



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2026 – 12:19 am BST

PDB ID : 9G6F / pdb_00009g6f
EMDB ID : EMD-51100
Title : Inactive 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 : 3KZI, 7NHO

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

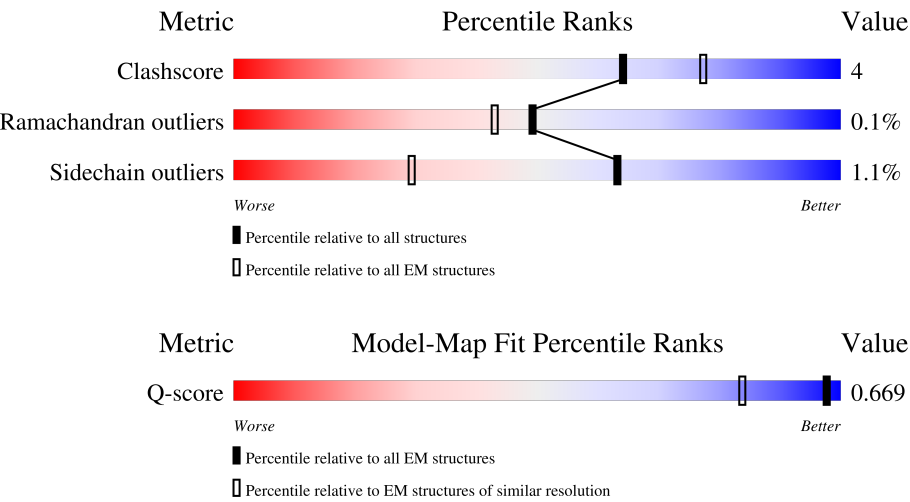
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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.



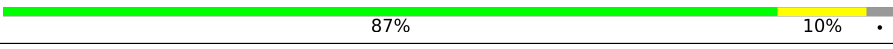
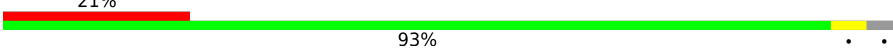
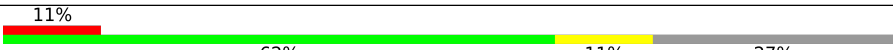
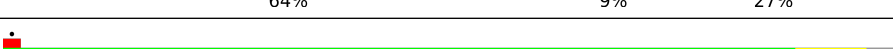
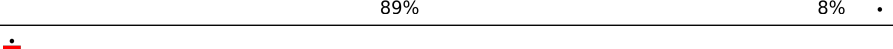
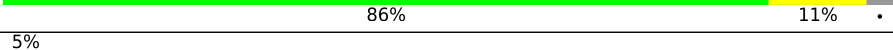
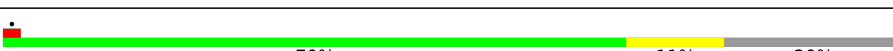
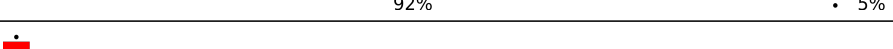
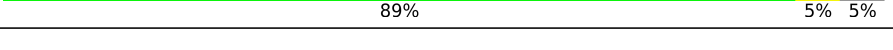
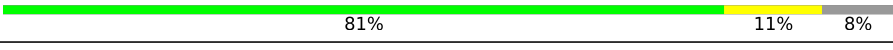
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

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% 11% 10%
1	a	360	78% 11% 10%
2	B	510	5% 91% 8% .
2	b	510	90% 9% .

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Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
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	T	32	
13	t	32	
14	X	41	
14	x	41	
15	Y	46	

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Mol	Chain	Length	Quality of chain
15	y	46	
16	Z	62	
16	z	62	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 42670 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	324	Total	C	N	O	S	0	0
			2544	1667	417	445	15		
1	a	324	Total	C	N	O	S	0	0
			2544	1667	417	445	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	504	Total	C	N	O	S	0	0
			3961	2601	661	686	13		
2	b	505	Total	C	N	O	S	0	0
			3968	2605	664	686	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	436	Total	C	N	O	S	0	0
			3377	2214	565	585	13		
3	c	436	Total	C	N	O	S	0	0
			3377	2214	565	585	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
			2712	1798	444	458	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	81	Total	C	N	O	0	0
			657	430	107	120		
5	e	81	Total	C	N	O	0	0
			650	427	106	117		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	33	Total	C	N	O	S	0	0
			265	182	43	39	1		
6	f	33	Total	C	N	O	S	0	0
			269	184	44	40	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
			288	196	45	46	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	28	Total	C	N	O	S	0	0
			206	145	29	31	1		
9	j	28	Total	C	N	O	S	0	0
			206	145	29	31	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
			285	199	42	44		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			285	199	42	44		

- 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
			287	192	46	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
			258	172	38	47	1		
12	m	33	Total	C	N	O	S	0	0
			258	172	38	47	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	30	Total	C	N	O	S	0	0
			258	181	36	39	2		
13	t	30	Total	C	N	O	S	0	0
			258	181	36	39	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	35	Total	C	N	O	0	0
			254	172	38	44		
14	x	35	Total	C	N	O	0	0
			254	172	38	44		

- Molecule 15 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	28	Total	C	N	O	S	0	0
			205	134	36	32	3		
15	y	28	Total	C	N	O	S	0	0
			196	131	30	32	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	61	Total	C	N	O	S	0	0
			467	321	70	74	2		
16	z	61	Total	C	N	O	S	0	0
			458	317	67	72	2		

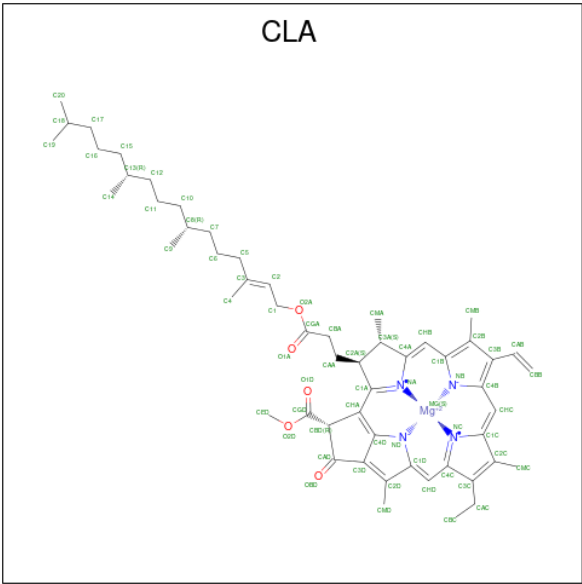
- Molecule 17 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 18 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Cl	0
			1	1	
18	a	1	Total	Cl	0
			1	1	

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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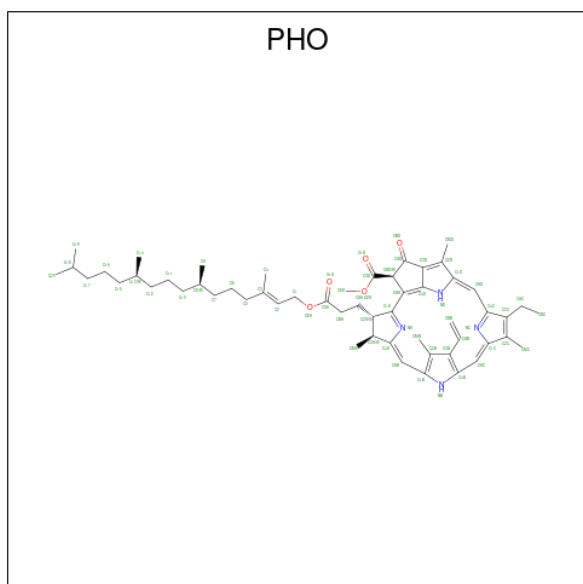
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total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

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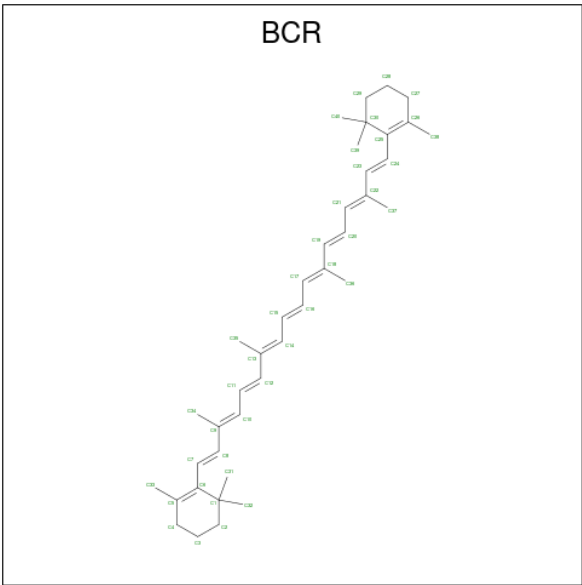
Mol	Chain	Residues	Atoms					AltConf
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 20 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



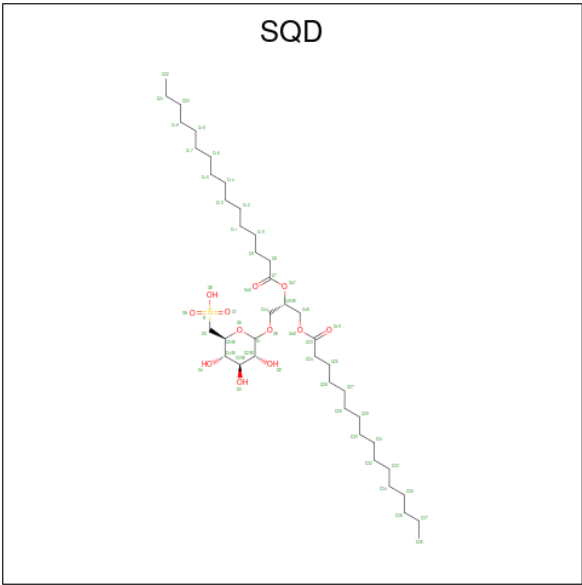
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	C	1	Total	C	0
			40	40	
21	C	1	Total	C	0
			40	40	
21	D	1	Total	C	0
			40	40	
21	K	1	Total	C	0
			40	40	
21	Y	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	
21	b	1	Total	C	0
			40	40	
21	b	1	Total	C	0
			40	40	
21	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms		AltConf
21	b	1	Total	C	0
			40	40	
21	c	1	Total	C	0
			40	40	
21	c	1	Total	C	0
			40	40	
21	d	1	Total	C	0
			40	40	
21	k	1	Total	C	0
			40	40	
21	y	1	Total	C	0
			40	40	

- Molecule 22 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



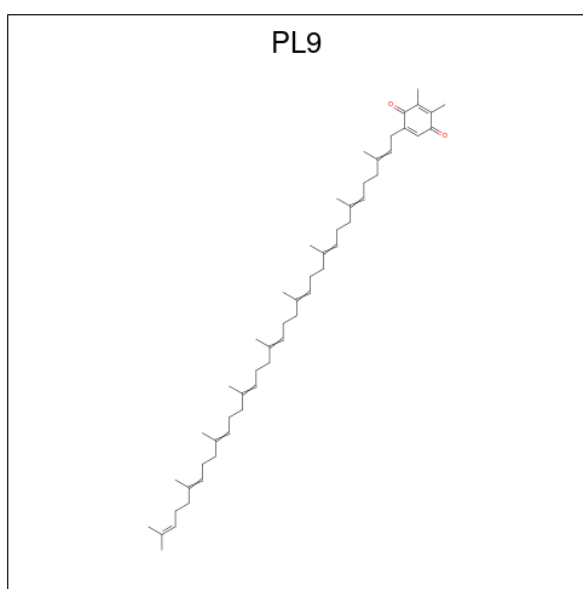
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	S	0
			50	37	12	1	
22	A	1	Total	C	O	S	0
			54	41	12	1	
22	F	1	Total	C	O	S	0
			33	23	9	1	
22	L	1	Total	C	O	S	0
			54	41	12	1	
22	a	1	Total	C	O	S	0
			54	41	12	1	

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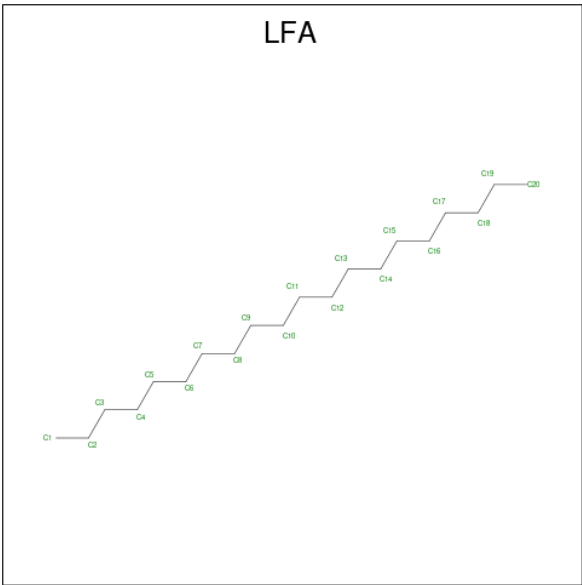
Mol	Chain	Residues	Atoms				AltConf
22	a	1	Total	C	O	S	0
			43	30	12	1	
22	f	1	Total	C	O	S	0
			45	32	12	1	
22	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 23 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 24 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



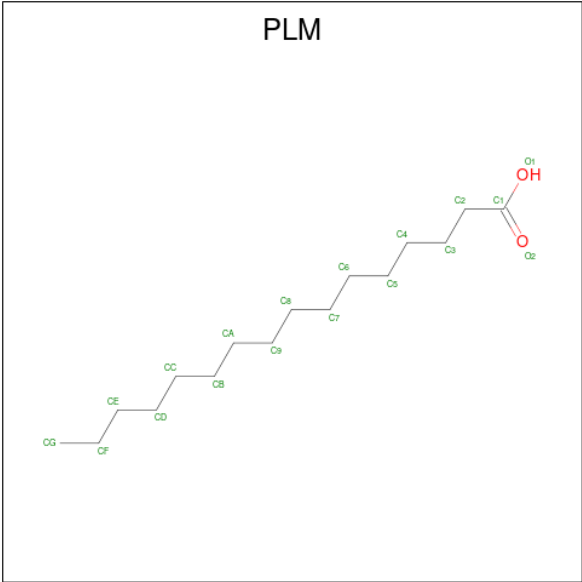
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	C	0
			15	15	
24	A	1	Total	C	0
			13	13	
24	B	1	Total	C	0
			13	13	
24	B	1	Total	C	0
			7	7	
24	B	1	Total	C	0
			11	11	
24	B	1	Total	C	0
			7	7	
24	C	1	Total	C	0
			7	7	
24	D	1	Total	C	0
			16	16	
24	D	1	Total	C	0
			13	13	
24	D	1	Total	C	0
			9	9	
24	H	1	Total	C	0
			14	14	
24	H	1	Total	C	0
			6	6	
24	I	1	Total	C	0
			7	7	
24	J	1	Total	C	0
			17	17	

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Mol	Chain	Residues	Atoms	AltConf
24	K	1	Total C 7 7	0
24	M	1	Total C 10 10	0
24	X	1	Total C 13 13	0
24	Z	1	Total C 8 8	0
24	a	1	Total C 11 11	0
24	b	1	Total C 12 12	0
24	b	1	Total C 11 11	0
24	b	1	Total C 9 9	0
24	b	1	Total C 9 9	0
24	b	1	Total C 7 7	0
24	d	1	Total C 15 15	0
24	d	1	Total C 8 8	0
24	h	1	Total C 8 8	0
24	h	1	Total C 6 6	0
24	h	1	Total C 7 7	0
24	i	1	Total C 11 11	0
24	k	1	Total C 7 7	0
24	m	1	Total C 9 9	0
24	x	1	Total C 13 13	0

- Molecule 25 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



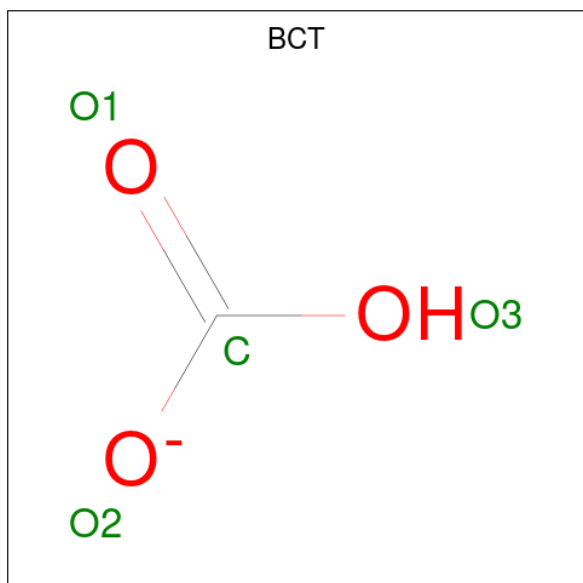
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			18	16	2	
25	A	1	Total	C	O	0
			11	9	2	
25	B	1	Total	C	O	0
			8	6	2	
25	B	1	Total	C	O	0
			12	10	2	
25	B	1	Total	C	O	0
			13	11	2	
25	B	1	Total	C	O	0
			16	14	2	
25	C	1	Total	C	O	0
			9	7	2	
25	D	1	Total	C	O	0
			18	16	2	
25	E	1	Total	C	O	0
			18	16	2	
25	H	1	Total	C	O	0
			10	8	2	
25	I	1	Total	C	O	0
			16	14	2	
25	I	1	Total	C	O	0
			18	16	2	
25	I	1	Total	C	O	0
			11	9	2	
25	a	1	Total	C	O	0
			17	15	2	

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Mol	Chain	Residues	Atoms			AltConf
25	a	1	Total	C	O	0
			12	10	2	
25	b	1	Total	C	O	0
			18	16	2	
25	b	1	Total	C	O	0
			9	7	2	
25	b	1	Total	C	O	0
			14	12	2	
25	b	1	Total	C	O	0
			13	11	2	
25	b	1	Total	C	O	0
			16	14	2	
25	e	1	Total	C	O	0
			18	16	2	
25	i	1	Total	C	O	0
			16	14	2	
25	i	1	Total	C	O	0
			13	11	2	
25	i	1	Total	C	O	0
			13	11	2	

- Molecule 26 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



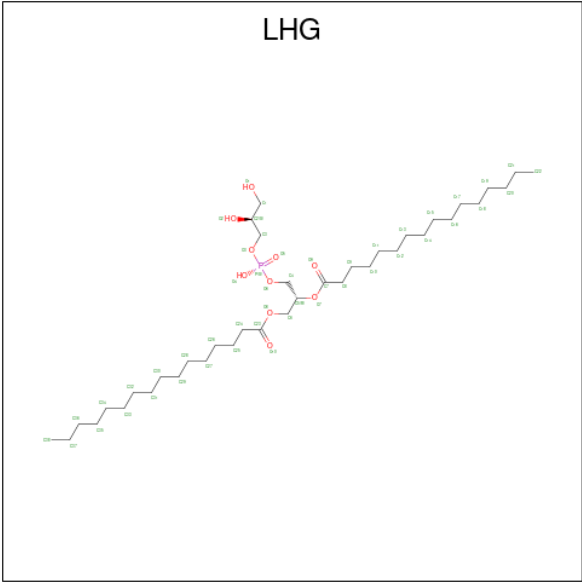
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			4	1	3	

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

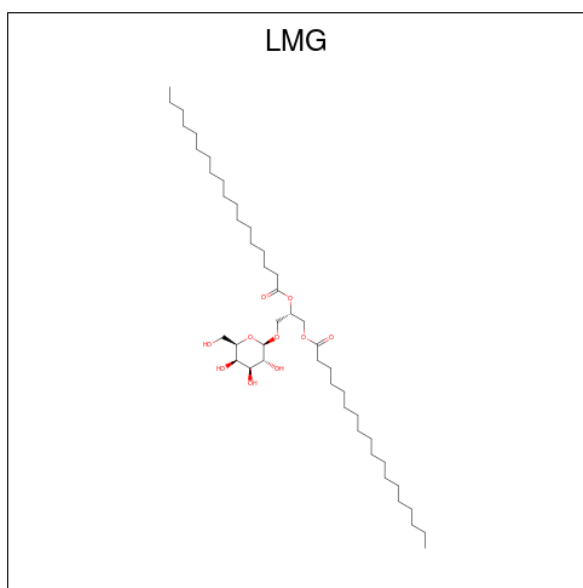
- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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

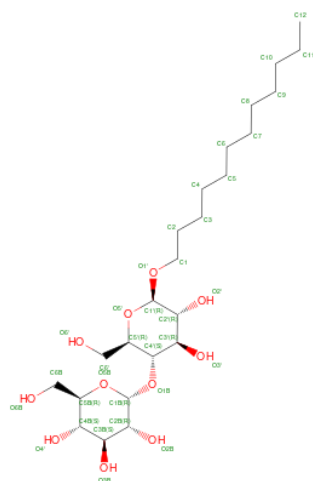
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula: $C_{45}H_{86}O_{10}$).



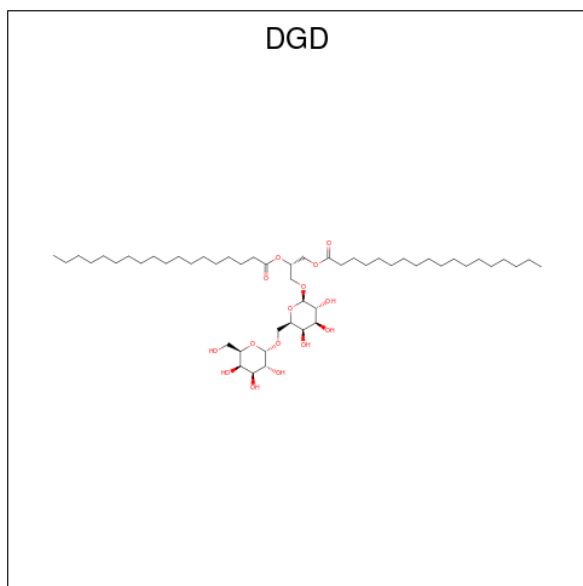
Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			42	32	10	
28	D	1	Total	C	O	0
			48	38	10	
28	b	1	Total	C	O	0
			51	41	10	
28	c	1	Total	C	O	0
			51	41	10	
28	c	1	Total	C	O	0
			51	41	10	
28	d	1	Total	C	O	0
			51	41	10	

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



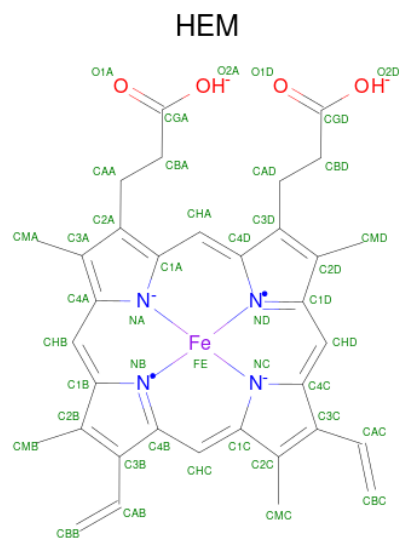
- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

C₅₁H₉₆O₁₅).



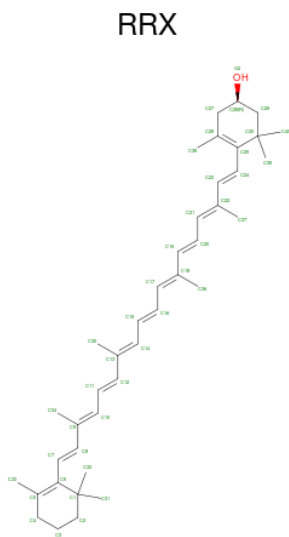
Mol	Chain	Residues	Atoms			AltConf
30	C	1	Total	C	O	0
			62	47	15	
30	D	1	Total	C	O	0
			44	35	9	
30	H	1	Total	C	O	0
			62	47	15	
30	J	1	Total	C	O	0
			54	39	15	
30	c	1	Total	C	O	0
			62	47	15	
30	c	1	Total	C	O	0
			62	47	15	
30	c	1	Total	C	O	0
			62	47	15	
30	d	1	Total	C	O	0
			47	36	11	
30	h	1	Total	C	O	0
			62	47	15	

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 32 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



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

- Molecule 33 is water.

Mol	Chain	Residues	Atoms	AltConf
33	A	72	Total O 72 72	1
33	B	137	Total O 137 137	1
33	C	59	Total O 59 59	0
33	D	87	Total O 87 87	0
33	E	8	Total O 8 8	0
33	H	22	Total O 22 22	0
33	K	2	Total O 2 2	0
33	L	5	Total O 5 5	0
33	M	2	Total O 2 2	0
33	T	4	Total O 4 4	0
33	X	3	Total O 3 3	0
33	a	70	Total O 70 70	1
33	b	146	Total O 146 146	1
33	c	61	Total O 61 61	0
33	d	86	Total O 86 86	0
33	e	7	Total O 7 7	0
33	f	1	Total O 1 1	0
33	h	19	Total O 19 19	0
33	k	1	Total O 1 1	0
33	l	7	Total O 7 7	0
33	m	2	Total O 2 2	0

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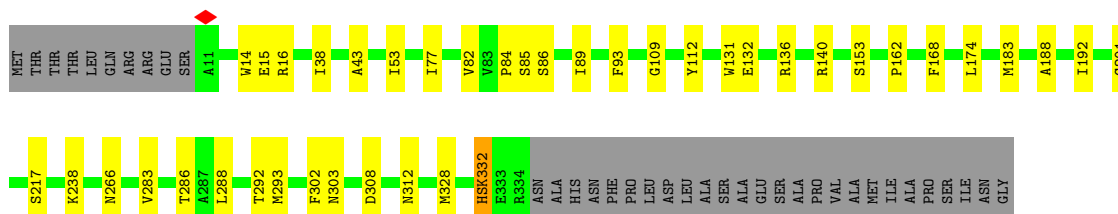
Mol	Chain	Residues	Atoms		AltConf
33	t	3	Total	O	0
			3	3	
33	x	5	Total	O	0
			5	5	

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.

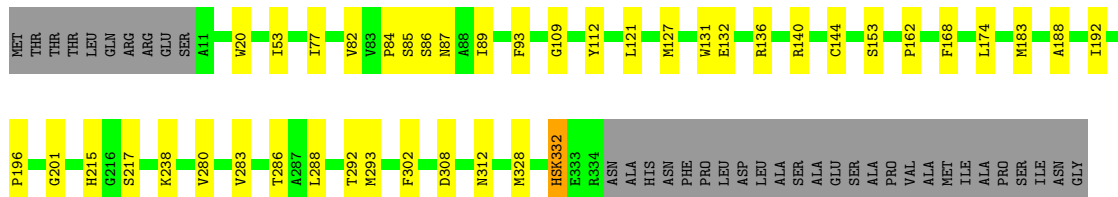
- Molecule 1: Photosystem II protein D1 1

Chain A: 

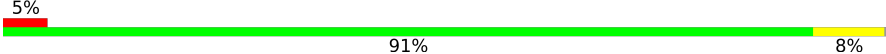


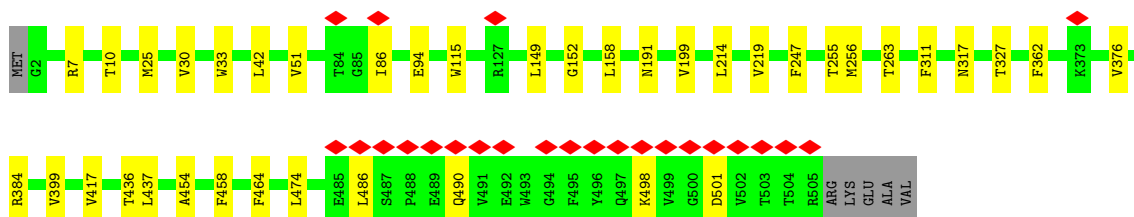
- Molecule 1: Photosystem II protein D1 1

Chain a: 



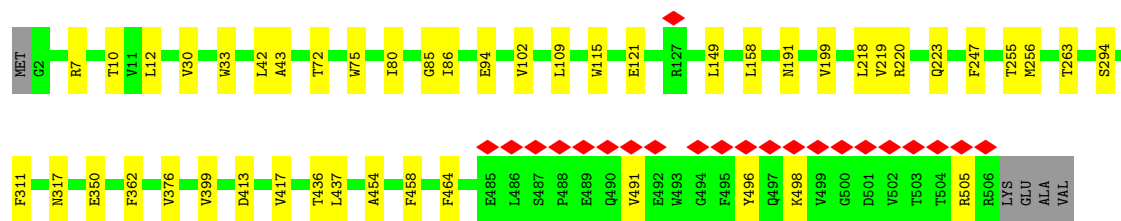
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 



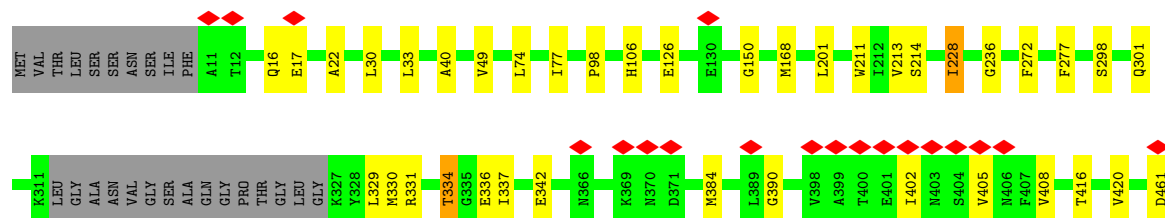
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 



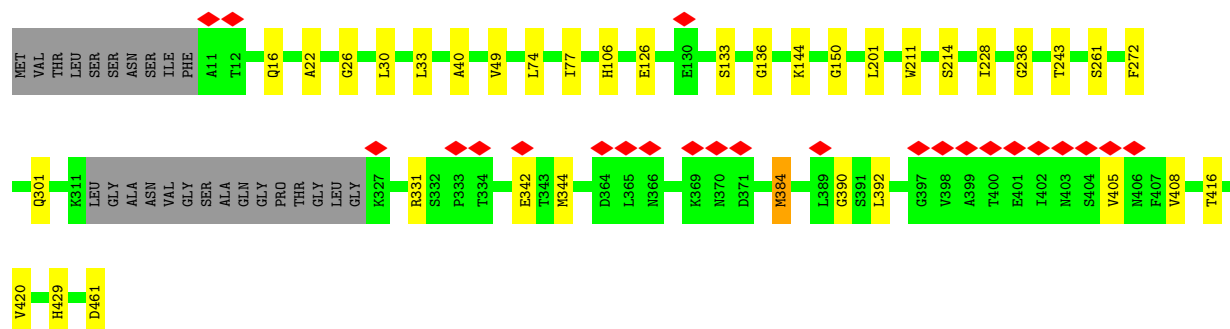
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 8% 5%



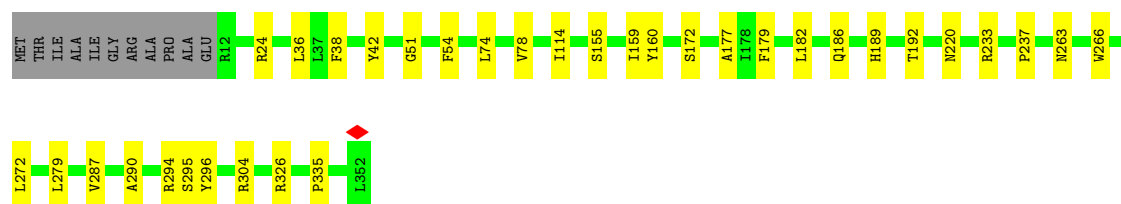
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 87% 8% 5%



• Molecule 4: Photosystem II D2 protein

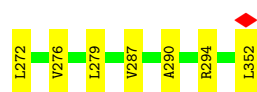
Chain D: 87% 10% 3%



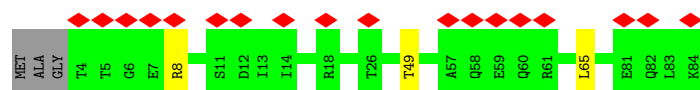
• Molecule 4: Photosystem II D2 protein

Chain d: 88% 9% 3%

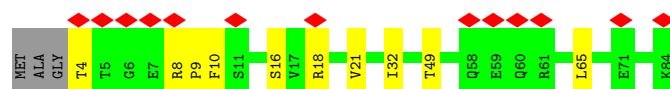
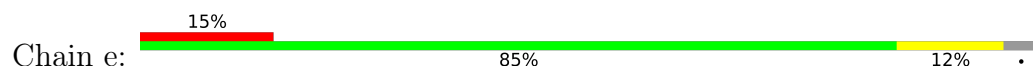




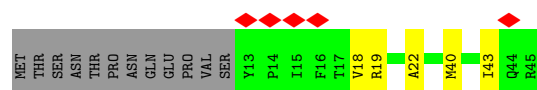
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



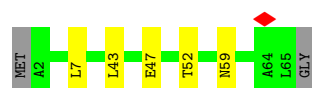
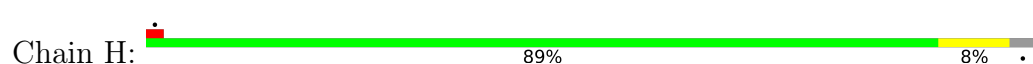
- Molecule 6: Cytochrome b559 subunit beta



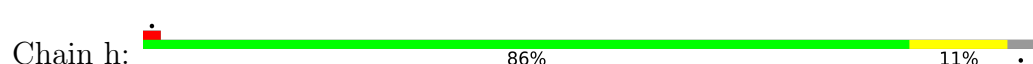
- Molecule 6: Cytochrome b559 subunit beta



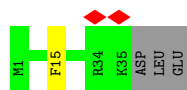
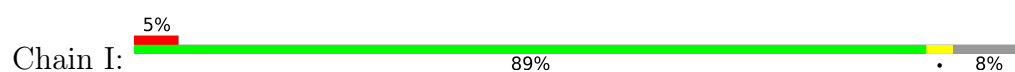
- Molecule 7: Photosystem II reaction center protein H



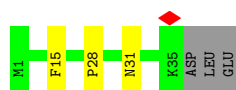
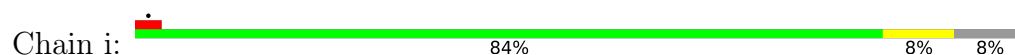
- Molecule 7: Photosystem II reaction center protein H



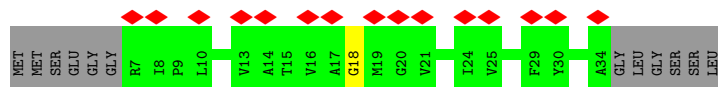
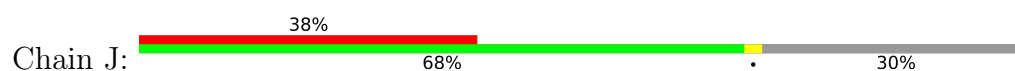
- Molecule 8: Photosystem II reaction center protein I



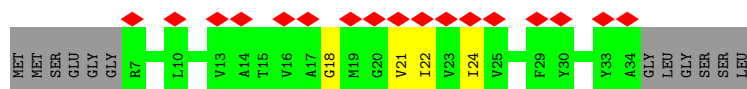
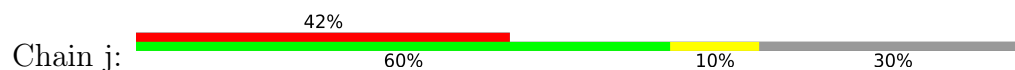
- Molecule 8: Photosystem II reaction center protein I



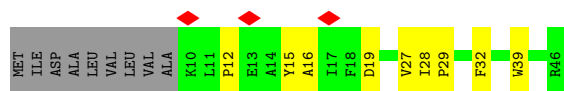
- Molecule 9: Photosystem II reaction center protein J



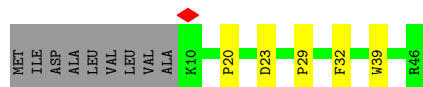
- Molecule 9: Photosystem II reaction center protein J



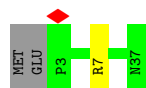
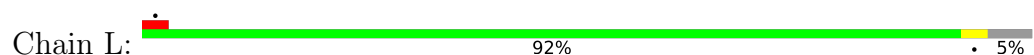
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

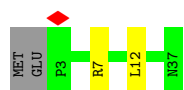


- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

Chain l:  89% 5% 5%



- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 17% 8%



- Molecule 12: Photosystem II reaction center protein M

Chain m:  81% 11% 8%



- Molecule 13: Photosystem II reaction center protein T

Chain T:  75% 19% 6%



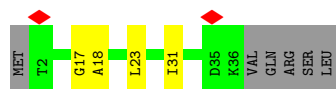
- Molecule 13: Photosystem II reaction center protein T

Chain t:  78% 16% 6%



- Molecule 14: Photosystem II reaction center X protein

Chain X:  5% 76% 10% 15%

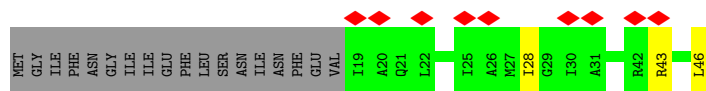


- Molecule 14: Photosystem II reaction center X protein

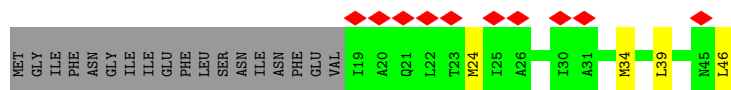
Chain x:  73% 12% 15%



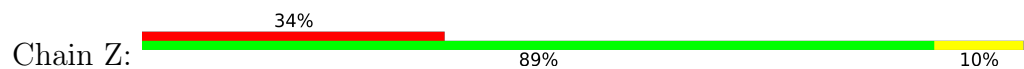
- Molecule 15: Photosystem II reaction center protein Ycf12



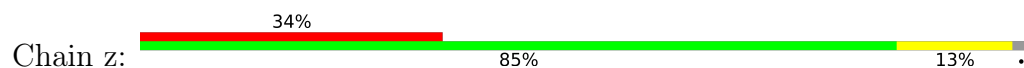
- Molecule 15: Photosystem II reaction center protein Ycf12



- Molecule 16: Photosystem II reaction center protein Z



- Molecule 16: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	417537	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	0.387	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.037	Depositor
Map size (Å)	137.5, 208.5, 104.5	wwPDB
Map dimensions	209, 417, 275	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: RRX, LHG, FME, LMT, PLM, HSK, HEM, CL, BCR, PHO, BCT, FE2, DGD, CLA, PL9, SQD, LFA, LMG

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	0.22	0/2613	0.45	0/3562
1	a	0.22	0/2613	0.44	0/3562
2	B	0.21	0/4101	0.42	0/5590
2	b	0.20	0/4108	0.43	2/5599 (0.0%)
3	C	0.21	0/3487	0.42	0/4750
3	c	0.20	0/3487	0.40	0/4750
4	D	0.22	0/2807	0.42	0/3827
4	d	0.23	0/2807	0.42	0/3827
5	E	0.21	0/676	0.46	0/923
5	e	0.19	0/669	0.43	0/914
6	F	0.27	0/274	0.58	0/374
6	f	0.26	0/278	0.57	0/379
7	H	0.21	0/519	0.46	0/708
7	h	0.21	0/519	0.47	0/708
8	I	0.21	0/285	0.50	0/385
8	i	0.20	0/285	0.47	0/385
9	J	0.18	0/212	0.36	0/291
9	j	0.18	0/212	0.38	0/291
10	K	0.30	0/295	0.72	2/407 (0.5%)
10	k	0.28	0/295	0.51	0/407
11	L	0.15	0/294	0.32	0/399
11	l	0.15	0/294	0.31	0/399
12	M	0.34	0/261	0.59	0/356
12	m	0.34	0/261	0.61	0/356
13	T	0.21	0/257	0.40	0/349
13	t	0.20	0/257	0.38	0/349
14	X	0.19	0/257	0.38	0/348
14	x	0.18	0/257	0.37	0/348
15	Y	0.19	0/206	0.50	0/275
15	y	0.23	0/197	0.58	0/265
16	Z	0.19	0/478	0.41	0/654

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	z	0.19	0/469	0.34	0/643
All	All	0.21	0/34030	0.44	4/46380 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	a	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	27	VAL	CA-C-N	7.20	124.77	120.24
10	K	27	VAL	C-N-CA	7.20	124.77	120.24
2	b	85	GLY	CA-C-N	5.41	131.72	121.97
2	b	85	GLY	C-N-CA	5.41	131.72	121.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	HSK	Mainchain
1	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	2544	0	2447	33	0
1	a	2544	0	2447	32	0
2	B	3961	0	3820	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3968	0	3827	34	0
3	C	3377	0	3286	26	0
3	c	3377	0	3286	24	0
4	D	2712	0	2617	27	0
4	d	2712	0	2617	23	0
5	E	657	0	644	3	0
5	e	650	0	636	6	0
6	F	265	0	271	5	0
6	f	269	0	277	4	0
7	H	506	0	529	4	0
7	h	506	0	529	6	0
8	I	288	0	307	1	0
8	i	288	0	307	2	0
9	J	206	0	213	1	0
9	j	206	0	213	2	0
10	K	285	0	290	5	0
10	k	285	0	290	3	0
11	L	287	0	299	2	0
11	l	287	0	299	2	0
12	M	258	0	276	5	0
12	m	258	0	276	2	0
13	T	258	0	261	4	0
13	t	258	0	261	4	0
14	X	254	0	282	2	0
14	x	254	0	282	2	0
15	Y	205	0	228	3	0
15	y	196	0	215	3	0
16	Z	467	0	501	2	0
16	z	458	0	488	5	0
17	A	1	0	0	0	0
17	a	1	0	0	0	0
18	A	1	0	0	0	0
18	a	1	0	0	0	0
19	A	260	0	288	6	0
19	B	1040	0	1152	21	0
19	C	845	0	936	17	0
19	D	130	0	144	5	0
19	a	260	0	288	6	0
19	b	1040	0	1152	25	0
19	c	845	0	936	17	0
19	d	130	0	144	5	0
20	A	64	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	64	0	74	3	0
20	a	64	0	74	0	0
20	d	64	0	74	2	0
21	A	40	0	56	1	0
21	B	160	0	224	5	0
21	C	80	0	112	2	0
21	D	40	0	56	0	0
21	K	40	0	56	2	0
21	Y	40	0	56	2	0
21	a	40	0	56	2	0
21	b	160	0	224	8	0
21	c	80	0	112	1	0
21	d	40	0	56	0	0
21	k	40	0	56	0	0
21	y	40	0	56	1	0
22	A	104	0	145	3	0
22	F	33	0	39	3	0
22	L	54	0	78	2	0
22	a	97	0	128	2	0
22	f	45	0	57	2	0
22	l	54	0	78	1	0
23	A	55	0	80	3	0
23	D	55	0	80	0	0
23	a	55	0	80	5	0
23	d	55	0	80	1	0
24	A	28	0	51	0	0
24	B	38	0	63	2	0
24	C	7	0	10	0	0
24	D	38	0	70	3	0
24	H	20	0	32	0	0
24	I	7	0	10	0	0
24	J	17	0	33	0	0
24	K	7	0	10	0	0
24	M	10	0	16	0	0
24	X	13	0	22	1	0
24	Z	8	0	12	0	0
24	a	11	0	18	0	0
24	b	48	0	76	1	0
24	d	23	0	41	1	0
24	h	21	0	30	0	0
24	i	11	0	18	0	0
24	k	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	m	9	0	14	0	0
24	x	13	0	25	0	0
25	A	29	0	45	1	0
25	B	49	0	66	0	0
25	C	9	0	10	1	0
25	D	18	0	31	2	0
25	E	18	0	31	0	0
25	H	10	0	12	0	0
25	I	45	0	69	0	0
25	a	29	0	42	2	0
25	b	70	0	103	1	0
25	e	18	0	31	0	0
25	i	42	0	60	0	0
26	A	4	0	0	0	0
26	d	4	0	0	0	0
27	A	46	0	65	1	0
27	D	98	0	148	1	0
27	L	49	0	74	2	0
27	a	95	0	139	4	0
27	d	98	0	148	0	0
27	l	49	0	74	1	0
28	B	51	0	72	2	0
28	C	93	0	126	3	0
28	D	48	0	66	1	0
28	b	51	0	72	4	0
28	c	102	0	144	1	0
28	d	51	0	72	3	0
29	C	30	0	33	2	0
29	D	59	0	81	3	0
29	M	70	0	92	1	0
29	b	20	0	24	1	0
29	d	58	0	76	1	0
29	i	35	0	46	0	0
29	m	70	0	92	1	0
29	t	24	0	35	1	0
29	z	35	0	46	3	0
30	C	62	0	82	1	0
30	D	44	0	57	1	0
30	H	62	0	82	0	0
30	J	54	0	66	4	0
30	c	186	0	246	4	0
30	d	47	0	59	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	h	62	0	82	2	0
31	F	43	0	30	1	0
31	f	43	0	30	0	0
32	H	41	0	56	0	0
32	x	41	0	56	0	0
33	A	72	0	0	0	0
33	B	137	0	0	0	0
33	C	59	0	0	0	0
33	D	87	0	0	1	0
33	E	8	0	0	0	0
33	H	22	0	0	0	0
33	K	2	0	0	0	0
33	L	5	0	0	1	0
33	M	2	0	0	0	0
33	T	4	0	0	0	0
33	X	3	0	0	0	0
33	a	70	0	0	0	0
33	b	146	0	0	0	0
33	c	61	0	0	0	0
33	d	86	0	0	0	0
33	e	7	0	0	0	0
33	f	1	0	0	0	0
33	h	19	0	0	0	0
33	k	1	0	0	0	0
33	l	7	0	0	1	0
33	m	2	0	0	0	0
33	t	3	0	0	0	0
33	x	5	0	0	0	0
All	All	42670	0	43454	350	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 4.

The worst 5 of 350 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)
3:c:30:LEU:HD21	19:c:512:CLA:H2A	1.74	0.68
3:C:30:LEU:HD21	19:C:513:CLA:H2A	1.75	0.68
23:A:410:PL9:H33	4:D:42:TYR:HB2	1.76	0.68
27:a:416:LHG:HC32	5:e:9:PRO:HA	1.77	0.66
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.80	0.64

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/360 (89%)	315 (98%)	6 (2%)	0	100	100
1	a	321/360 (89%)	316 (98%)	5 (2%)	0	100	100
2	B	502/510 (98%)	495 (99%)	5 (1%)	2 (0%)	30	34
2	b	503/510 (99%)	495 (98%)	7 (1%)	1 (0%)	43	51
3	C	432/461 (94%)	423 (98%)	9 (2%)	0	100	100
3	c	432/461 (94%)	425 (98%)	7 (2%)	0	100	100
4	D	339/352 (96%)	334 (98%)	5 (2%)	0	100	100
4	d	339/352 (96%)	333 (98%)	6 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
6	F	31/45 (69%)	30 (97%)	1 (3%)	0	100	100
6	f	31/45 (69%)	30 (97%)	1 (3%)	0	100	100
7	H	62/66 (94%)	62 (100%)	0	0	100	100
7	h	62/66 (94%)	61 (98%)	1 (2%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	26/40 (65%)	26 (100%)	0	0	100	100
9	j	26/40 (65%)	26 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	31 (100%)	0	0	100	100
13	T	28/32 (88%)	28 (100%)	0	0	100	100
13	t	28/32 (88%)	28 (100%)	0	0	100	100
14	X	33/41 (80%)	33 (100%)	0	0	100	100
14	x	33/41 (80%)	33 (100%)	0	0	100	100
15	Y	26/46 (56%)	26 (100%)	0	0	100	100
15	y	26/46 (56%)	26 (100%)	0	0	100	100
16	Z	59/62 (95%)	59 (100%)	0	0	100	100
16	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	4141/4512 (92%)	4079 (98%)	59 (1%)	3 (0%)	49	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	86	ILE
2	b	86	ILE
2	B	384	ARG

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	261/290 (90%)	261 (100%)	0	100	100
1	a	261/290 (90%)	261 (100%)	0	100	100
2	B	400/407 (98%)	396 (99%)	4 (1%)	68	81
2	b	400/407 (98%)	395 (99%)	5 (1%)	61	76
3	C	340/362 (94%)	336 (99%)	4 (1%)	63	78
3	c	340/362 (94%)	336 (99%)	4 (1%)	63	78
4	D	275/283 (97%)	274 (100%)	1 (0%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	275/283 (97%)	272 (99%)	3 (1%)	65	79
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	69/73 (94%)	67 (97%)	2 (3%)	37	51
6	F	26/39 (67%)	26 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	54/55 (98%)	54 (100%)	0	100	100
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	31/34 (91%)	31 (100%)	0	100	100
9	J	19/28 (68%)	19 (100%)	0	100	100
9	j	19/28 (68%)	17 (90%)	2 (10%)	6	6
10	K	28/37 (76%)	28 (100%)	0	100	100
10	k	28/37 (76%)	28 (100%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	100	100
11	l	33/35 (94%)	32 (97%)	1 (3%)	36	49
12	M	30/33 (91%)	30 (100%)	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	33	45
13	T	26/28 (93%)	26 (100%)	0	100	100
13	t	26/28 (93%)	26 (100%)	0	100	100
14	X	28/34 (82%)	26 (93%)	2 (7%)	13	16
14	x	28/34 (82%)	25 (89%)	3 (11%)	6	6
15	Y	20/37 (54%)	19 (95%)	1 (5%)	22	28
15	y	19/37 (51%)	18 (95%)	1 (5%)	20	26
16	Z	50/52 (96%)	48 (96%)	2 (4%)	28	38
16	z	48/52 (92%)	47 (98%)	1 (2%)	47	63
All	All	3380/3654 (92%)	3343 (99%)	37 (1%)	63	79

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	j	21	VAL
15	y	34	MET
9	j	22	ILE

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Mol	Chain	Res	Type
14	x	12	ILE
16	Z	25	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	289	GLN
4	d	250	ASN
2	b	374	ASN
3	c	361	ASN
10	k	40	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	HSK	A	332	1	9,11,12	1.83	1 (11%)	6,14,16	1.73	2 (33%)
1	HSK	a	332	1	9,11,12	1.82	1 (11%)	6,14,16	1.75	2 (33%)
8	FME	i	1	8	8,9,10	0.36	0	7,9,11	0.73	0
13	FME	T	1	13	8,9,10	0.38	0	7,9,11	1.38	1 (14%)
8	FME	I	1	8	8,9,10	0.36	0	7,9,11	0.76	0
13	FME	t	1	13	8,9,10	0.36	0	7,9,11	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HSK	A	332	1	-	2/5/6/8	0/1/1/1
1	HSK	a	332	1	-	2/5/6/8	0/1/1/1
8	FME	i	1	8	-	2/7/9/11	-
13	FME	T	1	13	-	3/7/9/11	-
8	FME	I	1	8	-	3/7/9/11	-
13	FME	t	1	13	-	4/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	HSK	CD2-NE2	-4.13	1.31	1.37
1	a	332	HSK	CD2-NE2	-4.11	1.31	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	332	HSK	ND1-CE1-NE2	-2.92	108.09	111.75
1	A	332	HSK	ND1-CE1-NE2	-2.89	108.13	111.75
13	T	1	FME	CA-N-CN	2.89	127.26	122.82
1	a	332	HSK	CD2-NE2-CE1	2.34	108.07	105.22
1	A	332	HSK	CD2-NE2-CE1	2.30	108.02	105.22

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	332	HSK	C-CA-CB-CG
1	A	332	HSK	N-CA-CB-CG
8	I	1	FME	C-CA-CB-CG
1	a	332	HSK	C-CA-CB-CG
1	a	332	HSK	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 212 ligands modelled in this entry, 4 are monoatomic - leaving 208 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	$\# Z > 2$
25	PLM	I	101	-	15,15,17	0.68	0	15,15,17	0.64	0
28	LMG	c	501	-	51,51,55	0.50	0	59,59,63	0.63	0
30	DGD	d	414	-	47,47,67	0.52	0	54,55,81	0.66	0
19	CLA	b	610	2	69,73,73	1.23	10 (14%)	83,113,113	1.35	9 (10%)
19	CLA	B	613	2	69,73,73	1.24	10 (14%)	83,113,113	1.31	7 (8%)
19	CLA	b	615	2	69,73,73	1.25	10 (14%)	83,113,113	1.31	7 (8%)
24	LFA	B	625	-	10,10,19	0.24	0	9,9,18	0.18	0
30	DGD	C	517	-	63,63,67	0.59	0	77,77,81	0.74	2 (2%)
29	LMT	b	602	-	20,20,36	0.50	0	25,25,47	0.86	1 (4%)
25	PLM	b	623	-	17,17,17	0.64	0	17,17,17	0.66	0
27	LHG	A	417	-	45,45,48	0.54	0	48,51,54	0.50	0
29	LMT	D	403	-	24,24,36	0.49	0	29,29,47	0.68	0
24	LFA	B	621	-	12,12,19	0.22	0	11,11,18	0.19	0
19	CLA	a	408	1	69,73,73	1.22	9 (13%)	83,113,113	1.36	7 (8%)
19	CLA	b	605	2	69,73,73	1.22	9 (13%)	83,113,113	1.30	8 (9%)
25	PLM	E	101	-	17,17,17	0.64	0	17,17,17	0.58	0
19	CLA	d	404	4	69,73,73	1.23	9 (13%)	83,113,113	1.28	4 (4%)
32	RRX	x	102	-	42,42,42	0.20	0	57,58,58	0.40	0
29	LMT	m	101	-	36,36,36	0.53	0	47,47,47	0.75	0
29	LMT	m	102	-	36,36,36	0.55	0	47,47,47	0.69	0
19	CLA	C	503	3	69,73,73	1.24	9 (13%)	83,113,113	1.31	8 (9%)
19	CLA	c	503	3	69,73,73	1.24	9 (13%)	83,113,113	1.34	5 (6%)
19	CLA	b	612	33	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)
24	LFA	A	412	-	14,14,19	0.24	0	13,13,18	0.20	0
25	PLM	b	631	-	15,15,17	0.69	0	15,15,17	0.63	0
29	LMT	d	412	-	24,24,36	0.52	0	29,29,47	0.69	0
24	LFA	X	101	-	12,12,19	0.22	0	11,11,18	0.25	0
19	CLA	b	606	2	69,73,73	1.26	8 (11%)	83,113,113	1.45	9 (10%)
29	LMT	D	402	-	36,36,36	0.53	0	47,47,47	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PLM	i	102	-	12,12,17	0.77	0	12,12,17	0.70	0
21	BCR	y	101	-	41,41,41	0.34	0	56,56,56	1.06	4 (7%)
29	LMT	C	502	-	31,31,36	0.64	0	42,42,47	0.85	1 (2%)
24	LFA	d	411	-	14,14,19	0.20	0	13,13,18	0.25	0
19	CLA	c	502	3	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
19	CLA	B	604	2	69,73,73	1.26	8 (11%)	83,113,113	1.48	10 (12%)
21	BCR	d	406	-	41,41,41	0.34	0	56,56,56	0.71	0
24	LFA	k	102	-	6,6,19	0.25	0	5,5,18	0.21	0
24	LFA	a	413	-	10,10,19	0.23	0	9,9,18	0.21	0
19	CLA	a	404	1	69,73,73	1.25	9 (13%)	83,113,113	1.36	8 (9%)
27	LHG	L	101	-	48,48,48	0.51	0	51,54,54	0.54	0
19	CLA	b	609	33	69,73,73	1.22	6 (8%)	83,113,113	1.37	8 (9%)
24	LFA	d	413	-	7,7,19	0.25	0	6,6,18	0.20	0
24	LFA	h	101	-	7,7,19	0.26	0	6,6,18	0.18	0
19	CLA	B	603	2	69,73,73	1.22	9 (13%)	83,113,113	1.29	9 (10%)
19	CLA	c	509	3	69,73,73	1.23	9 (13%)	83,113,113	1.36	9 (10%)
29	LMT	i	103	-	36,36,36	0.52	0	47,47,47	1.02	2 (4%)
19	CLA	B	616	2	69,73,73	1.24	8 (11%)	83,113,113	1.38	6 (7%)
22	SQD	F	102	-	31,32,54	2.37	8 (25%)	34,36,65	1.67	6 (17%)
25	PLM	C	520	-	8,8,17	0.91	0	8,8,17	0.89	0
19	CLA	c	510	3	69,73,73	1.22	8 (11%)	83,113,113	1.35	6 (7%)
19	CLA	b	608	2	69,73,73	1.24	9 (13%)	83,113,113	1.40	9 (10%)
21	BCR	C	521	-	41,41,41	0.37	0	56,56,56	1.11	5 (8%)
21	BCR	a	409	-	41,41,41	0.32	0	56,56,56	0.71	0
19	CLA	C	515	3	69,73,73	1.23	8 (11%)	83,113,113	1.34	9 (10%)
24	LFA	h	103	-	5,5,19	0.26	0	4,4,18	0.16	0
19	CLA	B	607	33	69,73,73	1.23	6 (8%)	83,113,113	1.38	8 (9%)
19	CLA	B	614	2	69,73,73	1.23	9 (13%)	83,113,113	1.33	9 (10%)
30	DGD	c	517	-	63,63,67	0.55	0	77,77,81	0.78	2 (2%)
28	LMG	b	622	-	51,51,55	0.50	0	59,59,63	0.61	0
20	PHO	D	401	-	58,69,69	1.16	3 (5%)	56,99,99	1.62	7 (12%)
19	CLA	C	511	3	69,73,73	1.22	8 (11%)	83,113,113	1.34	6 (7%)
19	CLA	C	513	3	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
30	DGD	c	516	-	63,63,67	0.58	0	77,77,81	0.75	2 (2%)
24	LFA	B	624	-	6,6,19	0.26	0	5,5,18	0.17	0
21	BCR	c	520	-	41,41,41	0.37	0	56,56,56	1.16	5 (8%)
24	LFA	b	629	-	8,8,19	0.23	0	7,7,18	0.21	0
24	LFA	i	105	-	10,10,19	0.24	0	9,9,18	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	c	508	33	69,73,73	1.23	8 (11%)	83,113,113	1.37	8 (9%)
19	CLA	B	610	33	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
24	LFA	b	632	-	6,6,19	0.27	0	5,5,18	0.18	0
19	CLA	B	615	2	69,73,73	1.22	8 (11%)	83,113,113	1.31	5 (6%)
21	BCR	b	620	-	41,41,41	0.36	0	56,56,56	0.92	3 (5%)
19	CLA	C	506	33	69,73,73	1.23	8 (11%)	83,113,113	1.36	7 (8%)
21	BCR	B	619	-	41,41,41	0.32	0	56,56,56	0.75	0
25	PLM	b	628	-	13,13,17	0.73	0	13,13,17	0.69	0
25	PLM	b	630	-	12,12,17	0.74	0	12,12,17	0.74	0
27	LHG	d	409	-	48,48,48	0.51	0	51,54,54	0.49	0
25	PLM	a	414	-	11,11,17	0.78	0	11,11,17	0.75	0
28	LMG	C	518	-	42,42,55	0.53	0	50,50,63	0.70	0
30	DGD	D	415	-	44,44,67	0.55	0	52,52,81	0.68	1 (1%)
22	SQD	a	412	-	42,43,54	1.67	7 (16%)	51,54,65	1.43	6 (11%)
24	LFA	I	103	-	6,6,19	0.26	0	5,5,18	0.18	0
19	CLA	B	611	2	69,73,73	1.23	10 (14%)	83,113,113	1.36	9 (10%)
23	PL9	a	411	-	55,55,55	1.08	3 (5%)	68,69,69	1.56	13 (19%)
28	LMG	c	518	-	51,51,55	0.48	0	59,59,63	0.58	0
22	SQD	l	102	-	53,54,54	1.52	9 (16%)	62,65,65	1.51	8 (12%)
31	HEM	F	101	5,6	50,50,50	1.45	7 (14%)	66,82,82	1.25	8 (12%)
19	CLA	A	407	1	69,73,73	1.23	10 (14%)	83,113,113	1.34	7 (8%)
19	CLA	c	507	3	69,73,73	1.24	9 (13%)	83,113,113	1.34	9 (10%)
25	PLM	B	627	-	15,15,17	0.70	0	15,15,17	0.61	0
25	PLM	D	405	-	17,17,17	0.64	0	17,17,17	0.62	0
29	LMT	M	102	-	36,36,36	0.55	0	47,47,47	0.73	0
19	CLA	a	405	33	69,73,73	1.22	8 (11%)	83,113,113	1.39	8 (9%)
19	CLA	A	404	33	69,73,73	1.22	8 (11%)	83,113,113	1.40	8 (9%)
24	LFA	C	519	-	6,6,19	0.27	0	5,5,18	0.16	0
19	CLA	c	512	3	69,73,73	1.24	10 (14%)	83,113,113	1.38	8 (9%)
24	LFA	D	404	-	15,15,19	0.17	0	14,14,18	0.37	0
30	DGD	c	519	-	63,63,67	0.55	0	77,77,81	0.71	1 (1%)
24	LFA	H	104	-	5,5,19	0.27	0	4,4,18	0.16	0
19	CLA	c	513	3	69,73,73	1.23	8 (11%)	83,113,113	1.35	7 (8%)
19	CLA	C	504	3	69,73,73	1.23	8 (11%)	83,113,113	1.34	5 (6%)
21	BCR	B	629	-	41,41,41	0.34	0	56,56,56	0.88	2 (3%)
24	LFA	K	102	-	6,6,19	0.25	0	5,5,18	0.20	0
27	LHG	D	412	-	48,48,48	0.52	0	51,54,54	0.51	0
30	DGD	J	101	-	55,55,67	0.54	0	69,69,81	0.86	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LFA	x	101	-	12,12,19	0.22	0	11,11,18	0.24	0
25	PLM	A	413	-	17,17,17	0.65	0	17,17,17	0.62	0
27	LHG	D	413	-	48,48,48	0.51	0	51,54,54	0.49	0
19	CLA	c	506	3	69,73,73	1.23	10 (14%)	83,113,113	1.35	6 (7%)
20	PHO	a	407	-	58,69,69	1.21	4 (6%)	56,99,99	1.54	7 (12%)
25	PLM	B	623	-	11,11,17	0.79	0	11,11,17	0.74	0
25	PLM	B	626	-	12,12,17	0.76	0	12,12,17	0.71	0
19	CLA	b	603	33	69,73,73	1.26	8 (11%)	83,113,113	1.28	5 (6%)
28	LMG	D	414	-	48,48,55	0.53	0	56,56,63	0.62	0
24	LFA	m	103	-	8,8,19	0.24	0	7,7,18	0.19	0
29	LMT	M	101	-	36,36,36	0.52	0	47,47,47	0.79	0
30	DGD	h	102	-	63,63,67	0.59	0	77,77,81	0.75	1 (1%)
19	CLA	a	406	33	69,73,73	1.22	8 (11%)	83,113,113	1.37	10 (12%)
23	PL9	A	410	-	55,55,55	1.07	3 (5%)	68,69,69	1.48	12 (17%)
19	CLA	b	604	2	69,73,73	1.22	9 (13%)	83,113,113	1.33	8 (9%)
19	CLA	A	403	1	69,73,73	1.24	9 (13%)	83,113,113	1.36	8 (9%)
19	CLA	B	612	2	69,73,73	1.23	9 (13%)	83,113,113	1.40	7 (8%)
19	CLA	b	617	2	69,73,73	1.22	8 (11%)	83,113,113	1.31	5 (6%)
19	CLA	C	507	3	69,73,73	1.24	10 (14%)	83,113,113	1.34	6 (7%)
19	CLA	c	514	3	69,73,73	1.22	9 (13%)	83,113,113	1.36	8 (9%)
24	LFA	J	102	-	16,16,19	0.24	0	15,15,18	0.20	0
27	LHG	l	101	-	48,48,48	0.51	0	51,54,54	0.53	0
19	CLA	B	605	2	69,73,73	1.24	8 (11%)	83,113,113	1.35	6 (7%)
22	SQD	L	102	-	53,54,54	1.52	9 (16%)	62,65,65	1.53	9 (14%)
24	LFA	D	407	-	8,8,19	0.25	0	7,7,18	0.21	0
19	CLA	b	616	2	69,73,73	1.23	9 (13%)	83,113,113	1.33	9 (10%)
25	PLM	I	104	-	10,10,17	0.84	0	10,10,17	0.81	0
29	LMT	d	401	-	35,35,36	0.53	0	46,46,47	0.74	0
19	CLA	D	408	4	69,73,73	1.24	9 (13%)	83,113,113	1.28	4 (4%)
22	SQD	a	410	-	53,54,54	1.49	6 (11%)	62,65,65	1.51	7 (11%)
21	BCR	b	601	-	41,41,41	0.31	0	56,56,56	1.44	9 (16%)
27	LHG	a	416	-	48,48,48	0.51	0	51,54,54	0.49	0
25	PLM	a	401	-	16,16,17	0.68	0	16,16,17	0.60	0
19	CLA	b	614	2	69,73,73	1.22	10 (14%)	83,113,113	1.39	7 (8%)
24	LFA	M	103	-	9,9,19	0.23	0	8,8,18	0.21	0
30	DGD	H	103	-	63,63,67	0.59	0	77,77,81	0.75	0
19	CLA	C	505	3	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
24	LFA	b	624	-	11,11,19	0.21	0	10,10,18	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PLM	A	415	-	10,10,17	0.83	0	10,10,17	0.77	0
21	BCR	D	410	-	41,41,41	0.34	0	56,56,56	0.71	0
25	PLM	i	101	-	15,15,17	0.67	0	15,15,17	0.67	0
28	LMG	C	501	-	51,51,55	0.51	0	59,59,63	0.62	0
24	LFA	Z	101	-	7,7,19	0.25	0	6,6,18	0.20	0
21	BCR	C	516	-	41,41,41	0.33	0	56,56,56	0.69	0
26	BCT	d	403	17	2,3,3	0.88	0	2,3,3	3.21	2 (100%)
19	CLA	B	601	33	69,73,73	1.27	8 (11%)	83,113,113	1.29	5 (6%)
19	CLA	c	505	33	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)
19	CLA	B	606	2	69,73,73	1.24	10 (14%)	83,113,113	1.39	8 (9%)
22	SQD	f	102	-	44,45,54	1.63	9 (20%)	53,56,65	1.56	8 (15%)
19	CLA	c	504	3	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
19	CLA	C	508	3	69,73,73	1.24	9 (13%)	83,113,113	1.33	9 (10%)
21	BCR	K	101	-	41,41,41	0.32	0	56,56,56	0.59	0
27	LHG	d	408	-	48,48,48	0.52	0	51,54,54	0.51	0
19	CLA	C	514	3	69,73,73	1.23	7 (10%)	83,113,113	1.35	7 (8%)
19	CLA	b	613	2	69,73,73	1.23	10 (14%)	83,113,113	1.37	9 (10%)
19	CLA	D	409	4	69,73,73	1.23	8 (11%)	83,113,113	1.32	5 (6%)
20	PHO	d	402	-	58,69,69	1.17	3 (5%)	56,99,99	1.59	6 (10%)
27	LHG	a	415	-	45,45,48	0.53	0	48,51,54	0.52	0
23	PL9	D	411	-	55,55,55	1.30	6 (10%)	68,69,69	1.51	14 (20%)
28	LMG	B	620	-	51,51,55	0.51	0	59,59,63	0.61	0
19	CLA	B	608	2	69,73,73	1.23	10 (14%)	83,113,113	1.33	9 (10%)
19	CLA	c	511	3	69,73,73	1.25	10 (14%)	83,113,113	1.25	4 (4%)
19	CLA	B	602	2	69,73,73	1.22	7 (10%)	83,113,113	1.34	8 (9%)
19	CLA	b	607	2	69,73,73	1.24	10 (14%)	83,113,113	1.36	5 (6%)
19	CLA	B	609	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
21	BCR	Y	101	-	41,41,41	0.35	0	56,56,56	1.00	2 (3%)
24	LFA	H	101	-	13,13,19	0.21	0	12,12,18	0.27	0
24	LFA	h	104	-	6,6,19	0.25	0	5,5,18	0.19	0
19	CLA	b	611	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
24	LFA	b	627	-	8,8,19	0.25	0	7,7,18	0.18	0
22	SQD	A	411	-	53,54,54	1.54	7 (13%)	62,65,65	1.32	6 (9%)
25	PLM	b	625	-	8,8,17	0.93	0	8,8,17	0.82	0
21	BCR	B	617	-	41,41,41	0.33	0	56,56,56	0.78	1 (1%)
24	LFA	B	628	-	6,6,19	0.26	0	5,5,18	0.15	0
20	PHO	A	406	-	58,69,69	1.22	5 (8%)	56,99,99	1.54	7 (12%)
31	HEM	f	101	5,6	50,50,50	1.43	7 (14%)	66,82,82	1.25	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	t	101	-	24,24,36	0.53	0	29,29,47	1.09	3 (10%)
29	LMT	z	101	-	36,36,36	0.52	0	47,47,47	0.97	4 (8%)
21	BCR	k	101	-	41,41,41	0.32	0	56,56,56	0.56	0
21	BCR	B	618	-	41,41,41	0.37	0	56,56,56	0.78	0
32	RRX	H	102	-	42,42,42	0.20	0	57,58,58	0.39	0
26	BCT	A	416	17	2,3,3	0.89	0	2,3,3	3.22	2 (100%)
22	SQD	A	409	-	49,50,54	1.53	6 (12%)	58,61,65	1.54	7 (12%)
19	CLA	C	509	33	69,73,73	1.23	8 (11%)	83,113,113	1.37	9 (10%)
19	CLA	b	618	2	69,73,73	1.23	8 (11%)	83,113,113	1.37	5 (6%)
24	LFA	b	626	-	10,10,19	0.24	0	9,9,18	0.21	0
21	BCR	c	515	-	41,41,41	0.32	0	56,56,56	0.68	0
25	PLM	H	105	-	9,9,17	0.90	0	9,9,17	0.79	0
21	BCR	b	619	-	41,41,41	0.32	0	56,56,56	0.85	2 (3%)
25	PLM	i	104	-	12,12,17	0.76	0	12,12,17	0.69	0
28	LMG	d	410	-	51,51,55	0.53	0	59,59,63	0.59	0
24	LFA	D	406	-	12,12,19	0.23	0	11,11,18	0.28	0
19	CLA	C	510	3	69,73,73	1.23	8 (11%)	83,113,113	1.37	8 (9%)
19	CLA	C	512	3	69,73,73	1.25	9 (13%)	83,113,113	1.26	5 (6%)
19	CLA	d	405	4	69,73,73	1.24	9 (13%)	83,113,113	1.31	5 (6%)
24	LFA	A	414	-	12,12,19	0.23	0	11,11,18	0.21	0
25	PLM	B	622	-	7,7,17	1.00	0	7,7,17	0.93	0
23	PL9	d	407	-	55,55,55	1.31	6 (10%)	68,69,69	1.51	13 (19%)
21	BCR	b	621	-	41,41,41	0.32	0	56,56,56	0.75	0
19	CLA	A	405	33	69,73,73	1.23	8 (11%)	83,113,113	1.36	9 (10%)
25	PLM	e	101	-	17,17,17	0.64	0	17,17,17	0.61	0
25	PLM	I	102	-	17,17,17	0.66	0	17,17,17	0.65	0
21	BCR	A	408	-	41,41,41	0.32	0	56,56,56	0.73	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
25	PLM	I	101	-	-	6/13/13/15	-
28	LMG	c	501	-	-	18/46/66/70	0/1/1/1
30	DGD	d	414	-	-	13/41/62/95	0/1/1/2
19	CLA	b	610	2	-	7/39/115/115	-
19	CLA	B	613	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	615	2	-	8/39/115/115	-
24	LFA	B	625	-	-	3/8/8/17	-
30	DGD	C	517	-	-	22/51/91/95	0/2/2/2
29	LMT	b	602	-	-	8/11/31/61	0/1/1/2
25	PLM	b	623	-	-	3/15/15/15	-
27	LHG	A	417	-	-	16/50/50/53	-
29	LMT	D	403	-	-	7/15/35/61	0/1/1/2
24	LFA	B	621	-	-	4/10/10/17	-
19	CLA	a	408	1	-	10/39/115/115	-
19	CLA	b	605	2	-	14/39/115/115	-
25	PLM	E	101	-	-	7/15/15/15	-
19	CLA	d	404	4	-	5/39/115/115	-
32	RRX	x	102	-	-	2/29/65/65	0/2/2/2
29	LMT	m	101	-	-	11/21/61/61	0/2/2/2
29	LMT	m	102	-	-	4/21/61/61	0/2/2/2
19	CLA	C	503	3	-	8/39/115/115	-
19	CLA	c	503	3	-	10/39/115/115	-
19	CLA	b	612	33	-	7/39/115/115	-
24	LFA	A	412	-	-	2/12/12/17	-
25	PLM	b	631	-	-	5/13/13/15	-
29	LMT	d	412	-	-	1/15/35/61	0/1/1/2
24	LFA	X	101	-	-	3/10/10/17	-
19	CLA	b	606	2	-	5/39/115/115	-
29	LMT	D	402	-	-	6/21/61/61	0/2/2/2
25	PLM	i	102	-	-	3/10/10/15	-
21	BCR	y	101	-	-	8/29/63/63	0/2/2/2
29	LMT	C	502	-	-	4/16/56/61	0/2/2/2
24	LFA	d	411	-	-	0/12/12/17	-
19	CLA	c	502	3	-	8/39/115/115	-
19	CLA	B	604	2	-	12/39/115/115	-
21	BCR	d	406	-	-	8/29/63/63	0/2/2/2
24	LFA	k	102	-	-	0/4/4/17	-
24	LFA	a	413	-	-	1/8/8/17	-
19	CLA	a	404	1	-	7/39/115/115	-
27	LHG	L	101	-	-	18/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	609	33	-	4/39/115/115	-
24	LFA	d	413	-	-	0/5/5/17	-
24	LFA	h	101	-	-	0/5/5/17	-
19	CLA	B	603	2	-	14/39/115/115	-
19	CLA	c	509	3	-	6/39/115/115	-
29	LMT	i	103	-	-	7/21/61/61	0/2/2/2
19	CLA	B	616	2	-	15/39/115/115	-
22	SQD	F	102	-	-	20/33/33/69	-
25	PLM	C	520	-	-	0/6/6/15	-
19	CLA	c	510	3	-	7/39/115/115	-
19	CLA	b	608	2	-	3/39/115/115	-
21	BCR	C	521	-	-	5/29/63/63	0/2/2/2
21	BCR	a	409	-	-	3/29/63/63	0/2/2/2
19	CLA	C	515	3	-	4/39/115/115	-
24	LFA	h	103	-	-	0/3/3/17	-
19	CLA	B	607	33	-	4/39/115/115	-
19	CLA	B	614	2	-	16/39/115/115	-
30	DGD	c	517	-	-	18/51/91/95	0/2/2/2
28	LMG	b	622	-	-	23/46/66/70	0/1/1/1
20	PHO	D	401	-	-	4/37/103/103	0/5/6/6
19	CLA	C	511	3	-	8/39/115/115	-
19	CLA	C	513	3	-	6/39/115/115	-
30	DGD	c	516	-	-	21/51/91/95	0/2/2/2
24	LFA	B	624	-	-	0/4/4/17	-
21	BCR	c	520	-	-	5/29/63/63	0/2/2/2
24	LFA	b	629	-	-	1/6/6/17	-
24	LFA	i	105	-	-	0/8/8/17	-
19	CLA	c	508	33	-	6/39/115/115	-
19	CLA	B	610	33	-	7/39/115/115	-
24	LFA	b	632	-	-	2/4/4/17	-
19	CLA	B	615	2	-	6/39/115/115	-
21	BCR	b	620	-	-	1/29/63/63	0/2/2/2
19	CLA	C	506	33	-	8/39/115/115	-
21	BCR	B	619	-	-	3/29/63/63	0/2/2/2
25	PLM	b	628	-	-	2/11/11/15	-
25	PLM	b	630	-	-	2/10/10/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	d	409	-	-	14/53/53/53	-
25	PLM	a	414	-	-	6/9/9/15	-
28	LMG	C	518	-	-	19/37/57/70	0/1/1/1
30	DGD	D	415	-	-	16/38/58/95	0/1/1/2
22	SQD	a	412	-	-	17/38/58/69	0/1/1/1
24	LFA	I	103	-	-	1/4/4/17	-
19	CLA	B	611	2	-	3/39/115/115	-
23	PL9	a	411	-	-	30/53/73/73	0/1/1/1
28	LMG	c	518	-	-	15/46/66/70	0/1/1/1
22	SQD	l	102	-	-	26/49/69/69	0/1/1/1
31	HEM	F	101	5,6	-	2/14/54/54	-
19	CLA	A	407	1	-	12/39/115/115	-
19	CLA	c	507	3	-	18/39/115/115	-
25	PLM	B	627	-	-	3/13/13/15	-
25	PLM	D	405	-	-	3/15/15/15	-
29	LMT	M	102	-	-	4/21/61/61	0/2/2/2
19	CLA	a	405	33	-	3/39/115/115	-
19	CLA	A	404	33	-	3/39/115/115	-
24	LFA	C	519	-	-	0/4/4/17	-
19	CLA	c	512	3	-	6/39/115/115	-
24	LFA	D	404	-	-	4/13/13/17	-
30	DGD	c	519	-	-	11/51/91/95	0/2/2/2
24	LFA	H	104	-	-	0/3/3/17	-
19	CLA	c	513	3	-	8/39/115/115	-
19	CLA	C	504	3	-	10/39/115/115	-
21	BCR	B	629	-	-	10/29/63/63	0/2/2/2
24	LFA	K	102	-	-	0/4/4/17	-
27	LHG	D	412	-	-	8/53/53/53	-
30	DGD	J	101	-	-	18/43/83/95	0/2/2/2
24	LFA	x	101	-	-	0/10/10/17	-
25	PLM	A	413	-	-	4/15/15/15	-
27	LHG	D	413	-	-	14/53/53/53	-
19	CLA	c	506	3	-	9/39/115/115	-
20	PHO	a	407	-	-	5/37/103/103	0/5/6/6
25	PLM	B	623	-	-	0/9/9/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PLM	B	626	-	-	3/10/10/15	-
19	CLA	b	603	33	-	17/39/115/115	-
28	LMG	D	414	-	-	12/43/63/70	0/1/1/1
24	LFA	m	103	-	-	1/6/6/17	-
29	LMT	M	101	-	-	7/21/61/61	0/2/2/2
30	DGD	h	102	-	-	13/51/91/95	0/2/2/2
19	CLA	a	406	33	-	11/39/115/115	-
23	PL9	A	410	-	-	21/53/73/73	0/1/1/1
19	CLA	b	604	2	-	6/39/115/115	-
19	CLA	A	403	1	-	7/39/115/115	-
19	CLA	B	612	2	-	6/39/115/115	-
19	CLA	b	617	2	-	7/39/115/115	-
19	CLA	C	507	3	-	9/39/115/115	-
19	CLA	c	514	3	-	4/39/115/115	-
24	LFA	J	102	-	-	2/14/14/17	-
27	LHG	l	101	-	-	25/53/53/53	-
19	CLA	B	605	2	-	8/39/115/115	-
22	SQD	L	102	-	-	25/49/69/69	0/1/1/1
24	LFA	D	407	-	-	0/6/6/17	-
19	CLA	b	616	2	-	14/39/115/115	-
25	PLM	I	104	-	-	5/8/8/15	-
29	LMT	d	401	-	-	2/20/60/61	0/2/2/2
19	CLA	D	408	4	-	5/39/115/115	-
22	SQD	a	410	-	-	21/49/69/69	0/1/1/1
21	BCR	b	601	-	-	9/29/63/63	0/2/2/2
27	LHG	a	416	-	-	21/53/53/53	-
25	PLM	a	401	-	-	5/14/14/15	-
19	CLA	b	614	2	-	7/39/115/115	-
24	LFA	M	103	-	-	1/7/7/17	-
30	DGD	H	103	-	-	12/51/91/95	0/2/2/2
19	CLA	C	505	3	-	6/39/115/115	-
24	LFA	b	624	-	-	1/9/9/17	-
25	PLM	A	415	-	-	5/8/8/15	-
21	BCR	D	410	-	-	8/29/63/63	0/2/2/2
25	PLM	i	101	-	-	3/13/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	C	501	-	-	22/46/66/70	0/1/1/1
24	LFA	Z	101	-	-	1/5/5/17	-
21	BCR	C	516	-	-	6/29/63/63	0/2/2/2
19	CLA	B	601	33	-	17/39/115/115	-
19	CLA	c	505	33	-	8/39/115/115	-
19	CLA	B	606	2	-	3/39/115/115	-
22	SQD	f	102	-	-	18/40/60/69	0/1/1/1
19	CLA	c	504	3	-	8/39/115/115	-
19	CLA	C	508	3	-	18/39/115/115	-
21	BCR	K	101	-	-	7/29/63/63	0/2/2/2
27	LHG	d	408	-	-	8/53/53/53	-
19	CLA	C	514	3	-	8/39/115/115	-
19	CLA	b	613	2	-	3/39/115/115	-
19	CLA	D	409	4	-	13/39/115/115	-
20	PHO	d	402	-	-	4/37/103/103	0/5/6/6
27	LHG	a	415	-	-	15/50/50/53	-
23	PL9	D	411	-	-	11/53/73/73	0/1/1/1
28	LMG	B	620	-	-	18/46/66/70	0/1/1/1
19	CLA	B	608	2	-	8/39/115/115	-
19	CLA	c	511	3	-	7/39/115/115	-
19	CLA	B	602	2	-	1/39/115/115	-
19	CLA	b	607	2	-	8/39/115/115	-
19	CLA	B	609	-	-	6/39/115/115	-
21	BCR	Y	101	-	-	7/29/63/63	0/2/2/2
24	LFA	H	101	-	-	5/11/11/17	-
24	LFA	h	104	-	-	1/4/4/17	-
19	CLA	b	611	-	-	6/39/115/115	-
24	LFA	b	627	-	-	0/6/6/17	-
22	SQD	A	411	-	-	22/49/69/69	0/1/1/1
25	PLM	b	625	-	-	3/6/6/15	-
21	BCR	B	617	-	-	5/29/63/63	0/2/2/2
24	LFA	B	628	-	-	2/4/4/17	-
20	PHO	A	406	-	-	4/37/103/103	0/5/6/6
31	HEM	f	101	5,6	-	5/14/54/54	-
29	LMT	t	101	-	-	7/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	z	101	-	-	5/21/61/61	0/2/2/2
21	BCR	k	101	-	-	7/29/63/63	0/2/2/2
21	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	RRX	H	102	-	-	2/29/65/65	0/2/2/2
22	SQD	A	409	-	-	22/45/65/69	0/1/1/1
19	CLA	C	509	33	-	12/39/115/115	-
19	CLA	b	618	2	-	15/39/115/115	-
24	LFA	b	626	-	-	2/8/8/17	-
21	BCR	c	515	-	-	6/29/63/63	0/2/2/2
25	PLM	H	105	-	-	2/7/7/15	-
21	BCR	b	619	-	-	5/29/63/63	0/2/2/2
25	PLM	i	104	-	-	5/10/10/15	-
28	LMG	d	410	-	-	14/46/66/70	0/1/1/1
24	LFA	D	406	-	-	3/10/10/17	-
19	CLA	C	510	3	-	5/39/115/115	-
19	CLA	C	512	3	-	7/39/115/115	-
19	CLA	d	405	4	-	11/39/115/115	-
24	LFA	A	414	-	-	2/10/10/17	-
25	PLM	B	622	-	-	2/5/5/15	-
23	PL9	d	407	-	-	6/53/73/73	0/1/1/1
21	BCR	b	621	-	-	3/29/63/63	0/2/2/2
19	CLA	A	405	33	-	13/39/115/115	-
25	PLM	e	101	-	-	3/15/15/15	-
25	PLM	I	102	-	-	4/15/15/15	-
21	BCR	A	408	-	-	3/29/63/63	0/2/2/2

