



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:10 PM UTC

PDB ID : 7PNK / pdb_00007pnk
EMDB ID : EMD-13548
Title : Unstacked compact Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-09-07
Resolution : 3.61 Å (reported)
Based on initial model : 6KAC

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:

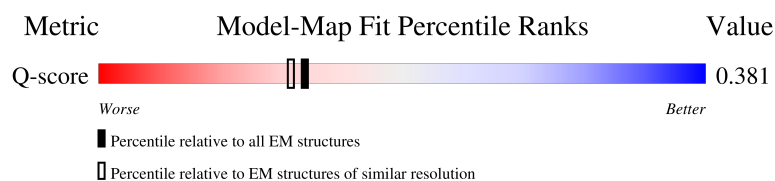
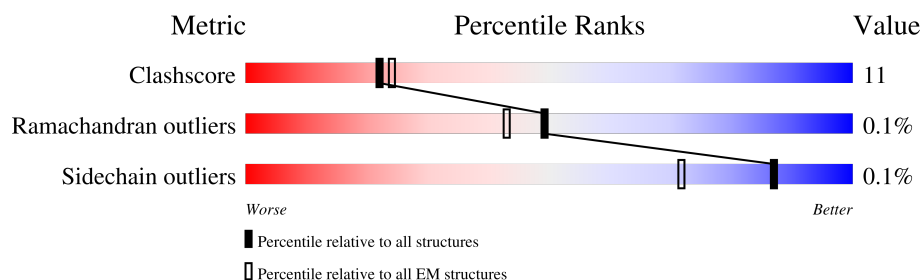
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.61 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.



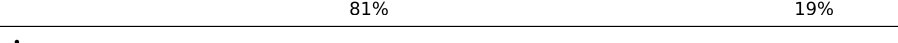
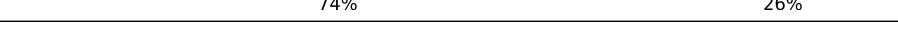
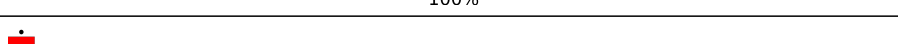
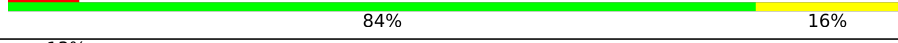
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11801 (3.11 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	336	
1	a	336	
2	B	484	
2	b	484	

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Mol	Chain	Length	Quality of chain
3	V	32	 81% 19%
3	v	32	 75% 25%
4	C	449	 81% 19%
4	c	449	 75% 24%
5	D	348	 79% 21%
5	d	348	 68% 32%
6	E	76	 79% 21%
6	e	76	 72% 28%
7	F	31	 74% 26%
7	f	31	 65% 32% .
8	H	67	 78% 21% .
8	h	67	 67% 33%
9	I	35	 80% 20%
9	i	35	 80% 20%
10	J	36	 100%
10	j	36	 86% 14%
11	K	37	 76% 24%
11	k	37	 86% 14%
12	L	38	 84% 16% 8%
12	l	38	 61% 39% 13%
13	M	31	 65% 35% 6%
13	m	31	 81% 19% 16%
14	O	238	 80% 20% 8%
14	o	238	 77% 23% 6%
15	P	187	79% 21% 79%

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Mol	Chain	Length	Quality of chain
15	p	187	
16	T	30	
16	t	30	
17	W	44	
17	w	44	
18	X	30	
18	x	30	
19	Z	61	
19	z	61	
20	N	222	
21	G	221	
22	S	243	
23	Y	222	
24	U	27	
24	u	27	

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
28	CLA	A	405	X	-	-	-
28	CLA	A	406	X	-	-	-
28	CLA	A	407	X	-	-	-
28	CLA	A	410	X	-	-	-
28	CLA	B	602	X	-	-	-
28	CLA	B	603	X	-	-	-
28	CLA	B	604	X	-	-	-
28	CLA	B	605	X	-	-	-
28	CLA	B	606	X	-	-	-
28	CLA	B	607	X	-	-	-
28	CLA	B	608	X	-	-	-
28	CLA	B	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	B	610	X	-	-	-
28	CLA	B	611	X	-	-	-
28	CLA	B	612	X	-	-	-
28	CLA	B	613	X	-	-	-
28	CLA	B	614	X	-	-	-
28	CLA	B	615	X	-	-	-
28	CLA	B	616	X	-	-	-
28	CLA	B	617	X	-	-	-
28	CLA	C	501	X	-	-	-
28	CLA	C	502	X	-	-	-
28	CLA	C	503	X	-	-	-
28	CLA	C	504	X	-	-	-
28	CLA	C	505	X	-	-	-
28	CLA	C	506	X	-	-	-
28	CLA	C	507	X	-	-	-
28	CLA	C	508	X	-	-	-
28	CLA	C	509	X	-	-	-
28	CLA	C	510	X	-	-	-
28	CLA	C	511	X	-	-	-
28	CLA	C	512	X	-	-	-
28	CLA	C	513	X	-	-	-
28	CLA	D	402	X	-	-	-
28	CLA	D	403	X	-	-	-
28	CLA	G	602	X	-	-	-
28	CLA	G	603	X	-	-	-
28	CLA	G	604	X	-	-	-
28	CLA	G	610	X	-	-	-
28	CLA	G	611	X	-	-	-
28	CLA	G	612	X	-	-	-
28	CLA	G	613	X	-	-	-
28	CLA	G	614	X	-	-	-
28	CLA	N	602	X	-	-	-
28	CLA	N	603	X	-	-	-
28	CLA	N	604	X	-	-	-
28	CLA	N	610	X	-	-	-
28	CLA	N	611	X	-	-	-
28	CLA	N	612	X	-	-	-
28	CLA	N	613	X	-	-	-
28	CLA	N	614	X	-	-	-
28	CLA	S	602	X	-	-	-
28	CLA	S	603	X	-	-	-
28	CLA	S	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	S	605	X	-	-	-
28	CLA	S	609	X	-	-	-
28	CLA	S	610	X	-	-	-
28	CLA	S	611	X	-	-	-
28	CLA	S	612	X	-	-	-
28	CLA	S	613	X	-	-	-
28	CLA	S	614	X	-	-	-
28	CLA	S	617	X	-	-	-
28	CLA	Y	602	X	-	-	-
28	CLA	Y	603	X	-	-	-
28	CLA	Y	604	X	-	-	-
28	CLA	Y	608	X	-	-	-
28	CLA	Y	610	X	-	-	-
28	CLA	Y	611	X	-	-	-
28	CLA	Y	612	X	-	-	-
28	CLA	Y	613	X	-	-	-
28	CLA	Y	614	X	-	-	-
28	CLA	a	405	X	-	-	-
28	CLA	a	406	X	-	-	-
28	CLA	a	407	X	-	-	-
28	CLA	a	410	X	-	-	-
28	CLA	b	602	X	-	-	-
28	CLA	b	603	X	-	-	-
28	CLA	b	604	X	-	-	-
28	CLA	b	605	X	-	-	-
28	CLA	b	606	X	-	-	-
28	CLA	b	607	X	-	-	-
28	CLA	b	608	X	-	-	-
28	CLA	b	609	X	-	-	-
28	CLA	b	610	X	-	-	-
28	CLA	b	611	X	-	-	-
28	CLA	b	612	X	-	-	-
28	CLA	b	613	X	-	-	-
28	CLA	b	614	X	-	-	-
28	CLA	b	615	X	-	-	-
28	CLA	b	616	X	-	-	-
28	CLA	b	617	X	-	-	-
28	CLA	c	501	X	-	-	-
28	CLA	c	502	X	-	-	-
28	CLA	c	503	X	-	-	-
28	CLA	c	504	X	-	-	-
28	CLA	c	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	c	506	X	-	-	-
28	CLA	c	507	X	-	-	-
28	CLA	c	508	X	-	-	-
28	CLA	c	509	X	-	-	-
28	CLA	c	510	X	-	-	-
28	CLA	c	511	X	-	-	-
28	CLA	c	512	X	-	-	-
28	CLA	c	513	X	-	-	-
28	CLA	d	402	X	-	-	-
28	CLA	d	403	X	-	-	-
34	C7Z	B	620	X	-	-	-
34	C7Z	b	620	X	-	-	-
39	LMK	C	527	X	-	-	-
39	LMK	c	527	X	-	-	-
43	RRX	H	101	X	-	-	-
43	RRX	h	101	X	-	-	-
46	CHL	G	601	X	-	-	-
46	CHL	G	605	X	-	-	-
46	CHL	G	606	X	-	-	-
46	CHL	G	607	X	-	-	-
46	CHL	G	608	X	-	-	-
46	CHL	G	609	X	-	-	-
46	CHL	N	601	X	-	-	-
46	CHL	N	605	X	-	-	-
46	CHL	N	606	X	-	-	-
46	CHL	N	607	X	-	-	-
46	CHL	N	608	X	-	-	-
46	CHL	N	609	X	-	-	-
46	CHL	S	601	X	-	-	-
46	CHL	S	606	X	-	-	-
46	CHL	S	607	X	-	-	-
46	CHL	S	608	X	-	-	-
46	CHL	Y	601	X	-	-	-
46	CHL	Y	605	X	-	-	-
46	CHL	Y	606	X	-	-	-
46	CHL	Y	607	X	-	-	-
46	CHL	Y	609	X	-	-	-
48	XAT	G	622	X	-	-	-
48	XAT	N	622	X	-	-	-

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 60673 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		
2	b	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	76	Total	C	N	O	S	0	0
			621	404	102	115			
6	e	76	Total	C	N	O	S	0	0
			621	404	102	115			

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	36	Total	C	N	O	S	0	0
			266	183	40	43			

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	36	Total	C	N	O	0	0
			266	183	40	43		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	7	ILE	THR	conflict	UNP A0A1C8XRM8
J	42	LEU	GLN	conflict	UNP A0A1C8XRM8
j	7	ILE	THR	conflict	UNP A0A1C8XRM8
j	42	LEU	GLN	conflict	UNP A0A1C8XRM8

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			234	159	33	42		
13	m	31	Total	C	N	O	0	0
			234	159	33	42		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	9	THR	ILE	conflict	UNP D0FXZ3
m	9	THR	ILE	conflict	UNP D0FXZ3

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1822	1153	296	367	6		
14	o	238	Total	C	N	O	S	0	0
			1822	1153	296	367	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	30	Total	C	N	O	0	0
			201	132	32	37		
18	x	30	Total	C	N	O	0	0
			201	132	32	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called Chlorophyll a-b binding protein of LHCII type I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

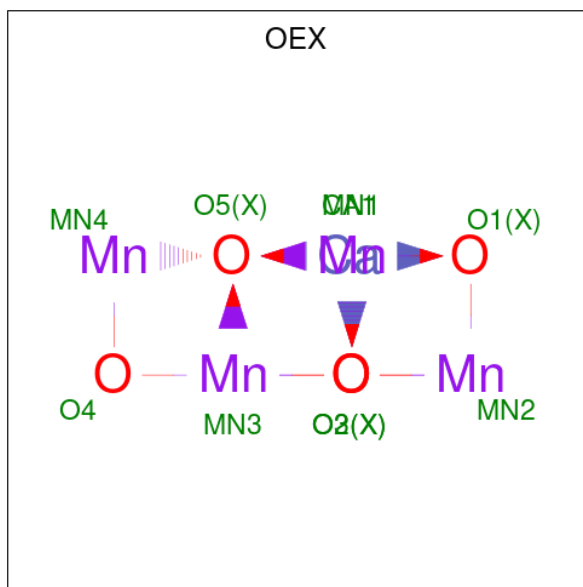
- Molecule 23 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	222	Total	C	N	O	S	0	0
			1670	1083	272	312	3		

- Molecule 24 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
24	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 25 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
25	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

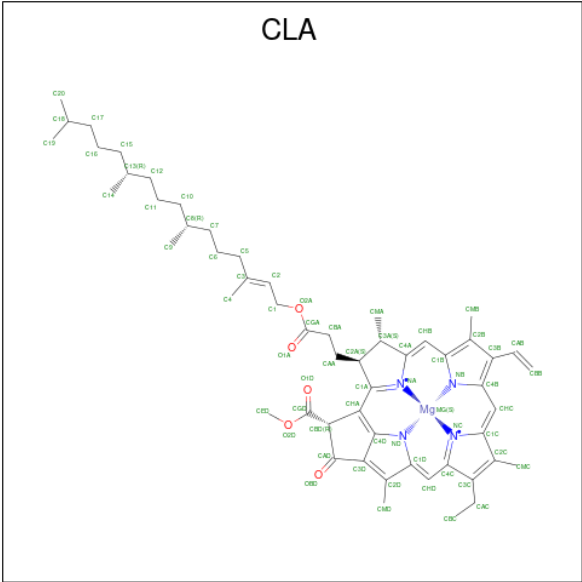
- Molecule 26 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 27 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total	Cl	0
			2	2	
27	a	2	Total	Cl	0
			2	2	

- Molecule 28 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	S	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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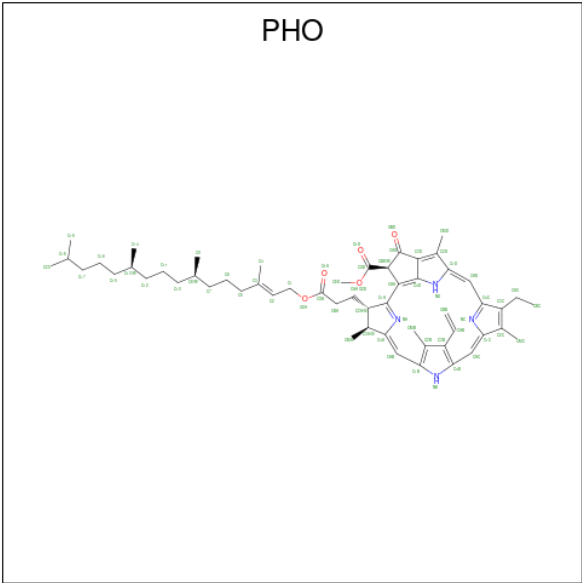
Mol	Chain	Residues	Atoms					AltConf
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total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

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

- Molecule 29 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



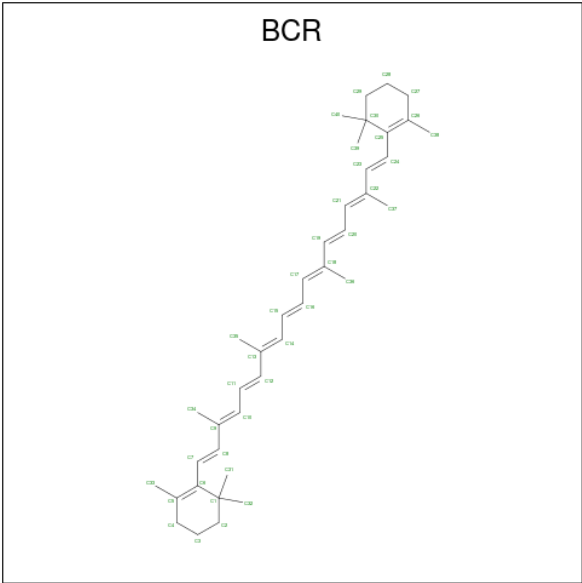
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	N	O	0
			64	55	4	5	
29	A	1	Total	C	N	O	0
			64	55	4	5	
29	a	1	Total	C	N	O	0
			64	55	4	5	

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

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



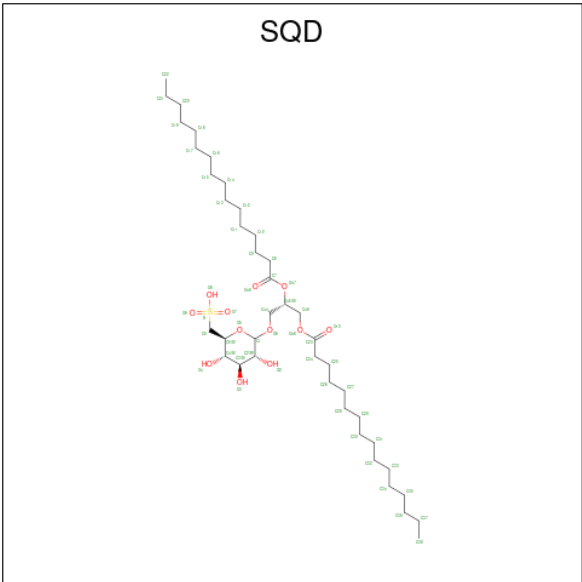
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	C	0
			40	40	
30	B	1	Total	C	0
			40	40	
30	B	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	D	1	Total	C	0
			40	40	
30	a	1	Total	C	0
			40	40	
30	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
30	b	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	d	1	Total C 40 40	0

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



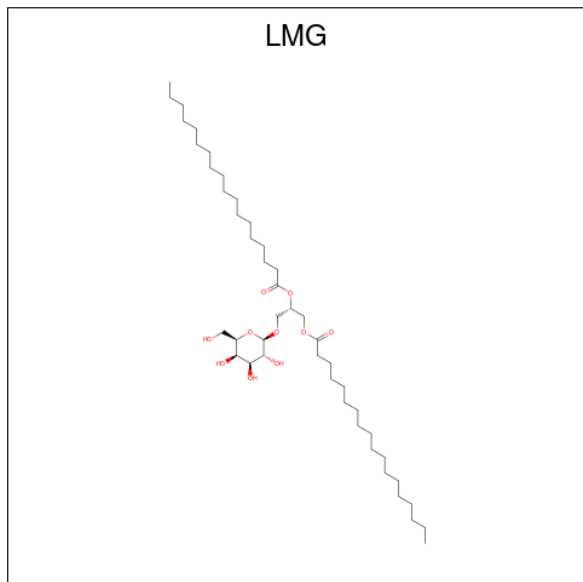
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C O S 51 38 12 1	0
31	B	1	Total C O S 42 29 12 1	0
31	B	1	Total C O S 54 41 12 1	0
31	C	1	Total C O S 54 41 12 1	0
31	M	1	Total C O S 42 29 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
31	a	1	Total	C	O	S	0
			51	38	12	1	
31	b	1	Total	C	O	S	0
			42	29	12	1	
31	b	1	Total	C	O	S	0
			54	41	12	1	
31	c	1	Total	C	O	S	0
			54	41	12	1	
31	m	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



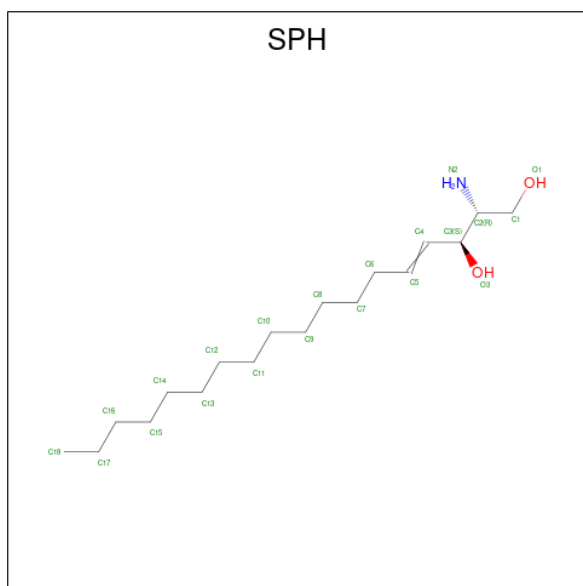
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O		0
			48	38	10		
32	B	1	Total	C	O		0
			44	34	10		
32	C	1	Total	C	O		0
			51	41	10		
32	C	1	Total	C	O		0
			55	45	10		
32	D	1	Total	C	O		0
			46	36	10		
32	H	1	Total	C	O		0
			48	38	10		

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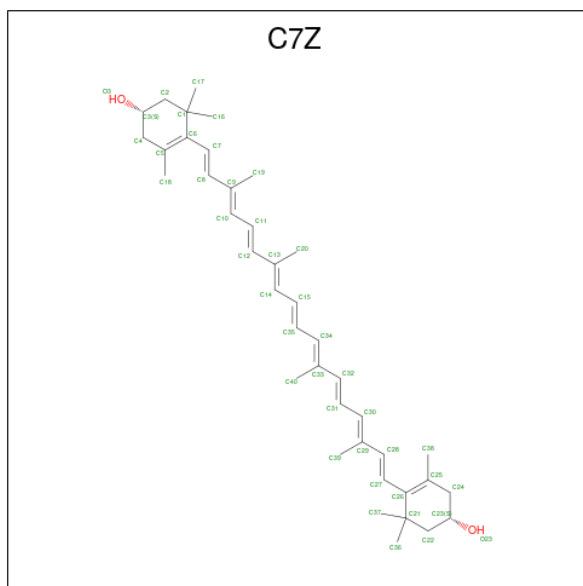
Mol	Chain	Residues	Atoms			AltConf
32	W	1	Total	C	O	0
			39	29	10	
32	a	1	Total	C	O	0
			48	38	10	
32	b	1	Total	C	O	0
			44	34	10	
32	c	1	Total	C	O	0
			51	41	10	
32	c	1	Total	C	O	0
			55	45	10	
32	d	1	Total	C	O	0
			46	36	10	
32	h	1	Total	C	O	0
			48	38	10	
32	w	1	Total	C	O	0
			39	29	10	

- Molecule 33 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



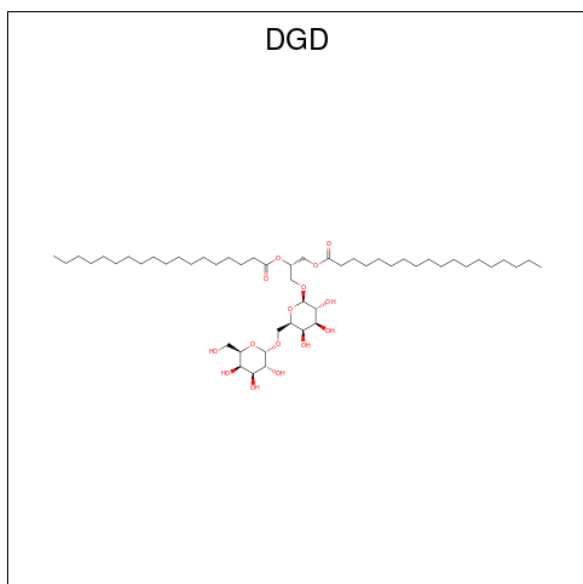
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			21	18	1	2	
33	Y	1	Total	C	N	O	0
			21	18	1	2	
33	a	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 34 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



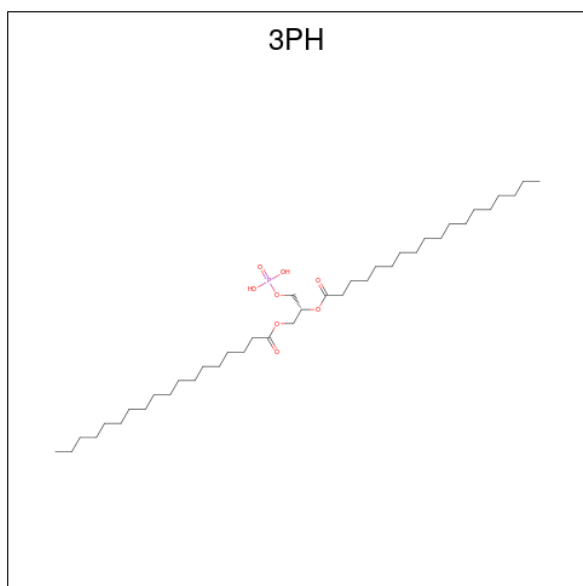
Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			42	40	2	
34	b	1	Total	C	O	0
			42	40	2	

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



Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			43	28	15	
35	C	1	Total	C	O	0
			55	40	15	
35	C	1	Total	C	O	0
			62	47	15	
35	C	1	Total	C	O	0
			59	44	15	
35	b	1	Total	C	O	0
			43	28	15	
35	c	1	Total	C	O	0
			55	40	15	
35	c	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			59	44	15	

- Molecule 36 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



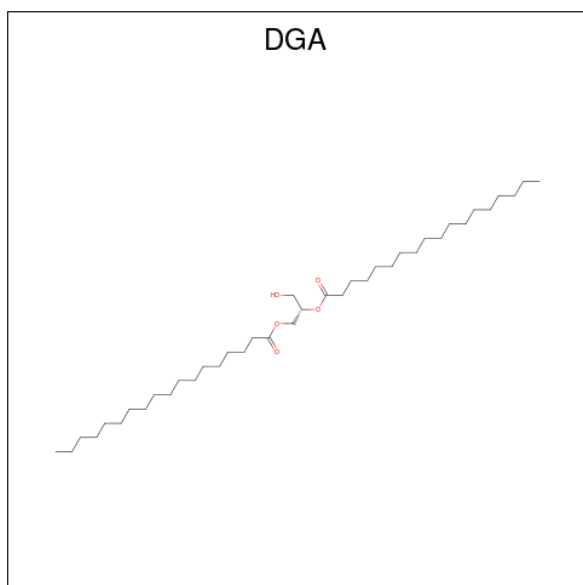
Mol	Chain	Residues	Atoms				AltConf
36	B	1	Total	C	O	P	0
			48	39	8	1	
36	T	1	Total	C	O	P	0
			48	39	8	1	
36	S	1	Total	C	O	P	0
			48	39	8	1	

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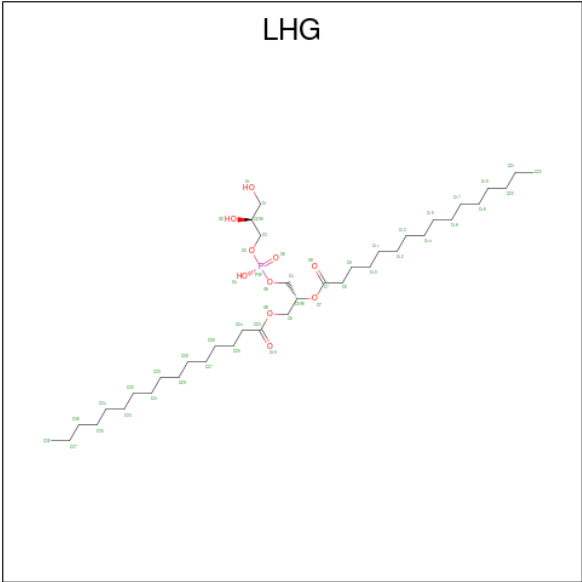
Mol	Chain	Residues	Atoms				AltConf
36	b	1	Total	C	O	P	0
			48	39	8	1	
36	t	1	Total	C	O	P	0
			48	39	8	1	

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



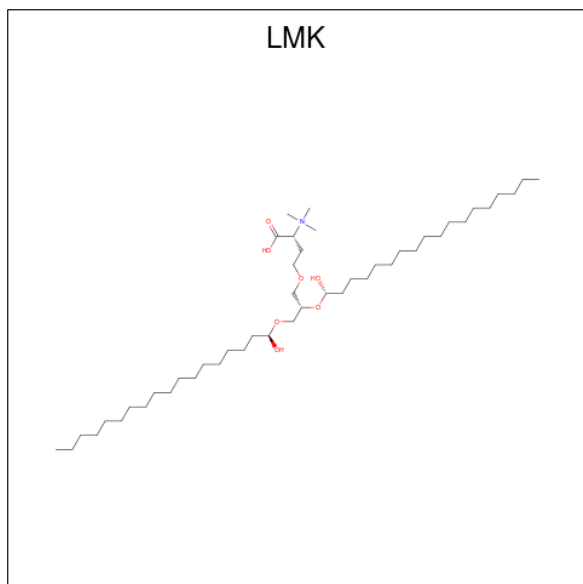
Mol	Chain	Residues	Atoms				AltConf
37	B	1	Total	C	O		0
			44	39	5		
37	C	1	Total	C	O		0
			44	39	5		
37	J	1	Total	C	O		0
			29	24	5		
37	b	1	Total	C	O		0
			44	39	5		
37	c	1	Total	C	O		0
			44	39	5		
37	j	1	Total	C	O		0
			29	24	5		

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



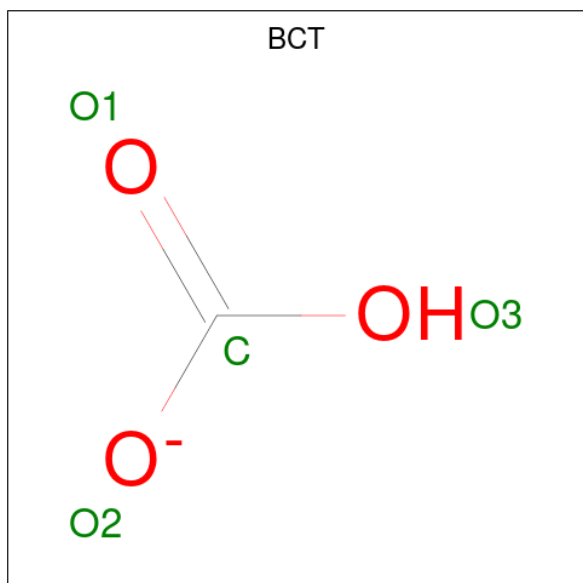
Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	C	O	P	0
			47	36	10	1	
38	D	1	Total	C	O	P	0
			44	33	10	1	
38	D	1	Total	C	O	P	0
			49	38	10	1	
38	D	1	Total	C	O	P	0
			39	28	10	1	
38	L	1	Total	C	O	P	0
			49	38	10	1	
38	N	1	Total	C	O	P	0
			49	38	10	1	
38	G	1	Total	C	O	P	0
			49	38	10	1	
38	S	1	Total	C	O	P	0
			45	34	10	1	
38	Y	1	Total	C	O	P	0
			49	38	10	1	
38	c	1	Total	C	O	P	0
			47	36	10	1	
38	d	1	Total	C	O	P	0
			44	33	10	1	
38	d	1	Total	C	O	P	0
			49	38	10	1	
38	d	1	Total	C	O	P	0
			39	28	10	1	
38	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 39 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$).



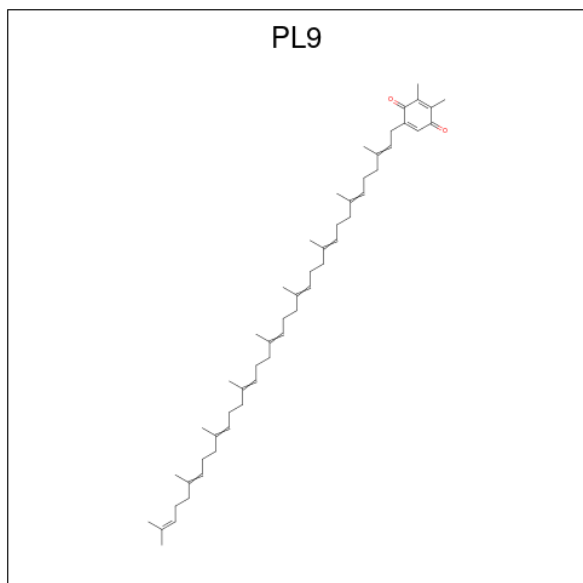
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
39	C	1	40	32	1	7	0
39	c	1	40	32	1	7	0

- Molecule 40 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



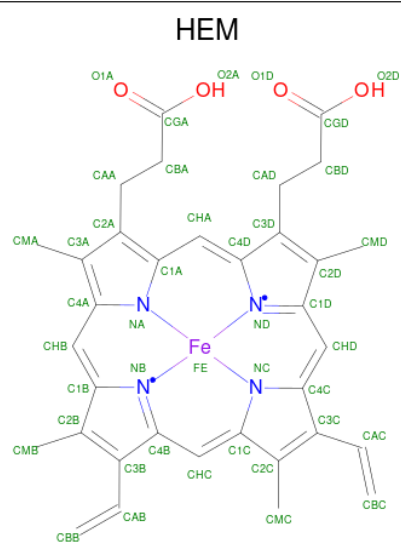
Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			4	1	3	
40	d	1	Total	C	O	0
			4	1	3	

- Molecule 41 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: $C_{53}H_{80}O_2$).



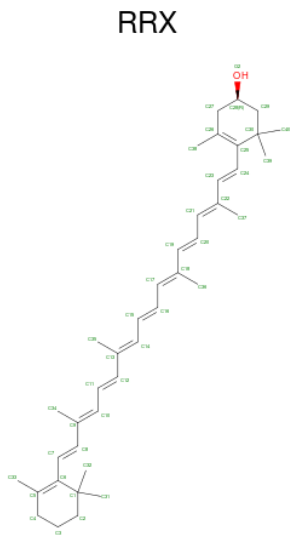
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			55	53	2	
41	d	1	Total	C	O	0
			55	53	2	

- Molecule 42 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



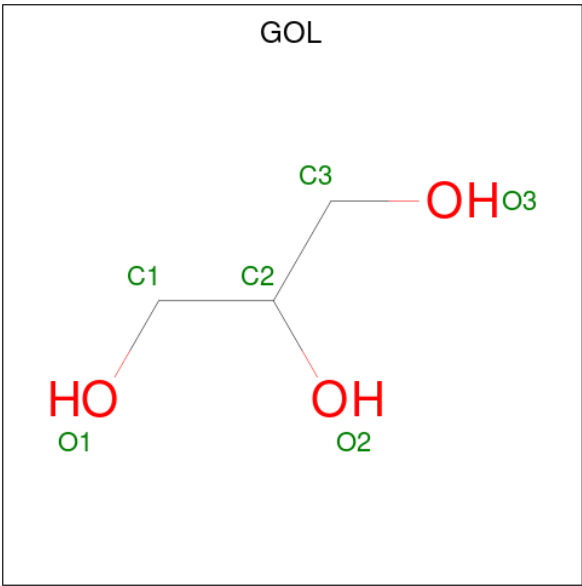
Mol	Chain	Residues	Atoms					AltConf
42	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
42	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 43 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



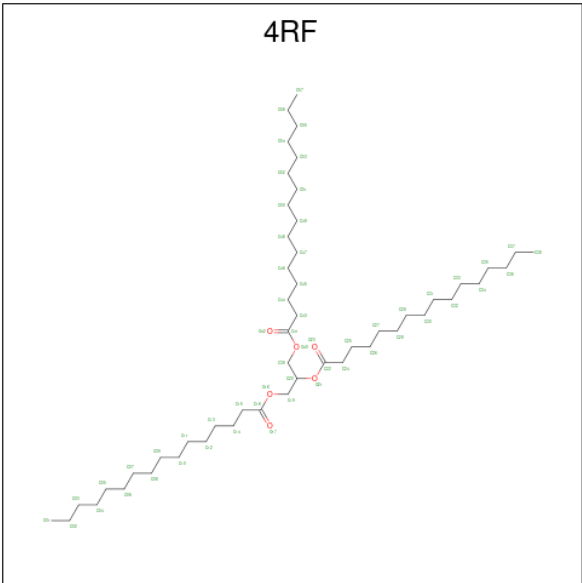
Mol	Chain	Residues	Atoms			AltConf
43	H	1	Total 41	C 40	O 1	0
43	h	1	Total 41	C 40	O 1	0

- Molecule 44 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
44	I	1	Total	C	O	0
			6	3	3	

- Molecule 45 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$).



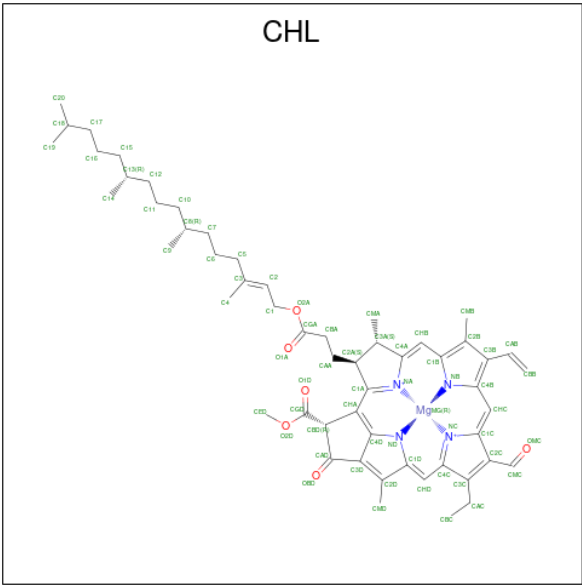
Mol	Chain	Residues	Atoms			AltConf
45	I	1	Total	C	O	0
			57	51	6	
45	K	1	Total	C	O	0
			57	51	6	

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Mol	Chain	Residues	Atoms			AltConf
45	i	1	Total	C	O	0
			57	51	6	
45	k	1	Total	C	O	0
			57	51	6	

- Molecule 46 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



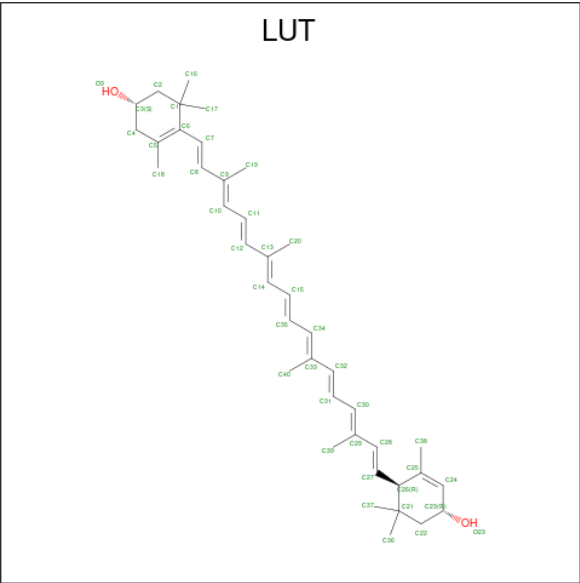
Mol	Chain	Residues	Atoms						AltConf
46	N	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O	0	
			50	39	1	4	6		
46	N	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	G	1	Total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

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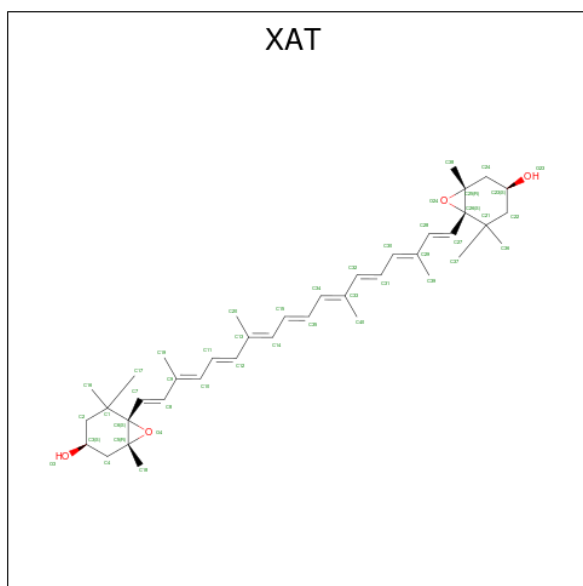
Mol	Chain	Residues	Atoms					AltConf
46	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	G	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
46	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	S	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
46	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
46	S	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
46	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 47 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



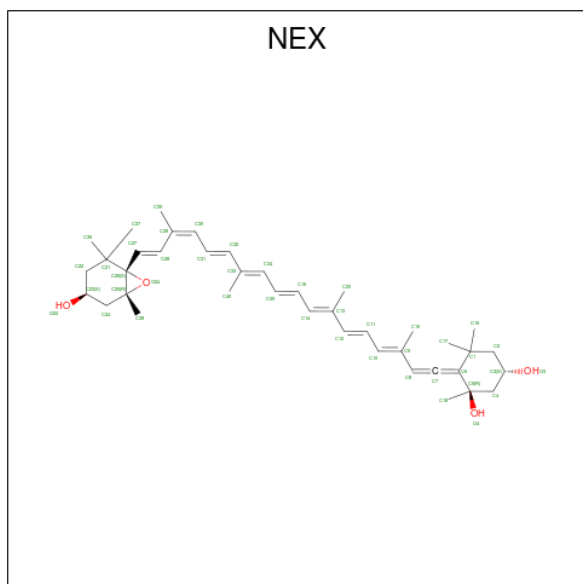
Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			42	40	2	
47	N	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			42	40	2	

- Molecule 48 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).



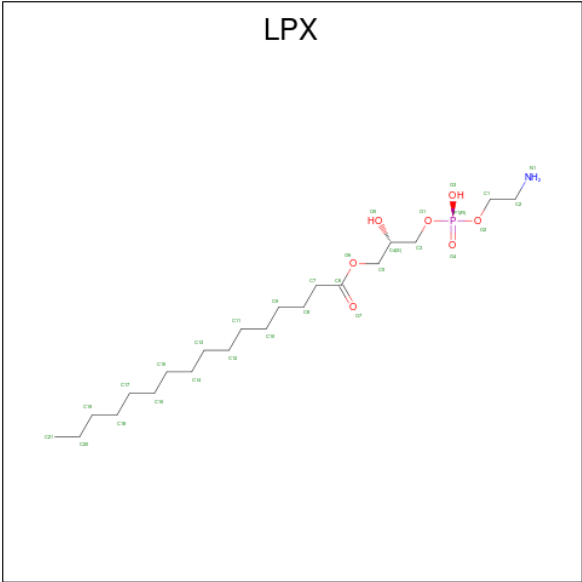
Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	Y	1	Total	C	O	0
			44	40	4	

- Molecule 49 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



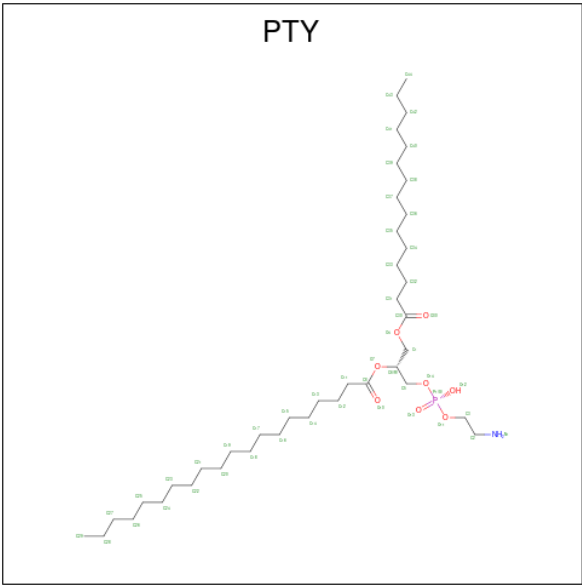
Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	S	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	

- Molecule 50 is (2S)-3-[[[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-hydroxypropyl]hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					AltConf
50	S	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 51 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).

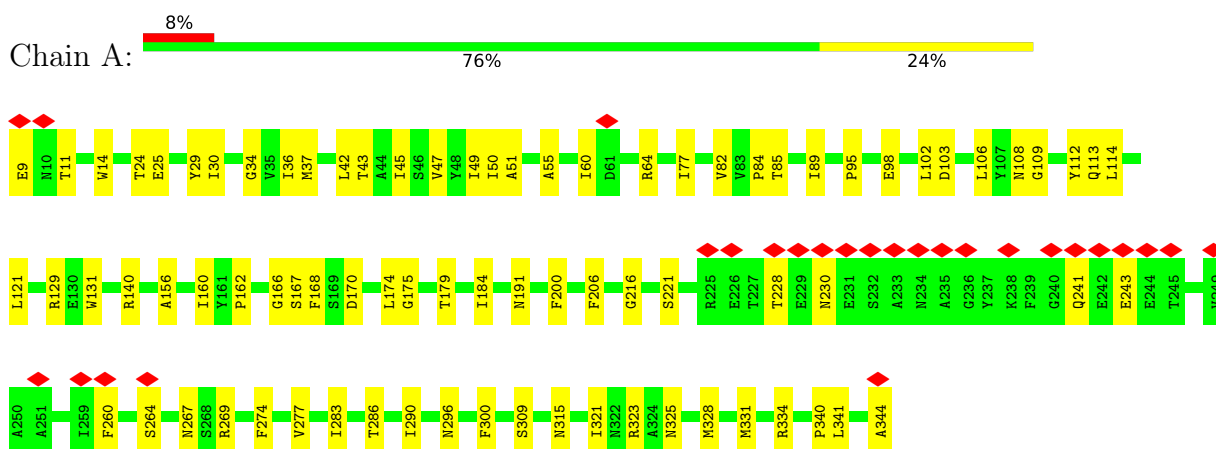


Mol	Chain	Residues	Atoms					AltConf
51	Y	1	Total	C	N	O	P	0
			50	40	1	8	1	
51	Y	1	Total	C	N	O	P	0
			19	9	1	8	1	

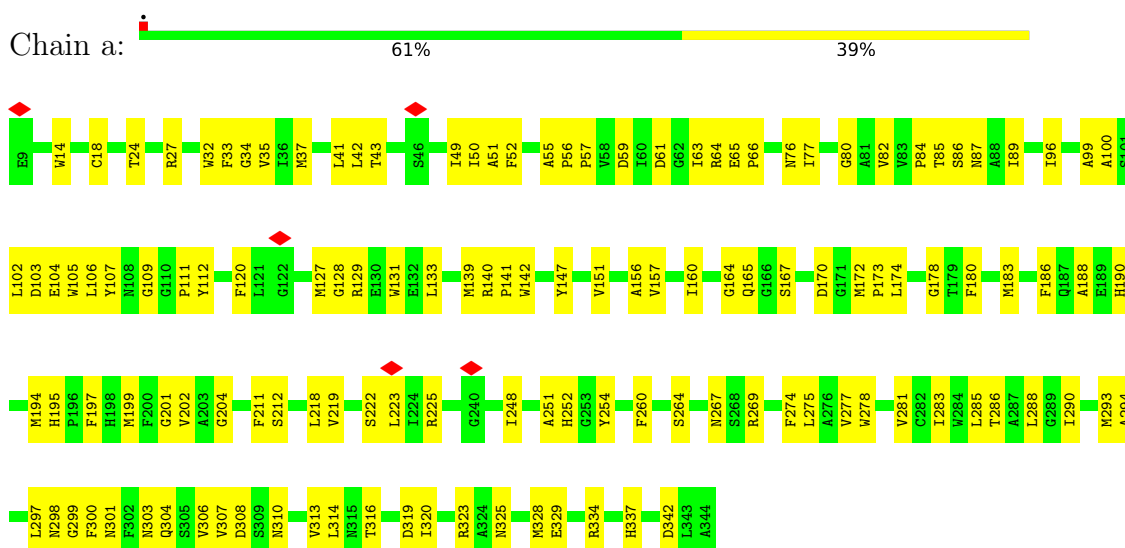
3 Residue-property plots

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.

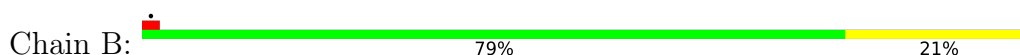
- Molecule 1: Photosystem II protein D1

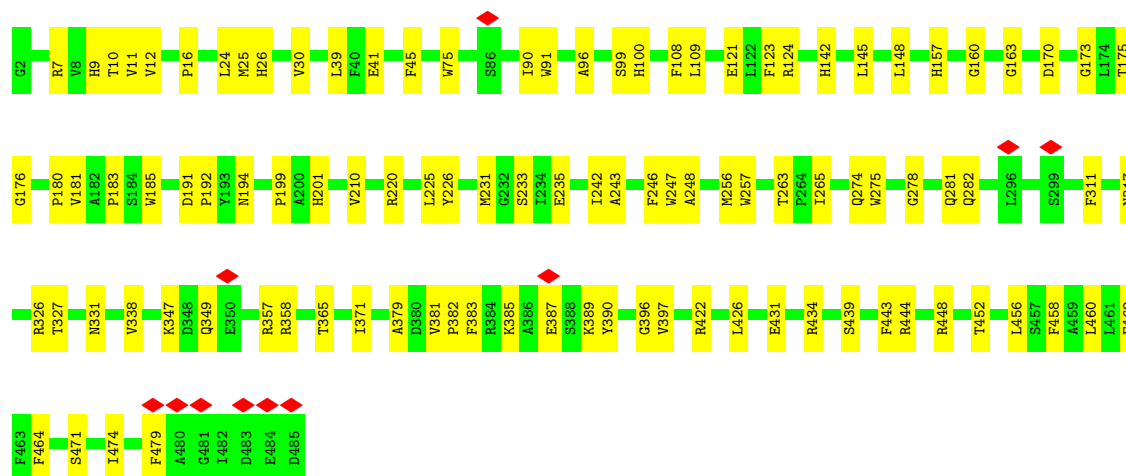


- Molecule 1: Photosystem II protein D1

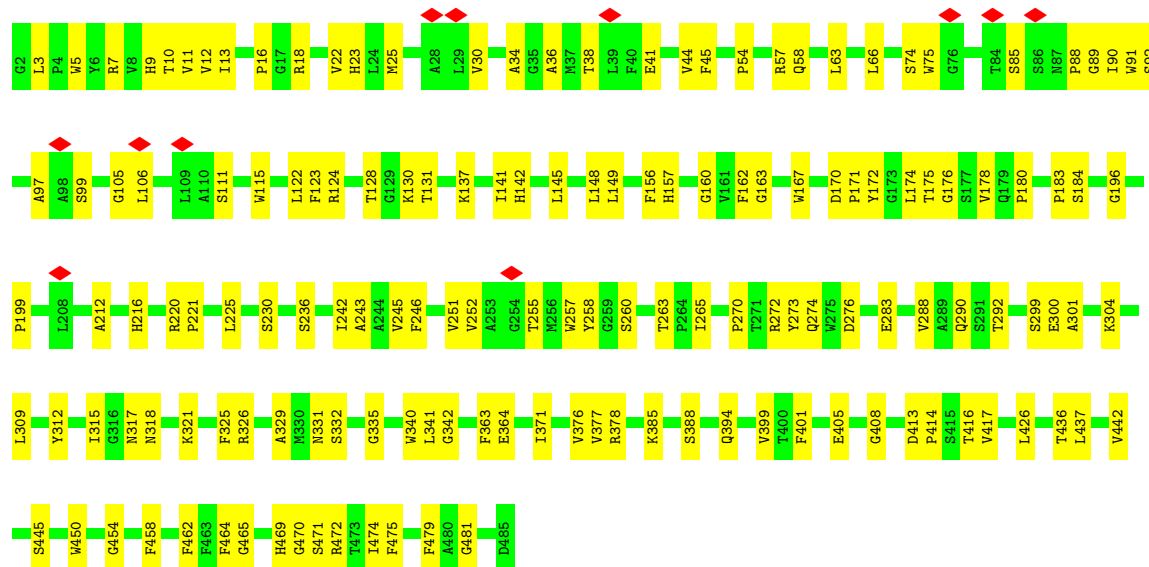


- Molecule 2: Photosystem II CP47 reaction center protein

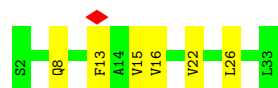
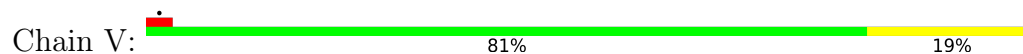




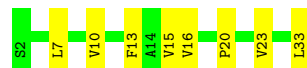
• Molecule 2: Photosystem II CP47 reaction center protein



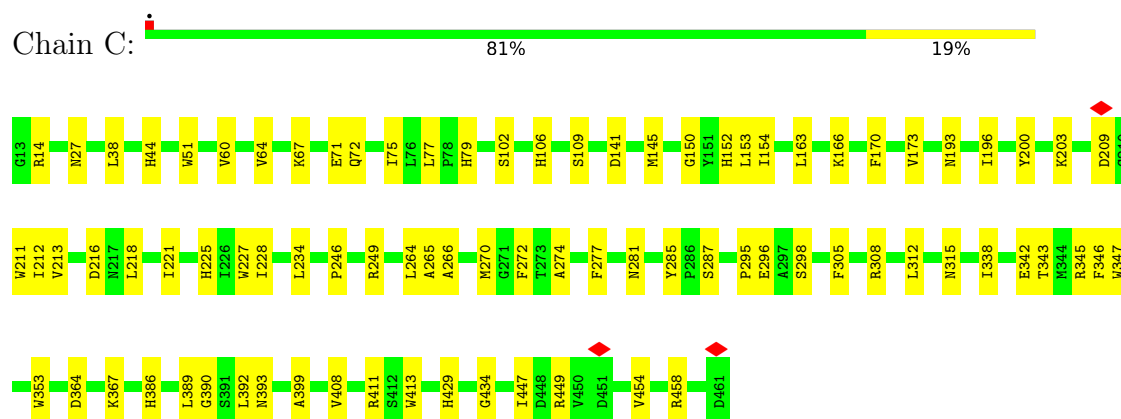
• Molecule 3: Photosystem II reaction center protein Ycf12



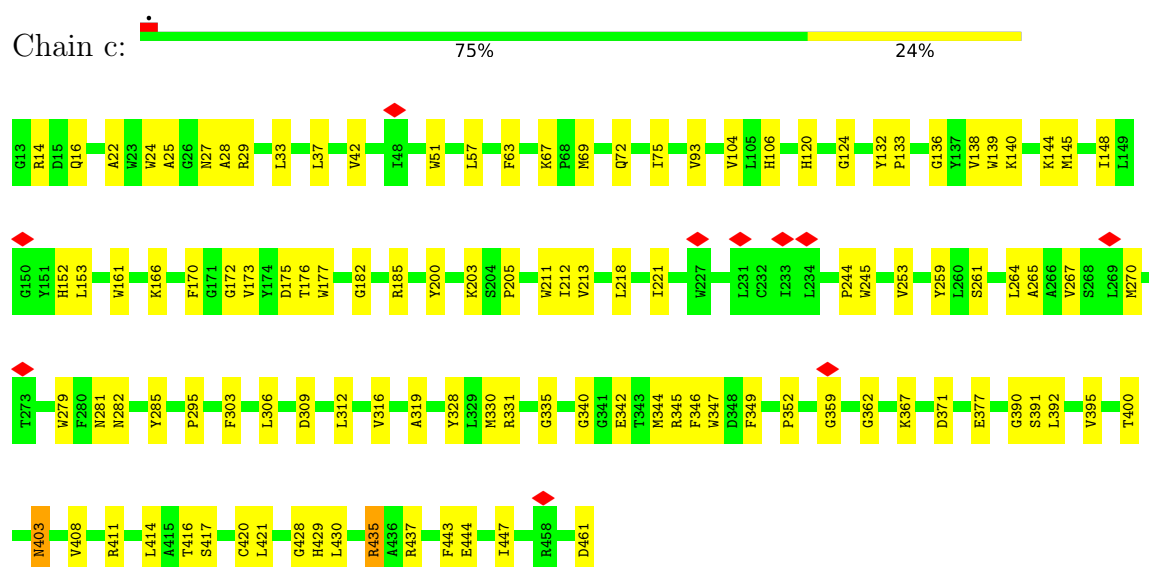
• Molecule 3: Photosystem II reaction center protein Ycf12



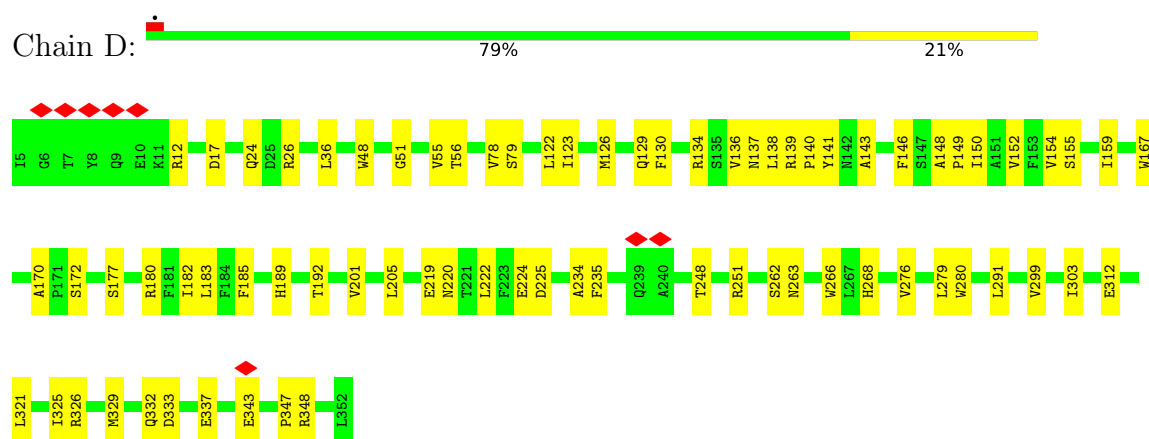
- Molecule 4: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II CP43 reaction center protein

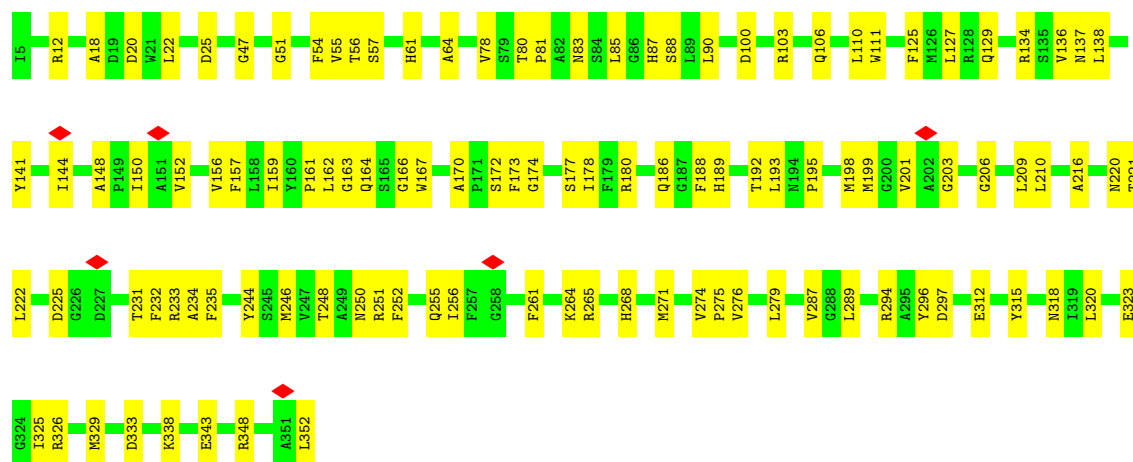


- Molecule 5: Photosystem II D2 protein



- Molecule 5: Photosystem II D2 protein

Chain d:  68% 32%



- Molecule 6: Cytochrome b559 subunit alpha

Chain E:  79% 21%



- Molecule 6: Cytochrome b559 subunit alpha

Chain e:  72% 28%



- Molecule 7: Cytochrome b559 subunit beta

Chain F:  74% 26%



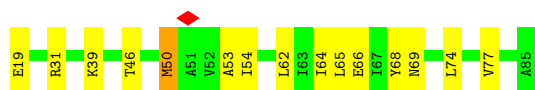
- Molecule 7: Cytochrome b559 subunit beta

Chain f:  65% 32%

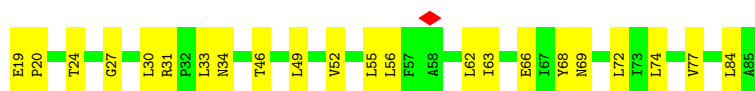


- Molecule 8: Photosystem II reaction center protein H

Chain H:  78% 21%



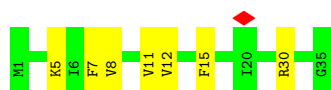
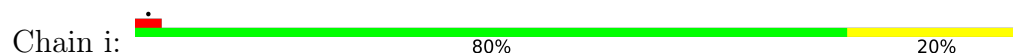
- Molecule 8: Photosystem II reaction center protein H



- Molecule 9: Photosystem II reaction center protein I



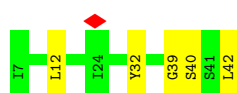
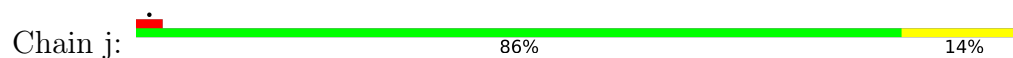
- Molecule 9: Photosystem II reaction center protein I



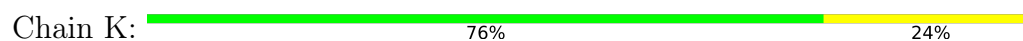
- Molecule 10: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein J



- Molecule 11: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein K

Chain k:  86% 14%



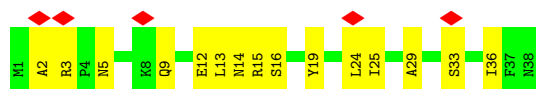
- Molecule 12: Photosystem II reaction center protein L

Chain L:  8% 84% 16%



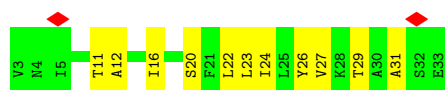
- Molecule 12: Photosystem II reaction center protein L

Chain l:  13% 61% 39%



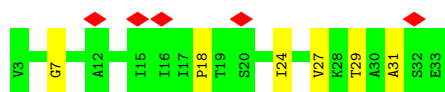
- Molecule 13: Photosystem II reaction center protein M

Chain M:  6% 65% 35%



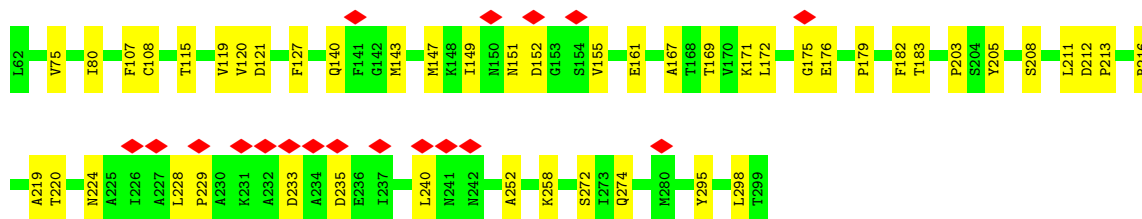
- Molecule 13: Photosystem II reaction center protein M

Chain m:  16% 81% 19%



- Molecule 14: PsbO

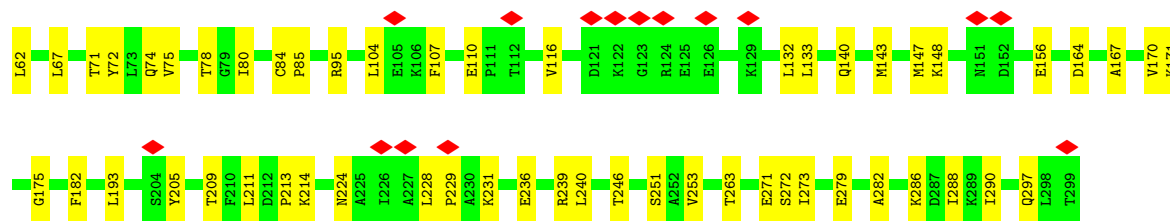
Chain O:  8% 80% 20%



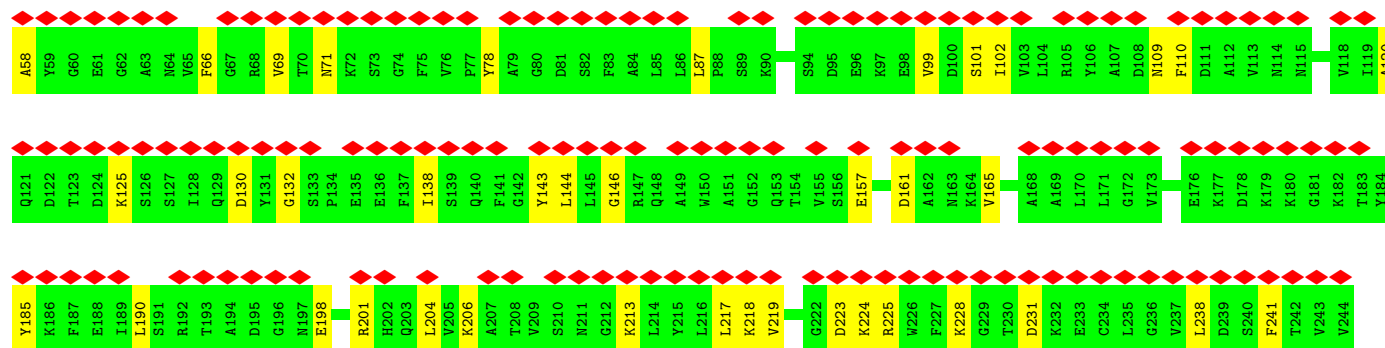
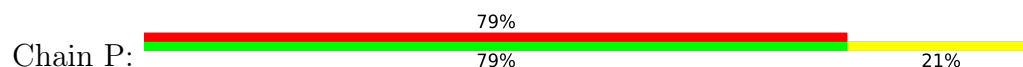
- Molecule 14: PsbO

Chain o:  6% 77% 23%

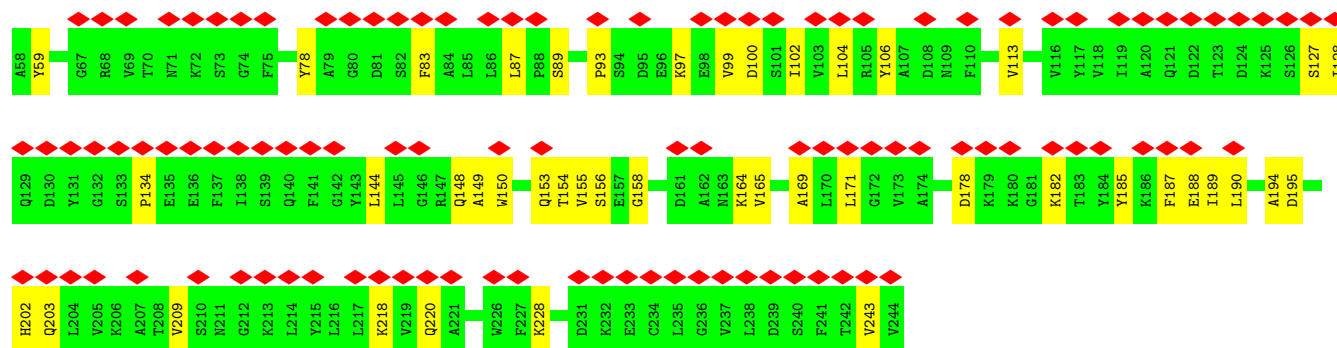
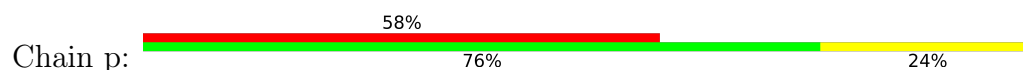




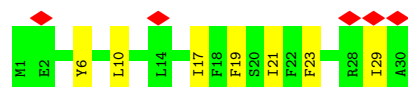
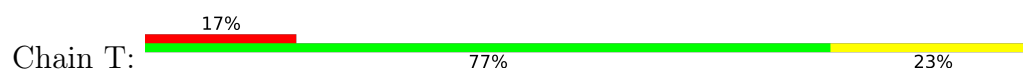
• Molecule 15: PsbP



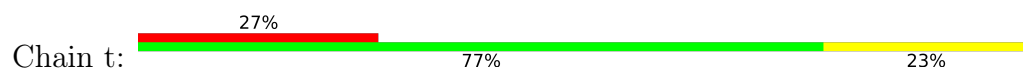
• Molecule 15: PsbP

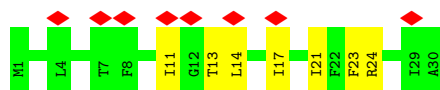


• Molecule 16: Photosystem II reaction center protein T

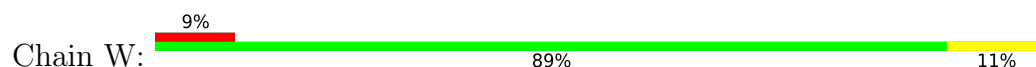


• Molecule 16: Photosystem II reaction center protein T

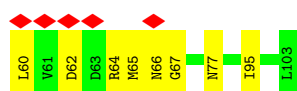
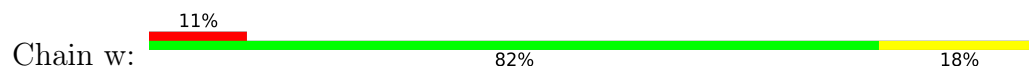




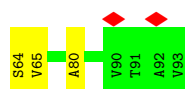
- Molecule 17: PsbW



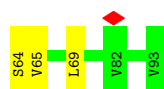
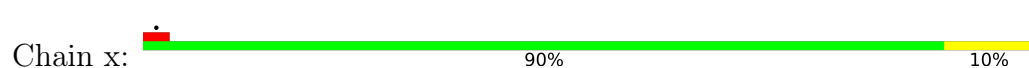
- Molecule 17: PsbW



- Molecule 18: PsbX



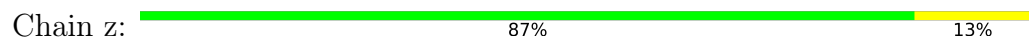
- Molecule 18: PsbX



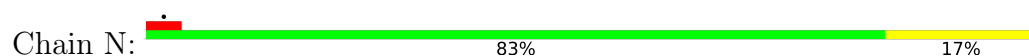
- Molecule 19: Photosystem II reaction center protein Z

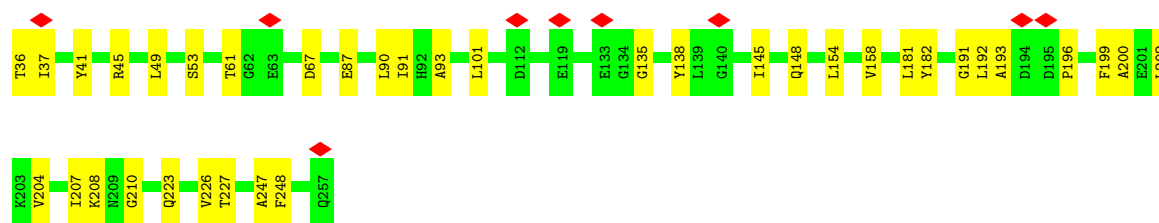


- Molecule 19: Photosystem II reaction center protein Z

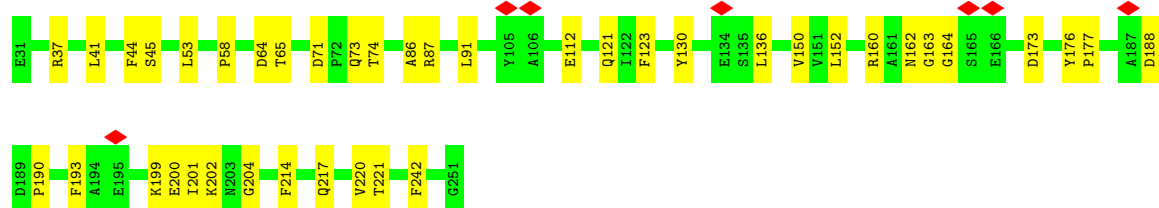
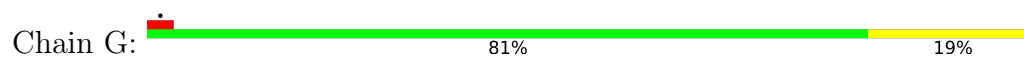


- Molecule 20: Chlorophyll a-b binding protein of LHCII type I, chloroplastic

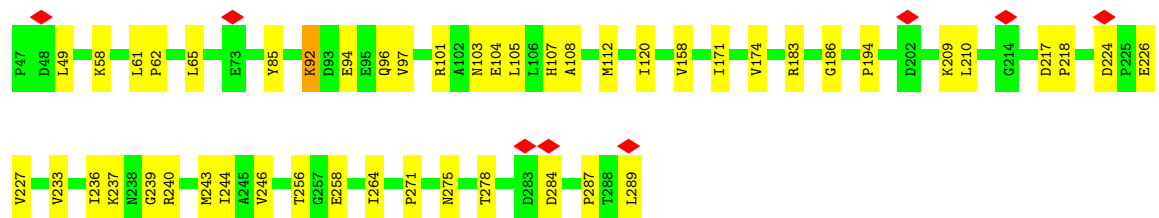
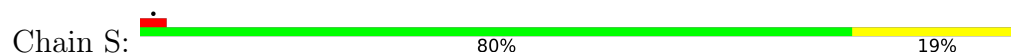




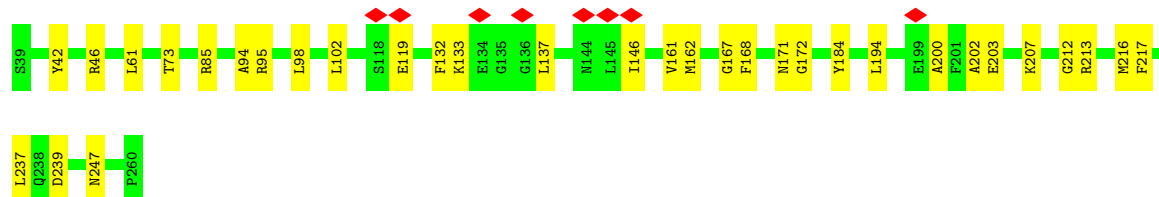
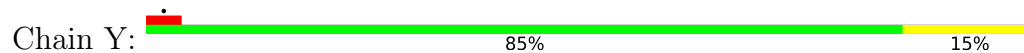
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



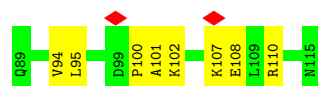
- Molecule 22: CP26



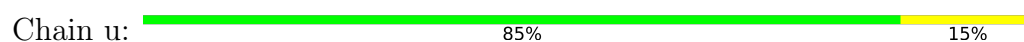
- Molecule 23: LHCII M1



- Molecule 24: PsbU



- Molecule 24: PsbU



Q89	
R90	
V91	
R92	
	M115

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21066	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	22.262	Depositor
Minimum map value	-13.270	Depositor
Average map value	0.035	Depositor
Map value standard deviation	1.121	Depositor
Recommended contour level	3.5	Depositor
Map size ($\text{\AA}$)	448.0, 448.0, 448.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.896, 0.896, 0.896	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: C7Z, 3PH, LPX, XAT, DGA, FE2, CHL, LMK, NEX, BCR, LHG, 4RF, CLA, RRX, BCT, PL9, SQD, HEM, CSD, CL, DGD, SPH, OEX, PHO, PTY, LUT, LMG, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.20	0/2723	0.44	0/3715
1	a	0.24	0/2723	0.58	1/3715 (0.0%)
2	B	0.16	0/3906	0.41	0/5319
2	b	0.18	0/3906	0.45	0/5319
3	V	0.16	0/228	0.40	0/311
3	v	0.19	0/228	0.56	0/311
4	C	0.17	0/3602	0.38	0/4913
4	c	0.19	0/3602	0.45	0/4913
5	D	0.18	0/2860	0.44	0/3899
5	d	0.21	0/2860	0.52	0/3899
6	E	0.17	0/639	0.46	0/870
6	e	0.19	0/639	0.44	0/870
7	F	0.17	0/259	0.36	0/351
7	f	0.23	0/259	0.66	1/351 (0.3%)
8	H	0.22	0/513	0.54	1/703 (0.1%)
8	h	0.22	0/513	0.53	0/703
9	I	0.20	0/287	0.51	0/386
9	i	0.25	0/287	0.54	0/386
10	J	0.13	0/272	0.32	0/369
10	j	0.14	0/272	0.38	0/369
11	K	0.24	0/308	0.53	0/423
11	k	0.29	0/308	0.61	0/423
12	L	0.15	0/321	0.35	0/435
12	l	0.23	0/321	0.47	0/435
13	M	0.26	0/237	0.59	0/323
13	m	0.25	0/237	0.60	0/323
14	O	0.17	0/1857	0.50	1/2508 (0.0%)
14	o	0.17	0/1857	0.45	0/2508
15	P	0.15	0/1473	0.44	1/1988 (0.1%)
15	p	0.15	0/1473	0.48	1/1988 (0.1%)
16	T	0.21	0/254	0.58	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.16	0/254	0.42	0/342
17	W	0.20	0/339	0.53	0/460
17	w	0.18	0/339	0.51	0/460
18	X	0.18	0/202	0.45	0/276
18	x	0.20	0/202	0.49	0/276
19	Z	0.14	0/469	0.35	0/641
19	z	0.22	0/469	0.49	0/641
20	N	0.18	0/1751	0.46	0/2386
21	G	0.17	0/1725	0.44	0/2348
22	S	0.18	0/1903	0.50	0/2590
23	Y	0.15	0/1719	0.35	0/2343
24	U	0.19	0/224	0.51	0/298
24	u	0.17	0/224	0.43	0/298
All	All	0.19	0/49044	0.46	6/66727 (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
4	c	0	1
5	d	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	199	MET	CB-CG-SD	6.32	131.66	112.70
15	p	155	VAL	N-CA-C	-6.30	106.99	113.10
7	f	39	MET	CB-CG-SD	-6.16	94.23	112.70
8	H	50	MET	CB-CG-SD	-6.05	94.54	112.70
14	O	120	VAL	N-CA-C	-5.59	107.83	113.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	c	435	ARG	Sidechain
5	d	136	VAL	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	A	2638	0	2541	70	0
1	a	2638	0	2541	118	0
2	B	3785	0	3663	80	0
2	b	3785	0	3663	116	0
3	V	227	0	261	6	0
3	v	227	0	261	6	0
4	C	3483	0	3376	70	0
4	c	3483	0	3376	95	0
5	D	2766	0	2655	66	0
5	d	2766	0	2655	101	0
6	E	621	0	605	12	0
6	e	621	0	605	19	0
7	F	252	0	265	9	0
7	f	252	0	265	10	0
8	H	503	0	532	16	0
8	h	503	0	532	18	0
9	I	279	0	288	7	0
9	i	279	0	288	6	0
10	J	266	0	286	0	0
10	j	266	0	286	6	0
11	K	297	0	312	8	0
11	k	297	0	312	5	0
12	L	313	0	325	7	0
12	l	313	0	325	15	0
13	M	234	0	258	11	0
13	m	234	0	258	8	0
14	O	1822	0	1789	29	0
14	o	1822	0	1789	35	0
15	P	1444	0	1403	30	0
15	p	1444	0	1403	29	0
16	T	247	0	260	7	0
16	t	247	0	260	7	0
17	W	332	0	323	4	0
17	w	332	0	323	6	0
18	X	201	0	224	2	0
18	x	201	0	224	2	0
19	Z	457	0	478	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	457	0	478	5	0
20	N	1703	0	1641	26	0
21	G	1680	0	1614	34	0
22	S	1856	0	1816	33	0
23	Y	1670	0	1622	23	0
24	U	224	0	226	7	0
24	u	224	0	226	3	0
25	A	10	0	0	1	0
25	a	10	0	0	0	0
26	A	1	0	0	0	0
26	a	1	0	0	0	0
27	A	2	0	0	1	0
27	a	2	0	0	0	0
28	A	240	0	240	16	0
28	B	1040	0	1149	65	0
28	C	845	0	932	43	0
28	D	130	0	144	12	0
28	G	466	0	468	19	0
28	N	468	0	468	15	0
28	S	625	0	586	18	0
28	Y	570	0	613	34	0
28	a	239	0	239	18	0
28	b	1040	0	1148	67	0
28	c	845	0	926	58	0
28	d	130	0	143	10	0
29	A	128	0	148	8	0
29	a	128	0	148	14	0
30	A	40	0	53	3	0
30	B	80	0	106	5	0
30	C	160	0	211	17	0
30	D	40	0	53	1	0
30	a	40	0	53	6	0
30	b	80	0	106	8	0
30	c	160	0	211	19	0
30	d	40	0	53	3	0
31	A	51	0	68	3	0
31	B	96	0	124	6	0
31	C	54	0	77	2	0
31	M	42	0	47	1	0
31	a	51	0	68	4	0
31	b	96	0	124	10	0
31	c	54	0	77	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	m	42	0	47	1	0
32	A	48	0	66	6	0
32	B	44	0	58	6	0
32	C	106	0	158	6	0
32	D	46	0	62	1	0
32	H	48	0	66	8	0
32	W	39	0	48	2	0
32	a	48	0	66	4	0
32	b	44	0	58	3	0
32	c	106	0	158	2	0
32	d	46	0	62	5	0
32	h	48	0	66	7	0
32	w	39	0	48	0	0
33	A	21	0	37	2	0
33	Y	21	0	37	2	0
33	a	21	0	37	2	0
34	B	42	0	0	0	0
34	b	42	0	0	0	0
35	B	43	0	44	1	0
35	C	176	0	226	14	0
35	b	43	0	44	2	0
35	c	176	0	226	20	0
36	B	48	0	75	1	0
36	S	48	0	75	4	0
36	T	48	0	75	1	0
36	b	48	0	75	2	0
36	t	48	0	75	2	0
37	B	44	0	76	4	0
37	C	44	0	76	3	0
37	J	29	0	40	1	0
37	b	44	0	76	4	0
37	c	44	0	76	2	0
37	j	29	0	40	3	0
38	C	47	0	67	5	0
38	D	132	0	183	14	0
38	G	49	0	74	4	0
38	L	49	0	74	5	0
38	N	49	0	74	4	0
38	S	45	0	63	4	0
38	Y	49	0	74	6	0
38	c	47	0	67	4	0
38	d	132	0	183	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	l	49	0	74	3	0
39	C	40	0	0	0	0
39	c	40	0	0	0	0
40	D	4	0	1	0	0
40	d	4	0	1	0	0
41	D	55	0	80	3	0
41	d	55	0	80	9	0
42	F	43	0	30	2	0
42	f	43	0	30	1	0
43	H	41	0	56	3	0
43	h	41	0	56	4	0
44	I	6	0	8	0	0
45	I	57	0	98	4	0
45	K	57	0	98	3	0
45	i	57	0	98	3	0
45	k	57	0	98	2	0
46	G	340	0	305	21	0
46	N	380	0	382	23	0
46	S	194	0	144	7	0
46	Y	310	0	306	14	0
47	G	84	0	110	5	0
47	N	84	0	110	9	0
47	S	84	0	110	8	0
47	Y	84	0	110	7	0
48	G	44	0	56	7	0
48	N	44	0	56	1	0
48	Y	44	0	56	3	0
49	G	44	0	54	2	0
49	N	44	0	54	3	0
49	S	44	0	54	1	0
49	Y	44	0	54	2	0
50	S	30	0	43	1	0
51	Y	69	0	90	7	0
All	All	60673	0	61750	1404	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 11.

