



# wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 12:15 PM UTC

PDB ID : 9EVX / pdb\_00009evx  
EMDB ID : EMD-50019  
Title : cryoEM structure of Photosystem II averaged across S2-S3 states at 1.71 Angstrom resolution  
Authors : Hussein, R.; Graca, A.; Zouni, A.; Messinger, J.; Schroder, W.P.  
Deposited on : 2024-04-02  
Resolution : 1.71 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

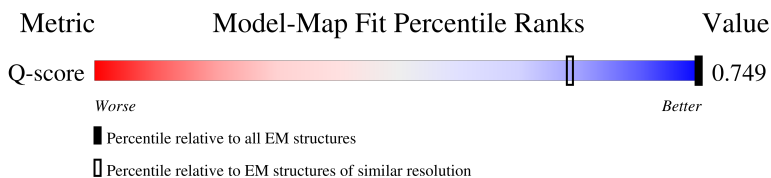
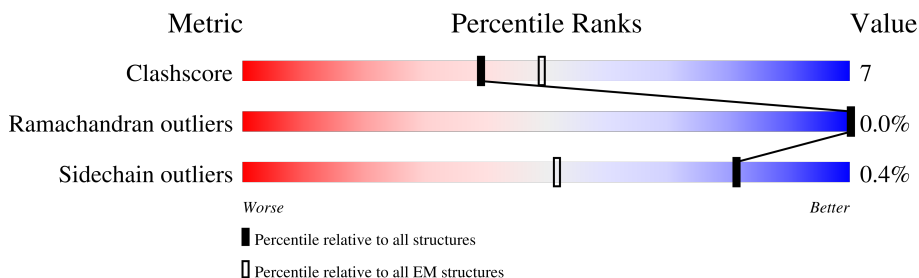
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 1.71 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.






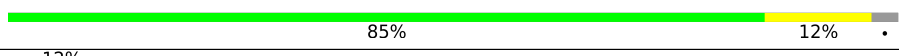
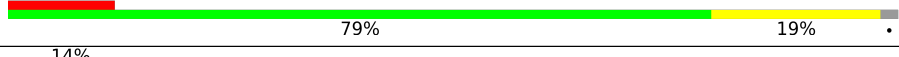



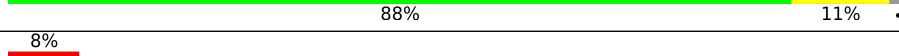
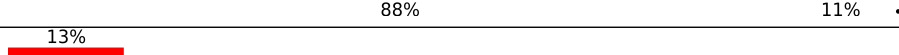
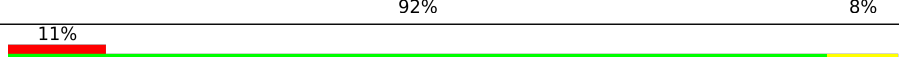
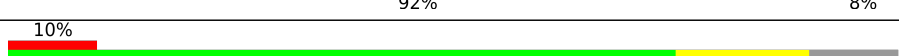

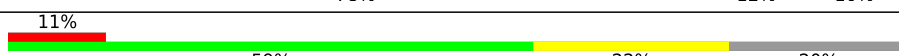
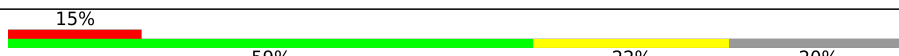
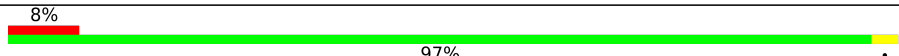
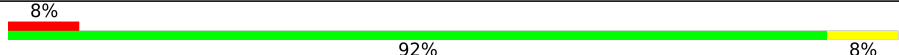




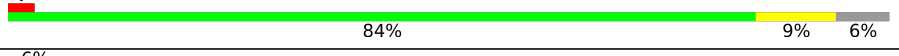

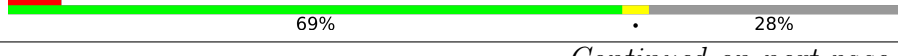

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	612 ( 1.21 - 2.21 )

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

Mol	Chain	Length	Quality of chain
1	A	344	 82% 15%
1	a	344	 82% 15%
2	B	510	 88% 11%
2	b	510	 88% 11%

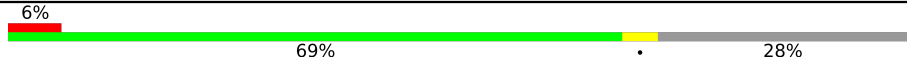

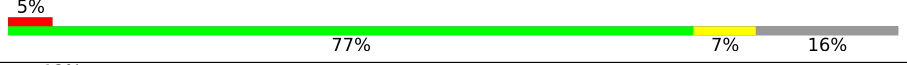


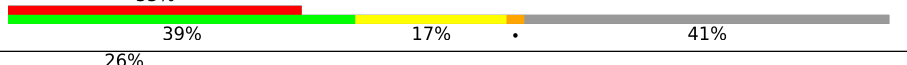
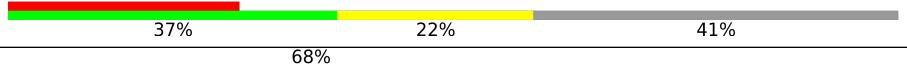

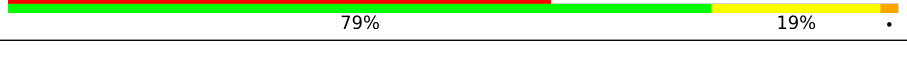
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Mol	Chain	Length	Quality of chain
3	C	461	 85% 12%
3	c	461	 85% 12%
4	D	352	 85% 12%
4	d	352	 85% 12%
5	E	84	 79% 19% 12%
5	e	84	 79% 19% 14%
6	F	45	 62% 13% 24%
6	f	45	 62% 13% 24%
7	H	66	 88% 11% 8%
7	h	66	 88% 11% 8%
8	I	38	 92% 8% 13%
8	i	38	 92% 8% 11%
9	J	40	 75% 15% 10%
9	j	40	 78% 12% 8%
10	K	46	 59% 22% 11%
10	k	46	 59% 22% 15%
11	L	37	 97% 8% 8%
11	l	37	 92% 8% 8%
12	M	36	 78% 11% 8% 8%
12	m	36	 81% 8% 6% 8%
13	O	272	 78% 12% 23% 11%
13	o	272	 79% 11% 20% 11%
14	T	32	 84% 9% 6% 6%
14	t	32	 84% 9% 6% 6%
15	U	134	 69% 28% 6%

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Mol	Chain	Length	Quality of chain
15	u	134	
16	V	163	
16	v	163	
17	X	41	
17	x	41	
18	Y	46	
18	y	46	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	419	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	419	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-

## 2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 104863 atoms, of which 52030 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	334	5164	1723	2530	433	463	15	3	0
1	a	334	5164	1723	2530	433	463	15	3	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	505	7852	2620	3858	667	694	13	3	0
2	b	505	7852	2620	3858	667	694	13	3	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	451	6899	2283	3408	585	610	13	2	0
3	c	451	6899	2283	3408	585	610	13	2	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	341	5338	1800	2621	444	461	12	0	0
4	d	341	5338	1800	2621	444	461	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	82	Total	C	H	N	O	0	0
			1301	431	640	107	123		
5	e	82	Total	C	H	N	O	0	0
			1301	431	640	107	123		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
6	F	34	Total	C	H	N	O	S	0	0
			557	187	282	45	42	1		
6	f	34	Total	C	H	N	O	S	0	0
			557	187	282	45	42	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace	
7	H	65	Total	C	H	N	O	S	2	0
			1045	338	534	83	87	3		
7	h	65	Total	C	H	N	O	S	2	0
			1045	338	534	83	87	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	41	CYS	PHE	variant	UNP Q8DJ43
h	41	CYS	PHE	variant	UNP Q8DJ43

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
8	I	38	Total	C	H	N	O	S	0	0
			641	211	328	48	53	1		
8	i	38	Total	C	H	N	O	S	0	0
			641	211	328	48	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
9	J	36	Total	C	H	N	O	S	0	0
			525	174	268	40	42	1		
9	j	36	Total	C	H	N	O	S	0	0
			525	174	268	40	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	37	Total	C	H	N	O	0	0
			598	204	305	43	46		
10	k	37	Total	C	H	N	O	0	0
			598	204	305	43	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
11	L	37	Total	C	H	N	O	S	2	0
			640	208	328	49	54	1		
11	l	37	Total	C	H	N	O	S	2	0
			640	208	328	49	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
12	M	33	Total	C	H	N	O	S	2	0
			545	177	281	38	48	1		
12	m	33	Total	C	H	N	O	S	2	0
			545	177	281	38	48	1		

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace	
13	O	243	Total	C	H	N	O	S	3	0
			3710	1171	1834	313	387	5		
13	o	243	Total	C	H	N	O	S	3	0
			3710	1171	1834	313	387	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
14	T	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		
14	t	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	97	Total	C	H	N	O	0	0
			1547	491	773	129	154		
15	u	97	Total	C	H	N	O	0	0
			1547	491	773	129	154		

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0
			2135	675	1071	177	208	4		
16	v	137	Total	C	H	N	O	S	0	0
			2135	675	1071	177	208	4		

- Molecule 17 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	38	Total	C	H	N	O	0	0
			593	188	312	45	48		
17	x	38	Total	C	H	N	O	0	0
			593	188	312	45	48		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Y	27	Total	C	H	N	O	S	0	0
			423	131	224	35	30	3		
18	y	27	Total	C	H	N	O	S	0	0
			425	131	226	35	30	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0
			995	328	516	72	77	2		
19	z	62	Total	C	H	N	O	S	0	0
			995	328	516	72	77	2		

- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Fe	0
			1	1	

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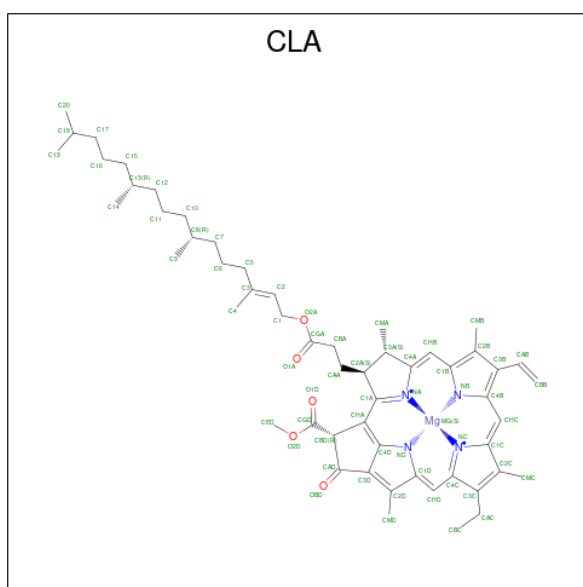
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Mol	Chain	Residues	Atoms	AltConf
20	a	1	Total Fe 1 1	0

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf	
22	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	A	1	Total	C	H	Mg	N	O	0
			102	44	48	1	4	5	
22	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 117	C 49	H 58	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	a	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	a	1	Total 102	C 44	H 48	Mg 1	N 4	O 5	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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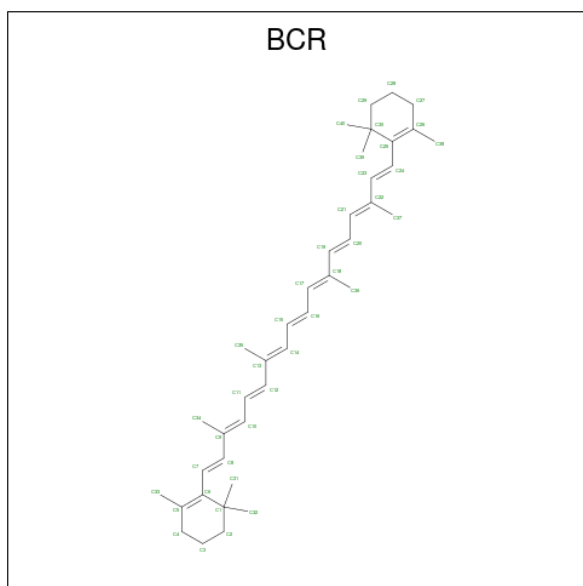
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 117	C 49	H 58	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
22	d	1	137	55	72	1	4	5	0

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



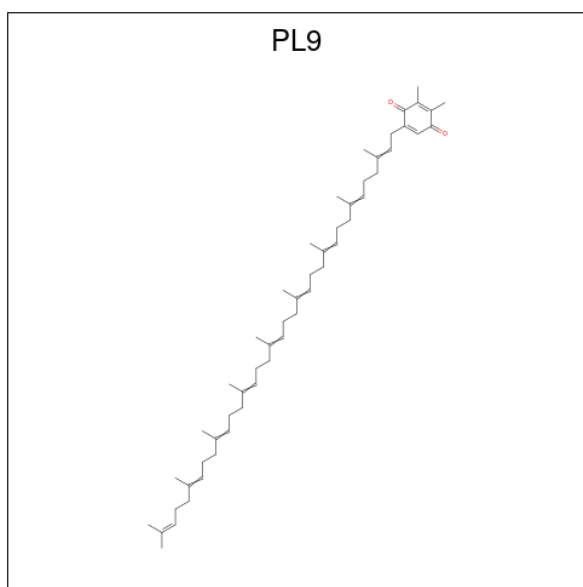
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	C	1	Total	C	H	0
			96	40	56	
23	C	1	Total	C	H	0
			96	40	56	
23	D	1	Total	C	H	0
			96	40	56	
23	H	1	Total	C	H	0
			96	40	56	
23	K	1	Total	C	H	0
			96	40	56	
23	K	1	Total	C	H	0
			96	40	56	

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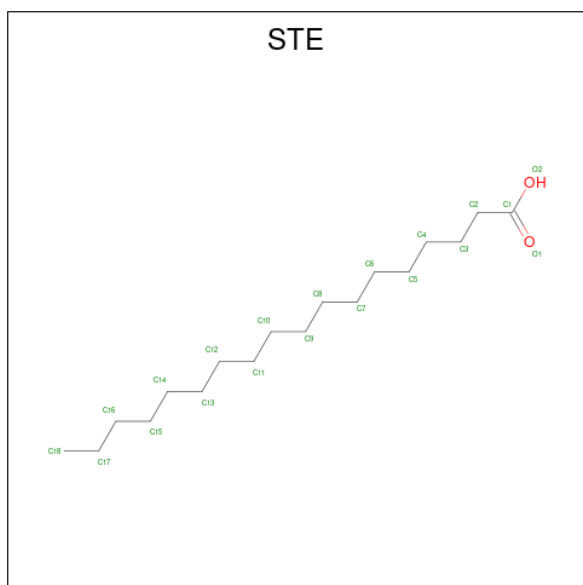
Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
23	T	1	96	40	56	0
23	a	1	96	40	56	0
23	b	1	96	40	56	0
23	b	1	96	40	56	0
23	b	1	96	40	56	0
23	c	1	96	40	56	0
23	c	1	96	40	56	0
23	d	1	96	40	56	0
23	h	1	96	40	56	0
23	k	1	96	40	56	0
23	k	1	96	40	56	0
23	t	1	96	40	56	0

- Molecule 24 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<sub>53</sub>H<sub>80</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
24	A	1	135	53	80	2	0
24	D	1	135	53	80	2	0
24	a	1	135	53	80	2	0
24	d	1	135	53	80	2	0

- Molecule 25 is STEARIC ACID (CCD ID: STE) (formula:  $C_{18}H_{36}O_2$ ).



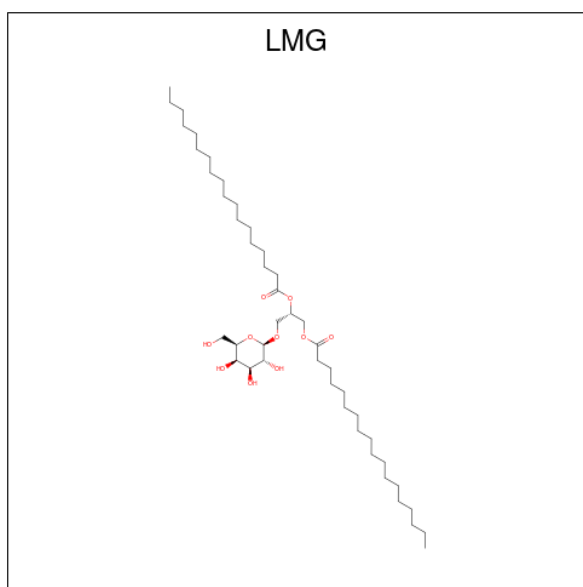
Mol	Chain	Residues	Atoms			AltConf	
25	A	1	Total	C	H	0	
			23	9	14		
25	A	1	Total	C	H	0	
			23	8	15		
25	A	1	Total	C	H	0	
			32	11	21		
25	A	1	Total	C	H	0	
			32	11	21		
25	A	1	Total	C	H	O	0
			28	10	16	2	
25	B	1	Total	C	H	O	0
			43	15	26	2	
25	B	1	Total	C	H	O	0
			28	10	16	2	
25	B	1	Total	C	H	0	
			32	12	20		
25	C	1	Total	C	H	O	0
			34	12	20	2	
25	C	1	Total	C	H	O	0
			28	10	16	2	
25	C	1	Total	C	H	0	
			23	8	15		
25	D	1	Total	C	H	O	0
			55	18	35	2	
25	D	1	Total	C	H	0	
			26	9	17		
25	E	1	Total	C	H	O	0
			28	10	16	2	
25	E	1	Total	C	H	0	
			35	12	23		
25	E	1	Total	C	H	O	0
			55	18	35	2	
25	I	1	Total	C	H	0	
			38	14	24		
25	J	1	Total	C	H	0	
			32	12	20		
25	K	1	Total	C	H	0	
			32	11	21		
25	M	1	Total	C	H	0	
			26	10	16		
25	T	1	Total	C	H	0	
			44	15	29		
25	a	1	Total	C	H	0	
			23	9	14		

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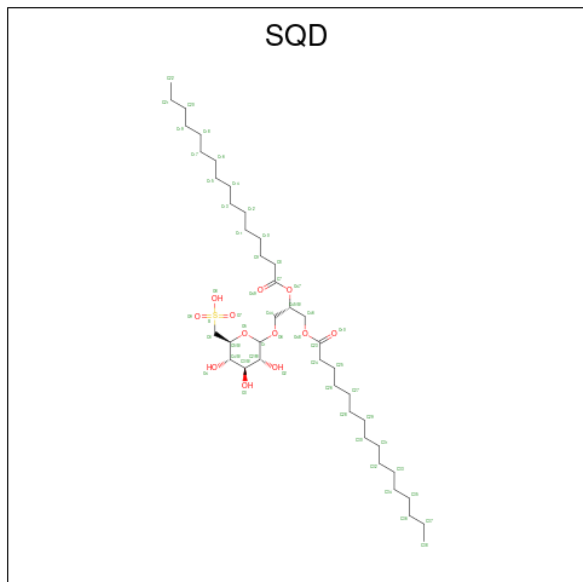
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
25	a	1	23	8	15		0
25	a	1	32	11	21		0
25	a	1	32	11	21		0
25	a	1	28	10	16	2	0
25	b	1	32	12	20		0
25	b	1	43	15	26	2	0
25	b	1	28	10	16	2	0
25	c	1	34	12	20	2	0
25	c	1	28	10	16	2	0
25	c	1	23	8	15		0
25	d	1	55	18	35	2	0
25	d	1	26	9	17		0
25	e	1	28	10	16	2	0
25	e	1	35	12	23		0
25	e	1	55	18	35	2	0
25	i	1	38	14	24		0
25	j	1	32	12	20		0
25	k	1	32	11	21		0
25	m	1	26	10	16		0
25	t	1	46	16	28	2	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



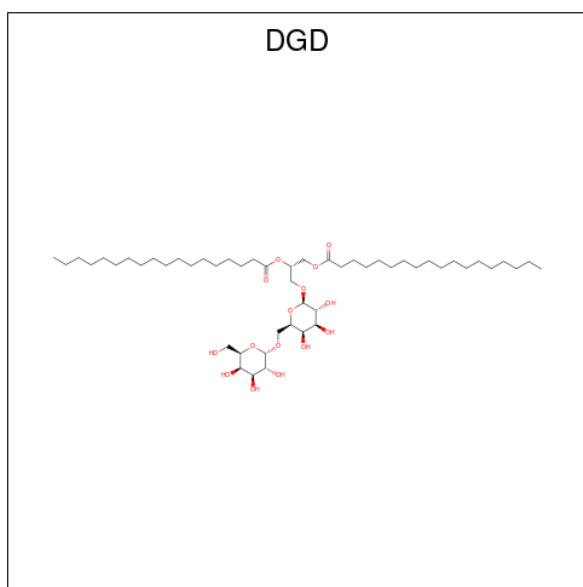
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
26	A	1	Total 114	C 38	H 66	O 10	0
26	B	1	Total 123	C 41	H 72	O 10	0
26	C	1	Total 114	C 38	H 66	O 10	0
26	C	1	Total 120	C 40	H 70	O 10	0
26	D	1	Total 83	C 29	H 49	O 5	0
26	D	1	Total 123	C 41	H 72	O 10	0
26	H	1	Total 98	C 34	H 59	O 5	0
26	a	1	Total 114	C 38	H 66	O 10	0
26	b	1	Total 123	C 41	H 72	O 10	0
26	c	1	Total 114	C 38	H 66	O 10	0
26	c	1	Total 120	C 40	H 70	O 10	0
26	d	1	Total 83	C 29	H 49	O 5	0
26	d	1	Total 123	C 41	H 72	O 10	0
26	h	1	Total 98	C 34	H 59	O 5	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



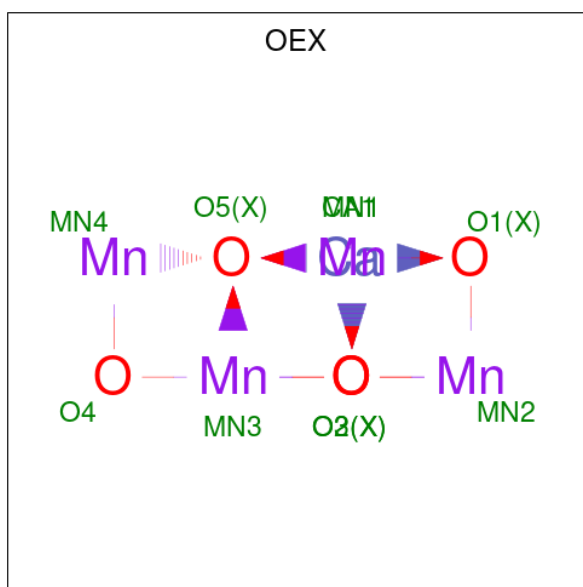
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	S	
27	A	1	Total	C	H	O	S	0
			122	39	70	12	1	
27	A	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	B	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	X	1	Total	C	H	O	S	0
			81	25	45	10	1	
27	a	1	Total	C	H	O	S	0
			122	39	70	12	1	
27	a	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	b	1	Total	C	H	O	S	0
			113	36	64	12	1	
27	x	1	Total	C	H	O	S	0
			81	25	45	10	1	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



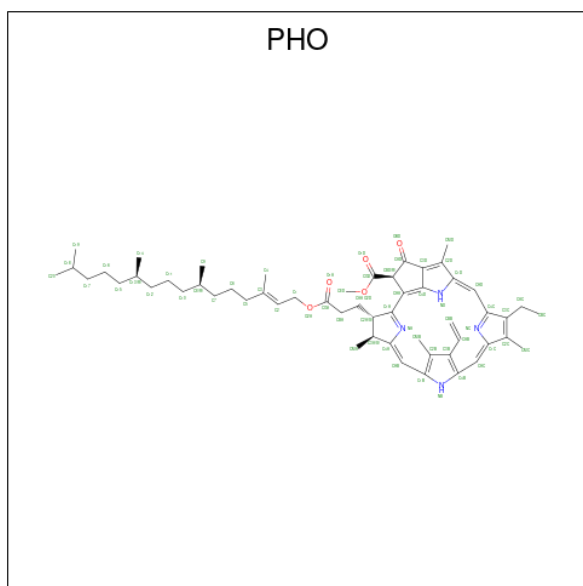
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
28	A	1	162	51	96	15	0
28	C	1	144	47	82	15	0
28	C	1	129	42	72	15	0
28	C	1	144	47	82	15	0
28	H	1	144	47	82	15	0
28	a	1	162	51	96	15	0
28	c	1	144	47	82	15	0
28	c	1	129	42	72	15	0
28	c	1	144	47	82	15	0
28	h	1	144	47	82	15	0

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



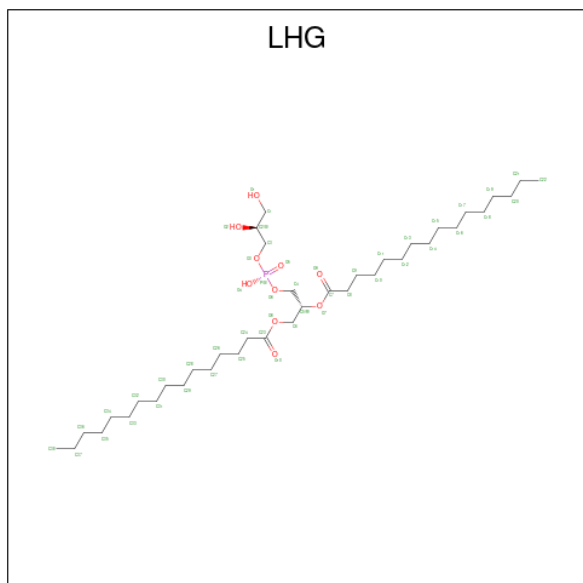
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	N		O
30	A	1	138	55	74	4	5	0
30	D	1	138	55	74	4	5	0

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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	N		O
30	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
30	d	1	Total	C	H	N	O	0
			138	55	74	4	5	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



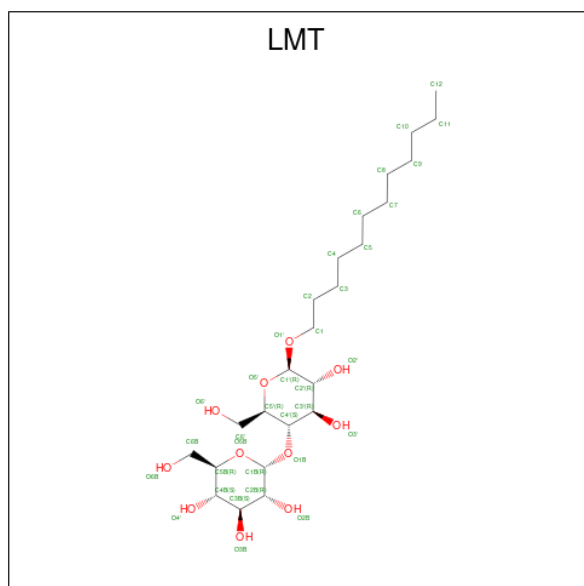
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	O		P
31	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	D	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	D	1	Total	C	H	O	P	0
			114	36	67	10	1	
31	D	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	L	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	a	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	d	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	d	1	Total	C	H	O	P	0
			114	36	67	10	1	
31	d	1	Total	C	H	O	P	0
			123	38	74	10	1	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
31	1	1	123	38	74	10	1	0

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



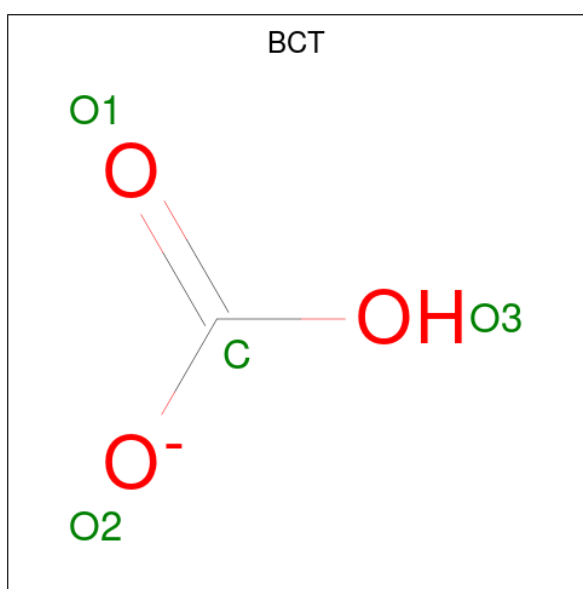
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
32	B	1	60	19	35	6	0
32	C	1	59	18	35	6	0
32	C	1	80	24	45	11	0
32	E	1	57	18	33	6	0
32	J	1	58	18	34	6	0
32	M	1	79	24	44	11	0
32	Z	1	79	24	44	11	0
32	b	1	60	19	35	6	0
32	c	1	59	18	35	6	0
32	c	1	80	24	45	11	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
32	e	1	Total 57	C 18	H 33	O 6	0
32	j	1	Total 58	C 18	H 34	O 6	0
32	m	1	Total 79	C 24	H 44	O 11	0
32	z	1	Total 79	C 24	H 44	O 11	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
33	D	1	Total 5	C 1	H 1	O 3	0
33	d	1	Total 5	C 1	H 1	O 3	0

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).



- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	172	Total 172	O 172	0
36	B	273	Total 273	O 273	0
36	C	200	Total 201	O 201	1
36	D	177	Total 177	O 177	0
36	E	38	Total 38	O 38	0
36	F	4	Total 4	O 4	0
36	H	28	Total 28	O 28	0
36	I	6	Total 6	O 6	0
36	J	14	Total 14	O 14	0
36	K	4	Total 4	O 4	0
36	L	16	Total 16	O 16	0
36	M	7	Total 7	O 7	0
36	O	99	Total 99	O 99	0
36	T	8	Total 8	O 8	0
36	U	61	Total 61	O 61	0
36	V	95	Total 95	O 95	0
36	X	9	Total 9	O 9	0
36	a	168	Total 168	O 168	0
36	b	273	Total 273	O 273	0
36	c	201	Total 202	O 202	1
36	d	177	Total 177	O 177	0

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Mol	Chain	Residues	Atoms		AltConf
36	e	38	Total 38	O 38	0
36	f	4	Total 4	O 4	0
36	h	28	Total 28	O 28	0
36	i	6	Total 6	O 6	0
36	j	14	Total 14	O 14	0
36	k	4	Total 4	O 4	0
36	l	13	Total 13	O 13	0
36	m	3	Total 3	O 3	0
36	o	99	Total 99	O 99	0
36	t	7	Total 7	O 7	0
36	u	55	Total 55	O 55	0
36	v	95	Total 95	O 95	0
36	x	9	Total 9	O 9	0

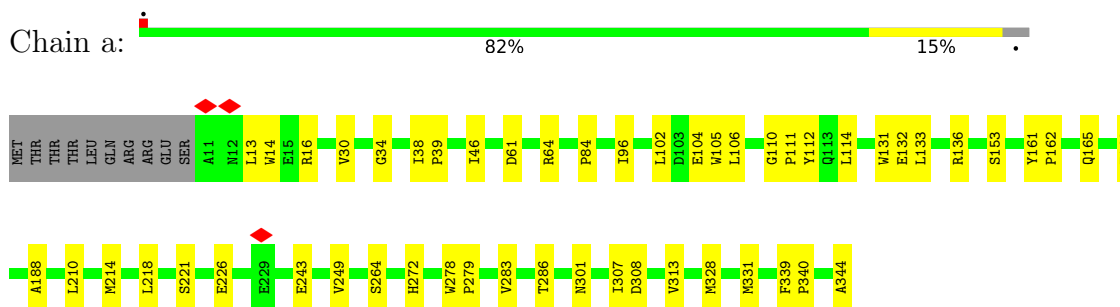
### 3 Residue-property plots [i](#)

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

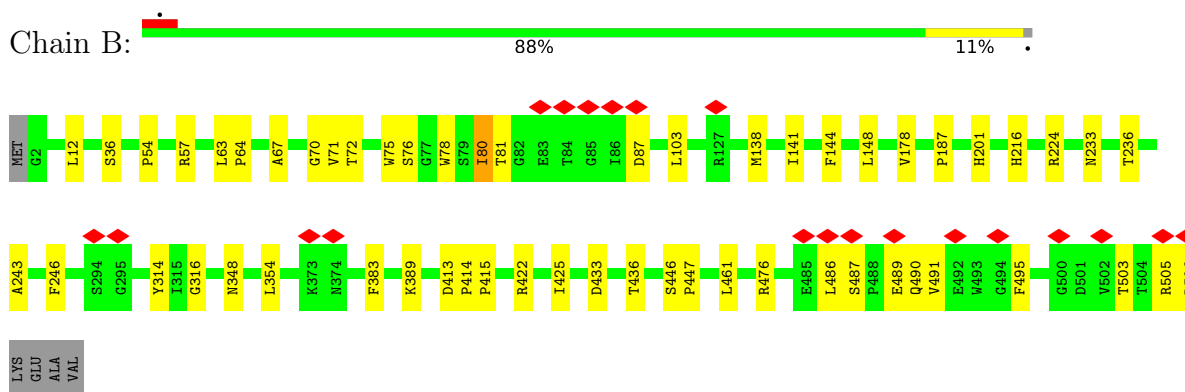
- Molecule 1: Photosystem II protein D1 1




- Molecule 1: Photosystem II protein D1 1

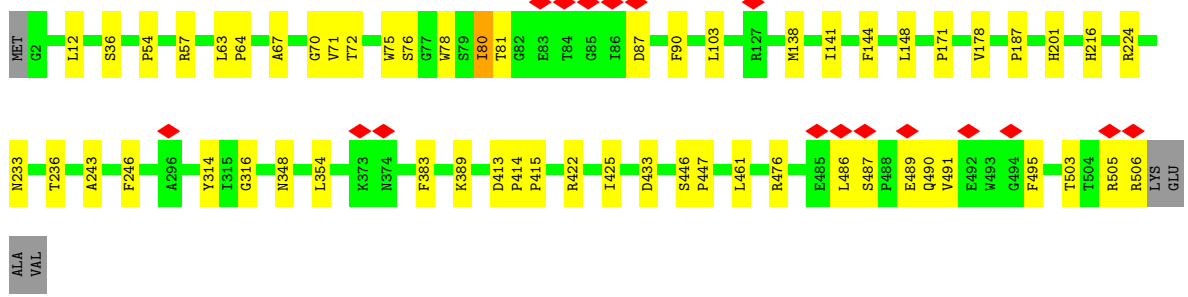


- Molecule 2: Photosystem II CP47 reaction center protein




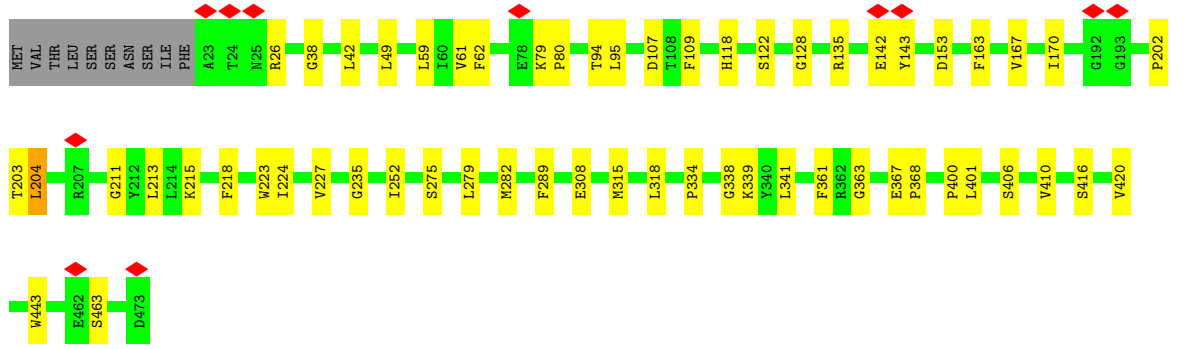
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  88% 11%




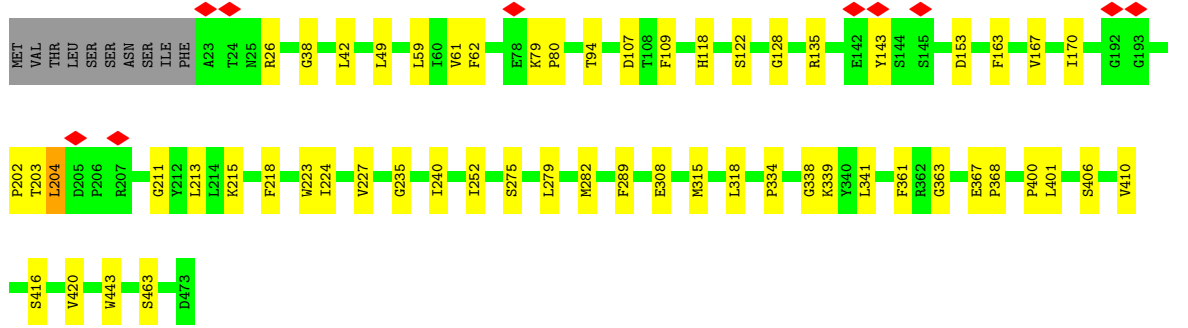
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  85% 12%




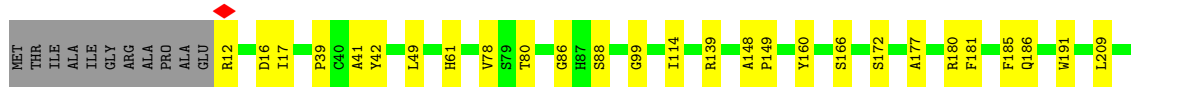
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  85% 12%



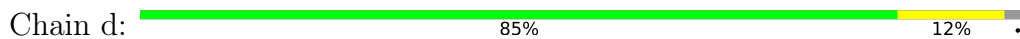
• Molecule 4: Photosystem II D2 protein

Chain D:  85% 12%

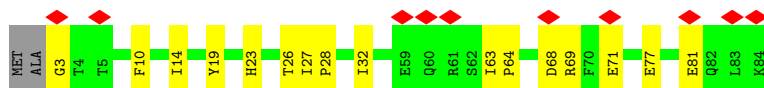
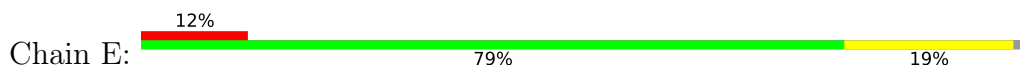




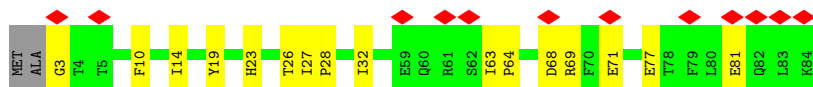
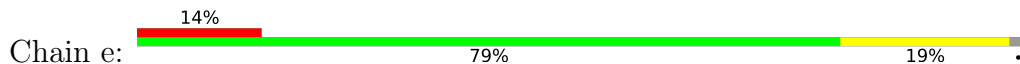
- Molecule 4: Photosystem II D2 protein



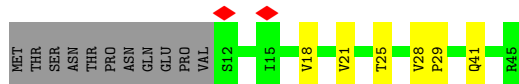
- Molecule 5: Cytochrome b559 subunit alpha



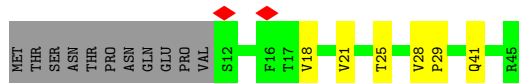
- Molecule 5: Cytochrome b559 subunit alpha



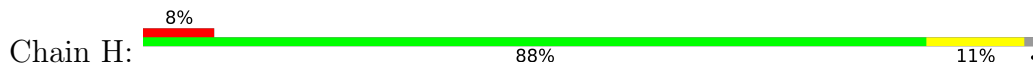
- Molecule 6: Cytochrome b559 subunit beta

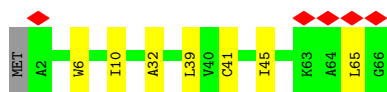


- Molecule 6: Cytochrome b559 subunit beta

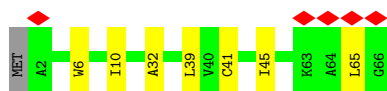
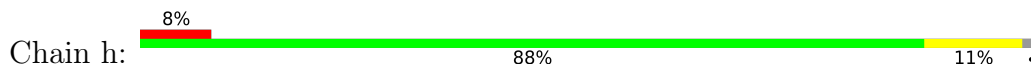


- Molecule 7: Photosystem II reaction center protein H

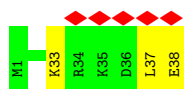
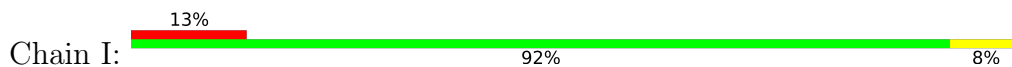




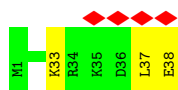
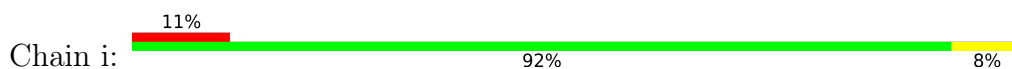
- Molecule 7: Photosystem II reaction center protein H



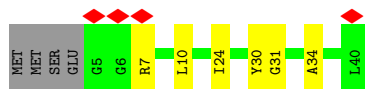
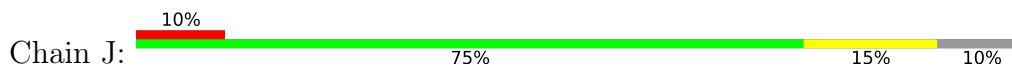
- Molecule 8: Photosystem II reaction center protein I



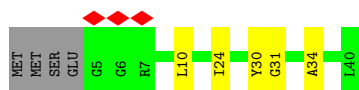
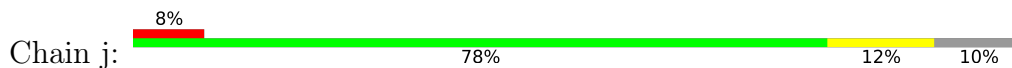
- Molecule 8: Photosystem II reaction center protein I



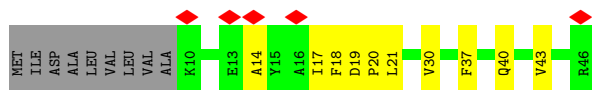
- Molecule 9: Photosystem II reaction center protein J



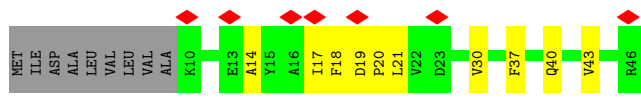
- Molecule 9: Photosystem II reaction center protein J



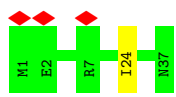
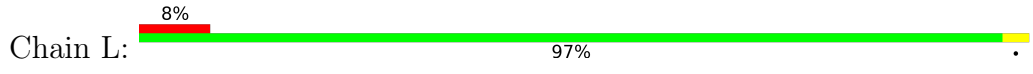
- Molecule 10: Photosystem II reaction center protein K



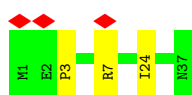
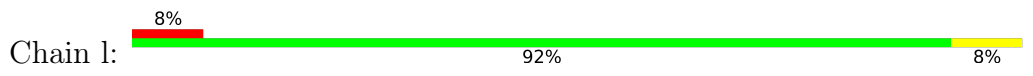
- Molecule 10: Photosystem II reaction center protein K



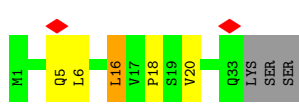
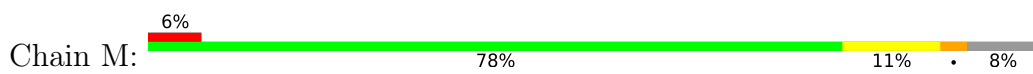
• Molecule 11: Photosystem II reaction center protein L



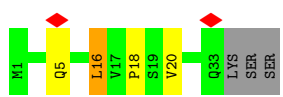
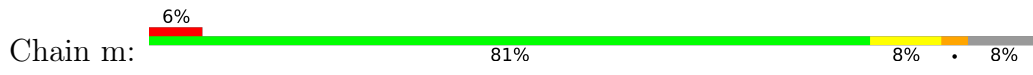
• Molecule 11: Photosystem II reaction center protein L



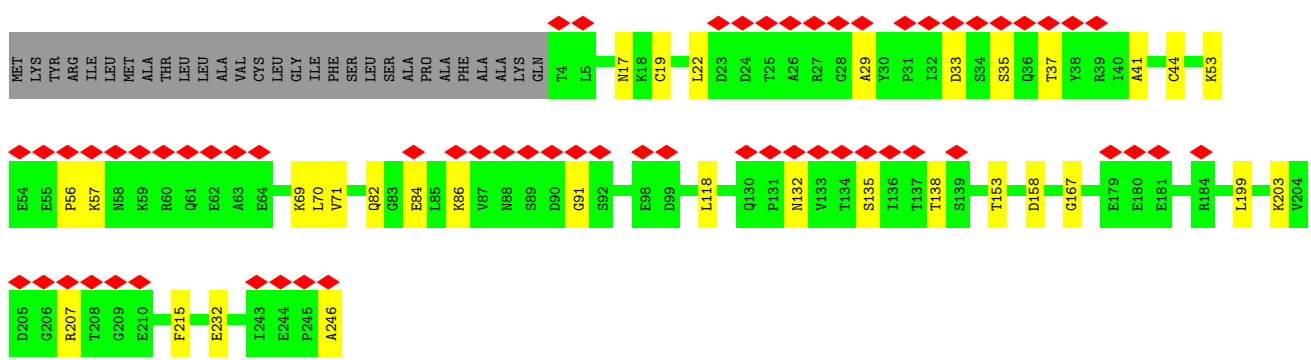
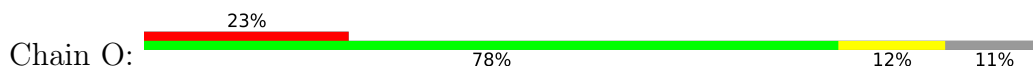
• Molecule 12: Photosystem II reaction center protein M



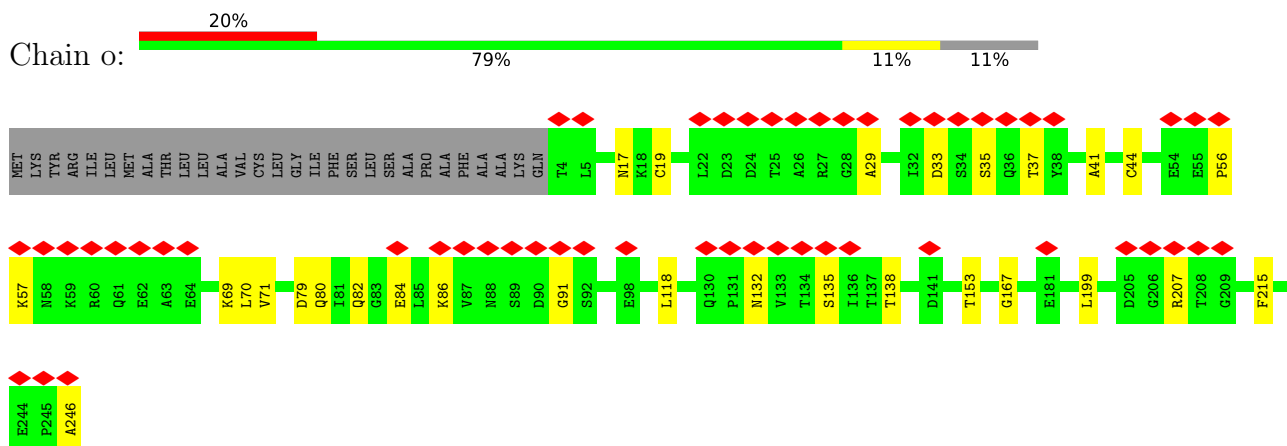
• Molecule 12: Photosystem II reaction center protein M



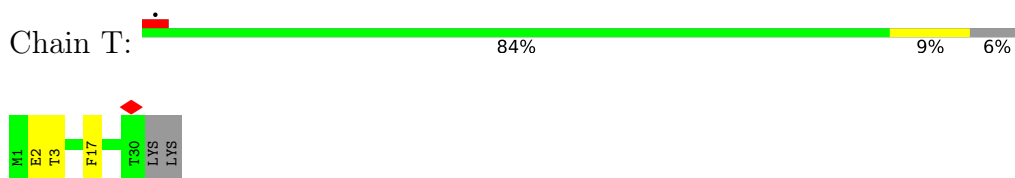
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



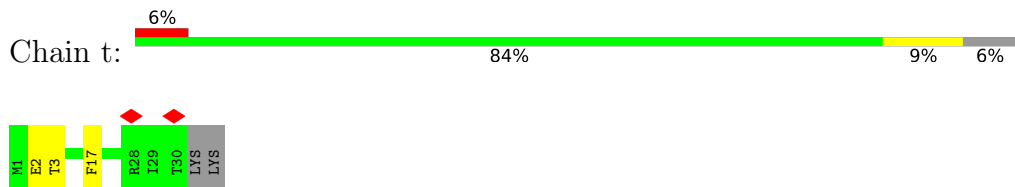
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



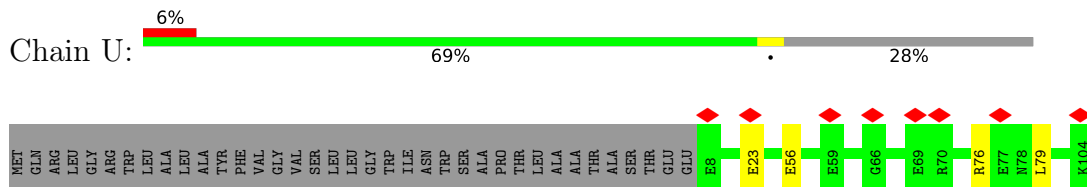
- Molecule 14: Photosystem II reaction center protein T



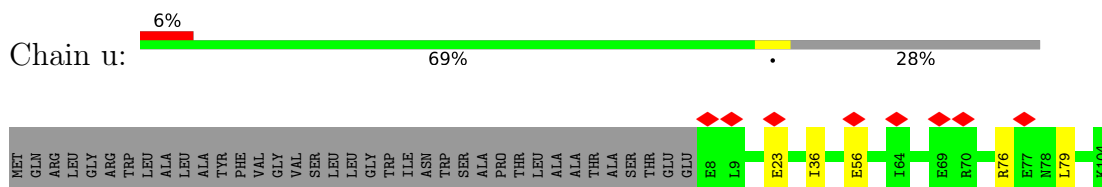
- Molecule 14: Photosystem II reaction center protein T



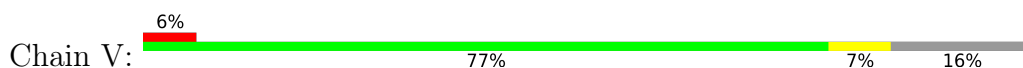
- Molecule 15: Photosystem II 12 kDa extrinsic protein

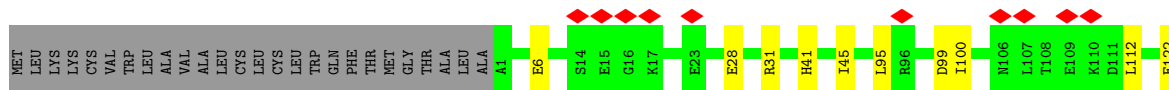


- Molecule 15: Photosystem II 12 kDa extrinsic protein

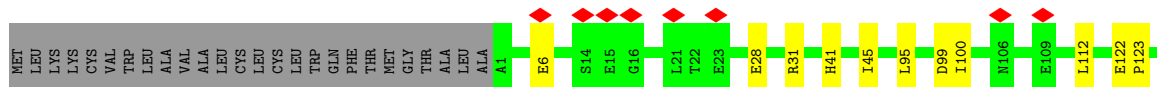
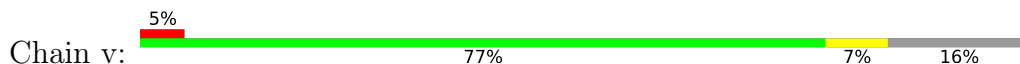


- Molecule 16: Cytochrome c-550

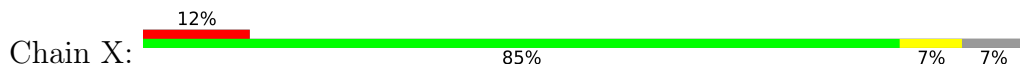




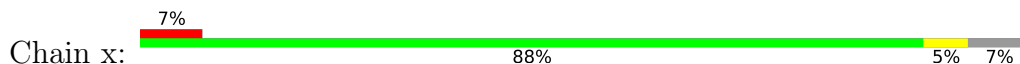
• Molecule 16: Cytochrome c-550



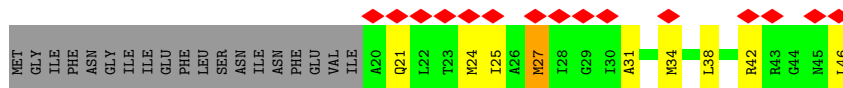
• Molecule 17: Photosystem II reaction center X protein



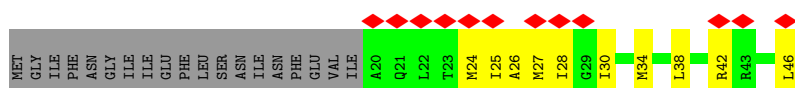
• Molecule 17: Photosystem II reaction center X protein



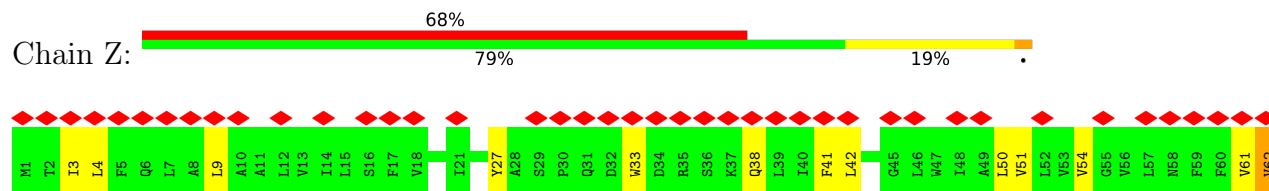
• Molecule 18: Photosystem II reaction center protein Ycf12



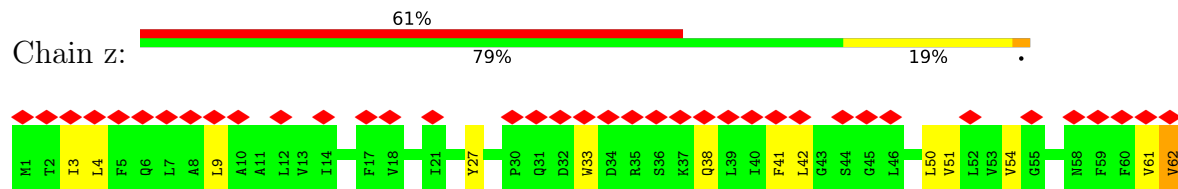
• Molecule 18: Photosystem II reaction center protein Ycf12



• Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	631270	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.426	Depositor
Minimum map value	-0.651	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	413.28, 413.28, 413.28	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.574, 0.574, 0.574	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, HEM, CLA, BCT, LMG, OEX, PL9, STE, HEC, SQD, FME, PHO, CL, LMT, DGD, FE2, LHG

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	0.17	0/2723	0.39	0/3713
1	a	0.17	0/2723	0.39	0/3713
2	B	0.16	0/4140	0.35	0/5641
2	b	0.16	0/4140	0.35	0/5641
3	C	0.16	0/3612	0.34	0/4917
3	c	0.16	0/3612	0.34	0/4917
4	D	0.17	0/2812	0.37	0/3832
4	d	0.17	0/2812	0.37	0/3832
5	E	0.14	0/680	0.32	0/929
5	e	0.14	0/680	0.34	0/929
6	F	0.19	0/284	0.34	0/387
6	f	0.19	0/284	0.34	0/387
7	H	0.12	0/539	0.28	0/736
7	h	0.13	0/539	0.28	0/736
8	I	0.15	0/310	0.34	0/419
8	i	0.15	0/310	0.36	0/419
9	J	0.16	0/263	0.32	0/356
9	j	0.16	0/263	0.33	0/356
10	K	0.19	0/303	0.34	0/416
10	k	0.19	0/303	0.35	0/416
11	L	0.12	0/327	0.27	0/444
11	l	0.13	0/327	0.27	0/444
12	M	0.14	0/264	0.33	0/363
12	m	0.14	0/264	0.33	0/363
13	O	0.13	0/1910	0.34	0/2594
13	o	0.13	0/1910	0.33	0/2594
14	T	0.15	0/257	0.35	0/349
14	t	0.15	0/257	0.35	0/349
15	U	0.12	0/785	0.27	0/1064
15	u	0.12	0/785	0.27	0/1064
16	V	0.13	0/1085	0.25	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.14	0/1085	0.25	0/1473
17	X	0.11	0/284	0.22	0/384
17	x	0.11	0/284	0.22	0/384
18	Y	0.14	0/200	0.32	0/268
18	y	0.16	0/200	0.33	0/268
19	Z	0.14	0/490	0.36	0/669
19	z	0.15	0/490	0.36	0/669
All	All	0.16	0/42536	0.34	0/57908

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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	2634	2530	2525	47	0
1	a	2634	2530	2525	47	0
2	B	3994	3858	3851	50	0
2	b	3994	3858	3851	51	0
3	C	3491	3408	3395	45	0
3	c	3491	3408	3395	45	0
4	D	2717	2621	2621	34	0
4	d	2717	2621	2621	32	0
5	E	661	640	640	13	0
5	e	661	640	640	13	0
6	F	275	282	282	4	0
6	f	275	282	282	4	0
7	H	511	534	523	10	0
7	h	511	534	523	11	0
8	I	313	328	328	3	0
8	i	313	328	328	3	0
9	J	257	268	268	6	0
9	j	257	268	268	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	293	305	305	9	0
10	k	293	305	305	10	0
11	L	312	328	316	1	0
11	l	312	328	316	2	0
12	M	264	281	271	11	0
12	m	264	281	271	10	0
13	O	1876	1834	1832	28	0
13	o	1876	1834	1832	23	0
14	T	258	261	261	2	0
14	t	258	261	261	2	0
15	U	774	773	773	2	0
15	u	774	773	773	3	0
16	V	1064	1071	1073	10	0
16	v	1064	1071	1073	10	0
17	X	281	312	312	3	0
17	x	281	312	312	2	0
18	Y	199	224	226	9	0
18	y	199	226	226	8	0
19	Z	479	516	516	15	0
19	z	479	516	516	16	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	2	0	0	1	0
21	a	2	0	0	1	0
22	A	244	251	251	5	0
22	B	1035	1139	1139	23	0
22	C	839	922	922	24	0
22	D	130	144	144	3	0
22	a	244	251	251	5	0
22	b	1035	1139	1139	24	0
22	c	839	922	922	23	0
22	d	130	144	144	1	0
23	A	40	56	56	4	0
23	B	120	168	168	10	0
23	C	80	112	112	7	0
23	D	40	56	56	5	0
23	H	40	56	56	6	0
23	K	80	112	112	5	0
23	T	40	56	56	7	0
23	a	40	56	56	2	0
23	b	120	168	168	8	0
23	c	80	112	112	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	d	40	56	56	4	0
23	h	40	56	56	7	0
23	k	80	112	112	5	0
23	t	40	56	56	11	0
24	A	55	80	80	10	0
24	D	55	80	80	1	0
24	a	55	80	80	12	0
24	d	55	80	80	1	0
25	A	51	87	87	4	0
25	B	41	62	62	3	0
25	C	34	51	51	0	0
25	D	29	52	52	2	0
25	E	44	74	74	2	0
25	I	14	24	24	0	0
25	J	12	20	20	1	0
25	K	11	21	21	0	0
25	M	10	16	16	0	0
25	T	15	29	26	0	0
25	a	51	87	87	6	0
25	b	41	62	62	2	0
25	c	34	51	51	0	0
25	d	29	52	52	2	0
25	e	44	74	74	2	0
25	i	14	24	24	0	0
25	j	12	20	20	1	0
25	k	11	21	21	1	0
25	m	10	16	16	0	0
25	t	18	28	28	1	0
26	A	48	66	66	1	0
26	B	51	72	72	1	0
26	C	98	136	136	7	0
26	D	85	121	121	2	0
26	H	39	59	59	6	0
26	a	48	66	66	1	0
26	b	51	72	72	1	0
26	c	98	136	136	6	0
26	d	85	121	121	2	0
26	h	39	59	59	6	0
27	A	106	147	149	4	0
27	B	54	77	78	3	0
27	X	36	45	46	3	0
27	a	106	147	149	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	b	49	64	65	3	0
27	x	36	45	46	3	0
28	A	66	96	96	6	0
28	C	181	236	236	2	0
28	H	62	82	82	0	0
28	a	66	96	96	10	0
28	c	181	236	236	1	0
28	h	62	82	82	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	64	74	74	1	0
30	D	64	74	74	0	0
30	a	64	74	74	0	0
30	d	64	74	74	0	0
31	A	49	74	74	1	0
31	D	145	215	215	5	0
31	L	49	74	74	0	0
31	a	49	74	74	1	0
31	d	145	215	215	7	0
31	l	49	74	74	0	0
32	B	25	35	34	0	0
32	C	59	80	80	2	0
32	E	24	33	34	1	0
32	J	24	34	34	2	0
32	M	35	44	45	0	0
32	Z	35	44	45	3	0
32	b	25	35	34	0	0
32	c	59	80	80	2	0
32	e	24	33	34	1	0
32	j	24	34	34	2	0
32	m	35	44	45	0	0
32	z	35	44	45	3	0
33	D	4	1	1	0	0
33	d	4	1	1	0	0
34	E	43	30	30	6	0
34	e	43	30	30	6	0
35	V	43	30	30	1	0
35	v	43	30	30	1	0
36	A	172	0	0	7	0
36	B	273	0	0	9	0
36	C	201	0	0	5	0
36	D	177	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	E	38	0	0	2	0
36	F	4	0	0	0	0
36	H	28	0	0	0	0
36	I	6	0	0	0	0
36	J	14	0	0	2	0
36	K	4	0	0	0	0
36	L	16	0	0	0	0
36	M	7	0	0	0	0
36	O	99	0	0	4	0
36	T	8	0	0	0	0
36	U	61	0	0	0	0
36	V	95	0	0	0	0
36	X	9	0	0	1	0
36	a	168	0	0	7	0
36	b	273	0	0	9	0
36	c	202	0	0	5	0
36	d	177	0	0	2	0
36	e	38	0	0	2	0
36	f	4	0	0	0	0
36	h	28	0	0	0	0
36	i	6	0	0	0	0
36	j	14	0	0	2	0
36	k	4	0	0	0	0
36	l	13	0	0	0	0
36	m	3	0	0	0	0
36	o	99	0	0	4	0
36	t	7	0	0	0	0
36	u	55	0	0	0	0
36	v	95	0	0	0	0
36	x	9	0	0	1	0
All	All	52833	52030	51925	741	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 7.