The worst 5 of 716 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	102	SQD	O47-C45	-7.07	1.38	1.46
22	F	102	SQD	C6-S	4.94	1.84	1.77
20	A	406	PHO	C4D-ND	-4.83	1.31	1.38
22	f	102	SQD	O48-C23	4.80	1.47	1.33
22	F	102	SQD	O47-C7	4.77	1.43	1.33

The worst 5 of 709 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	606	CLA	C4A-NA-C1A	8.07	110.33	106.71
19	B	604	CLA	C4A-NA-C1A	8.06	110.33	106.71
19	B	612	CLA	C4A-NA-C1A	8.04	110.32	106.71
19	B	607	CLA	C4A-NA-C1A	7.94	110.28	106.71
19	b	614	CLA	C4A-NA-C1A	7.93	110.27	106.71

There are no chirality outliers.

5 of 1578 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	403	CLA	CBD-CGD-O2D-CED
19	A	404	CLA	CHA-CBD-CGD-O1D
19	A	404	CLA	CHA-CBD-CGD-O2D
19	B	601	CLA	CHA-CBD-CGD-O1D
19	B	601	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

119 monomers are involved in 191 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	610	CLA	1	0
19	B	613	CLA	2	0
19	b	615	CLA	2	0
24	B	625	LFA	2	0
30	C	517	DGD	1	0
29	b	602	LMT	1	0
27	A	417	LHG	1	0
29	D	403	LMT	1	0
19	a	408	CLA	3	0
19	b	605	CLA	1	0
19	d	404	CLA	3	0
29	m	101	LMT	1	0
19	C	503	CLA	1	0
19	c	503	CLA	2	0
25	b	631	PLM	1	0
24	X	101	LFA	1	0
19	b	606	CLA	5	0
29	D	402	LMT	2	0
21	y	101	BCR	1	0
29	C	502	LMT	2	0
24	d	411	LFA	1	0
19	c	502	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	604	CLA	3	0
19	a	404	CLA	3	0
27	L	101	LHG	2	0
19	b	609	CLA	1	0
19	B	603	CLA	1	0
19	B	616	CLA	4	0
22	F	102	SQD	3	0
25	C	520	PLM	1	0
19	b	608	CLA	1	0
21	a	409	BCR	2	0
19	C	515	CLA	3	0
19	B	607	CLA	2	0
30	c	517	DGD	2	0
28	b	622	LMG	4	0
20	D	401	PHO	3	0
19	C	513	CLA	2	0
30	c	516	DGD	1	0
19	B	615	CLA	4	0
21	b	620	BCR	2	0
25	a	414	PLM	1	0
28	C	518	LMG	2	0
30	D	415	DGD	1	0
22	a	412	SQD	2	0
19	B	611	CLA	2	0
23	a	411	PL9	5	0
28	c	518	LMG	1	0
22	l	102	SQD	1	0
31	F	101	HEM	1	0
19	A	407	CLA	3	0
19	c	507	CLA	4	0
25	D	405	PLM	2	0
19	c	512	CLA	4	0
24	D	404	LFA	2	0
30	c	519	DGD	1	0
19	c	513	CLA	1	0
19	C	504	CLA	2	0
21	B	629	BCR	4	0
30	J	101	DGD	4	0
25	A	413	PLM	1	0
27	D	413	LHG	1	0
19	c	506	CLA	3	0
28	D	414	LMG	1	0

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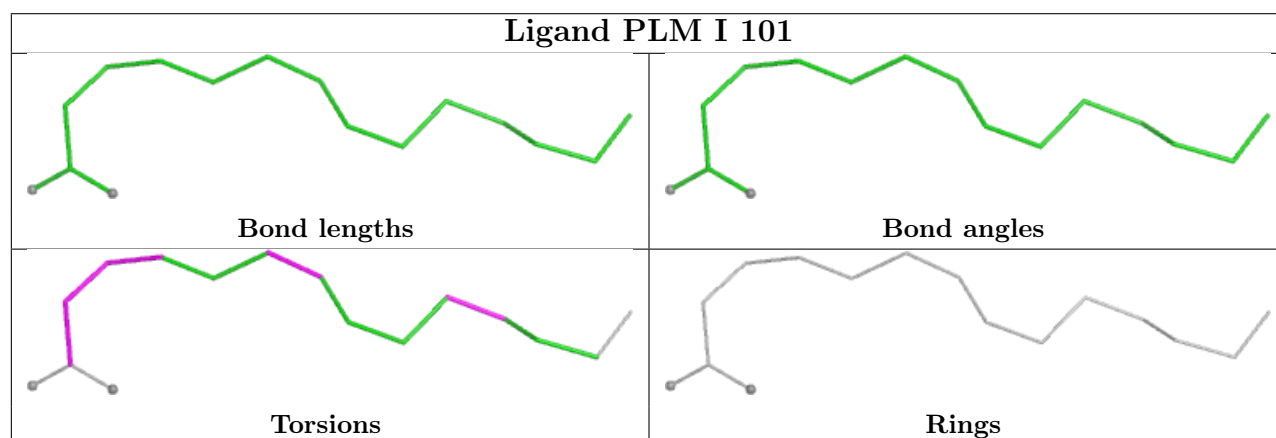
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29	M	101	LMT	1	0
30	h	102	DGD	2	0
23	A	410	PL9	3	0
19	b	604	CLA	2	0
19	A	403	CLA	3	0
19	B	612	CLA	2	0
19	b	617	CLA	5	0
19	C	507	CLA	2	0
19	c	514	CLA	1	0
27	l	101	LHG	1	0
19	B	605	CLA	1	0
22	L	102	SQD	2	0
29	d	401	LMT	1	0
19	D	408	CLA	3	0
21	b	601	BCR	3	0
27	a	416	LHG	3	0
25	a	401	PLM	1	0
19	b	614	CLA	3	0
19	C	505	CLA	1	0
28	C	501	LMG	1	0
21	C	516	BCR	2	0
19	c	505	CLA	2	0
19	B	606	CLA	1	0
22	f	102	SQD	2	0
19	c	504	CLA	1	0
19	C	508	CLA	4	0
21	K	101	BCR	2	0
19	C	514	CLA	1	0
19	b	613	CLA	2	0
19	D	409	CLA	2	0
20	d	402	PHO	2	0
27	a	415	LHG	1	0
28	B	620	LMG	2	0
19	B	608	CLA	1	0
19	B	602	CLA	3	0
19	b	607	CLA	4	0
19	B	609	CLA	1	0
21	Y	101	BCR	2	0
22	A	411	SQD	2	0
21	B	617	BCR	1	0
29	t	101	LMT	1	0
29	z	101	LMT	3	0

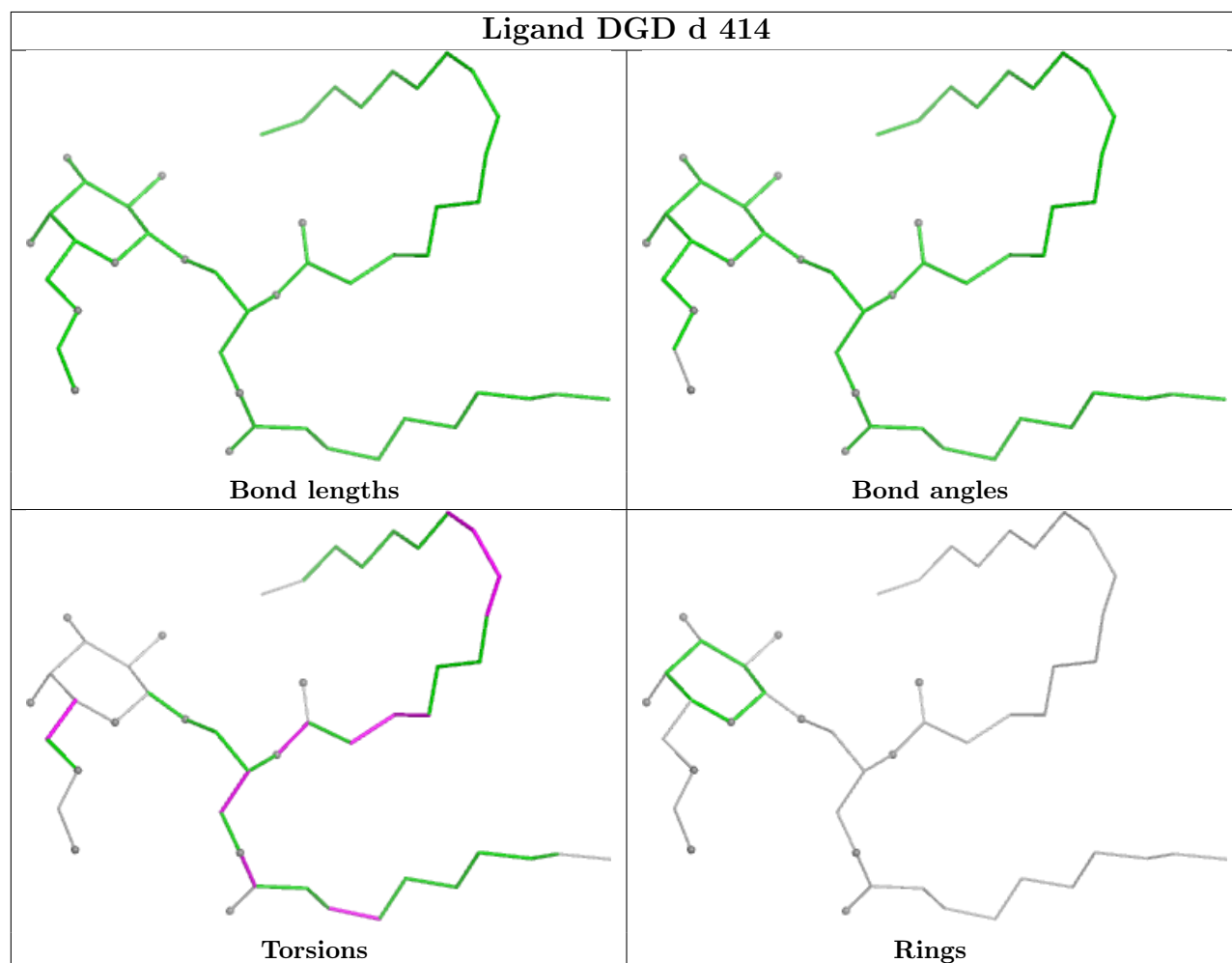
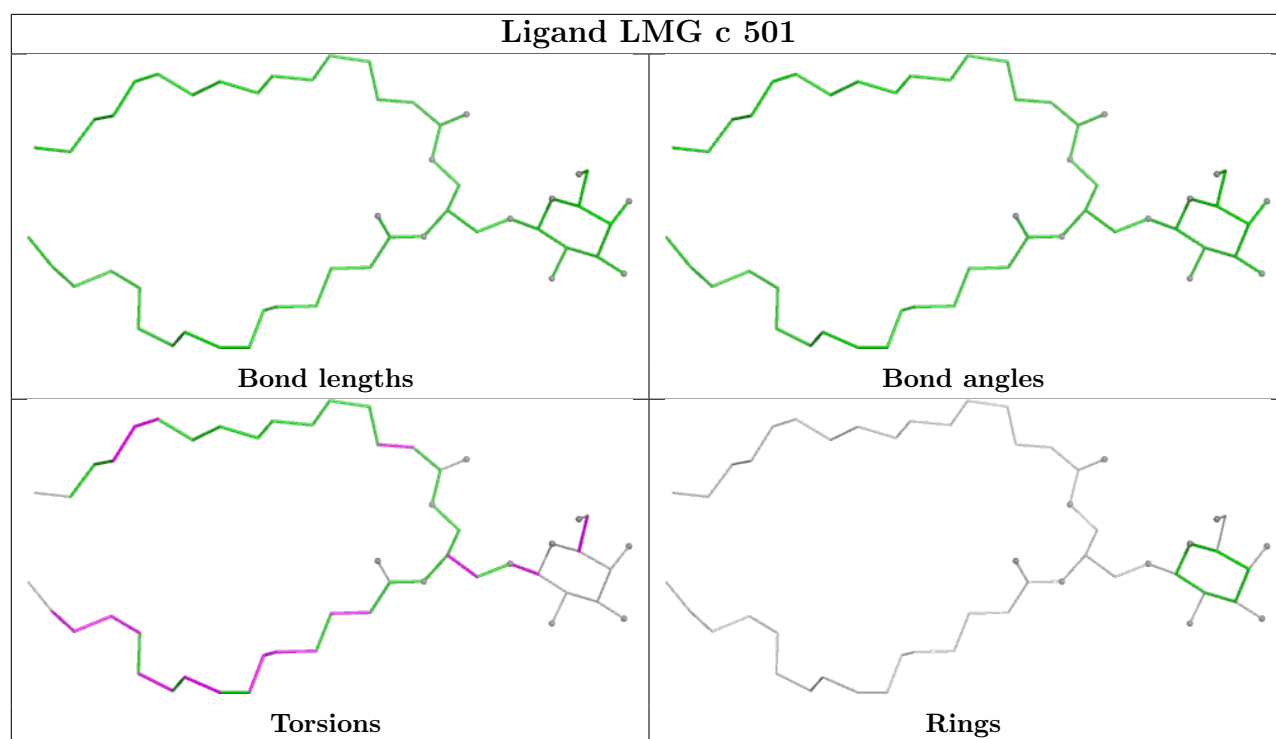
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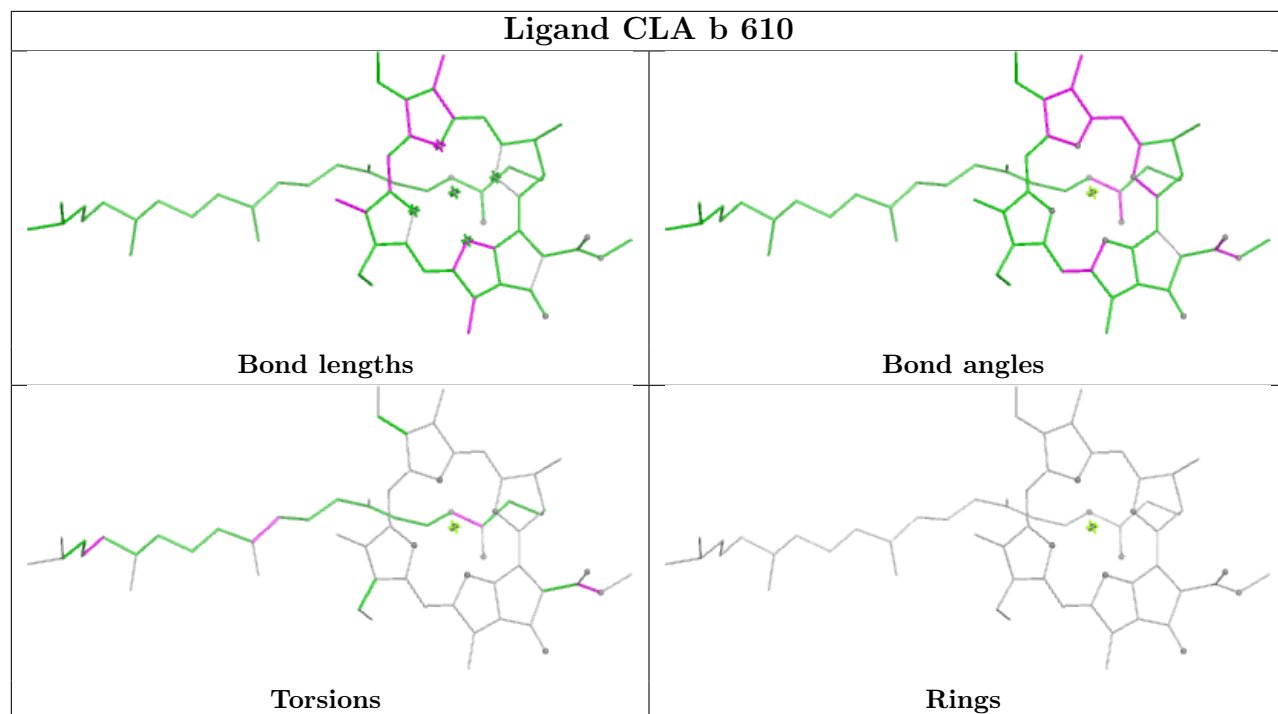
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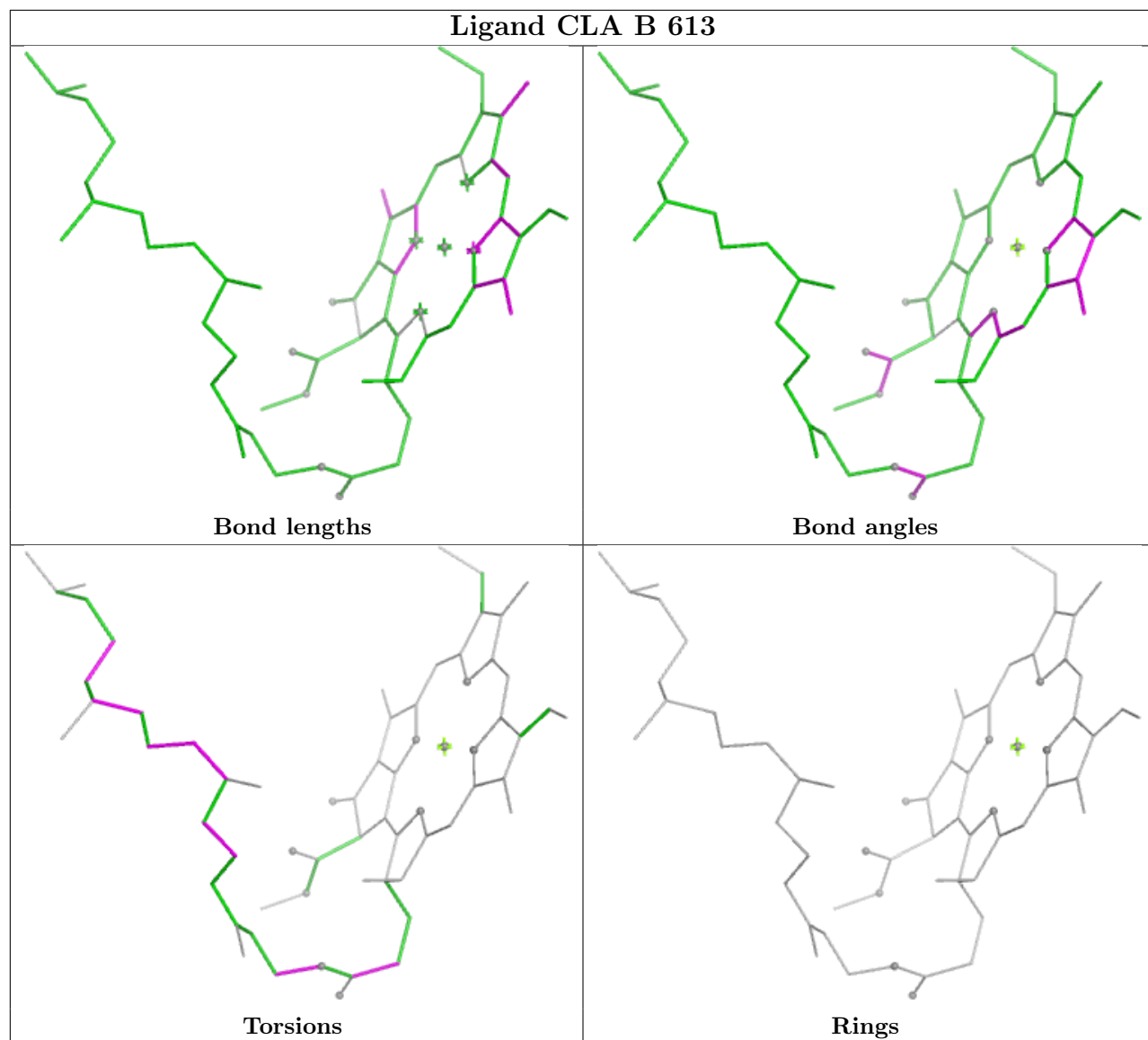
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	618	BCR	1	0
22	A	409	SQD	1	0
19	C	509	CLA	2	0
19	b	618	CLA	4	0
24	b	626	LFA	1	0
21	c	515	BCR	1	0
21	b	619	BCR	3	0
28	d	410	LMG	3	0
24	D	406	LFA	1	0
19	C	510	CLA	1	0
19	d	405	CLA	2	0
23	d	407	PL9	1	0
21	A	408	BCR	1	0

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

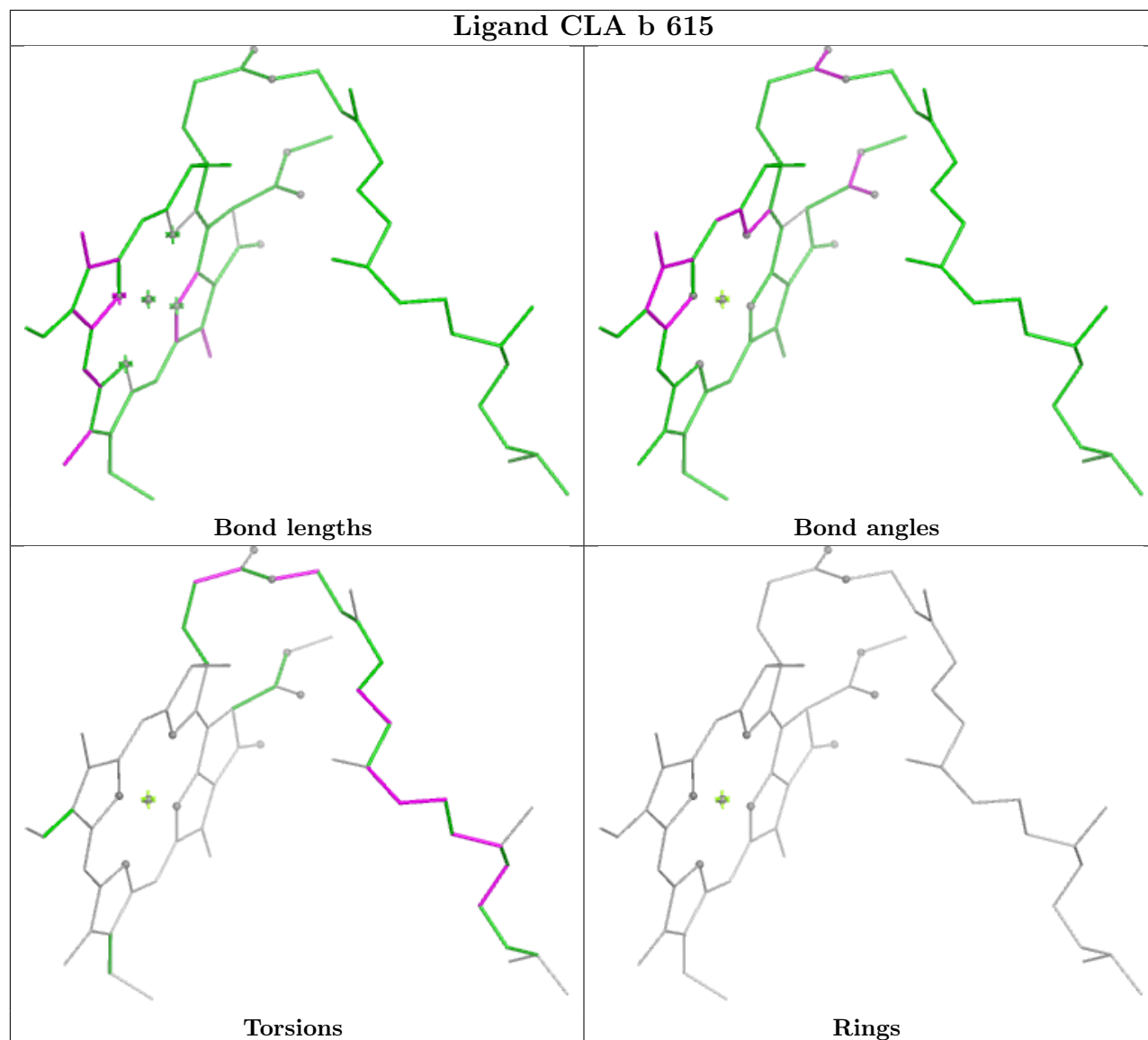




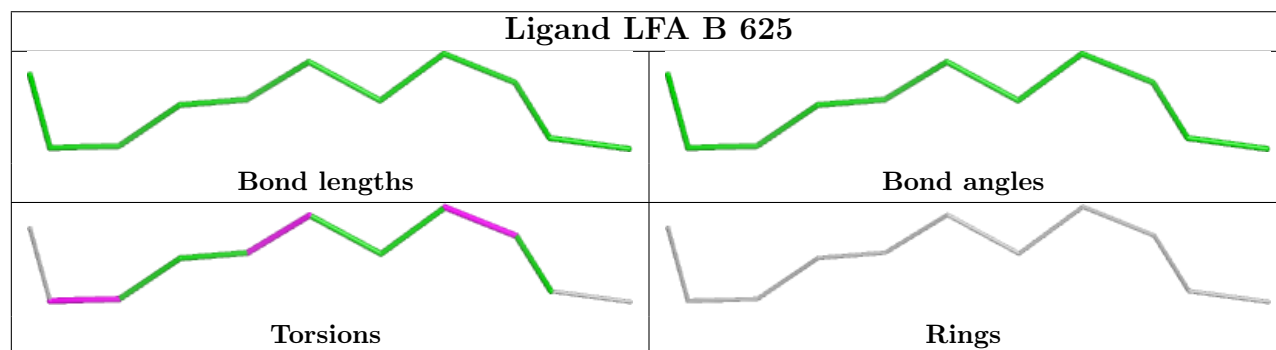


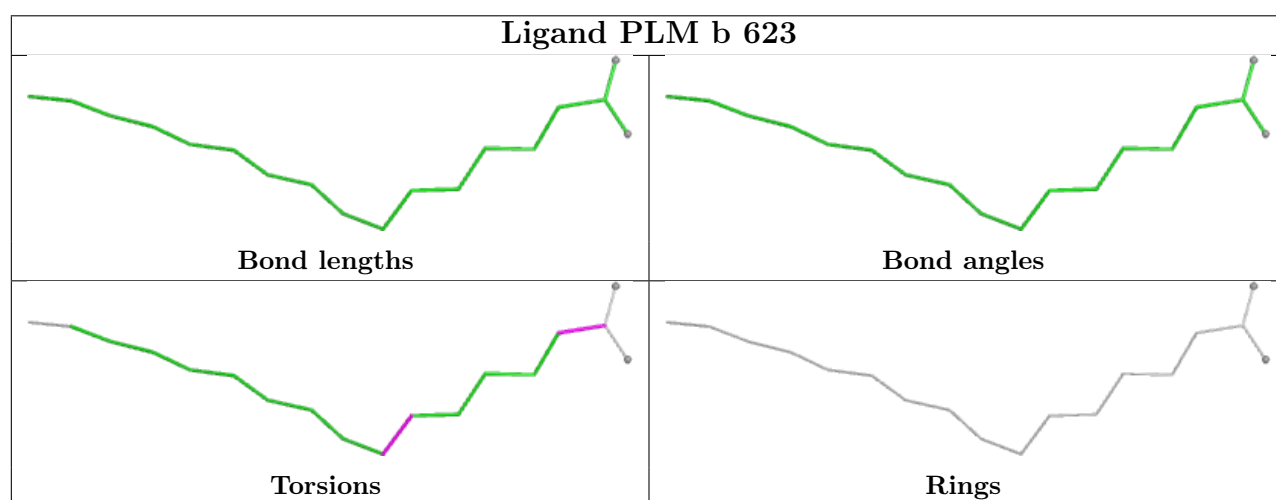
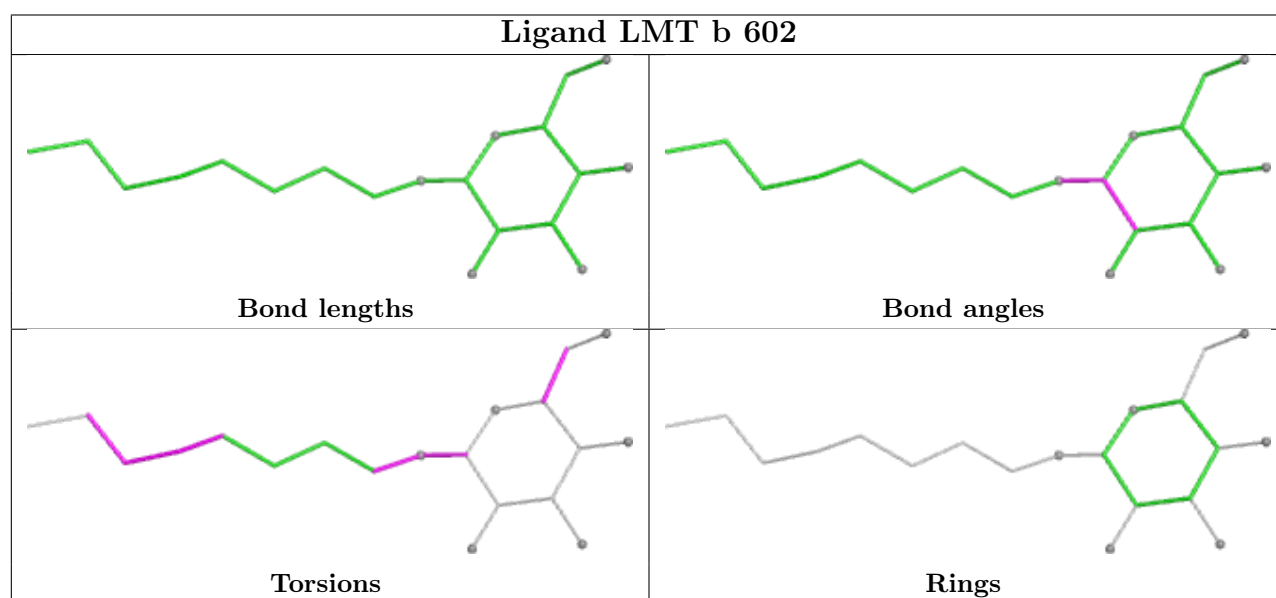
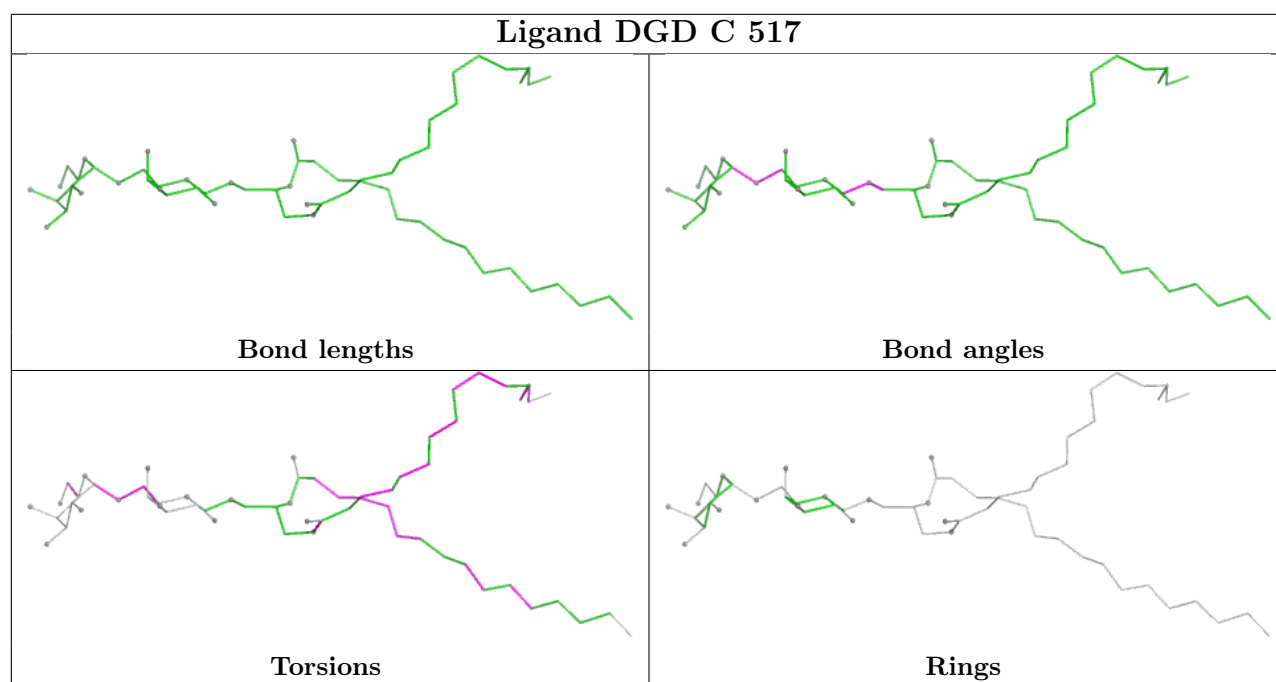


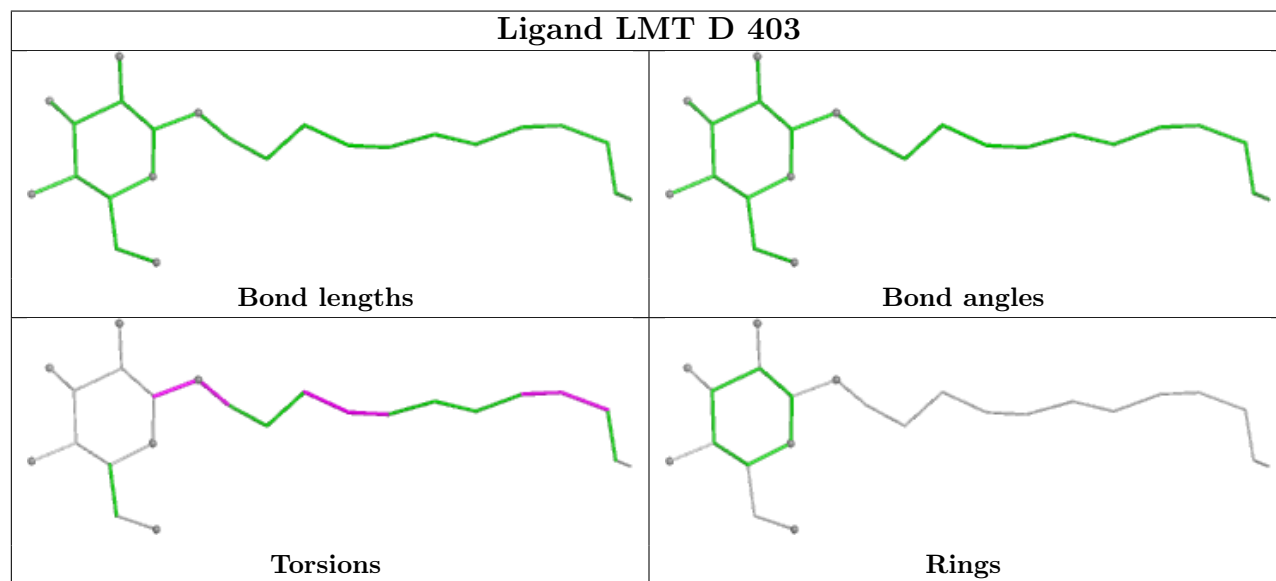
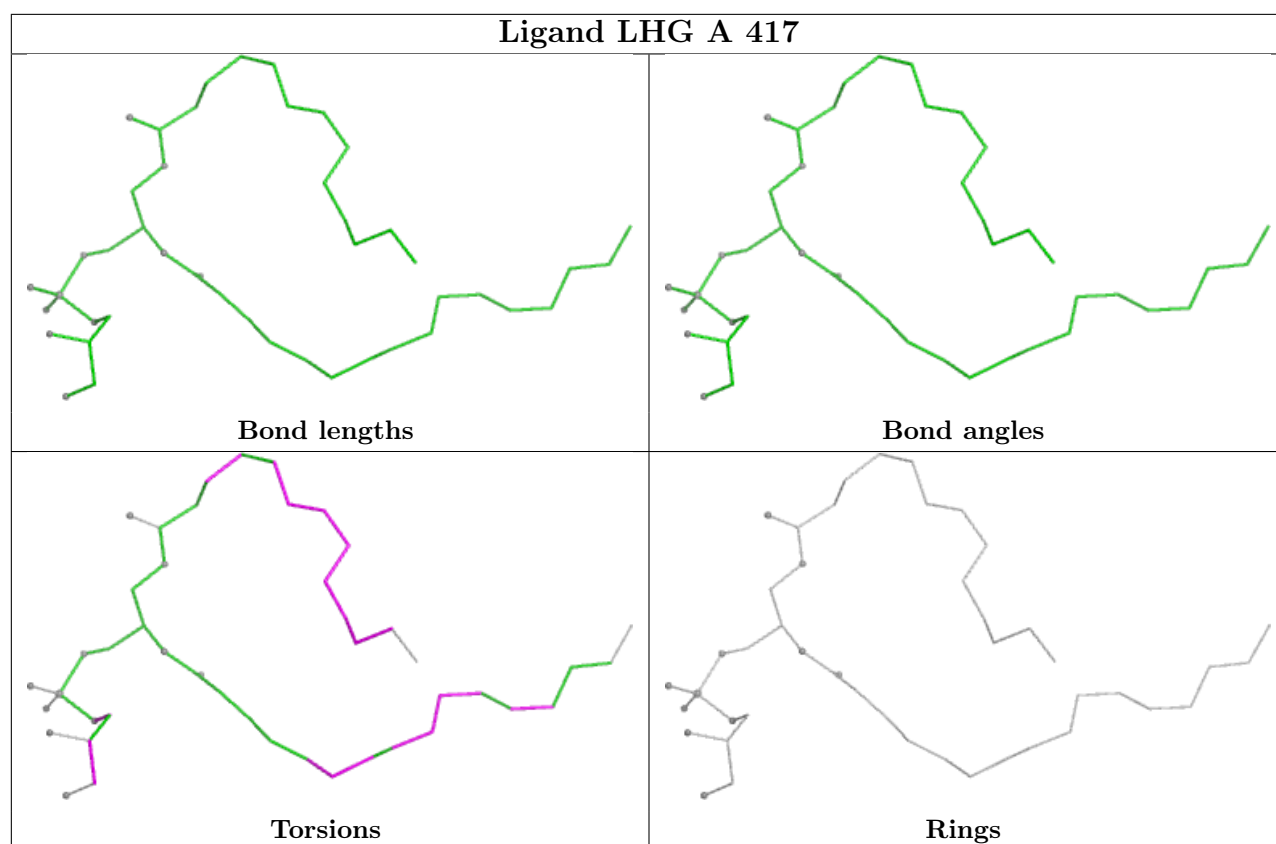
Ligand CLA b 615

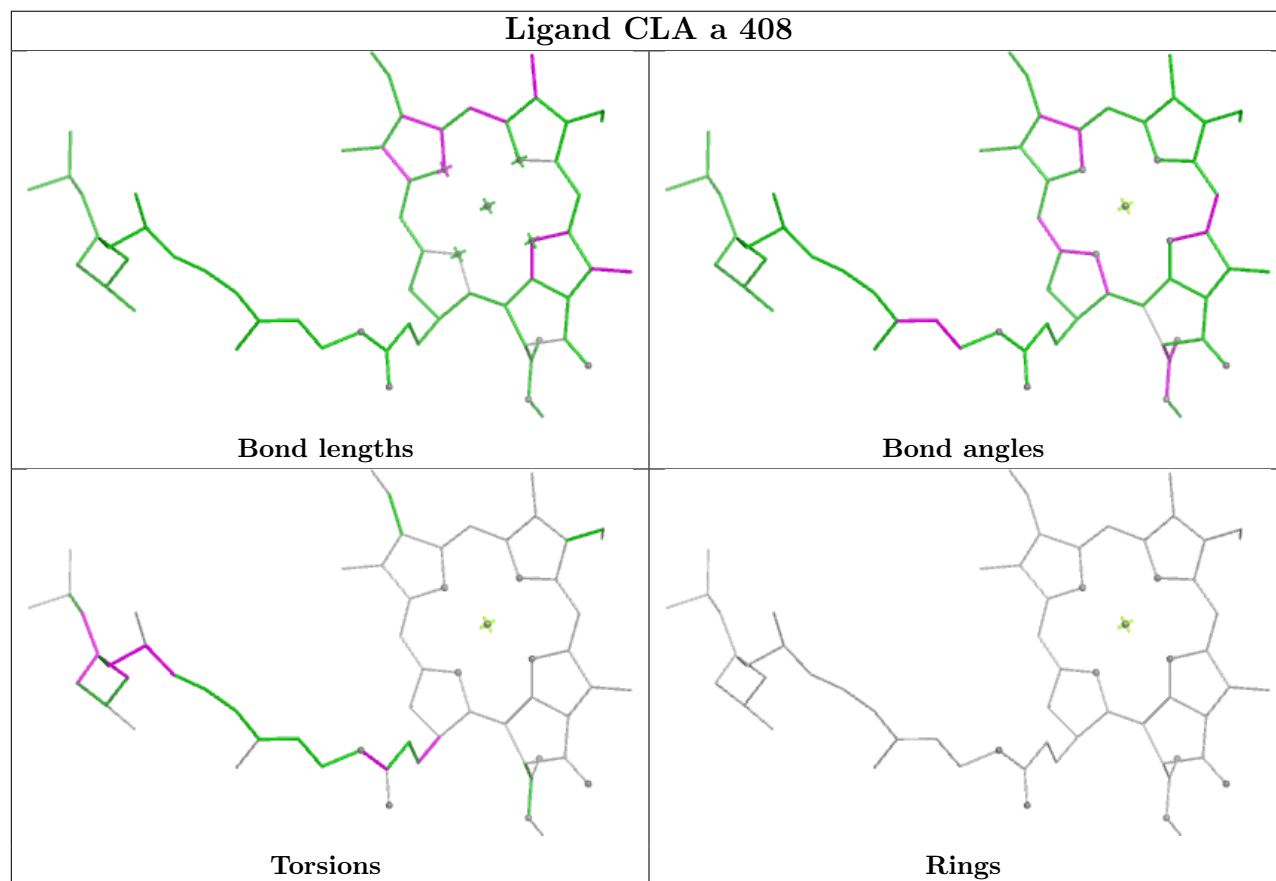
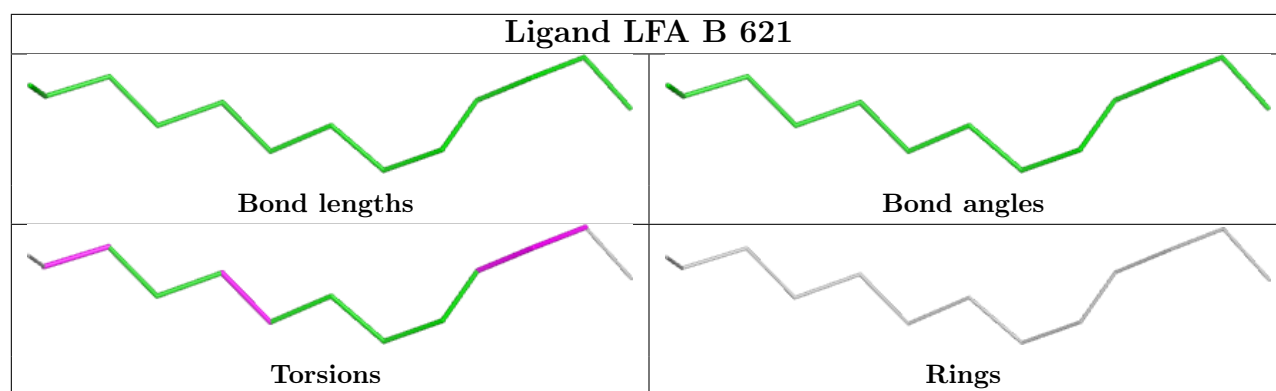


