



wwPDB EM Validation Summary Report ⓘ

Jul 24, 2025 – 04:42 pm BST

PDB ID : 9G6G / pdb_00009g6g
EMDB ID : EMD-51101
Title : Semi-active PSII dimer from native Peak4 PSII dimers
Authors : Zhao, Z.; Vercellino, I.; Nixon, P.J.; Sazanov, L.A.
Deposited on : 2024-07-18
Resolution : 2.20 Å (reported)
Based on initial models : 7NHO, 3KZI

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

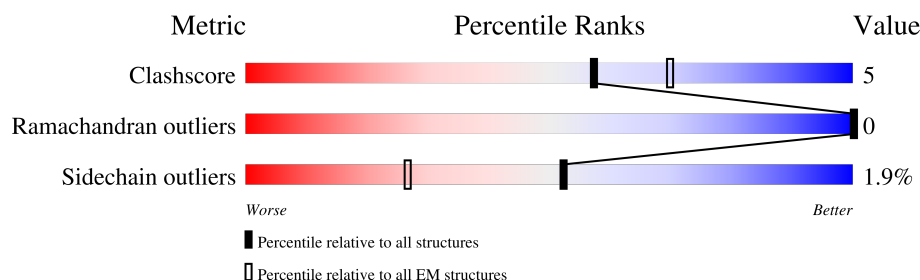
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	360	 79% 13% 8%
2	B	510	 91% 8% .
2	b	510	 90% 8% ..
3	C	461	 90% 8% .
3	c	461	 86% 9% 5%
4	D	352	 88% 8% ..
4	d	352	 86% 11% .
5	E	84	 87% 8% 5%

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Mol	Chain	Length	Quality of chain
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
14	T	32	
14	t	32	
15	U	134	
16	V	163	
17	X	41	
17	x	41	
18	Y	46	
18	y	46	
19	Z	62	

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Mol	Chain	Length	Quality of chain
19	z	62	
20	a	360	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	C	515	X	-	-	-
23	CLA	C	516	X	-	-	-
23	CLA	C	517	X	-	-	-
23	CLA	C	518	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	D	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	402	X	-	-	-
23	CLA	a	403	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	401	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	d	405	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 47004 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2599	1707	430	447	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	505	Total	C	N	O	S	0	0
			3941	2589	662	677	13		
2	b	504	Total	C	N	O	S	0	0
			3949	2595	655	686	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3460	2268	581	598	13		
3	c	437	Total	C	N	O	S	0	0
			3362	2211	562	576	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2709	1796	444	457	12		
4	d	341	Total	C	N	O	S	0	0
			2712	1798	444	458	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	80	Total	C	N	O	0	0
			644	422	105	117		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	76	Total	C	N	O	0	0
			603	400	96	107		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	35	Total	C	N	O	S	0	0
			280	190	46	43	1		
6	f	34	Total	C	N	O	S	0	0
			274	187	45	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	64	Total	C	N	O	S	0	0
			506	339	81	84	2		
7	h	64	Total	C	N	O	S	0	0
			506	339	81	84	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			284	194	45	44	1		
8	i	35	Total	C	N	O	S	0	0
			288	196	45	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	35	Total	C	N	O	S	0	0
			253	172	39	41	1		
9	j	29	Total	C	N	O	S	0	0
			216	150	33	32	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			289	201	42	46		
10	k	37	Total	C	N	O	0	0
			289	201	42	46		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	35	Total	C	N	O	0	0
			281	189	43	49		
11	l	35	Total	C	N	O	0	0
			287	192	46	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	33	Total	C	N	O	S	0	0
			254	170	38	45	1		
12	m	33	Total	C	N	O	S	0	0
			254	170	37	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	243	Total	C	N	O	S	0	0
			1794	1128	303	359	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total	C	N	O	S	0	0
			250	177	33	38	2		
14	t	30	Total	C	N	O	S	0	0
			254	179	36	37	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	97	Total	C	N	O	0	0
			755	481	128	146		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	137	Total	C	N	O	S	0	0
			1052	668	176	204	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	X	38	Total	C	N	O	0	0
			279	187	45	47		
17	x	38	Total	C	N	O	0	0
			278	187	45	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	31	Total	C	N	O	S	0	0
			227	152	39	34	2		
18	y	29	Total	C	N	O	S	0	0
			206	136	34	33	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			455	316	67	70	2		
19	z	61	Total	C	N	O	S	0	0
			459	317	68	73	1		

- Molecule 20 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	323	Total	C	N	O	S	0	0
			2531	1660	416	440	15		

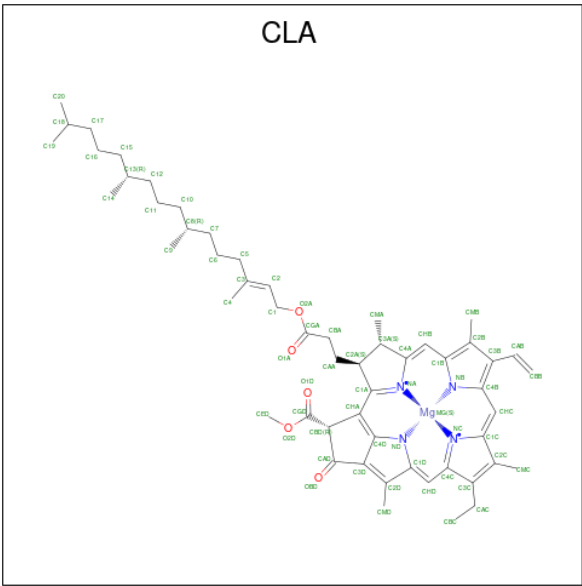
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Cl	0
			2	2	
22	a	1	Total	Cl	0
			1	1	

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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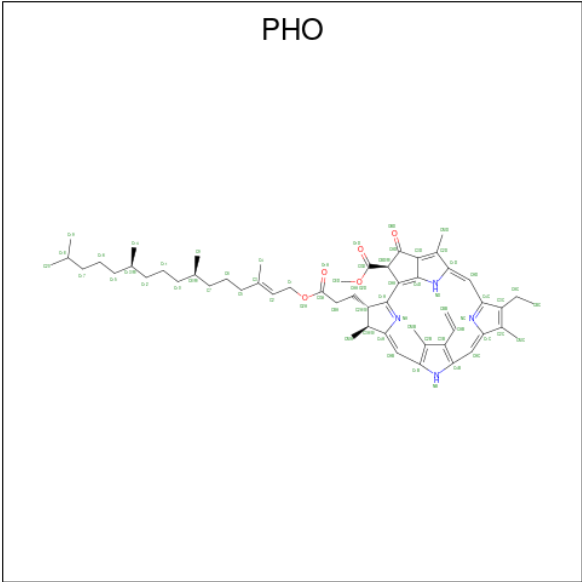
Mol	Chain	Residues	Atoms					AltConf
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total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

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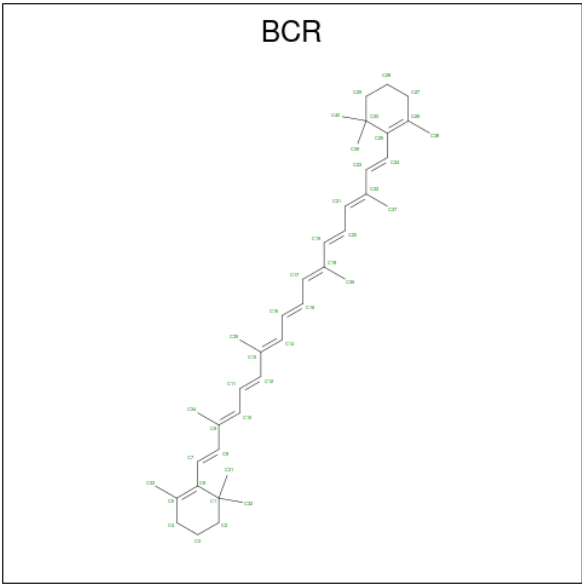
Mol	Chain	Residues	Atoms					AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total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

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



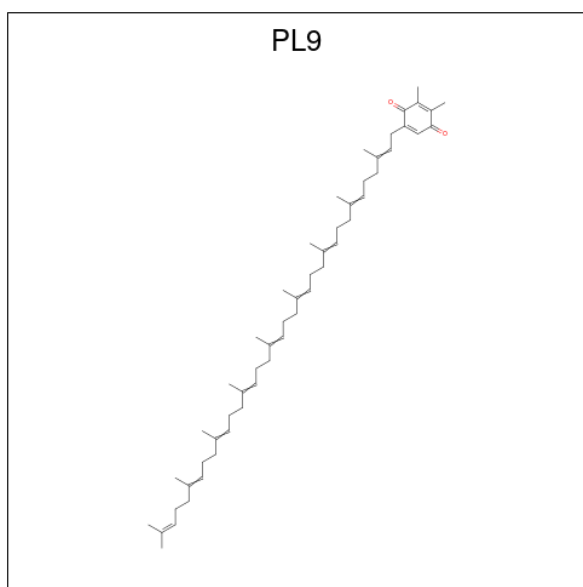
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



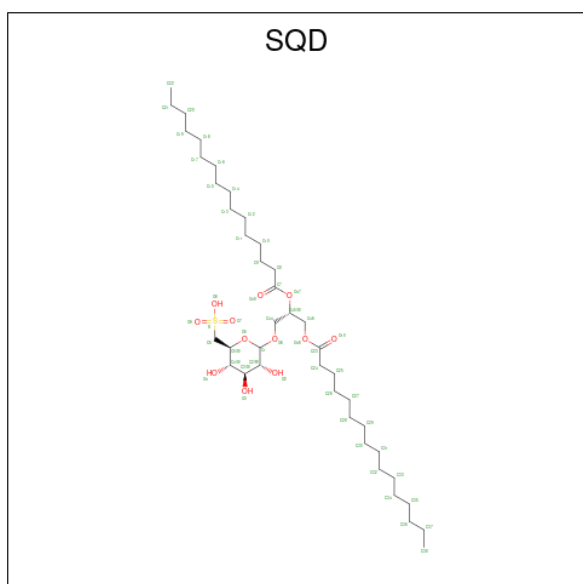
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	T	1	Total C 40 40	0
25	Y	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	f	1	Total C 40 40	0
25	i	1	Total C 40 40	0
25	j	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	t	1	Total C 40 40	0
25	z	1	Total C 40 40	0

- 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).



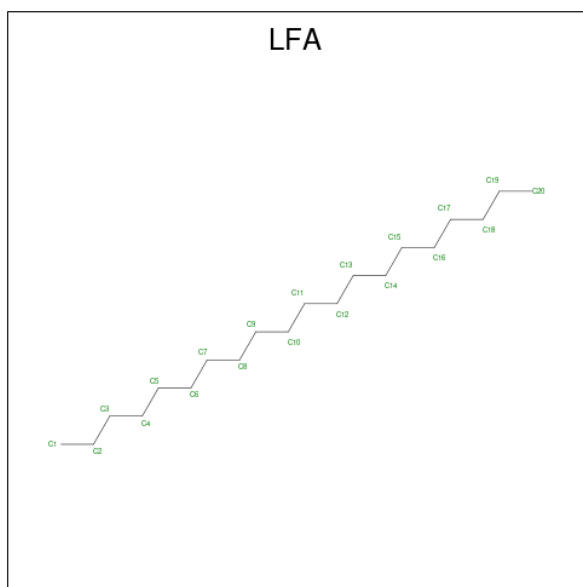
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			55	53	2	
26	D	1	Total	C	O	0
			55	53	2	
26	a	1	Total	C	O	0
			55	53	2	
26	d	1	Total	C	O	0
			55	53	2	

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



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	S	0
			54	41	12	1	
27	A	1	Total	C	O	S	0
			51	38	12	1	
27	B	1	Total	C	O	S	0
			54	41	12	1	
27	D	1	Total	C	O	S	0
			43	30	12	1	
27	F	1	Total	C	O	S	0
			45	32	12	1	
27	a	1	Total	C	O	S	0
			51	38	12	1	
27	a	1	Total	C	O	S	0
			45	32	12	1	
27	b	1	Total	C	O	S	0
			54	41	12	1	
27	d	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 28 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	C	0
			7	7	
28	A	1	Total	C	0
			7	7	
28	B	1	Total	C	0
			13	13	

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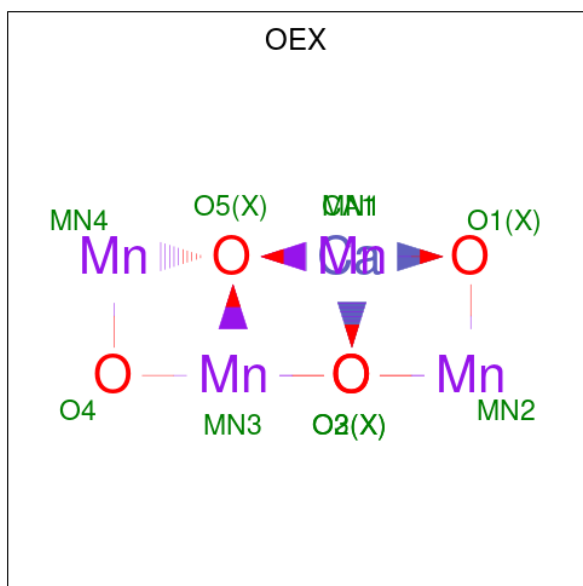
Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C 6 6	0
28	B	1	Total C 8 8	0
28	B	1	Total C 6 6	0
28	B	1	Total C 7 7	0
28	C	1	Total C 12 12	0
28	C	1	Total C 9 9	0
28	C	1	Total C 13 13	0
28	D	1	Total C 12 12	0
28	D	1	Total C 10 10	0
28	D	1	Total C 8 8	0
28	E	1	Total C 6 6	0
28	H	1	Total C 9 9	0
28	I	1	Total C 13 13	0
28	I	1	Total C 7 7	0
28	I	1	Total C 8 8	0
28	I	1	Total C 8 8	0
28	a	1	Total C 9 9	0
28	a	1	Total C 10 10	0
28	b	1	Total C 8 8	0
28	b	1	Total C 8 8	0
28	b	1	Total C 7 7	0

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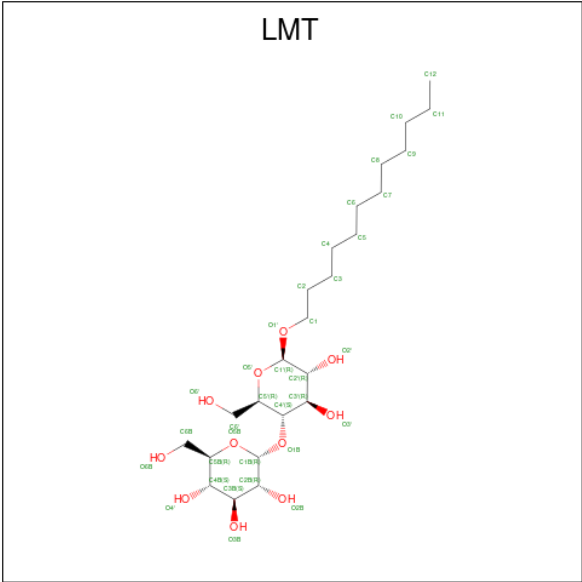
Mol	Chain	Residues	Atoms	AltConf
28	d	1	Total C 10 10	0
28	d	1	Total C 9 9	0
28	e	1	Total C 17 17	0
28	h	1	Total C 10 10	0
28	i	1	Total C 13 13	0
28	m	1	Total C 9 9	0

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



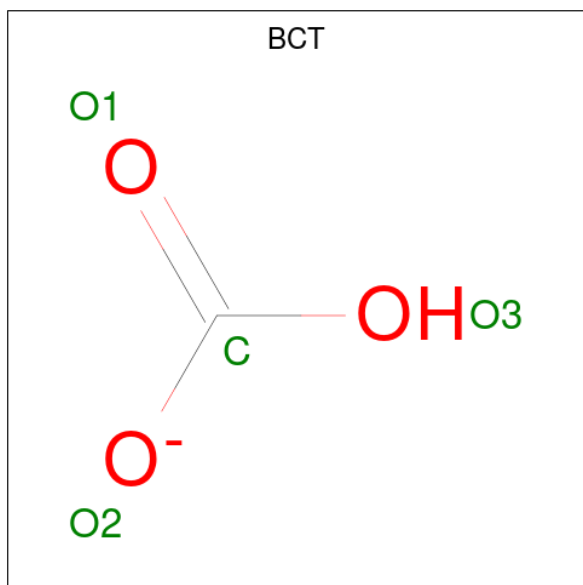
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			35	24	11	
30	B	1	Total	C	O	0
			35	24	11	
30	B	1	Total	C	O	0
			35	24	11	
30	C	1	Total	C	O	0
			35	24	11	
30	D	1	Total	C	O	0
			33	22	11	
30	E	1	Total	C	O	0
			35	24	11	
30	J	1	Total	C	O	0
			24	18	6	
30	M	1	Total	C	O	0
			35	24	11	
30	M	1	Total	C	O	0
			35	24	11	
30	T	1	Total	C	O	0
			24	18	6	
30	T	1	Total	C	O	0
			35	24	11	
30	a	1	Total	C	O	0
			35	24	11	
30	a	1	Total	C	O	0
			24	18	6	
30	c	1	Total	C	O	0
			29	18	11	

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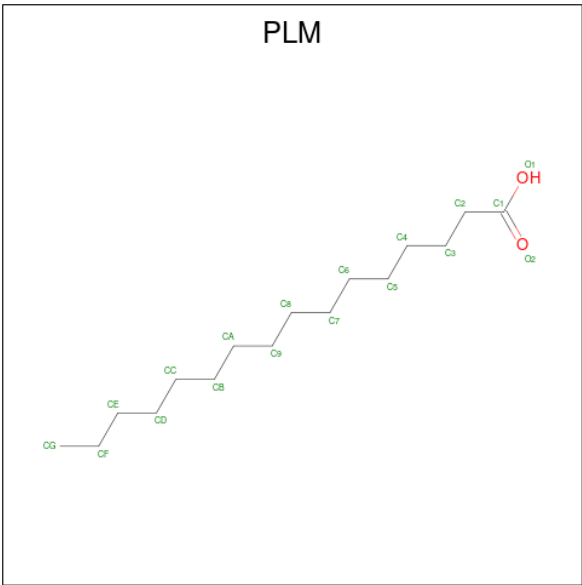
Mol	Chain	Residues	Atoms			AltConf
30	d	1	Total	C	O	0
			24	18	6	
30	f	1	Total	C	O	0
			34	23	11	
30	z	1	Total	C	O	0
			35	24	11	

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 32 is PALMITIC ACID (CCD ID: PLM) (formula: $\text{C}_{16}\text{H}_{32}\text{O}_2$).



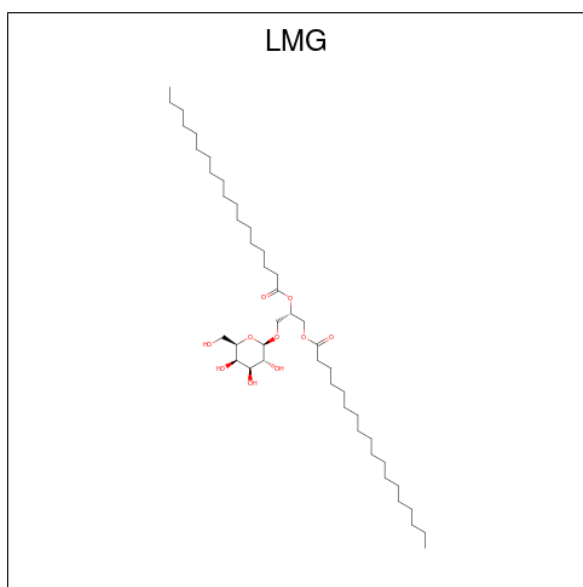
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			13	11	2	
32	B	1	Total	C	O	0
			15	13	2	
32	B	1	Total	C	O	0
			13	11	2	
32	C	1	Total	C	O	0
			13	11	2	
32	C	1	Total	C	O	0
			13	11	2	
32	C	1	Total	C	O	0
			13	11	2	
32	D	1	Total	C	O	0
			18	16	2	
32	D	1	Total	C	O	0
			11	9	2	
32	E	1	Total	C	O	0
			15	13	2	
32	E	1	Total	C	O	0
			16	14	2	
32	E	1	Total	C	O	0
			18	16	2	
32	J	1	Total	C	O	0
			16	14	2	
32	K	1	Total	C	O	0
			14	12	2	
32	a	1	Total	C	O	0
			11	9	2	

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Mol	Chain	Residues	Atoms			AltConf
32	b	1	Total	C	O	0
			15	13	2	
32	b	1	Total	C	O	0
			16	14	2	
32	b	1	Total	C	O	0
			11	9	2	
32	b	1	Total	C	O	0
			12	10	2	
32	c	1	Total	C	O	0
			9	7	2	
32	c	1	Total	C	O	0
			15	13	2	
32	c	1	Total	C	O	0
			10	8	2	
32	c	1	Total	C	O	0
			13	11	2	
32	d	1	Total	C	O	0
			16	14	2	
32	h	1	Total	C	O	0
			11	9	2	
32	i	1	Total	C	O	0
			15	13	2	
32	i	1	Total	C	O	0
			13	11	2	
32	k	1	Total	C	O	0
			12	10	2	
32	l	1	Total	C	O	0
			14	12	2	
32	x	1	Total	C	O	0
			18	16	2	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



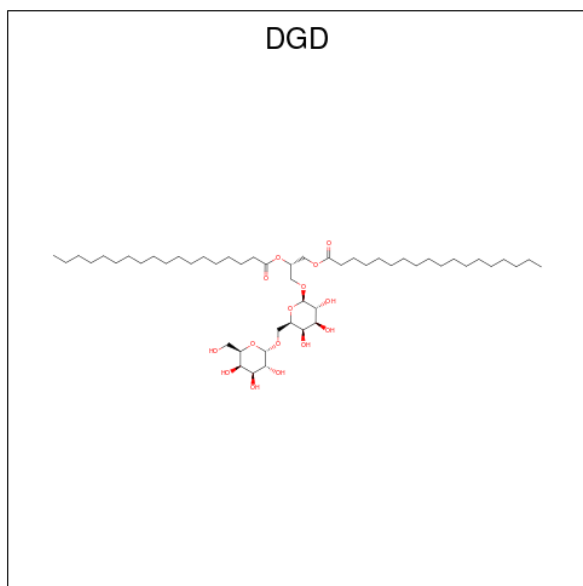
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			51	41	10	
33	C	1	Total	C	O	0
			48	38	10	
33	D	1	Total	C	O	0
			51	41	10	
33	I	1	Total	C	O	0
			51	41	10	
33	Y	1	Total	C	O	0
			51	41	10	
33	a	1	Total	C	O	0
			51	41	10	
33	b	1	Total	C	O	0
			51	41	10	
33	c	1	Total	C	O	0
			51	41	10	
33	d	1	Total	C	O	0
			51	41	10	
33	y	1	Total	C	O	0
			51	41	10	

- Molecule 34 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			6	3	3	

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



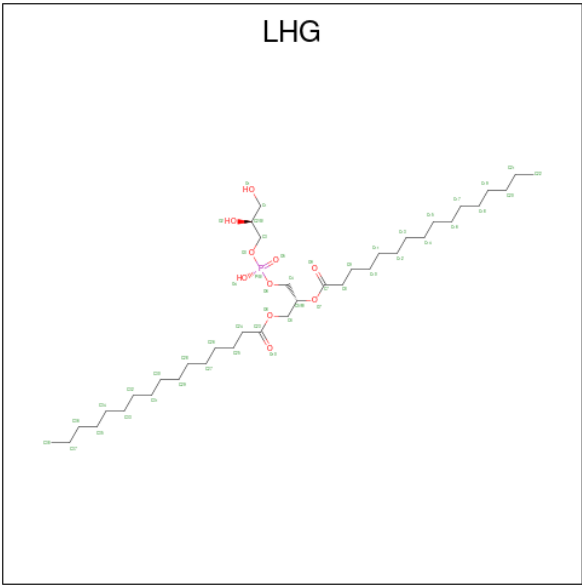
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			53	38	15	
35	C	1	Total	C	O	0
			62	47	15	

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Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			61	46	15	
35	D	1	Total	C	O	0
			47	36	11	
35	H	1	Total	C	O	0
			58	43	15	
35	c	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			51	41	10	
35	c	1	Total	C	O	0
			62	47	15	
35	d	1	Total	C	O	0
			46	35	11	
35	h	1	Total	C	O	0
			62	47	15	

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



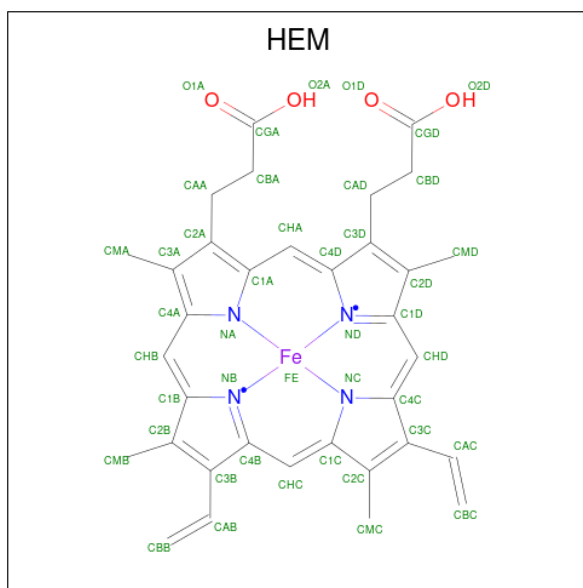
Mol	Chain	Residues	Atoms				AltConf
36	D	1	Total	C	O	P	0
			49	38	10	1	
36	D	1	Total	C	O	P	0
			49	38	10	1	
36	D	1	Total	C	O	P	0
			46	35	10	1	

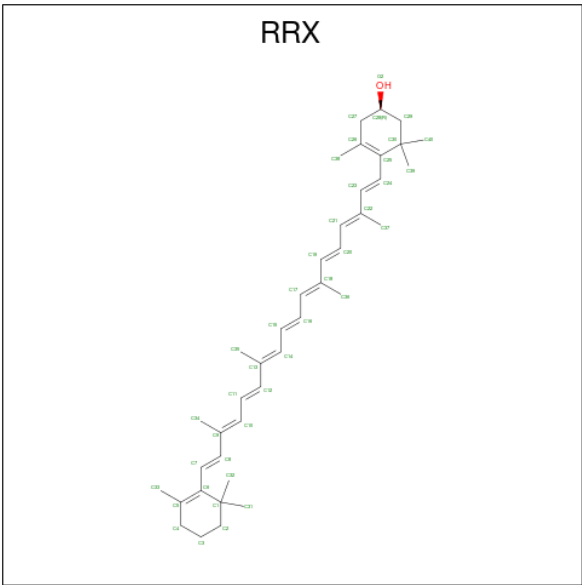
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Mol	Chain	Residues	Atoms				AltConf
36	E	1	Total	C	O	P	0
			49	38	10	1	
36	L	1	Total	C	O	P	0
			49	38	10	1	
36	a	1	Total	C	O	P	0
			46	35	10	1	
36	a	1	Total	C	O	P	0
			49	38	10	1	
36	d	1	Total	C	O	P	0
			49	38	10	1	
36	d	1	Total	C	O	P	0
			49	38	10	1	
36	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms			AltConf
38	H	1	Total	C	O	0
			41	40	1	
38	x	1	Total	C	O	0
			41	40	1	

- Molecule 39 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
39	O	1	Total	Ca	0
			1	1	

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	113	Total	O	0
			113	113	
40	B	135	Total	O	0
			135	135	
40	C	118	Total	O	1
			118	118	
40	D	103	Total	O	0
			103	103	
40	E	11	Total	O	0
			11	11	
40	F	4	Total	O	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
40	H	15	Total 15	O 15	0
40	I	1	Total 1	O 1	0
40	J	3	Total 3	O 3	0
40	K	2	Total 2	O 2	0
40	L	5	Total 5	O 5	0
40	M	5	Total 5	O 5	0
40	O	38	Total 38	O 38	0
40	T	5	Total 5	O 5	0
40	U	24	Total 24	O 24	0
40	V	36	Total 36	O 36	0
40	X	5	Total 5	O 5	0
40	Y	3	Total 3	O 3	0
40	Z	1	Total 1	O 1	0
40	a	64	Total 64	O 64	0
40	b	107	Total 107	O 107	0
40	c	52	Total 52	O 52	0
40	d	75	Total 75	O 75	0
40	e	6	Total 6	O 6	0
40	f	1	Total 1	O 1	0
40	h	8	Total 8	O 8	0
40	i	1	Total 1	O 1	0

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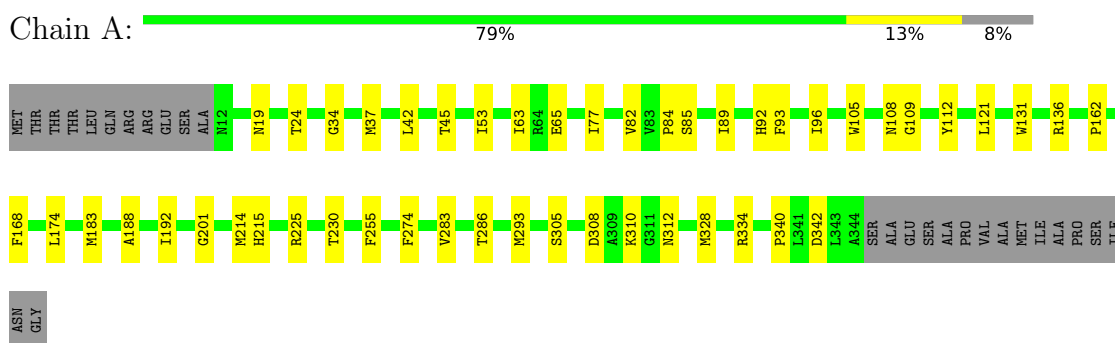
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Mol	Chain	Residues	Atoms		AltConf
40	j	3	Total 3	O 3	0
40	k	1	Total 1	O 1	0
40	l	7	Total 7	O 7	0
40	m	1	Total 1	O 1	0
40	t	3	Total 3	O 3	0
40	x	4	Total 4	O 4	0

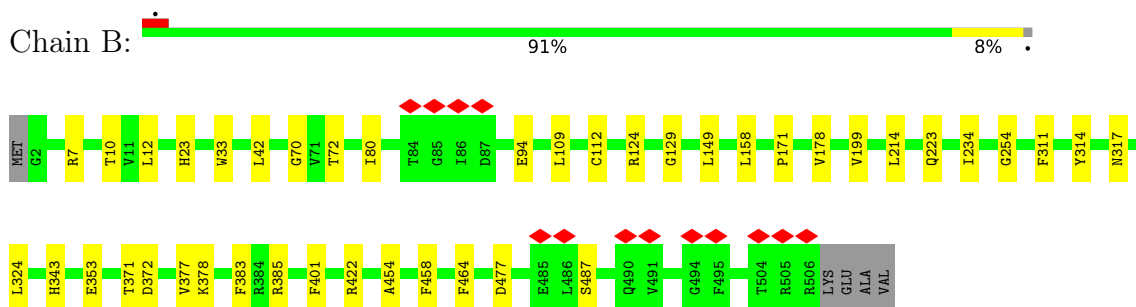
3 Residue-property plots [i](#)

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

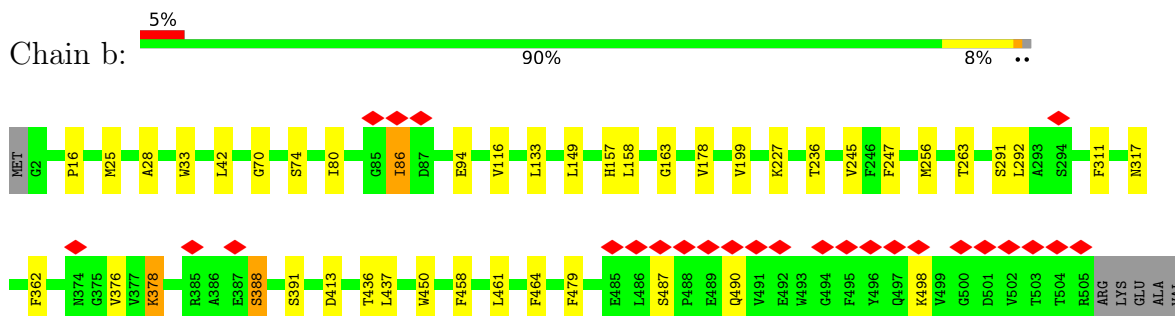
- Molecule 1: Photosystem II protein D1 1




- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein




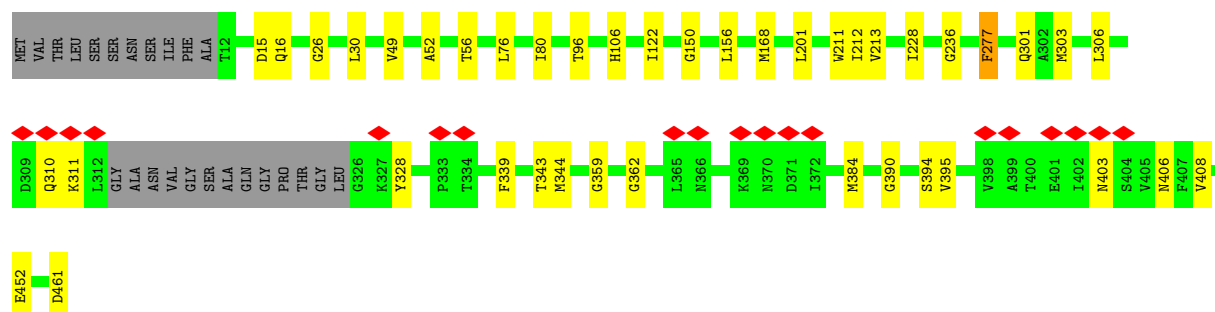
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  90% 8% .




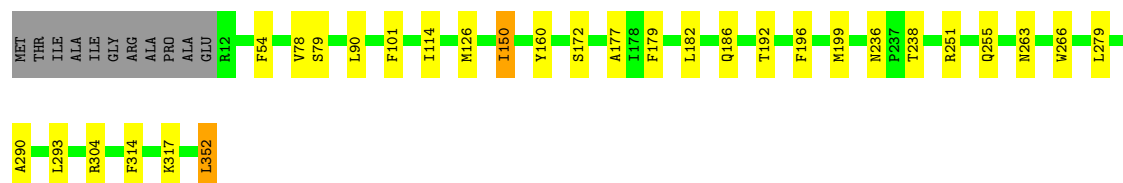
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  86% 9% 5%




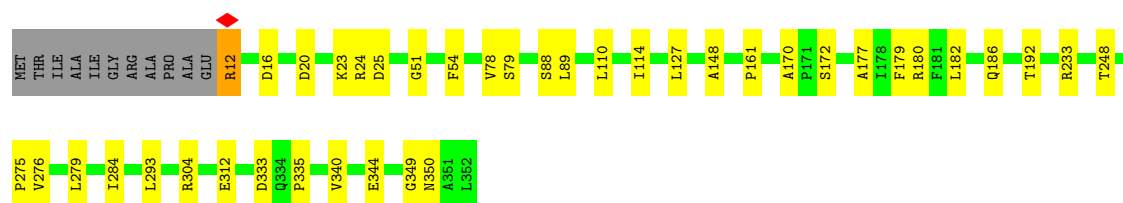
- Molecule 4: Photosystem II D2 protein

Chain D:  88% 8% . .




- Molecule 4: Photosystem II D2 protein

Chain d:  86% 11% .

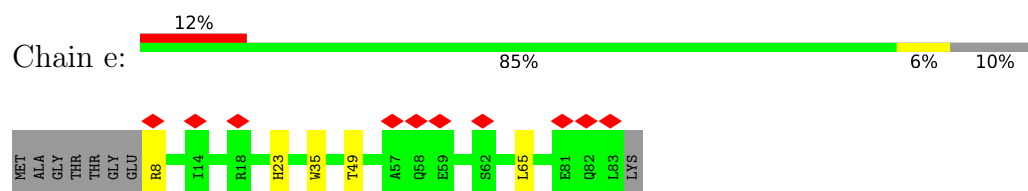


- Molecule 5: Cytochrome b559 subunit alpha

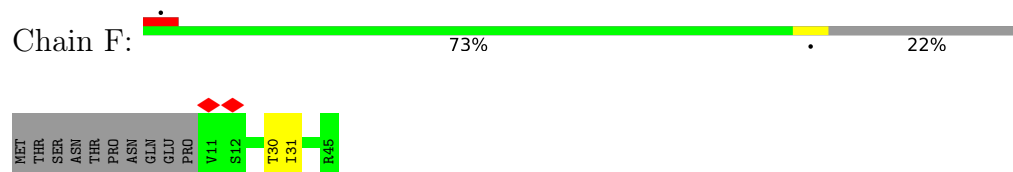
Chain E:  87% 8% 5%



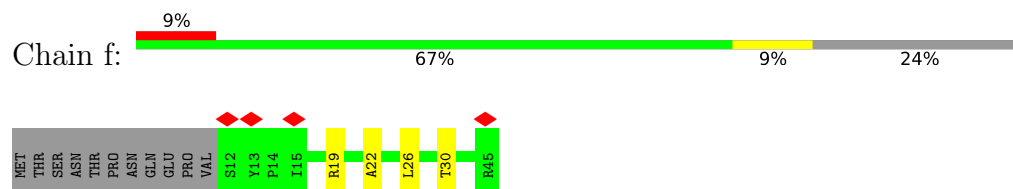
- Molecule 5: Cytochrome b559 subunit alpha



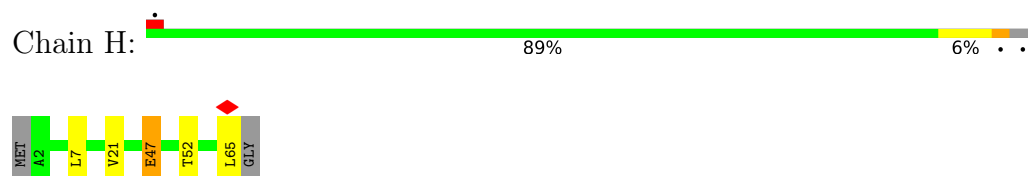
- Molecule 6: Cytochrome b559 subunit beta



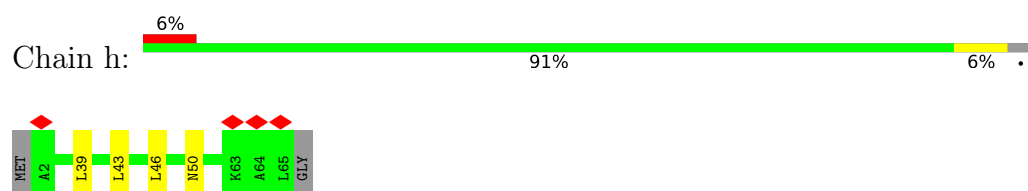
- Molecule 6: Cytochrome b559 subunit beta



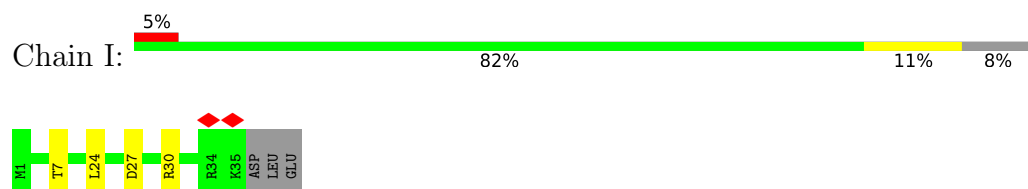
- Molecule 7: Photosystem II reaction center protein H



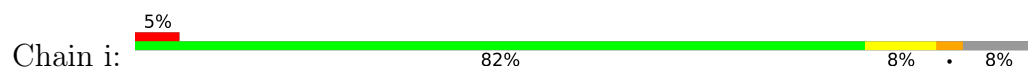
- Molecule 7: Photosystem II reaction center protein H

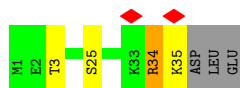


- Molecule 8: Photosystem II reaction center protein I

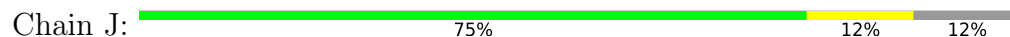


- Molecule 8: Photosystem II reaction center protein I

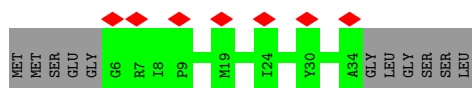




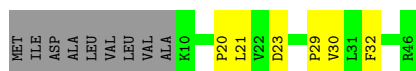
- Molecule 9: Photosystem II reaction center protein J



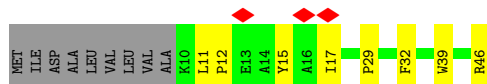
- Molecule 9: Photosystem II reaction center protein J



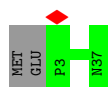
- Molecule 10: Photosystem II reaction center protein K



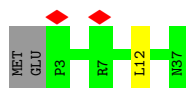
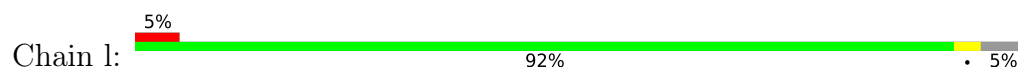
- Molecule 10: Photosystem II reaction center protein K




- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 14% • 8%




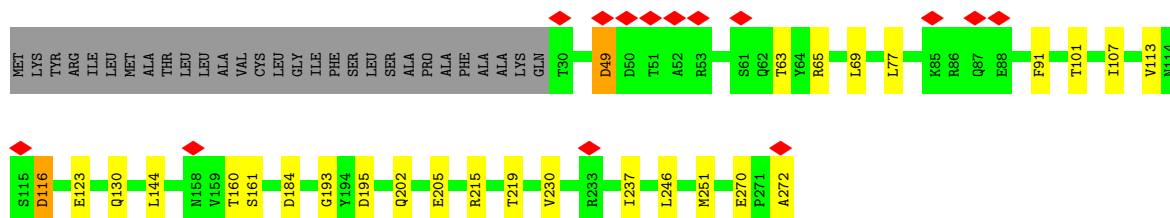
- Molecule 12: Photosystem II reaction center protein M

Chain m:  6% 64% 28% 8%




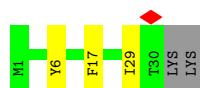
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  5% 79% 10% • 11%




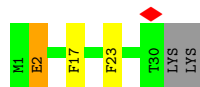
- Molecule 14: Photosystem II reaction center protein T

Chain T:  84% 9% 6%



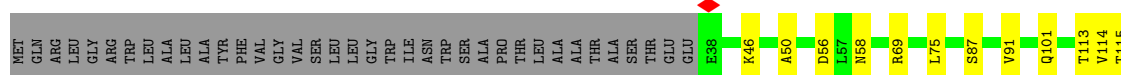
- Molecule 14: Photosystem II reaction center protein T

Chain t:  84% 6% • 6%

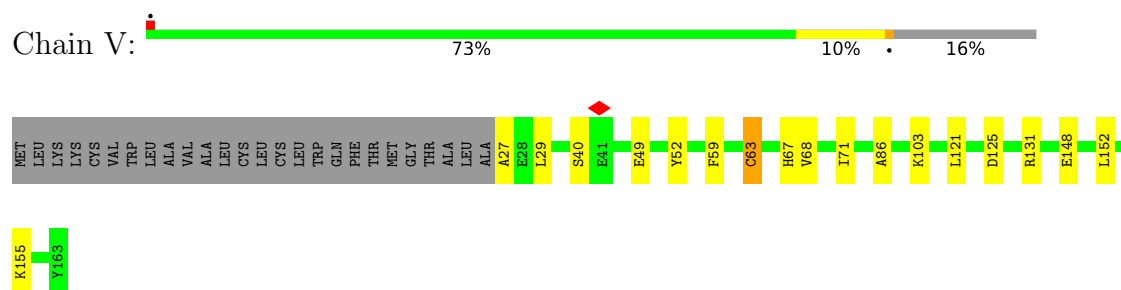


- Molecule 15: Photosystem II 12 kDa extrinsic protein

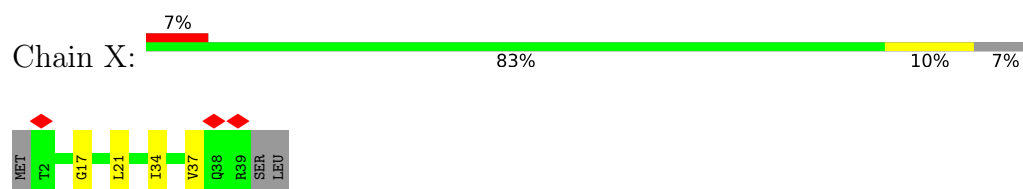
Chain U:  61% 11% 28%



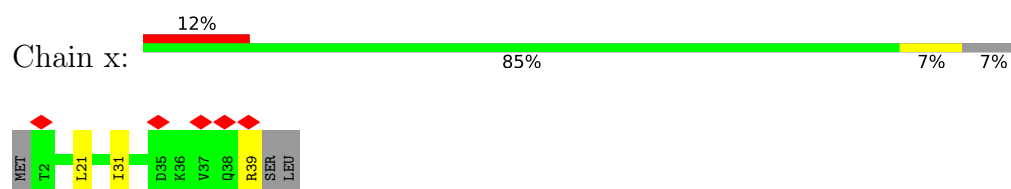
- Molecule 16: Cytochrome c-550



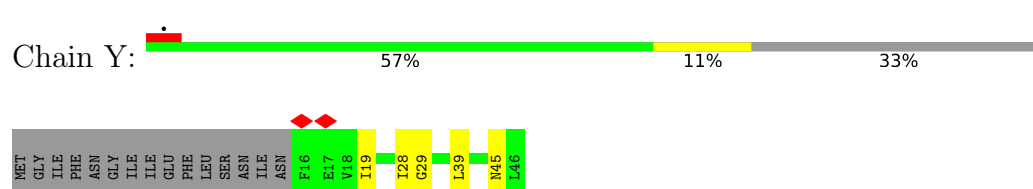
- Molecule 17: Photosystem II reaction center X protein



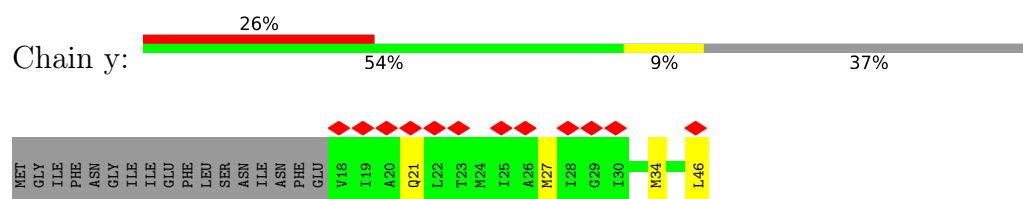
- Molecule 17: Photosystem II reaction center X protein



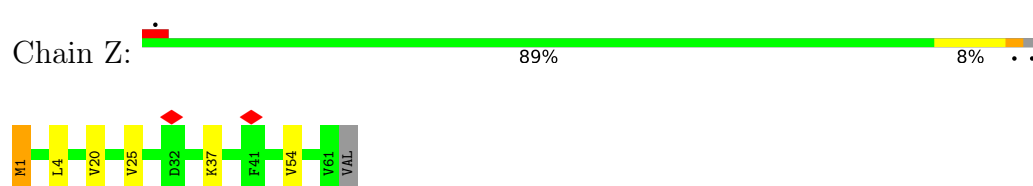
- Molecule 18: Photosystem II reaction center protein Ycf12



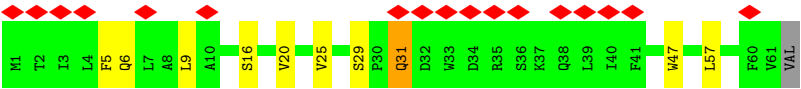
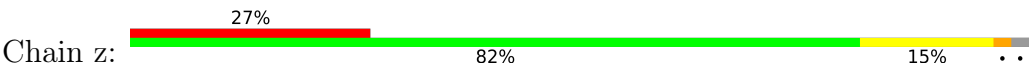
- Molecule 18: Photosystem II reaction center protein Ycf12



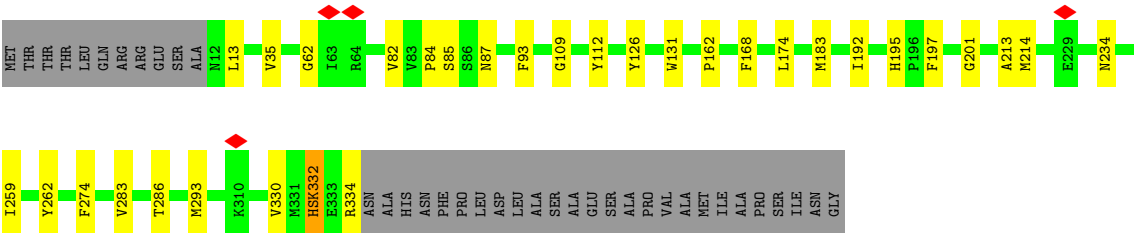
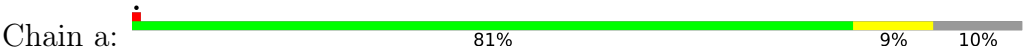
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein D1 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	272215	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.383	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.039	Depositor
Map size (Å)	137.0, 208.5, 119.0	wwPDB
Map dimensions	238, 417, 274	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LFA, CL, FE2, CA, LMG, PHO, PLM, LMT, GOL, HSK, FME, BCT, HEM, PL9, DGD, RRX, CLA, BCR, OEX, SQD, 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	0.24	0/2684	0.44	0/3663
2	B	0.22	0/4081	0.39	0/5565
2	b	0.22	0/4089	0.39	0/5576
3	C	0.22	0/3573	0.39	0/4868
3	c	0.20	0/3473	0.38	0/4734
4	D	0.24	0/2804	0.43	0/3822
4	d	0.22	0/2807	0.41	0/3827
5	E	0.20	0/663	0.38	0/907
5	e	0.22	0/622	0.44	0/853
6	F	0.24	0/289	0.44	0/394
6	f	0.22	0/283	0.45	0/387
7	H	0.21	0/519	0.39	0/708
7	h	0.20	0/519	0.39	0/708
8	I	0.20	0/281	0.42	0/380
8	i	0.23	0/285	0.56	0/385
9	J	0.20	0/259	0.42	0/351
9	j	0.15	0/222	0.33	0/303
10	K	0.30	0/299	0.49	0/412
10	k	0.28	0/299	0.54	0/412
11	L	0.18	0/288	0.32	0/392
11	l	0.18	0/294	0.33	0/399
12	M	0.27	0/257	0.49	0/351
12	m	0.31	0/257	0.56	0/351
13	O	0.19	0/1825	0.37	0/2485
14	T	0.21	0/249	0.36	0/339
14	t	0.20	0/253	0.34	0/344
15	U	0.17	0/766	0.36	0/1041
16	V	0.20	0/1073	0.35	0/1459
17	X	0.16	0/282	0.30	0/381
17	x	0.15	0/281	0.28	0/380
18	Y	0.28	0/229	0.45	0/309

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	y	0.25	0/207	0.44	0/278
19	Z	0.22	0/466	0.42	0/639
19	z	0.19	0/470	0.36	0/645
20	a	0.22	0/2600	0.43	0/3545
All	All	0.22	0/37848	0.40	0/51593

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
20	a	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	a	332	HSK	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2599	0	2500	35	0
2	B	3941	0	3786	30	0
2	b	3949	0	3798	29	0
3	C	3460	0	3376	26	0
3	c	3362	0	3267	27	0
4	D	2709	0	2613	22	0
4	d	2712	0	2617	32	0
5	E	644	0	627	5	0
5	e	603	0	581	4	0
6	F	280	0	284	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	274	0	282	3	0
7	H	506	0	529	4	0
7	h	506	0	529	5	0
8	I	284	0	303	4	0
8	i	288	0	307	2	0
9	J	253	0	265	4	0
9	j	216	0	227	0	0
10	K	289	0	294	4	0
10	k	289	0	294	4	0
11	L	281	0	288	0	0
11	l	287	0	299	0	0
12	M	254	0	272	5	0
12	m	254	0	270	9	0
13	O	1794	0	1736	14	0
14	T	250	0	245	2	0
14	t	254	0	257	3	0
15	U	755	0	748	9	0
16	V	1052	0	1053	11	0
17	X	279	0	307	2	0
17	x	278	0	310	3	0
18	Y	227	0	250	3	0
18	y	206	0	226	4	0
19	Z	455	0	486	3	0
19	z	459	0	487	5	0
20	a	2531	0	2434	24	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	1	0	0	0	0
23	A	260	0	288	10	0
23	B	1020	0	1113	23	0
23	C	845	0	936	23	0
23	D	130	0	144	6	0
23	a	195	0	216	7	0
23	b	1040	0	1152	23	0
23	c	845	0	936	25	0
23	d	195	0	216	7	0
24	A	64	0	74	1	0
24	D	64	0	74	2	0
24	a	64	0	74	2	0
24	d	64	0	74	2	0
25	A	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	120	0	168	4	0
25	C	120	0	168	6	0
25	D	40	0	56	1	0
25	T	40	0	56	3	0
25	Y	40	0	56	4	0
25	a	40	0	56	1	0
25	b	120	0	168	8	0
25	f	40	0	56	0	0
25	i	40	0	56	1	0
25	j	40	0	56	0	0
25	k	40	0	56	2	0
25	t	40	0	56	1	0
25	z	40	0	56	2	0
26	A	55	0	80	5	0
26	D	55	0	80	3	0
26	a	55	0	80	4	0
26	d	55	0	80	1	0
27	A	105	0	147	7	0
27	B	54	0	78	4	0
27	D	43	0	50	0	0
27	F	45	0	57	1	0
27	a	96	0	126	5	0
27	b	54	0	78	2	0
27	d	45	0	57	2	0
28	A	14	0	20	0	0
28	B	40	0	63	1	0
28	C	34	0	59	1	0
28	D	30	0	48	0	0
28	E	6	0	8	0	0
28	H	9	0	14	0	0
28	I	36	0	56	1	0
28	a	19	0	30	0	0
28	b	23	0	37	0	0
28	d	19	0	30	0	0
28	e	17	0	33	0	0
28	h	10	0	19	1	0
28	i	13	0	22	0	0
28	m	9	0	14	0	0
29	A	10	0	0	0	0
30	A	35	0	46	1	0
30	B	70	0	92	2	0
30	C	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D	33	0	39	3	0
30	E	35	0	46	0	0
30	J	24	0	35	0	0
30	M	70	0	92	3	0
30	T	59	0	81	0	0
30	a	59	0	81	1	0
30	c	29	0	31	1	0
30	d	24	0	35	1	0
30	f	34	0	41	1	0
30	z	35	0	46	0	0
31	A	4	0	0	0	0
31	a	4	0	0	0	0
32	A	13	0	18	2	0
32	B	28	0	40	0	0
32	C	39	0	54	1	0
32	D	29	0	45	4	0
32	E	49	0	77	1	0
32	J	16	0	24	0	0
32	K	14	0	20	1	0
32	a	11	0	14	0	0
32	b	54	0	76	1	0
32	c	47	0	62	2	0
32	d	16	0	24	1	0
32	h	11	0	14	0	0
32	i	28	0	40	0	0
32	k	12	0	16	0	0
32	l	14	0	20	0	0
32	x	18	0	31	0	0
33	B	51	0	72	5	0
33	C	48	0	66	1	0
33	D	51	0	72	4	0
33	I	51	0	72	3	0
33	Y	51	0	72	0	0
33	a	51	0	72	2	0
33	b	51	0	72	1	0
33	c	51	0	72	1	0
33	d	51	0	72	1	0
33	y	51	0	72	2	0
34	B	6	0	8	0	0
35	C	176	0	232	6	0
35	D	47	0	59	2	0
35	H	58	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	c	175	0	235	3	0
35	d	46	0	57	0	0
35	h	62	0	82	1	0
36	D	144	0	213	7	0
36	E	49	0	74	2	0
36	L	49	0	74	1	0
36	a	95	0	139	4	0
36	d	98	0	148	3	0
36	l	49	0	74	5	0
37	E	43	0	30	2	0
37	V	43	0	30	0	0
37	f	43	0	30	2	0
38	H	41	0	56	0	0
38	x	41	0	56	1	0
39	O	1	0	0	0	0
40	A	113	0	0	0	0
40	B	135	0	0	0	0
40	C	118	0	0	2	0
40	D	103	0	0	0	0
40	E	11	0	0	0	0
40	F	4	0	0	0	0
40	H	15	0	0	0	0
40	I	1	0	0	0	0
40	J	3	0	0	0	0
40	K	2	0	0	0	0
40	L	5	0	0	0	0
40	M	5	0	0	0	0
40	O	38	0	0	1	0
40	T	5	0	0	0	0
40	U	24	0	0	0	0
40	V	36	0	0	0	0
40	X	5	0	0	0	0
40	Y	3	0	0	0	0
40	Z	1	0	0	0	0
40	a	64	0	0	0	0
40	b	107	0	0	0	0
40	c	52	0	0	0	0
40	d	75	0	0	0	0
40	e	6	0	0	0	0
40	f	1	0	0	0	0
40	h	8	0	0	0	0
40	i	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	j	3	0	0	0	0
40	k	1	0	0	0	0
40	l	7	0	0	0	0
40	m	1	0	0	0	0
40	t	3	0	0	0	0
40	x	4	0	0	0	0
All	All	47004	0	47601	433	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 433 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)
25:T:101:BCR:H19C	25:b:619:BCR:H363	1.69	0.74
4:D:192:THR:HG23	23:D:404:CLA:HBC2	1.75	0.68
3:c:30:LEU:HD21	23:c:511:CLA:H2A	1.75	0.67
20:a:192:ILE:HG13	20:a:293:MET:HE1	1.77	0.67
30:a:411:LMT:O3B	4:d:304:ARG:NH2	2.28	0.66

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/360 (92%)	328 (99%)	3 (1%)	0	100	100
2	B	503/510 (99%)	496 (99%)	7 (1%)	0	100	100
2	b	502/510 (98%)	493 (98%)	9 (2%)	0	100	100
3	C	449/461 (97%)	440 (98%)	9 (2%)	0	100	100
3	c	433/461 (94%)	425 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	339/352 (96%)	334 (98%)	5 (2%)	0	100	100
4	d	339/352 (96%)	335 (99%)	4 (1%)	0	100	100
5	E	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
5	e	74/84 (88%)	72 (97%)	2 (3%)	0	100	100
6	F	33/45 (73%)	33 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	62/66 (94%)	59 (95%)	3 (5%)	0	100	100
7	h	62/66 (94%)	59 (95%)	3 (5%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
9	J	33/40 (82%)	33 (100%)	0	0	100	100
9	j	27/40 (68%)	27 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	33/37 (89%)	33 (100%)	0	0	100	100
11	l	33/37 (89%)	33 (100%)	0	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	31 (100%)	0	0	100	100
13	O	241/272 (89%)	235 (98%)	6 (2%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
17	X	36/41 (88%)	36 (100%)	0	0	100	100
17	x	36/41 (88%)	36 (100%)	0	0	100	100
18	Y	29/46 (63%)	29 (100%)	0	0	100	100
18	y	27/46 (59%)	26 (96%)	1 (4%)	0	100	100
19	Z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
20	a	320/360 (89%)	316 (99%)	4 (1%)	0	100	100
All	All	4654/5081 (92%)	4576 (98%)	78 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/291 (91%)	263 (99%)	2 (1%)	79	88
2	B	393/407 (97%)	390 (99%)	3 (1%)	79	88
2	b	398/407 (98%)	387 (97%)	11 (3%)	38	51
3	C	346/362 (96%)	343 (99%)	3 (1%)	75	86
3	c	335/362 (92%)	329 (98%)	6 (2%)	54	69
4	D	274/283 (97%)	271 (99%)	3 (1%)	70	82
4	d	275/283 (97%)	271 (98%)	4 (2%)	60	75
5	E	69/73 (94%)	68 (99%)	1 (1%)	62	77
5	e	63/73 (86%)	62 (98%)	1 (2%)	58	73
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	53 (98%)	1 (2%)	52	67
7	h	54/55 (98%)	54 (100%)	0	100	100
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	31/34 (91%)	29 (94%)	2 (6%)	14	16
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	20/28 (71%)	20 (100%)	0	100	100
10	K	29/37 (78%)	29 (100%)	0	100	100
10	k	29/37 (78%)	27 (93%)	2 (7%)	13	14
11	L	32/35 (91%)	32 (100%)	0	100	100
11	l	33/35 (94%)	32 (97%)	1 (3%)	36	48
12	M	29/33 (88%)	28 (97%)	1 (3%)	32	42
12	m	29/33 (88%)	27 (93%)	2 (7%)	13	14
13	O	189/228 (83%)	178 (94%)	11 (6%)	17	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	24/28 (86%)	23 (96%)	1 (4%)	25	33
14	t	25/28 (89%)	24 (96%)	1 (4%)	27	35
15	U	79/112 (70%)	78 (99%)	1 (1%)	65	78
16	V	114/138 (83%)	112 (98%)	2 (2%)	54	69
17	X	30/34 (88%)	28 (93%)	2 (7%)	13	15
17	x	30/34 (88%)	29 (97%)	1 (3%)	33	44
18	Y	22/37 (60%)	20 (91%)	2 (9%)	7	8
18	y	20/37 (54%)	19 (95%)	1 (5%)	20	26
19	Z	47/52 (90%)	44 (94%)	3 (6%)	14	17
19	z	48/52 (92%)	45 (94%)	3 (6%)	15	17
20	a	259/290 (89%)	257 (99%)	2 (1%)	79	88
All	All	3755/4133 (91%)	3682 (98%)	73 (2%)	52	67

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	312	GLU
19	z	20	VAL
5	e	8	ARG
12	m	4	ASN
13	O	270	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	44	HIS
7	h	50	ASN
3	c	299	GLN
4	d	186	GLN
17	x	33	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.34	0	7,9,11	0.99	0
8	FME	I	1	8	8,9,10	0.38	0	7,9,11	0.86	0
20	HSK	a	332	20	7,11,12	1.27	1 (14%)	3,14,16	0.92	0
14	FME	T	1	14	8,9,10	0.39	0	7,9,11	1.09	0
8	FME	i	1	8	8,9,10	0.37	0	7,9,11	0.99	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
14	FME	t	1	14	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
20	HSK	a	332	20	-	2/5/6/8	0/1/1/1
14	FME	T	1	14	-	0/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	332	HSK	CE1-ND1	-2.14	1.34	1.36

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	a	332	HSK	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
8	i	1	FME	CA-CB-CG-SD
20	a	332	HSK	N-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
14	t	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 228 ligands modelled in this entry, 6 are monoatomic - leaving 222 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	$\# Z > 2$
32	PLM	b	626	-	10,10,17	0.80	0	10,10,17	0.82	0
30	LMT	C	526	-	36,36,36	0.57	0	47,47,47	0.76	2 (4%)
32	PLM	A	418	-	12,12,17	0.76	0	12,12,17	0.72	0
28	LFA	C	523	-	12,12,19	0.22	0	11,11,18	0.25	0
23	CLA	b	609	-	65,73,73	1.40	7 (10%)	76,113,113	1.48	10 (13%)
23	CLA	B	610	40	65,73,73	1.47	6 (9%)	76,113,113	1.51	9 (11%)
25	BCR	k	101	-	41,41,41	0.34	0	56,56,56	0.64	0
30	LMT	c	517	-	30,30,36	0.59	0	41,41,47	0.80	0
23	CLA	B	613	-	65,73,73	1.41	7 (10%)	76,113,113	1.47	8 (10%)
28	LFA	a	418	-	9,9,19	0.24	0	8,8,18	0.26	0
23	CLA	C	517	-	65,73,73	1.43	6 (9%)	76,113,113	1.49	7 (9%)
27	SQD	A	411	-	53,54,54	1.55	8 (15%)	62,65,65	1.37	8 (12%)
30	LMT	D	417	-	34,34,36	0.55	0	45,45,47	0.77	0
32	PLM	i	102	-	12,12,17	0.74	0	12,12,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	b	619	-	41,41,41	0.36	0	56,56,56	0.80	0
30	LMT	d	403	-	24,24,36	0.54	0	29,29,47	0.61	0
35	DGD	D	411	-	47,47,67	0.50	0	54,55,81	0.66	1 (1%)
35	DGD	d	407	-	46,46,67	0.55	0	53,54,81	0.71	0
30	LMT	J	101	-	24,24,36	0.49	0	29,29,47	0.59	0
33	LMG	B	619	-	51,51,55	0.52	0	59,59,63	0.57	0
27	SQD	a	407	-	50,51,54	1.52	6 (12%)	59,62,65	1.63	8 (13%)
33	LMG	D	409	-	51,51,55	0.56	0	59,59,63	0.64	0
33	LMG	y	101	-	51,51,55	0.51	0	59,59,63	0.63	0
32	PLM	c	519	-	14,14,17	0.72	0	14,14,17	0.66	0
32	PLM	x	101	-	17,17,17	0.66	0	17,17,17	0.65	0
30	LMT	f	103	-	35,35,36	0.54	0	46,46,47	0.69	1 (2%)
28	LFA	b	624	-	7,7,19	0.26	0	6,6,18	0.12	0
32	PLM	c	520	-	9,9,17	0.86	0	9,9,17	0.86	0
30	LMT	T	102	-	24,24,36	0.49	0	29,29,47	0.59	0
23	CLA	B	615	-	65,73,73	1.40	7 (10%)	76,113,113	1.43	7 (9%)
27	SQD	d	408	-	44,45,54	1.61	8 (18%)	53,56,65	1.51	8 (15%)
23	CLA	B	602	-	65,73,73	1.42	7 (10%)	76,113,113	1.47	8 (10%)
30	LMT	B	626	-	36,36,36	0.54	0	47,47,47	1.04	2 (4%)
23	CLA	B	612	-	65,73,73	1.37	7 (10%)	76,113,113	1.51	6 (7%)
35	DGD	C	504	-	63,63,67	0.59	0	77,77,81	1.22	8 (10%)
23	CLA	b	608	40	65,73,73	1.44	7 (10%)	76,113,113	1.51	8 (10%)
23	CLA	d	405	-	65,73,73	1.43	7 (10%)	76,113,113	1.48	9 (11%)
30	LMT	T	103	-	36,36,36	0.51	0	47,47,47	0.89	1 (2%)
33	LMG	c	521	-	51,51,55	0.49	0	59,59,63	0.60	0
26	PL9	D	402	-	55,55,55	1.26	5 (9%)	68,69,69	1.52	14 (20%)
36	LHG	a	416	-	45,45,48	0.53	0	48,51,54	0.49	0
23	CLA	C	506	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	10 (13%)
25	BCR	a	406	-	41,41,41	0.37	0	56,56,56	0.79	0
25	BCR	z	101	-	41,41,41	0.40	0	56,56,56	0.98	1 (1%)
23	CLA	b	603	-	65,73,73	1.44	7 (10%)	76,113,113	1.46	7 (9%)
30	LMT	M	101	-	36,36,36	0.59	0	47,47,47	0.79	1 (2%)
33	LMG	a	408	-	51,51,55	0.54	0	59,59,63	0.68	0
23	CLA	A	405	40	65,73,73	1.38	6 (9%)	76,113,113	1.59	10 (13%)
23	CLA	B	605	-	65,73,73	1.44	7 (10%)	76,113,113	1.46	7 (9%)
23	CLA	B	606	-	65,73,73	1.43	6 (9%)	76,113,113	1.52	9 (11%)
23	CLA	D	404	-	65,73,73	1.43	7 (10%)	76,113,113	1.41	6 (7%)
25	BCR	b	620	-	41,41,41	0.35	0	56,56,56	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	604	-	65,73,73	1.43	7 (10%)	76,113,113	1.45	8 (10%)
30	LMT	M	102	-	36,36,36	0.58	0	47,47,47	0.71	0
36	LHG	E	101	-	48,48,48	0.51	0	51,54,54	0.50	0
24	PHO	d	402	-	51,69,69	0.67	0	47,99,99	1.06	5 (10%)
32	PLM	B	624	-	14,14,17	0.71	0	14,14,17	0.66	0
25	BCR	A	409	-	41,41,41	0.34	0	56,56,56	0.67	0
35	DGD	c	516	-	63,63,67	0.57	0	77,77,81	0.70	1 (1%)
29	OEX	A	414	40,1,3	0,15,15	-	-	-	-	-
25	BCR	j	101	-	41,41,41	0.36	0	56,56,56	1.05	5 (8%)
35	DGD	C	505	-	62,62,67	0.61	0	76,76,81	1.39	6 (7%)
33	LMG	C	525	-	48,48,55	0.50	0	56,56,63	0.83	3 (5%)
32	PLM	C	524	-	12,12,17	0.77	0	12,12,17	0.78	1 (8%)
36	LHG	d	409	-	48,48,48	0.52	0	51,54,54	0.50	0
23	CLA	b	610	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	8 (10%)
38	RRX	x	102	-	42,42,42	0.26	0	57,58,58	0.41	0
36	LHG	l	102	-	48,48,48	0.51	0	51,54,54	0.56	1 (1%)
23	CLA	C	514	-	65,73,73	1.39	6 (9%)	76,113,113	1.54	7 (9%)
23	CLA	a	405	-	65,73,73	1.44	7 (10%)	76,113,113	1.44	8 (10%)
23	CLA	B	603	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
23	CLA	D	405	-	65,73,73	1.43	6 (9%)	76,113,113	1.42	8 (10%)
25	BCR	i	103	-	41,41,41	0.34	0	56,56,56	0.65	0
28	LFA	B	629	-	6,6,19	0.25	0	5,5,18	0.16	0
36	LHG	D	408	-	45,45,48	0.53	0	48,51,54	0.50	0
36	LHG	L	101	-	48,48,48	0.51	0	51,54,54	0.57	0
23	CLA	B	604	-	65,73,73	1.40	6 (9%)	76,113,113	1.55	8 (10%)
23	CLA	d	401	40	65,73,73	1.40	6 (9%)	76,113,113	1.61	8 (10%)
25	BCR	C	527	-	41,41,41	0.36	0	56,56,56	0.71	0
25	BCR	b	618	-	41,41,41	0.39	0	56,56,56	0.76	0
28	LFA	m	101	-	8,8,19	0.23	0	7,7,18	0.20	0
25	BCR	f	101	-	41,41,41	0.33	0	56,56,56	0.89	3 (5%)
28	LFA	h	101	-	9,9,19	0.23	0	8,8,18	0.21	0
35	DGD	c	514	-	63,63,67	0.59	0	77,77,81	0.76	2 (2%)
28	LFA	D	412	-	11,11,19	0.24	0	10,10,18	0.21	0
28	LFA	B	625	-	7,7,19	0.24	0	6,6,18	0.21	0
23	CLA	C	518	-	65,73,73	1.41	6 (9%)	76,113,113	1.49	8 (10%)
23	CLA	c	505	-	65,73,73	1.44	8 (12%)	76,113,113	1.42	8 (10%)
27	SQD	A	415	-	50,51,54	1.49	5 (10%)	59,62,65	1.72	10 (16%)
28	LFA	B	622	-	12,12,19	0.23	0	11,11,18	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	510	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
32	PLM	b	623	-	15,15,17	0.70	0	15,15,17	0.64	0
30	LMT	E	106	-	36,36,36	0.54	0	47,47,47	0.76	1 (2%)
25	BCR	B	631	-	41,41,41	0.36	0	56,56,56	1.37	6 (10%)
30	LMT	A	416	-	36,36,36	0.50	0	47,47,47	1.26	5 (10%)
27	SQD	F	101	-	44,45,54	1.61	9 (20%)	53,56,65	1.57	9 (16%)
35	DGD	h	102	-	63,63,67	0.57	0	77,77,81	0.76	1 (1%)
23	CLA	C	511	-	65,73,73	1.44	7 (10%)	76,113,113	1.49	9 (11%)
28	LFA	I	101	-	12,12,19	0.24	0	11,11,18	0.30	0
32	PLM	J	102	-	15,15,17	0.70	0	15,15,17	0.67	0
32	PLM	i	101	-	14,14,17	0.73	0	14,14,17	0.65	0
32	PLM	b	622	-	14,14,17	0.69	0	14,14,17	0.67	0
27	SQD	b	601	-	53,54,54	1.48	9 (16%)	62,65,65	1.49	7 (11%)
33	LMG	d	411	-	51,51,55	0.53	0	59,59,63	0.60	0
28	LFA	I	104	-	7,7,19	0.24	0	6,6,18	0.19	0
23	CLA	c	513	-	65,73,73	1.43	8 (12%)	76,113,113	1.43	6 (7%)
23	CLA	A	404	-	65,73,73	1.41	6 (9%)	76,113,113	1.51	8 (10%)
23	CLA	c	509	-	65,73,73	1.40	6 (9%)	76,113,113	1.51	7 (9%)
28	LFA	A	413	-	6,6,19	0.26	0	5,5,18	0.17	0
27	SQD	a	410	-	44,45,54	1.63	7 (15%)	53,56,65	1.44	7 (13%)
36	LHG	D	406	-	48,48,48	0.51	0	51,54,54	0.47	0
27	SQD	D	410	-	42,43,54	1.67	8 (19%)	51,54,65	1.53	8 (15%)
37	HEM	E	105	5,6	41,50,50	1.45	4 (9%)	45,82,82	1.48	8 (17%)
30	LMT	a	411	-	36,36,36	0.53	0	47,47,47	0.90	3 (6%)
32	PLM	k	102	-	11,11,17	0.78	0	11,11,17	0.76	0
25	BCR	C	502	-	41,41,41	0.36	0	56,56,56	0.74	1 (1%)
23	CLA	d	404	-	65,73,73	1.44	7 (10%)	76,113,113	1.40	6 (7%)
28	LFA	b	625	-	7,7,19	0.26	0	6,6,18	0.22	0
25	BCR	B	618	-	41,41,41	0.32	0	56,56,56	0.83	2 (3%)
23	CLA	A	408	-	65,73,73	1.44	7 (10%)	76,113,113	1.43	8 (10%)
23	CLA	B	601	40	65,73,73	1.47	7 (10%)	76,113,113	1.38	6 (7%)
36	LHG	d	410	-	48,48,48	0.52	0	51,54,54	0.51	0
23	CLA	a	403	40	65,73,73	1.42	6 (9%)	76,113,113	1.47	10 (13%)
32	PLM	l	101	-	13,13,17	0.78	0	13,13,17	0.67	0
30	LMT	z	102	-	36,36,36	0.53	0	47,47,47	0.77	1 (2%)
32	PLM	d	413	-	15,15,17	0.68	0	15,15,17	0.65	0
37	HEM	f	102	5,6	41,50,50	1.46	4 (9%)	45,82,82	1.41	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PL9	d	406	-	55,55,55	1.23	5 (9%)	68,69,69	1.52	15 (22%)
23	CLA	B	611	-	65,73,73	1.43	7 (10%)	76,113,113	1.53	9 (11%)
23	CLA	c	510	-	65,73,73	1.46	7 (10%)	76,113,113	1.37	5 (6%)
33	LMG	Y	101	-	51,51,55	0.52	0	59,59,63	0.67	0
28	LFA	D	416	-	7,7,19	0.25	0	6,6,18	0.21	0
23	CLA	b	611	40	65,73,73	1.47	8 (12%)	76,113,113	1.40	9 (11%)
30	LMT	B	620	-	36,36,36	0.55	0	47,47,47	0.71	0
23	CLA	b	605	-	65,73,73	1.45	6 (9%)	76,113,113	1.53	9 (11%)
36	LHG	D	407	-	48,48,48	0.52	0	51,54,54	0.47	0
32	PLM	E	107	-	17,17,17	0.65	0	17,17,17	0.61	0
32	PLM	E	102	-	14,14,17	0.75	0	14,14,17	0.67	0
23	CLA	b	616	-	65,73,73	1.43	7 (10%)	76,113,113	1.43	7 (9%)
32	PLM	C	519	-	12,12,17	0.74	0	12,12,17	0.77	1 (8%)
23	CLA	B	614	-	65,73,73	1.45	7 (10%)	76,113,113	1.48	10 (13%)
23	CLA	C	513	-	65,73,73	1.39	7 (10%)	76,113,113	1.50	9 (11%)
32	PLM	B	628	-	12,12,17	0.76	0	12,12,17	0.73	0
32	PLM	D	414	-	17,17,17	0.62	0	17,17,17	0.65	0
28	LFA	d	412	-	9,9,19	0.21	0	8,8,18	0.25	0
23	CLA	C	507	-	65,73,73	1.44	7 (10%)	76,113,113	1.44	6 (7%)
23	CLA	b	607	-	65,73,73	1.45	7 (10%)	76,113,113	1.49	9 (11%)
35	DGD	c	515	-	51,51,67	0.52	0	59,59,81	0.75	2 (3%)
23	CLA	b	617	-	65,73,73	1.43	7 (10%)	76,113,113	1.46	7 (9%)
31	BCT	a	415	21	2,3,3	0.89	0	2,3,3	3.22	2 (100%)
32	PLM	D	415	-	10,10,17	0.83	0	10,10,17	0.79	0
23	CLA	C	508	-	65,73,73	1.44	6 (9%)	76,113,113	1.41	8 (10%)
28	LFA	C	520	-	11,11,19	0.26	0	10,10,18	0.19	0
36	LHG	a	417	-	48,48,48	0.50	0	51,54,54	0.49	0
27	SQD	B	630	-	53,54,54	1.51	8 (15%)	62,65,65	1.49	6 (9%)
28	LFA	B	623	-	5,5,19	0.25	0	4,4,18	0.16	0
23	CLA	B	608	-	65,73,73	1.41	6 (9%)	76,113,113	1.51	8 (10%)
32	PLM	K	101	-	13,13,17	0.74	0	13,13,17	0.70	0
32	PLM	b	628	-	11,11,17	0.78	0	11,11,17	0.74	0
23	CLA	A	406	40	65,73,73	1.44	6 (9%)	76,113,113	1.45	11 (14%)
23	CLA	C	516	3	65,73,73	1.40	7 (10%)	76,113,113	1.54	8 (10%)
28	LFA	H	103	-	8,8,19	0.24	0	7,7,18	0.18	0
23	CLA	C	512	40	65,73,73	1.40	6 (9%)	76,113,113	1.55	8 (10%)
32	PLM	E	103	-	15,15,17	0.67	0	15,15,17	0.68	0
32	PLM	a	413	-	10,10,17	0.85	0	10,10,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LFA	d	414	-	8,8,19	0.25	0	7,7,18	0.19	0
28	LFA	a	412	-	8,8,19	0.25	0	7,7,18	0.19	0
23	CLA	c	511	3	65,73,73	1.43	7 (10%)	76,113,113	1.54	8 (10%)
24	PHO	D	401	-	51,69,69	0.68	0	47,99,99	1.15	5 (10%)
23	CLA	c	502	-	65,73,73	1.42	7 (10%)	76,113,113	1.47	7 (9%)
33	LMG	b	621	-	51,51,55	0.53	0	59,59,63	0.61	0
32	PLM	c	518	-	8,8,17	0.92	0	8,8,17	0.88	0
32	PLM	C	522	-	12,12,17	0.76	0	12,12,17	0.70	0
25	BCR	T	101	-	41,41,41	0.36	0	56,56,56	1.50	6 (10%)
25	BCR	C	501	-	41,41,41	0.40	0	56,56,56	0.98	1 (1%)
23	CLA	C	515	-	65,73,73	1.42	6 (9%)	76,113,113	1.41	7 (9%)
28	LFA	A	412	-	6,6,19	0.26	0	5,5,18	0.18	0
23	CLA	B	616	-	45,53,73	1.72	7 (15%)	52,89,113	1.75	7 (13%)
23	CLA	c	503	-	65,73,73	1.45	6 (9%)	76,113,113	1.39	8 (10%)
23	CLA	b	613	-	65,73,73	1.38	7 (10%)	76,113,113	1.55	7 (9%)
23	CLA	c	506	-	65,73,73	1.45	7 (10%)	76,113,113	1.53	7 (9%)
35	DGD	C	503	-	54,54,67	0.67	0	68,68,81	0.73	1 (1%)
28	LFA	I	105	-	7,7,19	0.24	0	6,6,18	0.20	0
23	CLA	B	609	-	65,73,73	1.45	7 (10%)	76,113,113	1.46	7 (9%)
34	GOL	B	621	-	5,5,5	0.38	0	5,5,5	0.41	0
23	CLA	c	512	-	65,73,73	1.41	6 (9%)	76,113,113	1.48	6 (7%)
31	BCT	A	417	21	2,3,3	0.89	0	2,3,3	3.28	2 (100%)
32	PLM	h	103	-	10,10,17	0.82	0	10,10,17	0.78	0
33	LMG	I	103	-	51,51,55	0.53	0	59,59,63	0.64	0
38	RRX	H	102	-	42,42,42	0.24	0	57,58,58	0.43	0
25	BCR	D	403	-	41,41,41	0.35	0	56,56,56	0.87	2 (3%)
37	HEM	V	201	16	41,50,50	1.43	3 (7%)	45,82,82	1.52	10 (22%)
24	PHO	A	407	-	51,69,69	0.72	2 (3%)	47,99,99	0.95	3 (6%)
23	CLA	B	607	40	65,73,73	1.43	7 (10%)	76,113,113	1.49	8 (10%)
28	LFA	B	627	-	5,5,19	0.26	0	4,4,18	0.15	0
28	LFA	I	102	-	6,6,19	0.26	0	5,5,18	0.20	0
23	CLA	b	614	-	65,73,73	1.41	6 (9%)	76,113,113	1.41	8 (10%)
23	CLA	b	606	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
23	CLA	c	507	40	65,73,73	1.39	6 (9%)	76,113,113	1.53	8 (10%)
23	CLA	b	615	-	65,73,73	1.41	7 (10%)	76,113,113	1.43	8 (10%)
30	LMT	a	419	-	24,24,36	0.57	0	29,29,47	0.75	1 (3%)
32	PLM	c	522	-	12,12,17	0.79	0	12,12,17	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	504	40	65,73,73	1.42	7 (10%)	76,113,113	1.53	8 (10%)
23	CLA	b	602	40	65,73,73	1.47	6 (9%)	76,113,113	1.37	6 (7%)
23	CLA	b	612	-	65,73,73	1.42	7 (10%)	76,113,113	1.52	10 (13%)
28	LFA	E	104	-	5,5,19	0.27	0	4,4,18	0.17	0
26	PL9	A	410	-	55,55,55	1.27	5 (9%)	68,69,69	1.62	14 (20%)
23	CLA	a	402	-	65,73,73	1.39	6 (9%)	76,113,113	1.50	8 (10%)
28	LFA	b	627	-	6,6,19	0.27	0	5,5,18	0.17	0
26	PL9	a	409	-	55,55,55	1.17	3 (5%)	68,69,69	1.48	12 (17%)
25	BCR	t	101	-	41,41,41	0.37	0	56,56,56	0.86	1 (1%)
25	BCR	B	617	-	41,41,41	0.37	0	56,56,56	0.71	0
25	BCR	Y	102	-	41,41,41	0.36	0	56,56,56	0.95	1 (1%)
24	PHO	a	404	-	51,69,69	0.70	0	47,99,99	0.95	3 (6%)
28	LFA	i	104	-	12,12,19	0.23	0	11,11,18	0.19	0
23	CLA	c	501	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	10 (13%)
28	LFA	C	521	-	8,8,19	0.21	0	7,7,18	0.24	0
23	CLA	C	509	40	65,73,73	1.41	7 (10%)	76,113,113	1.55	8 (10%)
28	LFA	D	413	-	9,9,19	0.26	0	8,8,18	0.20	0
35	DGD	H	101	-	59,59,67	0.58	0	73,73,81	0.81	0
28	LFA	e	101	-	16,16,19	0.23	0	15,15,18	0.21	0
23	CLA	c	508	-	65,73,73	1.40	7 (10%)	76,113,113	1.52	9 (11%)