The worst 5 of 741 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)
2:B:389:LYS:NZ	36:B:701:HOH:O	1.92	1.03
2:b:389:LYS:NZ	36:b:701:HOH:O	1.92	1.01
1:a:243:GLU:OE2	36:a:501:HOH:O	1.84	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:OE2	36:A:501:HOH:O	1.84	0.93
10:K:21:LEU:HD13	18:Y:24:MET:HE3	1.50	0.92

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	7 (2%)	0	100	100
1	a	335/344 (97%)	328 (98%)	7 (2%)	0	100	100
2	B	506/510 (99%)	499 (99%)	7 (1%)	0	100	100
2	b	506/510 (99%)	499 (99%)	7 (1%)	0	100	100
3	C	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	43	31
3	c	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	43	31
4	D	339/352 (96%)	333 (98%)	6 (2%)	0	100	100
4	d	339/352 (96%)	333 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	80 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	65/66 (98%)	64 (98%)	1 (2%)	0	100	100
7	h	65/66 (98%)	64 (98%)	1 (2%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	37/37 (100%)	37 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	244/272 (90%)	233 (96%)	11 (4%)	0	100	100
13	o	244/272 (90%)	235 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
16	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
17	X	36/41 (88%)	36 (100%)	0	0	100	100
17	x	36/41 (88%)	36 (100%)	0	0	100	100
18	Y	25/46 (54%)	25 (100%)	0	0	100	100
18	y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
19	Z	60/62 (97%)	60 (100%)	0	0	100	100
19	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	5212/5618 (93%)	5109 (98%)	101 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER

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

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/280 (97%)	272 (100%)	0	100	100
1	a	272/280 (97%)	272 (100%)	0	100	100
2	B	406/407 (100%)	405 (100%)	1 (0%)	87	81
2	b	406/407 (100%)	405 (100%)	1 (0%)	87	81
3	C	354/362 (98%)	351 (99%)	3 (1%)	73	61
3	c	354/362 (98%)	351 (99%)	3 (1%)	73	61
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	276/283 (98%)	276 (100%)	0	100	100
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	71/73 (97%)	71 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	56/55 (102%)	56 (100%)	0	100	100
7	h	56/55 (102%)	56 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	6
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	37/35 (106%)	37 (100%)	0	100	100
11	l	37/35 (106%)	37 (100%)	0	100	100
12	M	30/32 (94%)	28 (93%)	2 (7%)	15	2
12	m	30/32 (94%)	28 (93%)	2 (7%)	15	2
13	O	207/228 (91%)	206 (100%)	1 (0%)	81	71
13	o	207/228 (91%)	206 (100%)	1 (0%)	81	71
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	83 (99%)	1 (1%)	63	46
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	46
16	V	117/138 (85%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/138 (85%)	117 (100%)	0	100	100
17	X	31/34 (91%)	31 (100%)	0	100	100
17	x	31/34 (91%)	31 (100%)	0	100	100
18	Y	20/37 (54%)	19 (95%)	1 (5%)	22	4
18	y	20/37 (54%)	20 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	27
19	z	52/52 (100%)	51 (98%)	1 (2%)	50	27
All	All	4310/4588 (94%)	4290 (100%)	20 (0%)	81	71

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	315	MET
13	o	118	LEU
19	z	62	VAL
15	u	23	GLU
12	M	16[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	165	GLN
19	z	38	GLN
2	b	274	GLN
13	o	155	ASN
2	b	157	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 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
8	FME	i	1	8	8,9,10	0.97	0	8,9,11	0.84	0
12	FME	m	1	12	8,9,10	0.95	0	8,9,11	0.74	0
8	FME	I	1	8	8,9,10	0.97	0	8,9,11	0.84	0
12	FME	M	1	12	8,9,10	0.96	0	8,9,11	0.74	0
14	FME	t	1	14	8,9,10	0.97	0	8,9,11	1.02	0
14	FME	T	1	14	8,9,10	0.97	0	8,9,11	1.02	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
8	FME	i	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
8	i	1	FME	O-C-CA-CB
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	CB-CA-N-CN
8	I	1	FME	CB-CG-SD-CE

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 212 ligands modelled in this entry, 6 are monoatomic - leaving 206 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$
27	SQD	a	412	-	52,54,54	1.54	7 (13%)	62,65,65	1.29	6 (9%)
23	BCR	b	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	6 (10%)
25	STE	B	621	-	16,16,19	0.59	0	16,16,19	1.09	0
25	STE	j	101	-	11,11,19	0.28	0	10,10,19	0.84	0
24	PL9	D	407	-	55,55,55	0.98	3 (5%)	68,69,69	1.44	11 (16%)
28	DGD	C	518	-	58,58,67	0.95	2 (3%)	72,72,81	1.30	5 (6%)
31	LHG	l	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.22	5 (9%)
27	SQD	B	620	-	52,54,54	1.55	8 (15%)	62,65,65	1.34	6 (9%)
22	CLA	C	512	-	69,73,73	1.22	8 (11%)	82,113,113	1.26	6 (7%)
28	DGD	C	517	-	63,63,67	0.86	1 (1%)	77,77,81	1.33	7 (9%)
22	CLA	b	616	-	69,73,73	1.37	11 (15%)	82,113,113	1.23	4 (4%)
25	STE	b	601	-	11,11,19	0.29	0	10,10,19	0.79	0
26	LMG	H	101	-	38,38,55	0.53	0	40,40,63	1.33	2 (5%)
23	BCR	H	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	8 (14%)
25	STE	c	521	-	11,11,19	0.72	0	11,11,19	1.14	0
22	CLA	c	509	-	69,73,73	1.20	9 (13%)	82,113,113	1.33	6 (7%)
28	DGD	a	413	-	67,67,67	0.91	3 (4%)	81,81,81	1.35	12 (14%)
35	HEC	v	201	16	46,50,50	1.85	5 (10%)	58,82,82	1.95	4 (6%)
22	CLA	B	604	-	69,73,73	1.34	9 (13%)	82,113,113	1.37	7 (8%)
22	CLA	c	506	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
30	PHO	D	401	-	58,69,69	2.20	11 (18%)	55,99,99	1.33	6 (10%)
31	LHG	d	411	-	48,48,48	0.65	1 (2%)	51,54,54	1.23	6 (11%)
31	LHG	D	409	-	48,48,48	0.63	2 (4%)	51,54,54	1.18	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	BCR	k	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.15	4 (7%)
23	BCR	b	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.12	4 (7%)
25	STE	d	412	-	19,19,19	0.56	0	19,19,19	1.01	0
25	STE	K	102	-	10,10,19	0.30	0	9,9,19	0.80	0
24	PL9	A	408	-	55,55,55	0.99	3 (5%)	68,69,69	1.50	11 (16%)
25	STE	C	522	-	7,7,19	0.30	0	6,6,19	0.72	0
22	CLA	A	405	36	64,68,73	1.21	8 (12%)	76,107,113	1.42	7 (9%)
25	STE	A	416	-	10,10,19	0.30	0	9,9,19	0.78	0
22	CLA	a	419	36	69,73,73	1.15	8 (11%)	82,113,113	1.20	7 (8%)
22	CLA	c	512	-	69,73,73	1.21	8 (11%)	82,113,113	1.28	6 (7%)
25	STE	A	414	-	7,7,19	0.30	0	6,6,19	0.69	0
26	LMG	D	402	-	33,33,55	0.60	0	35,35,63	1.22	2 (5%)
32	LMT	j	102	-	24,24,36	1.04	3 (12%)	29,29,47	1.10	2 (6%)
25	STE	t	101	-	17,17,19	0.59	0	17,17,19	1.08	0
25	STE	E	101	-	11,11,19	0.70	0	11,11,19	1.14	0
22	CLA	C	505	-	69,73,73	1.32	9 (13%)	82,113,113	1.25	4 (4%)
32	LMT	C	523	-	24,24,36	1.11	4 (16%)	29,29,47	1.26	2 (6%)
27	SQD	A	411	-	50,52,54	1.55	7 (14%)	60,63,65	1.43	9 (15%)
23	BCR	B	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.16	5 (8%)
30	PHO	d	401	-	58,69,69	2.21	11 (18%)	55,99,99	1.34	6 (10%)
32	LMT	b	624	-	25,25,36	0.99	2 (8%)	30,30,47	1.11	3 (10%)
24	PL9	d	407	-	55,55,55	0.98	3 (5%)	68,69,69	1.44	11 (16%)
28	DGD	H	103	-	63,63,67	0.94	2 (3%)	77,77,81	1.29	6 (7%)
25	STE	C	516	-	13,13,19	0.65	0	13,13,19	1.13	0
25	STE	a	409	-	8,8,19	0.31	0	7,7,19	0.74	0
23	BCR	K	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.17	5 (8%)
22	CLA	B	605	-	69,73,73	1.31	8 (11%)	82,113,113	1.20	7 (8%)
22	CLA	b	603	-	69,73,73	1.21	9 (13%)	82,113,113	1.22	6 (7%)
22	CLA	b	611	36	69,73,73	1.20	9 (13%)	82,113,113	1.31	4 (4%)
22	CLA	B	609	-	69,73,73	1.34	10 (14%)	82,113,113	1.26	8 (9%)
22	CLA	a	406	-	58,62,73	1.43	7 (12%)	68,99,113	1.32	5 (7%)
22	CLA	b	617	-	64,68,73	1.38	7 (10%)	76,107,113	1.33	5 (6%)
23	BCR	D	406	-	41,41,41	1.12	2 (4%)	56,56,56	1.15	4 (7%)
29	OEX	a	417	1,3,36	0,15,15	-	-	-	-	-
25	STE	e	102	-	11,11,19	0.29	0	10,10,19	0.82	0
27	SQD	X	101	-	34,36,54	1.47	5 (14%)	42,45,65	1.50	7 (16%)
31	LHG	d	410	-	46,46,48	0.69	1 (2%)	49,52,54	1.20	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	STE	E	103	-	19,19,19	0.56	0	19,19,19	1.06	0
25	STE	D	413	-	8,8,19	0.30	0	7,7,19	0.76	0
22	CLA	b	604	-	69,73,73	1.25	9 (13%)	82,113,113	1.12	5 (6%)
31	LHG	A	420	-	48,48,48	0.67	2 (4%)	51,54,54	1.30	7 (13%)
23	BCR	a	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.12	3 (5%)
33	BCT	d	403	20	3,3,3	1.14	0	2,3,3	4.53	2 (100%)
22	CLA	D	405	-	69,73,73	1.37	10 (14%)	82,113,113	1.23	6 (7%)
32	LMT	m	101	-	36,36,36	1.12	4 (11%)	47,47,47	0.98	2 (4%)
22	CLA	c	503	-	69,73,73	1.46	11 (15%)	82,113,113	1.15	5 (6%)
22	CLA	B	612	-	69,73,73	1.28	9 (13%)	82,113,113	1.33	5 (6%)
22	CLA	B	602	-	69,73,73	1.21	9 (13%)	82,113,113	1.22	6 (7%)
28	DGD	c	518	-	58,58,67	0.95	2 (3%)	72,72,81	1.30	5 (6%)
25	STE	b	623	-	11,11,19	0.69	0	11,11,19	1.21	1 (9%)
26	LMG	h	101	-	38,38,55	0.53	0	40,40,63	1.32	2 (5%)
23	BCR	C	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	5 (8%)
24	PL9	a	408	-	55,55,55	0.98	3 (5%)	68,69,69	1.51	11 (16%)
27	SQD	b	621	-	47,49,54	1.63	8 (17%)	57,60,65	1.32	6 (10%)
25	STE	B	622	-	11,11,19	0.69	0	11,11,19	1.20	1 (9%)
26	LMG	d	408	-	51,51,55	0.78	1 (1%)	59,59,63	1.30	6 (10%)
25	STE	a	415	-	10,10,19	0.31	0	9,9,19	0.73	0
22	CLA	A	419	36	69,73,73	1.15	7 (10%)	82,113,113	1.20	7 (8%)
25	STE	k	102	-	10,10,19	0.30	0	9,9,19	0.79	0
22	CLA	B	616	-	64,68,73	1.38	7 (10%)	76,107,113	1.33	5 (6%)
22	CLA	c	510	-	69,73,73	1.18	8 (11%)	82,113,113	1.20	4 (4%)
23	BCR	c	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	5 (8%)
22	CLA	b	613	-	69,73,73	1.29	9 (13%)	82,113,113	1.33	5 (6%)
22	CLA	B	607	36	69,73,73	1.18	7 (10%)	82,113,113	1.22	4 (4%)
22	CLA	D	404	-	69,73,73	1.35	9 (13%)	82,113,113	1.28	6 (7%)
26	LMG	c	524	-	50,50,55	0.74	1 (2%)	58,58,63	1.34	7 (12%)
34	HEM	E	105	6,5	50,50,50	1.48	7 (14%)	67,82,82	1.11	6 (8%)
22	CLA	c	513	-	69,73,73	1.15	8 (11%)	82,113,113	1.18	6 (7%)
22	CLA	b	610	-	69,73,73	1.33	10 (14%)	82,113,113	1.25	8 (9%)
22	CLA	c	504	36	63,67,73	1.22	8 (12%)	74,105,113	1.28	4 (5%)
22	CLA	C	501	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	6 (7%)
22	CLA	b	615	-	69,73,73	1.18	8 (11%)	82,113,113	1.20	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	BCR	h	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	7 (12%)
22	CLA	d	405	-	69,73,73	1.37	10 (14%)	82,113,113	1.24	5 (6%)
26	LMG	d	402	-	33,33,55	0.60	0	35,35,63	1.22	2 (5%)
28	DGD	h	103	-	63,63,67	0.94	2 (3%)	77,77,81	1.29	6 (7%)
25	STE	C	521	-	11,11,19	0.72	0	11,11,19	1.14	0
25	STE	c	516	-	13,13,19	0.65	0	13,13,19	1.13	0
22	CLA	B	613	-	69,73,73	1.32	10 (14%)	82,113,113	1.32	7 (8%)
22	CLA	b	605	-	69,73,73	1.35	9 (13%)	82,113,113	1.37	7 (8%)
30	PHO	A	418	-	58,69,69	2.20	10 (17%)	55,99,99	1.32	5 (9%)
25	STE	T	102	-	14,14,19	0.29	0	13,13,19	0.82	0
22	CLA	C	503	-	69,73,73	1.46	11 (15%)	82,113,113	1.15	5 (6%)
25	STE	a	414	-	7,7,19	0.29	0	6,6,19	0.69	0
25	STE	d	413	-	8,8,19	0.31	0	7,7,19	0.76	0
23	BCR	A	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.12	3 (5%)
32	LMT	J	102	-	24,24,36	1.03	3 (12%)	29,29,47	1.10	2 (6%)
34	HEM	e	105	6,5	50,50,50	1.48	6 (12%)	67,82,82	1.11	6 (8%)
26	LMG	D	408	-	51,51,55	0.78	1 (1%)	59,59,63	1.29	6 (10%)
28	DGD	A	413	-	67,67,67	0.92	2 (2%)	81,81,81	1.35	11 (13%)
23	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.13	5 (8%)
22	CLA	B	615	-	69,73,73	1.38	11 (15%)	82,113,113	1.24	4 (4%)
25	STE	B	625	-	11,11,19	0.29	0	10,10,19	0.79	0
22	CLA	B	606	-	69,73,73	1.19	9 (13%)	82,113,113	1.26	4 (4%)
31	LHG	D	411	-	48,48,48	0.65	1 (2%)	51,54,54	1.23	6 (11%)
32	LMT	M	102	-	36,36,36	1.12	5 (13%)	47,47,47	0.98	2 (4%)
25	STE	a	421	-	11,11,19	0.70	0	11,11,19	1.16	0
22	CLA	b	608	36	69,73,73	1.17	7 (10%)	82,113,113	1.22	4 (4%)
26	LMG	B	624	-	51,51,55	0.72	1 (1%)	59,59,63	1.34	6 (10%)
25	STE	e	101	-	11,11,19	0.72	0	11,11,19	1.14	0
25	STE	m	102	-	9,9,19	0.28	0	8,8,19	0.84	0
26	LMG	a	410	-	48,48,55	0.79	1 (2%)	56,56,63	1.26	5 (8%)
32	LMT	e	104	-	24,24,36	1.01	2 (8%)	29,29,47	1.09	2 (6%)
22	CLA	B	611	-	69,73,73	1.34	9 (13%)	82,113,113	1.31	8 (9%)
22	CLA	A	404	-	69,73,73	1.33	7 (10%)	82,113,113	1.18	3 (3%)
22	CLA	C	509	-	69,73,73	1.20	9 (13%)	82,113,113	1.33	6 (7%)
25	STE	A	421	-	11,11,19	0.70	0	11,11,19	1.16	0
27	SQD	A	412	-	52,54,54	1.54	7 (13%)	62,65,65	1.29	6 (9%)
22	CLA	a	404	-	69,73,73	1.33	7 (10%)	82,113,113	1.18	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	C	511	3	69,73,73	1.19	7 (10%)	82,113,113	1.27	5 (6%)
23	BCR	K	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.16	3 (5%)
22	CLA	b	607	-	69,73,73	1.19	9 (13%)	82,113,113	1.26	4 (4%)
22	CLA	c	501	-	69,73,73	1.15	8 (11%)	82,113,113	1.21	6 (7%)
23	BCR	T	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.18	5 (8%)
32	LMT	z	101	-	36,36,36	1.17	6 (16%)	47,47,47	0.98	1 (2%)
23	BCR	t	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	5 (8%)
25	STE	J	101	-	11,11,19	0.28	0	10,10,19	0.84	0
32	LMT	B	623	-	25,25,36	1.00	2 (8%)	30,30,47	1.11	3 (10%)
31	LHG	d	409	-	48,48,48	0.64	2 (4%)	51,54,54	1.18	5 (9%)
26	LMG	c	520	-	48,48,55	0.81	1 (2%)	56,56,63	1.31	6 (10%)
32	LMT	C	525	-	36,36,36	1.13	5 (13%)	47,47,47	0.92	2 (4%)
22	CLA	B	608	-	69,73,73	1.30	10 (14%)	82,113,113	1.22	5 (6%)
22	CLA	b	602	36	69,73,73	1.16	6 (8%)	82,113,113	1.19	6 (7%)
23	BCR	k	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
31	LHG	a	420	-	48,48,48	0.67	2 (4%)	51,54,54	1.29	7 (13%)
30	PHO	a	418	-	58,69,69	2.19	10 (17%)	55,99,99	1.32	6 (10%)
27	SQD	x	101	-	34,36,54	1.47	5 (14%)	42,45,65	1.50	7 (16%)
31	LHG	D	410	-	46,46,48	0.68	1 (2%)	49,52,54	1.19	4 (8%)
25	STE	i	101	-	13,13,19	0.26	0	12,12,19	0.87	0
22	CLA	b	614	-	69,73,73	1.32	10 (14%)	82,113,113	1.32	7 (8%)
22	CLA	c	507	36	69,73,73	1.19	8 (11%)	82,113,113	1.27	6 (7%)
25	STE	A	415	-	10,10,19	0.31	0	9,9,19	0.74	0
23	BCR	C	514	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	5 (8%)
22	CLA	B	614	-	69,73,73	1.19	8 (11%)	82,113,113	1.20	6 (7%)
22	CLA	C	502	-	69,73,73	1.26	10 (14%)	82,113,113	1.25	3 (3%)
22	CLA	C	508	-	69,73,73	1.30	10 (14%)	82,113,113	1.26	6 (7%)
26	LMG	C	524	-	50,50,55	0.74	1 (2%)	58,58,63	1.33	7 (12%)
22	CLA	c	505	-	69,73,73	1.32	9 (13%)	82,113,113	1.25	4 (4%)
32	LMT	Z	101	-	36,36,36	1.17	6 (16%)	47,47,47	0.98	1 (2%)
22	CLA	C	506	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
22	CLA	B	603	-	69,73,73	1.25	9 (13%)	82,113,113	1.12	5 (6%)
23	BCR	c	514	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	5 (8%)
23	BCR	d	406	-	41,41,41	1.13	2 (4%)	56,56,56	1.14	4 (7%)
25	STE	c	522	-	7,7,19	0.30	0	6,6,19	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	HEC	V	201	16	46,50,50	1.85	5 (10%)	58,82,82	1.95	4 (6%)
22	CLA	C	504	36	63,67,73	1.22	8 (12%)	74,105,113	1.28	4 (5%)
26	LMG	A	410	-	48,48,55	0.79	1 (2%)	56,56,63	1.26	5 (8%)
25	STE	D	412	-	19,19,19	0.57	0	19,19,19	1.01	0
32	LMT	c	525	-	36,36,36	1.13	5 (13%)	47,47,47	0.92	2 (4%)
22	CLA	C	510	-	69,73,73	1.18	8 (11%)	82,113,113	1.20	4 (4%)
23	BCR	B	617	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	6 (10%)
33	BCT	D	403	20	3,3,3	1.14	0	2,3,3	4.52	2 (100%)
22	CLA	B	610	36	69,73,73	1.20	8 (11%)	82,113,113	1.31	4 (4%)
32	LMT	E	104	-	24,24,36	1.01	2 (8%)	29,29,47	1.08	2 (6%)
25	STE	E	102	-	11,11,19	0.29	0	10,10,19	0.83	0
25	STE	b	622	-	16,16,19	0.60	0	16,16,19	1.09	0
22	CLA	a	405	36	64,68,73	1.20	6 (9%)	76,107,113	1.35	6 (7%)
22	CLA	c	511	3	69,73,73	1.19	8 (11%)	82,113,113	1.26	5 (6%)
31	LHG	L	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.21	5 (9%)
26	LMG	C	520	-	48,48,55	0.81	1 (2%)	56,56,63	1.30	6 (10%)
29	OEX	A	417	1,3,36	0,15,15	-	-	-	-	-
22	CLA	C	513	-	69,73,73	1.15	8 (11%)	82,113,113	1.18	6 (7%)
28	DGD	c	519	-	63,63,67	0.88	1 (1%)	77,77,81	1.26	5 (6%)
22	CLA	b	609	-	69,73,73	1.30	10 (14%)	82,113,113	1.22	5 (6%)
25	STE	a	416	-	10,10,19	0.30	0	9,9,19	0.77	0
25	STE	I	101	-	13,13,19	0.26	0	12,12,19	0.86	0
22	CLA	c	502	-	69,73,73	1.26	10 (14%)	82,113,113	1.25	3 (3%)
23	BCR	b	620	-	41,41,41	1.09	2 (4%)	56,56,56	1.16	6 (10%)
25	STE	e	103	-	19,19,19	0.57	0	19,19,19	1.06	0
22	CLA	d	404	-	69,73,73	1.35	9 (13%)	82,113,113	1.28	6 (7%)
22	CLA	b	606	-	69,73,73	1.31	8 (11%)	82,113,113	1.20	7 (8%)
22	CLA	C	507	36	69,73,73	1.19	8 (11%)	82,113,113	1.27	6 (7%)
22	CLA	c	508	-	69,73,73	1.30	10 (14%)	82,113,113	1.25	6 (7%)
22	CLA	b	612	-	69,73,73	1.34	9 (13%)	82,113,113	1.31	8 (9%)
25	STE	A	409	-	8,8,19	0.31	0	7,7,19	0.74	0
27	SQD	a	411	-	50,52,54	1.55	7 (14%)	60,63,65	1.43	9 (15%)
28	DGD	c	517	-	63,63,67	0.85	1 (1%)	77,77,81	1.33	7 (9%)
32	LMT	c	523	-	24,24,36	1.12	4 (16%)	29,29,47	1.29	2 (6%)
25	STE	M	101	-	9,9,19	0.28	0	8,8,19	0.84	0
28	DGD	C	519	-	63,63,67	0.88	1 (1%)	77,77,81	1.26	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	601	36	69,73,73	1.16	8 (11%)	82,113,113	1.19	6 (7%)
26	LMG	b	625	-	51,51,55	0.72	1 (1%)	59,59,63	1.34	6 (10%)
22	CLA	A	406	-	58,62,73	1.44	7 (12%)	68,99,113	1.32	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	a	412	-	-	19/49/69/69	0/1/1/1
23	BCR	b	618	-	-	2/29/63/63	0/2/2/2
25	STE	B	621	-	-	5/14/14/17	-
25	STE	j	101	-	-	2/9/9/17	-
24	PL9	D	407	-	-	7/53/73/73	0/1/1/1
28	DGD	C	518	-	-	15/46/86/95	0/2/2/2
31	LHG	l	101	-	-	15/53/53/53	-
27	SQD	B	620	-	-	29/49/69/69	0/1/1/1
22	CLA	C	512	-	1/1/20/20	12/39/115/115	-
28	DGD	C	517	-	-	18/51/91/95	0/2/2/2
22	CLA	b	616	-	1/1/20/20	7/39/115/115	-
25	STE	b	601	-	-	3/9/9/17	-
26	LMG	H	101	-	-	18/40/40/70	-
23	BCR	H	102	-	-	8/29/63/63	0/2/2/2
25	STE	c	521	-	-	7/9/9/17	-
22	CLA	c	509	-	1/1/20/20	5/39/115/115	-
28	DGD	a	413	-	-	26/55/95/95	0/2/2/2
35	HEC	v	201	16	-	6/14/54/54	-
22	CLA	B	604	-	1/1/20/20	7/39/115/115	-
22	CLA	c	506	-	1/1/20/20	13/39/115/115	-
30	PHO	D	401	-	-	0/37/103/103	0/5/6/6
31	LHG	d	411	-	-	9/53/53/53	-
31	LHG	D	409	-	-	12/53/53/53	-
23	BCR	k	103	-	-	2/29/63/63	0/2/2/2
23	BCR	b	619	-	-	3/29/63/63	0/2/2/2
25	STE	d	412	-	-	6/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	STE	K	102	-	-	5/8/8/17	-
24	PL9	A	408	-	-	20/53/73/73	0/1/1/1
25	STE	C	522	-	-	1/5/5/17	-
22	CLA	A	405	36	1/1/19/20	6/33/109/115	-
25	STE	A	416	-	-	5/8/8/17	-
22	CLA	a	419	36	1/1/20/20	2/39/115/115	-
22	CLA	c	512	-	1/1/20/20	11/39/115/115	-
25	STE	A	414	-	-	1/5/5/17	-
26	LMG	D	402	-	-	8/35/35/70	-
32	LMT	j	102	-	-	10/15/35/61	0/1/1/2
25	STE	t	101	-	-	10/15/15/17	-
25	STE	E	101	-	-	4/9/9/17	-
22	CLA	C	505	-	1/1/20/20	5/39/115/115	-
32	LMT	C	523	-	-	2/15/35/61	0/1/1/2
27	SQD	A	411	-	-	18/47/67/69	0/1/1/1
23	BCR	B	619	-	-	1/29/63/63	0/2/2/2
30	PHO	d	401	-	-	0/37/103/103	0/5/6/6
32	LMT	b	624	-	-	6/17/37/61	0/1/1/2
24	PL9	d	407	-	-	7/53/73/73	0/1/1/1
28	DGD	H	103	-	-	14/51/91/95	0/2/2/2
25	STE	C	516	-	-	7/11/11/17	-
25	STE	a	409	-	-	5/6/6/17	-
23	BCR	K	101	-	-	0/29/63/63	0/2/2/2
22	CLA	B	605	-	-	7/39/115/115	-
22	CLA	b	603	-	1/1/20/20	2/39/115/115	-
22	CLA	b	611	36	1/1/20/20	0/39/115/115	-
22	CLA	a	406	-	1/1/17/20	5/26/102/115	-
22	CLA	b	617	-	1/1/19/20	8/33/109/115	-
22	CLA	B	609	-	-	5/39/115/115	-
23	BCR	D	406	-	-	3/29/63/63	0/2/2/2
25	STE	e	102	-	-	6/9/9/17	-
27	SQD	X	101	-	-	12/28/48/69	0/1/1/1
31	LHG	d	410	-	-	11/51/51/53	-
25	STE	E	103	-	-	8/17/17/17	-
25	STE	D	413	-	-	1/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	604	-	1/1/20/20	8/39/115/115	-
31	LHG	A	420	-	-	23/53/53/53	-
23	BCR	a	407	-	-	0/29/63/63	0/2/2/2
22	CLA	D	405	-	-	5/39/115/115	-
32	LMT	m	101	-	-	3/21/61/61	0/2/2/2
22	CLA	c	503	-	-	5/39/115/115	-
22	CLA	B	612	-	1/1/20/20	5/39/115/115	-
22	CLA	B	602	-	1/1/20/20	2/39/115/115	-
28	DGD	c	518	-	-	15/46/86/95	0/2/2/2
25	STE	b	623	-	-	5/9/9/17	-
26	LMG	h	101	-	-	17/40/40/70	-
23	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	PL9	a	408	-	-	20/53/73/73	0/1/1/1
27	SQD	b	621	-	-	21/44/64/69	0/1/1/1
25	STE	B	622	-	-	5/9/9/17	-
26	LMG	d	408	-	-	16/46/66/70	0/1/1/1
25	STE	a	415	-	-	5/8/8/17	-
22	CLA	A	419	36	1/1/20/20	2/39/115/115	-
25	STE	k	102	-	-	5/8/8/17	-
22	CLA	B	616	-	1/1/19/20	8/33/109/115	-
22	CLA	c	510	-	1/1/20/20	6/39/115/115	-
23	BCR	c	515	-	-	0/29/63/63	0/2/2/2
22	CLA	b	613	-	1/1/20/20	5/39/115/115	-
22	CLA	B	607	36	1/1/20/20	2/39/115/115	-
22	CLA	D	404	-	-	6/39/115/115	-
26	LMG	c	524	-	-	20/45/65/70	0/1/1/1
34	HEM	E	105	6,5	-	0/14/54/54	-
22	CLA	c	513	-	1/1/20/20	8/39/115/115	-
22	CLA	c	504	36	1/1/18/20	5/32/108/115	-
22	CLA	b	610	-	-	5/39/115/115	-
22	CLA	C	501	-	1/1/20/20	1/39/115/115	-
22	CLA	b	615	-	1/1/20/20	12/39/115/115	-
23	BCR	h	102	-	-	8/29/63/63	0/2/2/2
22	CLA	d	405	-	-	5/39/115/115	-
26	LMG	d	402	-	-	8/35/35/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	h	103	-	-	14/51/91/95	0/2/2/2
25	STE	C	521	-	-	7/9/9/17	-
25	STE	c	516	-	-	8/11/11/17	-
22	CLA	B	613	-	1/1/20/20	5/39/115/115	-
22	CLA	b	605	-	1/1/20/20	7/39/115/115	-
30	PHO	A	418	-	-	2/37/103/103	0/5/6/6
25	STE	T	102	-	-	5/12/12/17	-
22	CLA	C	503	-	-	5/39/115/115	-
25	STE	a	414	-	-	1/5/5/17	-
25	STE	d	413	-	-	1/6/6/17	-
23	BCR	A	407	-	-	0/29/63/63	0/2/2/2
32	LMT	J	102	-	-	10/15/35/61	0/1/1/2
34	HEM	e	105	6,5	-	0/14/54/54	-
26	LMG	D	408	-	-	16/46/66/70	0/1/1/1
28	DGD	A	413	-	-	28/55/95/95	0/2/2/2
23	BCR	B	618	-	-	1/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/20/20	7/39/115/115	-
25	STE	B	625	-	-	4/9/9/17	-
22	CLA	B	606	-	1/1/20/20	8/39/115/115	-
31	LHG	D	411	-	-	9/53/53/53	-
32	LMT	M	102	-	-	3/21/61/61	0/2/2/2
25	STE	a	421	-	-	5/9/9/17	-
22	CLA	b	608	36	1/1/20/20	2/39/115/115	-
26	LMG	B	624	-	-	17/46/66/70	0/1/1/1
25	STE	e	101	-	-	4/9/9/17	-
25	STE	m	102	-	-	3/7/7/17	-
26	LMG	a	410	-	-	25/43/63/70	0/1/1/1
32	LMT	e	104	-	-	9/15/35/61	0/1/1/2
22	CLA	B	611	-	1/1/20/20	3/39/115/115	-
22	CLA	A	404	-	1/1/20/20	2/39/115/115	-
22	CLA	C	509	-	1/1/20/20	5/39/115/115	-
25	STE	A	421	-	-	5/9/9/17	-
27	SQD	A	412	-	-	19/49/69/69	0/1/1/1
22	CLA	a	404	-	1/1/20/20	2/39/115/115	-
22	CLA	C	511	3	1/1/20/20	0/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	K	103	-	-	2/29/63/63	0/2/2/2
22	CLA	b	607	-	1/1/20/20	8/39/115/115	-
22	CLA	c	501	-	1/1/20/20	1/39/115/115	-
23	BCR	T	101	-	-	3/29/63/63	0/2/2/2
32	LMT	z	101	-	-	12/21/61/61	0/2/2/2
23	BCR	t	102	-	-	3/29/63/63	0/2/2/2
25	STE	J	101	-	-	2/9/9/17	-
32	LMT	B	623	-	-	6/17/37/61	0/1/1/2
31	LHG	d	409	-	-	12/53/53/53	-
26	LMG	c	520	-	-	19/43/63/70	0/1/1/1
32	LMT	C	525	-	-	8/21/61/61	0/2/2/2
22	CLA	B	608	-	1/1/20/20	5/39/115/115	-
22	CLA	b	602	36	1/1/20/20	22/39/115/115	-
23	BCR	k	101	-	-	0/29/63/63	0/2/2/2
31	LHG	a	420	-	-	24/53/53/53	-
30	PHO	a	418	-	-	2/37/103/103	0/5/6/6
27	SQD	x	101	-	-	12/28/48/69	0/1/1/1
31	LHG	D	410	-	-	10/51/51/53	-
25	STE	i	101	-	-	6/11/11/17	-
22	CLA	b	614	-	1/1/20/20	5/39/115/115	-
22	CLA	c	507	36	1/1/20/20	8/39/115/115	-
25	STE	A	415	-	-	3/8/8/17	-
23	BCR	C	514	-	-	0/29/63/63	0/2/2/2
22	CLA	B	614	-	1/1/20/20	11/39/115/115	-
22	CLA	C	502	-	-	4/39/115/115	-
22	CLA	C	508	-	-	1/39/115/115	-
26	LMG	C	524	-	-	20/45/65/70	0/1/1/1
22	CLA	c	505	-	1/1/20/20	5/39/115/115	-
32	LMT	Z	101	-	-	12/21/61/61	0/2/2/2
22	CLA	C	506	-	1/1/20/20	13/39/115/115	-
22	CLA	B	603	-	1/1/20/20	8/39/115/115	-
23	BCR	c	514	-	-	0/29/63/63	0/2/2/2
23	BCR	d	406	-	-	3/29/63/63	0/2/2/2
25	STE	c	522	-	-	1/5/5/17	-
35	HEC	V	201	16	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	504	36	1/1/18/20	5/32/108/115	-
26	LMG	A	410	-	-	25/43/63/70	0/1/1/1
25	STE	D	412	-	-	6/17/17/17	-
32	LMT	c	525	-	-	8/21/61/61	0/2/2/2
22	CLA	C	510	-	1/1/20/20	6/39/115/115	-
23	BCR	B	617	-	-	2/29/63/63	0/2/2/2
22	CLA	B	610	36	1/1/20/20	0/39/115/115	-
32	LMT	E	104	-	-	9/15/35/61	0/1/1/2
25	STE	E	102	-	-	5/9/9/17	-
25	STE	b	622	-	-	5/14/14/17	-
22	CLA	a	405	36	1/1/19/20	2/33/109/115	-
22	CLA	c	511	3	1/1/20/20	0/39/115/115	-
31	LHG	L	101	-	-	15/53/53/53	-
26	LMG	C	520	-	-	19/43/63/70	0/1/1/1
22	CLA	C	513	-	1/1/20/20	9/39/115/115	-
28	DGD	c	519	-	-	15/51/91/95	0/2/2/2
22	CLA	b	609	-	1/1/20/20	5/39/115/115	-
25	STE	a	416	-	-	5/8/8/17	-
25	STE	I	101	-	-	6/11/11/17	-
22	CLA	c	502	-	-	4/39/115/115	-
23	BCR	b	620	-	-	1/29/63/63	0/2/2/2
25	STE	e	103	-	-	8/17/17/17	-
22	CLA	d	404	-	-	6/39/115/115	-
22	CLA	b	606	-	-	6/39/115/115	-
22	CLA	C	507	36	1/1/20/20	8/39/115/115	-
22	CLA	c	508	-	-	1/39/115/115	-
22	CLA	b	612	-	1/1/20/20	3/39/115/115	-
25	STE	A	409	-	-	5/6/6/17	-
27	SQD	a	411	-	-	18/47/67/69	0/1/1/1
28	DGD	c	517	-	-	18/51/91/95	0/2/2/2
32	LMT	c	523	-	-	2/15/35/61	0/1/1/2
25	STE	M	101	-	-	3/7/7/17	-
28	DGD	C	519	-	-	15/51/91/95	0/2/2/2
22	CLA	B	601	36	1/1/20/20	22/39/115/115	-
26	LMG	b	625	-	-	16/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	406	-	1/1/17/20	5/26/102/115	-

The worst 5 of 871 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	418	PHO	C1B-C2B	9.76	1.50	1.39
30	A	418	PHO	C1B-C2B	9.73	1.50	1.39
30	d	401	PHO	C1B-C2B	9.49	1.49	1.39
30	D	401	PHO	C1B-C2B	9.47	1.49	1.39
30	d	401	PHO	C3B-C4B	9.40	1.51	1.41

The worst 5 of 855 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	v	201	HEC	CBB-CAB-C3B	-8.79	109.87	127.43
35	V	201	HEC	CBB-CAB-C3B	-8.77	109.91	127.43
35	V	201	HEC	CBC-CAC-C3C	-8.11	111.22	127.43
35	v	201	HEC	CBC-CAC-C3C	-8.11	111.22	127.43
22	B	604	CLA	C4A-NA-C1A	8.11	110.38	106.68

5 of 56 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	404	CLA	ND
22	A	405	CLA	ND
22	A	406	CLA	ND
22	A	419	CLA	ND
22	B	601	CLA	ND

5 of 1520 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	406	CLA	C2-C3-C5-C6
22	A	406	CLA	C4-C3-C5-C6
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	C3A-C2A-CAA-CBA
22	B	614	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

146 monomers are involved in 325 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	412	SQD	5	0
23	b	618	BCR	3	0
25	B	621	STE	1	0
25	j	101	STE	1	0
24	D	407	PL9	1	0
28	C	518	DGD	2	0
27	B	620	SQD	3	0
22	C	512	CLA	4	0
22	b	616	CLA	2	0
26	H	101	LMG	6	0
23	H	102	BCR	6	0
22	c	509	CLA	3	0
28	a	413	DGD	10	0
35	v	201	HEC	1	0
22	B	604	CLA	1	0
31	d	411	LHG	1	0
31	D	409	LHG	2	0
23	k	103	BCR	3	0
23	b	619	BCR	5	0
25	d	412	STE	2	0
24	A	408	PL9	10	0
22	A	405	CLA	1	0
25	A	416	STE	1	0
22	a	419	CLA	1	0
22	c	512	CLA	4	0
26	D	402	LMG	1	0
32	j	102	LMT	2	0
25	t	101	STE	1	0
22	C	505	CLA	3	0
32	C	523	LMT	2	0
27	A	411	SQD	2	0
23	B	619	BCR	1	0
24	d	407	PL9	1	0
25	a	409	STE	1	0
23	K	101	BCR	1	0
22	B	605	CLA	1	0
22	b	603	CLA	3	0
22	B	609	CLA	3	0
22	a	406	CLA	1	0
22	b	617	CLA	1	0
23	D	406	BCR	5	0
25	e	102	STE	2	0
27	X	101	SQD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	d	410	LHG	4	0
31	A	420	LHG	1	0
23	a	407	BCR	2	0
22	D	405	CLA	1	0
22	B	612	CLA	2	0
22	B	602	CLA	3	0
28	c	518	DGD	1	0
25	b	623	STE	1	0
26	h	101	LMG	6	0
23	C	515	BCR	5	0
24	a	408	PL9	12	0
27	b	621	SQD	3	0
25	B	622	STE	2	0
26	d	408	LMG	1	0
25	a	415	STE	2	0
22	A	419	CLA	1	0
25	k	102	STE	1	0
22	B	616	CLA	1	0
22	c	510	CLA	1	0
23	c	515	BCR	4	0
22	b	613	CLA	2	0
22	B	607	CLA	1	0
22	D	404	CLA	2	0
26	c	524	LMG	5	0
34	E	105	HEM	6	0
22	c	513	CLA	4	0
22	b	610	CLA	3	0
22	C	501	CLA	3	0
22	b	615	CLA	1	0
23	h	102	BCR	7	0
26	d	402	LMG	1	0
22	B	613	CLA	1	0
30	A	418	PHO	1	0
23	A	407	BCR	4	0
32	J	102	LMT	2	0
34	e	105	HEM	6	0
26	D	408	LMG	1	0
28	A	413	DGD	6	0
23	B	618	BCR	6	0
22	B	615	CLA	2	0
22	B	606	CLA	2	0
31	D	411	LHG	1	0

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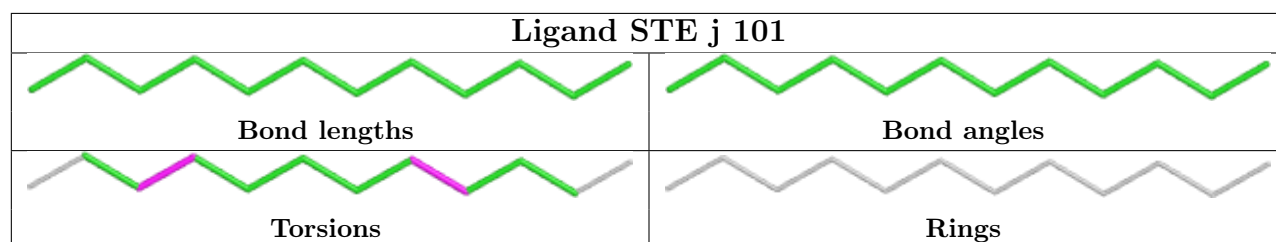
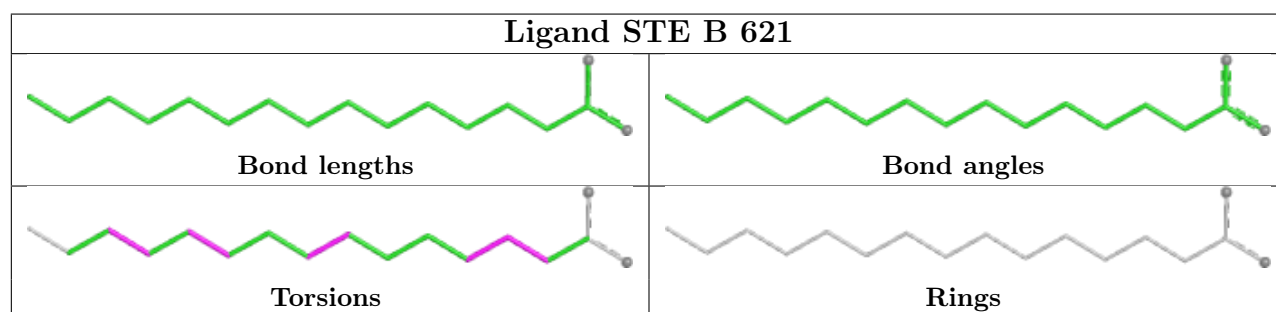
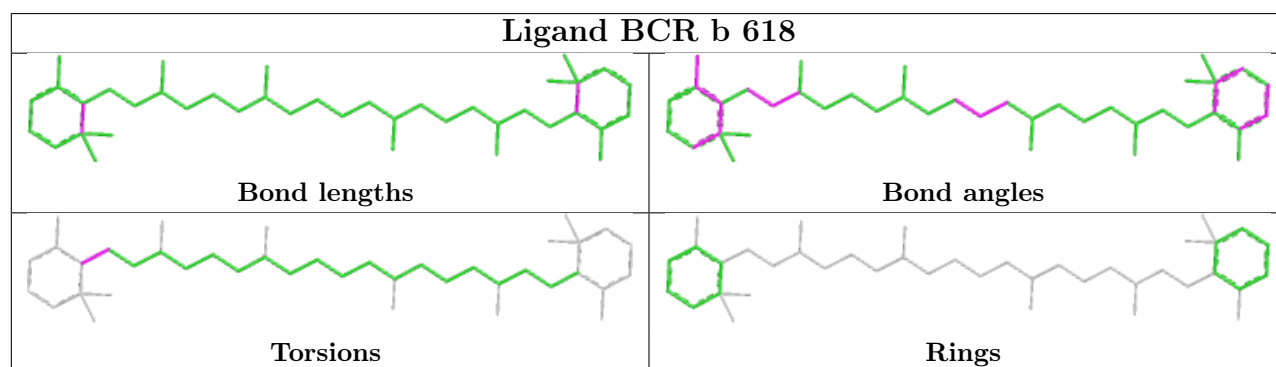
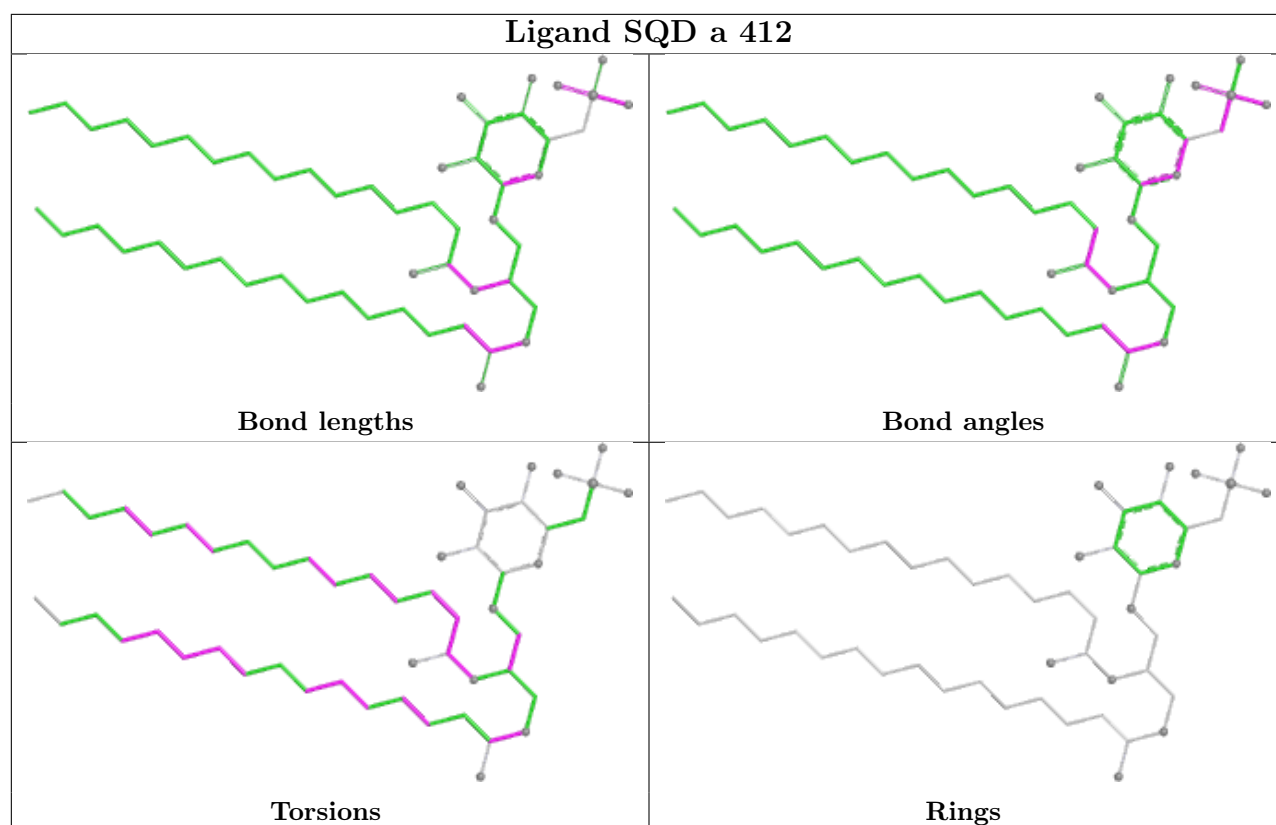
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	421	STE	2	0
22	b	608	CLA	1	0
26	B	624	LMG	1	0
26	a	410	LMG	1	0
32	e	104	LMT	1	0
22	A	404	CLA	2	0
22	C	509	CLA	3	0
25	A	421	STE	1	0
27	A	412	SQD	2	0
22	a	404	CLA	2	0
22	C	511	CLA	3	0
23	K	103	BCR	4	0
22	b	607	CLA	5	0
22	c	501	CLA	2	0
23	T	101	BCR	7	0
32	z	101	LMT	3	0
23	t	102	BCR	11	0
25	J	101	STE	1	0
31	d	409	LHG	2	0
26	c	520	LMG	1	0
22	B	608	CLA	2	0
22	b	602	CLA	4	0
23	k	101	BCR	2	0
31	a	420	LHG	1	0
27	x	101	SQD	3	0
31	D	410	LHG	2	0
22	b	614	CLA	1	0
25	A	415	STE	1	0
23	C	514	BCR	2	0
22	B	614	CLA	1	0
22	C	502	CLA	1	0
22	C	508	CLA	3	0
26	C	524	LMG	6	0
22	c	505	CLA	3	0
32	Z	101	LMT	3	0
23	c	514	BCR	3	0
23	d	406	BCR	4	0
35	V	201	HEC	1	0
26	A	410	LMG	1	0
25	D	412	STE	2	0
22	C	510	CLA	1	0
23	B	617	BCR	3	0

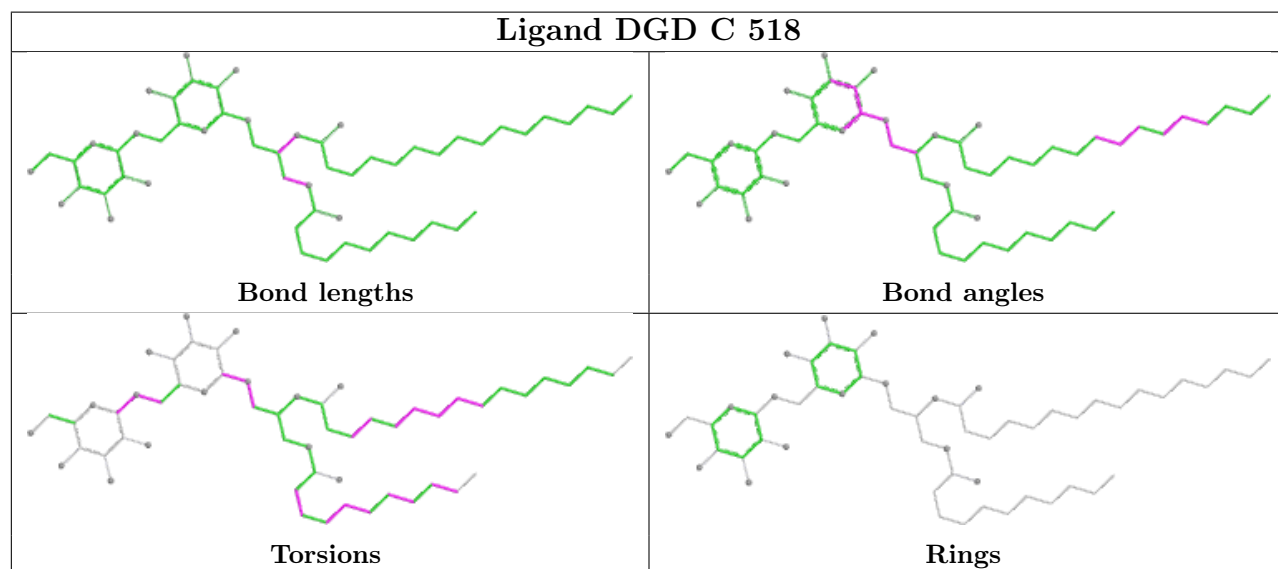
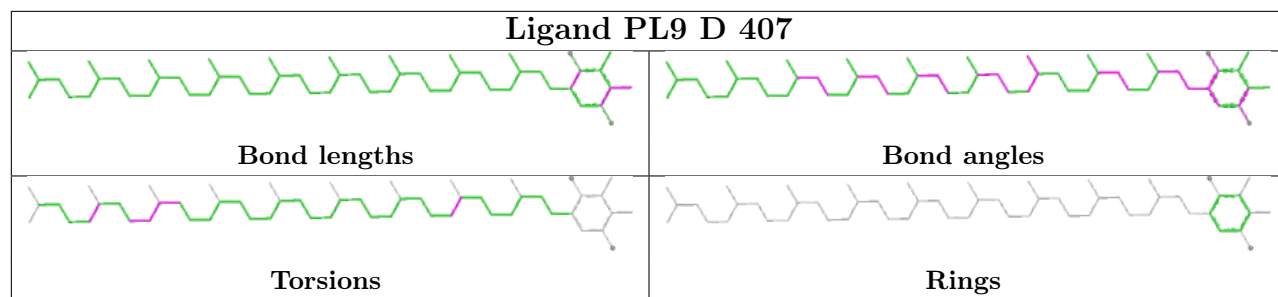
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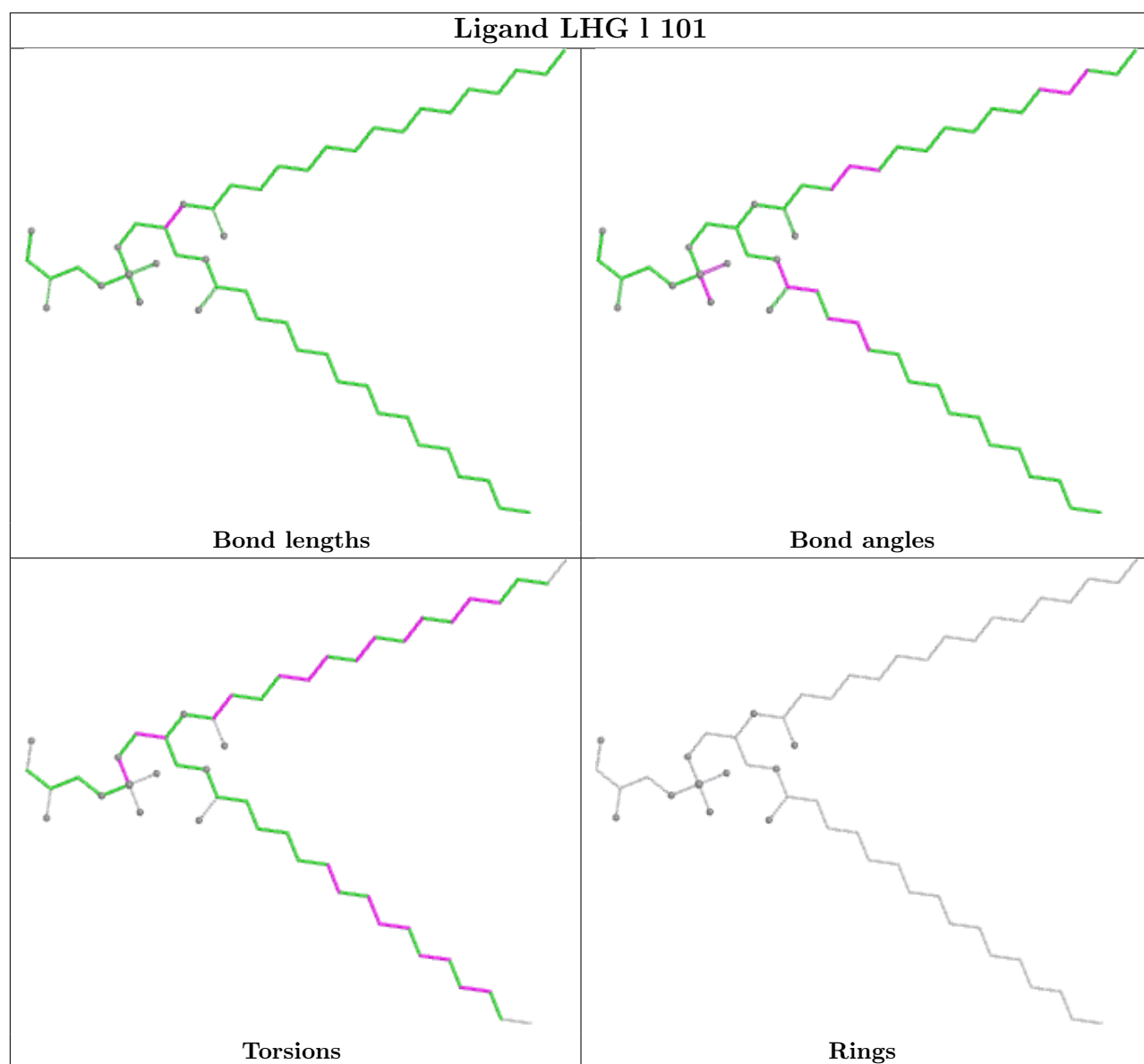
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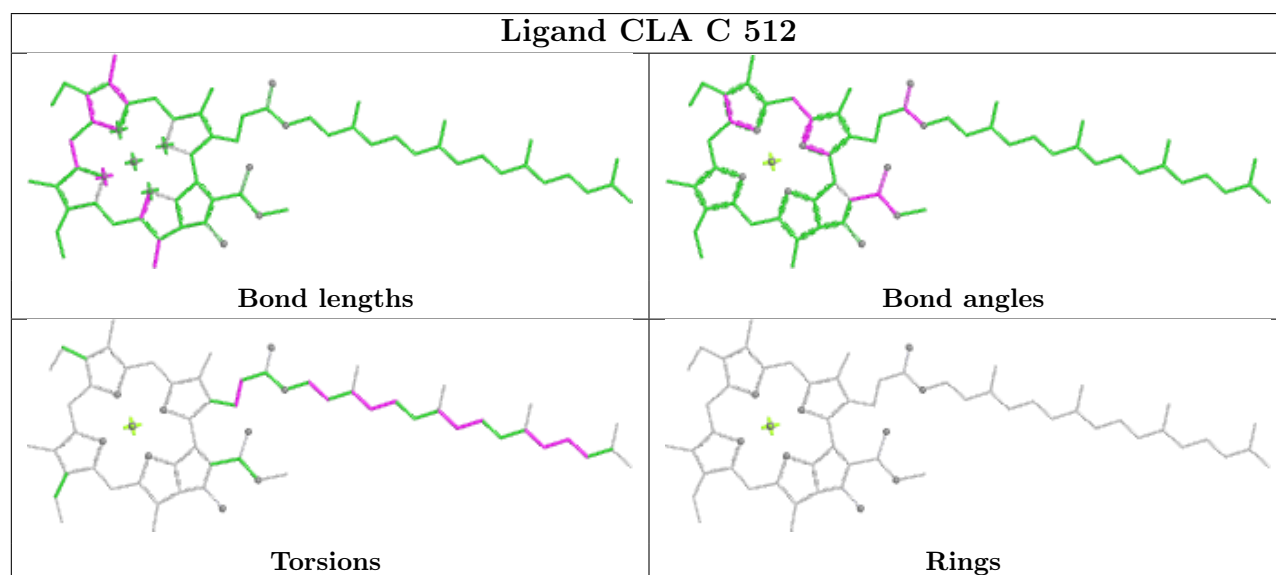
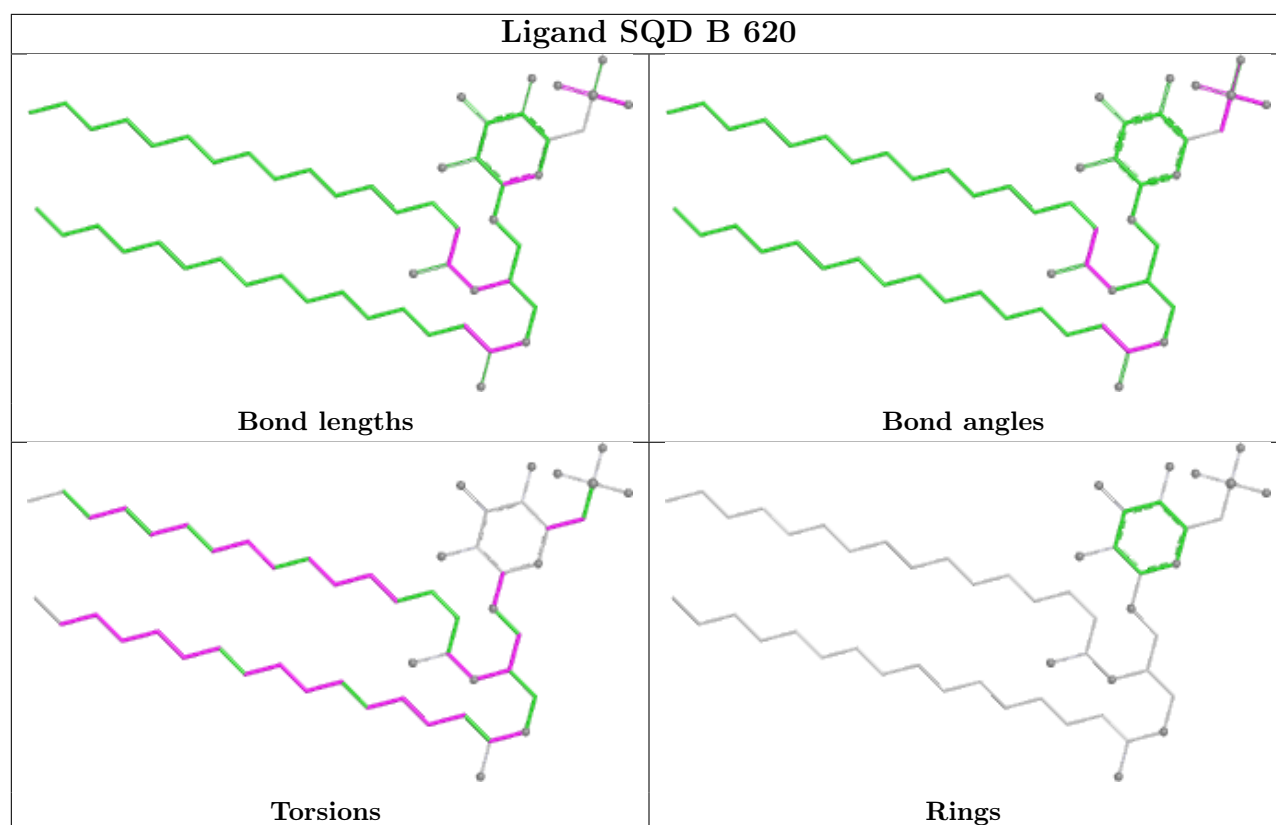
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	E	104	LMT	1	0
25	E	102	STE	2	0
25	b	622	STE	1	0
22	a	405	CLA	1	0
22	c	511	CLA	3	0
26	C	520	LMG	1	0
22	C	513	CLA	5	0
22	b	609	CLA	2	0
25	a	416	STE	1	0
22	c	502	CLA	1	0
22	d	404	CLA	1	0
22	b	606	CLA	1	0
22	c	508	CLA	4	0
25	A	409	STE	1	0
27	a	411	SQD	3	0
32	c	523	LMT	2	0
22	B	601	CLA	5	0
26	b	625	LMG	1	0
22	A	406	CLA	1	0