The worst 5 of 1404 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)
4:c:153:LEU:HD21	28:c:506:CLA:HAB	1.53	0.91
1:a:141:PRO:HD2	4:c:435:ARG:HH22	1.42	0.82
1:A:328:MET:HG3	5:D:325:ILE:HD11	1.61	0.82
8:h:56:LEU:HB3	43:h:101:RRX:H31	1.63	0.80
22:S:246:VAL:HG11	47:S:621:LUT:H12	1.62	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/336 (100%)	323 (96%)	12 (4%)	0	100	100
1	a	335/336 (100%)	317 (95%)	18 (5%)	0	100	100
2	B	481/484 (99%)	463 (96%)	18 (4%)	0	100	100
2	b	481/484 (99%)	465 (97%)	16 (3%)	0	100	100
3	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	v	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	428 (96%)	19 (4%)	0	100	100
4	c	447/449 (100%)	420 (94%)	27 (6%)	0	100	100
5	D	346/348 (99%)	334 (96%)	12 (4%)	0	100	100
5	d	346/348 (99%)	329 (95%)	17 (5%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	e	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	h	65/67 (97%)	62 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
9	i	33/35 (94%)	30 (91%)	3 (9%)	0	100	100
10	J	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
12	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m	29/31 (94%)	29 (100%)	0	0	100	100
14	O	236/238 (99%)	217 (92%)	18 (8%)	1 (0%)	30	59
14	o	236/238 (99%)	215 (91%)	20 (8%)	1 (0%)	30	59
15	P	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
15	p	185/187 (99%)	168 (91%)	17 (9%)	0	100	100
16	T	28/30 (93%)	27 (96%)	0	1 (4%)	2	20
16	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
17	W	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
18	X	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	204 (93%)	14 (6%)	2 (1%)	14	44
21	G	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
22	S	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	10	39
23	Y	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	24	55
24	U	25/27 (93%)	25 (100%)	0	0	100	100
24	u	25/27 (93%)	25 (100%)	0	0	100	100
All	All	6054/6142 (99%)	5755 (95%)	290 (5%)	9 (0%)	49	78

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	205	TYR
20	N	192	LEU
14	o	205	TYR
22	S	284	ASP
23	Y	146	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	276 (100%)	0	100	100
2	B	387/387 (100%)	387 (100%)	0	100	100
2	b	387/387 (100%)	387 (100%)	0	100	100
3	V	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	349 (100%)	1 (0%)	86	81
5	D	279/279 (100%)	278 (100%)	1 (0%)	84	79
5	d	279/279 (100%)	278 (100%)	1 (0%)	84	79
6	E	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
14	O	197/197 (100%)	197 (100%)	0	100	100
14	o	197/197 (100%)	197 (100%)	0	100	100
15	P	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	167 (99%)	1 (1%)	78	77
22	S	190/190 (100%)	190 (100%)	0	100	100
23	Y	167/167 (100%)	167 (100%)	0	100	100
24	U	26/26 (100%)	26 (100%)	0	100	100
24	u	26/26 (100%)	26 (100%)	0	100	100
All	All	4942/4940 (100%)	4938 (100%)	4 (0%)	87	87

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

Mol	Chain	Res	Type
5	D	332	GLN
21	G	73	GLN
4	c	403	ASN
5	d	83	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	315	ASN
4	c	189	ASN
1	a	335	ASN
2	b	317	ASN
4	c	373	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSD	B	218	2	4,7,8	1.03	0	1,8,10	0.17	0
2	CSD	b	218	2	4,7,8	1.09	0	1,8,10	0.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSD	B	218	2	-	1/2/6/8	-
2	CSD	b	218	2	-	2/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	218	CSD	N-CA-CB-SG
2	b	218	CSD	N-CA-CB-SG
2	b	218	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 250 ligands modelled in this entry, 6 are monoatomic - leaving 244 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	$\# Z > 2$
28	CLA	B	608	-	69,73,73	1.37	7 (10%)	82,113,113	1.89	16 (19%)
28	CLA	S	611	38	69,73,73	1.36	7 (10%)	82,113,113	1.93	19 (23%)
31	SQD	C	526	-	52,54,54	0.78	1 (1%)	62,65,65	0.84	2 (3%)
31	SQD	b	621	-	40,42,54	0.87	0	50,53,65	0.85	2 (4%)
35	DGD	C	519	-	63,63,67	1.24	7 (11%)	77,77,81	0.98	3 (3%)
46	CHL	S	607	-	37,51,74	1.68	8 (21%)	30,86,114	2.30	11 (36%)
28	CLA	B	609	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	17 (20%)
28	CLA	c	505	-	69,73,73	1.36	7 (10%)	82,113,113	2.01	18 (21%)
28	CLA	G	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	18 (21%)
36	3PH	b	624	-	47,47,47	0.88	4 (8%)	50,52,52	1.13	2 (4%)
28	CLA	a	405	-	69,73,73	1.33	6 (8%)	82,113,113	1.90	20 (24%)
46	CHL	S	608	-	55,69,74	1.35	8 (14%)	52,108,114	1.85	13 (25%)
33	SPH	a	414	-	19,20,20	0.68	1 (5%)	18,21,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	D	404	-	41,41,41	1.59	4 (9%)	56,56,56	4.41	15 (26%)
28	CLA	S	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.82	21 (25%)
28	CLA	G	603	-	69,73,73	1.34	6 (8%)	82,113,113	1.96	20 (24%)
28	CLA	b	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	21 (25%)
28	CLA	b	612	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	16 (19%)
28	CLA	N	602	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	21 (25%)
32	LMG	W	201	-	39,39,55	0.96	2 (5%)	47,47,63	1.17	2 (4%)
46	CHL	N	601	-	60,74,74	1.29	8 (13%)	58,114,114	1.72	12 (20%)
28	CLA	D	402	-	69,73,73	1.38	7 (10%)	82,113,113	1.84	18 (21%)
28	CLA	A	410	-	64,68,73	1.40	7 (10%)	76,107,113	1.98	19 (25%)
46	CHL	G	607	-	60,74,74	1.26	8 (13%)	58,114,114	1.71	12 (20%)
28	CLA	B	615	-	69,73,73	1.37	8 (11%)	82,113,113	1.89	16 (19%)
32	LMG	A	413	-	48,48,55	1.13	5 (10%)	56,56,63	1.19	4 (7%)
34	C7Z	b	620	-	43,43,43	5.47	26 (60%)	56,60,60	2.28	16 (28%)
28	CLA	N	610	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	20 (24%)
47	LUT	S	620	-	42,43,43	2.44	1 (2%)	51,60,60	1.87	13 (25%)
28	CLA	c	507	-	69,73,73	1.38	7 (10%)	82,113,113	1.91	19 (23%)
38	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.20	3 (7%)
32	LMG	D	411	-	46,46,55	1.04	4 (8%)	54,54,63	1.07	2 (3%)
49	NEX	Y	623	-	40,46,46	2.65	11 (27%)	50,70,70	1.78	12 (24%)
28	CLA	B	617	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	17 (20%)
28	CLA	c	503	-	69,73,73	1.37	7 (10%)	82,113,113	1.90	19 (23%)
35	DGD	b	623	-	44,44,67	0.88	1 (2%)	58,58,81	1.23	6 (10%)
35	DGD	c	518	-	56,56,67	1.06	4 (7%)	70,70,81	1.00	2 (2%)
30	BCR	C	514	-	41,41,41	1.61	4 (9%)	56,56,56	4.57	13 (23%)
28	CLA	S	614	-	59,63,73	1.46	6 (10%)	70,101,113	1.97	15 (21%)
47	LUT	N	620	-	42,43,43	2.48	1 (2%)	51,60,60	1.80	14 (27%)
46	CHL	G	609	-	60,74,74	1.48	10 (16%)	58,114,114	1.61	10 (17%)
28	CLA	S	613	-	59,63,73	1.47	7 (11%)	70,101,113	2.04	20 (28%)
28	CLA	Y	608	-	54,58,73	1.54	8 (14%)	64,95,113	2.07	18 (28%)
46	CHL	Y	601	23	60,74,74	1.29	9 (15%)	58,114,114	1.82	12 (20%)
28	CLA	S	602	-	64,68,73	1.40	7 (10%)	76,107,113	2.01	21 (27%)
28	CLA	Y	604	-	69,73,73	1.35	7 (10%)	82,113,113	1.86	19 (23%)
28	CLA	B	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.88	19 (23%)
28	CLA	Y	611	-	69,73,73	1.36	8 (11%)	82,113,113	1.83	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	C	516	-	41,41,41	1.60	4 (9%)	56,56,56	4.59	13 (23%)
28	CLA	C	509	-	69,73,73	1.36	7 (10%)	82,113,113	1.85	16 (19%)
30	BCR	d	404	-	41,41,41	1.61	4 (9%)	56,56,56	4.55	15 (26%)
28	CLA	Y	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	21 (25%)
35	DGD	B	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.15	3 (5%)
32	LMG	C	523	-	55,55,55	1.28	6 (10%)	63,63,63	1.11	4 (6%)
28	CLA	c	504	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	16 (19%)
30	BCR	A	411	-	41,41,41	1.61	4 (9%)	56,56,56	4.42	12 (21%)
37	DGA	B	625	-	43,43,43	1.16	2 (4%)	45,45,45	1.49	3 (6%)
28	CLA	C	501	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	20 (24%)
37	DGA	c	524	-	43,43,43	1.17	3 (6%)	45,45,45	1.49	3 (6%)
38	LHG	C	525	-	46,46,48	0.40	0	49,52,54	1.03	2 (4%)
45	4RF	k	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.88	3 (5%)
28	CLA	d	403	-	69,73,73	1.34	7 (10%)	82,113,113	1.91	17 (20%)
29	PHO	a	408	-	58,69,69	2.17	10 (17%)	55,99,99	1.50	7 (12%)
46	CHL	S	601	22	40,54,74	1.66	8 (20%)	34,90,114	2.13	11 (32%)
28	CLA	B	610	-	69,73,73	1.37	6 (8%)	82,113,113	1.75	16 (19%)
28	CLA	b	609	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	20 (24%)
35	DGD	c	520	-	60,60,67	1.18	6 (10%)	74,74,81	0.92	2 (2%)
45	4RF	i	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.90	3 (5%)
46	CHL	Y	609	-	60,74,74	1.32	9 (15%)	58,114,114	1.66	12 (20%)
42	HEM	F	101	7,6	50,50,50	1.50	9 (18%)	67,82,82	1.08	1 (1%)
28	CLA	b	604	-	69,73,73	1.36	7 (10%)	82,113,113	1.83	17 (20%)
51	PTY	Y	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)
35	DGD	C	518	-	56,56,67	1.07	4 (7%)	70,70,81	0.92	2 (2%)
46	CHL	G	601	21	60,74,74	1.35	8 (13%)	58,114,114	1.71	11 (18%)
49	NEX	N	623	-	40,46,46	2.68	11 (27%)	50,70,70	1.40	7 (14%)
28	CLA	G	604	-	53,57,73	1.55	8 (15%)	61,93,113	2.18	20 (32%)
28	CLA	N	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.93	19 (23%)
30	BCR	C	515	-	41,41,41	1.61	4 (9%)	56,56,56	4.40	12 (21%)
41	PL9	d	405	-	55,55,55	1.14	5 (9%)	68,69,69	1.57	12 (17%)
28	CLA	S	609	-	64,68,73	1.40	7 (10%)	76,107,113	1.94	19 (25%)
28	CLA	A	405	-	69,73,73	1.36	7 (10%)	82,113,113	1.83	16 (19%)
28	CLA	C	508	-	69,73,73	1.37	7 (10%)	82,113,113	1.81	17 (20%)
46	CHL	G	605	-	42,56,74	1.49	8 (19%)	36,92,114	2.17	12 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	a	411	-	41,41,41	1.63	4 (9%)	56,56,56	4.48	15 (26%)
25	OEX	a	401	1,4	0,15,15	-	-	-		
39	LMK	c	527	-	39,39,53	1.55	3 (7%)	39,46,60	1.29	2 (5%)
43	RRX	H	101	-	42,42,42	4.96	24 (57%)	56,58,58	2.83	21 (37%)
28	CLA	C	512	-	69,73,73	1.37	7 (10%)	82,113,113	1.88	17 (20%)
29	PHO	A	409	-	58,69,69	2.18	9 (15%)	55,99,99	1.65	9 (16%)
28	CLA	C	513	-	69,73,73	1.39	7 (10%)	82,113,113	1.89	17 (20%)
32	LMG	h	102	-	48,48,55	1.14	6 (12%)	56,56,63	1.18	3 (5%)
28	CLA	b	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.80	17 (20%)
28	CLA	B	616	-	69,73,73	1.36	7 (10%)	82,113,113	1.83	19 (23%)
28	CLA	b	615	-	69,73,73	1.36	7 (10%)	82,113,113	1.86	18 (21%)
28	CLA	Y	614	-	69,73,73	1.34	6 (8%)	82,113,113	1.85	19 (23%)
44	GOL	I	101	-	5,5,5	0.56	0	5,5,5	0.32	0
28	CLA	N	604	-	69,73,73	1.36	7 (10%)	82,113,113	1.94	20 (24%)
30	BCR	b	619	-	41,41,41	1.63	4 (9%)	56,56,56	4.54	11 (19%)
28	CLA	c	508	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	18 (21%)
30	BCR	c	514	-	41,41,41	1.58	4 (9%)	56,56,56	4.62	11 (19%)
28	CLA	B	604	-	69,73,73	1.37	8 (11%)	82,113,113	1.83	18 (21%)
28	CLA	b	610	-	69,73,73	1.36	6 (8%)	82,113,113	1.85	17 (20%)
28	CLA	b	606	-	69,73,73	1.34	6 (8%)	82,113,113	1.97	19 (23%)
28	CLA	C	502	-	69,73,73	1.35	6 (8%)	82,113,113	1.87	17 (20%)
28	CLA	S	612	-	49,53,73	1.61	7 (14%)	58,89,113	2.01	15 (25%)
28	CLA	b	605	-	69,73,73	1.37	8 (11%)	82,113,113	1.92	16 (19%)
38	LHG	S	624	28	44,44,48	0.42	0	47,50,54	1.14	3 (6%)
39	LMK	C	527	-	39,39,53	1.53	2 (5%)	39,46,60	1.50	2 (5%)
28	CLA	a	406	-	69,73,73	1.37	6 (8%)	82,113,113	1.82	18 (21%)
28	CLA	B	603	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	20 (24%)
28	CLA	S	604	-	59,63,73	1.46	6 (10%)	70,101,113	2.06	18 (25%)
28	CLA	G	614	-	53,57,73	1.53	7 (13%)	61,93,113	2.20	18 (29%)
41	PL9	D	405	-	55,55,55	1.10	4 (7%)	68,69,69	1.47	11 (16%)
46	CHL	N	608	-	44,58,74	1.52	7 (15%)	37,94,114	2.00	11 (29%)
31	SQD	A	412	-	49,51,54	0.80	0	59,62,65	0.86	2 (3%)
51	PTY	Y	627	-	18,18,49	1.33	3 (16%)	21,23,54	1.45	2 (9%)
30	BCR	B	618	-	41,41,41	1.66	5 (12%)	56,56,56	4.67	15 (26%)
28	CLA	c	511	-	69,73,73	1.37	7 (10%)	82,113,113	1.92	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	C7Z	B	620	-	43,43,43	5.45	26 (60%)	56,60,60	2.27	20 (35%)
28	CLA	b	607	-	69,73,73	1.36	7 (10%)	82,113,113	1.86	19 (23%)
28	CLA	c	509	-	69,73,73	1.37	6 (8%)	82,113,113	1.83	14 (17%)
29	PHO	a	409	-	58,69,69	2.15	9 (15%)	55,99,99	1.71	8 (14%)
28	CLA	N	612	-	49,53,73	1.61	8 (16%)	58,89,113	2.01	15 (25%)
36	3PH	S	626	-	47,47,47	0.87	4 (8%)	50,52,52	4.51	4 (8%)
48	XAT	N	622	-	41,47,47	0.68	1 (2%)	54,74,74	1.95	11 (20%)
38	LHG	d	409	-	48,48,48	0.39	0	51,54,54	1.00	2 (3%)
28	CLA	B	612	-	69,73,73	1.36	6 (8%)	82,113,113	1.83	17 (20%)
28	CLA	G	612	-	47,51,73	1.64	7 (14%)	55,86,113	2.08	14 (25%)
28	CLA	B	606	-	69,73,73	1.34	6 (8%)	82,113,113	1.96	19 (23%)
37	DGA	b	625	-	43,43,43	1.15	2 (4%)	45,45,45	1.52	3 (6%)
28	CLA	b	608	-	69,73,73	1.36	7 (10%)	82,113,113	1.87	17 (20%)
49	NEX	G	623	-	40,46,46	2.69	11 (27%)	50,70,70	1.85	9 (18%)
40	BCT	d	401	26	3,3,3	1.15	0	2,3,3	4.48	2 (100%)
38	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.04	3 (6%)
50	LPX	S	625	-	29,29,29	1.03	2 (6%)	31,33,33	0.98	1 (3%)
36	3PH	T	101	-	47,47,47	0.86	4 (8%)	50,52,52	1.13	2 (4%)
32	LMG	a	413	-	48,48,55	1.12	5 (10%)	56,56,63	1.15	3 (5%)
28	CLA	C	510	-	69,73,73	1.34	7 (10%)	82,113,113	1.94	16 (19%)
28	CLA	G	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	22 (26%)
38	LHG	D	409	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
47	LUT	S	621	-	42,43,43	2.43	1 (2%)	51,60,60	1.84	15 (29%)
28	CLA	S	605	-	54,58,73	1.57	9 (16%)	64,95,113	2.12	16 (25%)
31	SQD	m	101	-	40,42,54	0.87	0	50,53,65	0.90	2 (4%)
28	CLA	b	617	-	69,73,73	1.36	6 (8%)	82,113,113	1.85	18 (21%)
45	4RF	K	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.87	3 (5%)
46	CHL	S	606	-	38,52,74	1.80	8 (21%)	31,87,114	2.19	11 (35%)
28	CLA	c	510	-	69,73,73	1.32	6 (8%)	82,113,113	1.94	18 (21%)
32	LMG	b	622	-	44,44,55	0.97	3 (6%)	52,52,63	1.12	2 (3%)
35	DGD	C	520	-	60,60,67	1.17	6 (10%)	74,74,81	0.93	2 (2%)
28	CLA	A	407	-	54,58,73	1.53	6 (11%)	64,95,113	2.11	21 (32%)
30	BCR	c	516	-	41,41,41	1.61	4 (9%)	56,56,56	4.67	13 (23%)
47	LUT	G	620	-	42,43,43	2.45	1 (2%)	51,60,60	1.81	14 (27%)
48	XAT	Y	622	-	41,47,47	0.68	1 (2%)	54,74,74	3.72	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	3PH	t	101	-	47,47,47	0.88	4 (8%)	50,52,52	1.17	2 (4%)
28	CLA	a	407	-	53,57,73	1.55	7 (13%)	61,93,113	2.32	19 (31%)
28	CLA	D	403	-	69,73,73	1.36	6 (8%)	82,113,113	1.93	19 (23%)
28	CLA	N	614	-	53,57,73	1.55	8 (15%)	61,93,113	2.21	21 (34%)
32	LMG	c	523	-	55,55,55	1.28	6 (10%)	63,63,63	1.07	4 (6%)
32	LMG	d	411	-	46,46,55	1.04	4 (8%)	54,54,63	1.04	2 (3%)
28	CLA	C	504	-	69,73,73	1.34	6 (8%)	82,113,113	1.91	19 (23%)
28	CLA	Y	612	-	69,73,73	1.36	8 (11%)	82,113,113	1.89	19 (23%)
28	CLA	b	616	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	19 (23%)
28	CLA	c	501	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	19 (23%)
46	CHL	G	606	-	44,58,74	1.59	8 (18%)	37,94,114	2.19	11 (29%)
46	CHL	Y	607	-	60,74,74	1.10	7 (11%)	58,114,114	1.78	13 (22%)
33	SPH	Y	625	-	19,20,20	0.65	0	18,21,21	1.06	1 (5%)
49	NEX	S	623	-	40,46,46	2.70	12 (30%)	50,70,70	1.69	11 (22%)
28	CLA	B	611	-	69,73,73	1.38	7 (10%)	82,113,113	1.88	18 (21%)
28	CLA	A	406	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	16 (19%)
43	RRX	h	101	-	42,42,42	5.03	24 (57%)	56,58,58	2.48	20 (35%)
47	LUT	N	621	-	42,43,43	2.47	1 (2%)	51,60,60	1.90	12 (23%)
32	LMG	c	521	-	51,51,55	1.21	6 (11%)	59,59,63	1.03	2 (3%)
32	LMG	B	622	-	44,44,55	0.98	4 (9%)	52,52,63	1.11	2 (3%)
30	BCR	C	517	-	41,41,41	1.59	4 (9%)	56,56,56	4.47	15 (26%)
46	CHL	N	609	-	60,74,74	1.23	7 (11%)	58,114,114	1.69	12 (20%)
37	DGA	C	524	-	43,43,43	1.16	3 (6%)	45,45,45	1.53	3 (6%)
28	CLA	Y	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	22 (26%)
38	LHG	L	101	-	48,48,48	0.39	0	51,54,54	4.49	5 (9%)
25	OEX	A	401	1,4	0,15,15	-	-	-	-	-
32	LMG	w	201	-	39,39,55	0.95	2 (5%)	47,47,63	1.07	2 (4%)
30	BCR	c	517	-	41,41,41	1.62	4 (9%)	56,56,56	4.64	15 (26%)
28	CLA	B	607	-	69,73,73	1.36	7 (10%)	82,113,113	1.87	18 (21%)
28	CLA	N	611	-	53,57,73	1.54	6 (11%)	61,93,113	2.15	19 (31%)
28	CLA	S	617	-	54,58,73	1.53	7 (12%)	64,95,113	2.12	21 (32%)
28	CLA	c	513	-	69,73,73	1.35	7 (10%)	82,113,113	1.97	23 (28%)
47	LUT	Y	620	-	42,43,43	2.46	1 (2%)	51,60,60	1.82	14 (27%)
28	CLA	C	503	-	69,73,73	1.37	8 (11%)	82,113,113	1.89	18 (21%)
29	PHO	A	408	-	58,69,69	2.18	10 (17%)	55,99,99	1.50	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	DGA	j	101	-	28,28,43	1.32	3 (10%)	30,30,45	1.21	2 (6%)
28	CLA	d	402	-	69,73,73	1.38	7 (10%)	82,113,113	1.80	20 (24%)
38	LHG	G	624	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
46	CHL	N	605	20	60,74,74	1.32	8 (13%)	58,114,114	1.75	12 (20%)
46	CHL	G	608	-	38,52,74	1.64	8 (21%)	31,87,114	2.26	11 (35%)
46	CHL	Y	605	23	40,54,74	1.57	7 (17%)	34,90,114	2.17	10 (29%)
48	XAT	G	622	-	41,47,47	0.70	1 (2%)	54,74,74	1.91	12 (22%)
47	LUT	Y	621	-	42,43,43	2.45	1 (2%)	51,60,60	1.84	14 (27%)
38	LHG	d	410	-	38,38,48	0.42	0	41,44,54	1.15	3 (7%)
28	CLA	G	602	-	69,73,73	1.38	7 (10%)	82,113,113	1.88	18 (21%)
28	CLA	C	505	-	69,73,73	1.38	7 (10%)	82,113,113	1.83	16 (19%)
38	LHG	N	624	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
38	LHG	l	101	-	48,48,48	0.38	0	51,54,54	4.49	4 (7%)
28	CLA	b	602	-	69,73,73	1.36	7 (10%)	82,113,113	1.87	16 (19%)
31	SQD	b	626	-	52,54,54	0.78	0	62,65,65	0.84	2 (3%)
31	SQD	c	526	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
28	CLA	a	410	-	64,68,73	1.41	7 (10%)	76,107,113	1.93	19 (25%)
38	LHG	D	408	-	43,43,48	0.40	0	46,49,54	1.01	2 (4%)
28	CLA	N	613	-	69,73,73	1.37	8 (11%)	82,113,113	1.89	18 (21%)
28	CLA	Y	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.87	20 (24%)
28	CLA	c	502	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	18 (21%)
28	CLA	c	512	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	16 (19%)
31	SQD	M	101	-	40,42,54	0.87	0	50,53,65	0.88	2 (4%)
28	CLA	b	614	-	69,73,73	1.37	7 (10%)	82,113,113	1.85	17 (20%)
28	CLA	B	614	-	69,73,73	1.35	6 (8%)	82,113,113	1.86	17 (20%)
36	3PH	B	624	-	47,47,47	0.87	4 (8%)	50,52,52	1.14	2 (4%)
28	CLA	C	506	-	69,73,73	1.36	6 (8%)	82,113,113	1.85	16 (19%)
35	DGD	c	519	-	63,63,67	1.24	7 (11%)	77,77,81	0.95	2 (2%)
33	SPH	A	414	-	19,20,20	0.67	0	18,21,21	1.07	1 (5%)
31	SQD	B	626	-	52,54,54	0.79	0	62,65,65	0.85	2 (3%)
28	CLA	C	511	-	69,73,73	1.35	7 (10%)	82,113,113	1.93	18 (21%)
38	LHG	Y	624	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
32	LMG	C	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.10	4 (6%)
38	LHG	d	408	-	43,43,48	0.40	0	46,49,54	1.00	2 (4%)
31	SQD	a	412	-	49,51,54	0.80	1 (2%)	59,62,65	0.85	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	BCT	D	401	-	3,3,3	1.13	0	2,3,3	4.10	2 (100%)
45	4RF	I	102	-	56,56,56	1.06	3 (5%)	59,59,59	0.90	3 (5%)
28	CLA	c	506	-	69,73,73	1.36	6 (8%)	82,113,113	1.85	18 (21%)
46	CHL	N	607	-	60,74,74	1.25	7 (11%)	58,114,114	1.74	12 (20%)
47	LUT	G	621	-	42,43,43	2.44	1 (2%)	51,60,60	1.89	13 (25%)
28	CLA	Y	602	-	69,73,73	1.35	7 (10%)	82,113,113	1.87	21 (25%)
28	CLA	b	611	-	69,73,73	1.37	7 (10%)	82,113,113	1.91	19 (23%)
28	CLA	S	603	-	69,73,73	1.37	8 (11%)	82,113,113	1.98	19 (23%)
37	DGA	J	101	-	28,28,43	1.33	3 (10%)	30,30,45	1.26	2 (6%)
30	BCR	c	515	-	41,41,41	1.59	4 (9%)	56,56,56	4.42	14 (25%)
46	CHL	N	606	-	60,74,74	1.28	8 (13%)	58,114,114	1.81	13 (22%)
46	CHL	Y	606	-	60,74,74	1.34	8 (13%)	58,114,114	1.72	13 (22%)
42	HEM	f	101	7,6	50,50,50	1.46	7 (14%)	67,82,82	1.10	3 (4%)
31	SQD	B	621	-	40,42,54	0.86	0	50,53,65	0.86	2 (4%)
28	CLA	G	611	-	69,73,73	1.37	7 (10%)	82,113,113	1.87	19 (23%)
28	CLA	C	507	-	69,73,73	1.38	7 (10%)	82,113,113	1.91	20 (24%)
28	CLA	B	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.83	15 (18%)
30	BCR	B	619	-	41,41,41	1.62	4 (9%)	56,56,56	4.48	15 (26%)
30	BCR	b	618	-	41,41,41	1.64	4 (9%)	56,56,56	4.79	21 (37%)
32	LMG	H	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.12	2 (3%)
28	CLA	B	605	-	69,73,73	1.37	6 (8%)	82,113,113	2.02	18 (21%)

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
28	CLA	B	608	-	1/1/15/20	25/39/115/115	-
28	CLA	S	611	38	1/1/15/20	17/39/115/115	-
31	SQD	C	526	-	-	16/49/69/69	0/1/1/1
31	SQD	b	621	-	-	18/37/57/69	0/1/1/1
35	DGD	C	519	-	-	13/51/91/95	0/2/2/2
46	CHL	S	607	-	3/3/15/26	2/12/110/137	-
28	CLA	B	609	-	1/1/15/20	13/39/115/115	-
28	CLA	c	505	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	G	613	-	1/1/15/20	15/39/115/115	-
36	3PH	b	624	-	-	21/49/49/49	-
28	CLA	a	405	-	1/1/15/20	12/39/115/115	-
46	CHL	S	608	-	4/4/19/26	10/33/131/137	-
33	SPH	a	414	-	-	12/21/21/21	-
30	BCR	D	404	-	-	12/29/63/63	0/2/2/2
28	CLA	S	610	-	1/1/15/20	21/39/115/115	-
28	CLA	G	603	-	1/1/15/20	18/39/115/115	-
28	CLA	b	603	-	1/1/15/20	16/39/115/115	-
28	CLA	b	612	-	1/1/15/20	14/39/115/115	-
28	CLA	N	602	-	1/1/15/20	17/39/115/115	-
46	CHL	N	601	-	4/4/20/26	7/39/137/137	-
32	LMG	W	201	-	-	12/34/54/70	0/1/1/1
28	CLA	D	402	-	1/1/15/20	19/39/115/115	-
28	CLA	A	410	-	1/1/14/20	11/33/109/115	-
46	CHL	G	607	-	4/4/20/26	11/39/137/137	-
28	CLA	B	615	-	1/1/15/20	11/39/115/115	-
32	LMG	A	413	-	-	14/43/63/70	0/1/1/1
34	C7Z	b	620	-	1/1/12/26	14/29/67/67	0/2/2/2
28	CLA	N	610	-	1/1/15/20	22/39/115/115	-
47	LUT	S	620	-	-	2/29/67/67	0/2/2/2
28	CLA	c	507	-	1/1/15/20	18/39/115/115	-
38	LHG	D	410	-	-	30/43/43/53	-
32	LMG	D	411	-	-	9/41/61/70	0/1/1/1
49	NEX	Y	623	-	-	5/27/83/83	0/3/3/3
28	CLA	B	617	-	1/1/15/20	19/39/115/115	-
28	CLA	c	503	-	1/1/15/20	19/39/115/115	-
35	DGD	b	623	-	-	11/32/72/95	0/2/2/2
35	DGD	c	518	-	-	18/44/84/95	0/2/2/2
30	BCR	C	514	-	-	13/29/63/63	0/2/2/2
28	CLA	S	614	-	1/1/13/20	9/27/103/115	-
47	LUT	N	620	-	-	3/29/67/67	0/2/2/2
46	CHL	G	609	-	4/4/20/26	8/39/137/137	-
28	CLA	S	613	-	1/1/13/20	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	Y	608	-	1/1/12/20	9/21/97/115	-
46	CHL	Y	601	23	4/4/20/26	1/39/137/137	-
28	CLA	S	602	-	1/1/14/20	20/33/109/115	-
28	CLA	Y	604	-	1/1/15/20	16/39/115/115	-
28	CLA	B	602	-	1/1/15/20	21/39/115/115	-
28	CLA	Y	611	-	1/1/15/20	16/39/115/115	-
30	BCR	C	516	-	-	15/29/63/63	0/2/2/2
28	CLA	C	509	-	1/1/15/20	18/39/115/115	-
30	BCR	d	404	-	-	13/29/63/63	0/2/2/2
28	CLA	Y	603	-	1/1/15/20	16/39/115/115	-
35	DGD	B	623	-	-	14/32/72/95	0/2/2/2
32	LMG	C	523	-	-	18/50/70/70	0/1/1/1
28	CLA	c	504	-	1/1/15/20	20/39/115/115	-
30	BCR	A	411	-	-	11/29/63/63	0/2/2/2
37	DGA	B	625	-	-	25/45/45/45	-
28	CLA	C	501	-	1/1/15/20	18/39/115/115	-
37	DGA	c	524	-	-	23/45/45/45	-
38	LHG	C	525	-	-	32/51/51/53	-
45	4RF	k	101	-	-	30/59/59/59	-
28	CLA	d	403	-	1/1/15/20	22/39/115/115	-
29	PHO	a	408	-	-	5/37/103/103	0/5/6/6
46	CHL	S	601	22	3/3/16/26	5/15/113/137	-
28	CLA	B	610	-	1/1/15/20	14/39/115/115	-
28	CLA	b	609	-	1/1/15/20	19/39/115/115	-
35	DGD	c	520	-	-	7/48/88/95	0/2/2/2
45	4RF	i	101	-	-	31/59/59/59	-
46	CHL	Y	609	-	4/4/20/26	9/39/137/137	-
42	HEM	F	101	7,6	-	0/14/54/54	-
28	CLA	b	604	-	1/1/15/20	21/39/115/115	-
51	PTY	Y	626	-	-	18/53/53/53	-
35	DGD	C	518	-	-	14/44/84/95	0/2/2/2
46	CHL	G	601	21	4/4/20/26	8/39/137/137	-
49	NEX	N	623	-	-	2/27/83/83	1/3/3/3
28	CLA	G	604	-	1/1/11/20	11/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	N	603	-	1/1/15/20	19/39/115/115	-
30	BCR	C	515	-	-	11/29/63/63	0/2/2/2
41	PL9	d	405	-	-	21/53/73/73	0/1/1/1
28	CLA	S	609	-	1/1/14/20	12/33/109/115	-
28	CLA	A	405	-	1/1/15/20	14/39/115/115	-
28	CLA	C	508	-	1/1/15/20	8/39/115/115	-
46	CHL	G	605	-	4/4/16/26	4/18/116/137	-
30	BCR	a	411	-	-	9/29/63/63	0/2/2/2
39	LMK	c	527	-	2/2/6/6	11/46/46/60	-
43	RRX	H	101	-	1/1/11/25	6/29/65/65	0/2/2/2
28	CLA	C	512	-	1/1/15/20	21/39/115/115	-
29	PHO	A	409	-	-	4/37/103/103	0/5/6/6
28	CLA	C	513	-	1/1/15/20	20/39/115/115	-
32	LMG	h	102	-	-	11/43/63/70	0/1/1/1
28	CLA	b	613	-	1/1/15/20	18/39/115/115	-
28	CLA	B	616	-	1/1/15/20	15/39/115/115	-
28	CLA	b	615	-	1/1/15/20	12/39/115/115	-
28	CLA	Y	614	-	1/1/15/20	15/39/115/115	-
44	GOL	I	101	-	-	2/4/4/4	-
28	CLA	N	604	-	1/1/15/20	15/39/115/115	-
30	BCR	b	619	-	-	11/29/63/63	0/2/2/2
28	CLA	c	508	-	1/1/15/20	8/39/115/115	-
30	BCR	c	514	-	-	12/29/63/63	0/2/2/2
28	CLA	B	604	-	1/1/15/20	19/39/115/115	-
28	CLA	b	610	-	1/1/15/20	14/39/115/115	-
28	CLA	b	606	-	1/1/15/20	15/39/115/115	-
28	CLA	C	502	-	1/1/15/20	14/39/115/115	-
28	CLA	S	612	-	1/1/11/20	4/15/91/115	-
28	CLA	b	605	-	1/1/15/20	18/39/115/115	-
39	LMK	C	527	-	2/2/6/6	17/46/46/60	-
38	LHG	S	624	28	-	29/49/49/53	-
28	CLA	a	406	-	1/1/15/20	14/39/115/115	-
28	CLA	B	603	-	1/1/15/20	15/39/115/115	-
28	CLA	S	604	-	1/1/13/20	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	G	614	-	1/1/11/20	11/20/96/115	-
46	CHL	N	608	-	3/3/16/26	5/20/118/137	-
41	PL9	D	405	-	-	7/53/73/73	0/1/1/1
31	SQD	A	412	-	-	16/46/66/69	0/1/1/1
51	PTY	Y	627	-	-	11/20/20/53	-
30	BCR	B	618	-	-	7/29/63/63	0/2/2/2
28	CLA	c	511	-	1/1/15/20	14/39/115/115	-
34	C7Z	B	620	-	1/1/12/26	11/29/67/67	0/2/2/2
28	CLA	b	607	-	1/1/15/20	9/39/115/115	-
28	CLA	c	509	-	1/1/15/20	14/39/115/115	-
48	XAT	N	622	-	1/1/12/26	0/31/93/93	0/4/4/4
28	CLA	N	612	-	1/1/11/20	4/15/91/115	-
29	PHO	a	409	-	-	9/37/103/103	0/5/6/6
36	3PH	S	626	-	-	25/49/49/49	-
38	LHG	d	409	-	-	26/53/53/53	-
28	CLA	B	612	-	1/1/15/20	14/39/115/115	-
28	CLA	G	612	-	1/1/10/20	6/13/89/115	-
28	CLA	B	606	-	1/1/15/20	16/39/115/115	-
37	DGA	b	625	-	-	26/45/45/45	-
28	CLA	b	608	-	1/1/15/20	23/39/115/115	-
49	NEX	G	623	-	-	6/27/83/83	0/3/3/3
38	LHG	c	525	-	-	31/51/51/53	-
50	LPX	S	625	-	-	11/31/31/31	-
36	3PH	T	101	-	-	22/49/49/49	-
32	LMG	a	413	-	-	13/43/63/70	0/1/1/1
28	CLA	C	510	-	1/1/15/20	17/39/115/115	-
28	CLA	G	610	-	1/1/15/20	18/39/115/115	-
38	LHG	D	409	-	-	27/53/53/53	-
47	LUT	S	621	-	-	1/29/67/67	0/2/2/2
28	CLA	S	605	-	1/1/12/20	10/21/97/115	-
31	SQD	m	101	-	-	20/37/57/69	0/1/1/1
28	CLA	b	617	-	1/1/15/20	14/39/115/115	-
46	CHL	S	606	-	3/3/15/26	0/13/111/137	-
45	4RF	K	101	-	-	32/59/59/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	c	510	-	1/1/15/20	19/39/115/115	-
32	LMG	b	622	-	-	11/39/59/70	0/1/1/1
35	DGD	C	520	-	-	9/48/88/95	0/2/2/2
28	CLA	A	407	-	1/1/12/20	7/21/97/115	-
30	BCR	c	516	-	-	13/29/63/63	0/2/2/2
47	LUT	G	620	-	-	3/29/67/67	0/2/2/2
48	XAT	Y	622	-	-	1/31/93/93	0/4/4/4
36	3PH	t	101	-	-	26/49/49/49	-
28	CLA	a	407	-	1/1/11/20	11/20/96/115	-
28	CLA	D	403	-	1/1/15/20	16/39/115/115	-
28	CLA	N	614	-	1/1/11/20	8/20/96/115	-
32	LMG	c	523	-	-	14/50/70/70	0/1/1/1
32	LMG	d	411	-	-	8/41/61/70	0/1/1/1
28	CLA	C	504	-	1/1/15/20	13/39/115/115	-
28	CLA	Y	612	-	1/1/15/20	15/39/115/115	-
28	CLA	b	616	-	1/1/15/20	11/39/115/115	-
28	CLA	c	501	-	1/1/15/20	20/39/115/115	-
46	CHL	G	606	-	3/3/16/26	4/20/118/137	-
46	CHL	Y	607	-	4/4/20/26	8/39/137/137	-
33	SPH	Y	625	-	-	11/21/21/21	-
49	NEX	S	623	-	-	2/27/83/83	0/3/3/3
28	CLA	B	611	-	1/1/15/20	11/39/115/115	-
28	CLA	A	406	-	1/1/15/20	15/39/115/115	-
43	RRX	h	101	-	1/1/11/25	7/29/65/65	0/2/2/2
47	LUT	N	621	-	-	2/29/67/67	0/2/2/2
32	LMG	c	521	-	-	13/46/66/70	0/1/1/1
32	LMG	B	622	-	-	11/39/59/70	0/1/1/1
30	BCR	C	517	-	-	9/29/63/63	0/2/2/2
46	CHL	N	609	-	4/4/20/26	5/39/137/137	-
37	DGA	C	524	-	-	21/45/45/45	-
28	CLA	Y	610	-	1/1/15/20	15/39/115/115	-
38	LHG	L	101	-	-	41/53/53/53	-
32	LMG	w	201	-	-	10/34/54/70	0/1/1/1
30	BCR	c	517	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	607	-	1/1/15/20	13/39/115/115	-
28	CLA	N	611	-	1/1/11/20	9/20/96/115	-
28	CLA	S	617	-	1/1/12/20	7/21/97/115	-
28	CLA	c	513	-	1/1/15/20	12/39/115/115	-
47	LUT	Y	620	-	-	3/29/67/67	0/2/2/2
28	CLA	C	503	-	1/1/15/20	15/39/115/115	-
46	CHL	G	608	-	3/3/15/26	1/13/111/137	-
29	PHO	A	408	-	-	13/37/103/103	0/5/6/6
28	CLA	d	402	-	1/1/15/20	19/39/115/115	-
37	DGA	j	101	-	-	14/30/30/45	-
46	CHL	N	605	20	4/4/20/26	4/39/137/137	-
46	CHL	Y	605	23	3/3/16/26	3/15/113/137	-
38	LHG	G	624	-	-	28/53/53/53	-
48	XAT	G	622	-	2/2/12/26	0/31/93/93	0/4/4/4
47	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
38	LHG	d	410	-	-	23/43/43/53	-
28	CLA	G	602	-	1/1/15/20	22/39/115/115	-
28	CLA	C	505	-	1/1/15/20	17/39/115/115	-
38	LHG	N	624	-	-	32/53/53/53	-
38	LHG	l	101	-	-	37/53/53/53	-
28	CLA	b	602	-	1/1/15/20	26/39/115/115	-
31	SQD	b	626	-	-	22/49/69/69	0/1/1/1
31	SQD	c	526	-	-	13/49/69/69	0/1/1/1
28	CLA	a	410	-	1/1/14/20	5/33/109/115	-
38	LHG	D	408	-	-	23/48/48/53	-
28	CLA	N	613	-	1/1/15/20	17/39/115/115	-
28	CLA	Y	613	-	1/1/15/20	18/39/115/115	-
28	CLA	c	502	-	1/1/15/20	7/39/115/115	-
28	CLA	c	512	-	1/1/15/20	15/39/115/115	-
31	SQD	M	101	-	-	18/37/57/69	0/1/1/1
28	CLA	b	614	-	1/1/15/20	10/39/115/115	-
28	CLA	B	614	-	1/1/15/20	9/39/115/115	-
36	3PH	B	624	-	-	29/49/49/49	-
28	CLA	C	506	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	c	519	-	-	19/51/91/95	0/2/2/2
33	SPH	A	414	-	-	7/21/21/21	-
31	SQD	B	626	-	-	22/49/69/69	0/1/1/1
28	CLA	C	511	-	1/1/15/20	11/39/115/115	-
38	LHG	Y	624	-	-	29/53/53/53	-
32	LMG	C	521	-	-	13/46/66/70	0/1/1/1
38	LHG	d	408	-	-	30/48/48/53	-
31	SQD	a	412	-	-	21/46/66/69	0/1/1/1
46	CHL	N	607	-	4/4/20/26	10/39/137/137	-
45	4RF	I	102	-	-	27/59/59/59	-
28	CLA	c	506	-	1/1/15/20	18/39/115/115	-
47	LUT	G	621	-	-	4/29/67/67	0/2/2/2
28	CLA	Y	602	-	1/1/15/20	17/39/115/115	-
28	CLA	b	611	-	1/1/15/20	11/39/115/115	-
28	CLA	S	603	-	1/1/15/20	20/39/115/115	-
37	DGA	J	101	-	-	10/30/30/45	-
30	BCR	c	515	-	-	14/29/63/63	0/2/2/2
46	CHL	N	606	-	4/4/20/26	11/39/137/137	-
46	CHL	Y	606	-	4/4/20/26	7/39/137/137	-
42	HEM	f	101	7,6	-	1/14/54/54	-
31	SQD	B	621	-	-	14/37/57/69	0/1/1/1
28	CLA	G	611	-	1/1/15/20	15/39/115/115	-
28	CLA	C	507	-	1/1/15/20	20/39/115/115	-
28	CLA	B	613	-	1/1/15/20	16/39/115/115	-
30	BCR	B	619	-	-	6/29/63/63	0/2/2/2
30	BCR	b	618	-	-	7/29/63/63	0/2/2/2
32	LMG	H	102	-	-	9/43/63/70	0/1/1/1
28	CLA	B	605	-	1/1/15/20	13/39/115/115	-

The worst 5 of 1341 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	620	C7Z	C25-C26	16.39	1.62	1.34
34	B	620	C7Z	C25-C26	16.21	1.61	1.34
43	h	101	RRX	C26-C25	15.98	1.61	1.34
43	H	101	RRX	C26-C25	15.64	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	620	C7Z	C5-C6	15.48	1.60	1.34

The worst 5 of 2900 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	l	101	LHG	O7-C7-C8	23.00	161.24	111.48
38	L	101	LHG	O7-C7-C8	22.80	160.81	111.48
36	S	626	3PH	O21-C21-C22	22.29	159.71	111.48
30	b	618	BCR	C10-C11-C12	19.59	179.96	123.20
30	B	618	BCR	C10-C11-C12	19.27	179.02	123.20

5 of 194 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	A	405	CLA	ND
28	A	406	CLA	ND
28	A	407	CLA	ND
28	A	410	CLA	ND
28	B	602	CLA	ND

5 of 3328 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	405	CLA	C1A-C2A-CAA-CBA
28	A	405	CLA	C3A-C2A-CAA-CBA
28	A	405	CLA	CBD-CGD-O2D-CED
28	A	406	CLA	C1A-C2A-CAA-CBA
28	A	406	CLA	C3A-C2A-CAA-CBA

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	N	623	NEX	C1-C2-C3-C4-C5-C6

228 monomers are involved in 667 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	608	CLA	7	0
28	S	611	CLA	6	0
31	C	526	SQD	2	0
31	b	621	SQD	6	0
35	C	519	DGD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	S	607	CHL	1	0
28	B	609	CLA	6	0
28	c	505	CLA	4	0
28	G	613	CLA	4	0
36	b	624	3PH	2	0
28	a	405	CLA	9	0
46	S	608	CHL	2	0
33	a	414	SPH	2	0
30	D	404	BCR	1	0
28	S	610	CLA	2	0
28	G	603	CLA	5	0
28	b	603	CLA	2	0
28	b	612	CLA	5	0
28	N	602	CLA	2	0
32	W	201	LMG	2	0
46	N	601	CHL	7	0
28	D	402	CLA	8	0
28	A	410	CLA	3	0
46	G	607	CHL	7	0
28	B	615	CLA	6	0
32	A	413	LMG	6	0
28	N	610	CLA	4	0
47	S	620	LUT	4	0
28	c	507	CLA	4	0
38	D	410	LHG	5	0
32	D	411	LMG	1	0
49	Y	623	NEX	2	0
28	B	617	CLA	4	0
28	c	503	CLA	6	0
35	b	623	DGD	2	0
35	c	518	DGD	6	0
30	C	514	BCR	5	0
28	S	614	CLA	2	0
47	N	620	LUT	5	0
46	G	609	CHL	7	0
28	S	613	CLA	1	0
28	Y	608	CLA	2	0
46	Y	601	CHL	3	0
28	S	602	CLA	3	0
28	Y	604	CLA	1	0
28	B	602	CLA	3	0
28	Y	611	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	C	516	BCR	4	0
28	C	509	CLA	2	0
30	d	404	BCR	3	0
28	Y	603	CLA	5	0
35	B	623	DGD	1	0
32	C	523	LMG	4	0
28	c	504	CLA	3	0
30	A	411	BCR	3	0
37	B	625	DGA	4	0
28	C	501	CLA	5	0
37	c	524	DGA	2	0
38	C	525	LHG	5	0
45	k	101	4RF	2	0
28	d	403	CLA	5	0
29	a	408	PHO	7	0
46	S	601	CHL	2	0
28	B	610	CLA	3	0
28	b	609	CLA	10	0
35	c	520	DGD	6	0
45	i	101	4RF	3	0
46	Y	609	CHL	5	0
42	F	101	HEM	2	0
28	b	604	CLA	1	0
51	Y	626	PTY	7	0
35	C	518	DGD	6	0
46	G	601	CHL	4	0
49	N	623	NEX	3	0
28	G	604	CLA	4	0
28	N	603	CLA	2	0
30	C	515	BCR	6	0
41	d	405	PL9	9	0
28	S	609	CLA	1	0
28	A	405	CLA	9	0
28	C	508	CLA	3	0
46	G	605	CHL	1	0
30	a	411	BCR	6	0
43	H	101	RRX	3	0
28	C	512	CLA	2	0
29	A	409	PHO	4	0
28	C	513	CLA	6	0
32	h	102	LMG	7	0
28	b	613	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	616	CLA	4	0
28	b	615	CLA	4	0
28	Y	614	CLA	8	0
28	N	604	CLA	2	0
30	b	619	BCR	4	0
28	c	508	CLA	5	0
30	c	514	BCR	6	0
28	B	604	CLA	3	0
28	b	610	CLA	6	0
28	b	606	CLA	2	0
28	C	502	CLA	3	0
28	b	605	CLA	6	0
38	S	624	LHG	4	0
28	a	406	CLA	7	0
28	B	603	CLA	6	0
28	S	604	CLA	1	0
28	G	614	CLA	1	0
41	D	405	PL9	3	0
31	A	412	SQD	3	0
30	B	618	BCR	1	0
28	c	511	CLA	7	0
28	b	607	CLA	7	0
28	c	509	CLA	4	0
29	a	409	PHO	7	0
36	S	626	3PH	4	0
48	N	622	XAT	1	0
38	d	409	LHG	7	0
28	B	612	CLA	5	0
28	G	612	CLA	1	0
28	B	606	CLA	5	0
37	b	625	DGA	4	0
28	b	608	CLA	3	0
49	G	623	NEX	2	0
38	c	525	LHG	4	0
50	S	625	LPX	1	0
36	T	101	3PH	1	0
32	a	413	LMG	4	0
28	C	510	CLA	2	0
28	G	610	CLA	2	0
38	D	409	LHG	5	0
47	S	621	LUT	4	0
28	S	605	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	m	101	SQD	1	0
28	b	617	CLA	3	0
45	K	101	4RF	3	0
46	S	606	CHL	2	0
28	c	510	CLA	7	0
32	b	622	LMG	3	0
35	C	520	DGD	5	0
30	c	516	BCR	3	0
47	G	620	LUT	3	0
48	Y	622	XAT	3	0
36	t	101	3PH	2	0
28	a	407	CLA	1	0
28	D	403	CLA	4	0
28	N	614	CLA	1	0
32	c	523	LMG	1	0
32	d	411	LMG	5	0
28	C	504	CLA	3	0
28	Y	612	CLA	3	0
28	b	616	CLA	2	0
28	c	501	CLA	1	0
46	G	606	CHL	1	0
46	Y	607	CHL	4	0
33	Y	625	SPH	2	0
49	S	623	NEX	1	0
28	B	611	CLA	3	0
28	A	406	CLA	5	0
43	h	101	RRX	4	0
47	N	621	LUT	4	0
32	c	521	LMG	1	0
32	B	622	LMG	6	0
30	C	517	BCR	2	0
46	N	609	CHL	5	0
37	C	524	DGA	3	0
28	Y	610	CLA	3	0
38	L	101	LHG	5	0
25	A	401	OEX	1	0
30	c	517	BCR	6	0
28	B	607	CLA	5	0
28	N	611	CLA	1	0
28	c	513	CLA	8	0
47	Y	620	LUT	3	0
28	C	503	CLA	2	0

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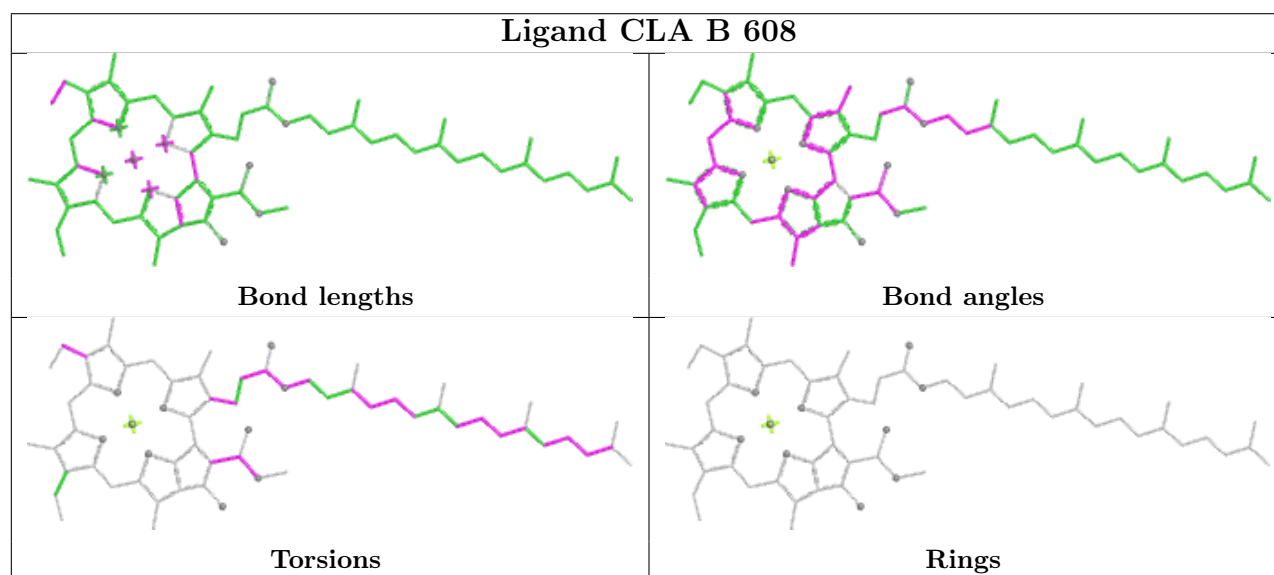
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37	j	101	DGA	3	0
28	d	402	CLA	5	0
38	G	624	LHG	4	0
46	N	605	CHL	5	0
46	G	608	CHL	3	0
46	Y	605	CHL	1	0
48	G	622	XAT	7	0
47	Y	621	LUT	4	0
38	d	410	LHG	3	0
28	G	602	CLA	3	0
28	C	505	CLA	6	0
38	N	624	LHG	4	0
38	l	101	LHG	3	0
28	b	602	CLA	4	0
31	b	626	SQD	4	0
31	c	526	SQD	2	0
28	a	410	CLA	3	0
38	D	408	LHG	4	0
28	N	613	CLA	3	0
28	Y	613	CLA	7	0
28	c	502	CLA	5	0
28	c	512	CLA	4	0
31	M	101	SQD	1	0
28	b	614	CLA	9	0
28	B	614	CLA	6	0
36	B	624	3PH	1	0
28	C	506	CLA	7	0
35	c	519	DGD	10	0
33	A	414	SPH	2	0
31	B	626	SQD	3	0
28	C	511	CLA	1	0
38	Y	624	LHG	6	0
32	C	521	LMG	2	0
38	d	408	LHG	3	0
31	a	412	SQD	4	0
45	I	102	4RF	4	0
28	c	506	CLA	5	0
46	N	607	CHL	4	0
47	G	621	LUT	2	0
28	Y	602	CLA	4	0
28	b	611	CLA	5	0

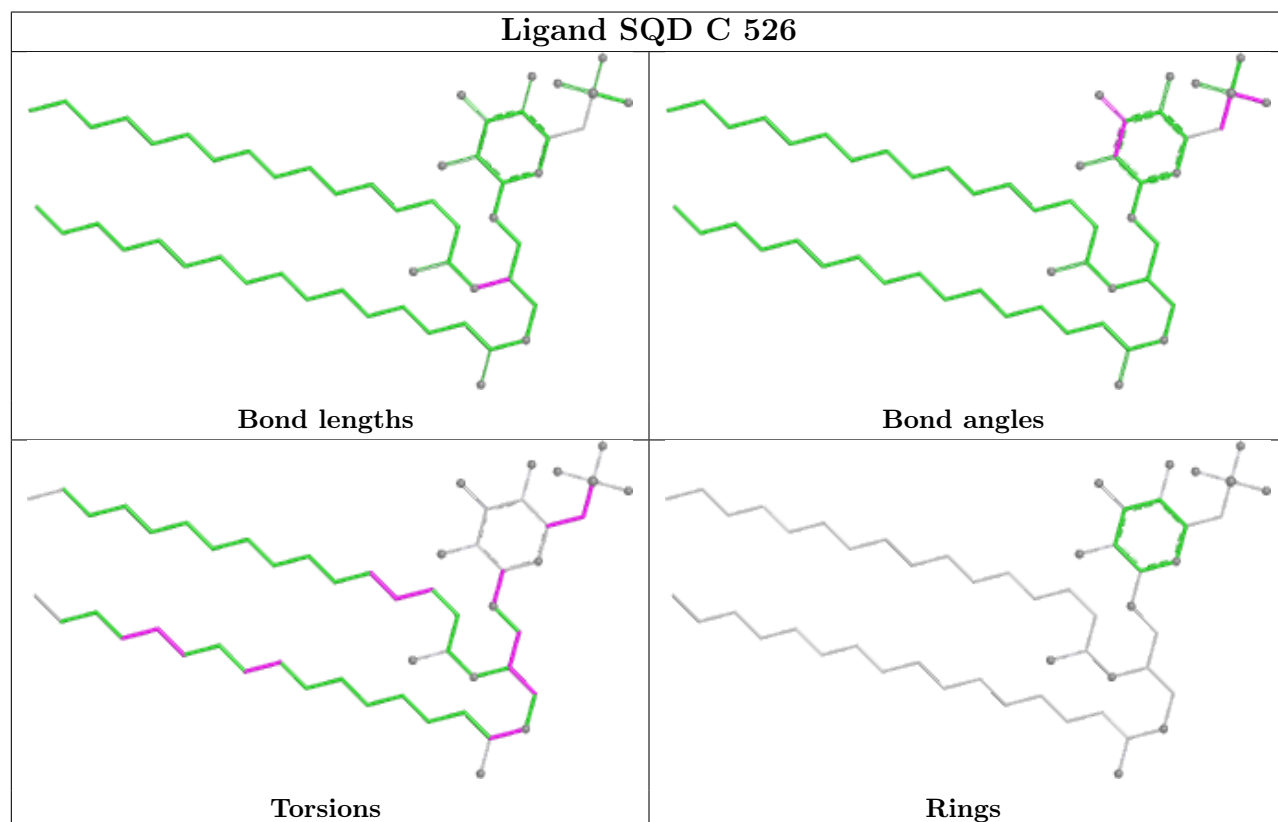
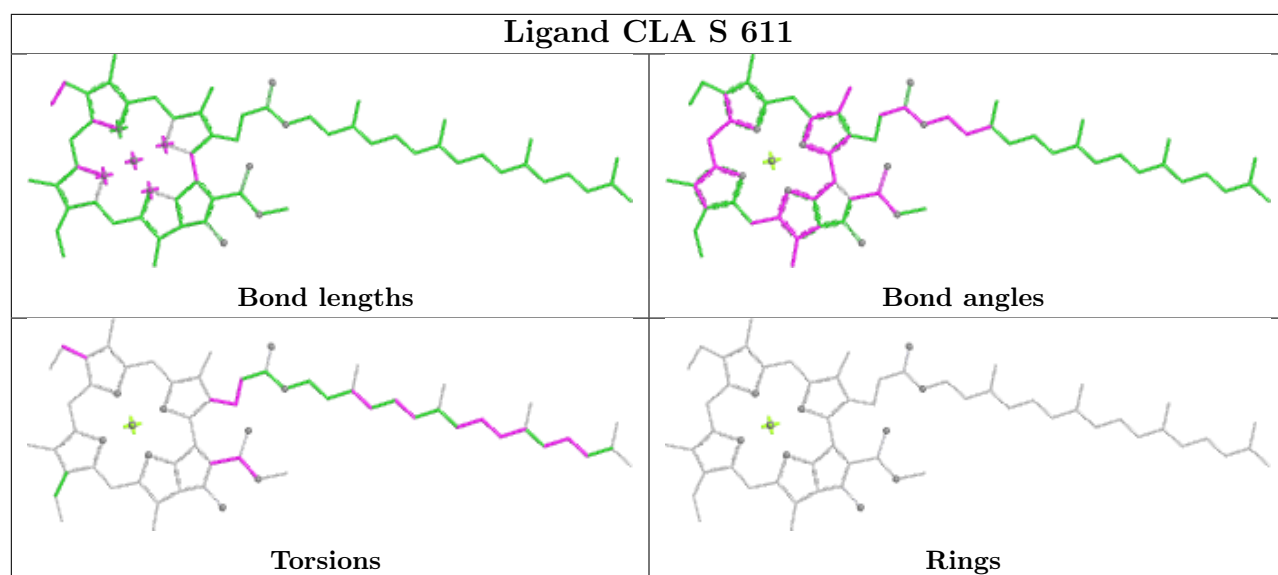
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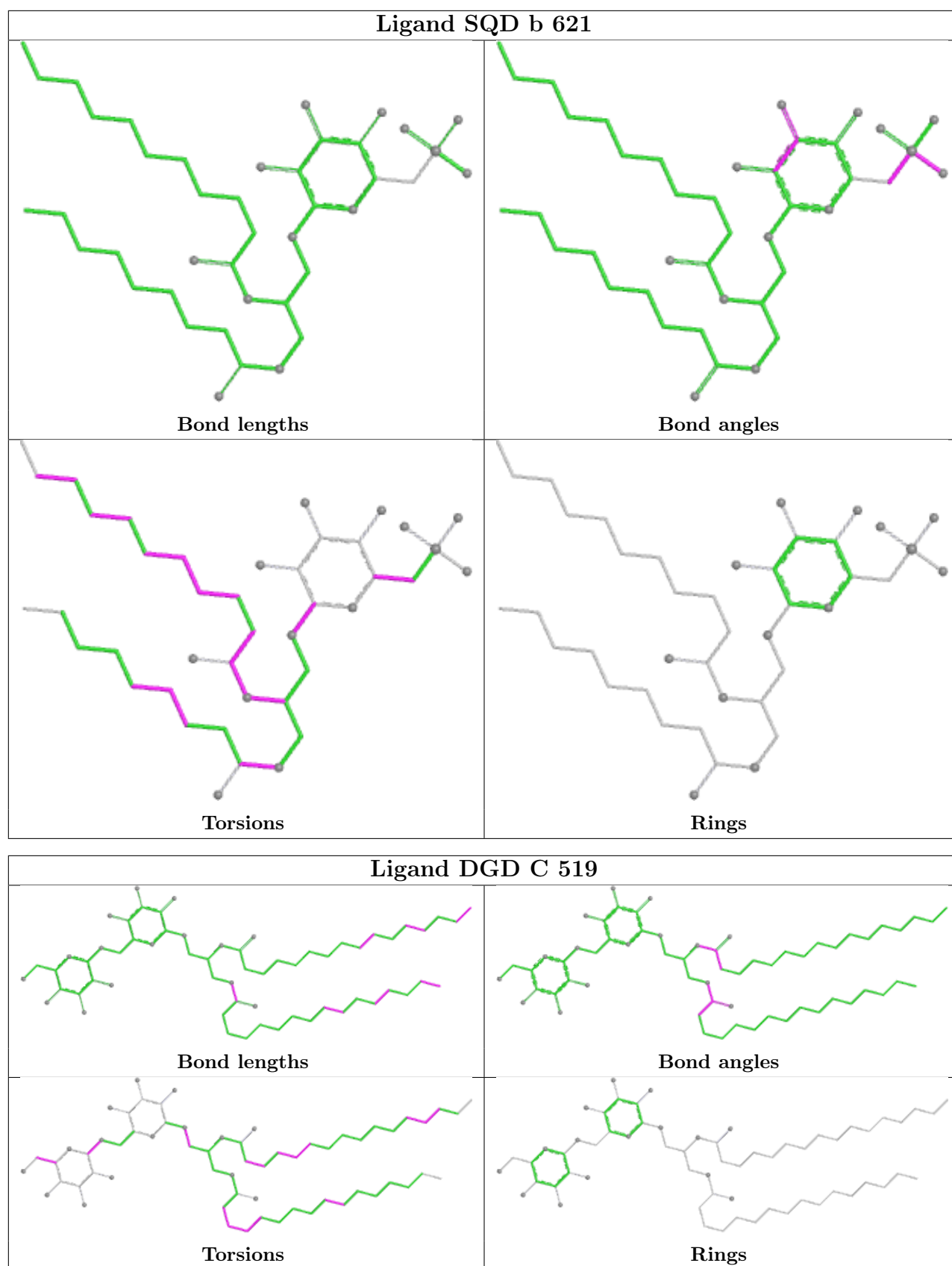
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	S	603	CLA	2	0
37	J	101	DGA	1	0
30	c	515	BCR	4	0
46	N	606	CHL	4	0
46	Y	606	CHL	2	0
42	f	101	HEM	1	0
31	B	621	SQD	3	0
28	C	507	CLA	6	0
28	B	613	CLA	5	0
30	B	619	BCR	4	0
30	b	618	BCR	4	0
32	H	102	LMG	8	0
28	B	605	CLA	5	0

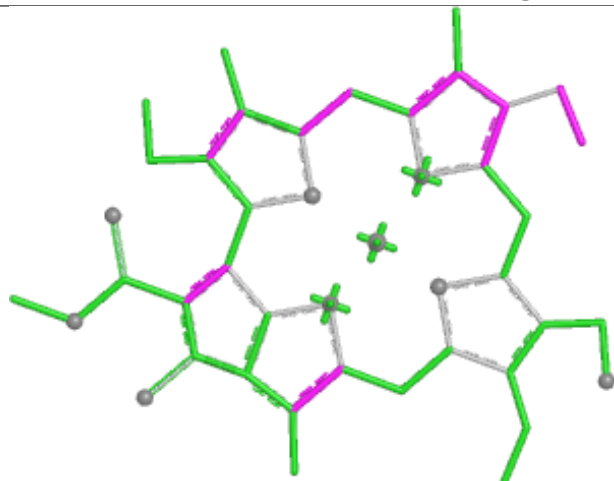
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



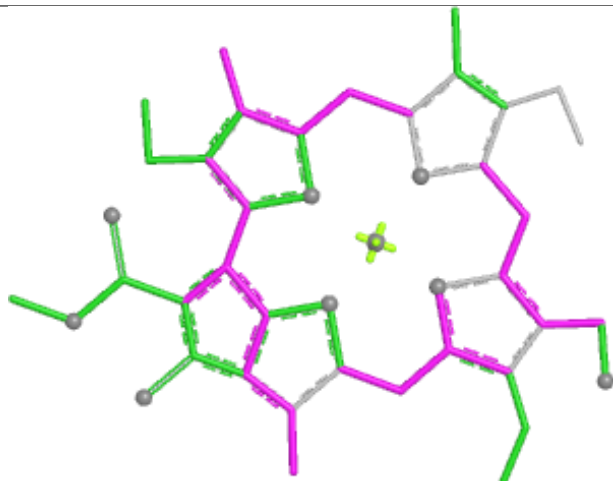




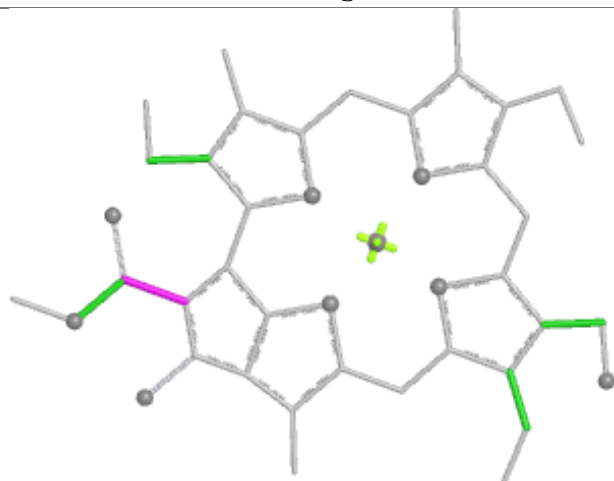
Ligand CHL S 607



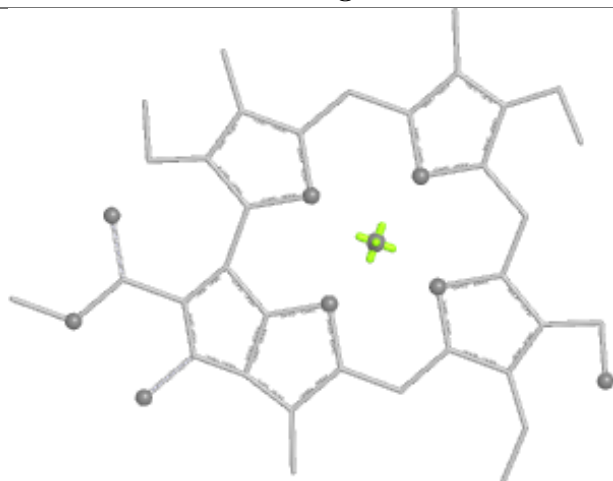
Bond lengths



Bond angles

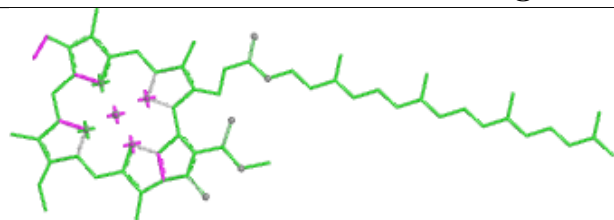


Torsions

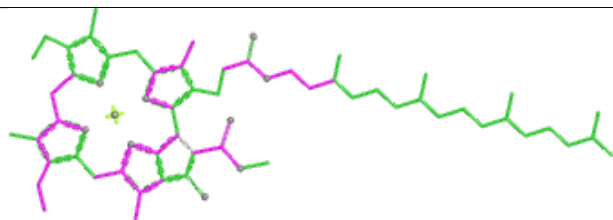


Rings

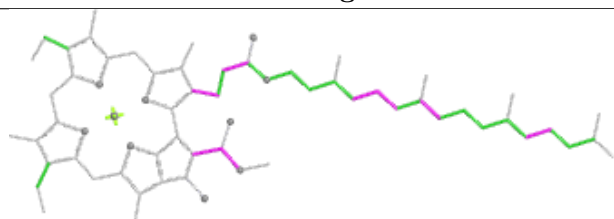
Ligand CLA B 609



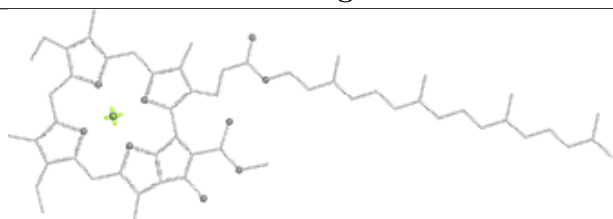
Bond lengths



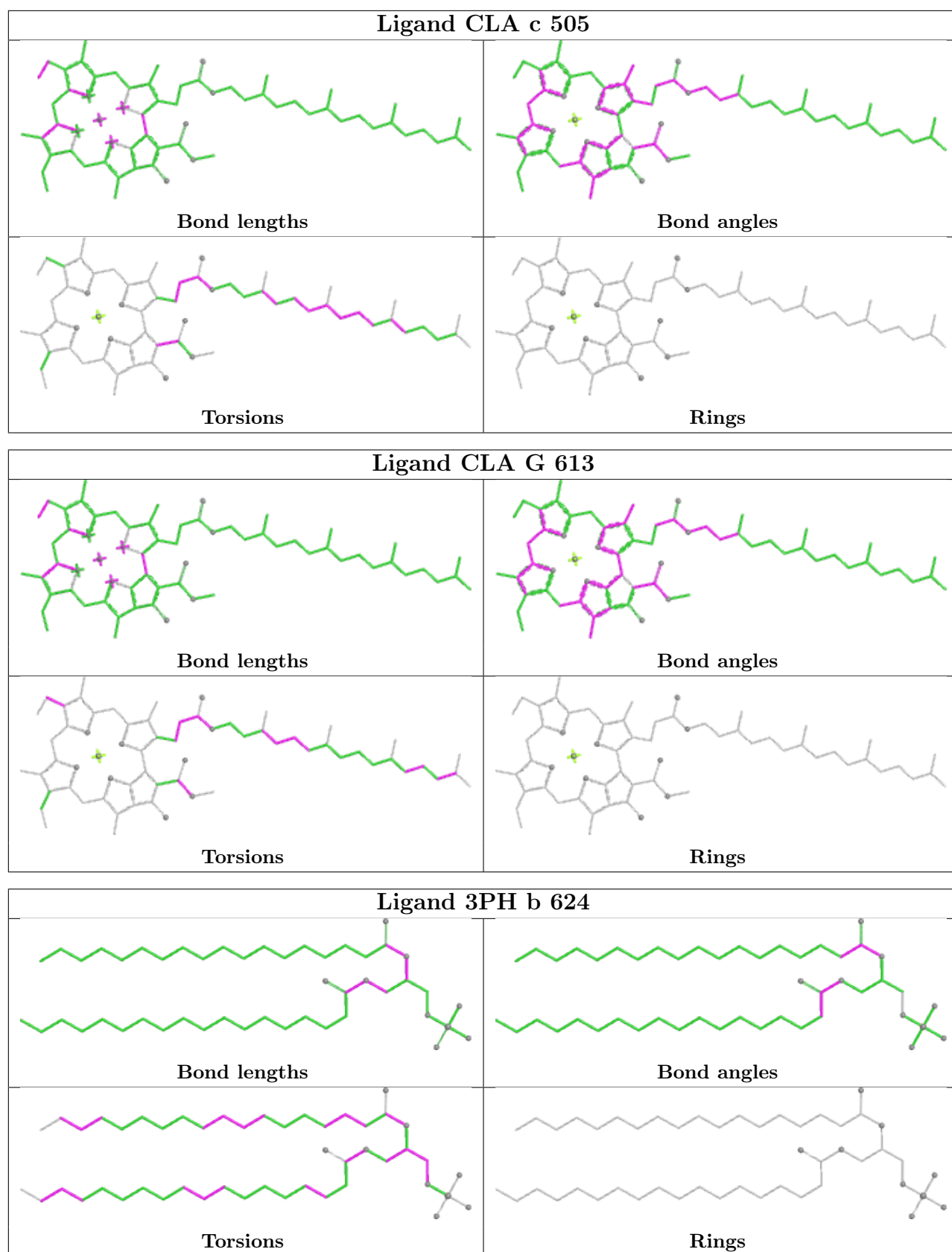
Bond angles

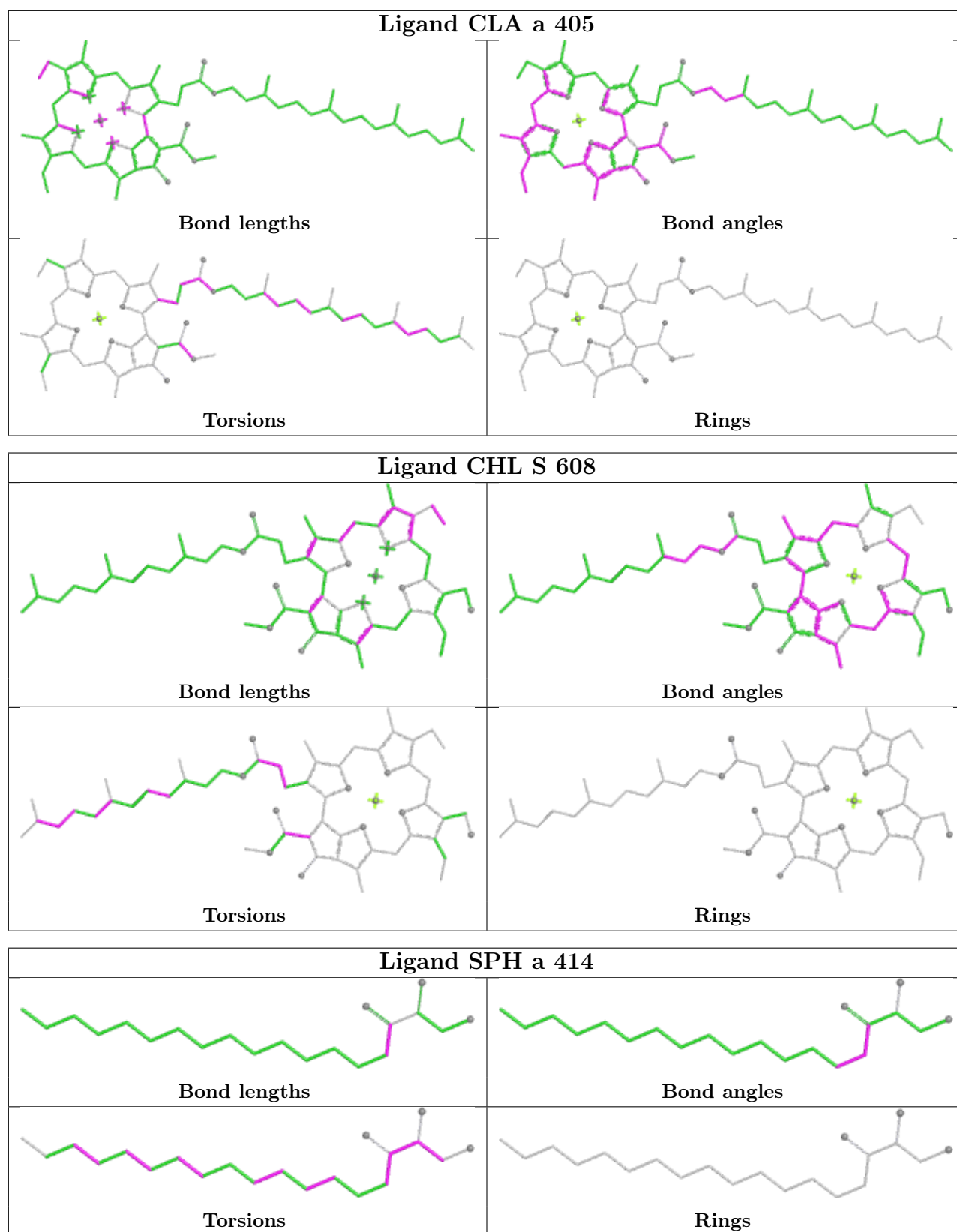


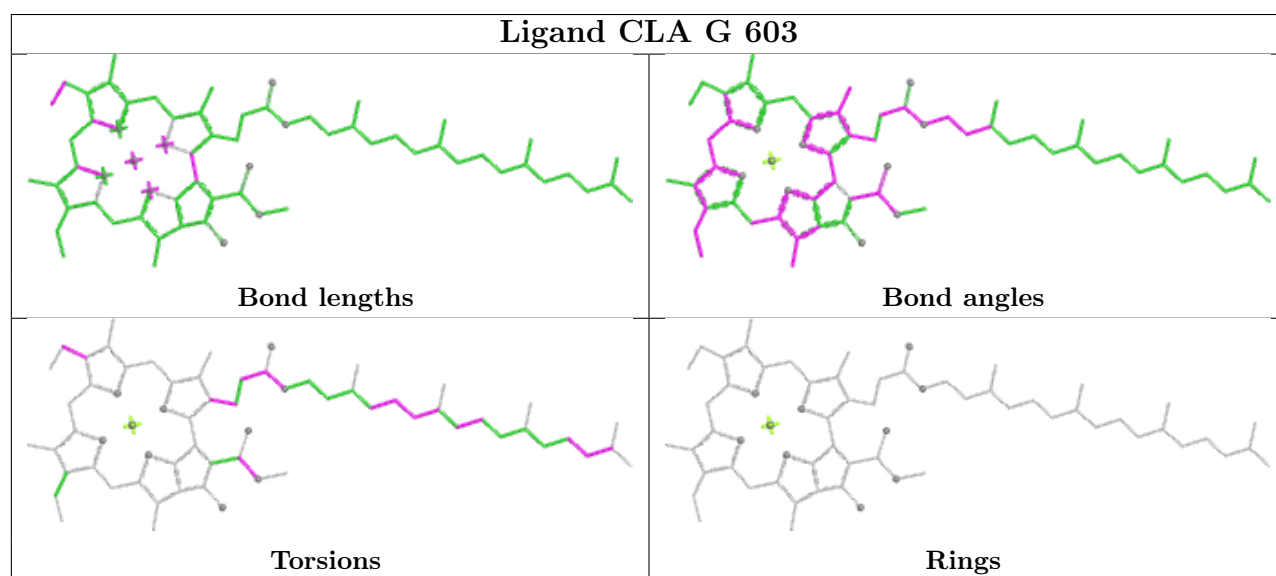
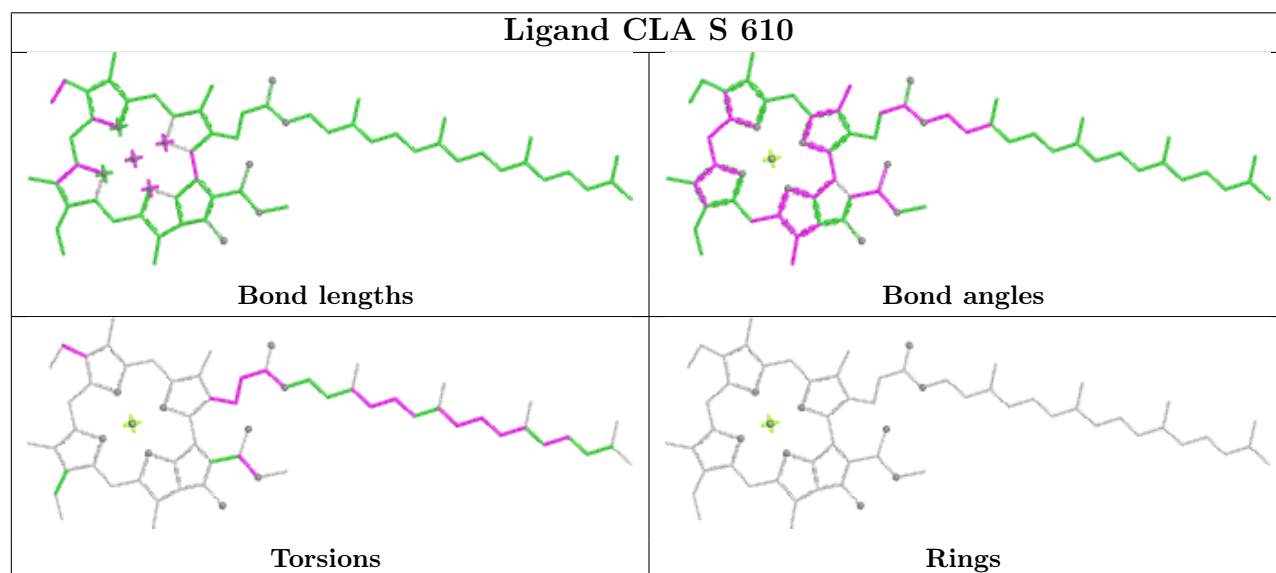
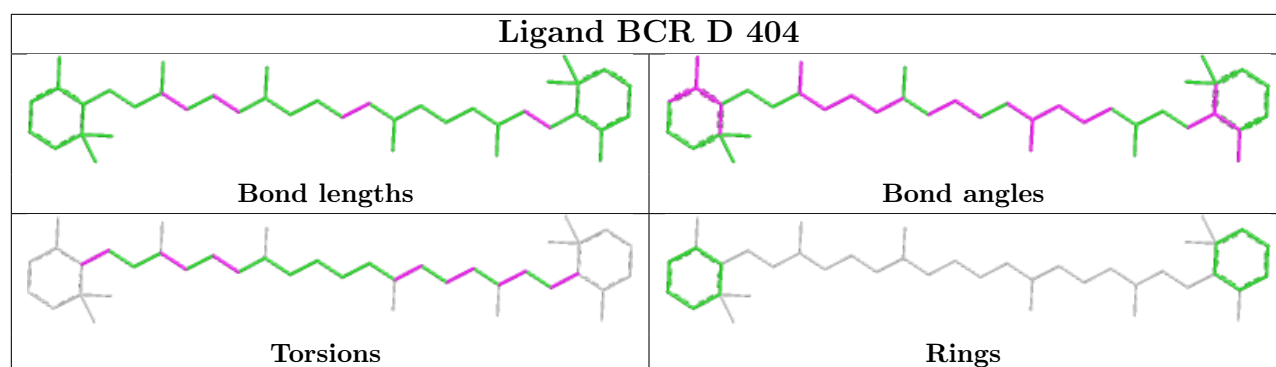
Torsions

