



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 05:02 PM UTC

PDB ID : 7RF3 / pdb_00007rf3
Title : RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.26 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 2.26 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)

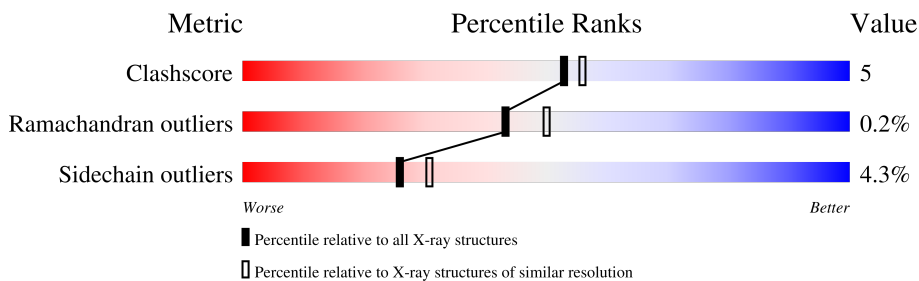
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$









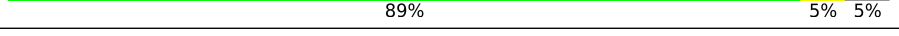

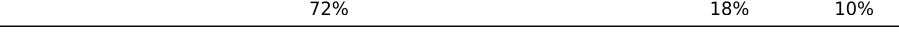
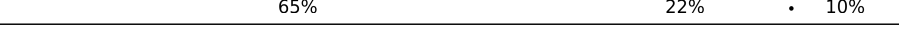

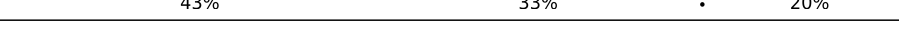


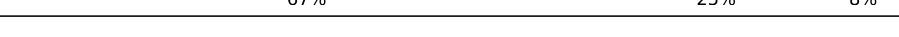

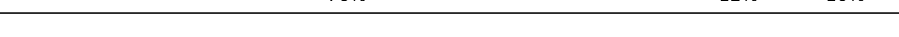






Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	344	86% 10% ..
1	a	344	85% 11% ..
2	B	510	87% 11% ..
2	b	510	87% 11% ..
3	C	461	87% 8% .
3	c	461	87% 10% ..

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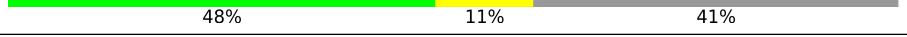


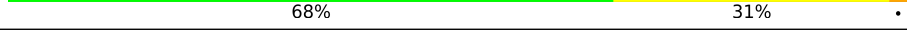
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
4	D	352	 88% 9%
4	d	352	 83% 12%
5	E	84	 86% 11%
5	e	84	 71% 25%
6	F	45	 71% 24%
6	f	45	 62% 9% 24%
7	H	66	 88% 11%
7	h	66	 80% 14% 5%
8	I	38	 89% 5% 5%
8	i	38	 82% 13% 5%
9	J	40	 72% 18% 10%
9	j	40	 65% 22% 10%
10	K	46	 70% 11% 20%
10	k	46	 43% 33% 20%
11	L	37	 89% 11%
11	l	37	 86% 8% 3%
12	M	36	 67% 25% 8%
12	m	36	 72% 14% 11%
13	O	272	 76% 12% 10%
13	o	272	 76% 12% 10%
14	R	41	 49% 20% 32%
14	r	41	 39% 24% 5% 32%
15	T	32	 81% 9% 6%
15	t	32	 84% 9% 6%
16	U	134	 65% 7% 28%

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Mol	Chain	Length	Quality of chain
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	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	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	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	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	411	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	609	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	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	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	d	402	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103278 atoms, of which 51563 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	334	5141	1717	2519	431	459	15	0	0	0
1	a	334	5129	1714	2510	431	459	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	505	7878	2631	3873	666	695	13	0	5	0
2	b	505	7814	2610	3836	665	690	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	442	6781	2249	3355	571	593	13	0	2	0
3	c	451	6926	2290	3426	587	610	13	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	D	341	5338	1800	2621	444	461	12	0	0	0
4	d	341	5350	1804	2627	444	463	12	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	H	65	Total	C	H	N	O	S	0	0	0
			1042	341	532	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
8	I	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
11	L	37	620	202	316	48	53	1	0	0	0
11	l	36	600	197	304	47	52		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
12	M	33	525	171	269	37	47	1	0	0	0
12	m	32	518	168	267	36	46	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
13	O	244	3700	1168	1830	313	385	4	0	1	0
13	o	244	3720	1170	1846	317	383	4	0	0	0

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
14	R	28	459	151	238	38	32	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
15	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
15	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

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

- Molecule 17 is a protein called Cytochrome c-550.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
19	Y	27	Total 413	C 128	H 217	N 35	O 30	S 3	0	0	0
19	y	30	Total 459	C 144	H 241	N 35	O 36	S 3	0	0	0

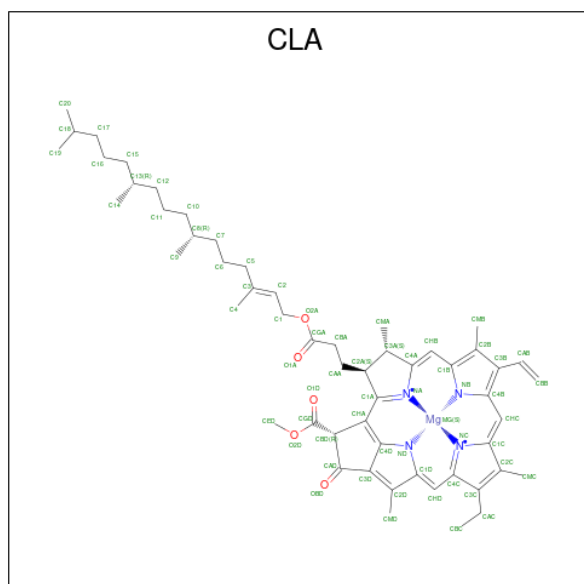
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
20	Z	62	Total 995	C 328	H 516	N 72	O 77	S 2	0	0	0
20	z	62	Total 986	C 326	H 509	N 72	O 77	S 2	0	0	0

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total Fe 1 1	0	0
21	a	1	Total Fe 1 1	0	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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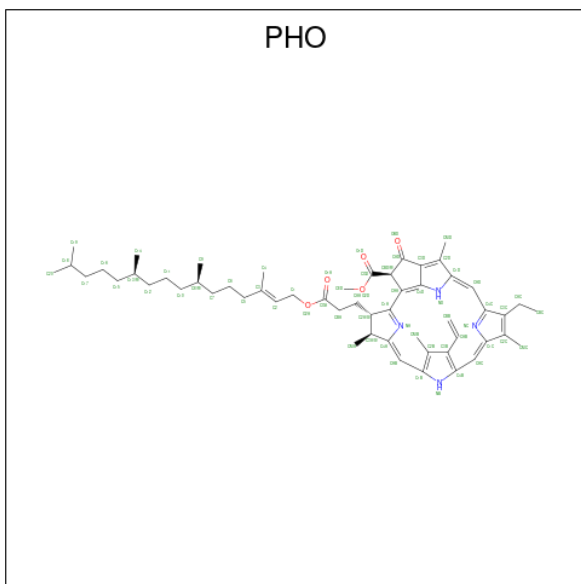
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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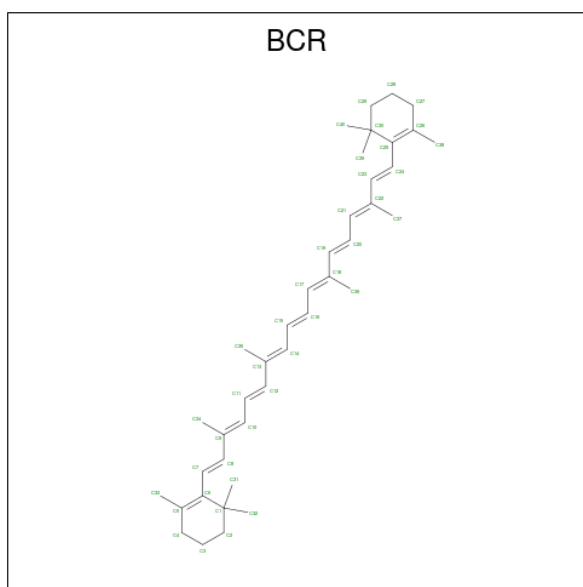
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total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

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	C	1	Total	C	H	0	0
			96	40	56		
24	D	1	Total	C	H	0	0
			96	40	56		
24	H	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	T	1	Total	C	H	0	0
			96	40	56		
24	Z	1	Total	C	H	0	0
			96	40	56		
24	a	1	Total	C	H	0	0
			96	40	56		
24	b	1	Total	C	H	0	0
			96	40	56		
24	b	1	Total	C	H	0	0
			96	40	56		

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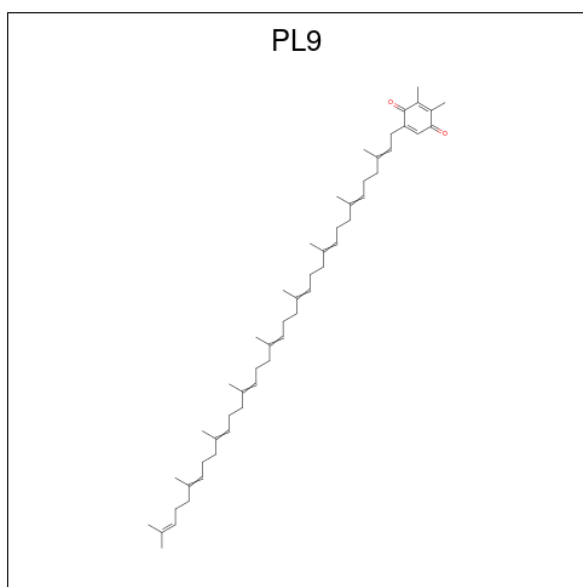
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40	56		
24	x	1	Total	C	H	0	0
			96	40	56		

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

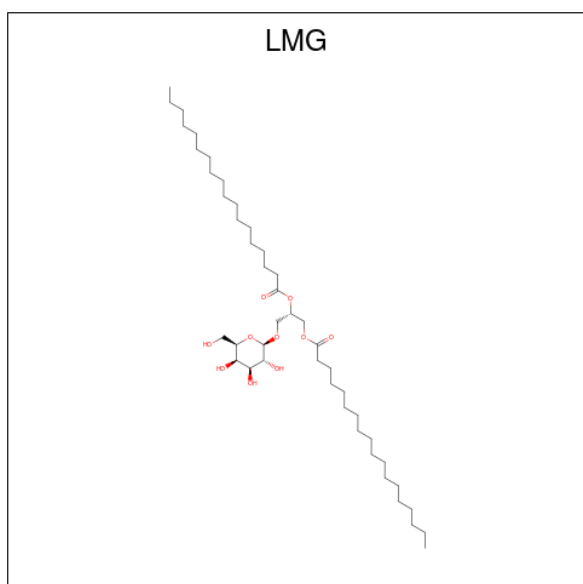
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



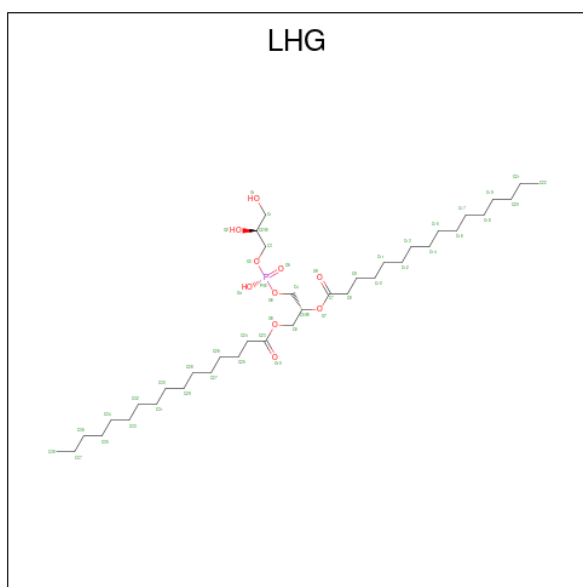
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
26	A	1	135	53	80	2	0	0
26	D	1	135	53	80	2	0	0
26	a	1	135	53	80	2	0	0
26	d	1	135	53	80	2	0	0

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



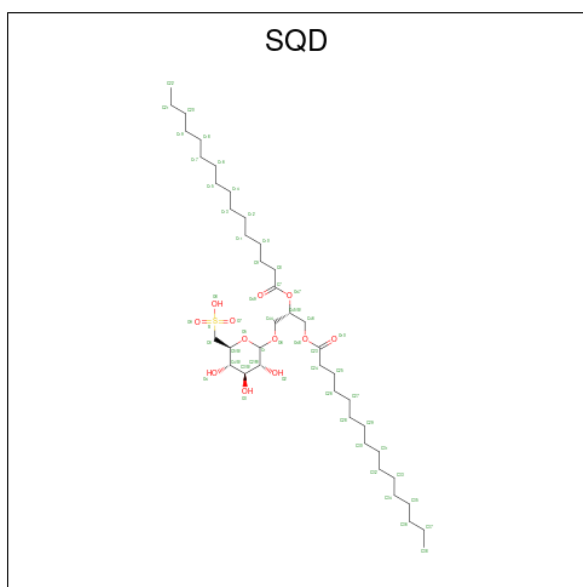
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	d	1	Total	C	H	O	0	0
			57	21	34	2		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



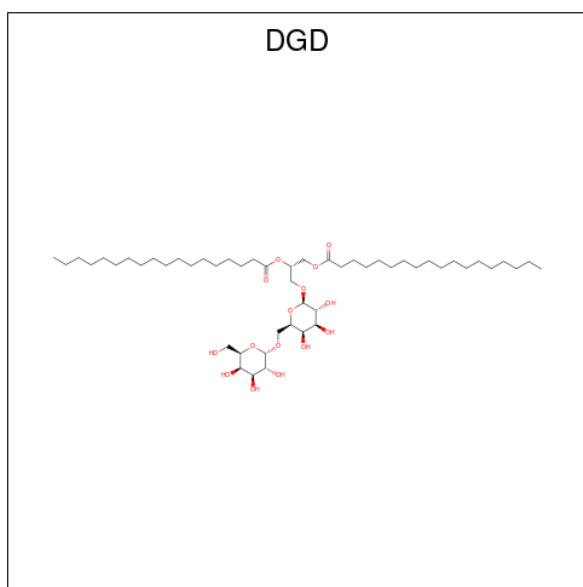
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
28	A	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
28	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	b	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
28	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
28	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



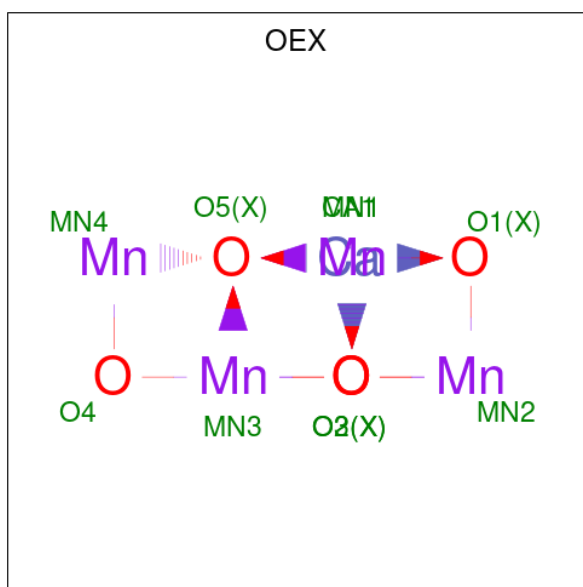
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



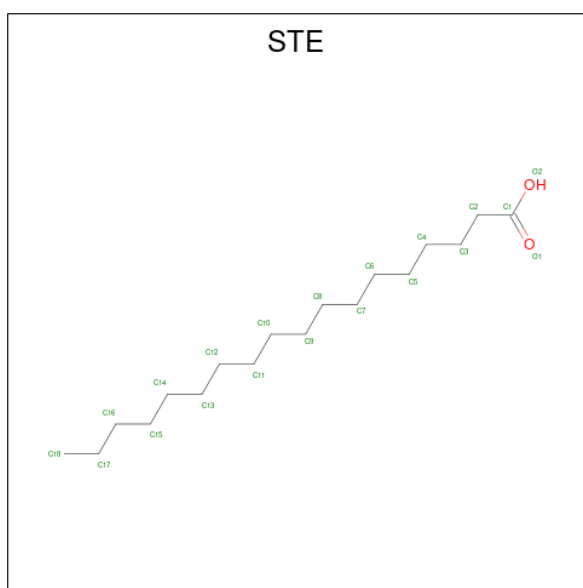
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
30	A	1	Total 162	C 51	H 96	O 15	0	0
30	B	1	Total 119	C 39	H 75	O 5	0	0
30	C	1	Total 144	C 47	H 82	O 15	0	0
30	C	1	Total 143	C 47	H 81	O 15	0	0
30	C	1	Total 144	C 47	H 82	O 15	0	0
30	H	1	Total 144	C 47	H 82	O 15	0	0
30	c	1	Total 144	C 47	H 82	O 15	0	0
30	c	1	Total 144	C 47	H 82	O 15	0	0
30	c	1	Total 144	C 47	H 82	O 15	0	0
30	h	1	Total 144	C 47	H 82	O 15	0	0

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
32	B	1	43	15	26	2	0	0
32	B	1	28	10	16	2	0	0

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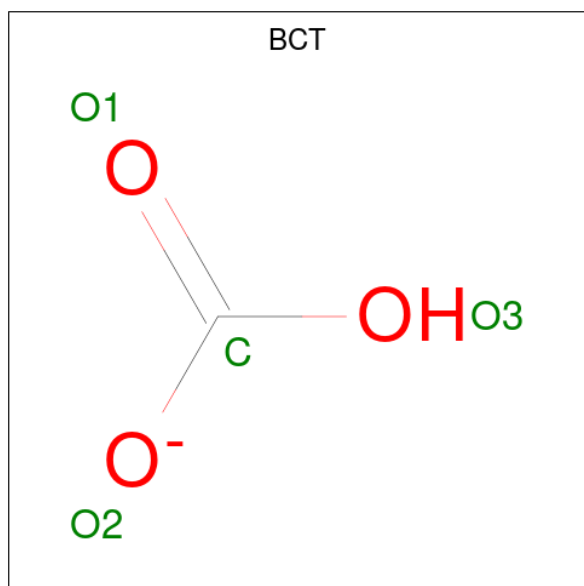
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 46 16 28 2	0	0
32	B	1	Total C H 47 16 31	0	0
32	B	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	D	1	Total C H O 55 18 35 2	0	0
32	E	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 44 15 29	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	c	1	Total C H O 55 18 35 2	0	0

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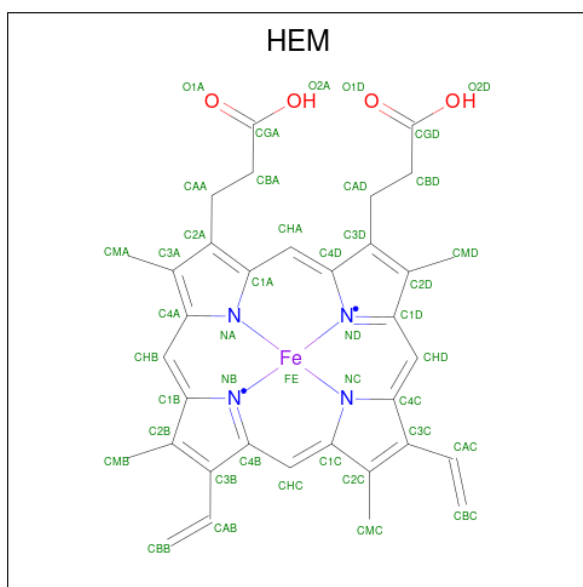
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	k	1	Total	C	H	O	0	0
			28	10	16	2		
32	l	1	Total	C	H		0	0
			53	18	35			
32	m	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H	O	0	0
			34	12	20	2		
32	t	1	Total	C	H		0	0
			26	10	16			
32	x	1	Total	C	H	O	0	0
			55	18	35	2		

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



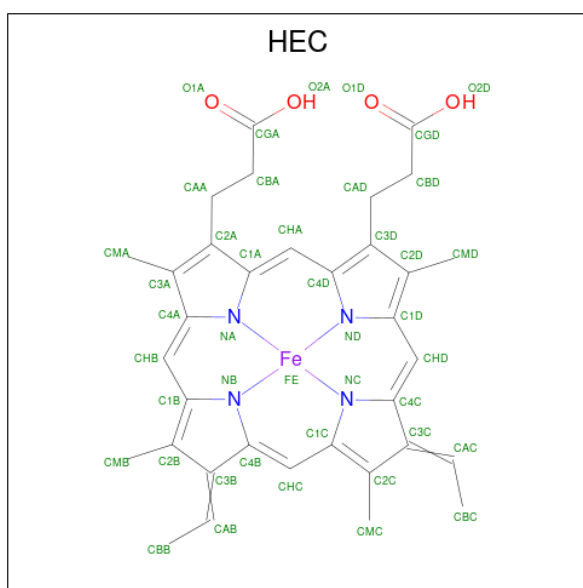
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
34	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
34	e	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
35	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	124	Total O 124 124	0	0
36	B	170	Total O 170 170	0	0
36	C	137	Total O 137 137	0	0
36	D	106	Total O 106 106	0	0
36	E	26	Total O 26 26	0	0
36	F	8	Total O 8 8	0	0
36	H	20	Total O 20 20	0	0
36	I	9	Total O 9 9	0	0
36	J	9	Total O 9 9	0	0
36	K	7	Total O 7 7	0	0
36	L	11	Total O 11 11	0	0
36	M	10	Total O 10 10	0	0
36	O	82	Total O 82 82	0	0
36	R	1	Total O 1 1	0	0
36	T	9	Total O 9 9	0	0
36	U	32	Total O 32 32	0	0
36	V	46	Total O 46 46	0	0
36	X	11	Total O 11 11	0	0
36	Y	3	Total O 3 3	0	0
36	Z	4	Total O 4 4	0	0
36	a	111	Total O 111 111	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	b	140	Total 140	O 140	0	0
36	c	115	Total 115	O 115	0	0
36	d	102	Total 102	O 102	0	0
36	e	19	Total 19	O 19	0	0
36	f	10	Total 10	O 10	0	0
36	h	22	Total 22	O 22	0	0
36	i	10	Total 10	O 10	0	0
36	j	10	Total 10	O 10	0	0
36	k	7	Total 7	O 7	0	0
36	l	7	Total 7	O 7	0	0
36	m	7	Total 7	O 7	0	0
36	o	79	Total 79	O 79	0	0
36	r	12	Total 12	O 12	0	0
36	t	10	Total 10	O 10	0	0
36	u	40	Total 40	O 40	0	0
36	v	39	Total 39	O 39	0	0
36	x	5	Total 5	O 5	0	0
36	y	5	Total 5	O 5	0	0
36	z	6	Total 6	O 6	0	0

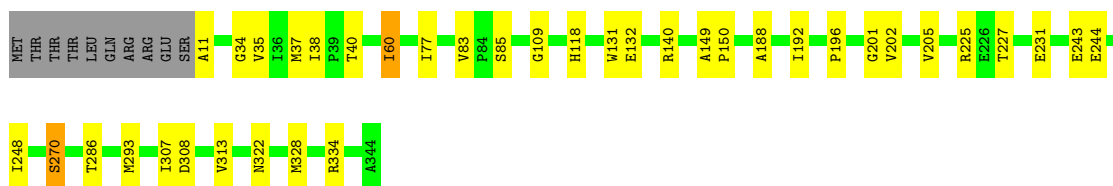
3 Residue-property plots [i](#)

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. 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. 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.


Note EDS failed to run properly.

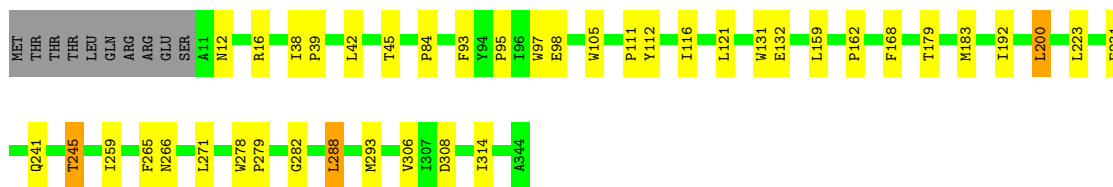
- Molecule 1: Photosystem II protein D1 1

Chain A:  86% 10% ..




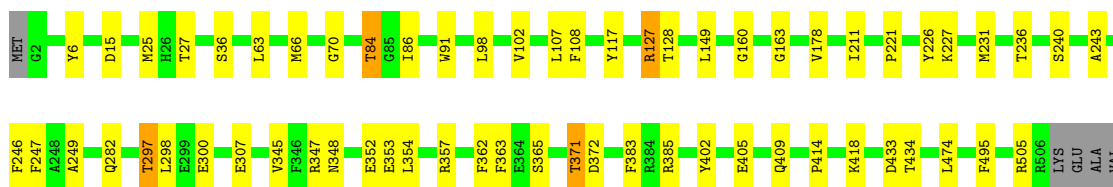
- Molecule 1: Photosystem II protein D1 1

Chain a:  85% 11% ..



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  87% 11% ..



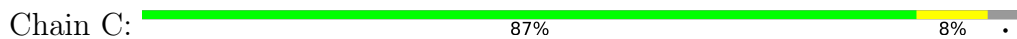
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  87% 11% ..

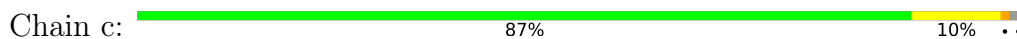




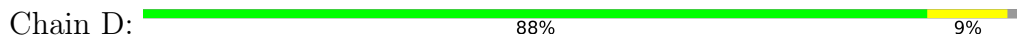
• Molecule 3: Photosystem II CP43 reaction center protein



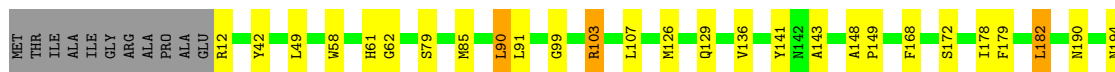
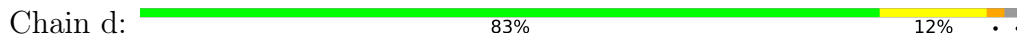
• Molecule 3: Photosystem II CP43 reaction center protein



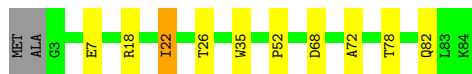
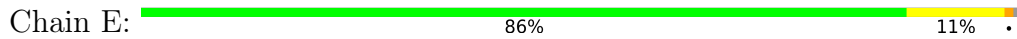
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



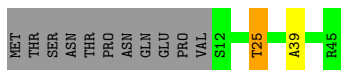
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  71% 25% ..



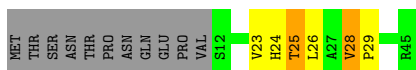
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  71% .. 24%




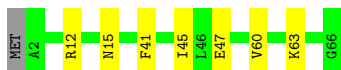
- Molecule 6: Cytochrome b559 subunit beta

Chain f:  62% 9% . 24%




- Molecule 7: Photosystem II reaction center protein H

Chain H:  88% 11% .




- Molecule 7: Photosystem II reaction center protein H

Chain h:  80% 14% . 5%




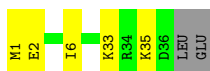
- Molecule 8: Photosystem II reaction center protein I

Chain I:  89% 5% 5%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  82% 13% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  72% 18% 10%



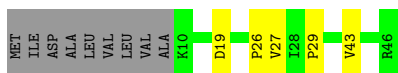
- Molecule 9: Photosystem II reaction center protein J

Chain j:  65% 22% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  70% 11% 20%



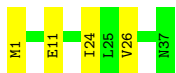
- Molecule 10: Photosystem II reaction center protein K

Chain k:  43% 33% 20%




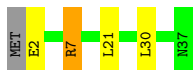
- Molecule 11: Photosystem II reaction center protein L

Chain L:  89% 11%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  86% 8% 8%



- Molecule 12: Photosystem II reaction center protein M

Chain M:  67% 25% 8%




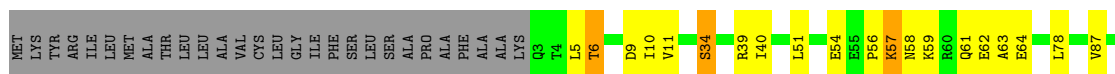
- Molecule 12: Photosystem II reaction center protein M

Chain m:  72% 14% 11%




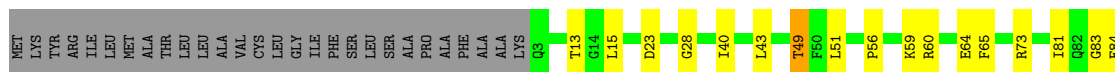
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  76% 12% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  76% 12% 10%

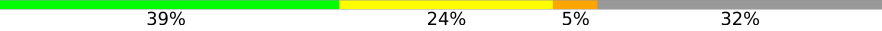


- Molecule 14: Photosystem II protein Y

Chain R:  49% 20% 32%




- Molecule 14: Photosystem II protein Y

Chain r:  39% 24% 5% 32%




- Molecule 15: Photosystem II reaction center protein T

Chain T:  81% 9% 6% 6%

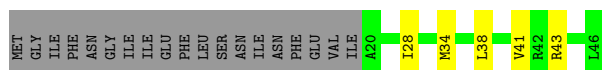


- Molecule 15: Photosystem II reaction center protein T

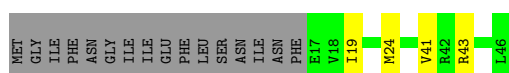
Chain t:  84% 9% 6%



- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 221.64Å 307.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.54 – 2.26	Depositor
% Data completeness (in resolution range)	99.8 (33.54-2.26)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.27Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.178 , 0.238	Depositor
Wilson B-factor (Å ²)	30.1	Xtrriage
Anisotropy	0.248	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	103278	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, PHO, STE, CL, OEX, LMG, HEM, BCR, BCT, FME, HEC, CLA, SQD, PL9, DGD, 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	0.60	1/2707 (0.0%)	0.67	0/3692
1	a	0.58	0/2704	0.65	0/3688
2	B	0.56	0/4161	0.63	0/5669
2	b	0.53	0/4118	0.62	0/5611
3	C	0.54	0/3547	0.62	0/4830
3	c	0.50	0/3619	0.60	0/4926
4	D	0.58	0/2812	0.64	0/3832
4	d	0.56	0/2821	0.65	0/3844
5	E	0.45	0/688	0.54	0/940
5	e	0.43	0/683	0.57	0/932
6	F	0.48	0/284	0.60	0/387
6	f	0.51	0/284	0.62	0/387
7	H	0.59	0/523	0.59	0/713
7	h	0.50	0/511	0.59	0/697
8	I	0.55	0/293	0.65	0/396
8	i	0.55	0/293	0.53	0/396
9	J	0.45	0/263	0.54	0/356
9	j	0.40	0/263	0.55	0/356
10	K	0.44	0/303	0.63	0/416
10	k	0.41	0/303	0.54	0/416
11	L	0.62	0/311	0.62	0/422
11	l	0.60	0/303	0.63	0/412
12	M	0.65	0/249	0.66	0/341
12	m	0.59	0/244	0.64	0/334
13	O	0.54	0/1904	0.65	0/2585
13	o	0.56	0/1905	0.64	0/2583
14	R	0.41	0/227	0.54	0/313
14	r	0.36	0/227	0.45	0/313
15	T	0.60	0/257	0.60	0/349
15	t	0.60	0/255	0.58	0/346
16	U	0.51	0/785	0.60	0/1064
16	u	0.54	0/785	0.64	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.54	0/1085	0.63	0/1473
17	v	0.52	0/1085	0.58	0/1473
18	X	0.45	0/284	0.58	0/384
18	x	0.39	0/289	0.49	0/391
19	Y	0.43	0/197	0.51	0/264
19	y	0.35	0/219	0.47	0/294
20	Z	0.40	0/490	0.50	0/669
20	z	0.35	0/488	0.44	0/666
All	All	0.54	1/42769 (0.0%)	0.62	0/58224

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	V	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ILE	CA-CB	-7.55	1.50	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

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	2622	2519	2519	23	0
1	a	2619	2510	2510	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4005	3873	3867	42	0
2	b	3978	3836	3836	37	0
3	C	3426	3355	3343	25	0
3	c	3500	3426	3426	28	0
4	D	2717	2621	2621	22	0
4	d	2723	2627	2627	31	0
5	E	666	651	651	7	0
5	e	664	648	648	18	0
6	F	275	282	282	2	0
6	f	275	282	282	5	0
7	H	510	532	532	5	0
7	h	498	518	518	5	0
8	I	296	311	311	0	0
8	i	296	311	311	2	0
9	J	257	268	268	5	0
9	j	257	268	268	7	0
10	K	293	305	305	1	0
10	k	293	305	305	12	0
11	L	304	316	316	4	0
11	l	296	304	304	1	0
12	M	256	269	269	9	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	20	0
13	o	1874	1846	1846	21	0
14	R	221	238	238	3	0
14	r	221	238	238	7	0
15	T	258	261	261	5	0
15	t	256	256	256	1	0
16	U	774	773	773	5	0
16	u	774	773	773	5	1
17	V	1064	1071	1073	11	1
17	v	1064	1071	1073	14	0
18	X	281	312	312	4	0
18	x	286	316	314	4	0
19	Y	196	217	217	2	0
19	y	218	241	241	2	0
20	Z	479	516	516	8	0
20	z	477	509	509	11	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	2	0
22	B	1035	1139	1139	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	839	922	922	8	0
22	D	195	216	216	3	0
22	a	260	288	288	2	0
22	b	1035	1139	1139	15	0
22	c	839	919	919	15	0
22	d	130	144	144	4	0
23	A	64	74	74	0	0
23	D	64	74	74	1	0
23	a	64	74	74	1	0
23	d	64	74	74	1	0
24	A	40	56	56	0	0
24	B	120	168	168	4	0
24	C	40	56	56	1	0
24	D	40	56	56	1	0
24	H	40	56	56	0	0
24	K	80	112	112	2	0
24	T	40	56	56	3	0
24	Z	40	56	56	2	0
24	a	40	56	56	1	0
24	b	120	168	168	2	0
24	c	40	56	56	2	0
24	d	40	56	56	3	0
24	k	120	168	168	0	0
24	t	40	56	56	3	0
24	x	40	56	56	1	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	3	0
26	D	55	80	80	1	0
26	a	55	80	80	3	0
26	d	55	80	80	0	0
27	A	48	66	66	3	0
27	C	48	66	66	1	0
27	D	112	157	156	1	0
27	M	51	72	72	1	0
27	a	49	68	68	0	0
27	b	55	86	86	0	0
27	c	85	113	113	1	0
27	d	67	92	92	1	0
27	m	51	72	72	0	0
28	A	47	67	67	2	0
28	B	49	74	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	49	74	74	2	0
28	E	49	74	74	2	0
28	L	49	74	74	6	0
28	b	49	74	74	1	0
28	d	88	125	125	5	0
28	e	42	57	57	3	0
28	l	49	74	74	1	0
29	A	91	135	135	5	0
29	B	54	78	77	1	0
29	F	36	45	45	0	0
29	L	49	65	64	2	0
29	a	90	133	132	6	0
29	f	41	48	48	2	0
30	A	66	96	96	3	0
30	B	44	75	75	4	0
30	C	186	245	243	6	0
30	H	62	82	81	1	0
30	c	186	246	244	4	0
30	h	62	82	81	0	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	B	75	117	114	5	0
32	C	40	63	60	0	0
32	D	20	35	35	3	0
32	E	12	16	16	0	0
32	H	18	35	35	3	0
32	I	15	26	26	1	0
32	J	12	16	16	1	0
32	M	40	67	64	1	0
32	a	12	16	16	0	0
32	b	82	141	138	5	0
32	c	20	35	35	0	0
32	d	17	26	26	0	0
32	j	12	16	16	1	0
32	k	12	16	16	2	0
32	l	18	35	35	1	0
32	m	12	16	16	0	0
32	t	24	36	36	0	0
32	x	20	35	35	2	0
33	D	4	1	1	1	0
33	a	4	1	1	0	0
34	F	43	30	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	e	43	30	30	4	0
35	V	43	30	30	1	0
35	v	43	30	30	0	0
36	A	124	0	0	7	0
36	B	170	0	0	13	0
36	C	137	0	0	4	0
36	D	106	0	0	6	0
36	E	26	0	0	1	0
36	F	8	0	0	0	0
36	H	20	0	0	1	0
36	I	9	0	0	0	0
36	J	9	0	0	1	0
36	K	7	0	0	0	0
36	L	11	0	0	1	0
36	M	10	0	0	2	0
36	O	82	0	0	3	0
36	R	1	0	0	0	0
36	T	9	0	0	4	0
36	U	32	0	0	1	0
36	V	46	0	0	3	0
36	X	11	0	0	0	0
36	Y	3	0	0	0	0
36	Z	4	0	0	0	0
36	a	111	0	0	4	0
36	b	140	0	0	5	0
36	c	115	0	0	1	0
36	d	102	0	0	1	0
36	e	19	0	0	3	0
36	f	10	0	0	0	0
36	h	22	0	0	0	0
36	i	10	0	0	0	0
36	j	10	0	0	1	0
36	k	7	0	0	2	0
36	l	7	0	0	1	0
36	m	7	0	0	0	0
36	o	79	0	0	5	0
36	r	12	0	0	0	0
36	t	10	0	0	0	0
36	u	40	0	0	0	0
36	v	39	0	0	3	0
36	x	5	0	0	0	0
36	y	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	z	6	0	0	0	0
All	All	51715	51563	51525	508	1

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 5.

The worst 5 of 508 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:15:ASP:OD1	36:B:704:HOH:O	1.88	0.92
2:B:354:LEU:O	36:B:702:HOH:O	1.87	0.91
2:B:84:THR:O	36:B:703:HOH:O	1.87	0.91
11:L:11:GLU:OE1	36:L:201:HOH:O	1.88	0.90
1:a:266:ASN:ND2	36:a:501:HOH:O	2.01	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:70:GLU:OE2	16:u:76:ARG:HE[3_457]	1.56	0.04

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 X-ray entries followed by that with respect to entries of similar resolution.

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	332/344 (96%)	327 (98%)	5 (2%)	0	100 100
1	a	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36 40
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100 100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100 100
3	C	442/461 (96%)	431 (98%)	10 (2%)	1 (0%)	43 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	43	50
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	328 (96%)	12 (4%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	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	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	27 (90%)	3 (10%)	0	100	100
13	O	243/272 (89%)	232 (96%)	8 (3%)	3 (1%)	10	7
13	o	242/272 (89%)	229 (95%)	11 (4%)	2 (1%)	16	14
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	8
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	17
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	2	1
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	3
20	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	5231/5700 (92%)	5087 (97%)	132 (2%)	12 (0%)	43	50

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO
3	c	416	SER
16	u	53	ALA

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 X-ray entries followed by that with respect to entries of similar resolution.