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
32	PLM	b	626	-	-	0/8/8/15	-
30	LMT	C	526	-	-	11/21/61/61	0/2/2/2
32	PLM	A	418	-	-	5/10/10/15	-
28	LFA	C	523	-	-	1/10/10/17	-
23	CLA	b	609	-	1/1/15/20	5/37/115/115	-
23	CLA	B	610	40	1/1/15/20	10/37/115/115	-
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
30	LMT	c	517	-	-	10/15/55/61	0/2/2/2
23	CLA	B	613	-	1/1/15/20	10/37/115/115	-
28	LFA	a	418	-	-	5/7/7/17	-
23	CLA	C	517	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	411	-	-	19/49/69/69	0/1/1/1
30	LMT	D	417	-	-	5/19/59/61	0/2/2/2
32	PLM	i	102	-	-	2/10/10/15	-
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
30	LMT	d	403	-	-	4/15/35/61	0/1/1/2
35	DGD	D	411	-	-	22/41/62/95	0/1/1/2
35	DGD	d	407	-	-	18/40/61/95	0/1/1/2
30	LMT	J	101	-	-	9/15/35/61	0/1/1/2
33	LMG	B	619	-	-	16/46/66/70	0/1/1/1
27	SQD	a	407	-	-	17/46/66/69	0/1/1/1
33	LMG	D	409	-	-	9/46/66/70	0/1/1/1
33	LMG	y	101	-	-	27/46/66/70	0/1/1/1
32	PLM	c	519	-	-	4/12/12/15	-
32	PLM	x	101	-	-	6/15/15/15	-
30	LMT	f	103	-	-	13/20/60/61	0/2/2/2
28	LFA	b	624	-	-	0/5/5/17	-
32	PLM	c	520	-	-	0/7/7/15	-
30	LMT	T	102	-	-	9/15/35/61	0/1/1/2
23	CLA	B	615	-	1/1/15/20	8/37/115/115	-
27	SQD	d	408	-	-	17/40/60/69	0/1/1/1
23	CLA	B	602	-	1/1/15/20	5/37/115/115	-
30	LMT	B	626	-	-	4/21/61/61	0/2/2/2
23	CLA	B	612	-	1/1/15/20	8/37/115/115	-
35	DGD	C	504	-	-	24/51/91/95	0/2/2/2
23	CLA	b	608	40	1/1/15/20	5/37/115/115	-
23	CLA	d	405	-	1/1/15/20	12/37/115/115	-
30	LMT	T	103	-	-	2/21/61/61	0/2/2/2
33	LMG	c	521	-	-	16/46/66/70	0/1/1/1
26	PL9	D	402	-	-	18/53/73/73	0/1/1/1
36	LHG	a	416	-	-	13/50/50/53	-
23	CLA	C	506	-	1/1/15/20	5/37/115/115	-
25	BCR	a	406	-	-	2/29/63/63	0/2/2/2
25	BCR	z	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	603	-	1/1/15/20	11/37/115/115	-
30	LMT	M	101	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	a	408	-	-	21/46/66/70	0/1/1/1
23	CLA	A	405	40	1/1/15/20	6/37/115/115	-
23	CLA	B	605	-	1/1/15/20	5/37/115/115	-
23	CLA	B	606	-	1/1/15/20	7/37/115/115	-
23	CLA	D	404	-	1/1/15/20	3/37/115/115	-
25	BCR	b	620	-	-	2/29/63/63	0/2/2/2
23	CLA	b	604	-	1/1/15/20	10/37/115/115	-
30	LMT	M	102	-	-	5/21/61/61	0/2/2/2
36	LHG	E	101	-	-	19/53/53/53	-
24	PHO	d	402	-	-	2/37/103/103	0/5/6/6
32	PLM	B	624	-	-	5/12/12/15	-
25	BCR	A	409	-	-	3/29/63/63	0/2/2/2
35	DGD	c	516	-	-	13/51/91/95	0/2/2/2
25	BCR	j	101	-	-	12/29/63/63	0/2/2/2
35	DGD	C	505	-	-	27/50/90/95	0/2/2/2
33	LMG	C	525	-	-	15/43/63/70	0/1/1/1
32	PLM	C	524	-	-	4/10/10/15	-
36	LHG	d	409	-	-	12/53/53/53	-
23	CLA	b	610	-	1/1/15/20	7/37/115/115	-
38	RRX	x	102	-	-	2/29/65/65	0/2/2/2
36	LHG	l	102	-	-	20/53/53/53	-
23	CLA	C	514	-	1/1/15/20	3/37/115/115	-
23	CLA	a	405	-	1/1/15/20	12/37/115/115	-
23	CLA	B	603	-	1/1/15/20	13/37/115/115	-
23	CLA	D	405	-	1/1/15/20	7/37/115/115	-
25	BCR	i	103	-	-	2/29/63/63	0/2/2/2
28	LFA	B	629	-	-	0/4/4/17	-
36	LHG	D	408	-	-	11/50/50/53	-
36	LHG	L	101	-	-	22/53/53/53	-
23	CLA	B	604	-	1/1/15/20	12/37/115/115	-
23	CLA	d	401	40	1/1/15/20	4/37/115/115	-
25	BCR	C	527	-	-	4/29/63/63	0/2/2/2
25	BCR	b	618	-	-	4/29/63/63	0/2/2/2
28	LFA	m	101	-	-	3/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	f	101	-	-	9/29/63/63	0/2/2/2
28	LFA	h	101	-	-	2/7/7/17	-
35	DGD	c	514	-	-	25/51/91/95	0/2/2/2
28	LFA	D	412	-	-	0/9/9/17	-
28	LFA	B	625	-	-	1/5/5/17	-
23	CLA	C	518	-	1/1/15/20	7/37/115/115	-
23	CLA	c	505	-	1/1/15/20	6/37/115/115	-
27	SQD	A	415	-	-	23/46/66/69	0/1/1/1
28	LFA	B	622	-	-	3/10/10/17	-
23	CLA	C	510	-	1/1/15/20	9/37/115/115	-
32	PLM	b	623	-	-	5/13/13/15	-
30	LMT	E	106	-	-	7/21/61/61	0/2/2/2
25	BCR	B	631	-	-	10/29/63/63	0/2/2/2
30	LMT	A	416	-	-	10/21/61/61	0/2/2/2
27	SQD	F	101	-	-	16/40/60/69	0/1/1/1
35	DGD	h	102	-	-	15/51/91/95	0/2/2/2
23	CLA	C	511	-	1/1/15/20	13/37/115/115	-
28	LFA	I	101	-	-	1/10/10/17	-
32	PLM	J	102	-	-	3/13/13/15	-
32	PLM	i	101	-	-	4/12/12/15	-
32	PLM	b	622	-	-	3/12/12/15	-
27	SQD	b	601	-	-	21/49/69/69	0/1/1/1
33	LMG	d	411	-	-	14/46/66/70	0/1/1/1
28	LFA	I	104	-	-	0/5/5/17	-
23	CLA	c	513	-	1/1/15/20	9/37/115/115	-
23	CLA	A	404	-	1/1/15/20	10/37/115/115	-
23	CLA	c	509	-	1/1/15/20	5/37/115/115	-
28	LFA	A	413	-	-	0/4/4/17	-
27	SQD	a	410	-	-	15/40/60/69	0/1/1/1
36	LHG	D	406	-	-	11/53/53/53	-
27	SQD	D	410	-	-	25/38/58/69	0/1/1/1
37	HEM	E	105	5,6	-	3/12/54/54	-
30	LMT	a	411	-	-	9/21/61/61	0/2/2/2
32	PLM	k	102	-	-	7/9/9/15	-
25	BCR	C	502	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	404	-	1/1/15/20	5/37/115/115	-
28	LFA	b	625	-	-	0/5/5/17	-
25	BCR	B	618	-	-	3/29/63/63	0/2/2/2
23	CLA	A	408	-	1/1/15/20	9/37/115/115	-
23	CLA	B	601	40	1/1/15/20	10/37/115/115	-
36	LHG	d	410	-	-	16/53/53/53	-
23	CLA	a	403	40	1/1/15/20	6/37/115/115	-
32	PLM	l	101	-	-	7/11/11/15	-
30	LMT	z	102	-	-	8/21/61/61	0/2/2/2
32	PLM	d	413	-	-	8/13/13/15	-
37	HEM	f	102	5,6	-	2/12/54/54	-
26	PL9	d	406	-	-	8/53/73/73	0/1/1/1
23	CLA	B	611	-	1/1/15/20	5/37/115/115	-
23	CLA	c	510	-	1/1/15/20	6/37/115/115	-
33	LMG	Y	101	-	-	17/46/66/70	0/1/1/1
28	LFA	D	416	-	-	0/5/5/17	-
23	CLA	b	611	40	1/1/15/20	11/37/115/115	-
30	LMT	B	620	-	-	10/21/61/61	0/2/2/2
23	CLA	b	605	-	1/1/15/20	10/37/115/115	-
36	LHG	D	407	-	-	16/53/53/53	-
32	PLM	E	107	-	-	5/15/15/15	-
32	PLM	E	102	-	-	6/12/12/15	-
23	CLA	b	616	-	1/1/15/20	4/37/115/115	-
32	PLM	C	519	-	-	3/10/10/15	-
23	CLA	B	614	-	1/1/15/20	16/37/115/115	-
23	CLA	C	513	-	1/1/15/20	5/37/115/115	-
32	PLM	B	628	-	-	4/10/10/15	-
32	PLM	D	414	-	-	9/15/15/15	-
28	LFA	d	412	-	-	0/7/7/17	-
23	CLA	C	507	-	1/1/15/20	8/37/115/115	-
23	CLA	b	607	-	1/1/15/20	5/37/115/115	-
35	DGD	c	515	-	-	16/46/66/95	0/1/1/2
23	CLA	b	617	-	1/1/15/20	15/37/115/115	-
32	PLM	D	415	-	-	3/8/8/15	-
23	CLA	C	508	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LFA	C	520	-	-	0/9/9/17	-
36	LHG	a	417	-	-	26/53/53/53	-
27	SQD	B	630	-	-	23/49/69/69	0/1/1/1
28	LFA	B	623	-	-	0/3/3/17	-
23	CLA	B	608	-	1/1/15/20	5/37/115/115	-
32	PLM	K	101	-	-	2/11/11/15	-
32	PLM	b	628	-	-	5/9/9/15	-
23	CLA	A	406	40	1/1/15/20	10/37/115/115	-
23	CLA	C	516	3	1/1/15/20	6/37/115/115	-
28	LFA	H	103	-	-	0/6/6/17	-
23	CLA	C	512	40	1/1/15/20	11/37/115/115	-
32	PLM	E	103	-	-	5/13/13/15	-
32	PLM	a	413	-	-	3/8/8/15	-
28	LFA	d	414	-	-	2/6/6/17	-
28	LFA	a	412	-	-	2/6/6/17	-
23	CLA	c	511	3	1/1/15/20	6/37/115/115	-
24	PHO	D	401	-	-	9/37/103/103	0/5/6/6
23	CLA	c	502	-	1/1/15/20	12/37/115/115	-
33	LMG	b	621	-	-	12/46/66/70	0/1/1/1
32	PLM	c	518	-	-	2/6/6/15	-
32	PLM	C	522	-	-	6/10/10/15	-
25	BCR	T	101	-	-	8/29/63/63	0/2/2/2
25	BCR	C	501	-	-	4/29/63/63	0/2/2/2
23	CLA	C	515	-	1/1/15/20	7/37/115/115	-
28	LFA	A	412	-	-	0/4/4/17	-
23	CLA	B	616	-	1/1/11/20	5/13/91/115	-
23	CLA	c	503	-	1/1/15/20	3/37/115/115	-
23	CLA	b	613	-	1/1/15/20	5/37/115/115	-
23	CLA	c	506	-	1/1/15/20	17/37/115/115	-
35	DGD	C	503	-	-	21/42/82/95	0/2/2/2
28	LFA	I	105	-	-	0/5/5/17	-
23	CLA	B	609	-	1/1/15/20	7/37/115/115	-
34	GOL	B	621	-	-	2/4/4/4	-
23	CLA	c	512	-	1/1/15/20	10/37/115/115	-
32	PLM	h	103	-	-	5/8/8/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	I	103	-	-	22/46/66/70	0/1/1/1
38	RRX	H	102	-	-	2/29/65/65	0/2/2/2
25	BCR	D	403	-	-	9/29/63/63	0/2/2/2
37	HEM	V	201	16	-	2/12/54/54	-
24	PHO	A	407	-	-	3/37/103/103	0/5/6/6
23	CLA	B	607	40	1/1/15/20	8/37/115/115	-
28	LFA	B	627	-	-	0/3/3/17	-
28	LFA	I	102	-	-	0/4/4/17	-
23	CLA	b	614	-	1/1/15/20	6/37/115/115	-
23	CLA	b	606	-	1/1/15/20	11/37/115/115	-
23	CLA	c	507	40	1/1/15/20	14/37/115/115	-
23	CLA	b	615	-	1/1/15/20	19/37/115/115	-
30	LMT	a	419	-	-	11/15/35/61	0/1/1/2
32	PLM	c	522	-	-	3/10/10/15	-
23	CLA	c	504	40	1/1/15/20	7/37/115/115	-
23	CLA	b	602	40	1/1/15/20	17/37/115/115	-
23	CLA	b	612	-	1/1/15/20	3/37/115/115	-
28	LFA	E	104	-	-	0/3/3/17	-
26	PL9	A	410	-	-	28/53/73/73	0/1/1/1
23	CLA	a	402	-	1/1/15/20	8/37/115/115	-
28	LFA	b	627	-	-	0/4/4/17	-
26	PL9	a	409	-	-	14/53/73/73	0/1/1/1
25	BCR	t	101	-	-	6/29/63/63	0/2/2/2
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
25	BCR	Y	102	-	-	6/29/63/63	0/2/2/2
24	PHO	a	404	-	-	6/37/103/103	0/5/6/6
28	LFA	i	104	-	-	1/10/10/17	-
23	CLA	c	501	-	1/1/15/20	4/37/115/115	-
28	LFA	C	521	-	-	1/6/6/17	-
23	CLA	C	509	40	1/1/15/20	10/37/115/115	-
28	LFA	D	413	-	-	1/7/7/17	-
35	DGD	H	101	-	-	7/47/87/95	0/2/2/2
28	LFA	e	101	-	-	6/14/14/17	-
23	CLA	c	508	-	1/1/15/20	6/37/115/115	-

The worst 5 of 567 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C4B-NB	7.30	1.41	1.35
23	B	610	CLA	C4B-NB	7.27	1.41	1.35
23	b	607	CLA	C4B-NB	7.26	1.41	1.35
23	B	601	CLA	C4B-NB	7.24	1.41	1.35
23	b	610	CLA	C4B-NB	7.22	1.41	1.35

The worst 5 of 800 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C4A-NA-C1A	8.39	110.48	106.71
23	B	604	CLA	C4A-NA-C1A	8.26	110.42	106.71
23	C	512	CLA	C4A-NA-C1A	8.15	110.37	106.71
23	b	608	CLA	C4A-NA-C1A	8.09	110.34	106.71
23	B	607	CLA	C4A-NA-C1A	7.94	110.28	106.71

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	406	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND

5 of 1761 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404	CLA	CBD-CGD-O2D-CED
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	A	406	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

146 monomers are involved in 245 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	418	PLM	2	0
23	b	609	CLA	3	0
23	B	610	CLA	2	0
25	k	101	BCR	2	0
30	c	517	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	613	CLA	1	0
23	C	517	CLA	5	0
27	A	411	SQD	2	0
30	D	417	LMT	3	0
25	b	619	BCR	5	0
30	d	403	LMT	1	0
35	D	411	DGD	2	0
33	B	619	LMG	5	0
27	a	407	SQD	2	0
33	D	409	LMG	4	0
33	y	101	LMG	2	0
32	c	519	PLM	1	0
30	f	103	LMT	1	0
23	B	615	CLA	3	0
27	d	408	SQD	2	0
23	B	612	CLA	2	0
35	C	504	DGD	3	0
23	b	608	CLA	1	0
23	d	405	CLA	3	0
33	c	521	LMG	1	0
26	D	402	PL9	3	0
36	a	416	LHG	1	0
23	C	506	CLA	3	0
25	a	406	BCR	1	0
25	z	101	BCR	2	0
23	b	603	CLA	1	0
30	M	101	LMT	1	0
33	a	408	LMG	2	0
23	A	405	CLA	2	0
23	B	605	CLA	2	0
23	D	404	CLA	2	0
25	b	620	BCR	2	0
23	b	604	CLA	2	0
30	M	102	LMT	2	0
36	E	101	LHG	2	0
24	d	402	PHO	2	0
25	A	409	BCR	1	0
35	c	516	DGD	1	0
35	C	505	DGD	1	0
33	C	525	LMG	1	0
32	C	524	PLM	1	0
36	d	409	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	610	CLA	1	0
38	x	102	RRX	1	0
36	l	102	LHG	5	0
23	a	405	CLA	3	0
23	B	603	CLA	3	0
23	D	405	CLA	4	0
25	i	103	BCR	1	0
36	D	408	LHG	5	0
36	L	101	LHG	1	0
23	B	604	CLA	4	0
23	d	401	CLA	1	0
25	C	527	BCR	3	0
25	b	618	BCR	1	0
28	h	101	LFA	1	0
35	c	514	DGD	1	0
23	C	518	CLA	2	0
23	c	505	CLA	2	0
27	A	415	SQD	5	0
28	B	622	LFA	1	0
23	C	510	CLA	3	0
25	B	631	BCR	3	0
30	A	416	LMT	1	0
27	F	101	SQD	1	0
35	h	102	DGD	1	0
23	C	511	CLA	1	0
32	b	622	PLM	1	0
27	b	601	SQD	2	0
33	d	411	LMG	1	0
28	I	104	LFA	1	0
23	c	513	CLA	4	0
23	A	404	CLA	2	0
23	c	509	CLA	1	0
27	a	410	SQD	3	0
36	D	406	LHG	1	0
37	E	105	HEM	2	0
30	a	411	LMT	1	0
23	d	404	CLA	3	0
23	A	408	CLA	3	0
23	B	601	CLA	2	0
36	d	410	LHG	2	0
23	a	403	CLA	1	0
32	d	413	PLM	1	0

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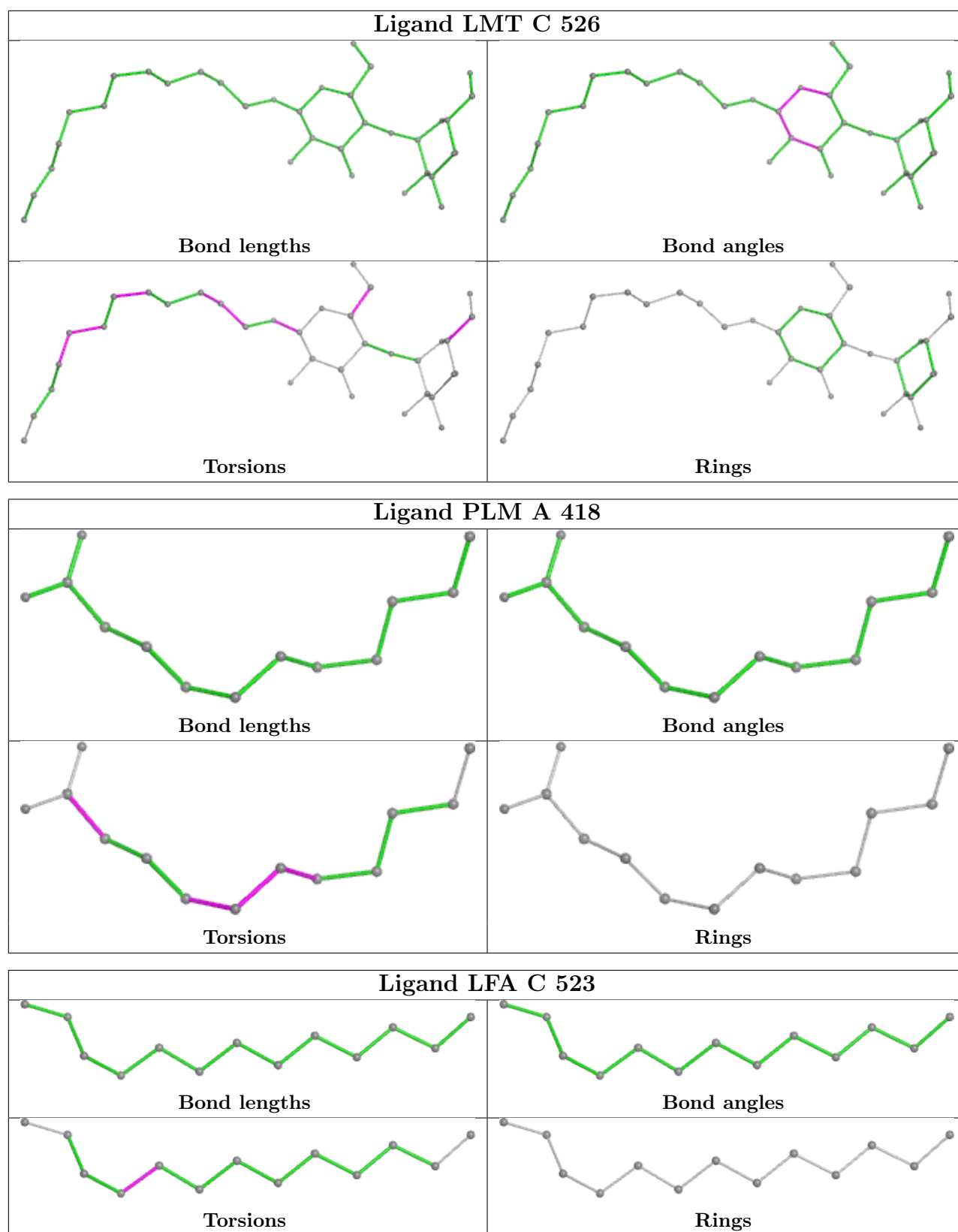
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	f	102	HEM	2	0
26	d	406	PL9	1	0
23	B	611	CLA	1	0
23	c	510	CLA	2	0
30	B	620	LMT	2	0
23	b	605	CLA	2	0
36	D	407	LHG	1	0
32	E	102	PLM	1	0
23	b	616	CLA	5	0
23	B	614	CLA	3	0
23	C	513	CLA	3	0
32	D	414	PLM	4	0
23	C	507	CLA	1	0
35	c	515	DGD	1	0
23	b	617	CLA	6	0
23	C	508	CLA	1	0
28	C	520	LFA	1	0
36	a	417	LHG	3	0
27	B	630	SQD	4	0
32	K	101	PLM	1	0
23	A	406	CLA	3	0
23	C	516	CLA	4	0
23	C	512	CLA	1	0
23	c	511	CLA	5	0
24	D	401	PHO	2	0
23	c	502	CLA	2	0
33	b	621	LMG	1	0
32	c	518	PLM	1	0
25	T	101	BCR	3	0
25	C	501	BCR	3	0
23	C	515	CLA	1	0
23	B	616	CLA	2	0
23	c	503	CLA	5	0
23	b	613	CLA	1	0
23	c	506	CLA	1	0
35	C	503	DGD	2	0
23	c	512	CLA	2	0
33	I	103	LMG	3	0
25	D	403	BCR	1	0
24	A	407	PHO	1	0
23	B	607	CLA	1	0
23	b	606	CLA	3	0

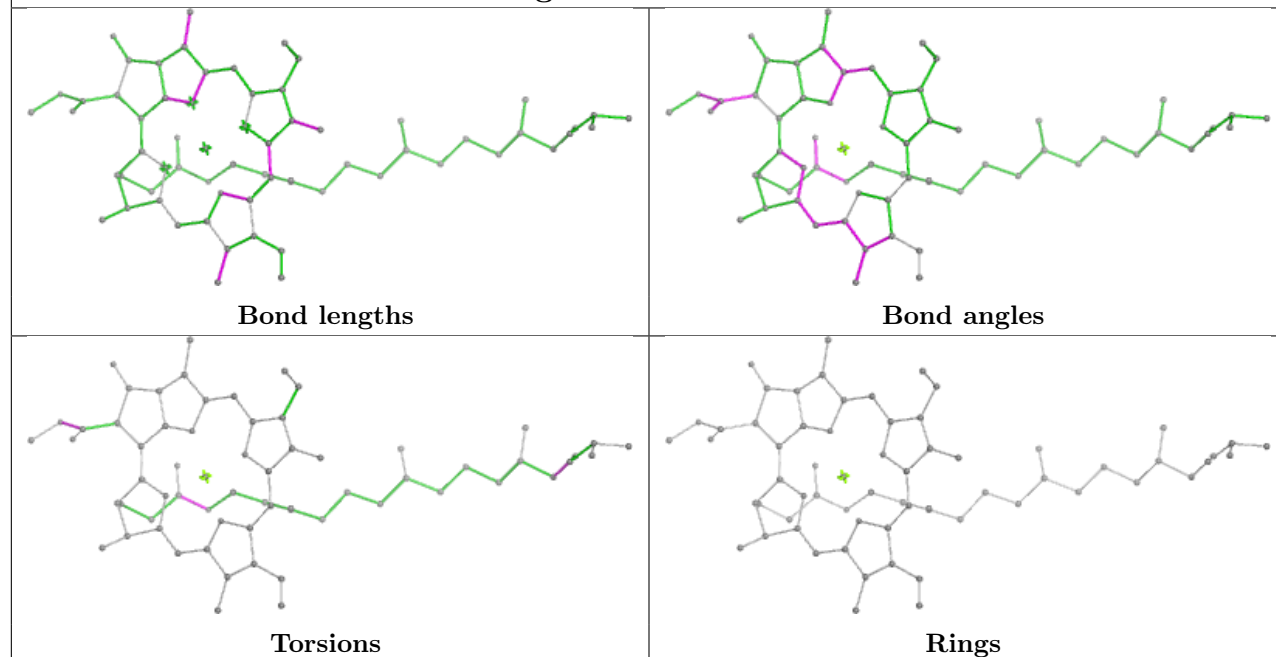
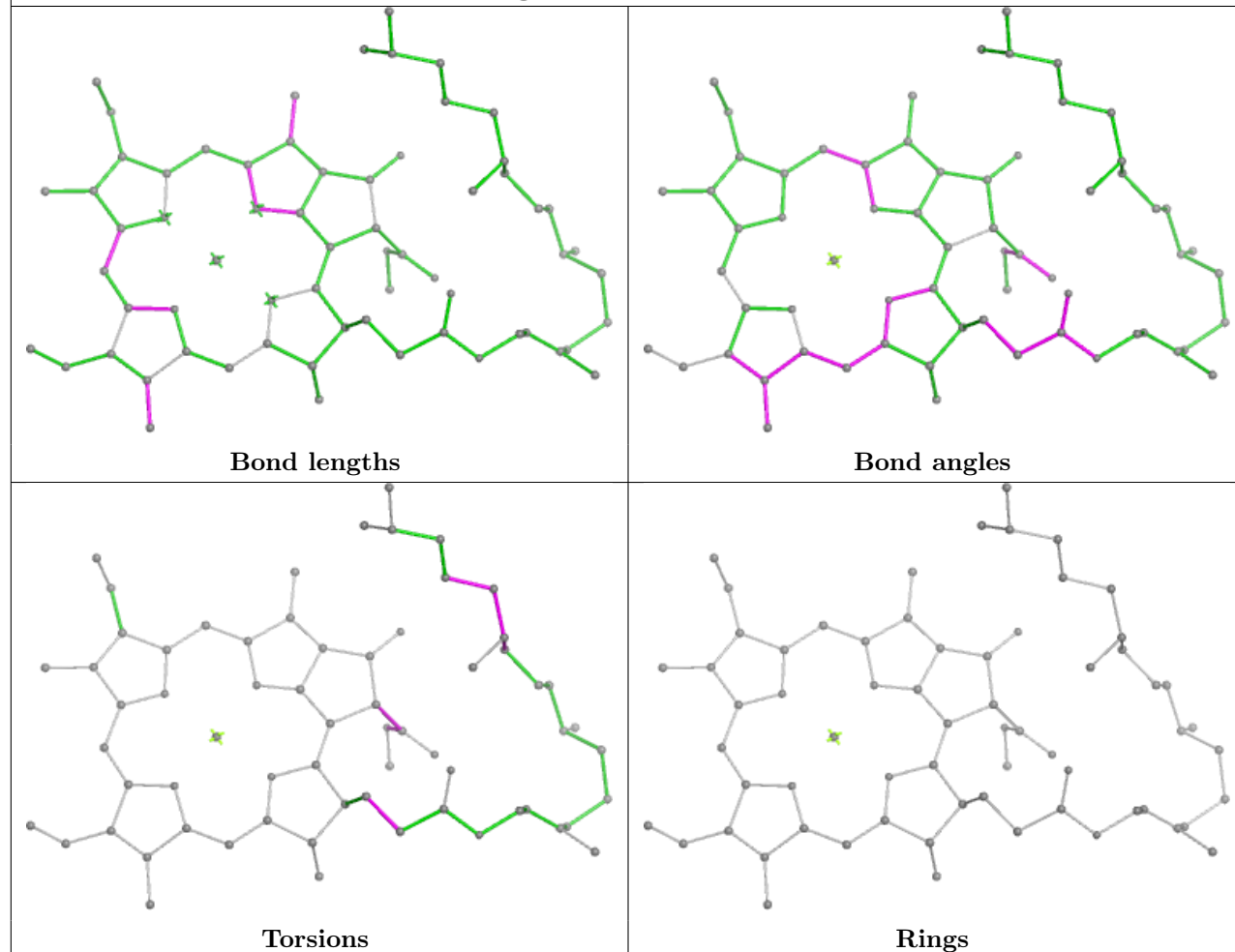
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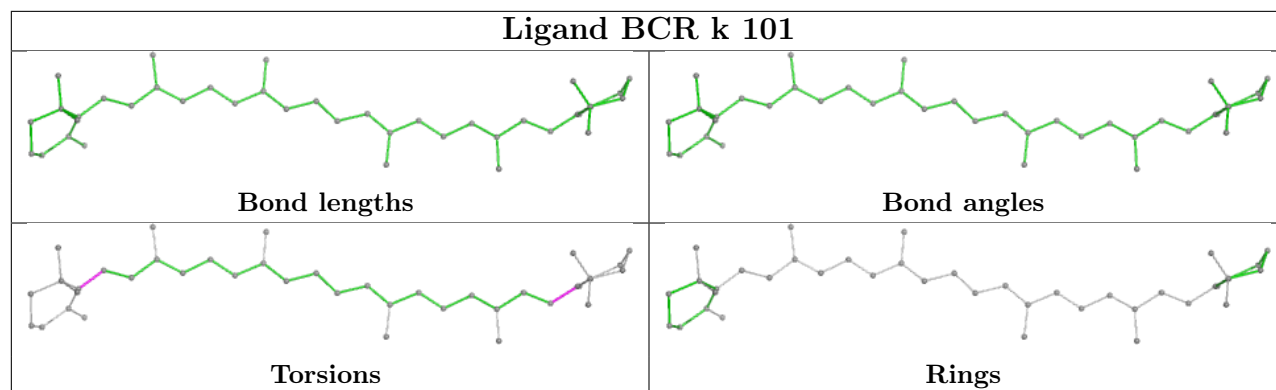
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	507	CLA	1	0
23	b	615	CLA	2	0
23	c	504	CLA	2	0
23	b	602	CLA	2	0
23	b	612	CLA	2	0
26	A	410	PL9	5	0
23	a	402	CLA	3	0
26	a	409	PL9	4	0
25	t	101	BCR	1	0
25	B	617	BCR	2	0
25	Y	102	BCR	4	0
24	a	404	PHO	2	0
23	c	501	CLA	2	0
35	H	101	DGD	1	0
23	c	508	CLA	2	0

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

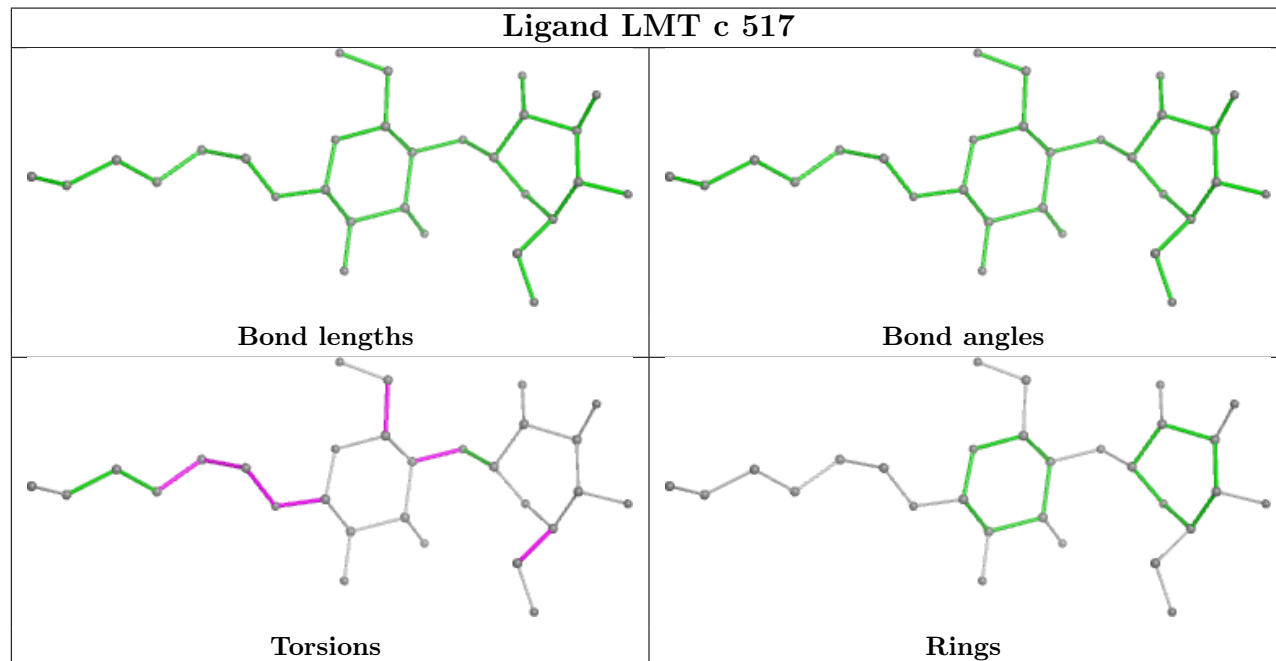


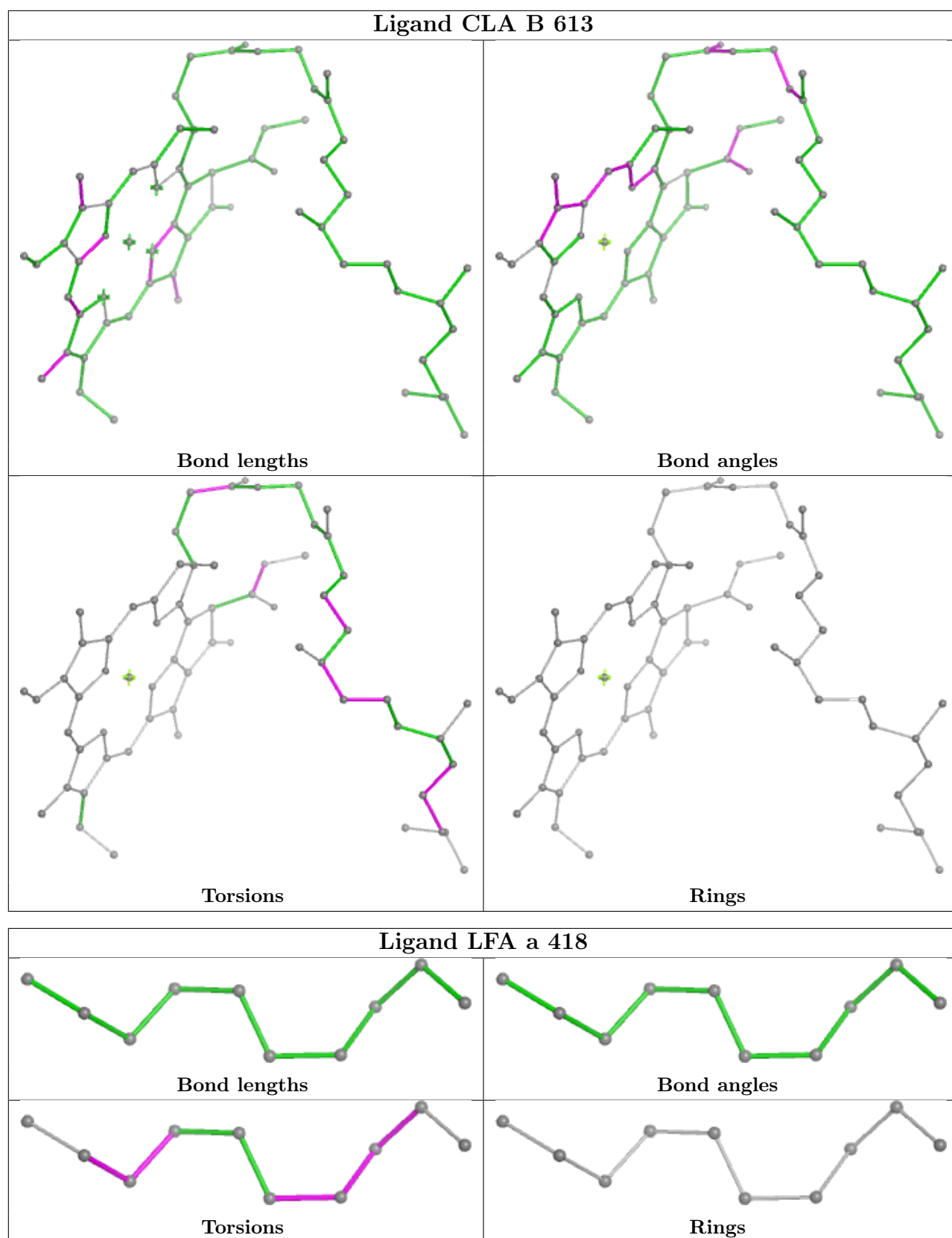
Ligand CLA b 609**Ligand CLA B 610**

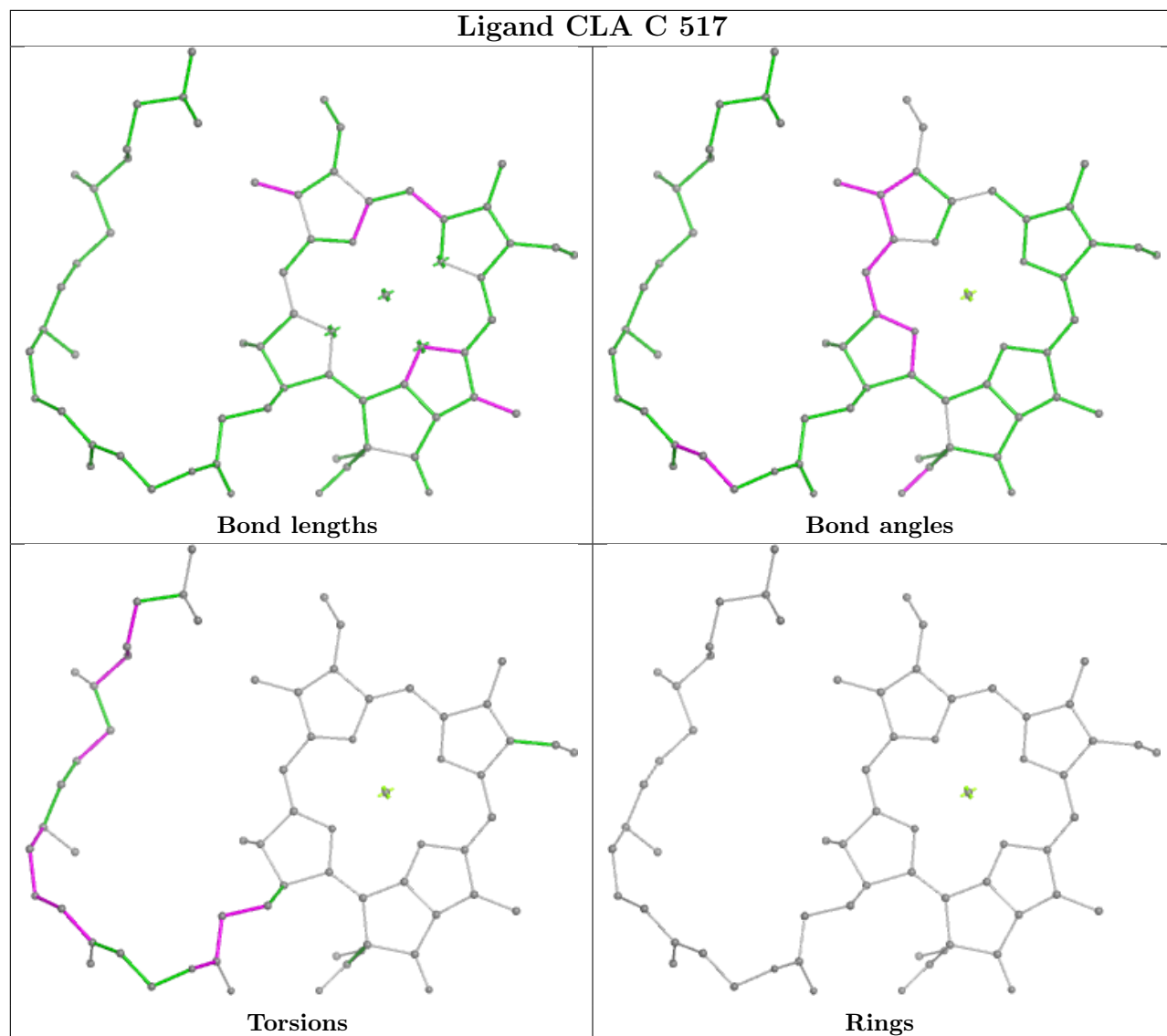
Ligand BCR k 101

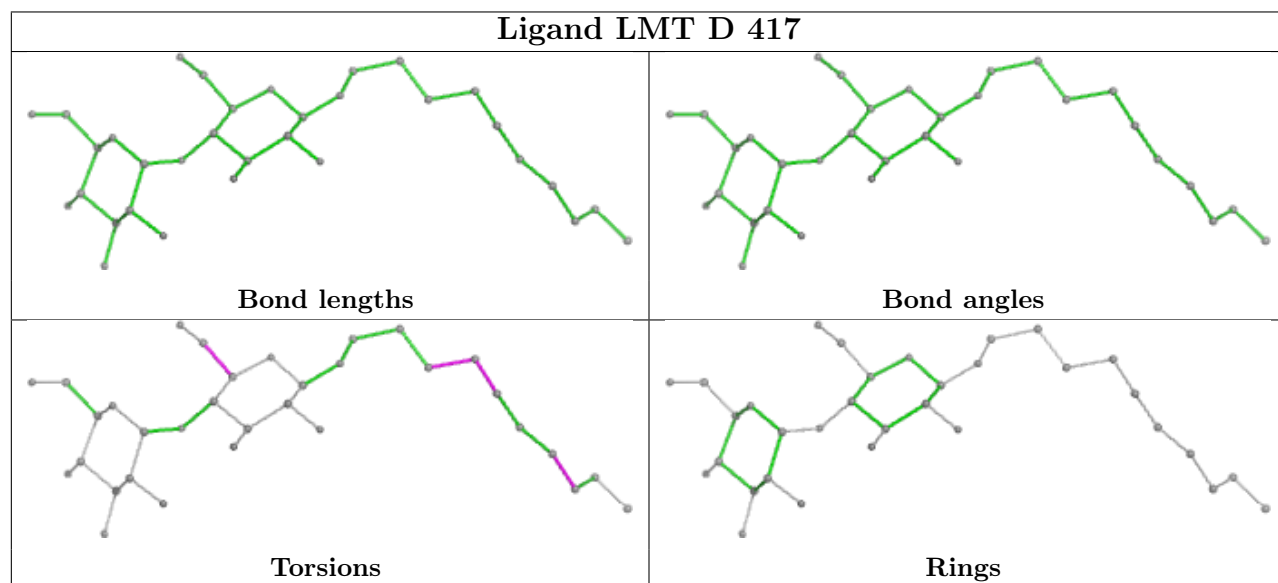
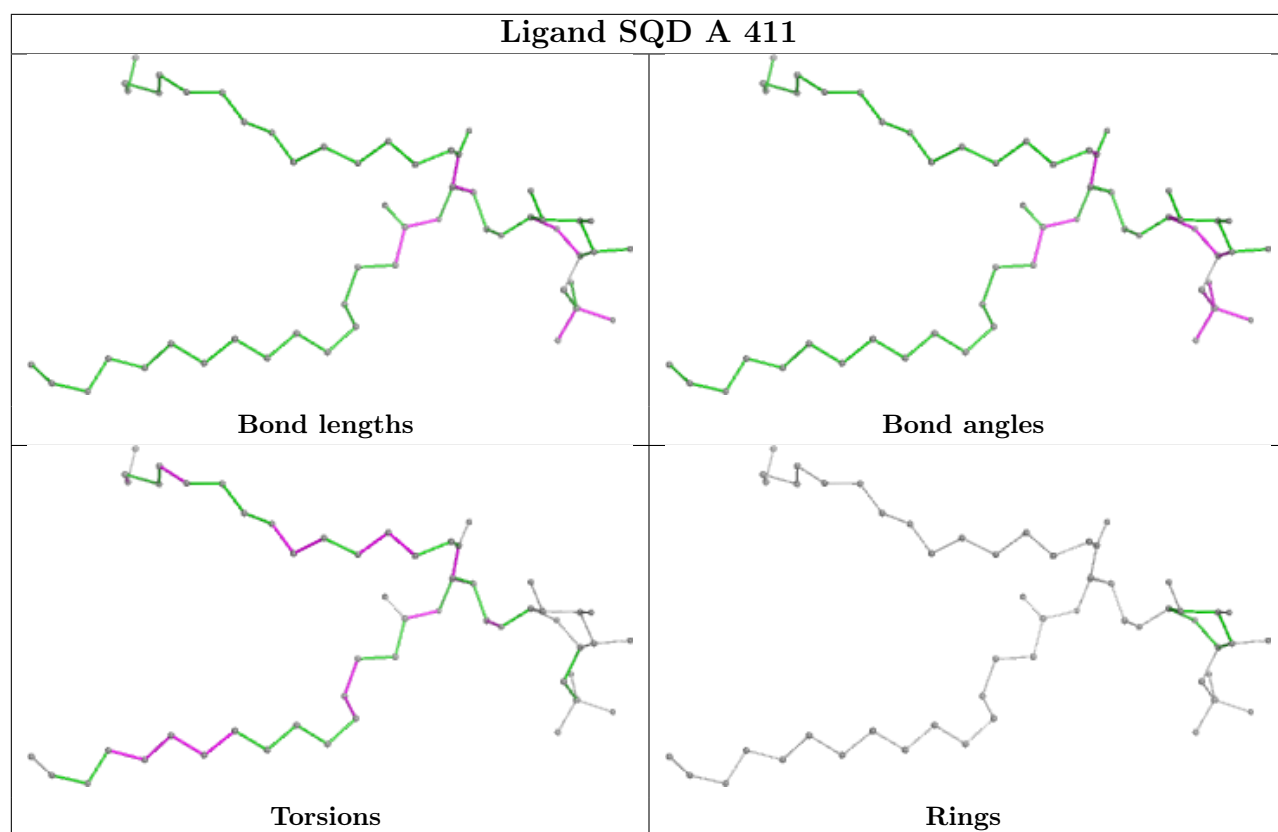


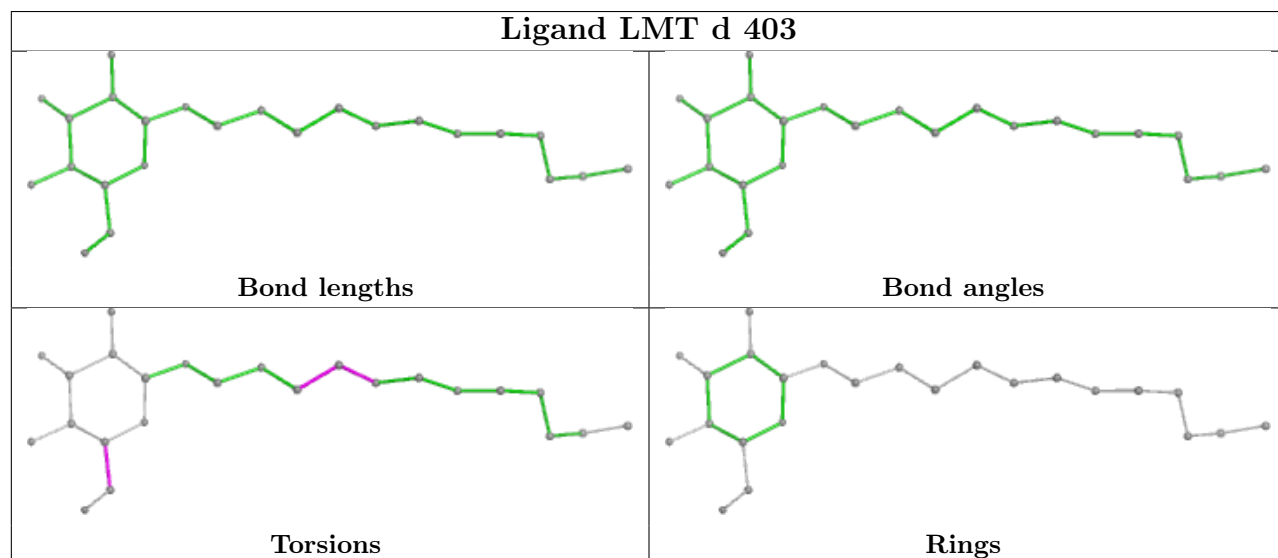
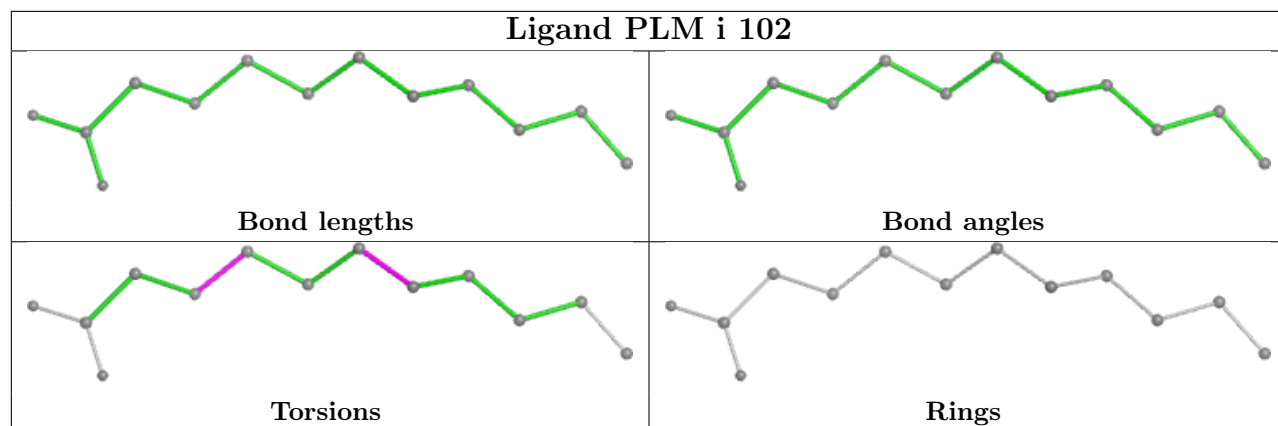
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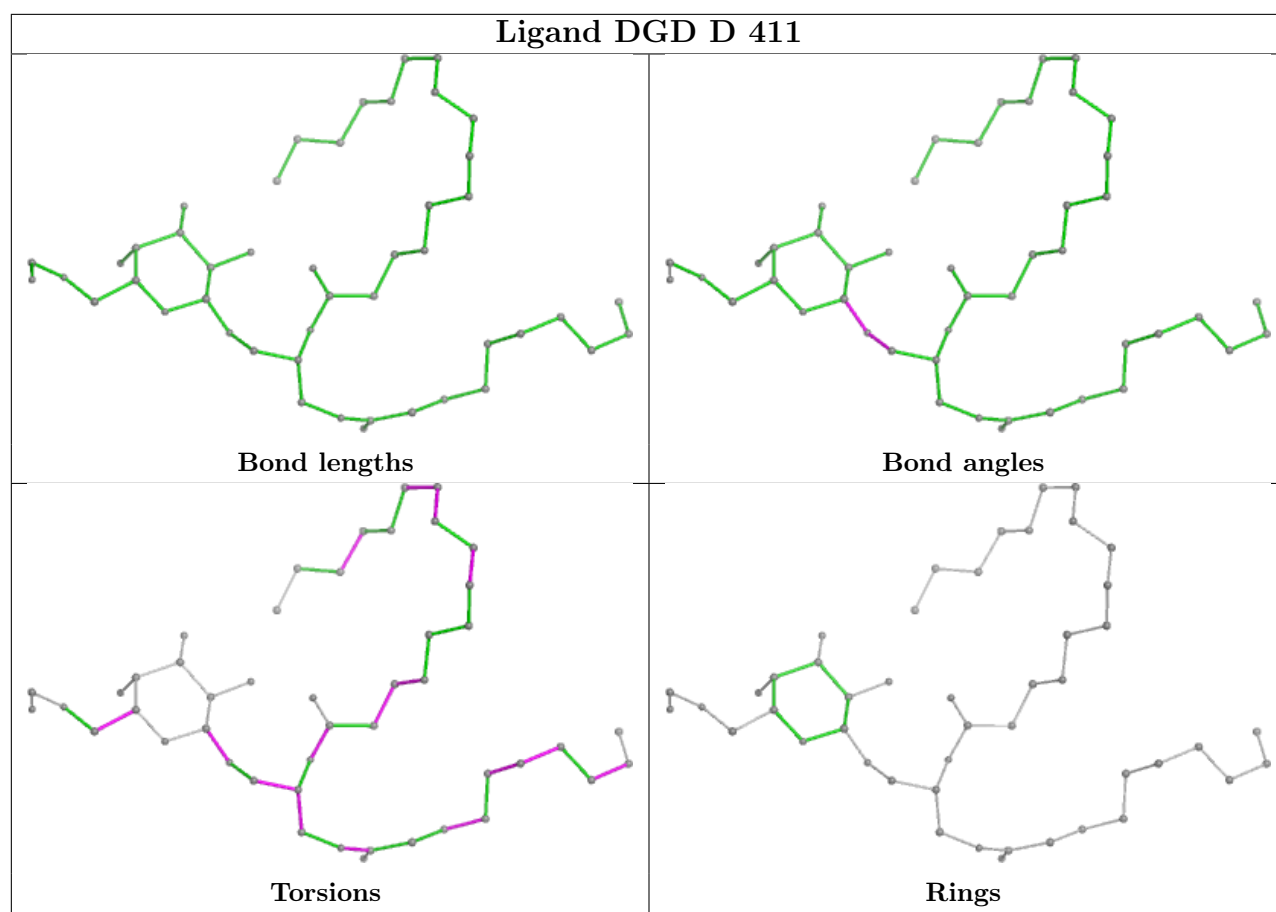


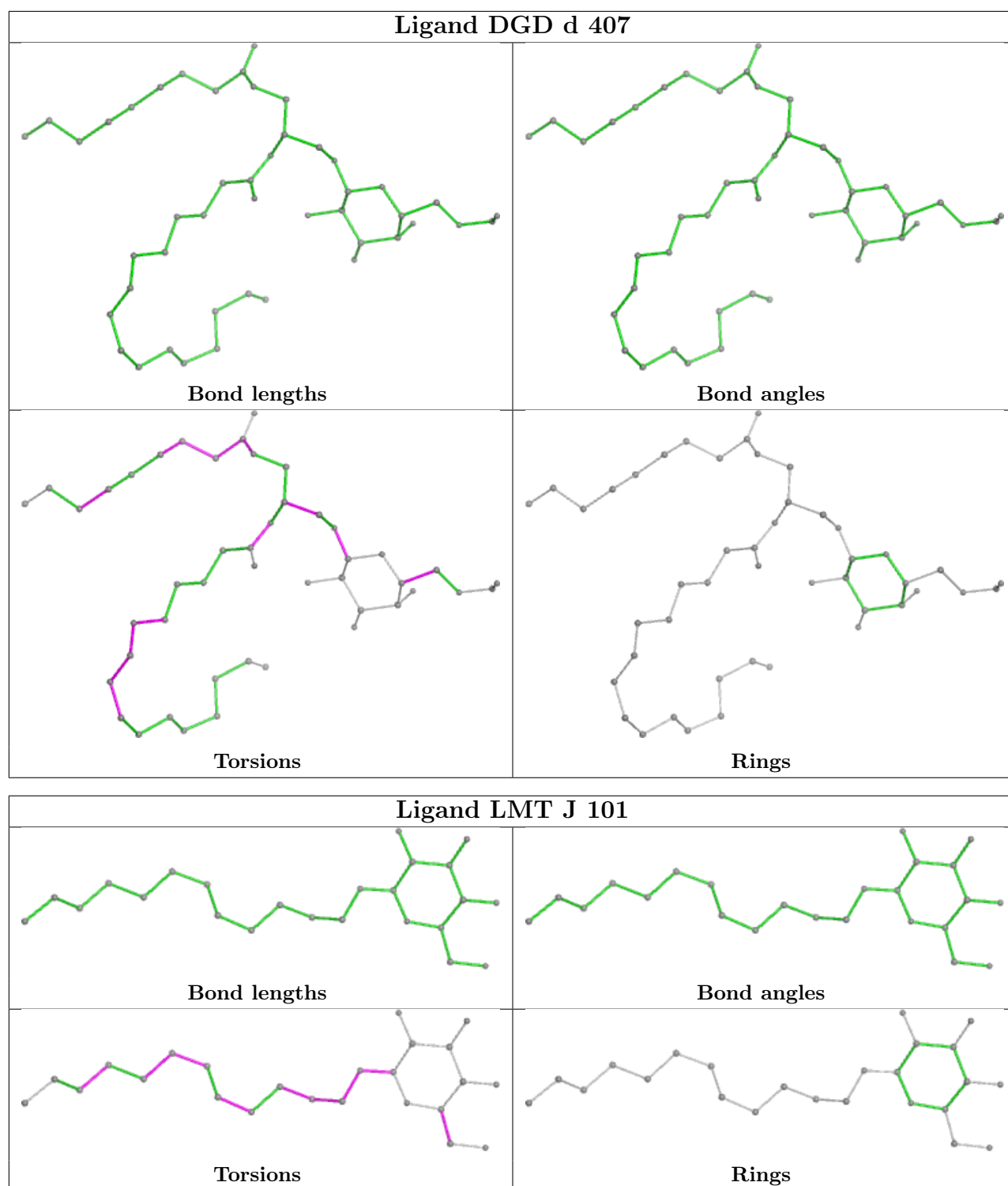


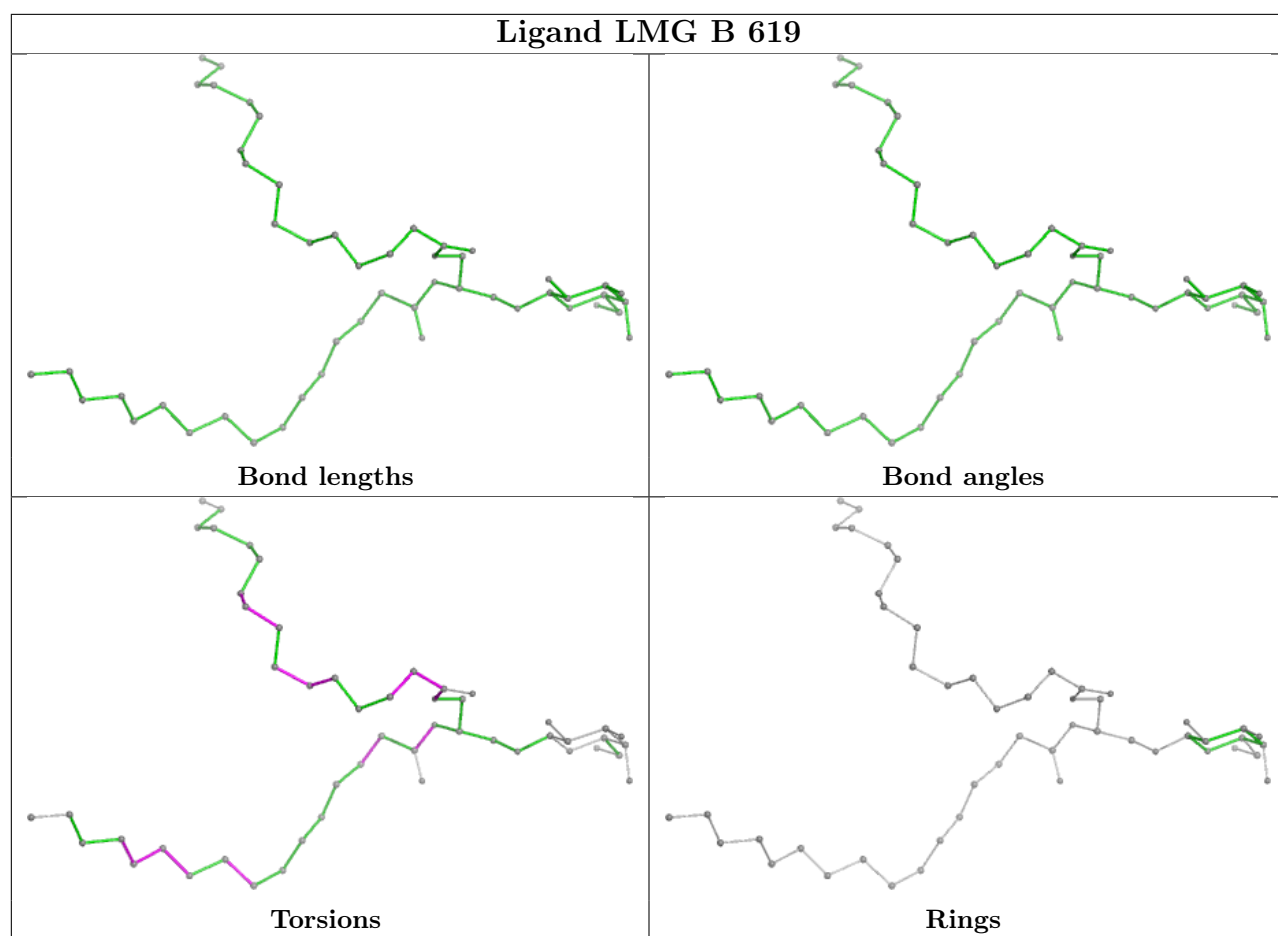


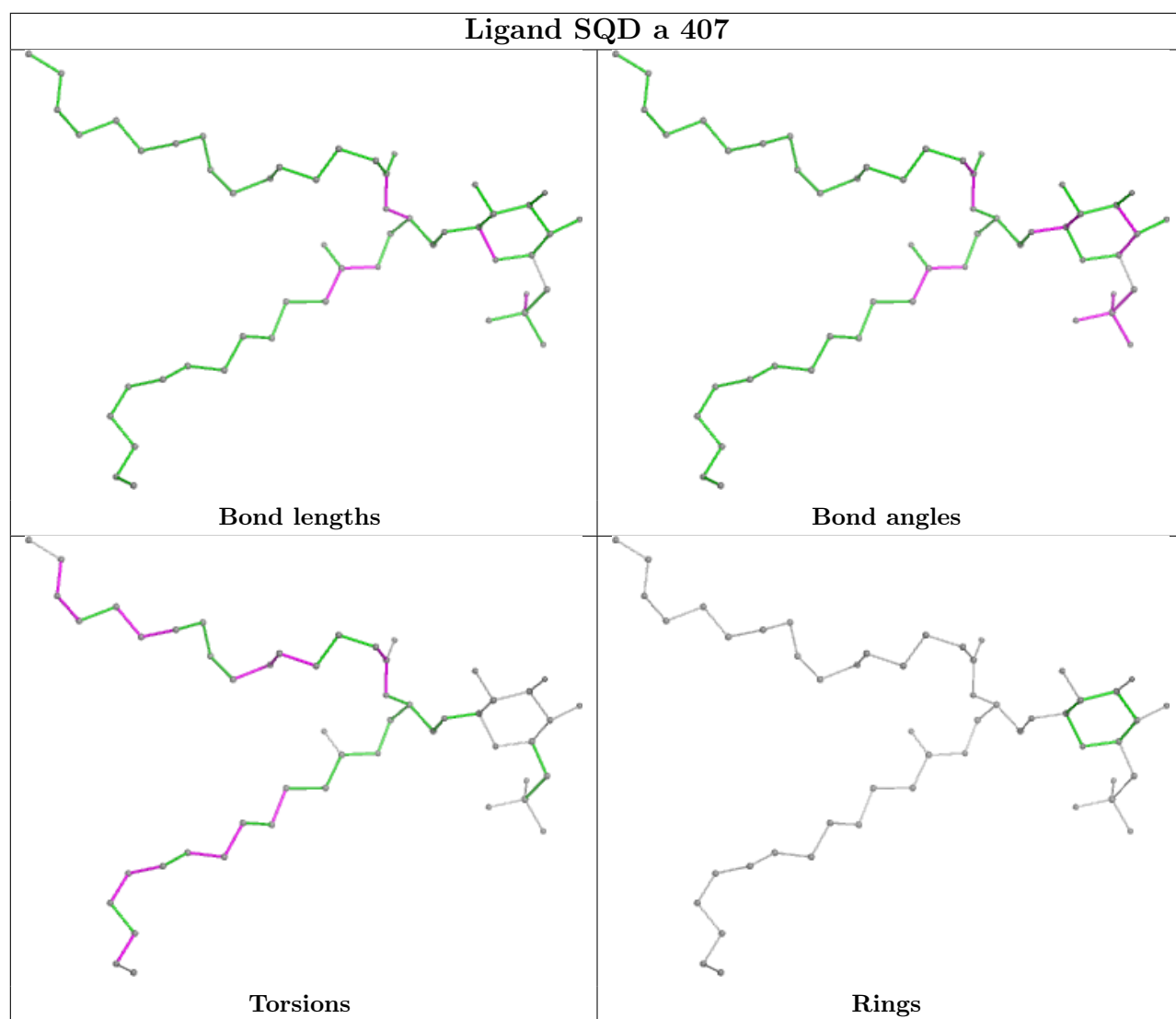


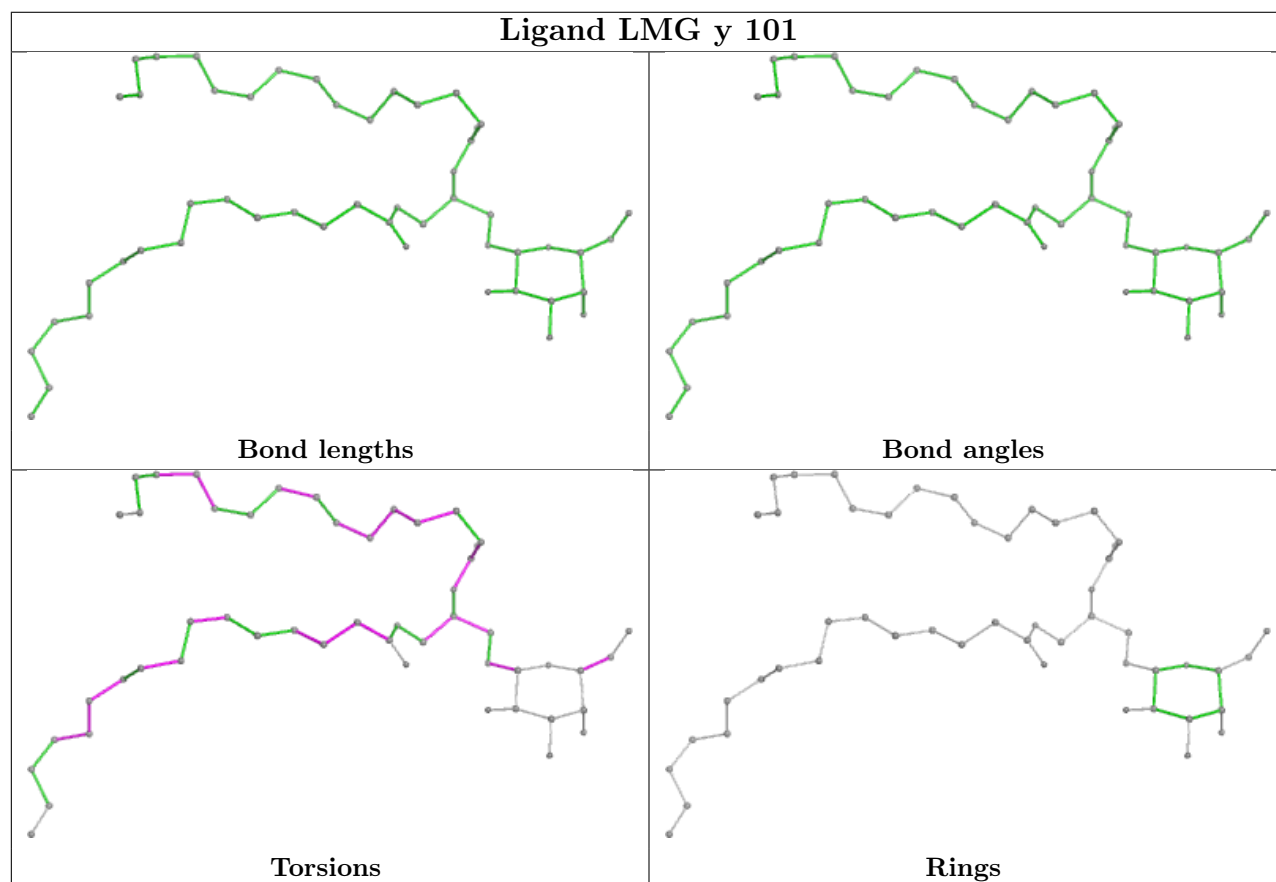
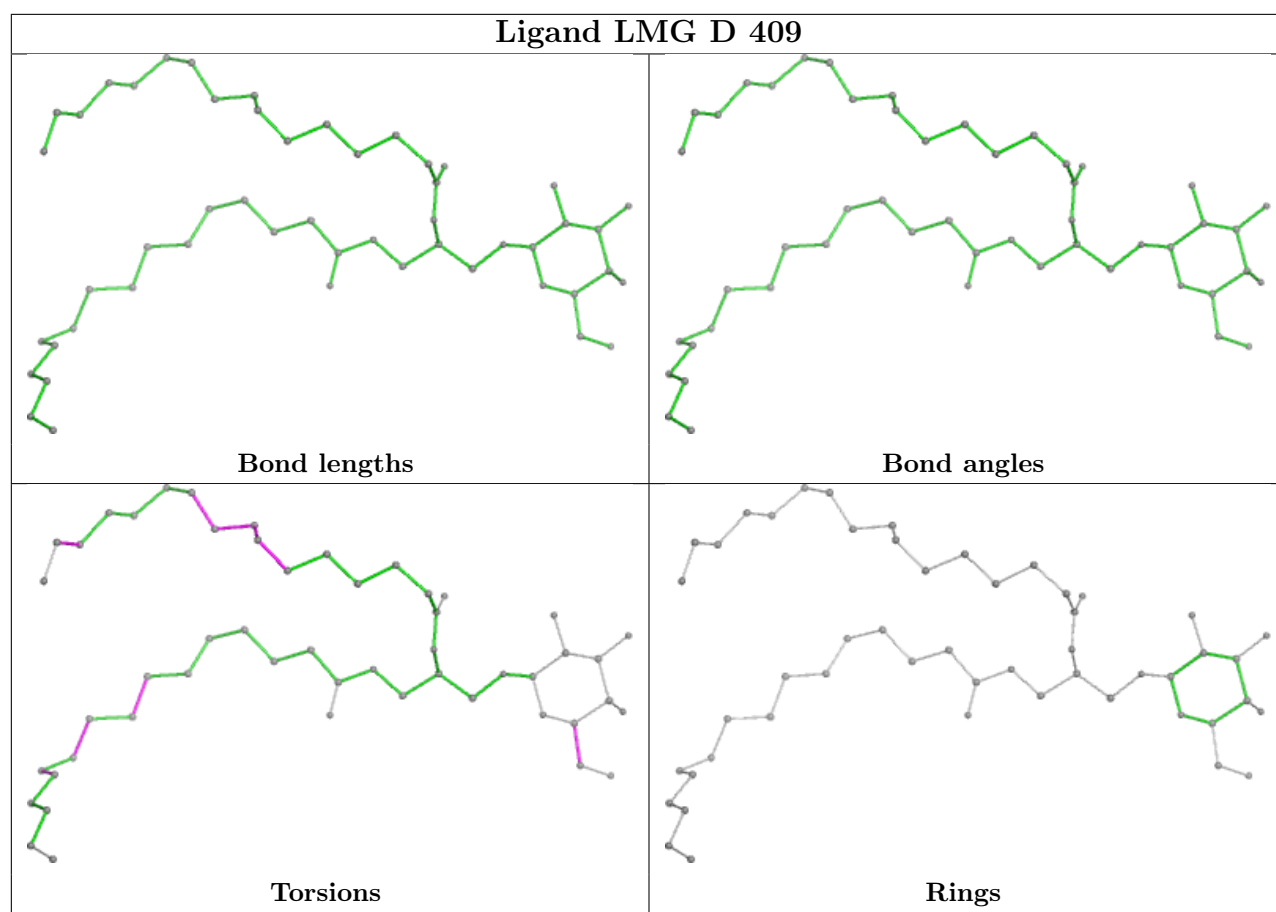


