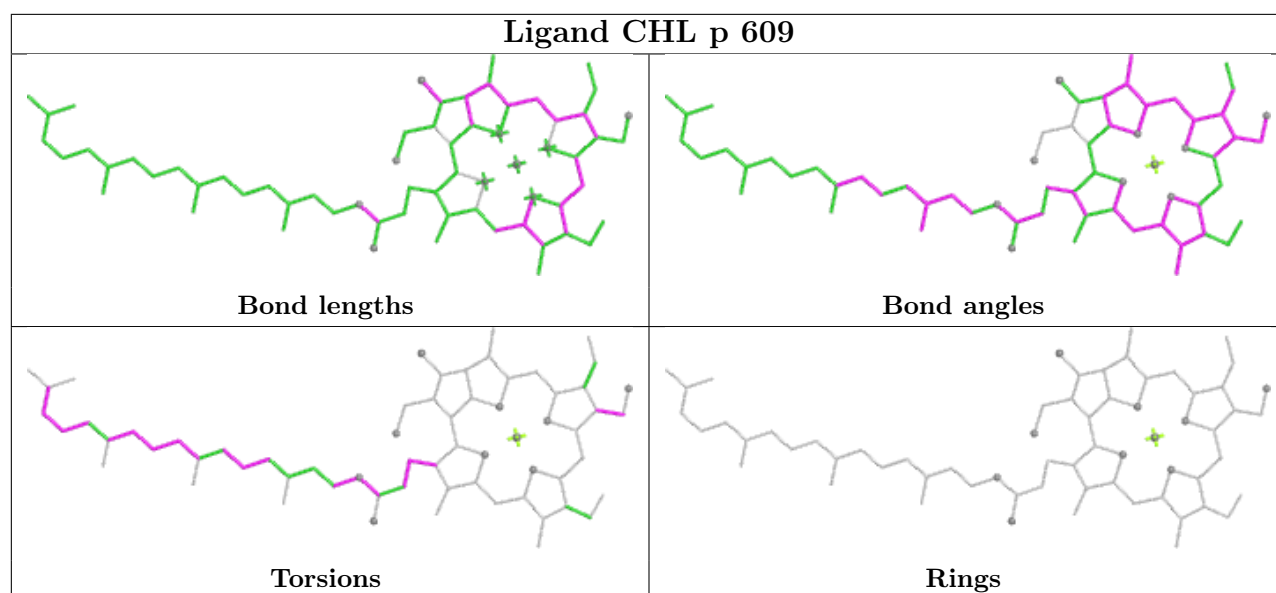


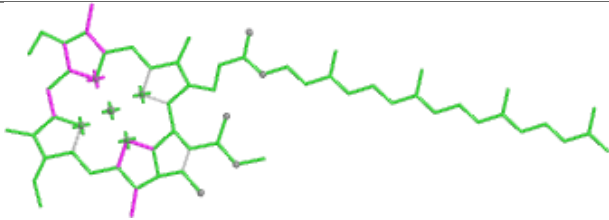
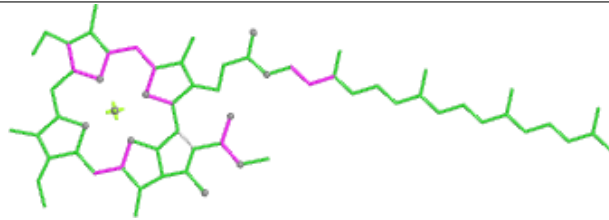
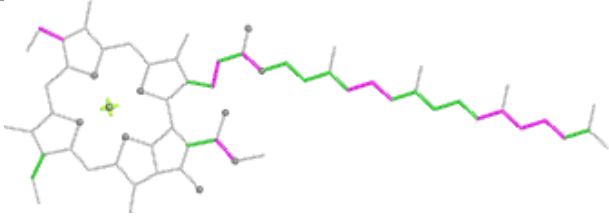
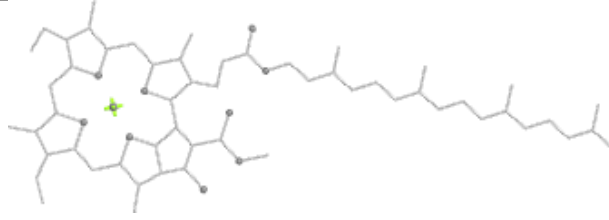
Ligand CLA q 609

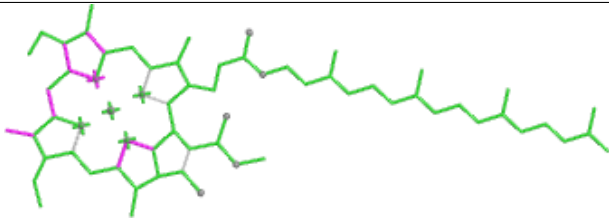
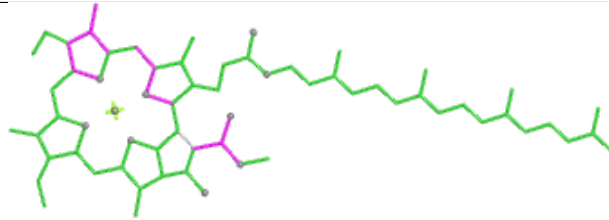
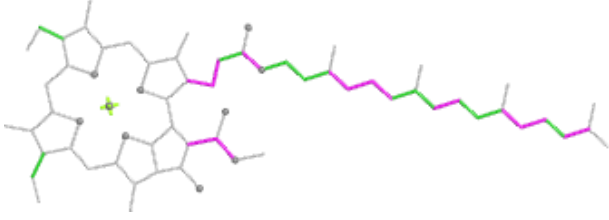
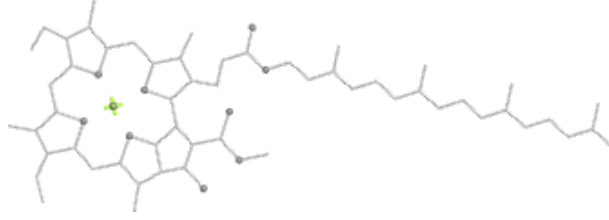


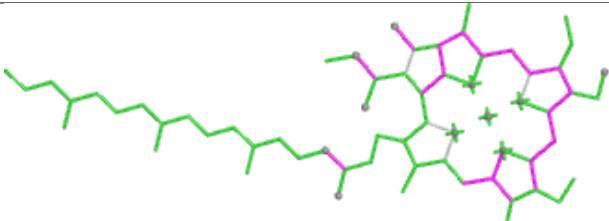
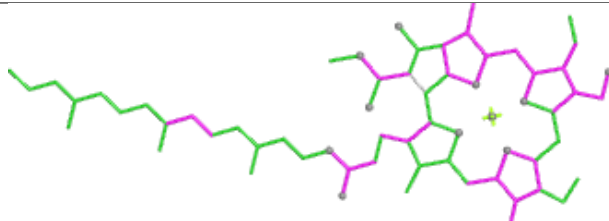
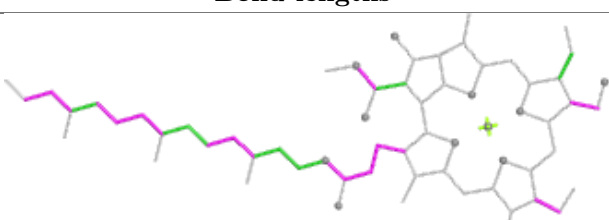
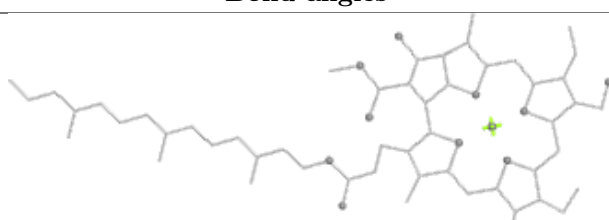
Ligand CLA 0 604

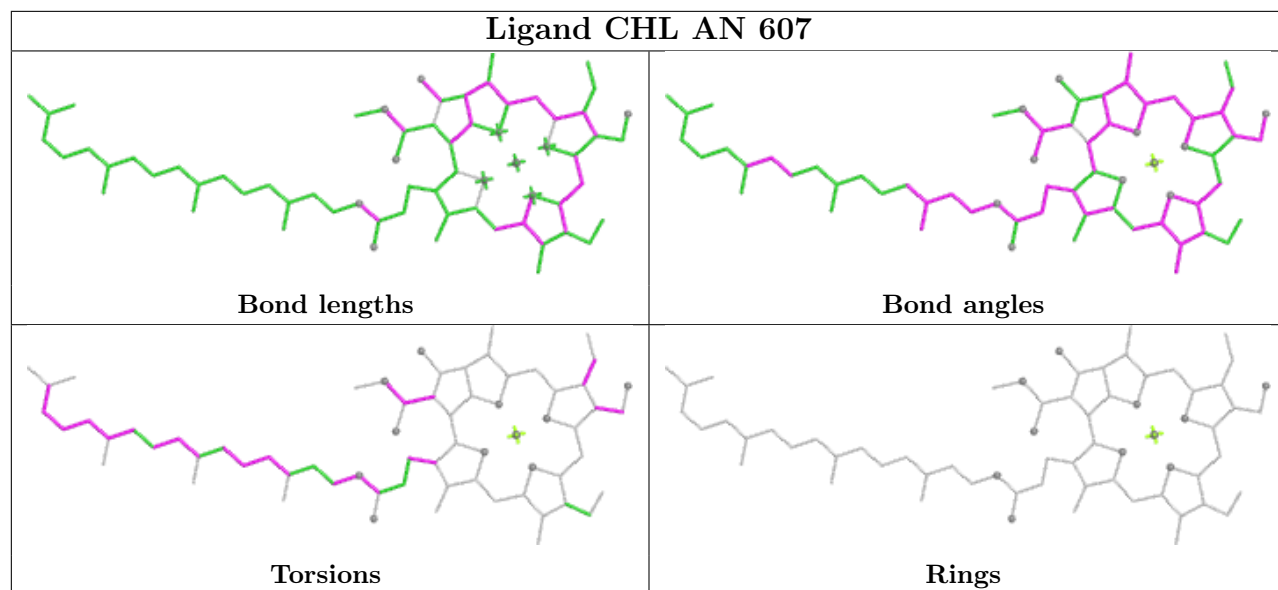




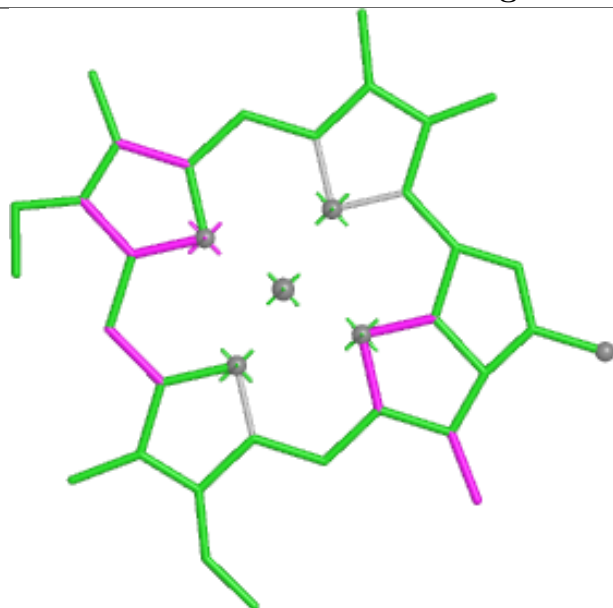
Ligand CLA P 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AL 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

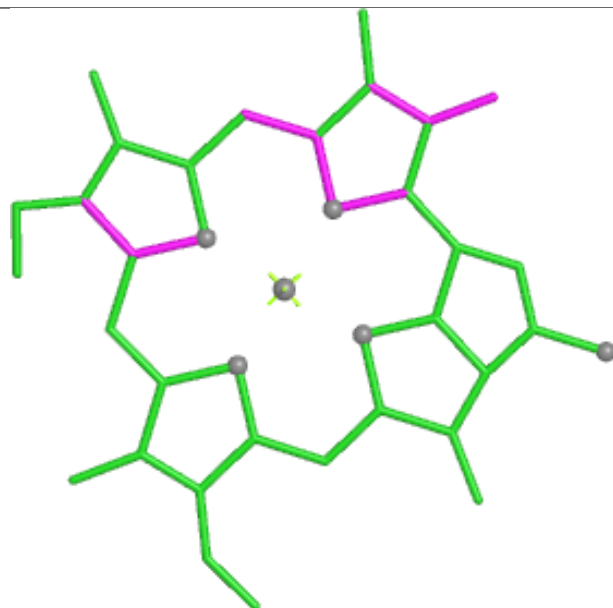
Ligand CHL q 605	
	
Bond lengths	Bond angles
	
Torsions	Rings



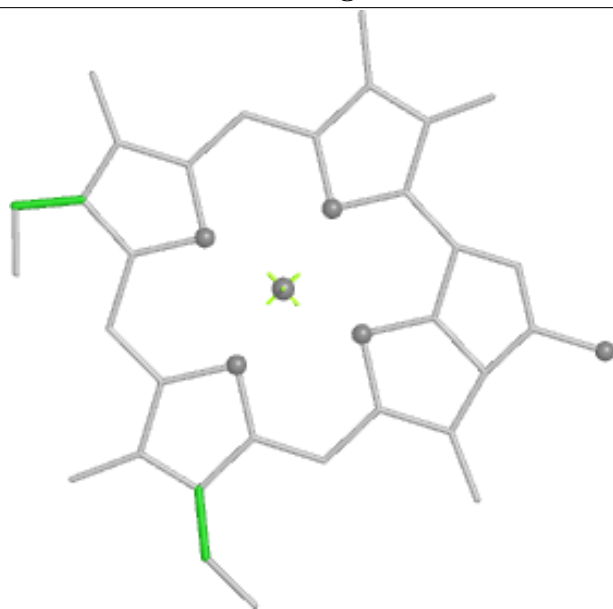
Ligand CLA AN 604



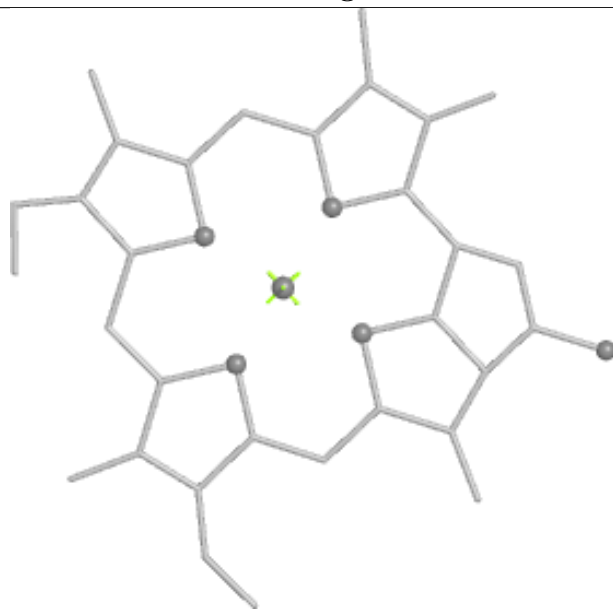
Bond lengths



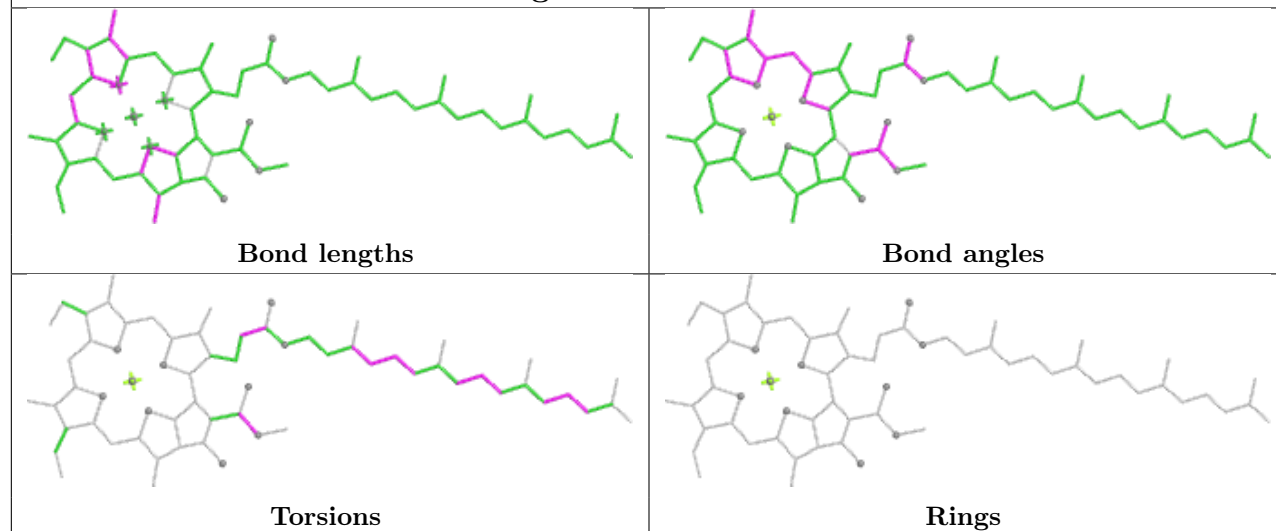
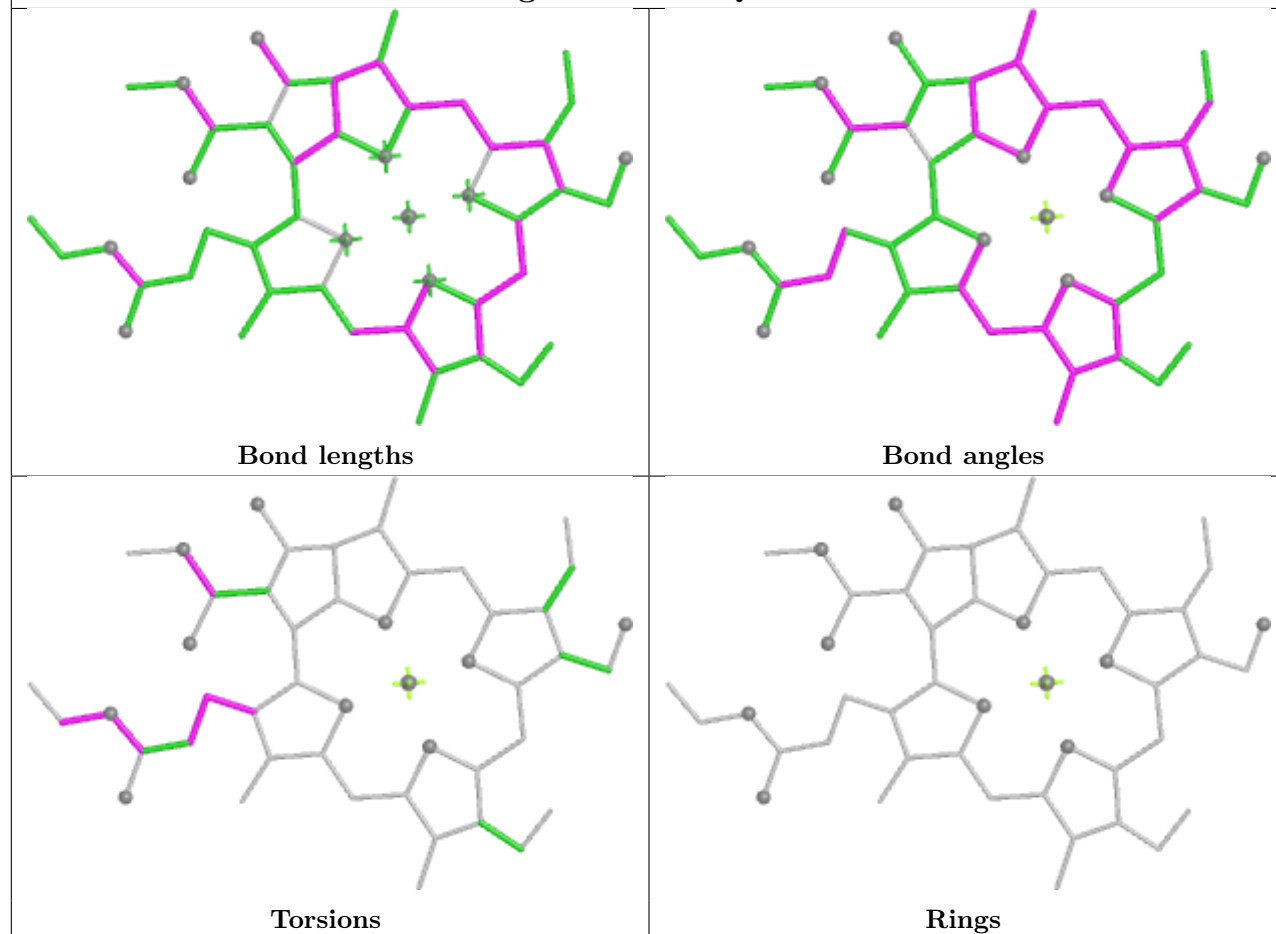
Bond angles

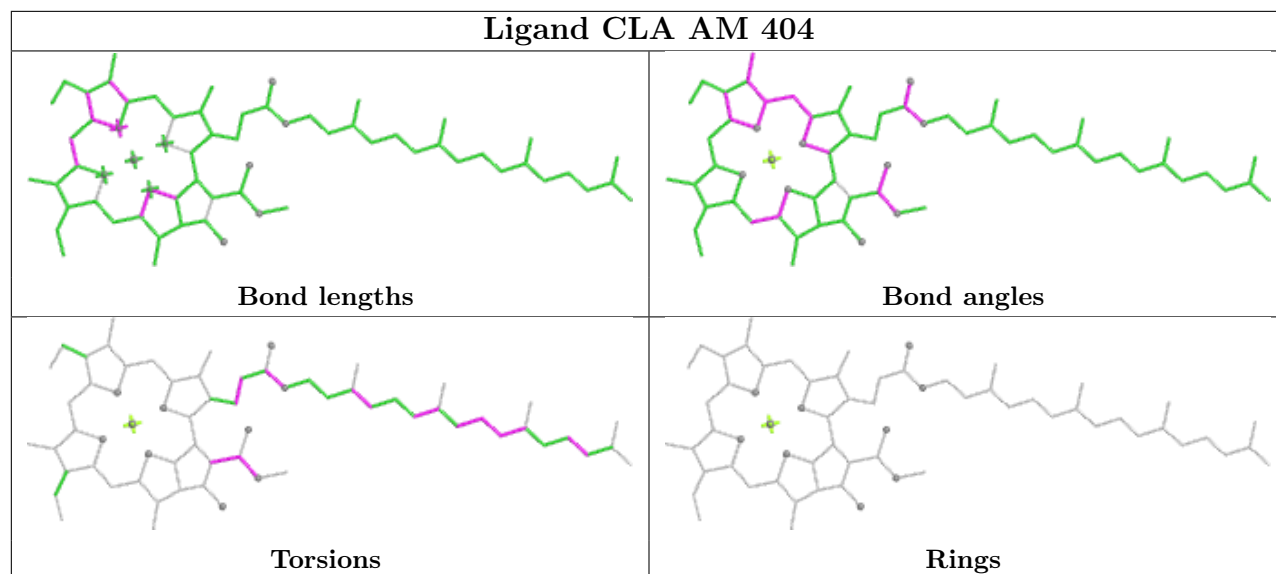
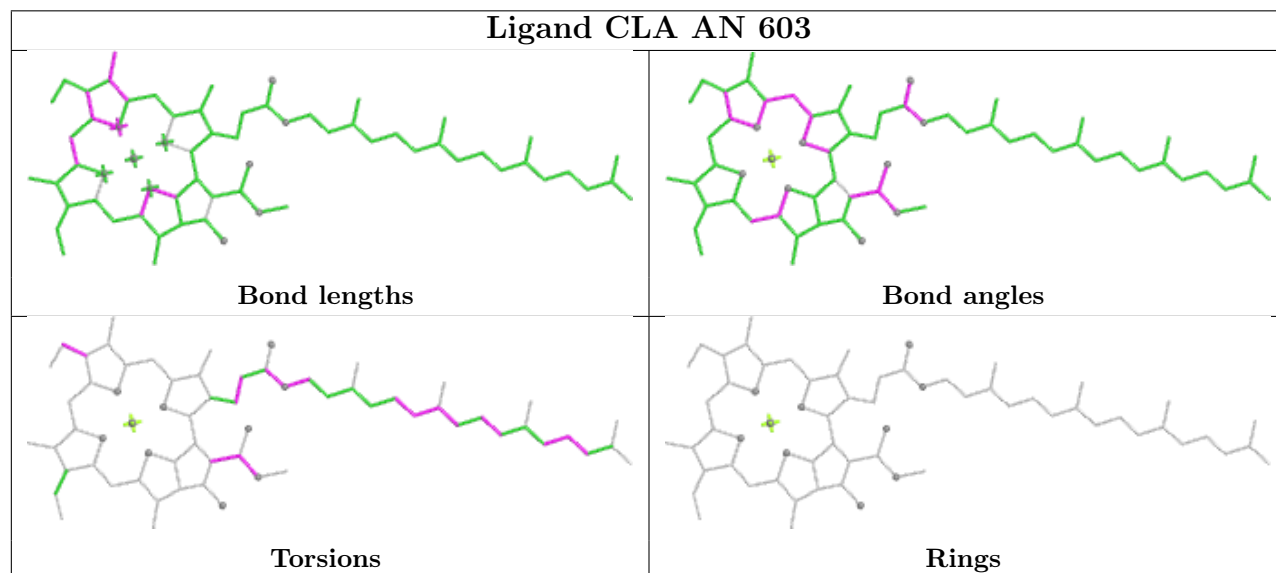
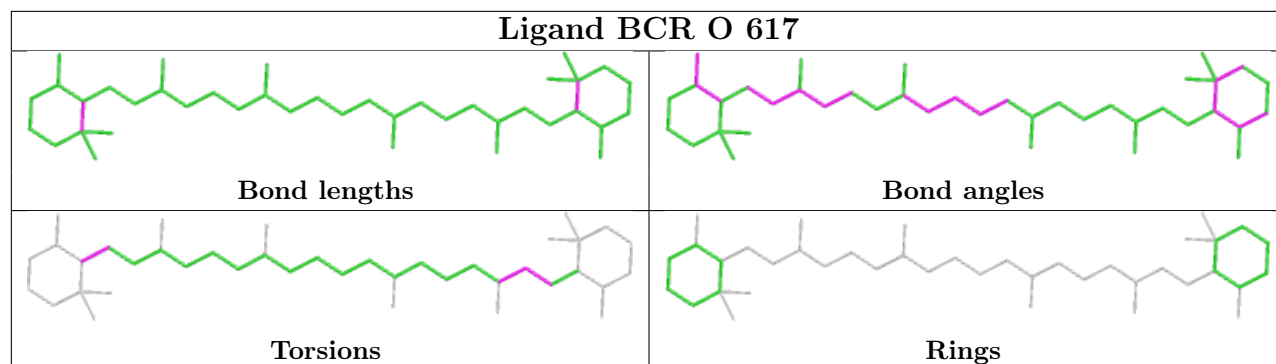


Torsions

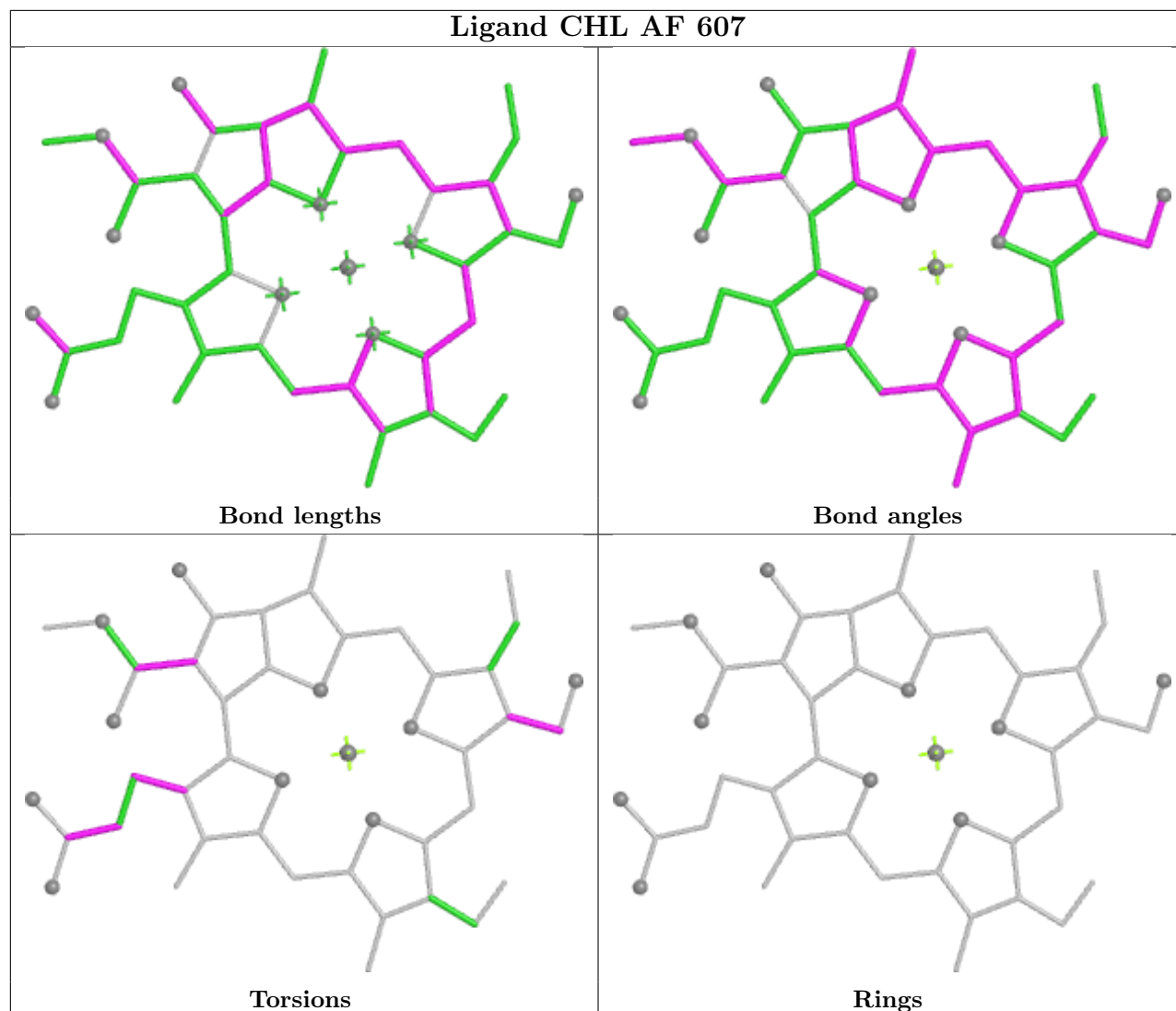


Rings

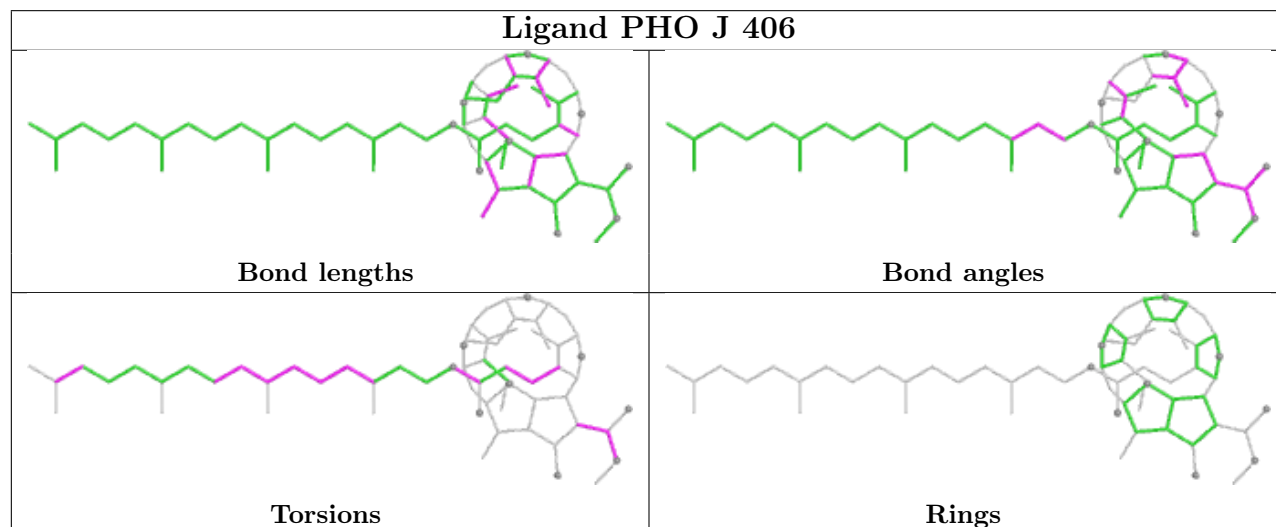
Ligand CLA O 613**Ligand CHL AQ 605**

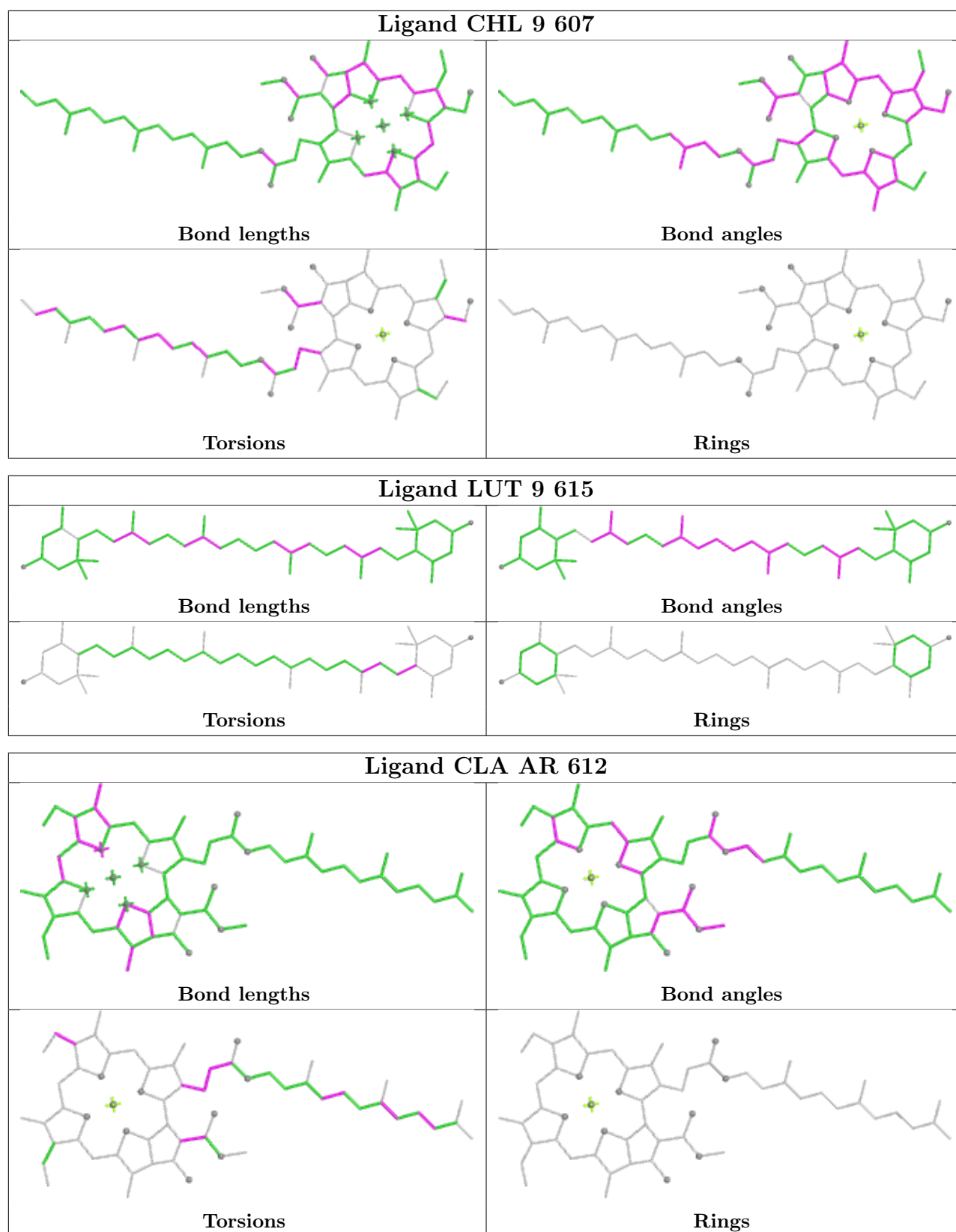
Ligand CLA AM 404**Ligand CLA AN 603****Ligand BCR O 617**

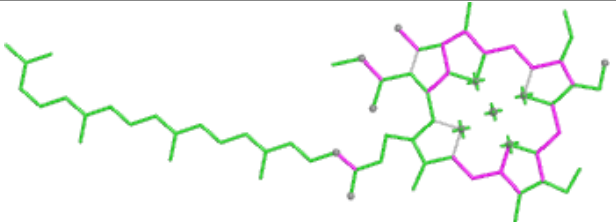
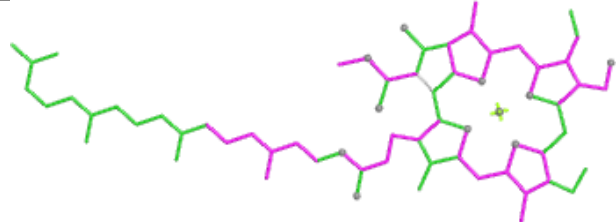
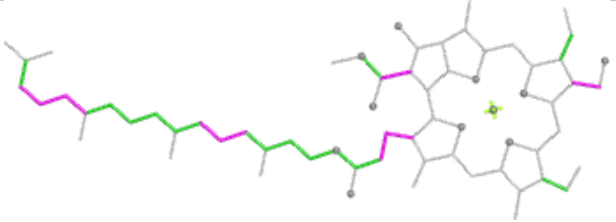
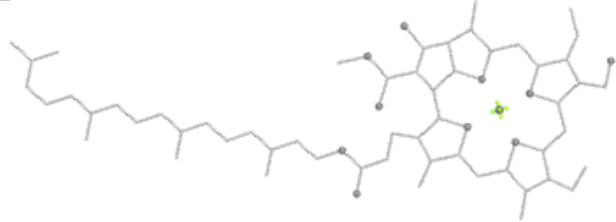
Ligand CHL AF 607

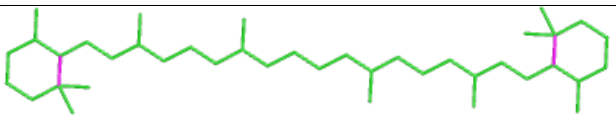
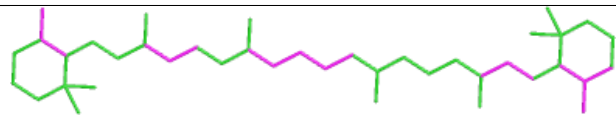
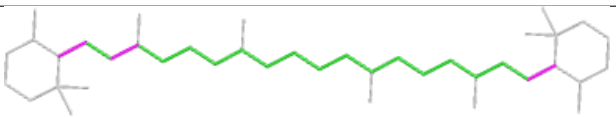
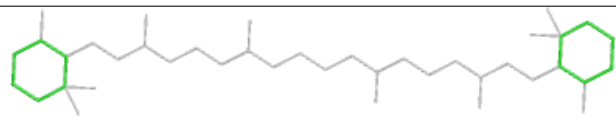


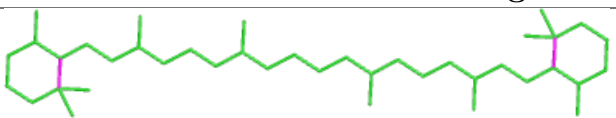
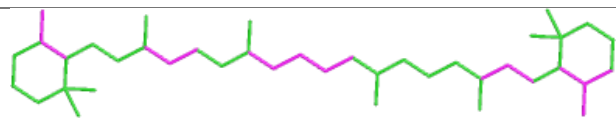
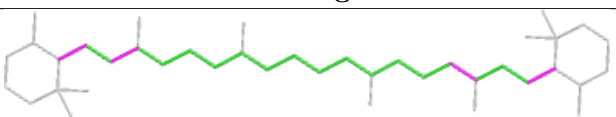
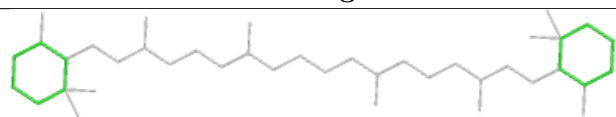
Ligand PHO J 406

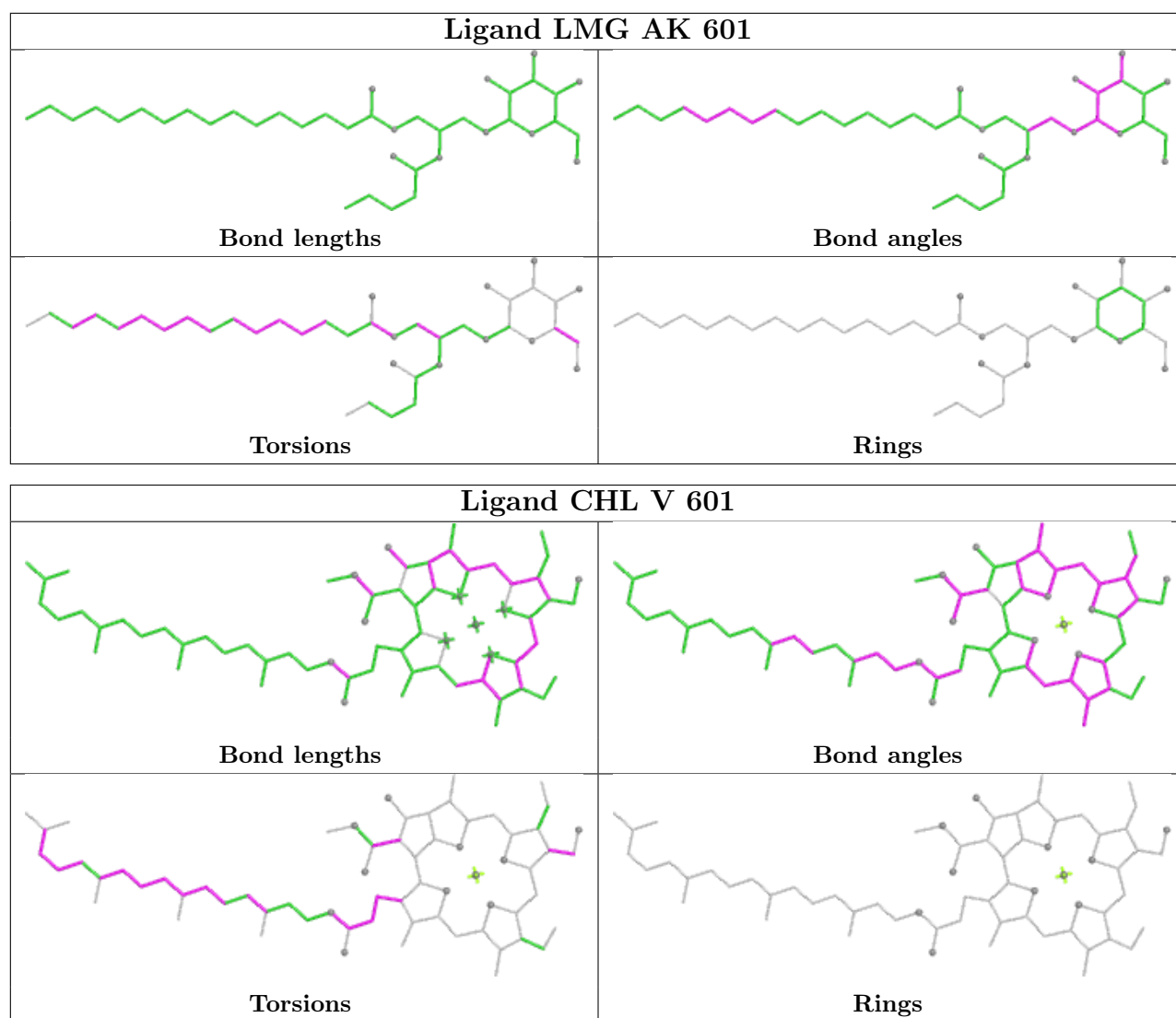


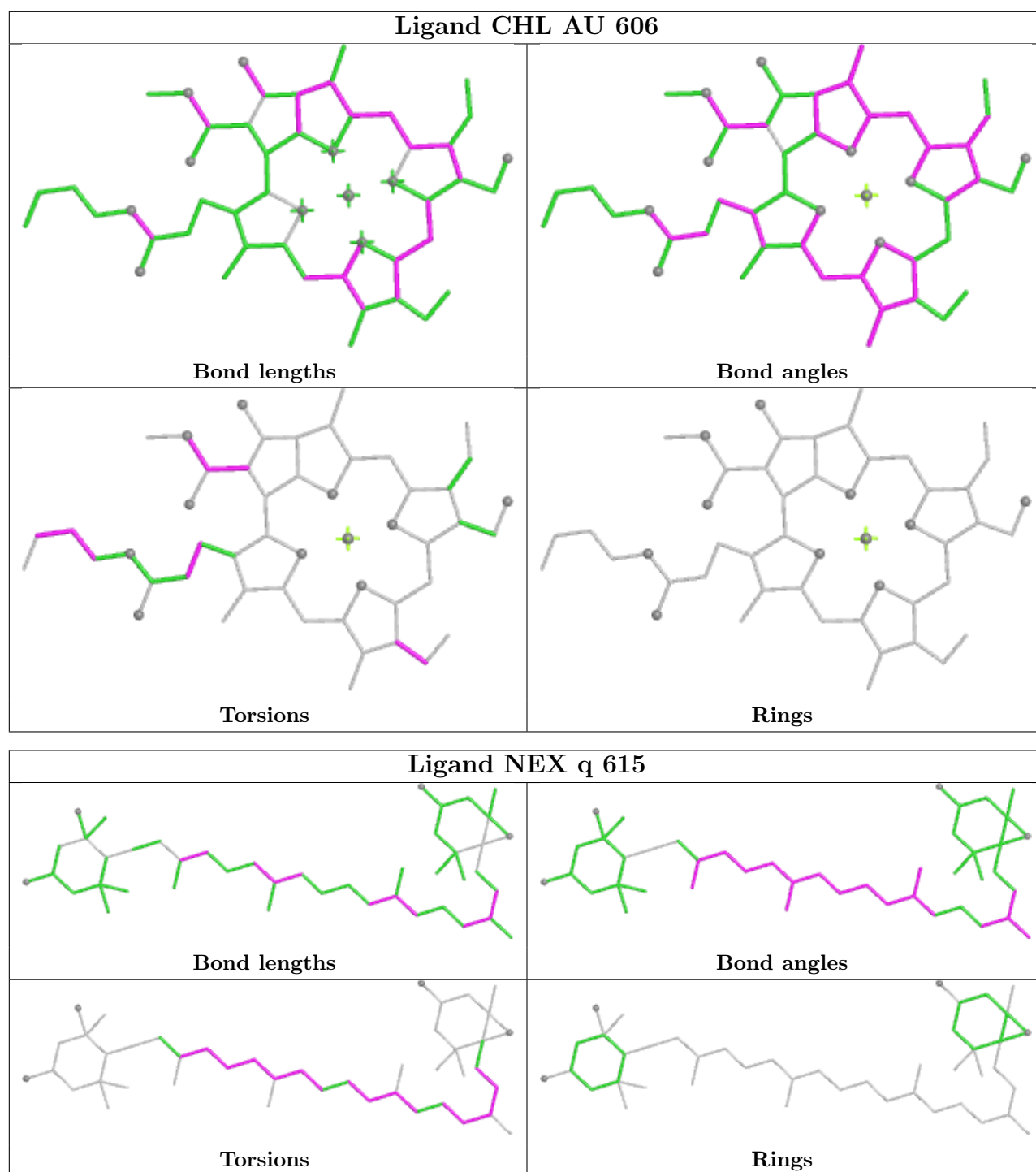


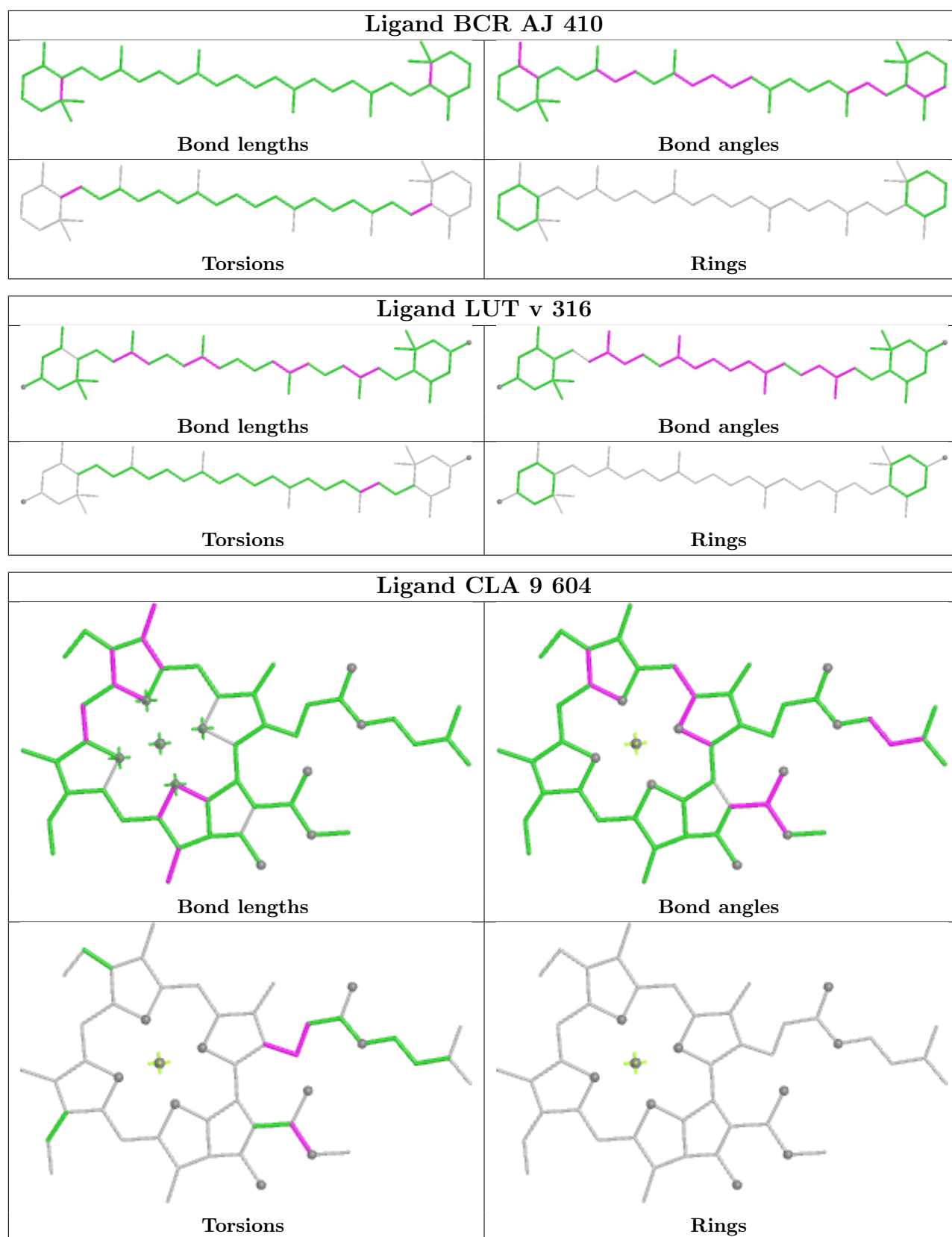
Ligand CHL p 608	
	Bond lengths
	Bond angles
	Torsions
	Rings

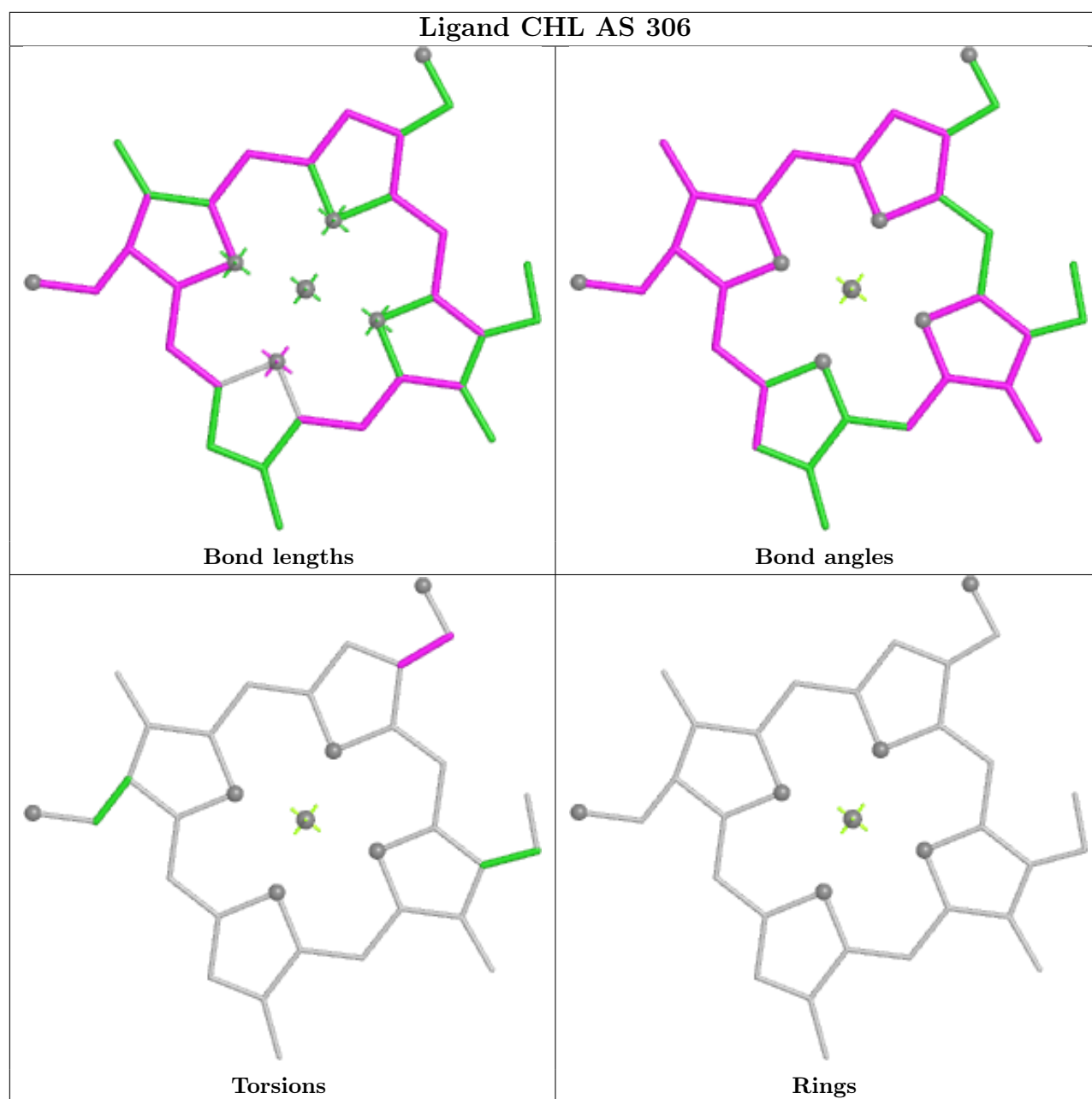
Ligand BCR k 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand BCR P 515	
	Bond lengths
	Bond angles
	Torsions
	Rings

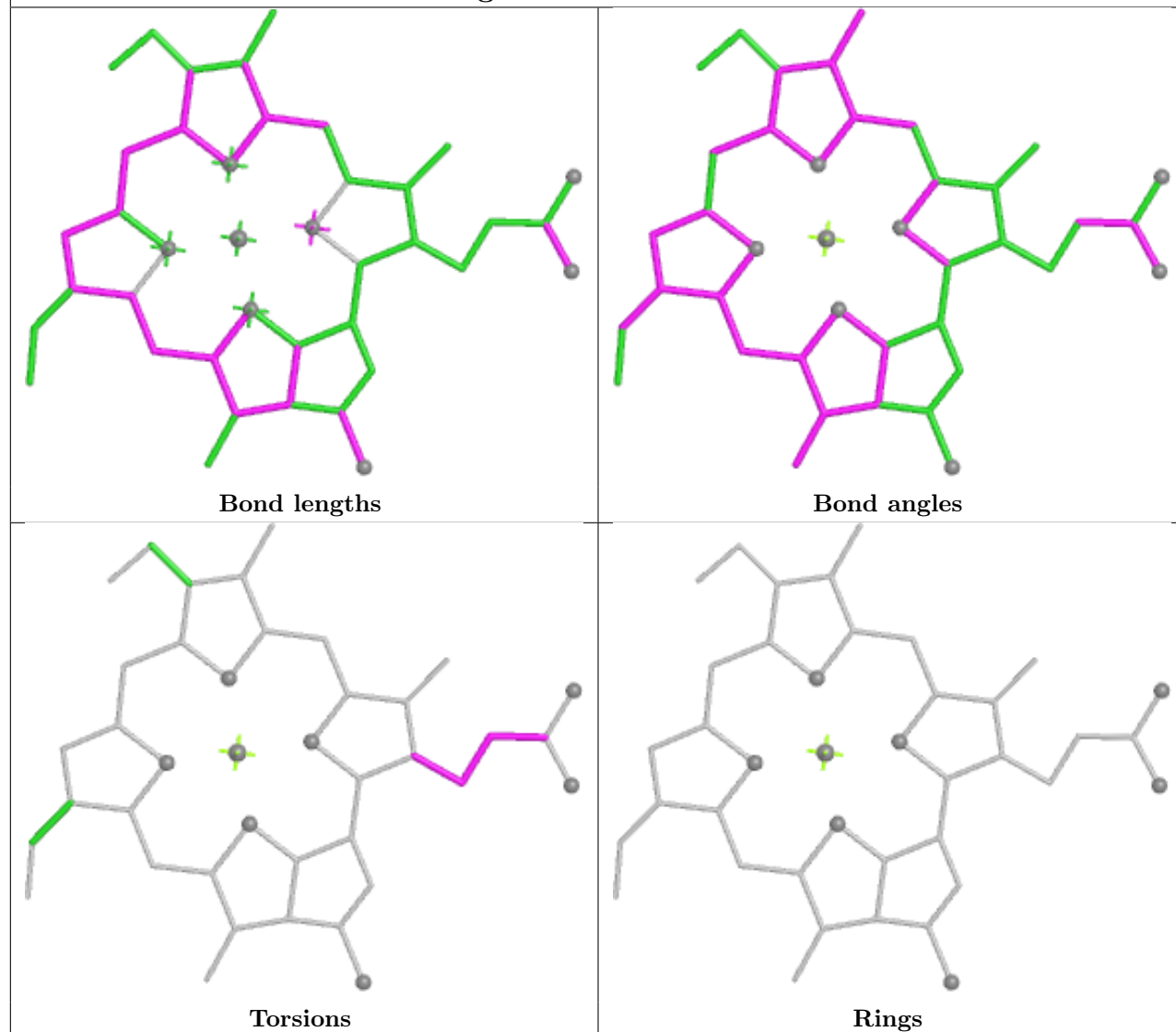




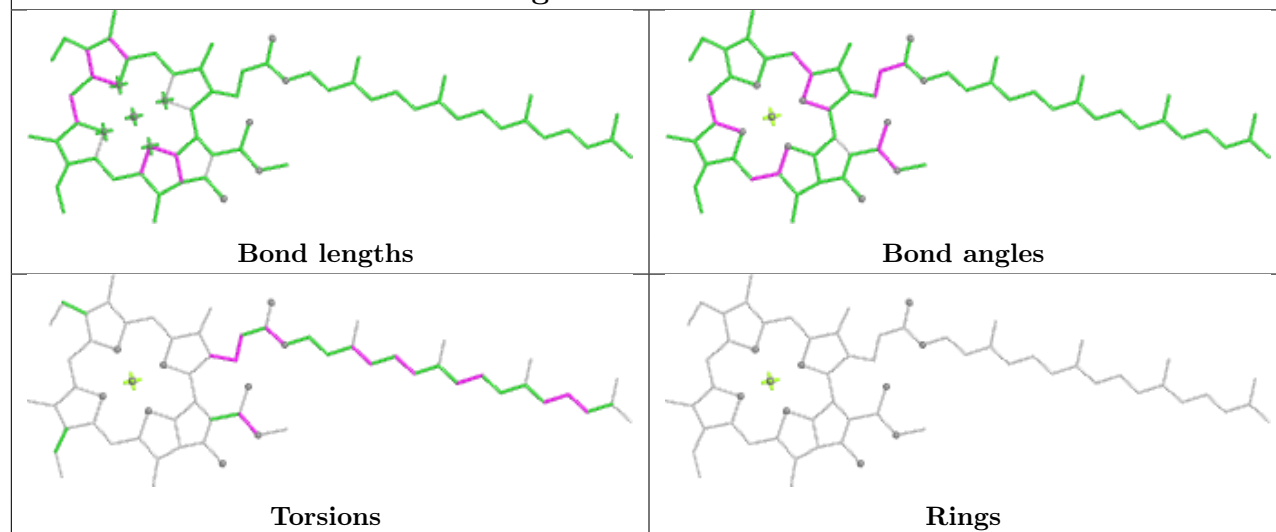


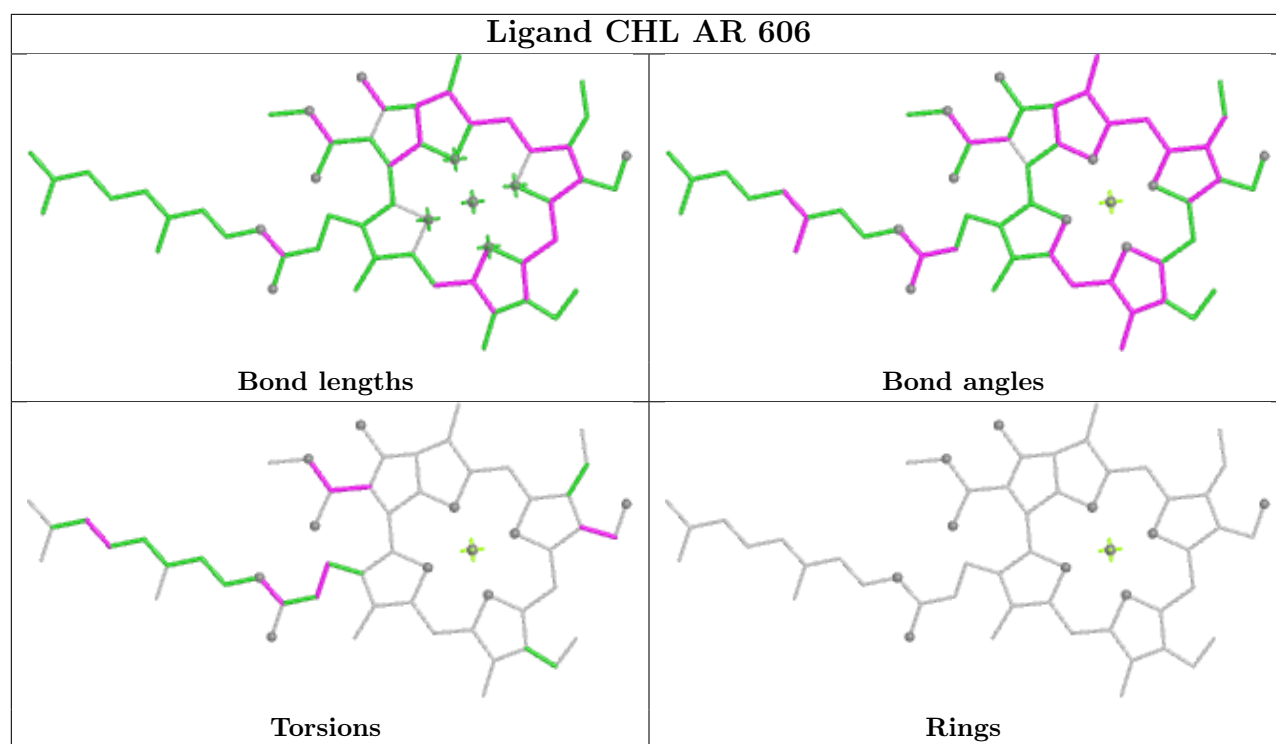


Ligand CHL AB 605

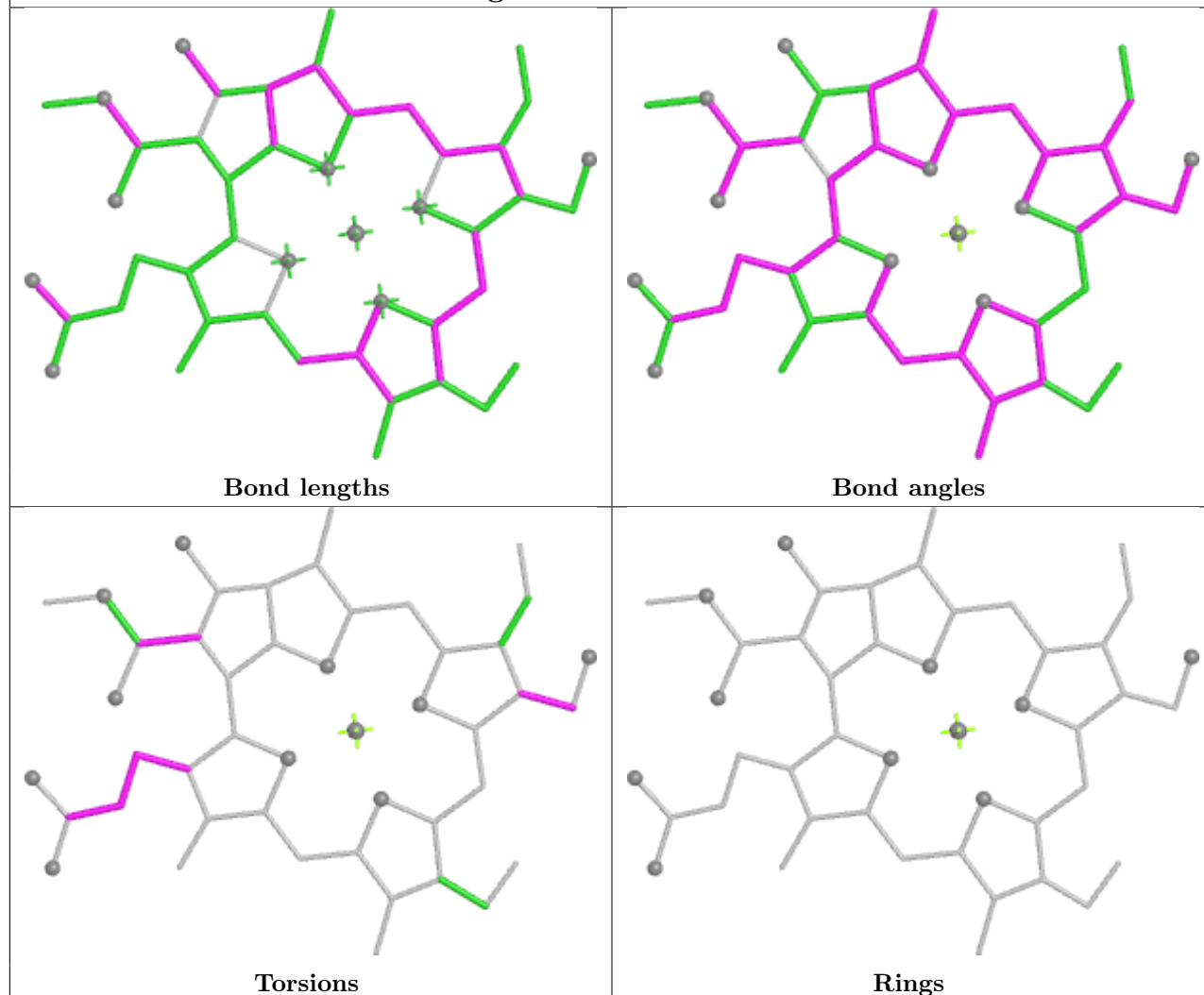


Ligand CLA O 608

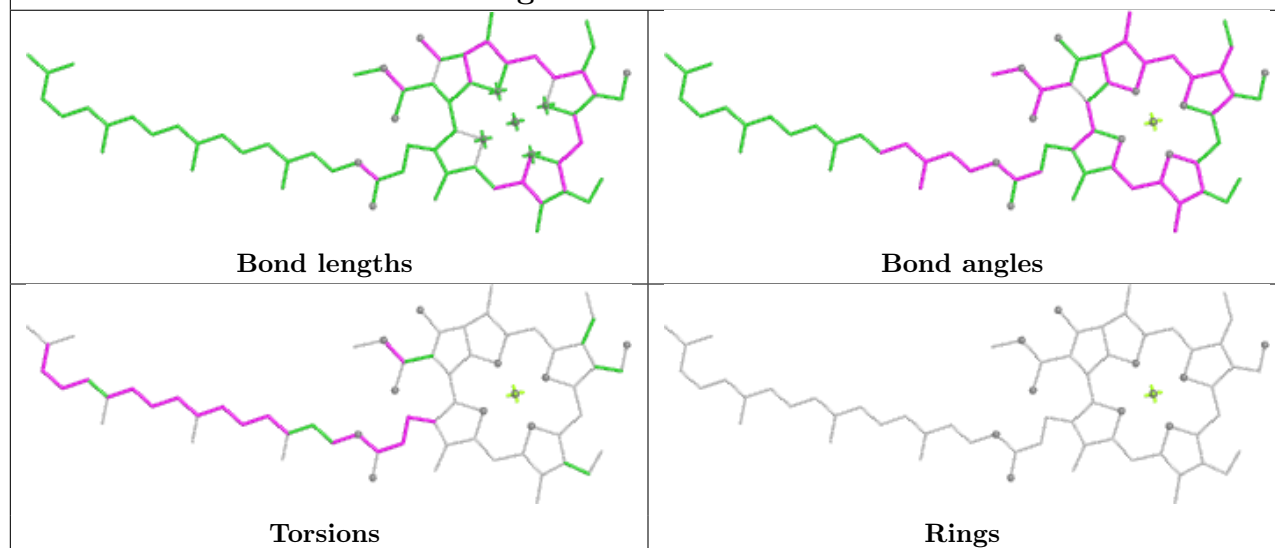


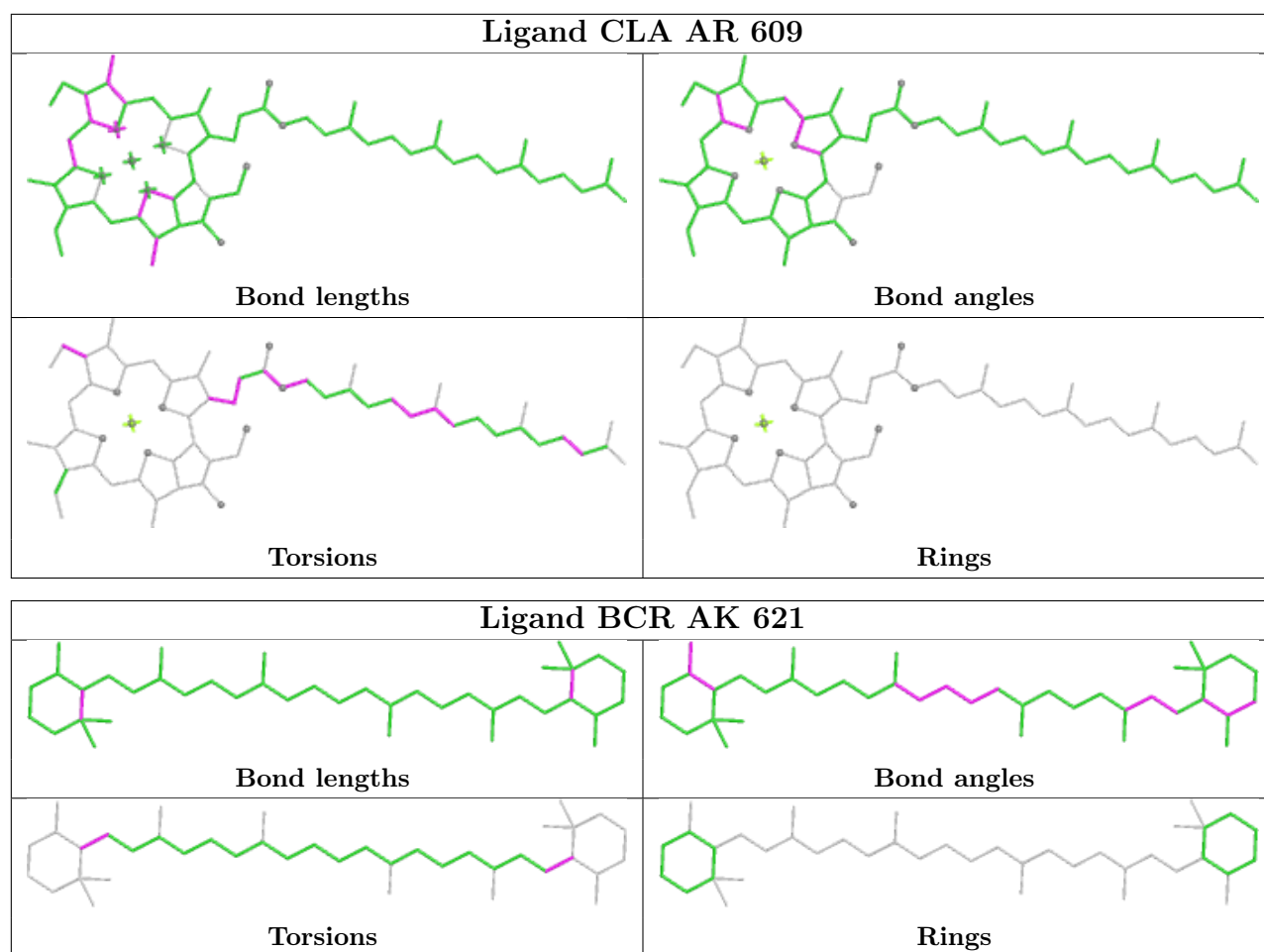


Ligand CHL AD 307

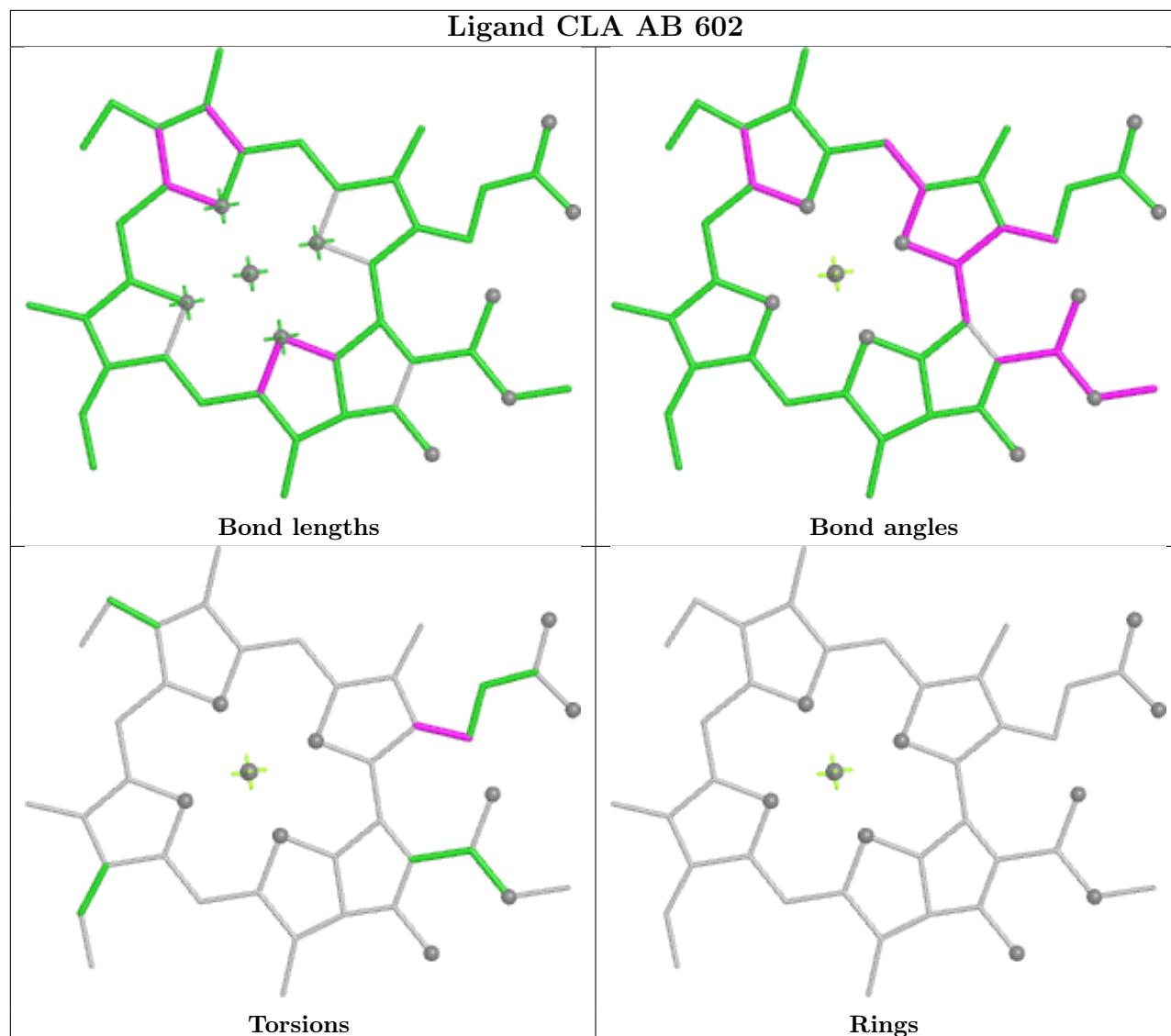


Ligand CHL AU 601

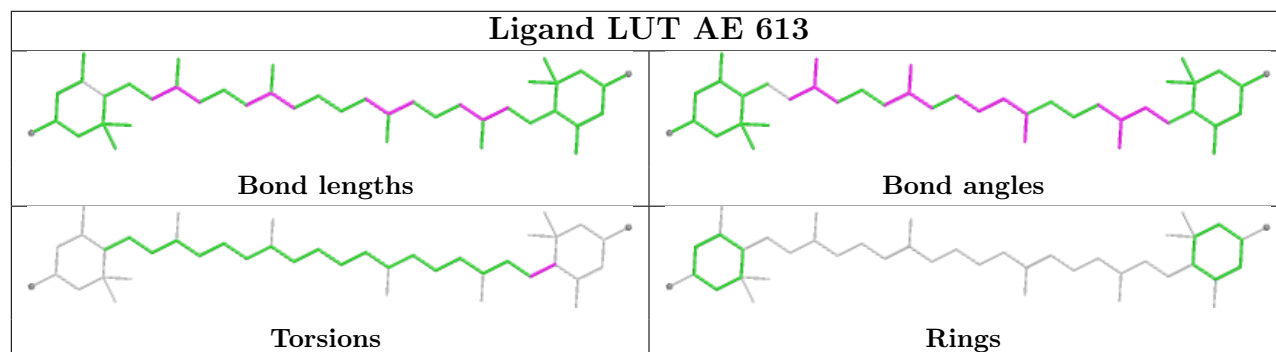


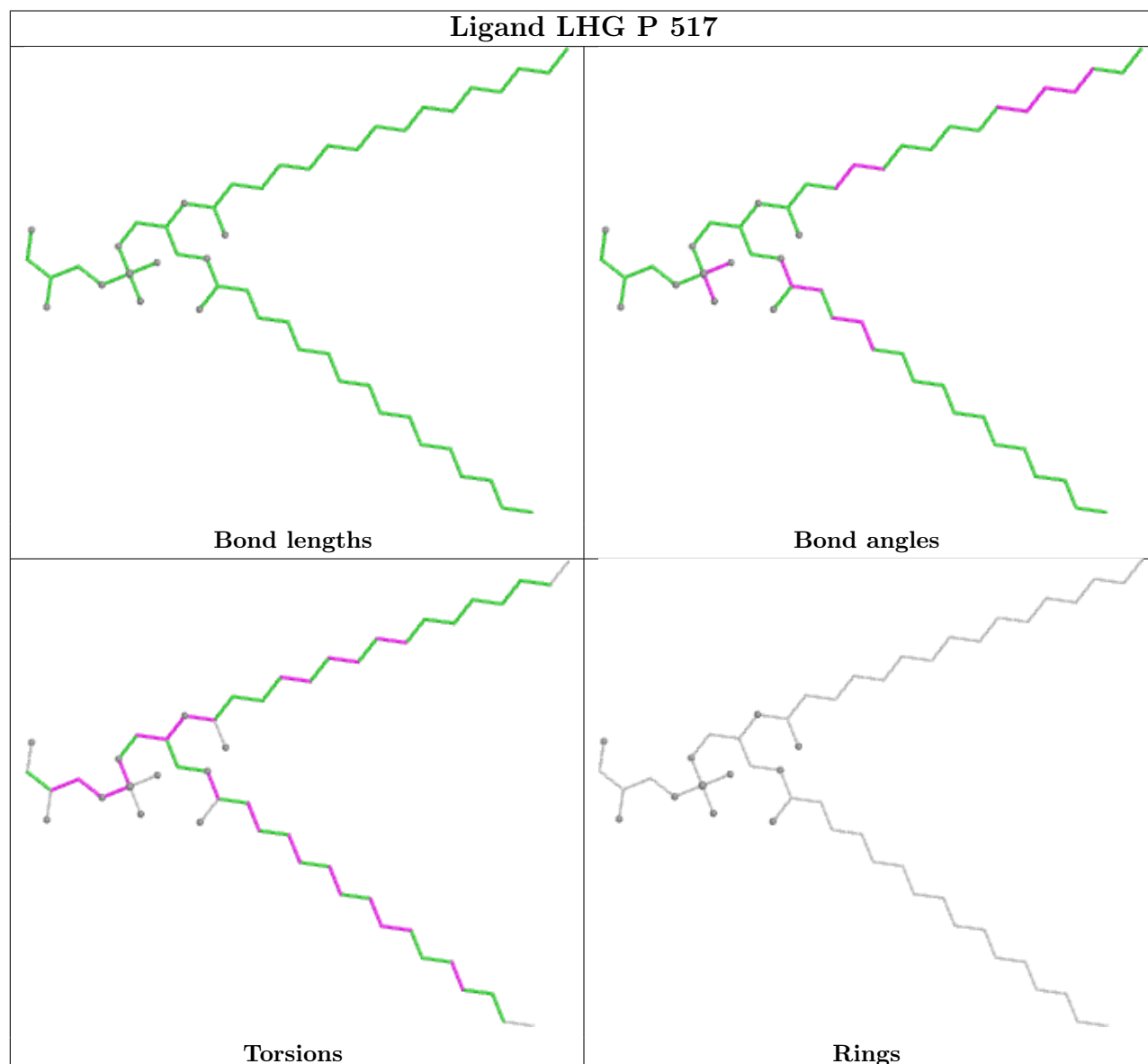
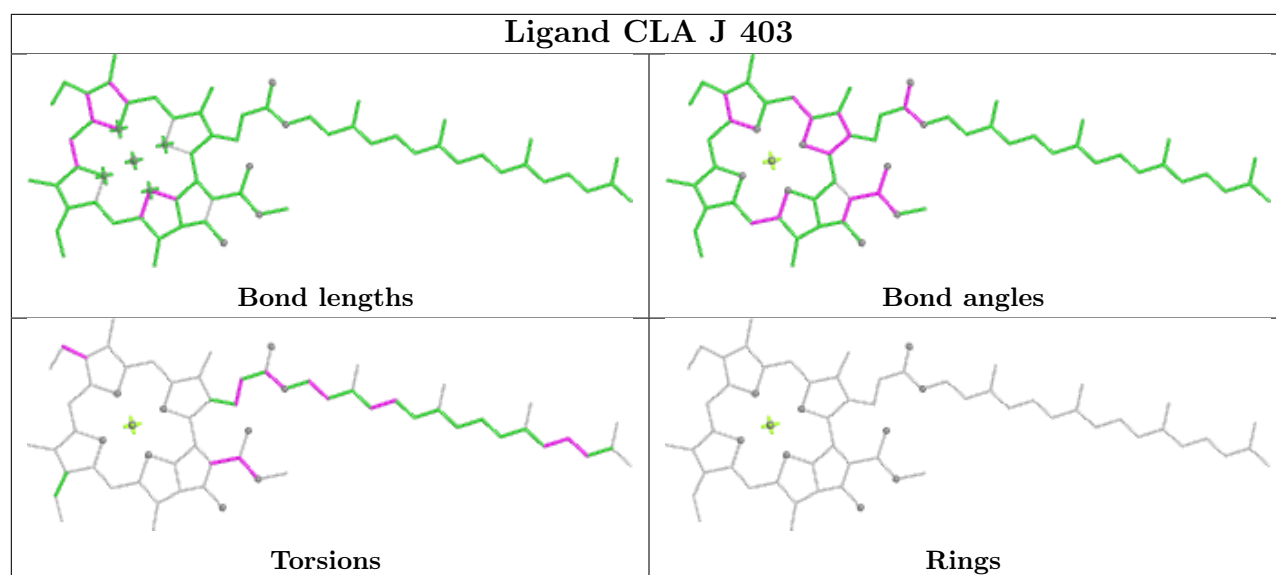


Ligand CLA AB 602

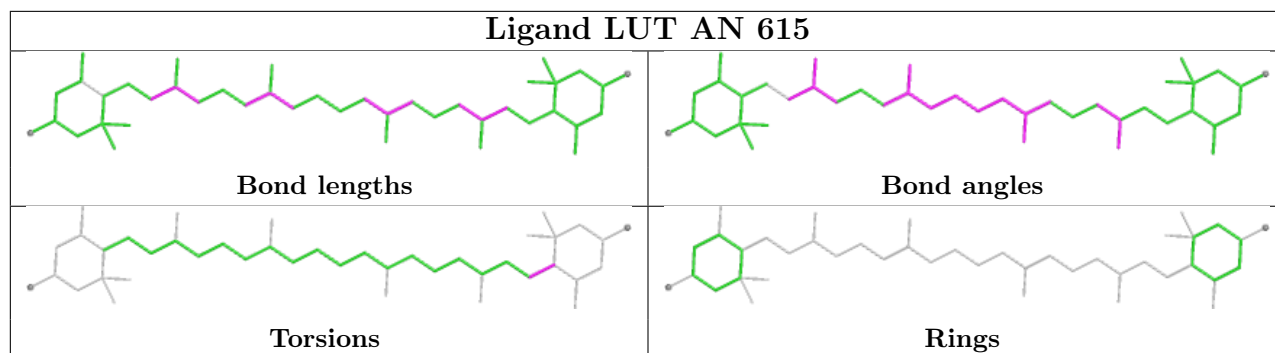


Ligand LUT AE 613

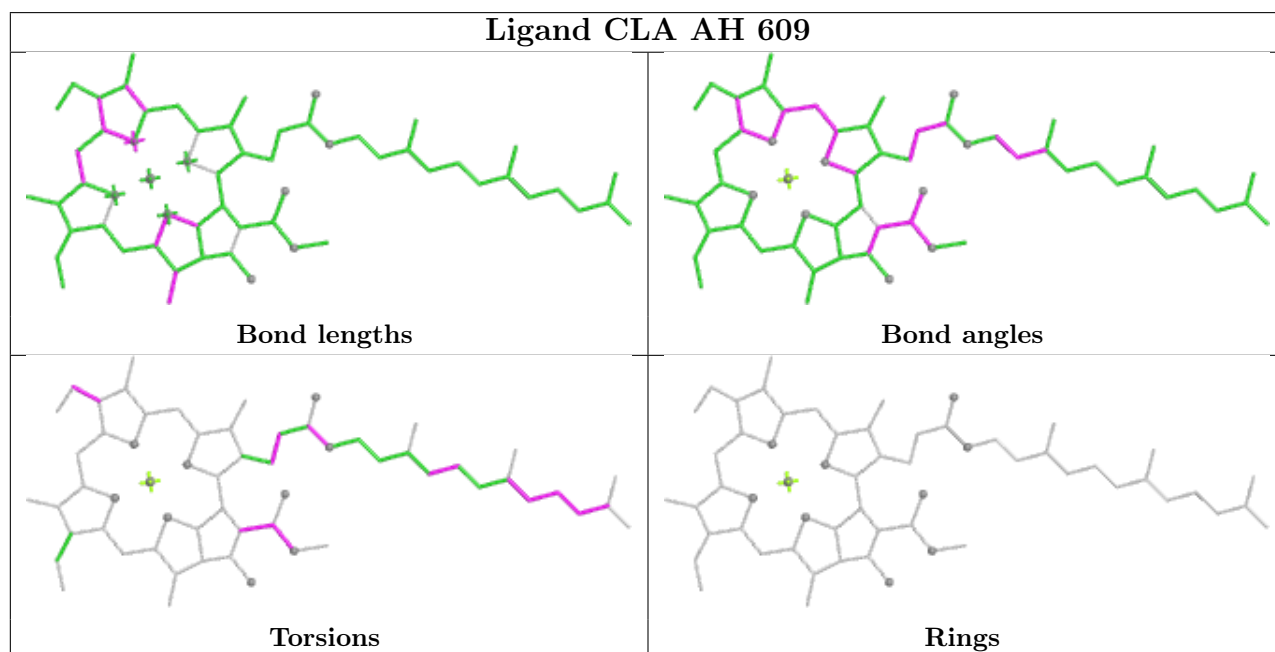




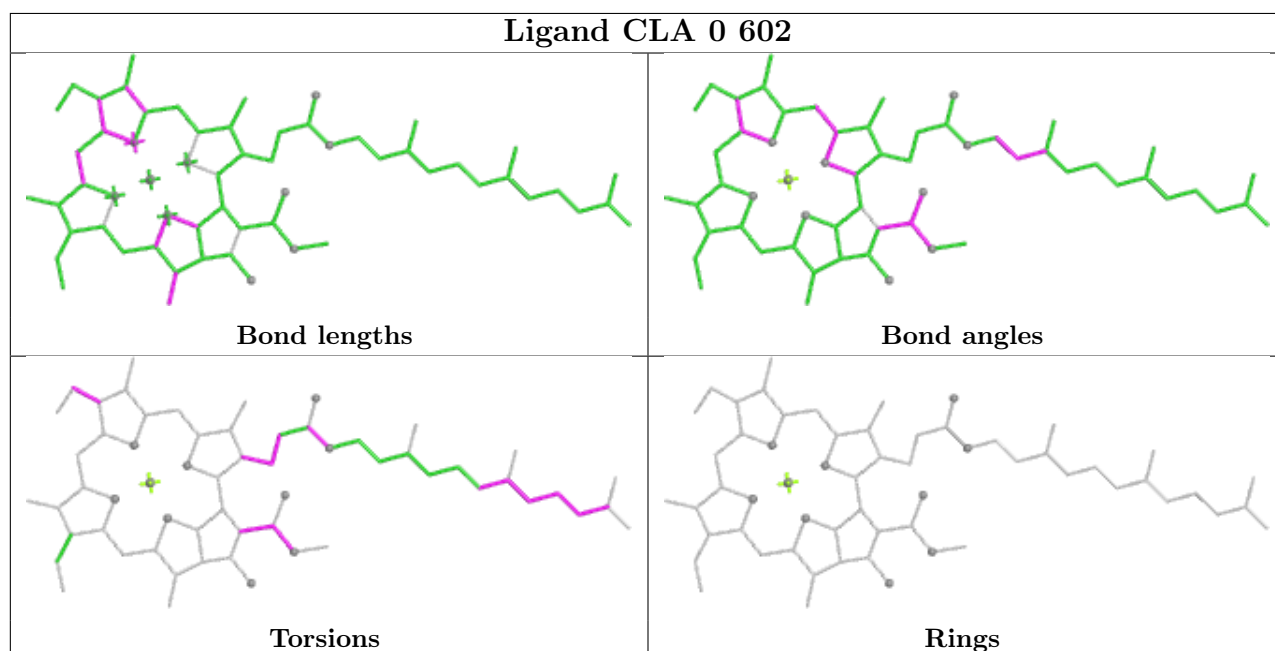
Ligand LUT AN 615



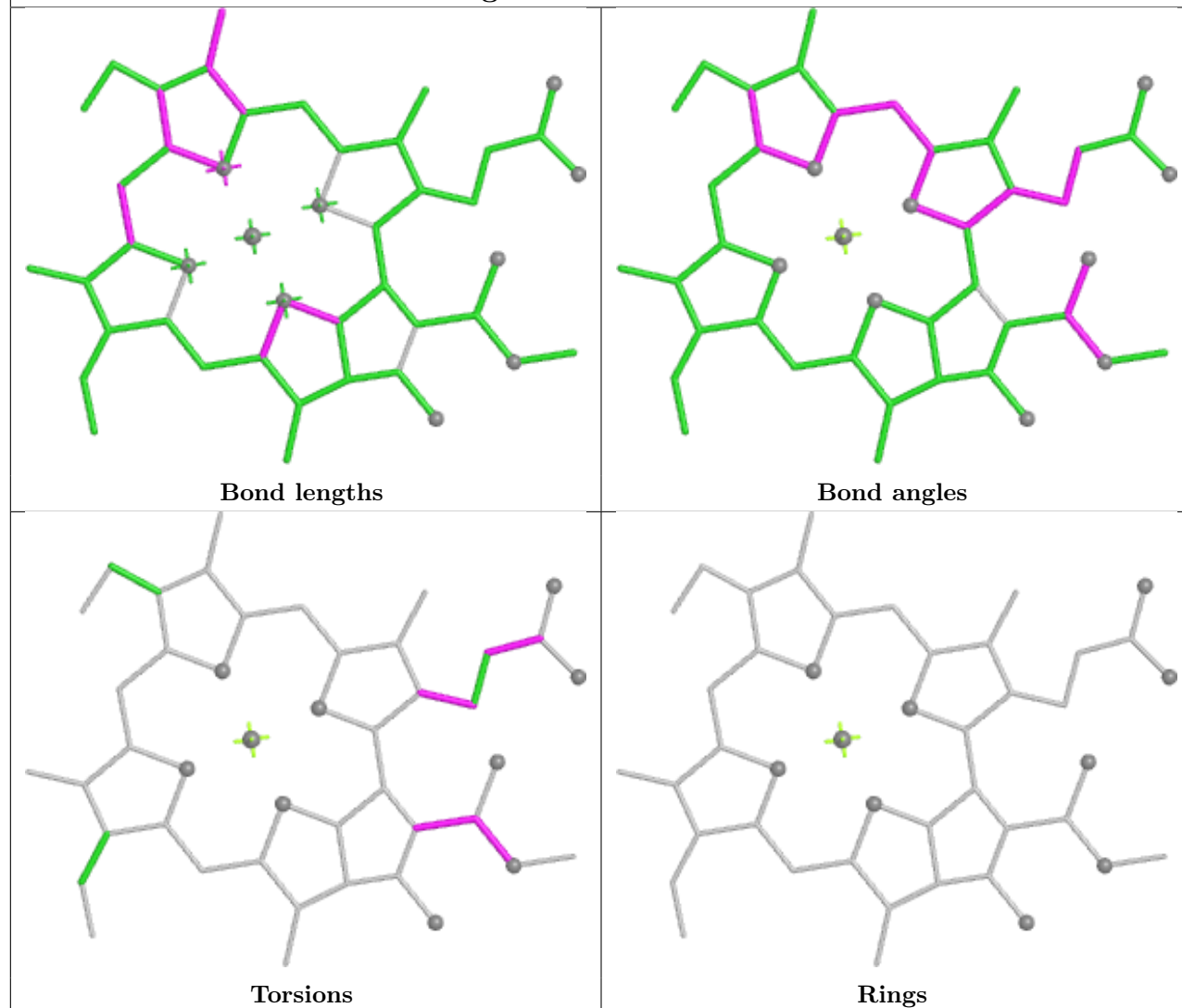
Ligand CLA AH 609



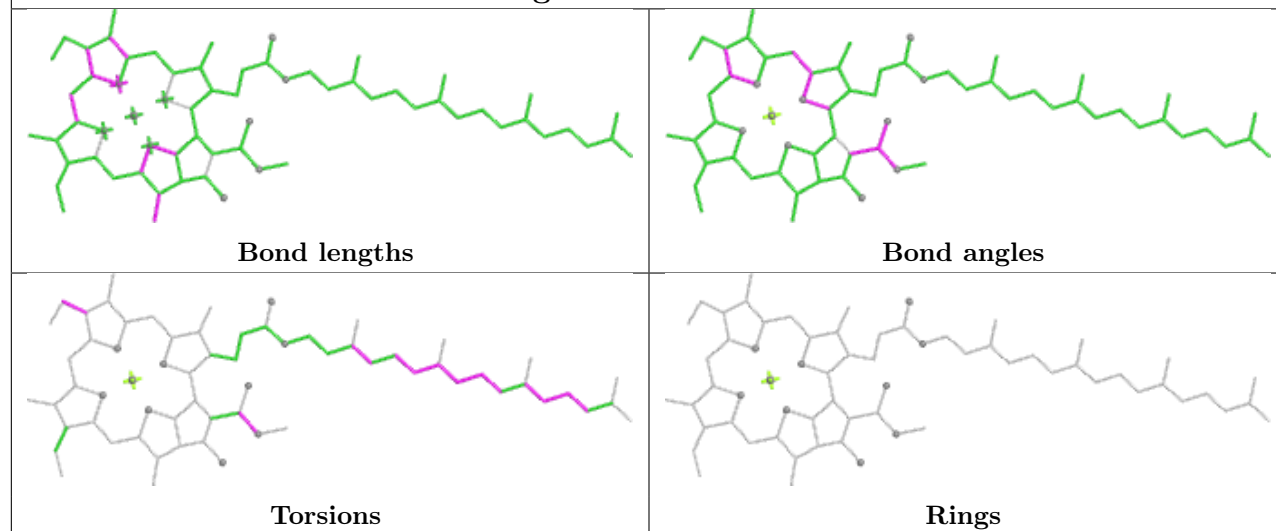
Ligand CLA 0 602

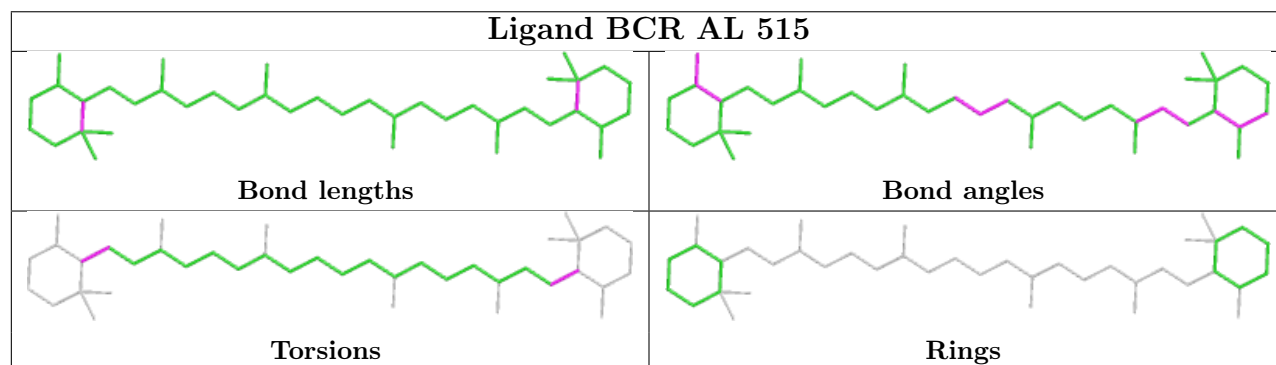
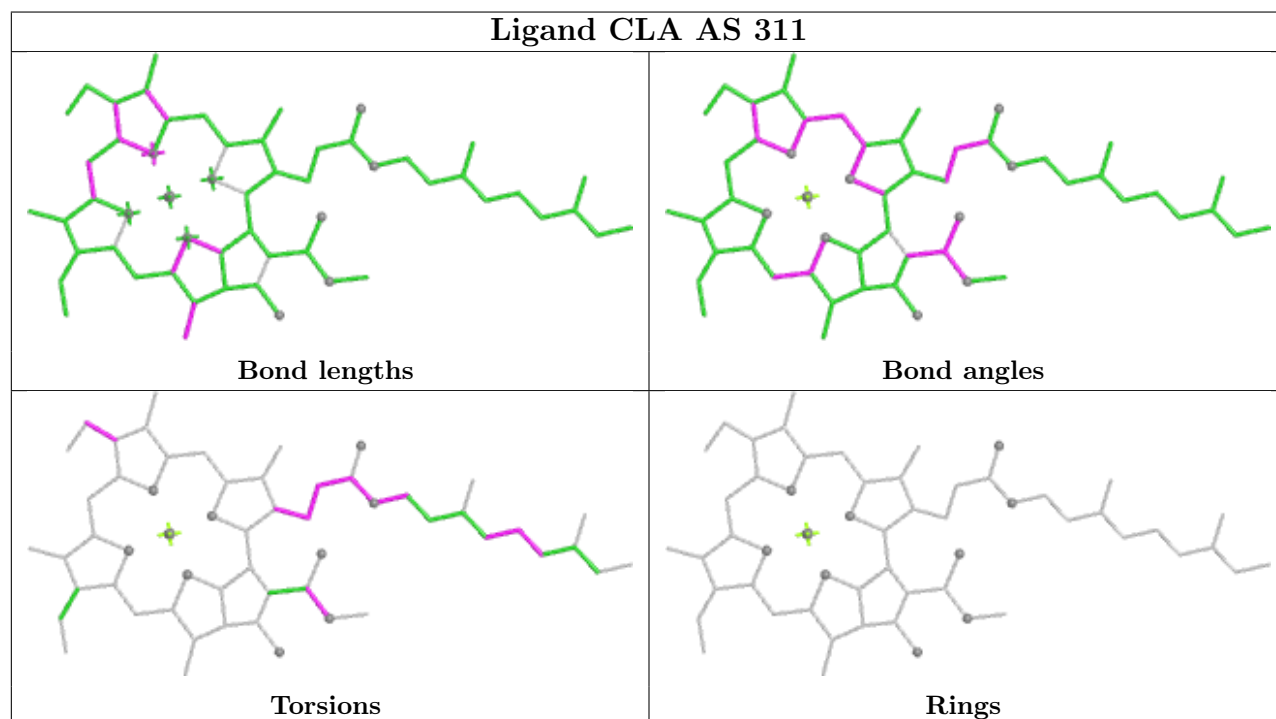
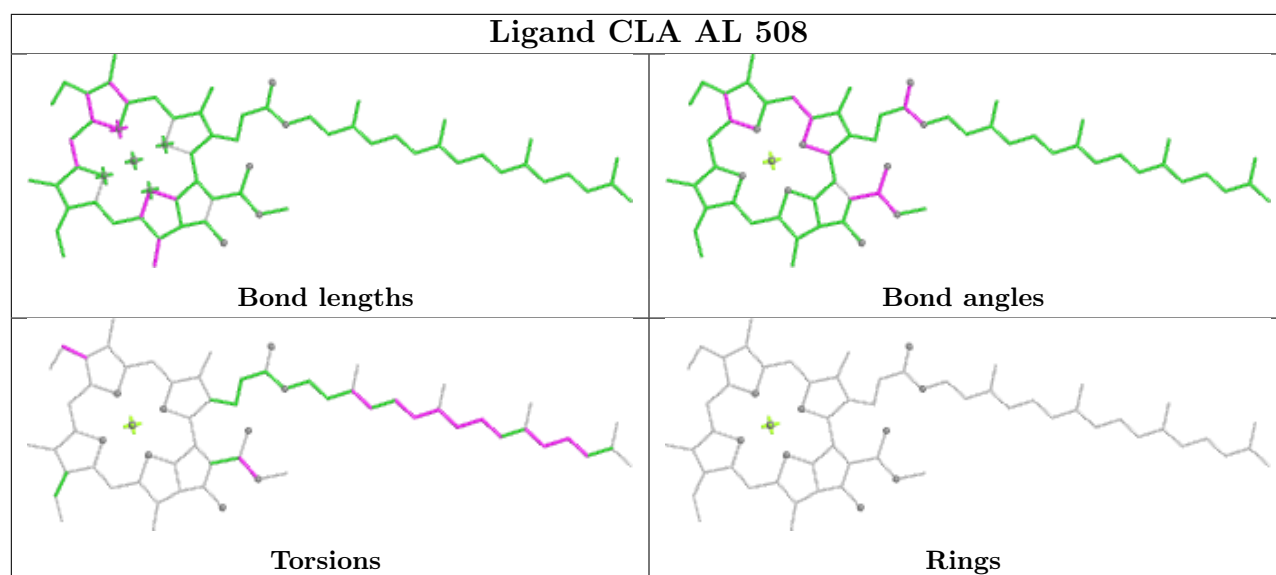


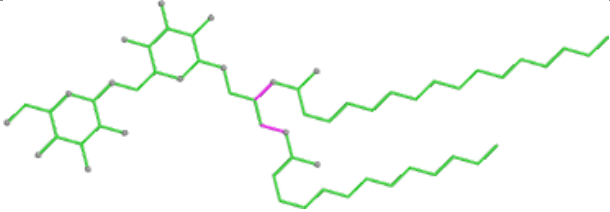
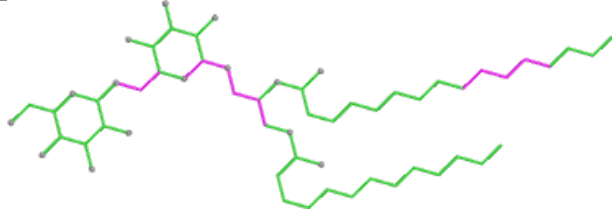
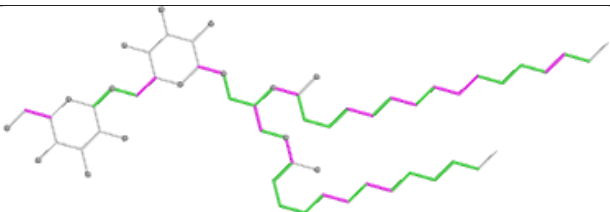
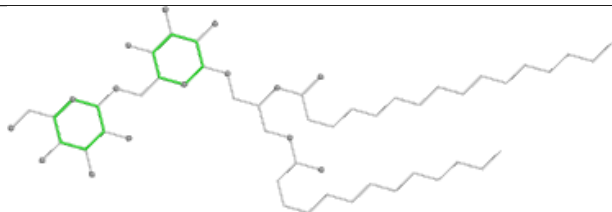
Ligand CLA AE 611

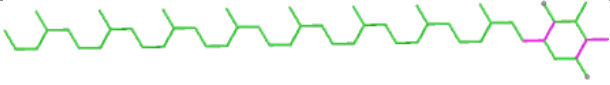
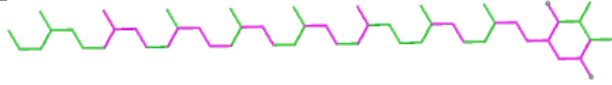
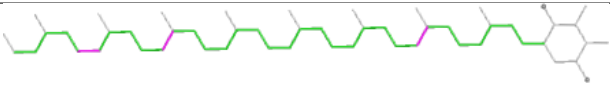
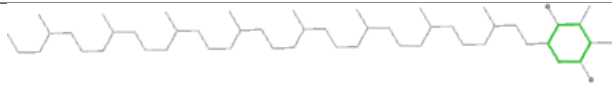


Ligand CLA P 507

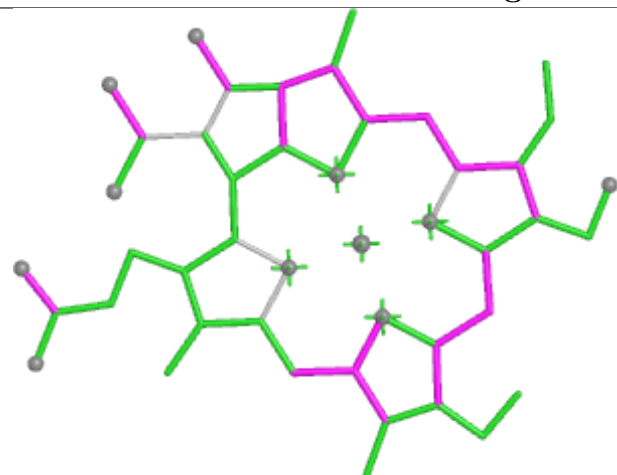




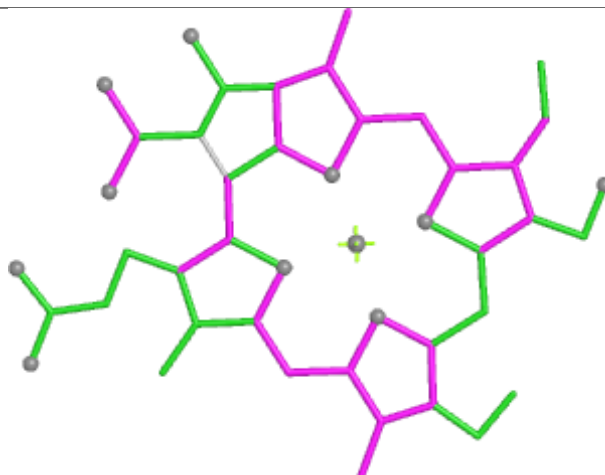
Ligand DGD AJ 401			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand PL9 AM 405			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