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	270/280 (96%)	264 (98%)	6 (2%)	45	56
1	a	269/280 (96%)	260 (97%)	9 (3%)	33	42
2	B	408/407 (100%)	395 (97%)	13 (3%)	34	43
2	b	402/407 (99%)	391 (97%)	11 (3%)	39	49
3	C	346/362 (96%)	339 (98%)	7 (2%)	48	59
3	c	354/362 (98%)	338 (96%)	16 (4%)	24	29
4	D	276/283 (98%)	272 (99%)	4 (1%)	59	70
4	d	277/283 (98%)	262 (95%)	15 (5%)	20	21
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	48
5	e	71/73 (97%)	67 (94%)	4 (6%)	19	20
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	39
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	61
7	h	53/55 (96%)	49 (92%)	4 (8%)	12	11
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	16
8	i	32/34 (94%)	30 (94%)	2 (6%)	16	16
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	20 (83%)	4 (17%)	2	0
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	5
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	12
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	12
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	24
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	35
14	R	22/33 (67%)	19 (86%)	3 (14%)	3	2
14	r	22/33 (67%)	17 (77%)	5 (23%)	1	0
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	36
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	34
16	U	84/112 (75%)	81 (96%)	3 (4%)	31	39
16	u	84/112 (75%)	83 (99%)	1 (1%)	63	74
17	V	117/138 (85%)	109 (93%)	8 (7%)	14	14
17	v	117/138 (85%)	110 (94%)	7 (6%)	17	18
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	6
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	14
19	Y	19/37 (51%)	18 (95%)	1 (5%)	20	22
19	y	22/37 (60%)	21 (96%)	1 (4%)	24	29
20	Z	52/52 (100%)	42 (81%)	10 (19%)	1	0
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	5
All	All	4321/4654 (93%)	4134 (96%)	187 (4%)	26	31

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	416	SER
9	j	7	ARG
4	d	178	ILE
4	d	329	MET
10	k	35	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
5	e	82	GLN
6	f	44	GLN
13	o	61	GLN
13	O	88	ASN
13	O	36	GLN

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	$\# Z > 2$
15	FME	t	1	15	8,9,10	1.17	1 (12%)	8,9,11	0.89	0
12	FME	M	1	12	8,9,10	1.01	0	8,9,11	1.35	2 (25%)
8	FME	I	1	8	8,9,10	1.05	0	8,9,11	0.74	0
15	FME	T	1	15	8,9,10	0.86	0	8,9,11	1.28	1 (12%)
12	FME	m	1	12	8,9,10	1.12	1 (12%)	8,9,11	0.58	0
8	FME	i	1	8	8,9,10	0.88	0	8,9,11	0.92	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
15	FME	t	1	15	-	2/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	4/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.51	1.42	1.46
12	m	1	FME	CA-N	-2.48	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	CB-CA-N	2.38	114.85	110.52
12	M	1	FME	CA-N-CN	-2.37	119.18	122.82
15	T	1	FME	C-CA-N	2.03	113.42	109.50

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	i	1	FME	N-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
15	t	1	FME	O-C-CA-CB
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	i	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 186 ligands modelled in this entry, 6 are monoatomic - leaving 180 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
22	CLA	c	510	-	69,73,73	1.43	8 (11%)	82,113,113	1.39	10 (12%)
24	BCR	c	514	-	41,41,41	1.16	4 (9%)	56,56,56	1.31	6 (10%)
30	DGD	h	101	-	63,63,67	1.22	10 (15%)	77,77,81	1.48	14 (18%)
22	CLA	b	615	-	69,73,73	1.57	11 (15%)	82,113,113	1.28	8 (9%)
32	STE	D	412	-	19,19,19	0.65	0	19,19,19	1.21	0
30	DGD	B	623	-	43,43,67	1.24	6 (13%)	45,45,81	1.27	5 (11%)
22	CLA	b	609	-	69,73,73	1.50	10 (14%)	82,113,113	1.48	9 (10%)
22	CLA	c	504	36	64,68,73	1.24	9 (14%)	76,107,113	1.25	7 (9%)
22	CLA	c	501	-	69,73,73	1.18	9 (13%)	82,113,113	1.48	8 (9%)
22	CLA	a	411	36	69,73,73	1.29	10 (14%)	82,113,113	1.49	11 (13%)
22	CLA	c	505	-	69,73,73	1.08	7 (10%)	82,113,113	1.29	6 (7%)
32	STE	C	519	-	11,11,19	0.81	0	11,11,19	1.42	2 (18%)
24	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	5 (8%)
32	STE	t	103	-	9,9,19	0.41	0	8,8,19	0.64	0
32	STE	j	101	-	11,11,19	0.99	0	11,11,19	0.86	0
22	CLA	a	405	-	69,73,73	1.42	10 (14%)	82,113,113	1.24	8 (9%)
27	LMG	d	408	-	21,21,55	0.69	1 (4%)	20,20,63	1.05	0
29	SQD	L	101	-	47,49,54	0.95	2 (4%)	57,60,65	2.19	16 (28%)
30	DGD	c	515	-	63,63,67	1.14	7 (11%)	77,77,81	1.37	10 (12%)
27	LMG	a	414	-	49,49,55	0.92	2 (4%)	57,57,63	1.36	5 (8%)
22	CLA	B	614	-	69,73,73	1.43	6 (8%)	82,113,113	1.46	11 (13%)
28	LHG	L	102	-	48,48,48	0.92	2 (4%)	51,54,54	1.18	4 (7%)
24	BCR	B	617	-	41,41,41	1.29	4 (9%)	56,56,56	1.31	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	c	520	-	48,48,55	1.10	5 (10%)	56,56,63	1.25	6 (10%)
32	STE	M	103	-	9,9,19	0.40	0	8,8,19	0.74	0
22	CLA	c	512	-	69,73,73	1.29	9 (13%)	82,113,113	1.48	13 (15%)
24	BCR	B	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.12	2 (3%)
27	LMG	A	410	-	48,48,55	0.94	3 (6%)	56,56,63	1.29	5 (8%)
29	SQD	A	412	-	50,52,54	1.06	5 (10%)	60,63,65	1.94	10 (16%)
28	LHG	l	101	-	48,48,48	0.69	0	51,54,54	1.28	5 (9%)
24	BCR	k	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.23	5 (8%)
22	CLA	B	612	-	69,73,73	1.09	4 (5%)	82,113,113	1.37	10 (12%)
32	STE	H	103	-	17,17,19	0.54	0	16,16,19	0.55	0
22	CLA	c	511	3	69,73,73	1.63	11 (15%)	82,113,113	1.30	4 (4%)
32	STE	x	102	-	19,19,19	0.66	0	19,19,19	1.13	1 (5%)
32	STE	a	415	-	11,11,19	0.96	1 (9%)	11,11,19	0.97	1 (9%)
32	STE	M	102	-	14,14,19	0.75	0	14,14,19	1.16	2 (14%)
22	CLA	B	610	36	69,73,73	1.33	8 (11%)	82,113,113	1.27	8 (9%)
22	CLA	B	616	-	64,68,73	1.31	8 (12%)	76,107,113	1.65	9 (11%)
26	PL9	a	410	-	55,55,55	0.85	2 (3%)	68,69,69	1.74	14 (20%)
22	CLA	b	606	-	69,73,73	1.42	6 (8%)	82,113,113	1.52	5 (6%)
22	CLA	C	510	-	69,73,73	1.36	12 (17%)	82,113,113	1.37	8 (9%)
24	BCR	b	619	-	41,41,41	1.23	2 (4%)	56,56,56	1.40	8 (14%)
30	DGD	A	414	-	67,67,67	1.23	8 (11%)	81,81,81	1.32	9 (11%)
32	STE	b	625	-	19,19,19	0.80	1 (5%)	19,19,19	0.87	0
28	LHG	b	623	-	48,48,48	1.02	4 (8%)	51,54,54	1.26	7 (13%)
22	CLA	d	403	-	69,73,73	1.26	10 (14%)	82,113,113	1.13	8 (9%)
32	STE	B	624	-	11,11,19	0.86	0	11,11,19	0.98	0
32	STE	c	519	-	19,19,19	0.61	0	19,19,19	1.21	1 (5%)
22	CLA	C	513	-	69,73,73	1.28	12 (17%)	82,113,113	1.28	10 (12%)
24	BCR	B	619	-	41,41,41	1.32	3 (7%)	56,56,56	1.44	8 (14%)
28	LHG	d	406	-	48,48,48	0.74	1 (2%)	51,54,54	1.27	5 (9%)
22	CLA	B	606	-	69,73,73	1.40	5 (7%)	82,113,113	1.58	7 (8%)
29	SQD	F	102	-	34,36,54	0.95	3 (8%)	42,45,65	2.00	11 (26%)
26	PL9	A	409	-	55,55,55	1.12	2 (3%)	68,69,69	1.66	13 (19%)
22	CLA	b	604	-	69,73,73	1.12	8 (11%)	82,113,113	1.55	9 (10%)
22	CLA	C	507	36	69,73,73	1.12	7 (10%)	82,113,113	1.29	7 (8%)
22	CLA	c	513	-	69,73,73	1.23	10 (14%)	82,113,113	1.23	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	C	514	-	41,41,41	1.27	5 (12%)	56,56,56	1.27	4 (7%)
22	CLA	B	609	-	69,73,73	1.21	9 (13%)	82,113,113	1.30	7 (8%)
32	STE	C	521	-	11,11,19	0.62	0	11,11,19	1.40	3 (27%)
31	OEX	a	416	1,36,3	0,15,15	-	-	-	-	-
34	HEM	F	101	5,6	50,50,50	1.43	7 (14%)	67,82,82	1.09	5 (7%)
26	PL9	D	407	-	55,55,55	1.47	8 (14%)	68,69,69	1.69	14 (20%)
22	CLA	C	501	-	69,73,73	1.46	10 (14%)	82,113,113	1.28	9 (10%)
22	CLA	b	601	36	69,73,73	1.42	6 (8%)	82,113,113	1.47	6 (7%)
27	LMG	D	410	-	31,31,55	0.88	1 (3%)	33,33,63	1.20	2 (6%)
28	LHG	E	101	-	48,48,48	0.97	4 (8%)	51,54,54	1.26	8 (15%)
24	BCR	t	101	-	41,41,41	1.26	3 (7%)	56,56,56	1.32	8 (14%)
28	LHG	B	621	-	48,48,48	1.03	3 (6%)	51,54,54	1.35	7 (13%)
32	STE	J	101	-	11,11,19	0.59	0	11,11,19	1.48	2 (18%)
22	CLA	A	405	-	58,62,73	1.63	8 (13%)	68,99,113	1.46	8 (11%)
24	BCR	K	102	-	41,41,41	1.19	3 (7%)	56,56,56	1.28	6 (10%)
35	HEC	V	201	17	46,50,50	1.74	4 (8%)	58,82,82	2.22	11 (18%)
22	CLA	B	604	-	69,73,73	1.33	9 (13%)	82,113,113	1.66	16 (19%)
32	STE	E	102	-	11,11,19	0.86	0	11,11,19	0.97	1 (9%)
33	BCT	a	409	21	3,3,3	1.35	0	2,3,3	3.77	2 (100%)
27	LMG	c	518	-	37,37,55	0.98	1 (2%)	45,45,63	1.34	7 (15%)
28	LHG	D	409	-	48,48,48	0.81	3 (6%)	51,54,54	1.34	7 (13%)
24	BCR	d	404	-	41,41,41	1.18	2 (4%)	56,56,56	1.20	6 (10%)
29	SQD	a	413	-	35,35,54	1.11	2 (5%)	37,37,65	1.34	4 (10%)
30	DGD	C	515	-	63,63,67	1.26	8 (12%)	77,77,81	1.40	8 (10%)
22	CLA	a	402	-	69,73,73	1.35	11 (15%)	82,113,113	1.24	7 (8%)
32	STE	C	520	-	15,15,19	0.56	0	14,14,19	0.59	0
22	CLA	b	612	-	69,73,73	1.13	6 (8%)	82,113,113	1.27	9 (10%)
22	CLA	C	509	-	69,73,73	1.14	7 (10%)	82,113,113	1.42	10 (12%)
31	OEX	A	415	1,36,3	0,15,15	-	-	-	-	-
22	CLA	C	502	-	69,73,73	1.21	10 (14%)	82,113,113	1.31	11 (13%)
30	DGD	C	516	-	63,63,67	1.24	7 (11%)	77,77,81	1.48	12 (15%)
30	DGD	c	517	-	63,63,67	1.14	6 (9%)	77,77,81	1.50	14 (18%)
22	CLA	B	611	-	69,73,73	1.19	9 (13%)	82,113,113	1.37	11 (13%)
26	PL9	d	405	-	55,55,55	1.46	7 (12%)	68,69,69	1.70	13 (19%)
24	BCR	H	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.36	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	M	104	-	14,14,19	0.41	0	13,13,19	0.83	0
22	CLA	C	503	-	69,73,73	1.50	8 (11%)	82,113,113	1.73	8 (9%)
22	CLA	b	603	-	69,73,73	1.27	11 (15%)	82,113,113	1.52	12 (14%)
24	BCR	A	406	-	41,41,41	1.07	3 (7%)	56,56,56	1.39	11 (19%)
22	CLA	b	608	-	69,73,73	1.19	7 (10%)	82,113,113	1.09	6 (7%)
29	SQD	a	412	-	52,54,54	0.99	3 (5%)	62,65,65	1.85	13 (20%)
22	CLA	c	503	-	69,73,73	1.28	7 (10%)	82,113,113	1.47	7 (8%)
22	CLA	b	607	36	69,73,73	1.22	10 (14%)	82,113,113	1.32	6 (7%)
22	CLA	C	511	3	69,73,73	1.27	9 (13%)	82,113,113	1.34	9 (10%)
22	CLA	b	613	-	69,73,73	1.17	10 (14%)	82,113,113	1.42	12 (14%)
22	CLA	d	402	-	69,73,73	1.24	6 (8%)	82,113,113	1.36	6 (7%)
22	CLA	B	603	-	69,73,73	1.53	7 (10%)	82,113,113	1.40	17 (20%)
22	CLA	b	616	-	64,68,73	1.22	8 (12%)	76,107,113	1.50	9 (11%)
22	CLA	c	508	-	68,72,73	1.30	12 (17%)	80,111,113	1.41	10 (12%)
32	STE	l	102	-	17,17,19	0.43	0	16,16,19	0.79	0
22	CLA	B	602	-	69,73,73	1.40	9 (13%)	82,113,113	1.31	12 (14%)
24	BCR	Z	101	-	41,41,41	1.14	4 (9%)	56,56,56	1.46	10 (17%)
22	CLA	c	509	-	69,73,73	1.64	9 (13%)	82,113,113	1.28	6 (7%)
30	DGD	C	517	-	63,63,67	1.16	6 (9%)	77,77,81	1.34	11 (14%)
27	LMG	M	101	-	51,51,55	0.96	3 (5%)	59,59,63	1.36	6 (10%)
22	CLA	B	605	-	69,73,73	1.25	9 (13%)	82,113,113	1.36	8 (9%)
24	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	6 (10%)
27	LMG	d	409	-	44,44,55	1.05	4 (9%)	52,52,63	1.36	6 (11%)
22	CLA	c	502	-	69,73,73	1.26	11 (15%)	82,113,113	1.25	11 (13%)
32	STE	b	626	-	9,9,19	0.43	0	8,8,19	0.67	0
24	BCR	D	406	-	41,41,41	1.23	2 (4%)	56,56,56	1.16	5 (8%)
28	LHG	e	102	-	41,41,48	0.94	3 (7%)	44,47,54	1.32	4 (9%)
22	CLA	A	402	-	69,73,73	1.41	7 (10%)	82,113,113	1.27	8 (9%)
22	CLA	b	602	-	69,73,73	1.25	8 (11%)	82,113,113	1.51	11 (13%)
24	BCR	x	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
27	LMG	C	518	-	48,48,55	1.05	6 (12%)	56,56,63	1.37	5 (8%)
27	LMG	D	408	-	51,51,55	0.99	4 (7%)	59,59,63	1.27	6 (10%)
23	PHO	A	404	-	58,69,69	1.79	12 (20%)	55,99,99	1.73	13 (23%)
32	STE	I	101	-	14,14,19	0.54	0	13,13,19	0.58	0
22	CLA	a	403	36	69,73,73	1.26	8 (11%)	82,113,113	1.48	14 (17%)
32	STE	B	625	-	17,17,19	0.76	0	17,17,19	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	t	102	-	13,13,19	0.68	0	13,13,19	1.14	1 (7%)
22	CLA	C	505	-	69,73,73	1.39	10 (14%)	82,113,113	1.33	10 (12%)
32	STE	m	102	-	11,11,19	0.65	0	11,11,19	1.28	1 (9%)
22	CLA	B	615	-	69,73,73	1.30	8 (11%)	82,113,113	1.34	10 (12%)
30	DGD	c	516	-	63,63,67	1.08	5 (7%)	77,77,81	1.39	11 (14%)
27	LMG	D	411	-	26,26,55	0.95	2 (7%)	26,26,63	1.34	3 (11%)
22	CLA	B	608	-	69,73,73	1.46	8 (11%)	82,113,113	1.33	13 (15%)
22	CLA	b	614	-	69,73,73	1.49	11 (15%)	82,113,113	1.34	7 (8%)
35	HEC	v	201	17	46,50,50	1.82	7 (15%)	58,82,82	1.95	8 (13%)
24	BCR	b	617	-	41,41,41	1.24	3 (7%)	56,56,56	1.37	8 (14%)
22	CLA	C	504	36	63,67,73	1.24	9 (14%)	74,105,113	1.24	7 (9%)
32	STE	d	410	-	16,16,19	0.65	0	16,16,19	1.04	0
22	CLA	b	605	-	69,73,73	1.17	7 (10%)	82,113,113	1.47	10 (12%)
32	STE	b	624	-	15,15,19	0.93	1 (6%)	15,15,19	0.73	0
22	CLA	B	607	36	69,73,73	1.26	9 (13%)	82,113,113	1.46	10 (12%)
34	HEM	e	101	5,6	50,50,50	1.43	7 (14%)	67,82,82	1.21	6 (8%)
22	CLA	D	404	36	69,73,73	1.14	4 (5%)	82,113,113	1.30	7 (8%)
27	LMG	m	101	-	51,51,55	1.09	4 (7%)	59,59,63	1.47	8 (13%)
23	PHO	d	401	-	58,69,69	2.03	11 (18%)	55,99,99	1.52	9 (16%)
24	BCR	b	618	-	41,41,41	1.34	5 (12%)	56,56,56	1.32	10 (17%)
24	BCR	k	103	-	41,41,41	1.04	2 (4%)	56,56,56	1.17	7 (12%)
22	CLA	A	403	36	69,73,73	1.27	10 (14%)	82,113,113	1.19	10 (12%)
28	LHG	d	407	-	38,38,48	0.84	2 (5%)	41,44,54	1.21	2 (4%)
29	SQD	A	413	-	38,38,54	1.06	3 (7%)	40,40,65	1.54	6 (15%)
24	BCR	T	101	-	41,41,41	1.26	5 (12%)	56,56,56	1.34	5 (8%)
33	BCT	D	402	21	3,3,3	1.16	0	2,3,3	2.80	1 (50%)
32	STE	b	620	-	15,15,19	0.56	0	14,14,19	0.70	0
23	PHO	a	404	-	58,69,69	1.97	12 (20%)	55,99,99	1.60	9 (16%)
32	STE	k	104	-	11,11,19	0.96	1 (9%)	11,11,19	1.15	1 (9%)
22	CLA	C	506	-	69,73,73	1.21	7 (10%)	82,113,113	1.15	8 (9%)
22	CLA	b	610	36	69,73,73	1.26	9 (13%)	82,113,113	1.29	10 (12%)
22	CLA	c	507	36	69,73,73	1.40	9 (13%)	82,113,113	1.28	6 (7%)
27	LMG	b	622	-	55,55,55	1.13	6 (10%)	63,63,63	1.46	8 (12%)
29	SQD	B	622	-	52,54,54	0.98	3 (5%)	62,65,65	1.89	13 (20%)
30	DGD	H	102	-	63,63,67	1.43	14 (22%)	77,77,81	1.38	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	B	627	-	11,11,19	0.78	0	11,11,19	1.09	1 (9%)
22	CLA	C	508	-	69,73,73	1.45	9 (13%)	82,113,113	1.24	9 (10%)
22	CLA	D	405	-	69,73,73	1.67	8 (11%)	82,113,113	1.45	14 (17%)
22	CLA	c	506	-	69,73,73	1.25	9 (13%)	82,113,113	1.19	6 (7%)
24	BCR	a	406	-	41,41,41	1.11	4 (9%)	56,56,56	1.17	2 (3%)
22	CLA	B	601	36	69,73,73	1.62	9 (13%)	82,113,113	1.27	5 (6%)
32	STE	B	626	-	15,15,19	0.47	0	14,14,19	0.72	0
22	CLA	C	512	-	69,73,73	1.27	5 (7%)	82,113,113	1.50	11 (13%)
23	PHO	D	401	-	58,69,69	2.07	12 (20%)	55,99,99	1.41	8 (14%)
32	STE	B	620	-	16,16,19	0.86	1 (6%)	16,16,19	0.87	1 (6%)
22	CLA	B	613	-	69,73,73	1.32	10 (14%)	82,113,113	1.34	9 (10%)
22	CLA	D	403	-	69,73,73	1.23	7 (10%)	82,113,113	1.44	9 (10%)
22	CLA	b	611	-	69,73,73	1.25	8 (11%)	82,113,113	1.43	8 (9%)
28	LHG	A	411	-	46,46,48	1.02	3 (6%)	49,52,54	1.25	3 (6%)
29	SQD	f	101	-	39,41,54	1.13	4 (10%)	49,52,65	1.77	9 (18%)
32	STE	b	621	-	19,19,19	0.68	0	19,19,19	0.90	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
22	CLA	c	510	-	1/1/20/20	9/39/115/115	-
24	BCR	c	514	-	-	4/29/63/63	0/2/2/2
30	DGD	h	101	-	-	16/51/91/95	0/2/2/2
22	CLA	b	615	-	1/1/20/20	9/39/115/115	-
32	STE	D	412	-	-	10/17/17/17	-
30	DGD	B	623	-	-	24/45/45/95	-
22	CLA	b	609	-	1/1/20/20	6/39/115/115	-
22	CLA	c	504	36	1/1/19/20	11/33/109/115	-
22	CLA	c	501	-	1/1/20/20	3/39/115/115	-
22	CLA	a	411	36	1/1/20/20	12/39/115/115	-
22	CLA	c	505	-	1/1/20/20	9/39/115/115	-
32	STE	C	519	-	-	6/9/9/17	-
24	BCR	k	101	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	t	103	-	-	4/7/7/17	-
32	STE	j	101	-	-	2/9/9/17	-
22	CLA	a	405	-	1/1/20/20	10/39/115/115	-
27	LMG	d	408	-	-	9/17/17/70	-
29	SQD	L	101	-	-	26/44/64/69	0/1/1/1
30	DGD	c	515	-	-	25/51/91/95	0/2/2/2
27	LMG	a	414	-	-	21/44/64/70	0/1/1/1
22	CLA	B	614	-	1/1/20/20	12/39/115/115	-
28	LHG	L	102	-	-	20/53/53/53	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
27	LMG	c	520	-	-	26/43/63/70	0/1/1/1
32	STE	M	103	-	-	3/7/7/17	-
22	CLA	c	512	-	1/1/20/20	20/39/115/115	-
24	BCR	B	618	-	-	6/29/63/63	0/2/2/2
27	LMG	A	410	-	-	24/43/63/70	0/1/1/1
29	SQD	A	412	-	-	17/47/67/69	0/1/1/1
28	LHG	l	101	-	-	18/53/53/53	-
24	BCR	k	102	-	-	12/29/63/63	0/2/2/2
22	CLA	B	612	-	1/1/20/20	9/39/115/115	-
32	STE	H	103	-	-	10/15/15/17	-
22	CLA	c	511	3	1/1/20/20	12/39/115/115	-
32	STE	x	102	-	-	13/17/17/17	-
32	STE	a	415	-	-	3/9/9/17	-
32	STE	M	102	-	-	4/12/12/17	-
22	CLA	B	610	36	1/1/20/20	4/39/115/115	-
22	CLA	B	616	-	1/1/19/20	8/33/109/115	-
26	PL9	a	410	-	-	26/53/73/73	0/1/1/1
22	CLA	b	606	-	1/1/20/20	9/39/115/115	-
22	CLA	C	510	-	1/1/20/20	8/39/115/115	-
24	BCR	b	619	-	-	14/29/63/63	0/2/2/2
30	DGD	A	414	-	-	27/55/95/95	0/2/2/2
32	STE	b	625	-	-	5/17/17/17	-
28	LHG	b	623	-	-	24/53/53/53	-
22	CLA	d	403	-	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	B	624	-	-	6/9/9/17	-
32	STE	c	519	-	-	12/17/17/17	-
22	CLA	C	513	-	-	16/39/115/115	-
24	BCR	B	619	-	-	6/29/63/63	0/2/2/2
28	LHG	d	406	-	-	20/53/53/53	-
22	CLA	B	606	-	1/1/20/20	10/39/115/115	-
29	SQD	F	102	-	-	11/28/48/69	0/1/1/1
26	PL9	A	409	-	-	25/53/73/73	0/1/1/1
22	CLA	b	604	-	1/1/20/20	8/39/115/115	-
22	CLA	C	507	36	1/1/20/20	9/39/115/115	-
22	CLA	c	513	-	1/1/20/20	9/39/115/115	-
24	BCR	C	514	-	-	6/29/63/63	0/2/2/2
22	CLA	B	609	-	-	4/39/115/115	-
32	STE	C	521	-	-	1/9/9/17	-
34	HEM	F	101	5,6	-	3/14/54/54	-
26	PL9	D	407	-	-	6/53/73/73	0/1/1/1
22	CLA	C	501	-	1/1/20/20	3/39/115/115	-
22	CLA	b	601	36	1/1/20/20	17/39/115/115	-
27	LMG	D	410	-	-	17/33/33/70	-
28	LHG	E	101	-	-	24/53/53/53	-
24	BCR	t	101	-	-	8/29/63/63	0/2/2/2
28	LHG	B	621	-	-	16/53/53/53	-
32	STE	J	101	-	-	5/9/9/17	-
22	CLA	A	405	-	1/1/17/20	6/26/102/115	-
24	BCR	K	102	-	-	4/29/63/63	0/2/2/2
35	HEC	V	201	17	-	6/14/54/54	-
22	CLA	B	604	-	1/1/20/20	11/39/115/115	-
32	STE	E	102	-	-	7/9/9/17	-
27	LMG	c	518	-	-	8/31/51/70	0/1/1/1
28	LHG	D	409	-	-	19/53/53/53	-
24	BCR	d	404	-	-	5/29/63/63	0/2/2/2
29	SQD	a	413	-	-	16/37/37/69	-
30	DGD	C	515	-	-	22/51/91/95	0/2/2/2
22	CLA	a	402	-	1/1/20/20	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	C	520	-	-	4/13/13/17	-
22	CLA	b	612	-	1/1/20/20	15/39/115/115	-
22	CLA	C	509	-	1/1/20/20	7/39/115/115	-
22	CLA	C	502	-	1/1/20/20	6/39/115/115	-
30	DGD	C	516	-	-	25/51/91/95	0/2/2/2
30	DGD	c	517	-	-	19/51/91/95	0/2/2/2
22	CLA	B	611	-	1/1/20/20	6/39/115/115	-
26	PL9	d	405	-	-	18/53/73/73	0/1/1/1
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
32	STE	M	104	-	-	8/12/12/17	-
22	CLA	C	503	-	1/1/20/20	4/39/115/115	-
22	CLA	b	603	-	1/1/20/20	13/39/115/115	-
24	BCR	A	406	-	-	3/29/63/63	0/2/2/2
22	CLA	b	608	-	-	7/39/115/115	-
29	SQD	a	412	-	-	22/49/69/69	0/1/1/1
22	CLA	c	503	-	1/1/20/20	11/39/115/115	-
22	CLA	b	607	36	1/1/20/20	12/39/115/115	-
22	CLA	C	511	3	1/1/20/20	11/39/115/115	-
22	CLA	b	613	-	1/1/20/20	8/39/115/115	-
22	CLA	d	402	-	1/1/20/20	7/39/115/115	-
22	CLA	B	603	-	1/1/20/20	10/39/115/115	-
22	CLA	b	616	-	1/1/19/20	8/33/109/115	-
22	CLA	c	508	-	1/1/19/20	13/38/114/115	-
32	STE	l	102	-	-	13/15/15/17	-
22	CLA	B	602	-	1/1/20/20	9/39/115/115	-
24	BCR	Z	101	-	-	10/29/63/63	0/2/2/2
22	CLA	c	509	-	1/1/20/20	16/39/115/115	-
30	DGD	C	517	-	-	12/51/91/95	0/2/2/2
27	LMG	M	101	-	-	27/46/66/70	0/1/1/1
22	CLA	B	605	-	1/1/20/20	10/39/115/115	-
24	BCR	K	101	-	-	11/29/63/63	0/2/2/2
27	LMG	d	409	-	-	12/39/59/70	0/1/1/1
22	CLA	c	502	-	1/1/20/20	15/39/115/115	-
32	STE	b	626	-	-	5/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	D	406	-	-	6/29/63/63	0/2/2/2
28	LHG	e	102	-	-	25/46/46/53	-
22	CLA	A	402	-	1/1/20/20	2/39/115/115	-
22	CLA	b	602	-	1/1/20/20	11/39/115/115	-
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
27	LMG	C	518	-	-	20/43/63/70	0/1/1/1
27	LMG	D	408	-	-	17/46/66/70	0/1/1/1
23	PHO	A	404	-	-	3/37/103/103	0/5/6/6
32	STE	I	101	-	-	7/12/12/17	-
22	CLA	a	403	36	1/1/20/20	14/39/115/115	-
32	STE	B	625	-	-	10/15/15/17	-
32	STE	t	102	-	-	3/11/11/17	-
22	CLA	C	505	-	1/1/20/20	10/39/115/115	-
32	STE	m	102	-	-	4/9/9/17	-
22	CLA	B	615	-	1/1/20/20	7/39/115/115	-
30	DGD	c	516	-	-	21/51/91/95	0/2/2/2
27	LMG	D	411	-	-	15/22/22/70	-
22	CLA	B	608	-	-	2/39/115/115	-
22	CLA	b	614	-	1/1/20/20	21/39/115/115	-
35	HEC	v	201	17	-	6/14/54/54	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
22	CLA	C	504	36	1/1/18/20	10/32/108/115	-
32	STE	d	410	-	-	7/14/14/17	-
22	CLA	b	605	-	1/1/20/20	9/39/115/115	-
32	STE	b	624	-	-	8/13/13/17	-
22	CLA	B	607	36	1/1/20/20	10/39/115/115	-
34	HEM	e	101	5,6	-	1/14/54/54	-
22	CLA	D	404	36	1/1/20/20	5/39/115/115	-
27	LMG	m	101	-	-	23/46/66/70	0/1/1/1
23	PHO	d	401	-	-	6/37/103/103	0/5/6/6
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
24	BCR	k	103	-	-	8/29/63/63	0/2/2/2
22	CLA	A	403	36	1/1/20/20	5/39/115/115	-
28	LHG	d	407	-	-	14/43/43/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	A	413	-	-	13/39/39/69	-
24	BCR	T	101	-	-	11/29/63/63	0/2/2/2
32	STE	b	620	-	-	7/13/13/17	-
23	PHO	a	404	-	-	6/37/103/103	0/5/6/6
32	STE	k	104	-	-	2/9/9/17	-
22	CLA	C	506	-	1/1/20/20	12/39/115/115	-
22	CLA	b	610	36	1/1/20/20	7/39/115/115	-
22	CLA	c	507	36	1/1/20/20	12/39/115/115	-
27	LMG	b	622	-	-	24/50/70/70	0/1/1/1
29	SQD	B	622	-	-	16/49/69/69	0/1/1/1
30	DGD	H	102	-	-	20/51/91/95	0/2/2/2
32	STE	B	627	-	-	7/9/9/17	-
22	CLA	C	508	-	-	5/39/115/115	-
22	CLA	D	405	-	-	9/39/115/115	-
22	CLA	c	506	-	1/1/20/20	13/39/115/115	-
24	BCR	a	406	-	-	5/29/63/63	0/2/2/2
22	CLA	B	601	36	1/1/20/20	19/39/115/115	-
32	STE	B	626	-	-	6/13/13/17	-
22	CLA	C	512	-	1/1/20/20	21/39/115/115	-
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
32	STE	B	620	-	-	8/14/14/17	-
22	CLA	B	613	-	1/1/20/20	14/39/115/115	-
22	CLA	D	403	-	1/1/20/20	7/39/115/115	-
22	CLA	b	611	-	1/1/20/20	10/39/115/115	-
28	LHG	A	411	-	-	22/51/51/53	-
29	SQD	f	101	-	-	12/36/56/69	0/1/1/1
32	STE	b	621	-	-	9/17/17/17	-

The worst 5 of 930 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	C1B-C2B	8.96	1.49	1.39
22	D	405	CLA	MG-NB	-8.64	1.88	2.05
23	D	401	PHO	C3B-C4B	8.45	1.50	1.41
23	D	401	PHO	C1B-C2B	8.45	1.48	1.39
23	a	404	PHO	C1B-C2B	8.38	1.48	1.39

The worst 5 of 1221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	V	201	HEC	CBB-CAB-C3B	-11.03	105.38	127.43
22	C	503	CLA	C4A-NA-C1A	10.19	111.33	106.68
22	B	616	CLA	C4A-NA-C1A	9.47	111.00	106.68
29	a	412	SQD	O6-C1-C2	8.95	121.87	108.27
29	A	412	SQD	O6-C1-C2	8.85	121.72	108.27

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	405	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND

5 of 1926 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	601	CLA	CAD-CBD-CGD-O2D
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

116 monomers are involved in 179 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	510	CLA	2	0
24	c	514	BCR	2	0
22	b	615	CLA	3	0
32	D	412	STE	3	0
30	B	623	DGD	4	0
22	c	501	CLA	2	0
22	a	411	CLA	1	0
32	j	101	STE	1	0
22	a	405	CLA	1	0
27	d	408	LMG	1	0
29	L	101	SQD	2	0
30	c	515	DGD	1	0
22	B	614	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	L	102	LHG	6	0
24	B	617	BCR	1	0
27	c	520	LMG	1	0
22	c	512	CLA	1	0
24	B	618	BCR	2	0
27	A	410	LMG	3	0
29	A	412	SQD	4	0
28	l	101	LHG	1	0
32	H	103	STE	3	0
22	c	511	CLA	5	0
32	x	102	STE	2	0
26	a	410	PL9	3	0
22	b	606	CLA	2	0
22	C	510	CLA	1	0
30	A	414	DGD	3	0
32	b	625	STE	1	0
28	b	623	LHG	1	0
22	d	403	CLA	3	0
32	B	624	STE	2	0
24	B	619	BCR	1	0
28	d	406	LHG	3	0
22	B	606	CLA	3	0
26	A	409	PL9	3	0
22	b	604	CLA	1	0
22	C	507	CLA	1	0
22	c	513	CLA	1	0
24	C	514	BCR	1	0
22	B	609	CLA	1	0
34	F	101	HEM	2	0
26	D	407	PL9	1	0
22	b	601	CLA	2	0
28	E	101	LHG	2	0
24	t	101	BCR	3	0
28	B	621	LHG	4	0
32	J	101	STE	1	0
35	V	201	HEC	1	0
22	B	604	CLA	2	0
28	D	409	LHG	2	0
24	d	404	BCR	3	0
29	a	413	SQD	2	0
22	C	509	CLA	2	0
22	C	502	CLA	1	0

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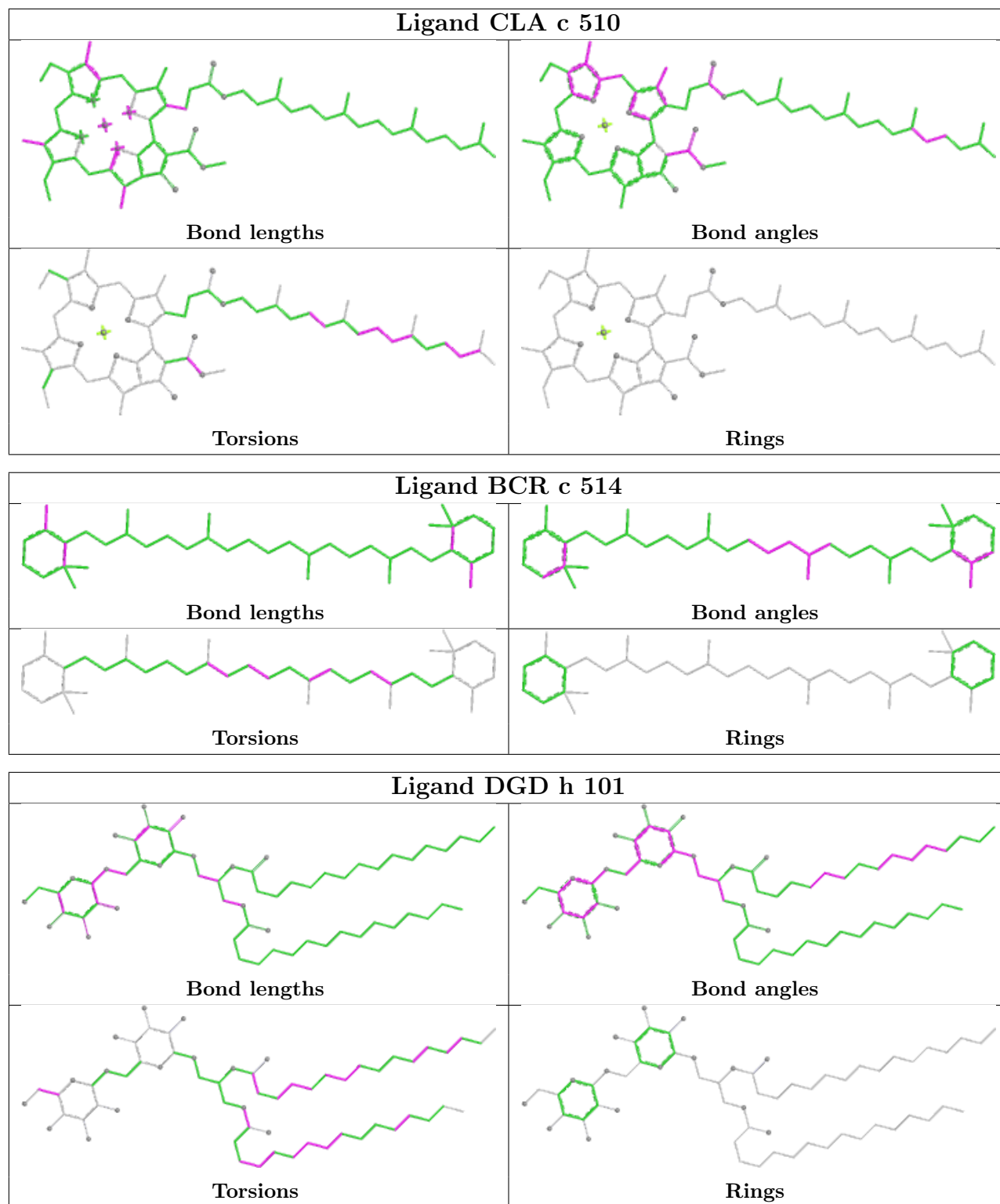
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	B	611	CLA	3	0
32	M	104	STE	1	0
29	a	412	SQD	4	0
22	c	503	CLA	3	0
22	b	607	CLA	1	0
22	C	511	CLA	2	0
22	d	402	CLA	1	0
22	B	603	CLA	2	0
22	b	616	CLA	2	0
22	c	508	CLA	1	0
32	l	102	STE	1	0
22	B	602	CLA	2	0
24	Z	101	BCR	2	0
30	C	517	DGD	2	0
27	M	101	LMG	1	0
22	B	605	CLA	4	0
24	K	101	BCR	2	0
22	c	502	CLA	1	0
32	b	626	STE	1	0
24	D	406	BCR	1	0
28	e	102	LHG	3	0
22	A	402	CLA	1	0
22	b	602	CLA	1	0
24	x	101	BCR	1	0
27	C	518	LMG	1	0
27	D	408	LMG	1	0
32	I	101	STE	1	0
22	B	615	CLA	1	0
30	c	516	DGD	2	0
22	b	614	CLA	2	0
24	b	617	BCR	1	0
22	C	504	CLA	1	0
22	b	605	CLA	2	0
32	b	624	STE	1	0
34	e	101	HEM	4	0
22	D	404	CLA	3	0
23	d	401	PHO	1	0
24	b	618	BCR	1	0
22	A	403	CLA	1	0
28	d	407	LHG	2	0

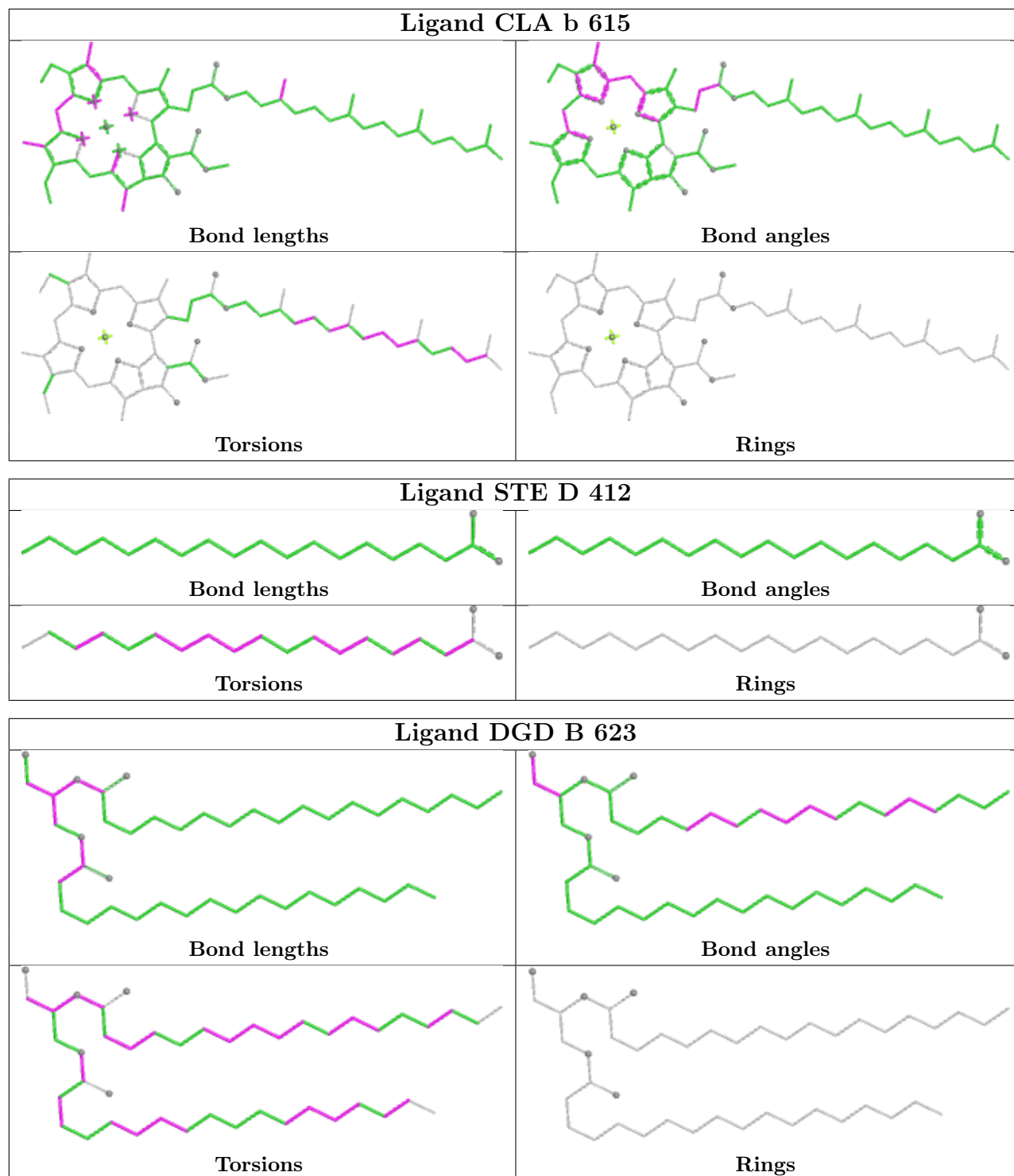
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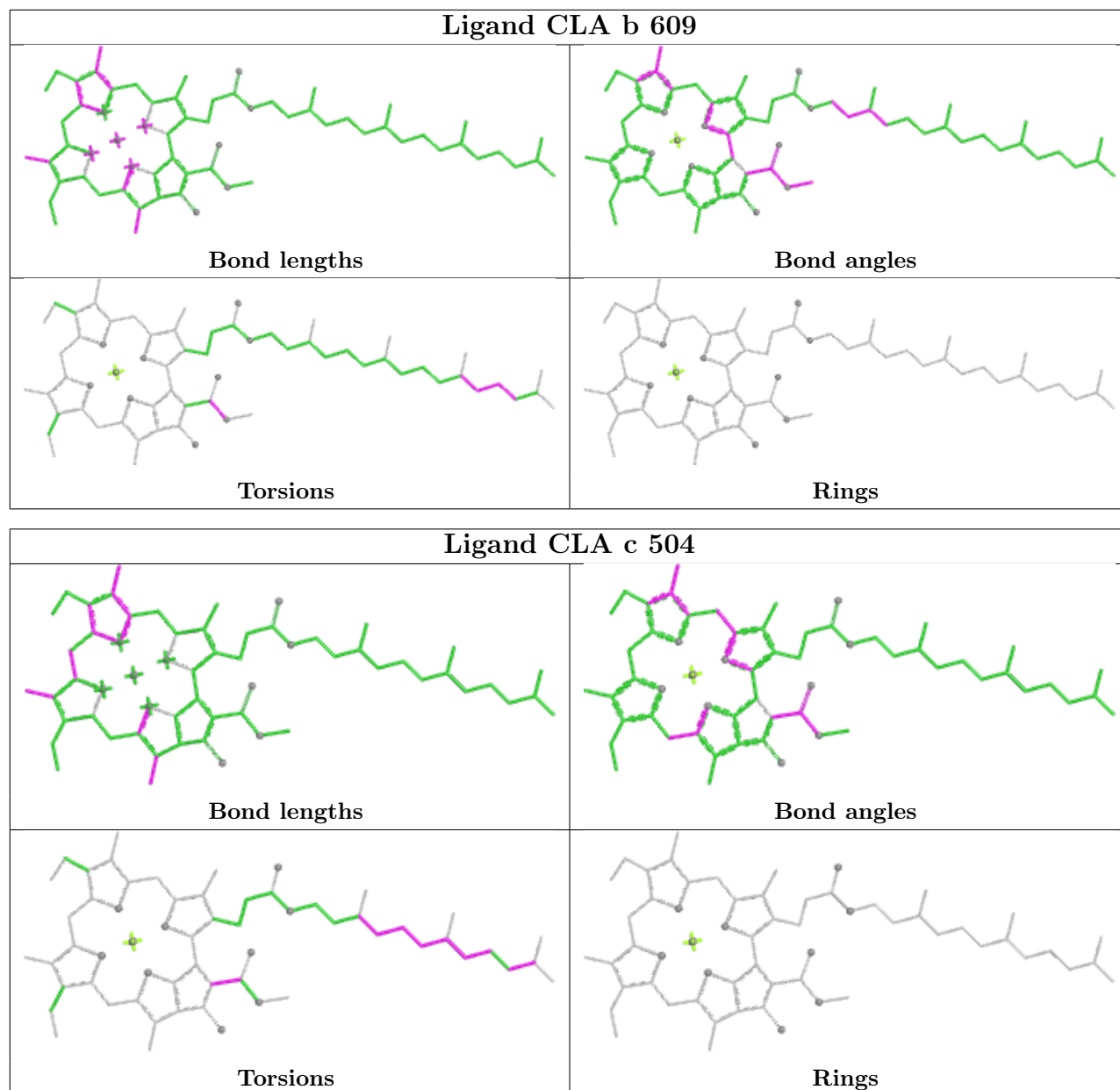
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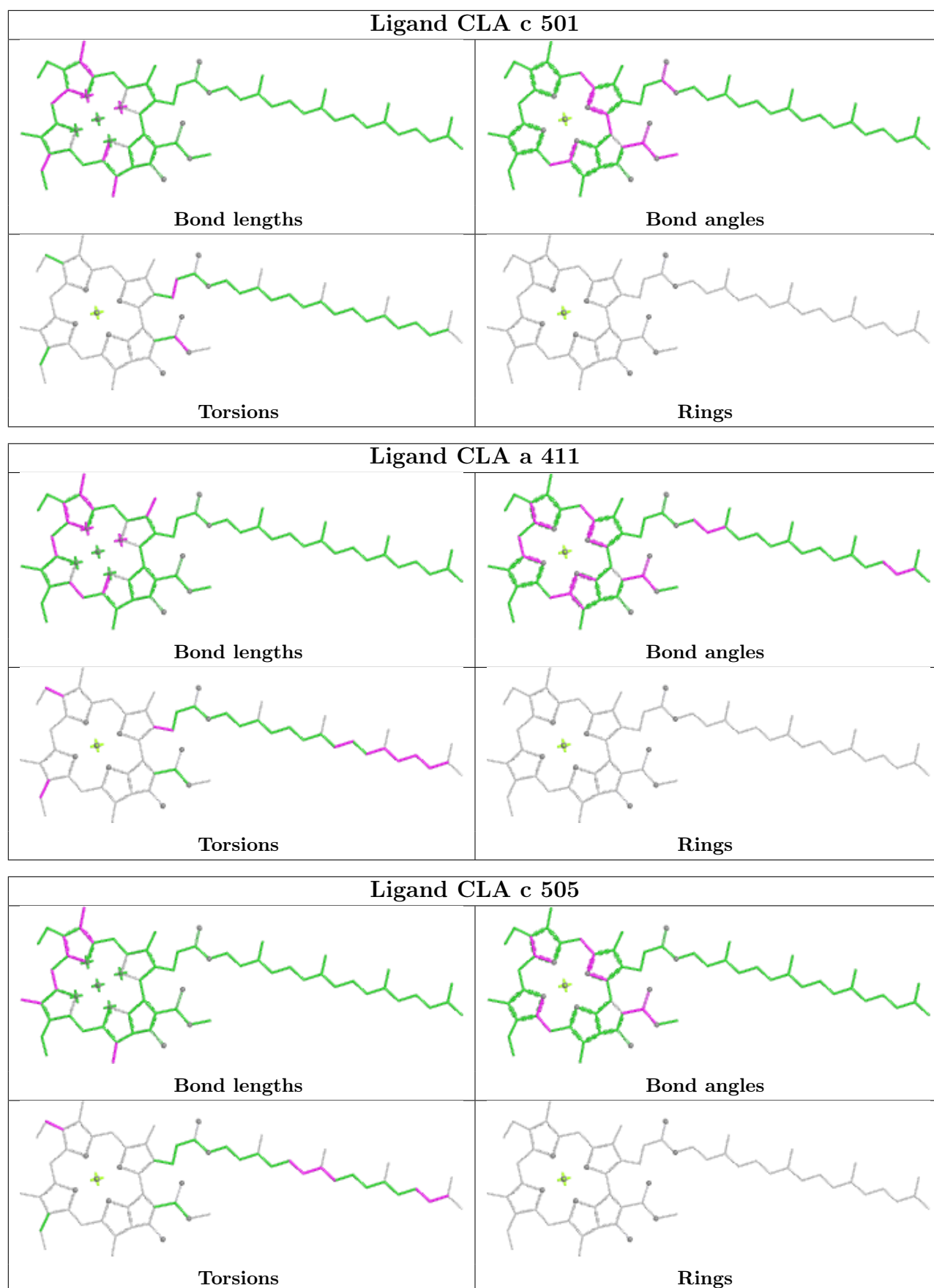
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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24	T	101	BCR	3	0
33	D	402	BCT	1	0
32	b	620	STE	1	0
23	a	404	PHO	1	0
32	k	104	STE	2	0
22	b	610	CLA	2	0
22	c	507	CLA	1	0
29	B	622	SQD	1	0
30	H	102	DGD	1	0
32	B	627	STE	2	0
24	a	406	BCR	1	0
22	B	601	CLA	3	0
23	D	401	PHO	1	0
32	B	620	STE	1	0
22	B	613	CLA	3	0
28	A	411	LHG	2	0
29	f	101	SQD	2	0
32	b	621	STE	1	0