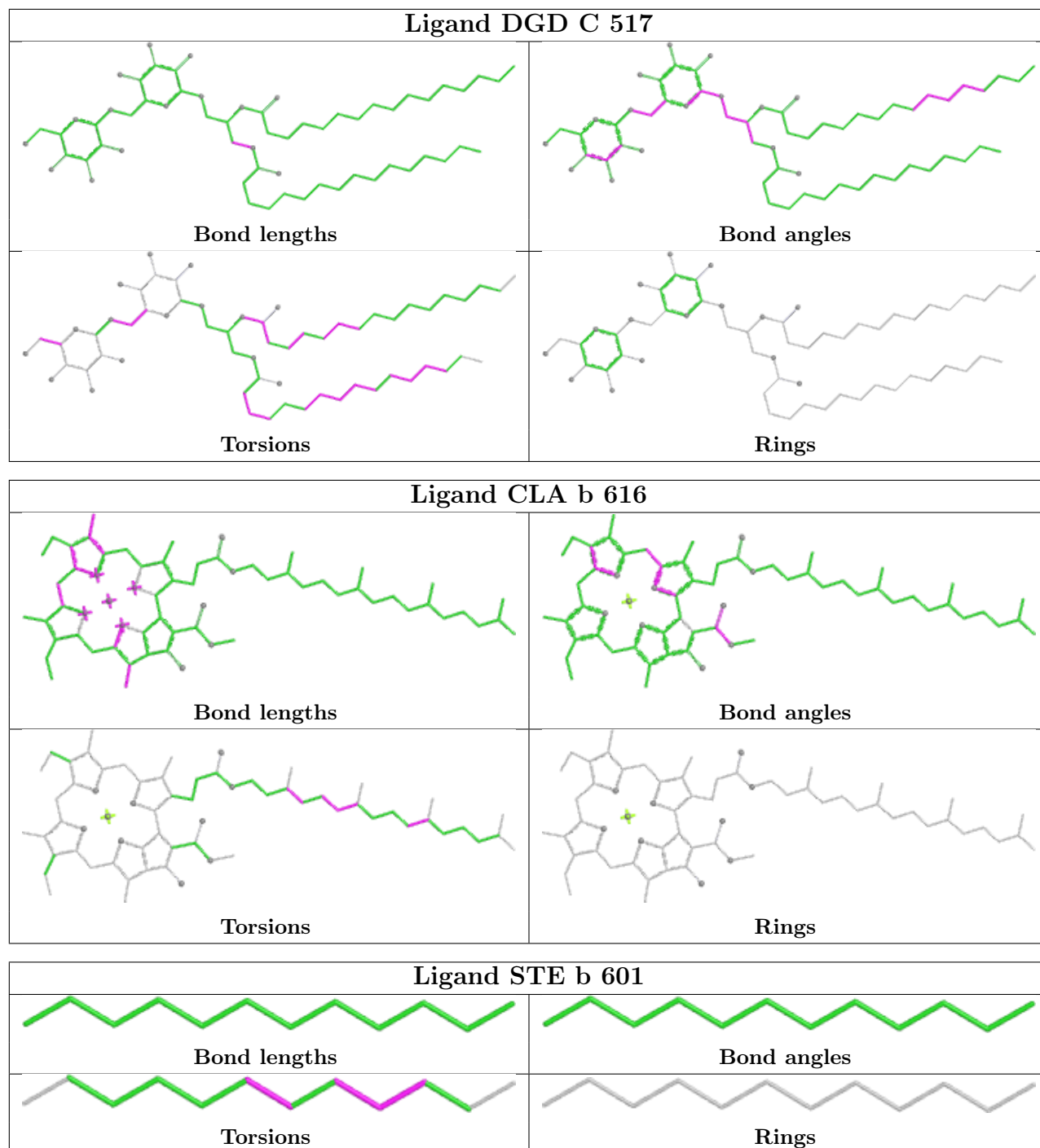
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

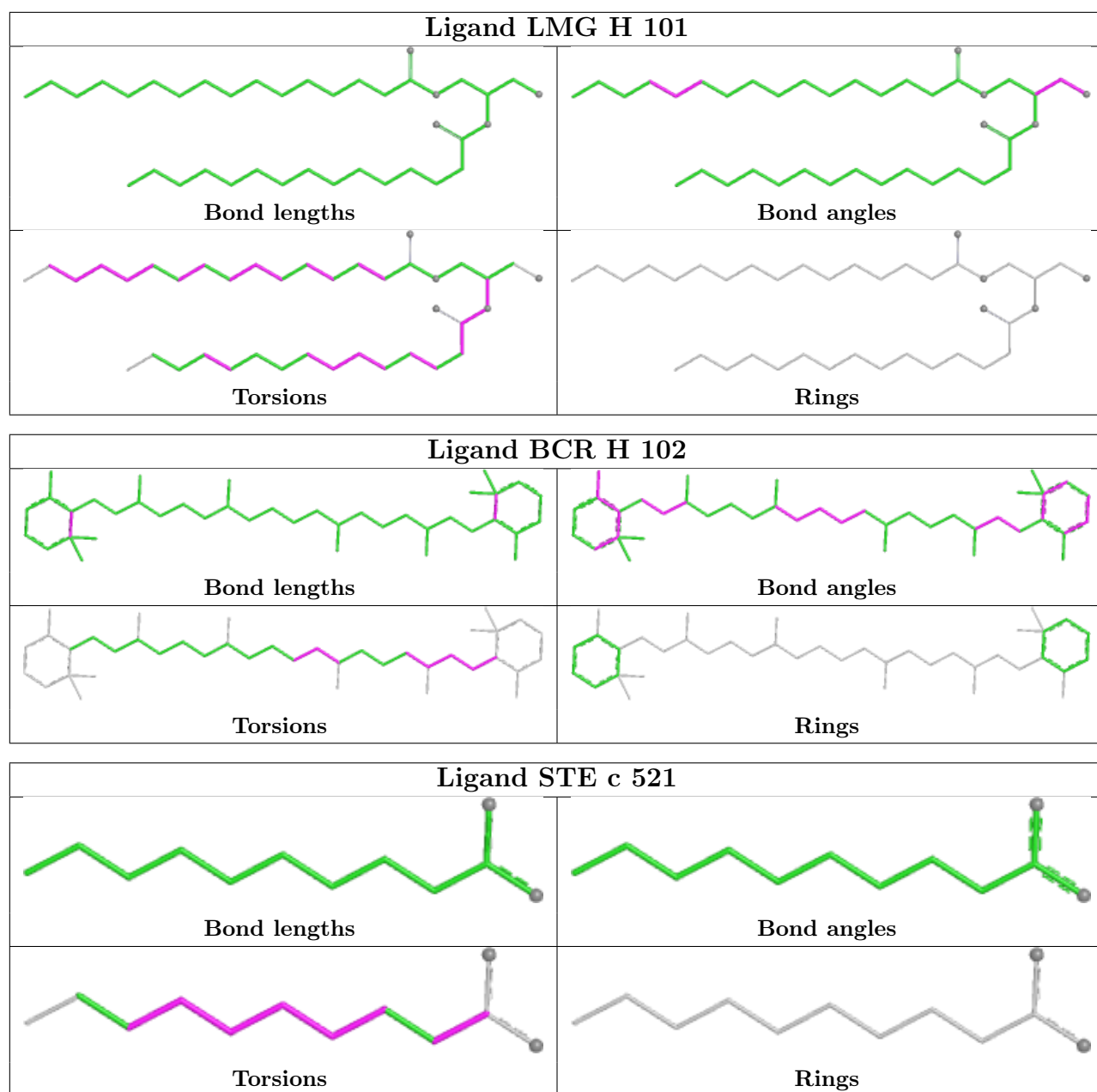


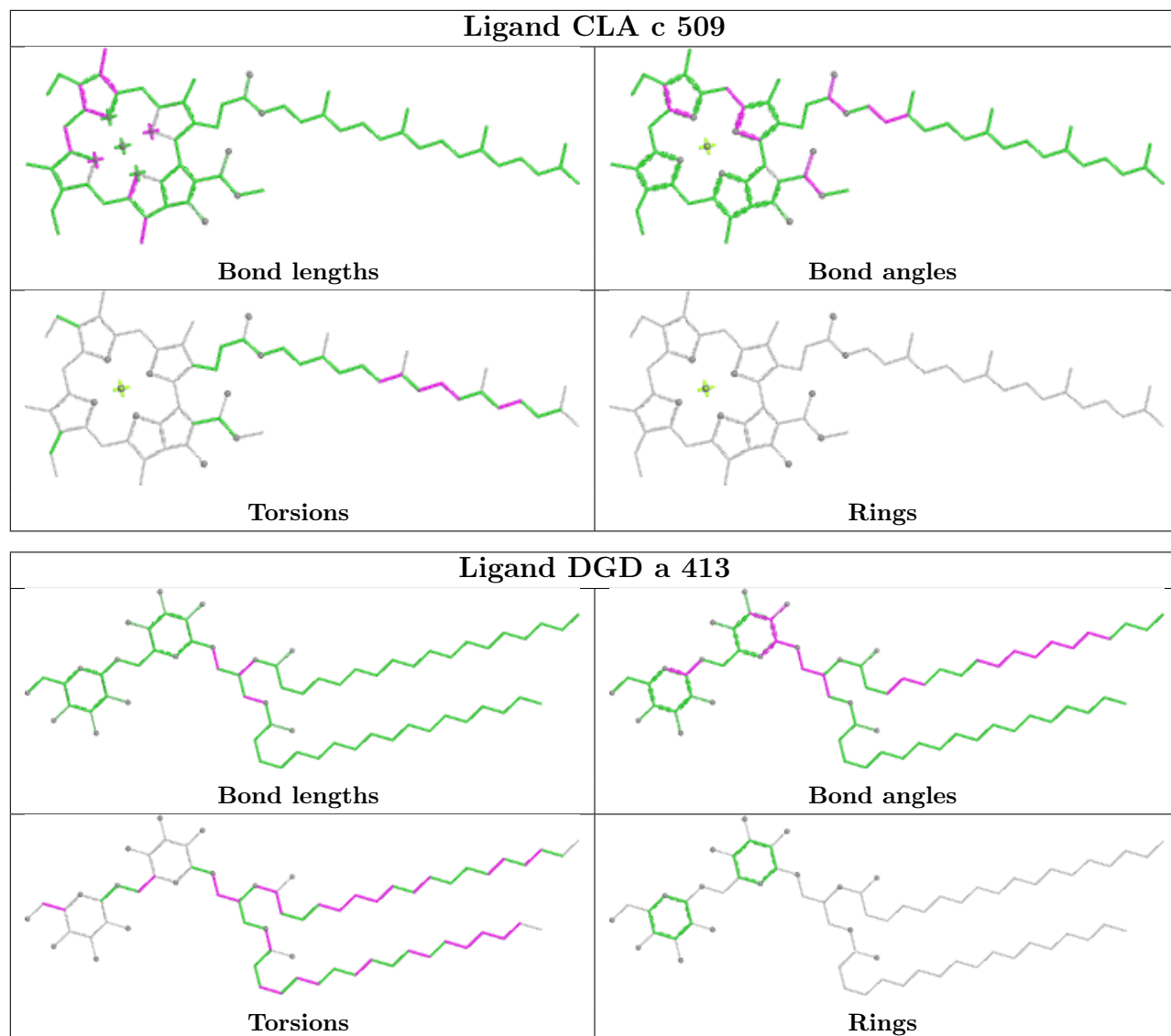


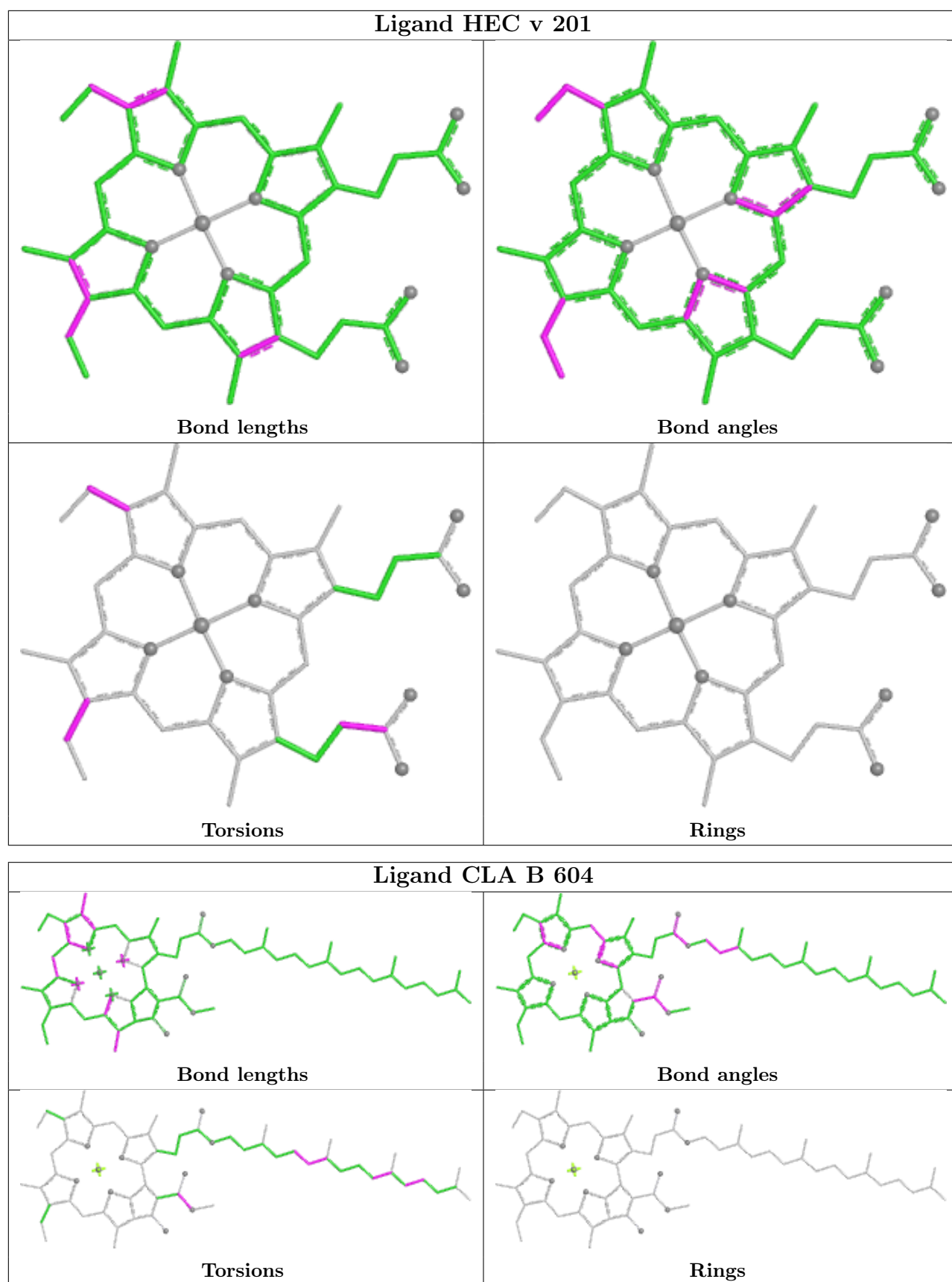


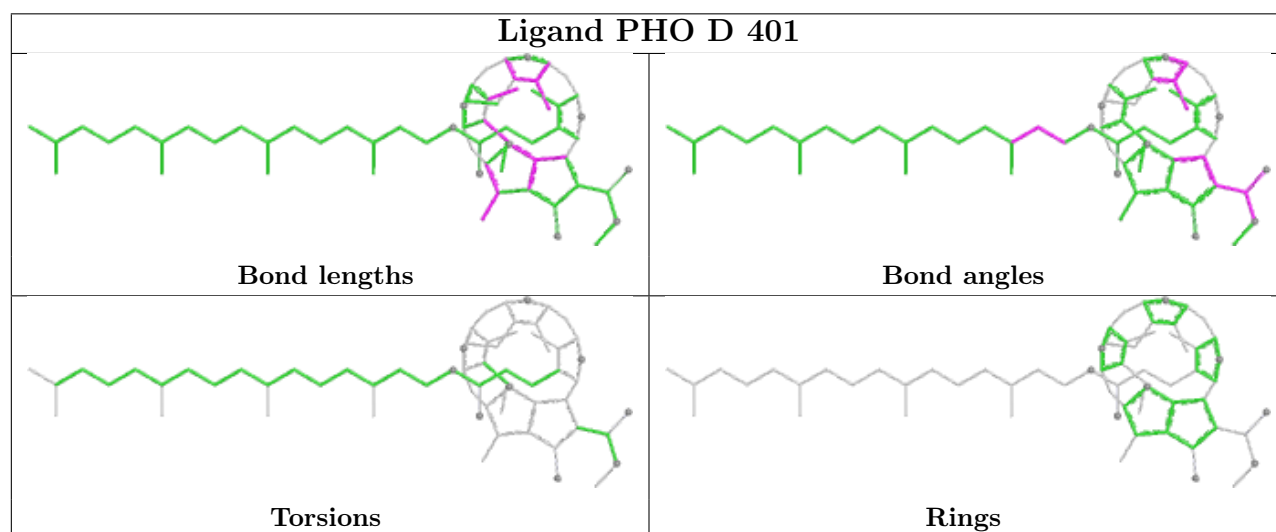
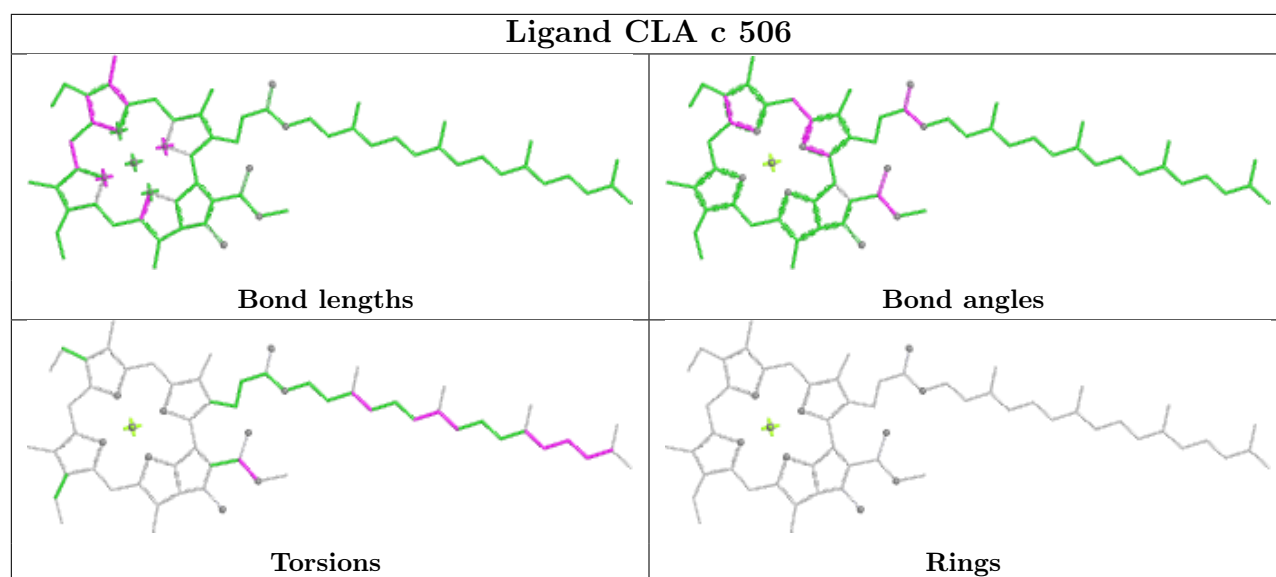


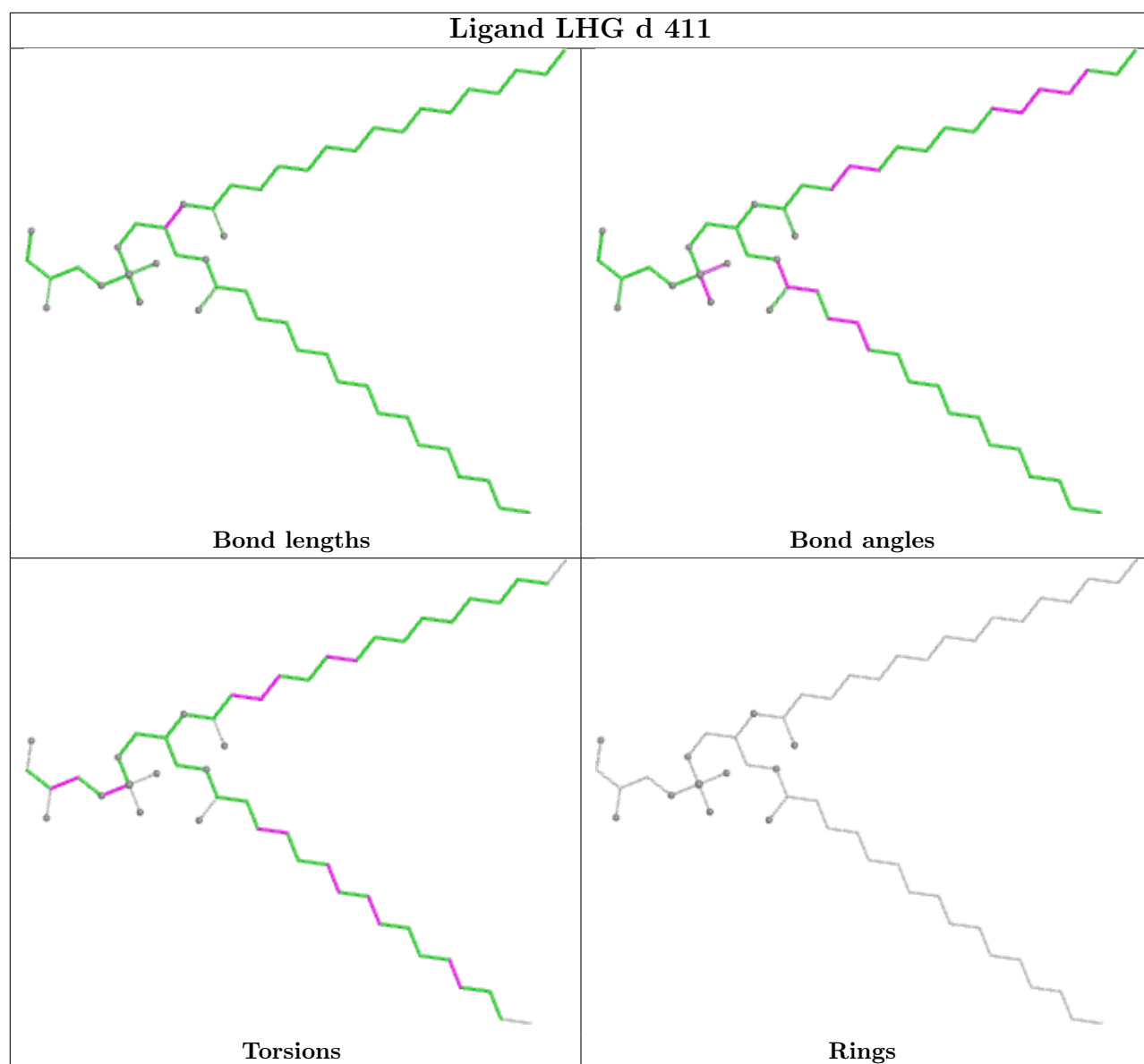


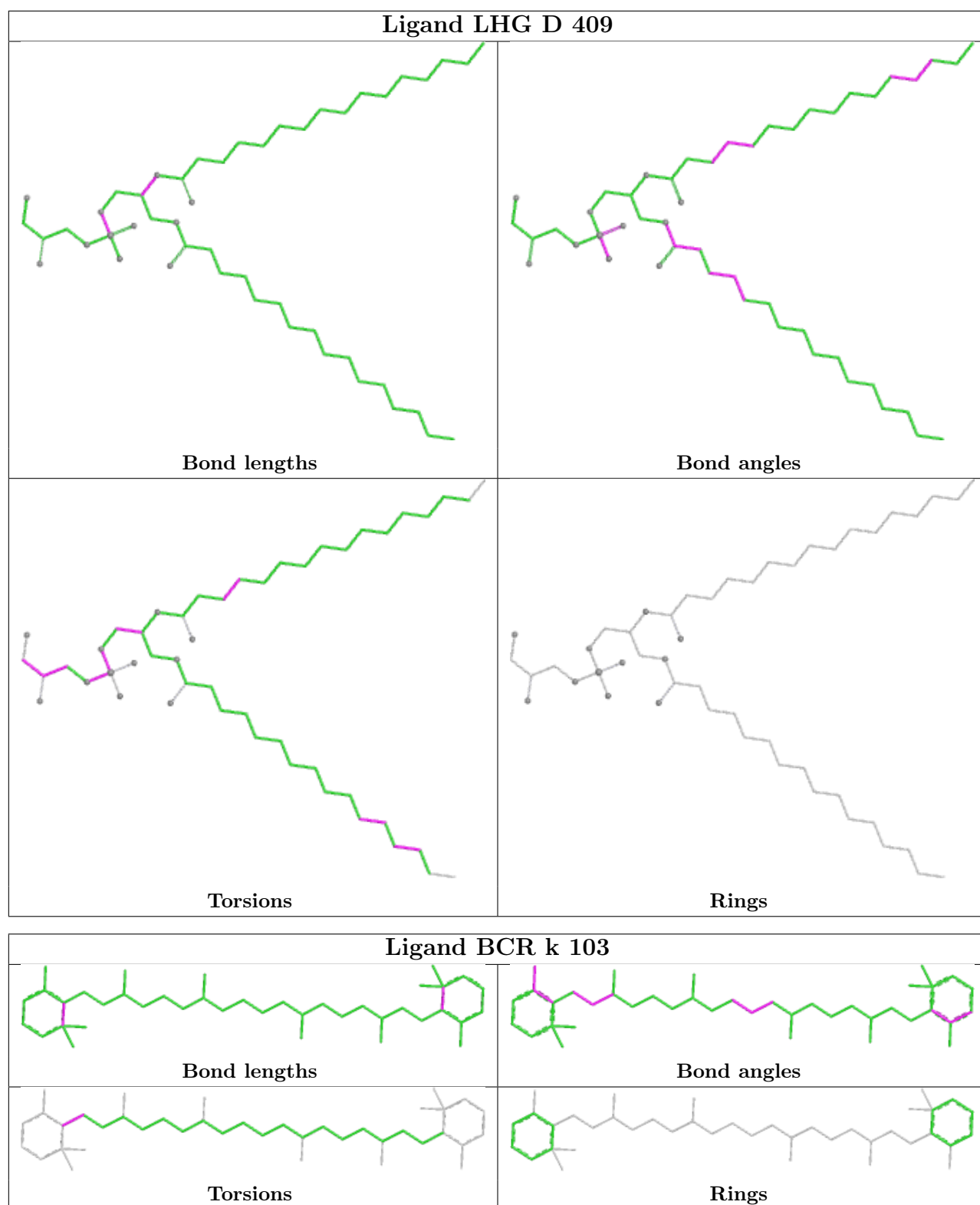


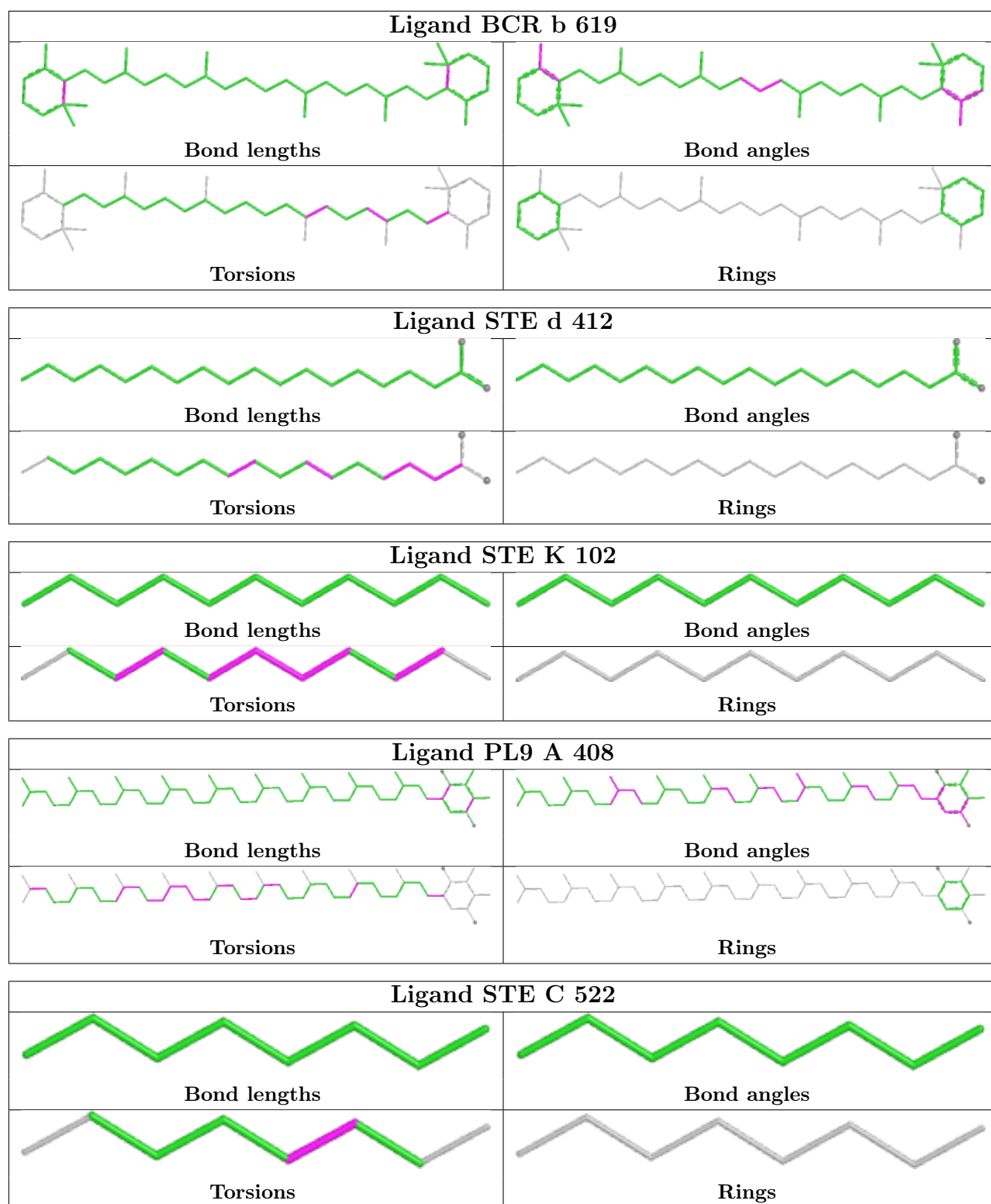


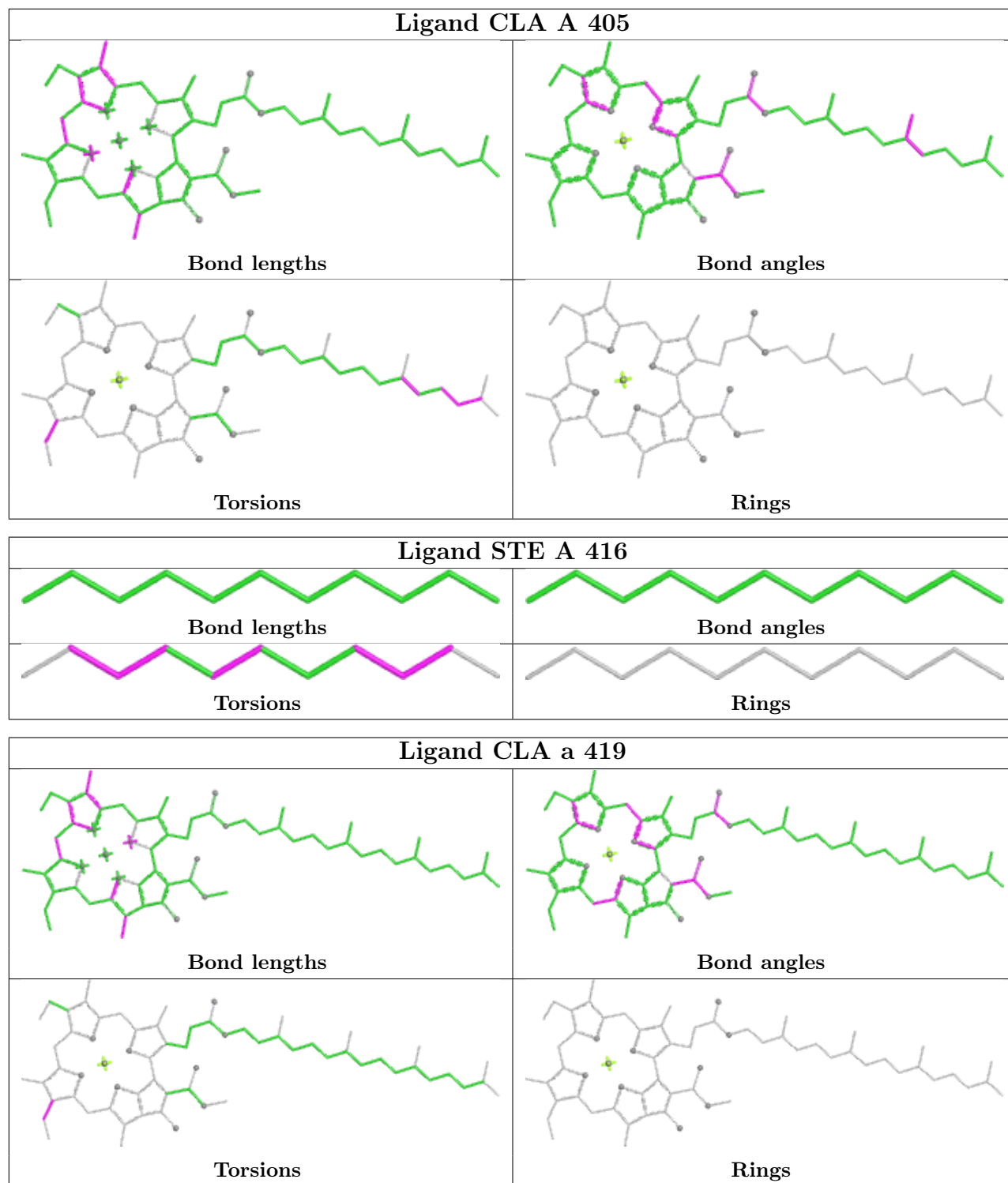


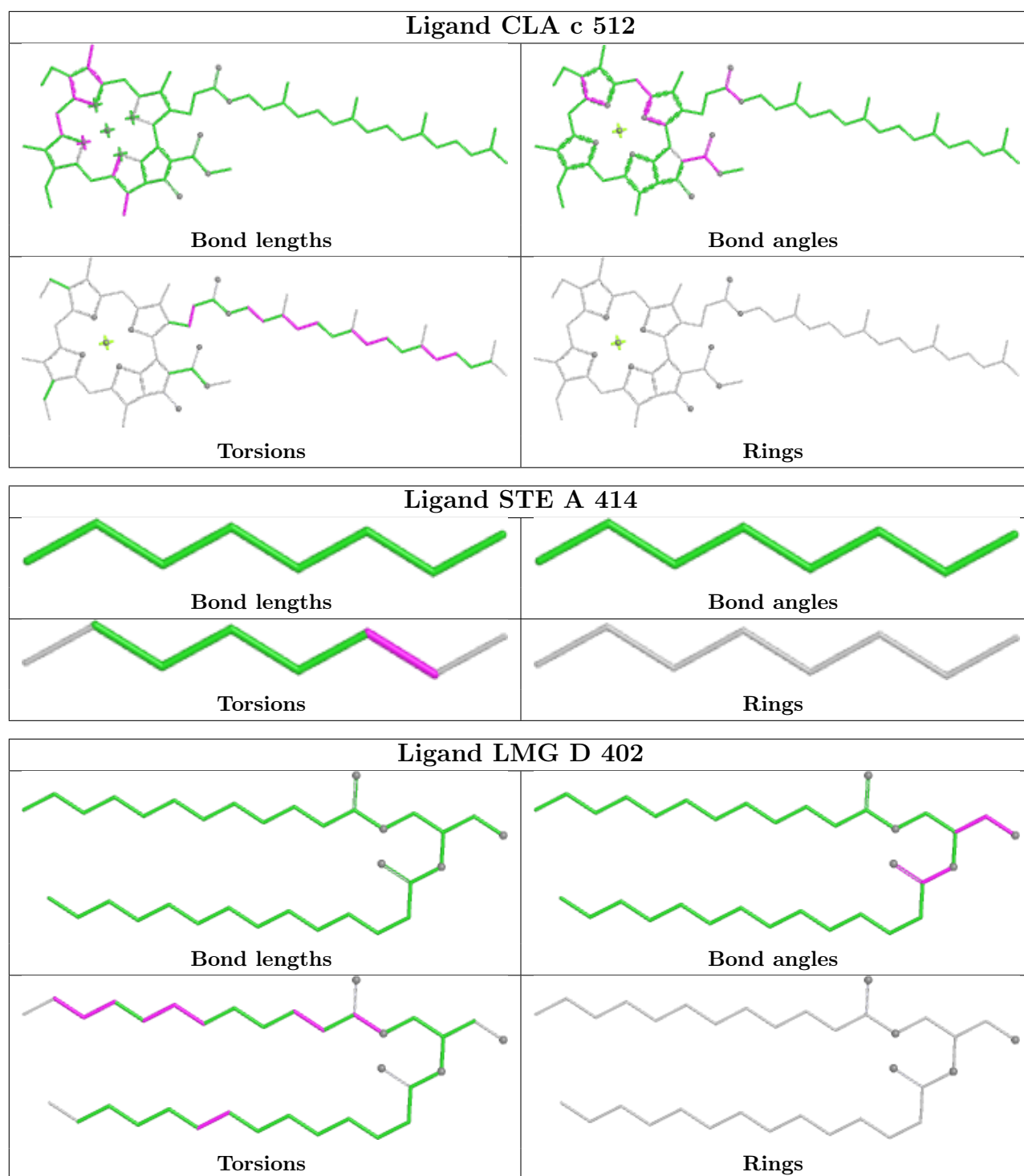


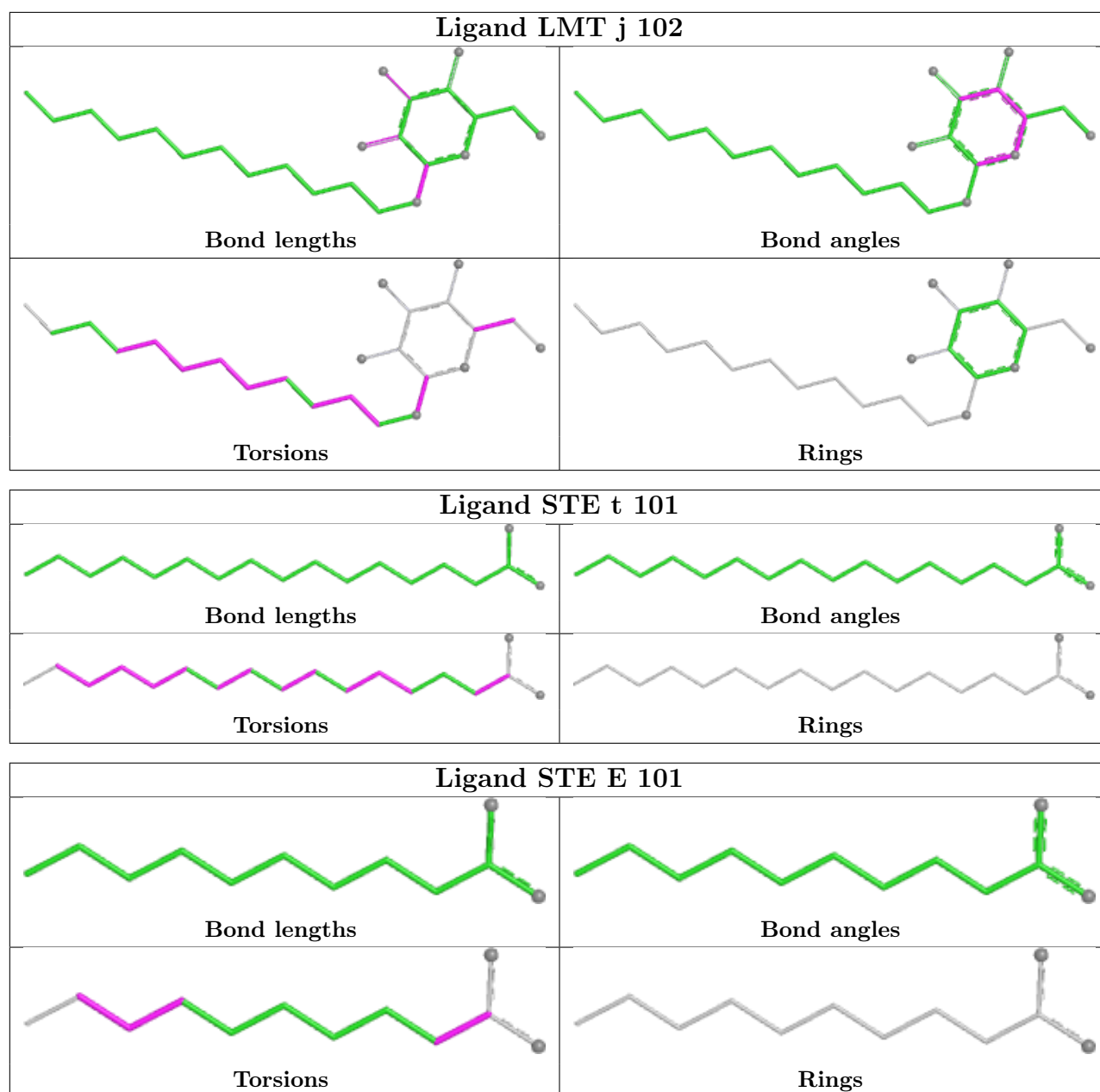


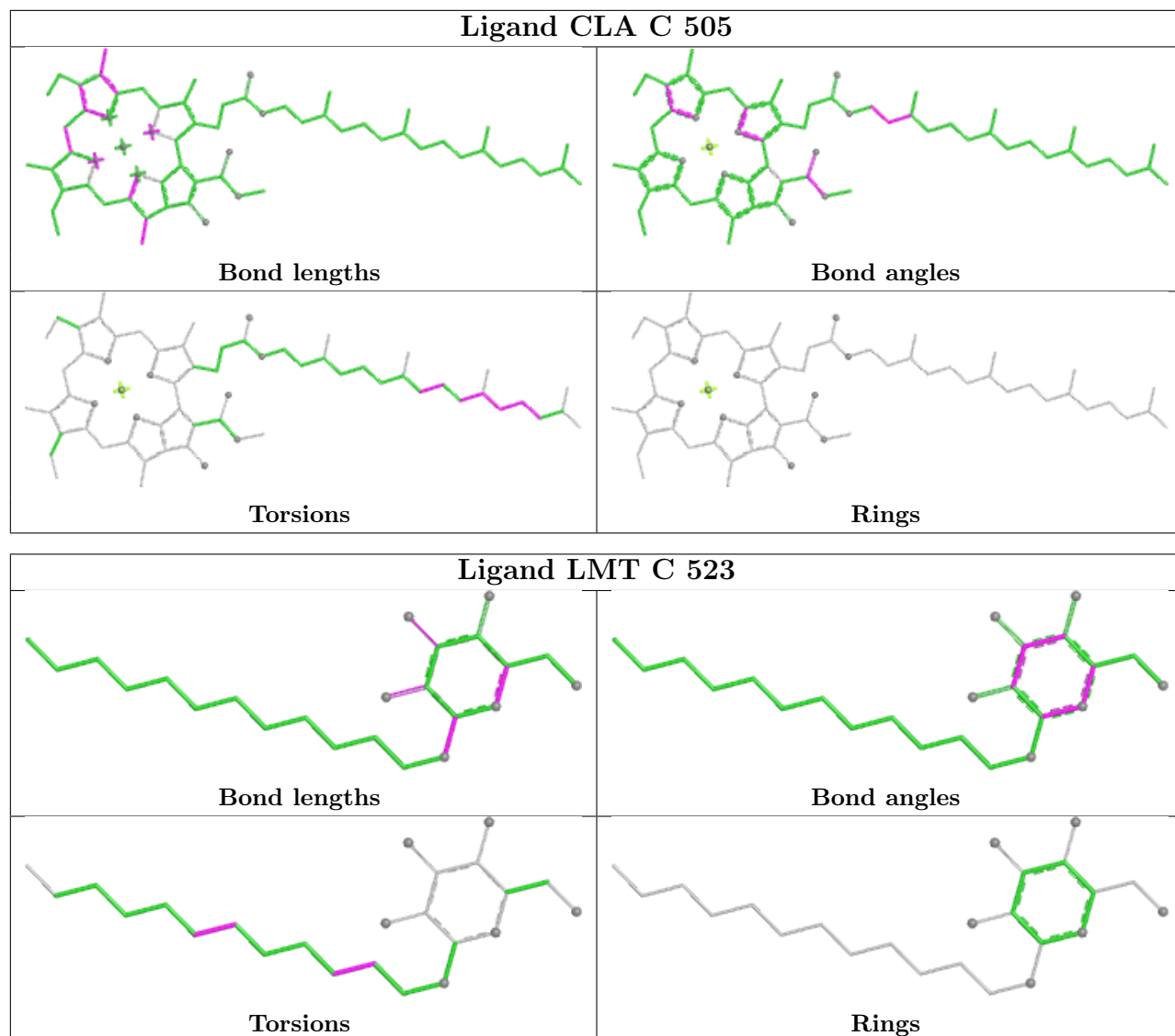


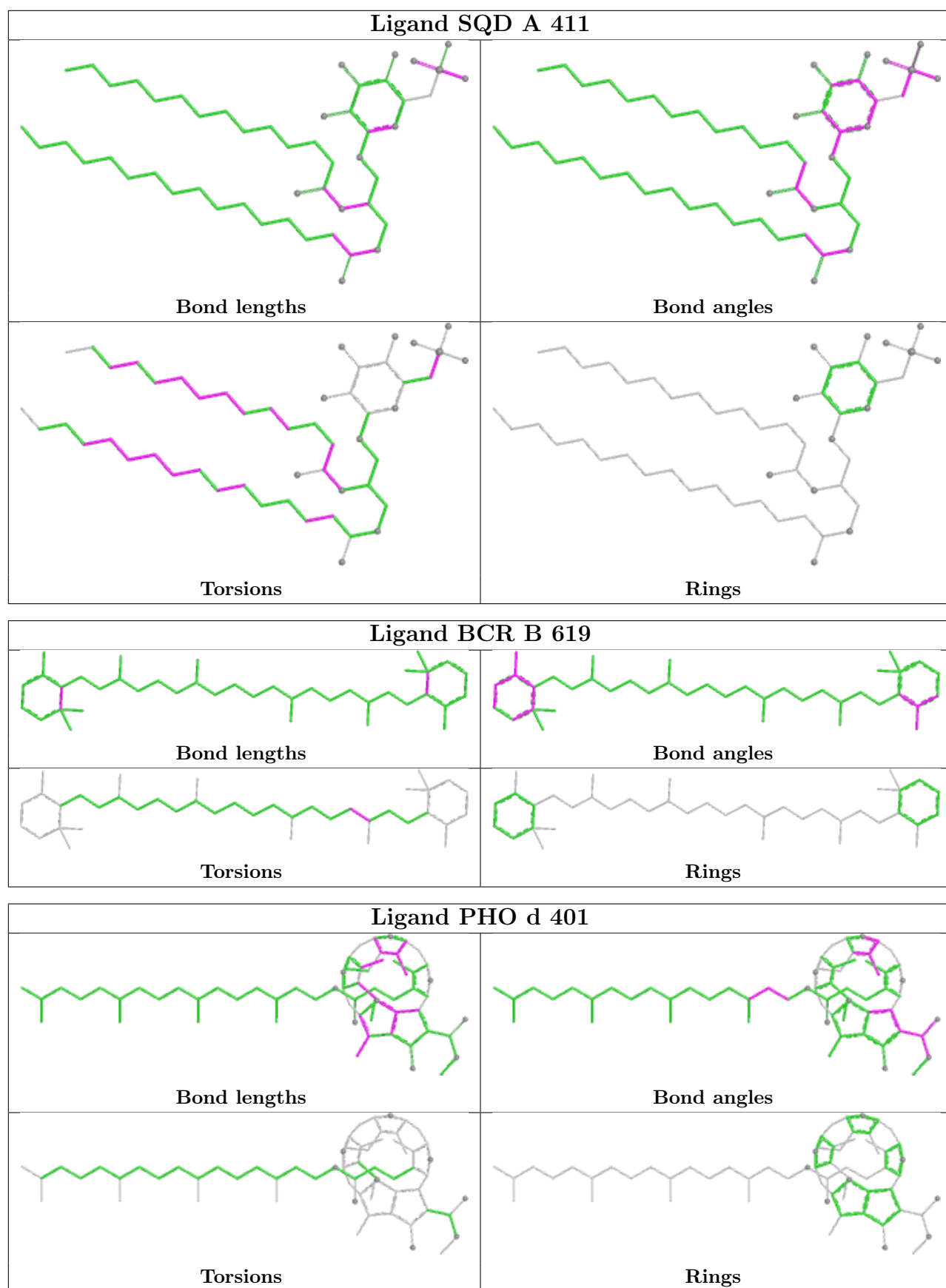


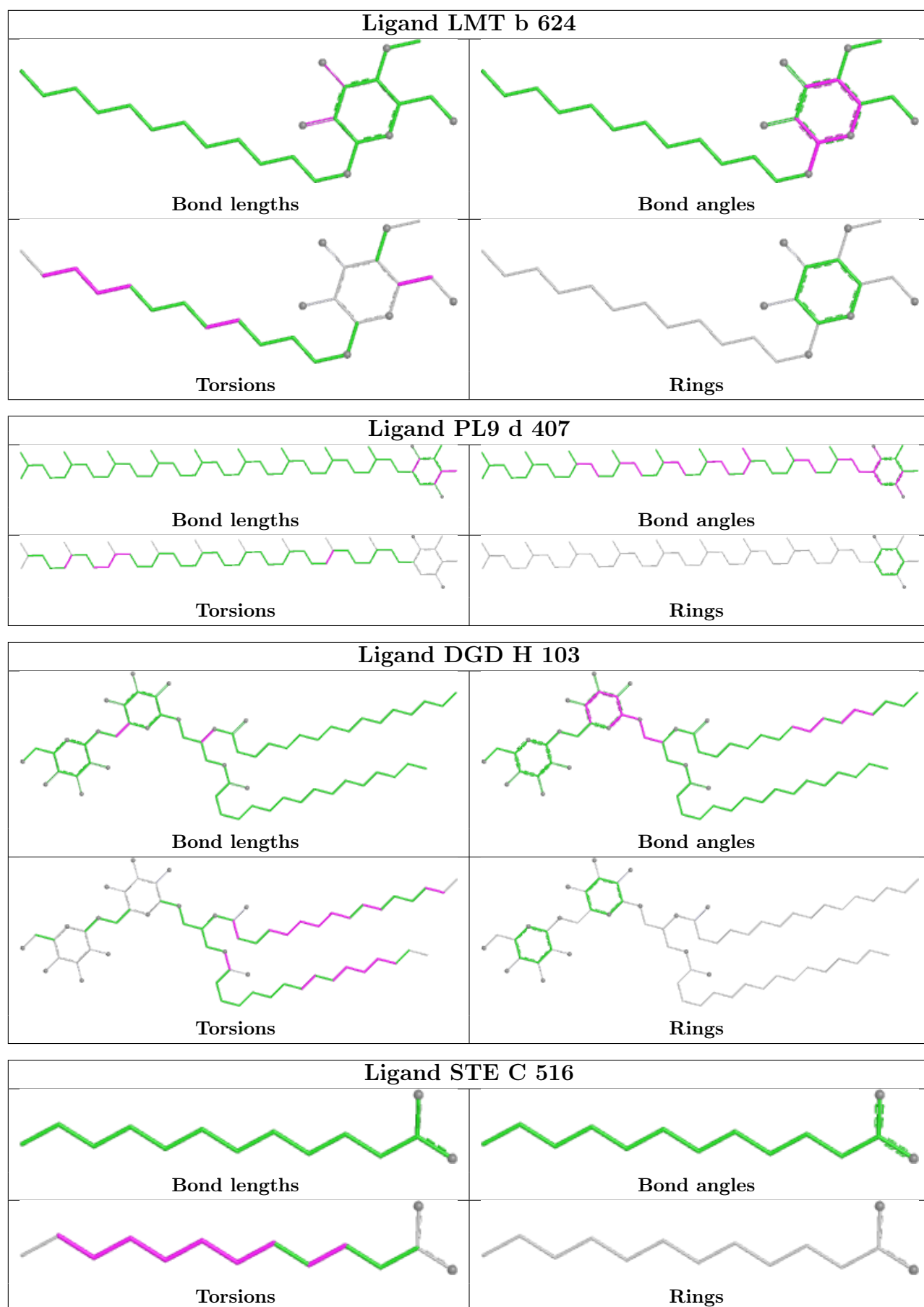


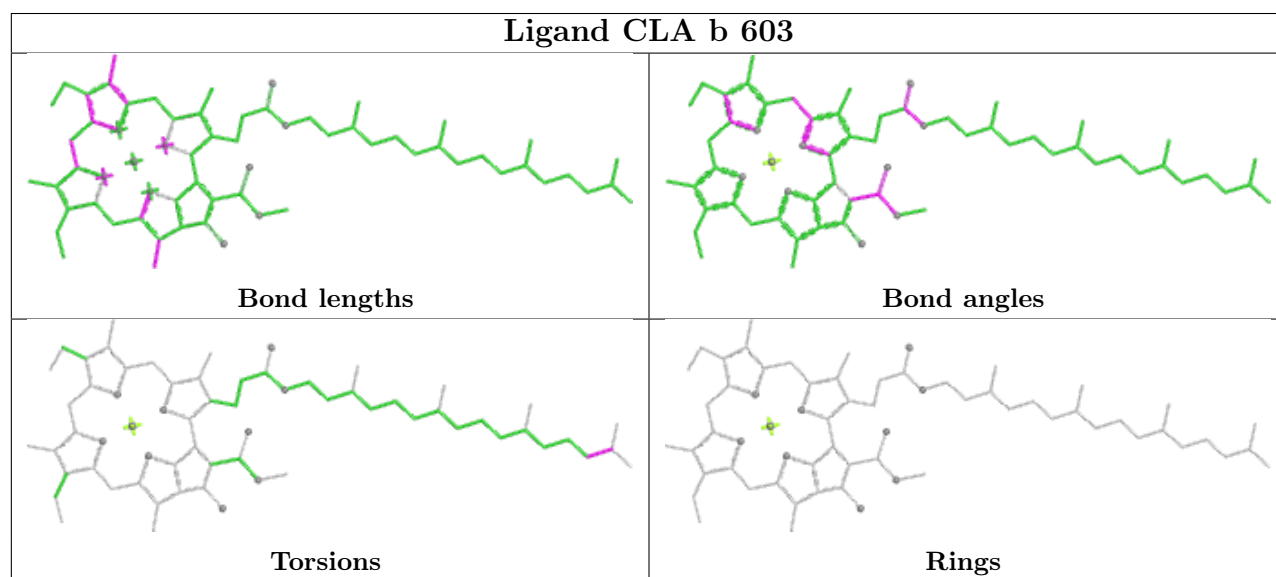
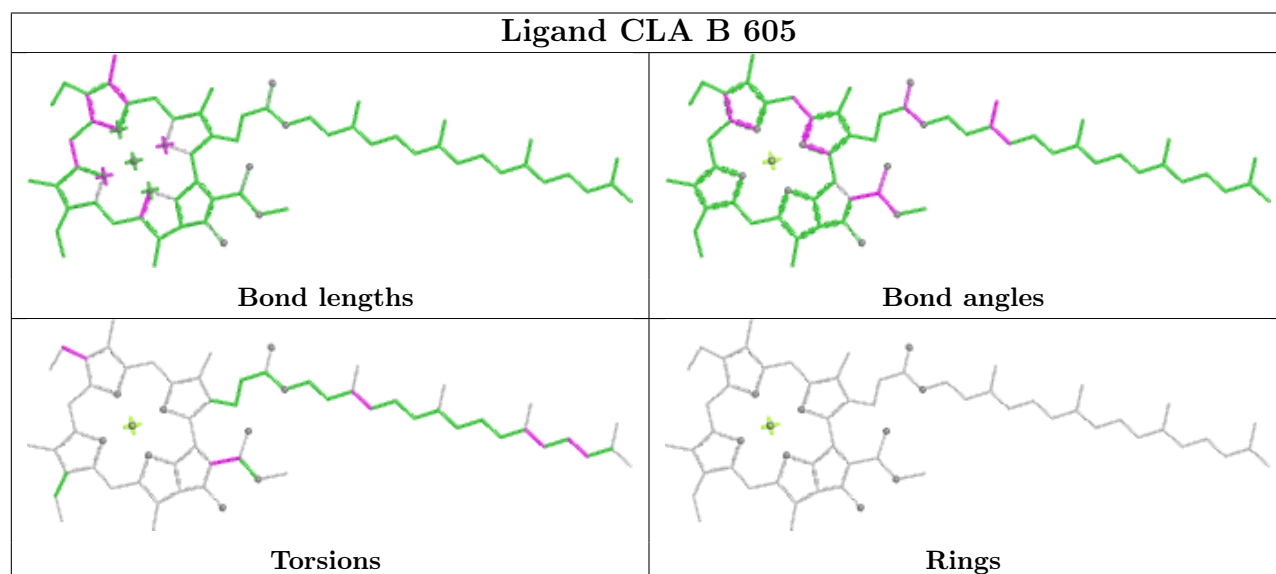
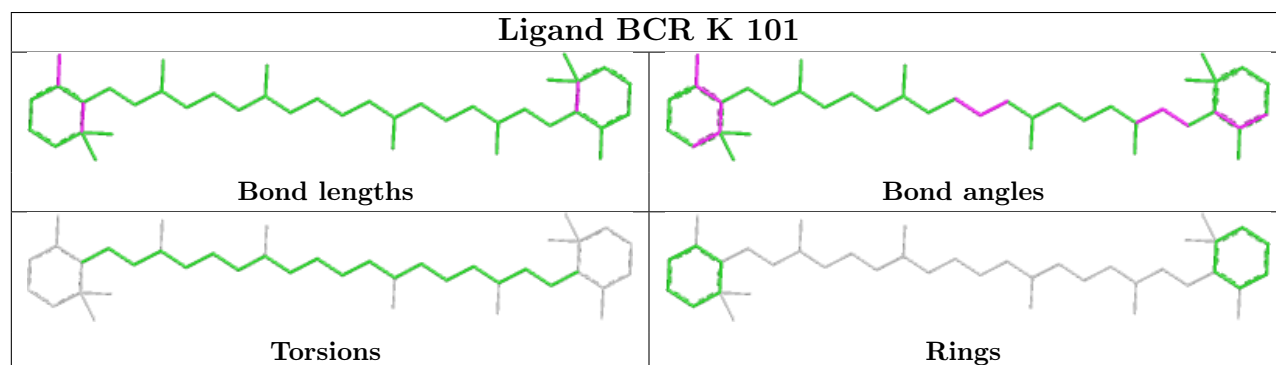
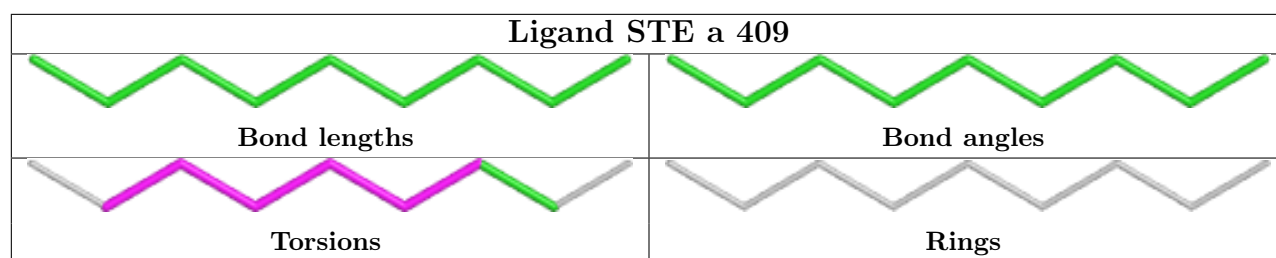