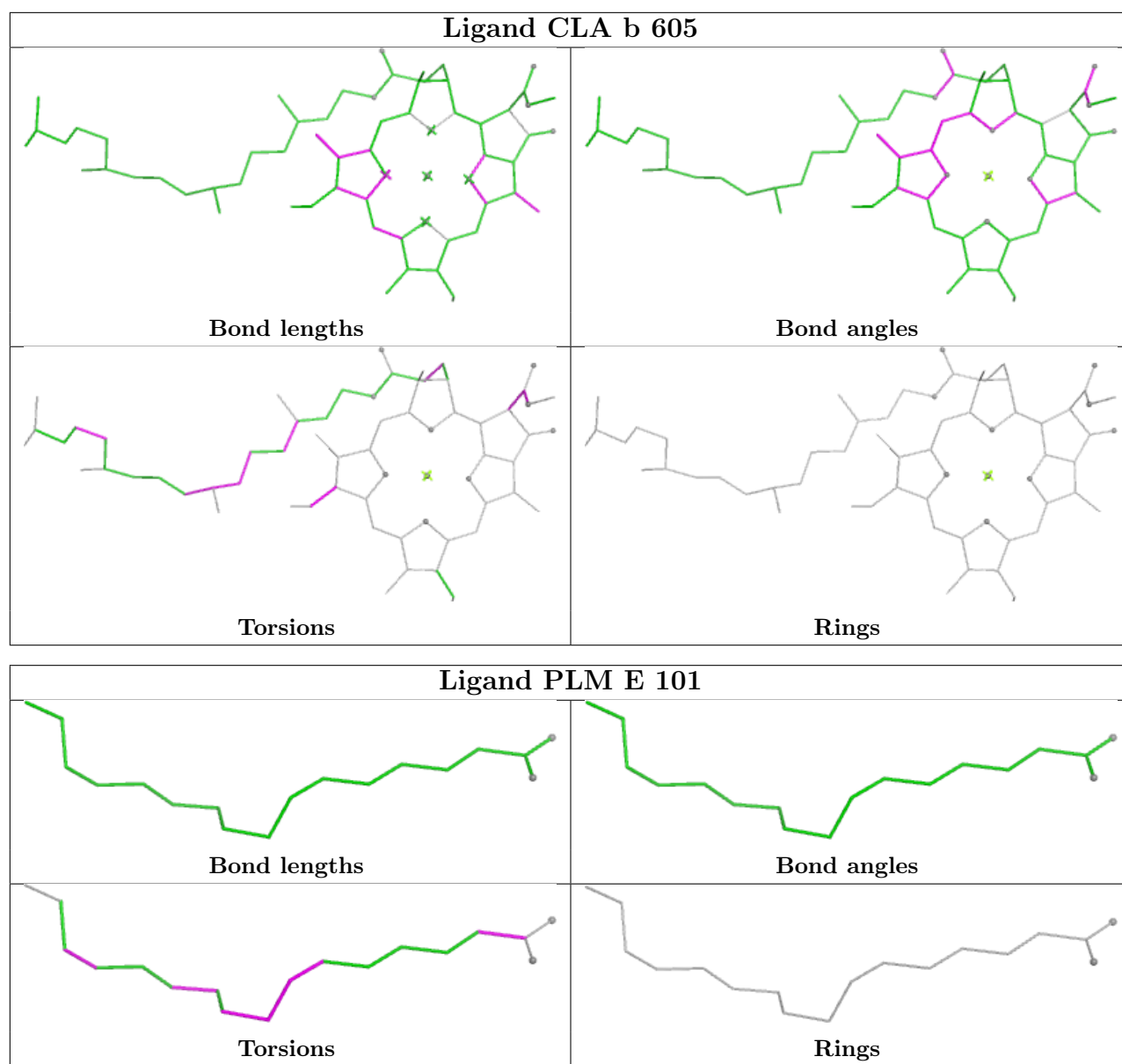
Ligand LFA B 625

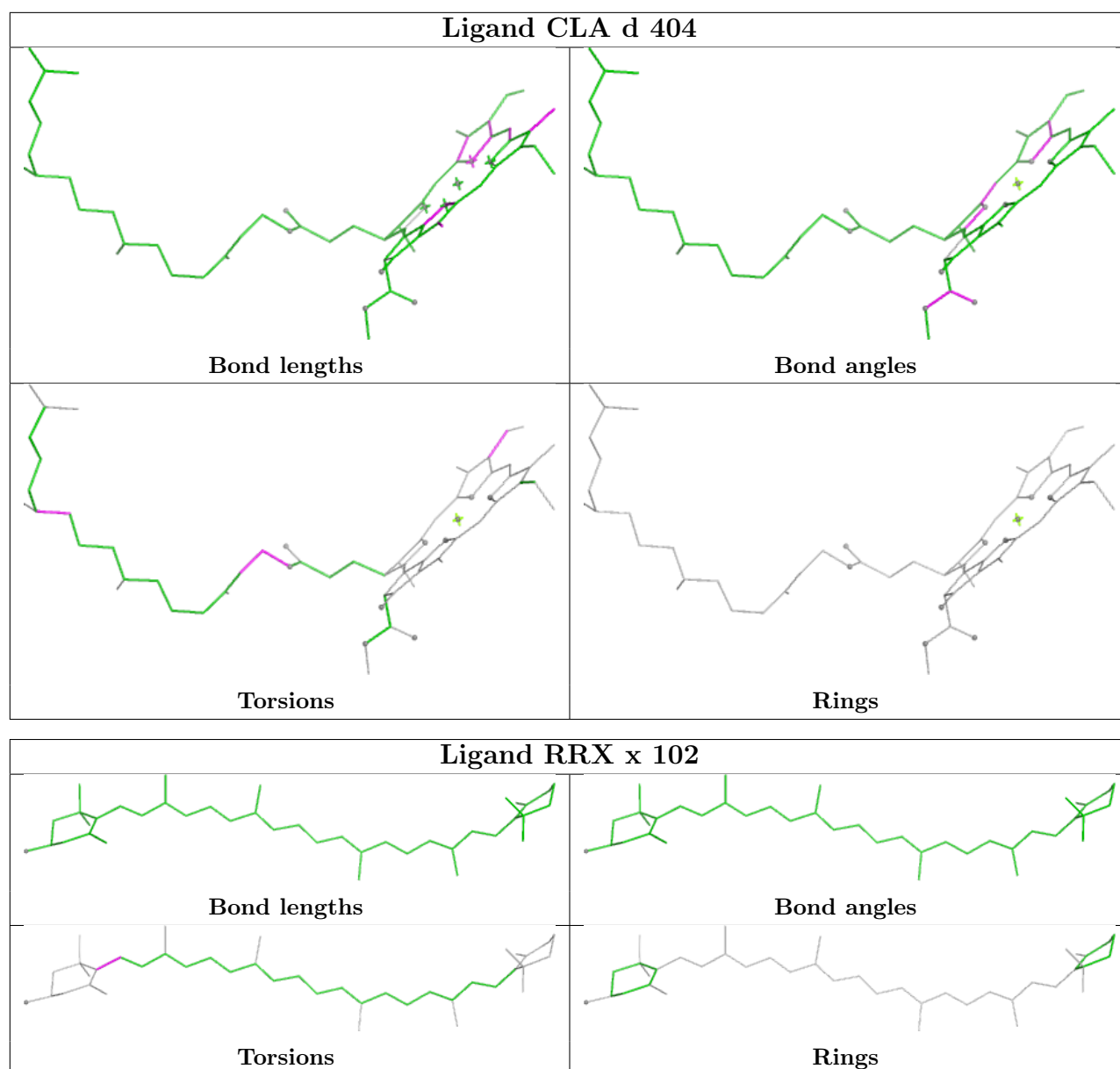


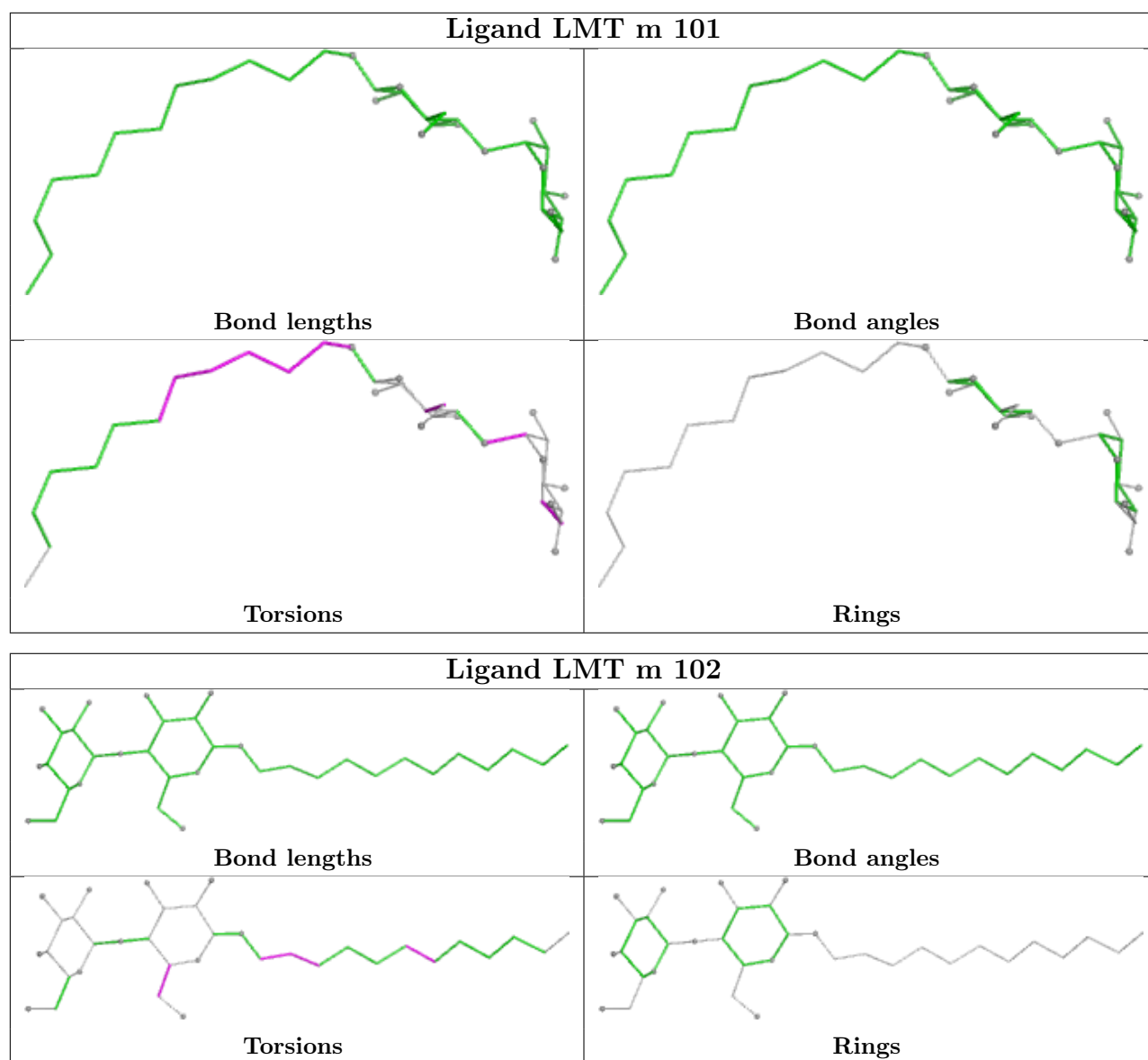


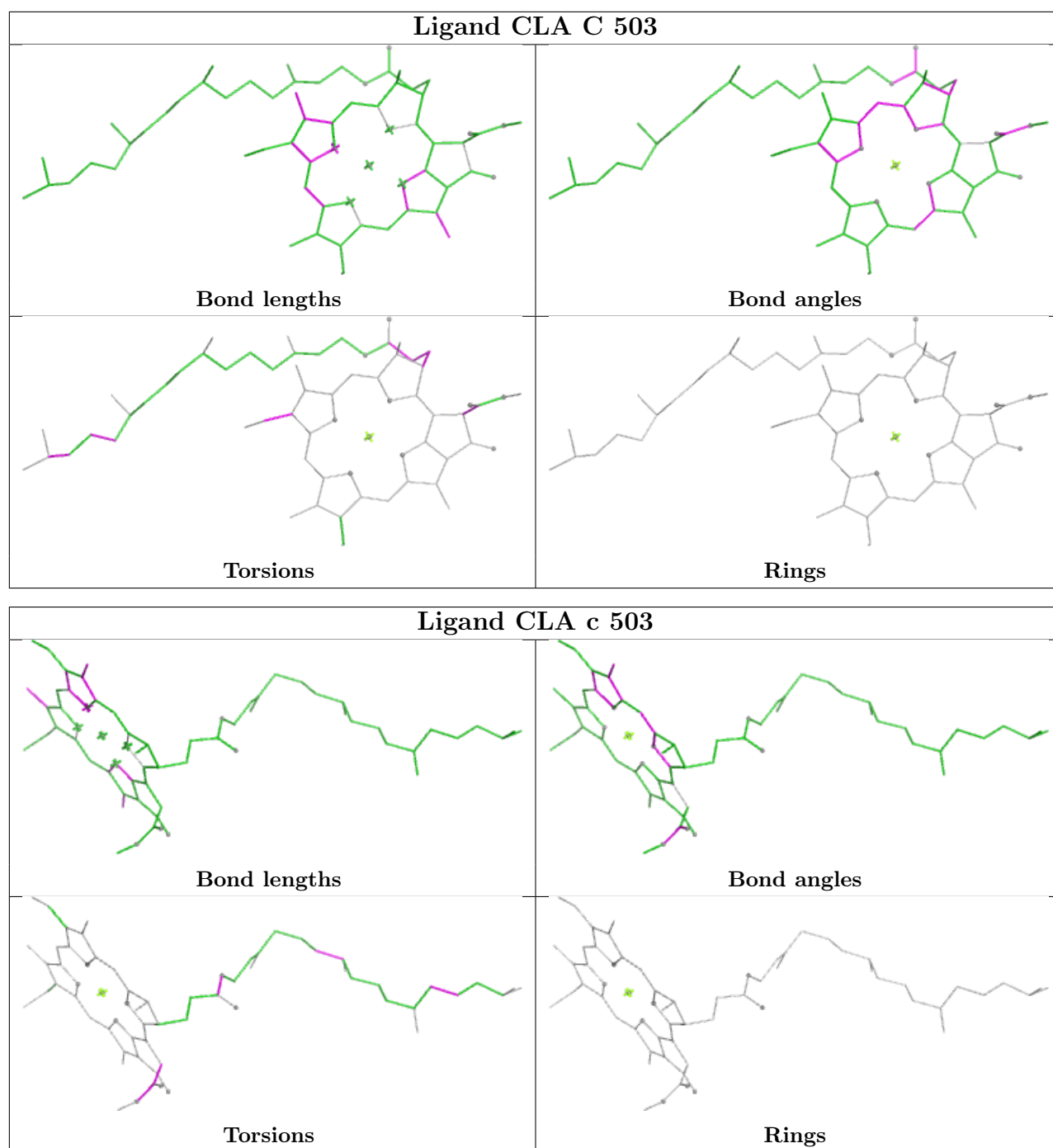


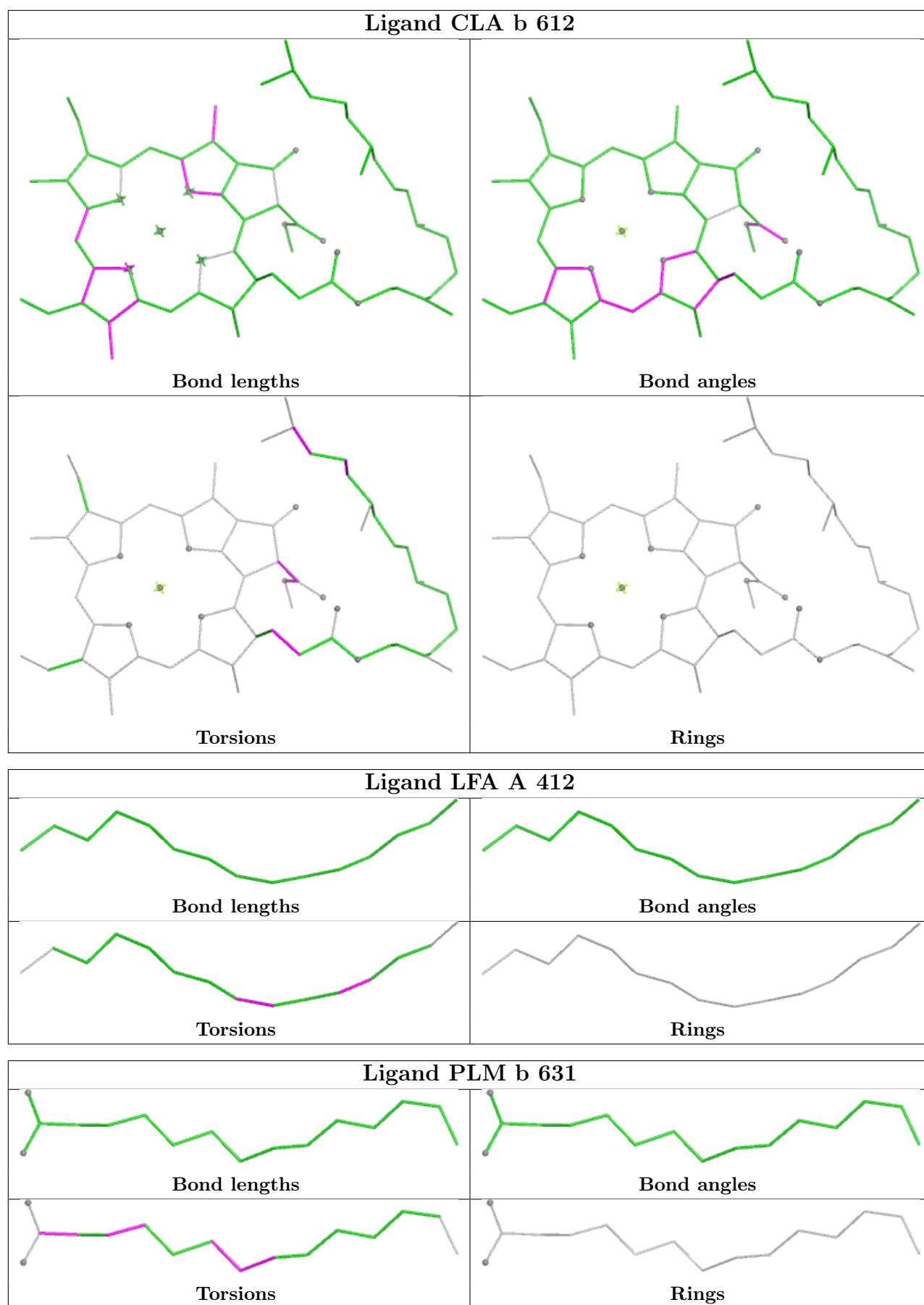


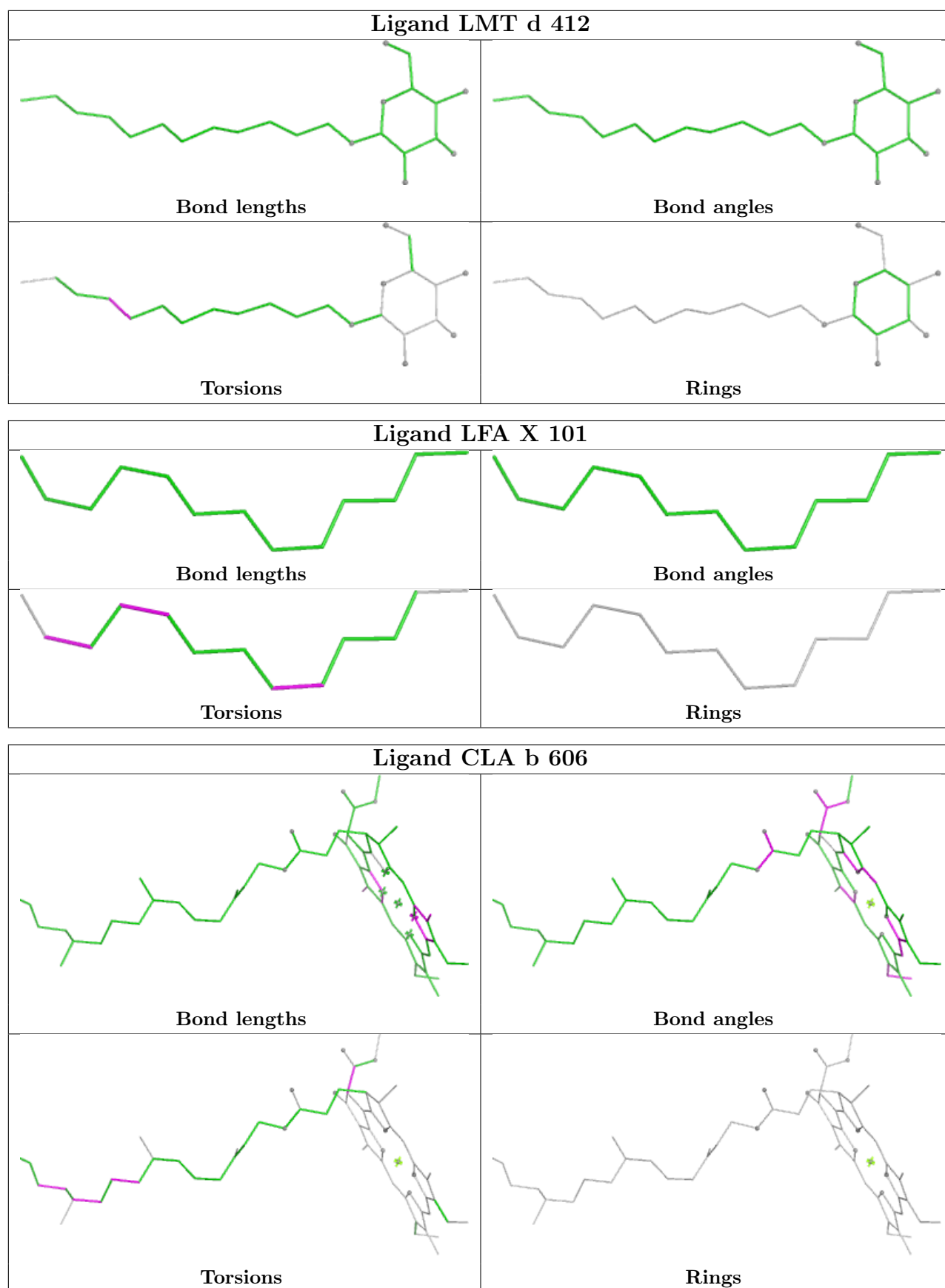


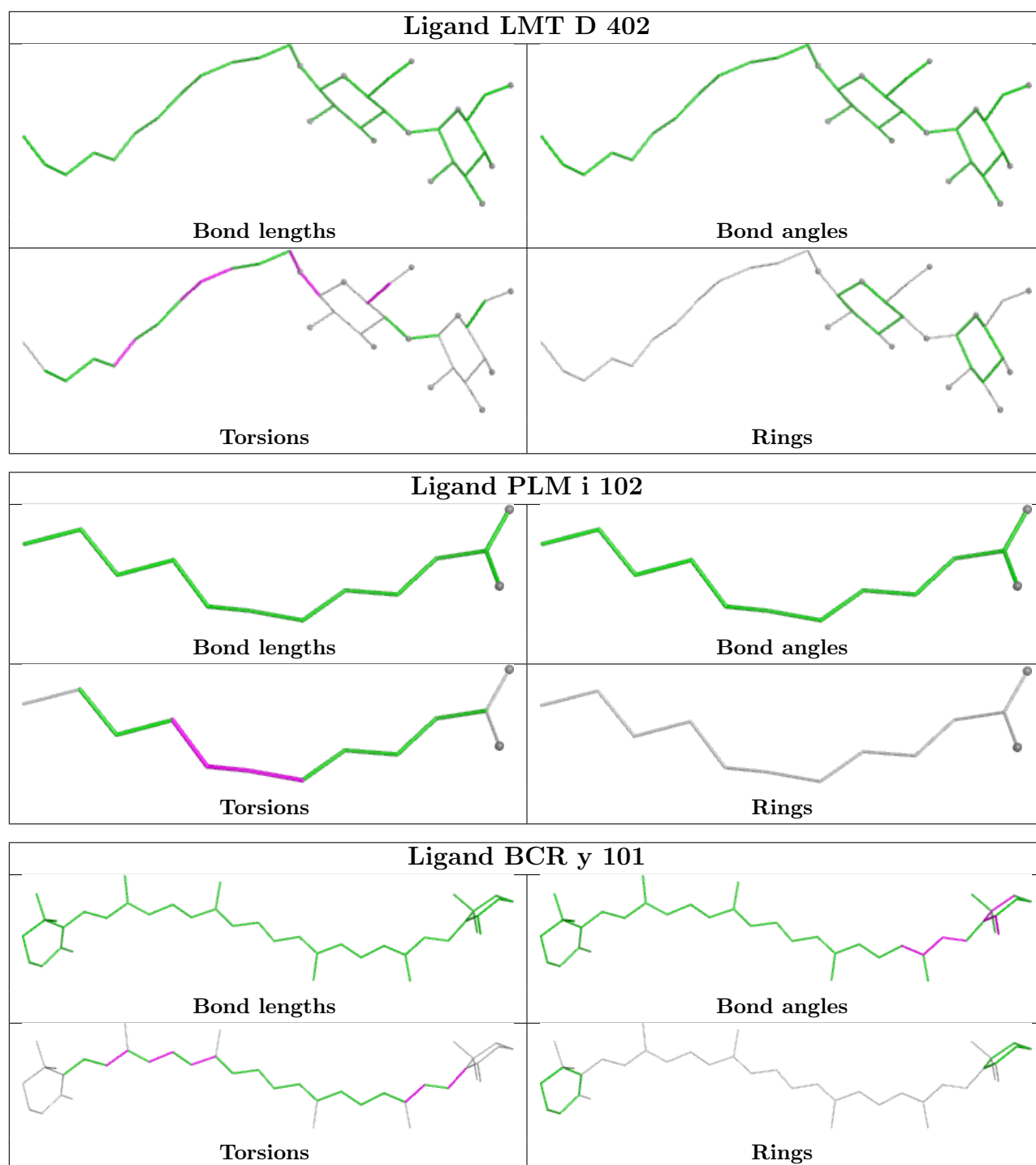


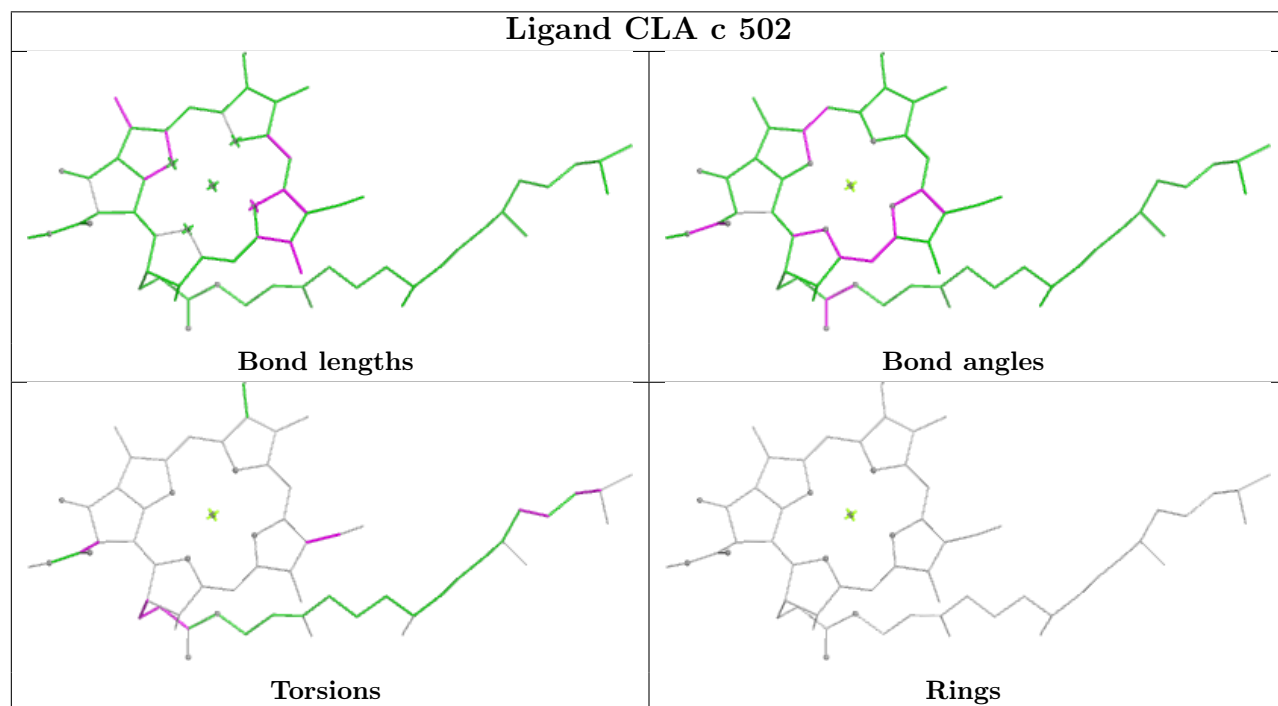
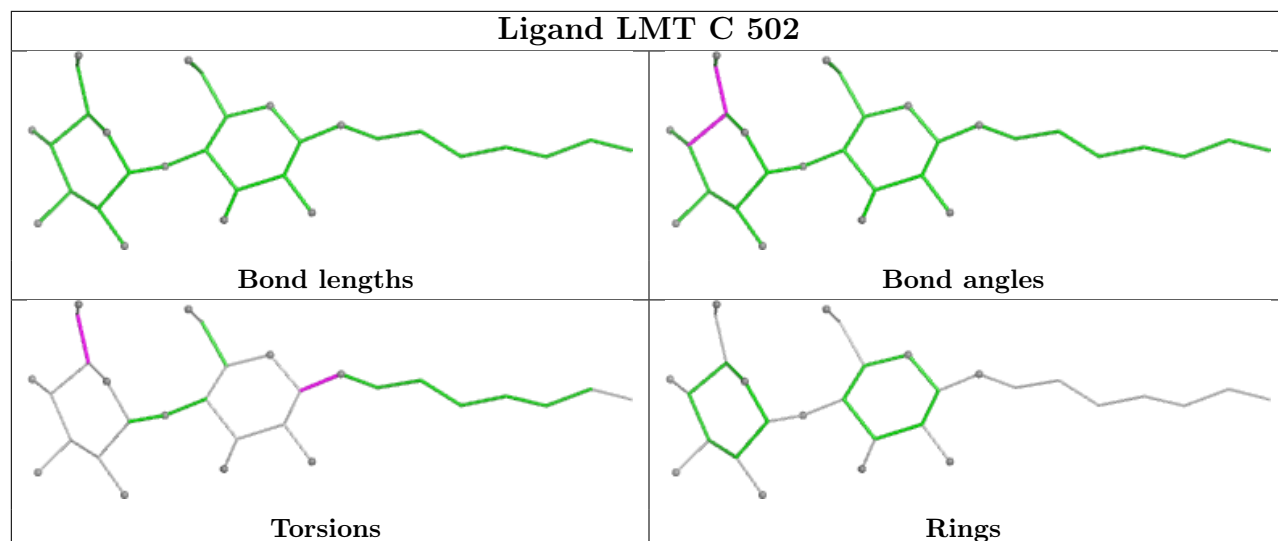


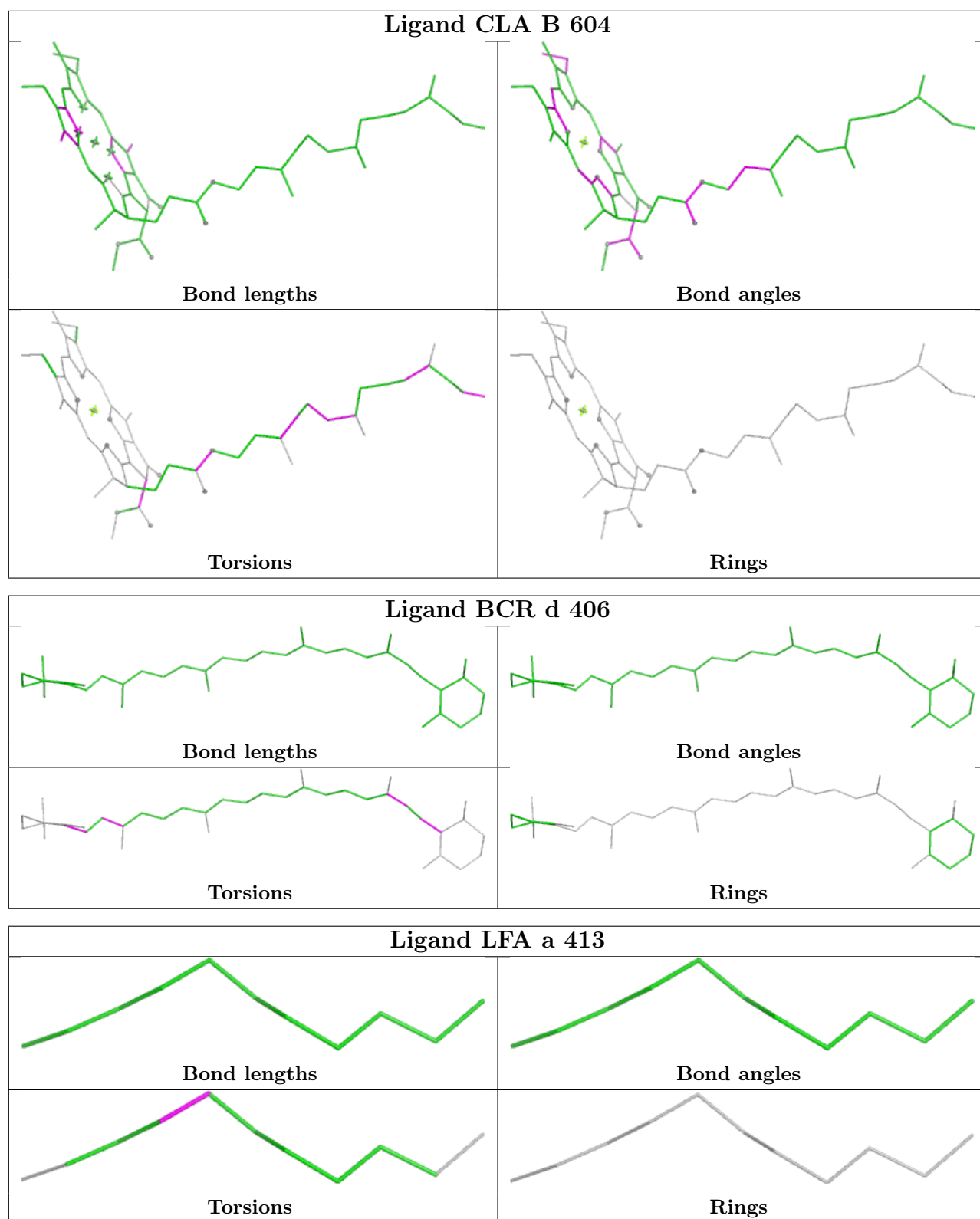


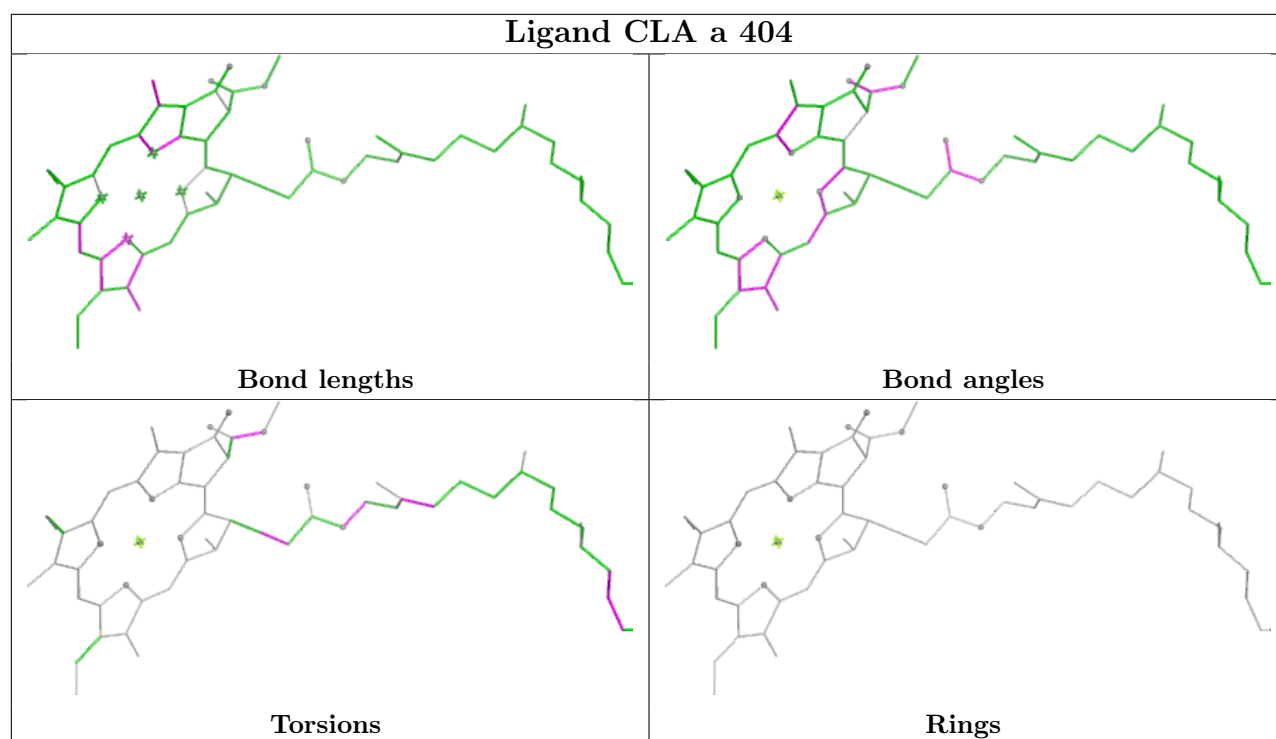


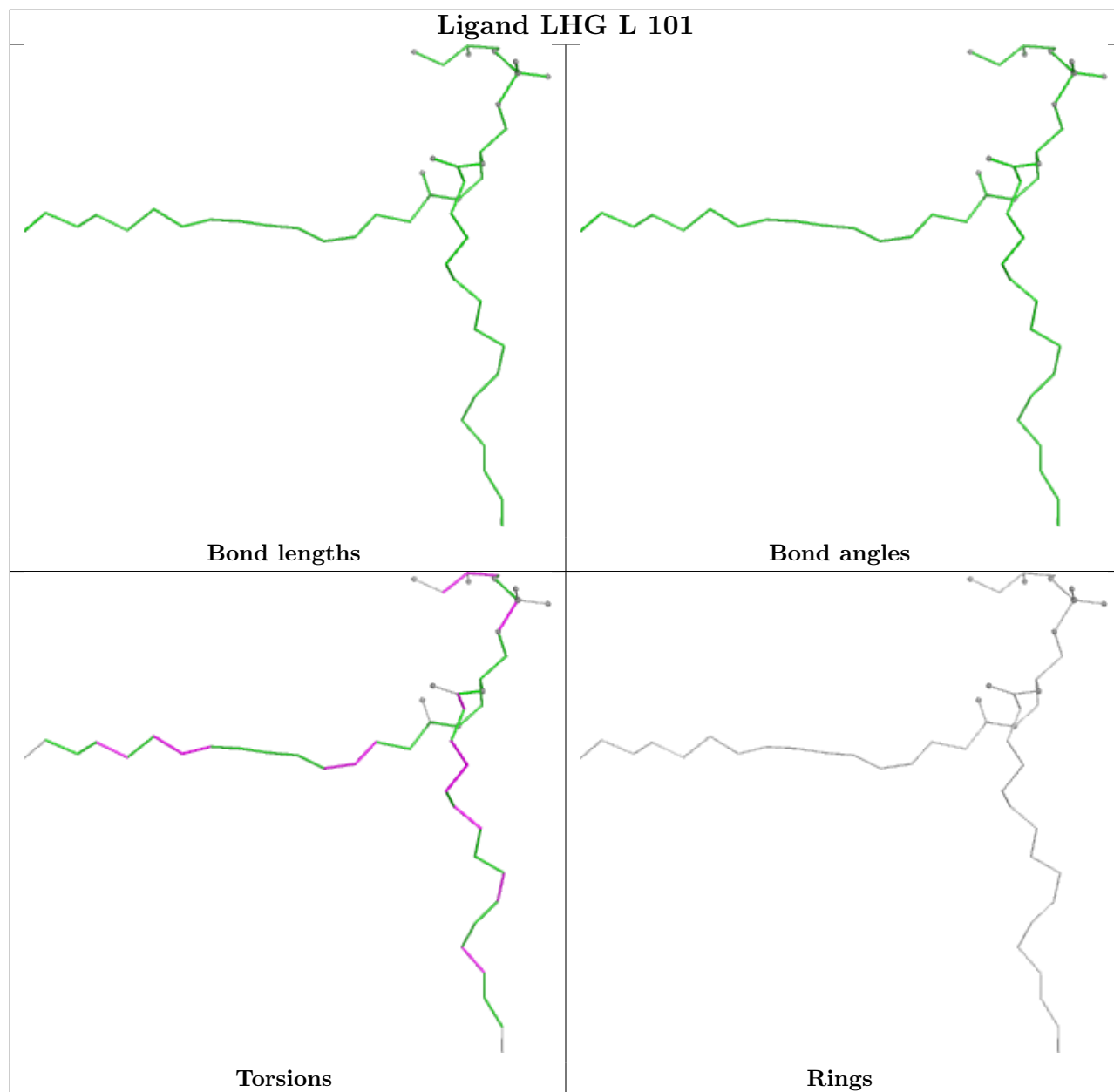


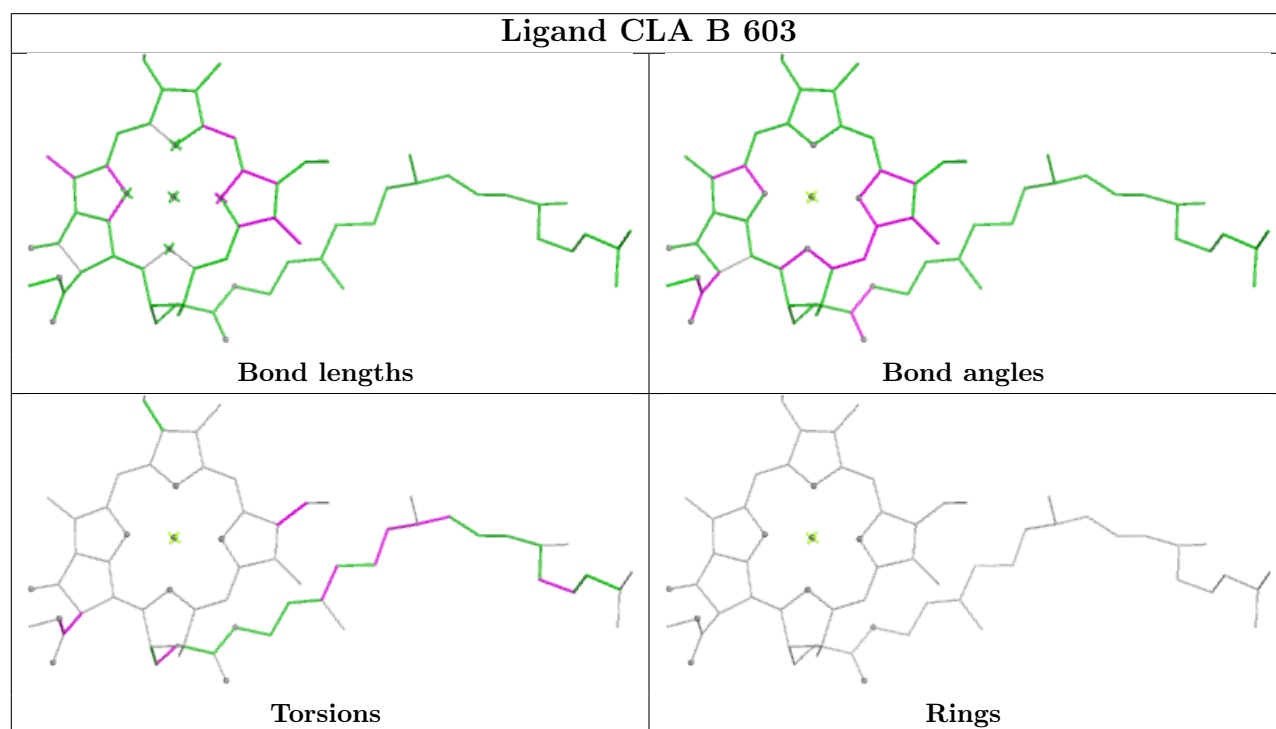
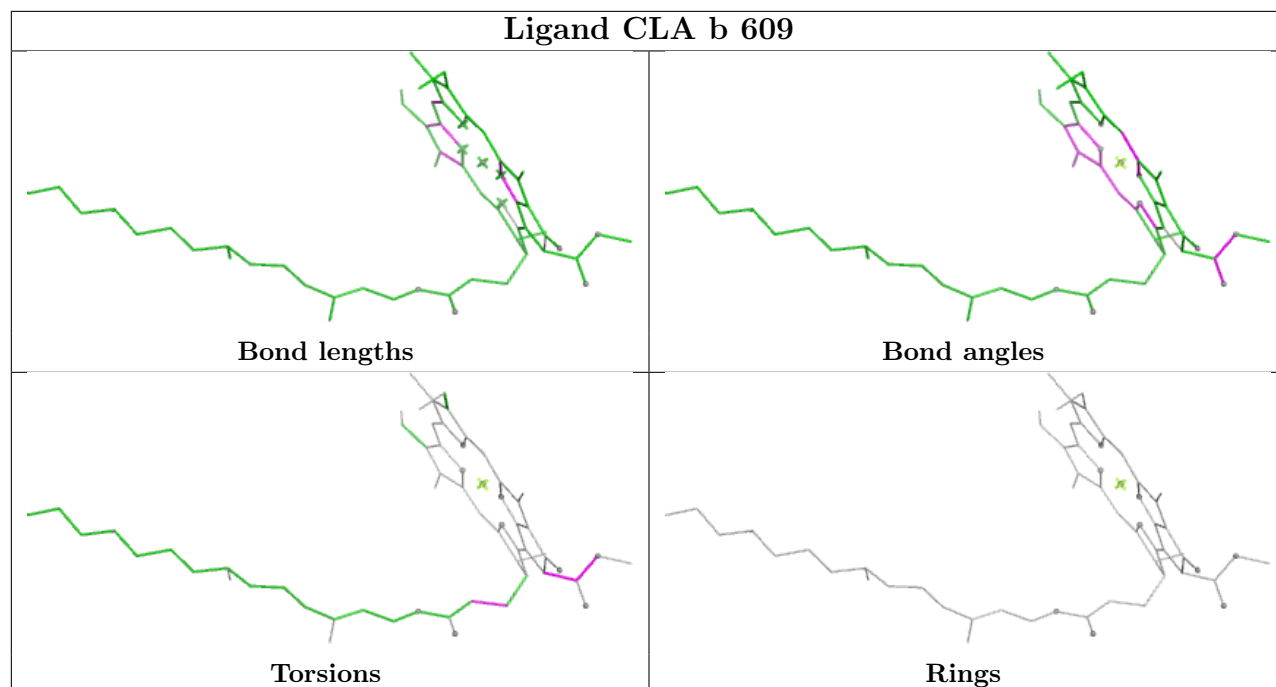


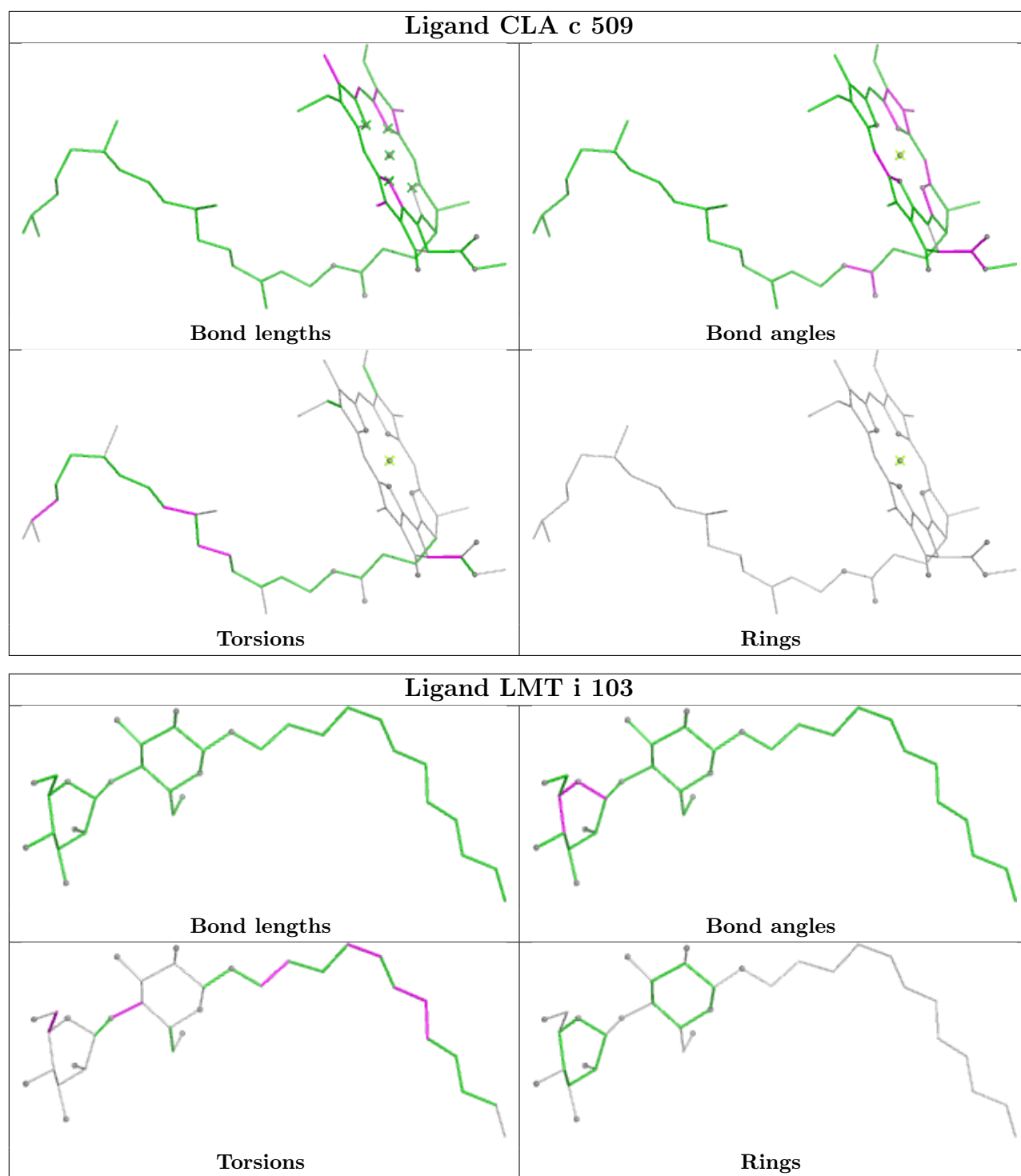


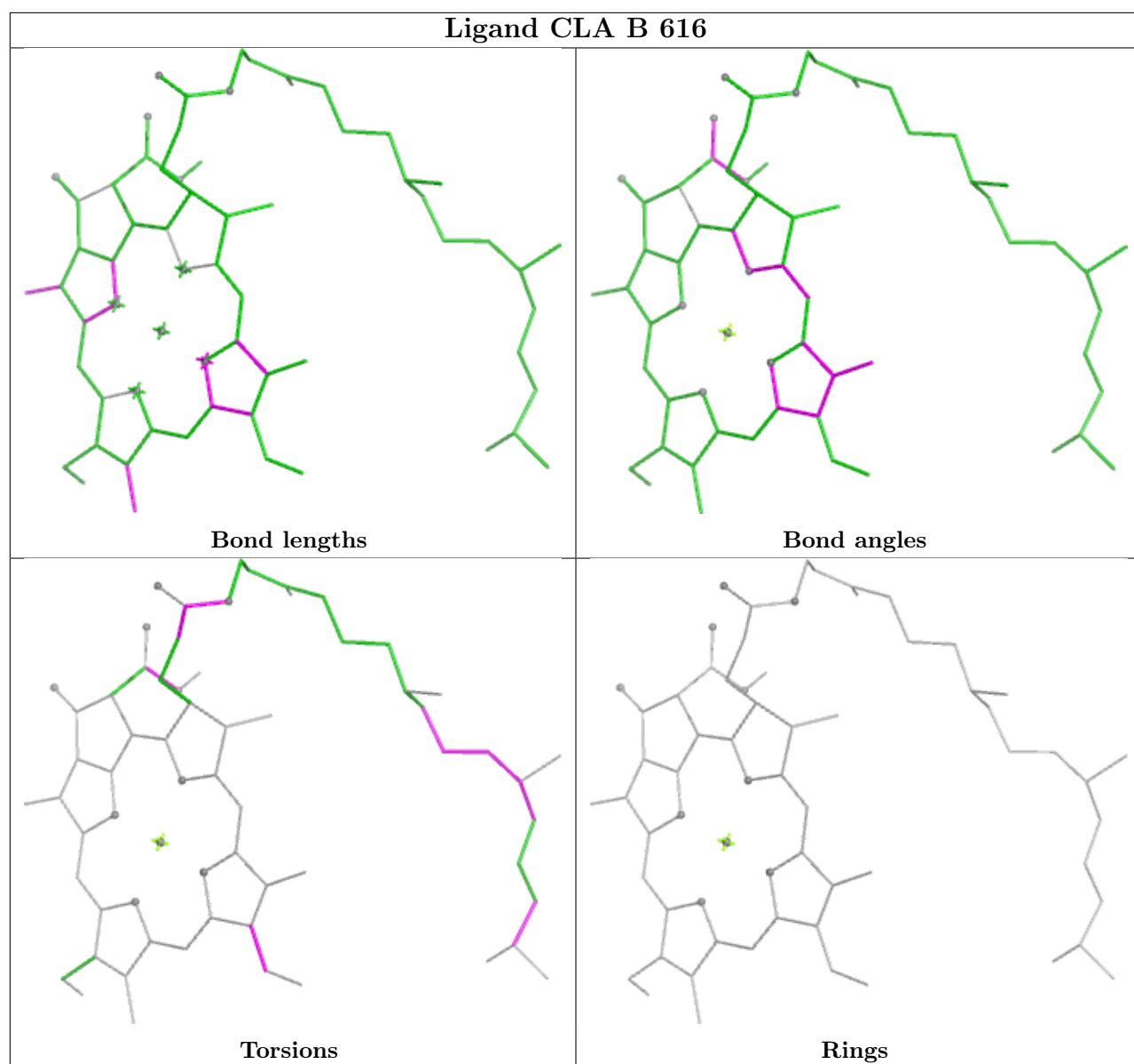


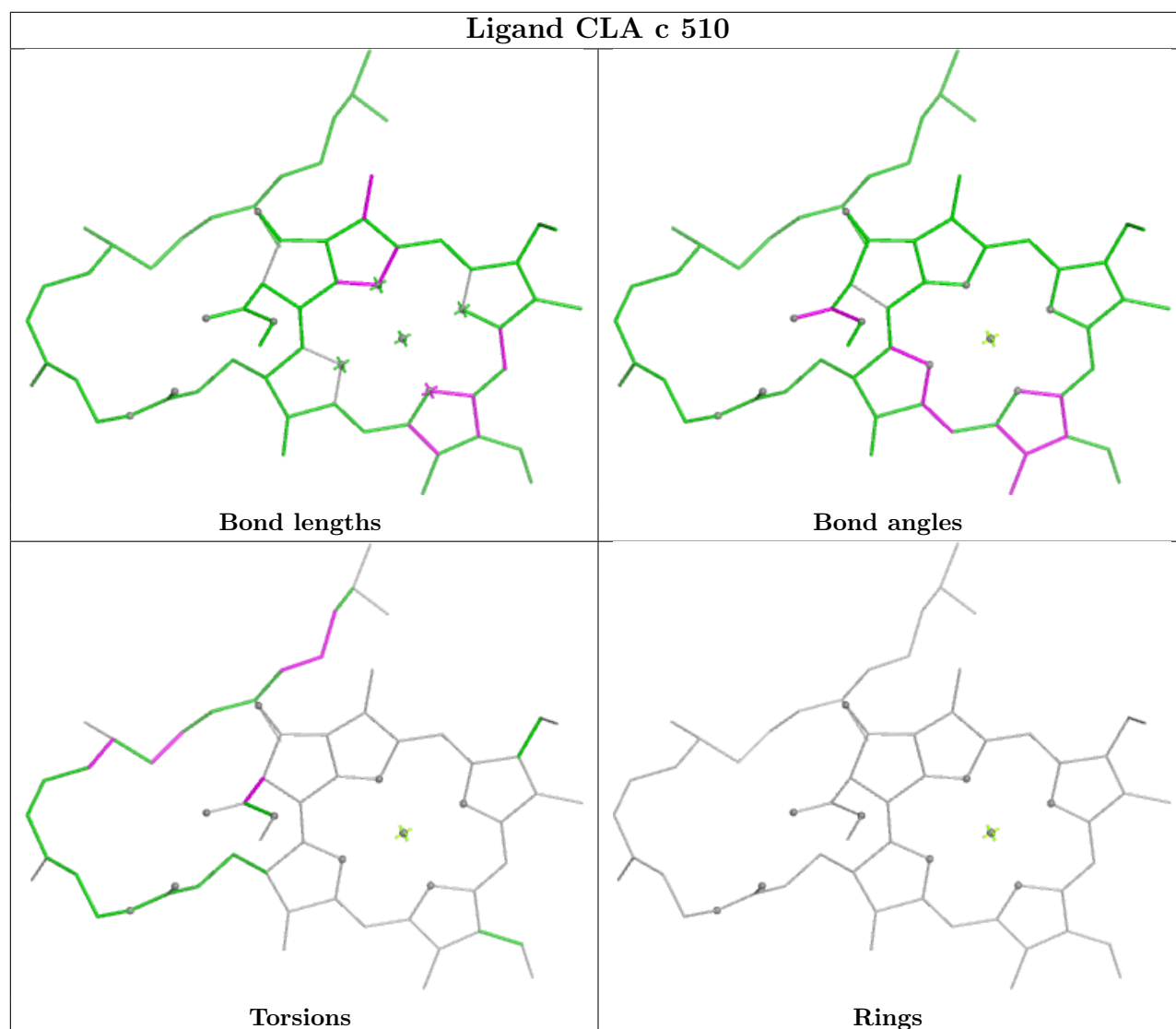
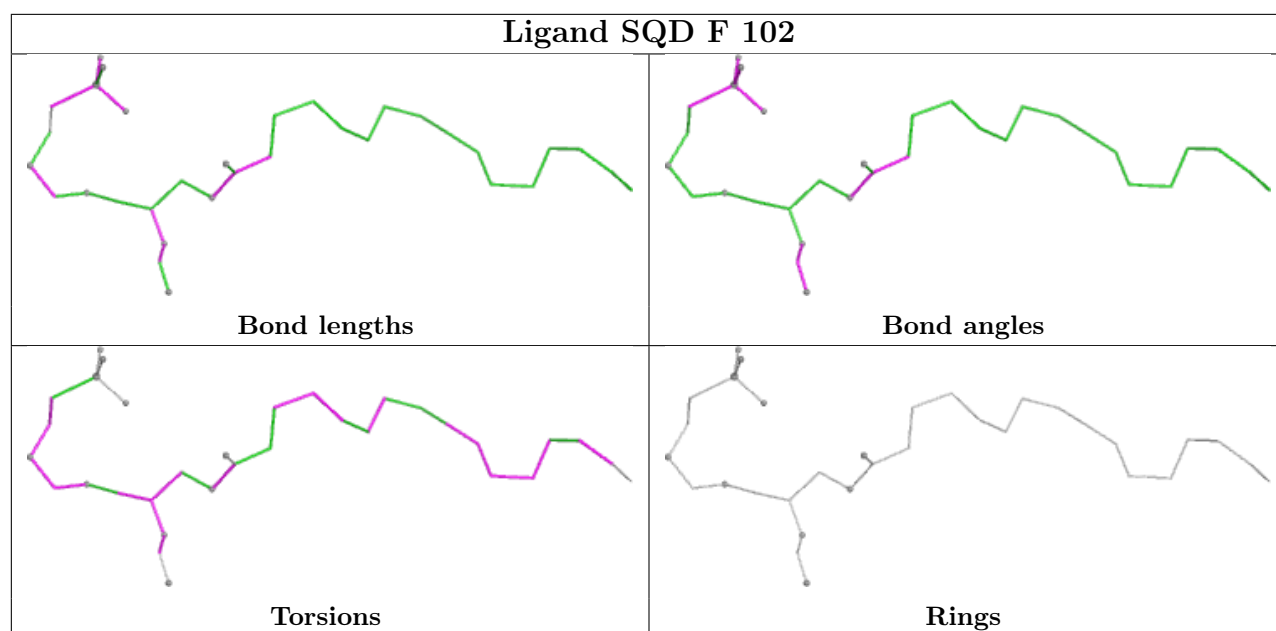


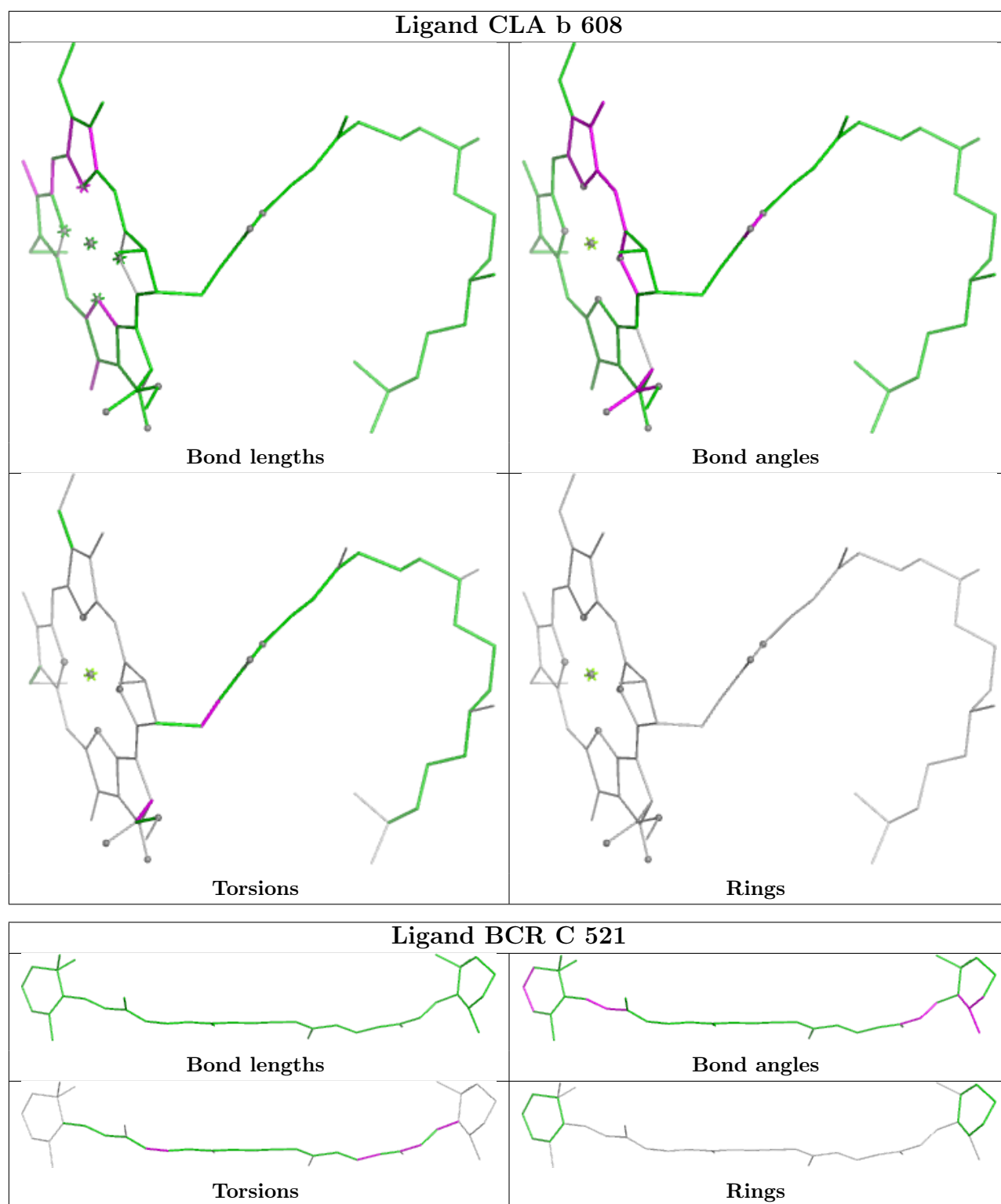


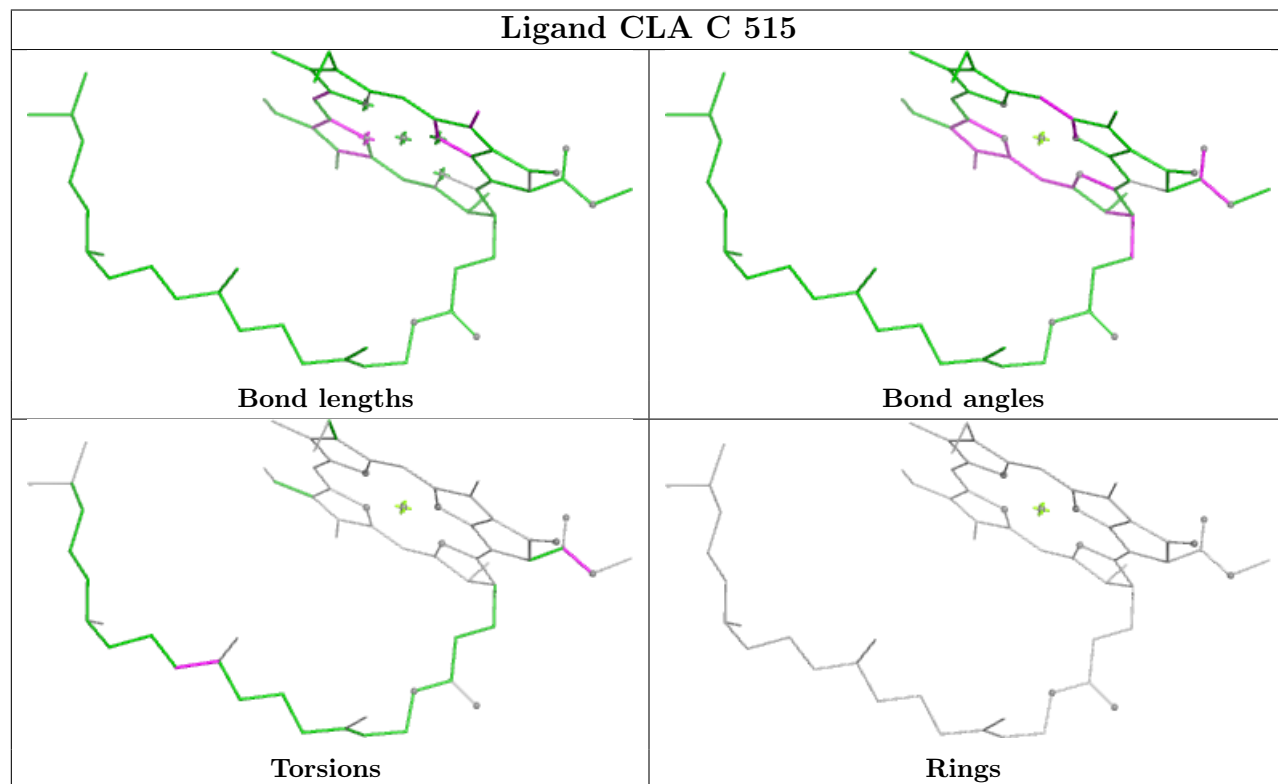
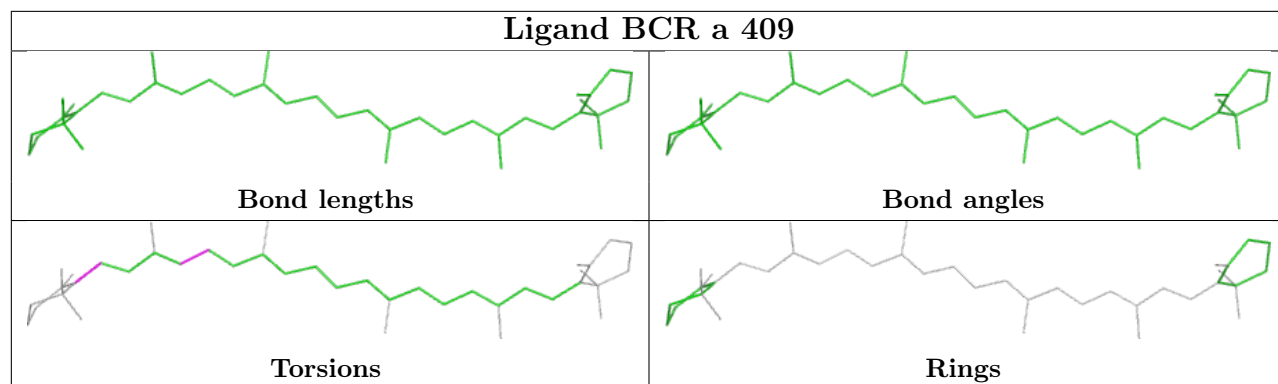


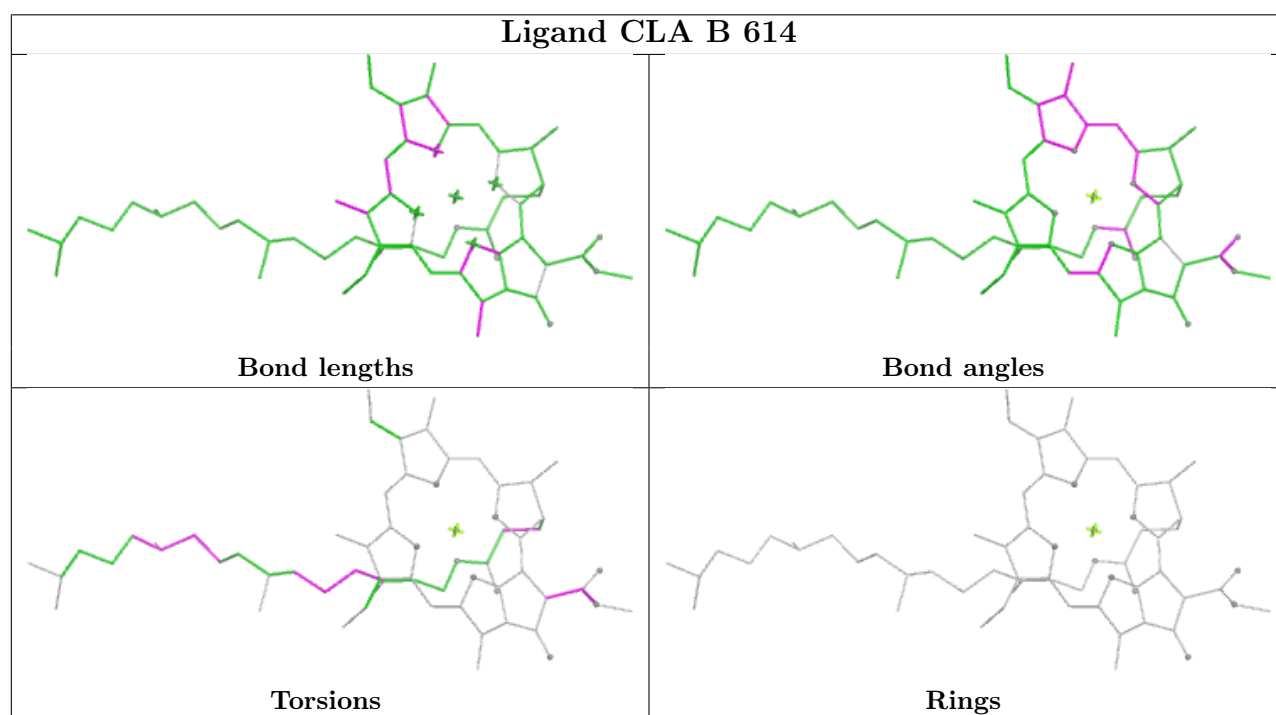
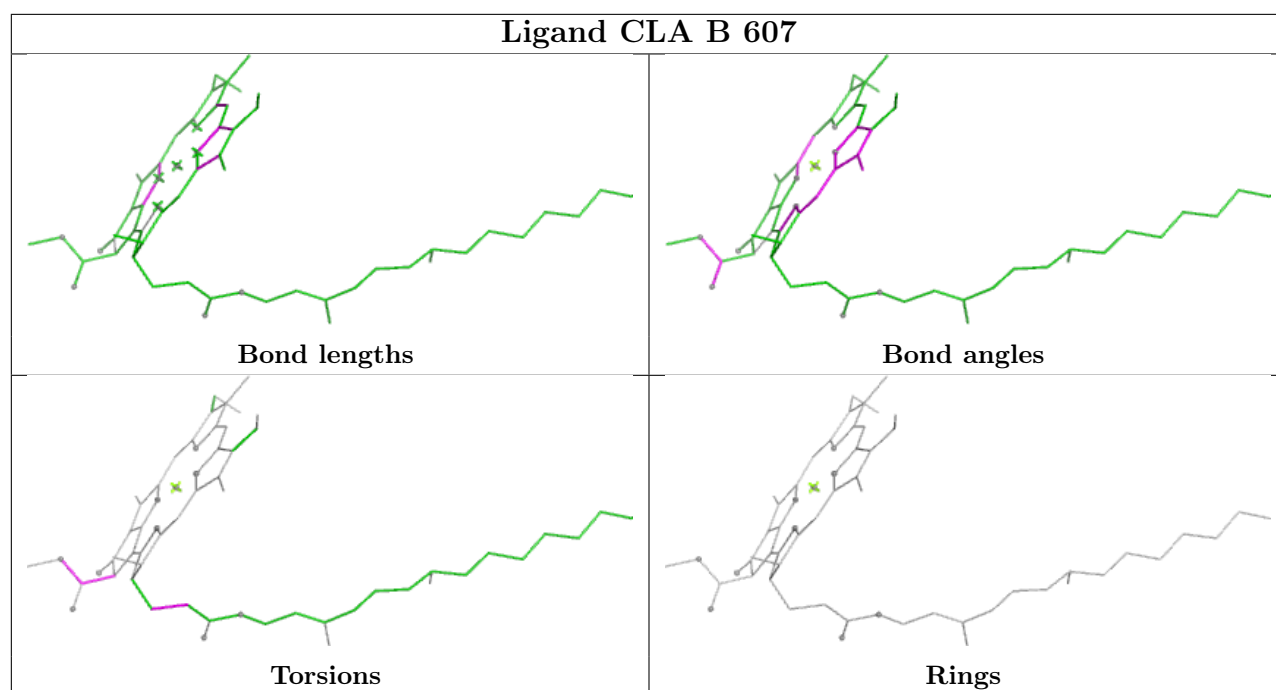