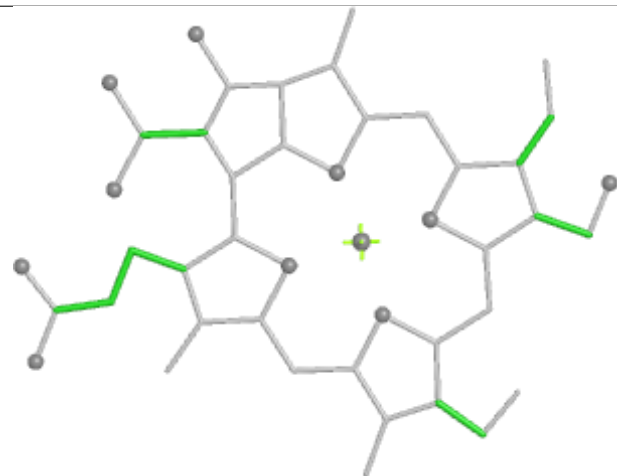
Ligand CHL AB 601



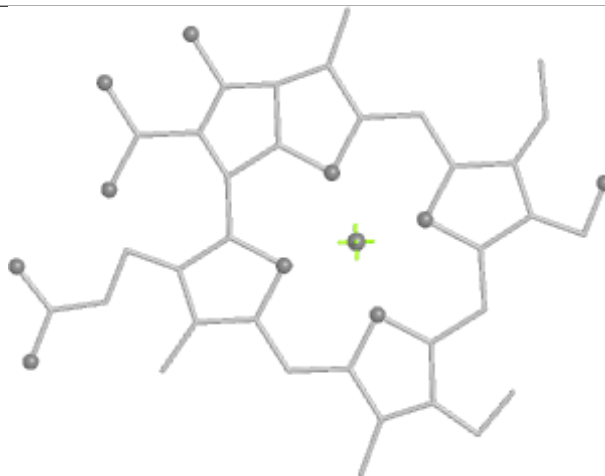
Bond lengths



Bond angles

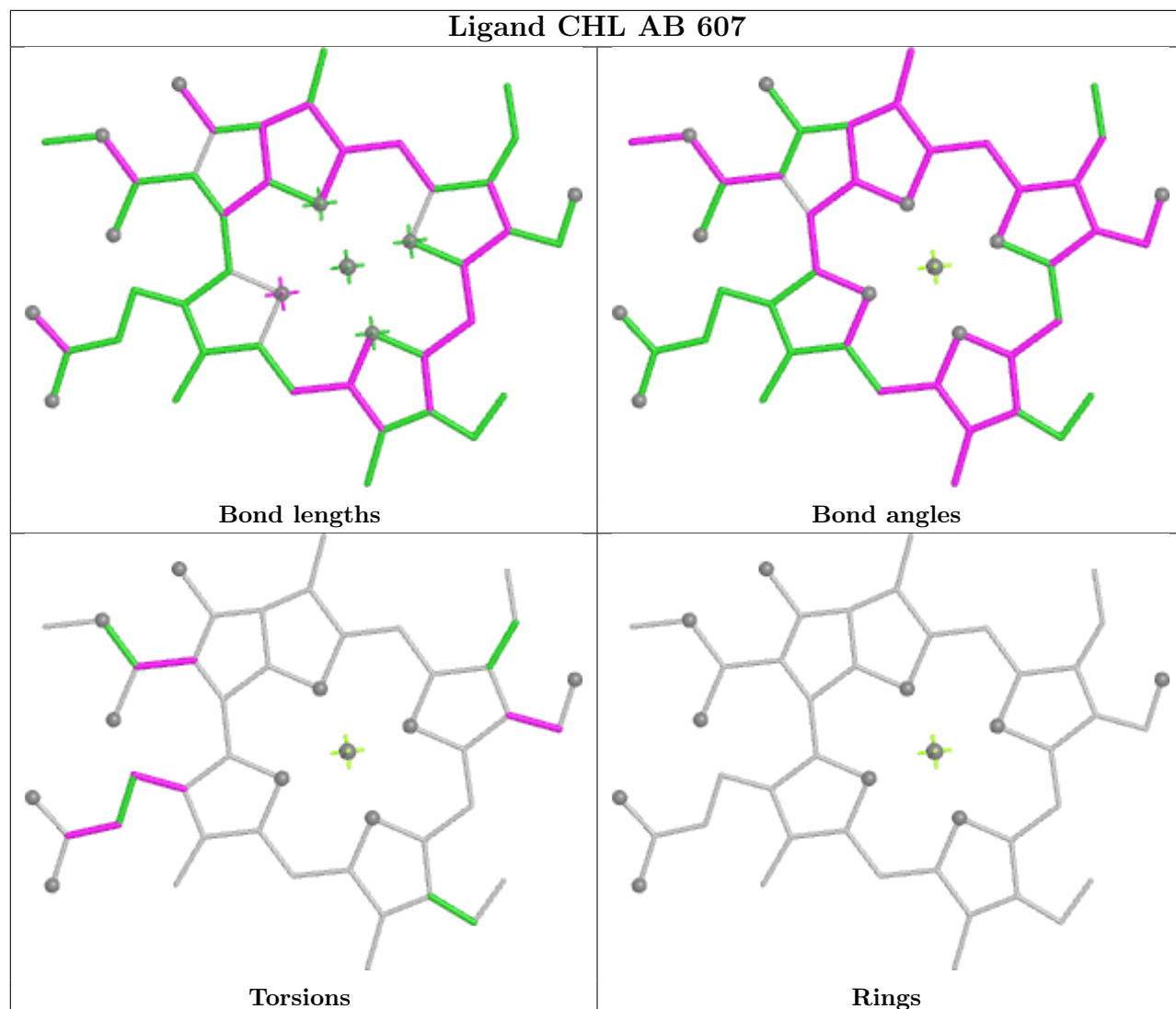


Torsions

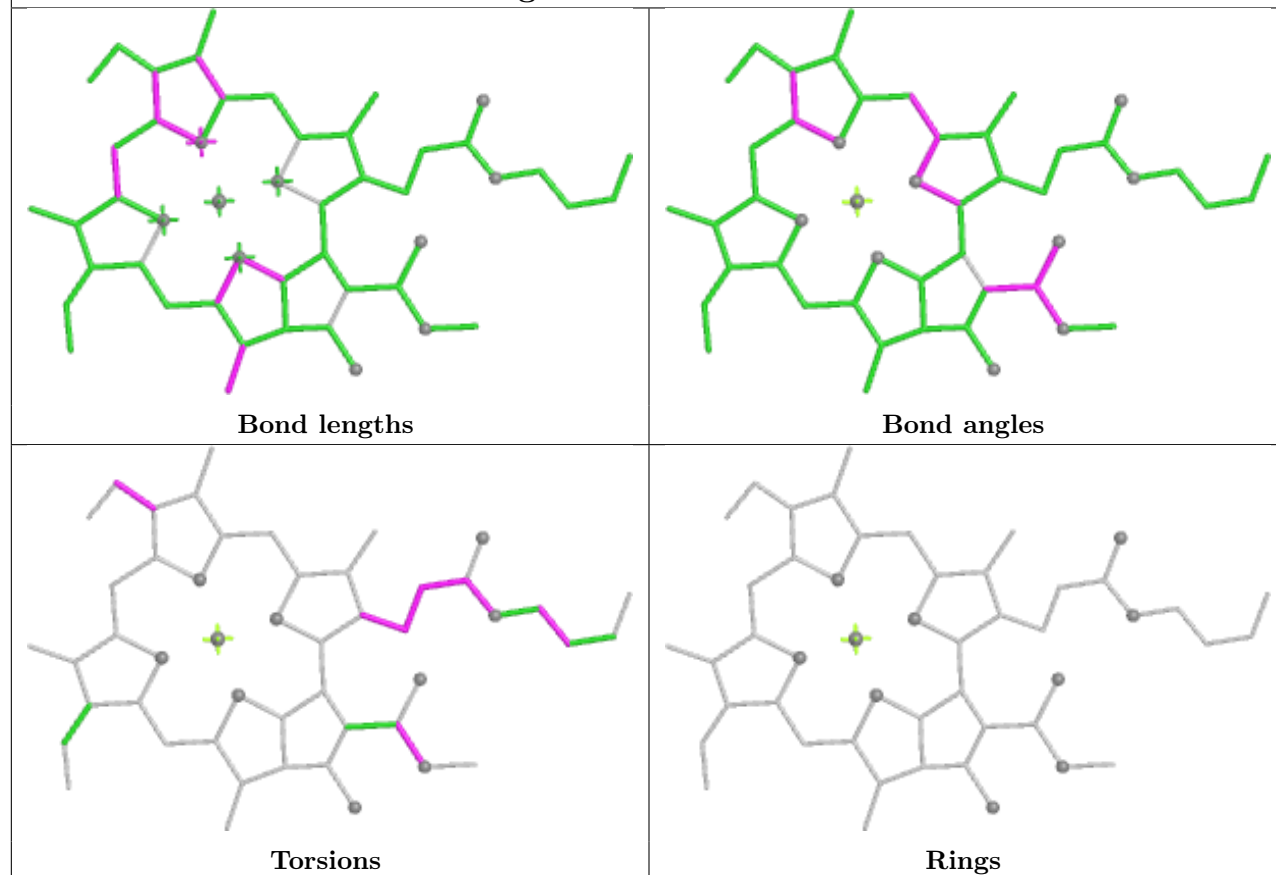


Rings

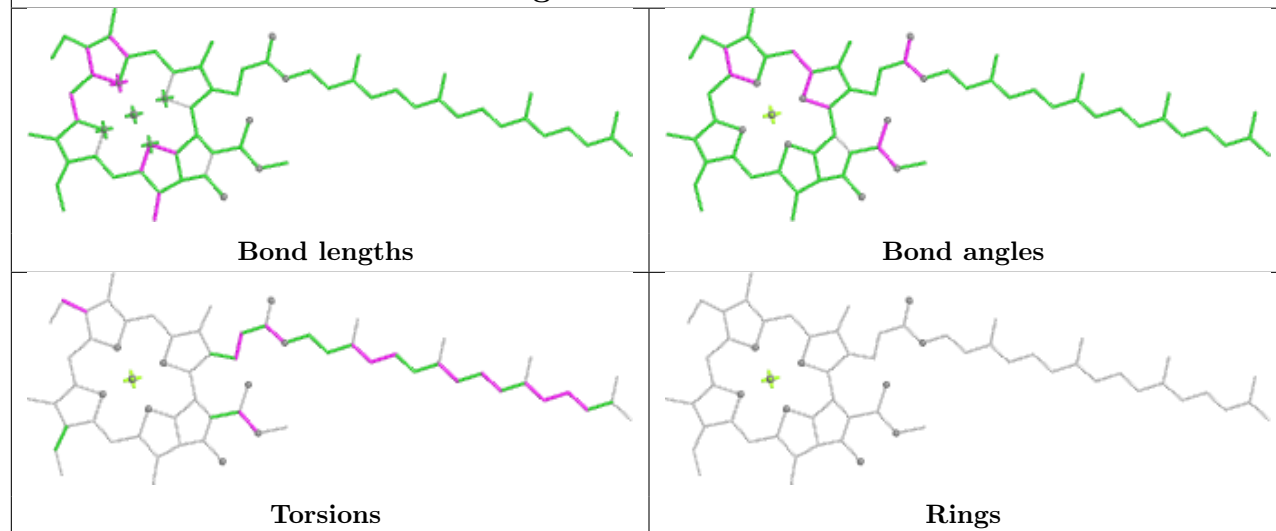
Ligand CHL AB 607



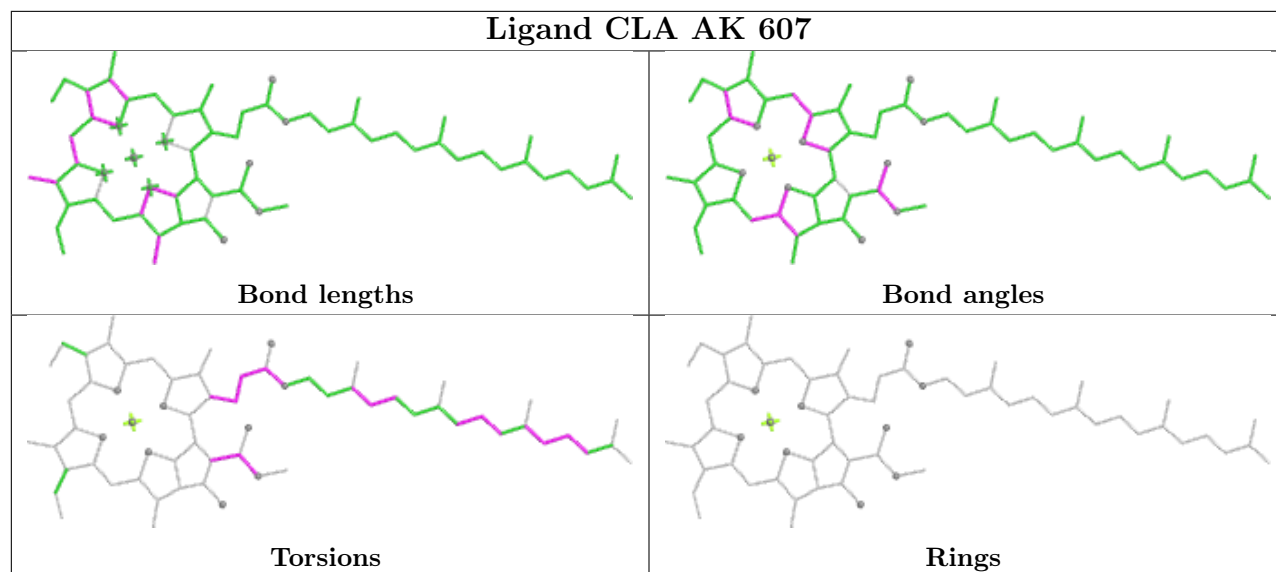
Ligand CLA AR 610



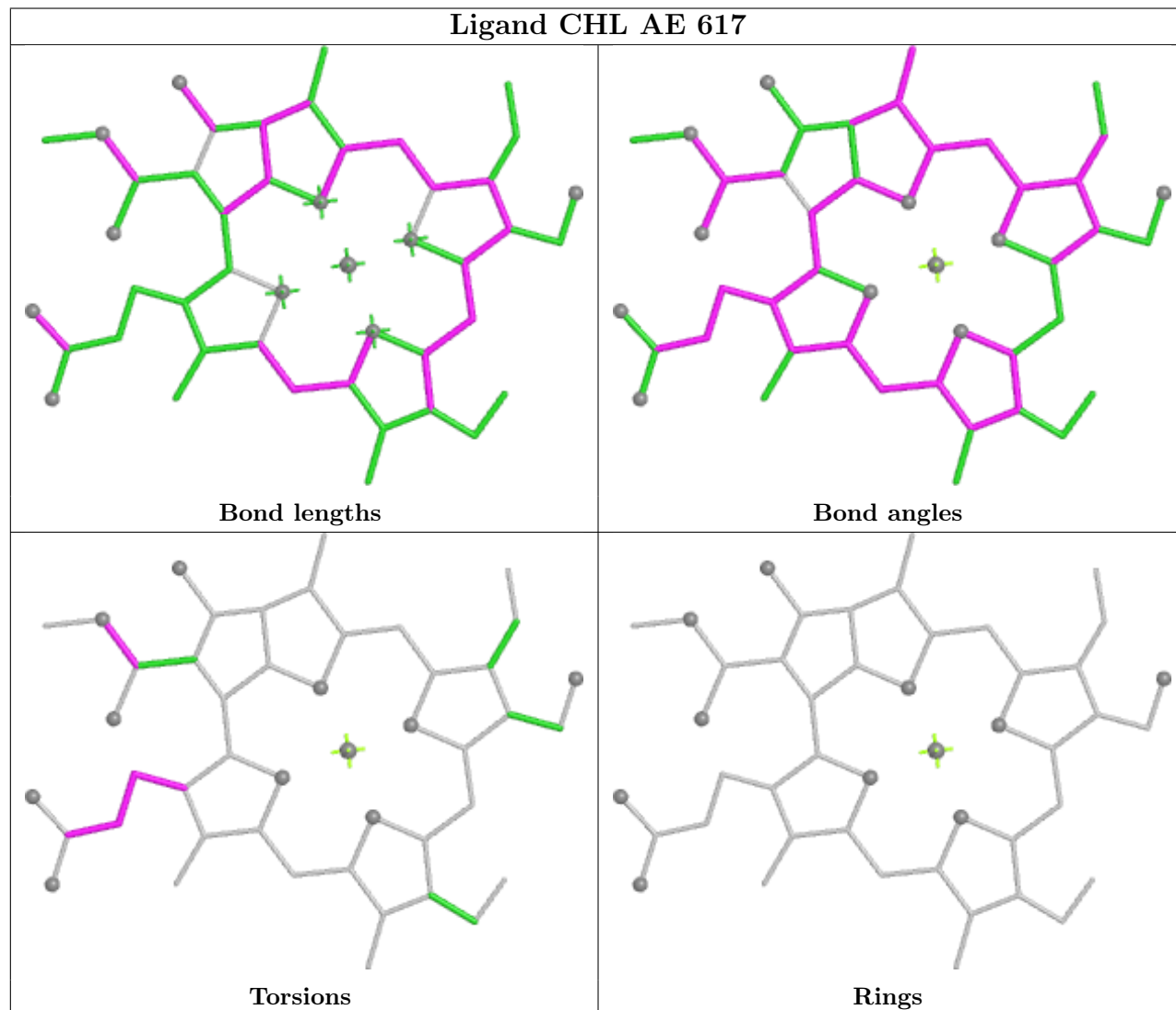
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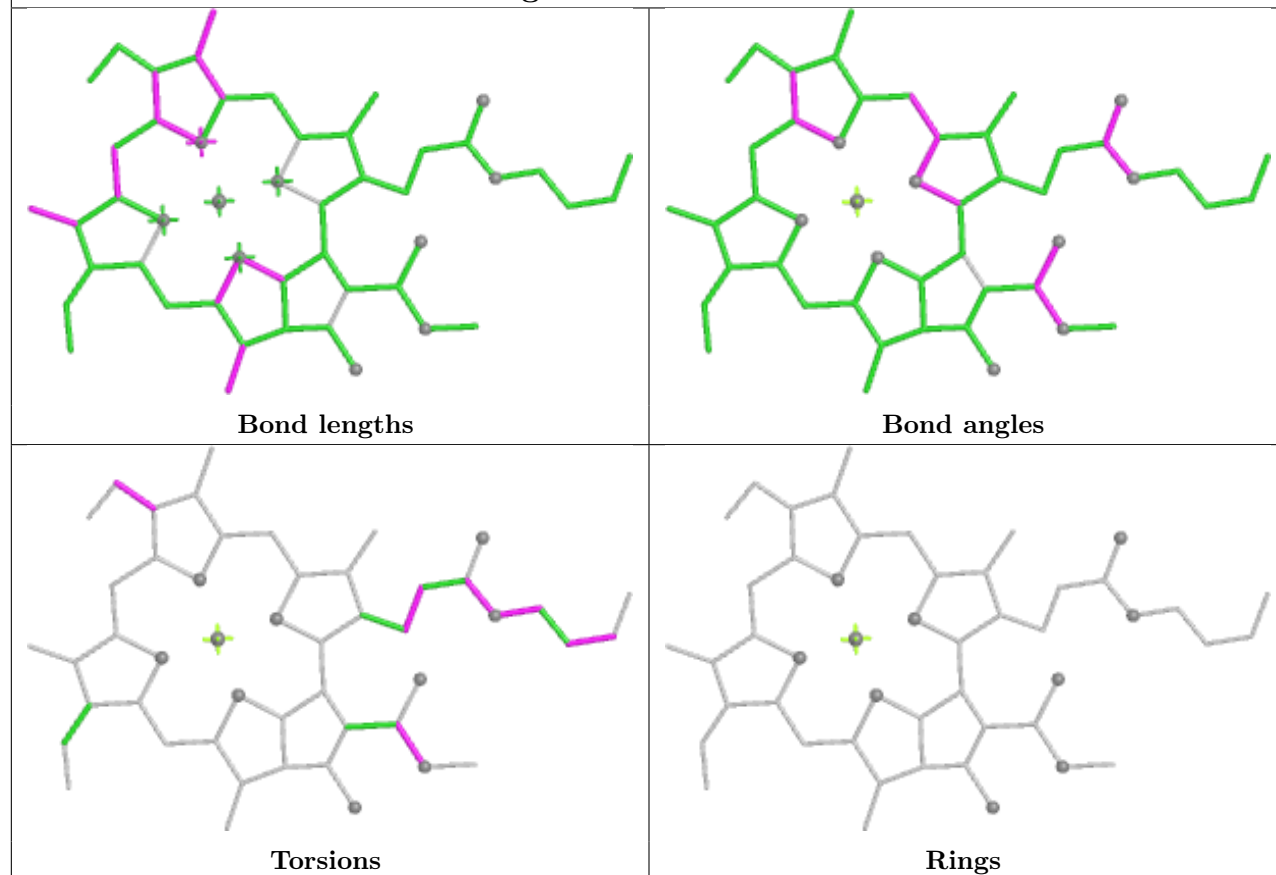
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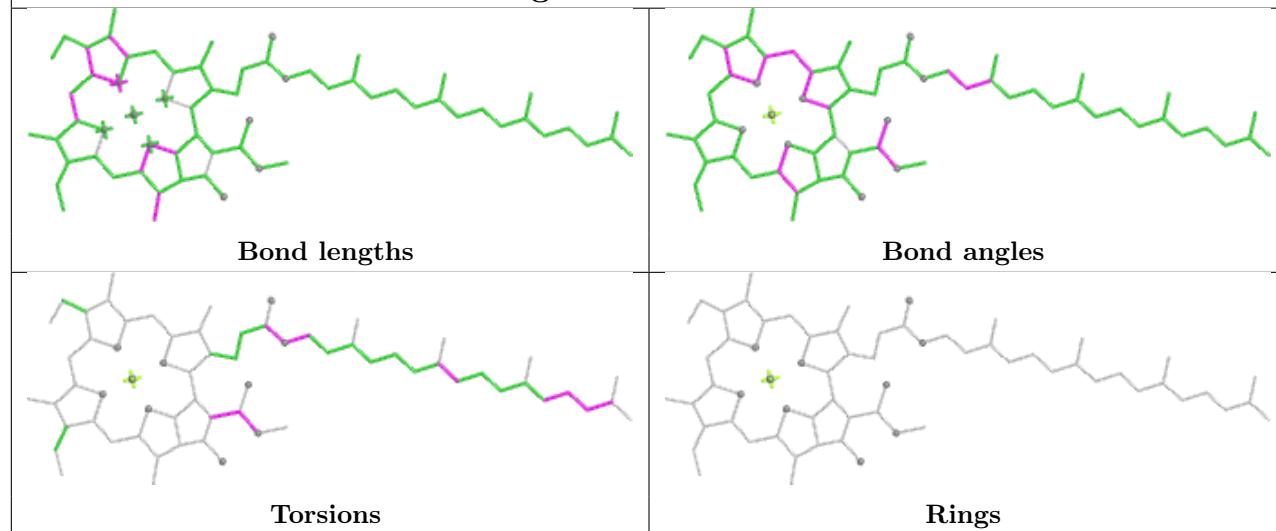
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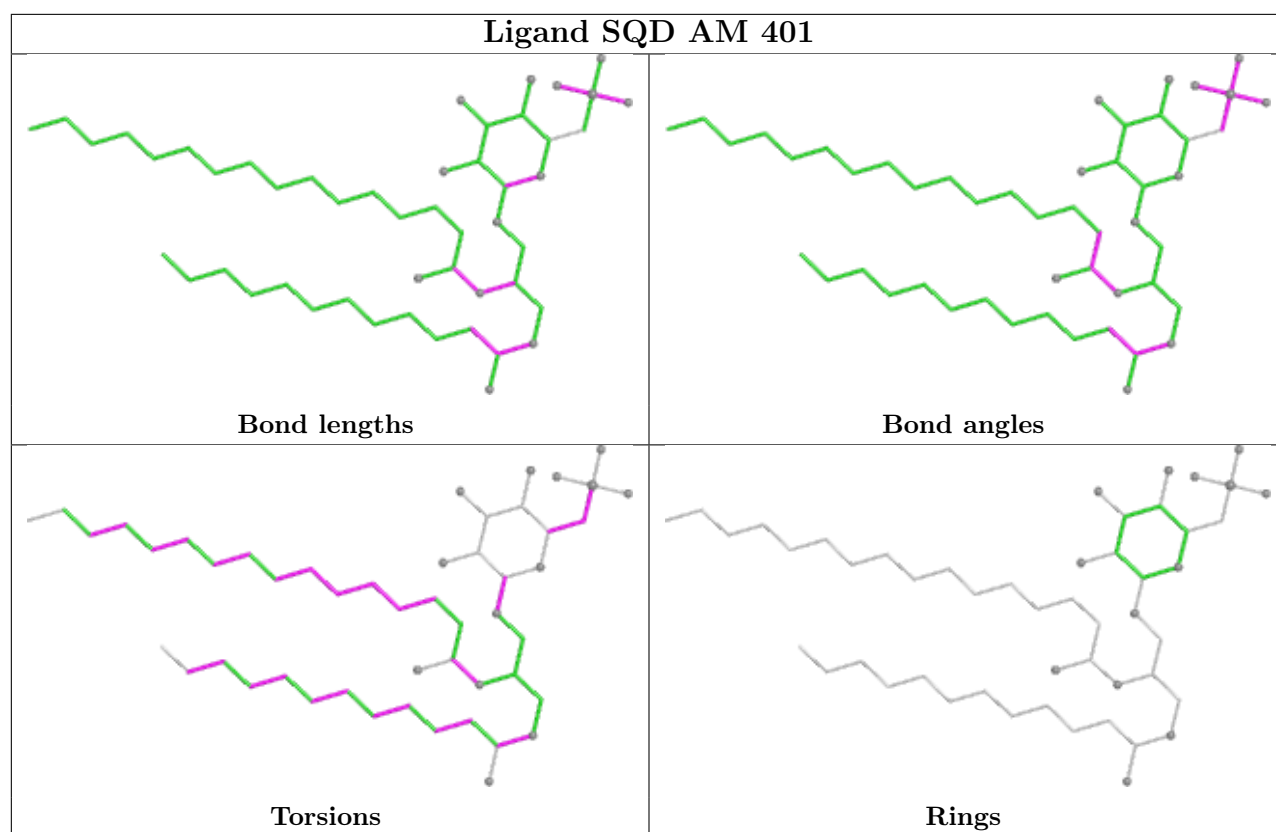


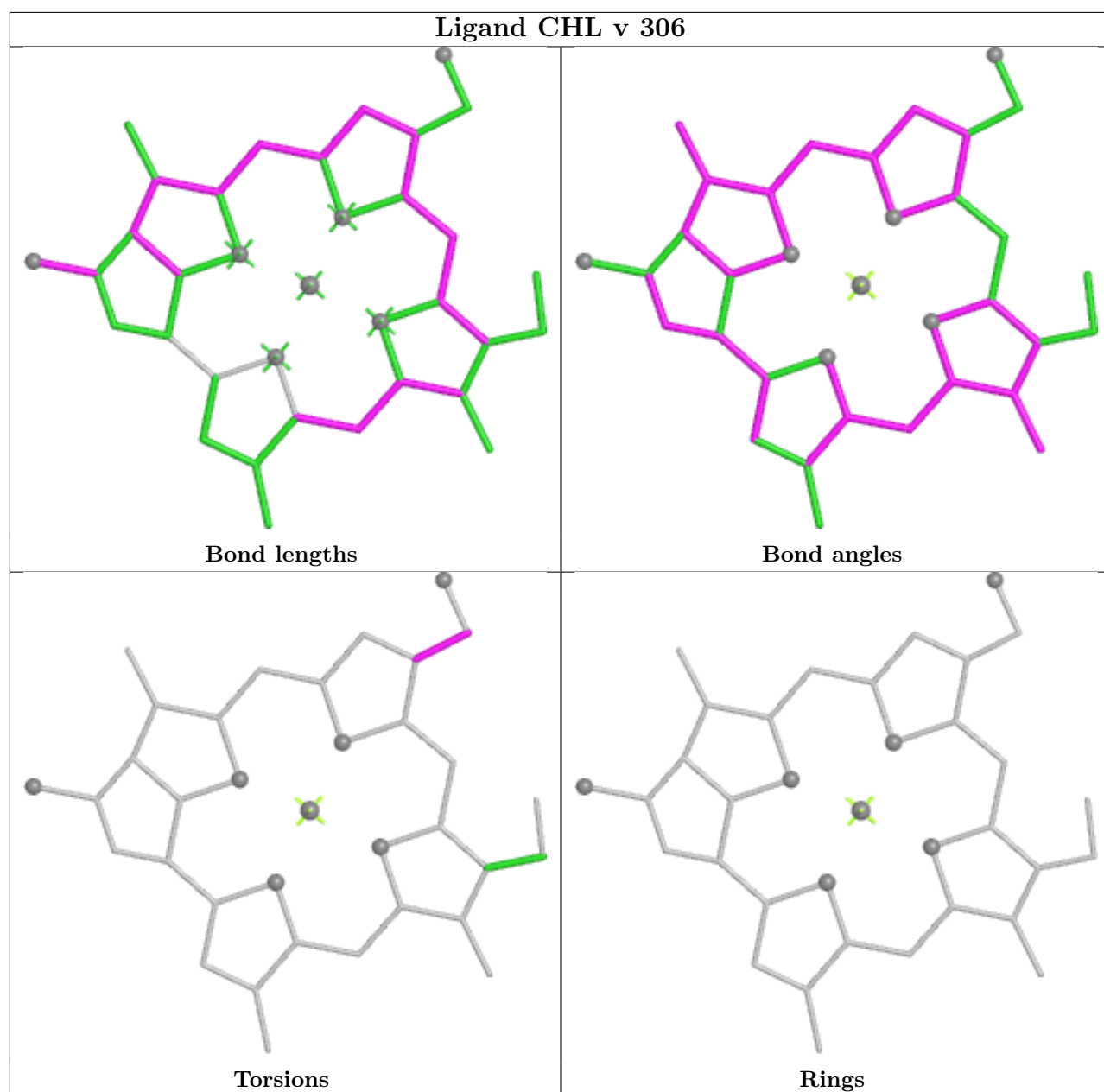
Ligand CLA AS 312

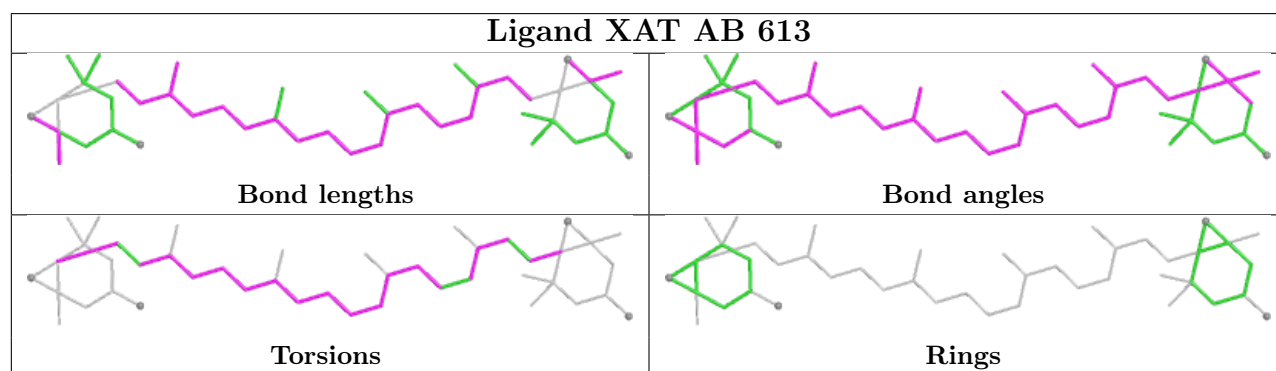
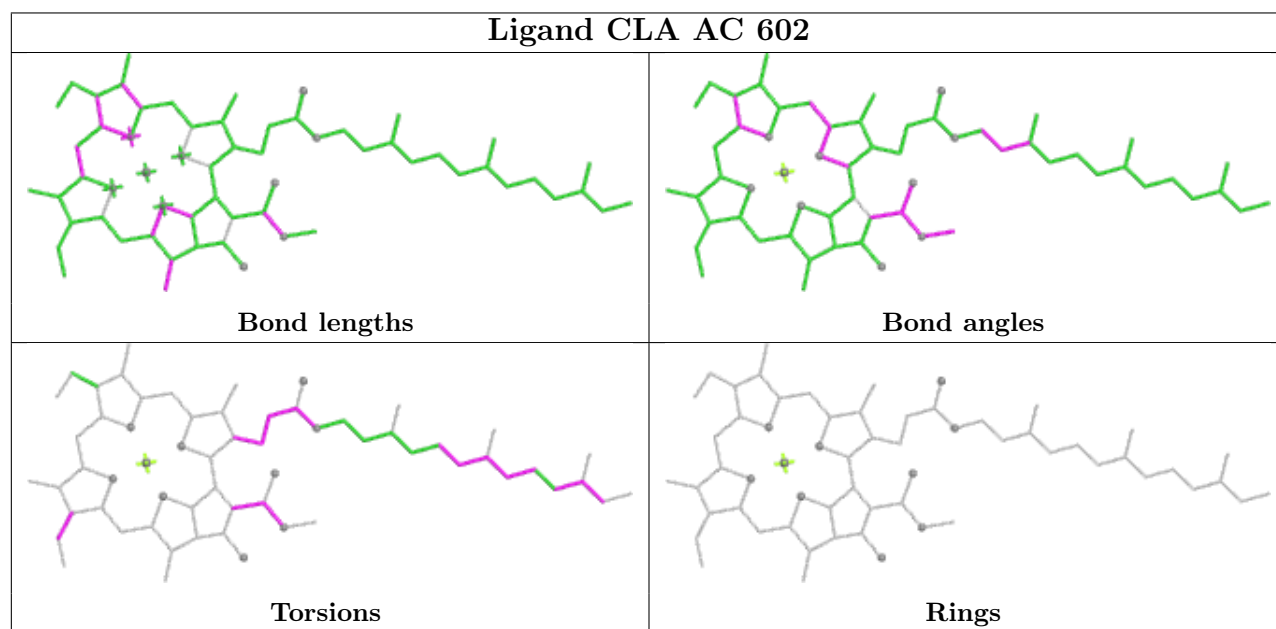
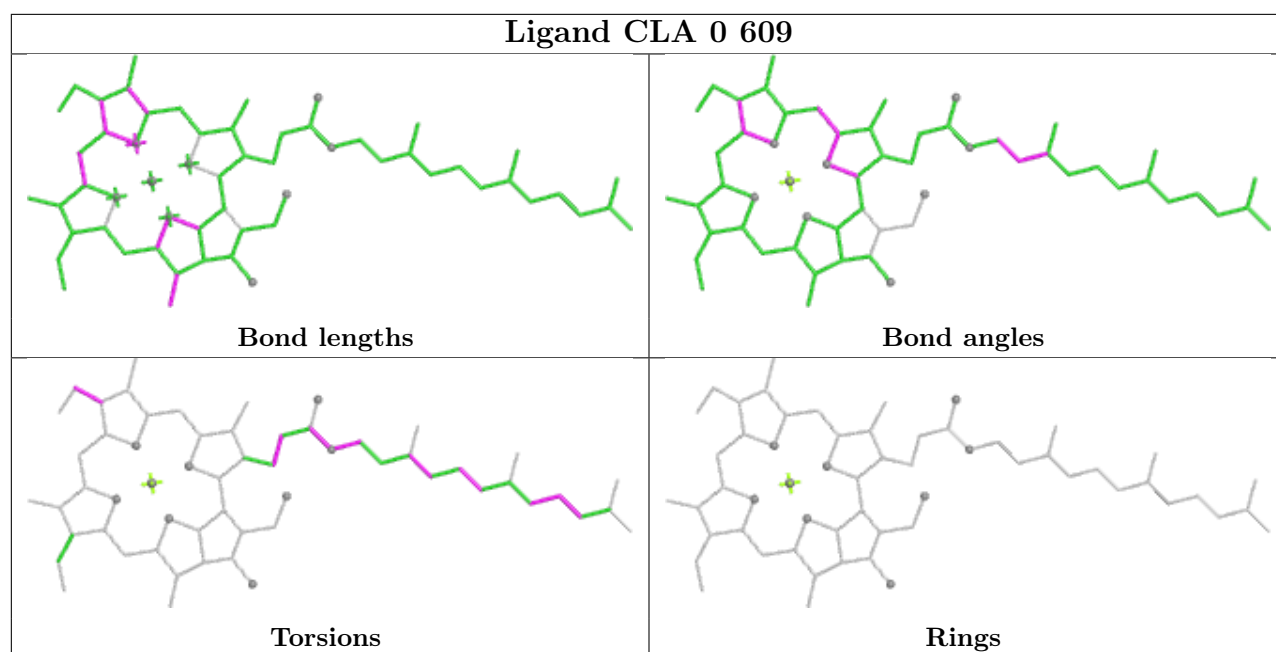


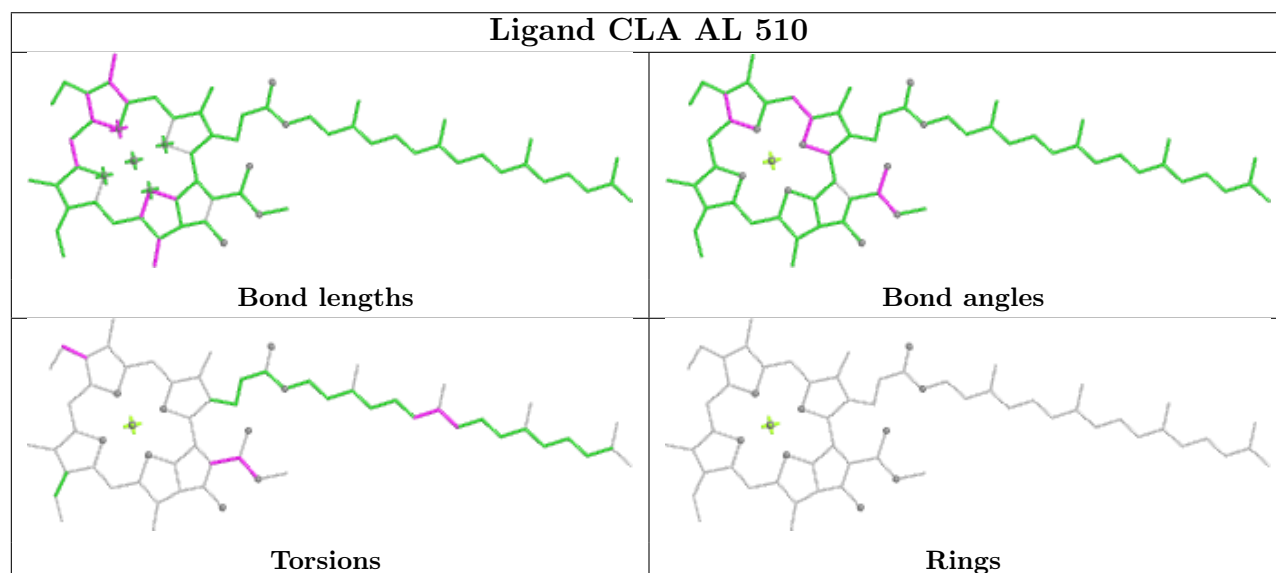
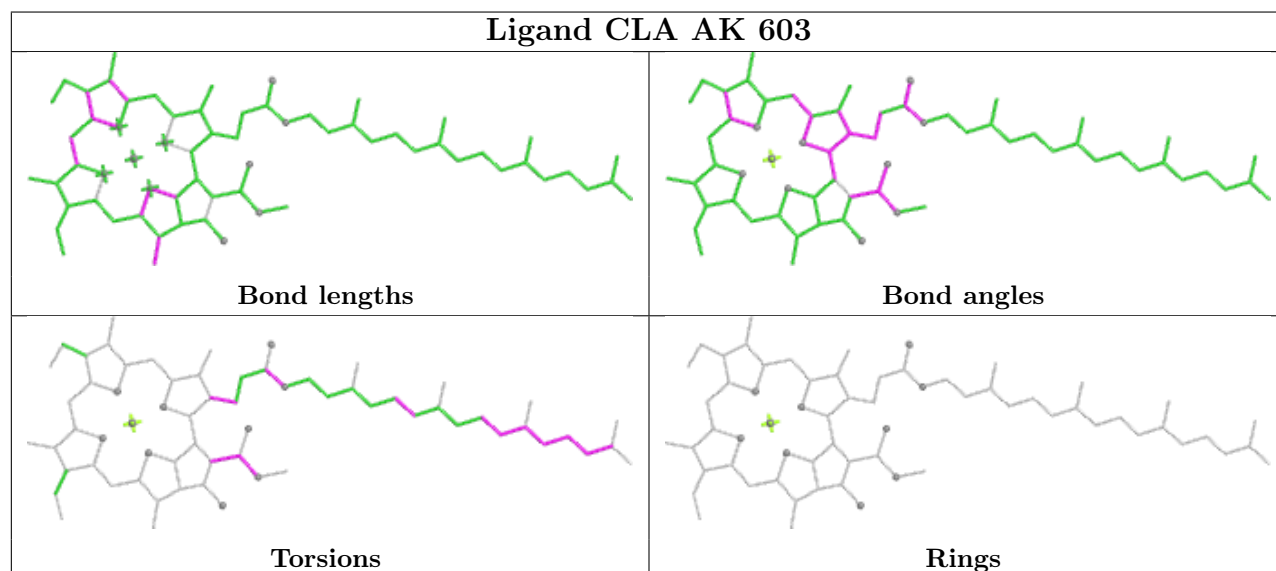
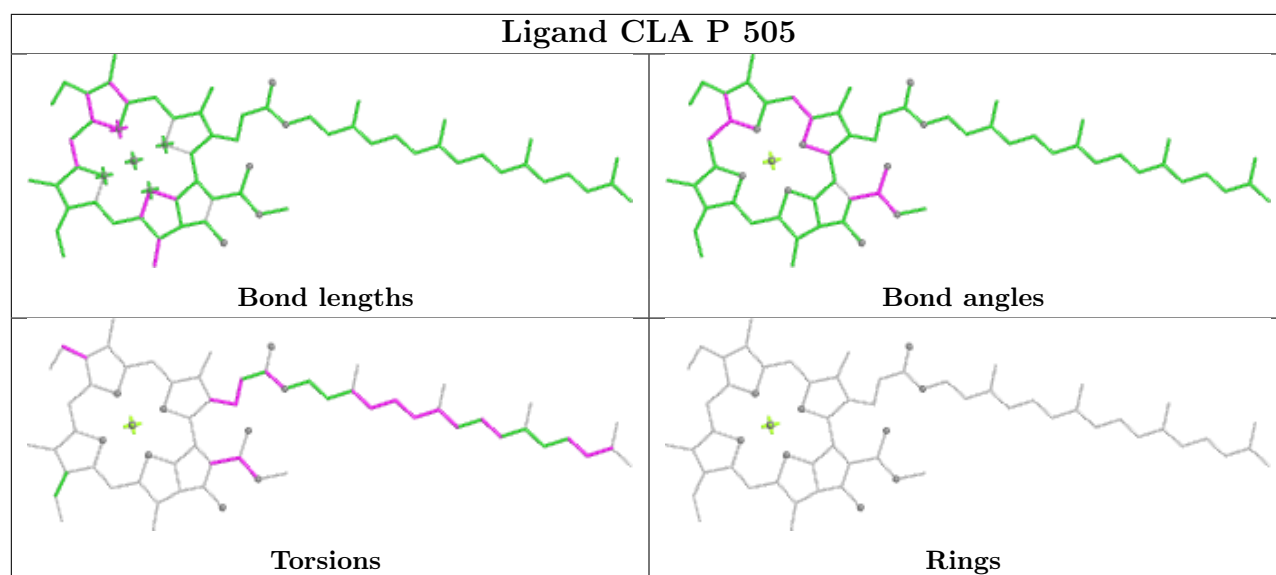
Ligand CLA O 610



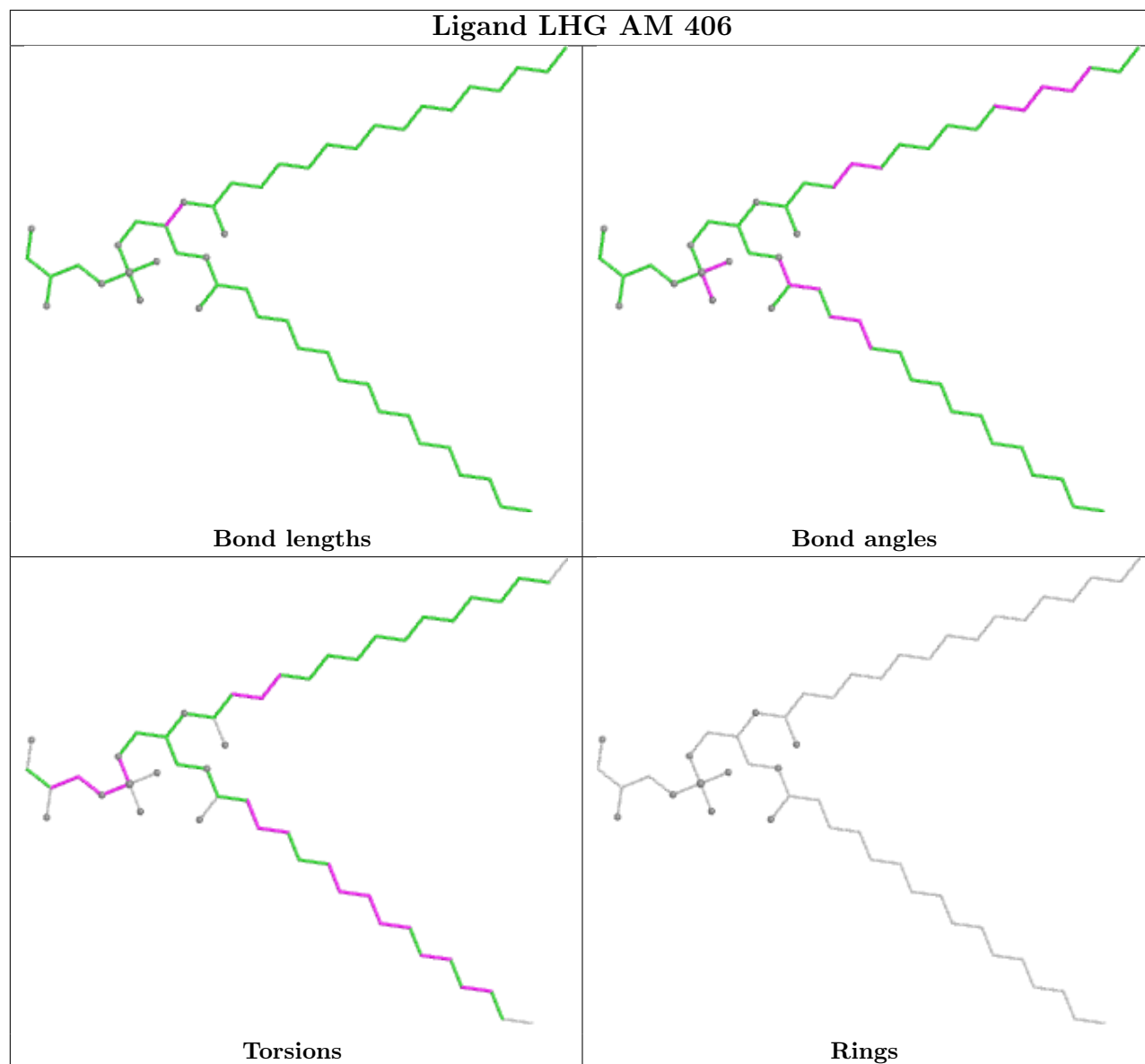




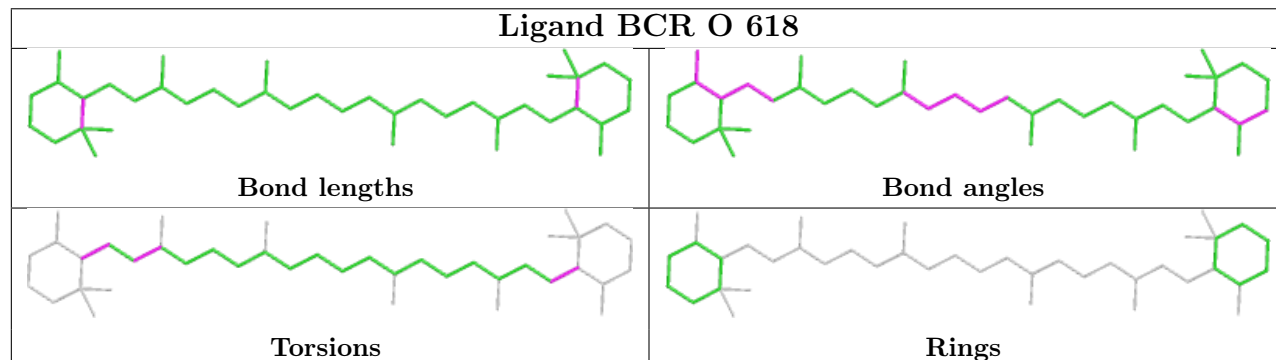




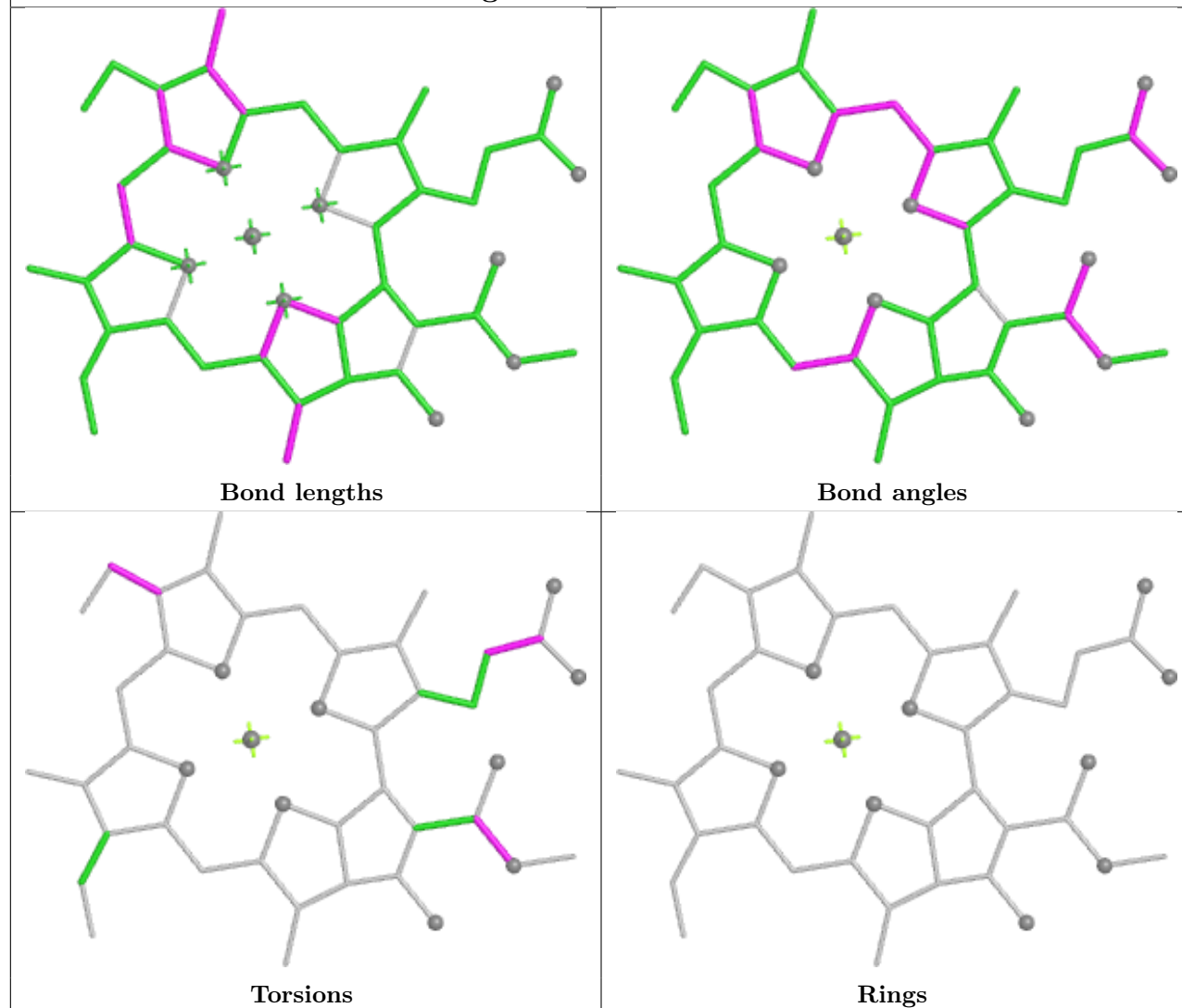
Ligand LHG AM 406



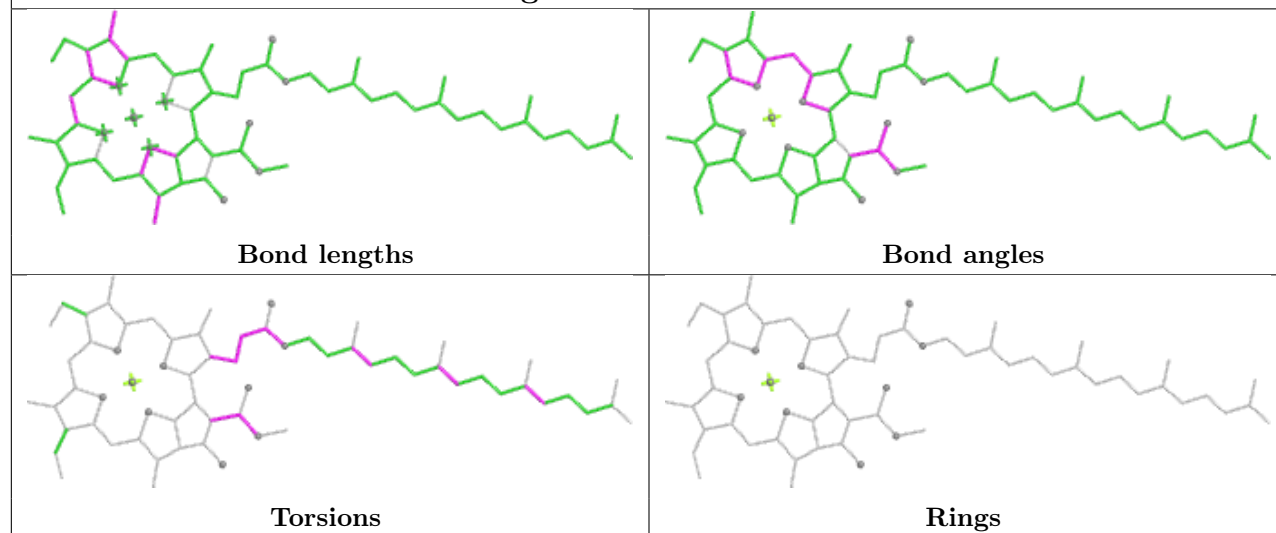
Ligand BCR O 618



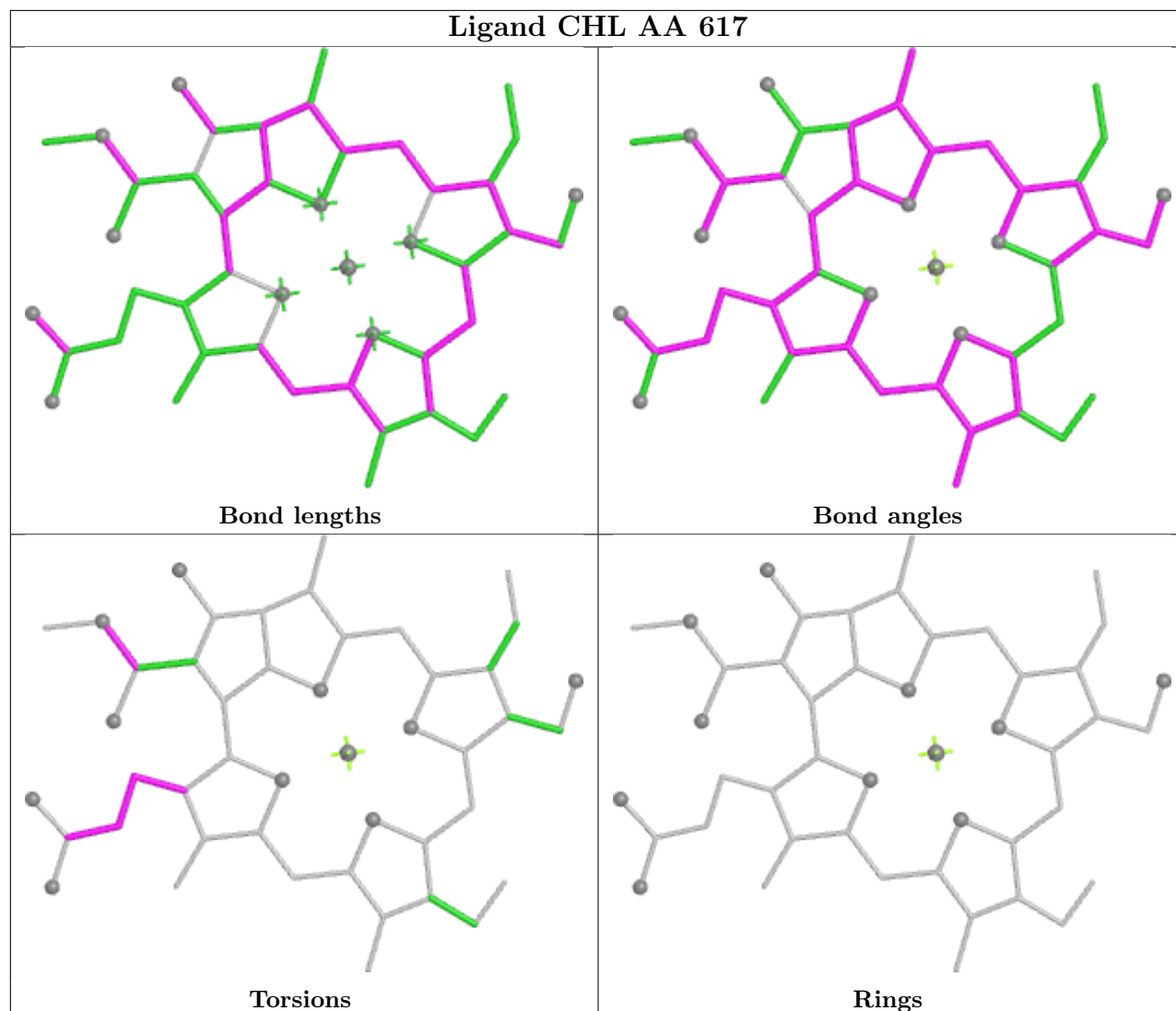
Ligand CLA AF 603

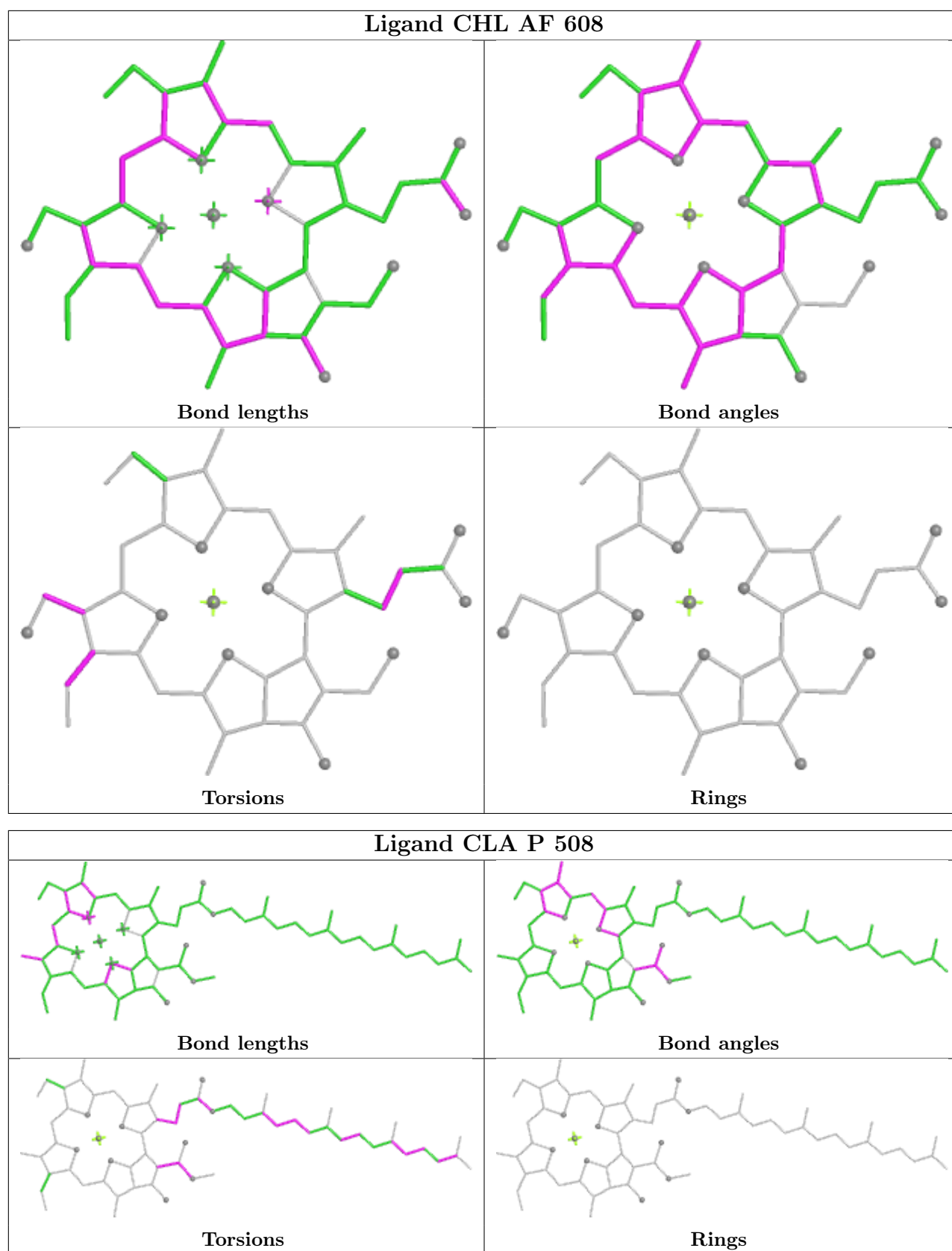


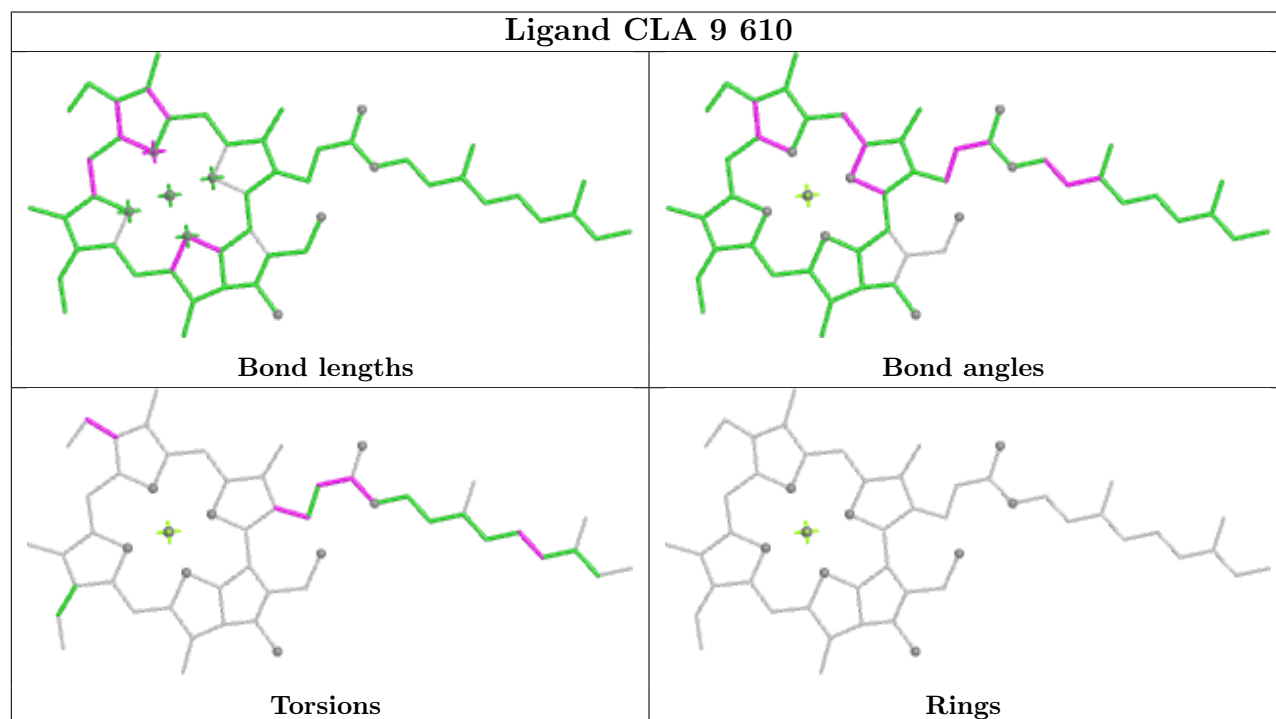
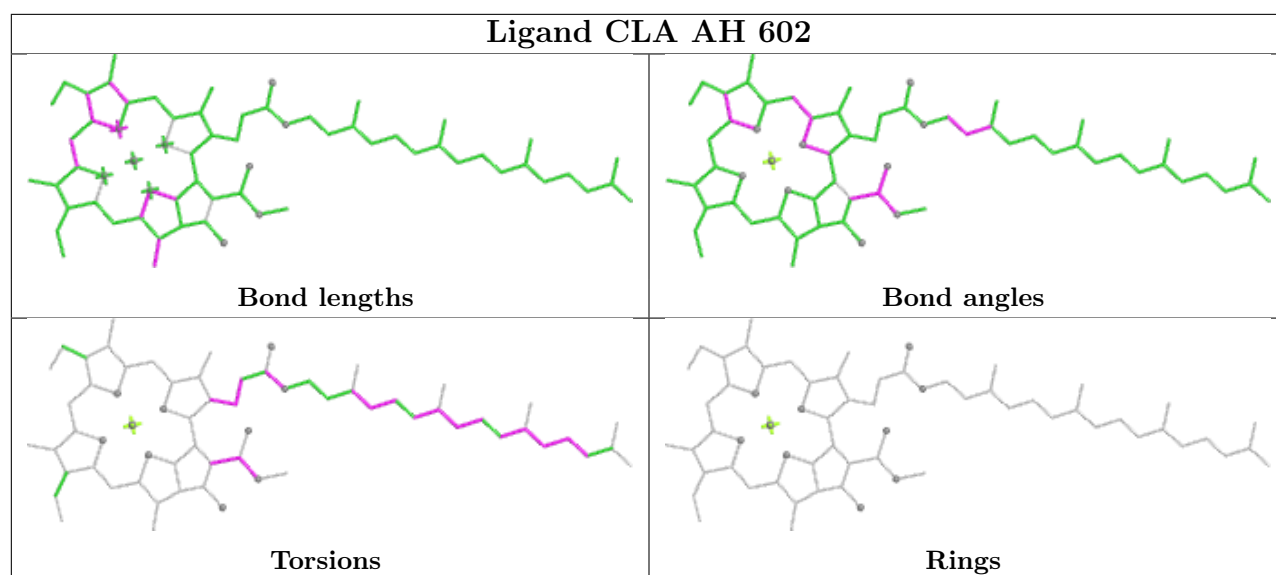
Ligand CLA AL 502

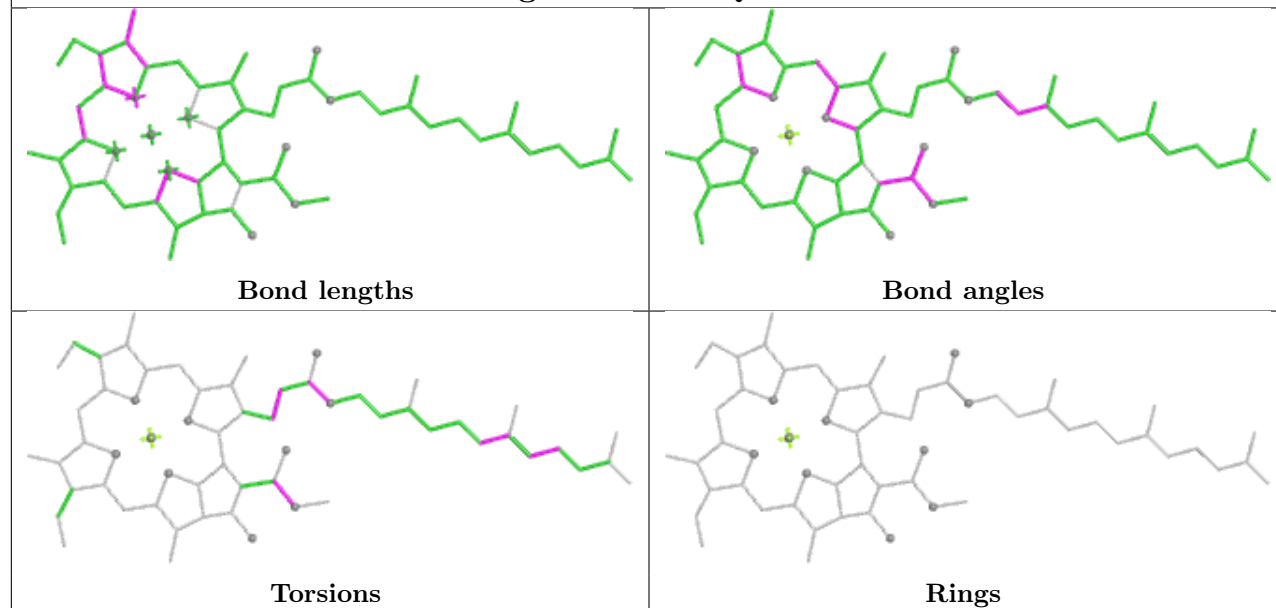
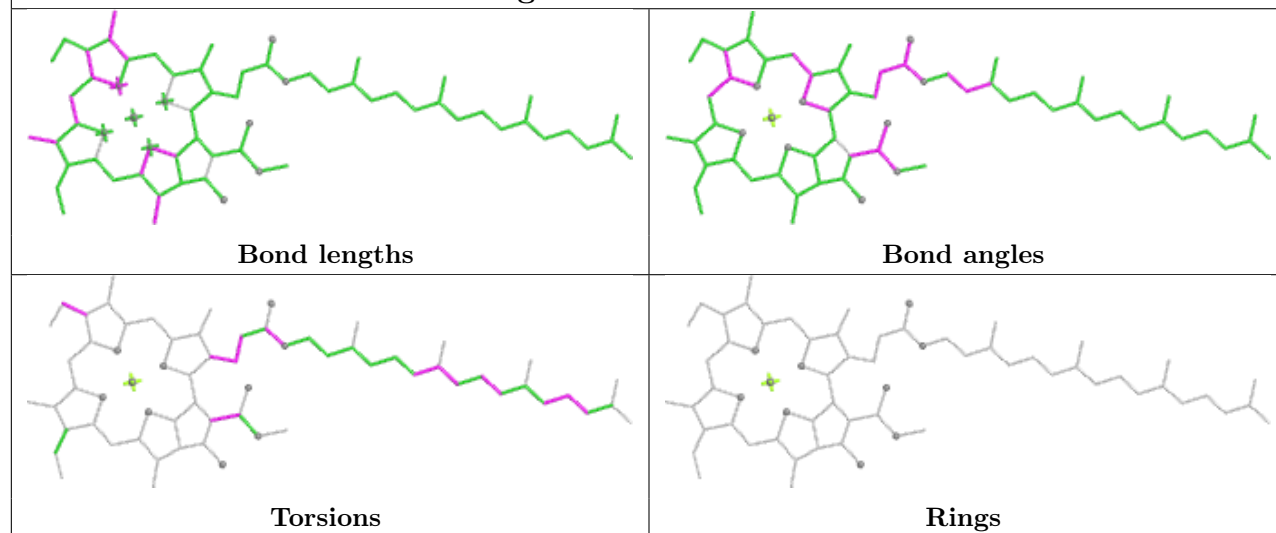


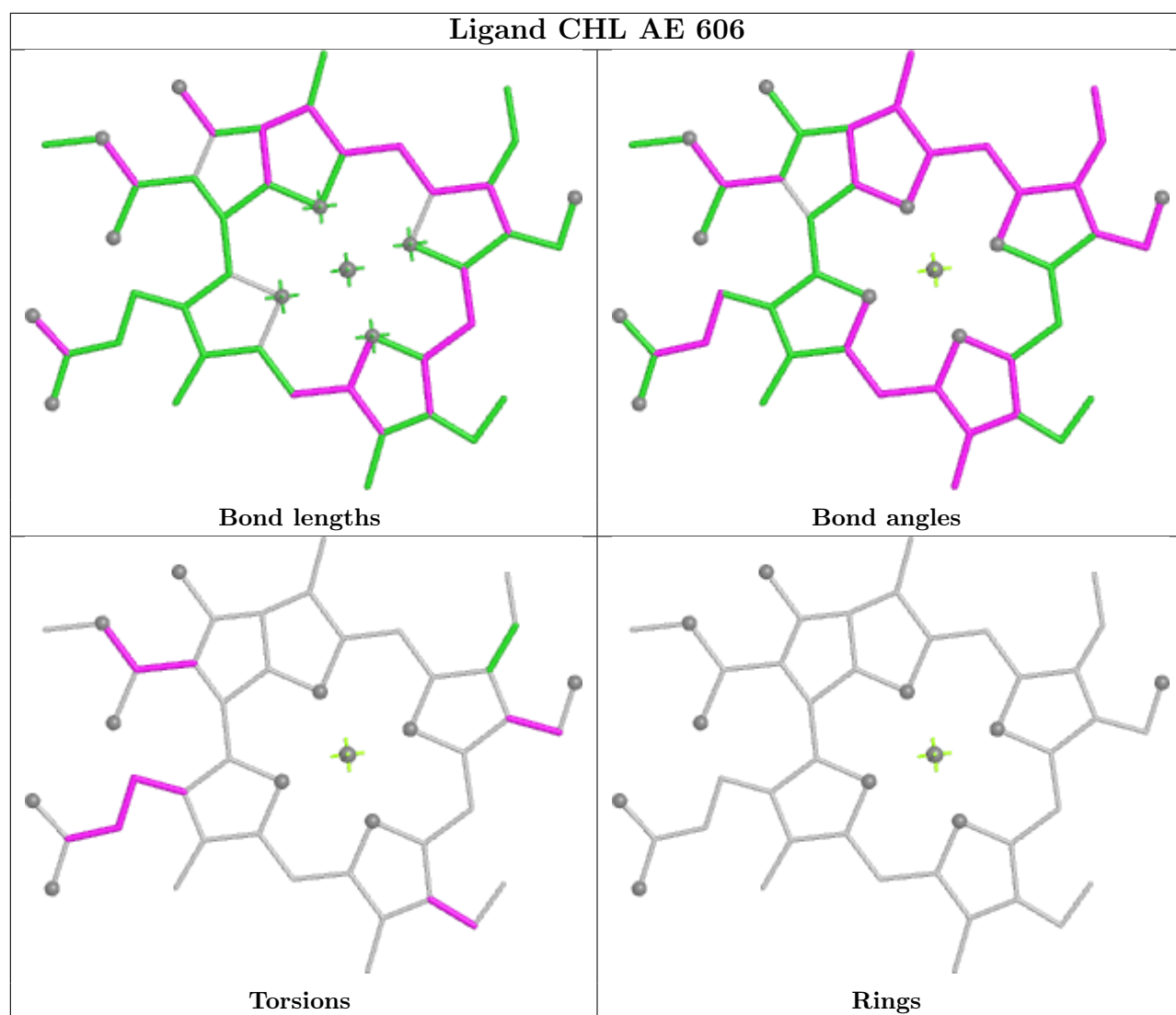
Ligand CHL AA 617



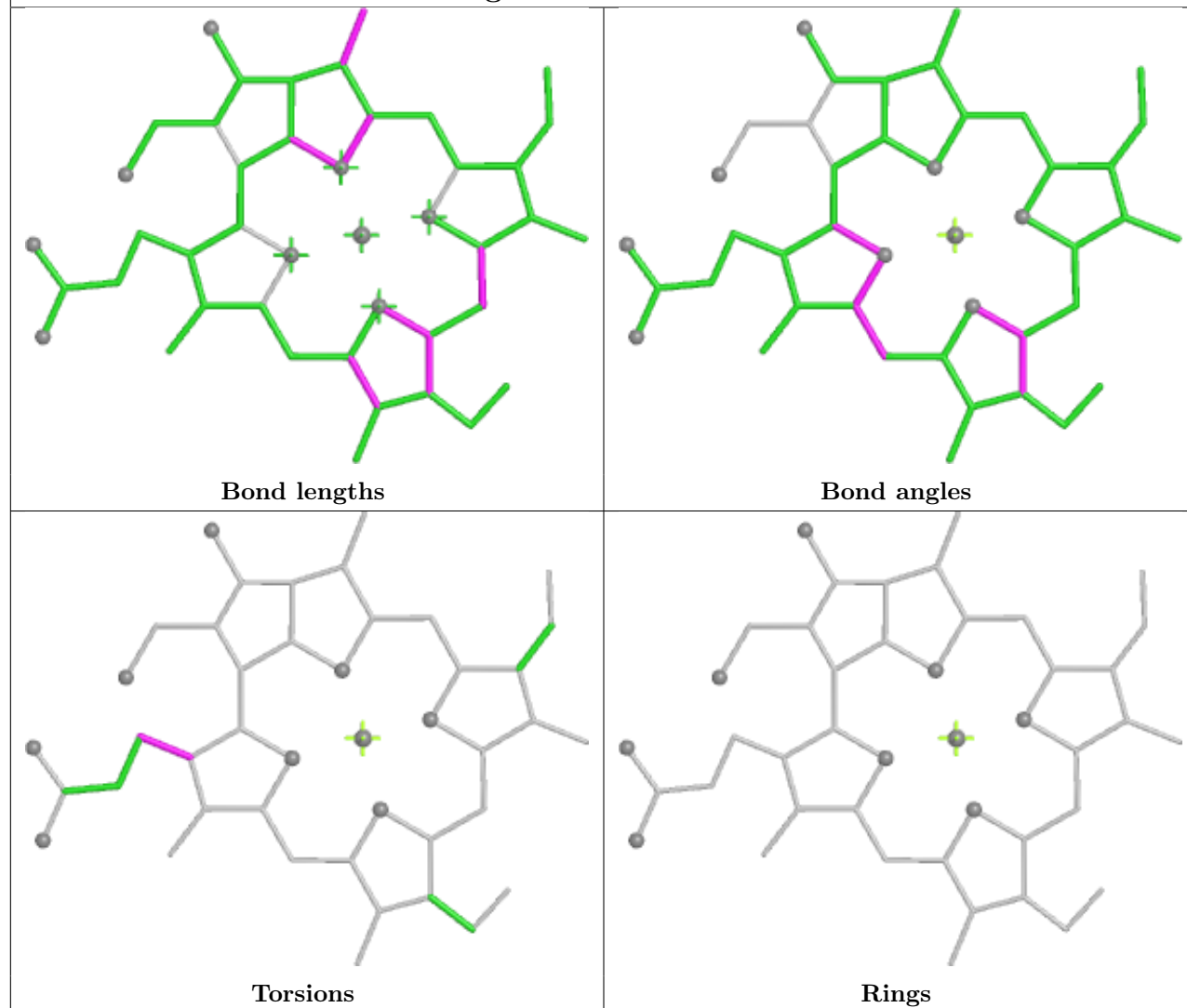




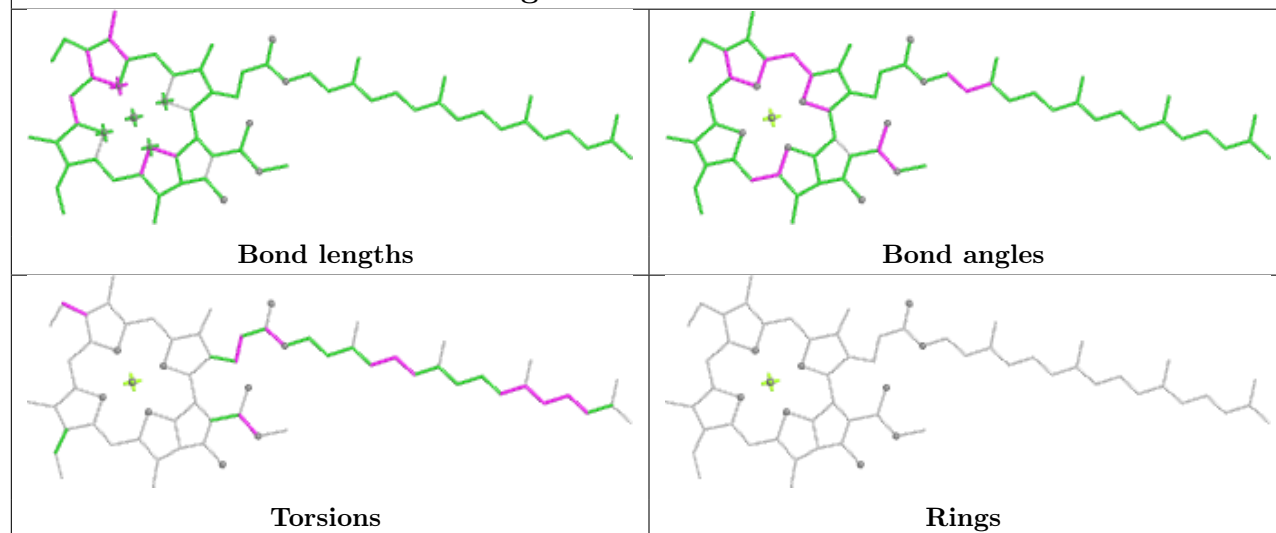
Ligand CLA AQ 613**Ligand CLA AK 614**



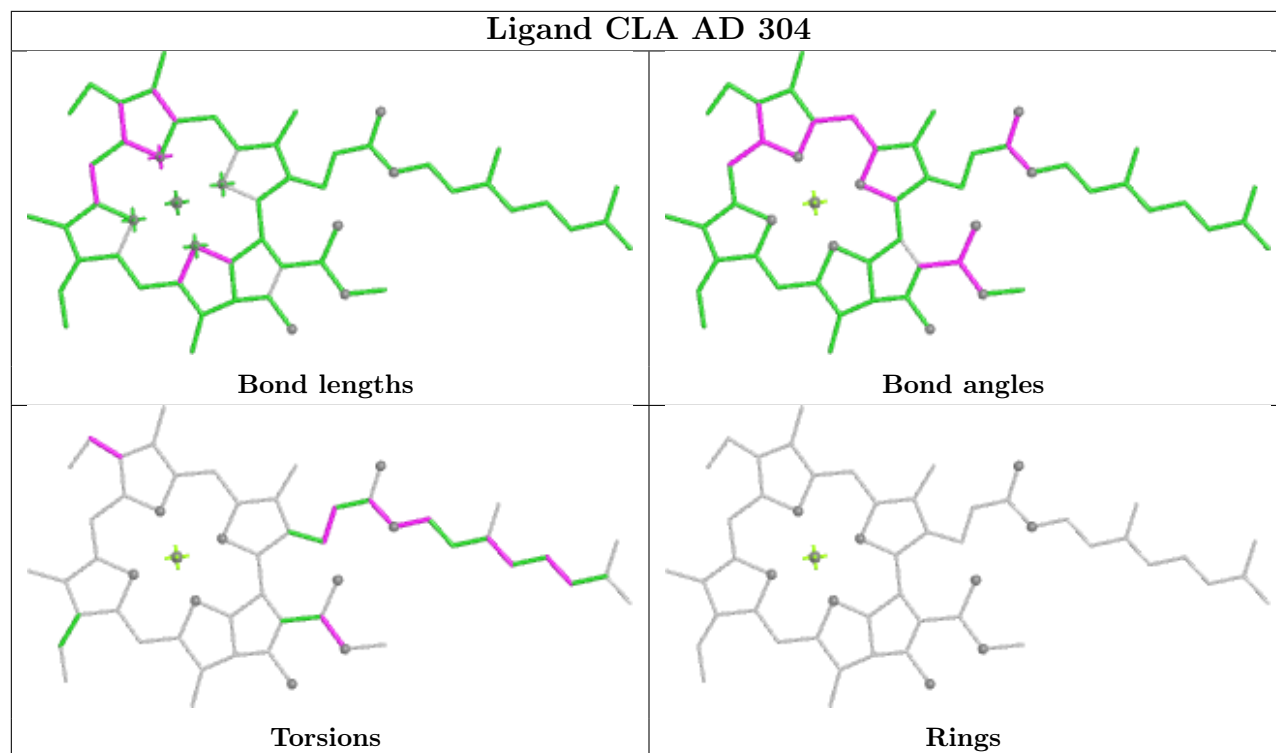
Ligand CLA AS 309



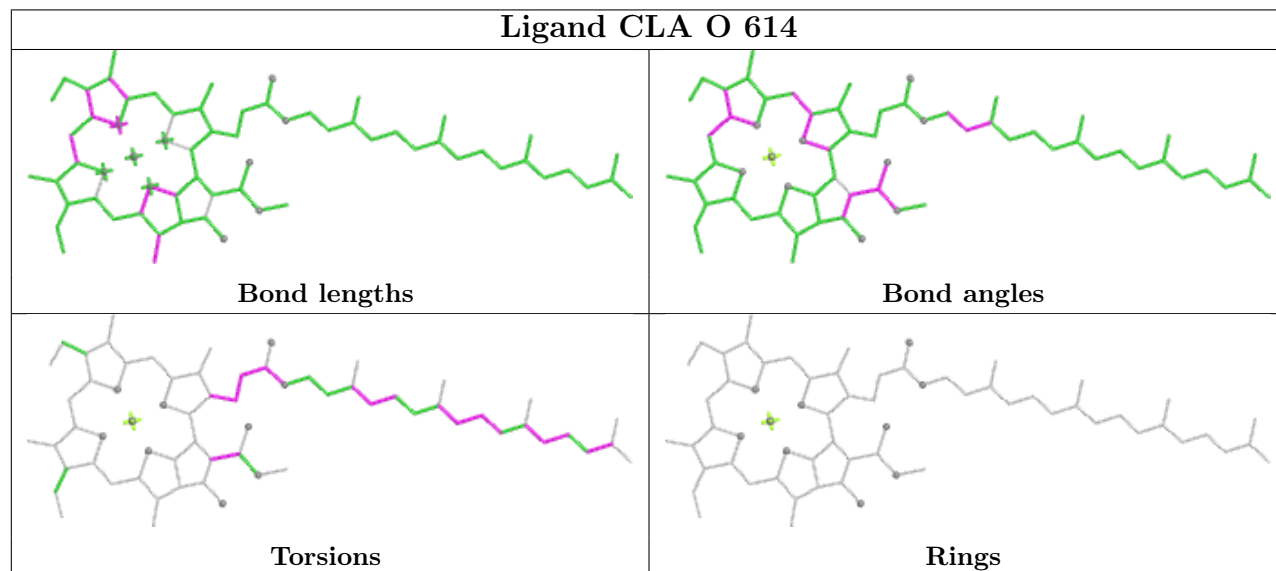
Ligand CLA AL 507



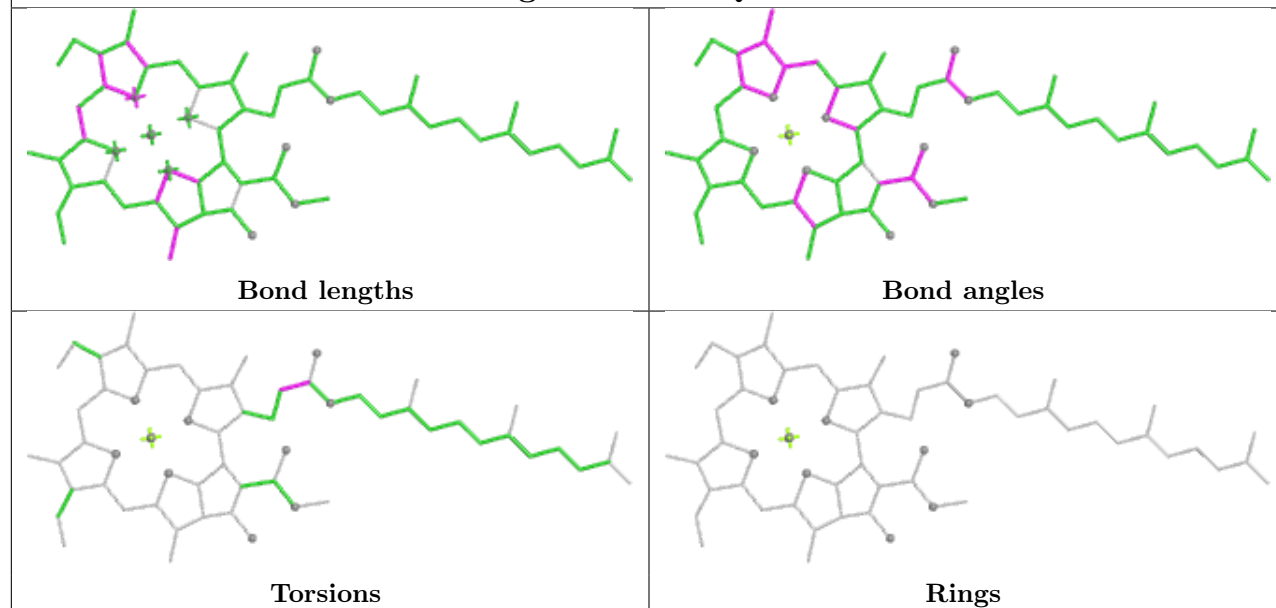
Ligand CLA AD 304



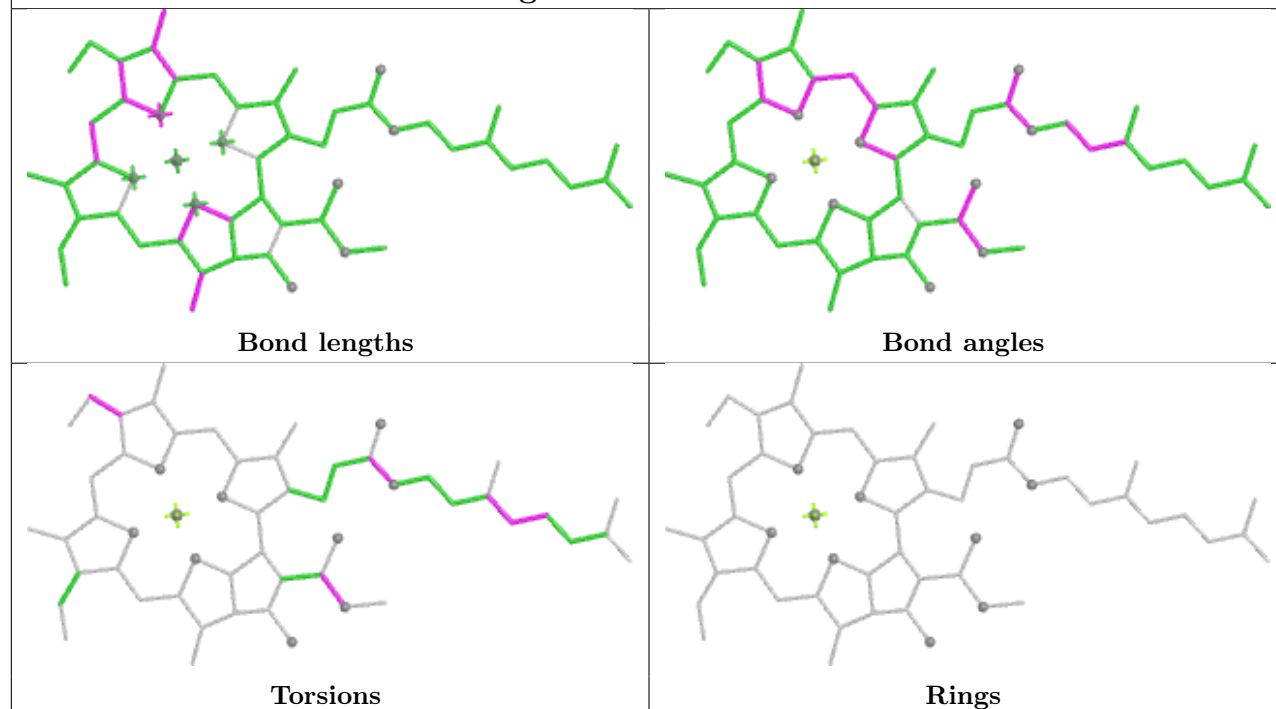
Ligand CLA O 614

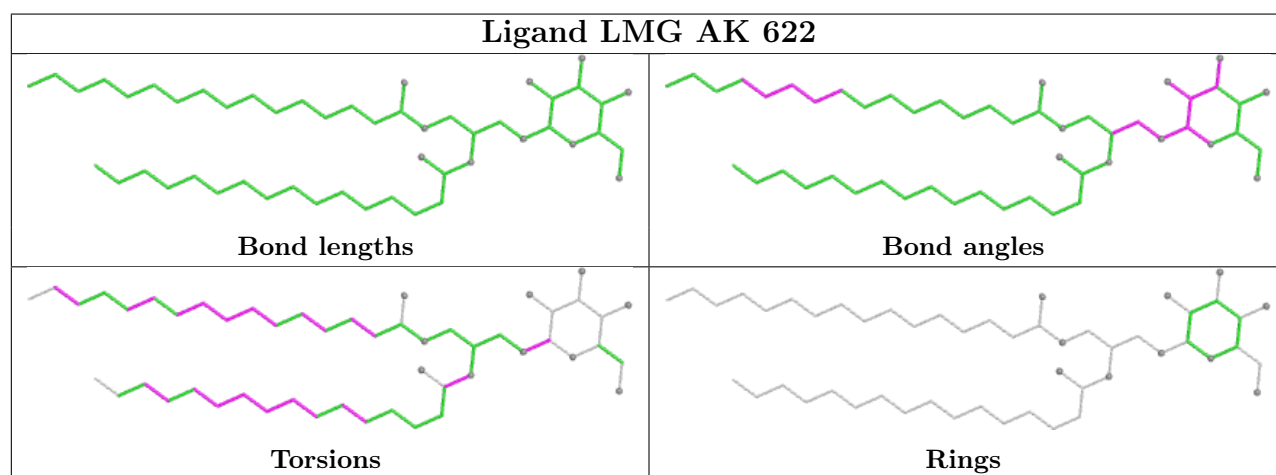
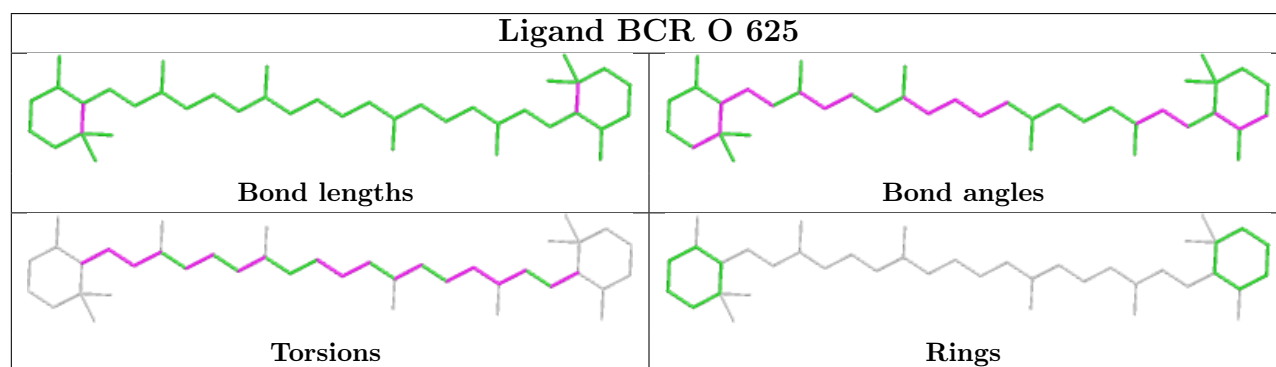
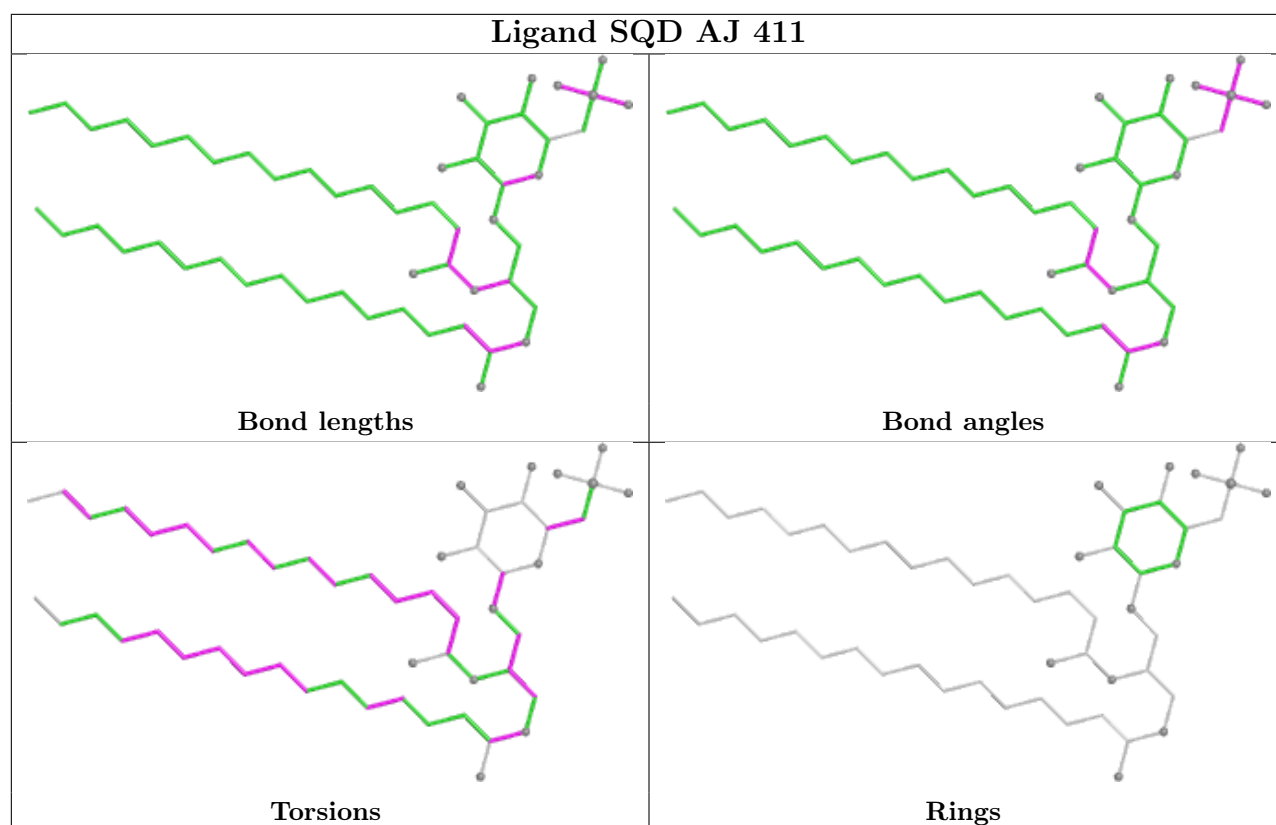


Ligand CLA AQ 612

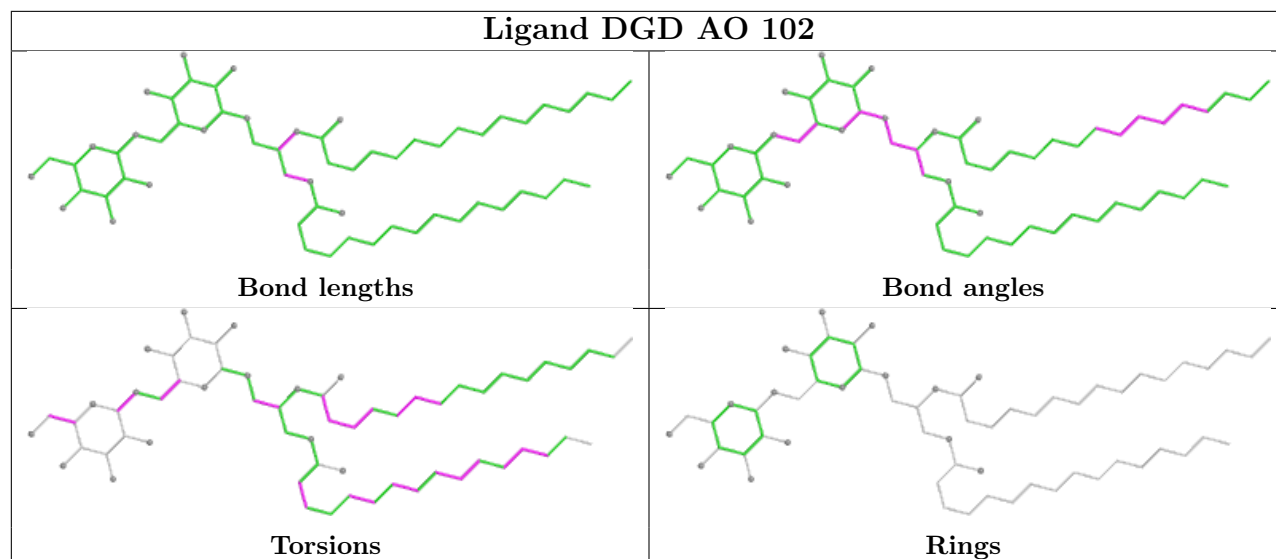


Ligand CLA AC 603

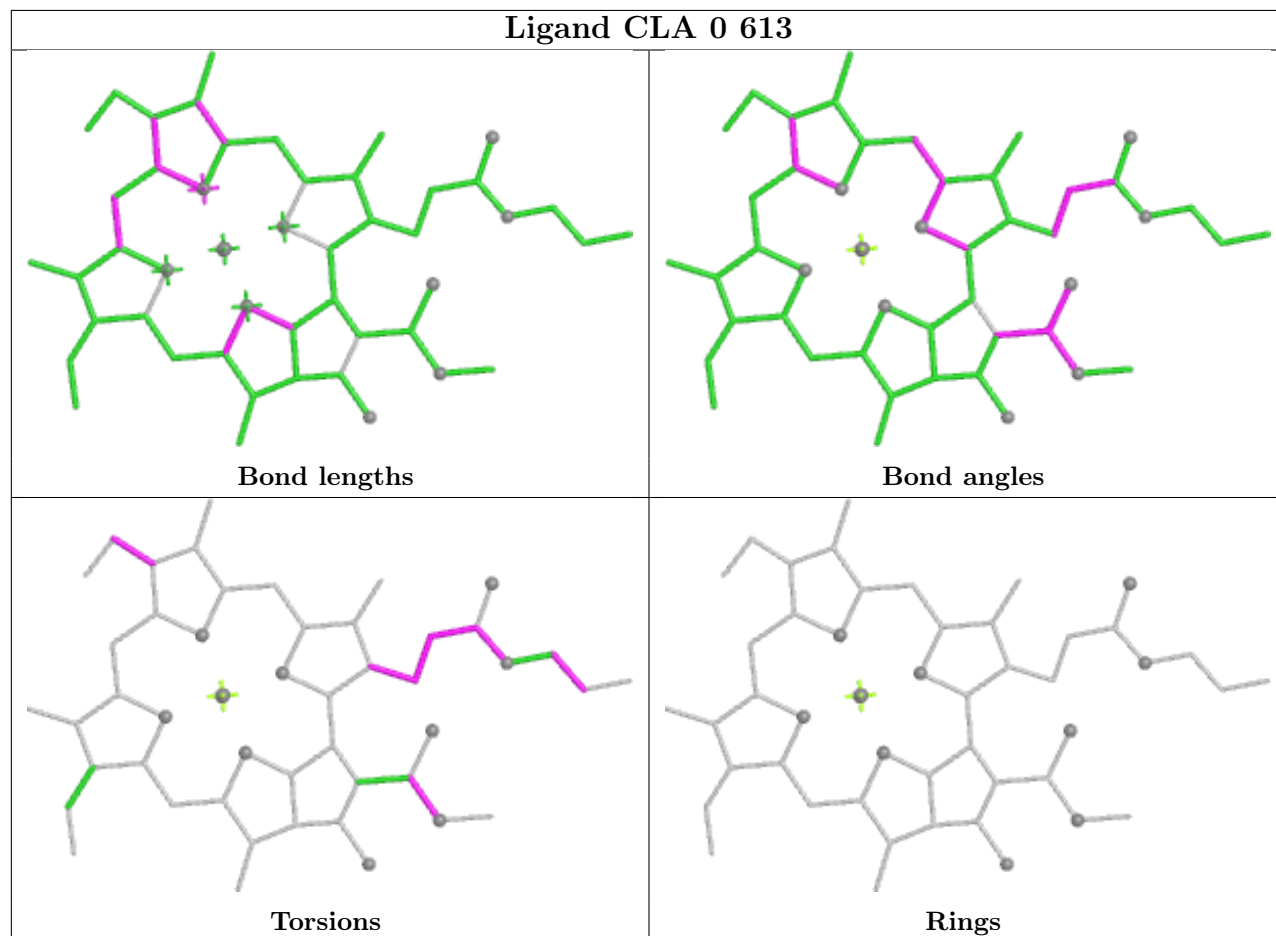




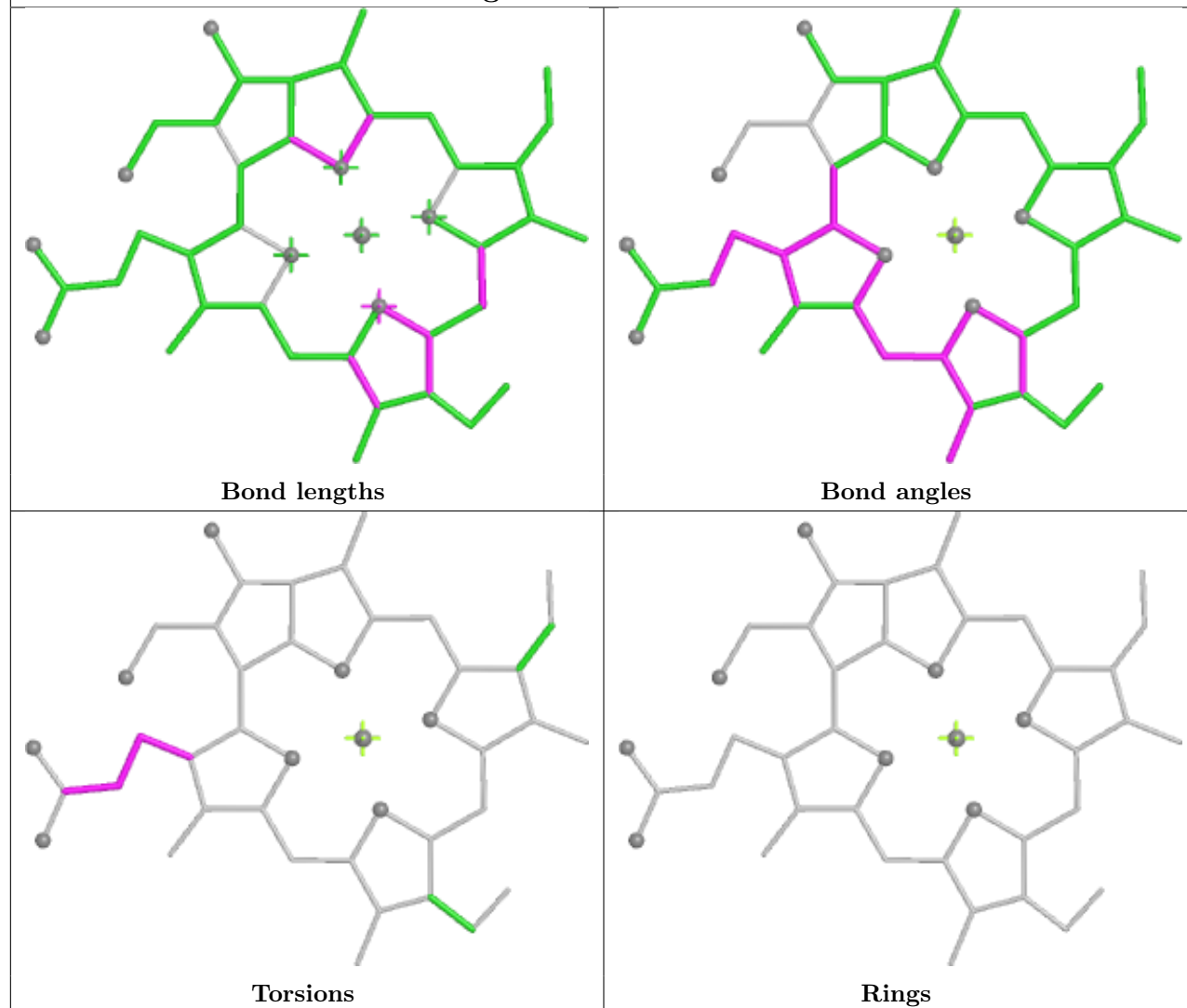
Ligand DGD AO 102



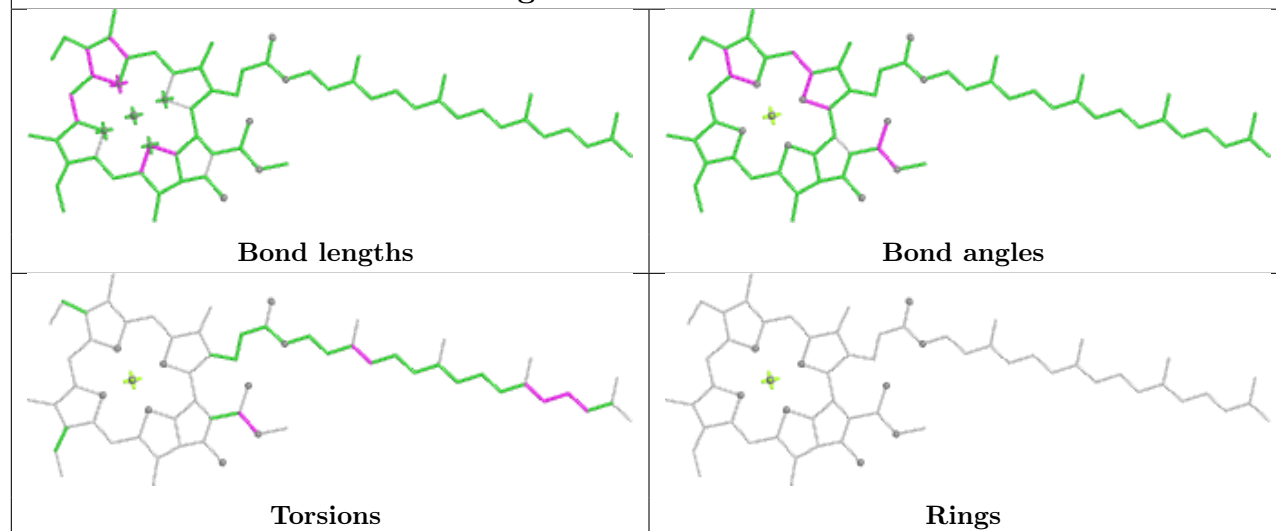
Ligand CLA 0 613



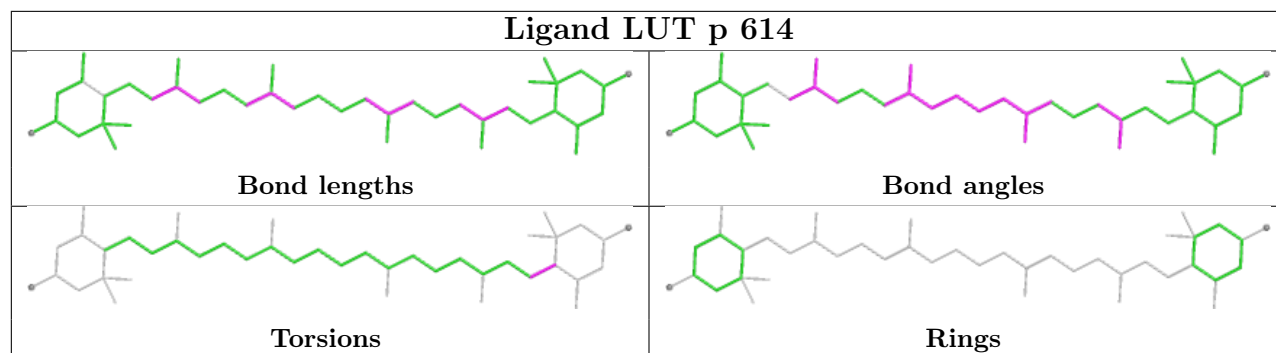
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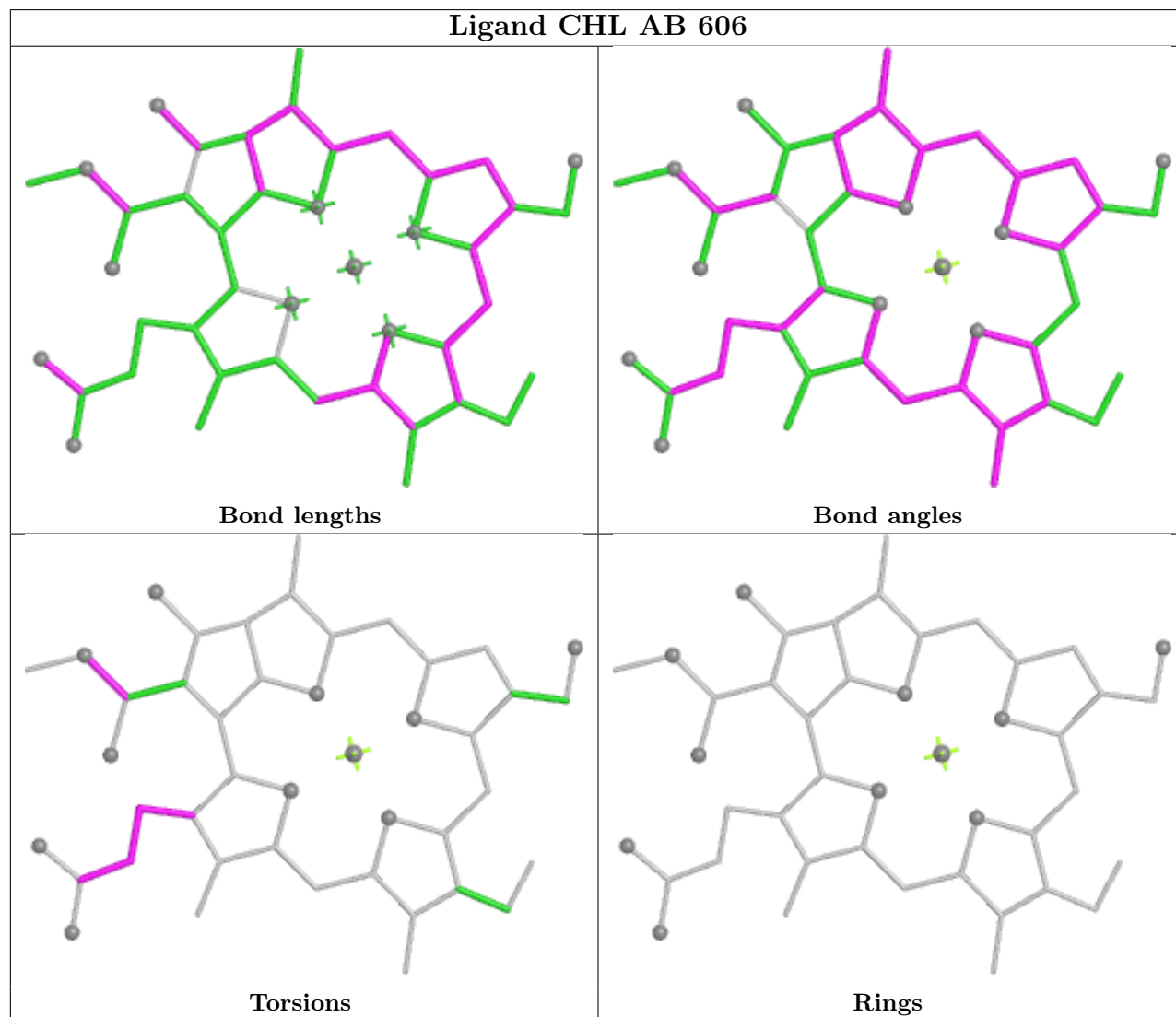
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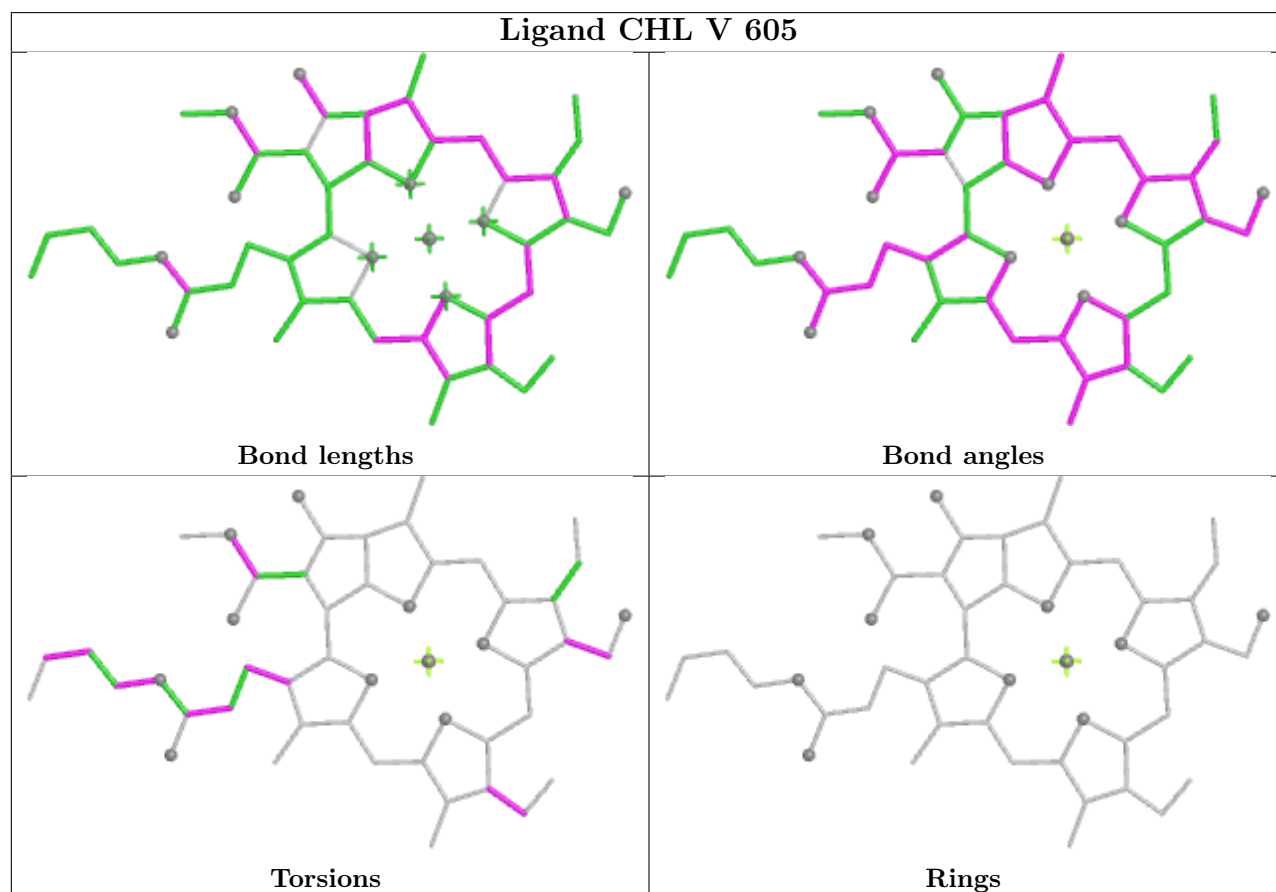
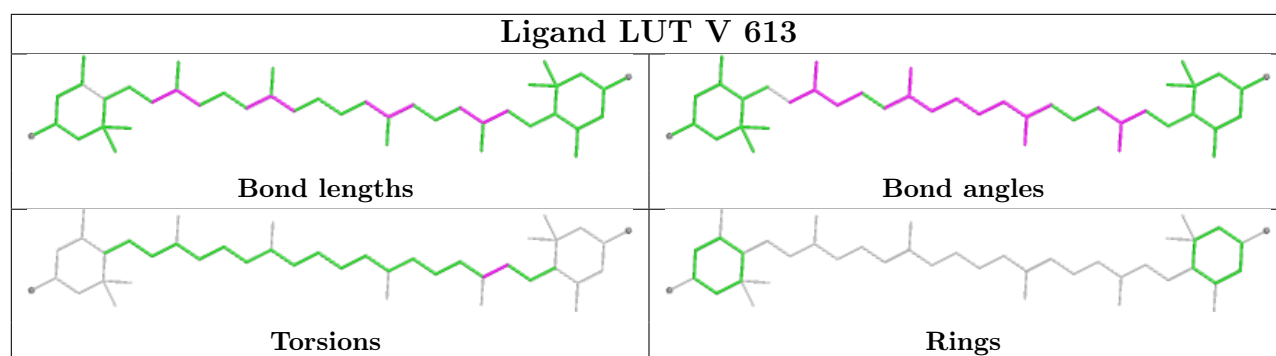