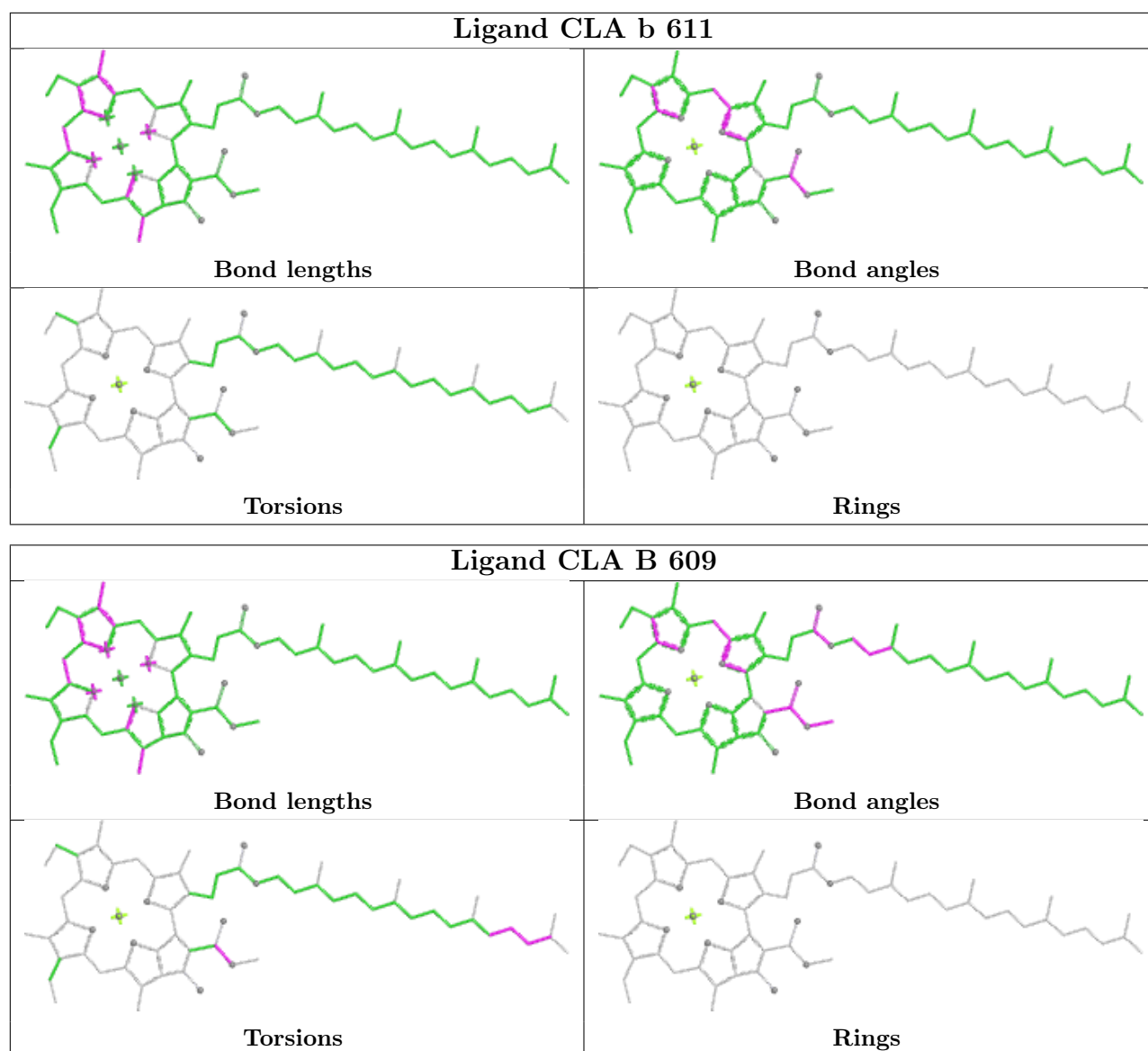


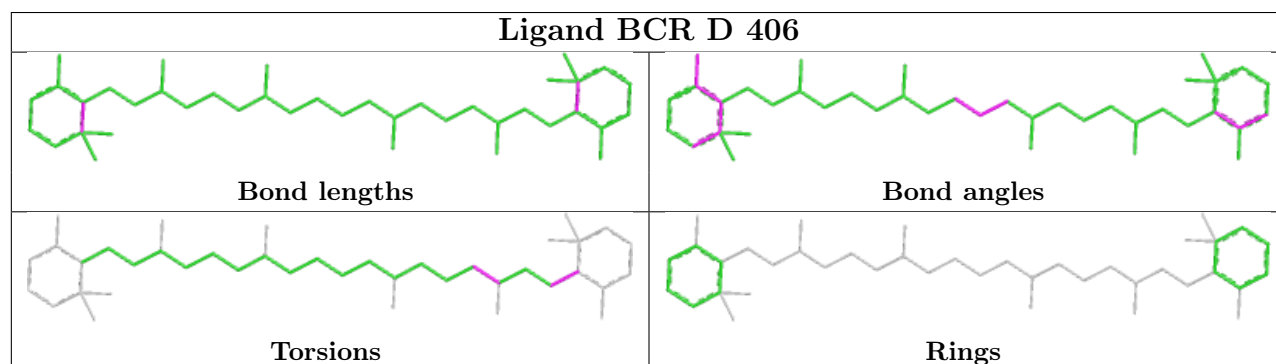
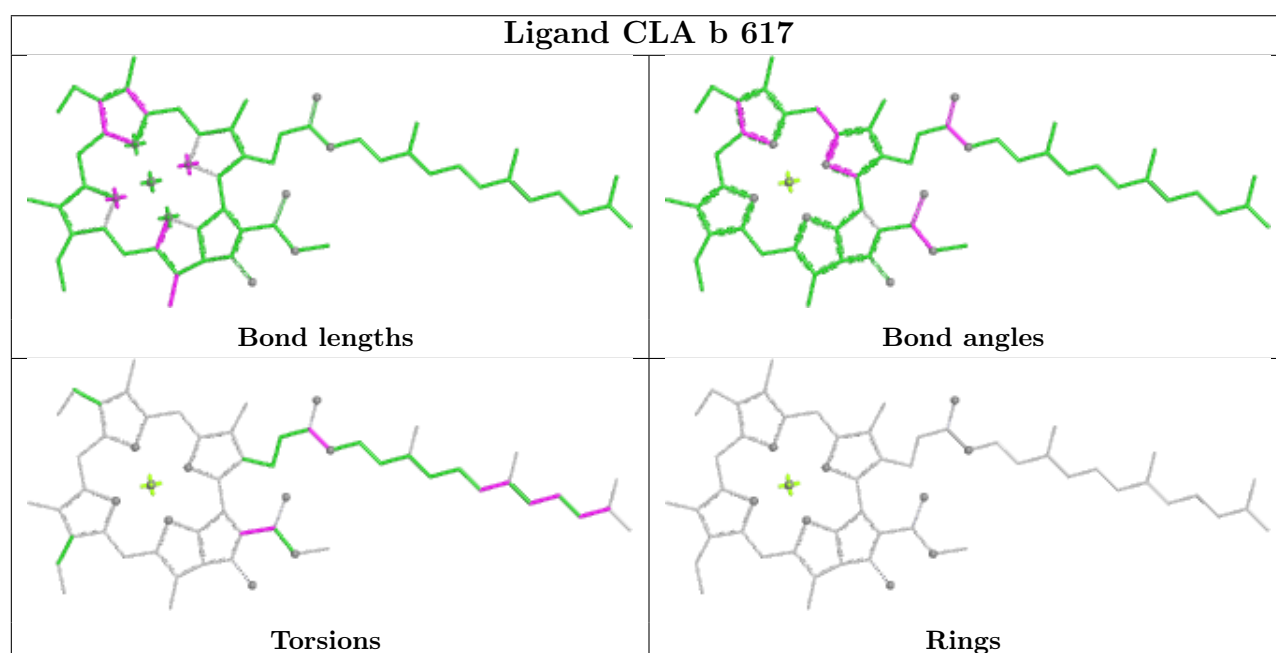
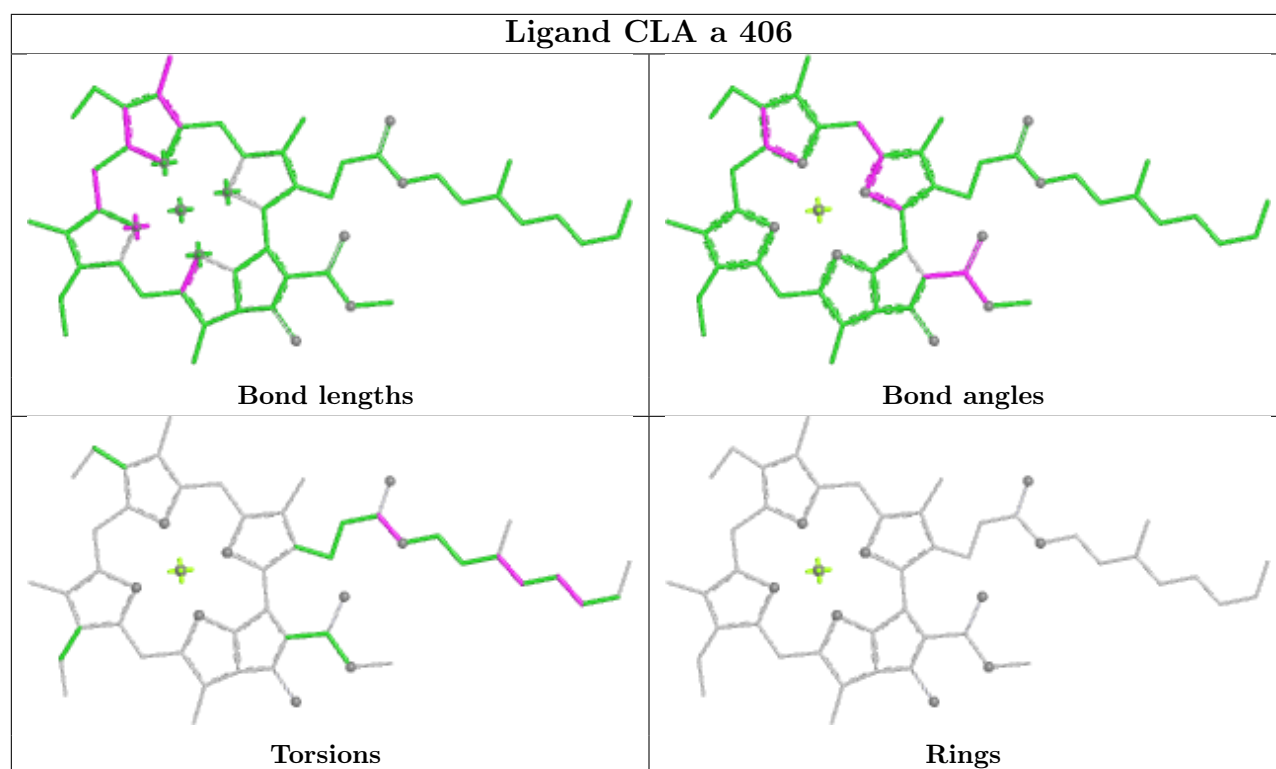


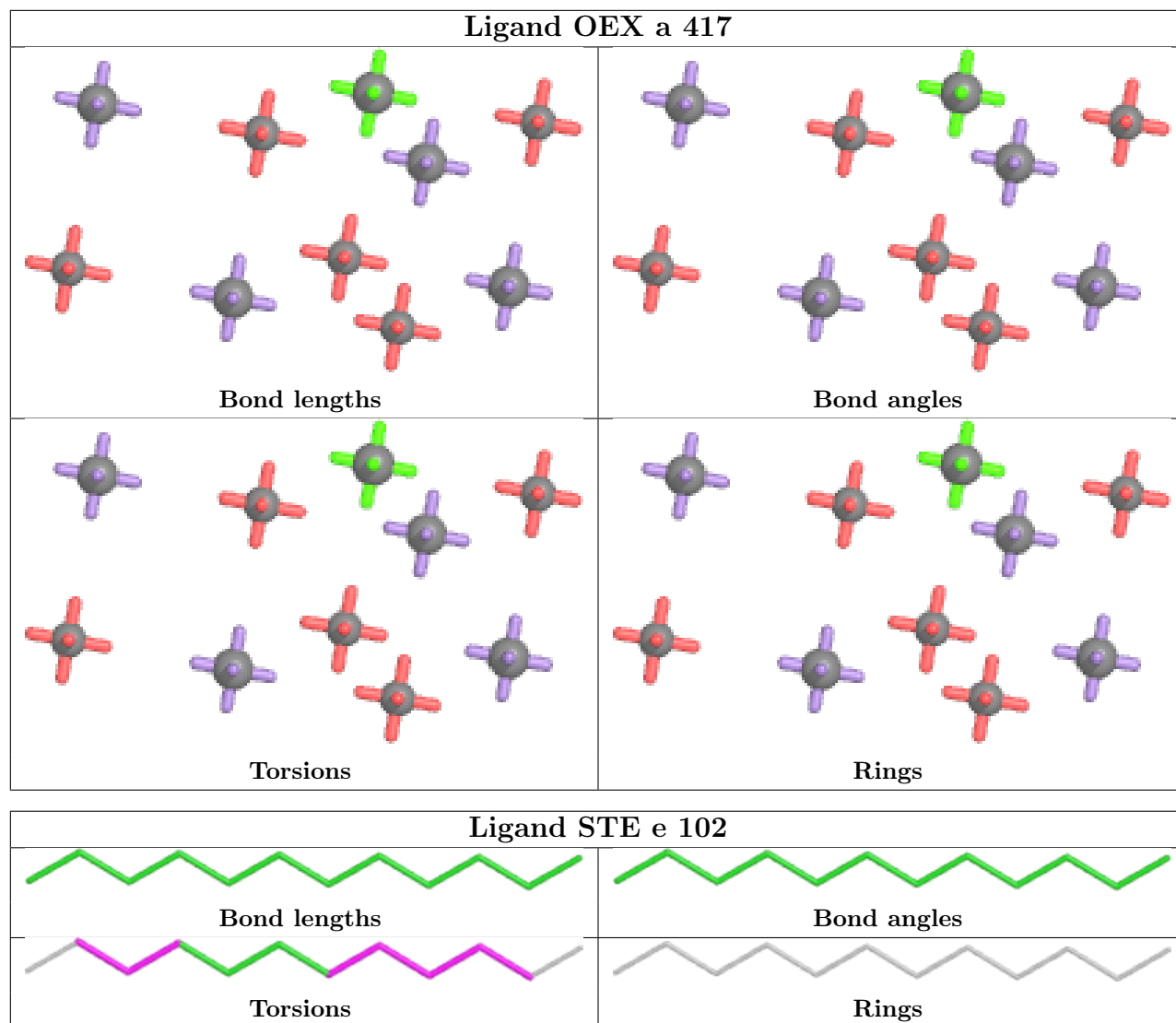


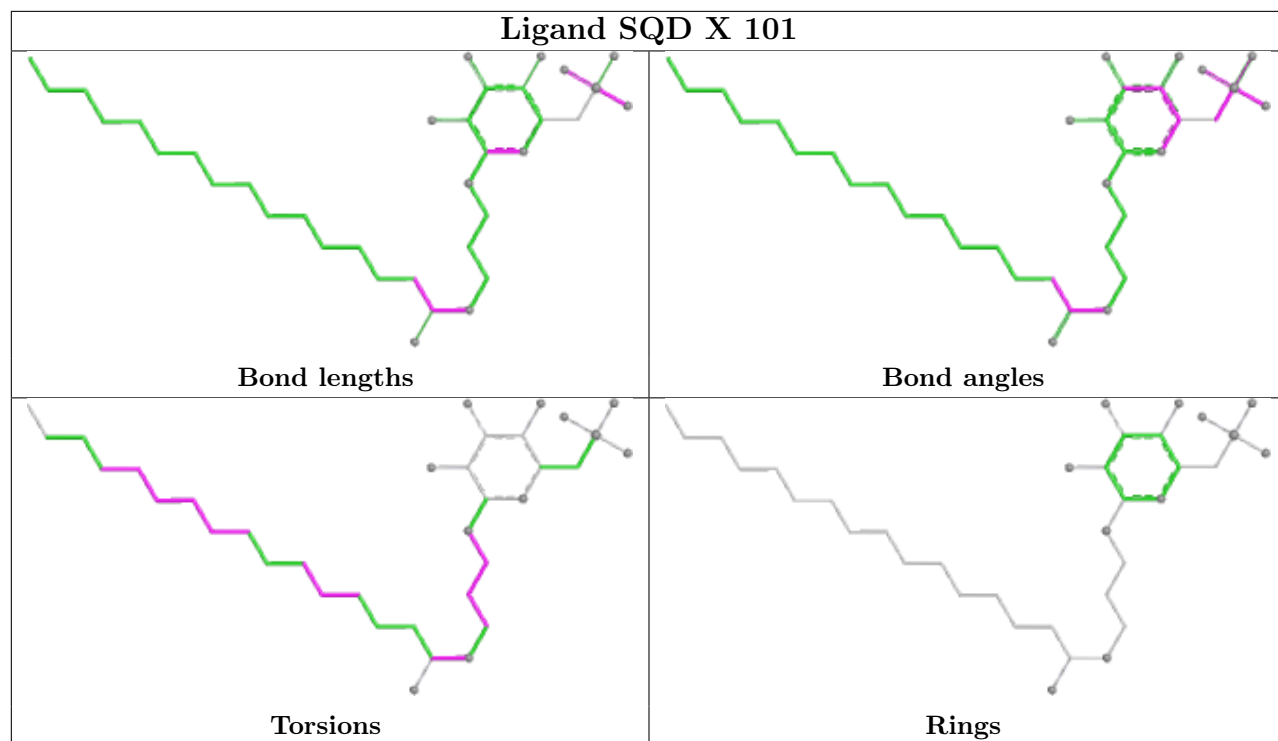


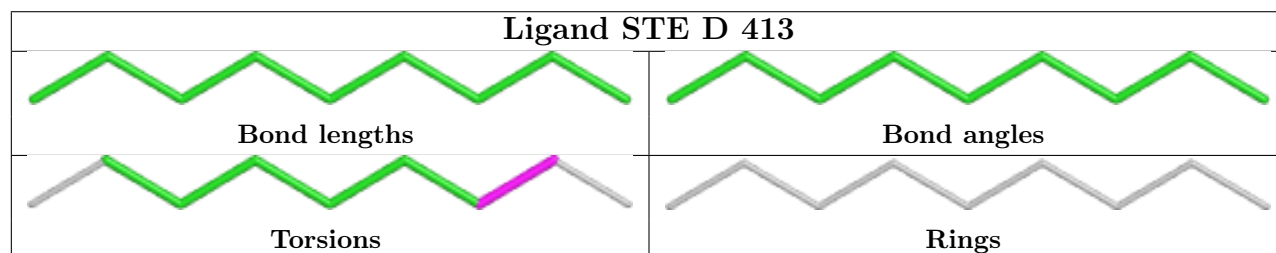
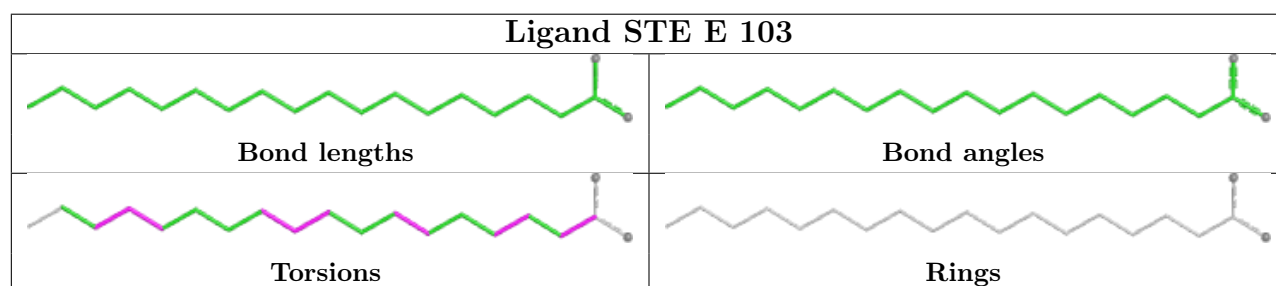
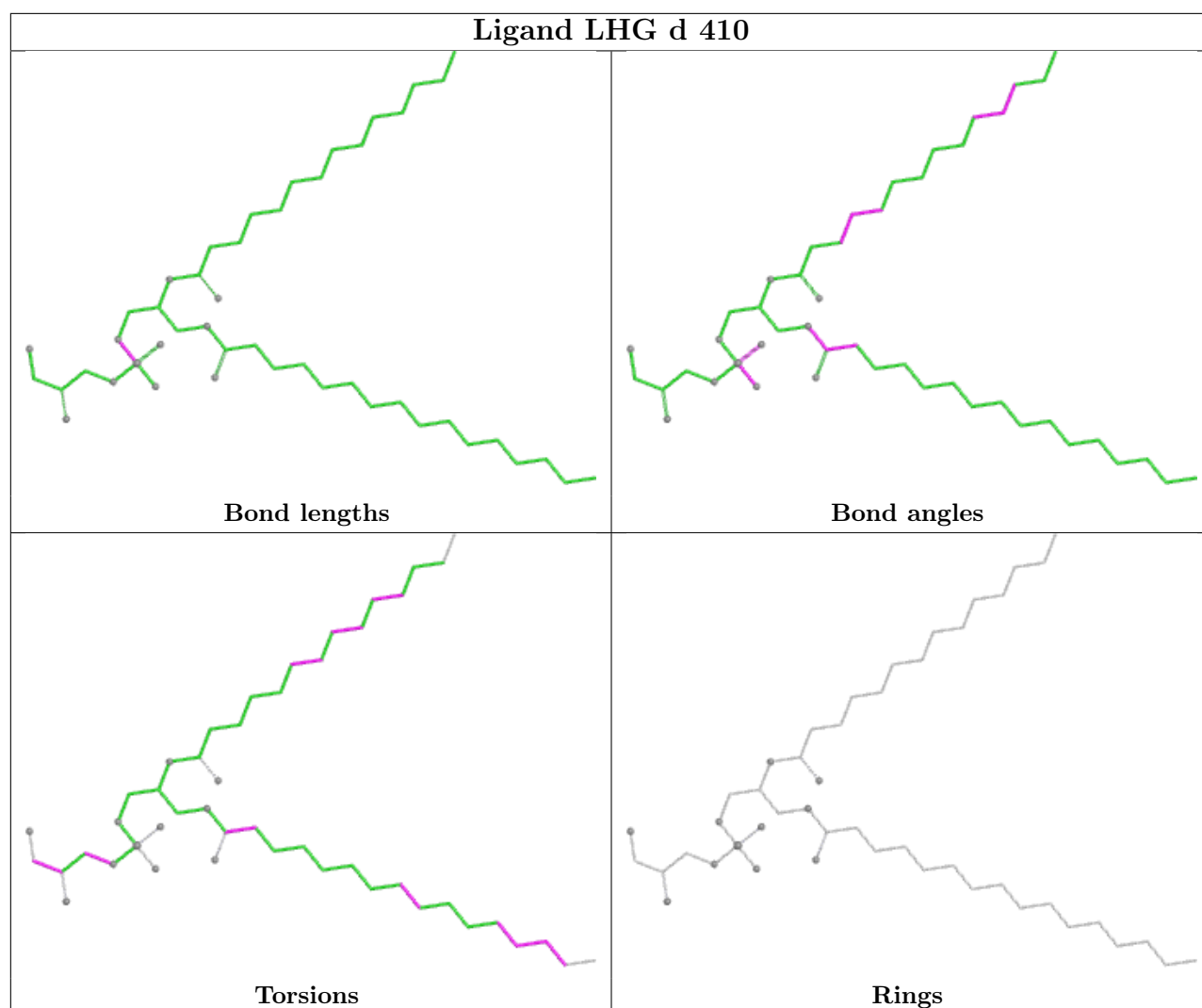


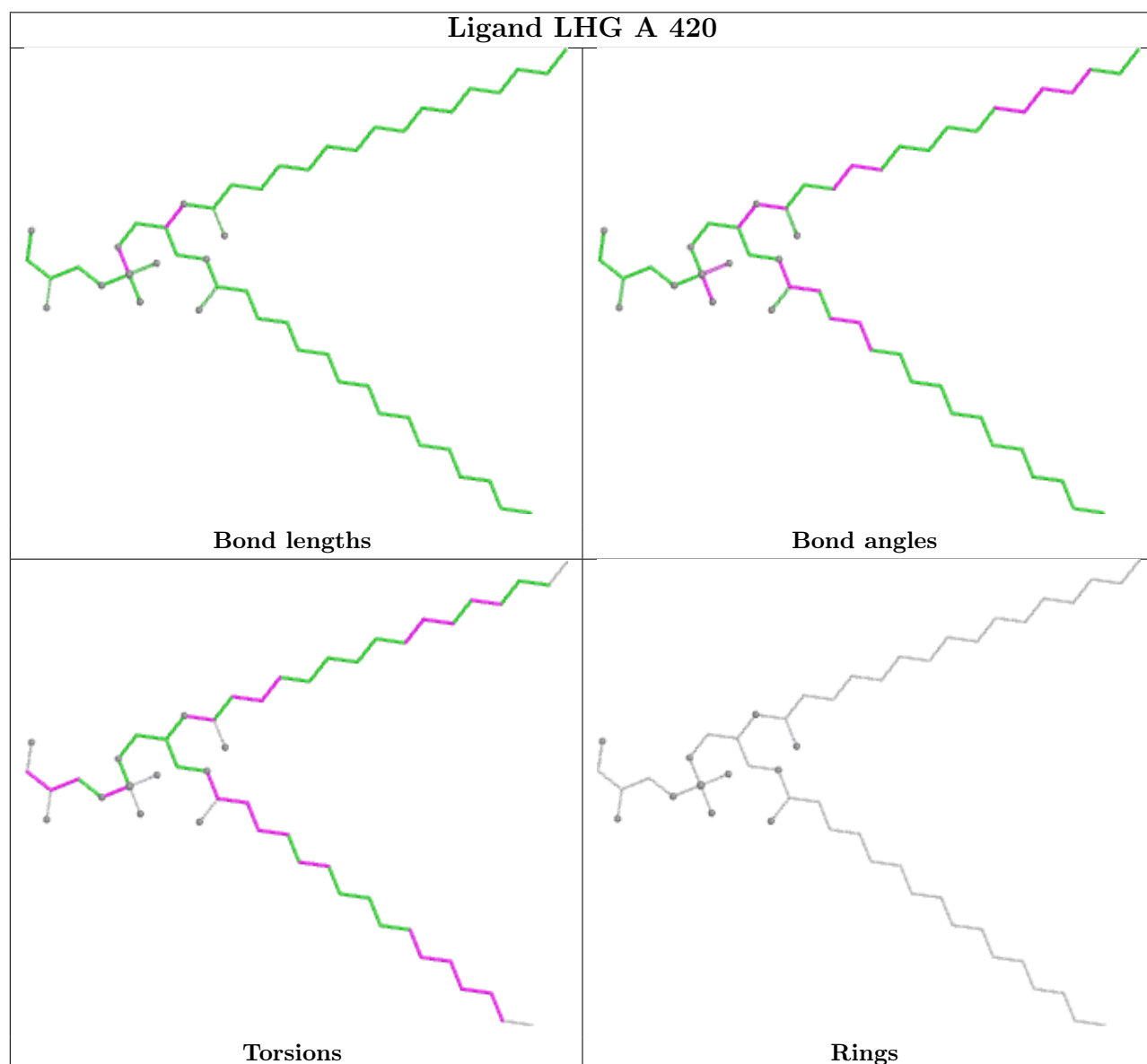
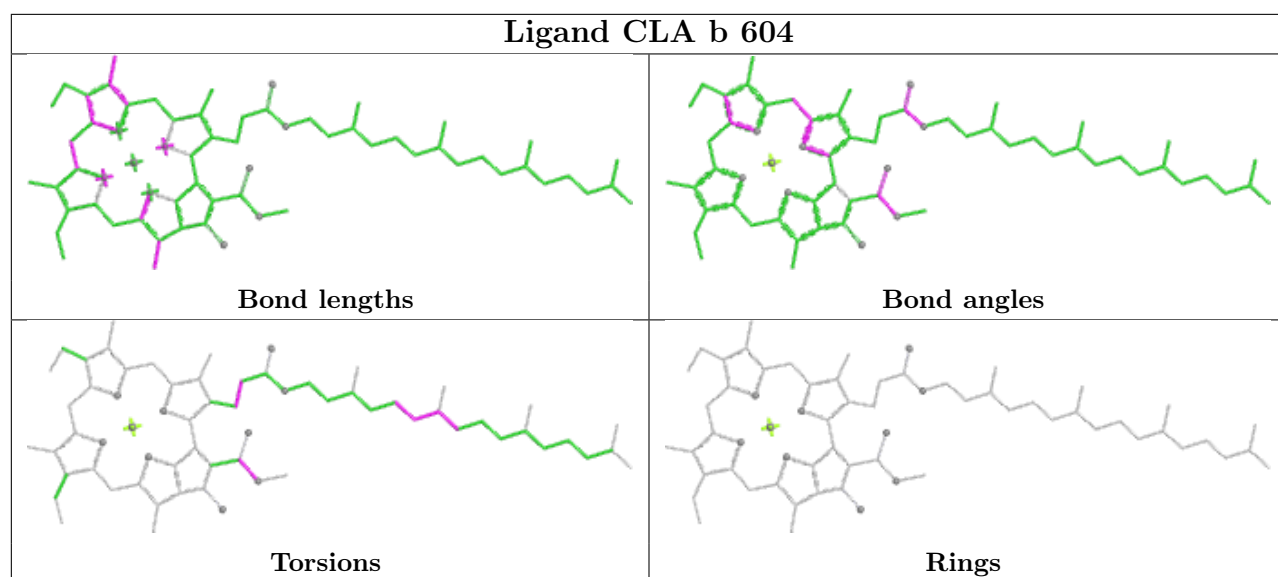


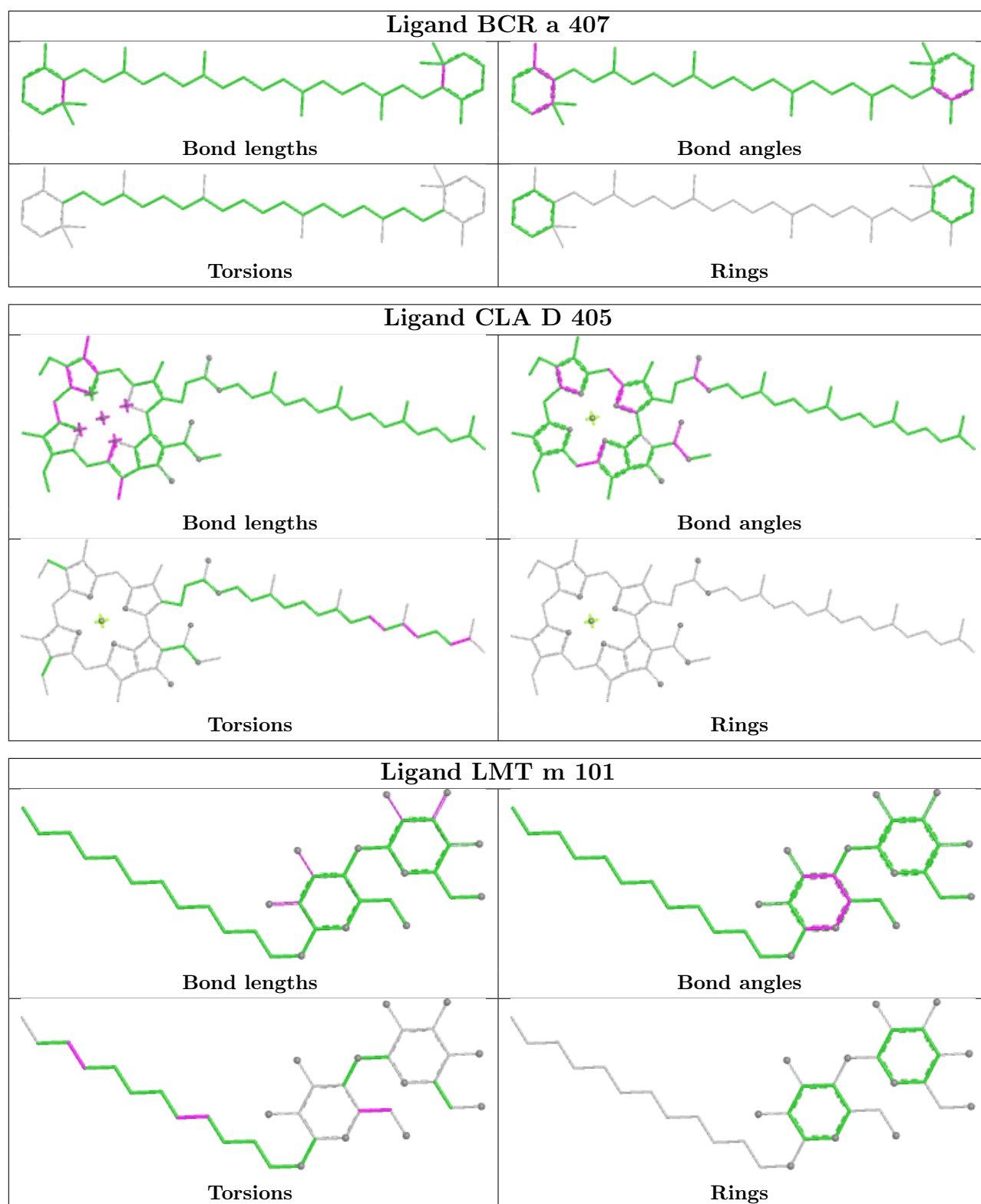


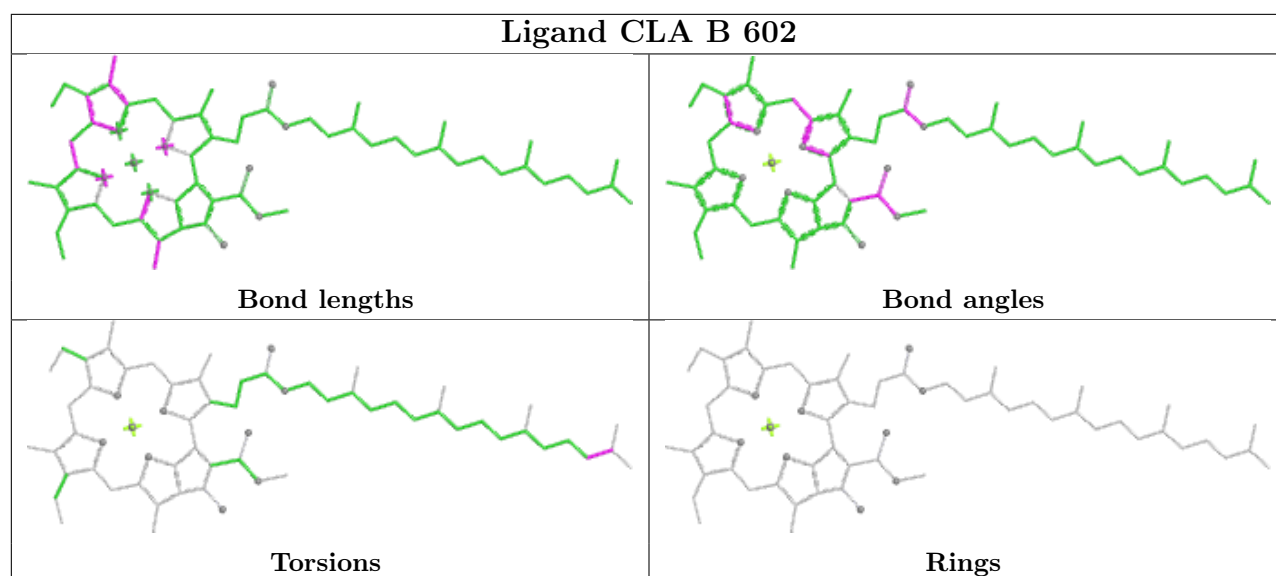
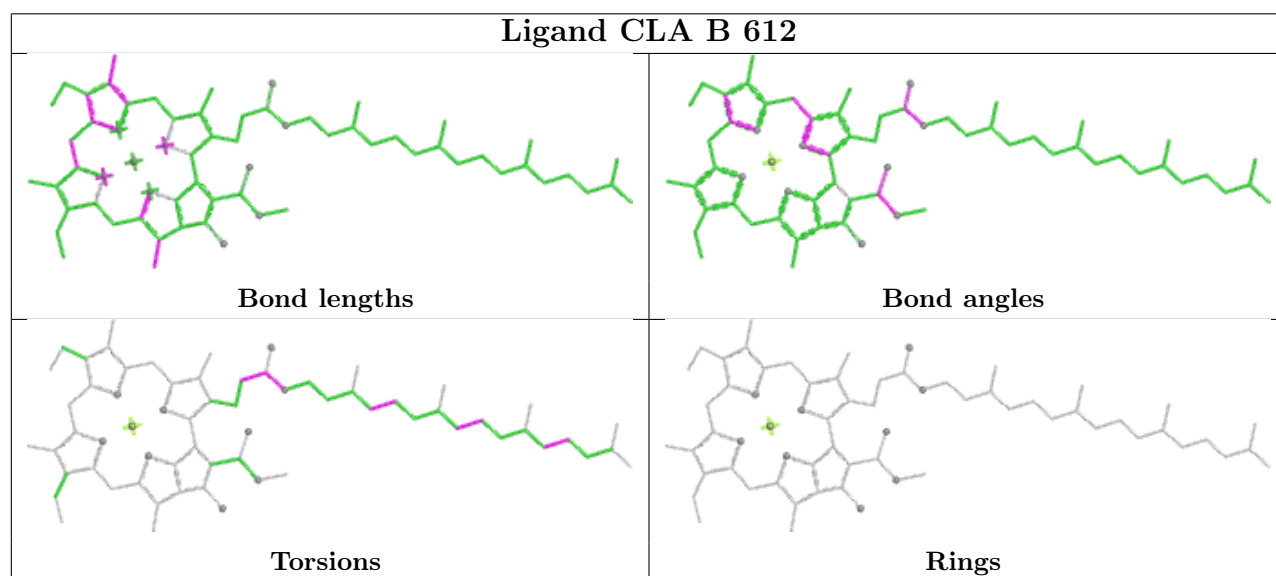
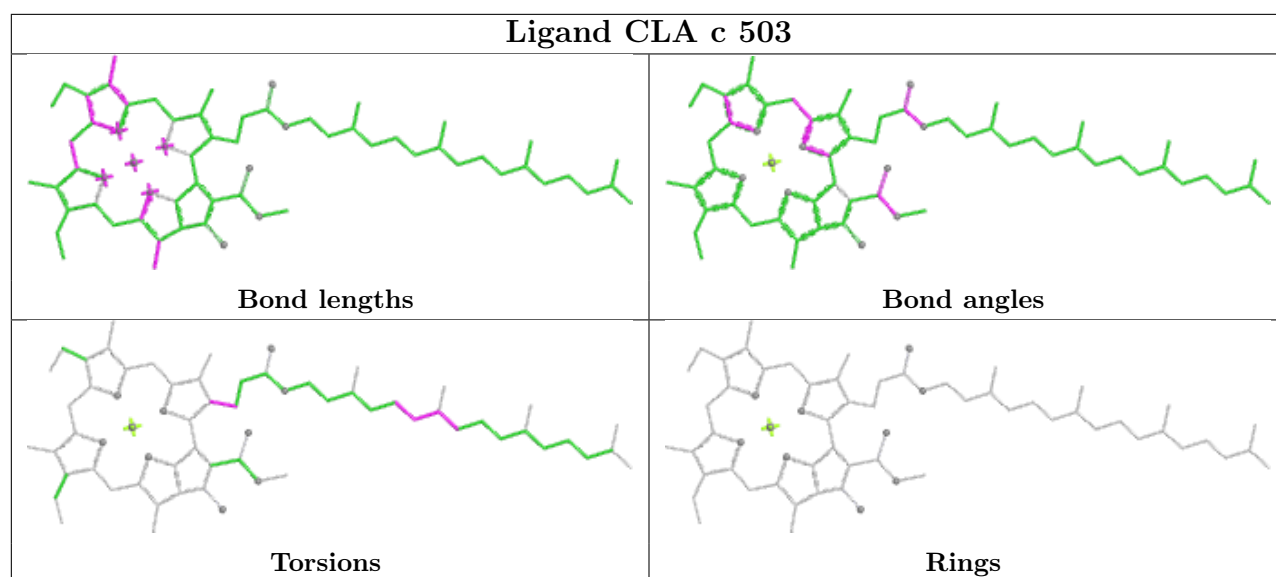


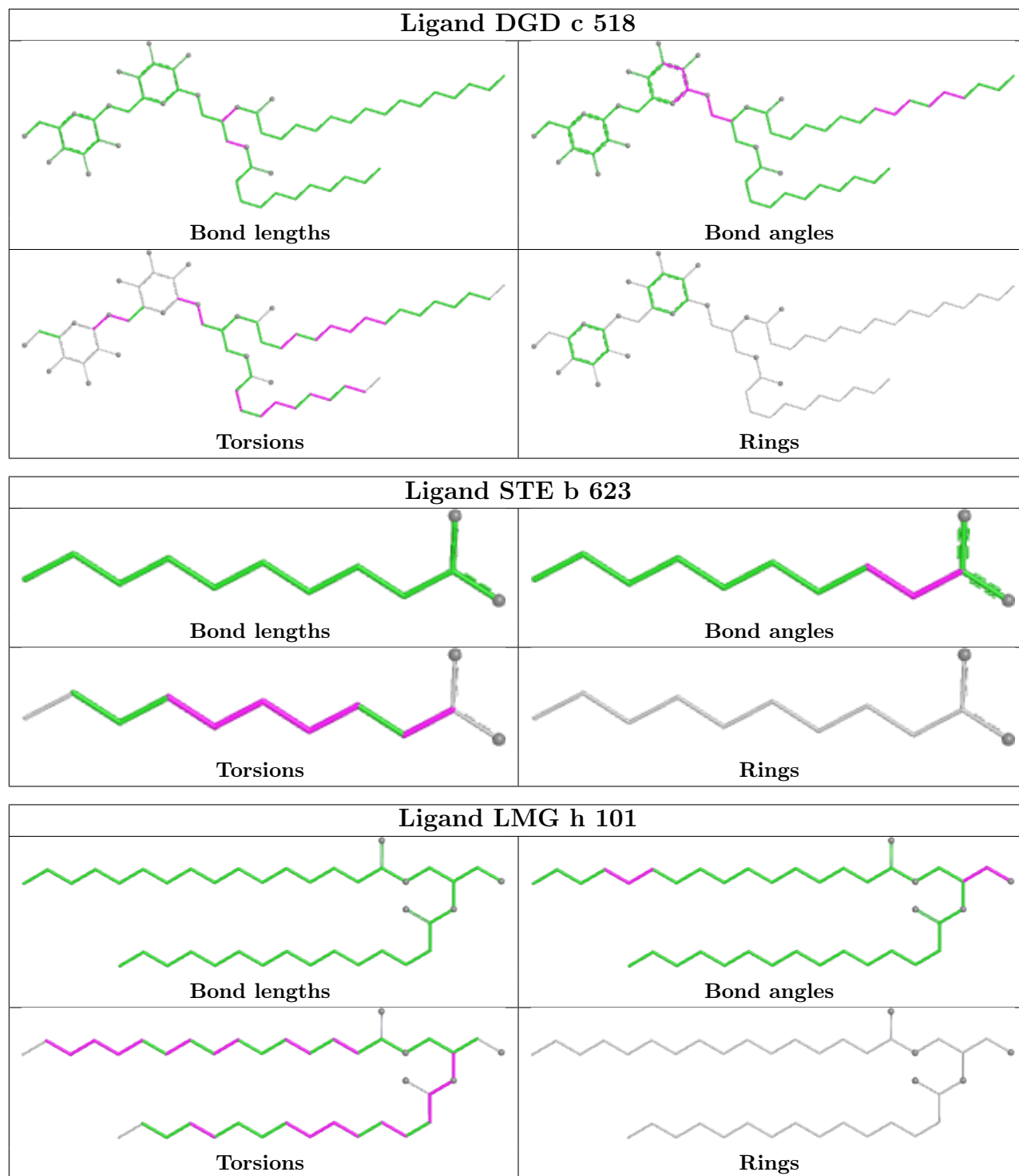


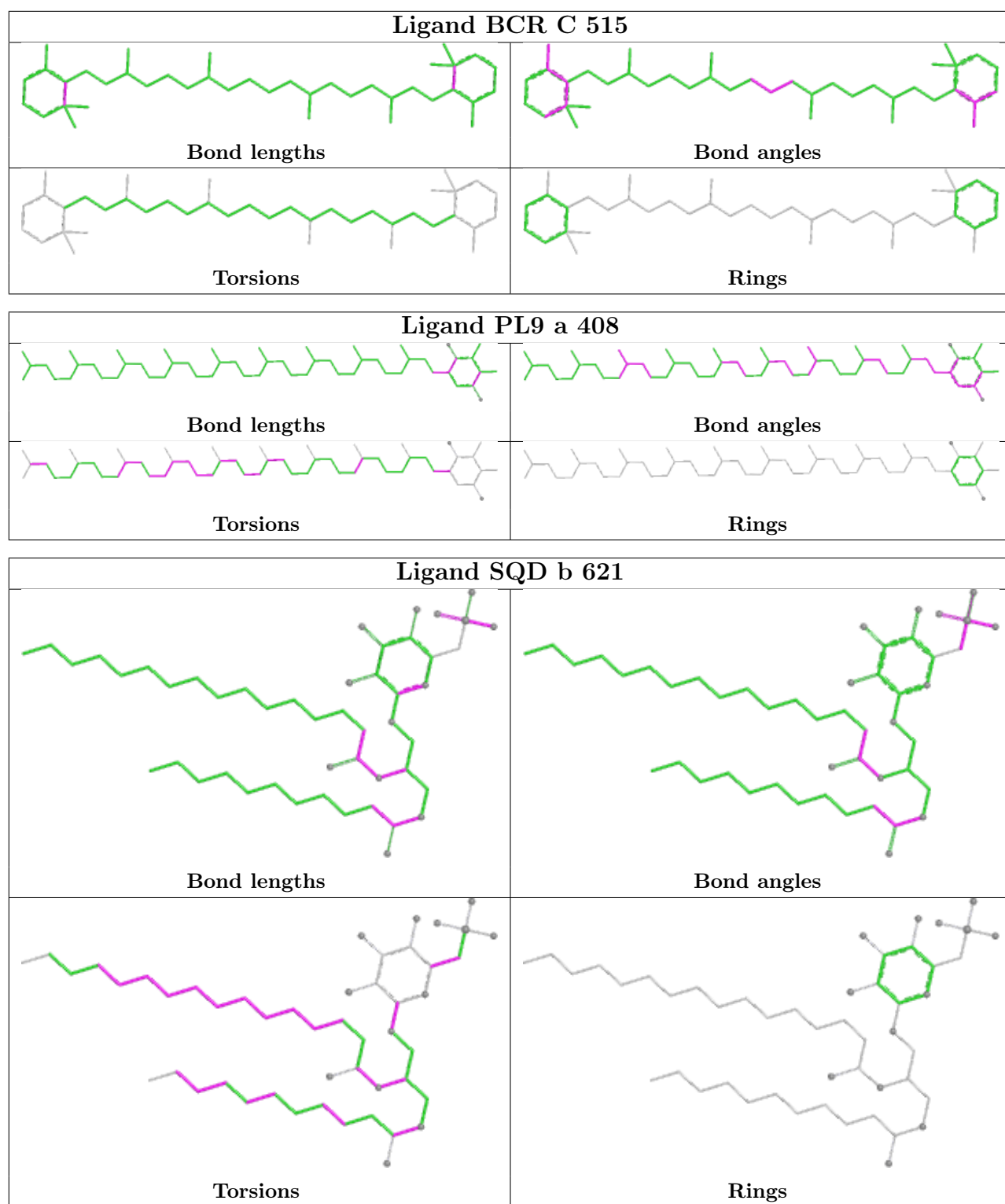


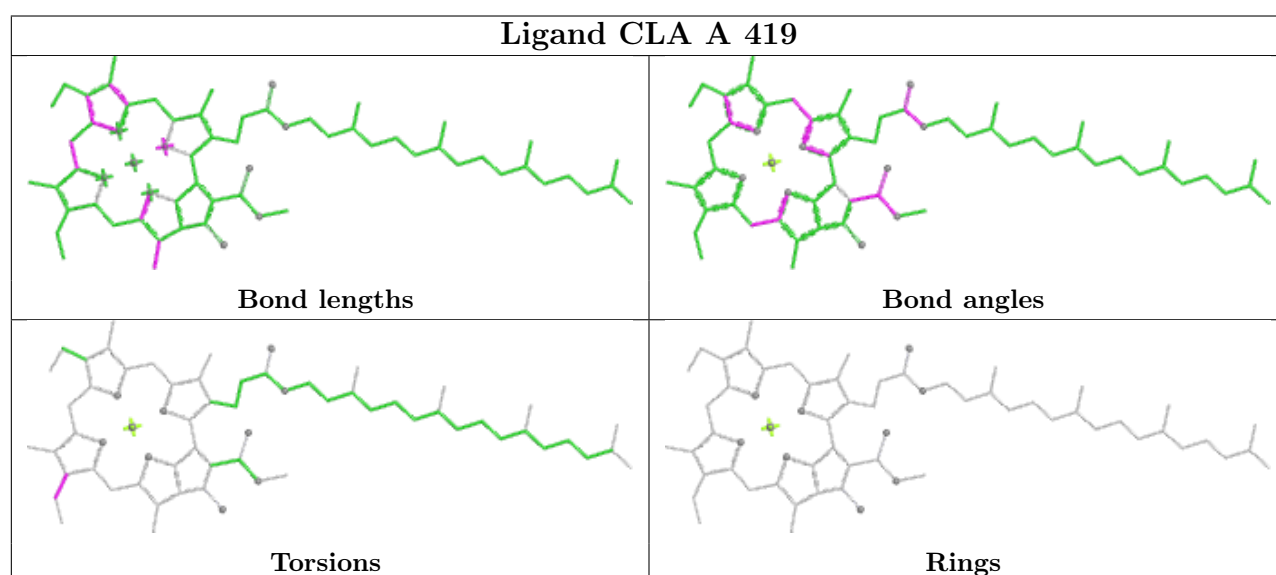
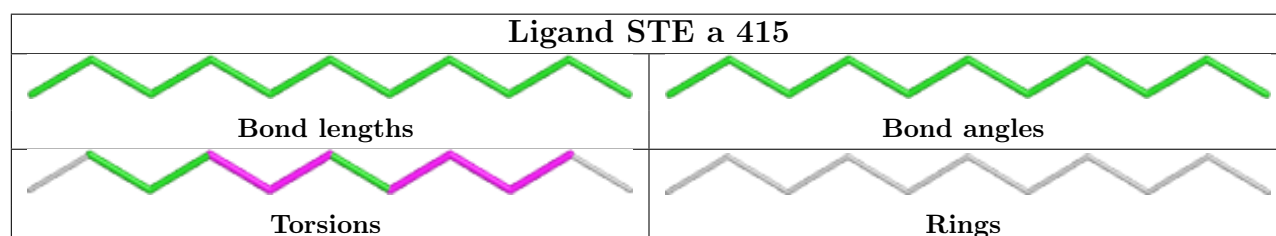
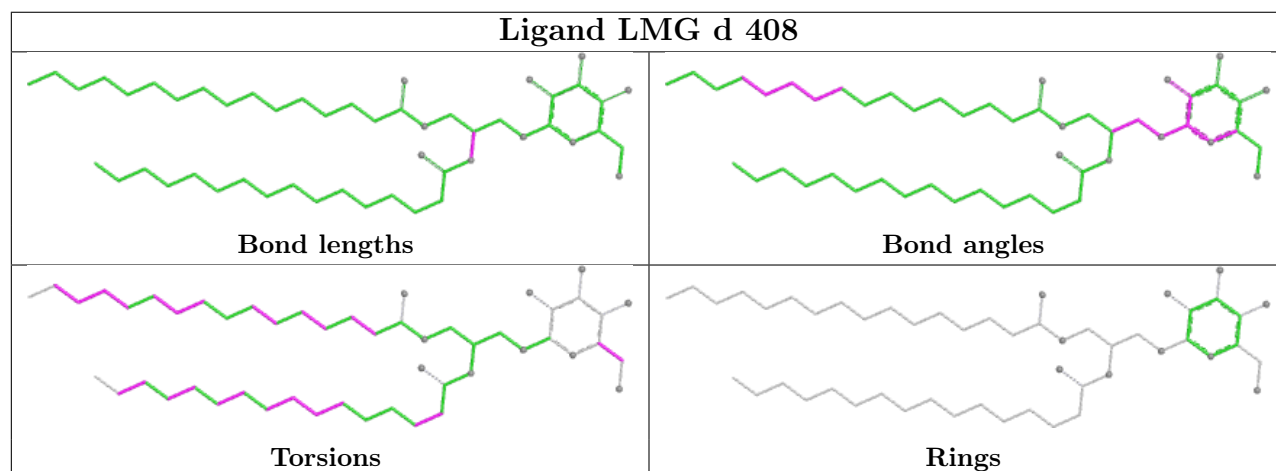
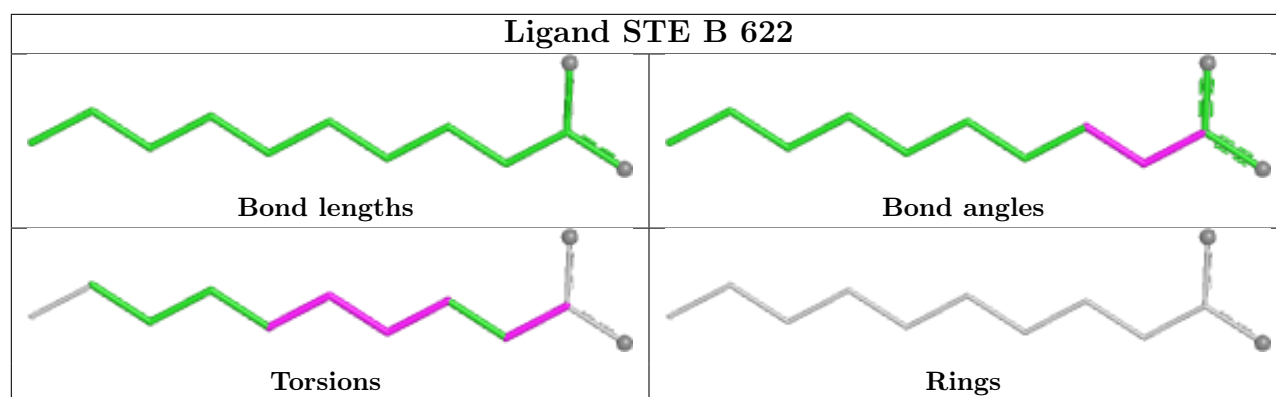