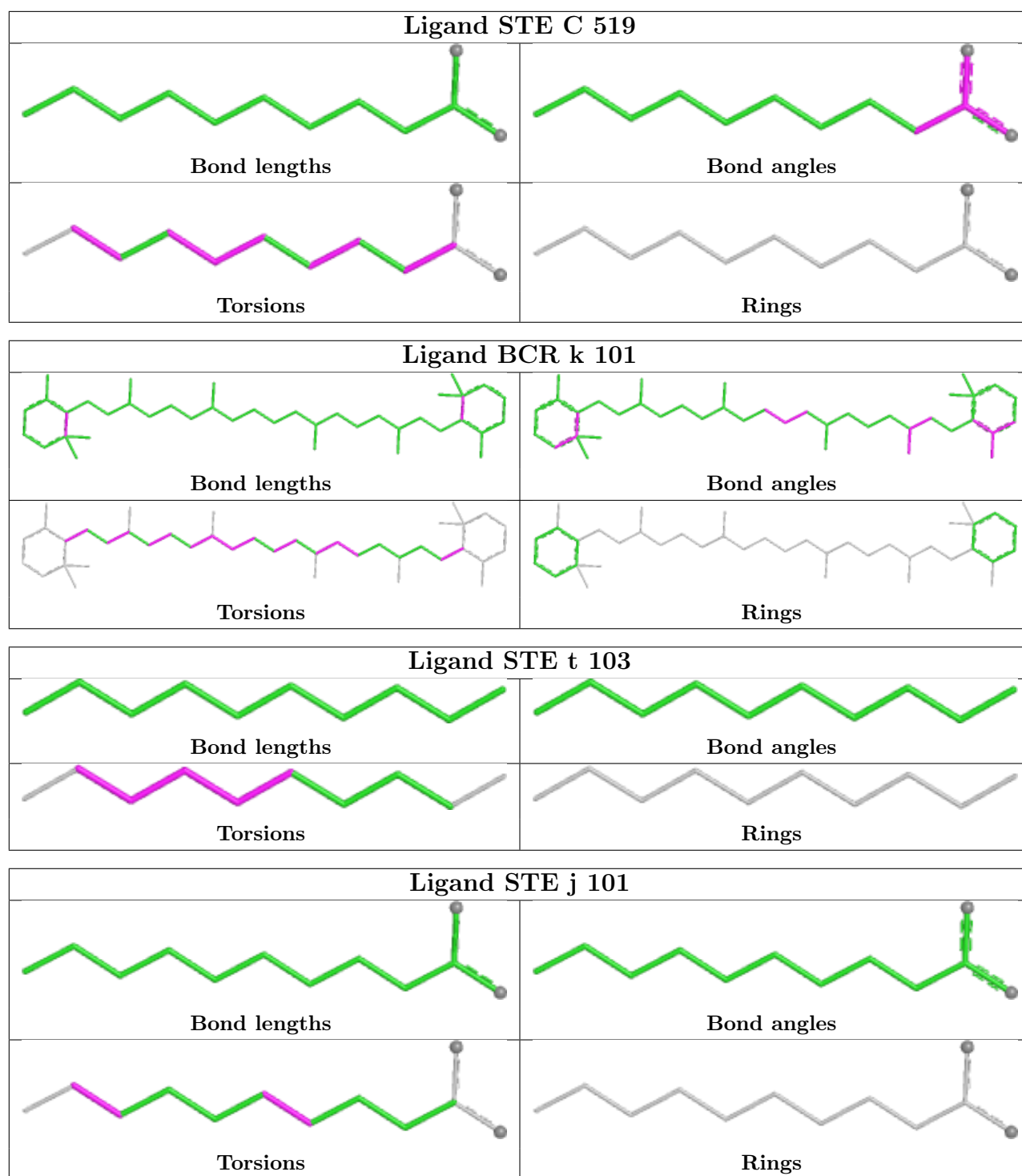
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

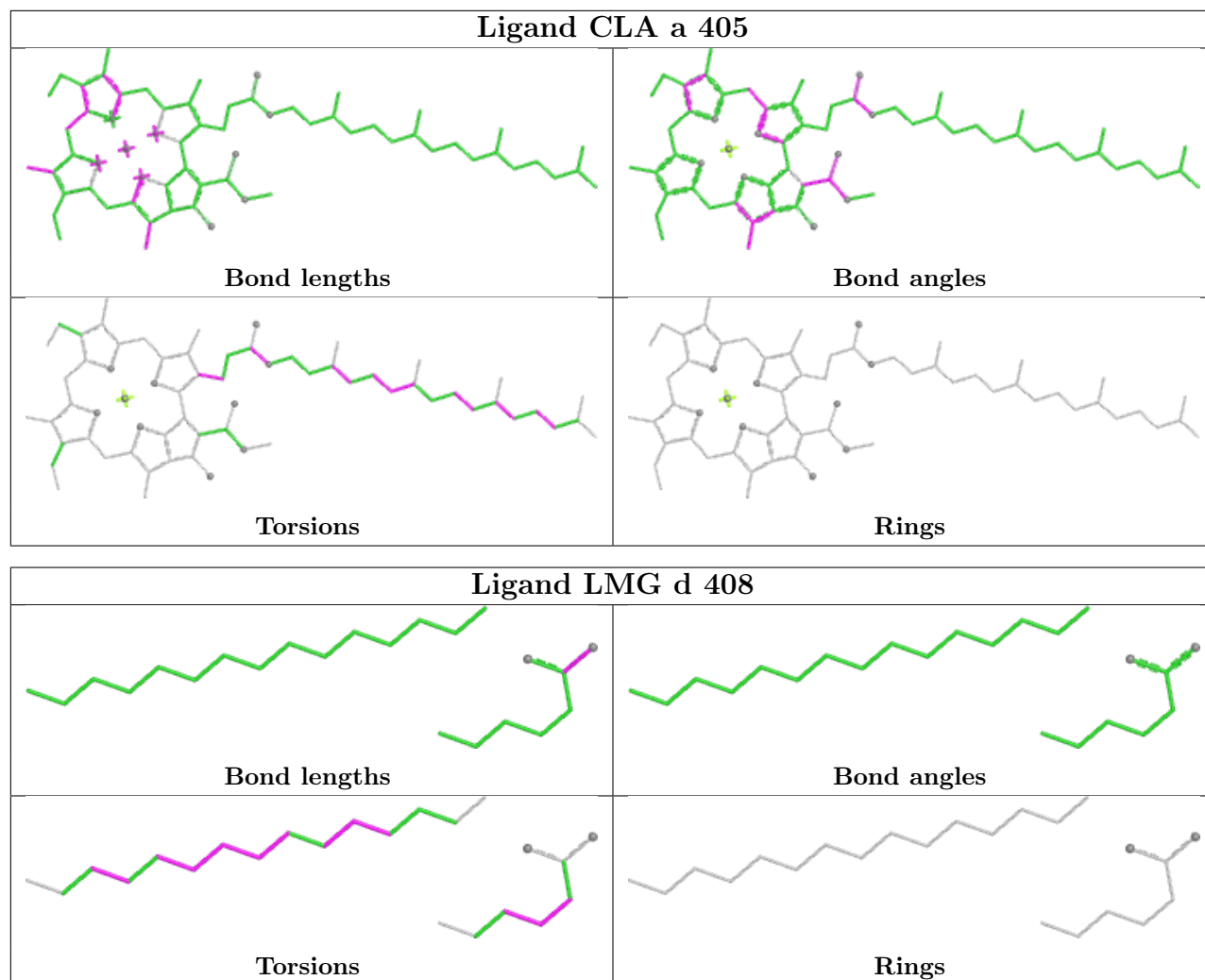


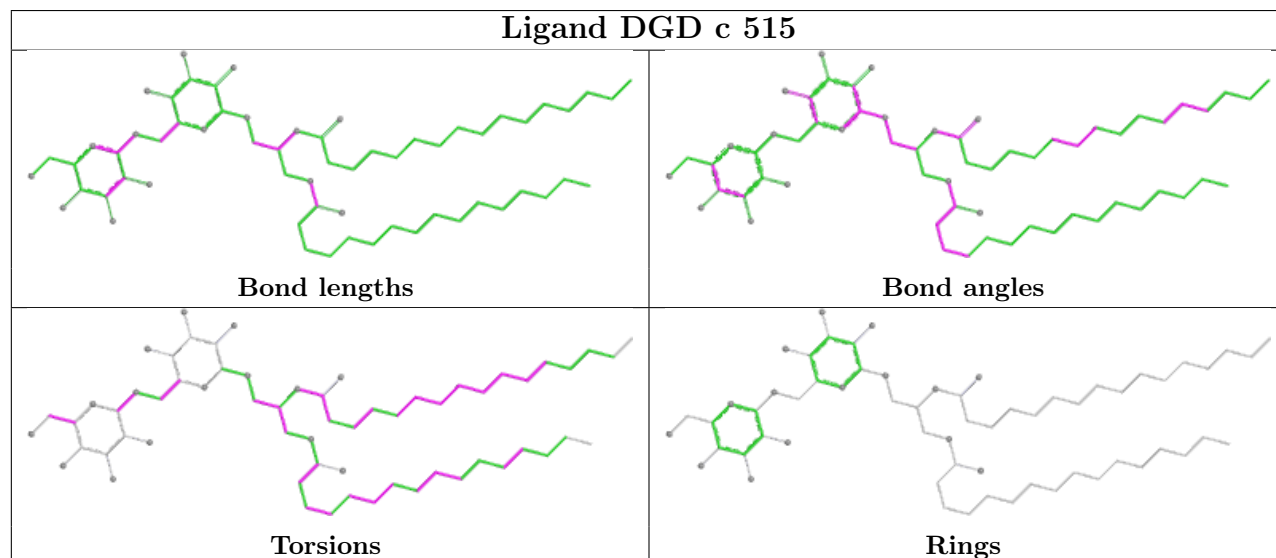
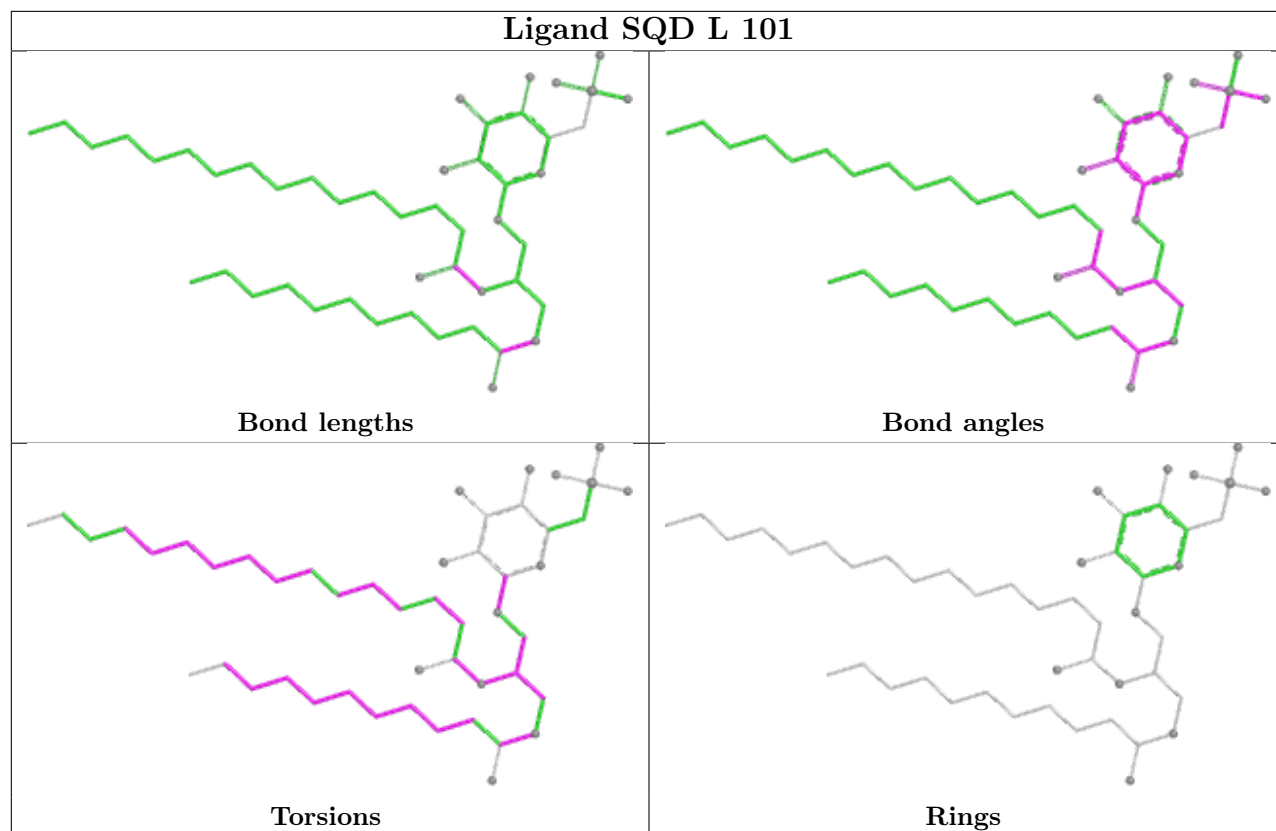


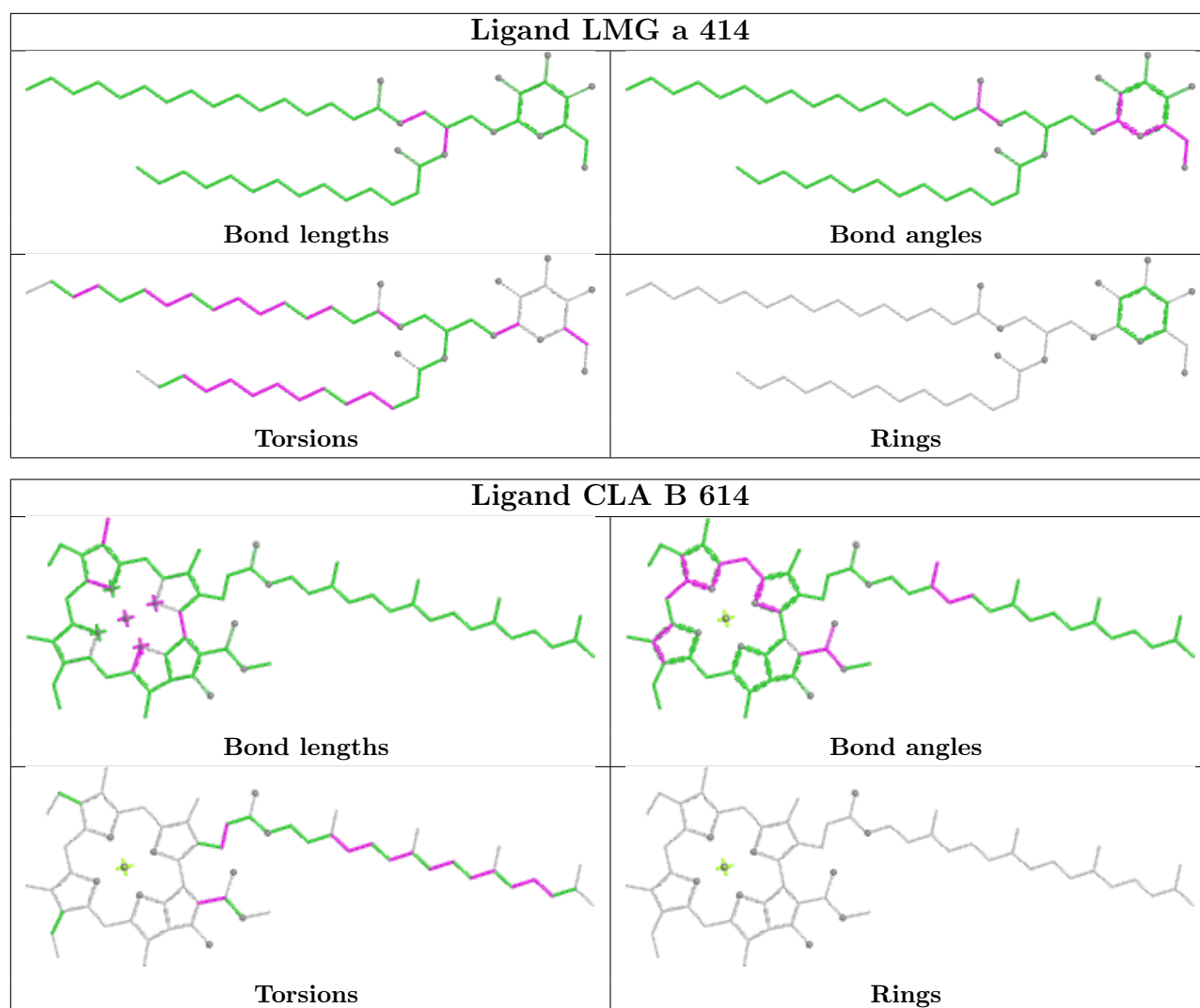


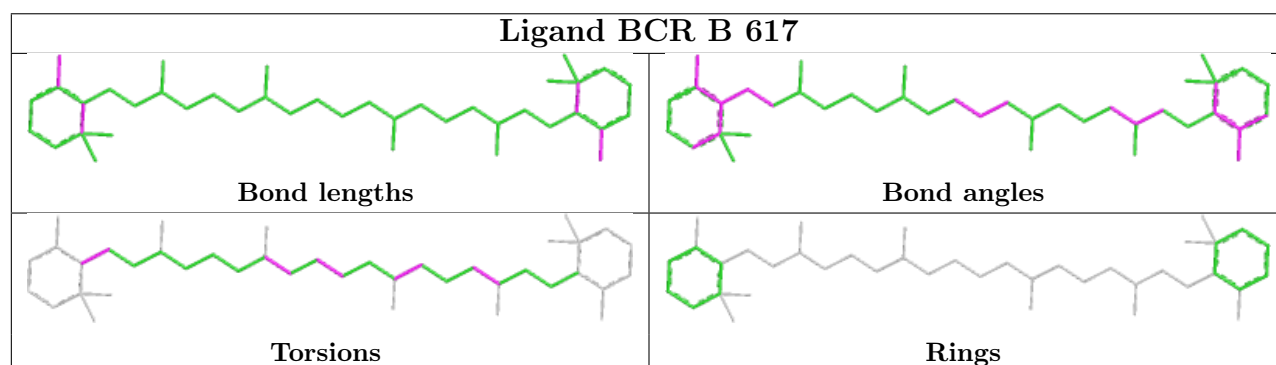
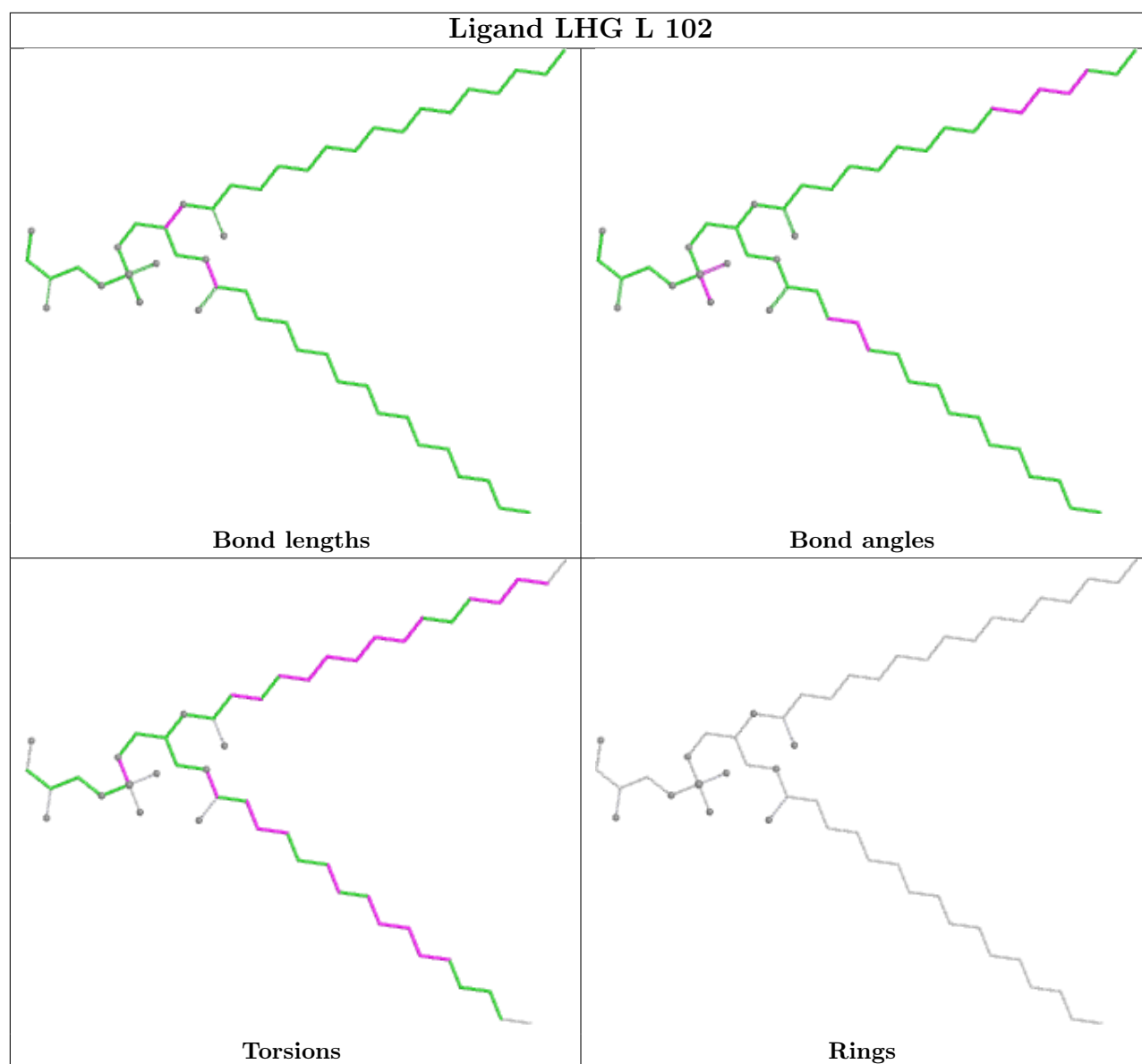


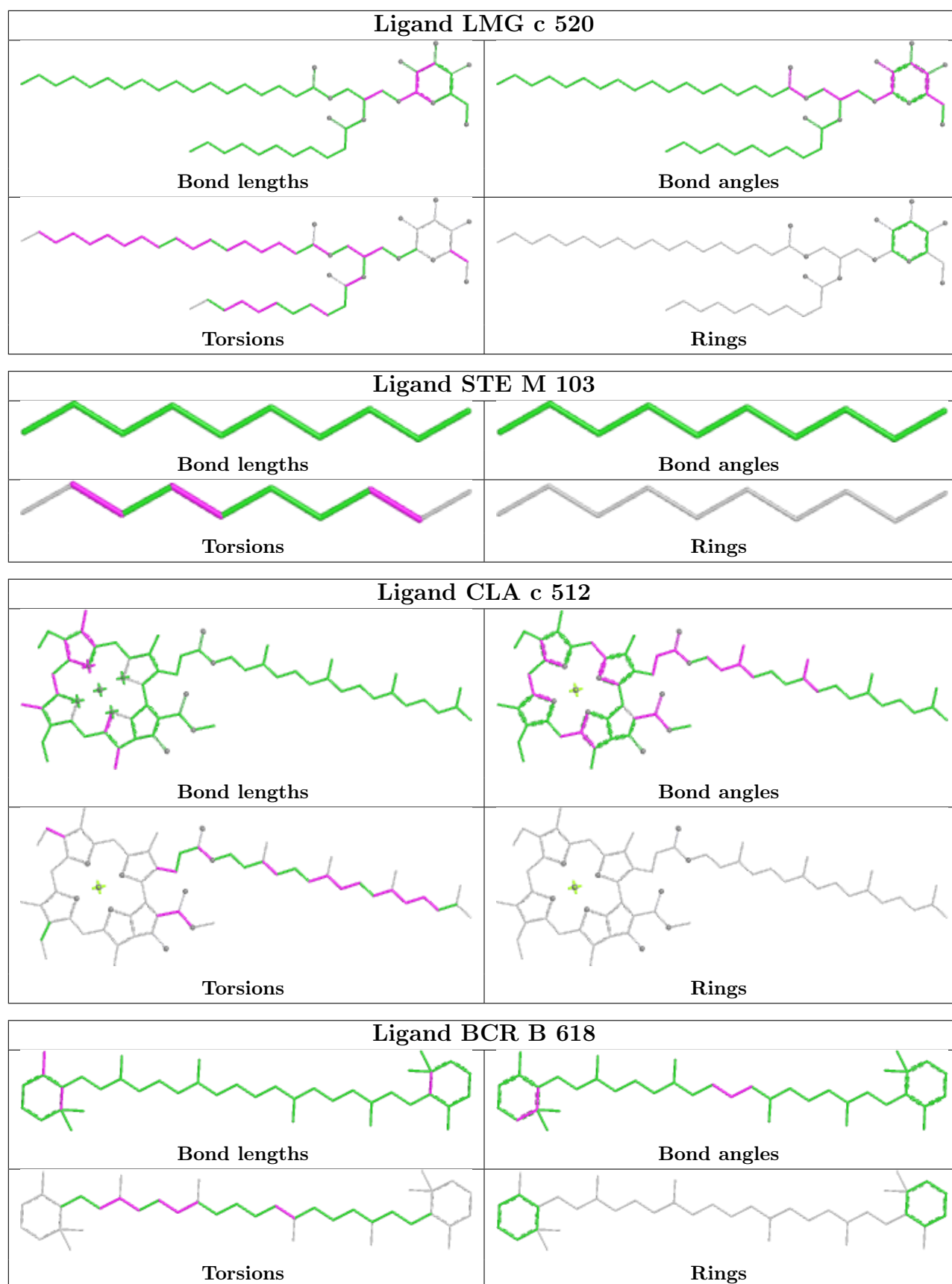


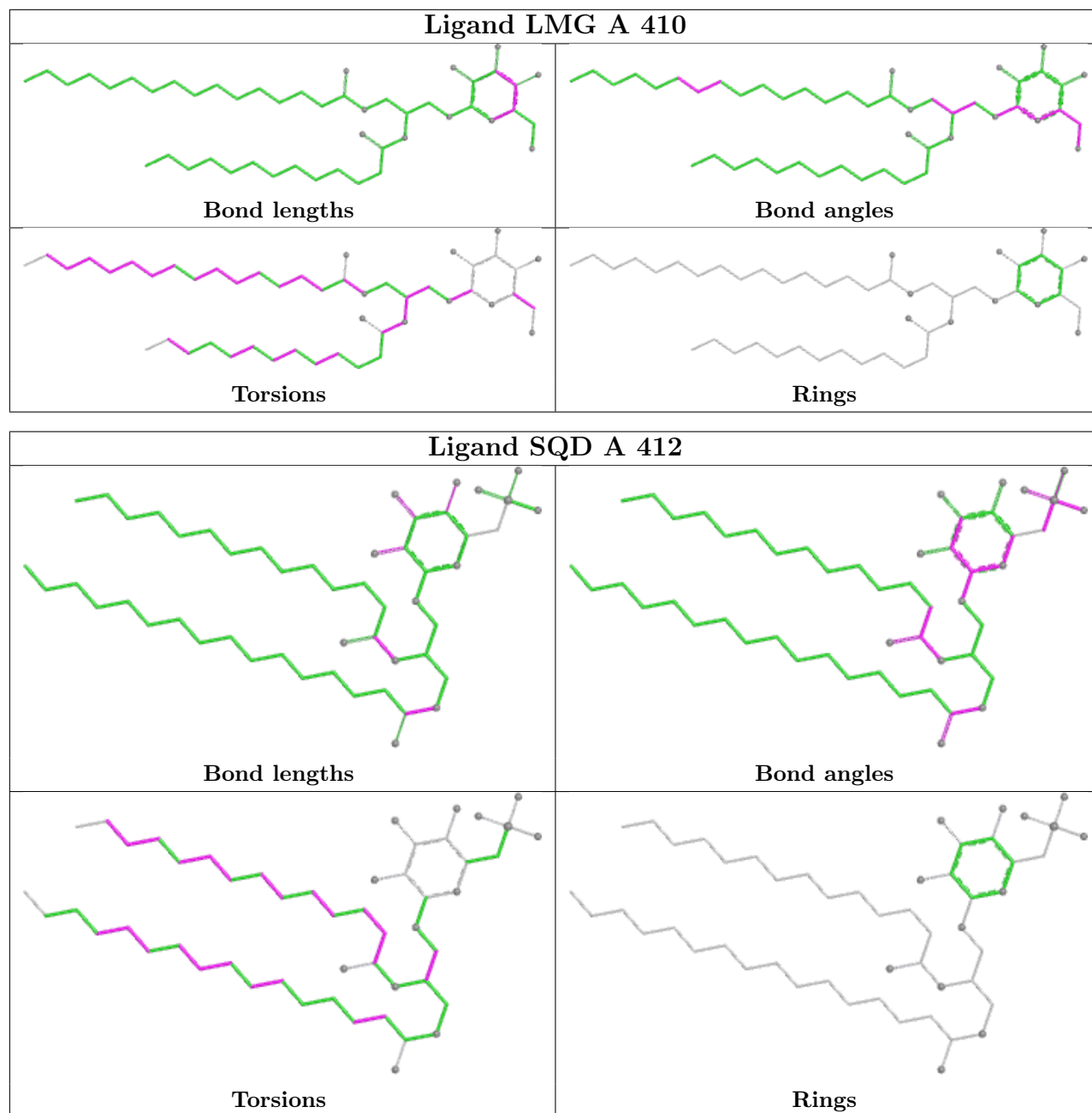


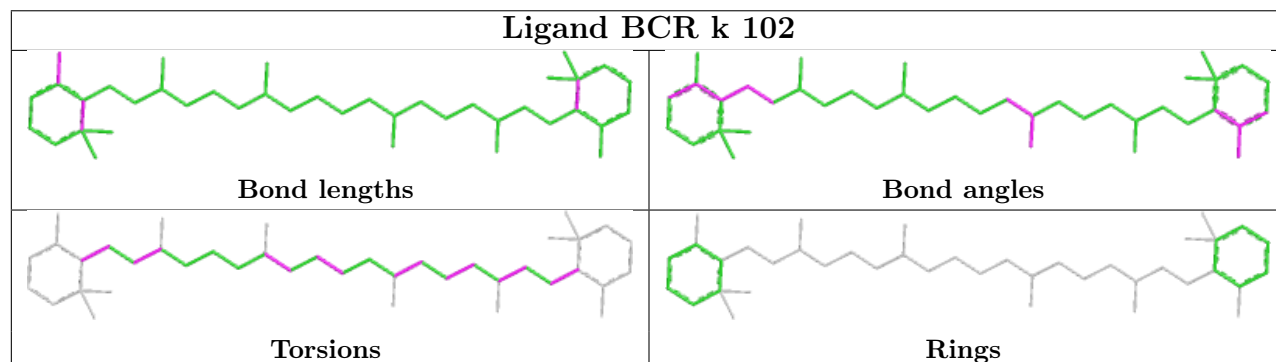
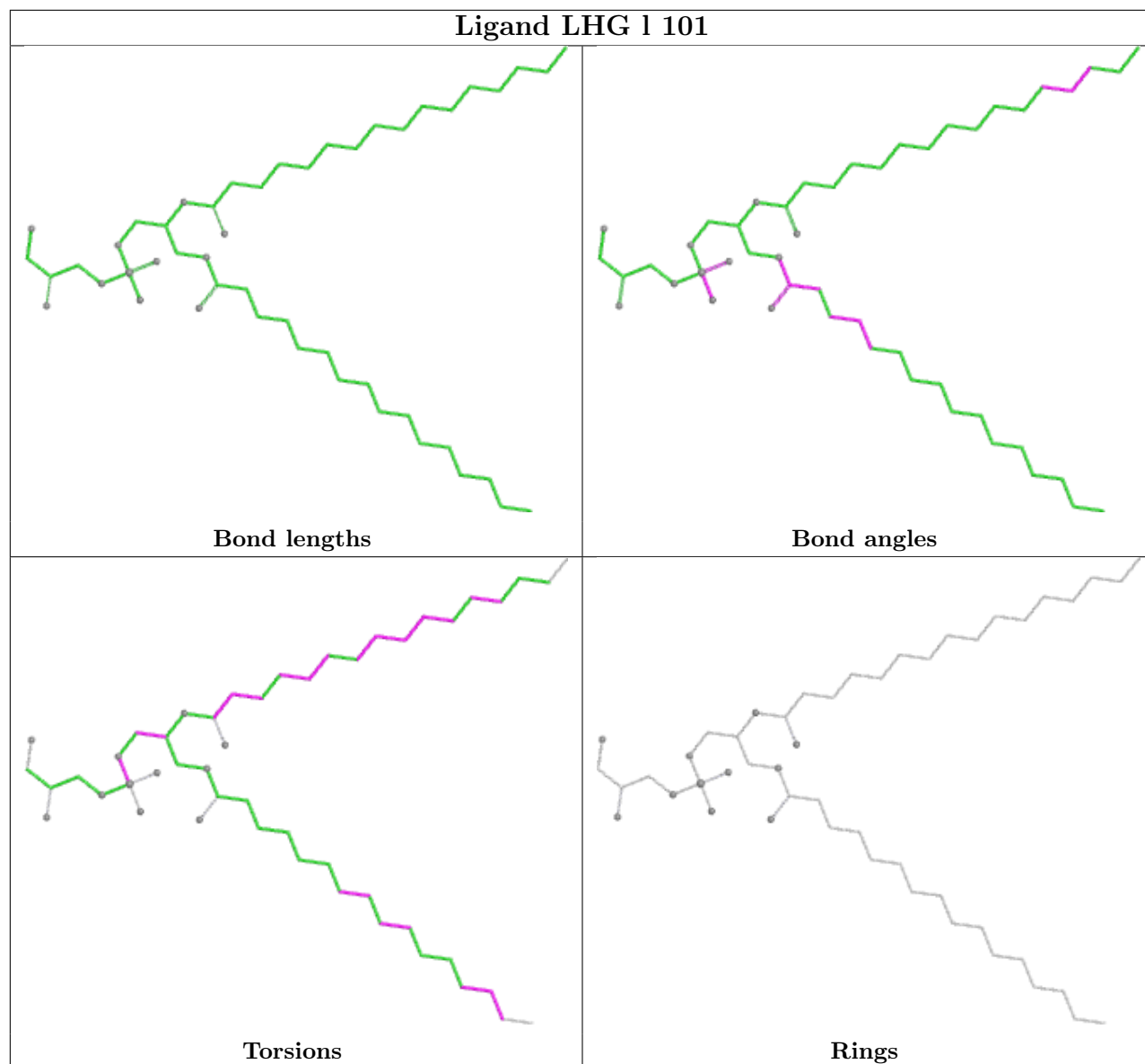