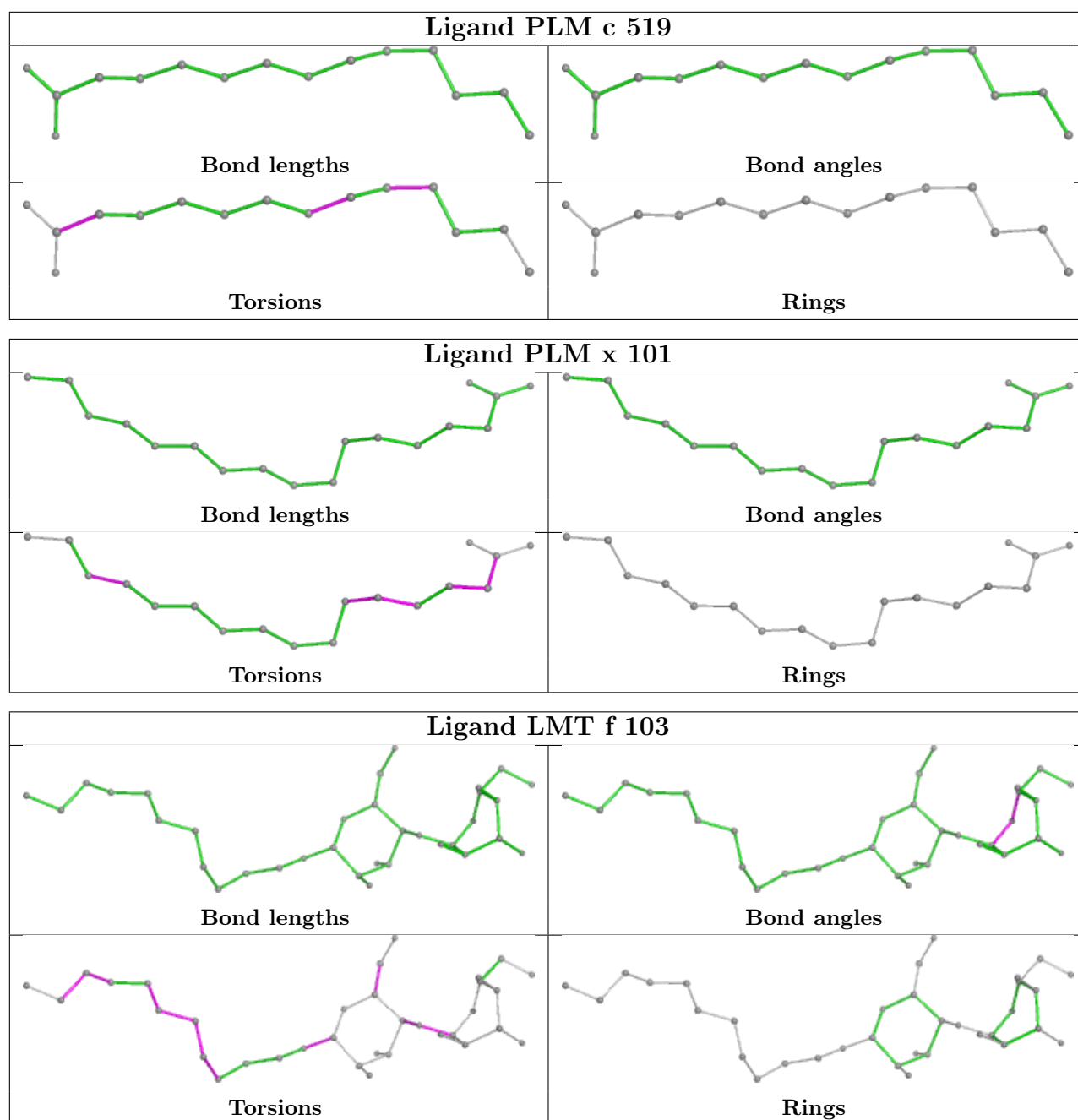


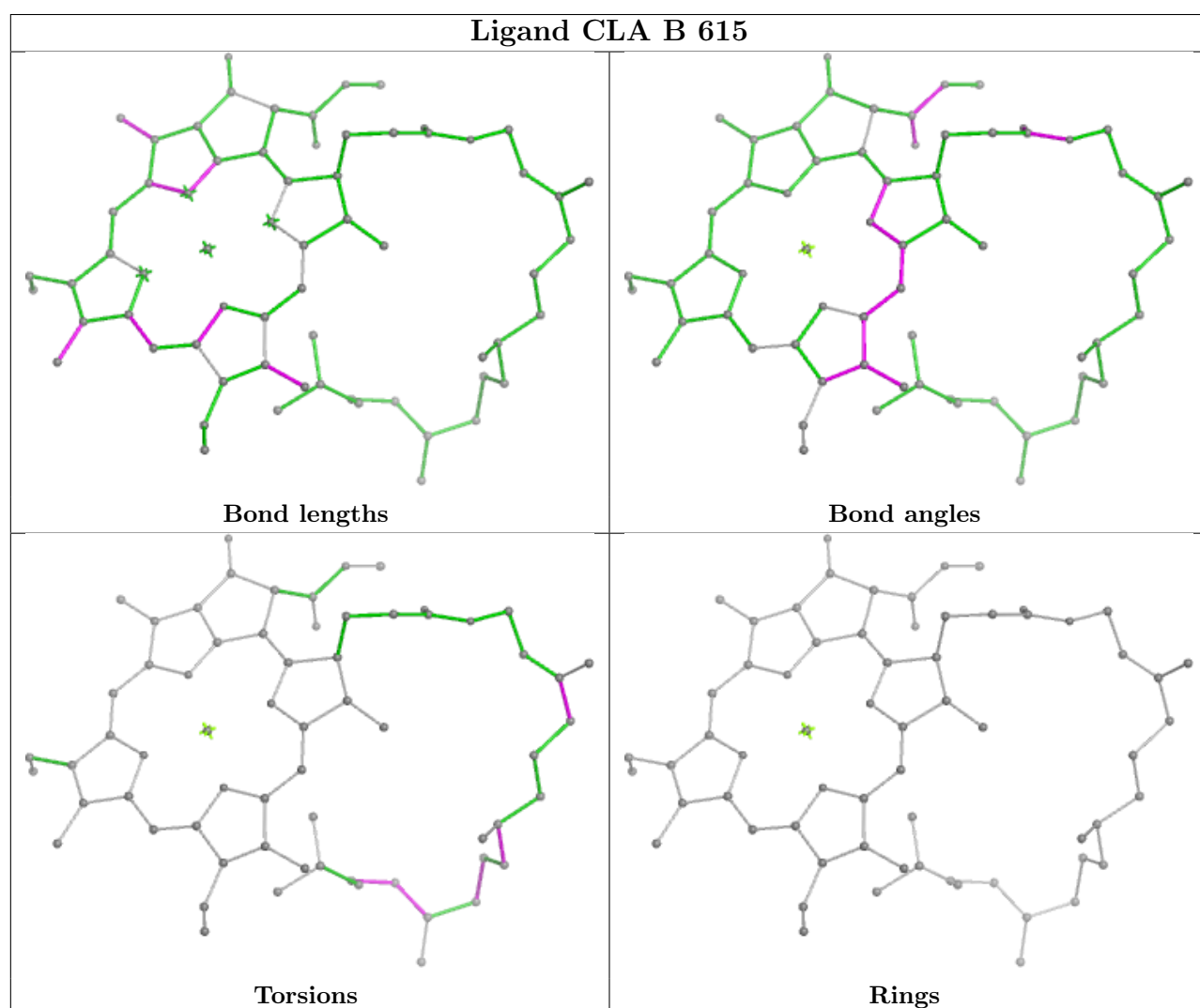
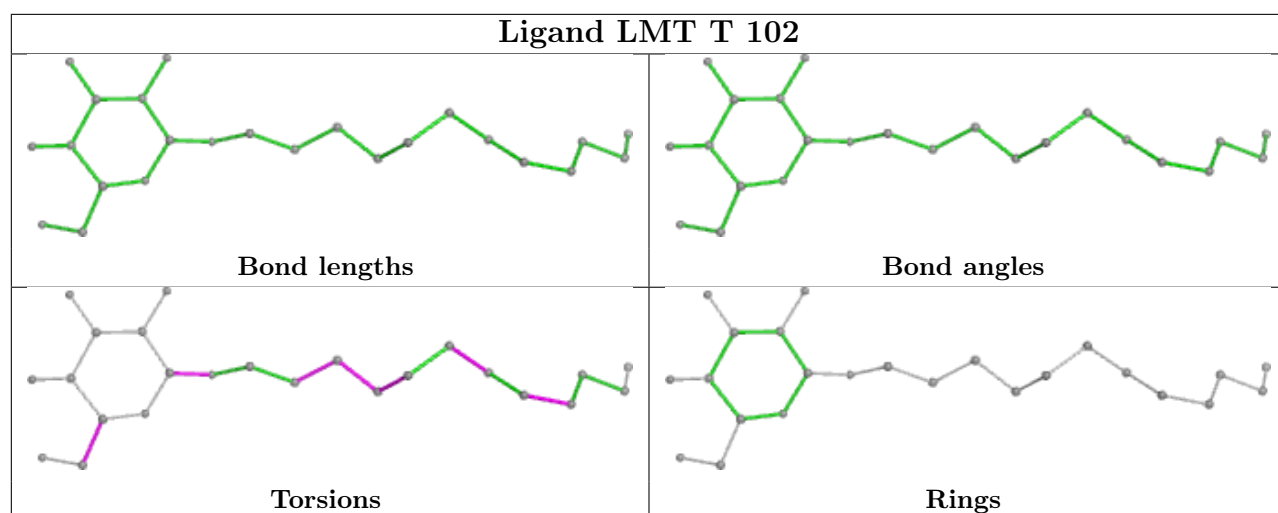


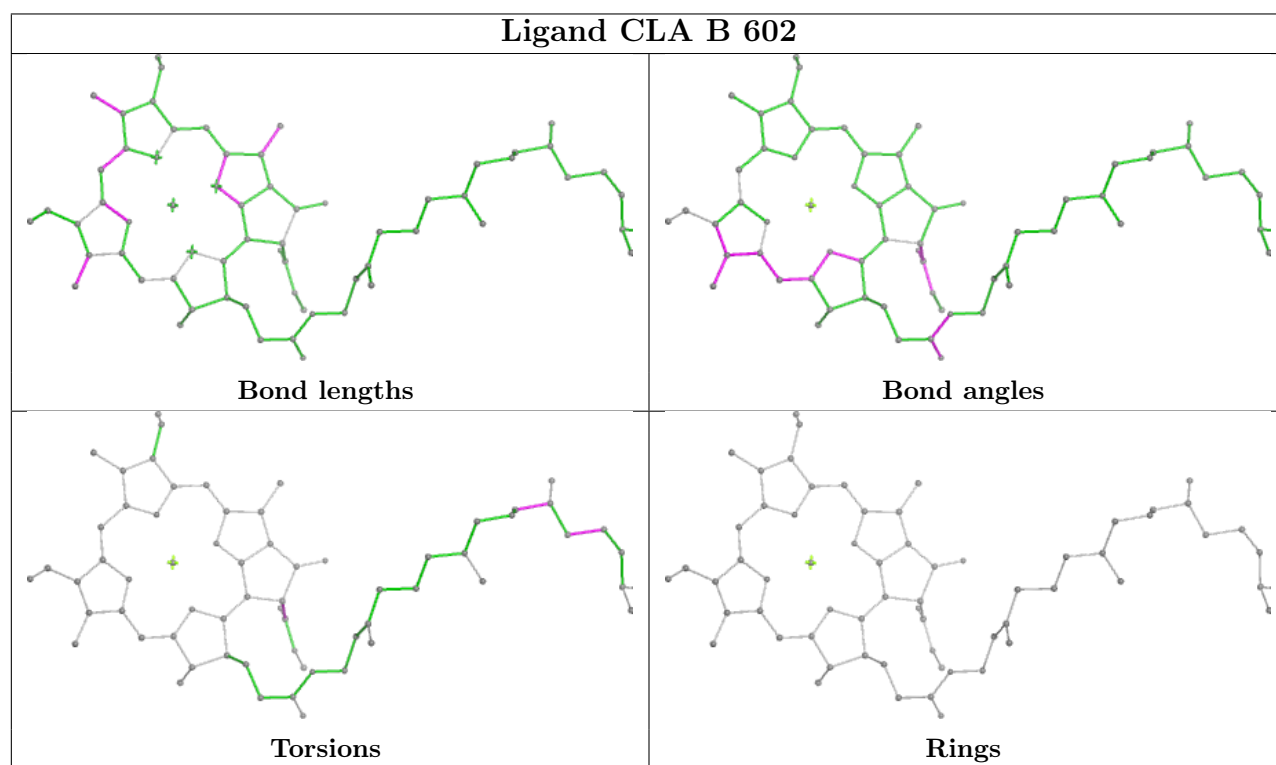
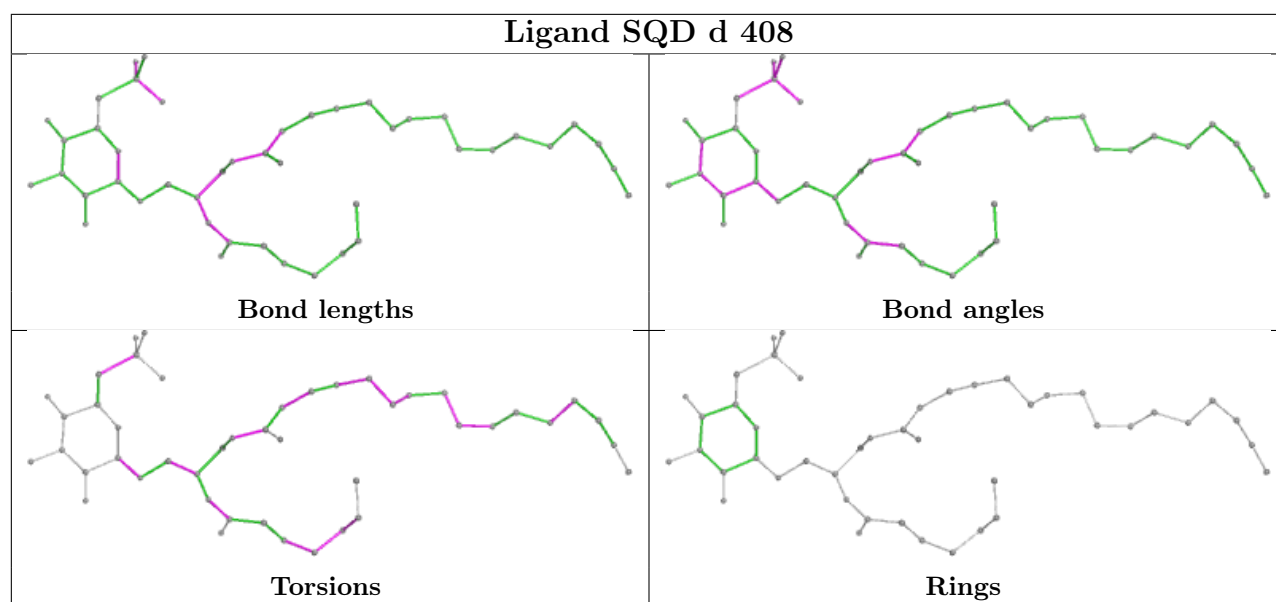


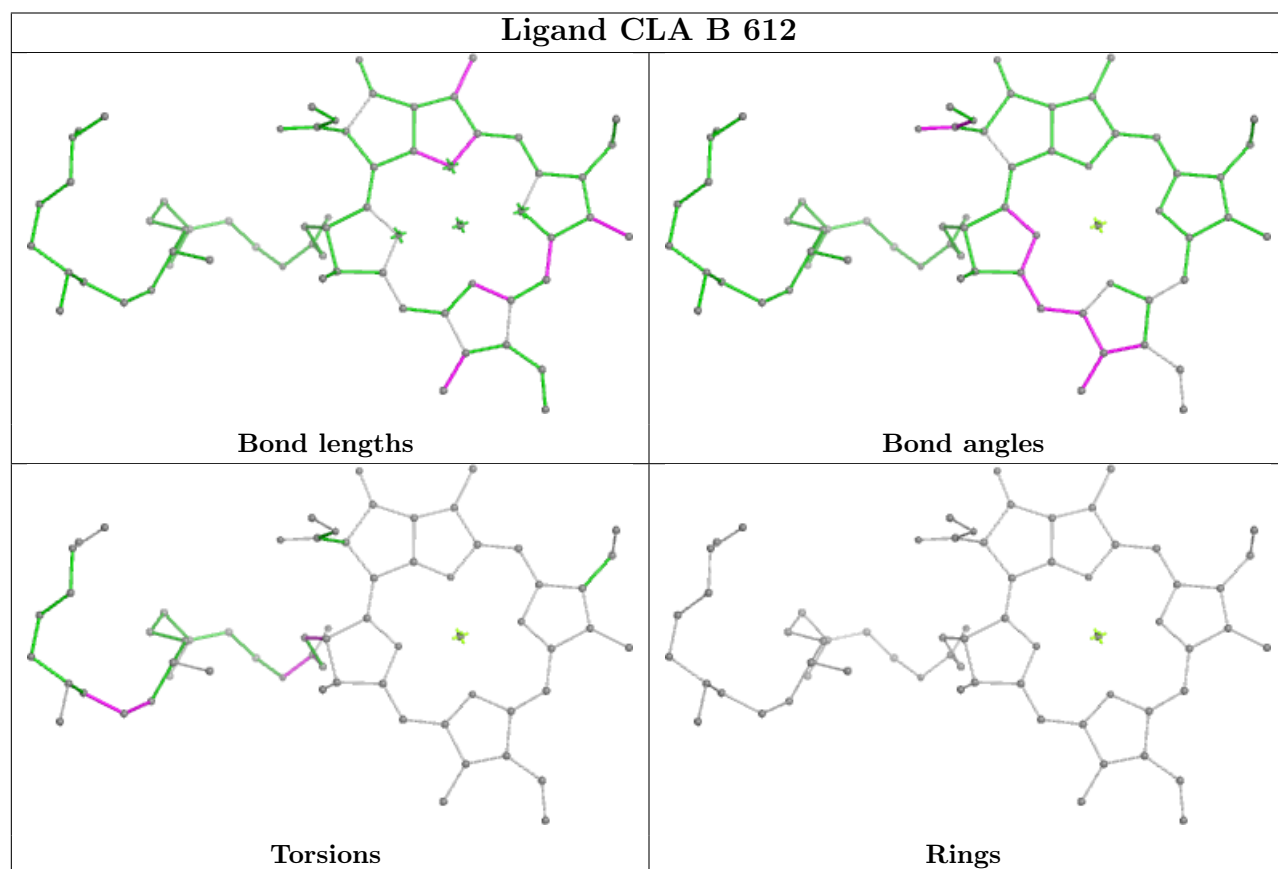
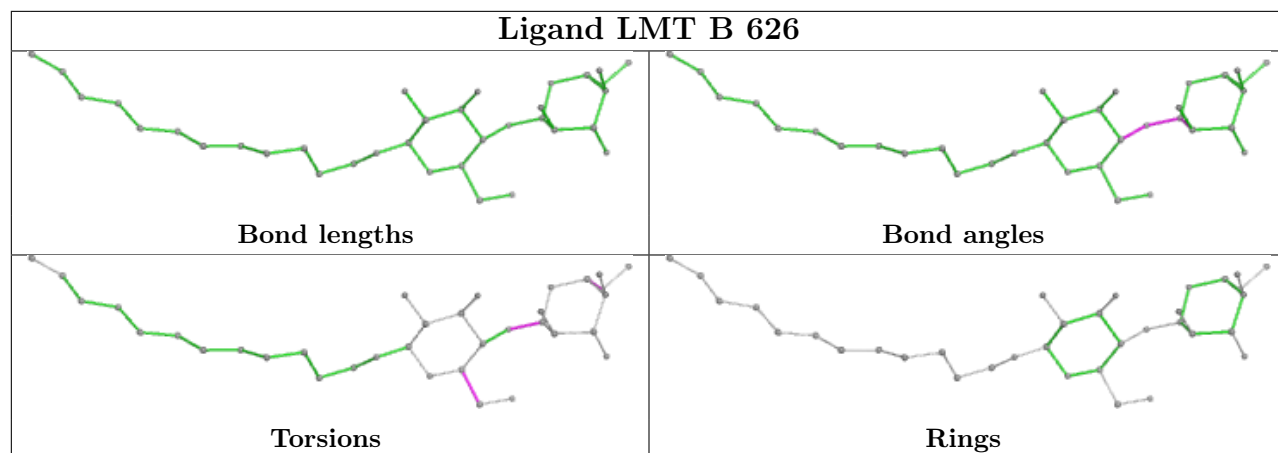


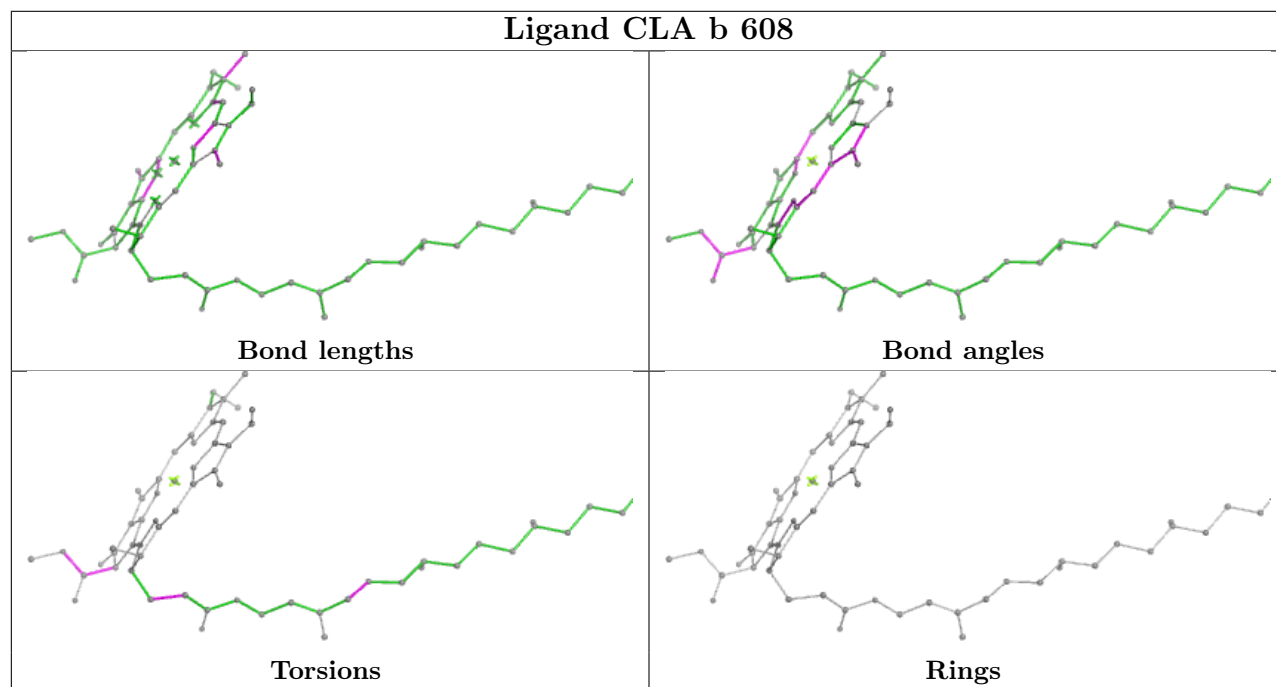
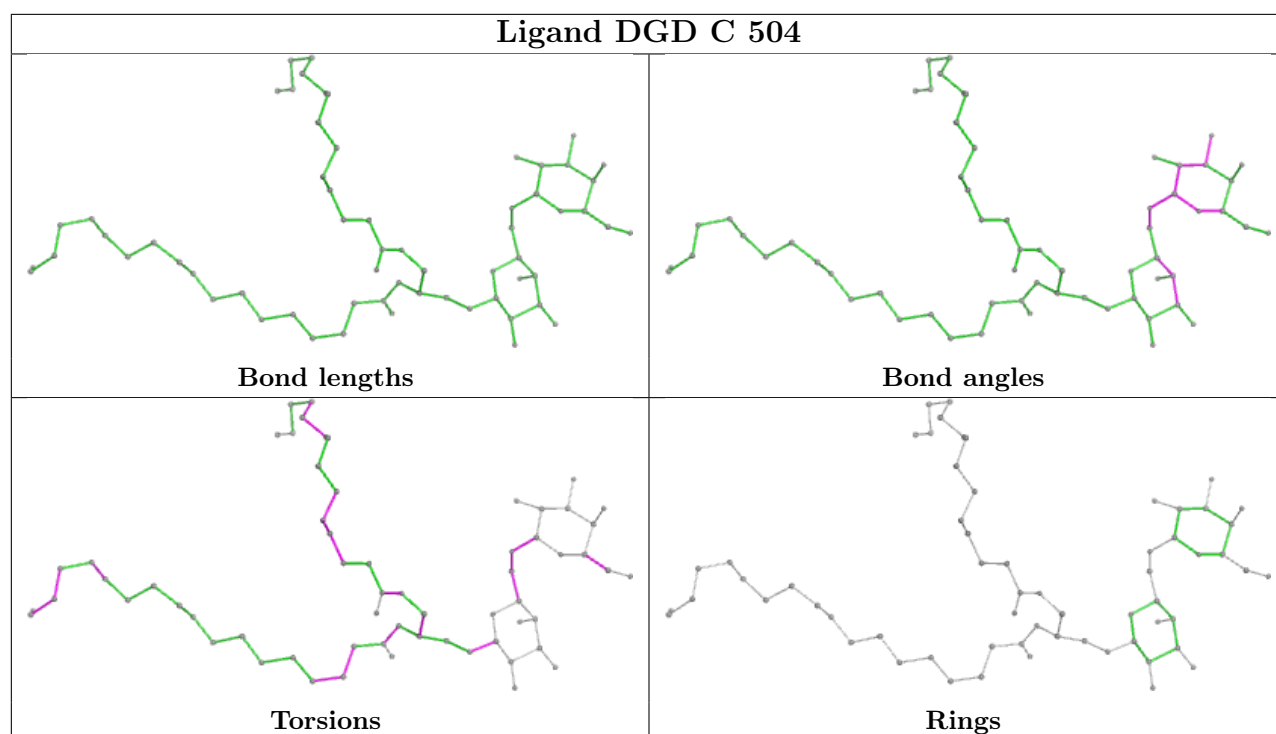


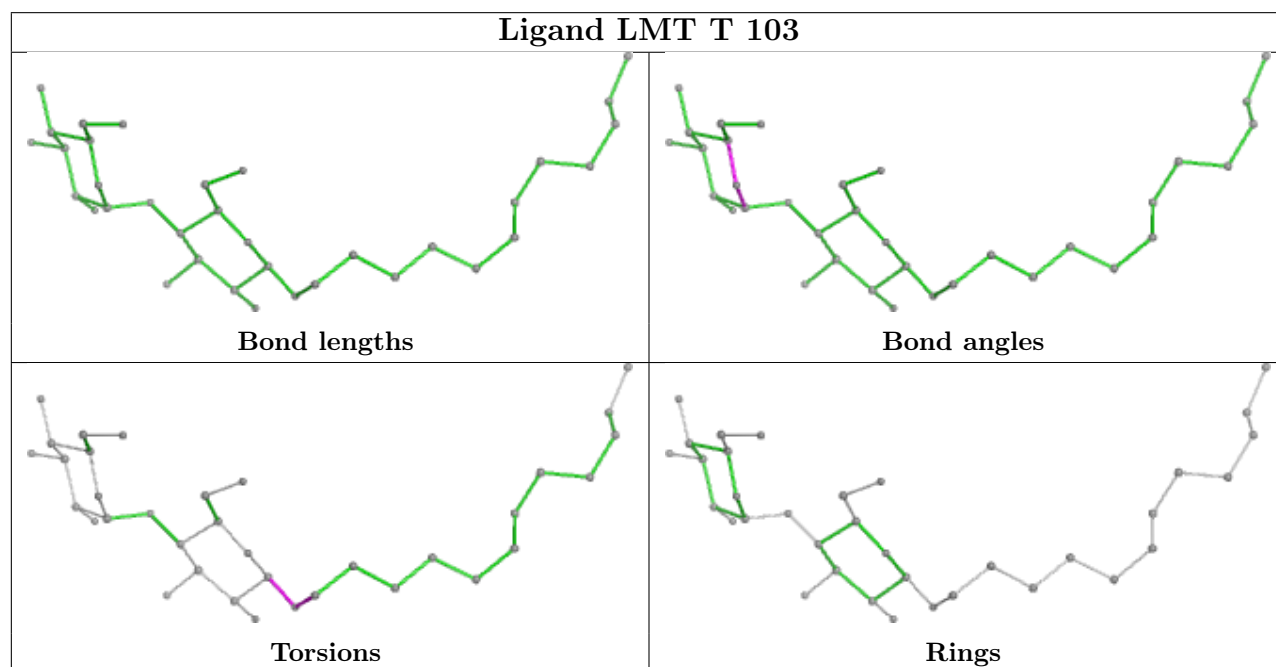
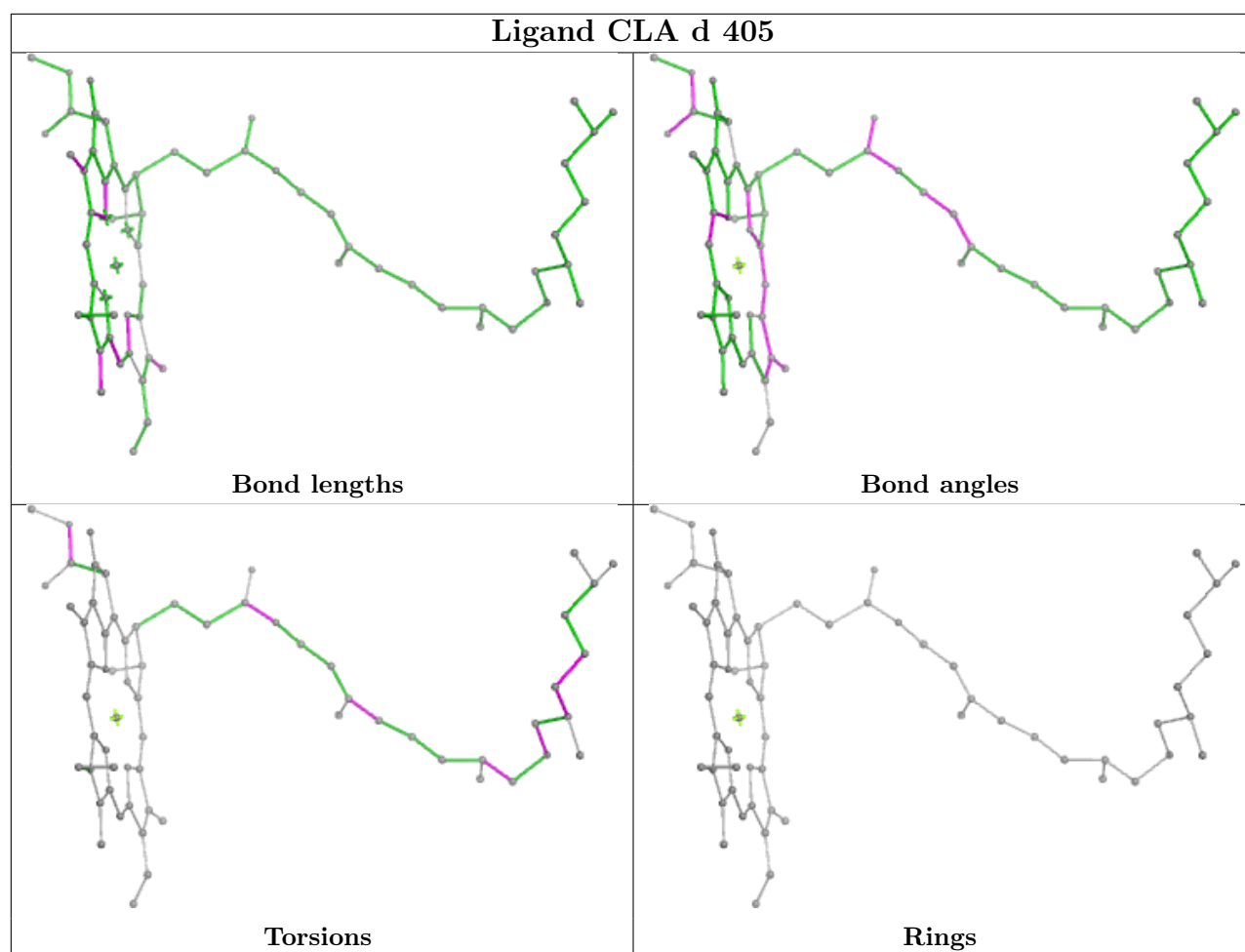


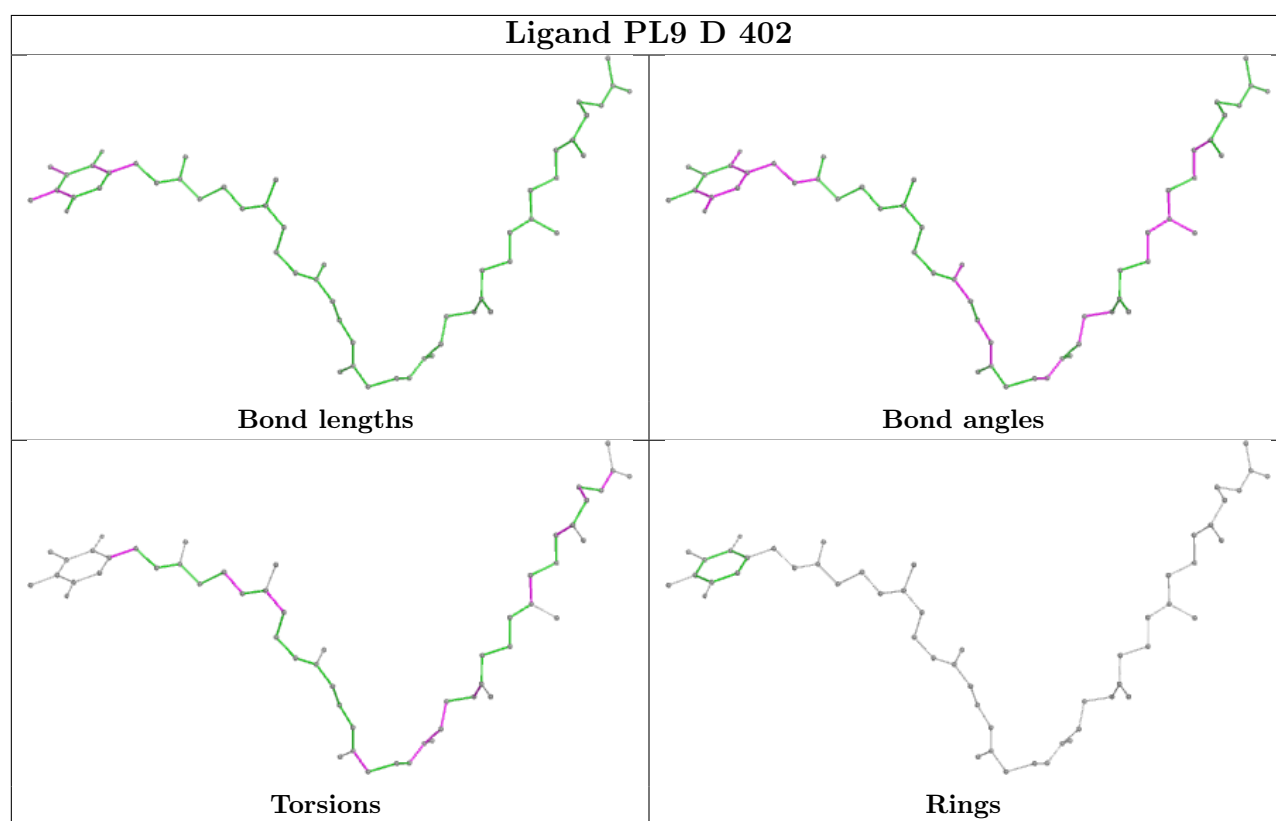
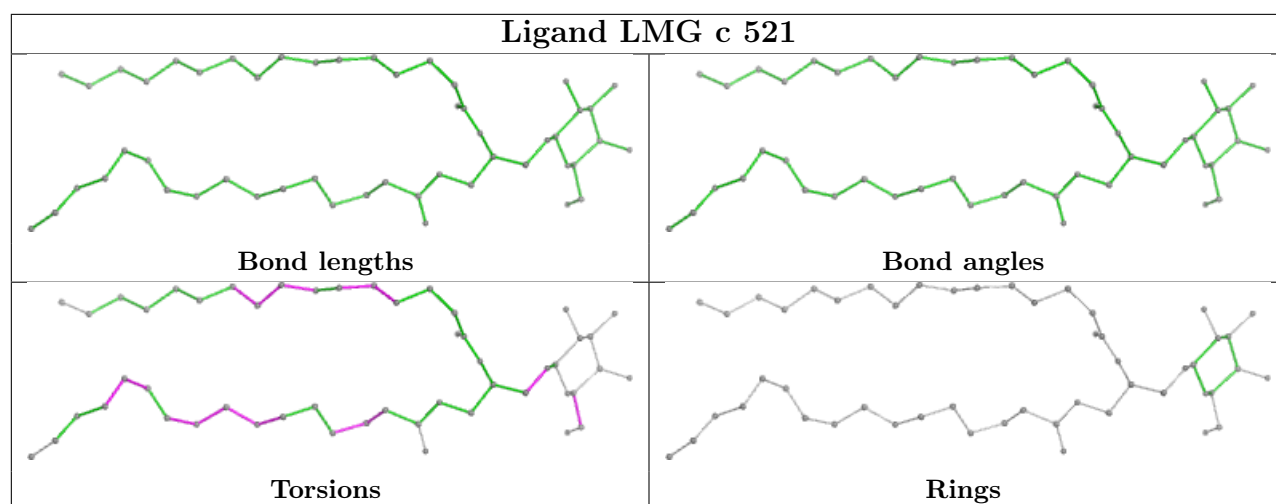


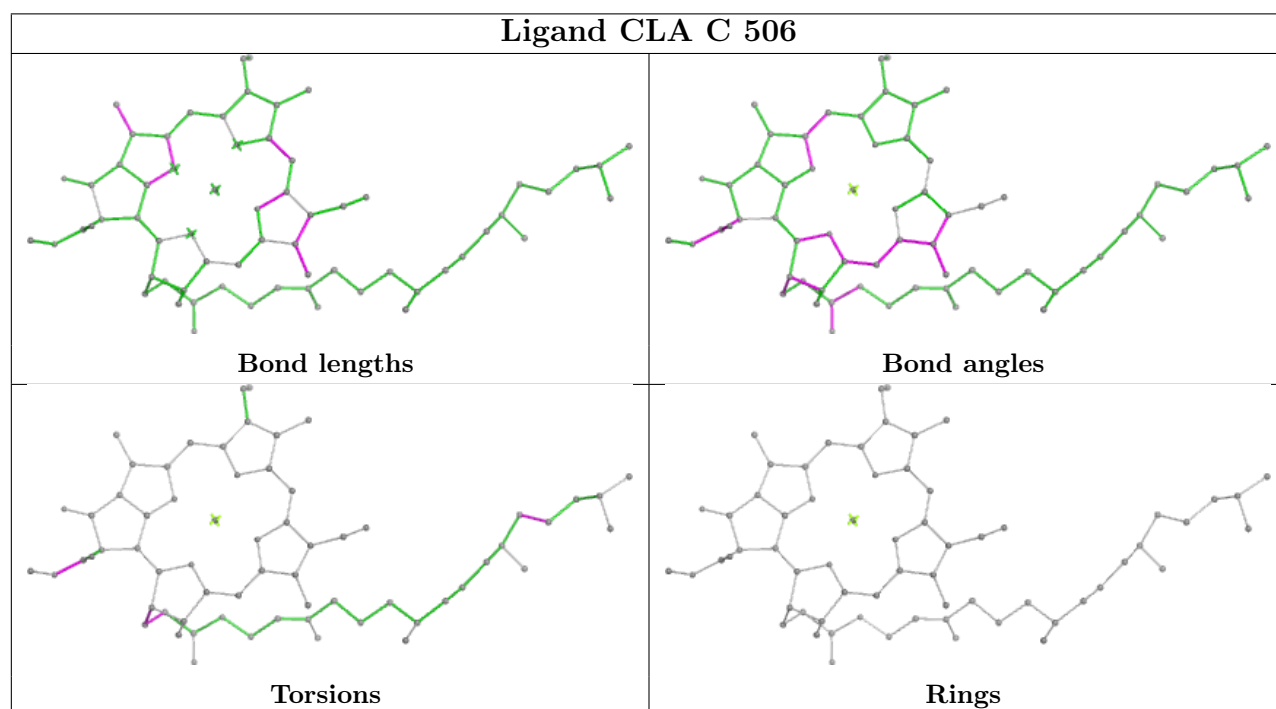
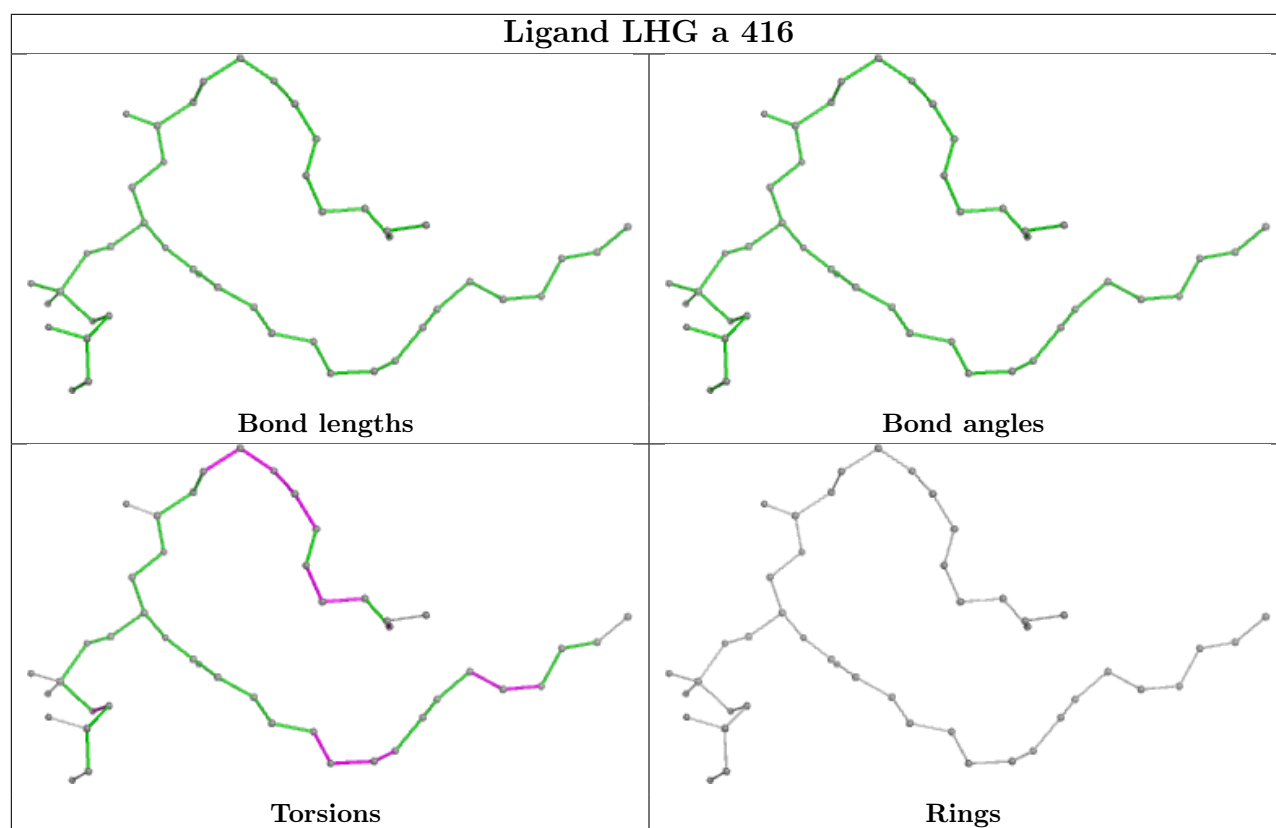


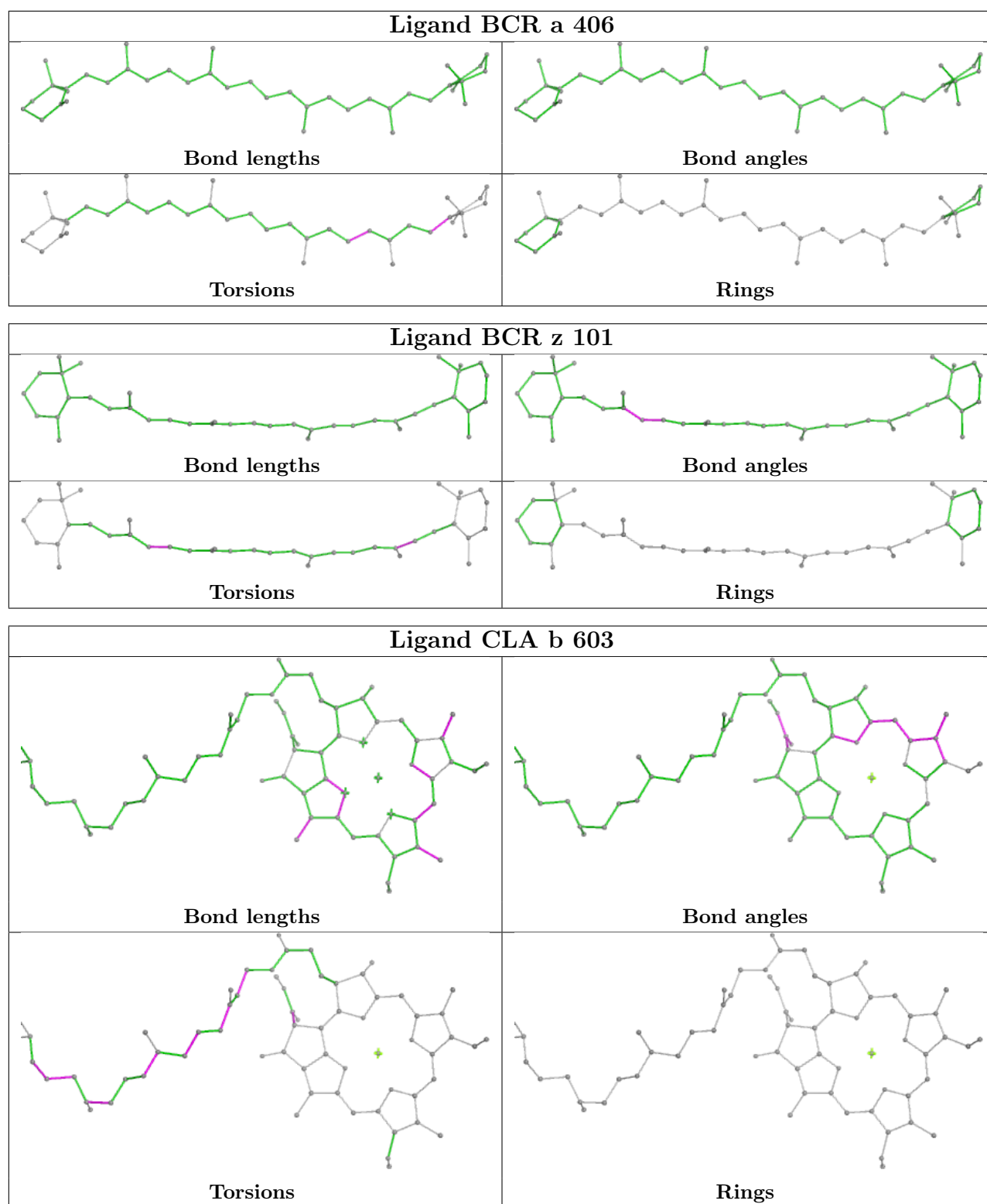


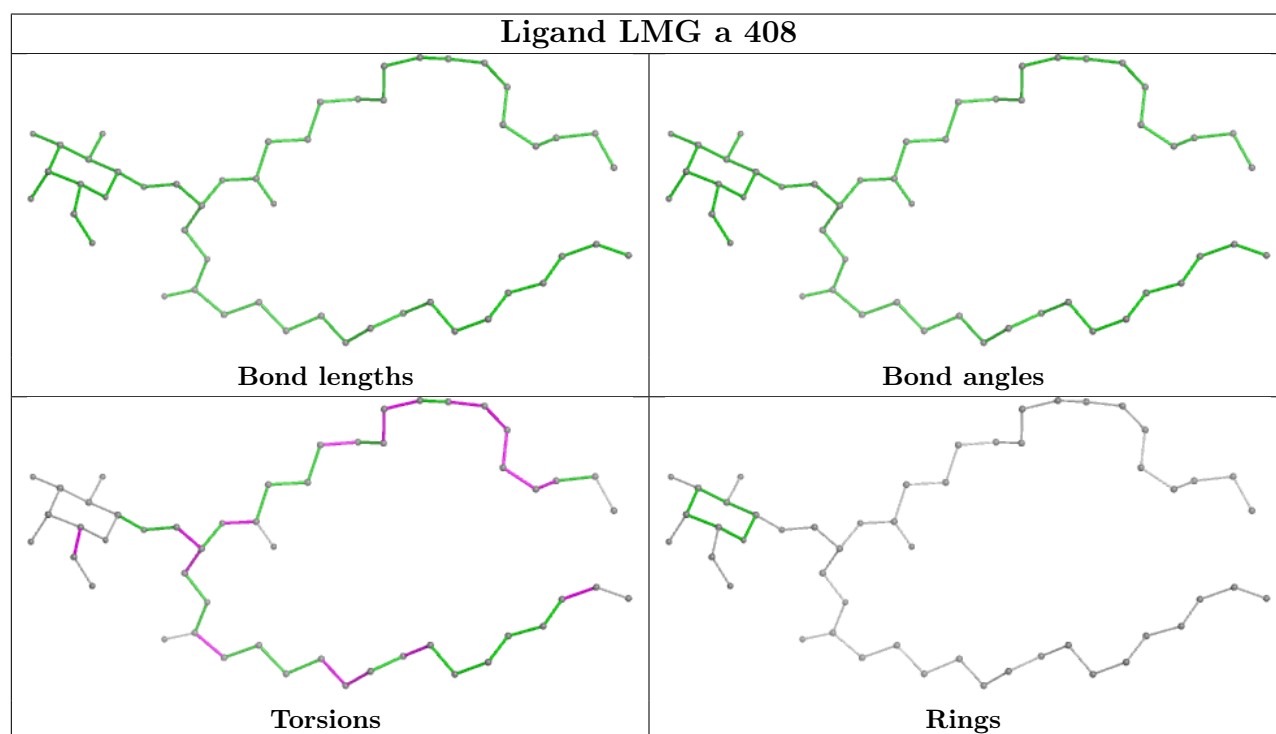
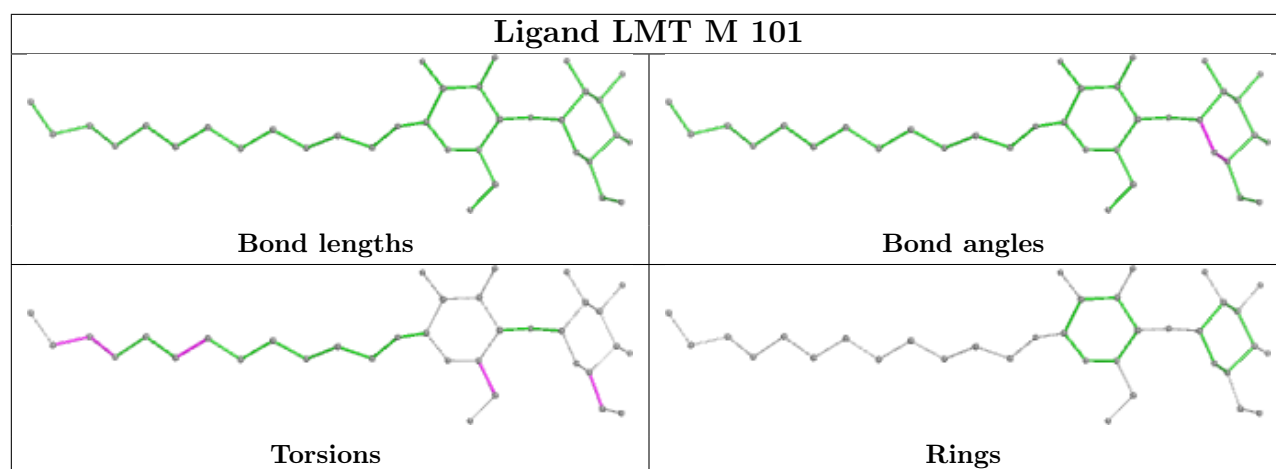




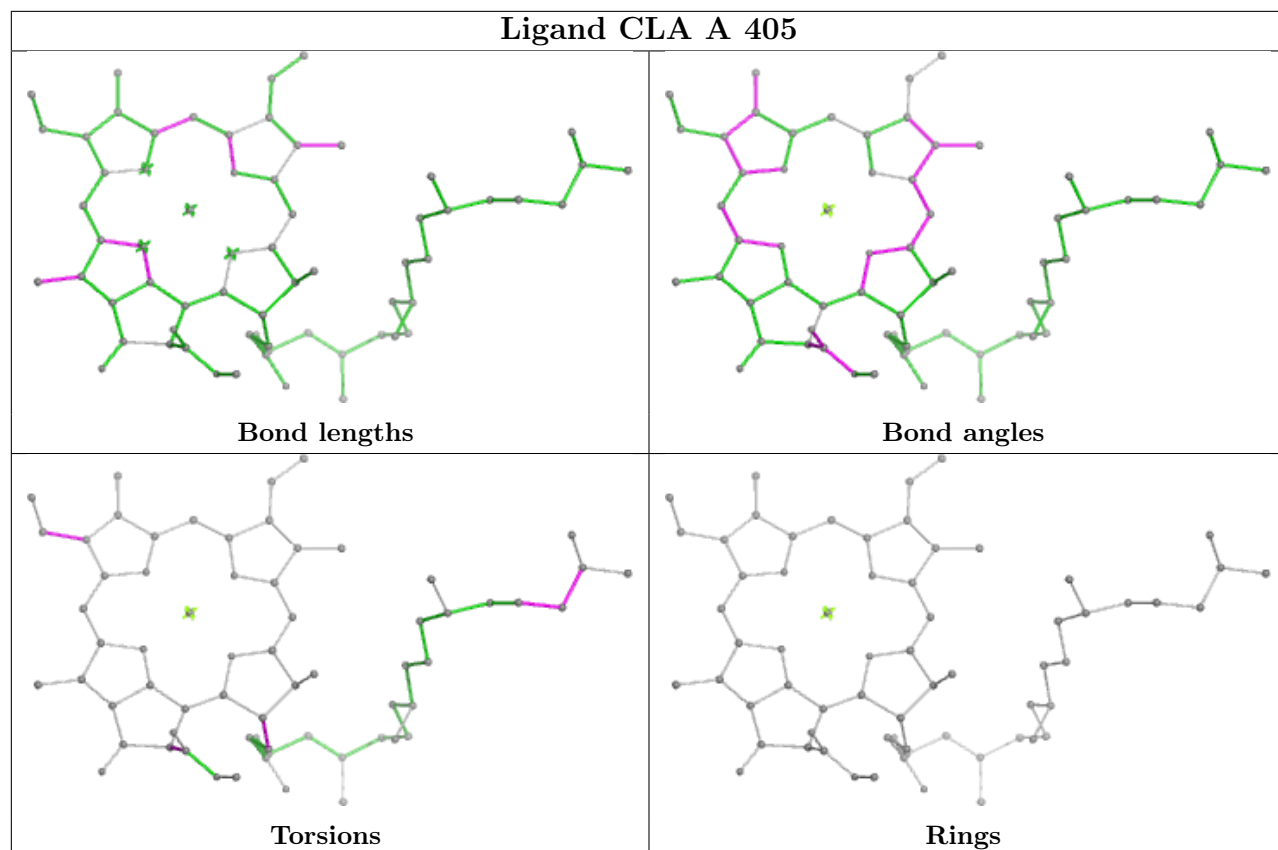




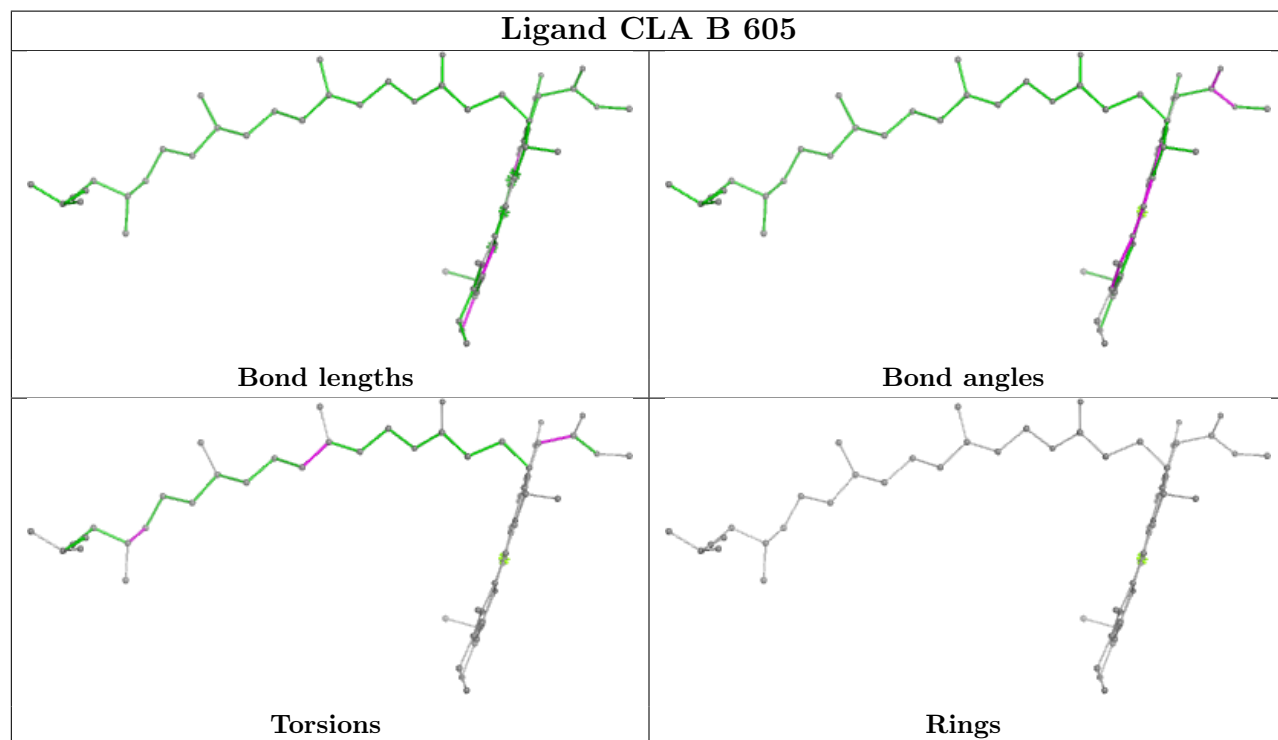


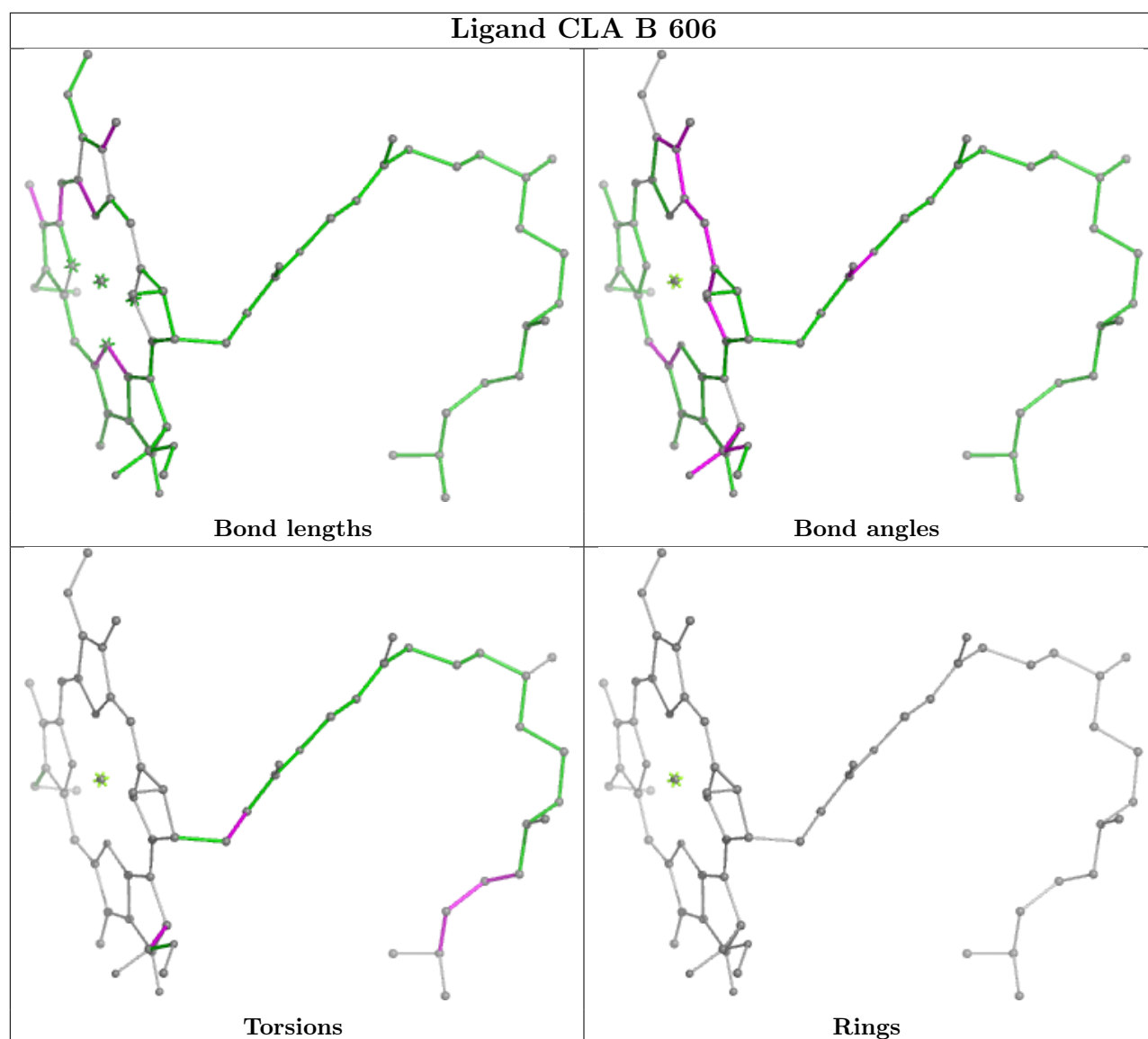


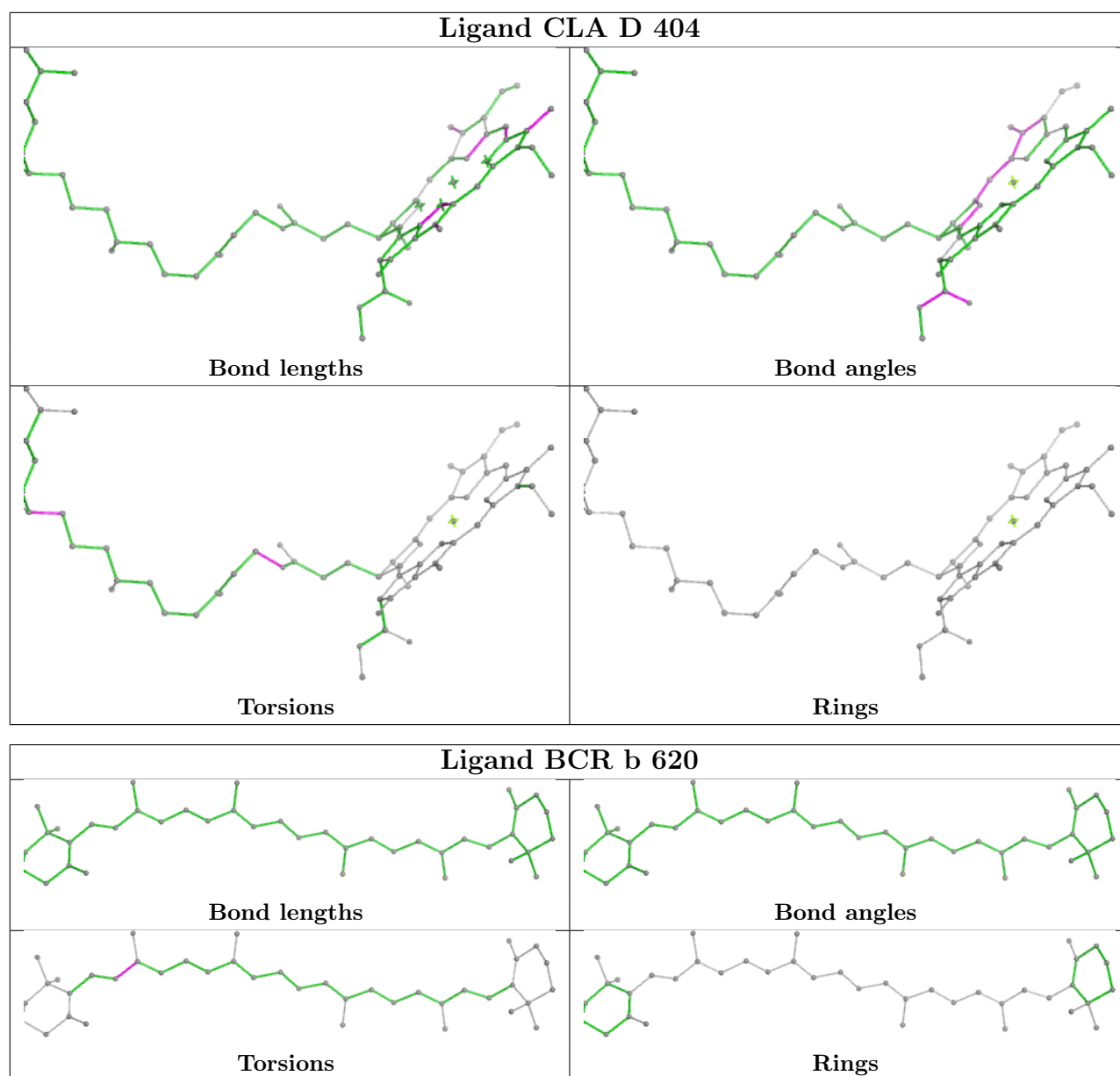
Ligand CLA A 405

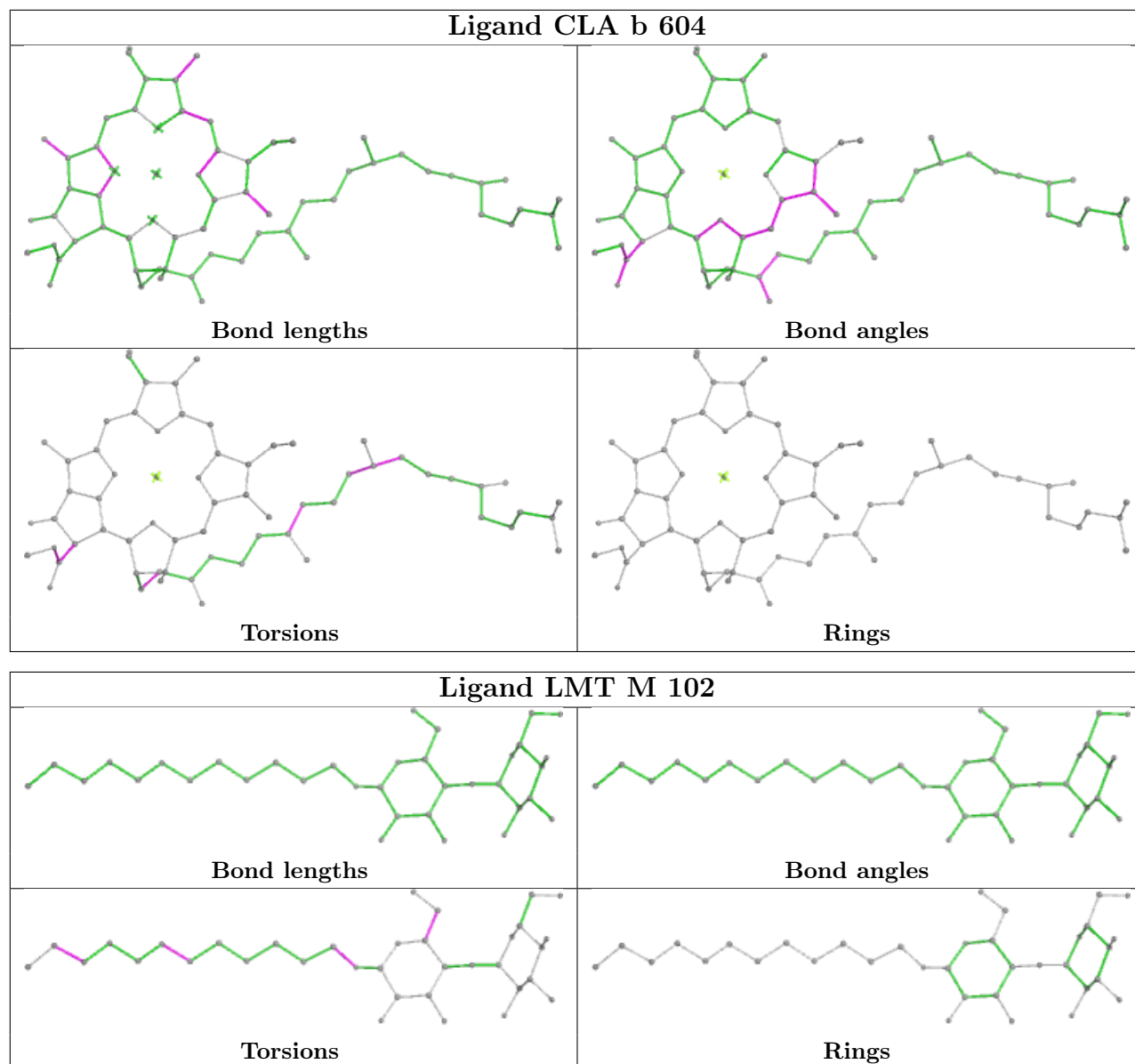


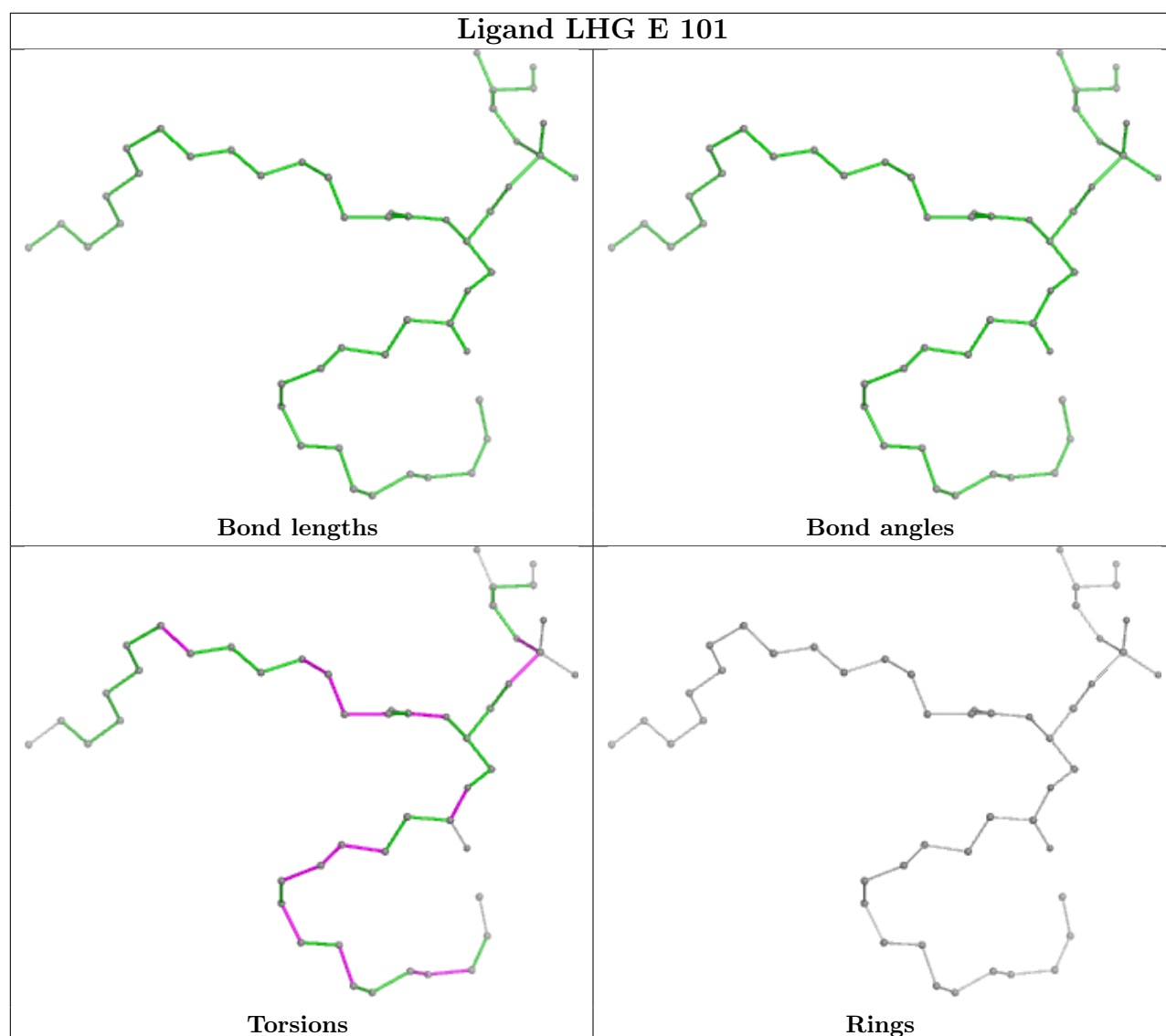
Ligand CLA B 605

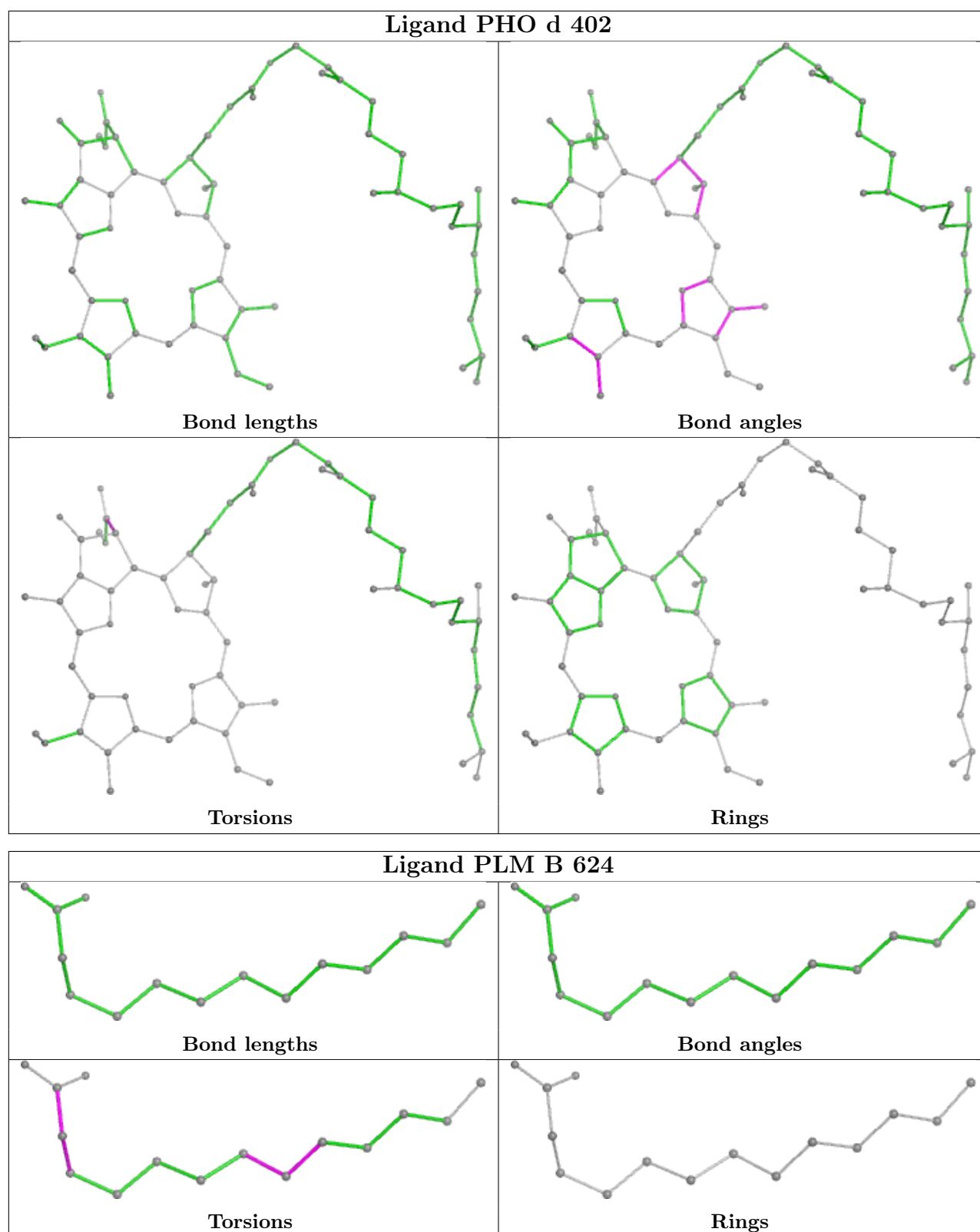


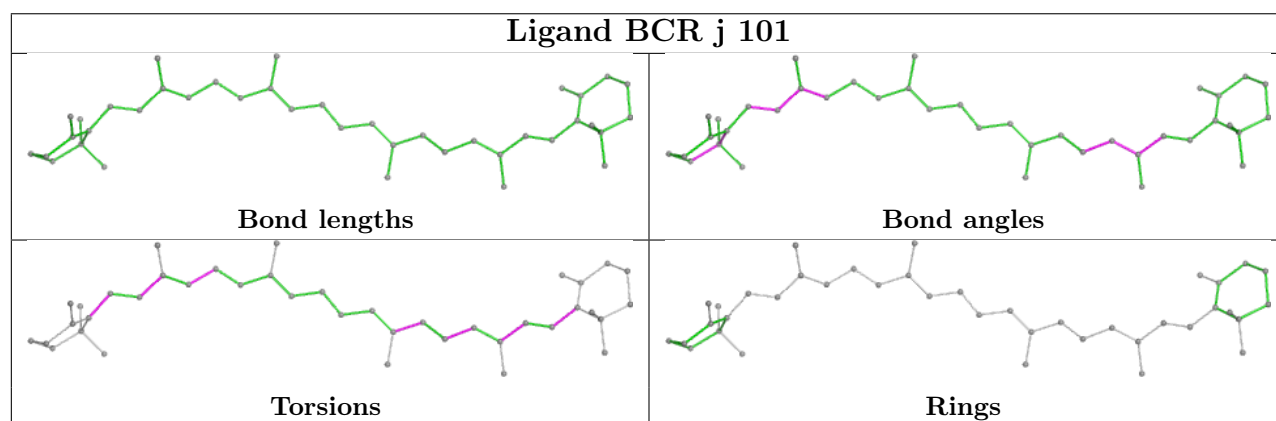
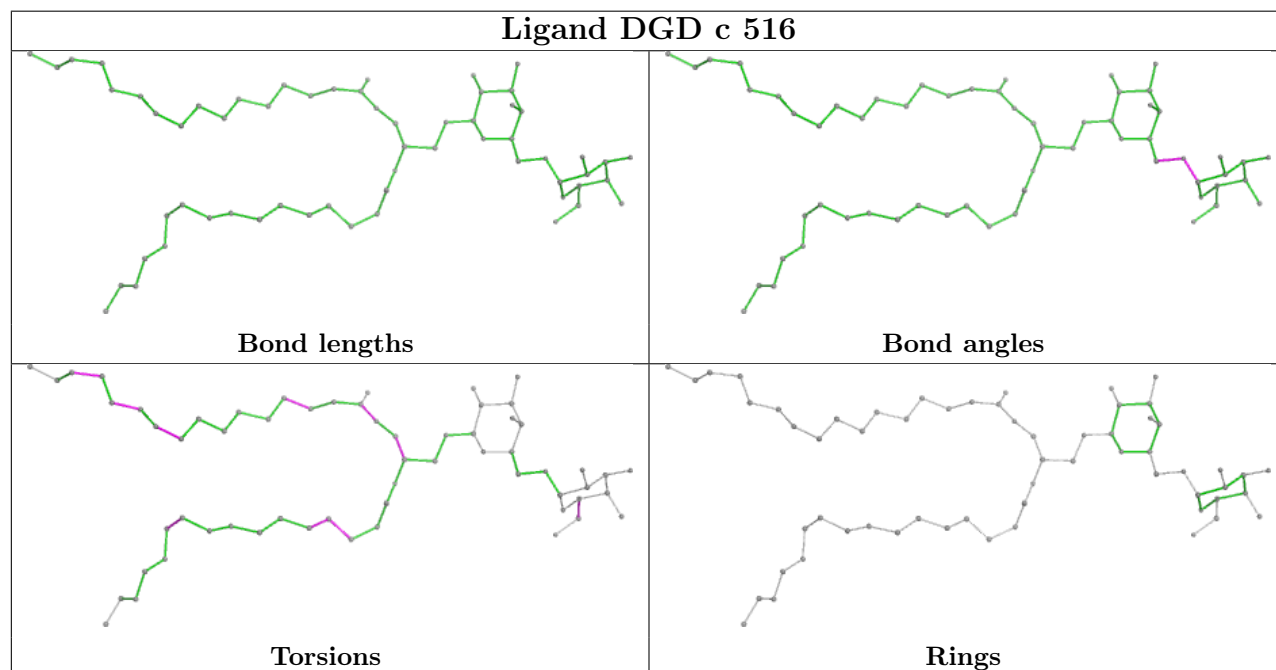
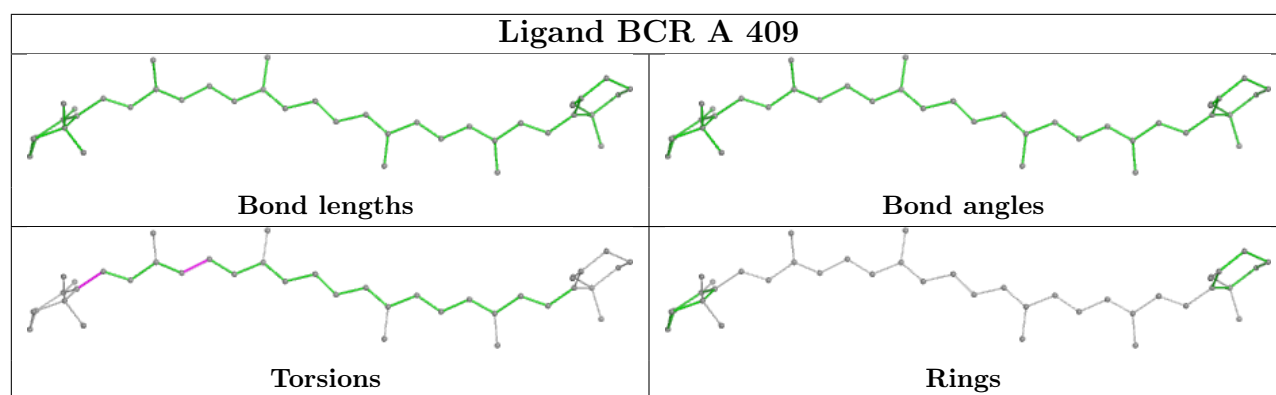