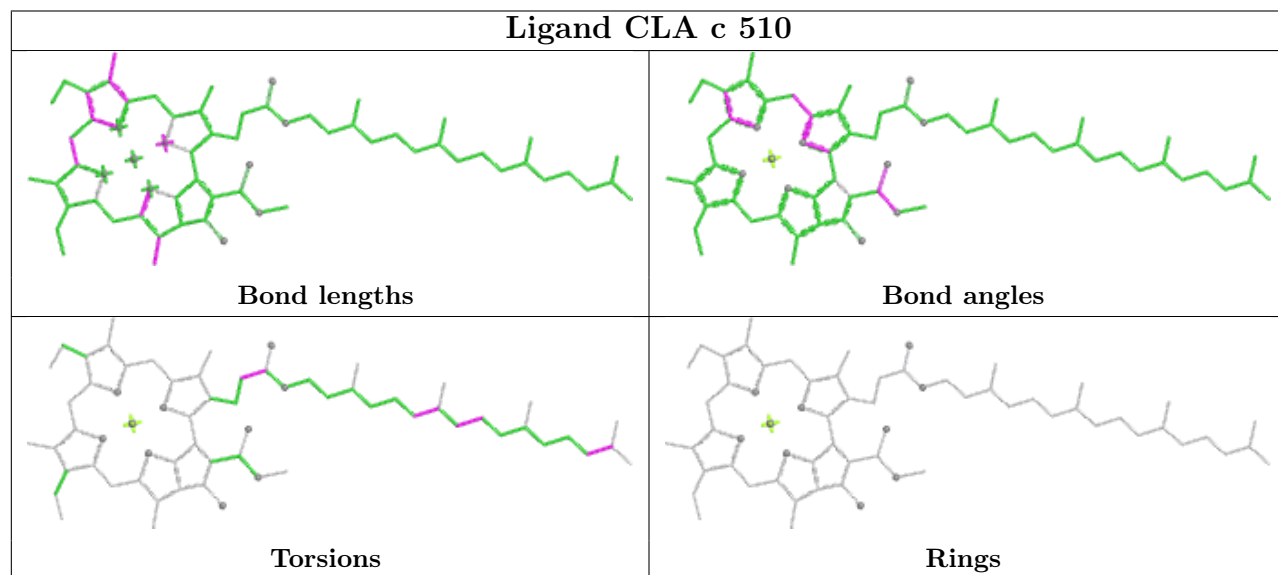
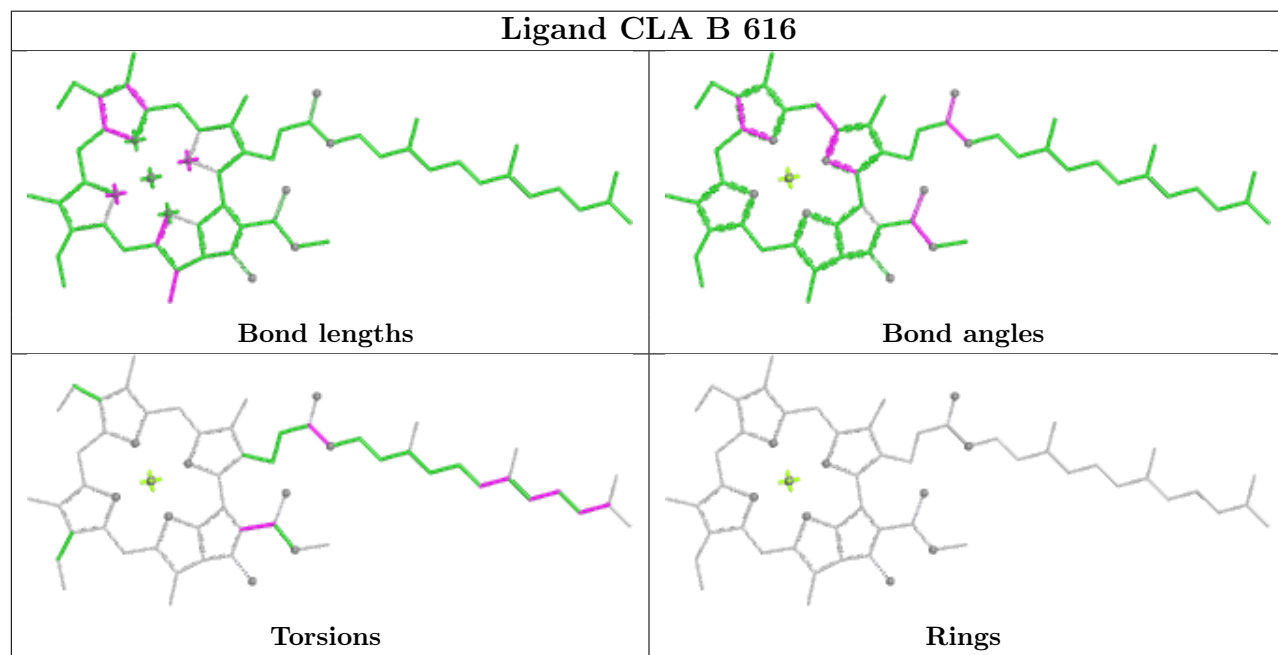
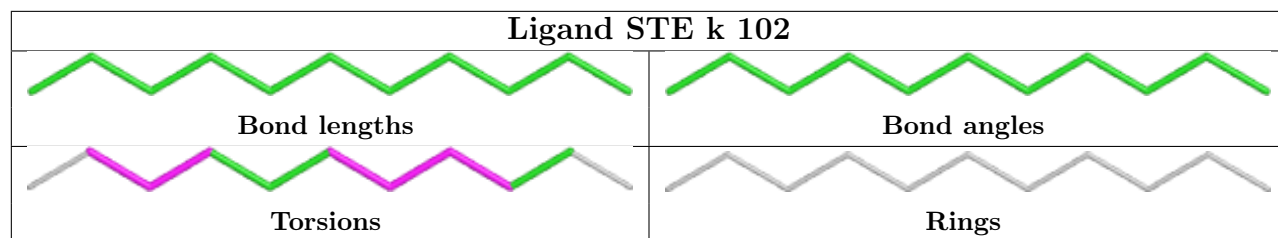


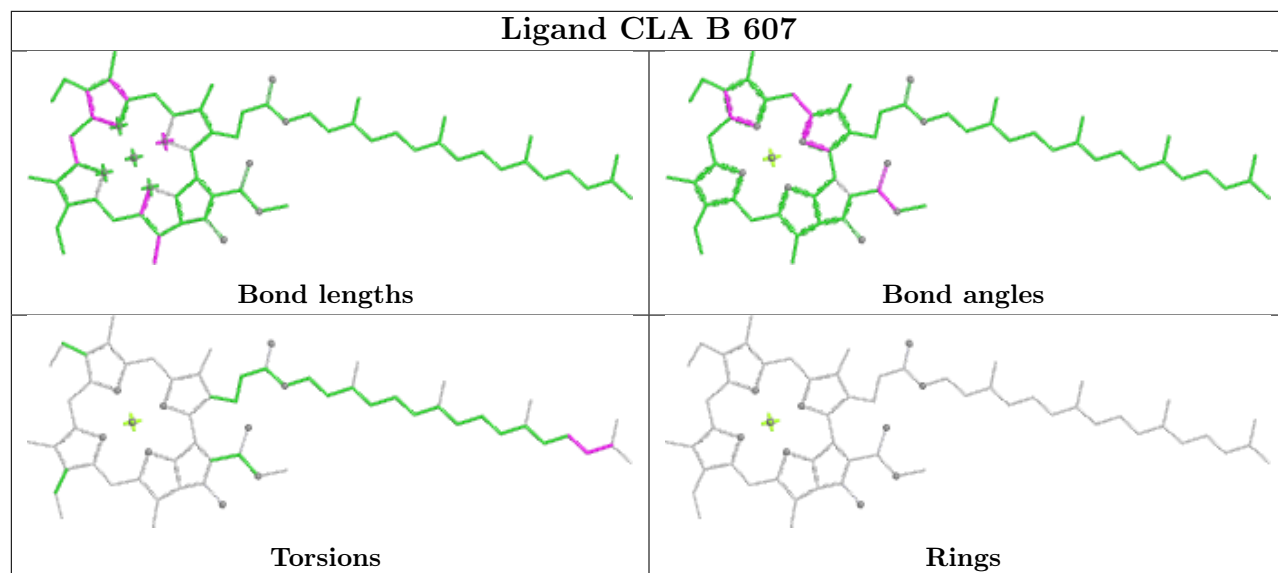
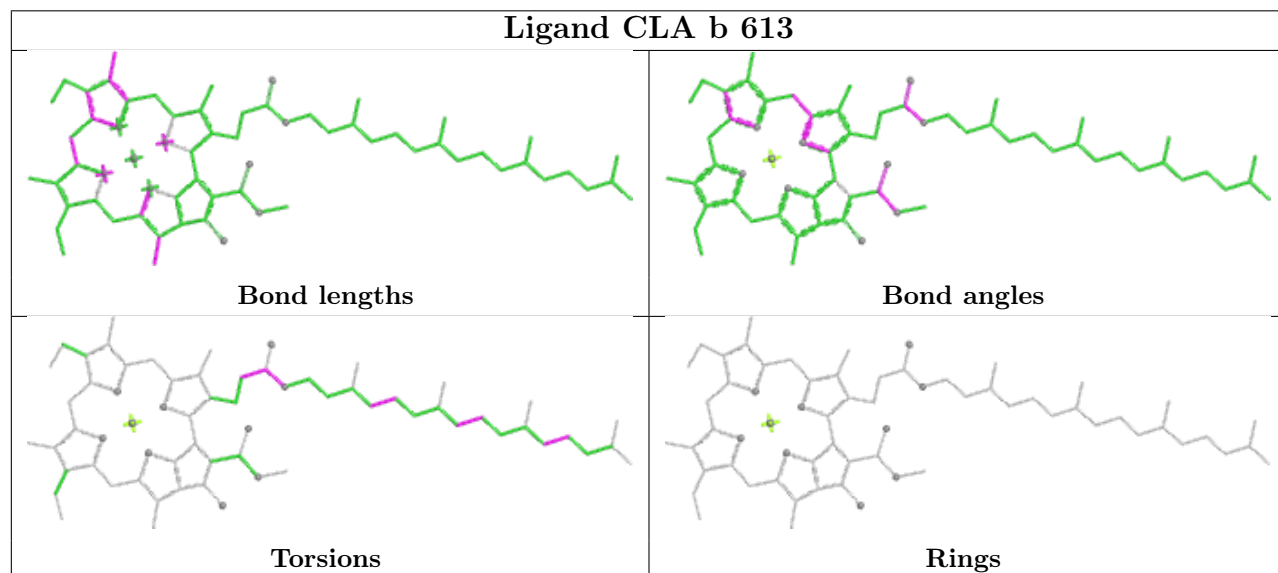
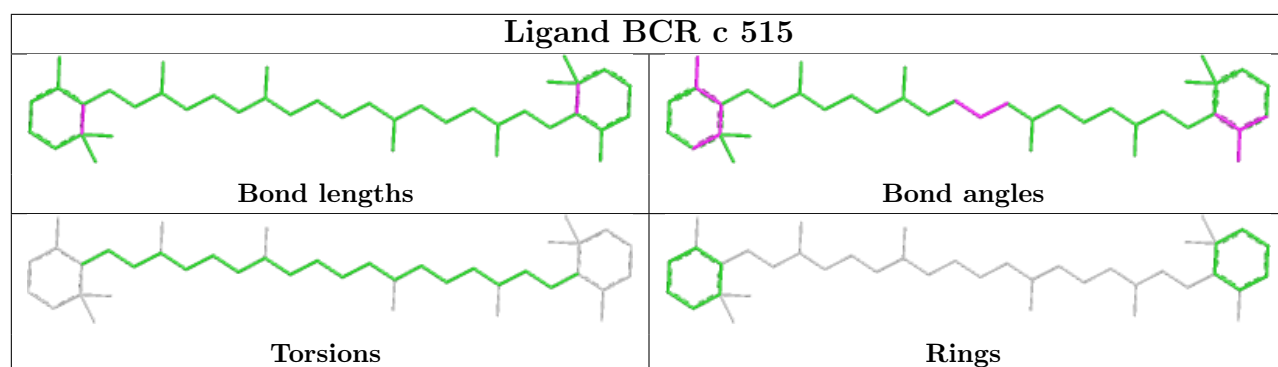


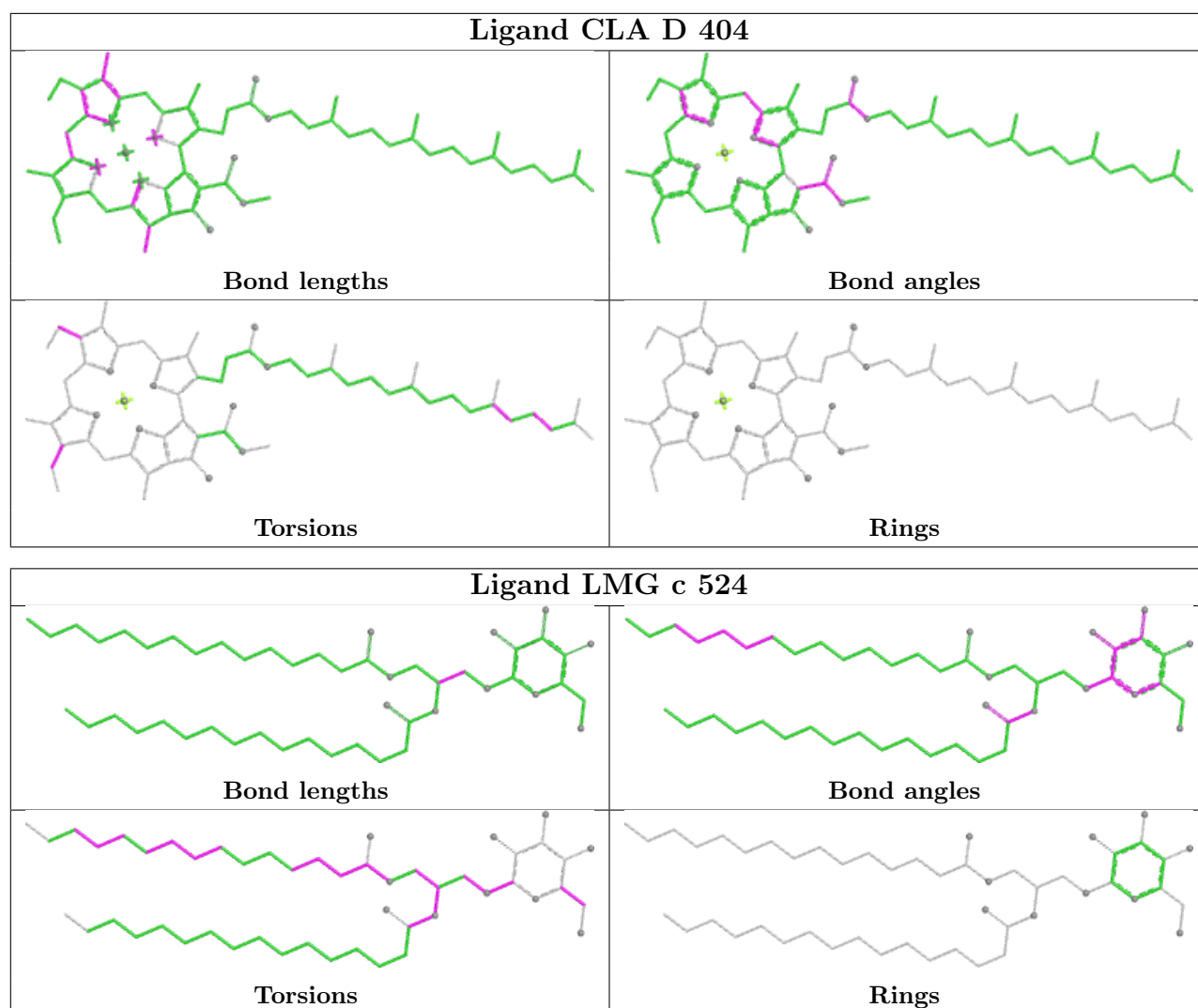


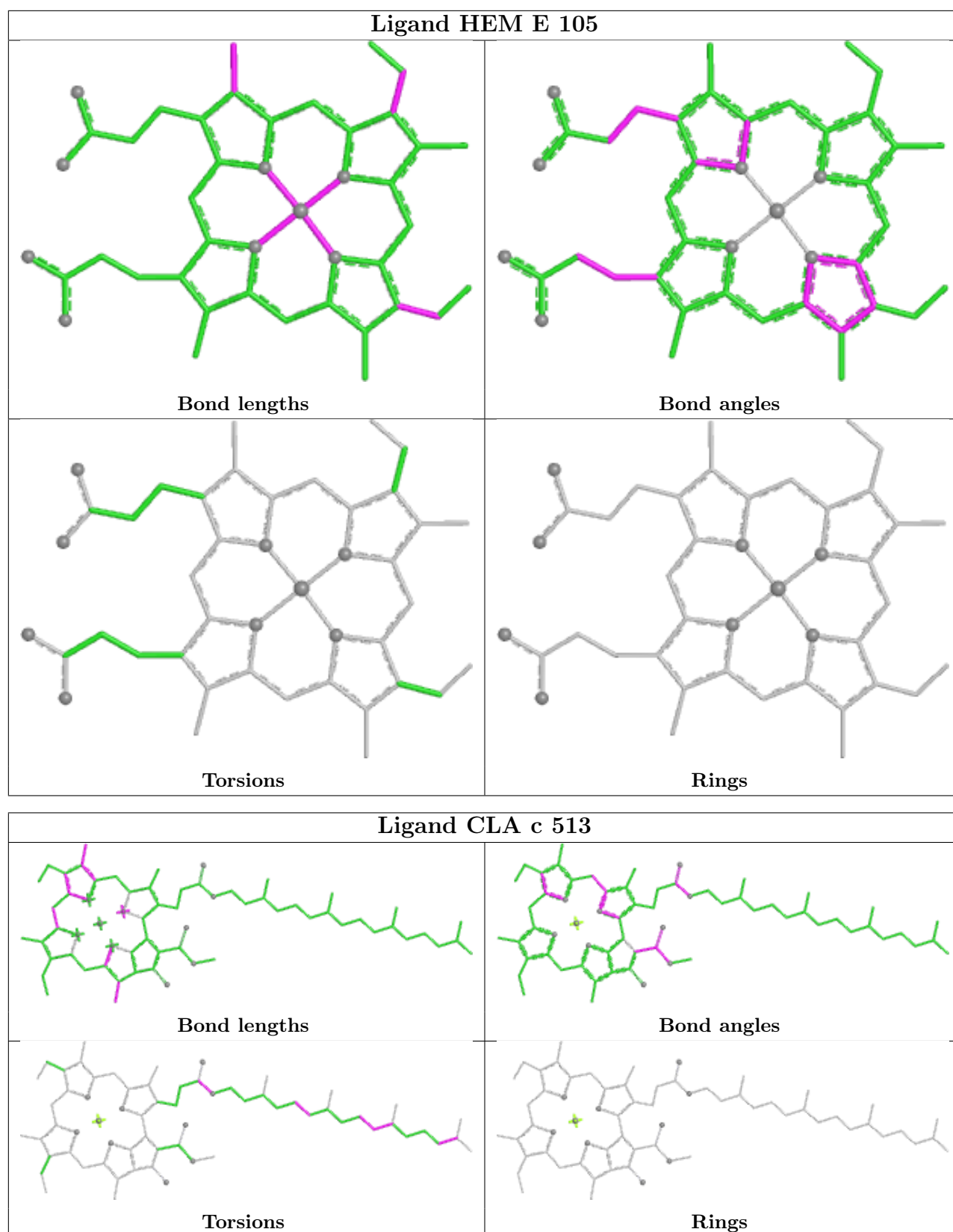


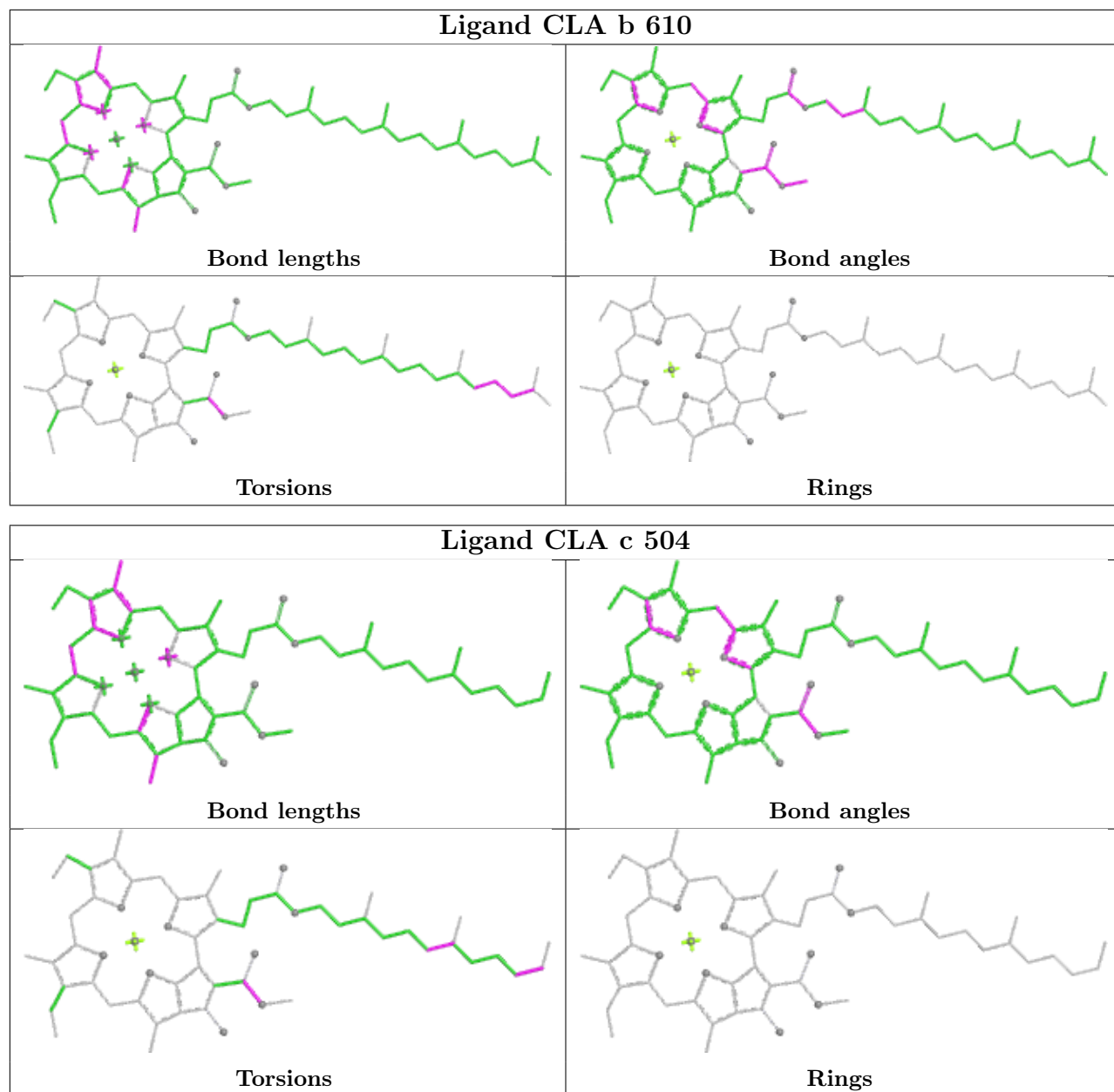


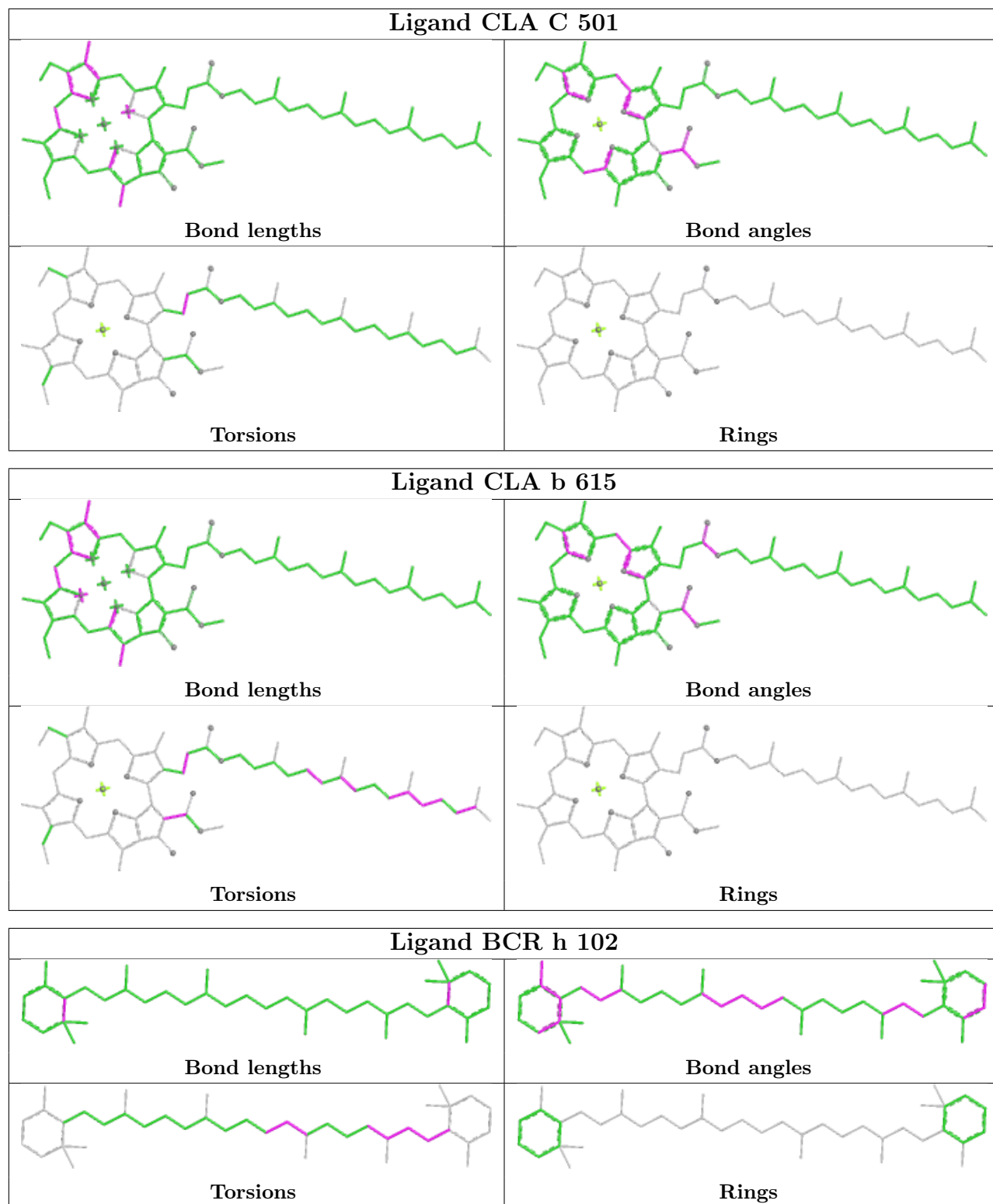


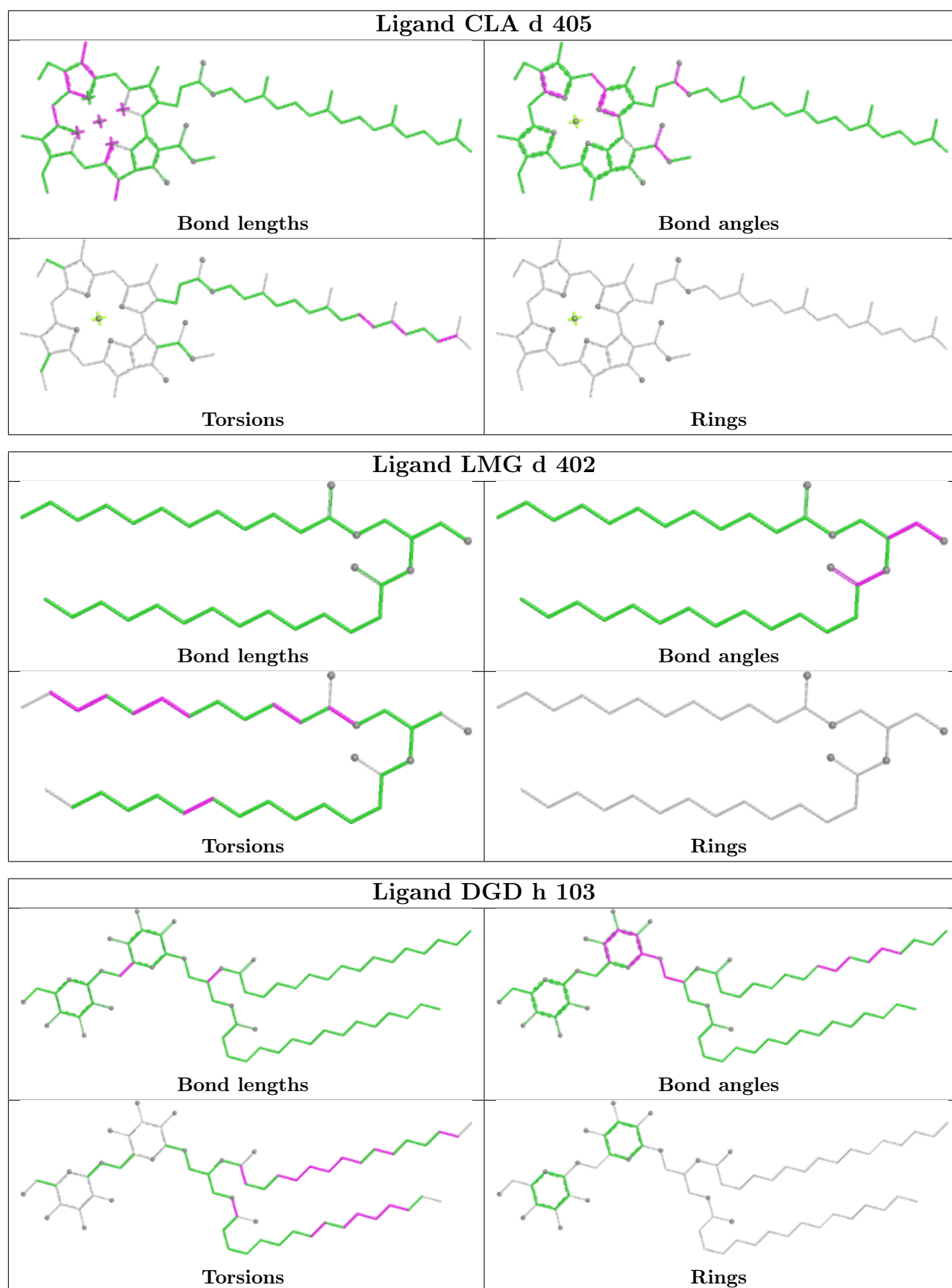


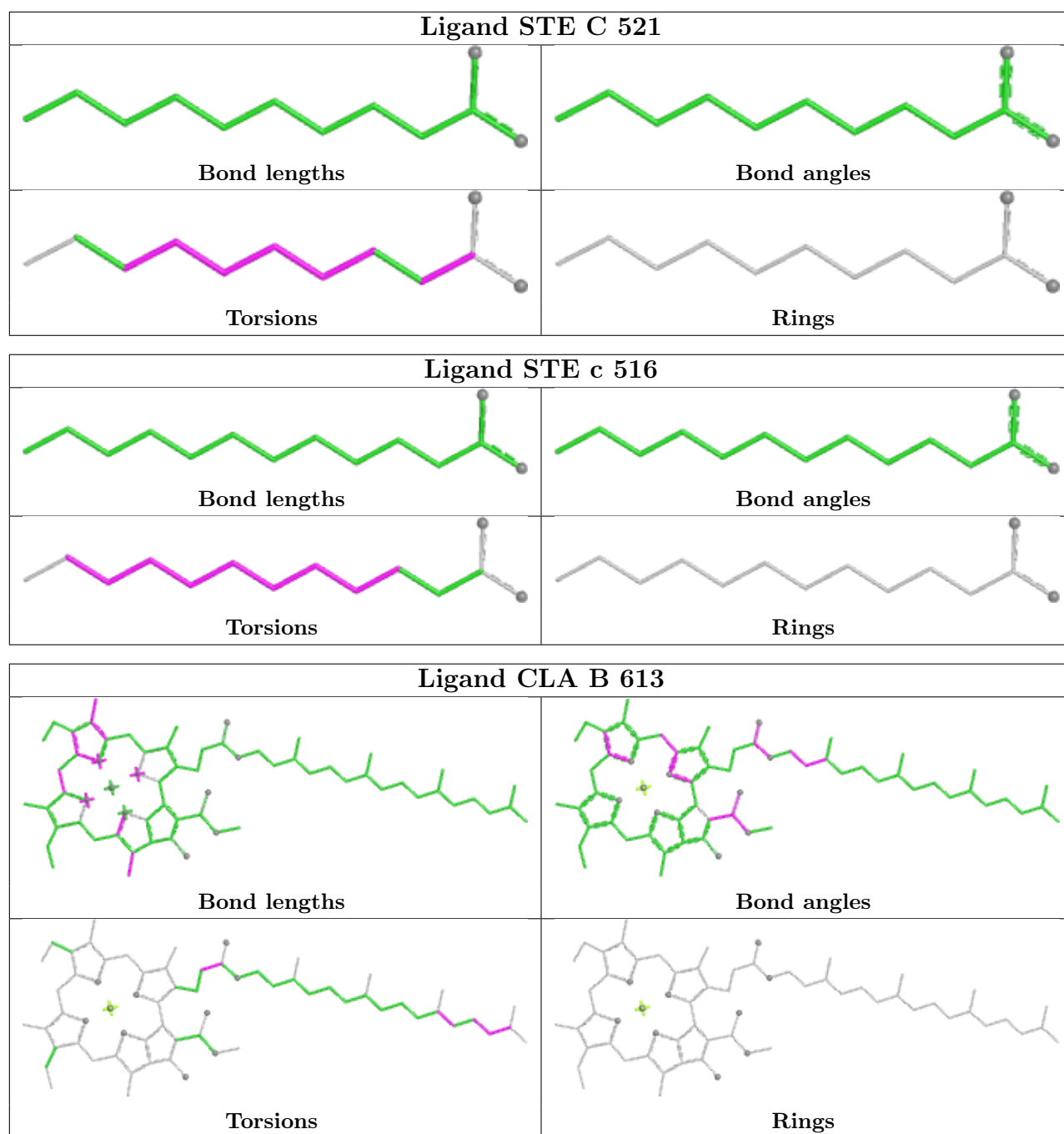


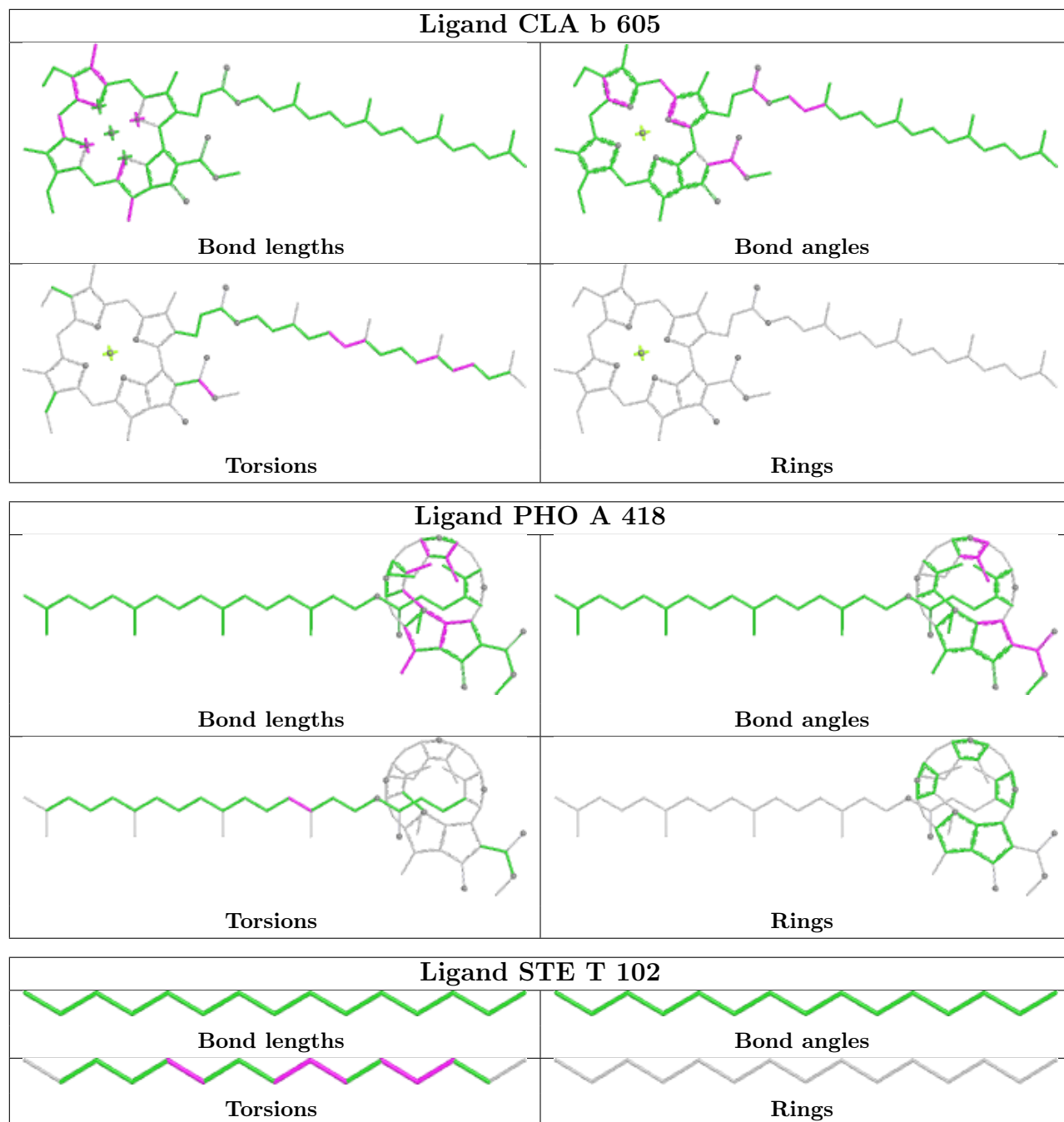


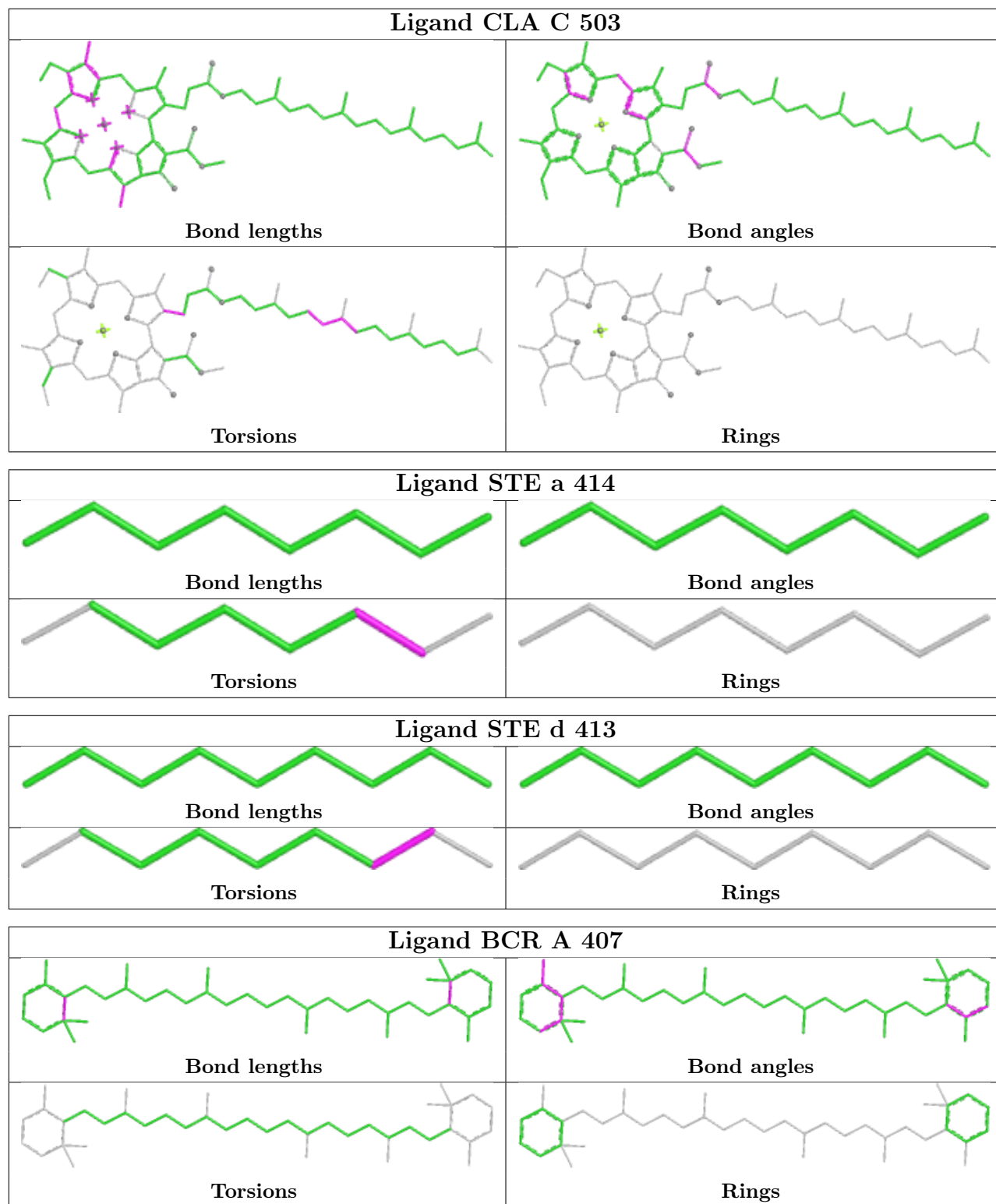


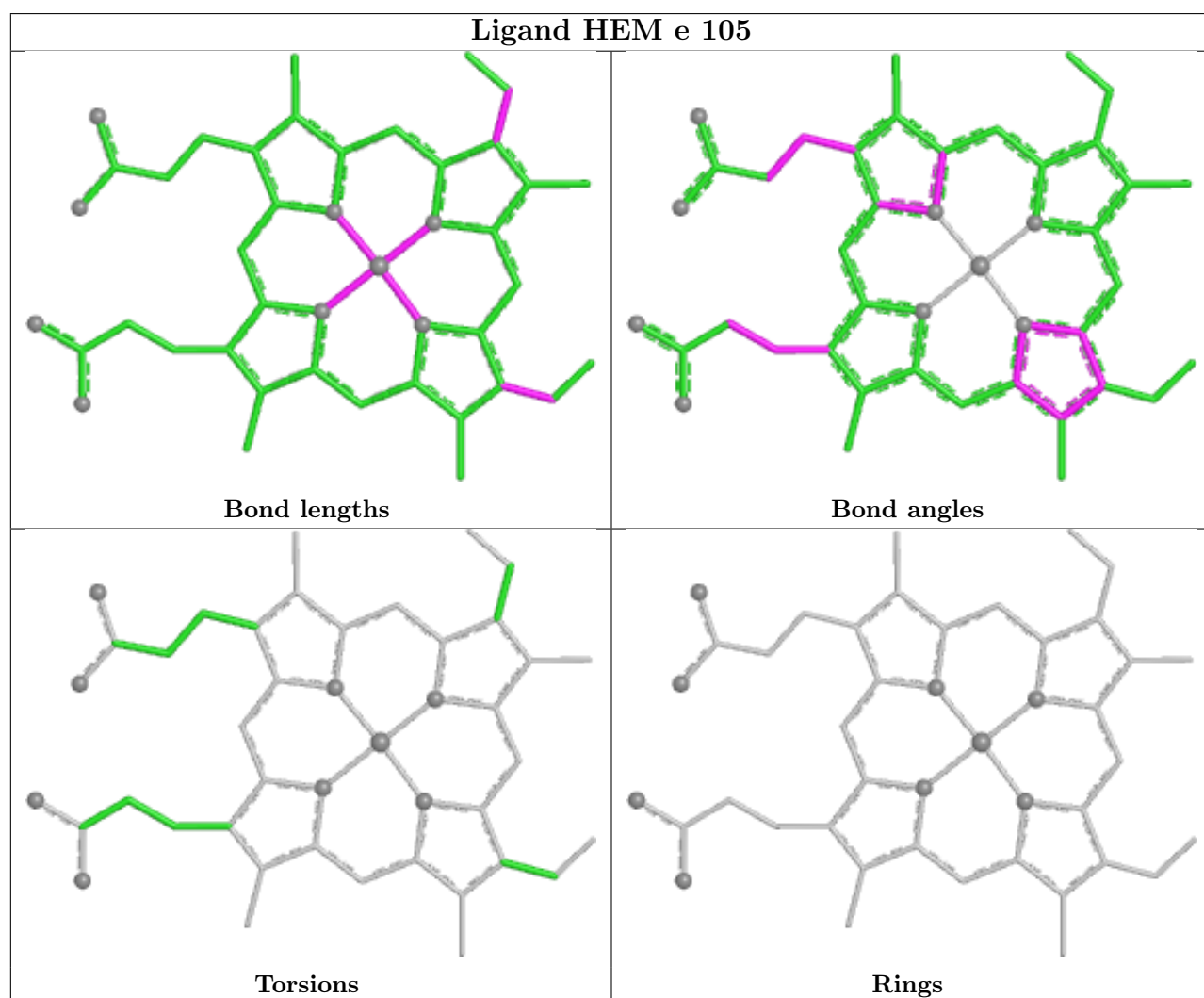
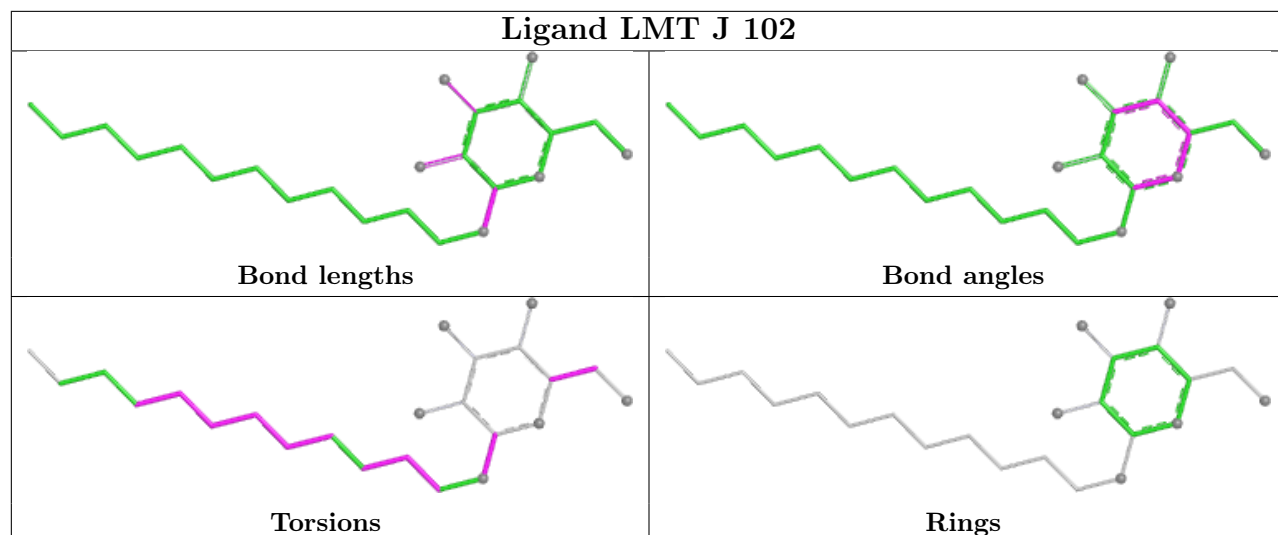


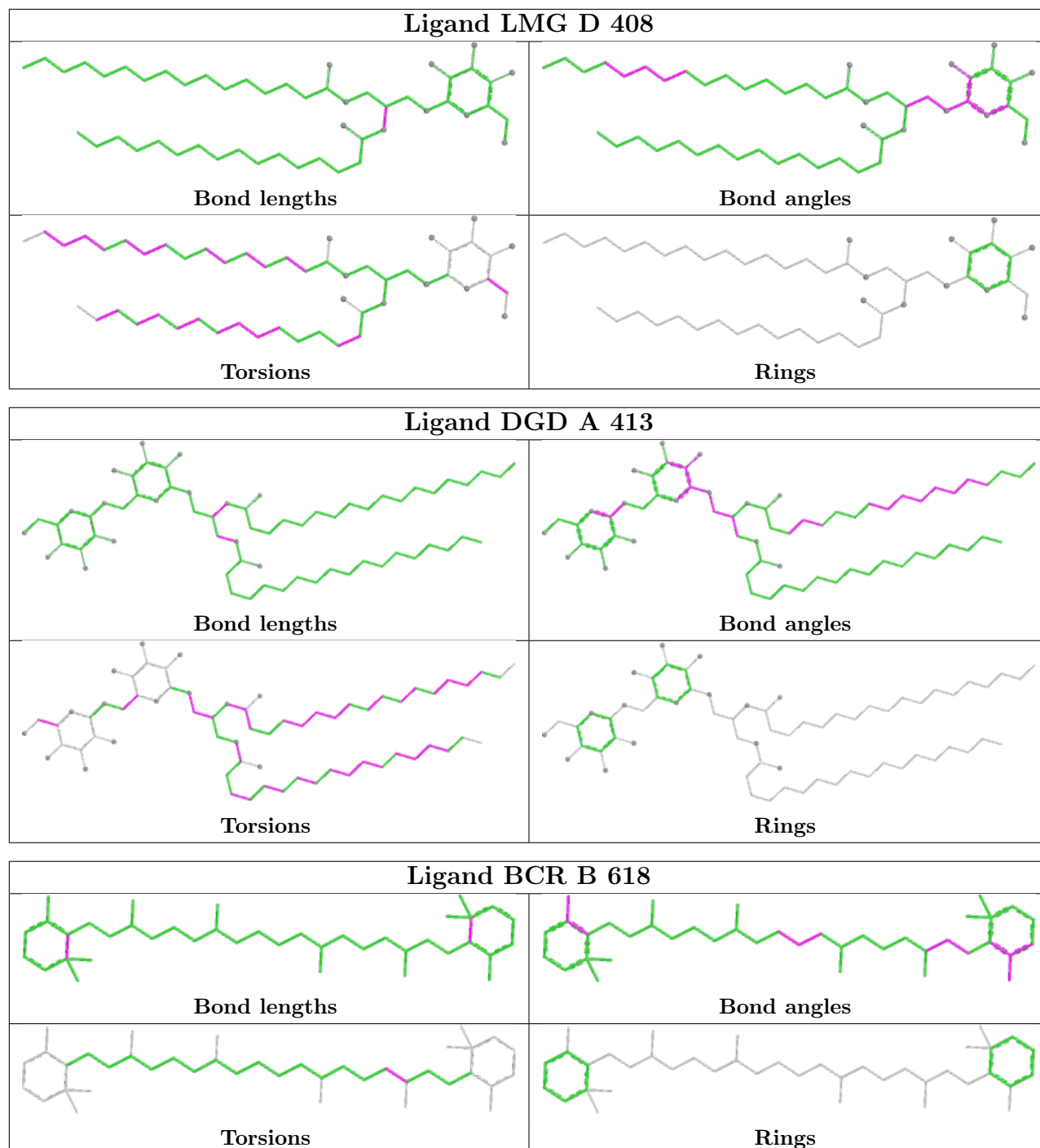


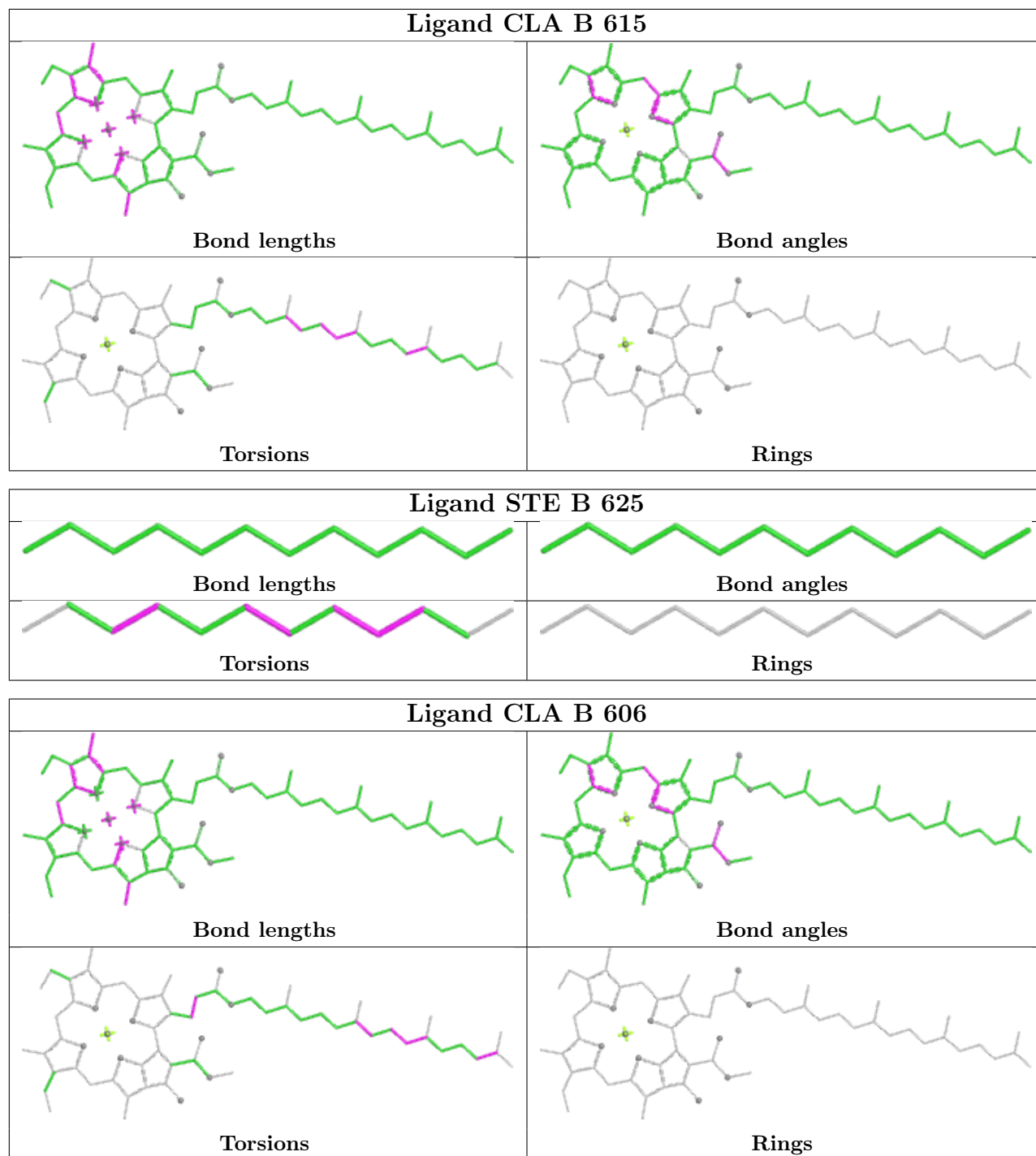


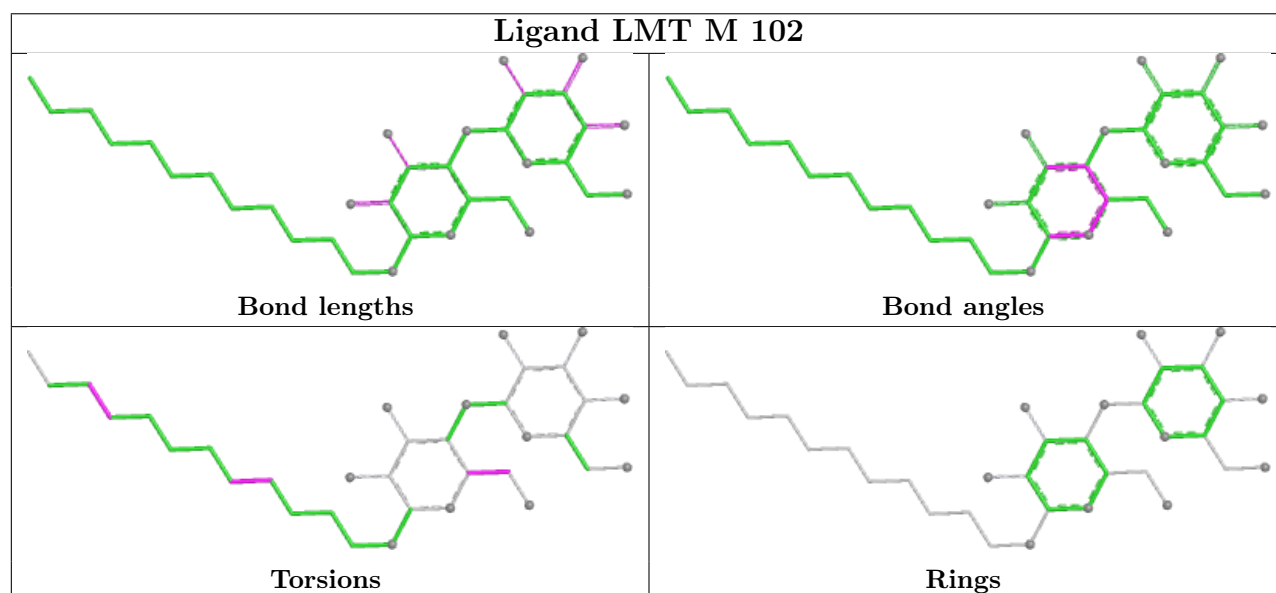
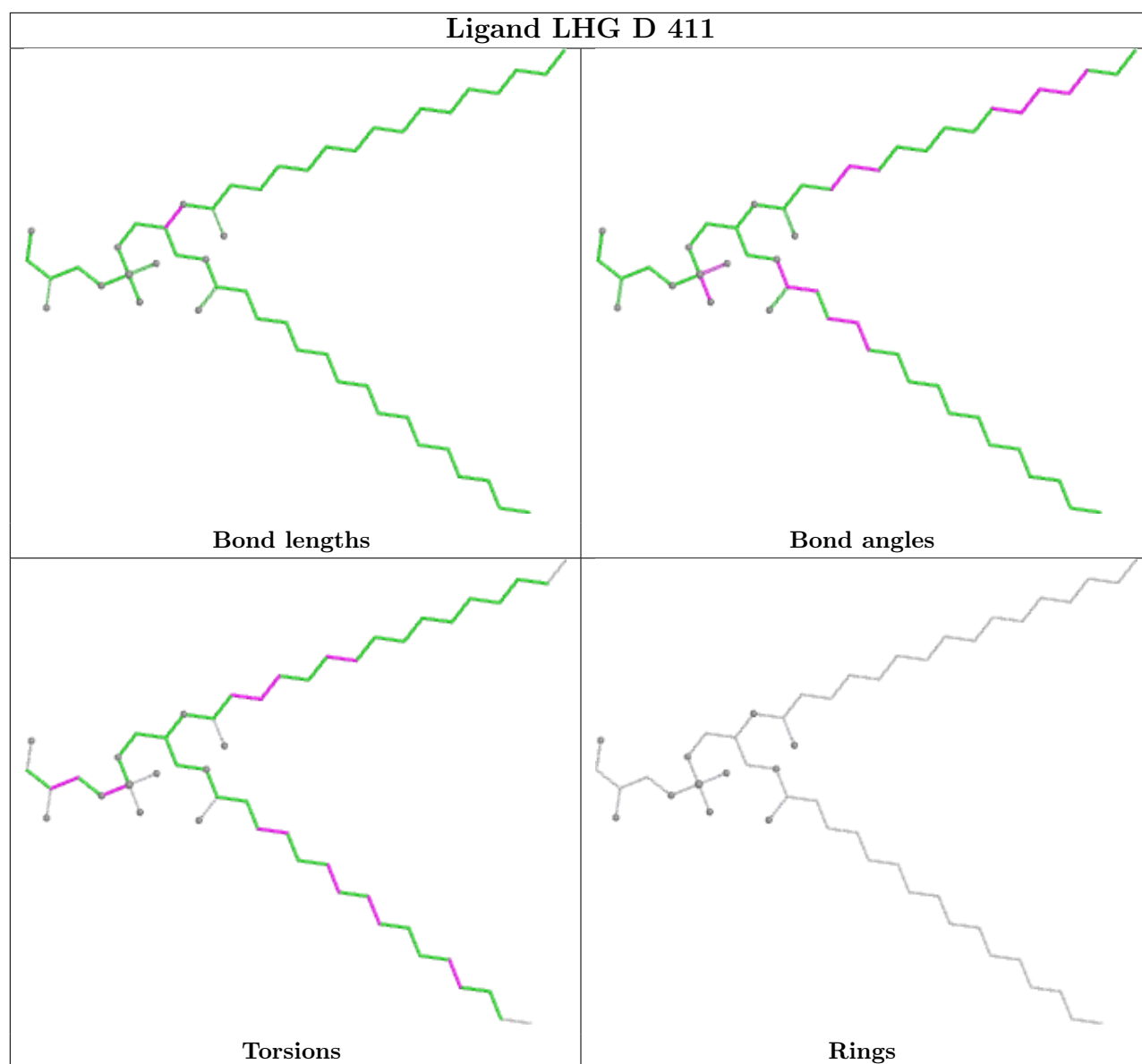