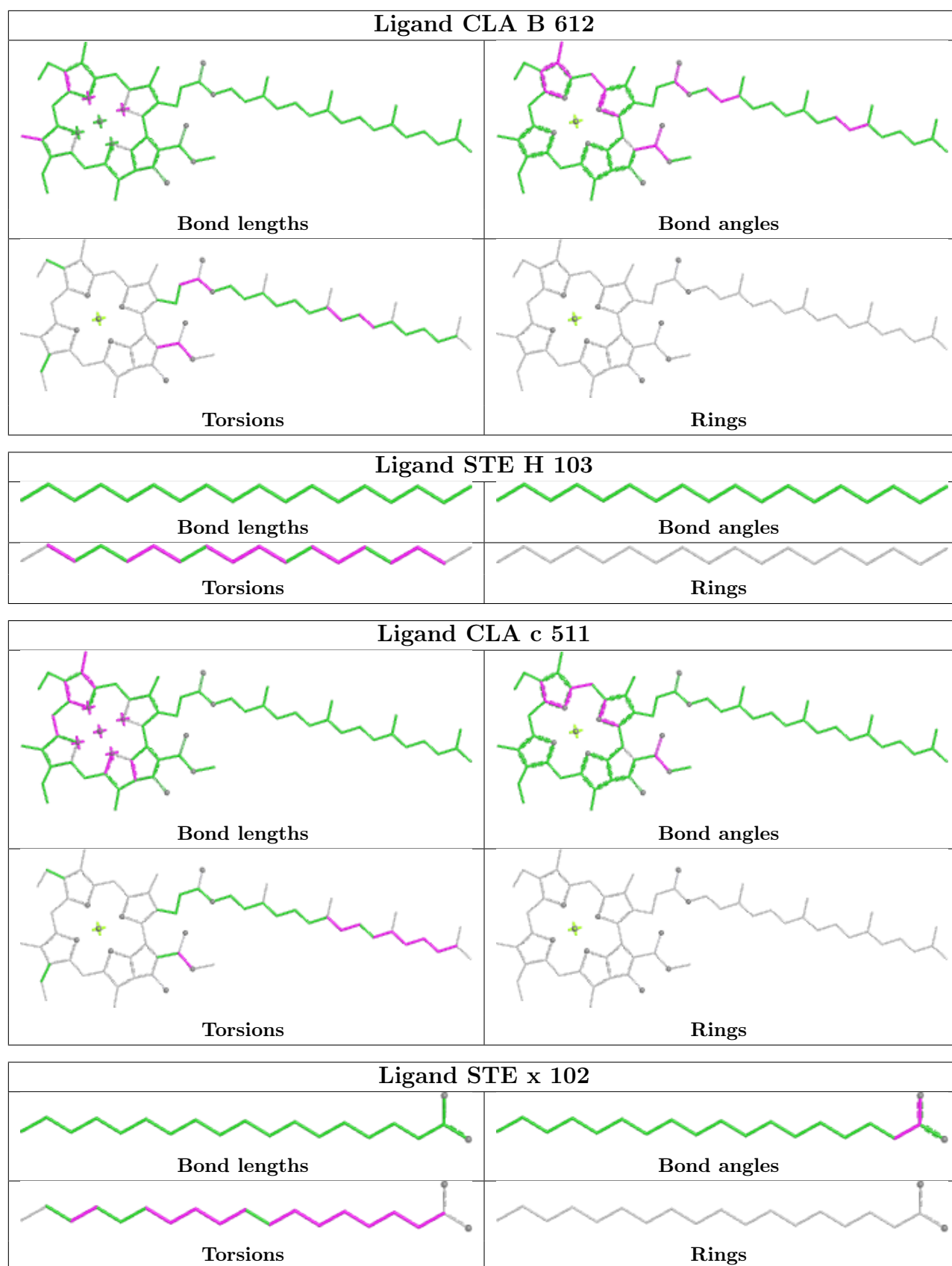


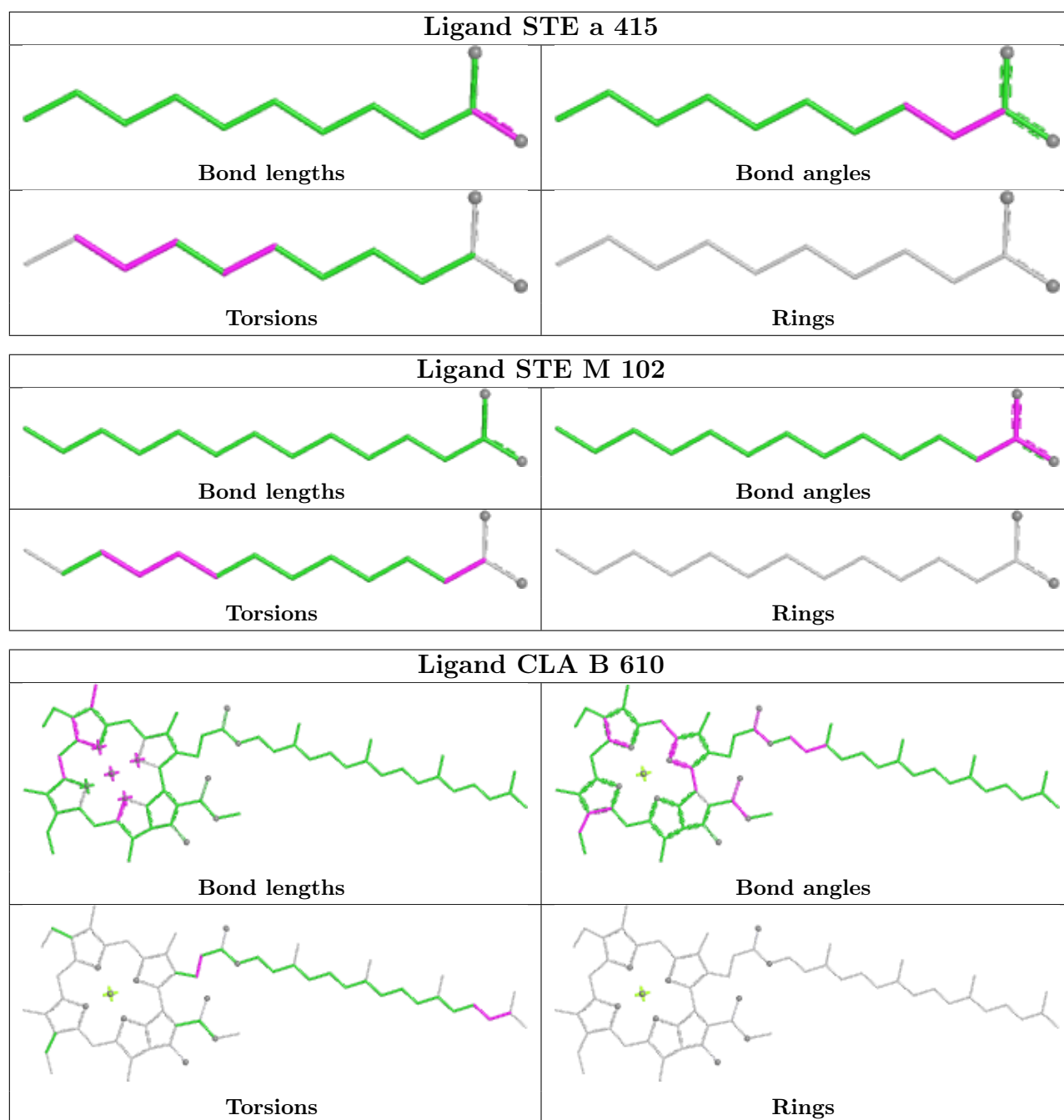


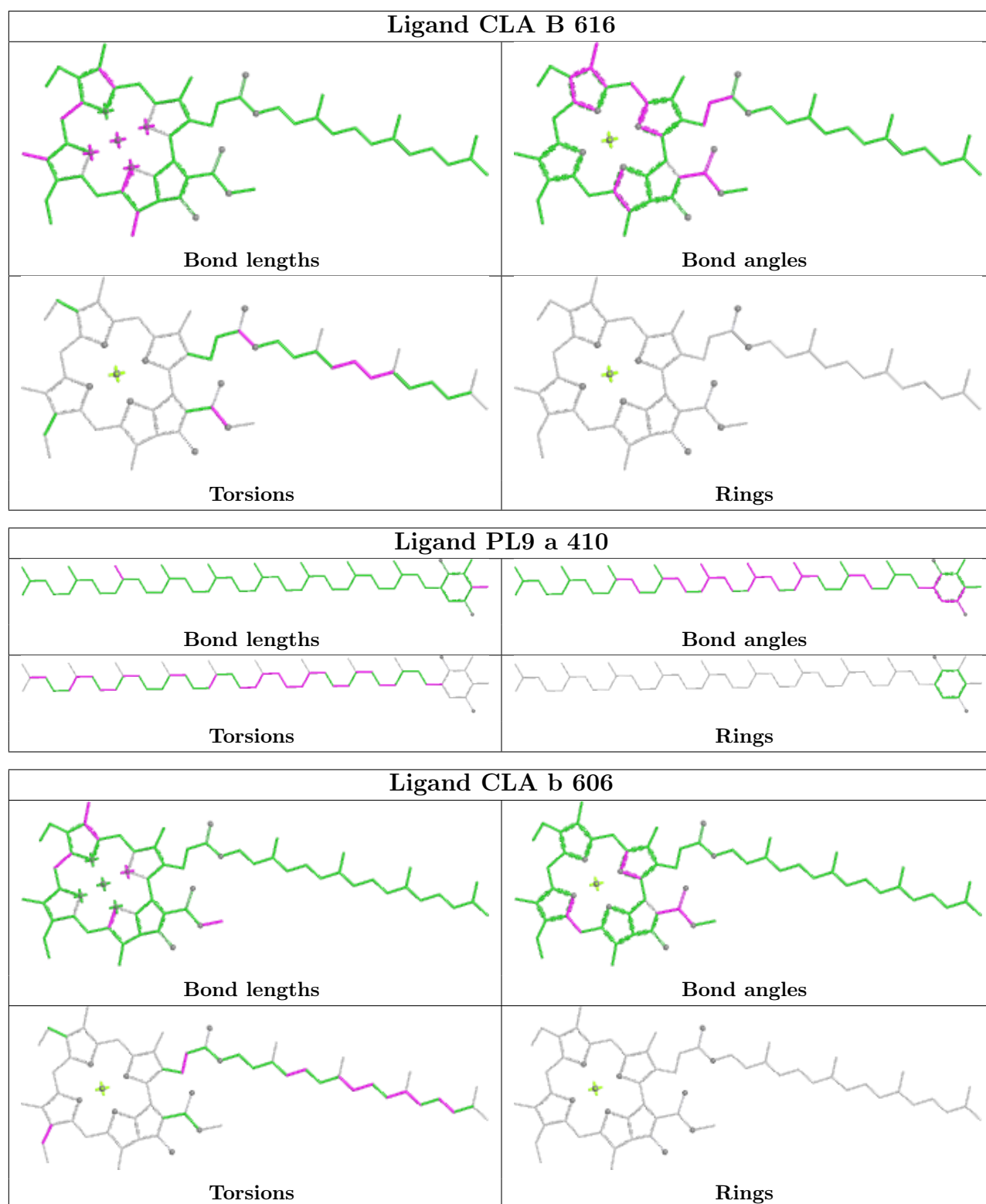


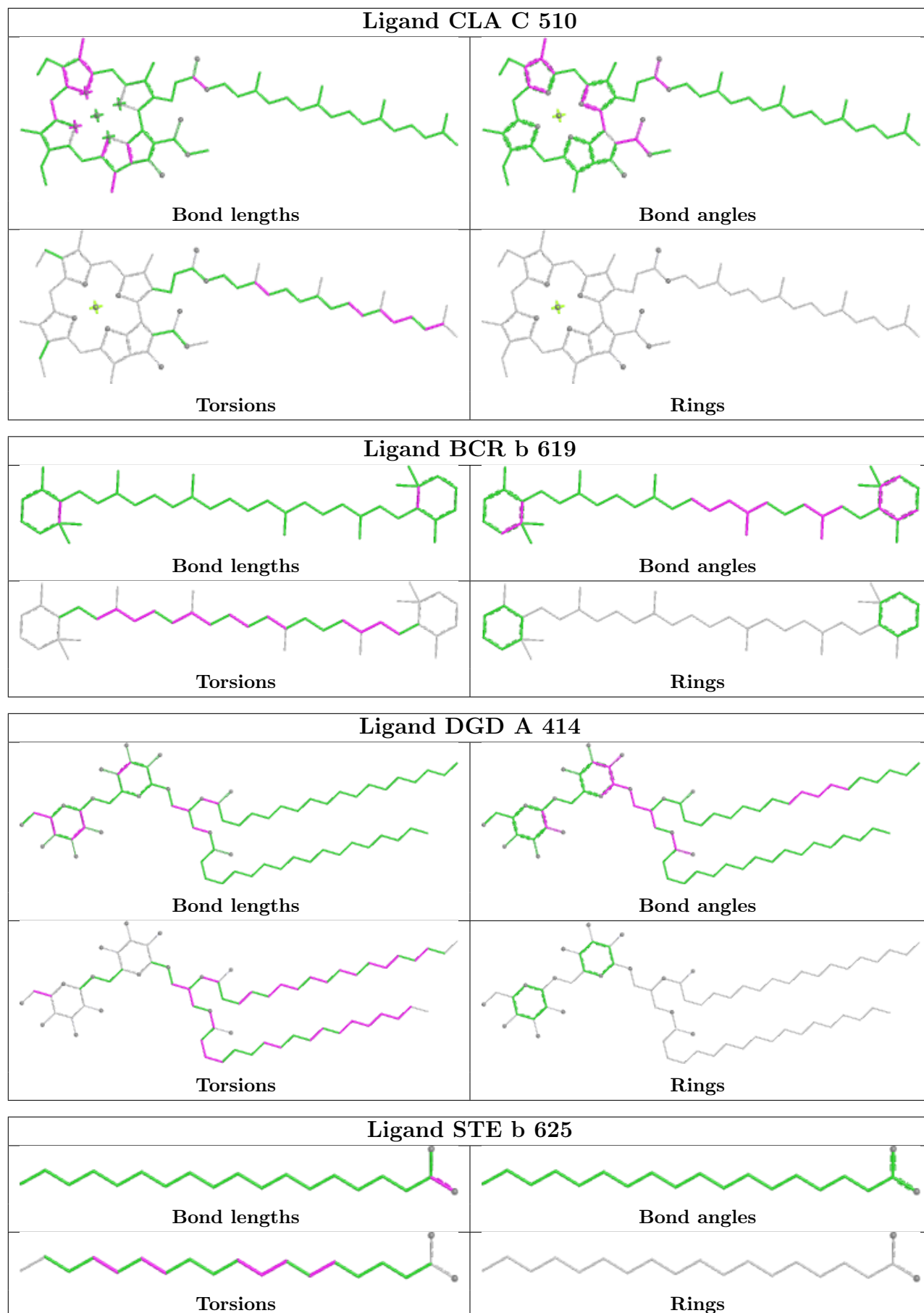


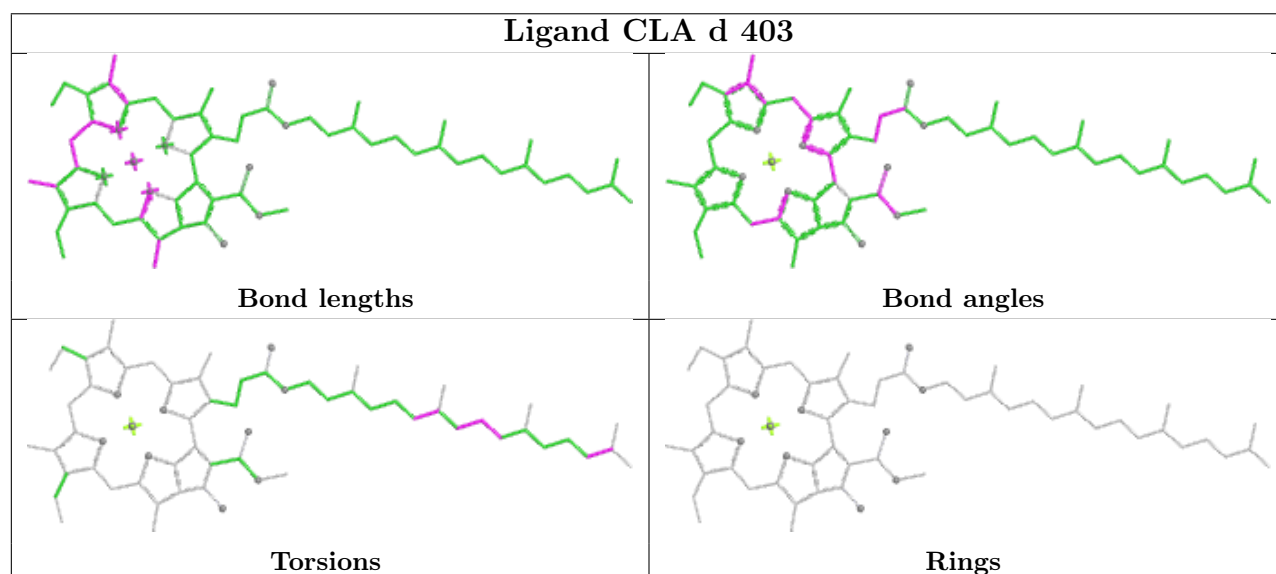
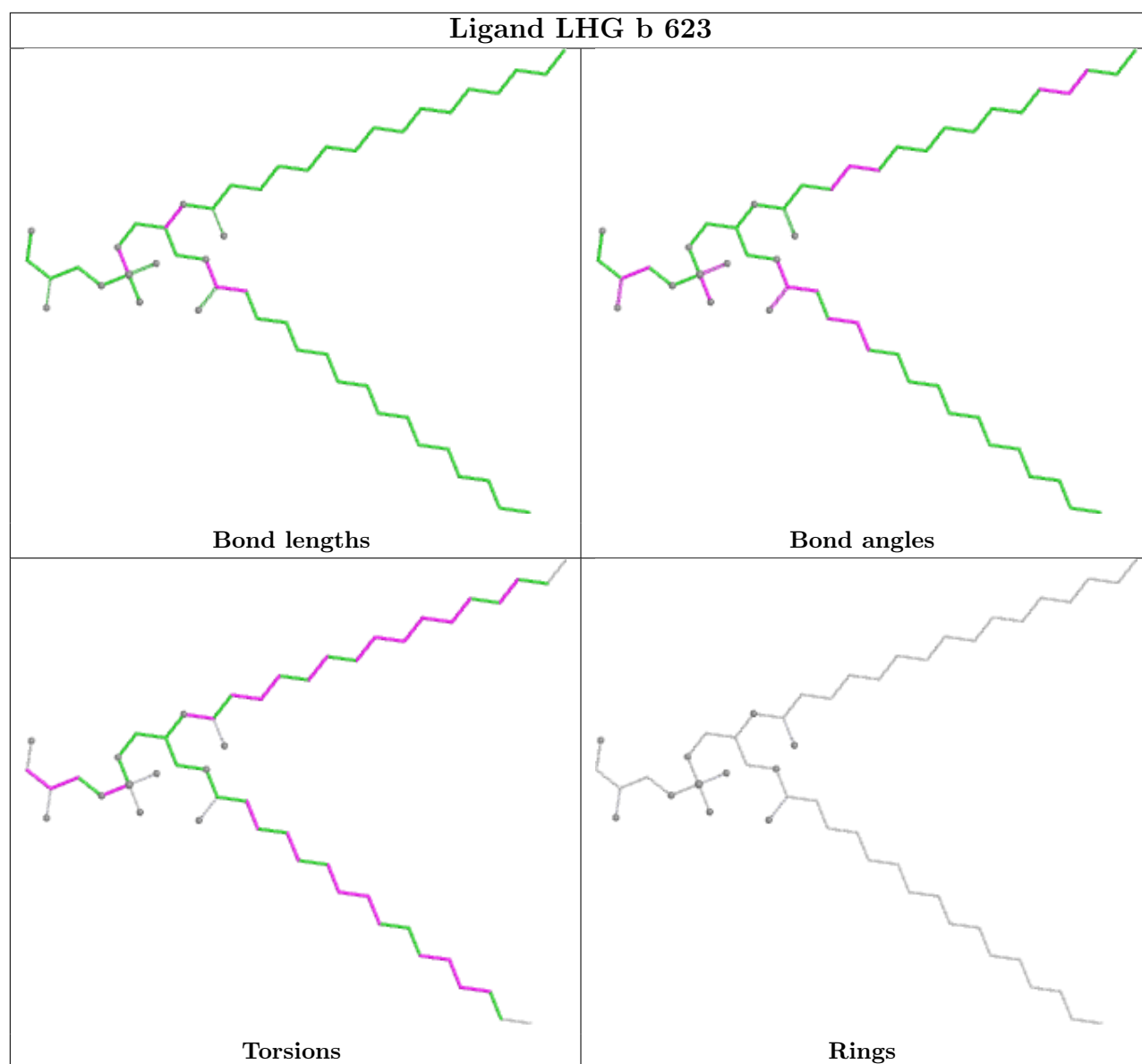


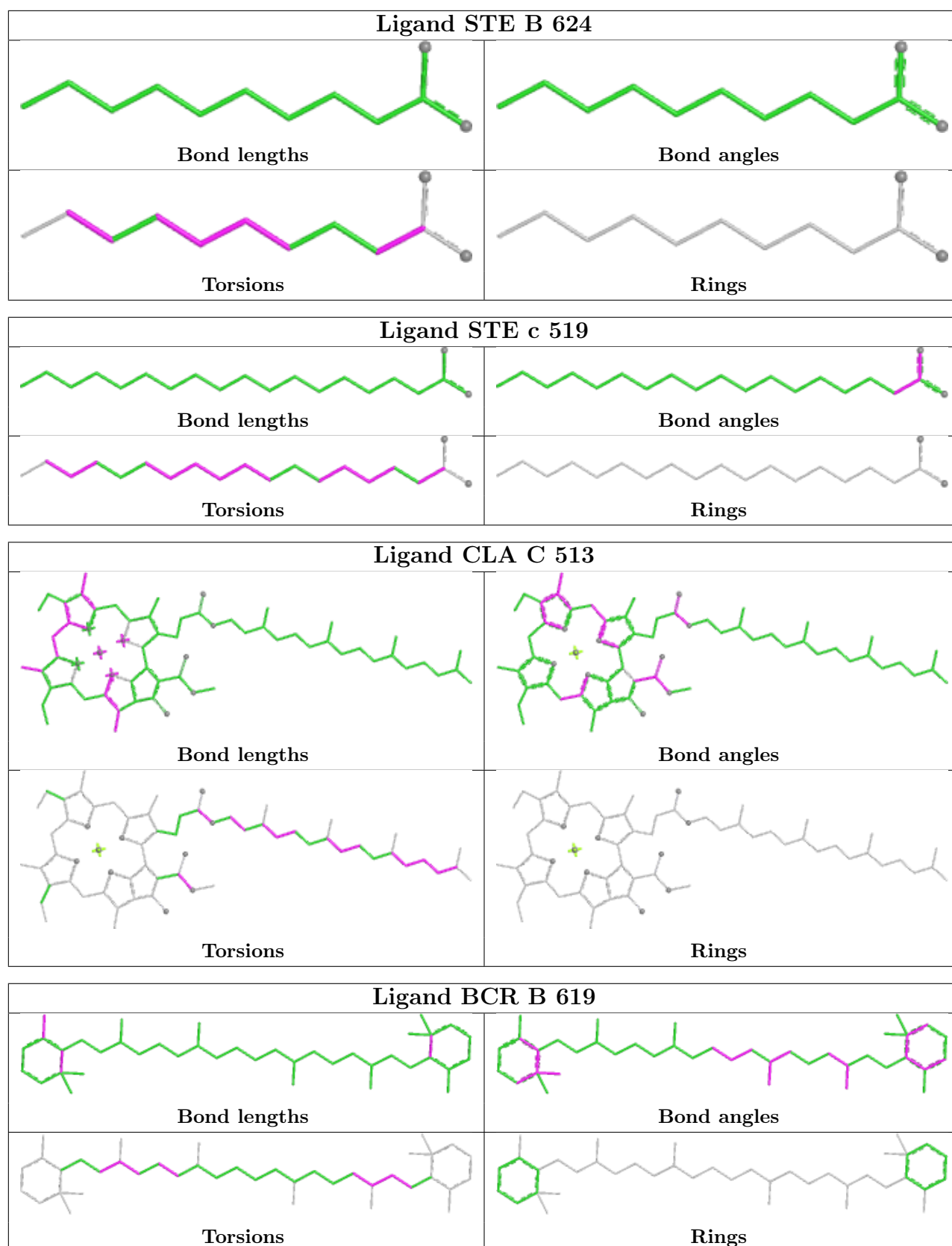


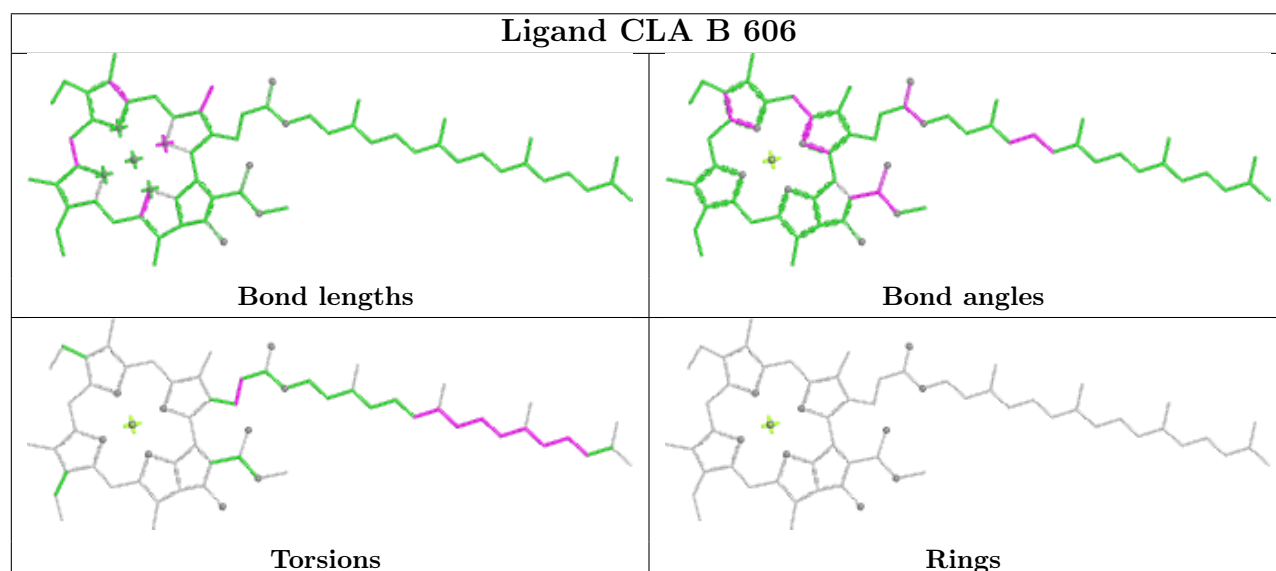
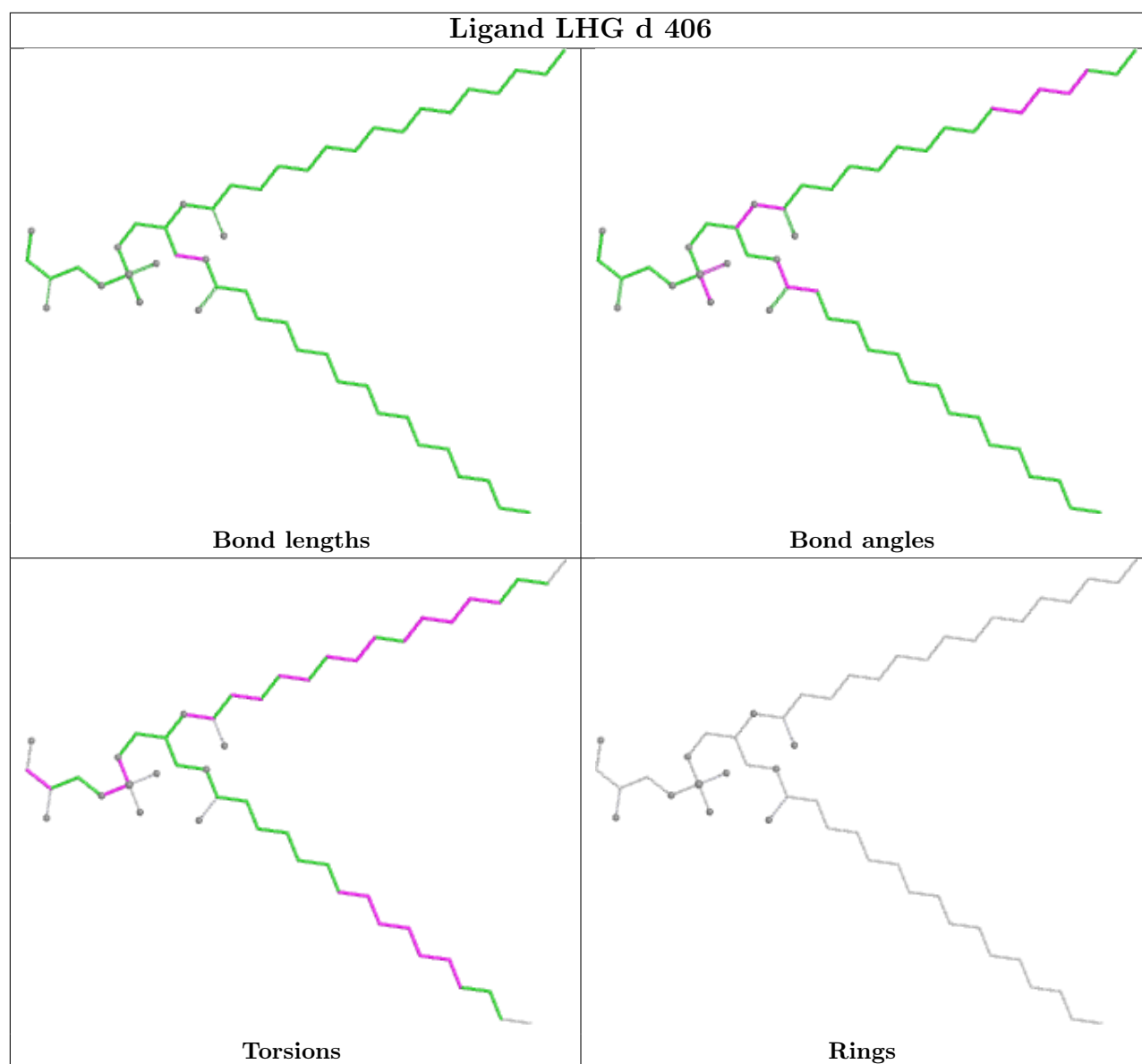


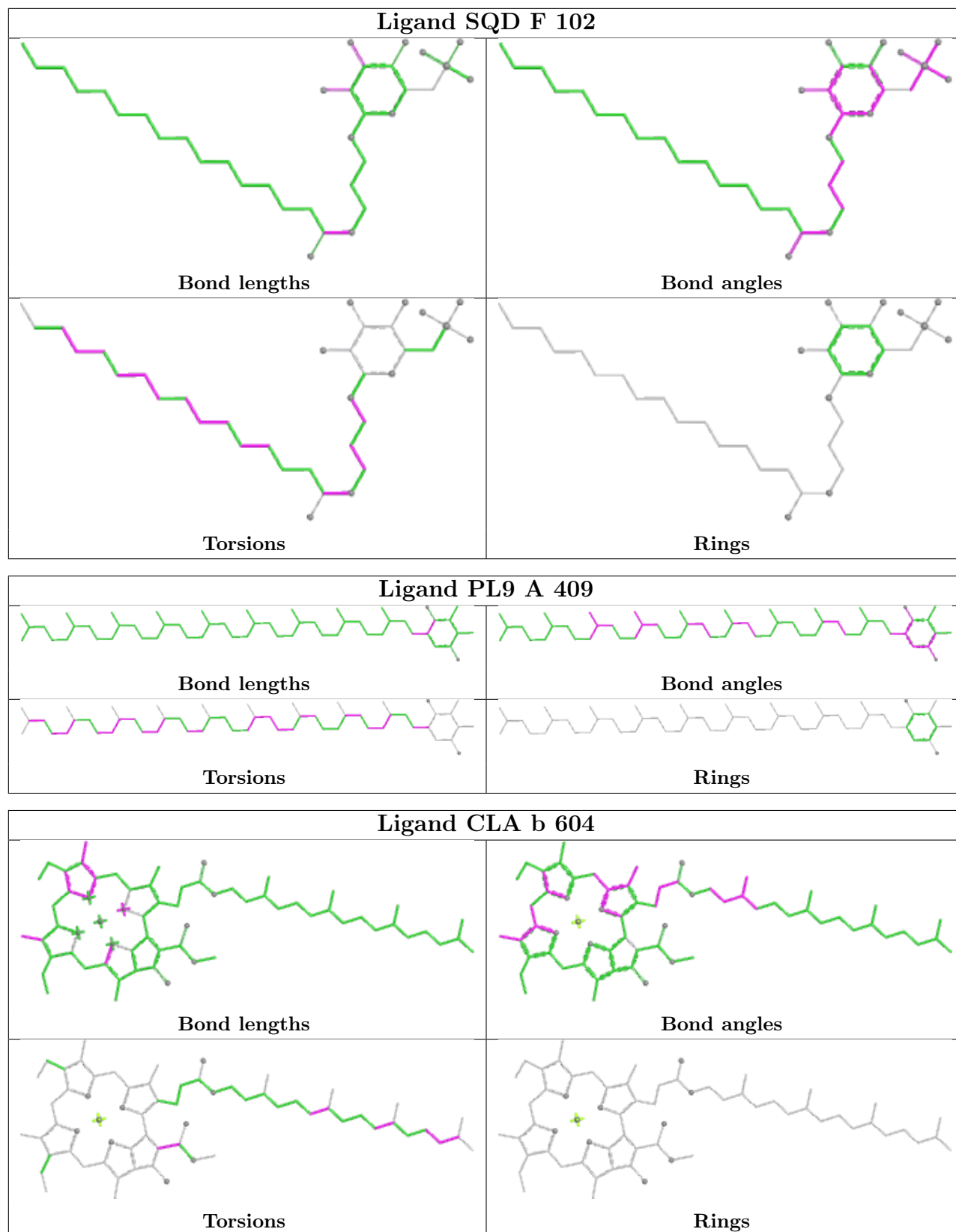


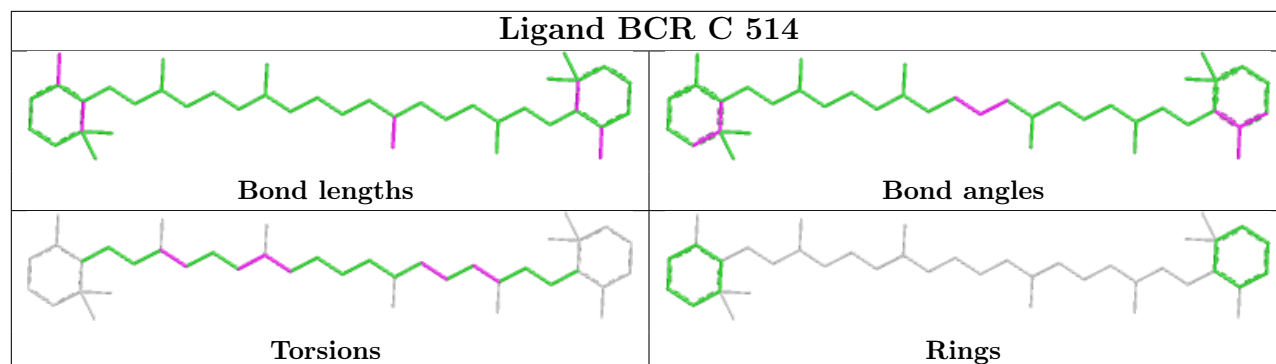
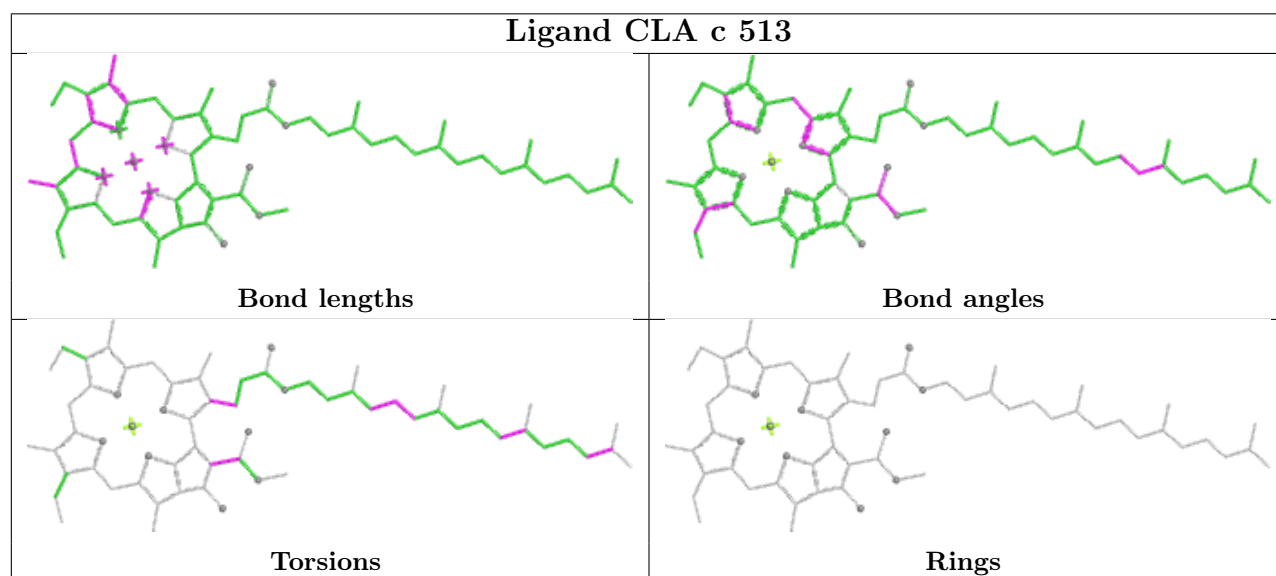
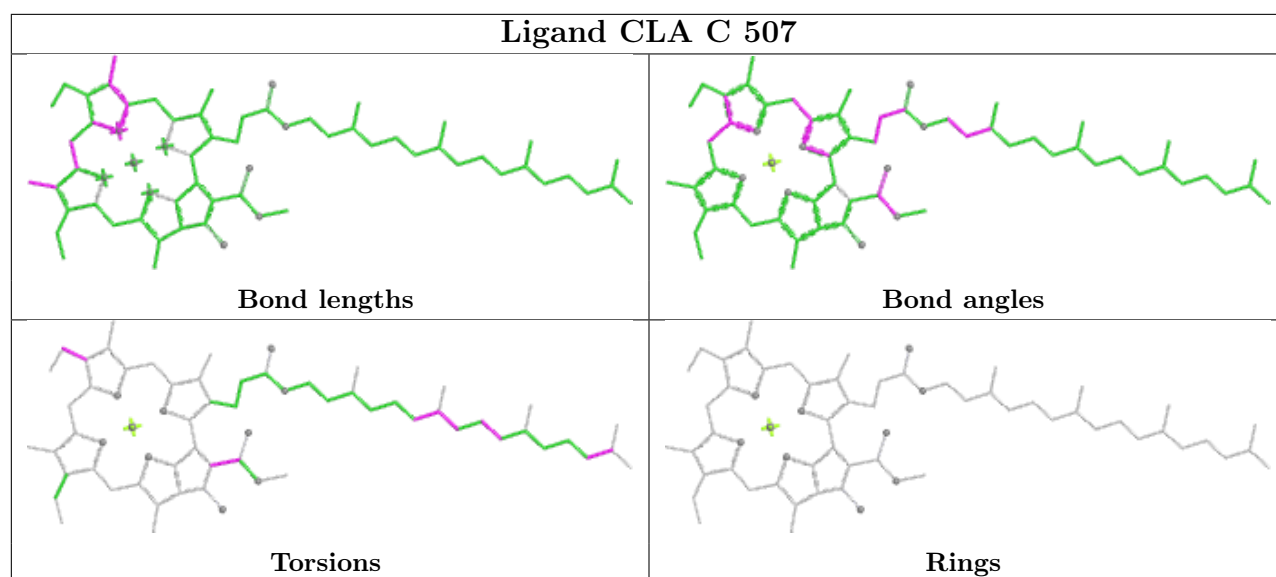


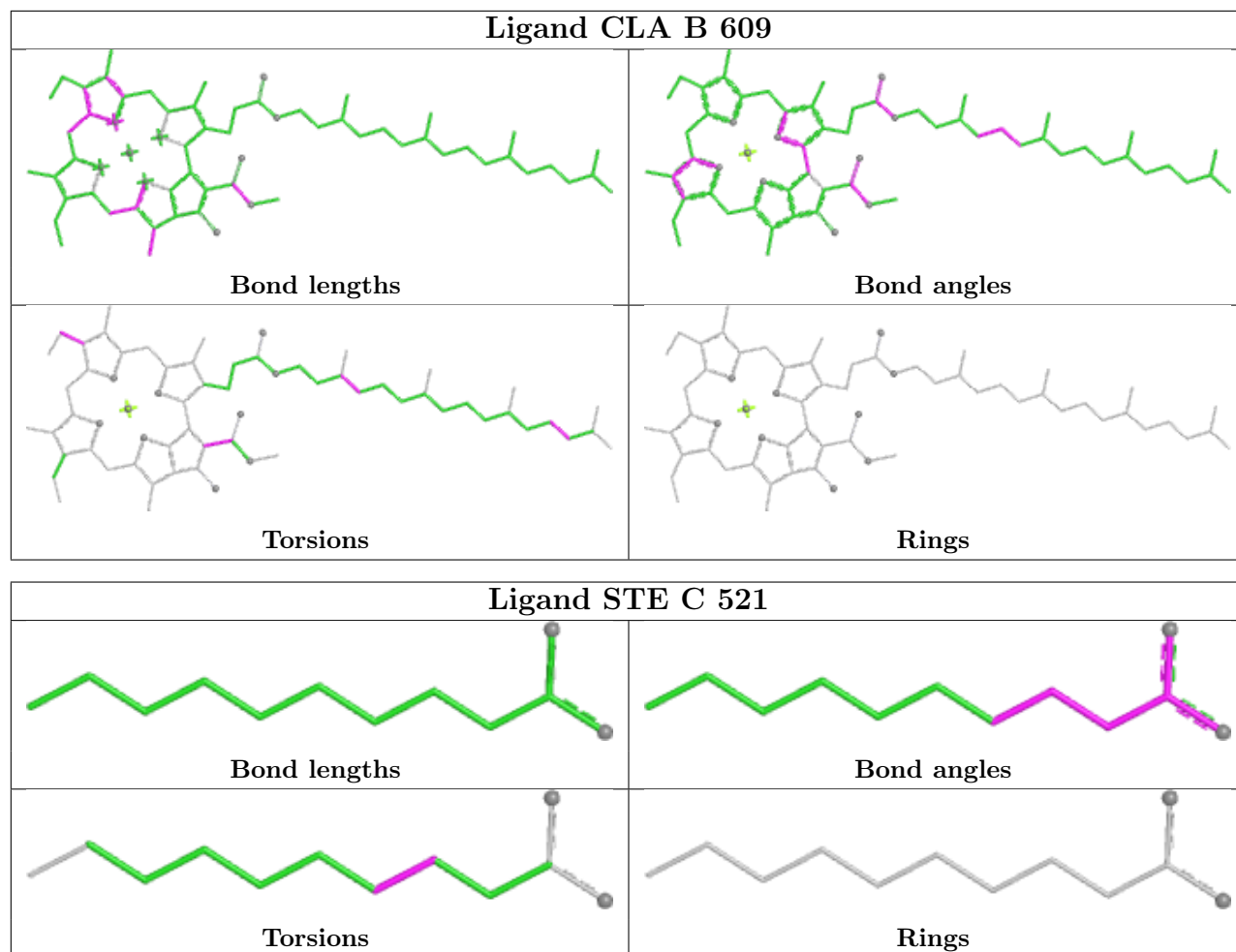


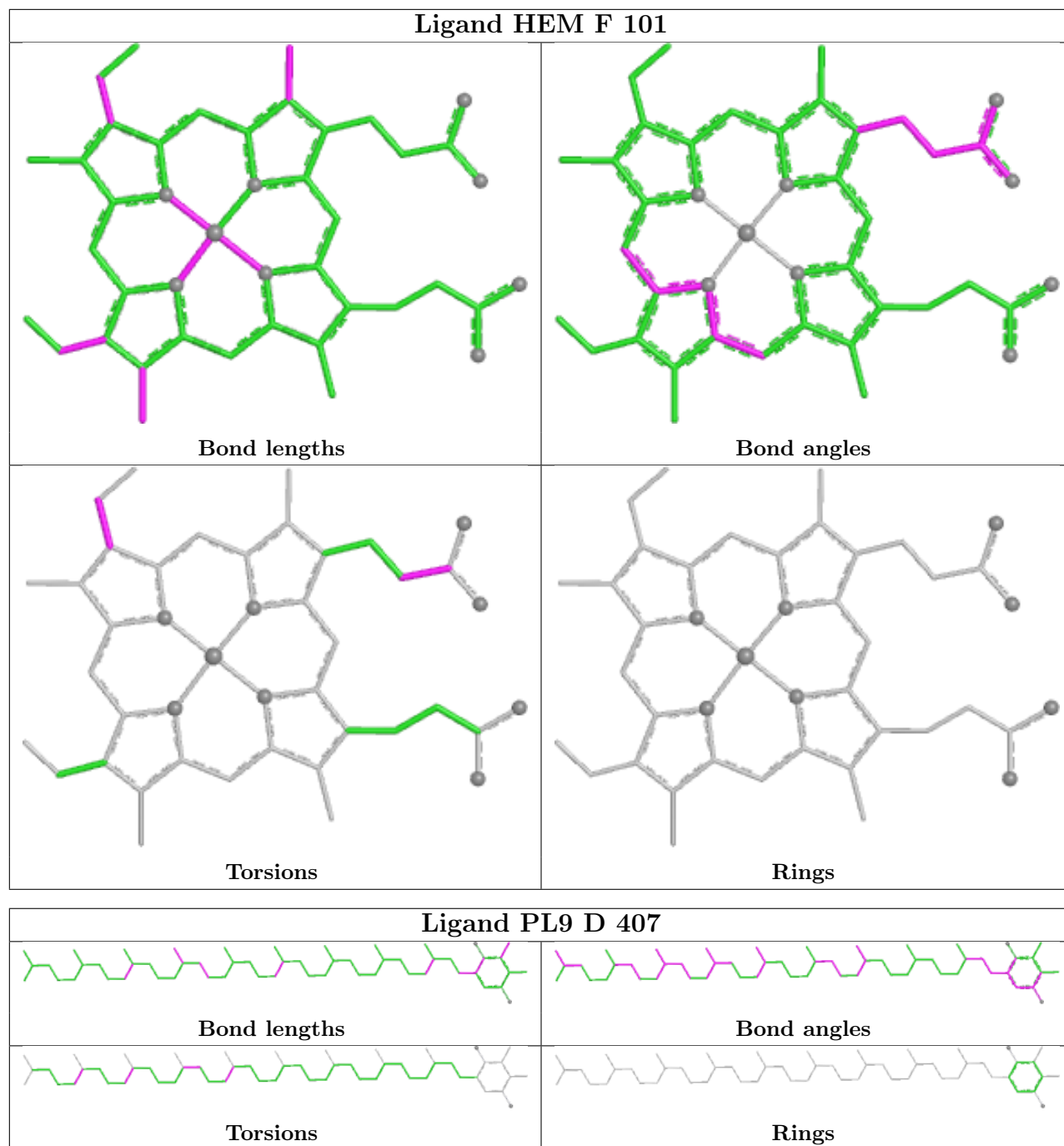


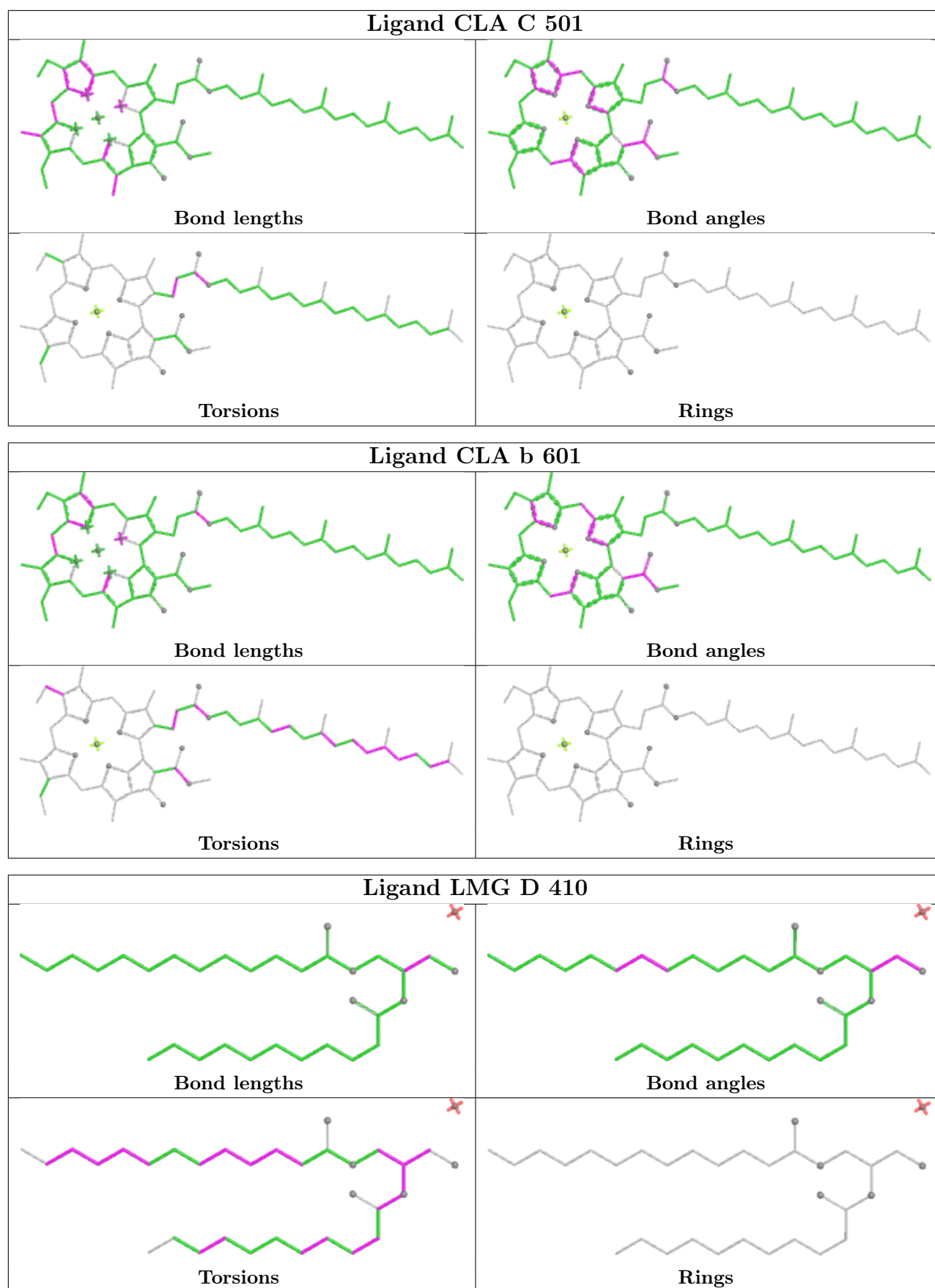


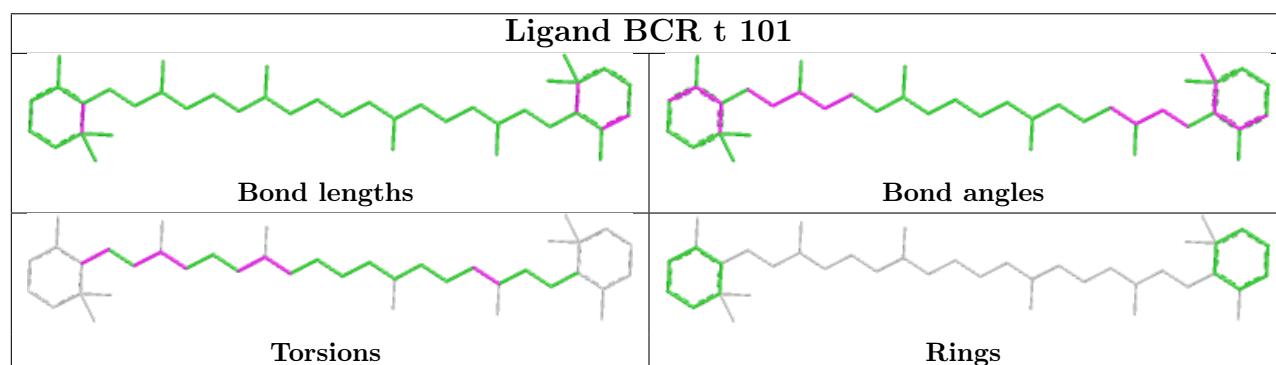
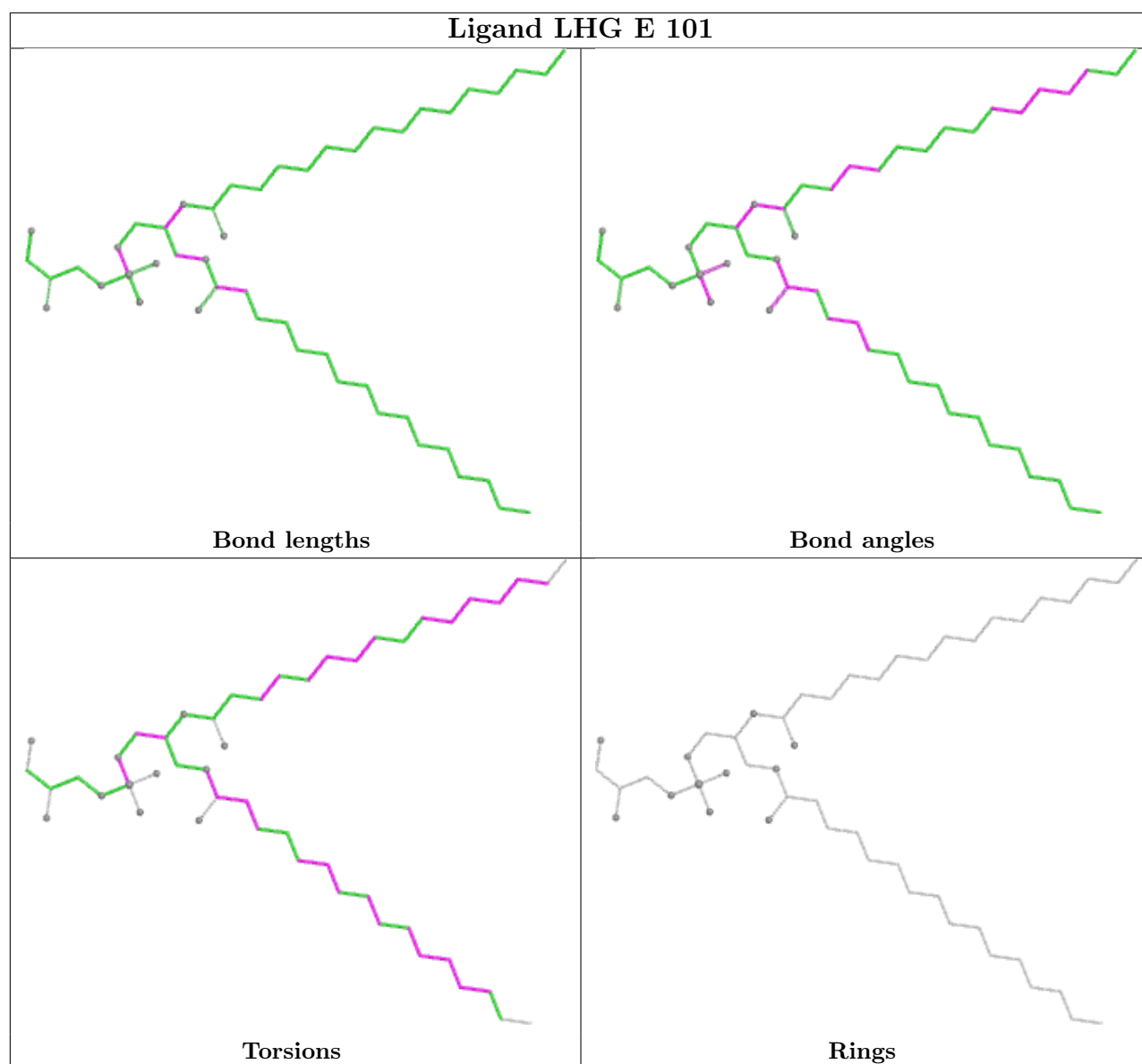