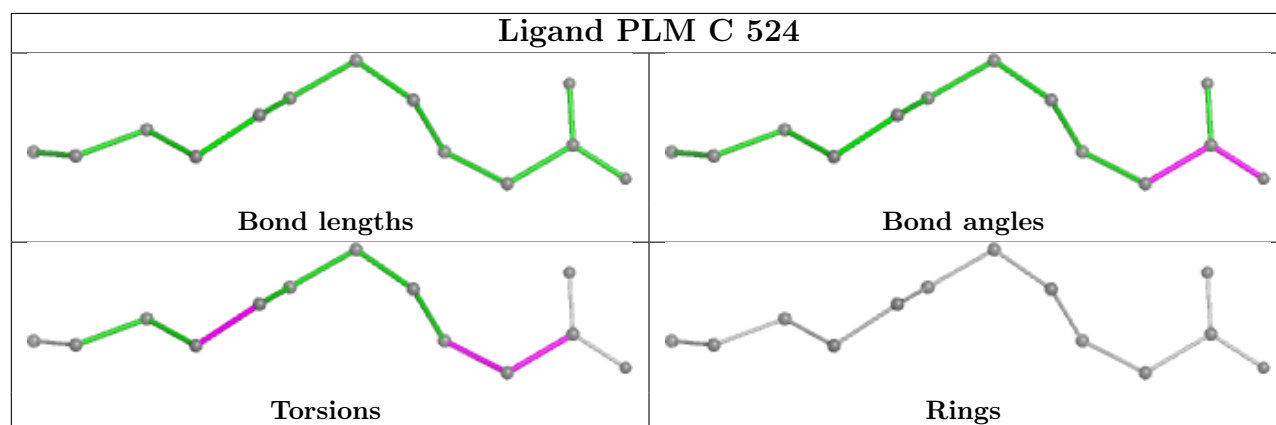
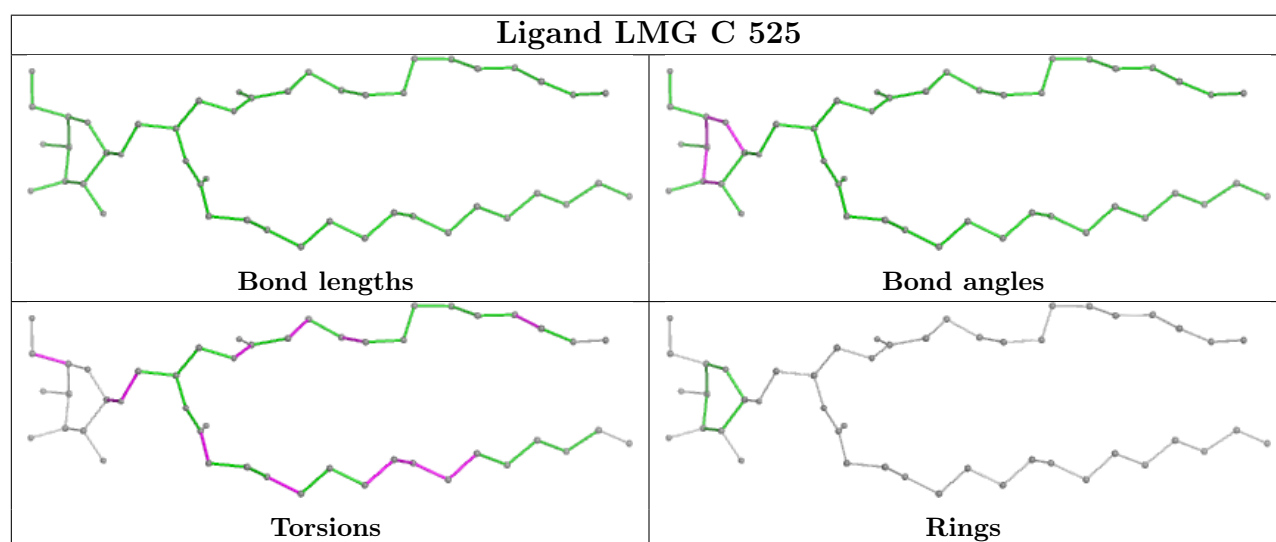
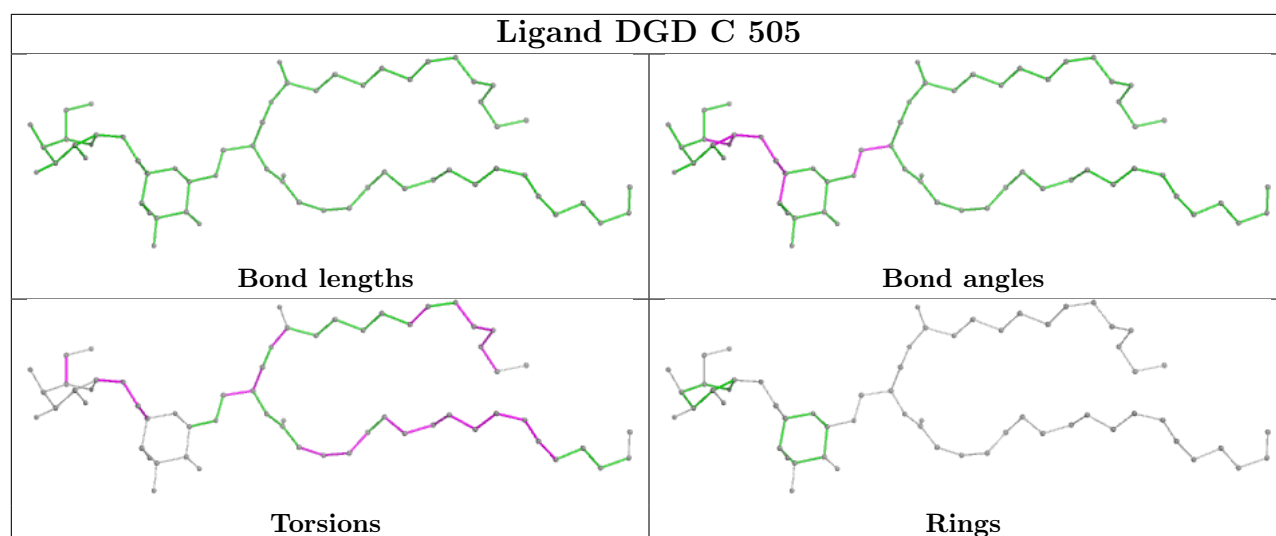


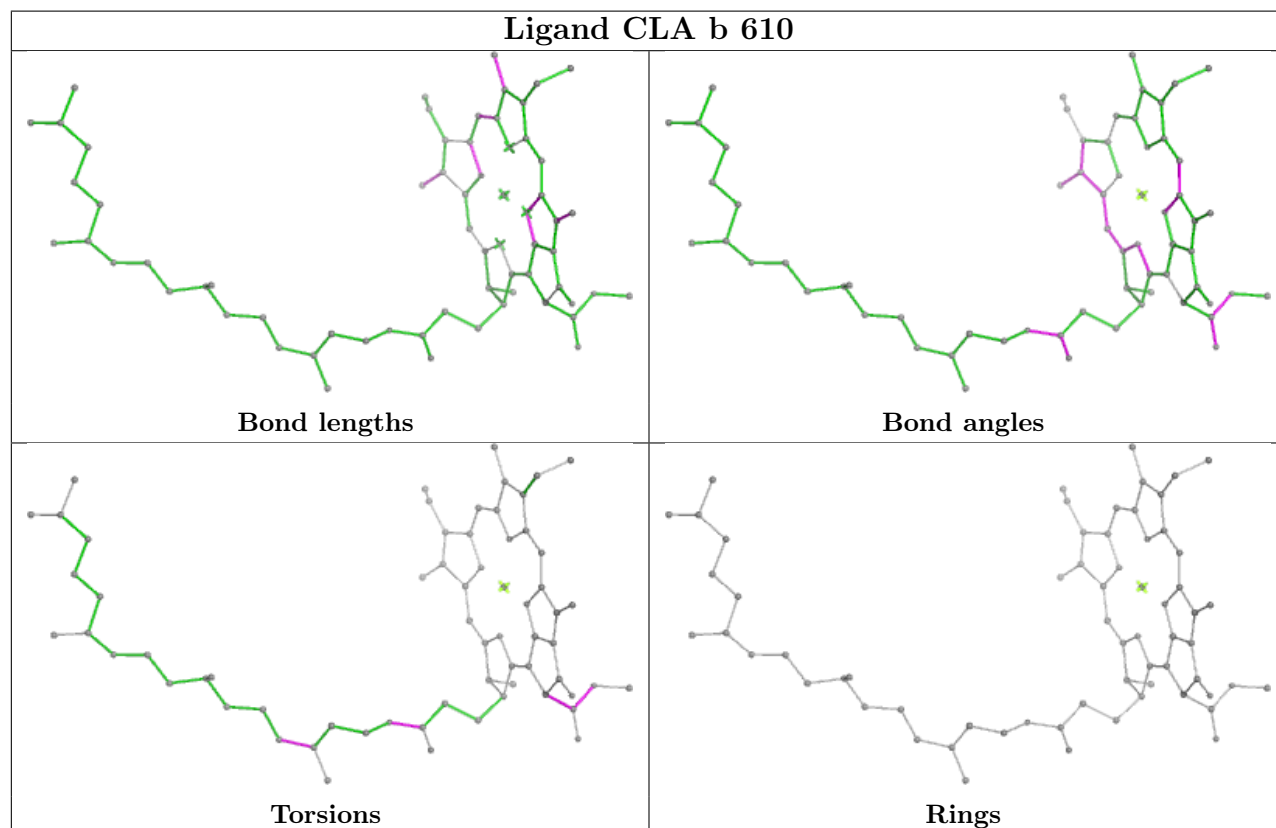
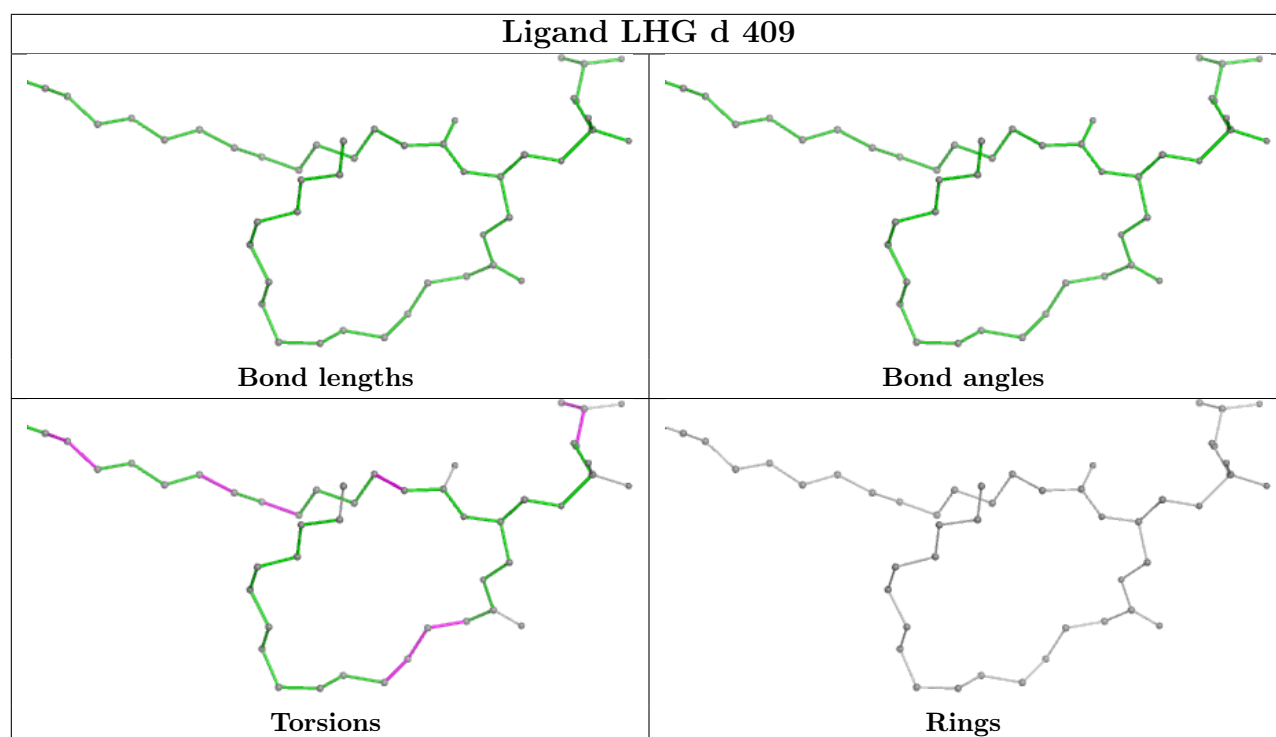


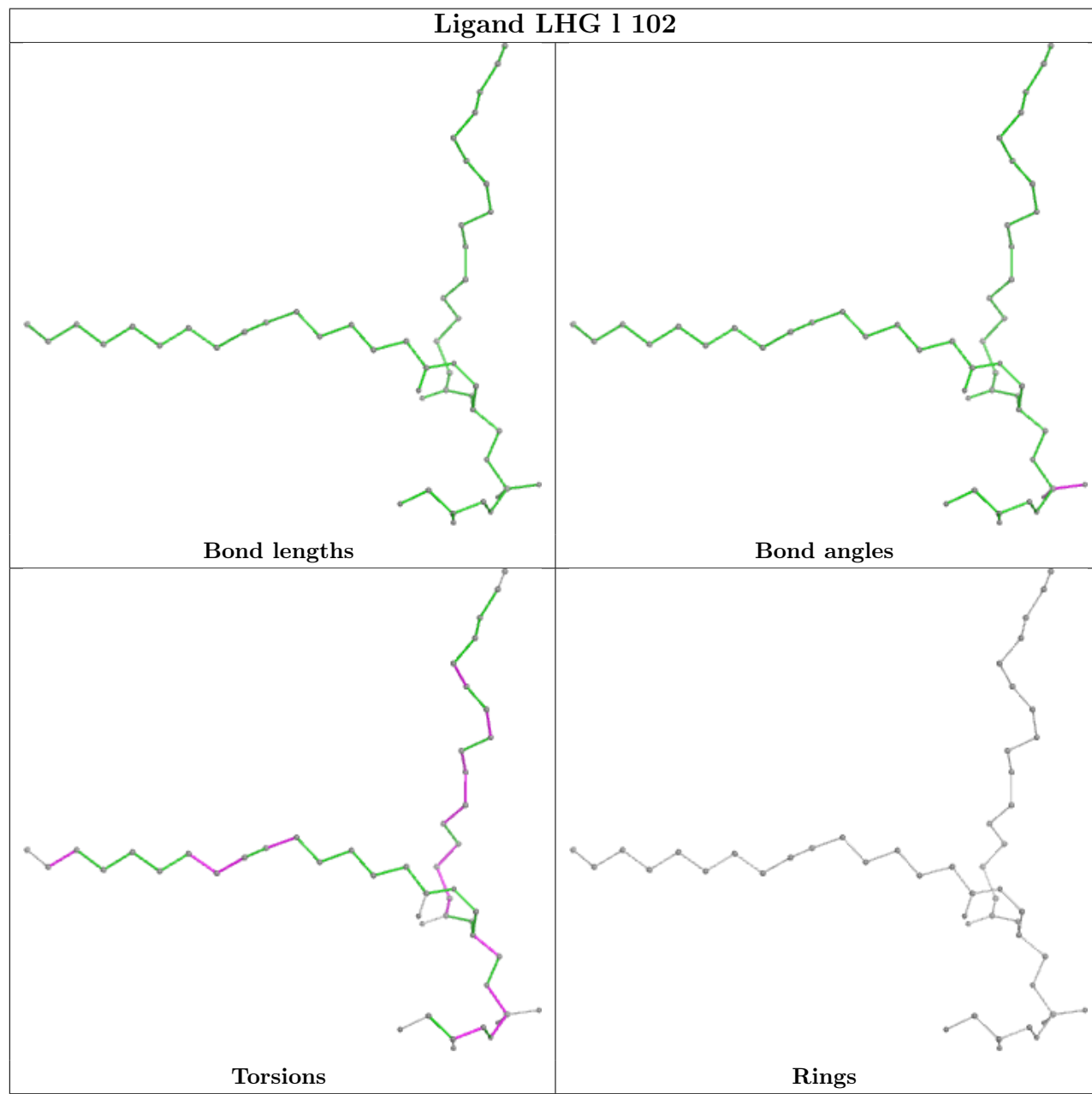
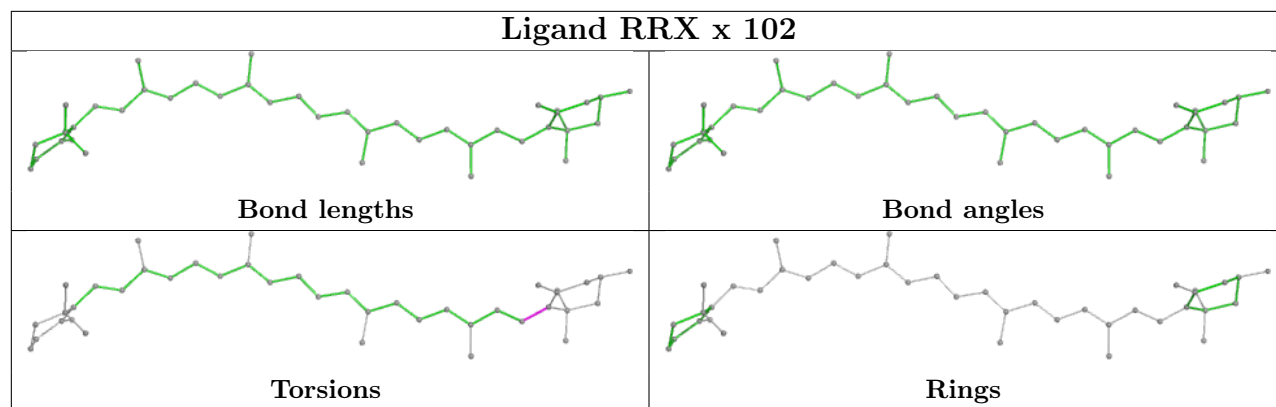


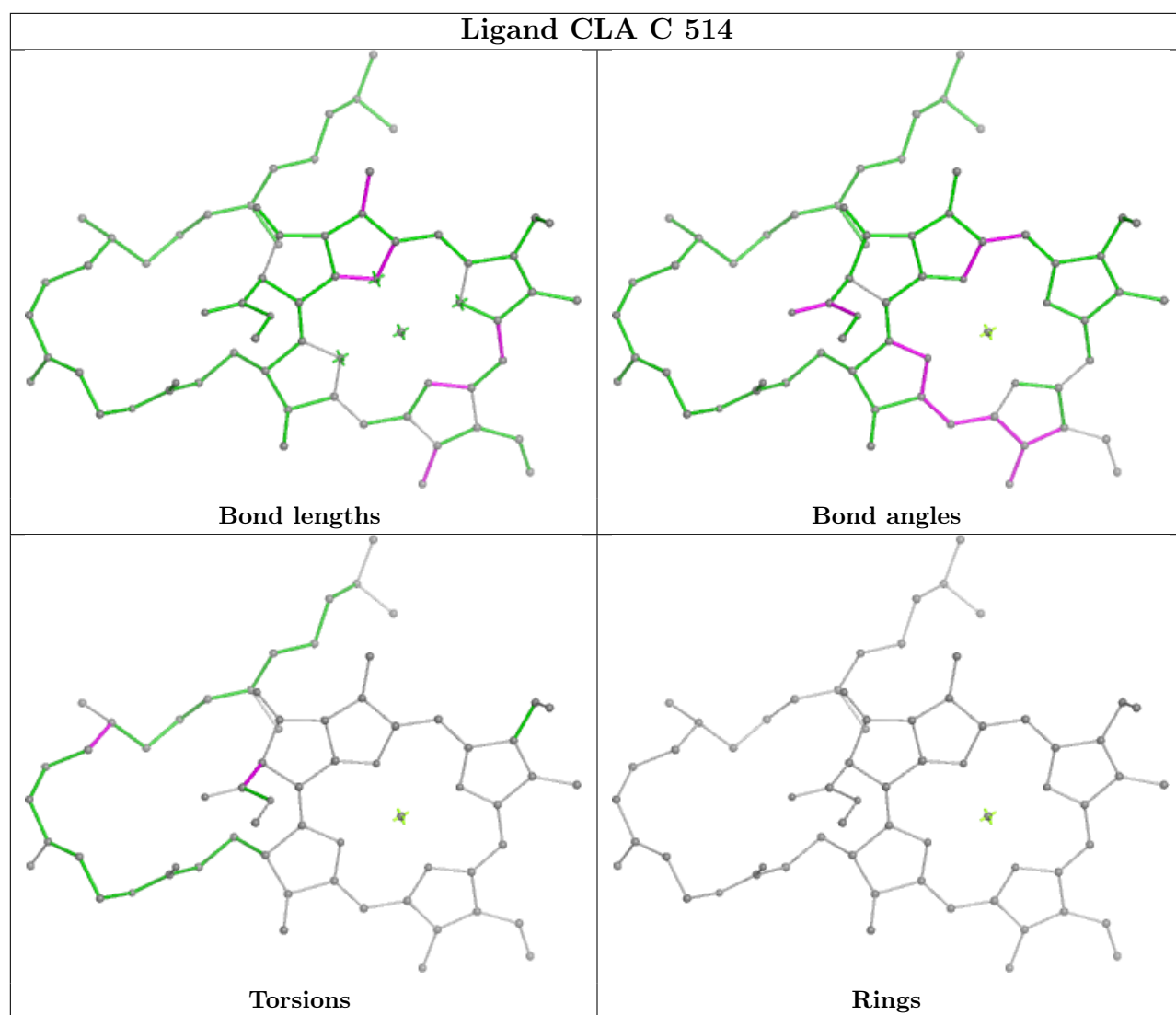


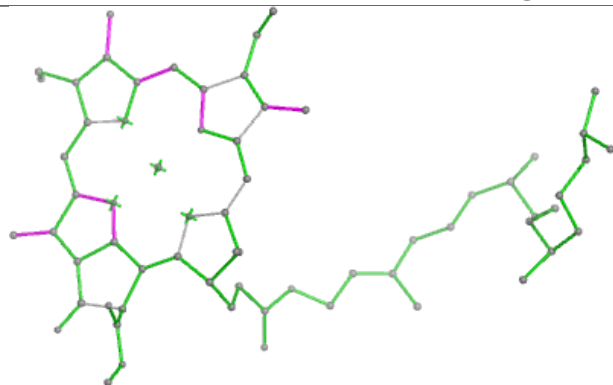
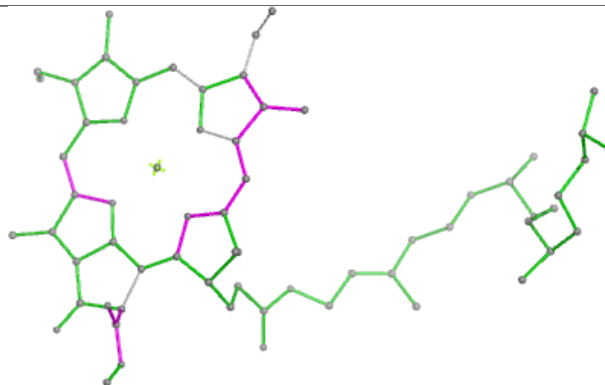
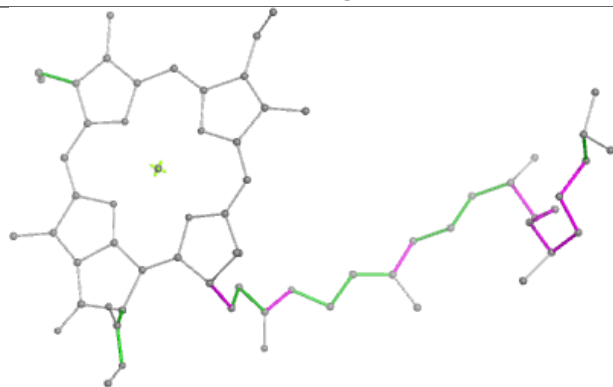
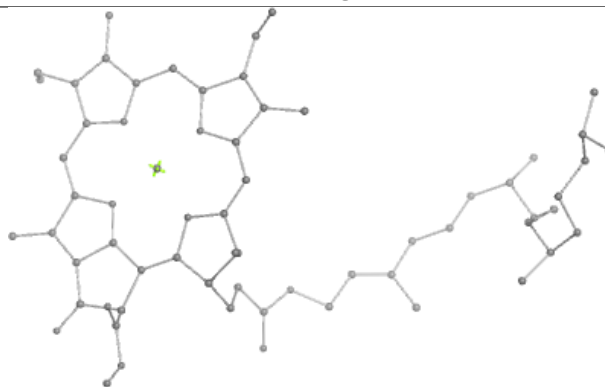
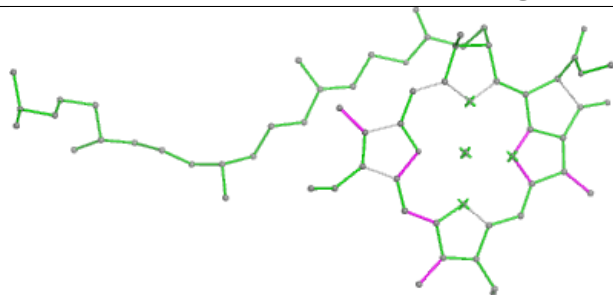
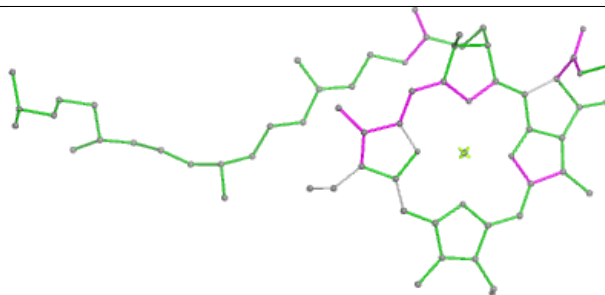
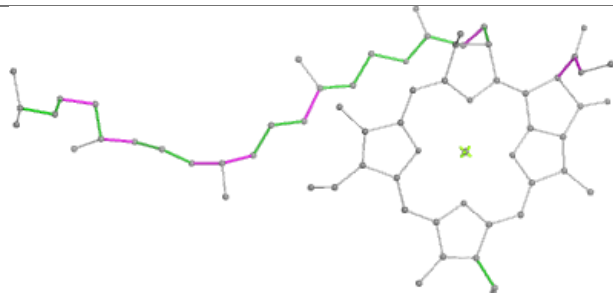
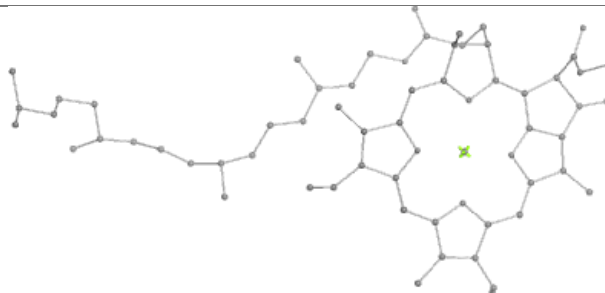


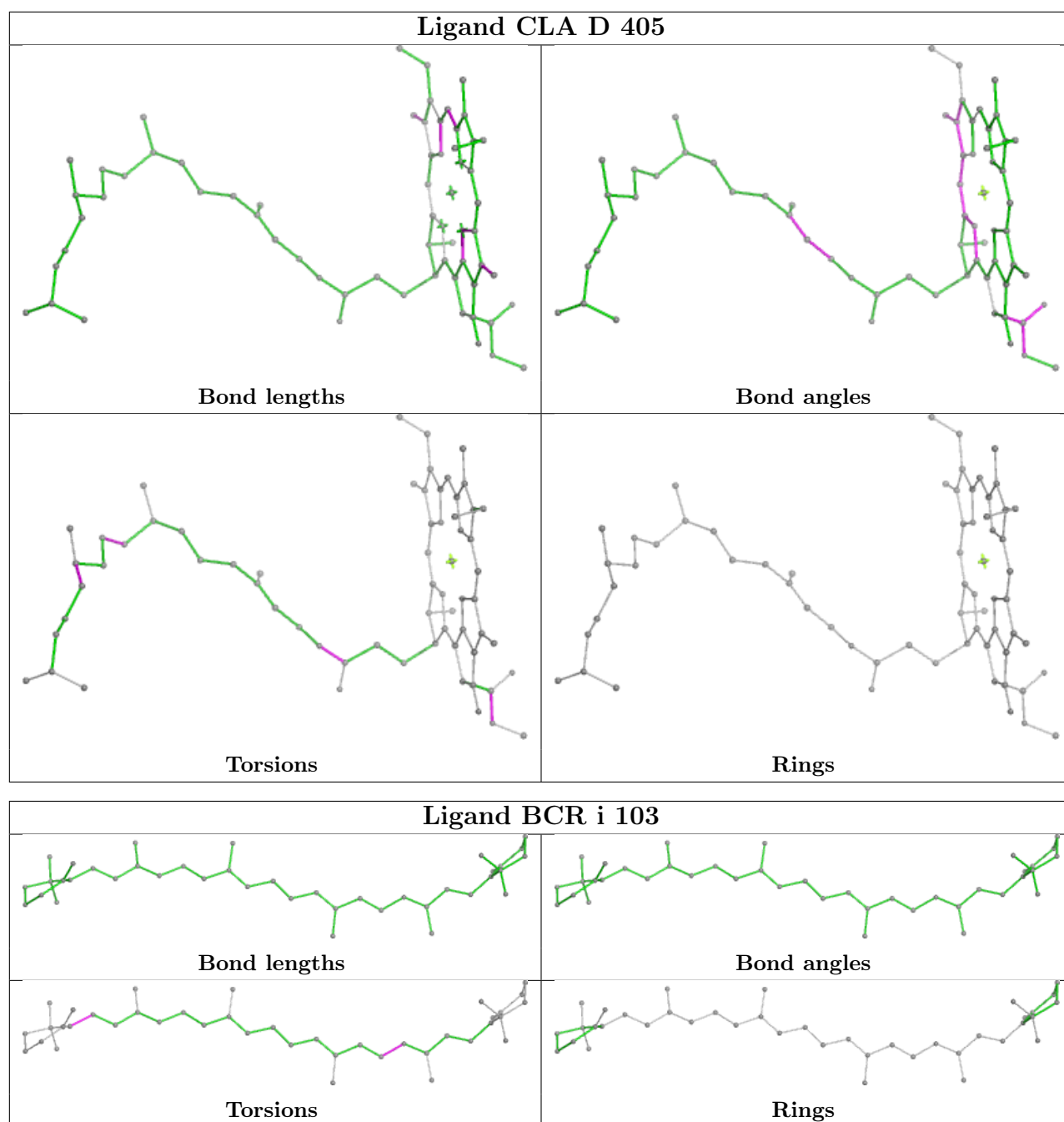


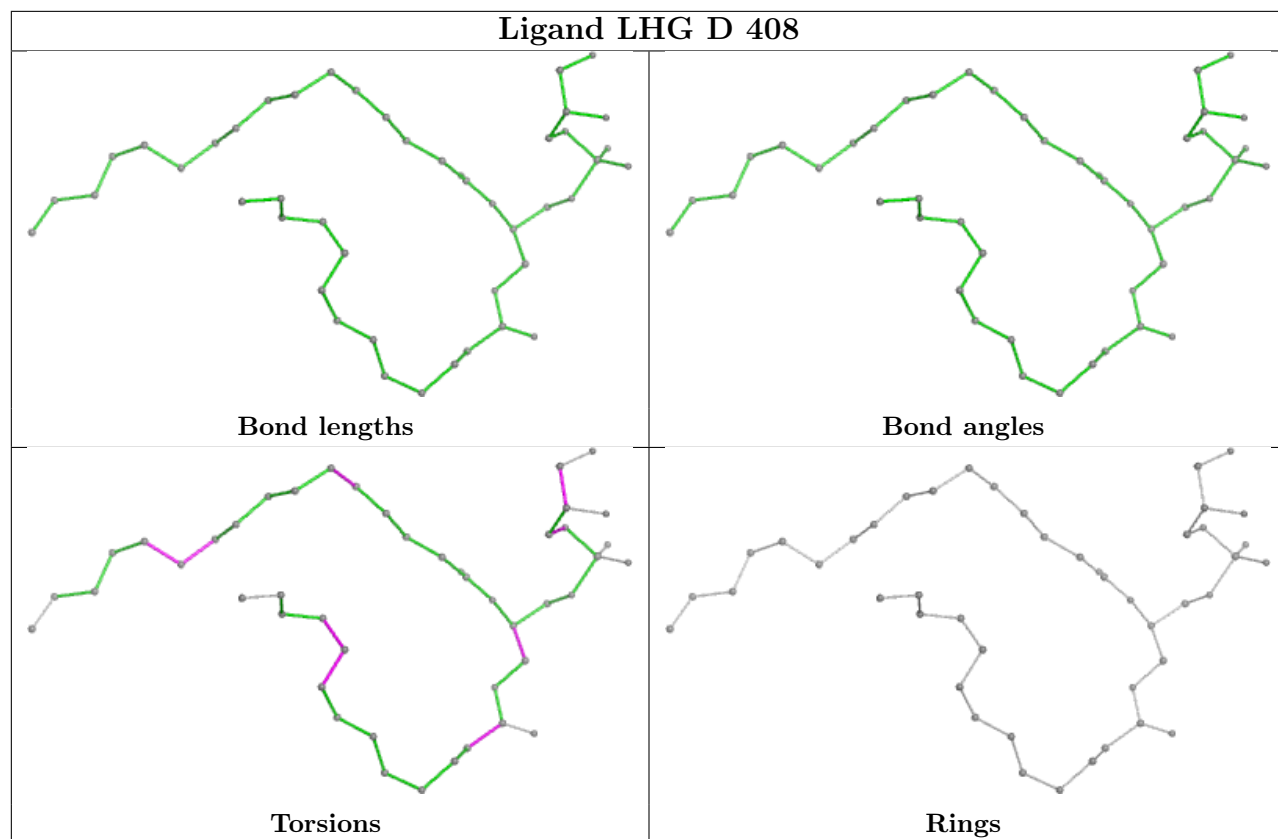


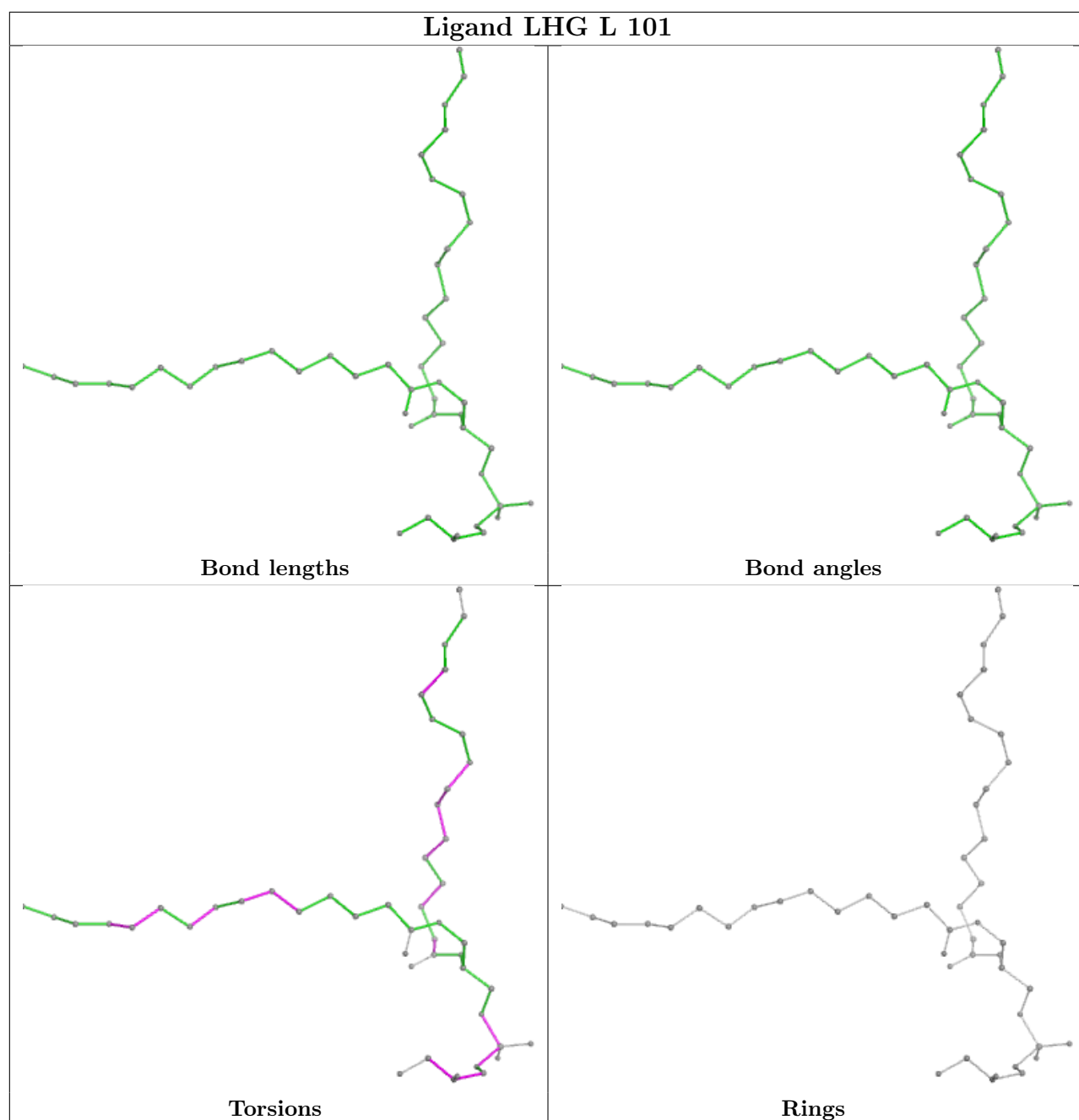


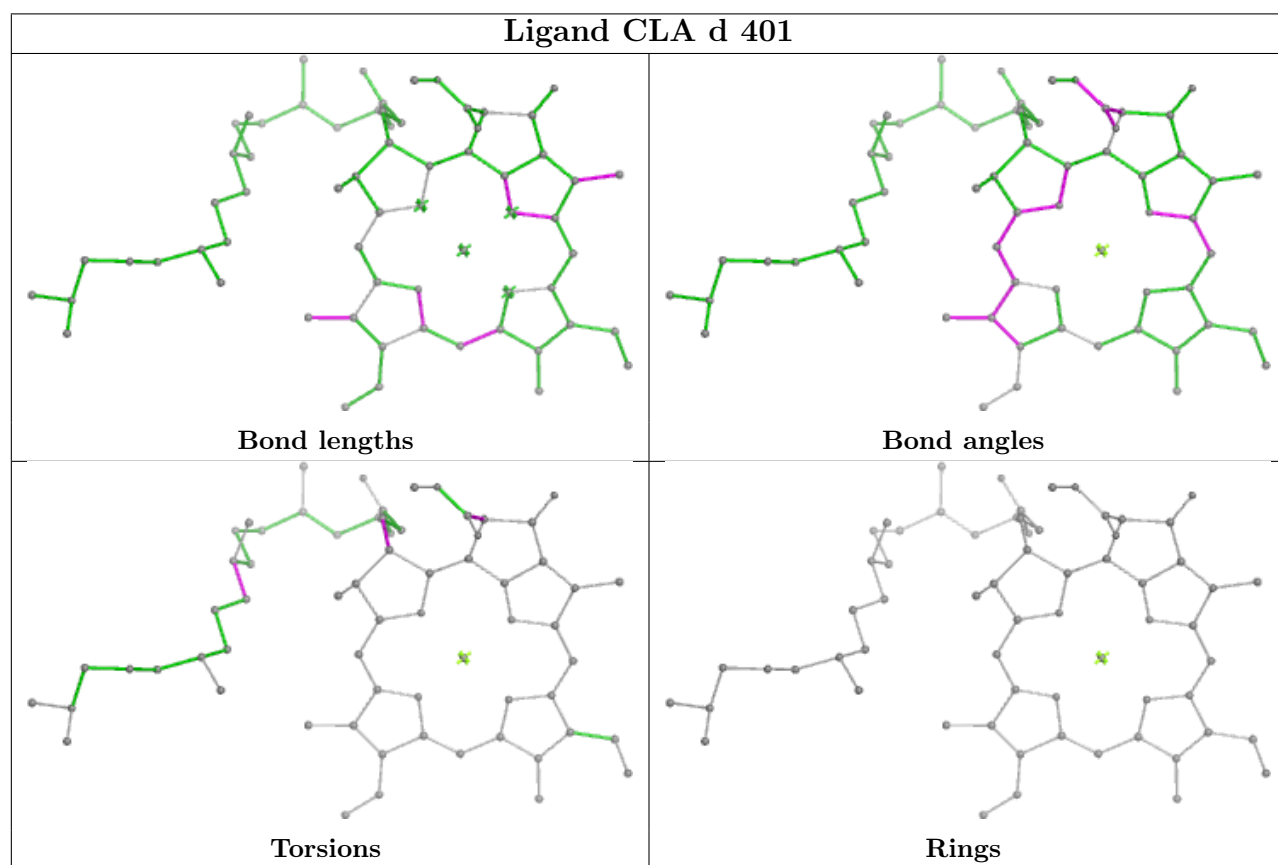
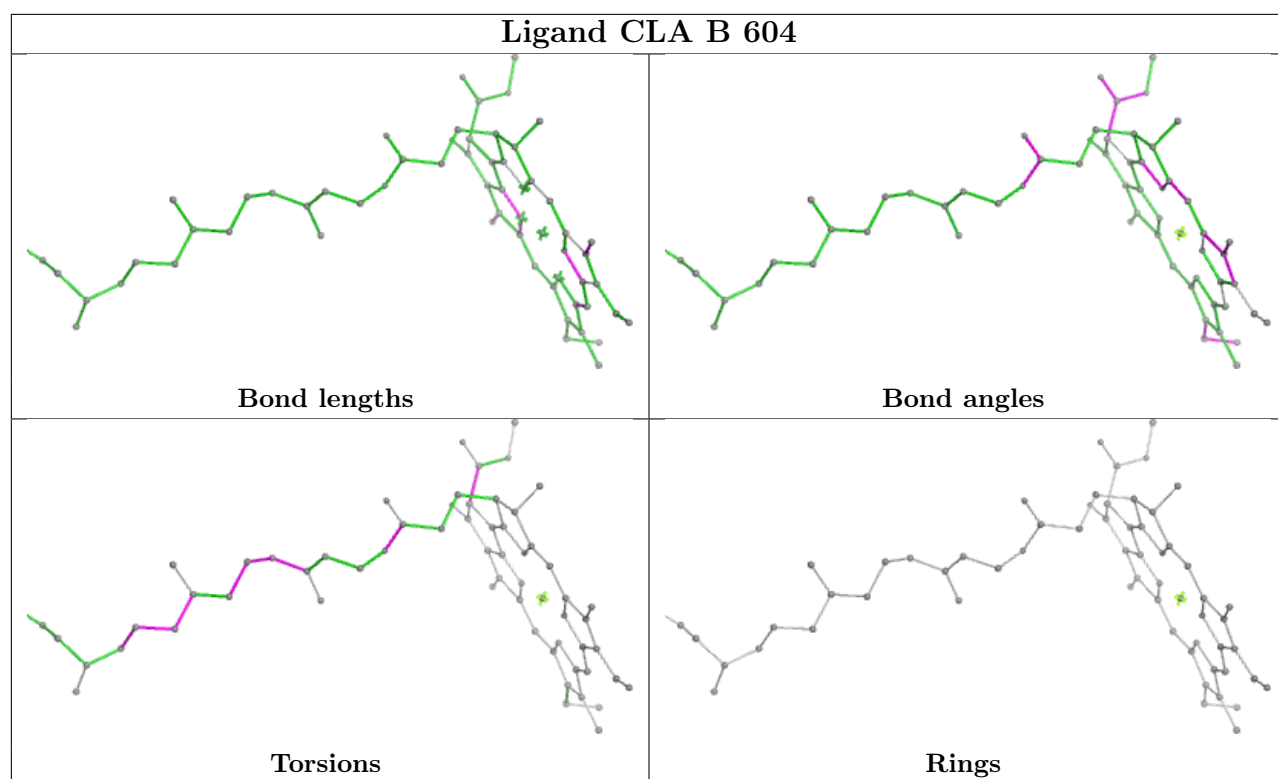


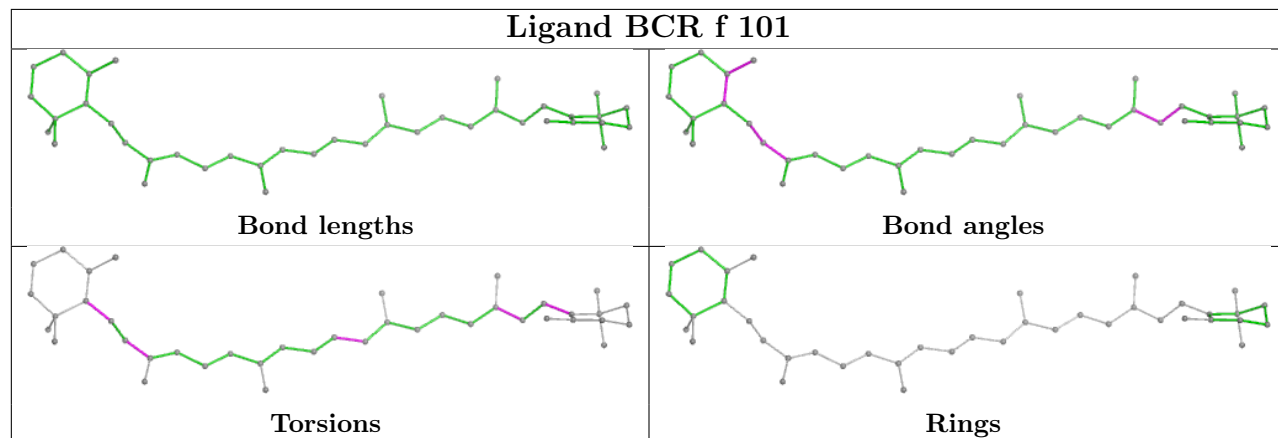
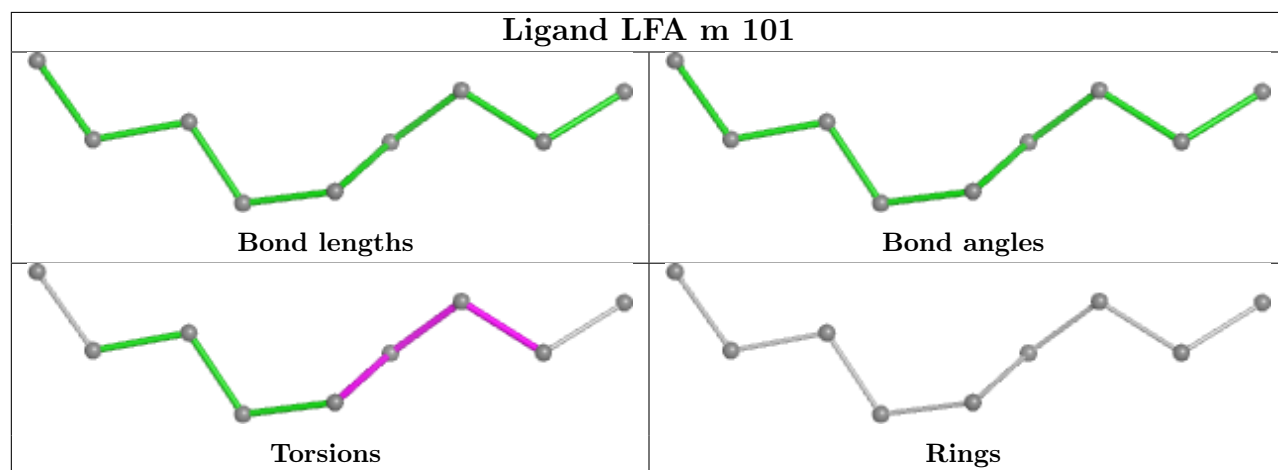
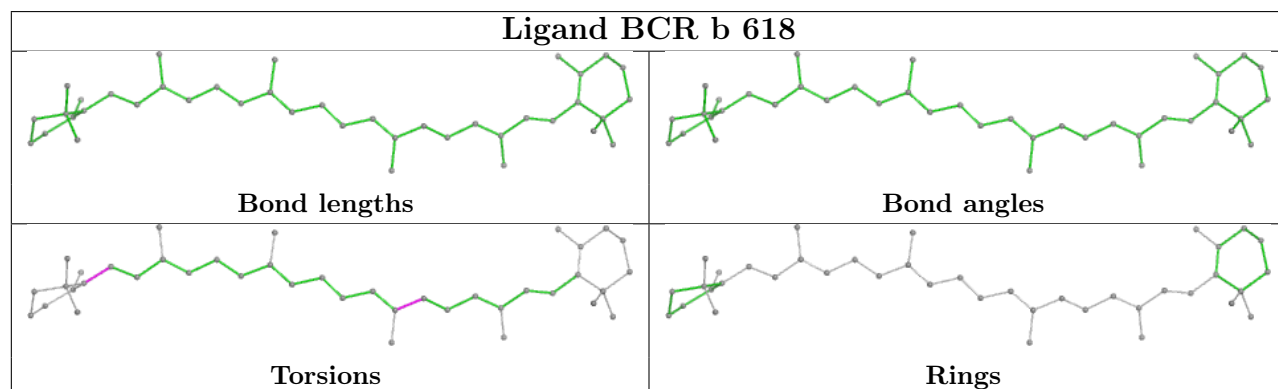
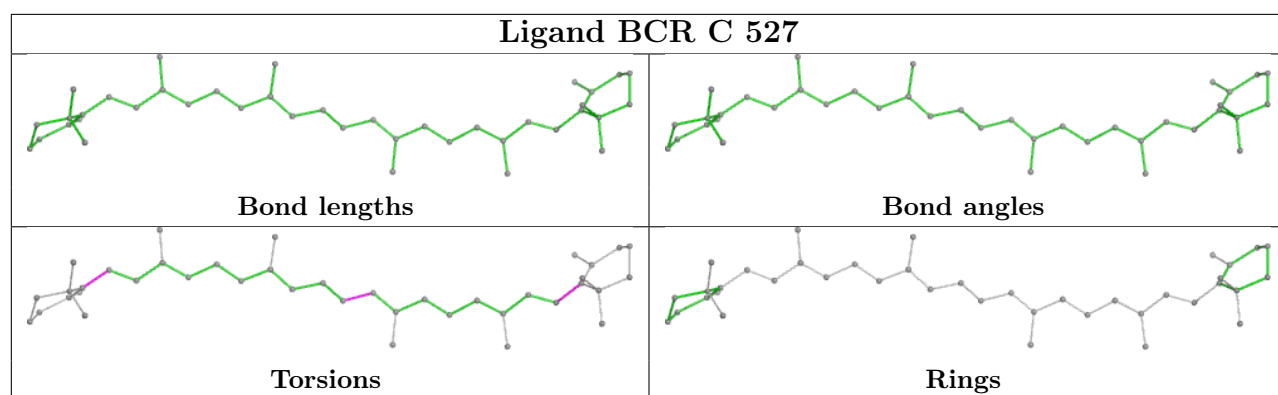
Ligand CLA a 405**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 603****Bond lengths****Bond angles****Torsions****Rings**

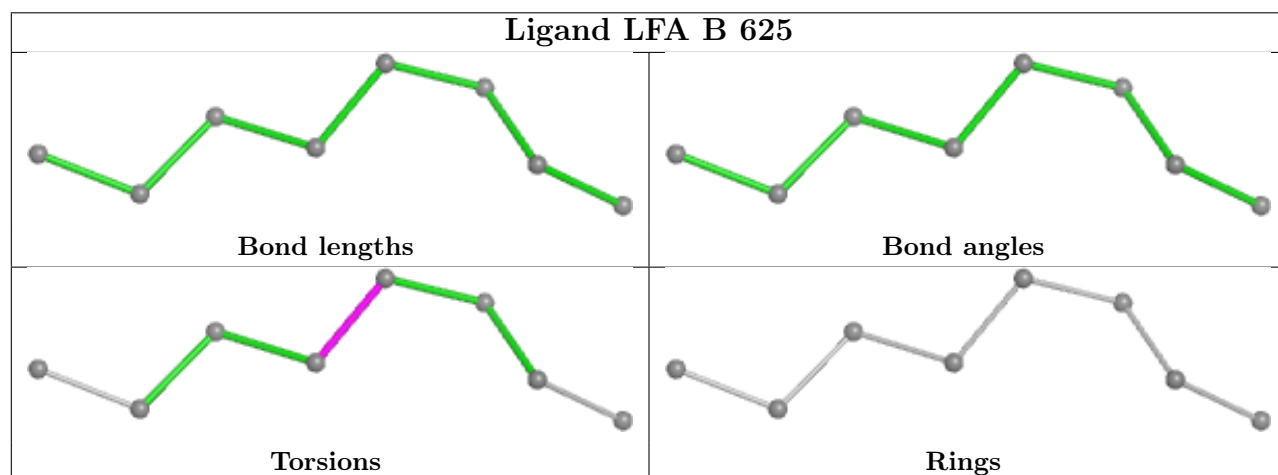
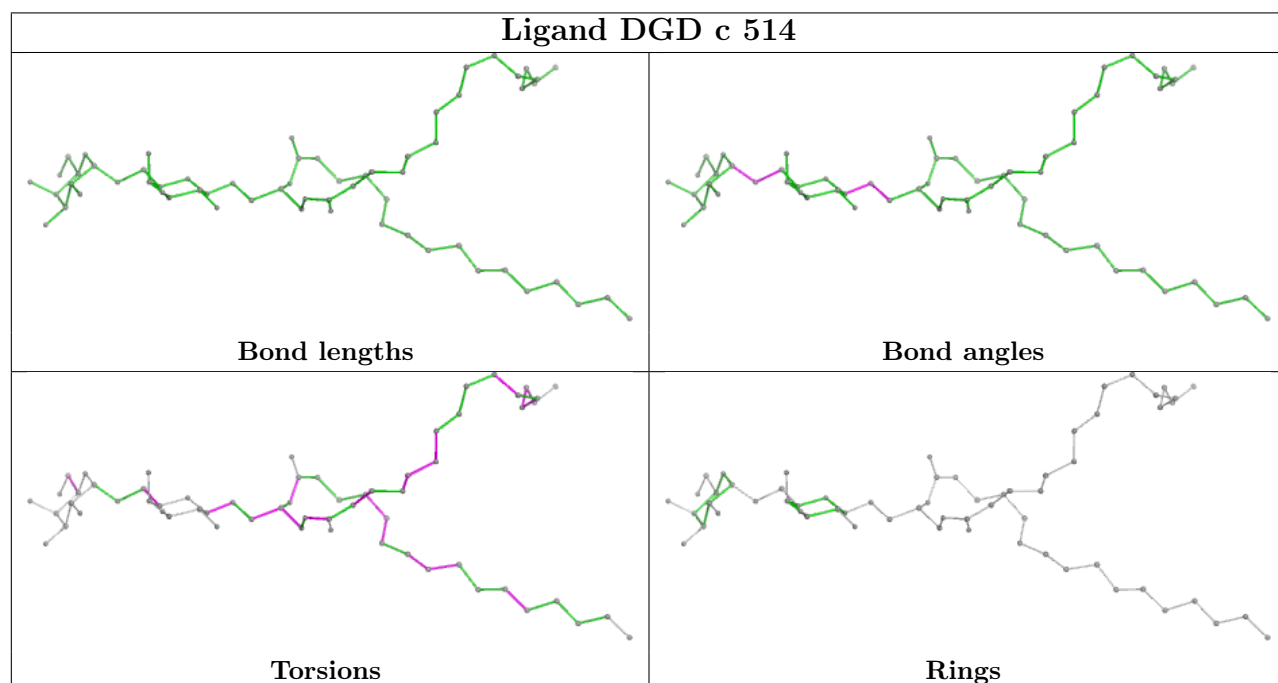
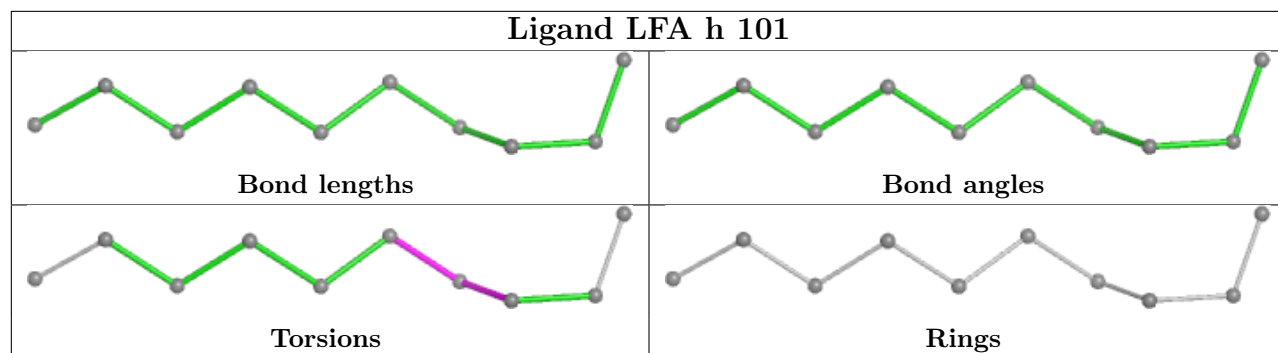


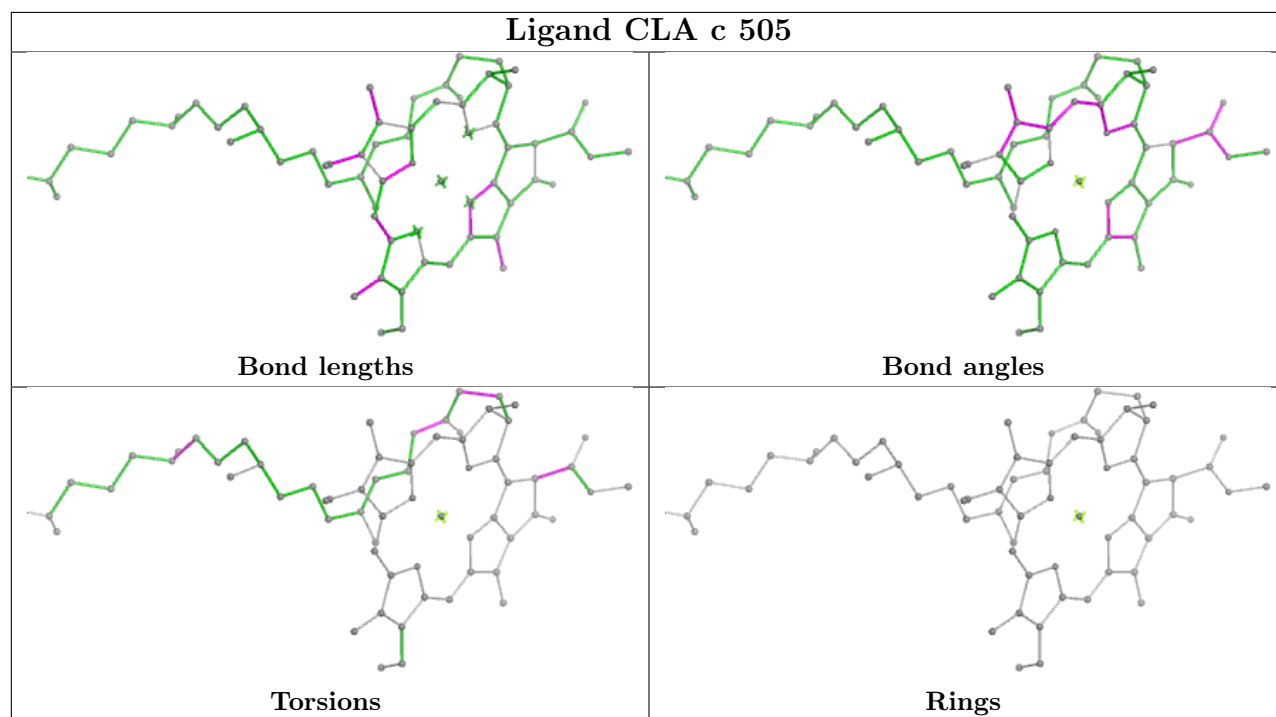
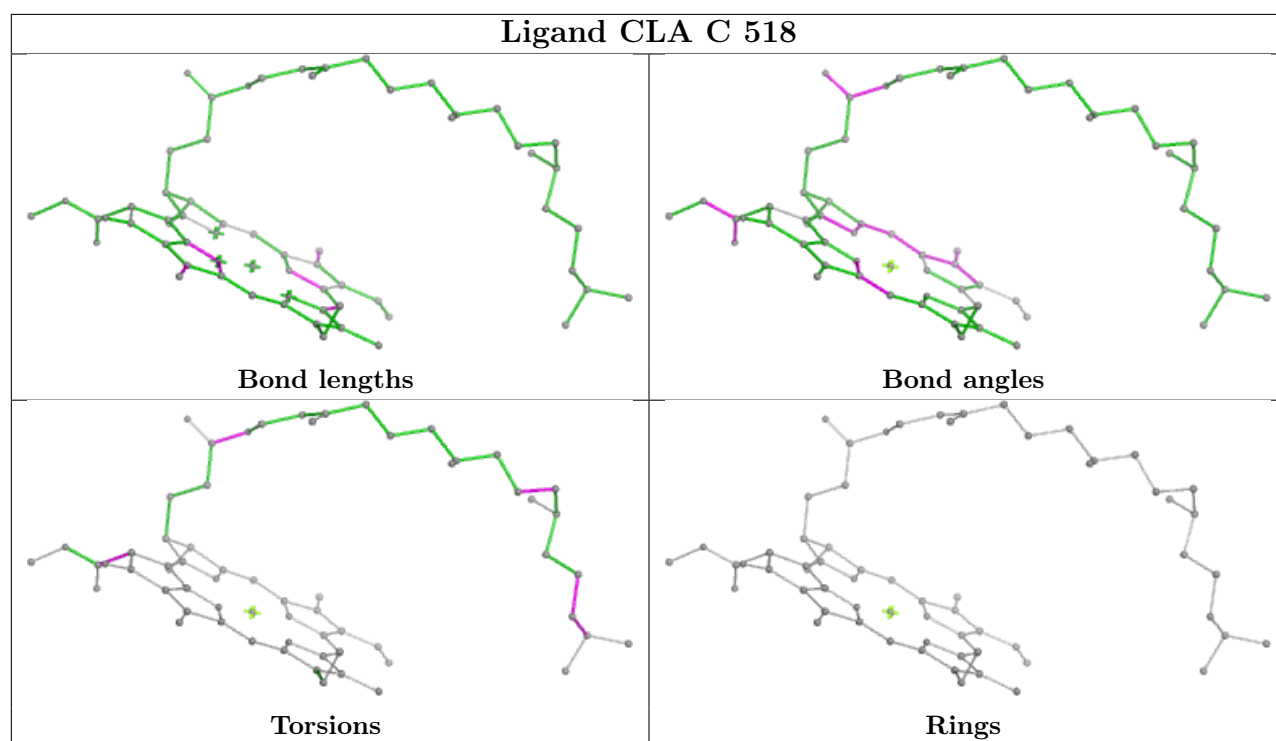


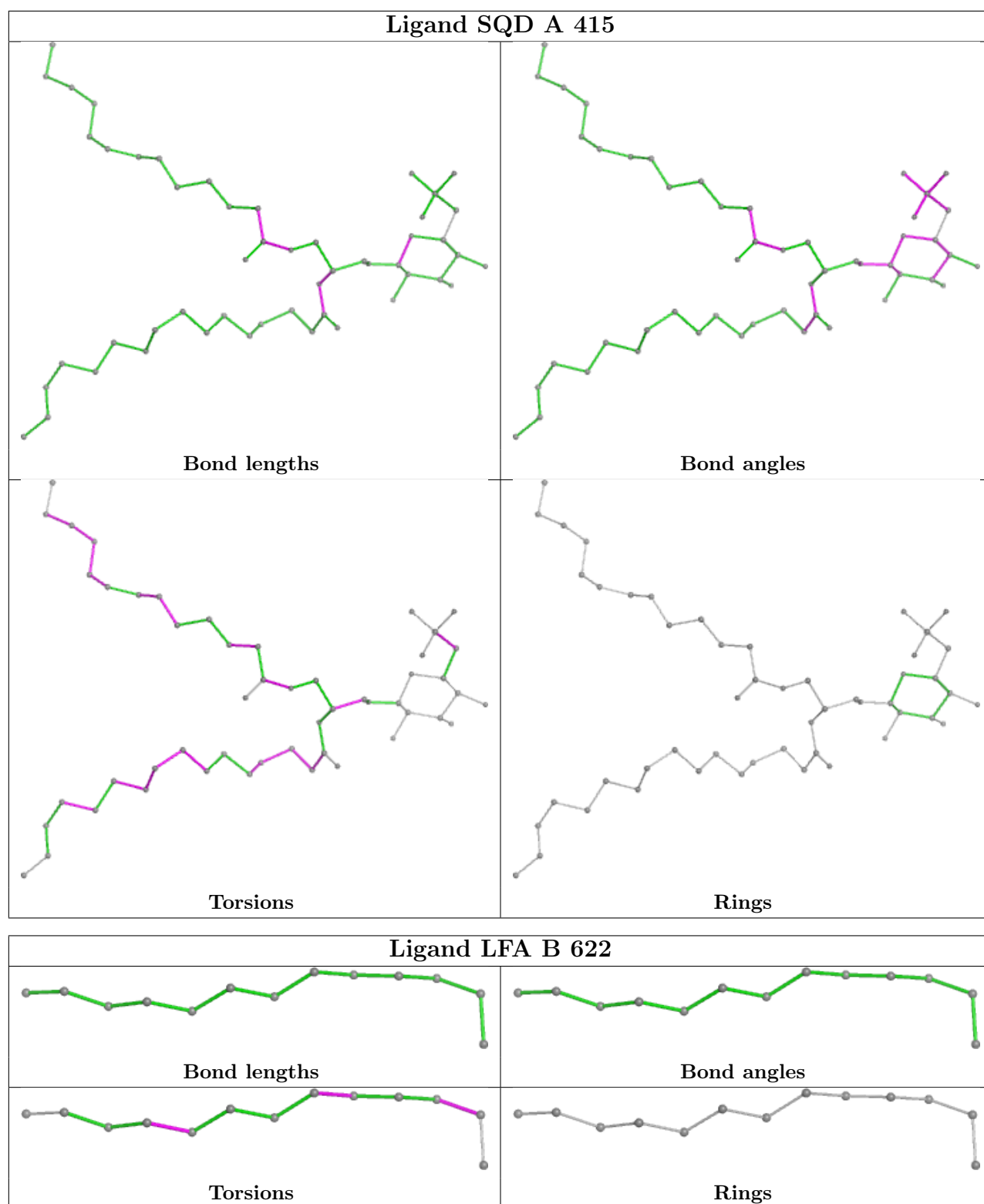


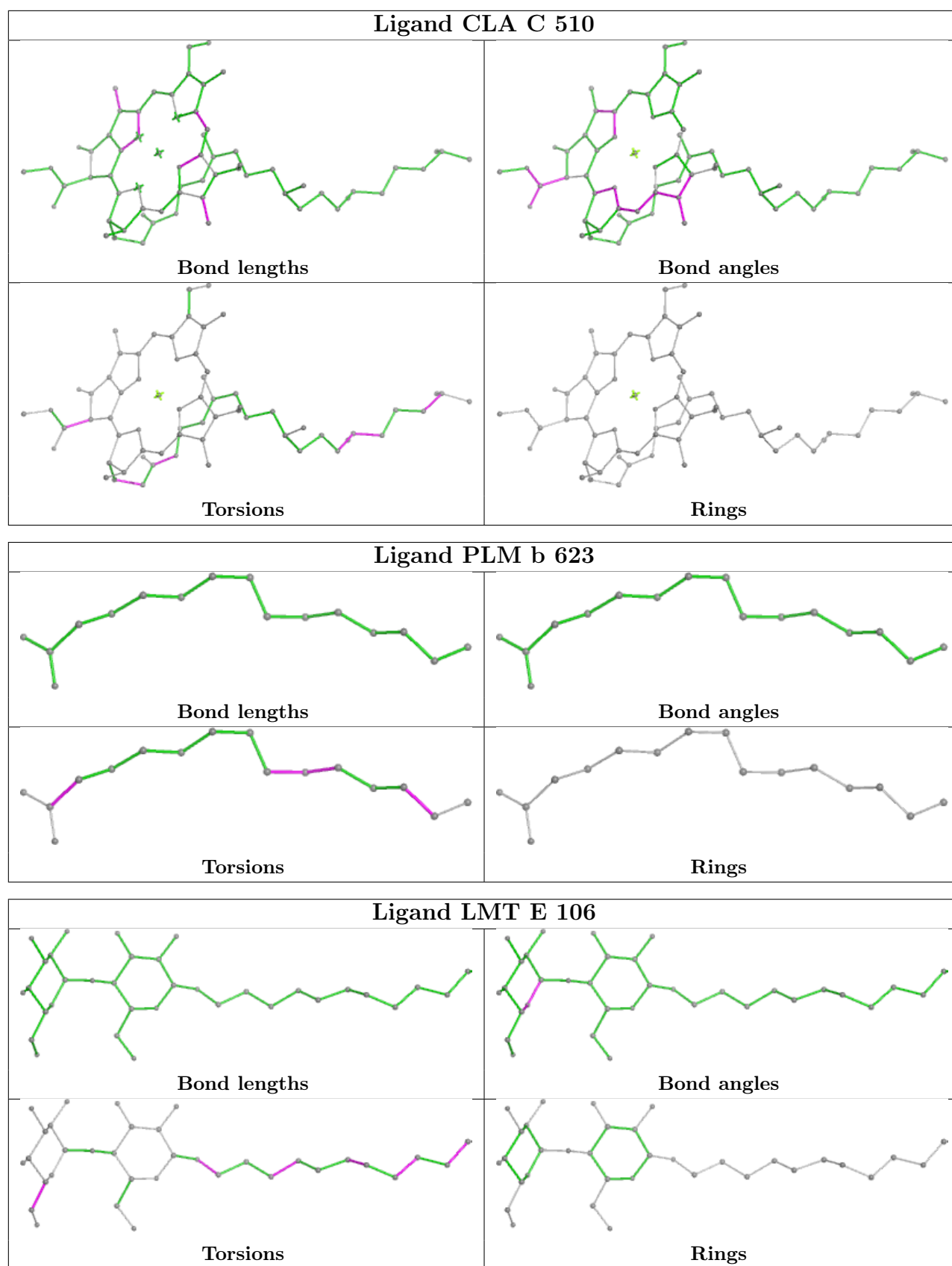


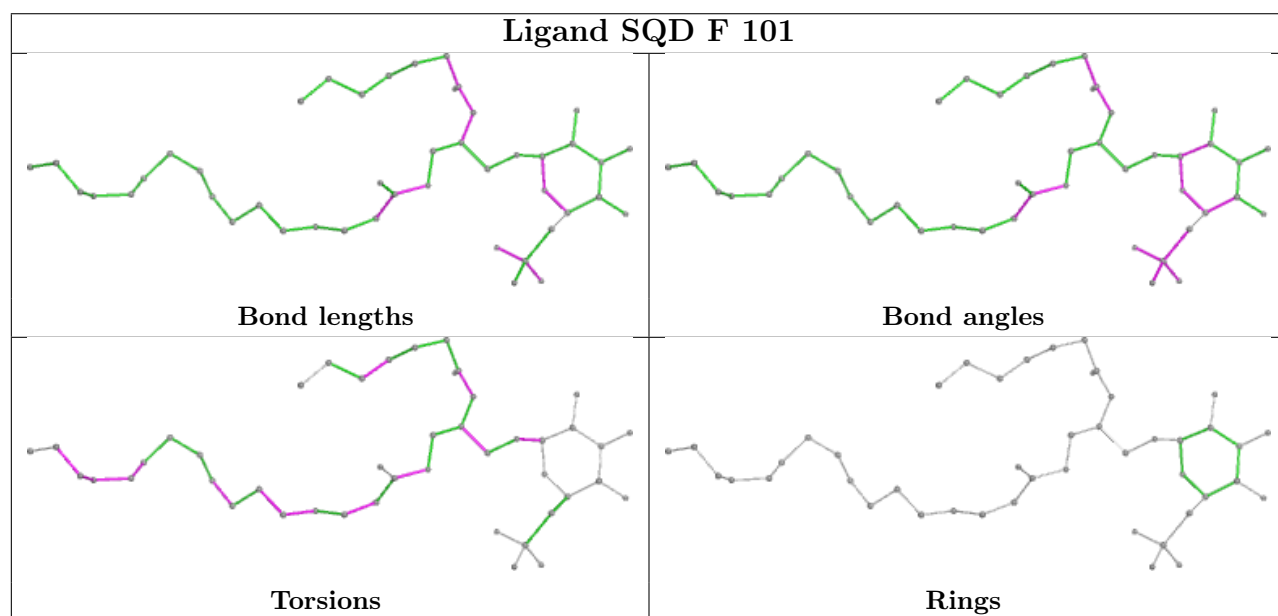
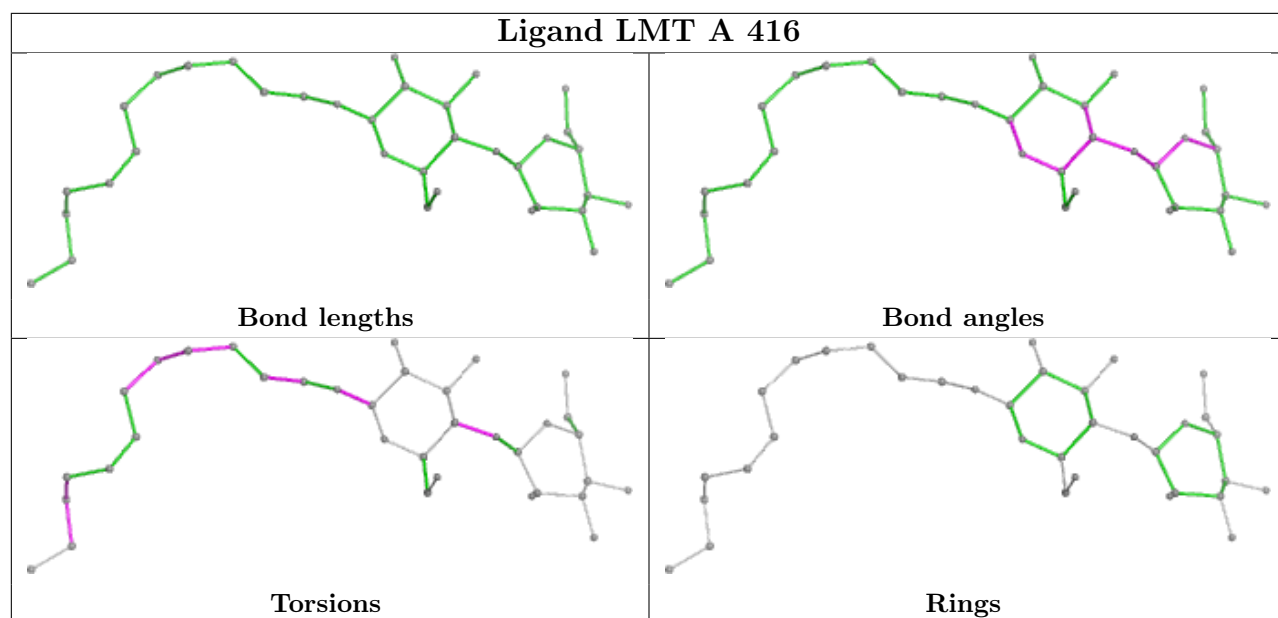
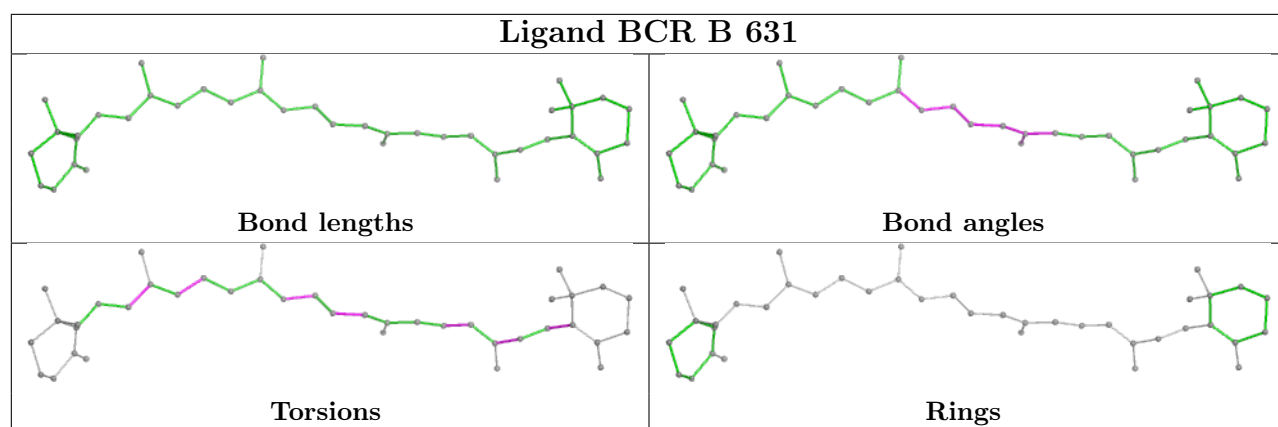