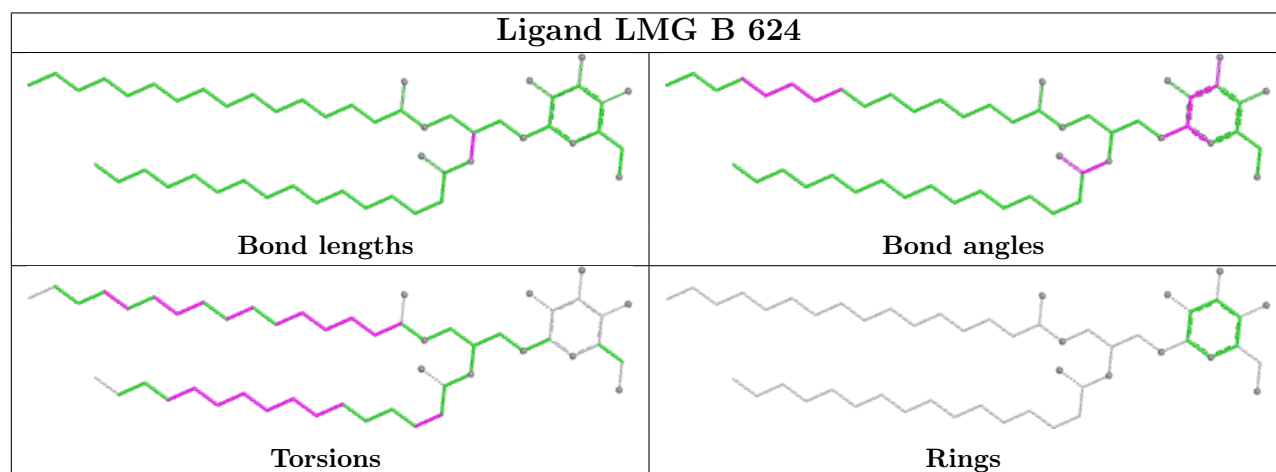
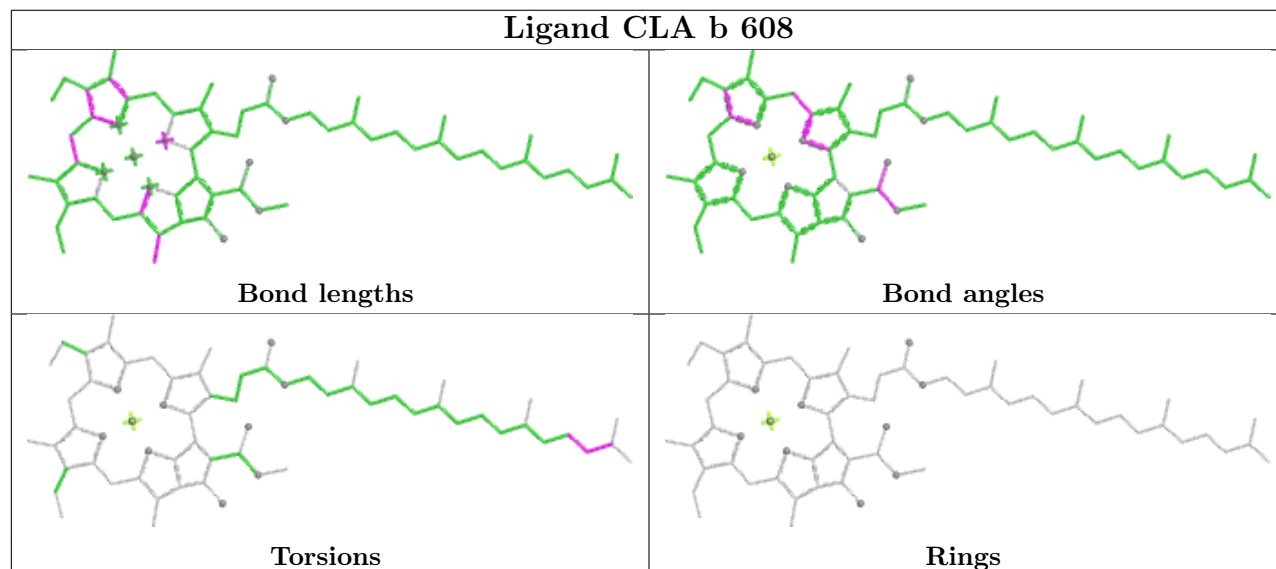
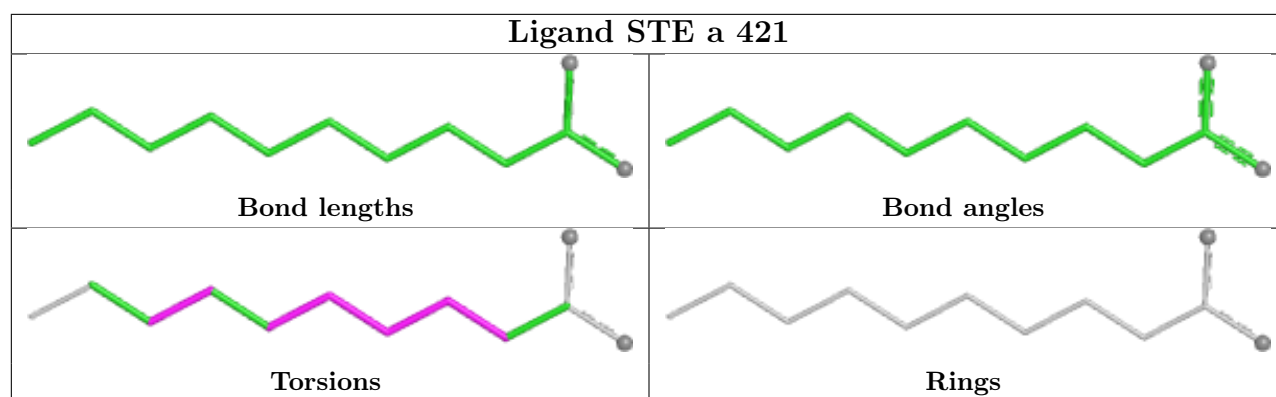


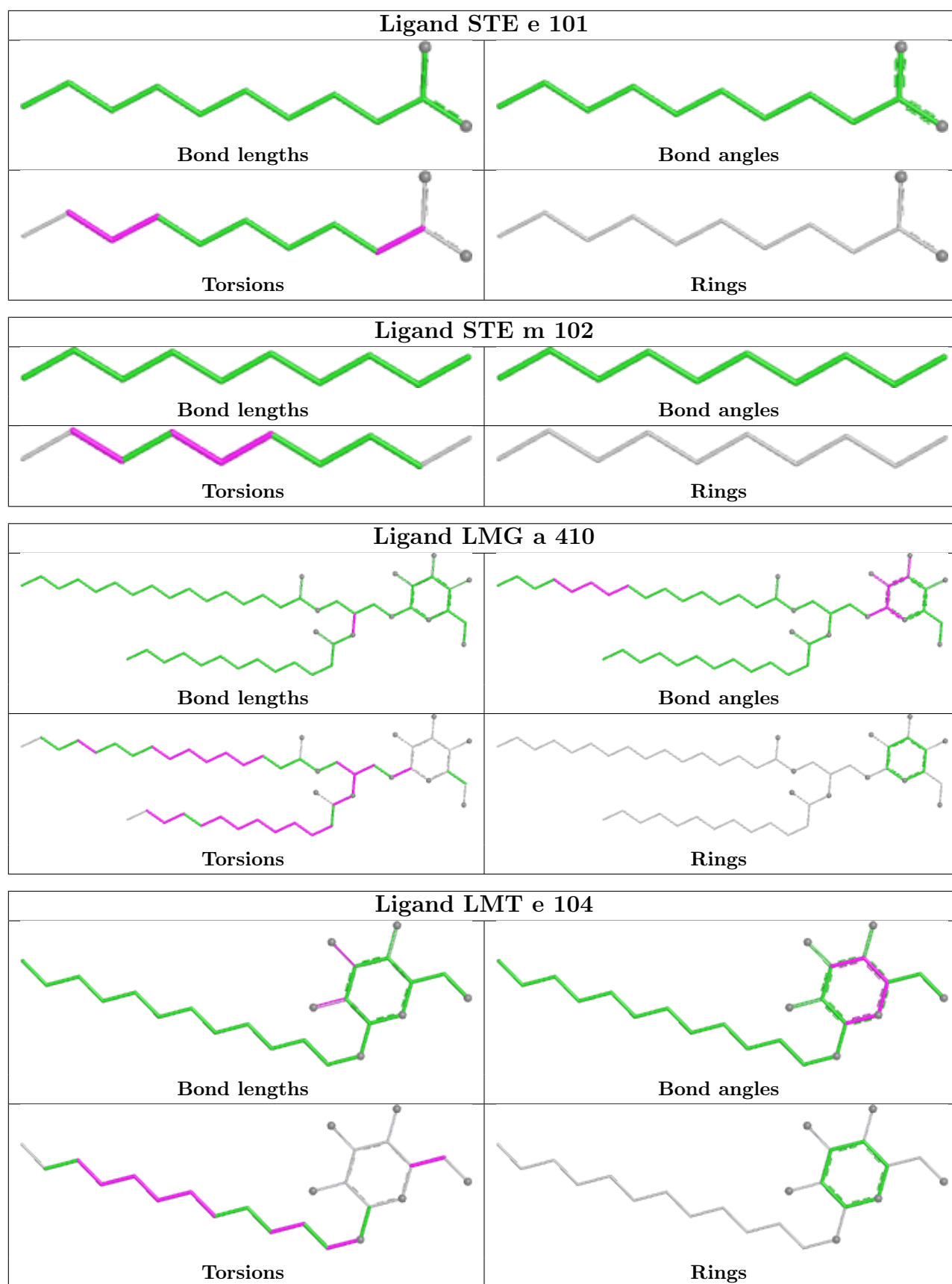


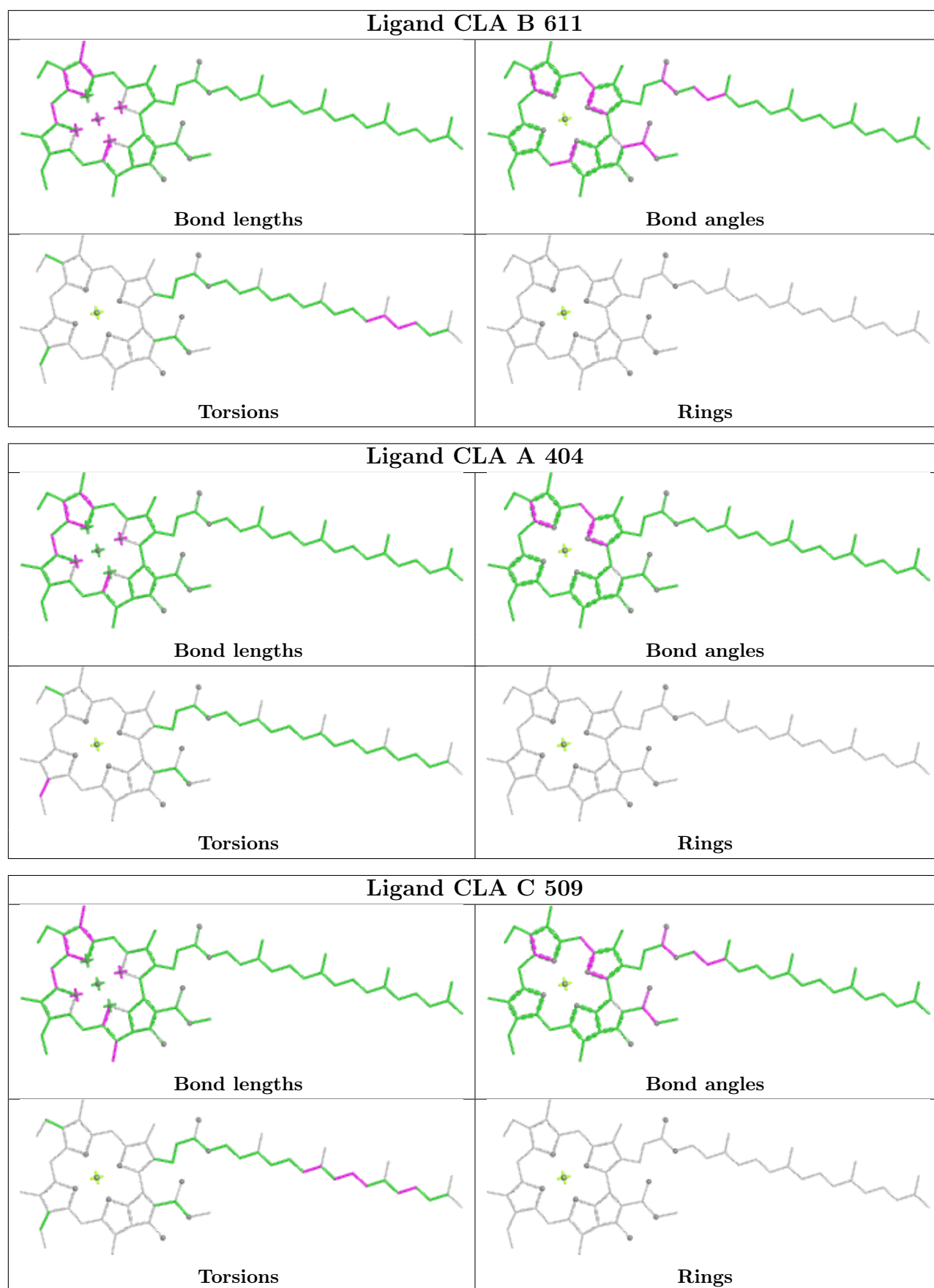


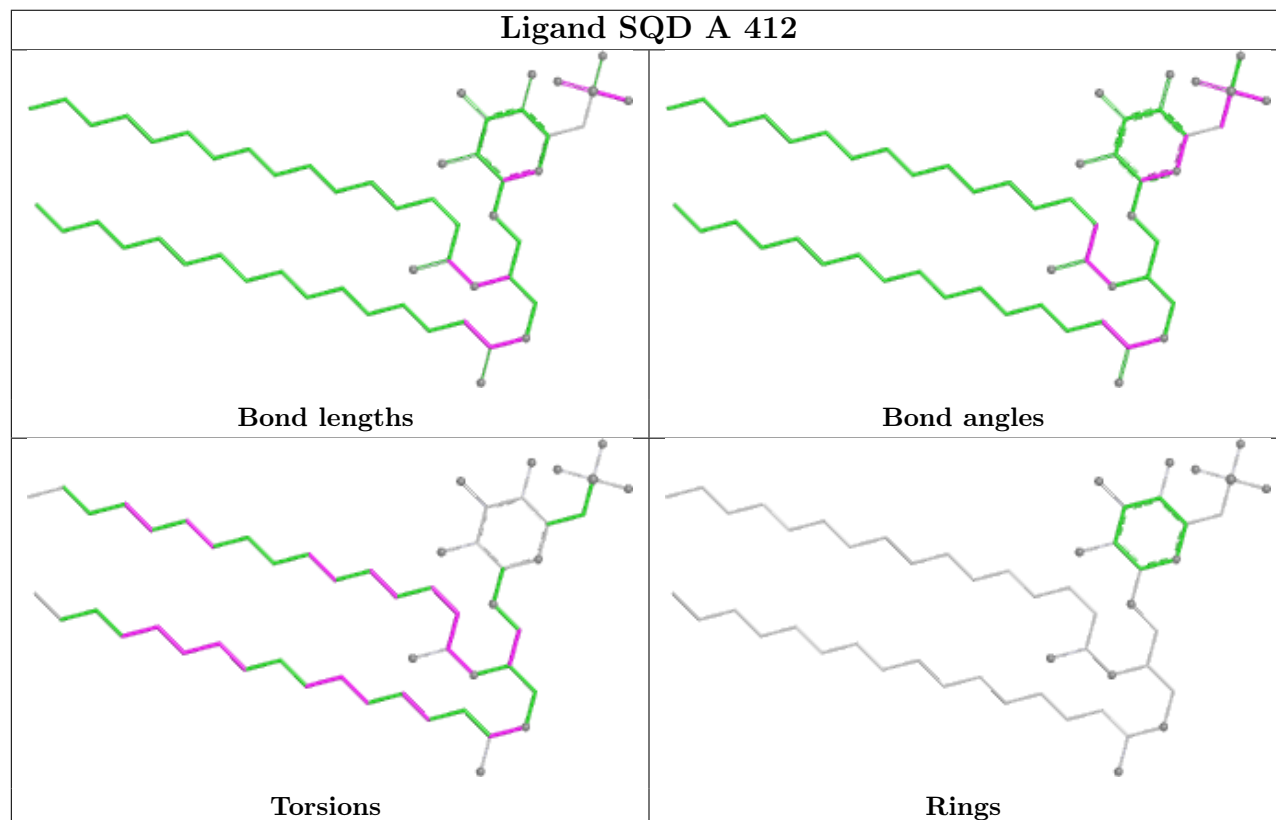
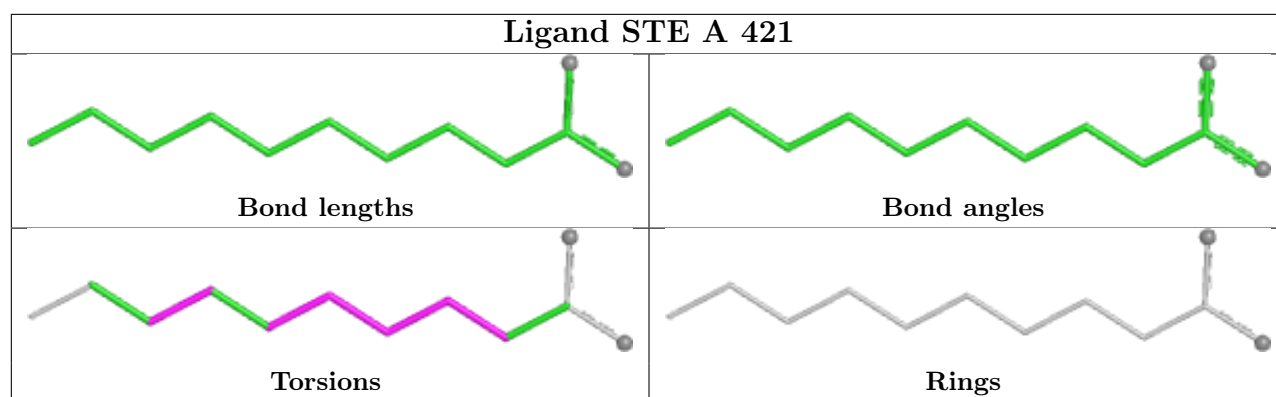


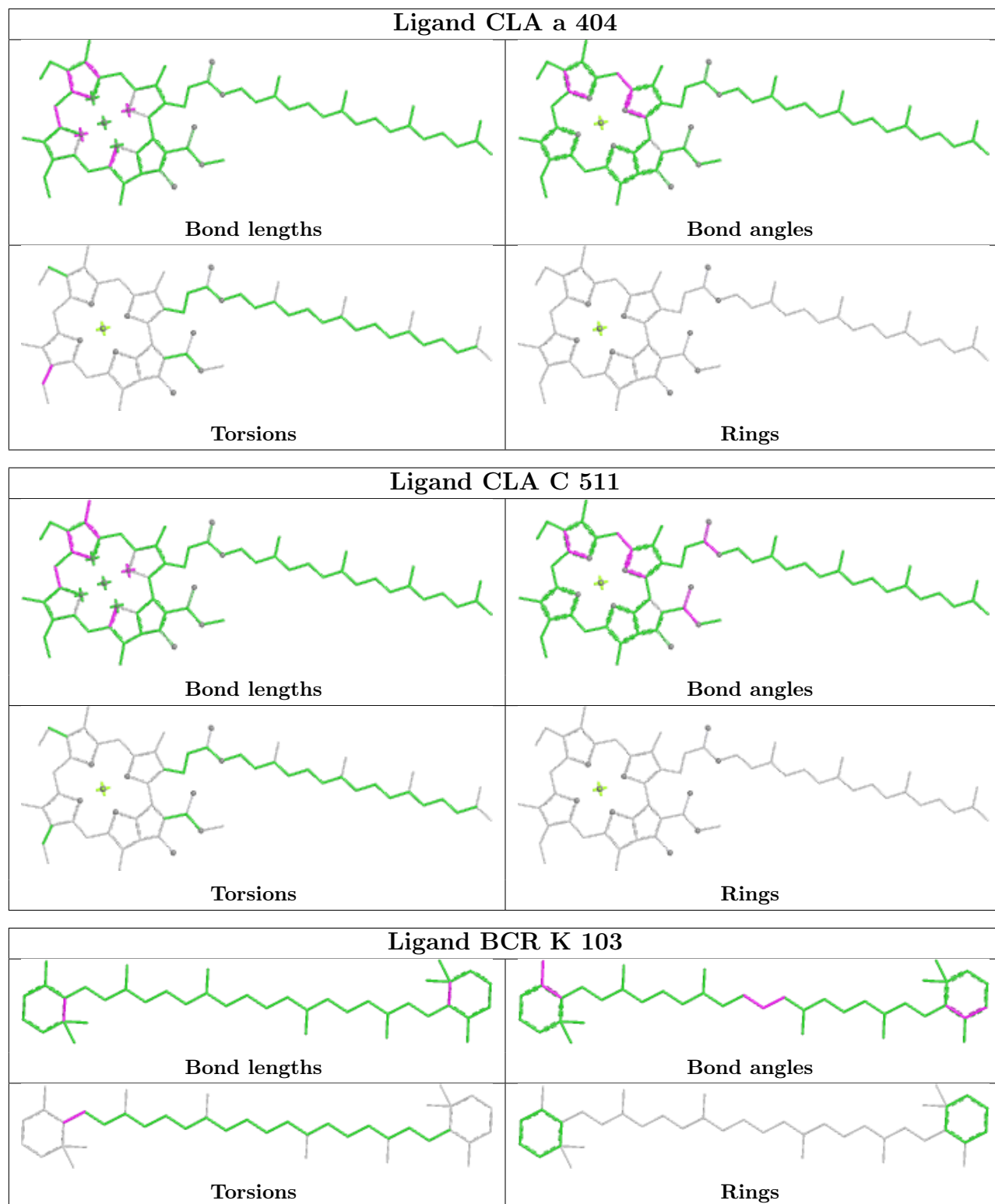


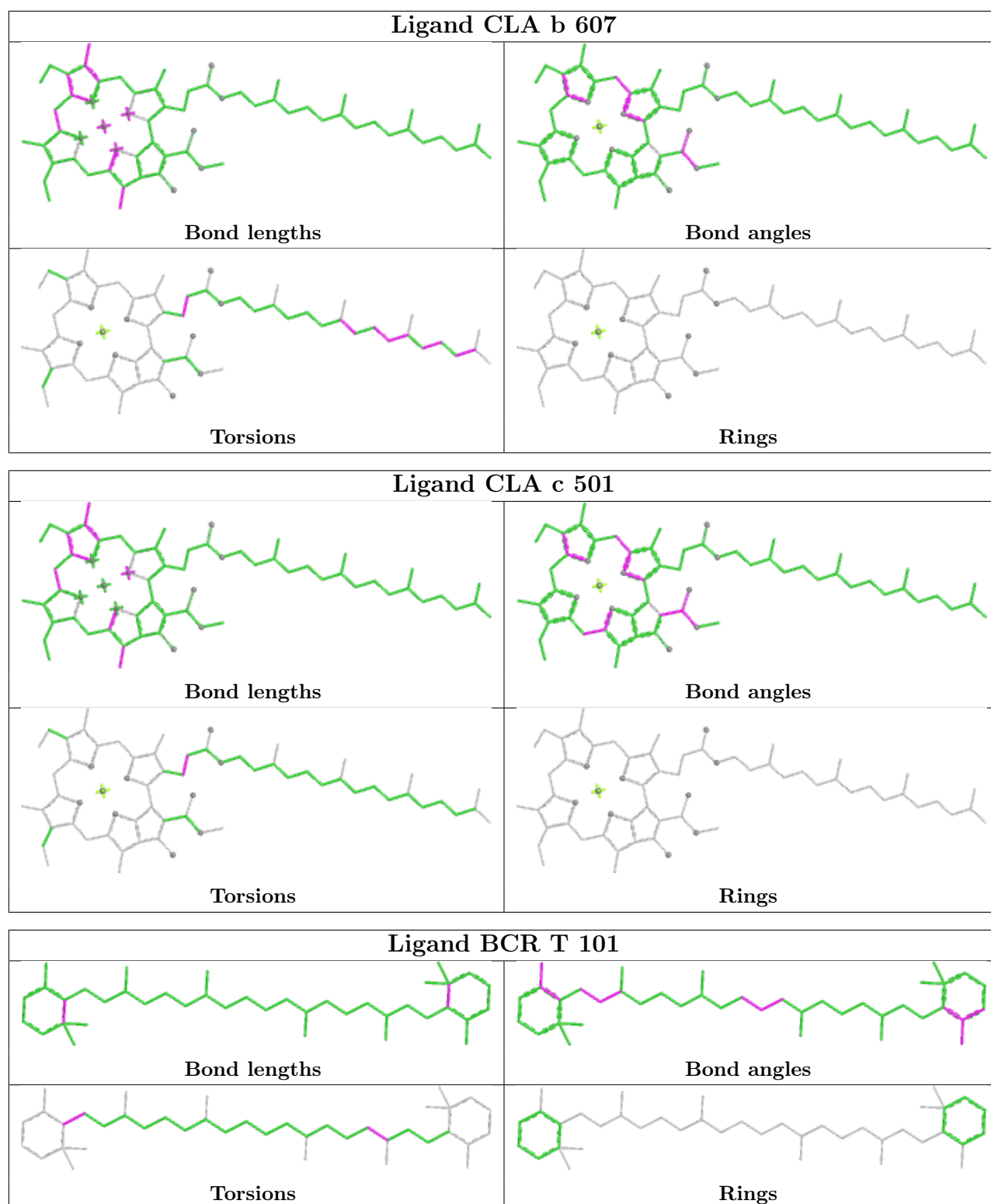


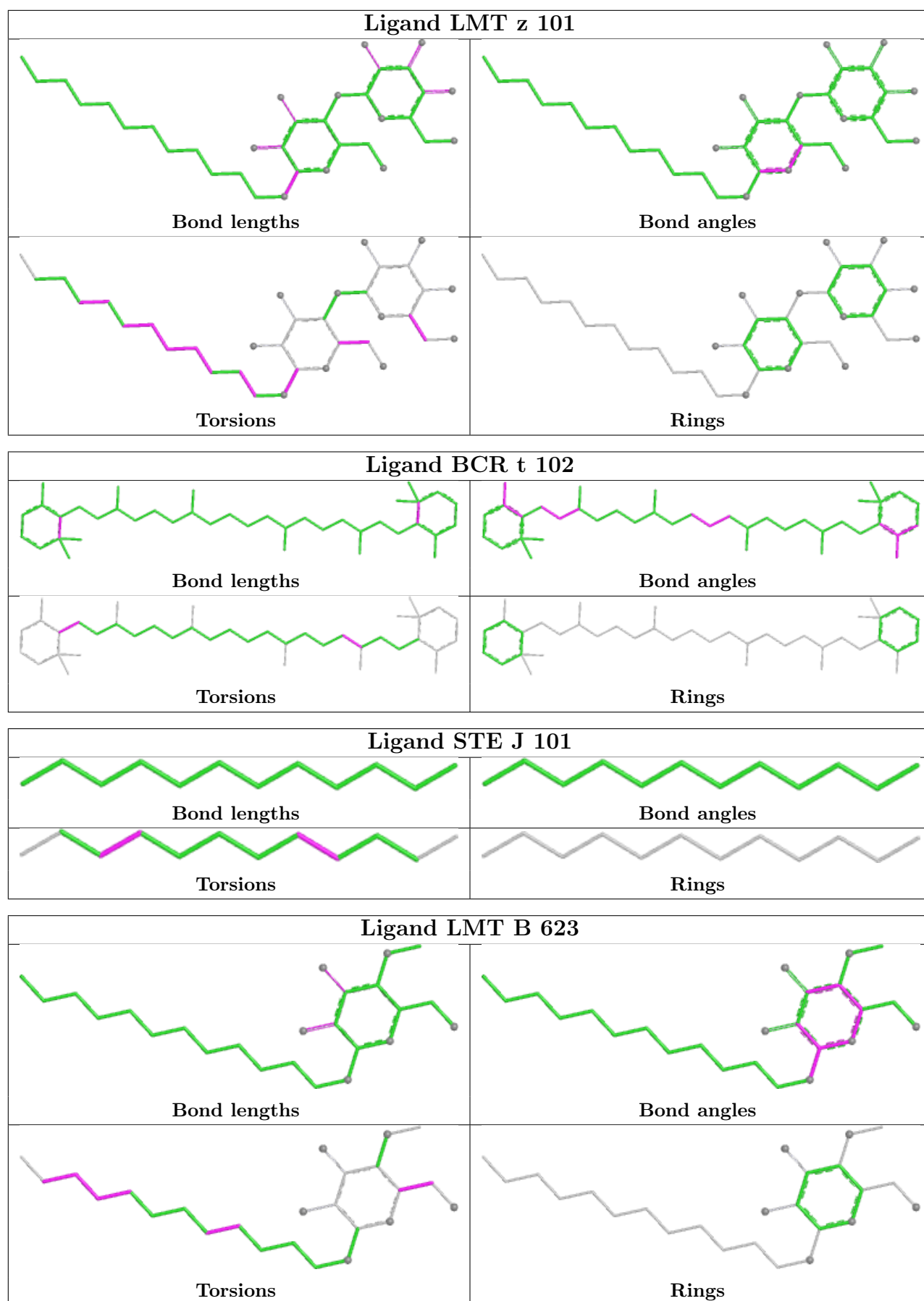


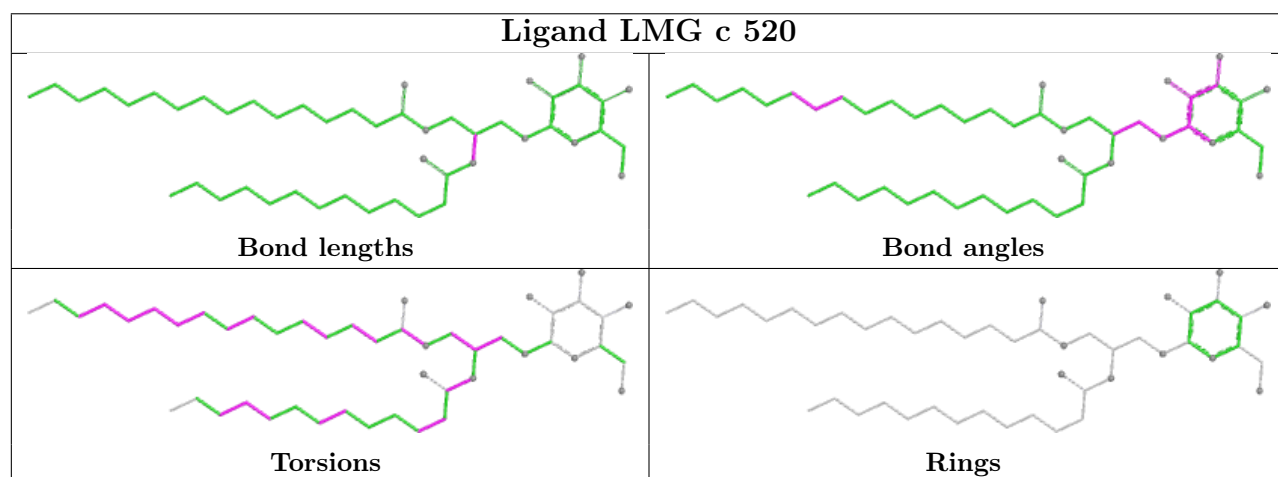
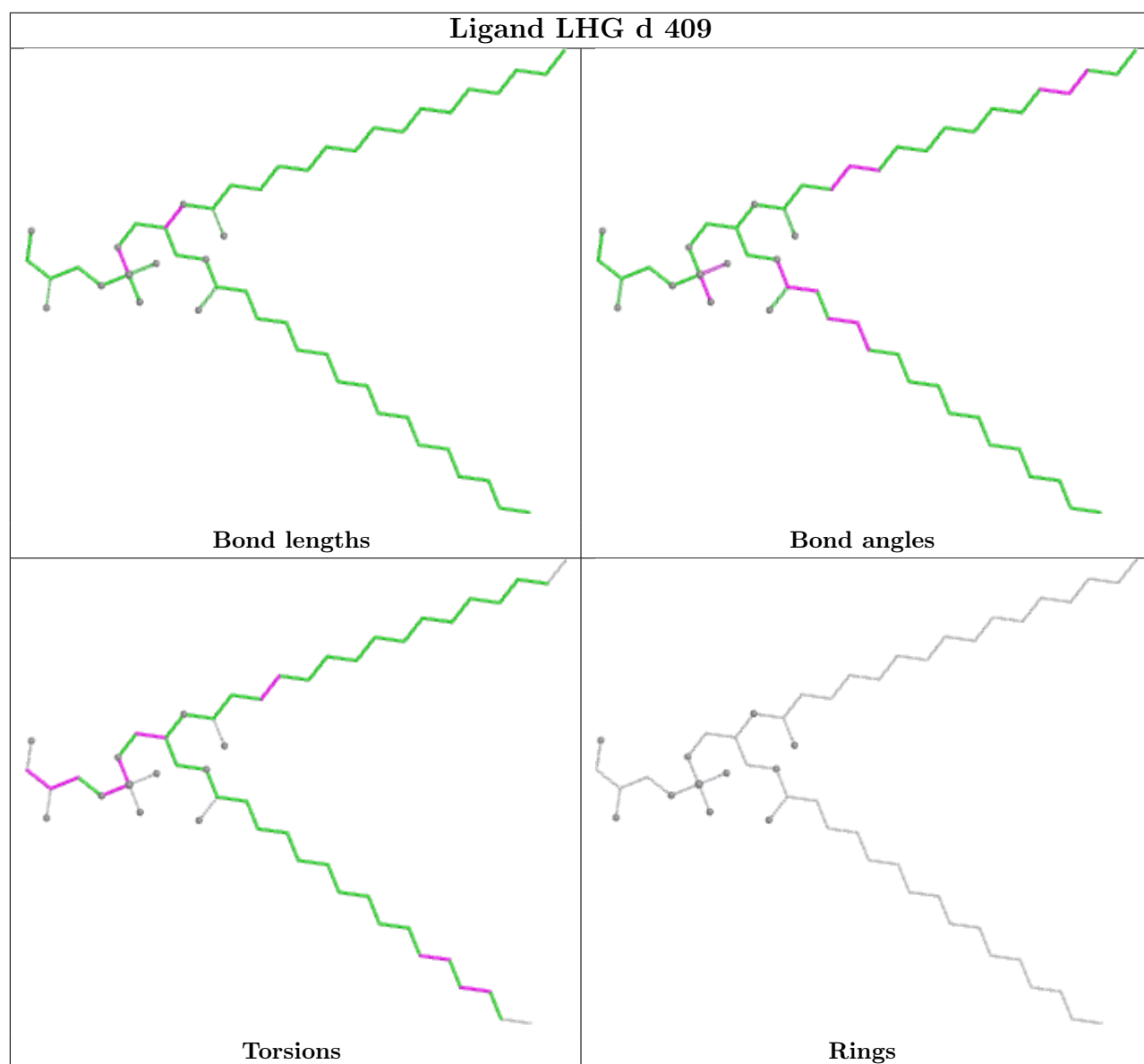


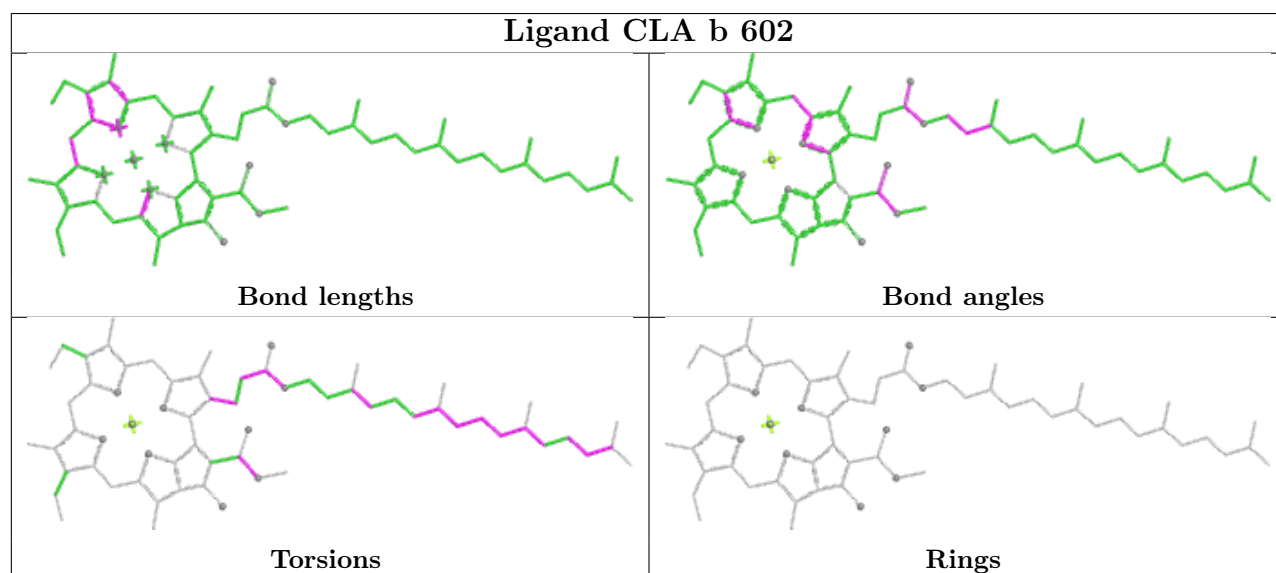
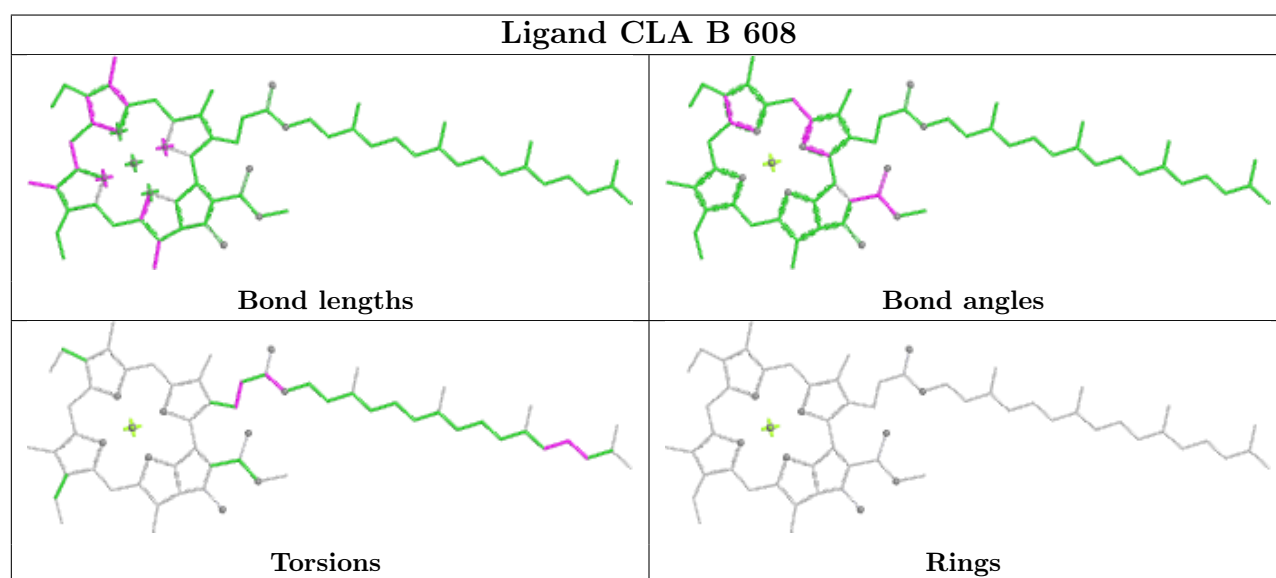
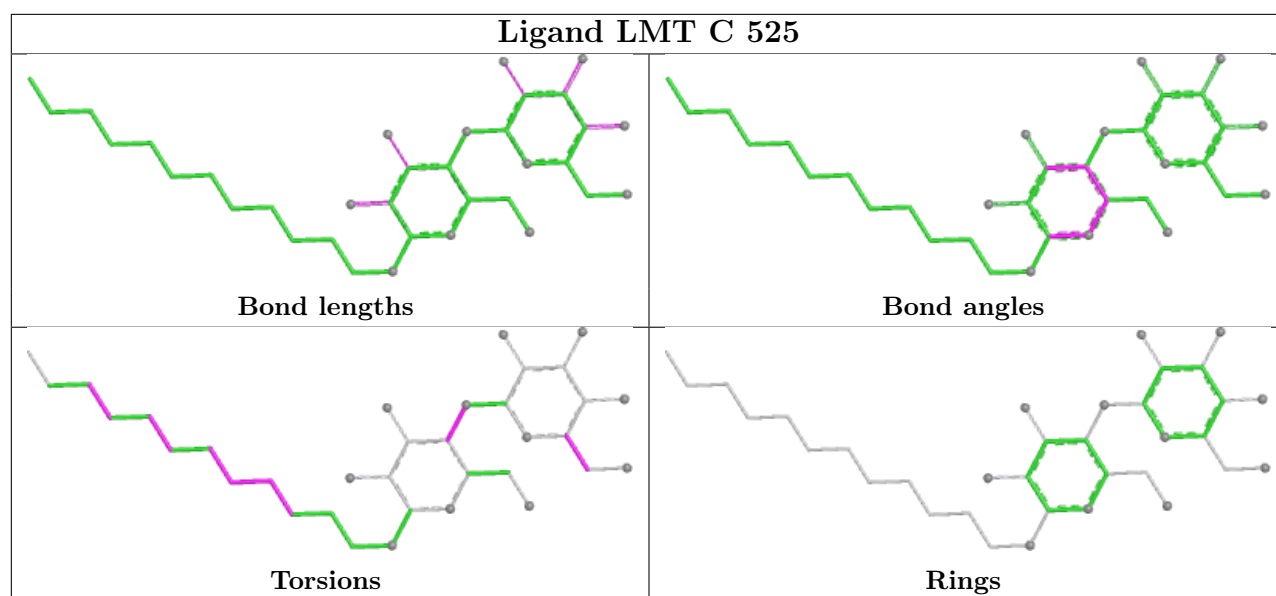


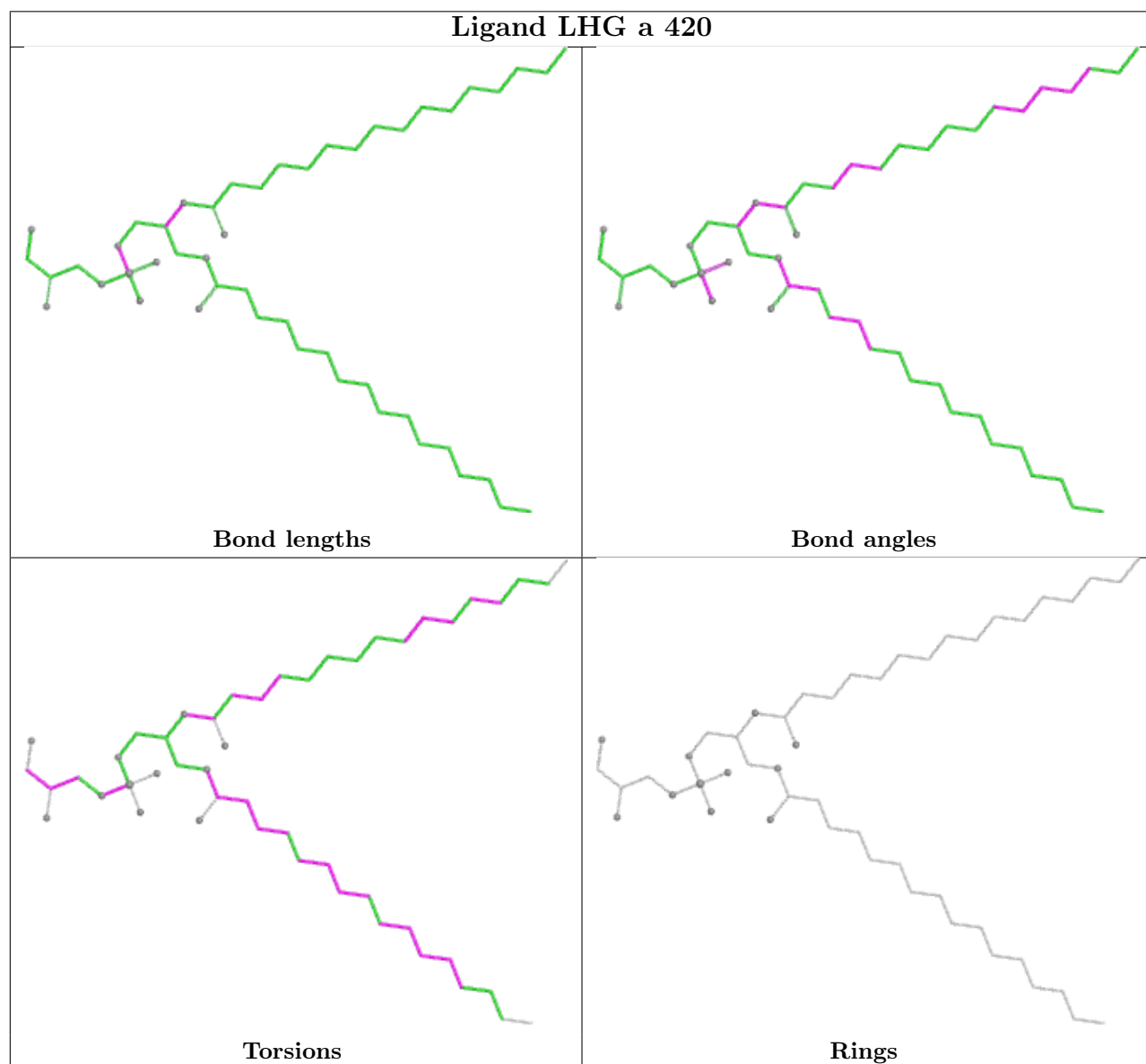
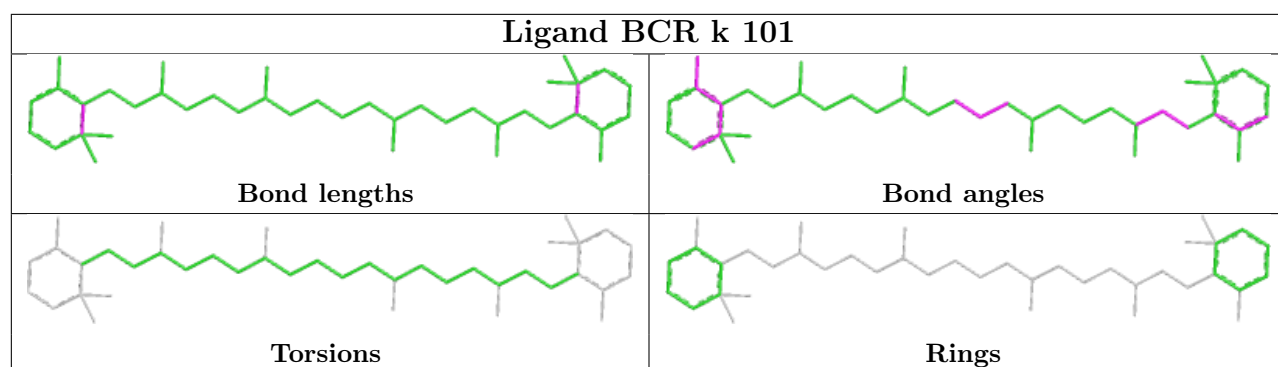


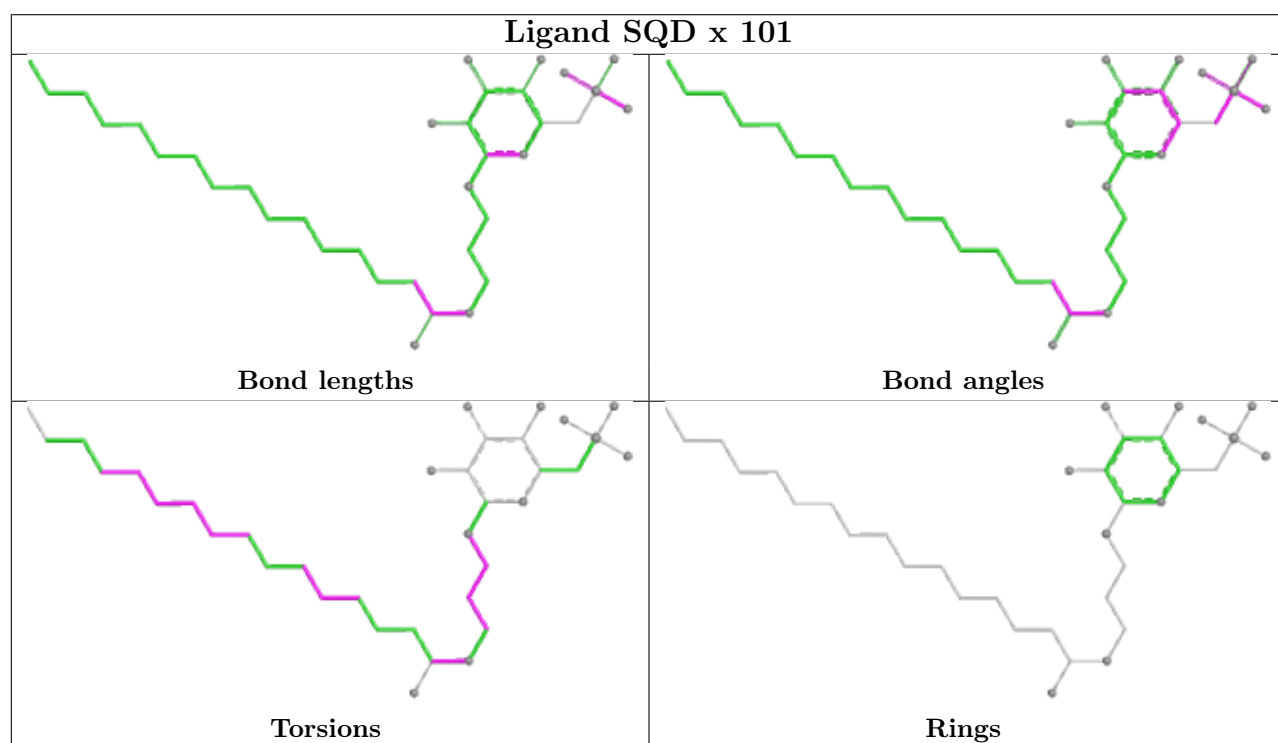
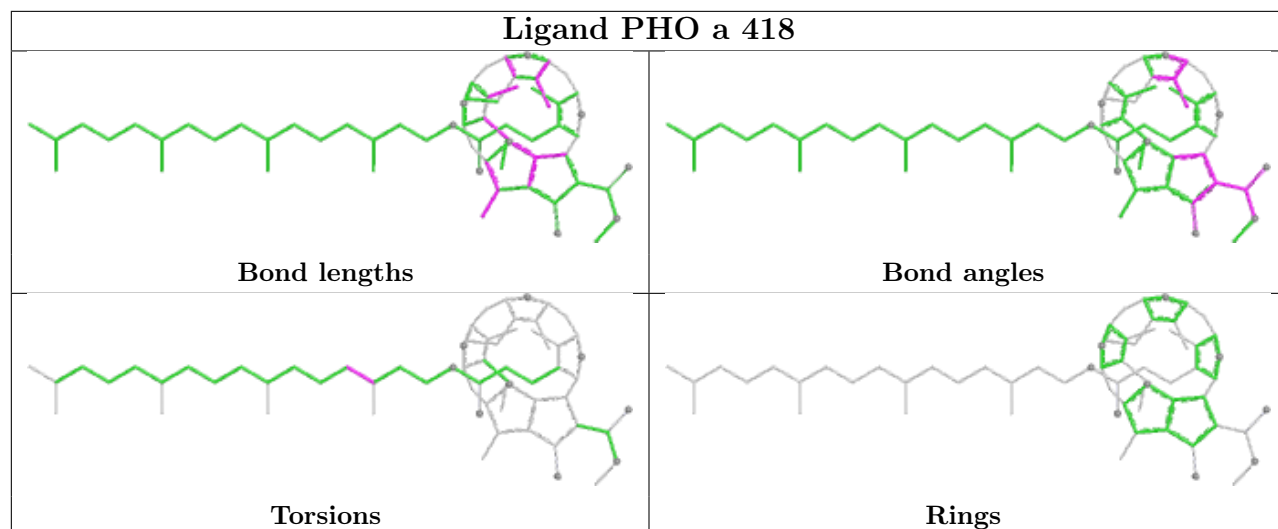