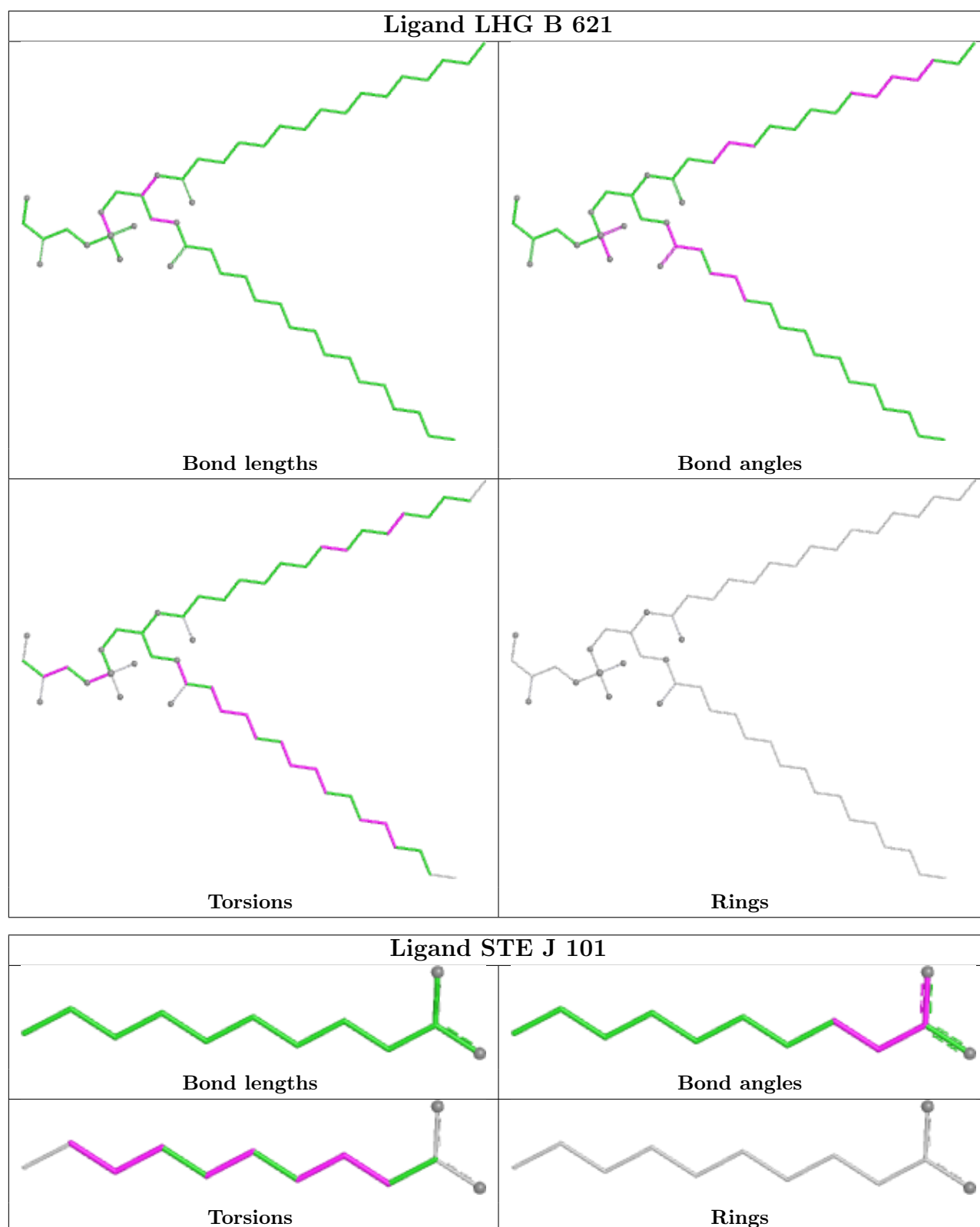


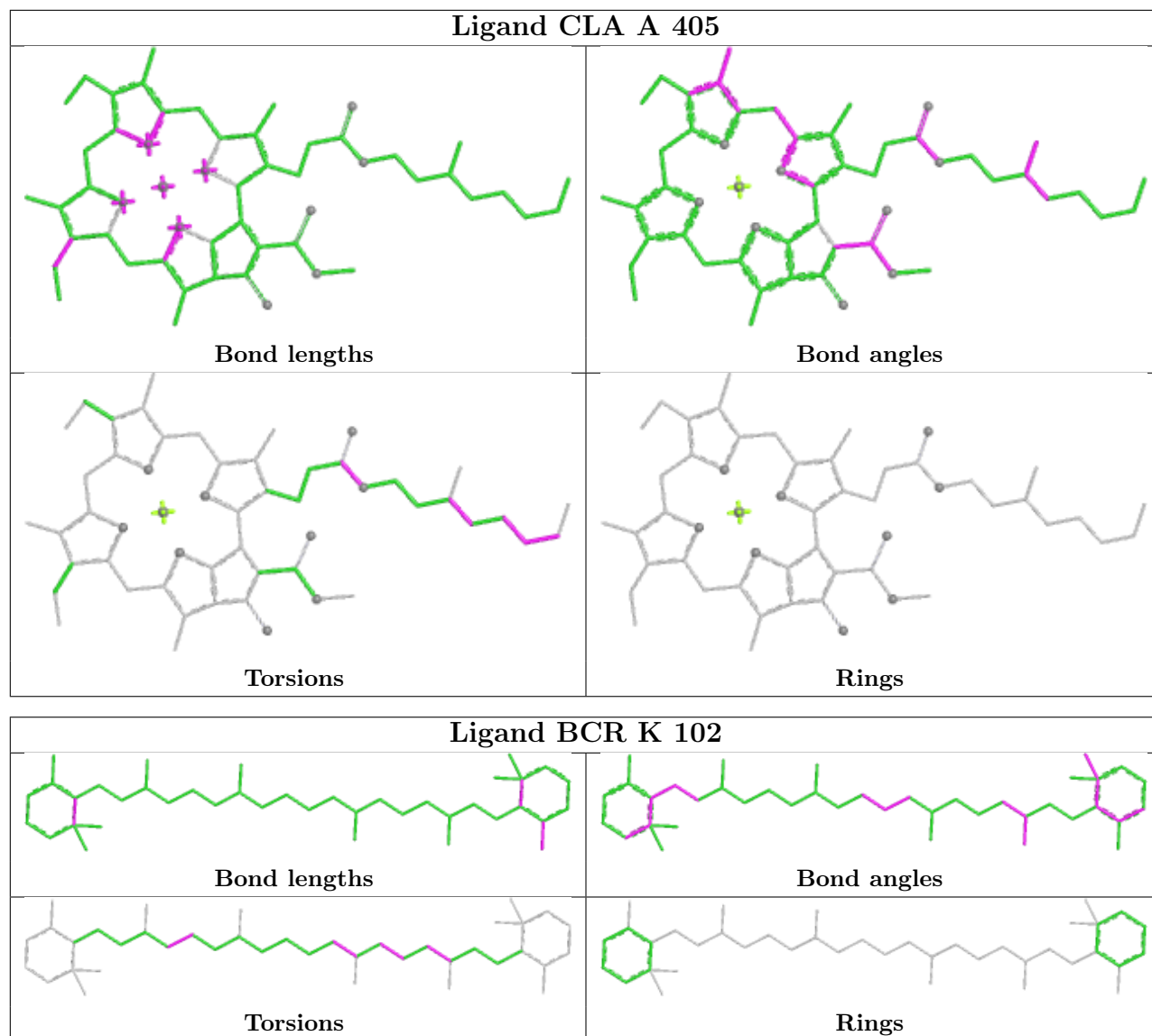


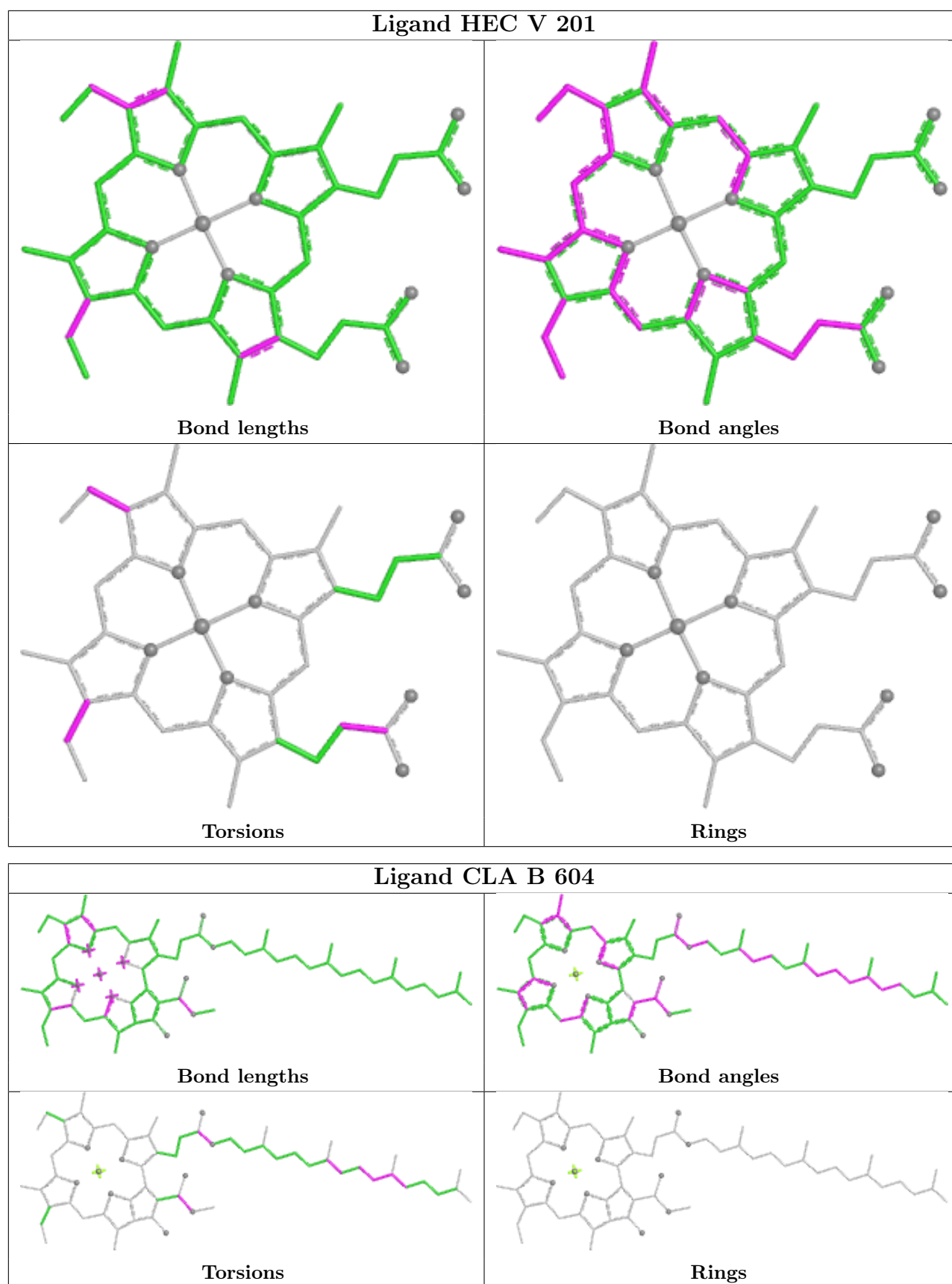


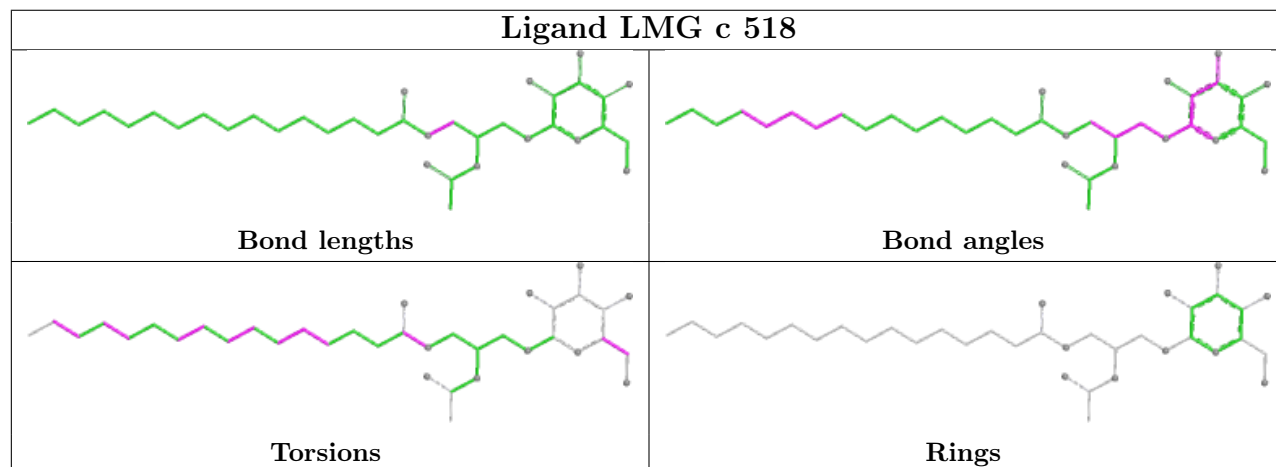
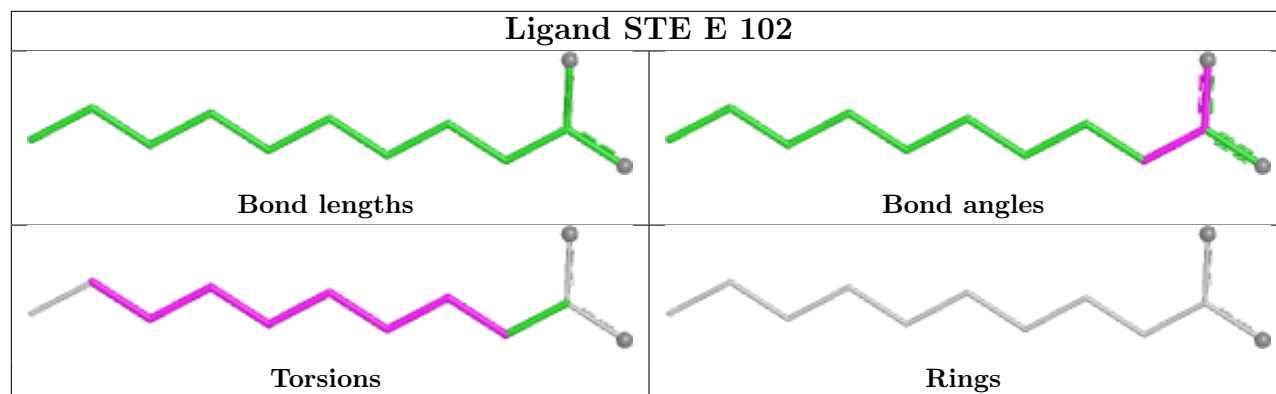


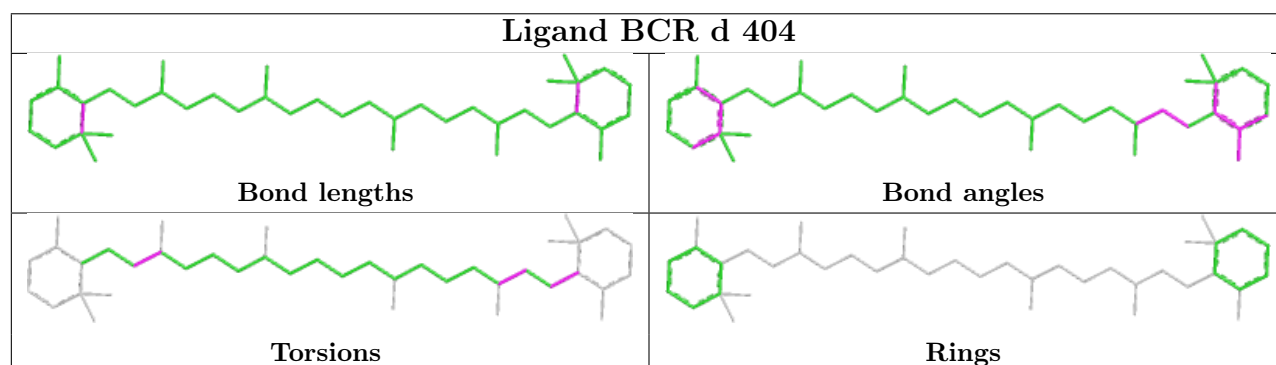
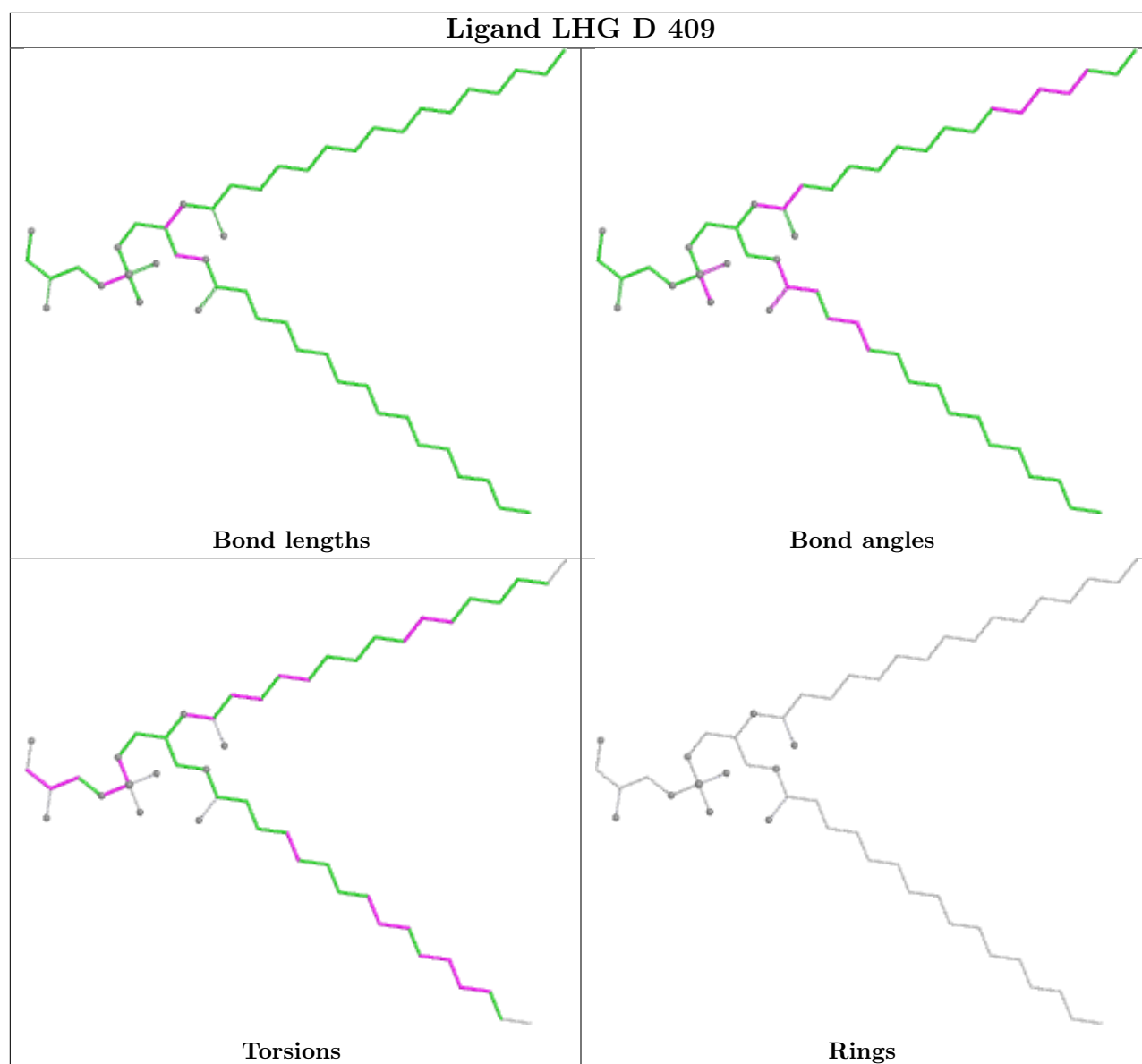


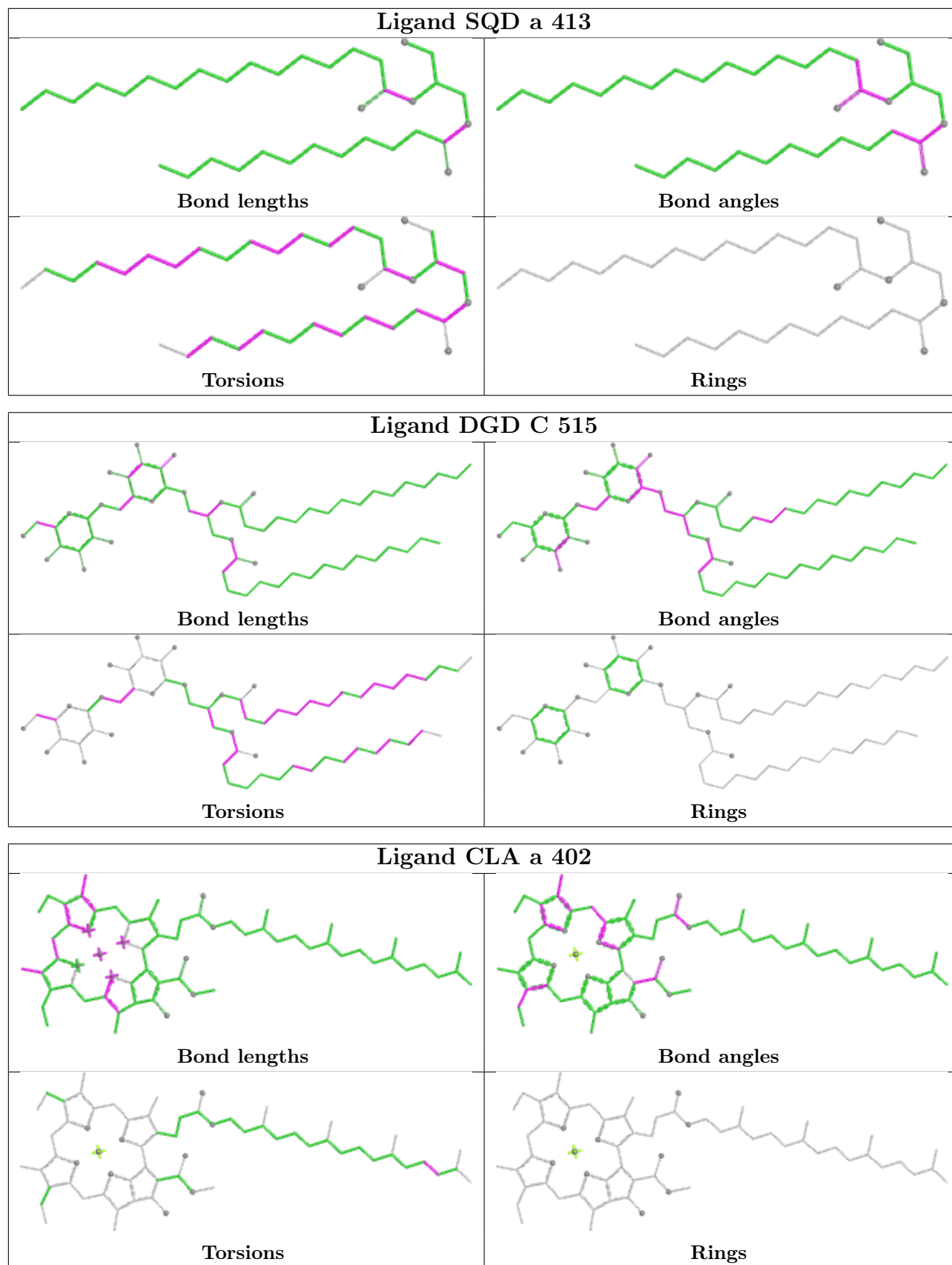


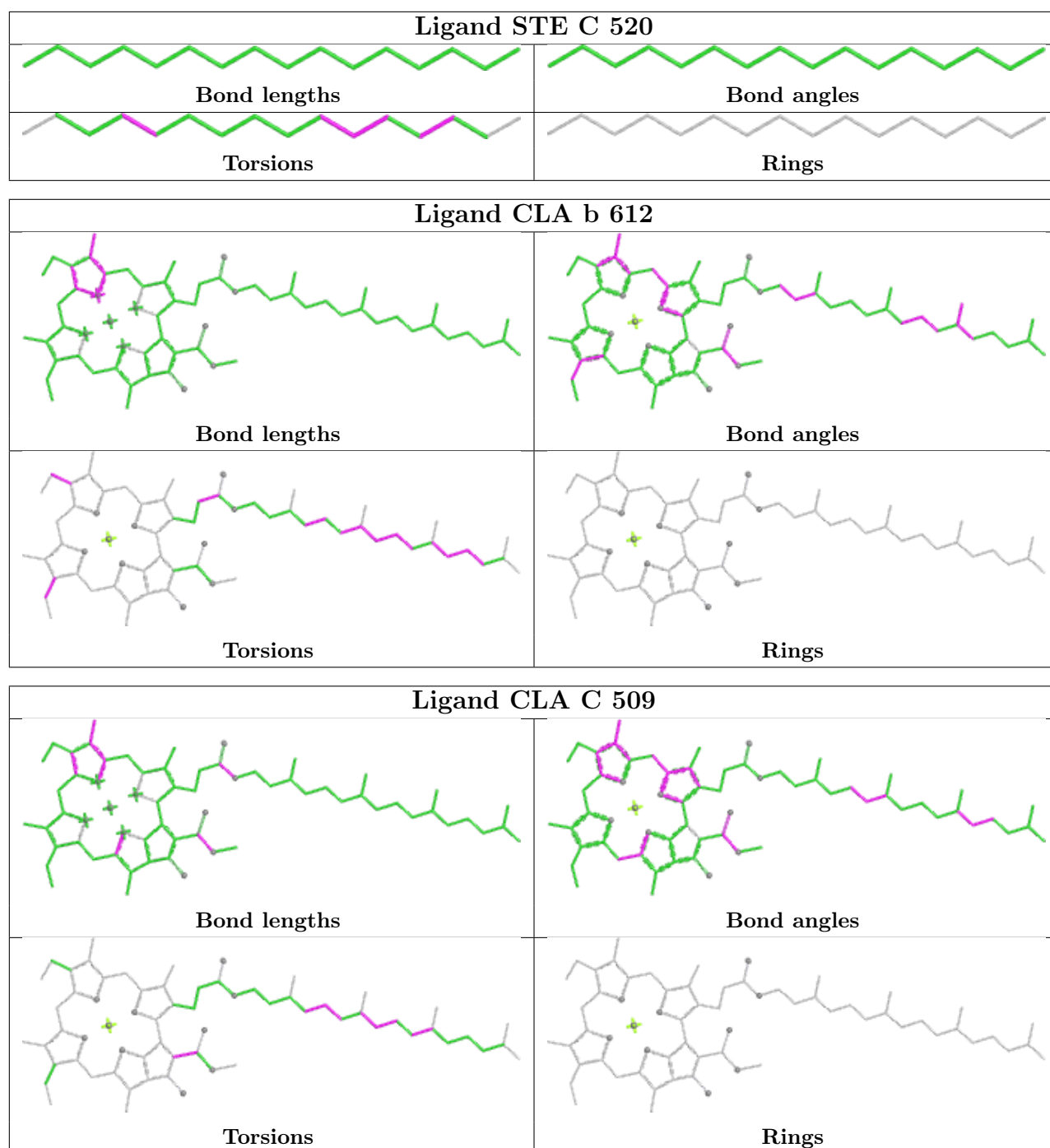


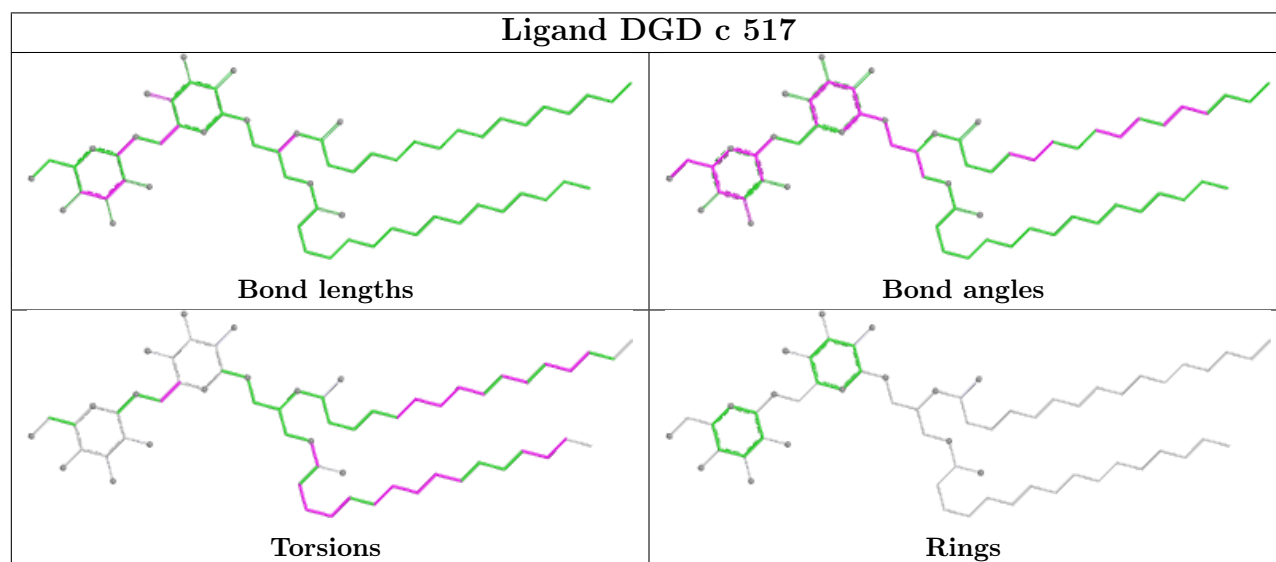
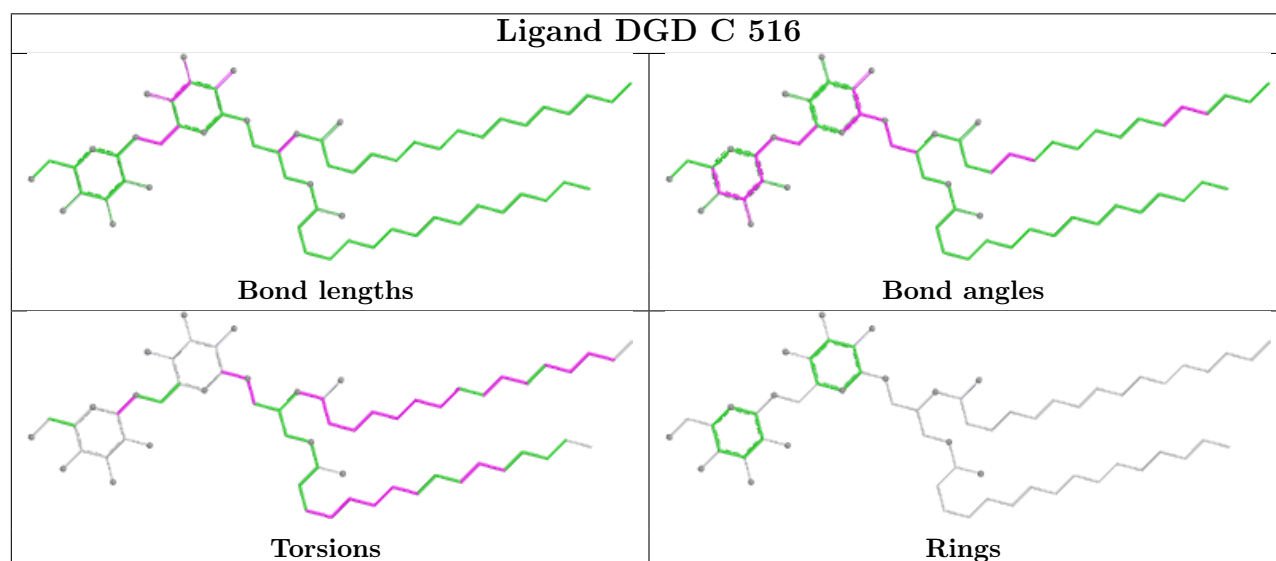
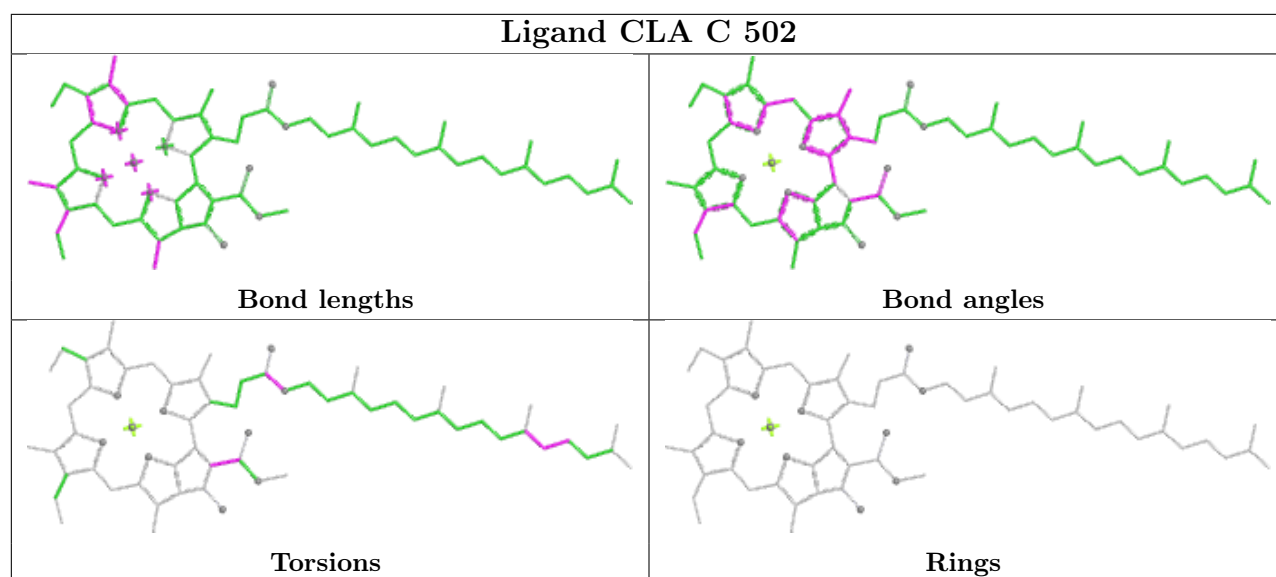


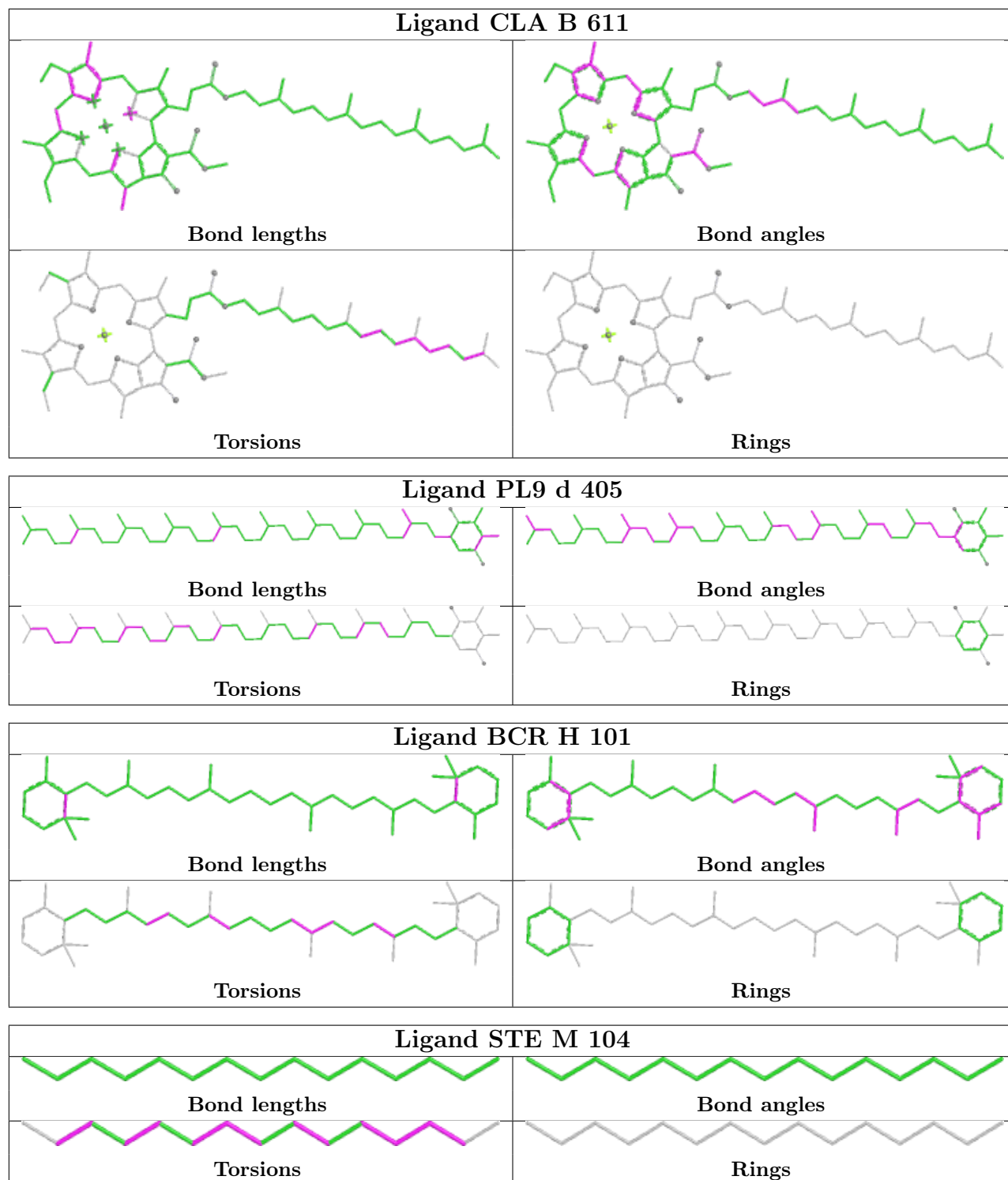


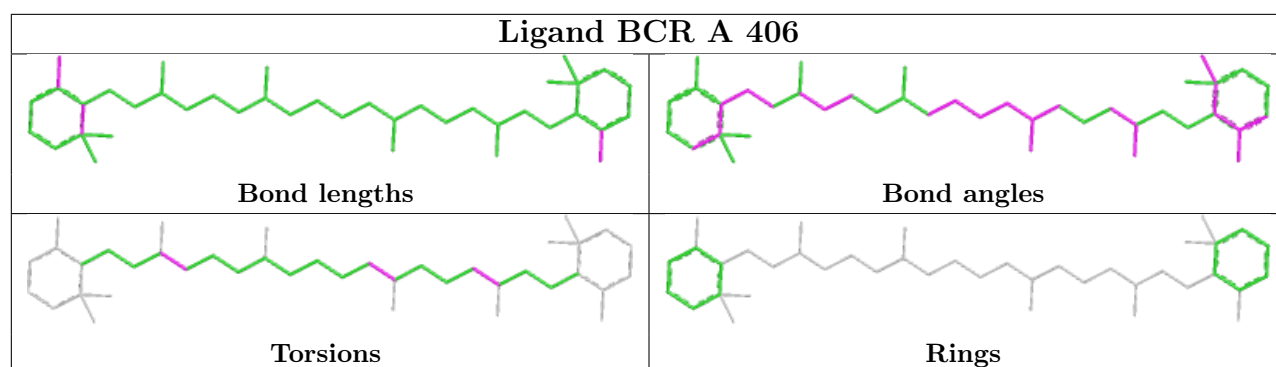
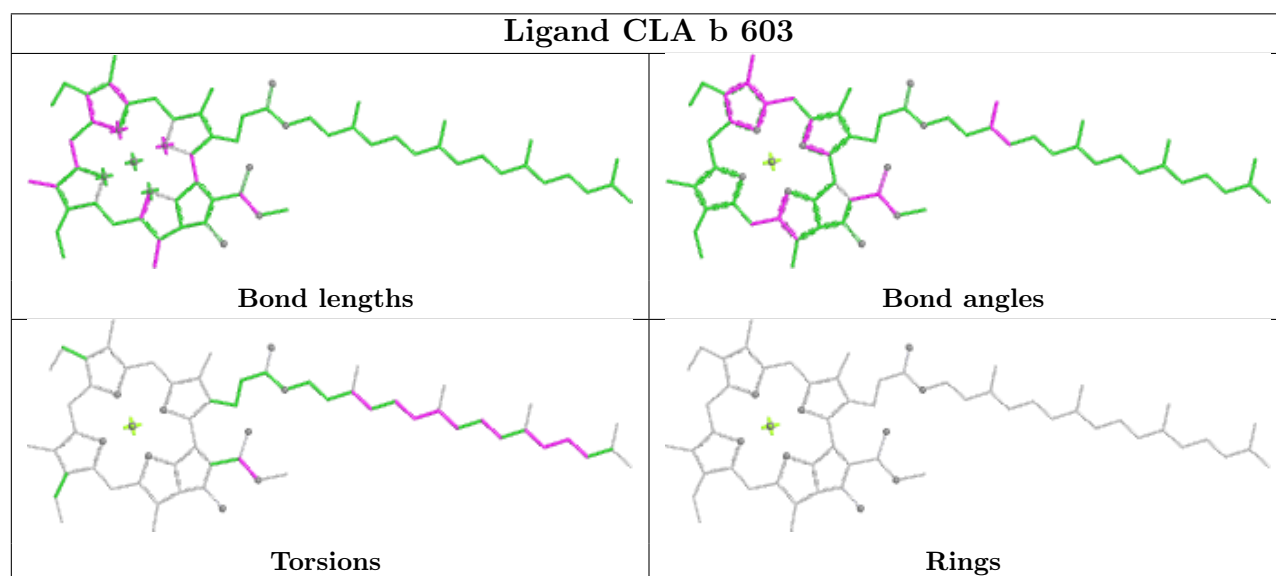
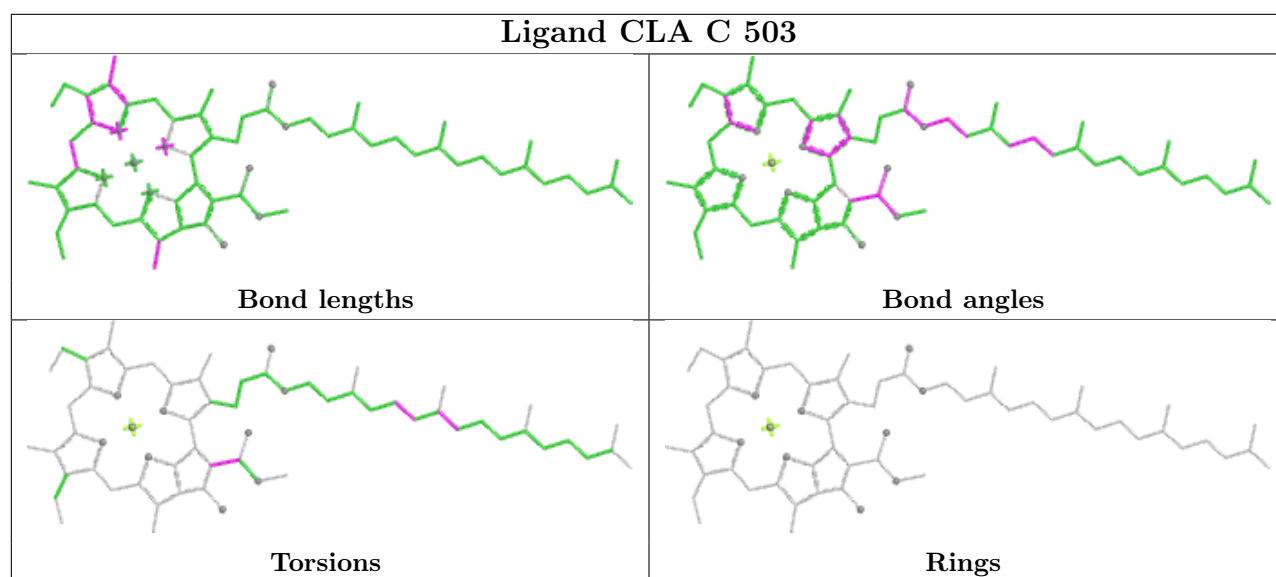