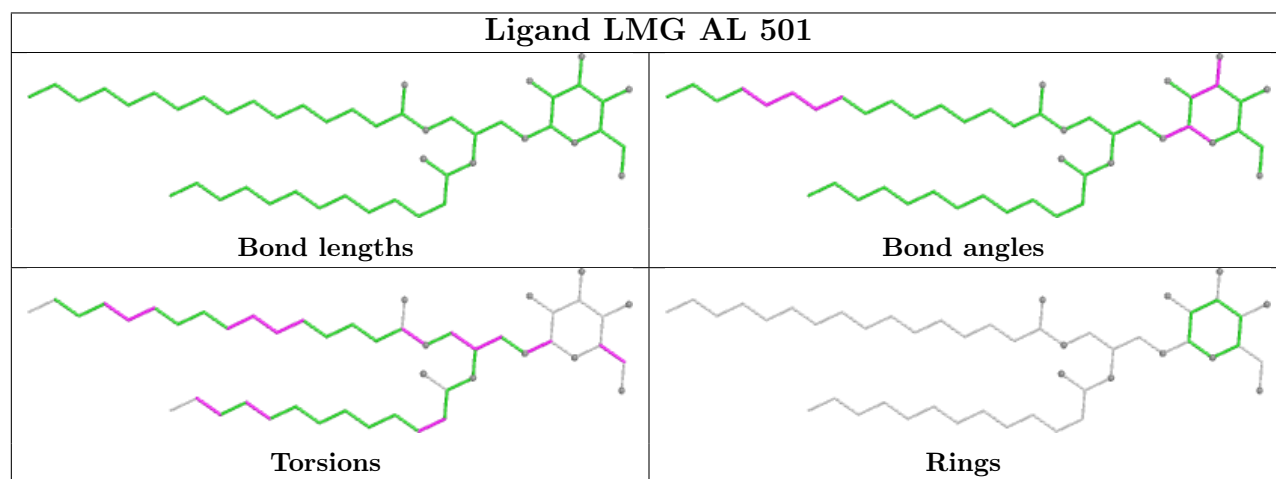
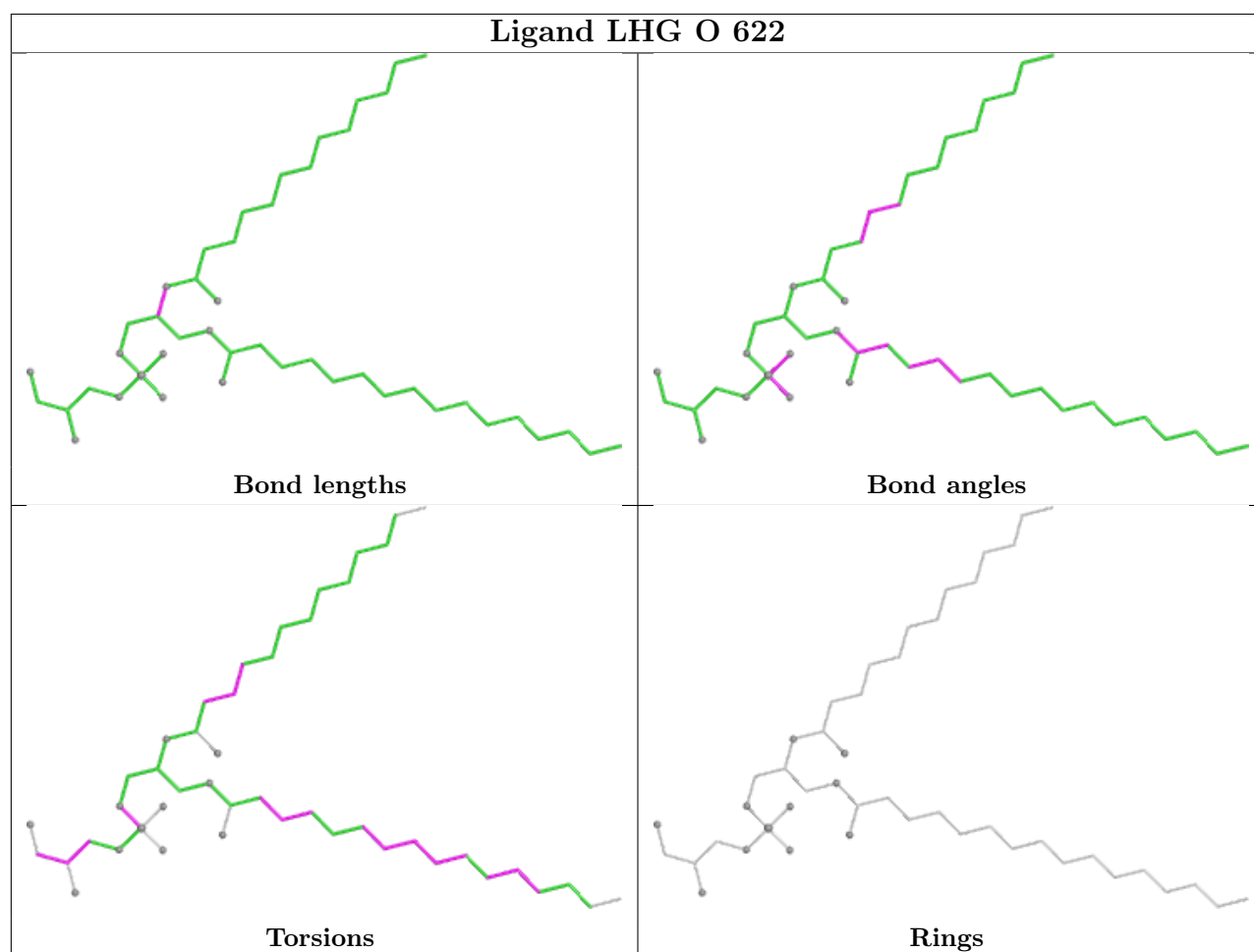
Ligand LUT p 614

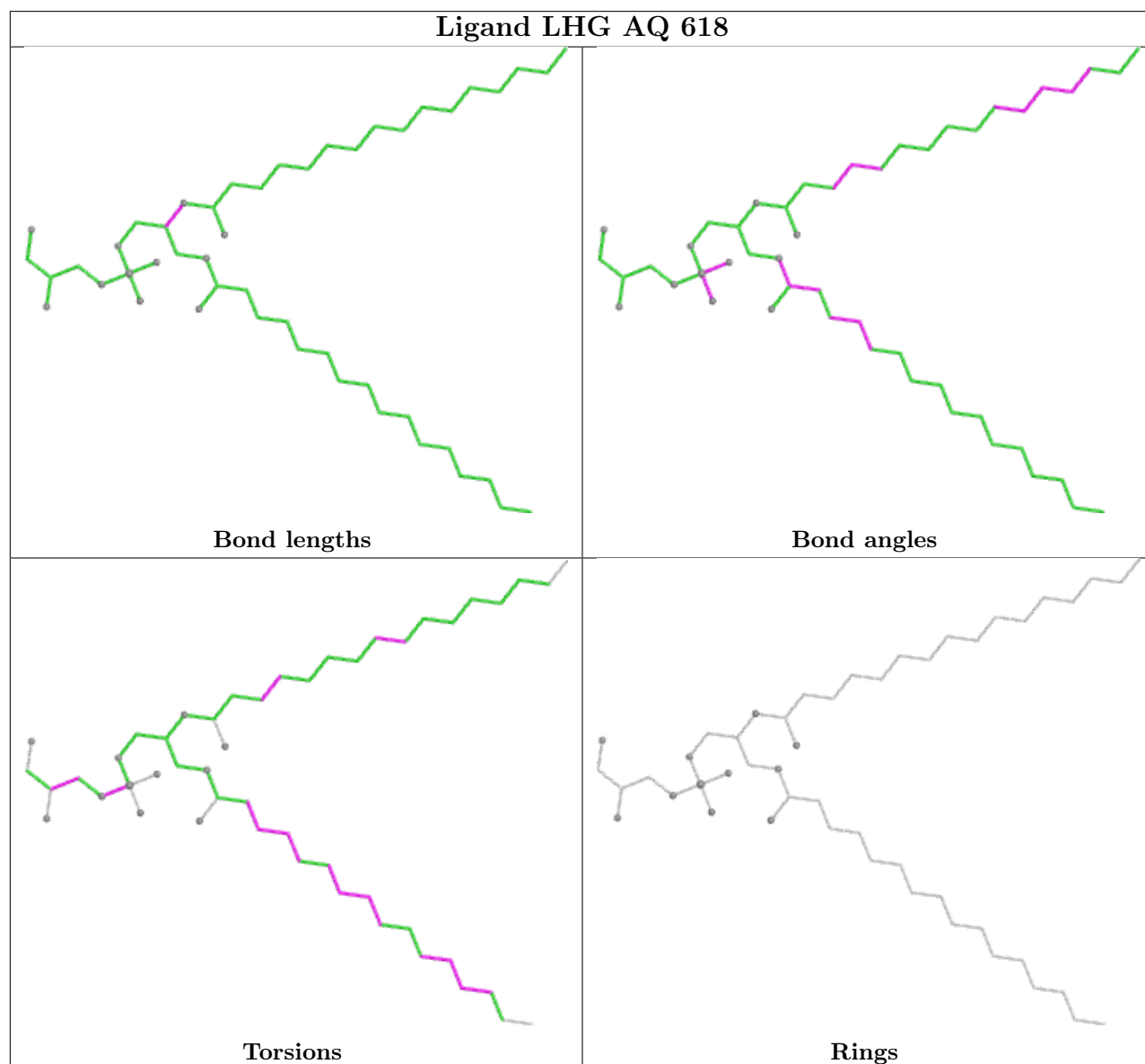
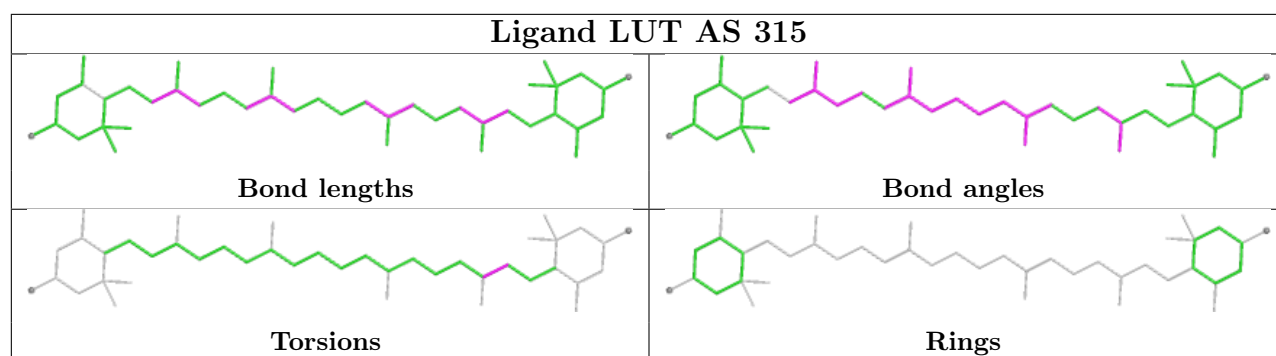


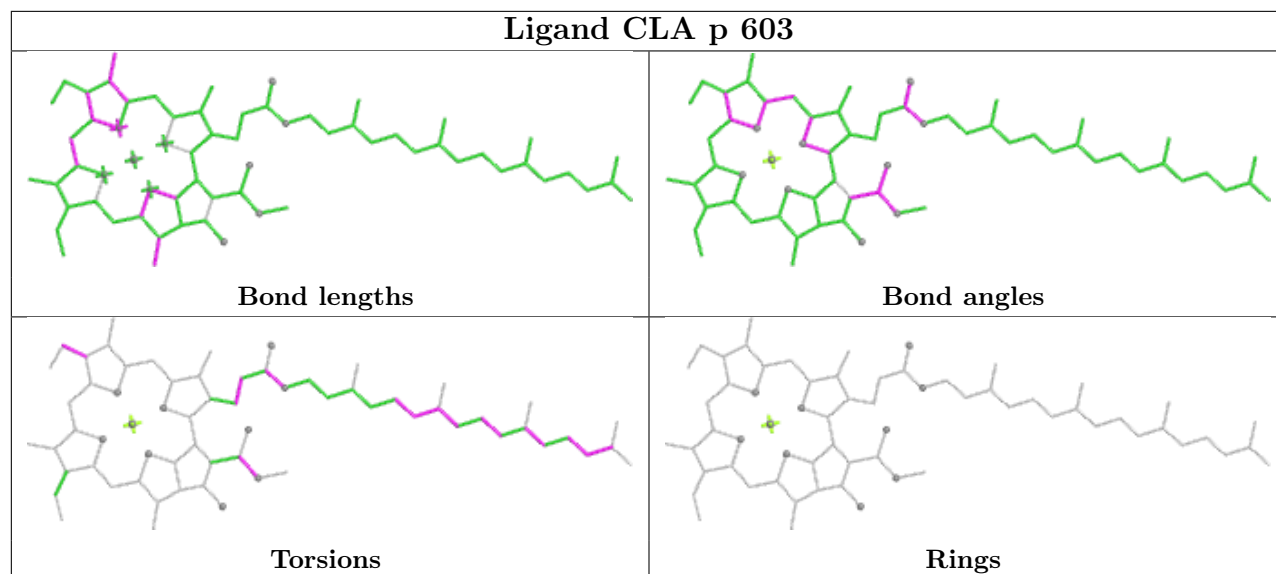
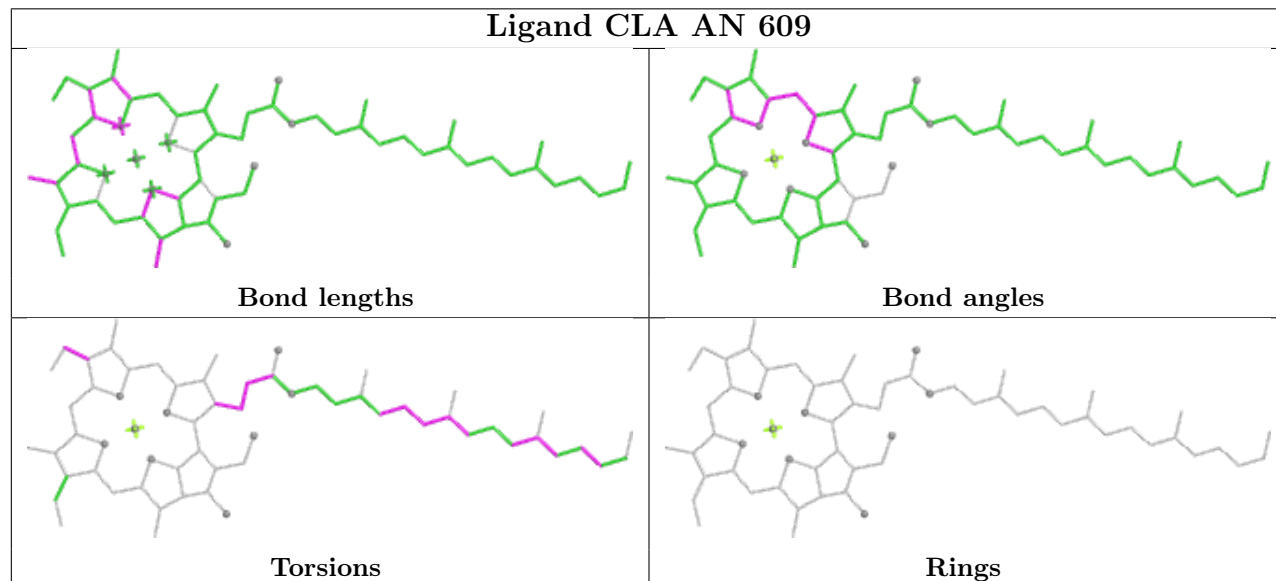
Ligand CHL AB 606



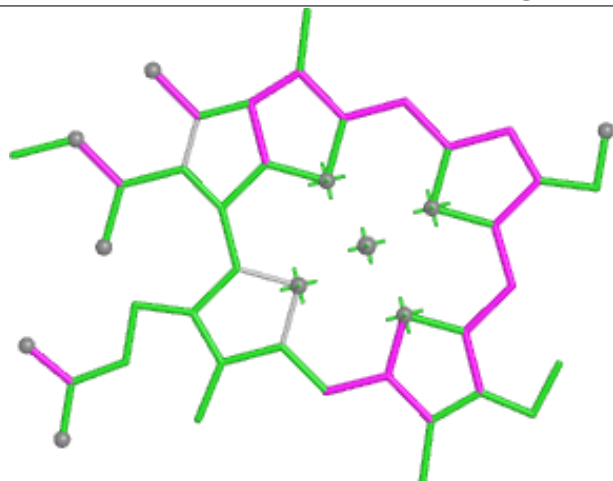




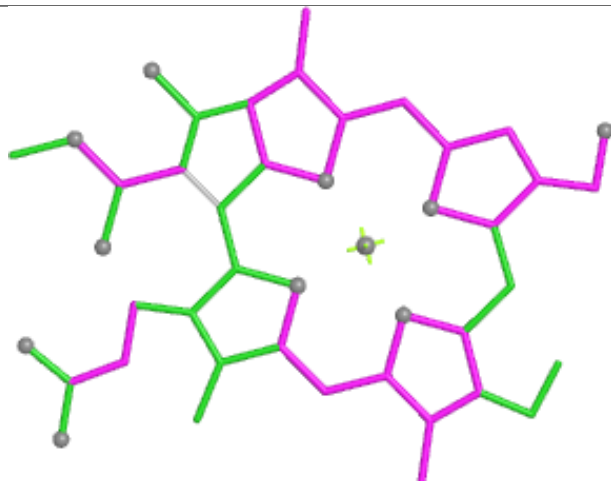


Ligand CLA p 603**Ligand CLA AN 609**

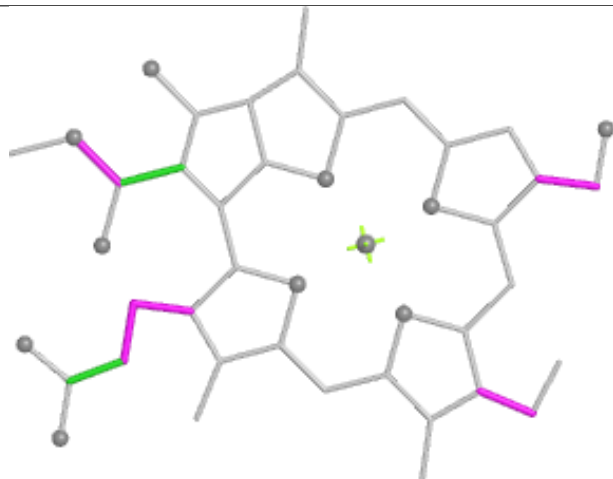
Ligand CHL 9 608



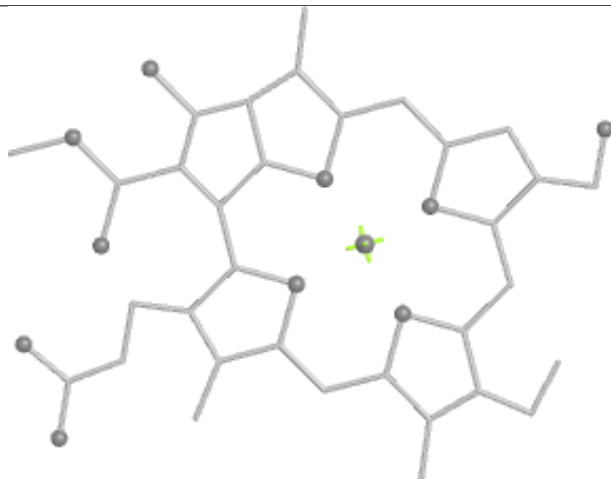
Bond lengths



Bond angles

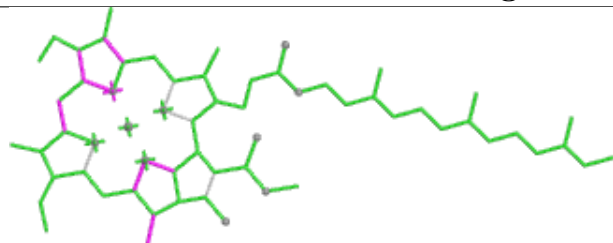


Torsions

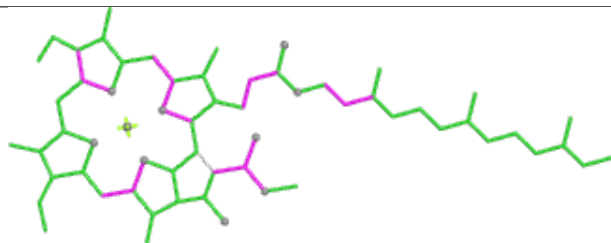


Rings

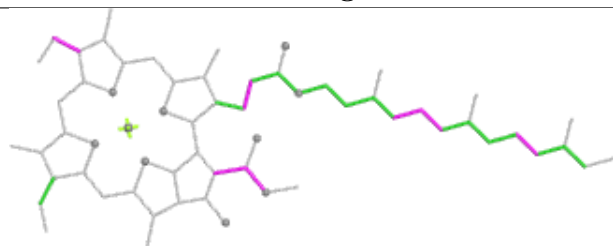
Ligand CLA AA 602



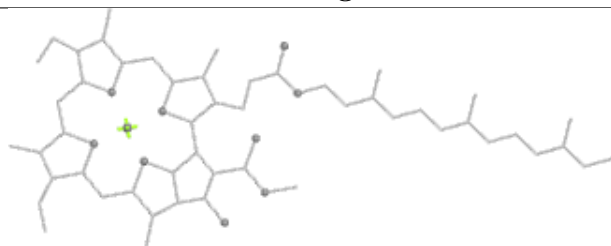
Bond lengths



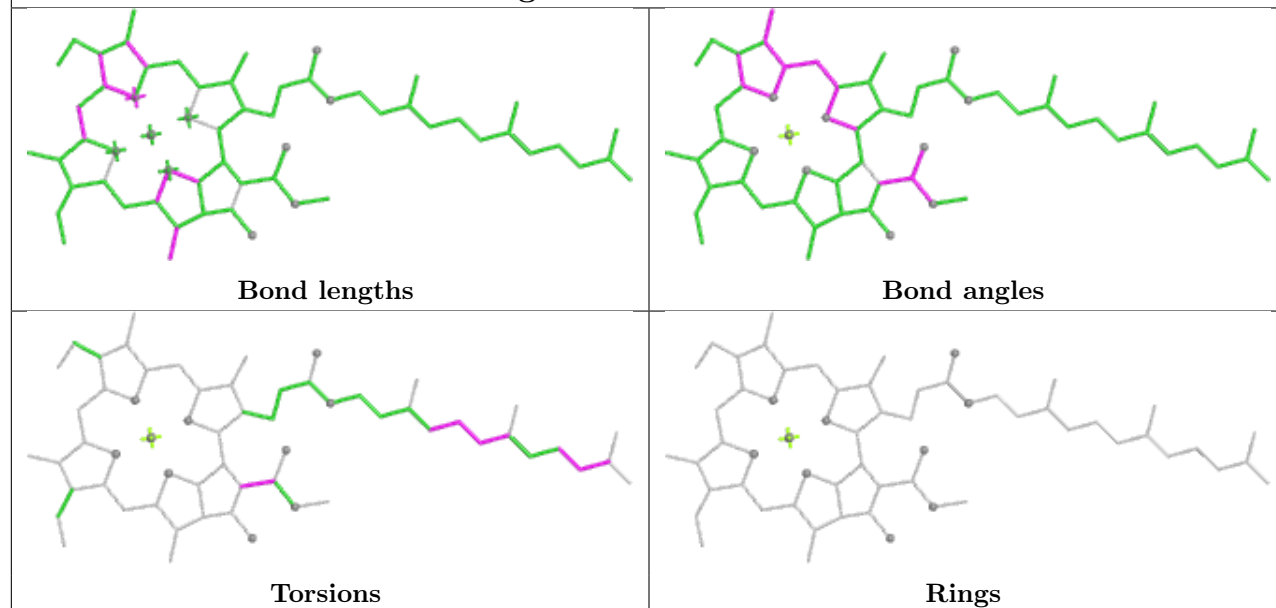
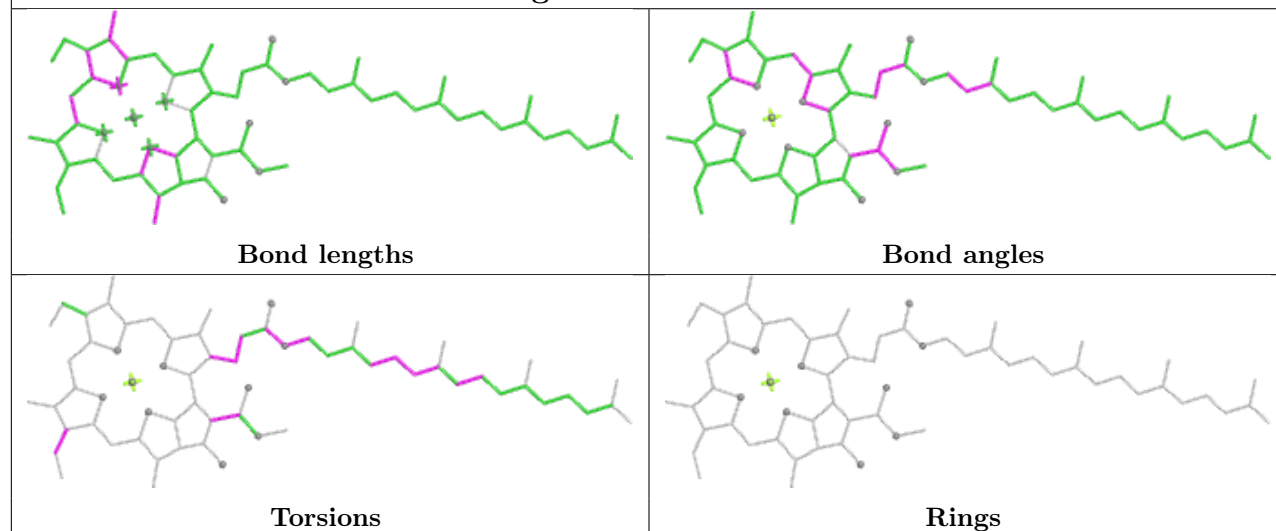
Bond angles

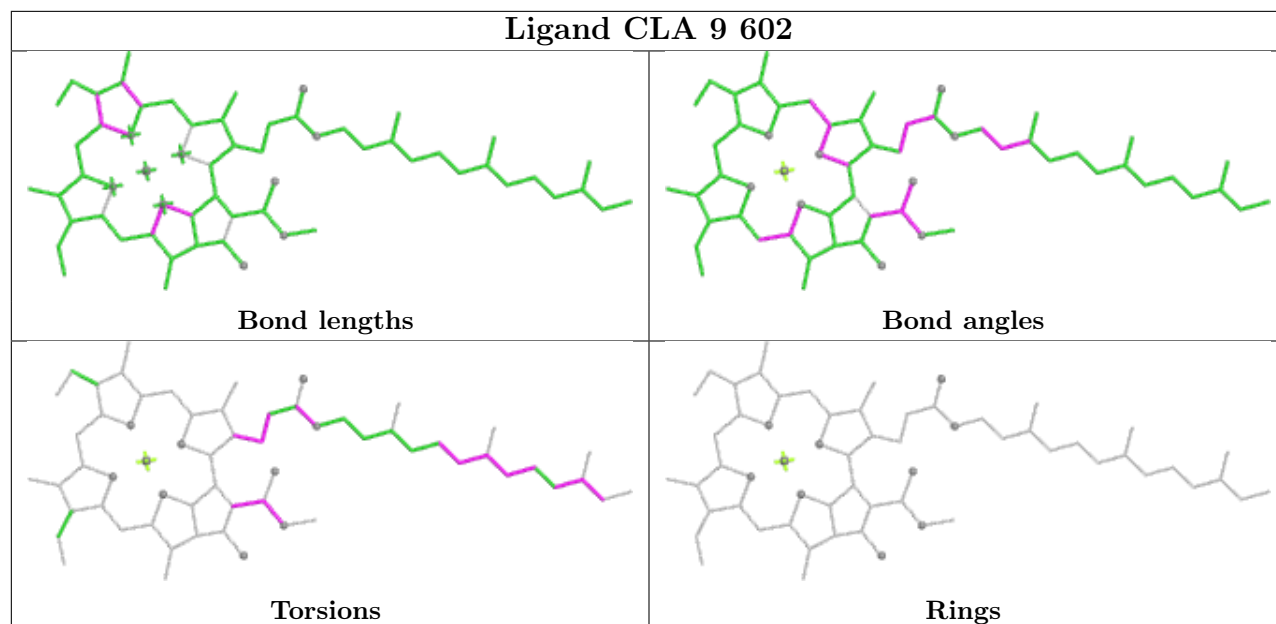
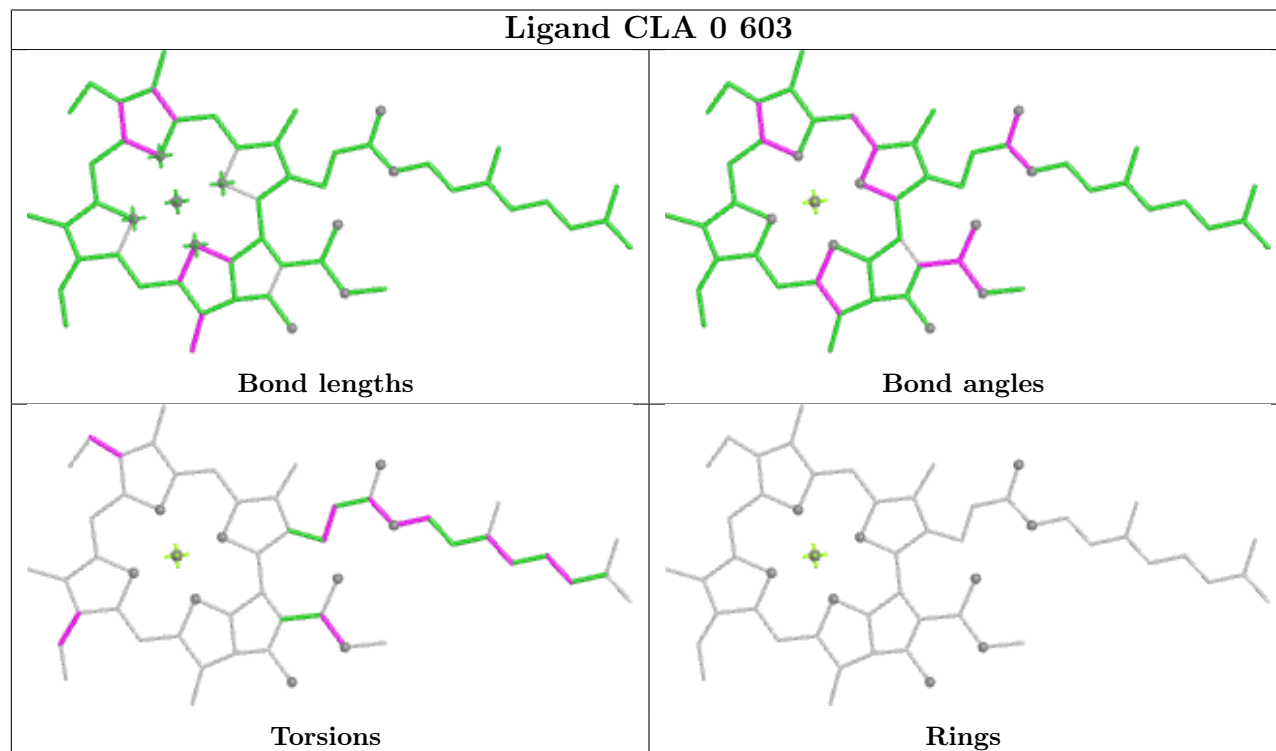


Torsions

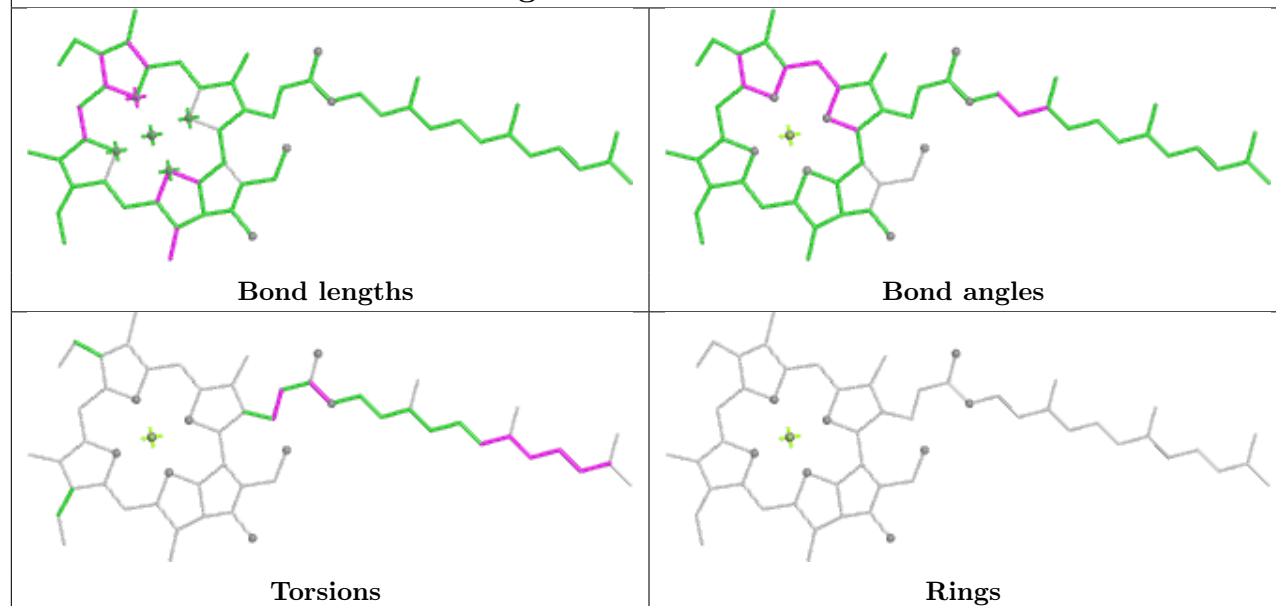


Rings

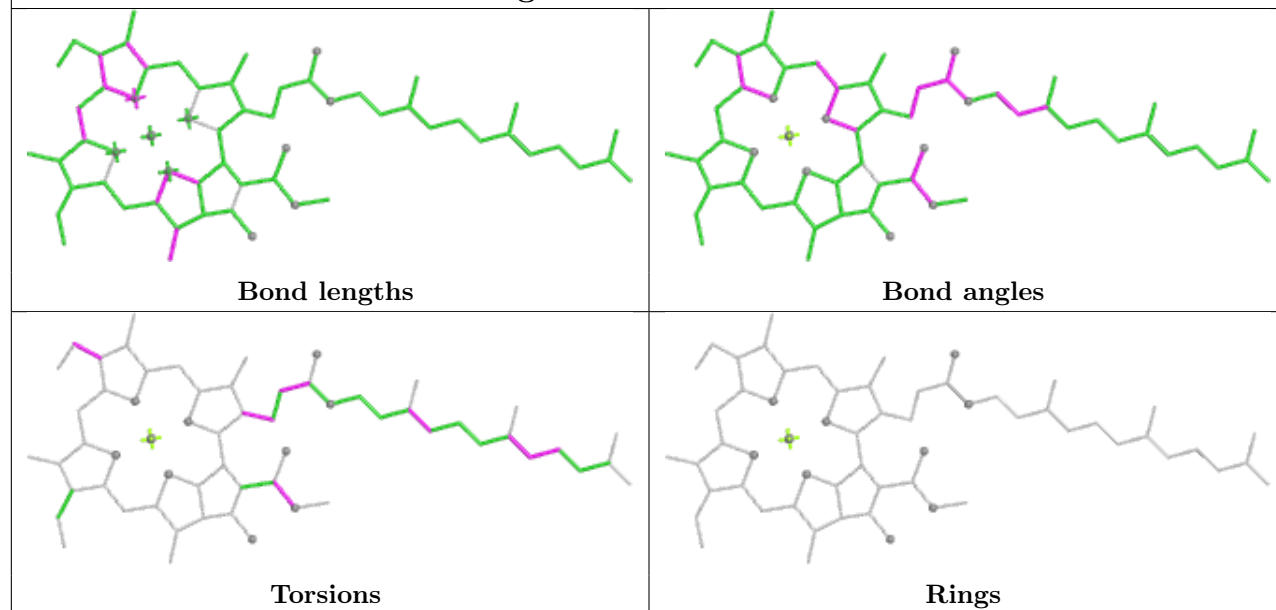
Ligand CLA AR 603**Ligand CLA O 604**

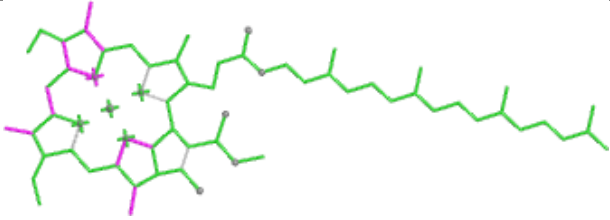
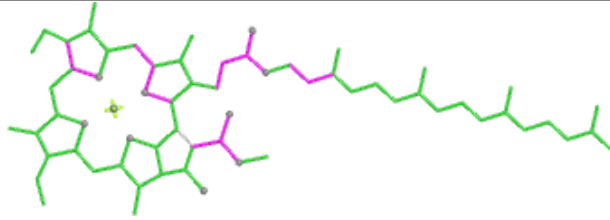
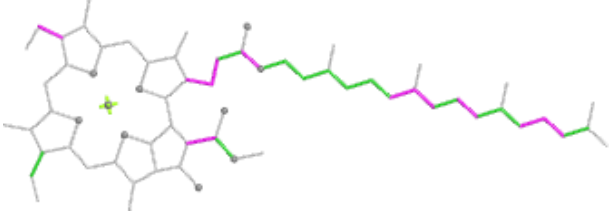
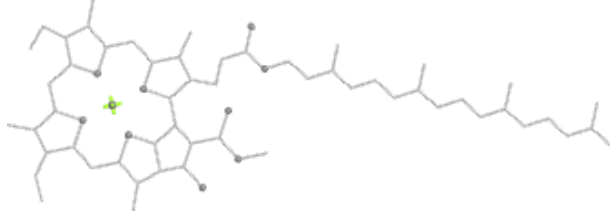
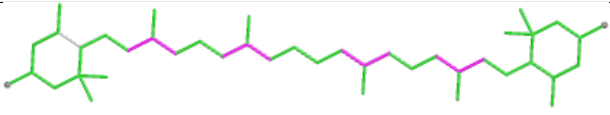
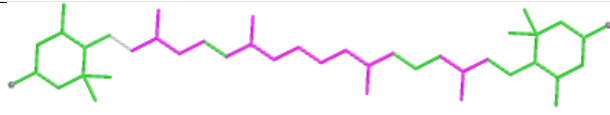
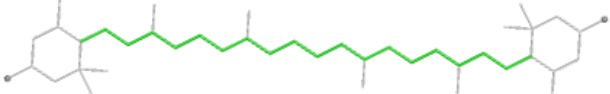
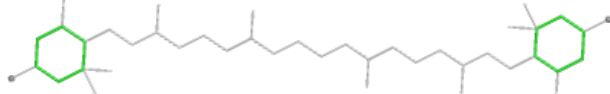
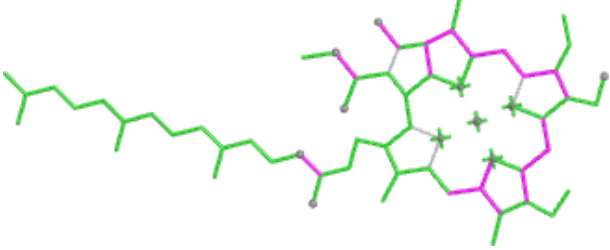
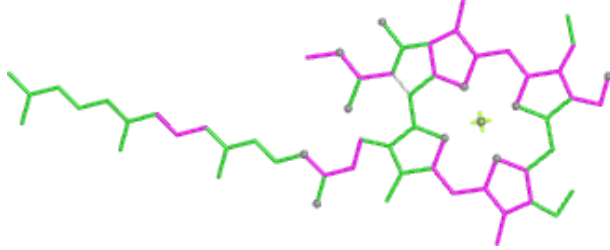
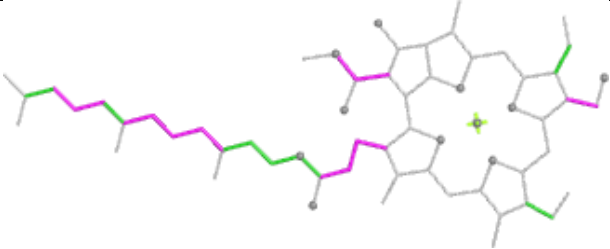
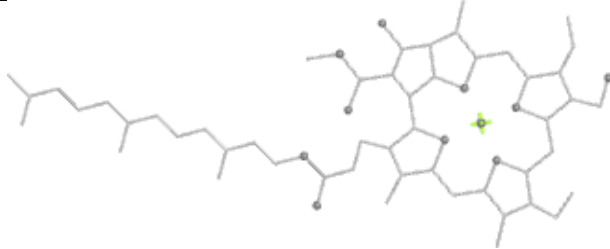
Ligand CLA 9 602**Ligand CLA 0 603**

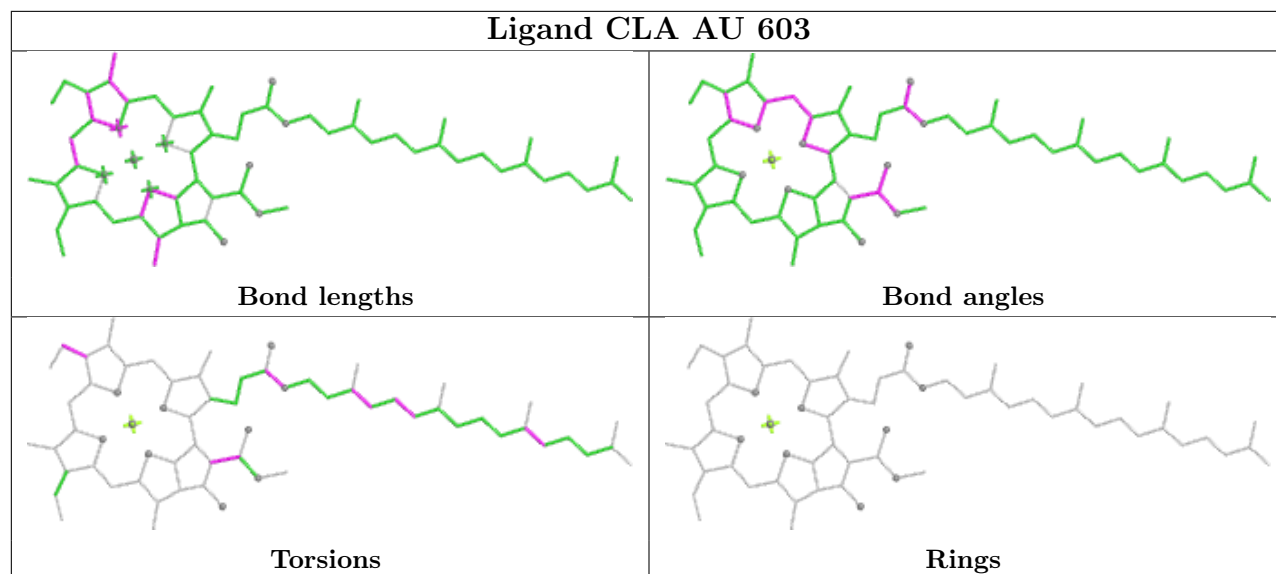
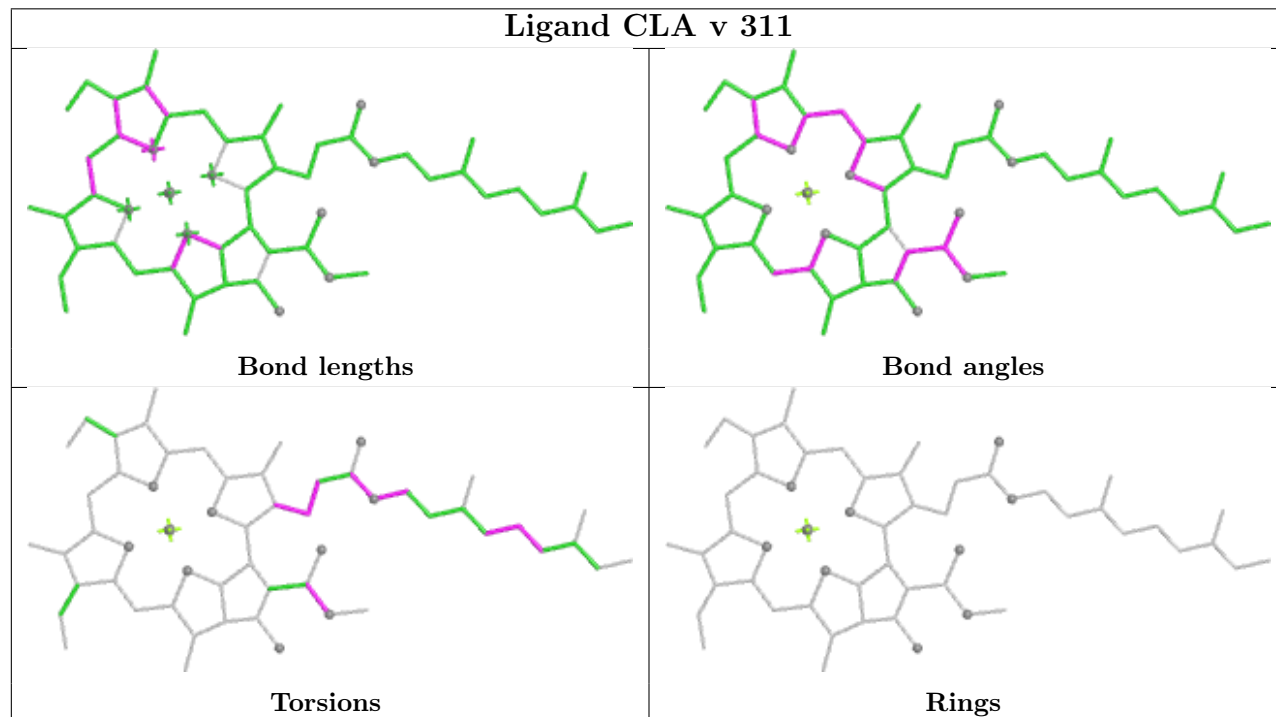
Ligand CLA AR 602

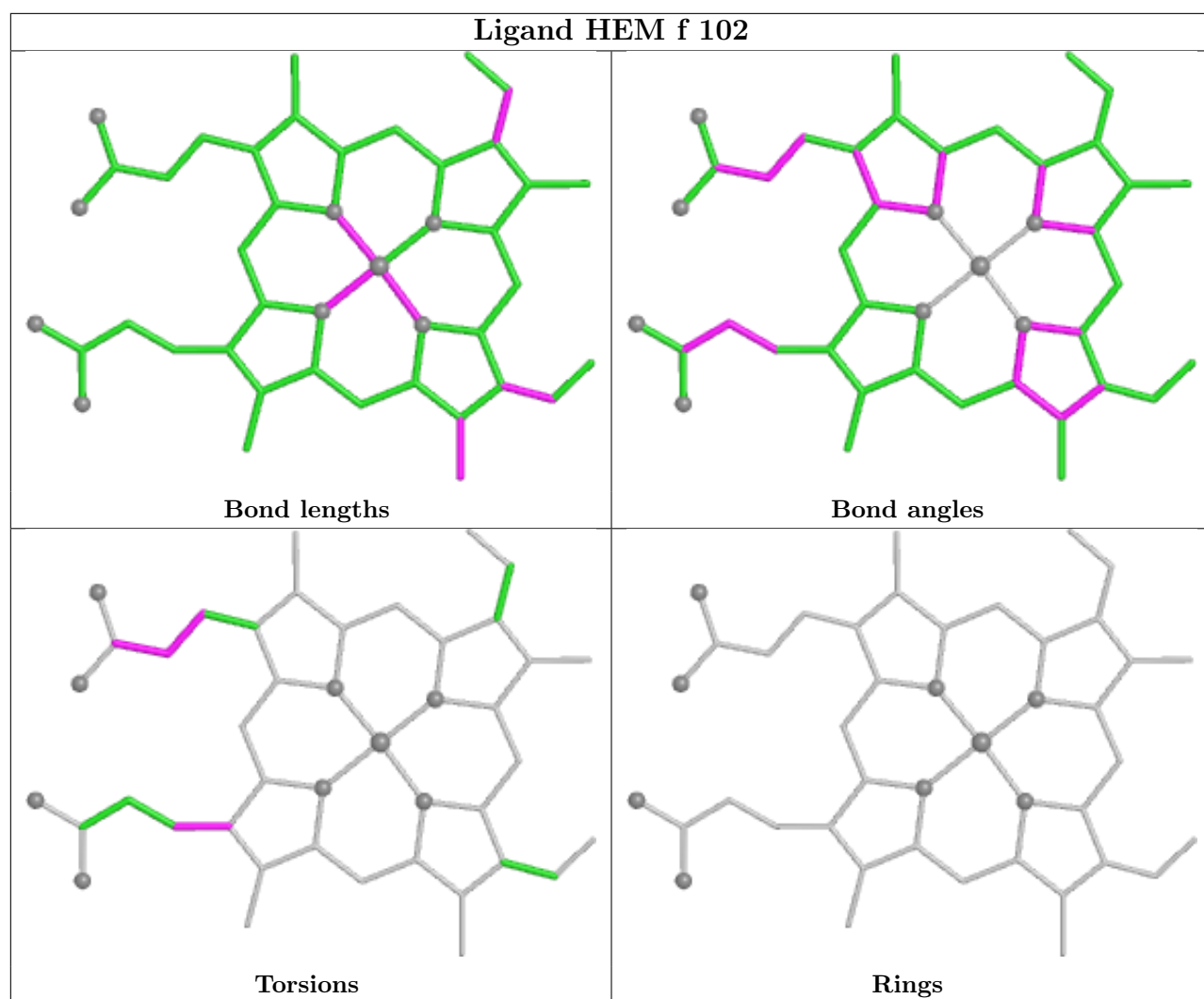


Ligand CLA AH 610

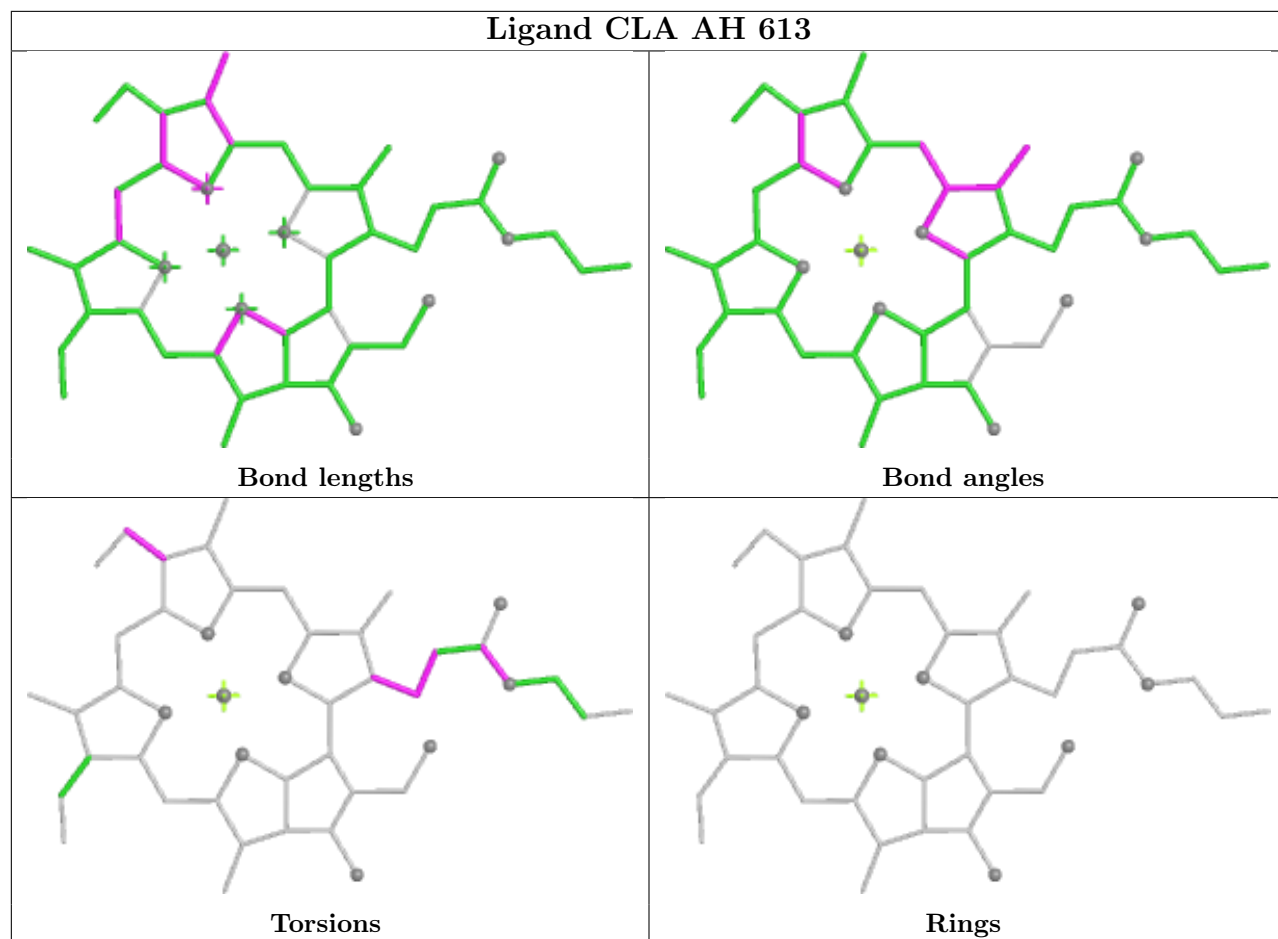


Ligand CLA O 612	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT AD 314	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL AA 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

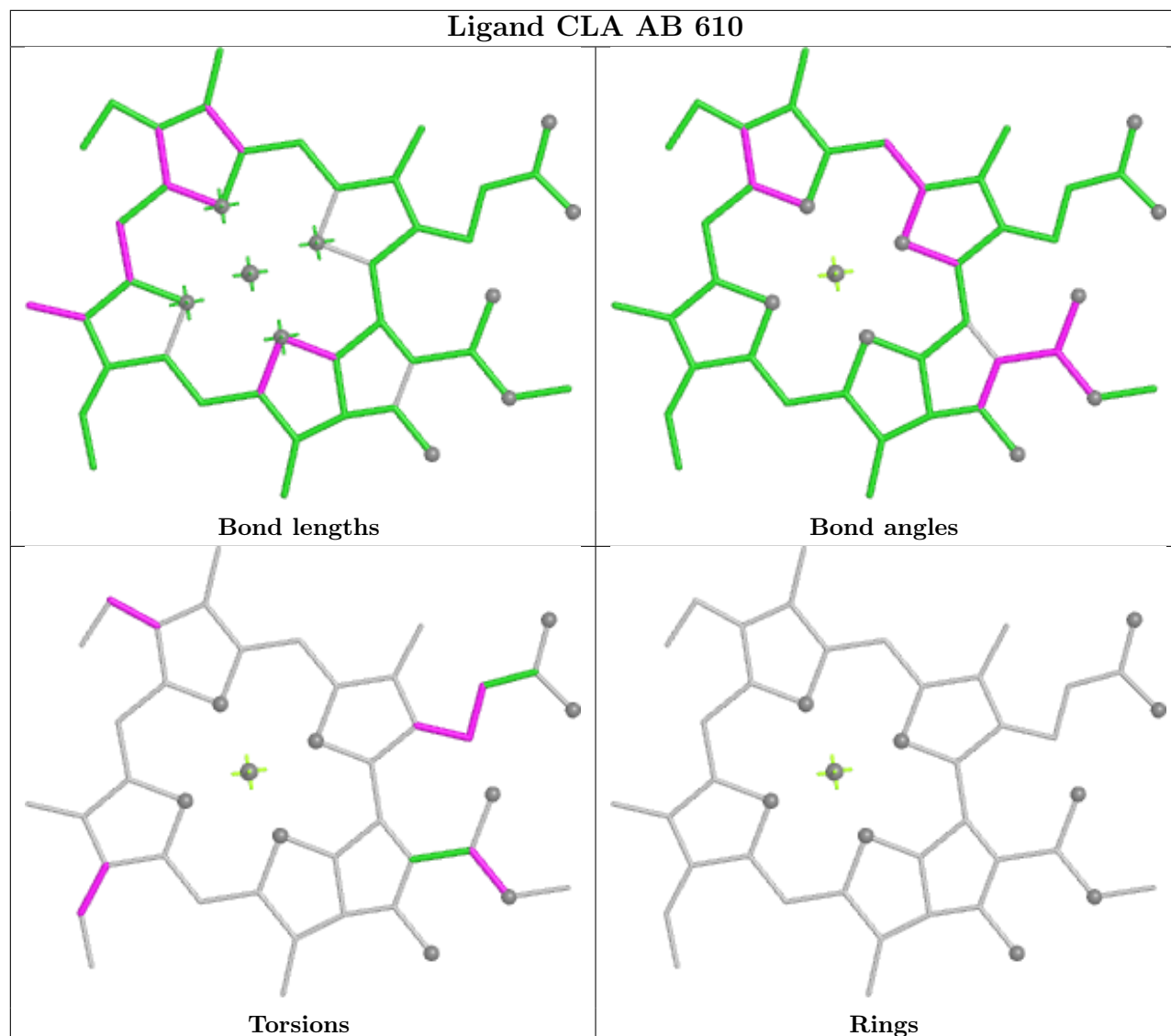
Ligand CLA AU 603**Ligand CLA v 311**



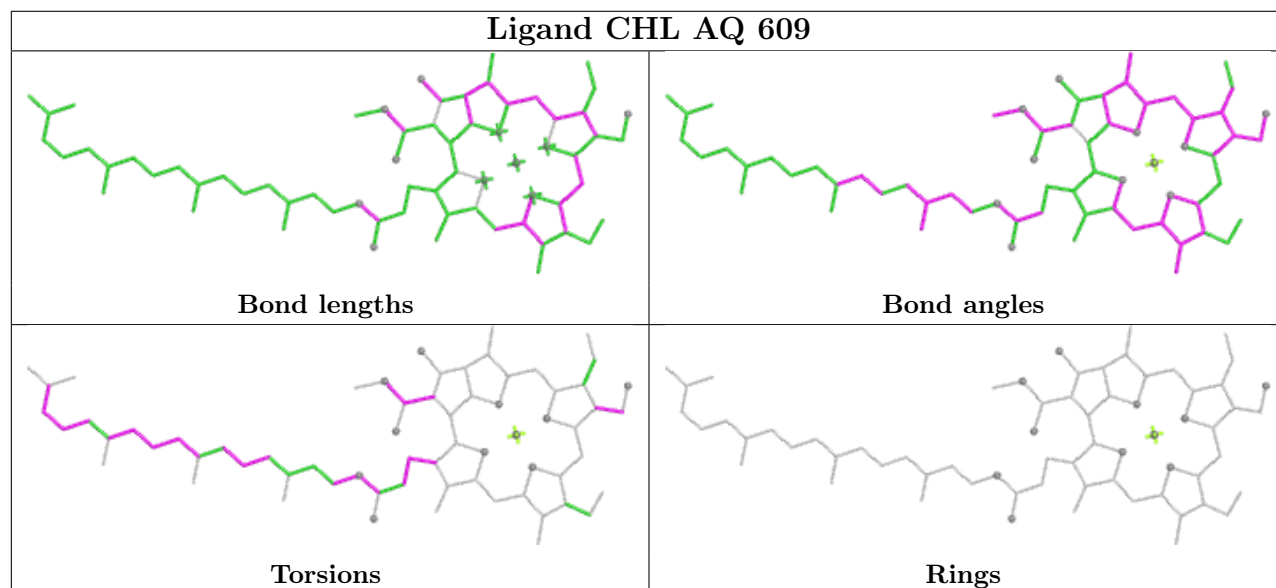
Ligand CLA AH 613

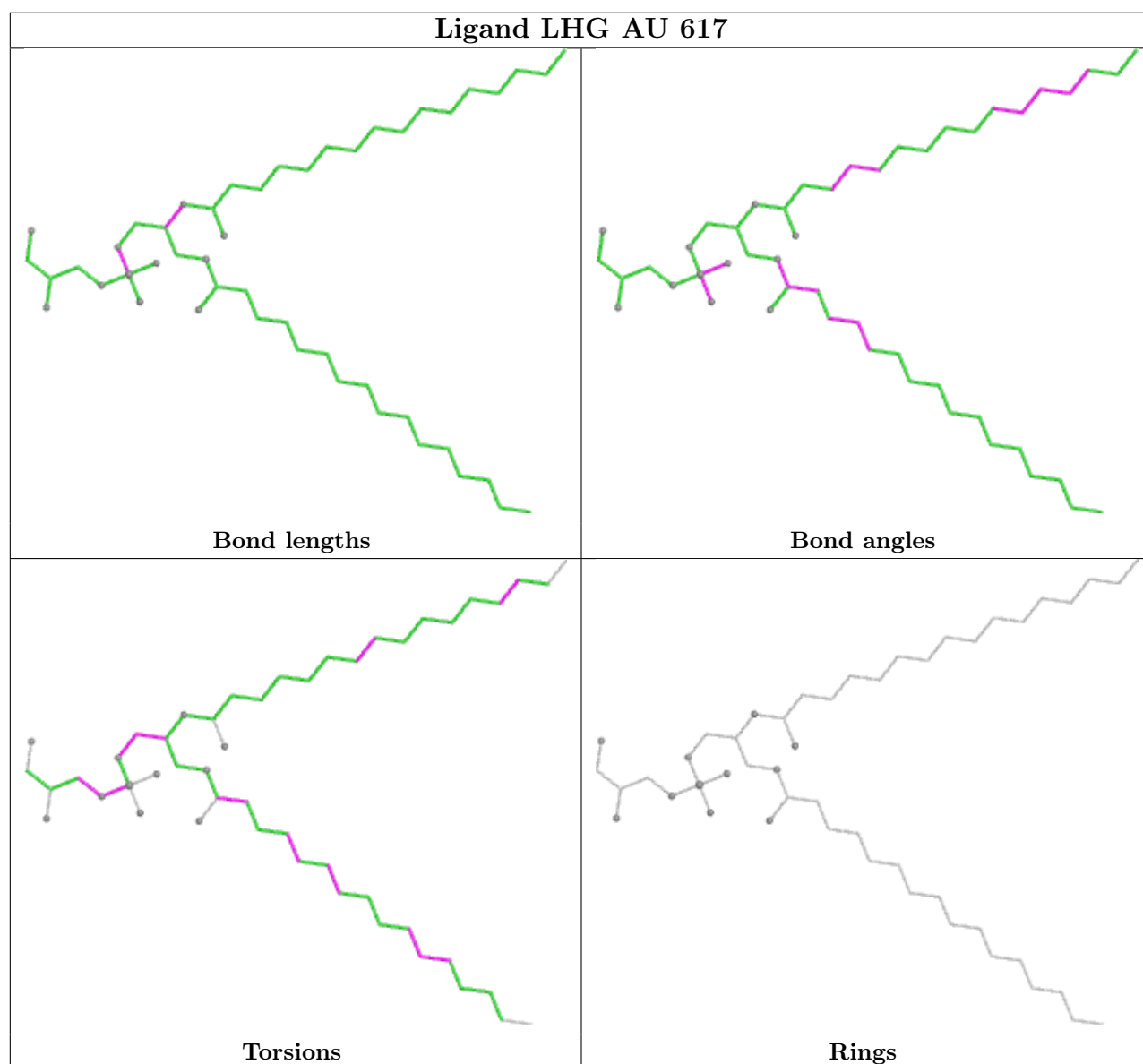
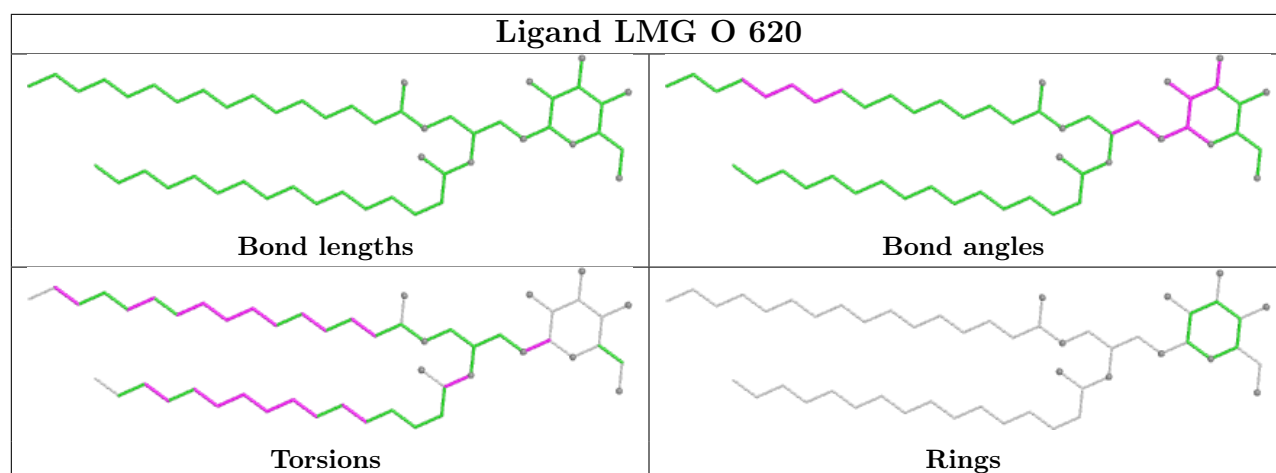


Ligand CLA AB 610

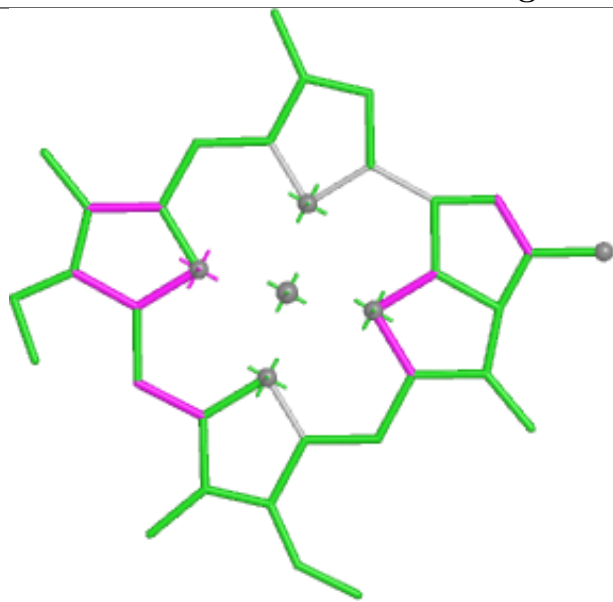


Ligand CHL AQ 609

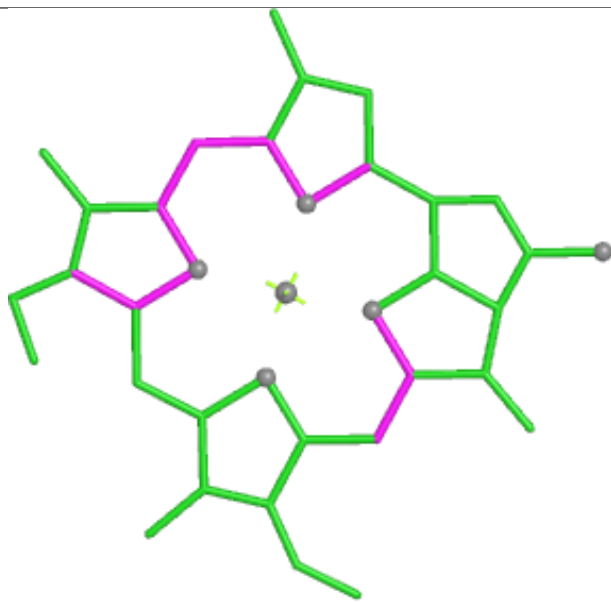




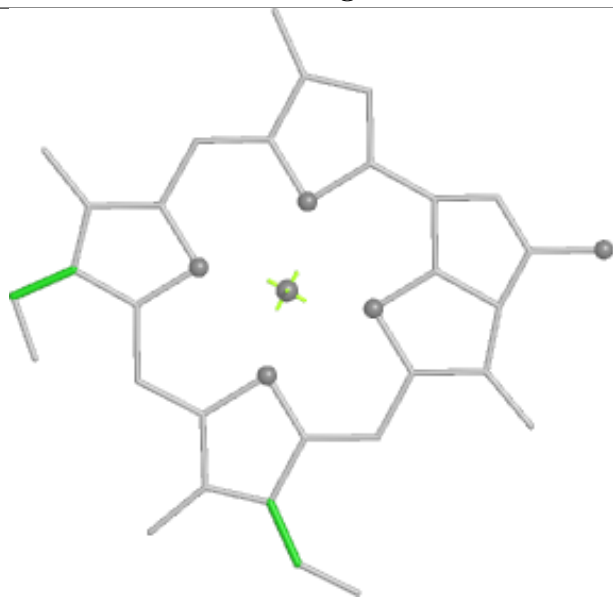
Ligand CLA 9 614



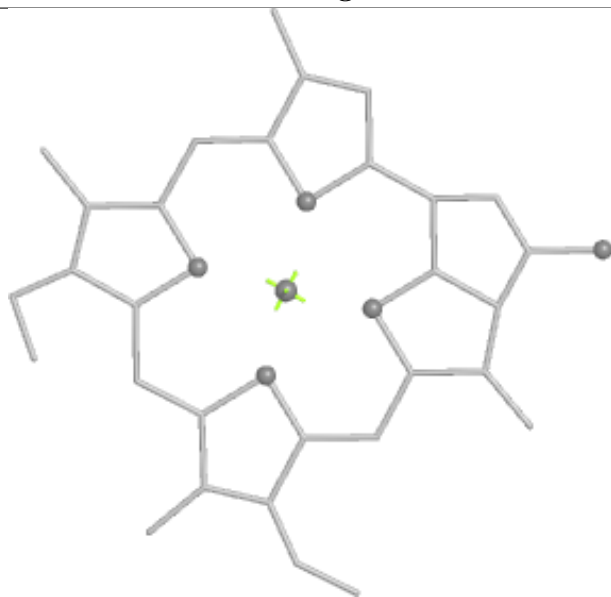
Bond lengths



Bond angles

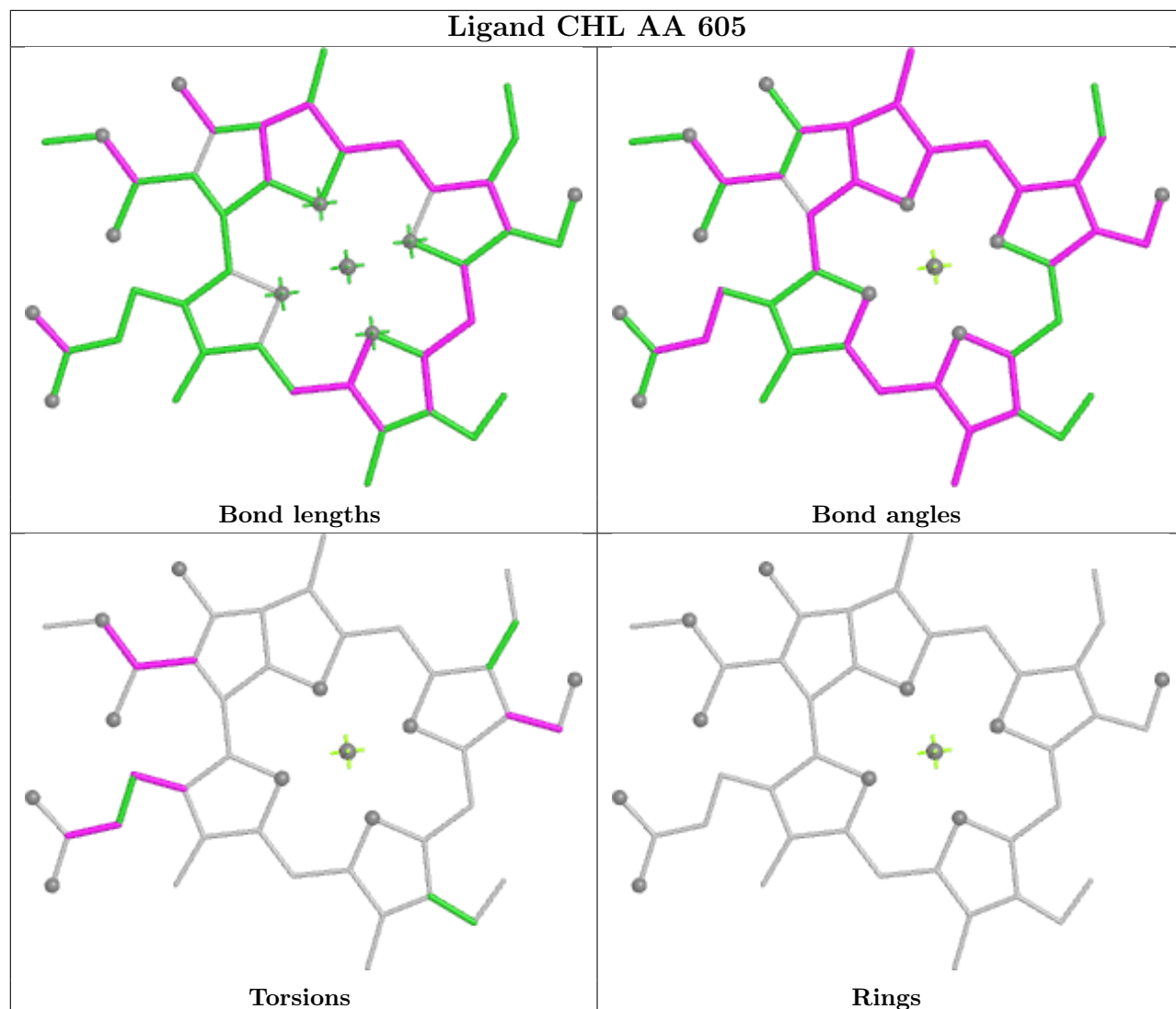


Torsions

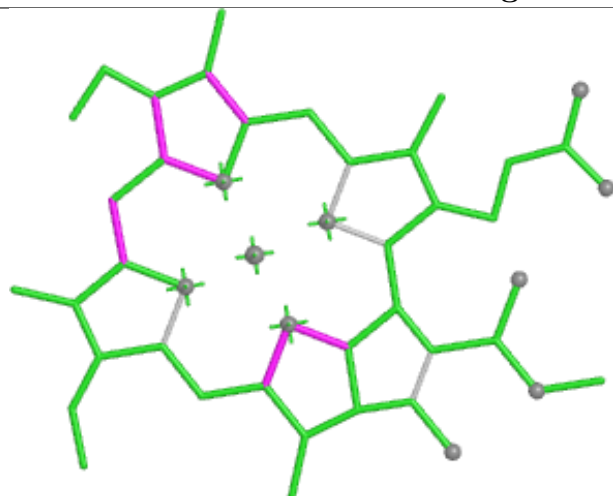


Rings

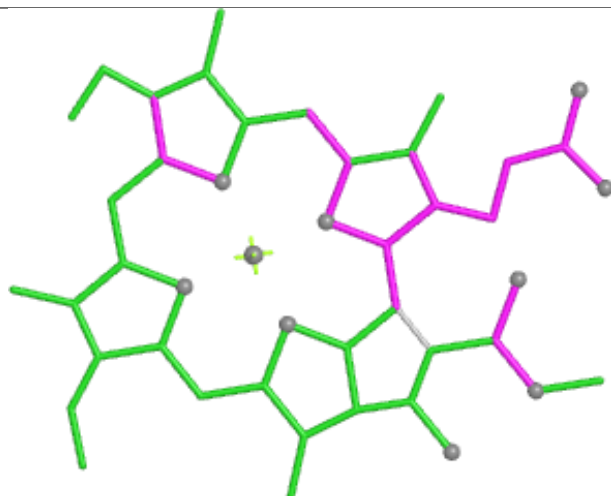
Ligand CHL AA 605



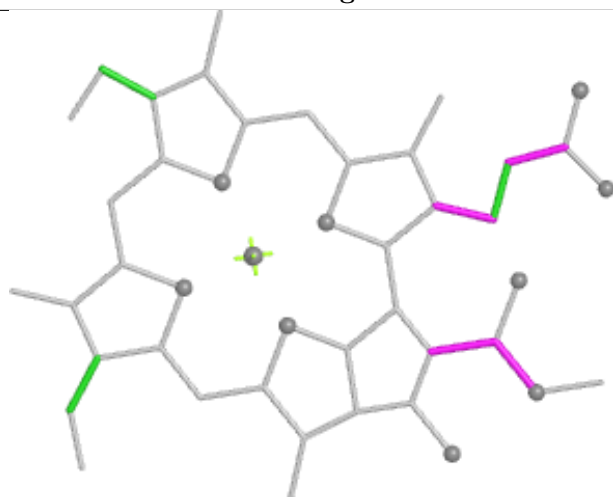
Ligand CLA AB 611



Bond lengths



Bond angles

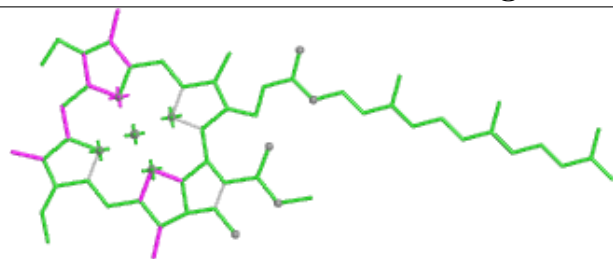


Torsions

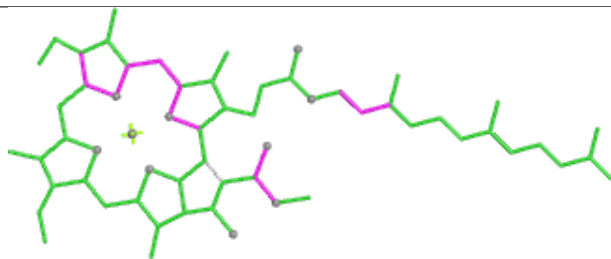


Rings

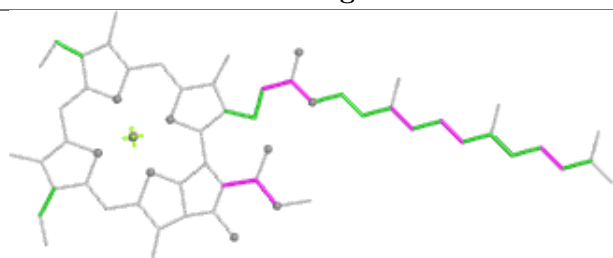
Ligand CLA AH 611



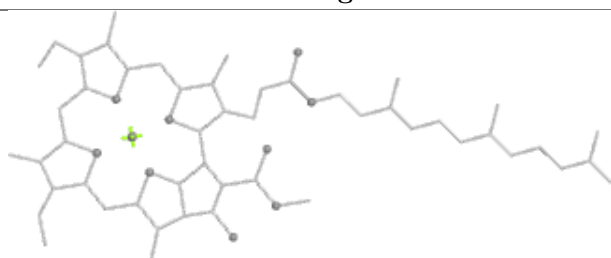
Bond lengths



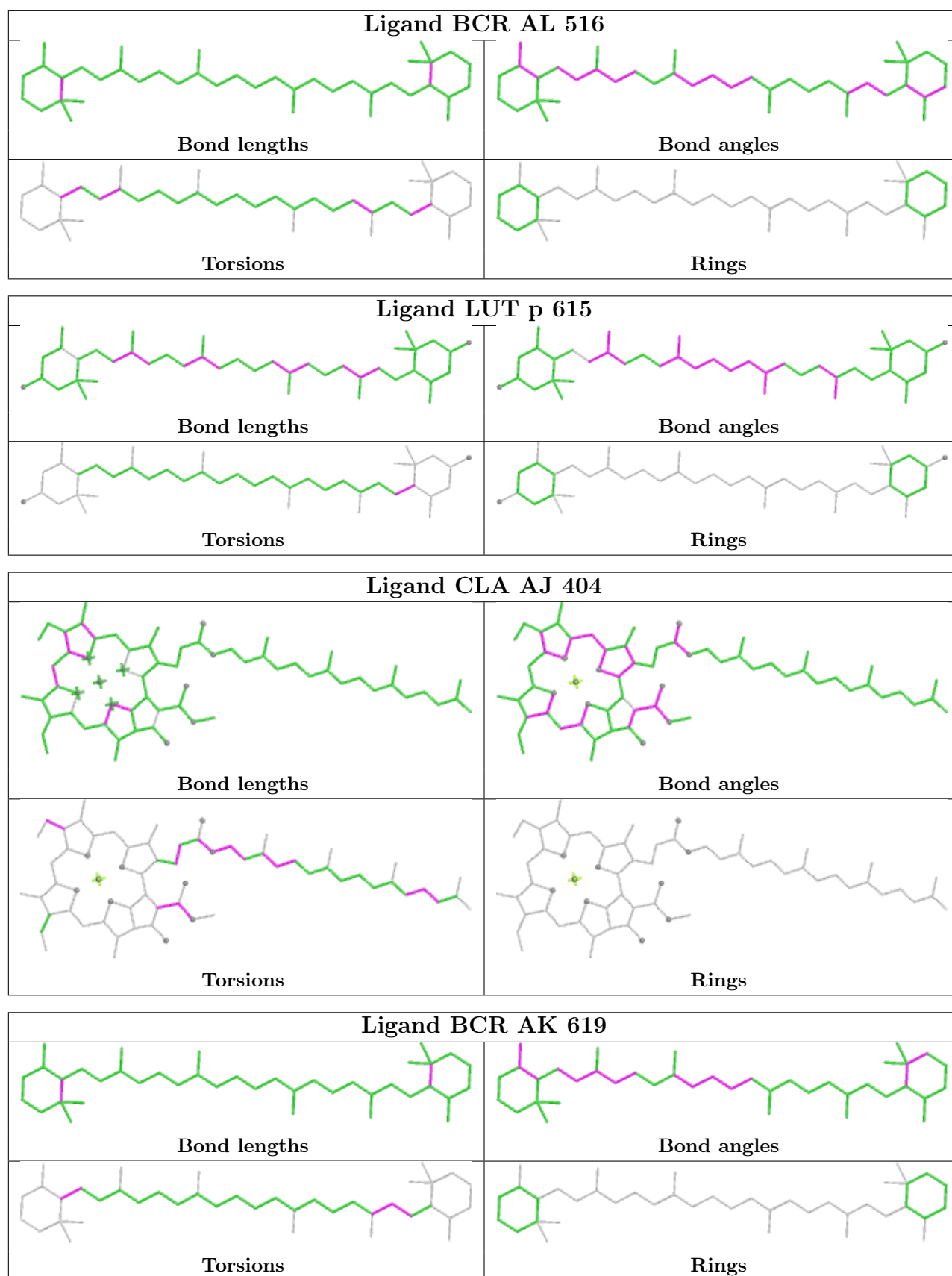
Bond angles

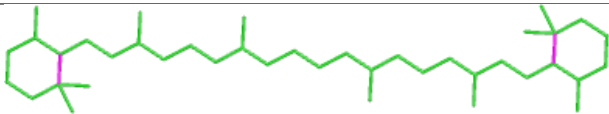
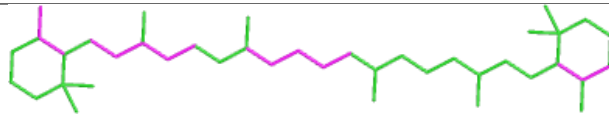
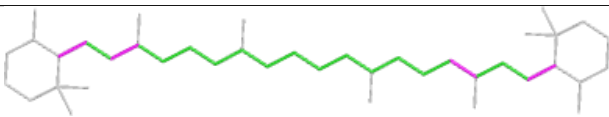
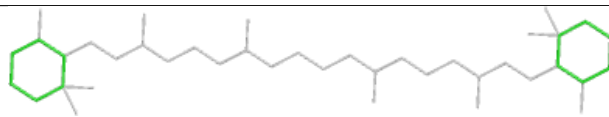


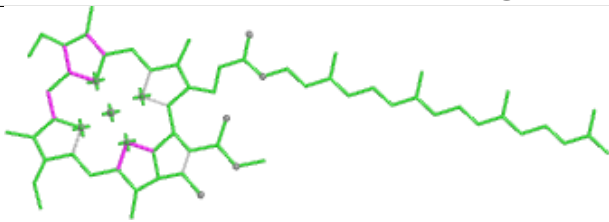
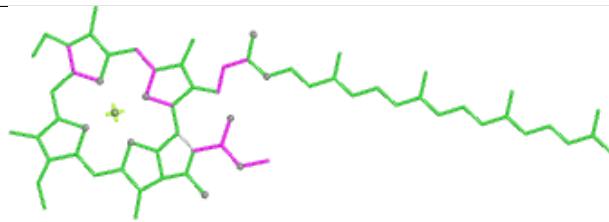
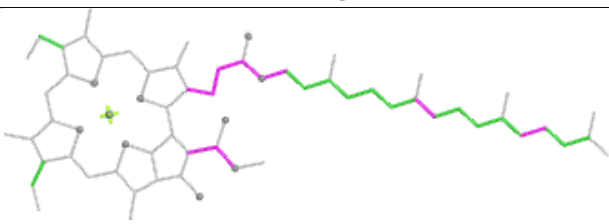
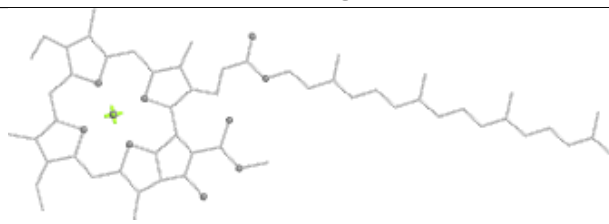
Torsions

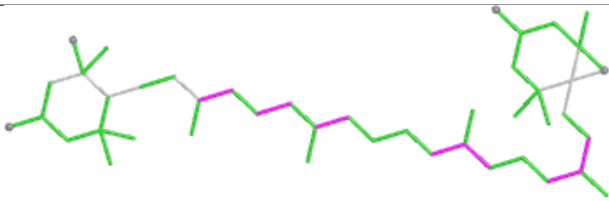
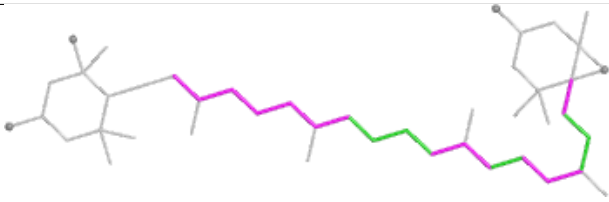


Rings

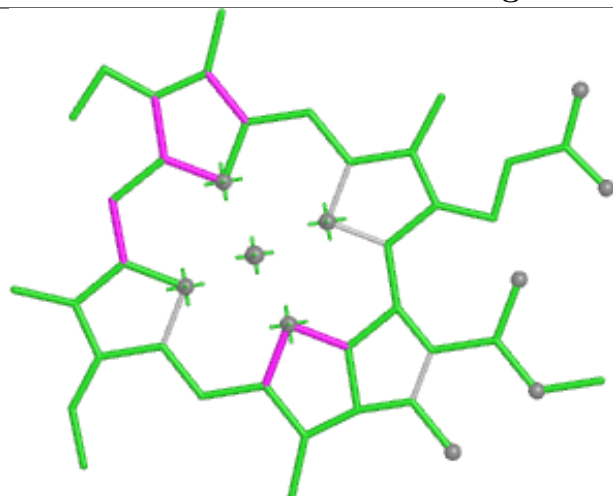


Ligand BCR P 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

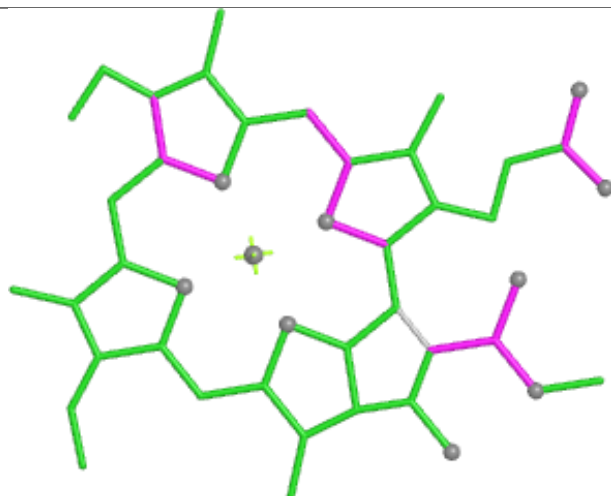
Ligand CLA AL 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NEX AA 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

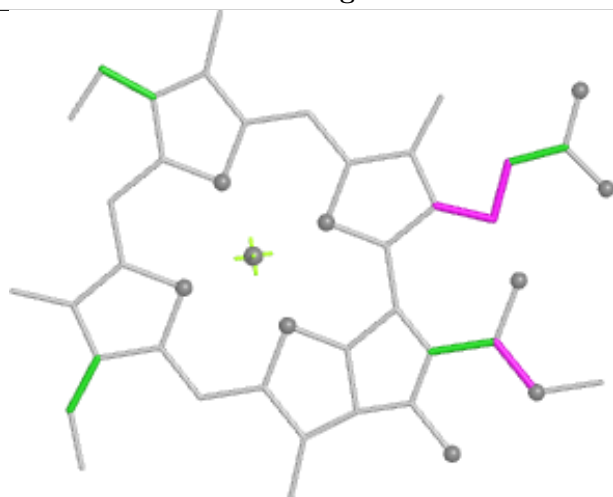
Ligand CLA AE 612



Bond lengths



Bond angles

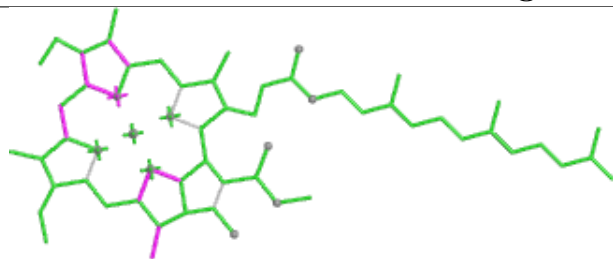


Torsions

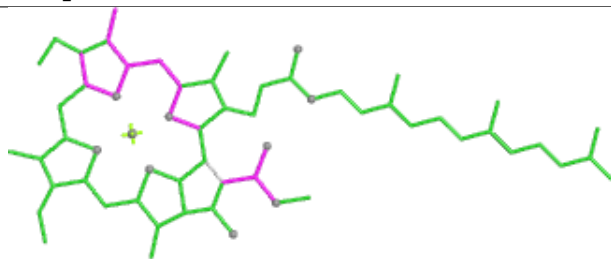


Rings

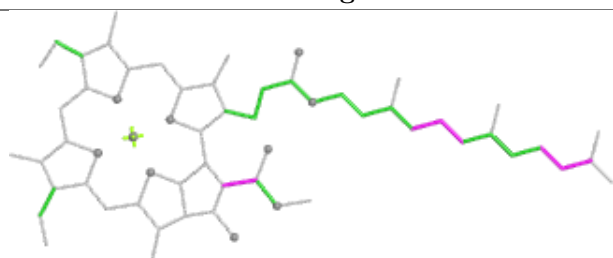
Ligand CLA q 603



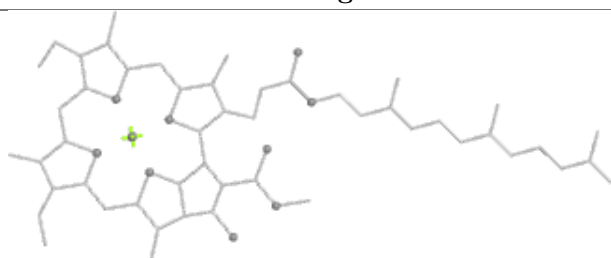
Bond lengths



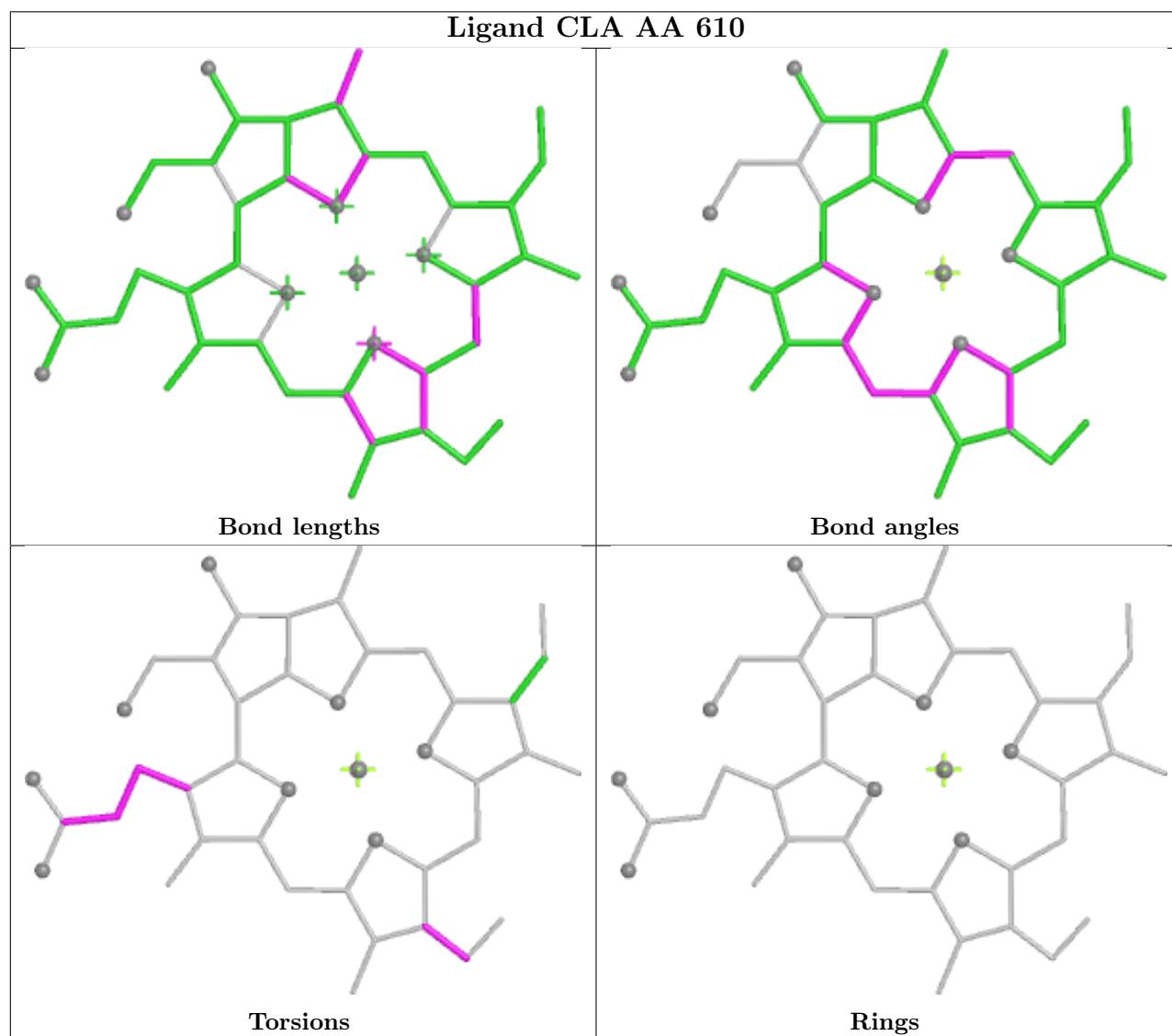
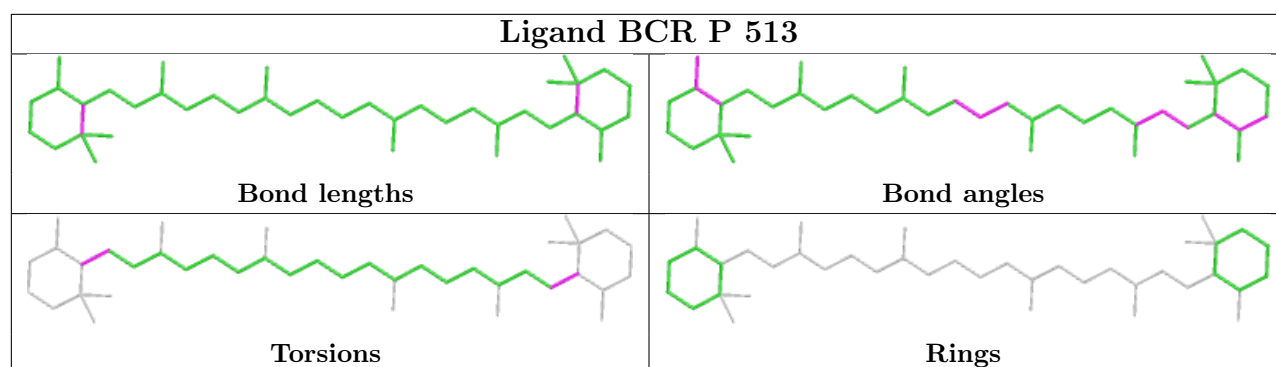
Bond angles

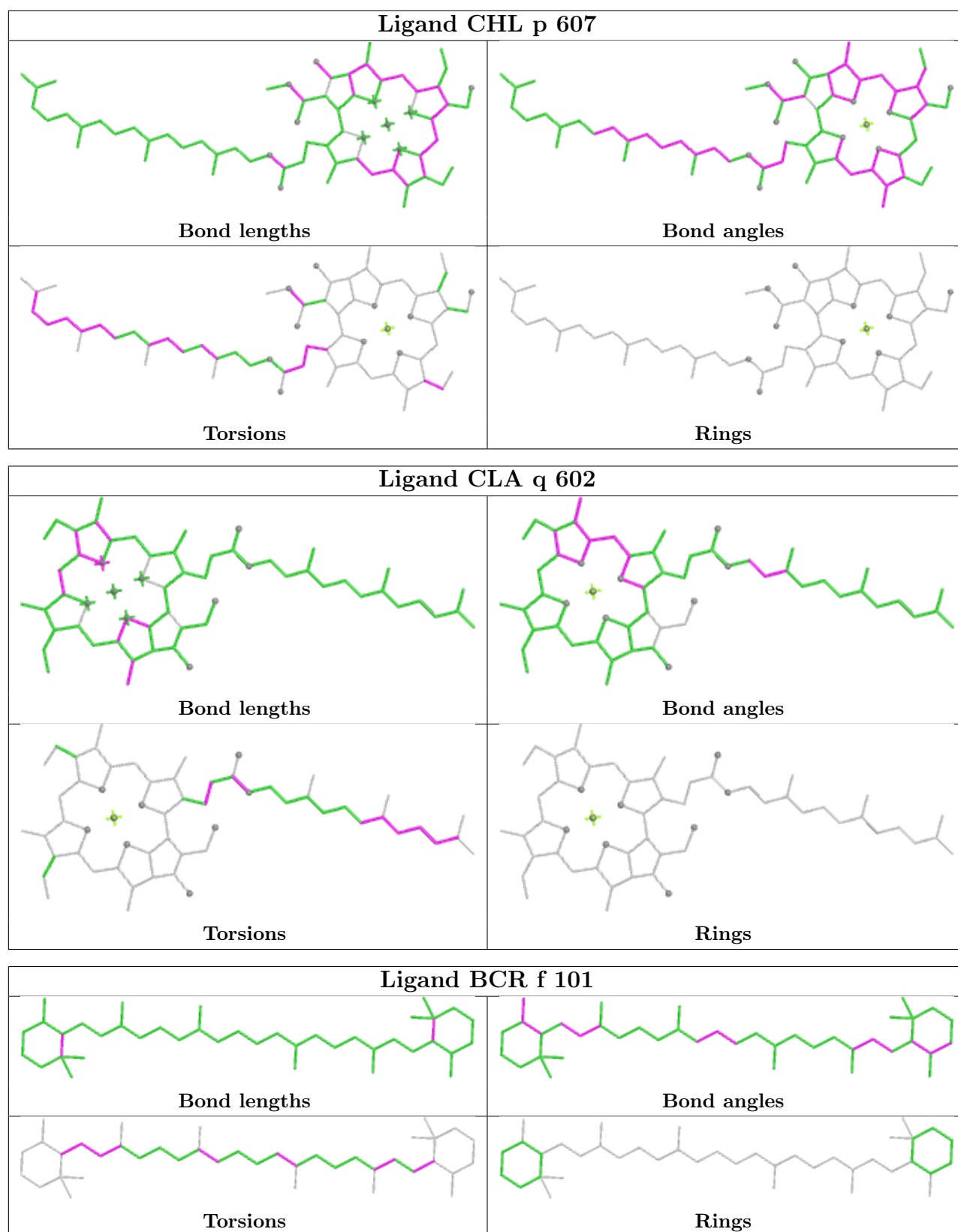


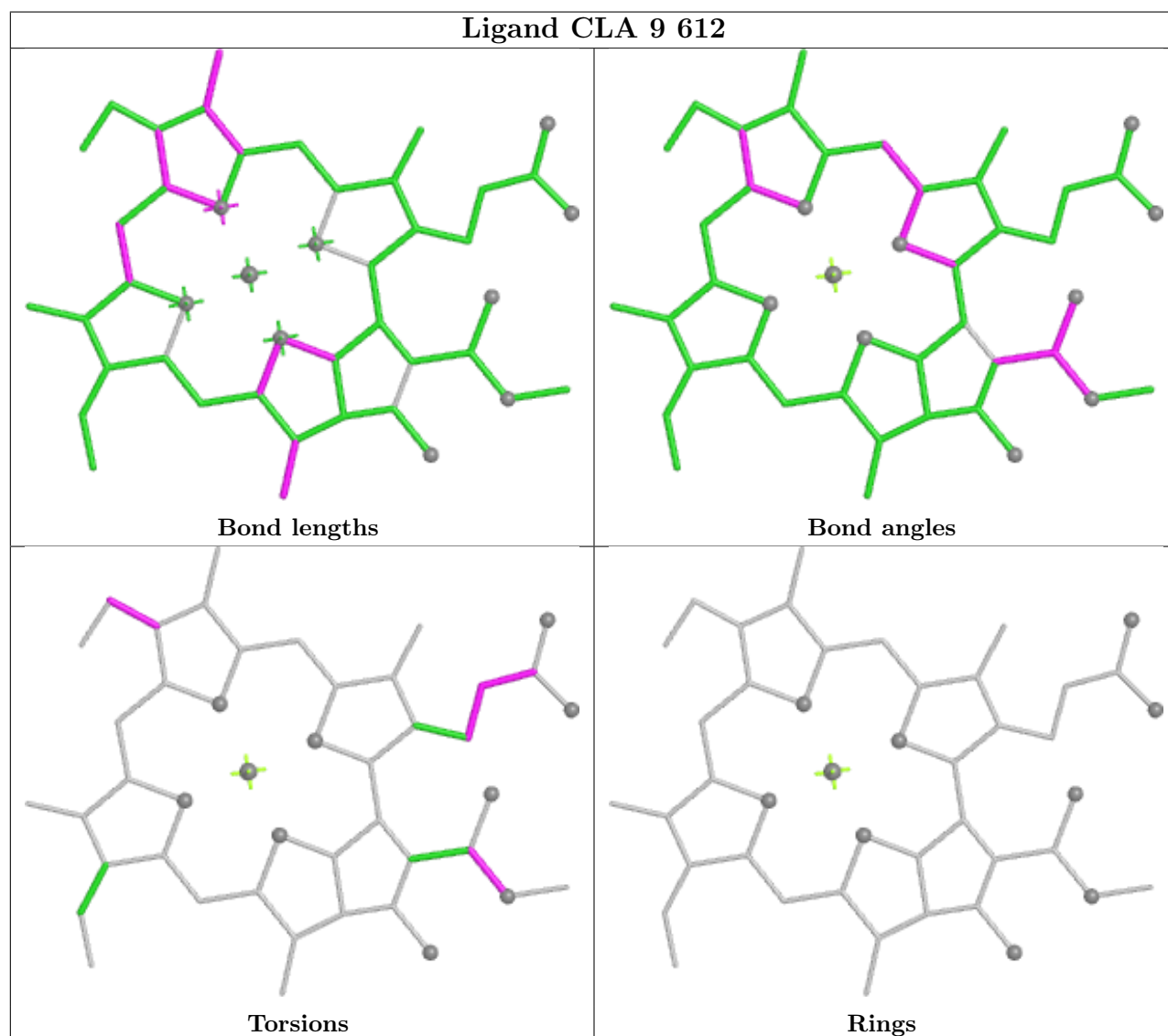
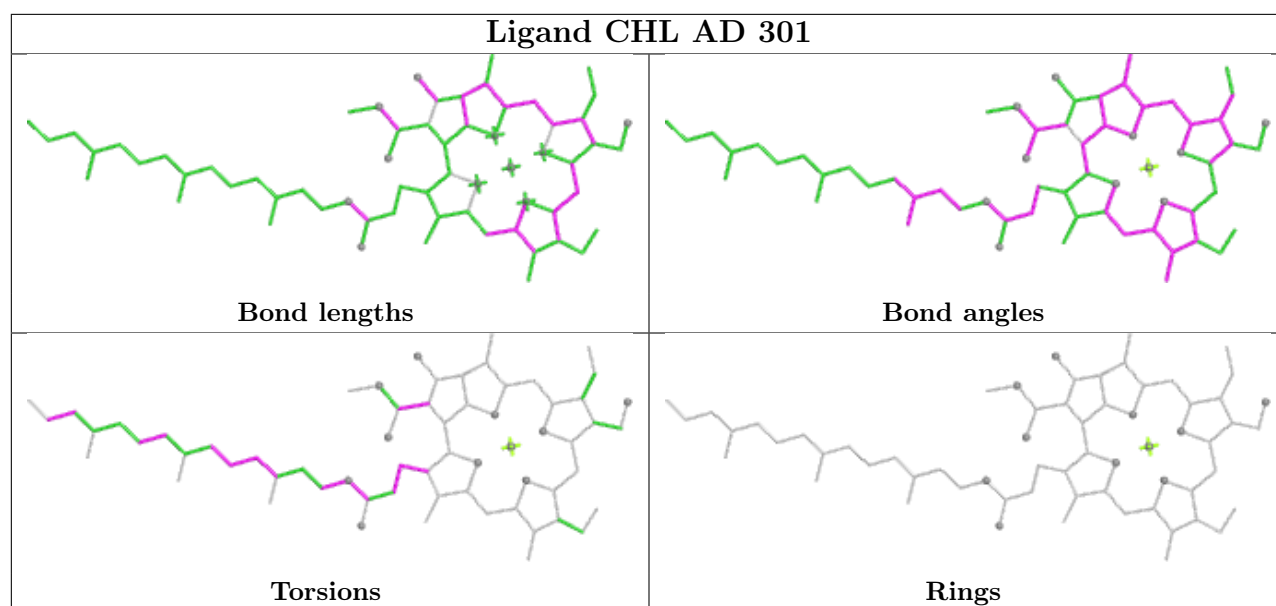
Torsions