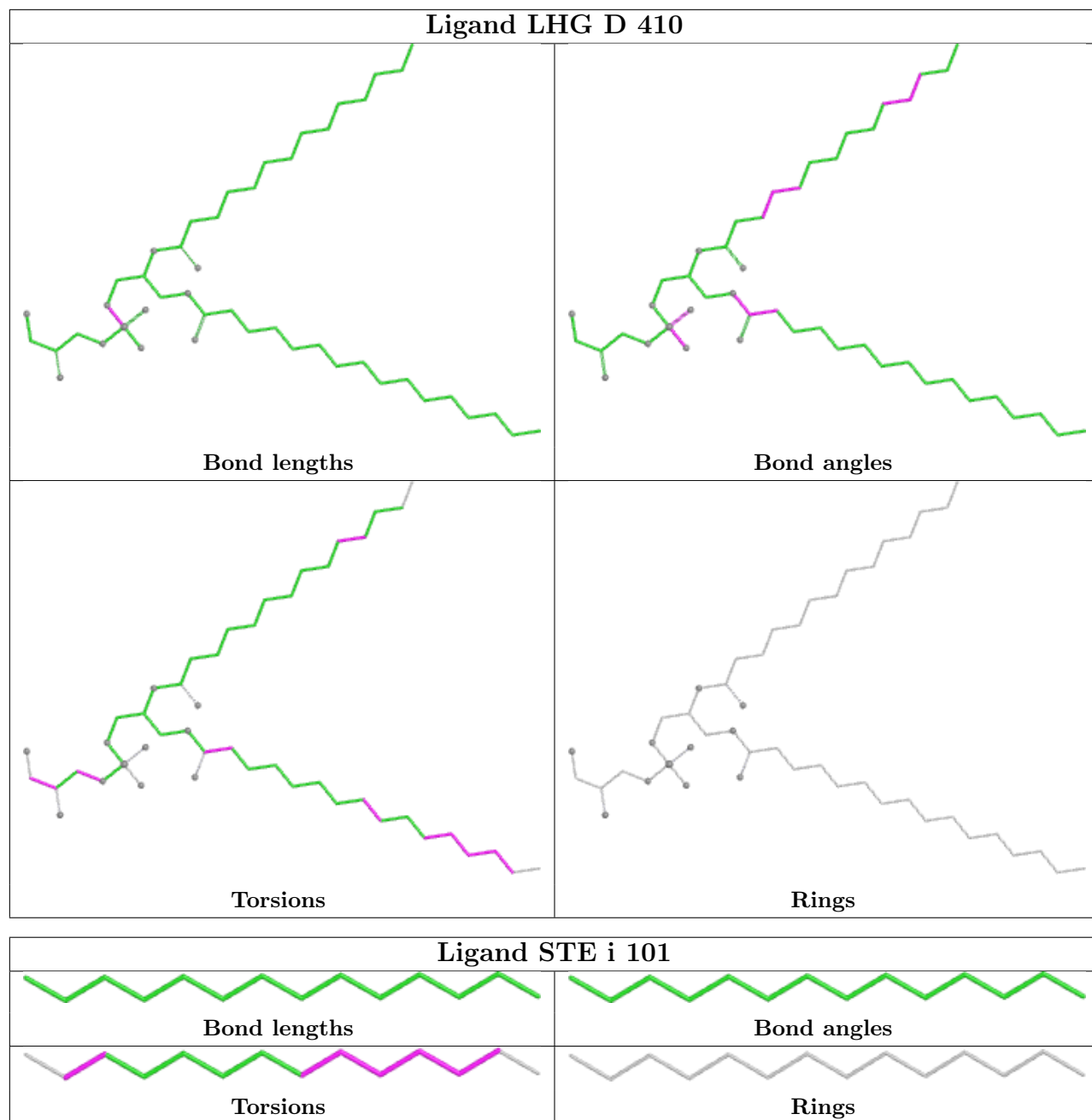


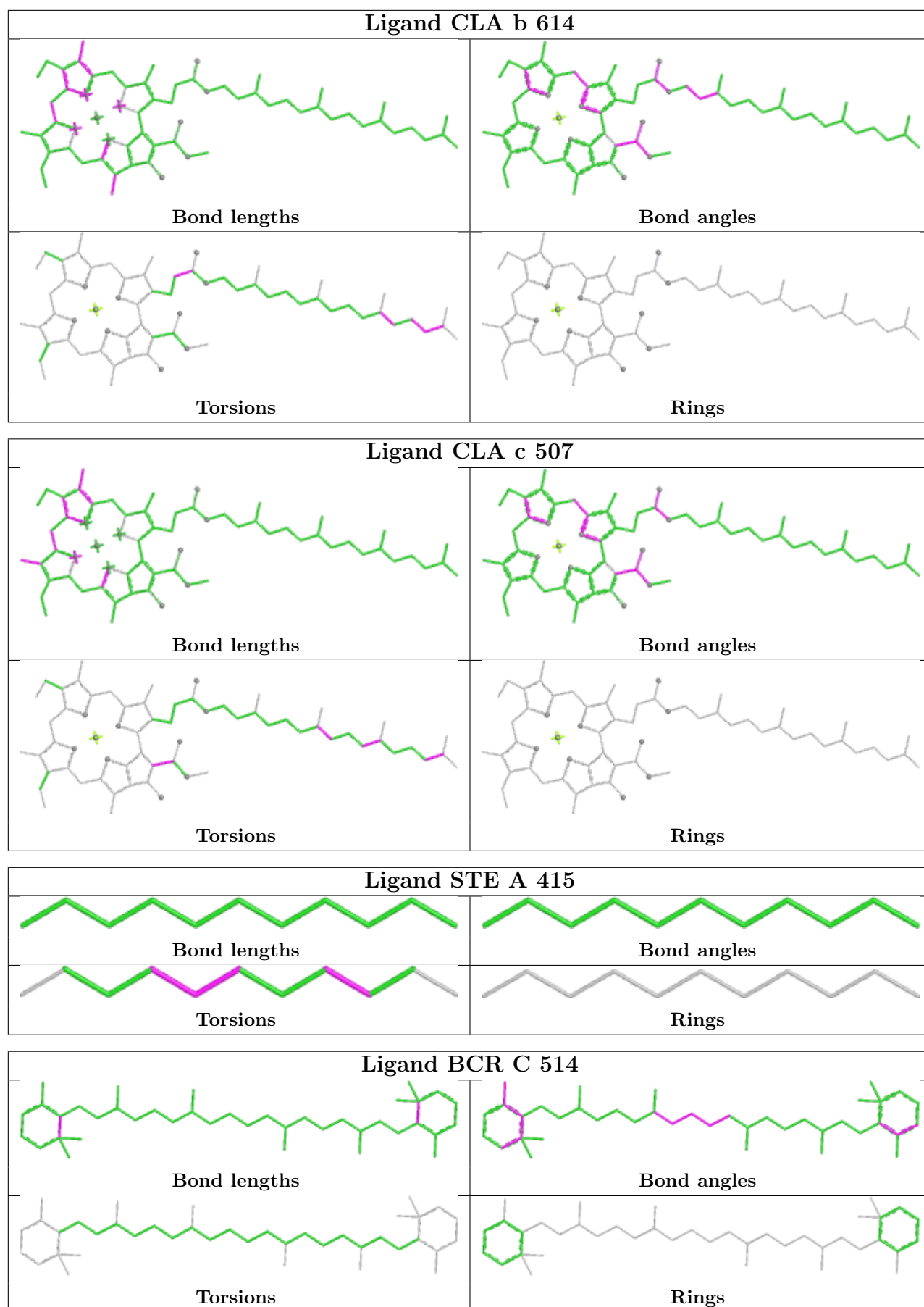


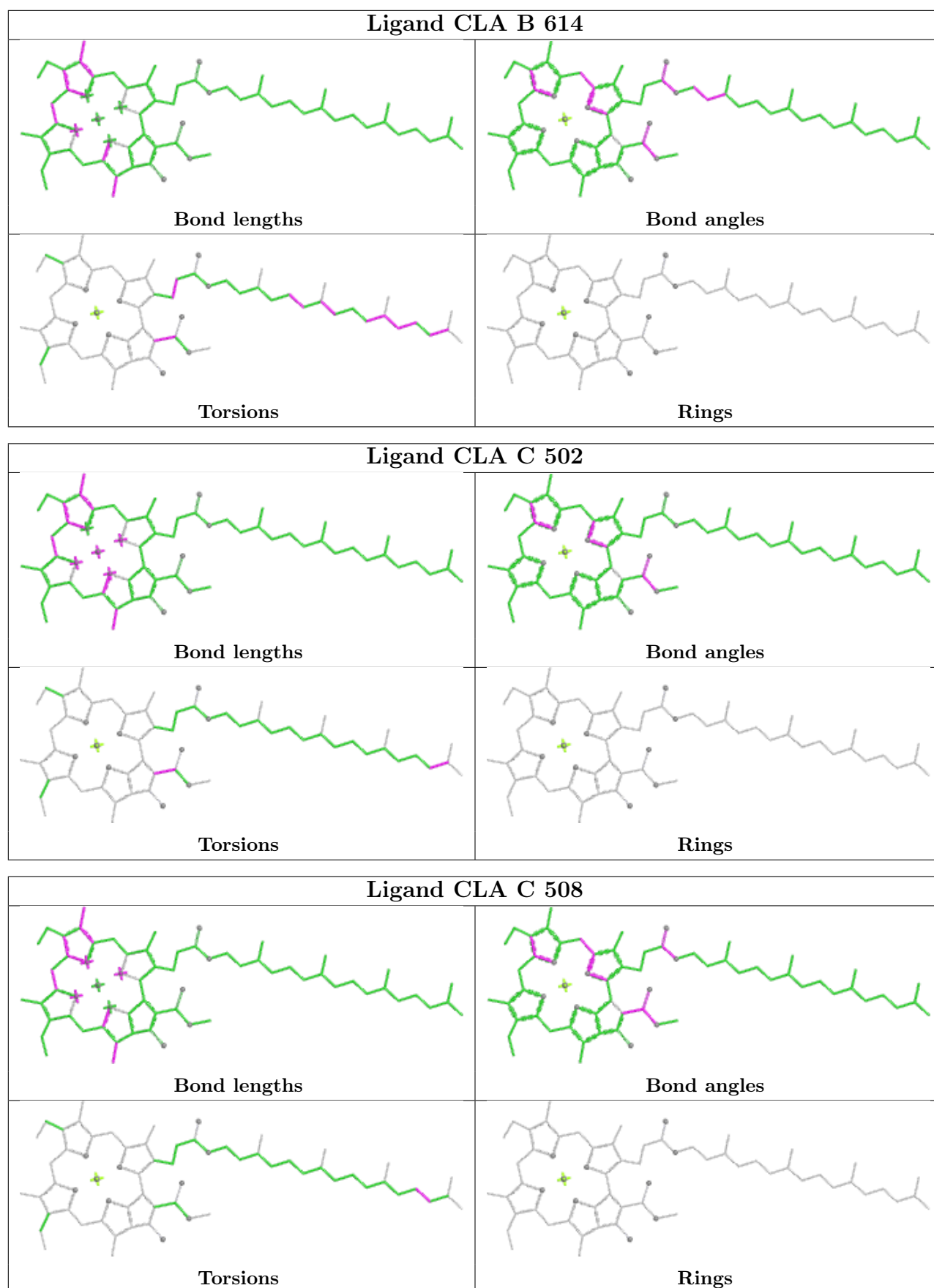


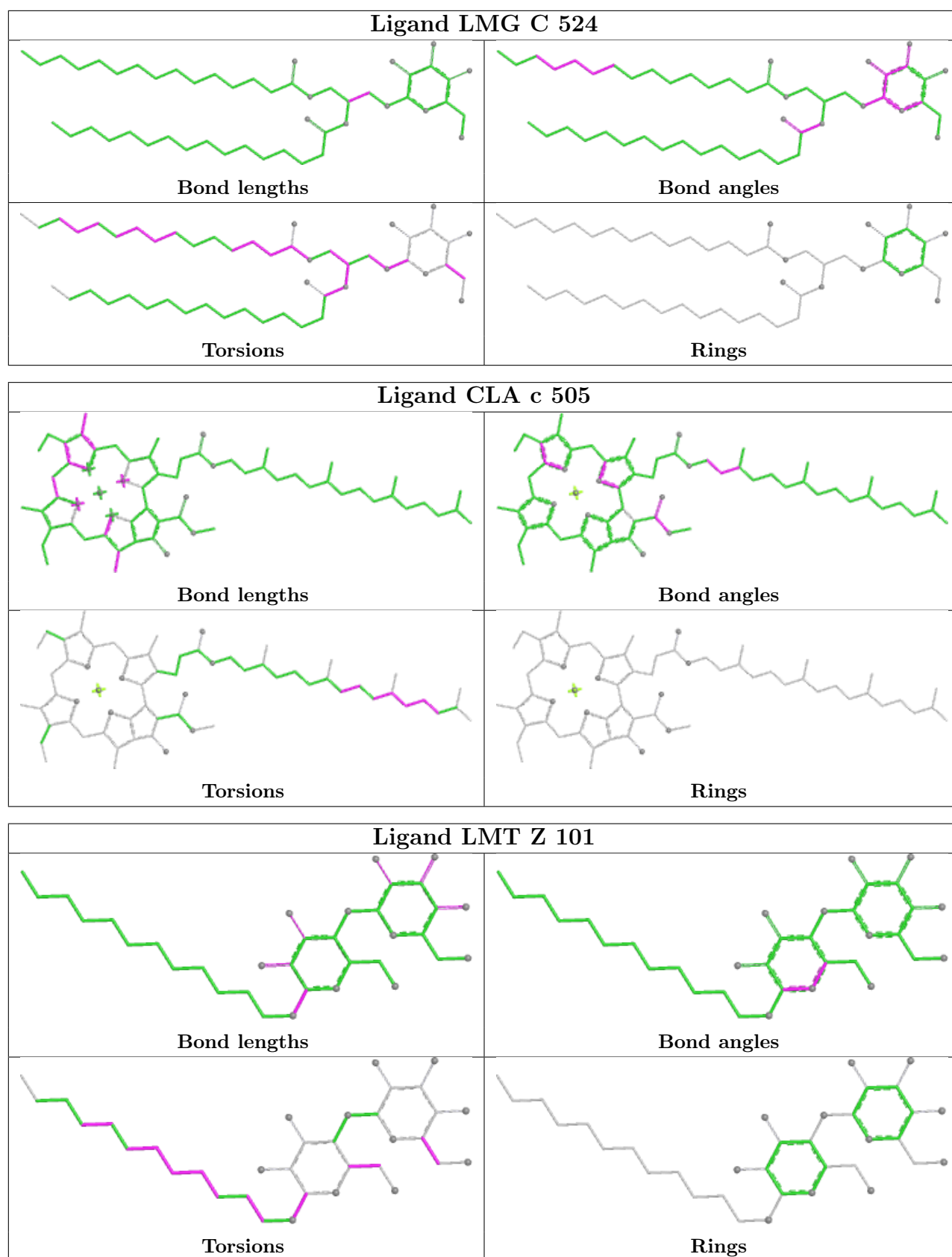


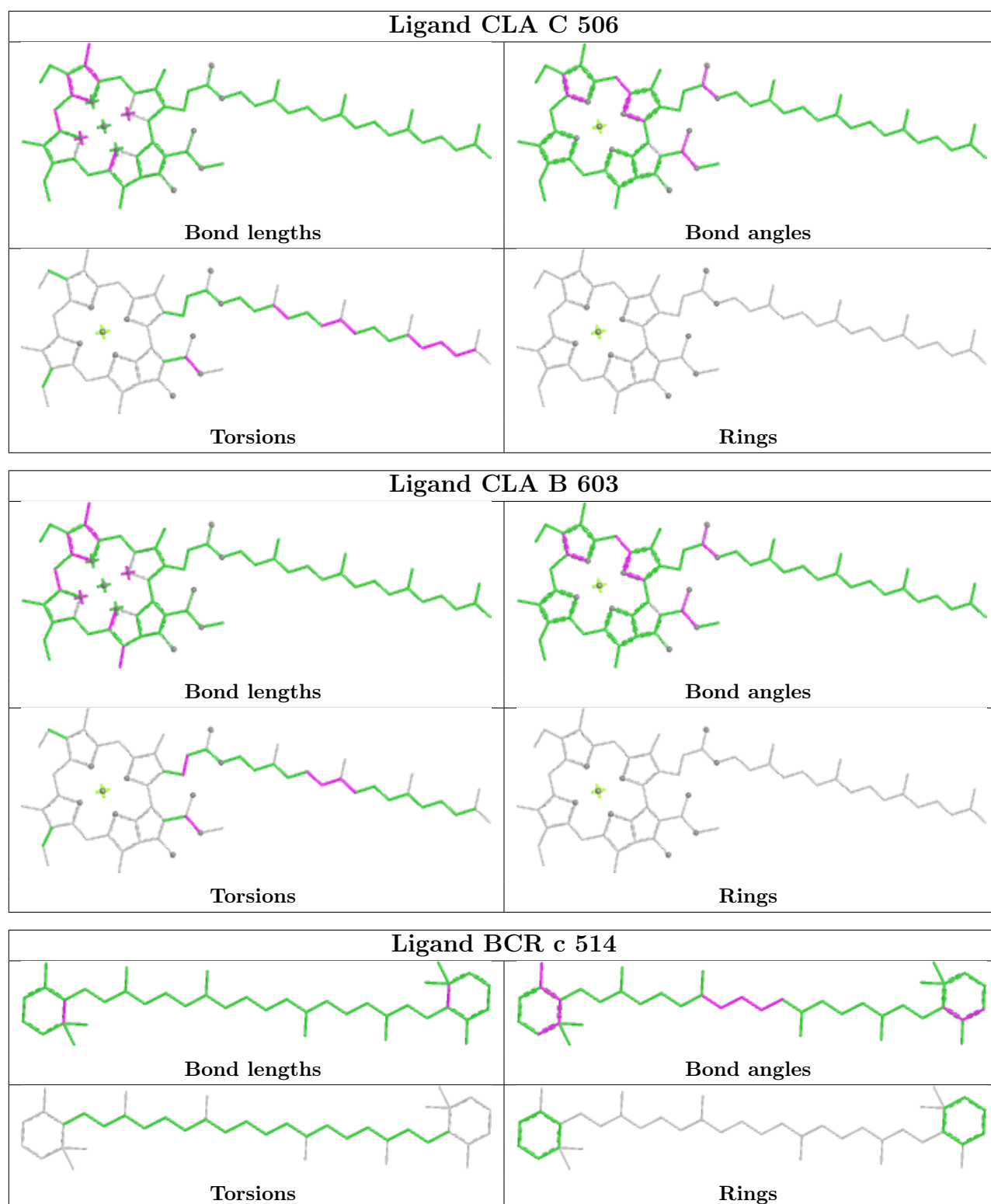


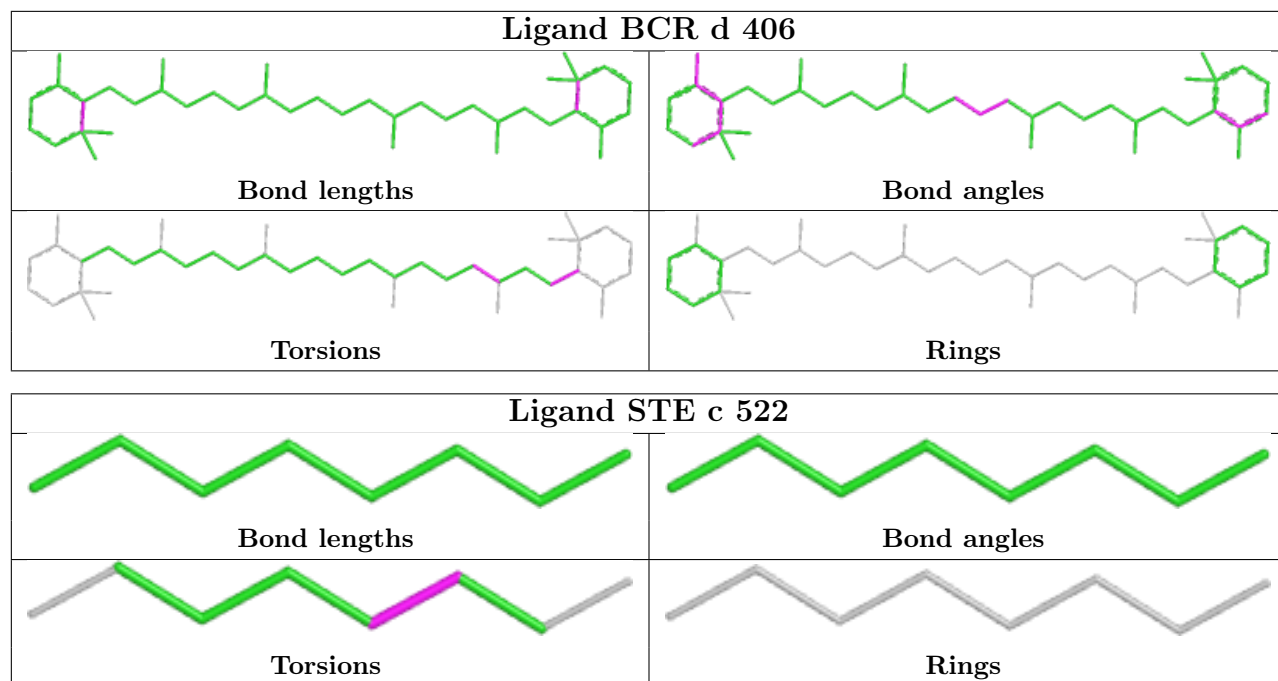


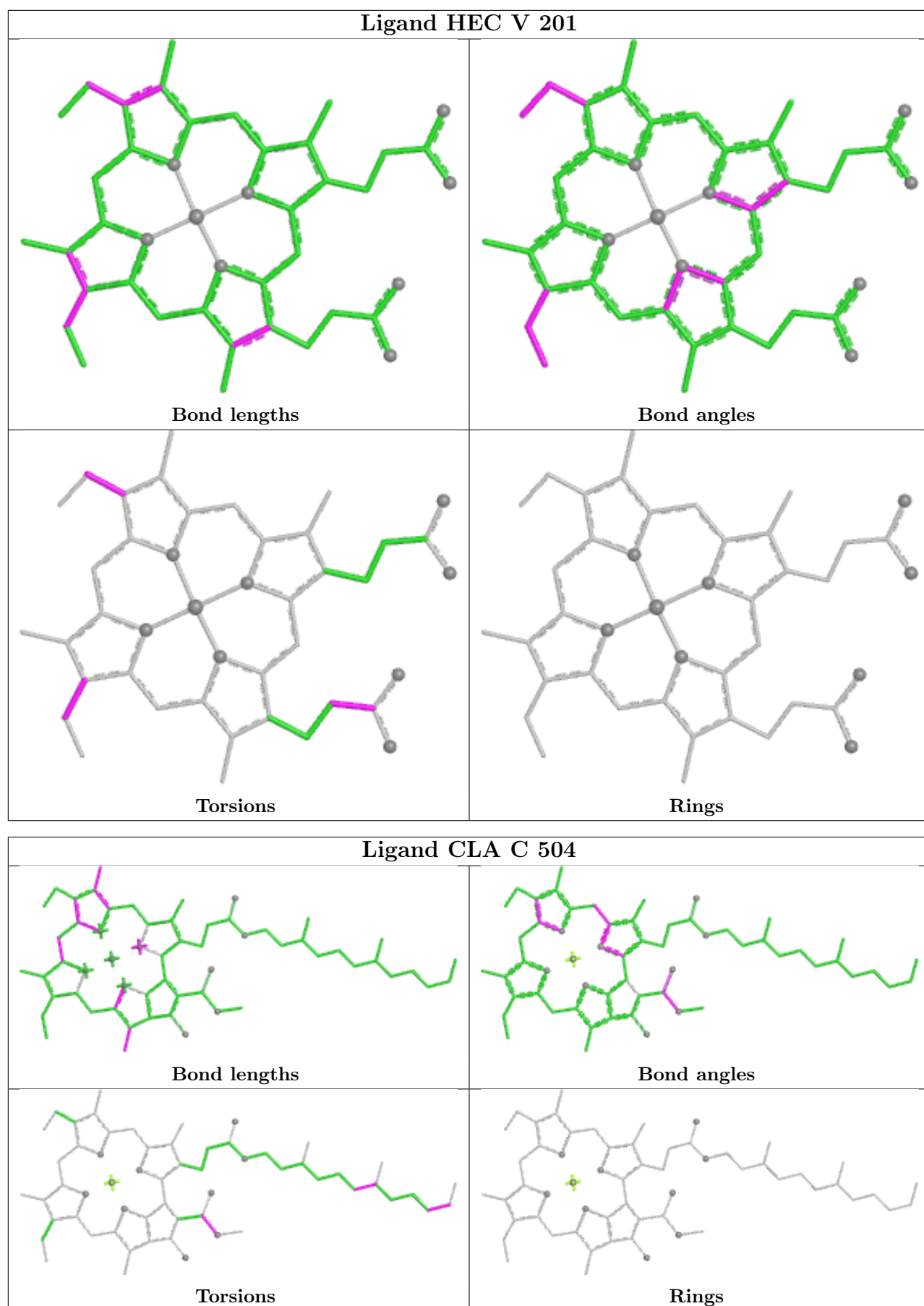


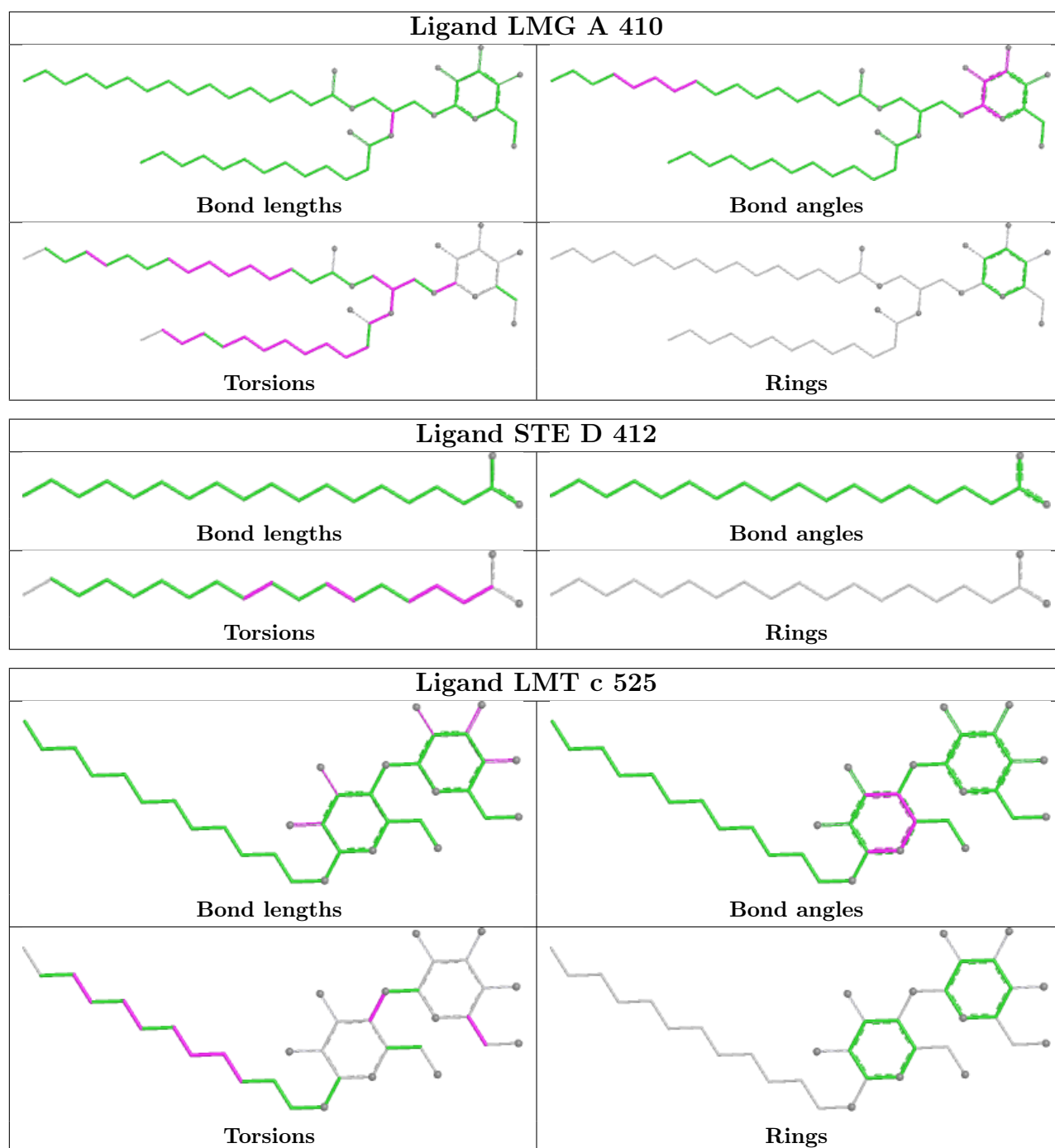


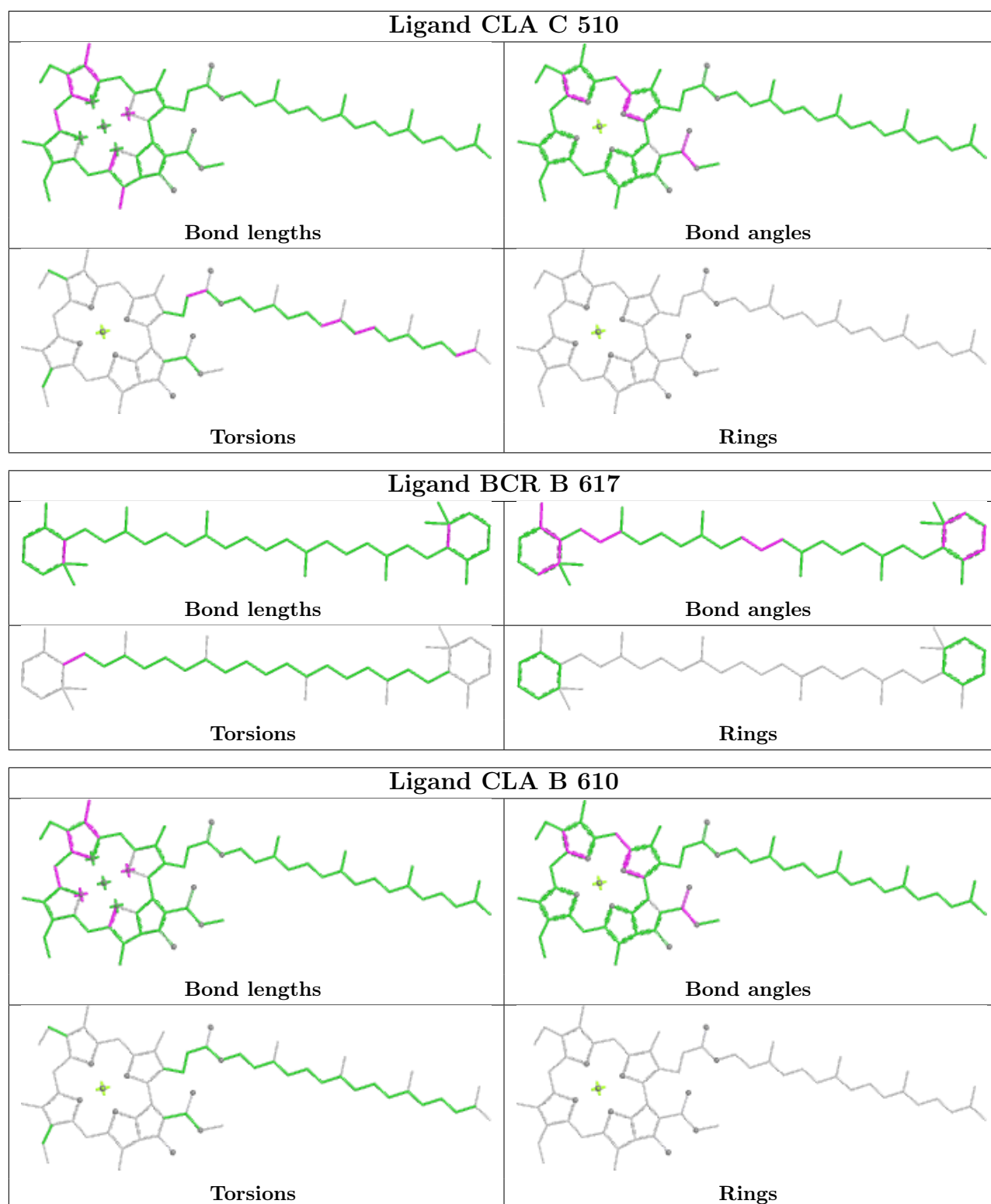


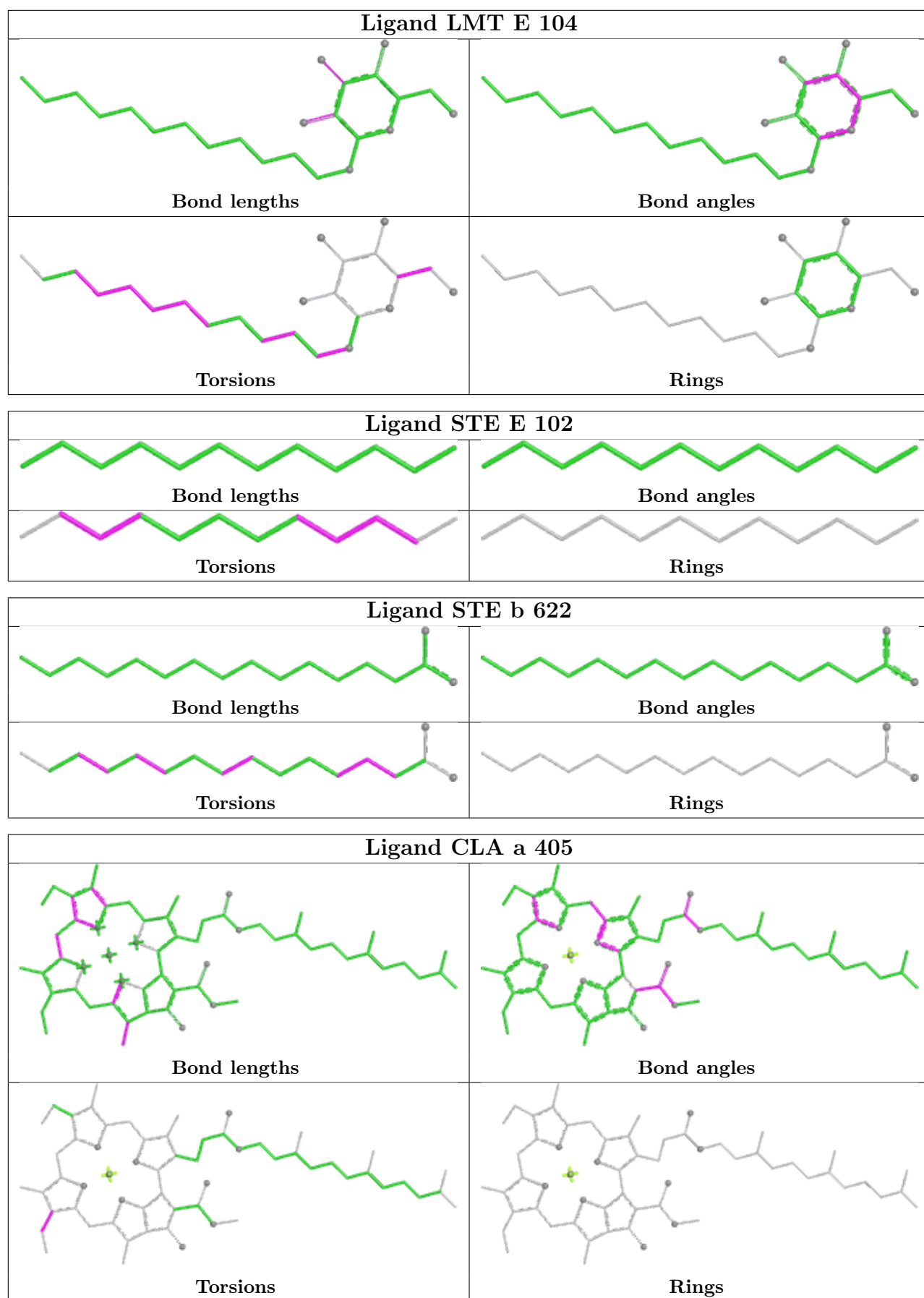


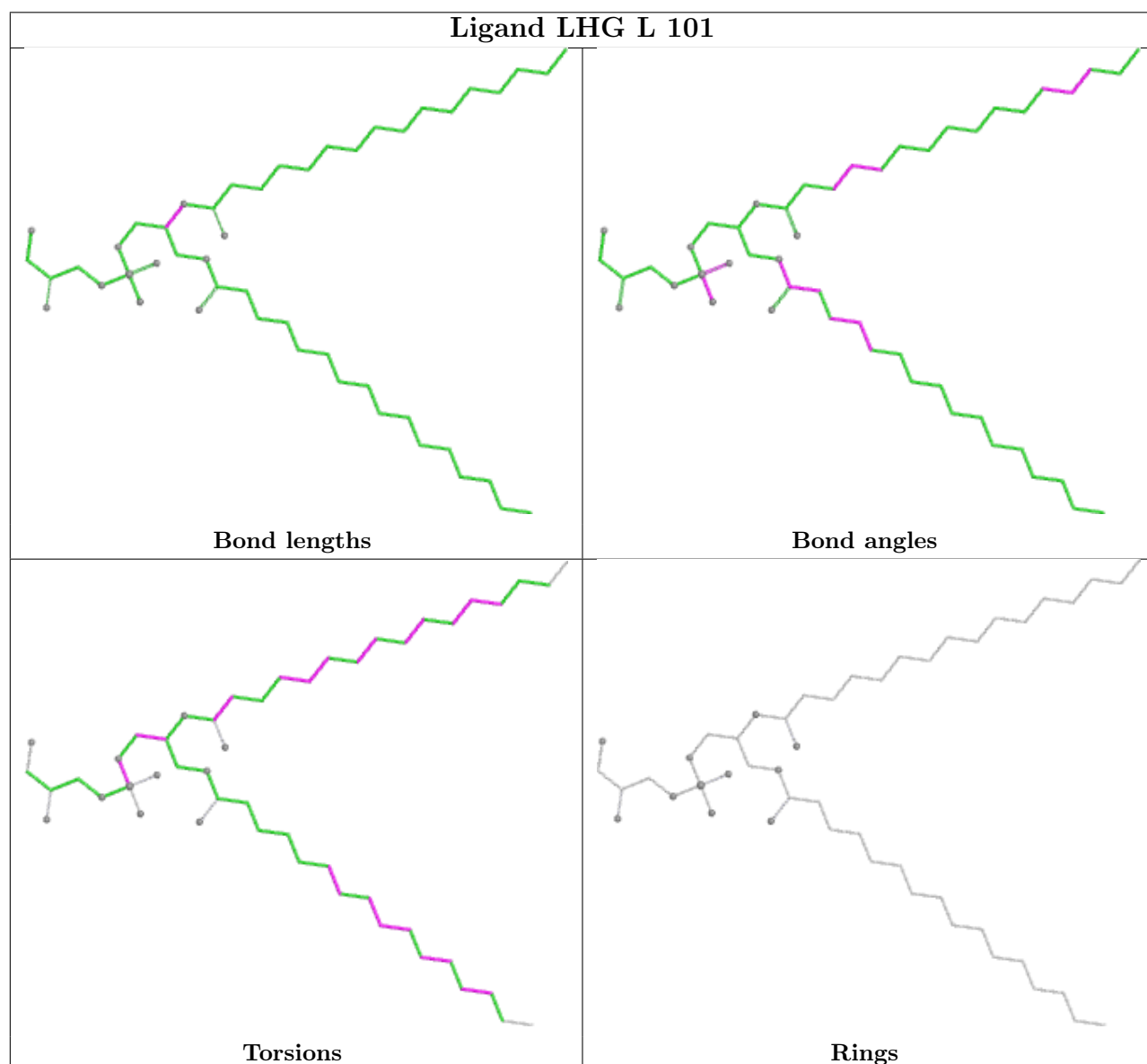
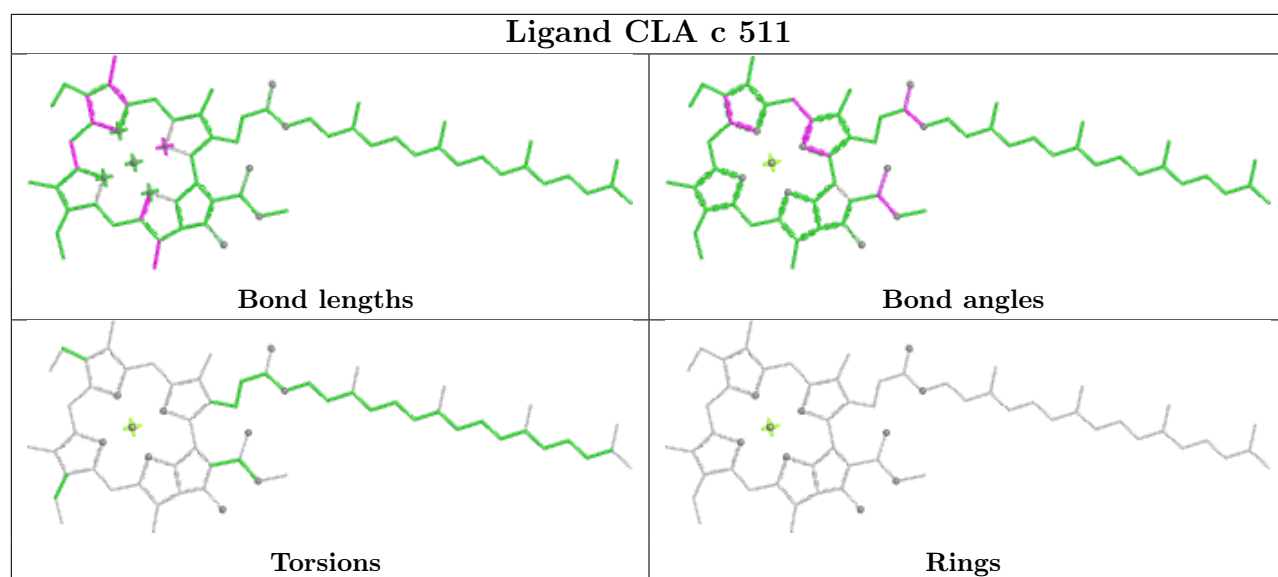


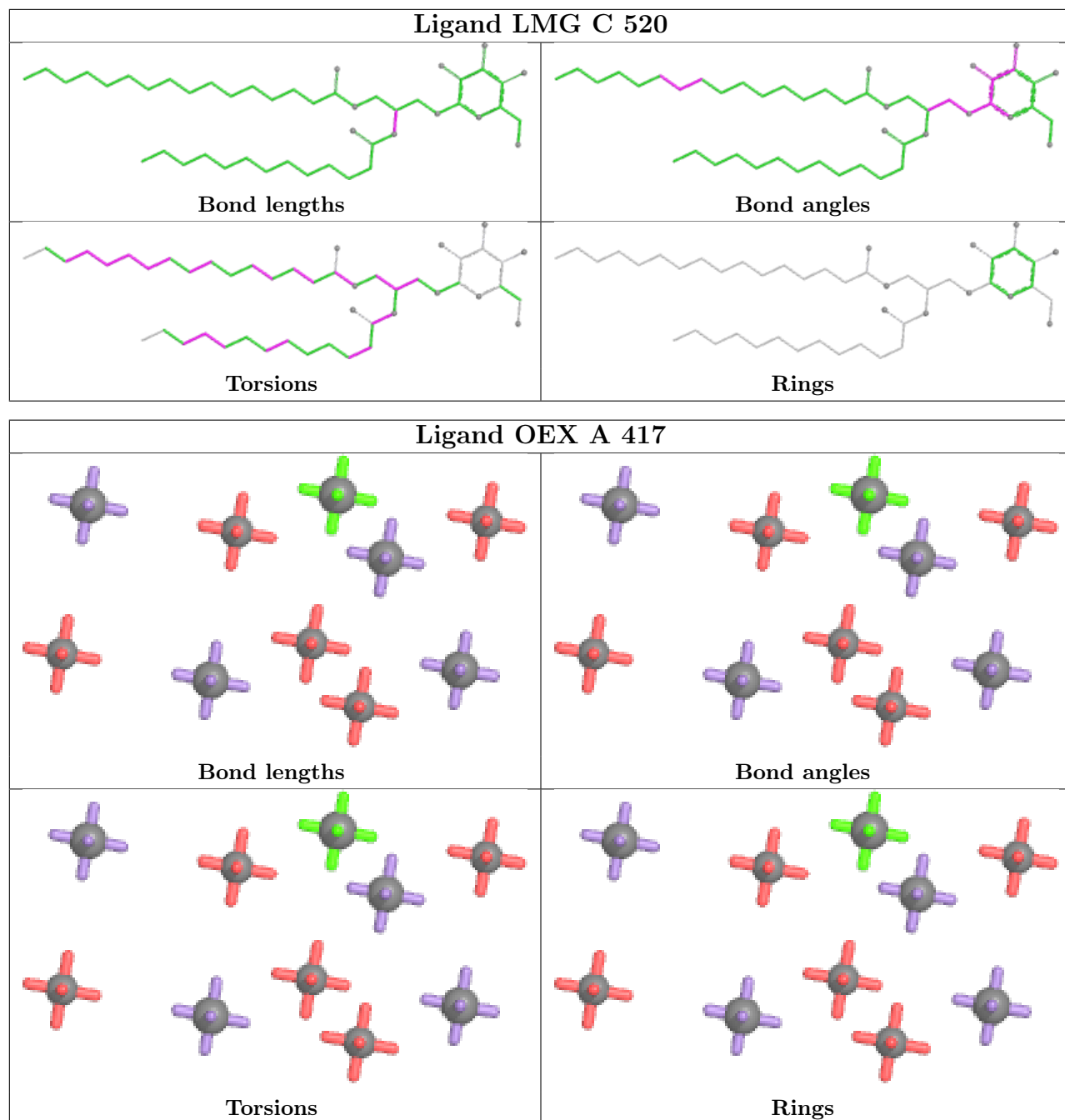


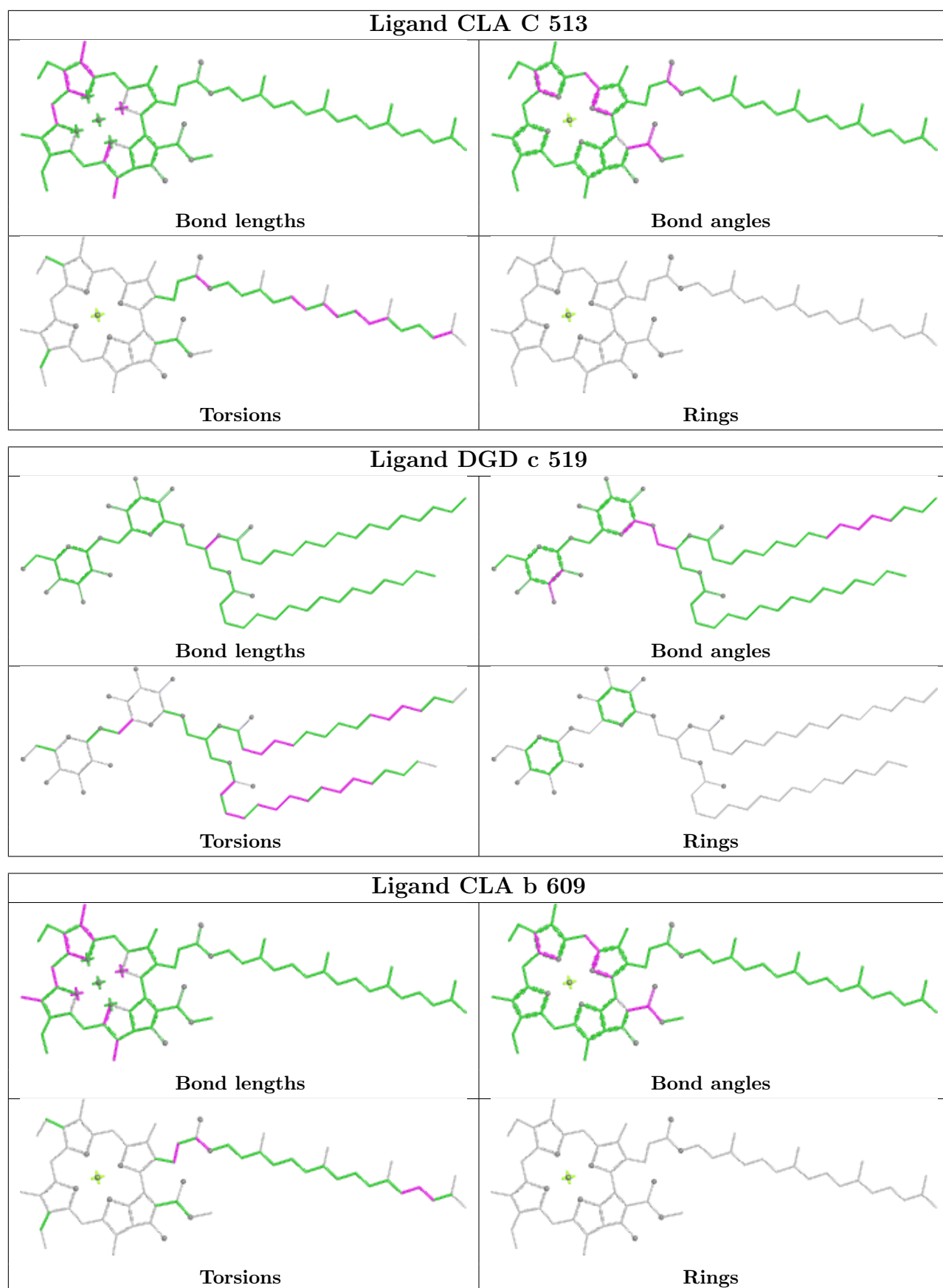


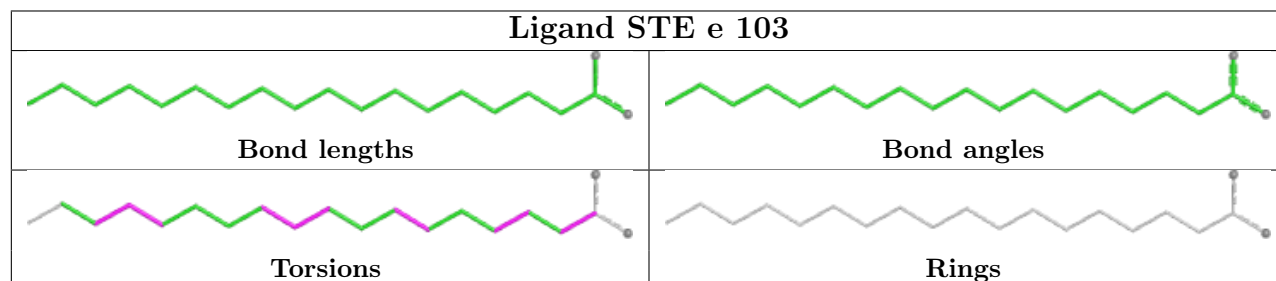
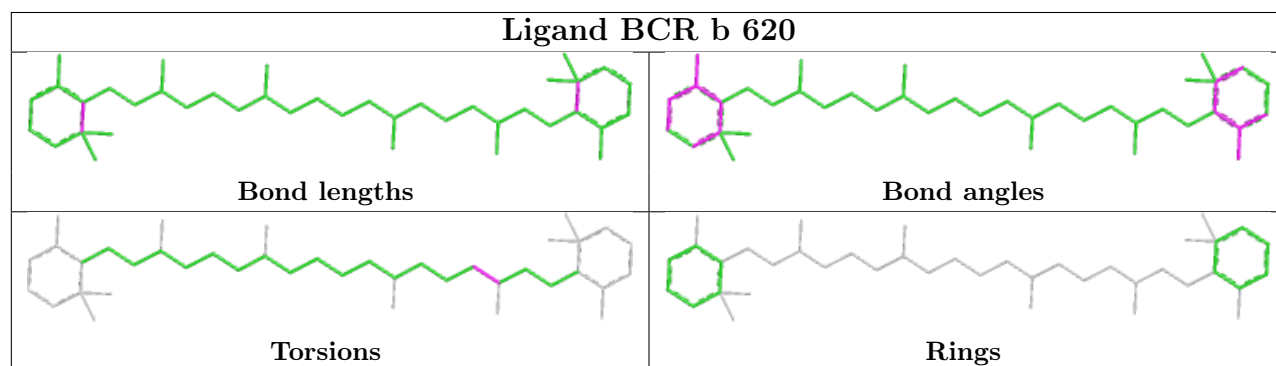
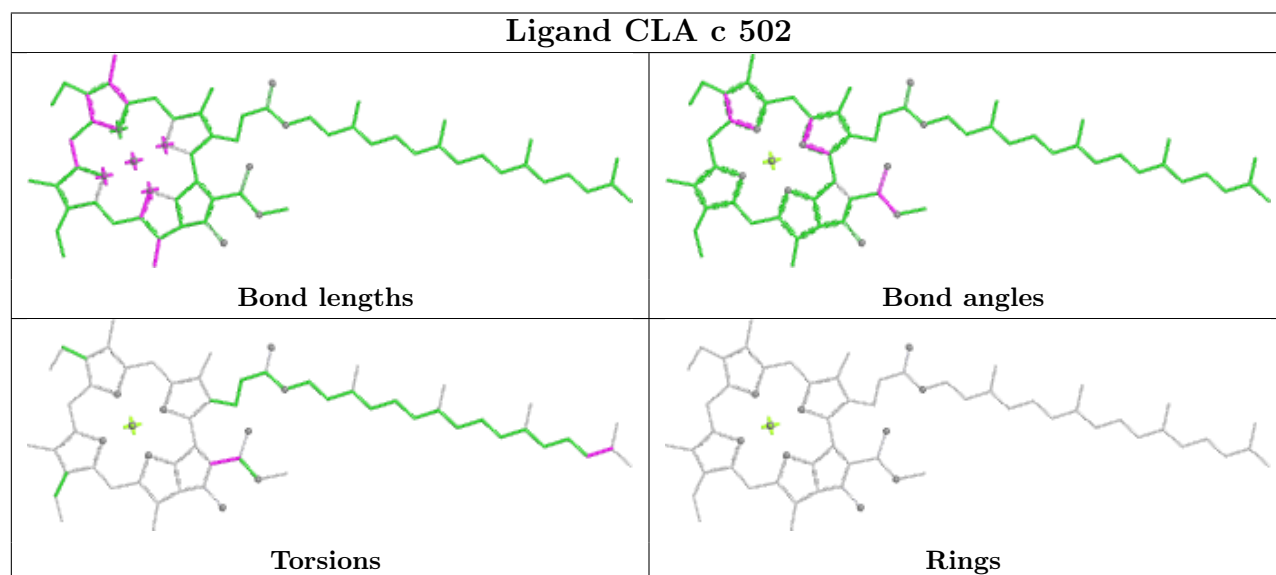
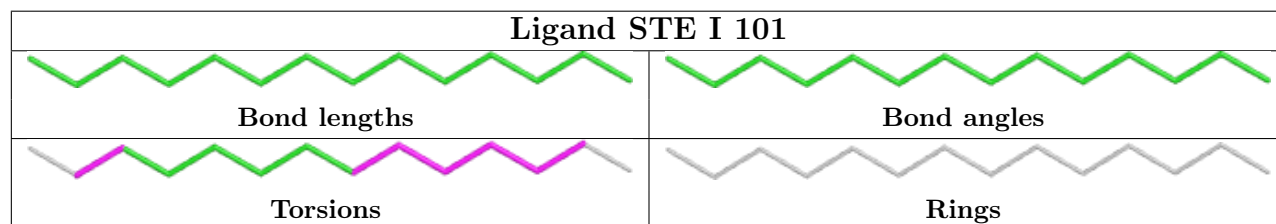
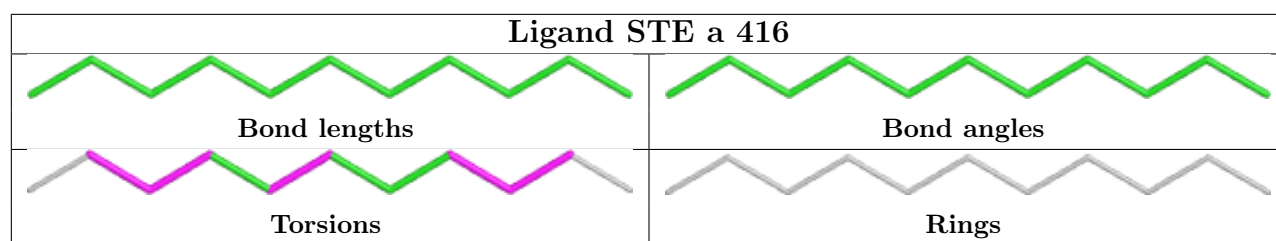


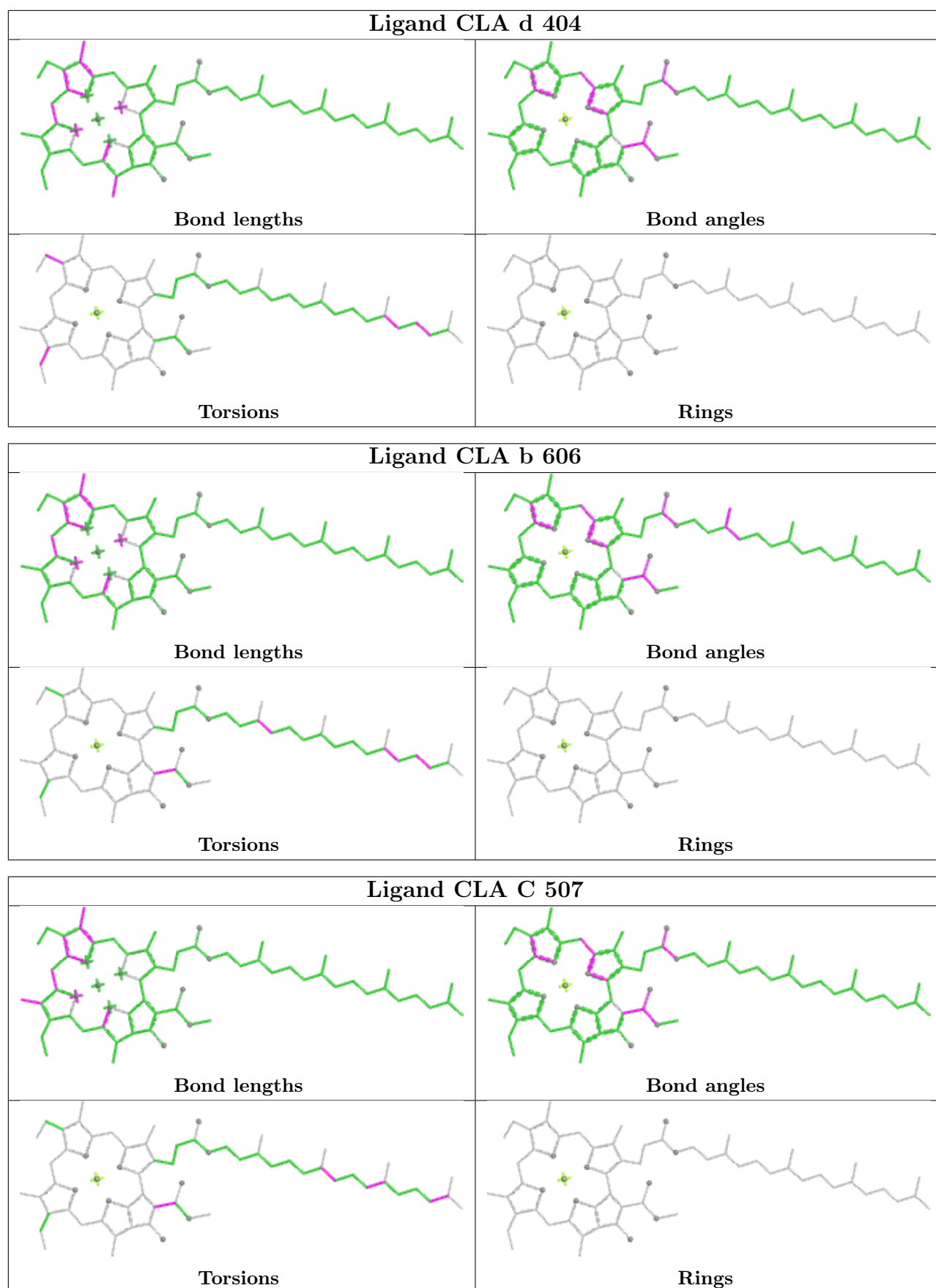


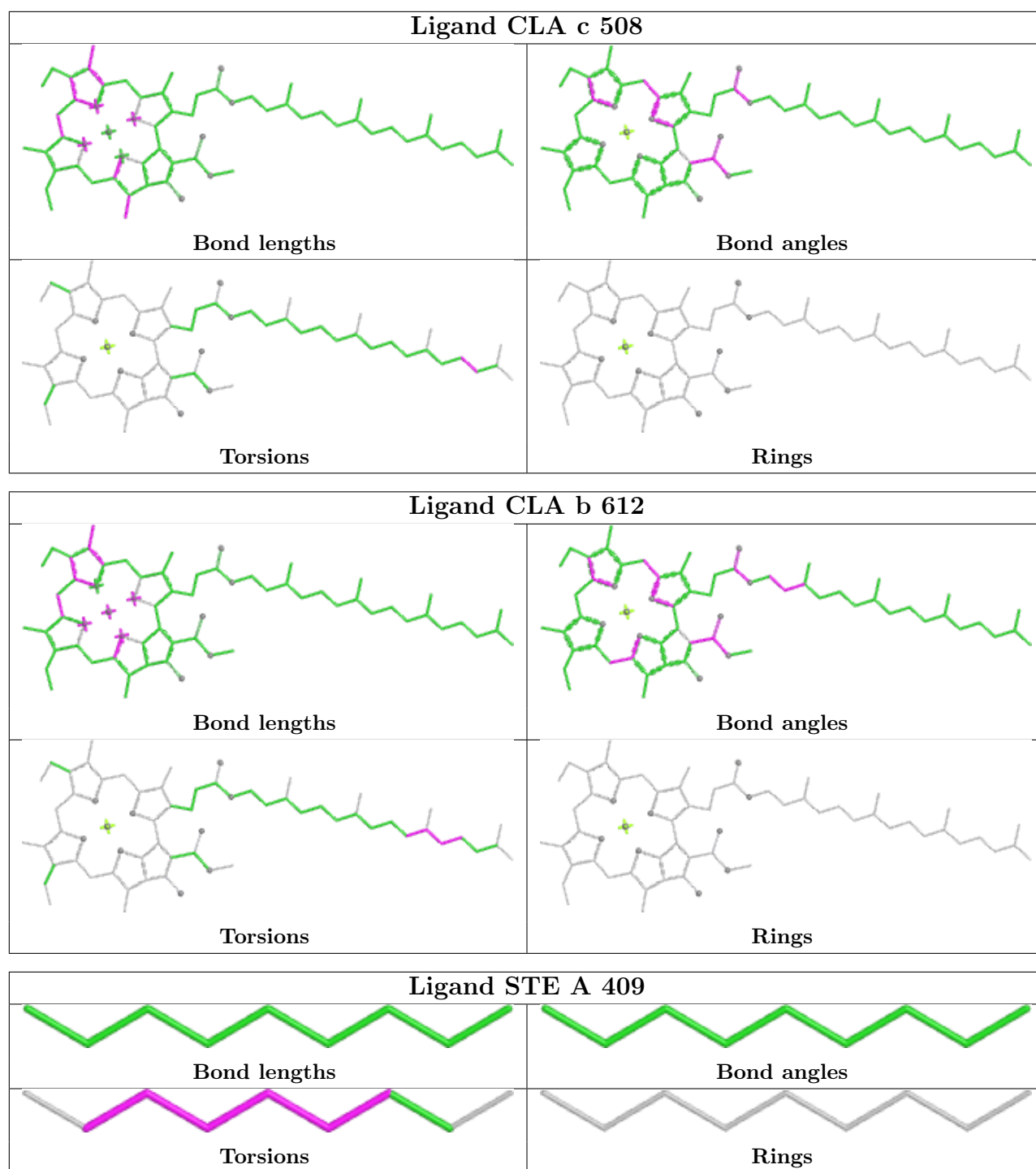


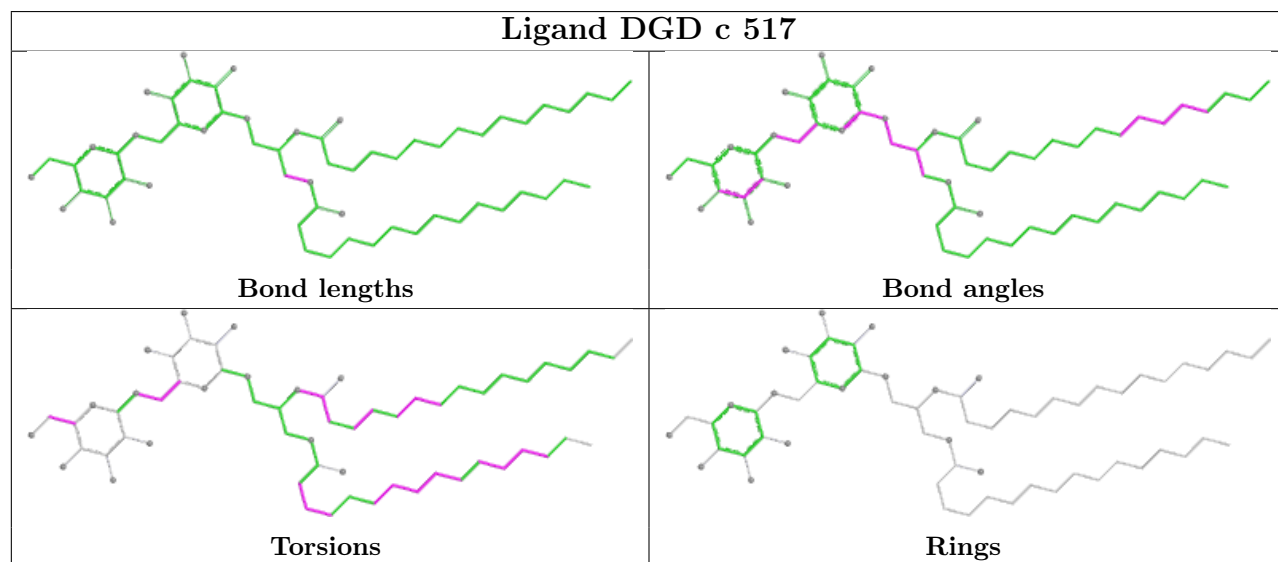
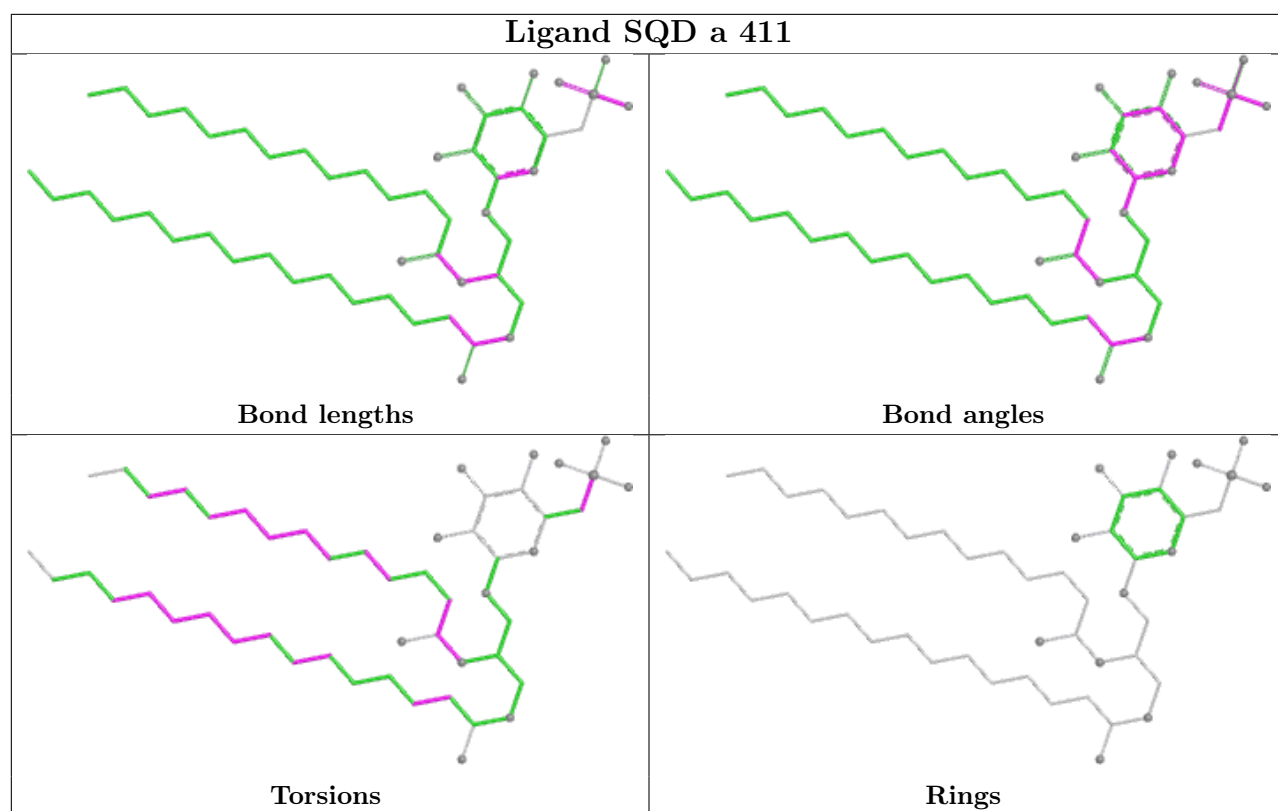