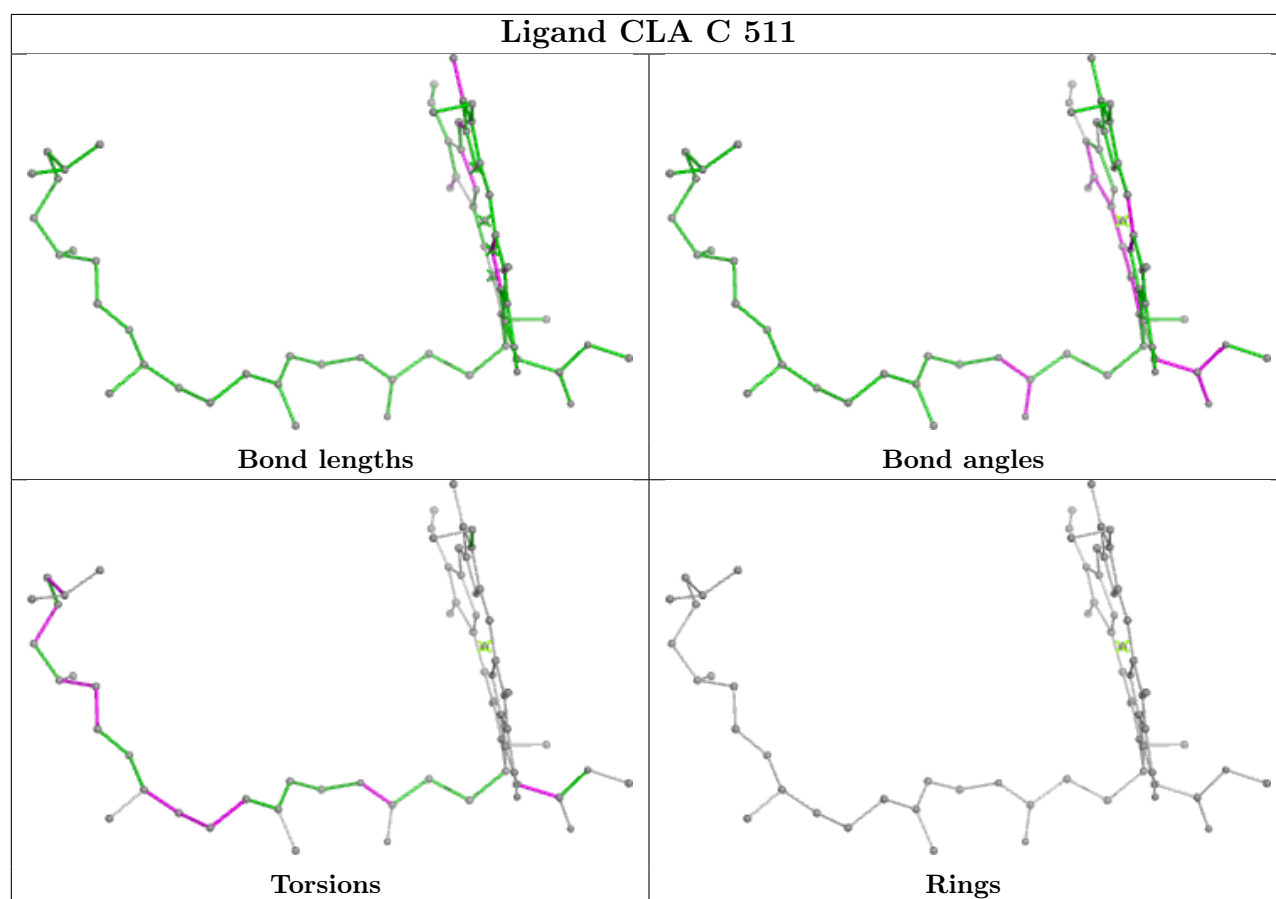
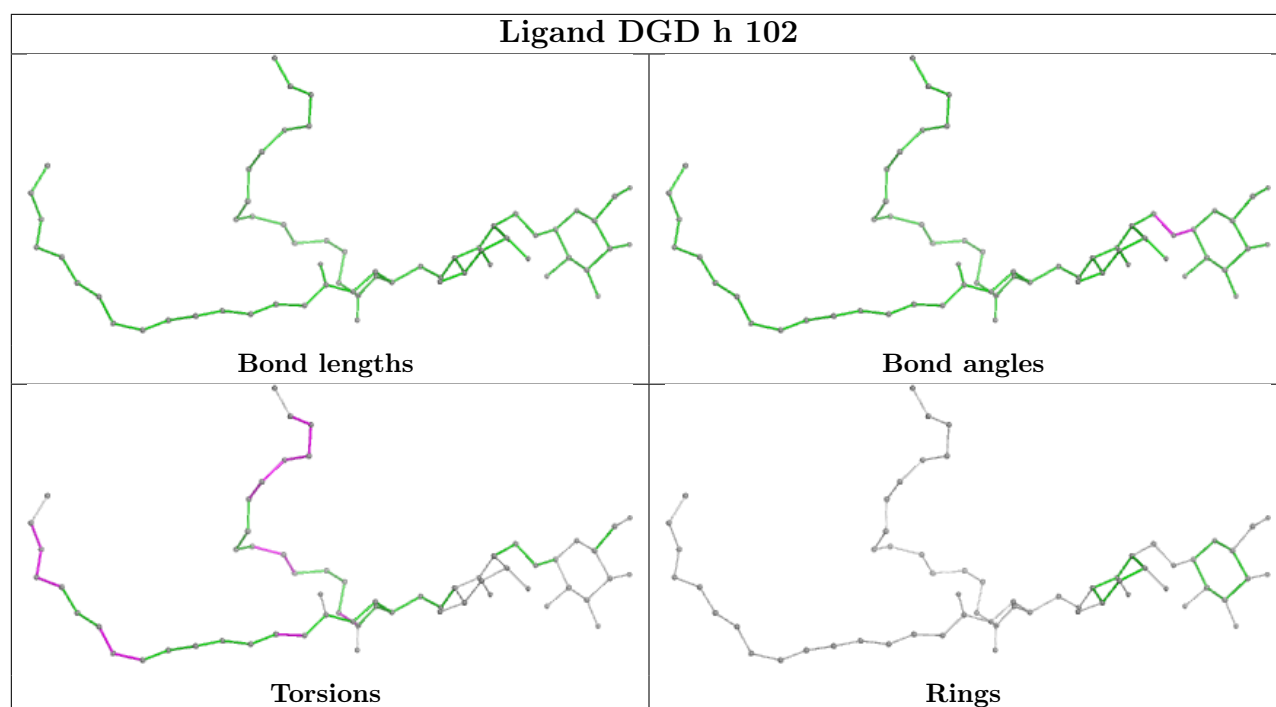


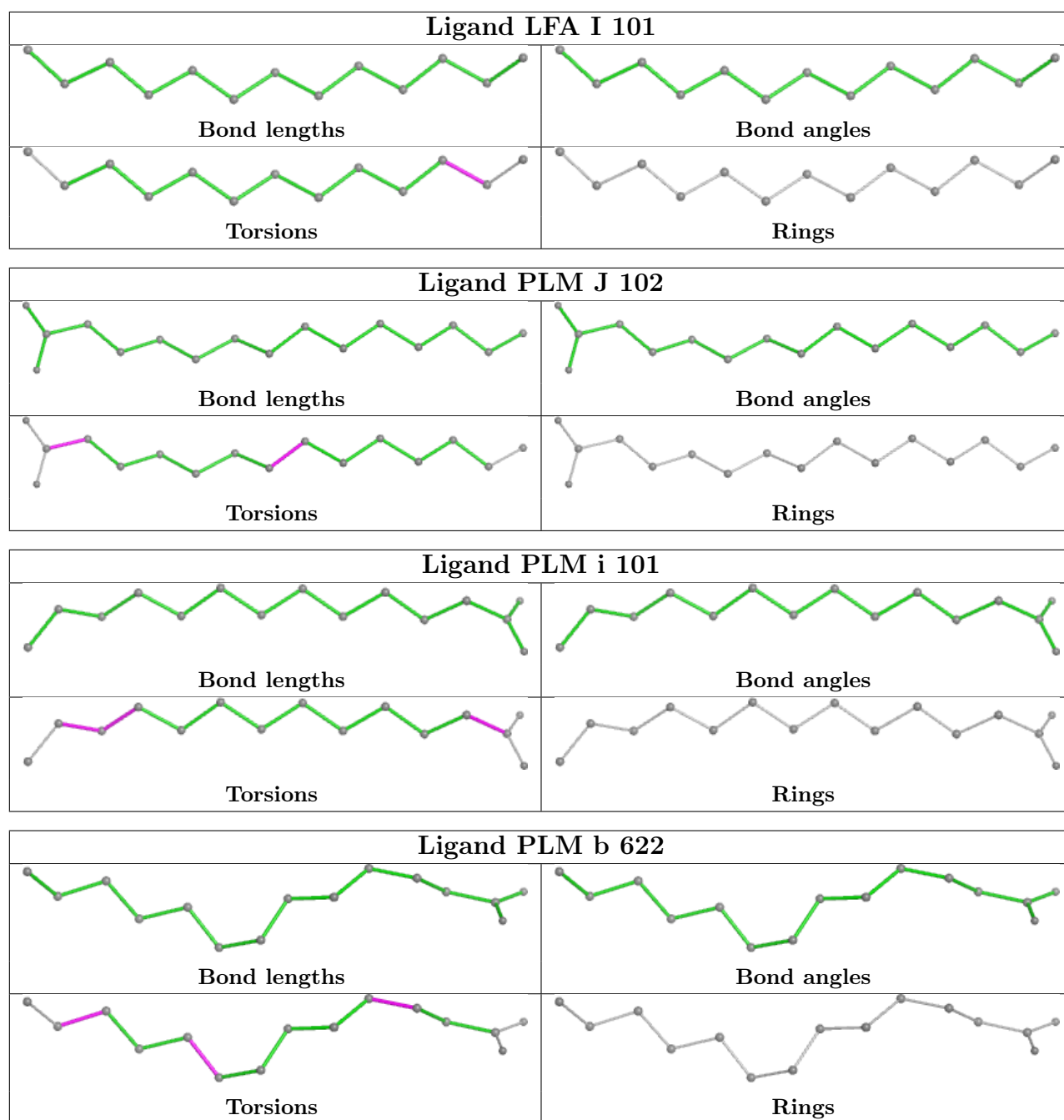


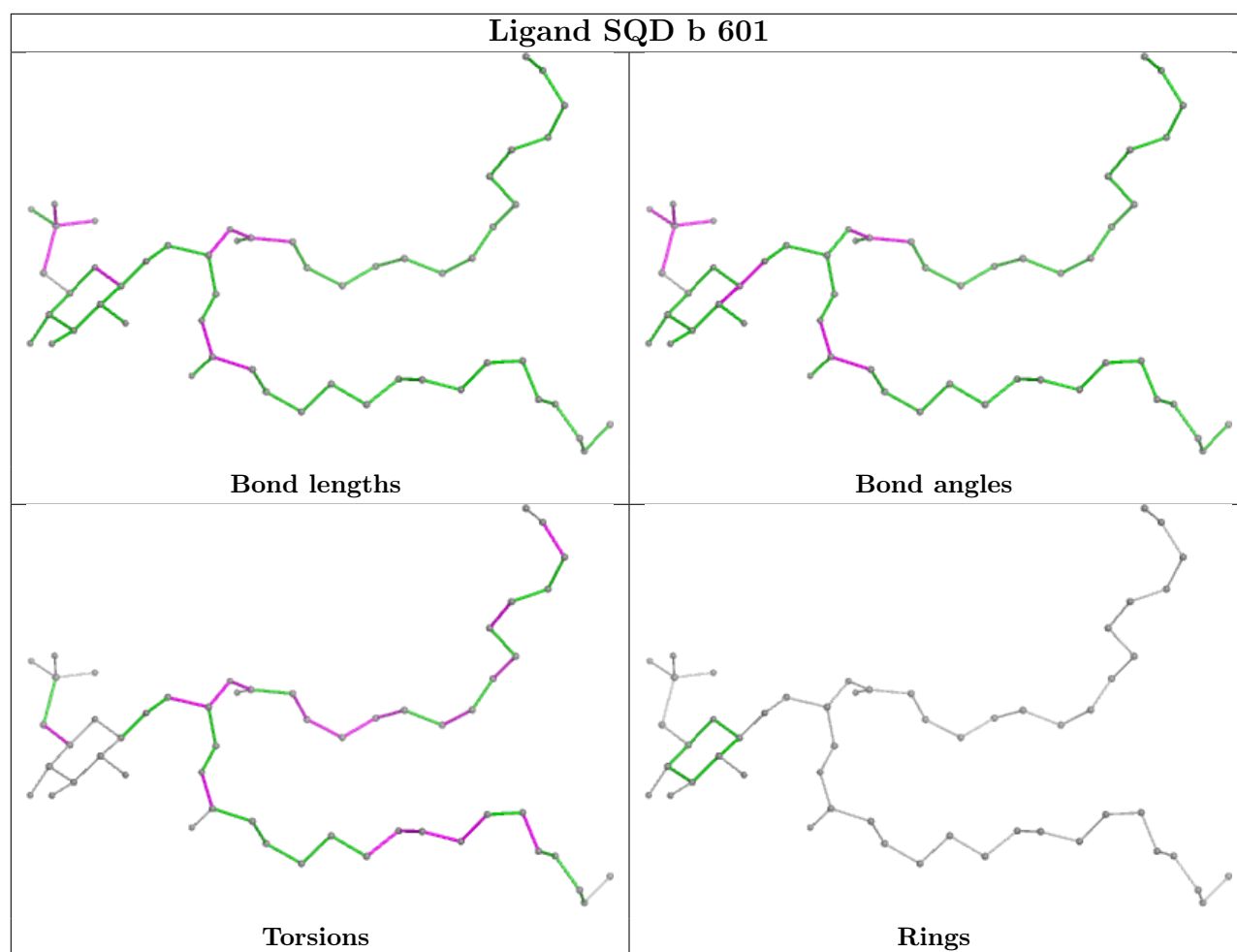


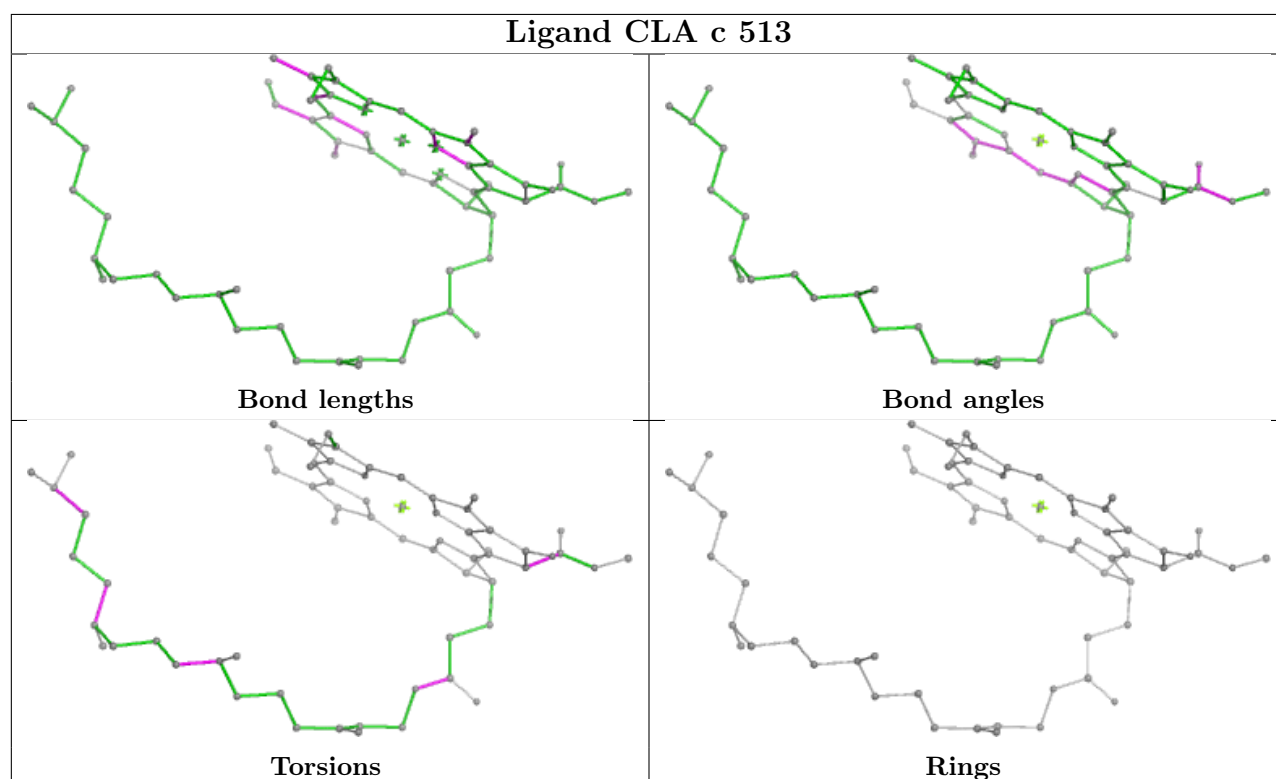
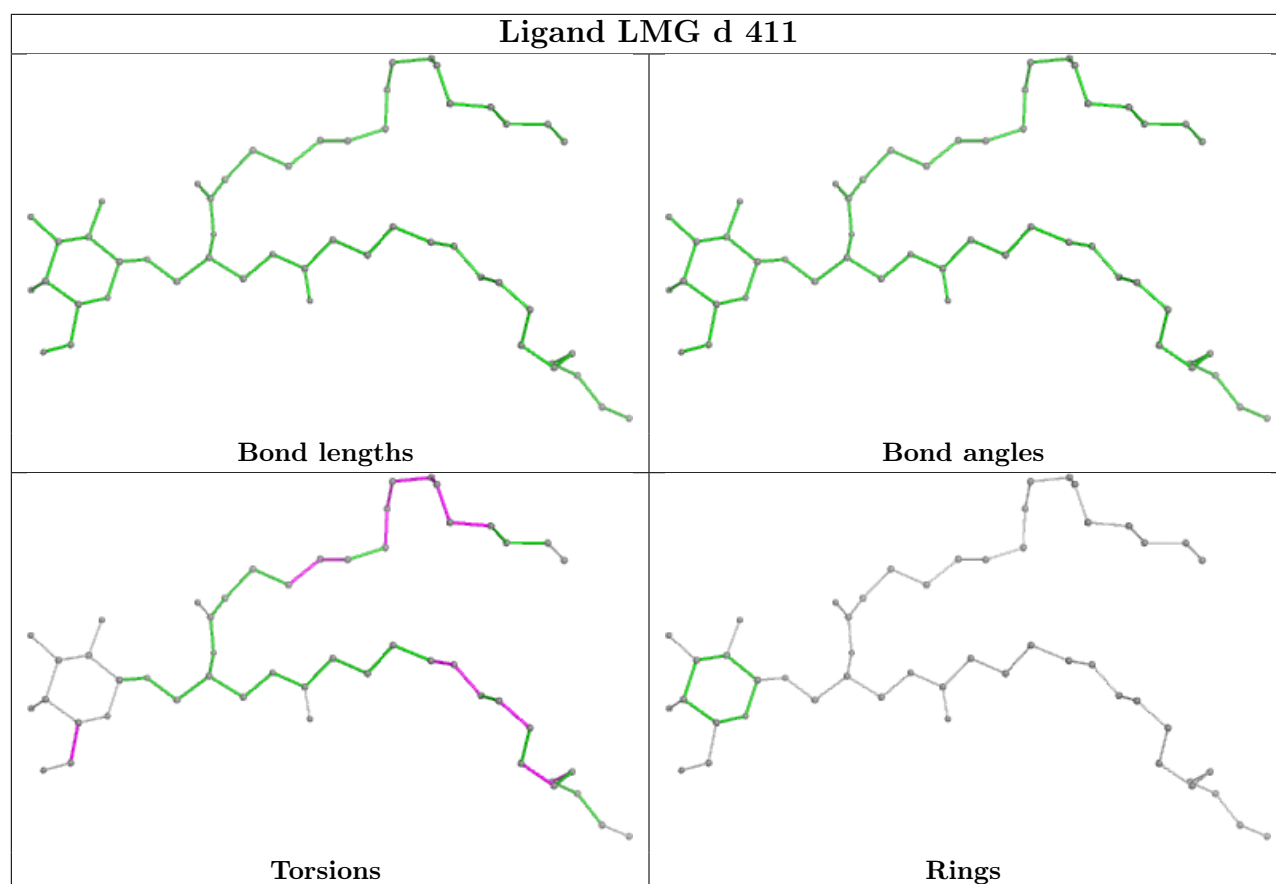


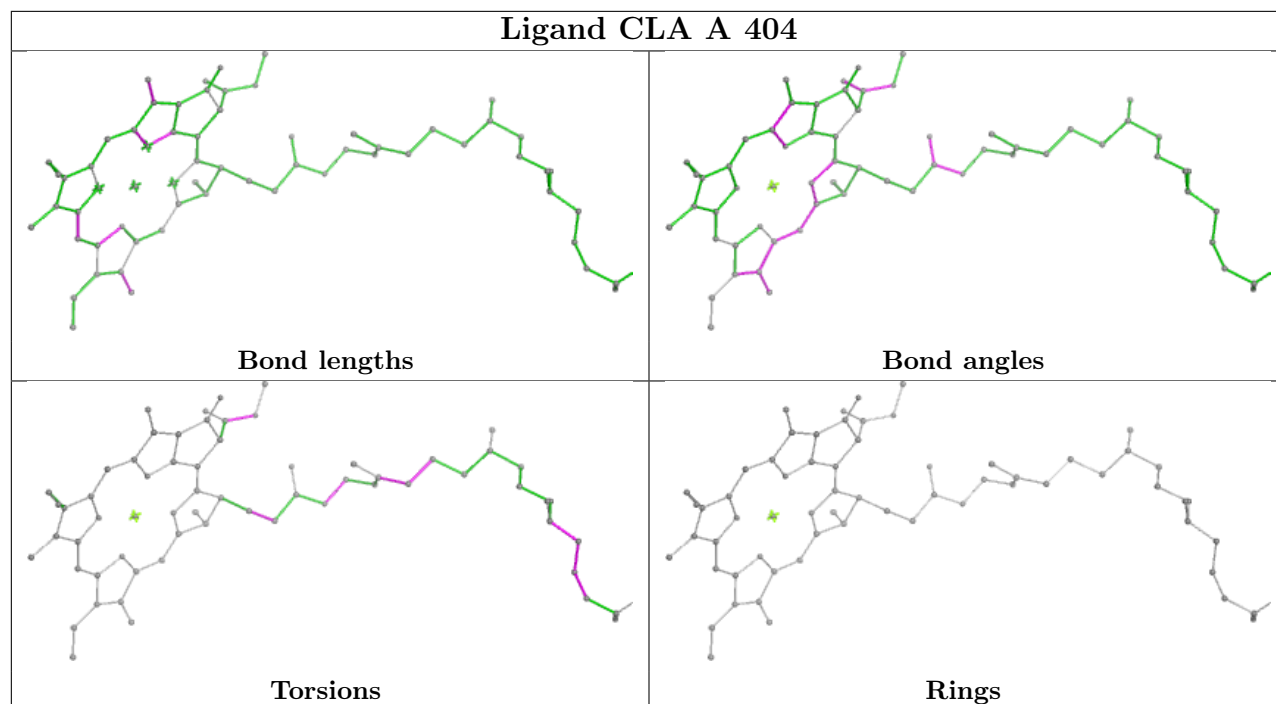
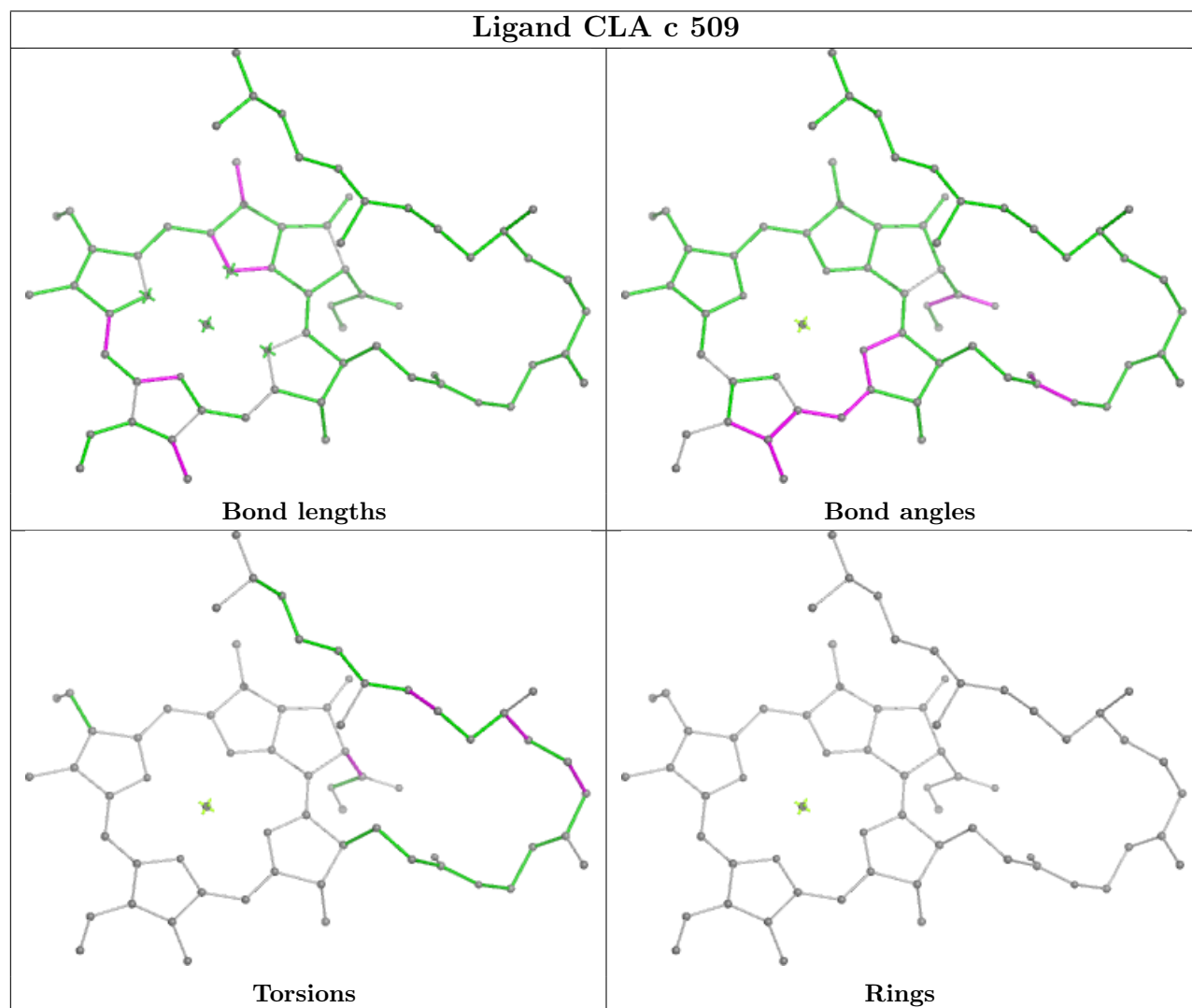




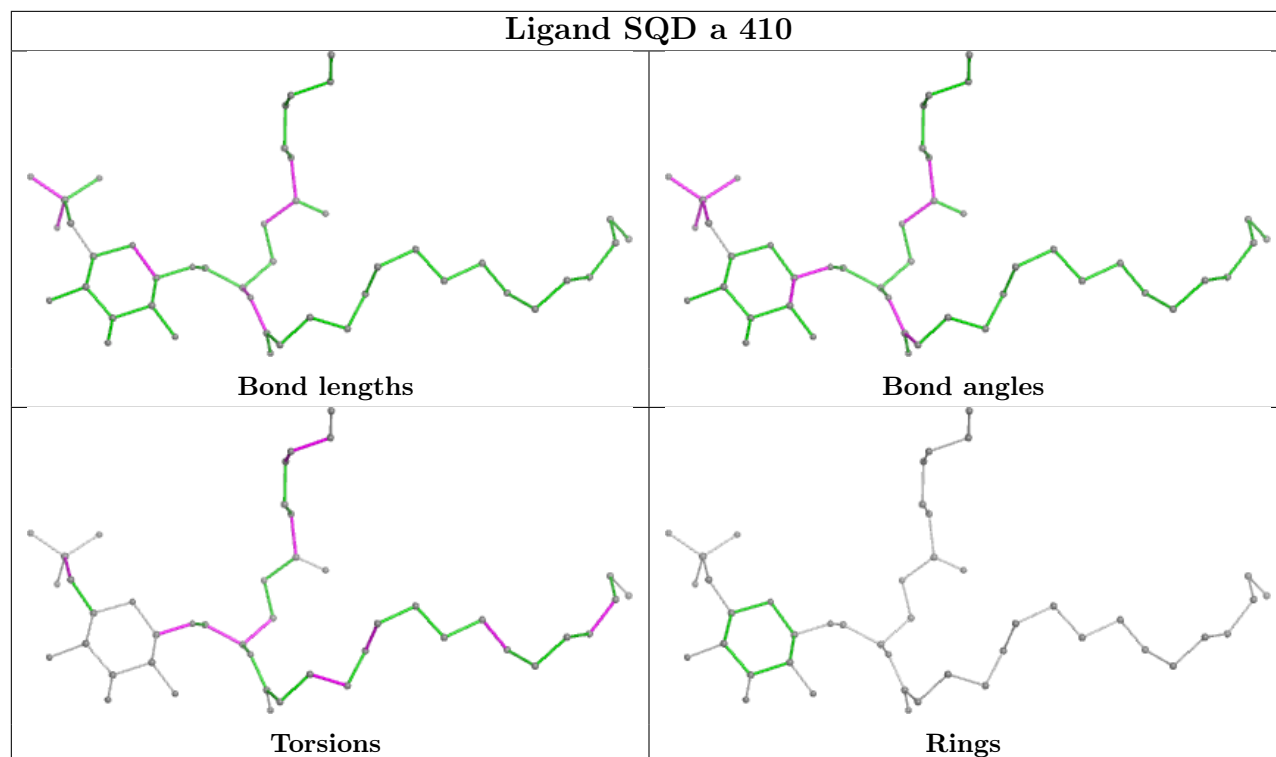




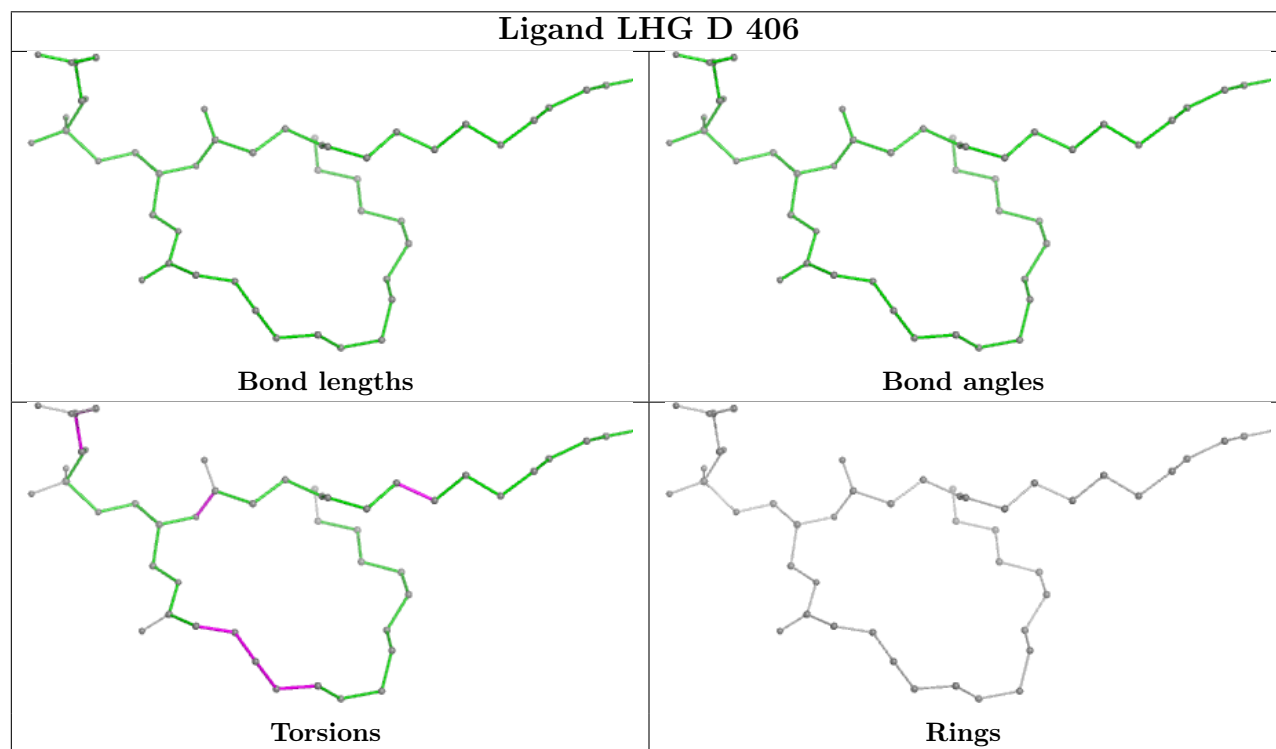


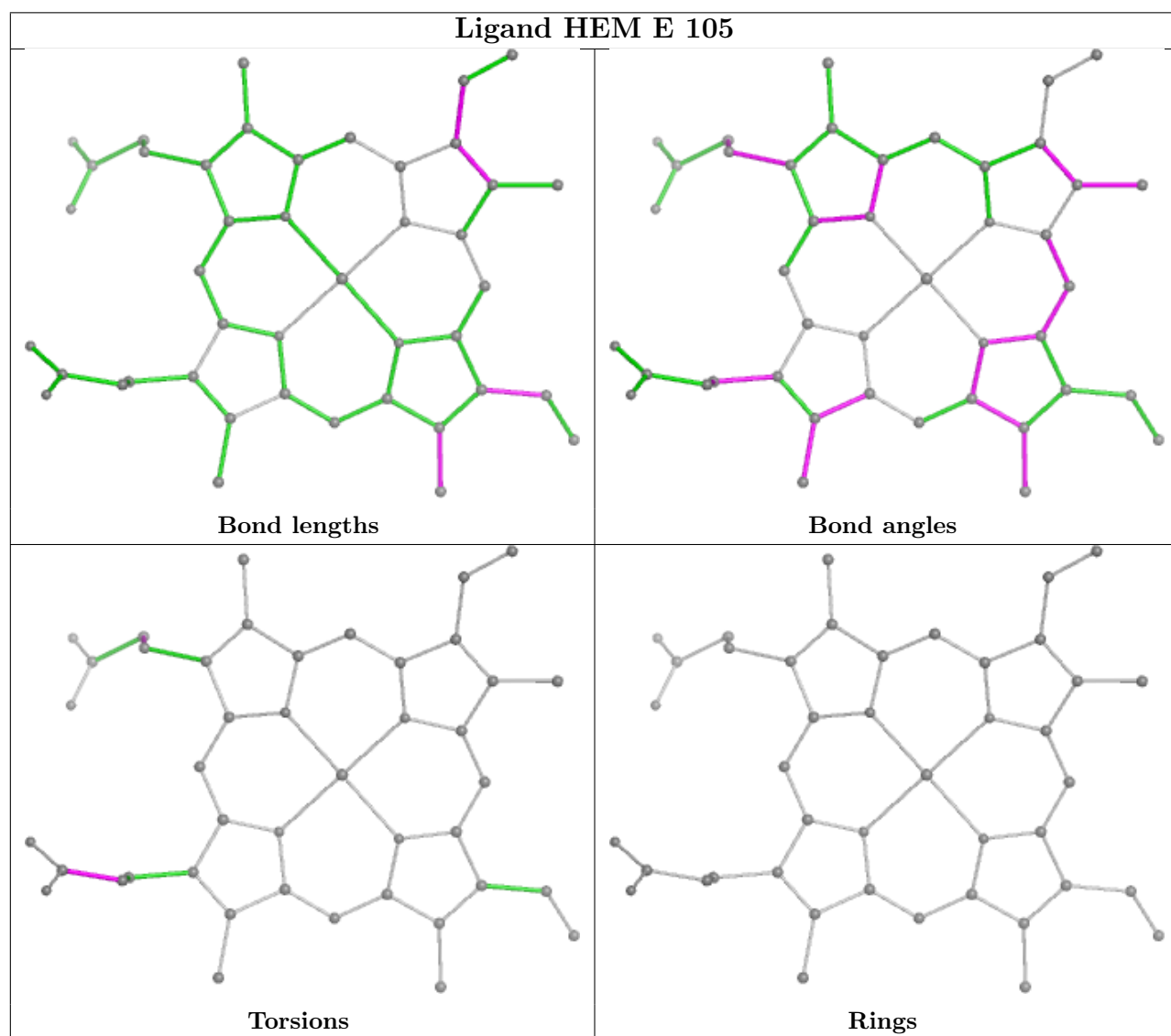
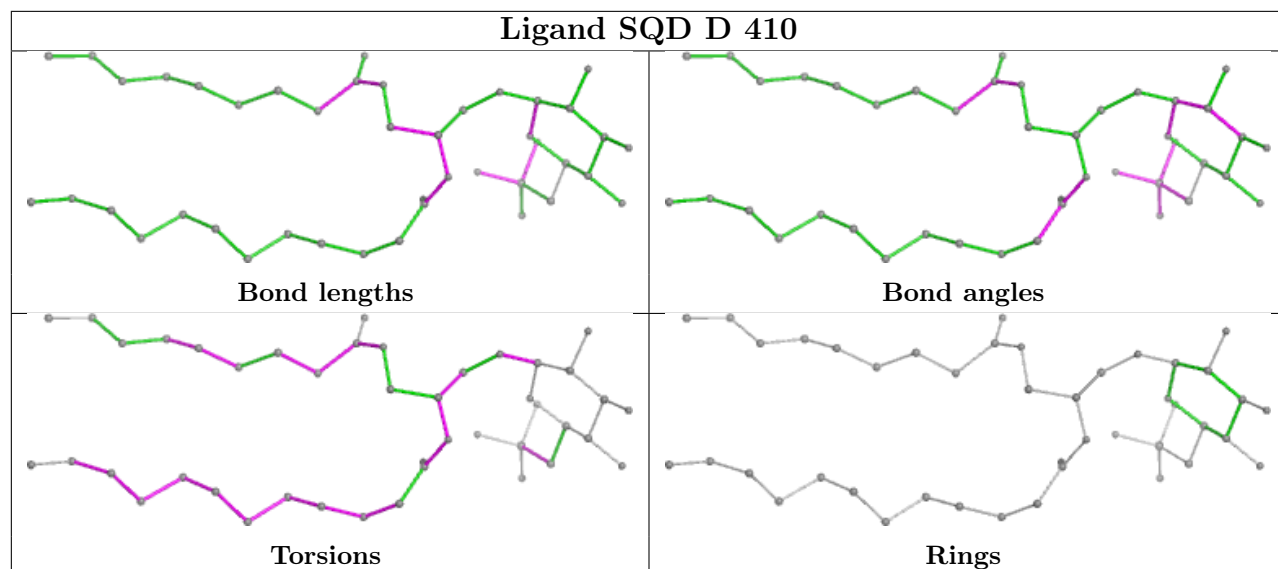
Ligand CLA A 404**Ligand CLA c 509**

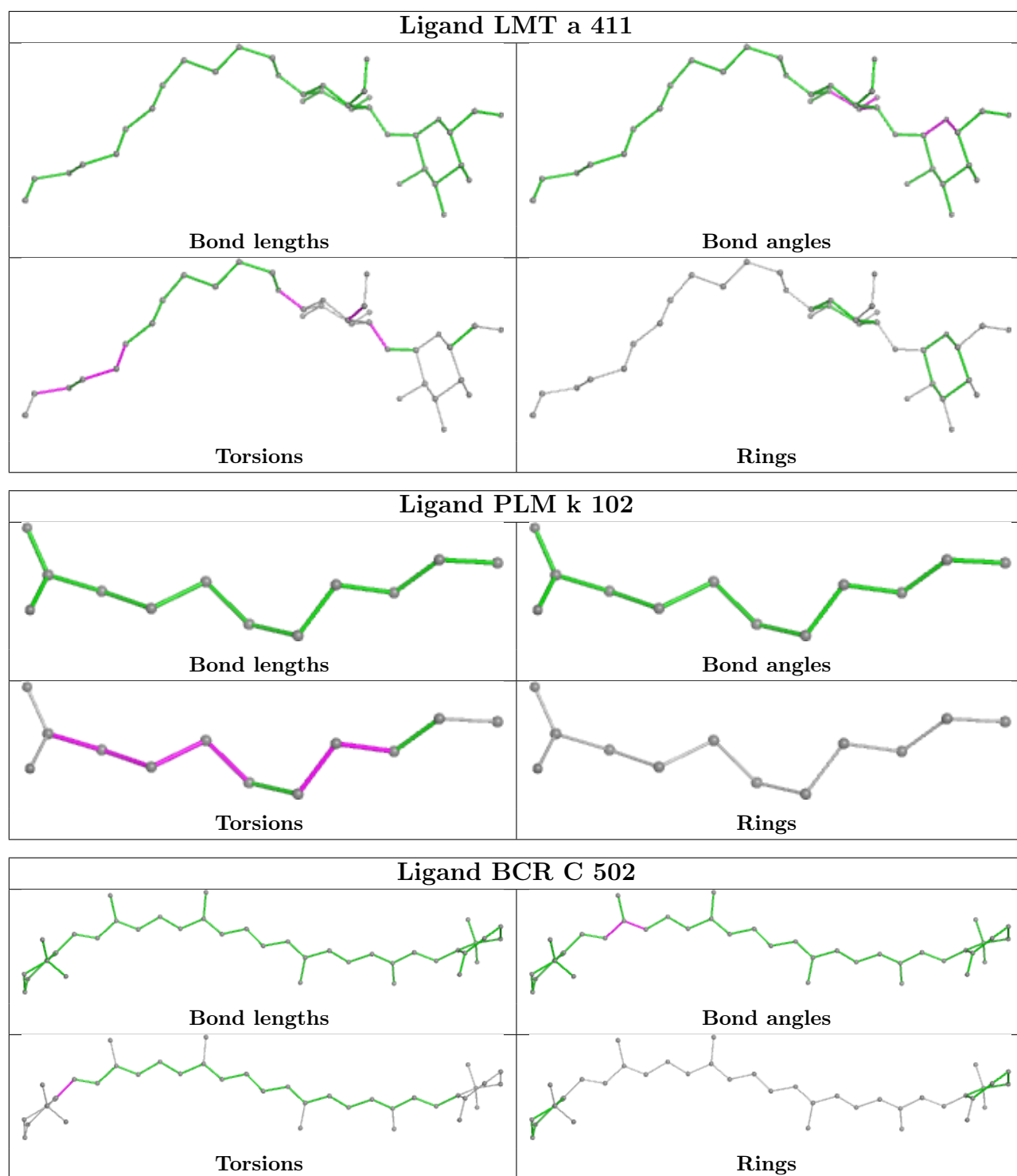
Ligand SQD a 410

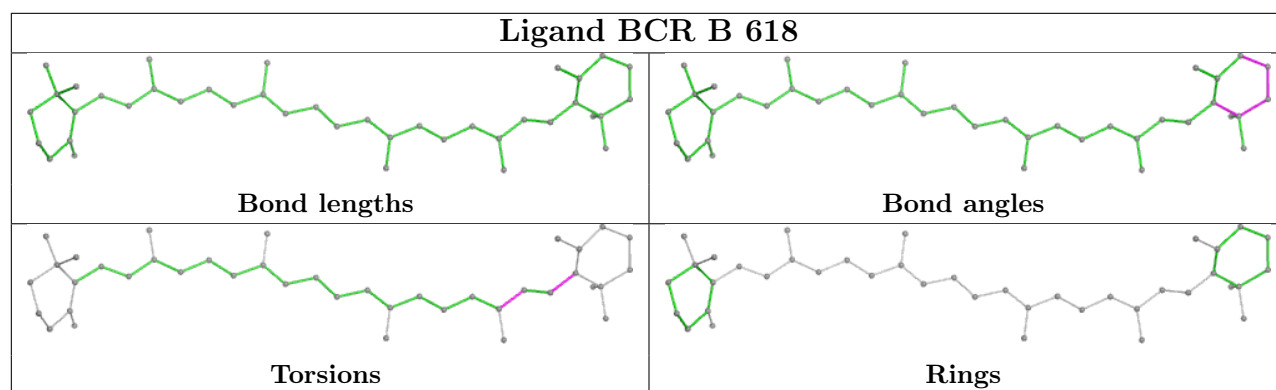
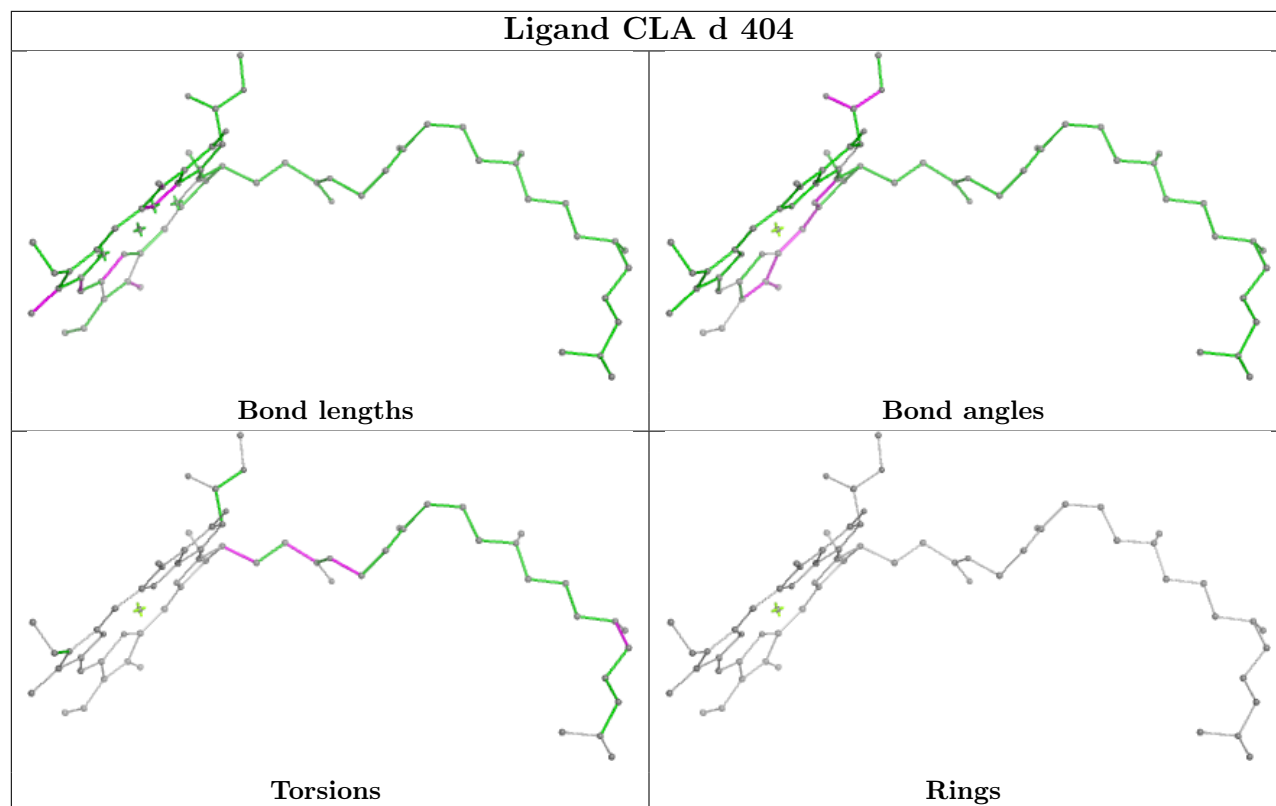