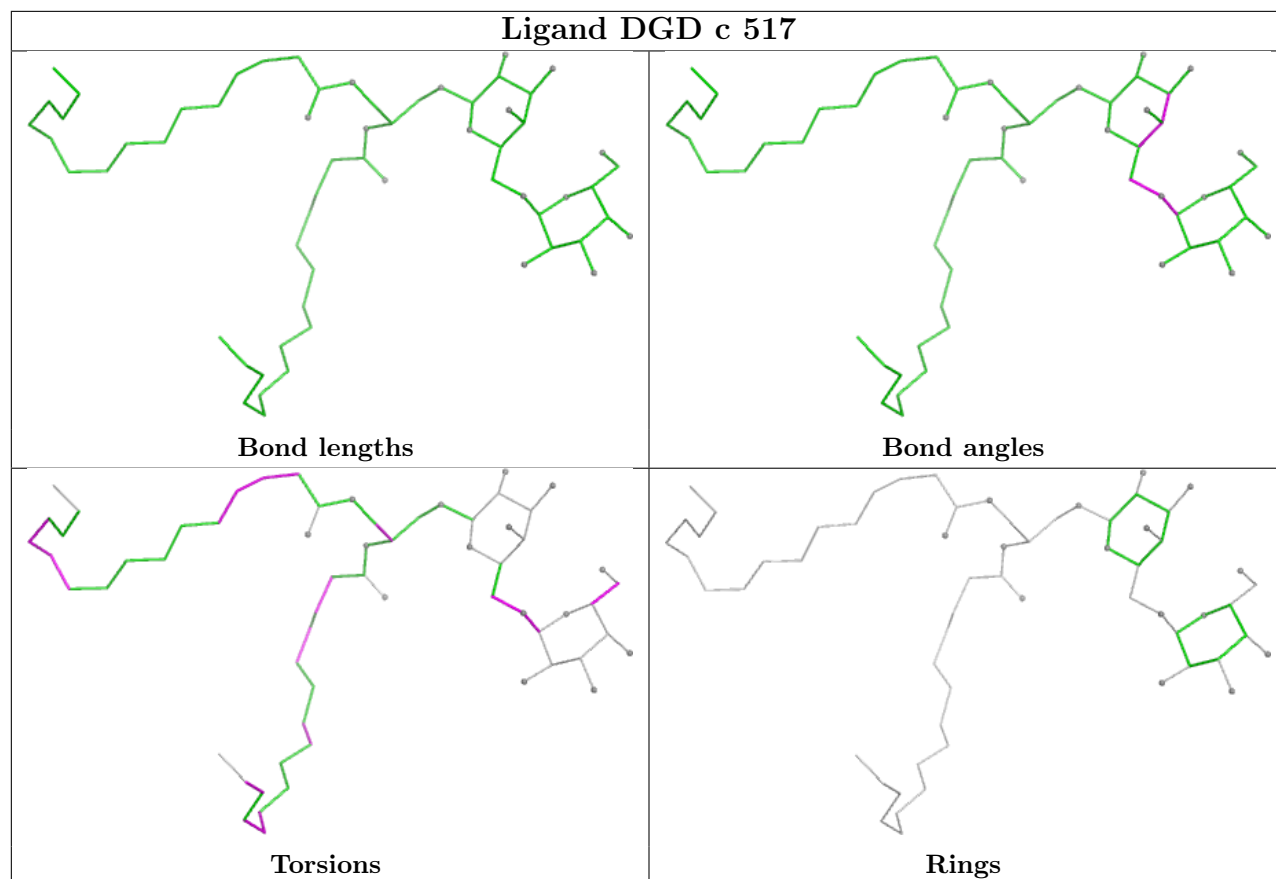


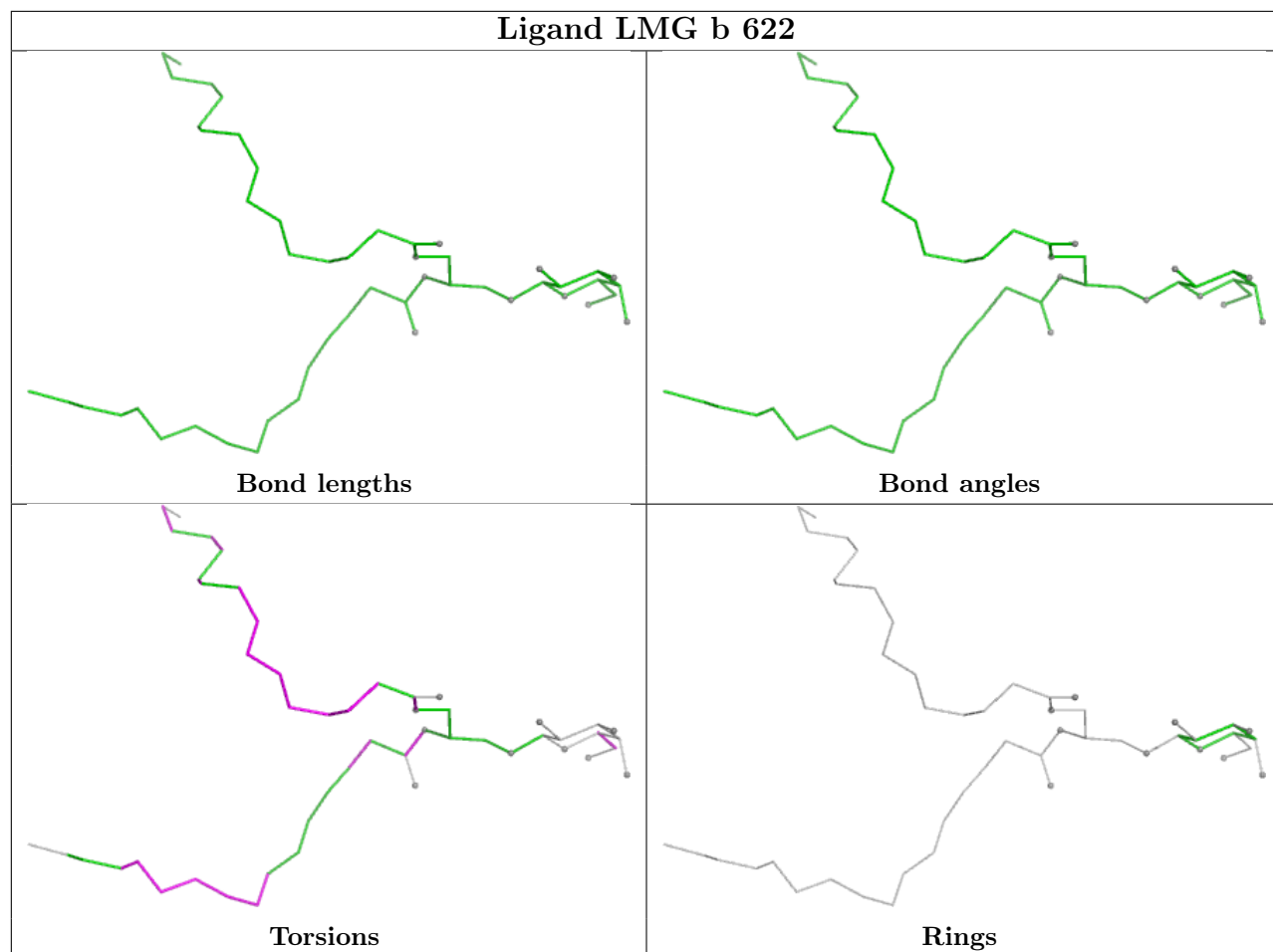


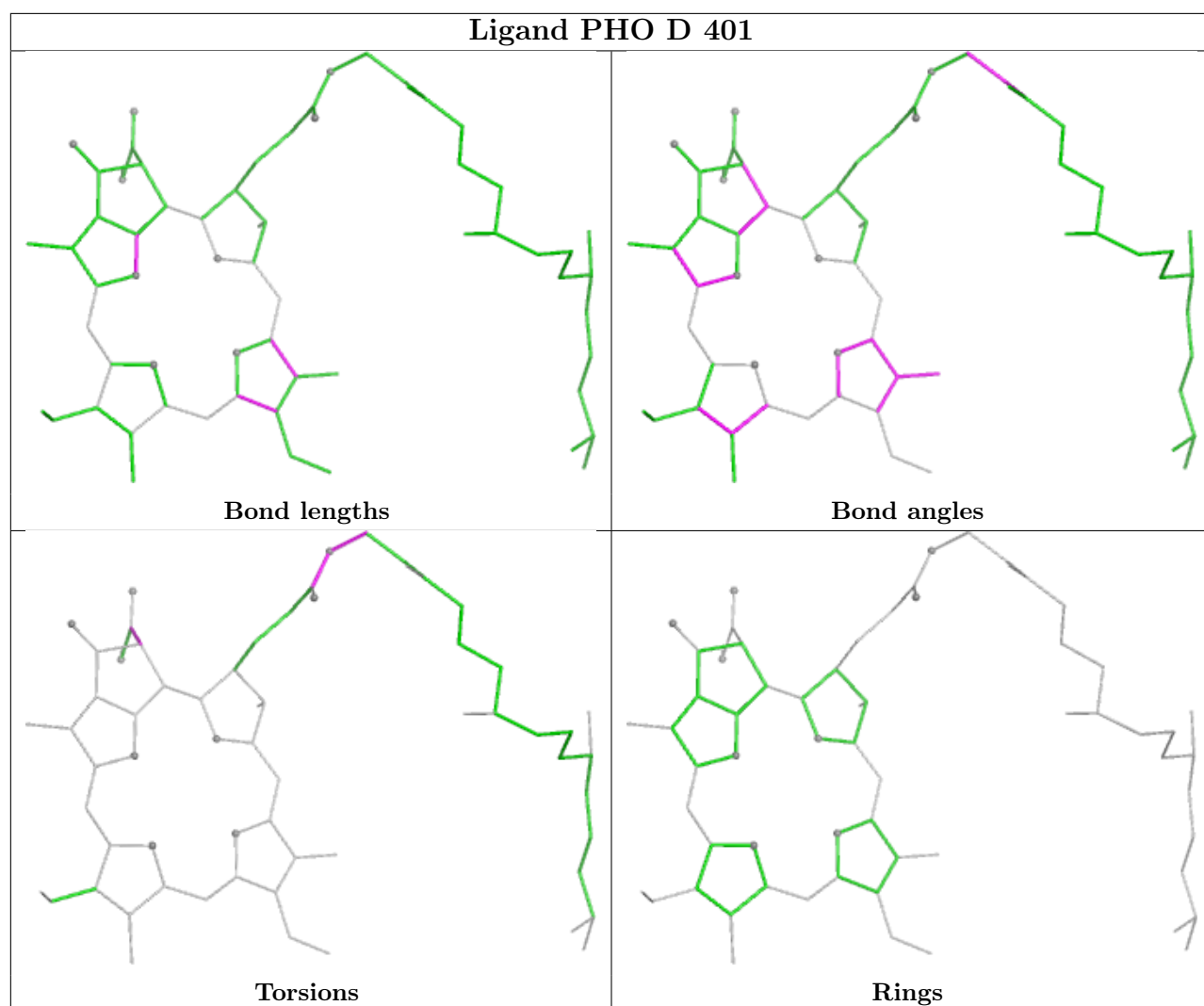


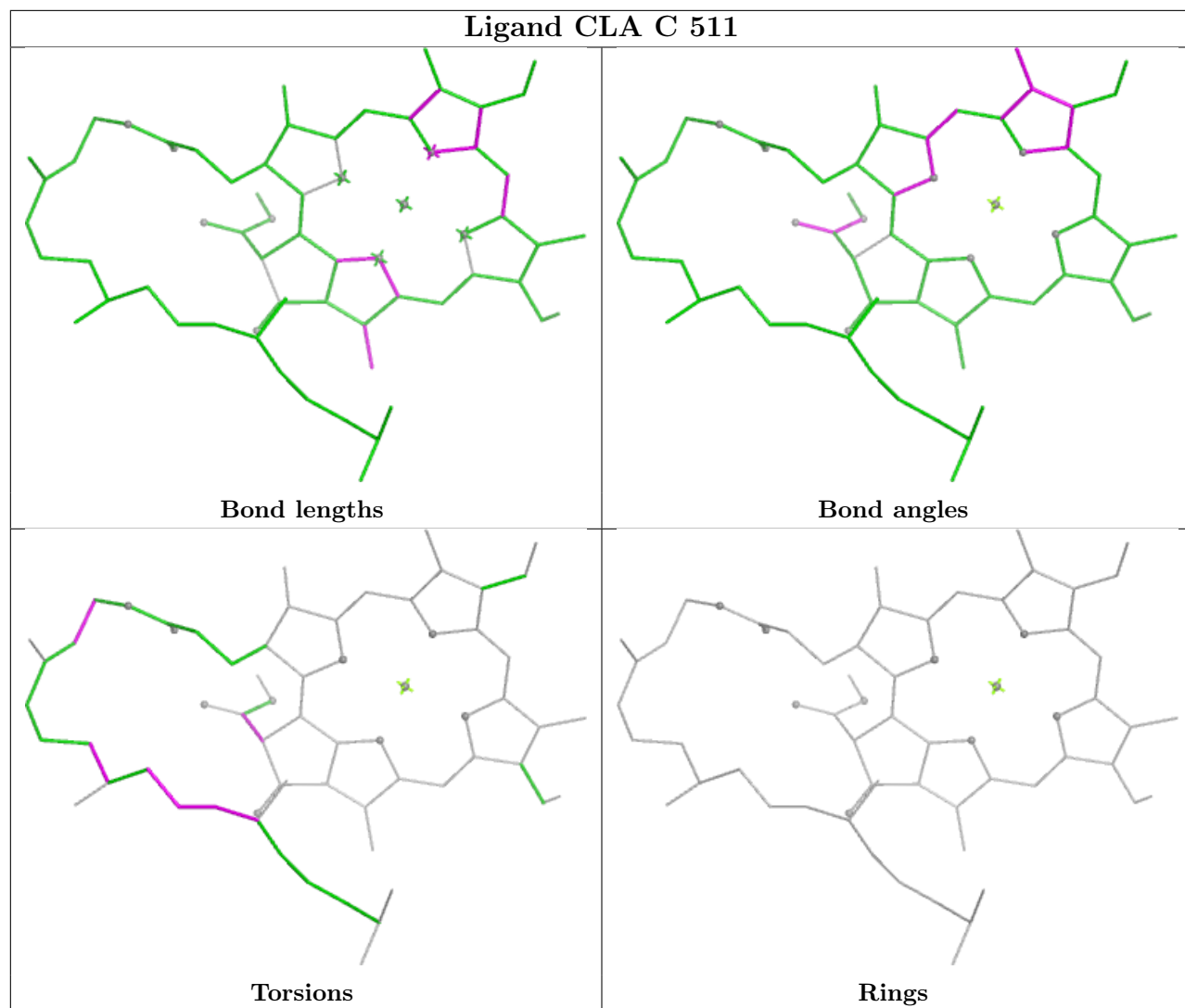


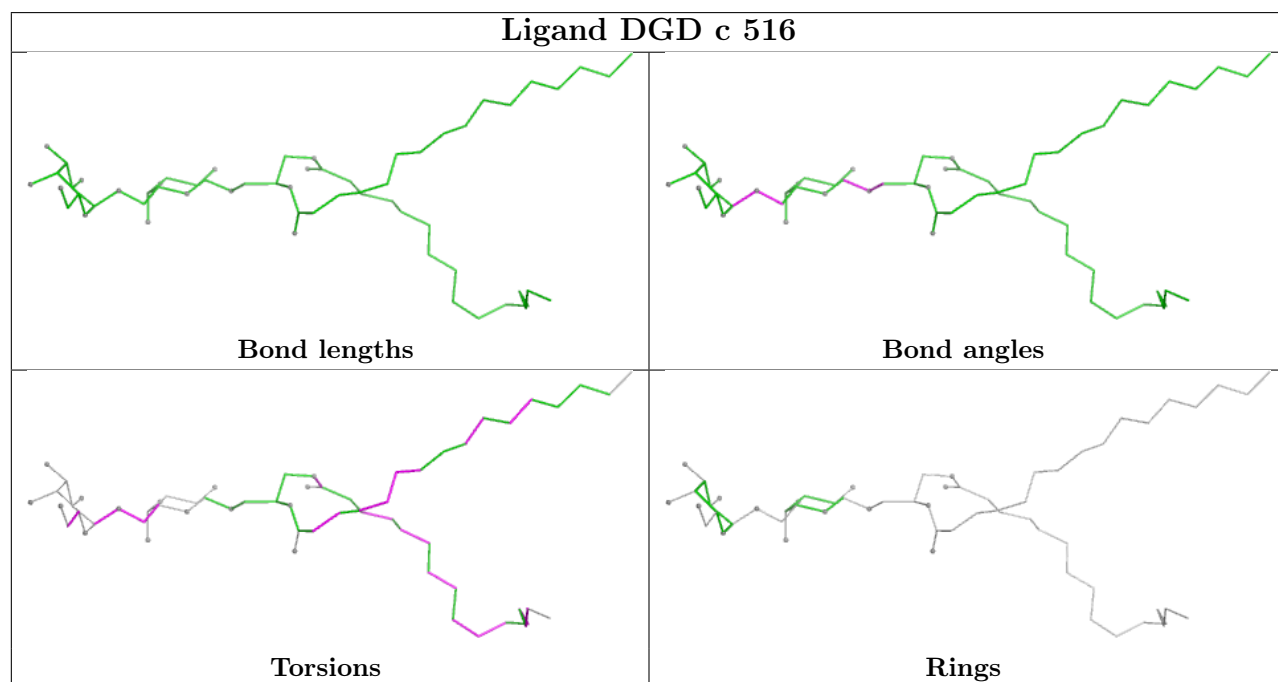
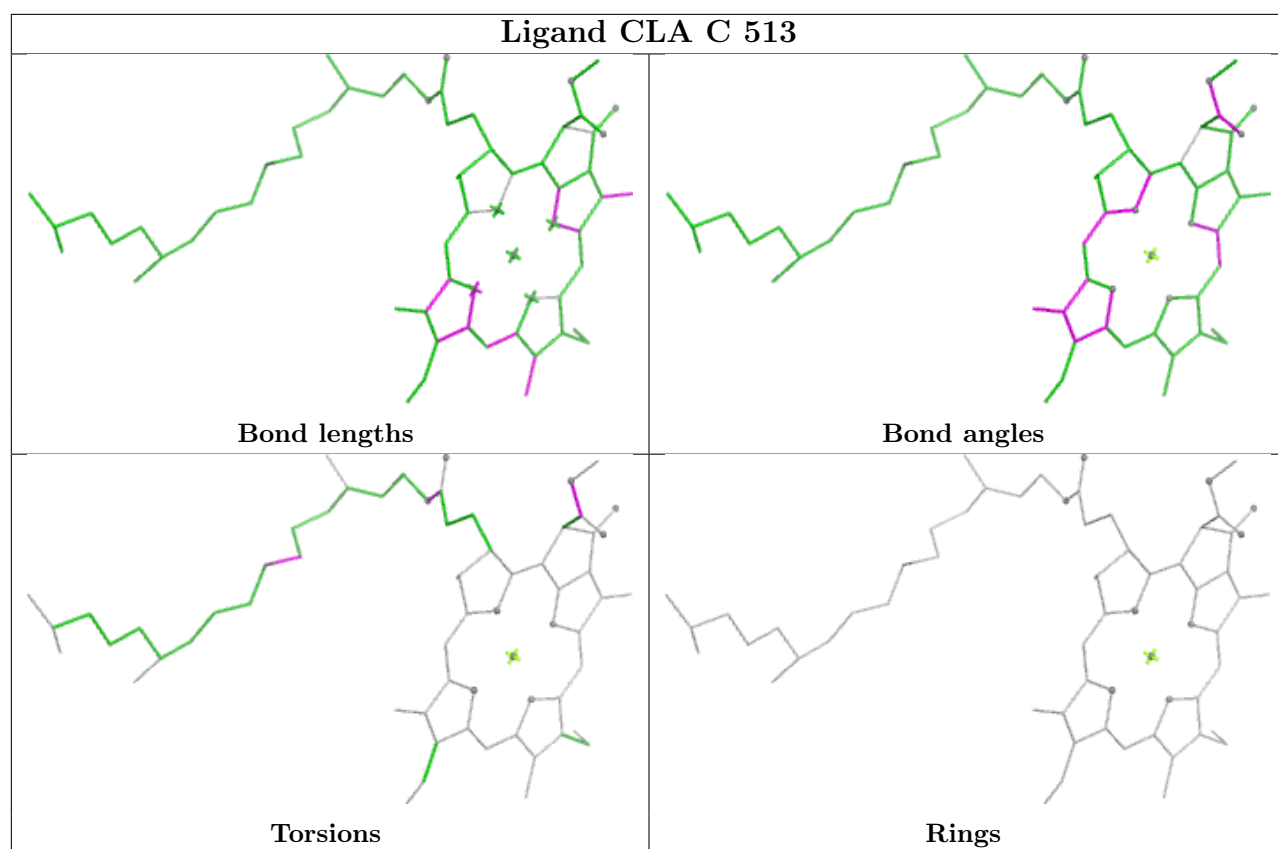


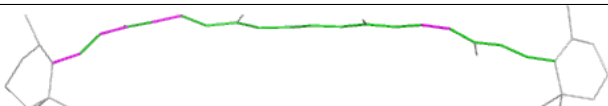
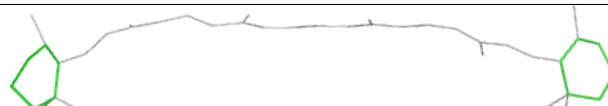


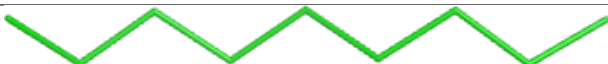
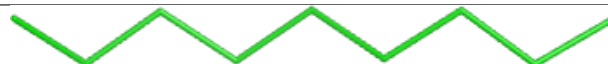
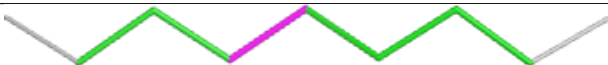


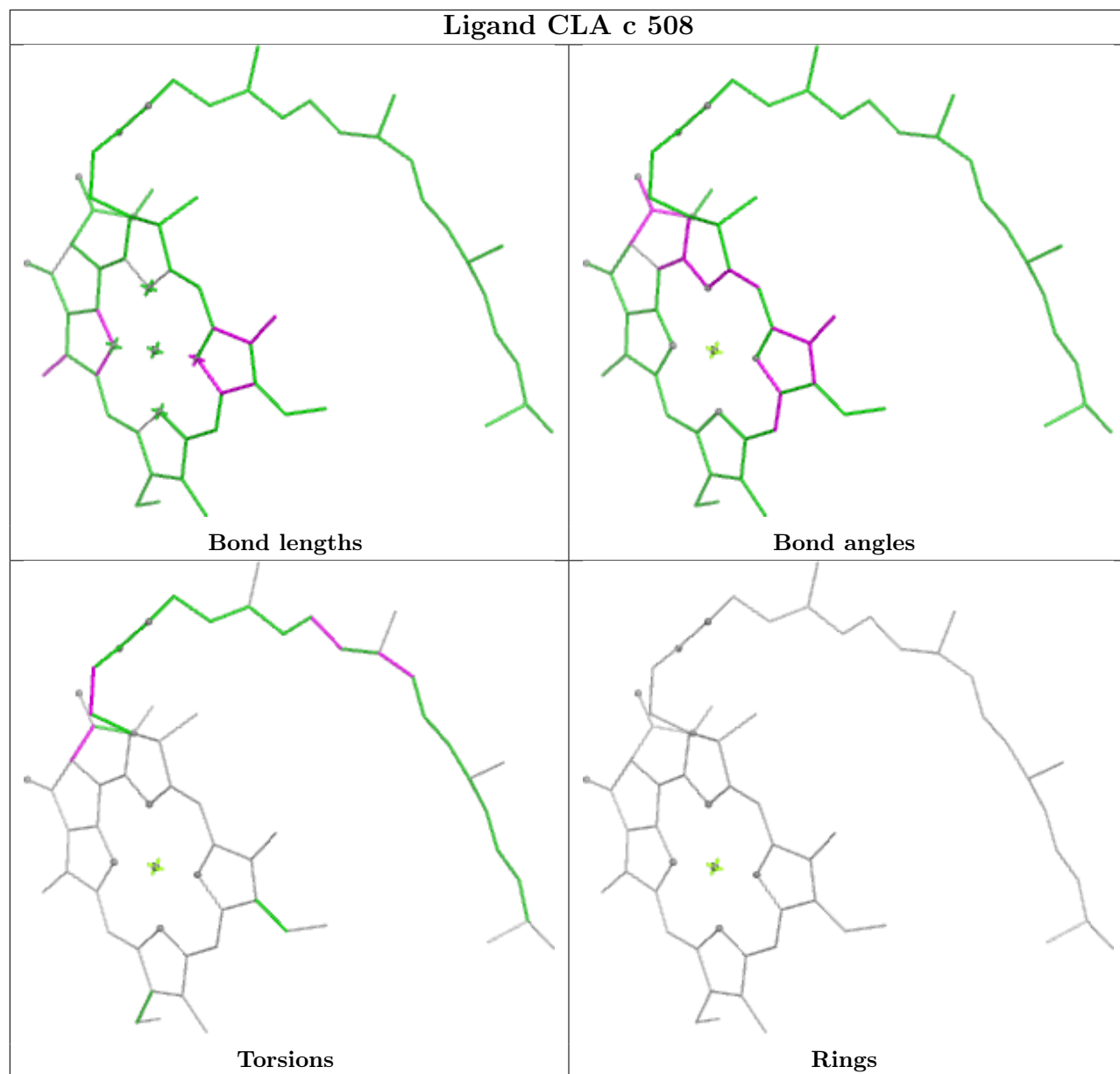


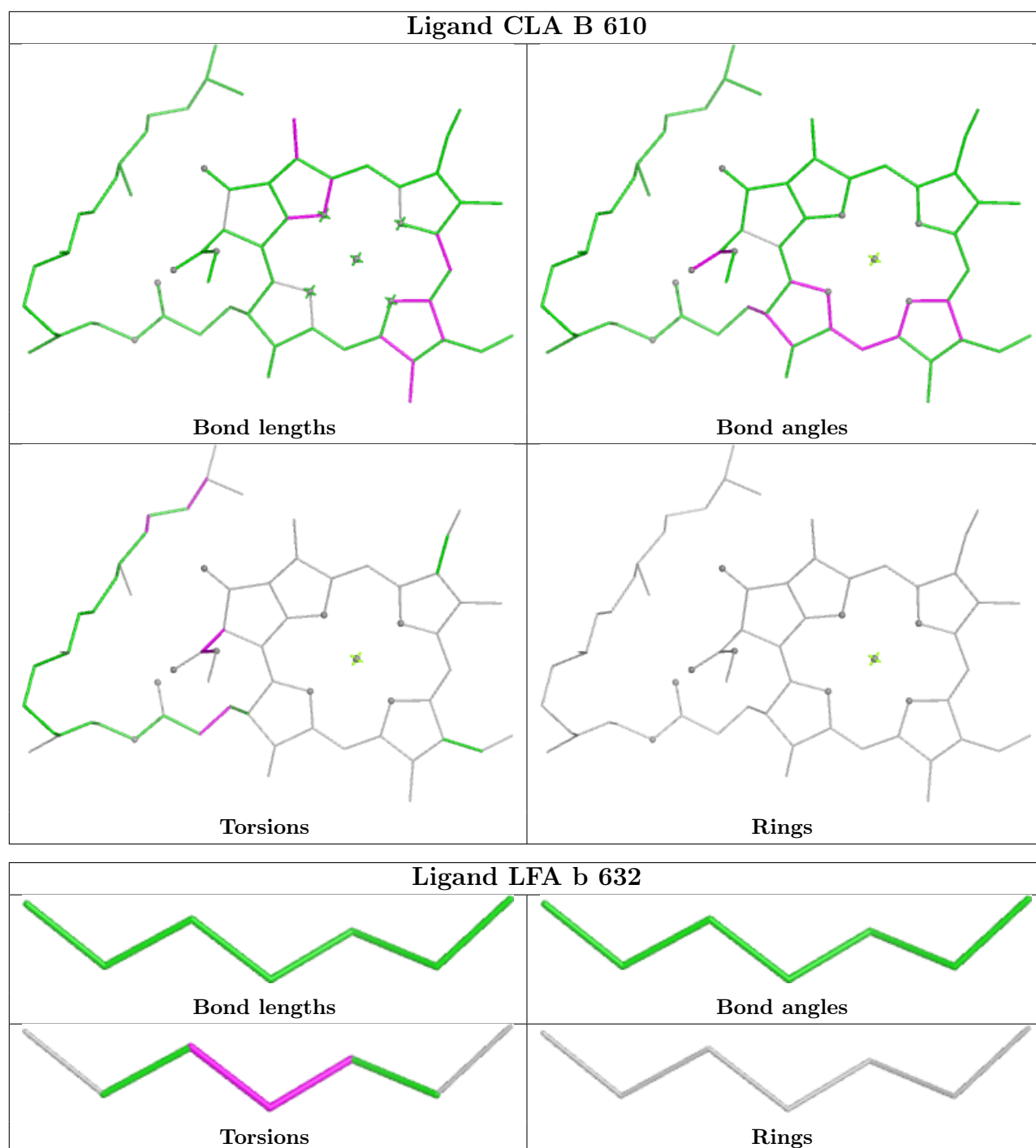


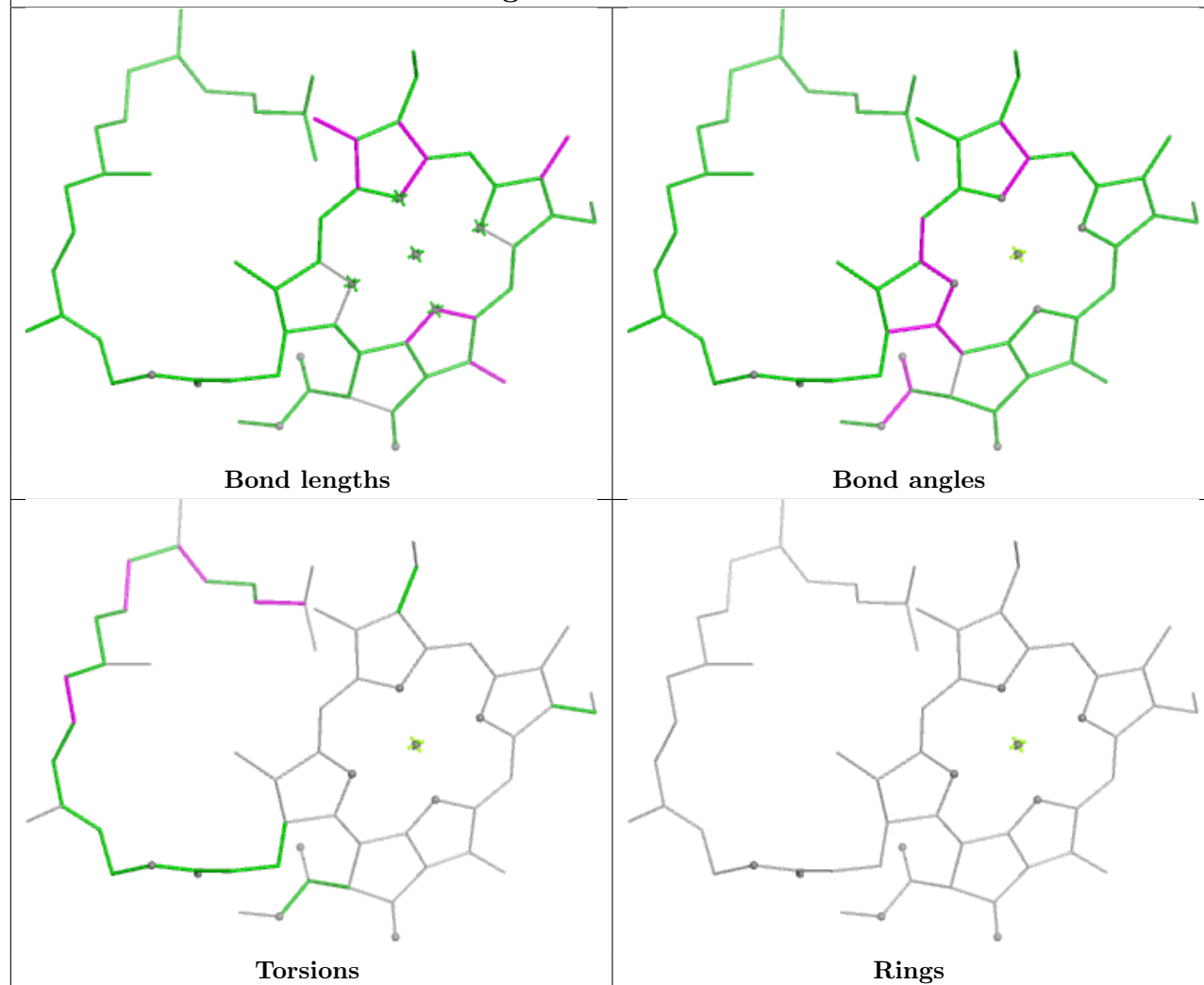
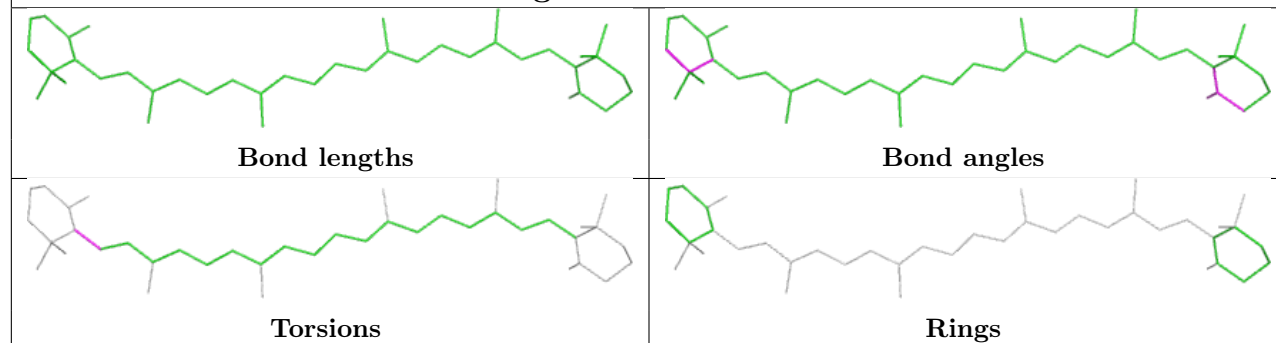


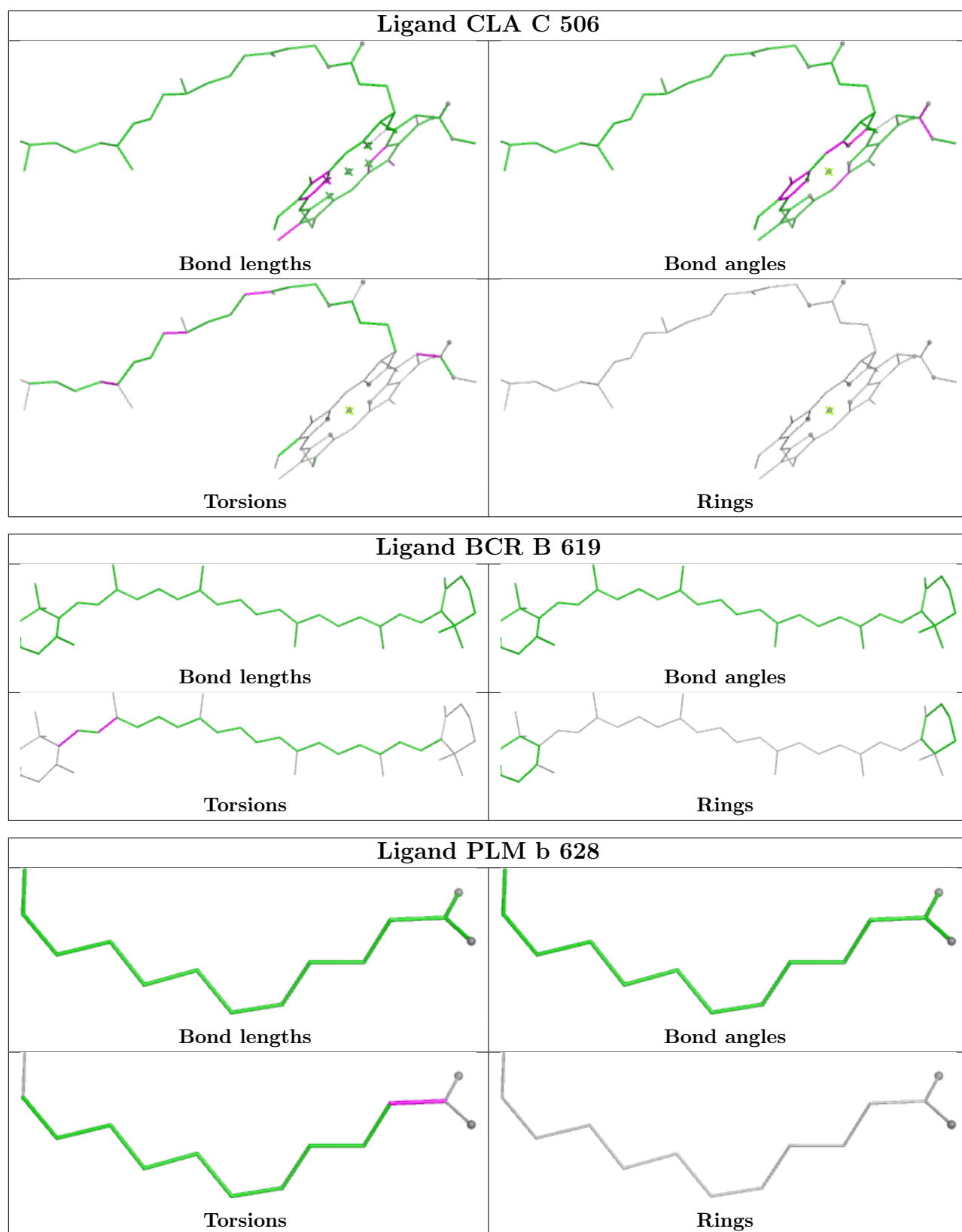
Ligand BCR c 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

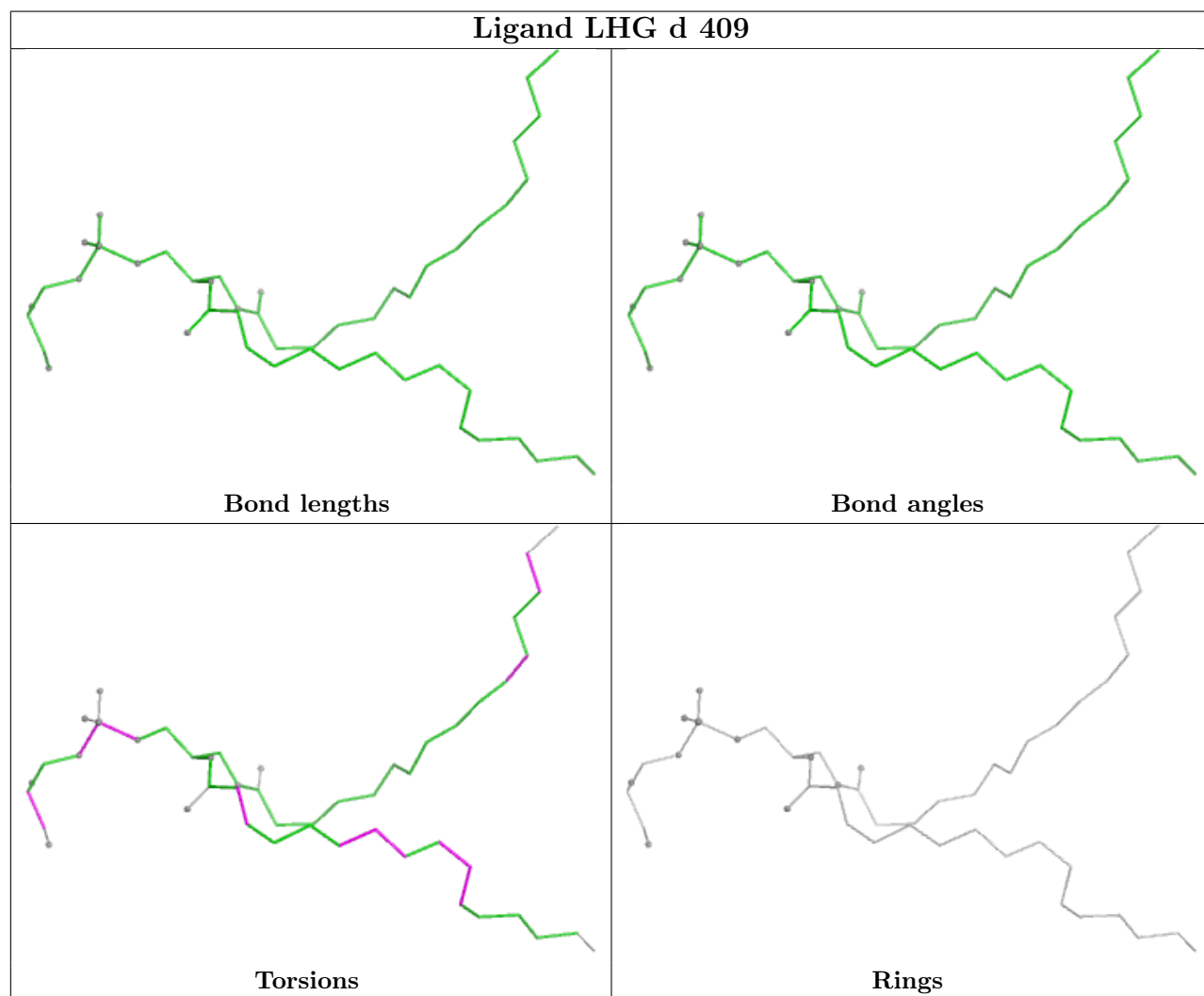
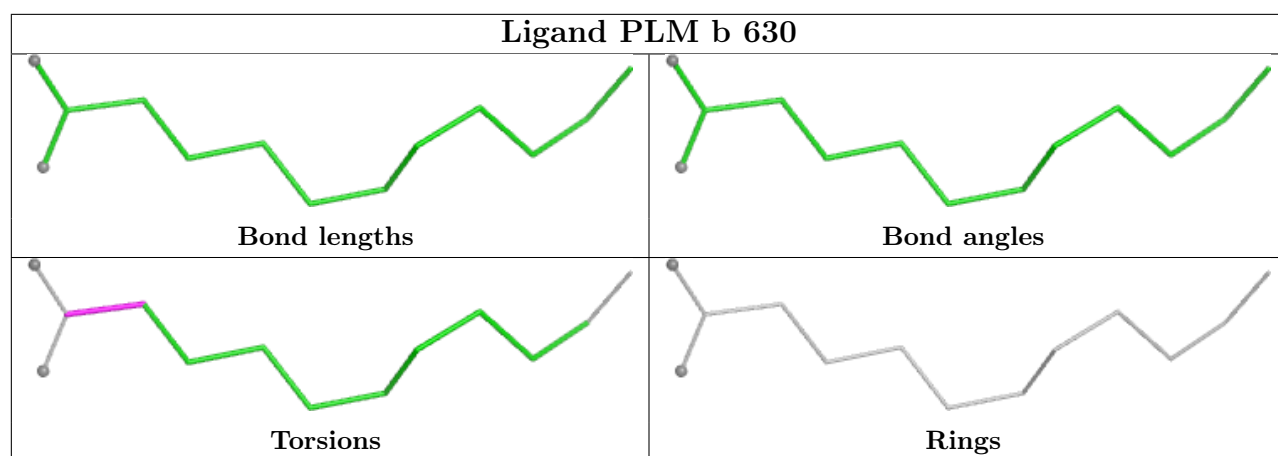
Ligand LFA b 629	
 Bond lengths	 Bond angles
 Torsions	 Rings

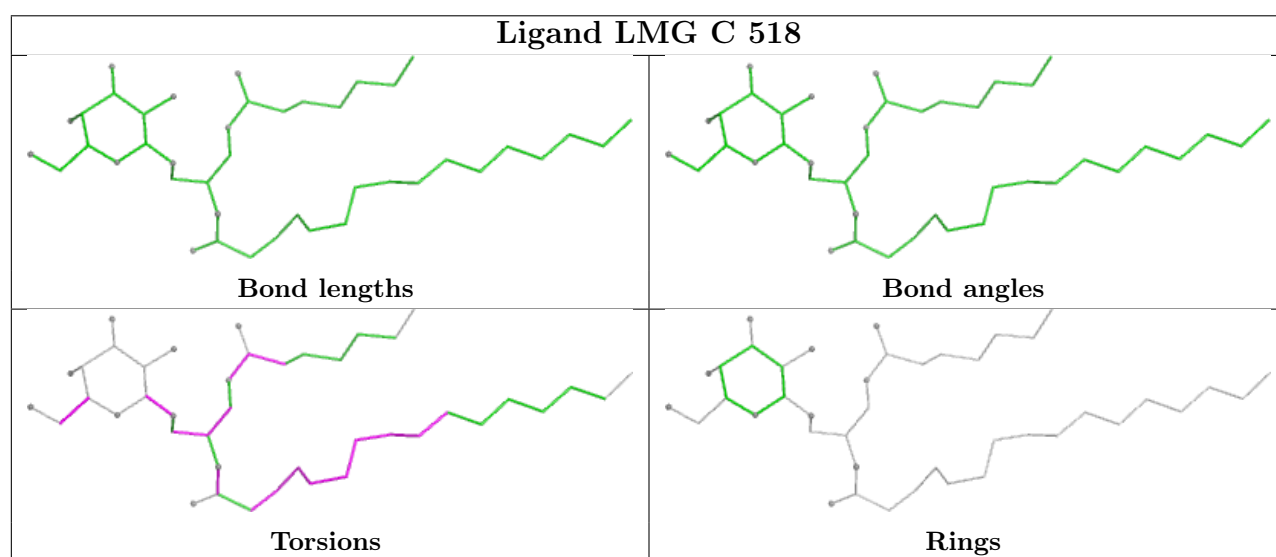
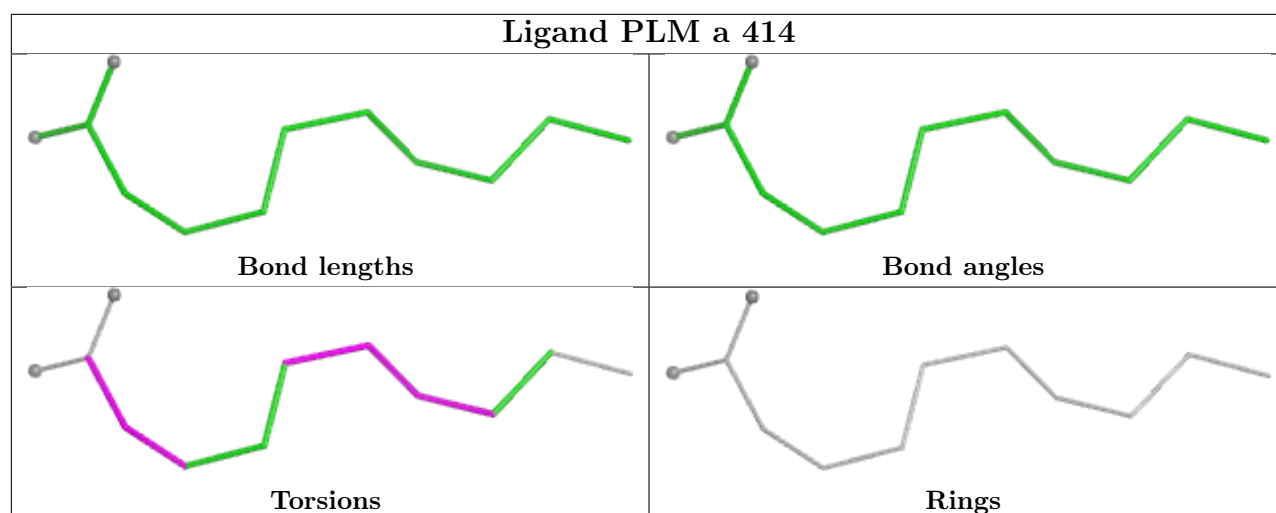


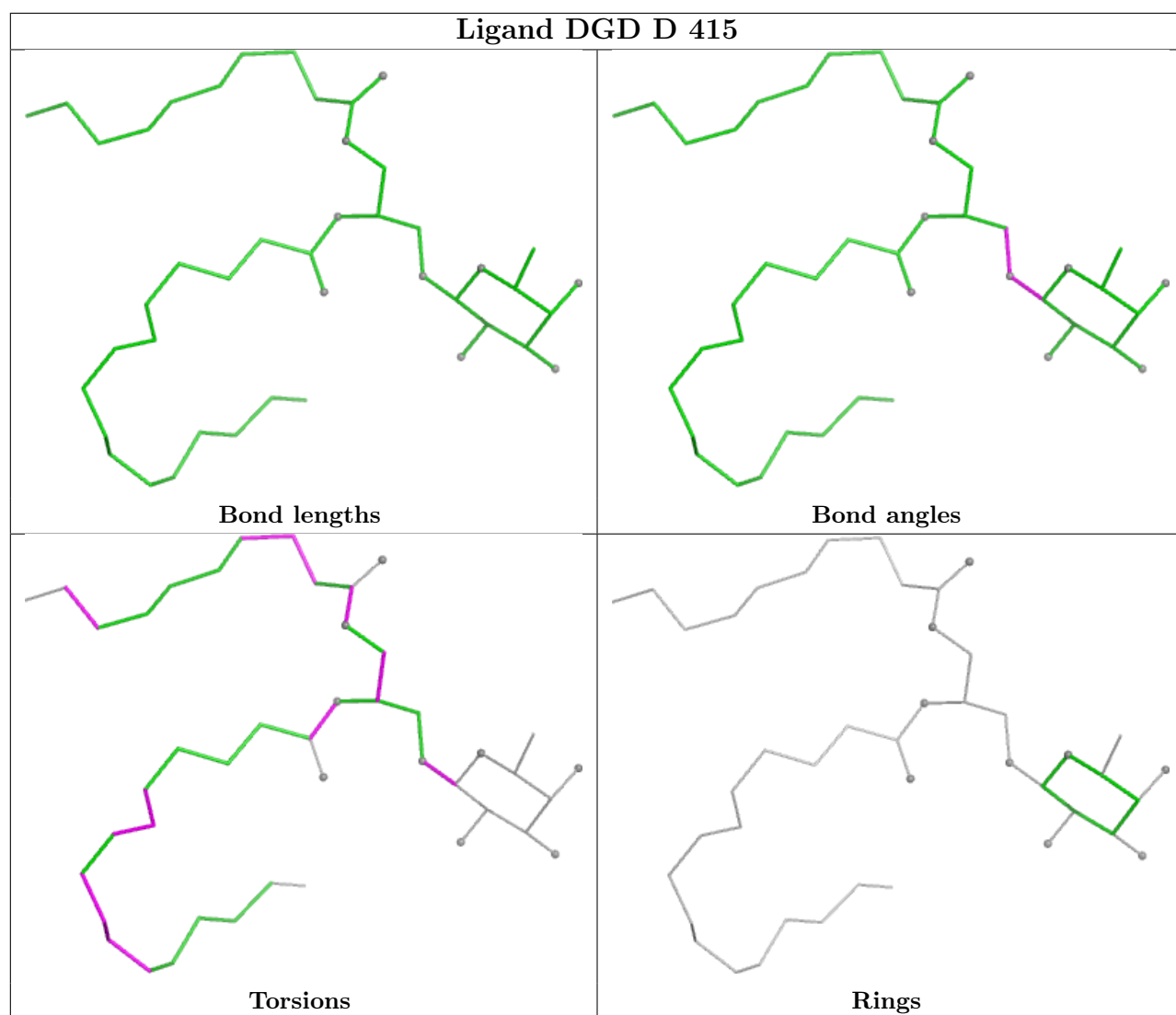


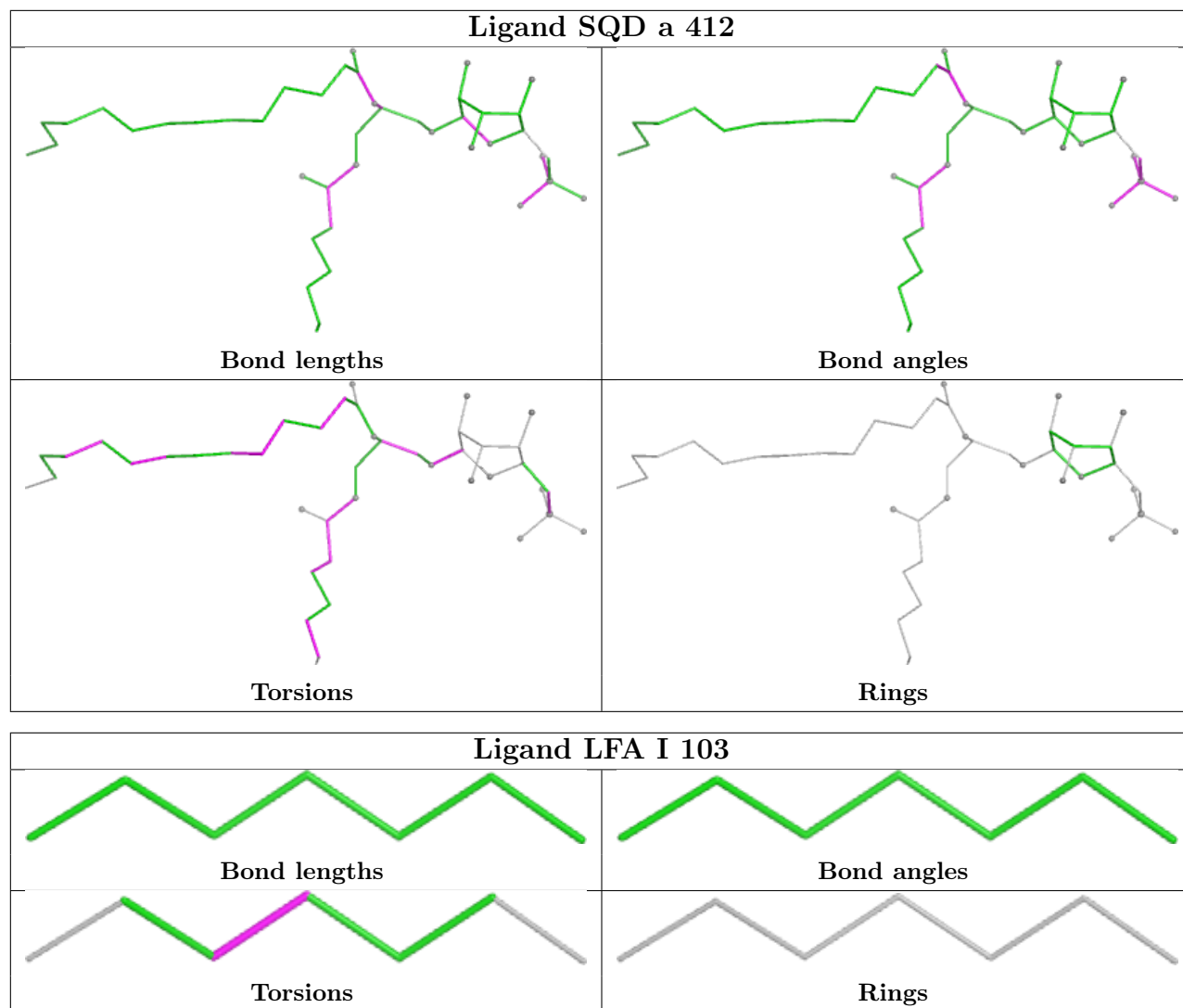
Ligand CLA B 615**Ligand BCR b 620**

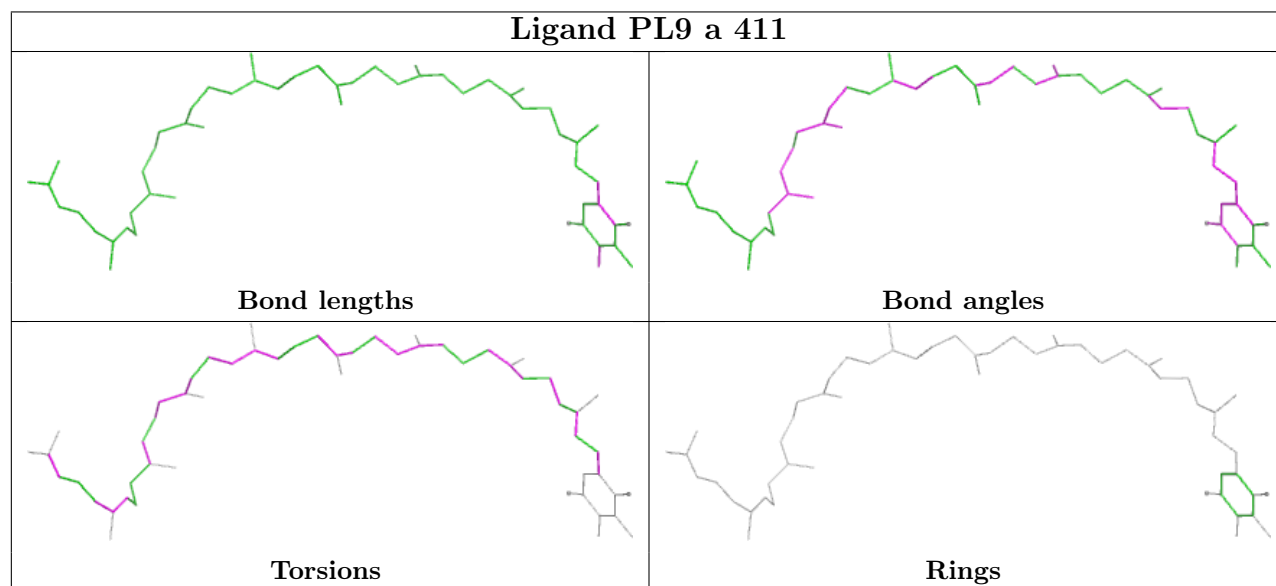
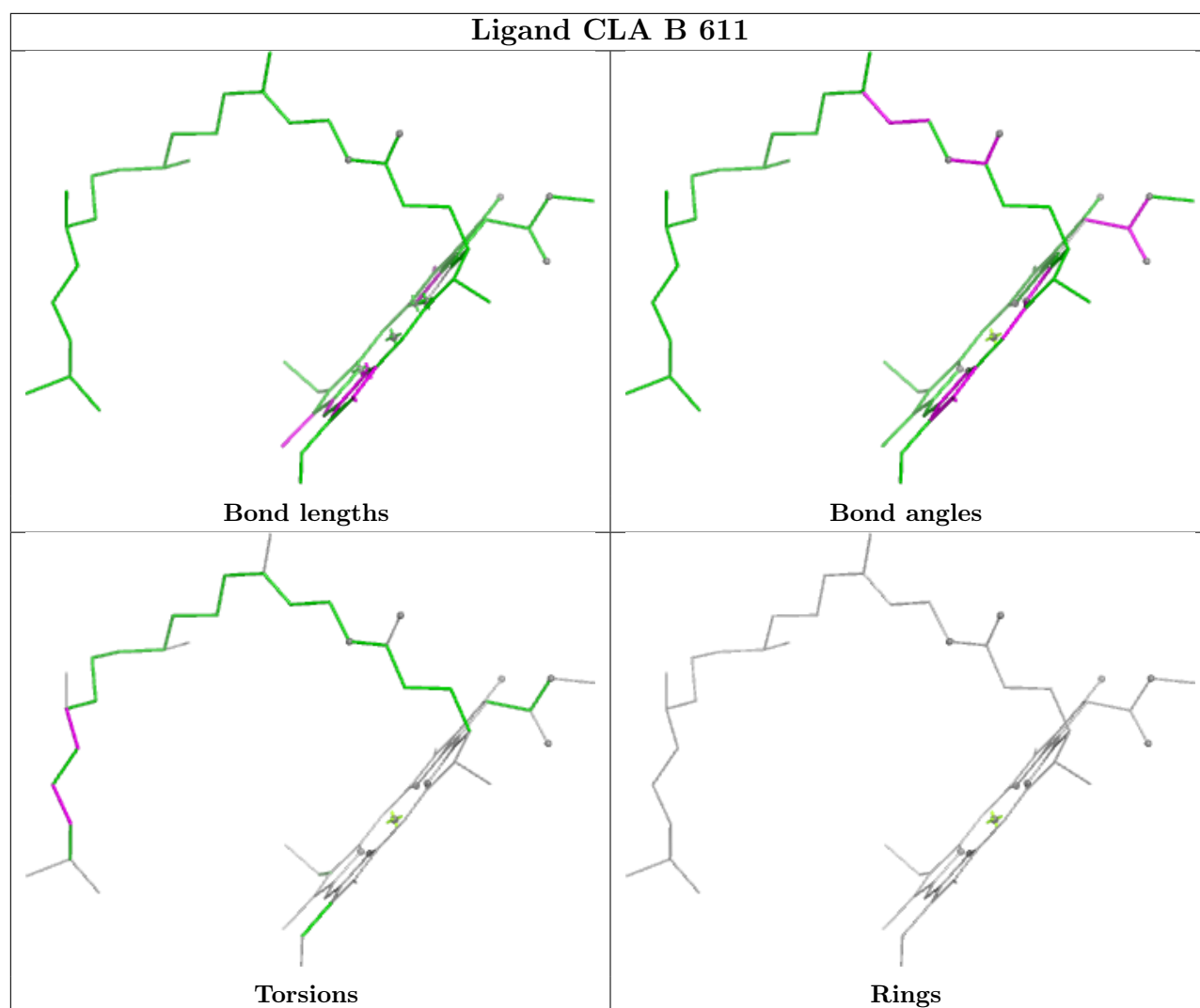


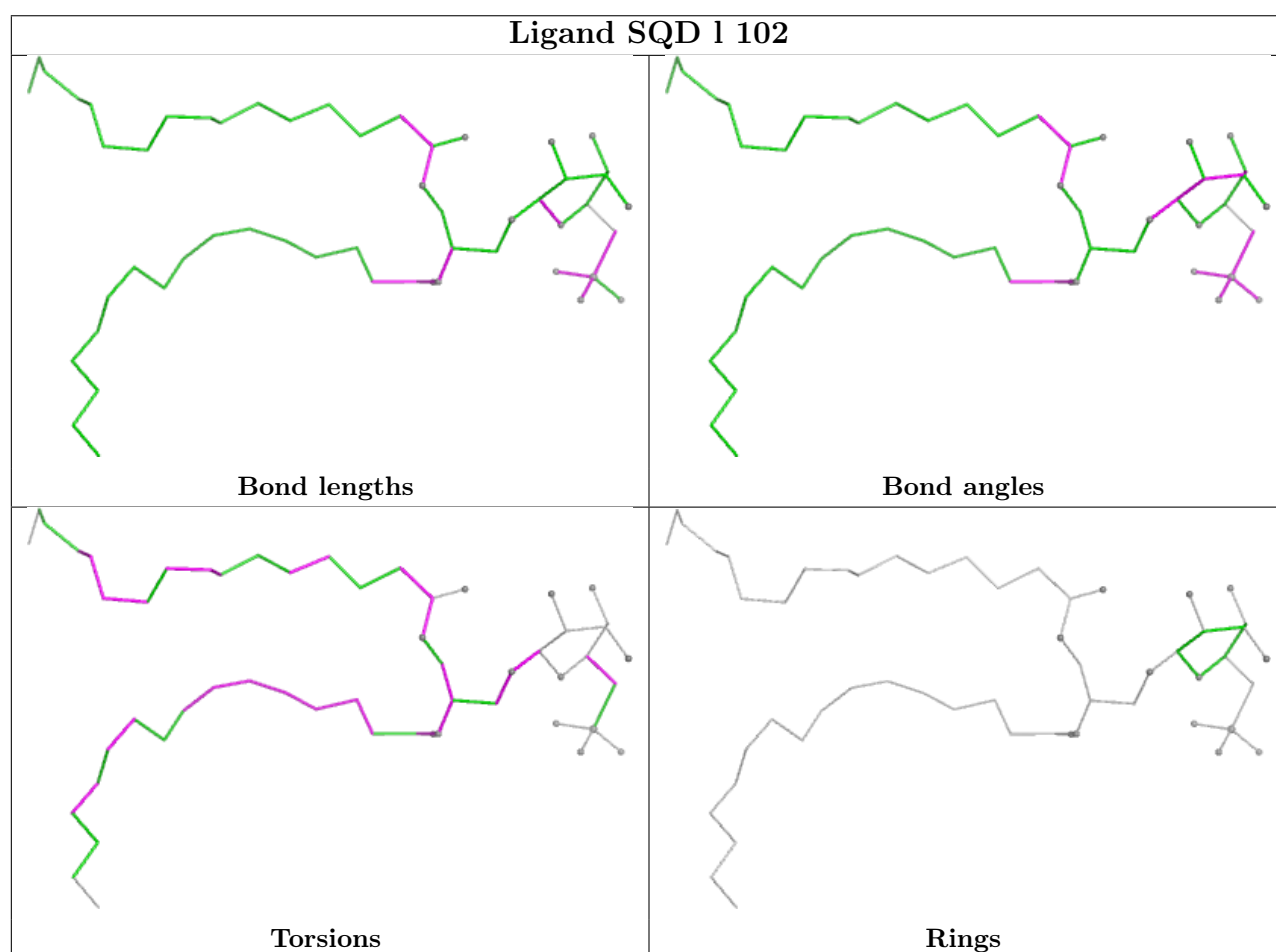
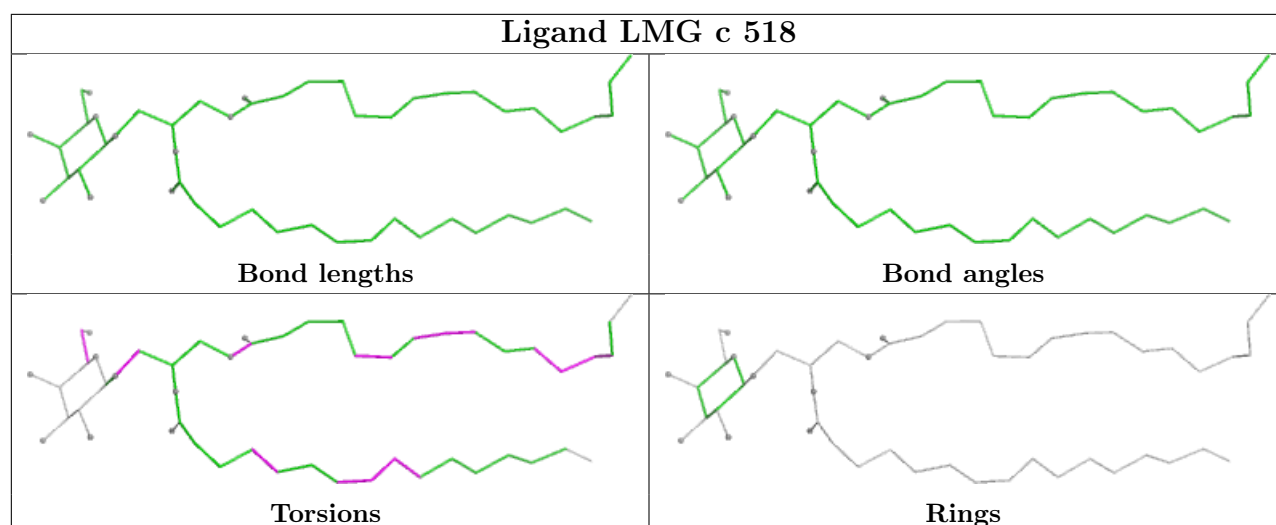