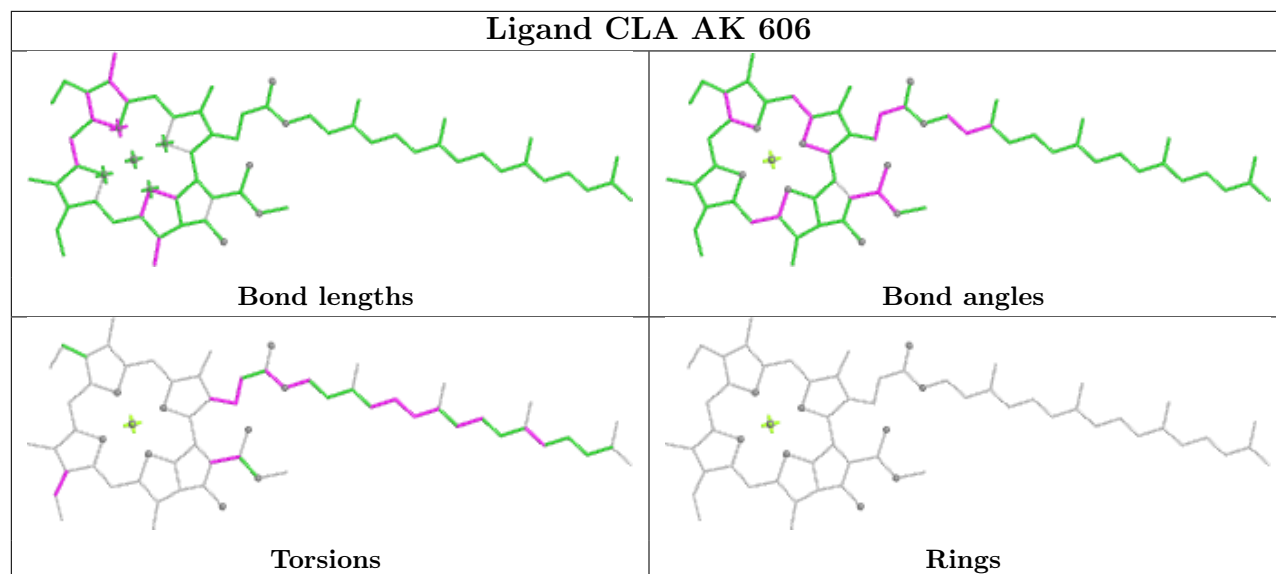
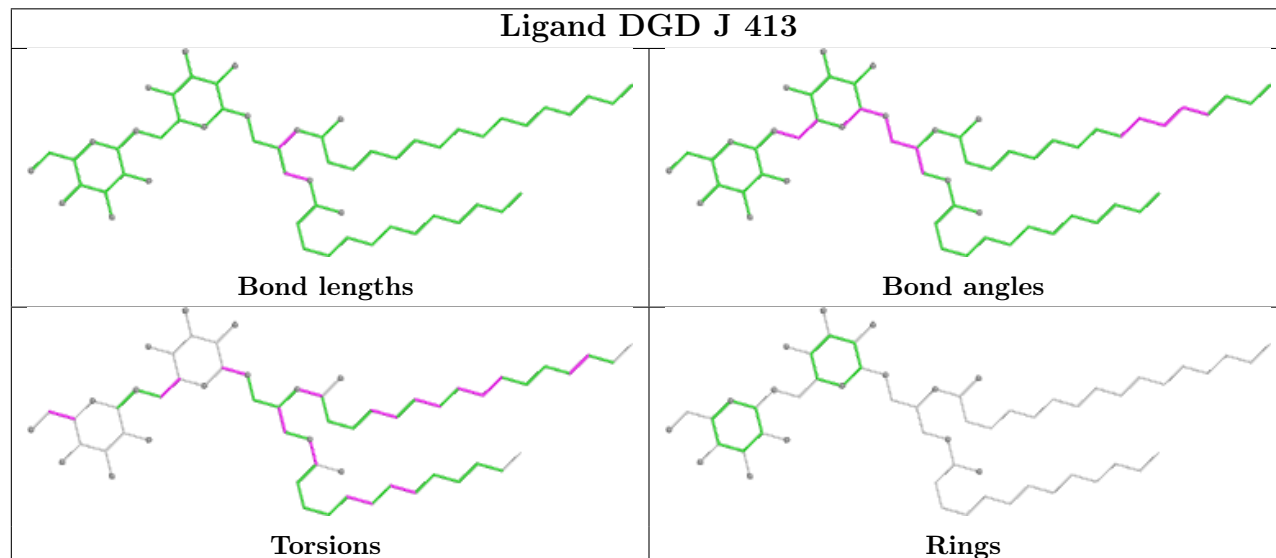
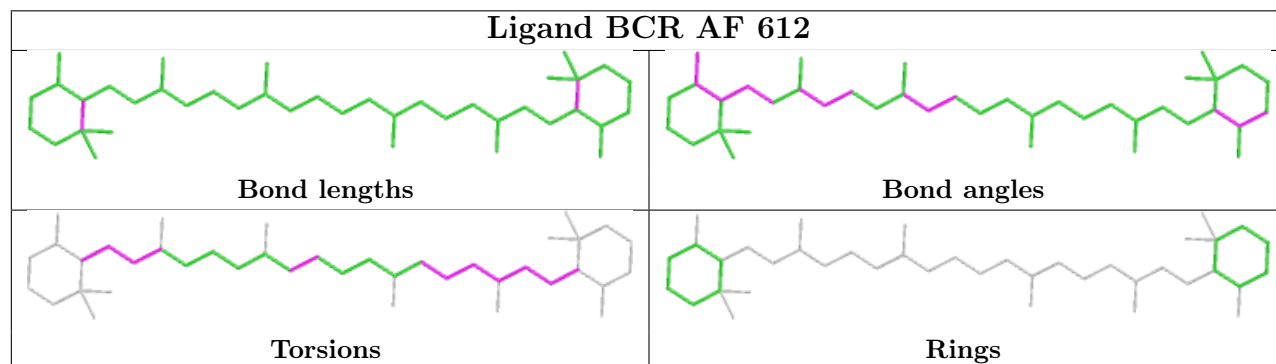


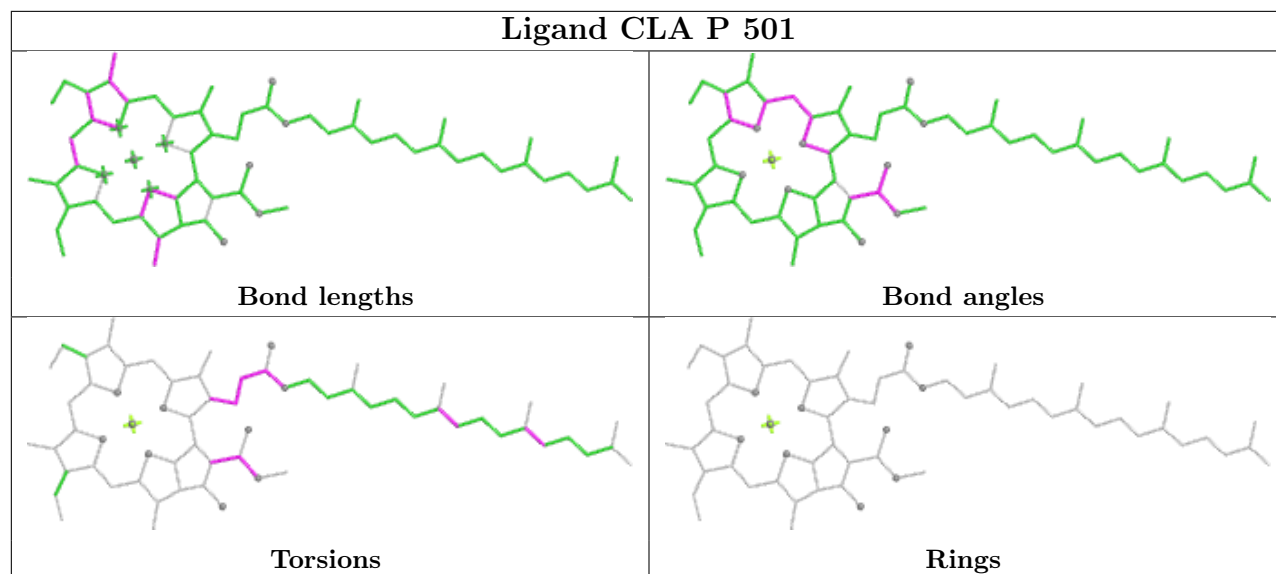
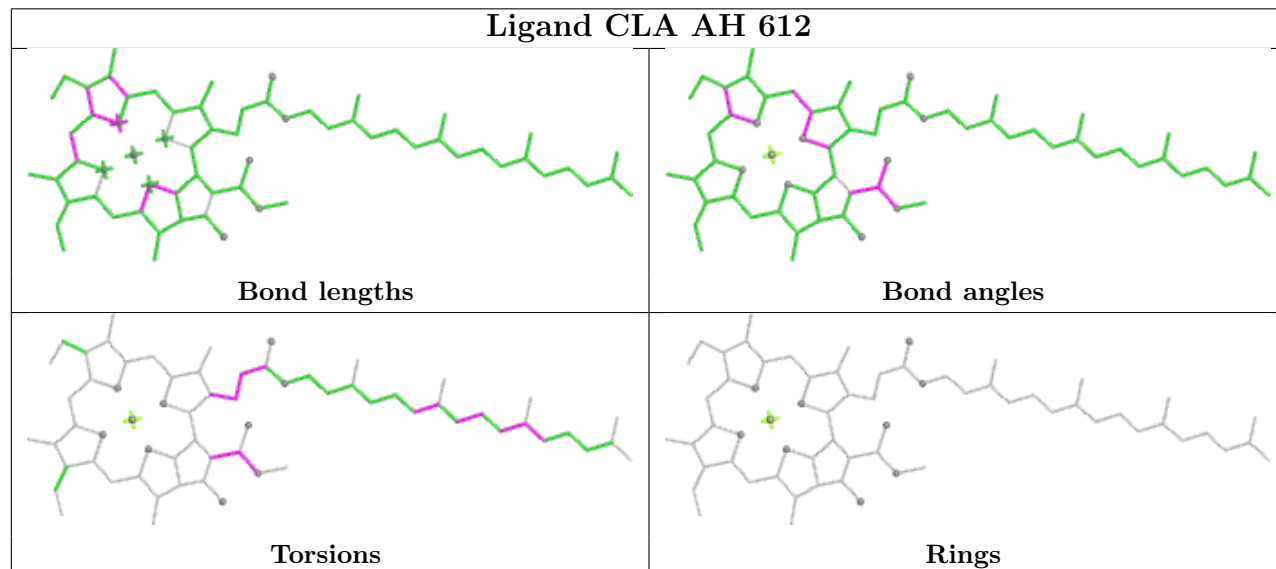
Rings

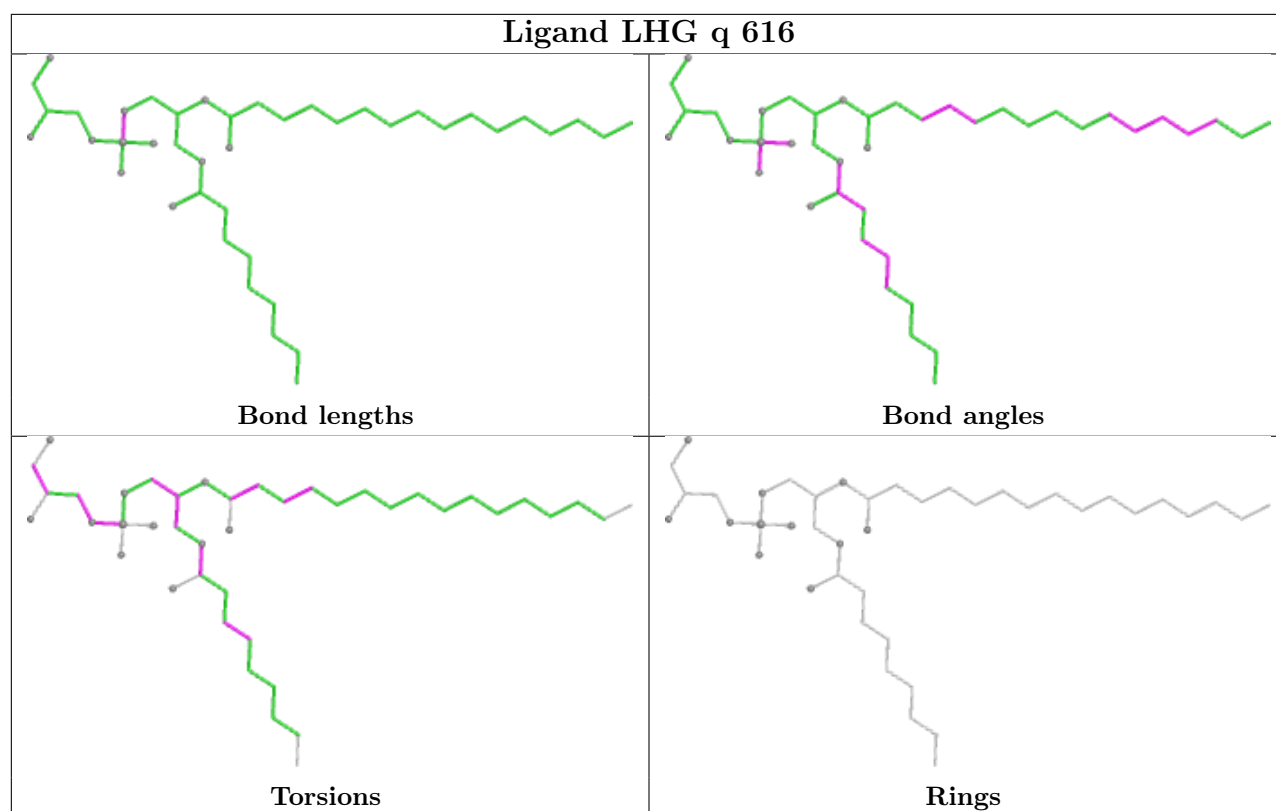


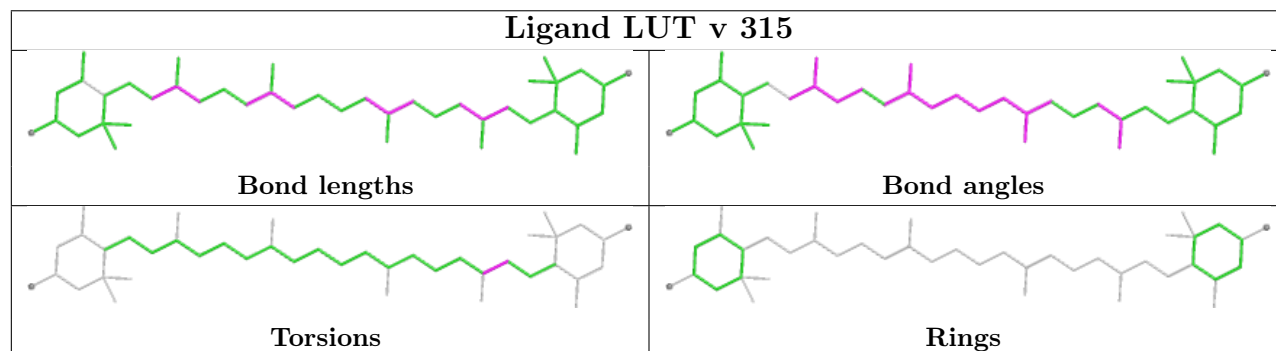
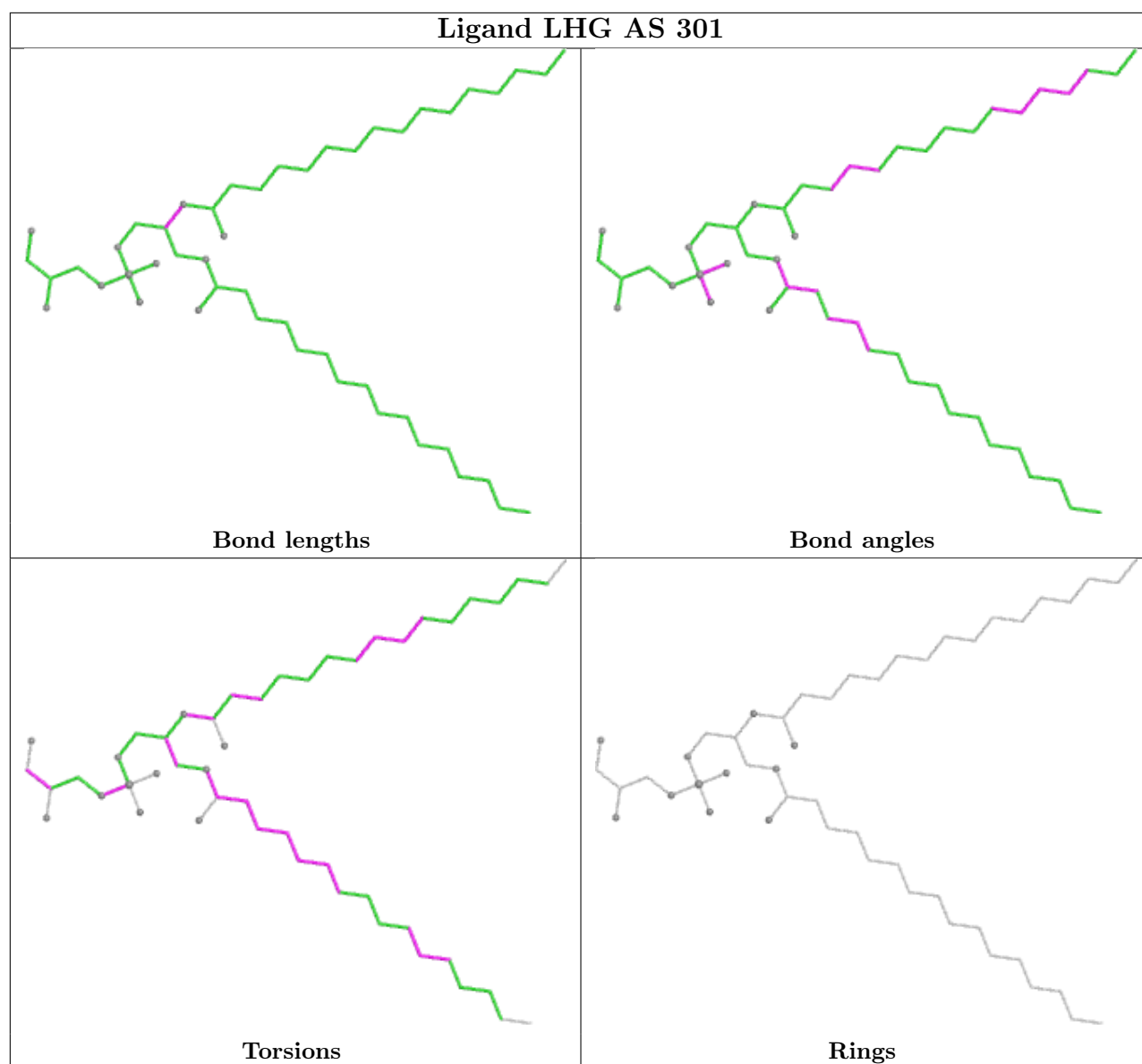


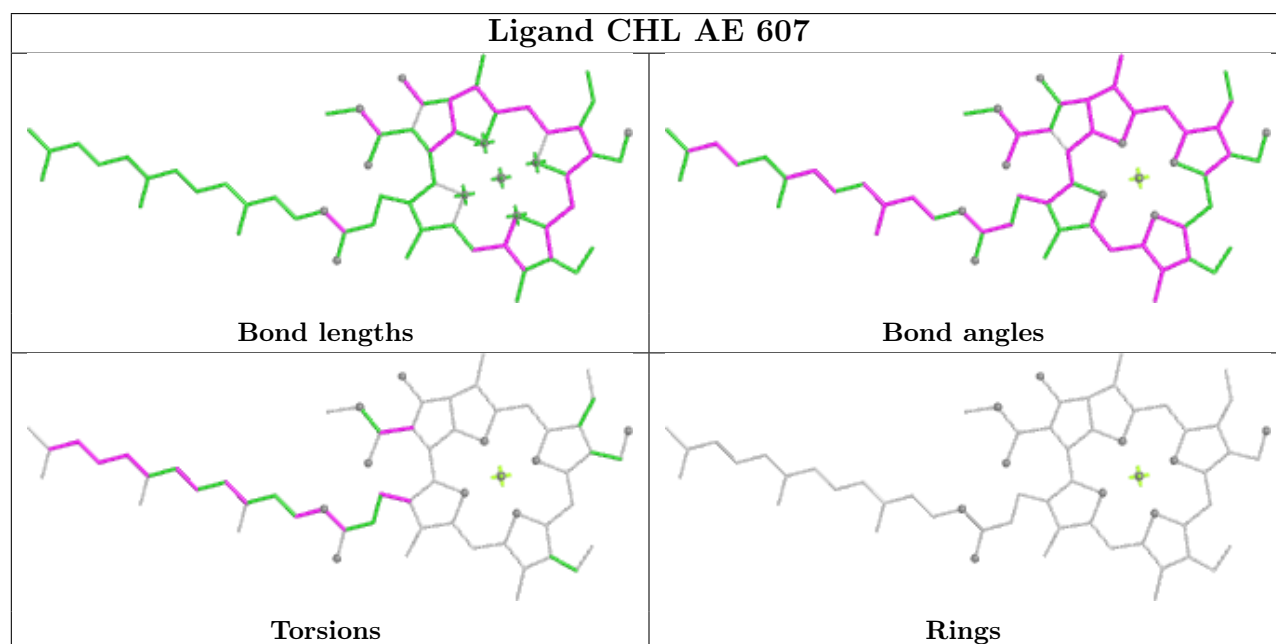
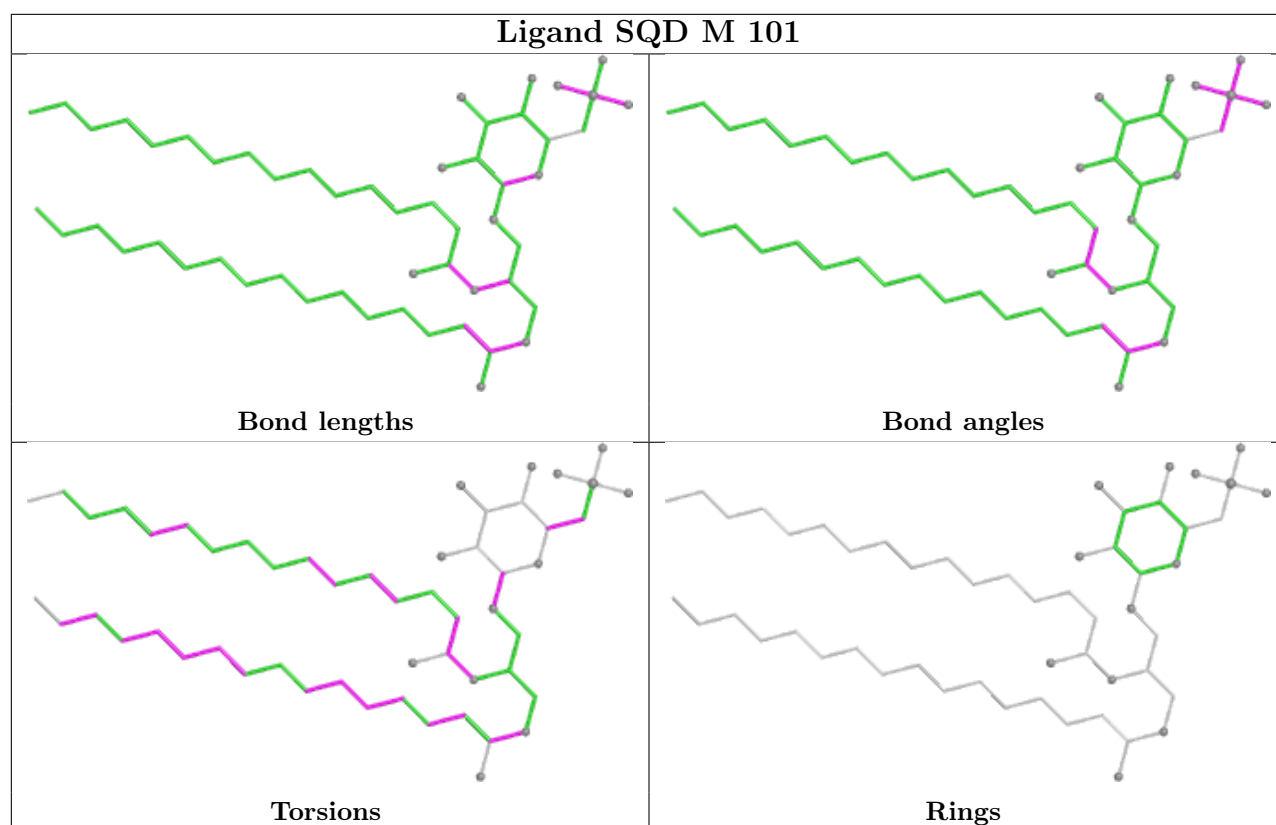


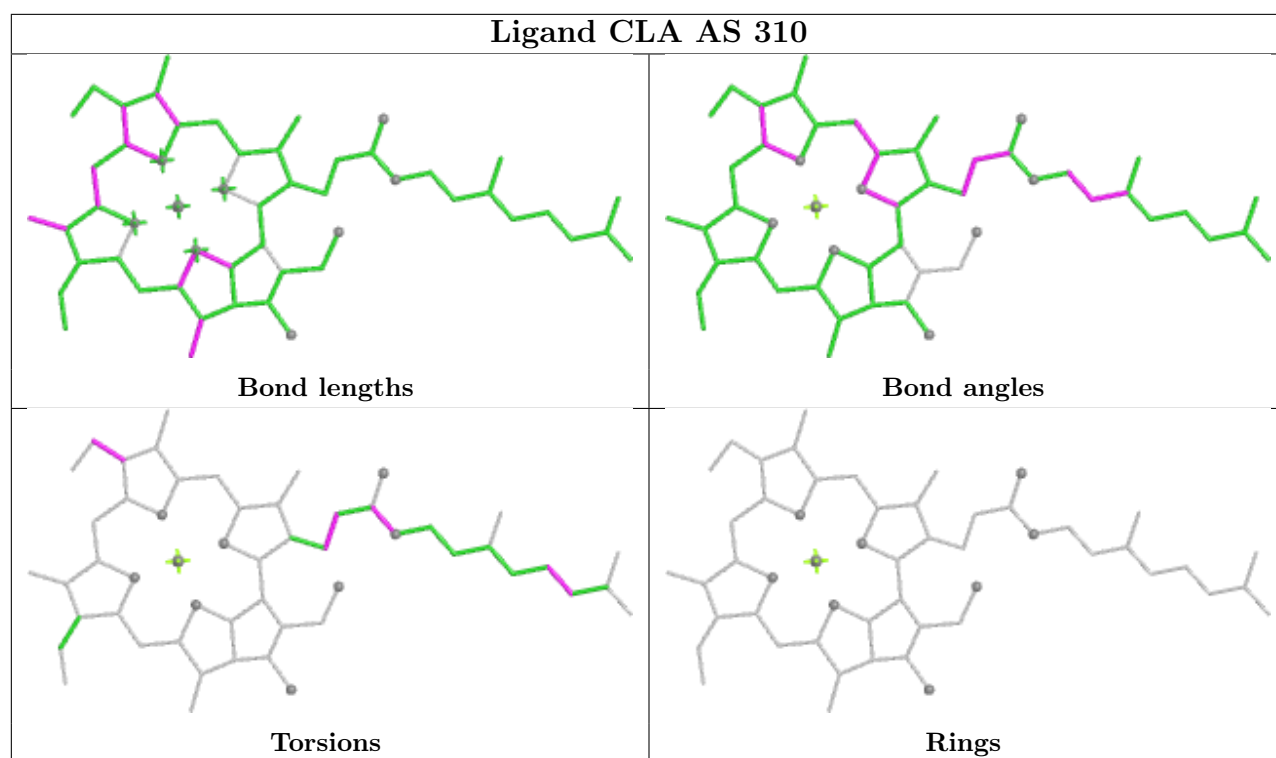
Ligand CLA AK 606**Ligand DGD J 413****Ligand BCR AF 612**

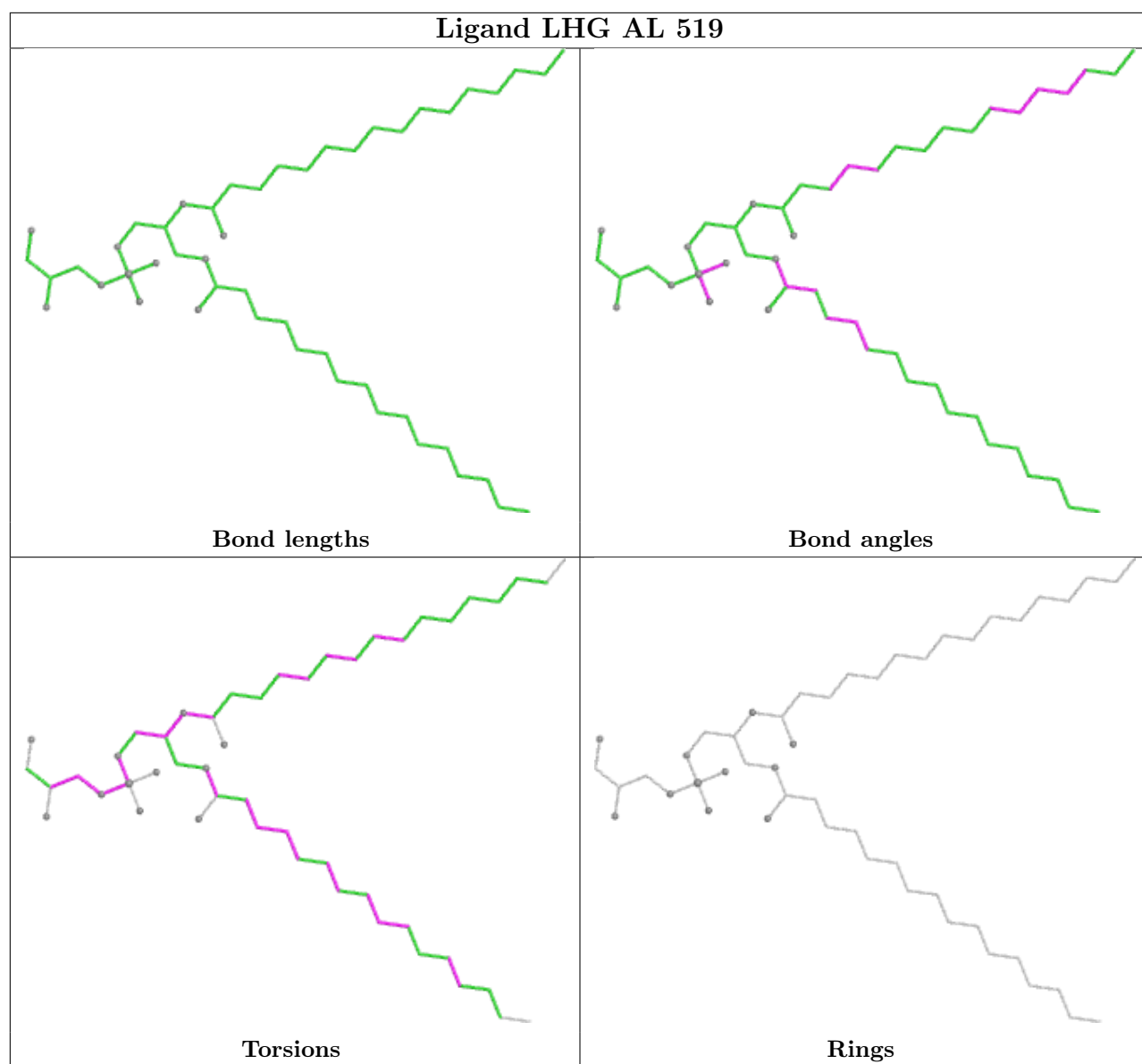
Ligand CLA P 501**Ligand CLA AH 612**



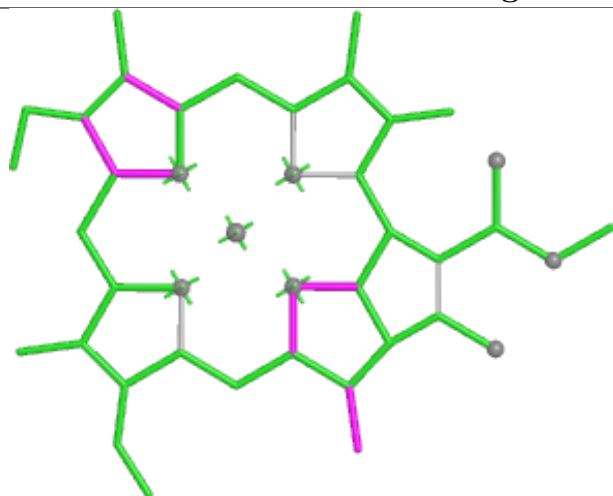








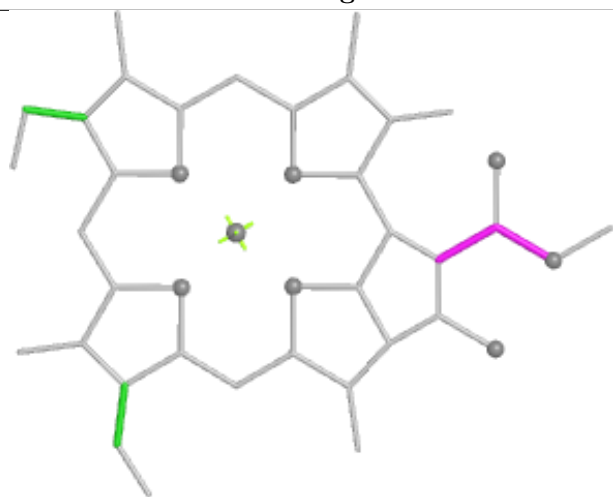
Ligand CLA AC 612



Bond lengths



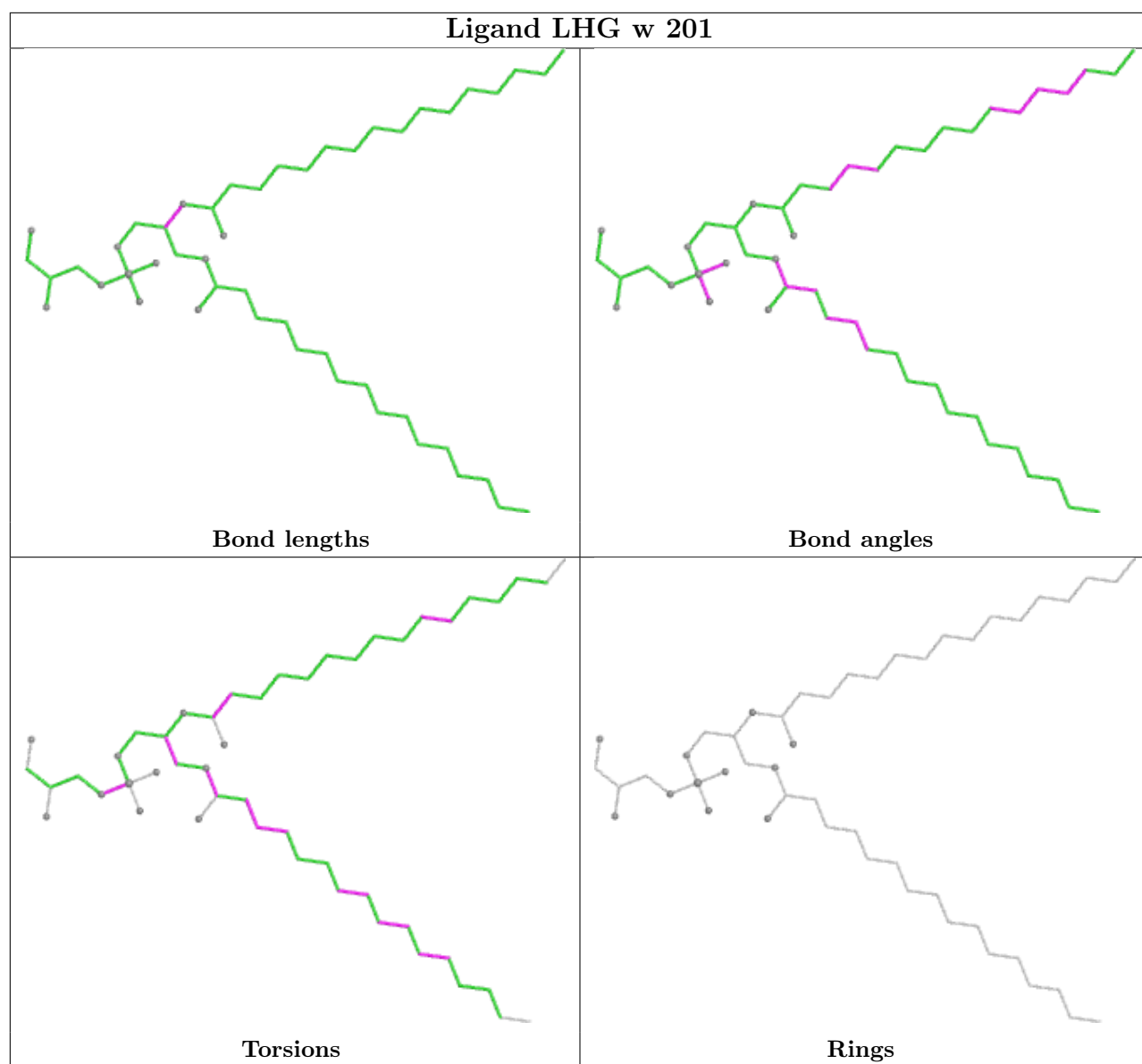
Bond angles



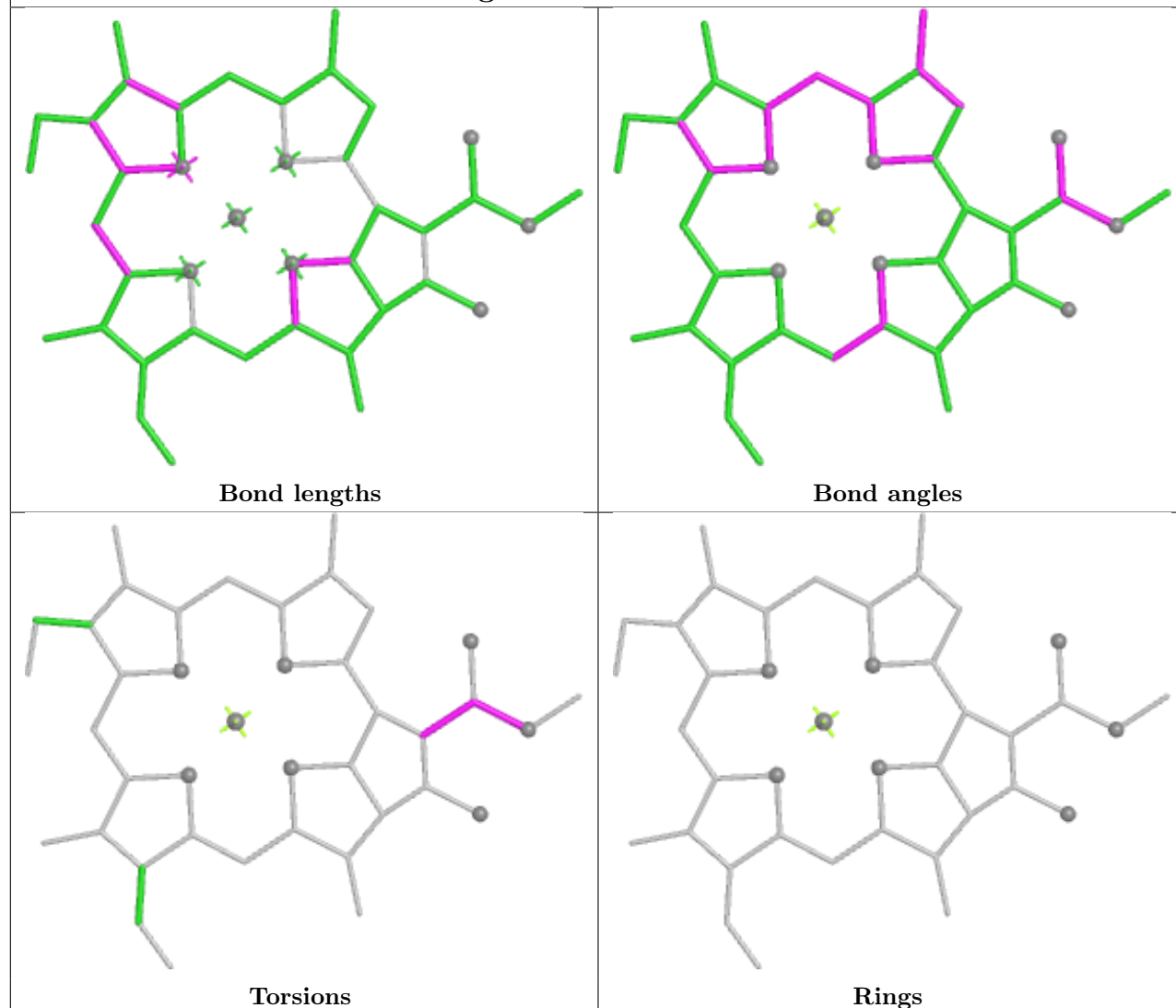
Torsions



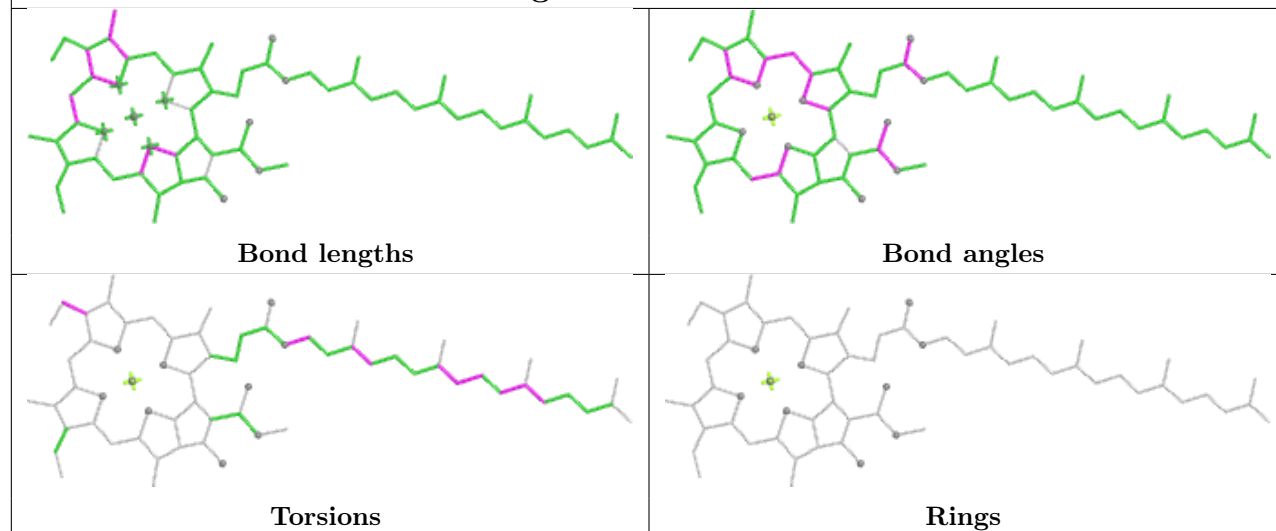
Rings

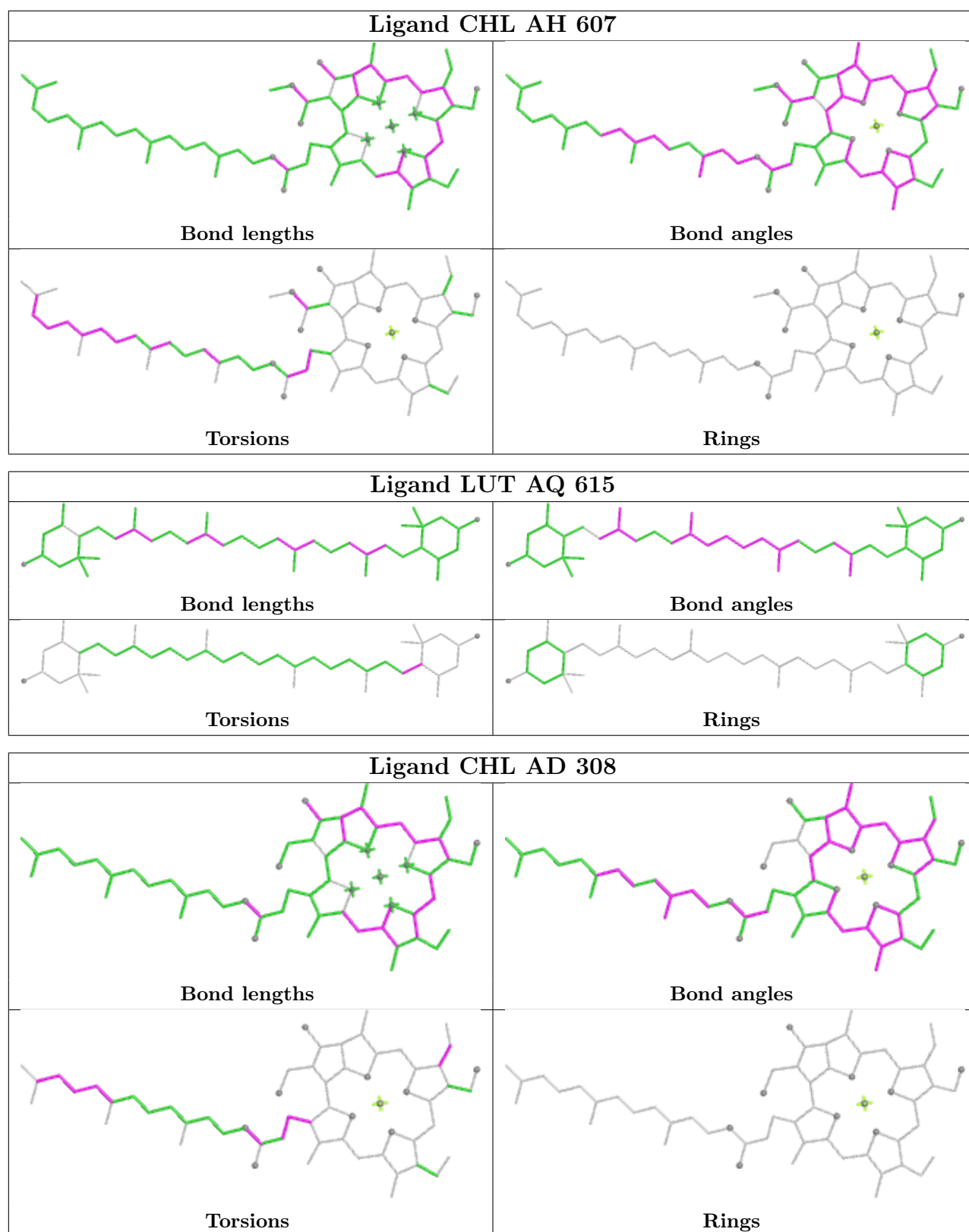


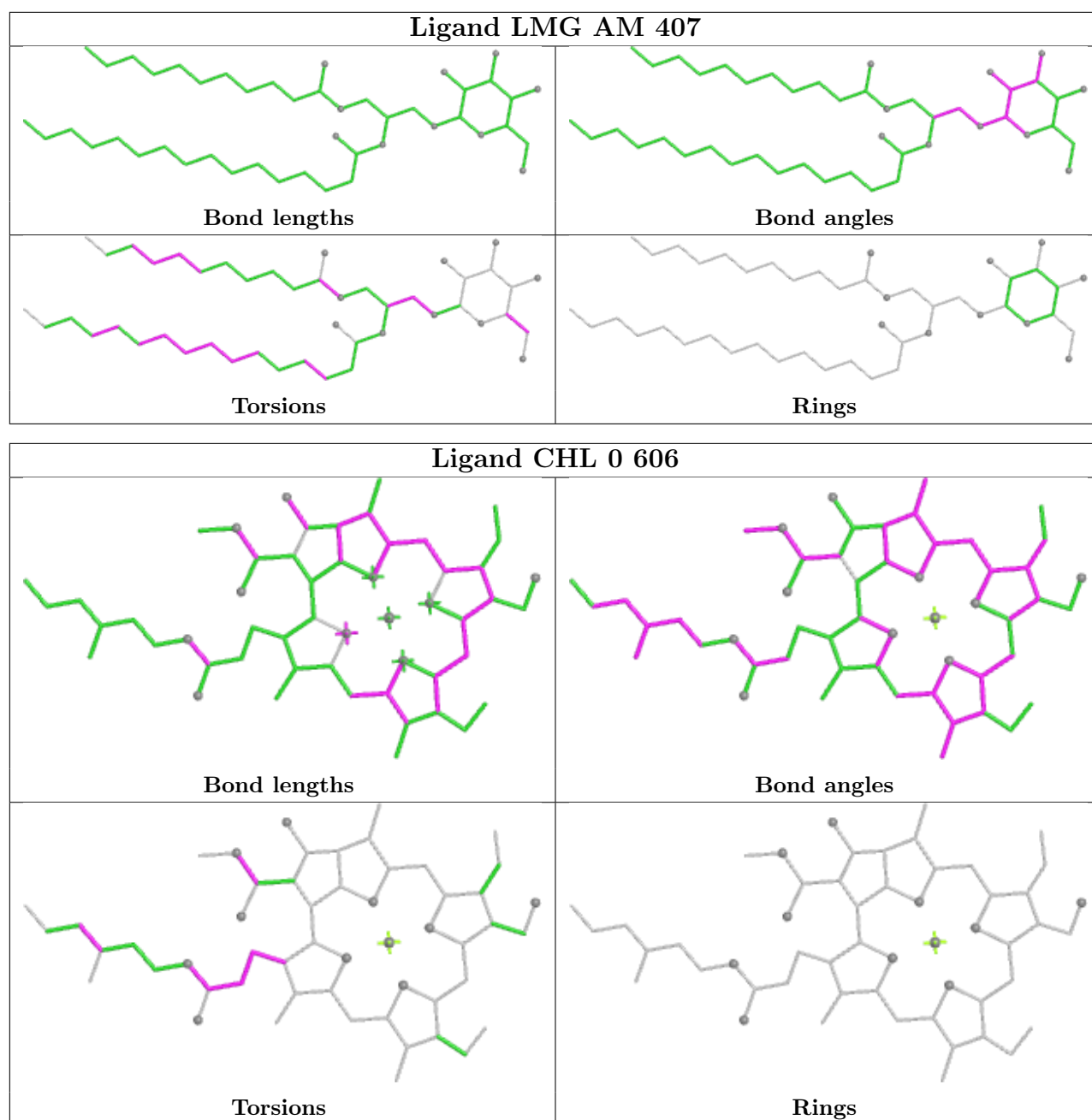
Ligand CLA AB 609



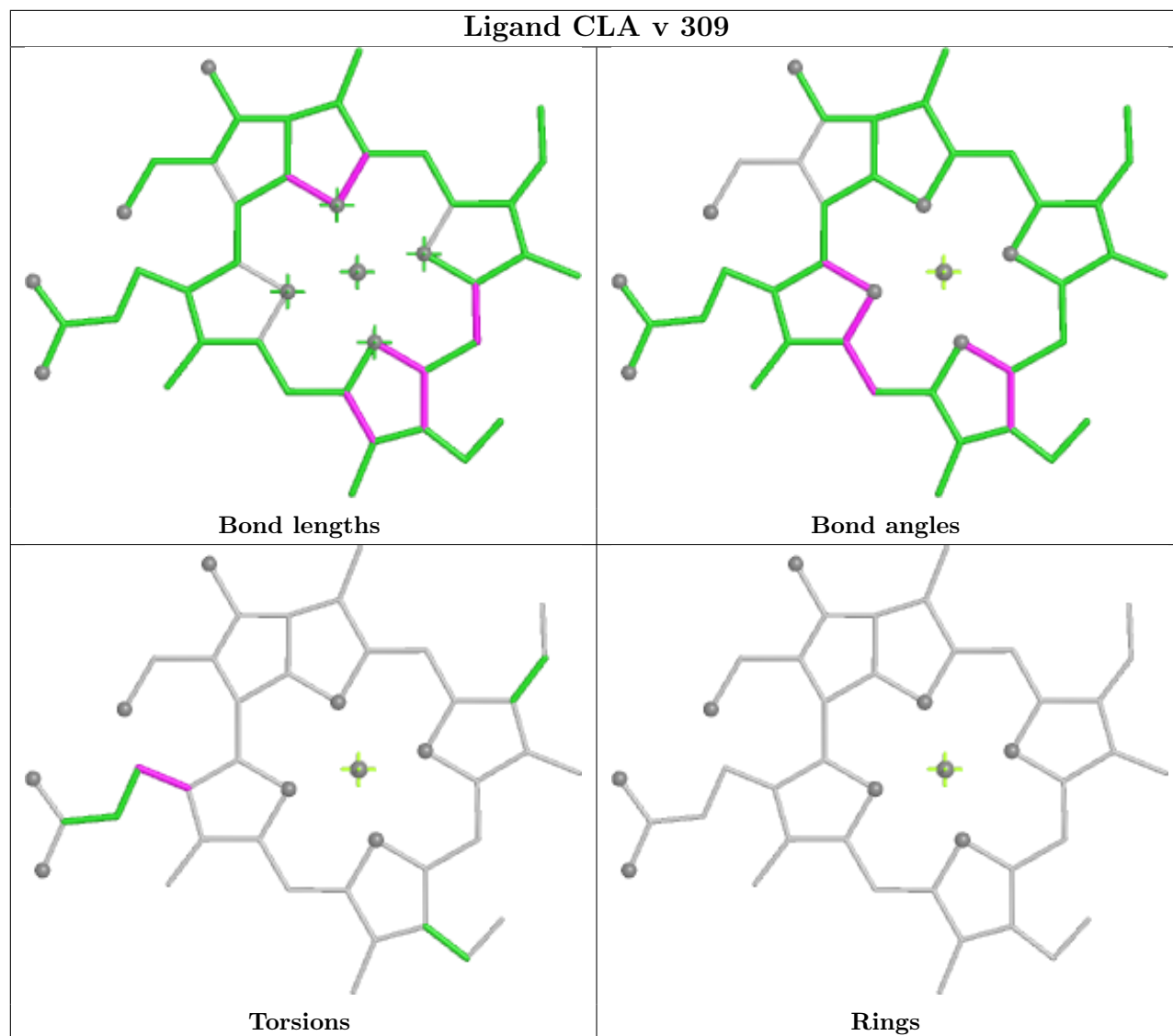
Ligand CLA O 615



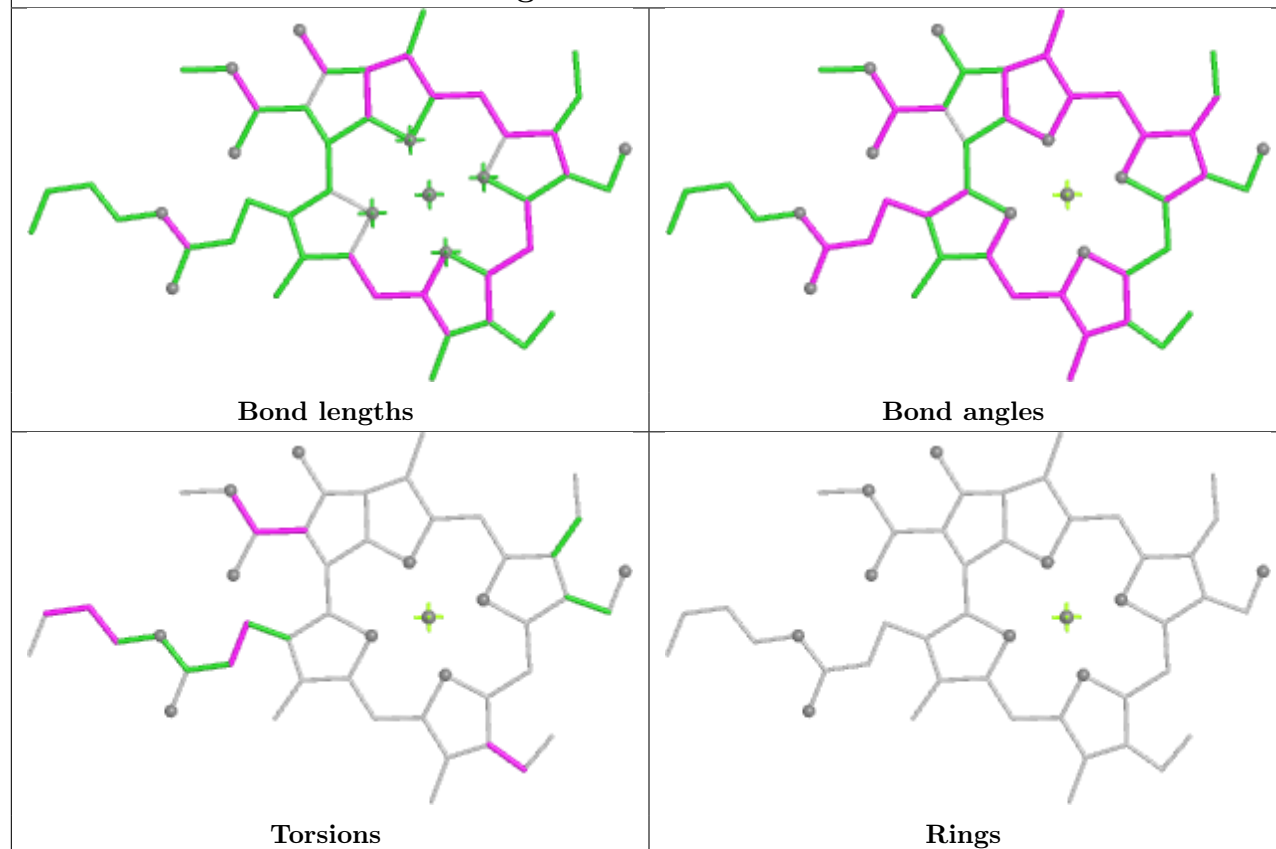




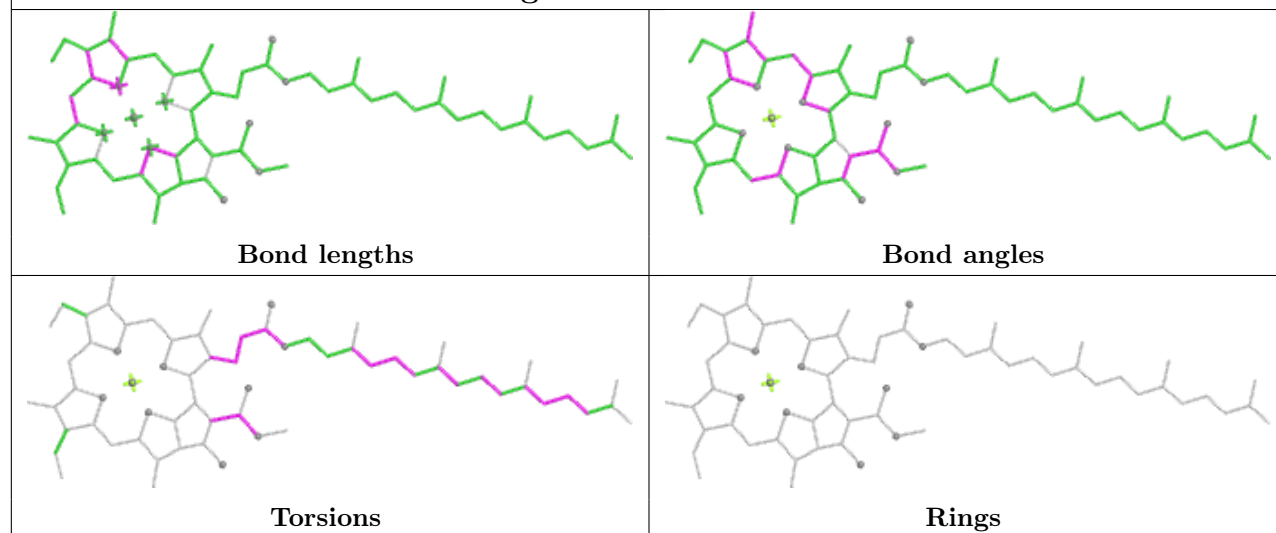
Ligand CLA v 309

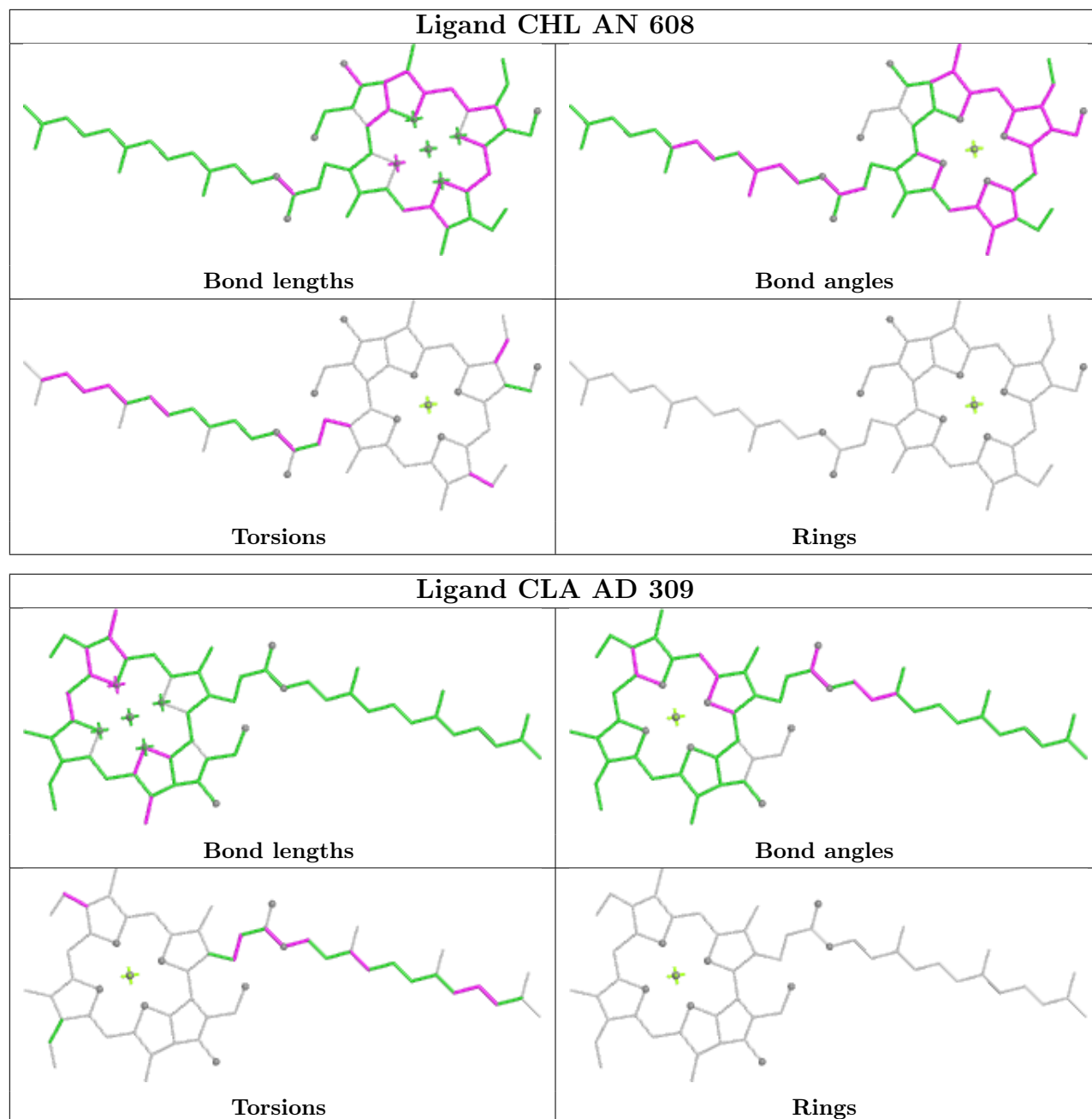


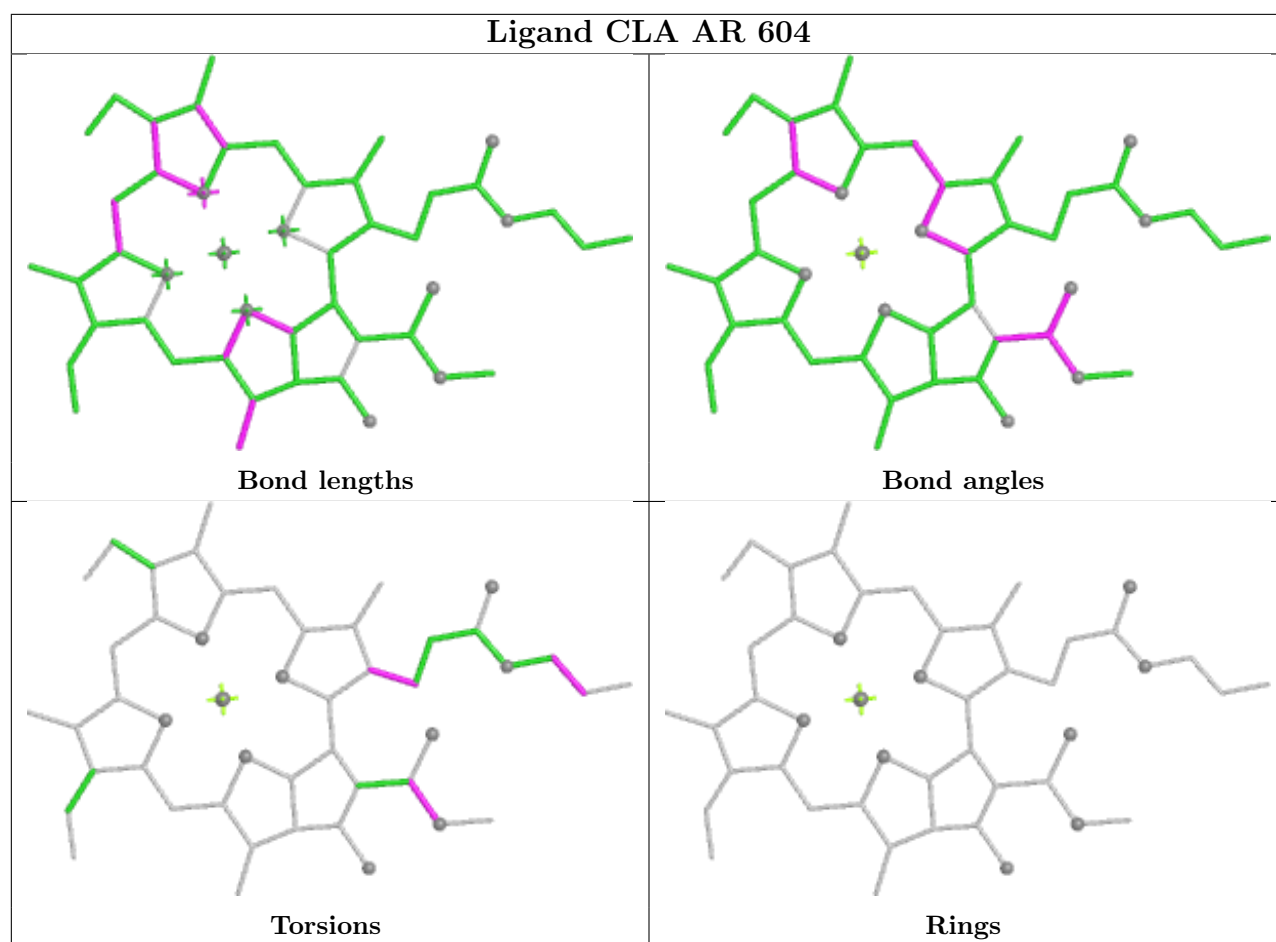
Ligand CHL AH 606

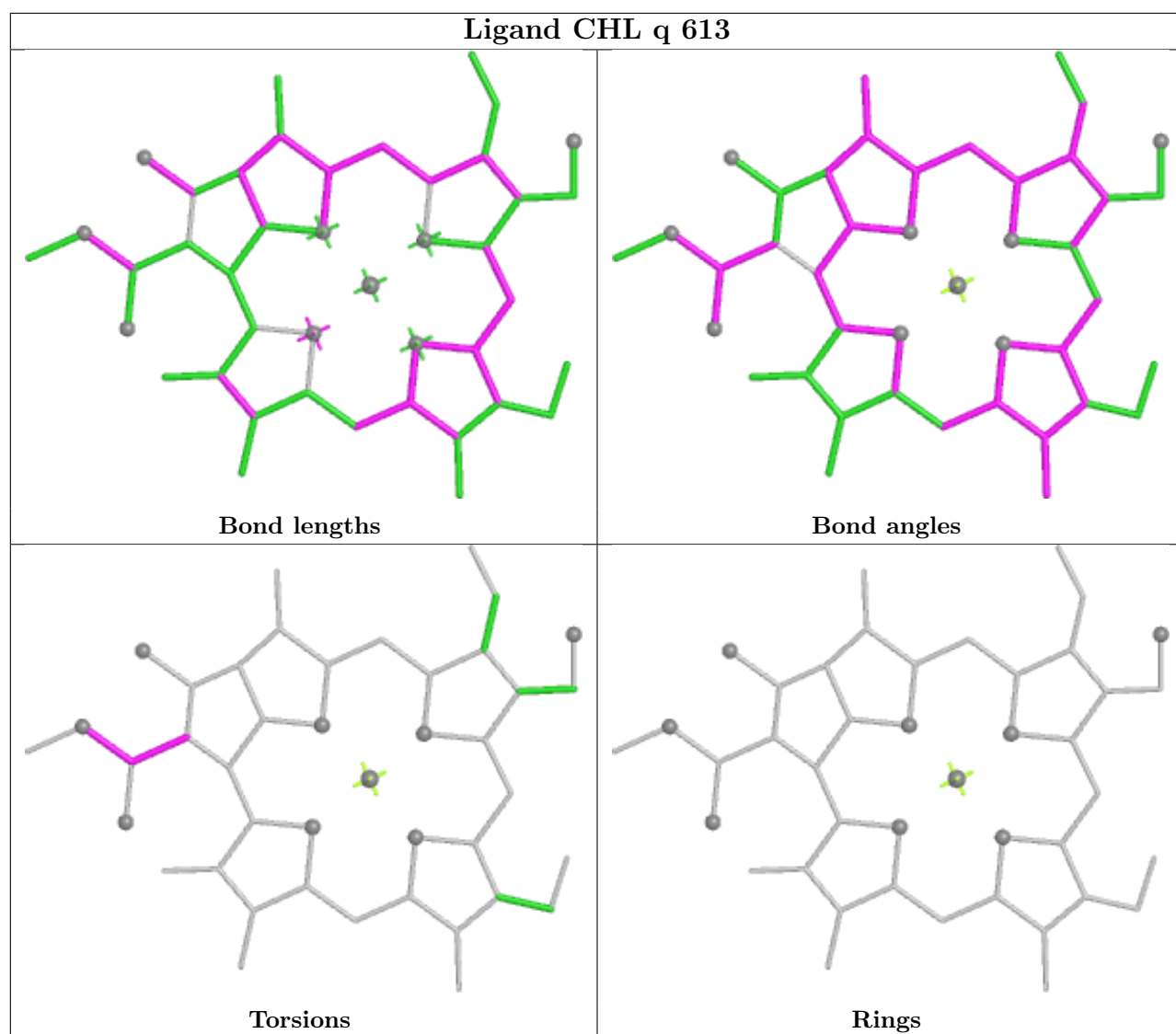


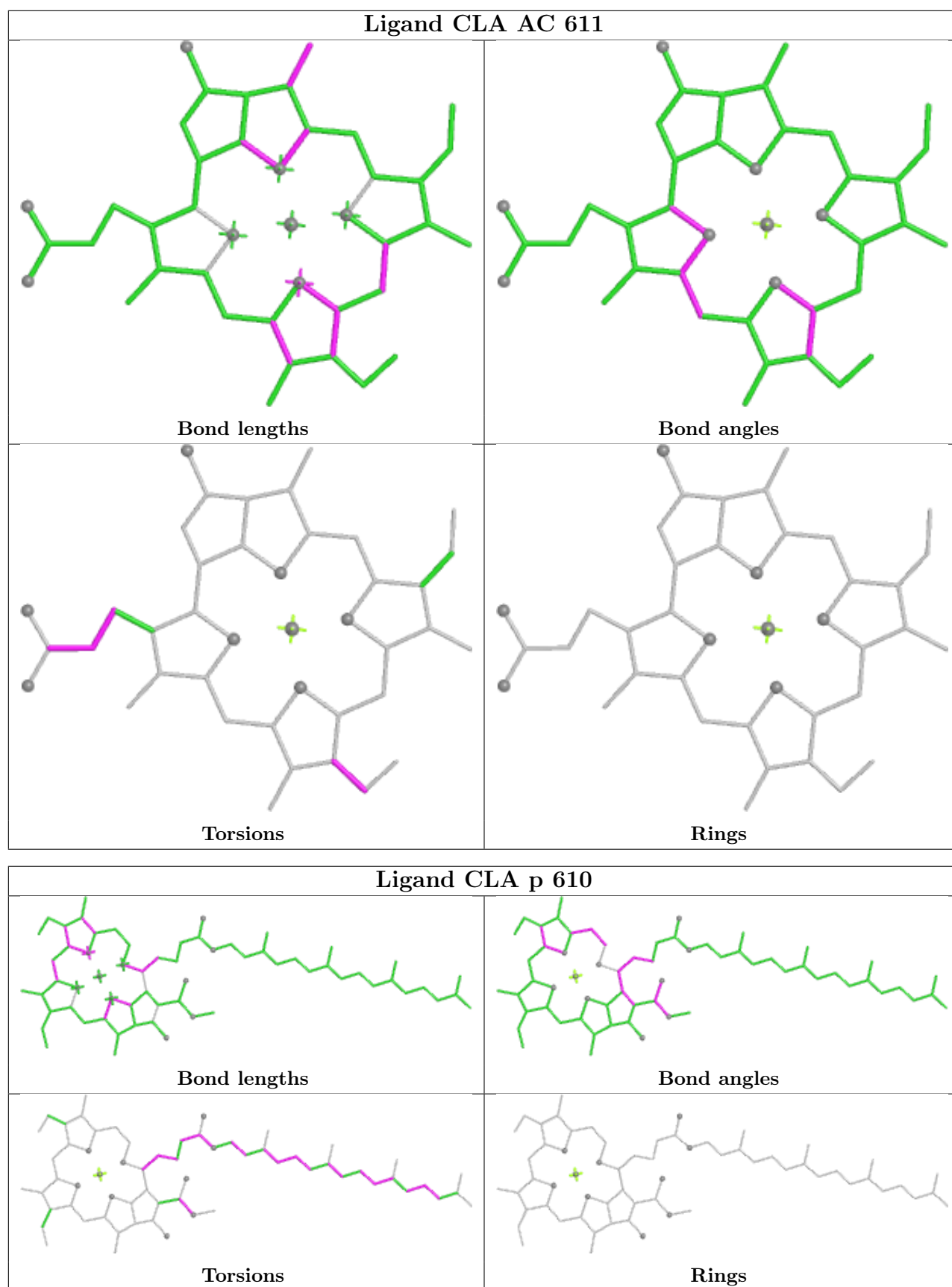
Ligand CLA AL 504

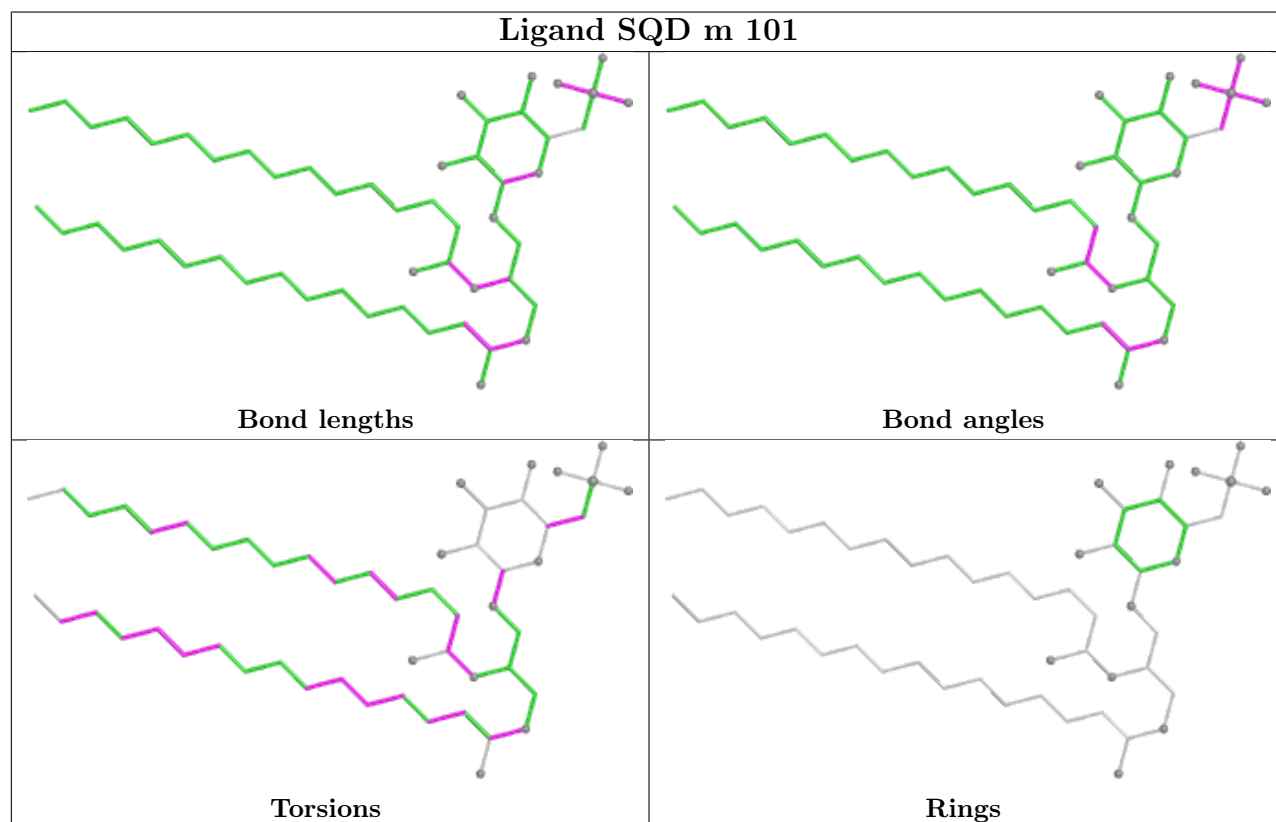
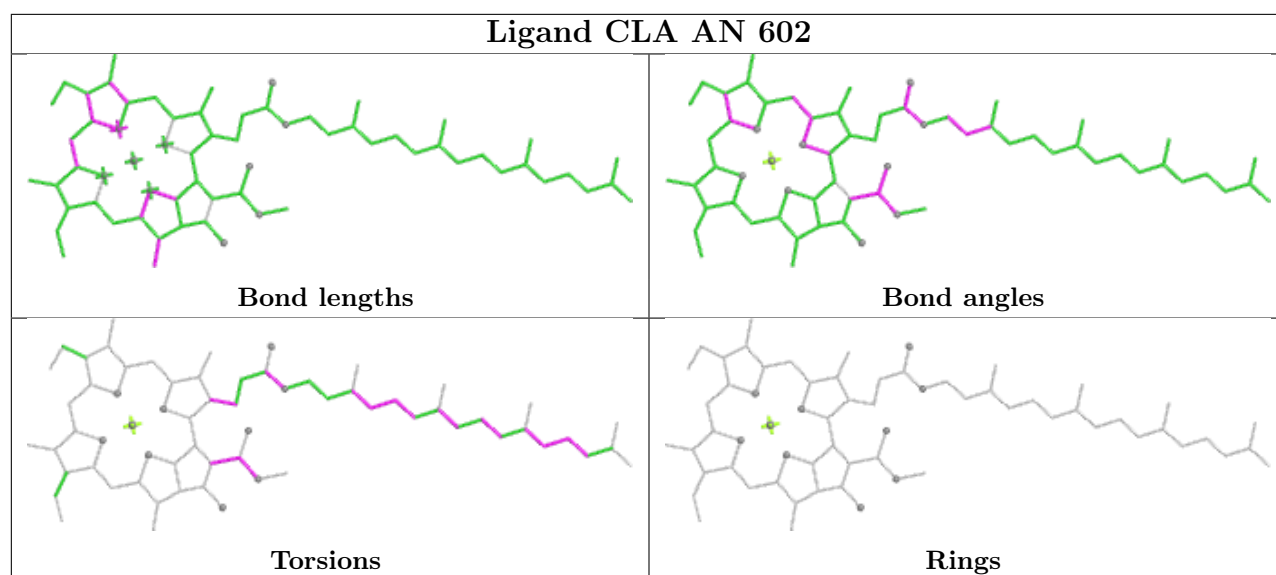


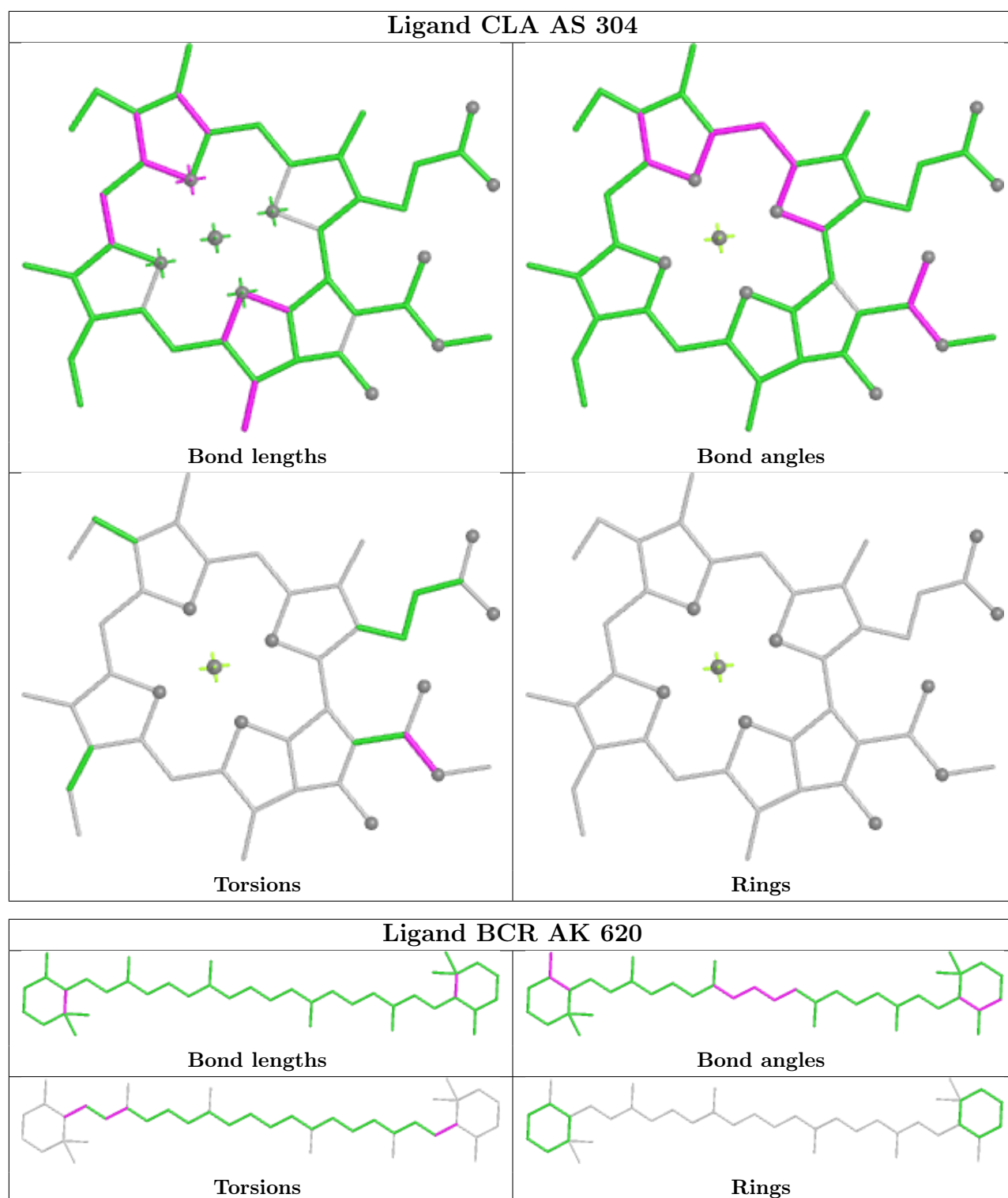




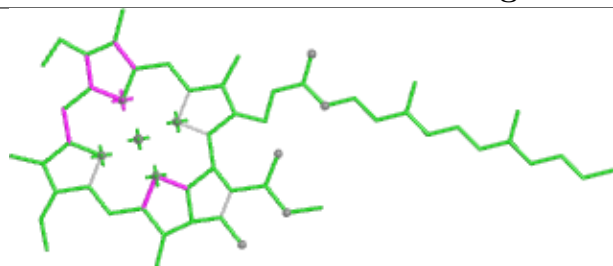




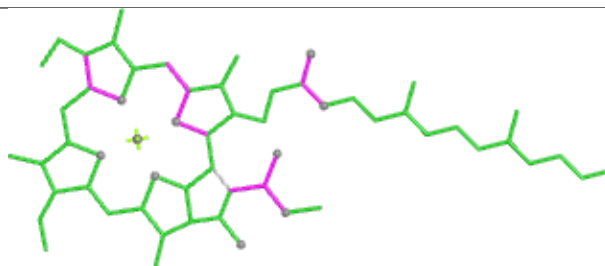




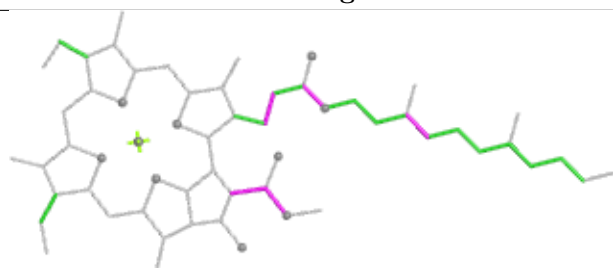
Ligand CLA AD 312



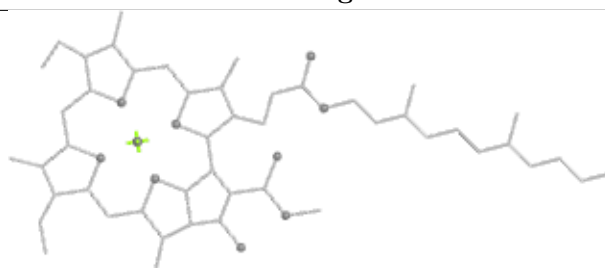
Bond lengths



Bond angles

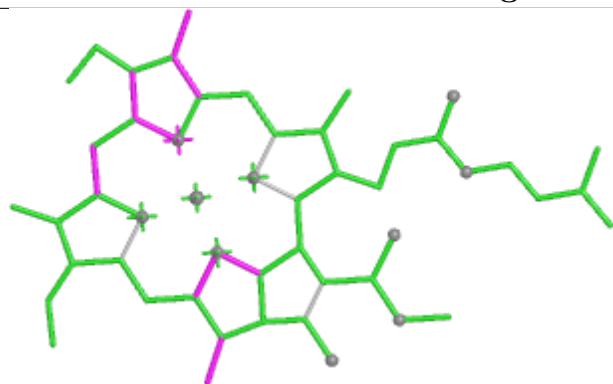


Torsions

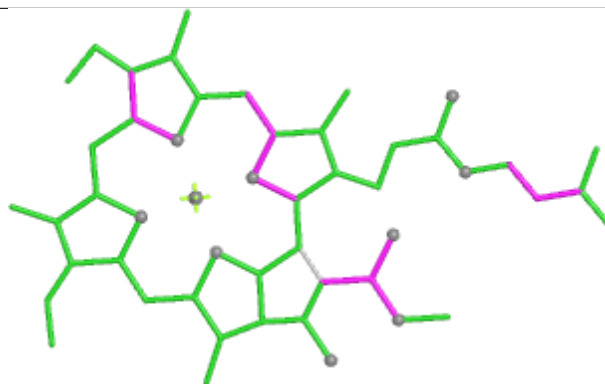


Rings

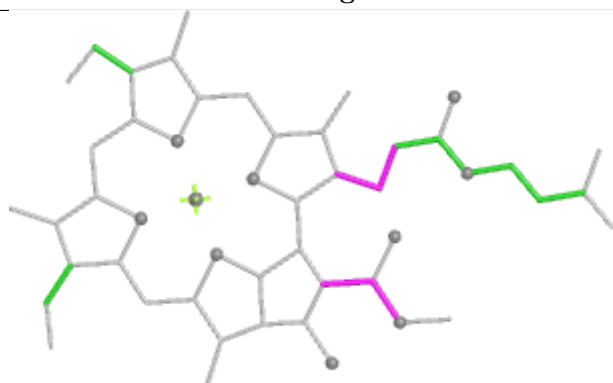
Ligand CLA AU 604



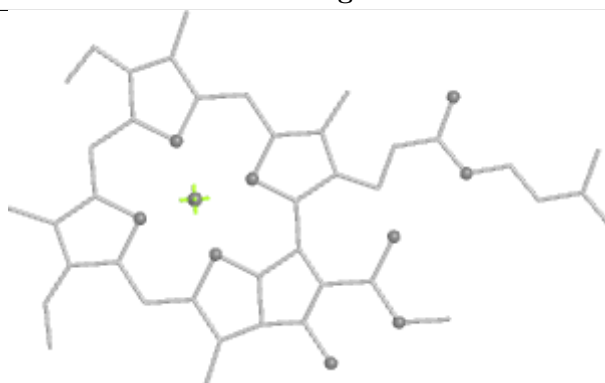
Bond lengths



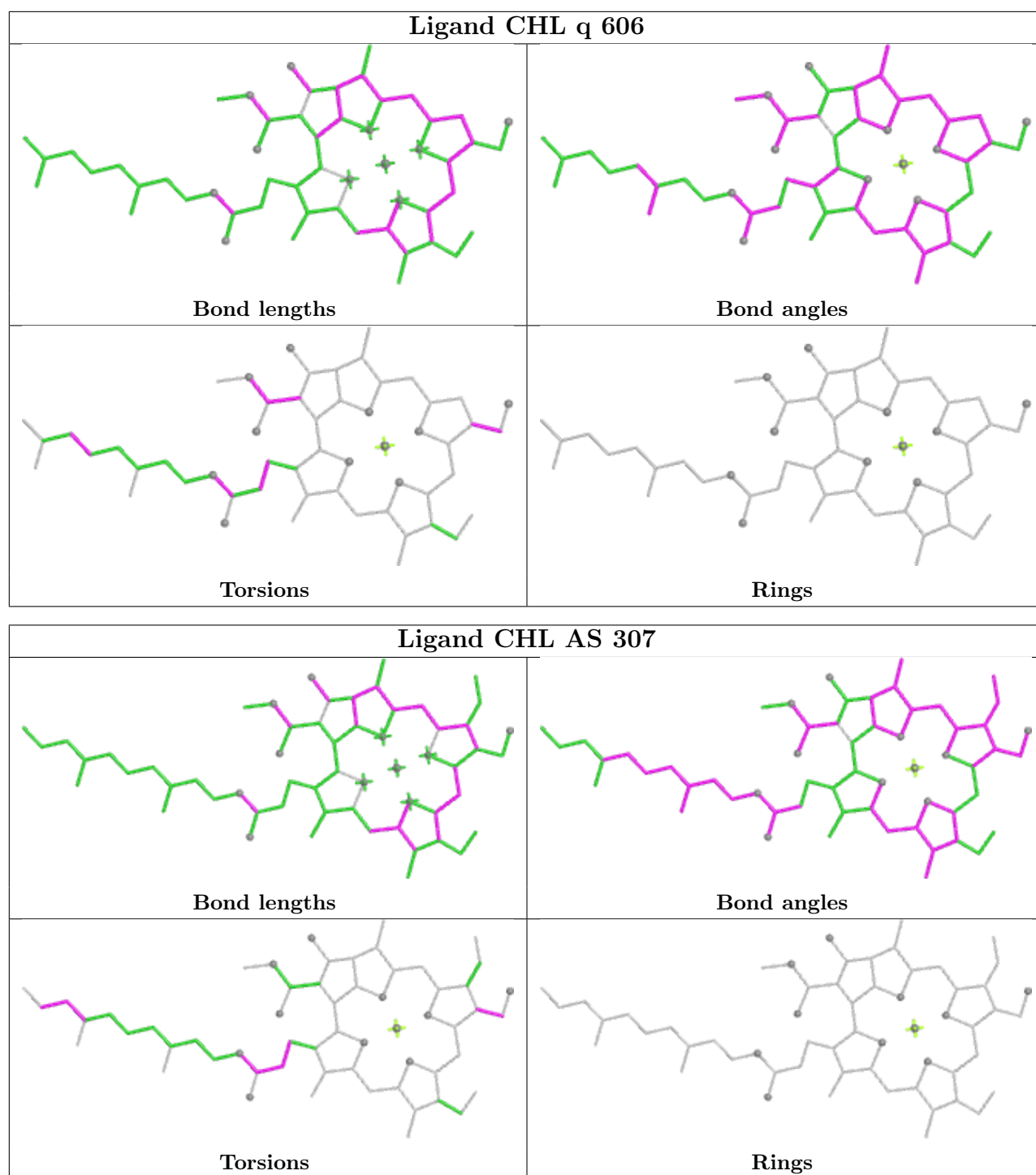
Bond angles

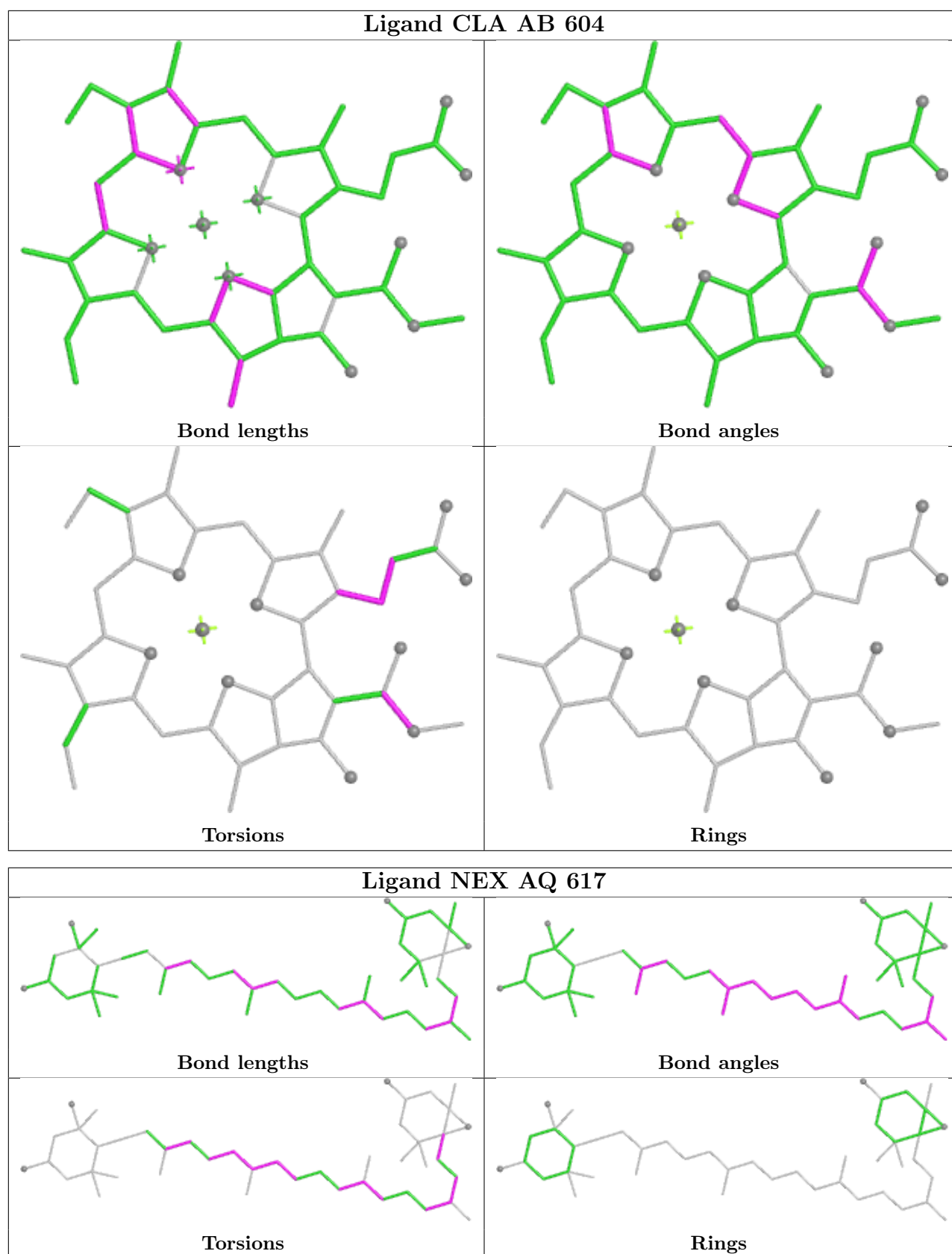


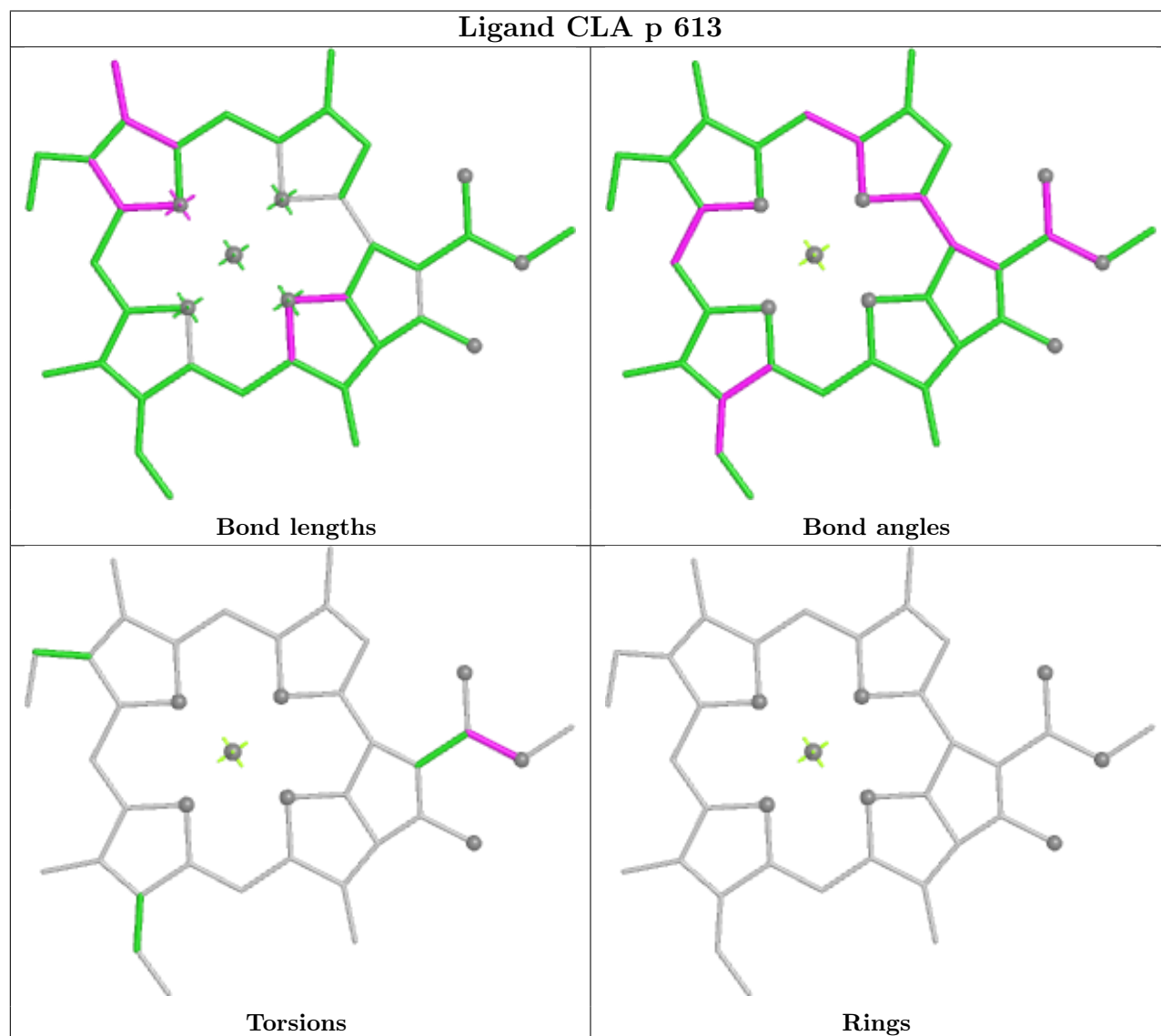
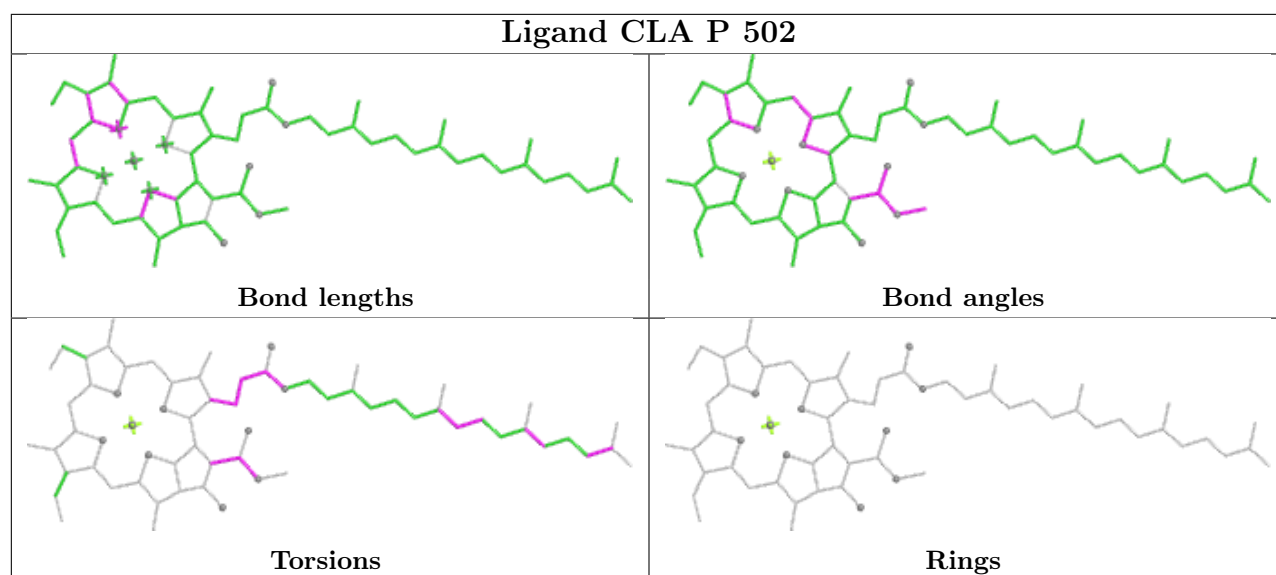
Torsions

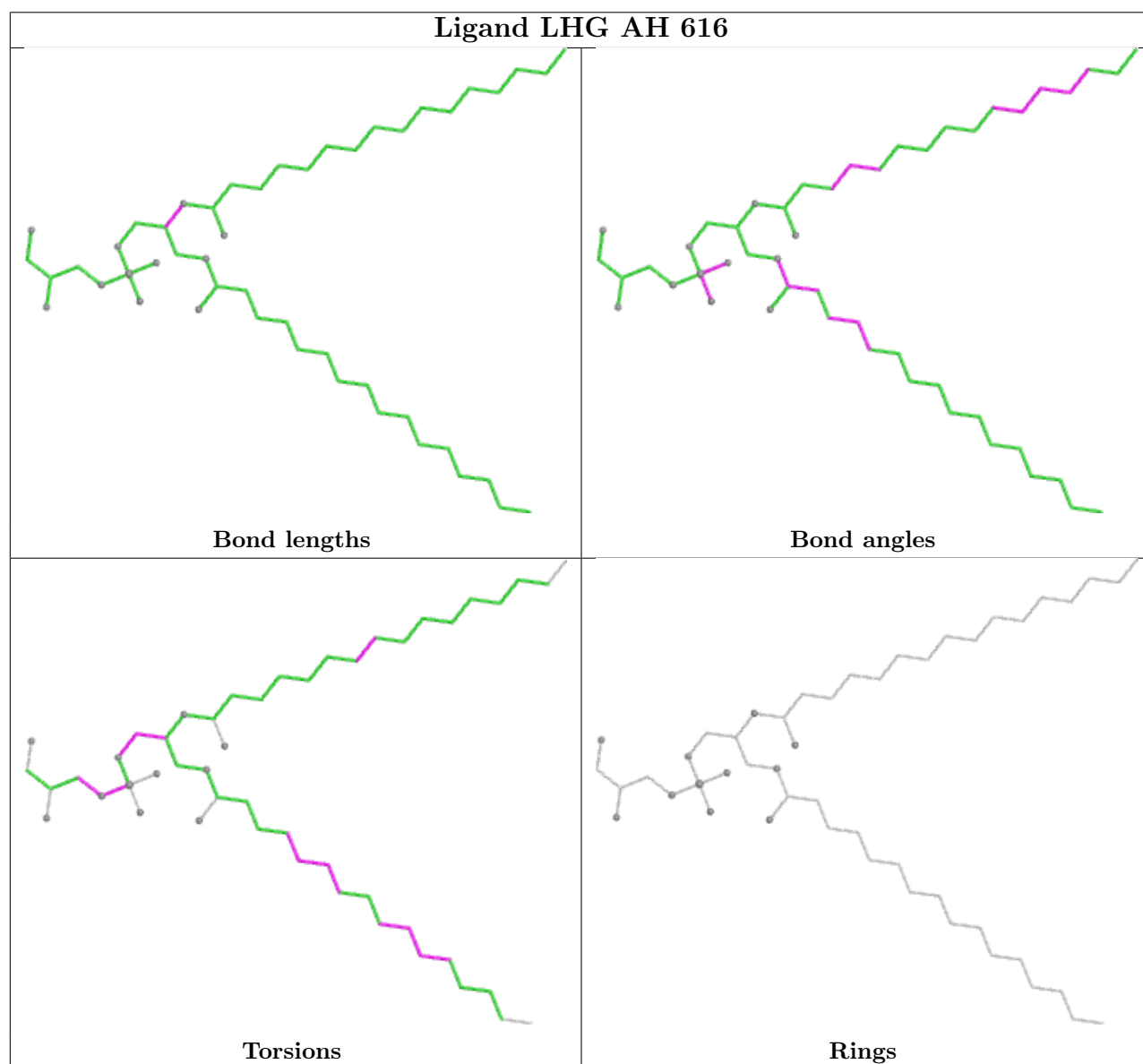
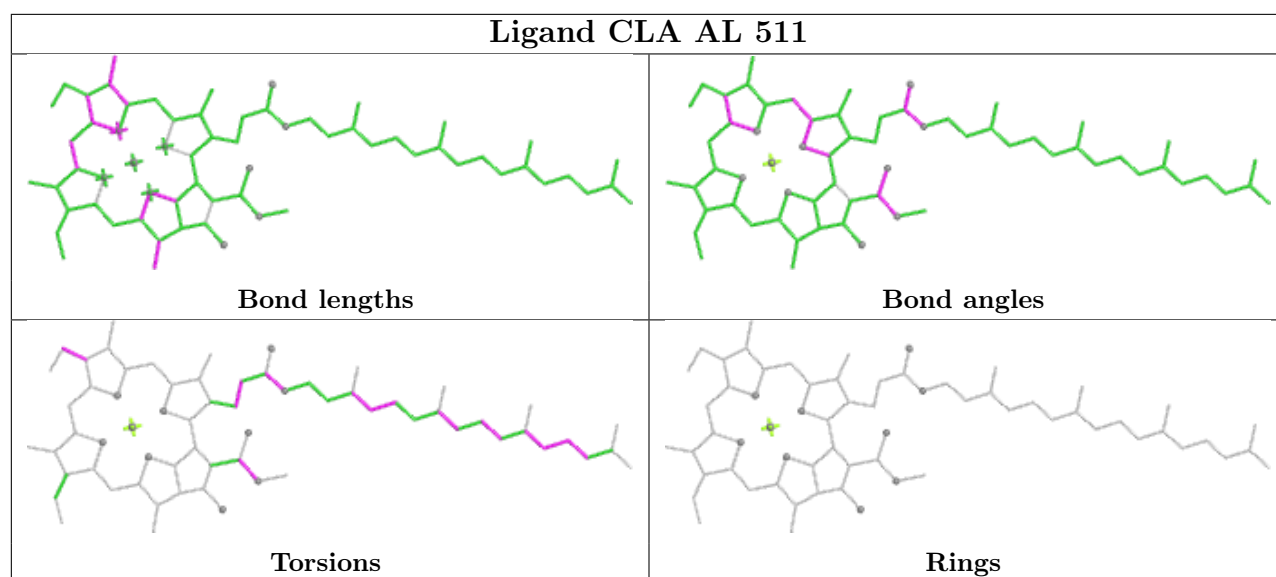