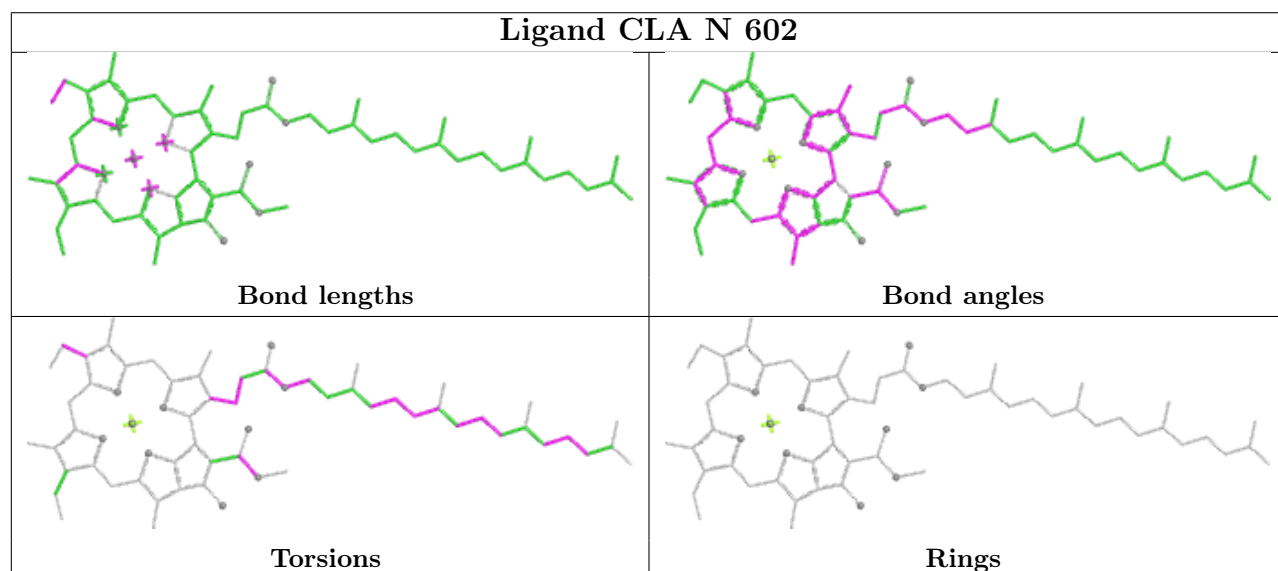
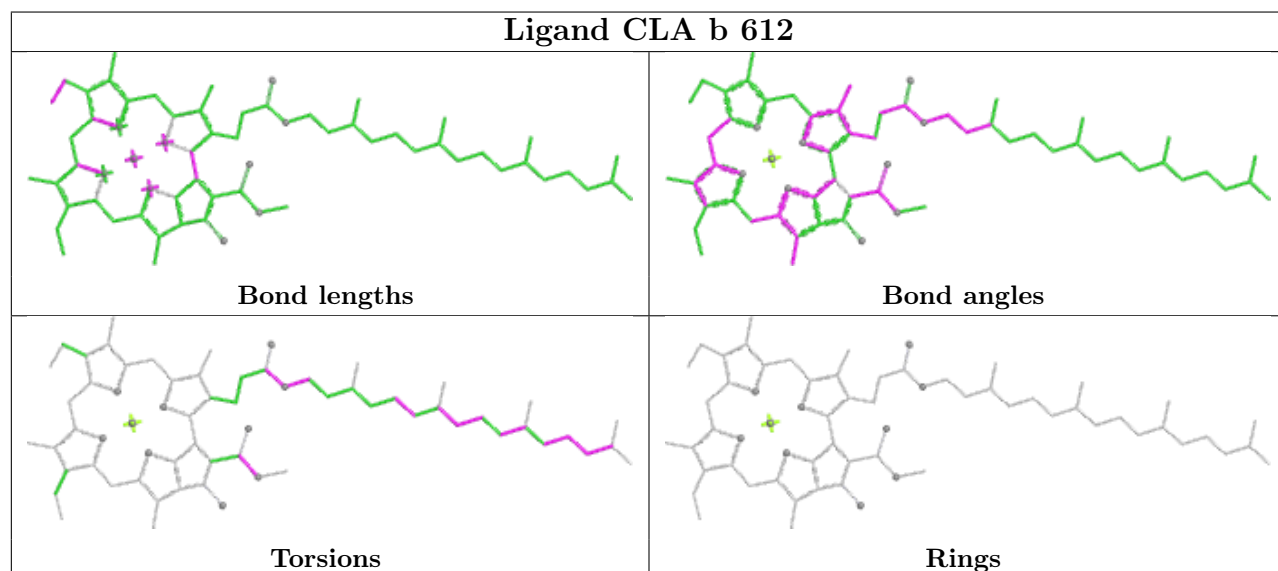
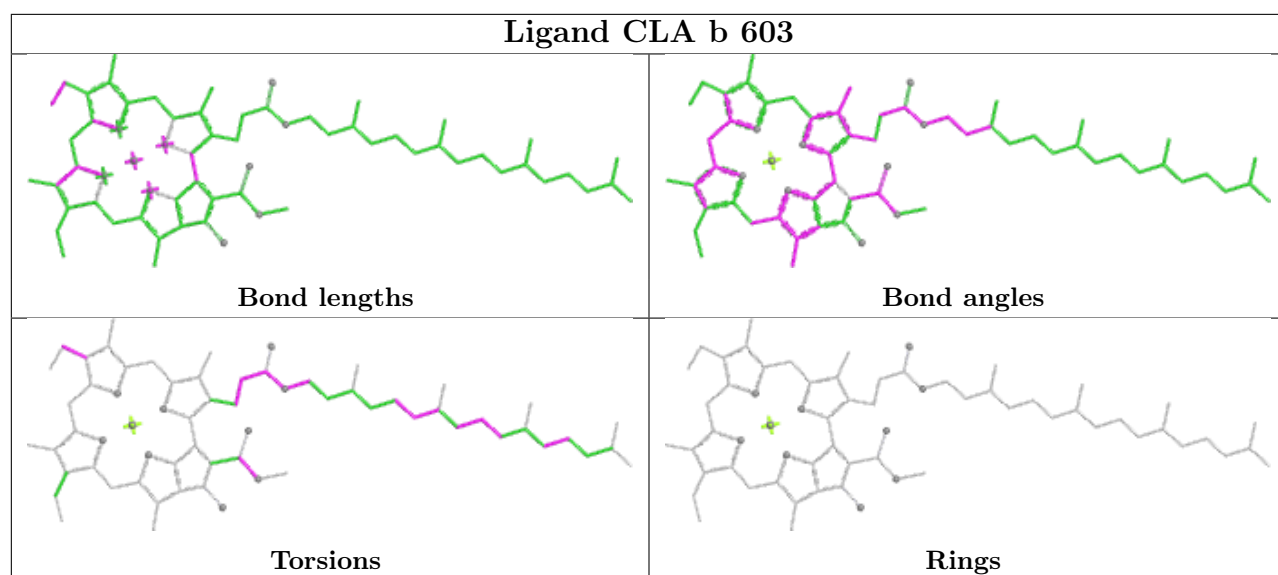


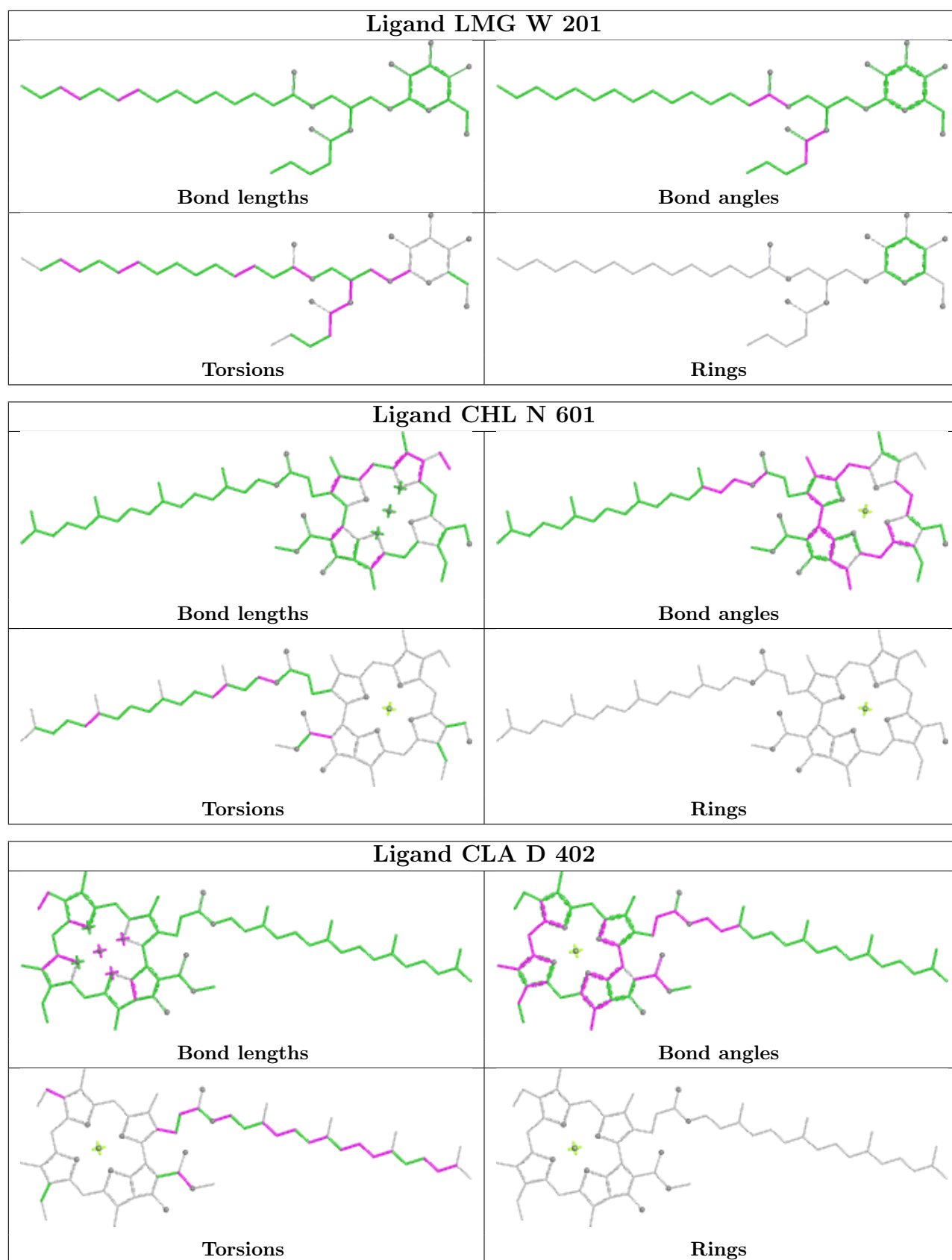
Rings

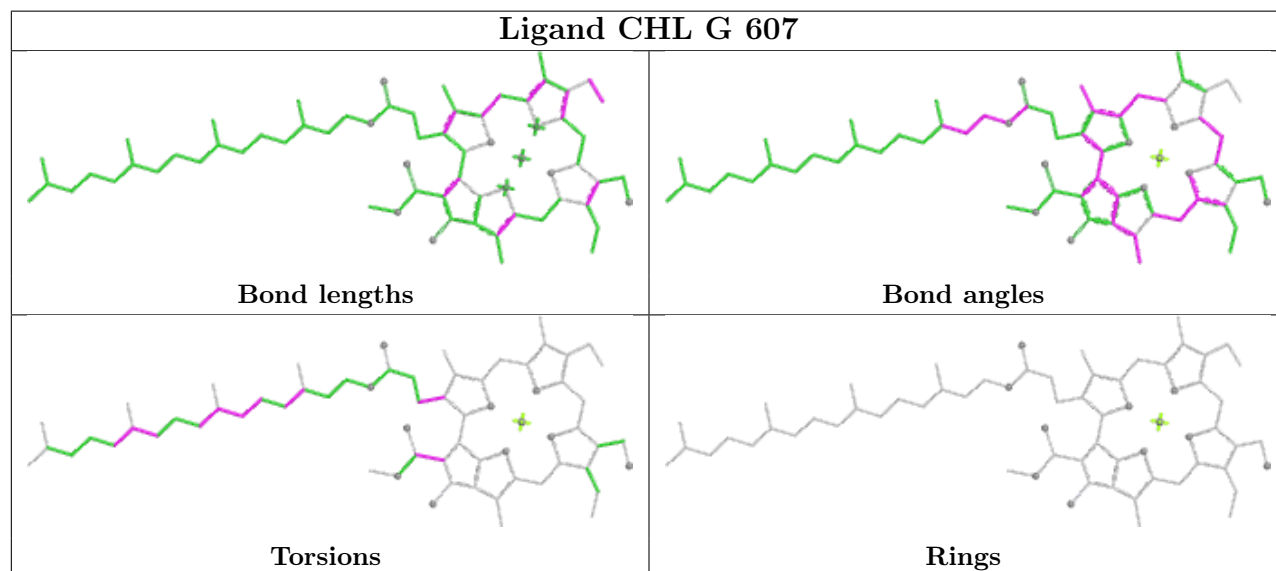
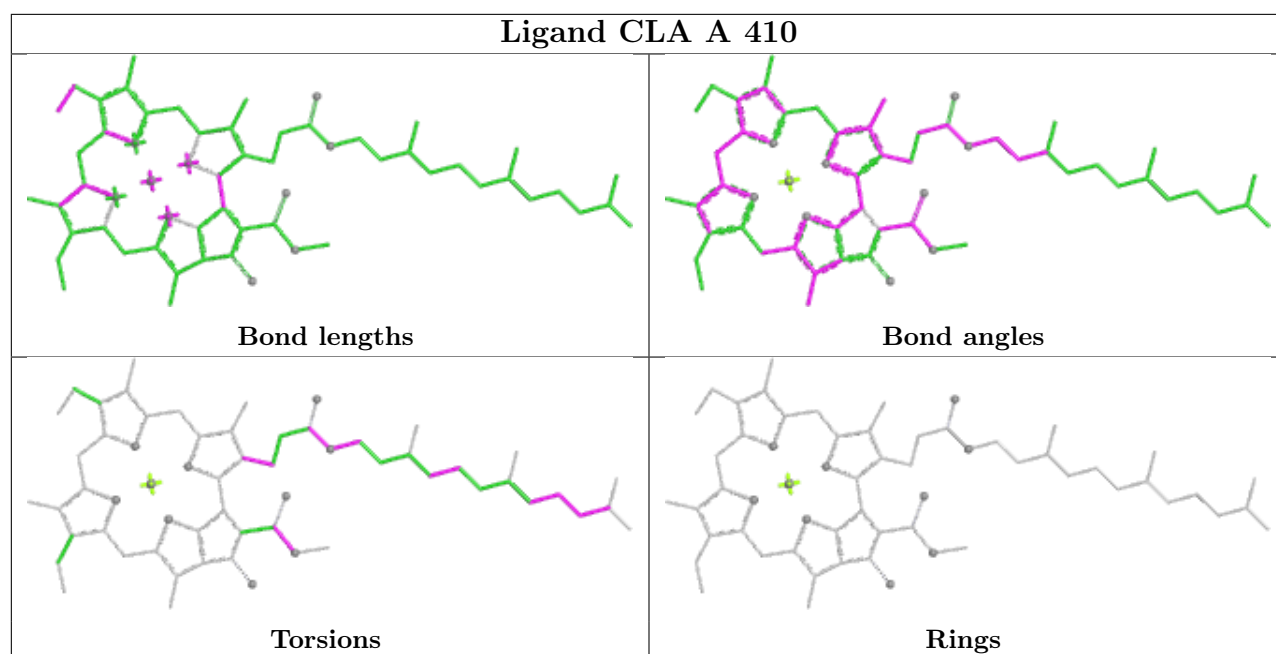


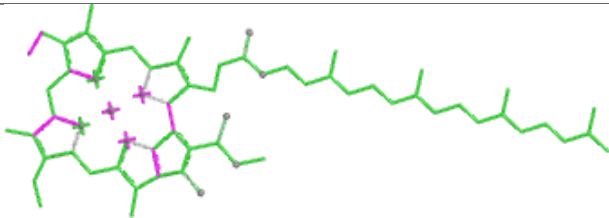
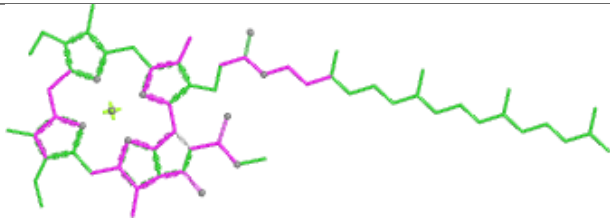
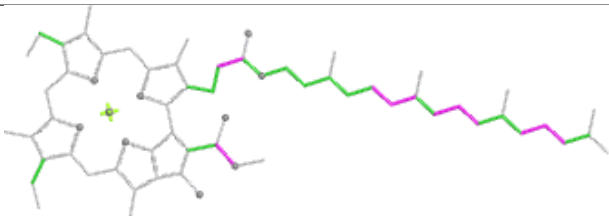
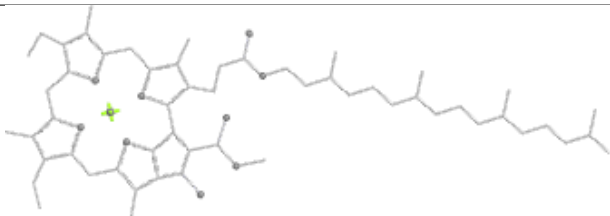


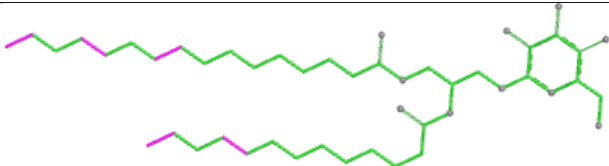
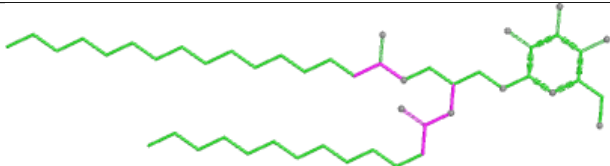
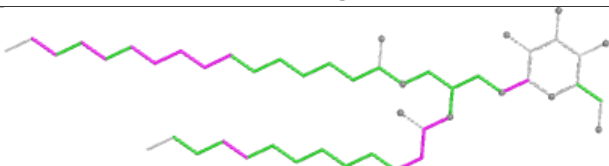
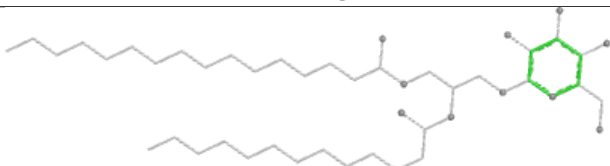


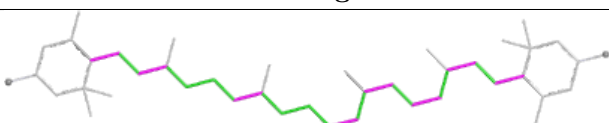
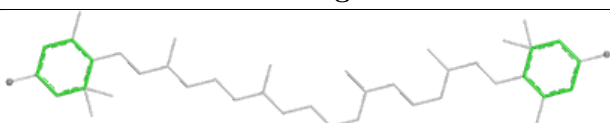


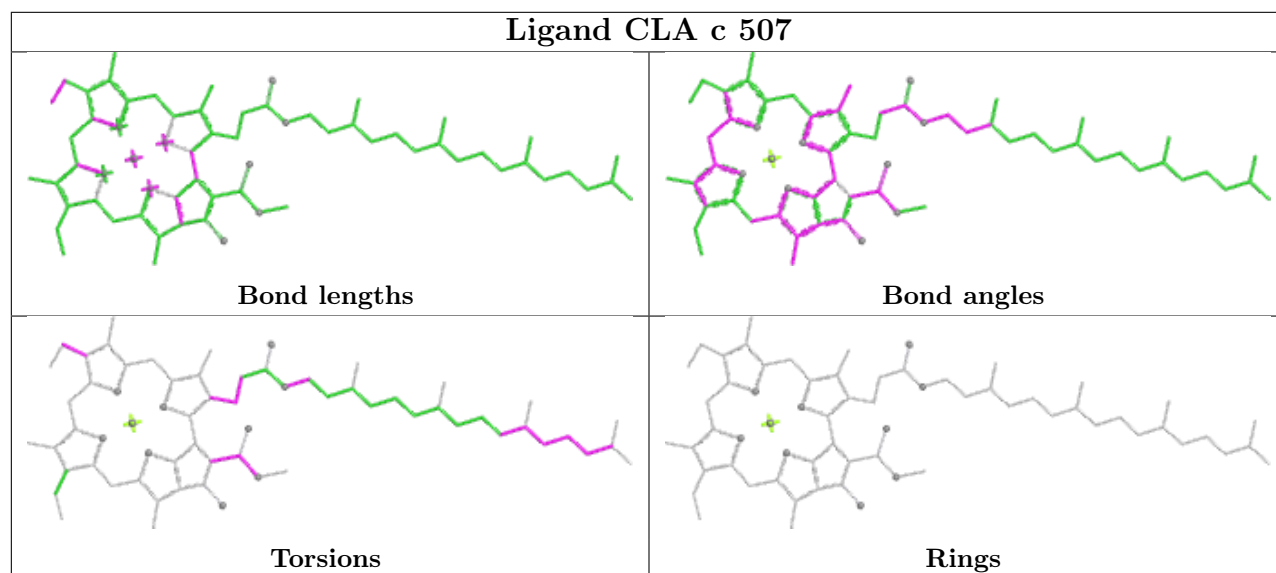
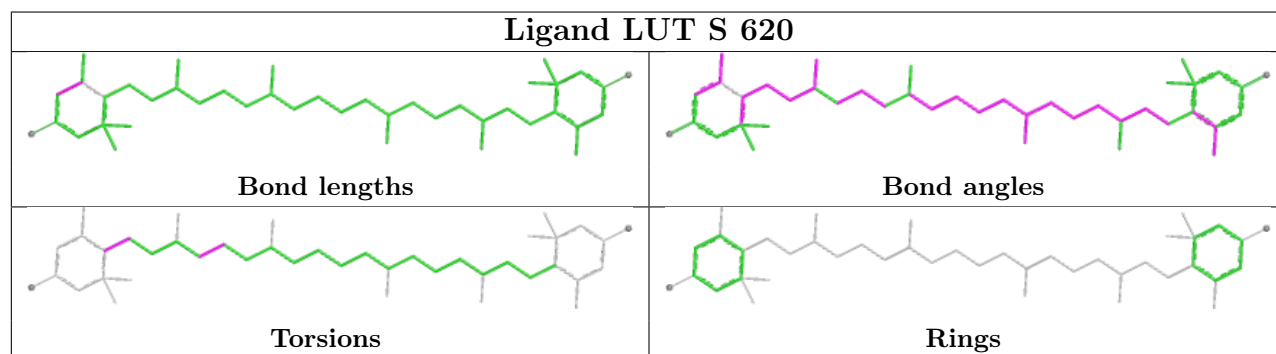
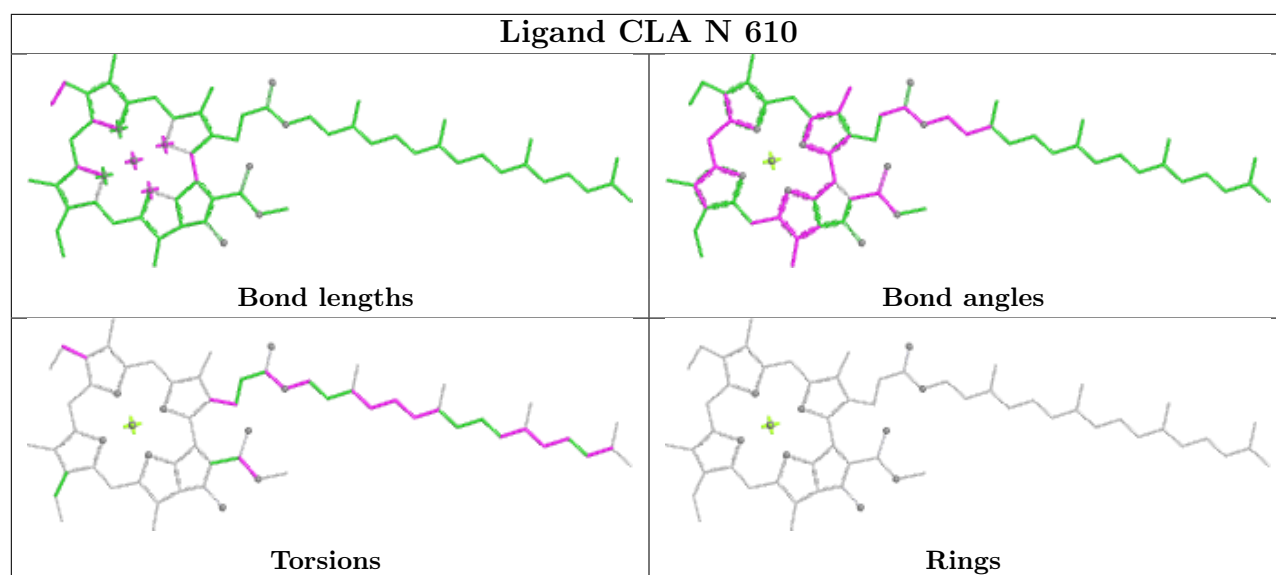


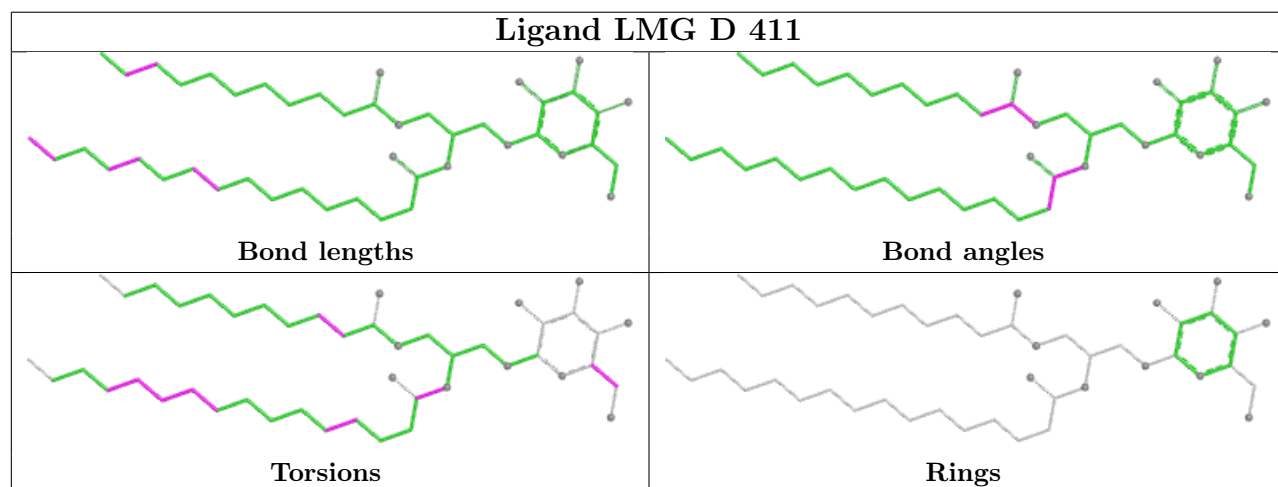
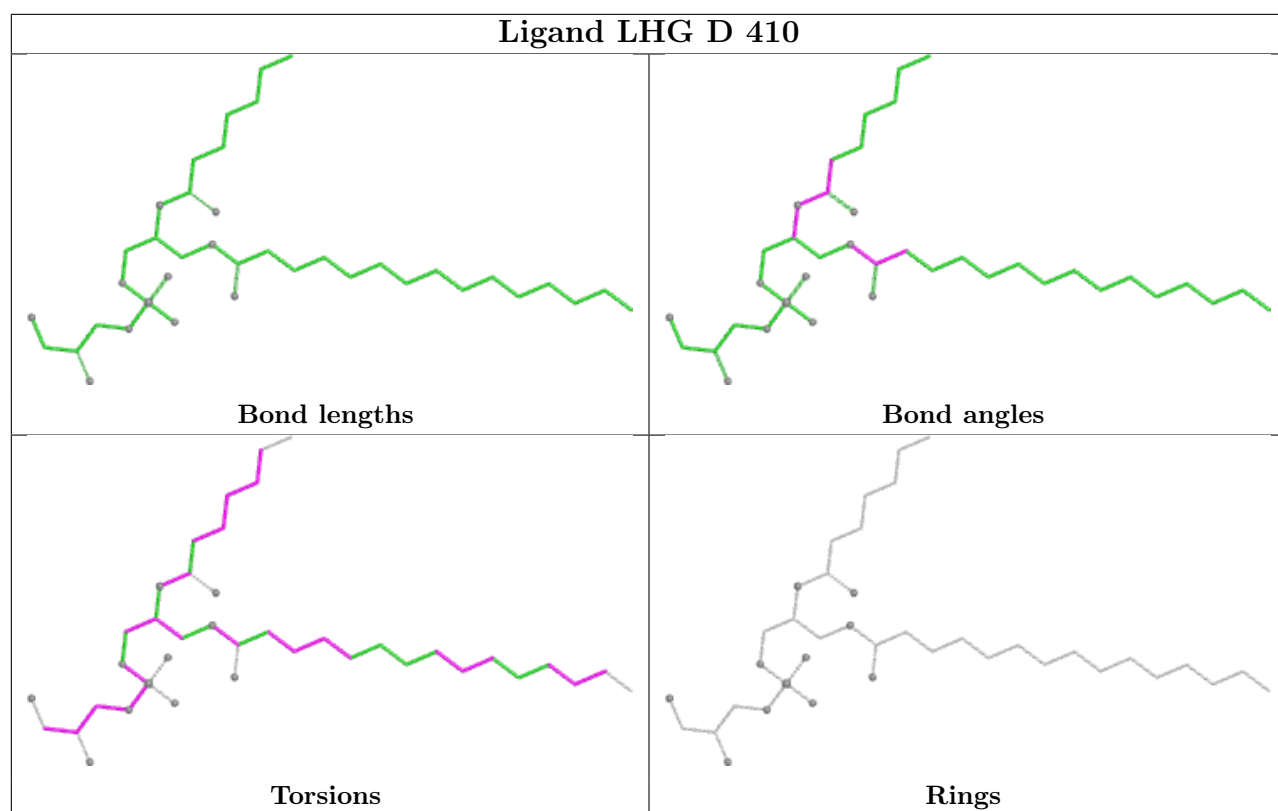


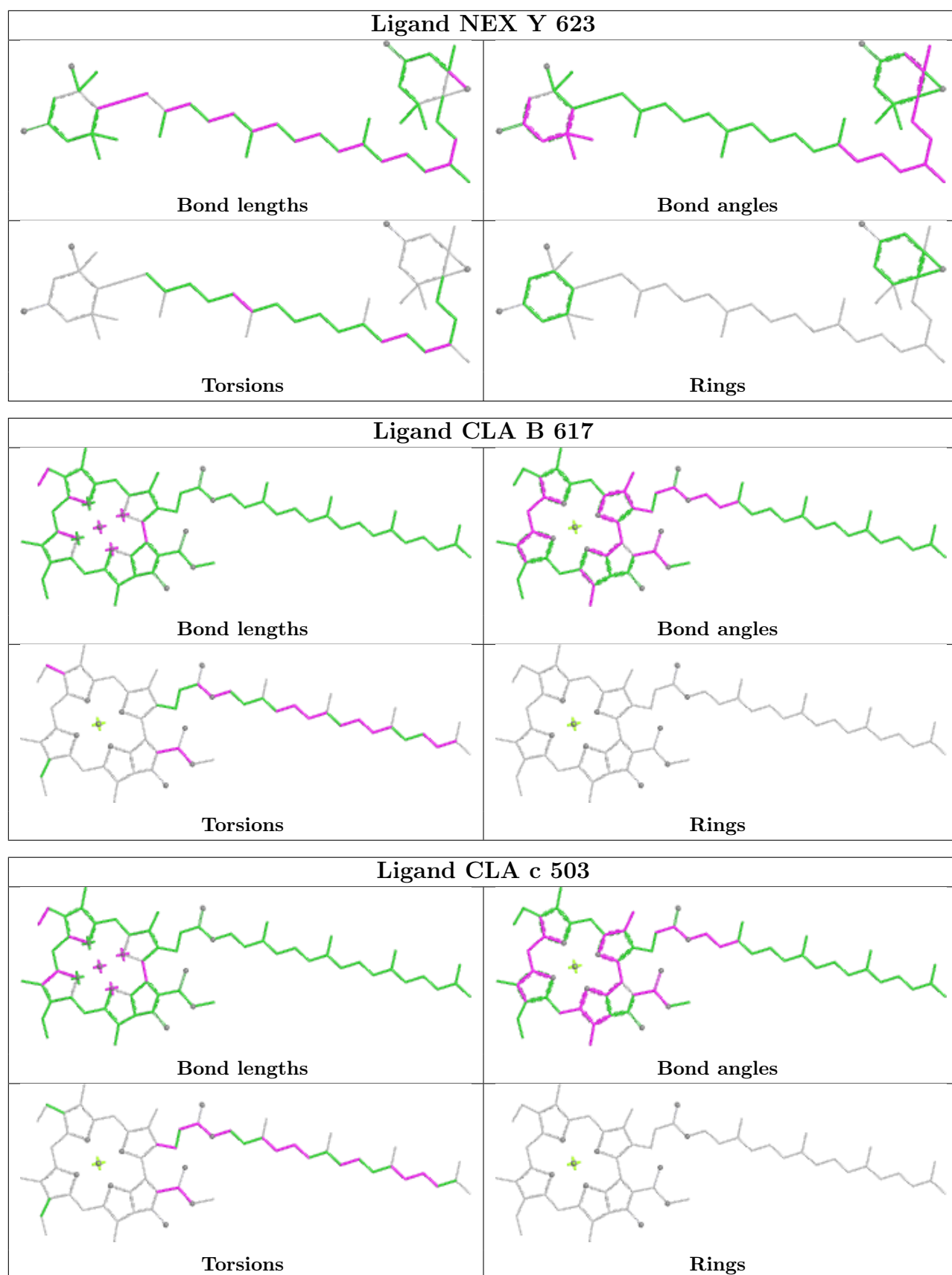
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

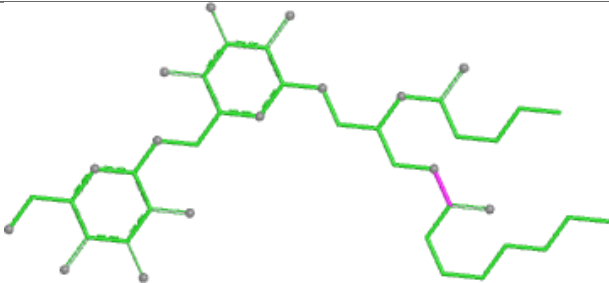
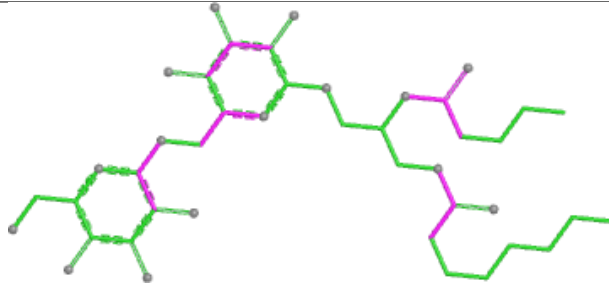
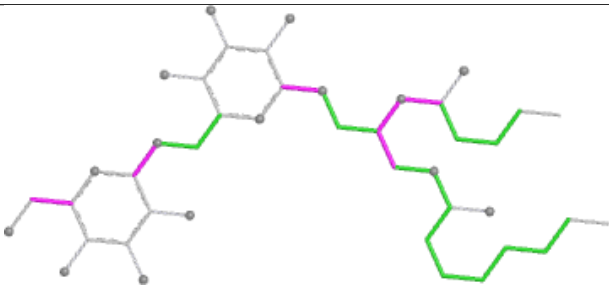
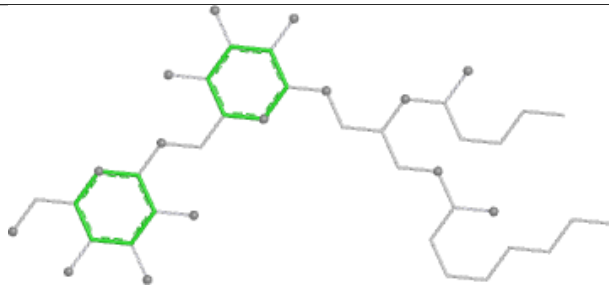
Ligand LMG A 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

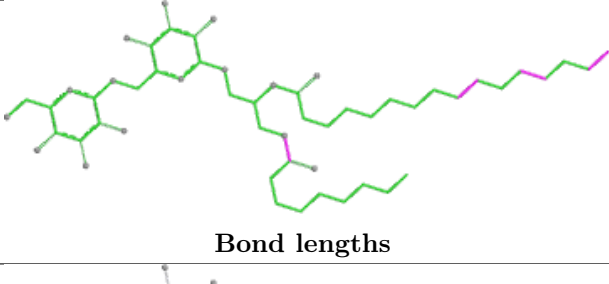
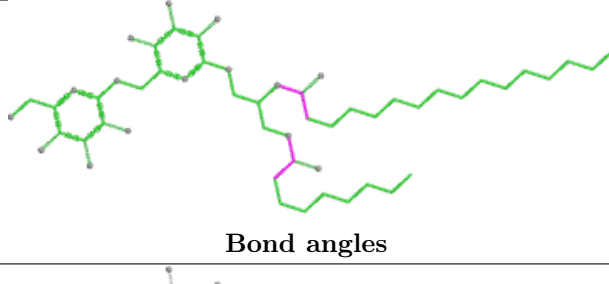
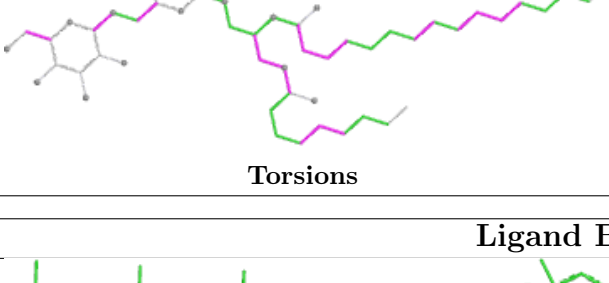
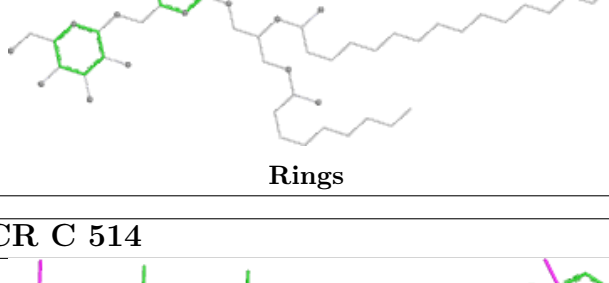
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Bond lengths	Bond angles
	
Torsions	Rings

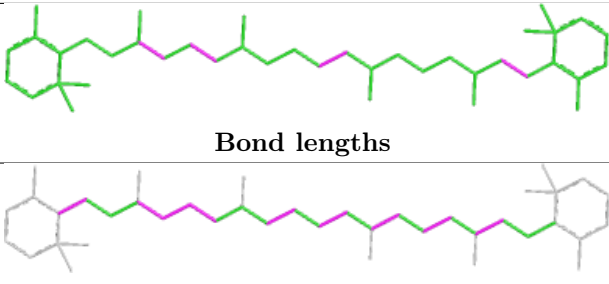
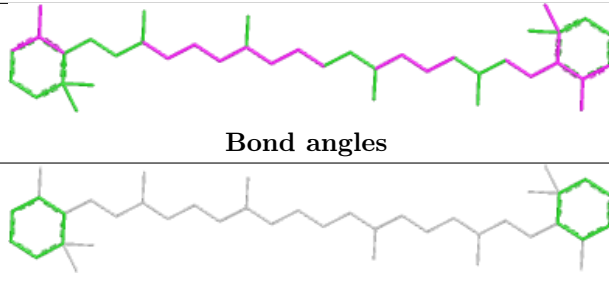


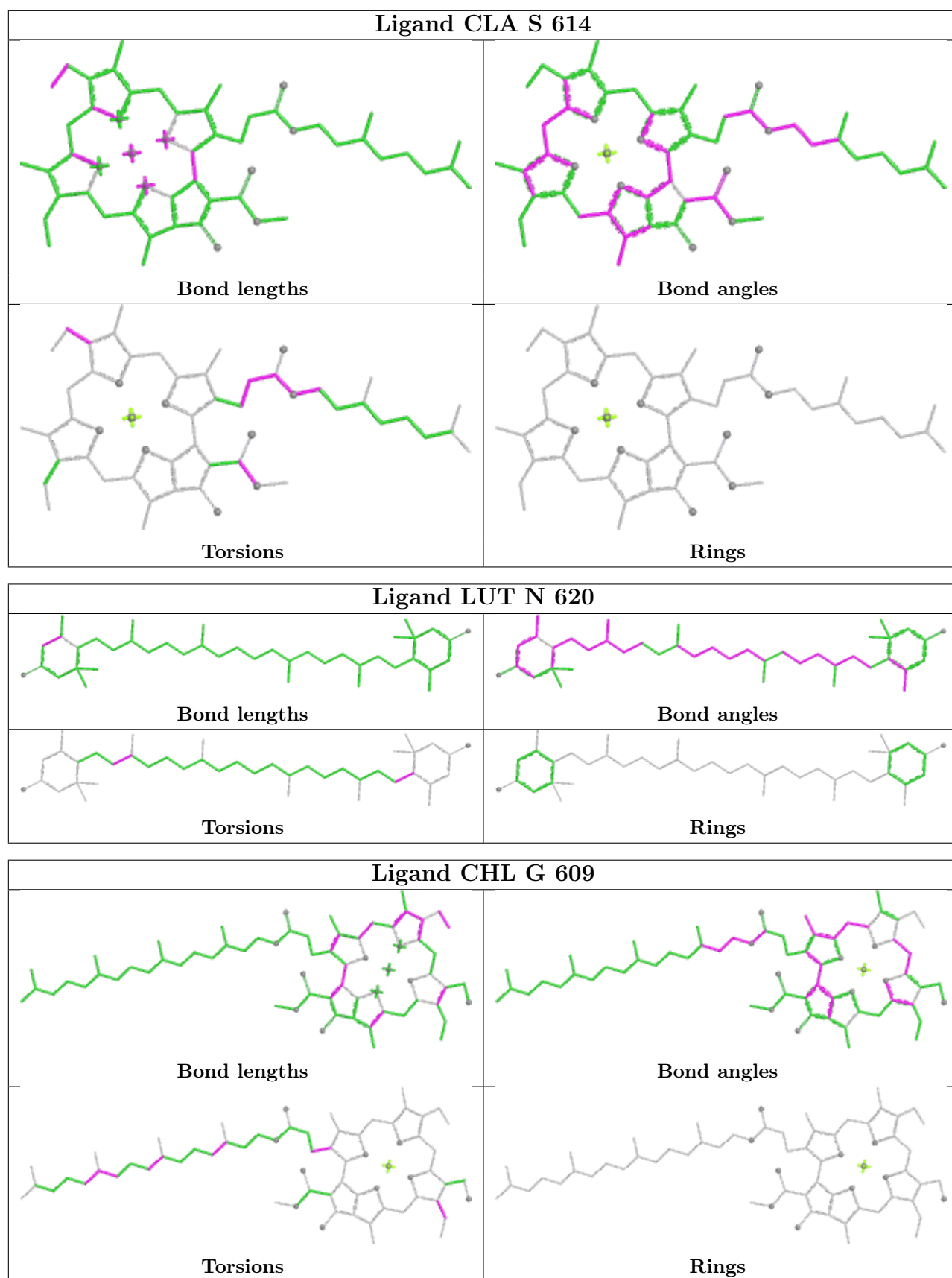




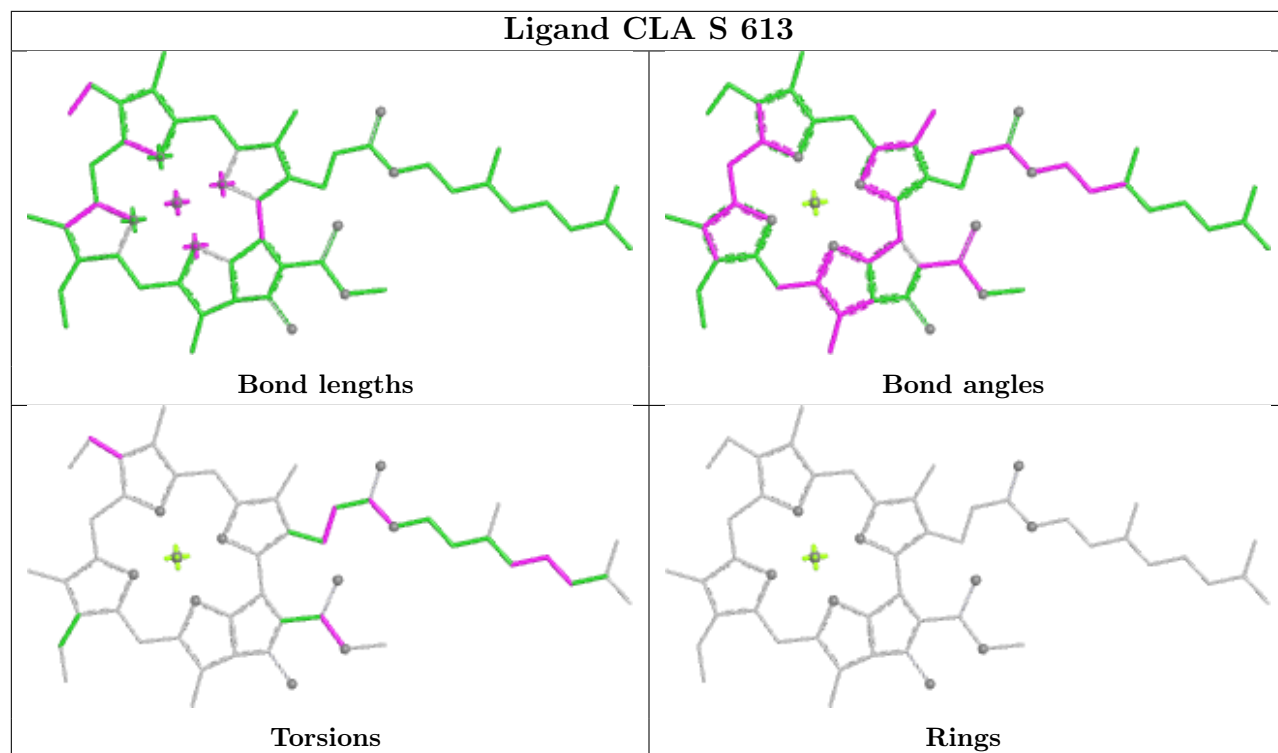
Ligand DGD b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

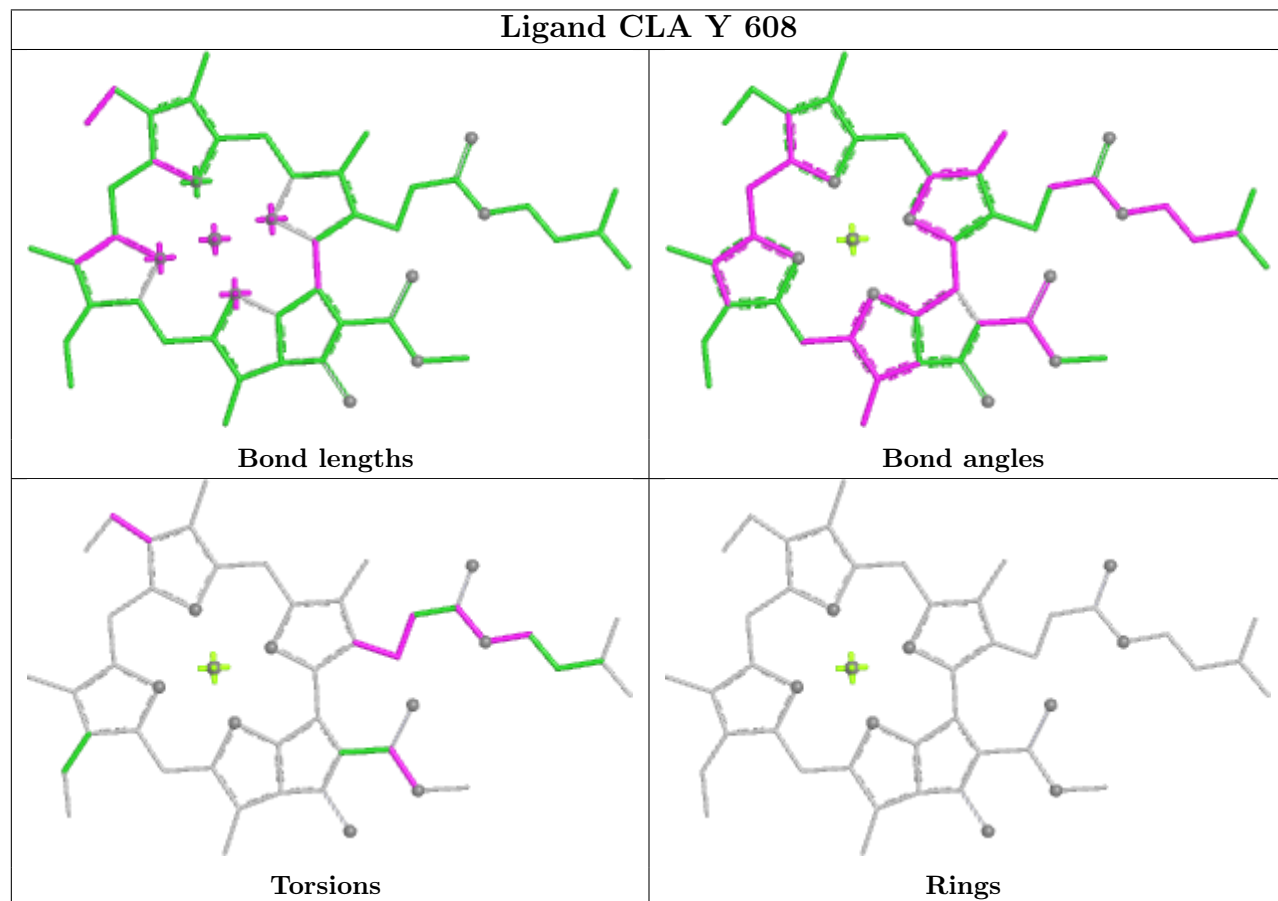
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Bond lengths	Bond angles
Torsions	Rings

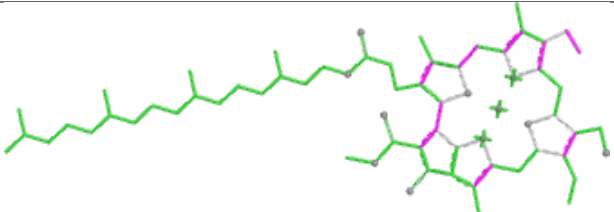
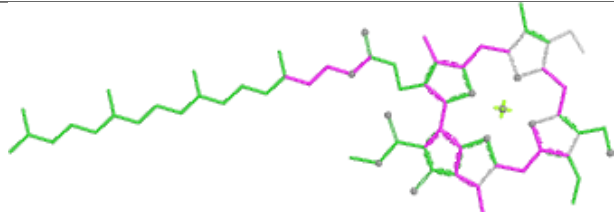
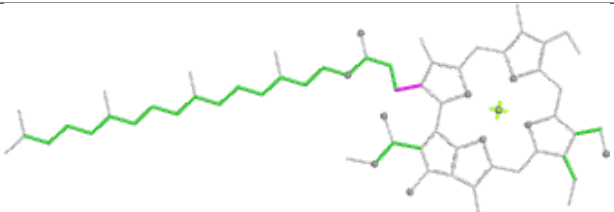
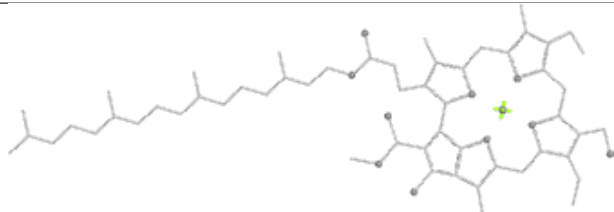


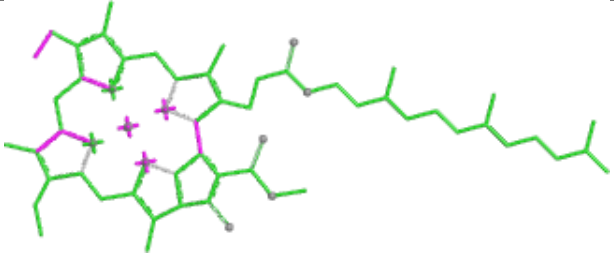
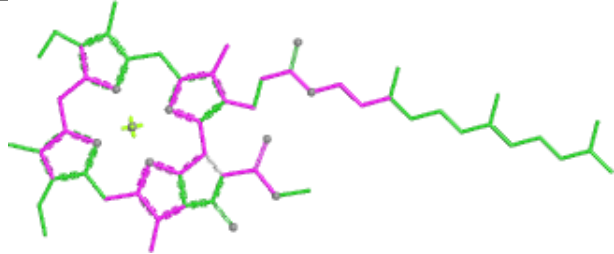
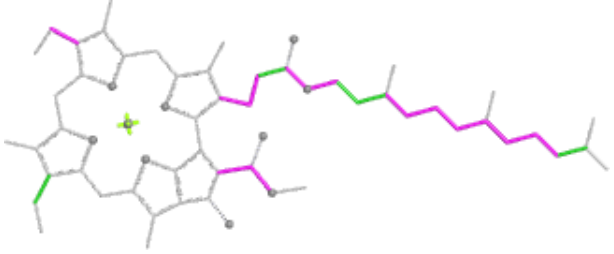
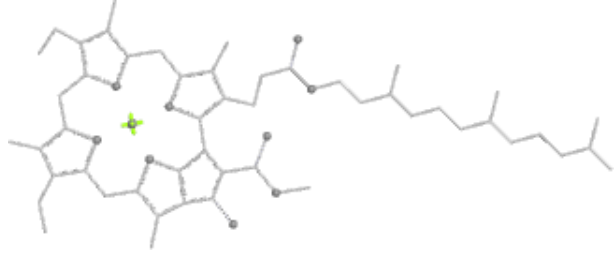
Ligand CLA S 613

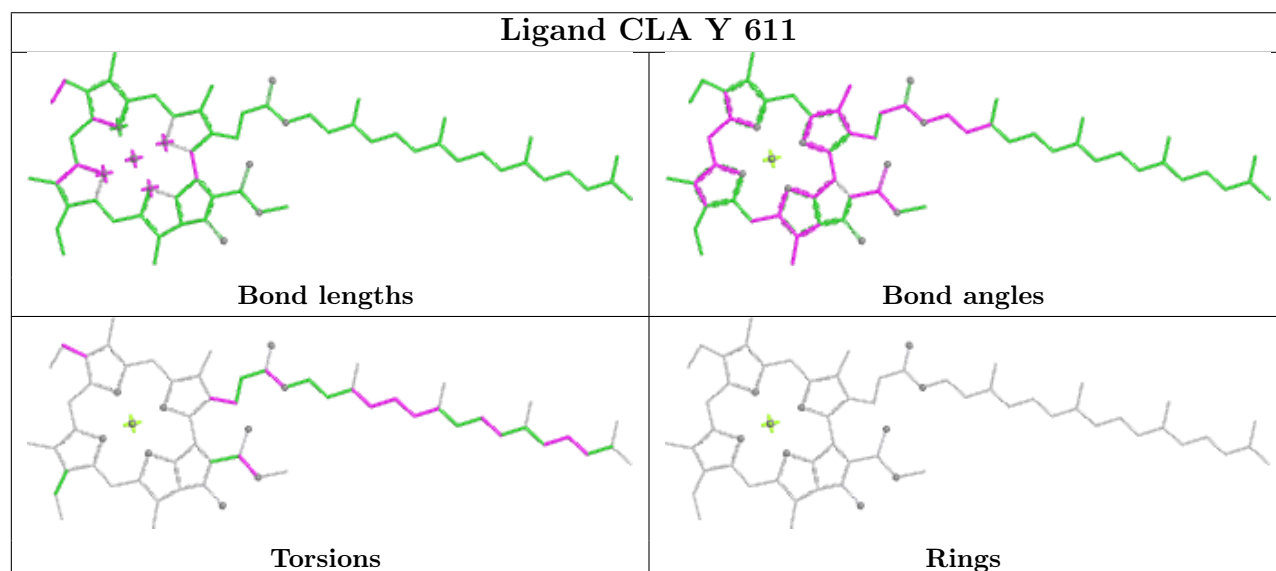
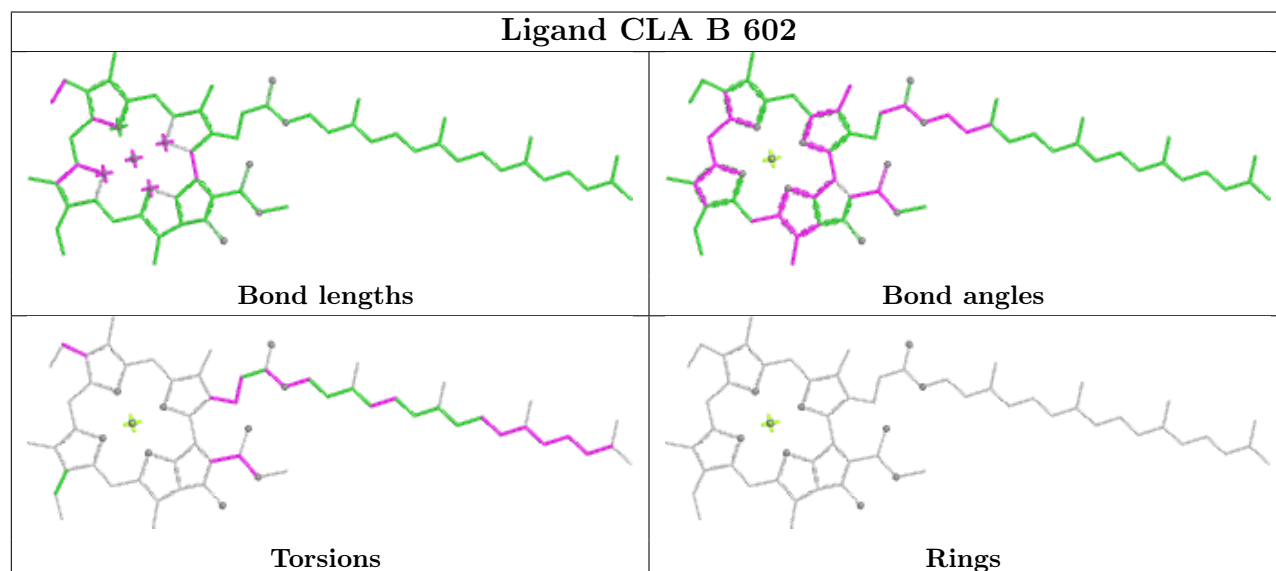
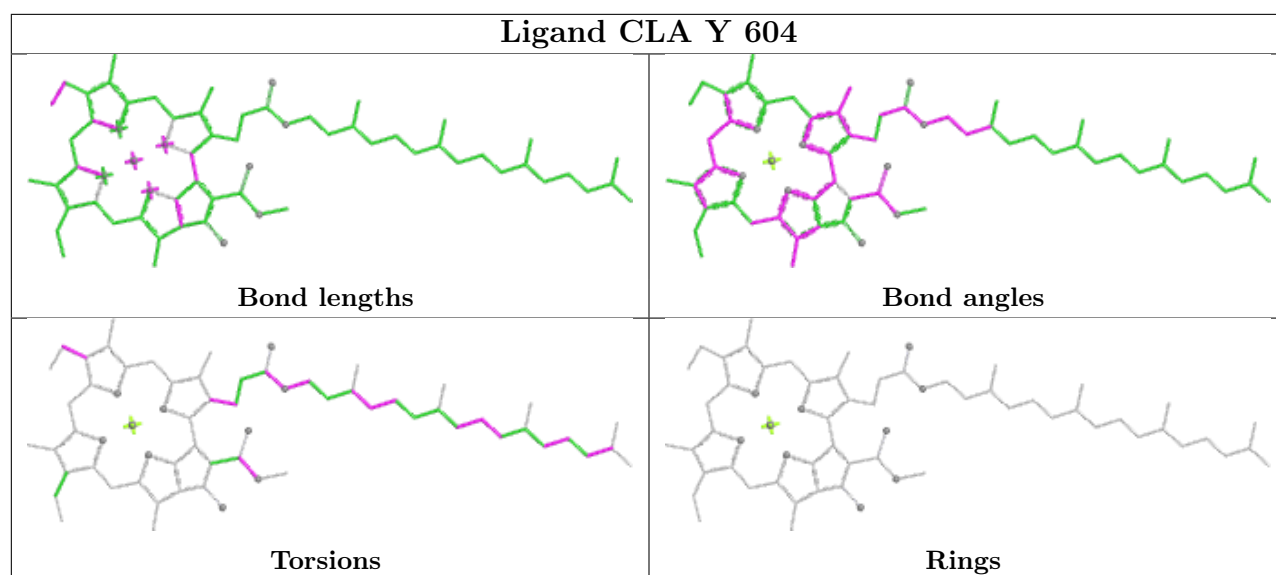


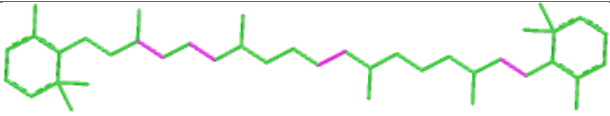
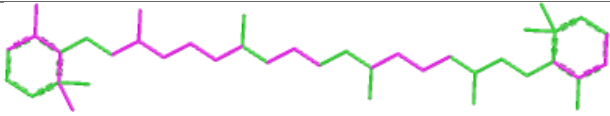
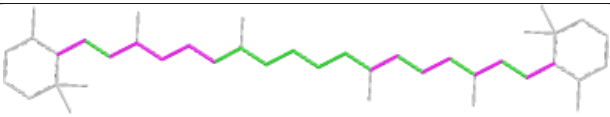
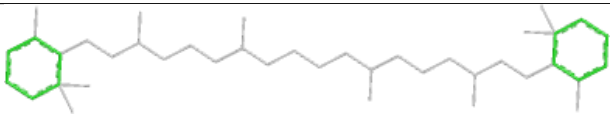
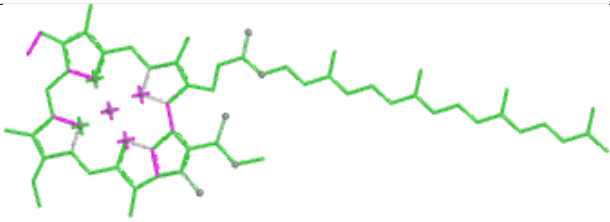
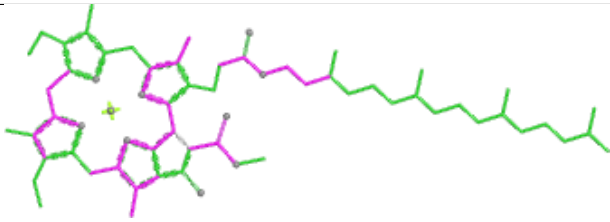
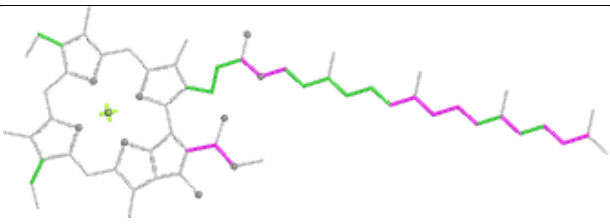
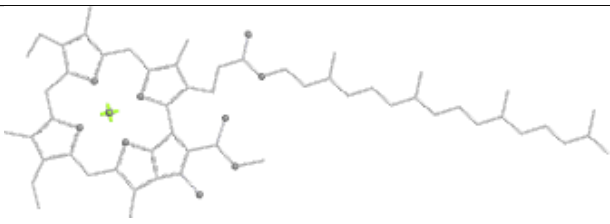
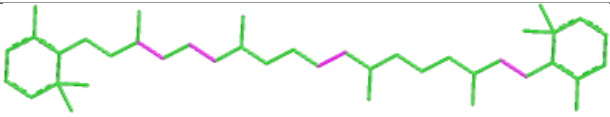
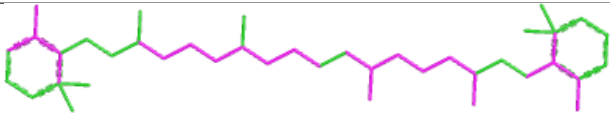
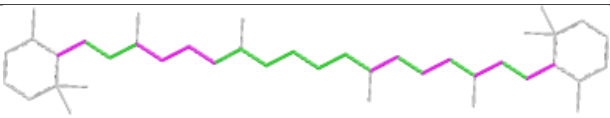
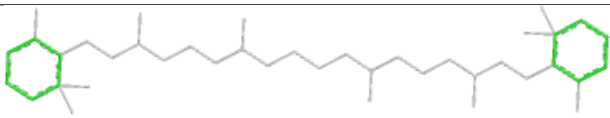
Ligand CLA Y 608

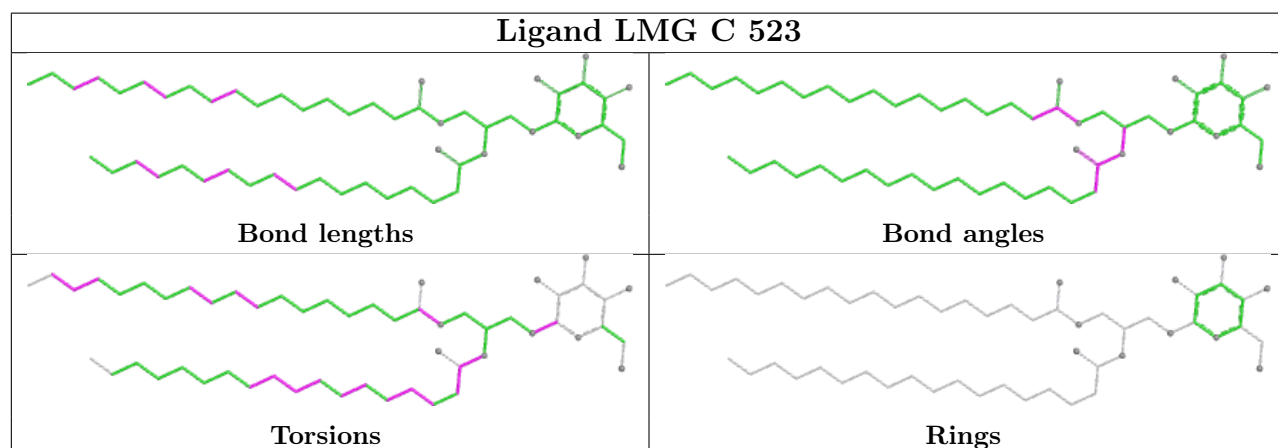
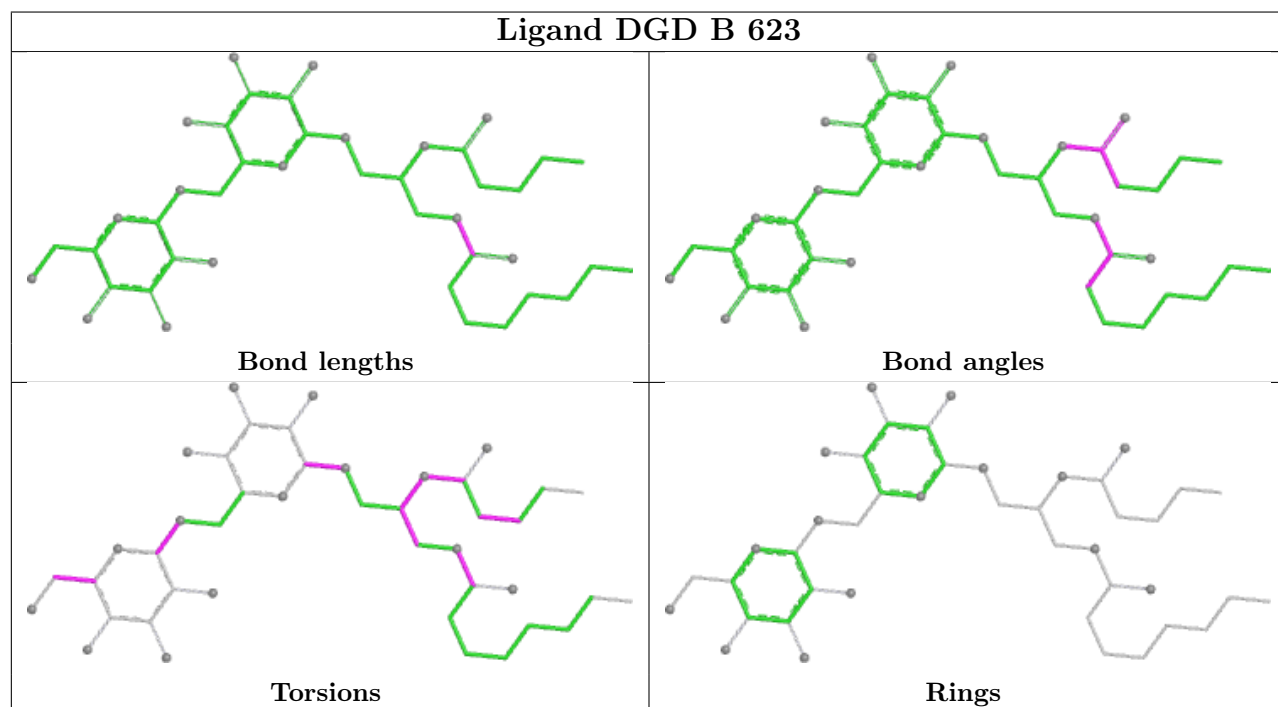
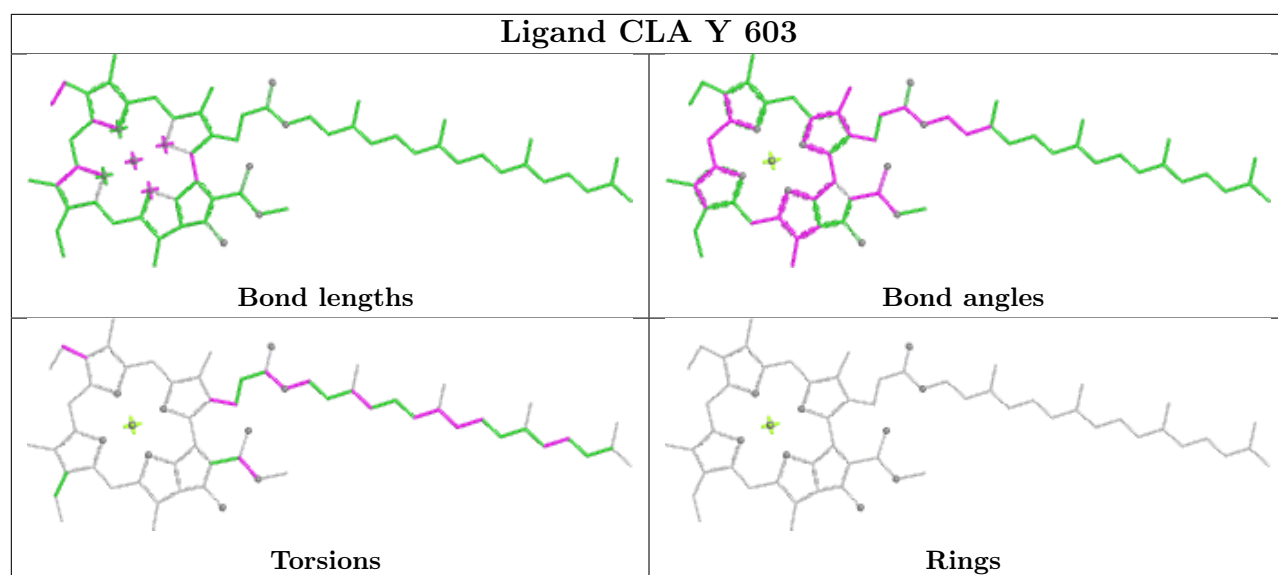


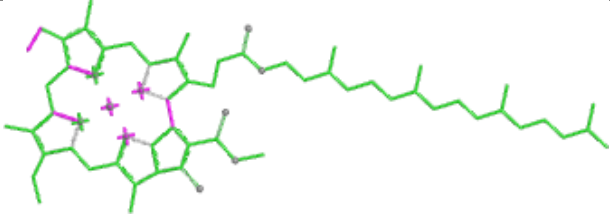
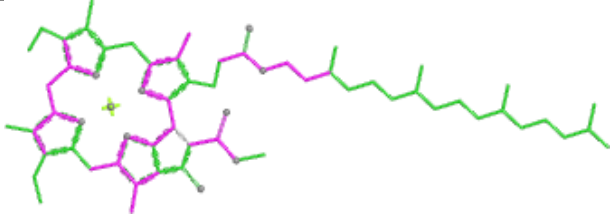
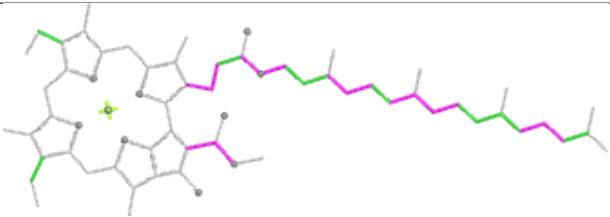
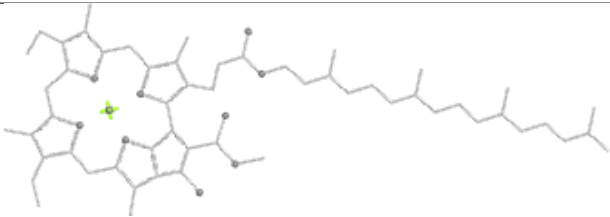
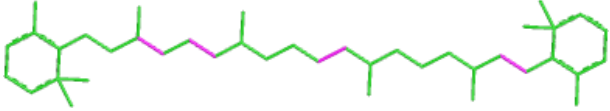
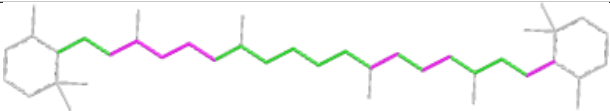
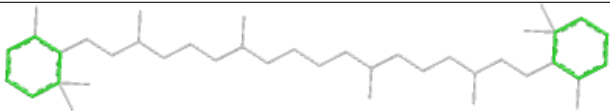
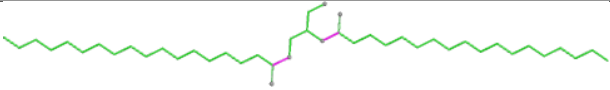
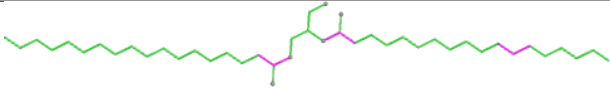
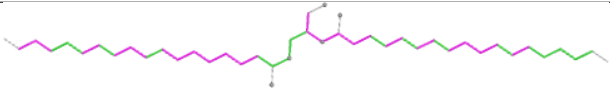
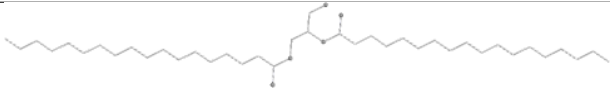
Ligand CHL Y 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

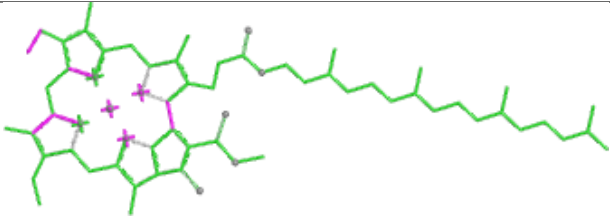
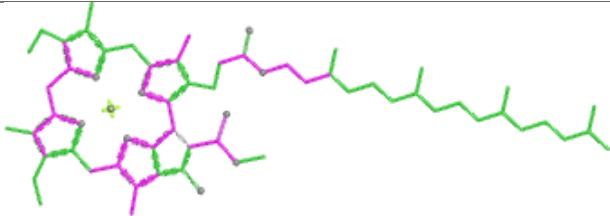
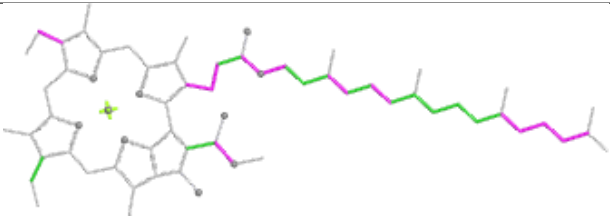
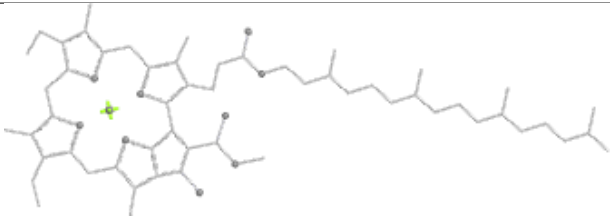
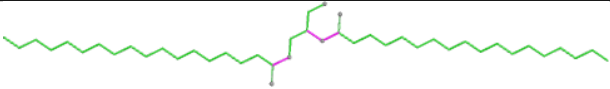
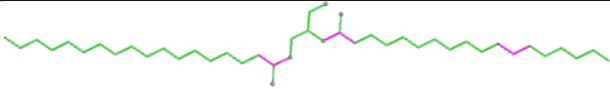
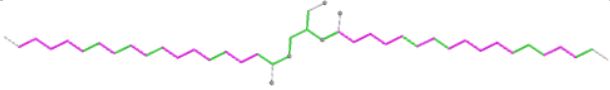
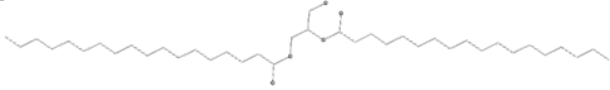
Ligand CLA S 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