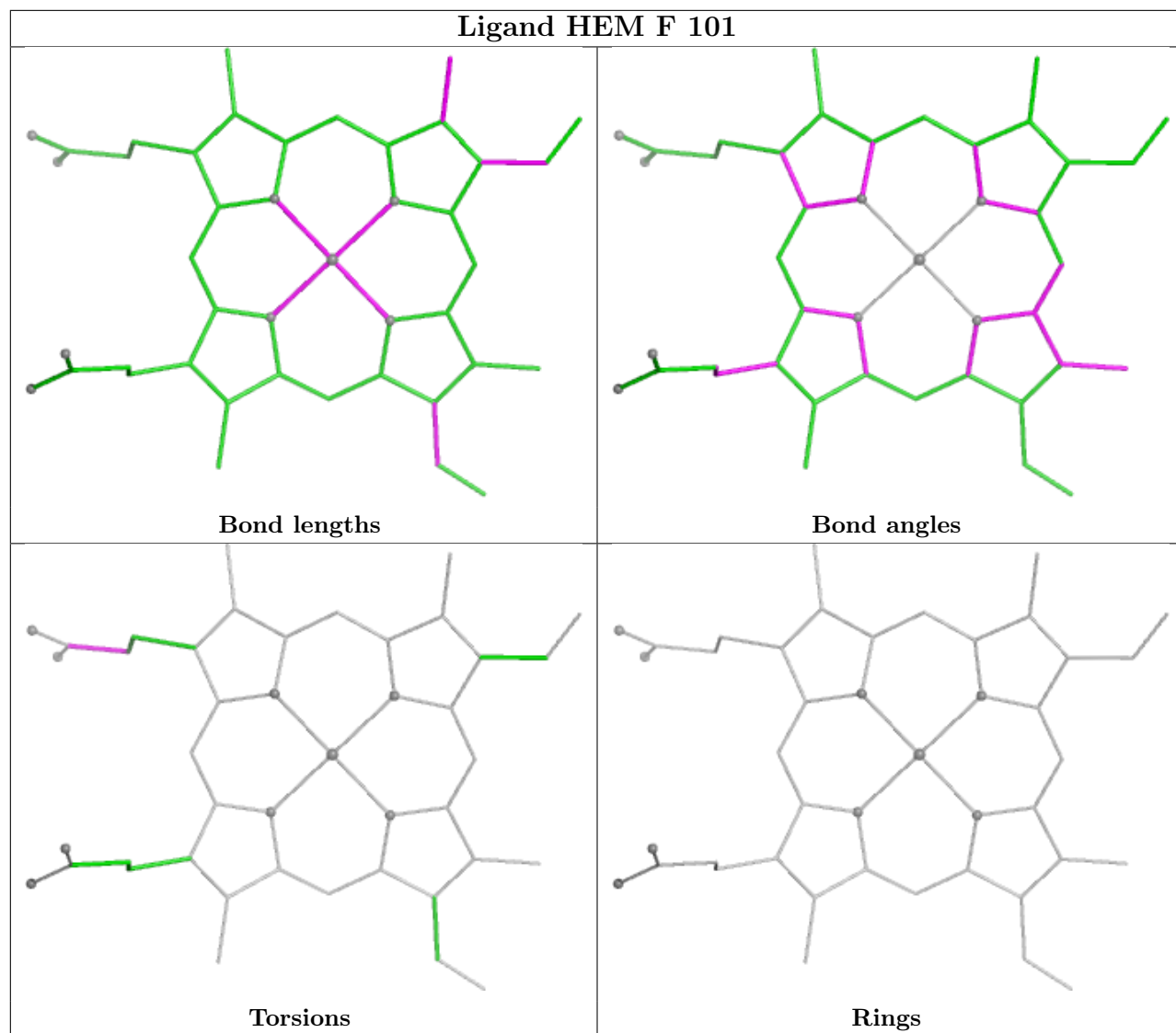




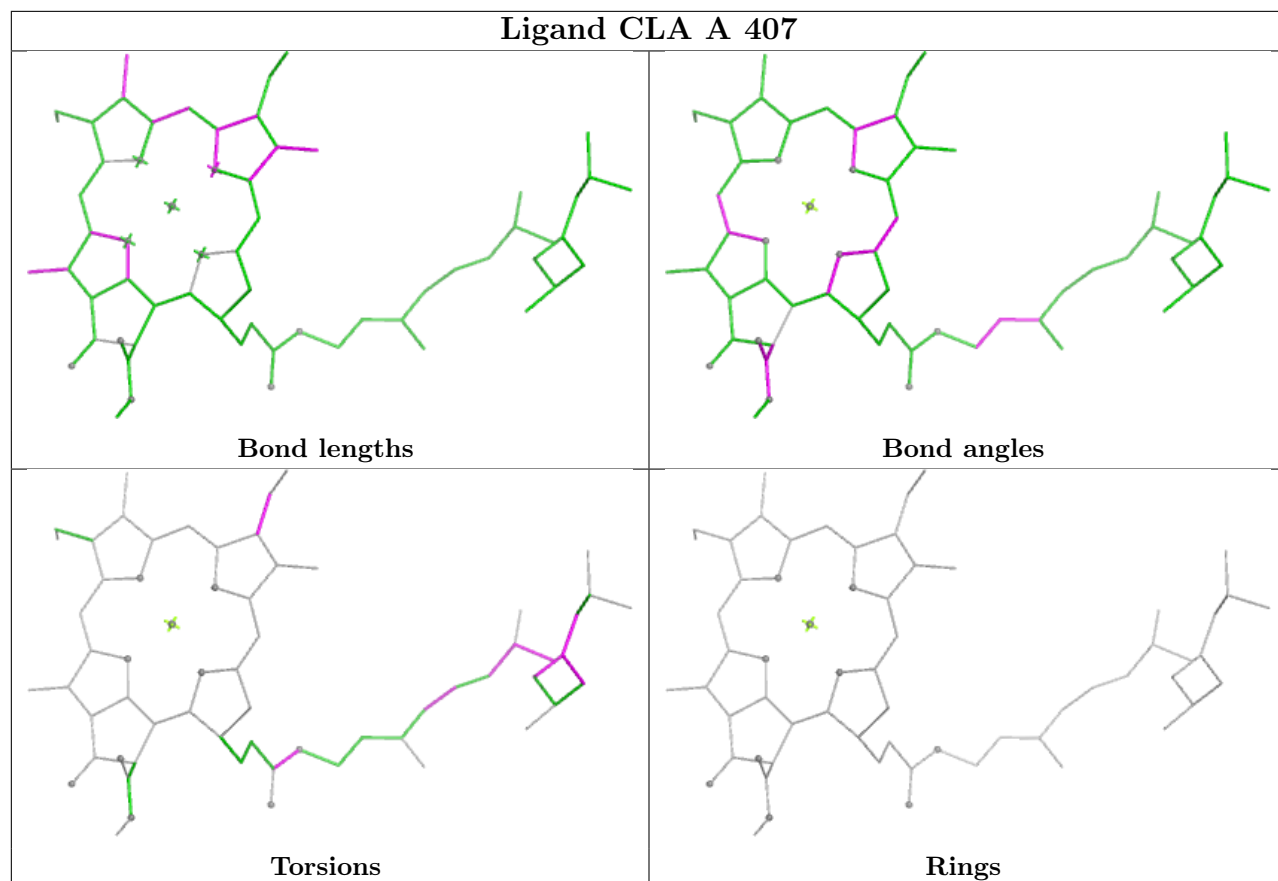




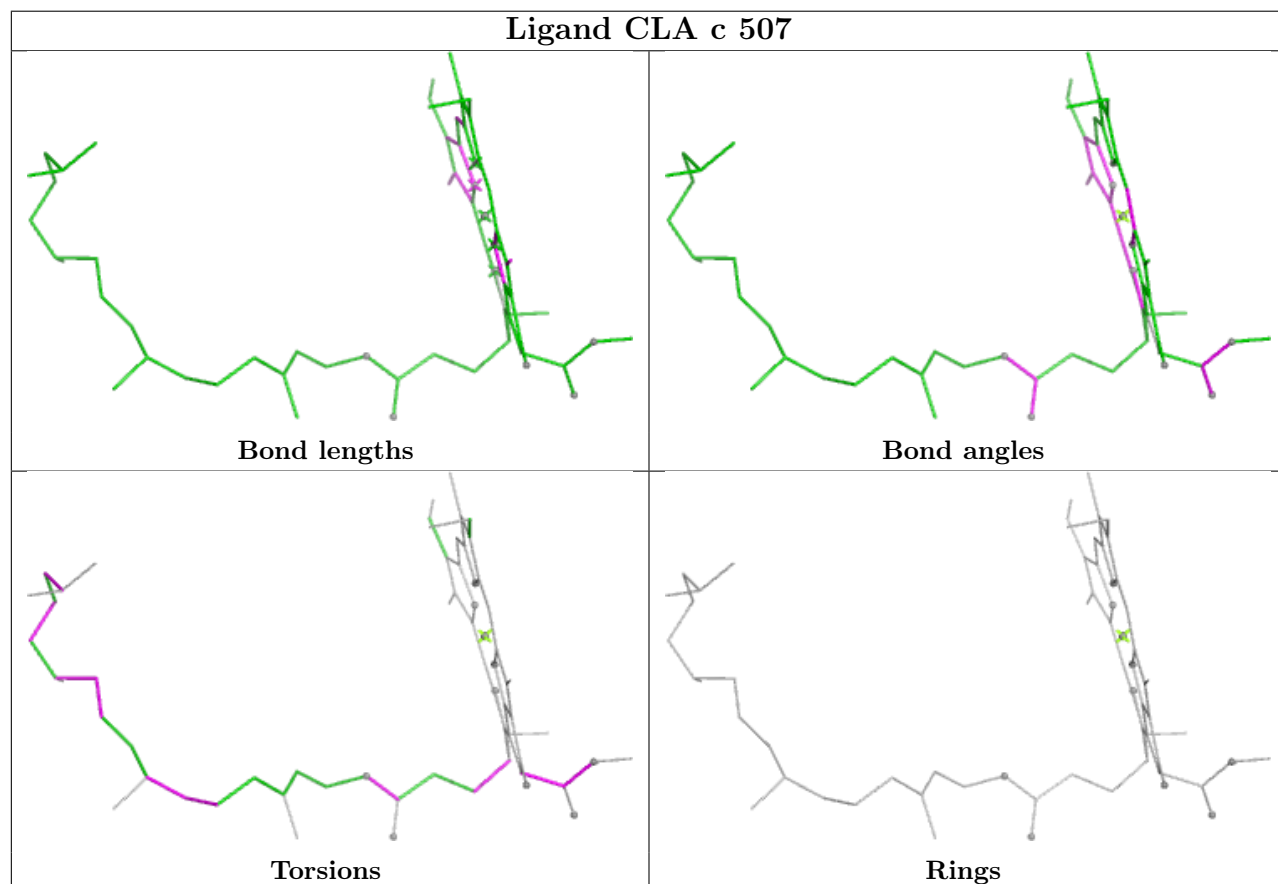


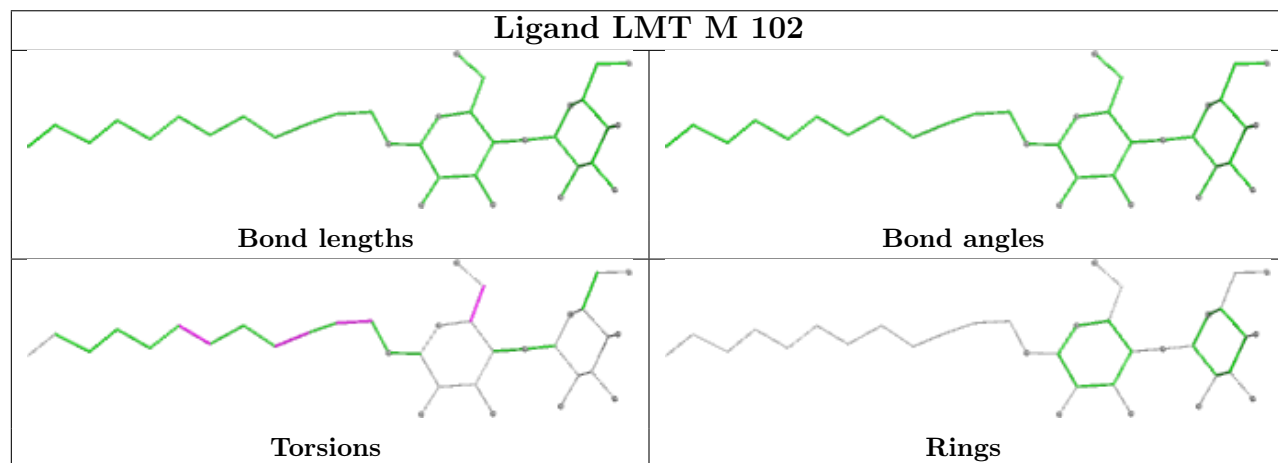
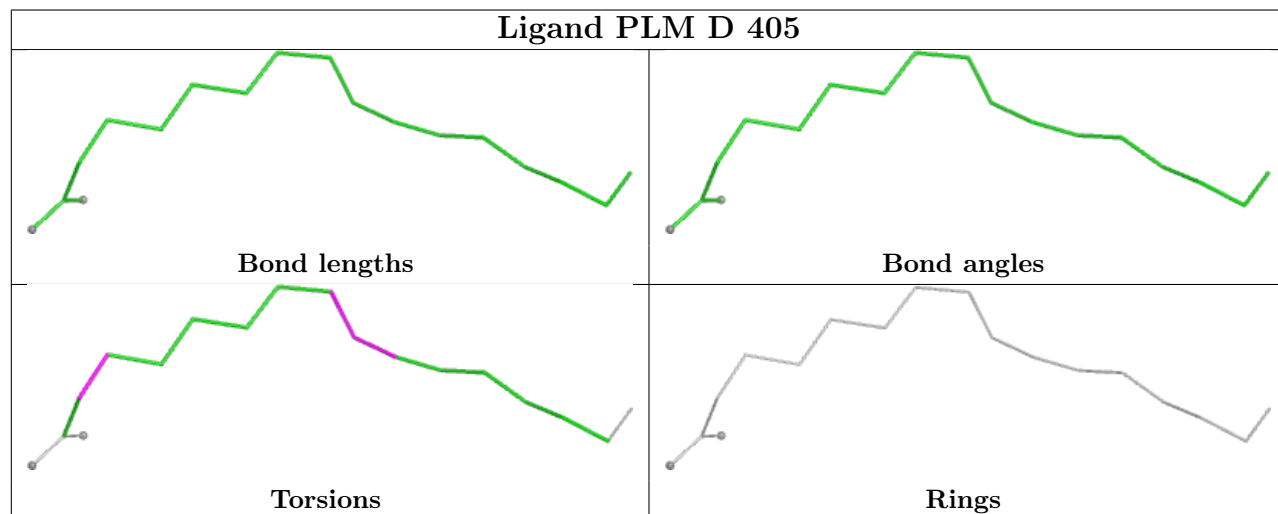
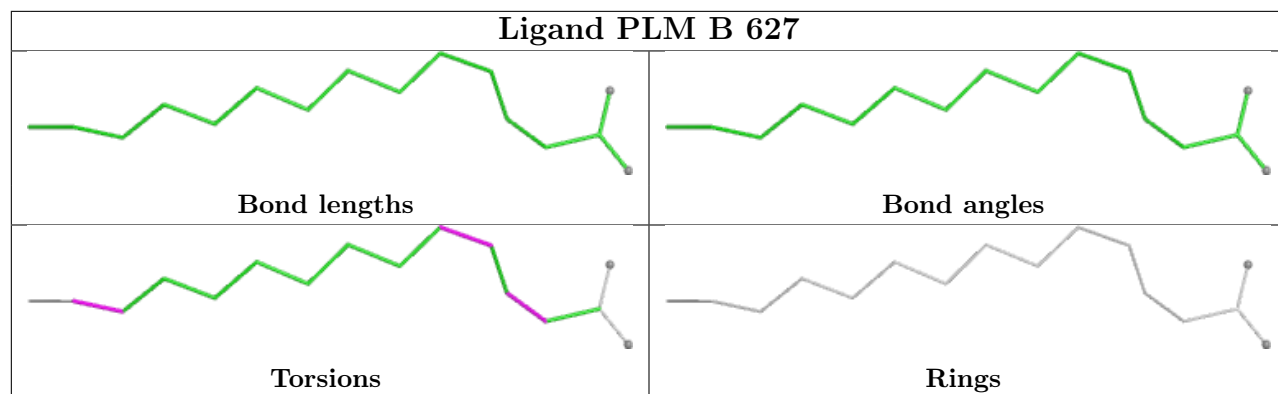


Ligand CLA A 407

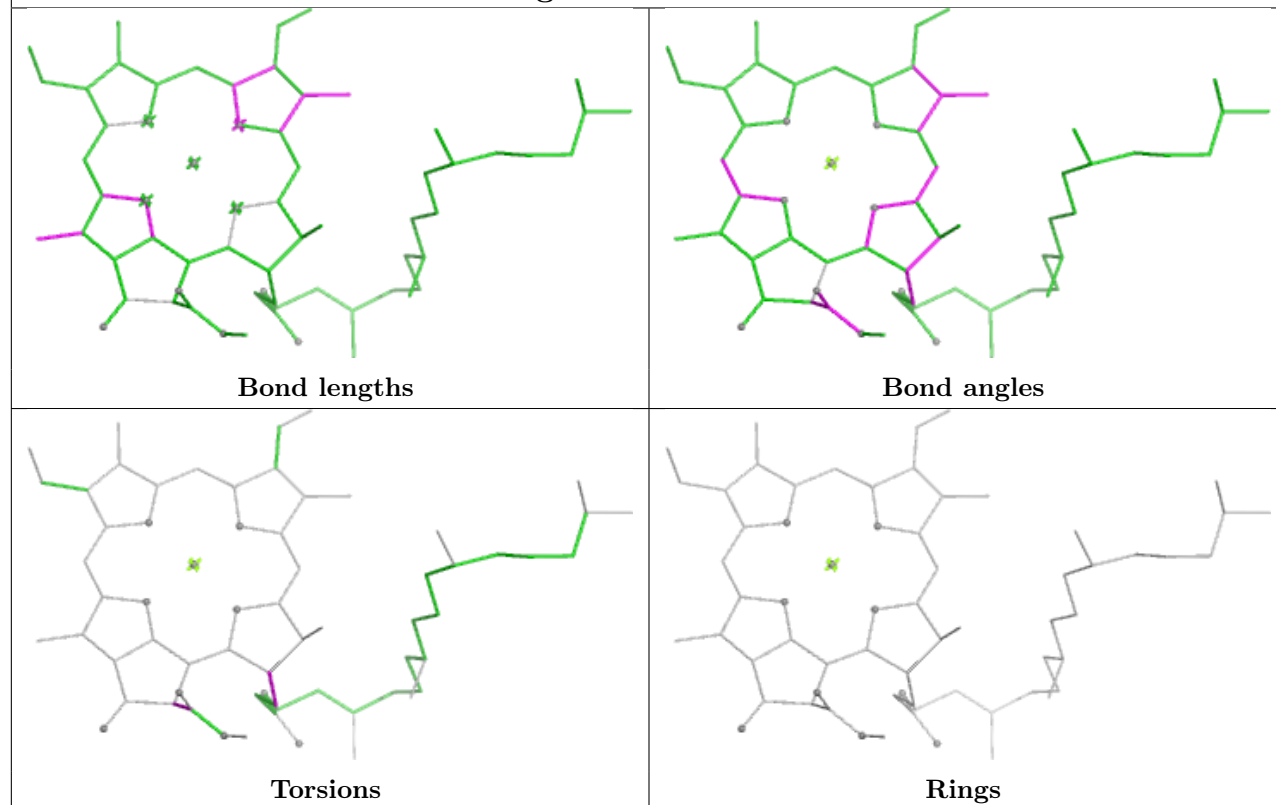


Ligand CLA c 507

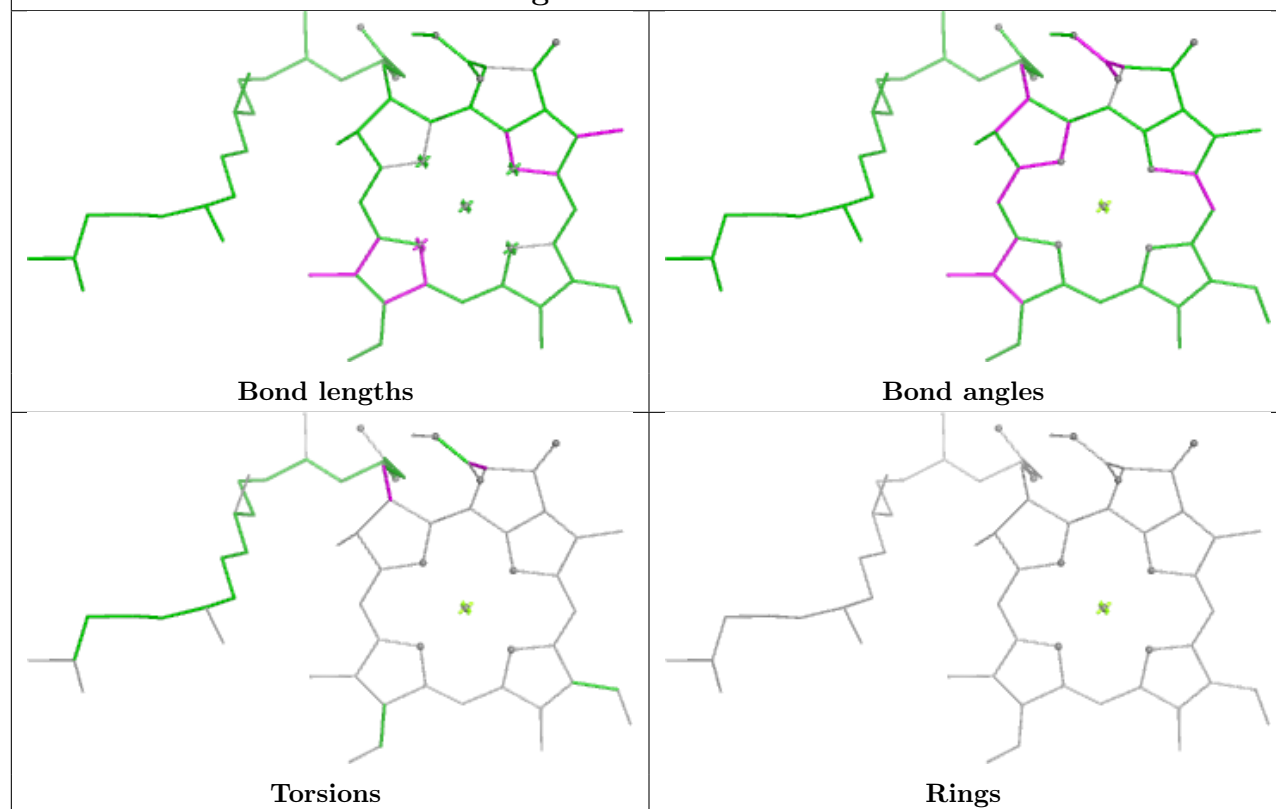


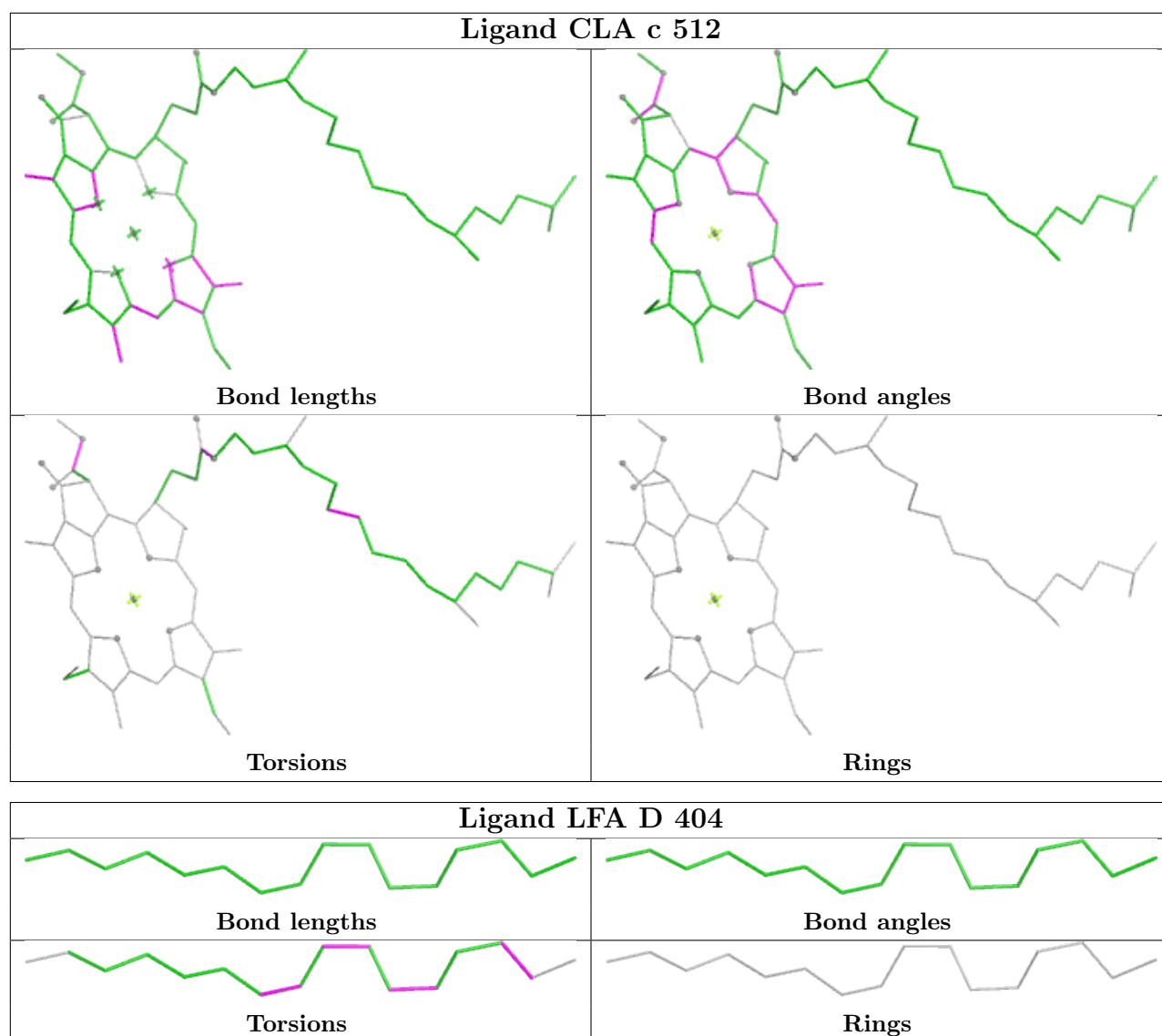


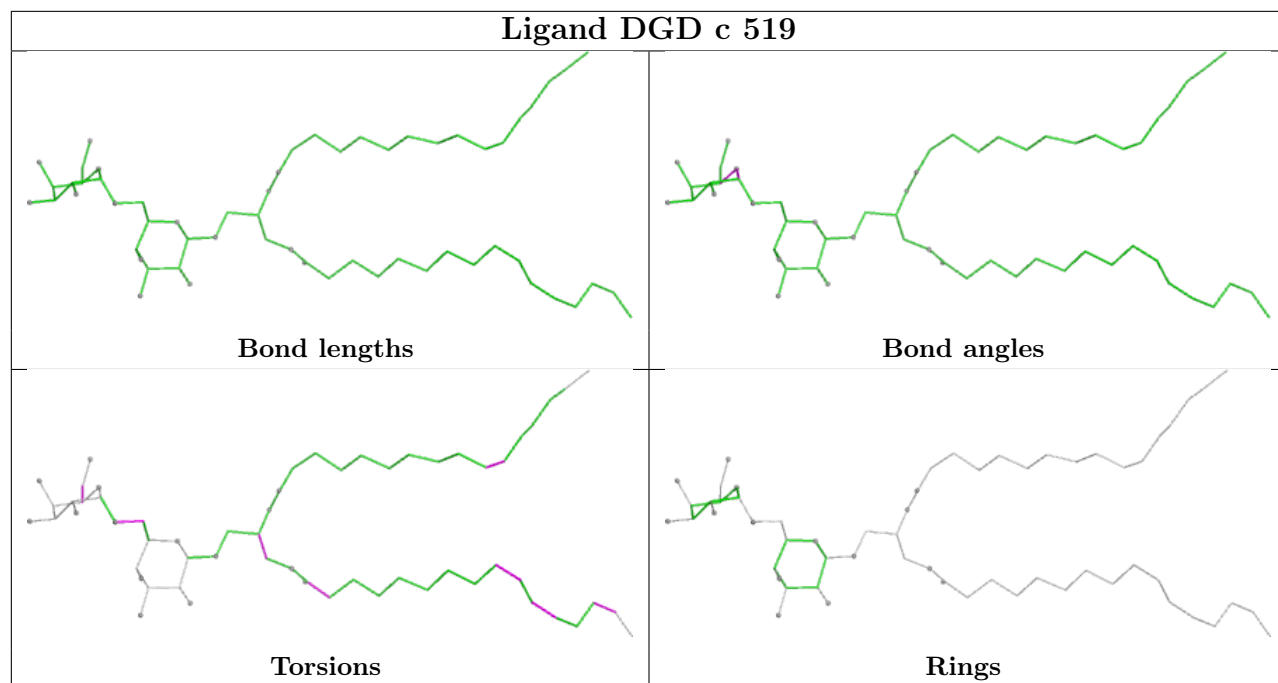
Ligand CLA a 405

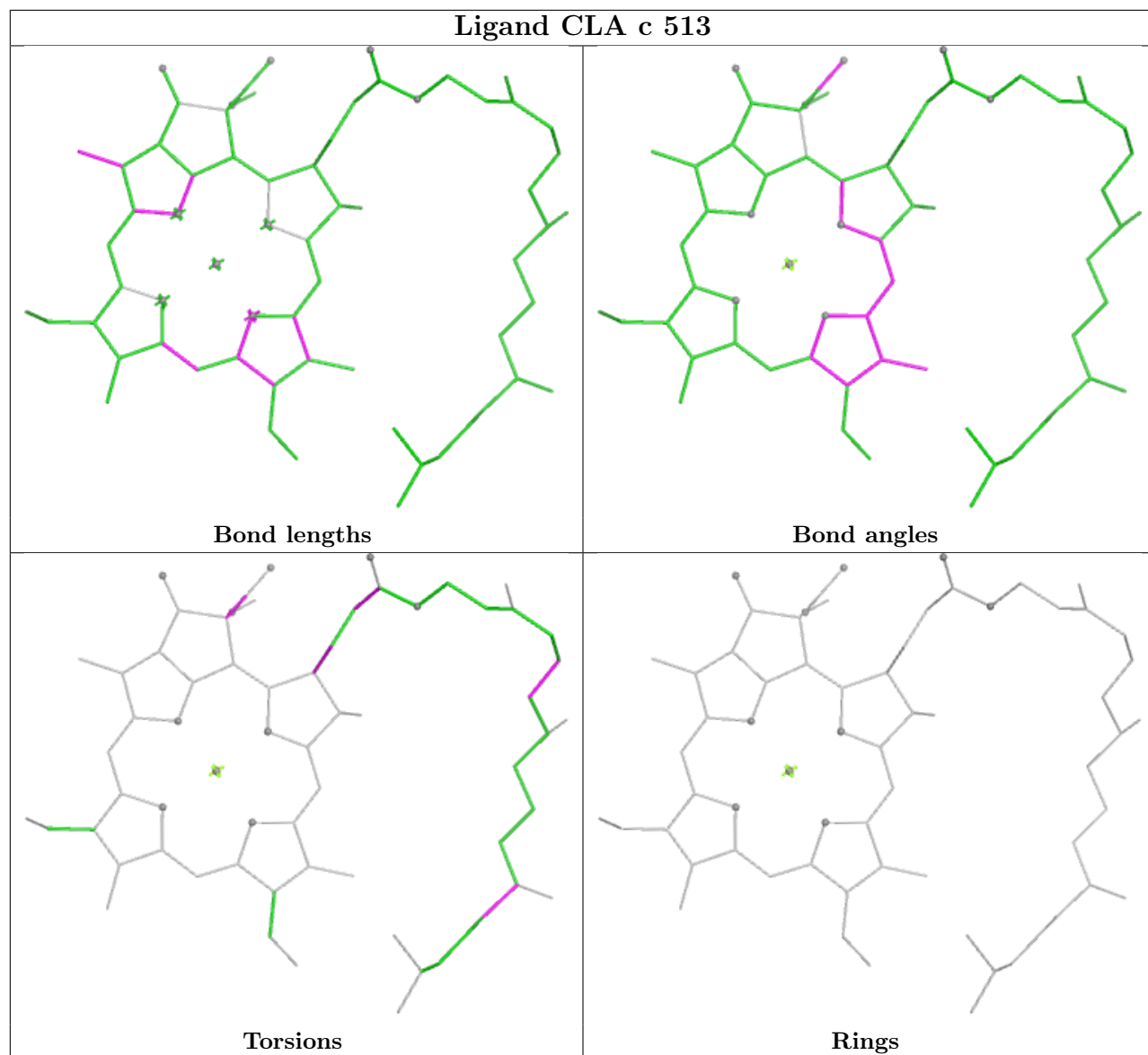


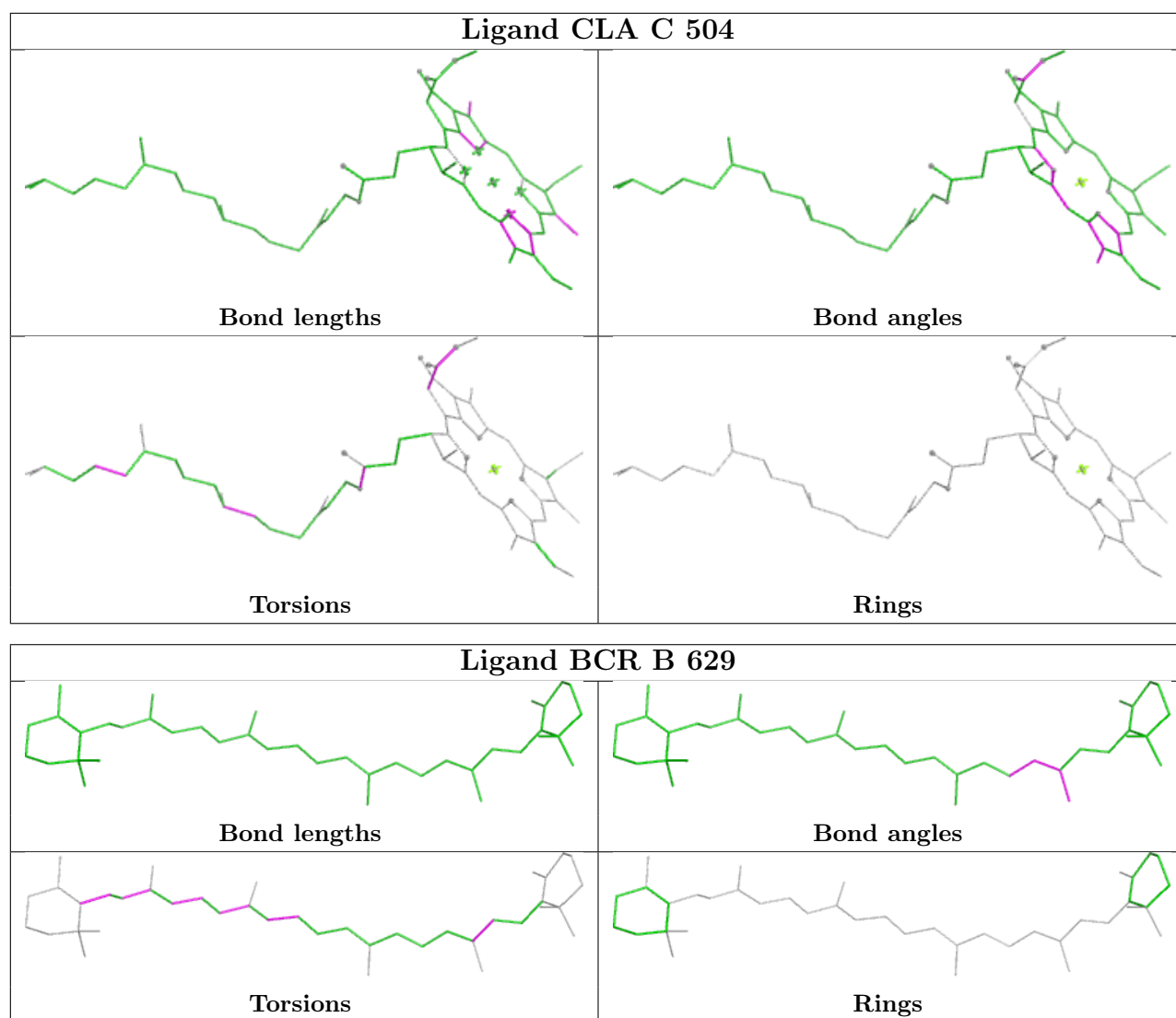
Ligand CLA A 404

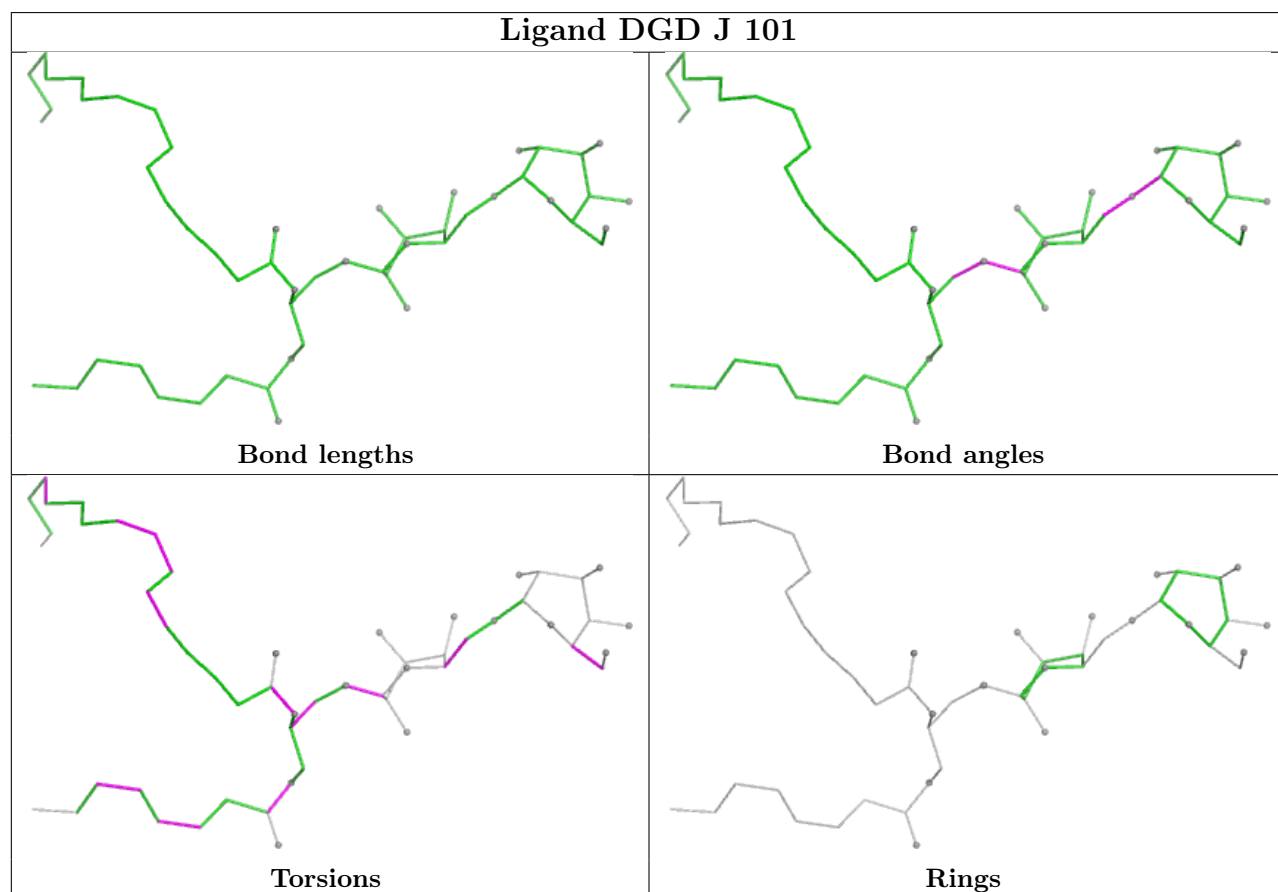
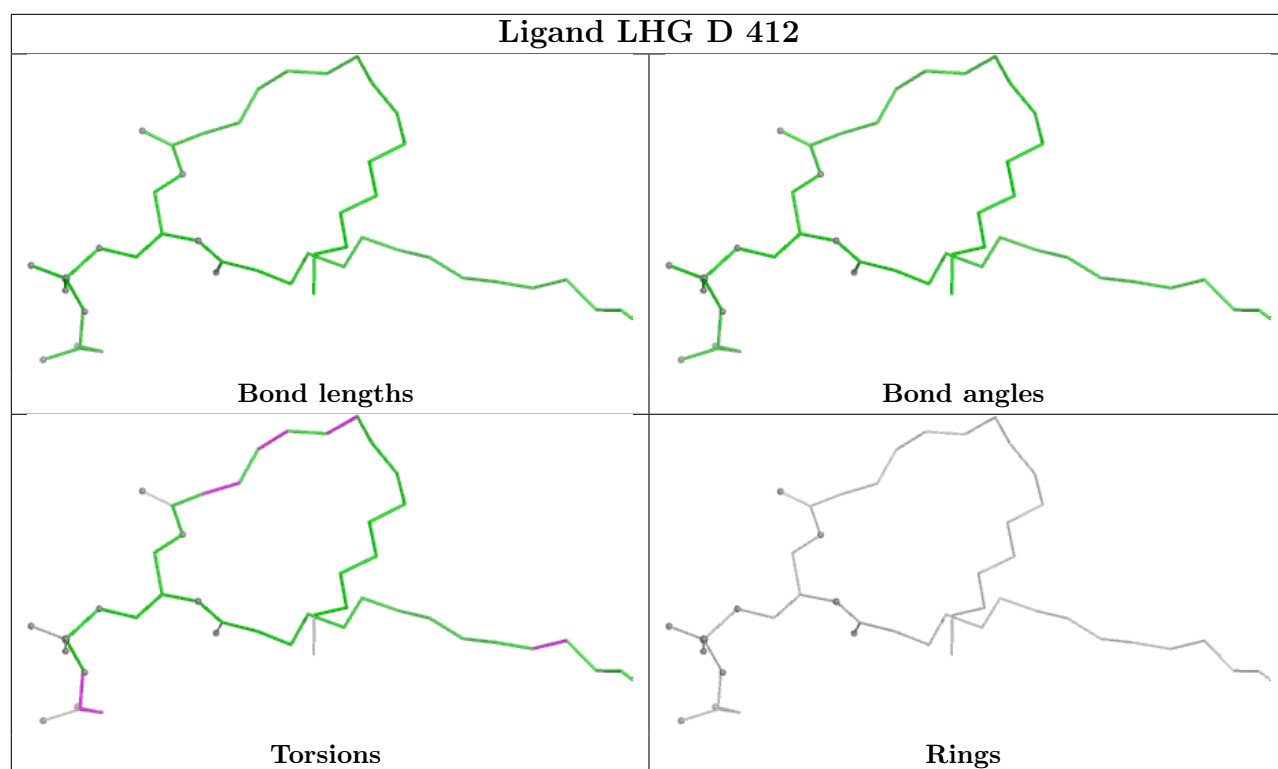


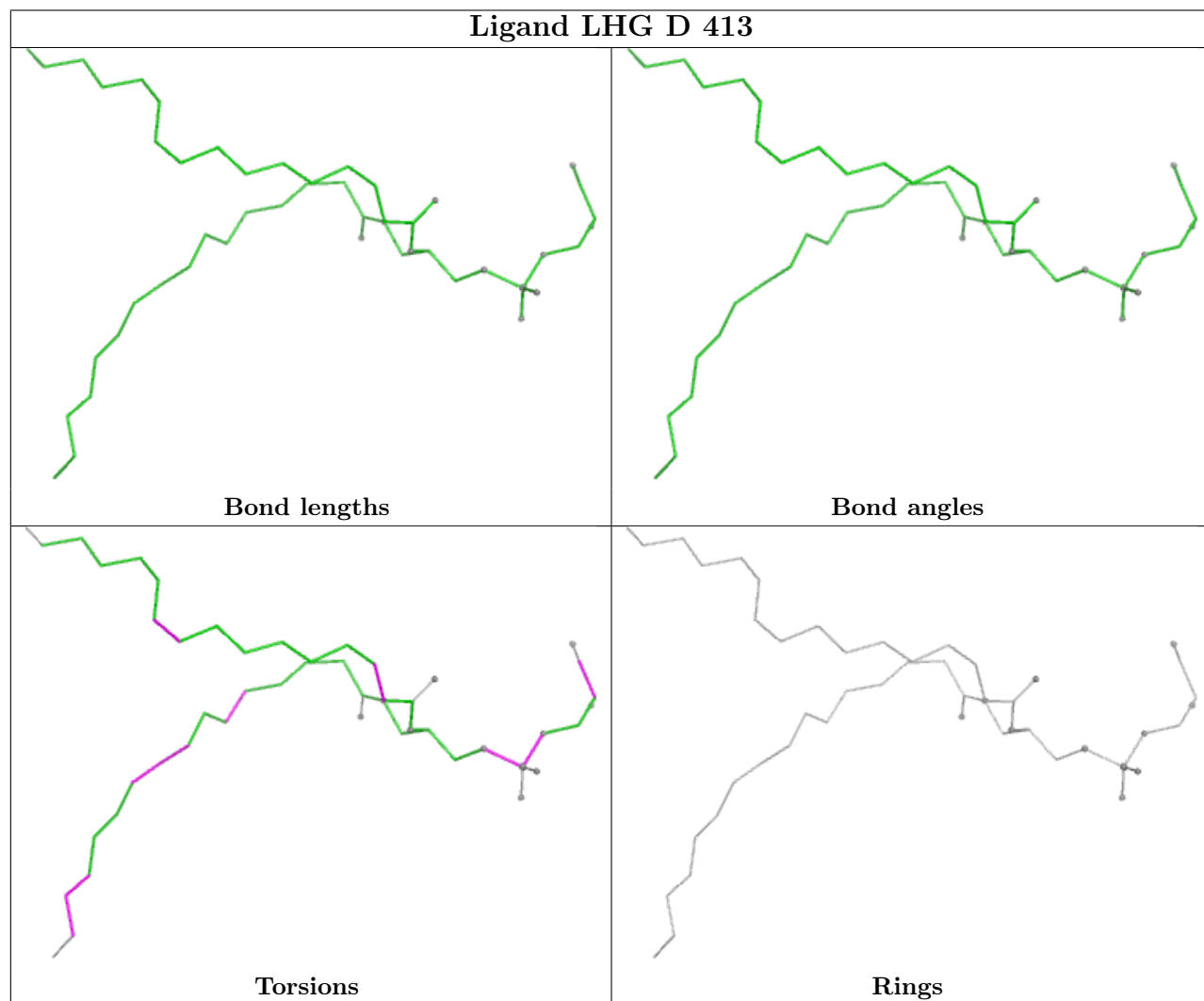
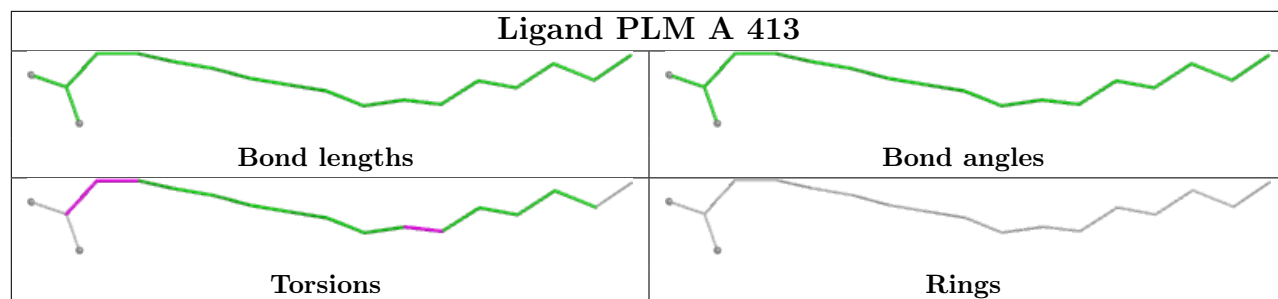


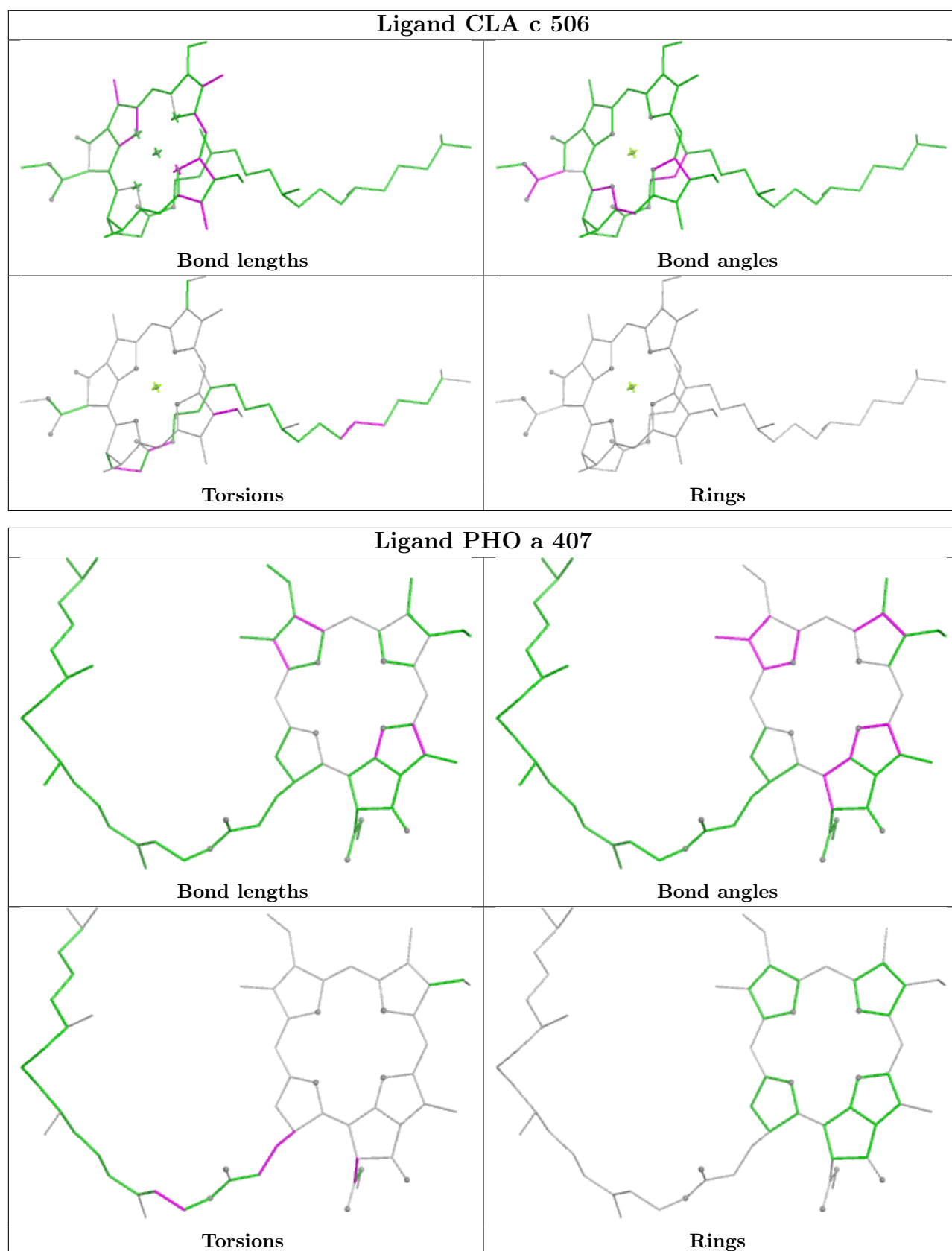


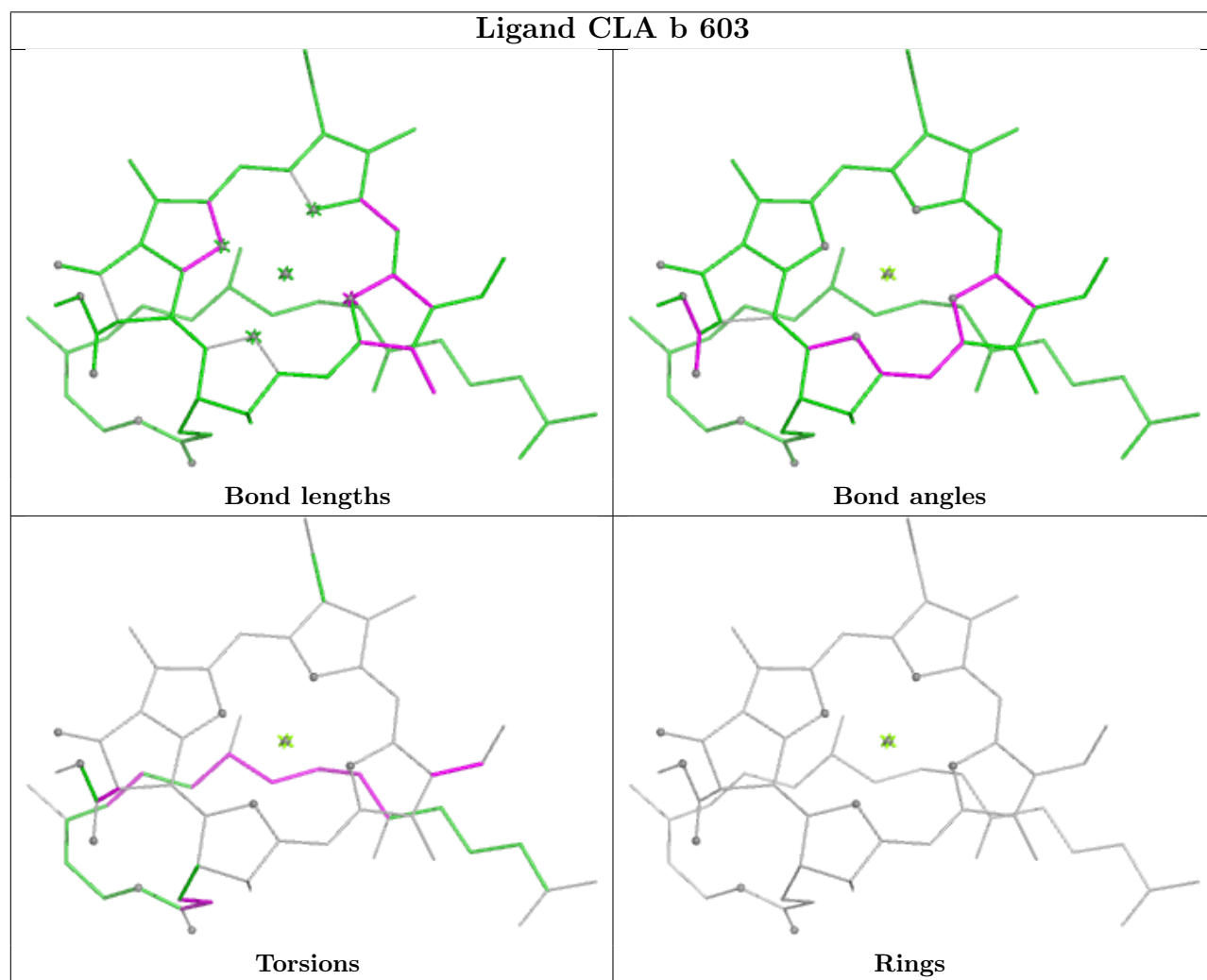
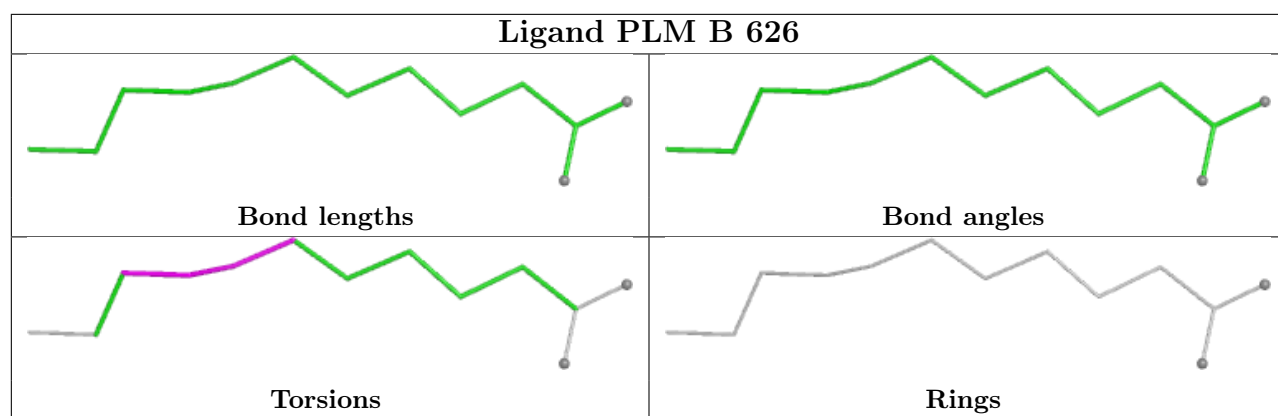


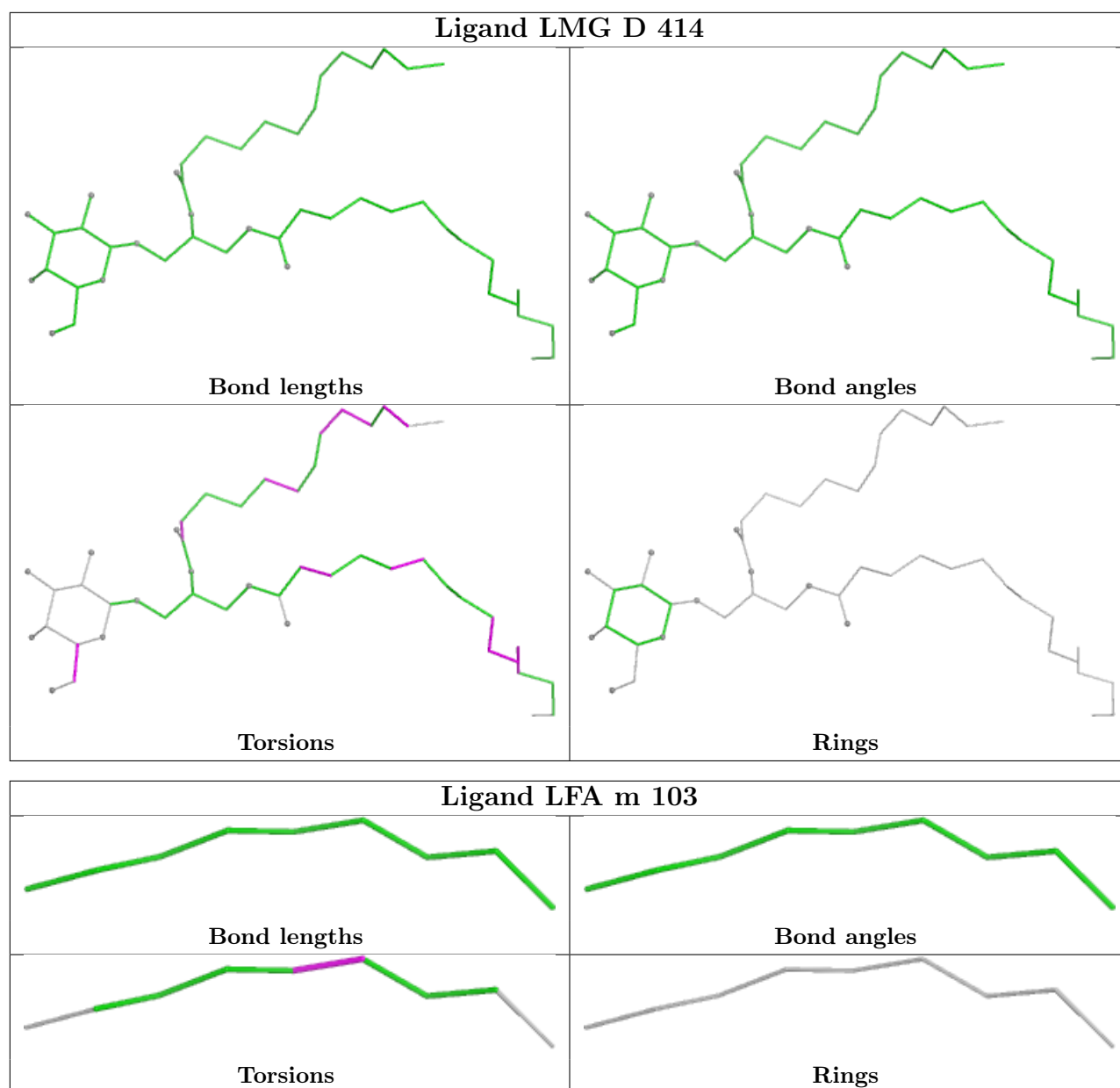


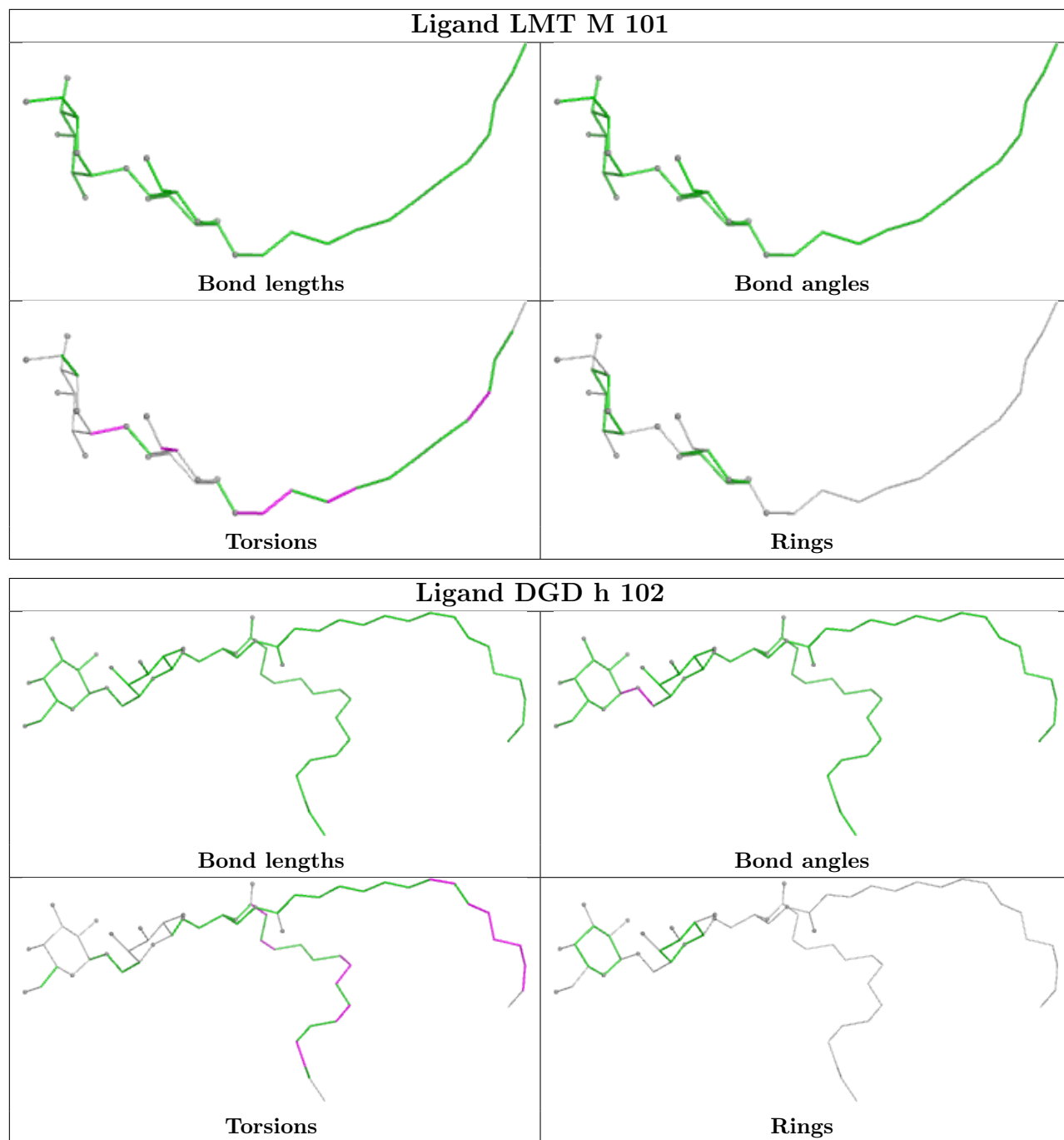


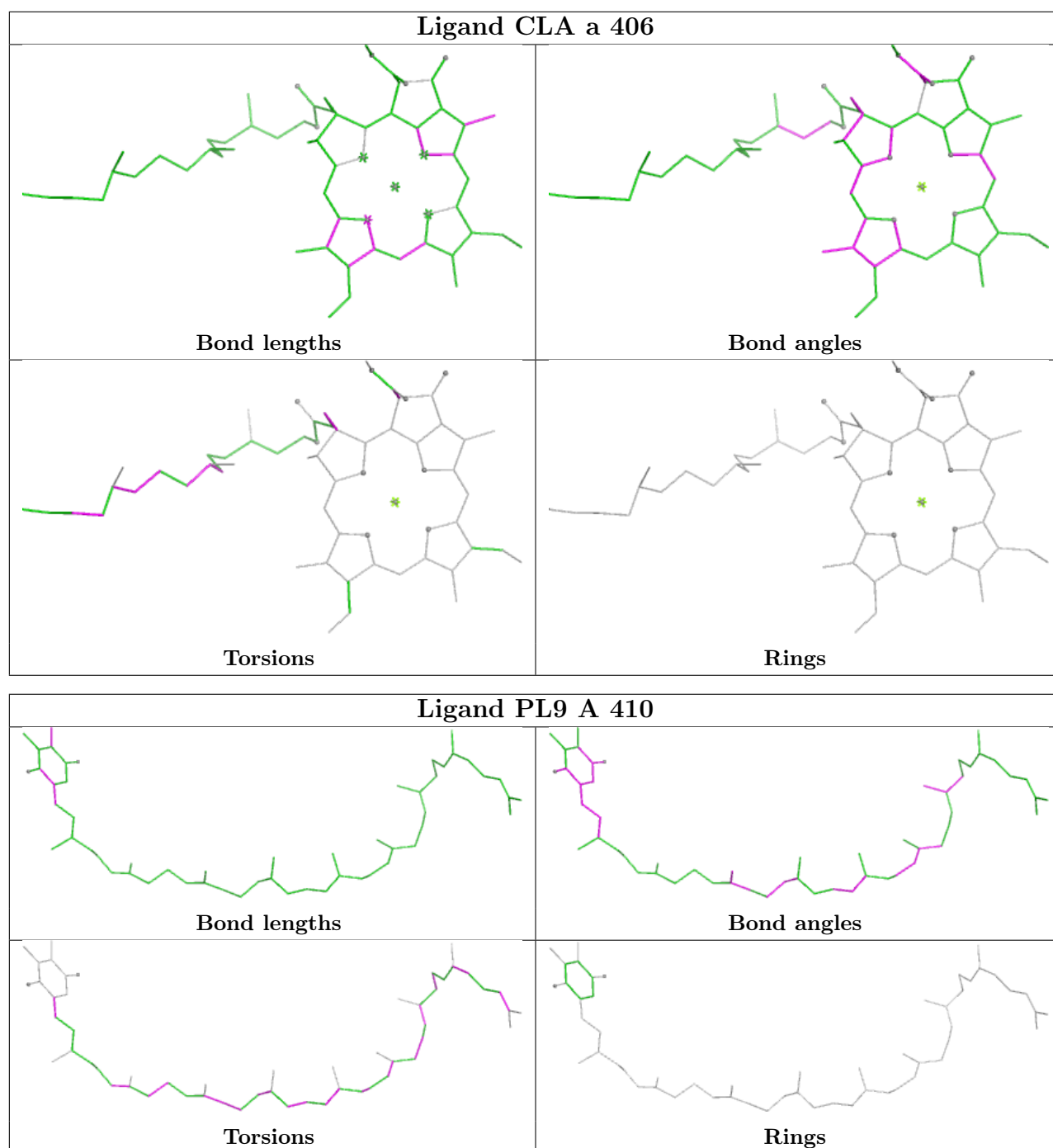


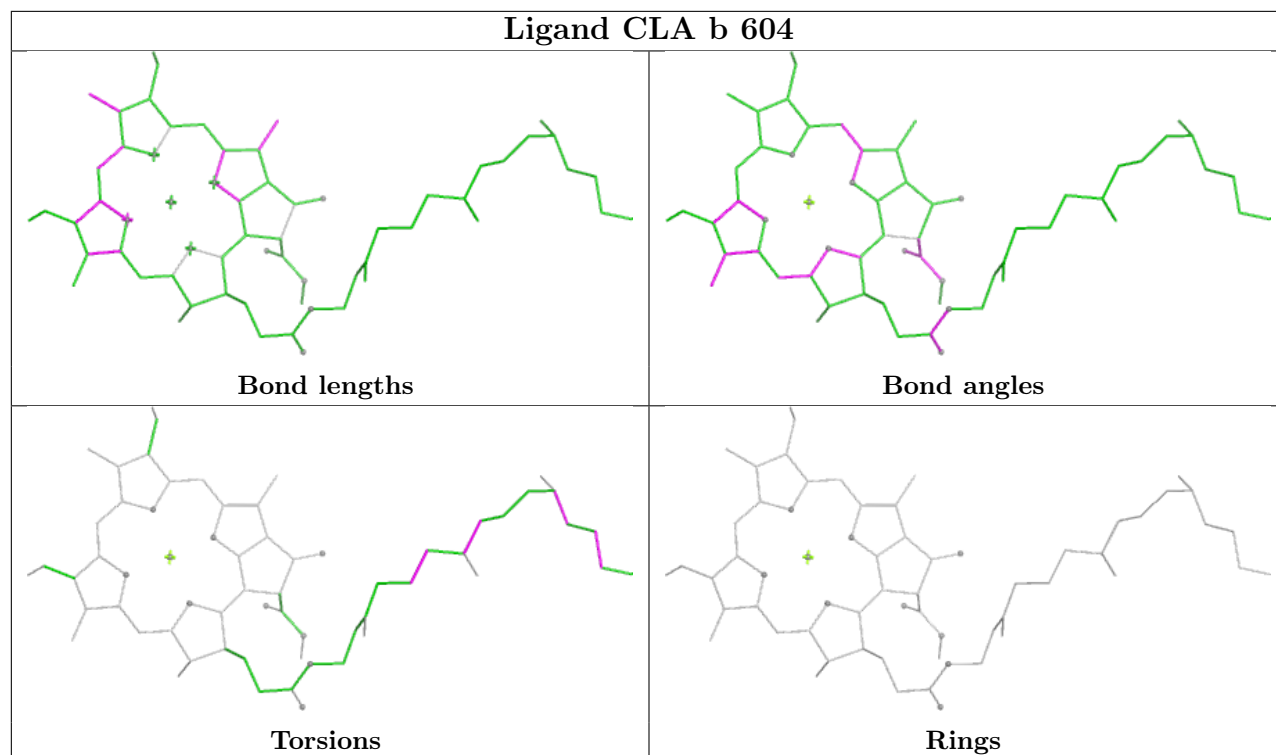
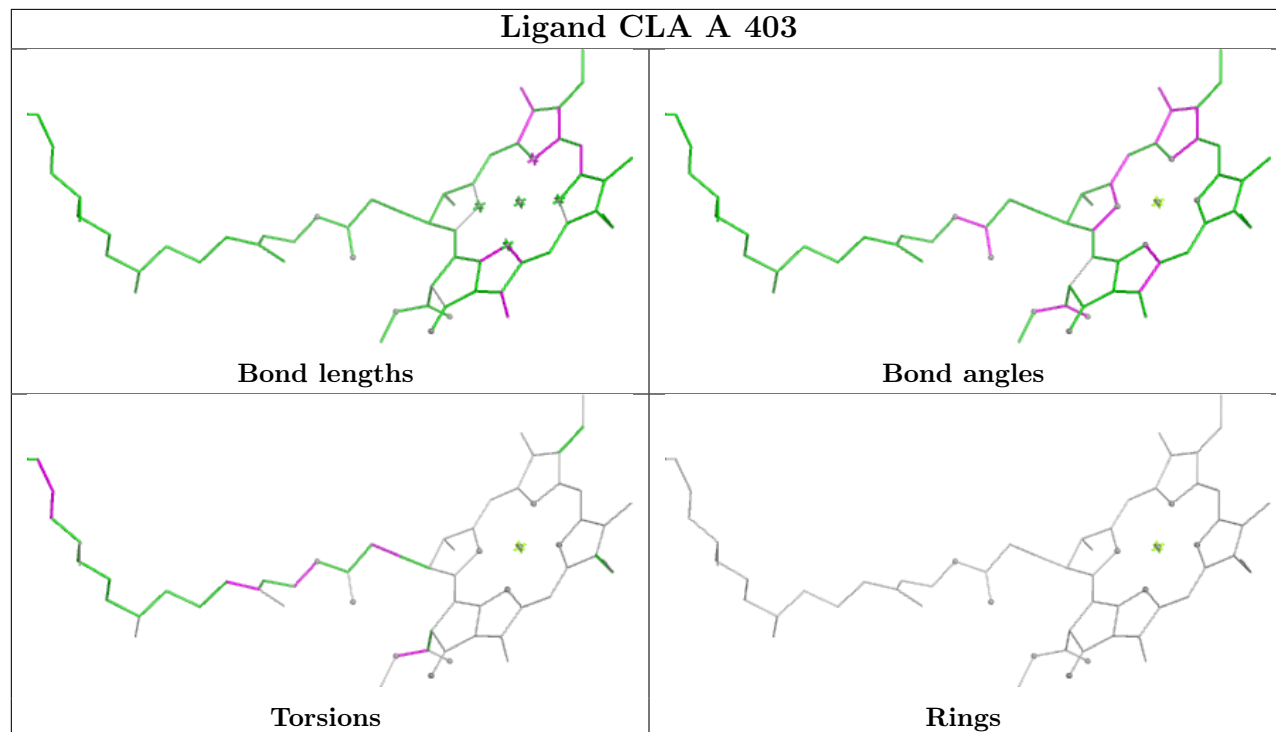