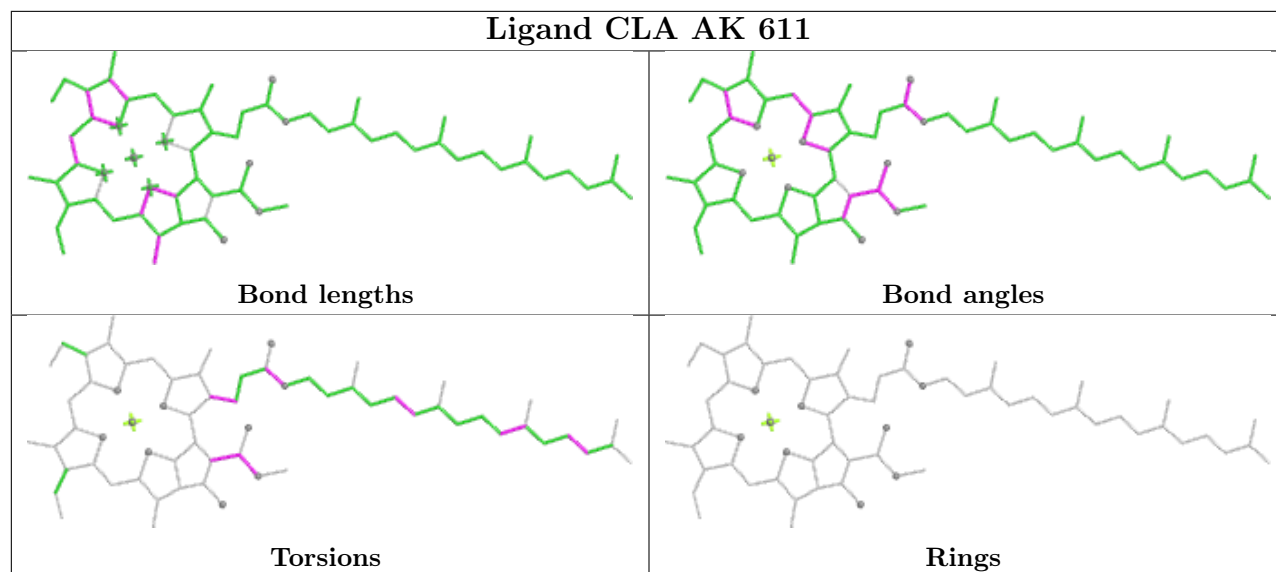
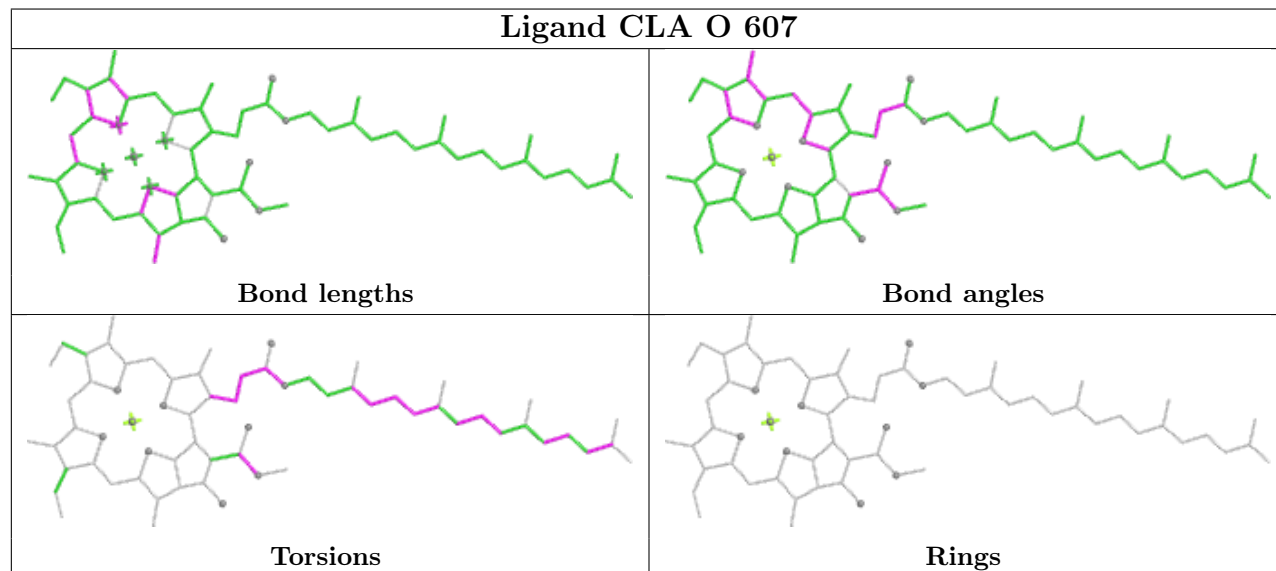
Rings

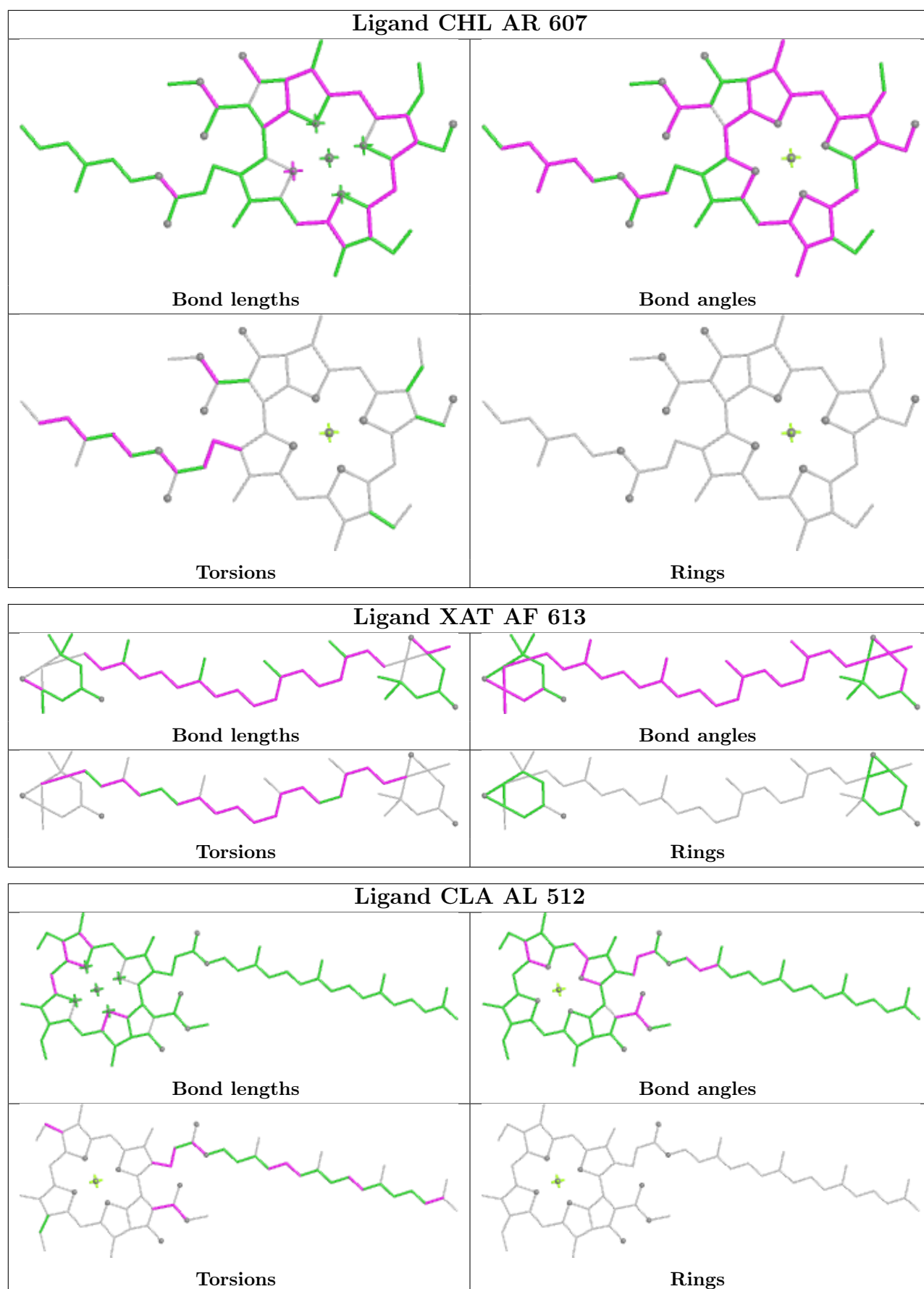


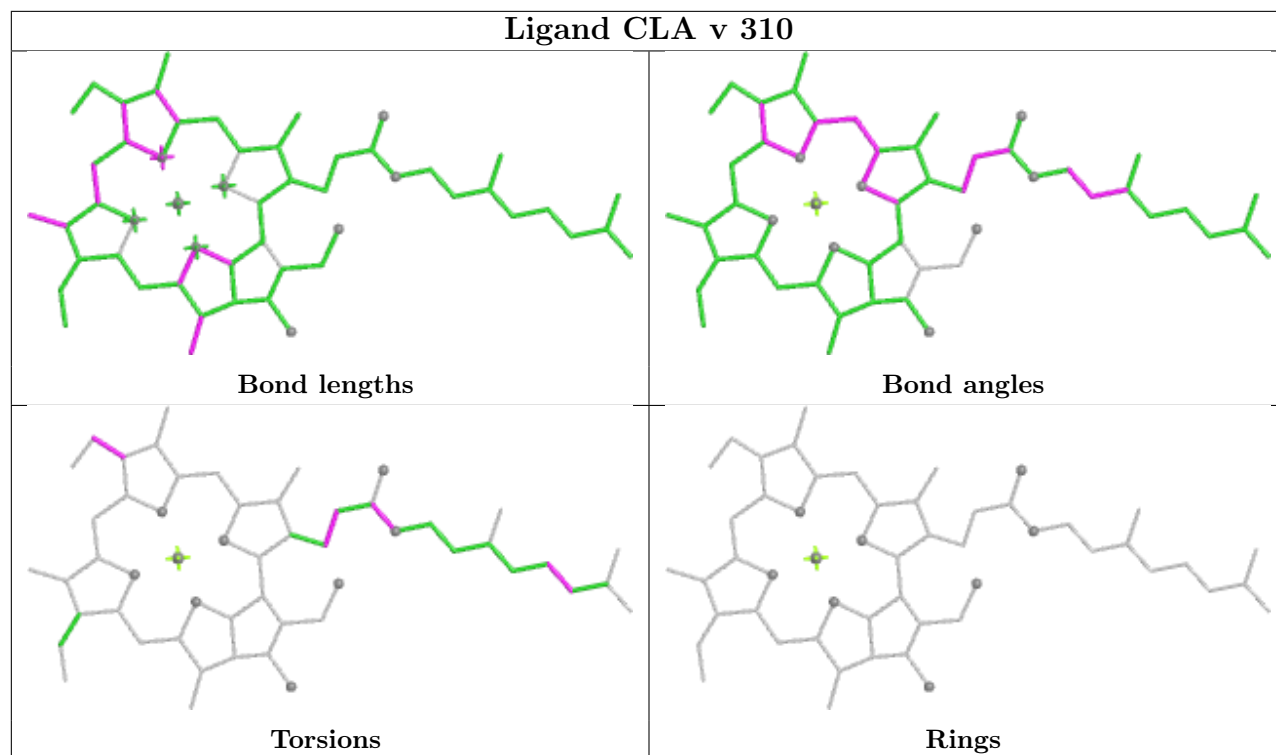
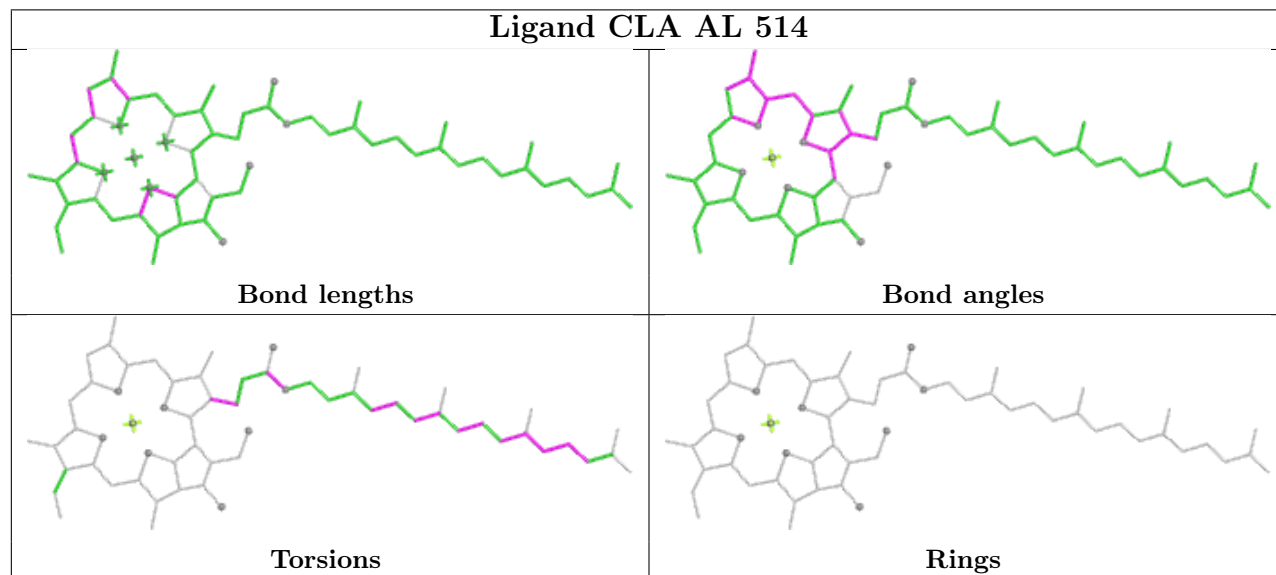


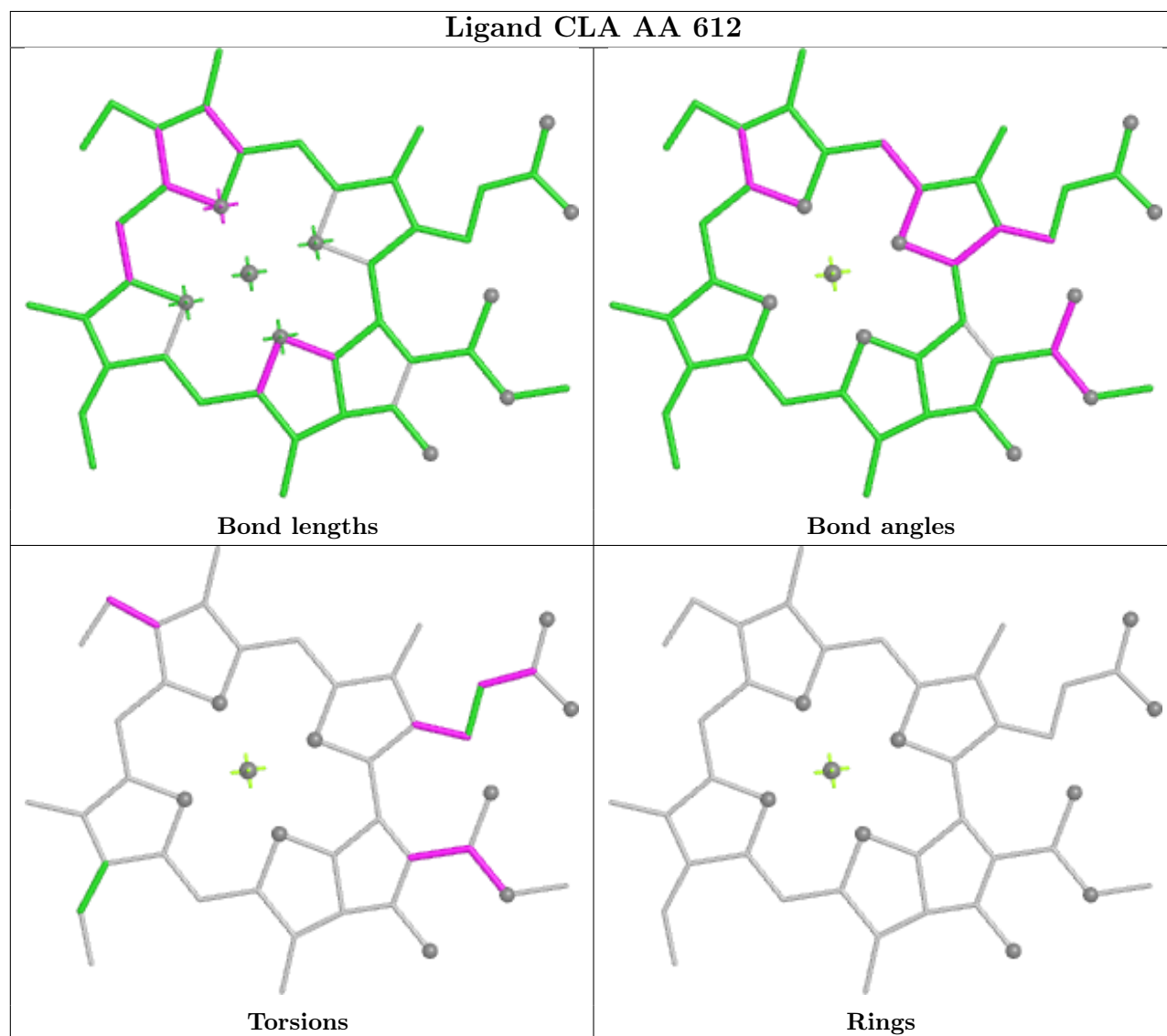
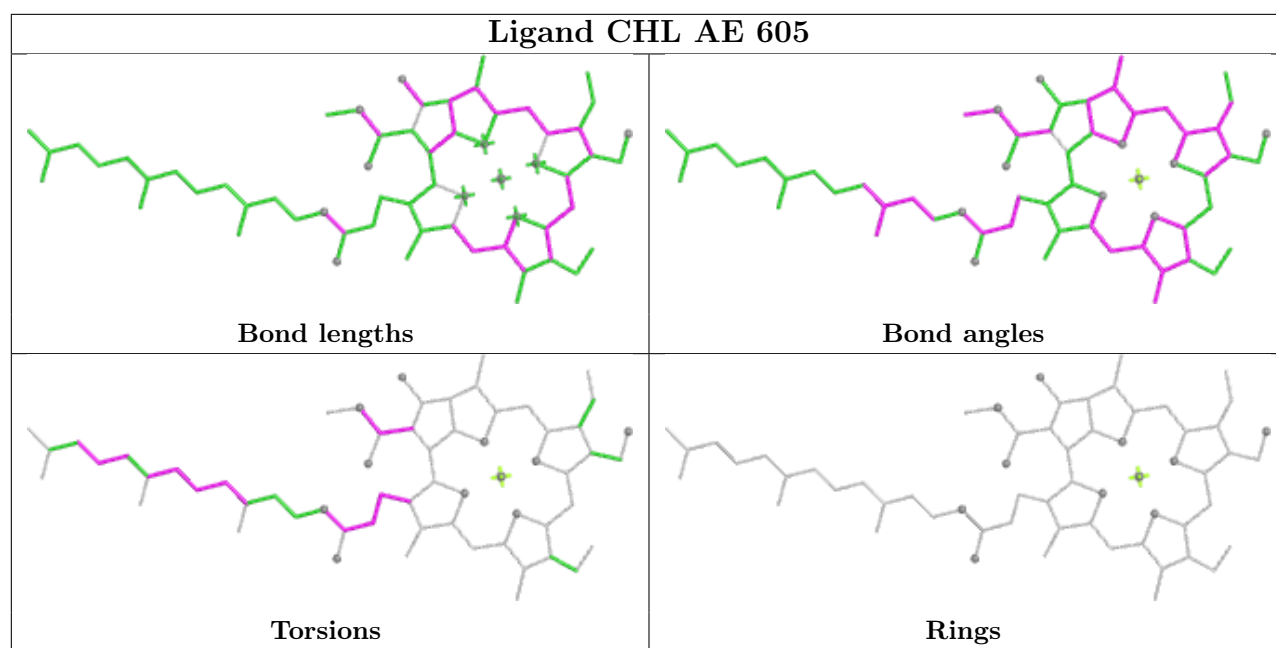


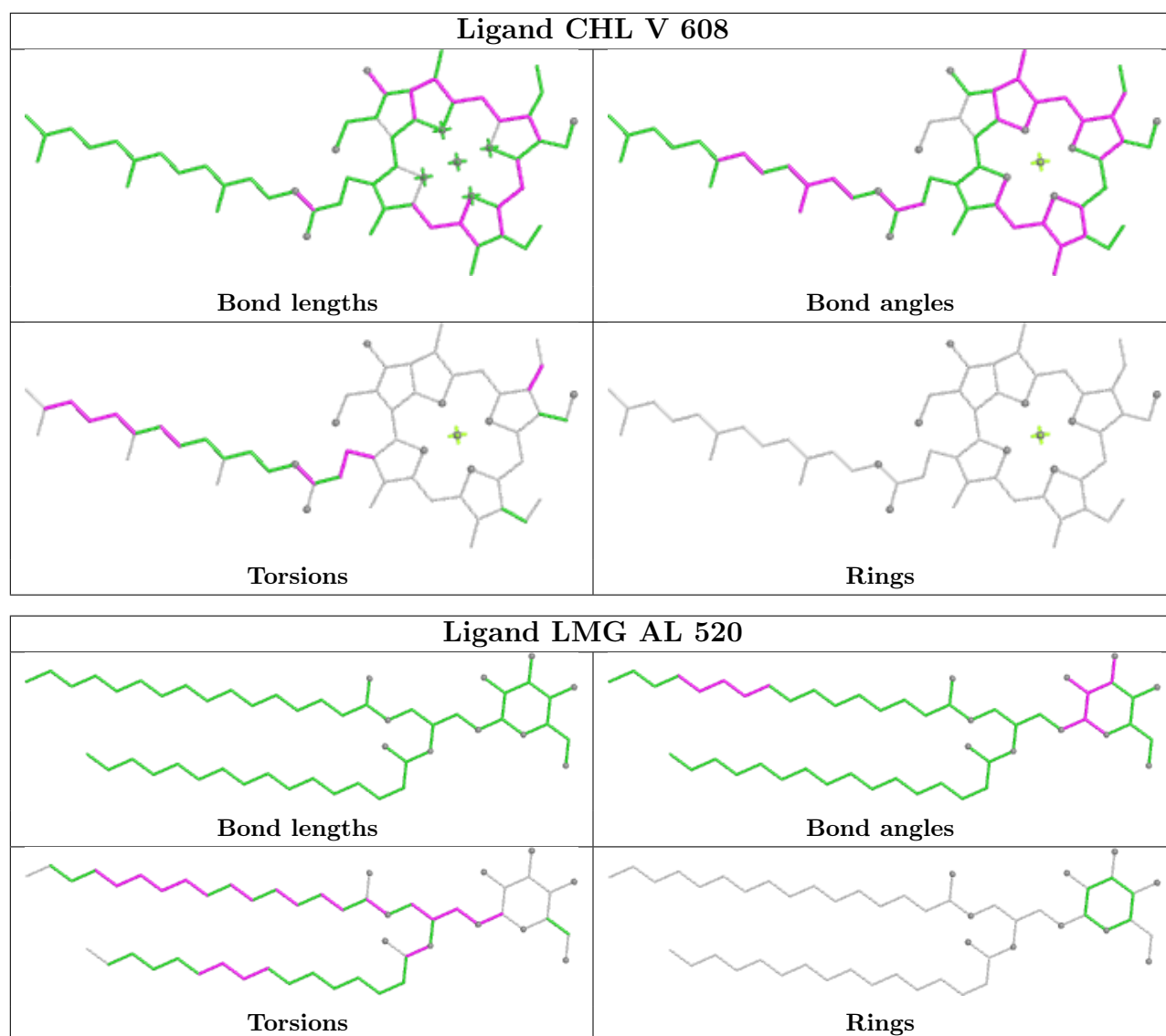


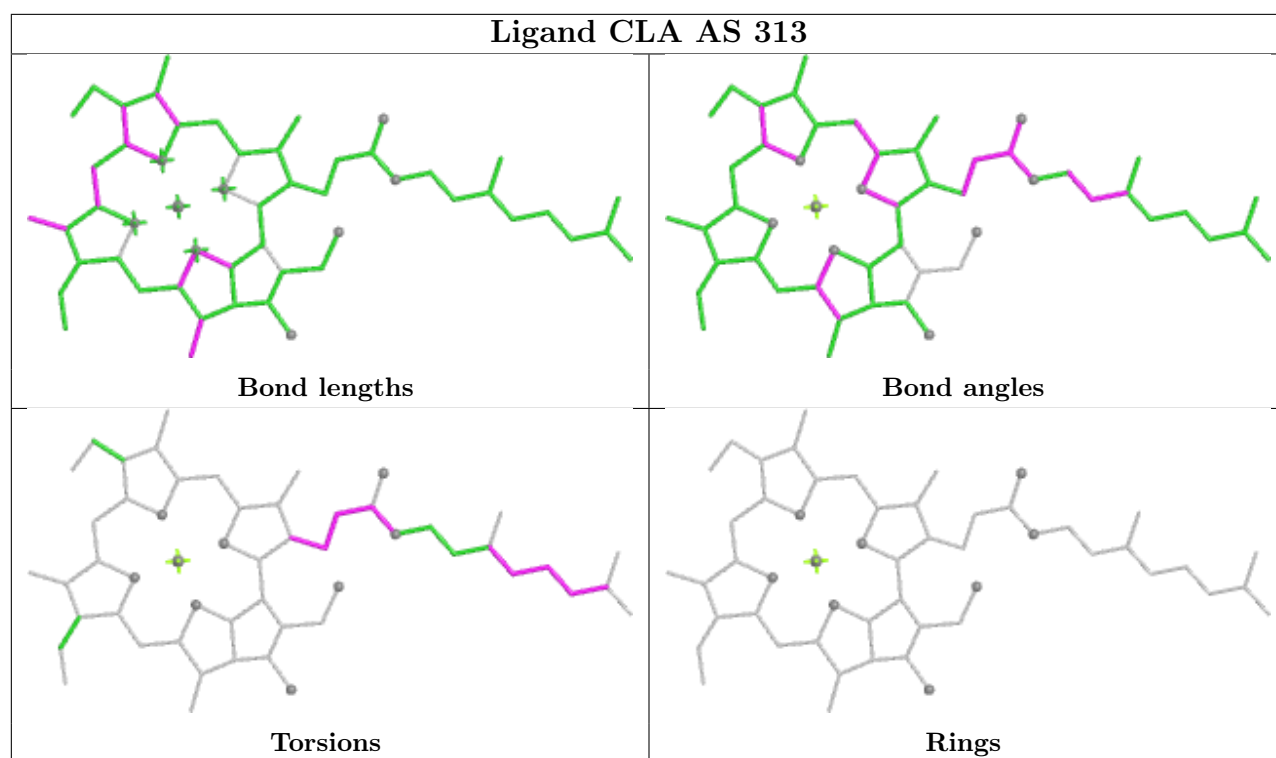
Ligand CLA AK 611**Ligand CLA O 607**



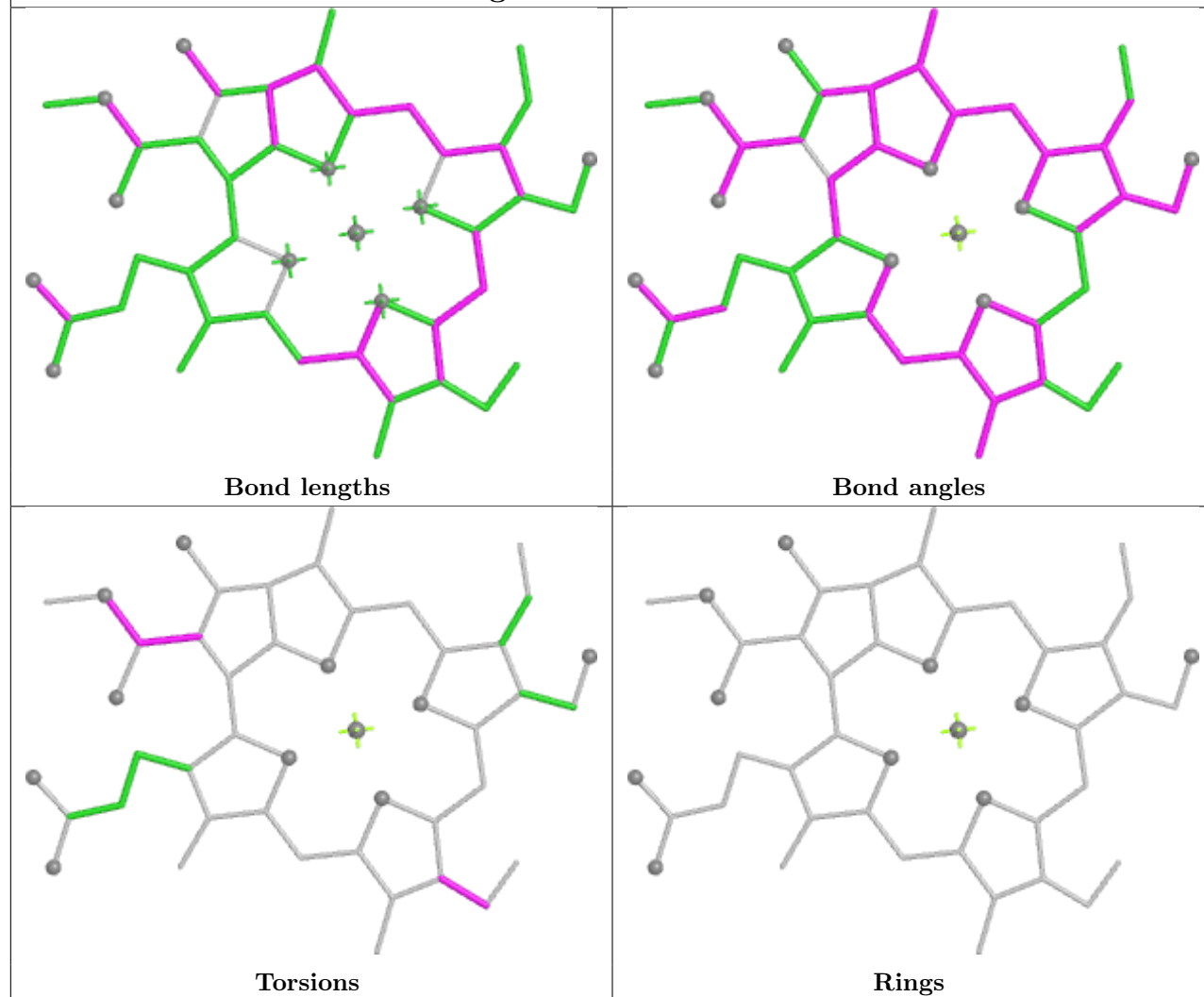
Ligand CLA v 310**Ligand CLA AL 514**



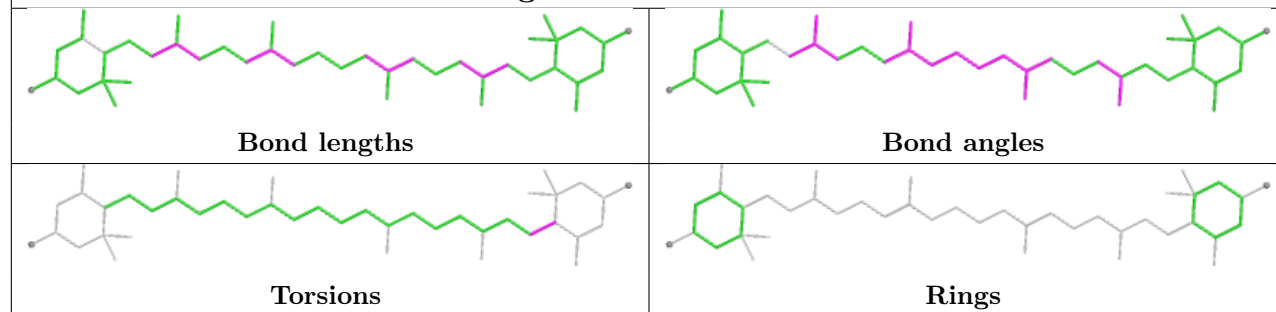




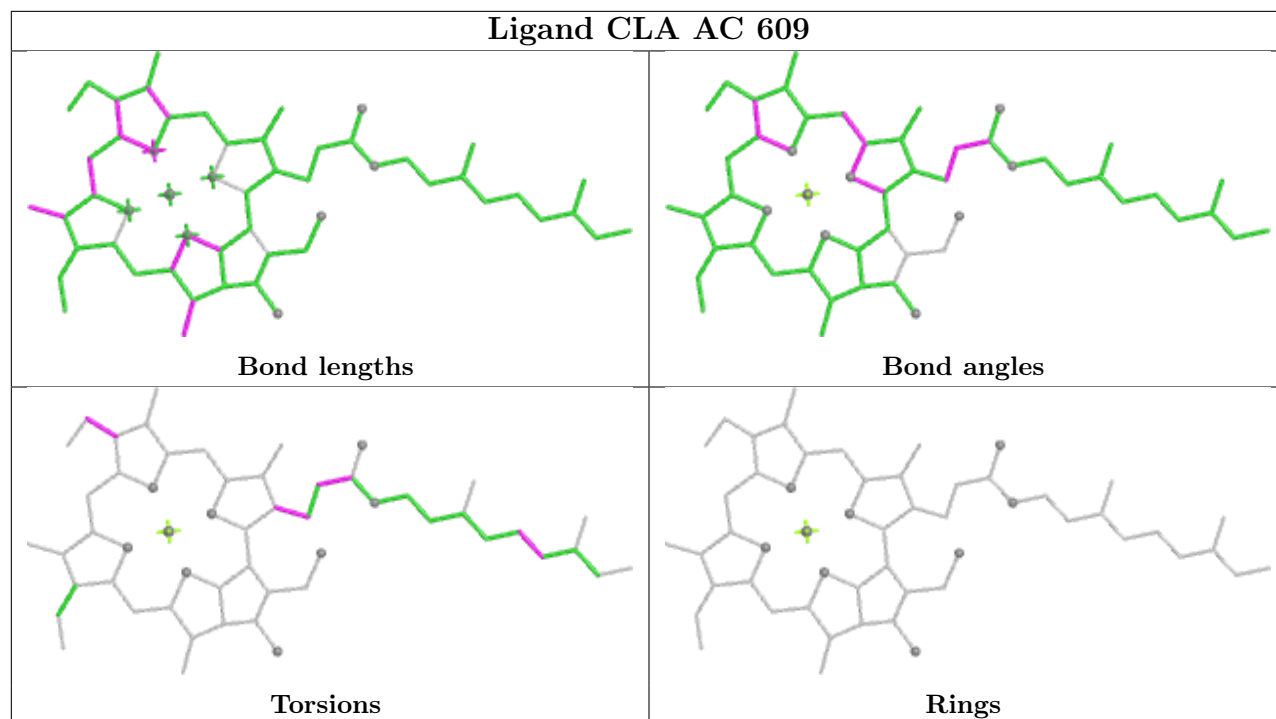
Ligand CHL AC 606



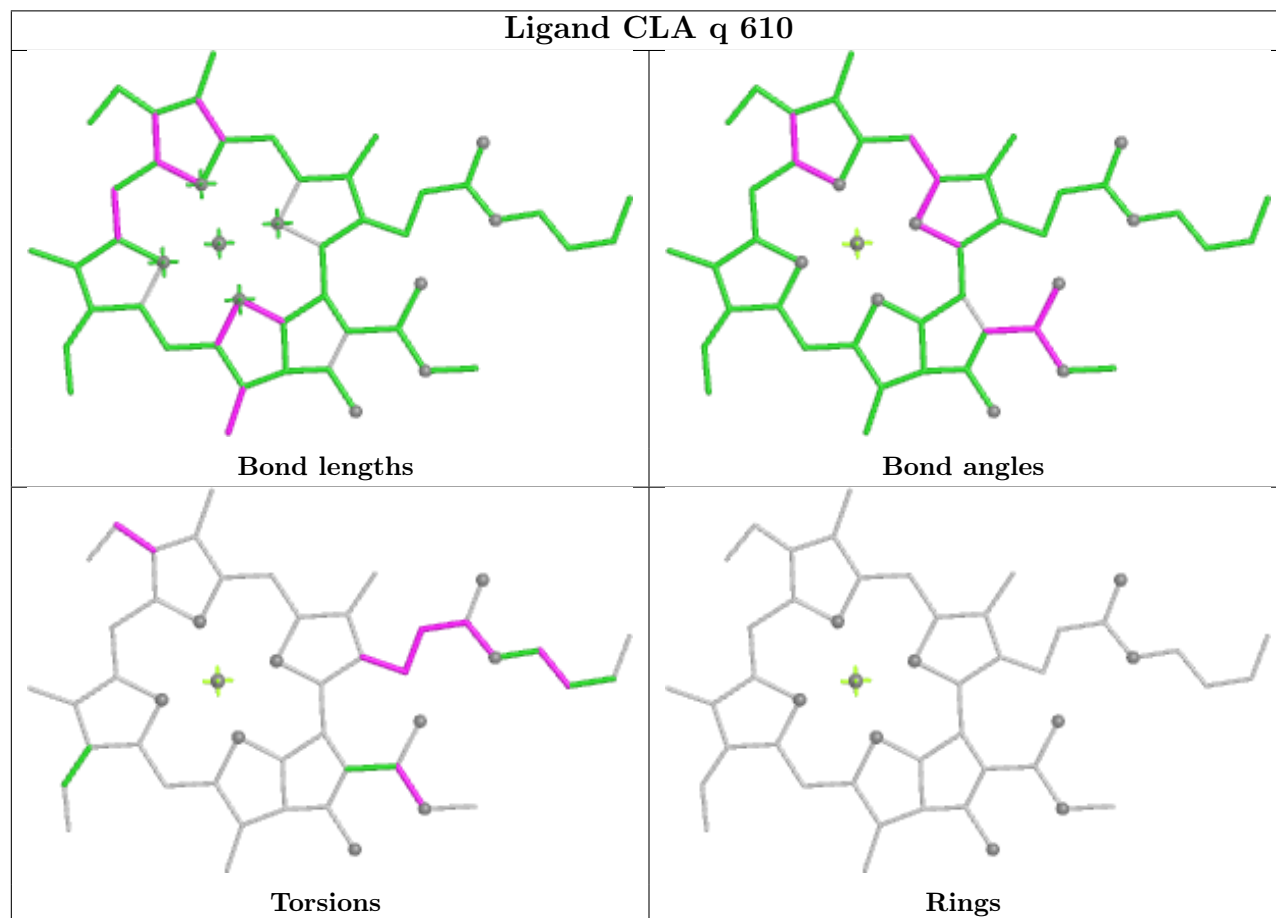
Ligand LUT AH 615



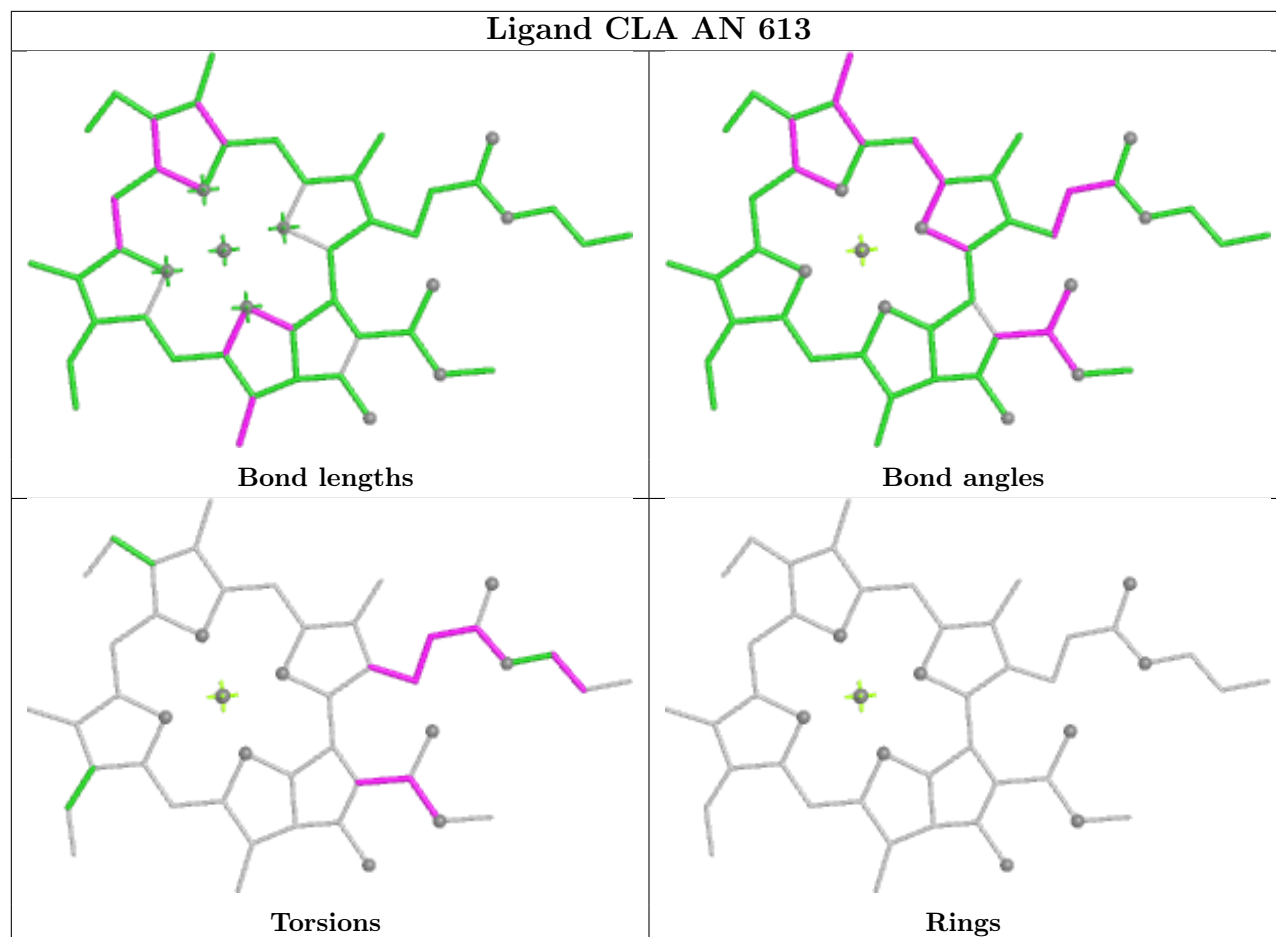
Ligand CLA AC 609



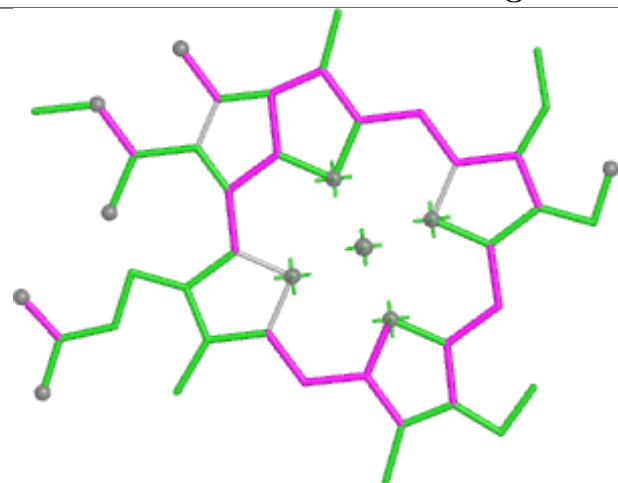
Ligand CLA q 610



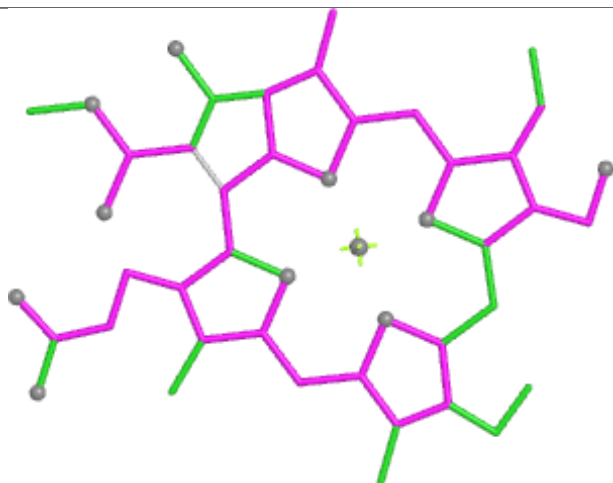
Ligand CLA AN 613



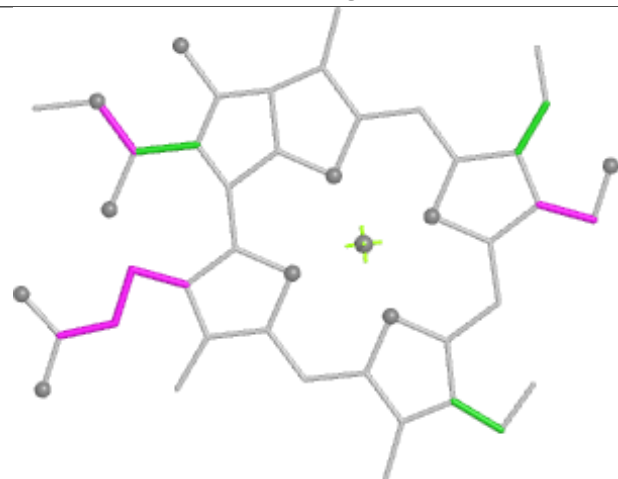
Ligand CHL AE 616



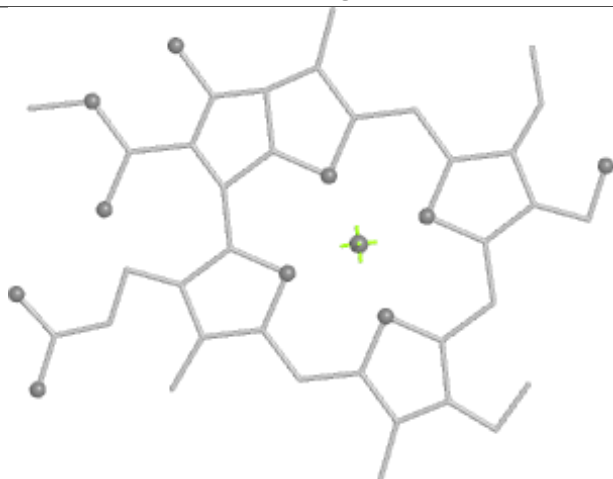
Bond lengths



Bond angles

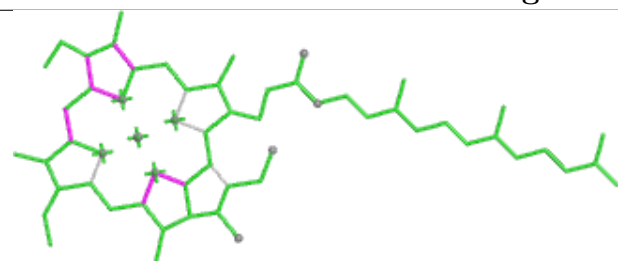


Torsions

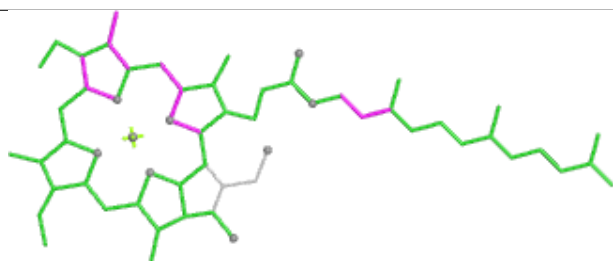


Rings

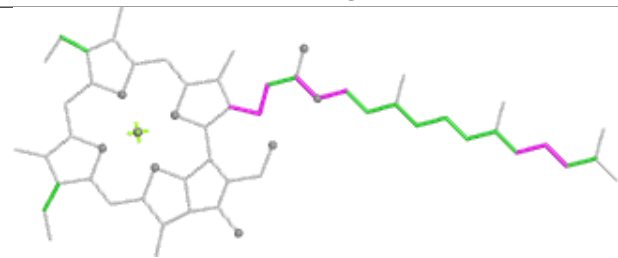
Ligand CLA J 407



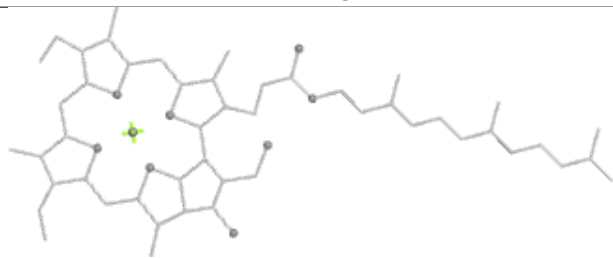
Bond lengths



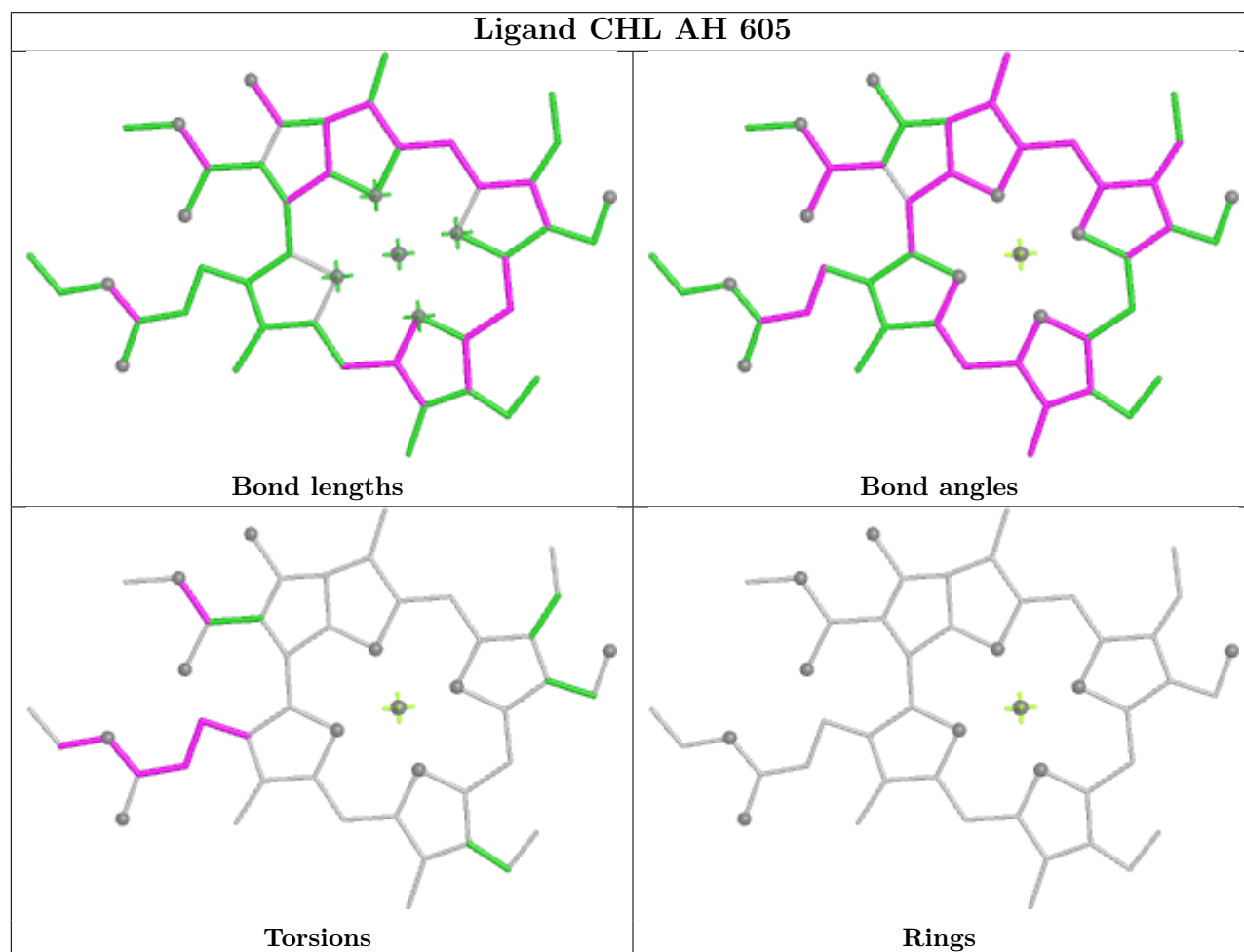
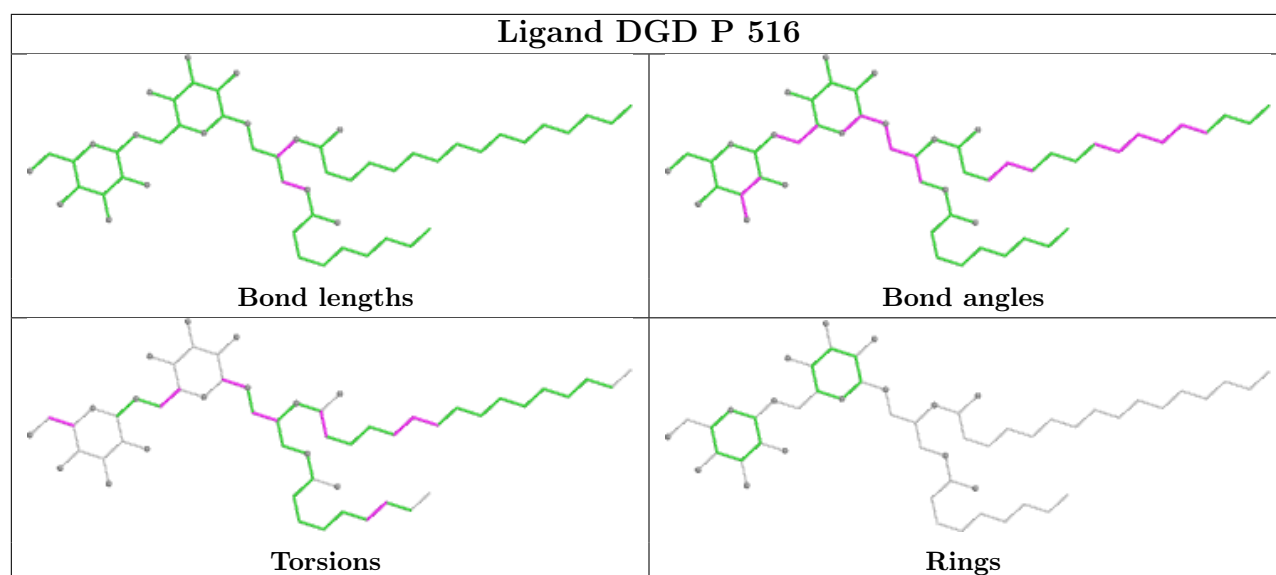
Bond angles

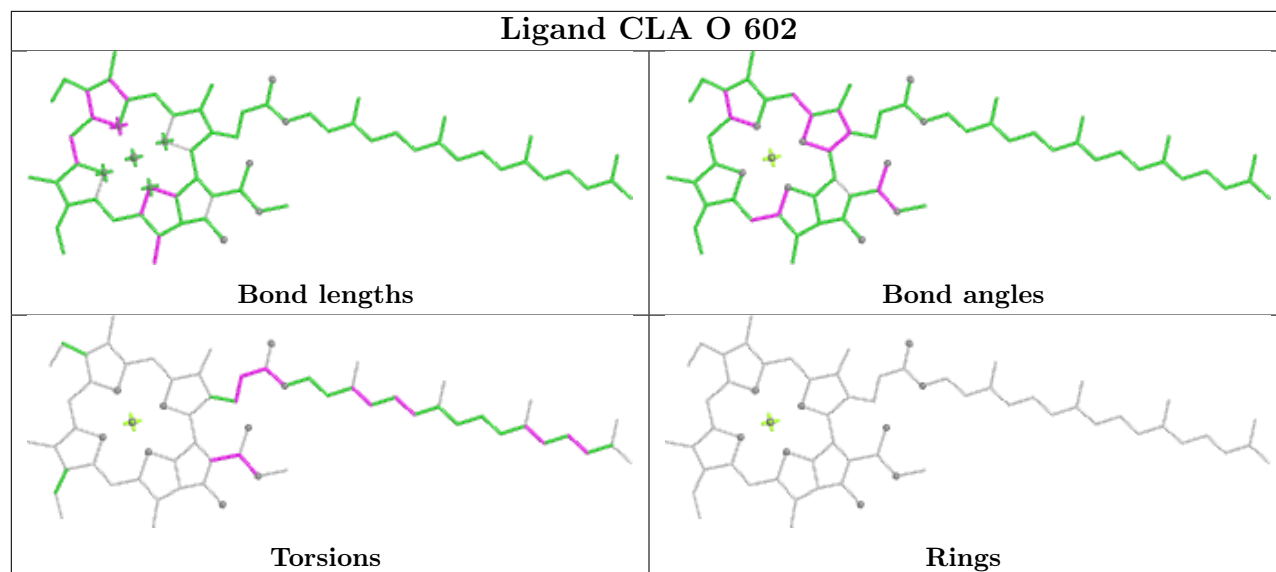
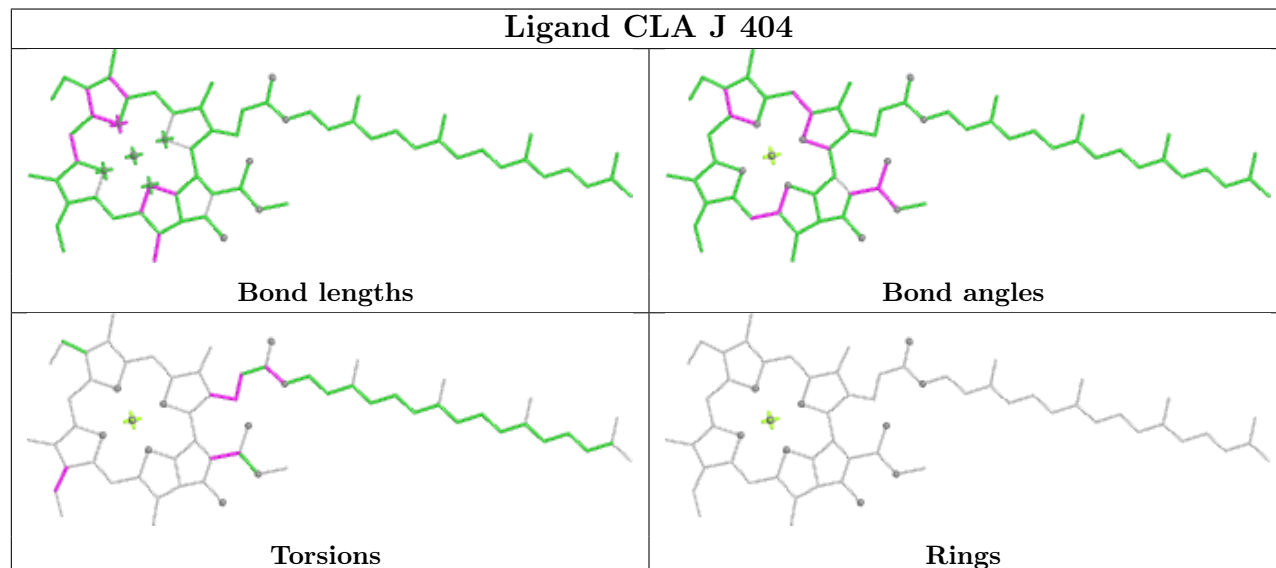


Torsions

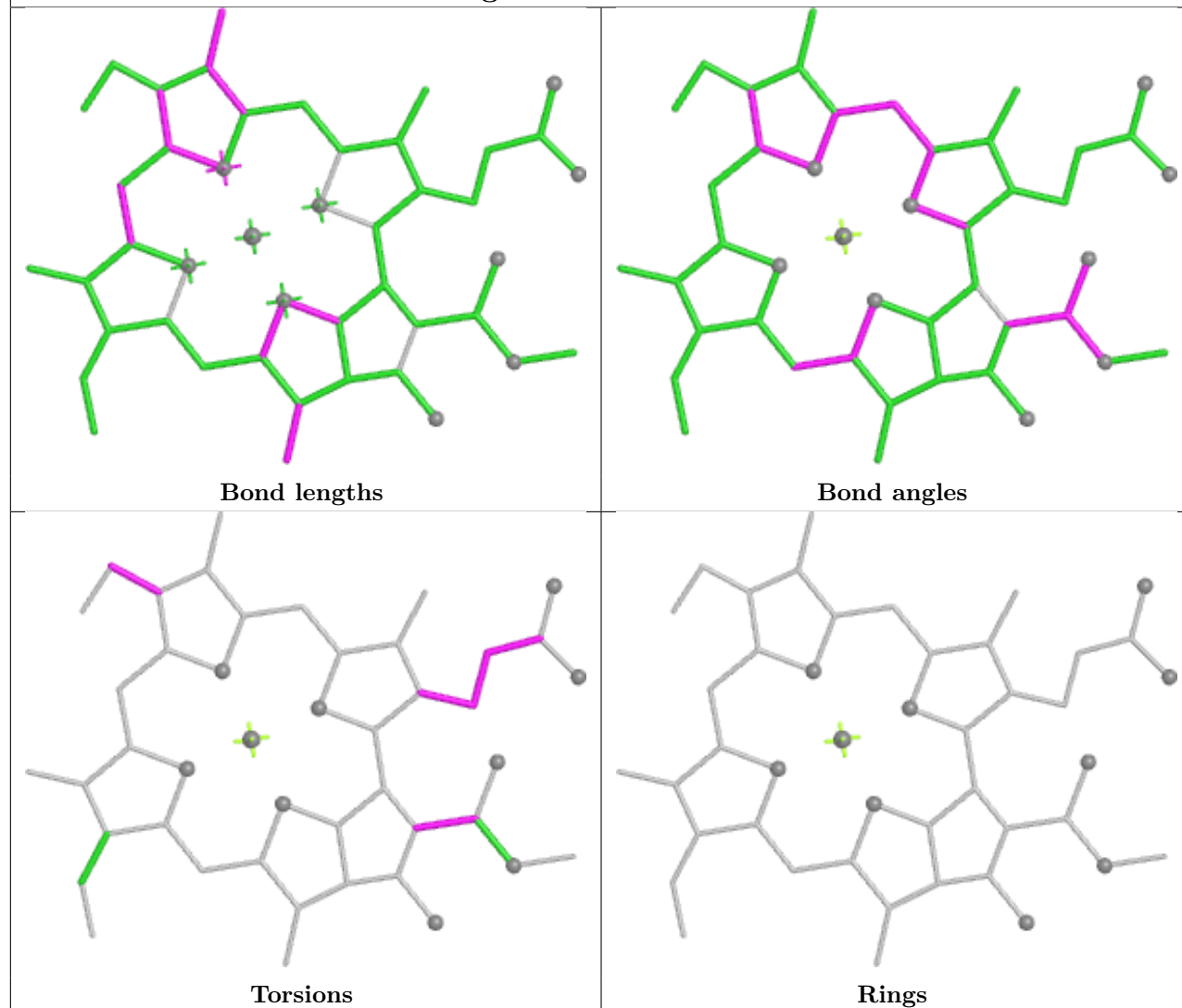


Rings

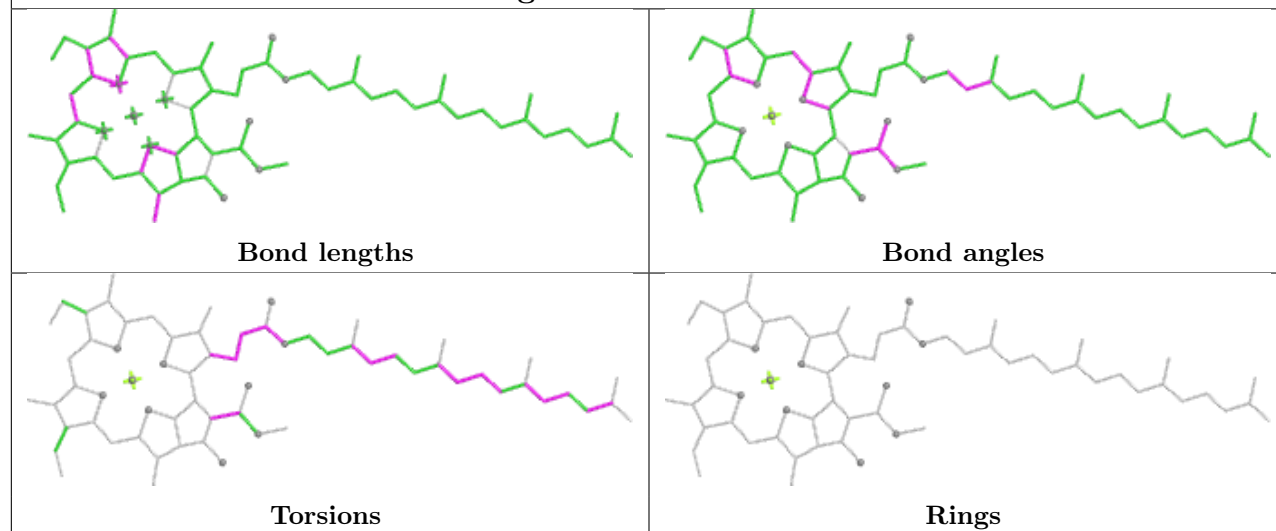


Ligand CLA O 602**Ligand CLA J 404**

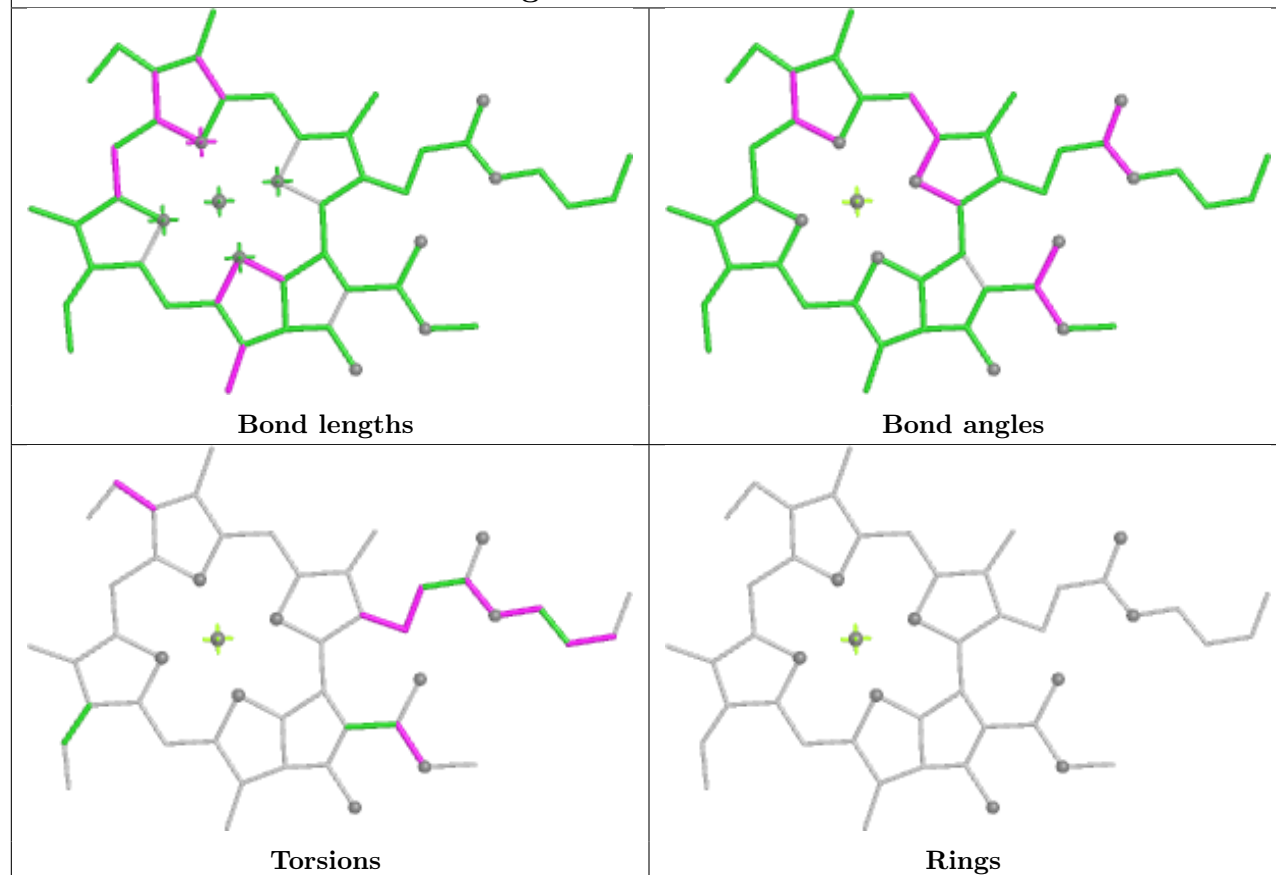
Ligand CLA AE 609



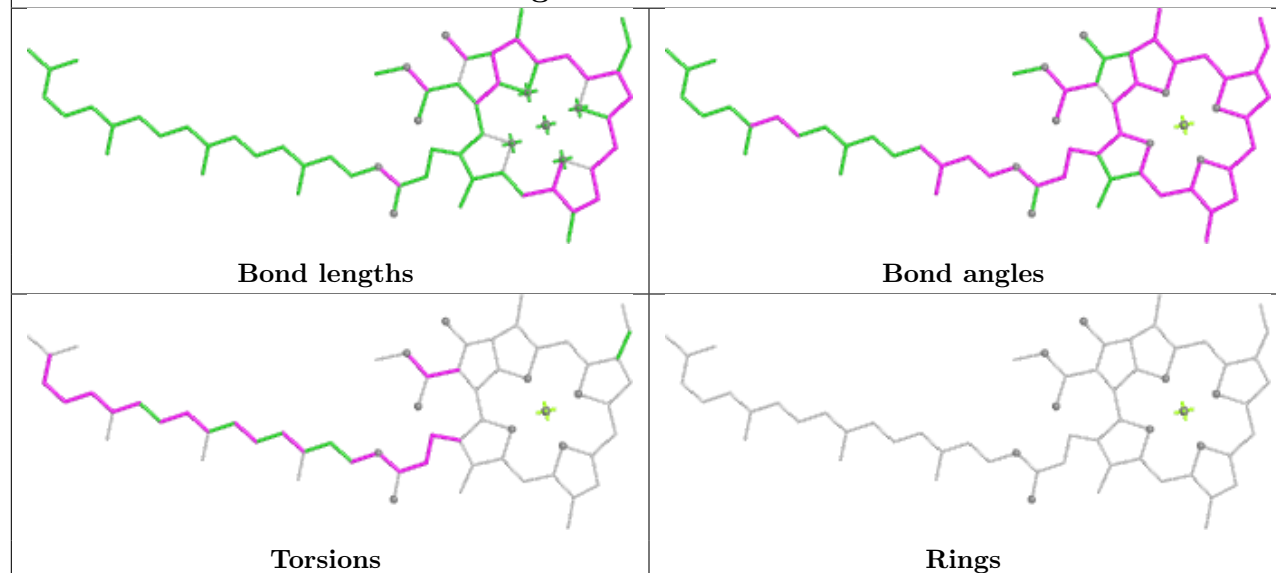
Ligand CLA AK 616

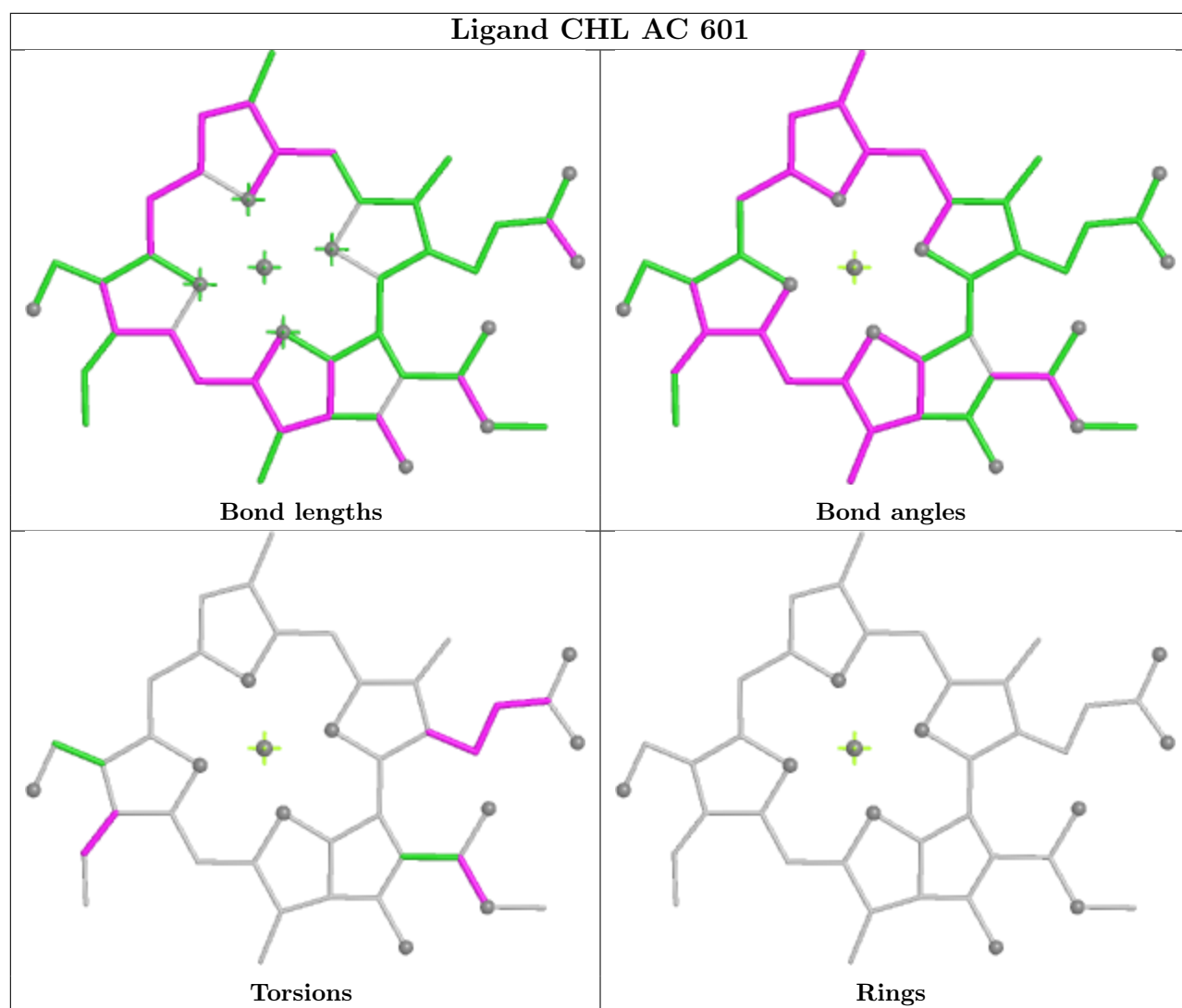


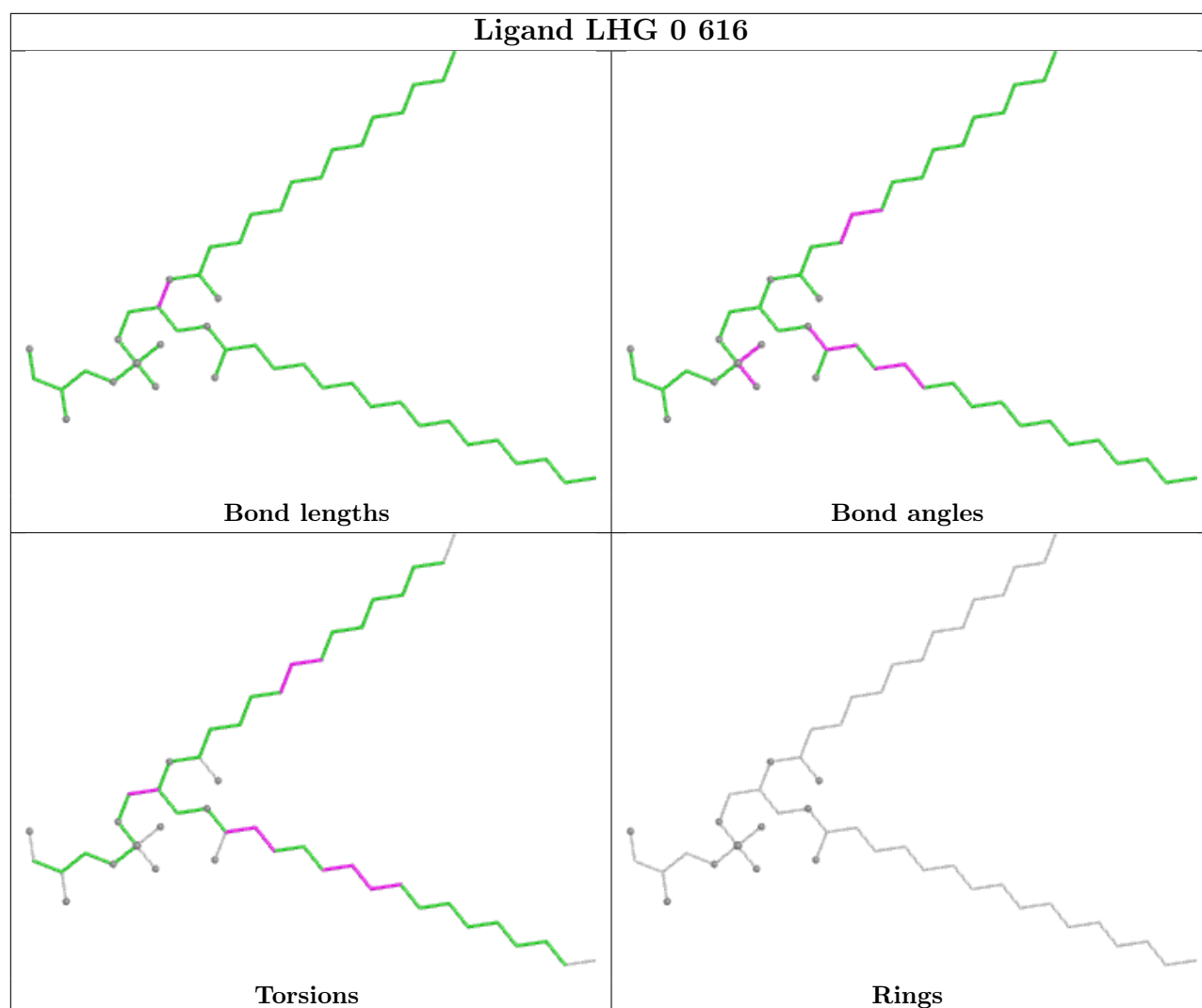
Ligand CLA AS 314



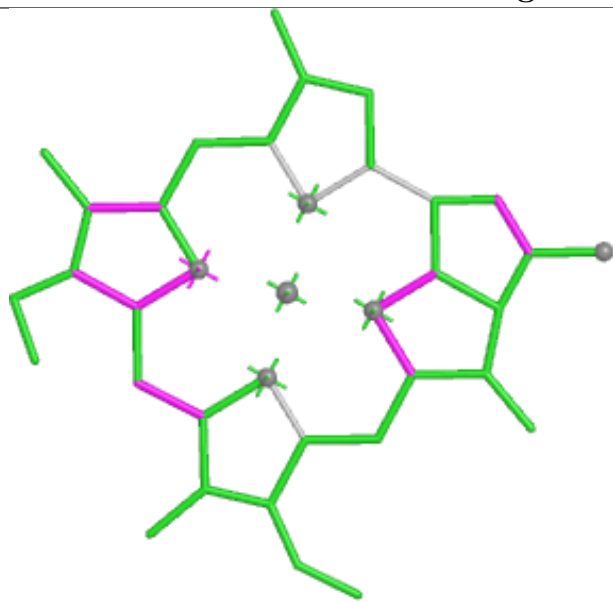
Ligand CHL V 607



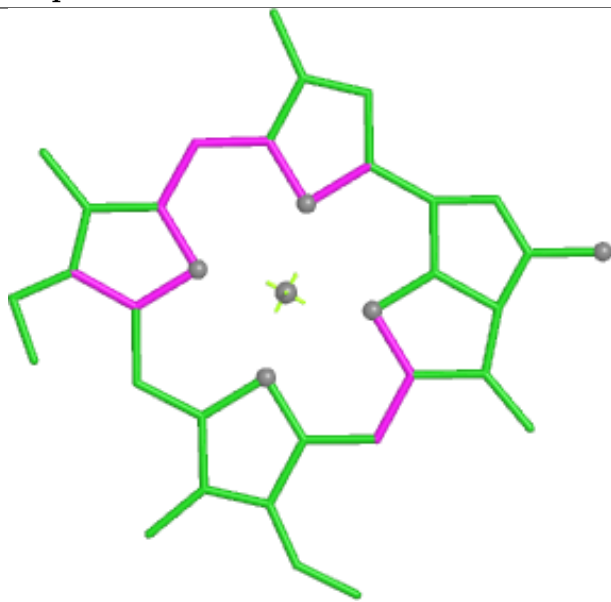




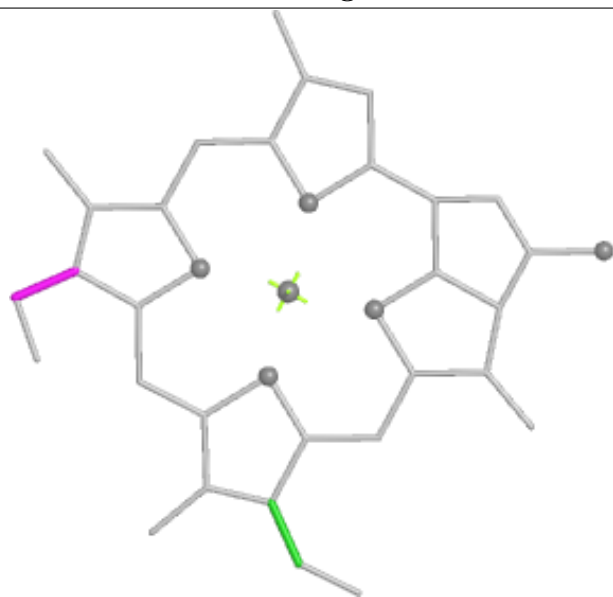
Ligand CLA p 611



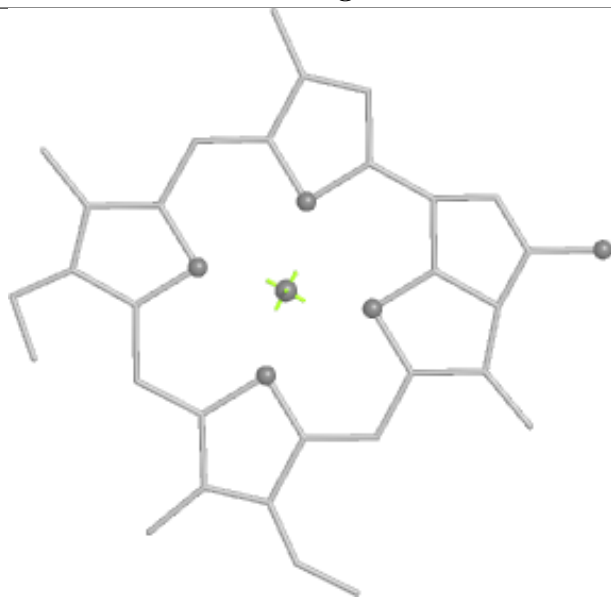
Bond lengths



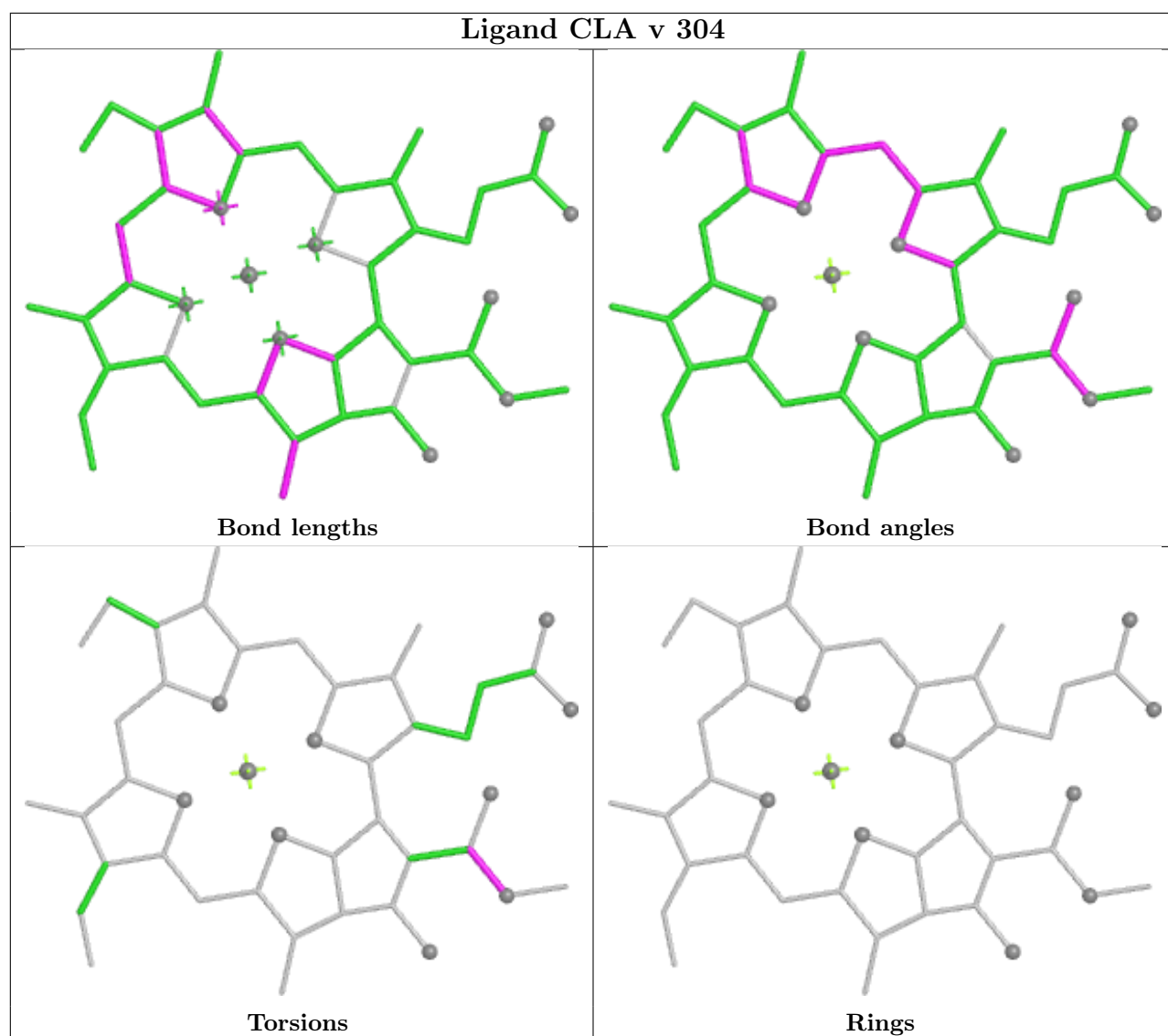
Bond angles



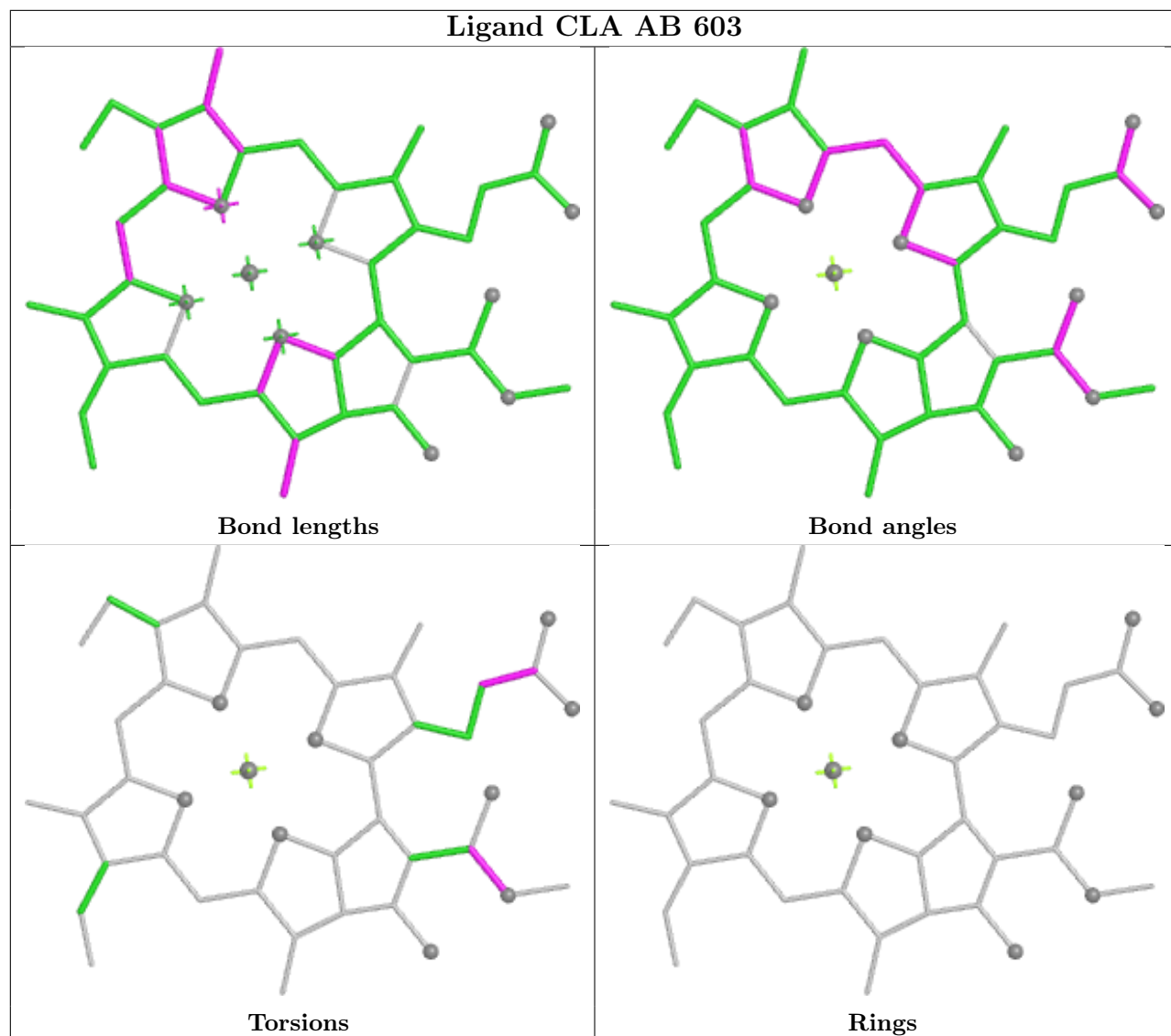
Torsions



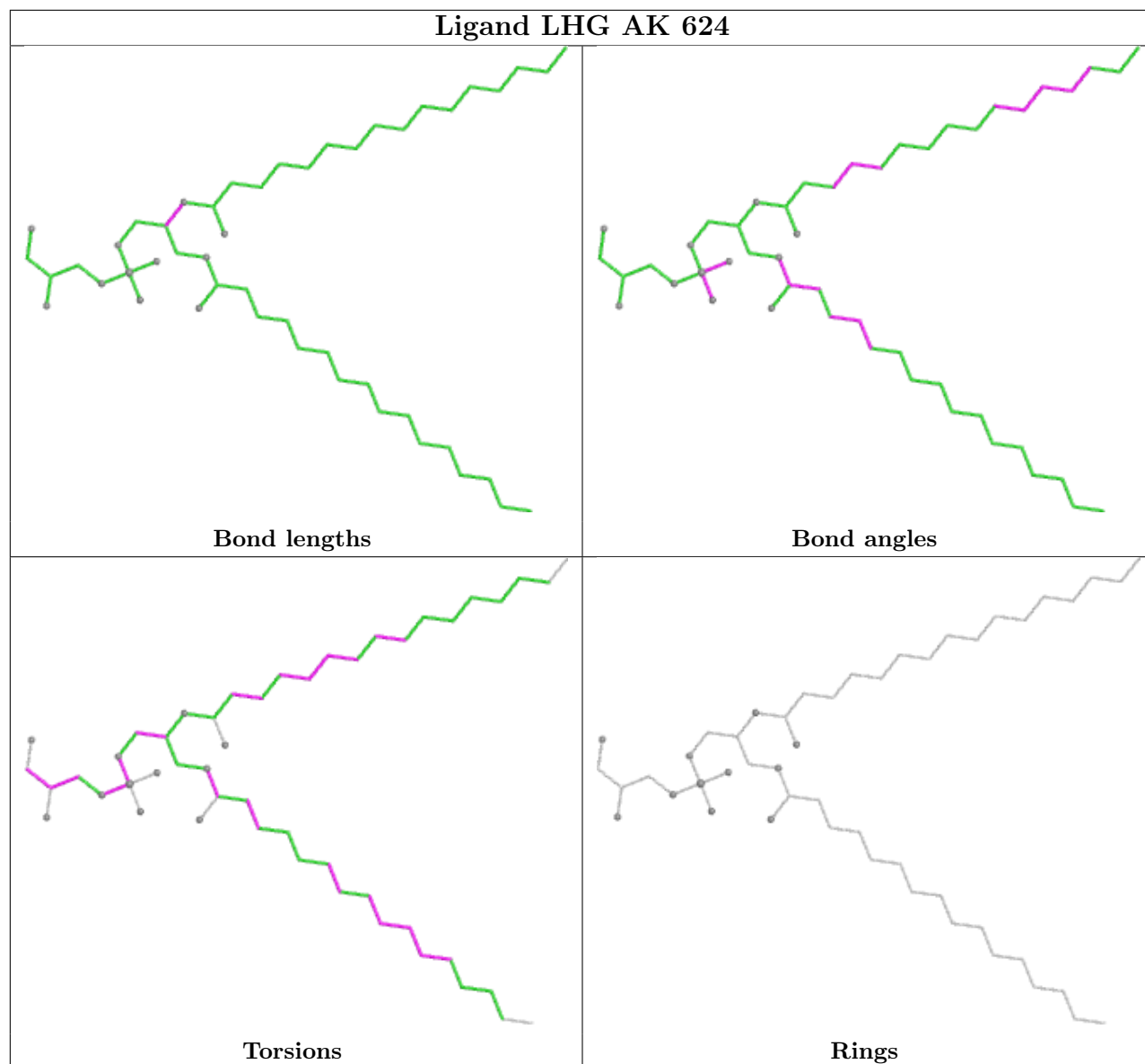
Rings



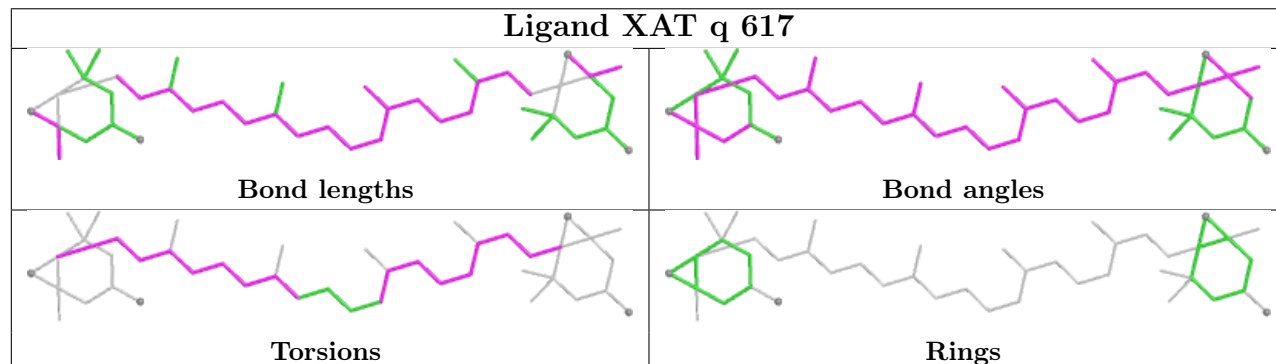
Ligand CLA AB 603



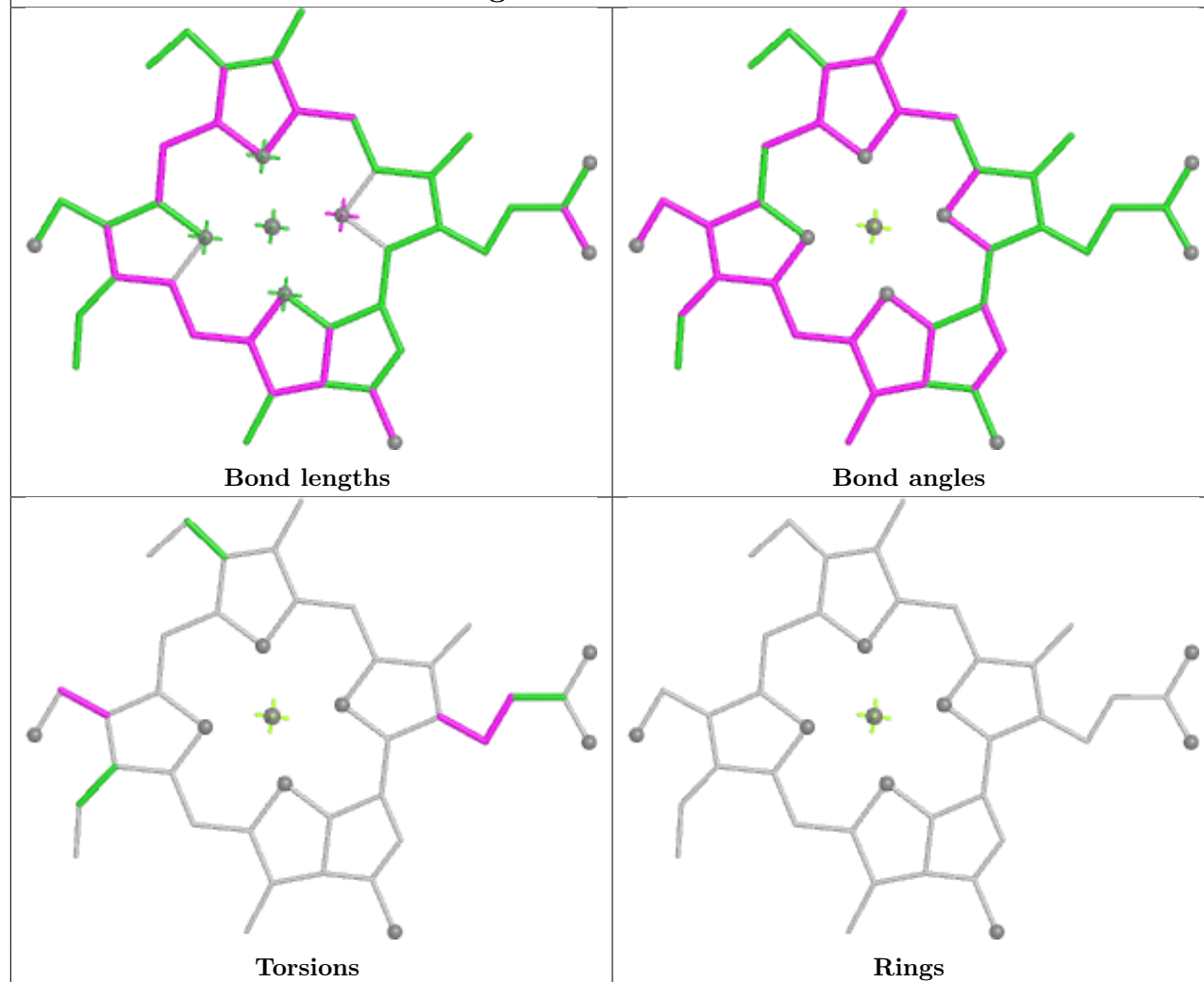
Ligand LHG AK 624



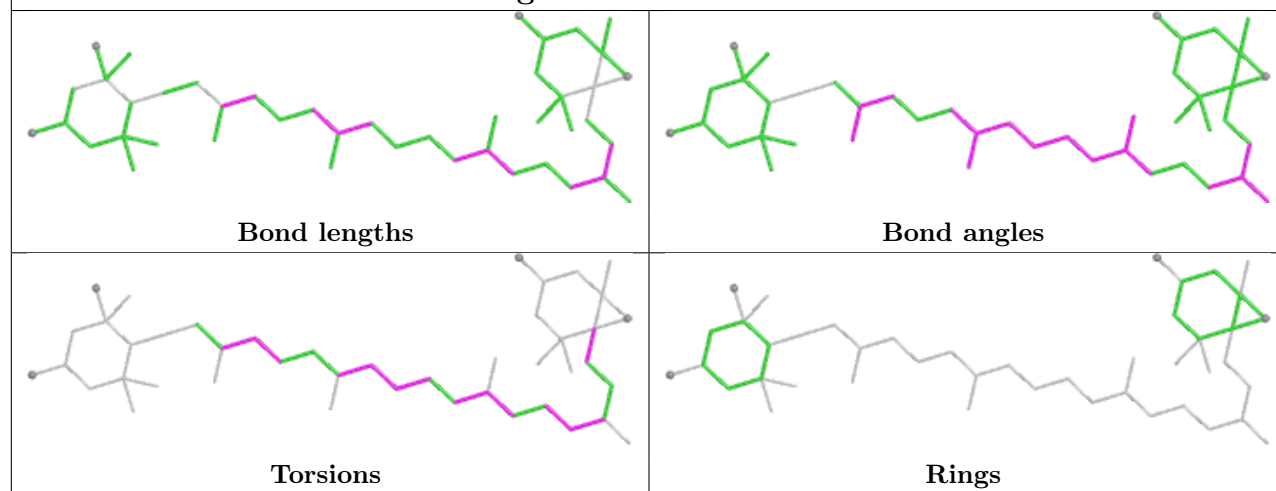
Ligand XAT q 617

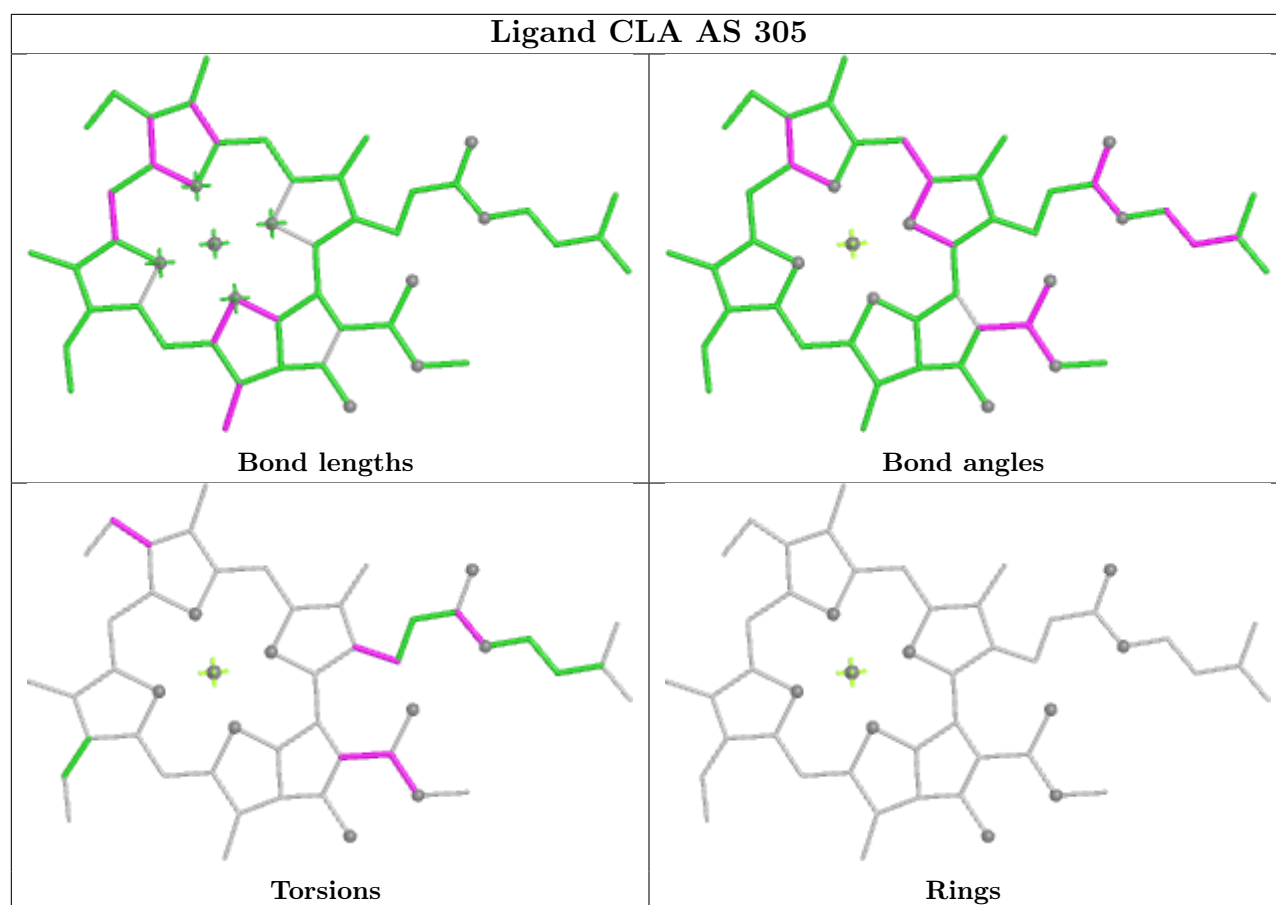


Ligand CHL AB 608

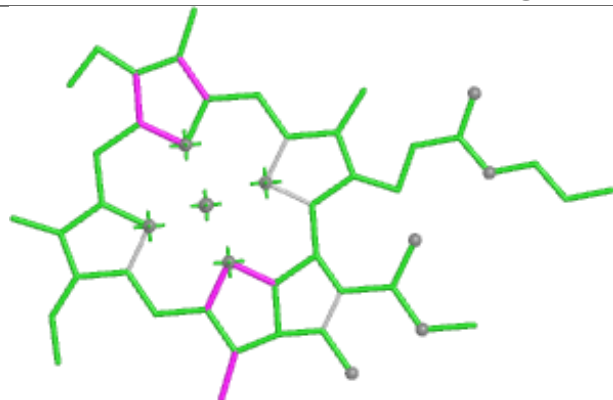


Ligand NEX AC 616

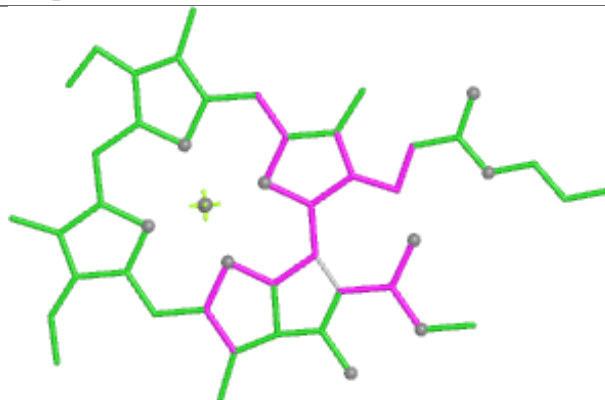




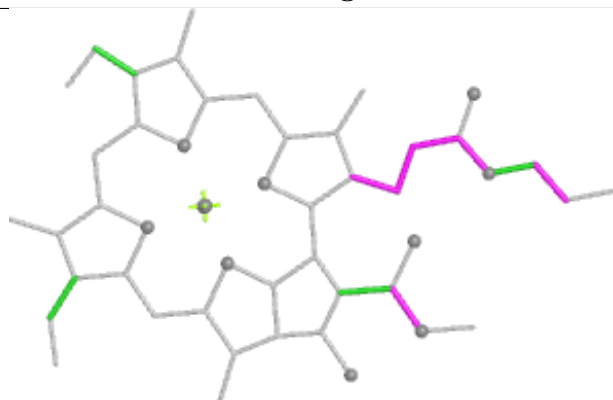
Ligand CLA p 618



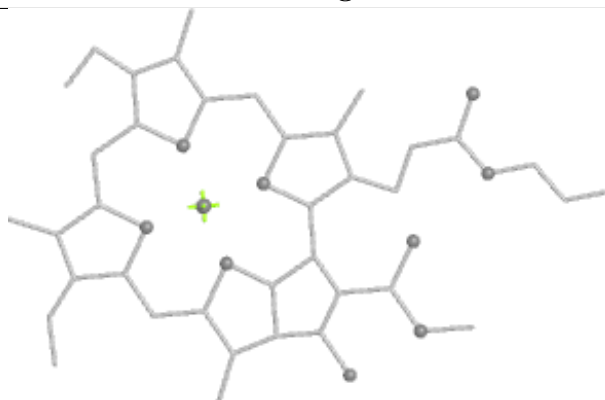
Bond lengths



Bond angles

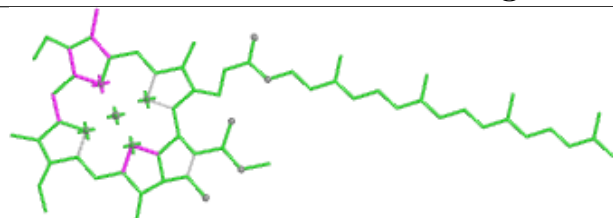


Torsions

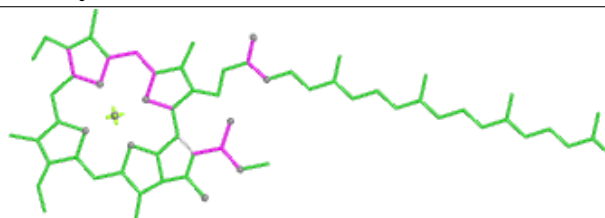


Rings

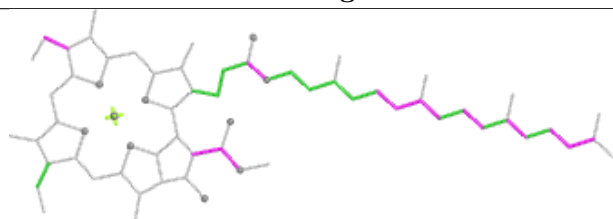
Ligand CLA AQ 603



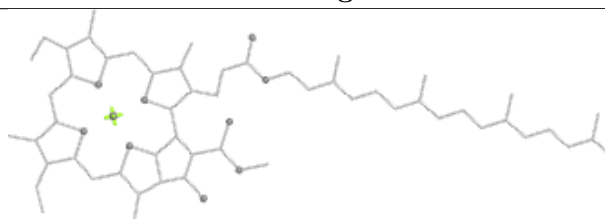
Bond lengths



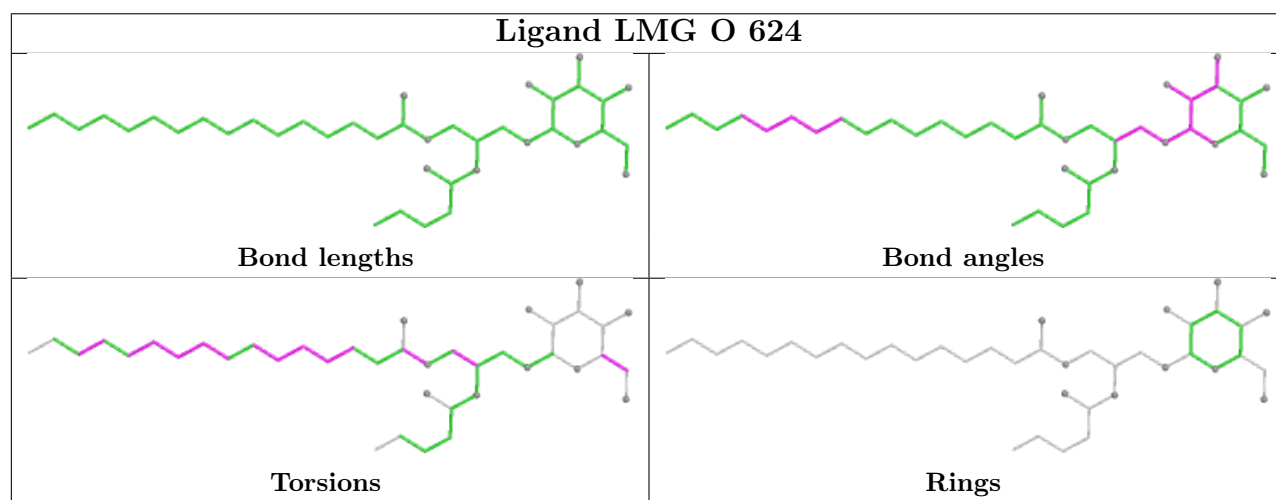
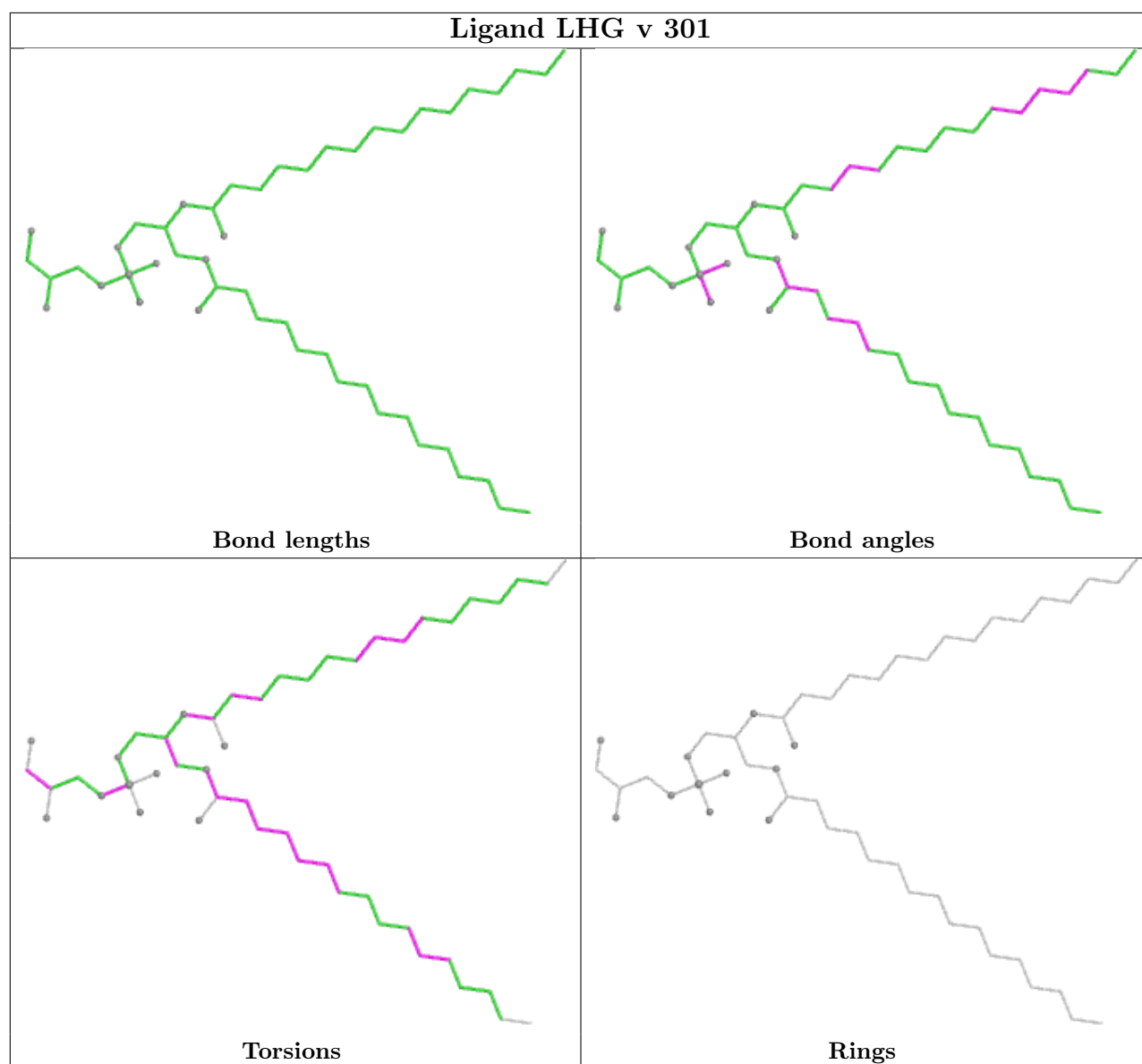
Bond angles