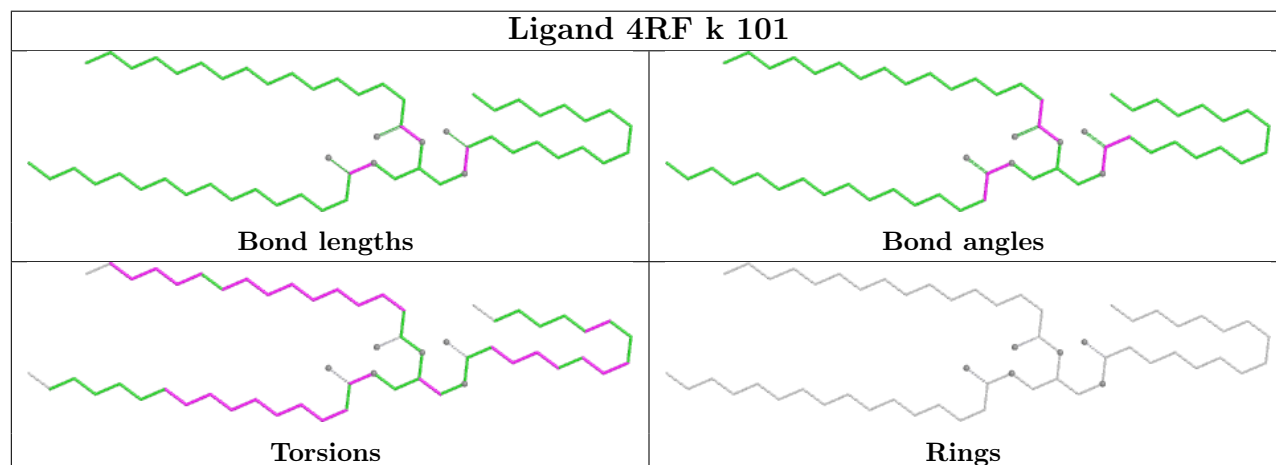
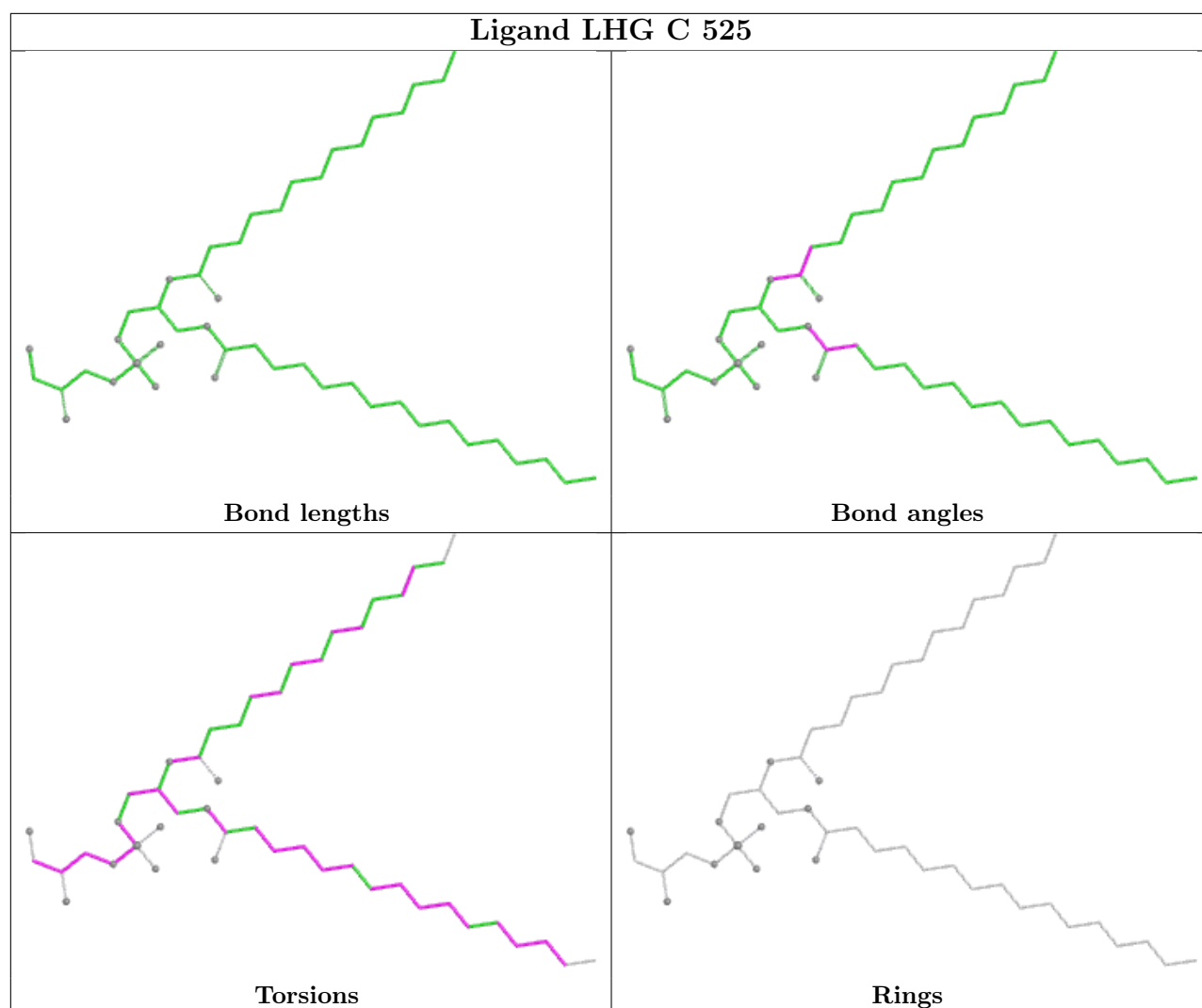


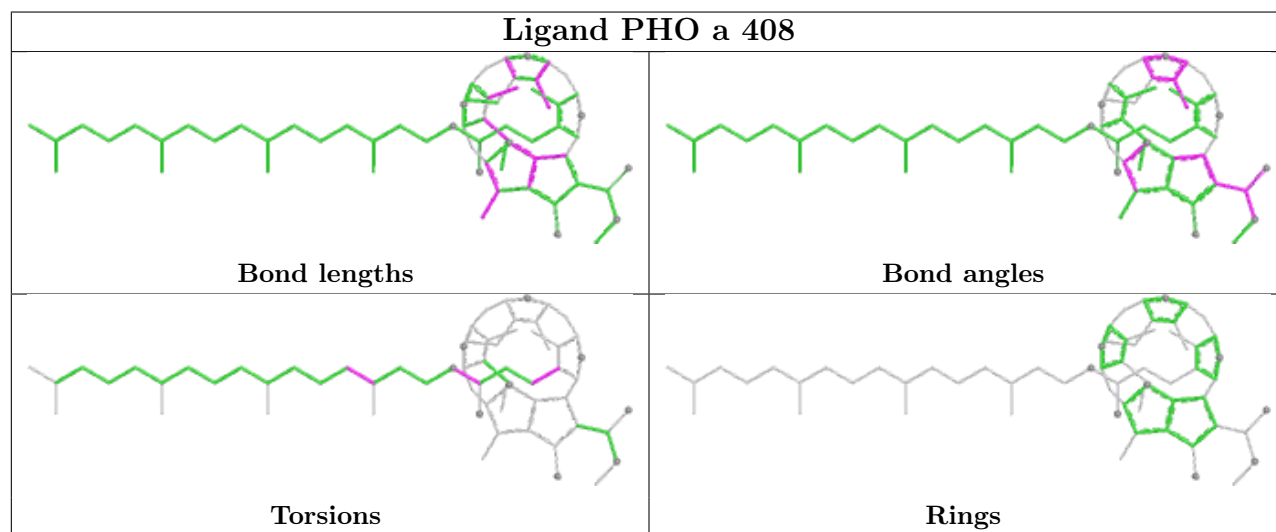
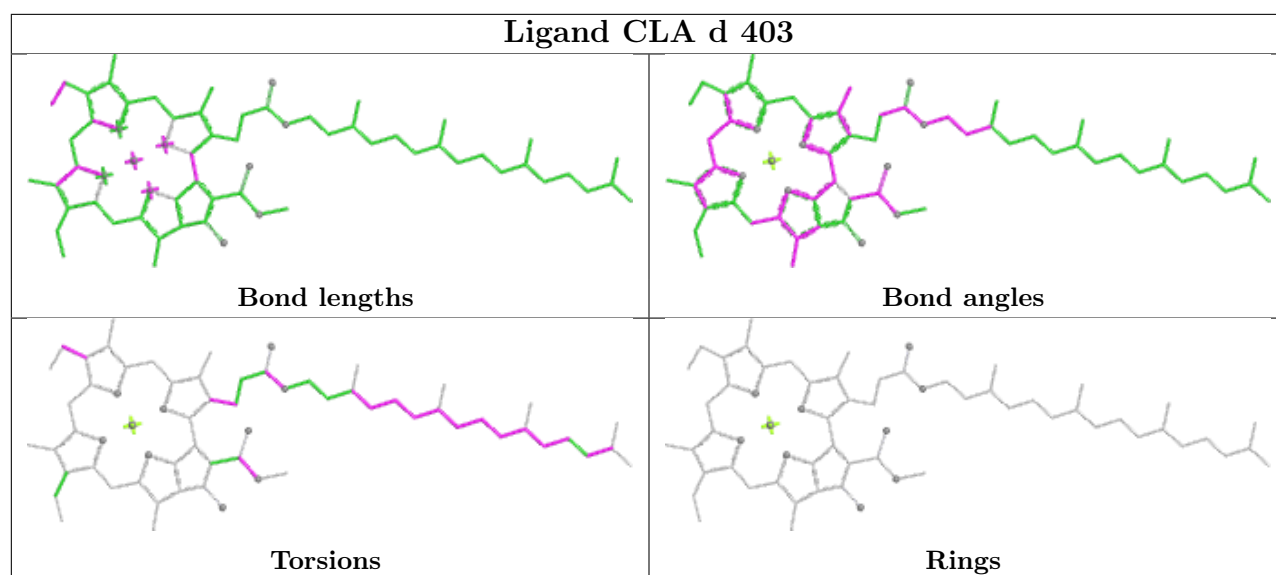
Ligand BCR C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings



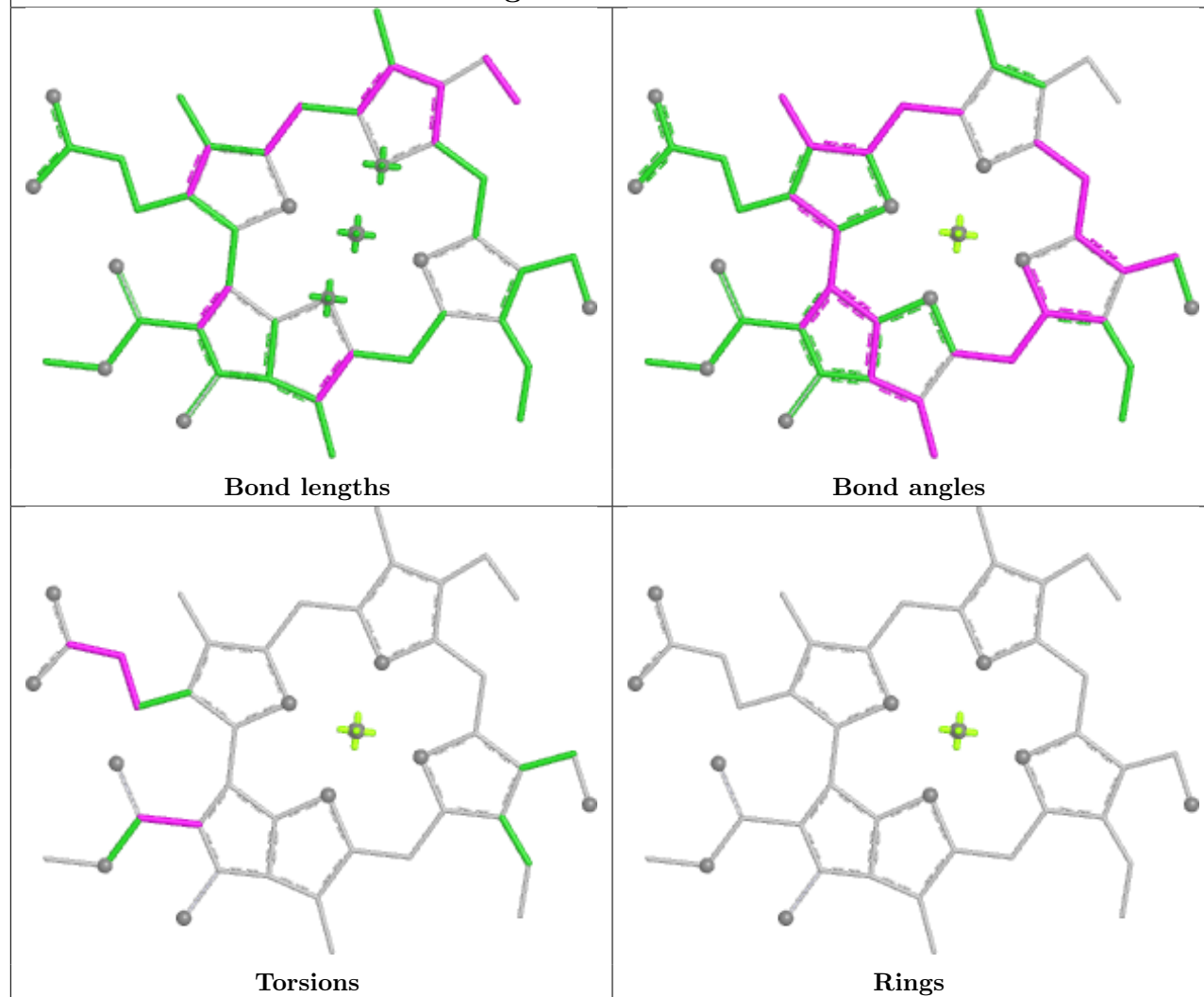
Ligand CLA c 504	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 411	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGA B 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGA c 524	
 Bond lengths	 Bond angles
 Torsions	 Rings

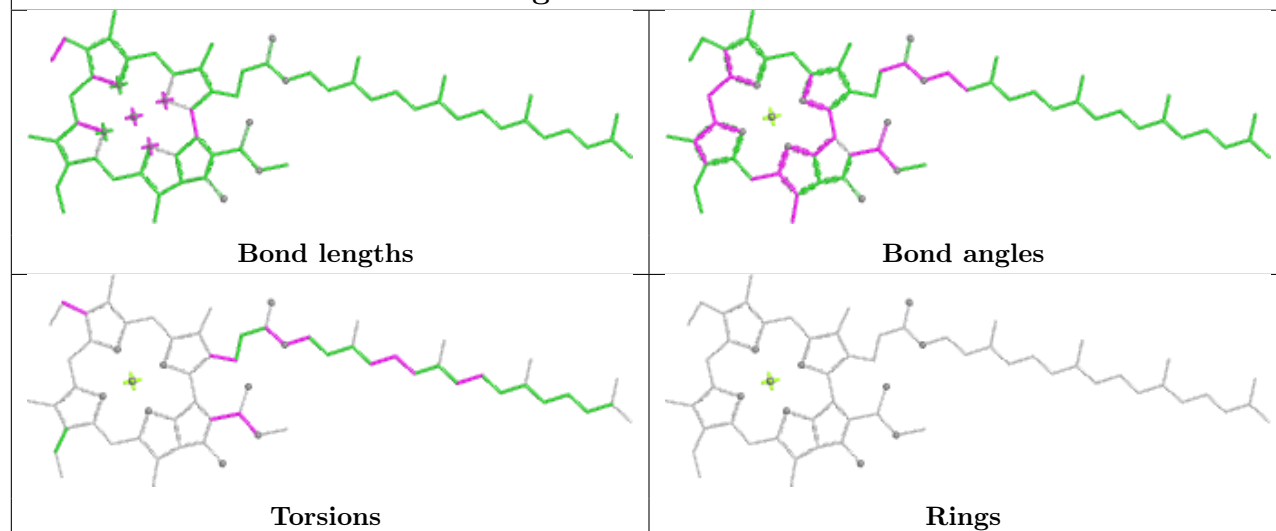


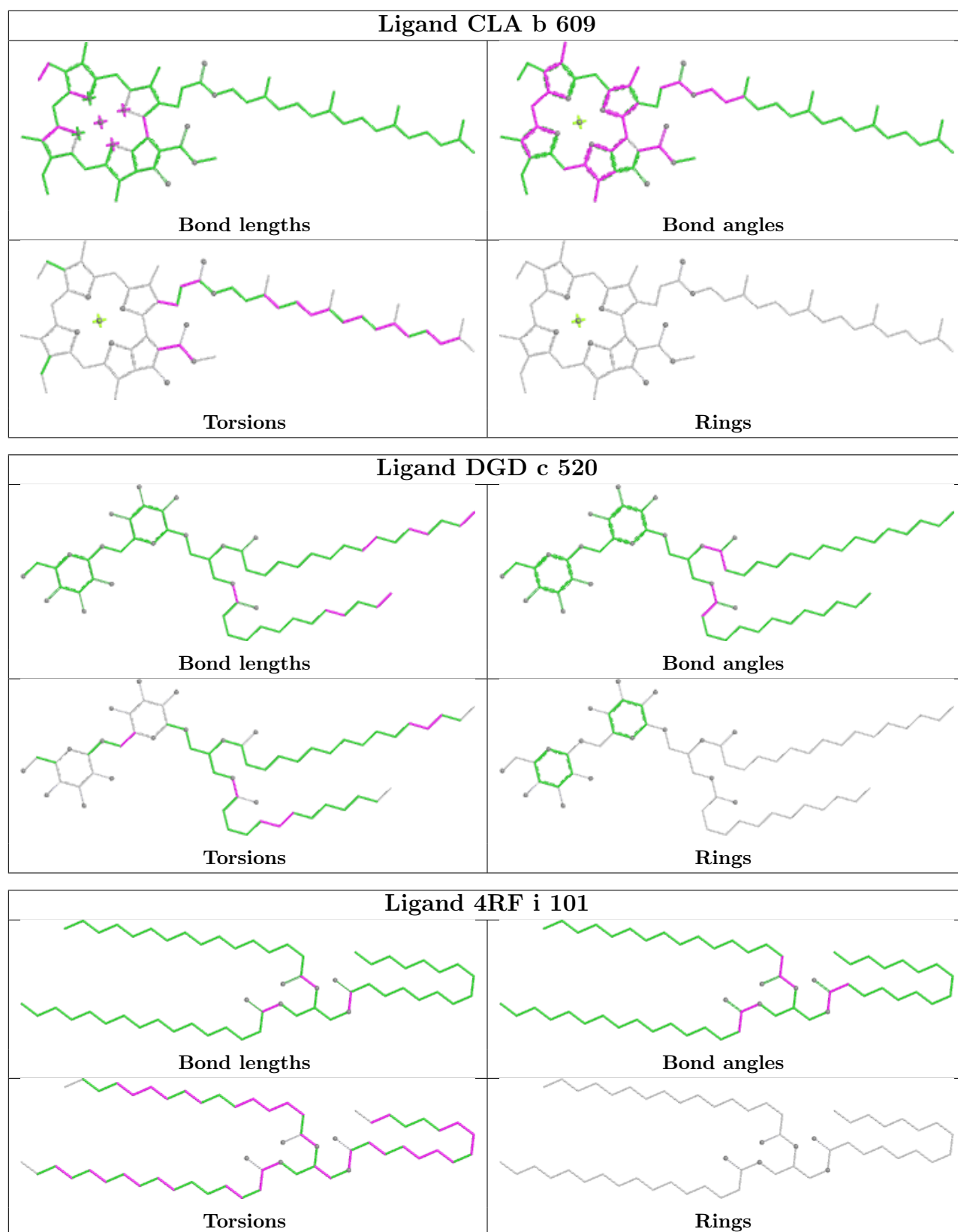


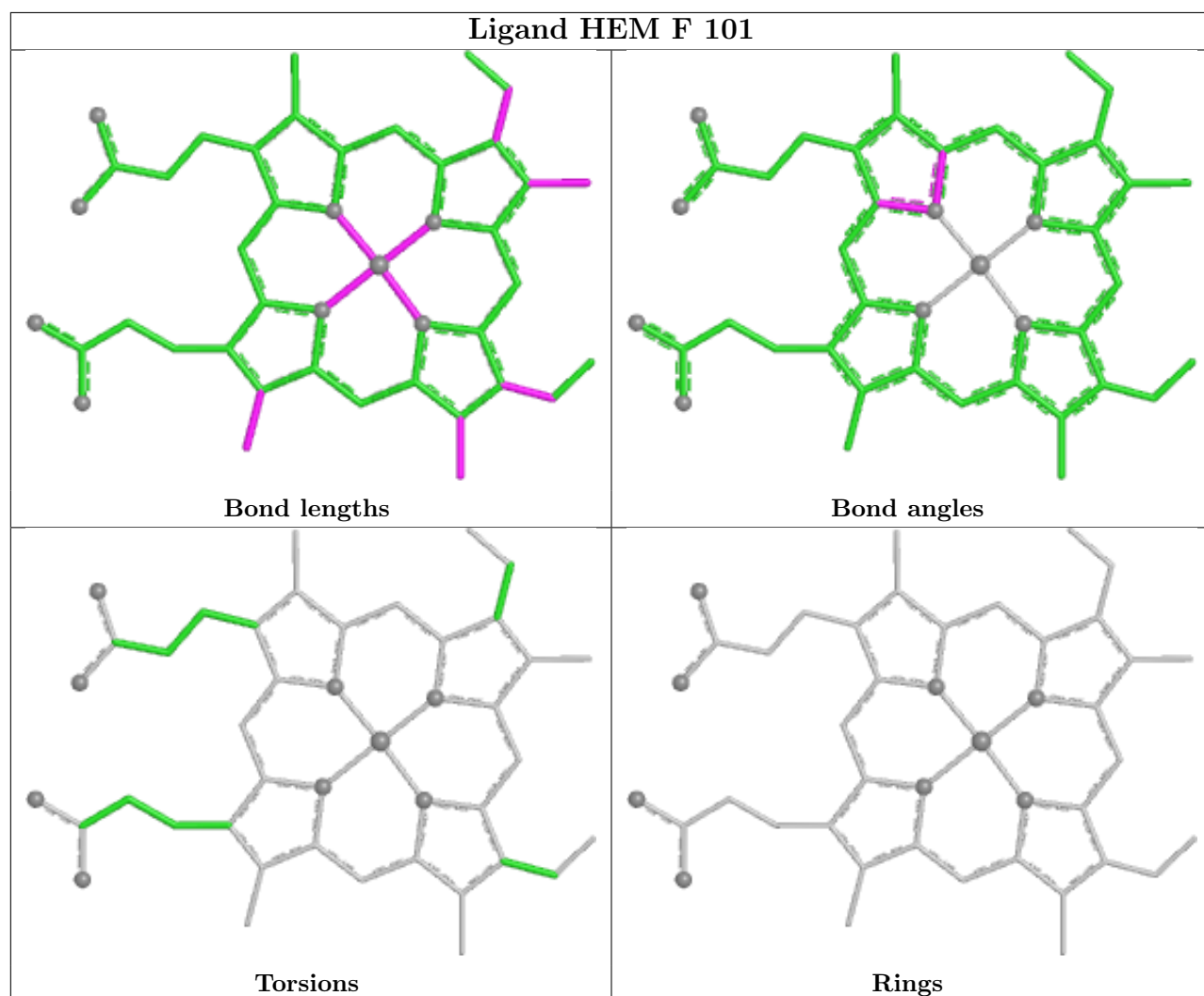
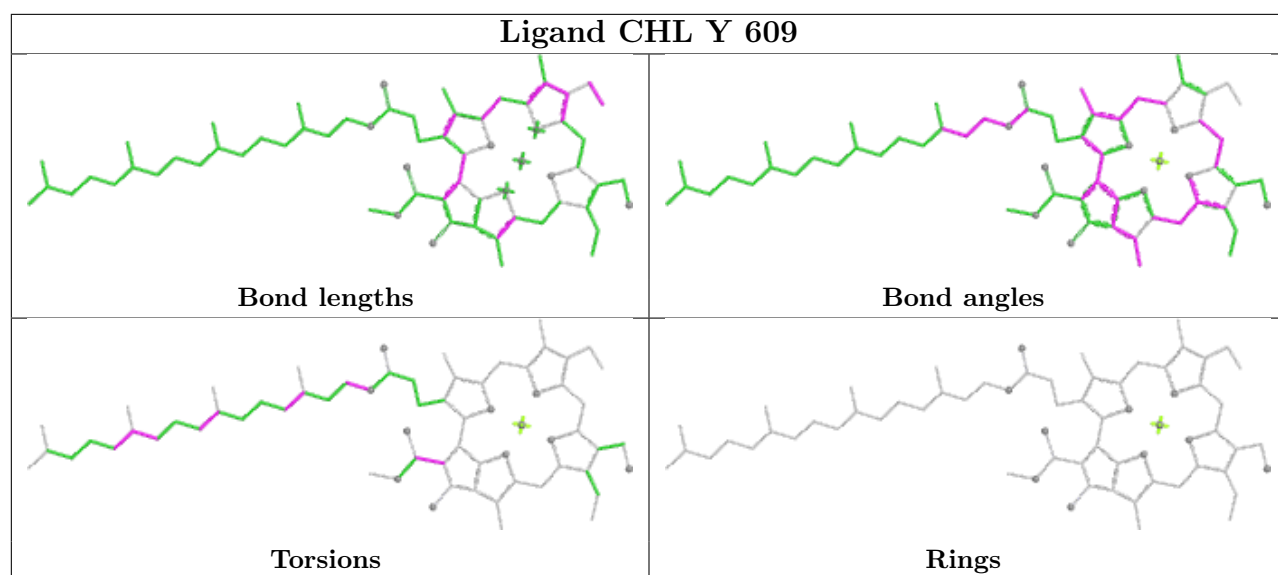
Ligand CHL S 601

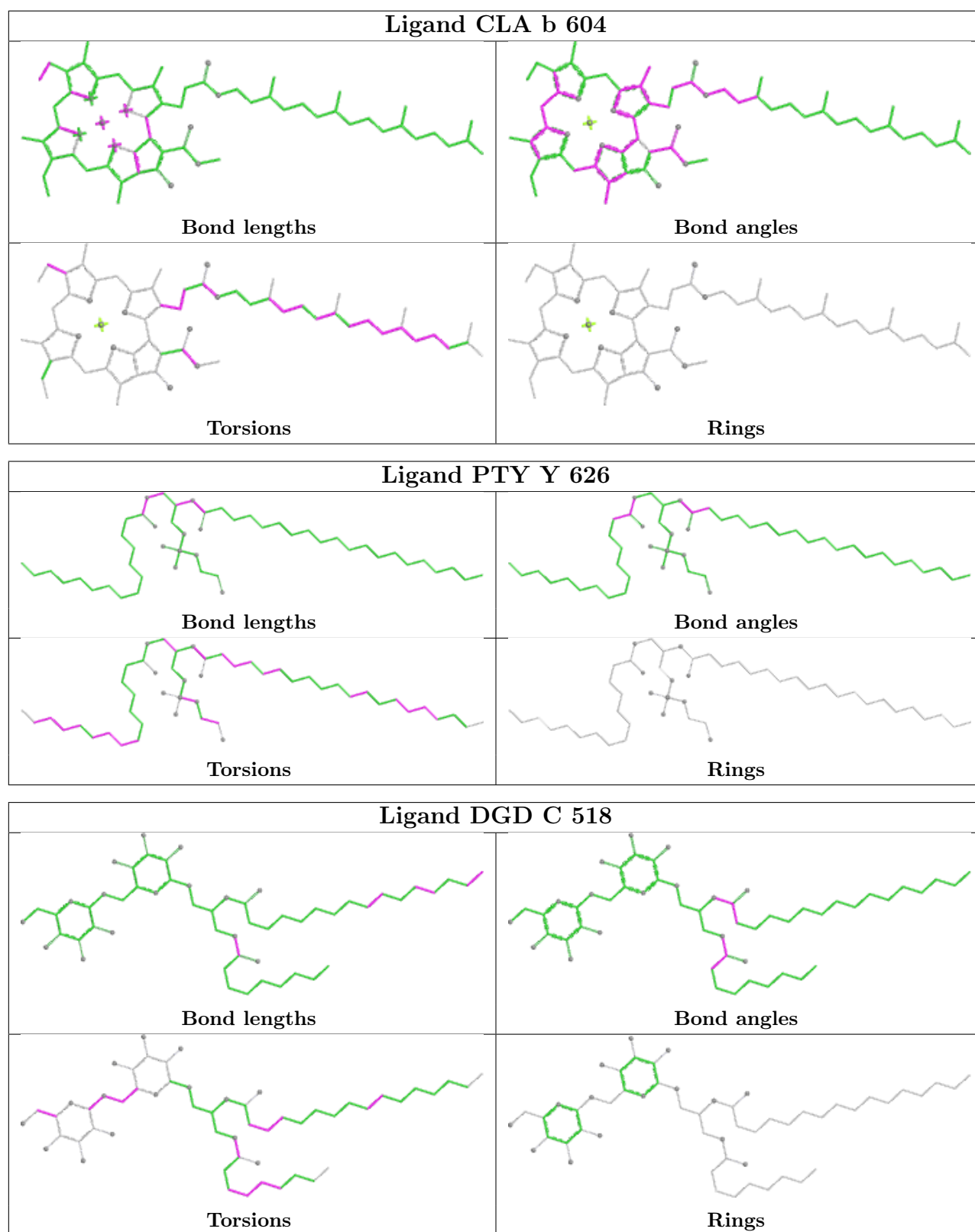


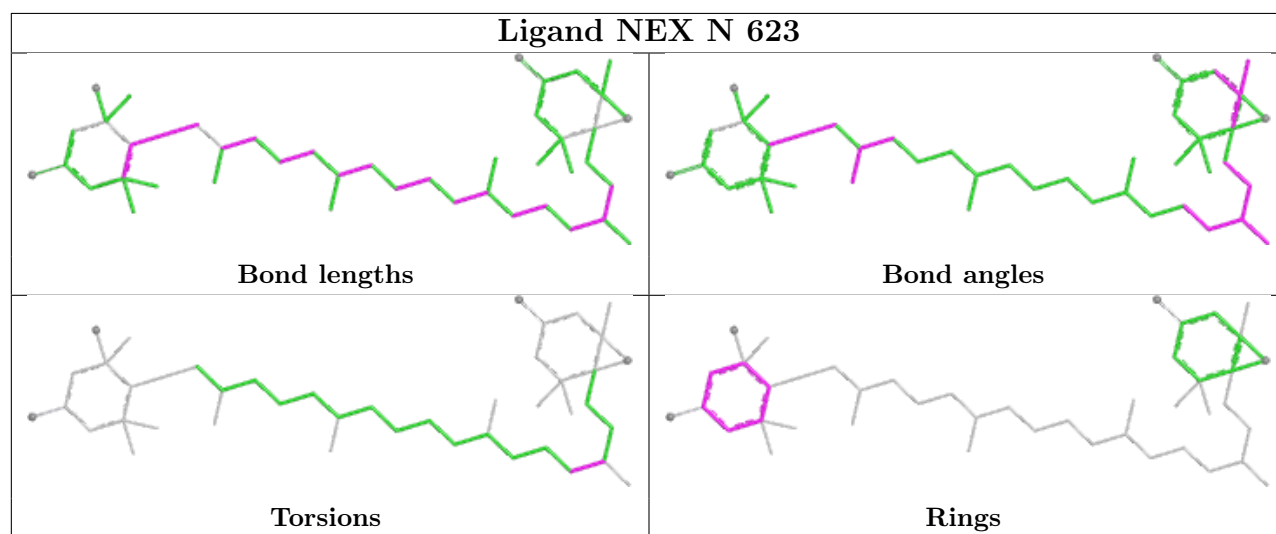
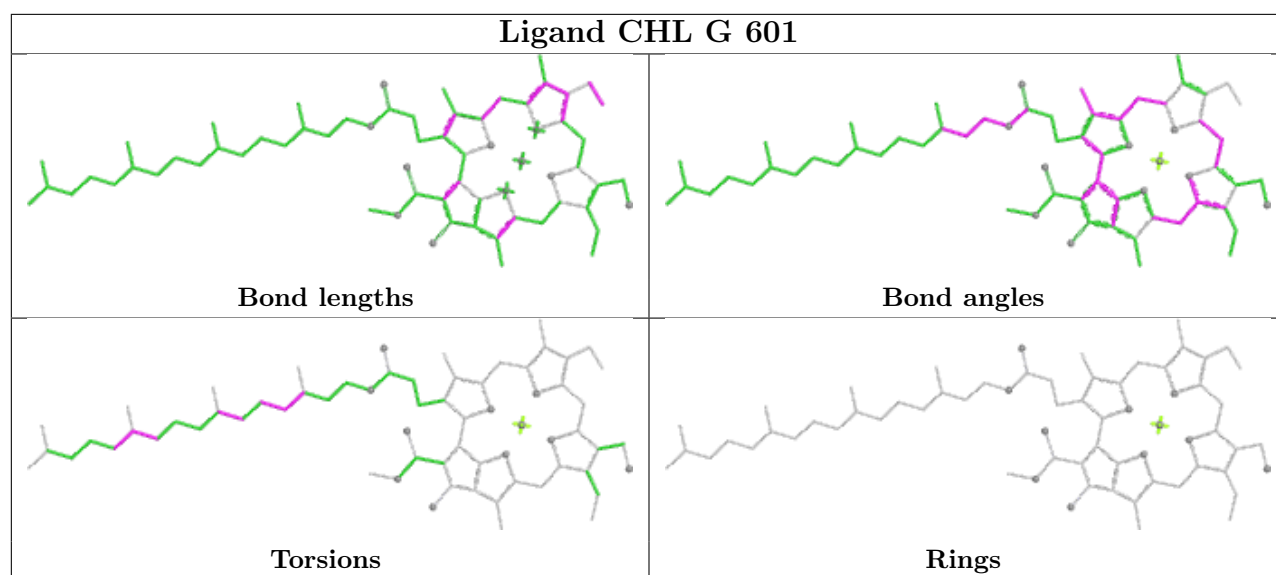
Ligand CLA B 610



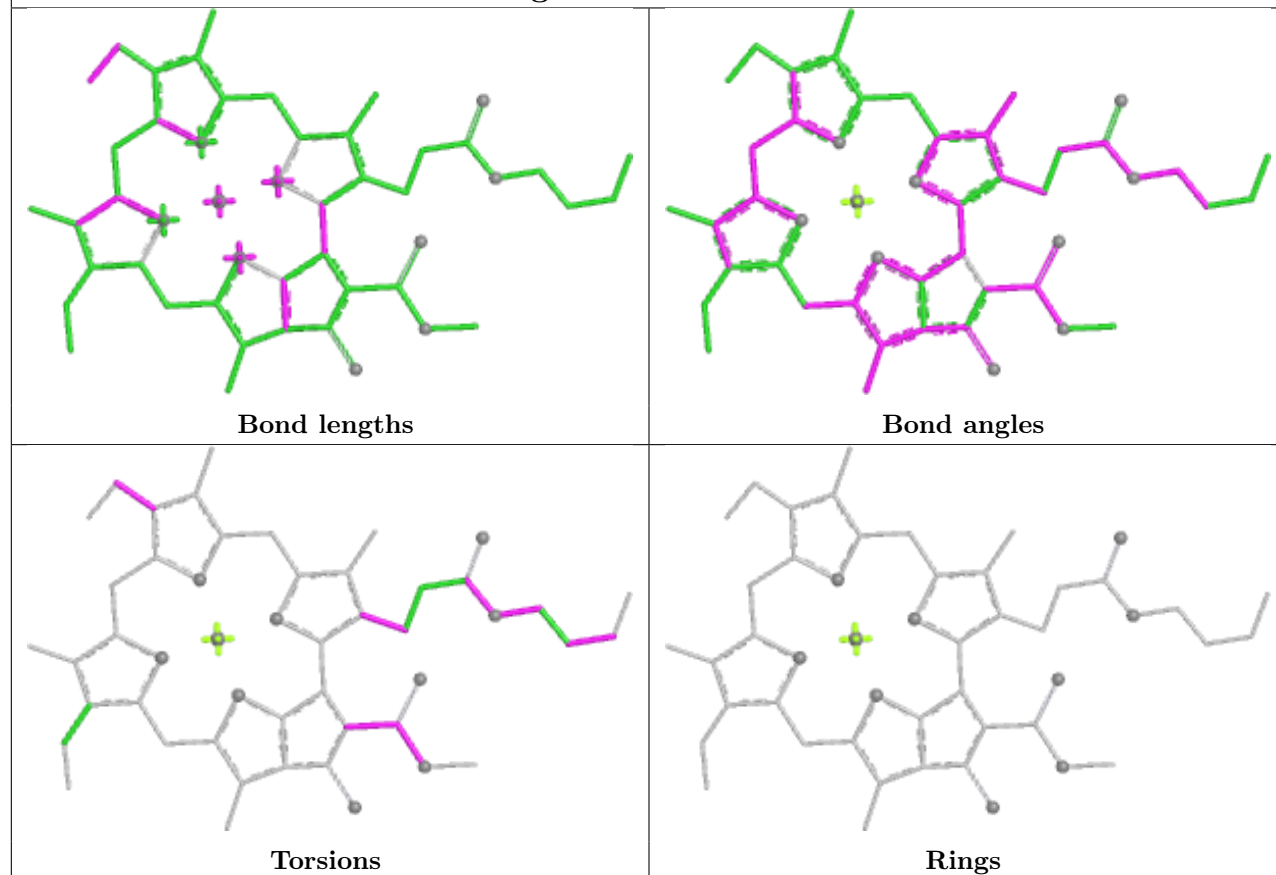




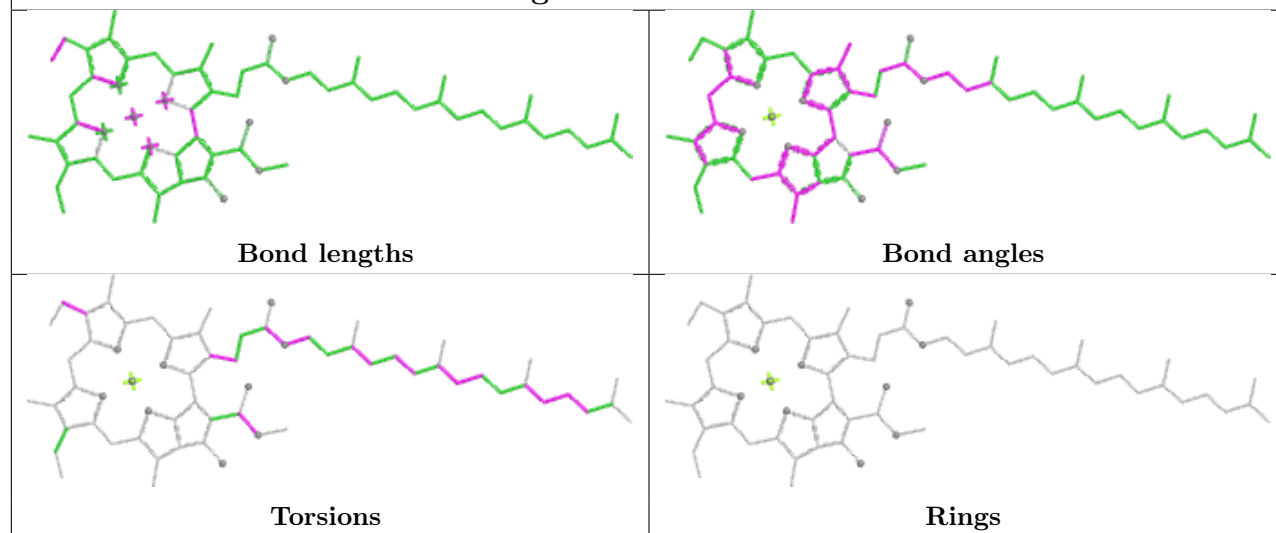


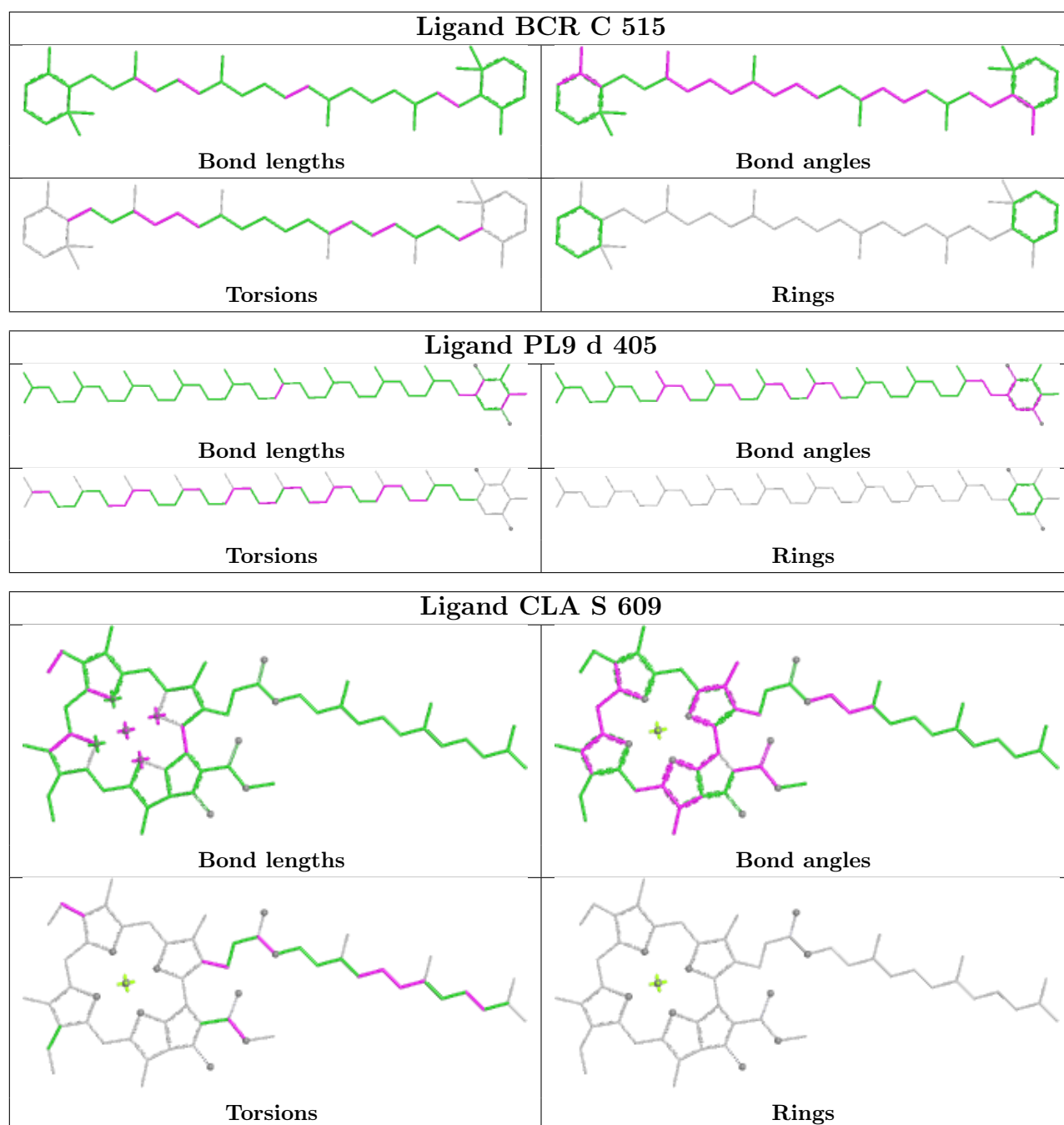


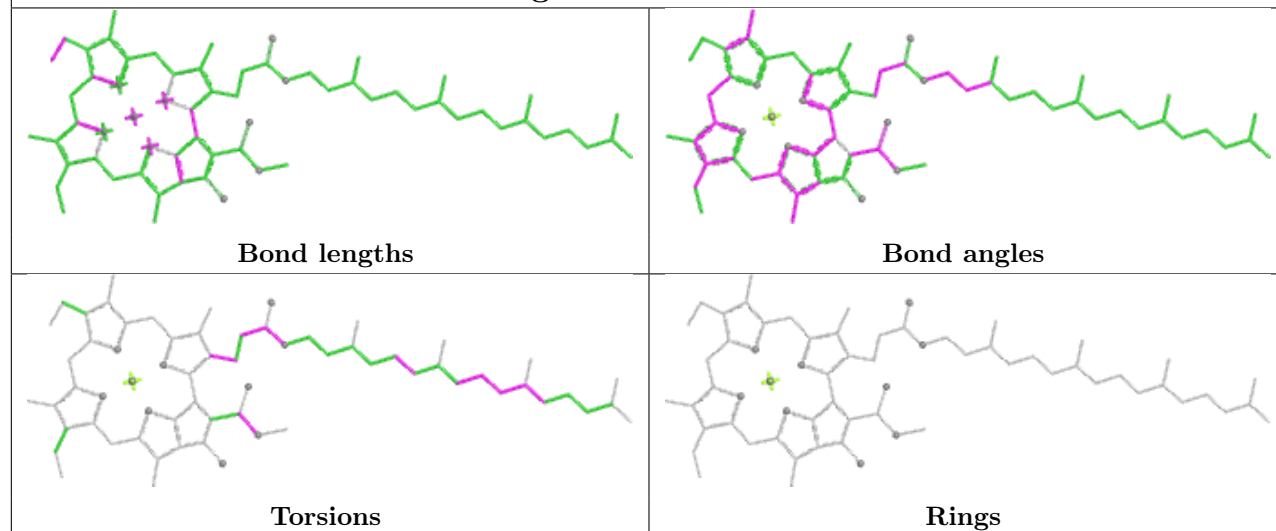
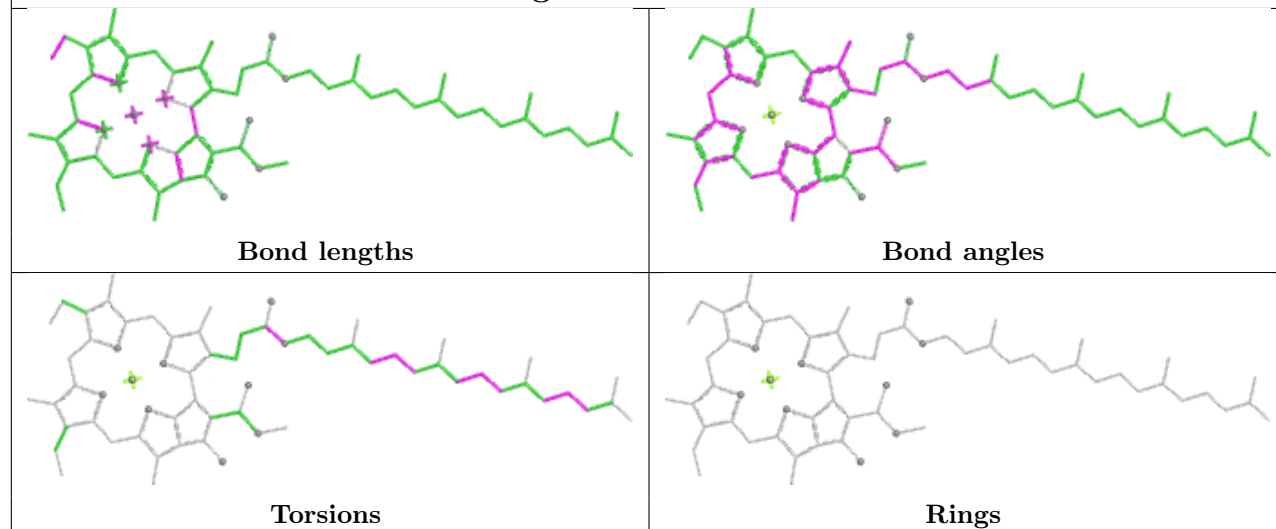
Ligand CLA G 604

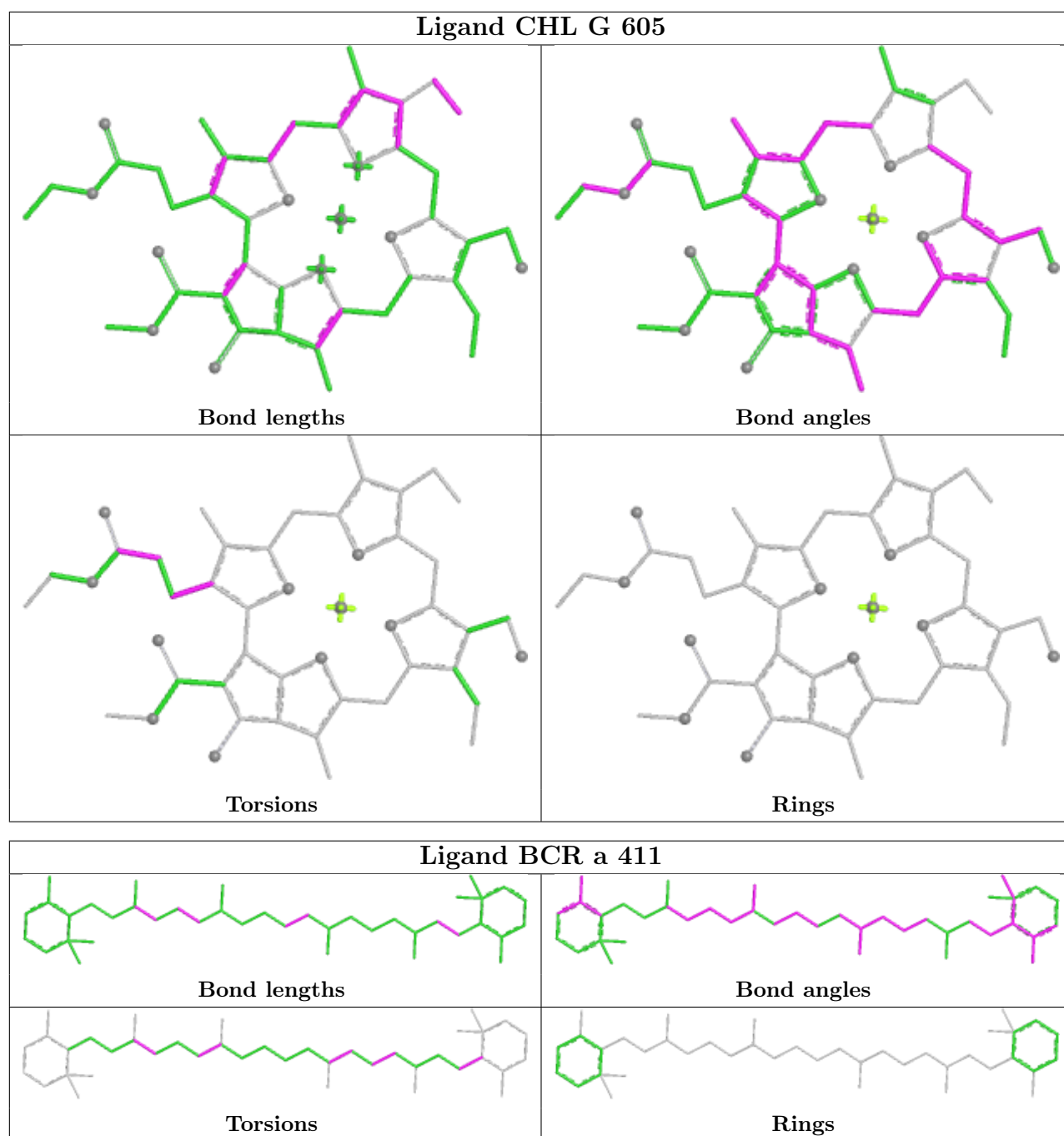


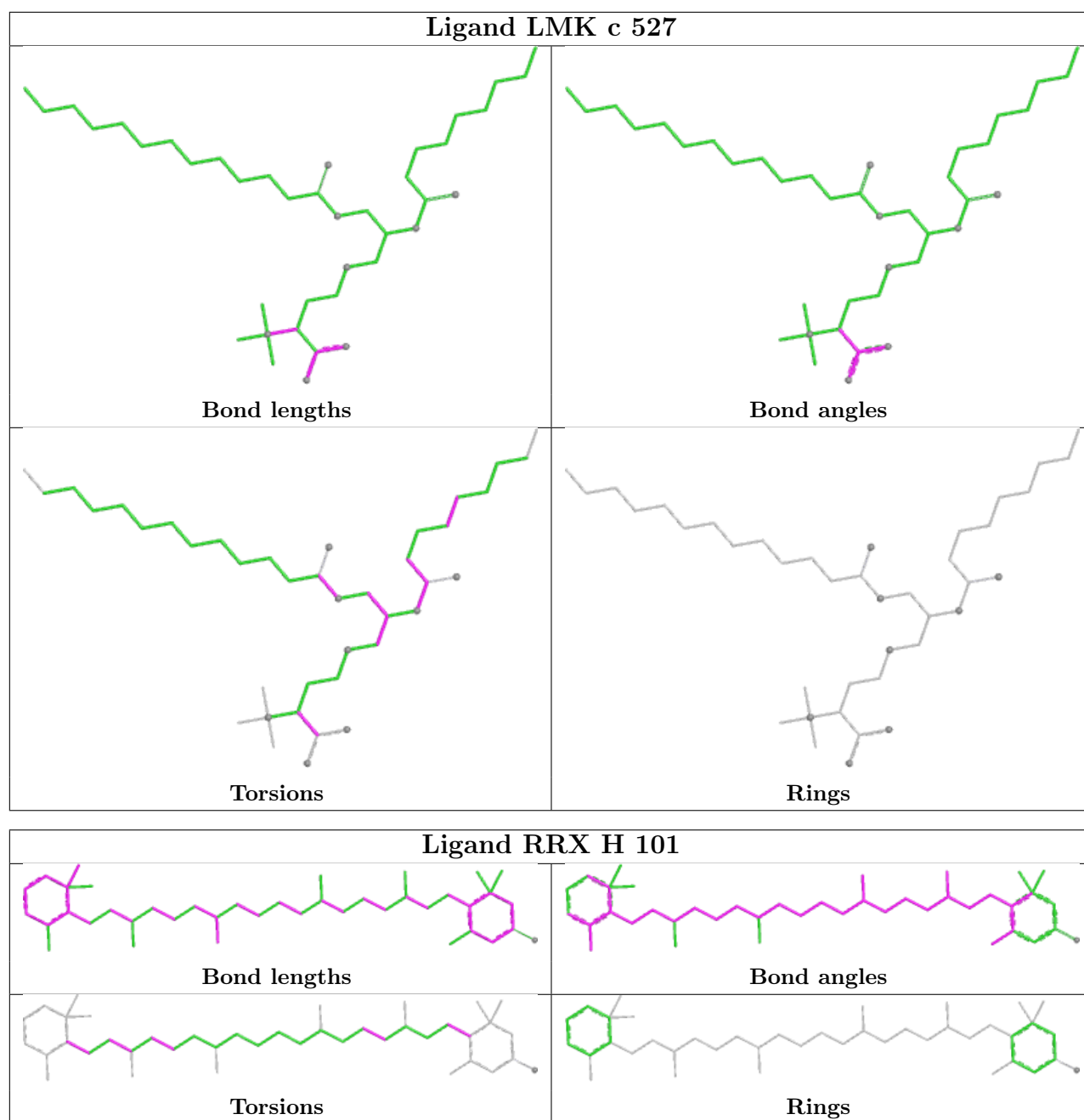
Ligand CLA N 603

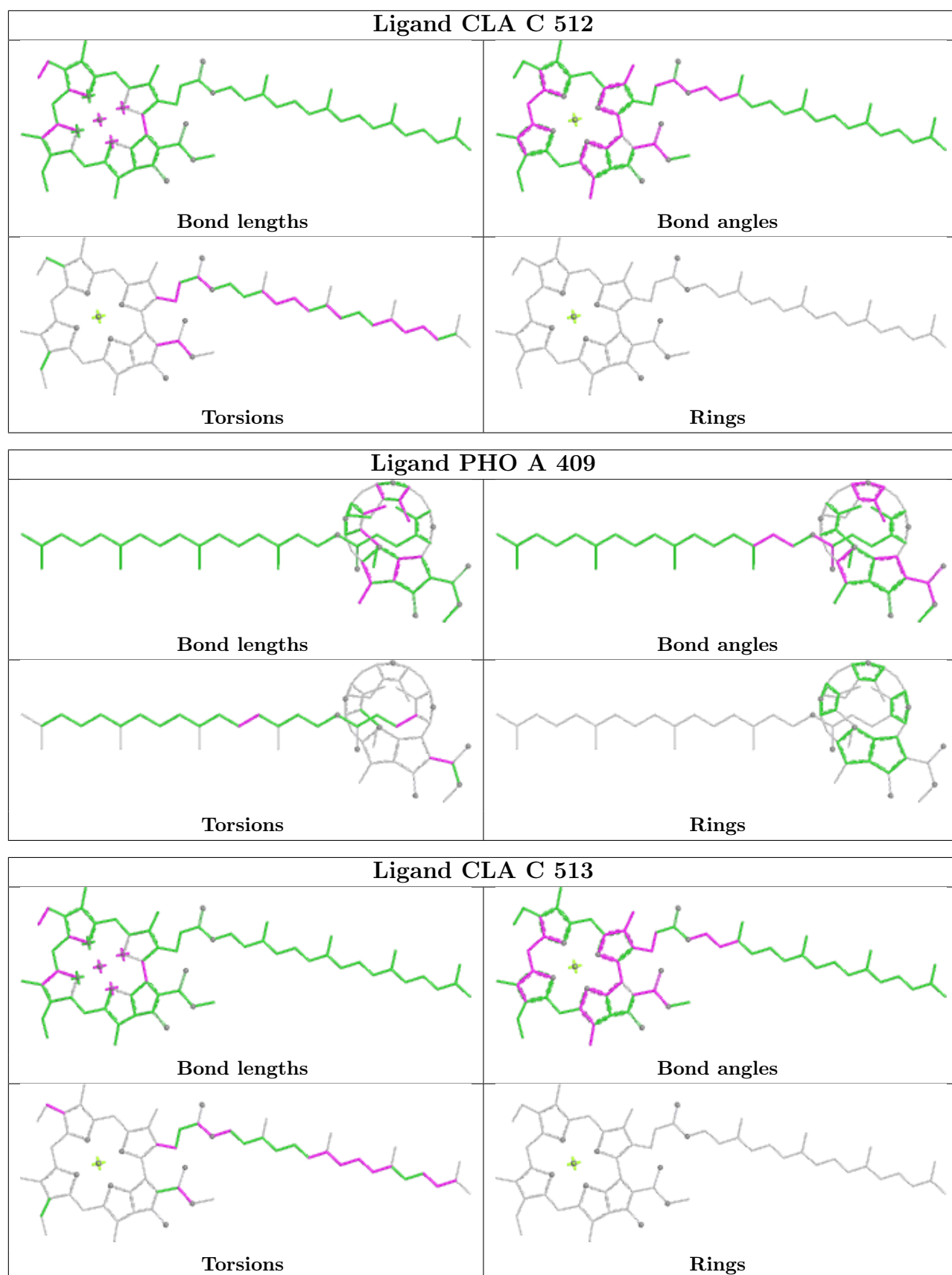


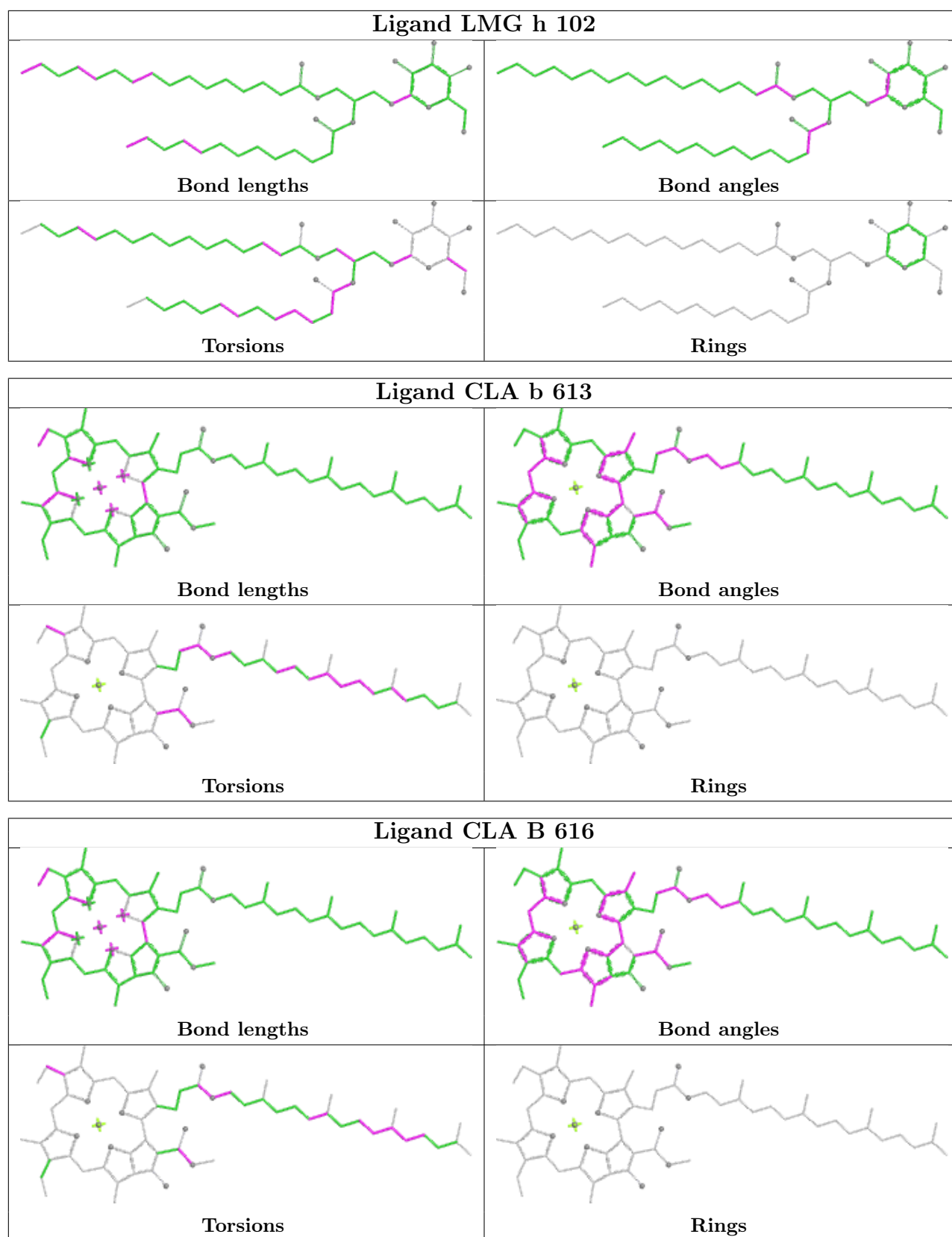


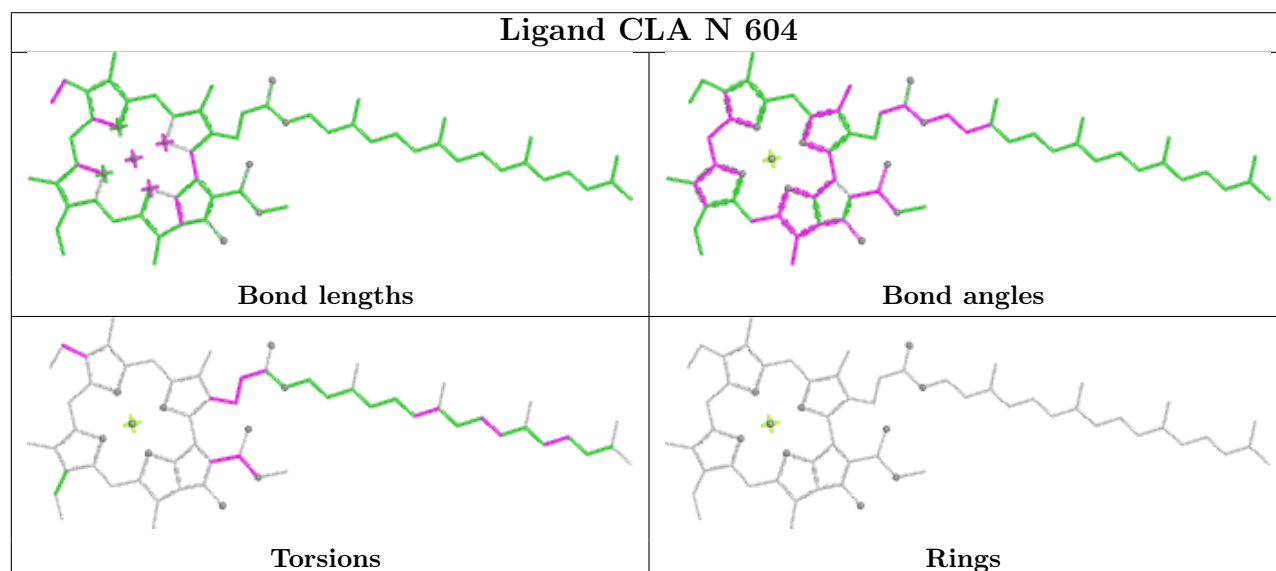
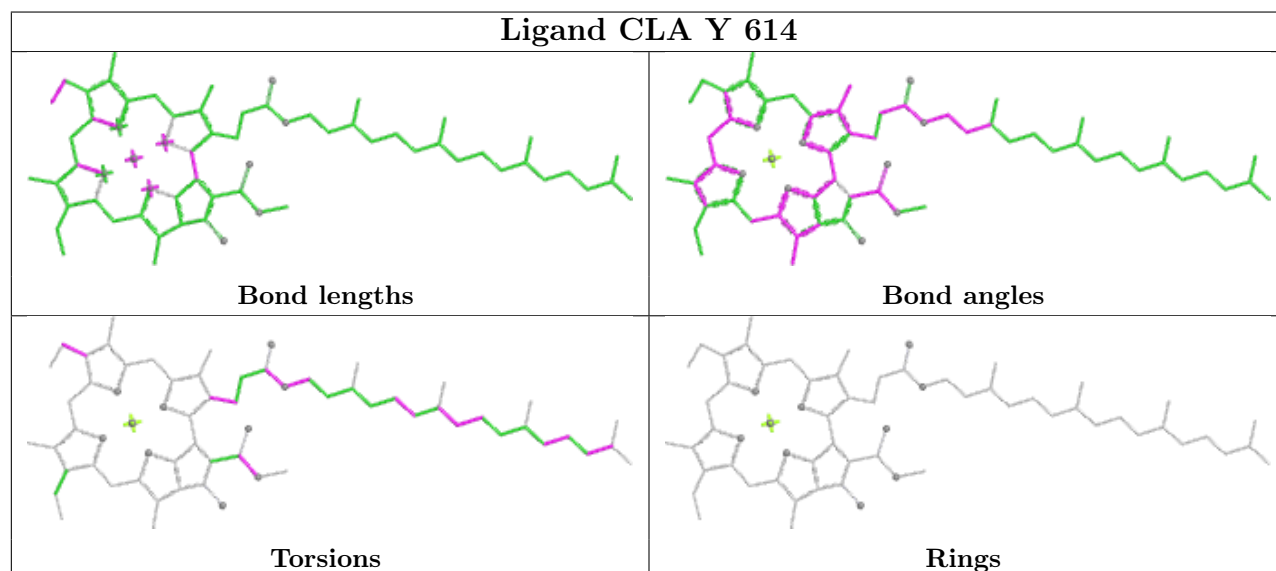
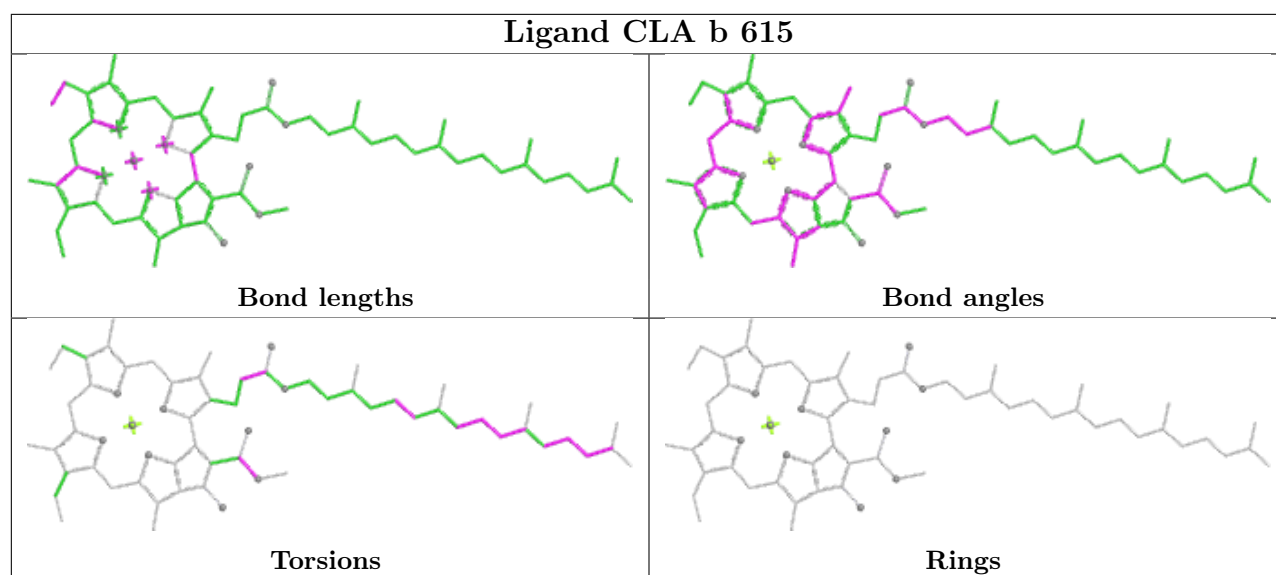
Ligand CLA A 405**Ligand CLA C 508**

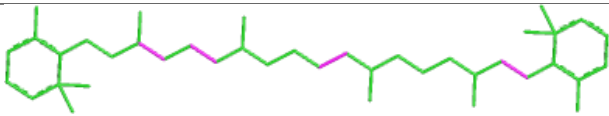
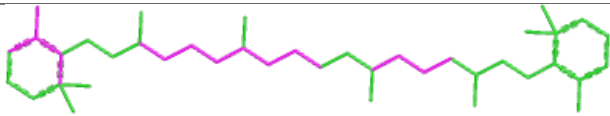
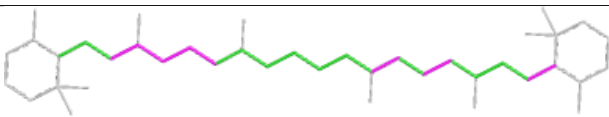
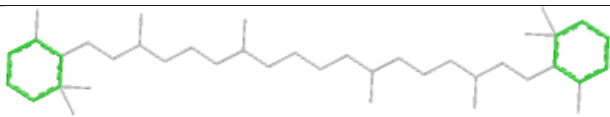


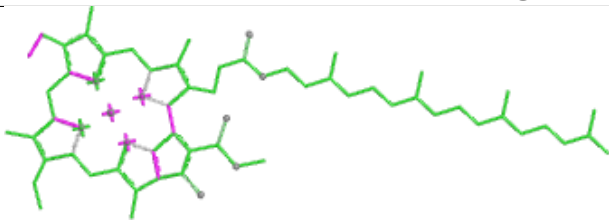
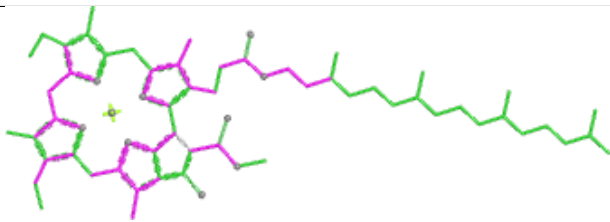
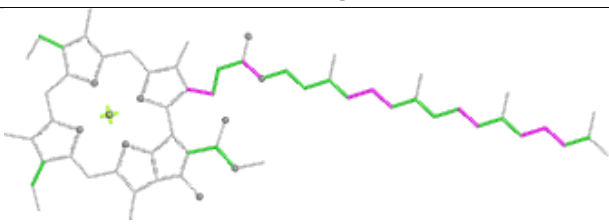
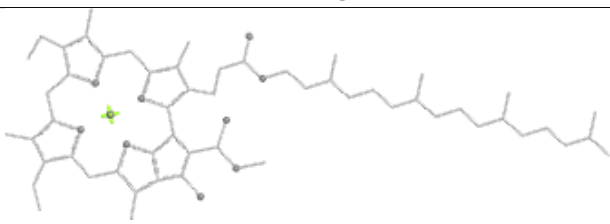


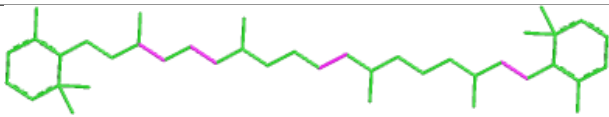
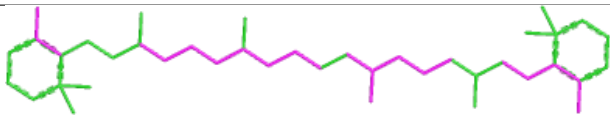
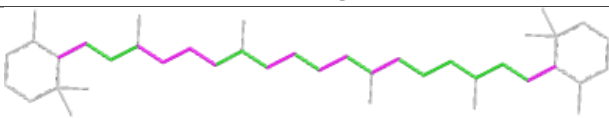
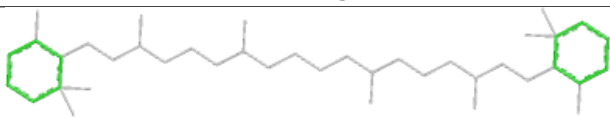


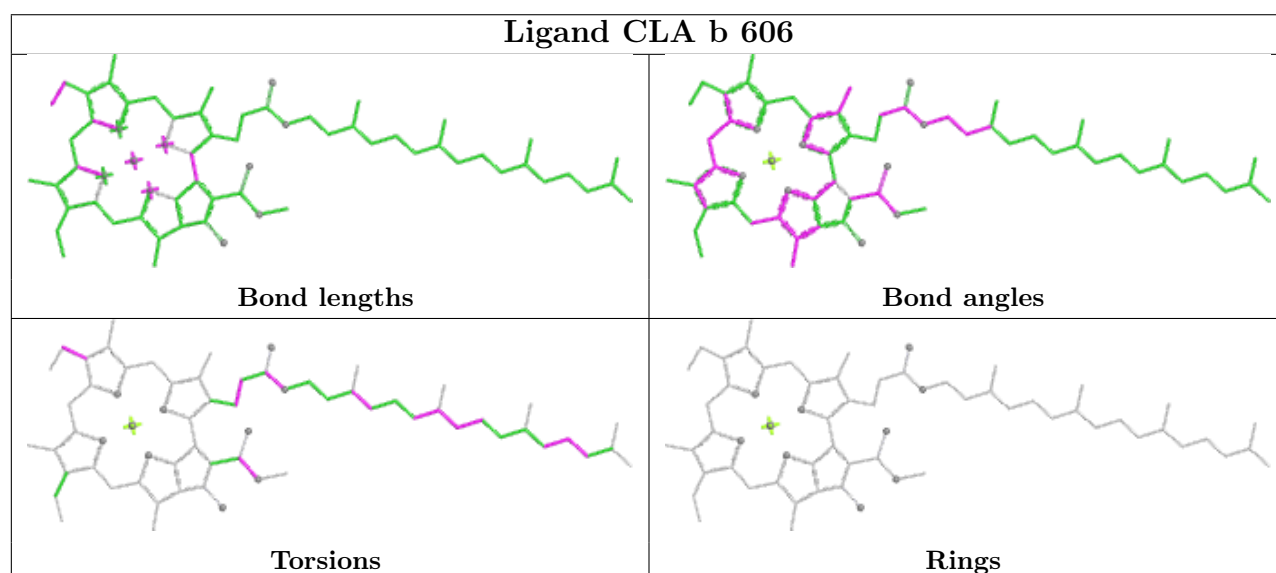
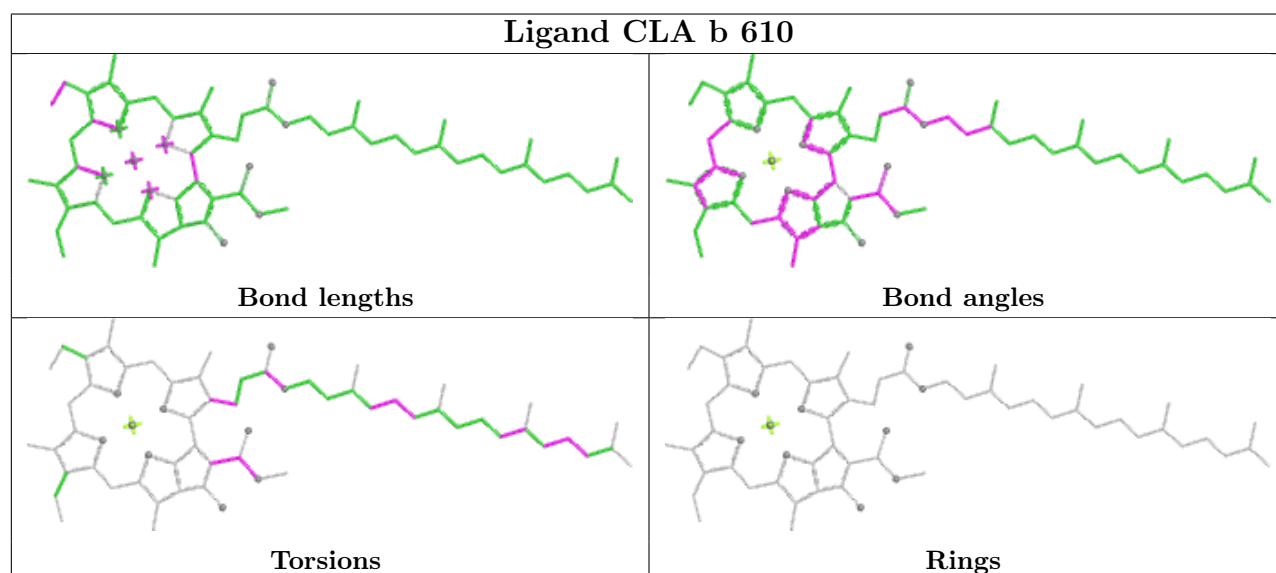
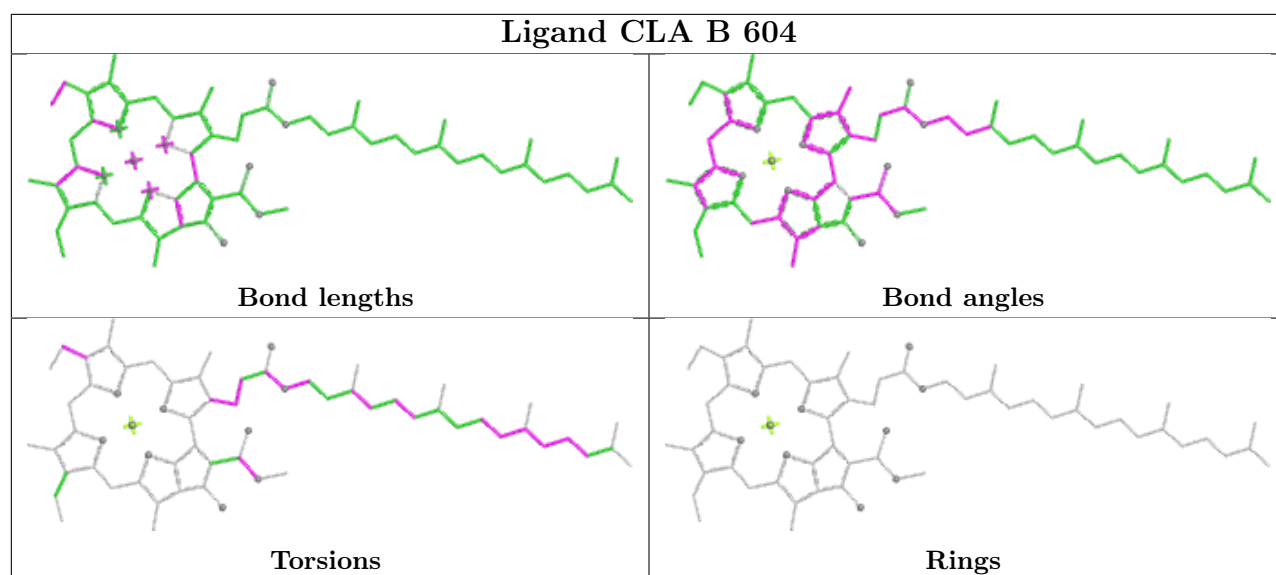