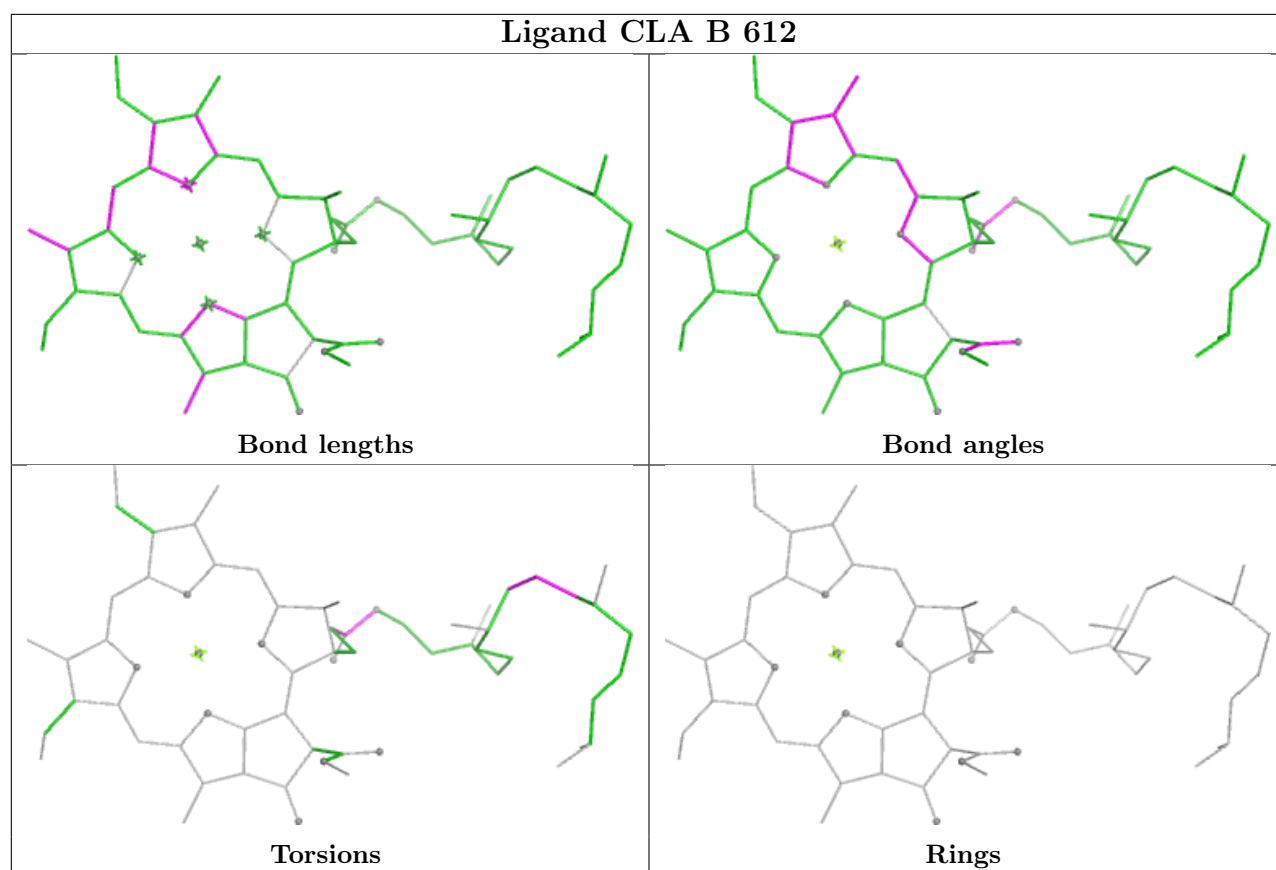




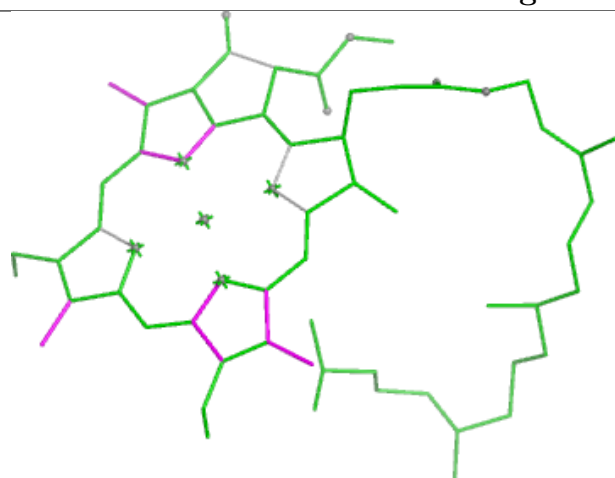




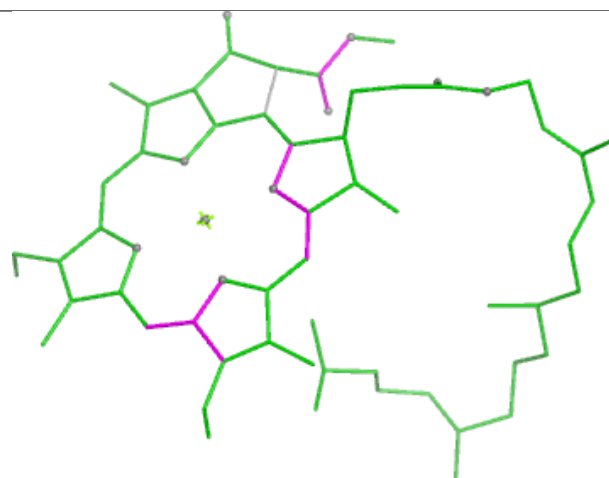
Ligand CLA b 604**Ligand CLA A 403**



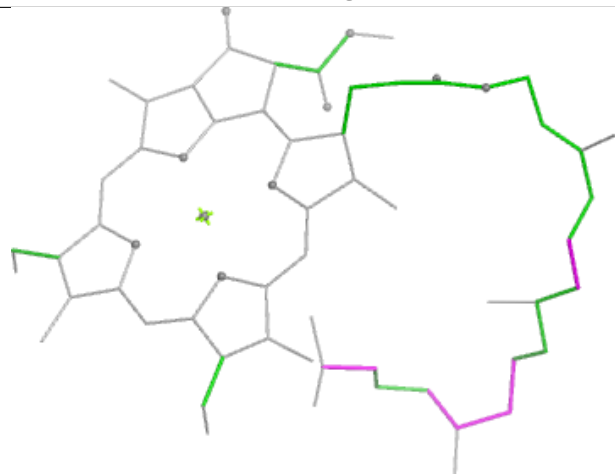
Ligand CLA b 617



Bond lengths



Bond angles

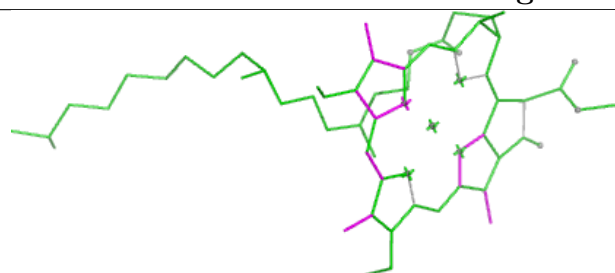


Torsions

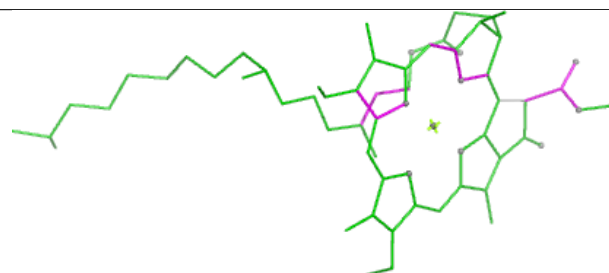


Rings

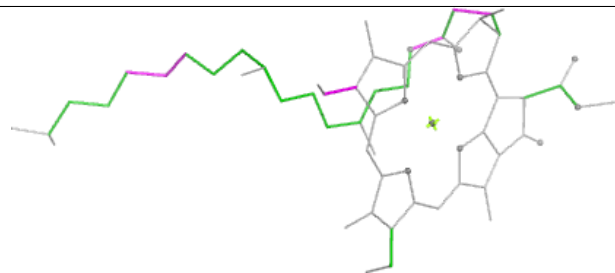
Ligand CLA C 507



Bond lengths



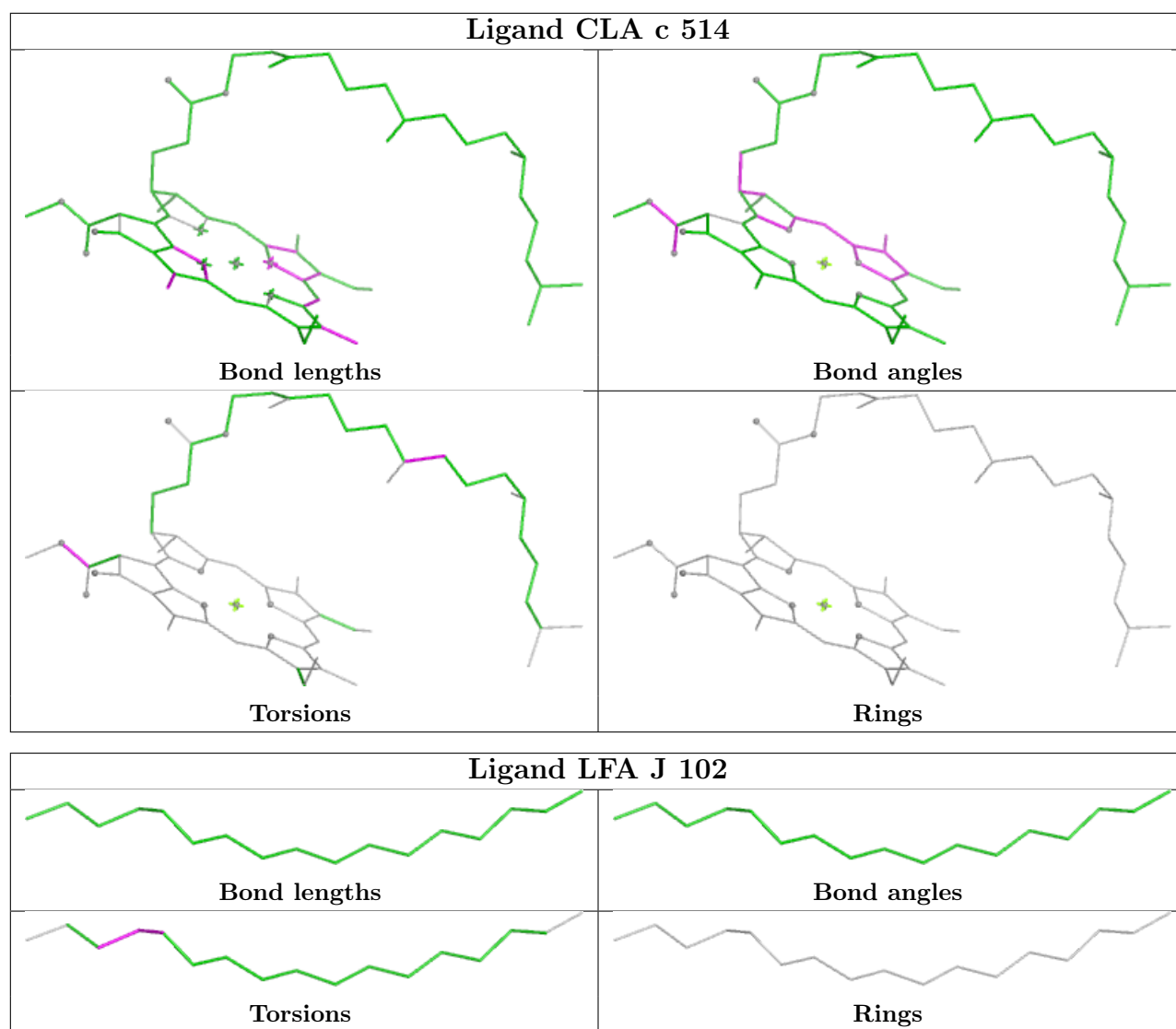
Bond angles

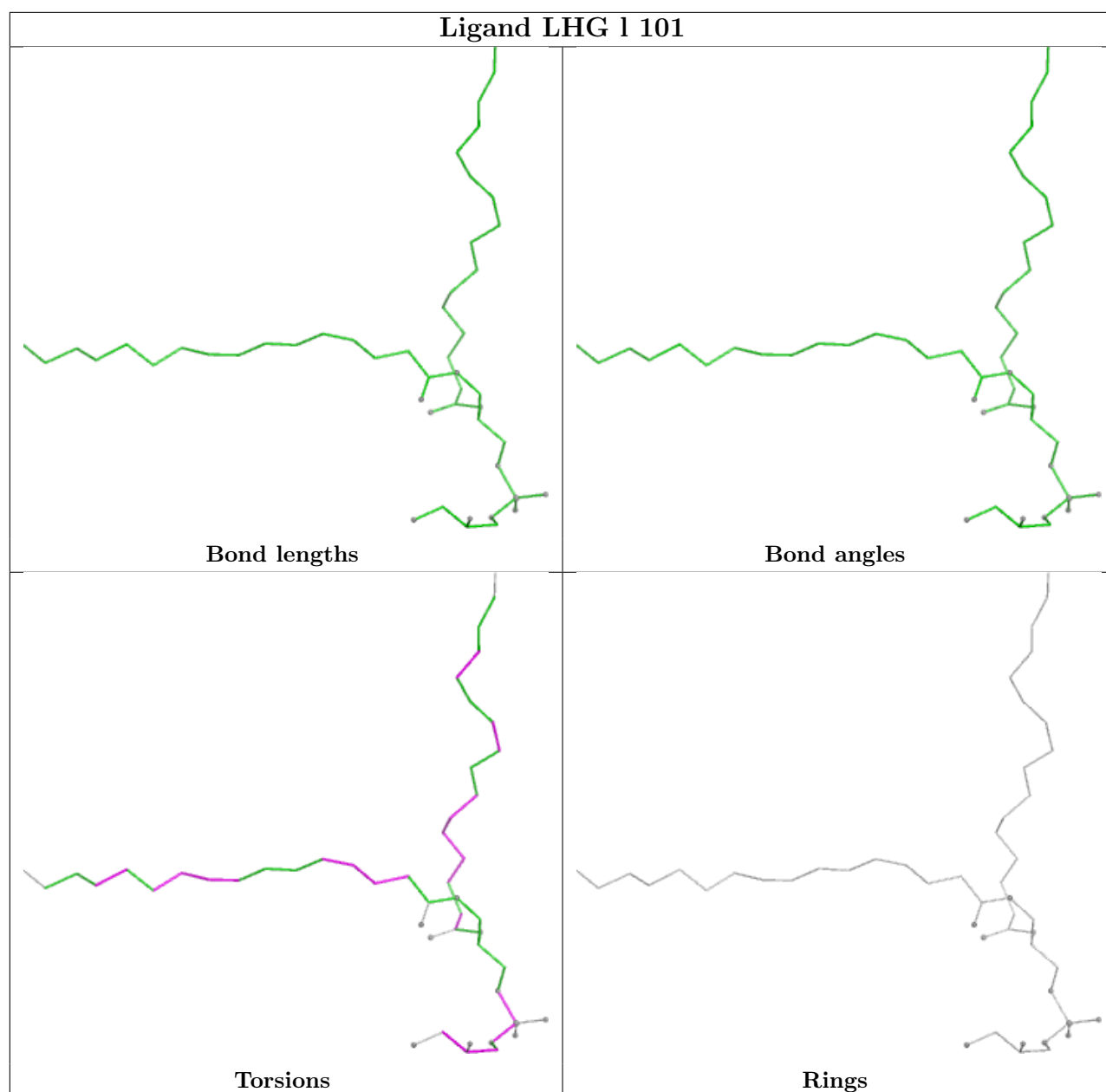


Torsions

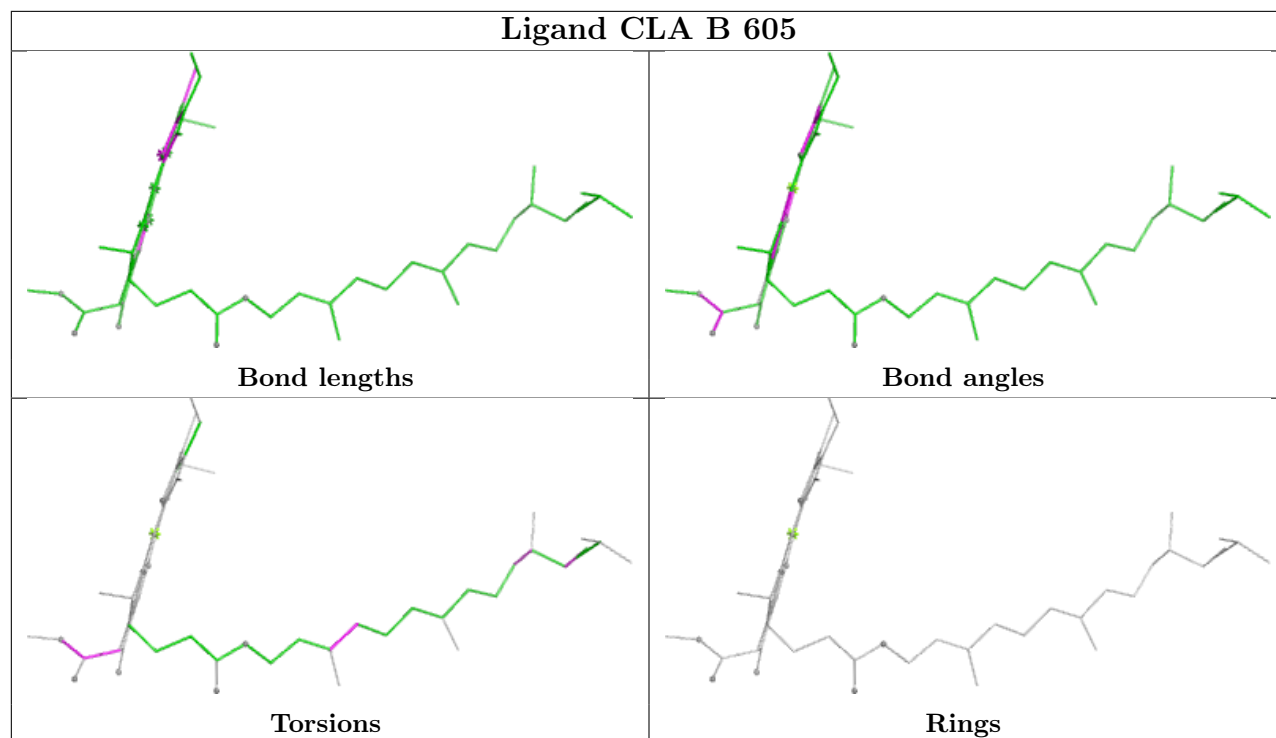


Rings

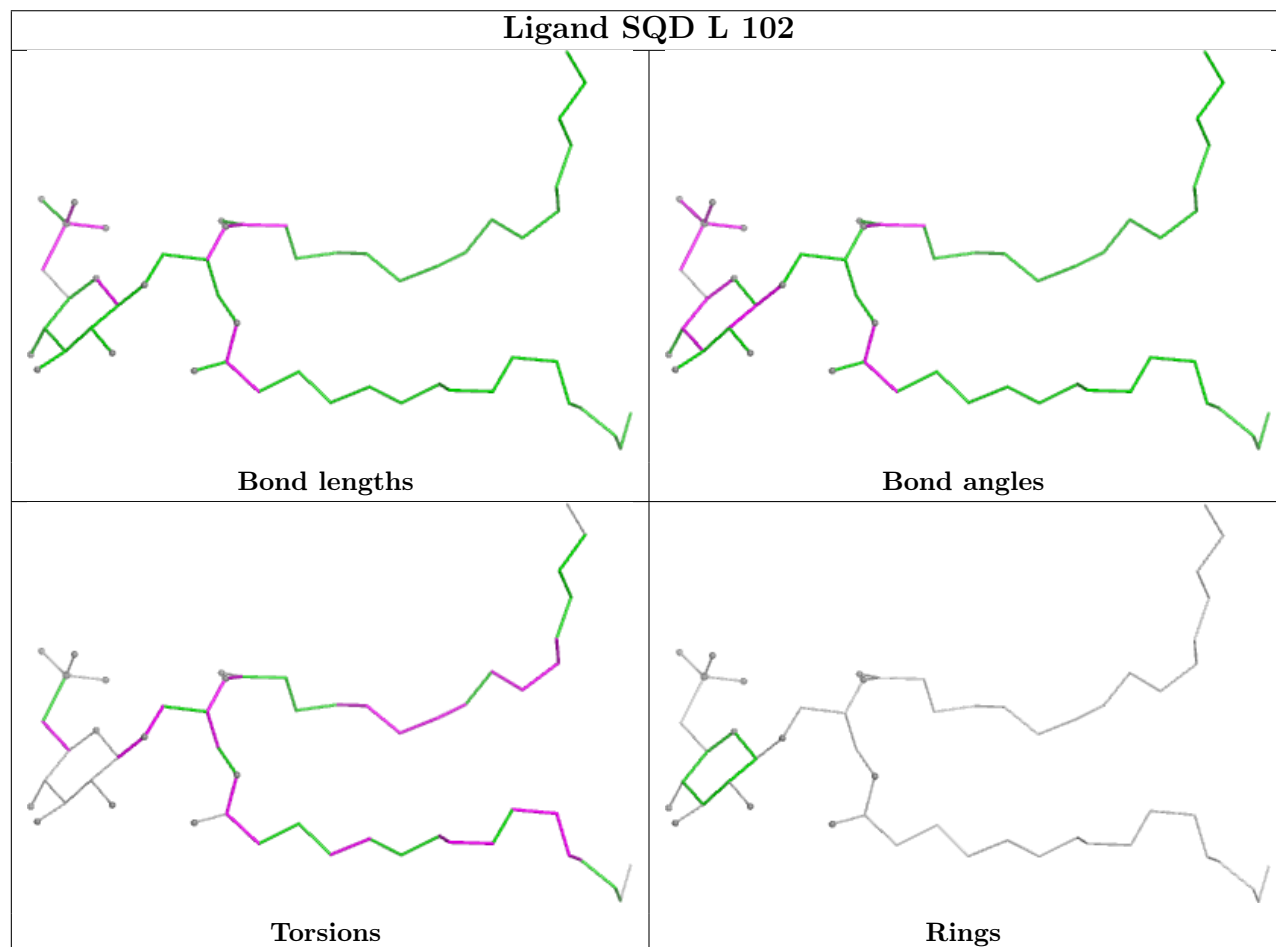


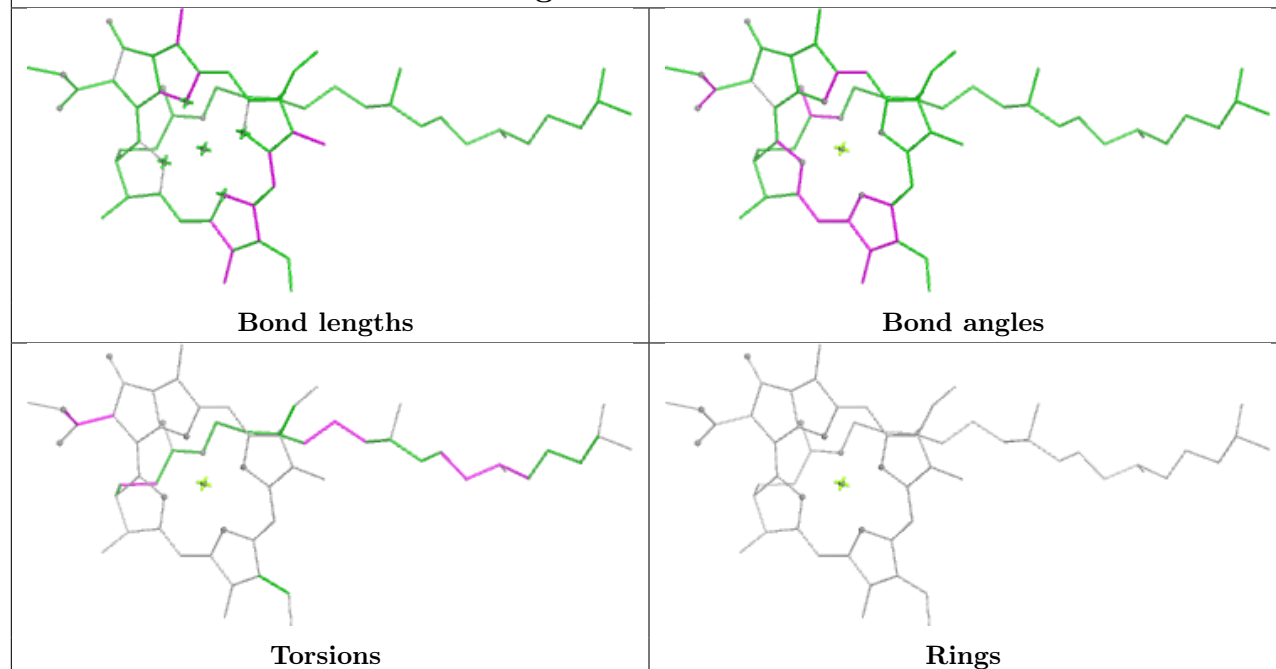
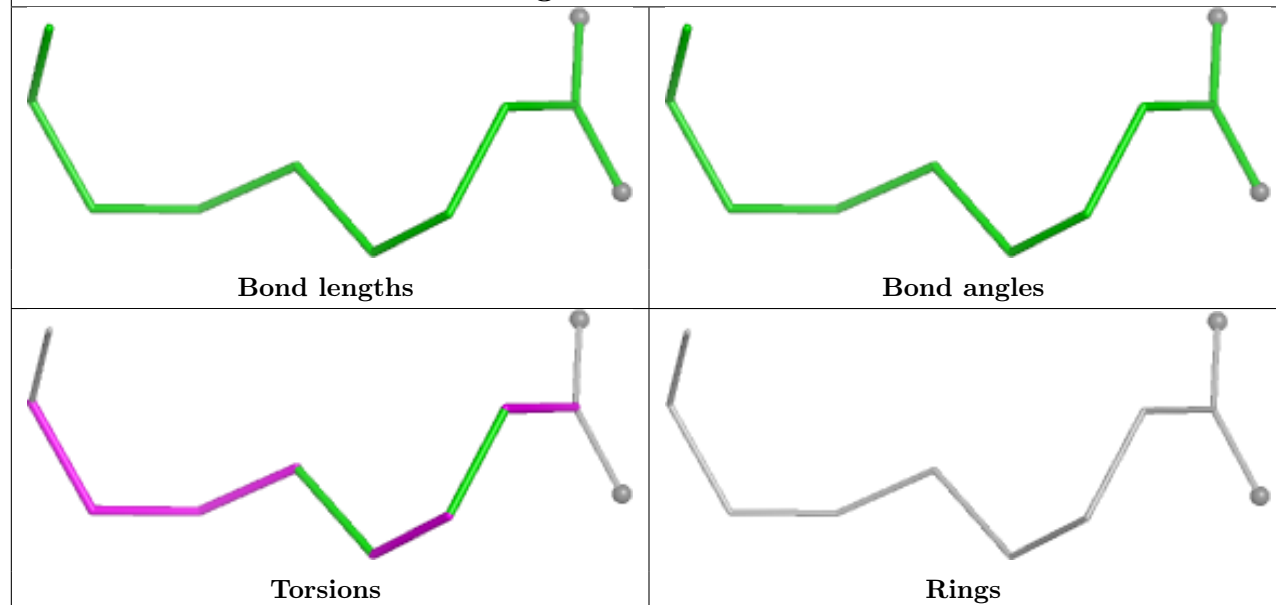


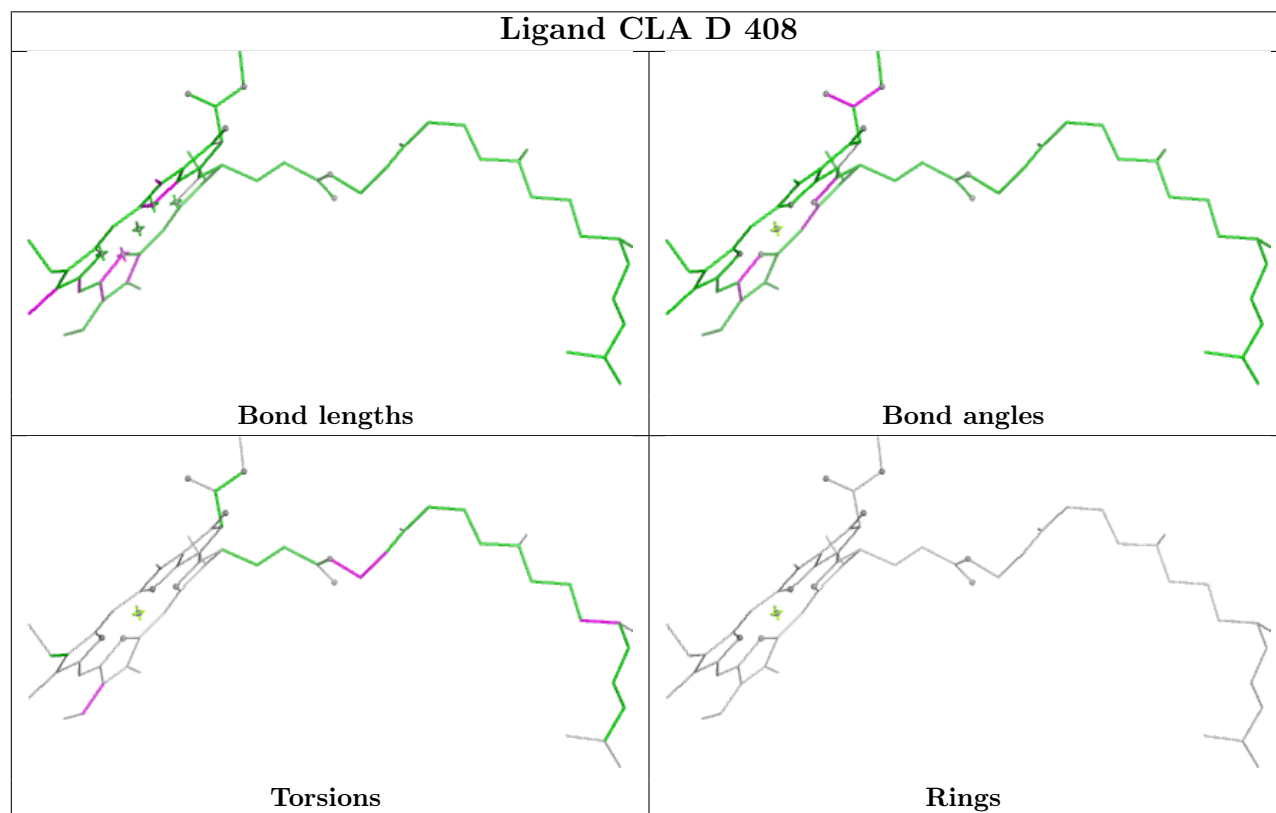
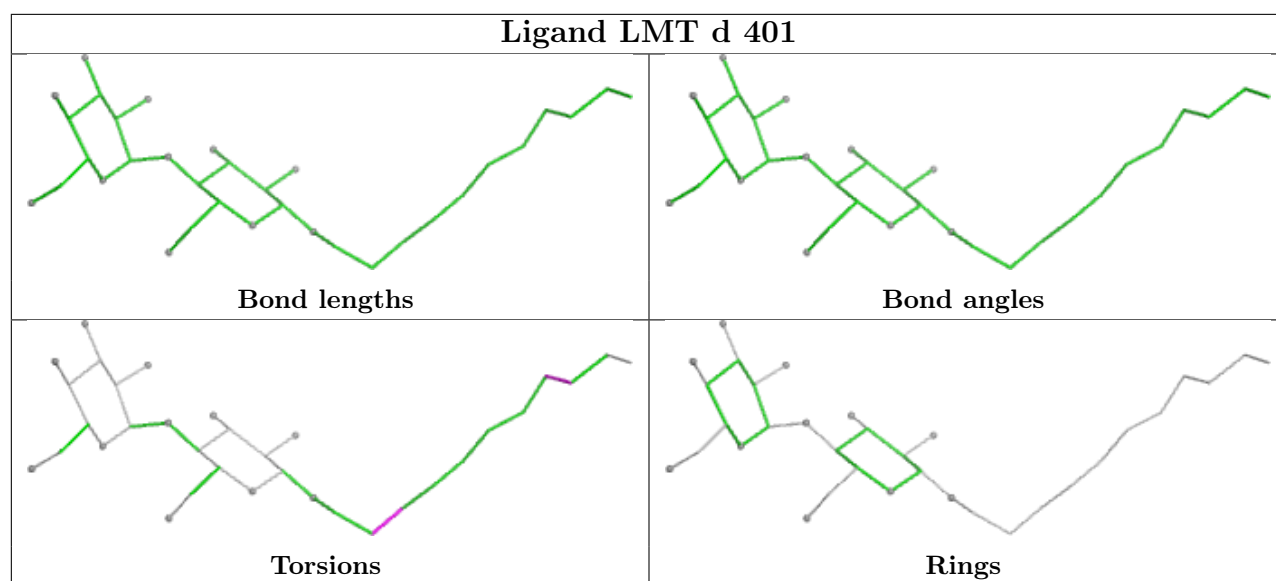
Ligand CLA B 605

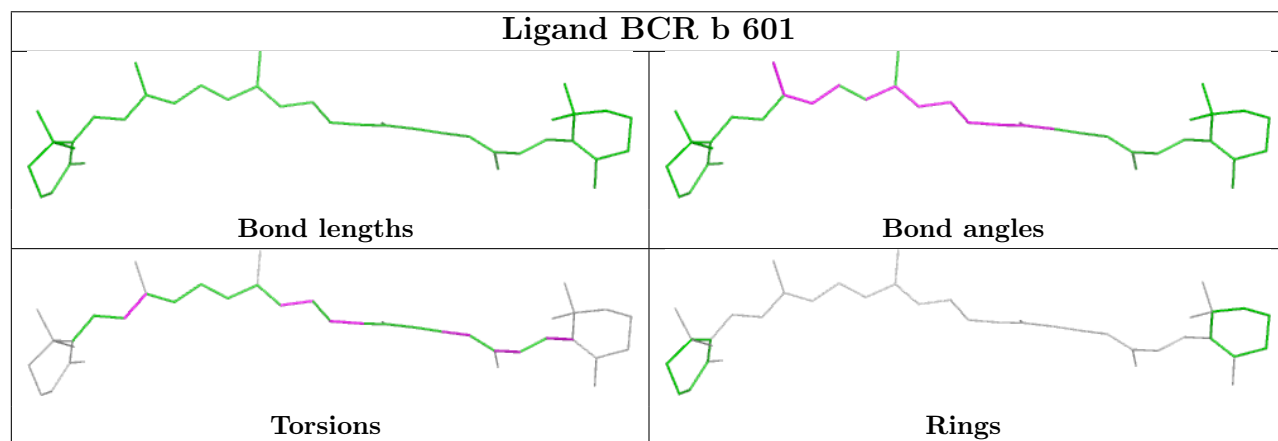
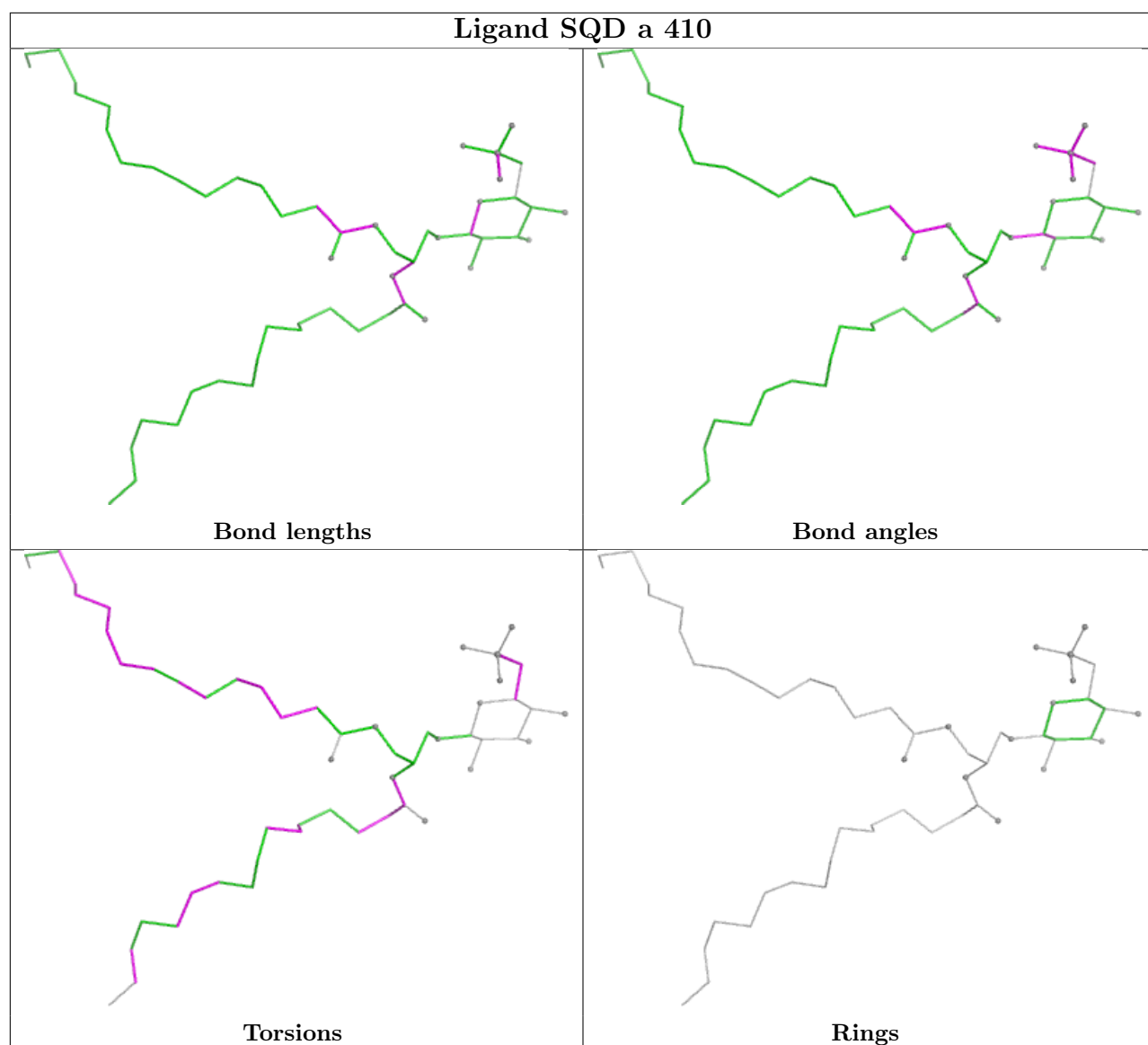


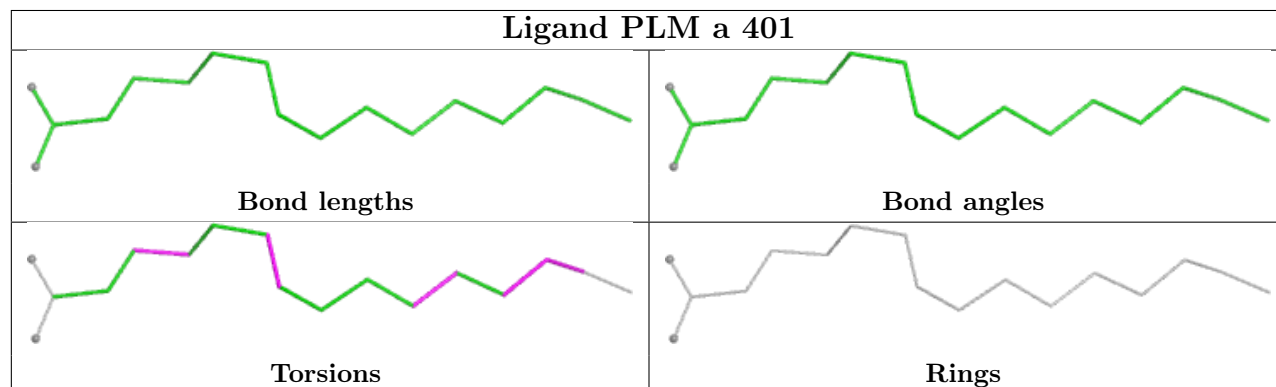
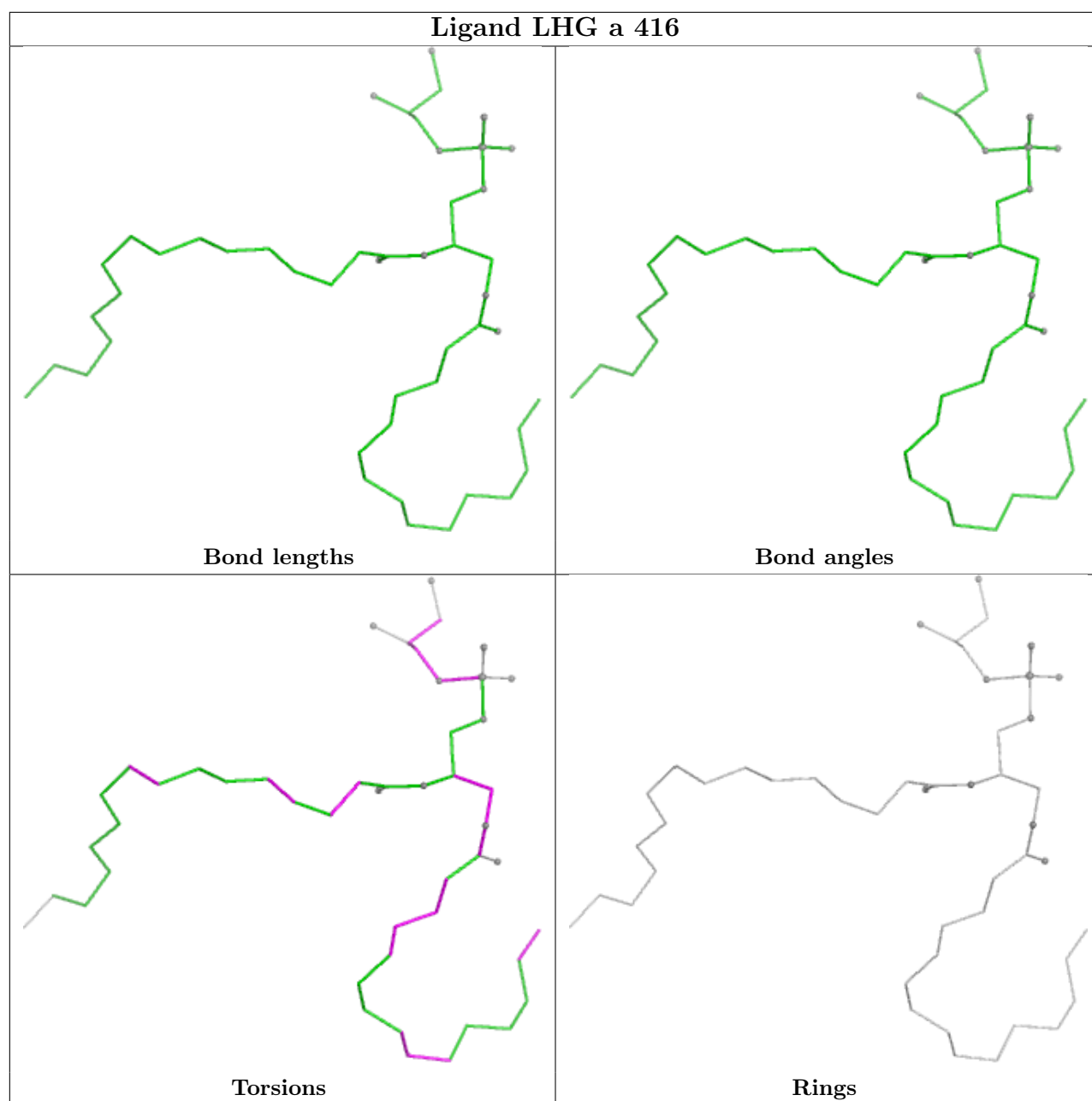
Ligand SQD L 102

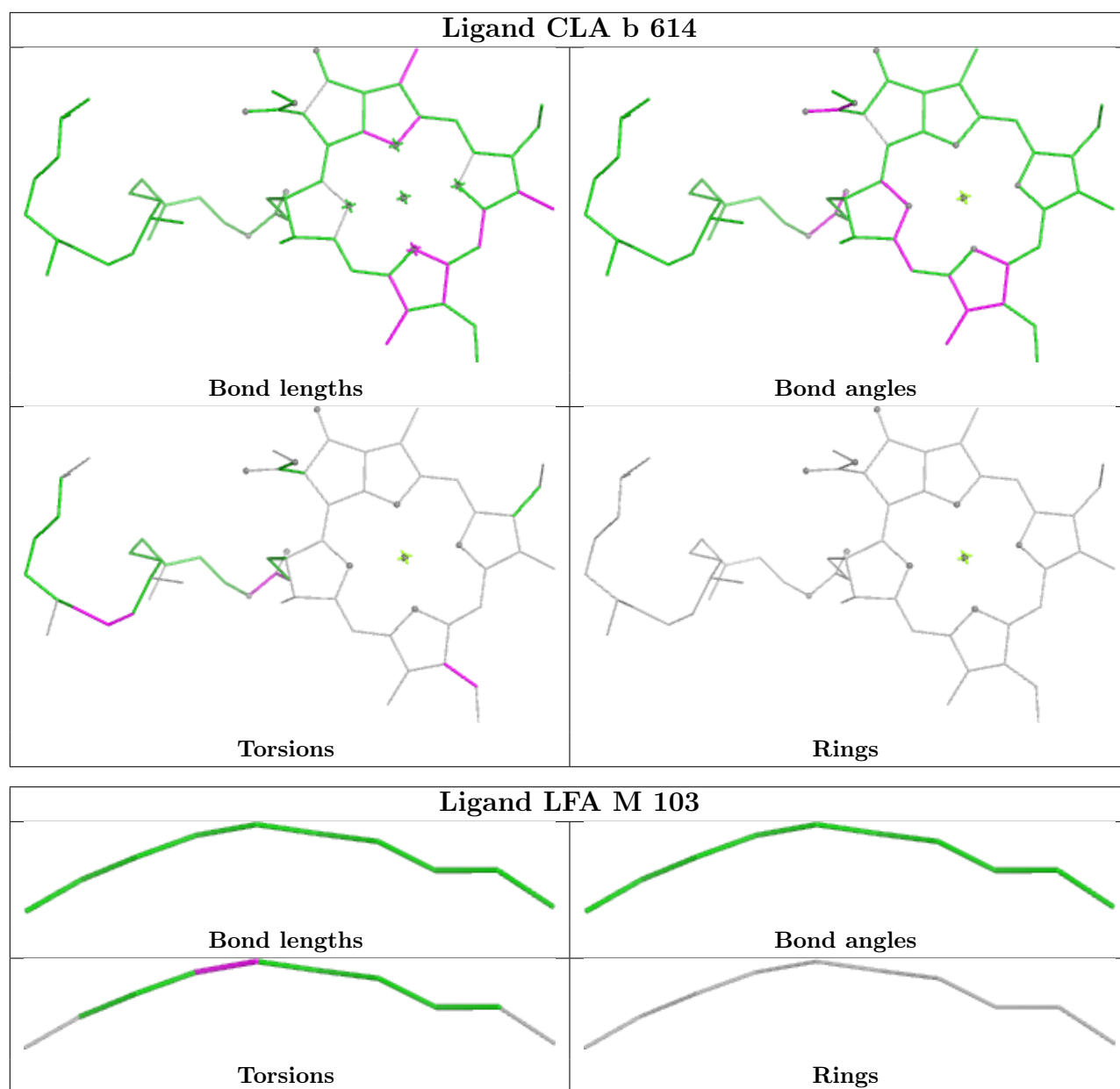


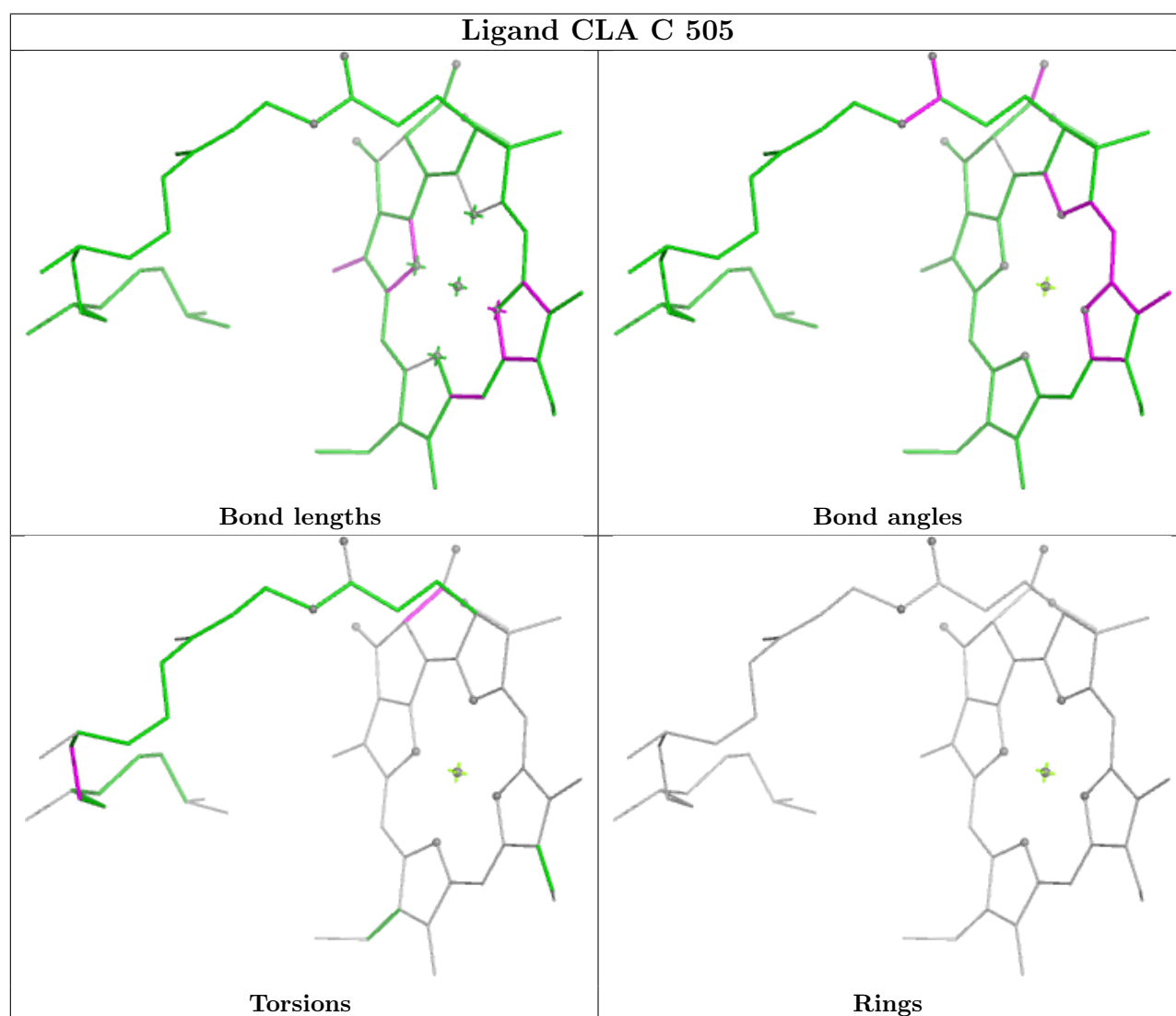
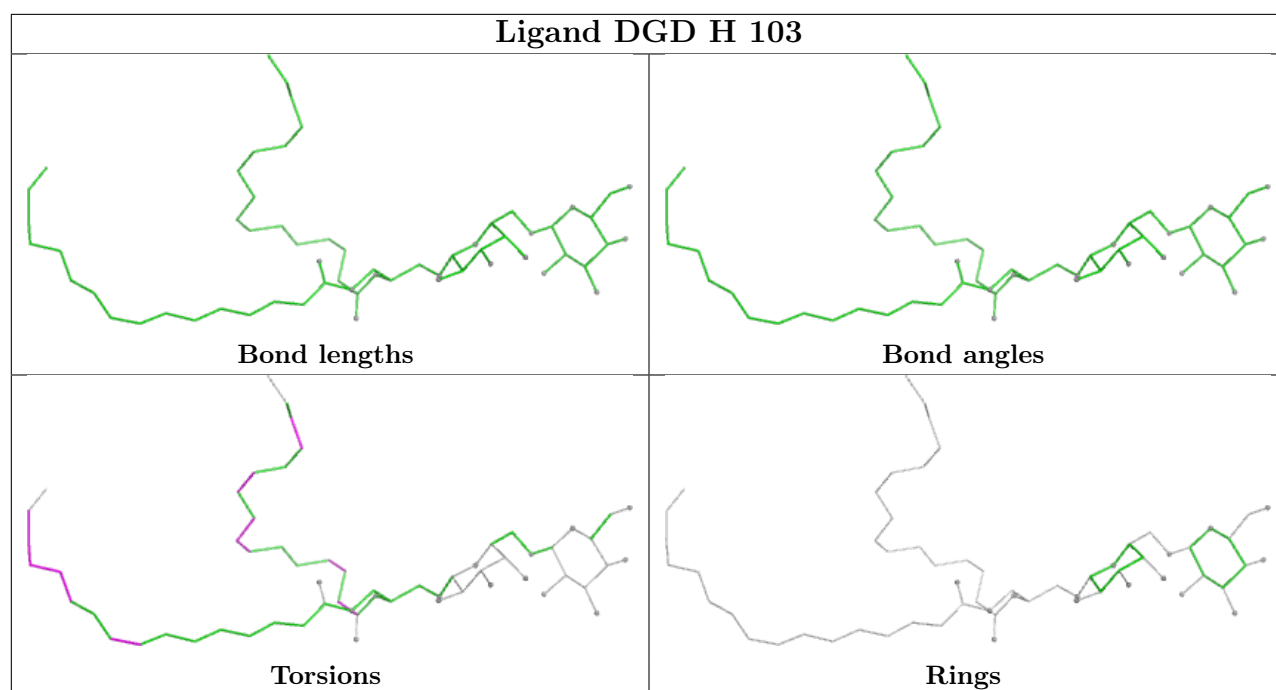
Ligand CLA b 616**Ligand PLM I 104**

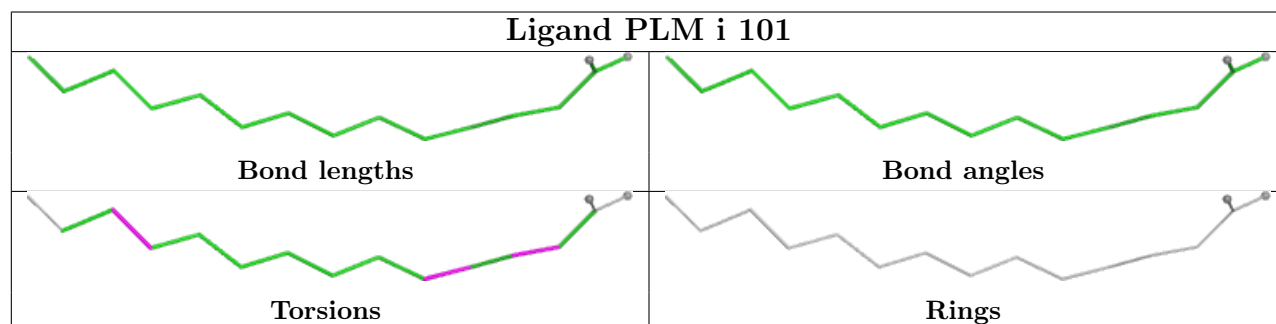
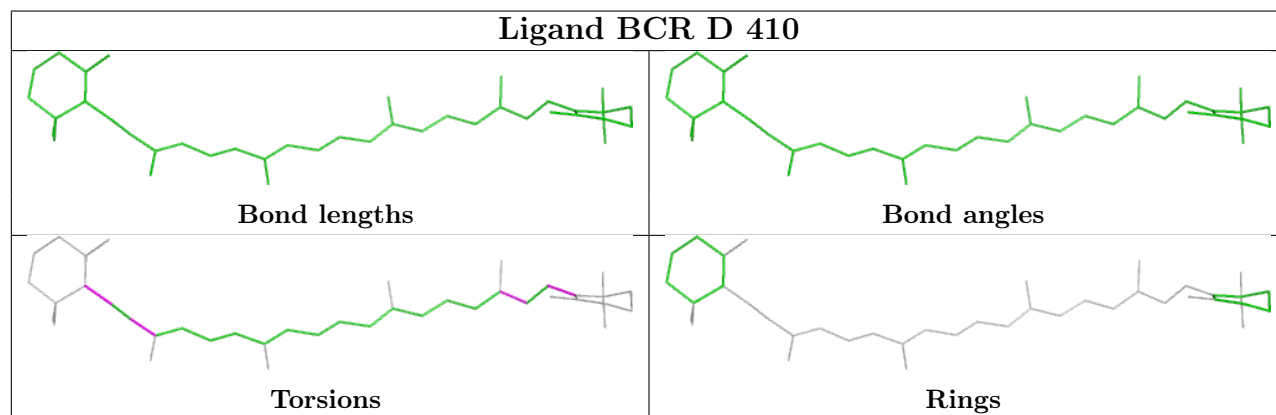
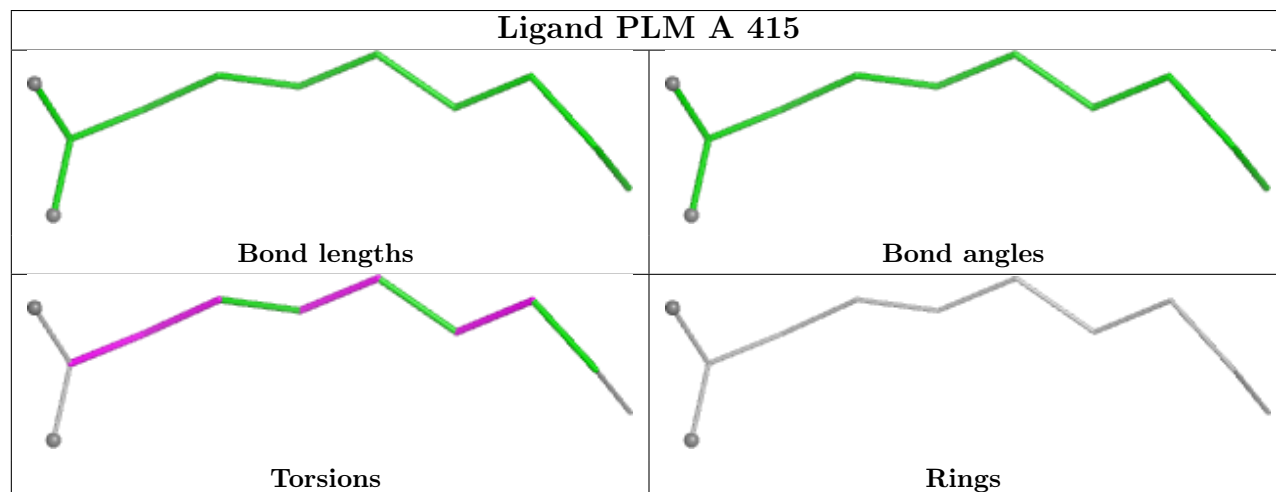
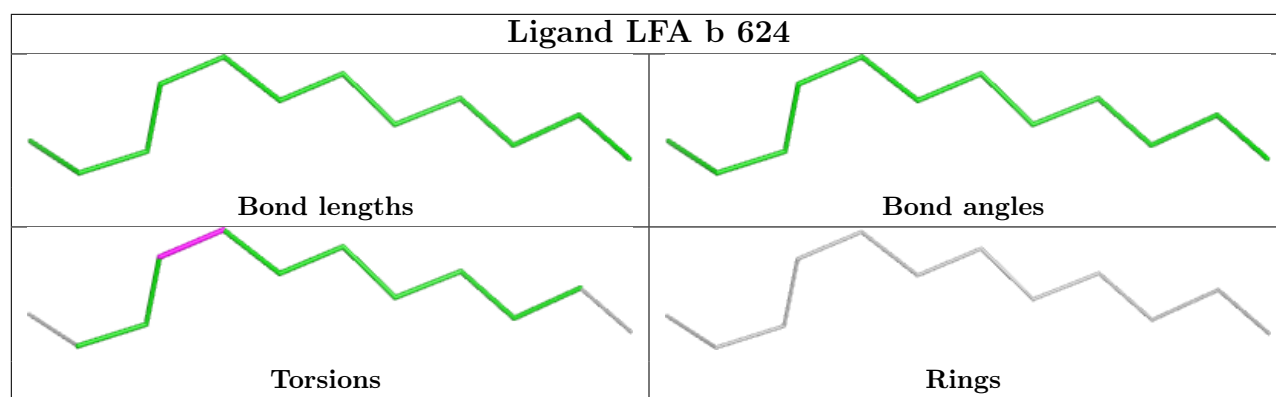