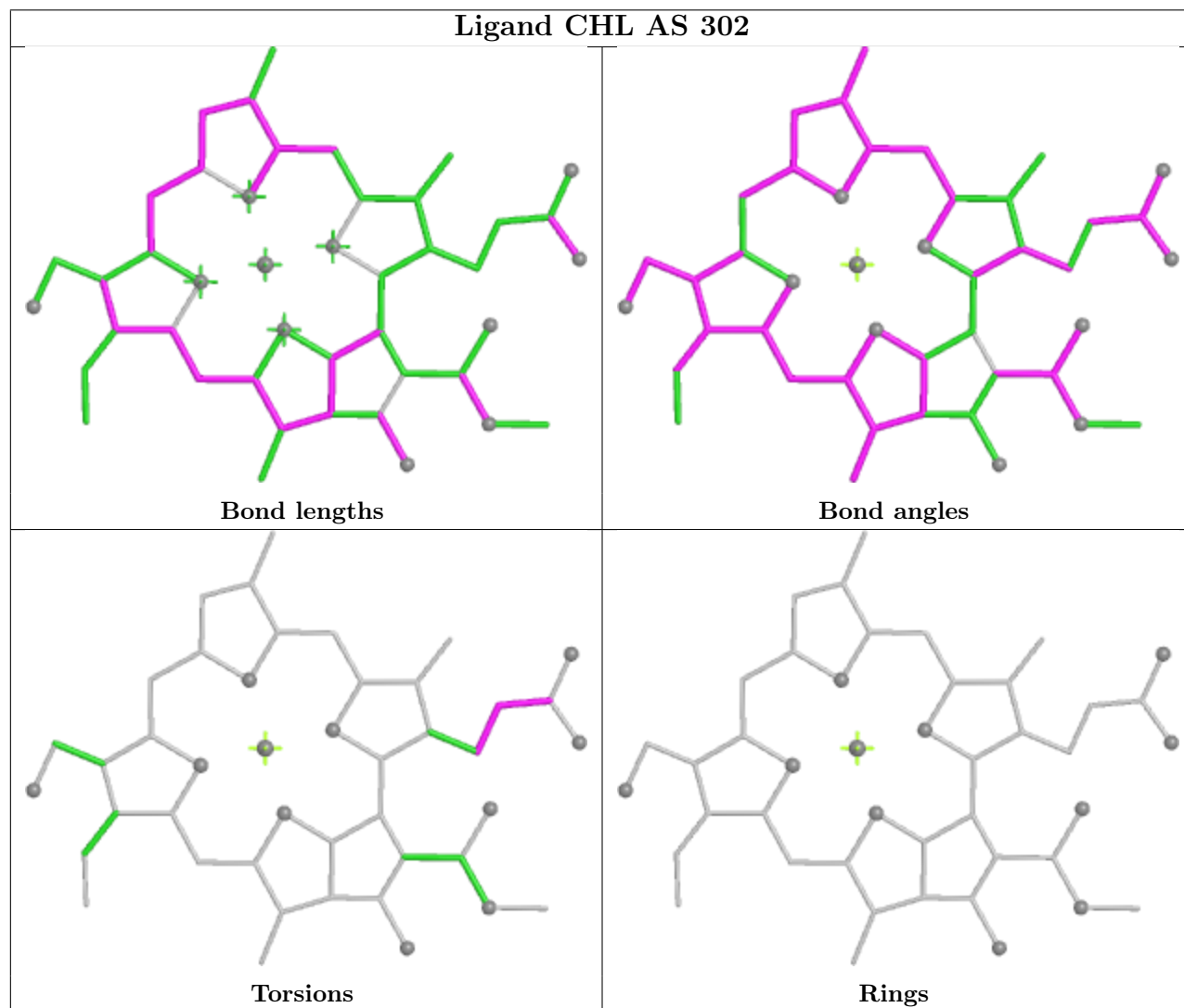
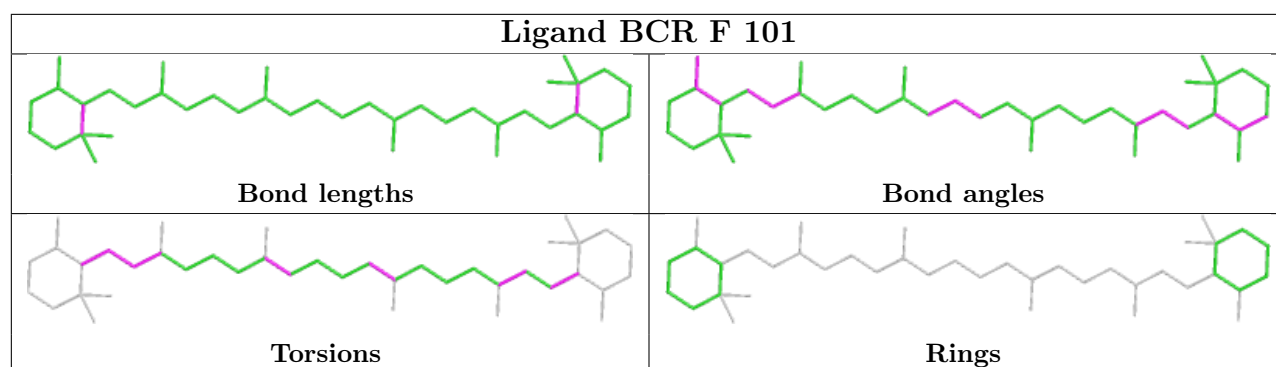


Torsions

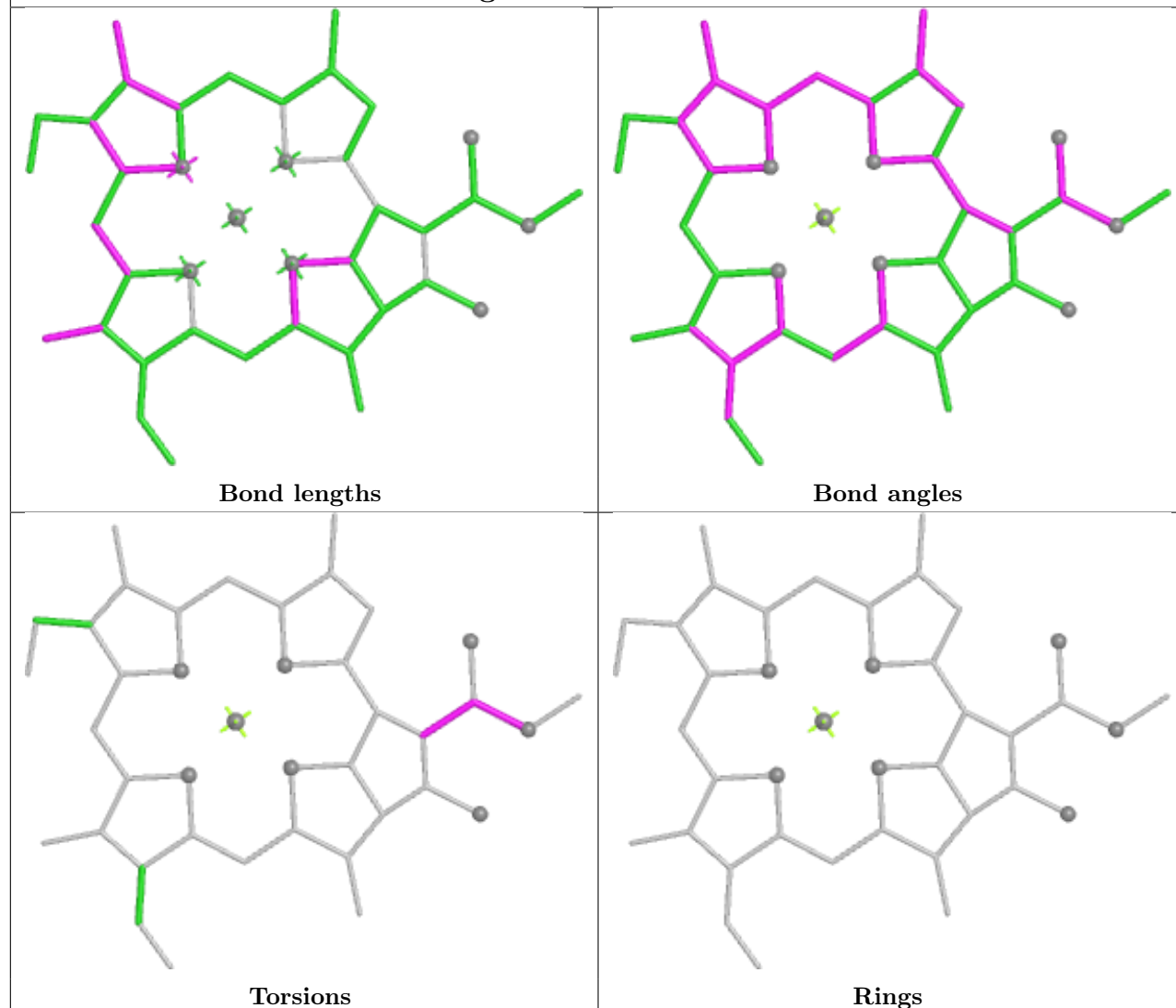


Rings

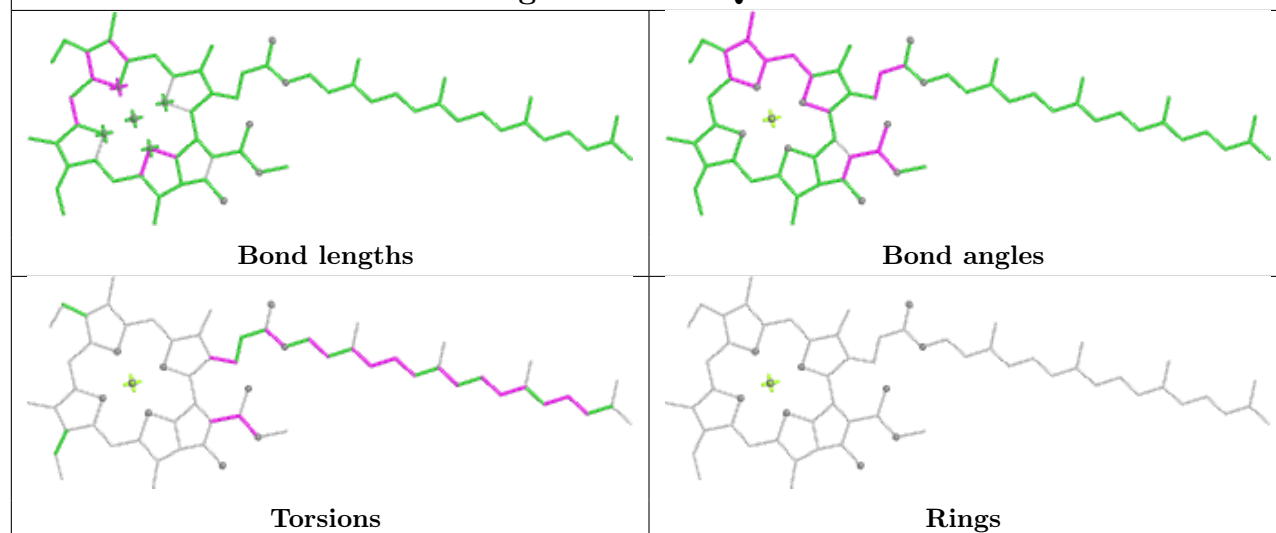




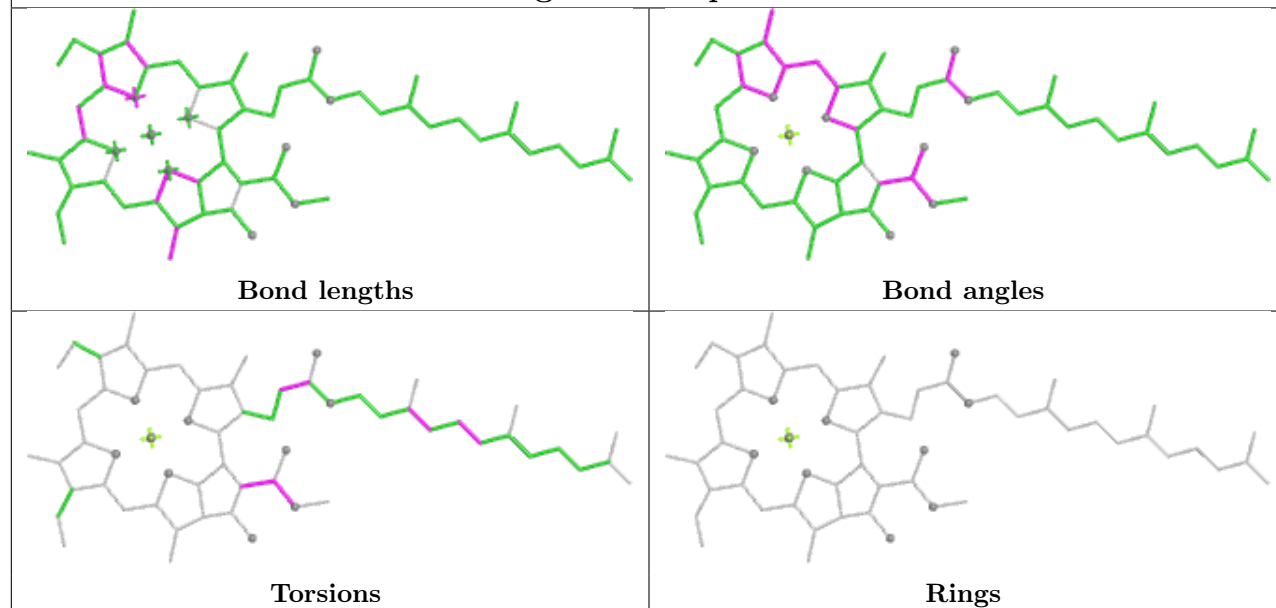
Ligand CLA AF 609



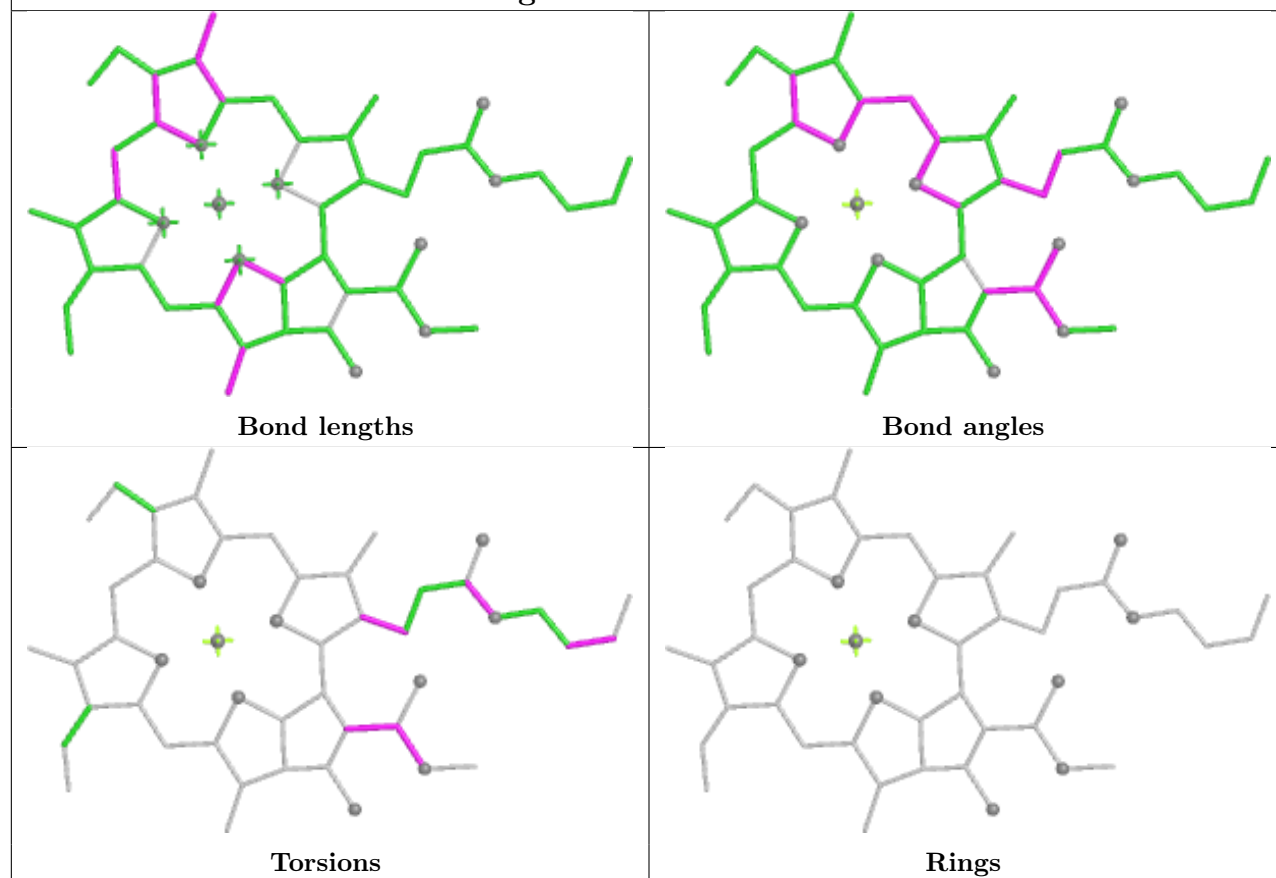
Ligand CLA AQ 610

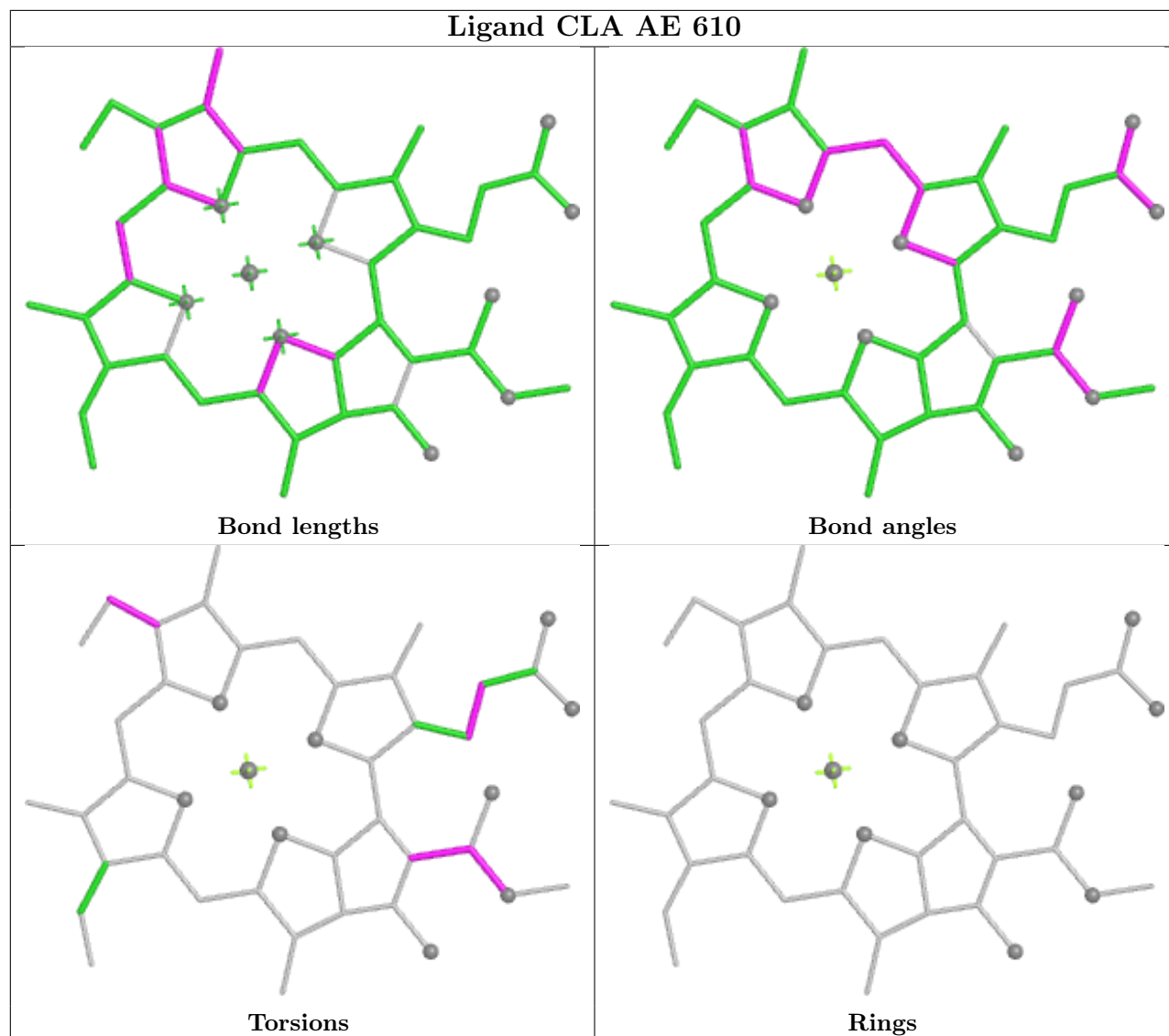
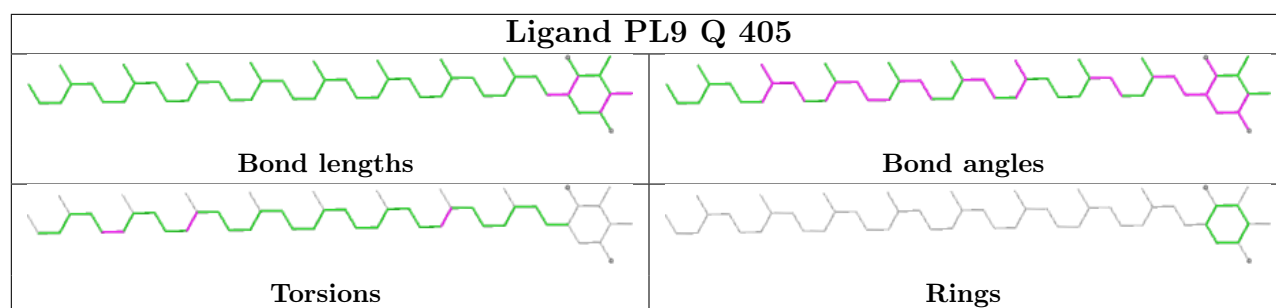


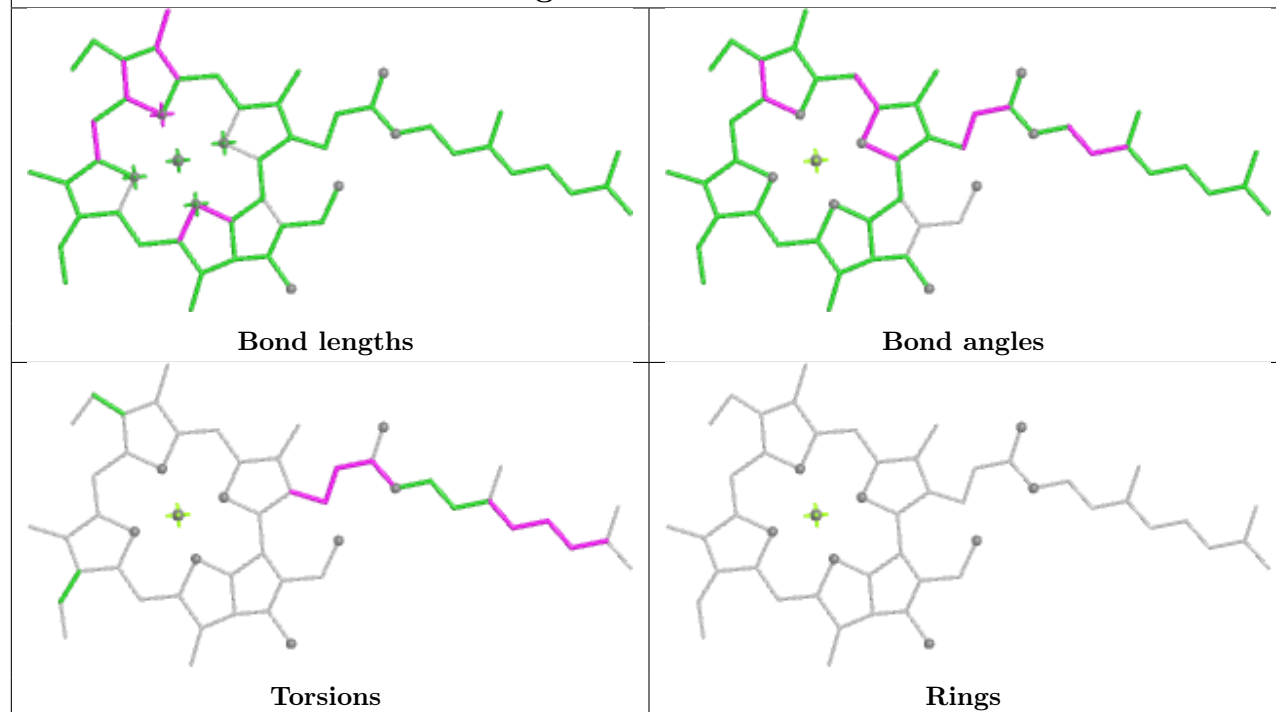
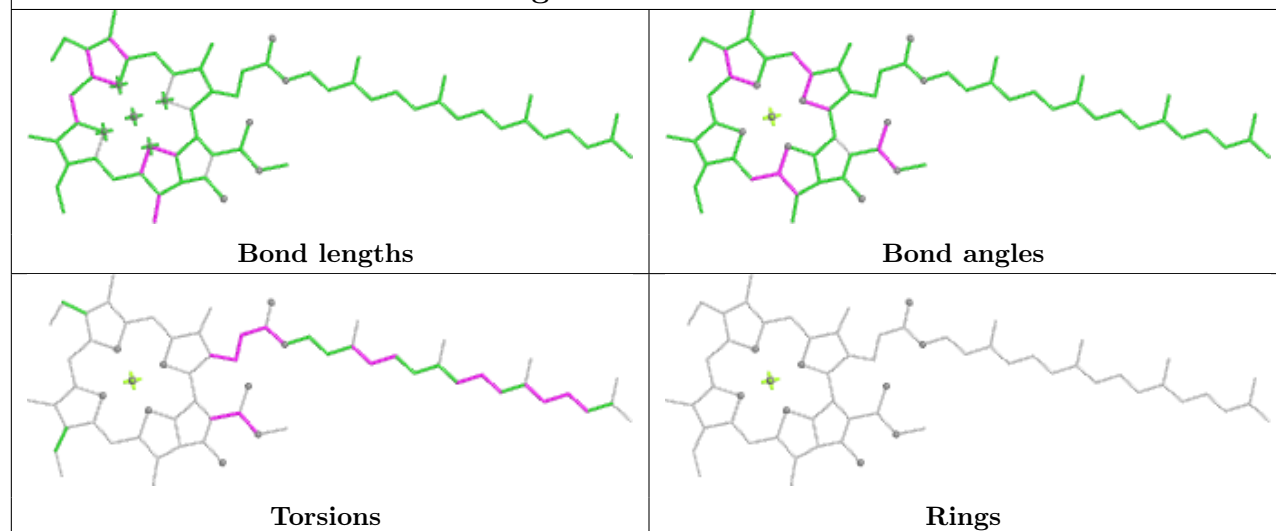
Ligand CLA p 612



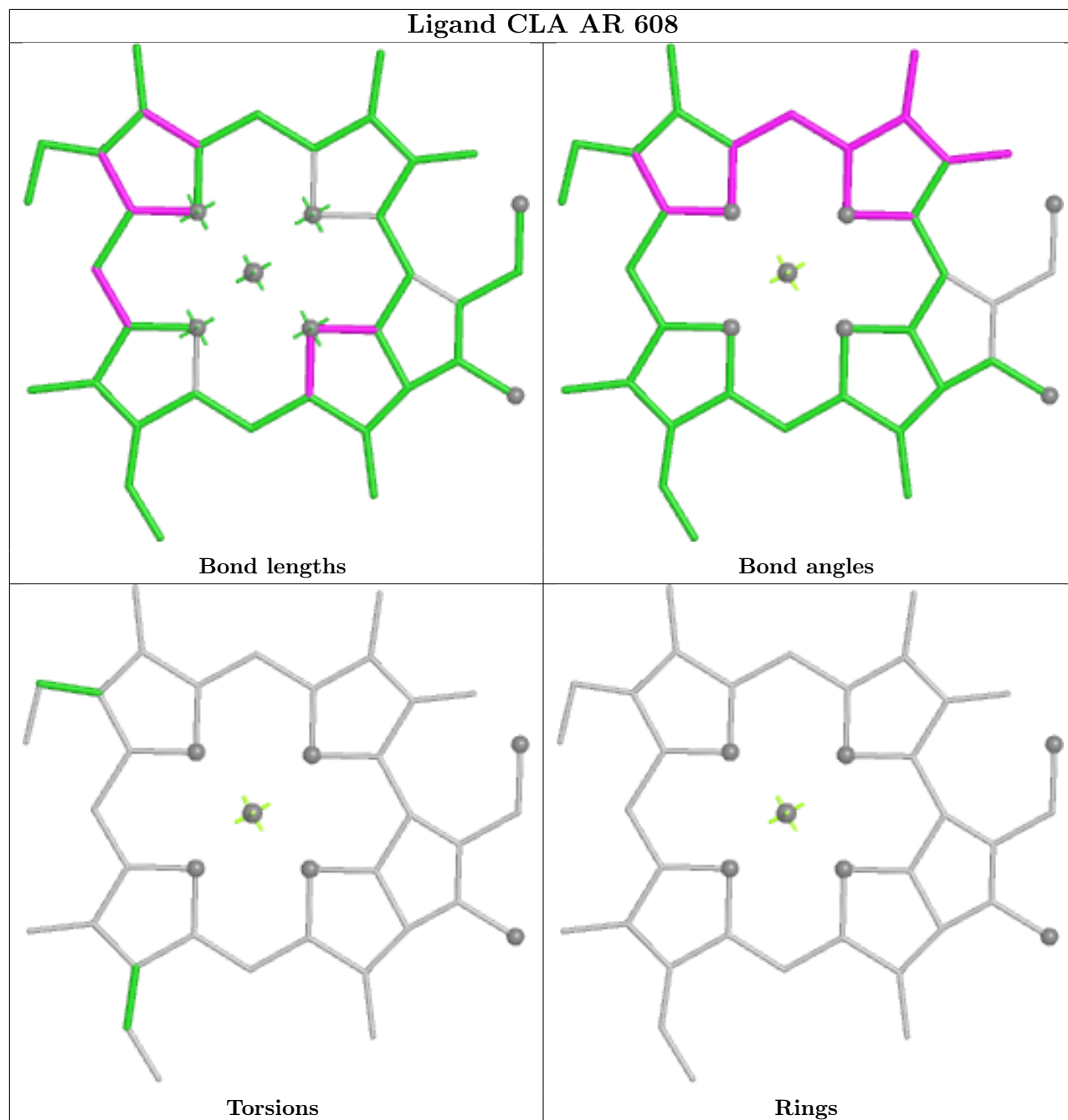
Ligand CLA AR 601



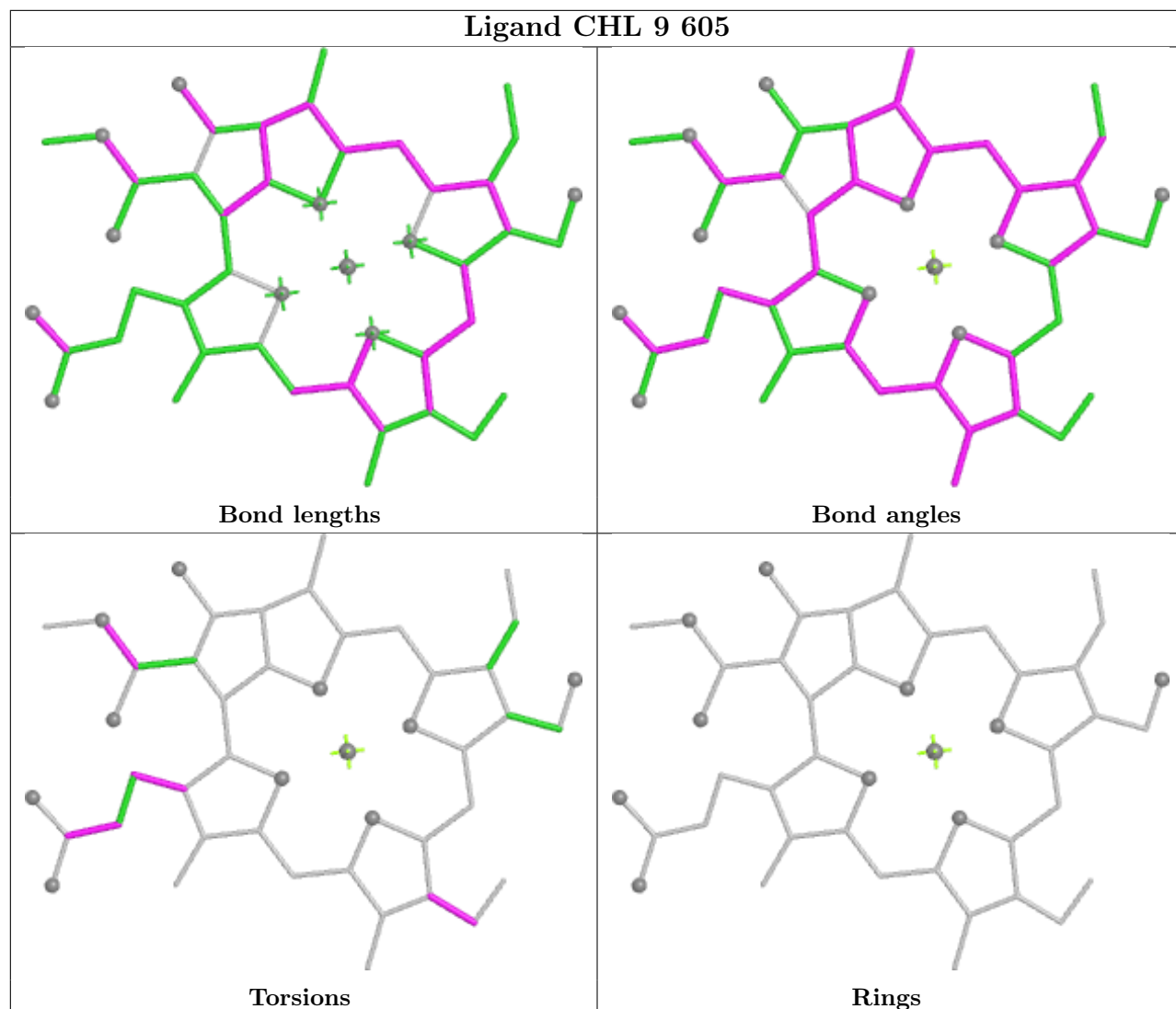


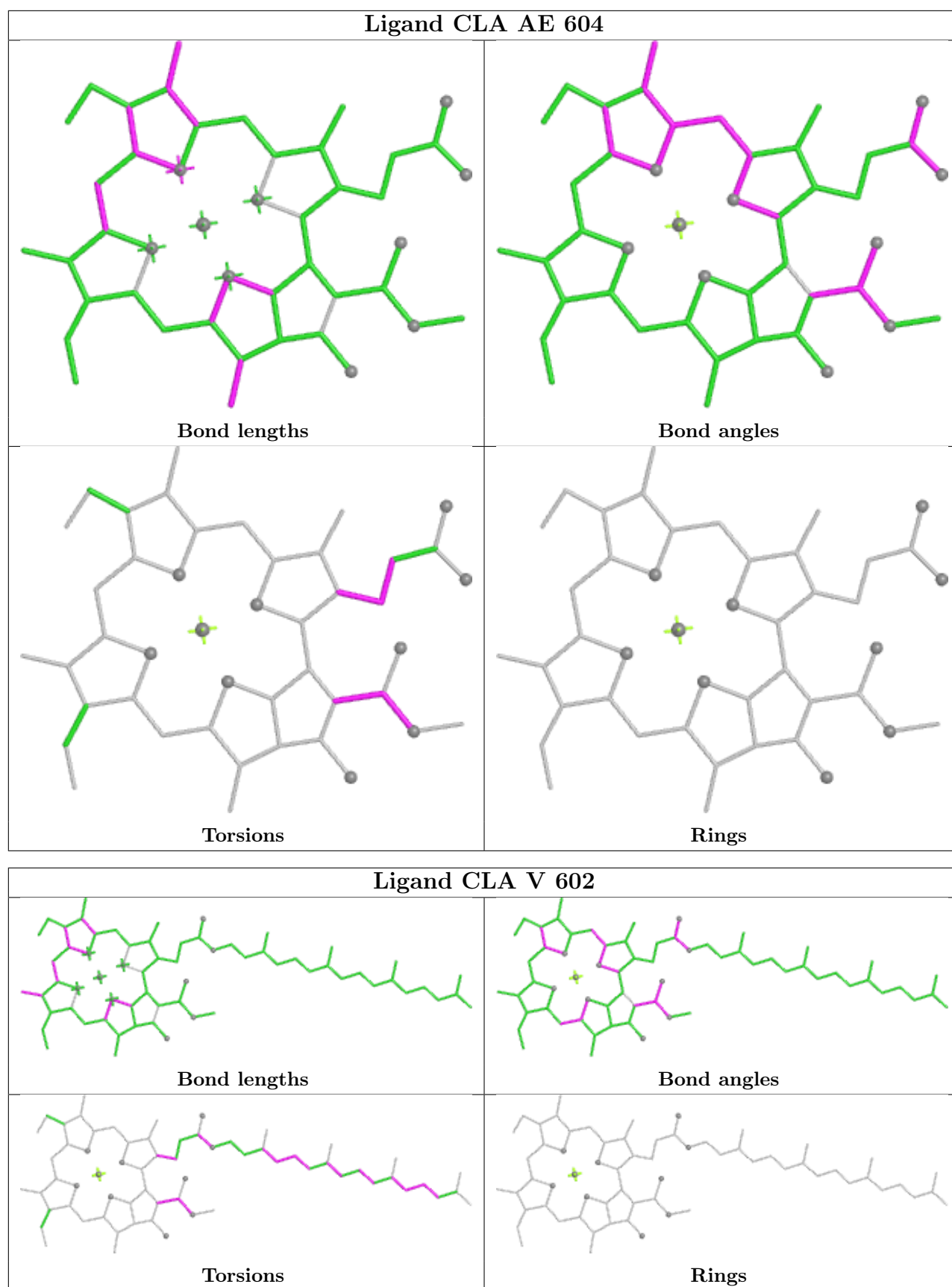
Ligand CLA v 313**Ligand CLA O 605**

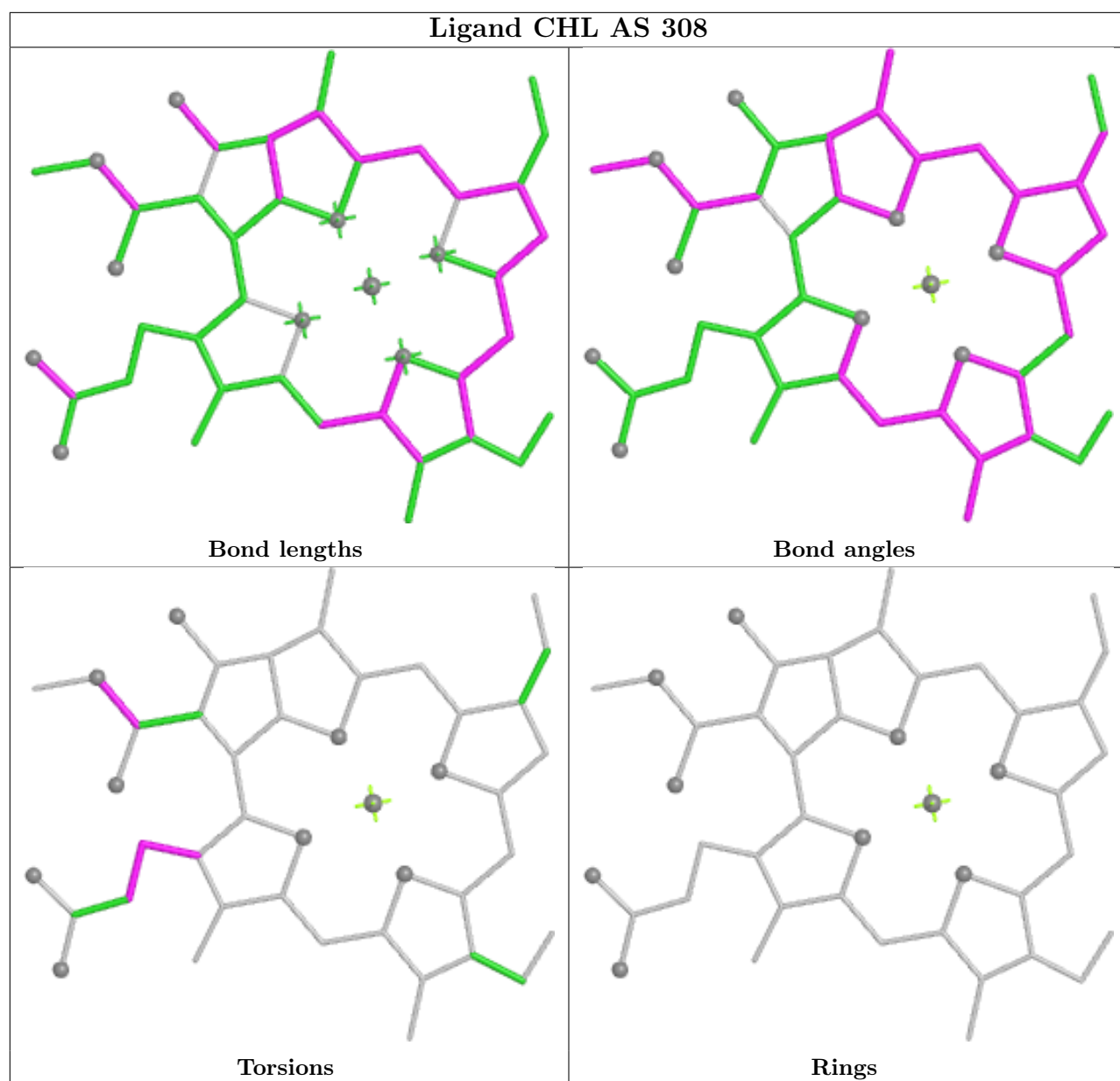
Ligand CLA AR 608



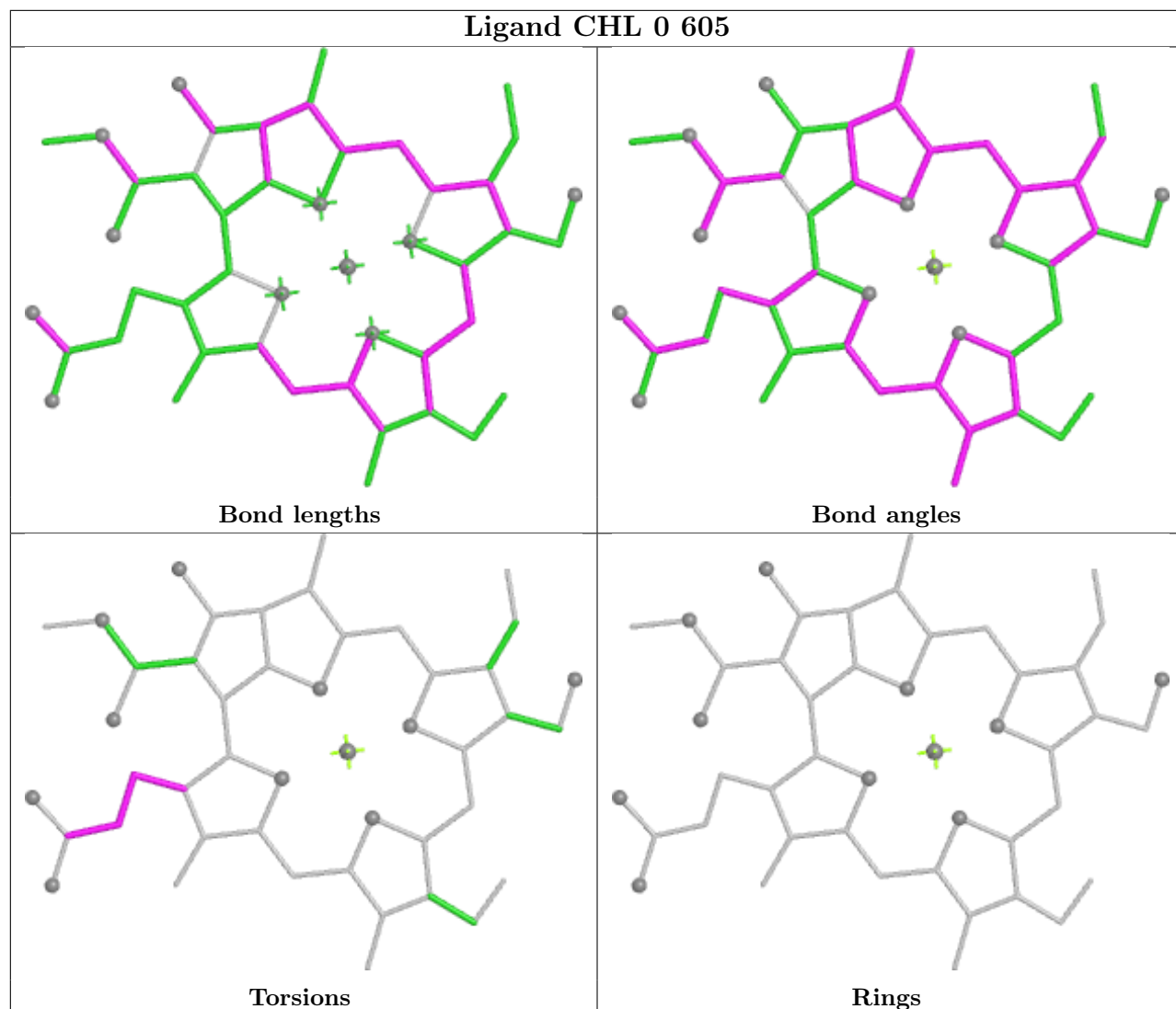
Ligand CHL 9 605



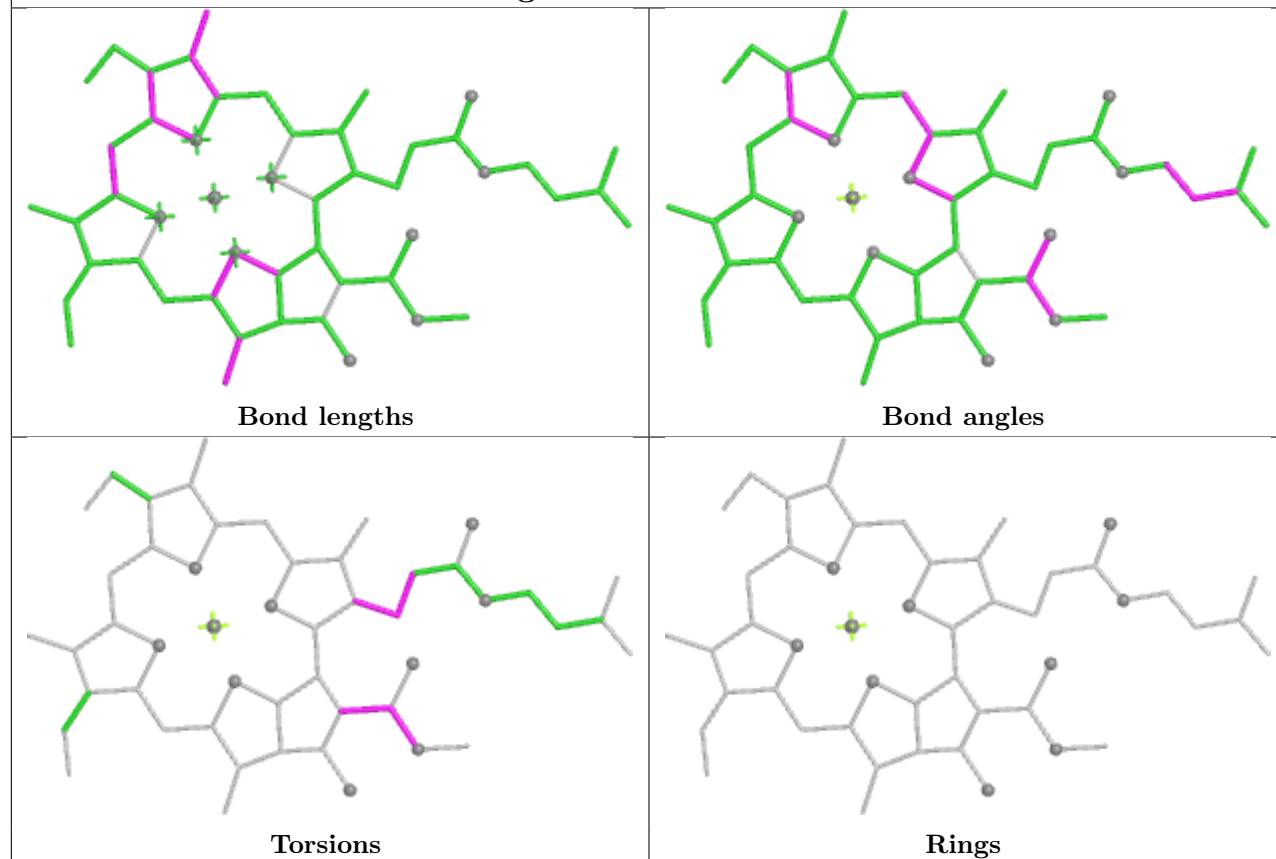




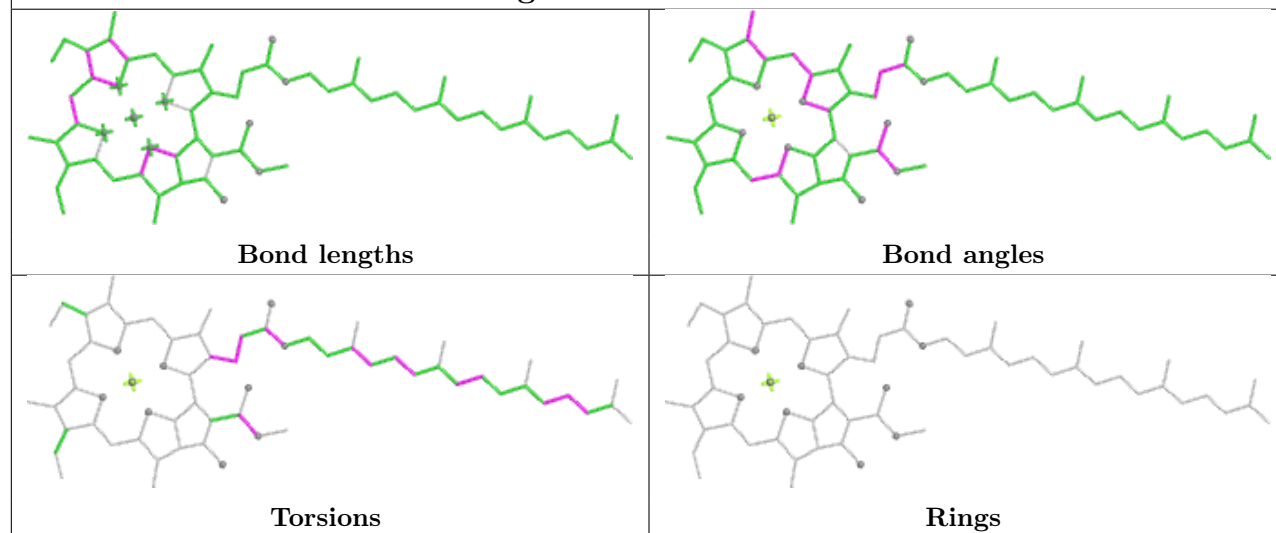
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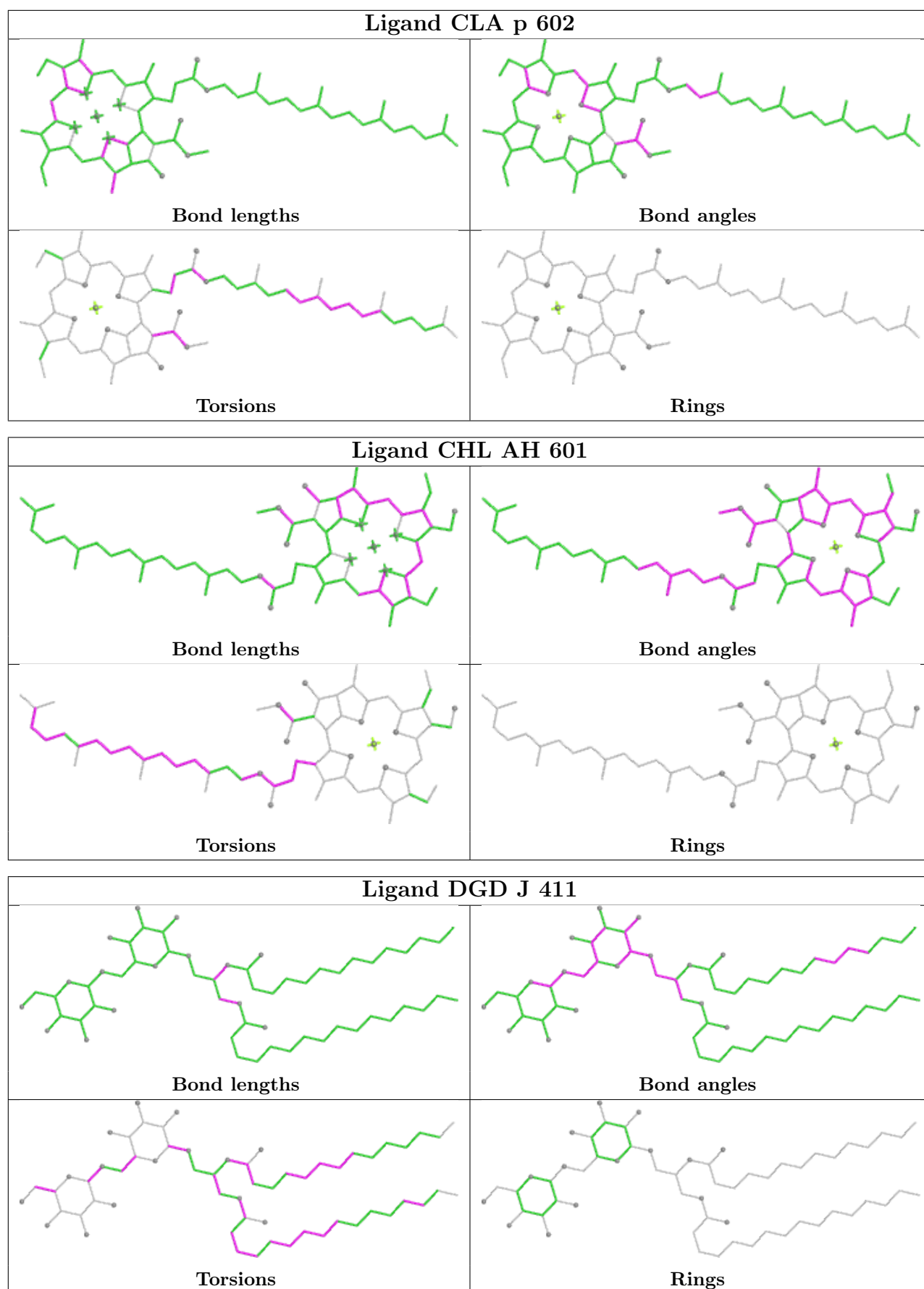


Ligand CLA AH 604

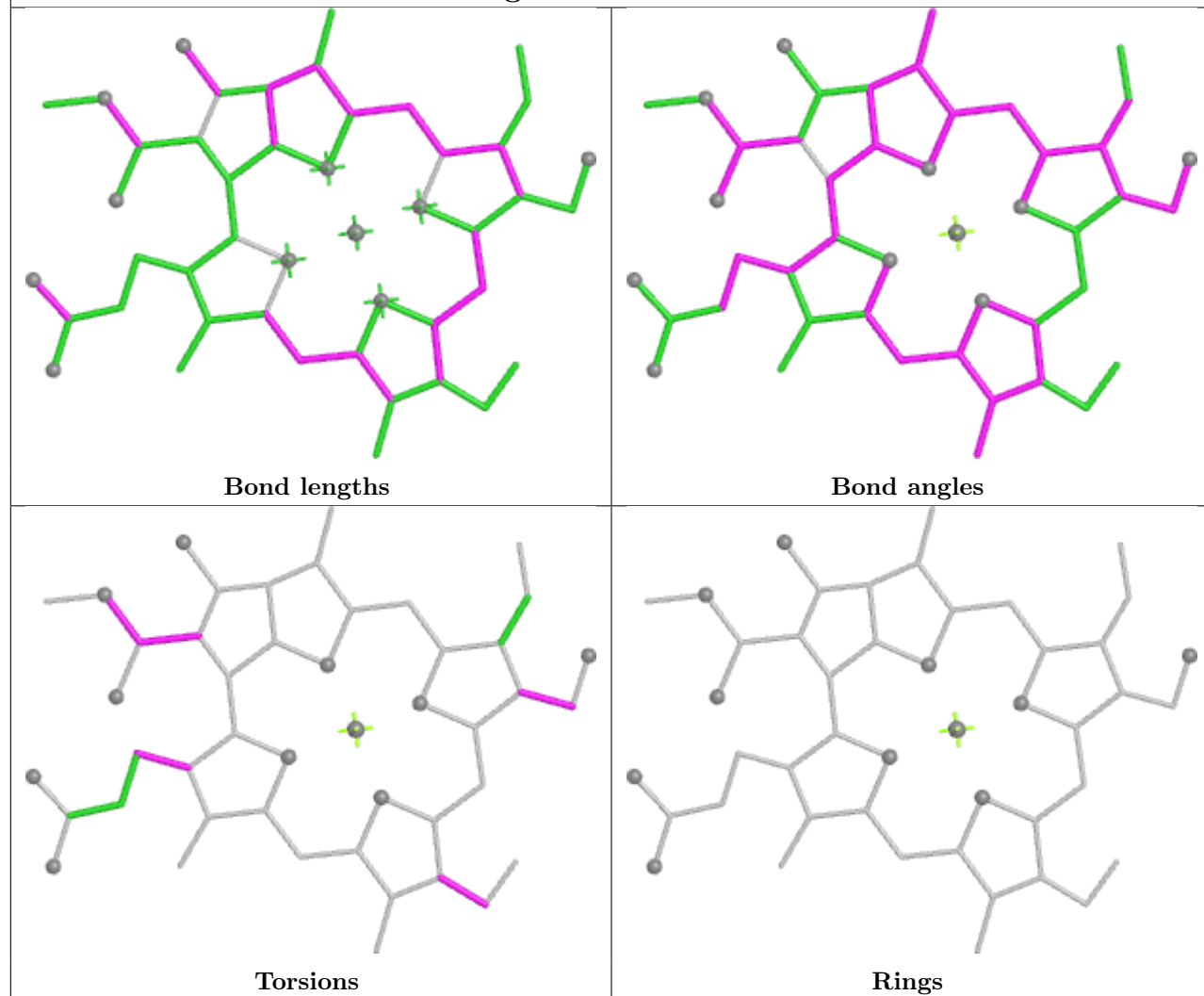


Ligand CLA AK 610

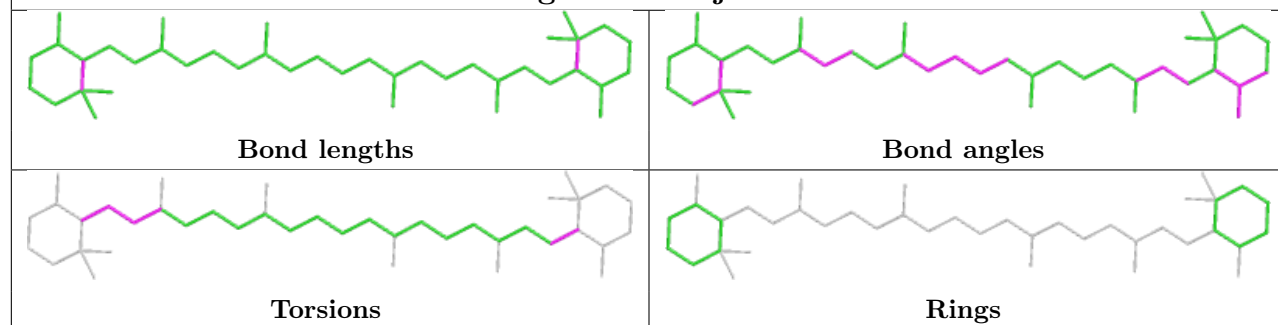


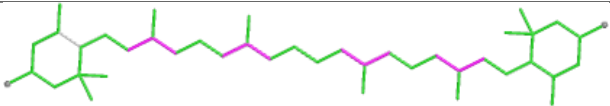
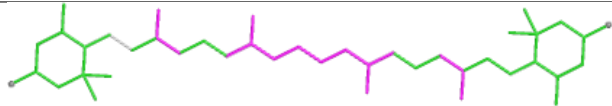
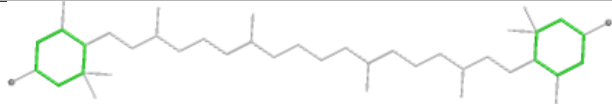


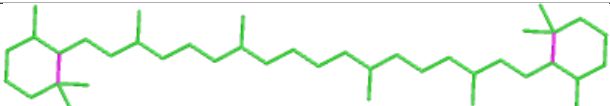
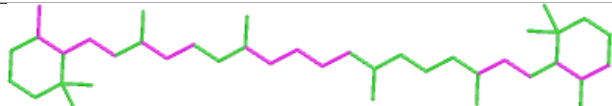
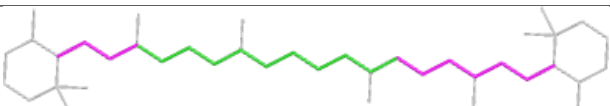
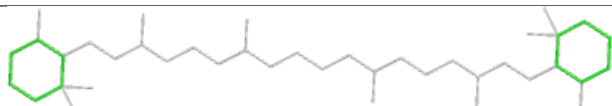
Ligand CHL 9 606

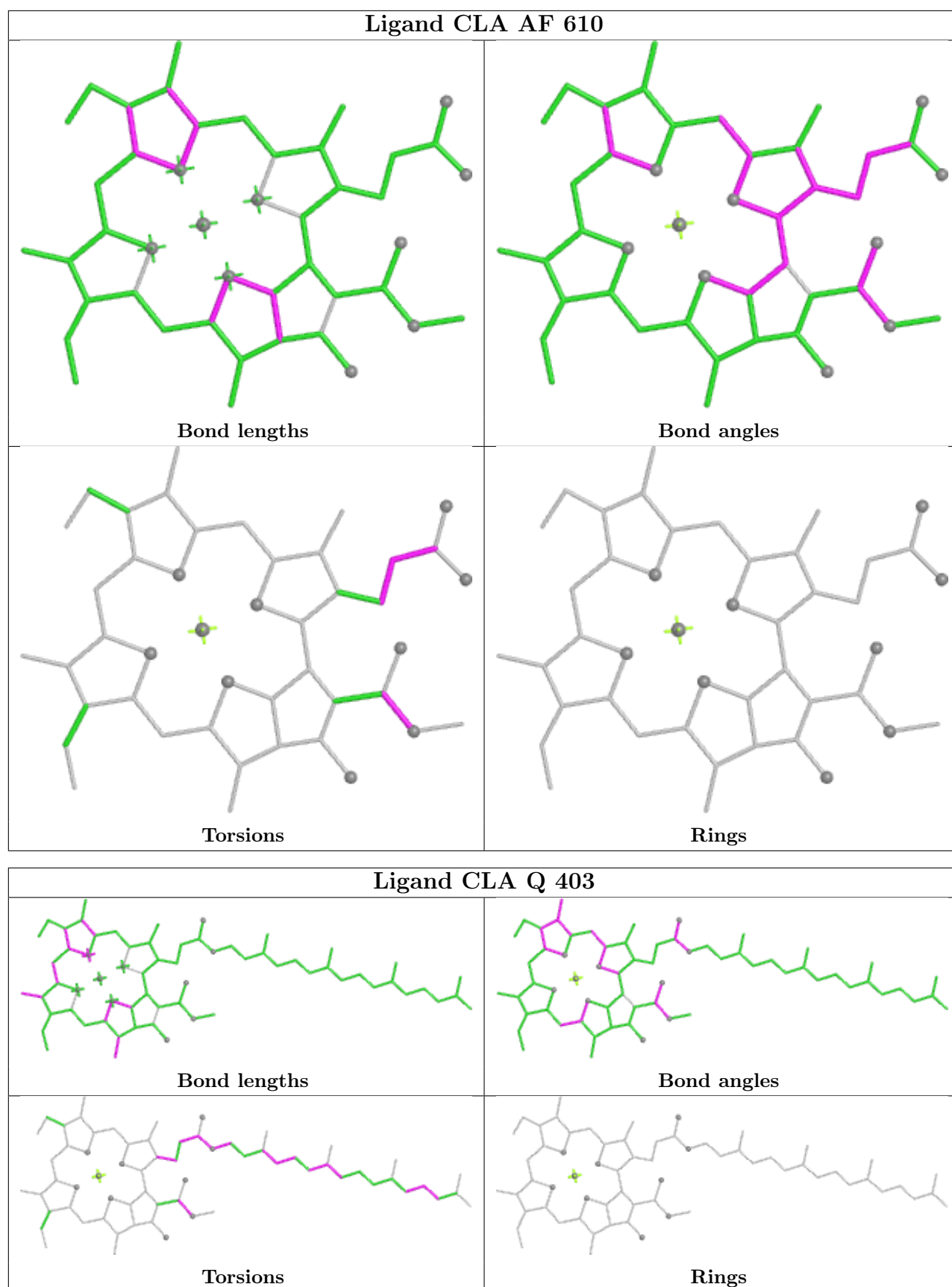


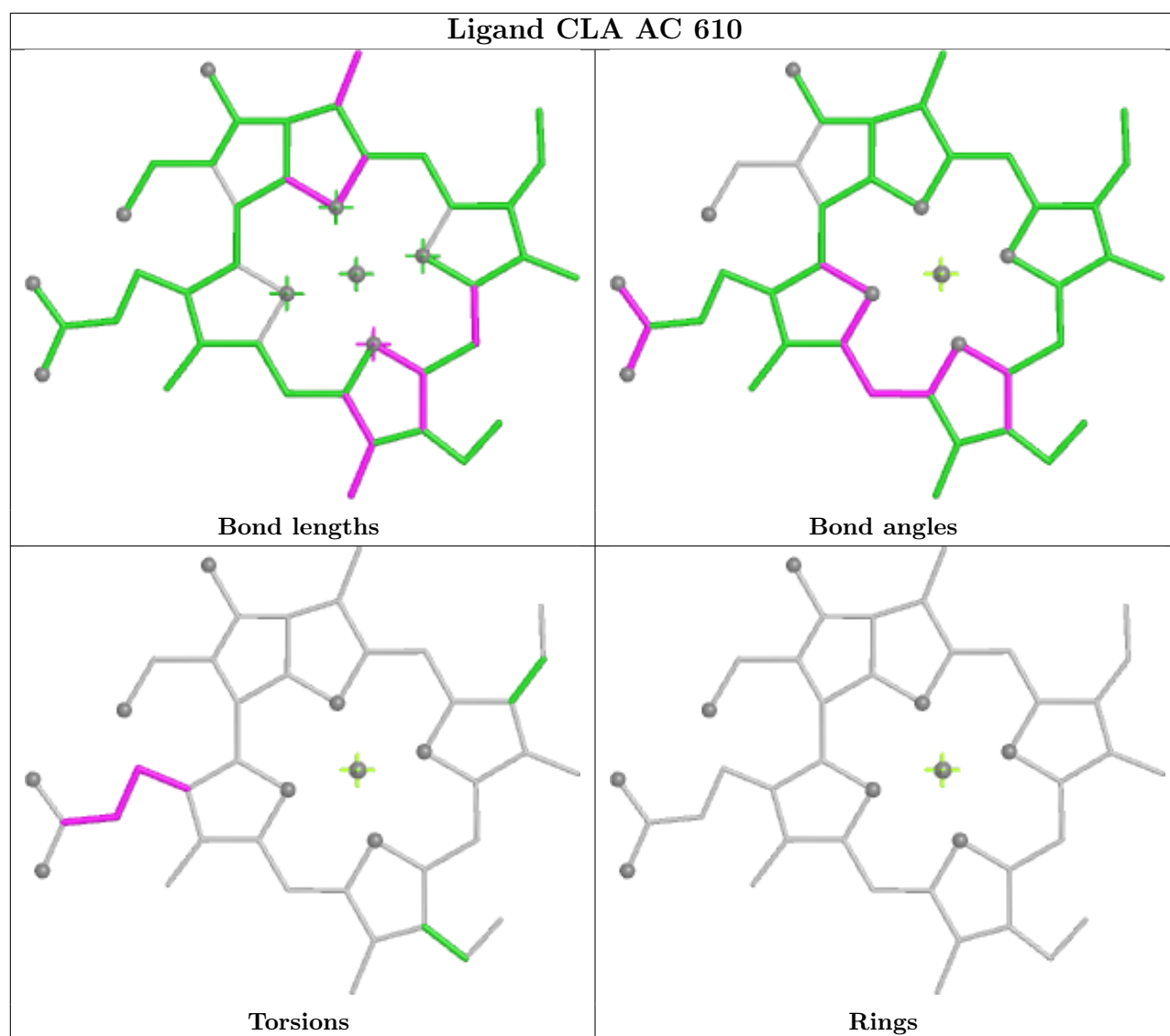
Ligand BCR j 101



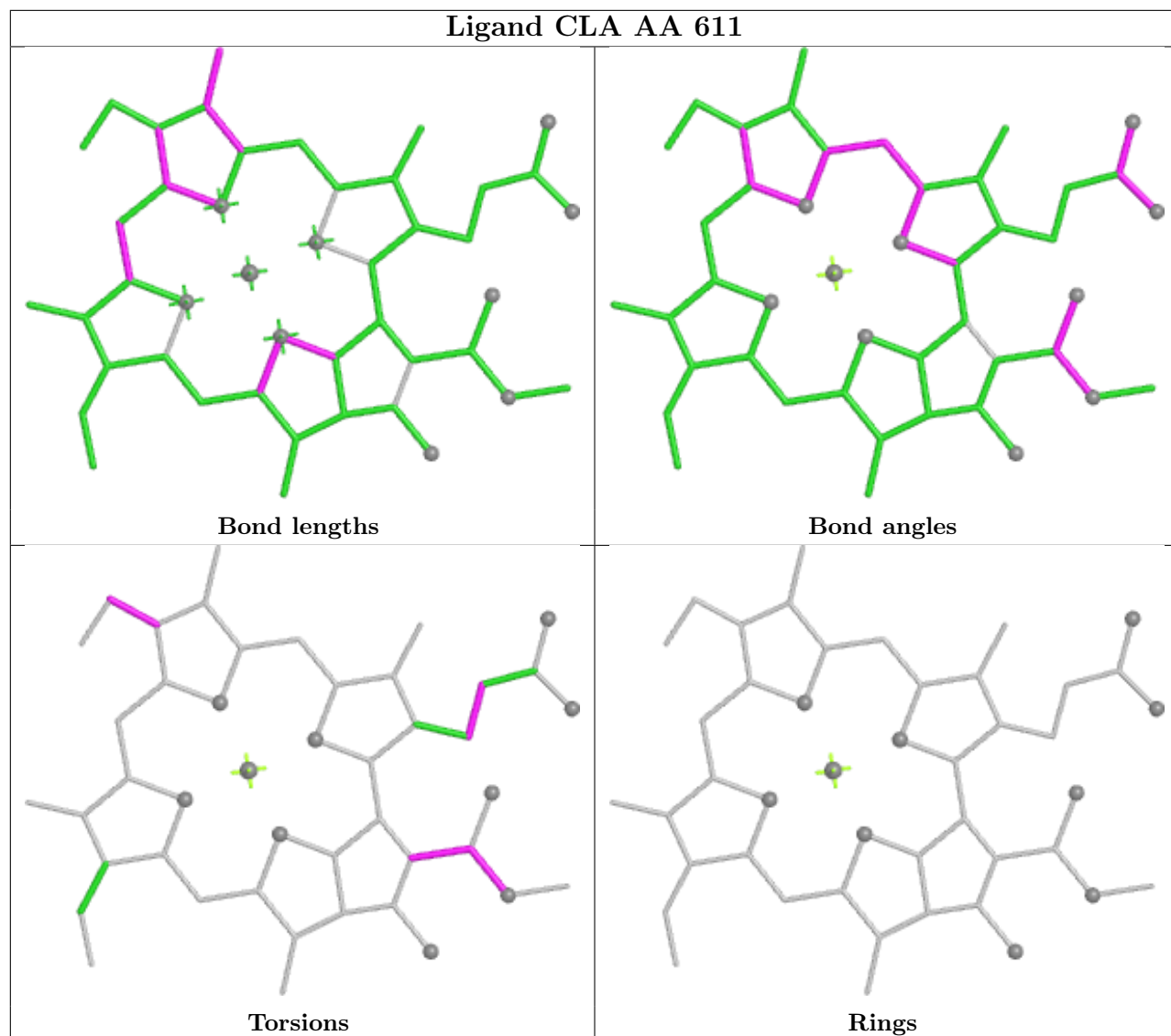
Ligand LUT AD 315			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR AB 612			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

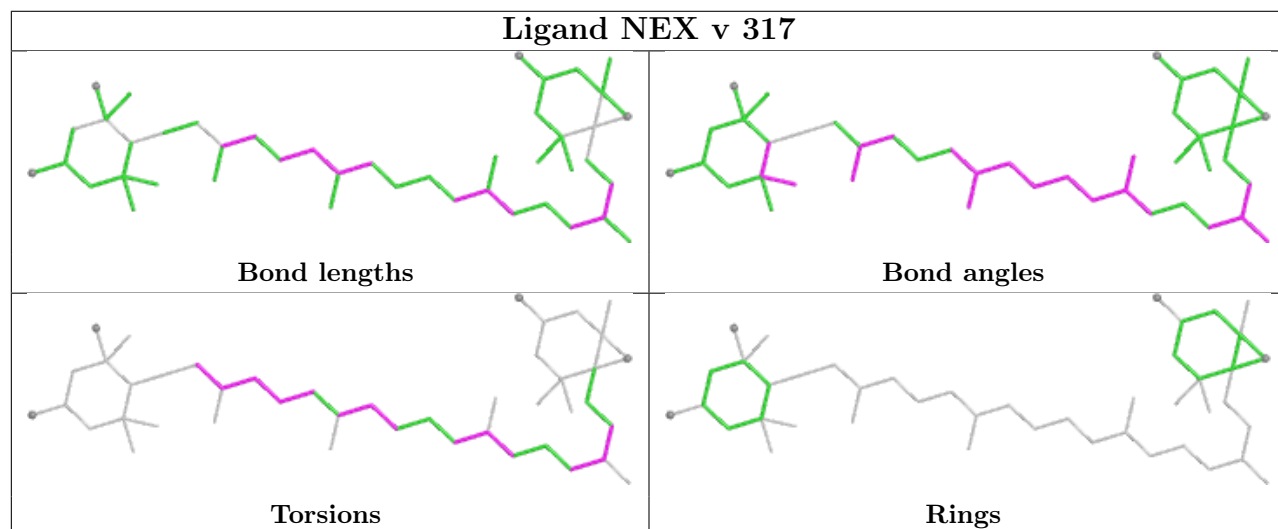




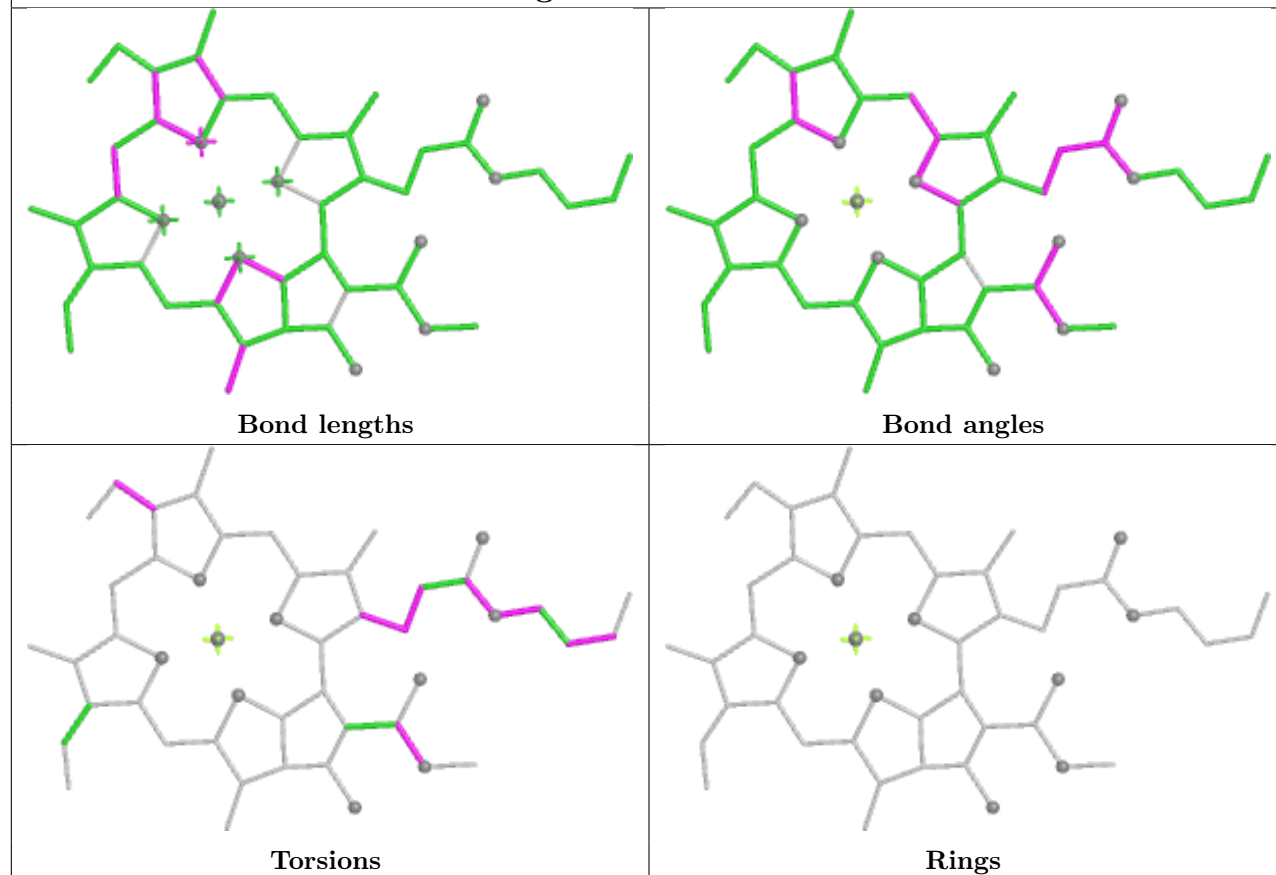
Ligand CLA AA 611



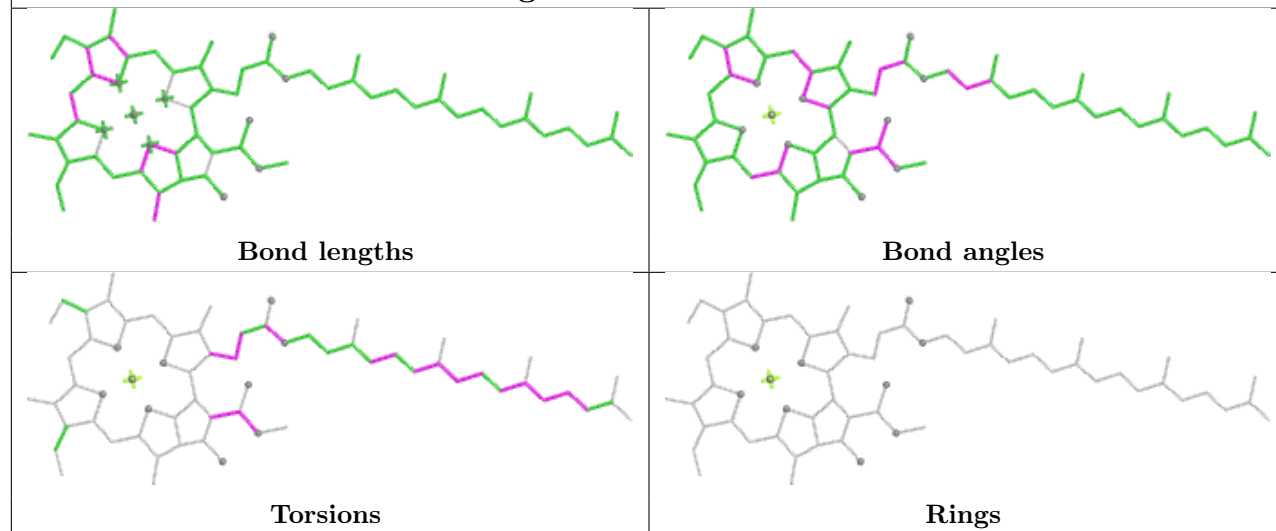
Ligand NEX v 317

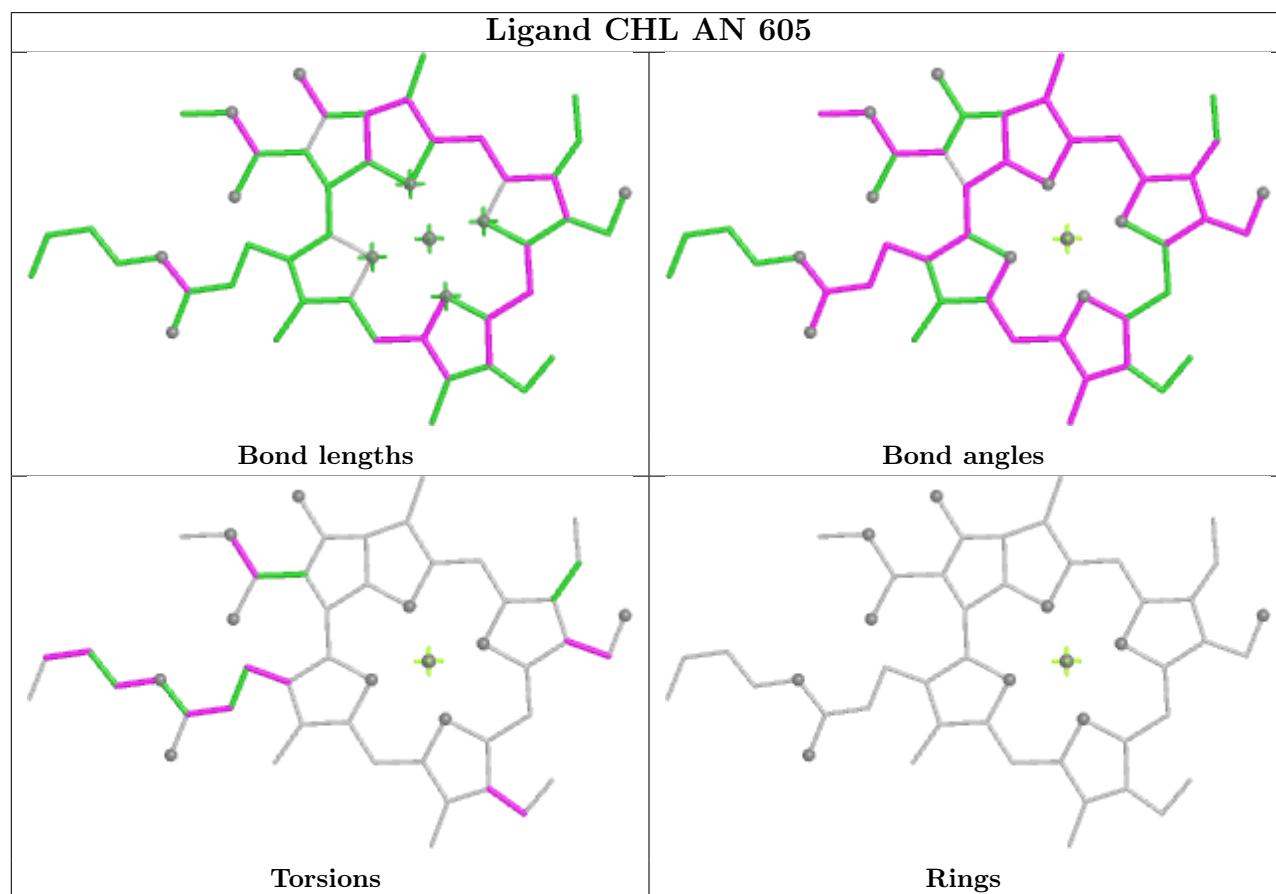
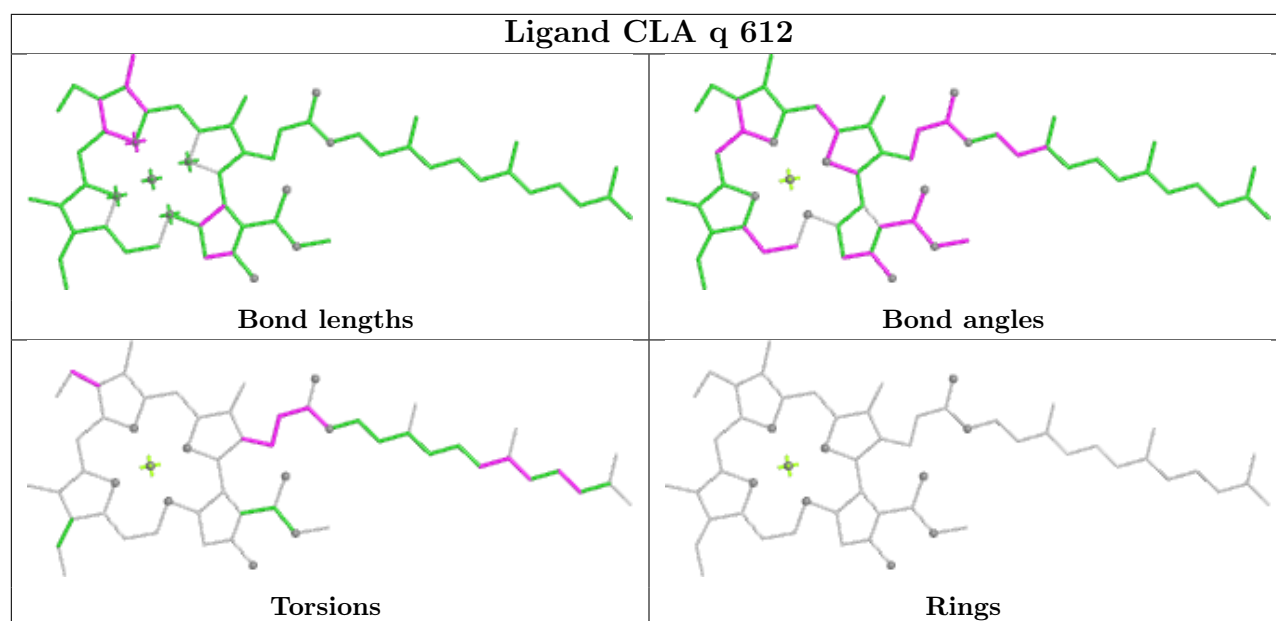


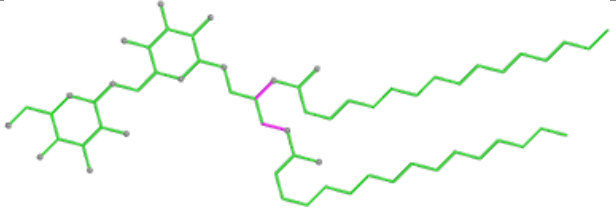
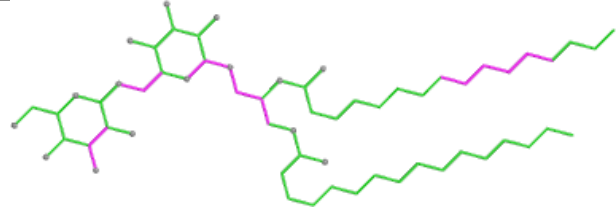
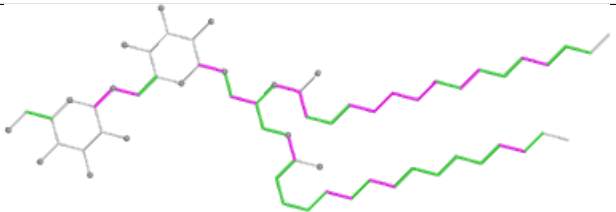
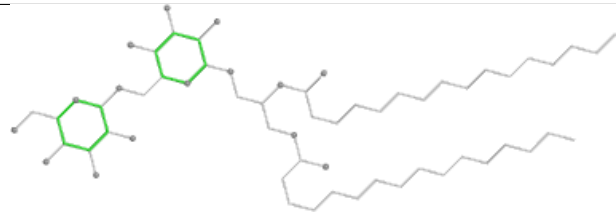
Ligand CLA v 314

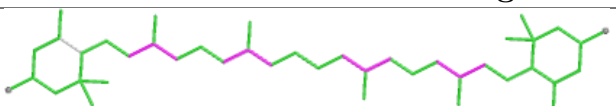
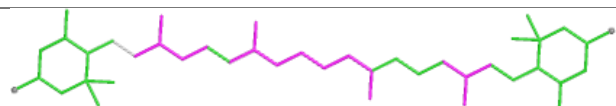
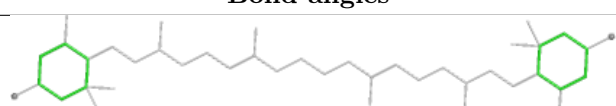


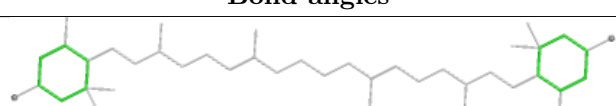
Ligand CLA AU 602

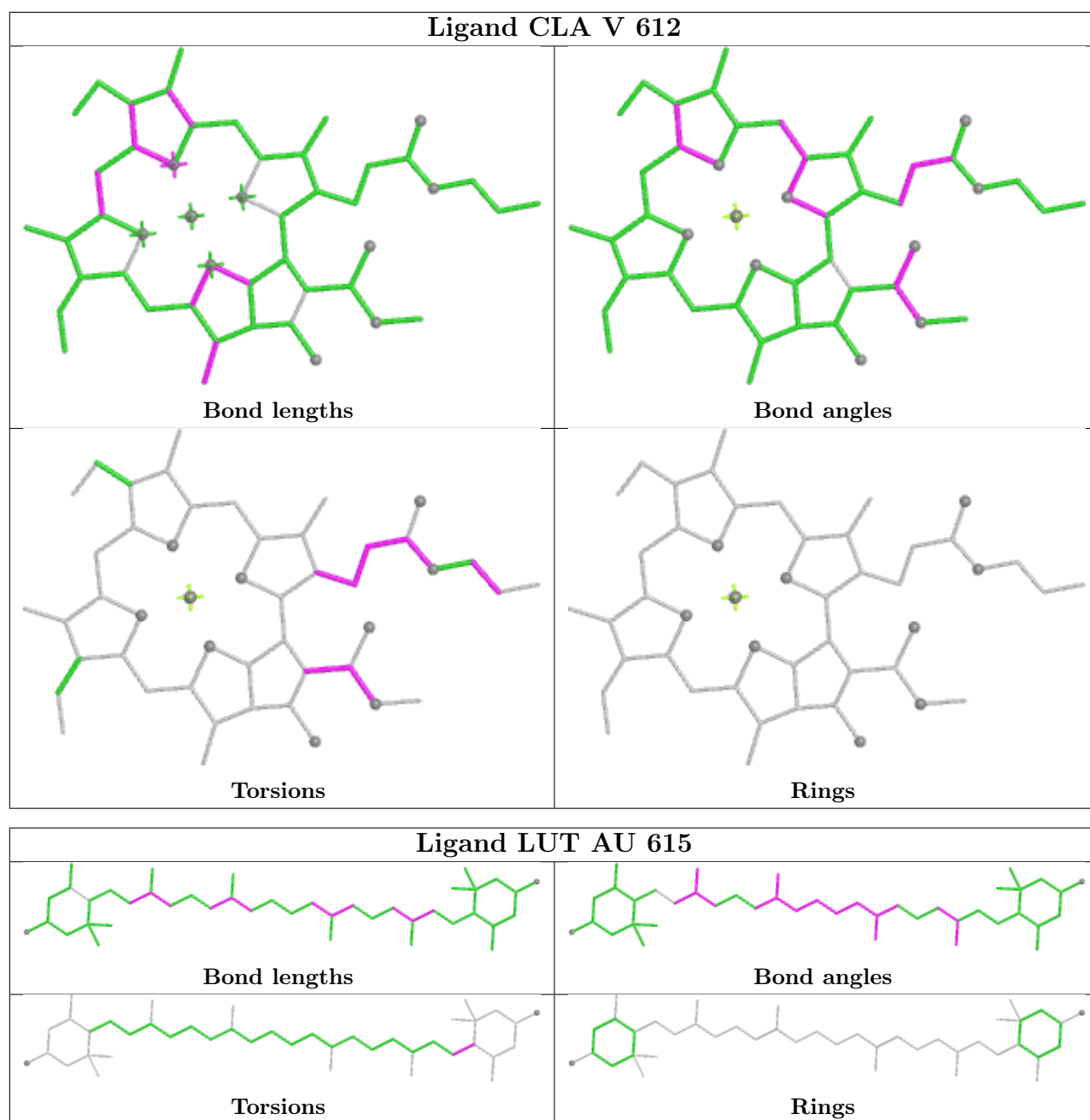


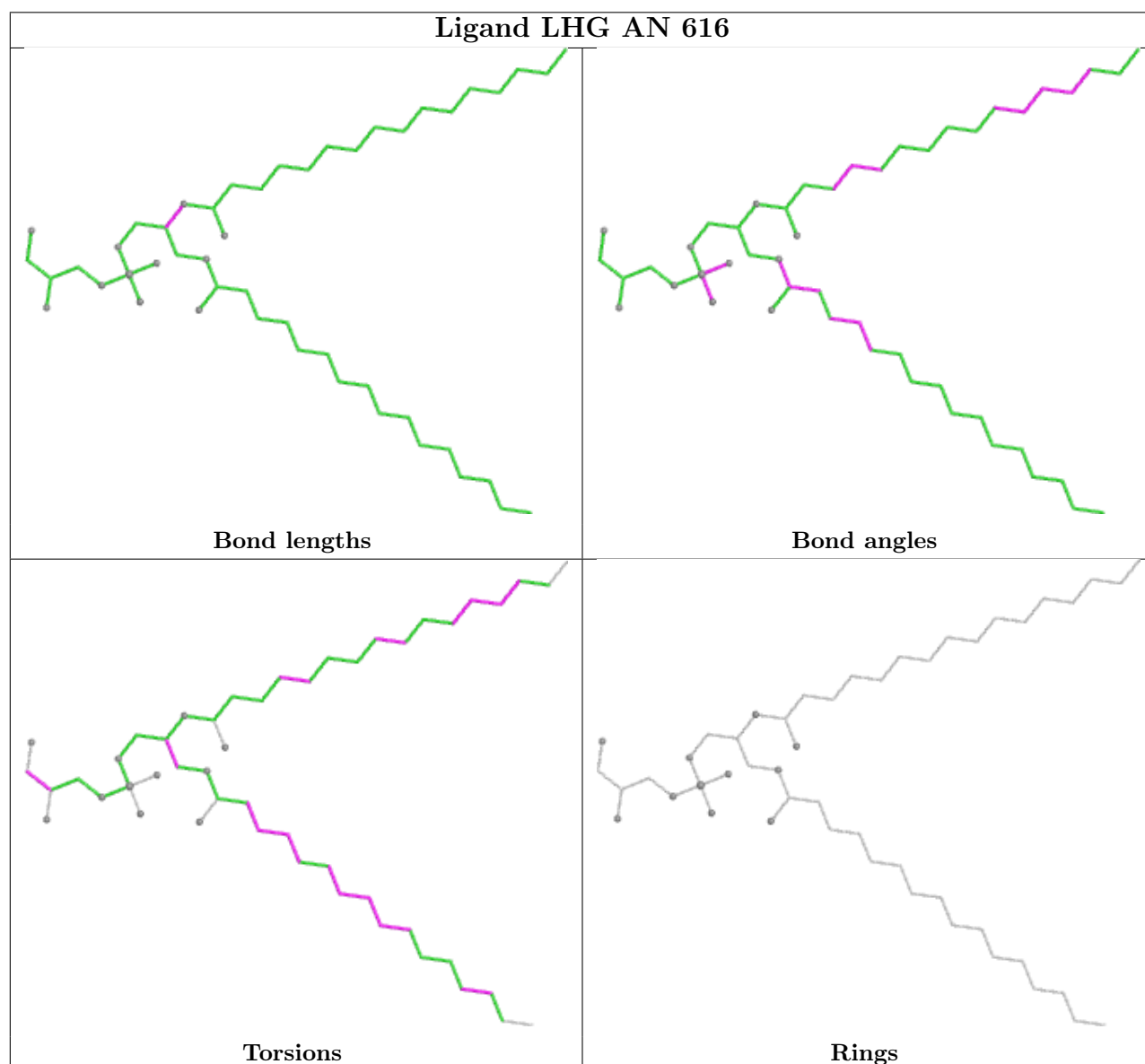
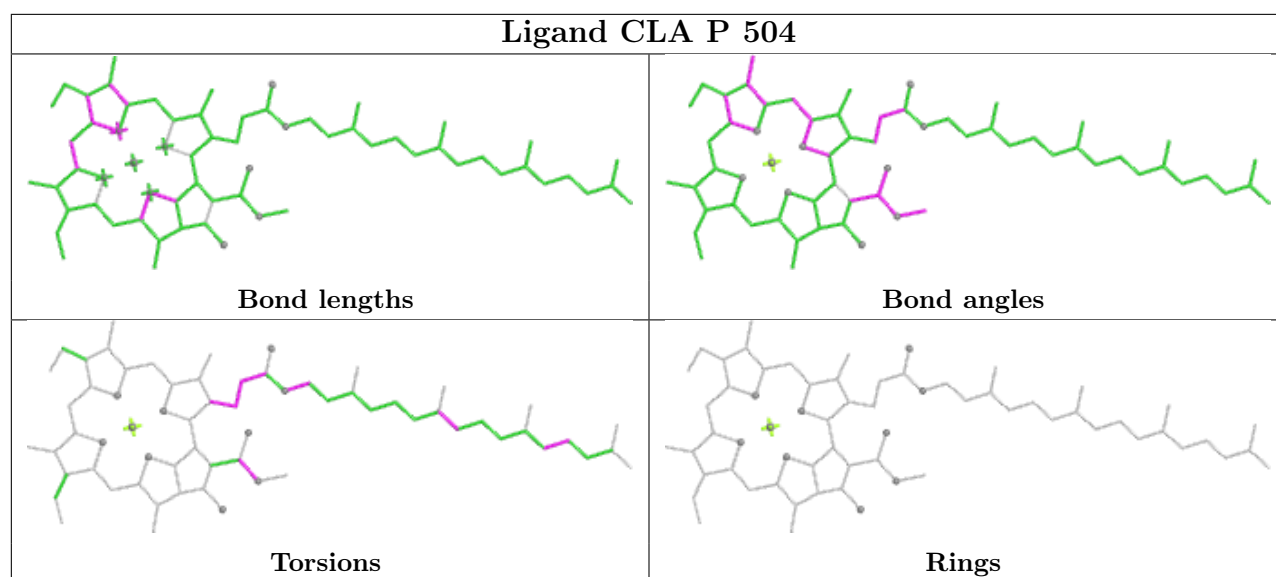


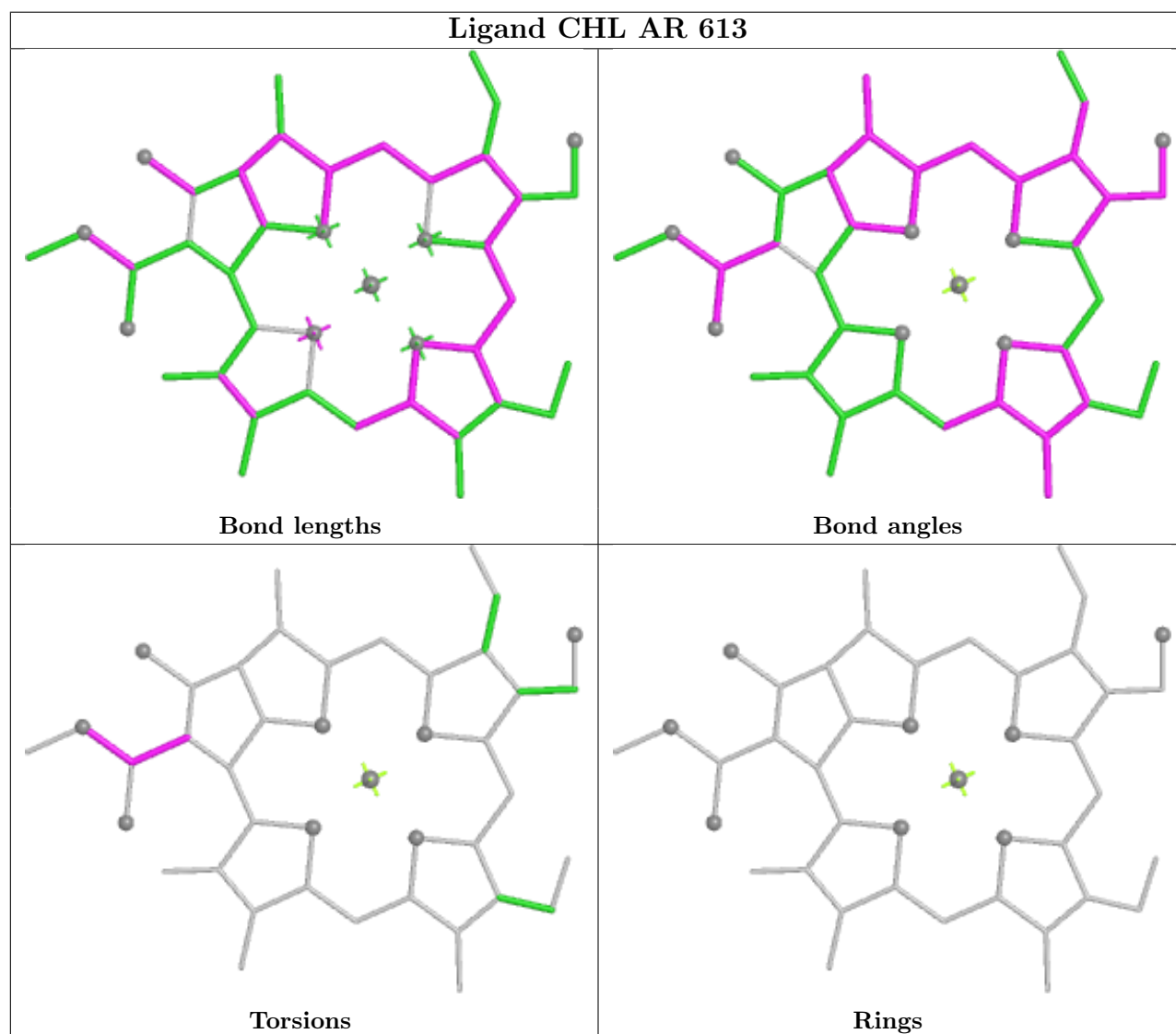
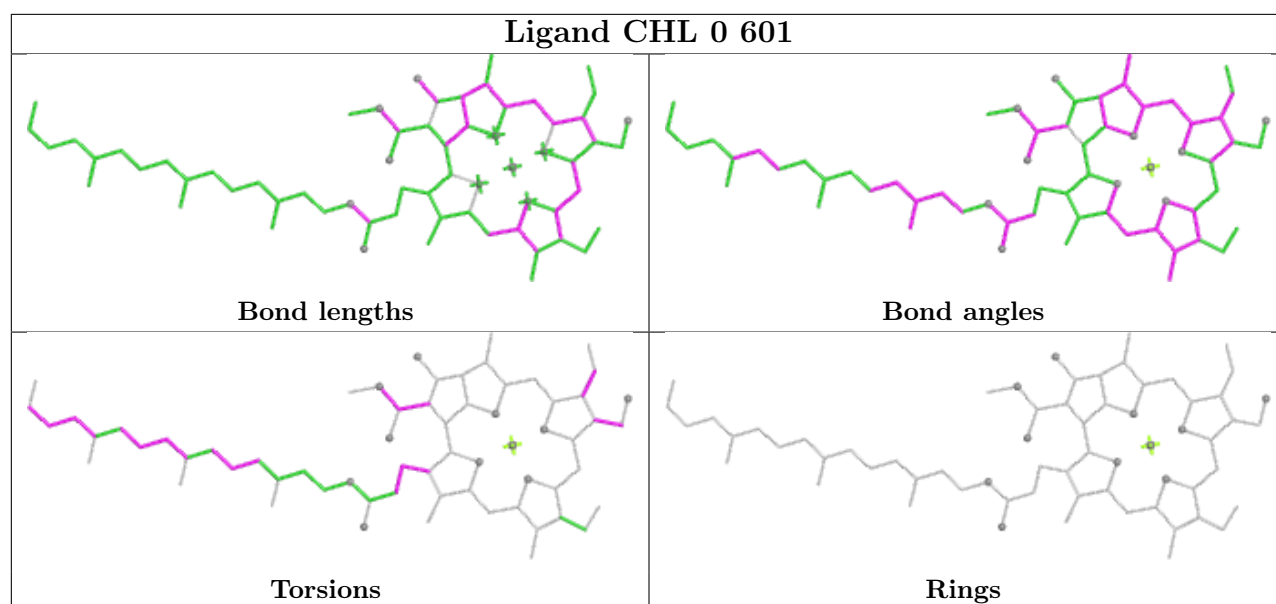
Ligand DGD AL 518	
	Bond lengths
	Bond angles
	Torsions
	Rings