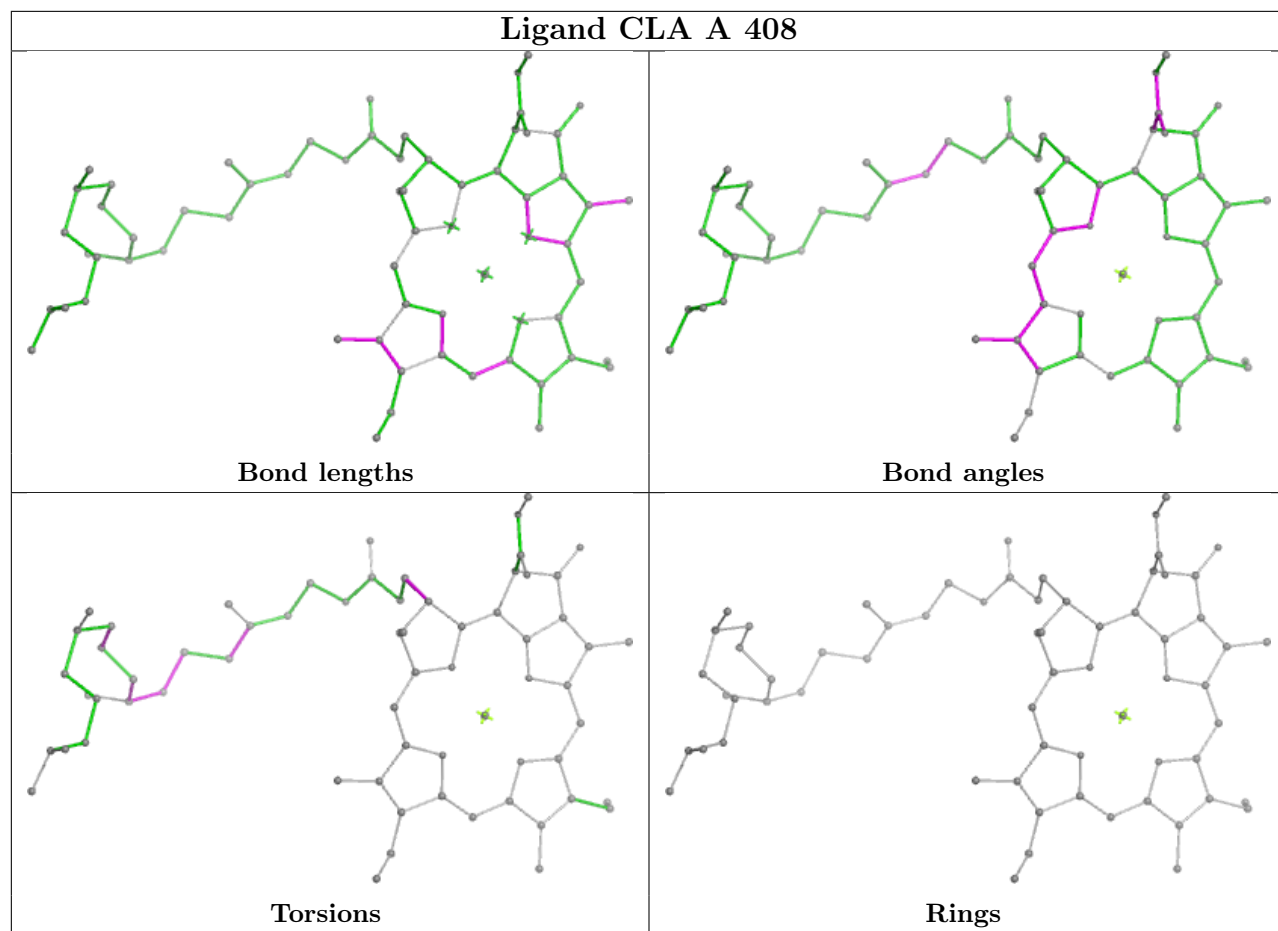
Ligand LHG D 406



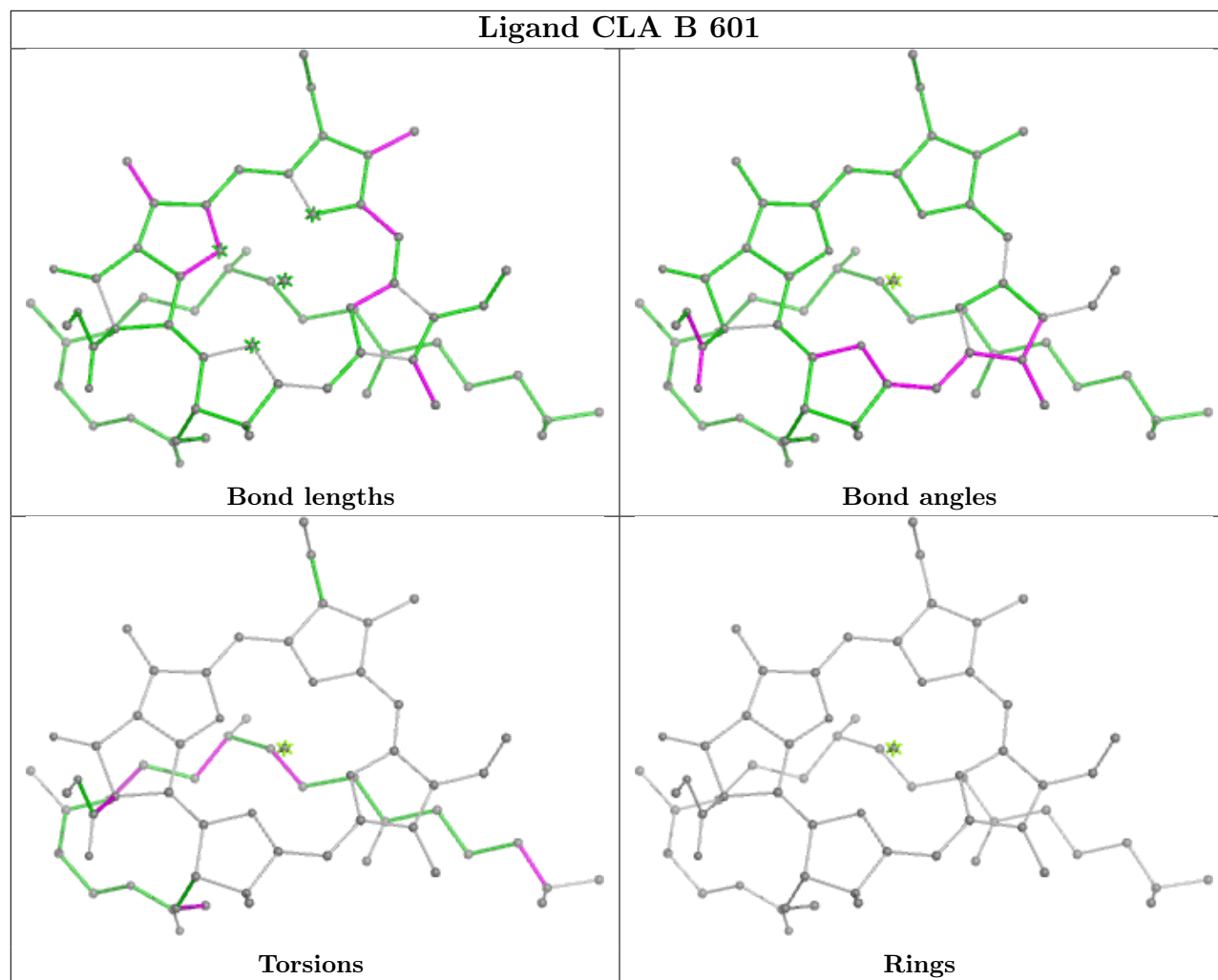


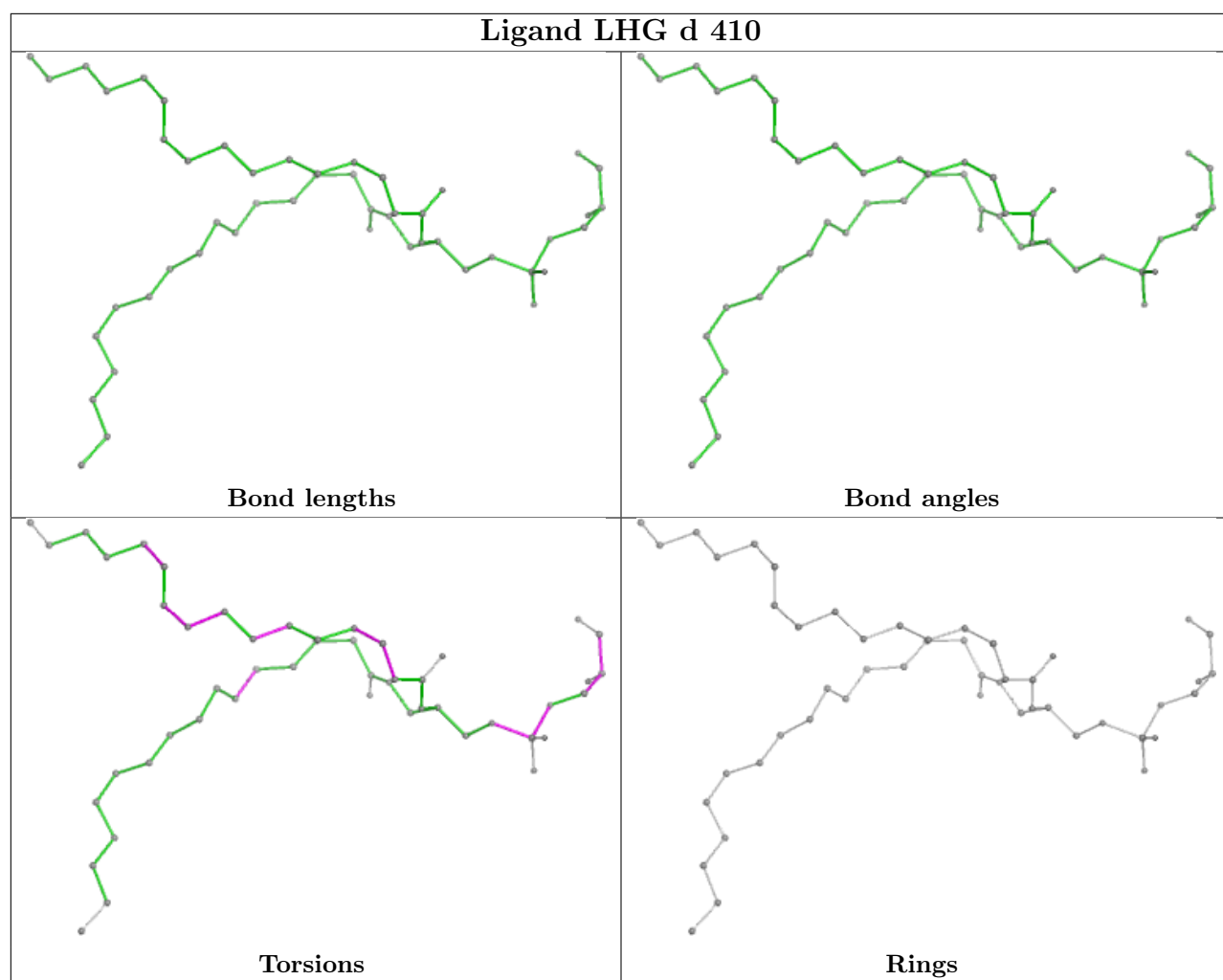


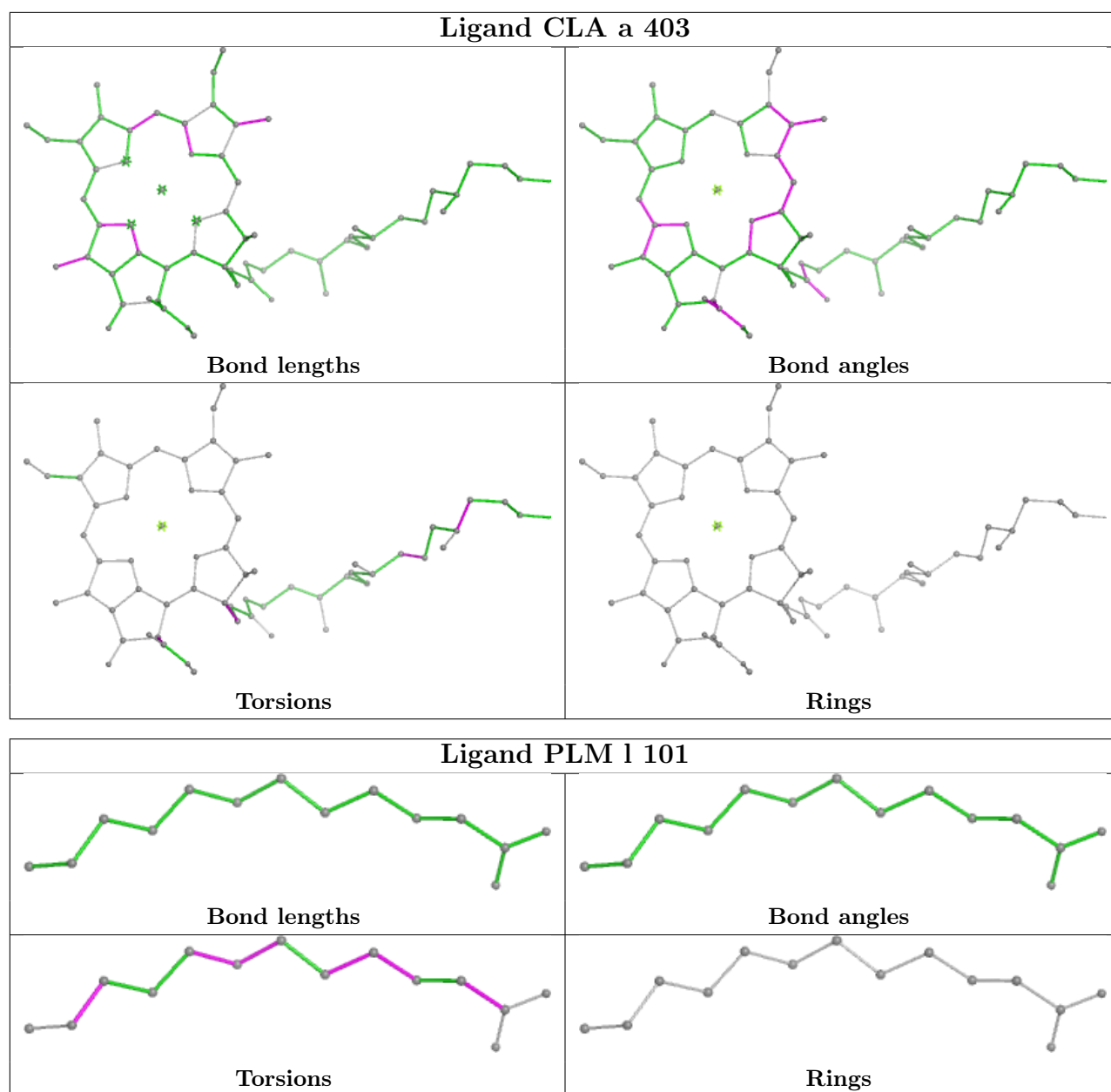


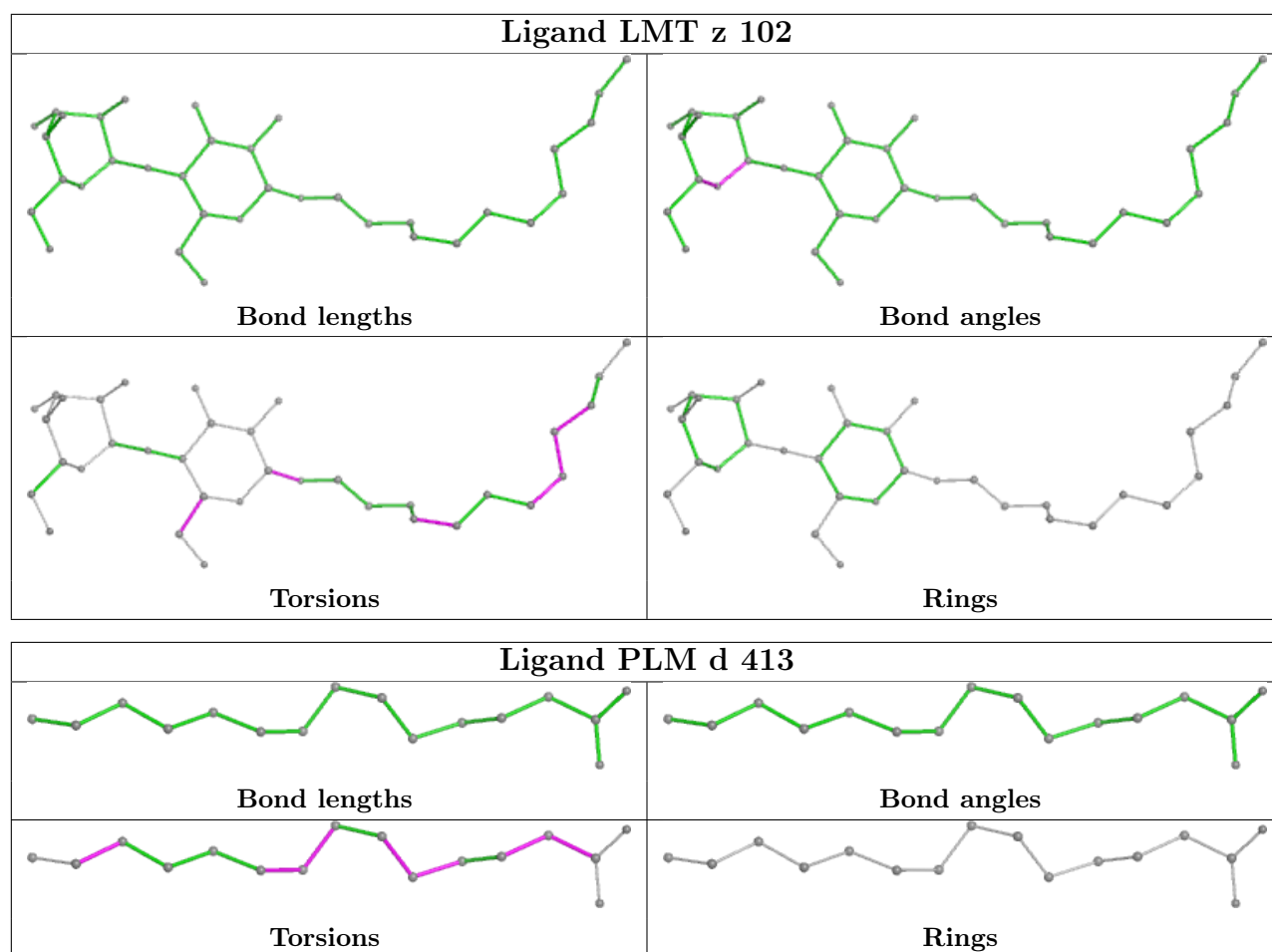


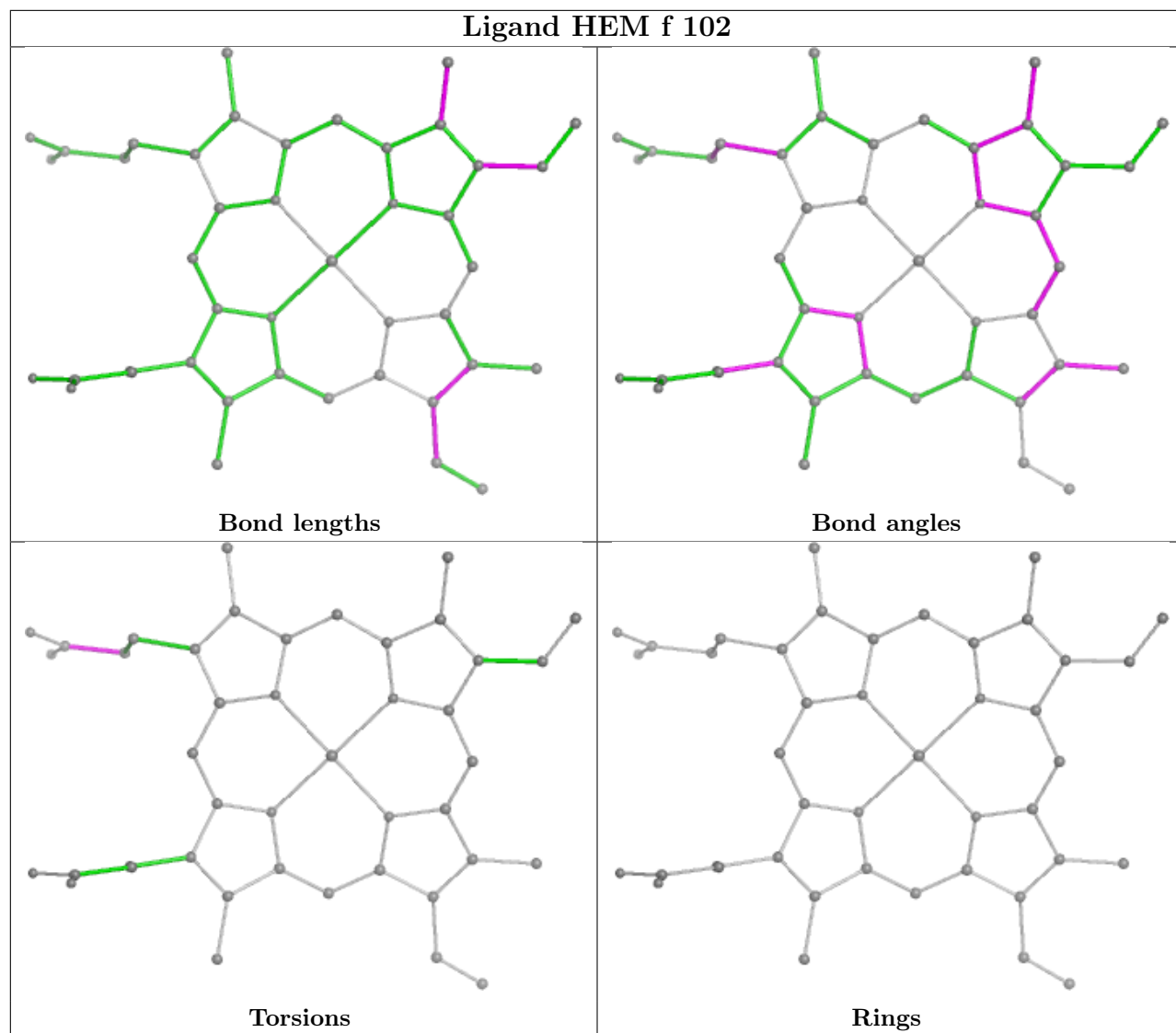
Ligand CLA B 601

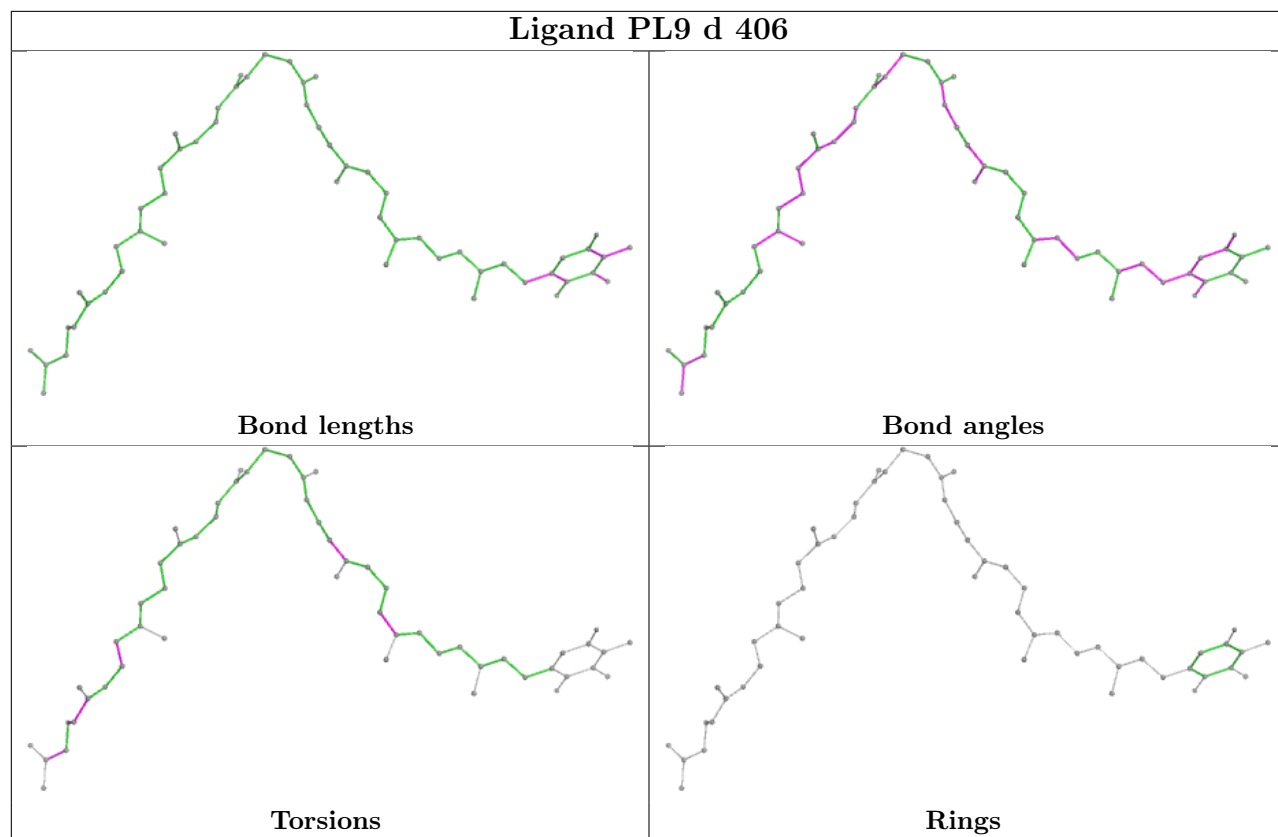


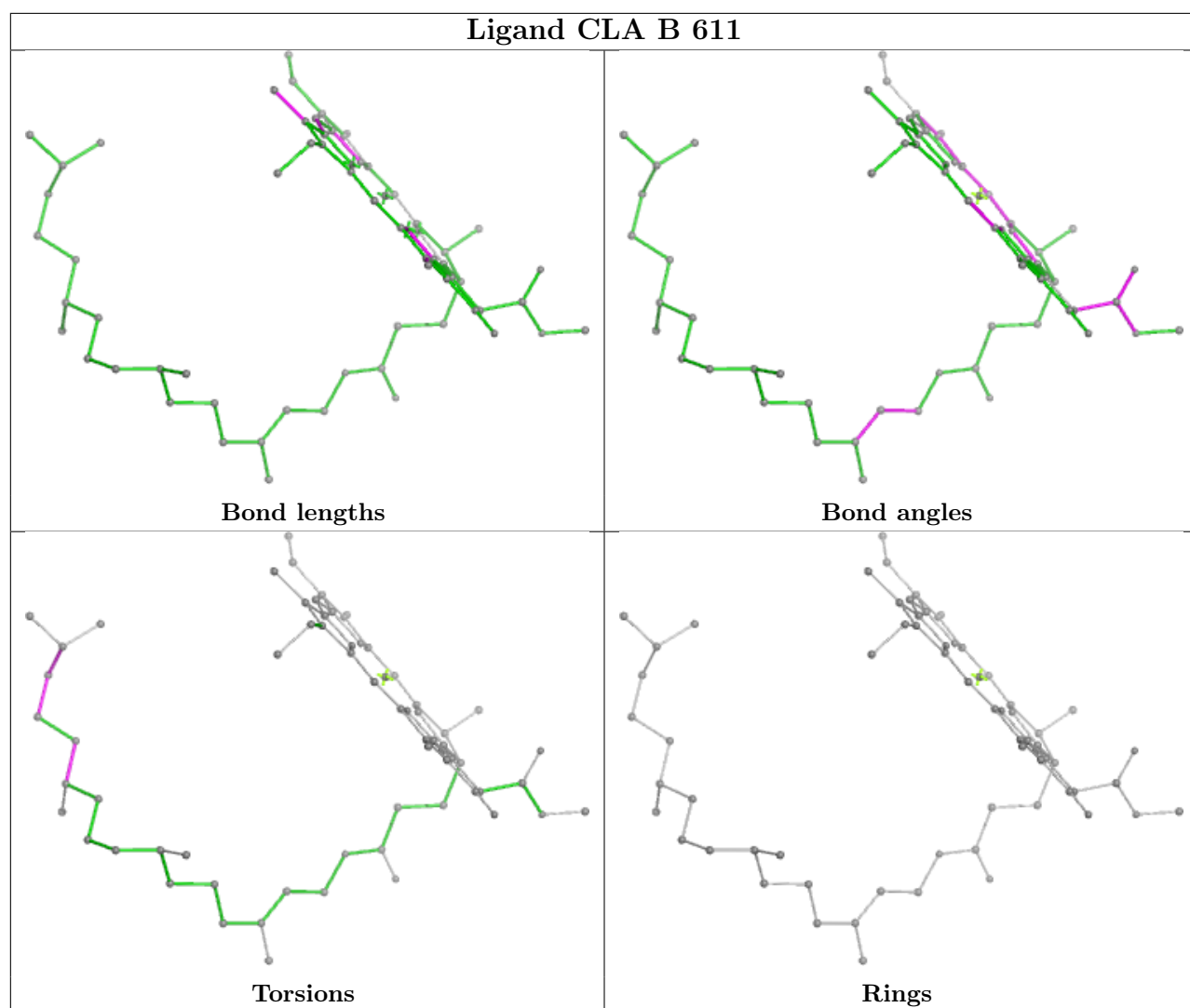




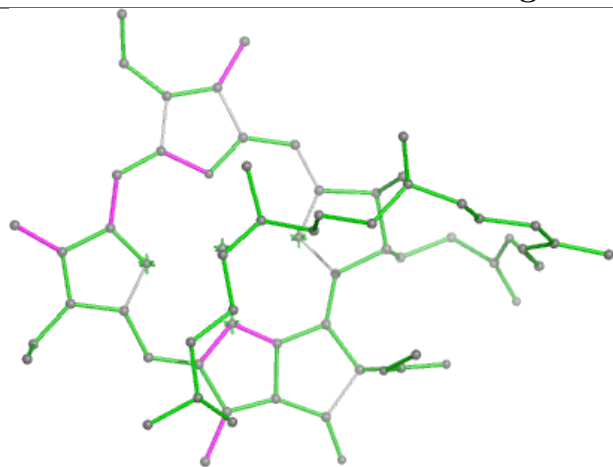




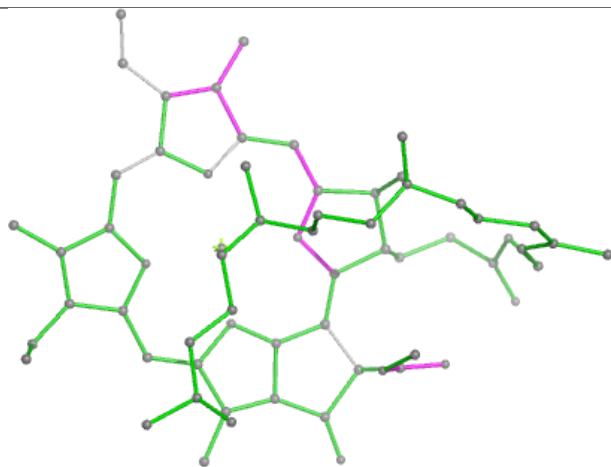




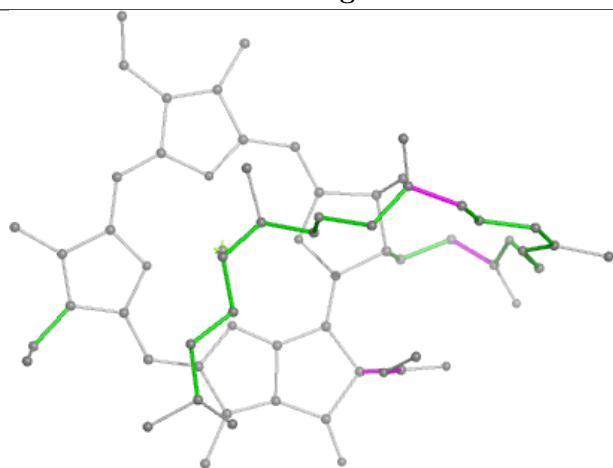
Ligand CLA c 510



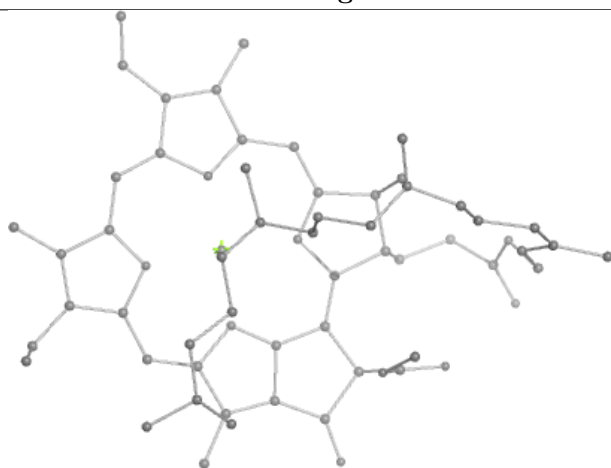
Bond lengths



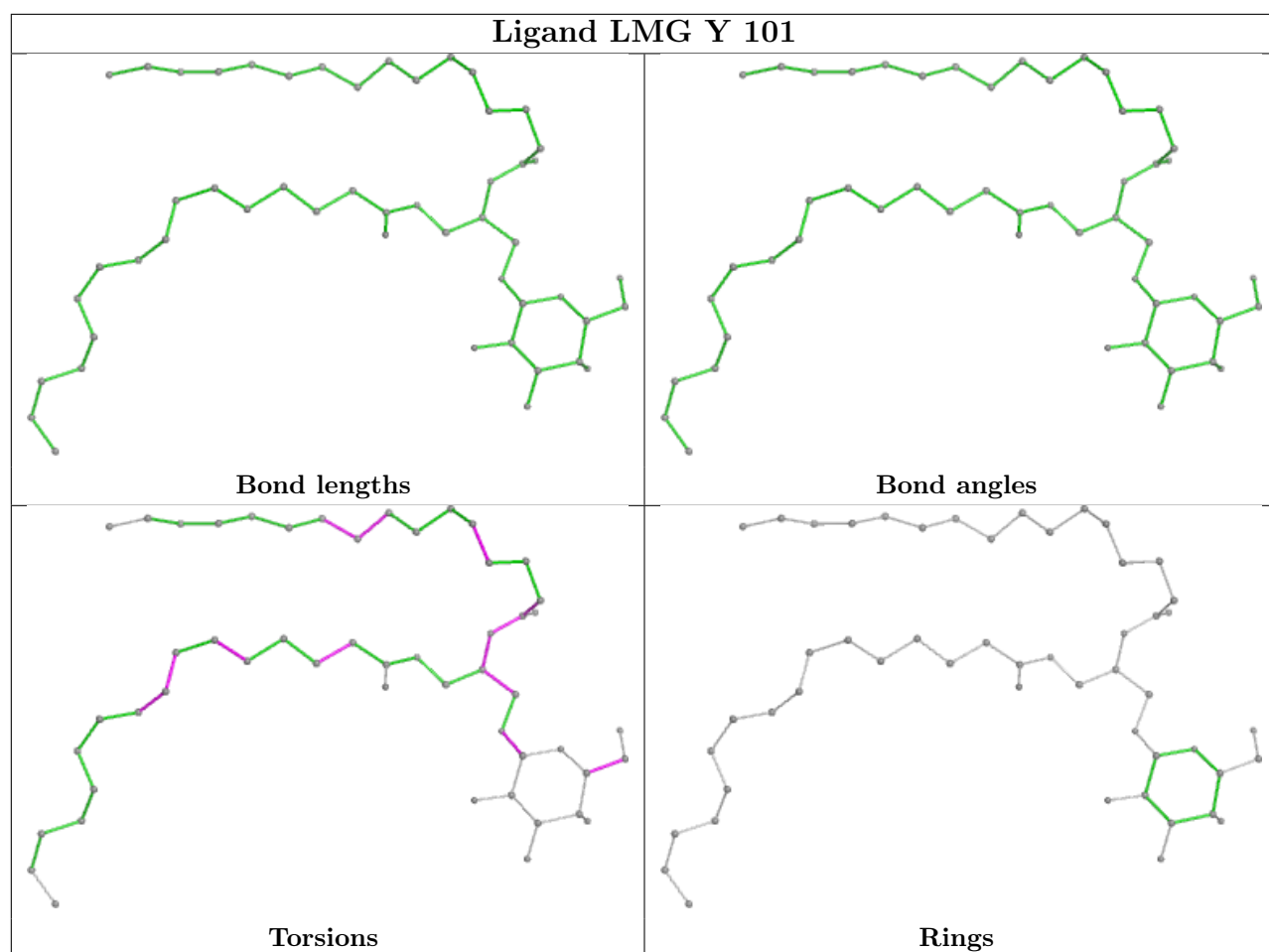
Bond angles



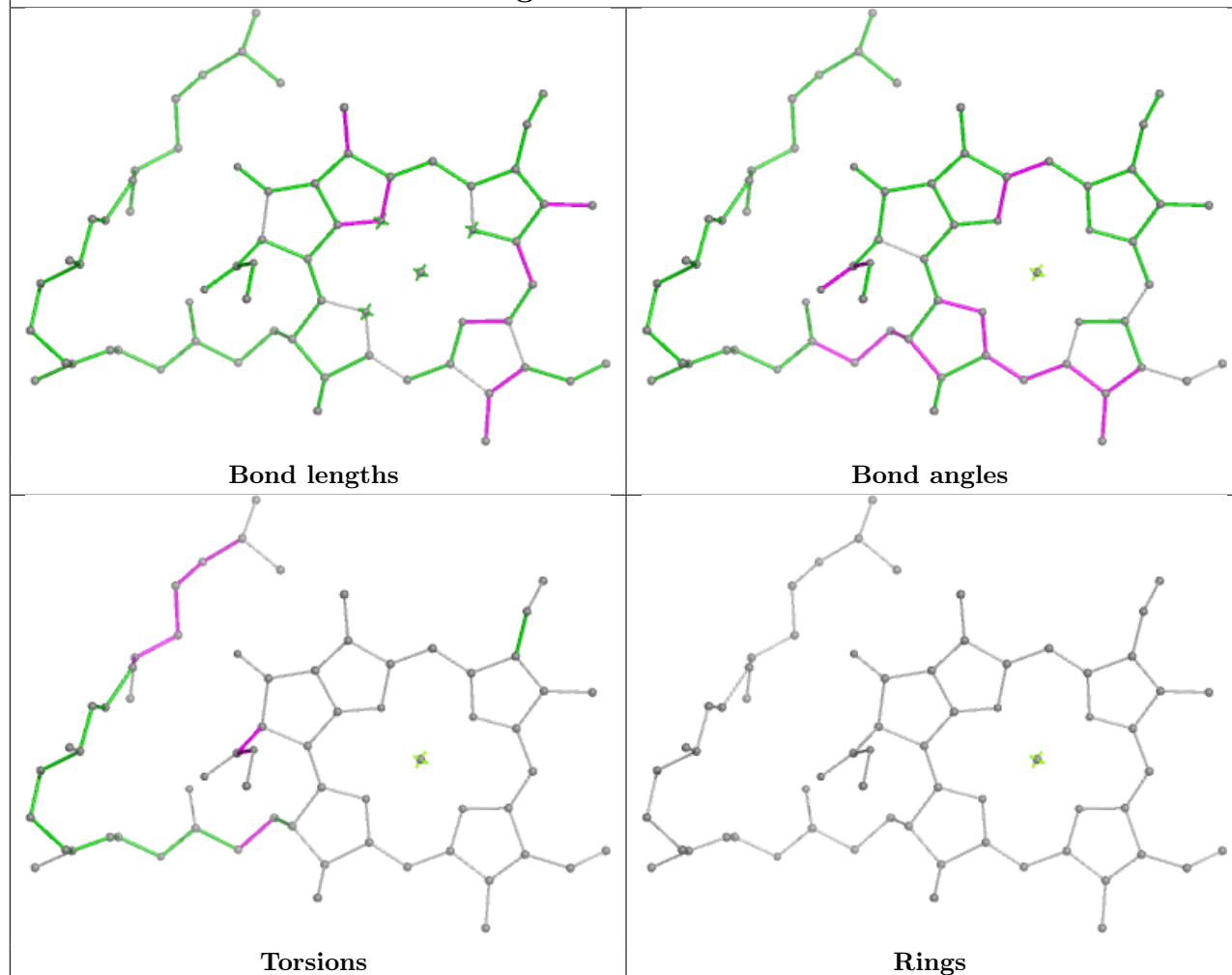
Torsions



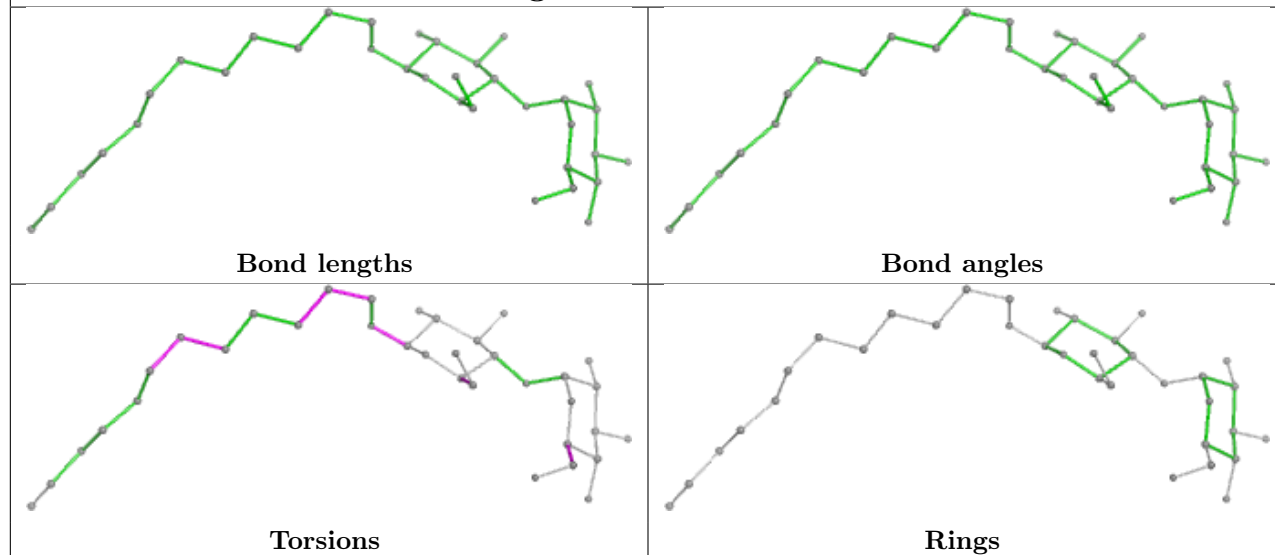
Rings

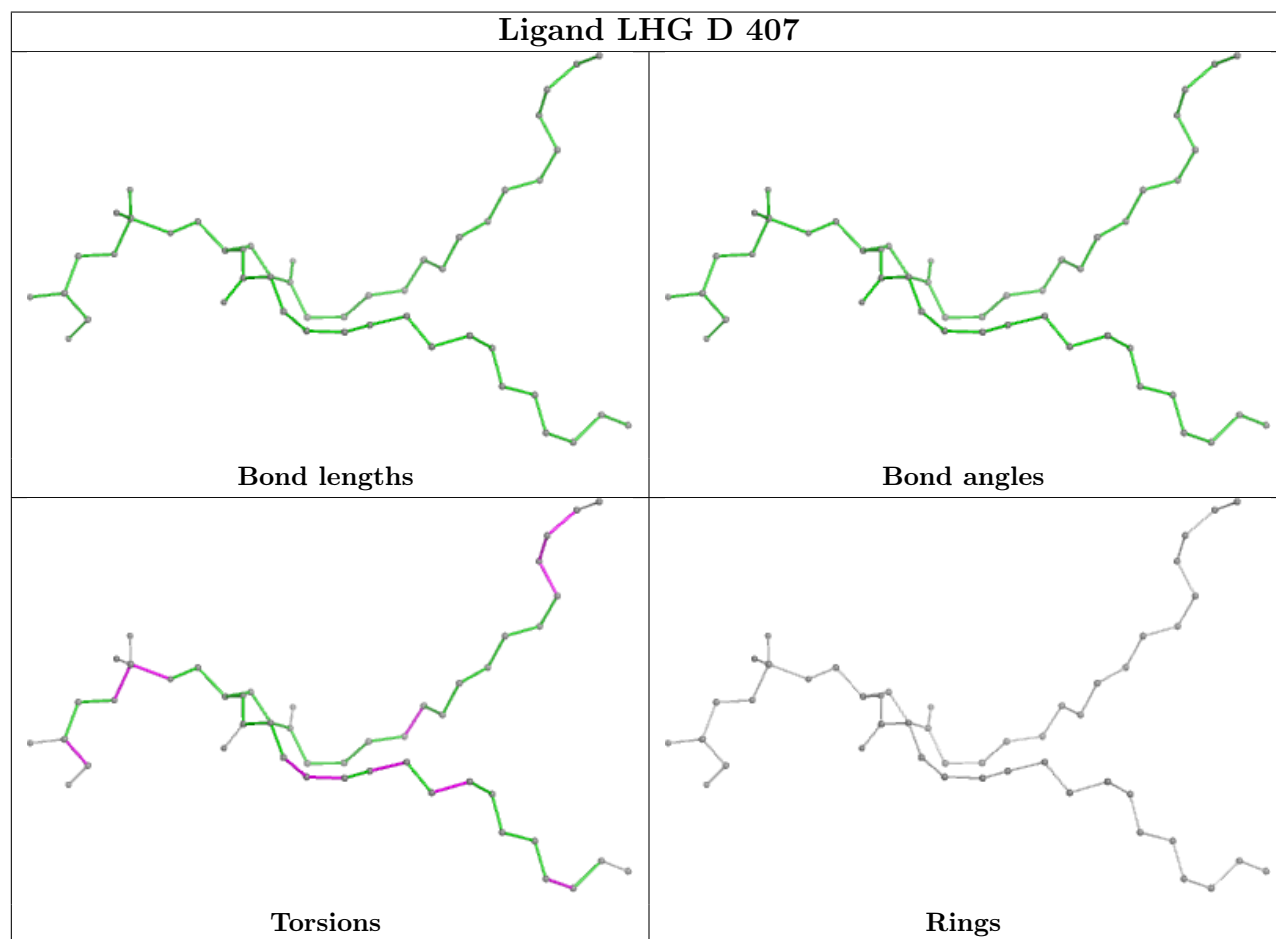
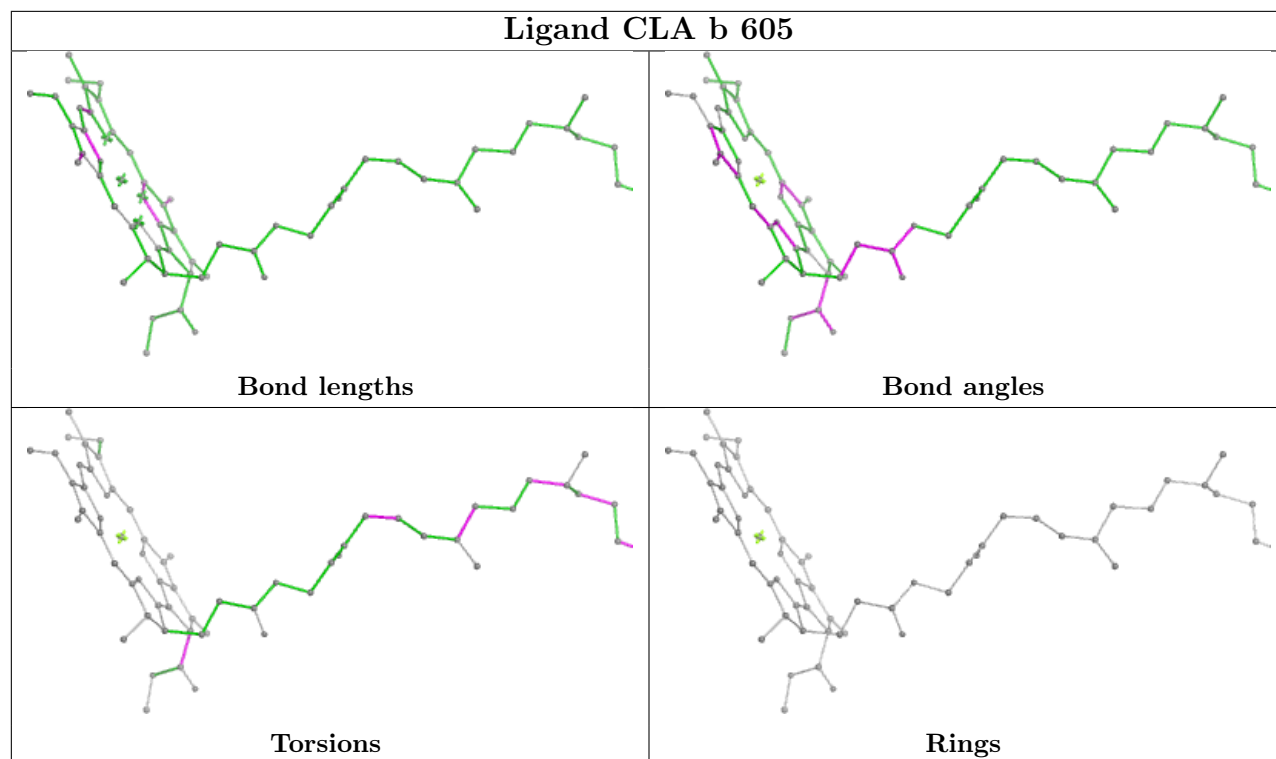


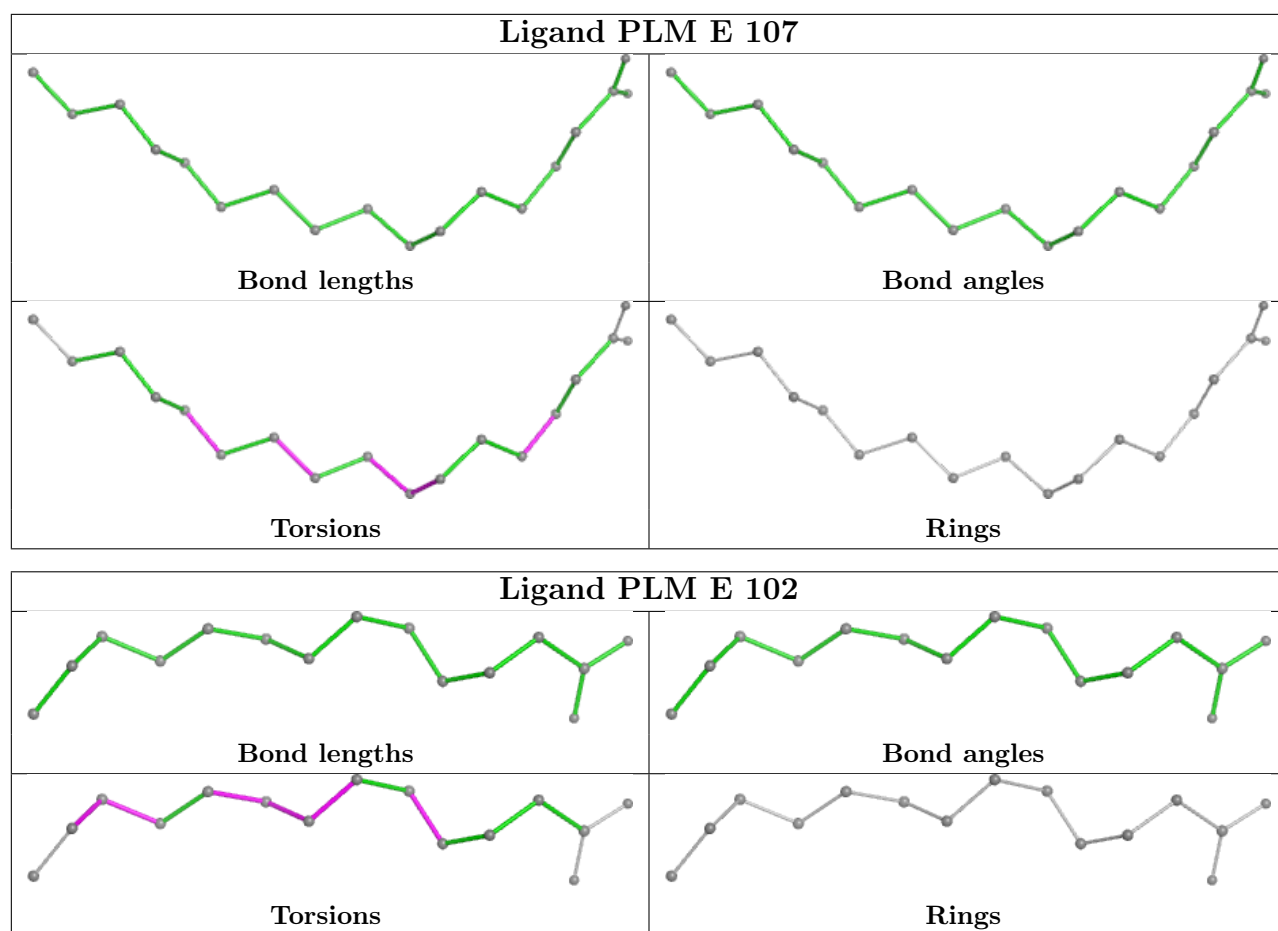
Ligand CLA b 611



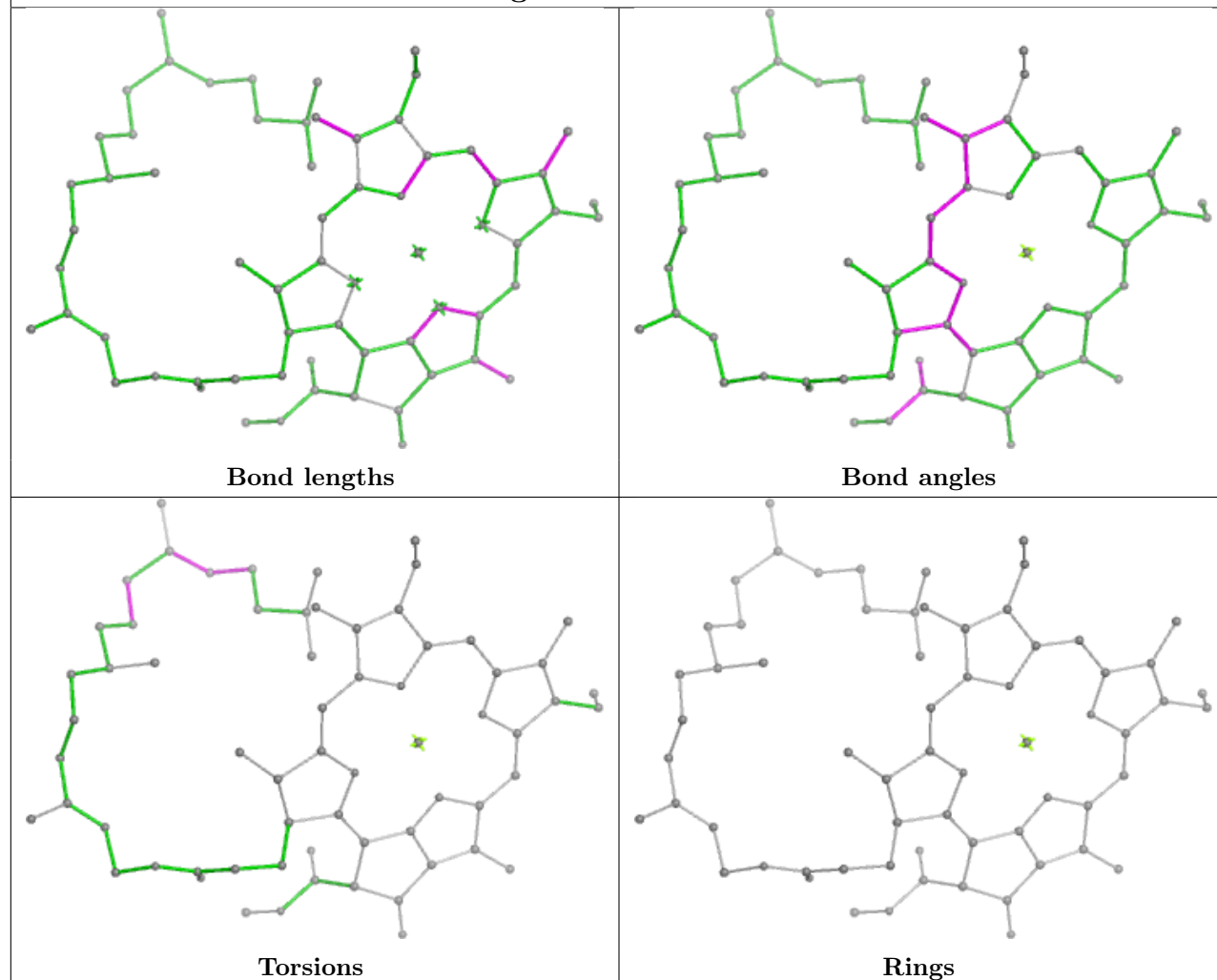
Ligand LMT B 620



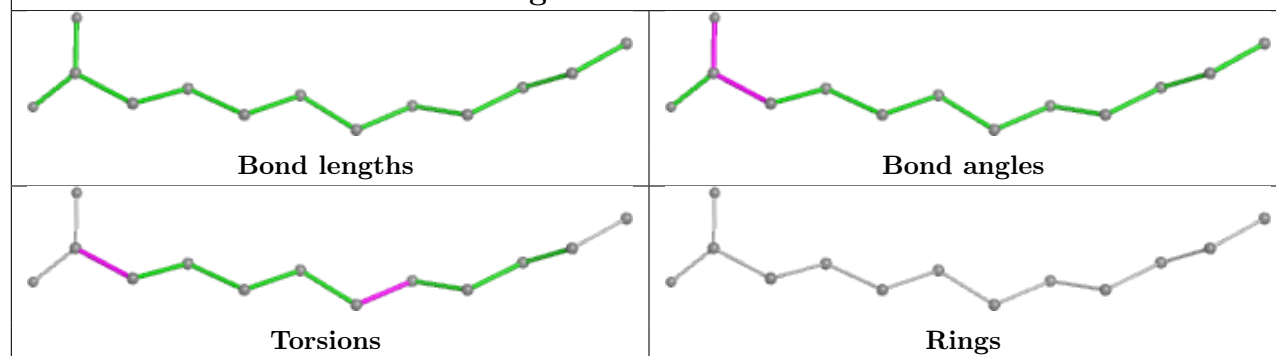


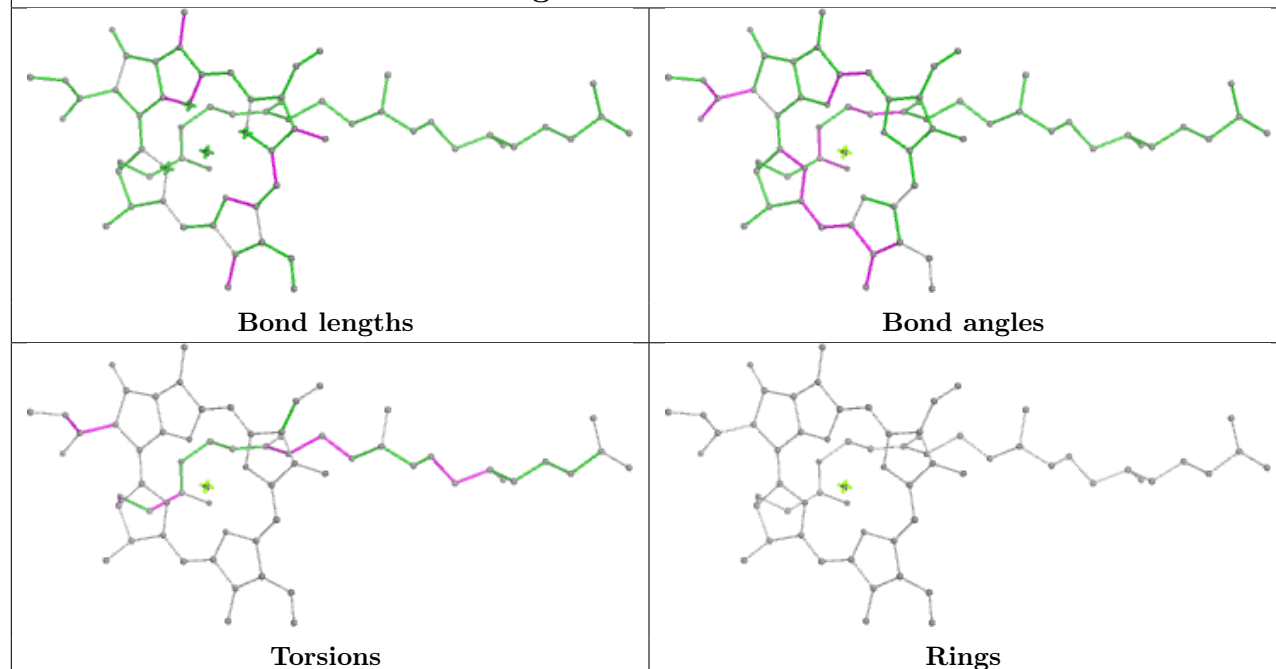
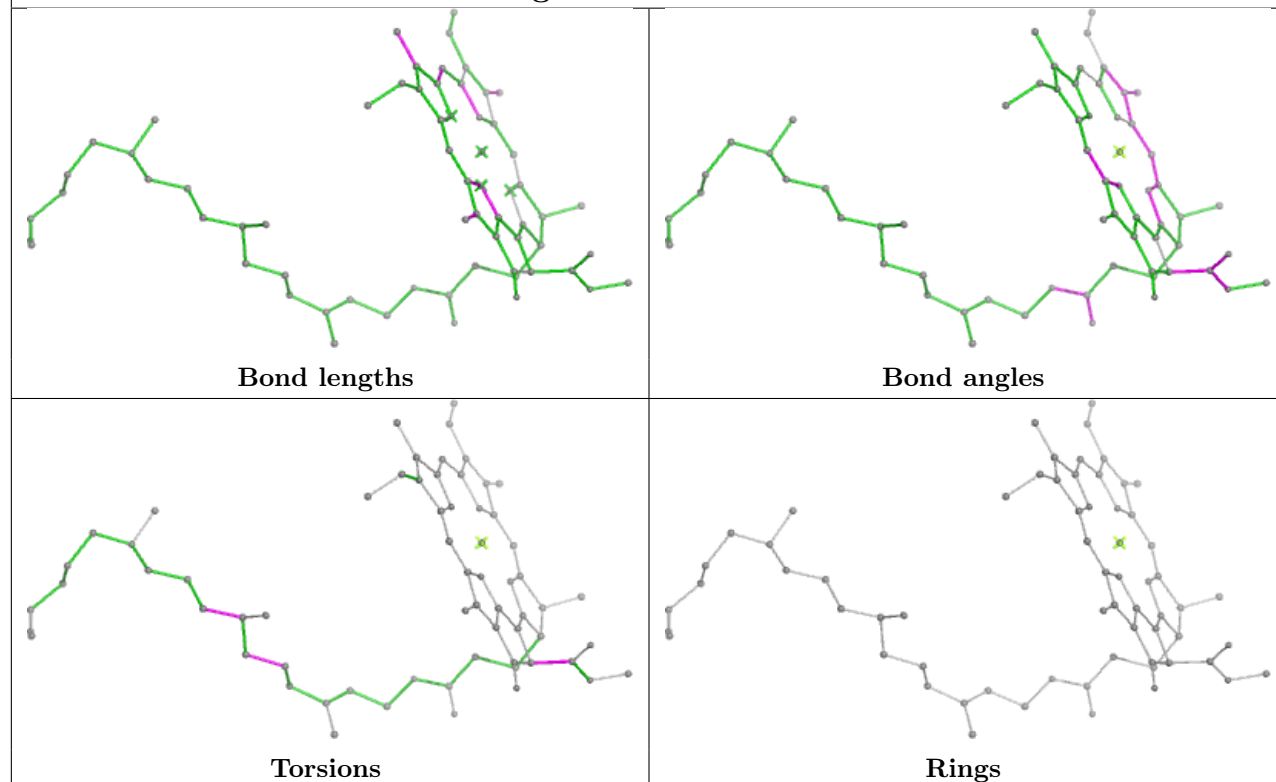


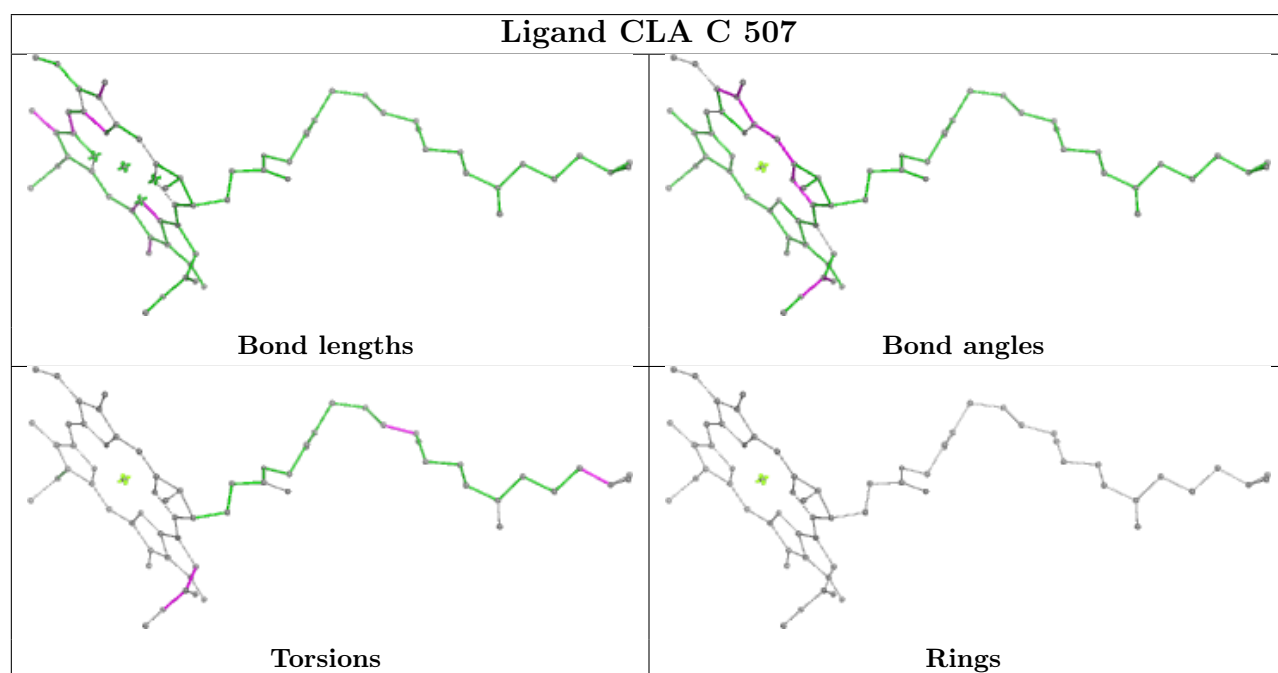
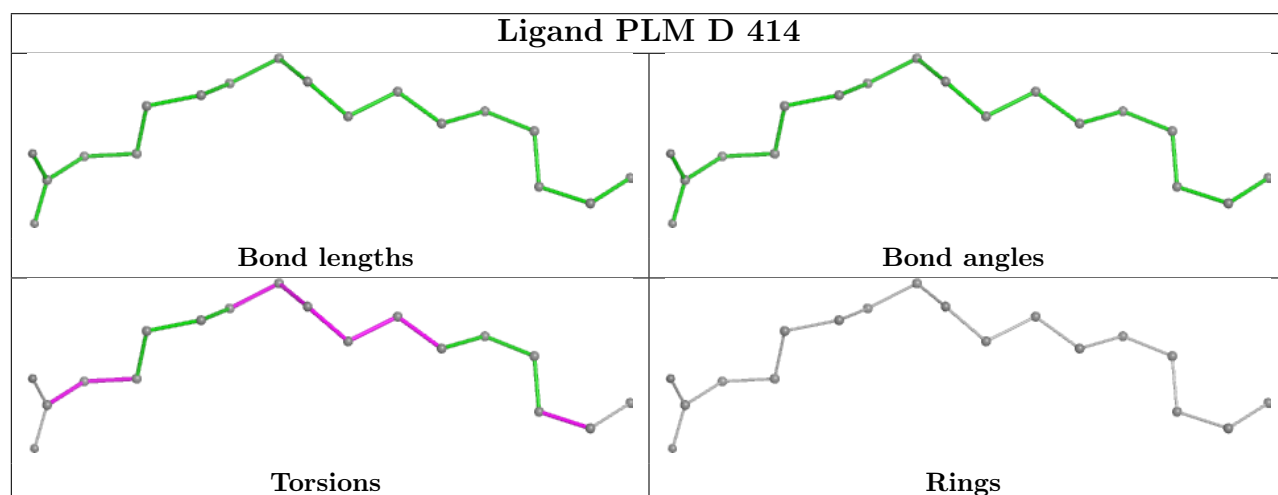
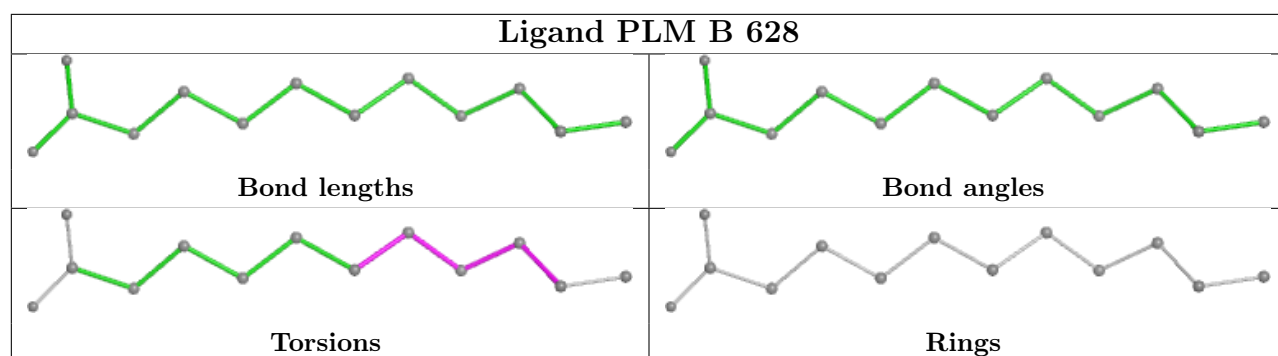
Ligand CLA b 616

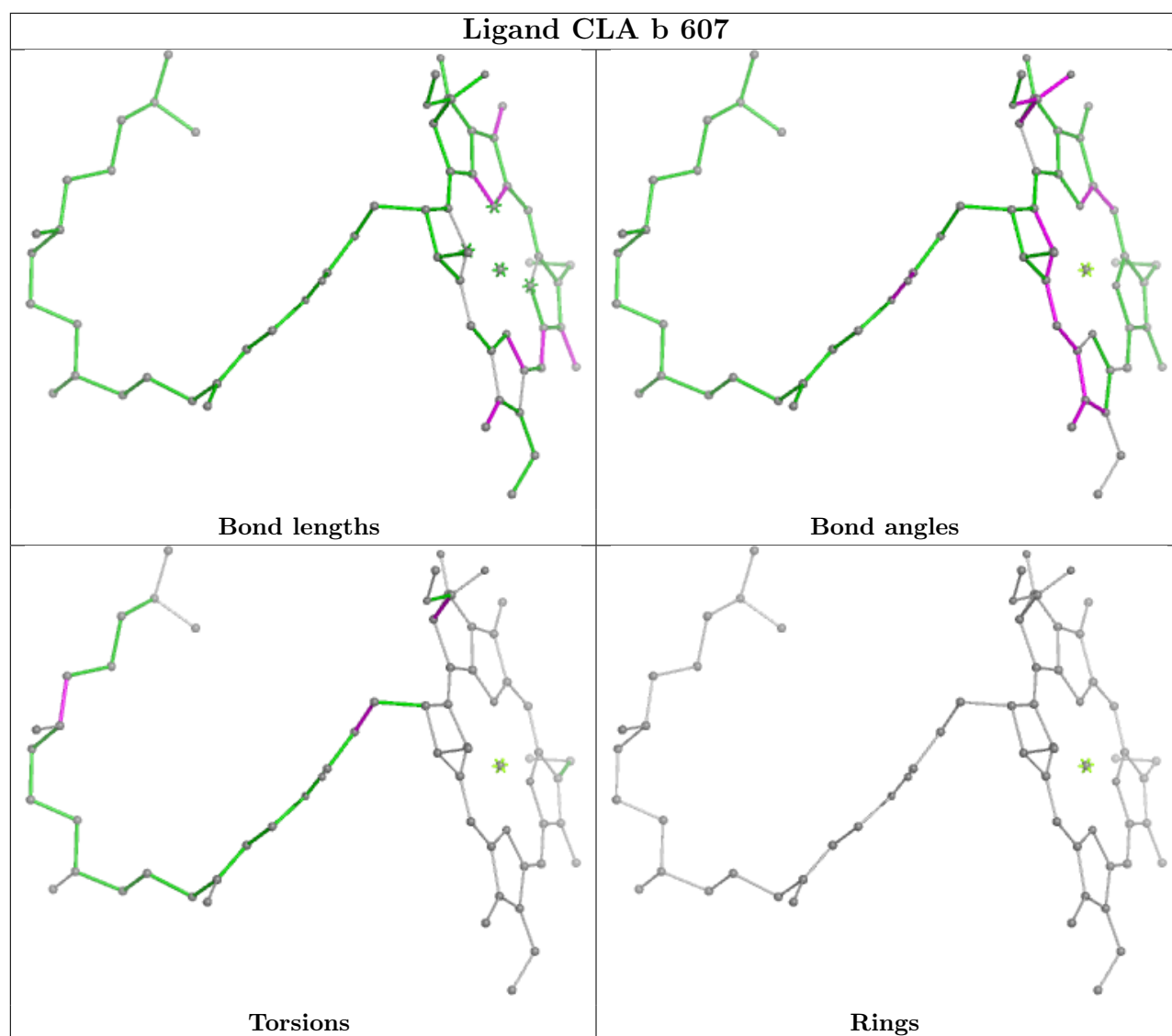


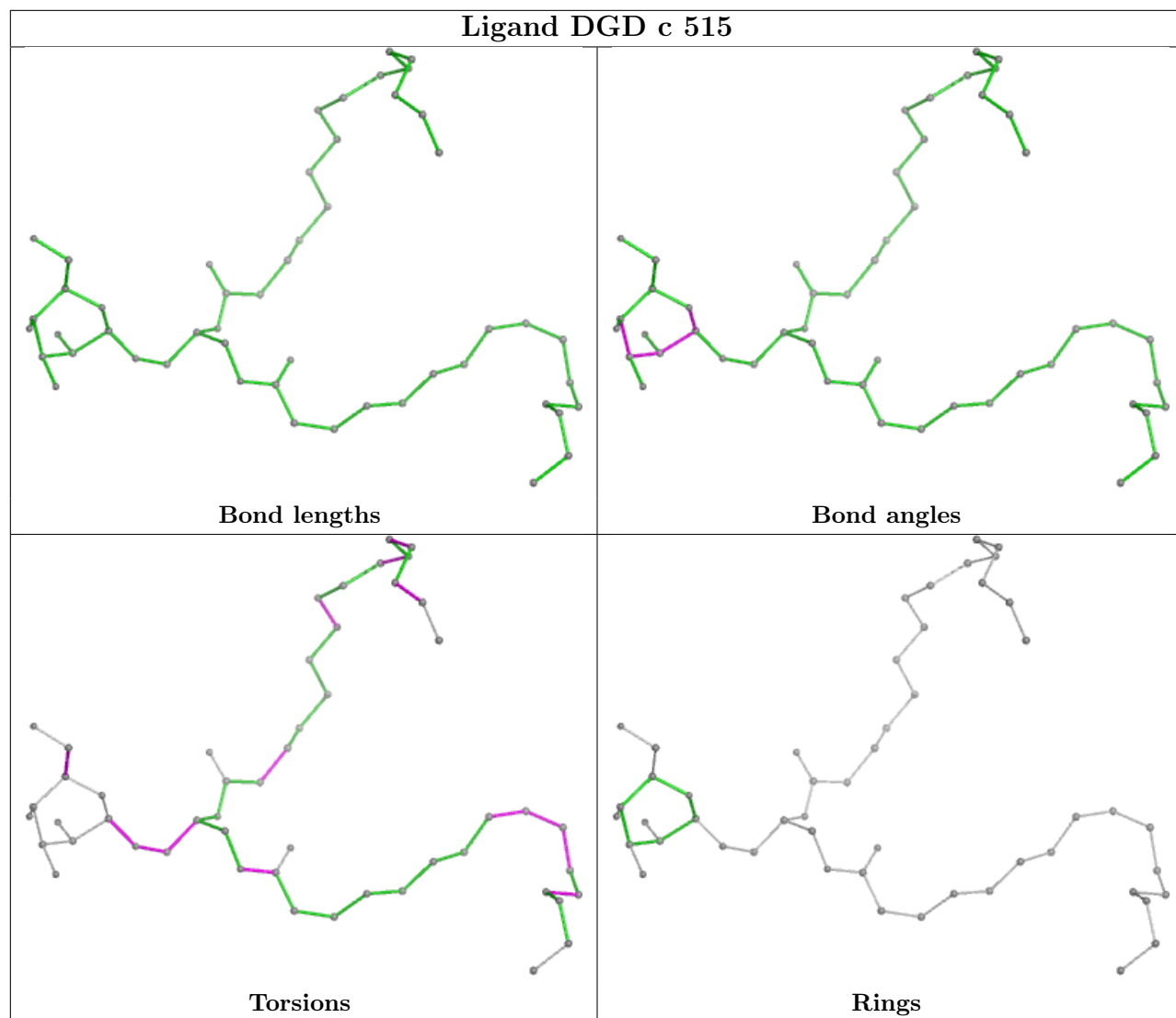
Ligand PLM C 519



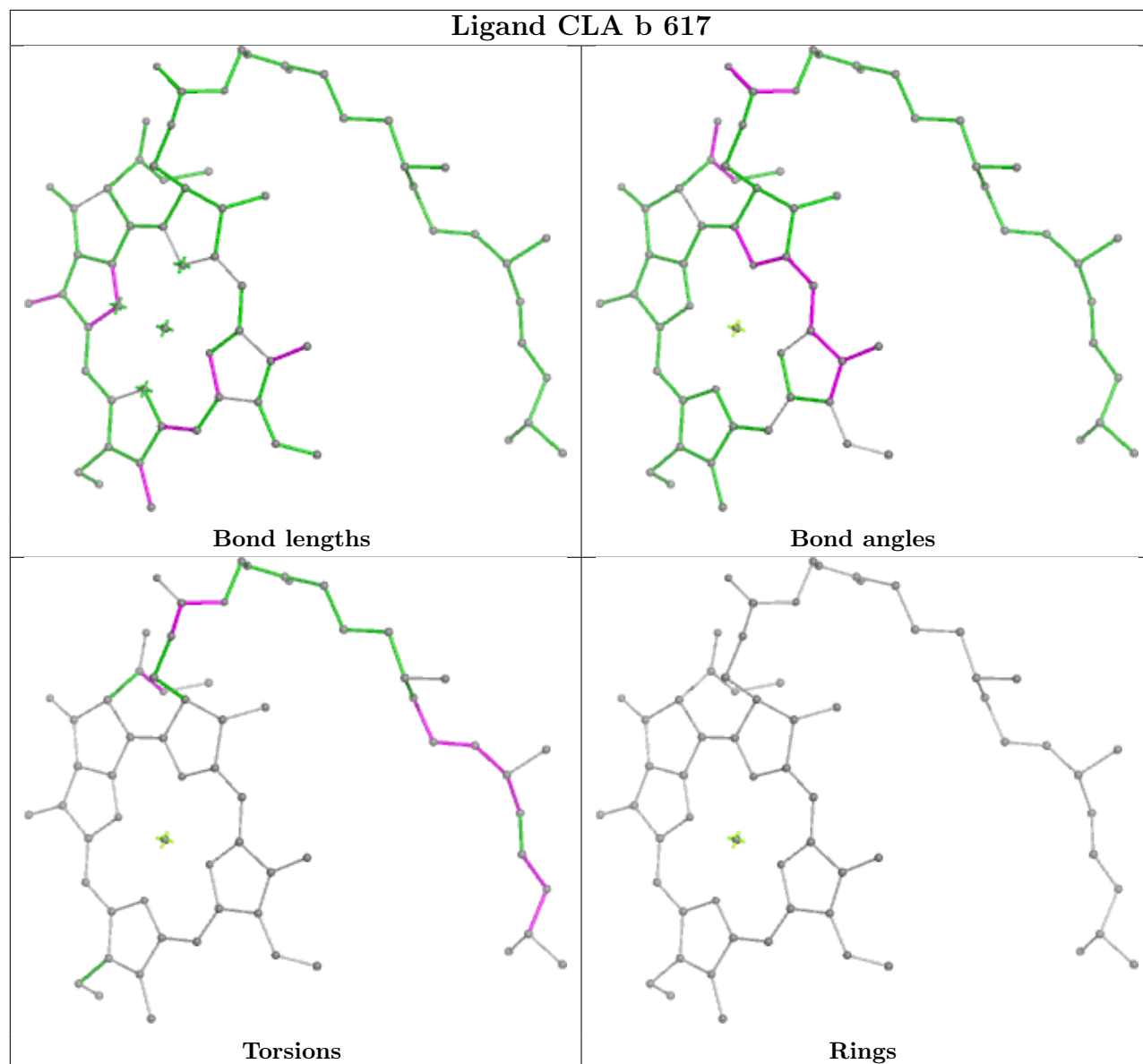
Ligand CLA B 614**Ligand CLA C 513**



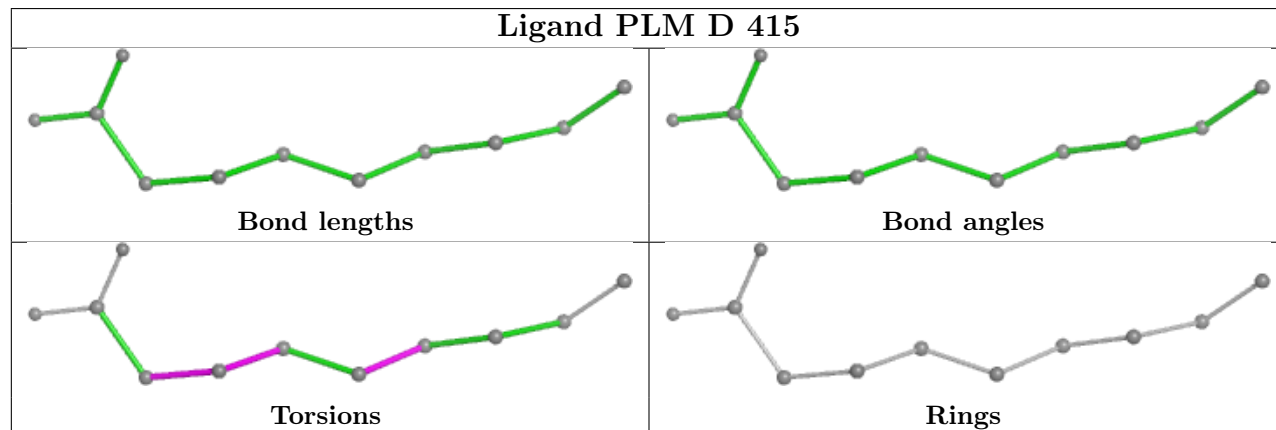




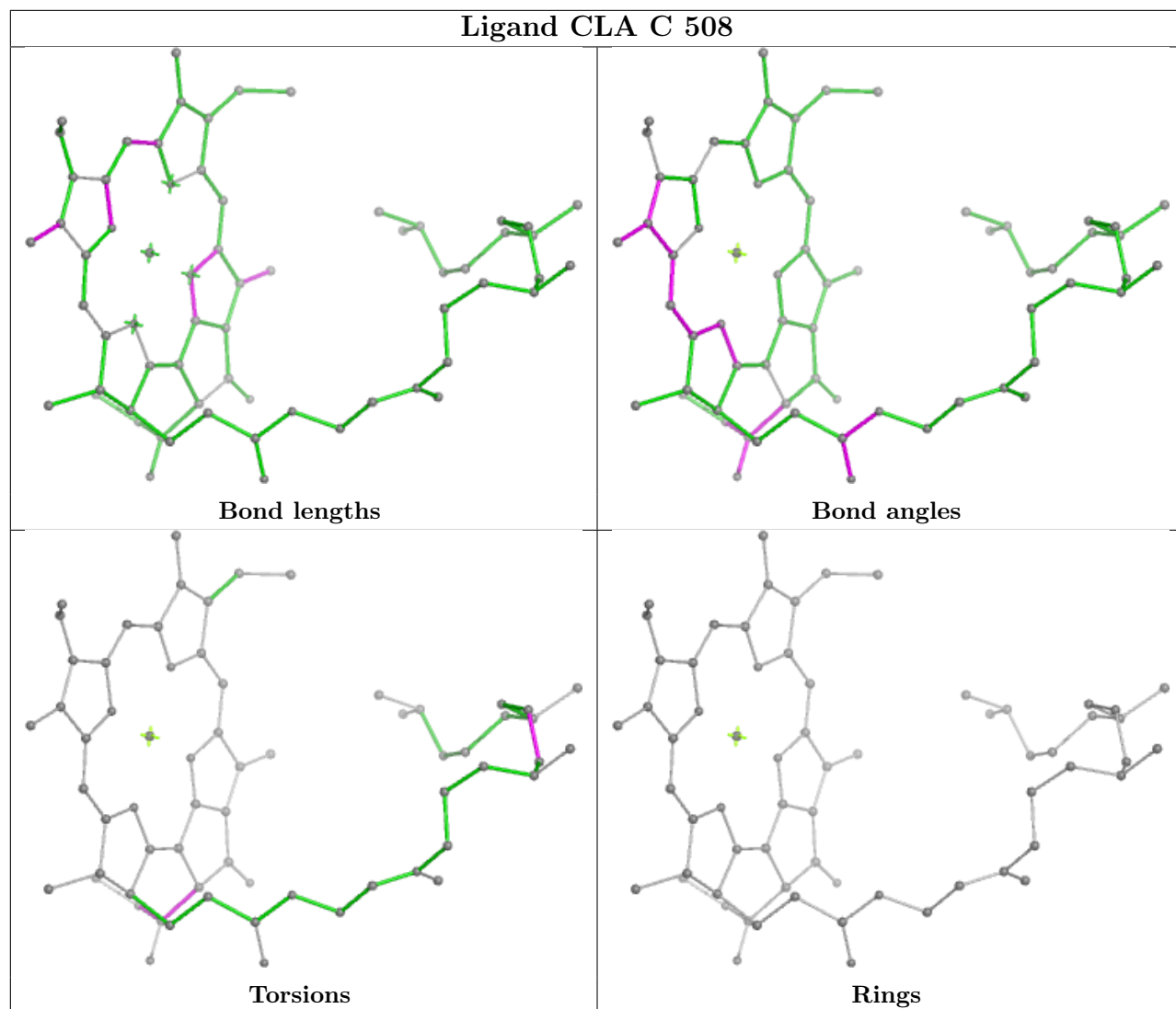
Ligand CLA b 617

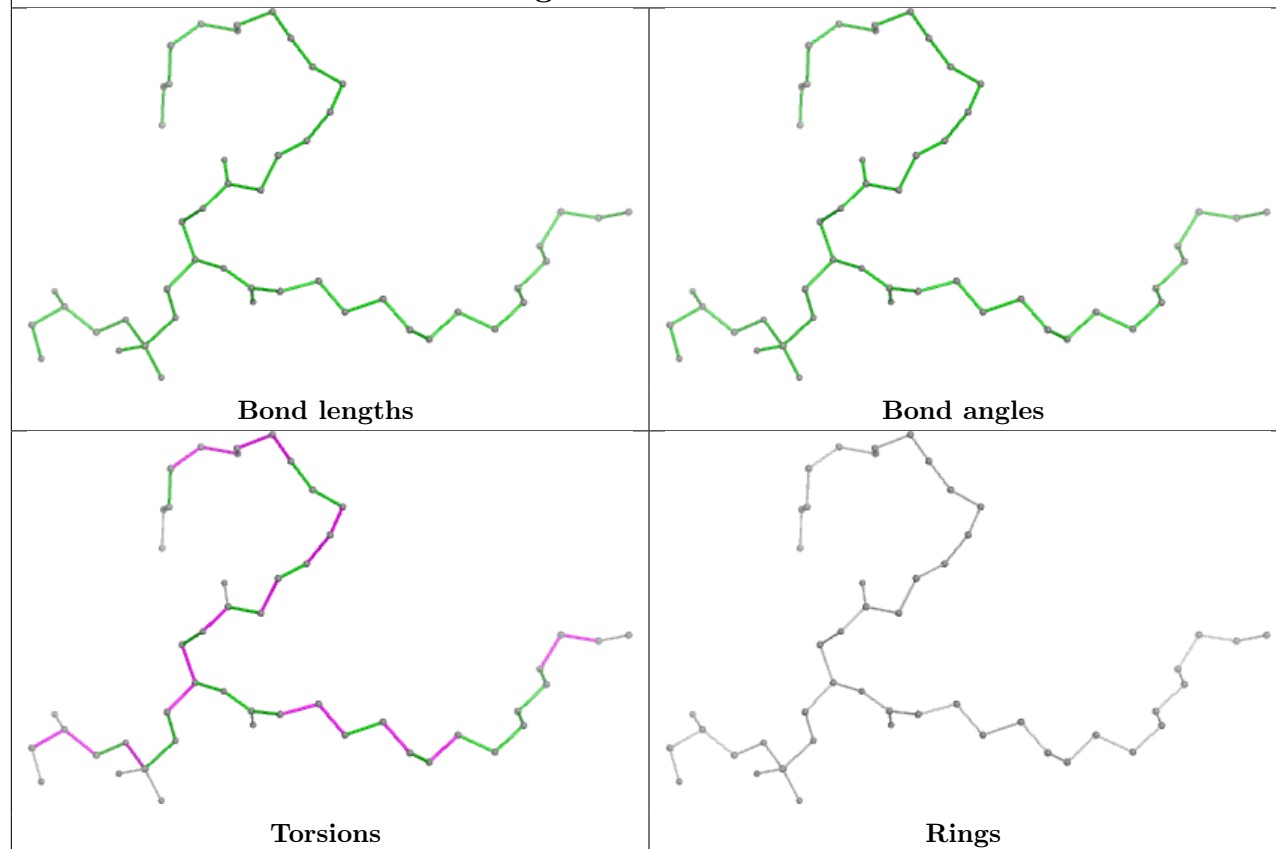
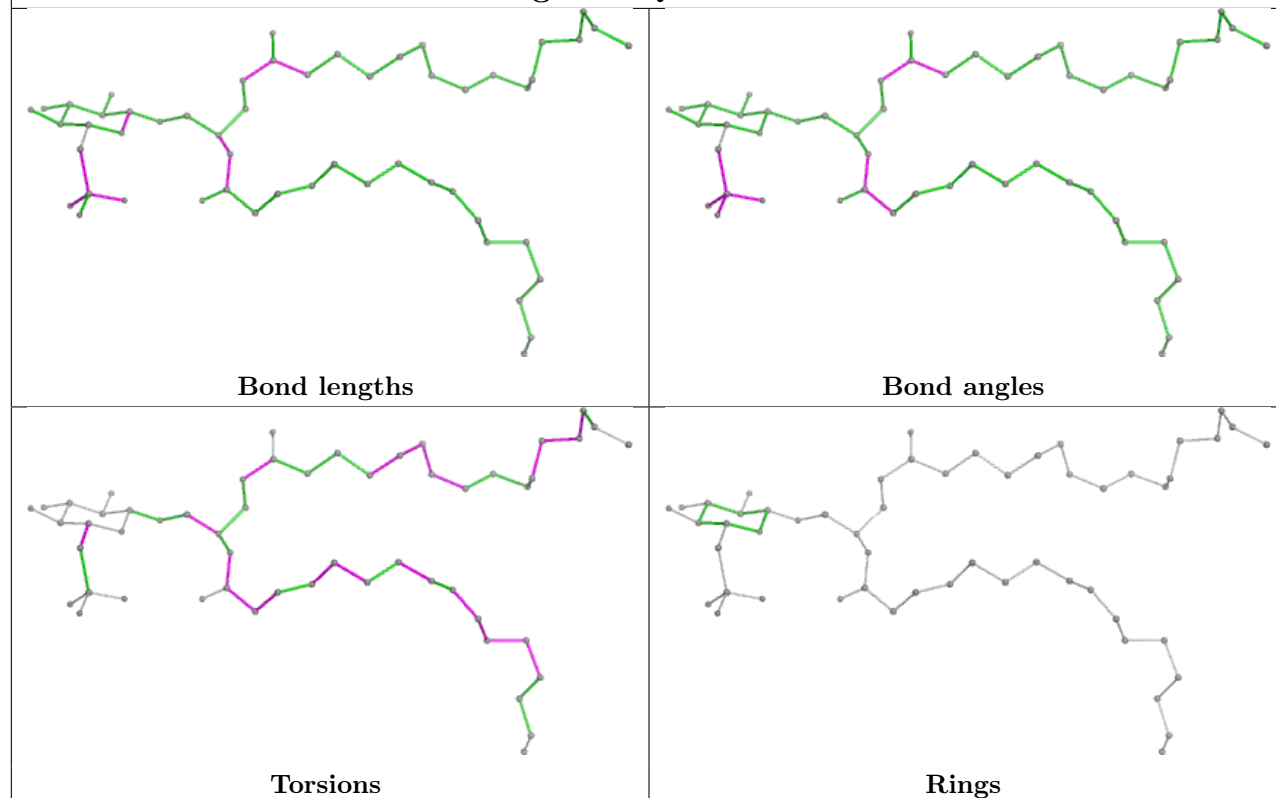


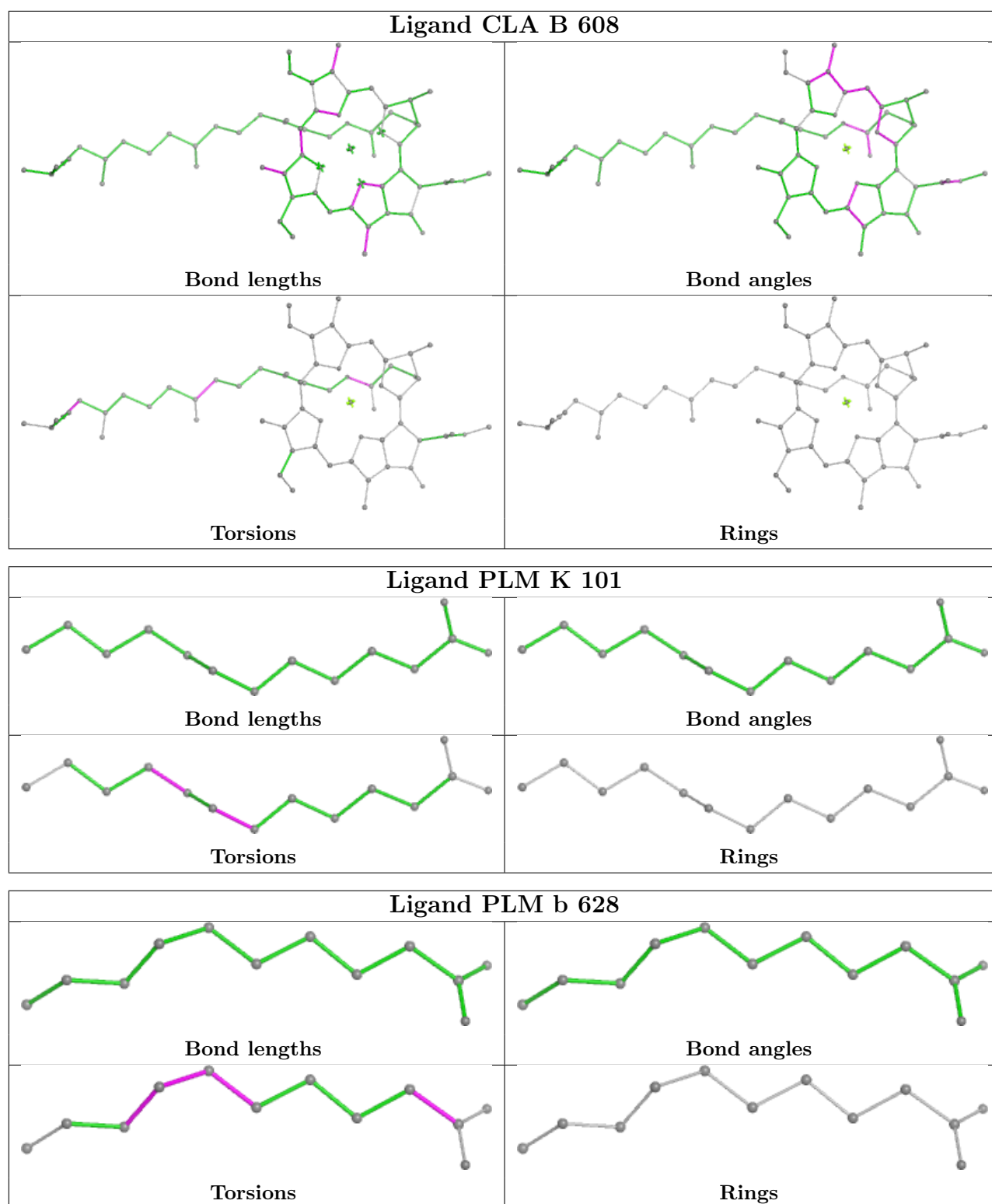
Ligand PLM D 415

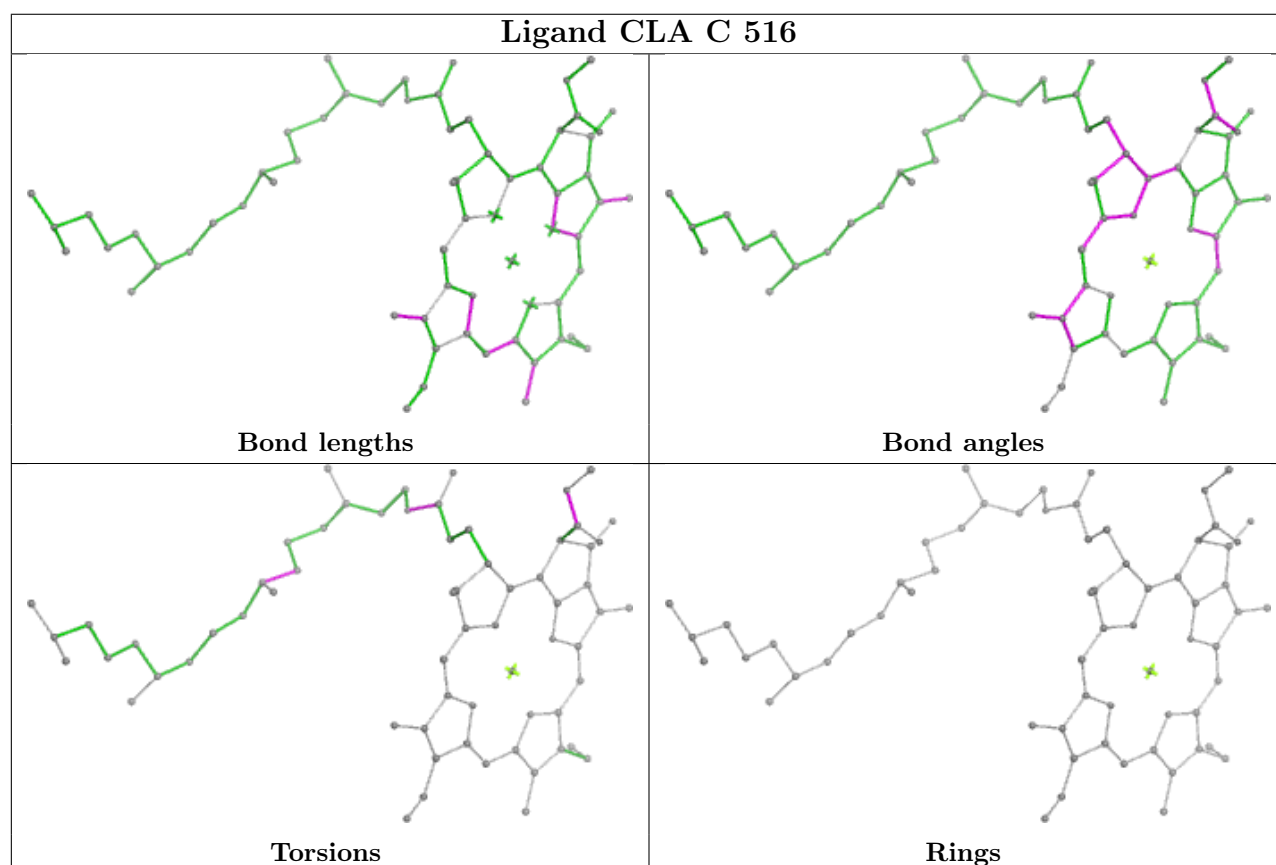
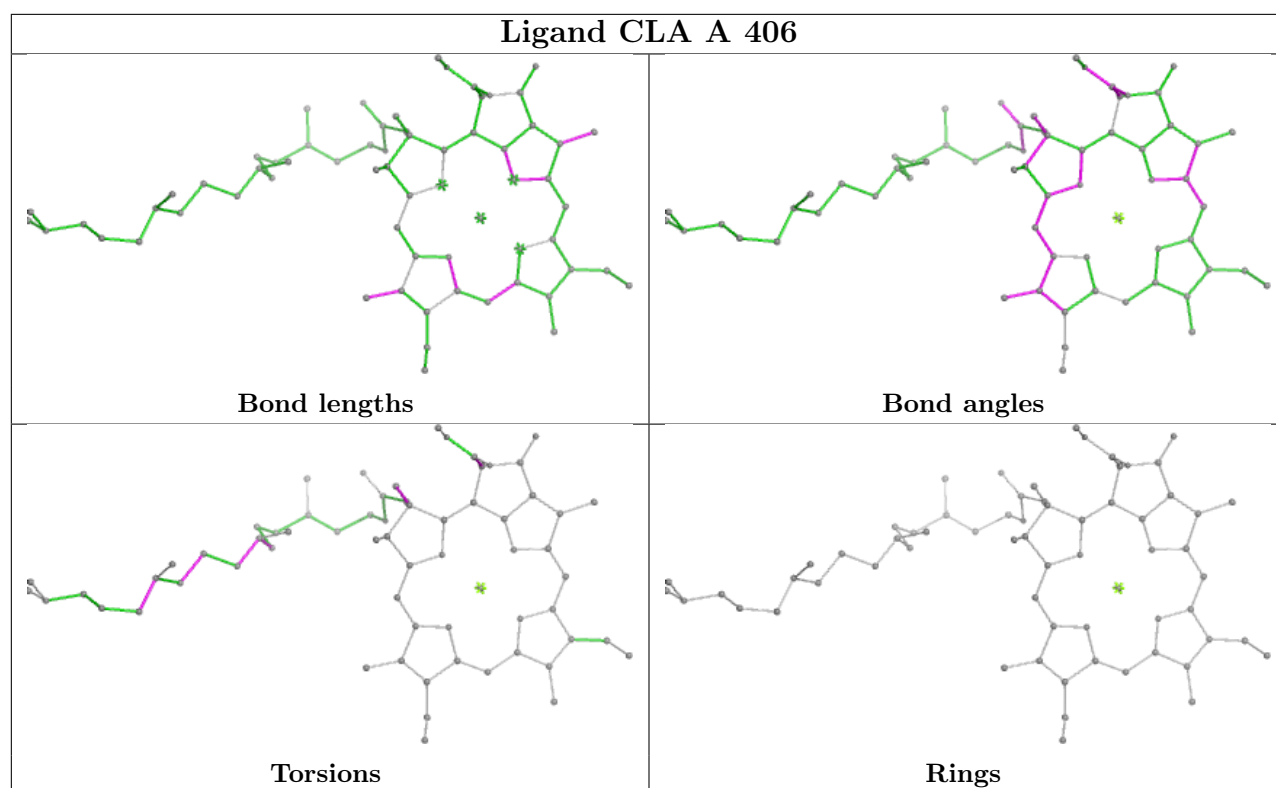