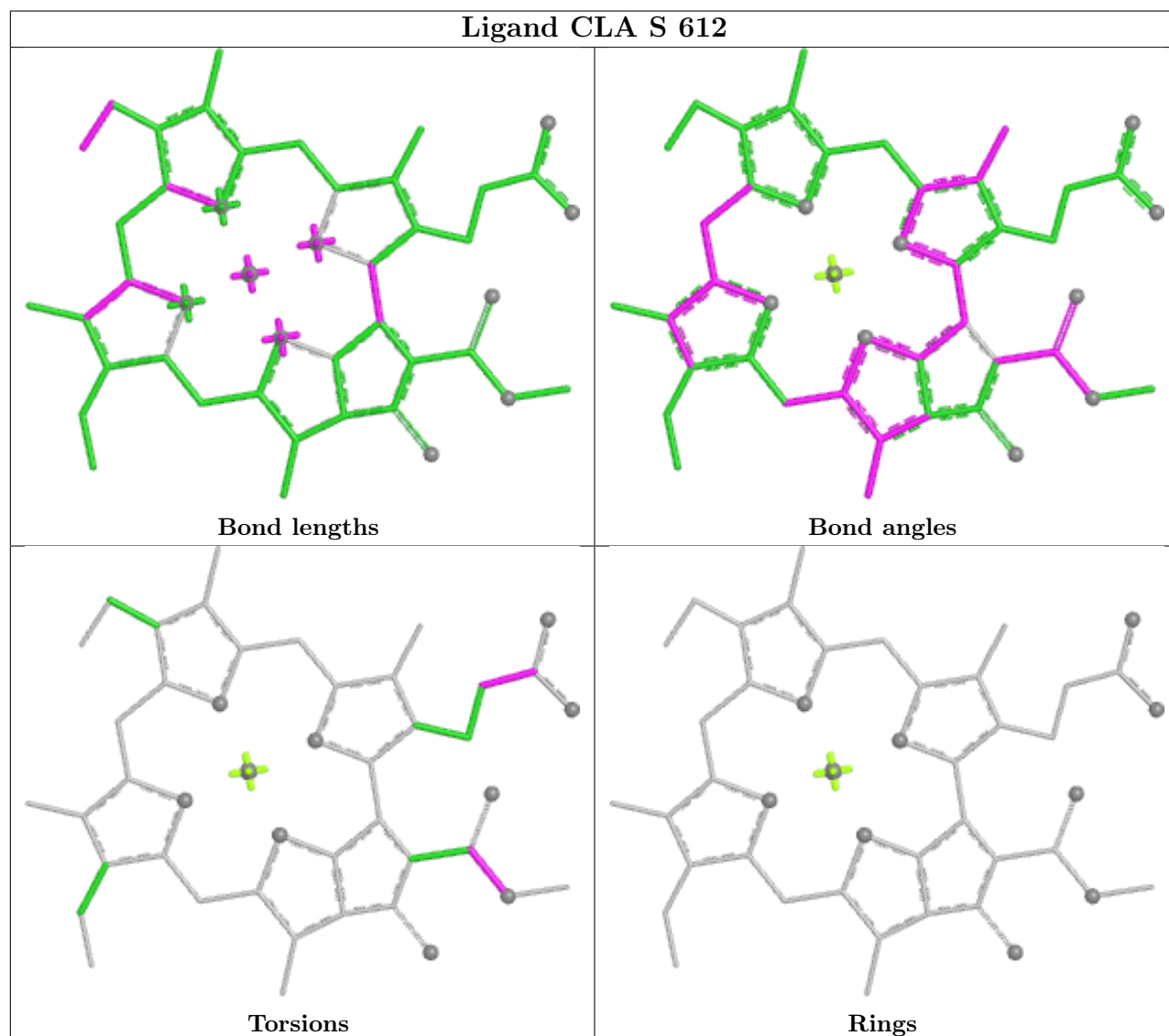
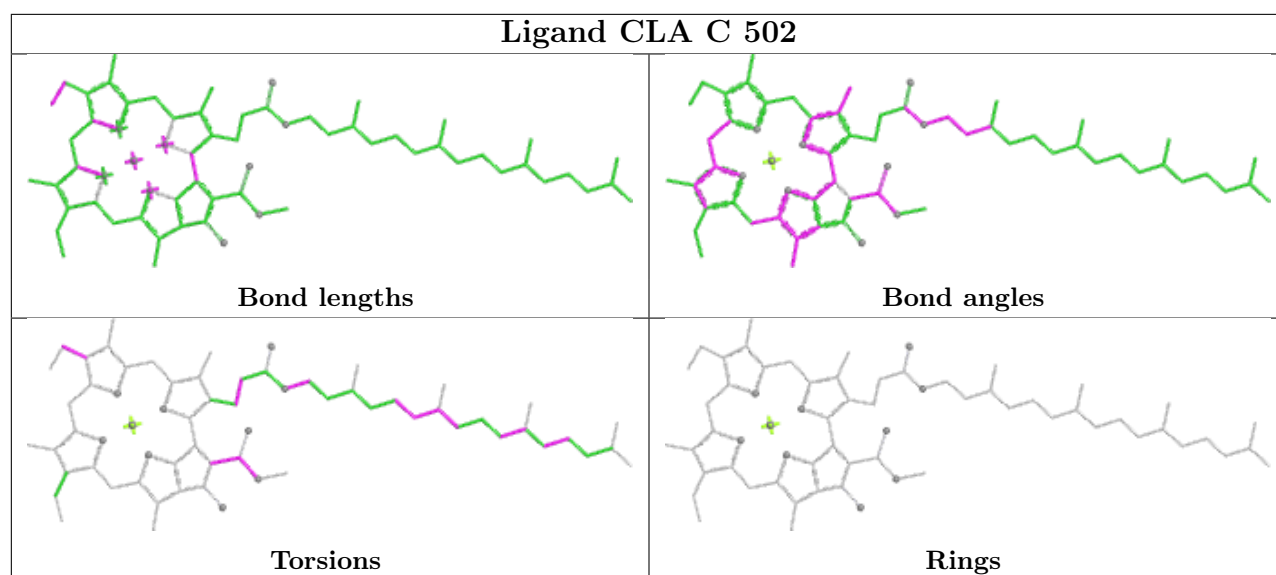


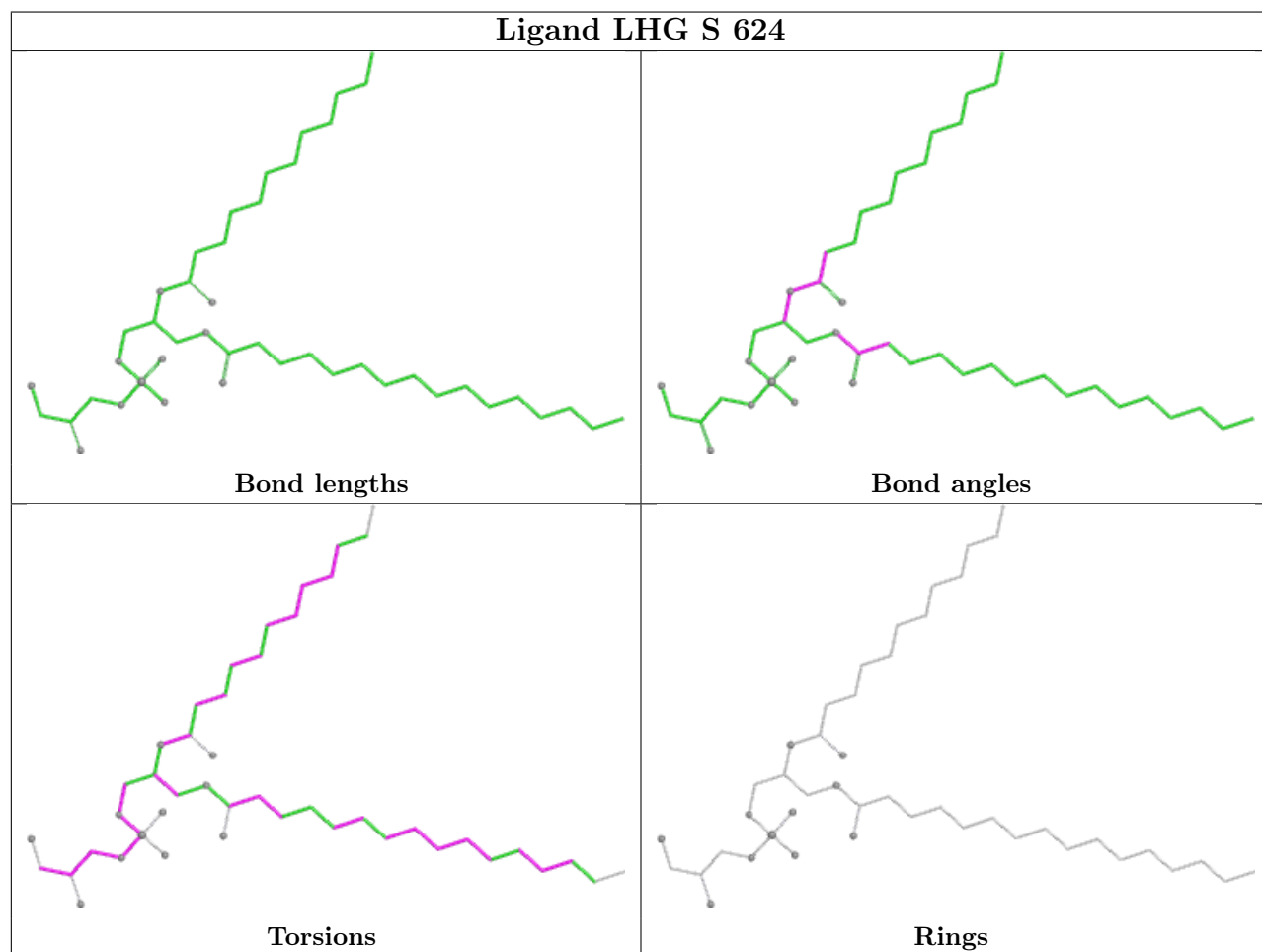
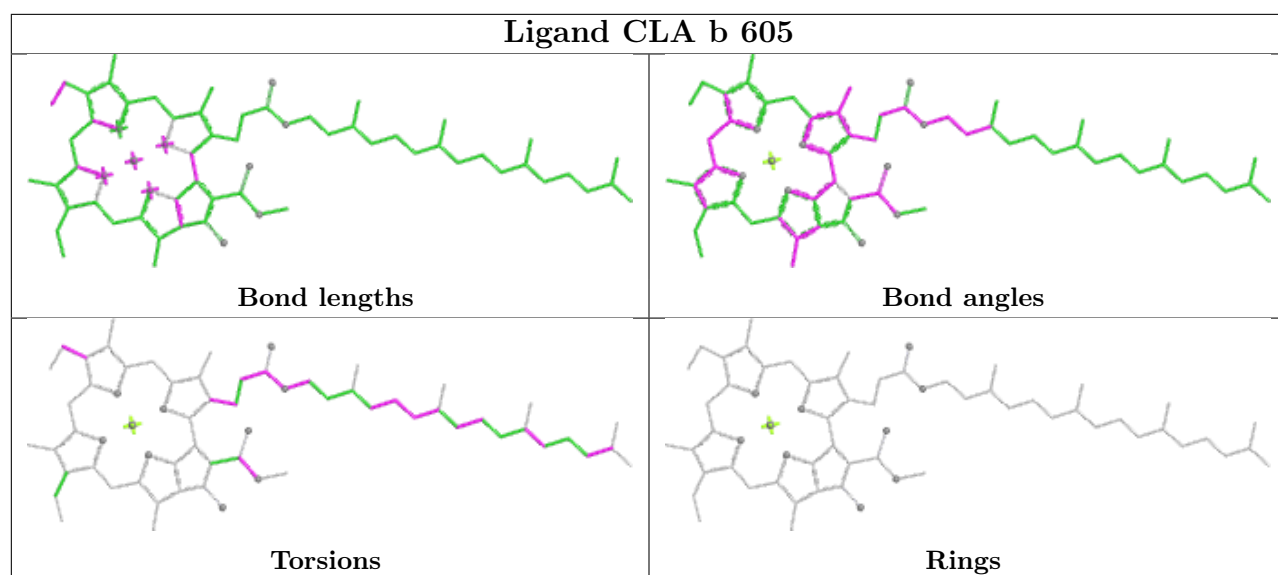
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

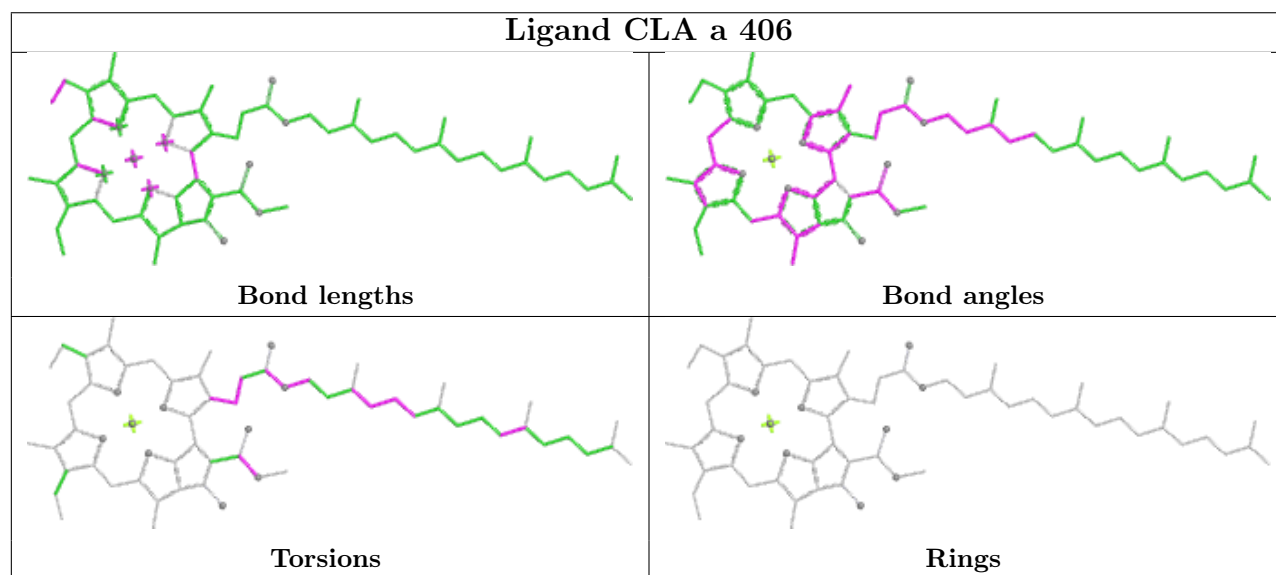
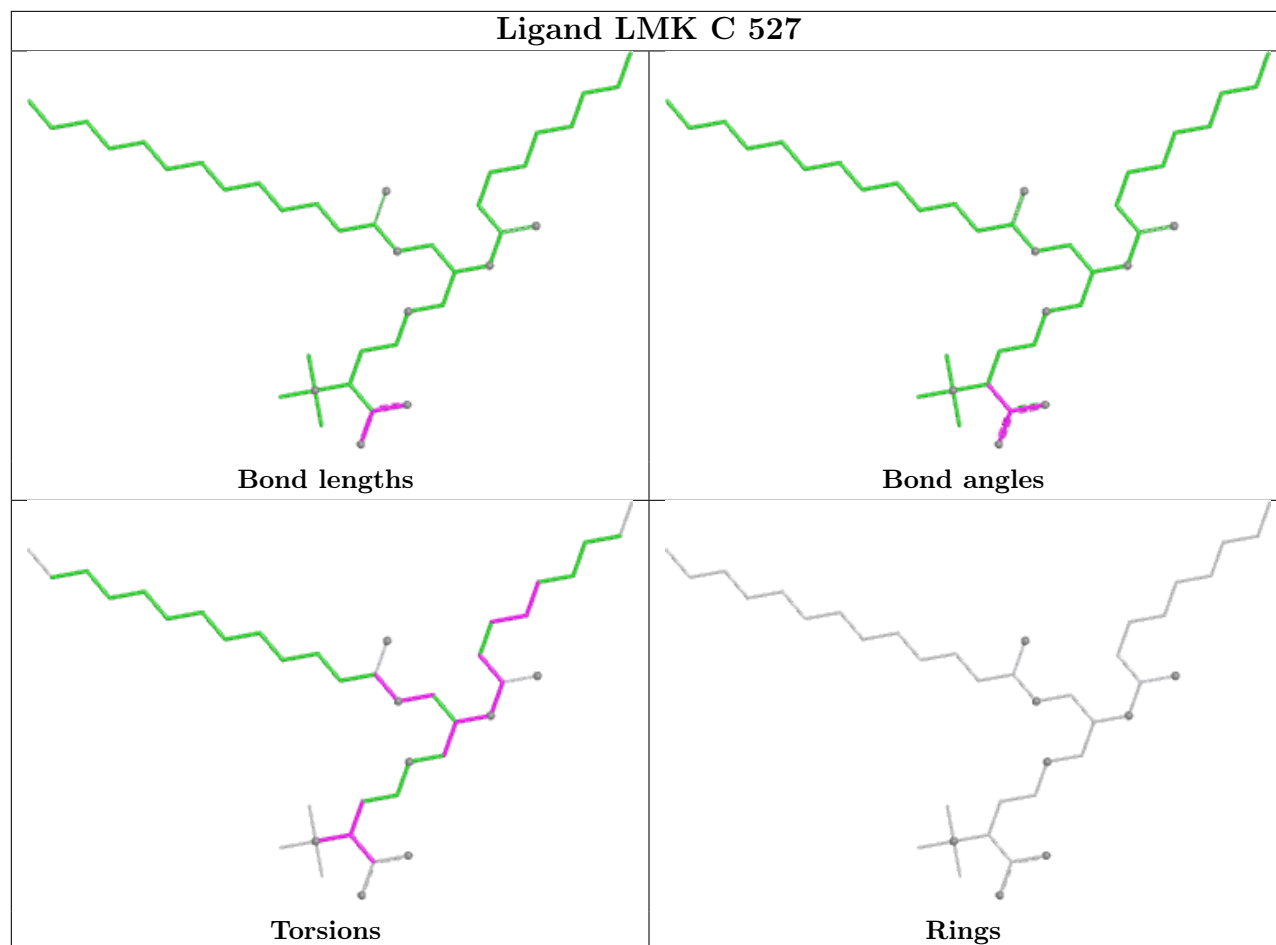
Ligand CLA c 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

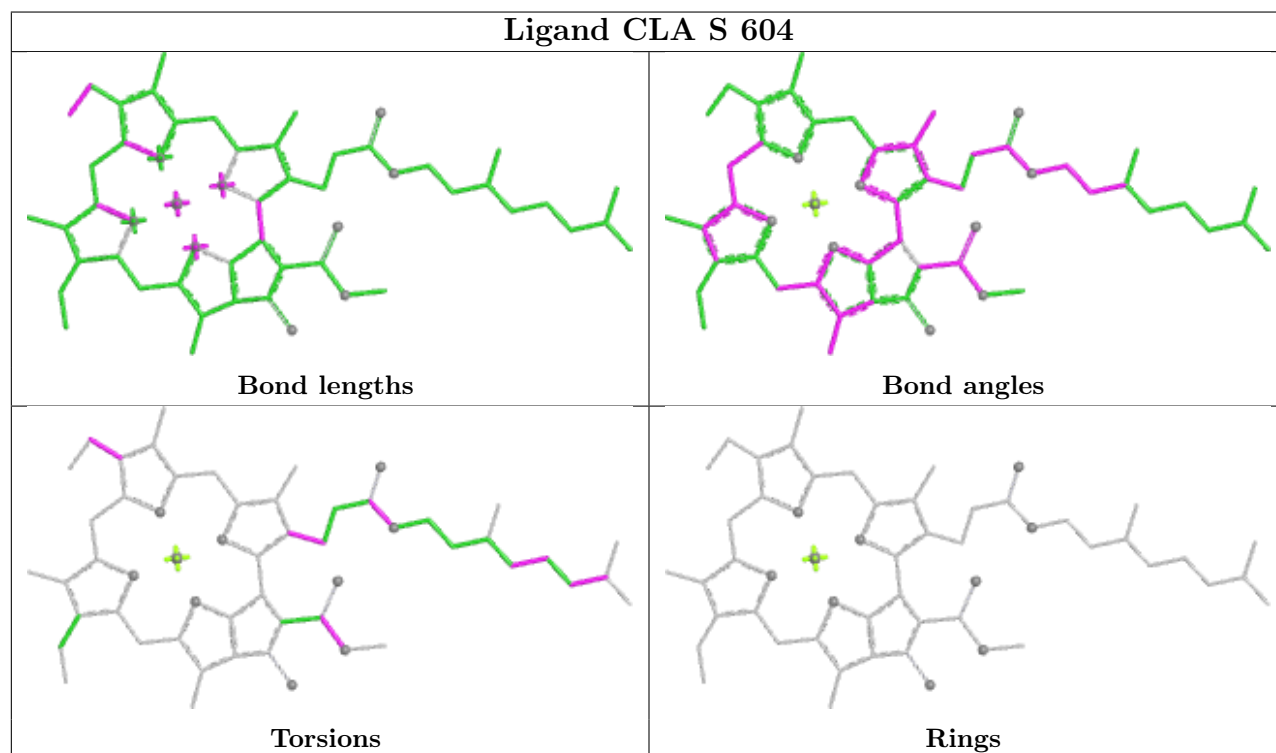
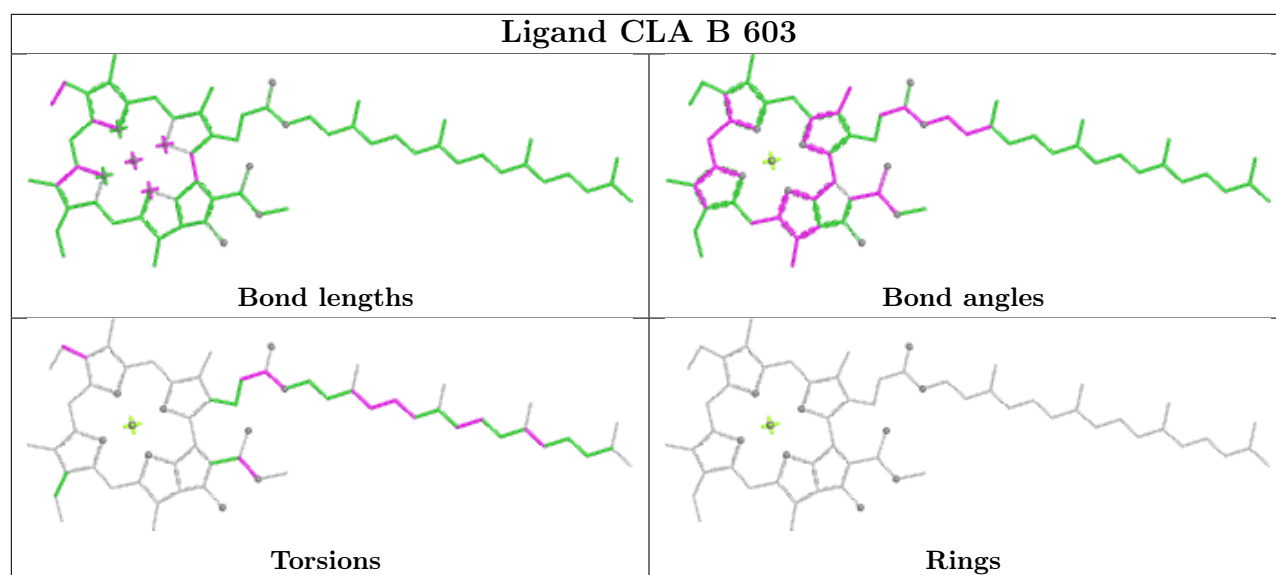
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

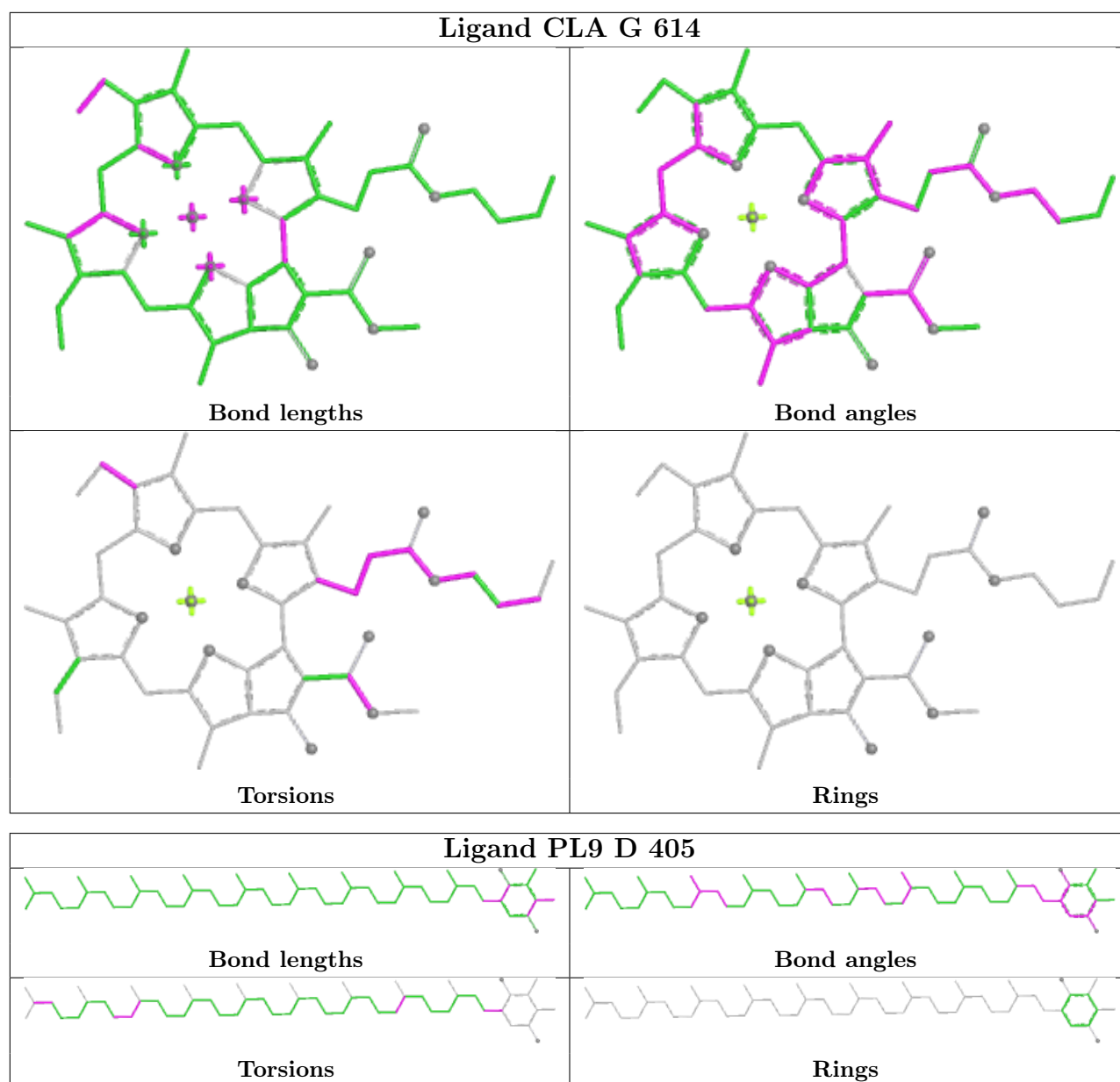


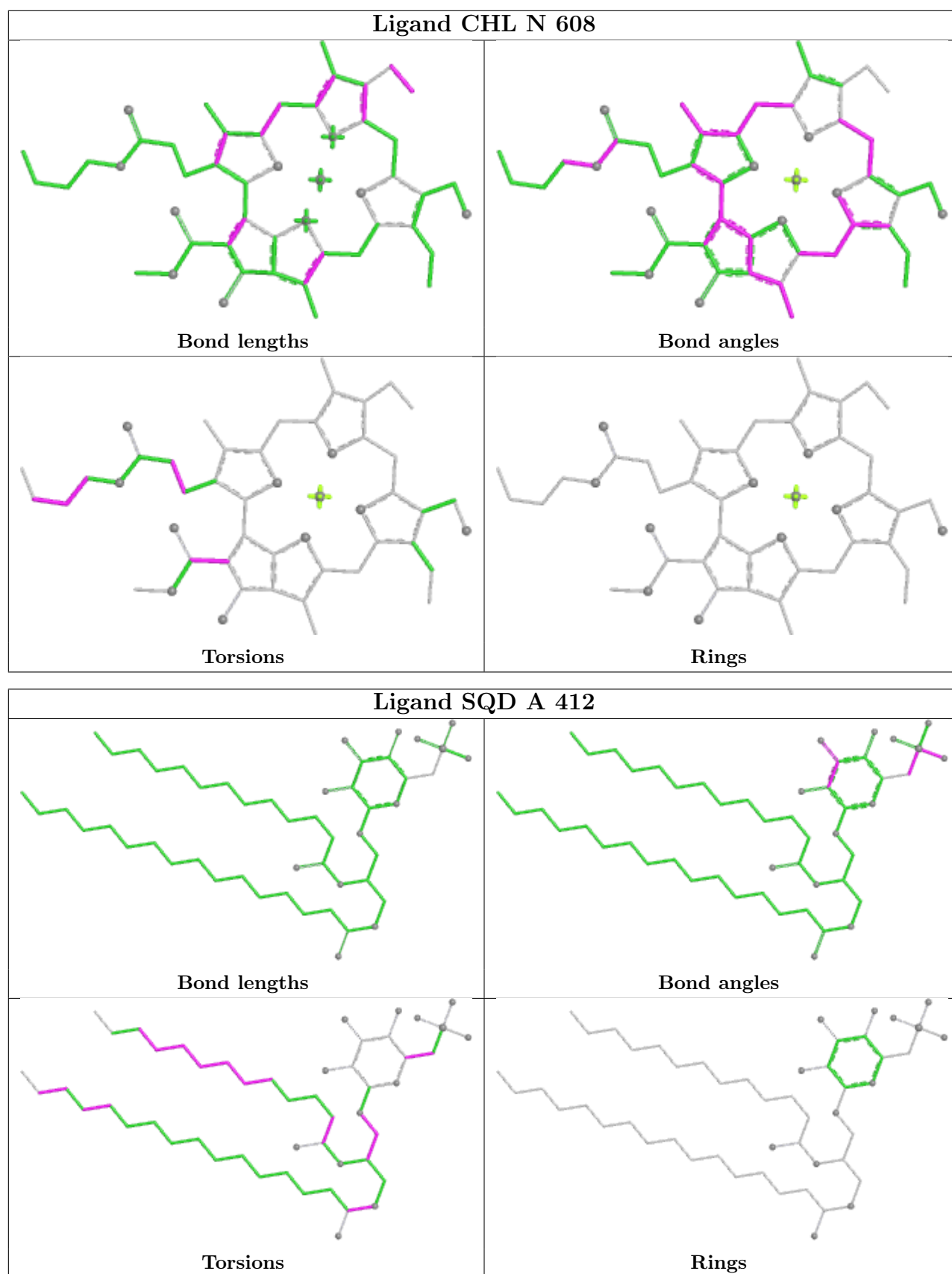


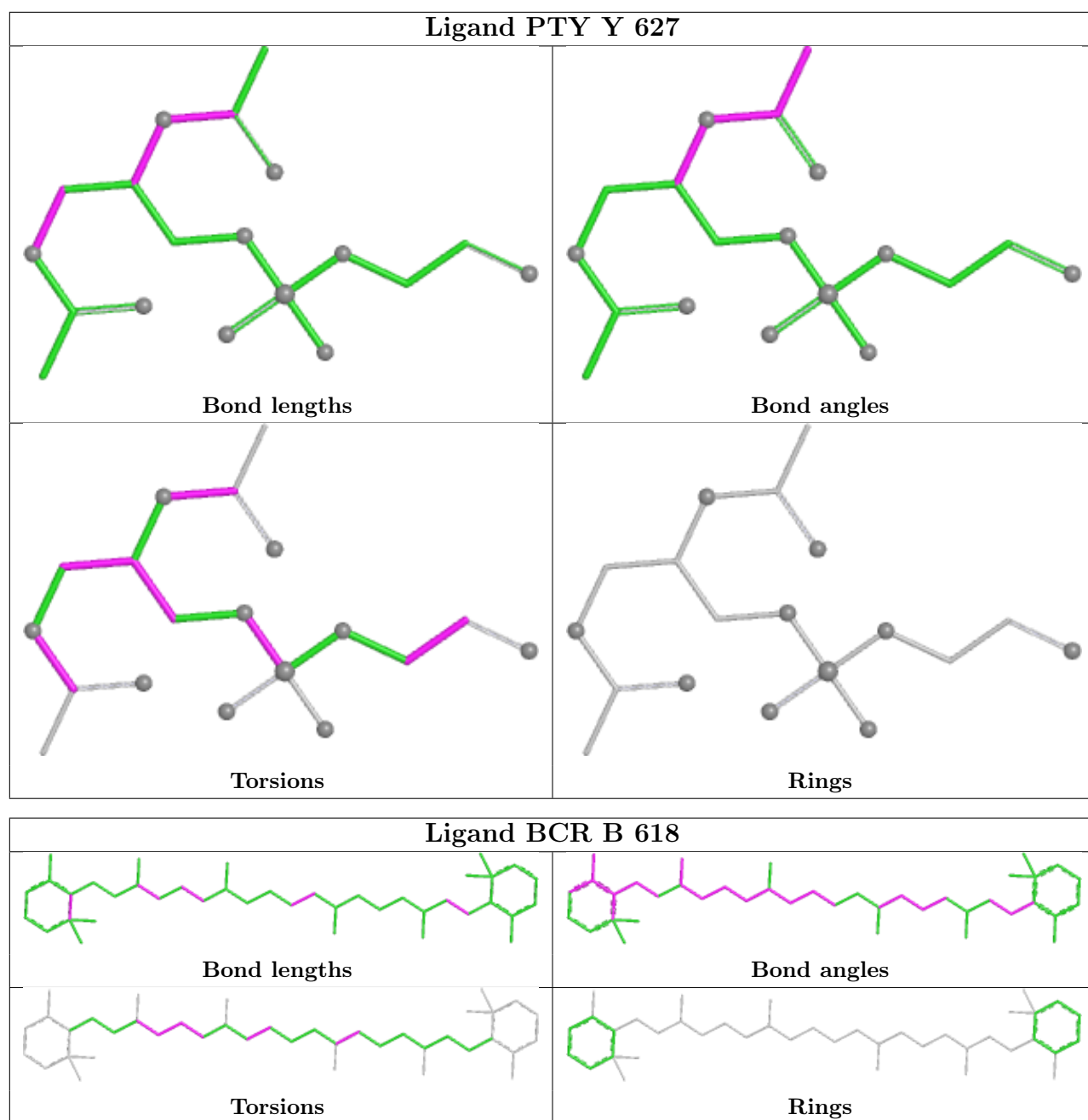


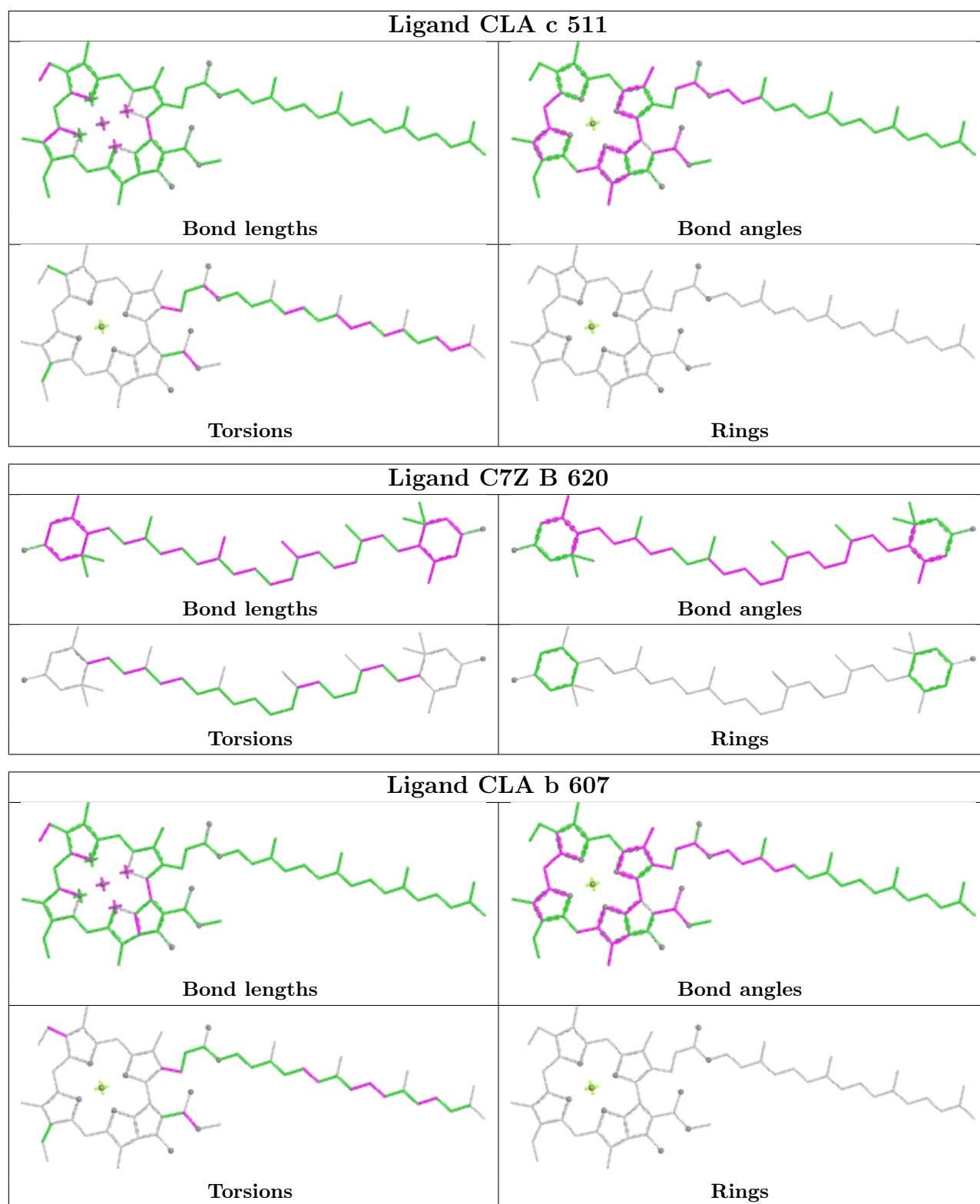


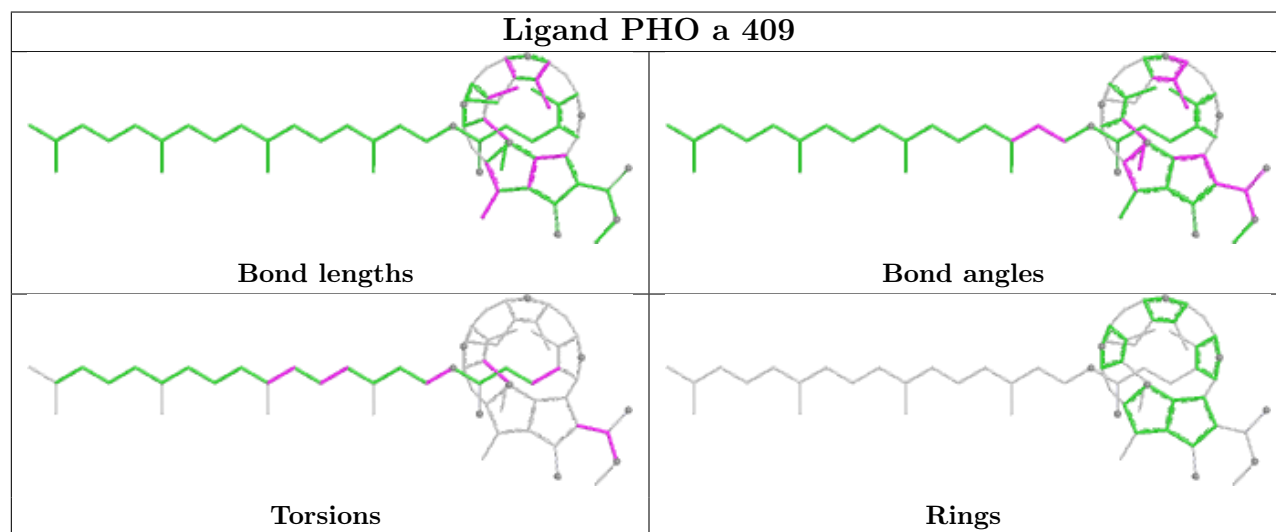
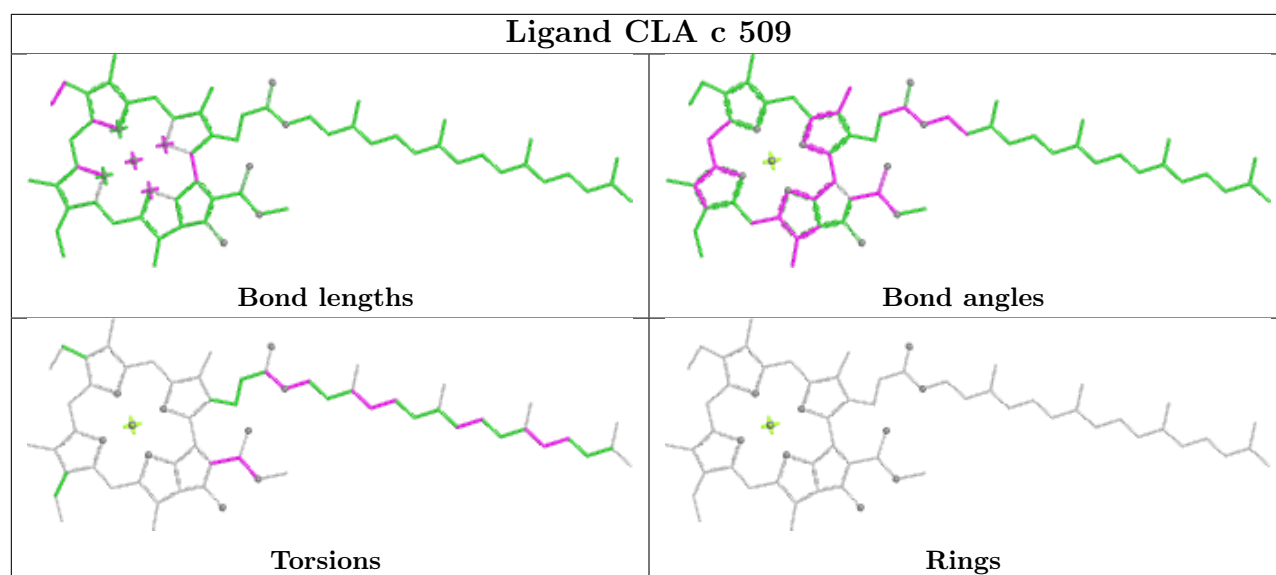


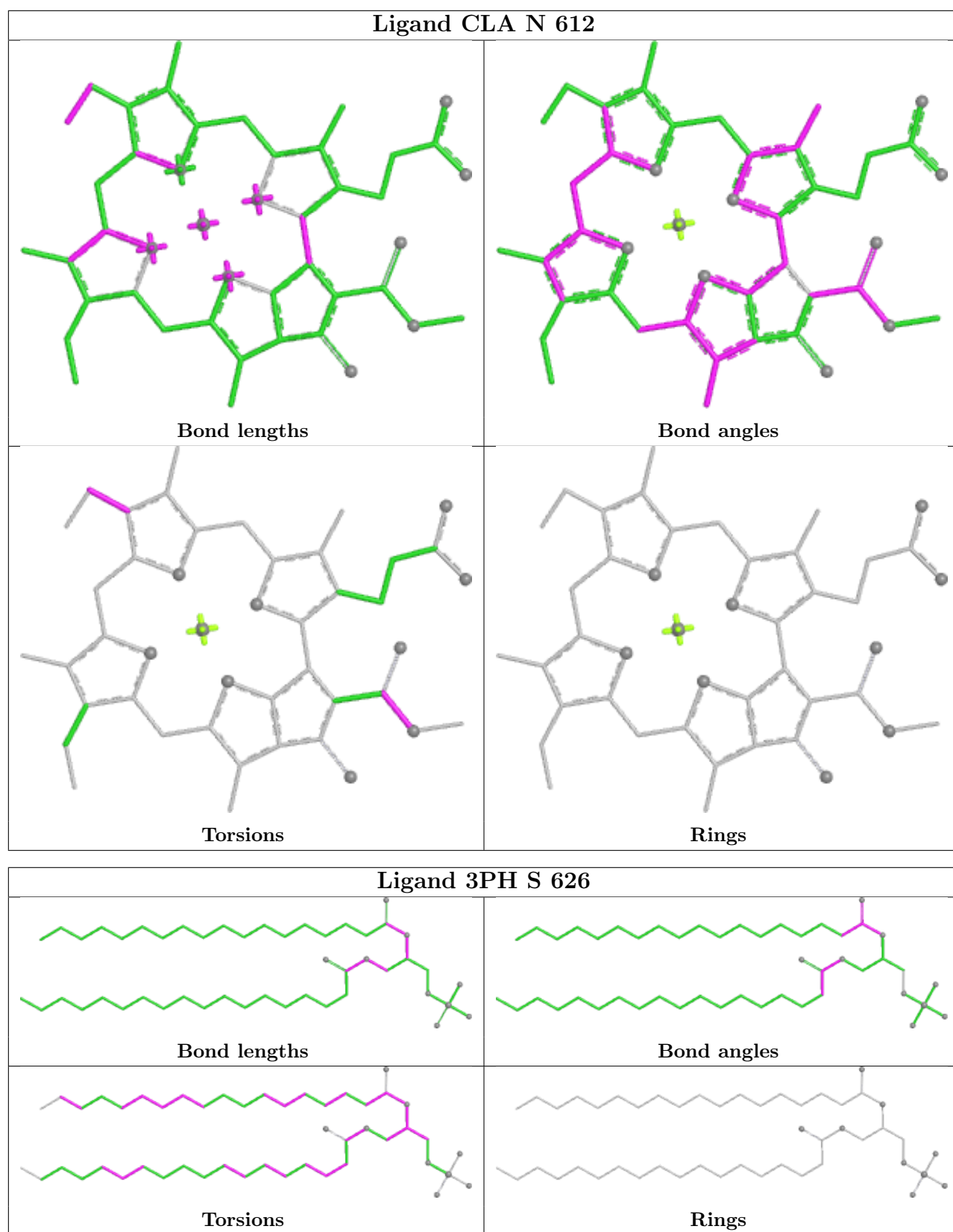


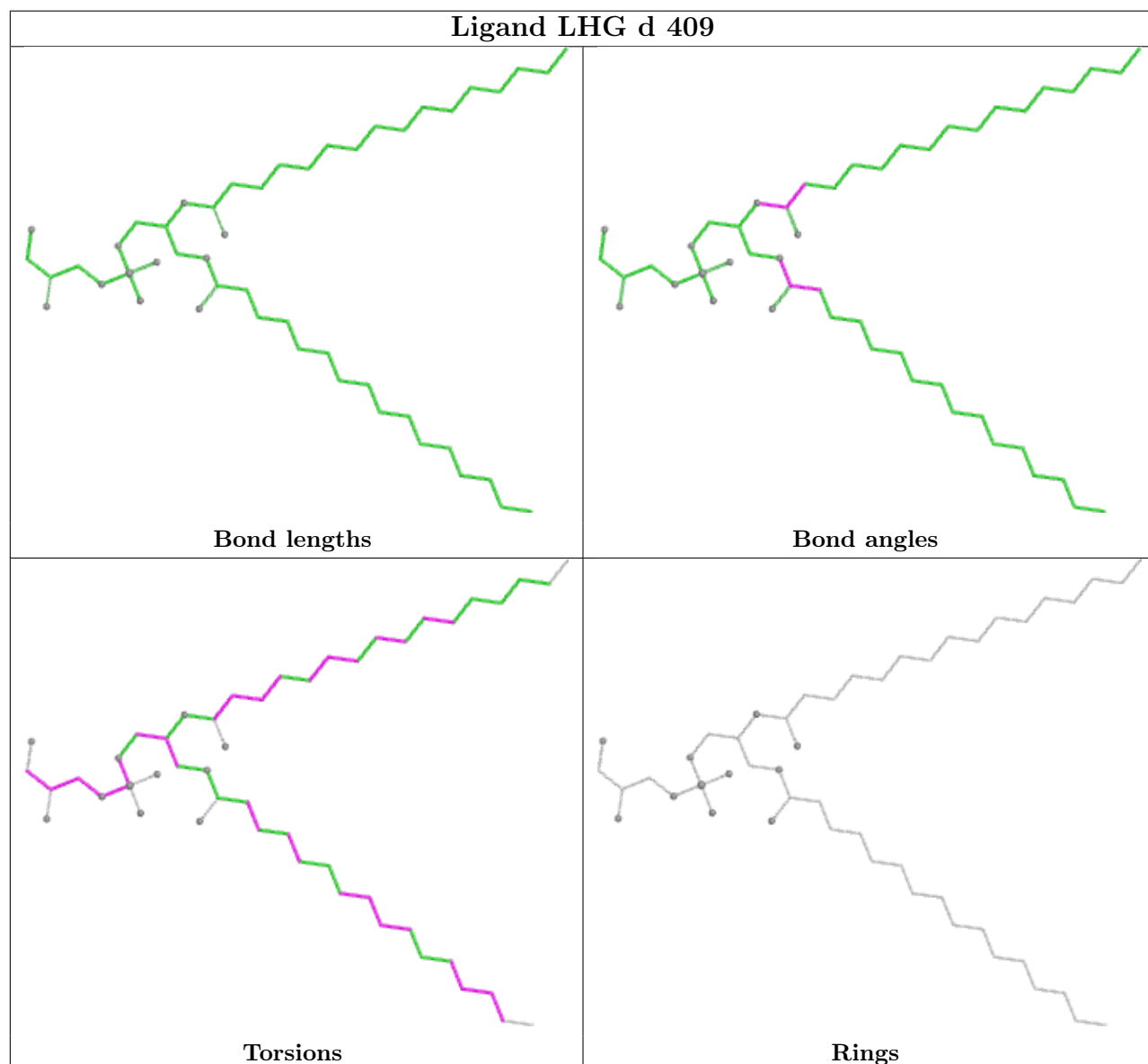
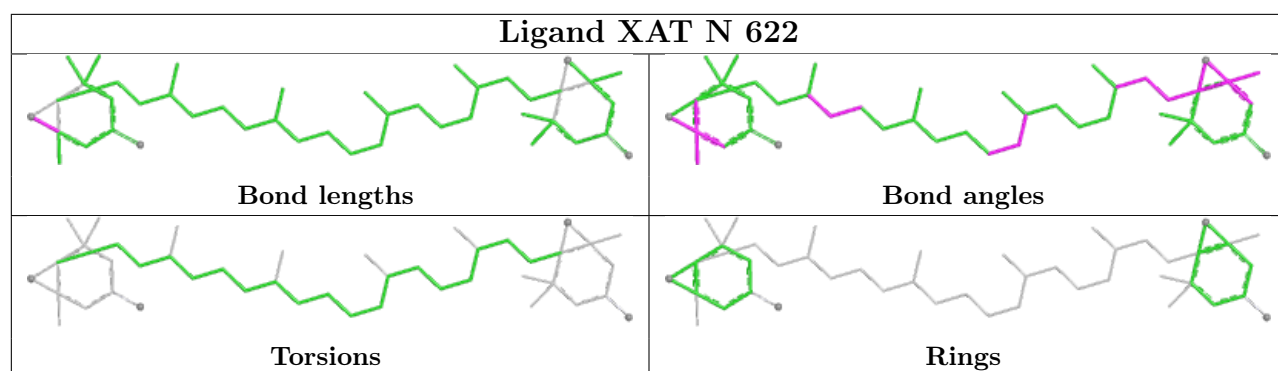




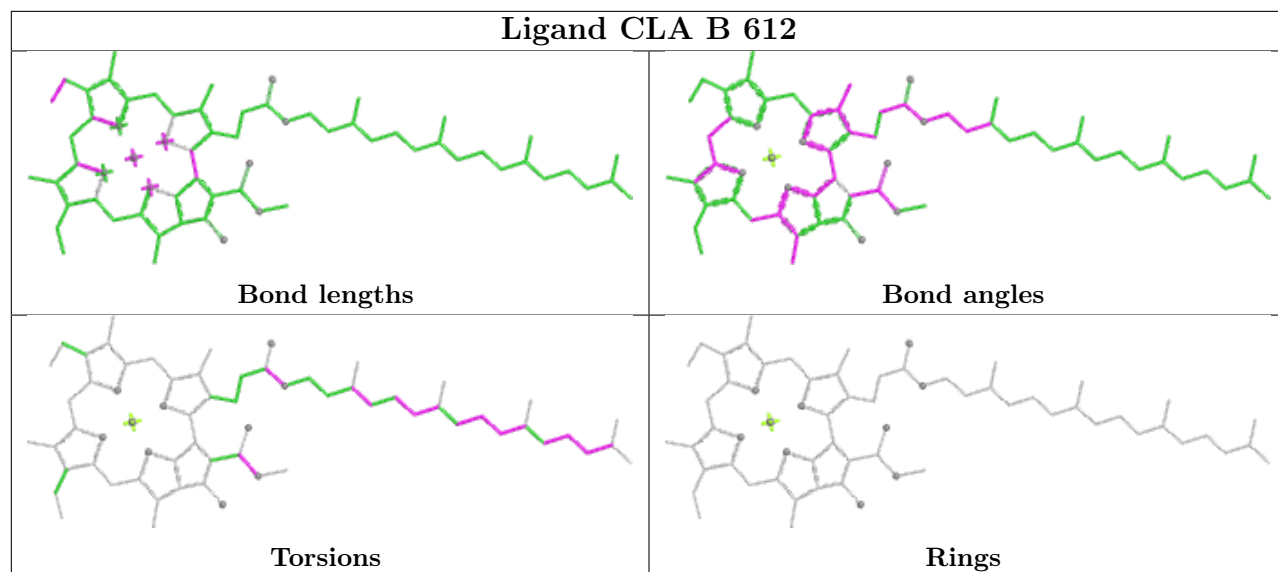




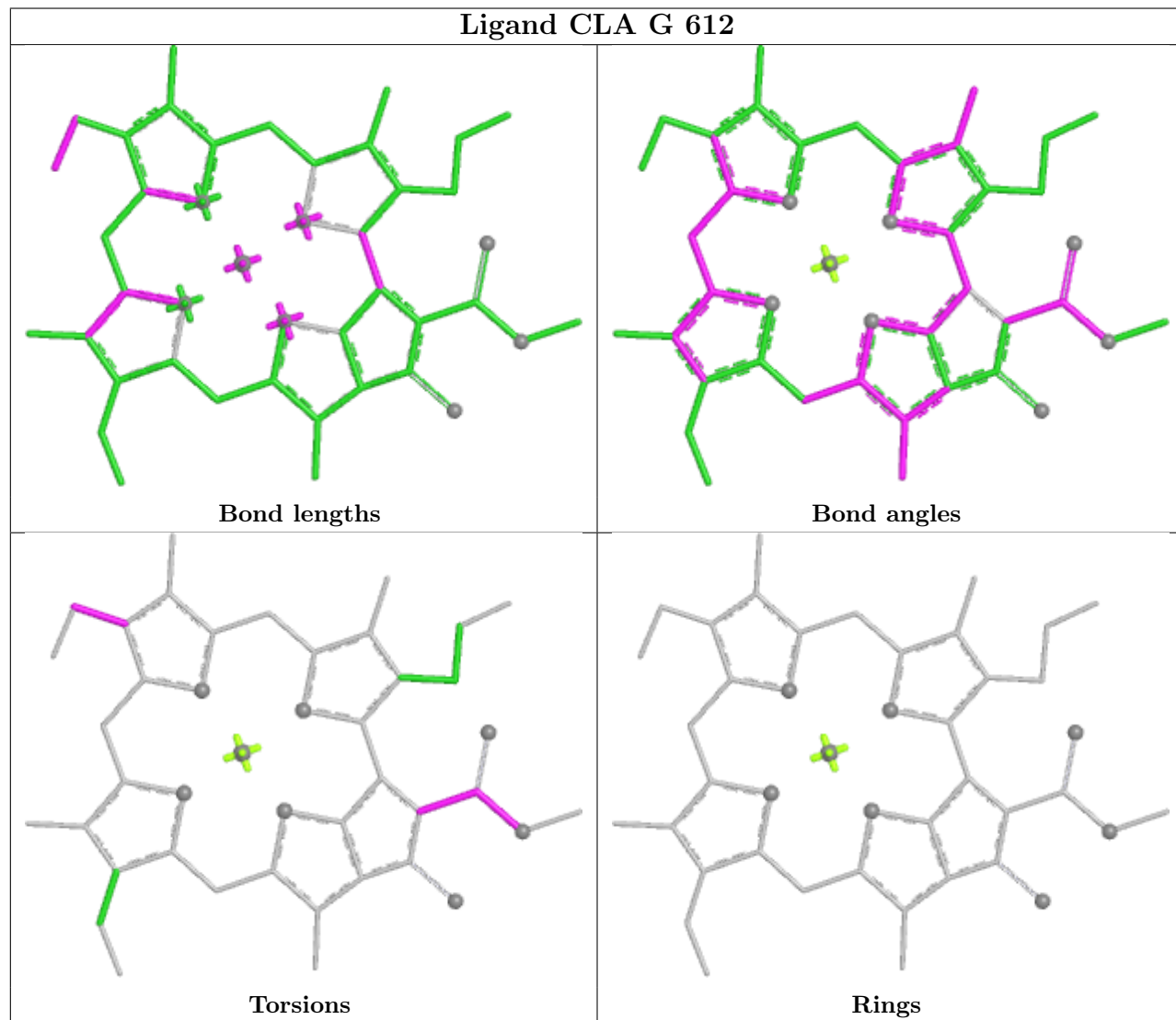


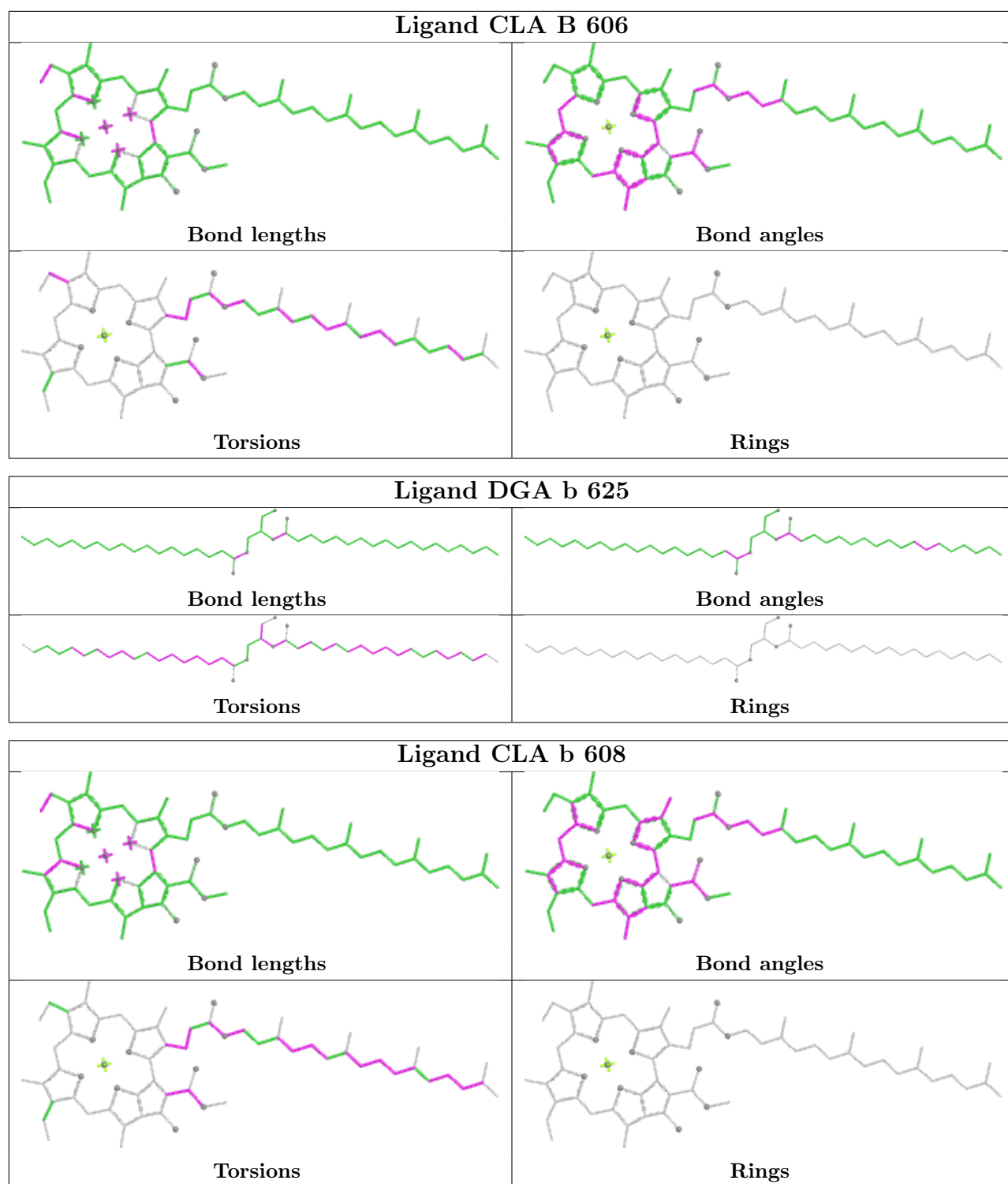


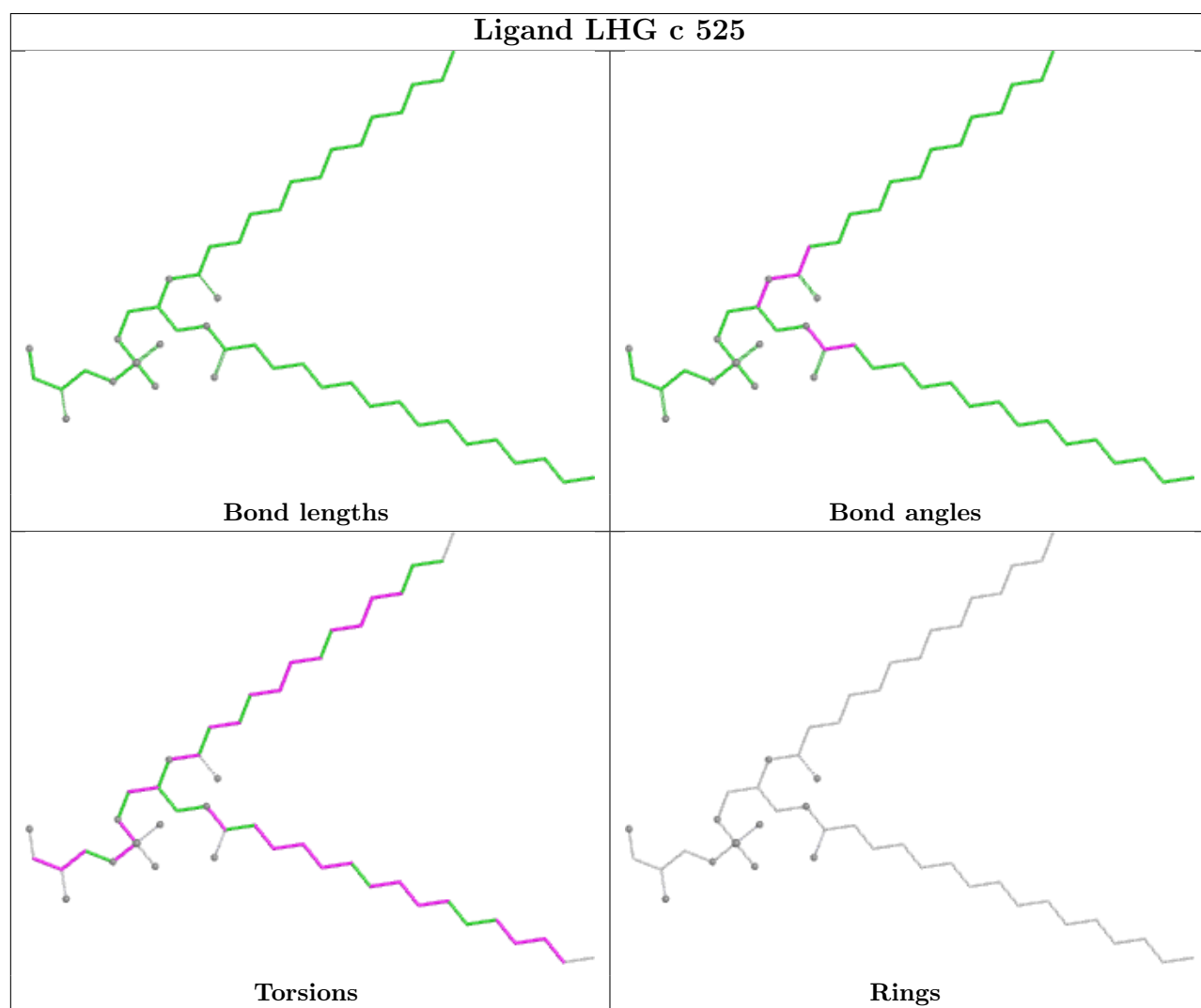
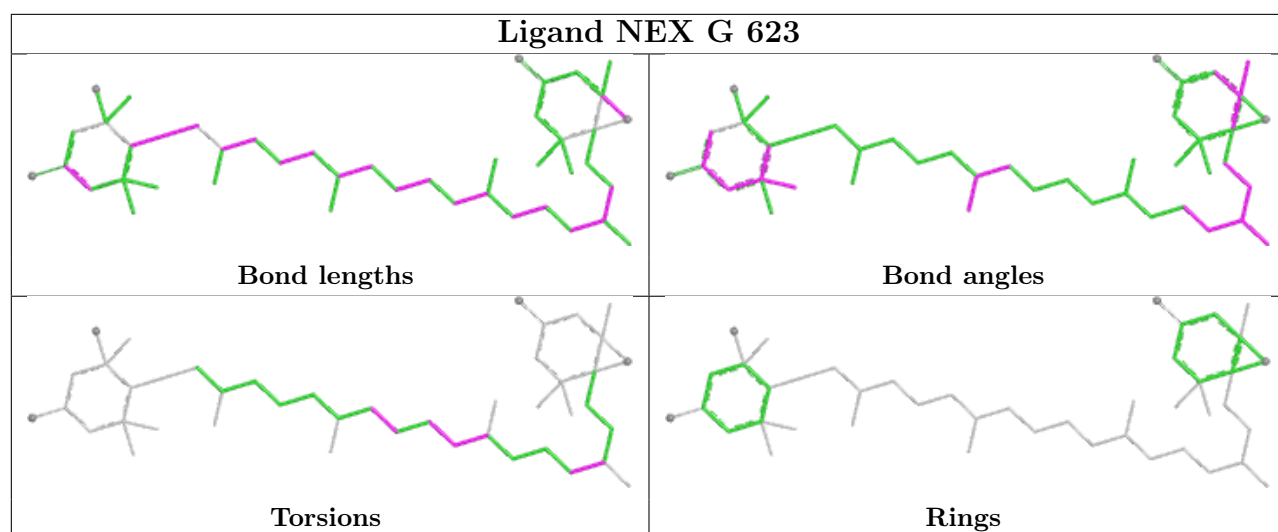
Ligand CLA B 612

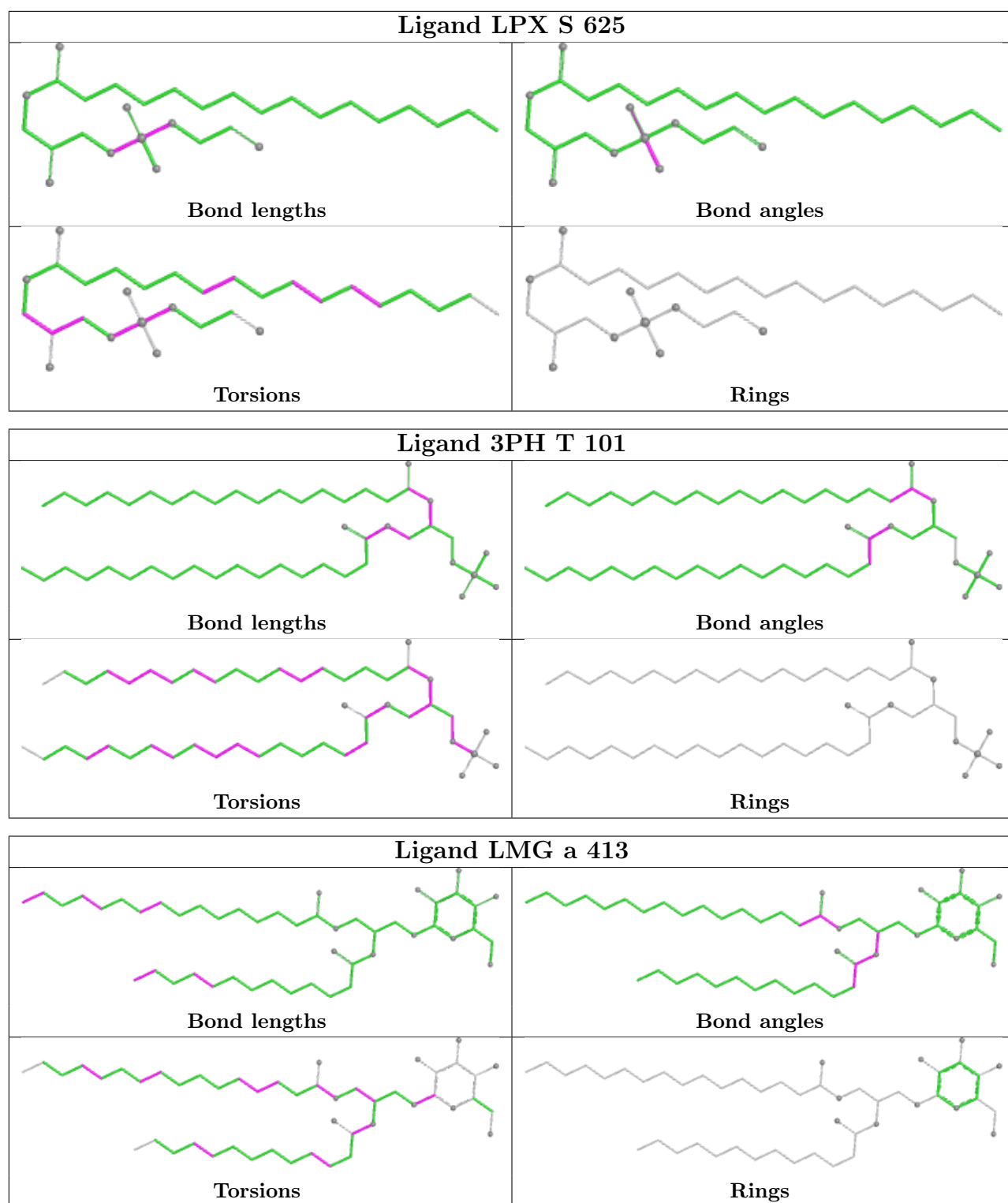


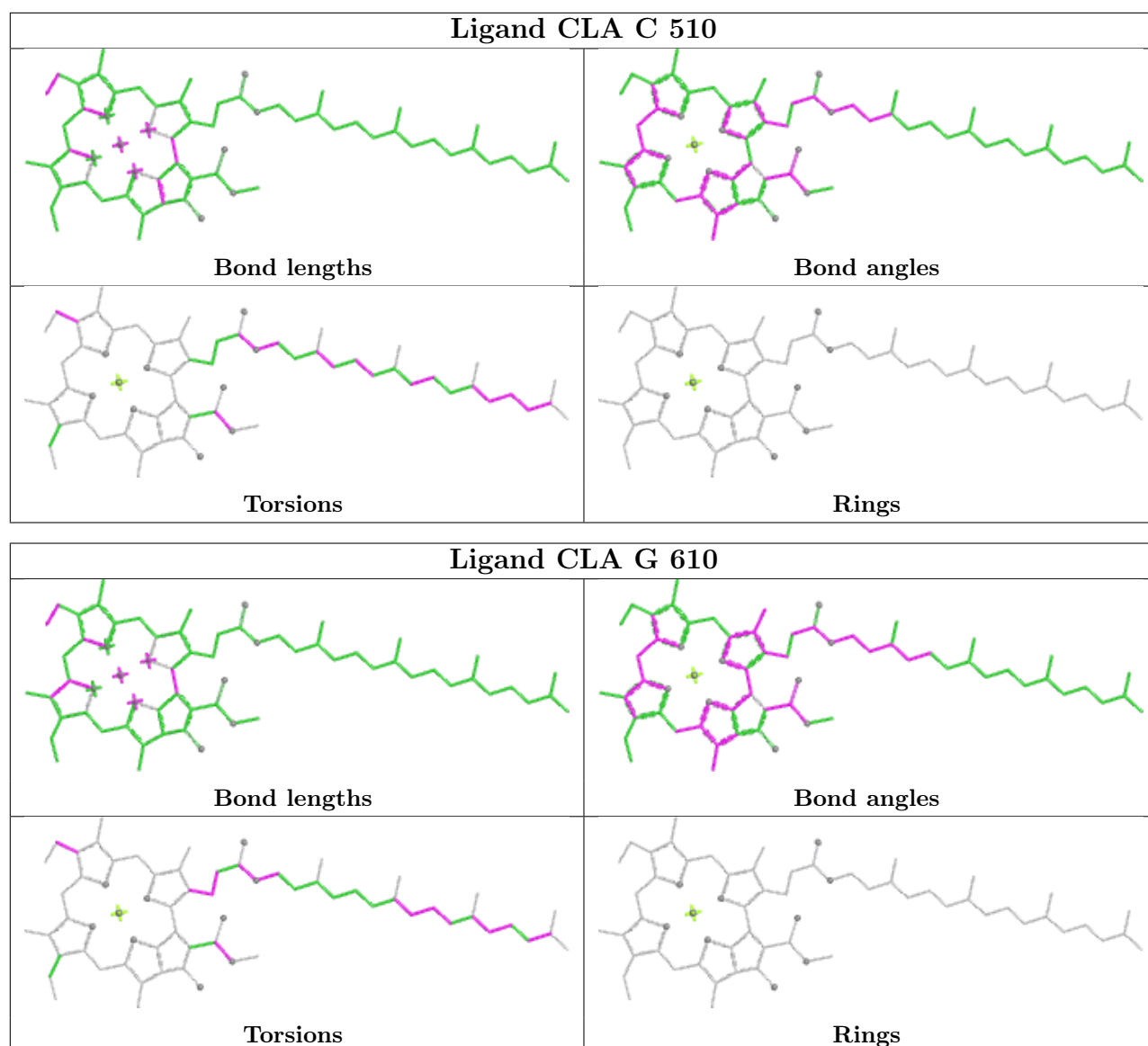
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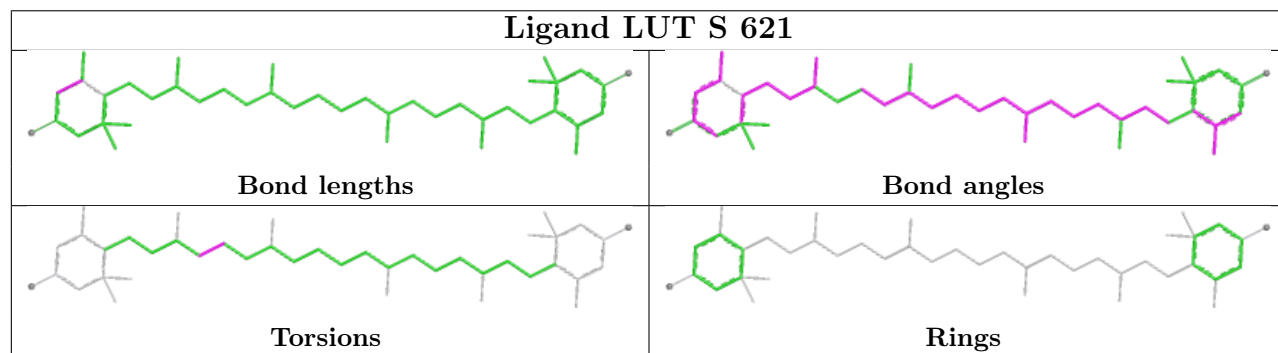
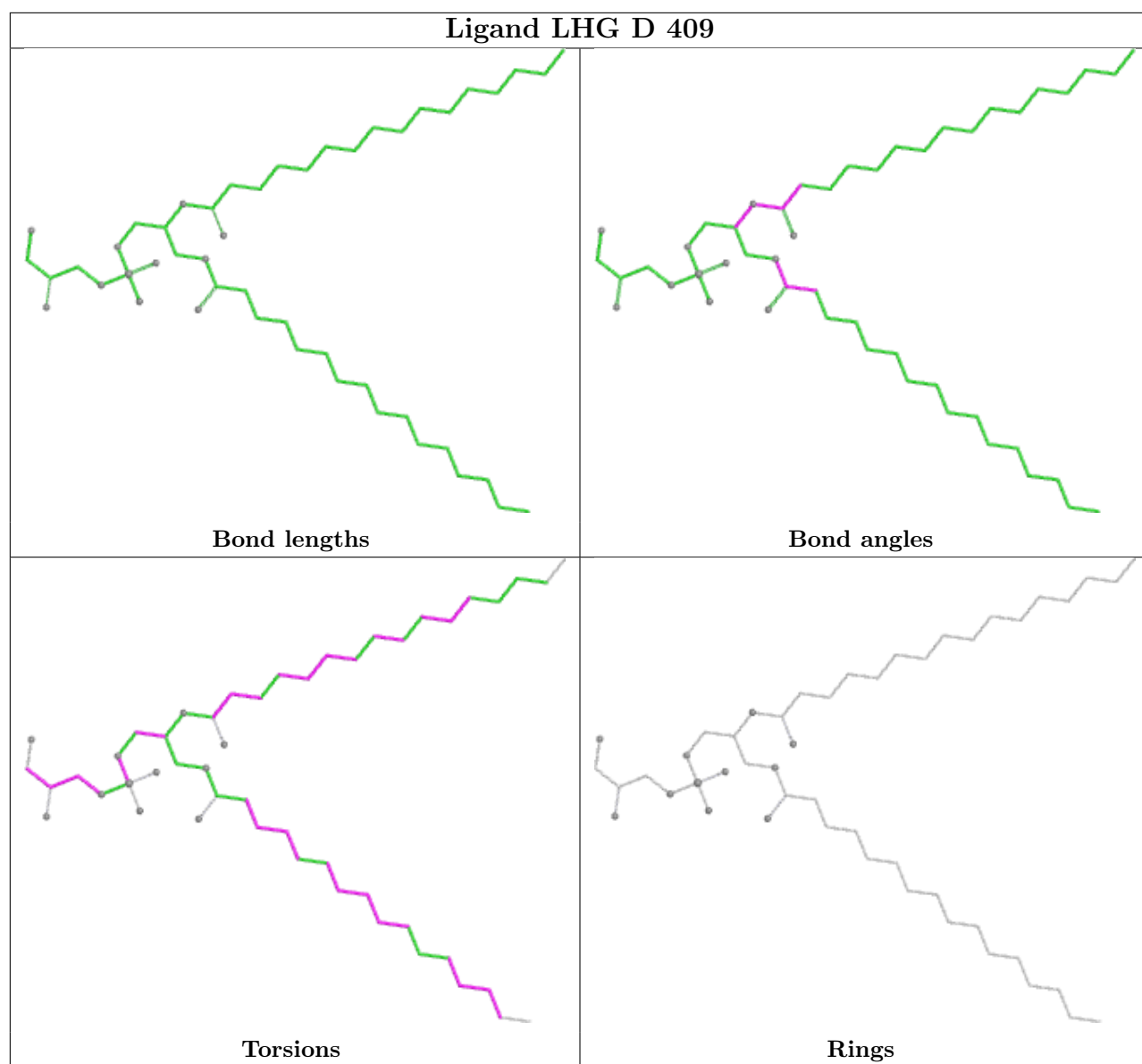