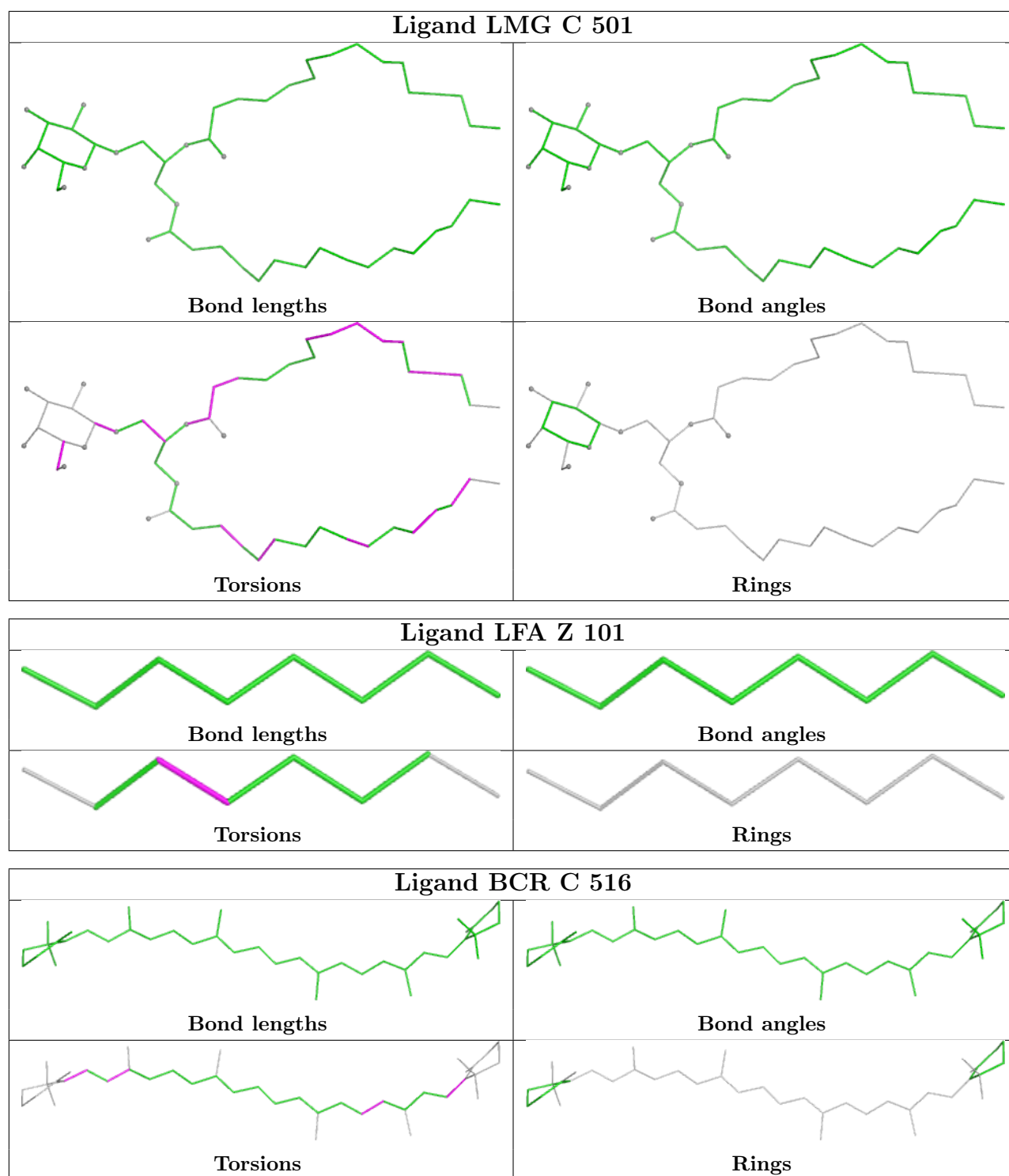


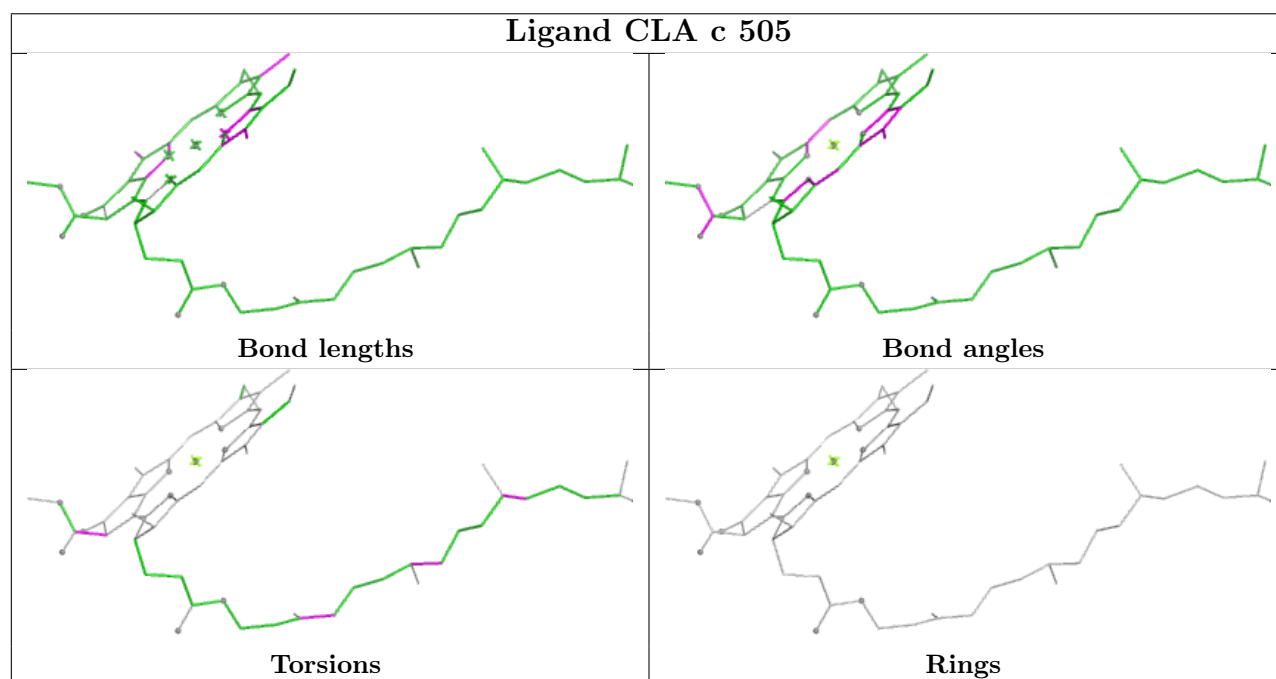
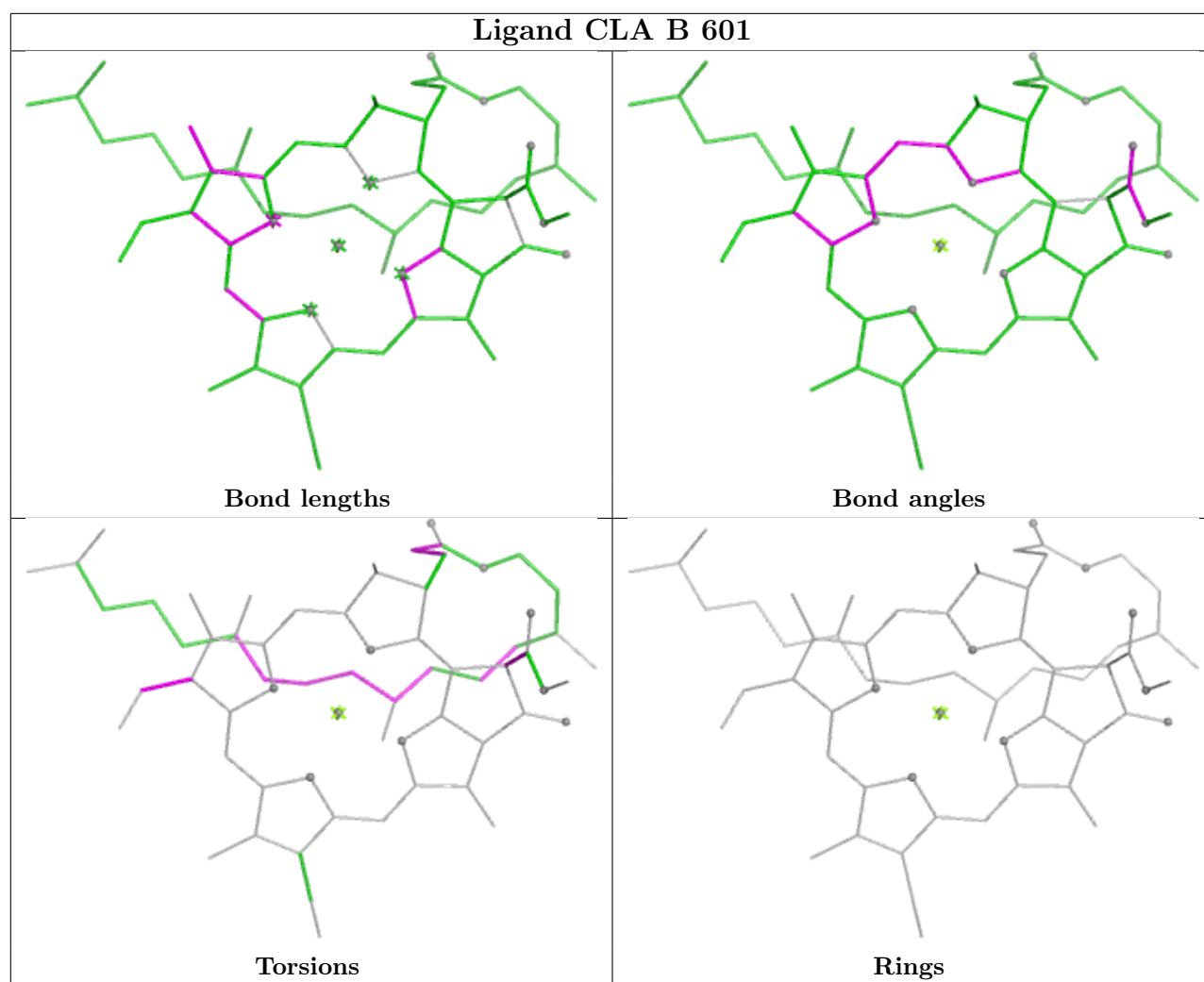


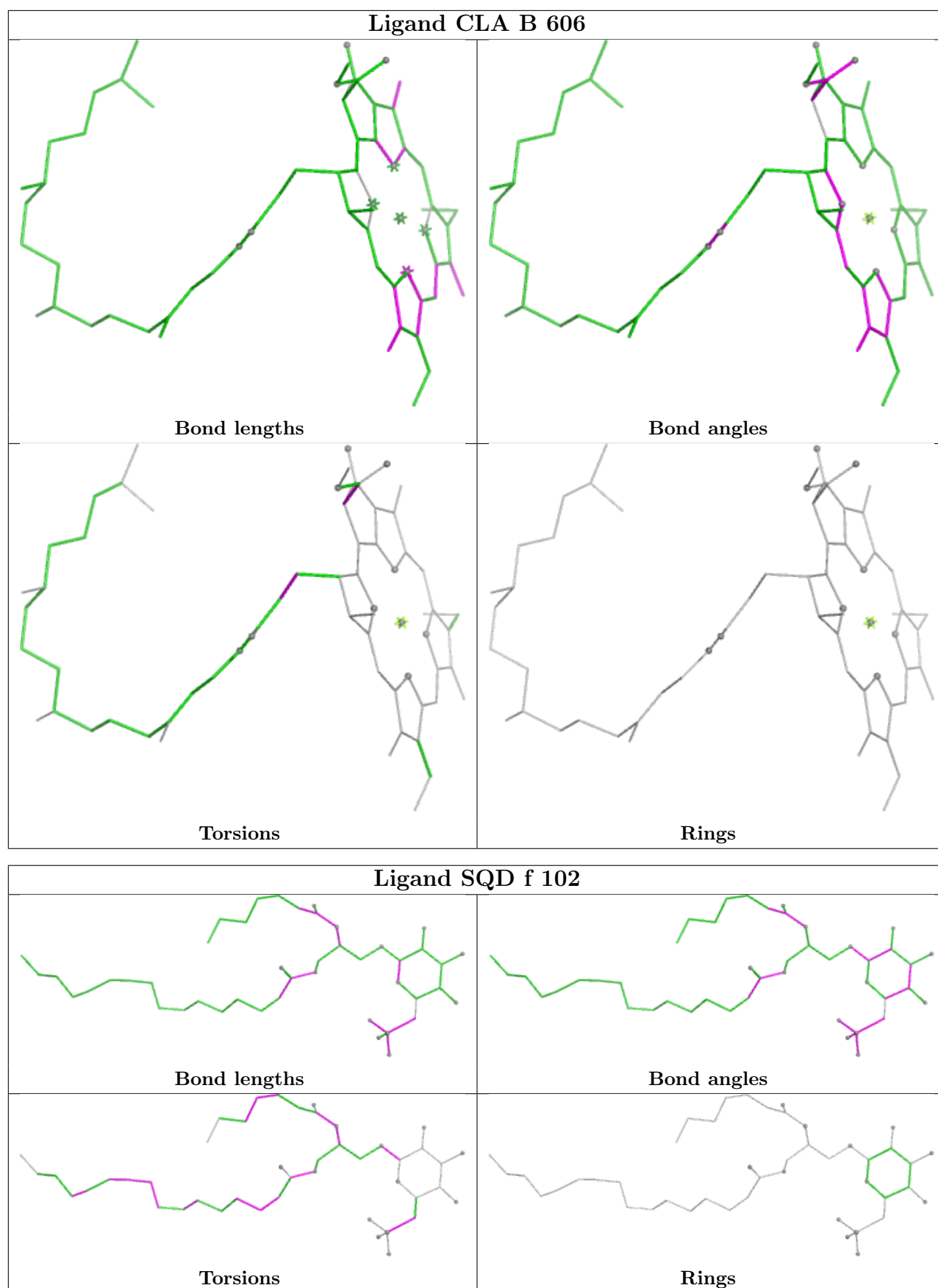




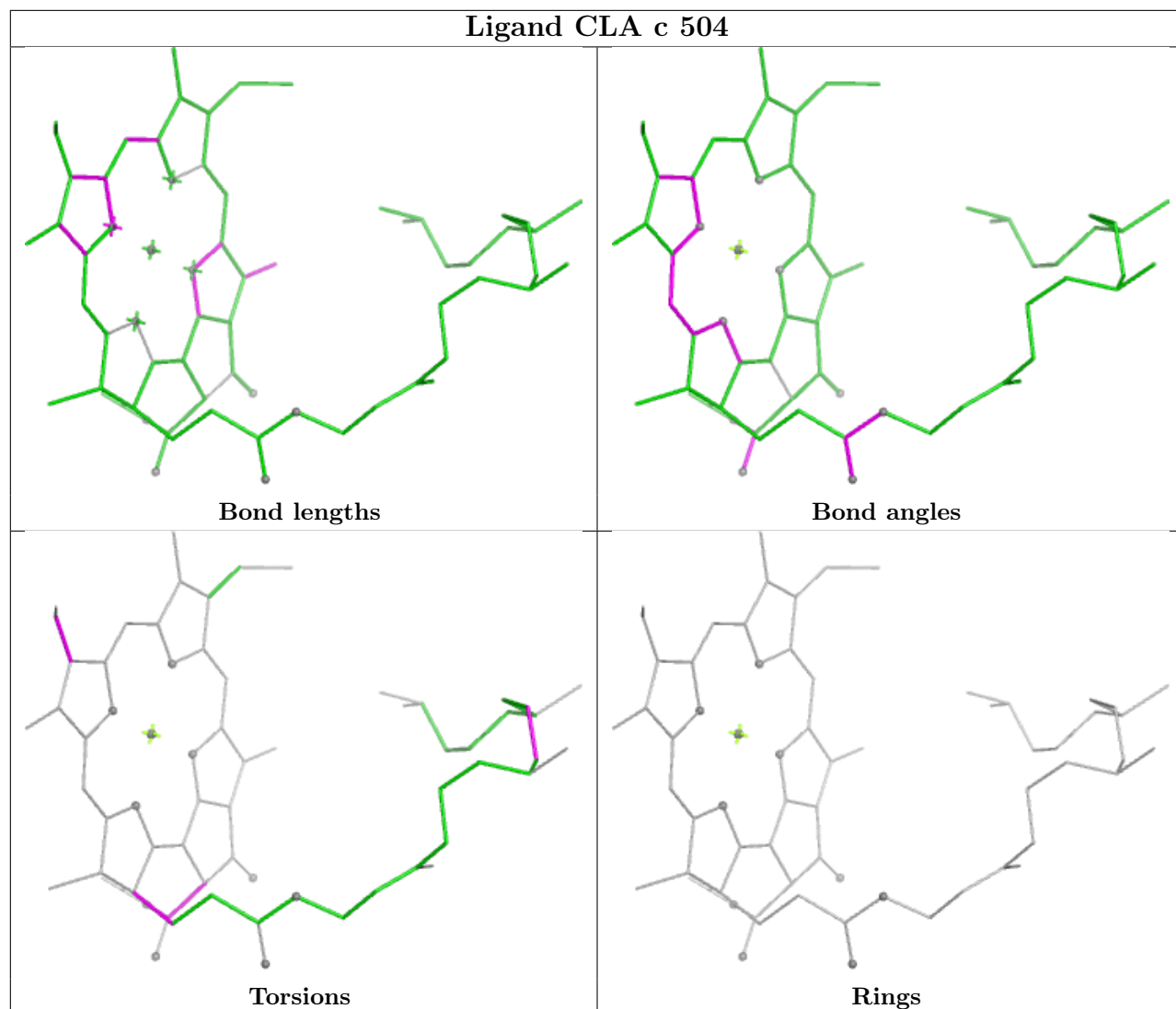


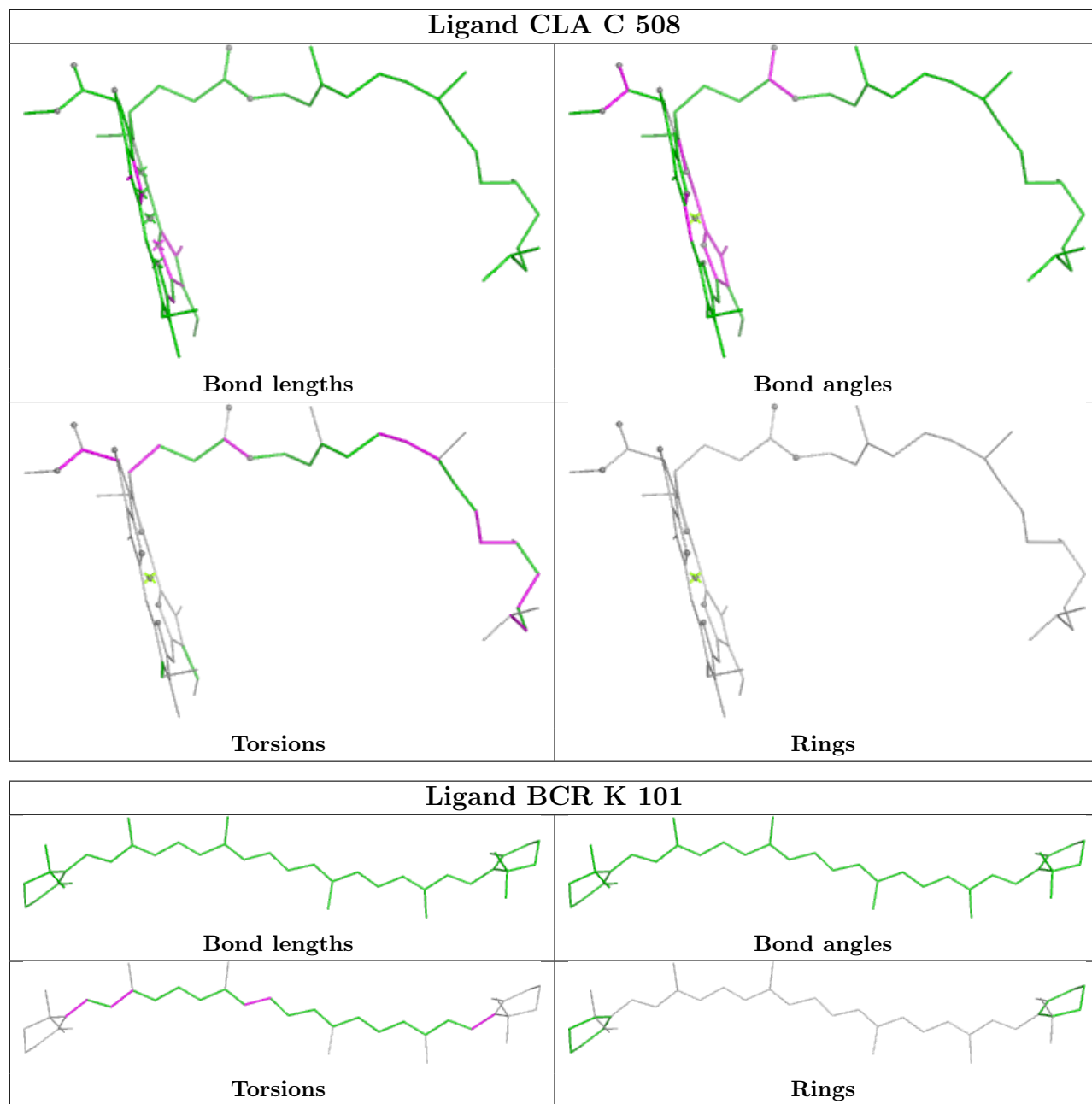


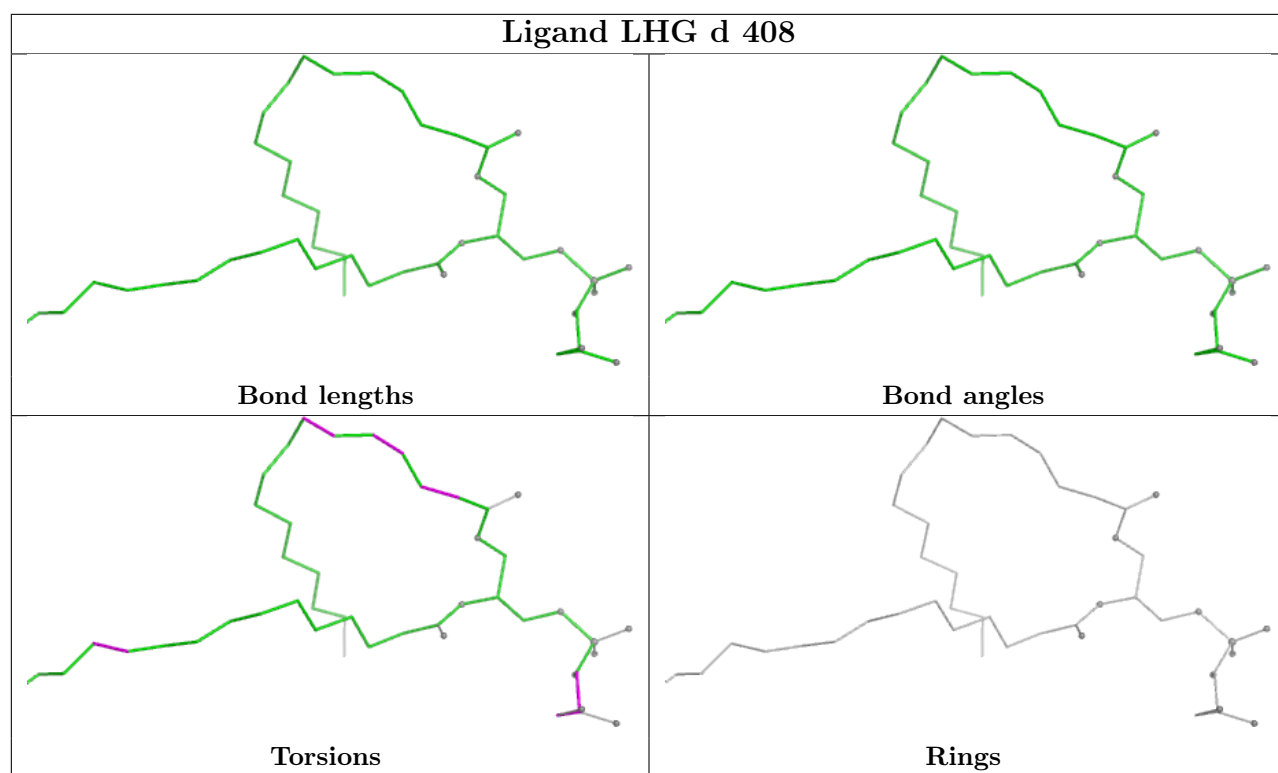


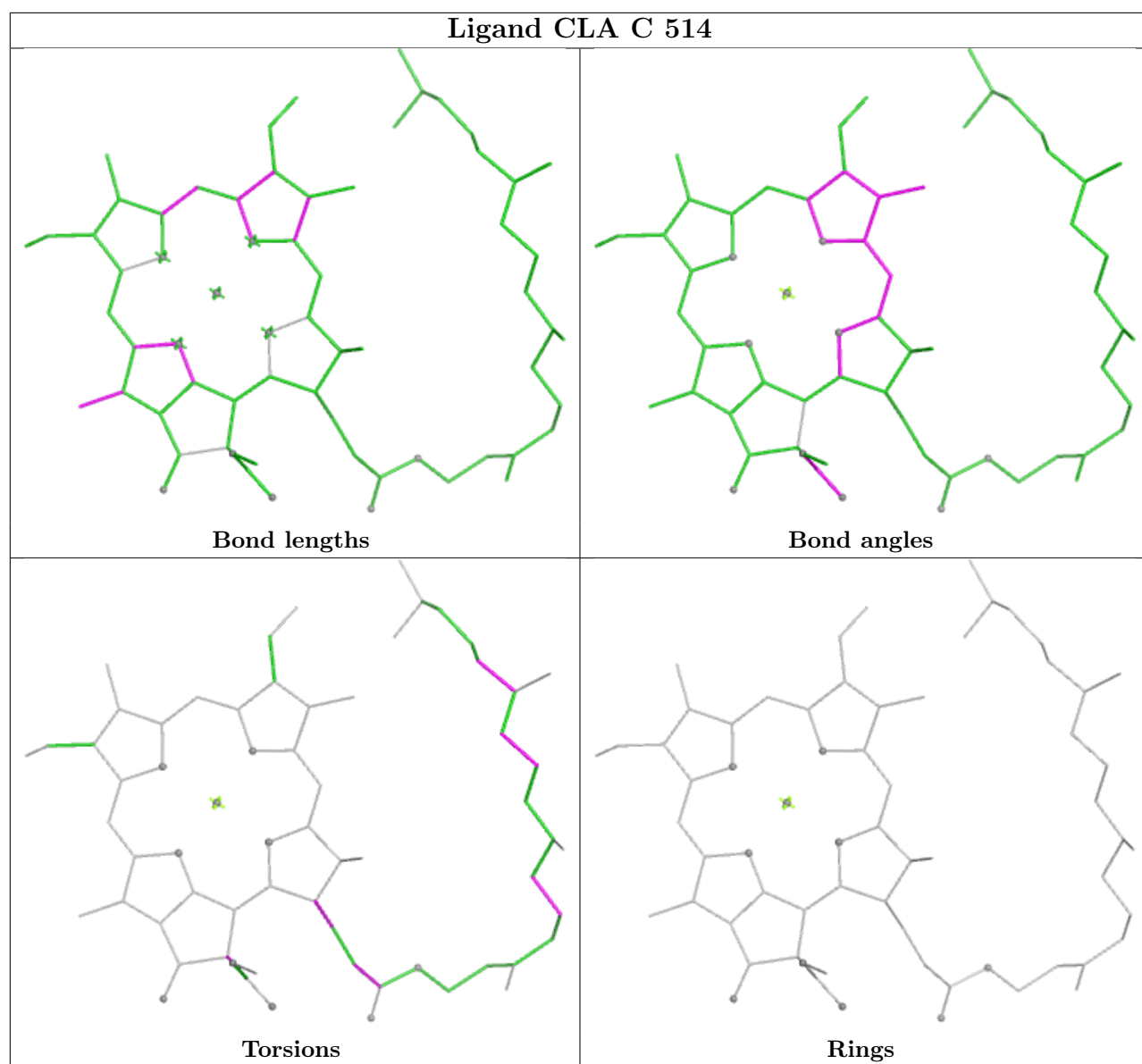


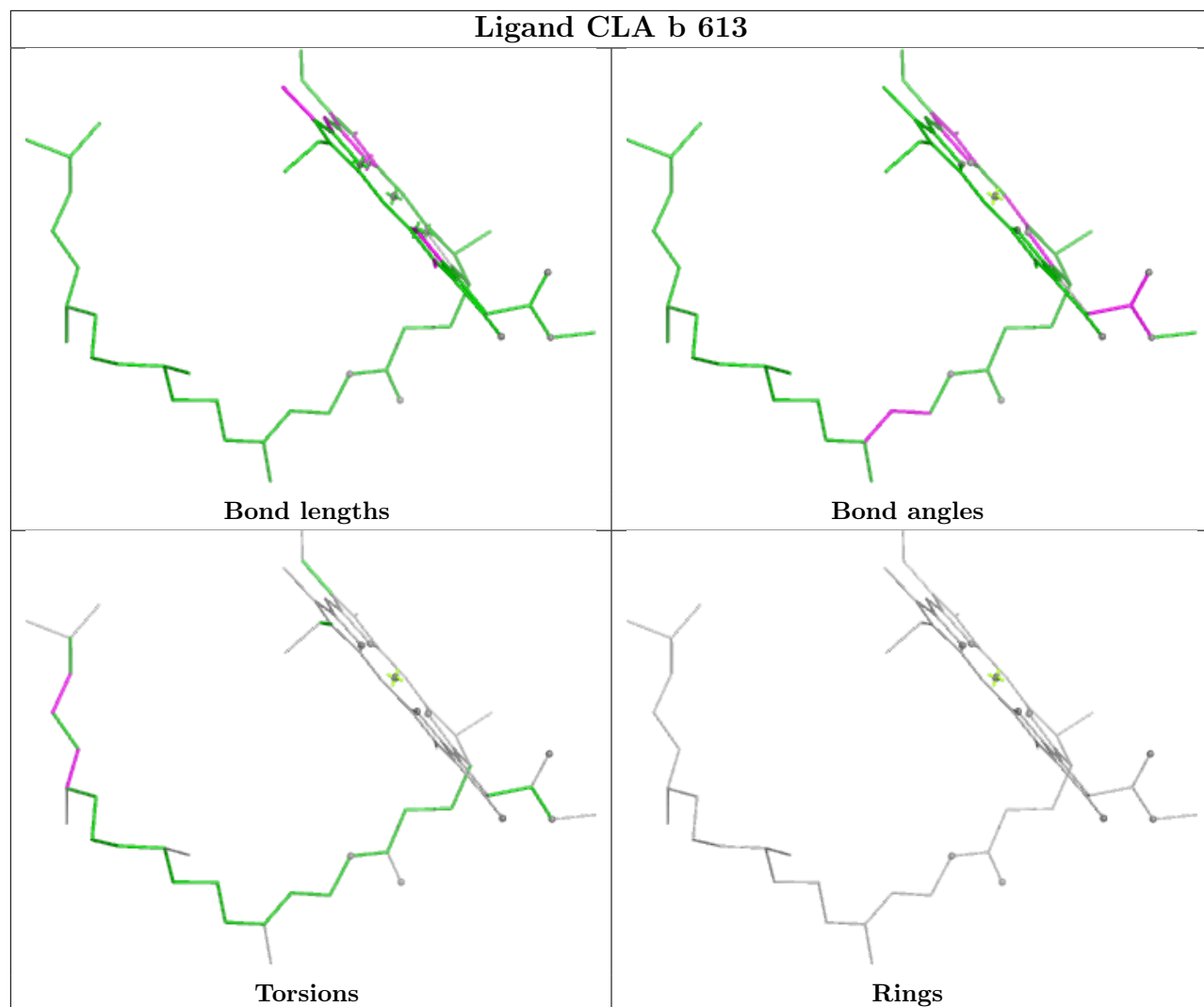
Ligand CLA c 504

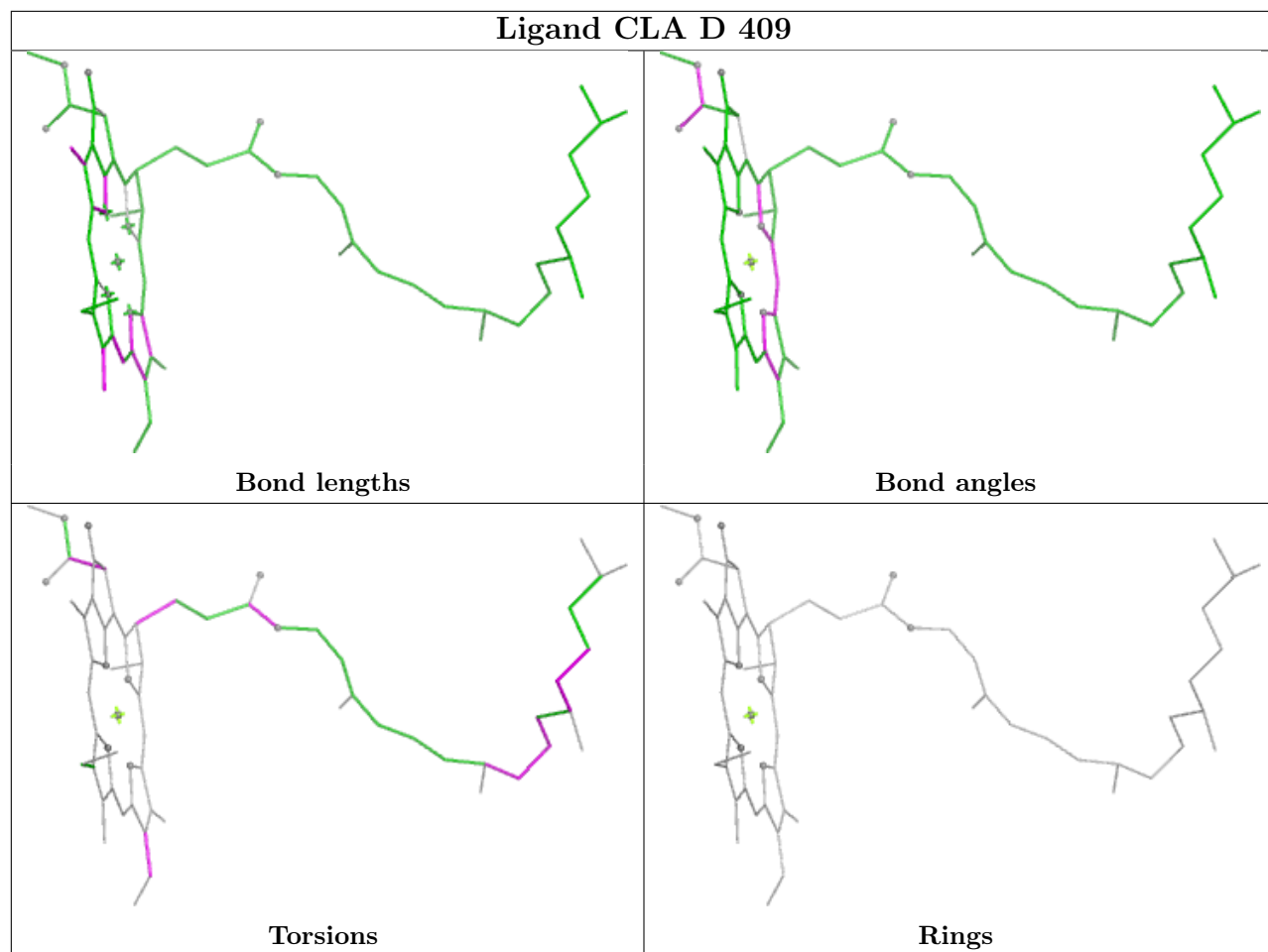


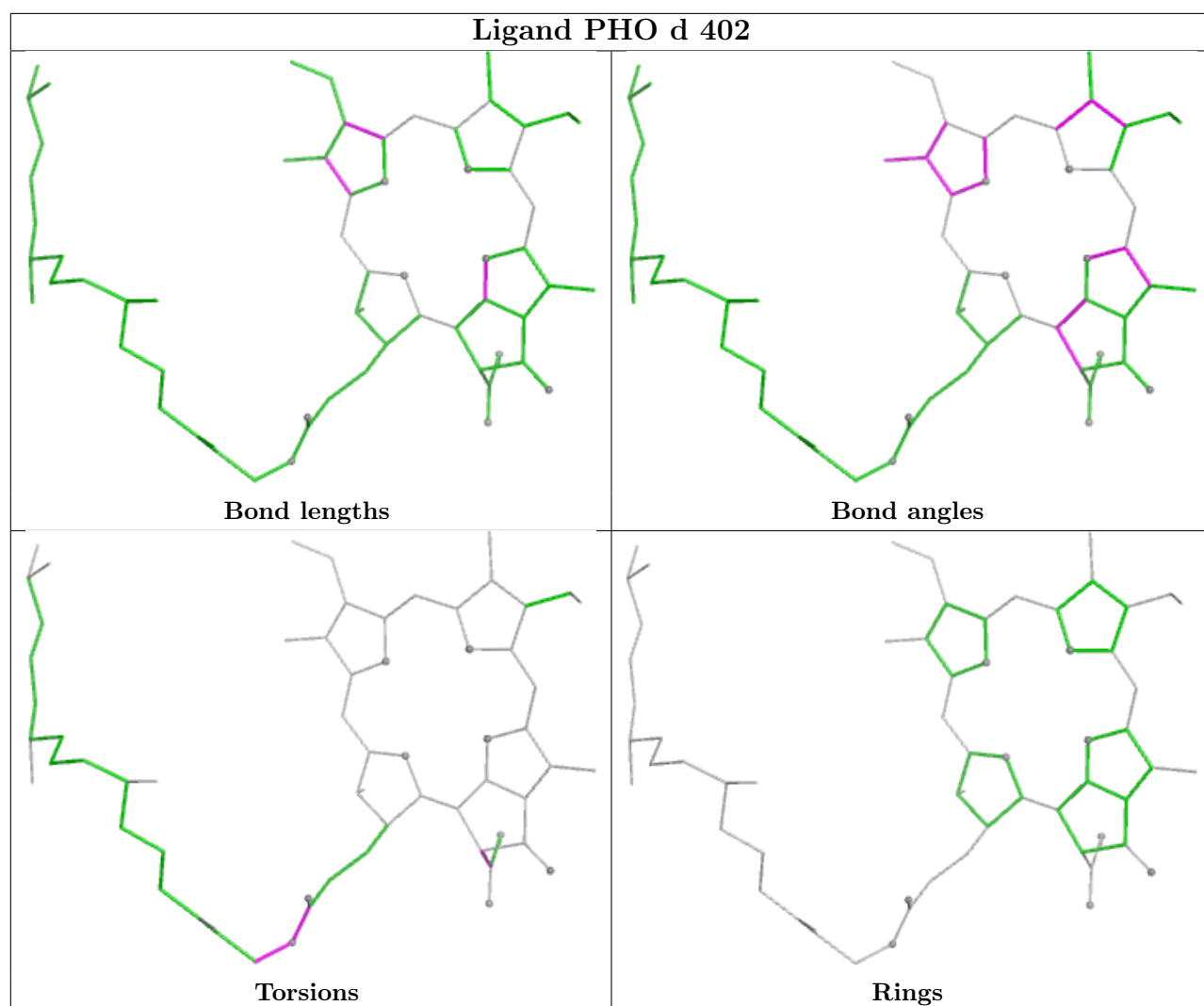


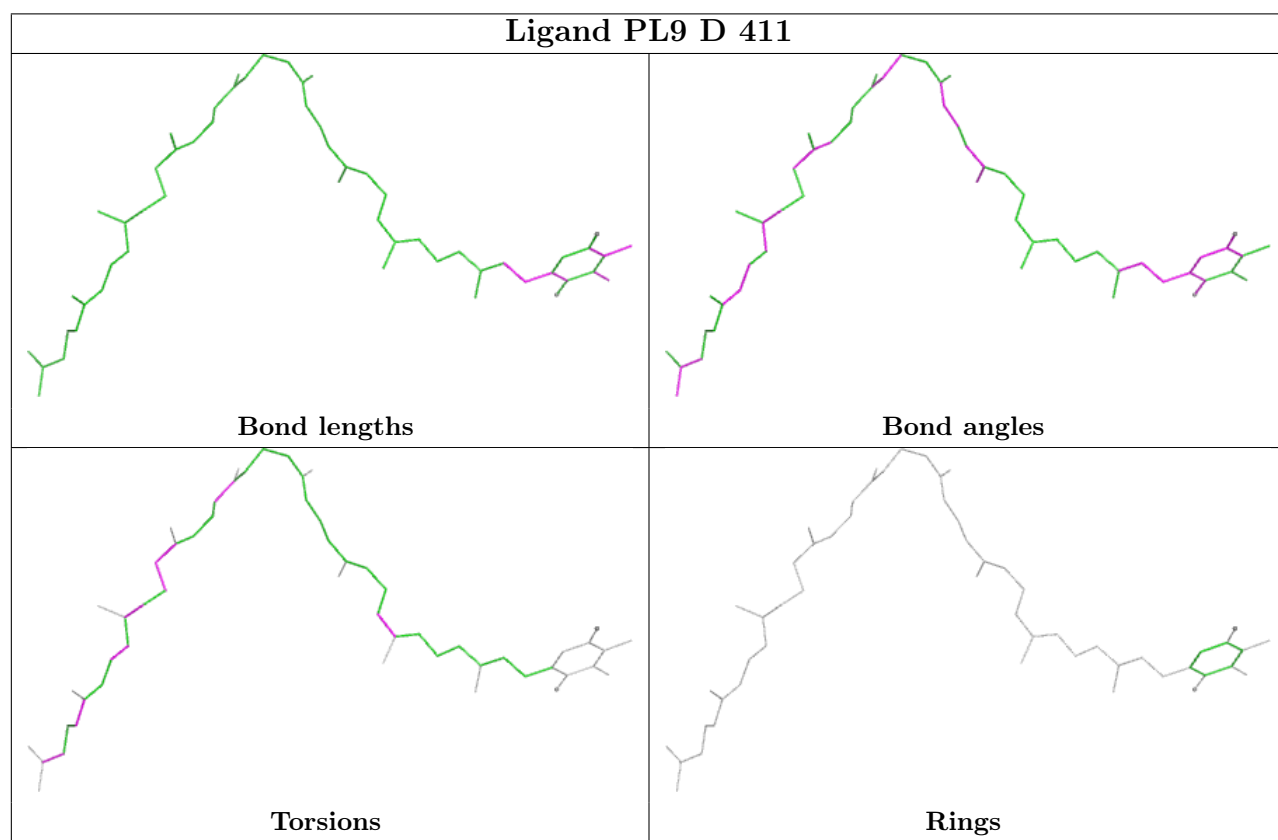
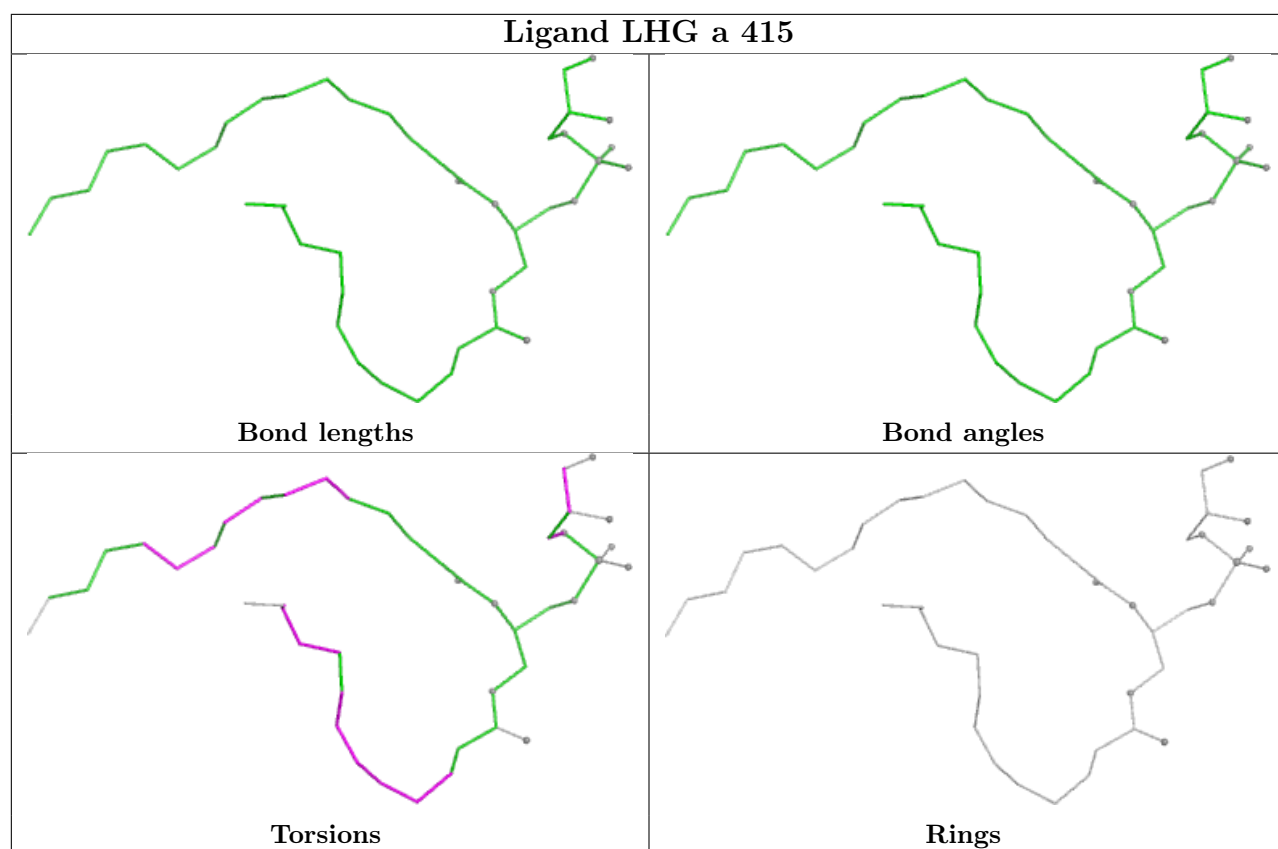


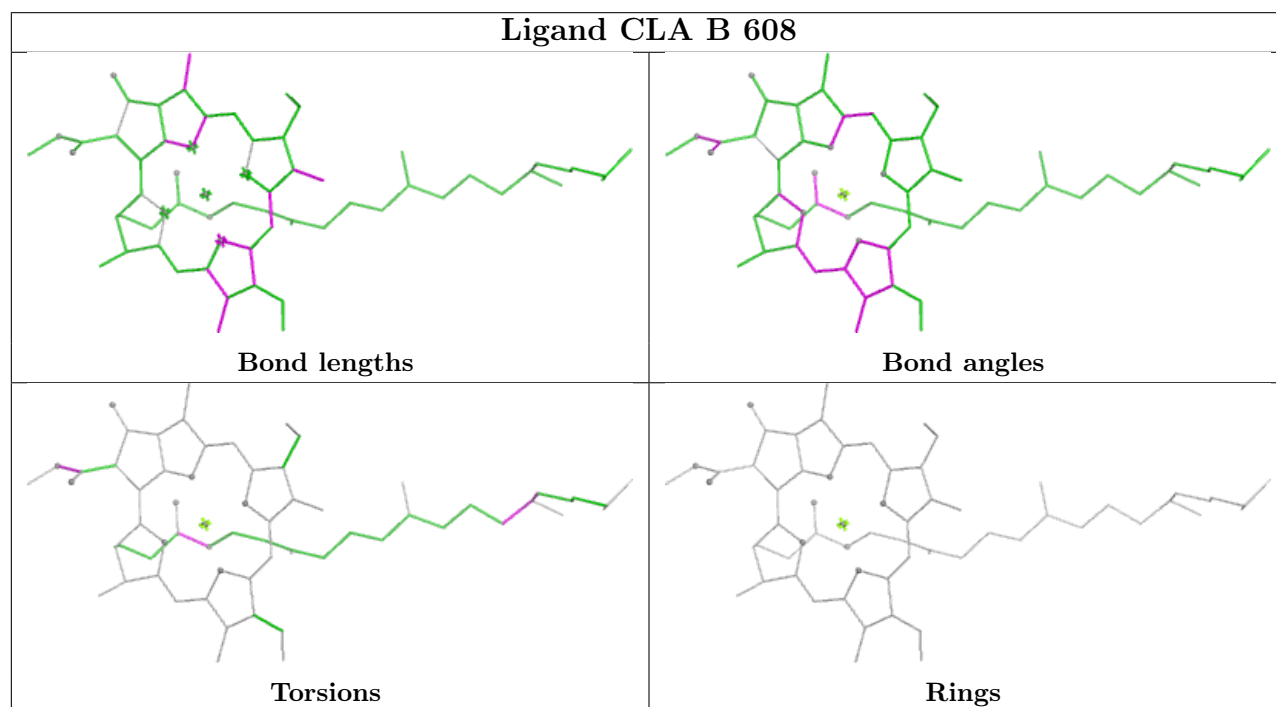
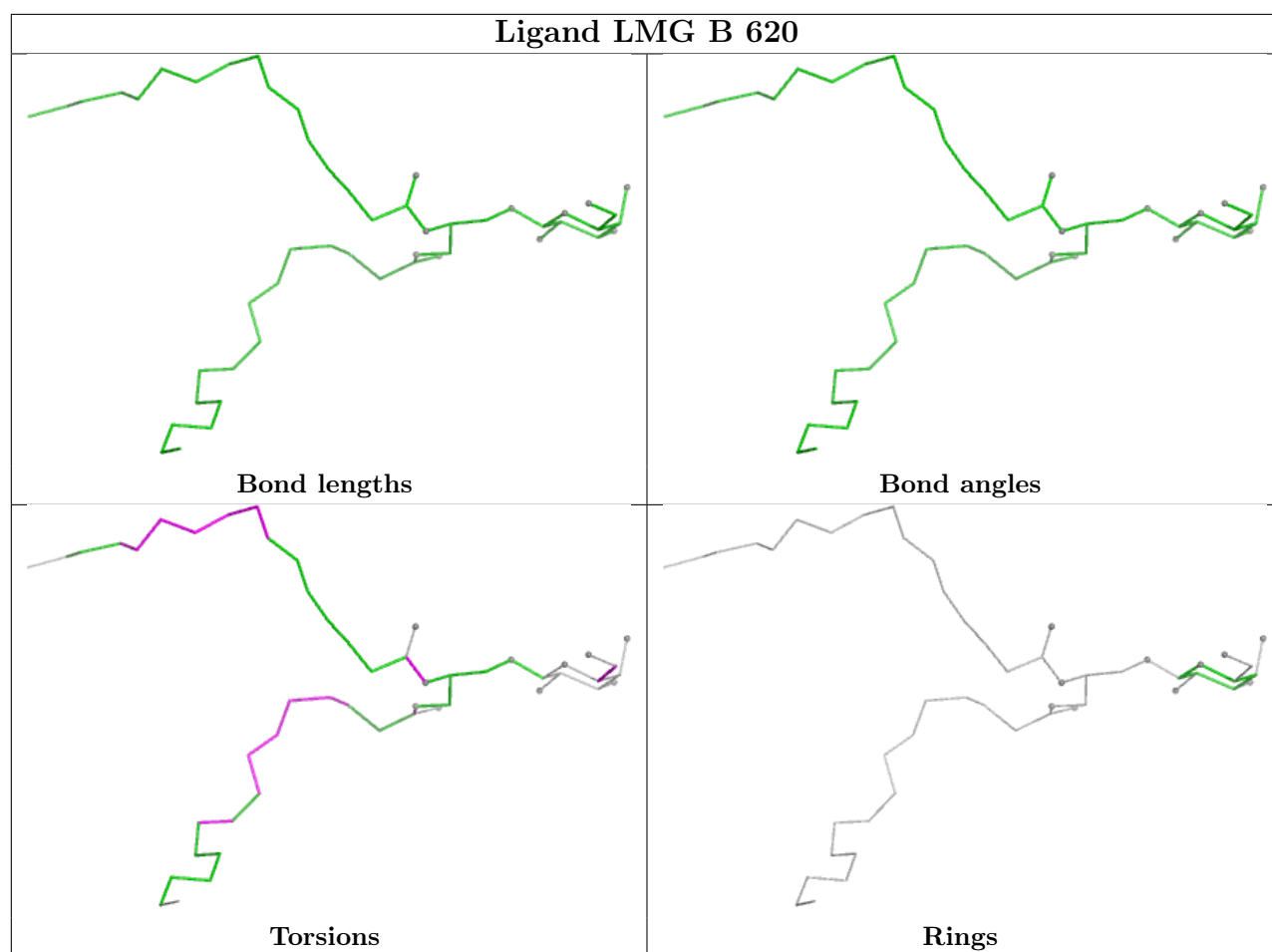




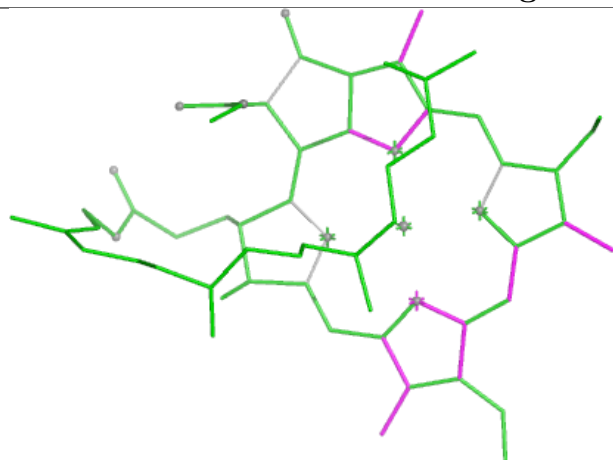




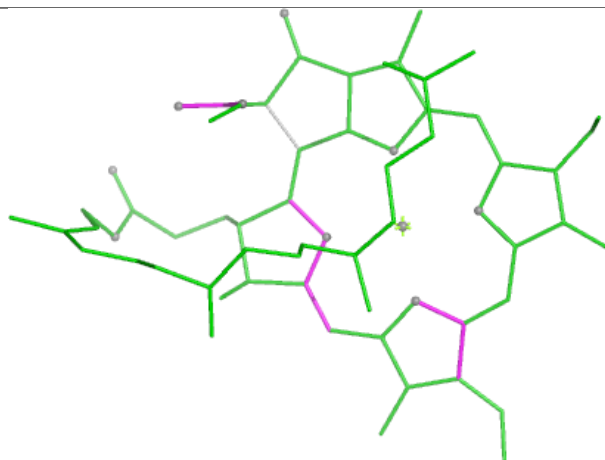




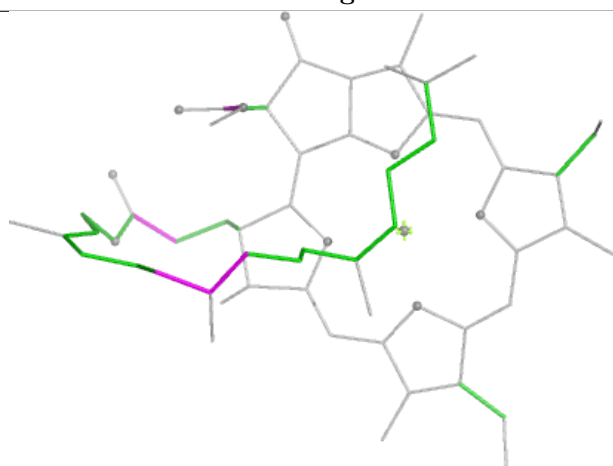
Ligand CLA c 511



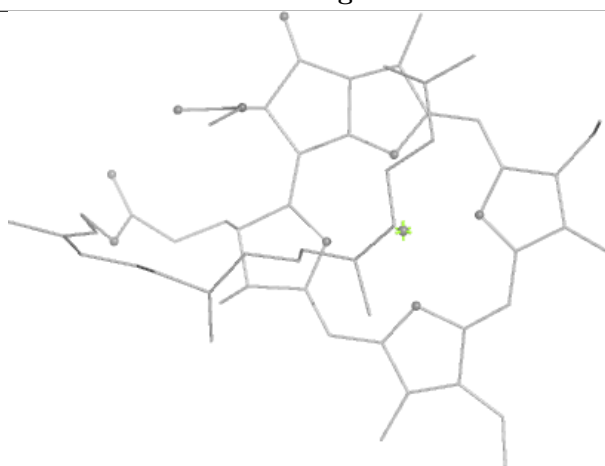
Bond lengths



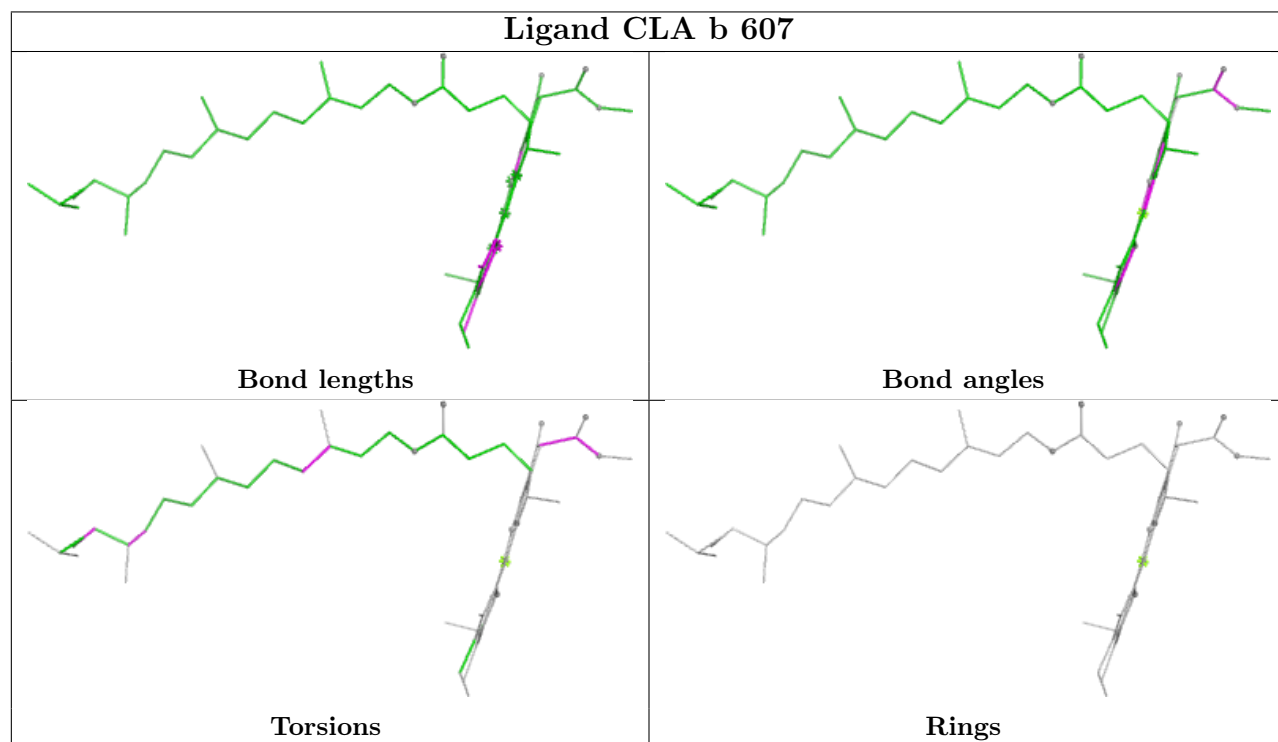
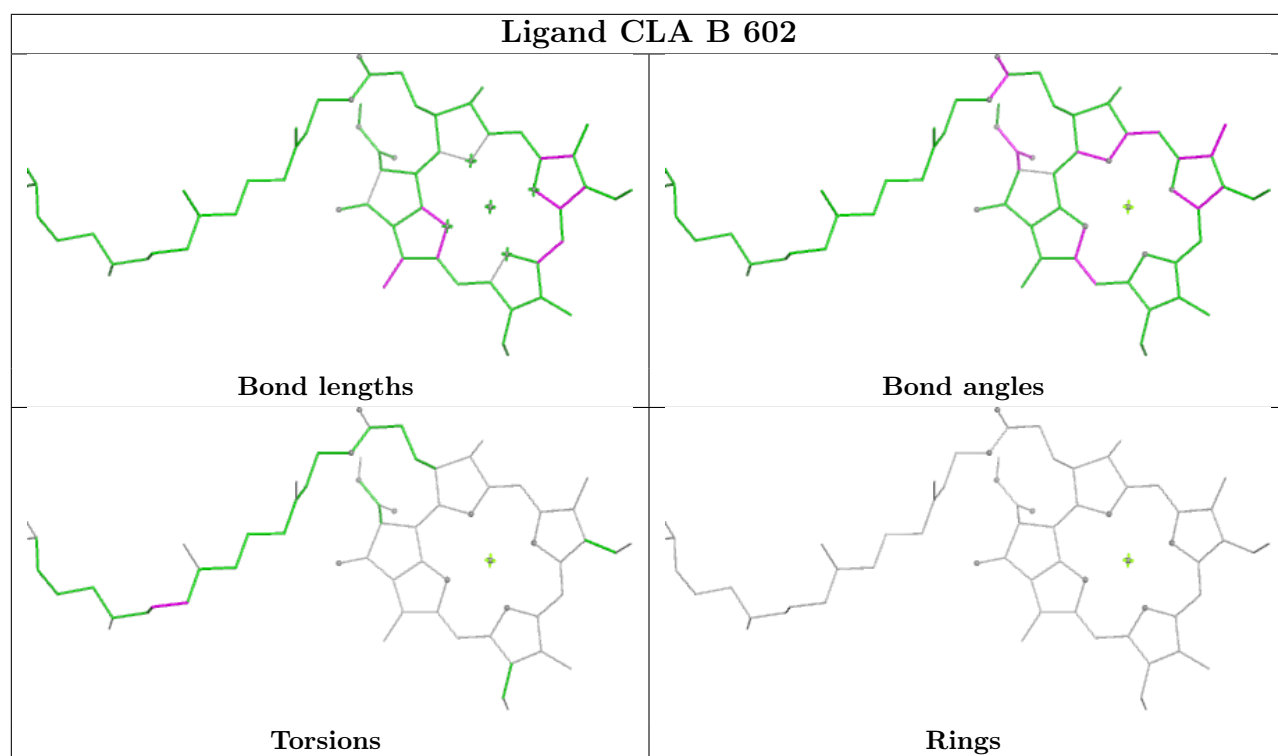
Bond angles

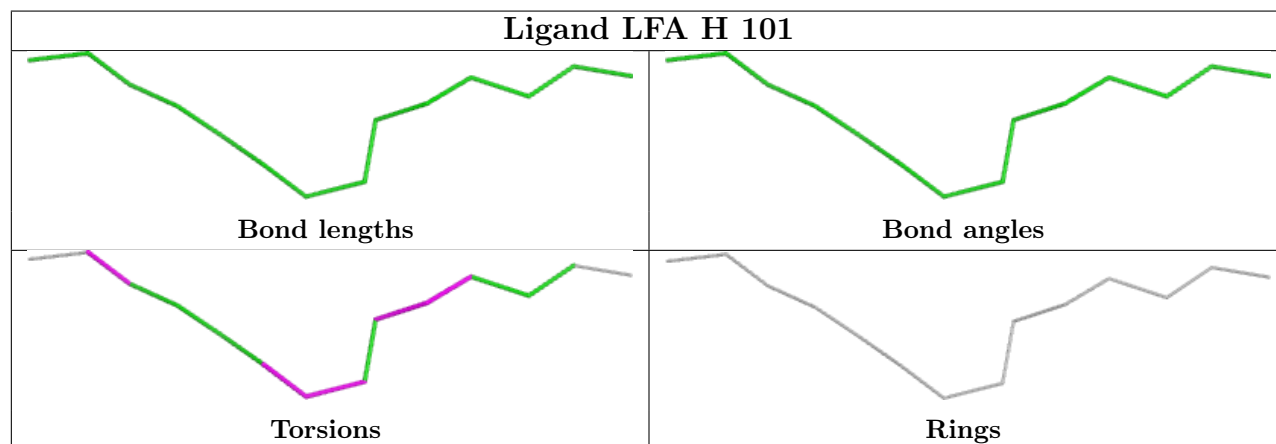
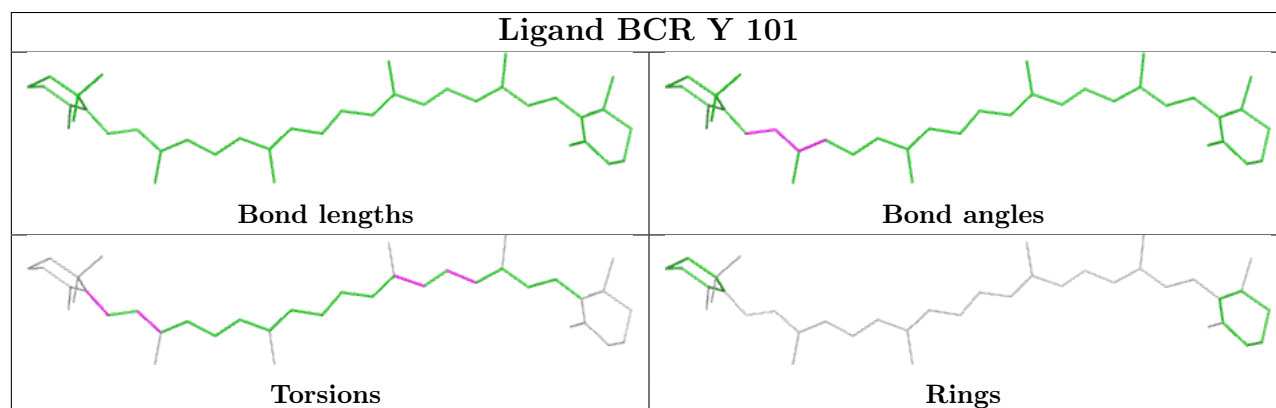
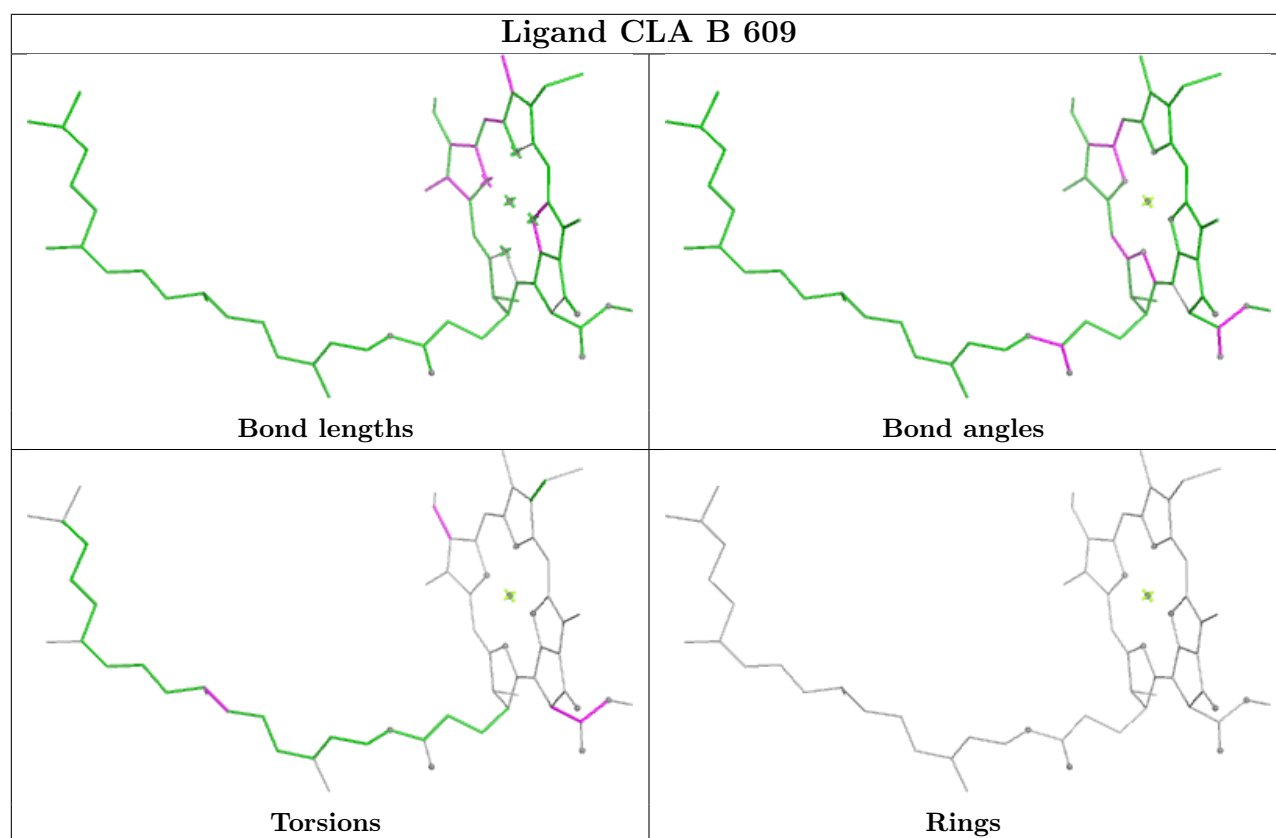