Ligand CLA C 508

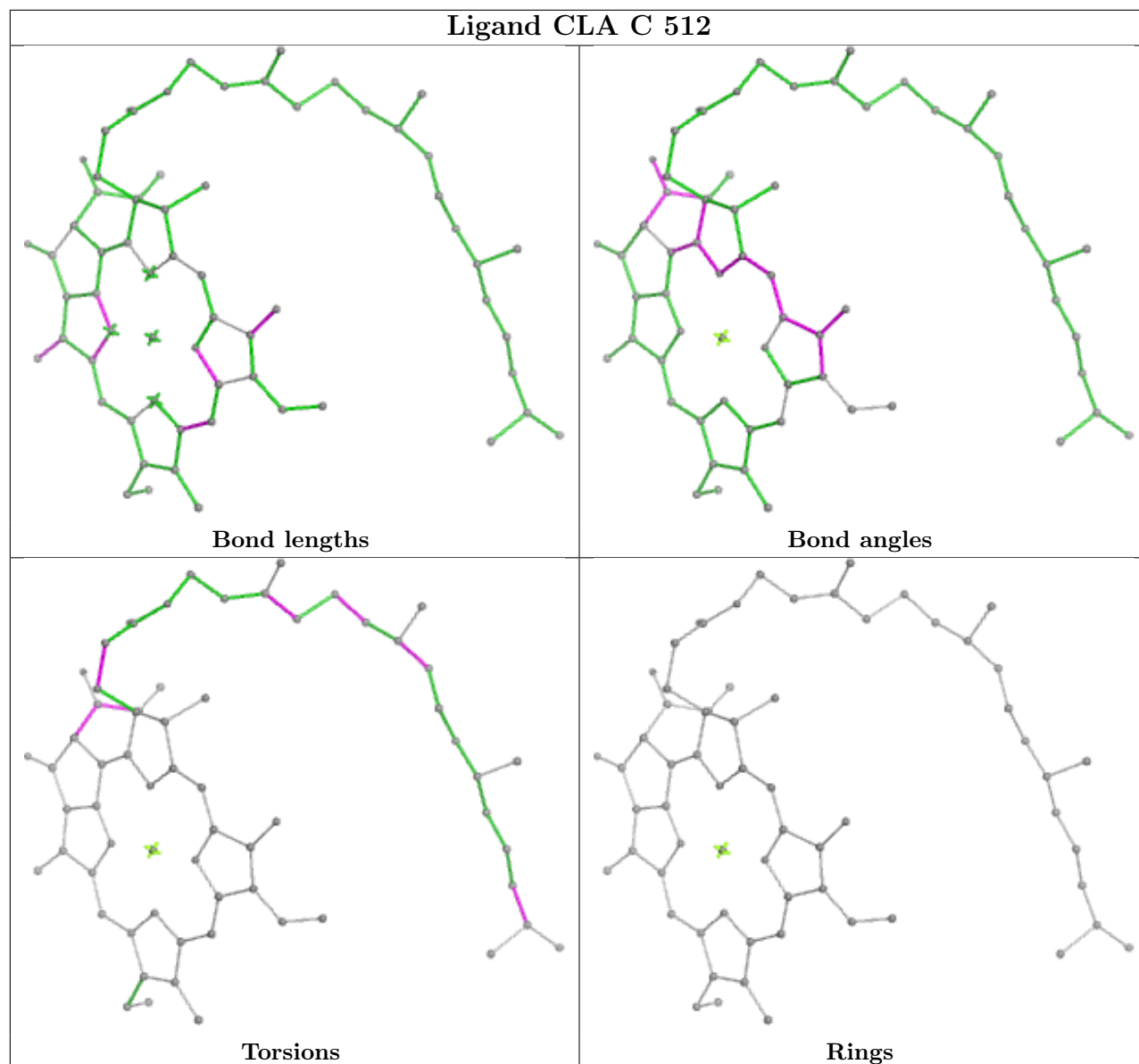


Ligand LHG a 417**Ligand SQD B 630**

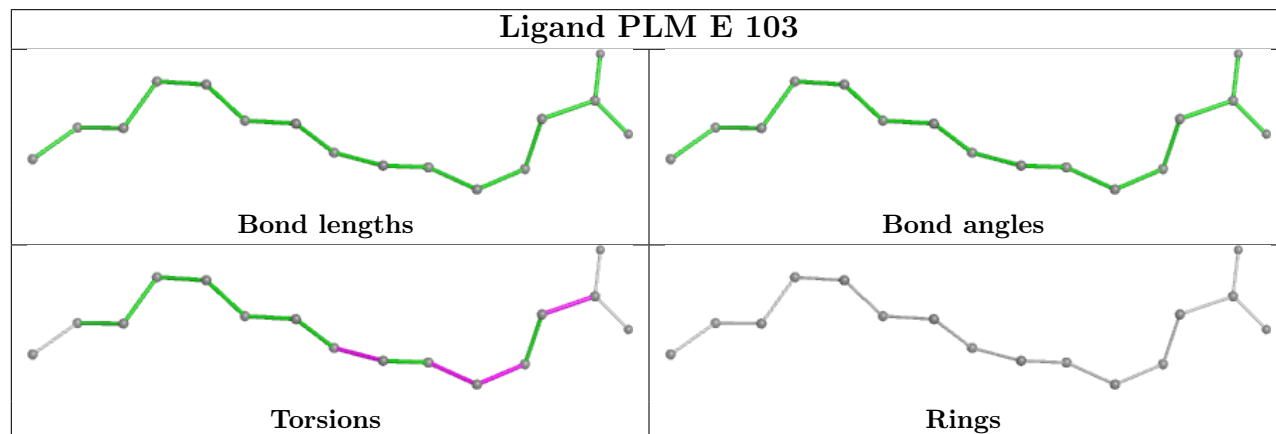


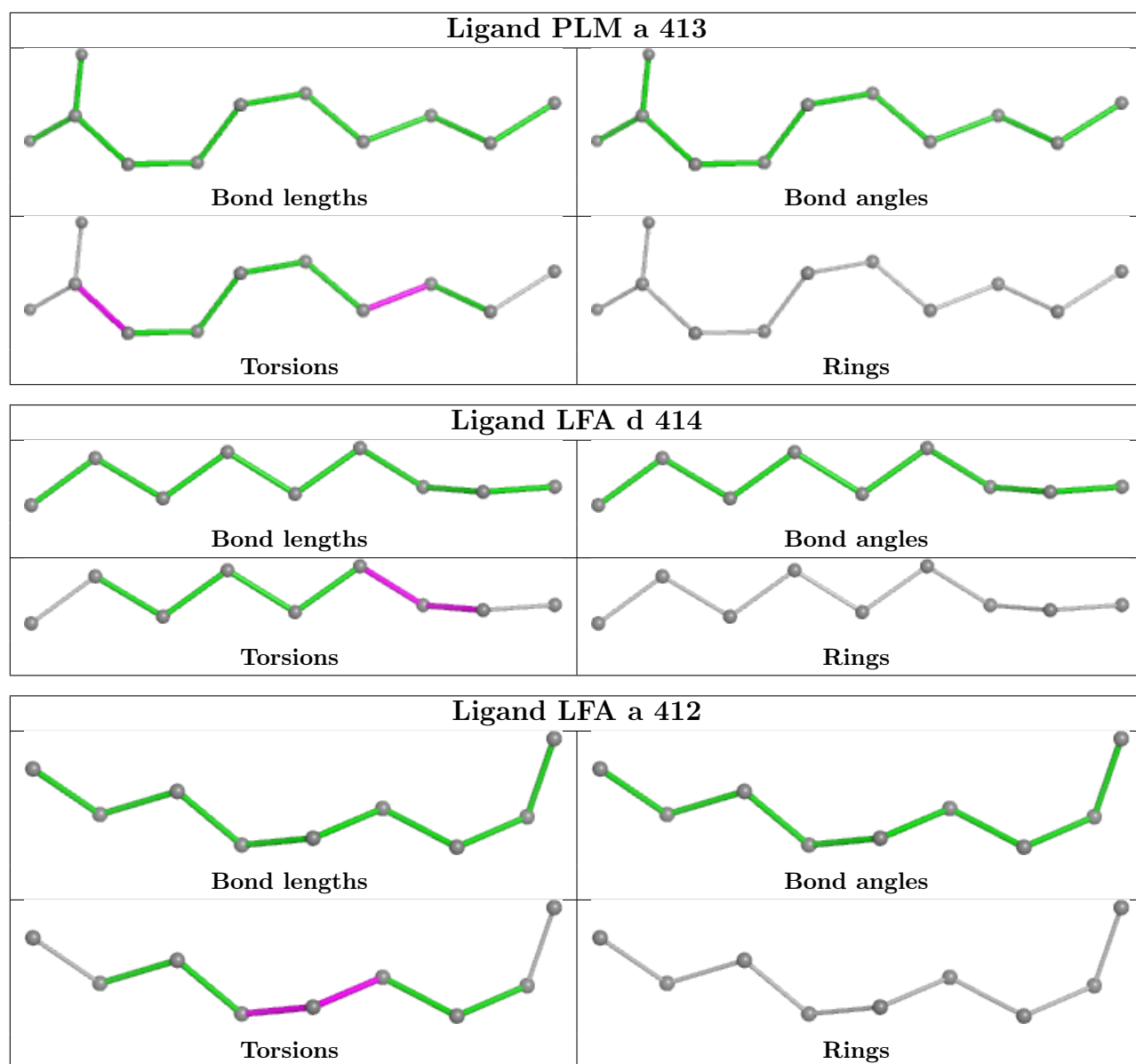


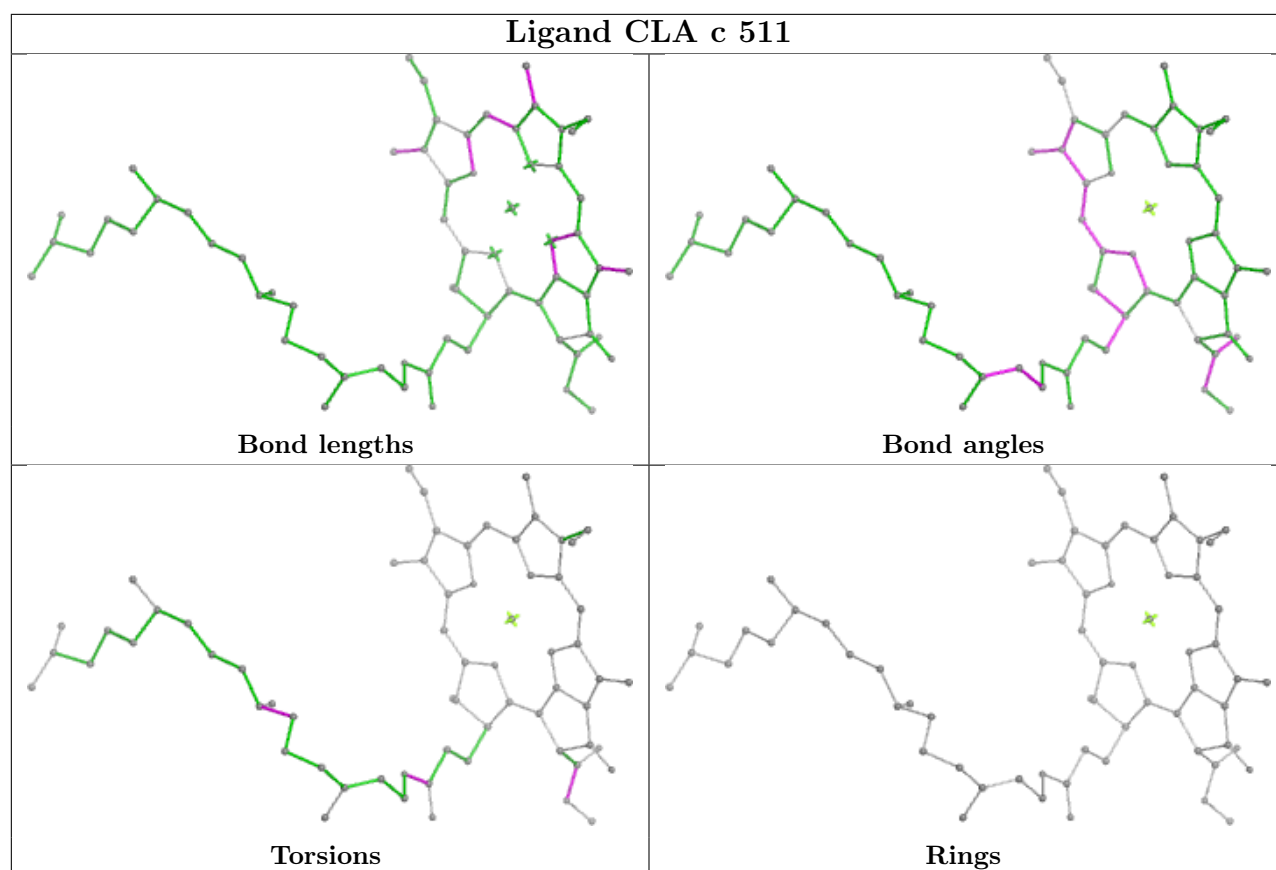
Ligand CLA C 512

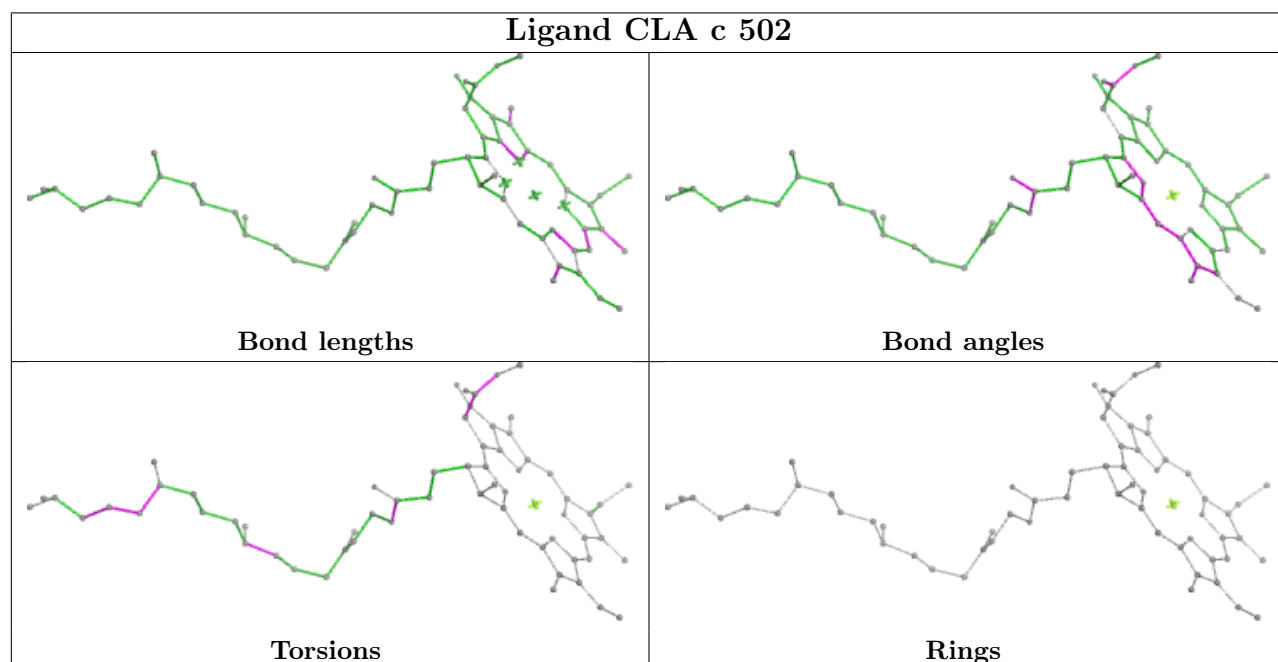
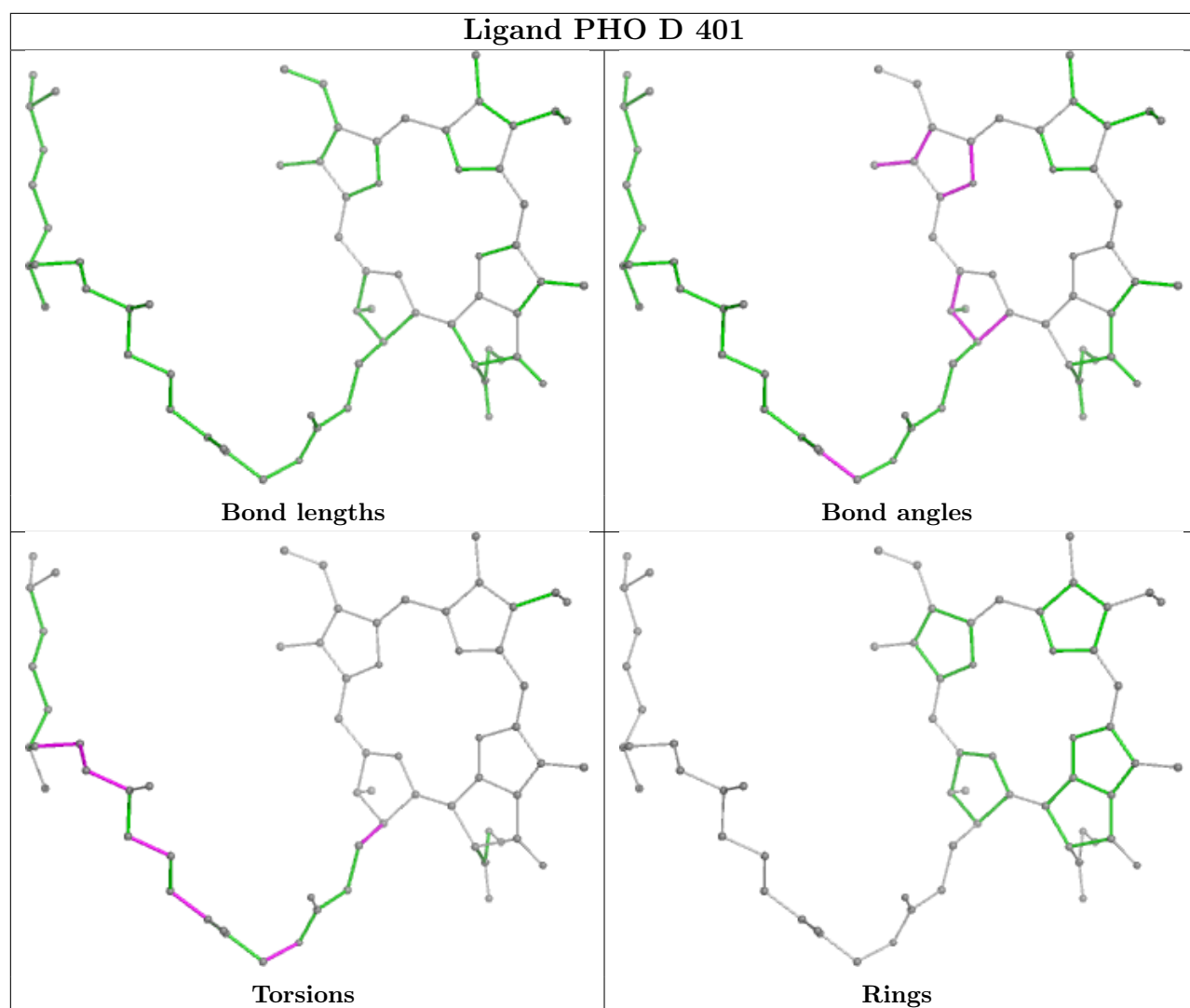


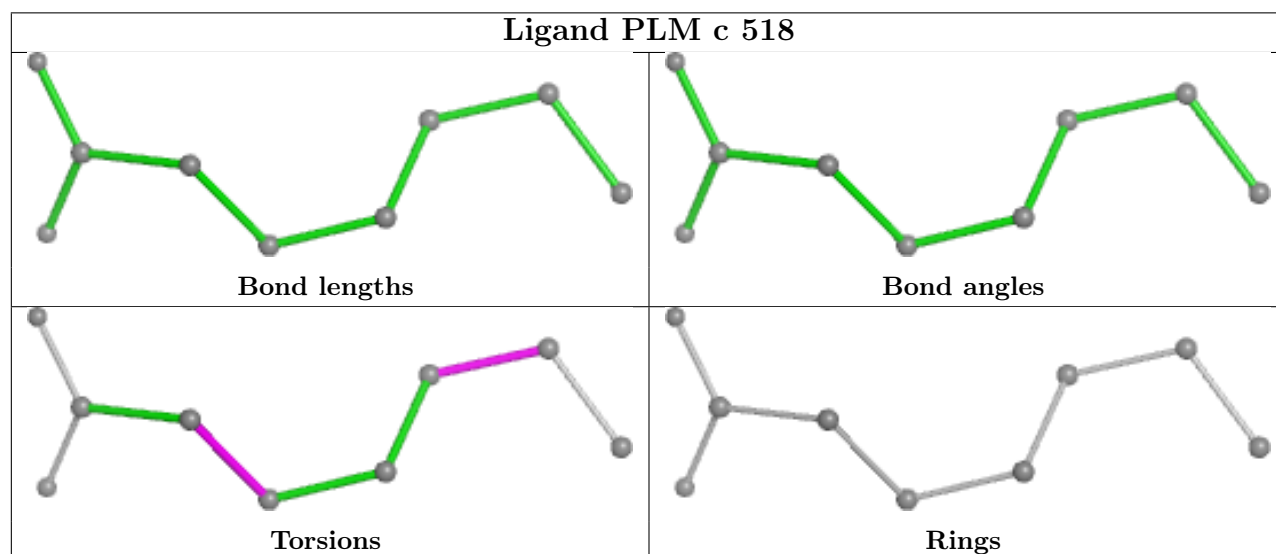
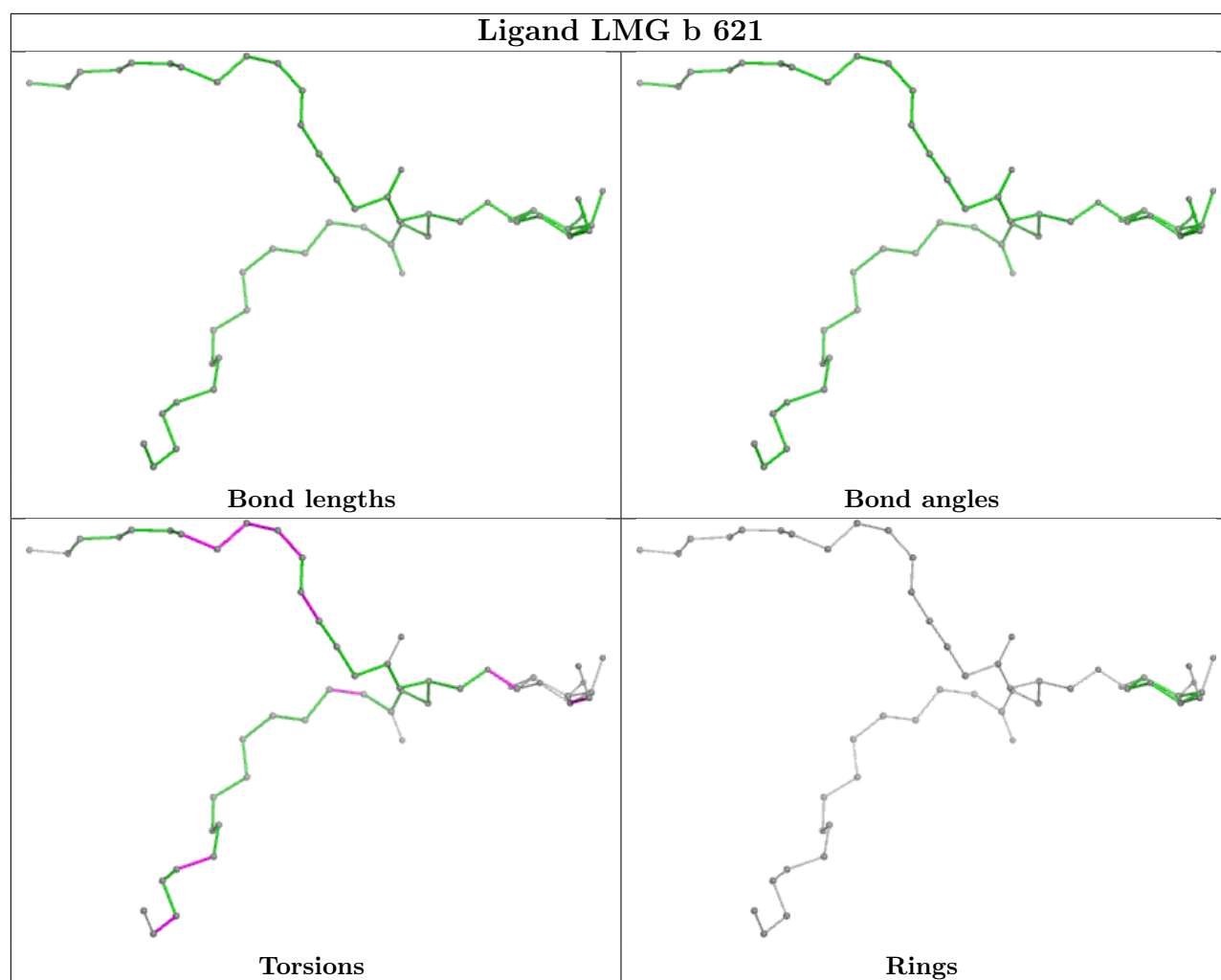
Ligand PLM E 103

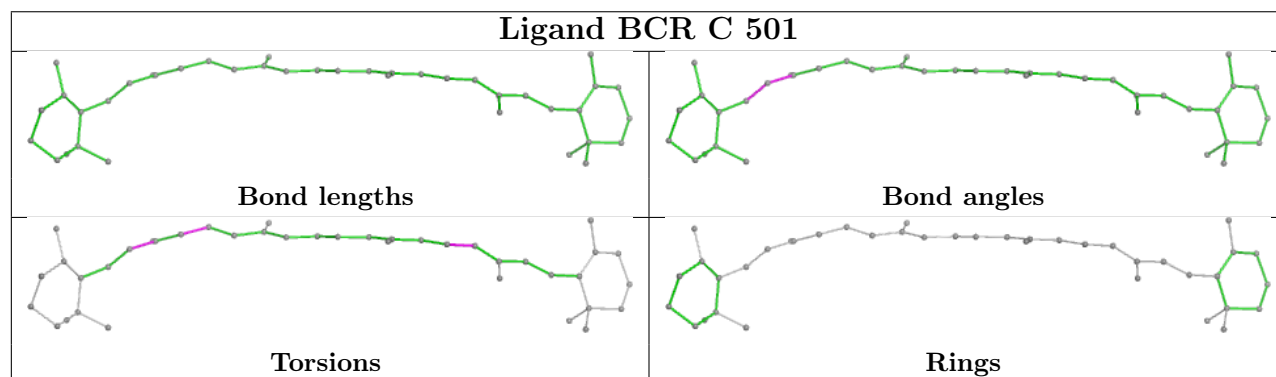
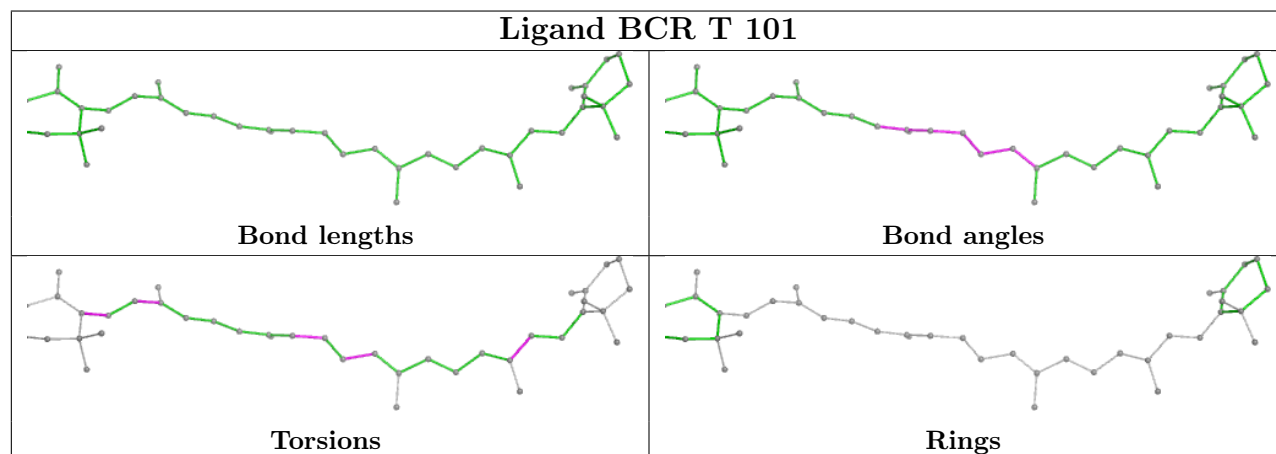
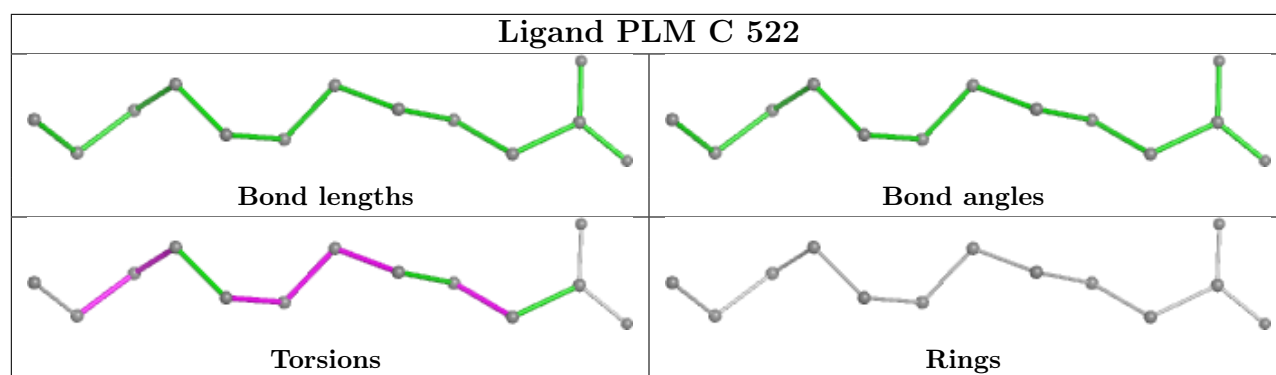


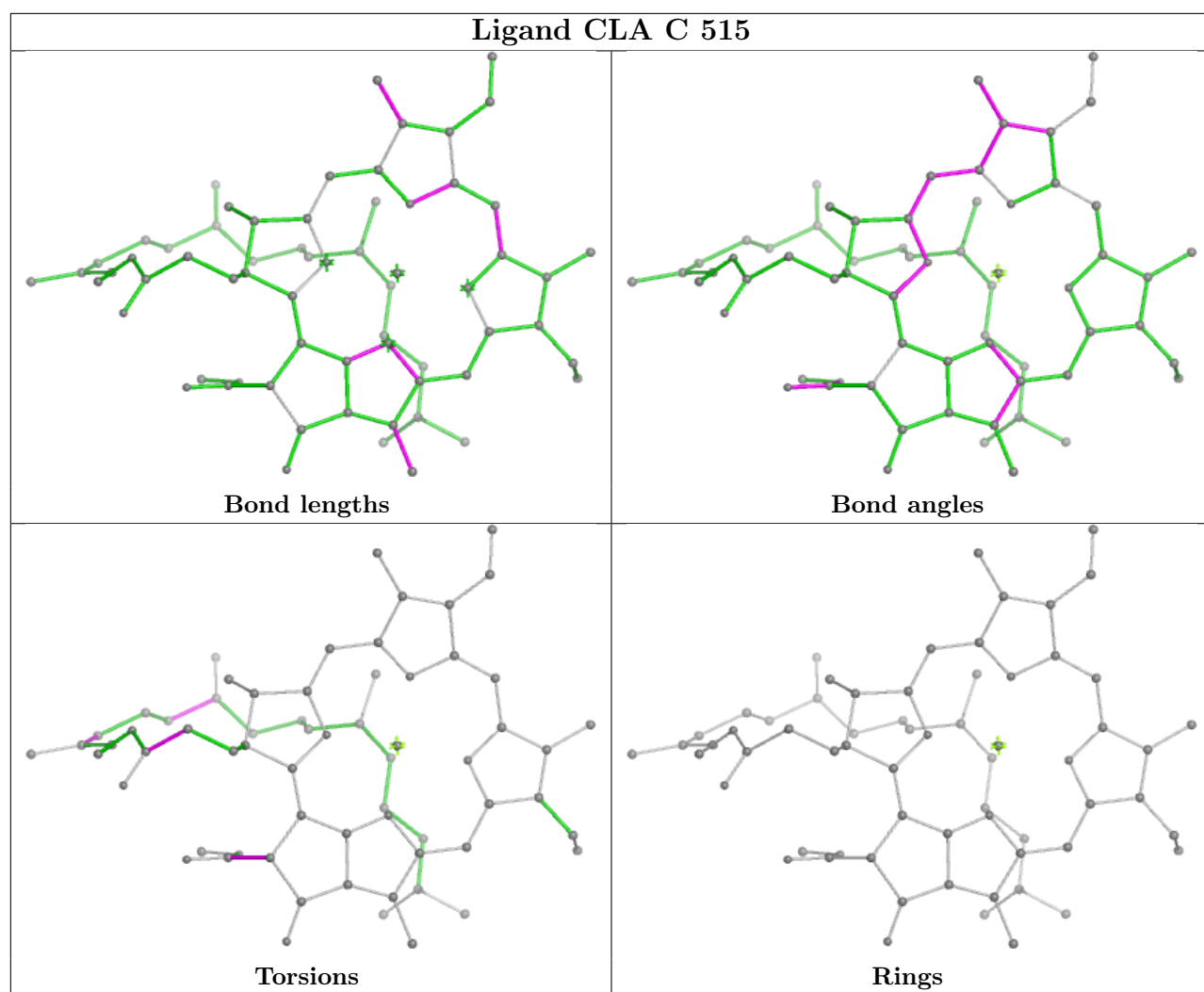




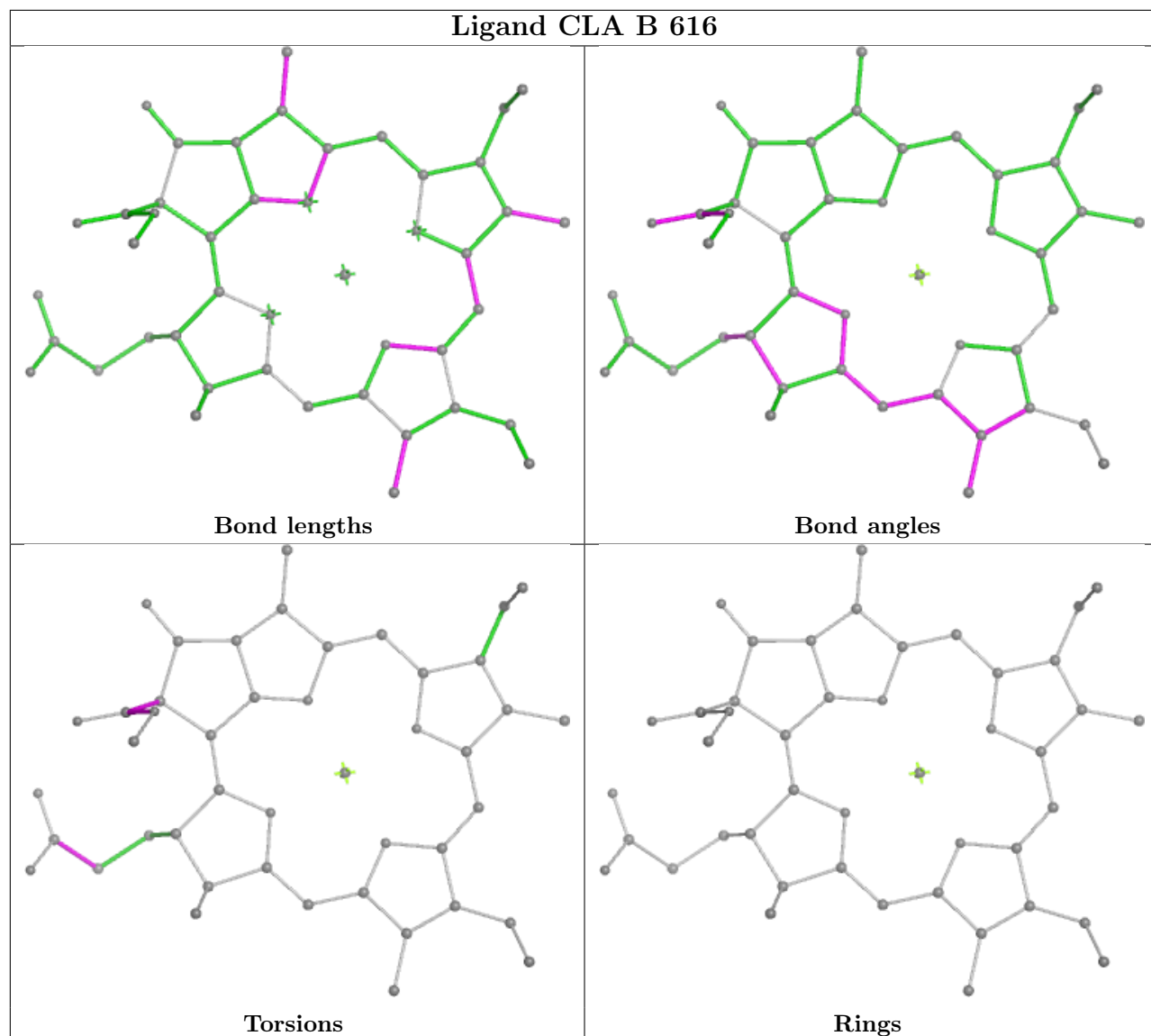




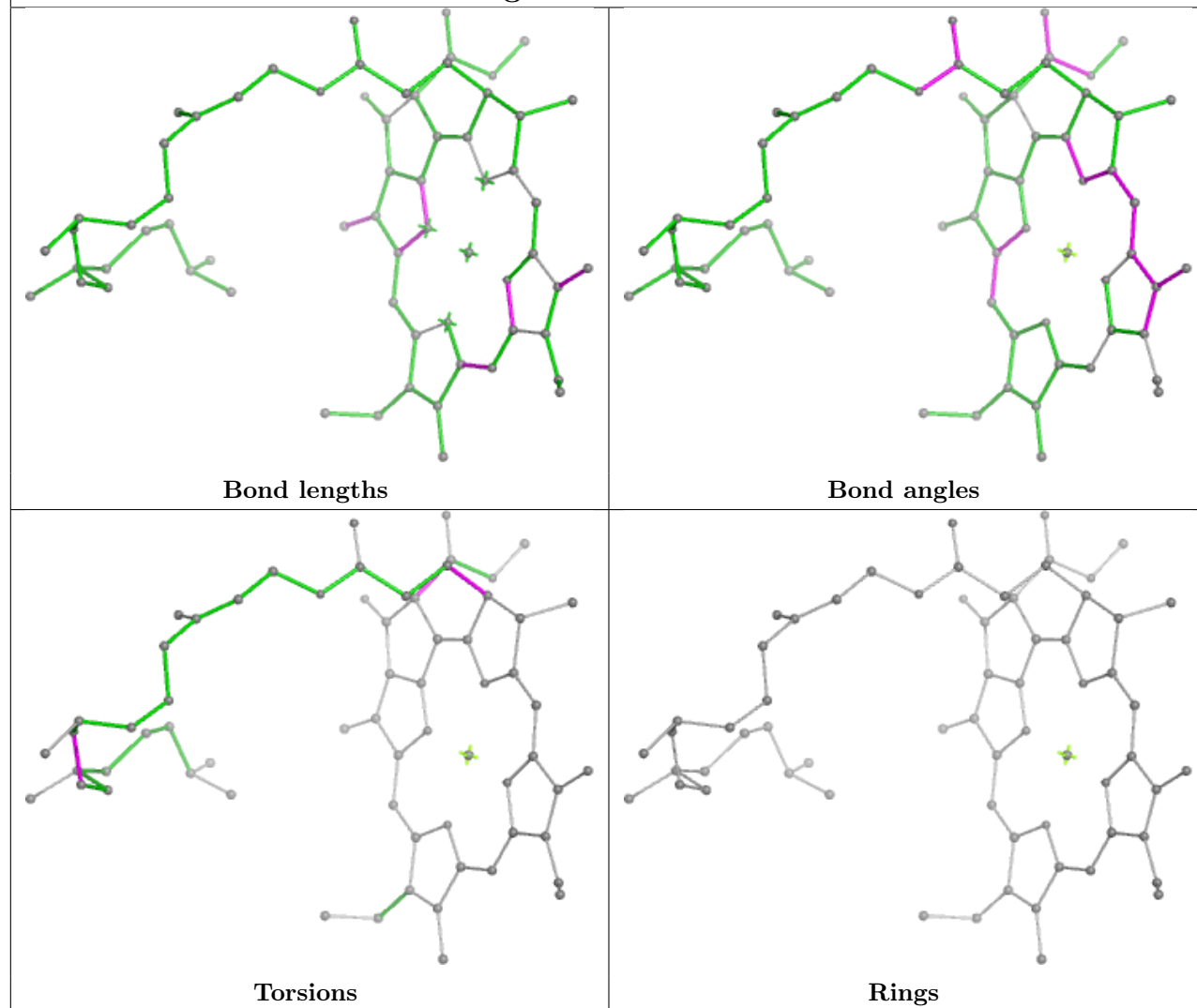




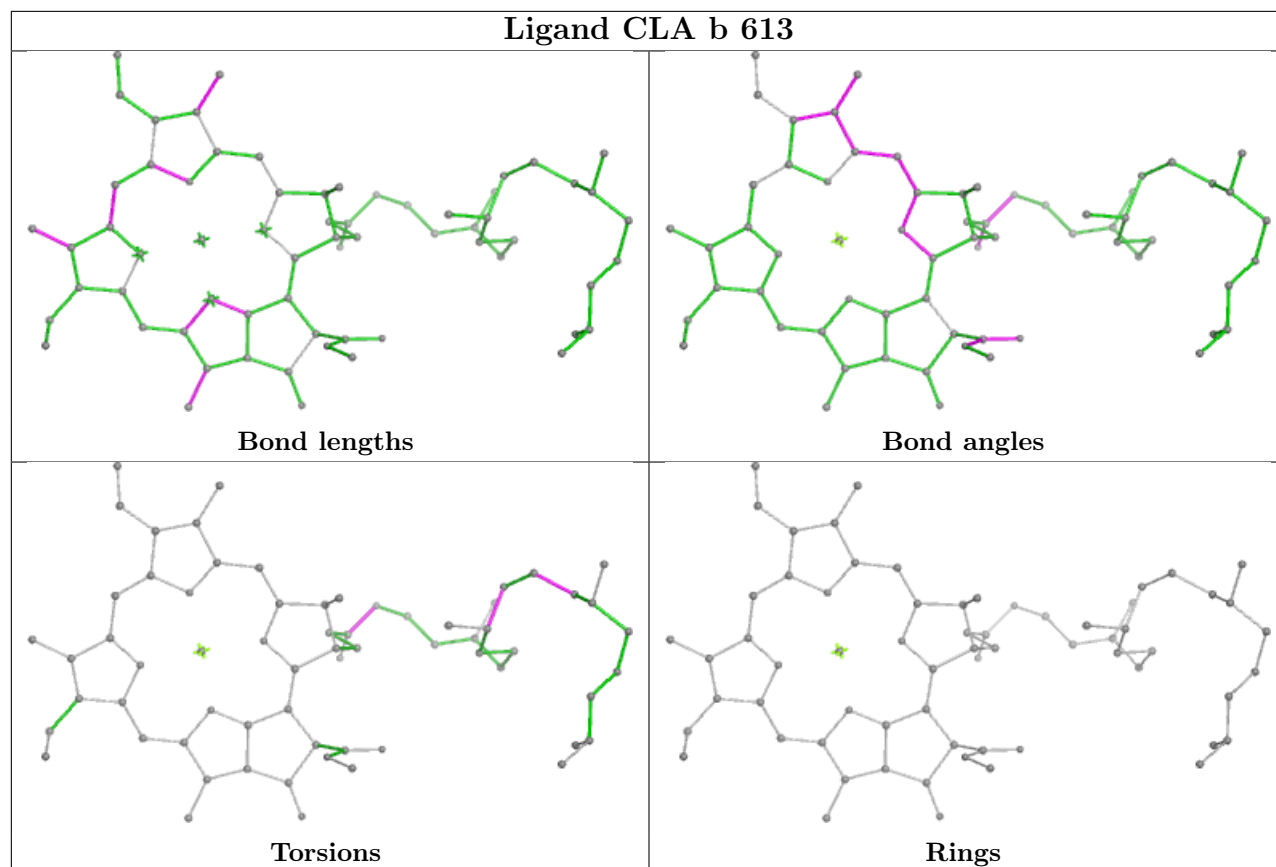
Ligand CLA B 616



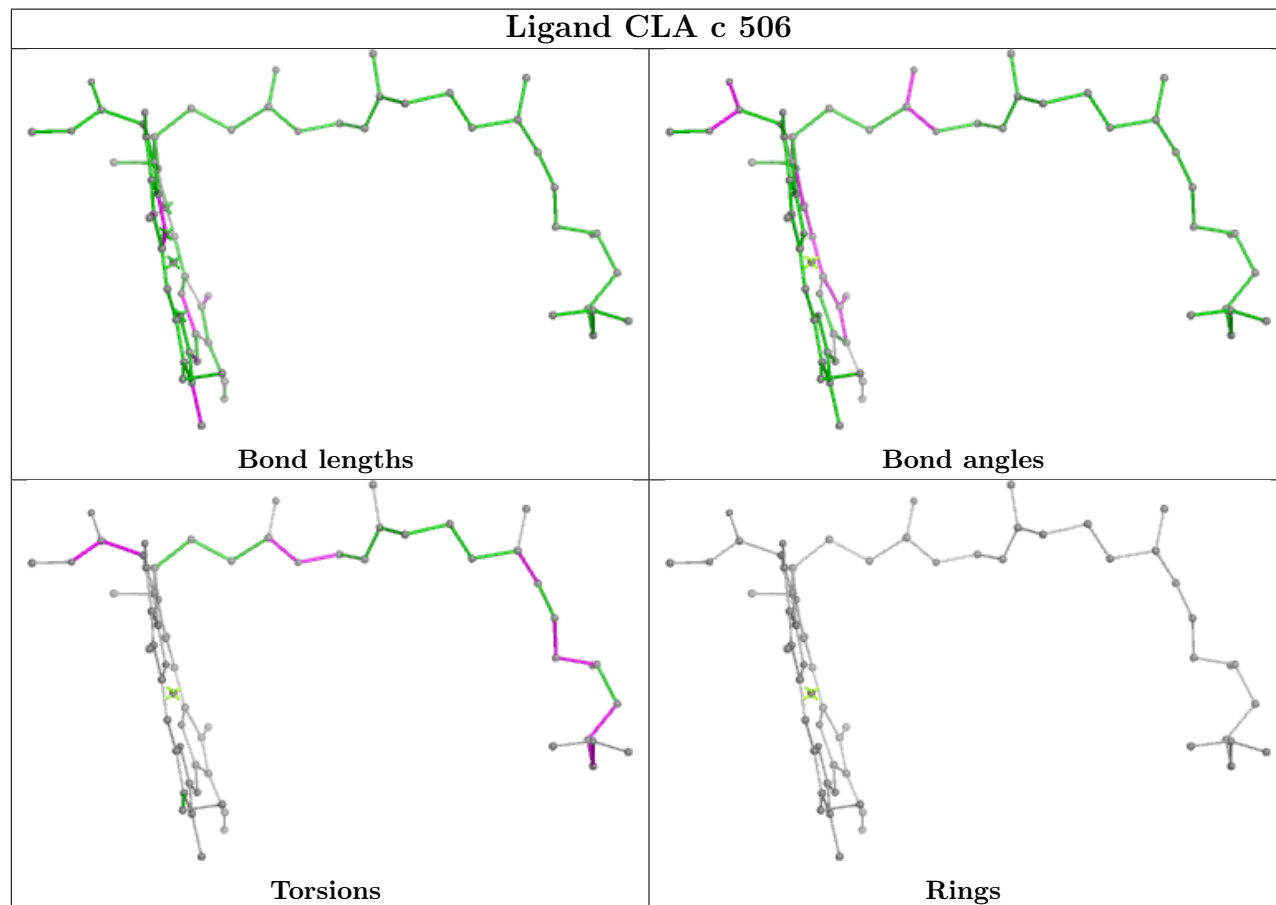
Ligand CLA c 503

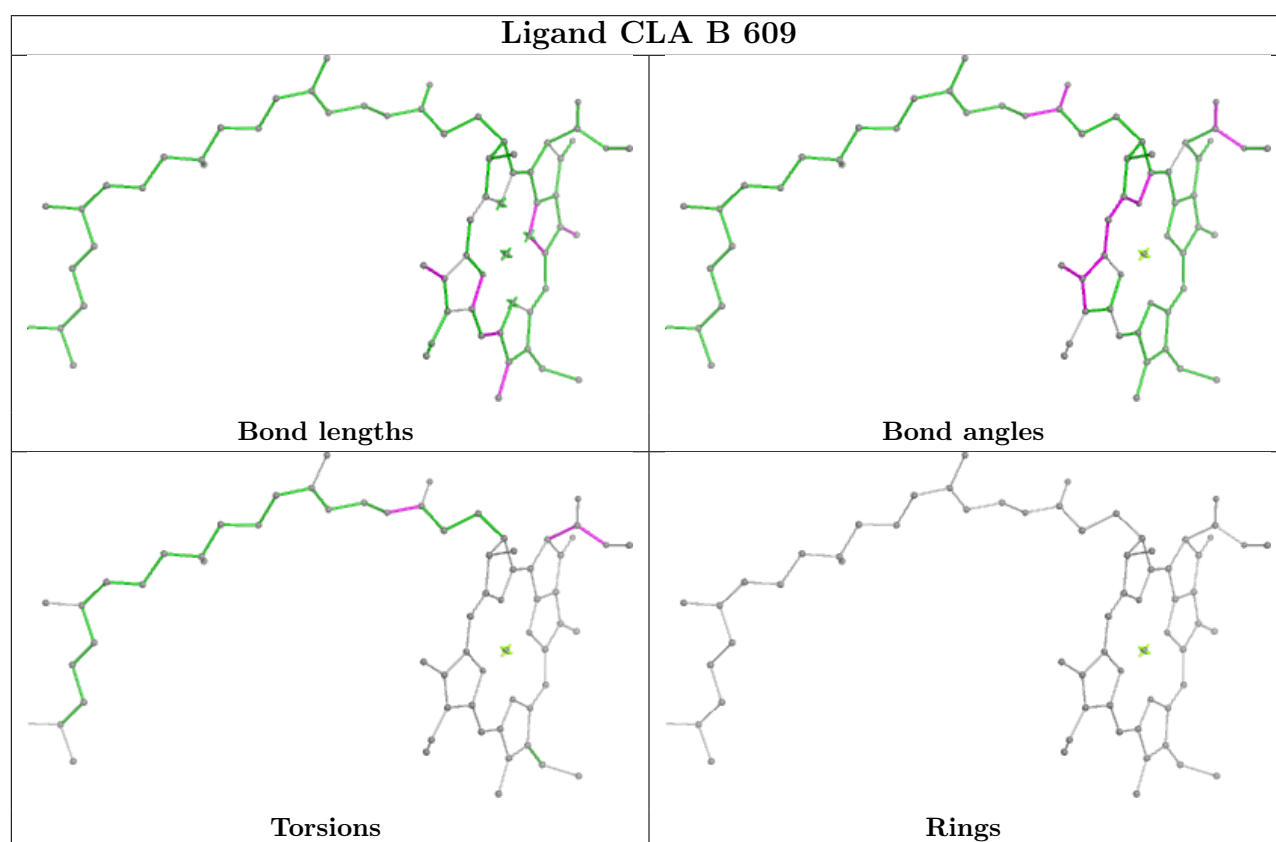
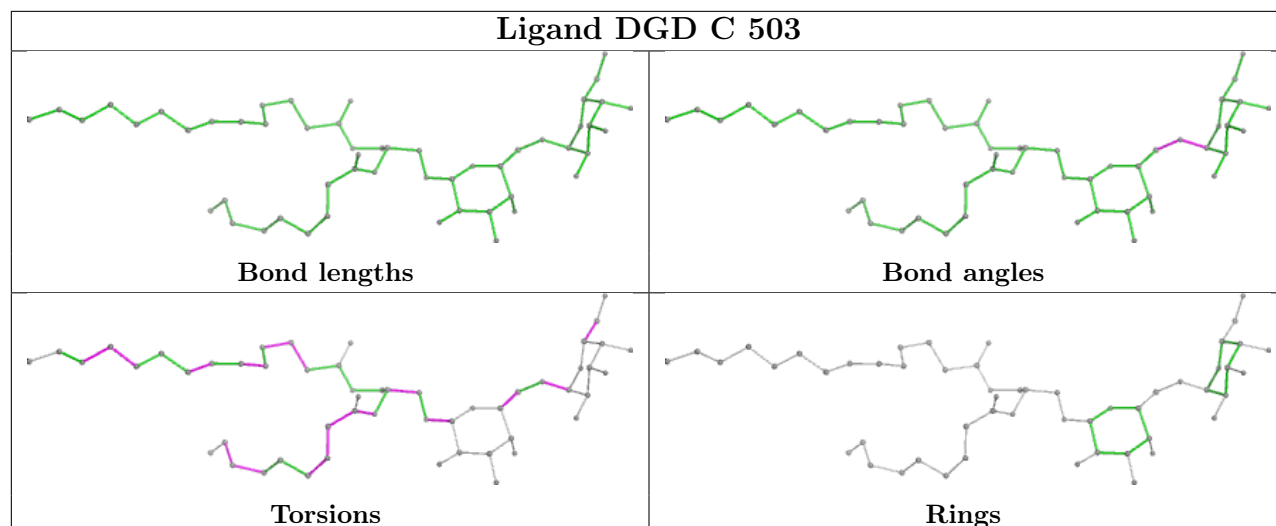


Ligand CLA b 613

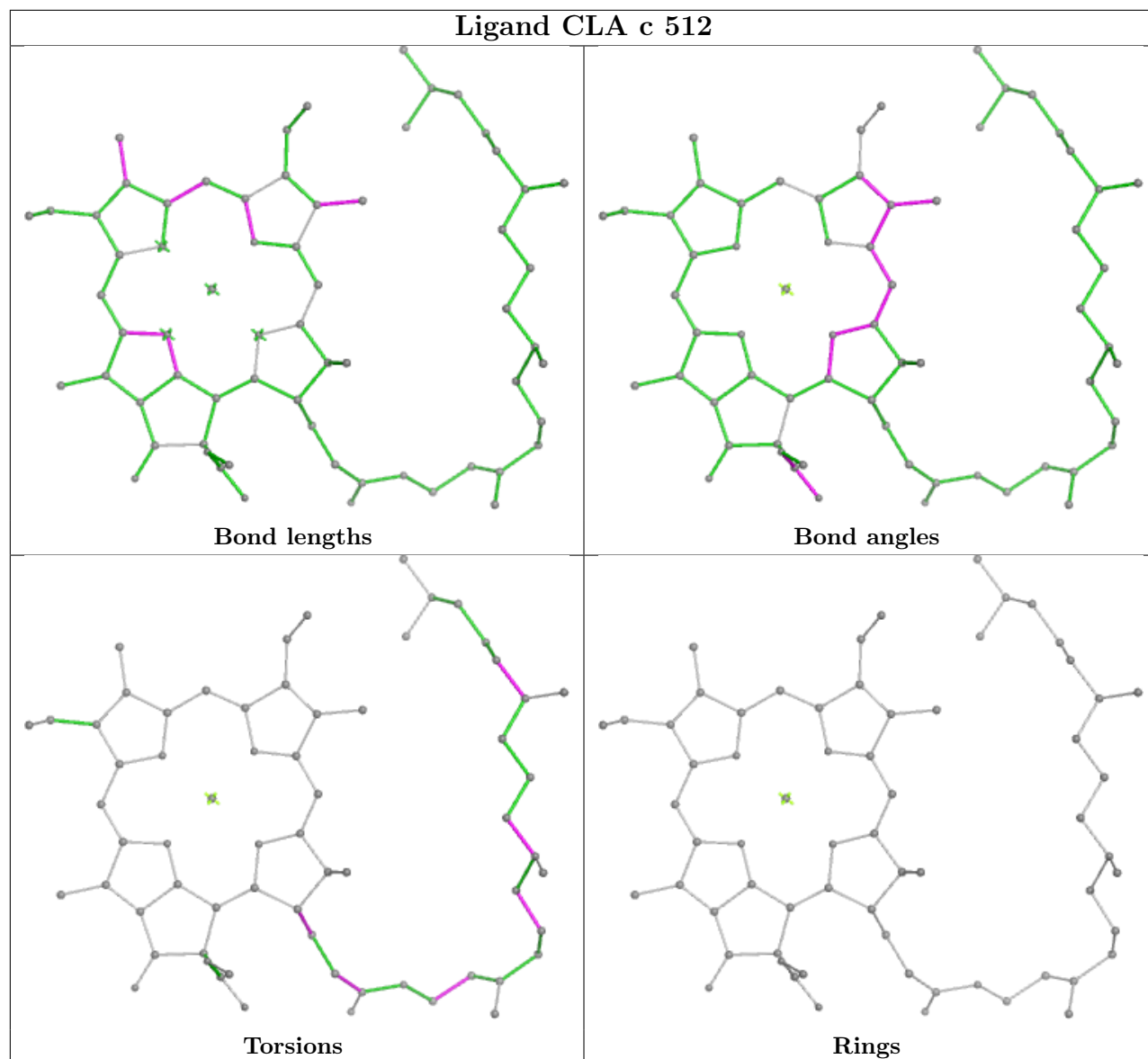


Ligand CLA c 506

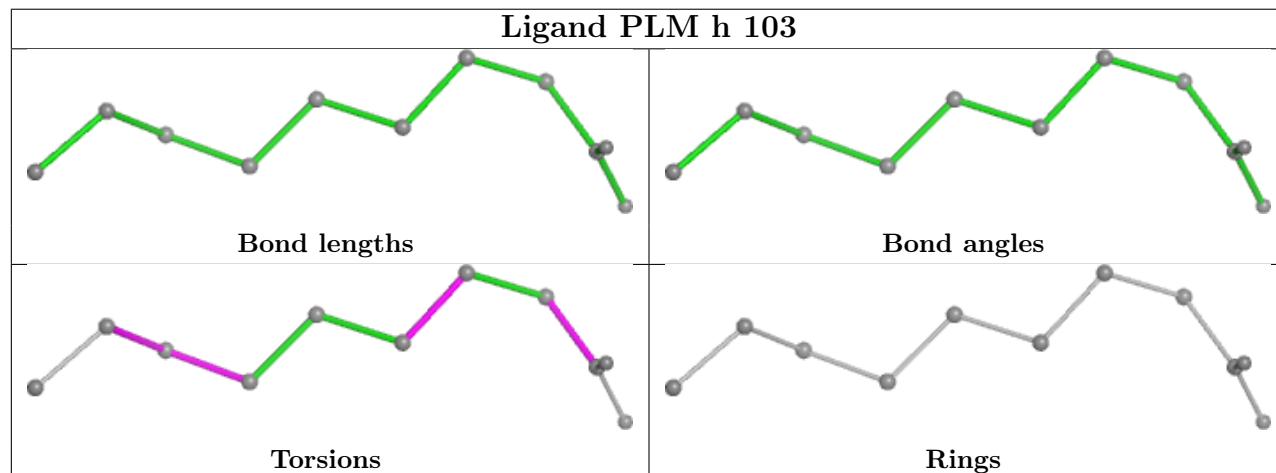




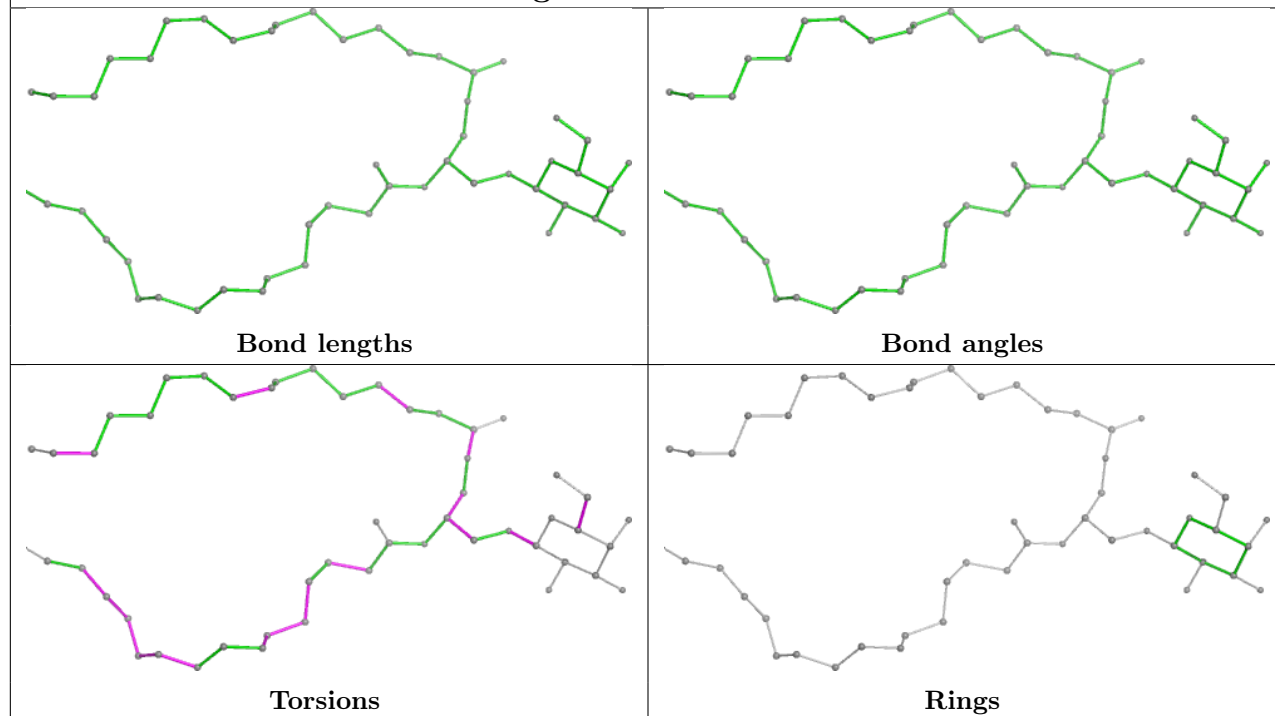
Ligand CLA c 512



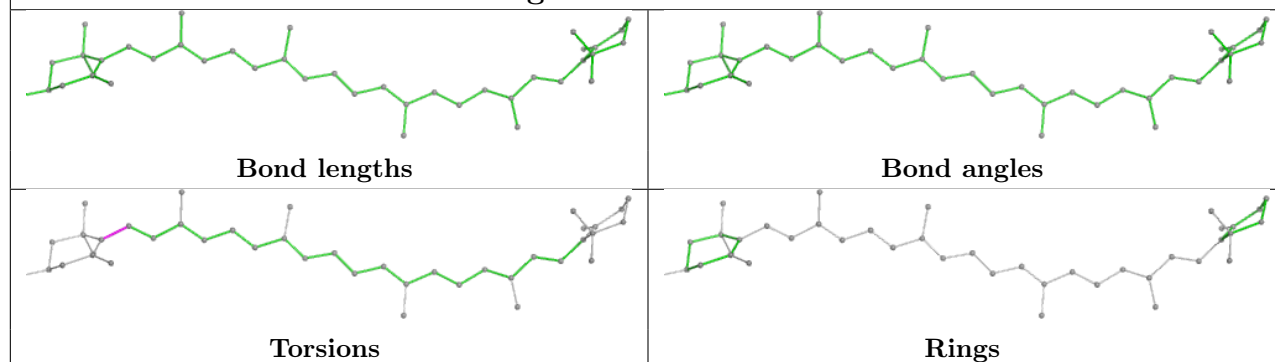
Ligand PLM h 103



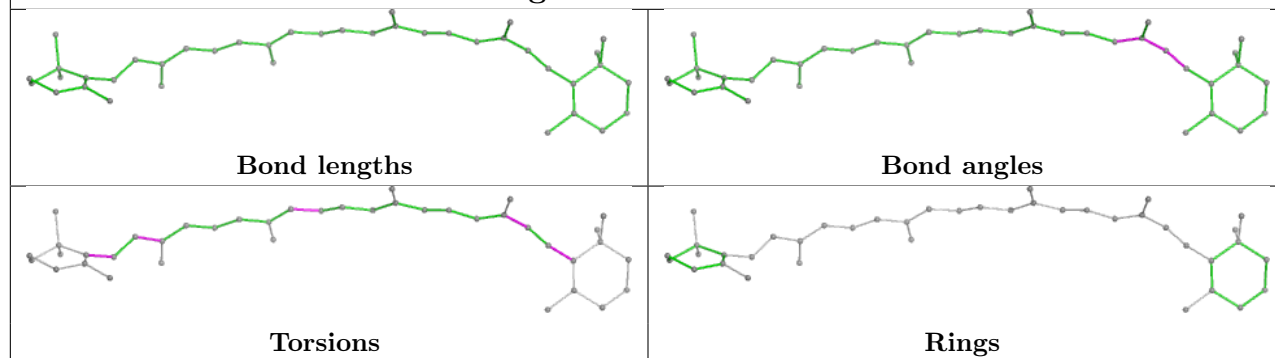
Ligand LMG I 103

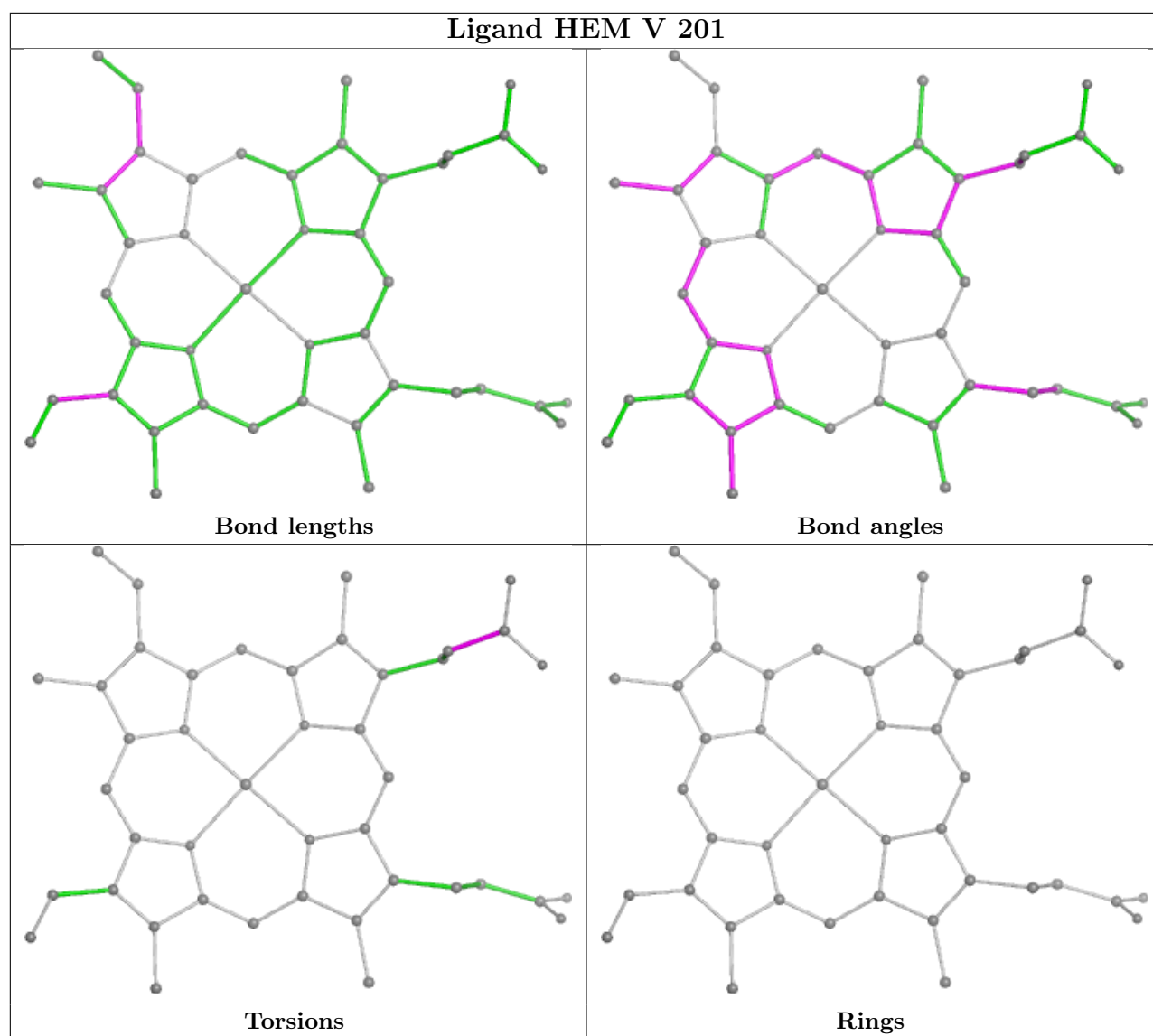


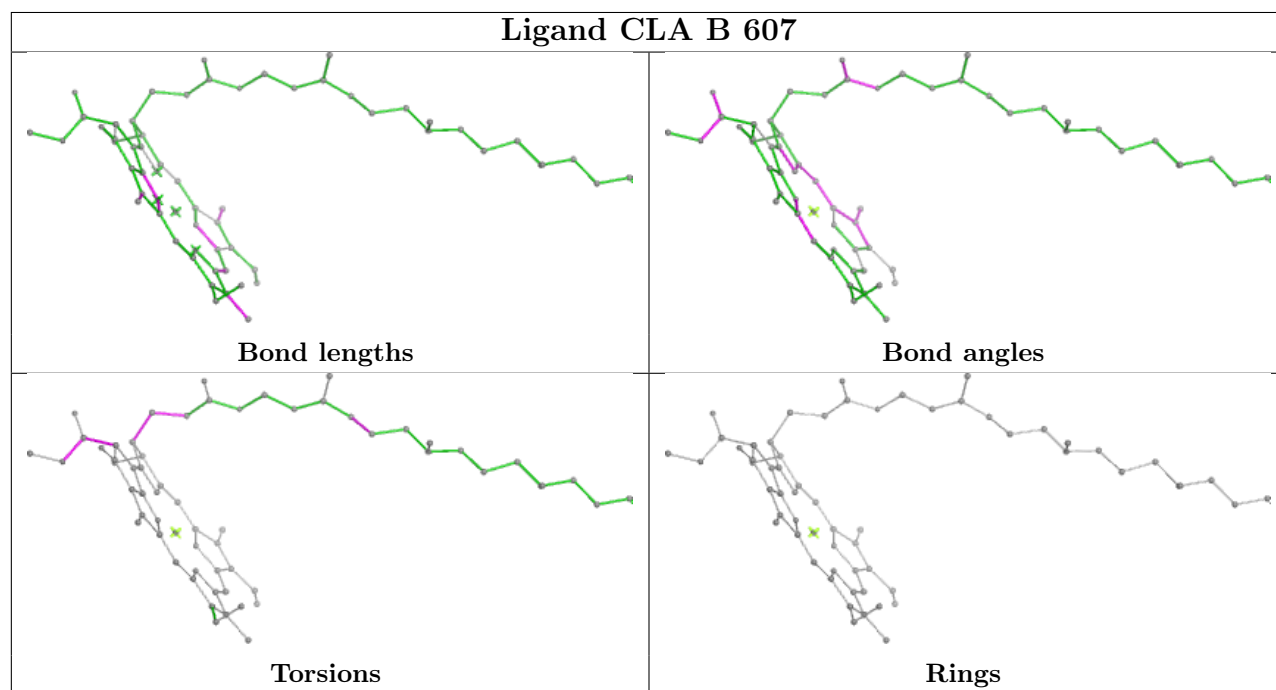
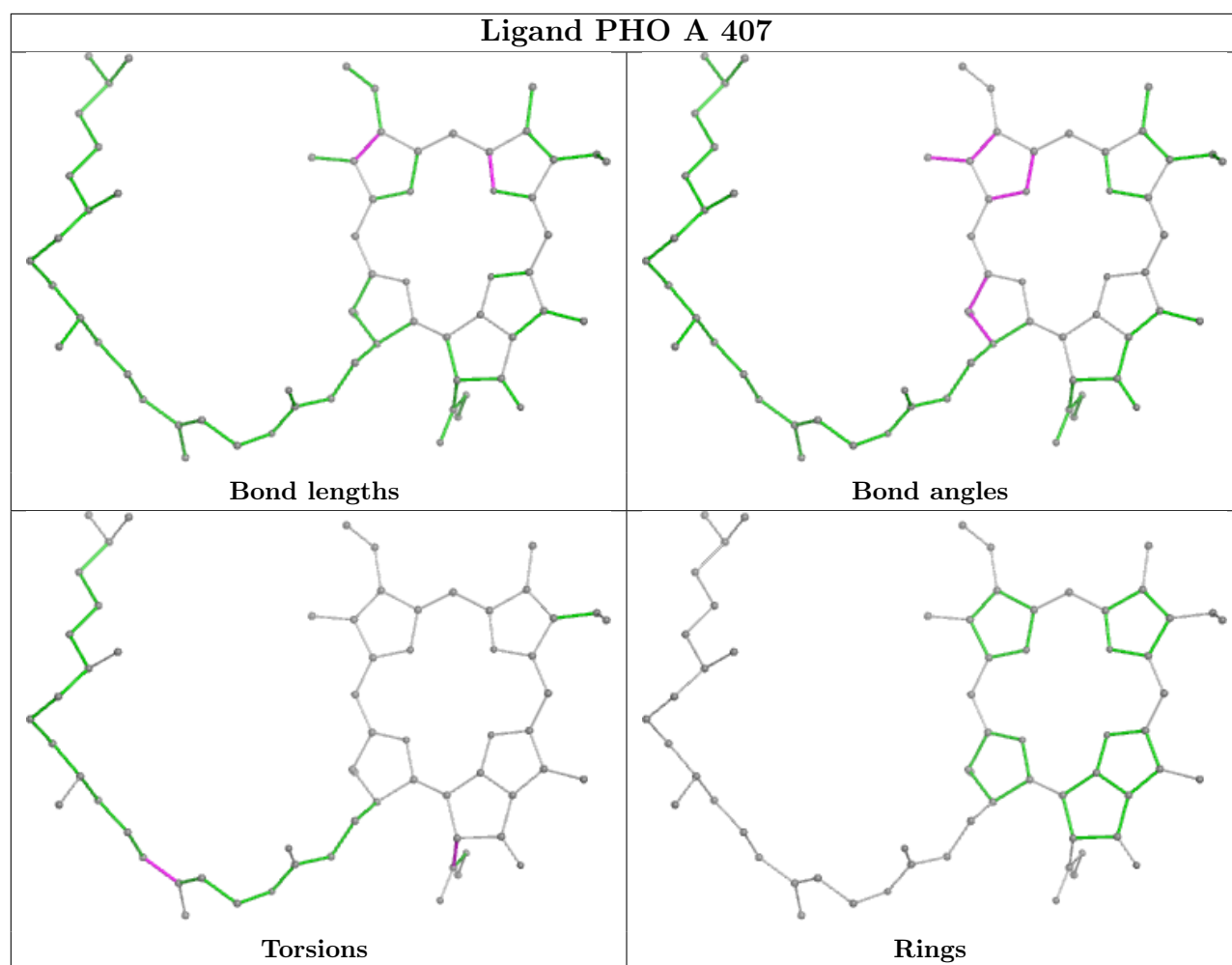
Ligand RRX H 102