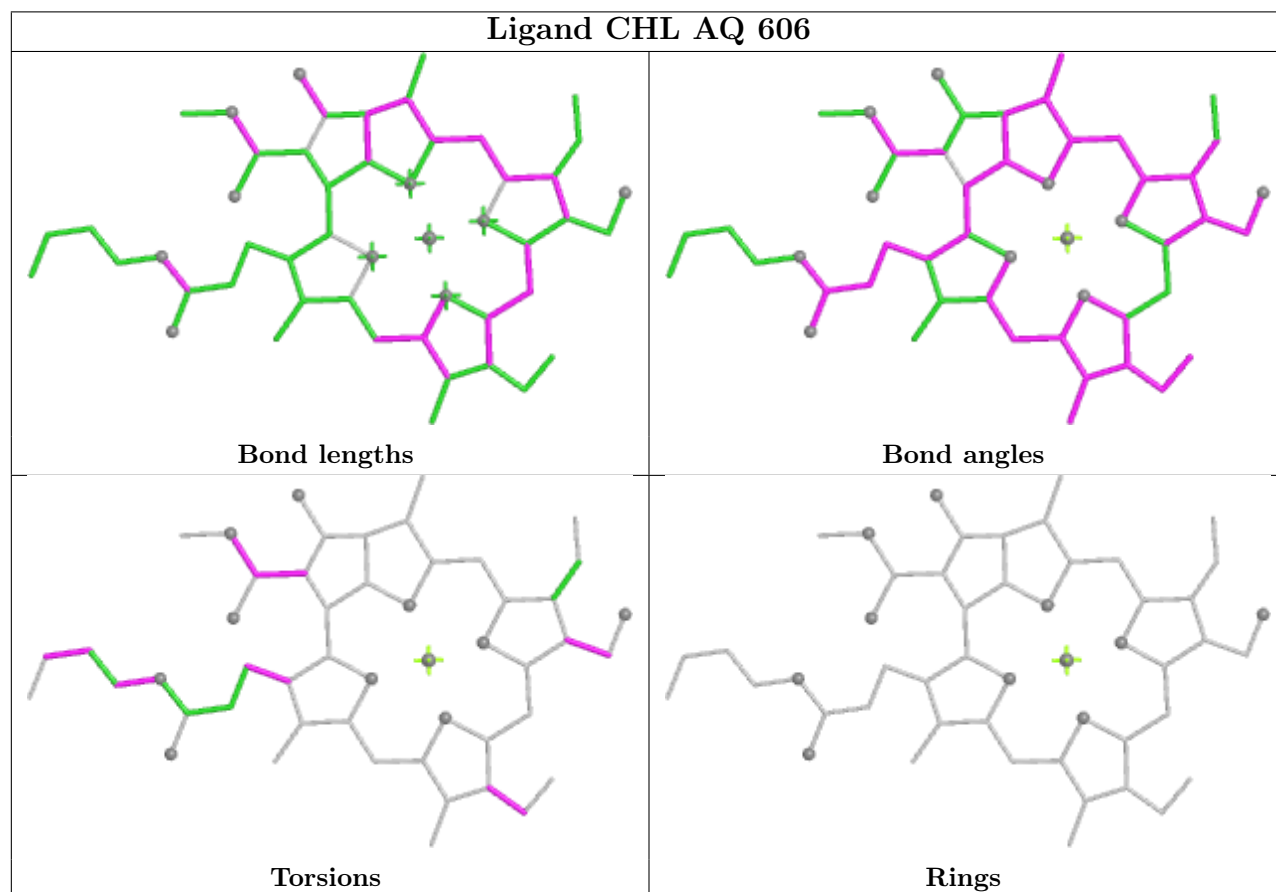
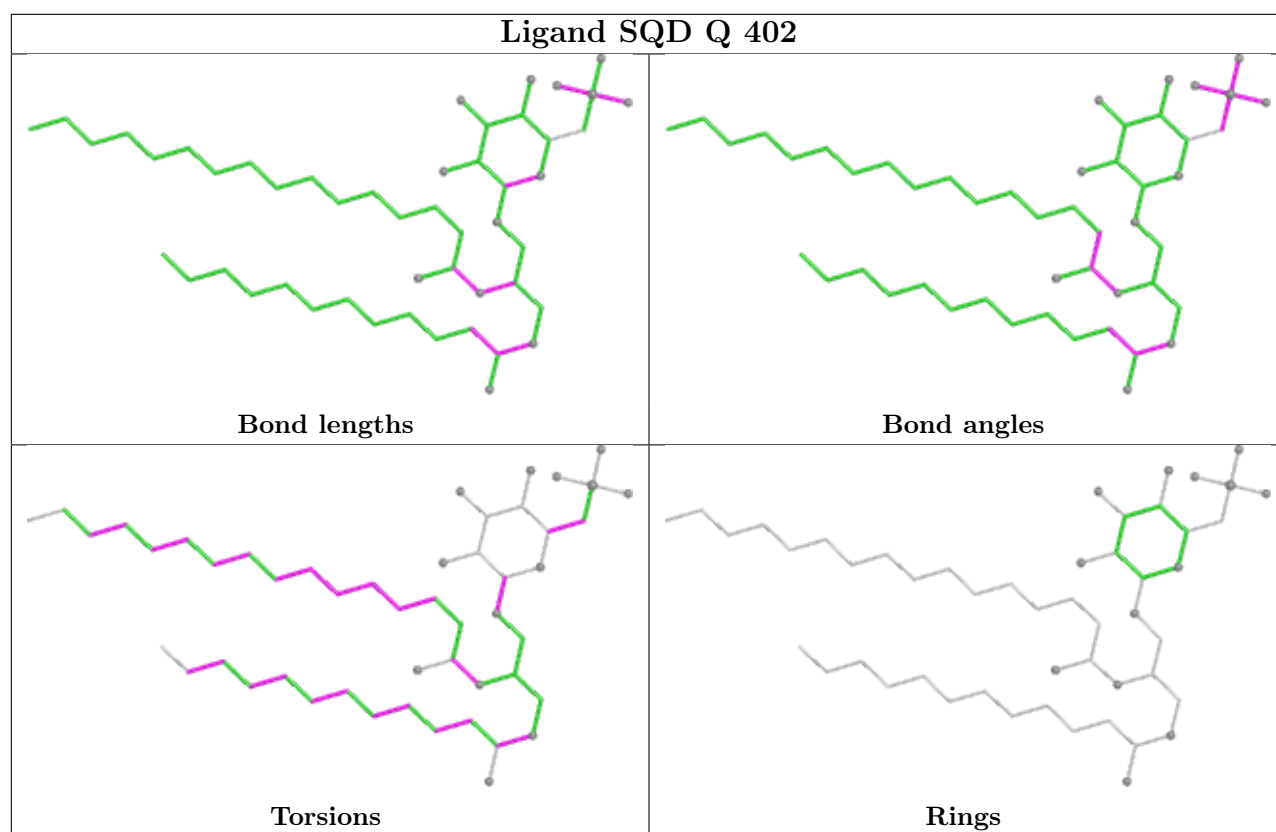
Ligand LUT AE 614	
	Bond lengths
	Bond angles
	Torsions
	Rings

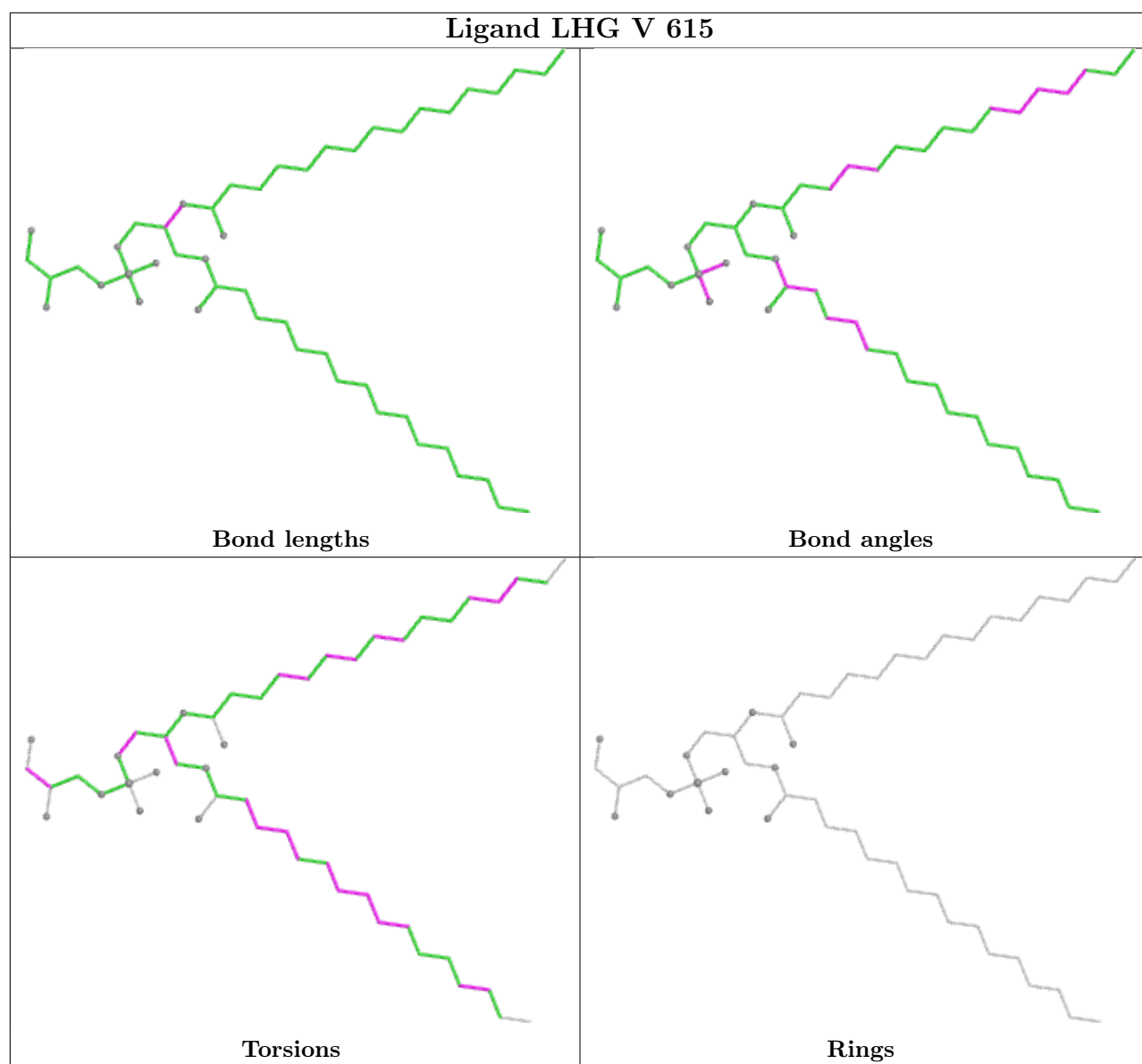
Ligand LUT AA 614	
	Bond lengths
	Bond angles
	Torsions
	Rings

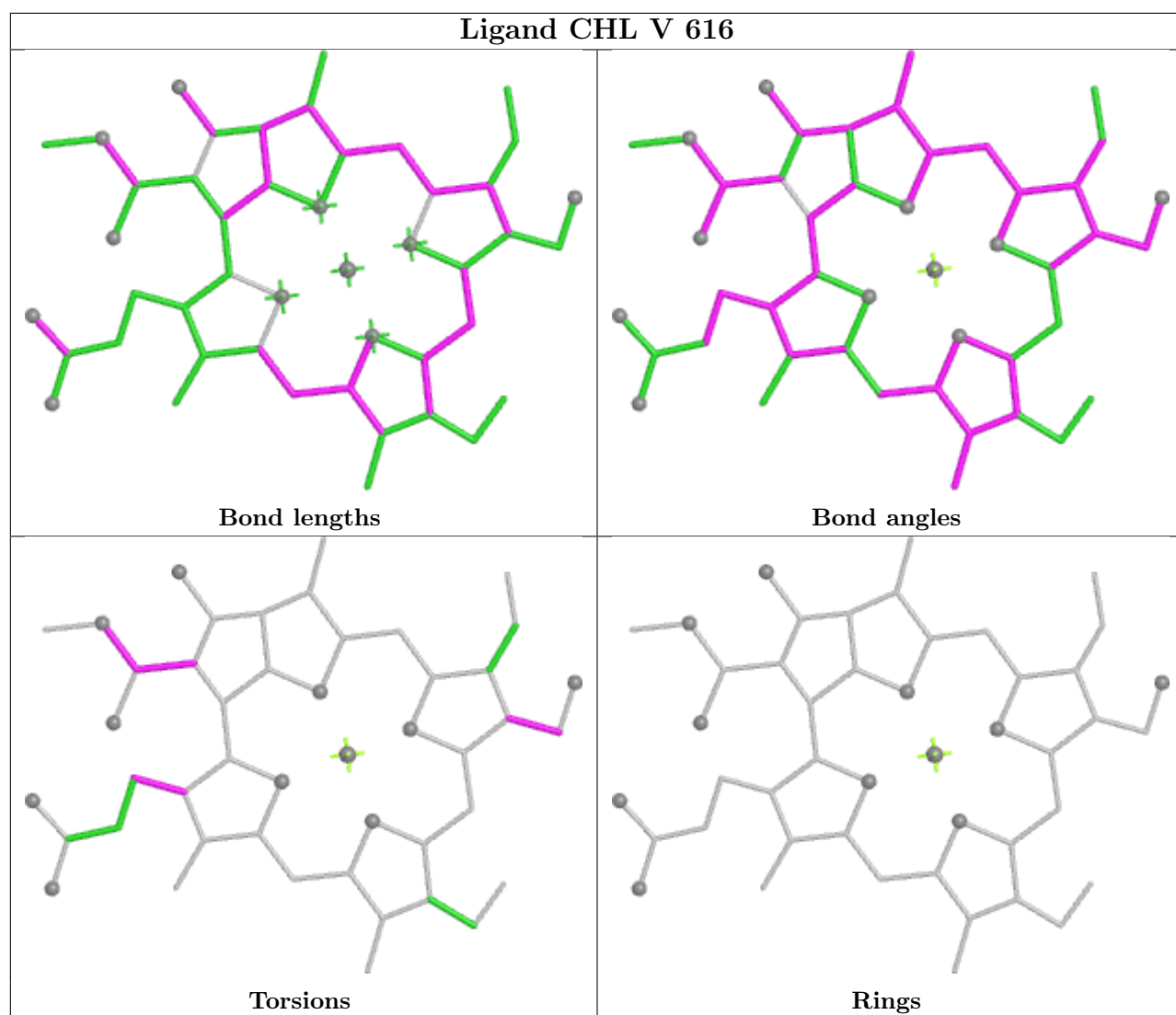


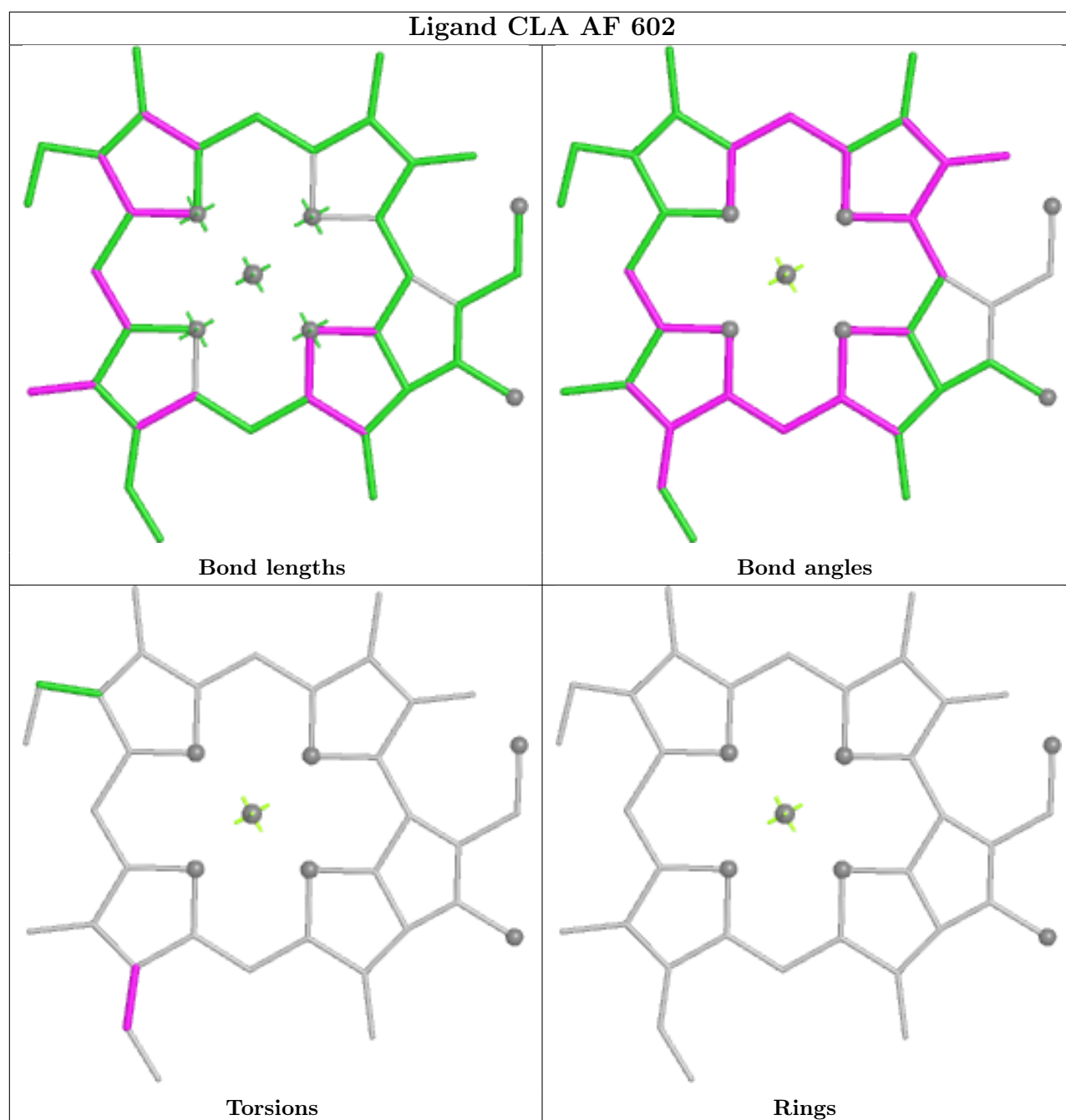




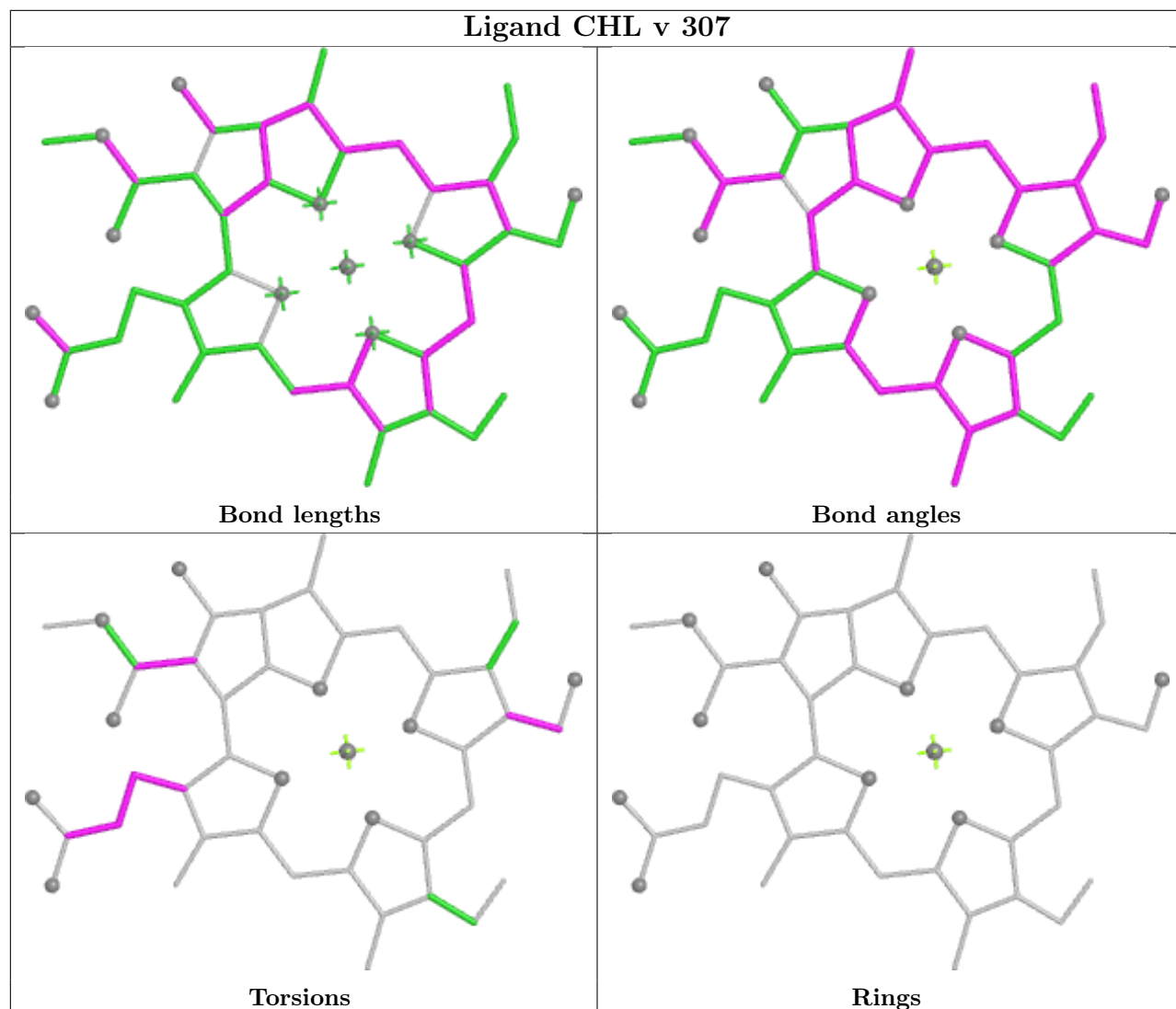




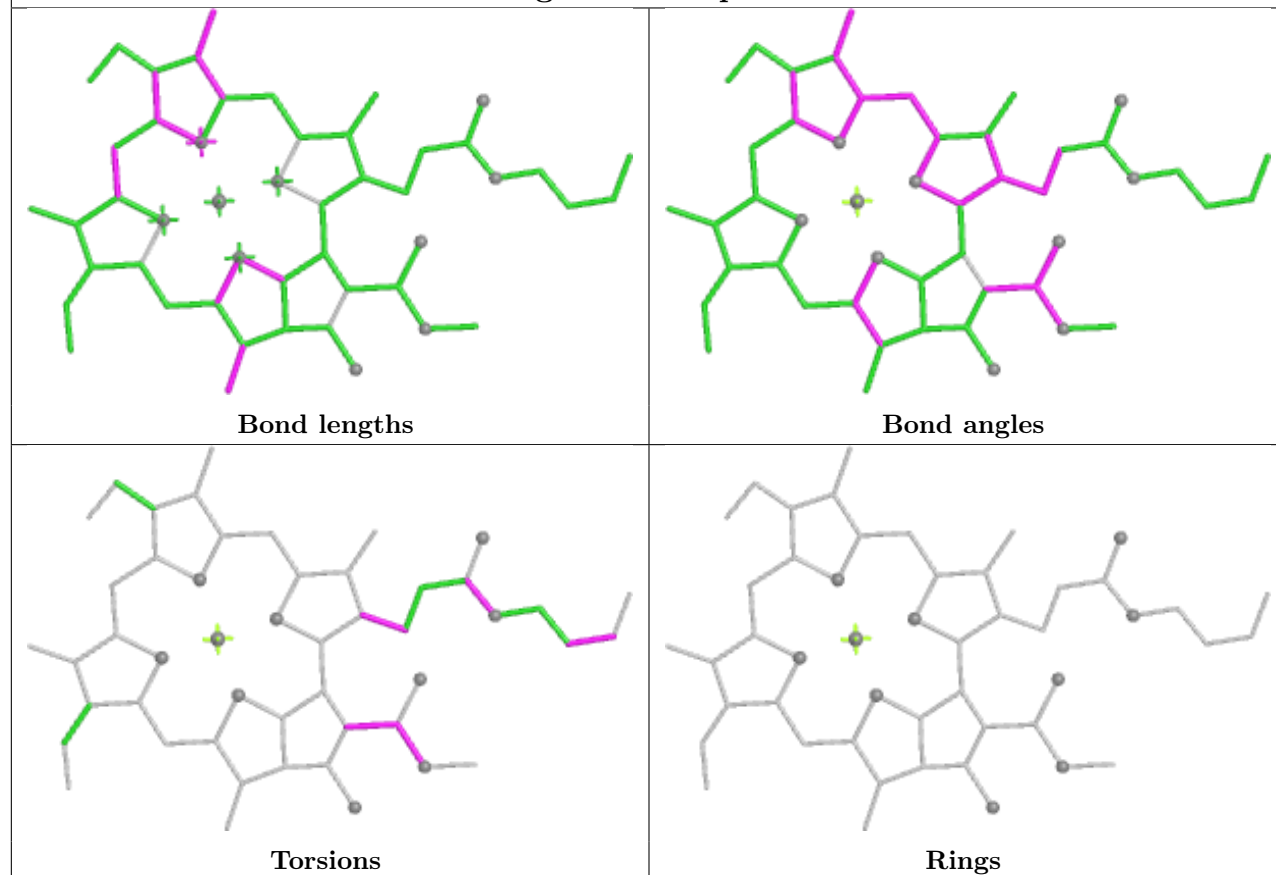




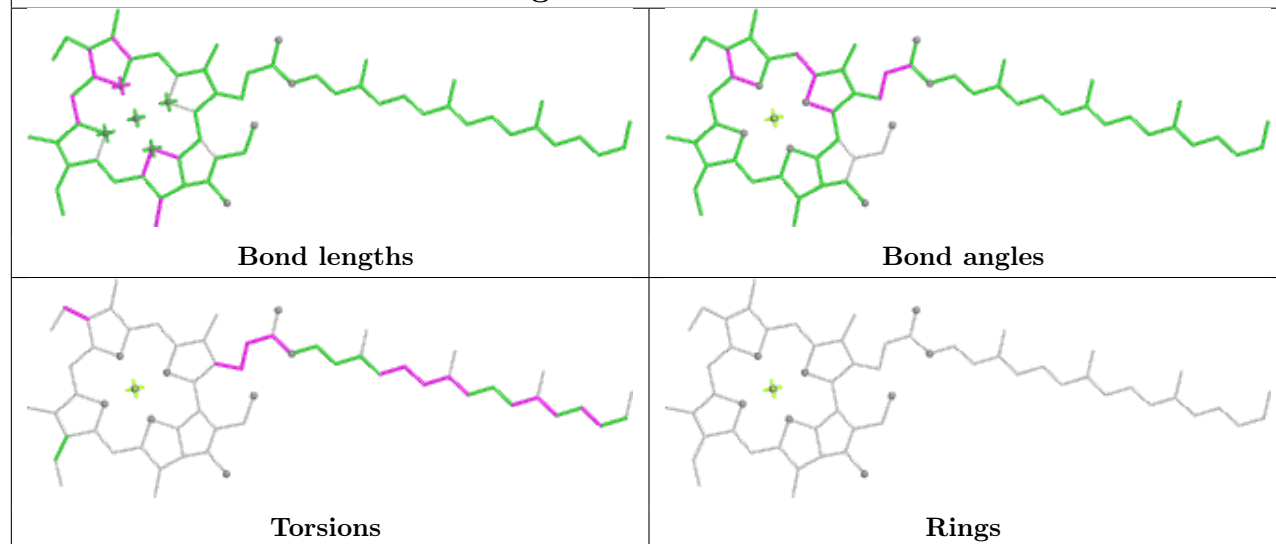
Ligand CHL v 307



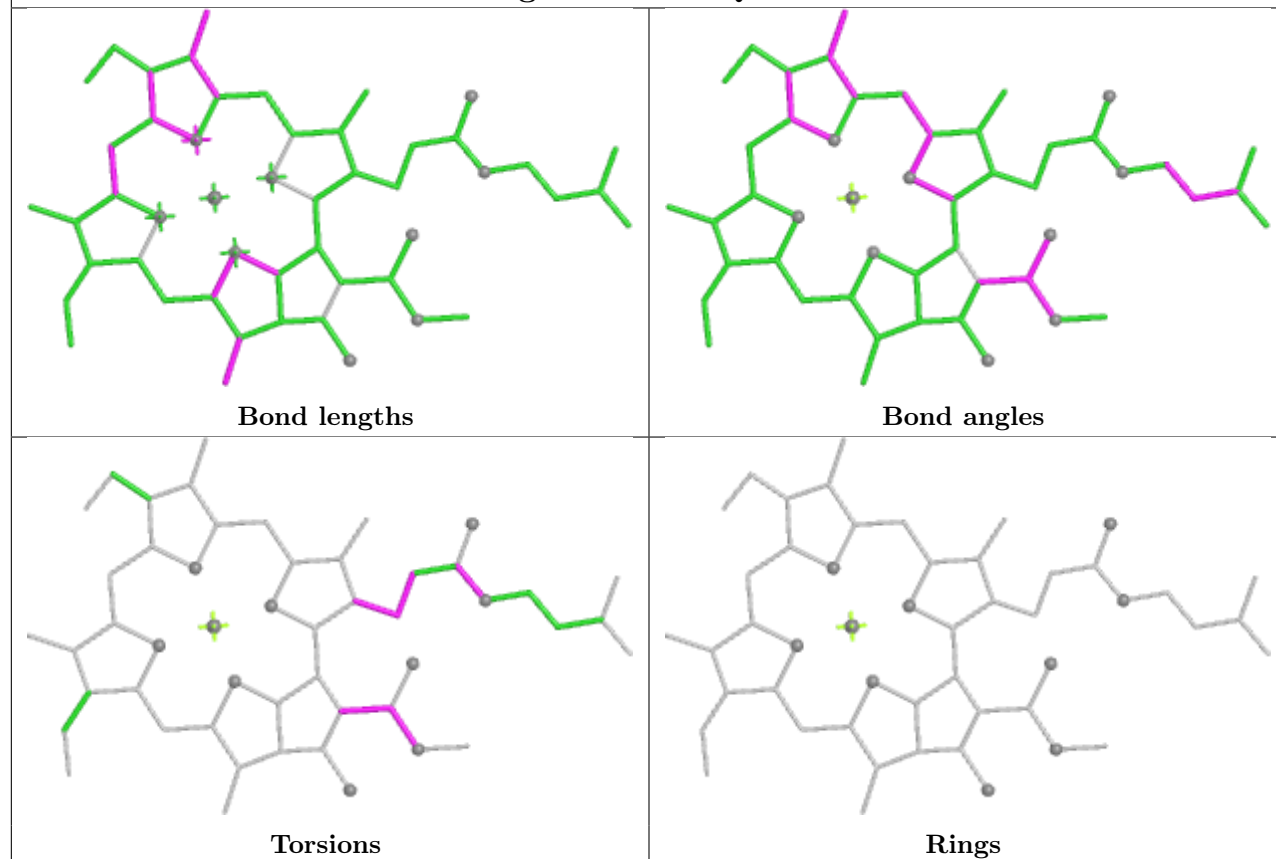
Ligand CLA q 601



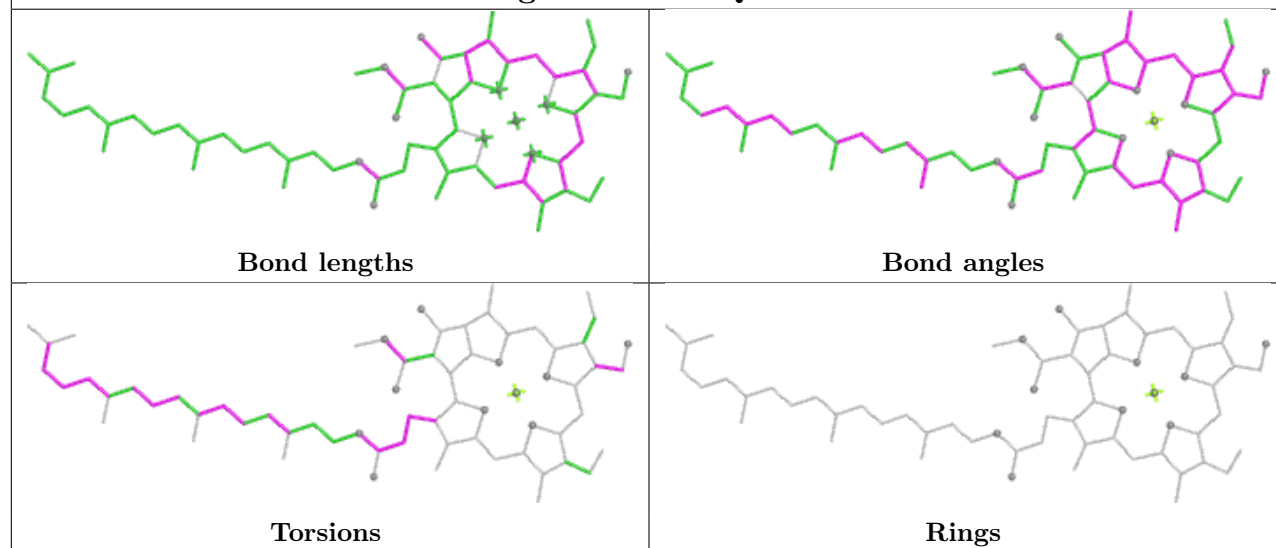
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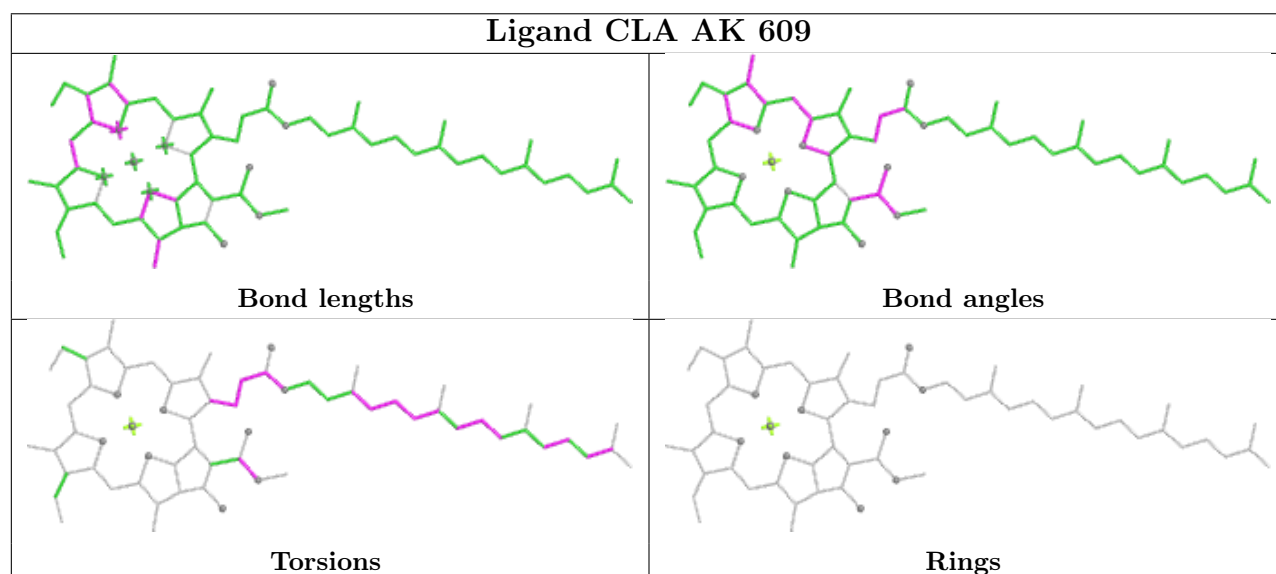
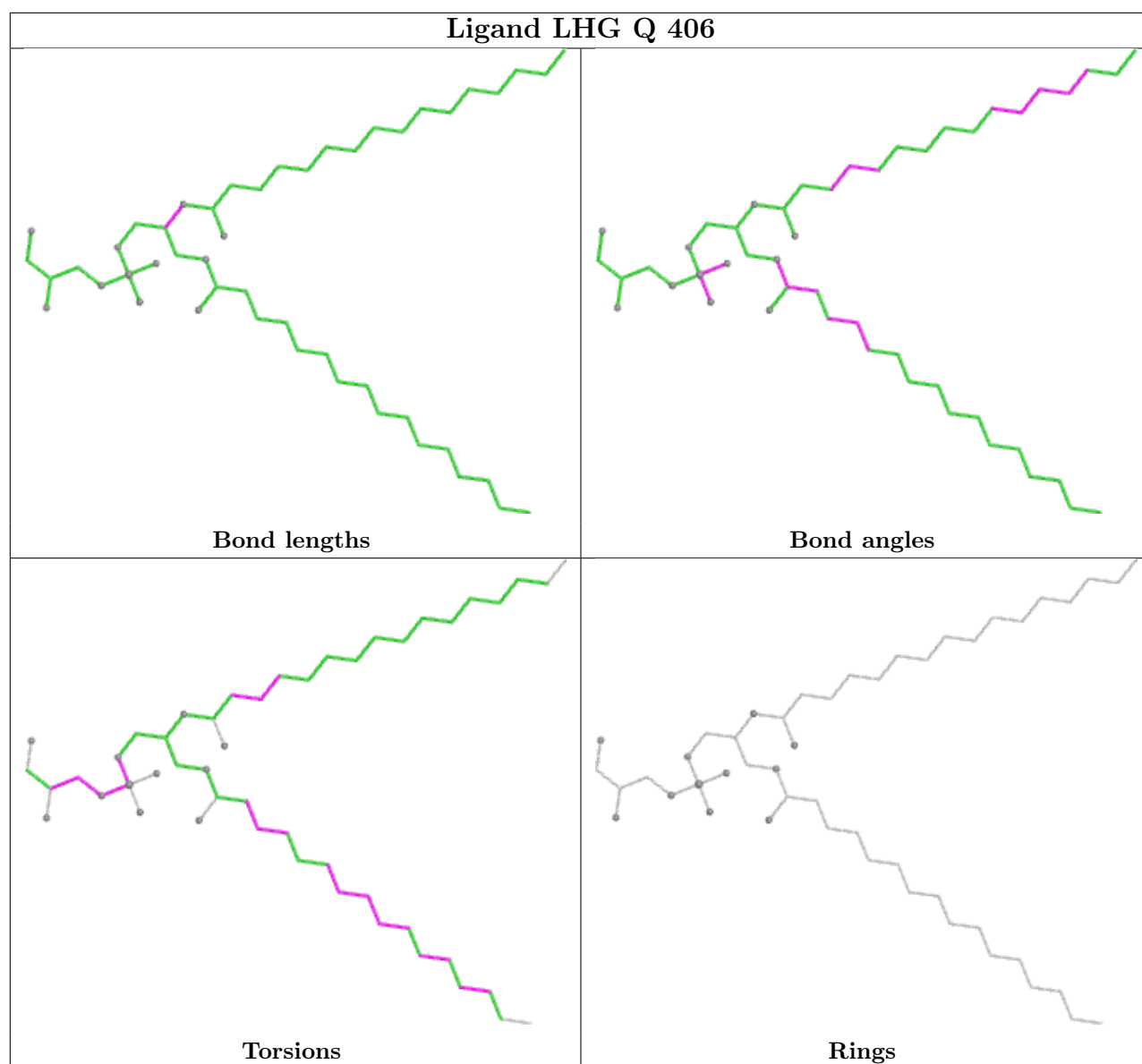


Ligand CLA AQ 604

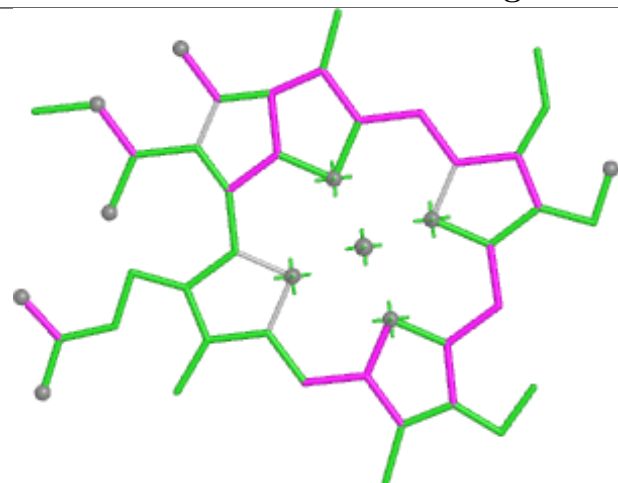


Ligand CHL AQ 601

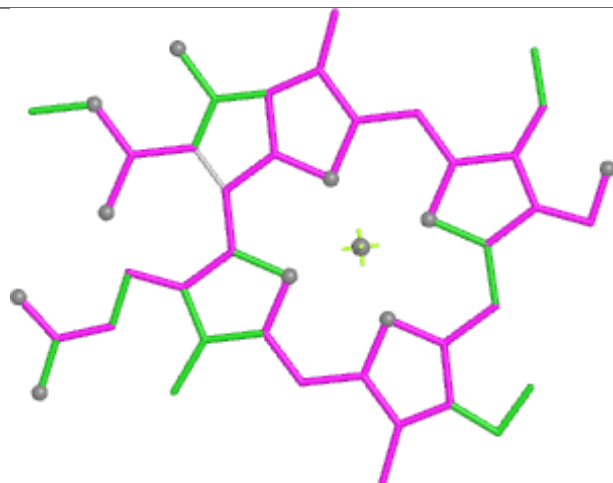




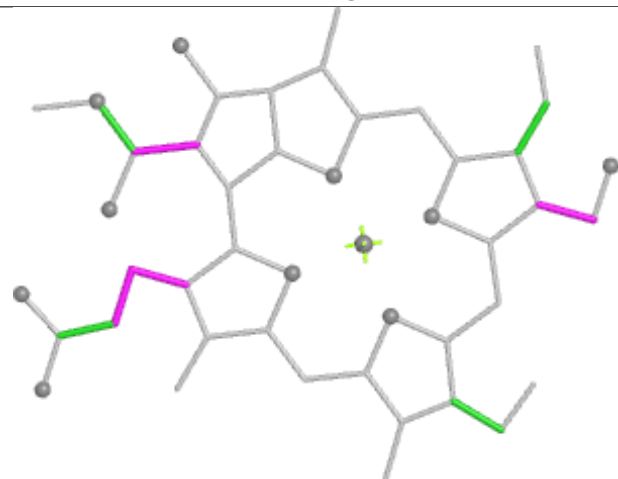
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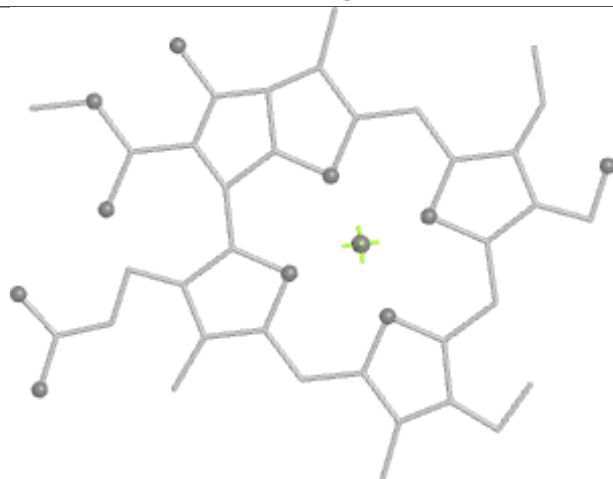
Bond lengths



Bond angles



Torsions

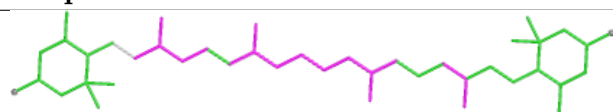


Rings

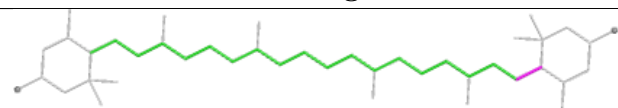
Ligand LUT q 614



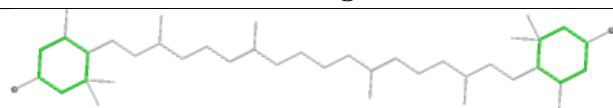
Bond lengths



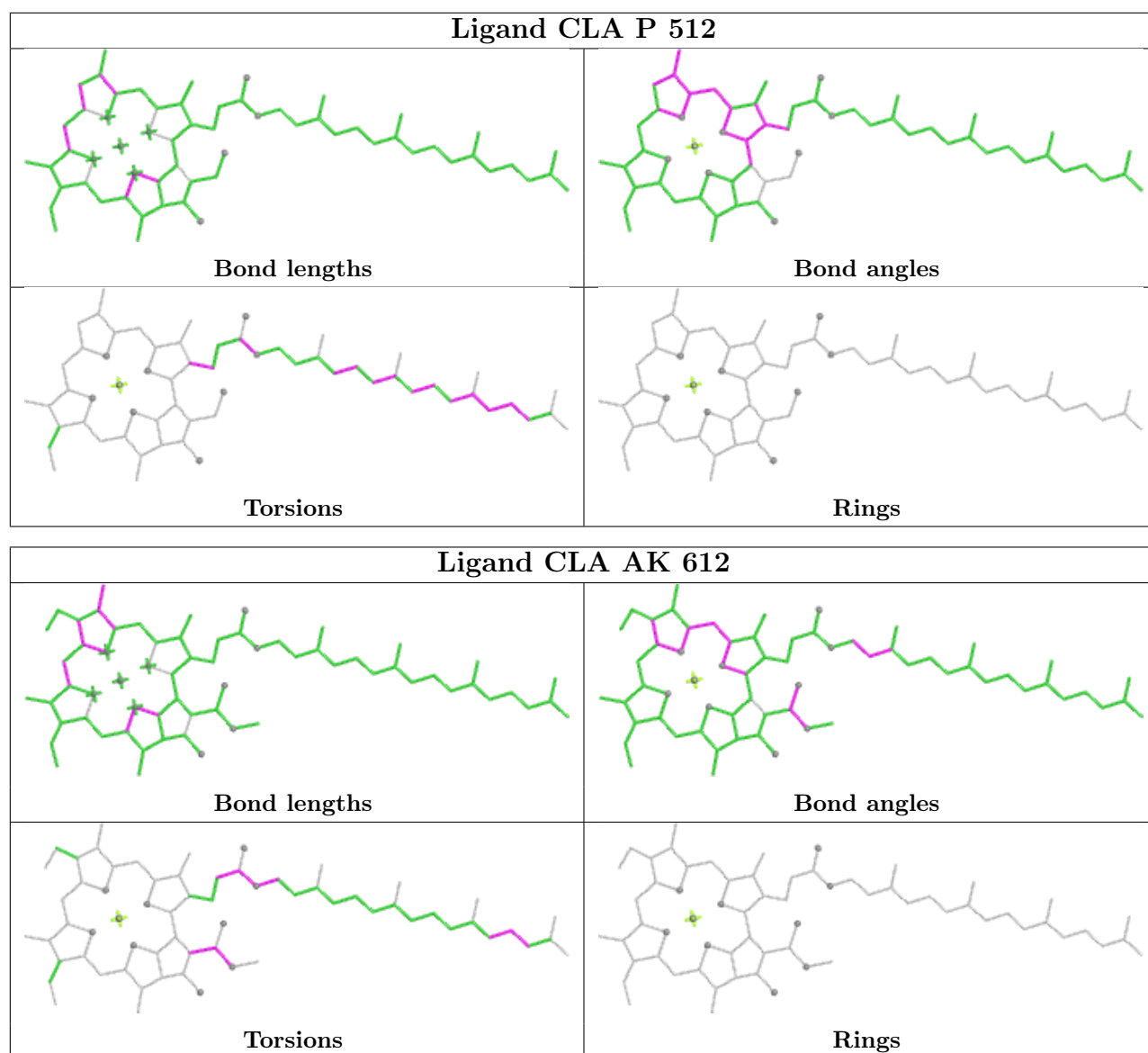
Bond angles



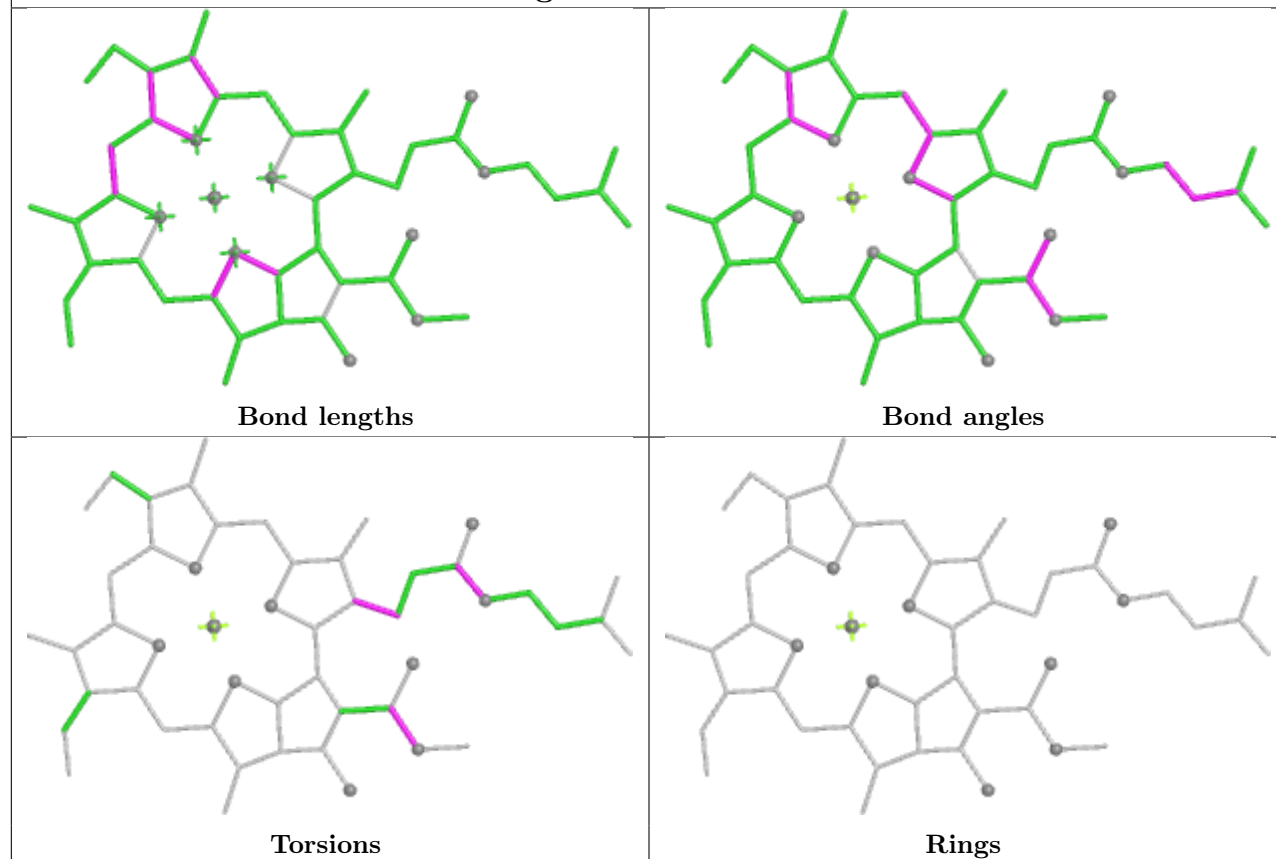
Torsions



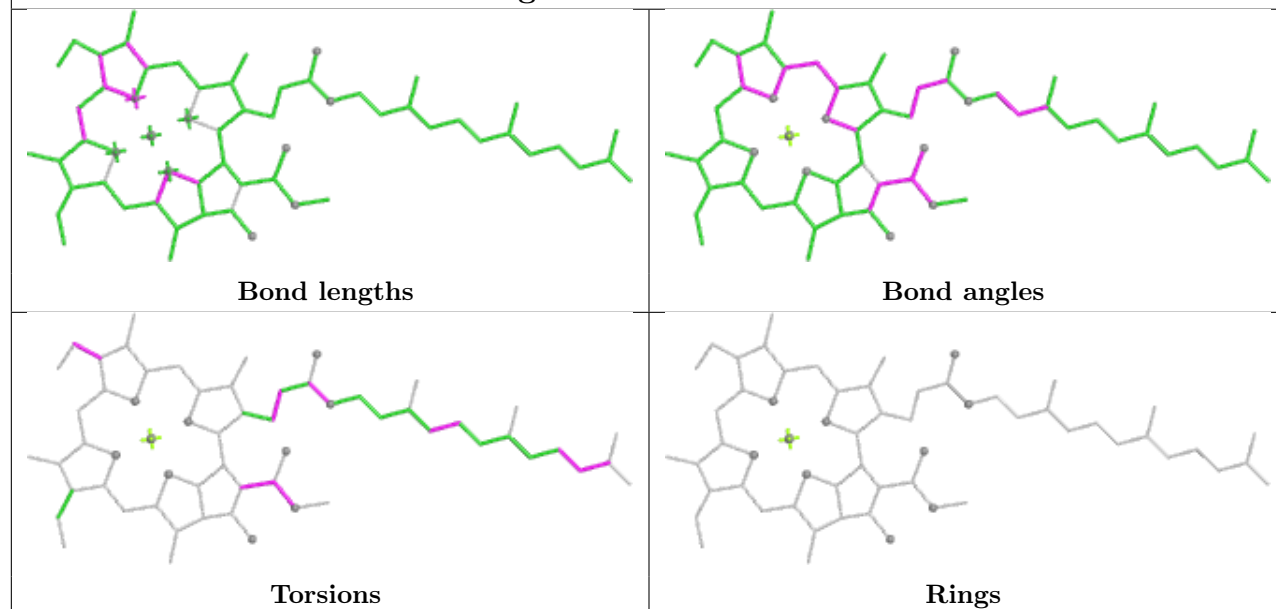
Rings



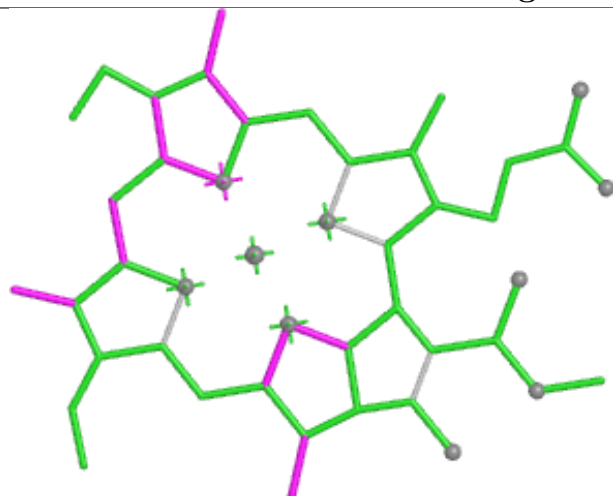
Ligand CLA v 305



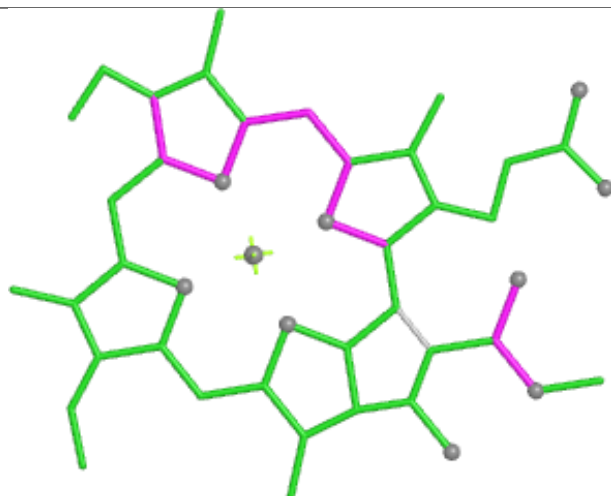
Ligand CLA AU 609



Ligand CLA 0 611



Bond lengths



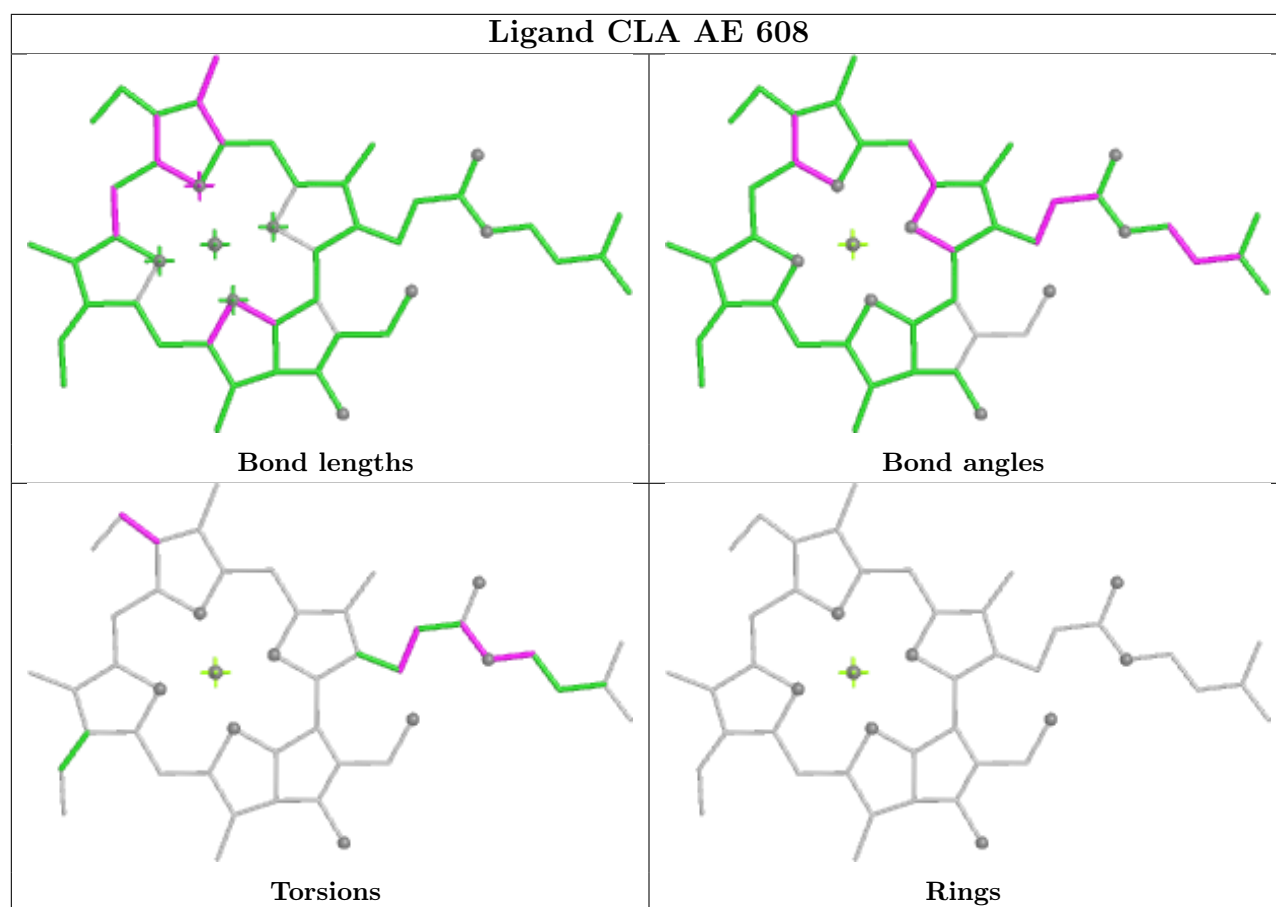
Bond angles



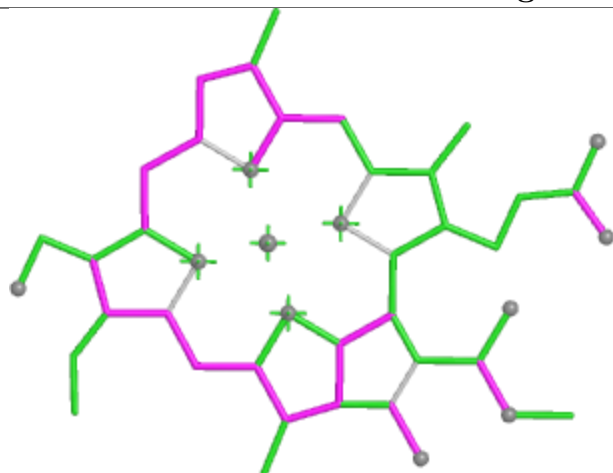
Torsions



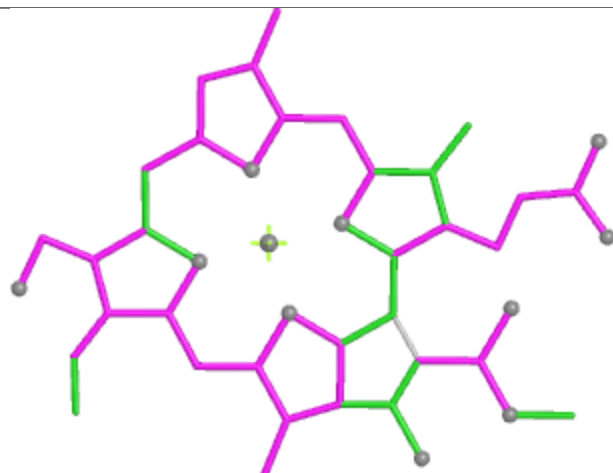
Rings



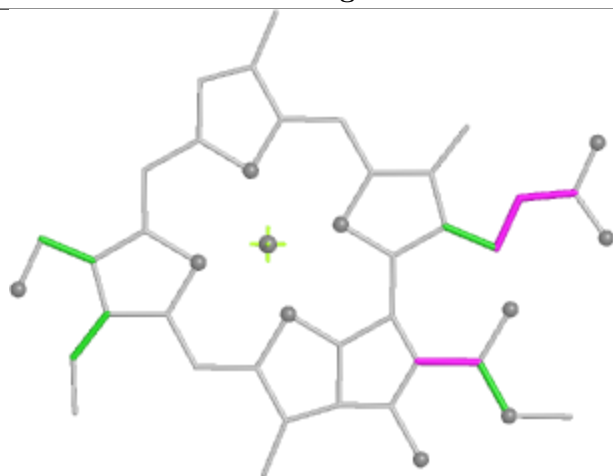
Ligand CHL v 302



Bond lengths



Bond angles

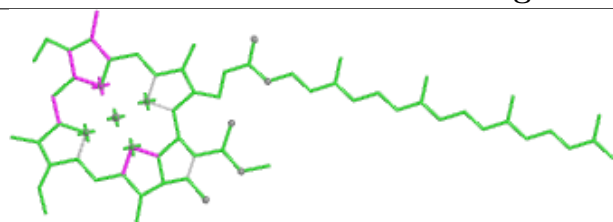


Torsions

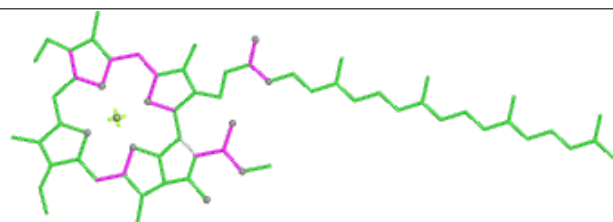


Rings

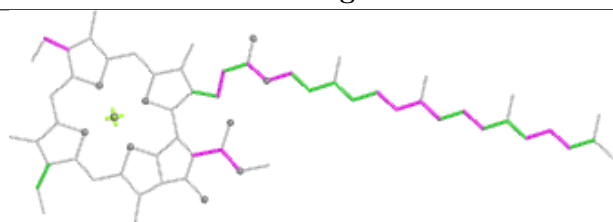
Ligand CLA V 603



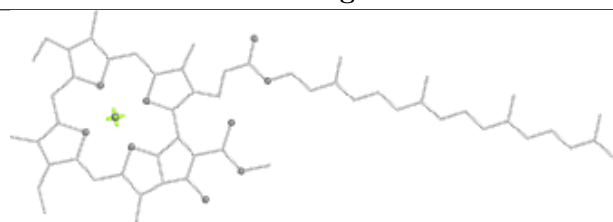
Bond lengths



Bond angles

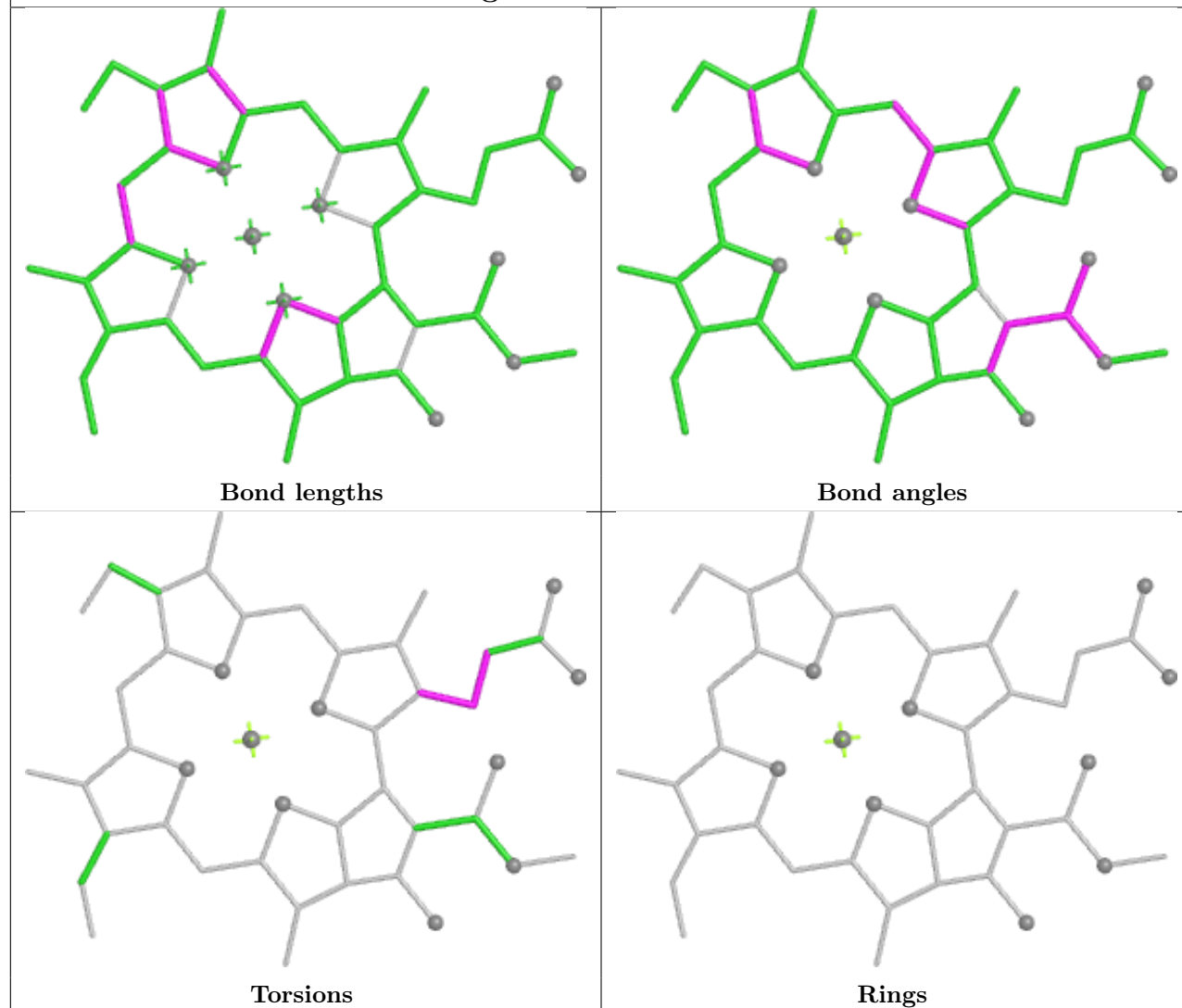


Torsions

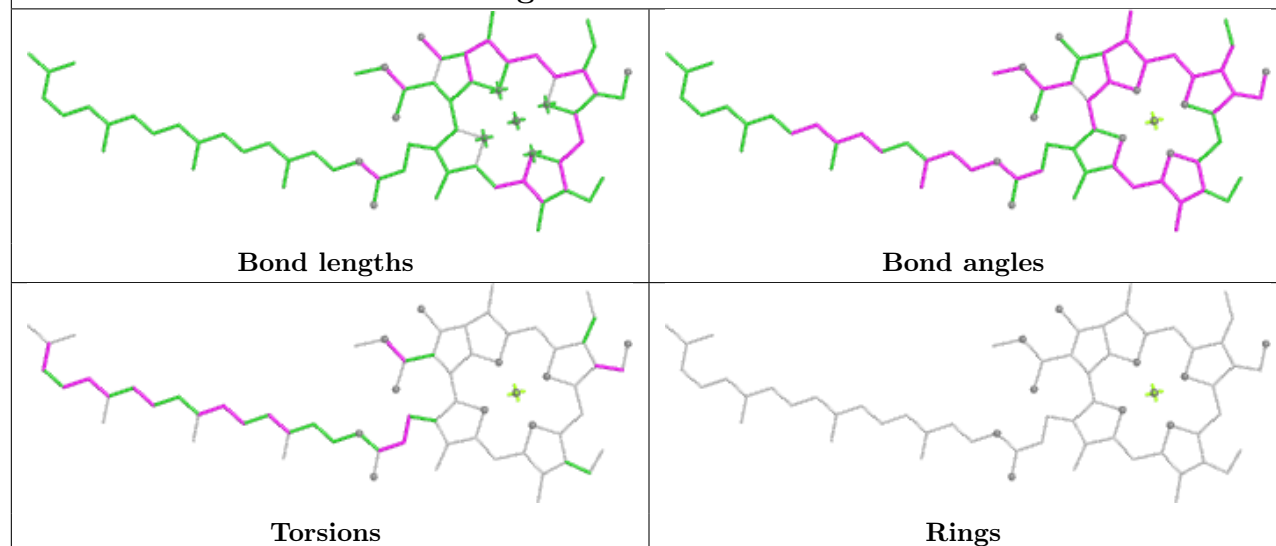


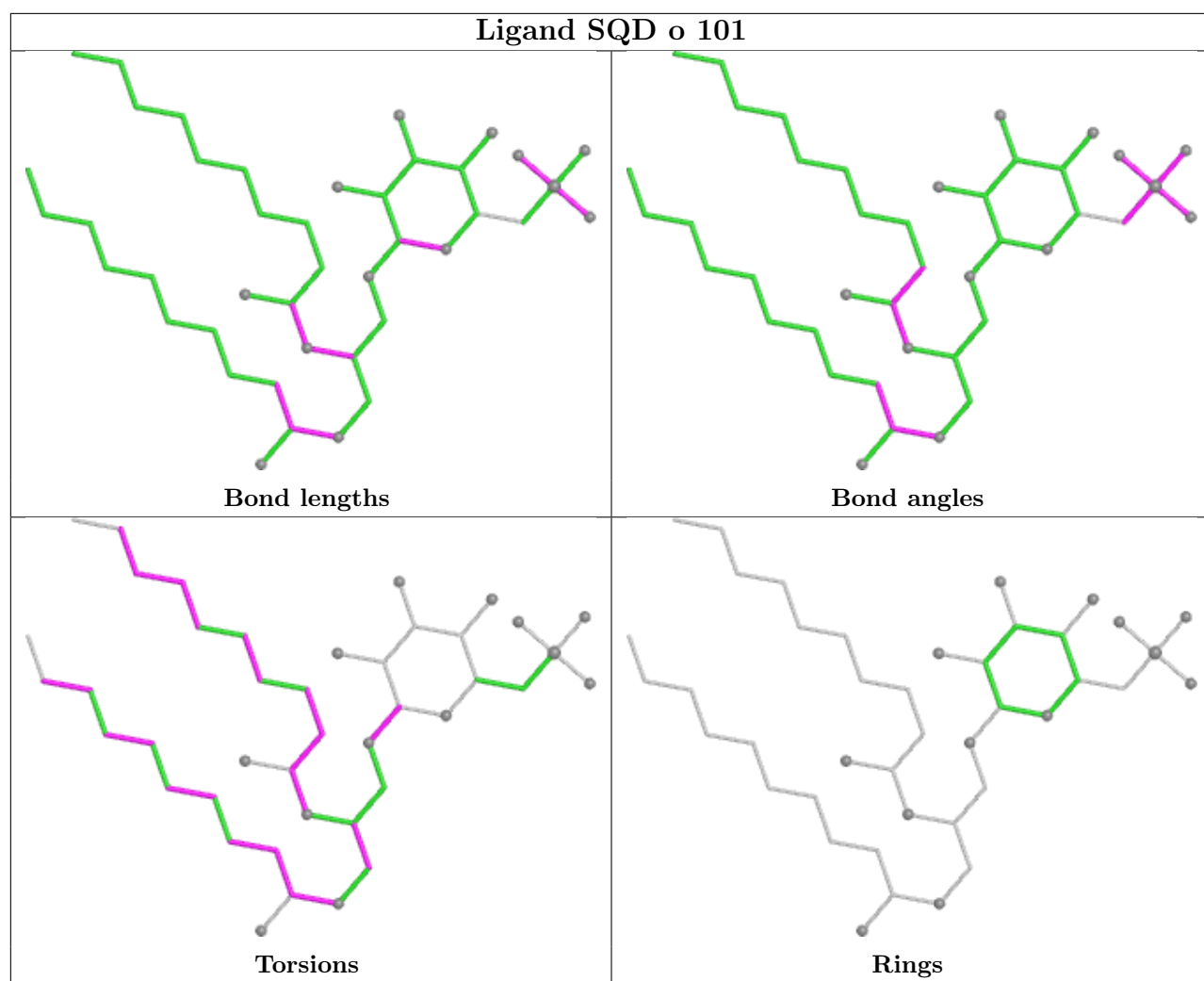
Rings

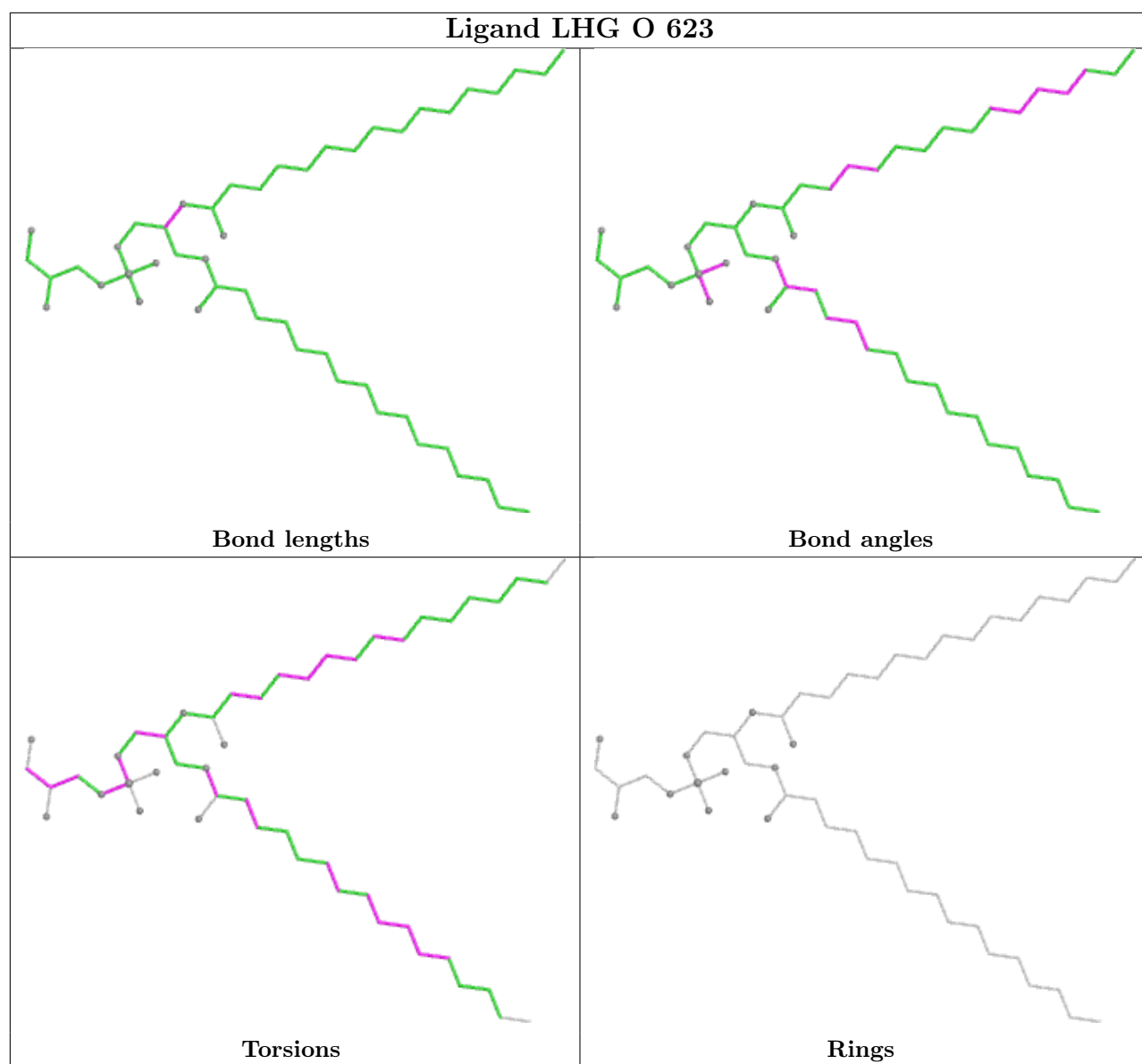
Ligand CLA AF 604

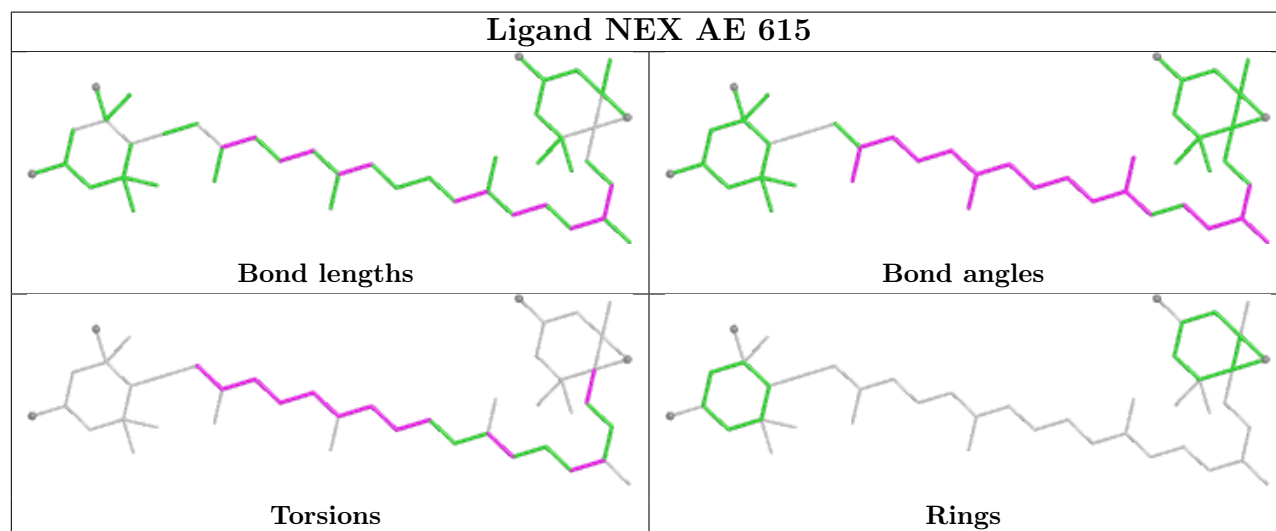
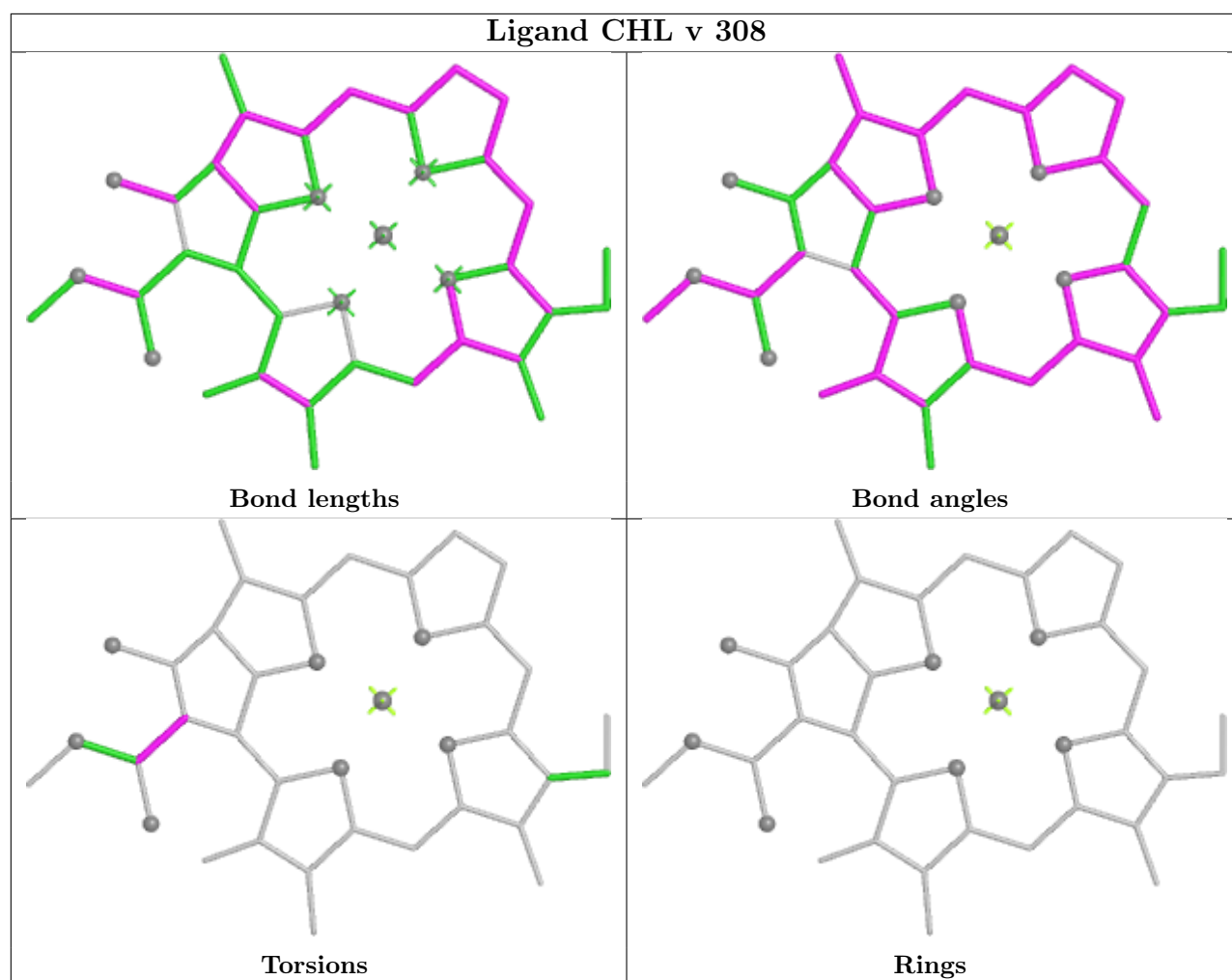


Ligand CHL AN 606

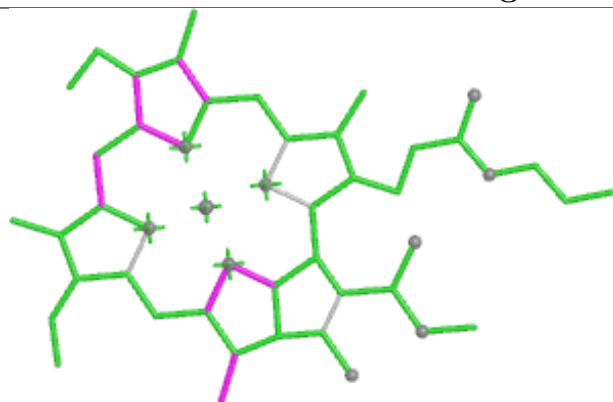




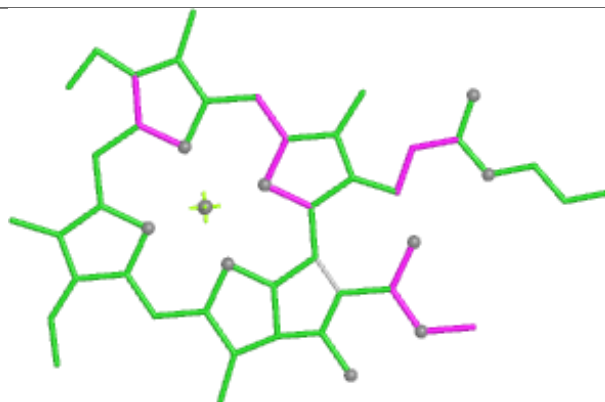




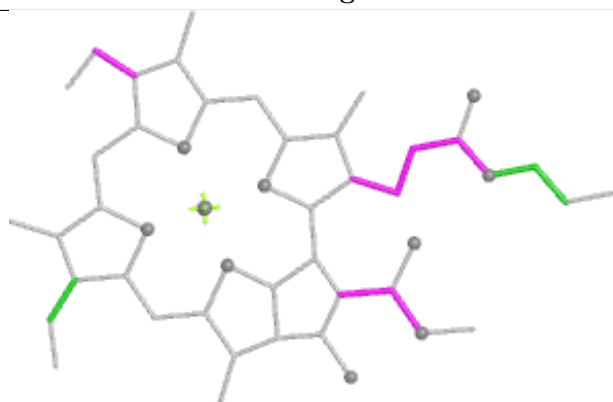
Ligand CLA AD 313



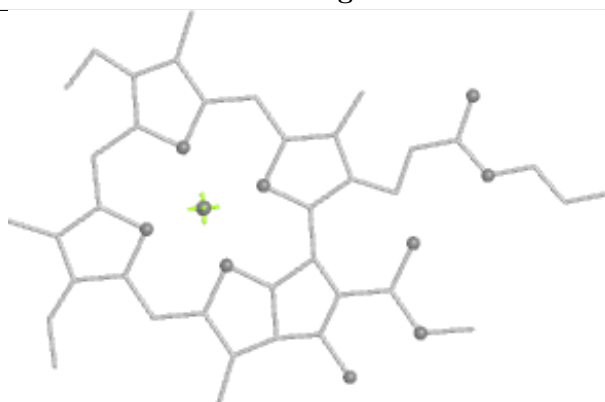
Bond lengths



Bond angles

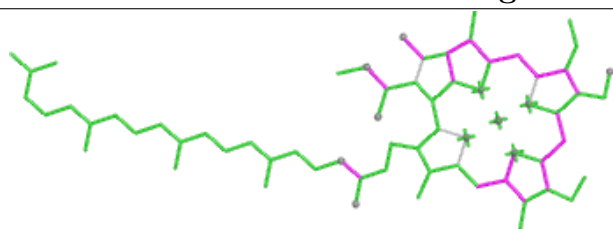


Torsions

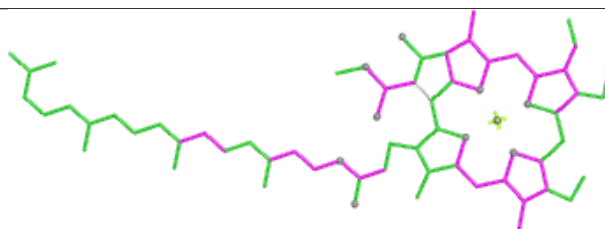


Rings

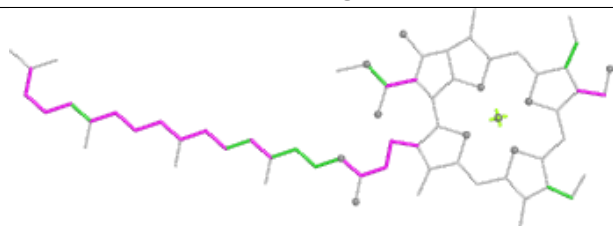
Ligand CHL AN 601



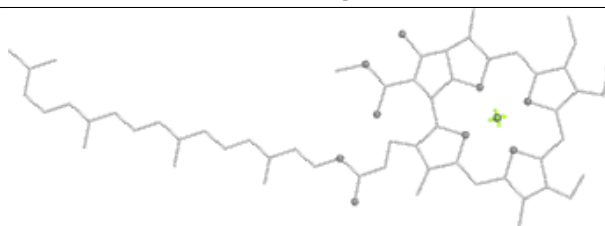
Bond lengths



Bond angles

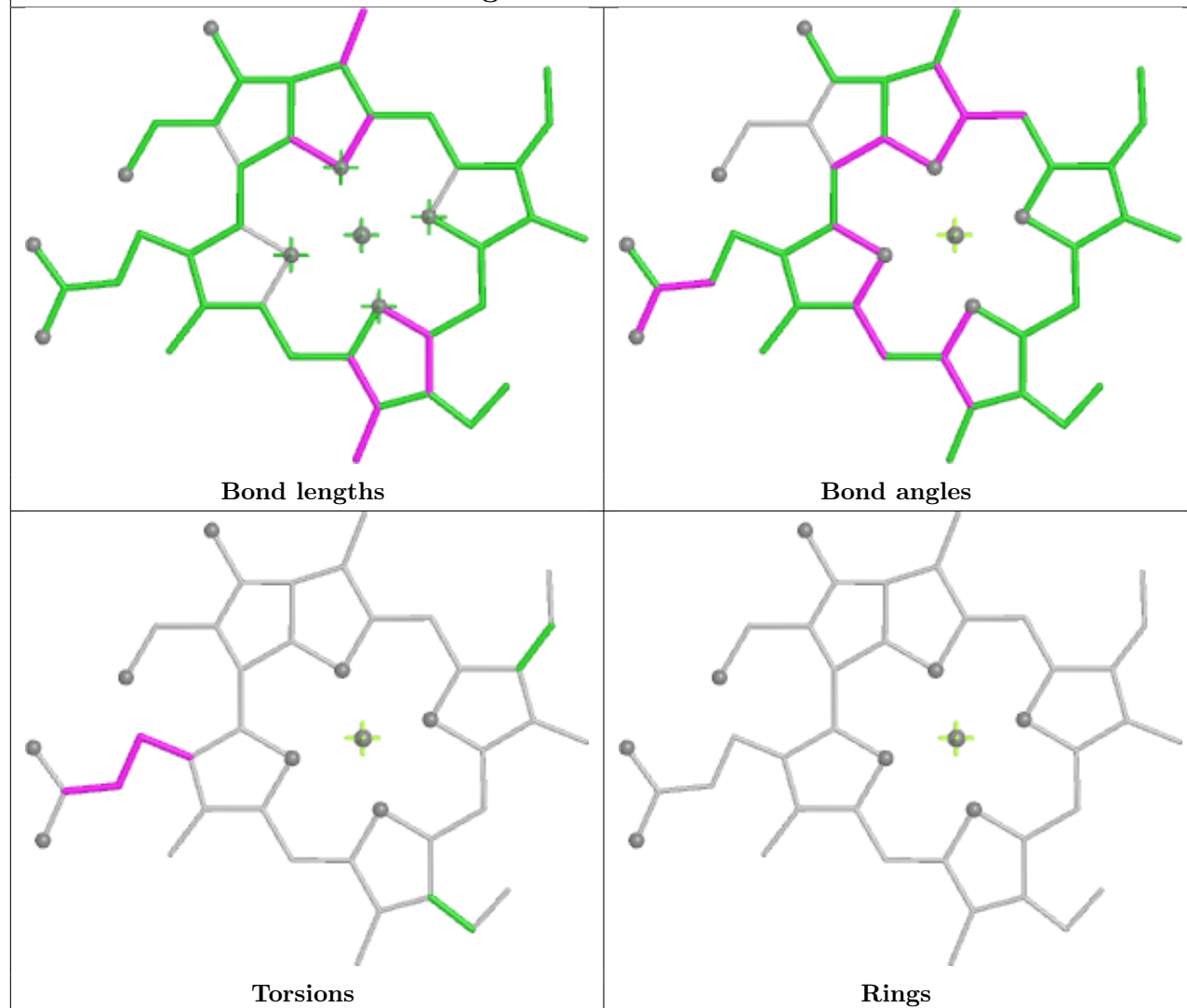


Torsions

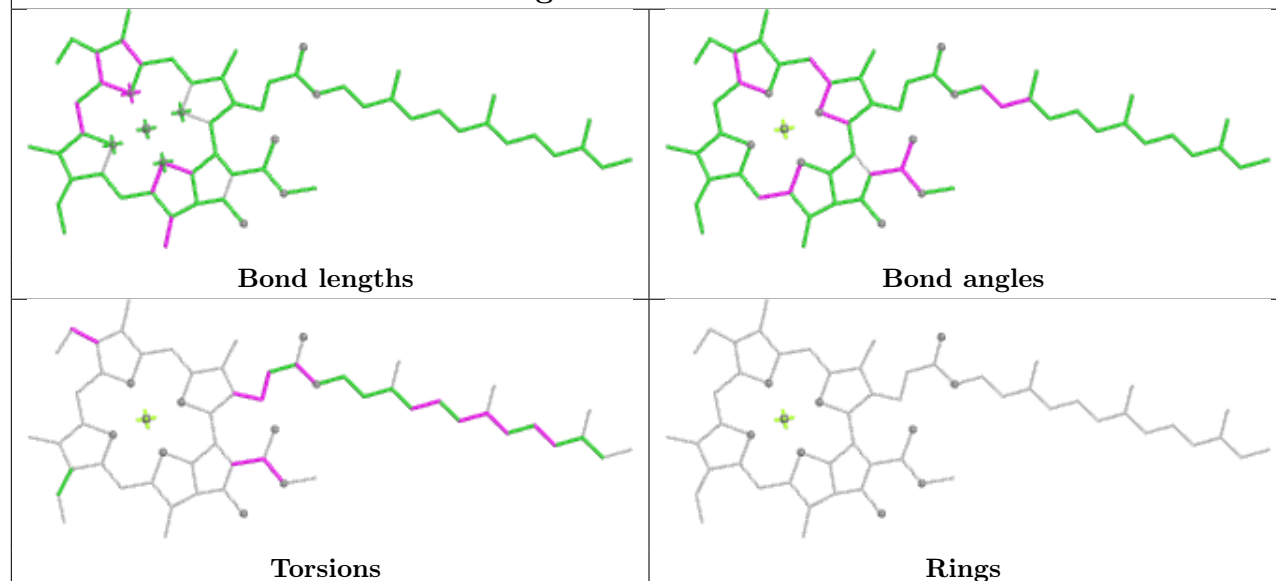


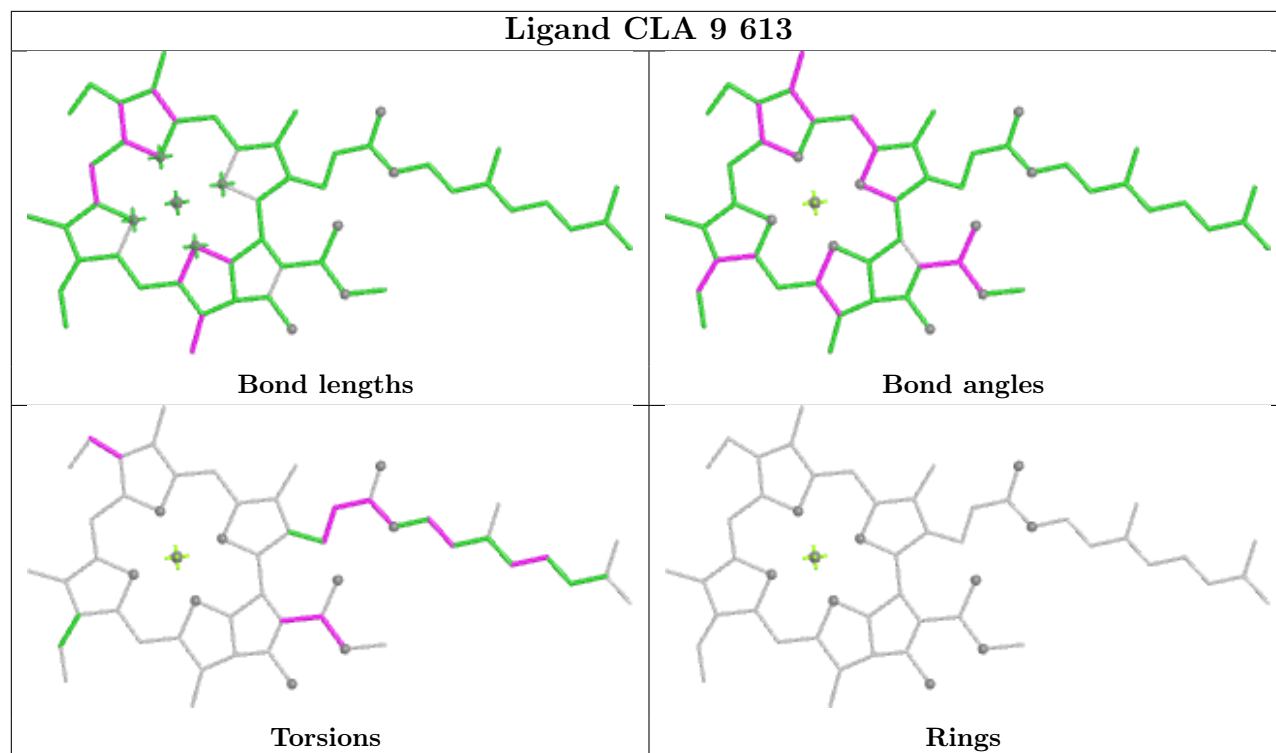
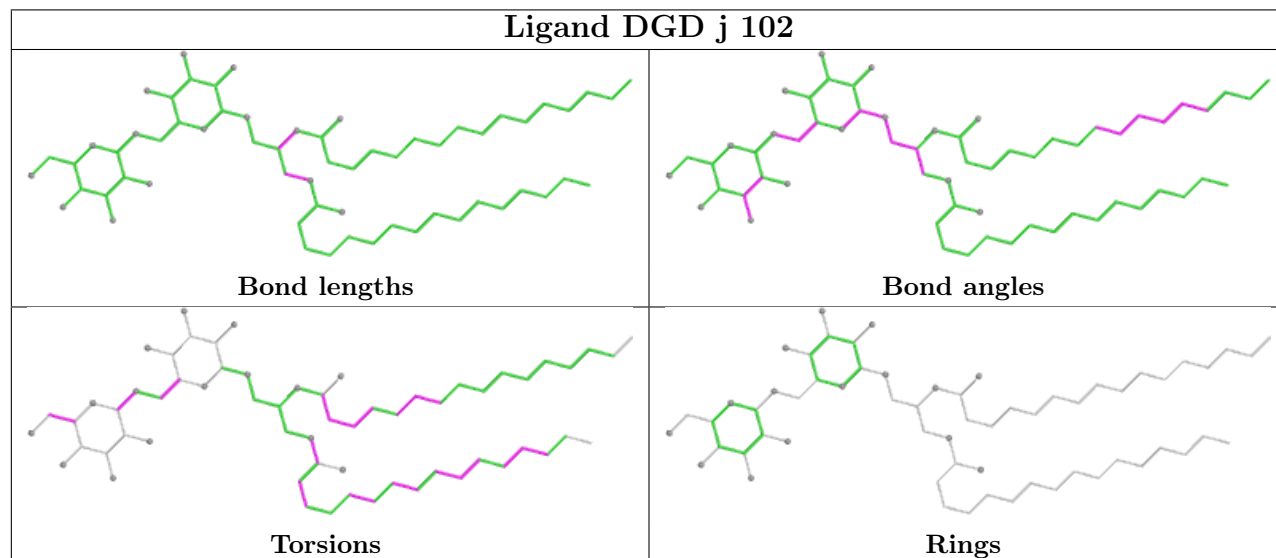
Rings

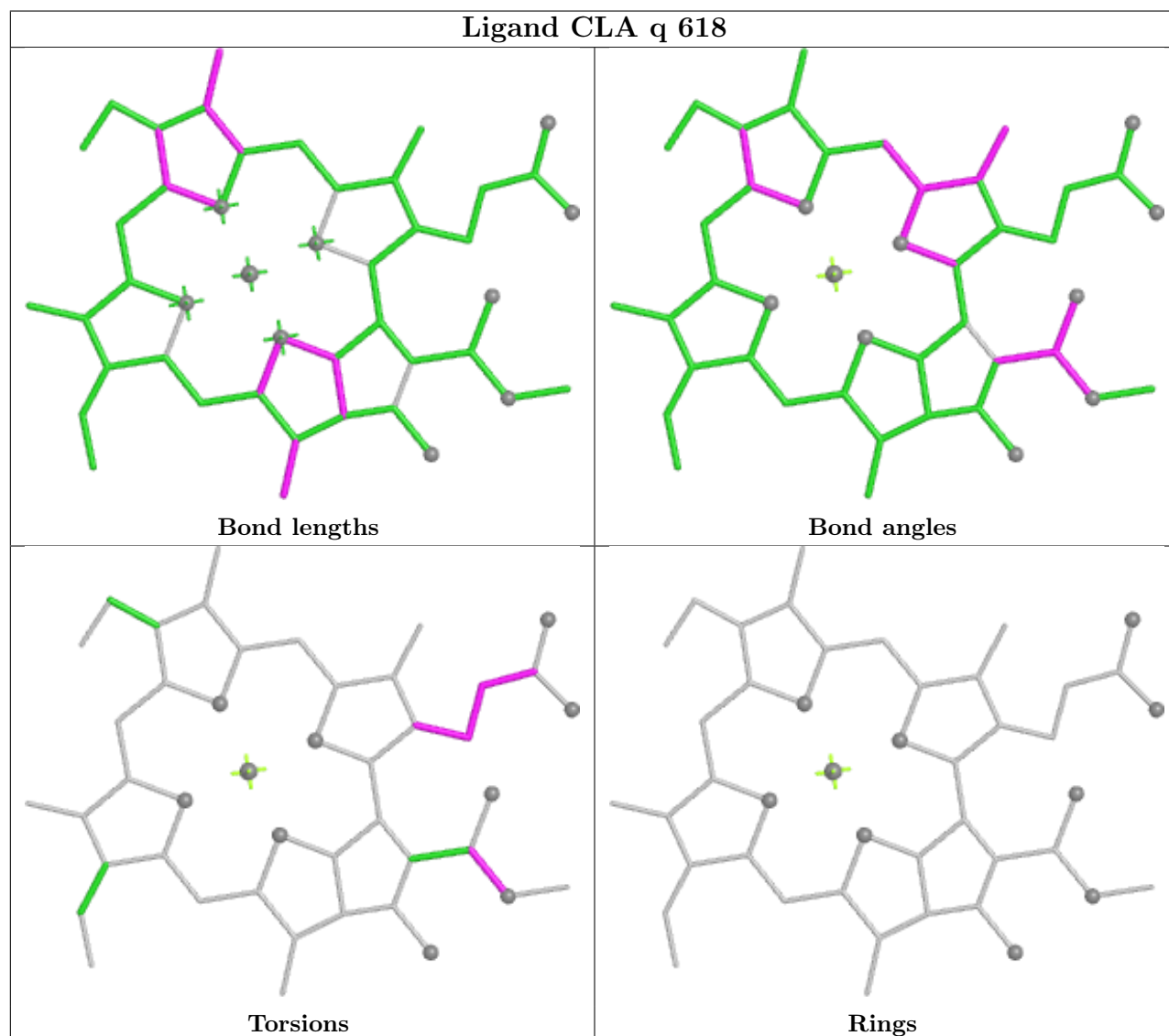
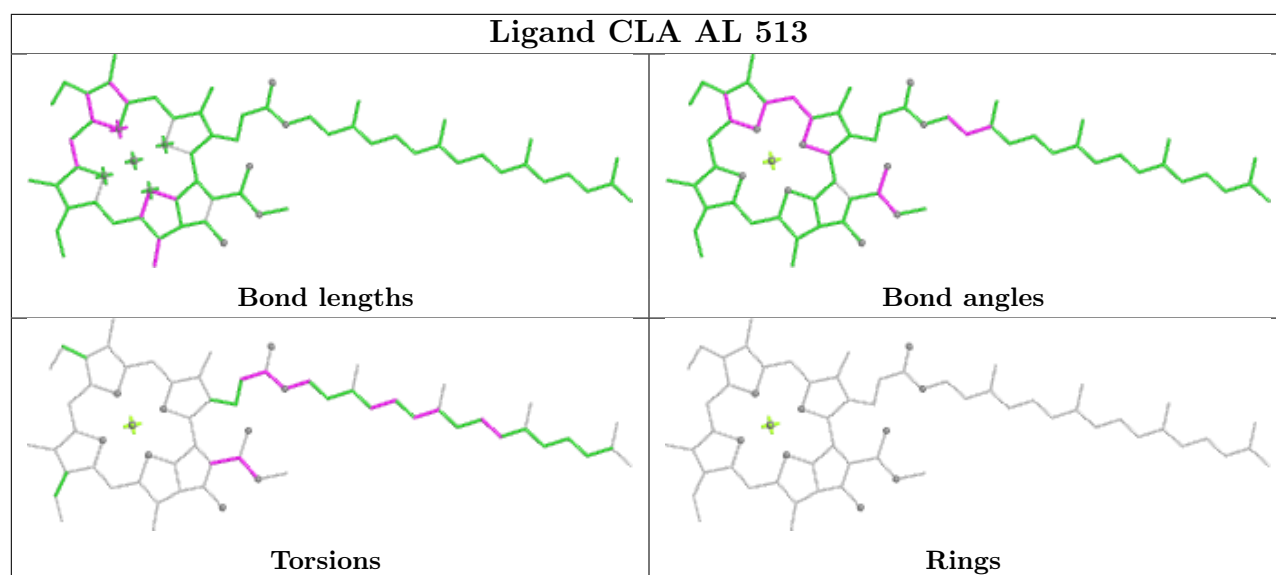
Ligand CLA AR 617

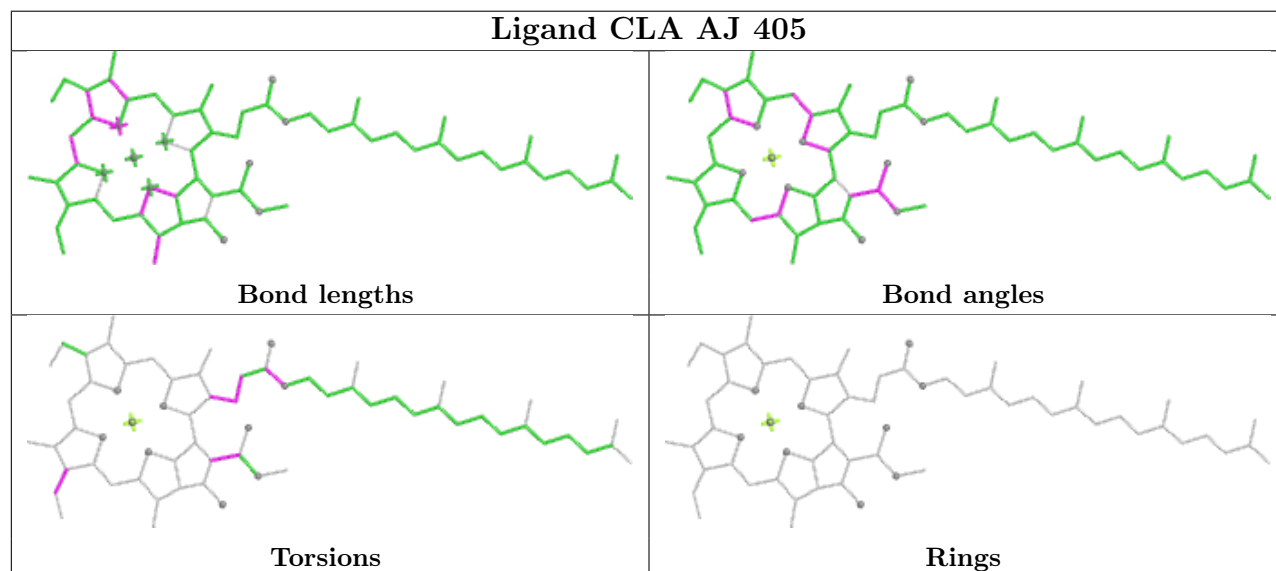
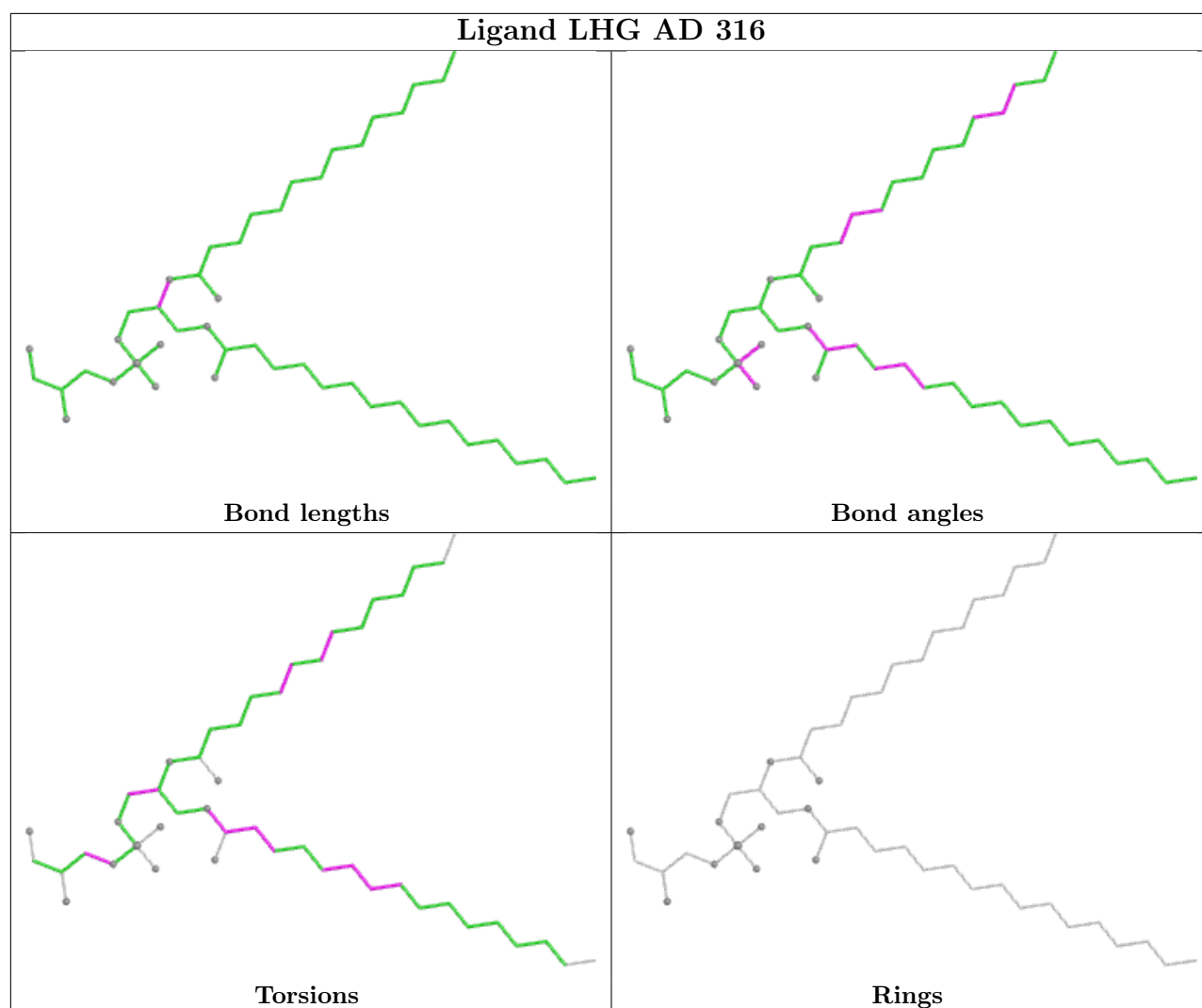


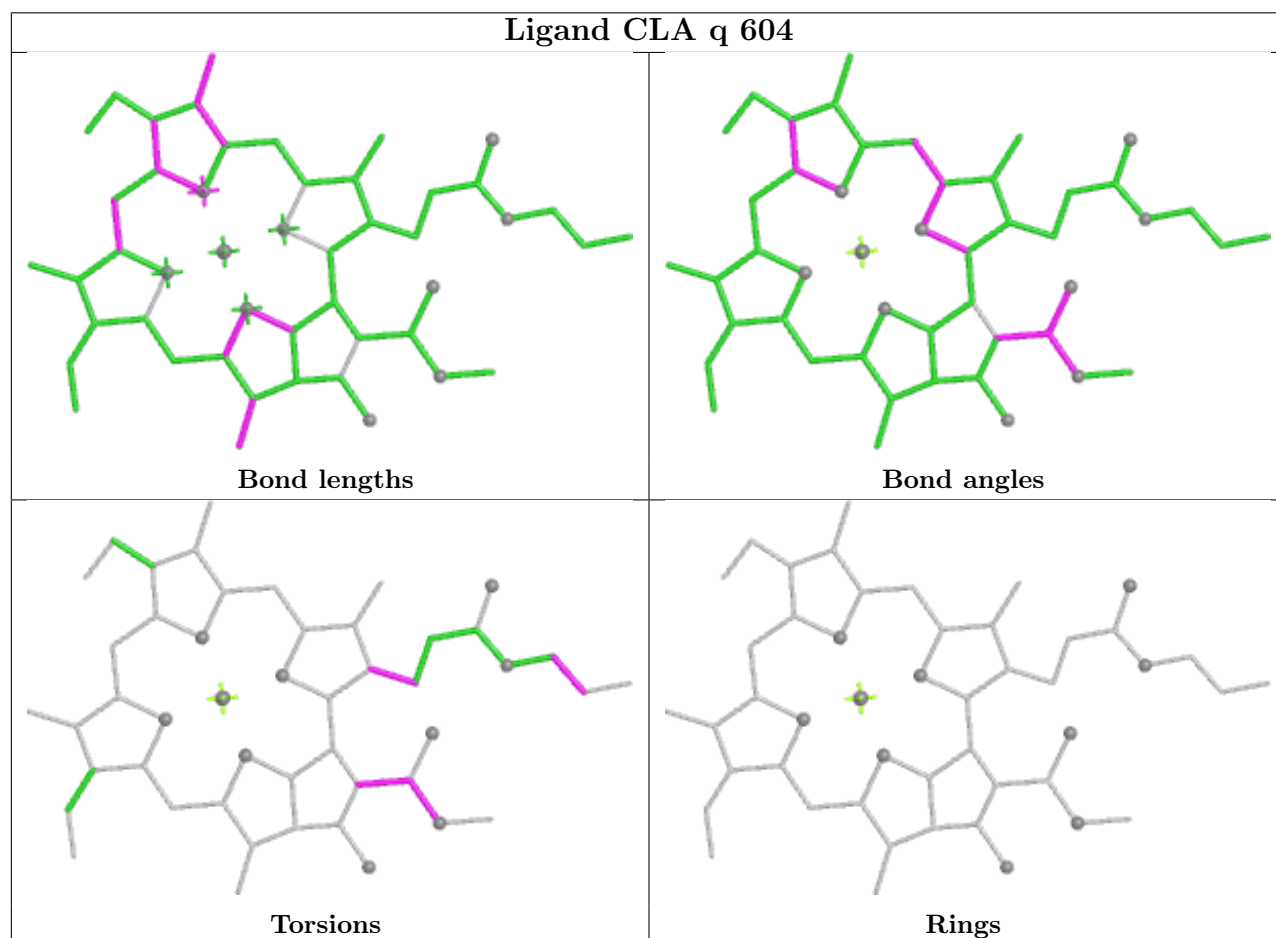
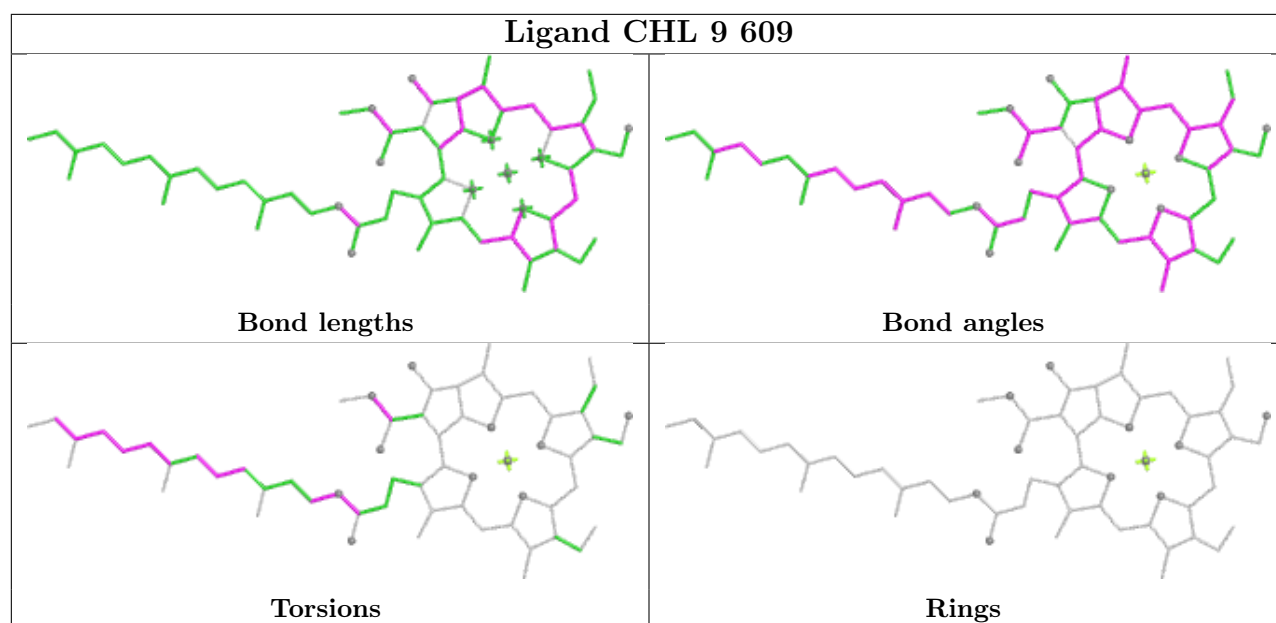
Ligand CLA v 303