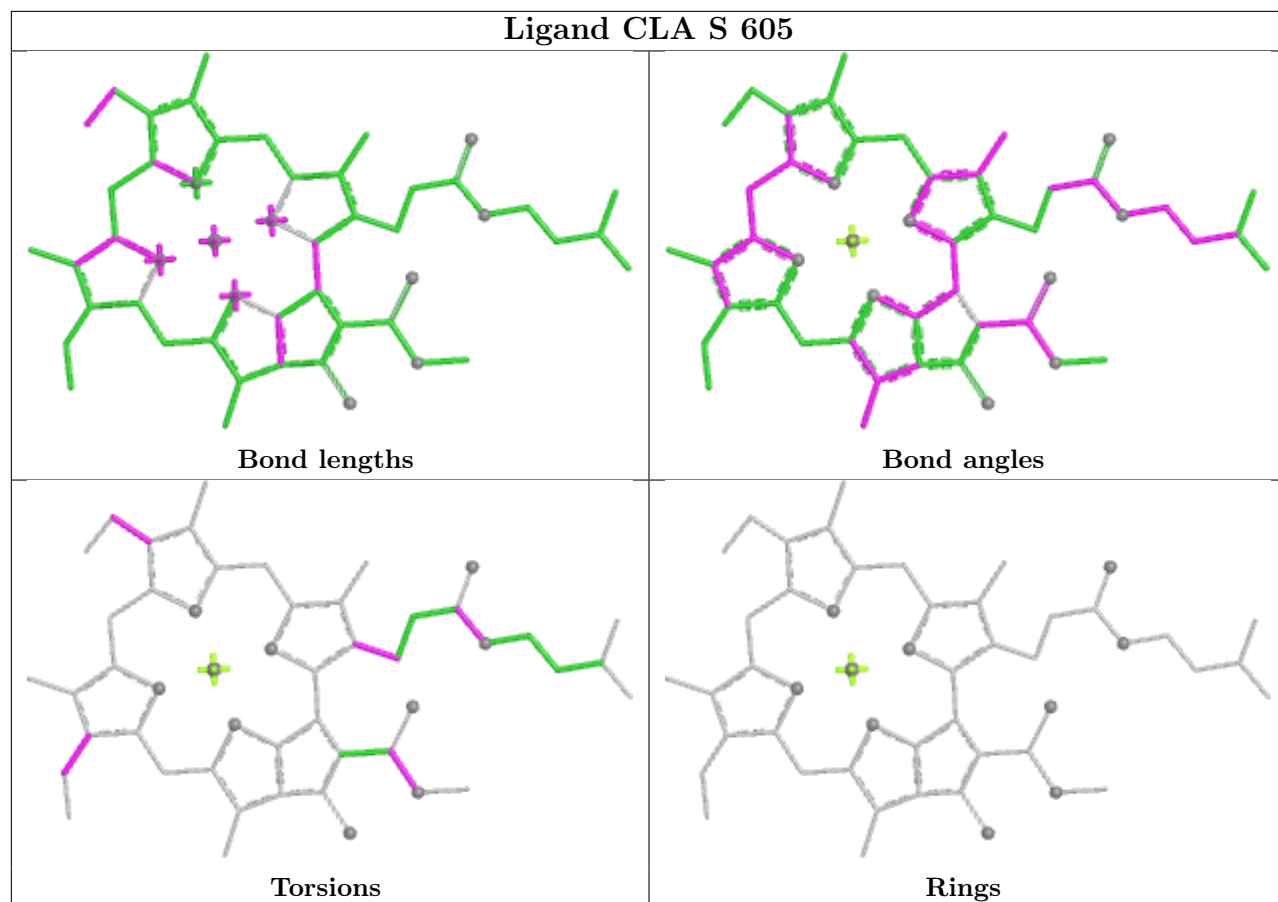


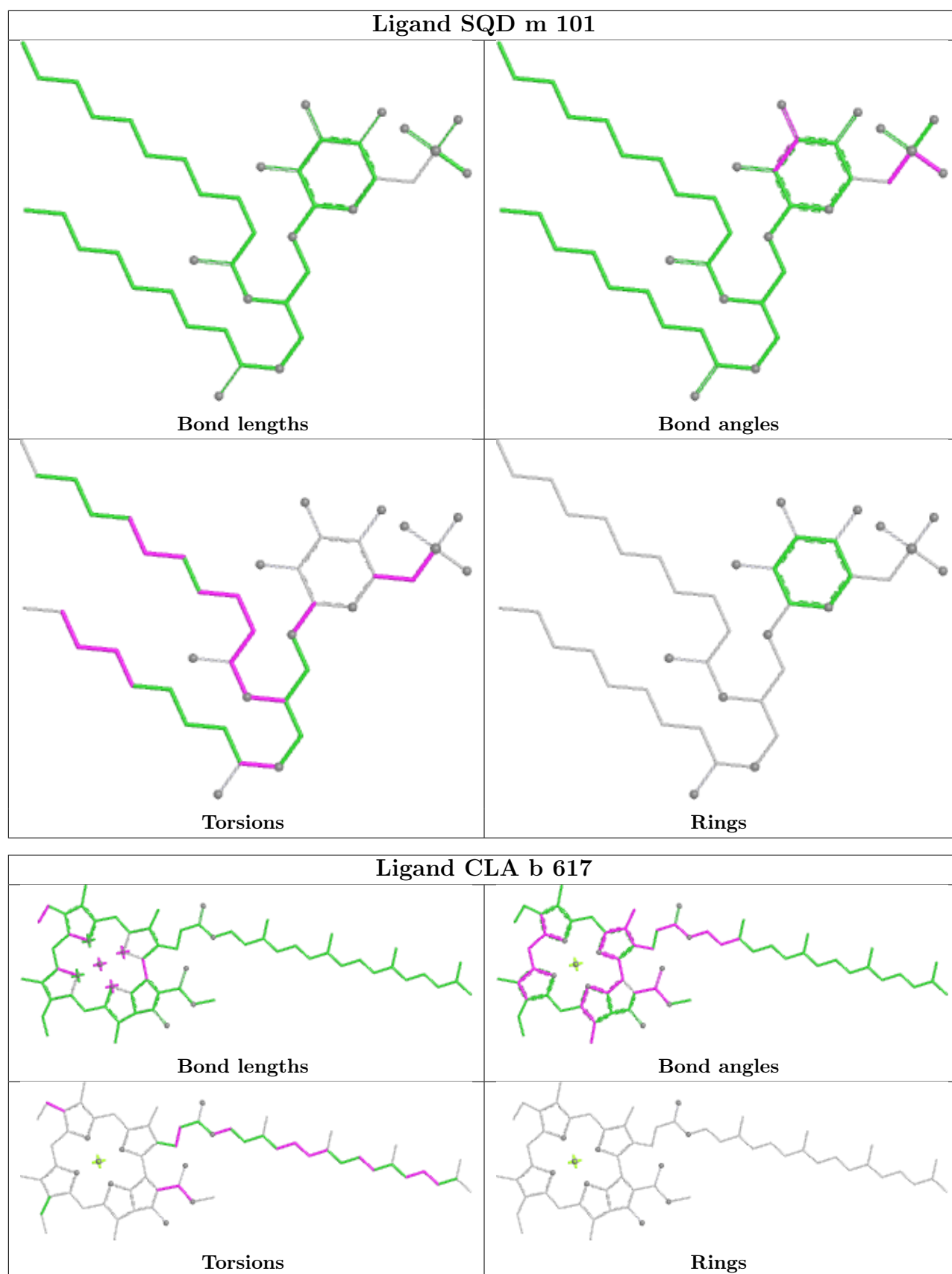




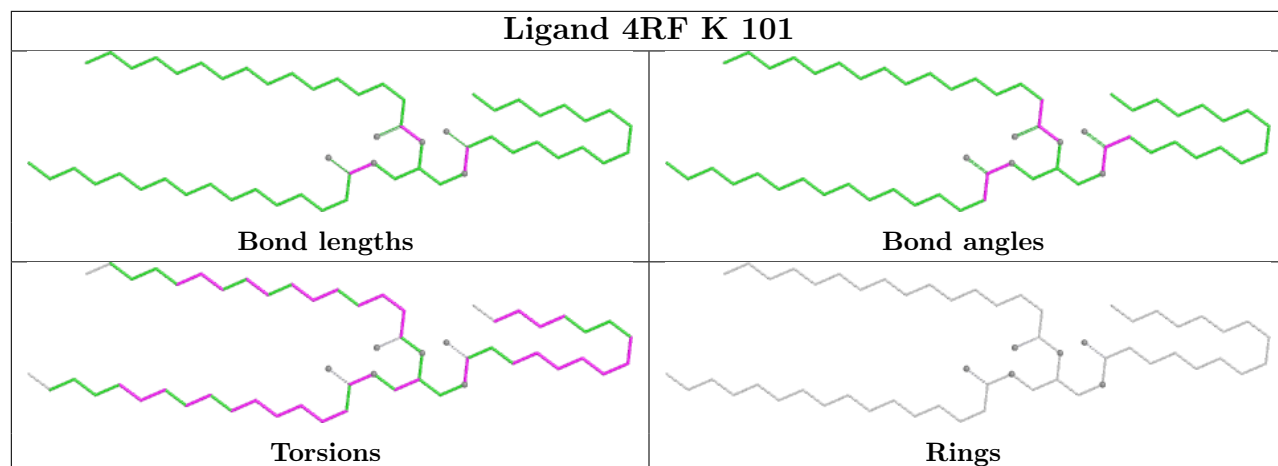


Ligand CLA S 605

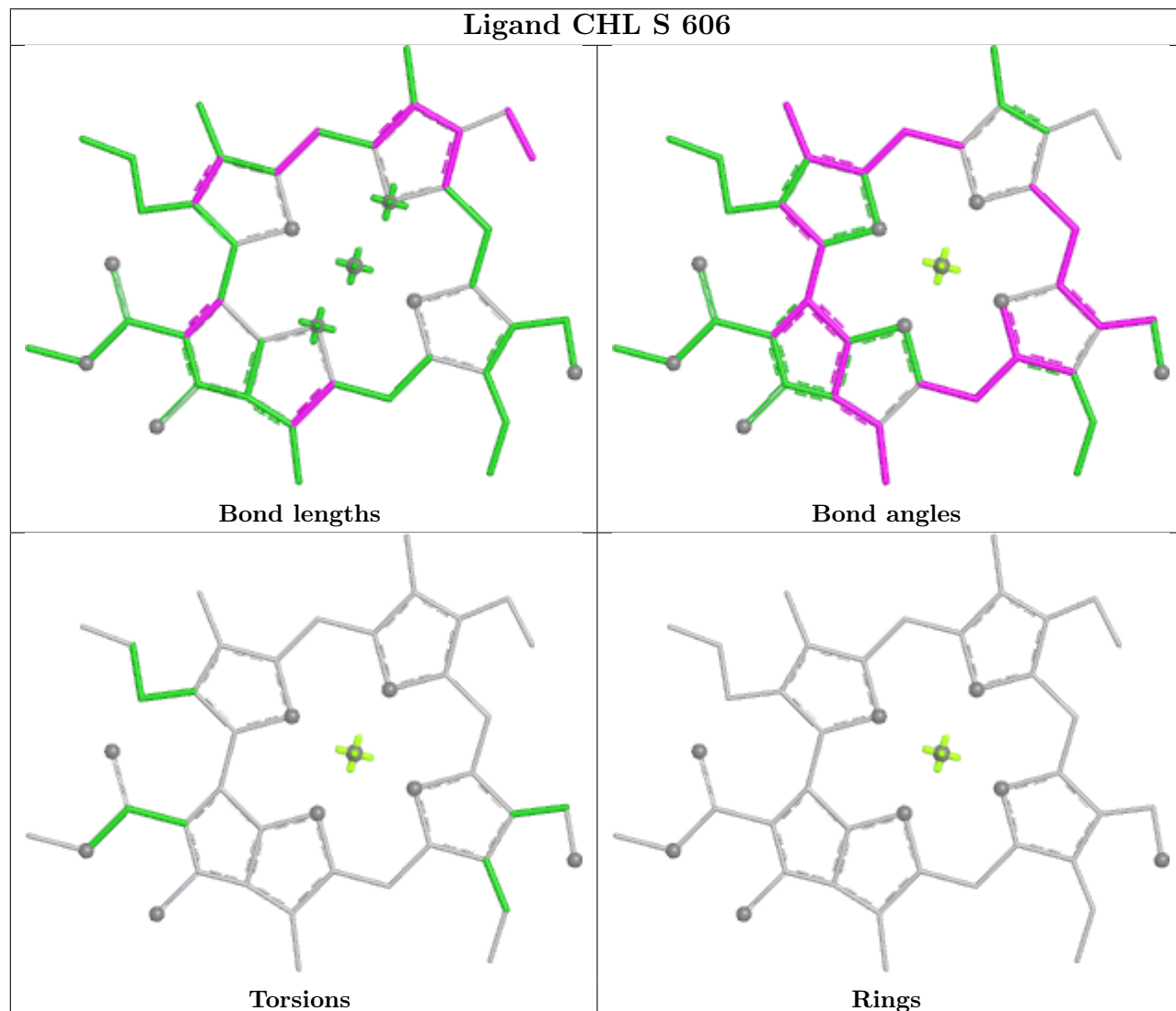


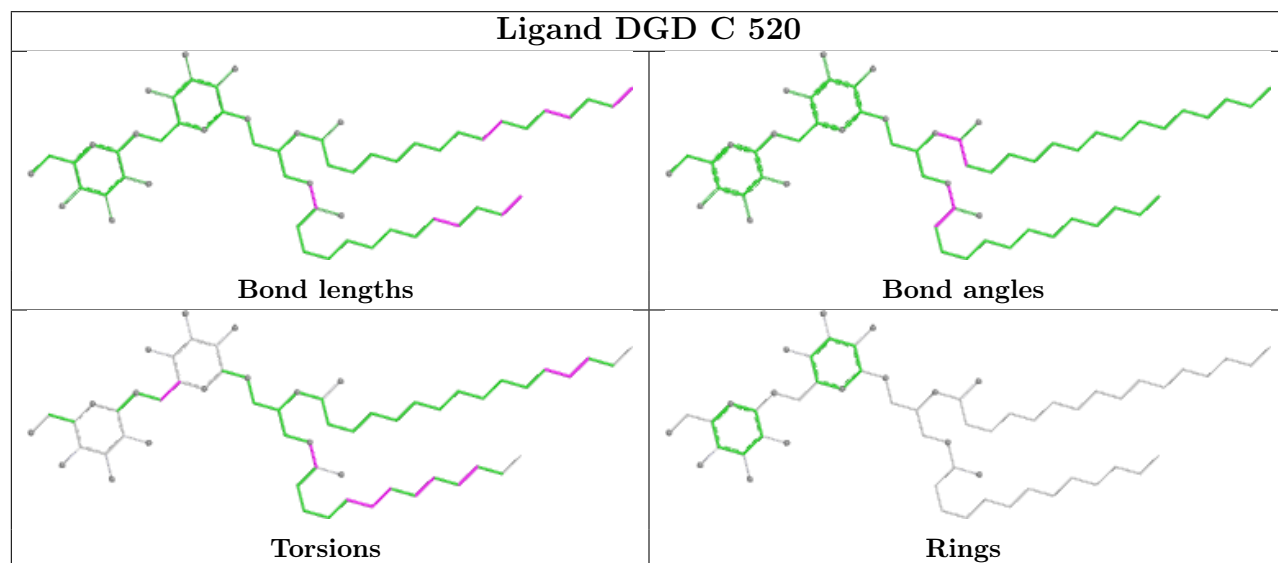
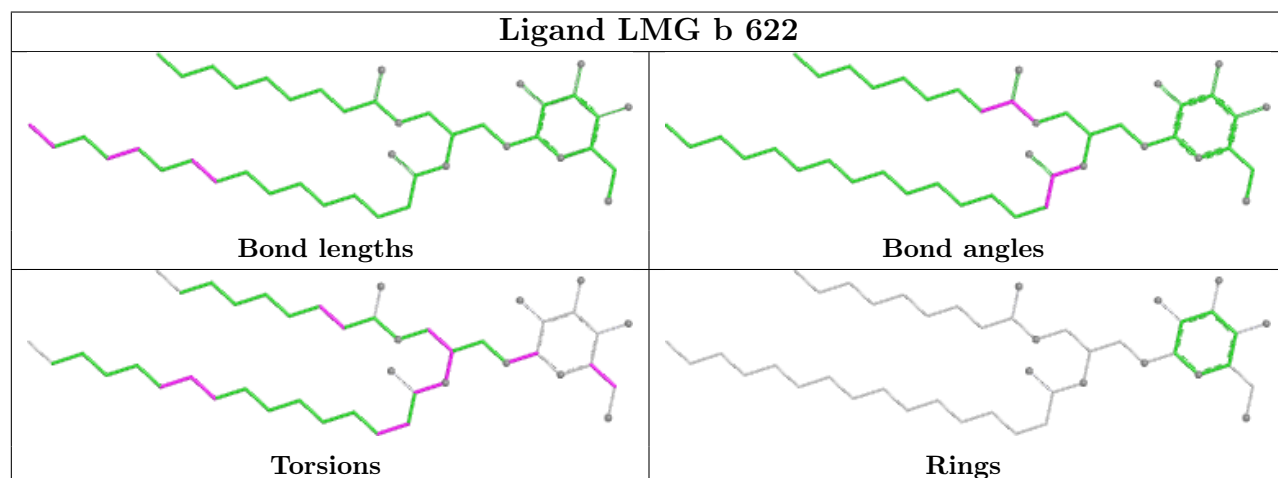
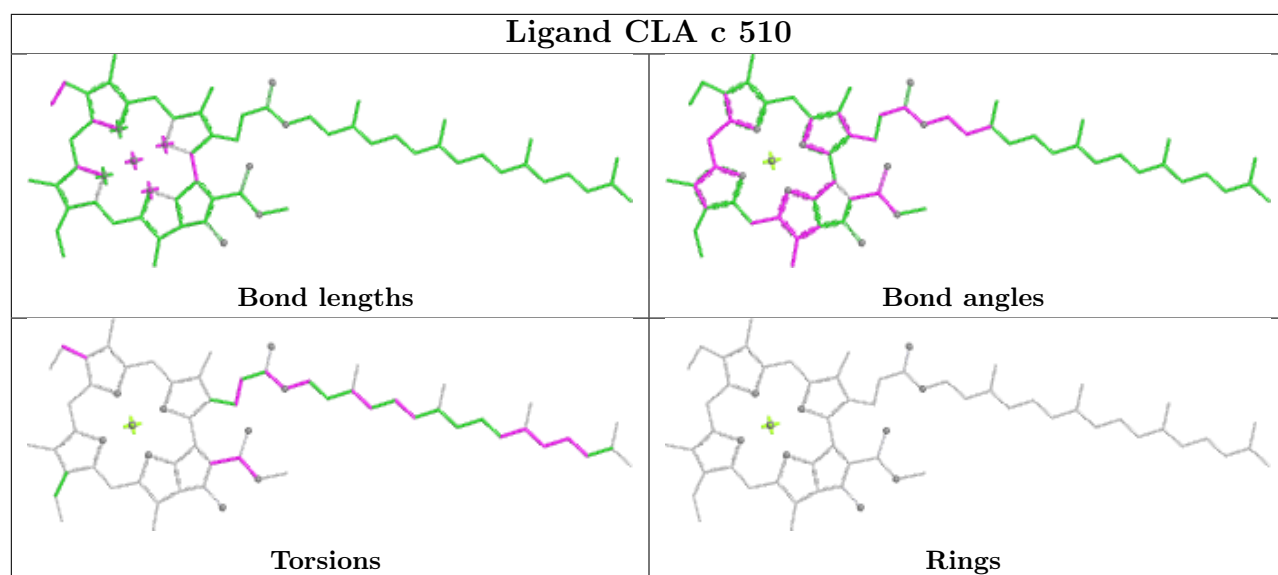


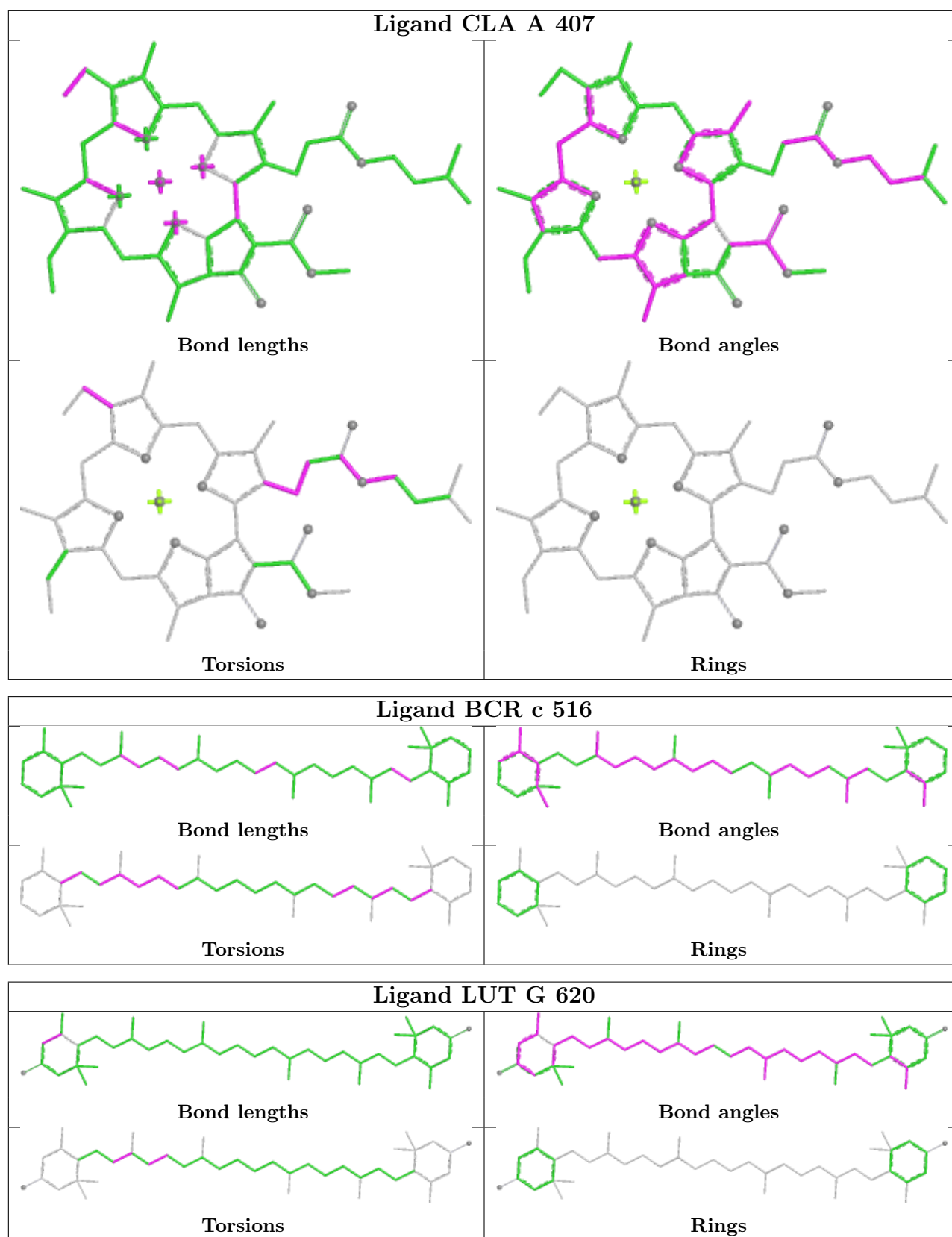
Ligand 4RF K 101

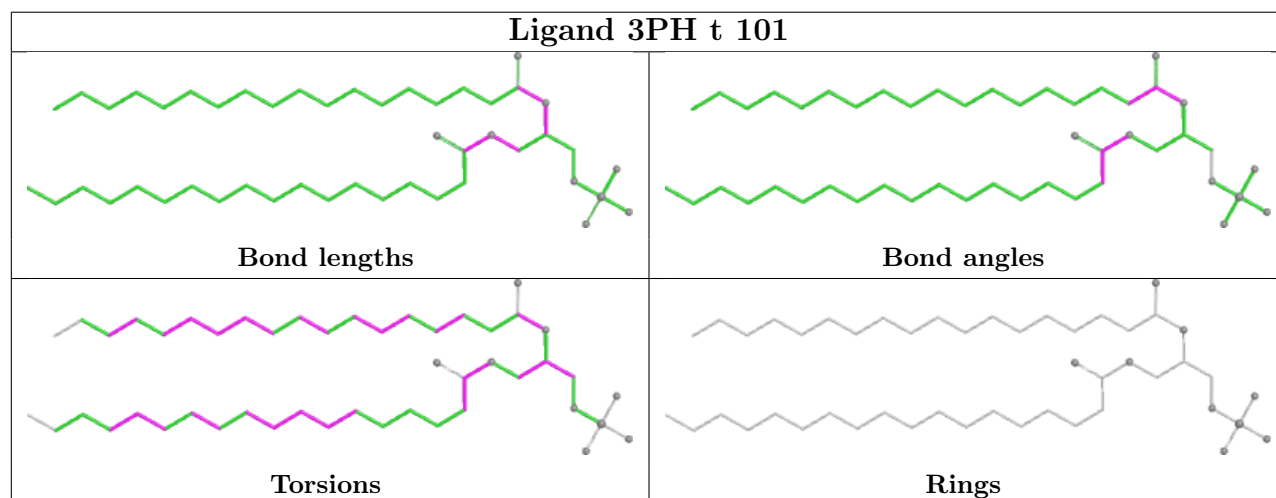
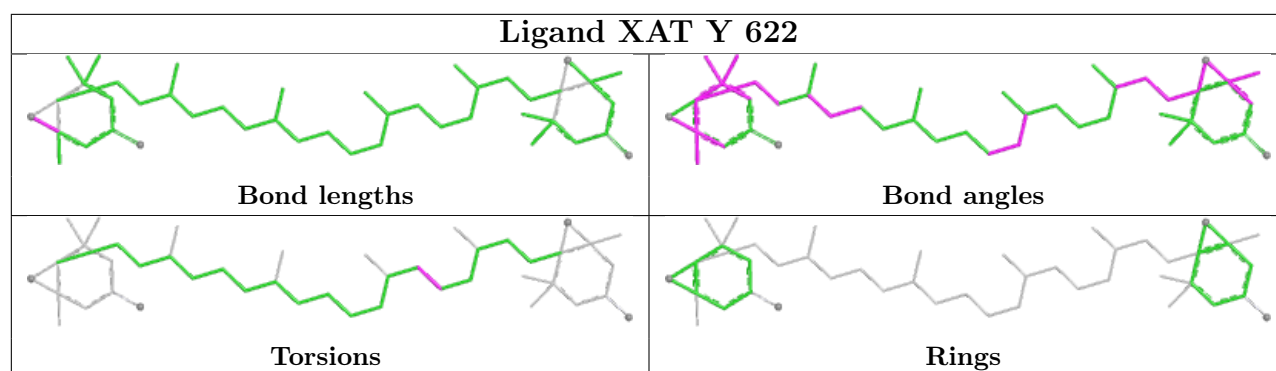


Ligand CHL S 606

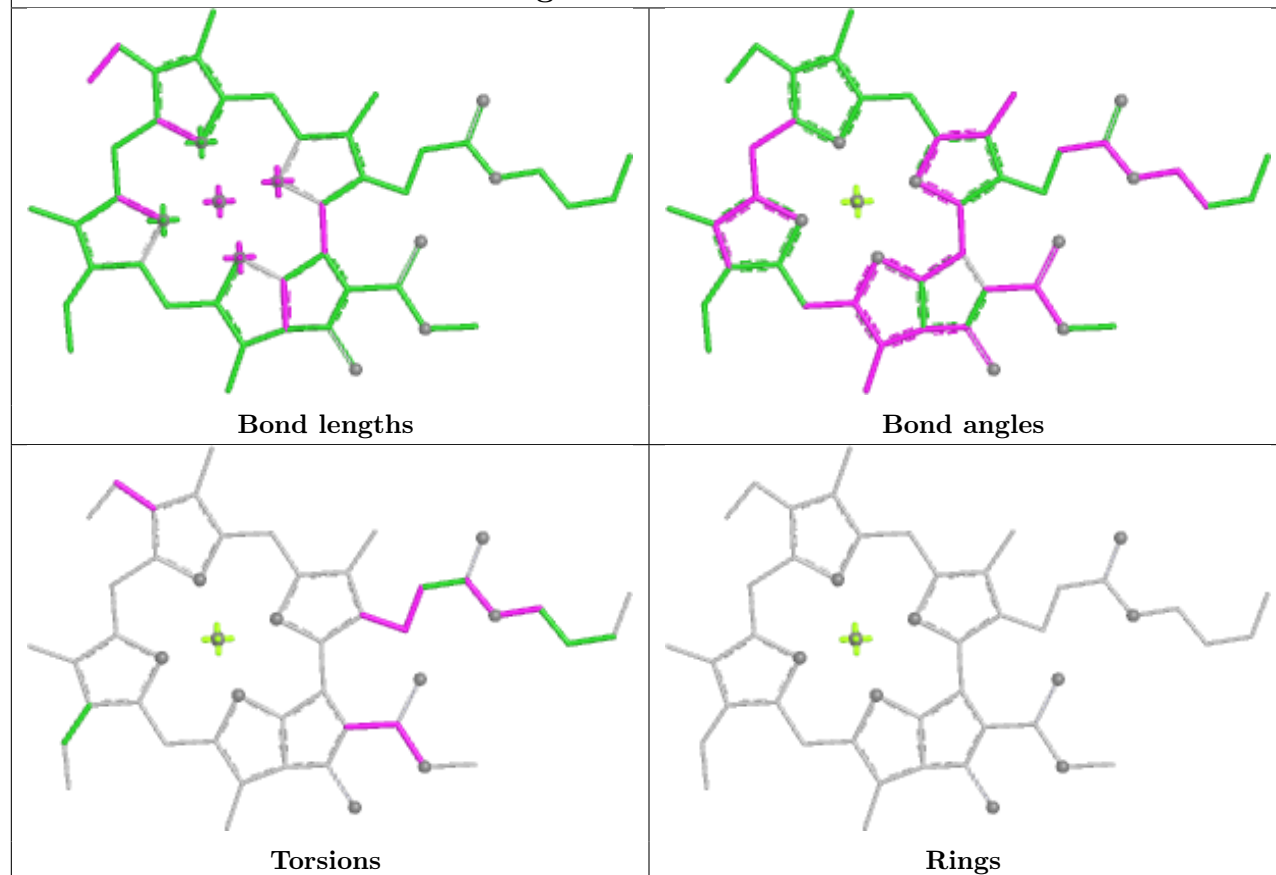




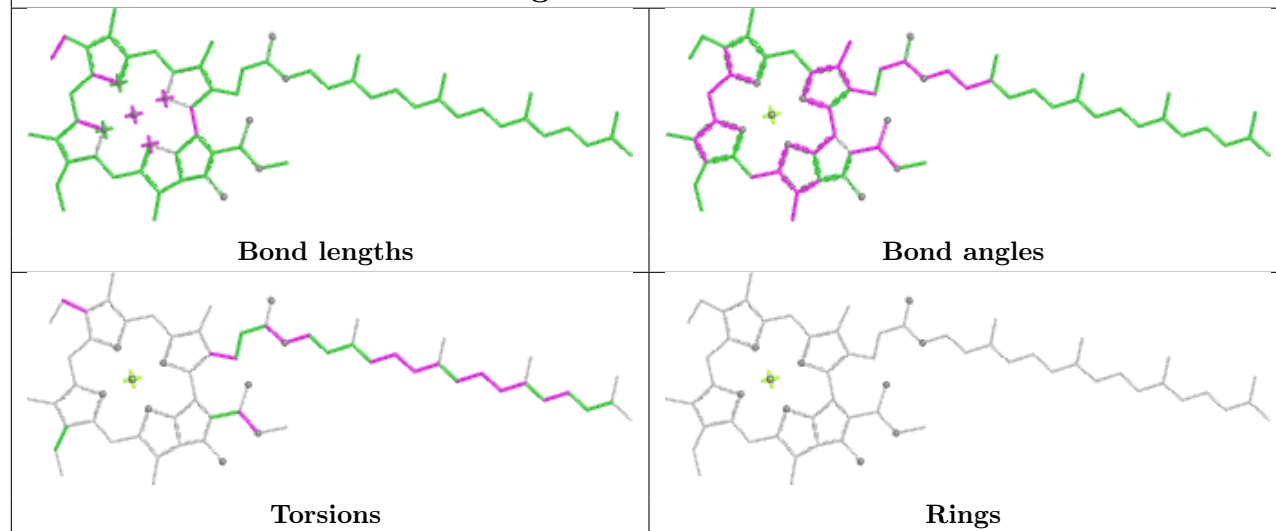


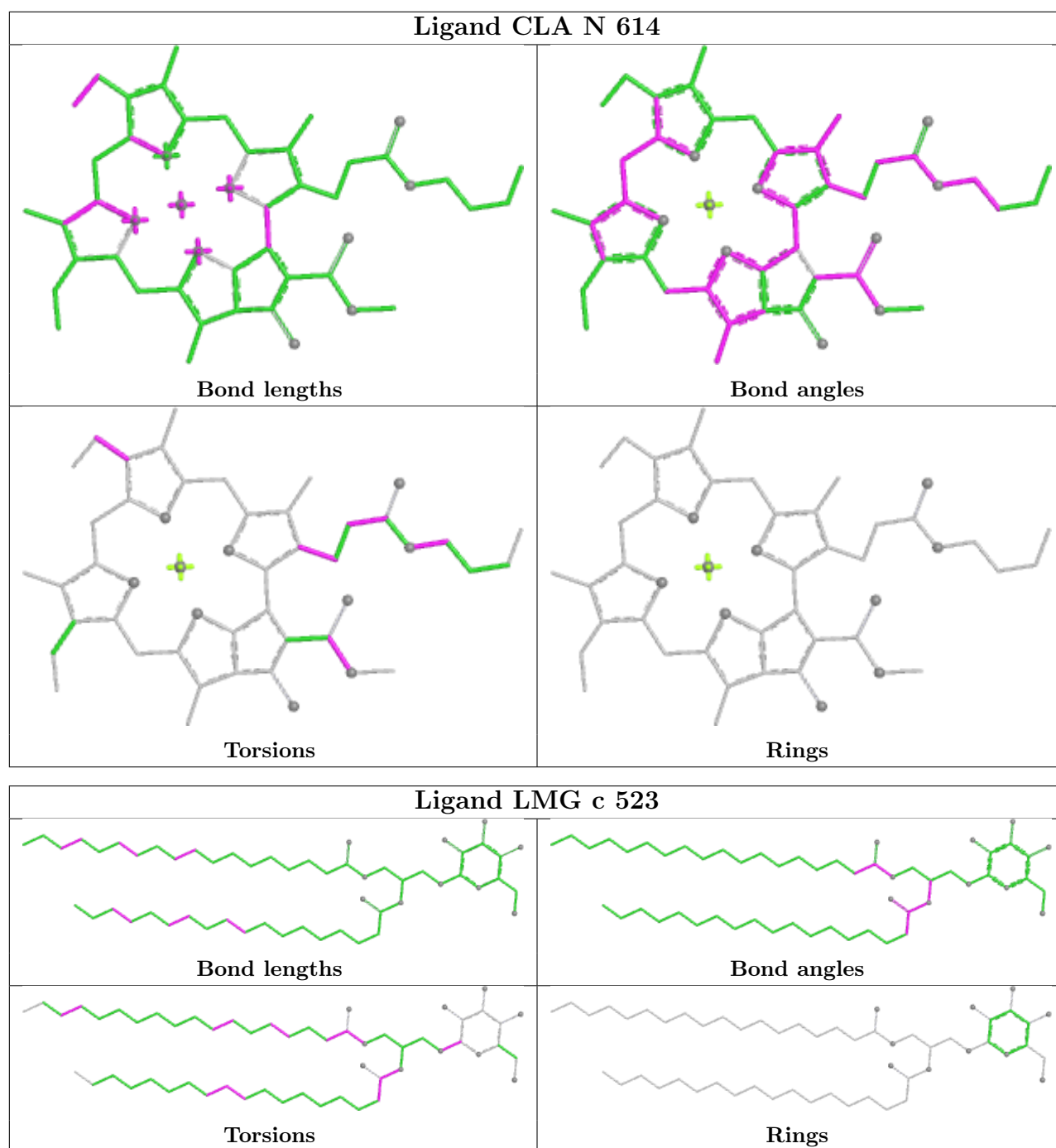


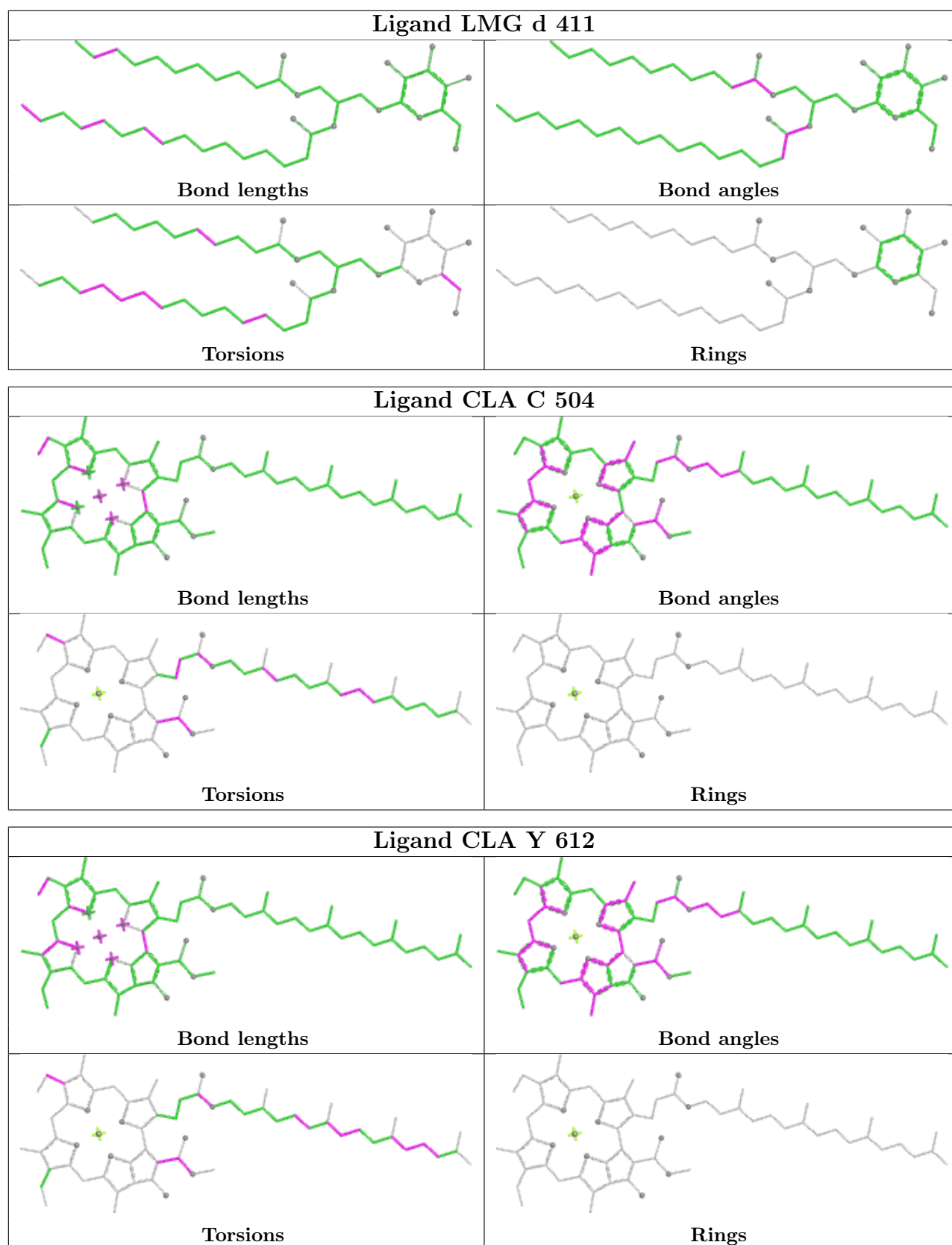
Ligand CLA a 407

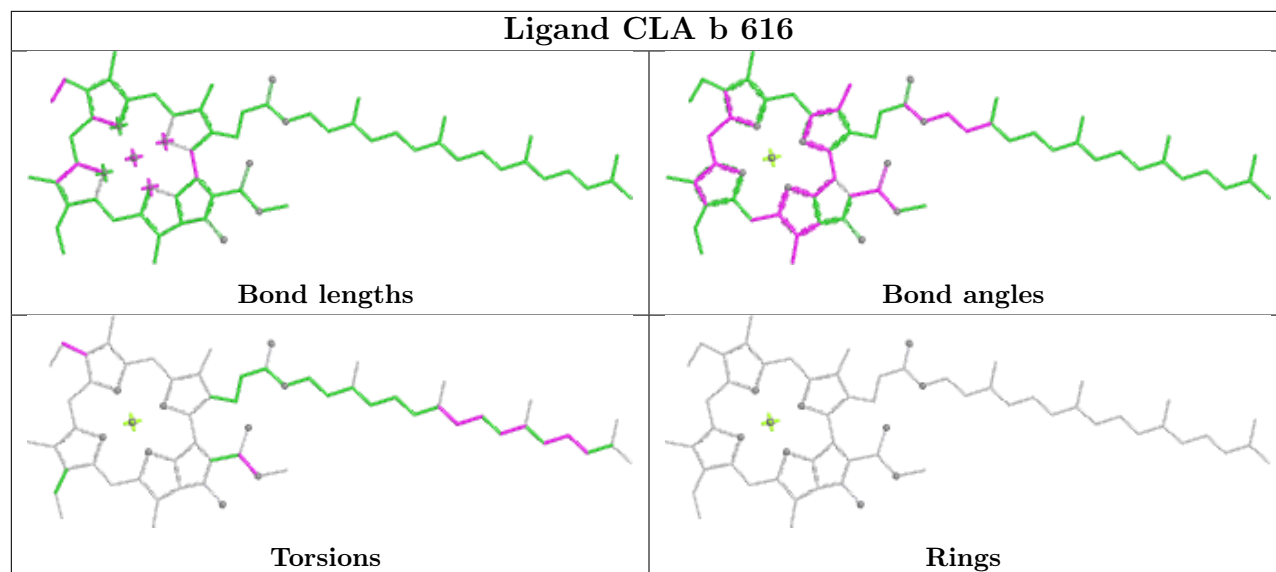
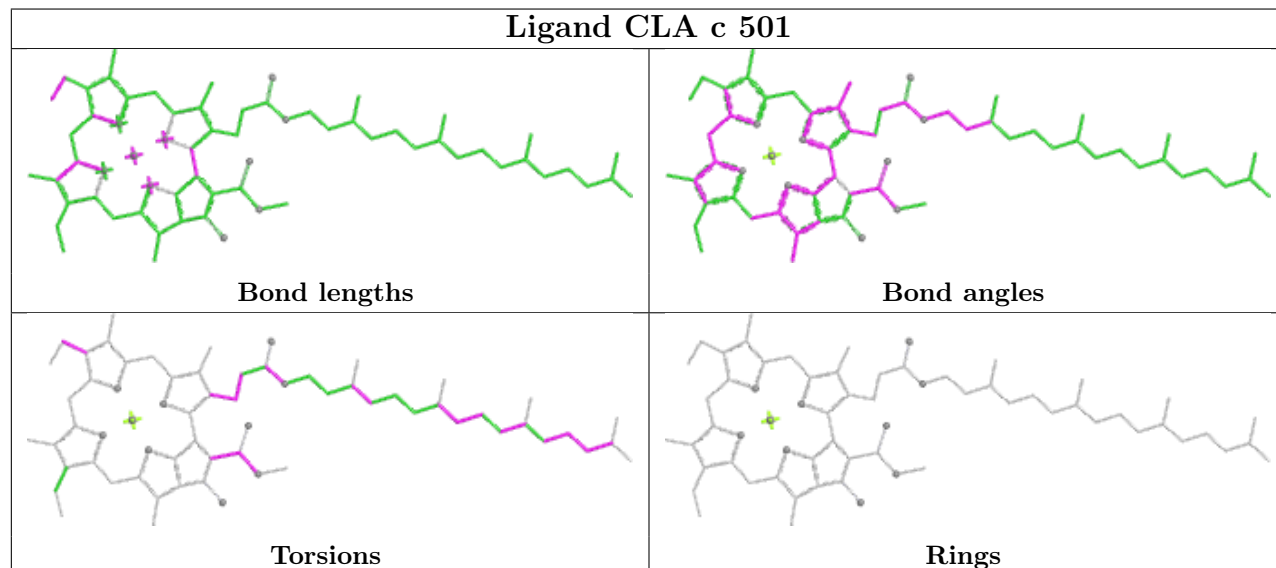


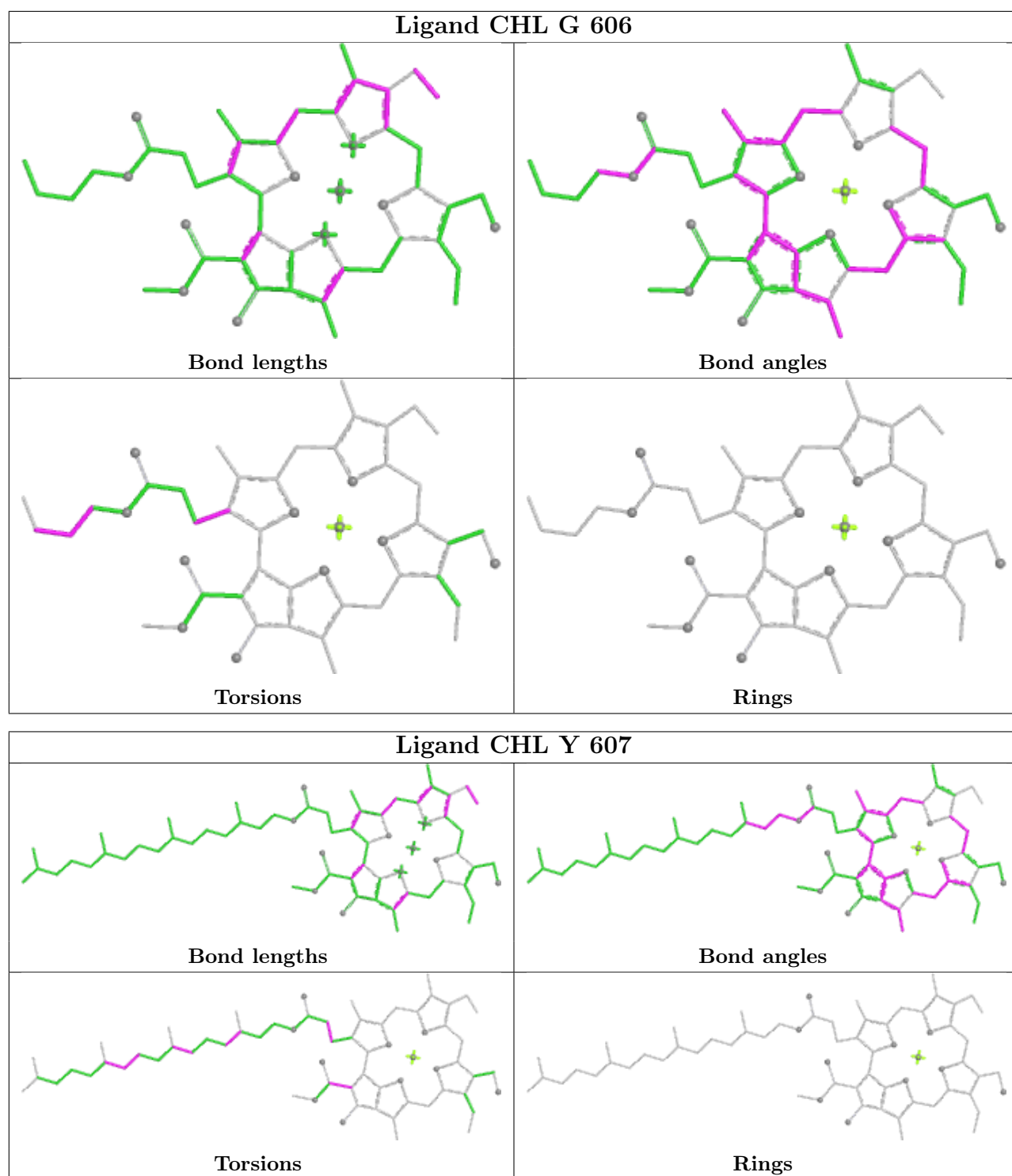
Ligand CLA D 403

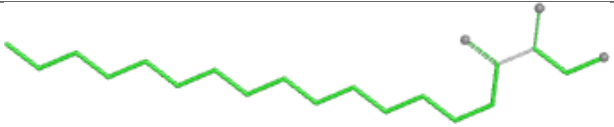
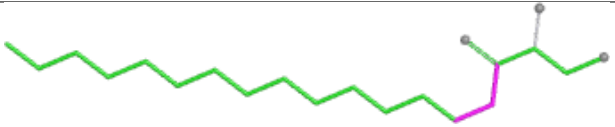
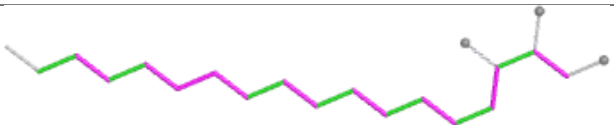
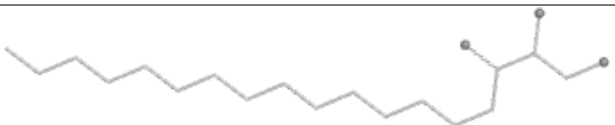
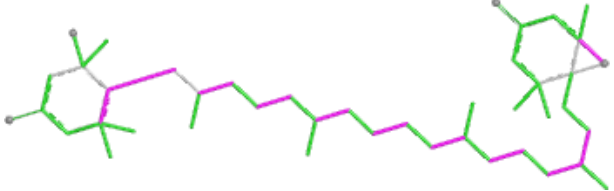
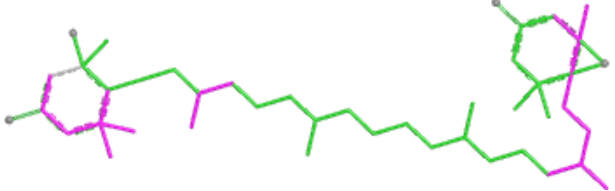
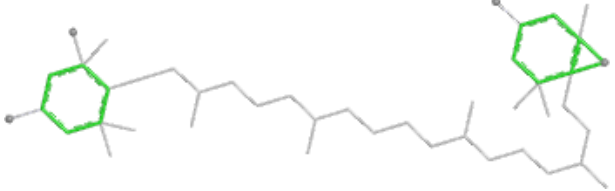
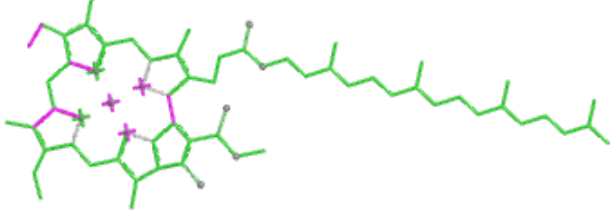
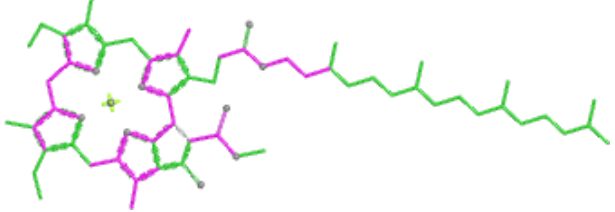
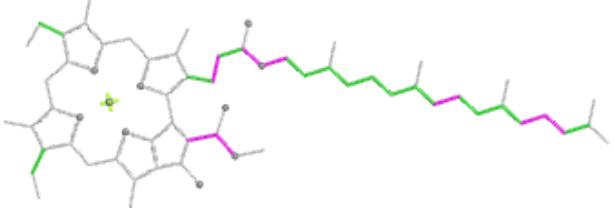
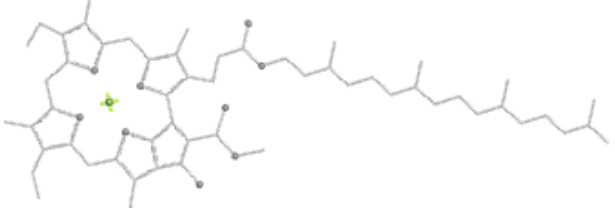


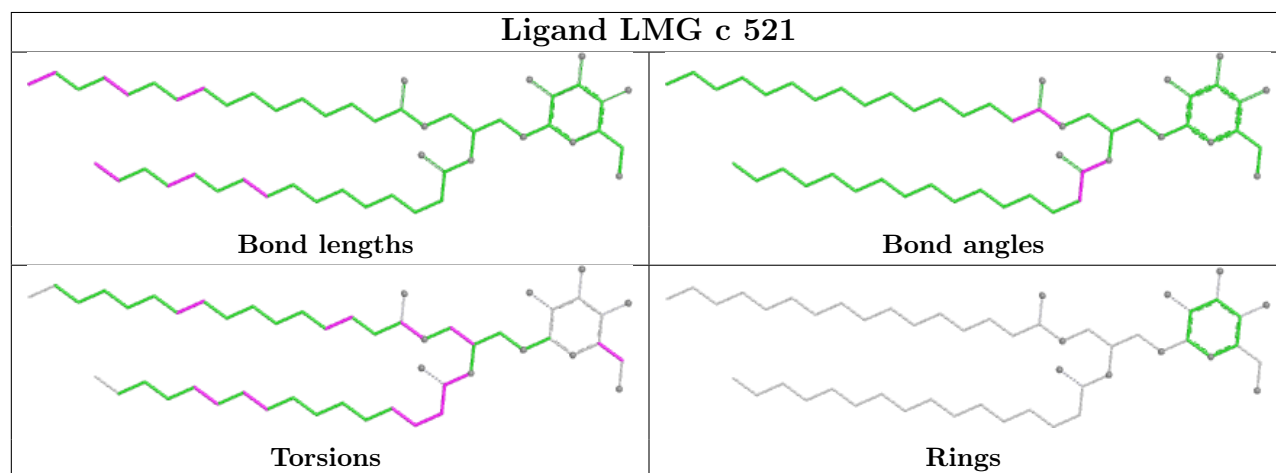
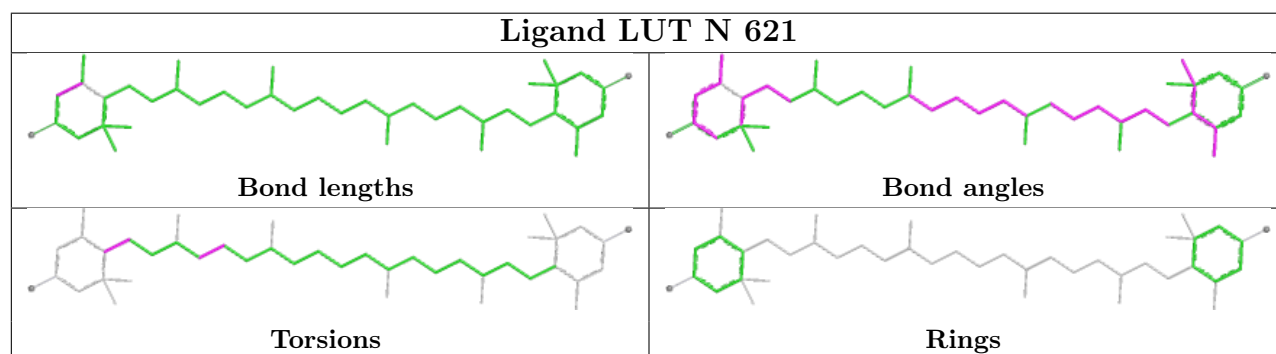
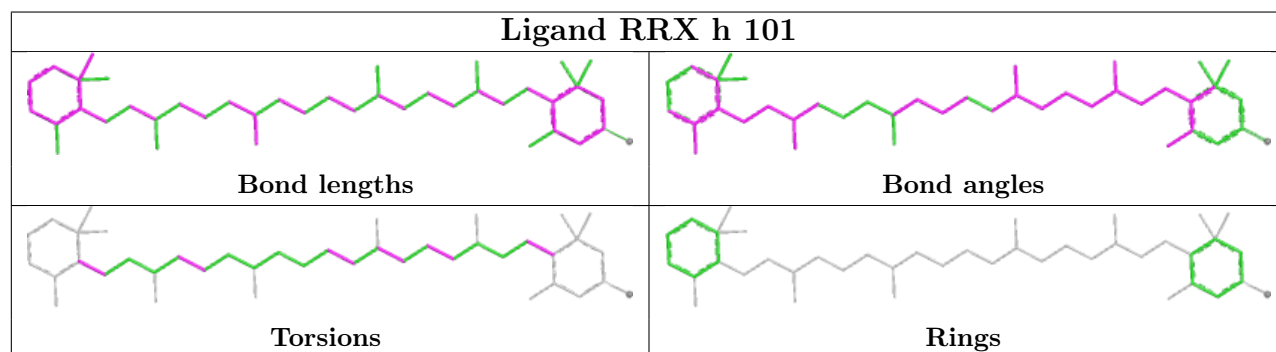
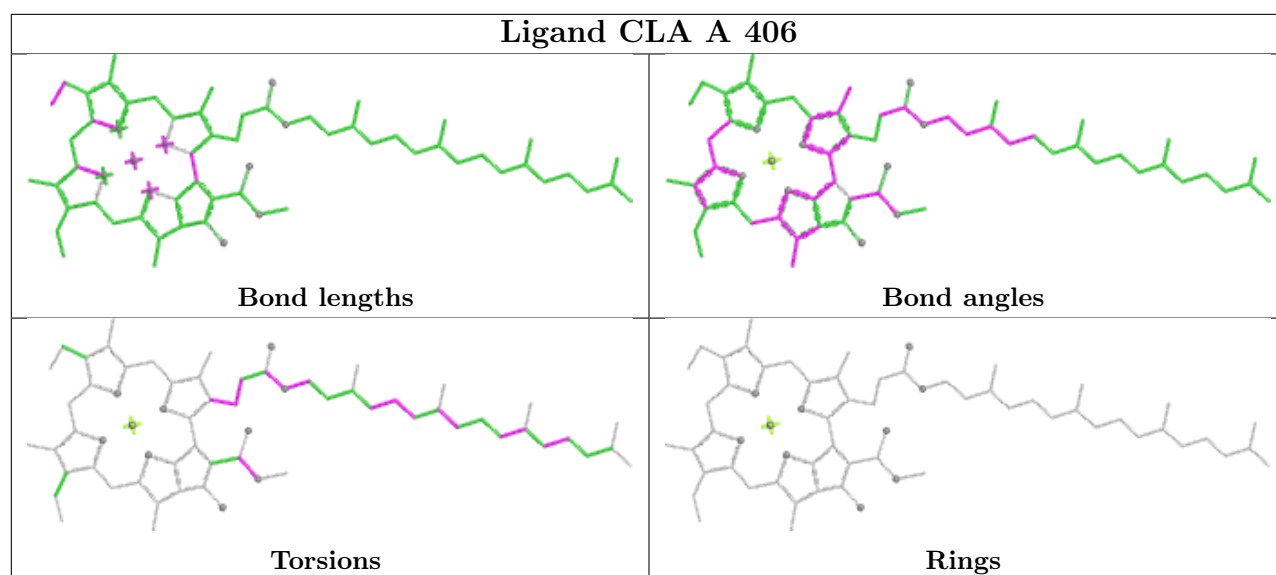


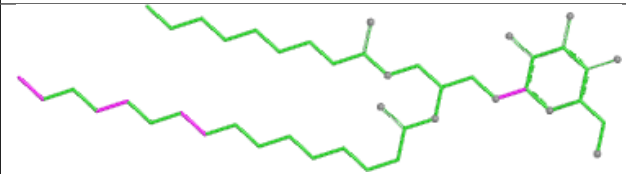
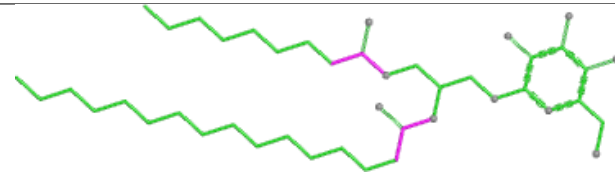
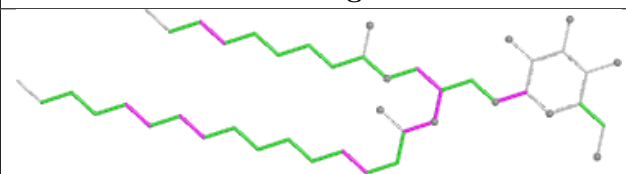
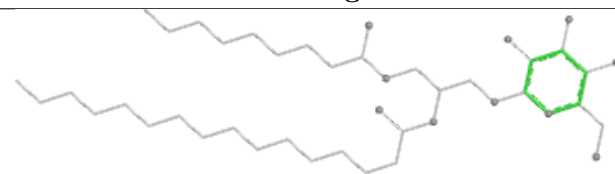
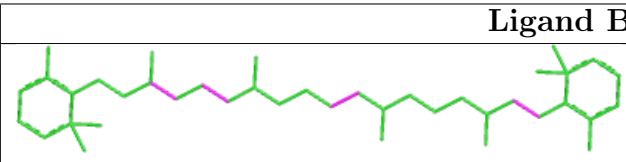
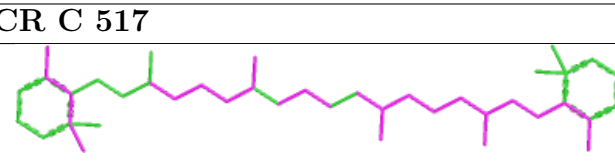
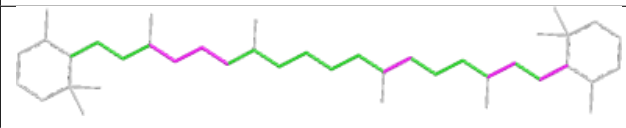
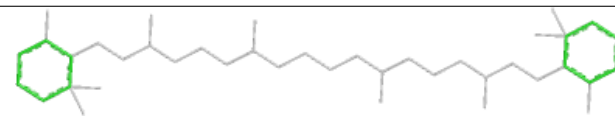
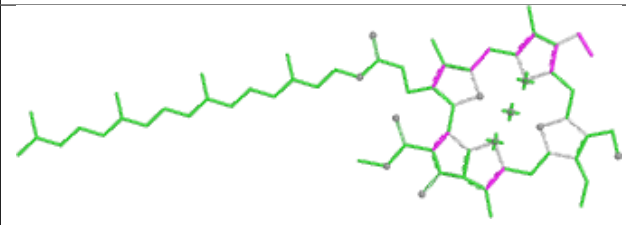
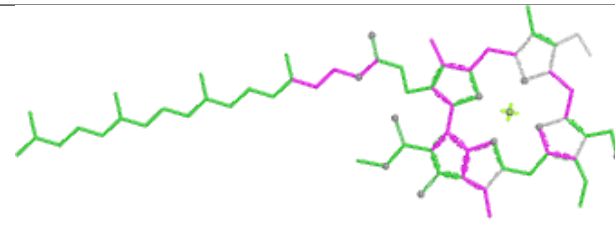
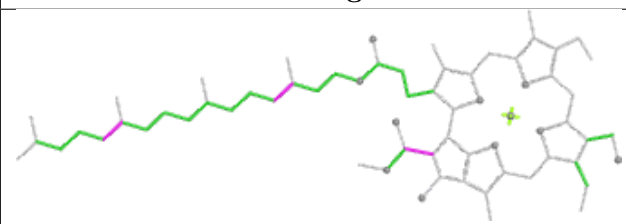
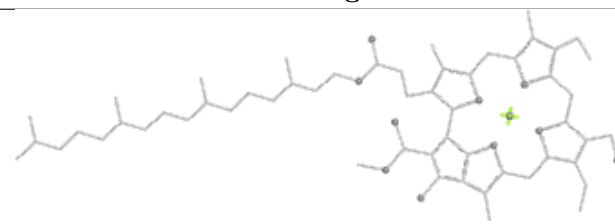
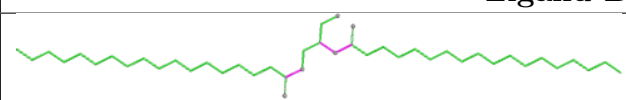
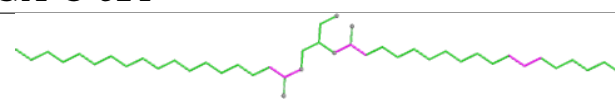
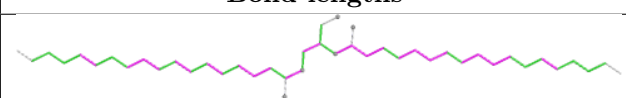
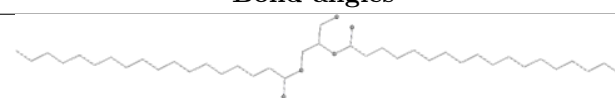


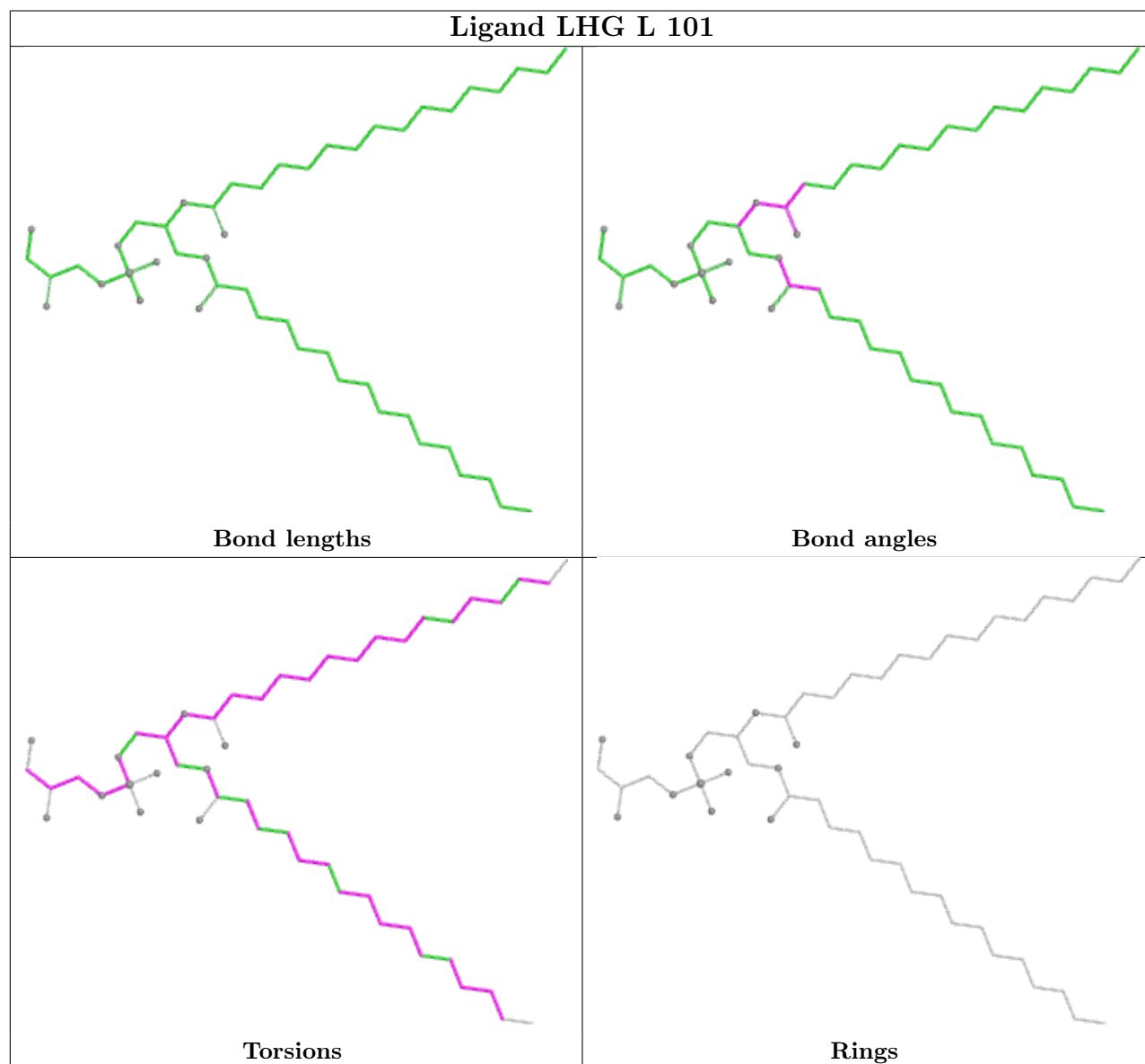
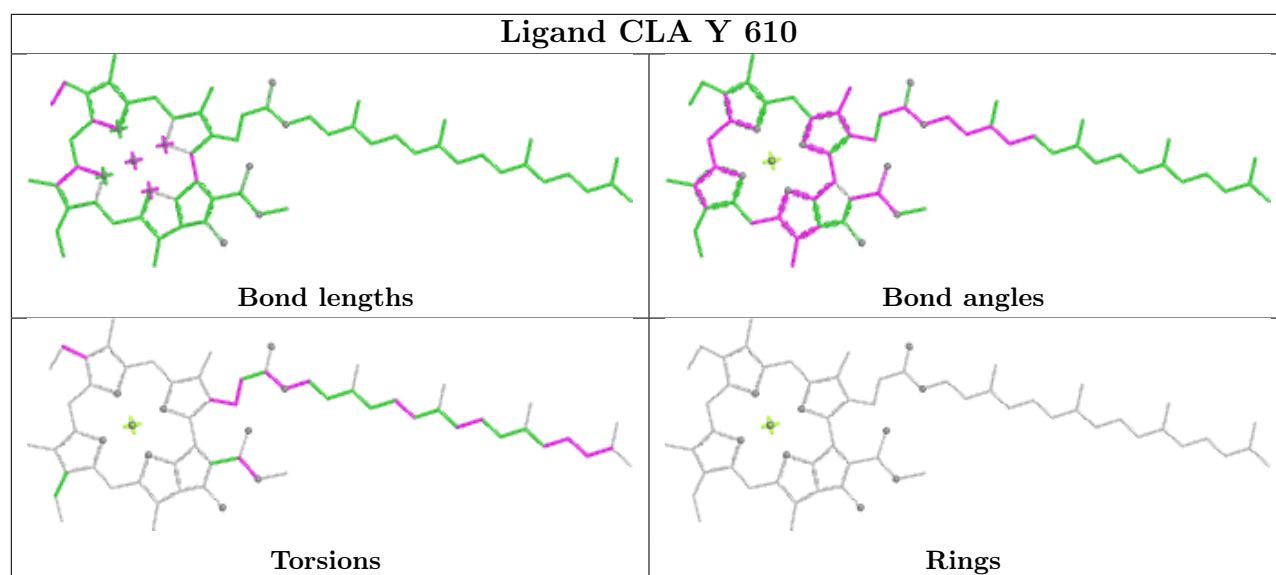
Ligand CLA b 616**Ligand CLA c 501**

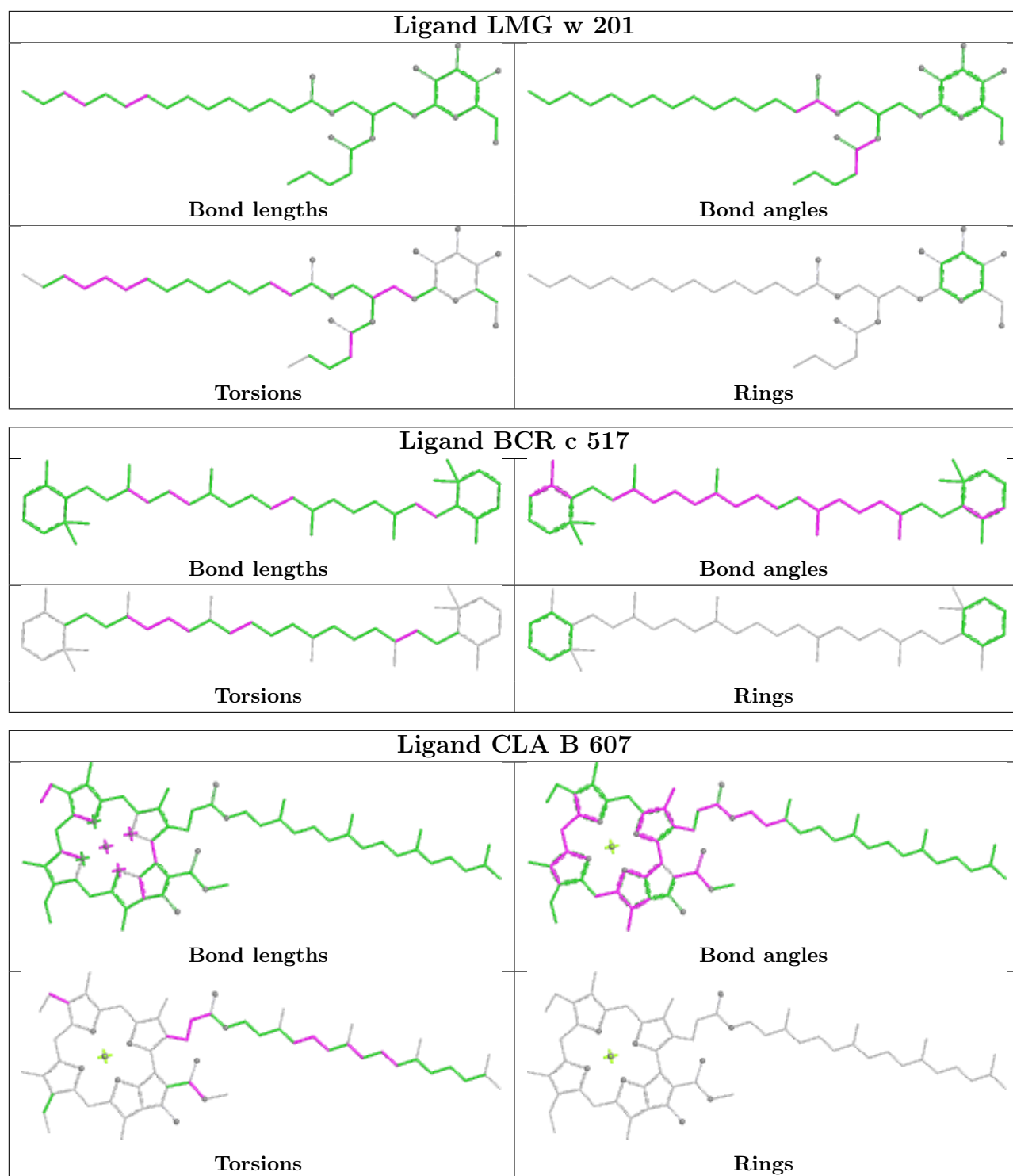


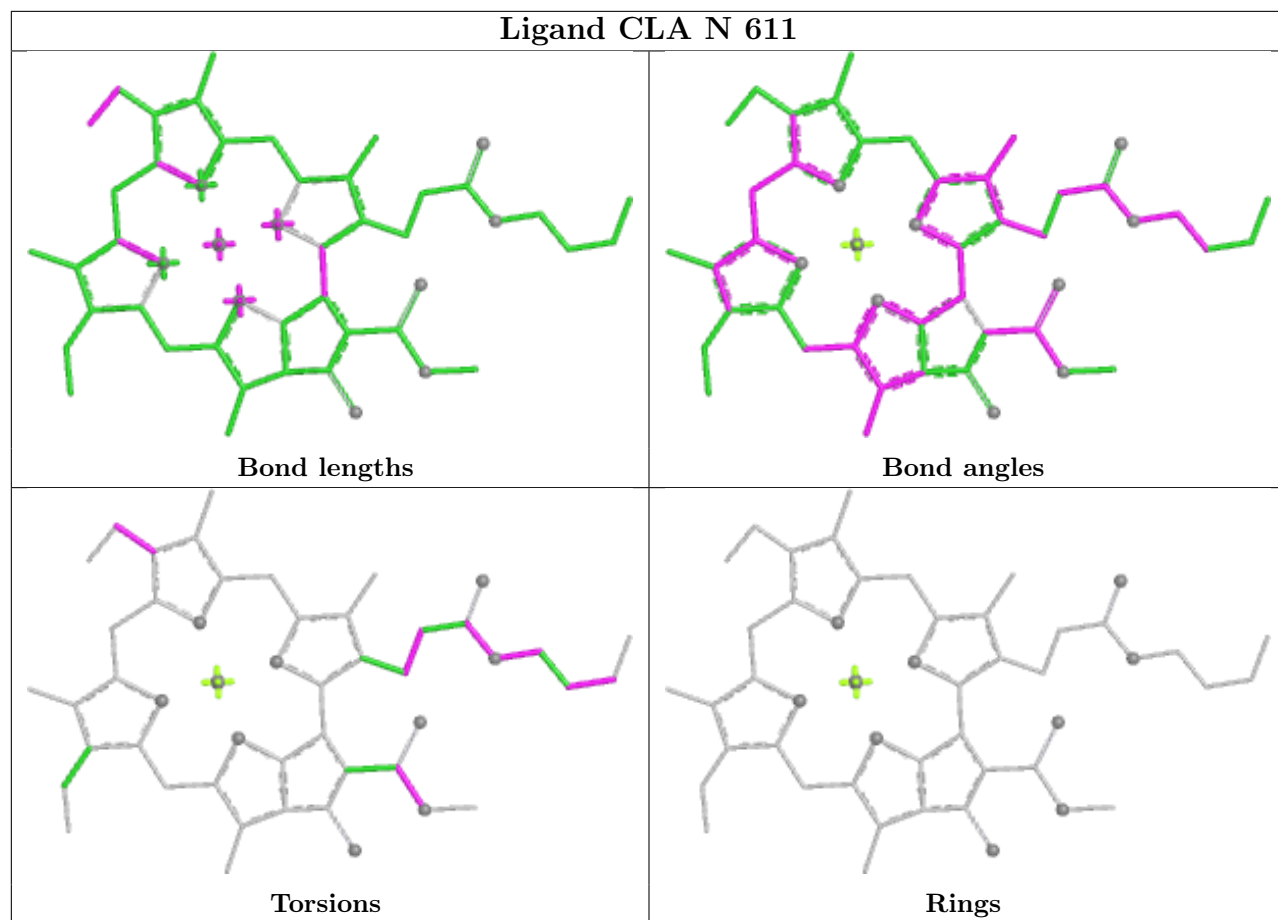
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand NEX S 623	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings



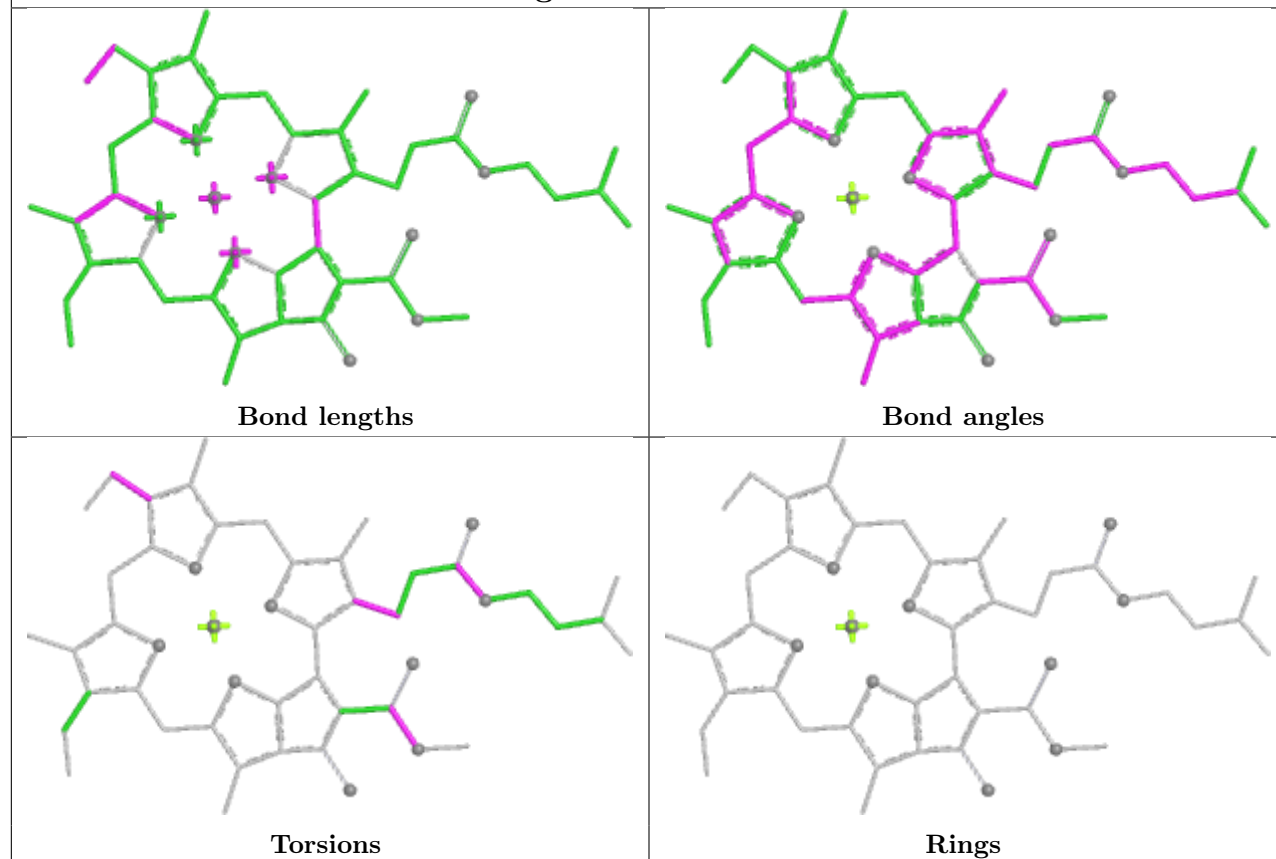
Ligand LMG B 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL N 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGA C 524	
 Bond lengths	 Bond angles
 Torsions	 Rings