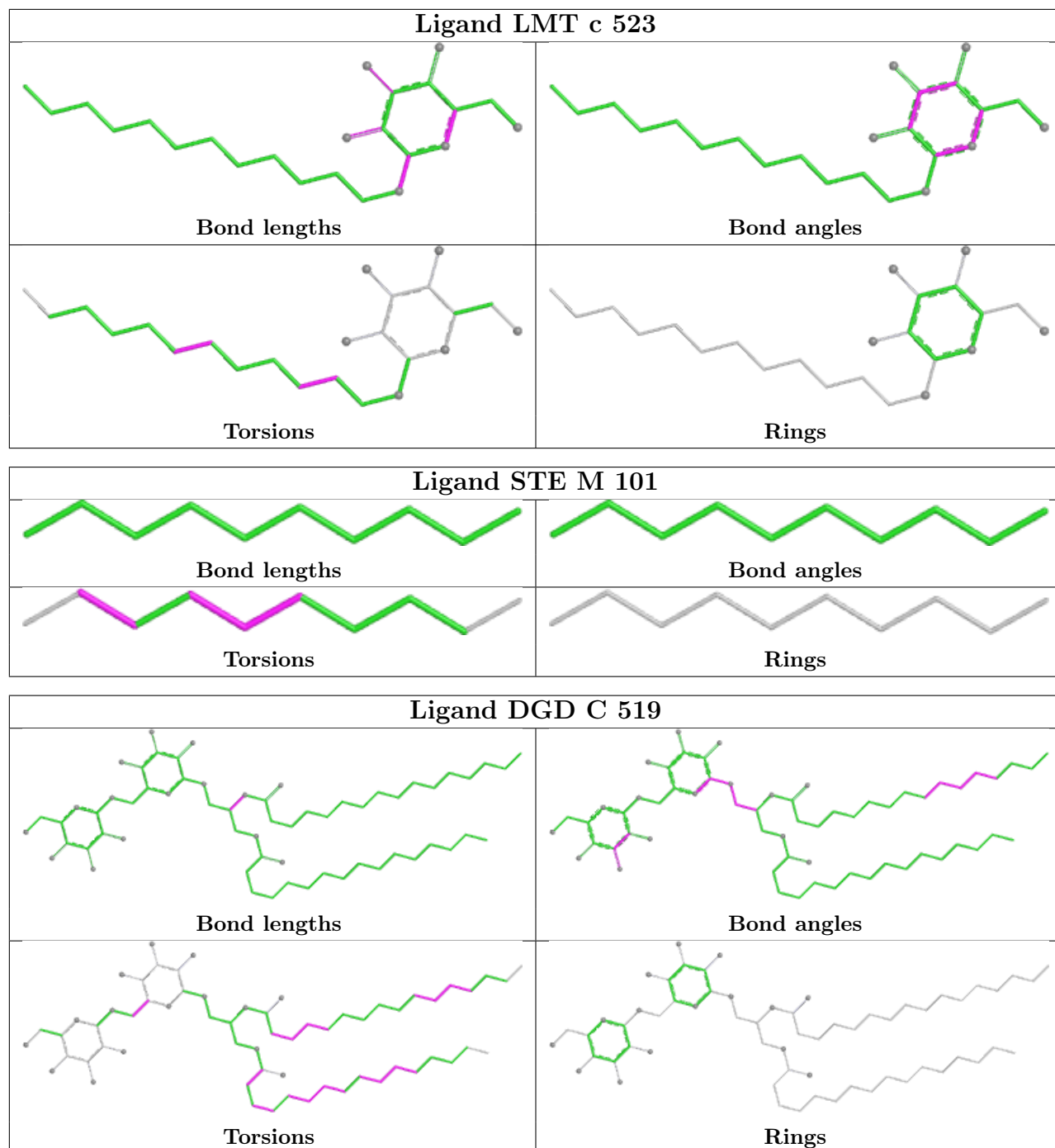


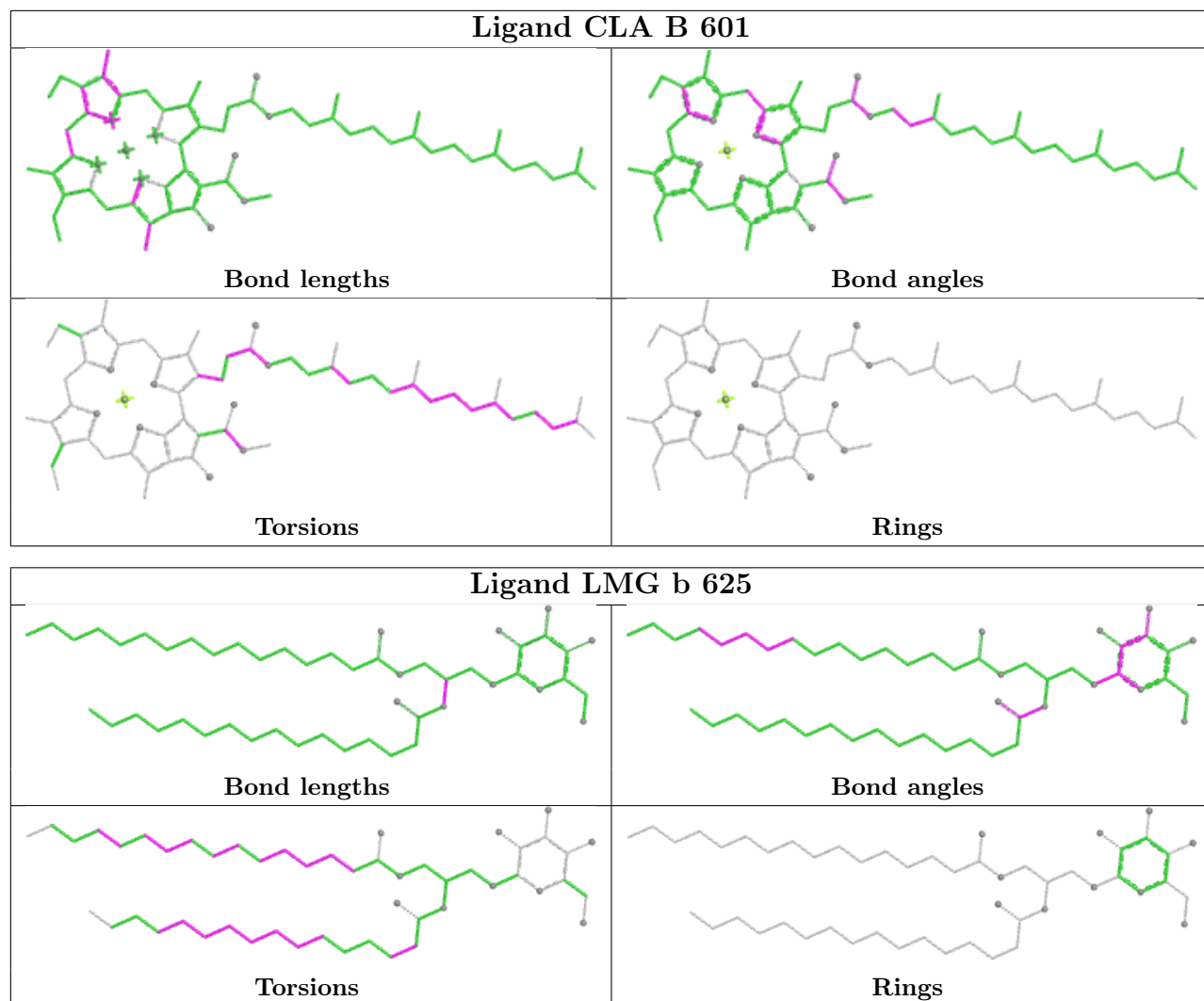


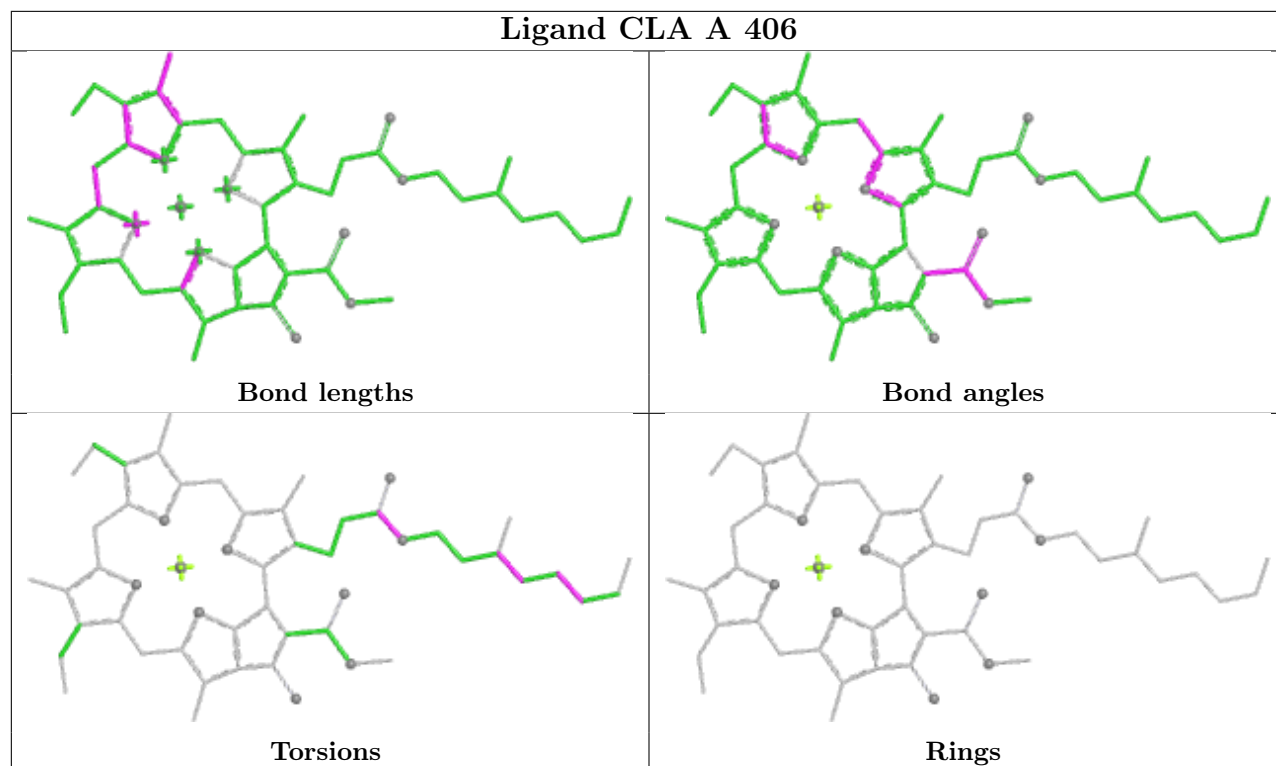












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

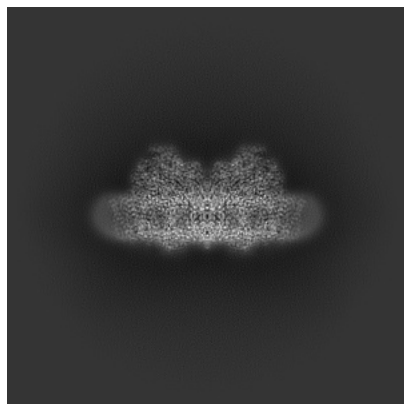
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50019. These allow visual inspection of the internal detail of the map and identification of artifacts.

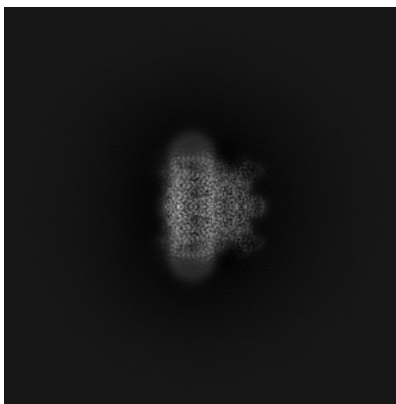
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

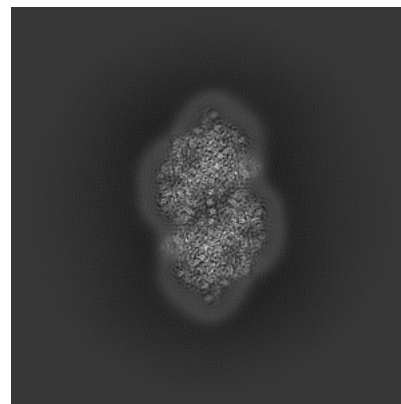
#### 6.1.1 Primary map



X

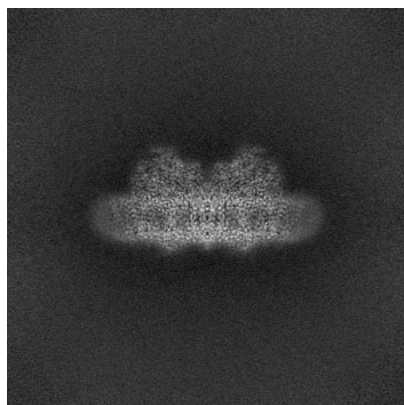


Y

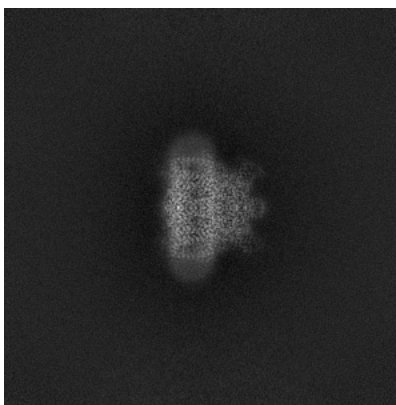


Z

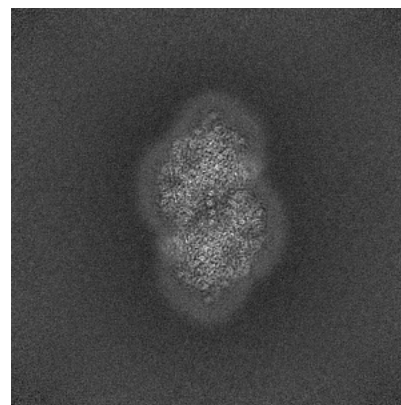
#### 6.1.2 Raw map



X



Y

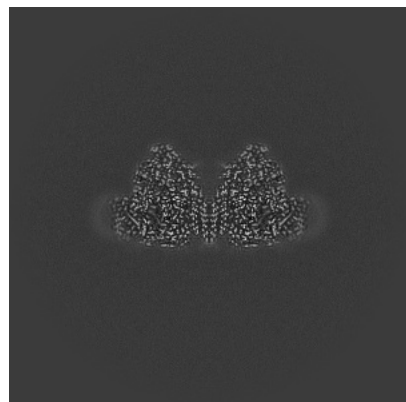


Z

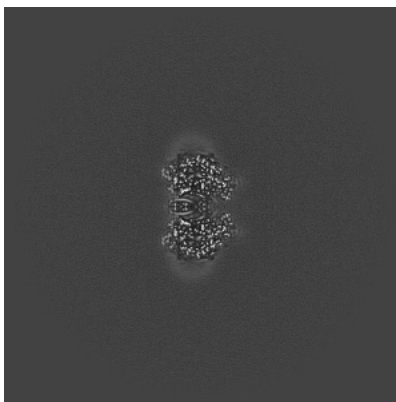
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

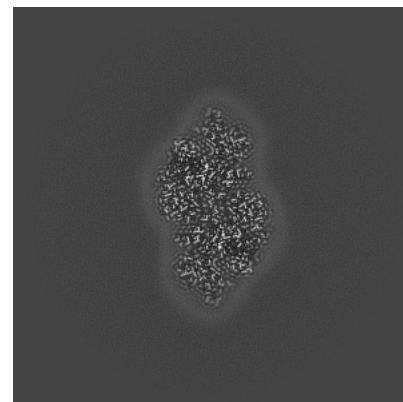
### 6.2.1 Primary map



X Index: 360

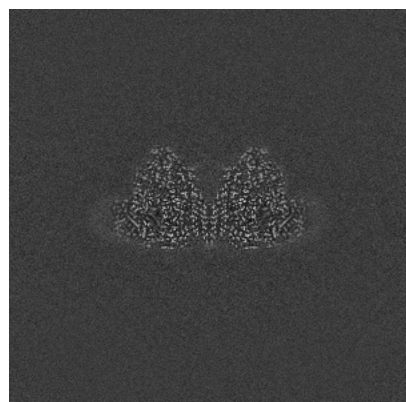


Y Index: 360

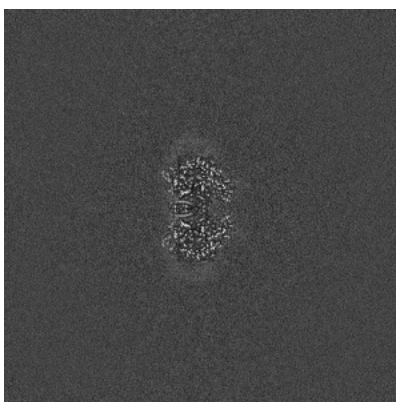


Z Index: 360

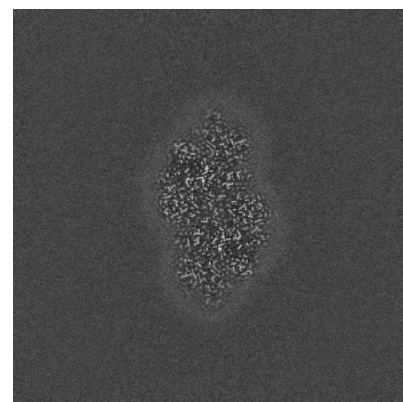
### 6.2.2 Raw map



X Index: 360



Y Index: 360

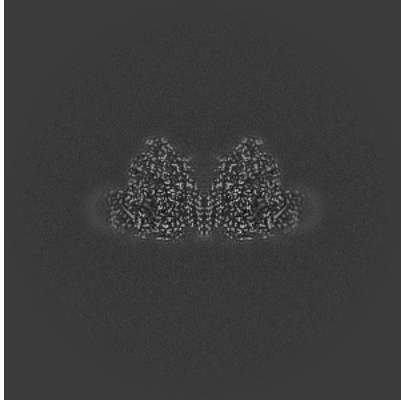


Z Index: 360

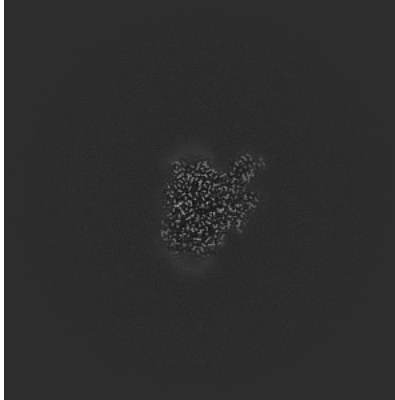
The images above show central slices of the map in three orthogonal directions.

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

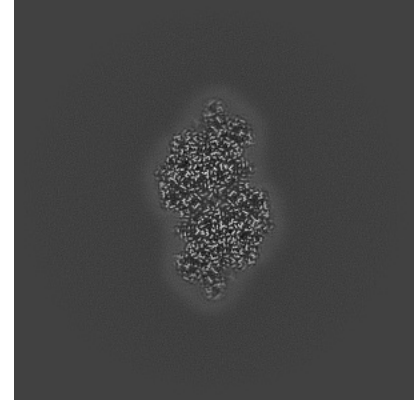
### 6.3.1 Primary map



X Index: 360

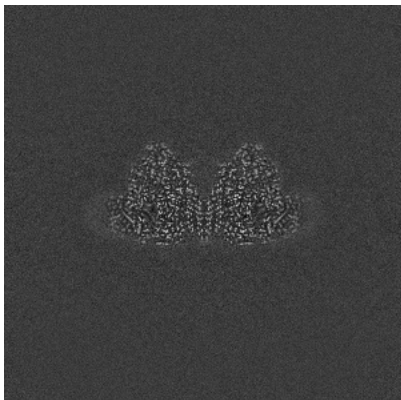


Y Index: 420

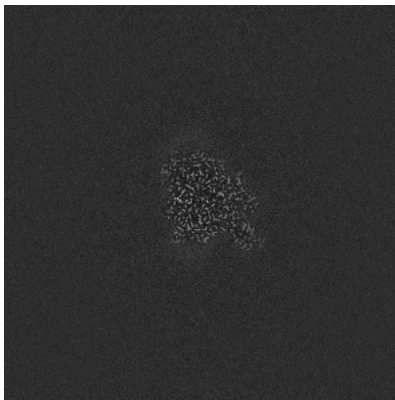


Z Index: 369

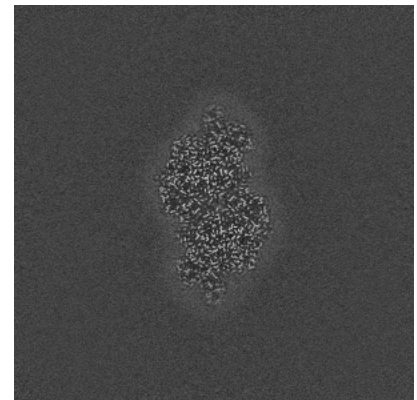
### 6.3.2 Raw map



X Index: 360



Y Index: 300

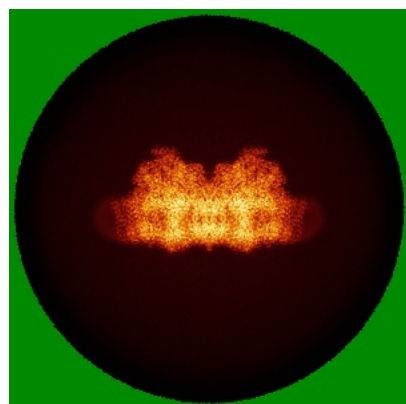


Z Index: 369

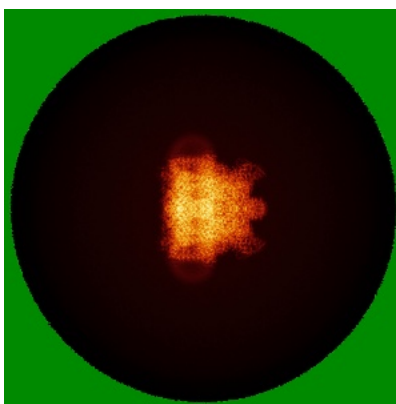
The images above show the largest variance slices of the map in three orthogonal directions.

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

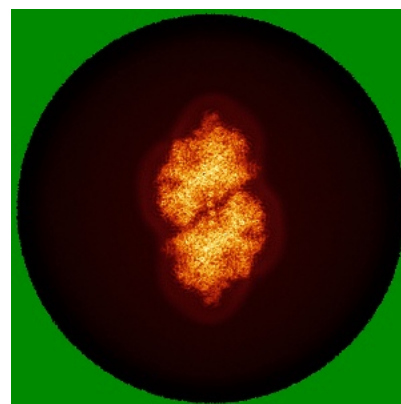
### 6.4.1 Primary map



X

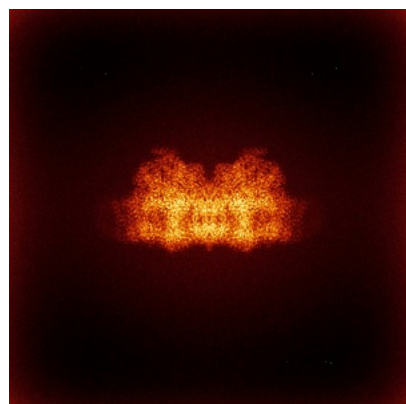


Y

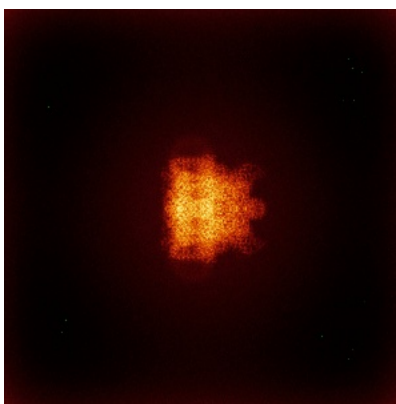


Z

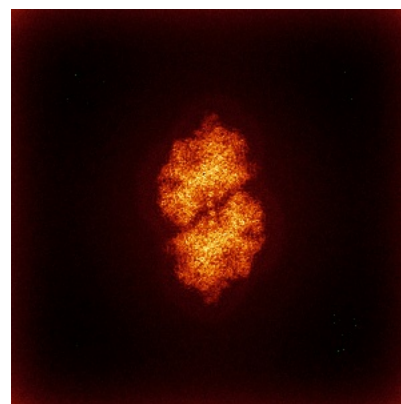
### 6.4.2 Raw map



X



Y

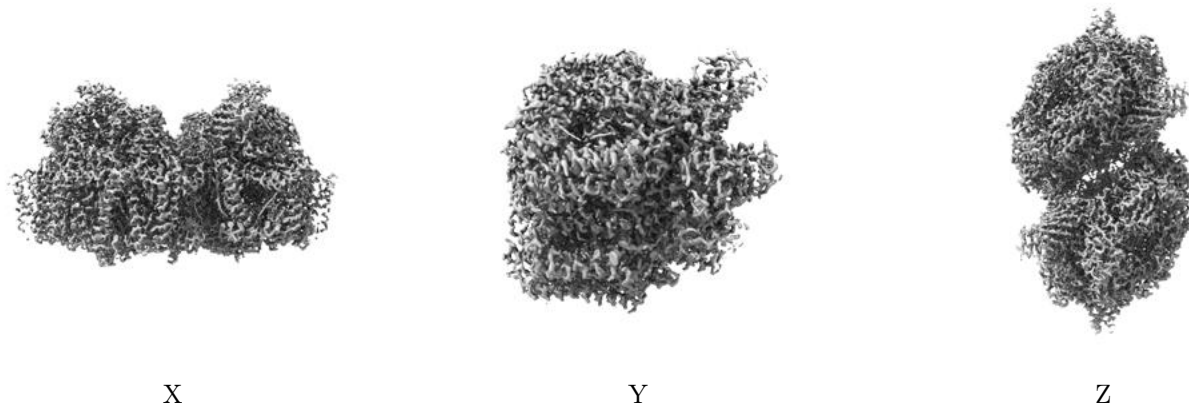


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

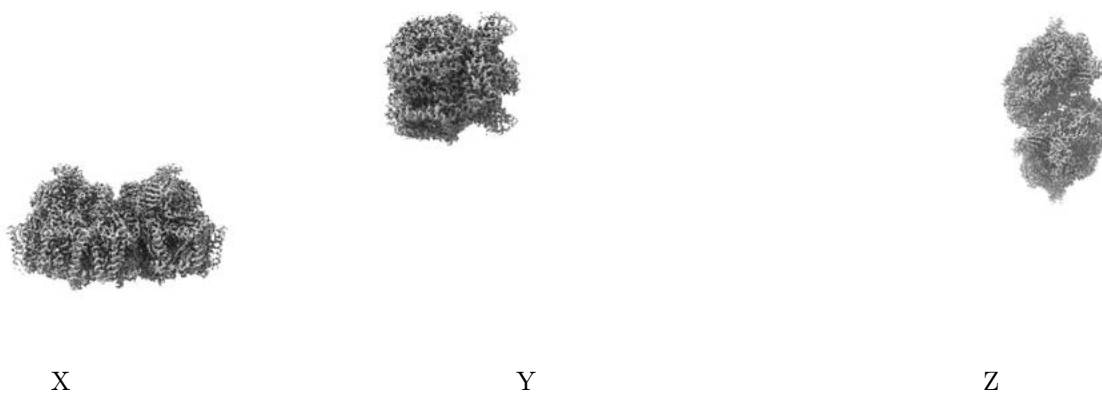
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

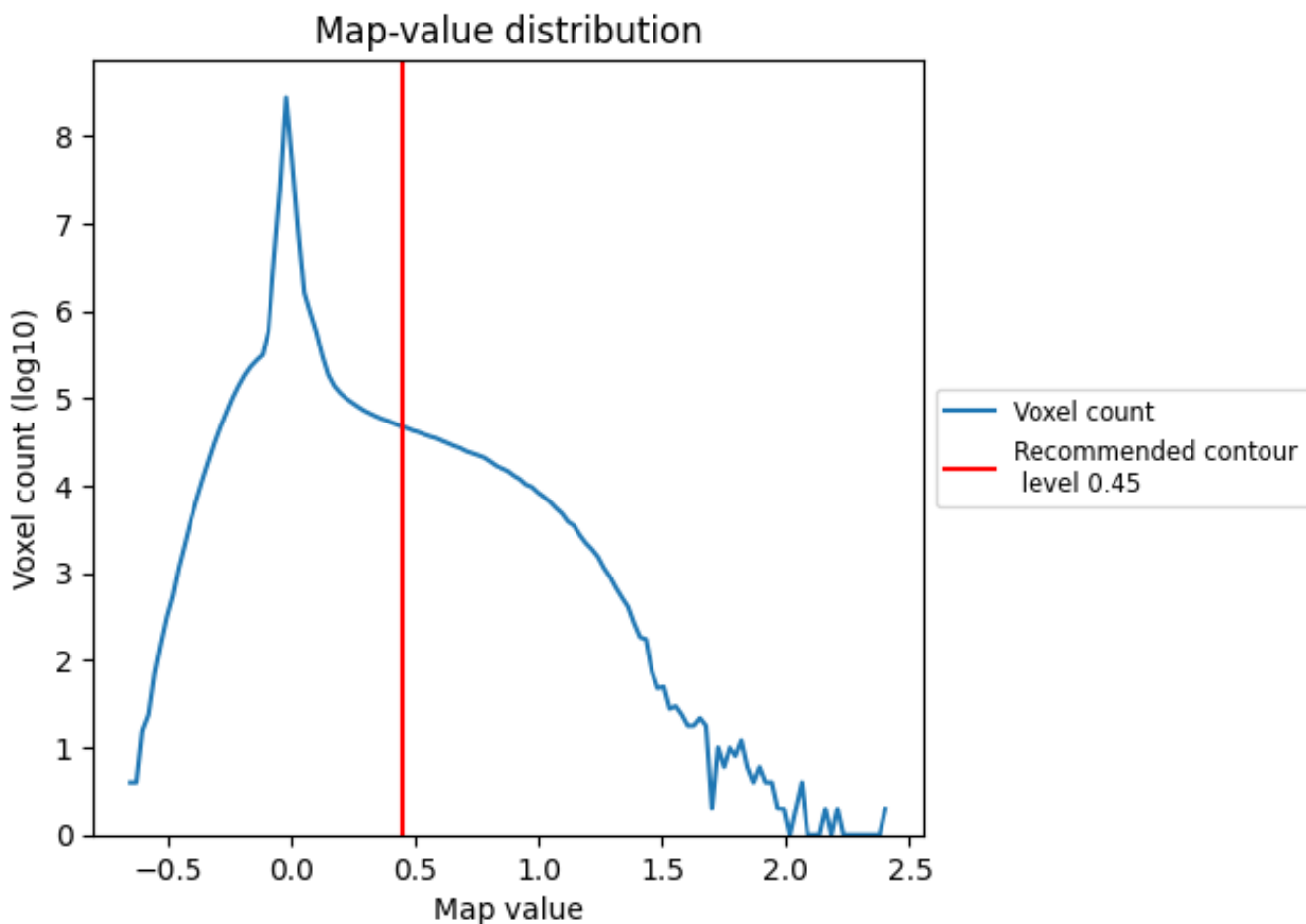
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

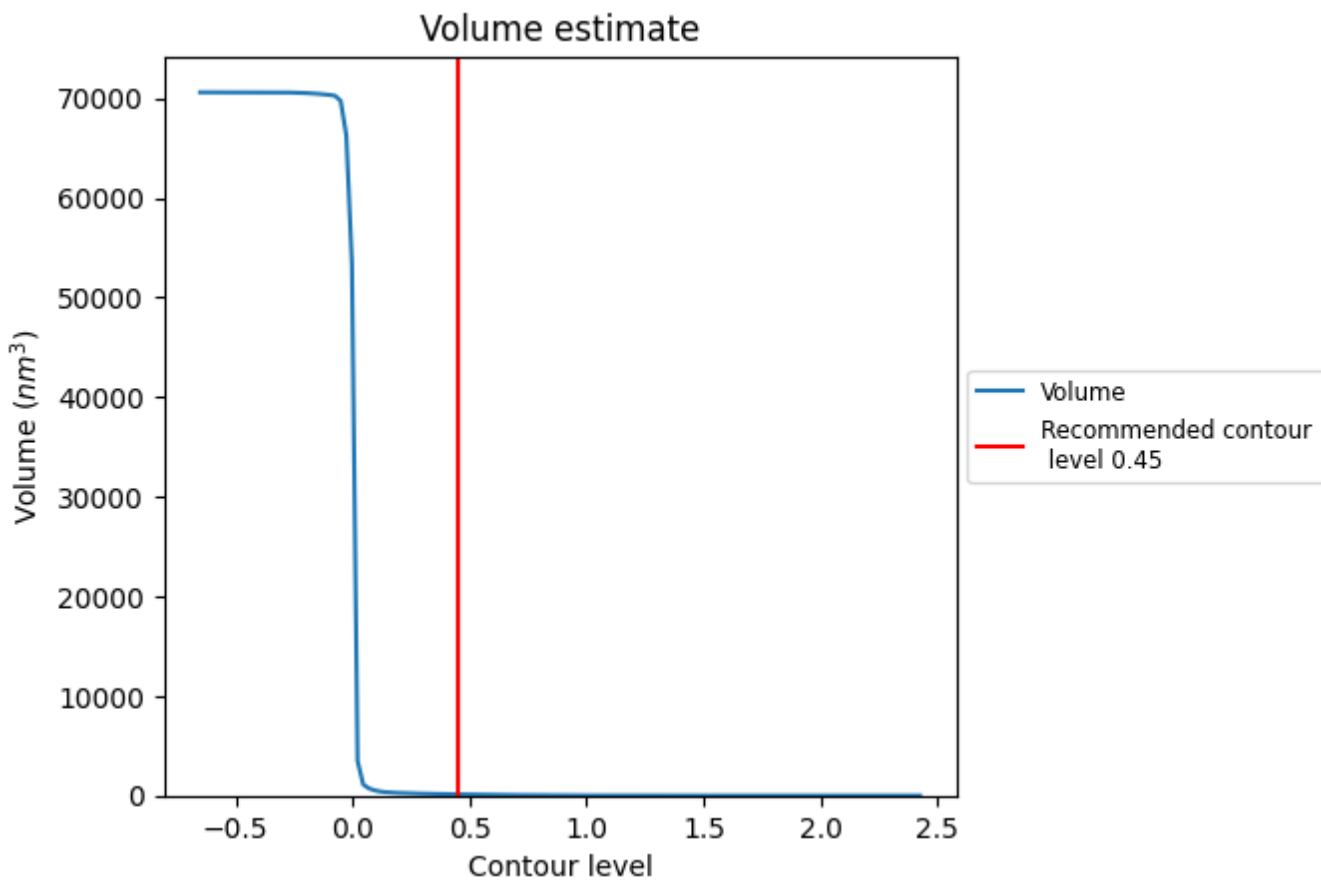
This section contains the results of statistical analysis of the map.

### 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.

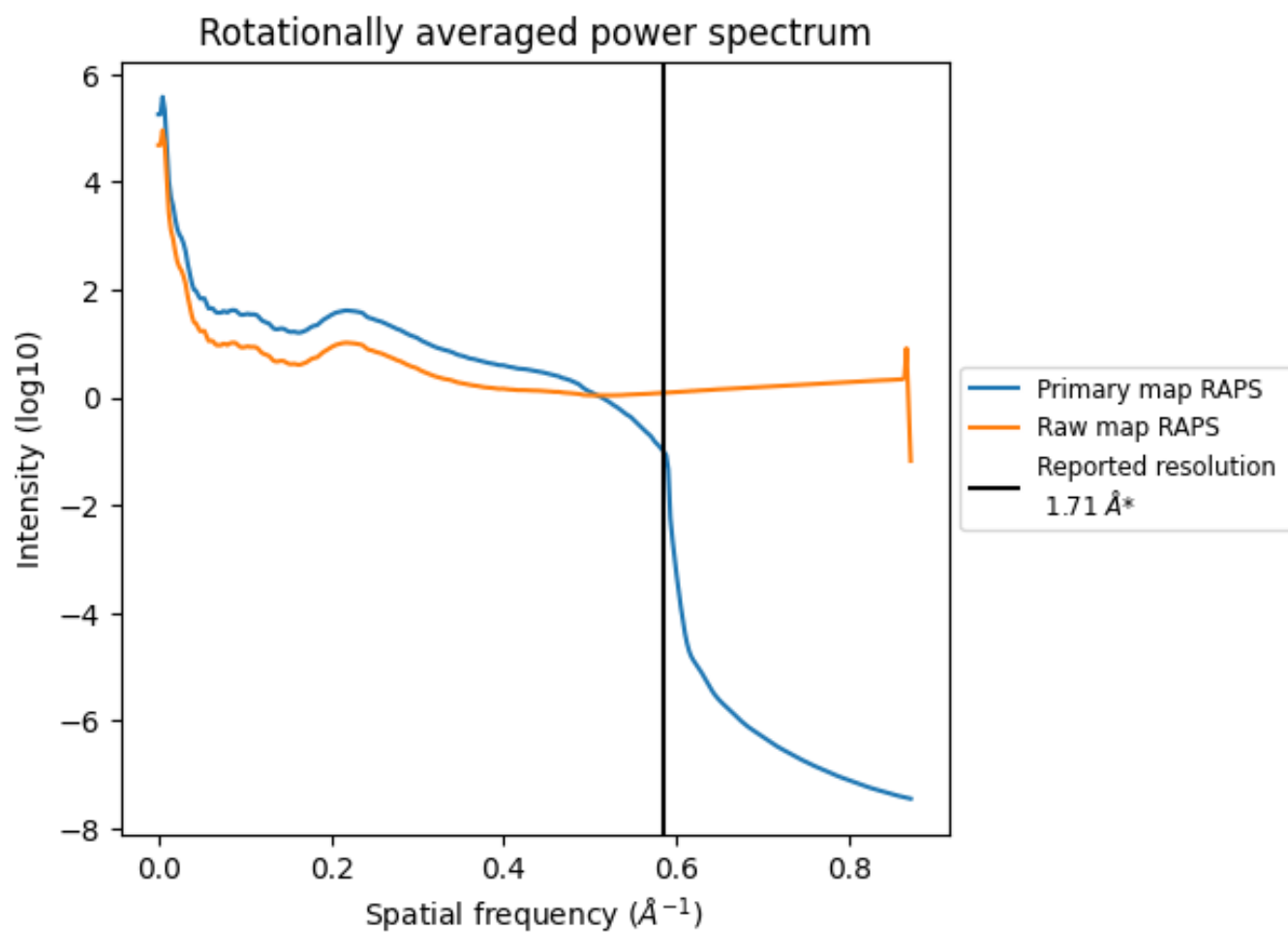
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm<sup>3</sup>; this corresponds to an approximate mass of 109 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

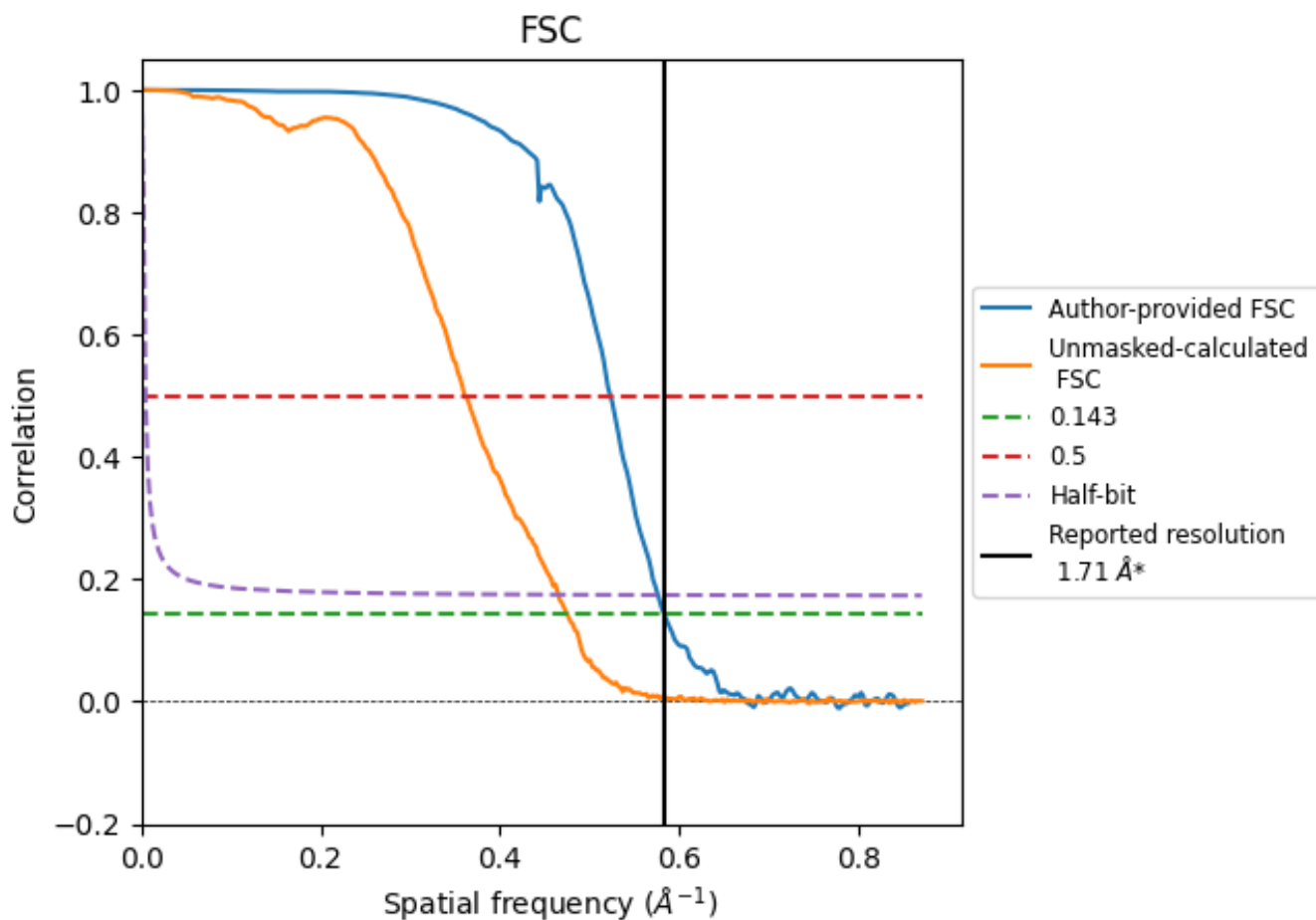


\*Reported resolution corresponds to spatial frequency of 0.585 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.585 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

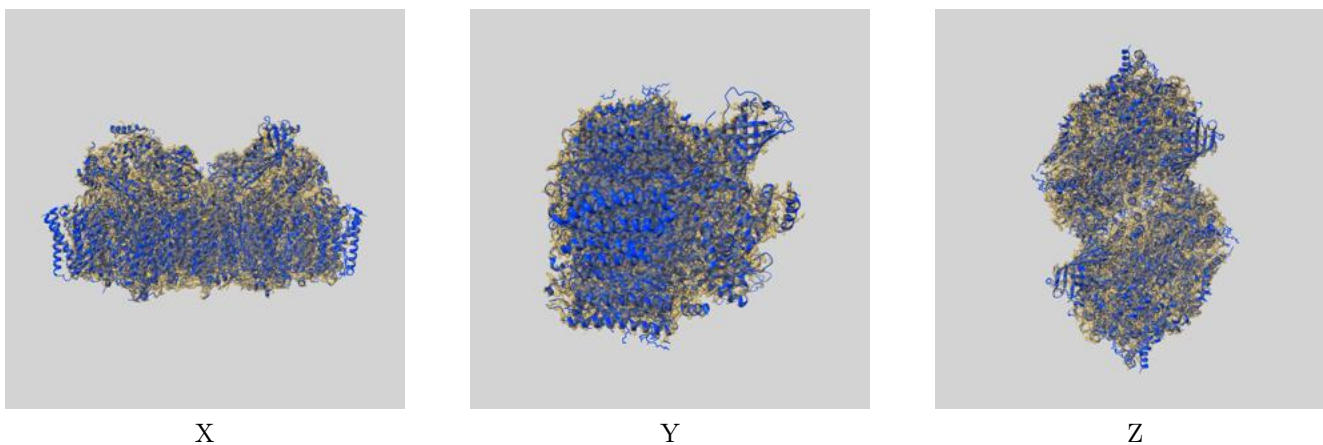
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.71	-	-
Author-provided FSC curve	1.71	1.91	1.73
Unmasked-calculated*	2.10	2.77	2.15

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.10 differs from the reported value 1.71 by more than 10 %

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

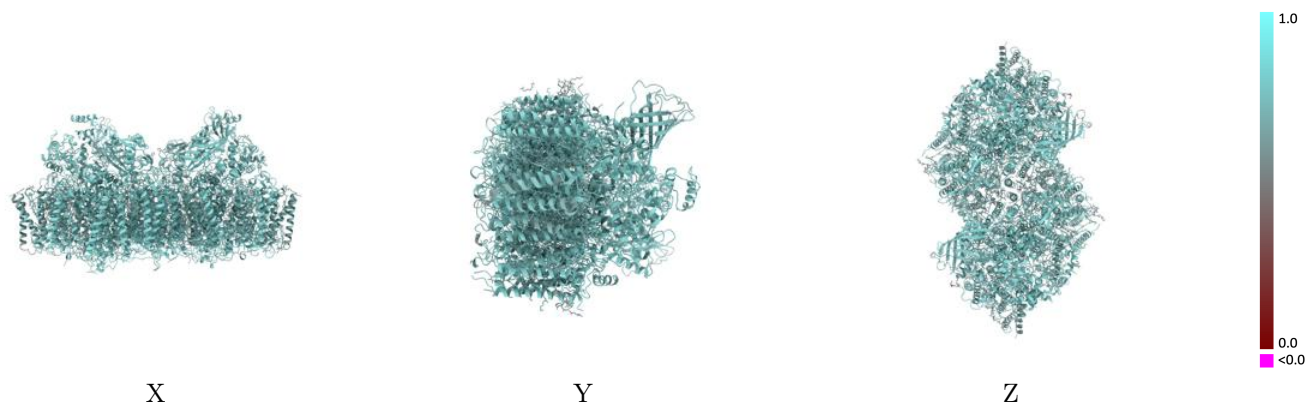
This section contains information regarding the fit between EMDB map EMD-50019 and PDB model 9EVX. Per-residue inclusion information can be found in section 3 on page 29.

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



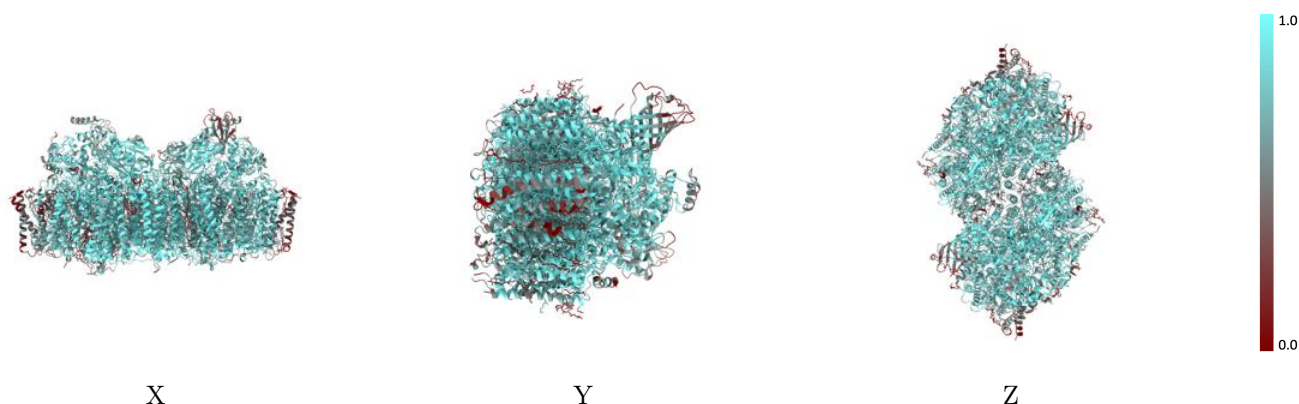
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



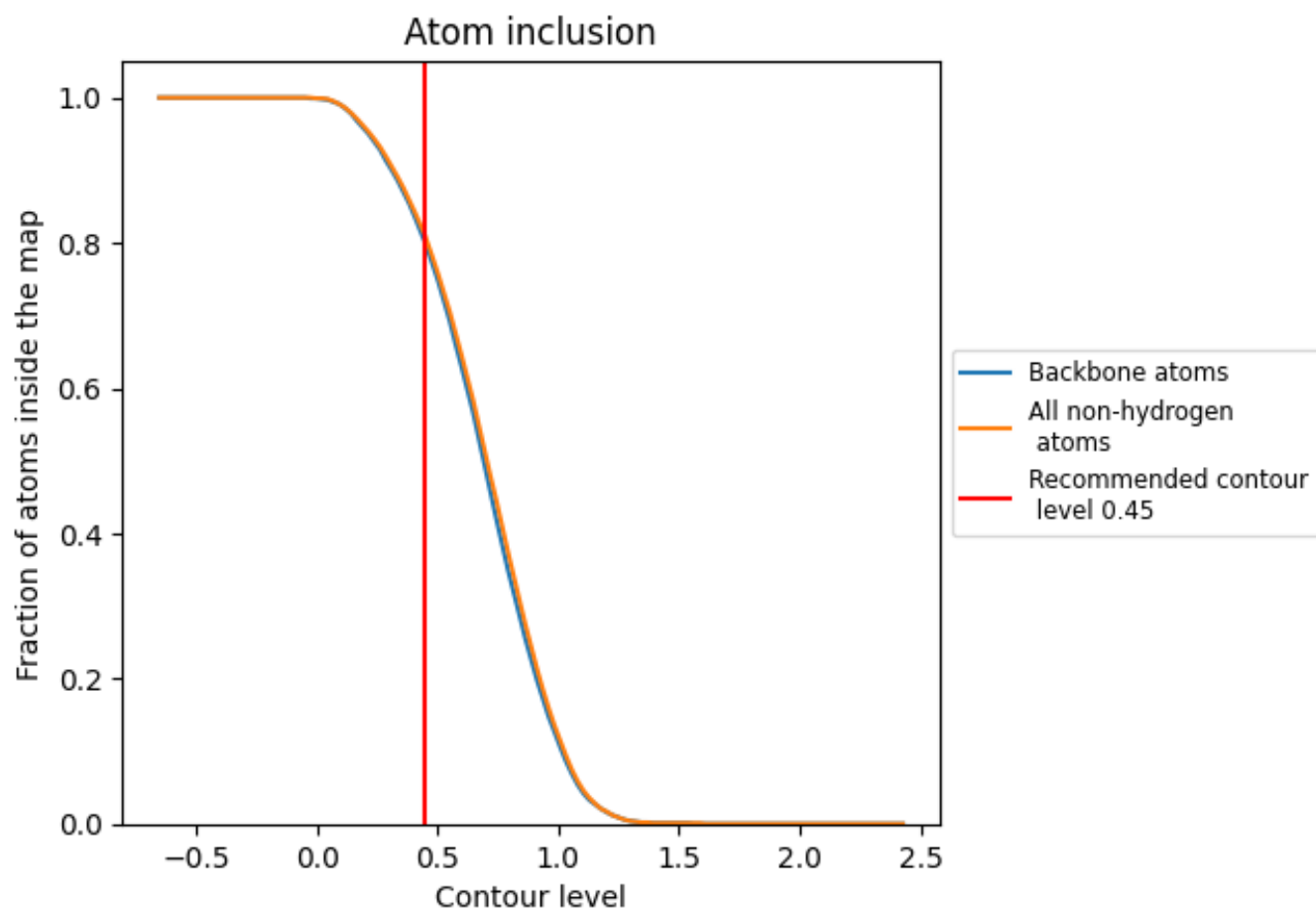
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).







































































## 9.4 Atom inclusion [i](#)

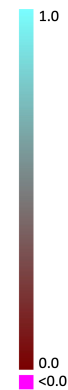


At the recommended contour level, 80% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary









The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.7490
A	 0.8620	 0.7700
B	 0.8650	 0.7580
C	 0.8280	 0.7430
D	 0.9200	 0.7740
E	 0.6740	 0.7180
F	 0.8070	 0.7480
H	 0.7480	 0.7330
I	 0.7760	 0.7400
J	 0.6490	 0.7220
K	 0.7580	 0.7240
L	 0.8560	 0.7730
M	 0.8230	 0.7650
O	 0.6540	 0.7220
T	 0.8380	 0.7700
U	 0.7510	 0.7380
V	 0.7740	 0.7400
X	 0.6100	 0.7120
Y	 0.3950	 0.6670
Z	 0.3280	 0.6400
a	 0.8630	 0.7680
b	 0.8670	 0.7610
c	 0.8290	 0.7420
d	 0.9230	 0.7760
e	 0.6780	 0.7250
f	 0.8550	 0.7490
h	 0.7570	 0.7350
i	 0.7830	 0.7380
j	 0.6700	 0.7280
k	 0.7470	 0.7310
l	 0.8730	 0.7740
m	 0.8230	 0.7690
o	 0.6590	 0.7240
t	 0.8230	 0.7690
u	 0.7500	 0.7460



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Chain	Atom inclusion	Q-score
v	 0.7880	 0.7410
x	 0.6160	 0.7190
y	 0.4200	 0.6760
z	 0.3520	 0.6440