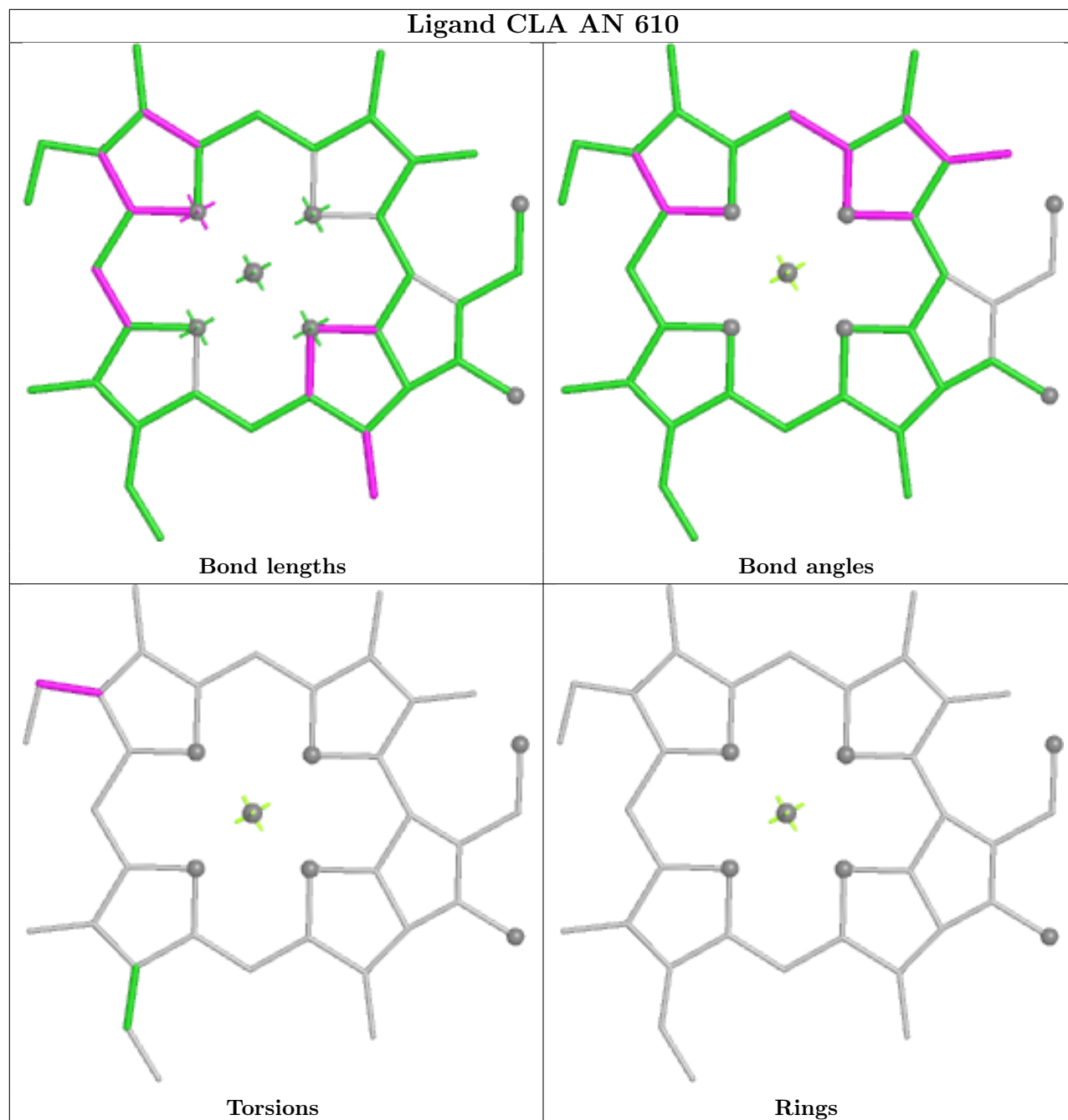
Ligand CLA 9 613**Ligand DGD j 102**

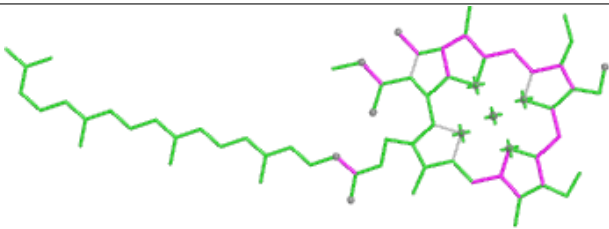
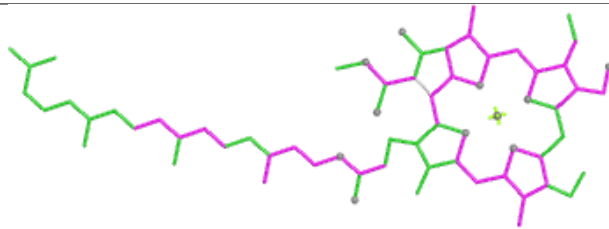
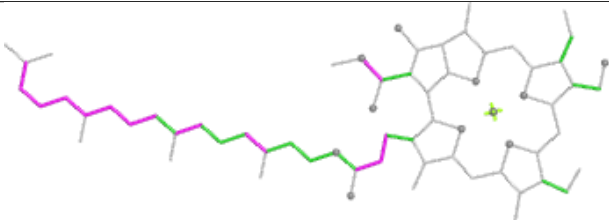
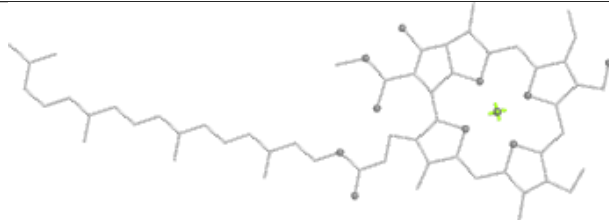


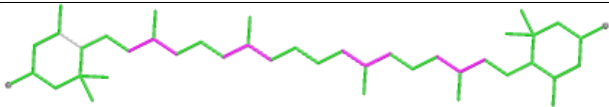
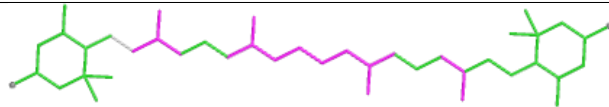
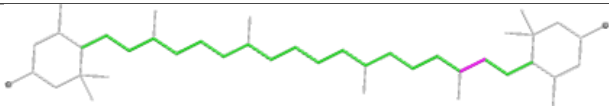
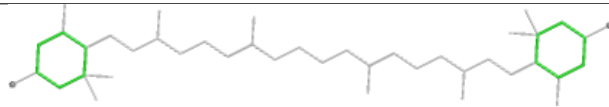


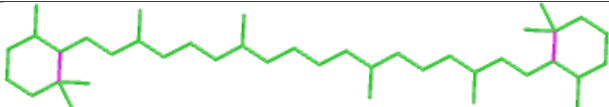
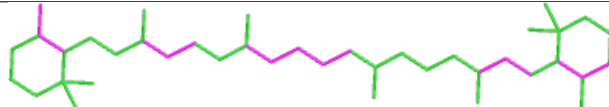
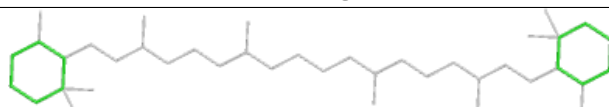


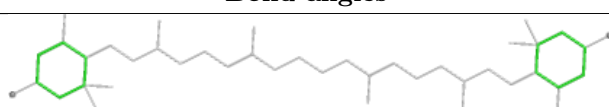
Ligand CLA AN 610

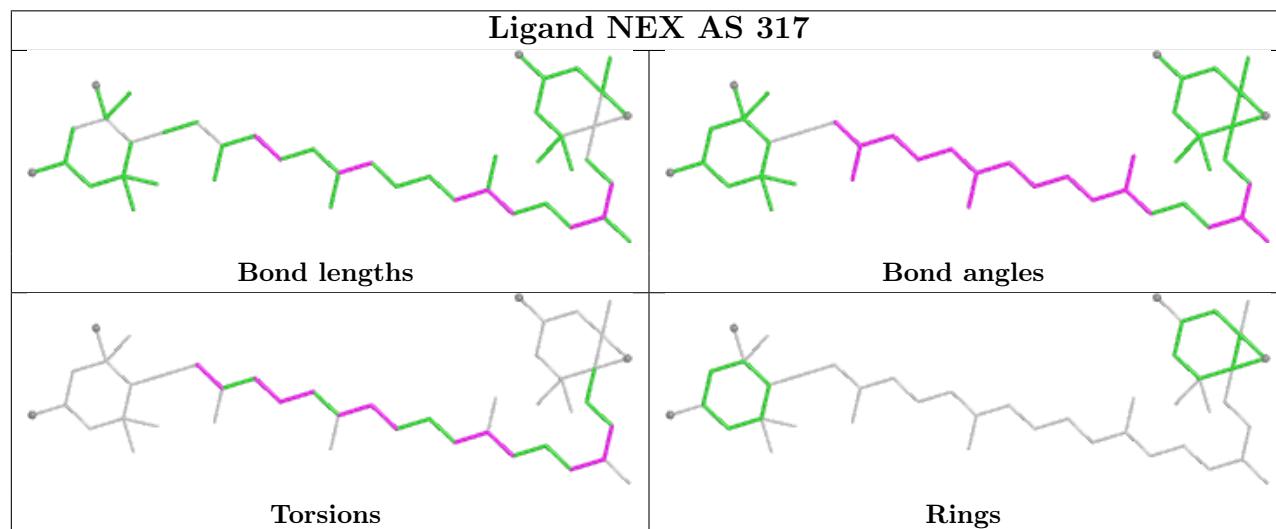
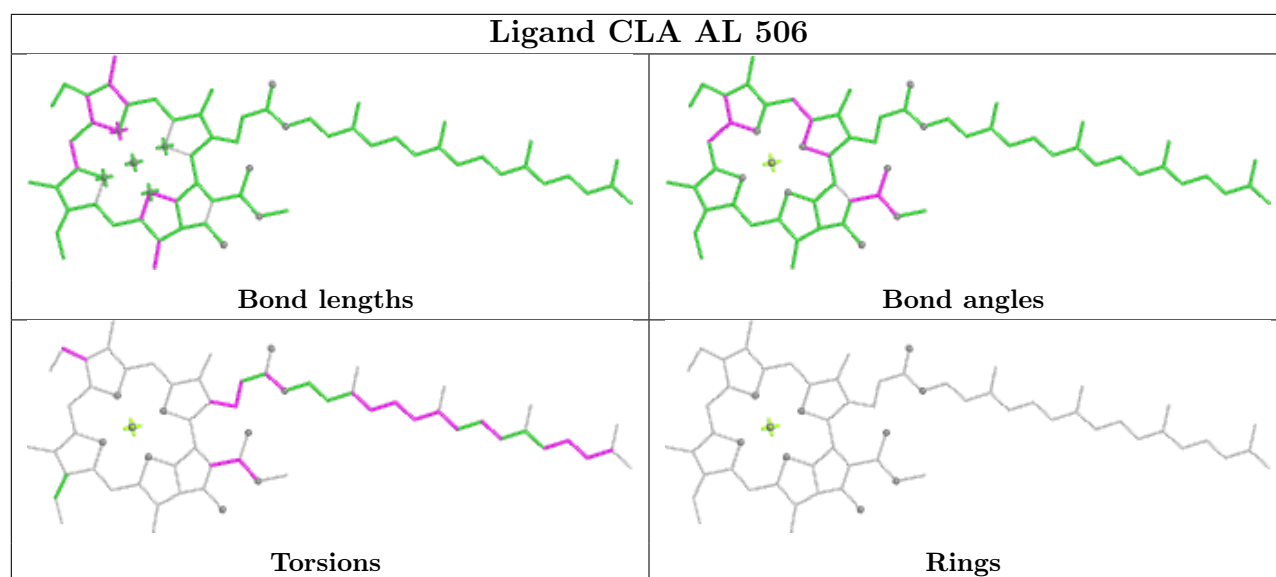


Ligand CHL AU 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

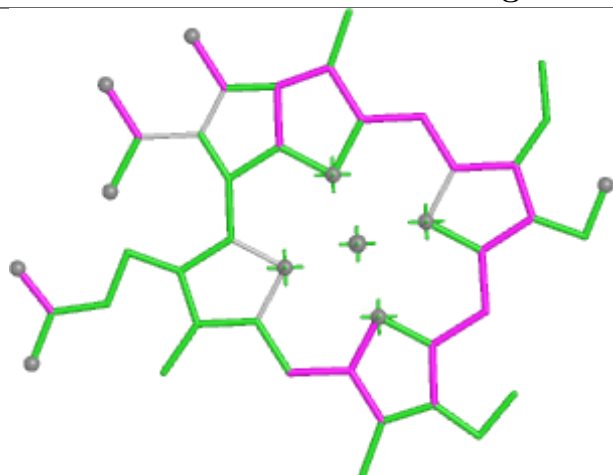
Ligand LUT AH 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

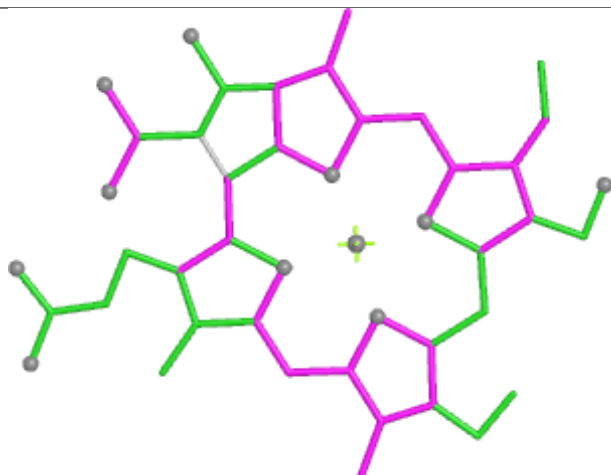
Ligand LUT AA 615	
	
Bond lengths	Bond angles
	
Torsions	Rings



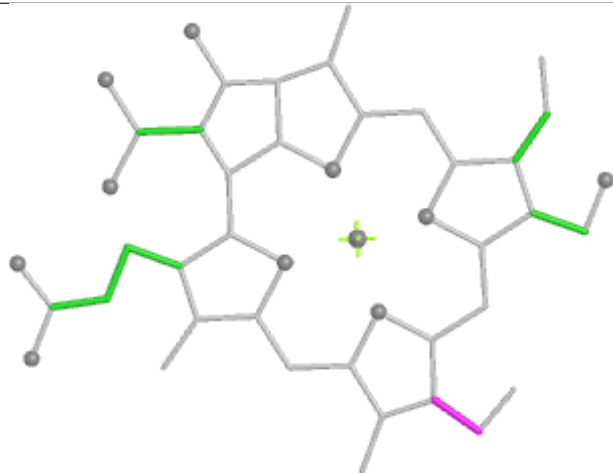
Ligand CHL AF 601



Bond lengths



Bond angles

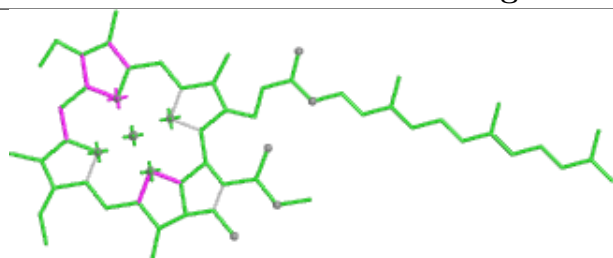


Torsions

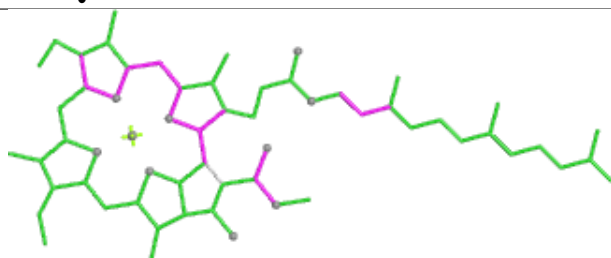


Rings

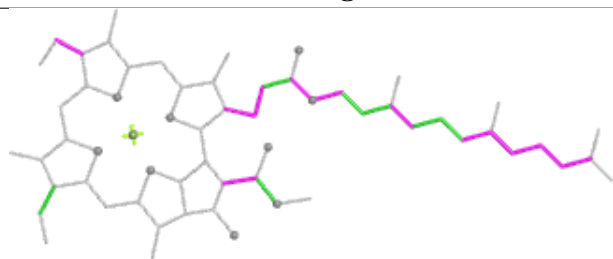
Ligand CLA AQ 611



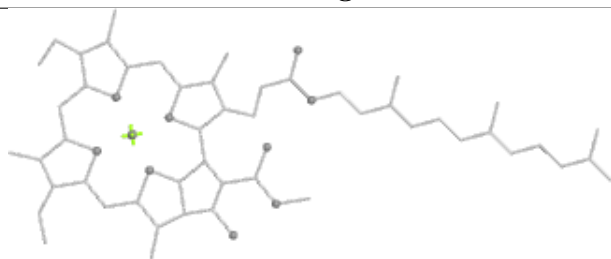
Bond lengths



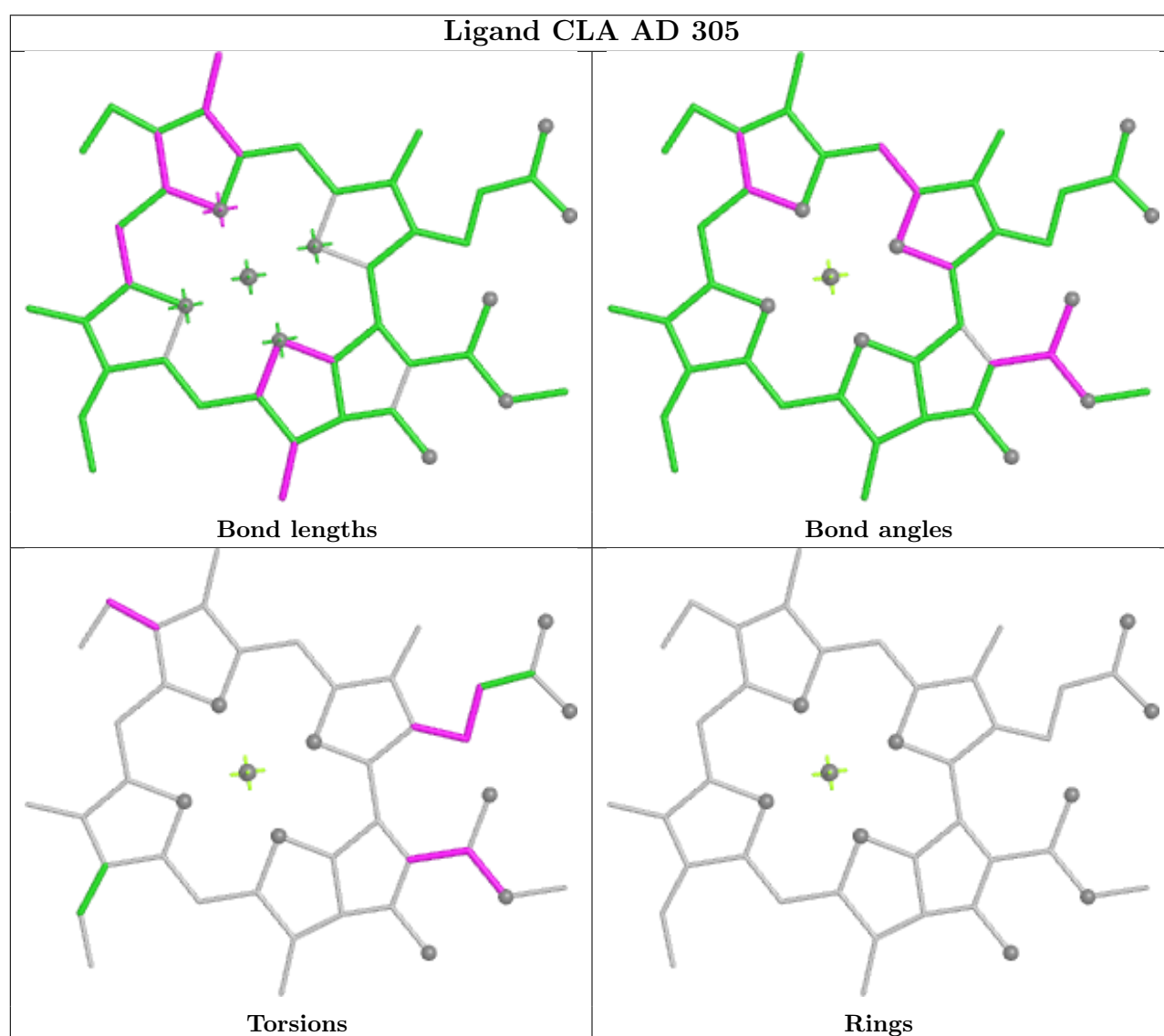
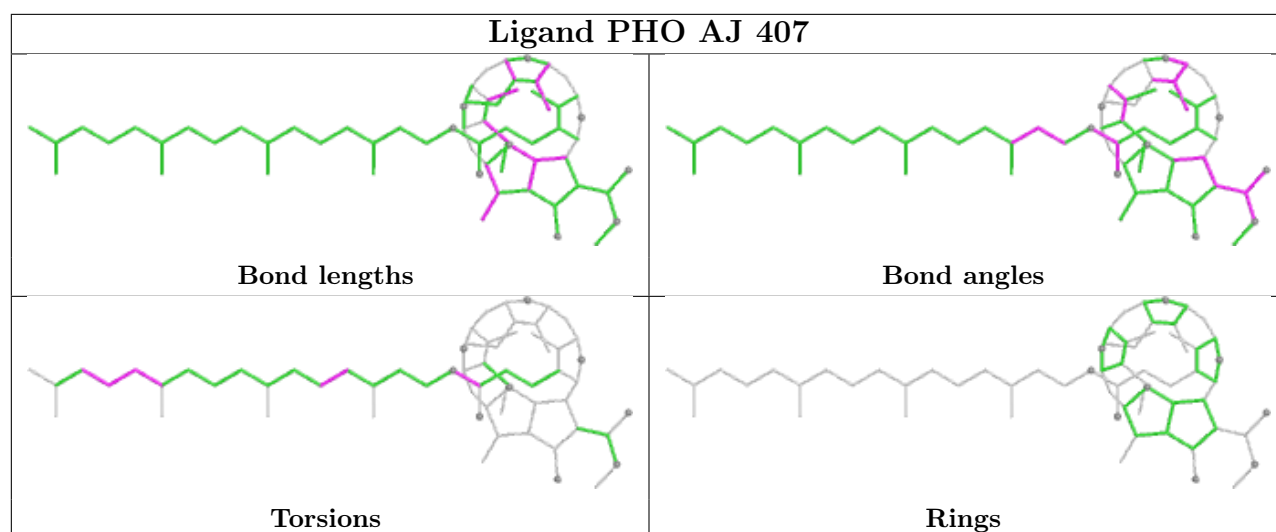
Bond angles



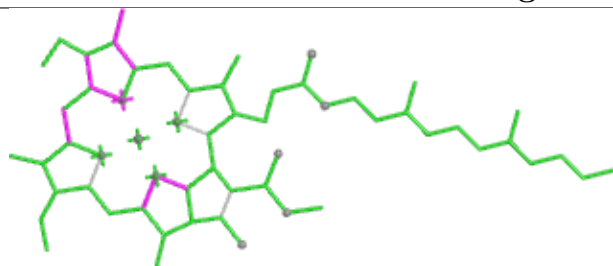
Torsions



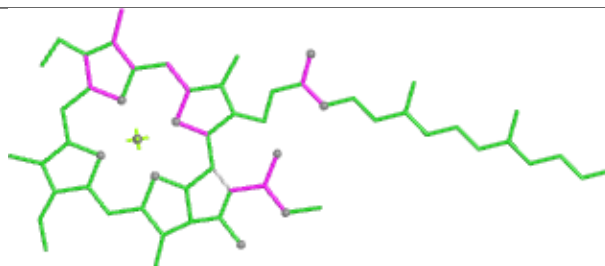
Rings



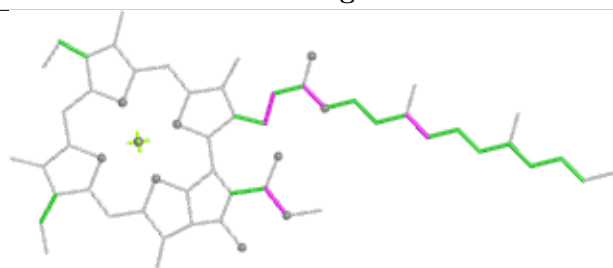
Ligand CLA 0 612



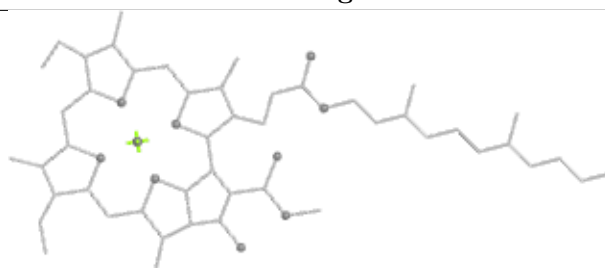
Bond lengths



Bond angles

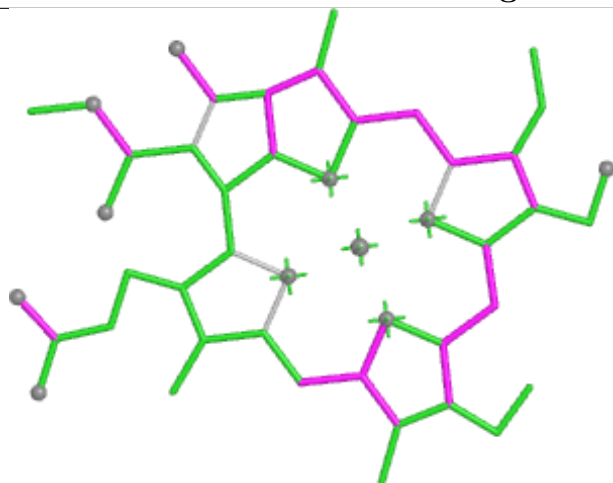


Torsions

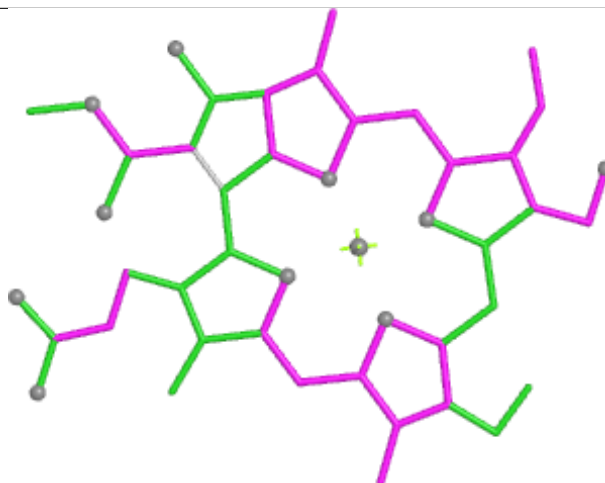


Rings

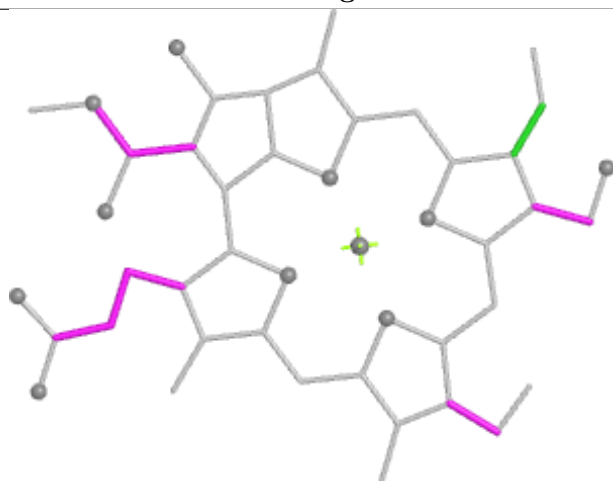
Ligand CHL AA 607



Bond lengths



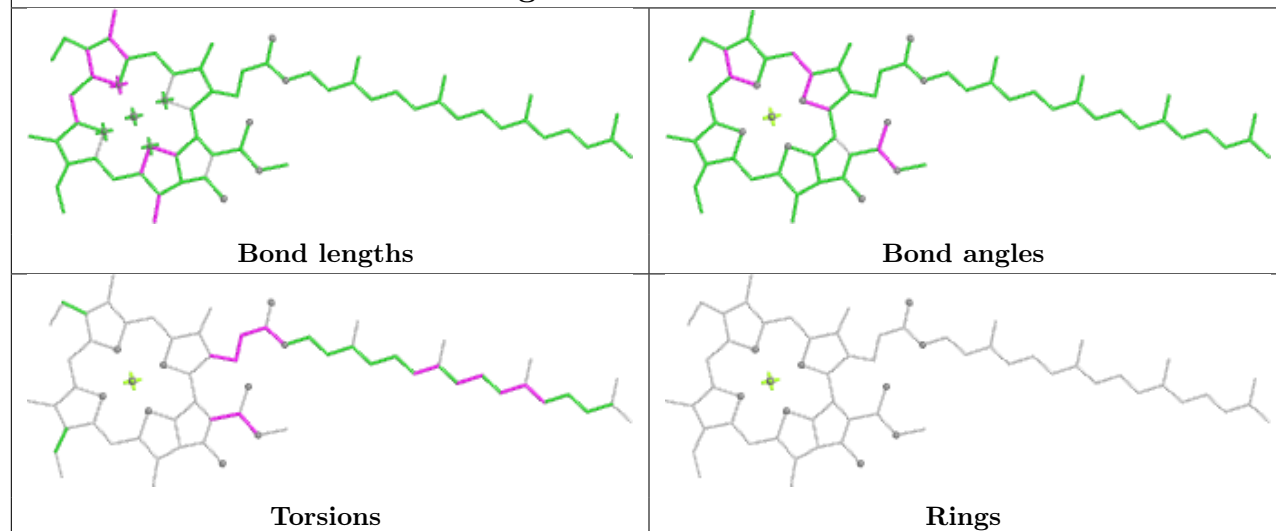
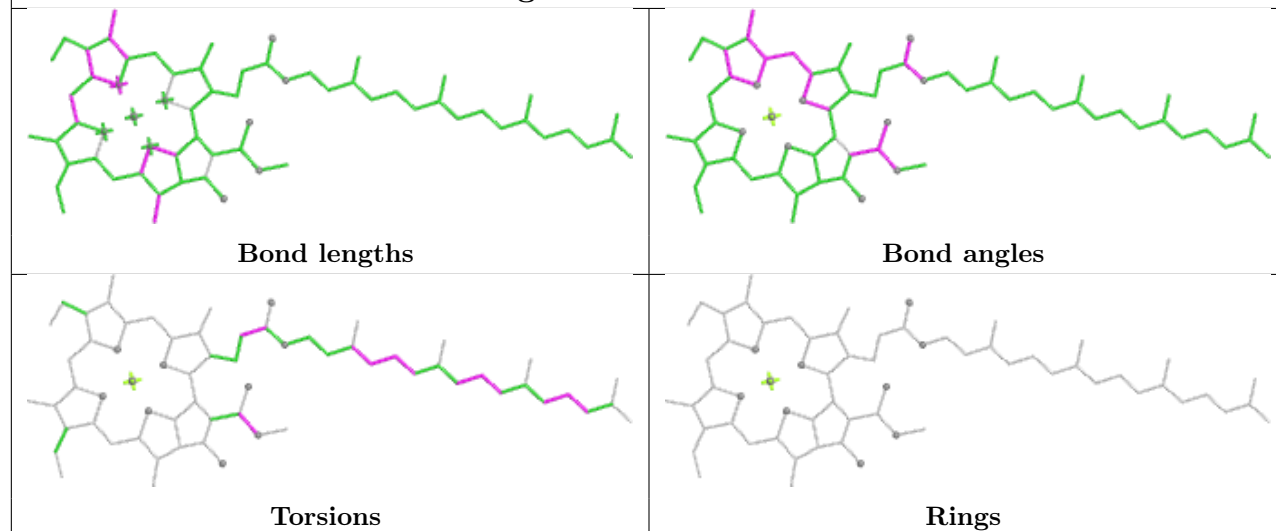
Bond angles

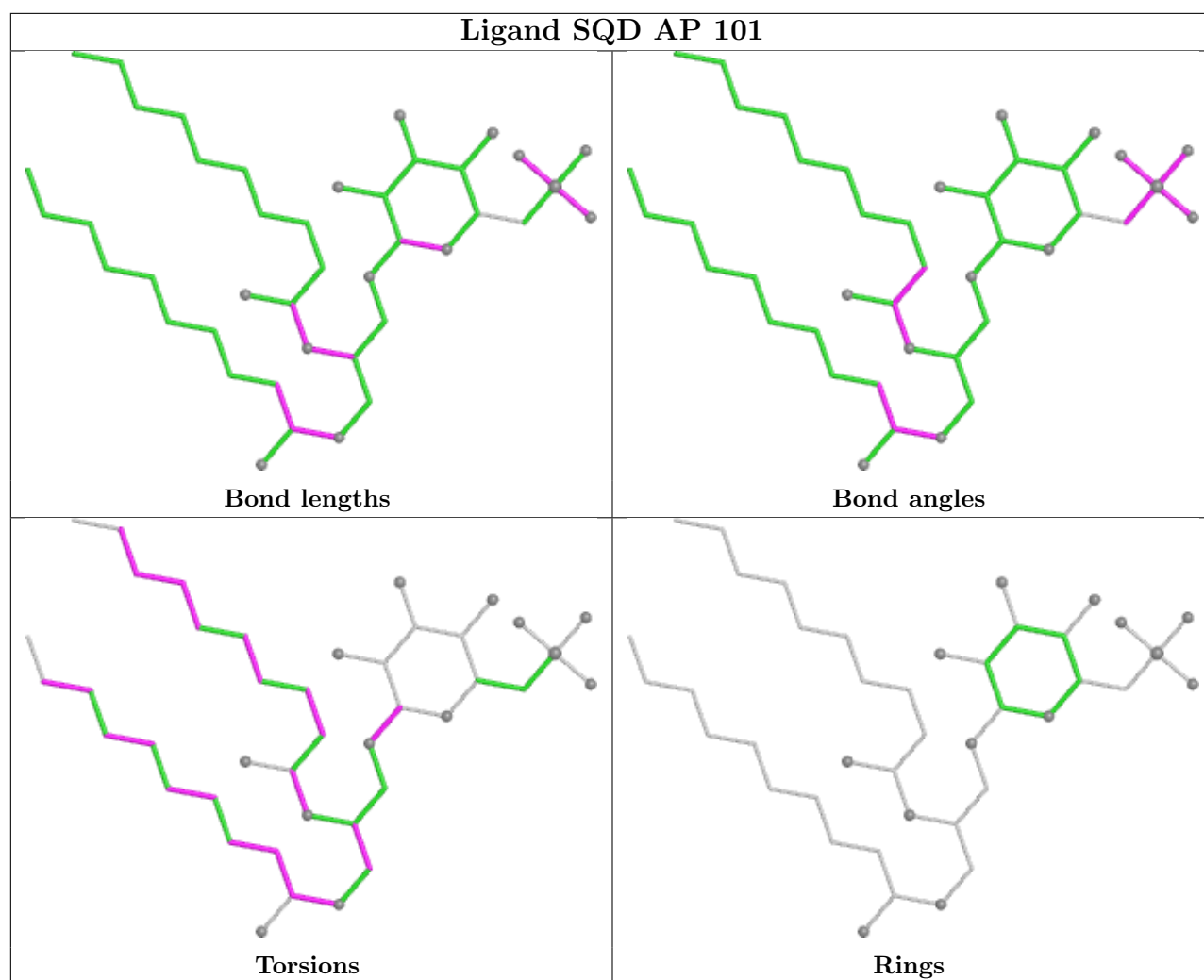


Torsions

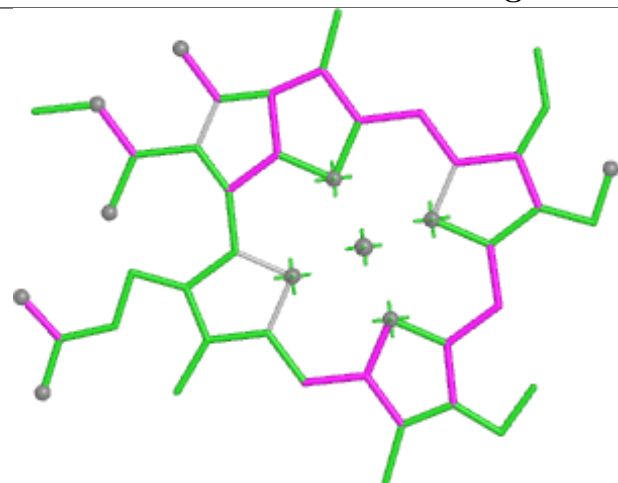


Rings

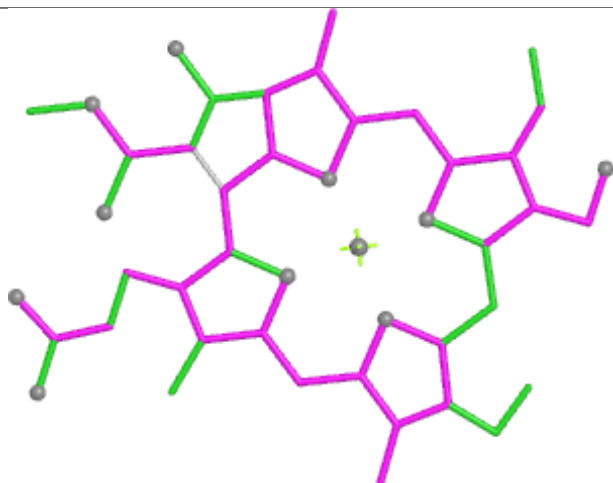
Ligand CLA AU 612**Ligand CLA AK 615**



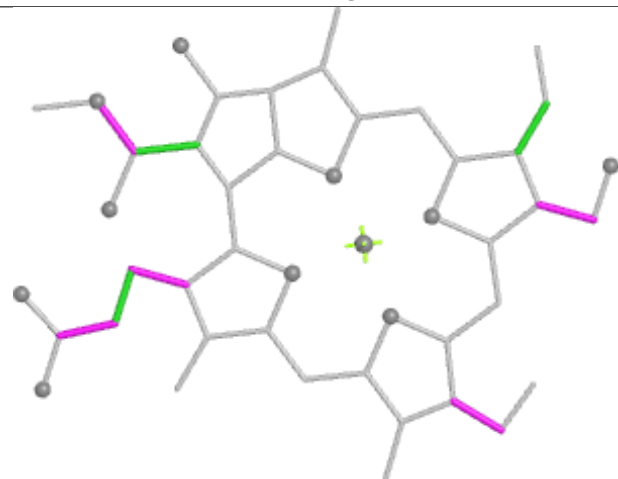
Ligand CHL AC 605



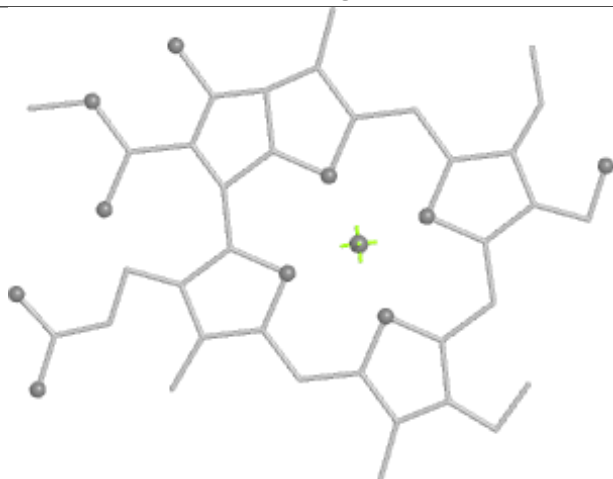
Bond lengths



Bond angles

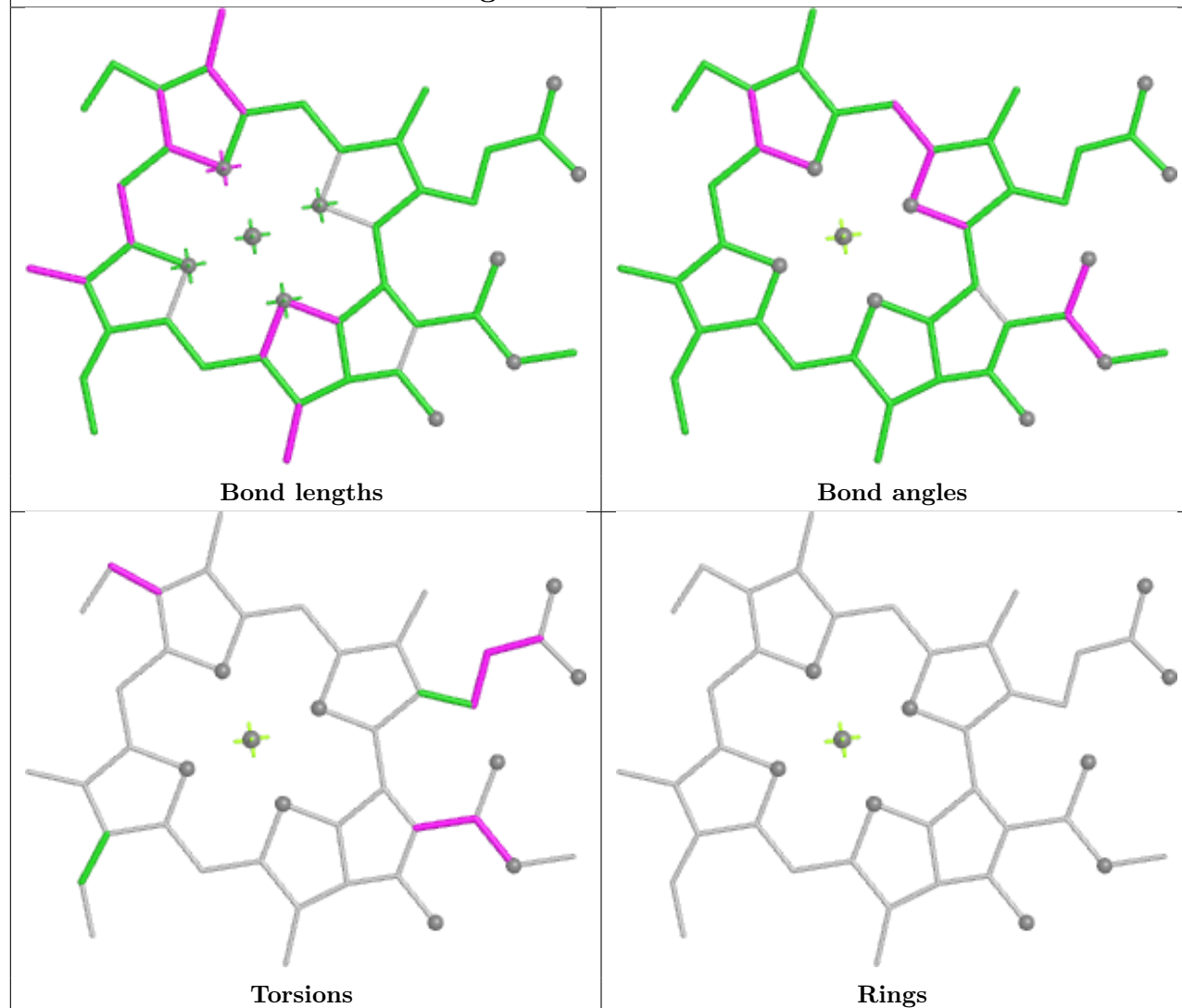


Torsions

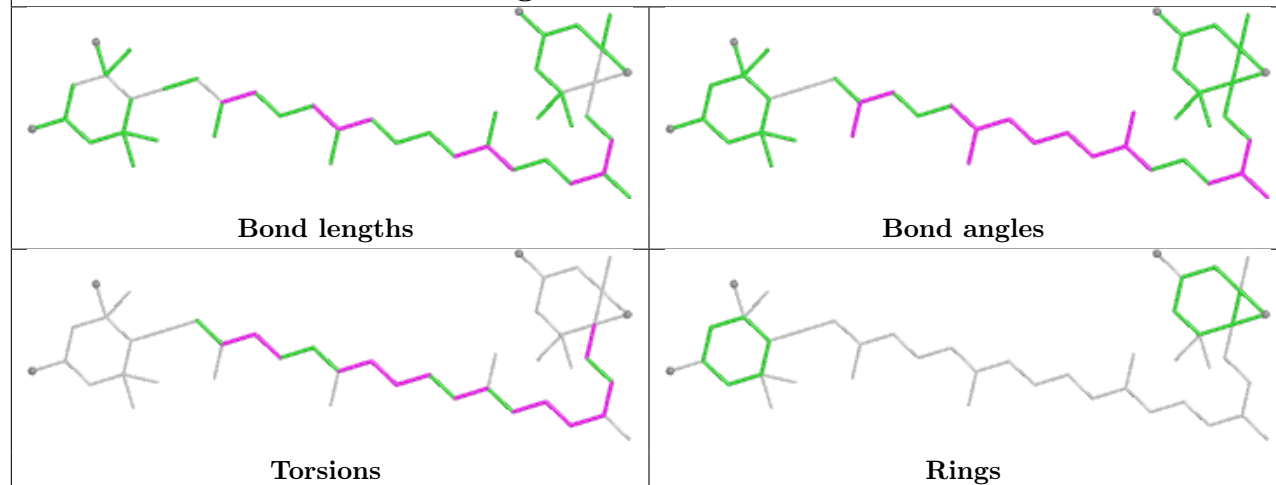


Rings

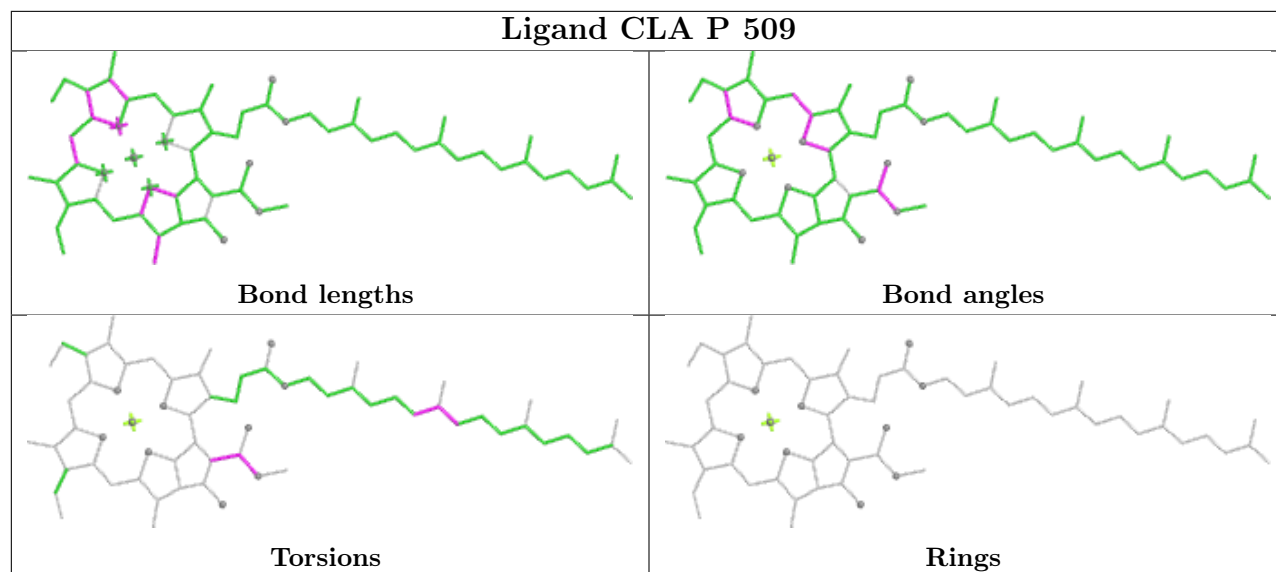
Ligand CLA AD 311



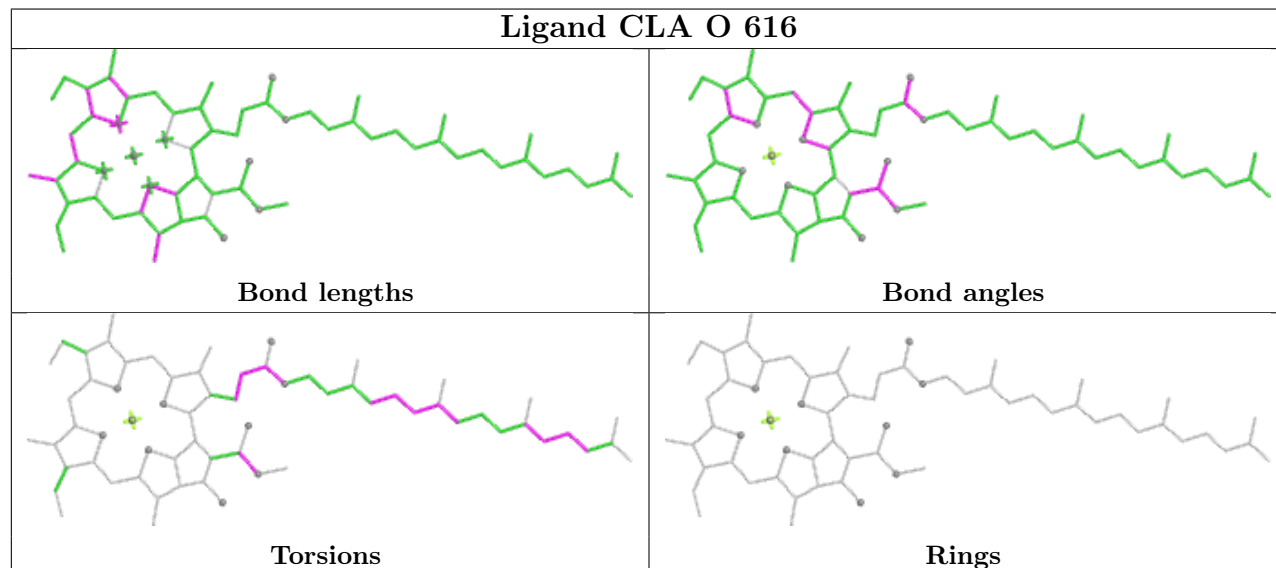
Ligand NEX AU 616



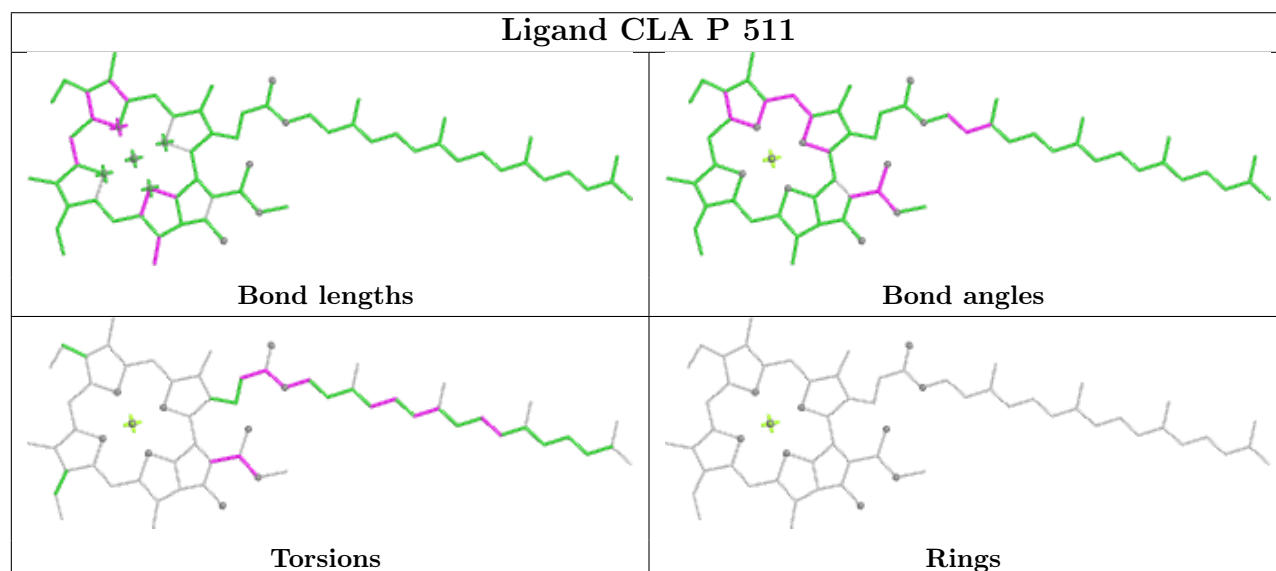
Ligand CLA P 509

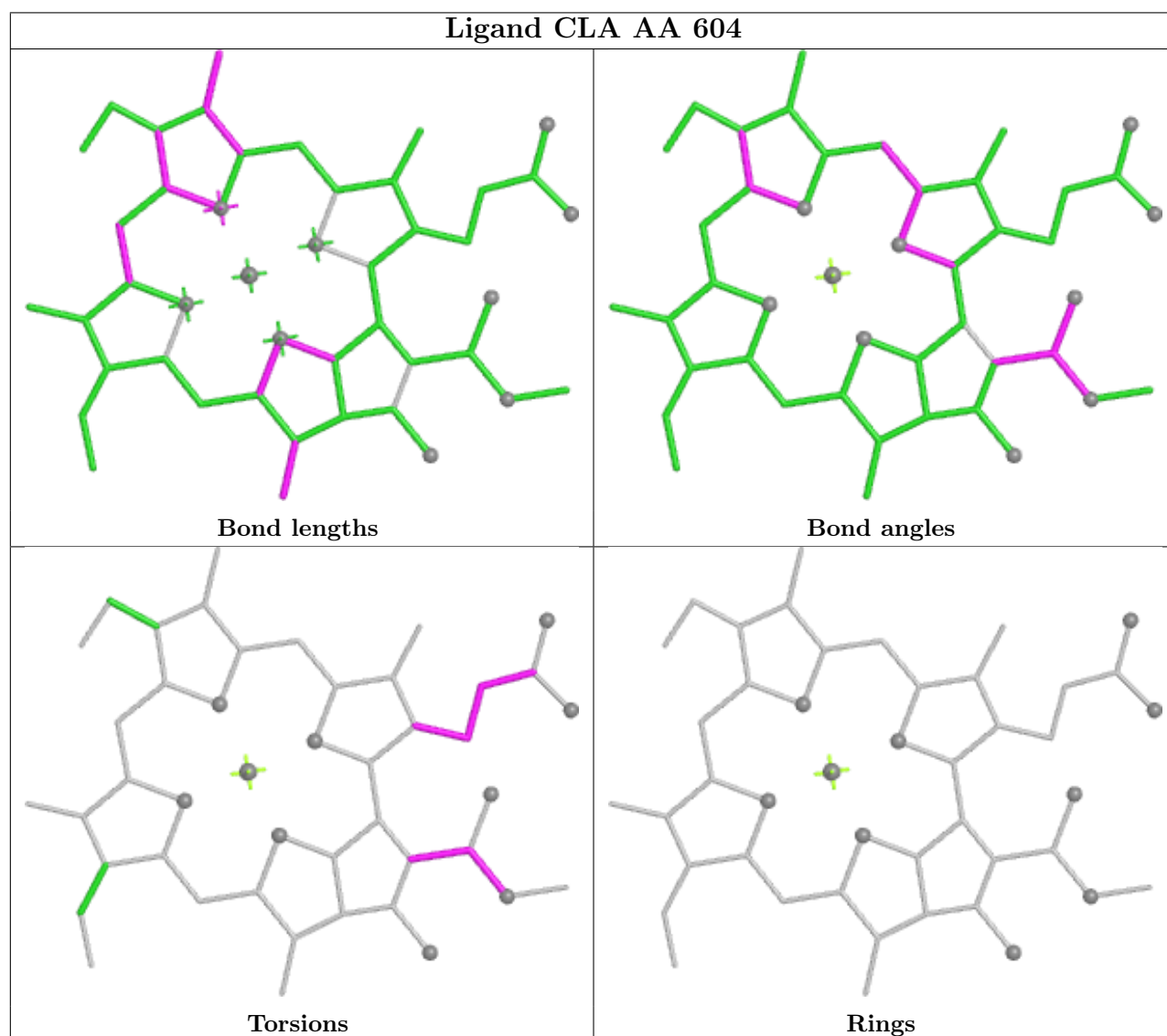
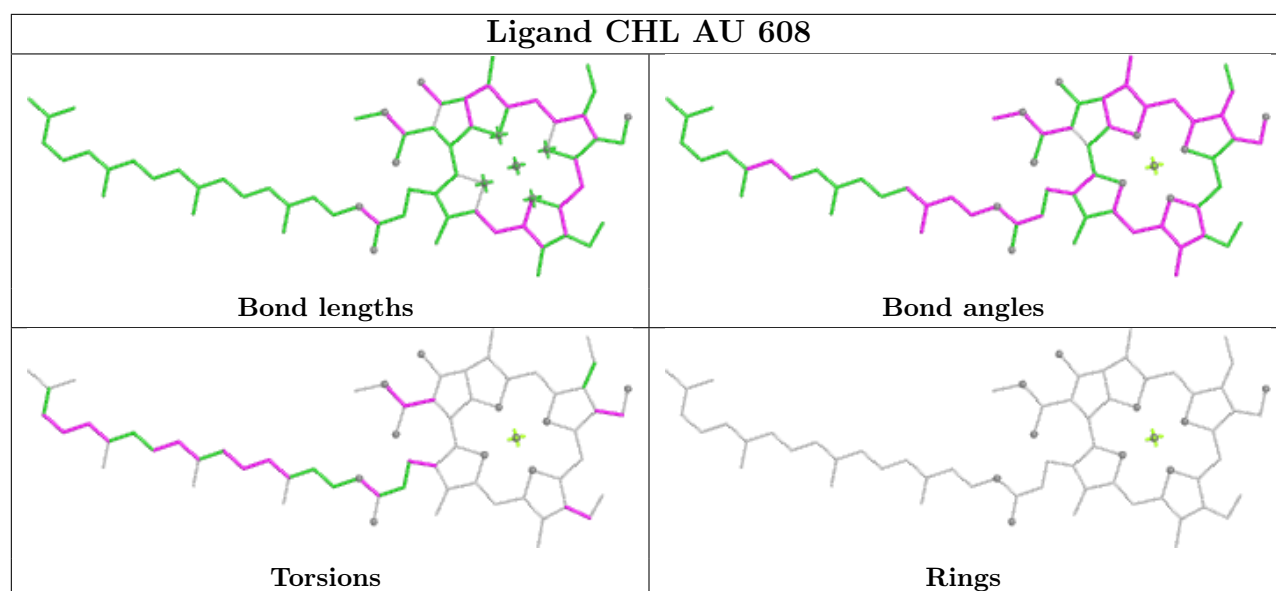


Ligand CLA O 616

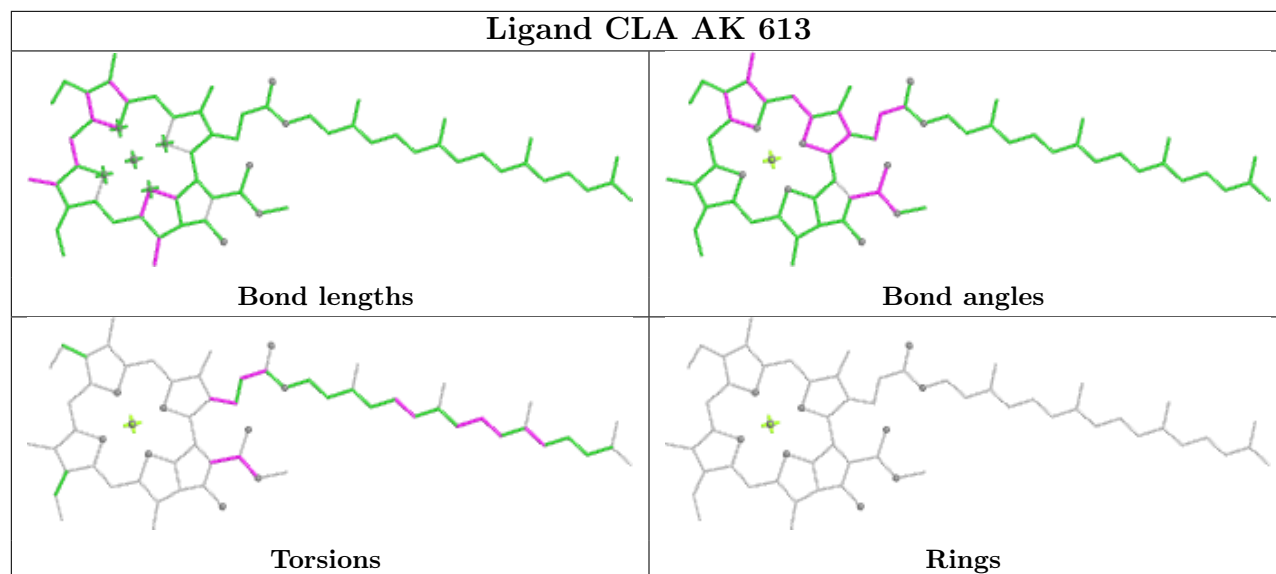


Ligand CLA P 511

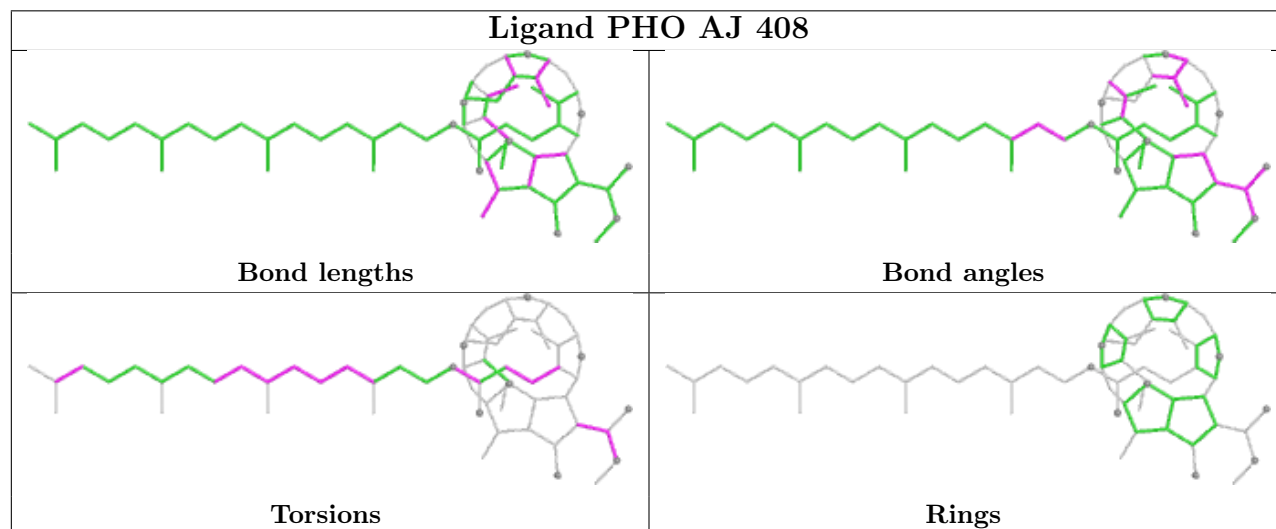




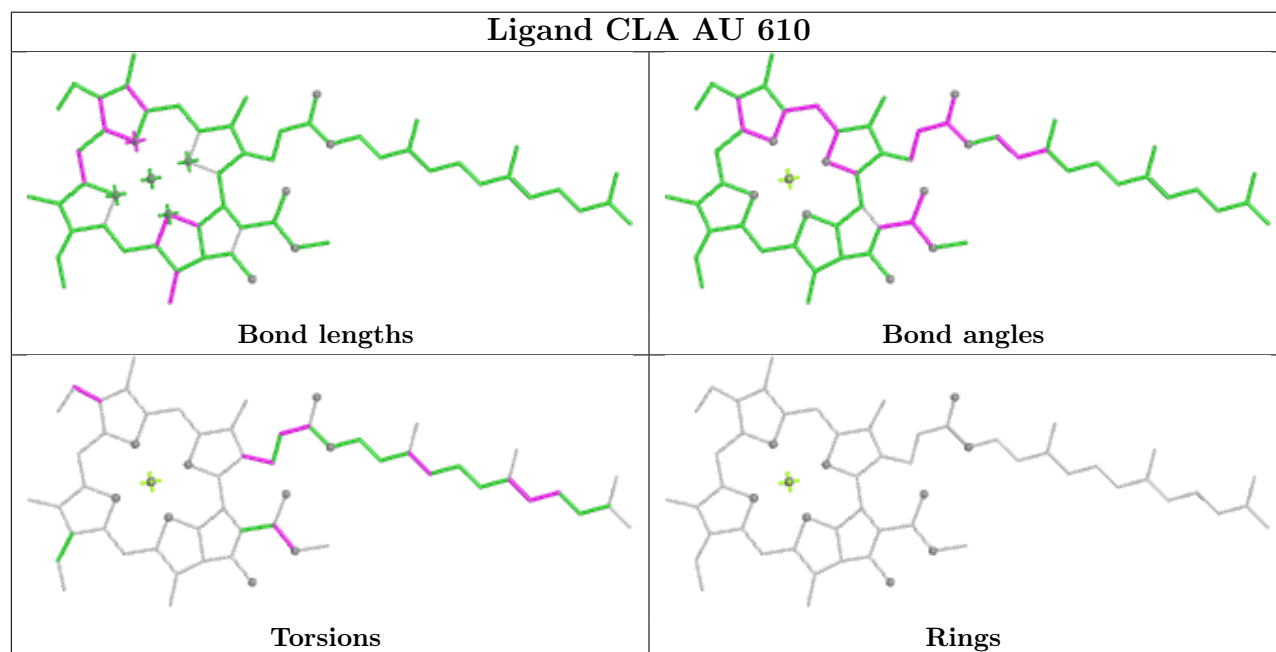
Ligand CLA AK 613

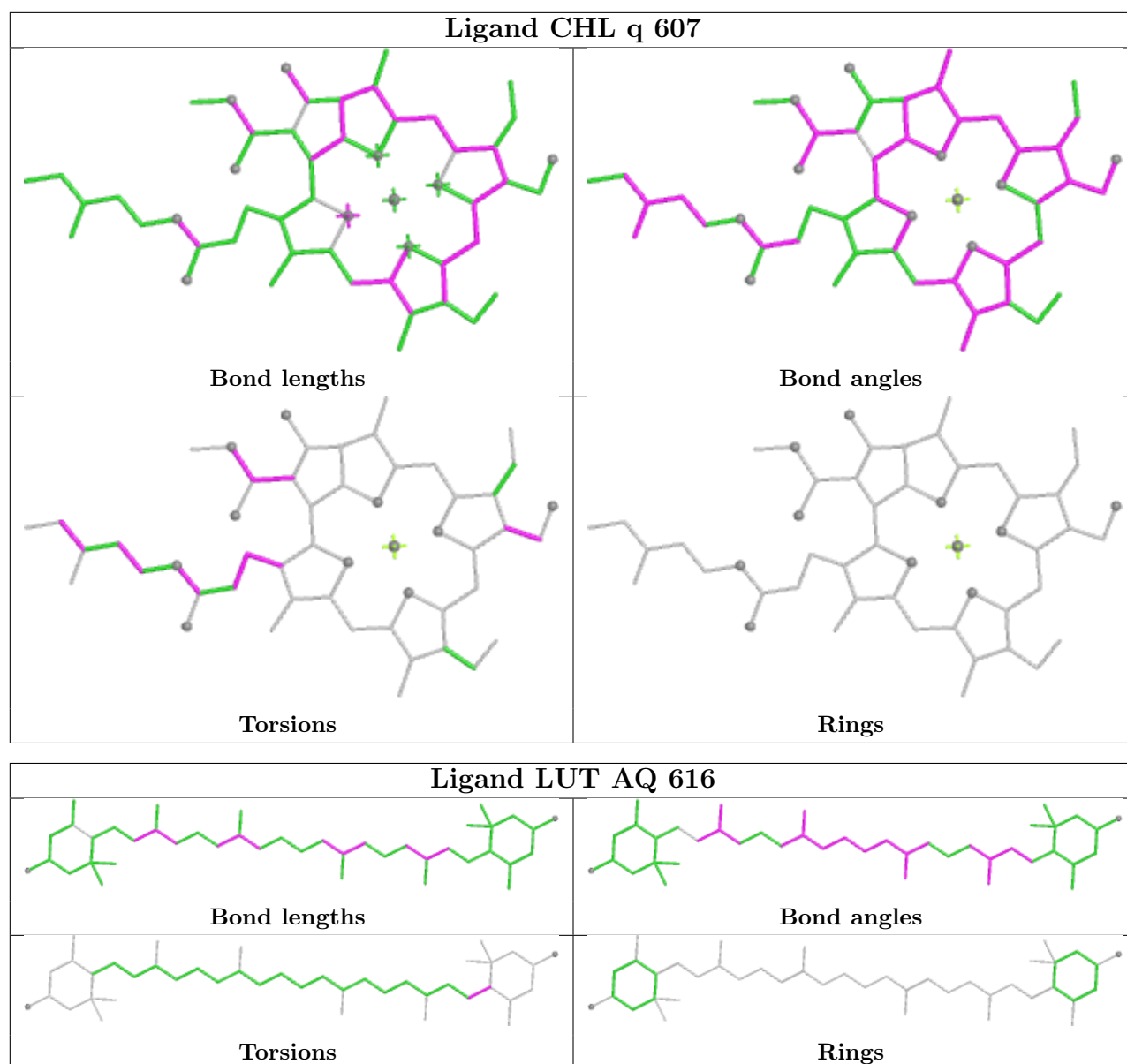


Ligand PHO AJ 408

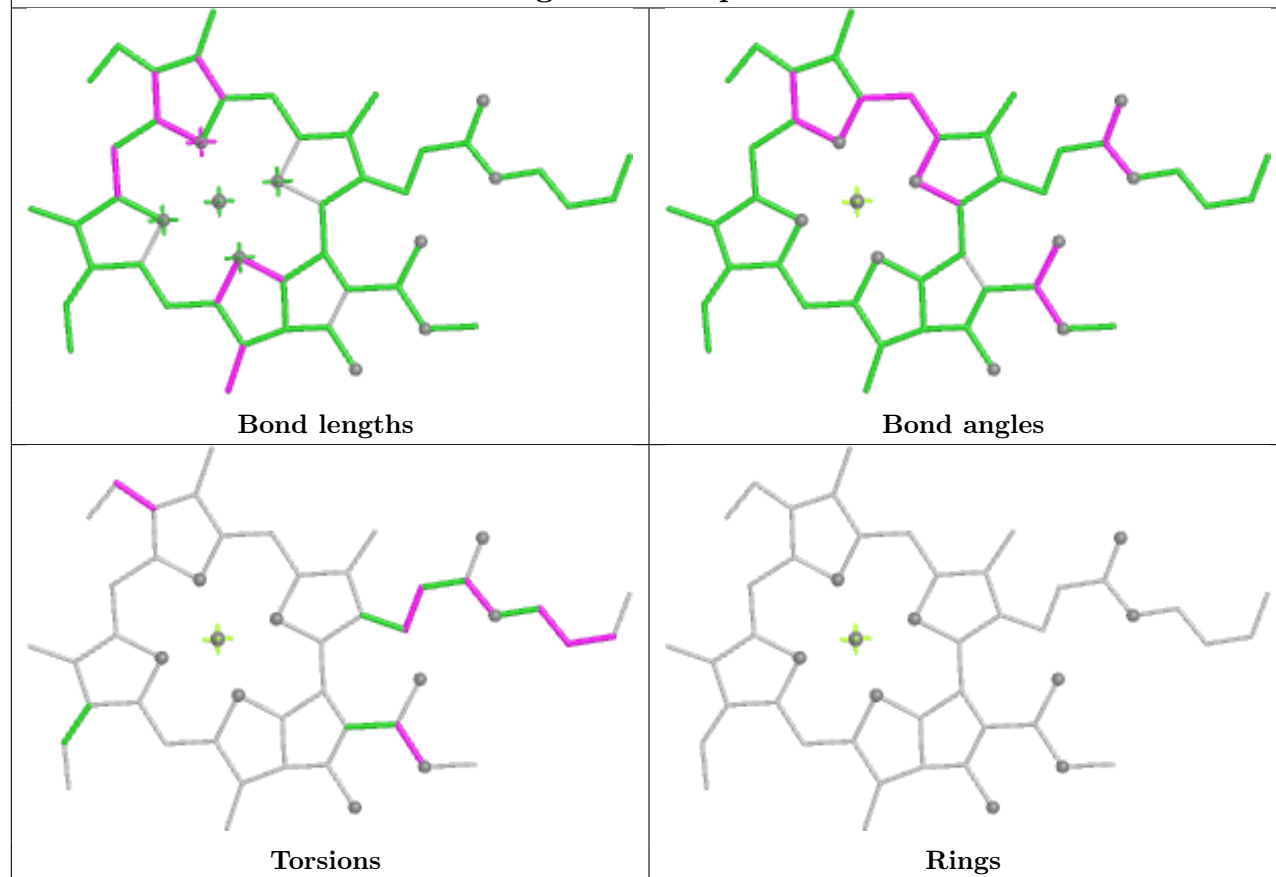


Ligand CLA AU 610

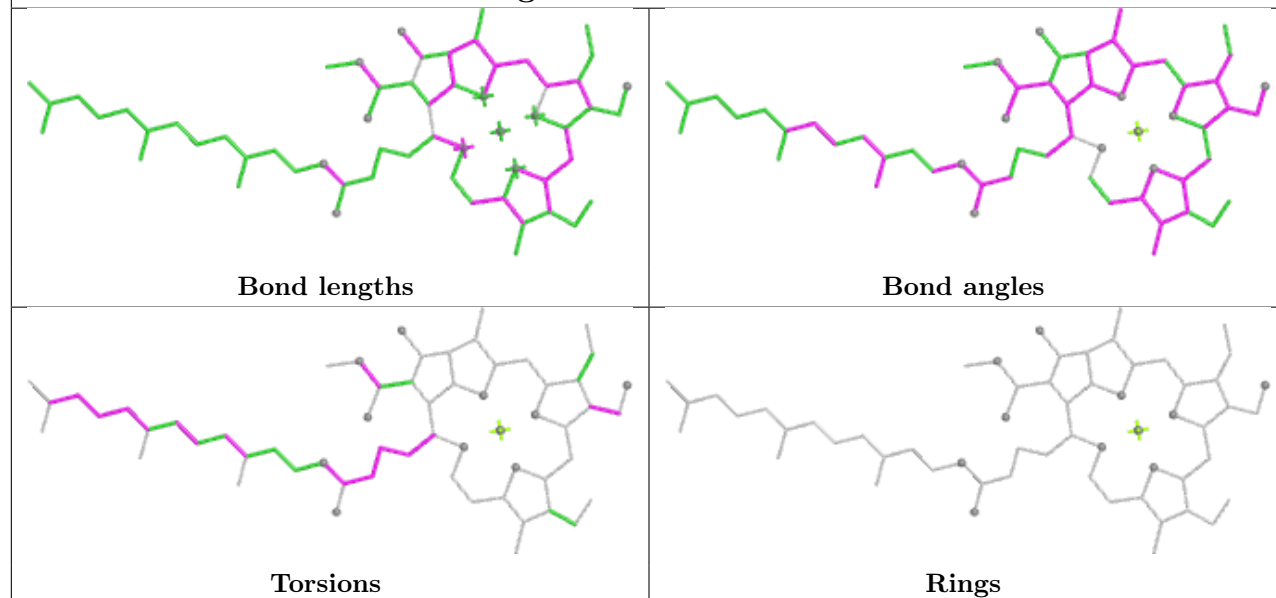


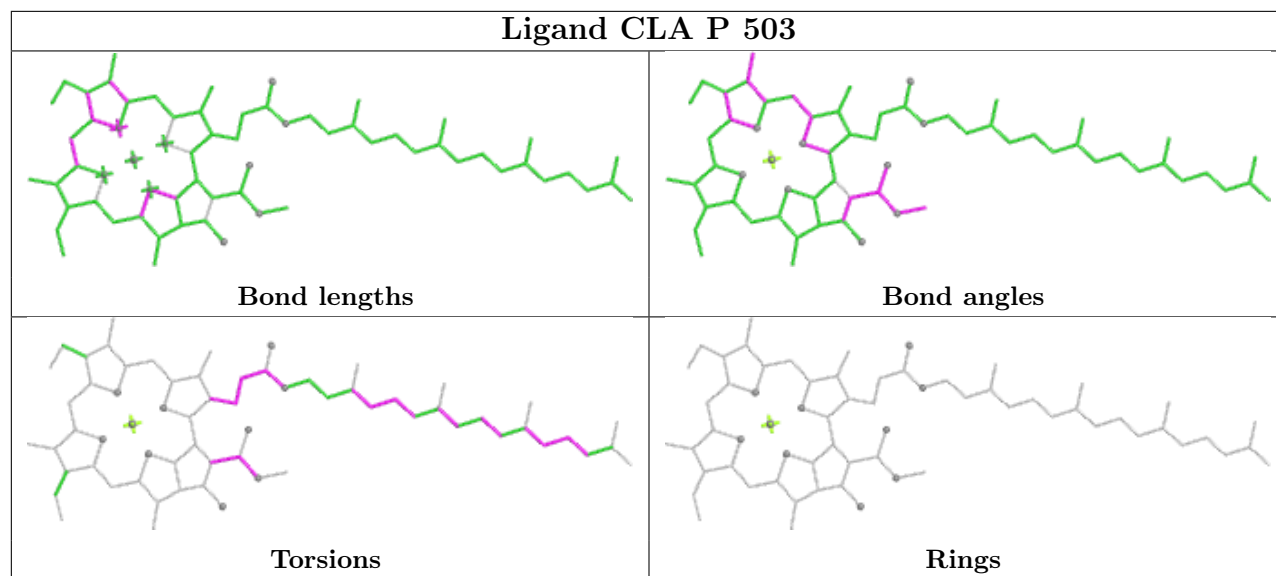


Ligand CLA q 611



Ligand CHL AA 608





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

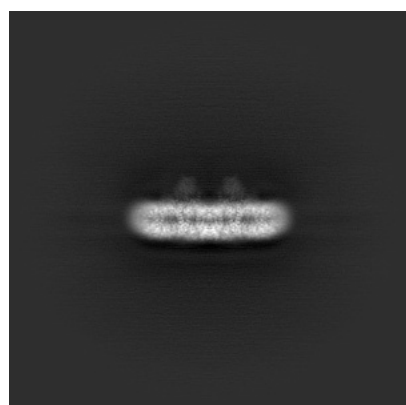
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63018. These allow visual inspection of the internal detail of the map and identification of artifacts.

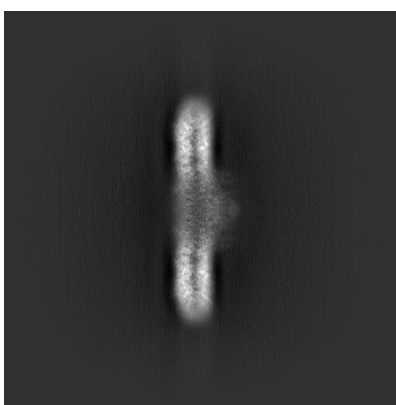
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

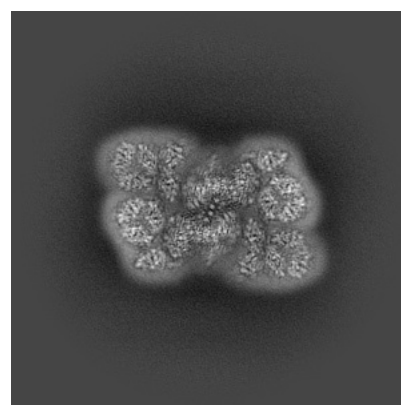
6.1.1 Primary map



X



Y

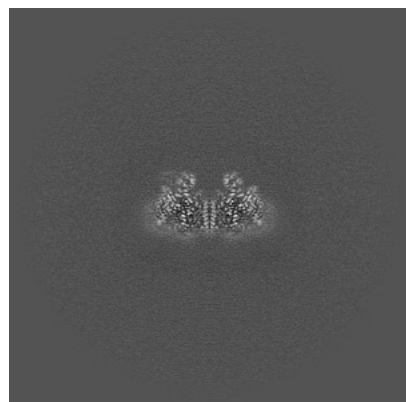


Z

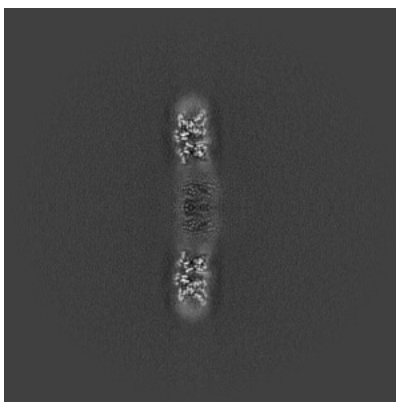
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

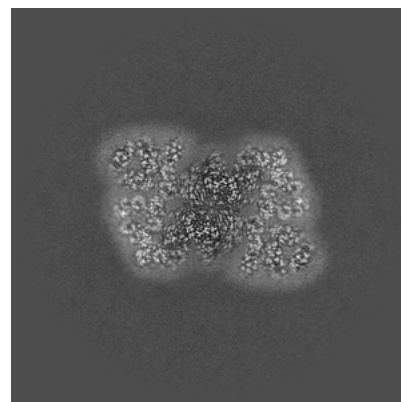
6.2.1 Primary map



X Index: 216



Y Index: 216

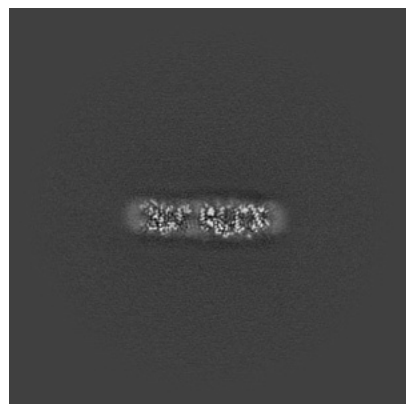


Z Index: 216

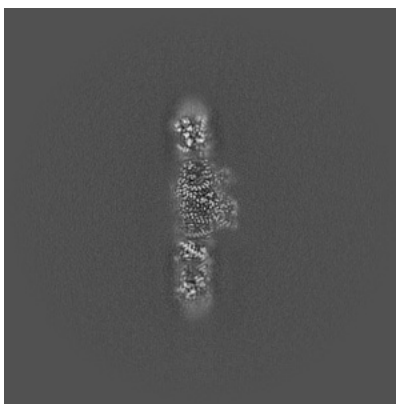
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

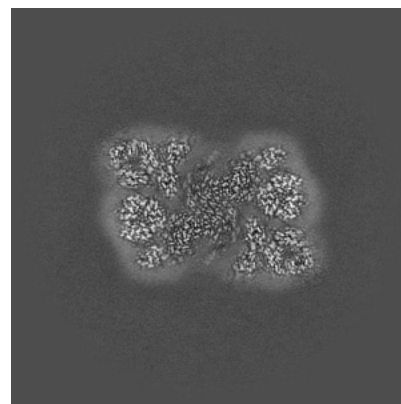
6.3.1 Primary map



X Index: 283



Y Index: 241

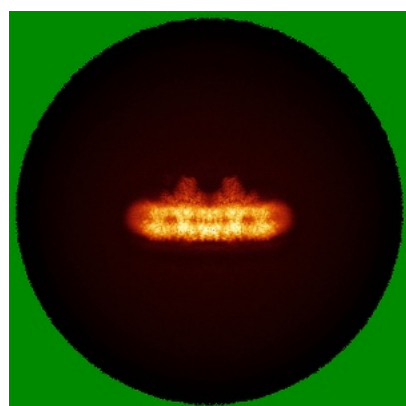


Z Index: 198

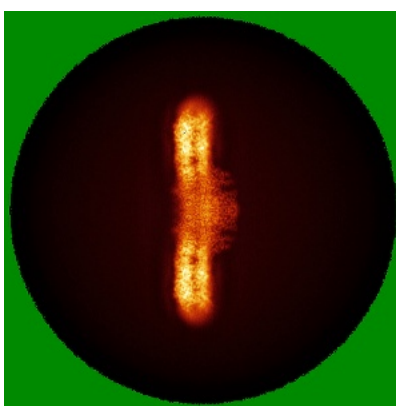
The images above show the largest variance slices of the map in three orthogonal directions.

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

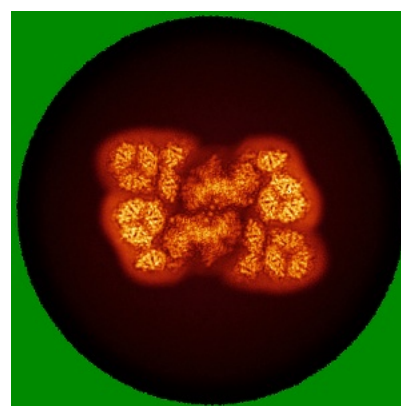
6.4.1 Primary map



X



Y

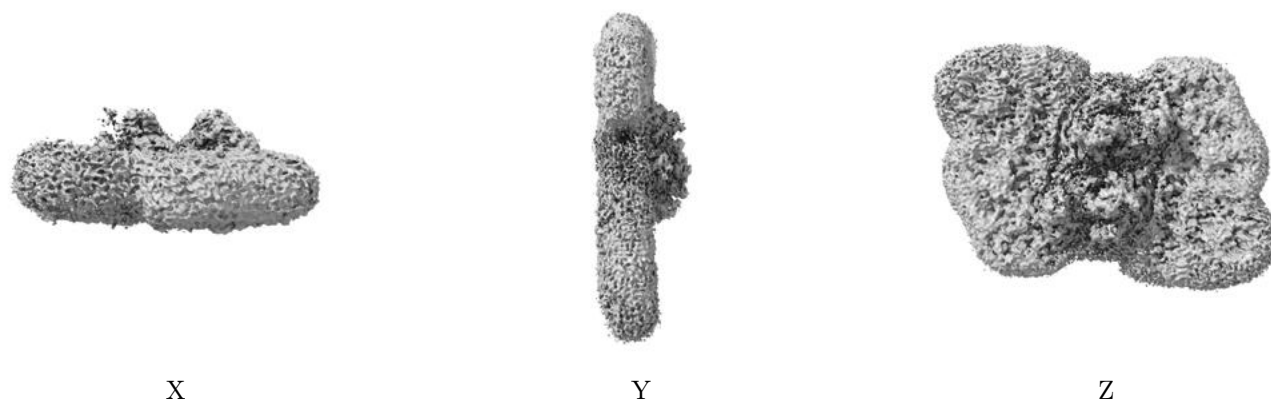


Z

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

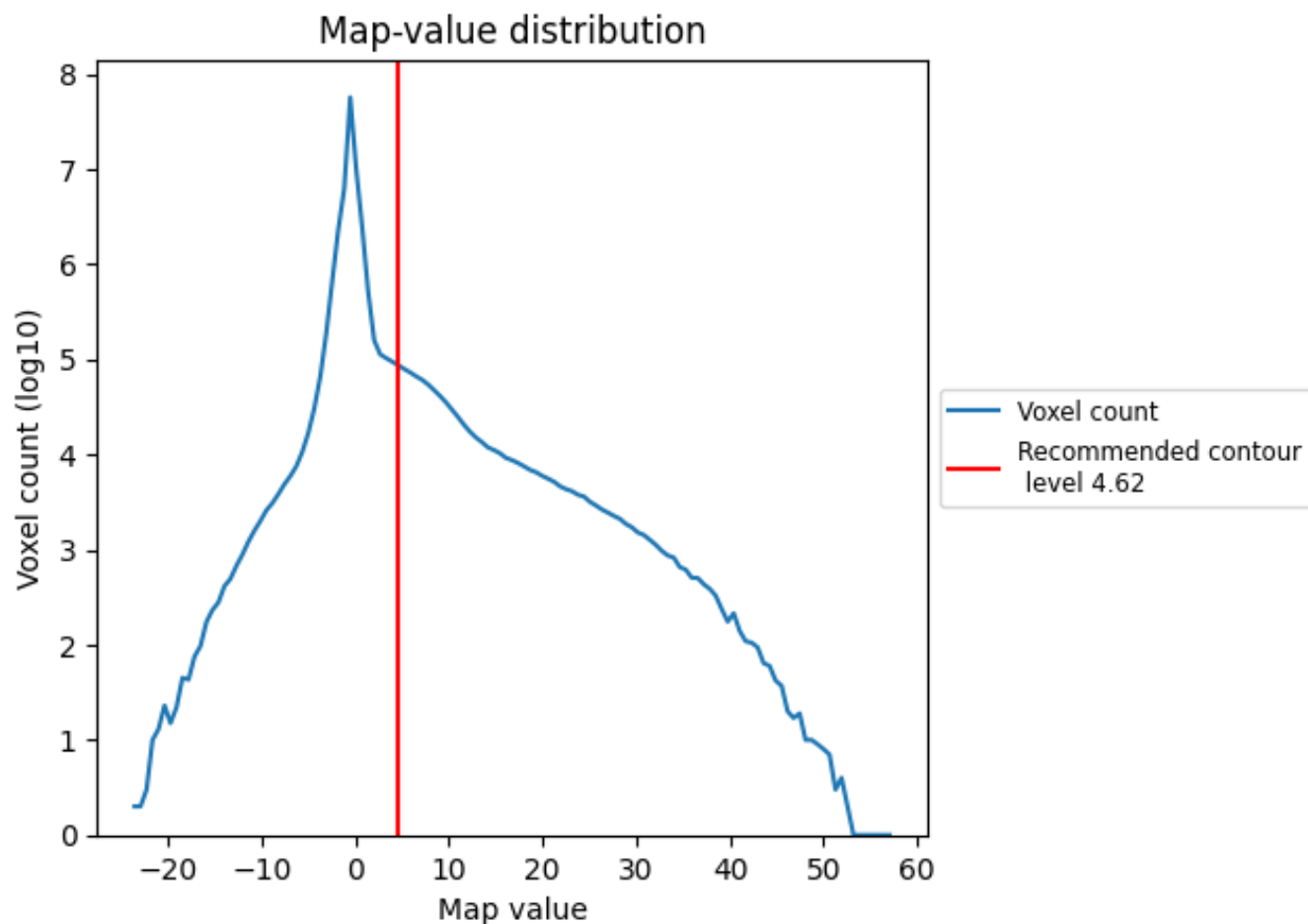
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

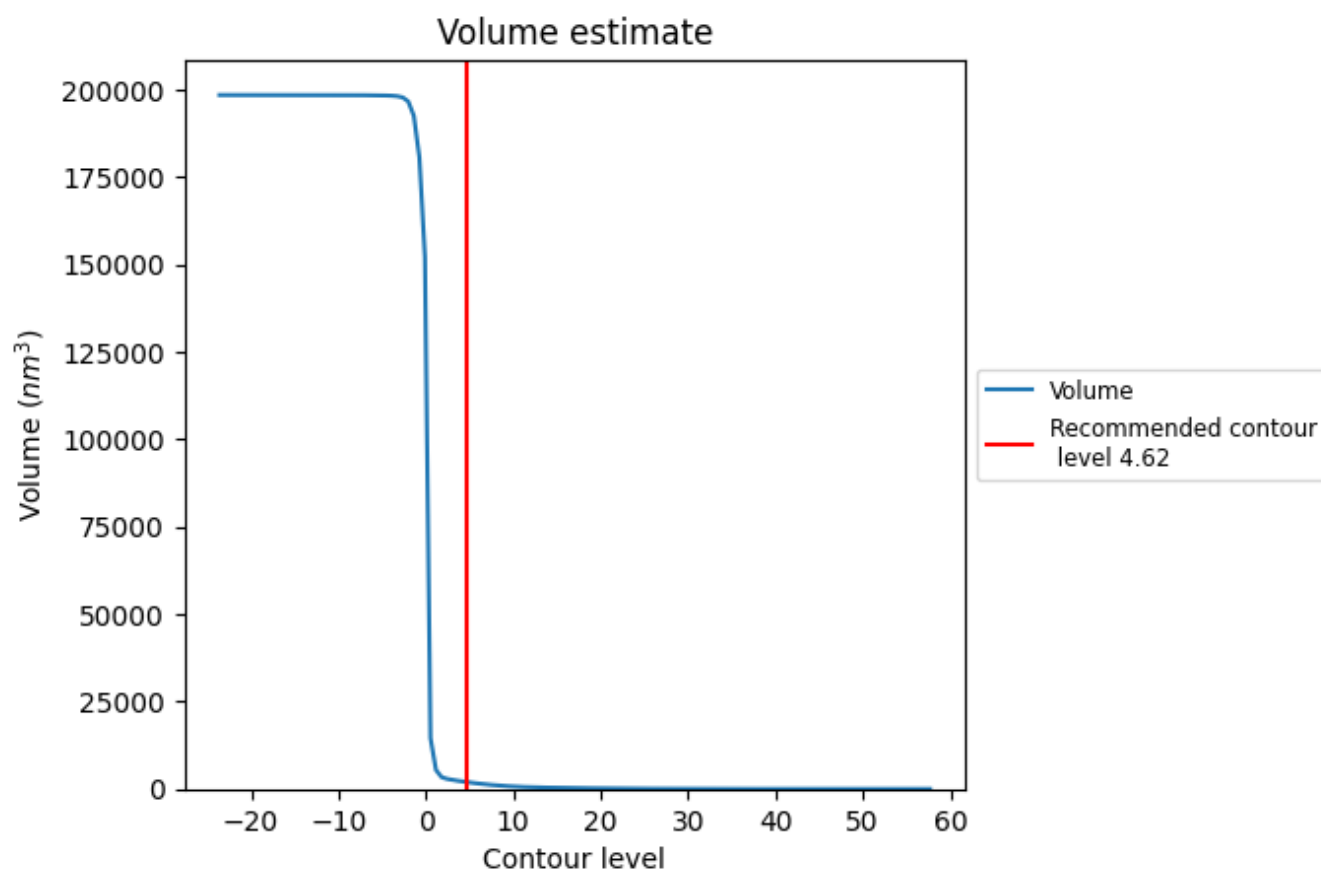
This section contains the results of statistical analysis of the map.

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.

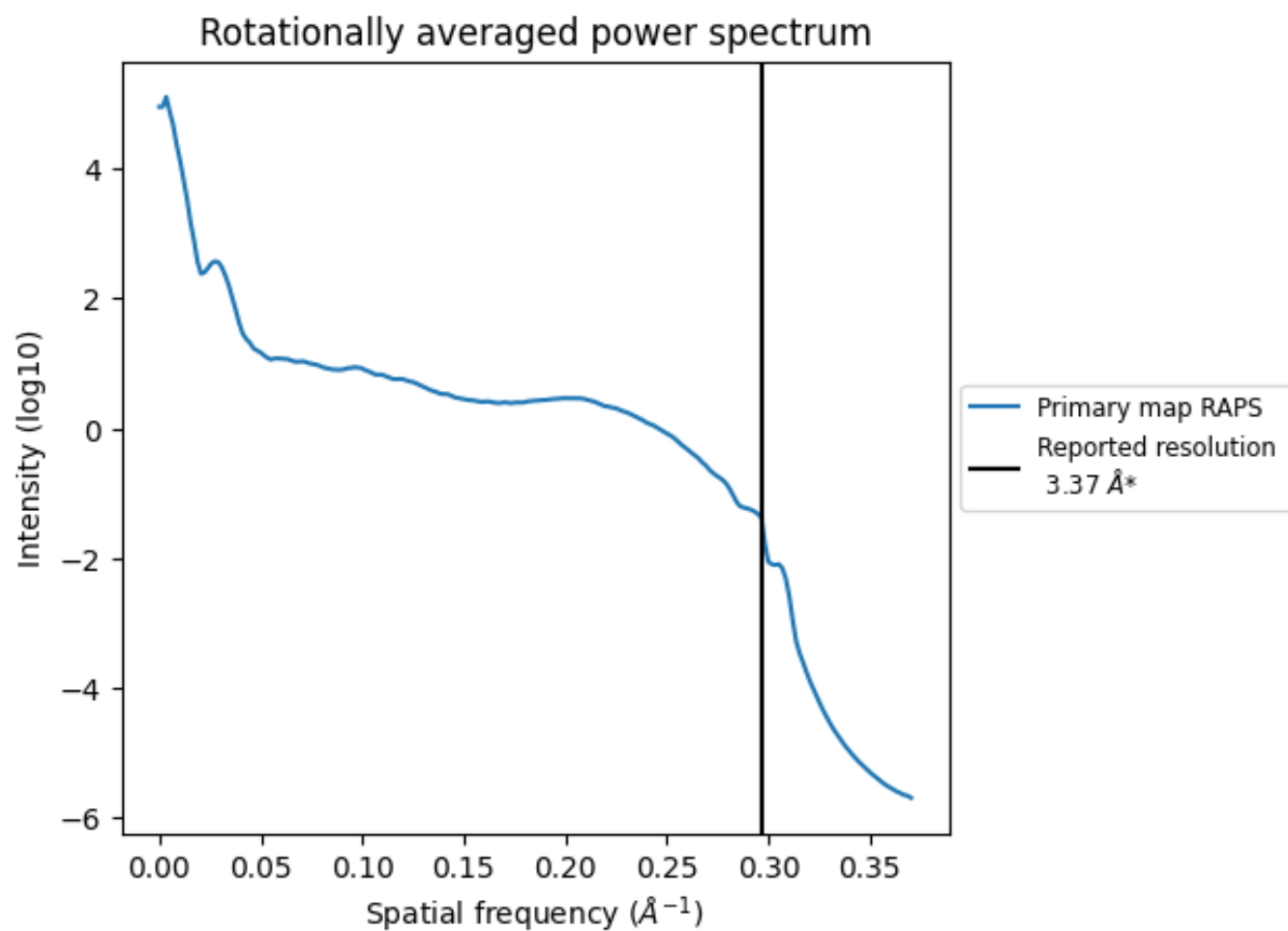
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1986 nm^3 ; this corresponds to an approximate mass of 1794 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 0.297 Å⁻¹

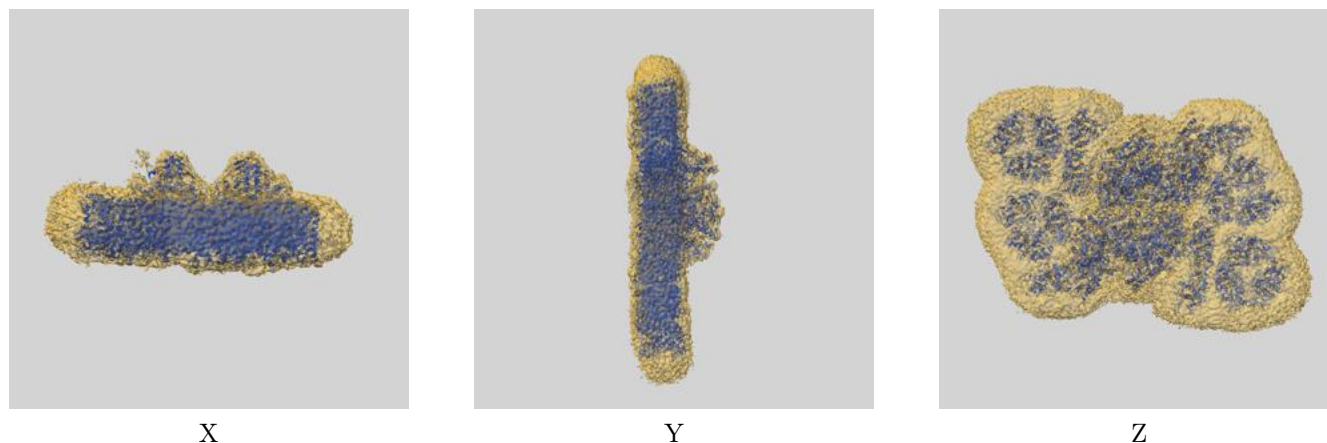
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

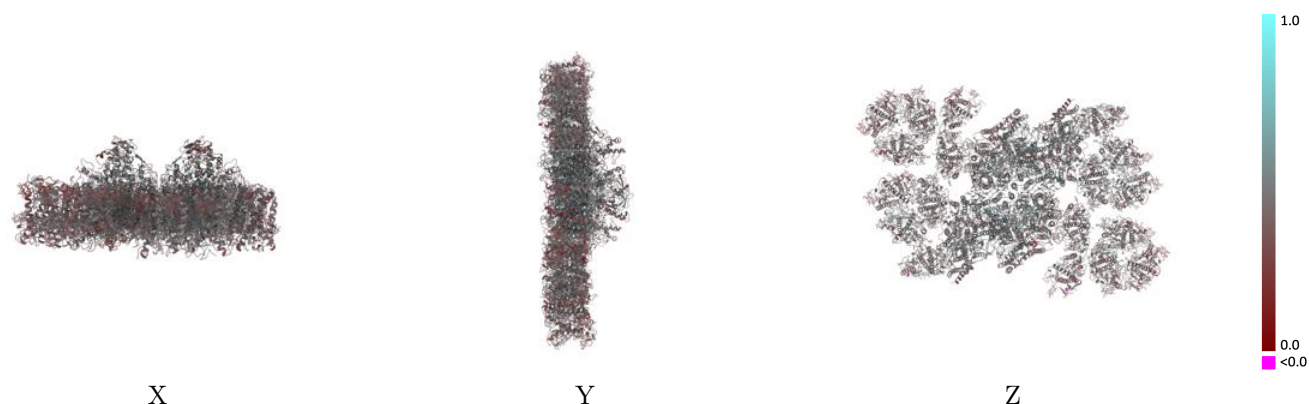
This section contains information regarding the fit between EMDB map EMD-63018 and PDB model 9LE8. Per-residue inclusion information can be found in section [3](#) on page [39](#).

9.1 Map-model overlay [i](#)



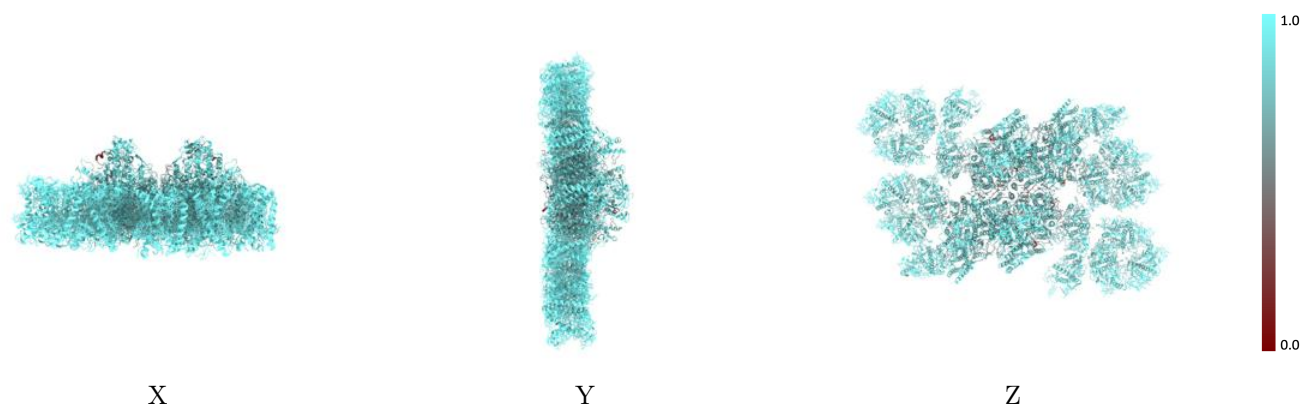
The images above show the 3D surface view of the map at the recommended contour level 4.62 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



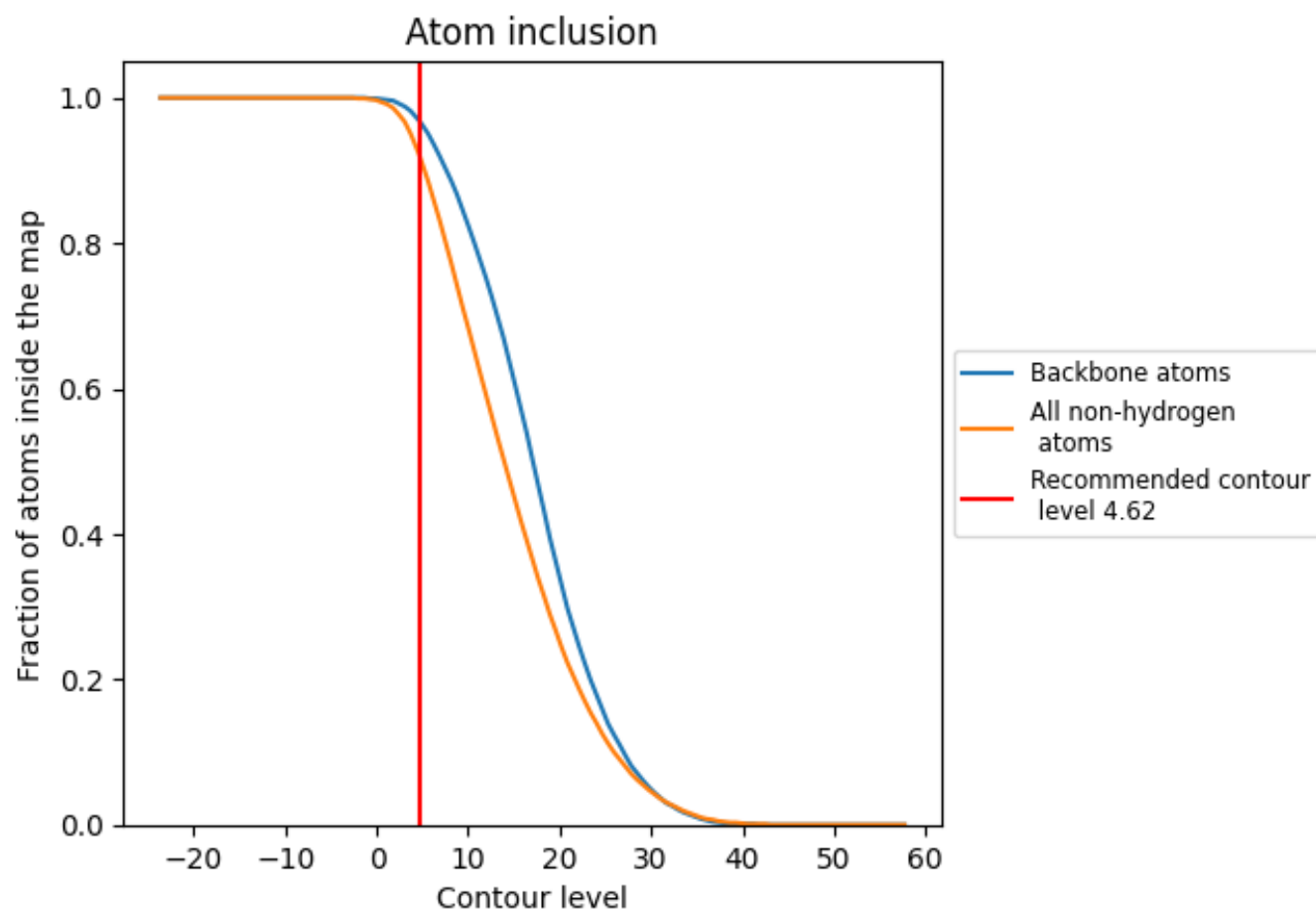
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.62).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (4.62) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9230	 0.4360
0	 0.9700	 0.4170
9	 0.9640	 0.4100
AA	 0.9680	 0.3850
AB	 0.9600	 0.3670
AC	 0.9650	 0.4080
AD	 0.9660	 0.4130
AE	 0.9710	 0.3860
AF	 0.9680	 0.3800
AG	 0.8560	 0.4660
AH	 0.9510	 0.4410
AI	 0.9500	 0.3810
AJ	 0.8850	 0.4830
AK	 0.8770	 0.4650
AL	 0.9060	 0.4700
AM	 0.9180	 0.4930
AN	 0.9700	 0.4220
AO	 0.8140	 0.3990
AP	 0.8640	 0.4630
AQ	 0.9680	 0.4390
AR	 0.9180	 0.3920
AS	 0.9780	 0.4110
AT	 0.8600	 0.4620
AU	 0.9490	 0.4440
AV	 0.9480	 0.3860
E	 0.9120	 0.3980
F	 0.8630	 0.4070
I	 0.9220	 0.4780
J	 0.8850	 0.4830
K	 0.9280	 0.4550
M	 0.7990	 0.4550
O	 0.8770	 0.4620
P	 0.9130	 0.4710
Q	 0.9160	 0.4950
U	 0.5710	 0.3300



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Chain	Atom inclusion	Q-score
V	 0.9700	 0.4140
W	 0.7290	 0.3890
X	 0.7340	 0.2920
e	 0.9190	 0.3930
f	 0.8500	 0.3930
i	 0.8970	 0.4690
j	 0.8200	 0.3990
k	 0.9260	 0.4460
m	 0.7790	 0.4500
o	 0.8760	 0.4650
p	 0.9720	 0.4480
q	 0.9130	 0.3990
u	 0.5400	 0.3160
v	 0.9760	 0.4190
w	 0.7180	 0.4010
x	 0.7100	 0.3010