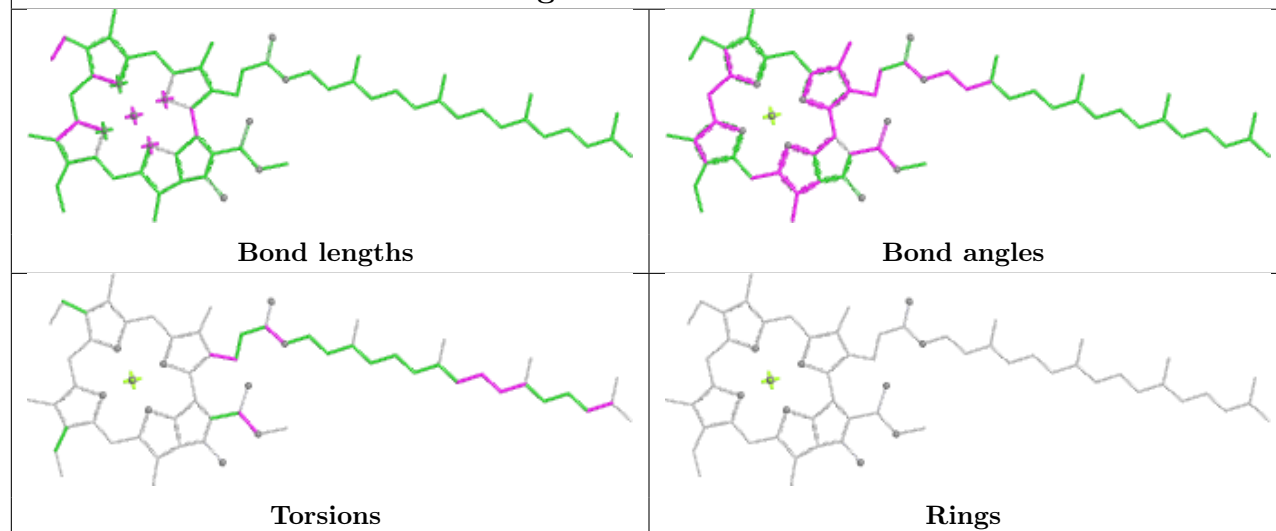


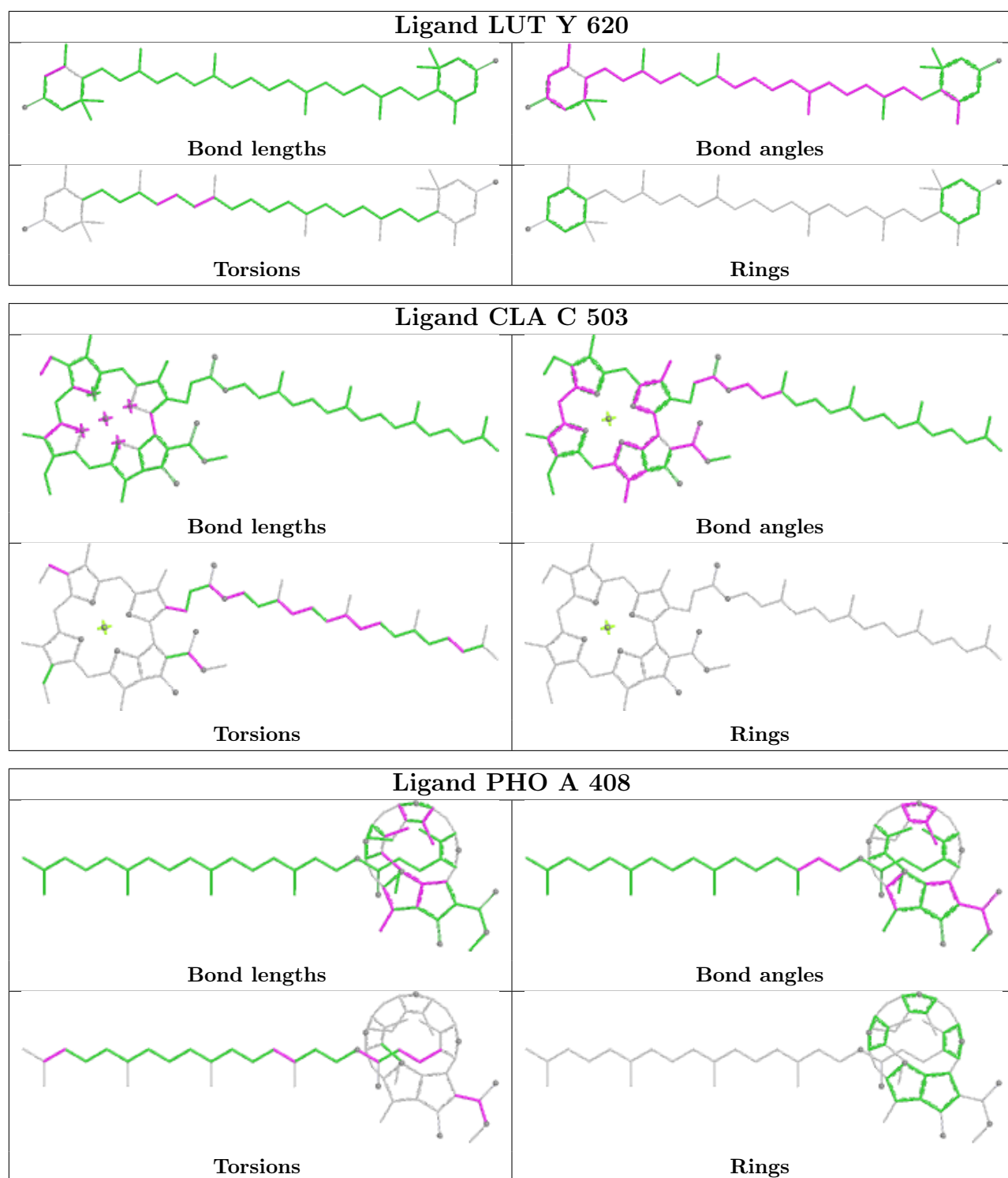


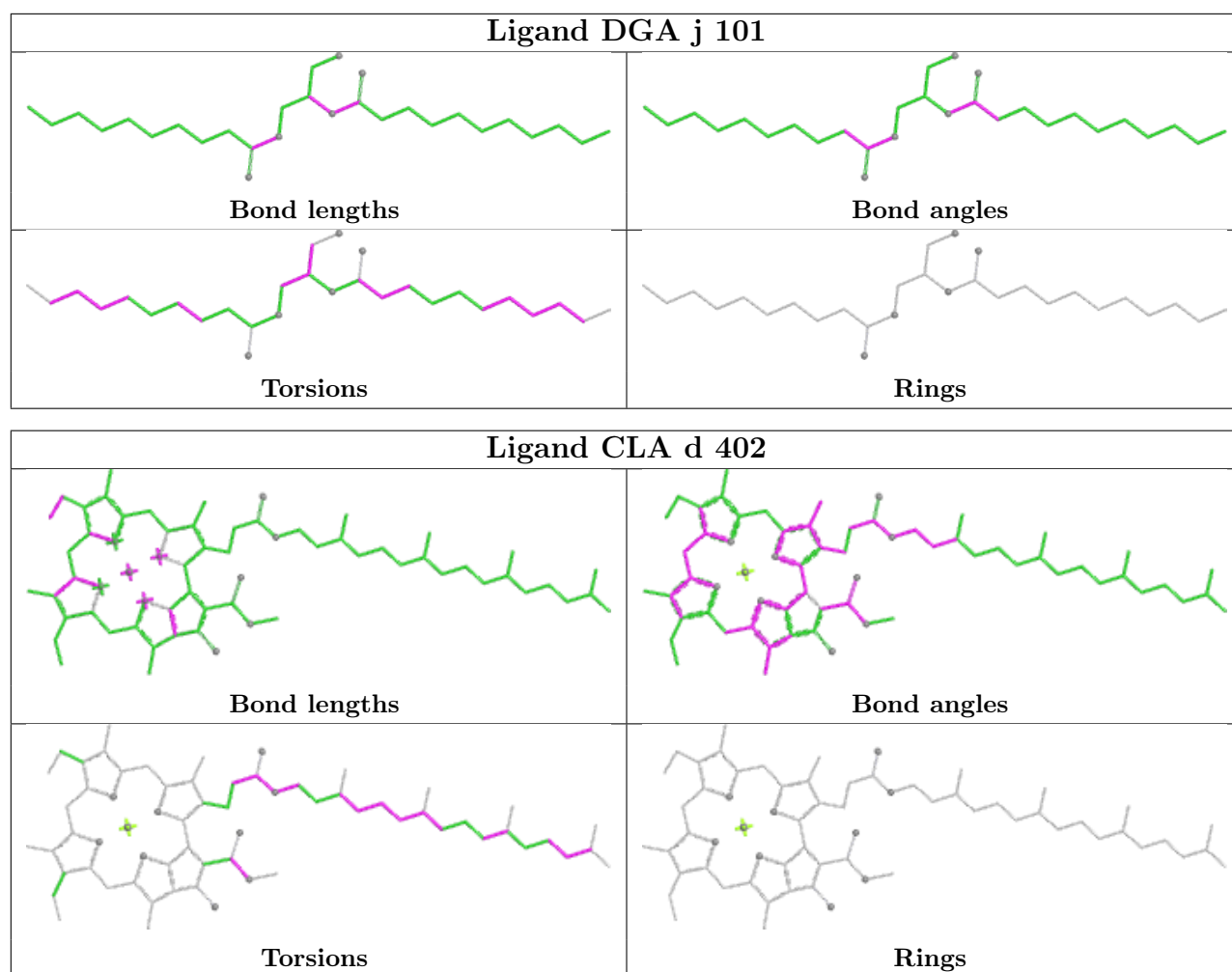
Ligand CLA S 617

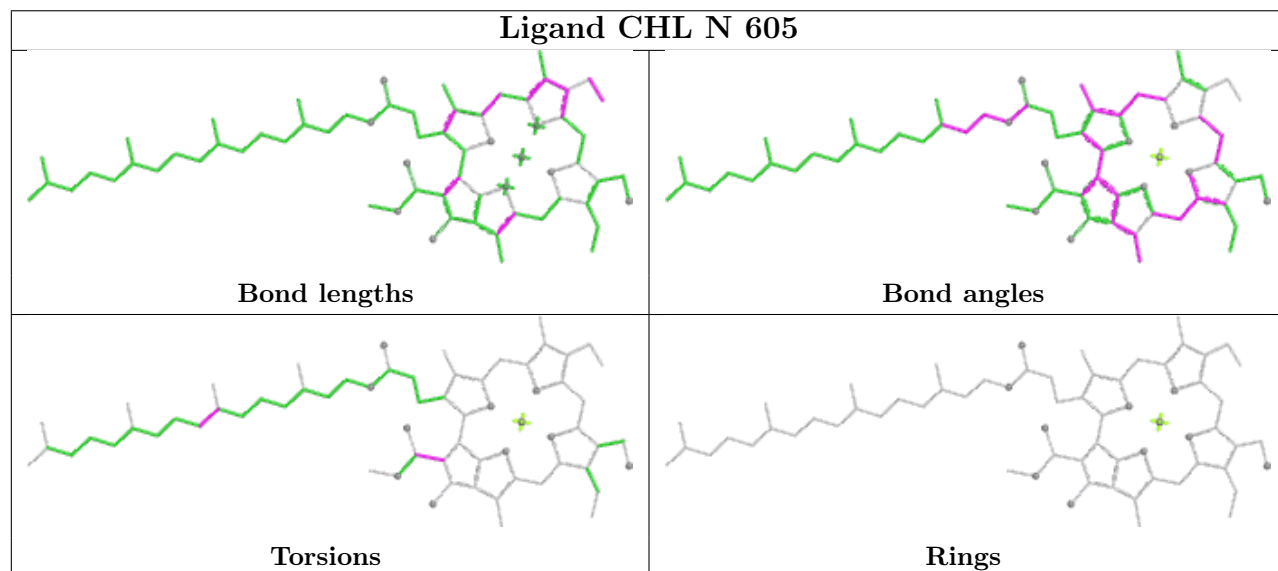
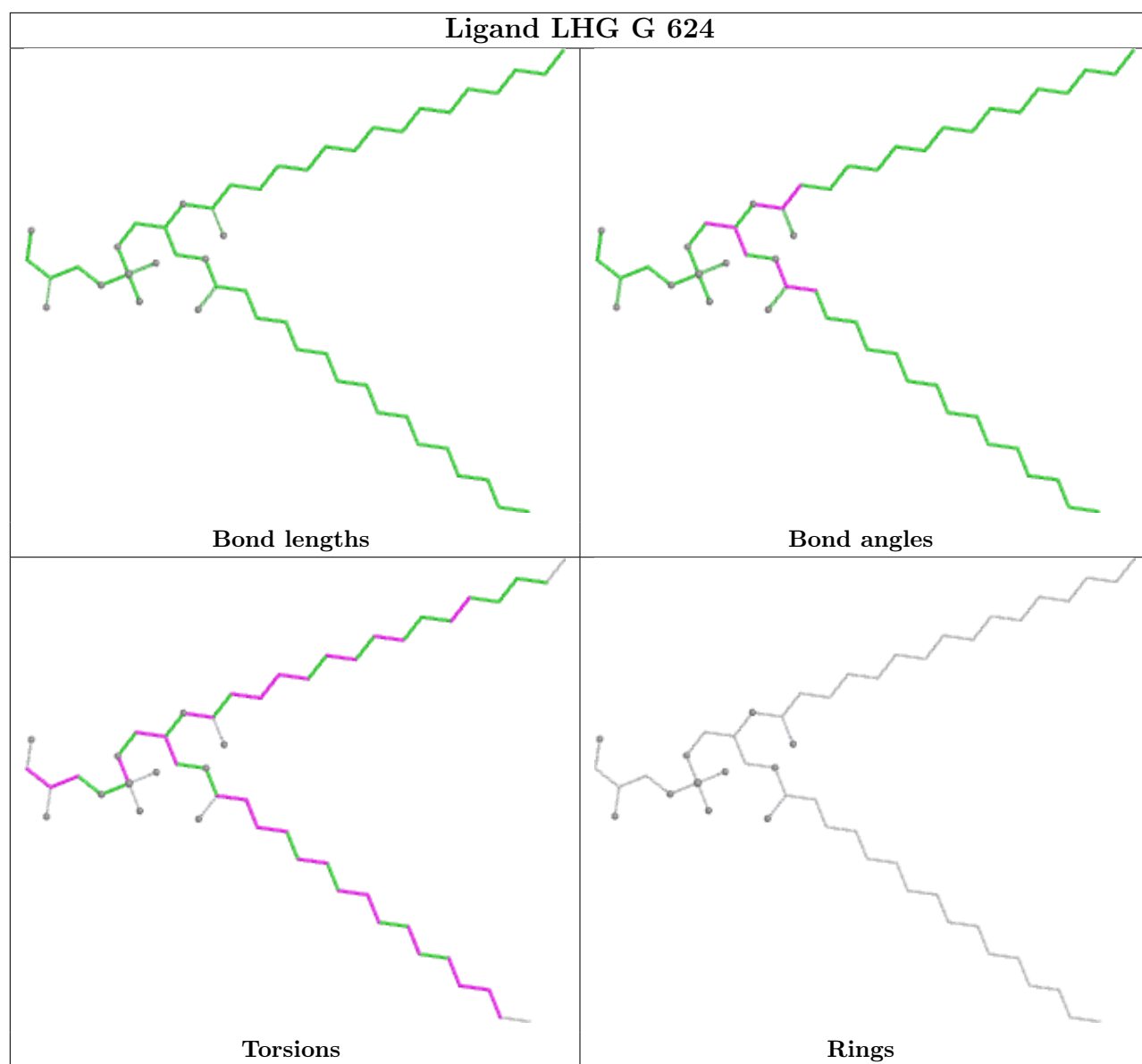


Ligand CLA c 513

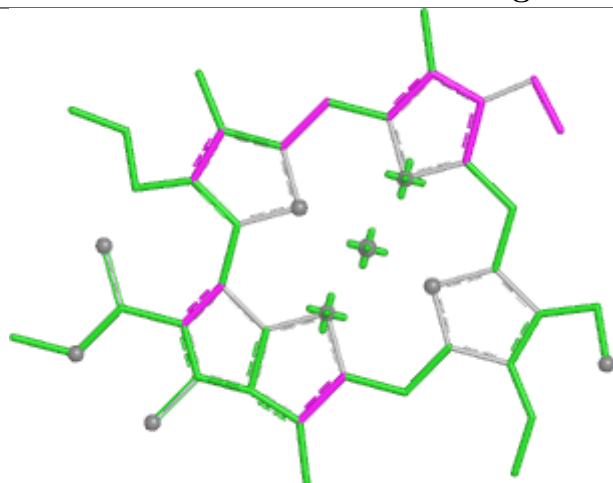




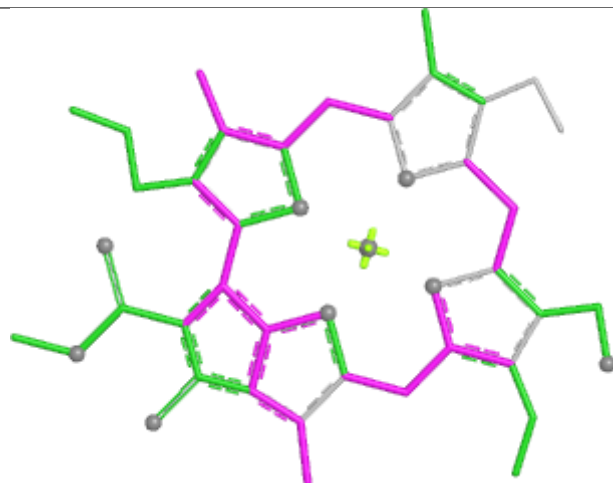




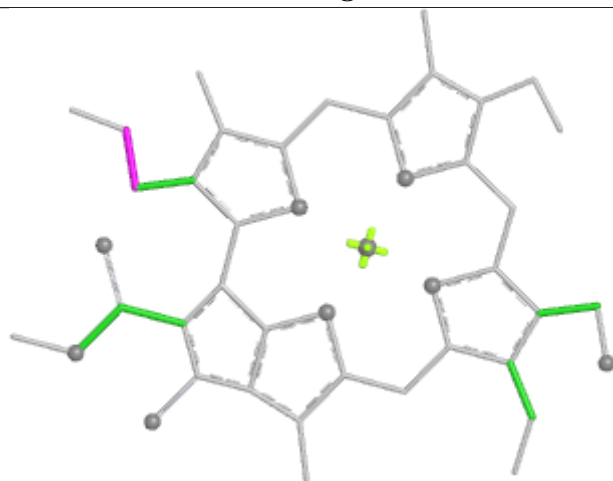
Ligand CHL G 608



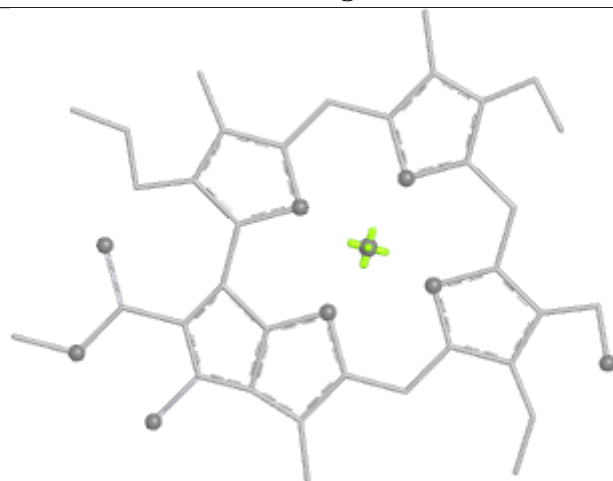
Bond lengths



Bond angles

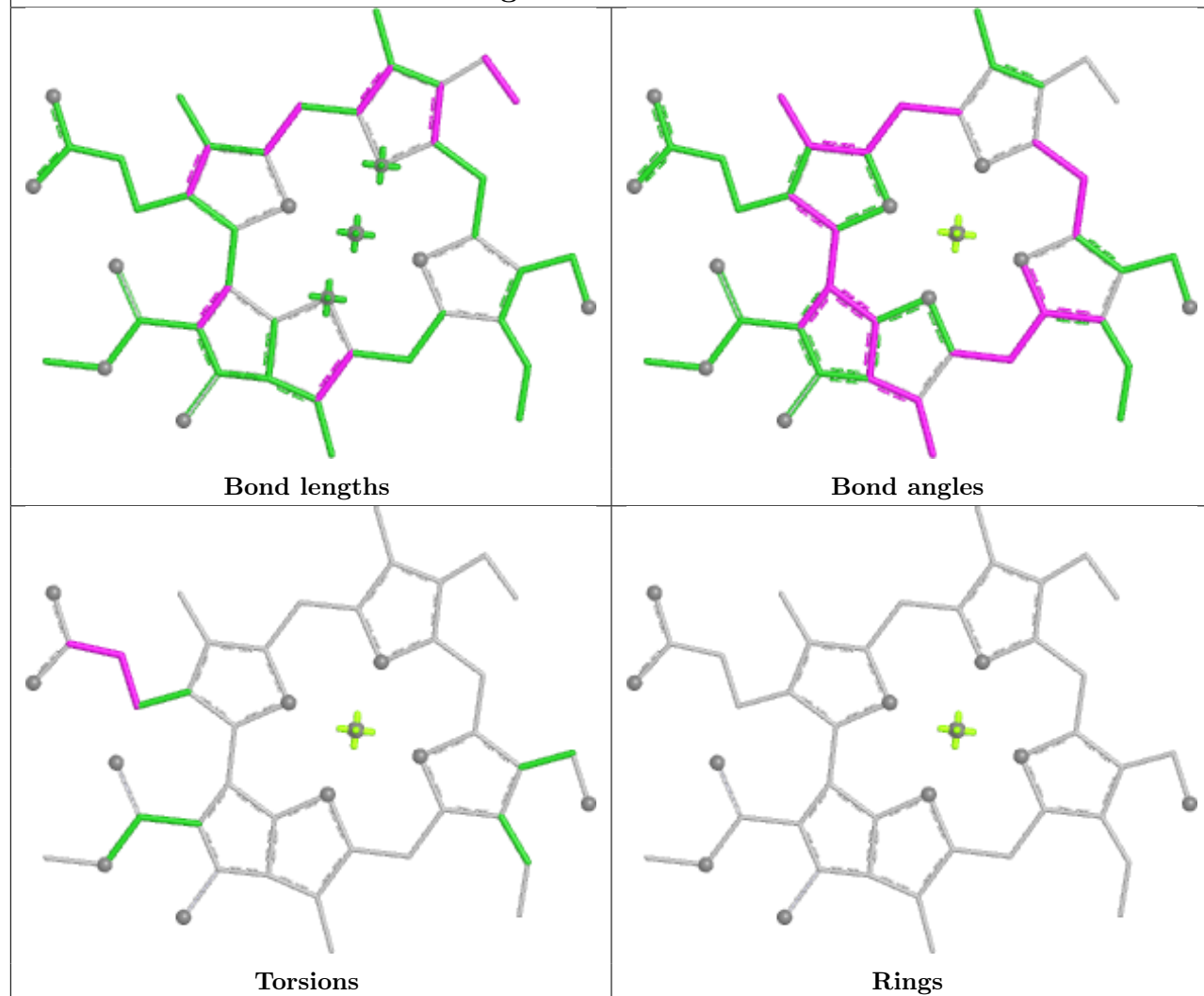


Torsions

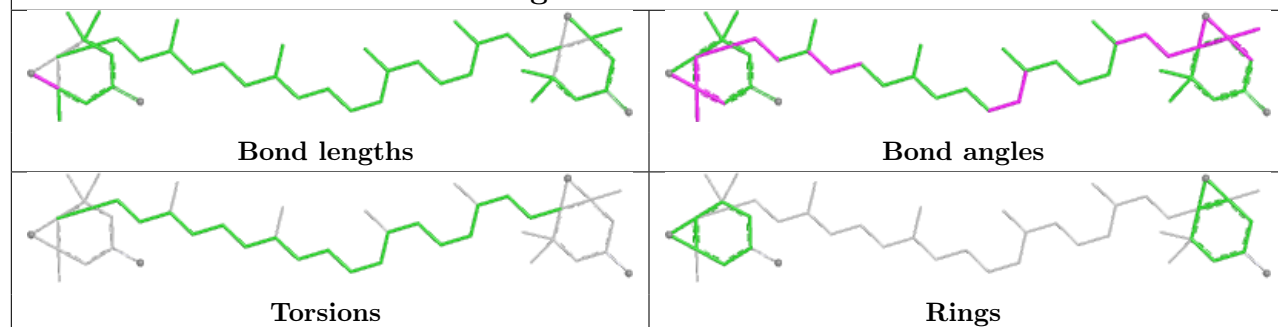


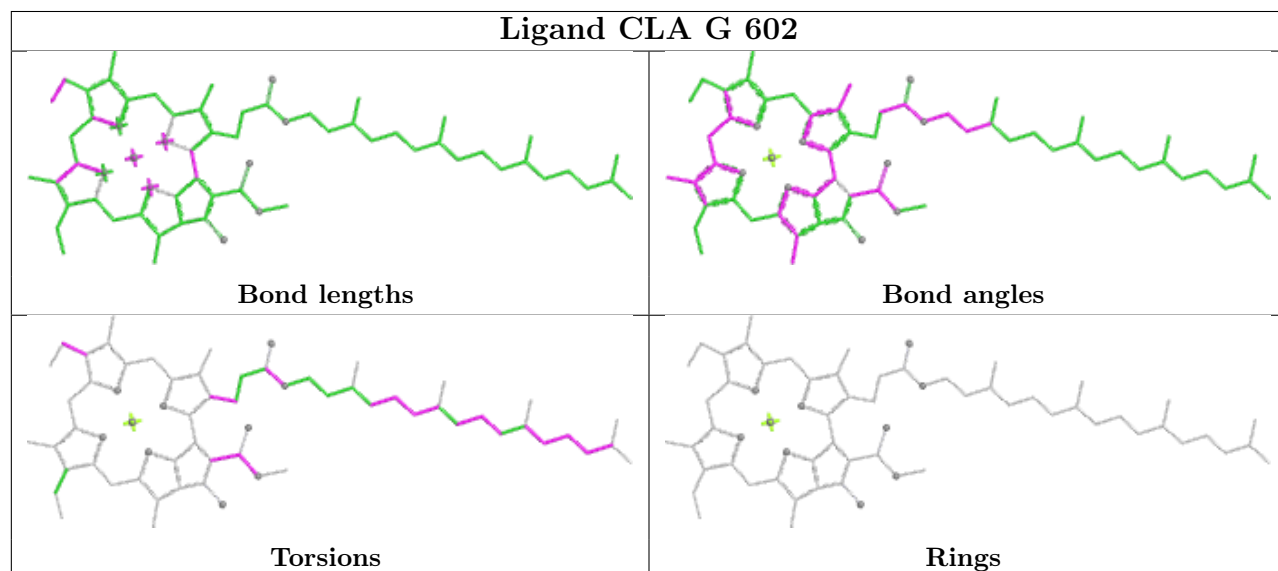
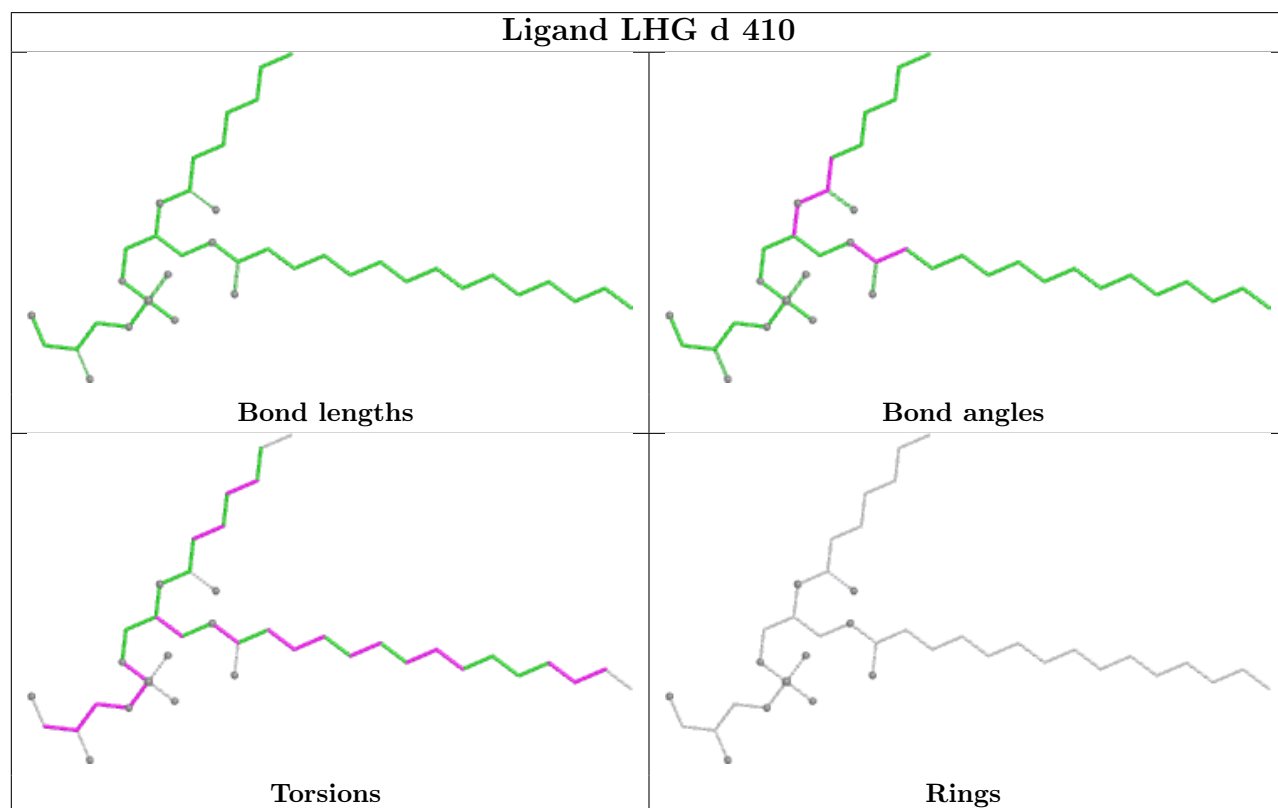
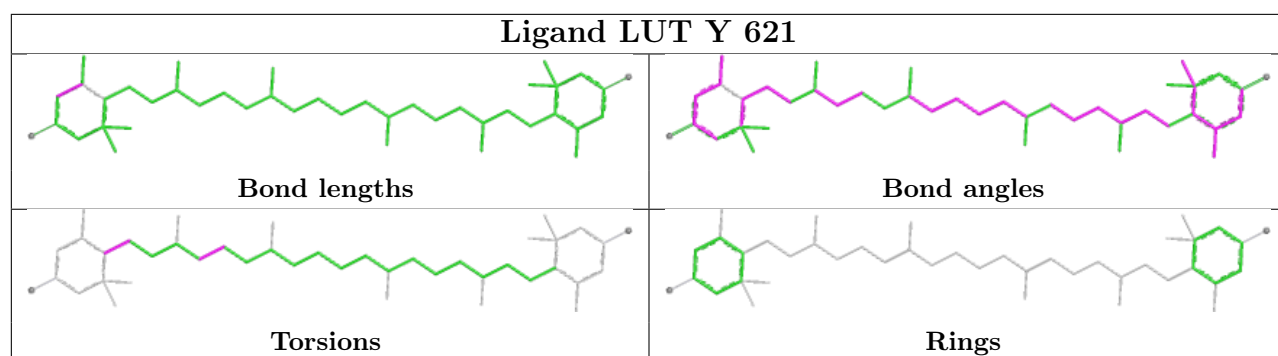
Rings

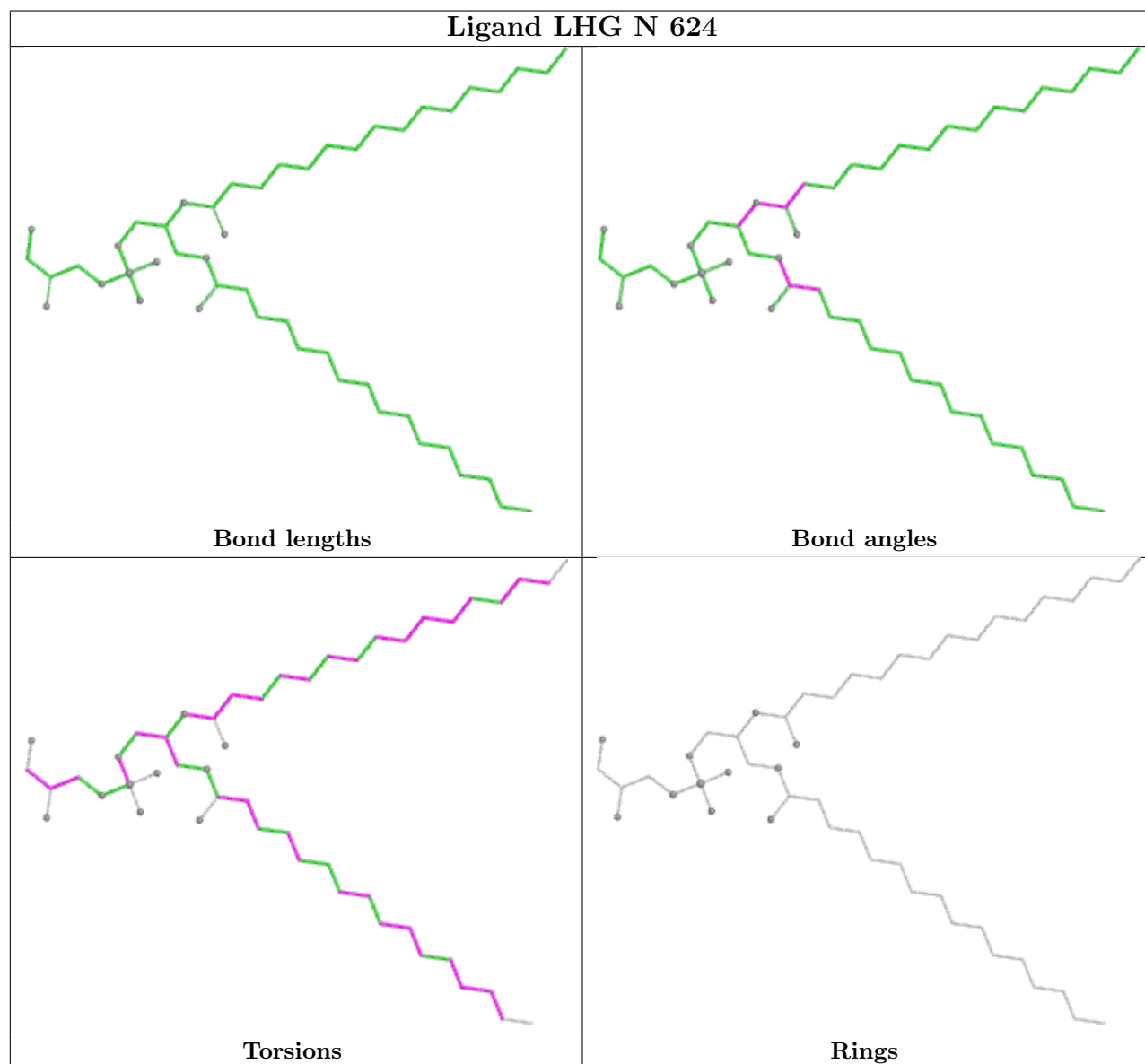
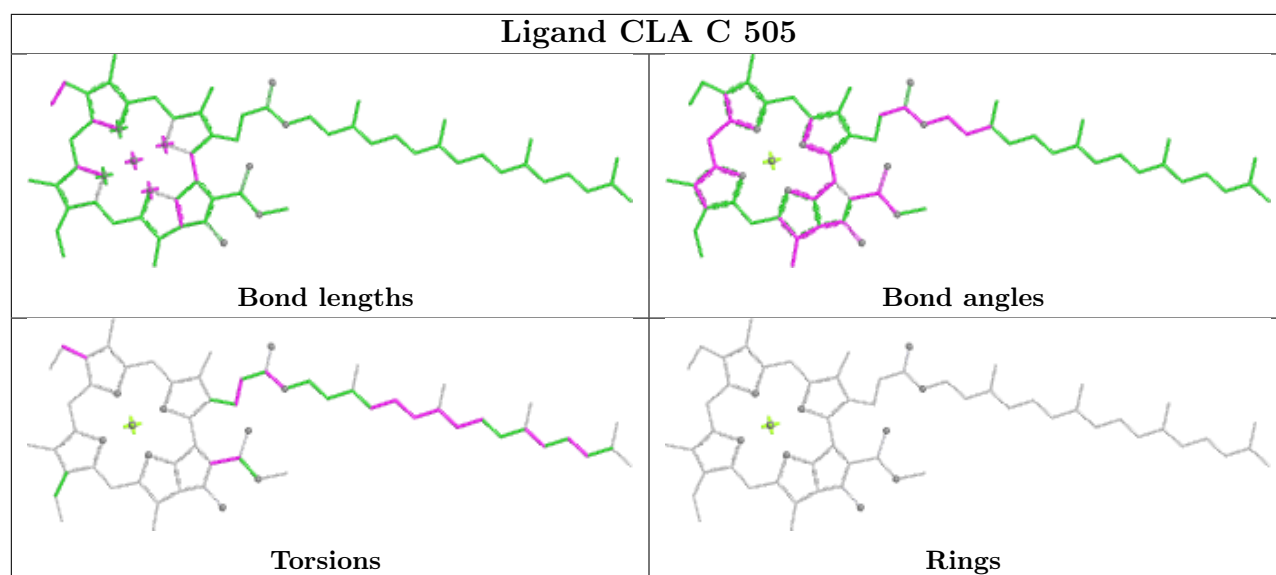
Ligand CHL Y 605

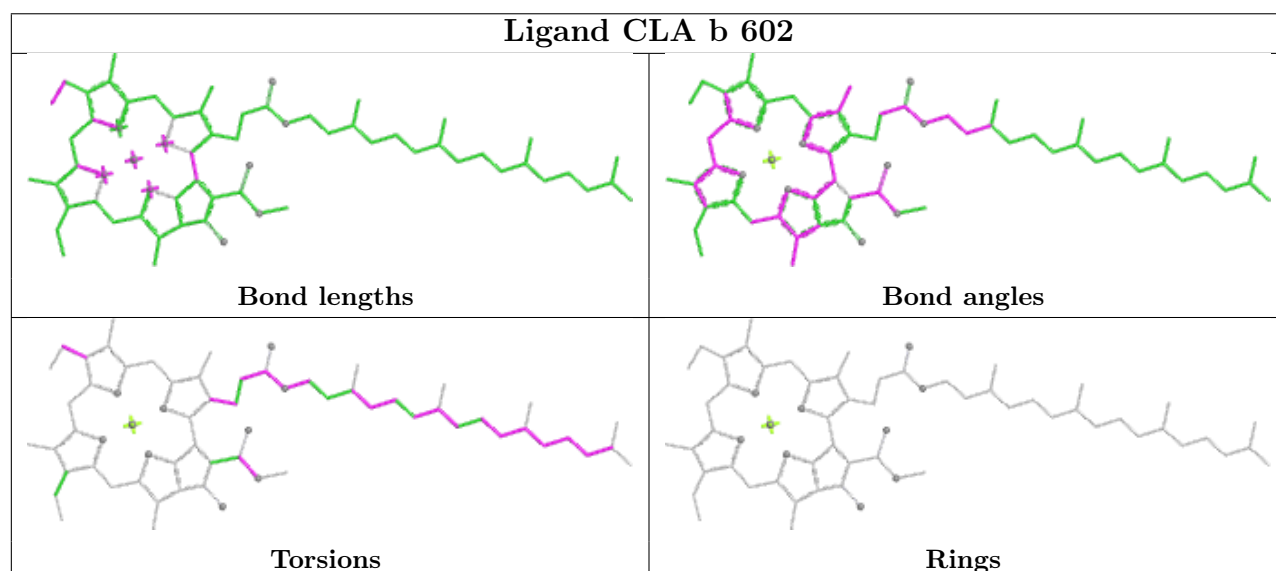
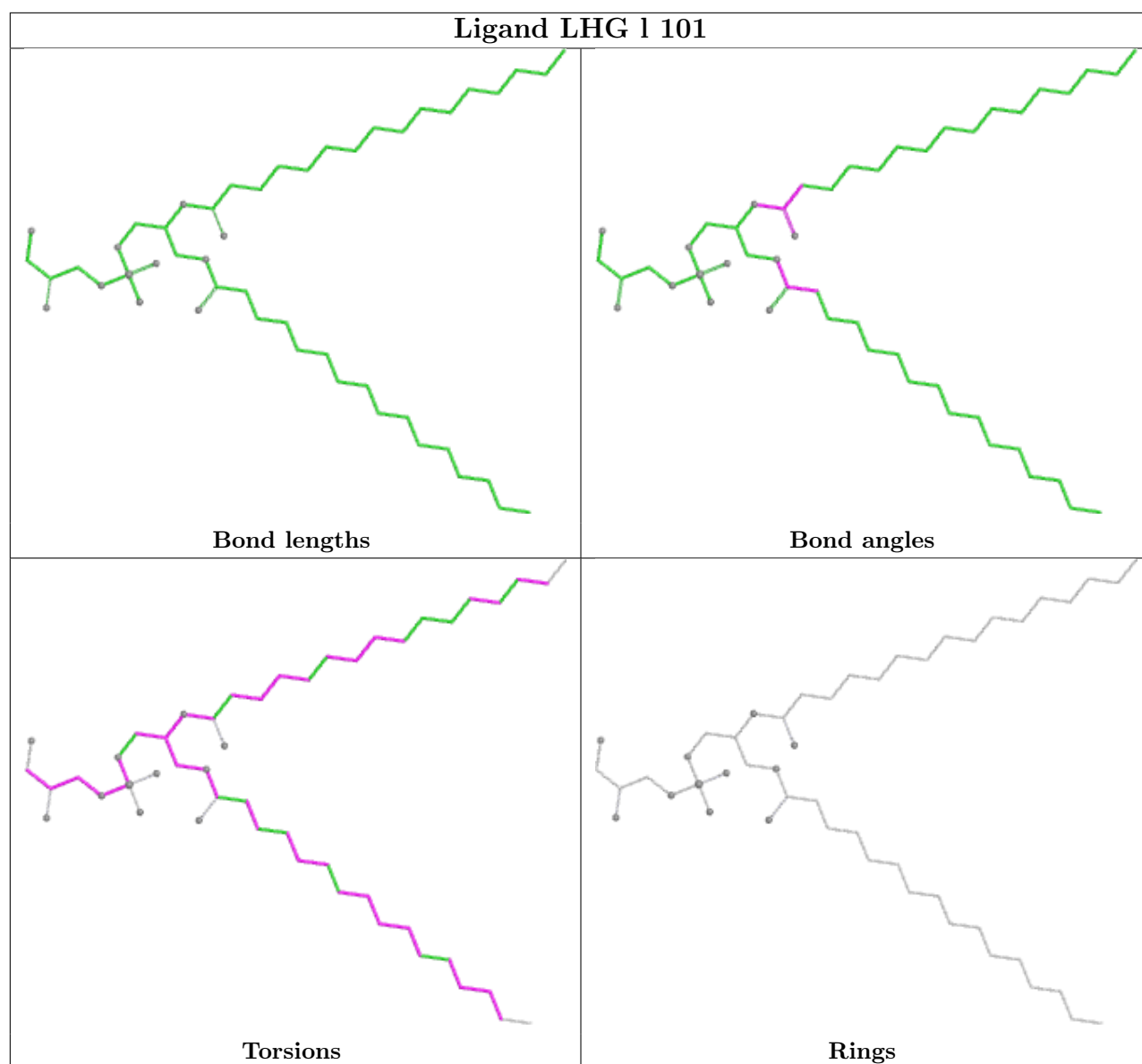


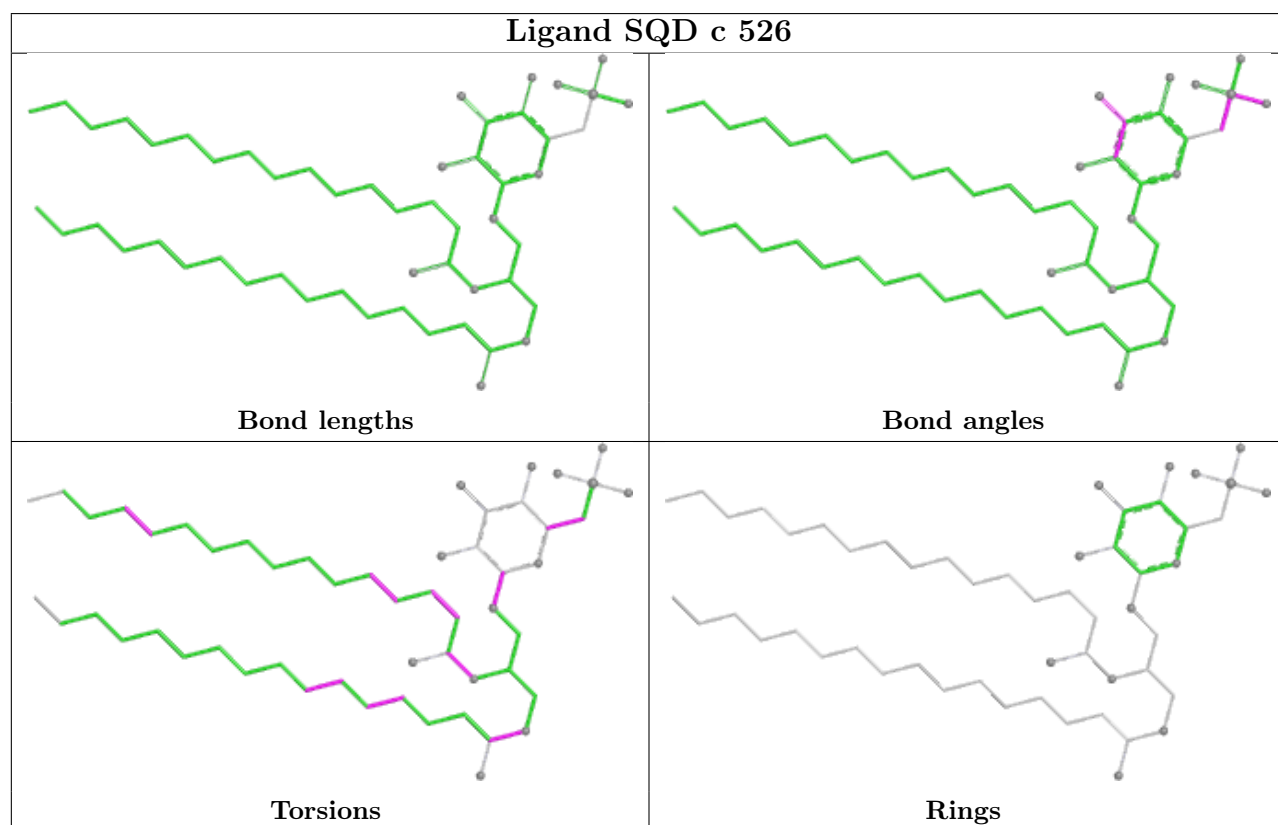
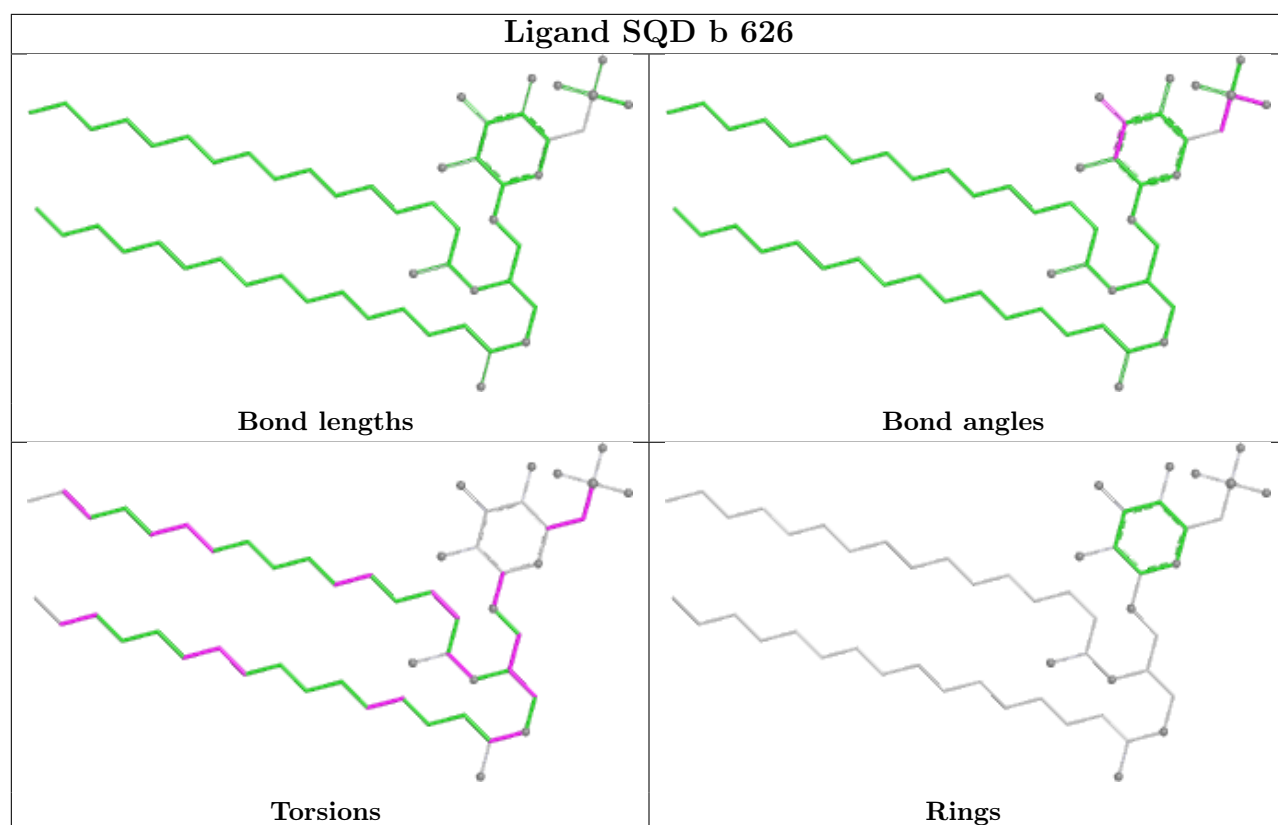
Ligand XAT G 622

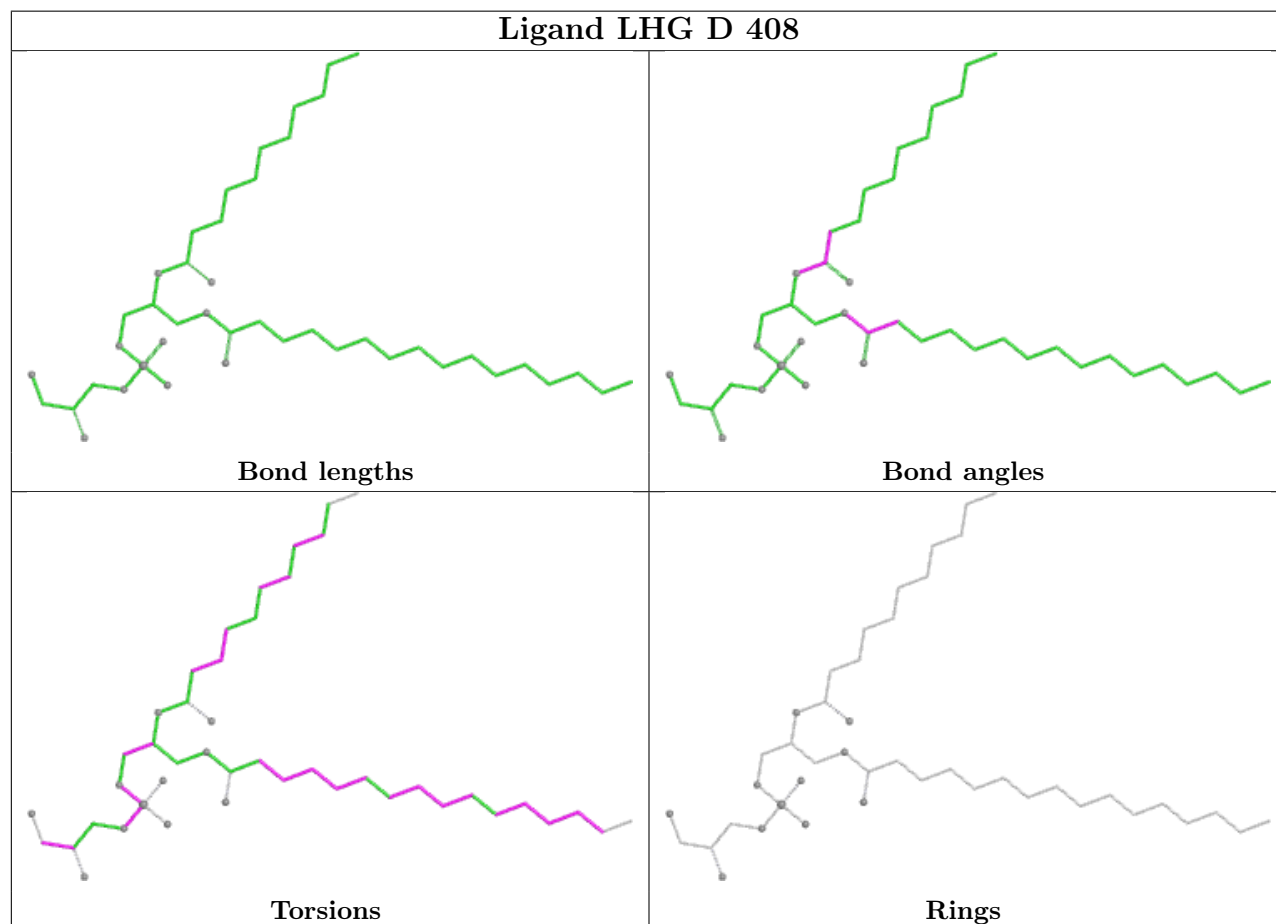
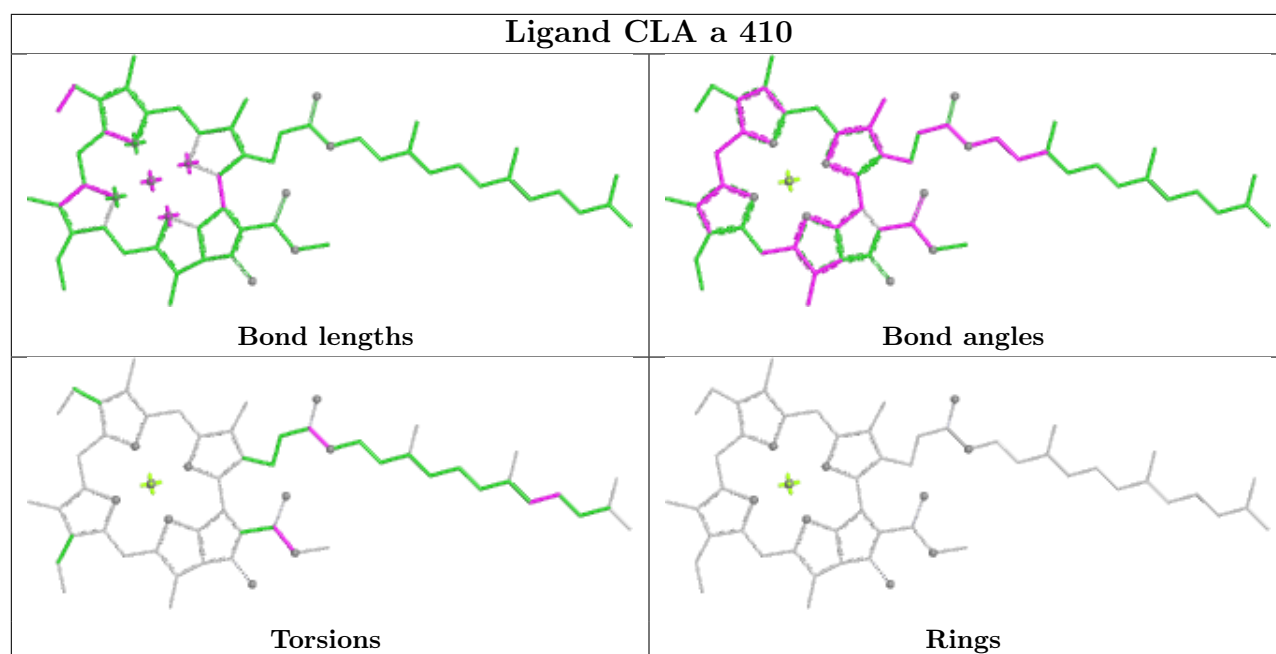


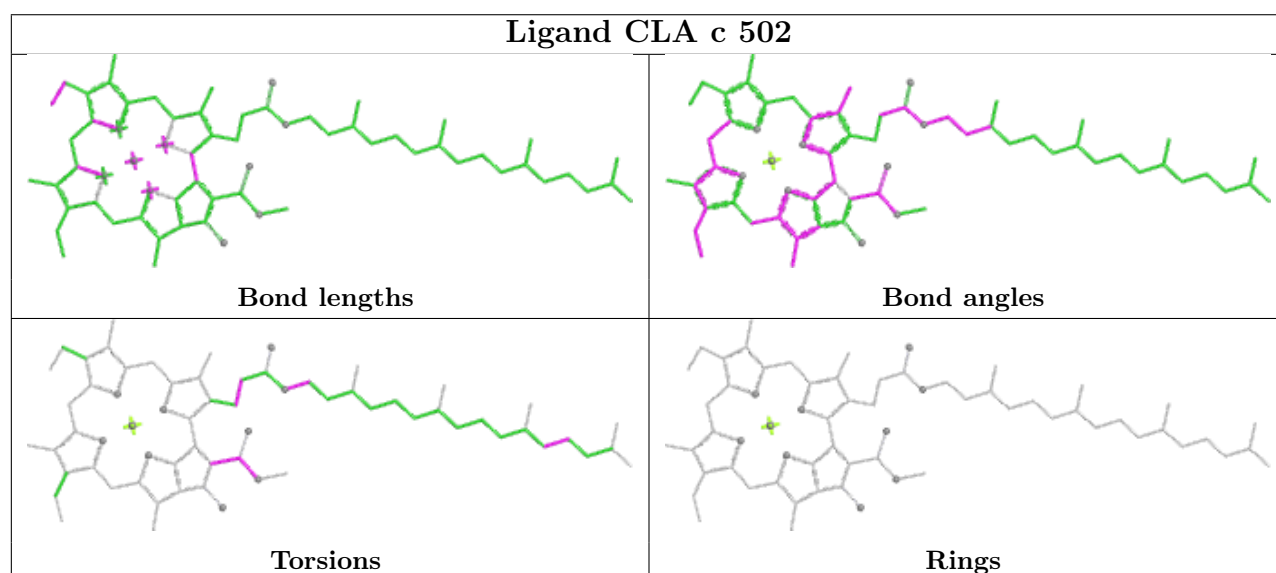
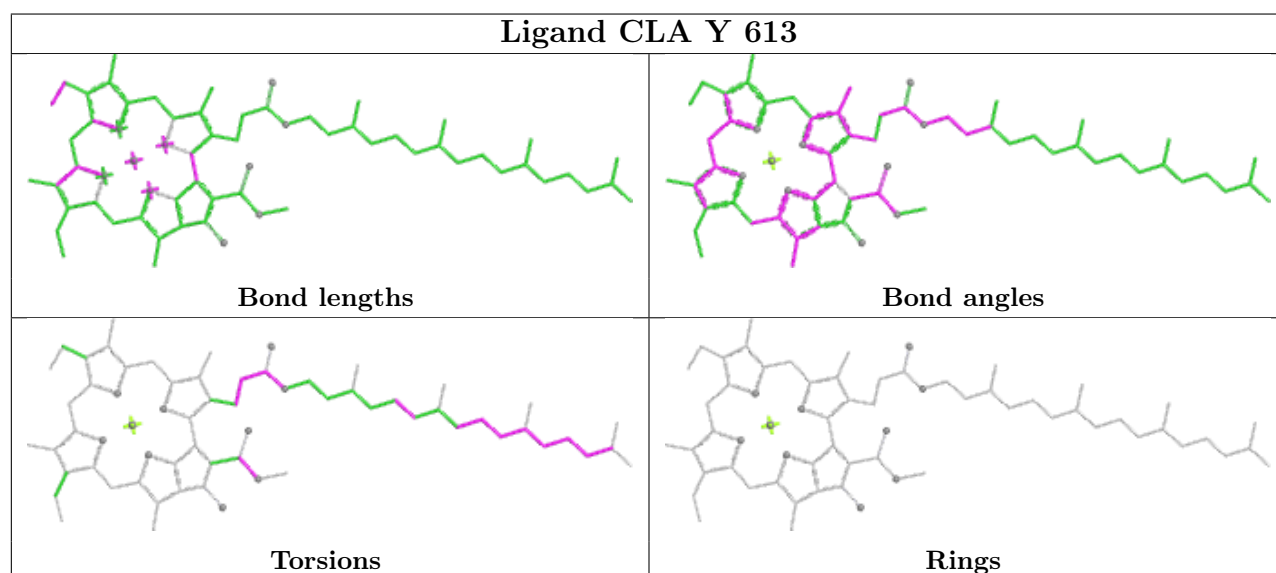
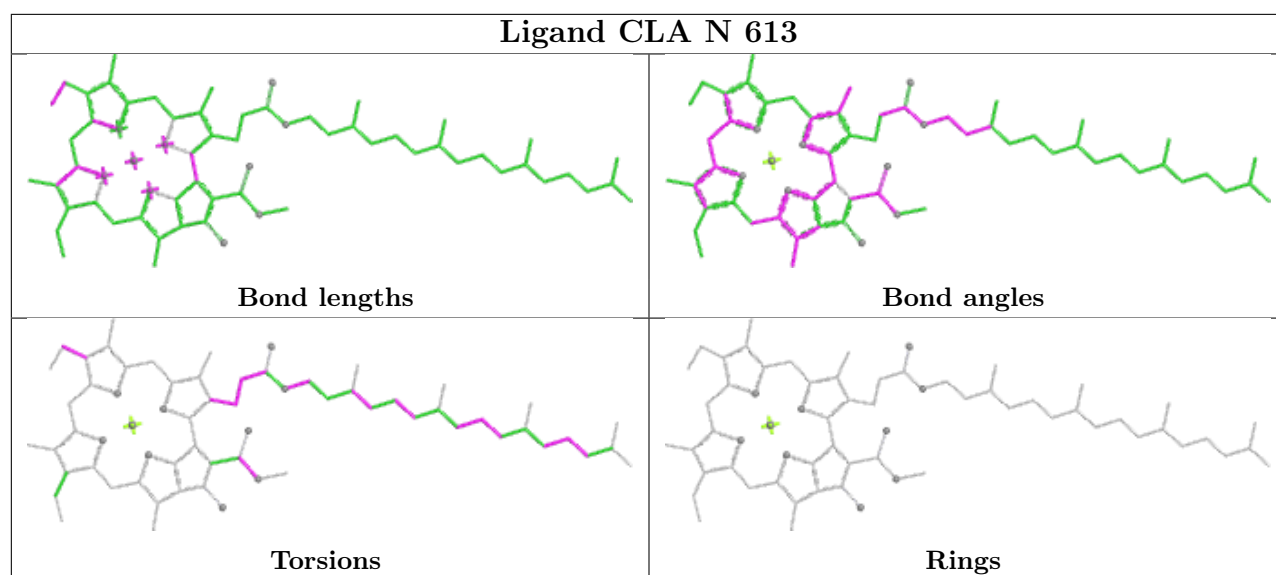


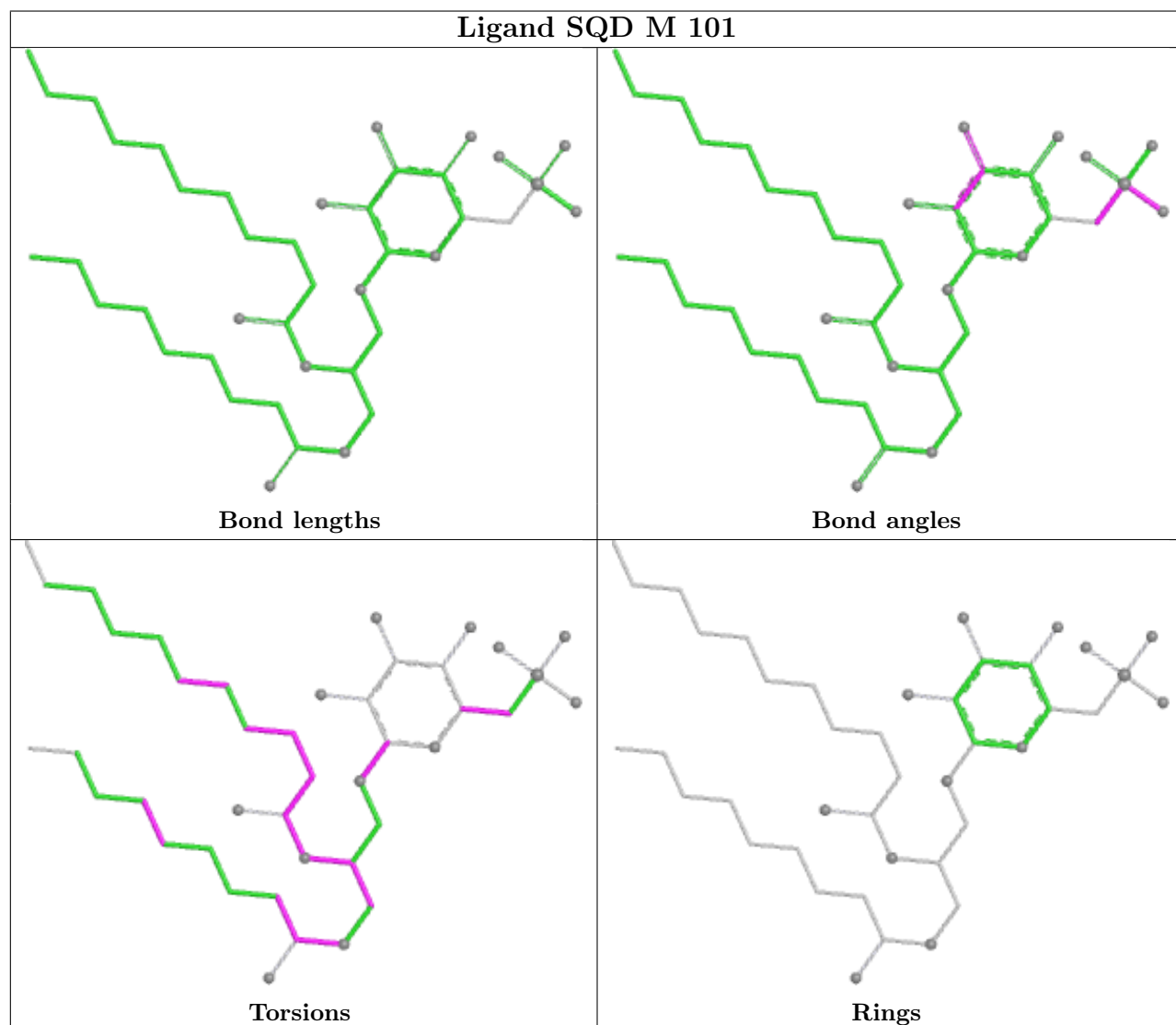
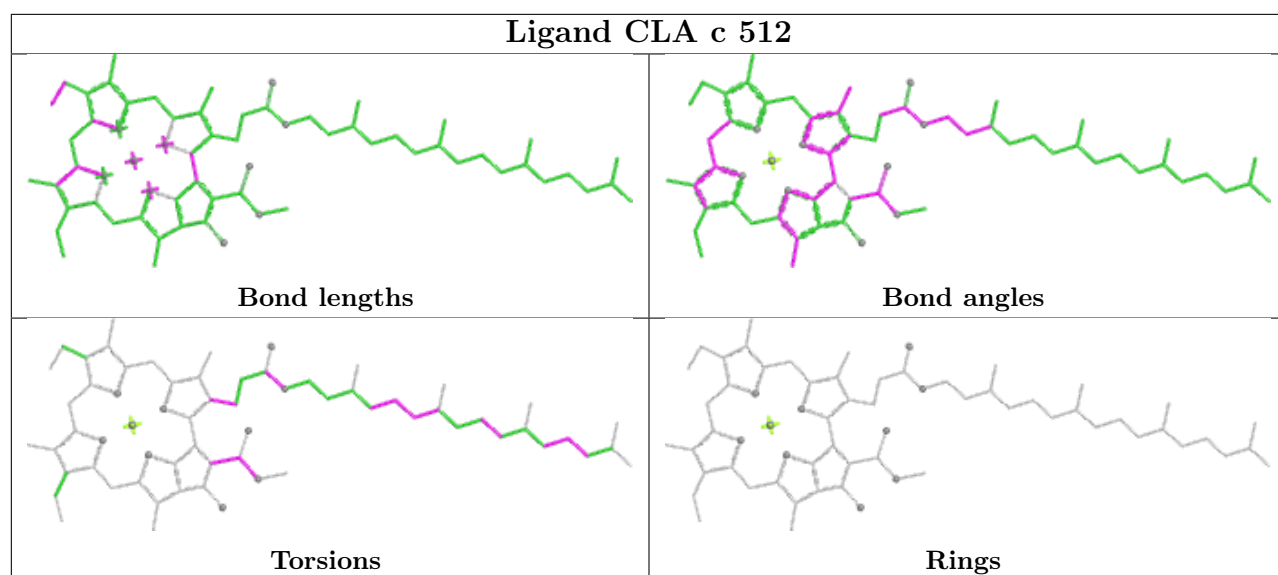


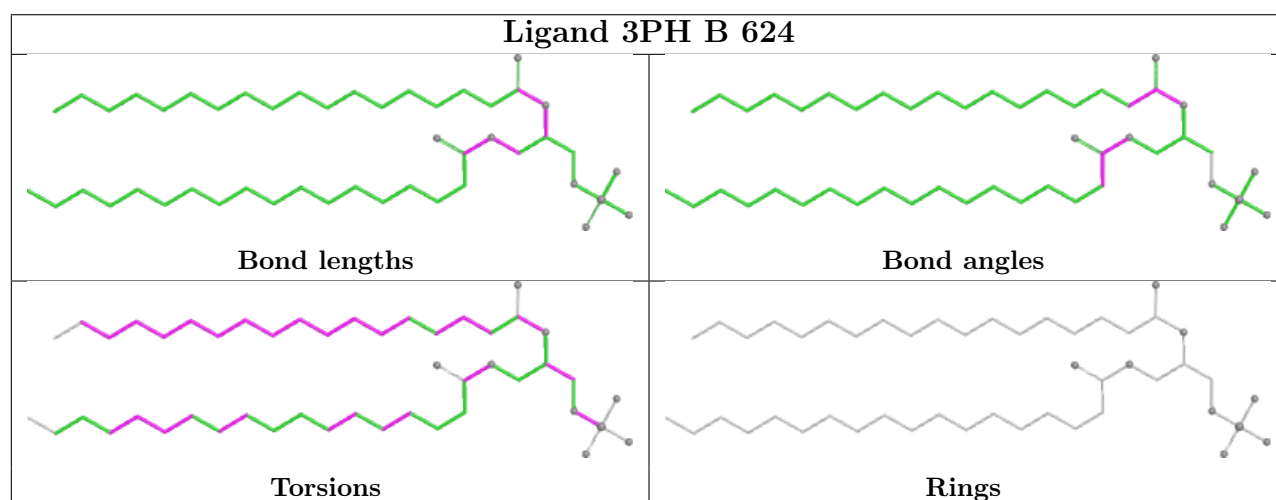
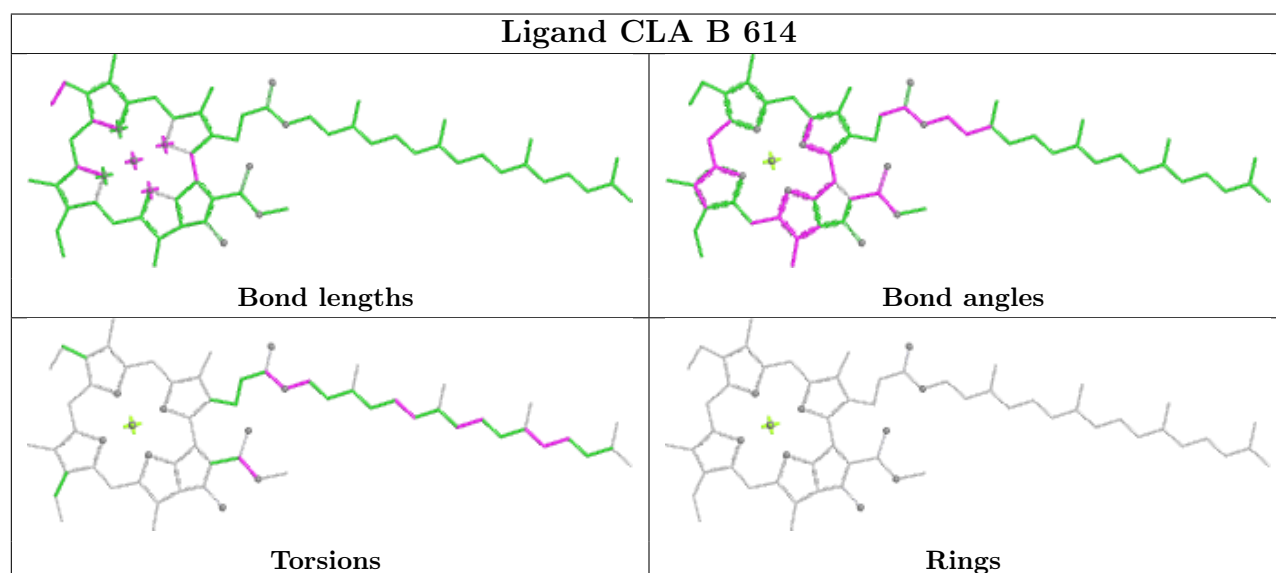
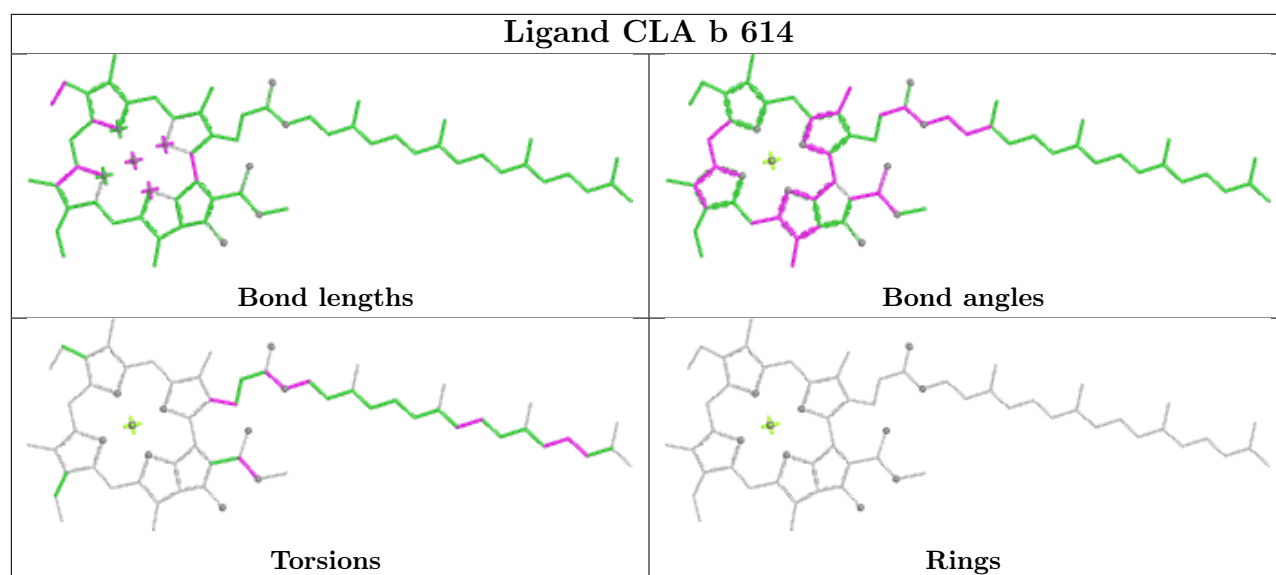


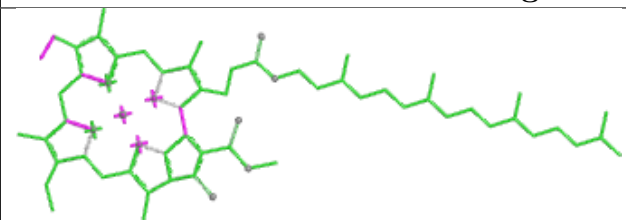
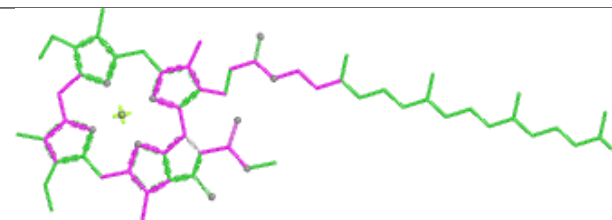
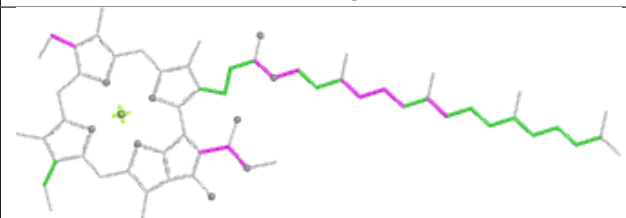
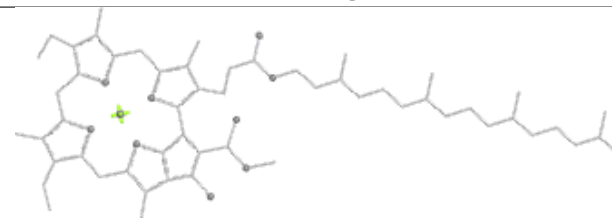


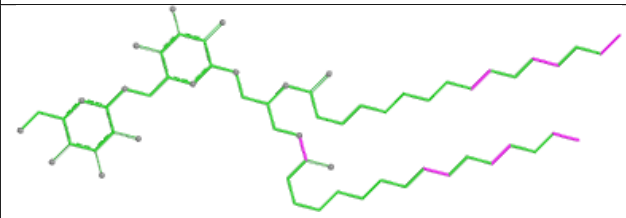
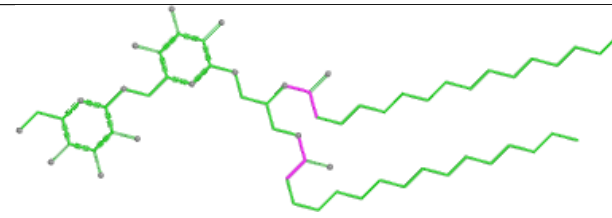
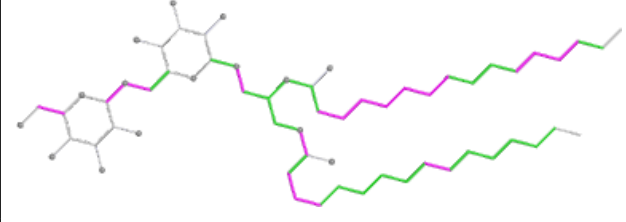
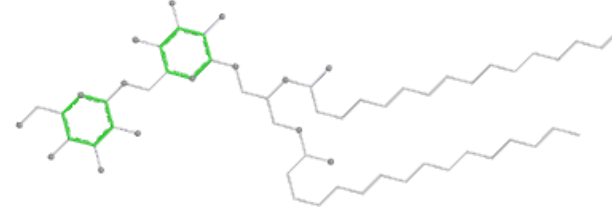


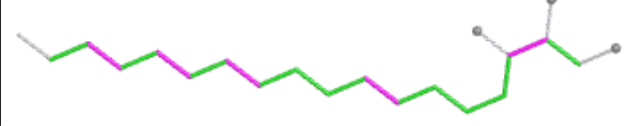
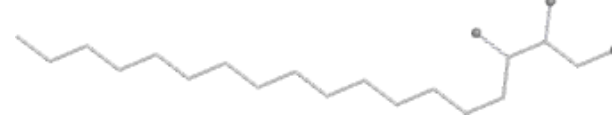