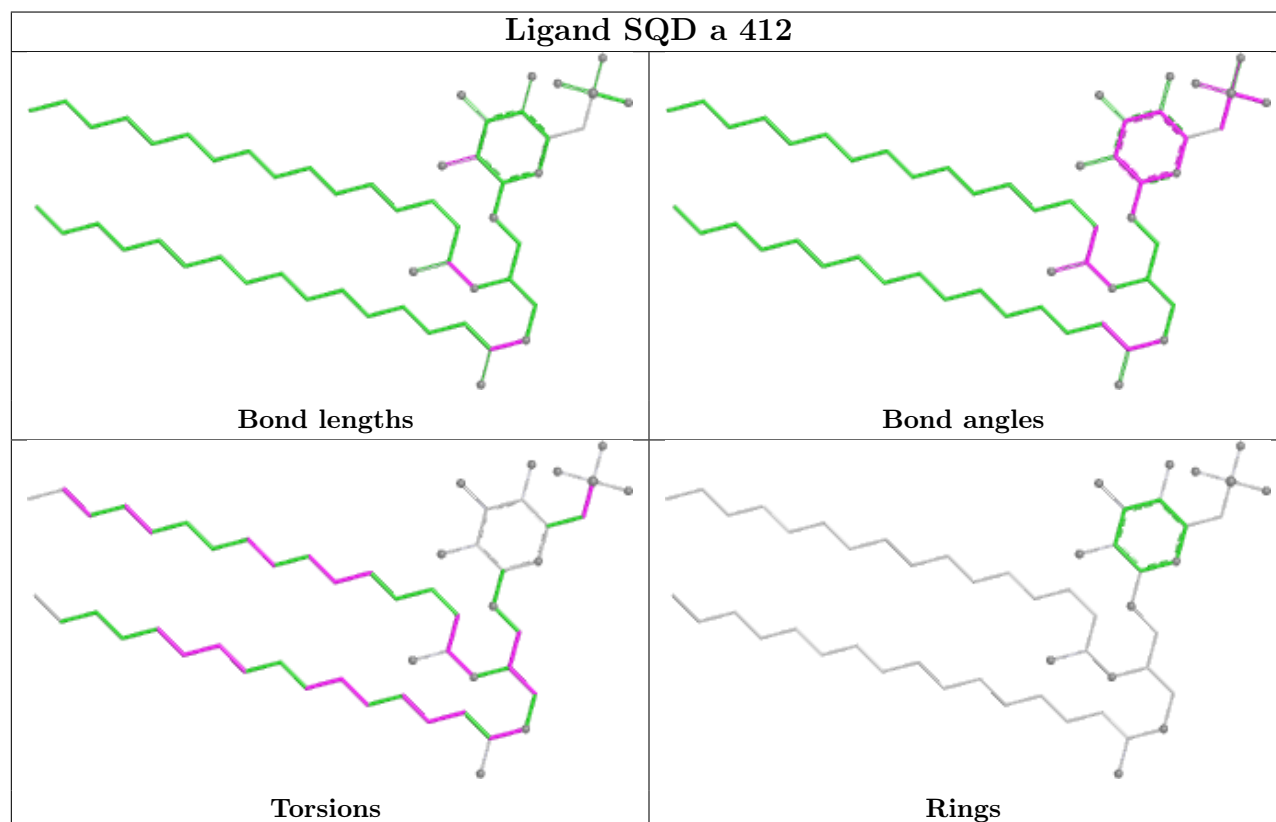
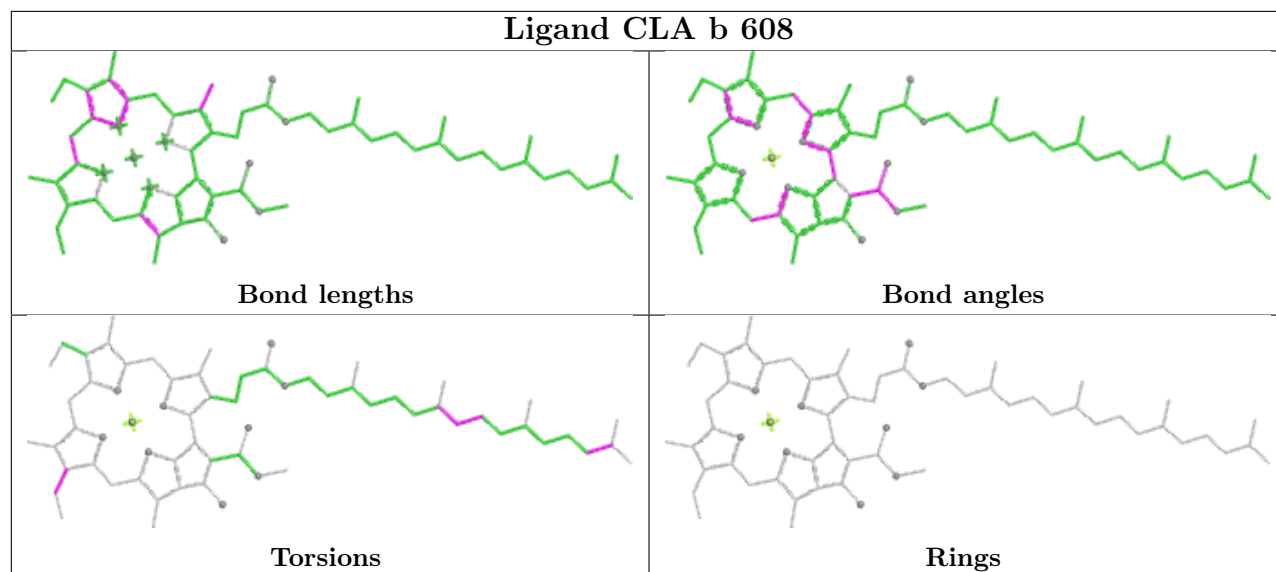


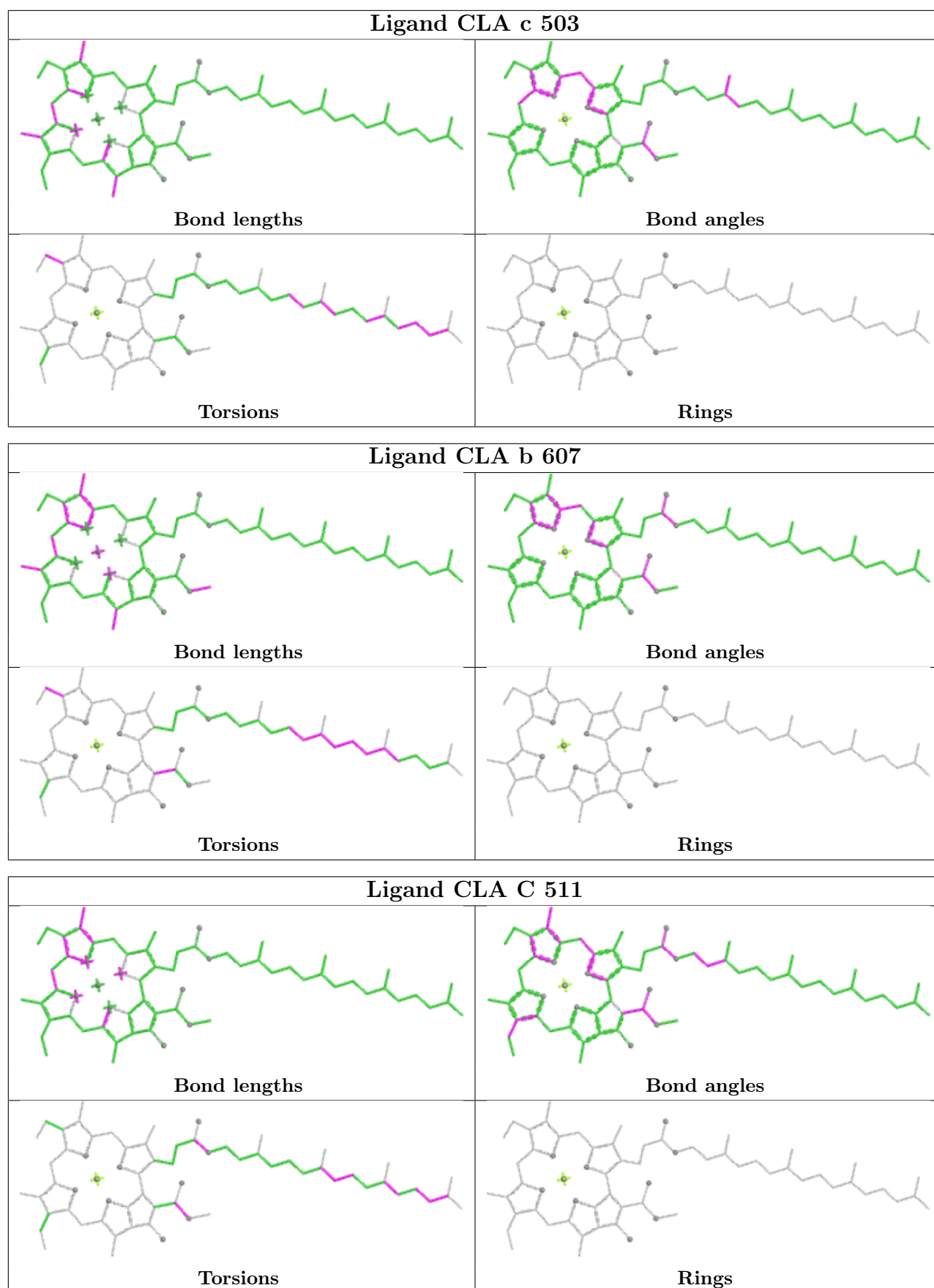


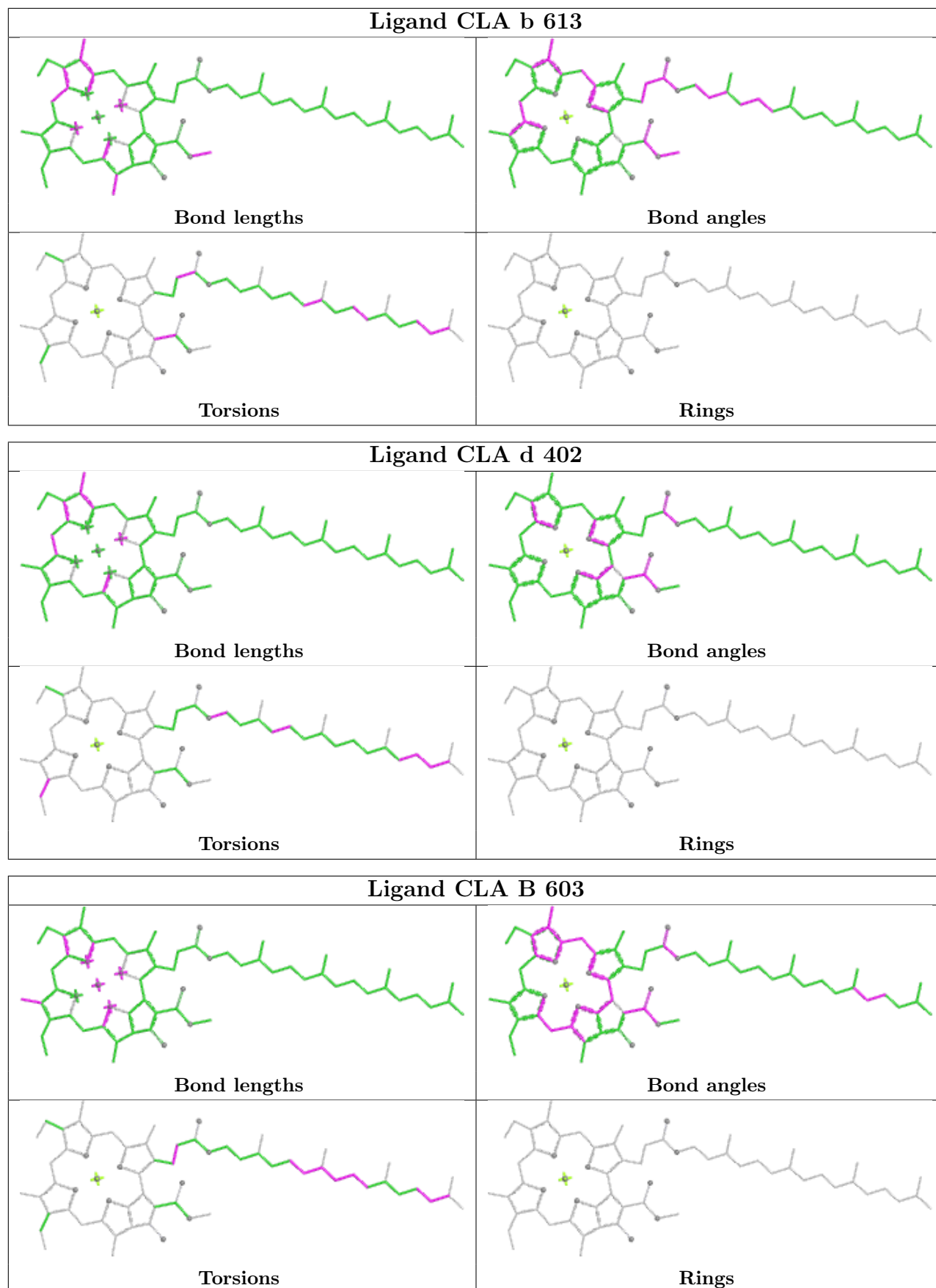


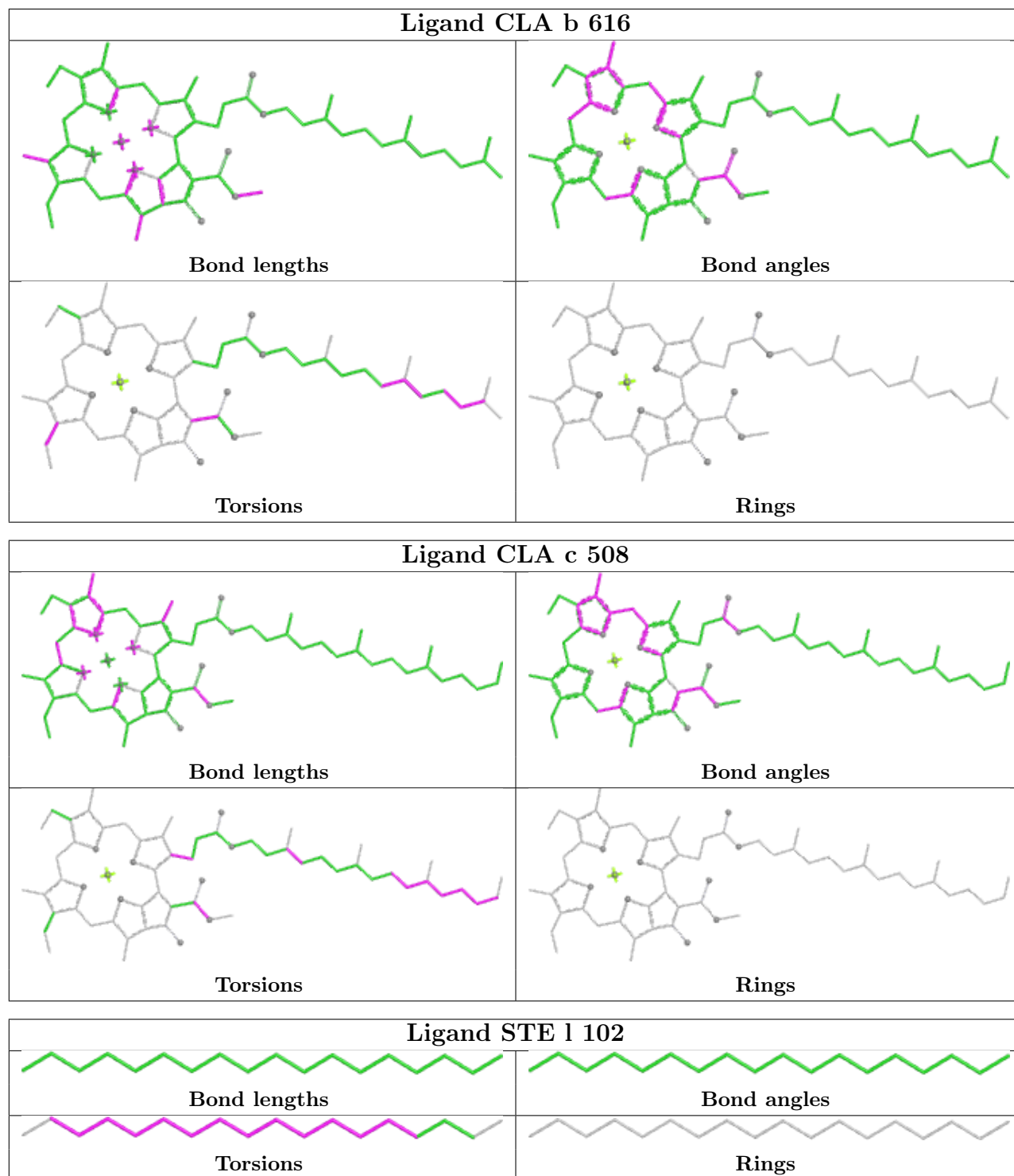


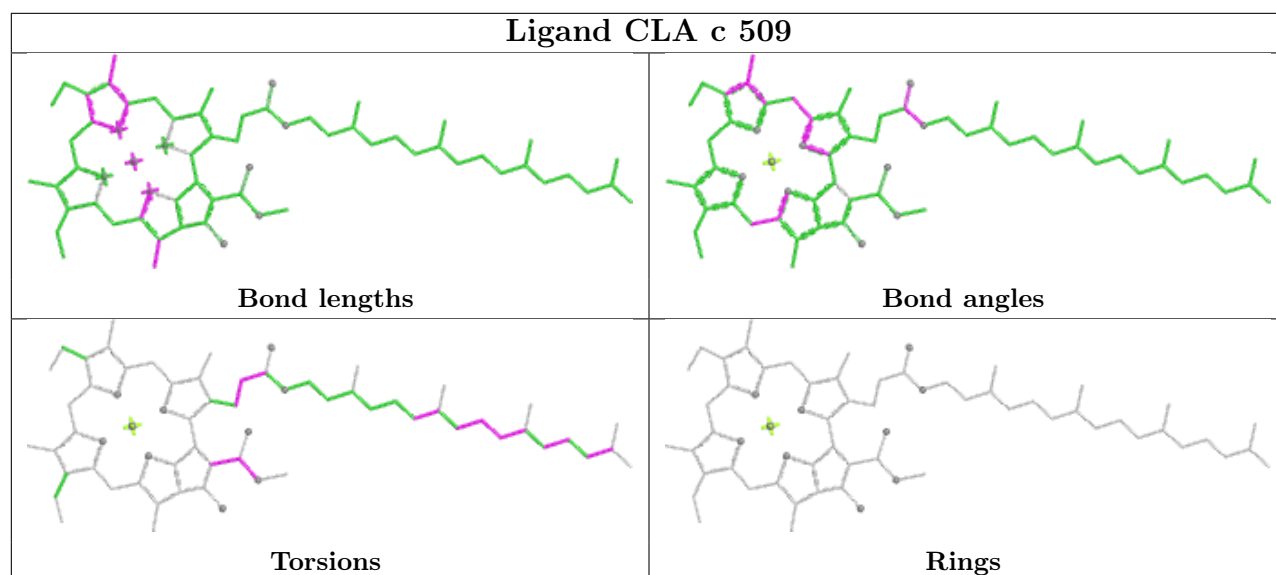
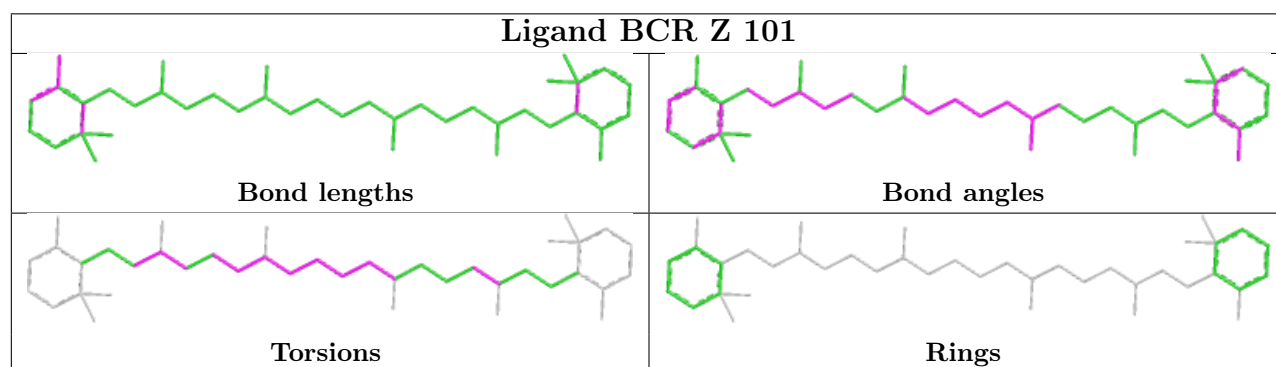
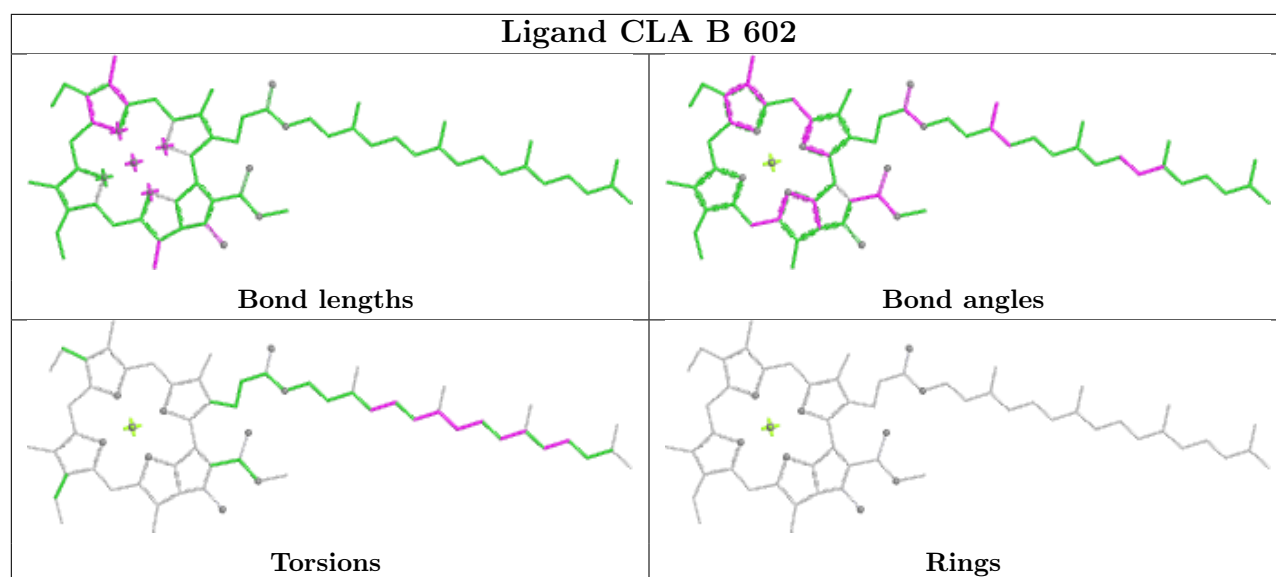


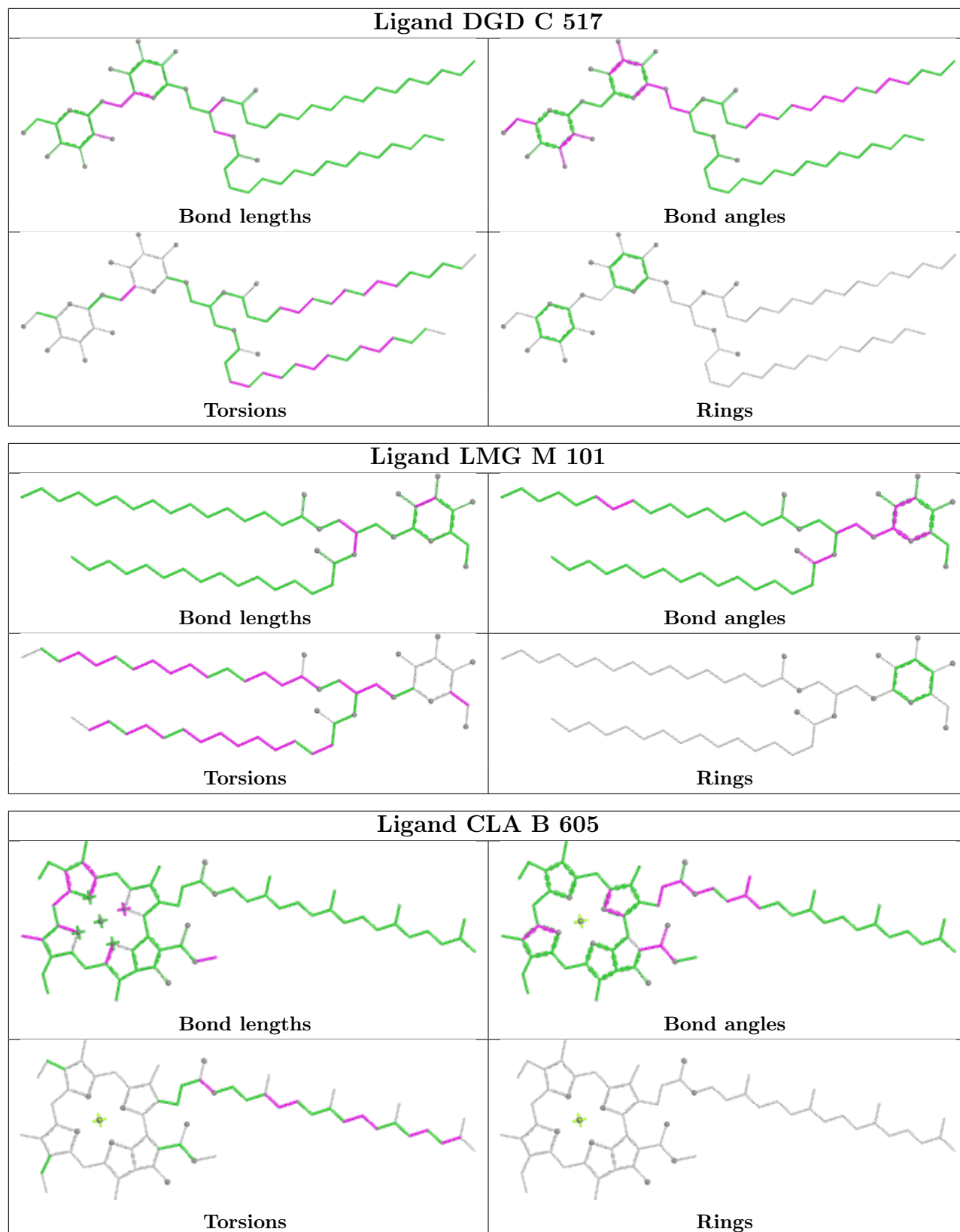


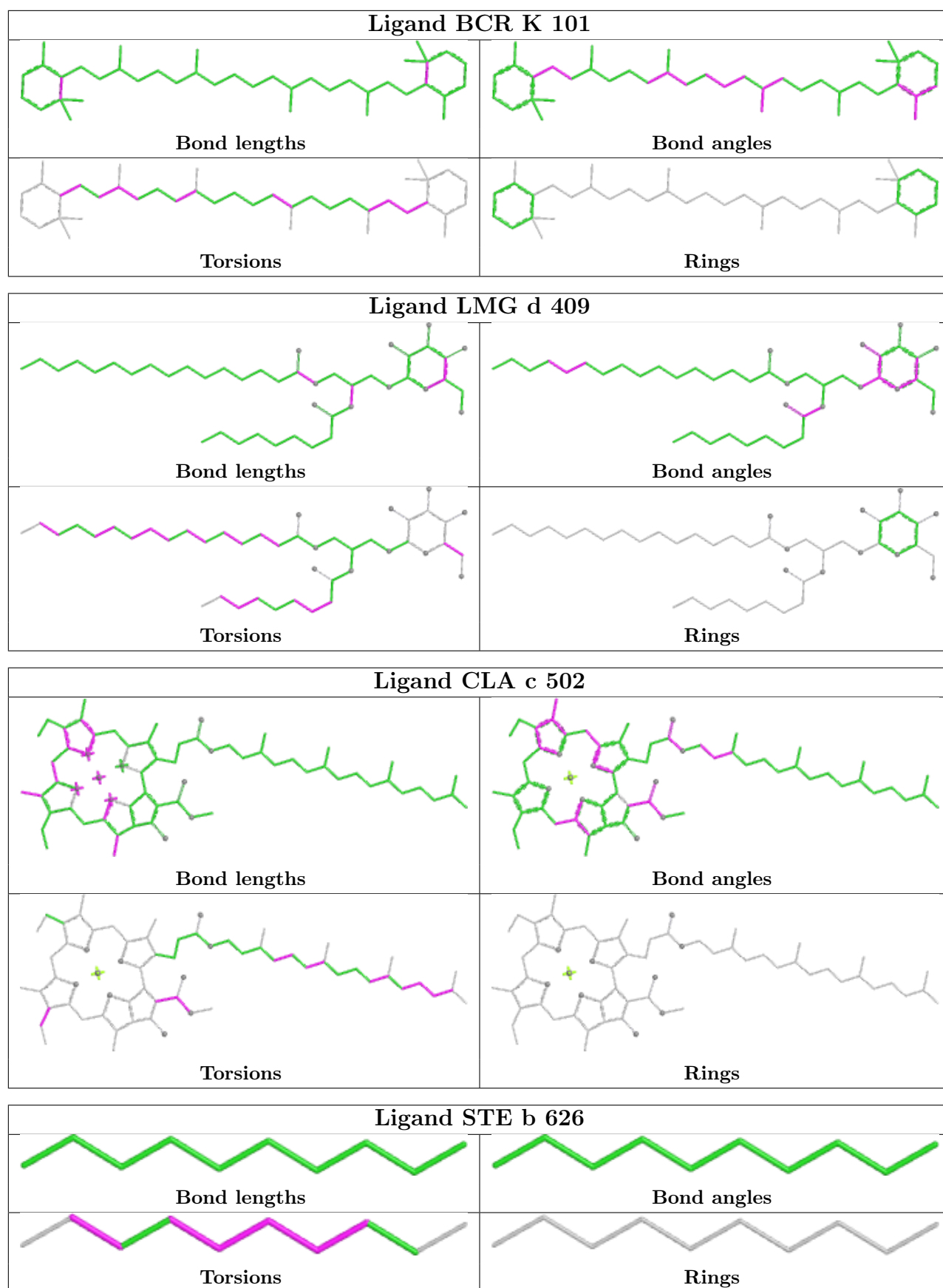


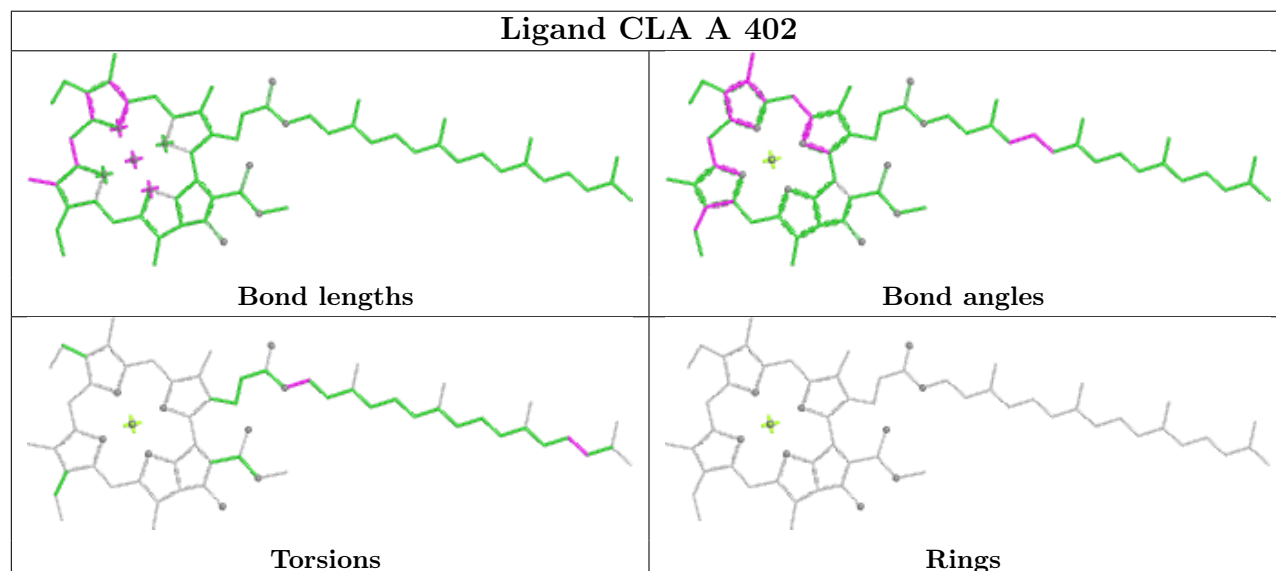
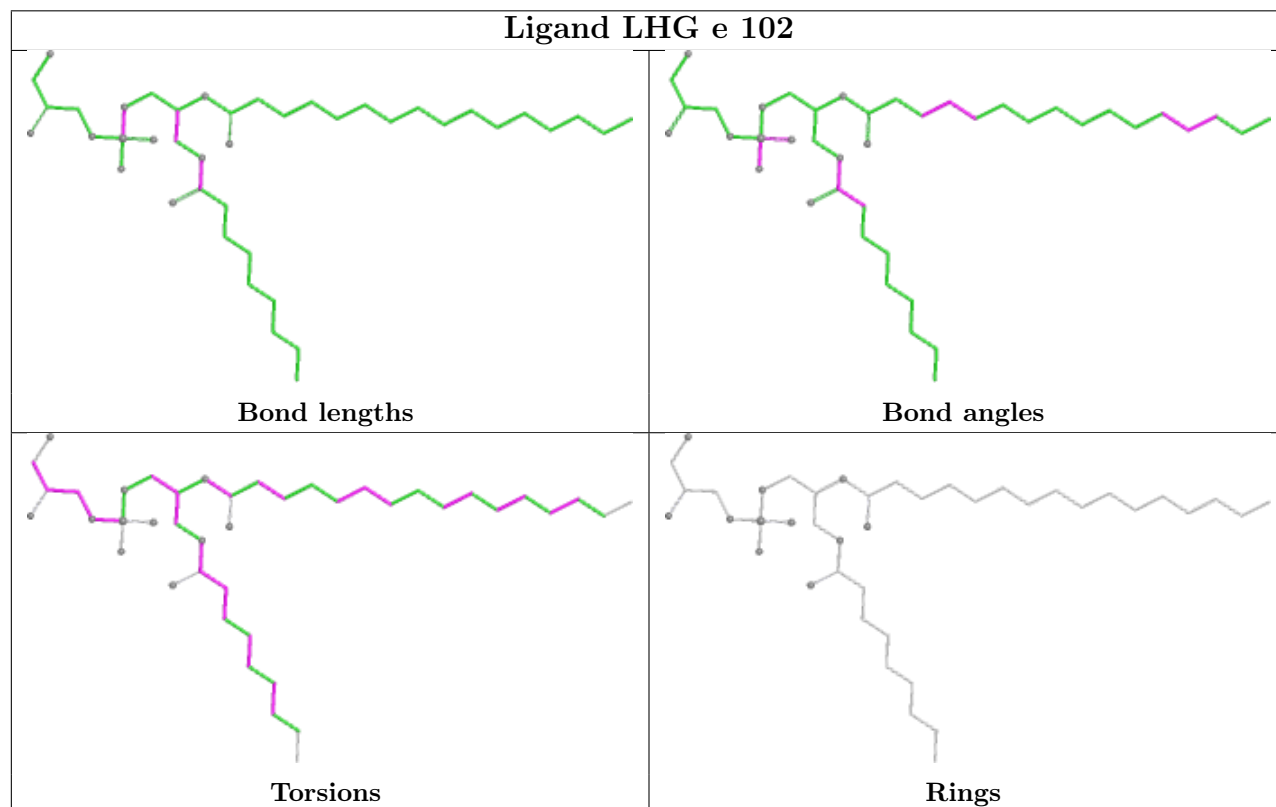
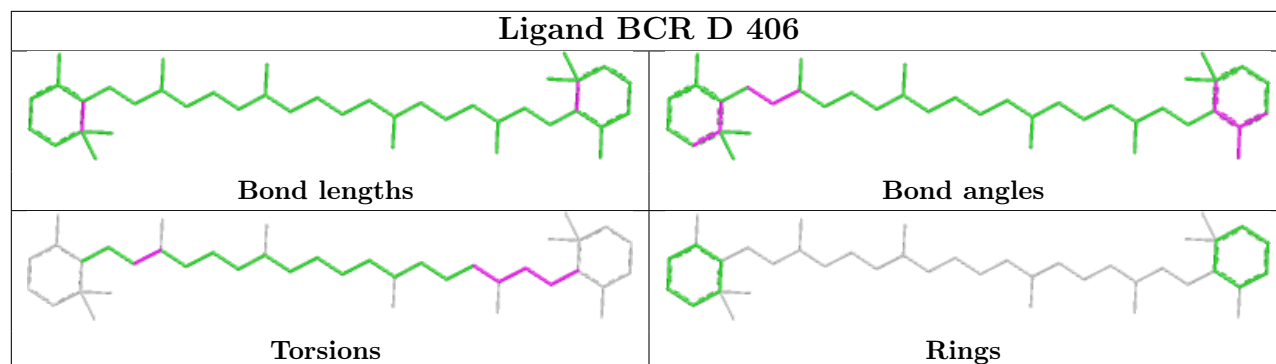