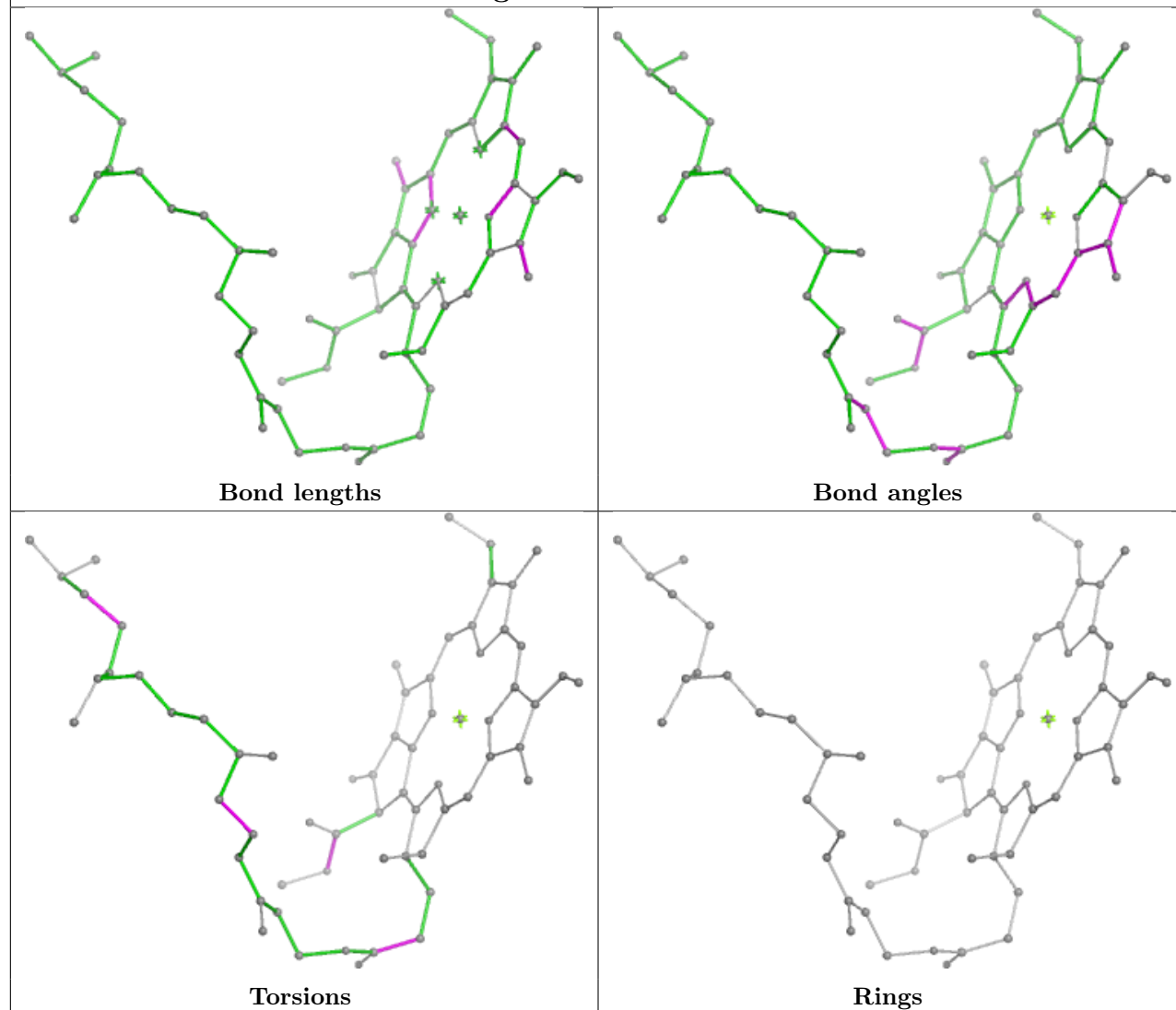
Ligand BCR D 403

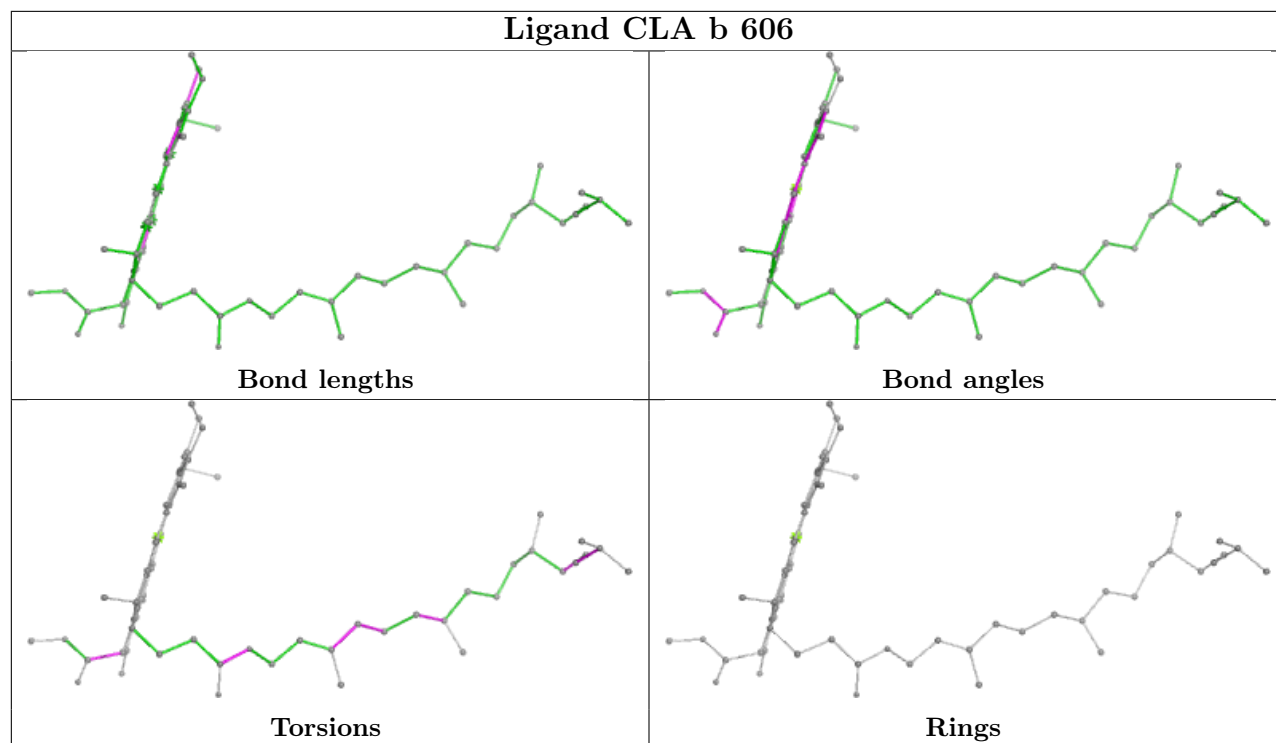




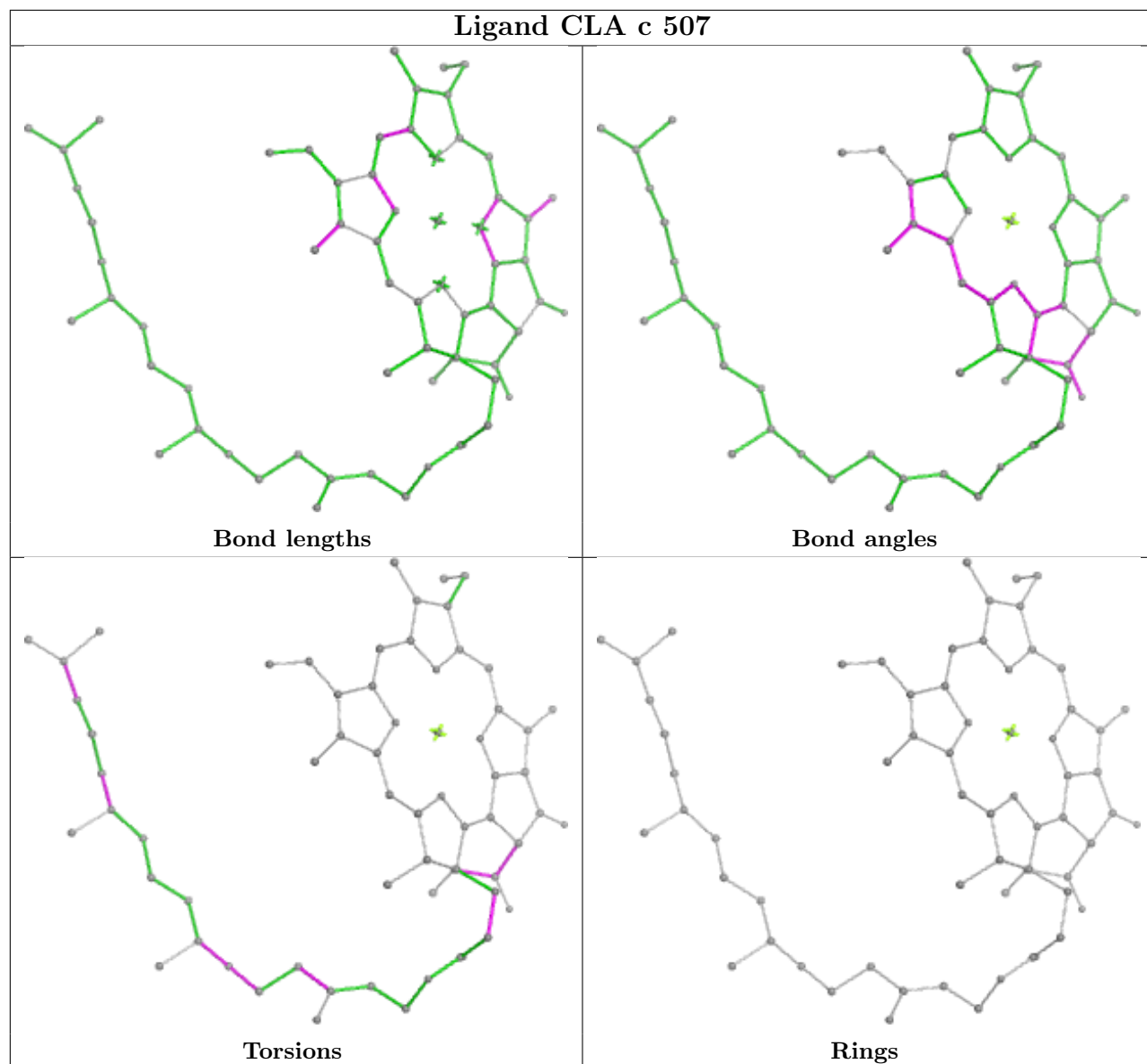


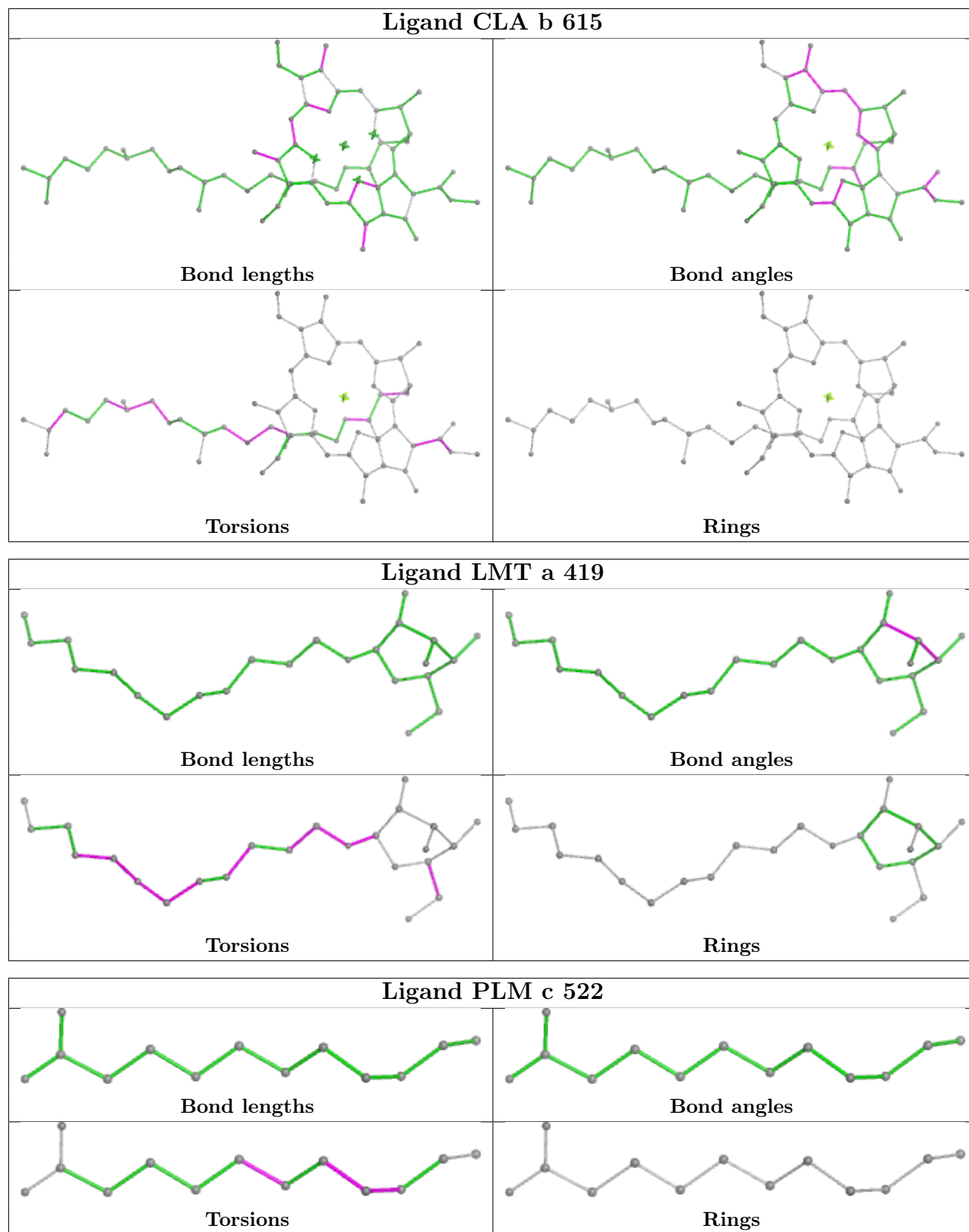
Ligand CLA b 614

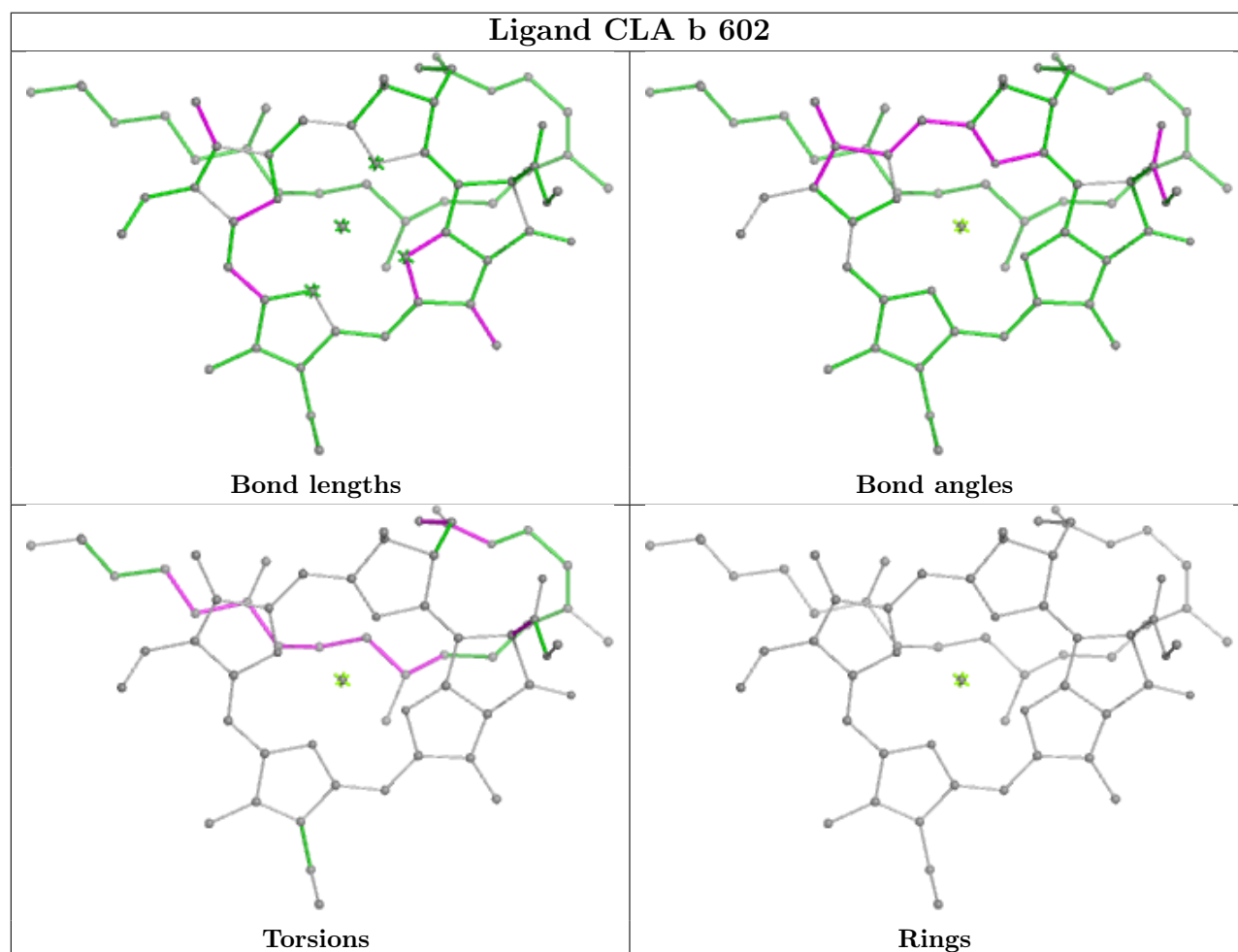
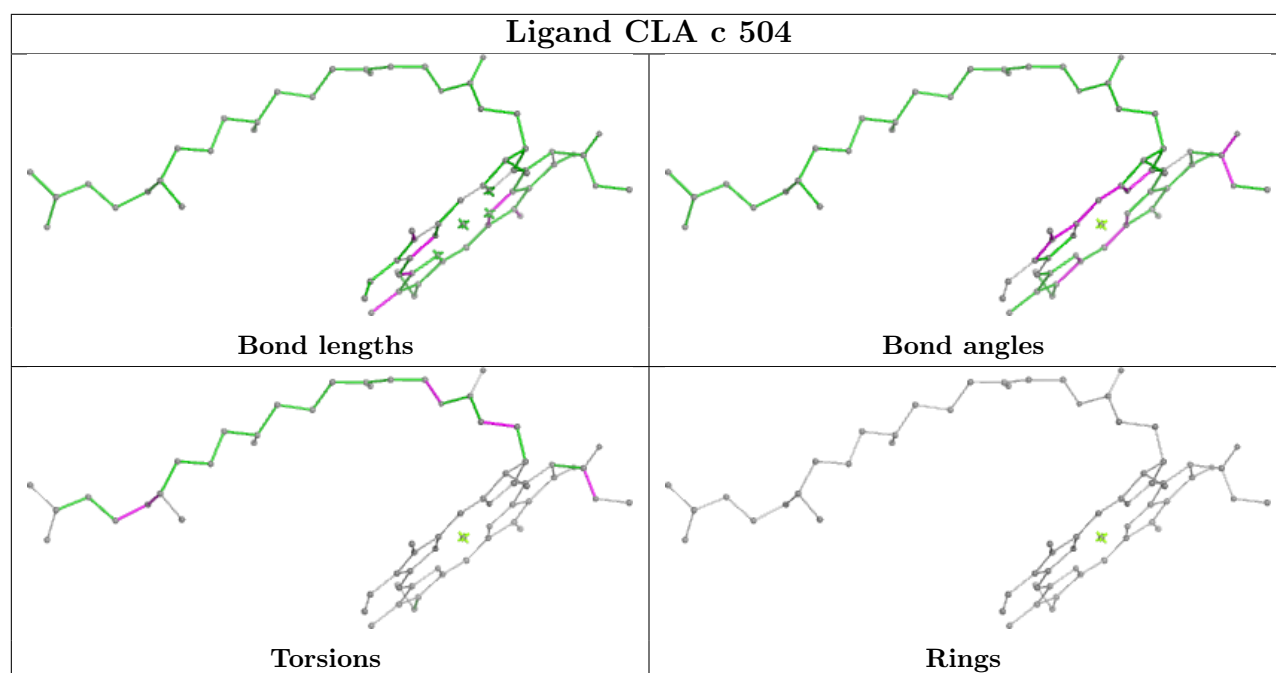


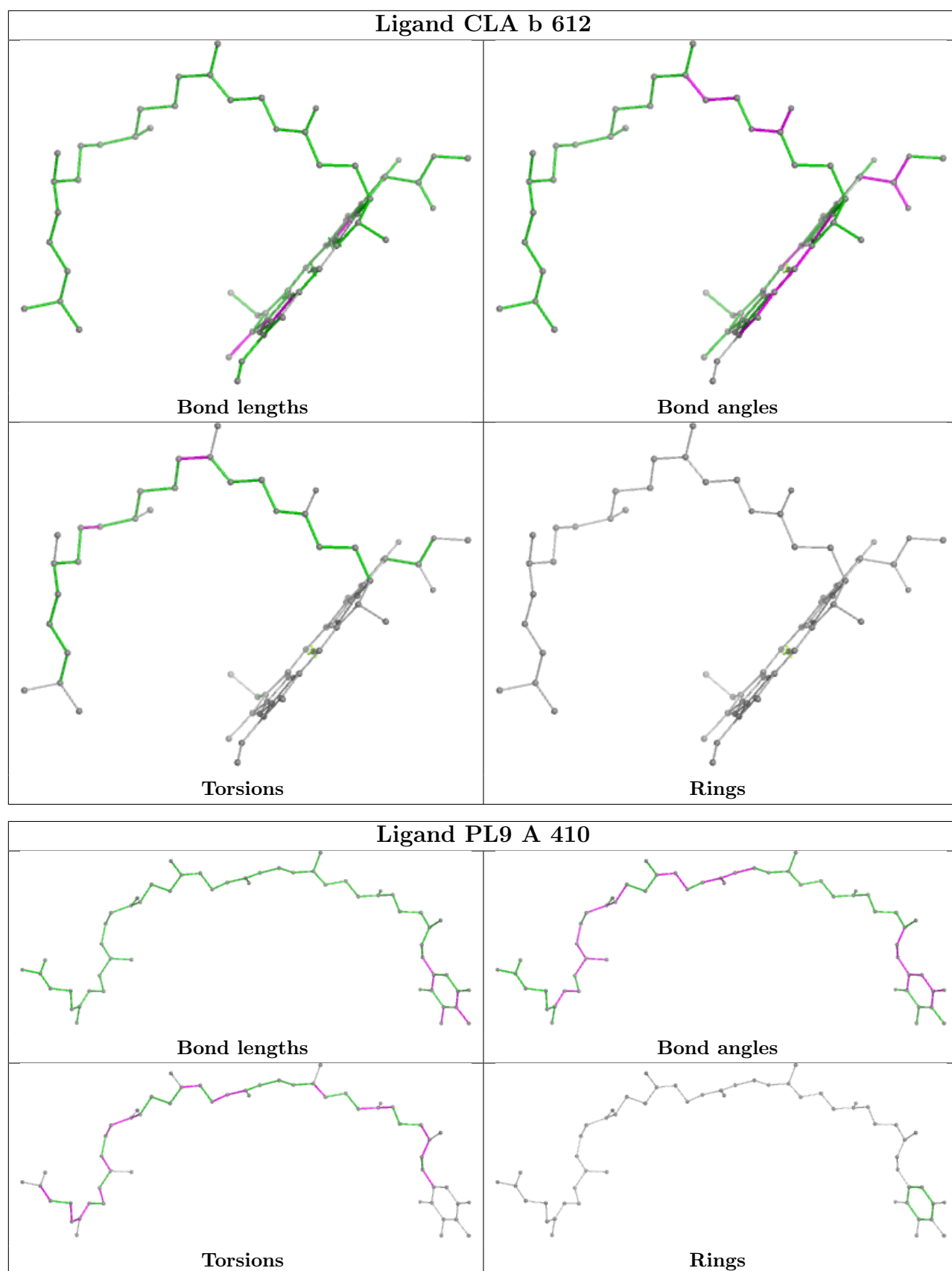


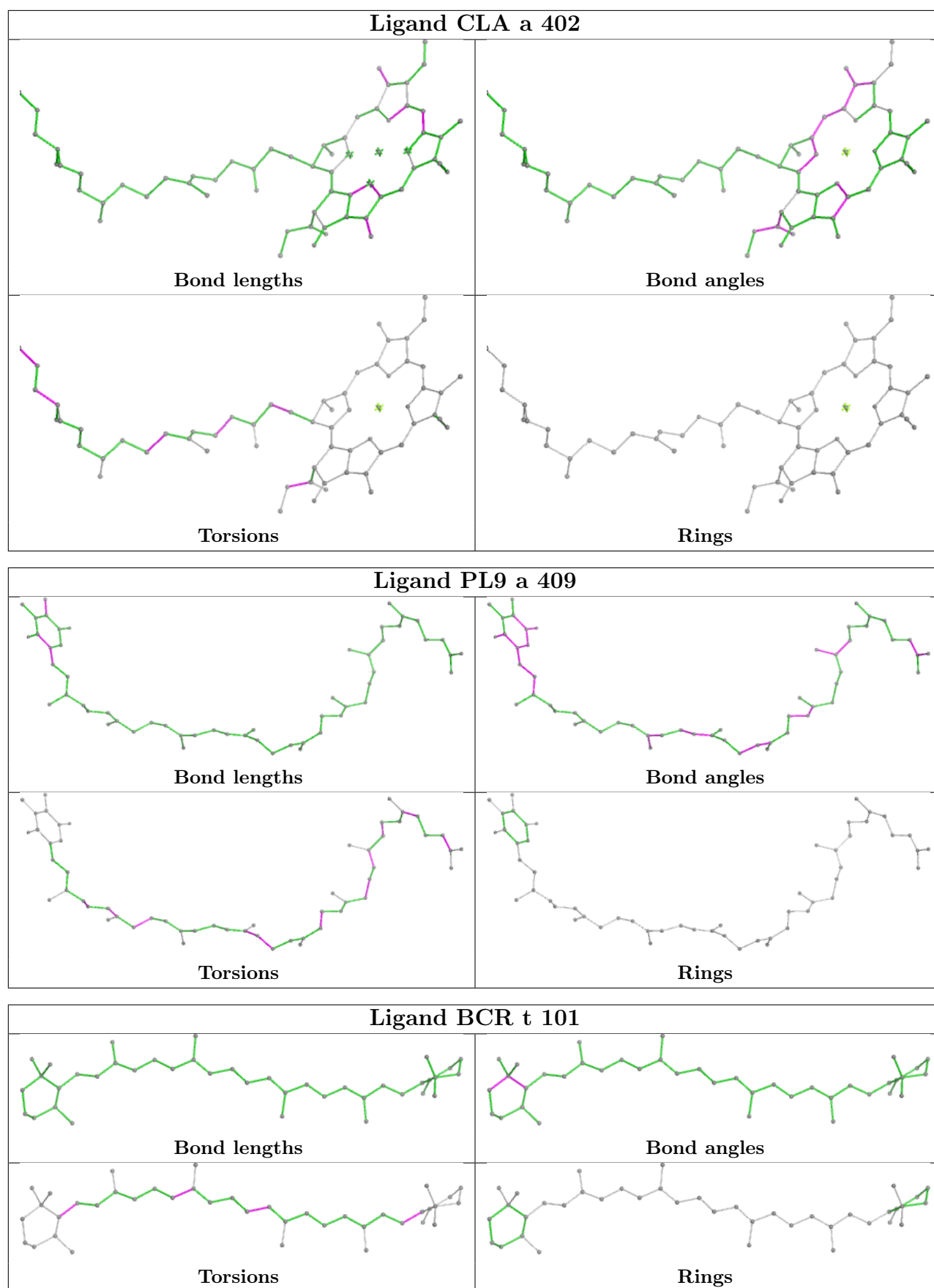
Ligand CLA c 507

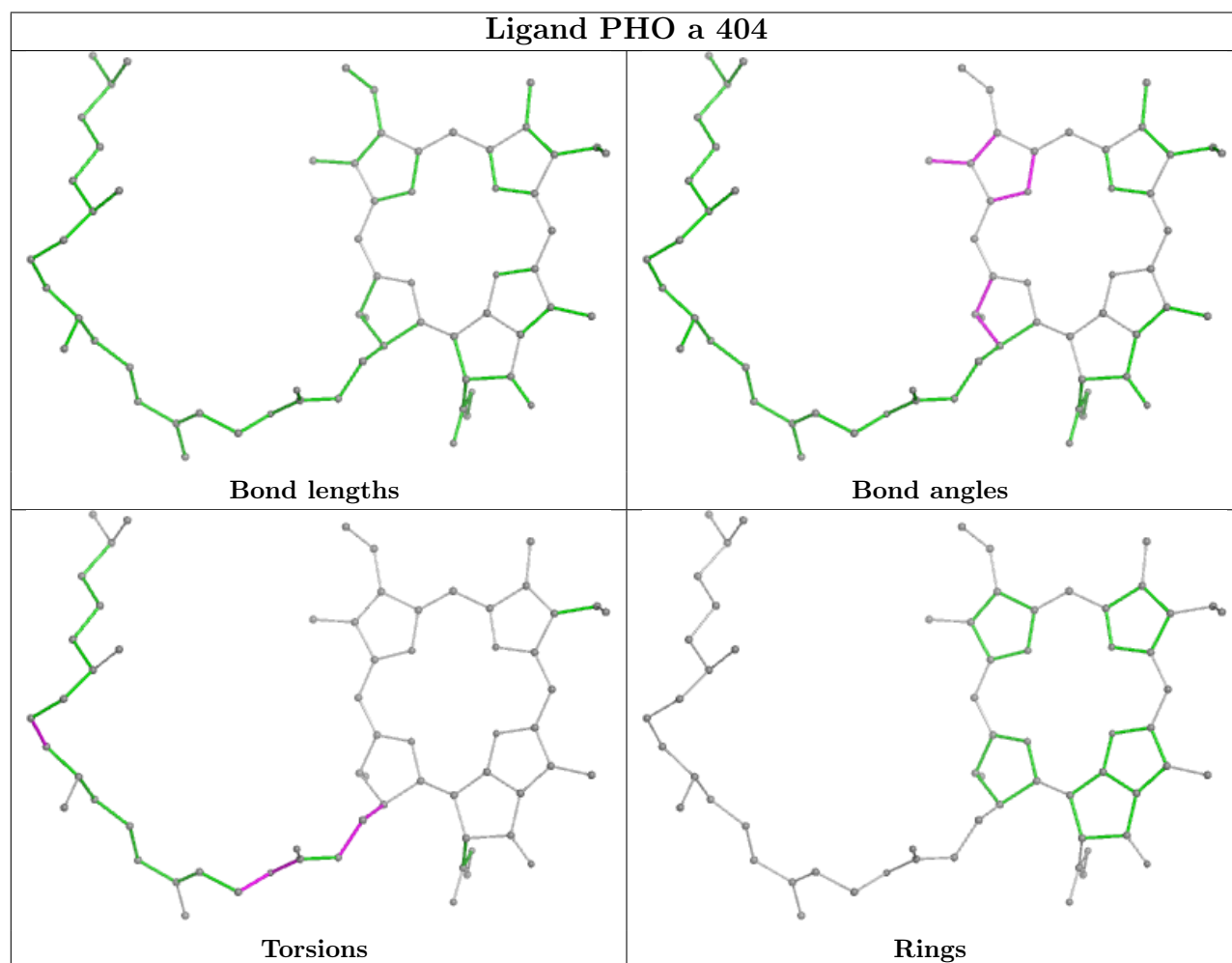
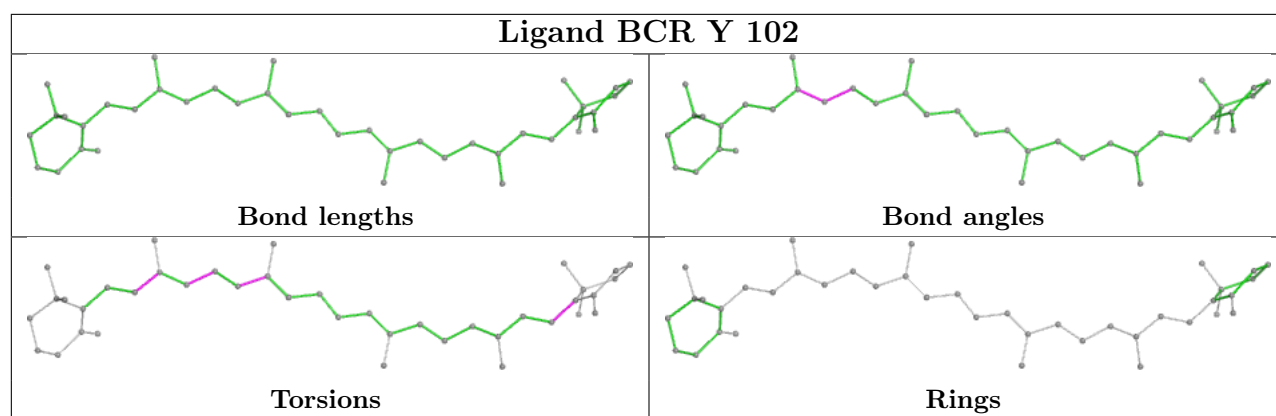


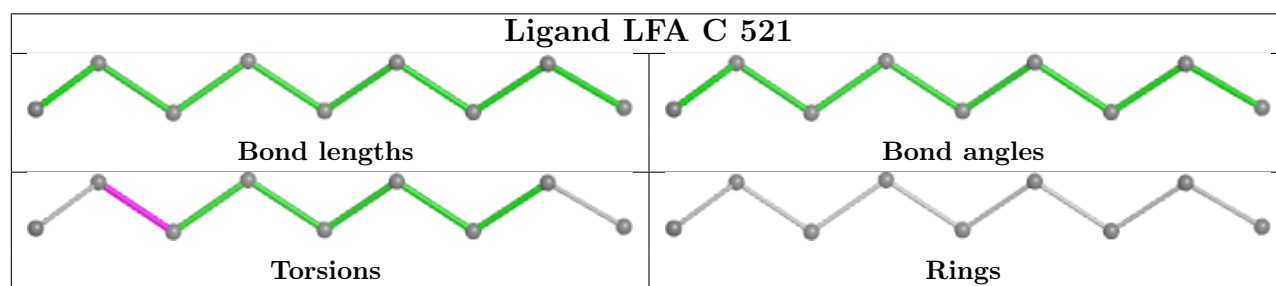
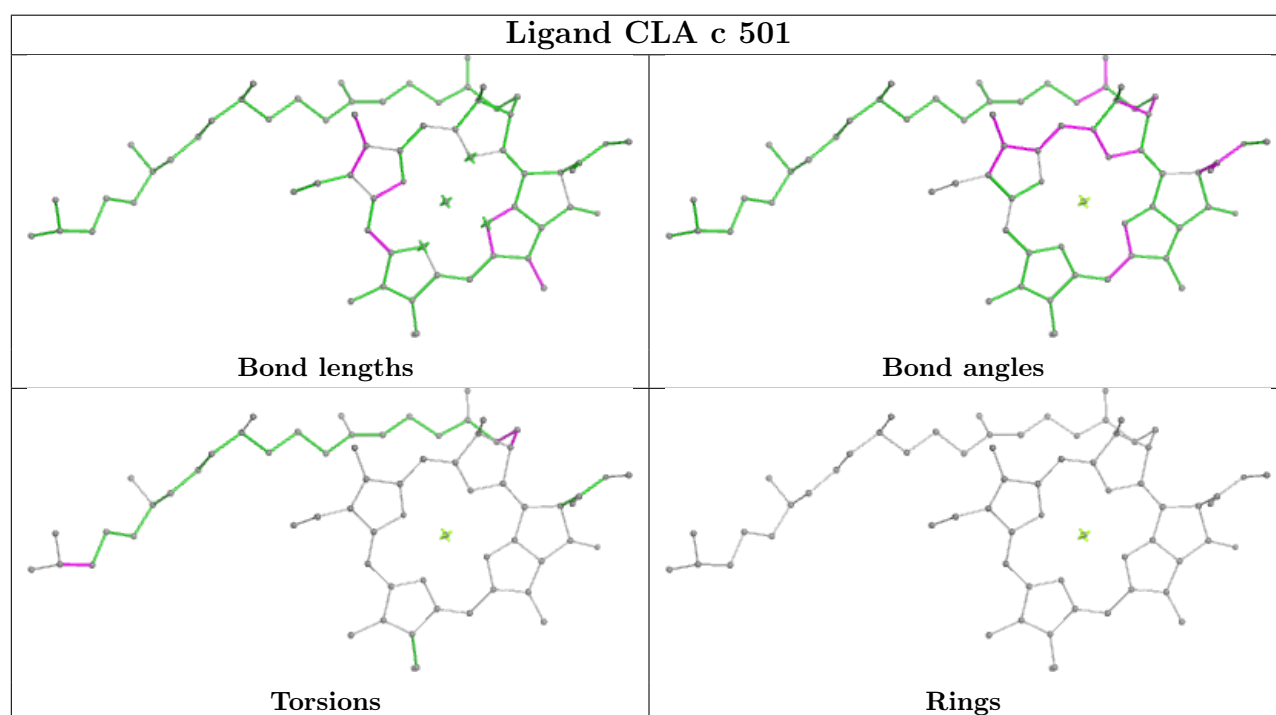
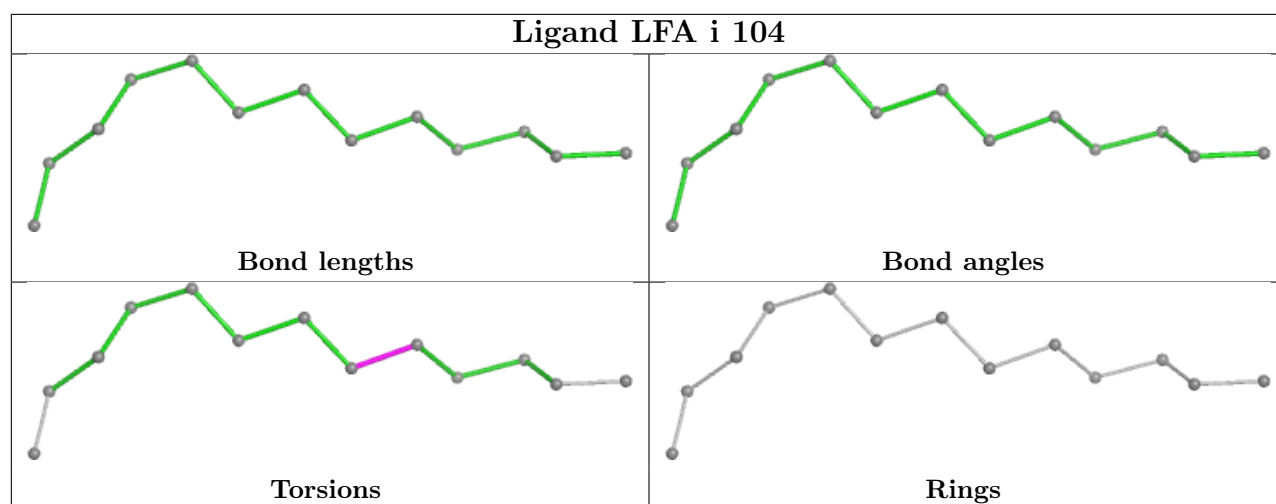


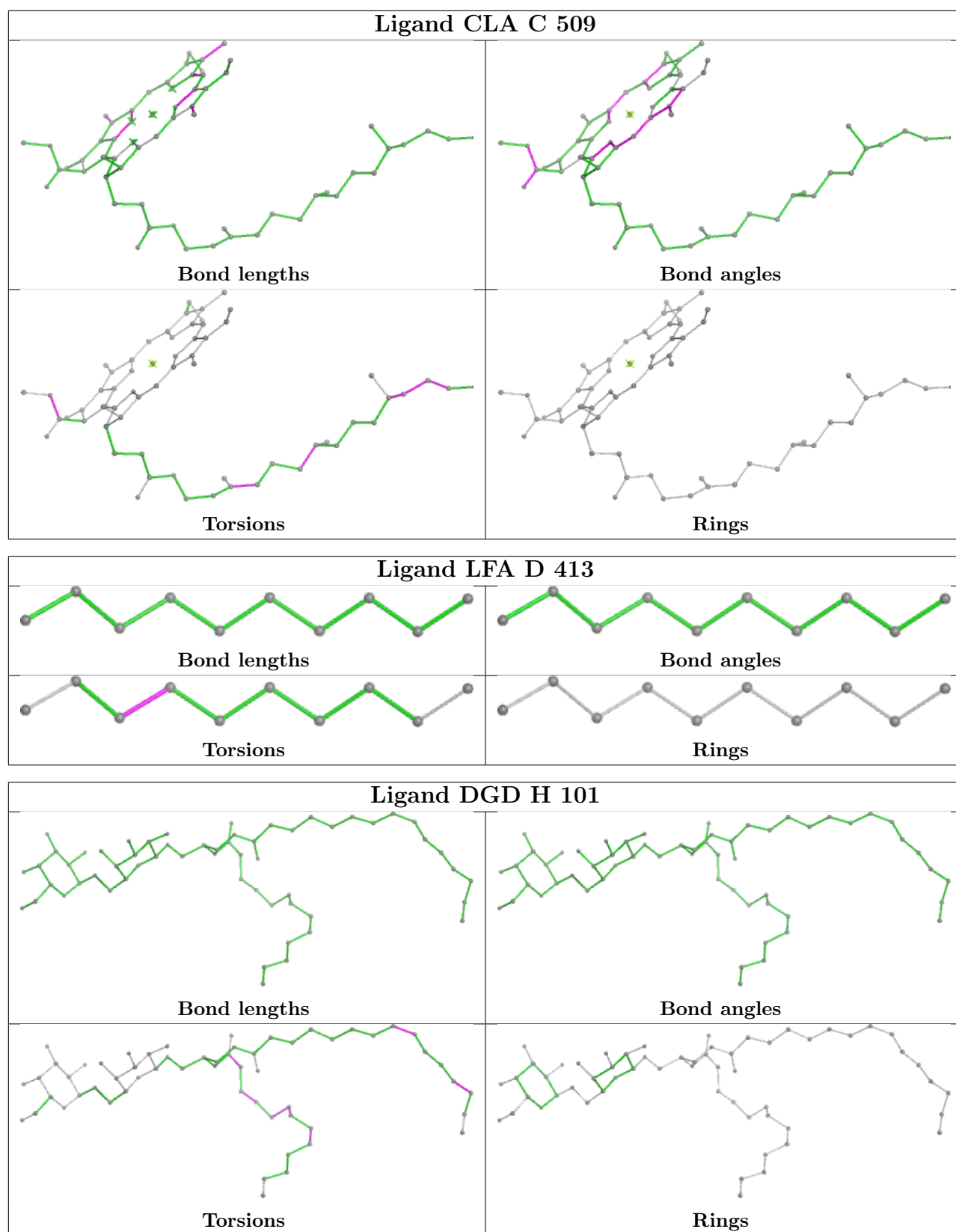


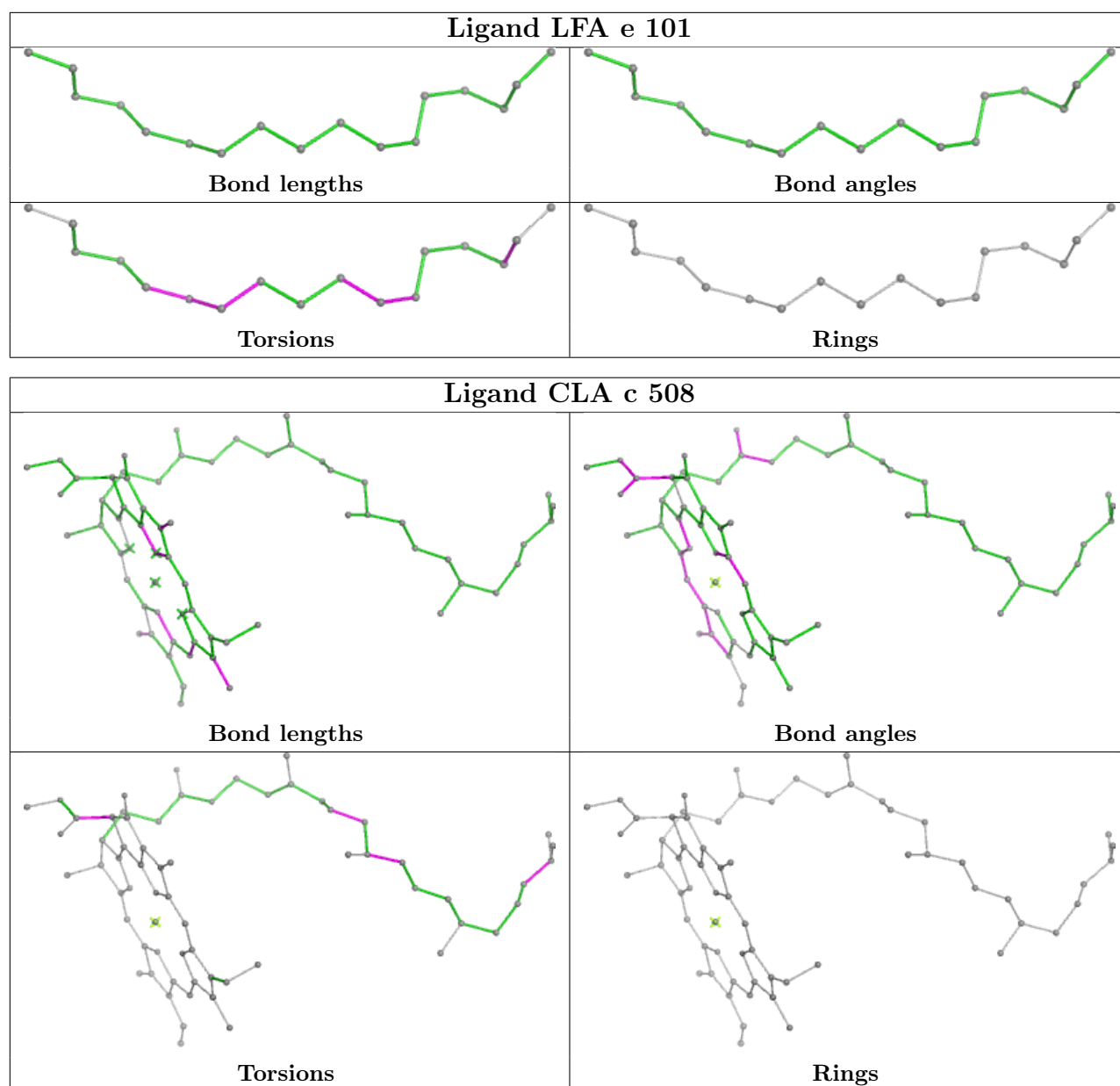












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

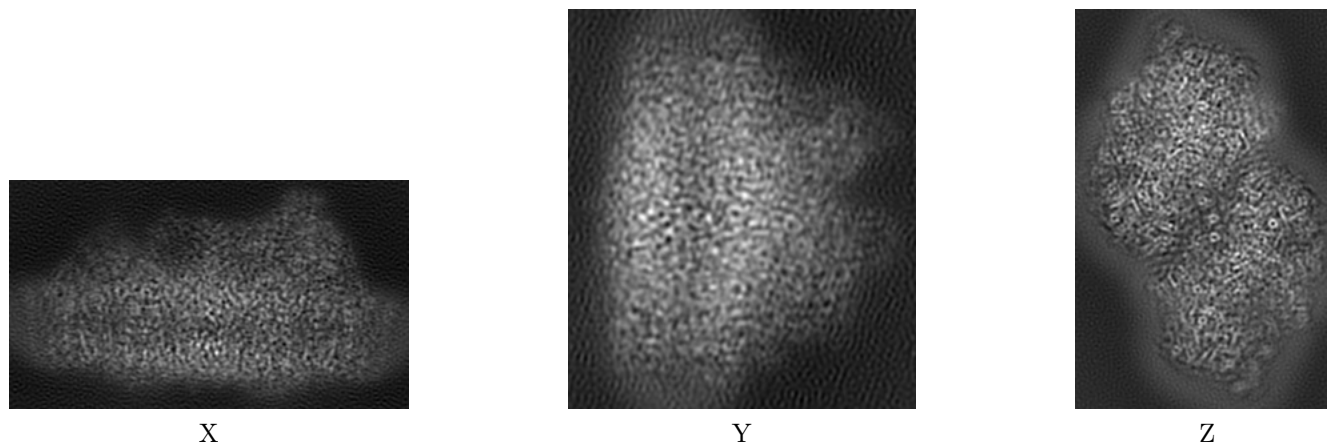
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51101. These allow visual inspection of the internal detail of the map and identification of artifacts.

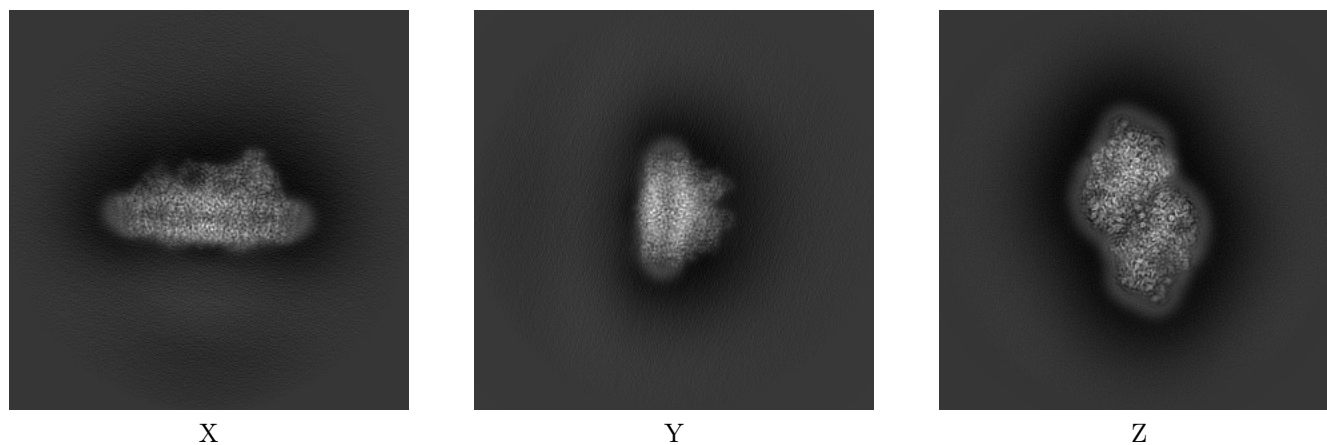
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



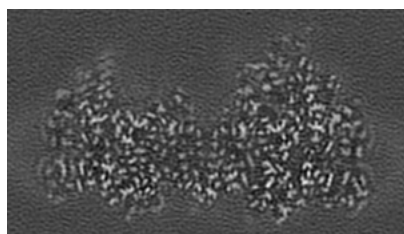
6.1.2 Raw map



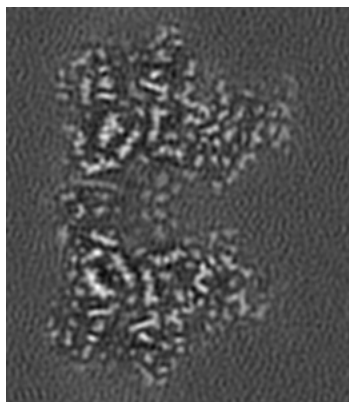
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

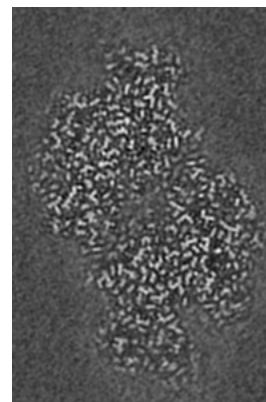
6.2.1 Primary map



X Index: 137

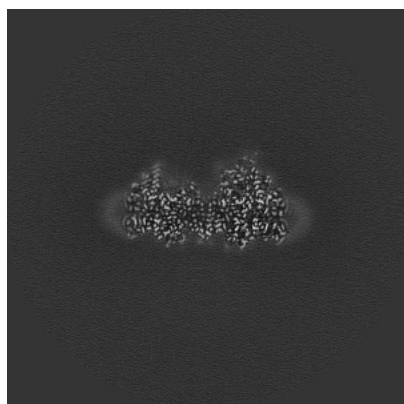


Y Index: 208

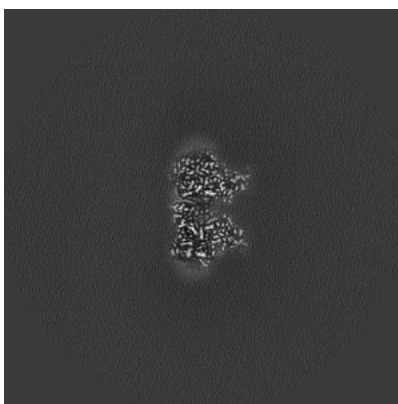


Z Index: 119

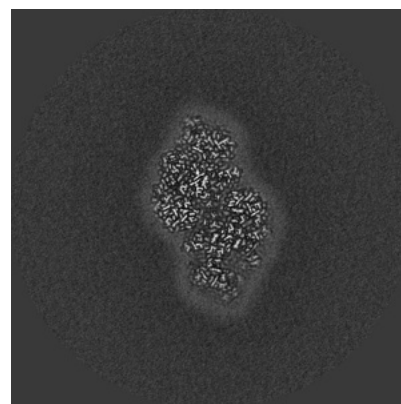
6.2.2 Raw map



X Index: 200



Y Index: 200

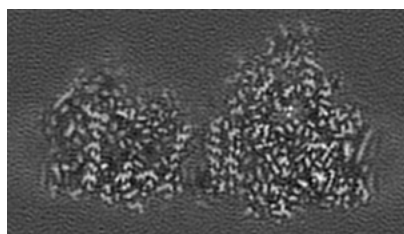


Z Index: 200

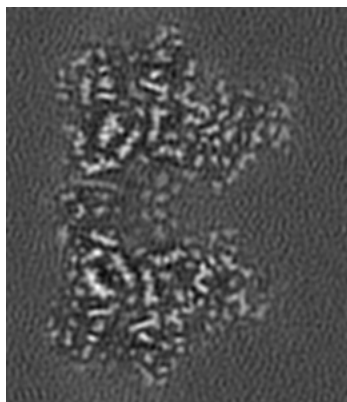
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

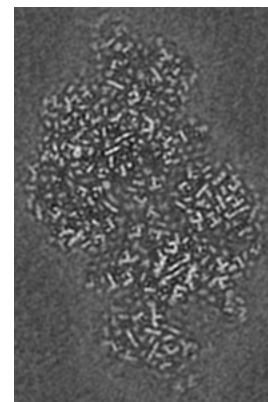
6.3.1 Primary map



X Index: 129

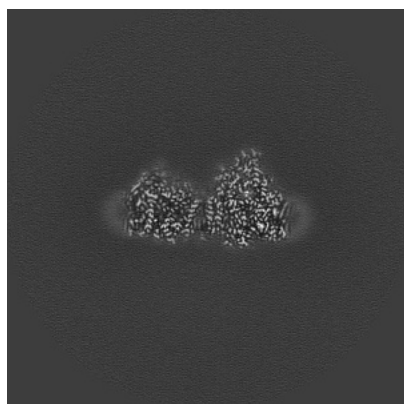


Y Index: 208

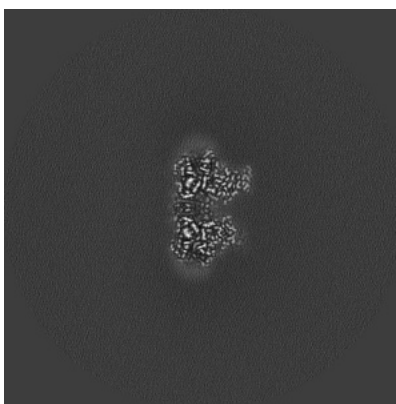


Z Index: 105

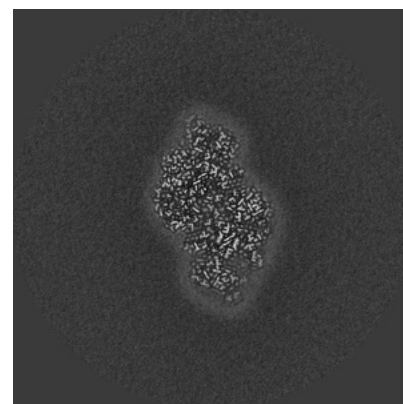
6.3.2 Raw map



X Index: 196



Y Index: 198

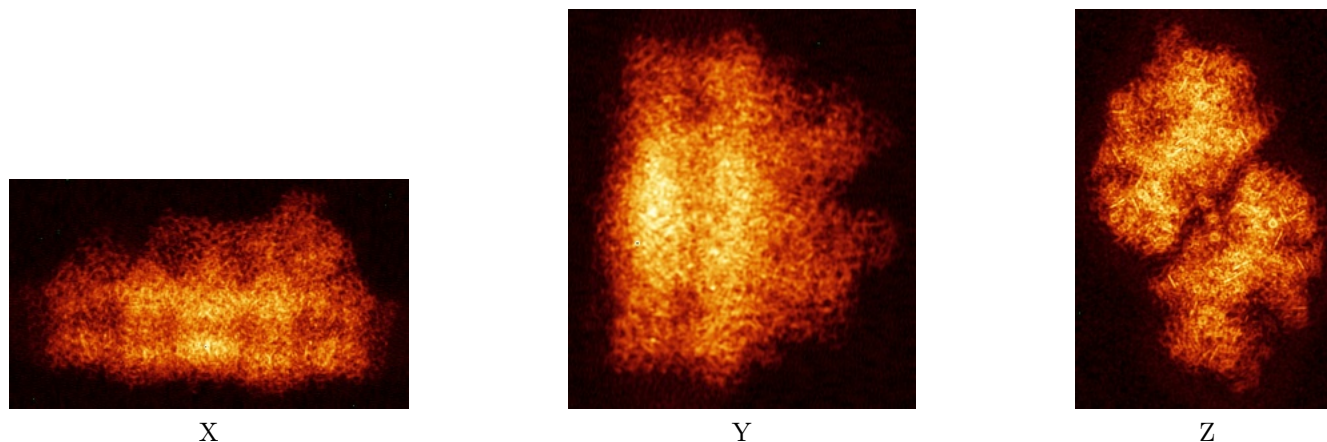


Z Index: 202

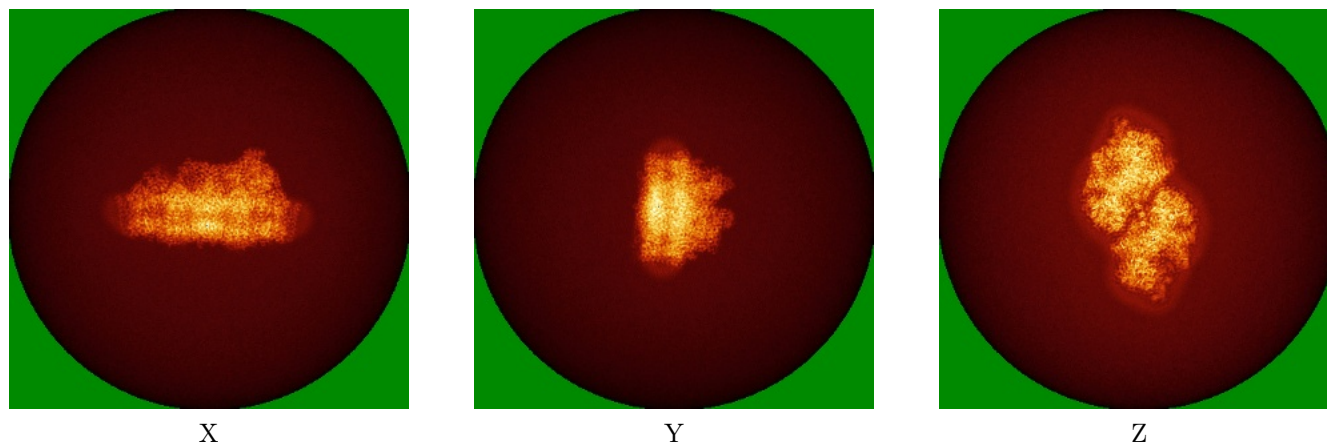
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



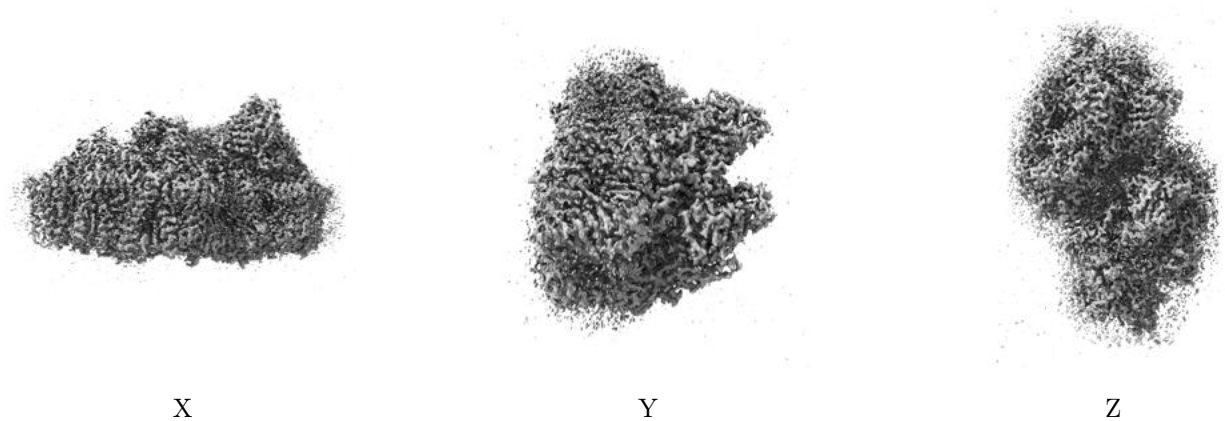
6.4.2 Raw map



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

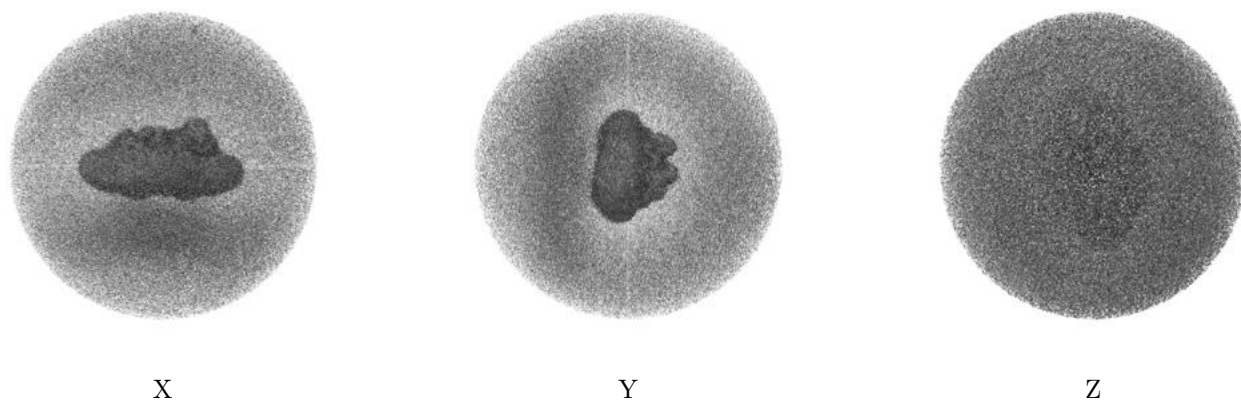
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.039. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

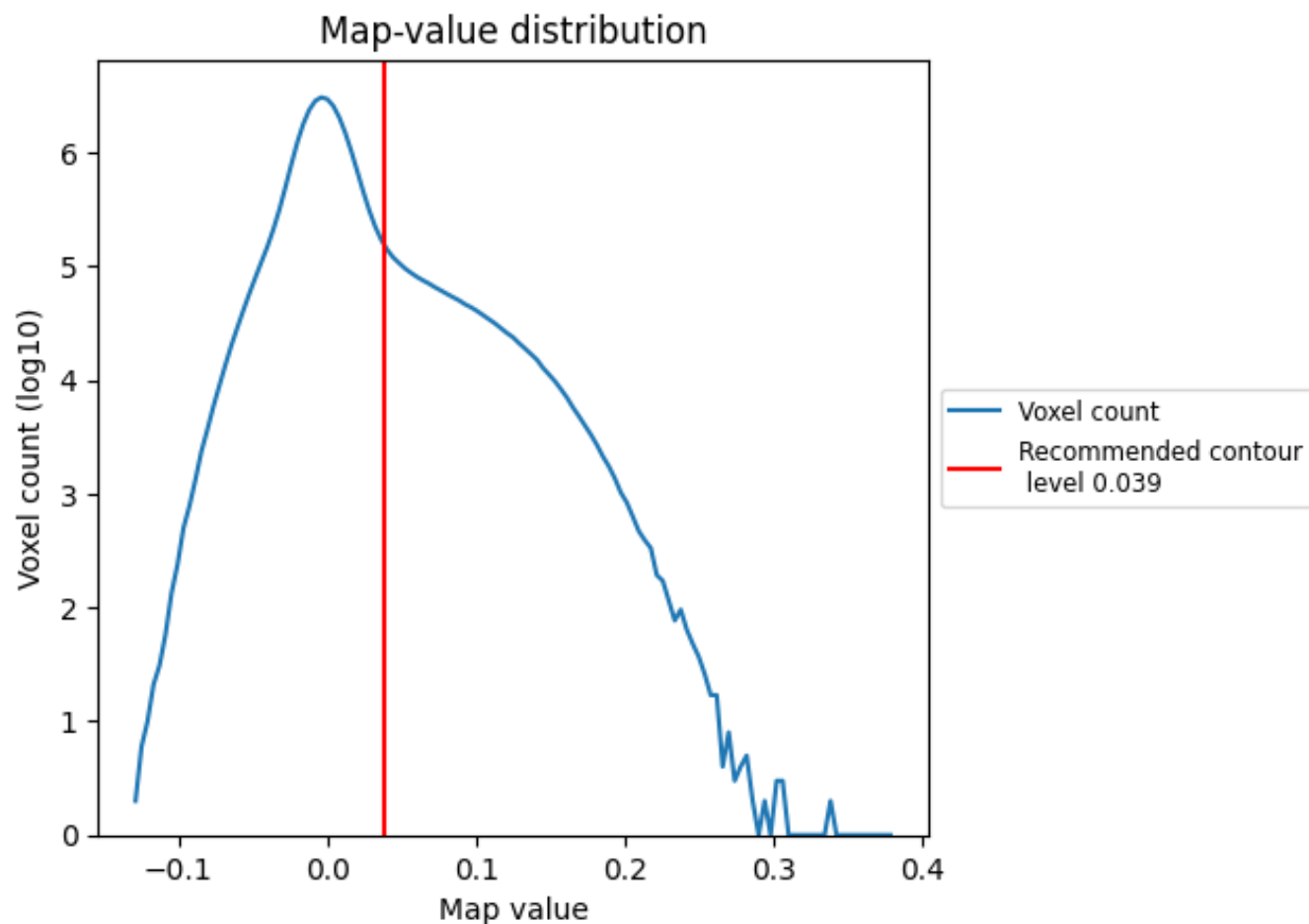
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

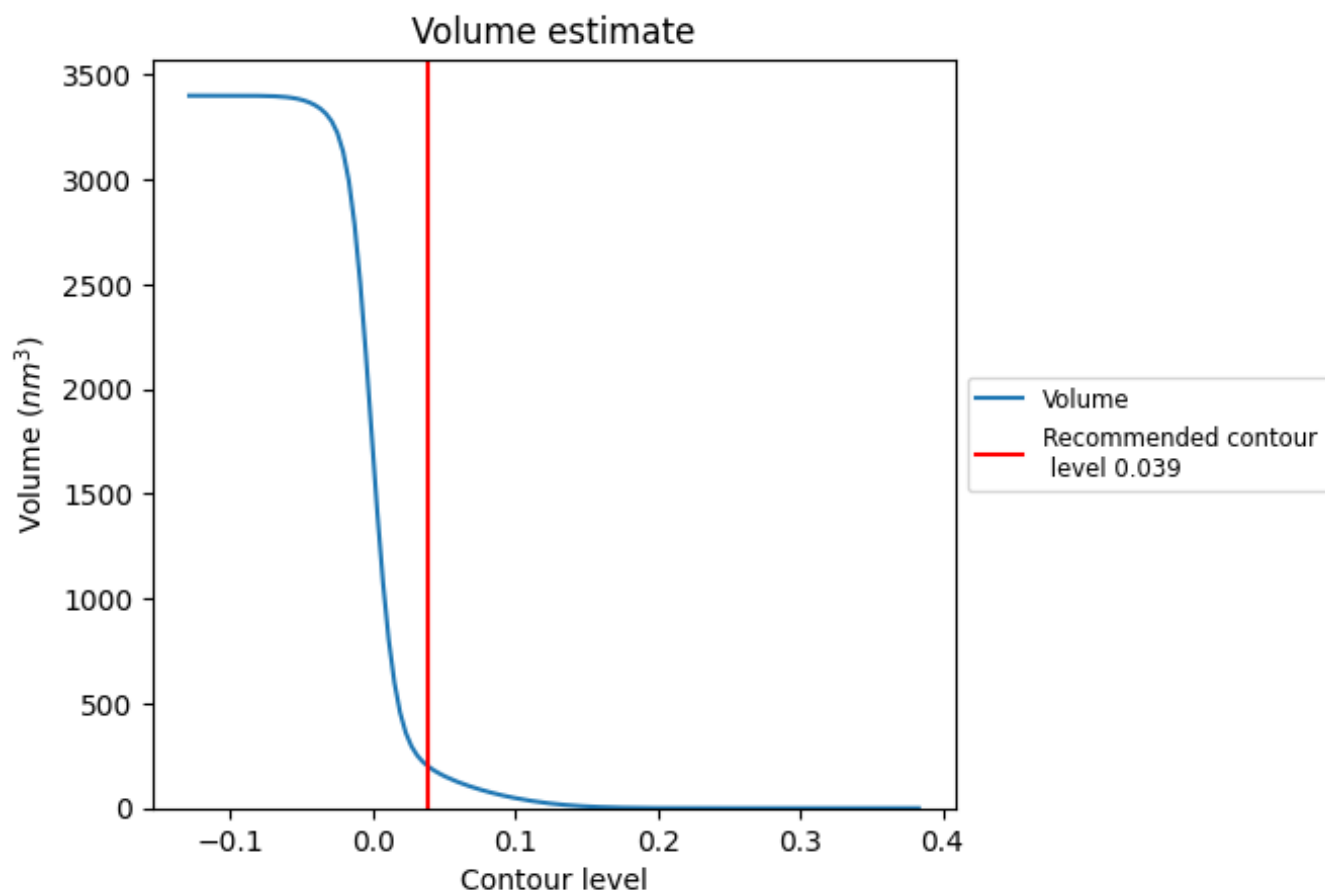
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 kDa.

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

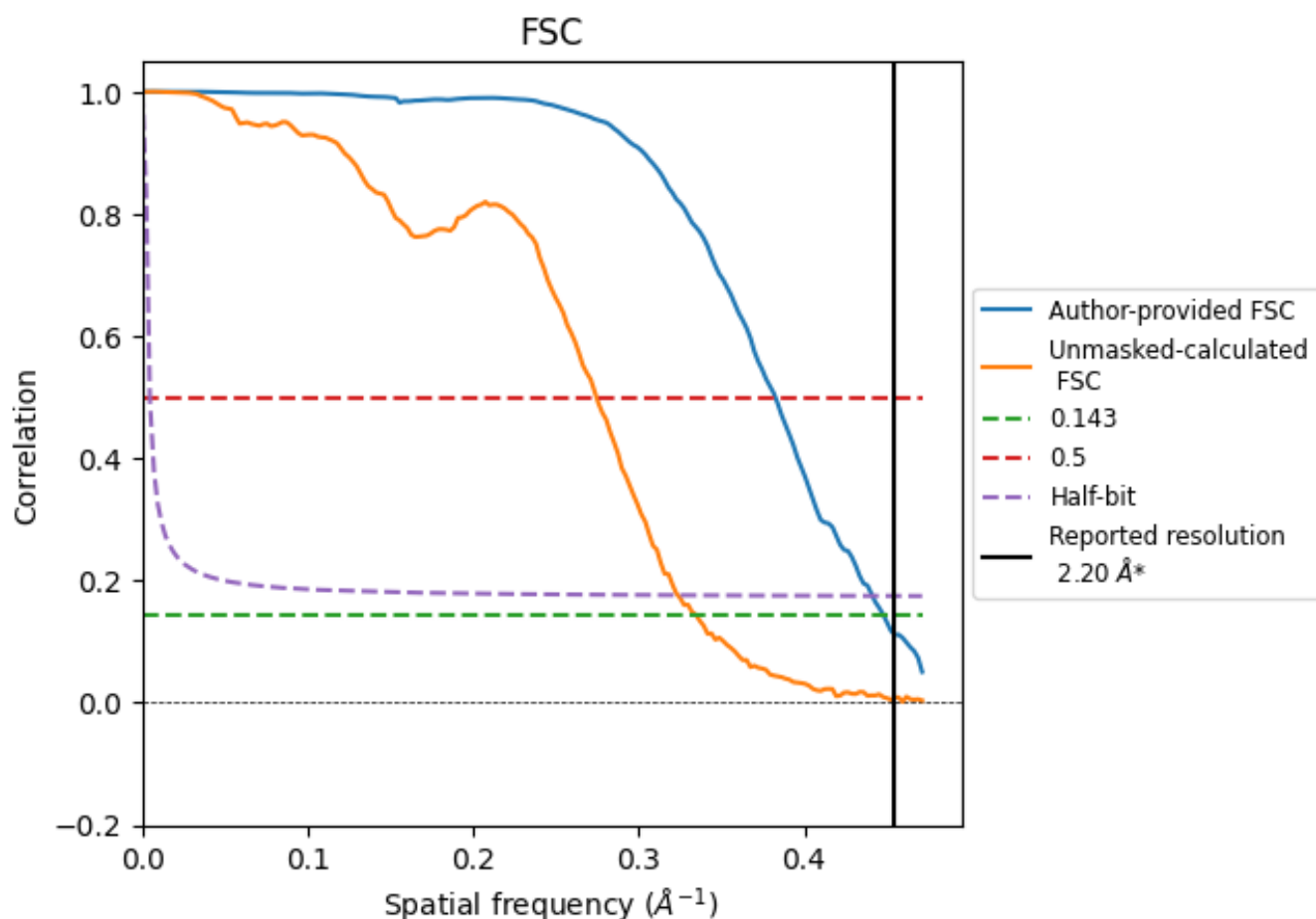
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 \AA^{-1}

8.2 Resolution estimates [i](#)

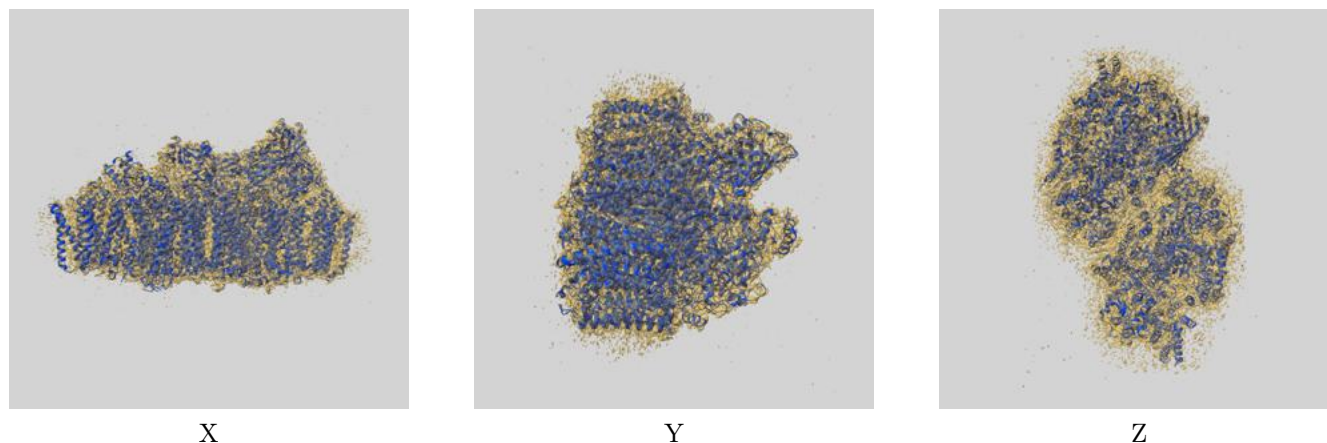
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.23	2.61	2.27
Unmasked-calculated*	2.99	3.64	3.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

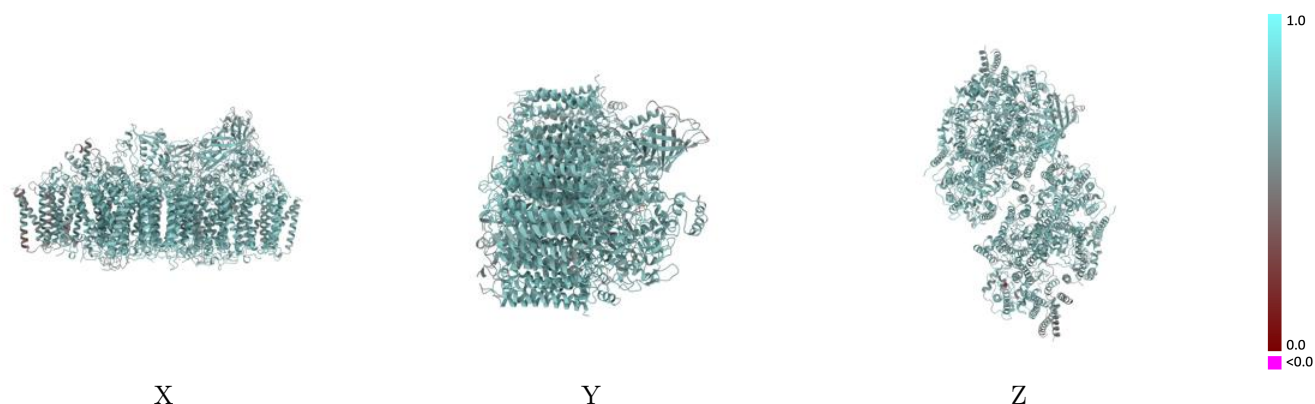
This section contains information regarding the fit between EMDB map EMD-51101 and PDB model 9G6G. Per-residue inclusion information can be found in section 3 on page 31.

9.1 Map-model overlay [i](#)



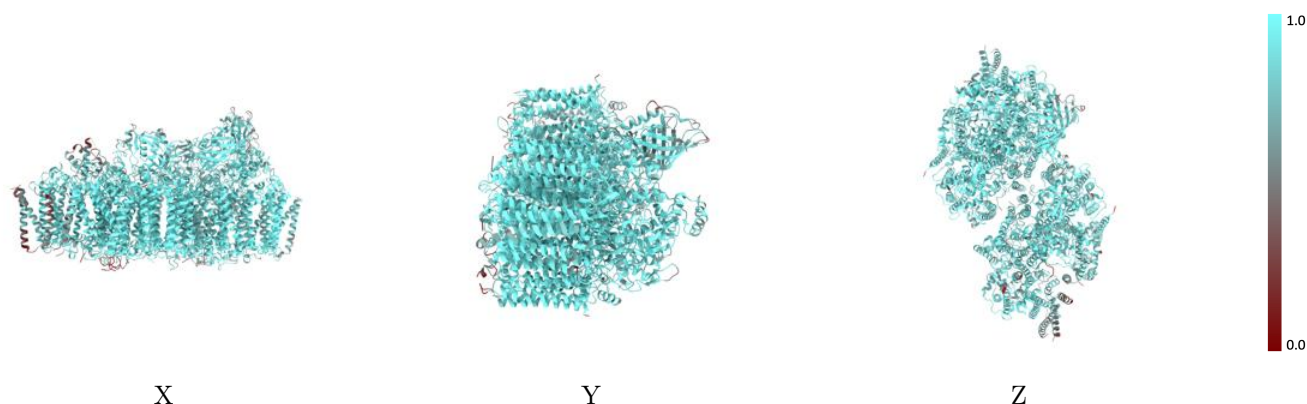
The images above show the 3D surface view of the map at the recommended contour level 0.039 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



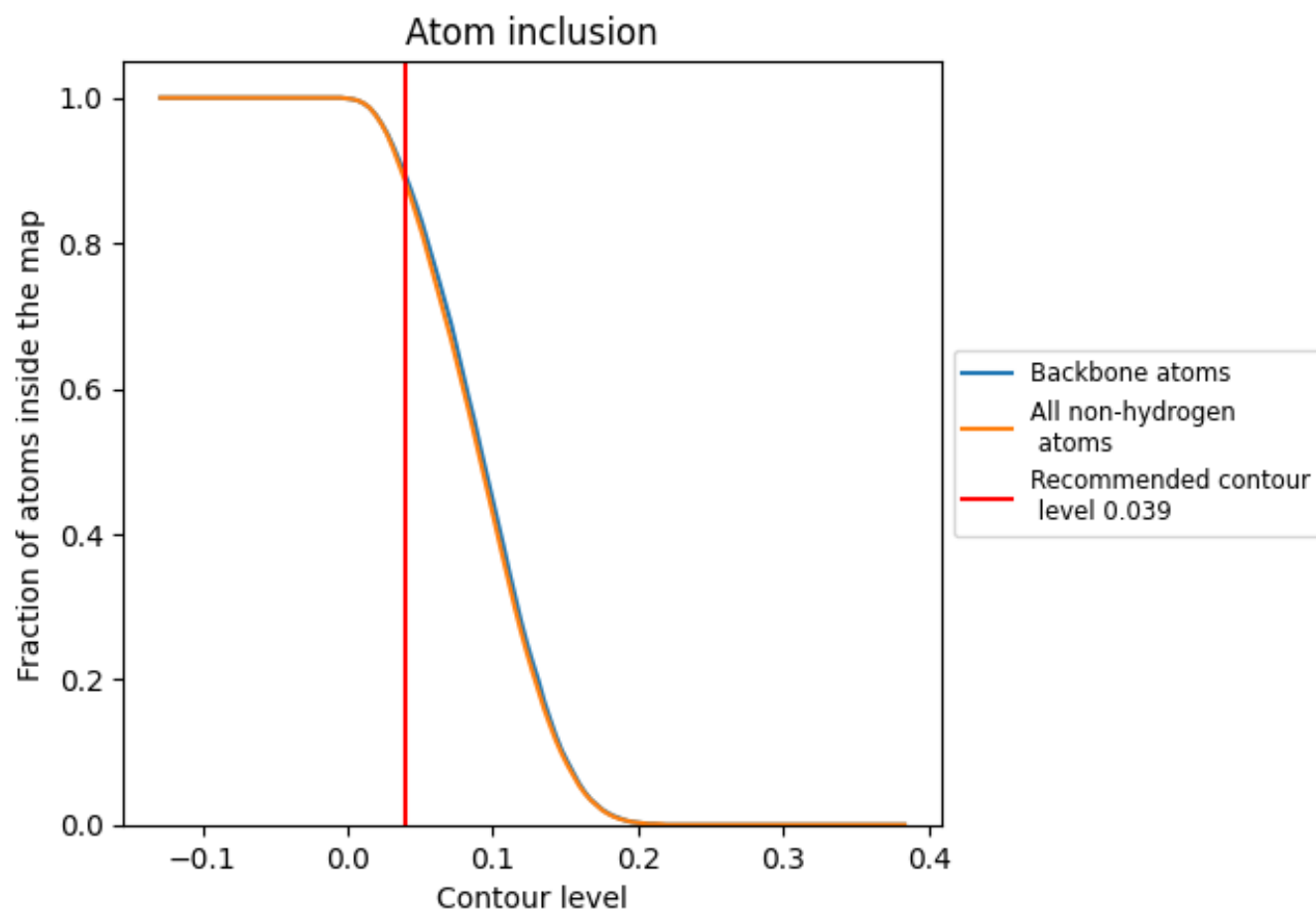
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.039).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.039) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.6690
A	 0.9490	 0.6990
B	 0.9210	 0.6870
C	 0.9350	 0.6810
D	 0.9400	 0.6980
E	 0.8190	 0.6460
F	 0.8310	 0.6720
H	 0.9300	 0.6870
I	 0.8690	 0.6600
J	 0.8820	 0.6530
K	 0.9360	 0.6660
L	 0.9360	 0.6960
M	 0.8730	 0.6690
O	 0.8310	 0.6340
T	 0.8470	 0.6530
U	 0.8700	 0.6400
V	 0.9050	 0.6600
X	 0.8410	 0.6620
Y	 0.7640	 0.6210
Z	 0.8140	 0.6280
a	 0.9030	 0.6820
b	 0.8910	 0.6710
c	 0.8490	 0.6480
d	 0.9280	 0.6900
e	 0.7440	 0.5950
f	 0.7450	 0.6030
h	 0.9000	 0.6640
i	 0.8850	 0.6640
j	 0.5860	 0.5650
k	 0.8460	 0.6250
l	 0.8890	 0.6970
m	 0.8970	 0.6670
t	 0.9340	 0.6960
x	 0.8060	 0.6400
y	 0.4270	 0.5060
z	 0.5860	 0.5420