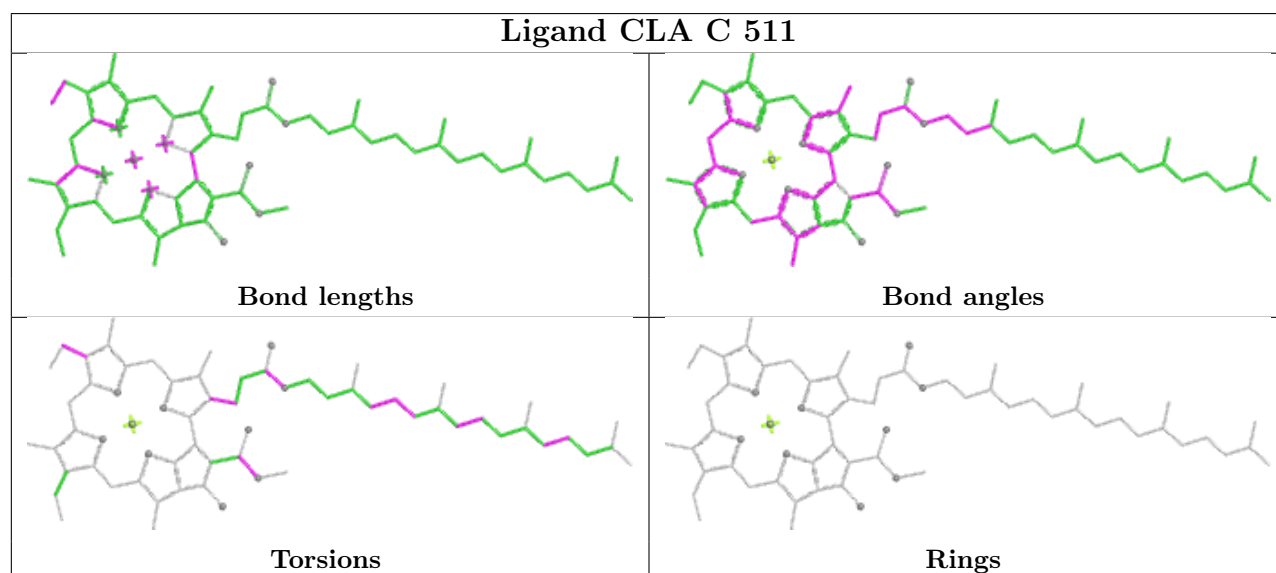
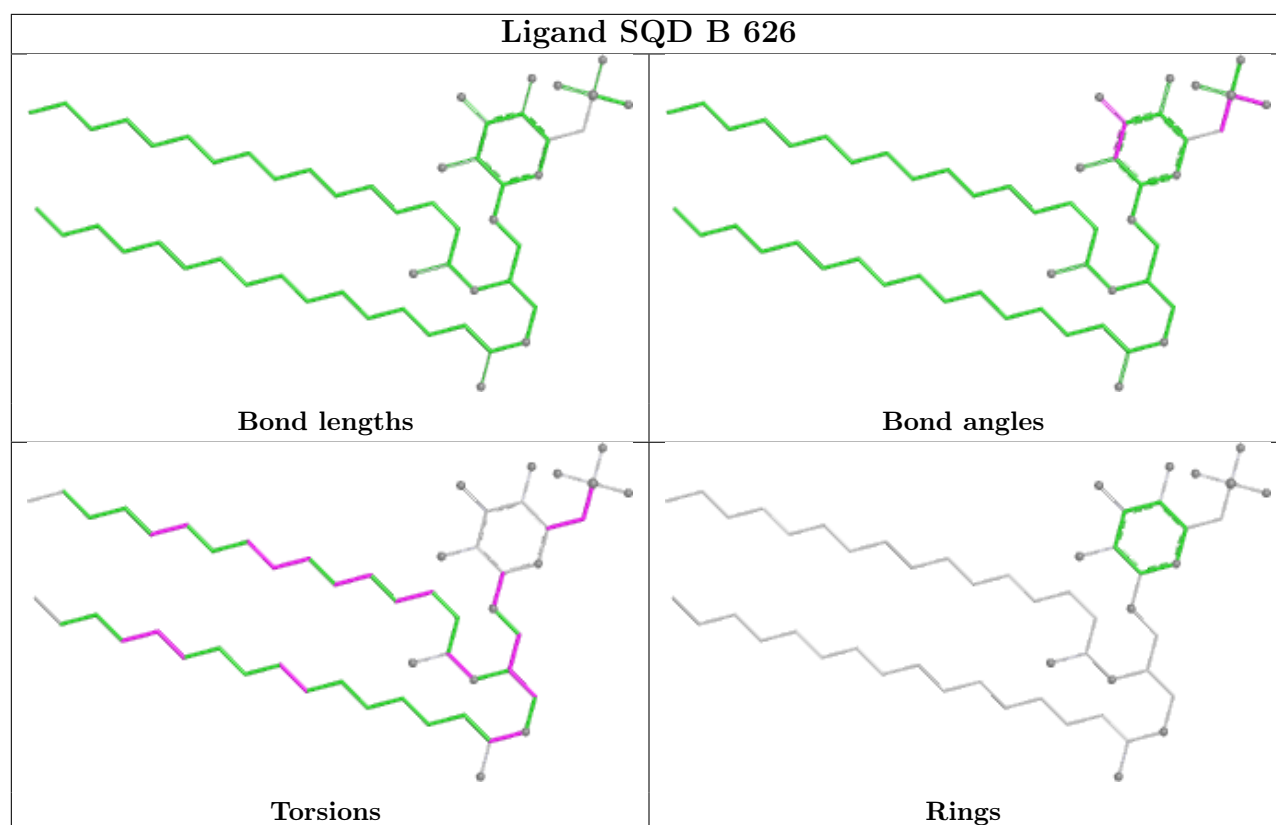


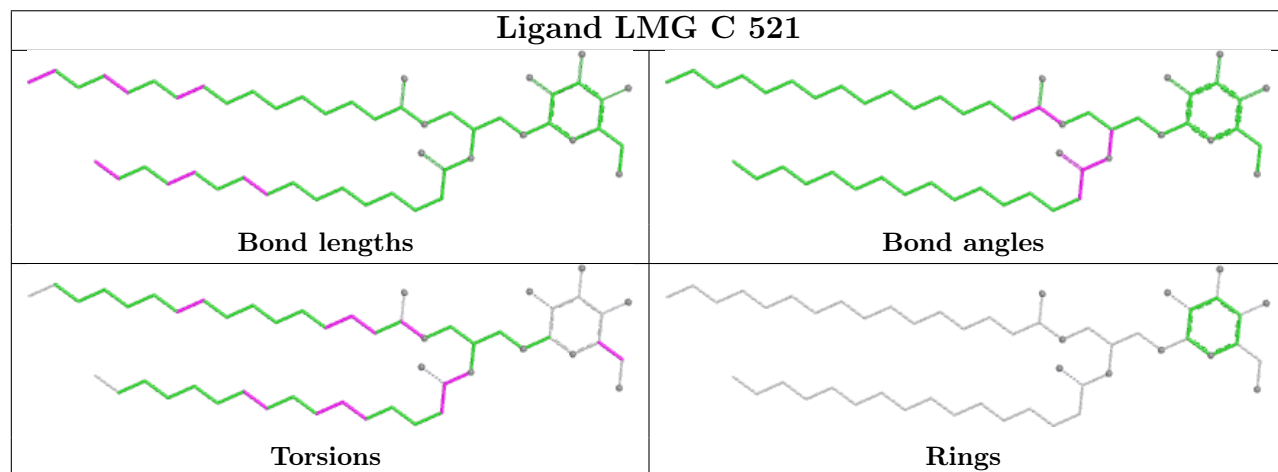
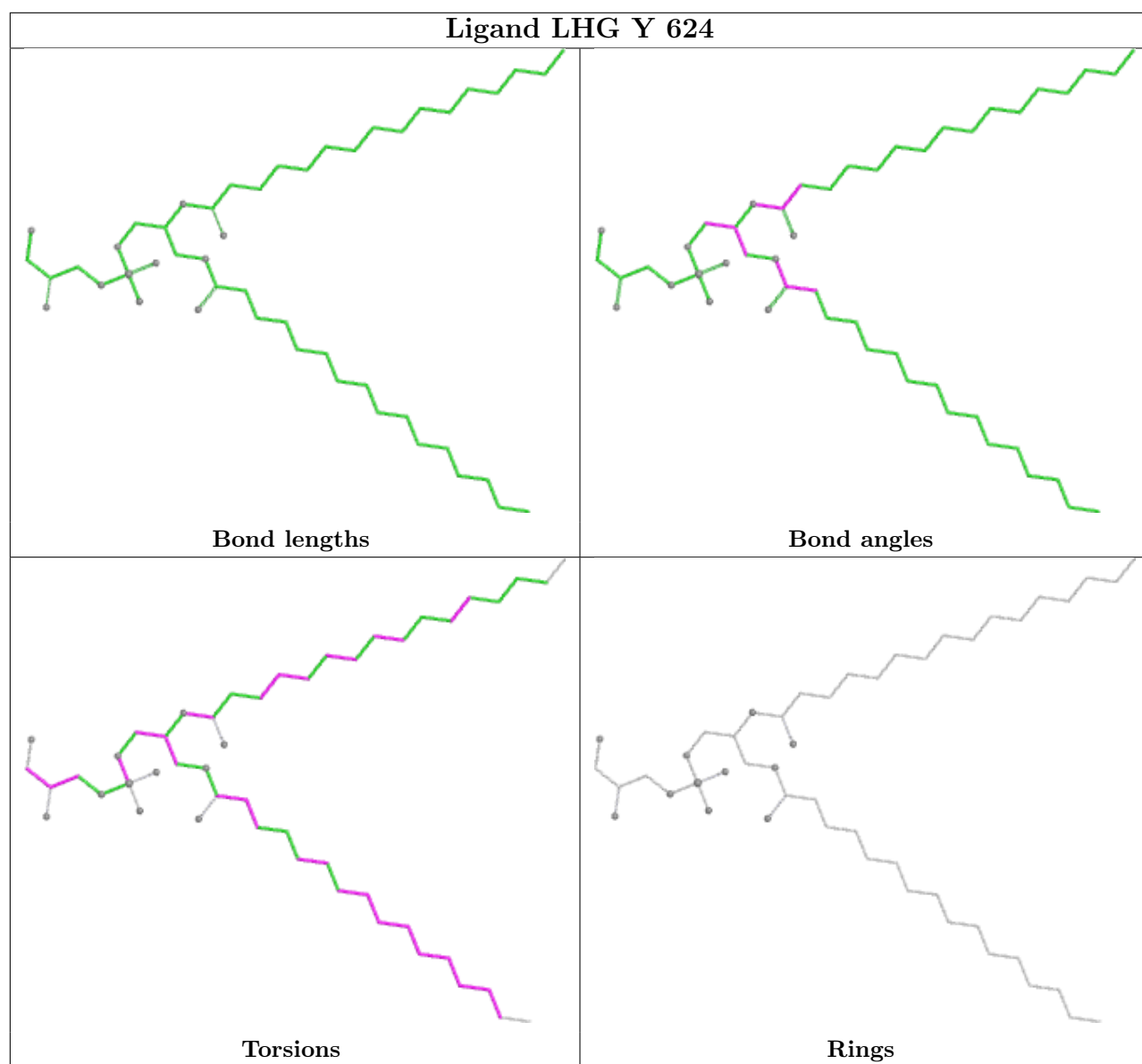


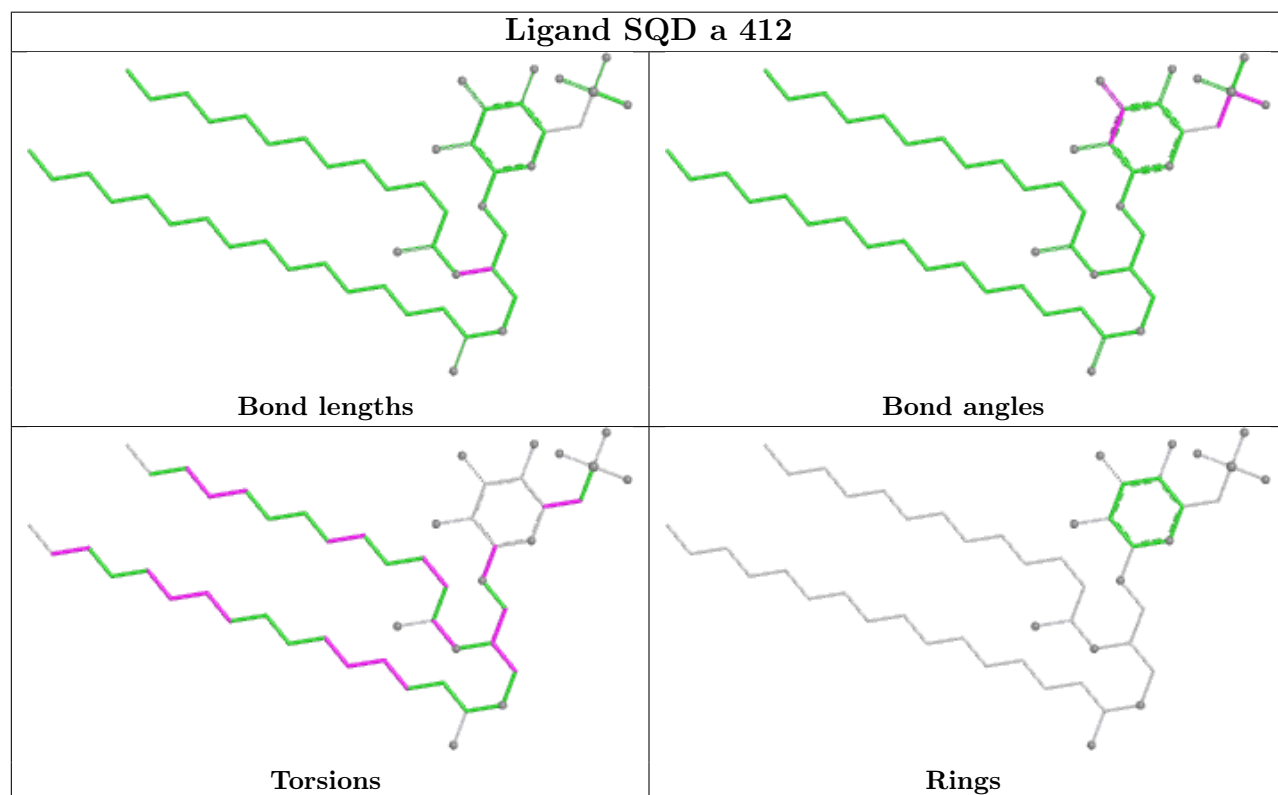
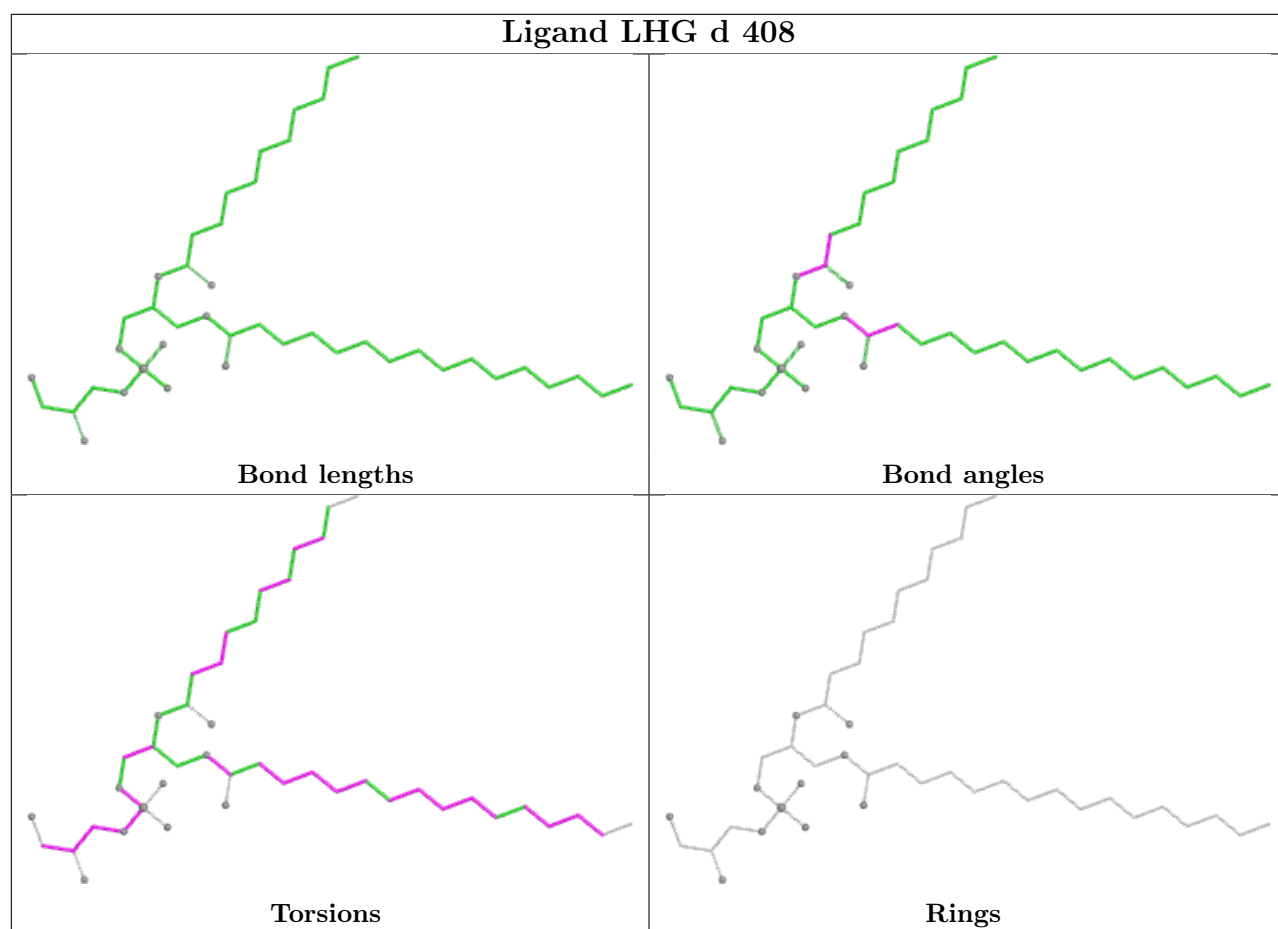
Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

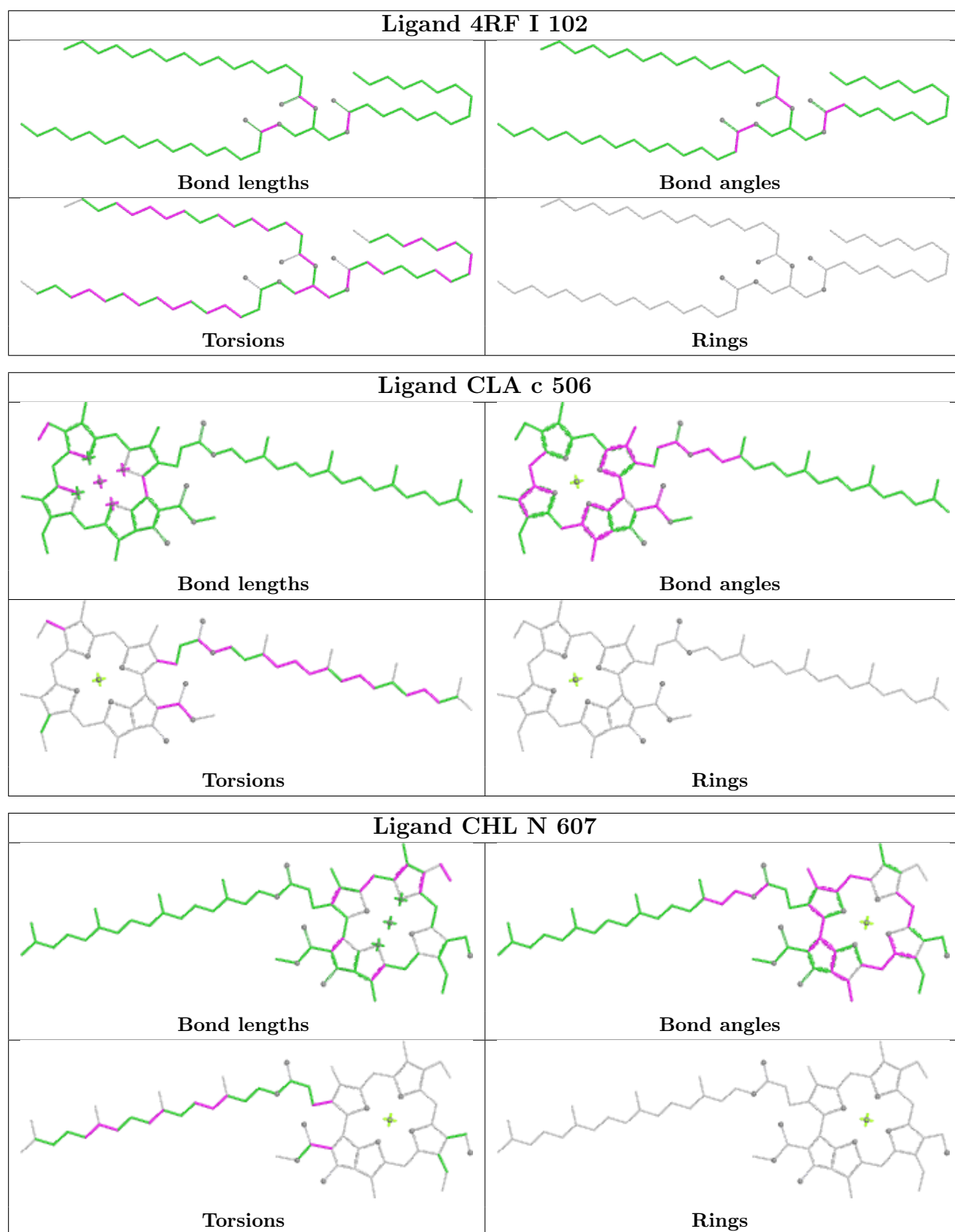
Ligand DGD c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

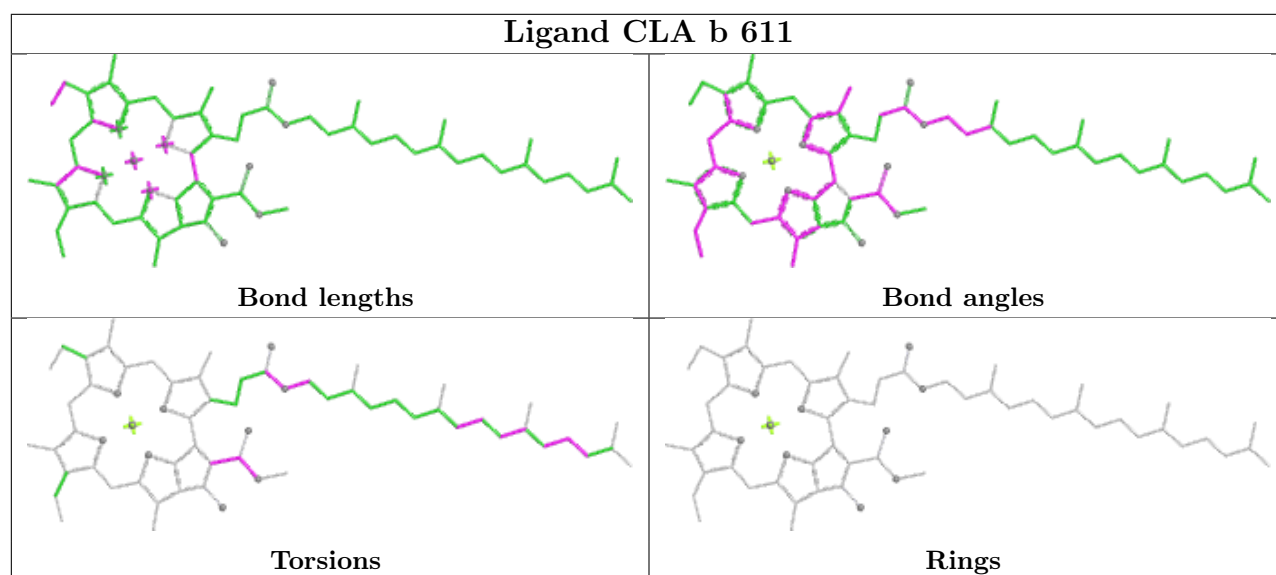
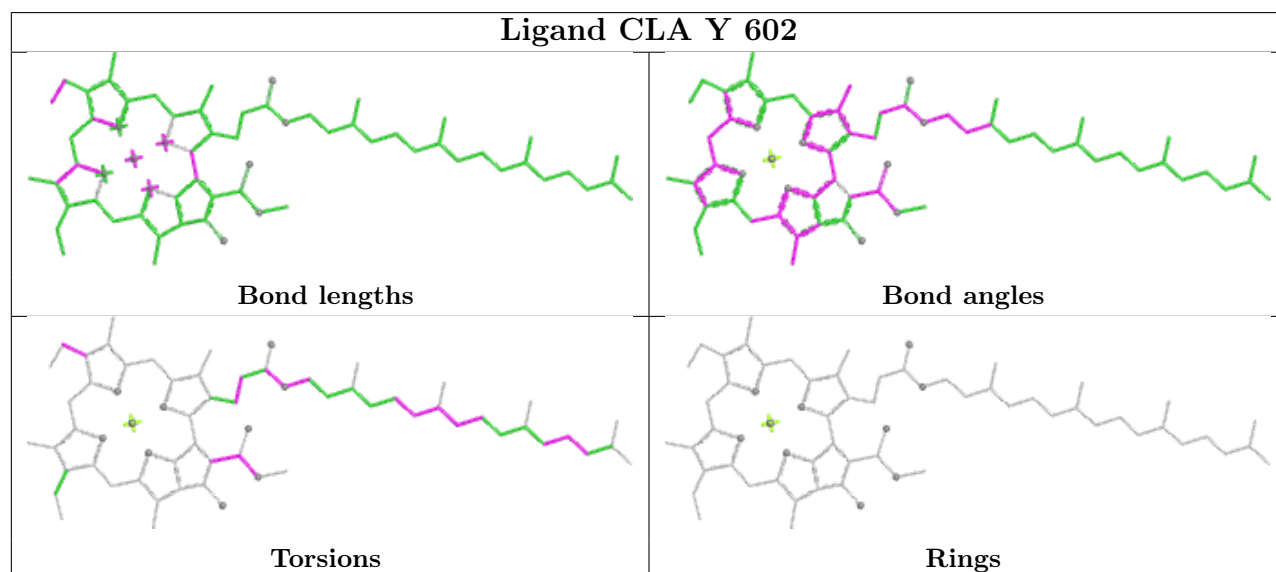
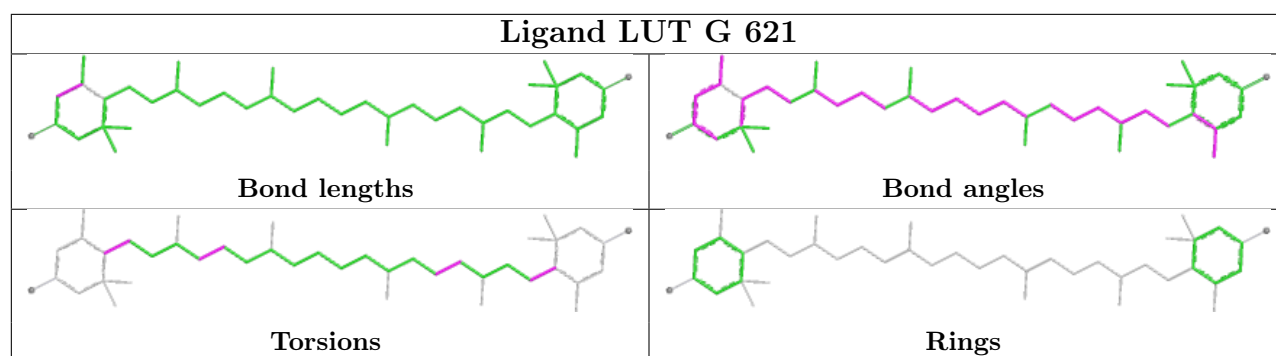
Ligand SPH A 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

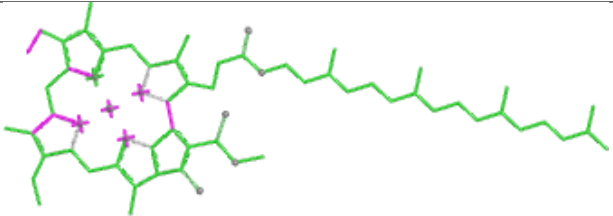
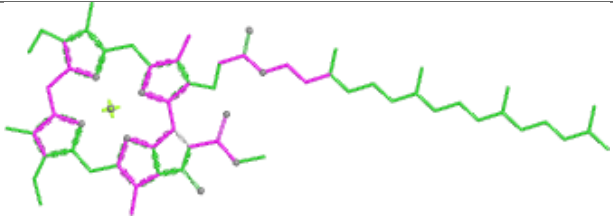
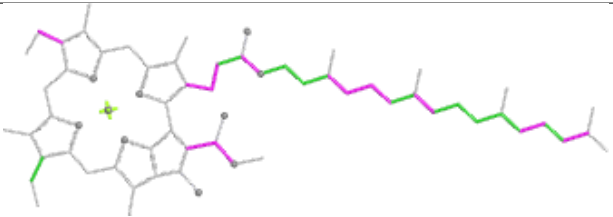
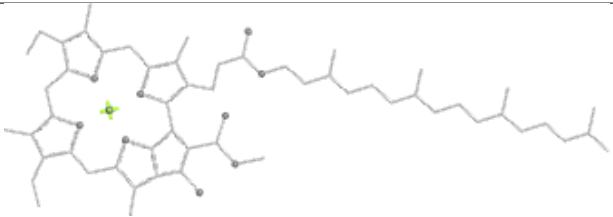
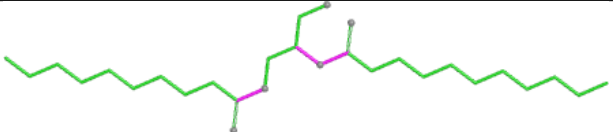
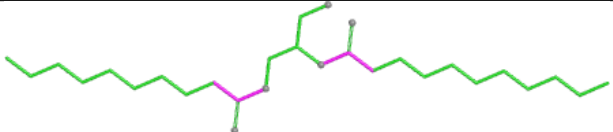
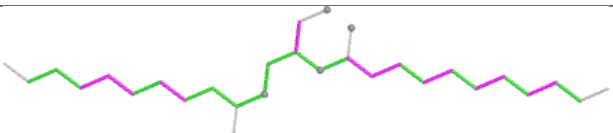
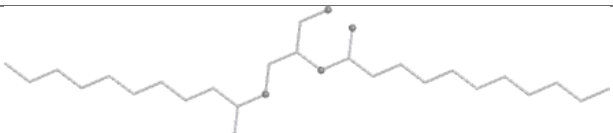
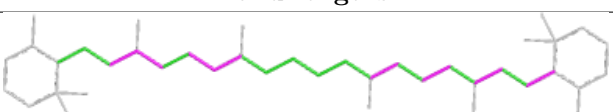
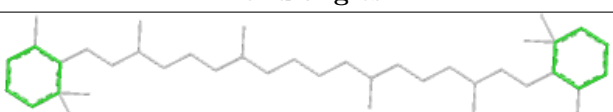


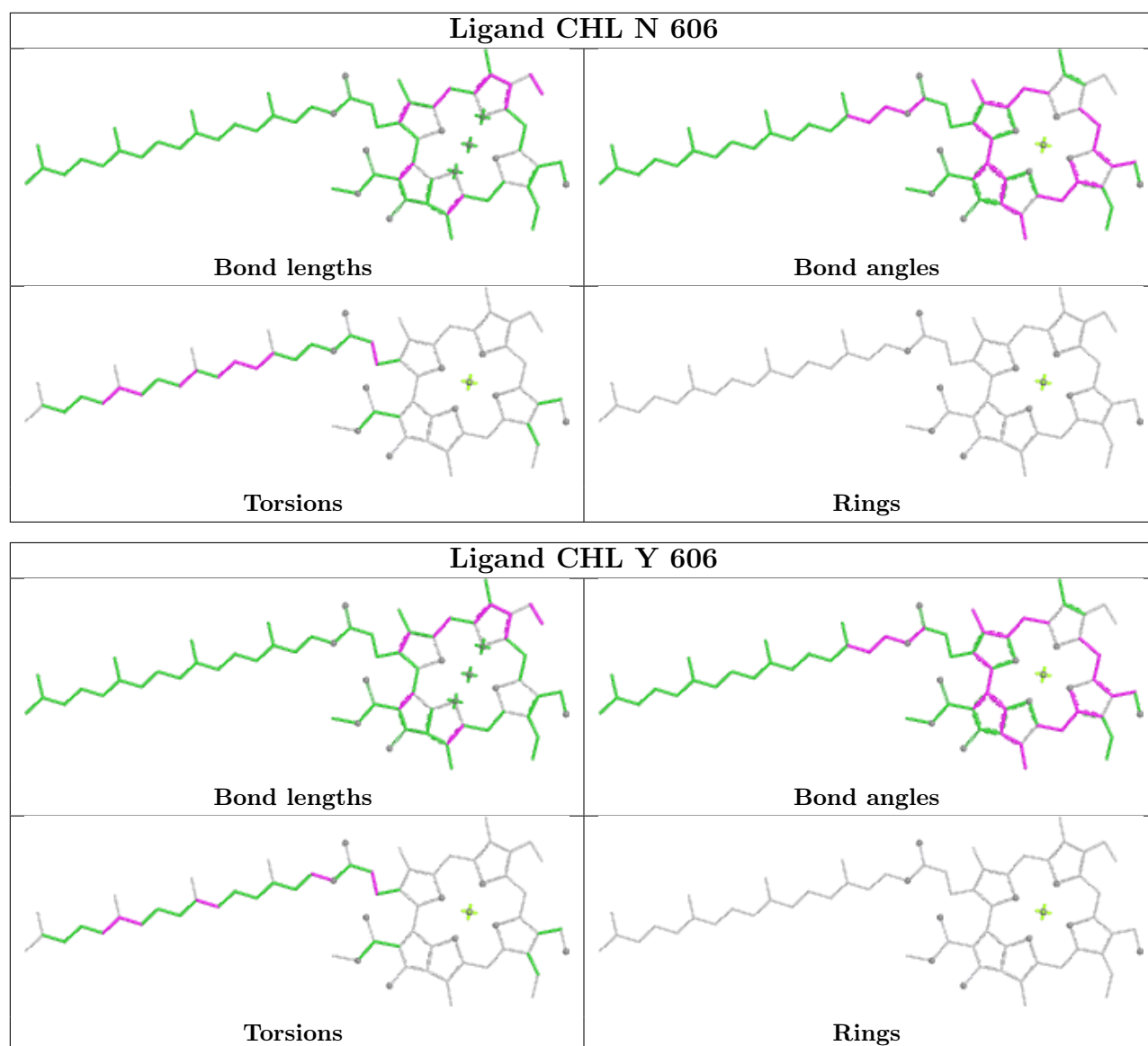




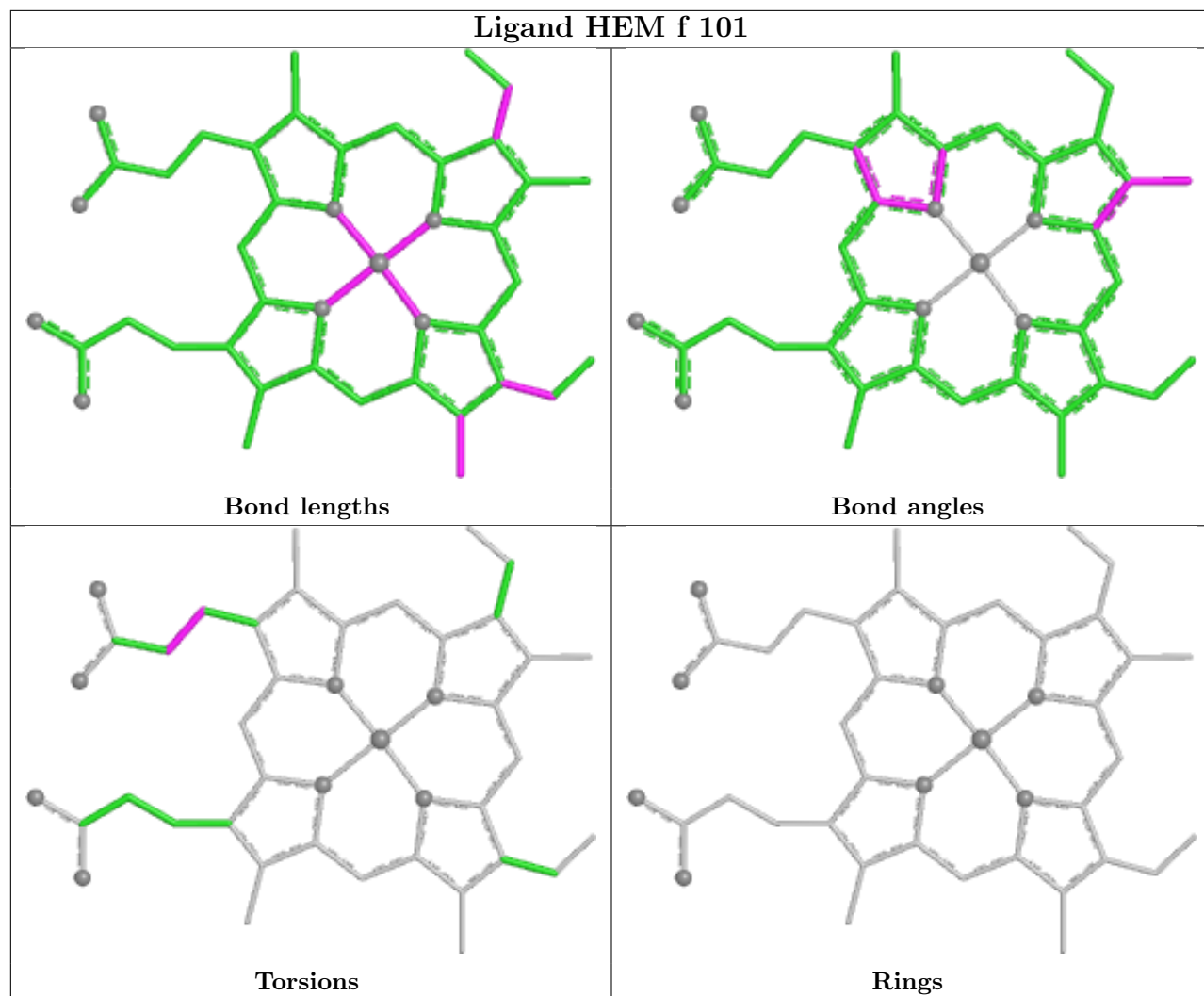


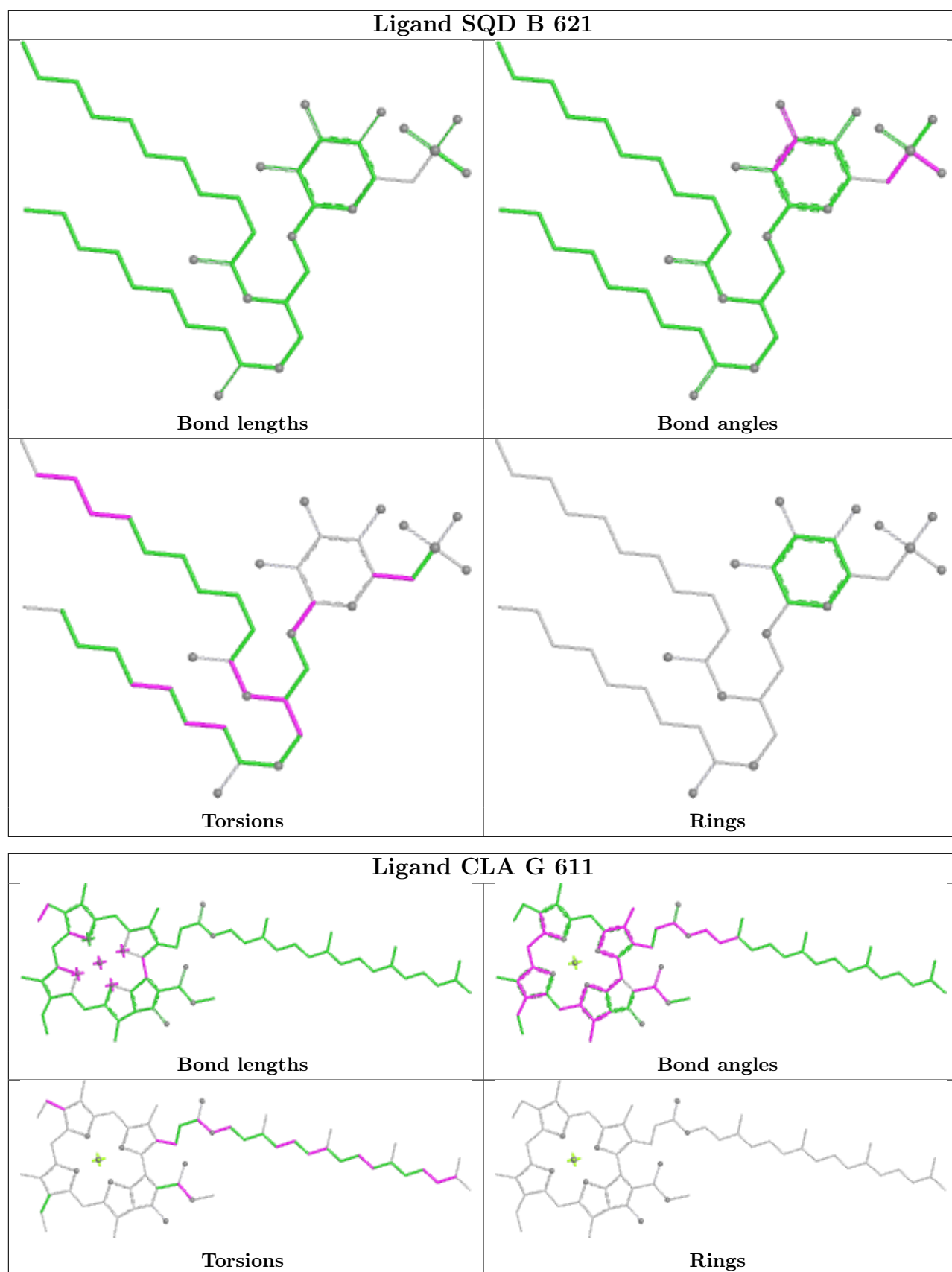


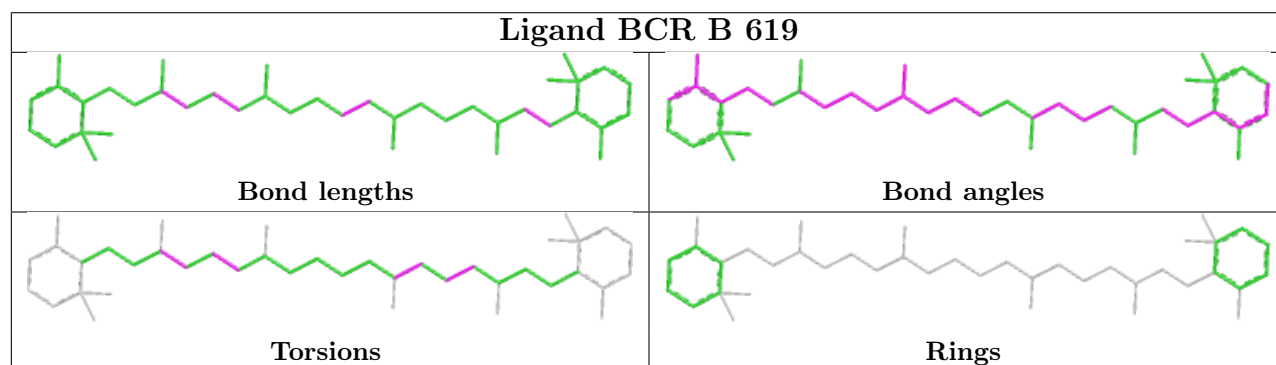
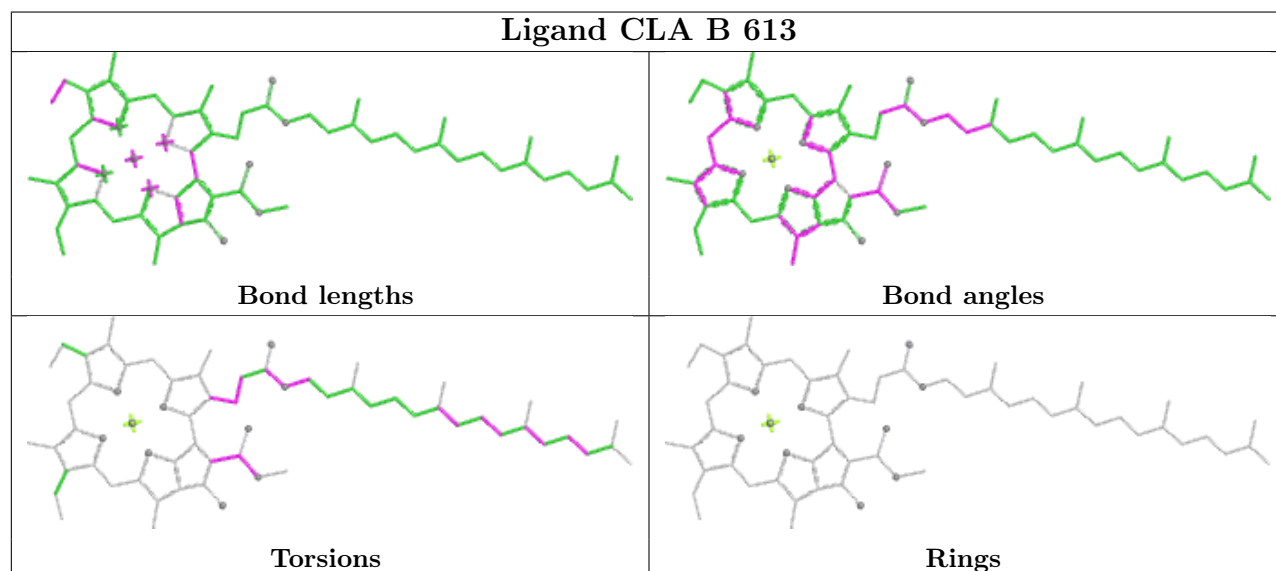
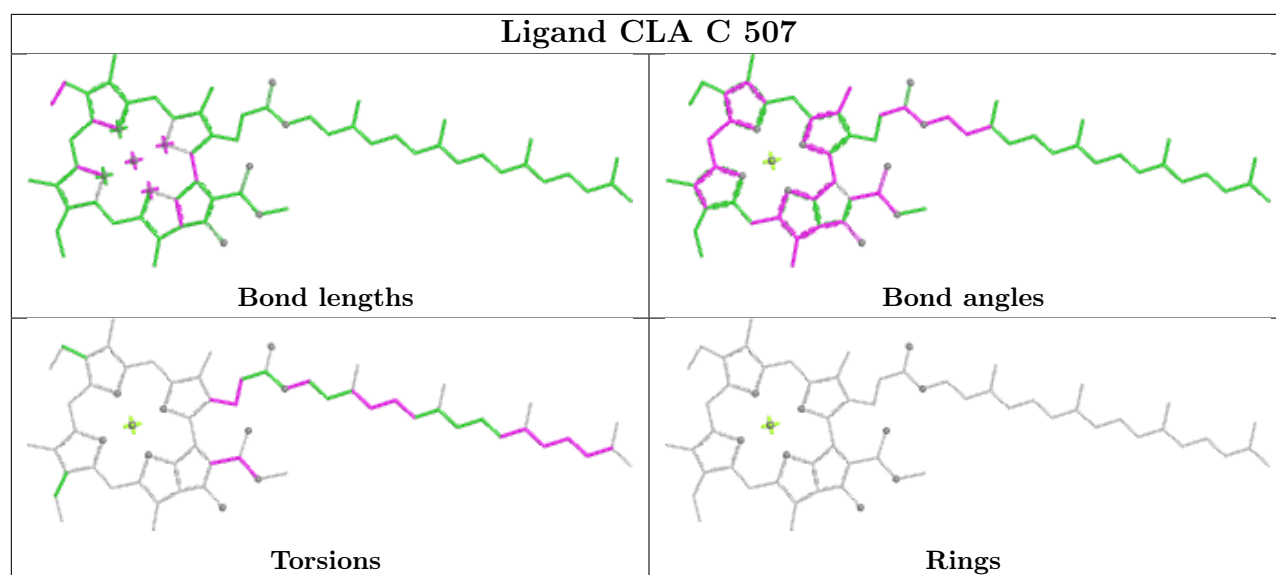
Ligand CLA S 603	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGA J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

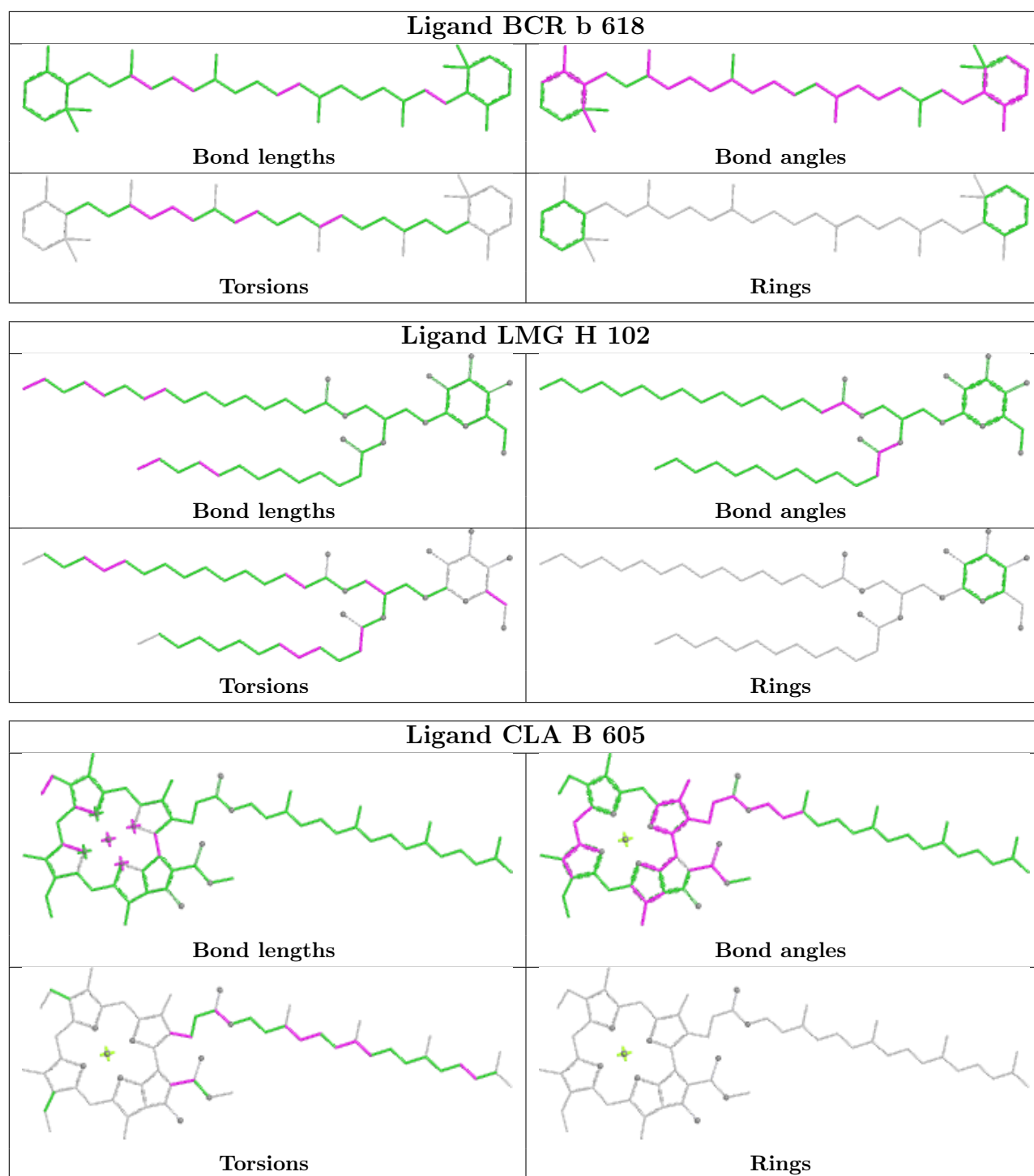


Ligand HEM f 101









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.

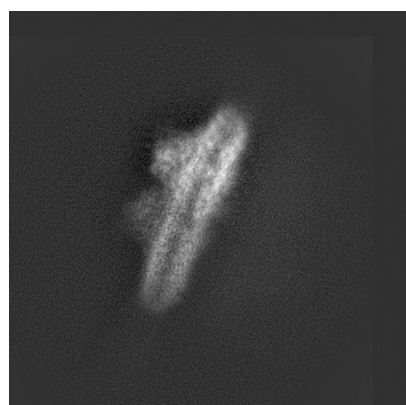
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13548. These allow visual inspection of the internal detail of the map and identification of artifacts.

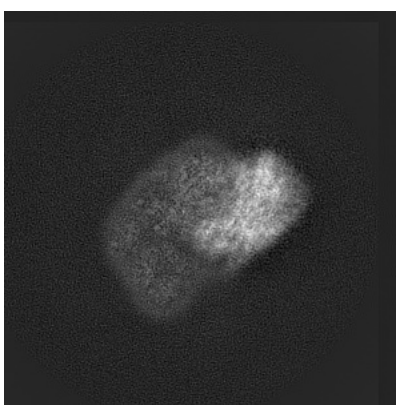
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

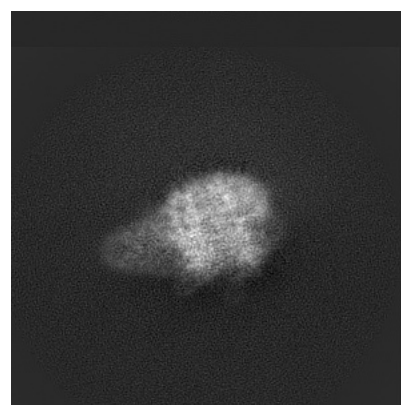
6.1.1 Primary map



X



Y

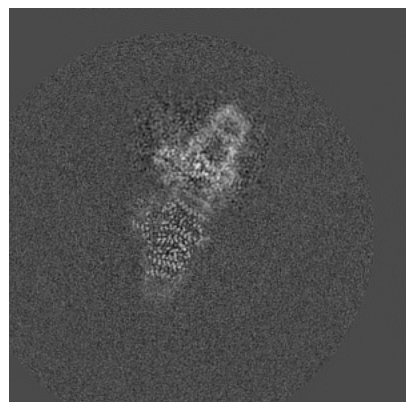


Z

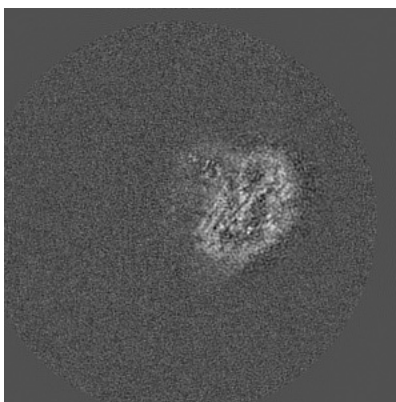
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

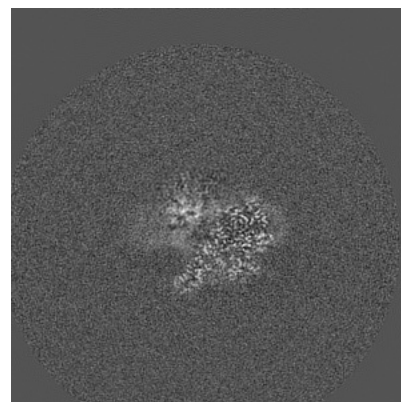
6.2.1 Primary map



X Index: 250



Y Index: 250

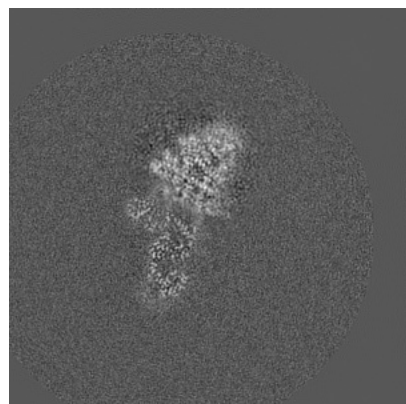


Z Index: 250

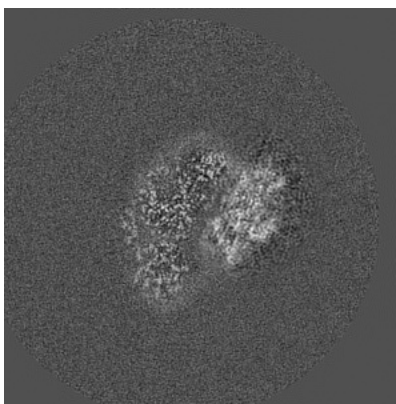
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

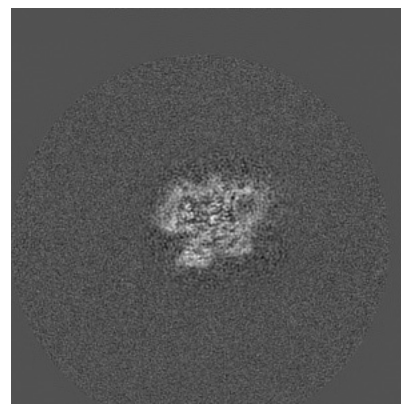
6.3.1 Primary map



X Index: 225



Y Index: 219

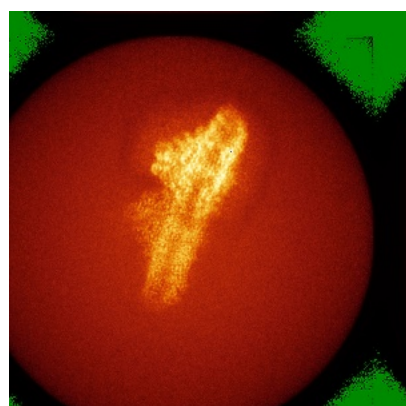


Z Index: 304

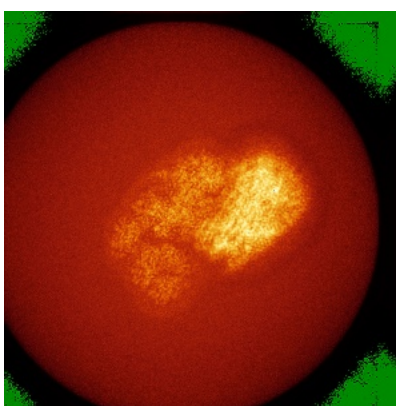
The images above show the largest variance slices of the map in three orthogonal directions.

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

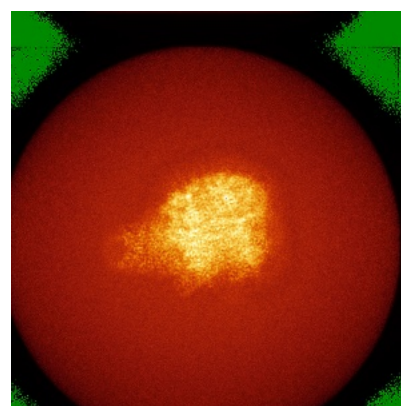
6.4.1 Primary map



X



Y

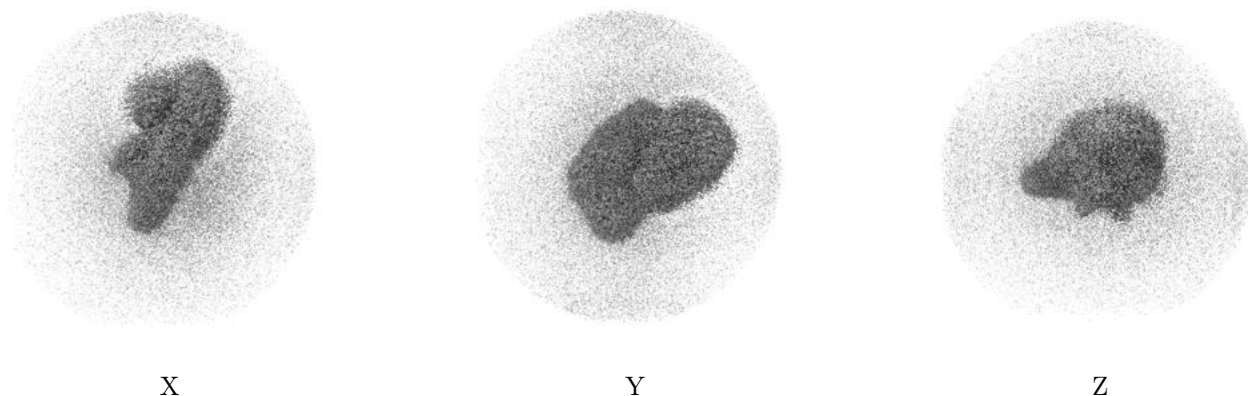


Z

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

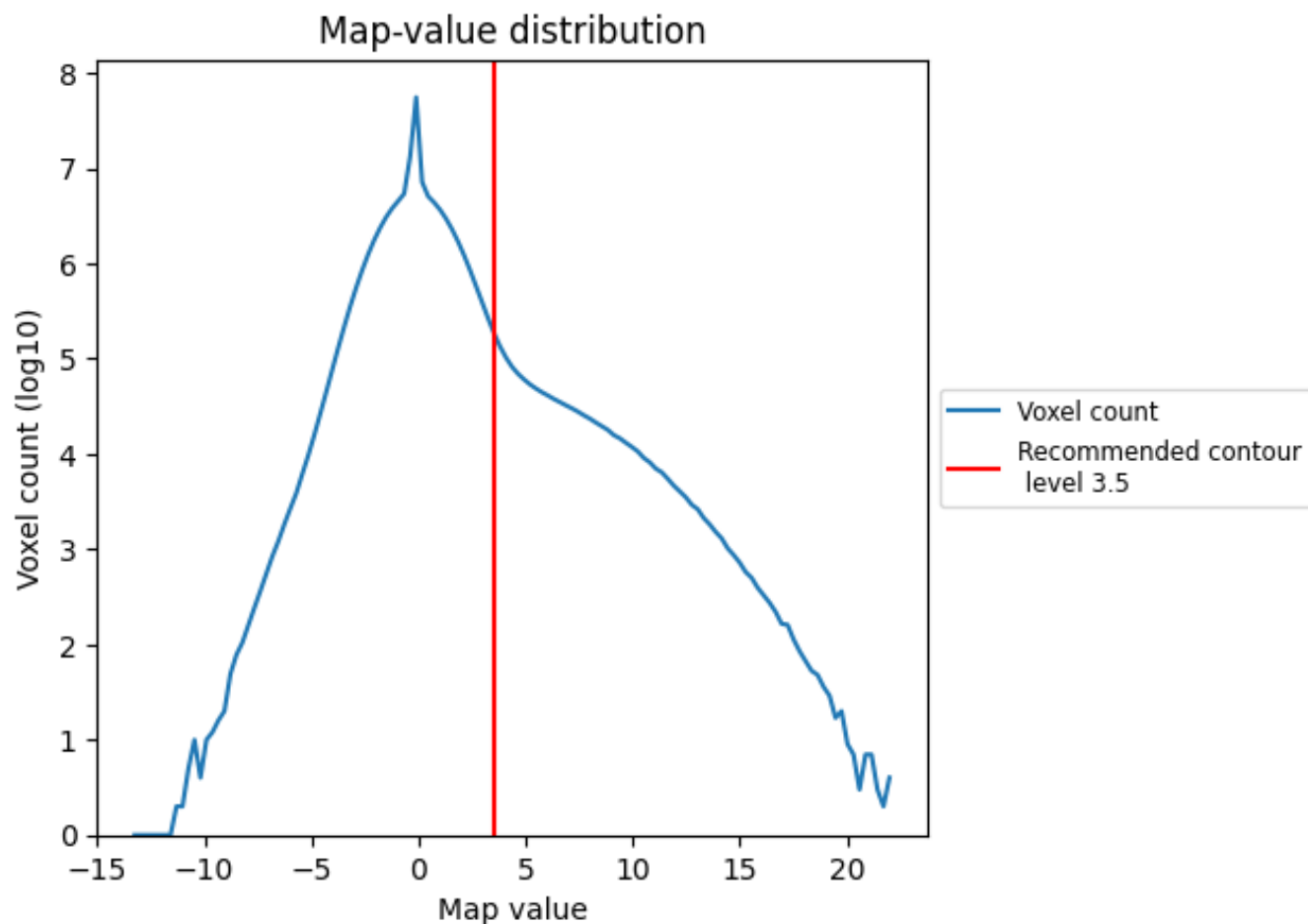
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

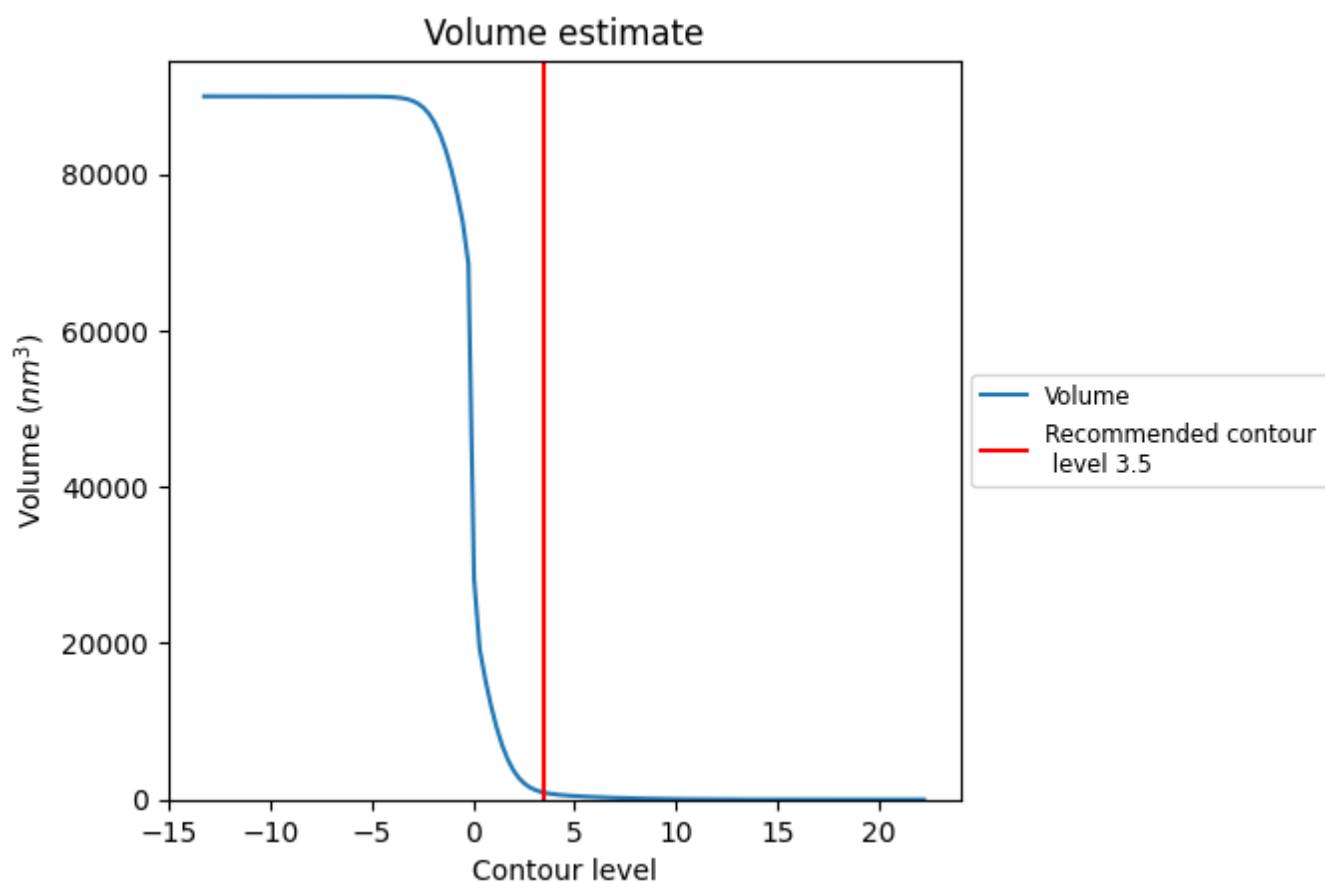
This section contains the results of statistical analysis of the map.

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.

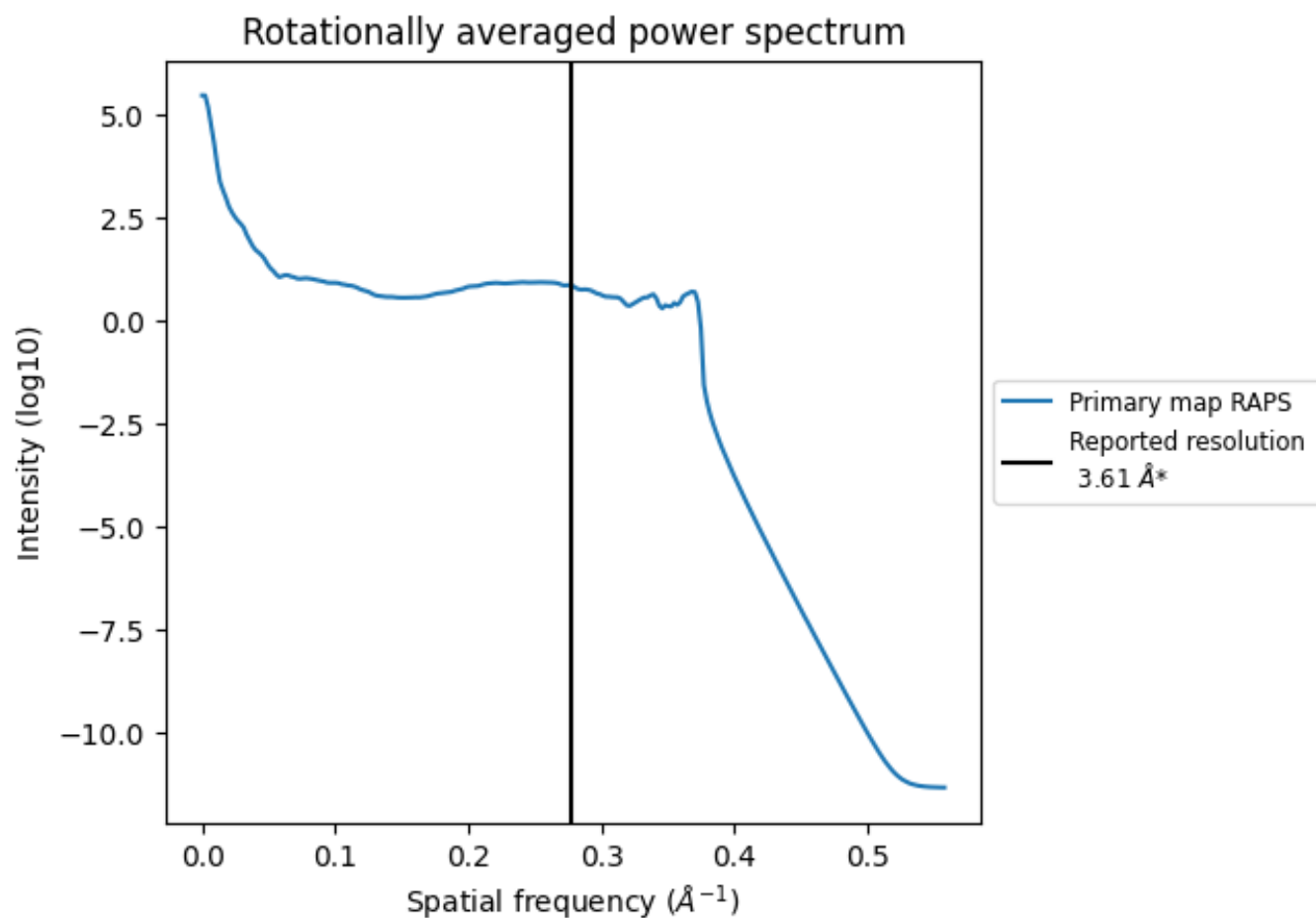
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 898 nm³; this corresponds to an approximate mass of 811 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 ⓘ

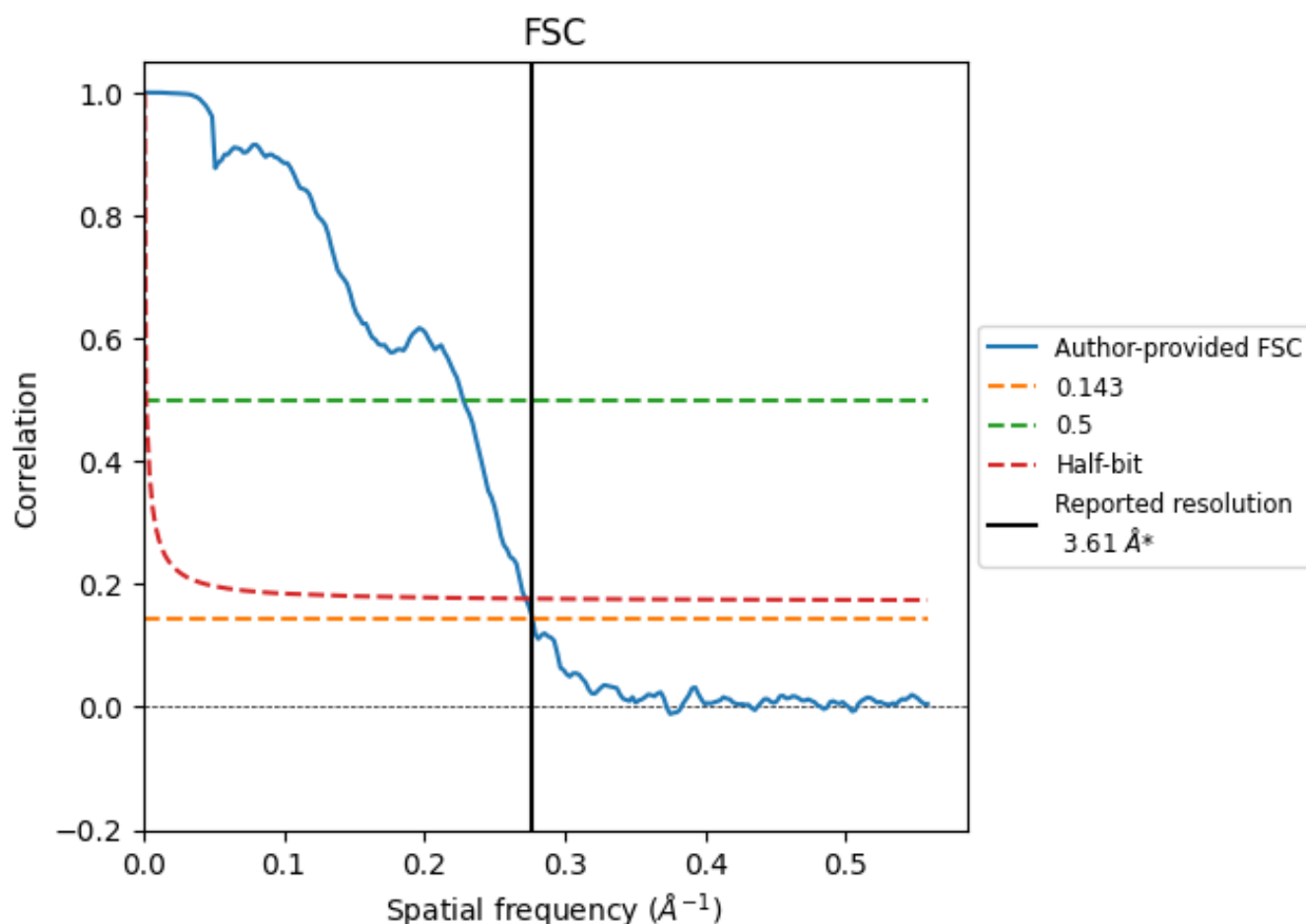


*Reported resolution corresponds to spatial frequency of 0.277 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.277 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	3.61	4.39	3.67
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

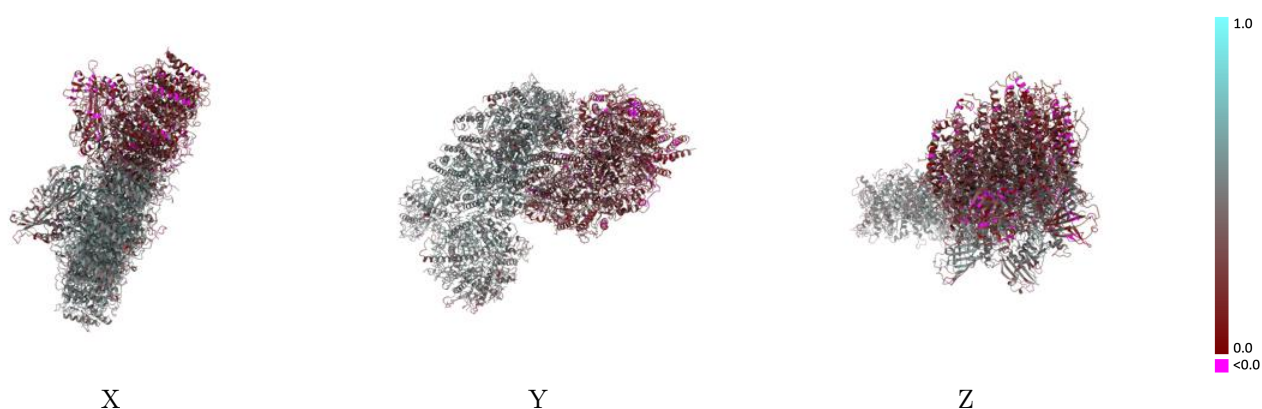
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13548 and PDB model 7PNK. Per-residue inclusion information can be found in section 3 on page 37.

9.1 Map-model overlay [i](#)

This section was not generated.

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

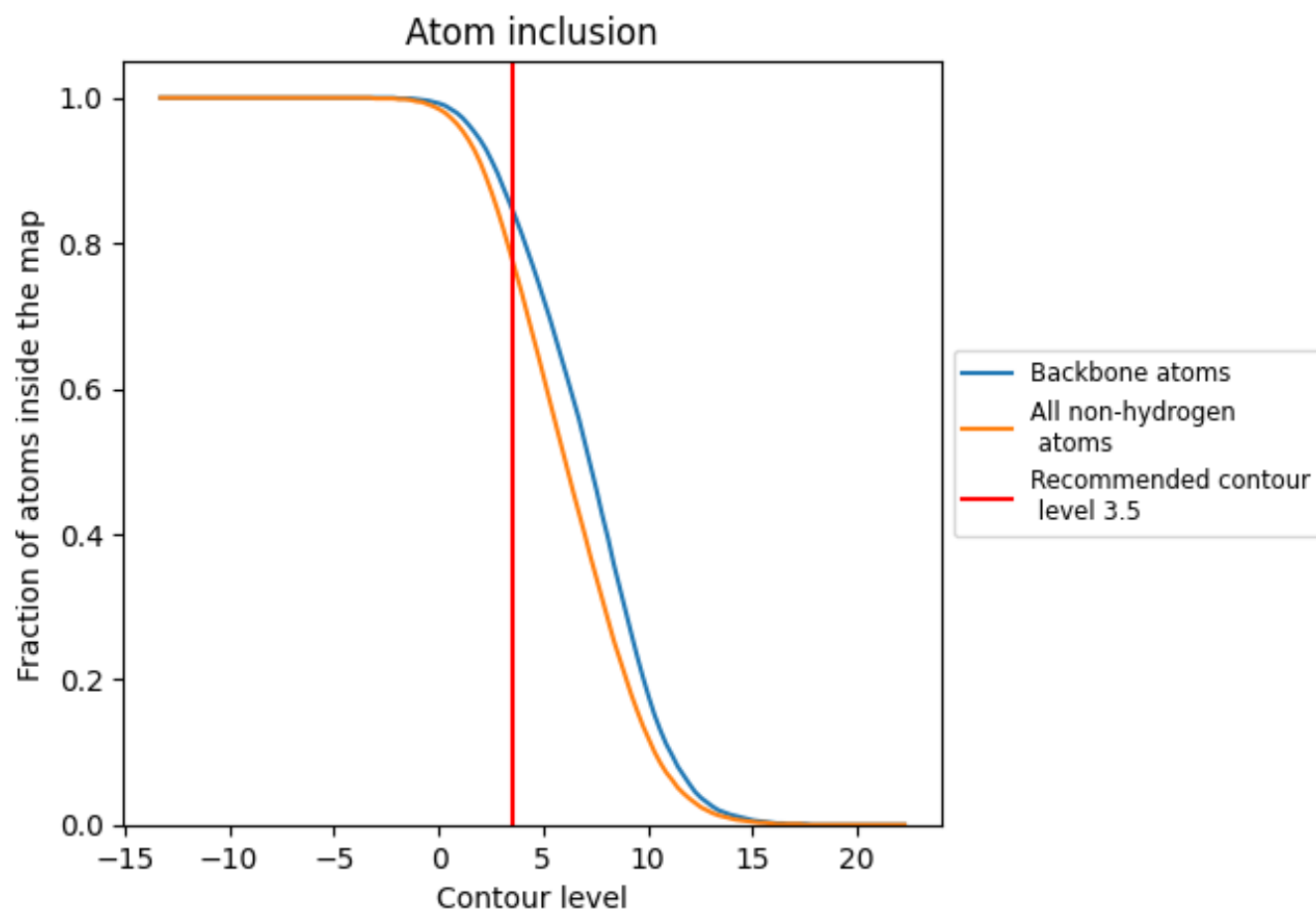


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.3810
A	 0.7720	 0.5100
B	 0.8000	 0.4910
C	 0.8120	 0.5310
D	 0.8180	 0.5240
E	 0.8140	 0.4740
F	 0.8080	 0.4820
G	 0.7440	 0.4420
H	 0.7960	 0.4790
I	 0.6840	 0.4500
J	 0.7280	 0.4740
K	 0.7340	 0.4710
L	 0.7490	 0.4910
M	 0.6470	 0.3770
N	 0.7750	 0.4800
O	 0.7230	 0.4310
P	 0.2770	 0.3450
S	 0.7710	 0.4780
T	 0.5970	 0.4100
U	 0.6330	 0.3920
V	 0.7600	 0.4840
W	 0.6560	 0.4540
X	 0.7510	 0.4430
Y	 0.7500	 0.4910
Z	 0.7910	 0.4930
a	 0.8530	 0.2340
b	 0.8320	 0.2570
c	 0.8620	 0.2170
d	 0.8790	 0.2770
e	 0.9490	 0.2380
f	 0.8950	 0.2490
h	 0.8330	 0.2430
i	 0.7810	 0.2010
j	 0.8760	 0.2850
k	 0.8860	 0.2450



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Chain	Atom inclusion	Q-score
l	 0.6840	 0.1810
m	 0.6650	 0.2260
o	 0.8250	 0.2010
p	 0.3550	 0.1570
t	 0.6010	 0.2440
u	 0.9400	 0.2420
v	 0.8980	 0.2180
w	 0.7950	 0.1740
x	 0.8660	 0.1970
z	 0.8970	 0.1980