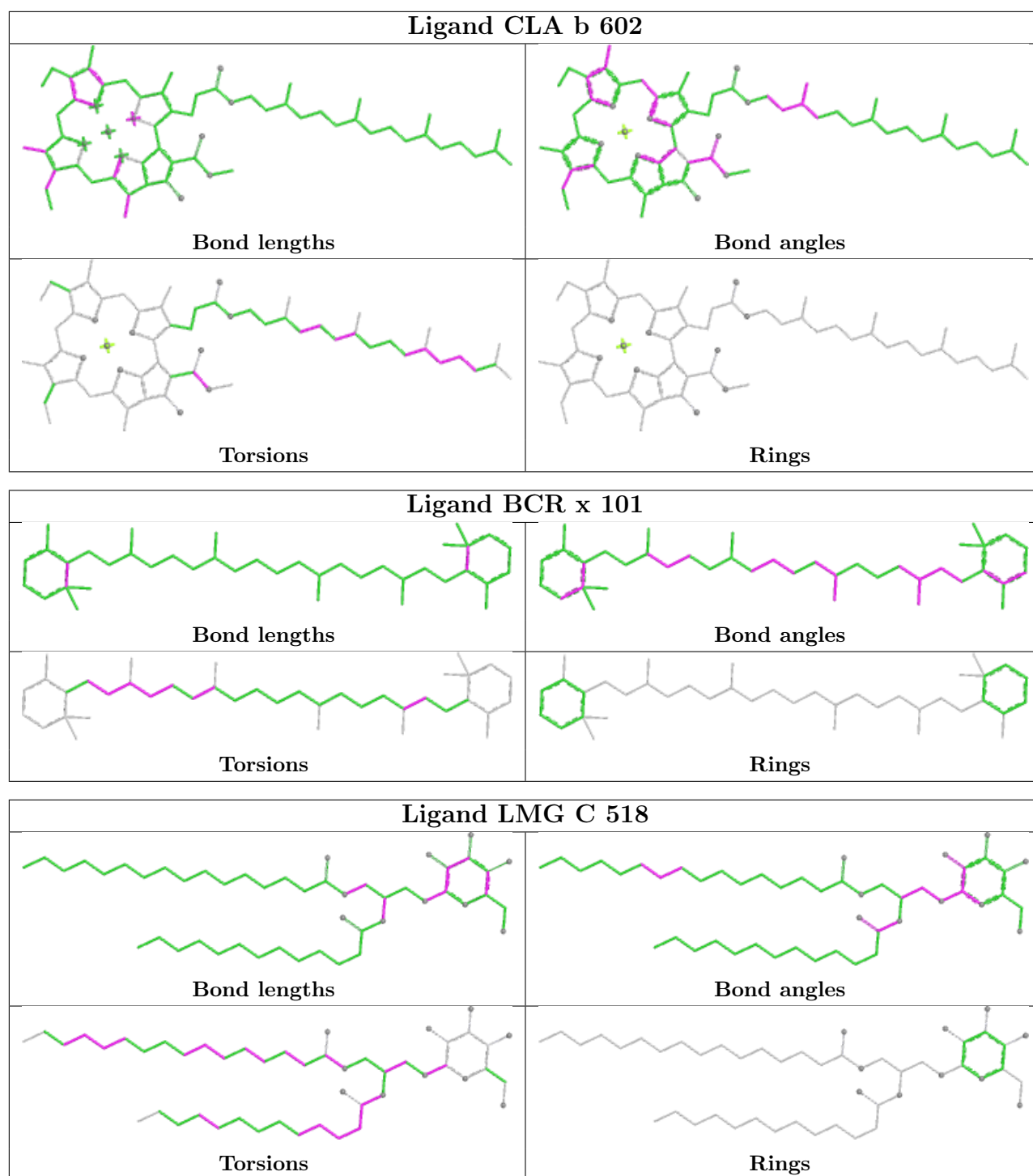


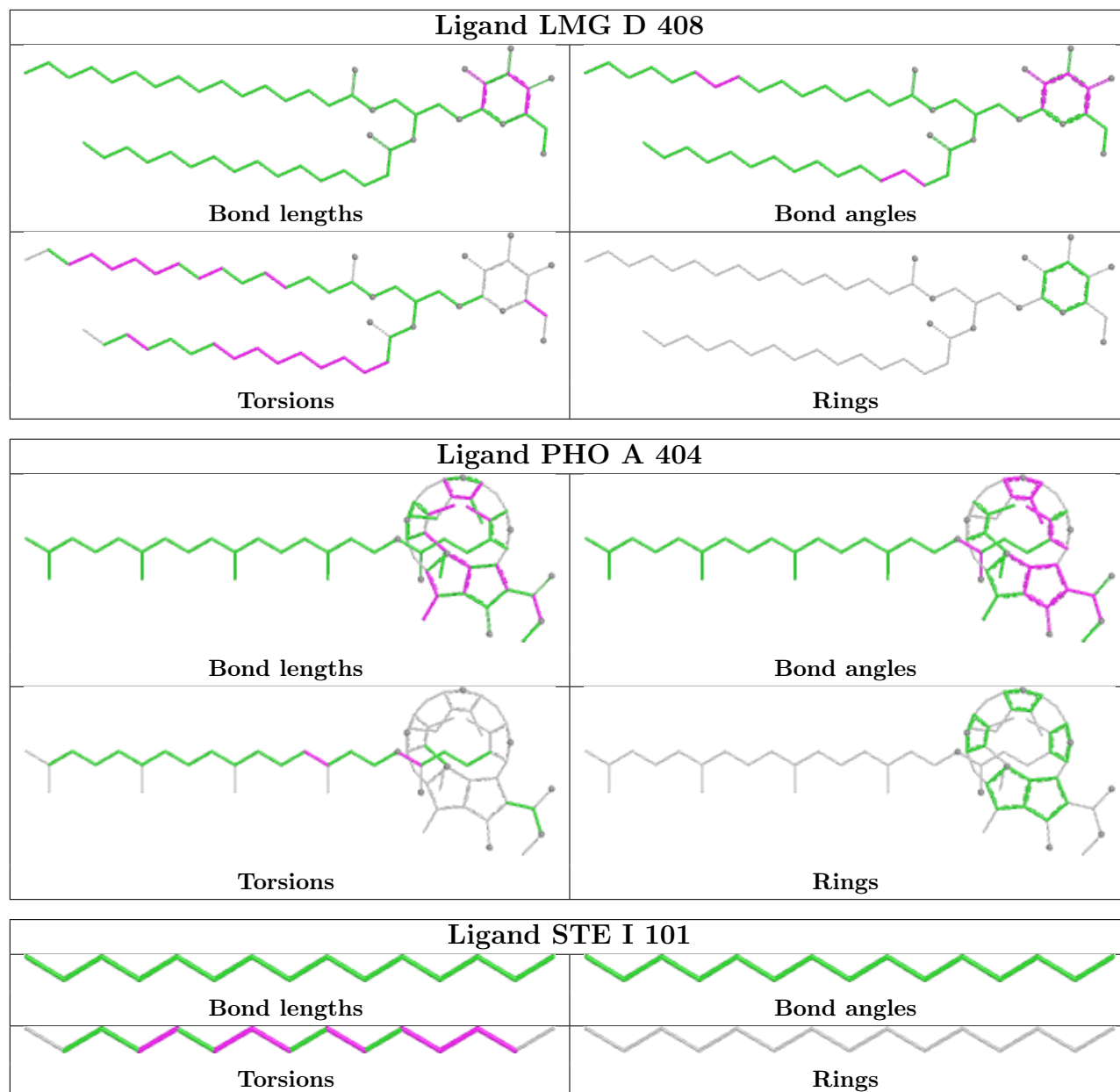


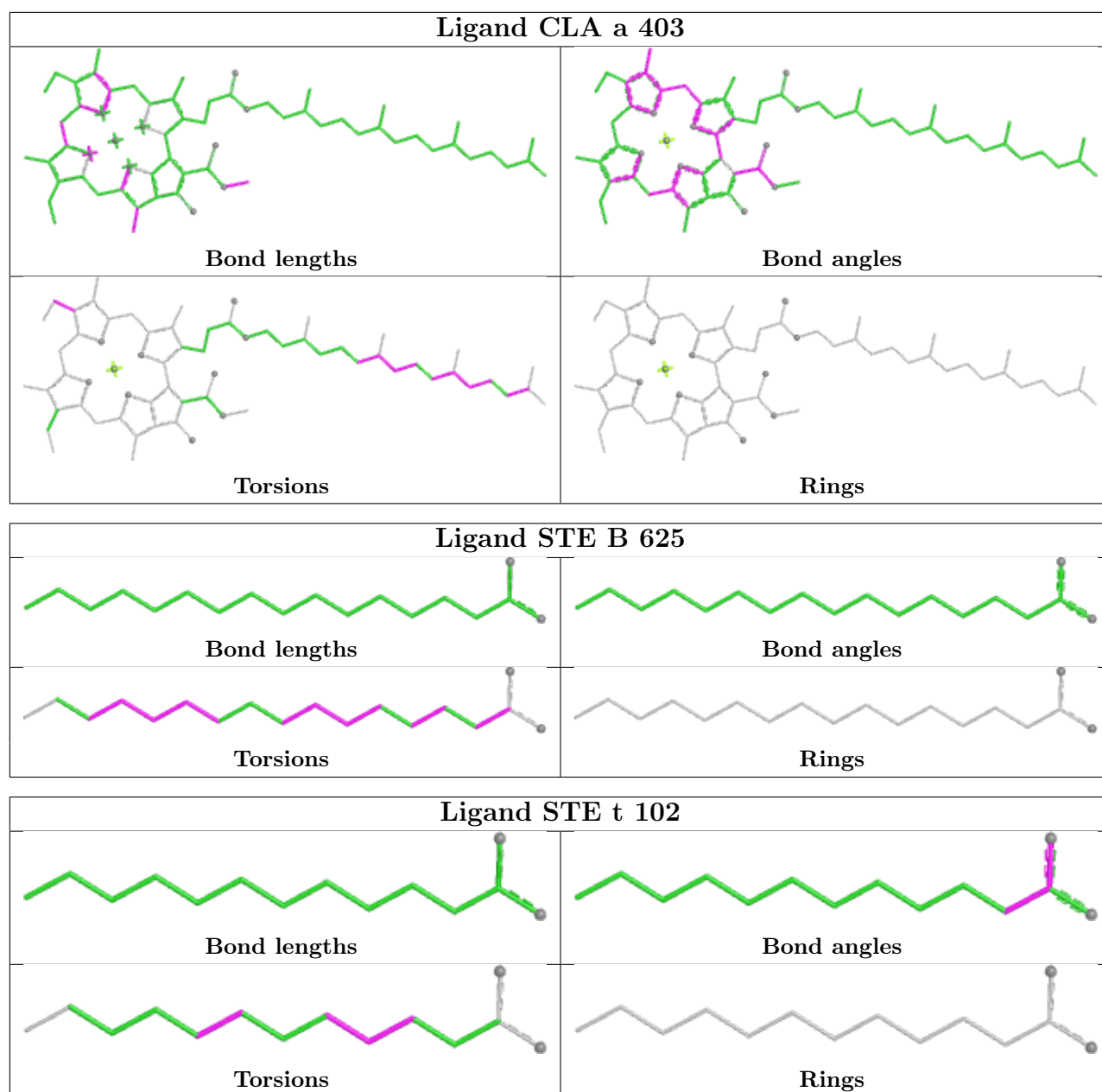


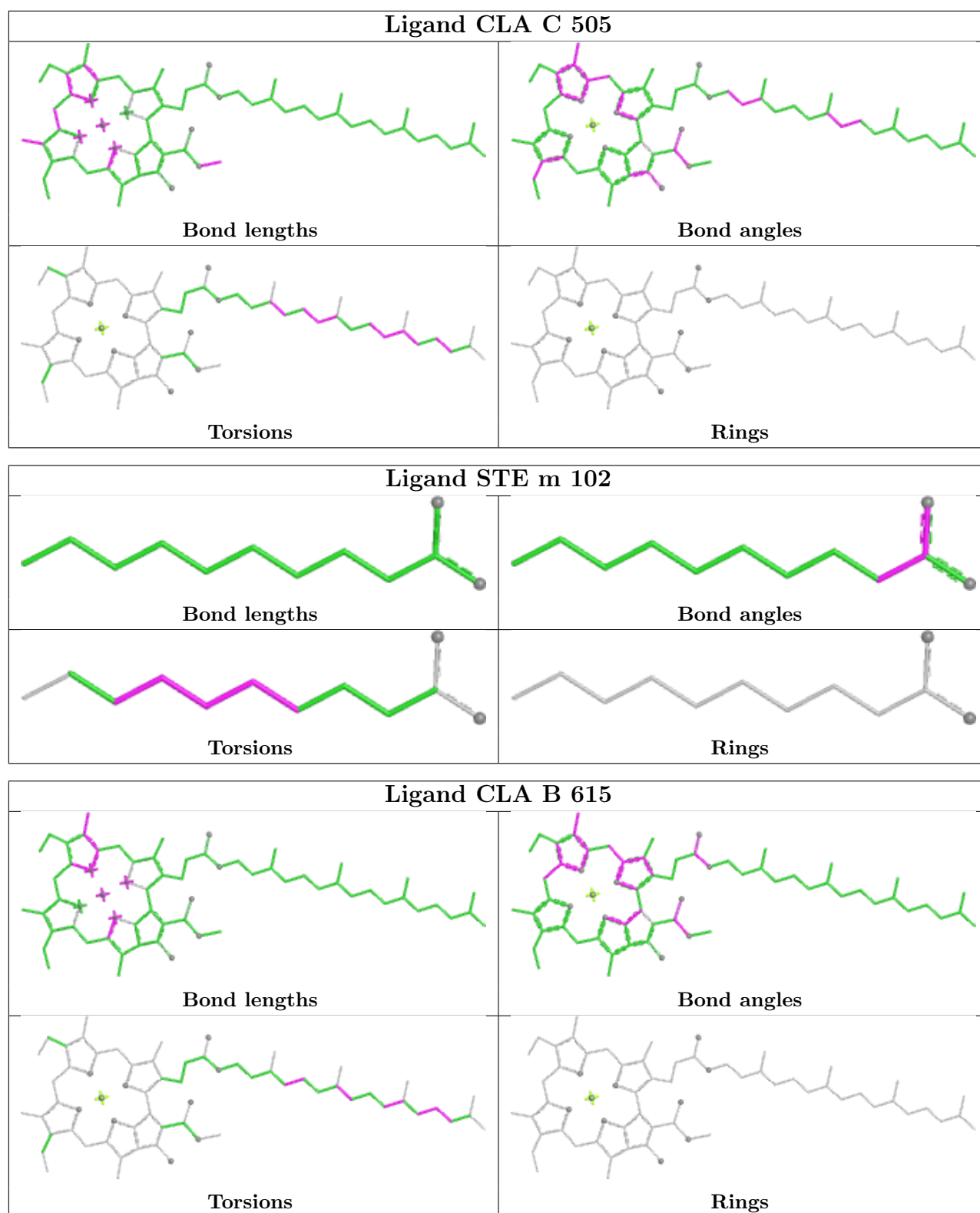


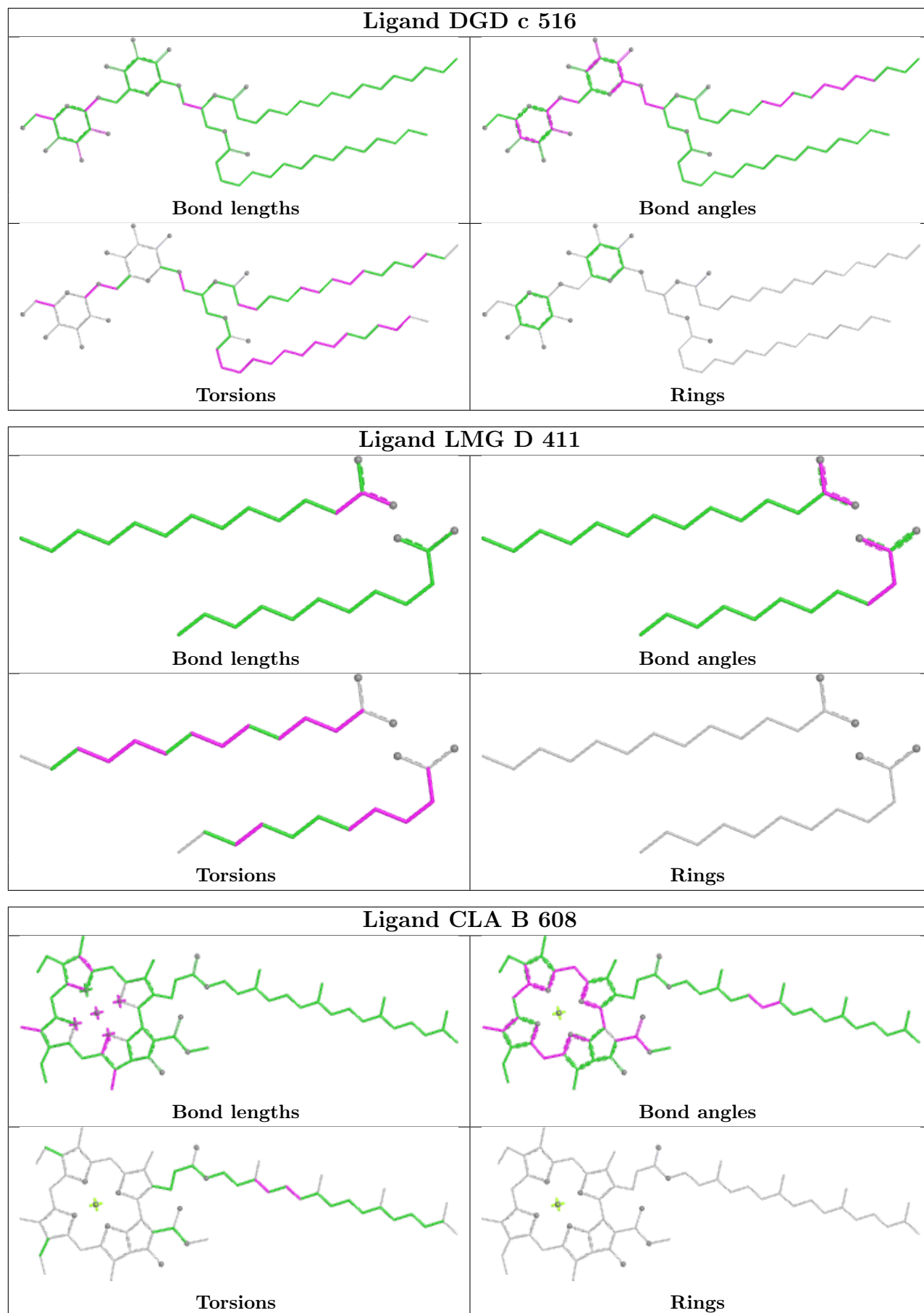


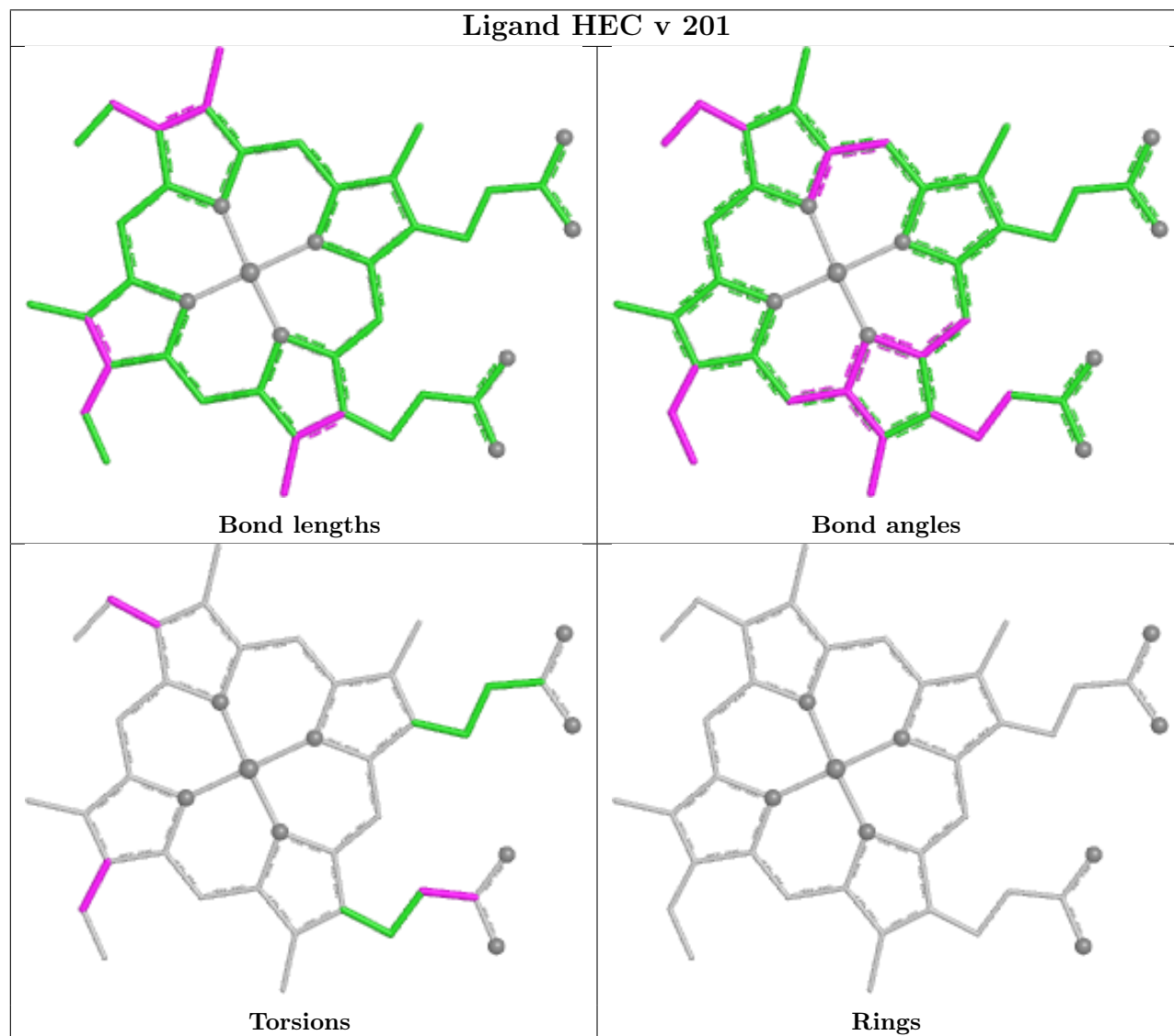
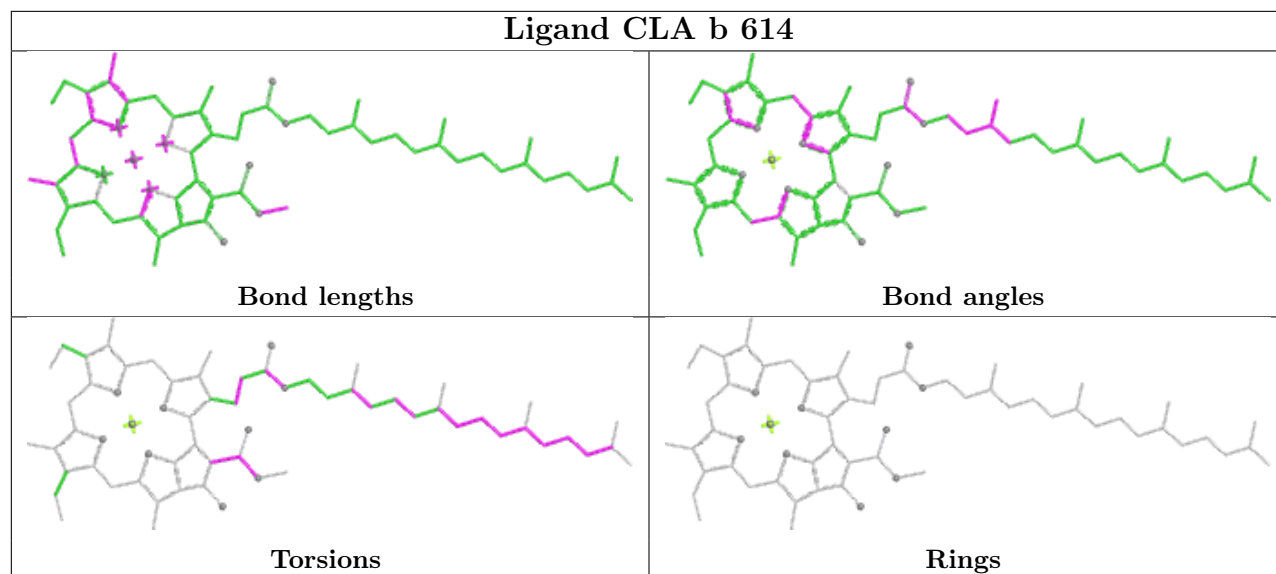


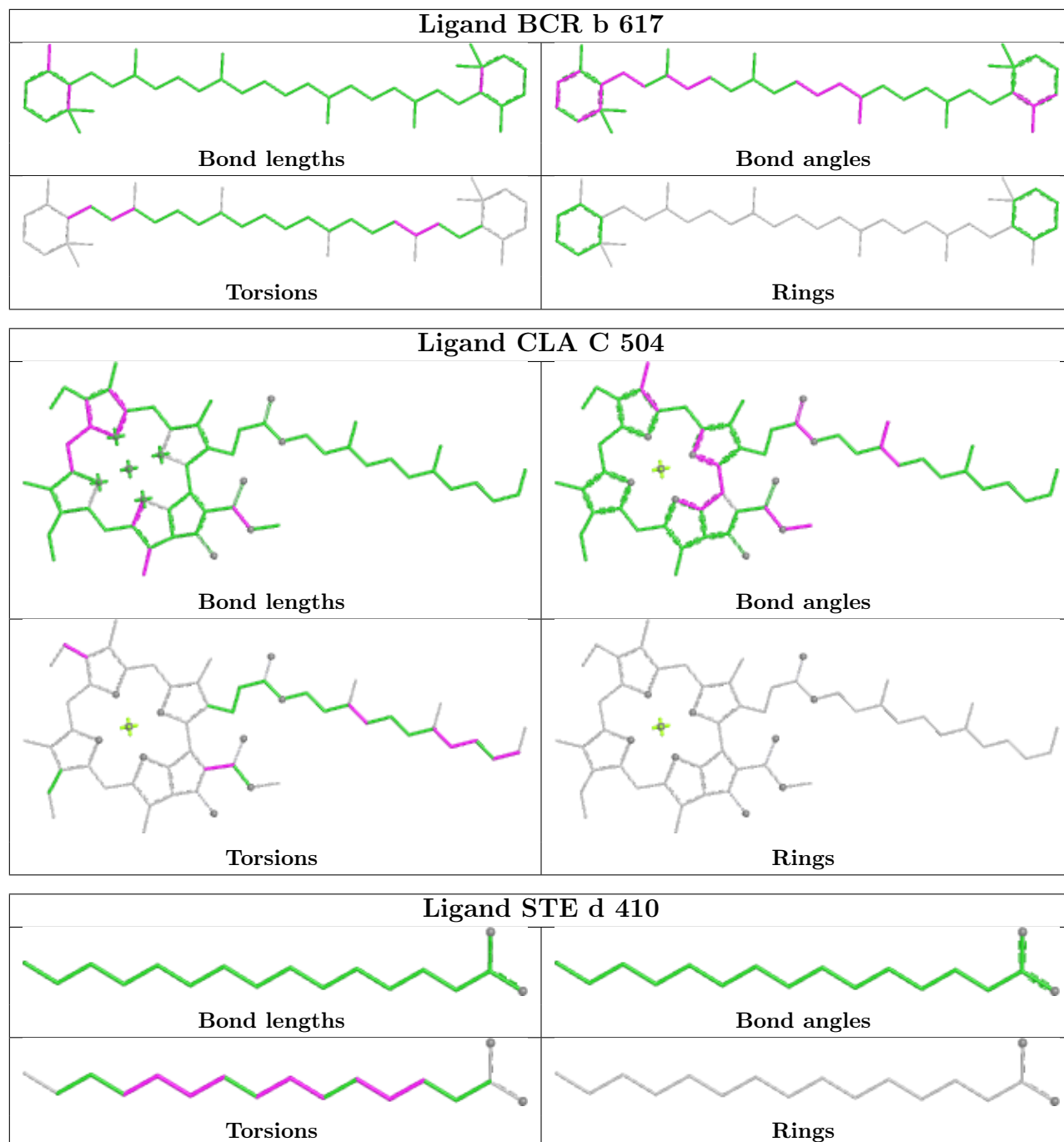


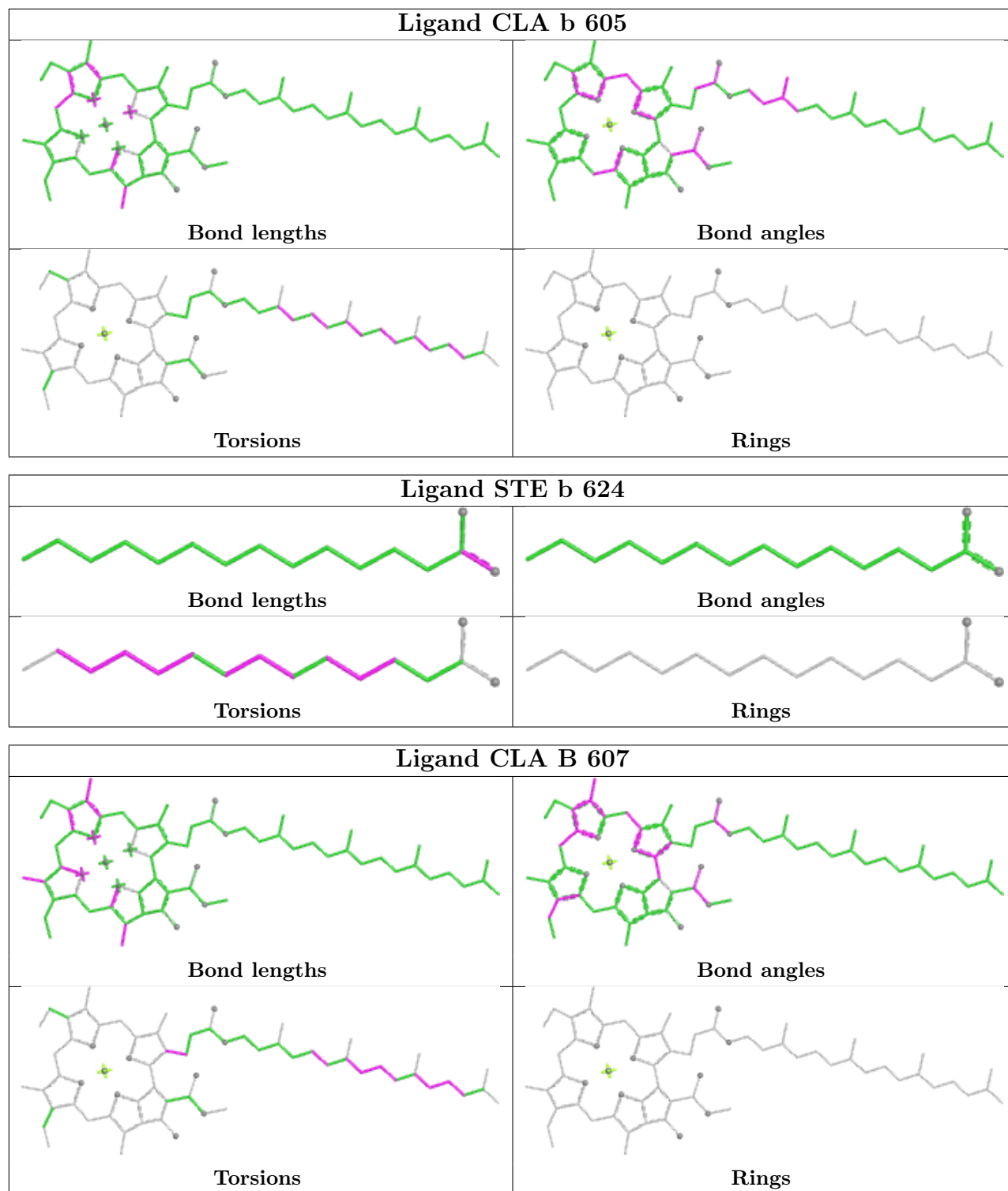


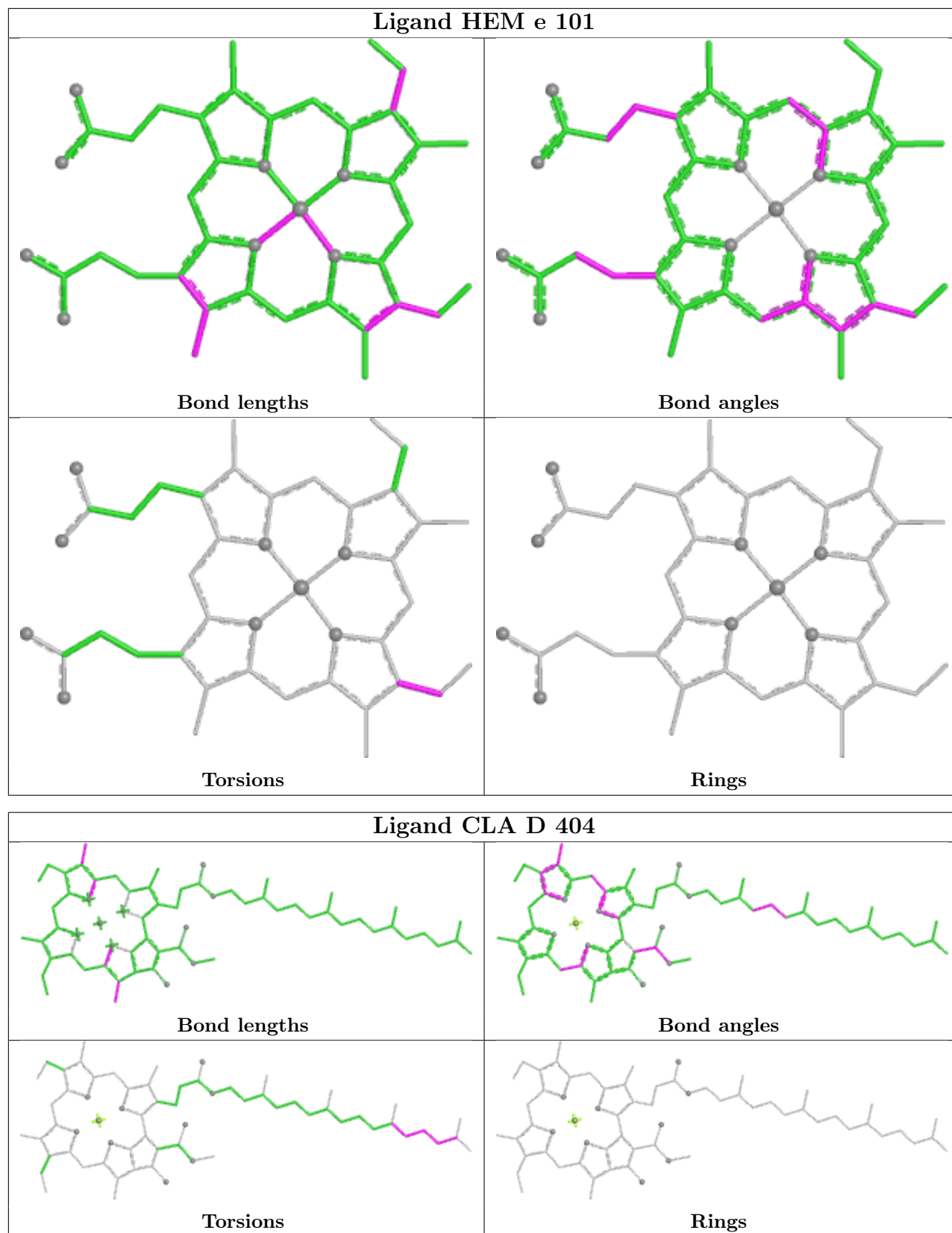


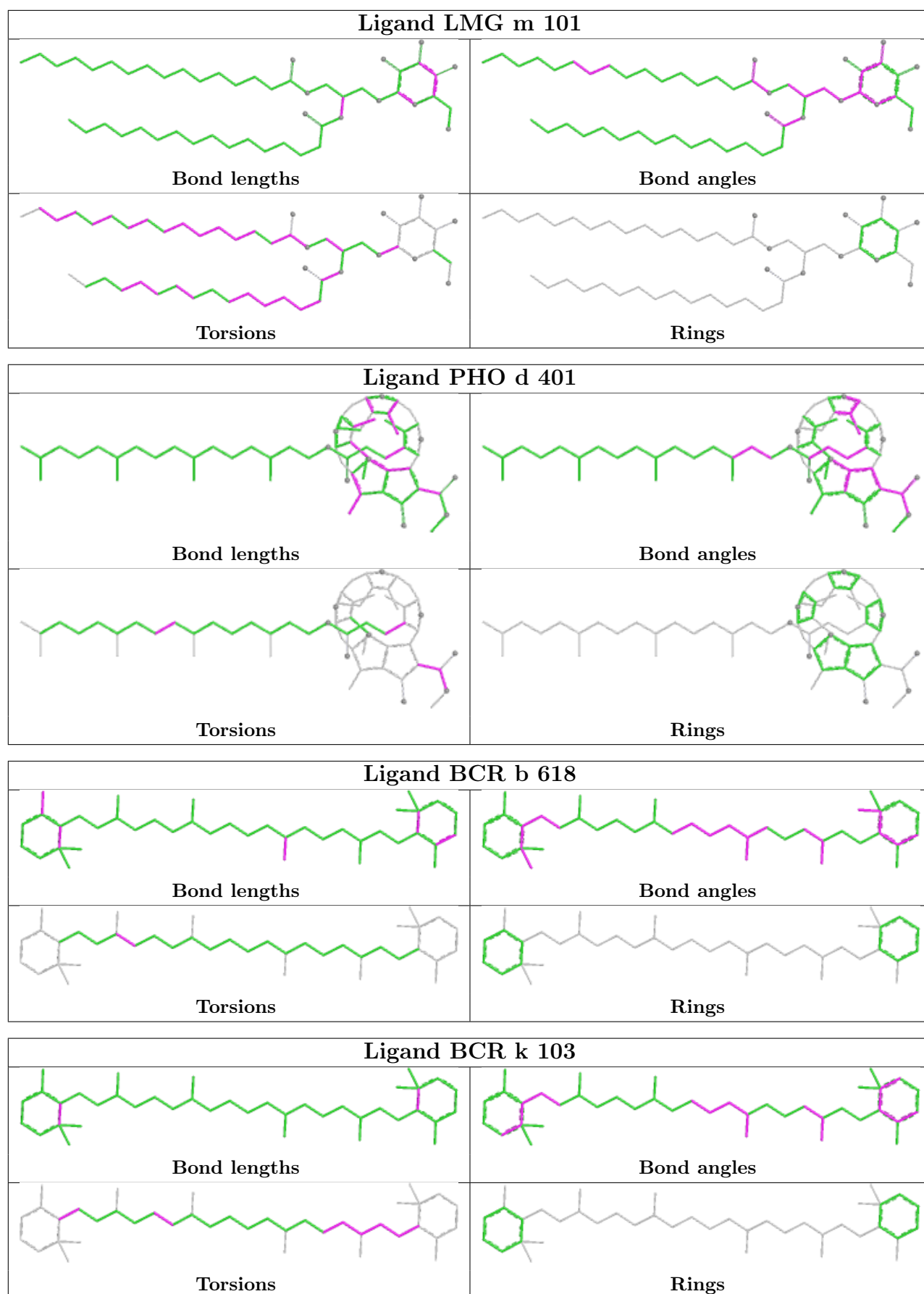


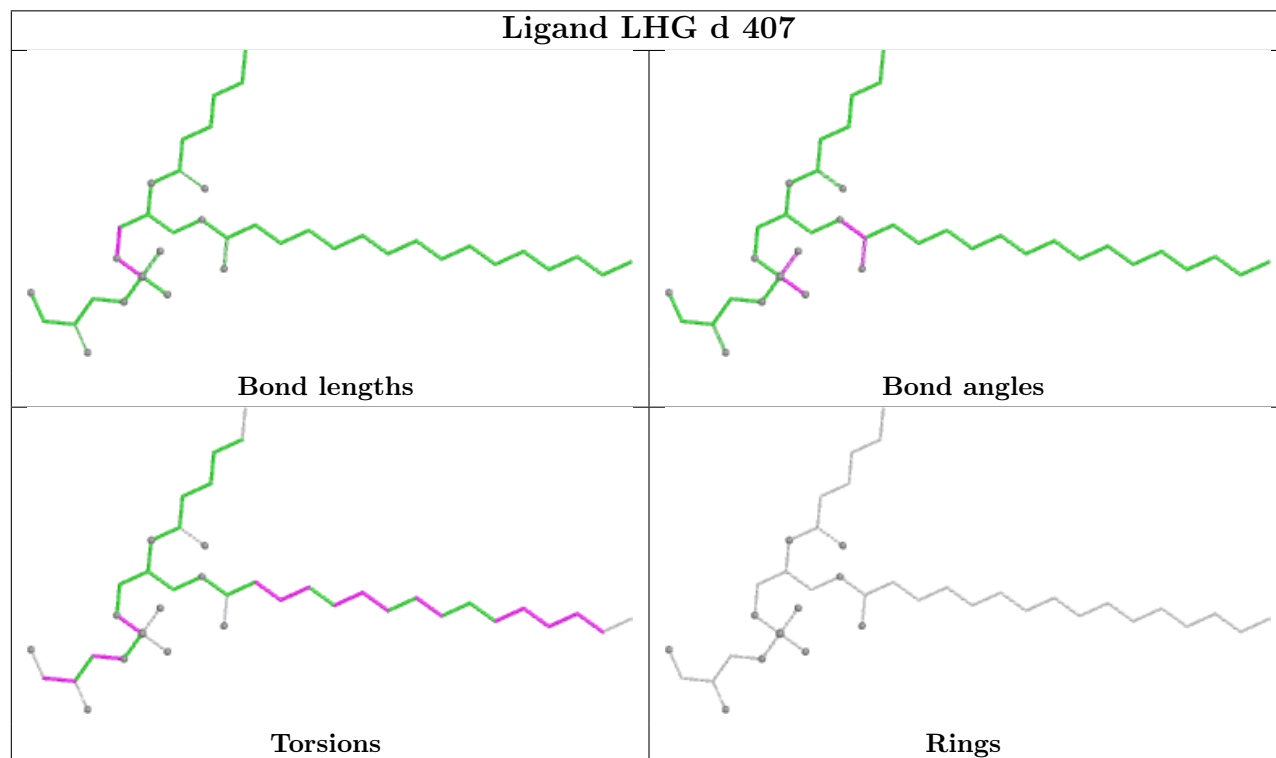
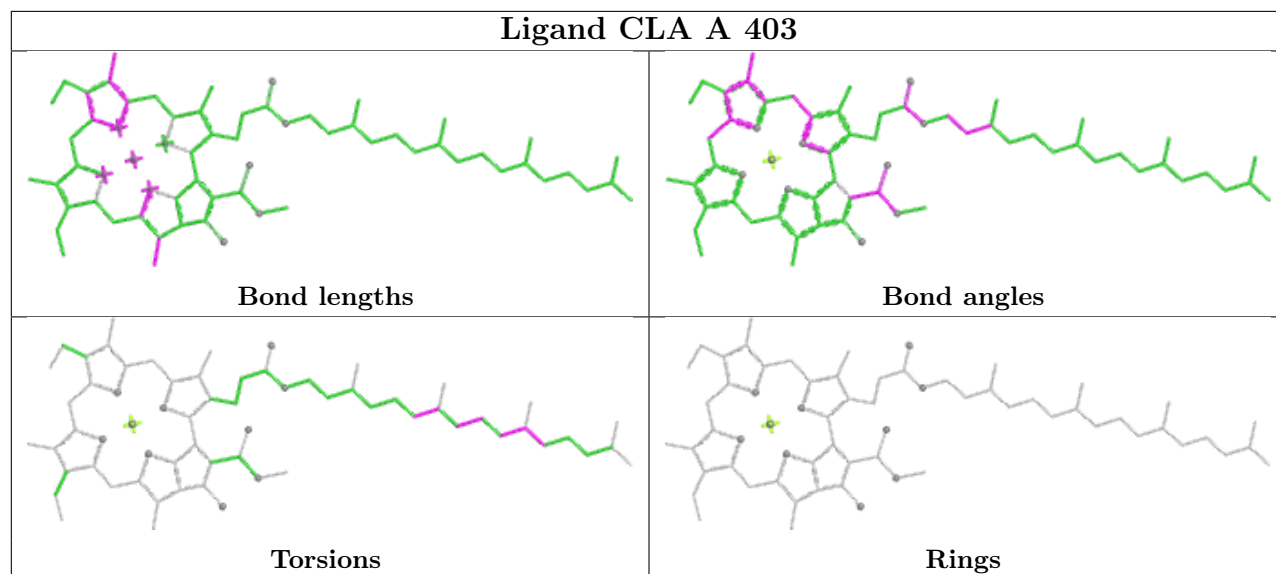


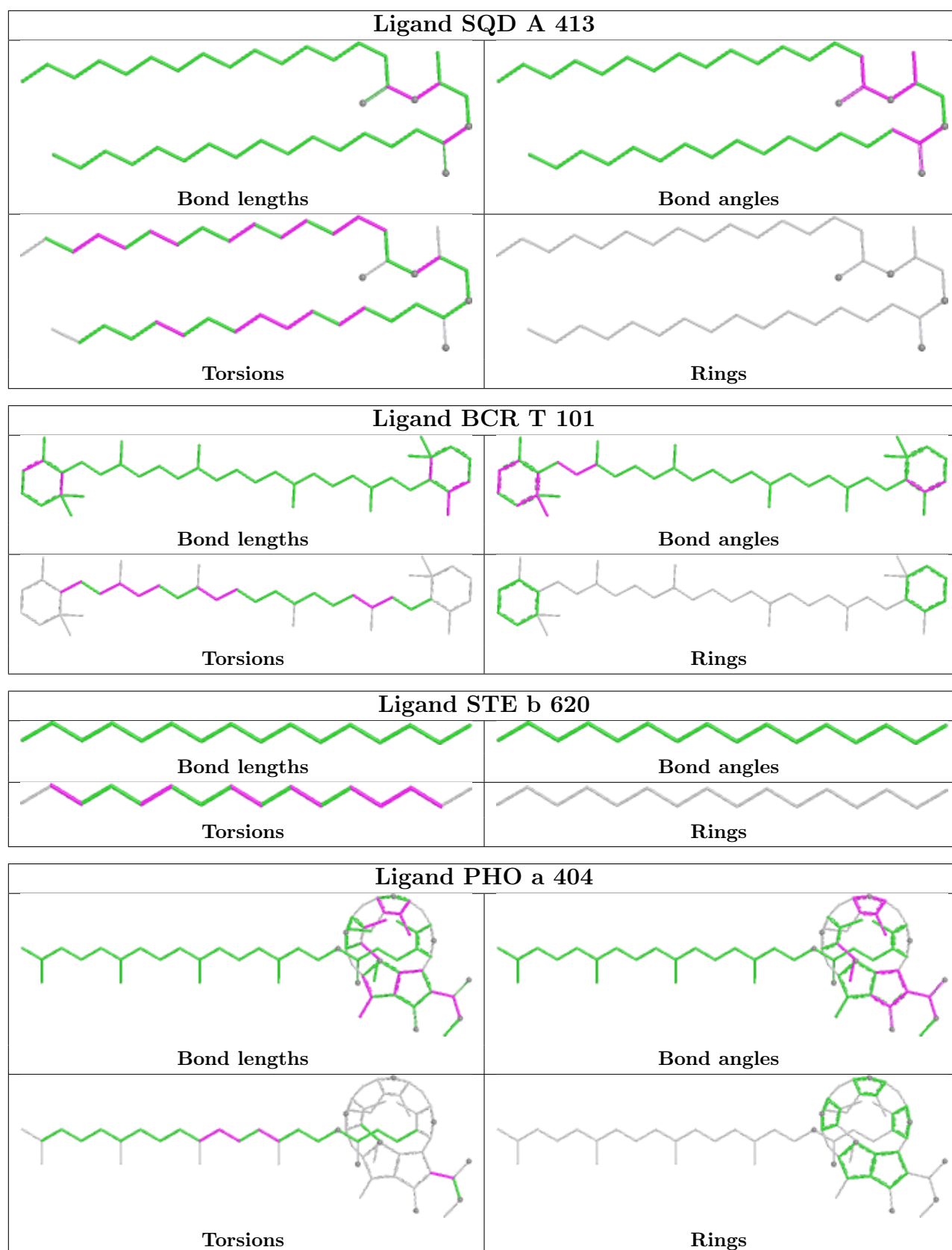


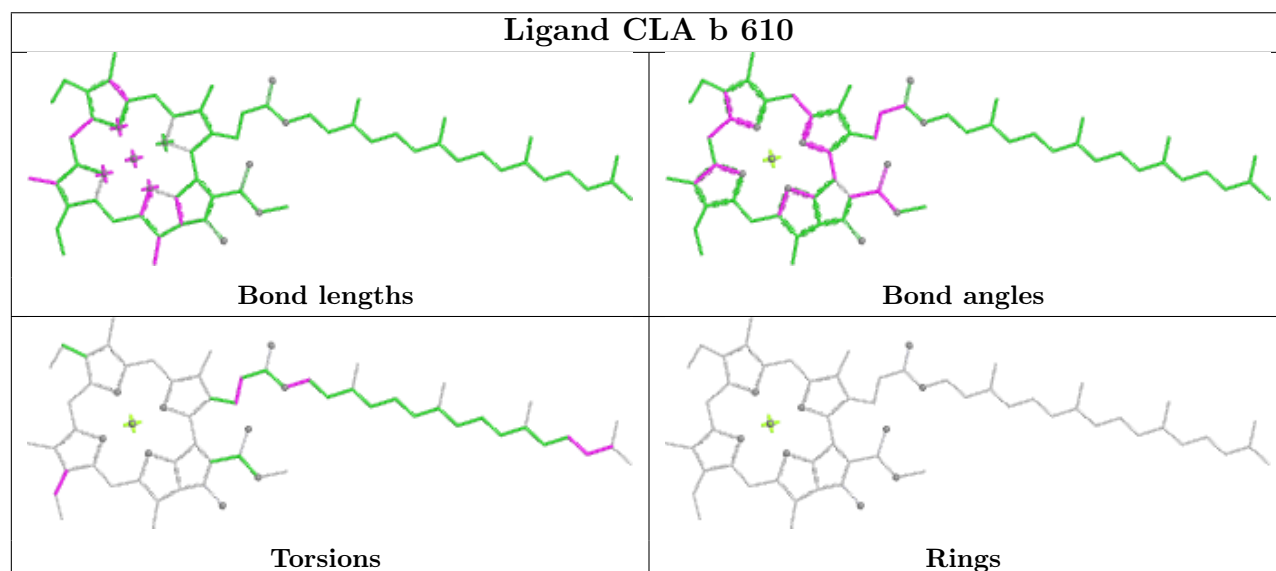
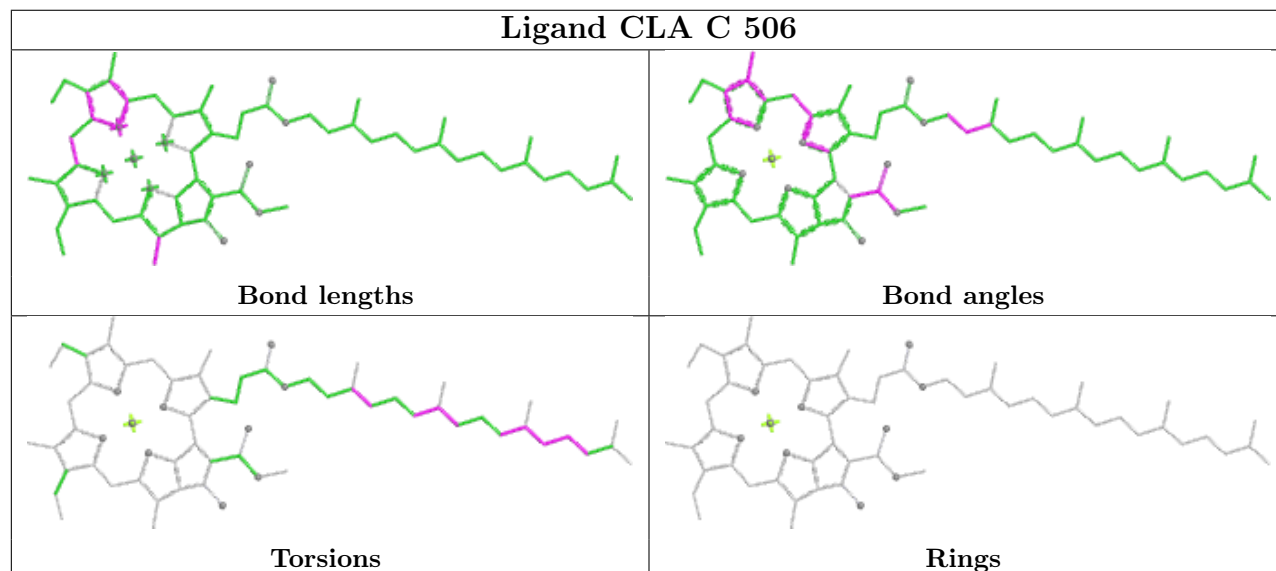
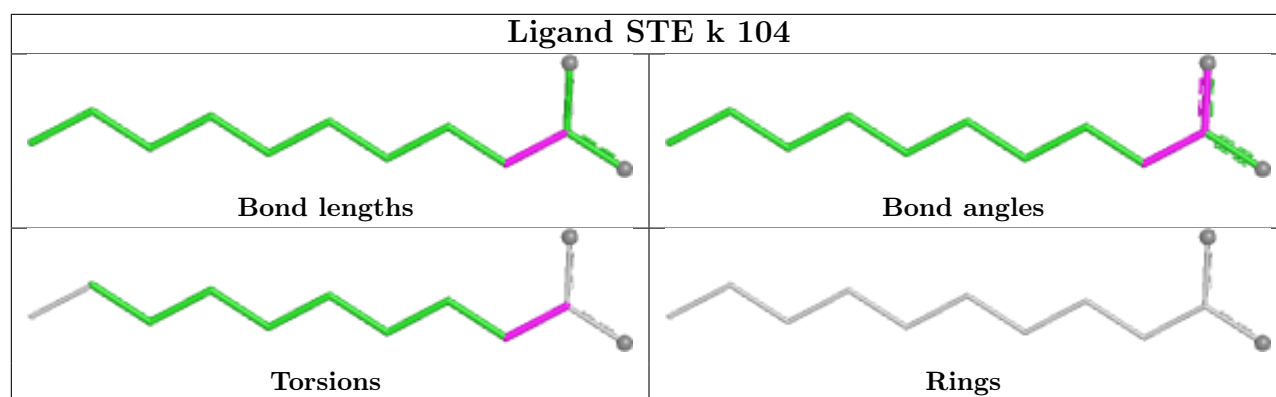


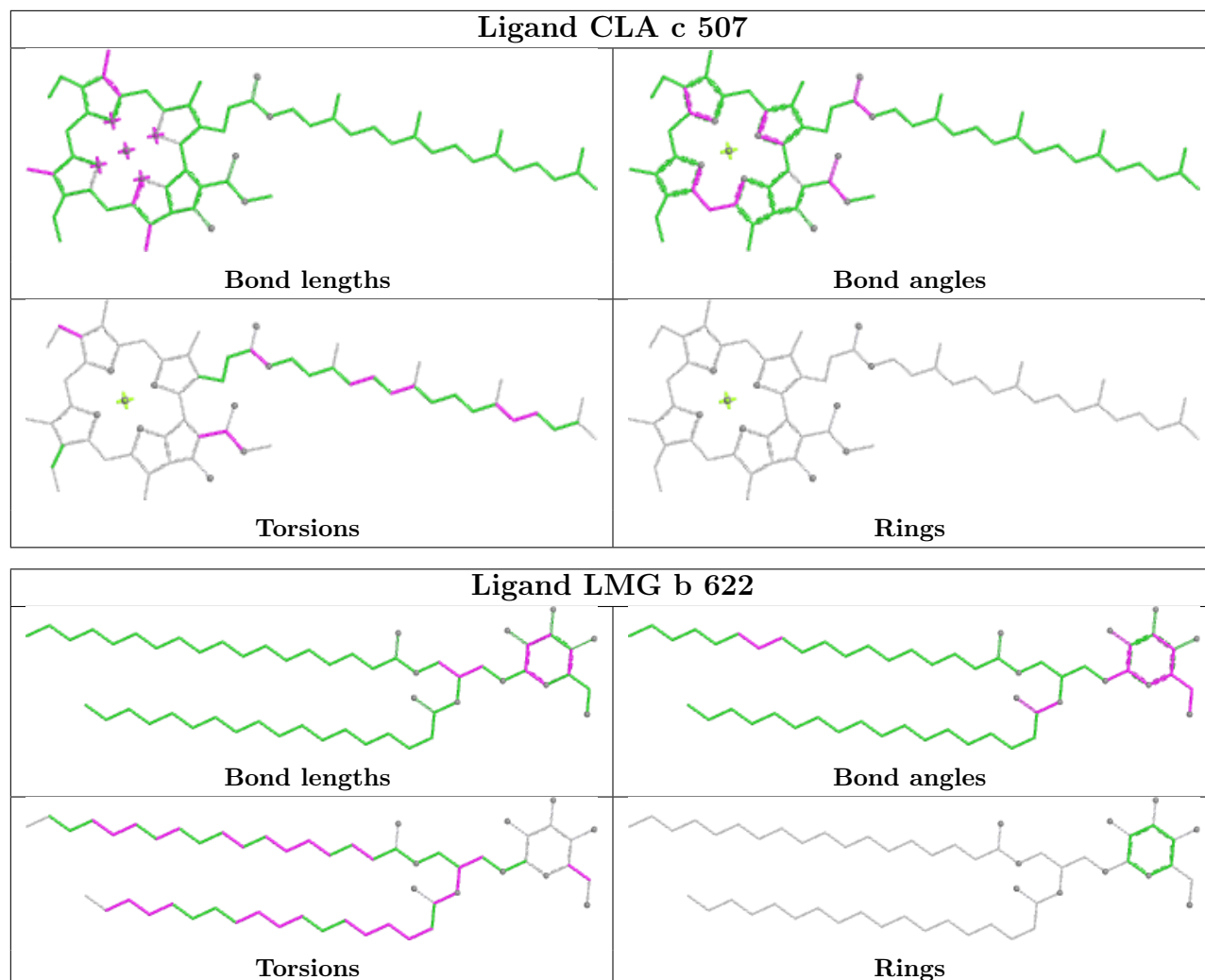


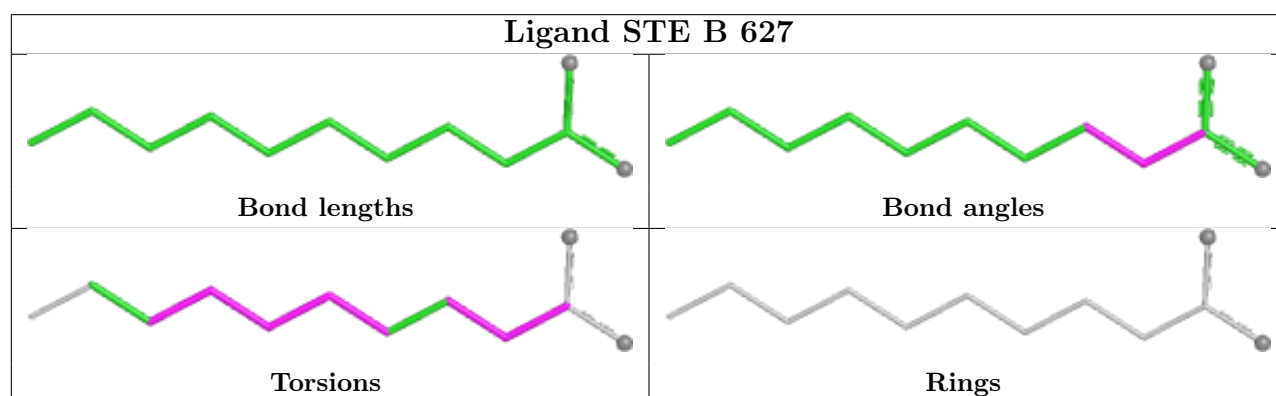
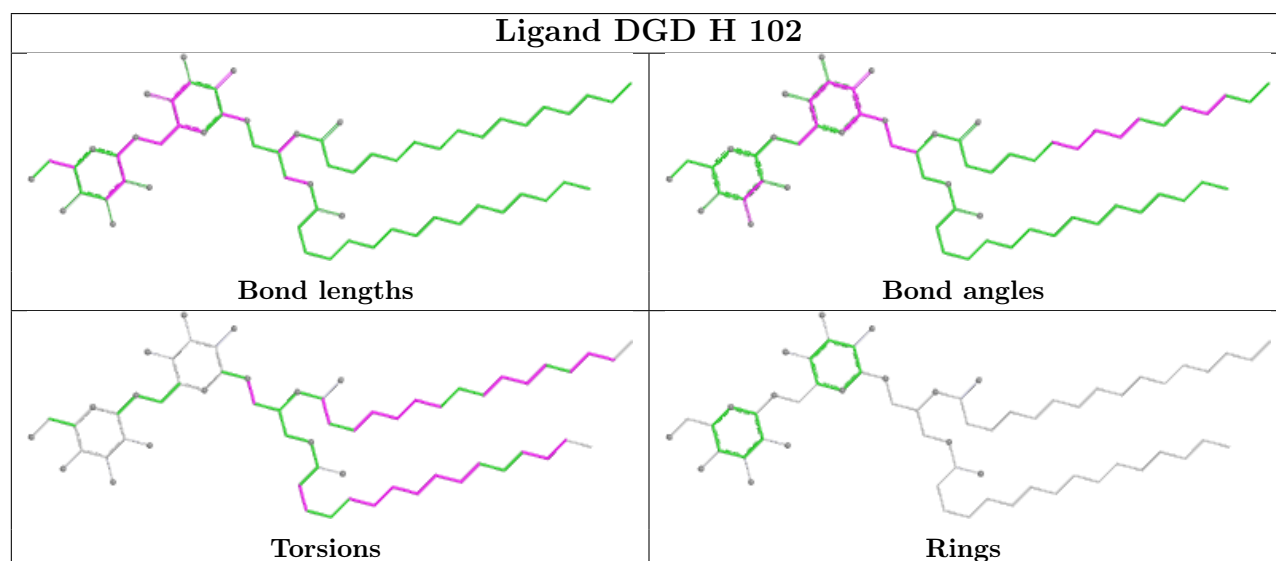
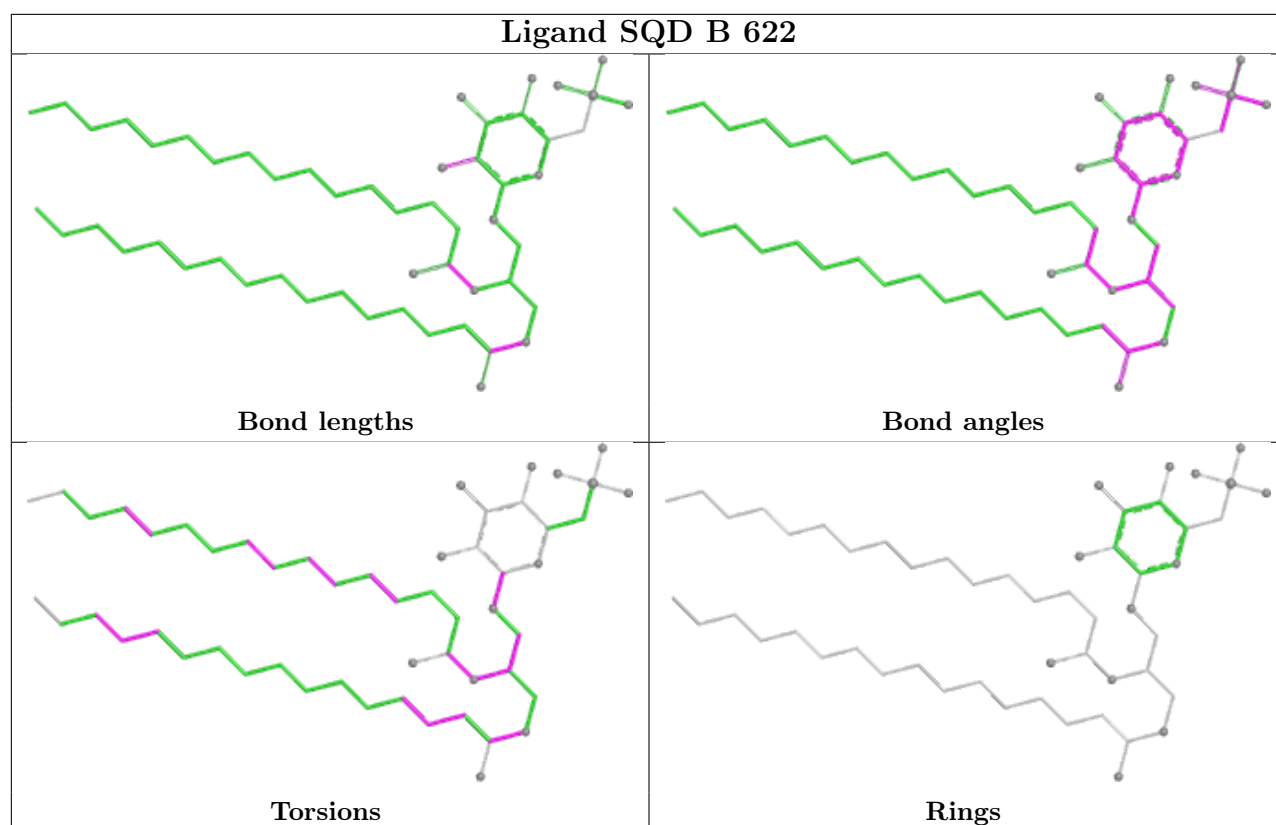


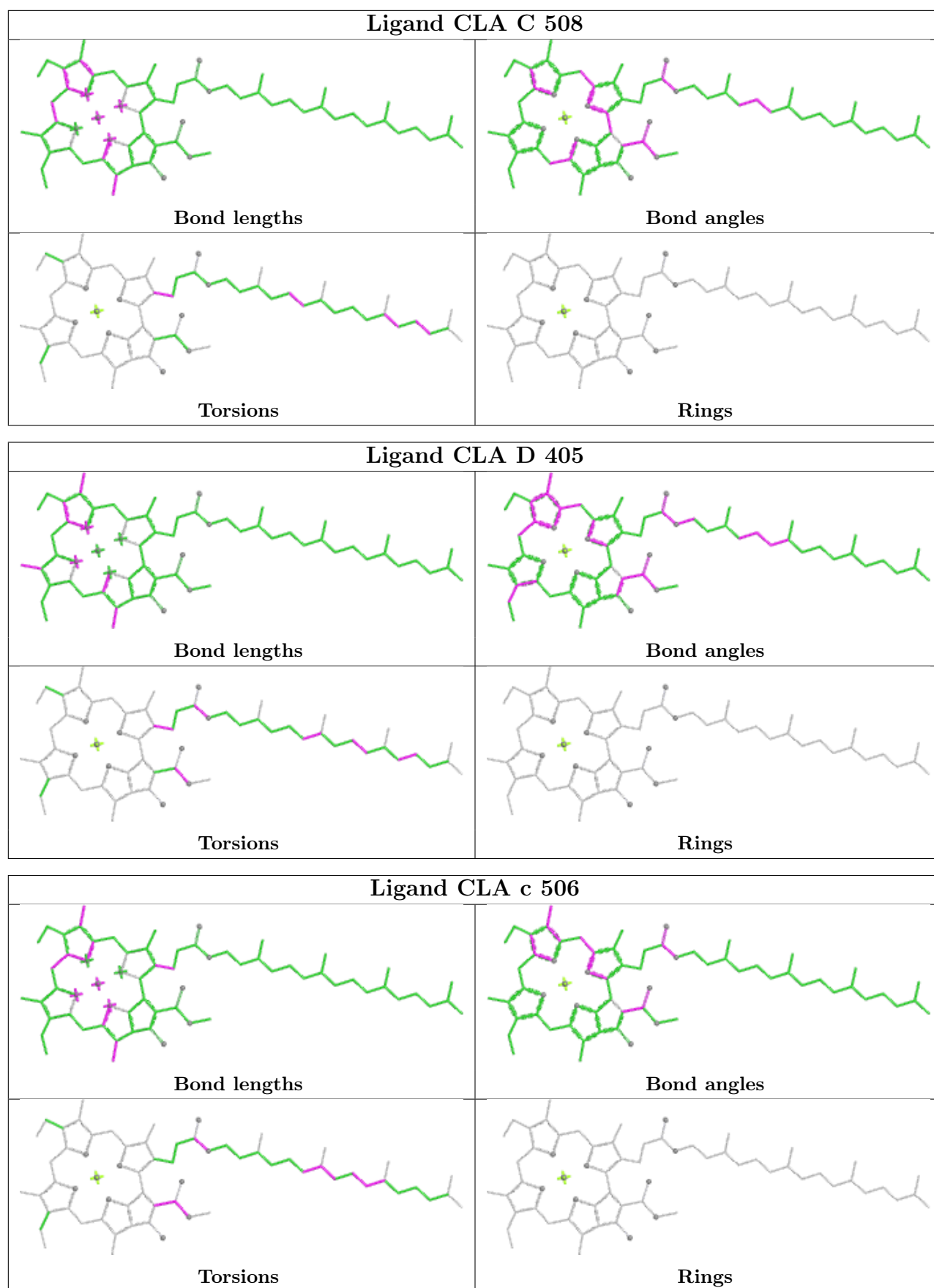


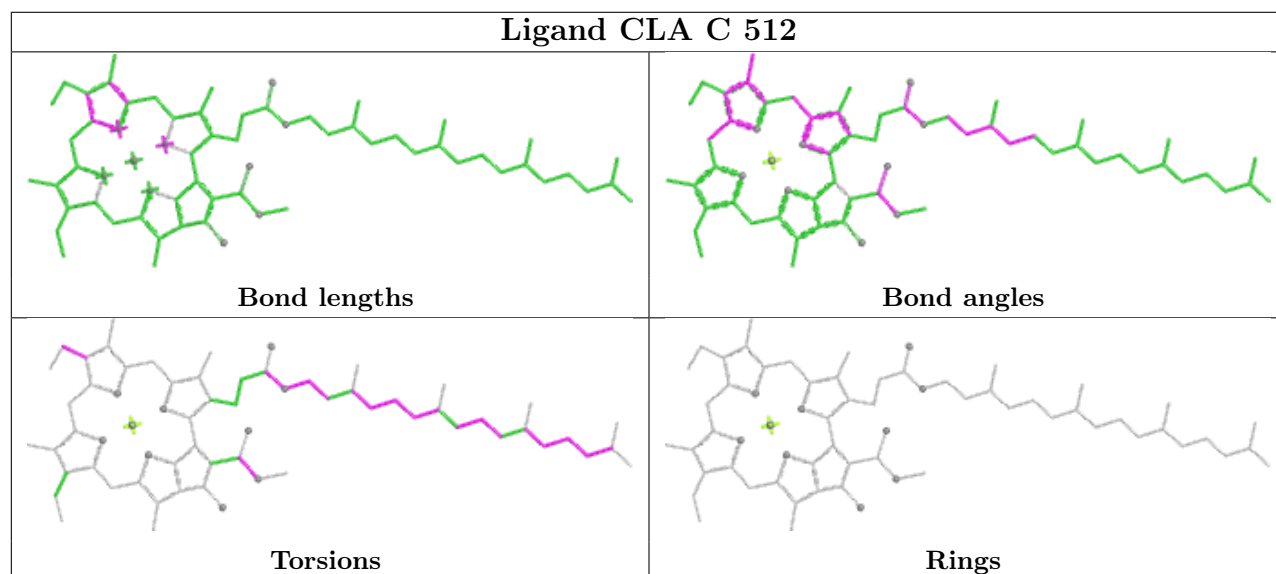
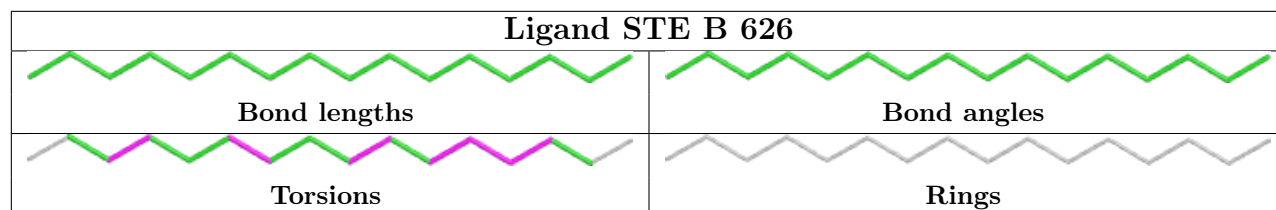
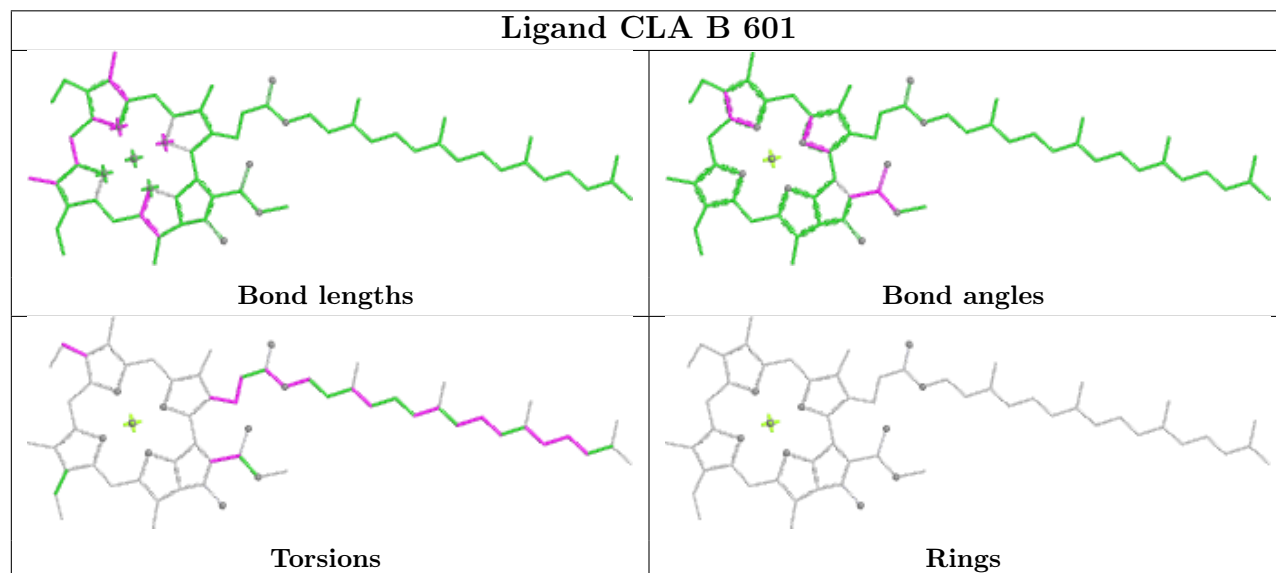
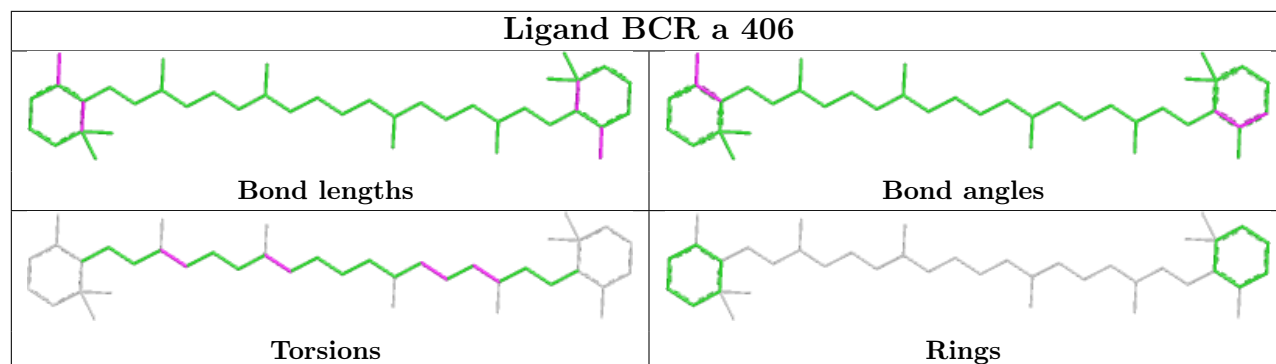


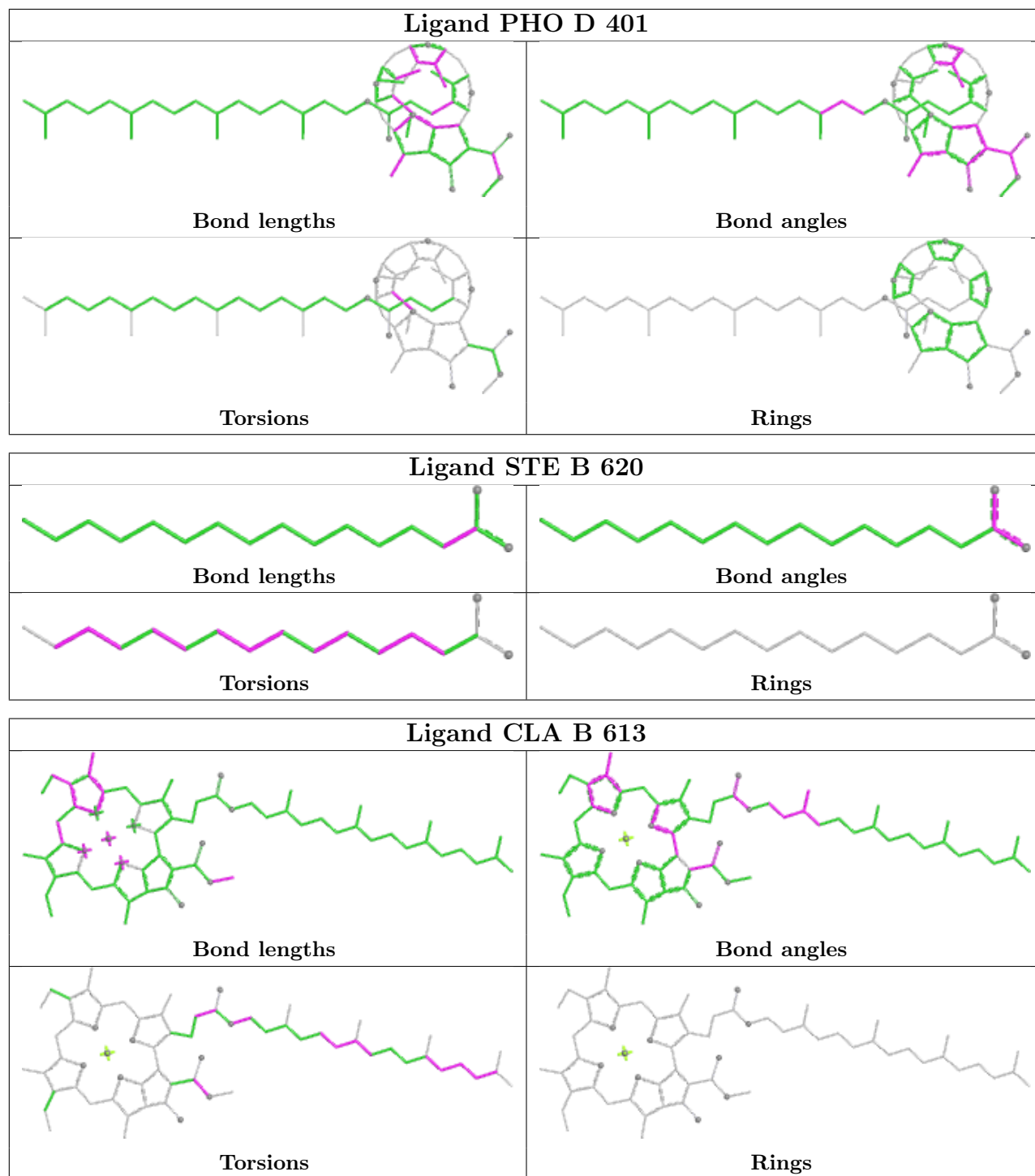


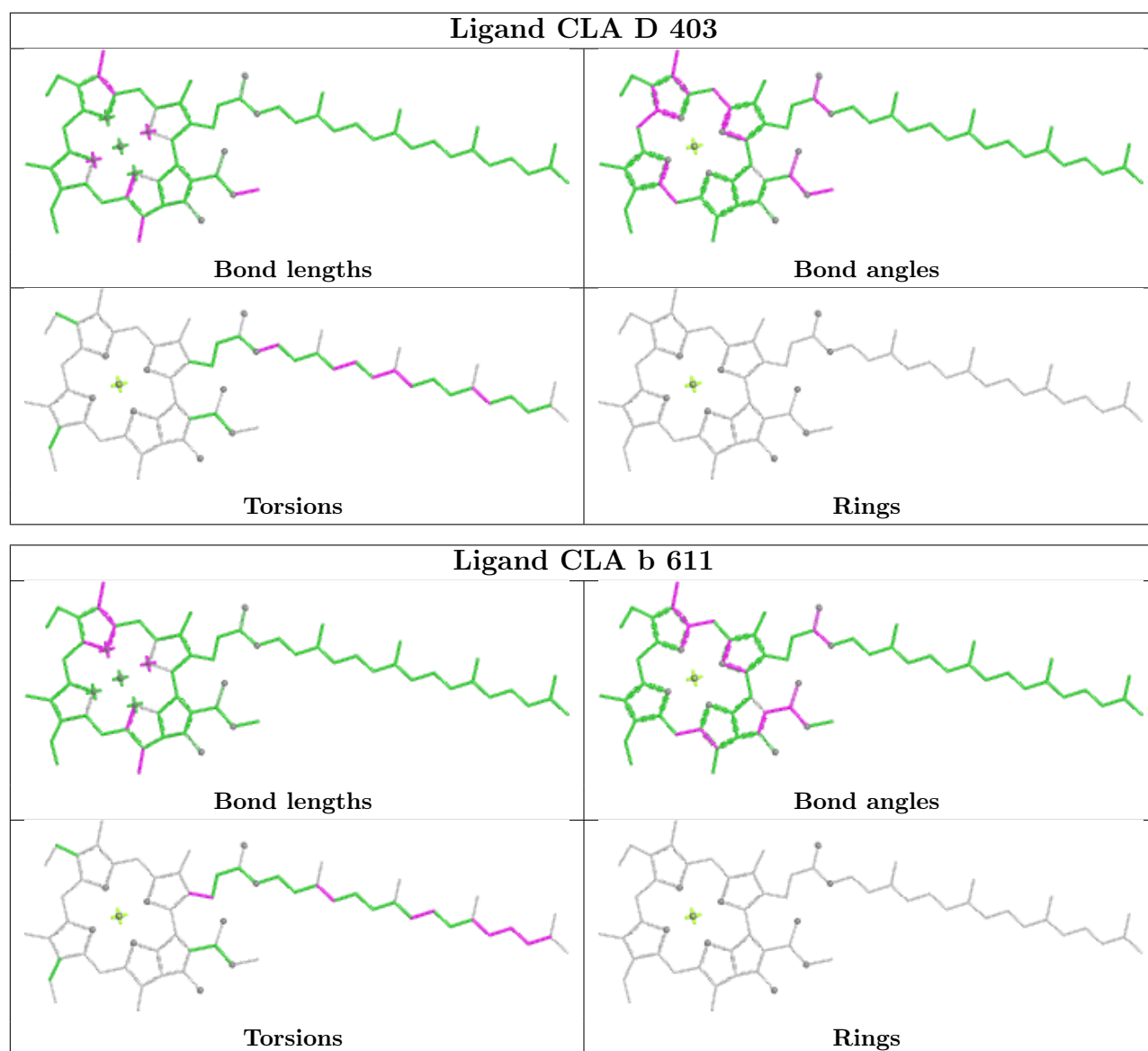


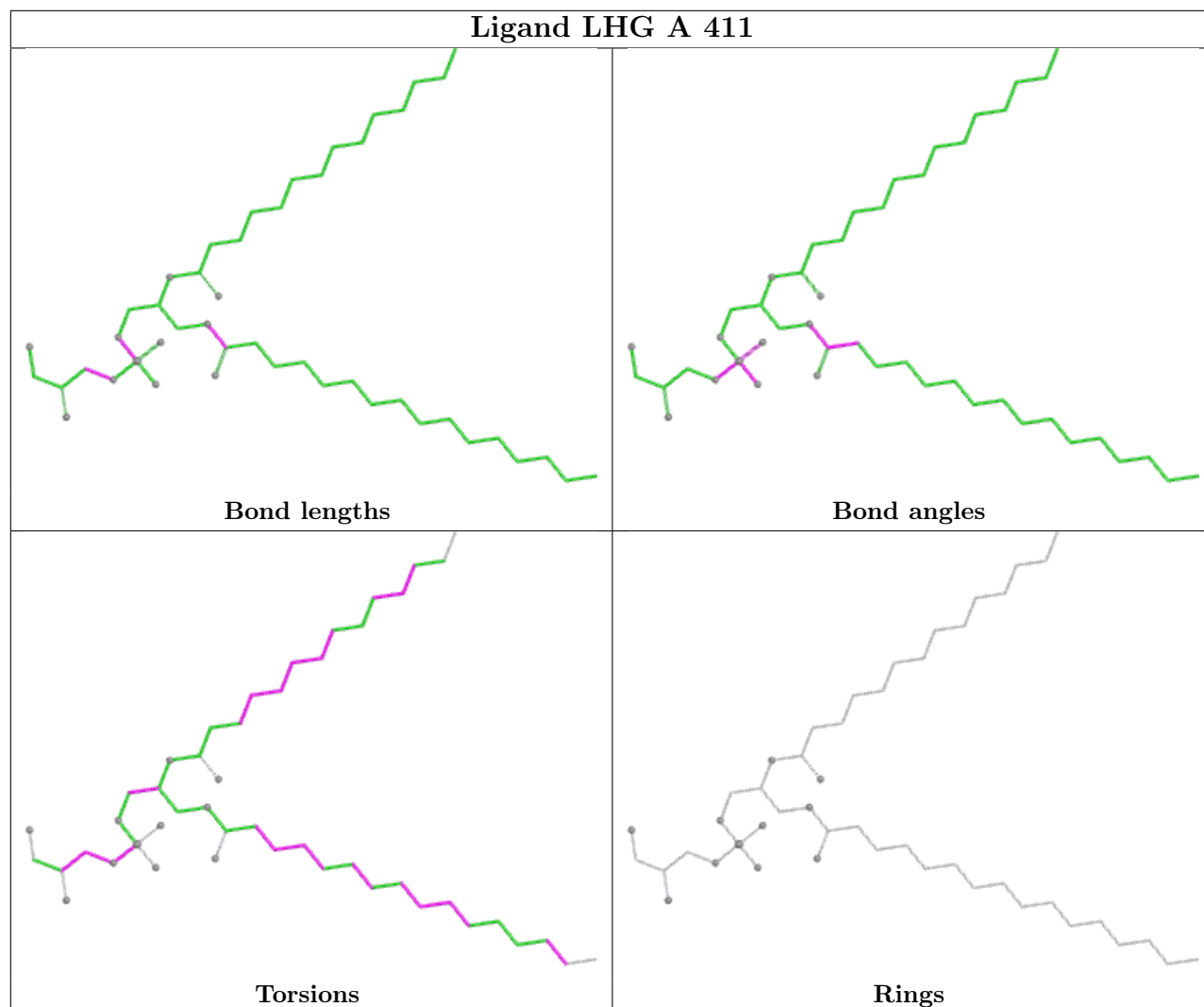


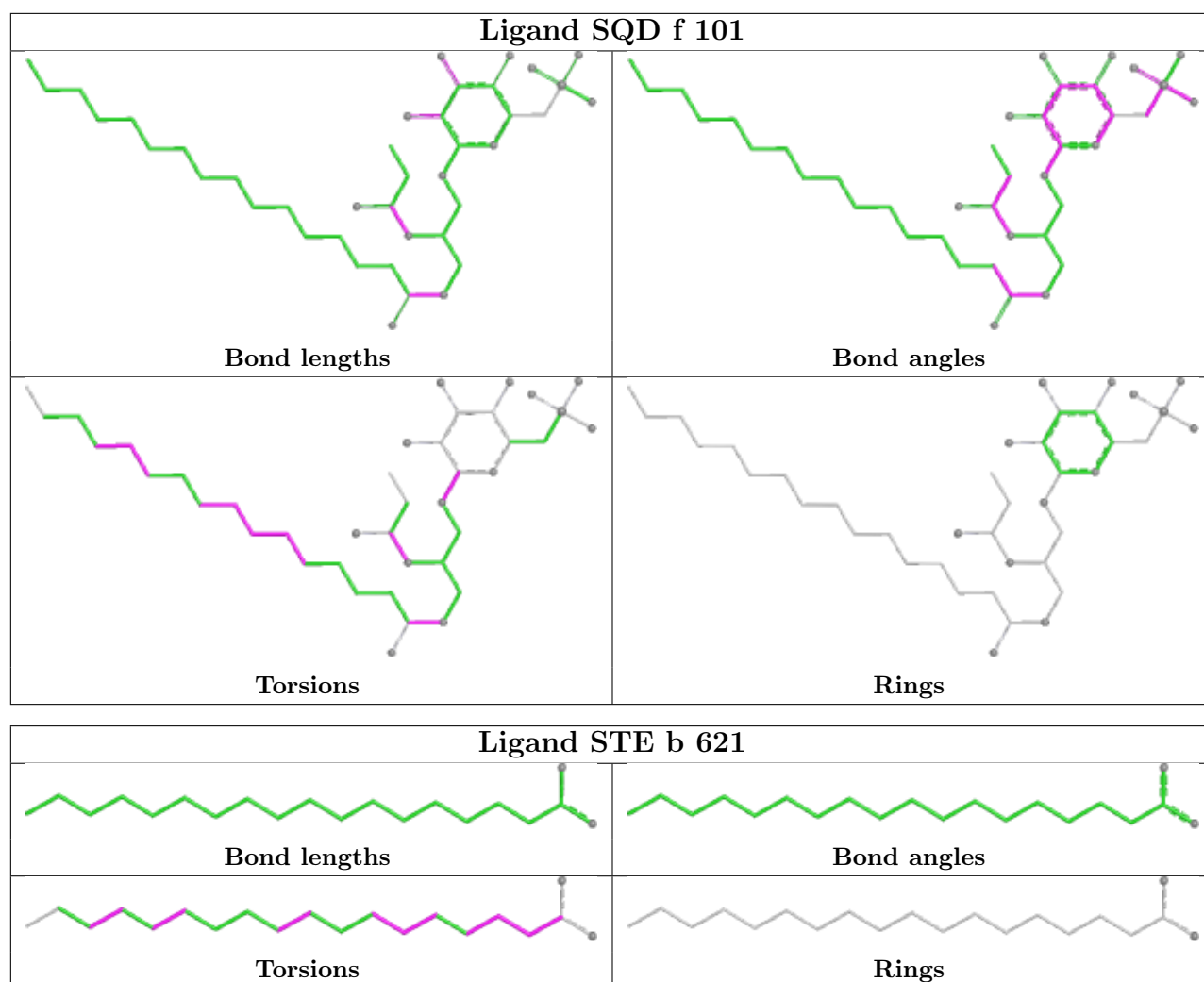












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.