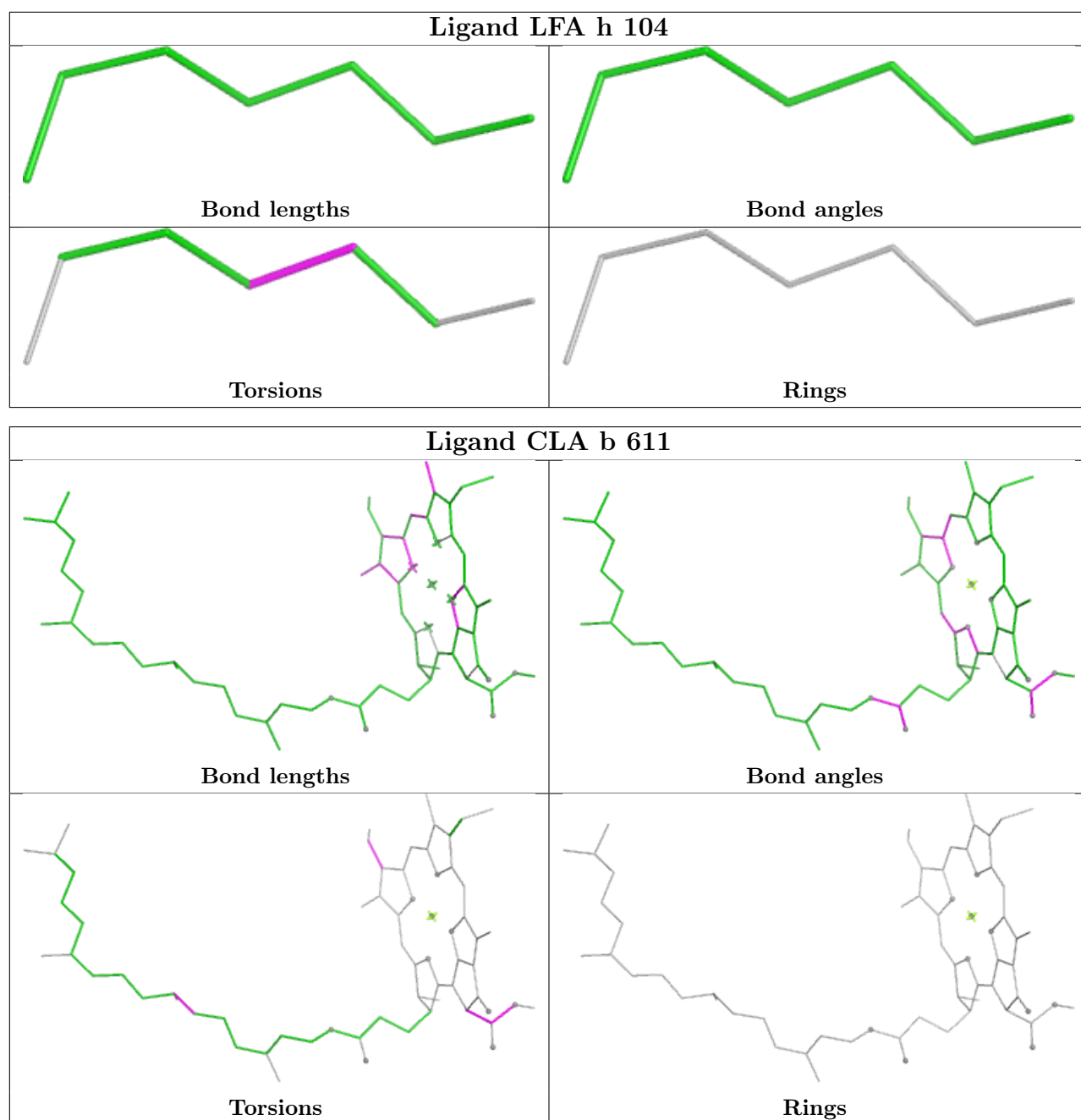
Torsions

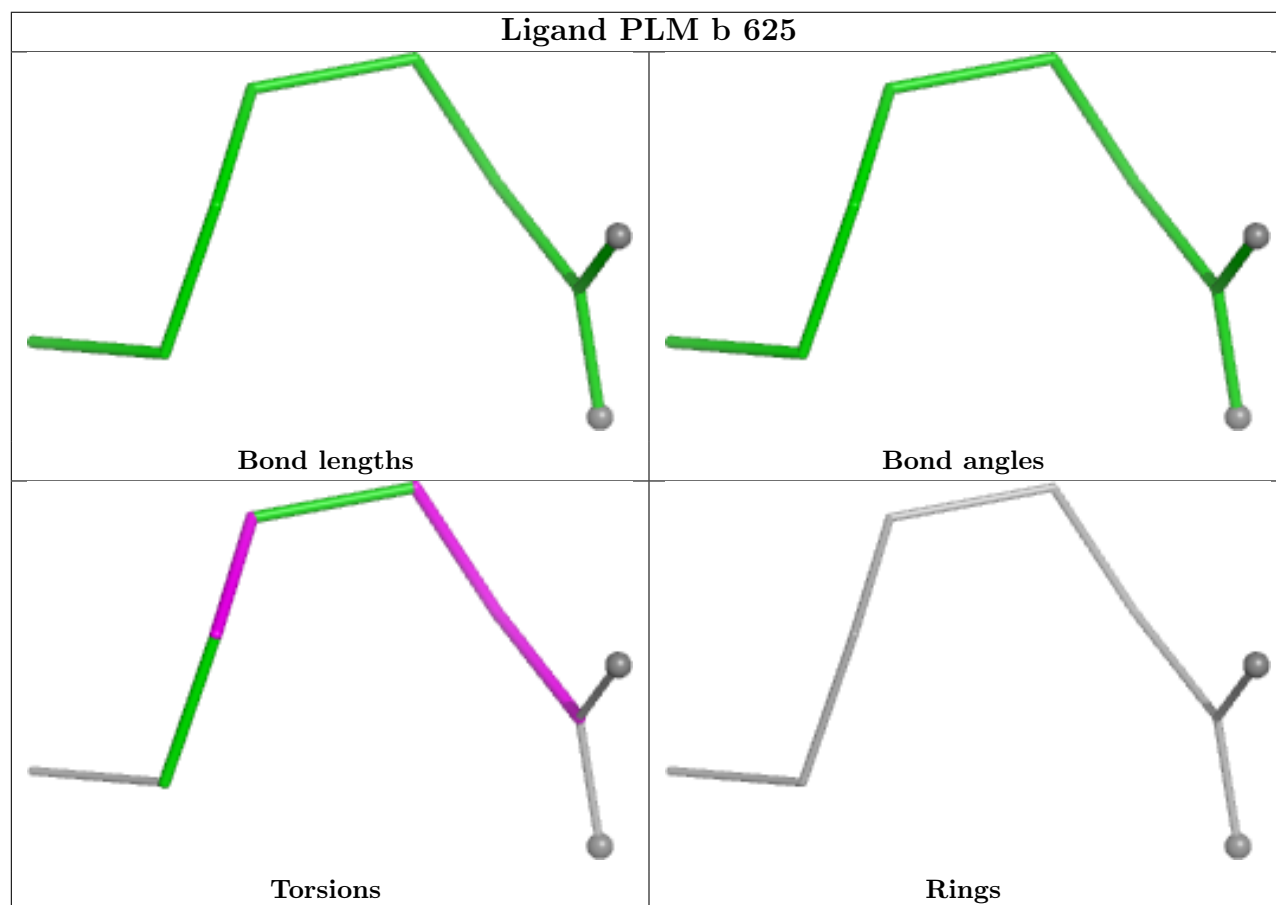
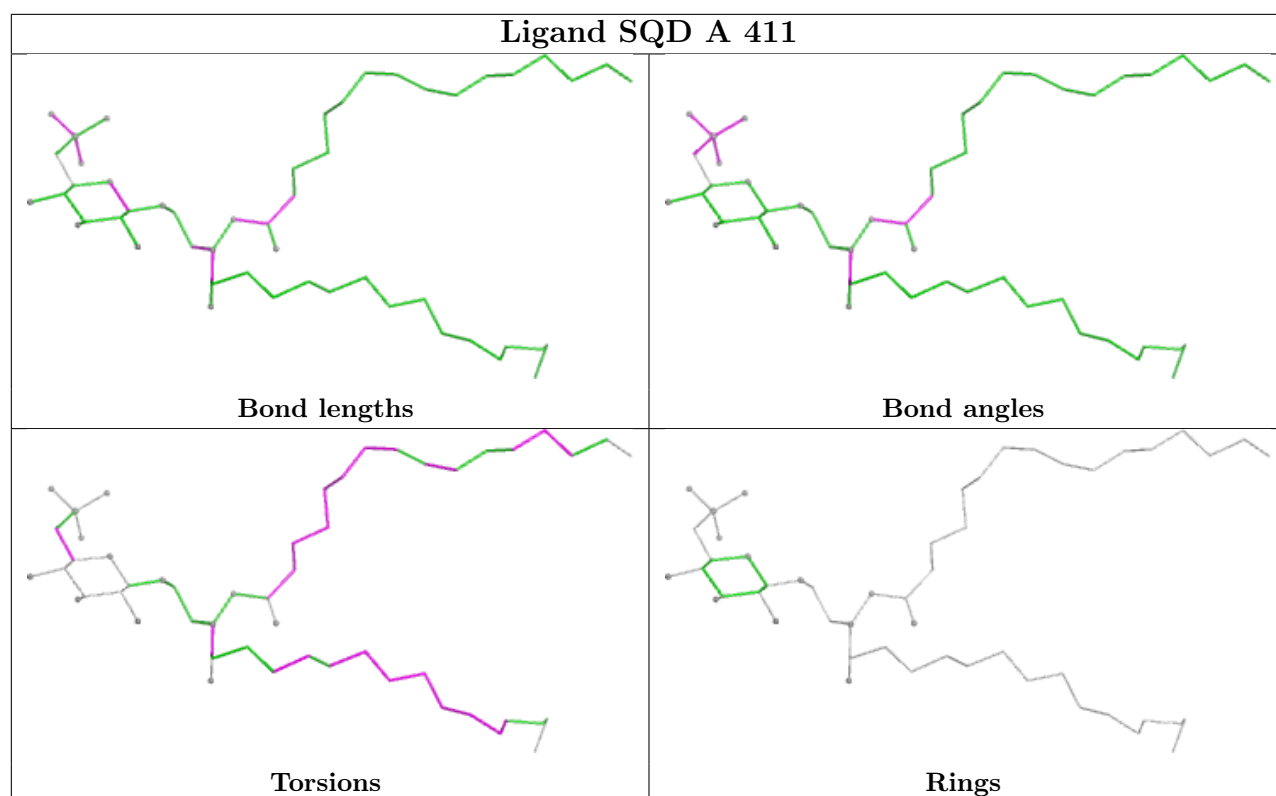


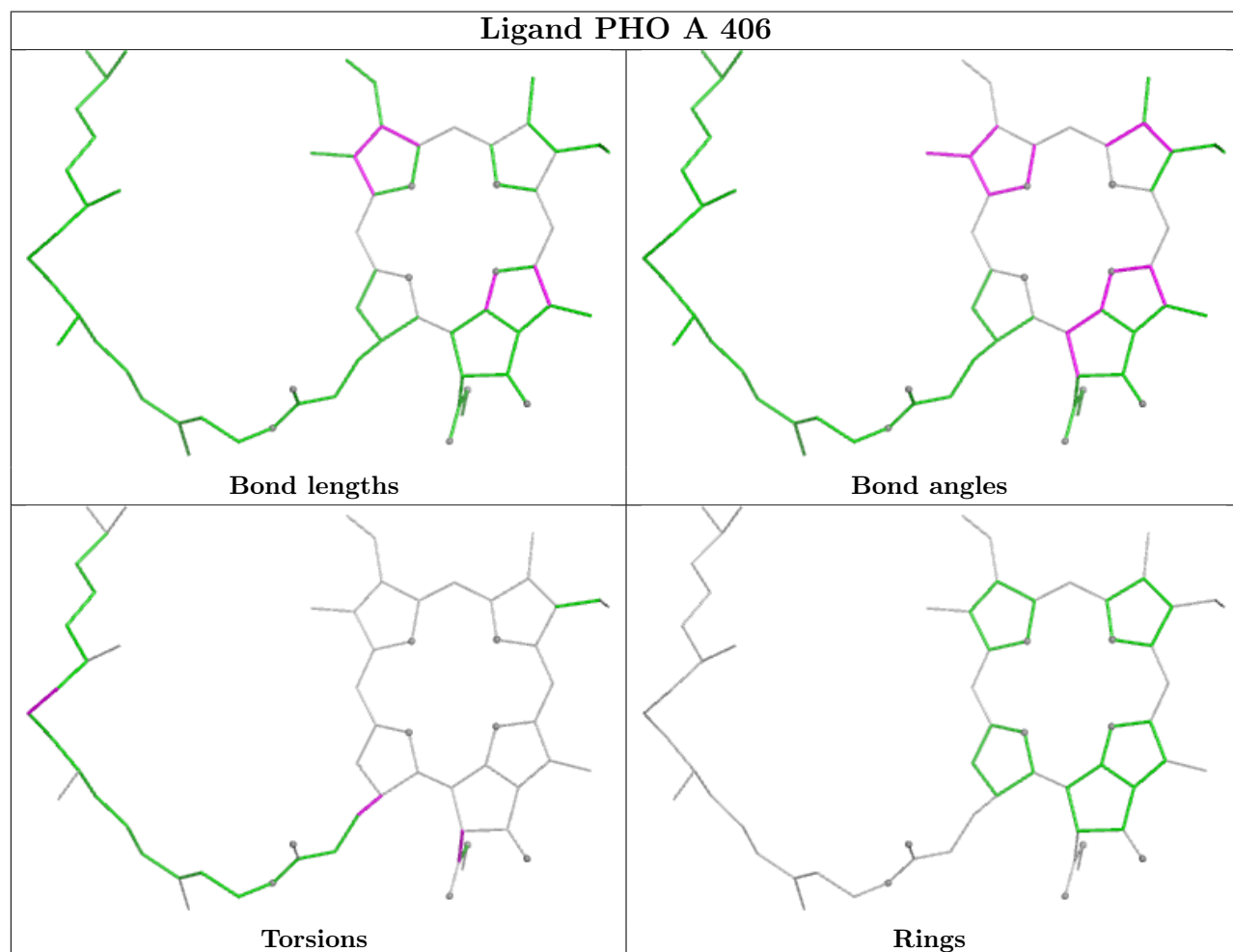
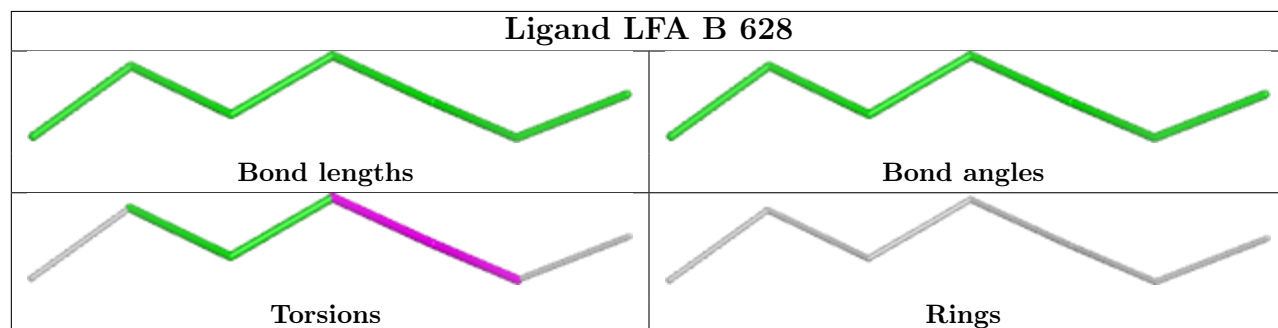
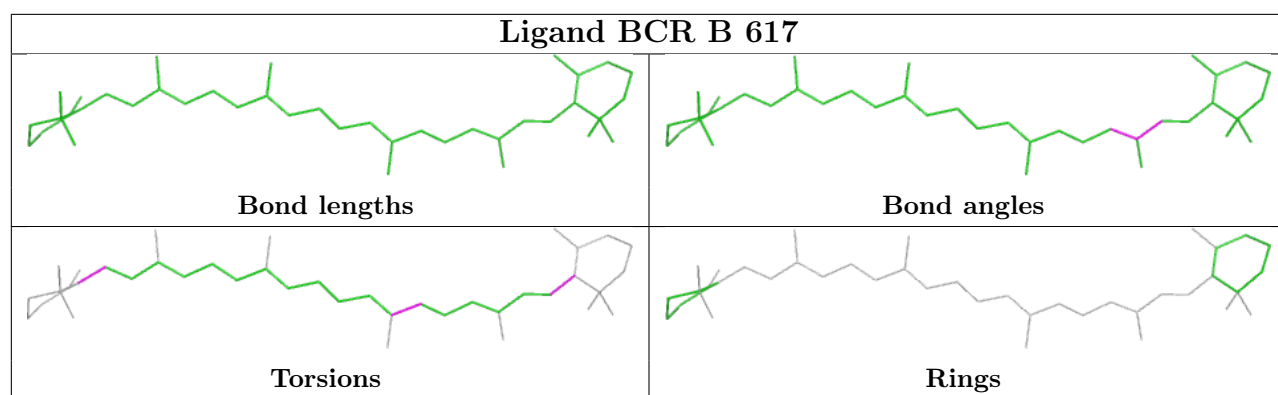
Rings

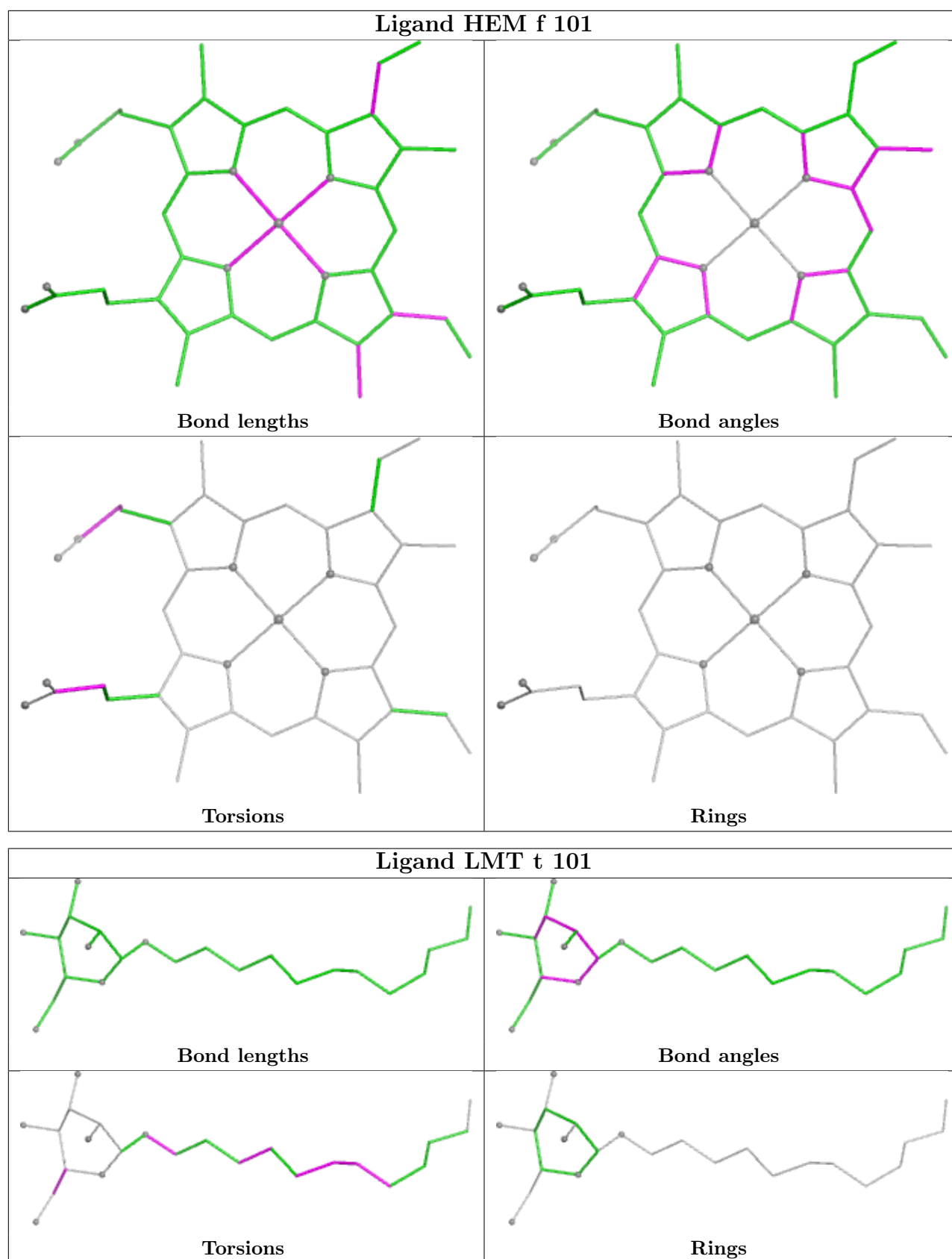


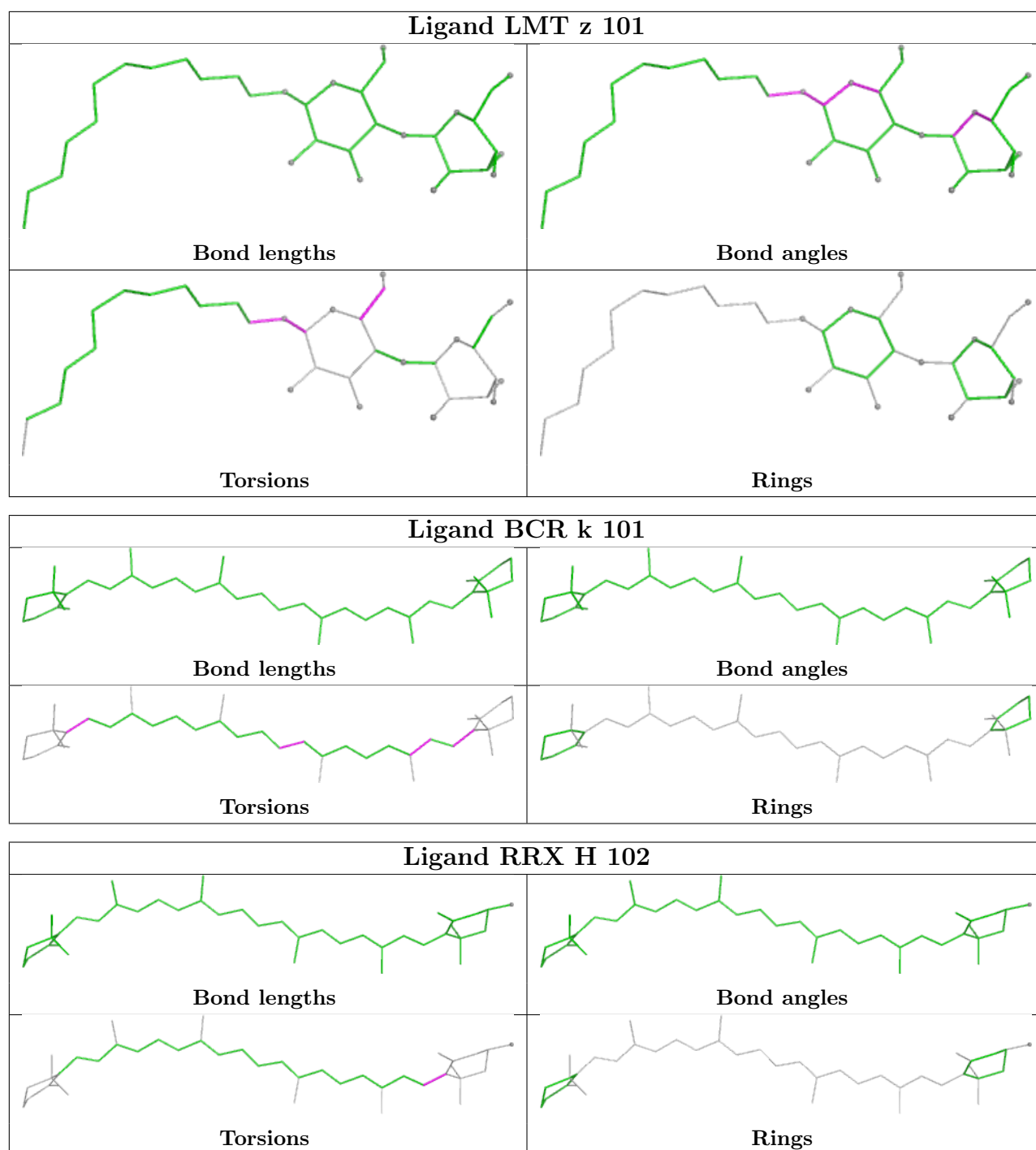


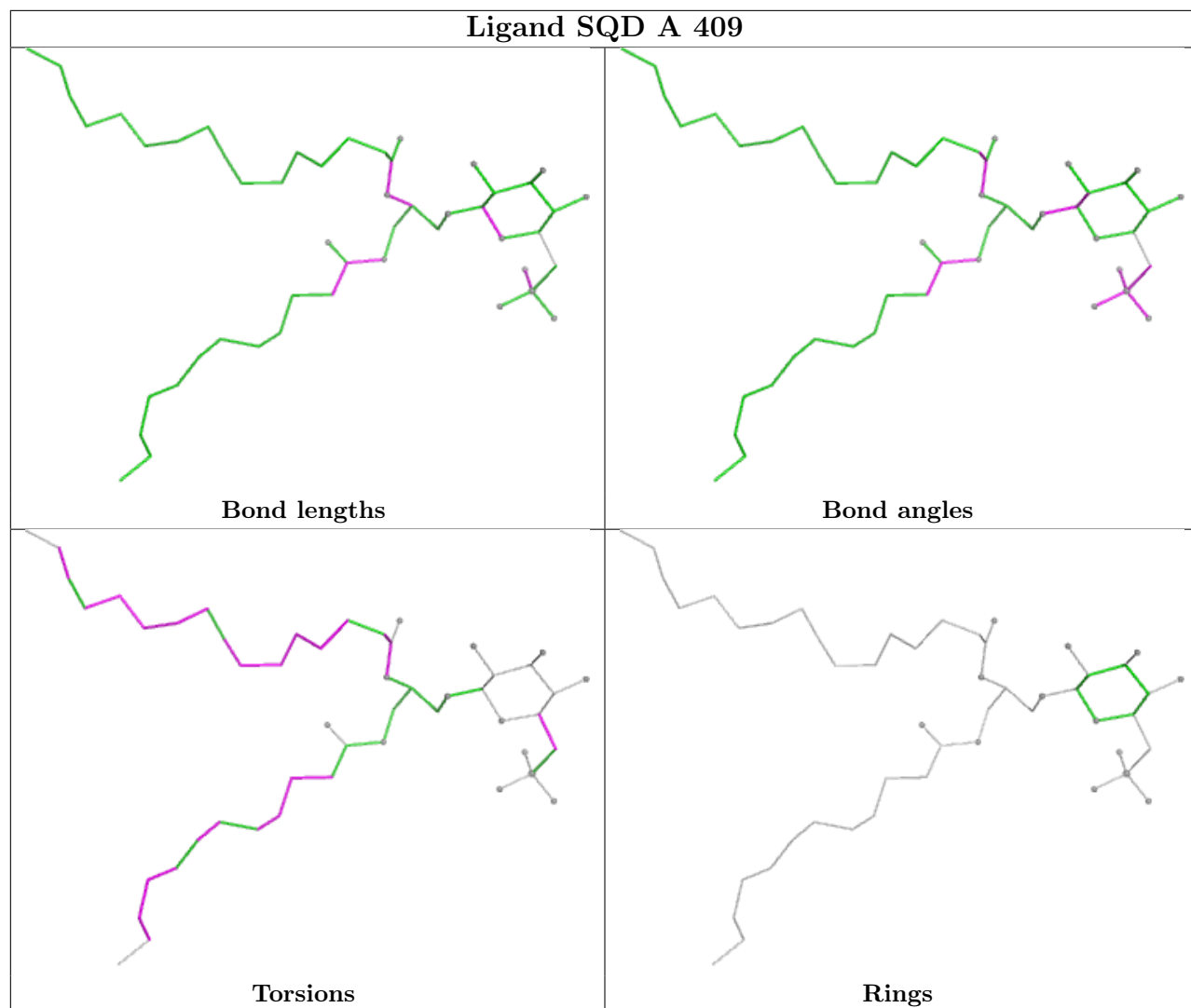


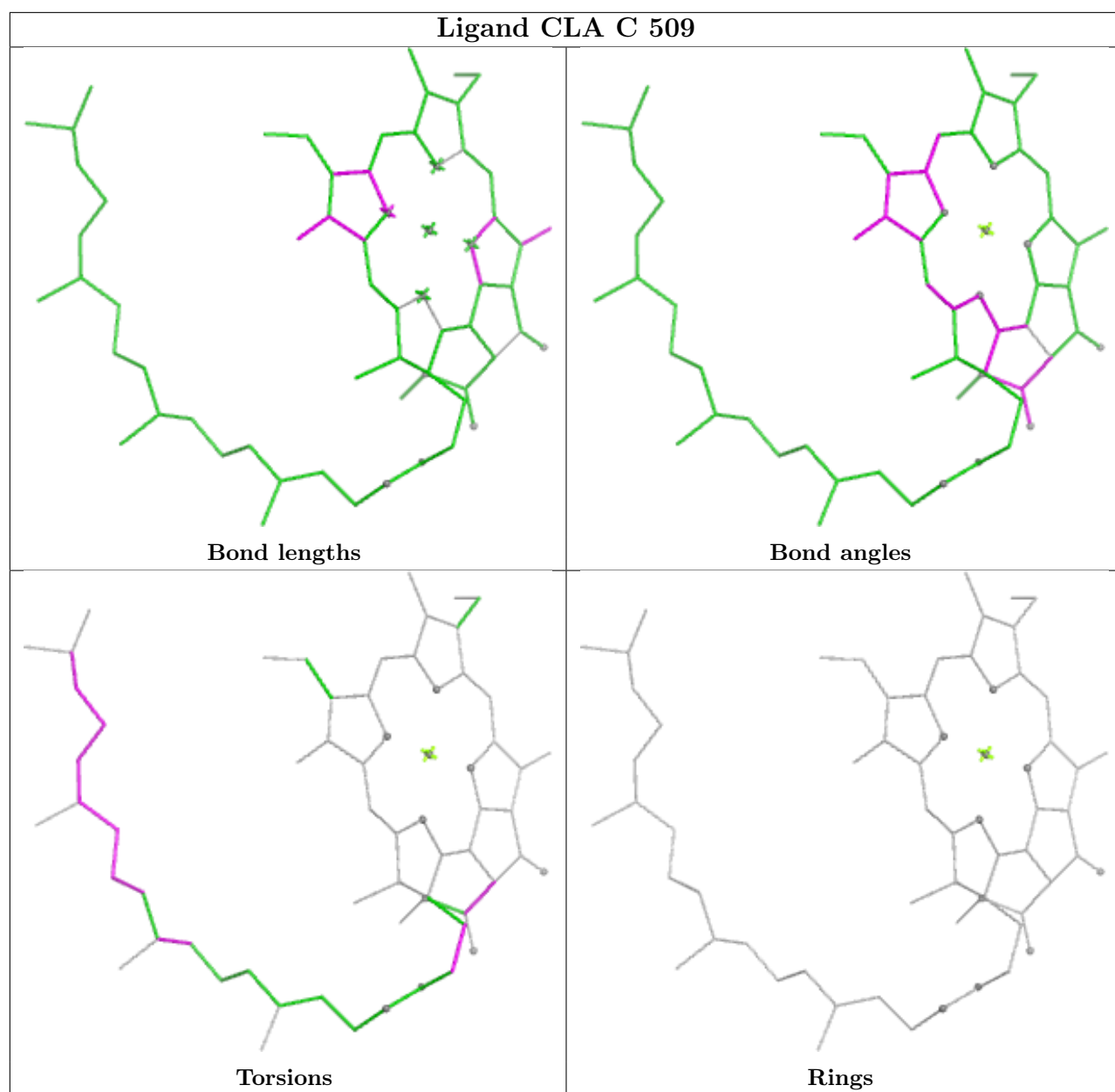


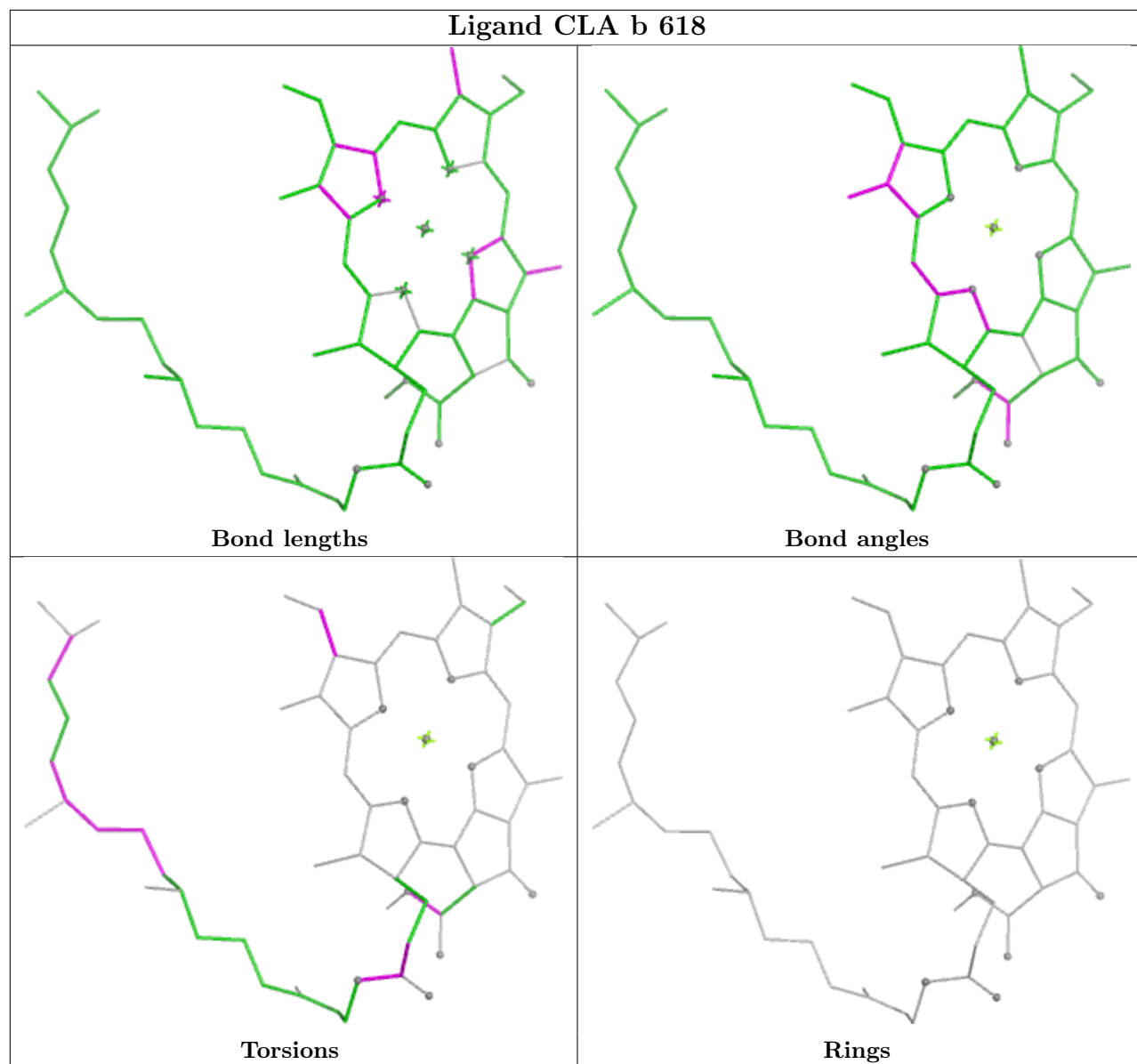


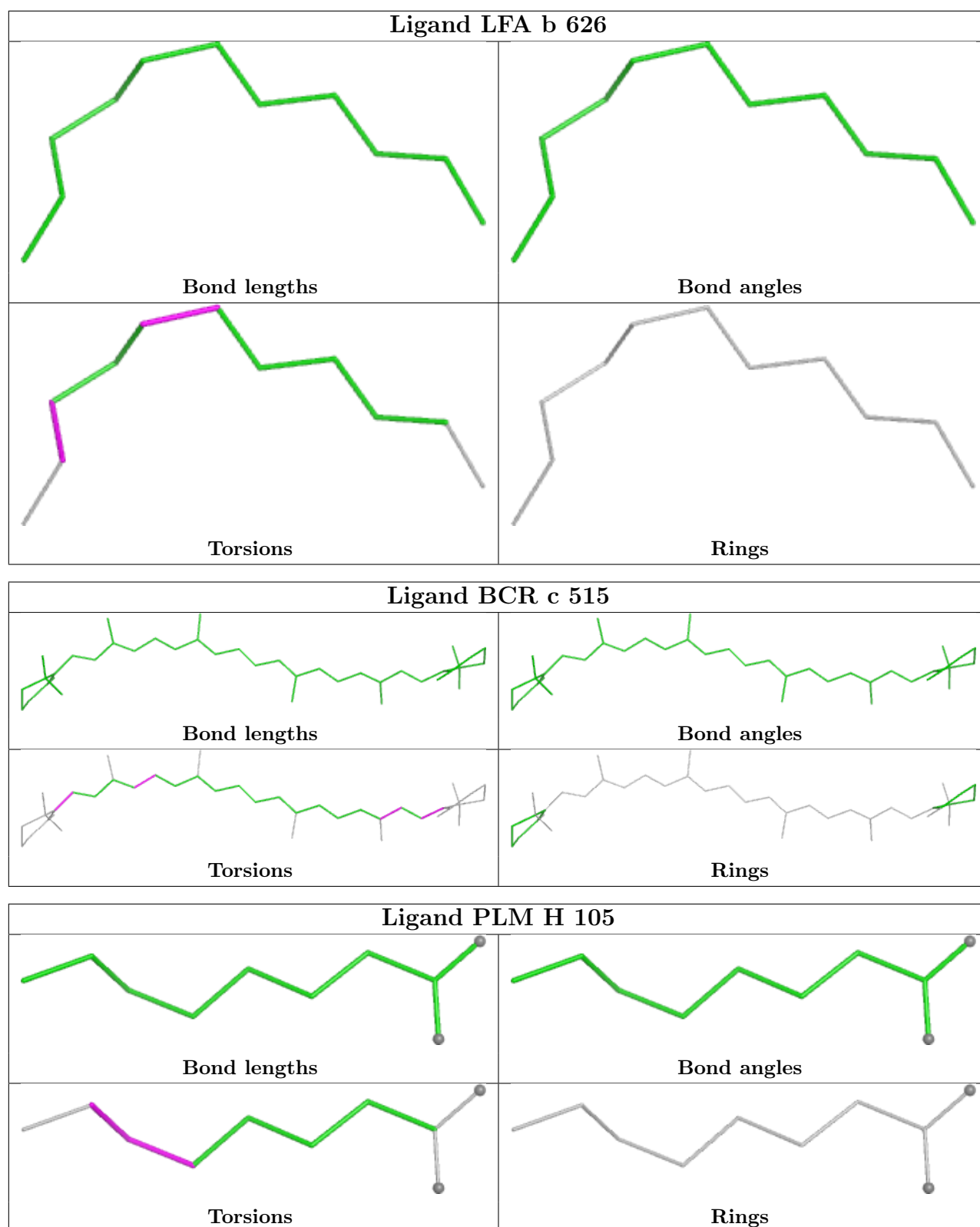


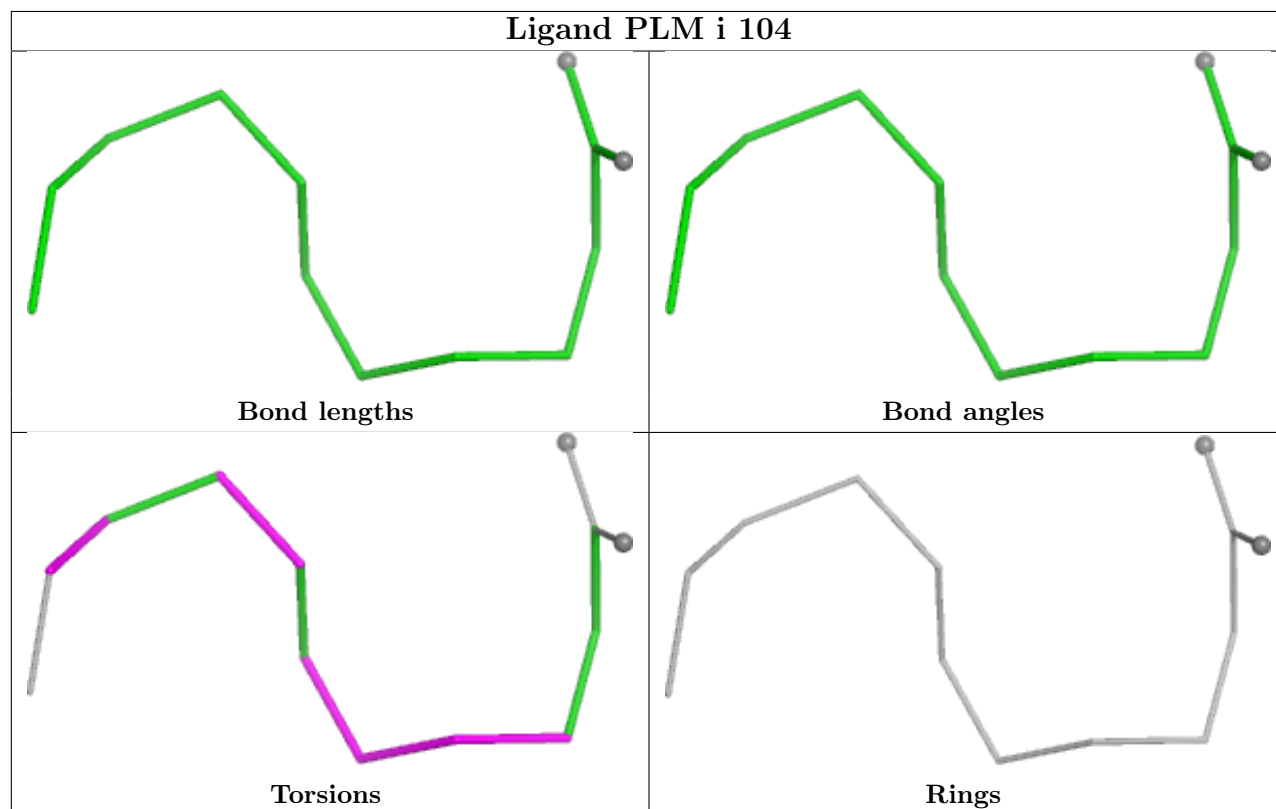
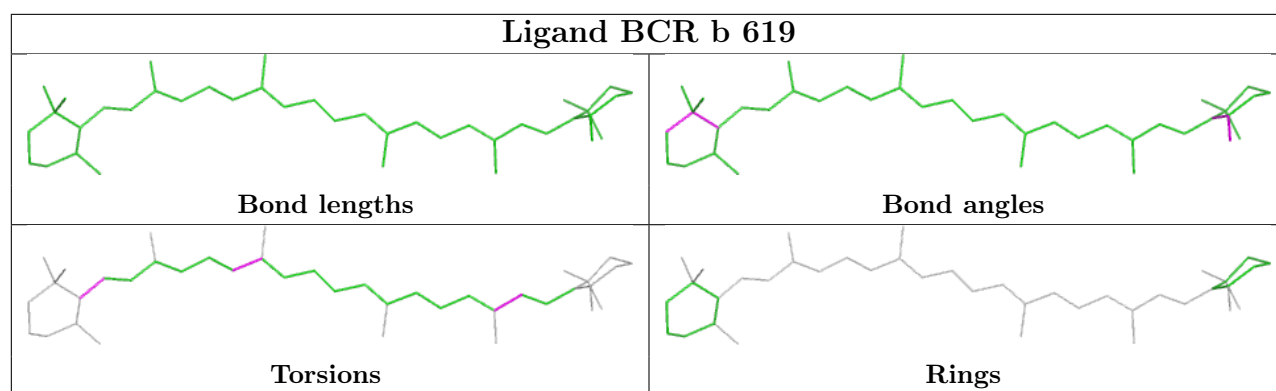


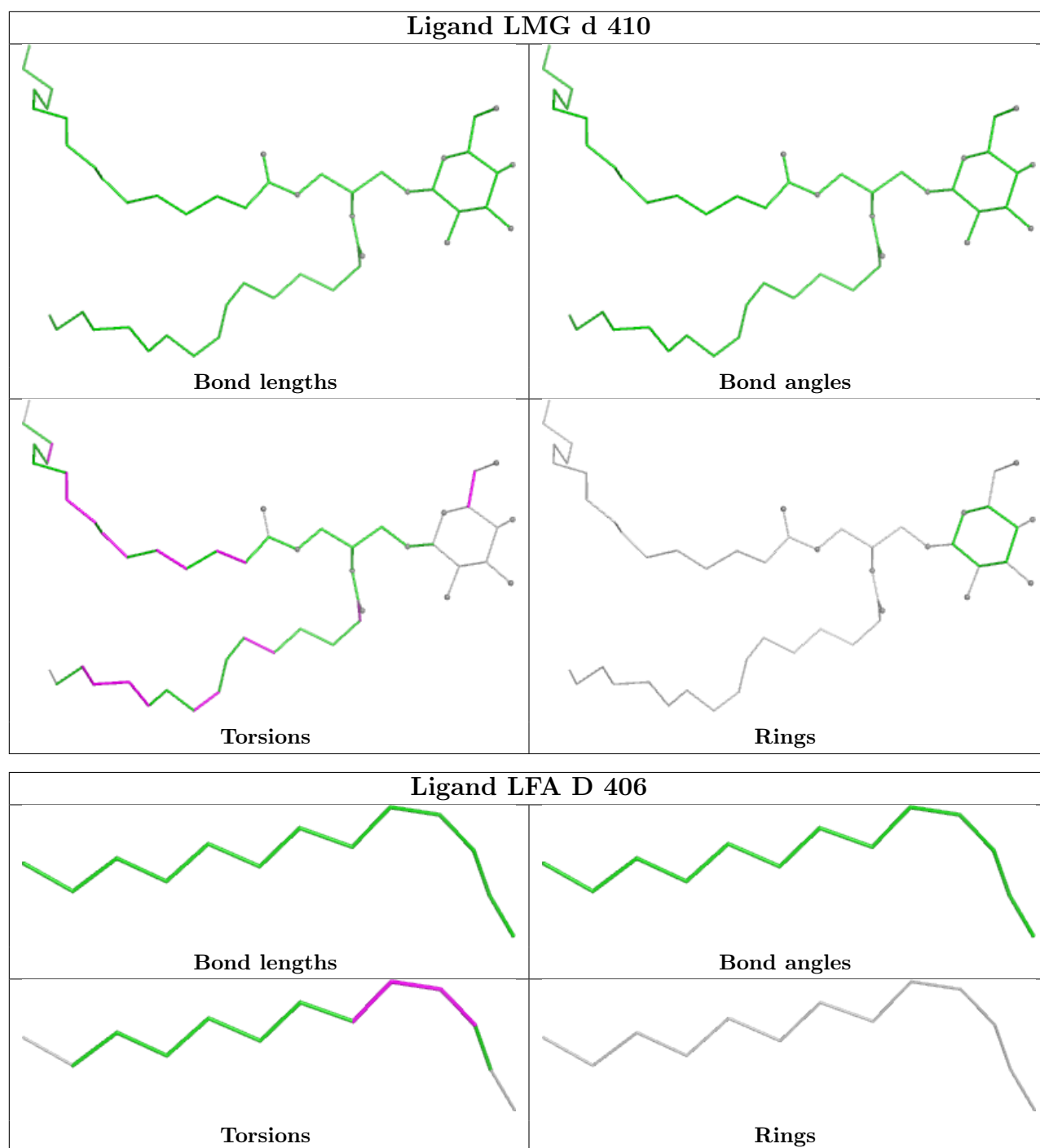


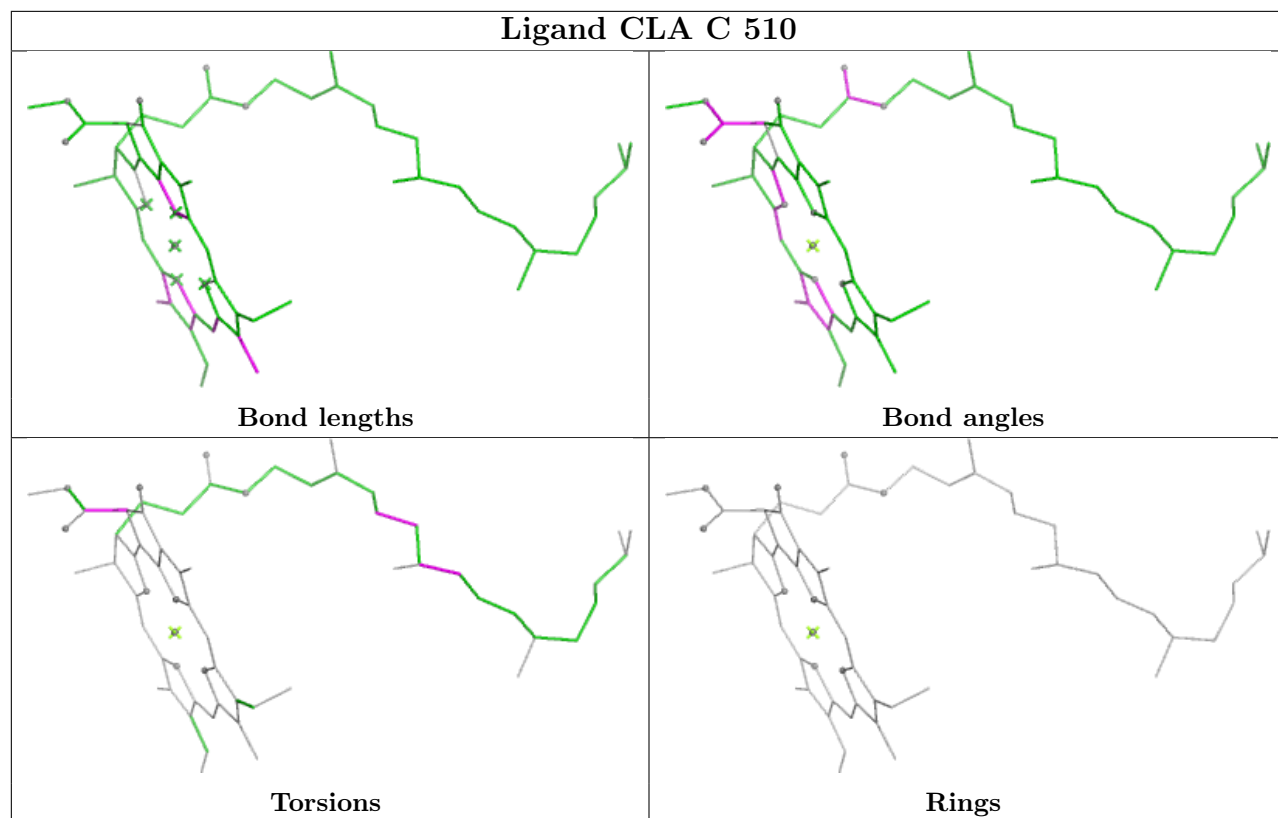




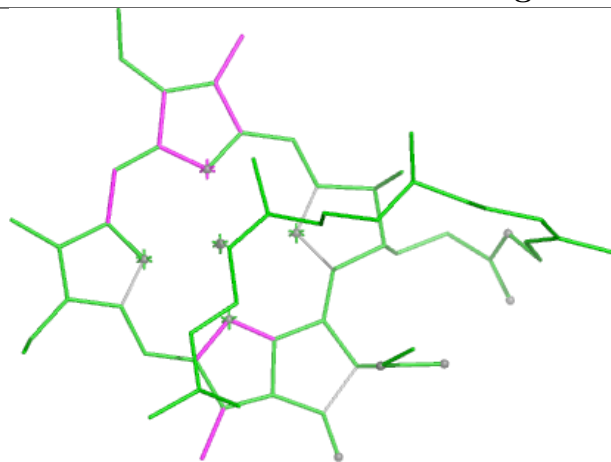




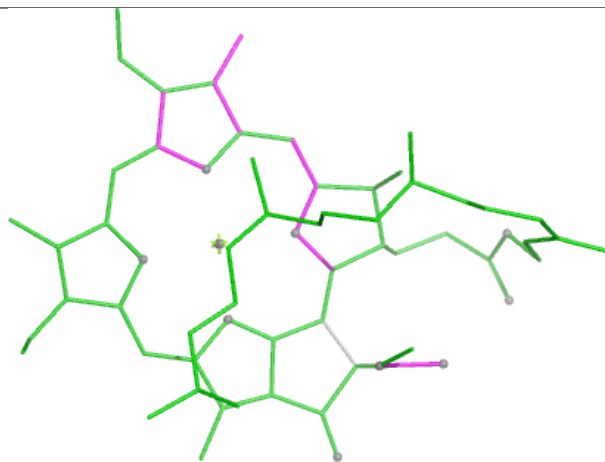




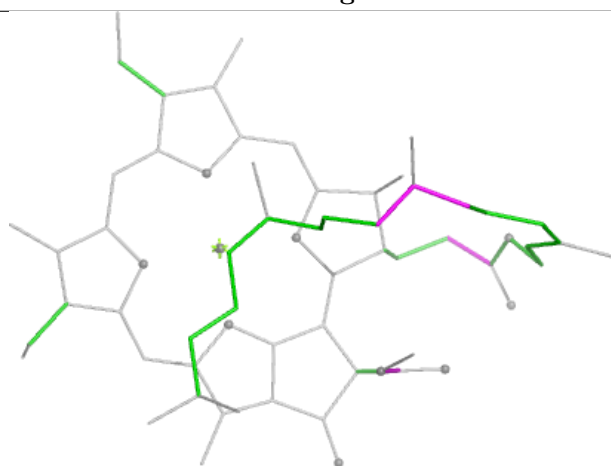
Ligand CLA C 512



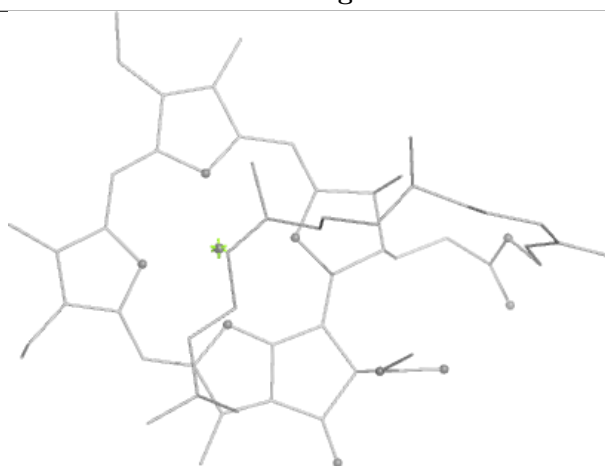
Bond lengths



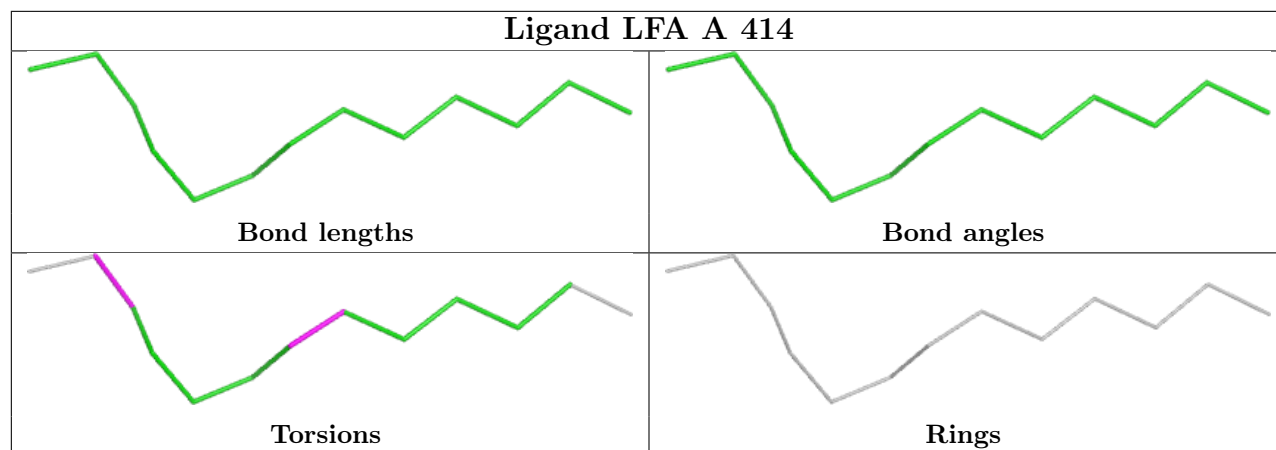
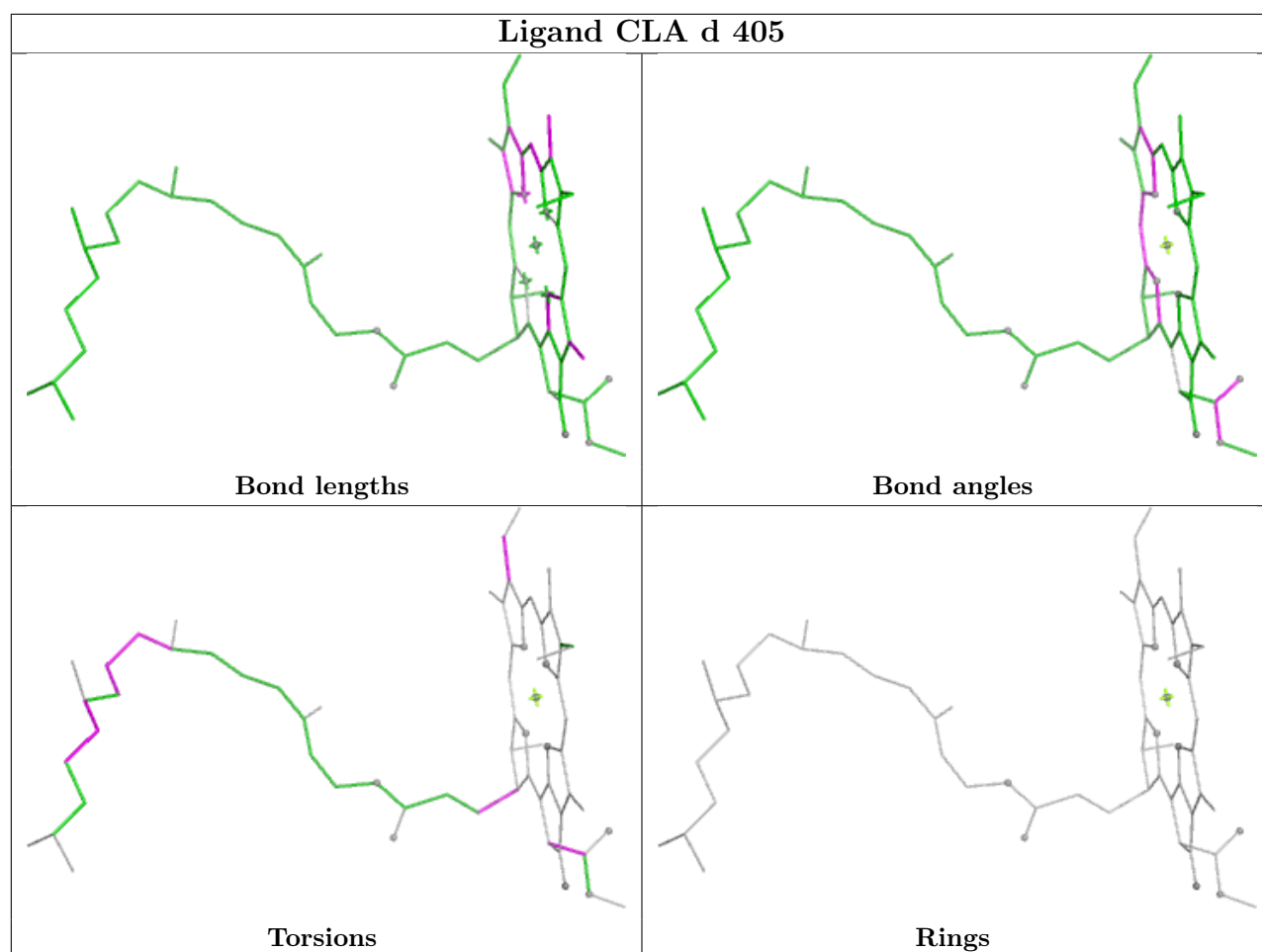
Bond angles

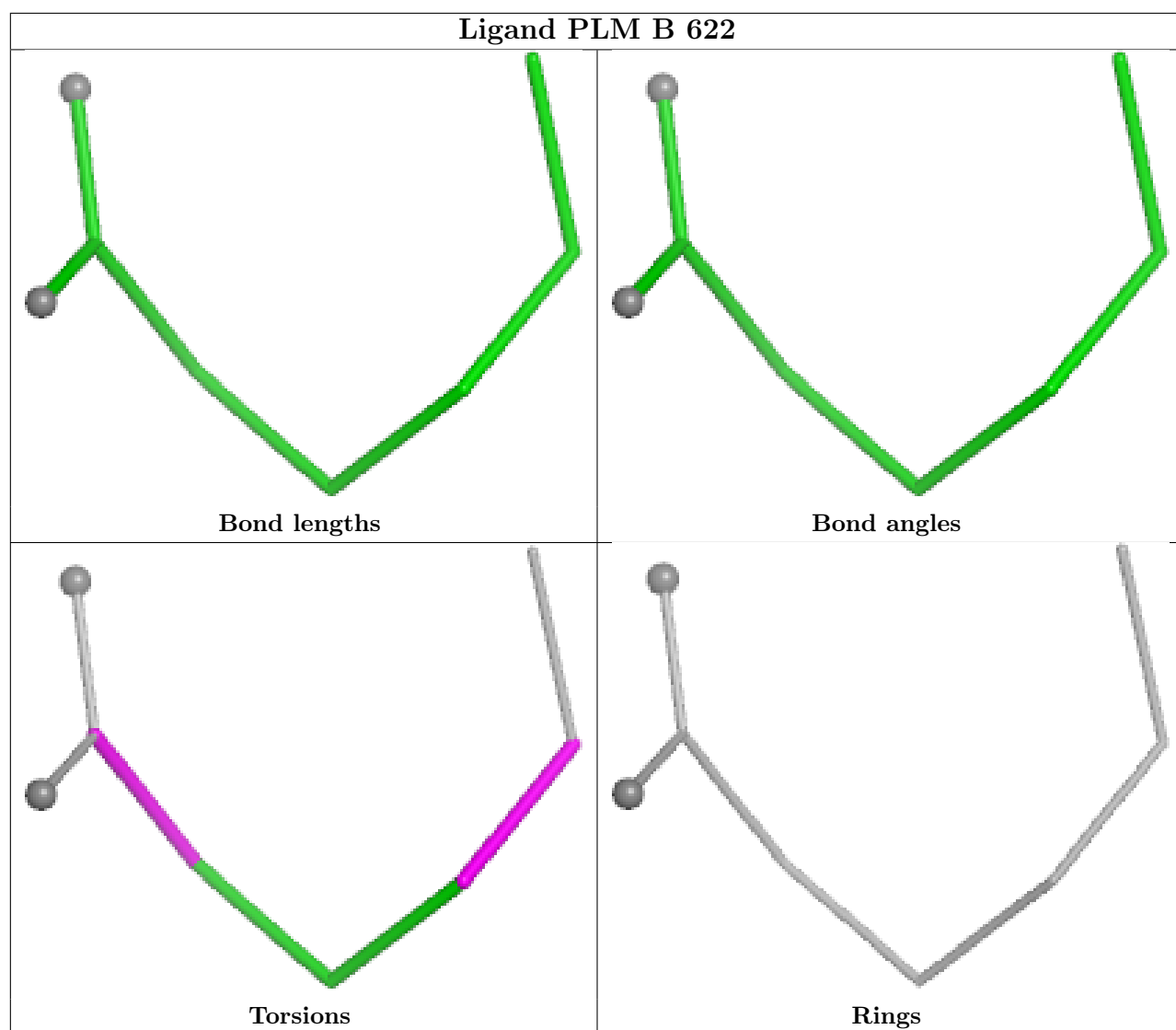


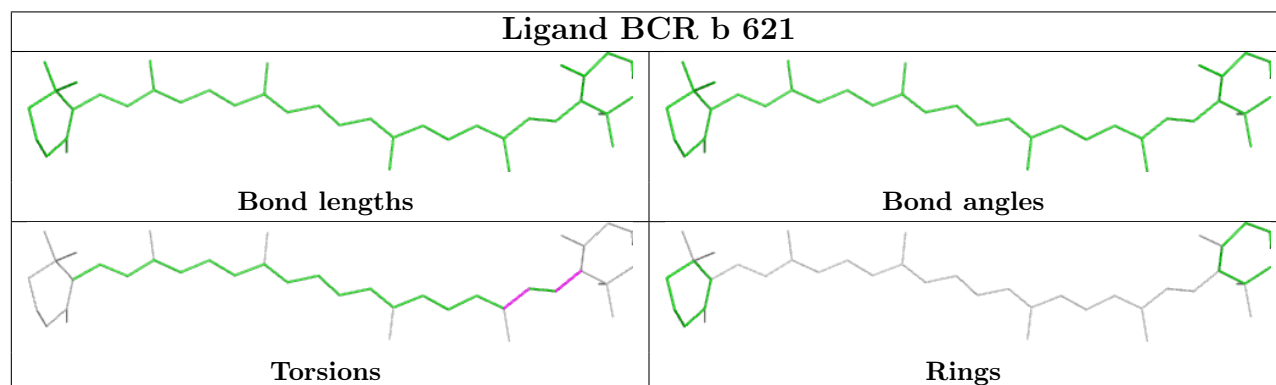
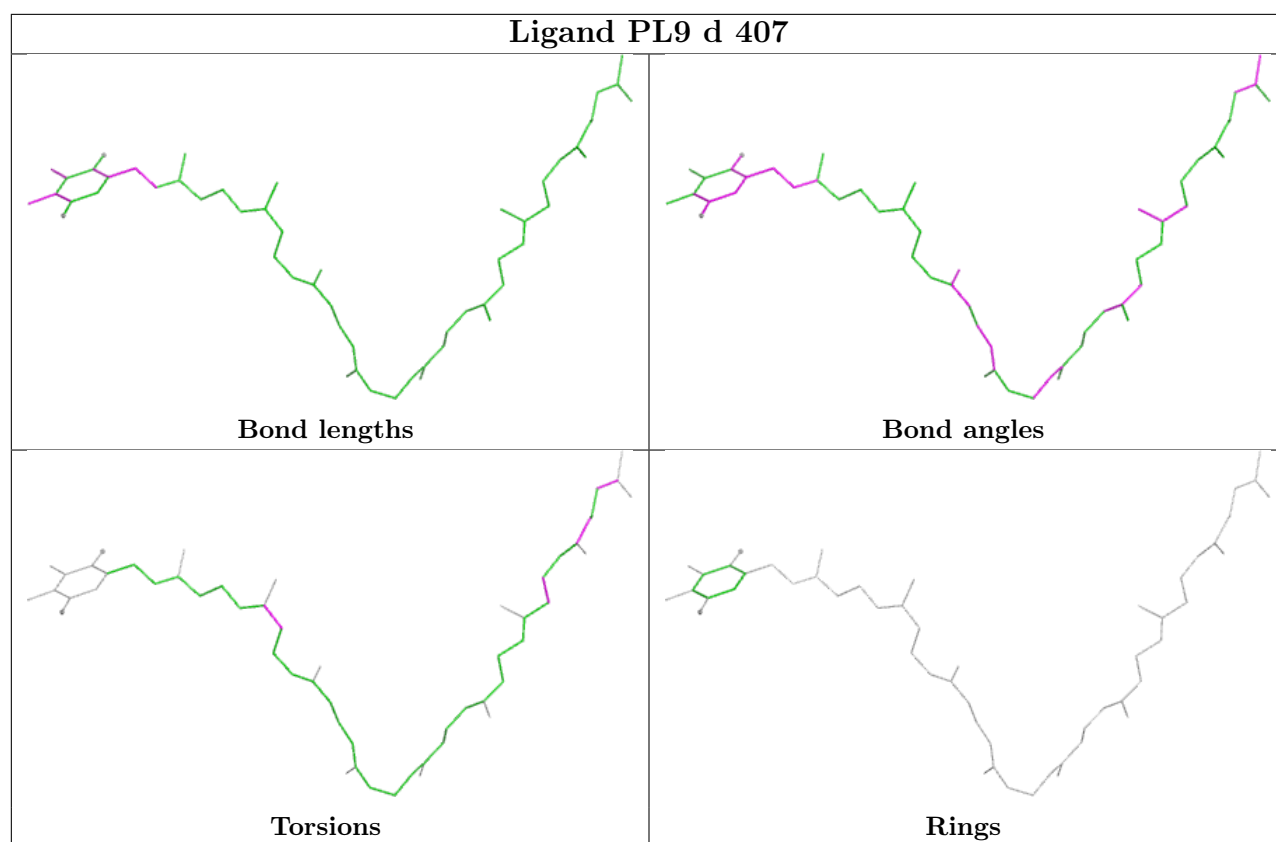
Torsions

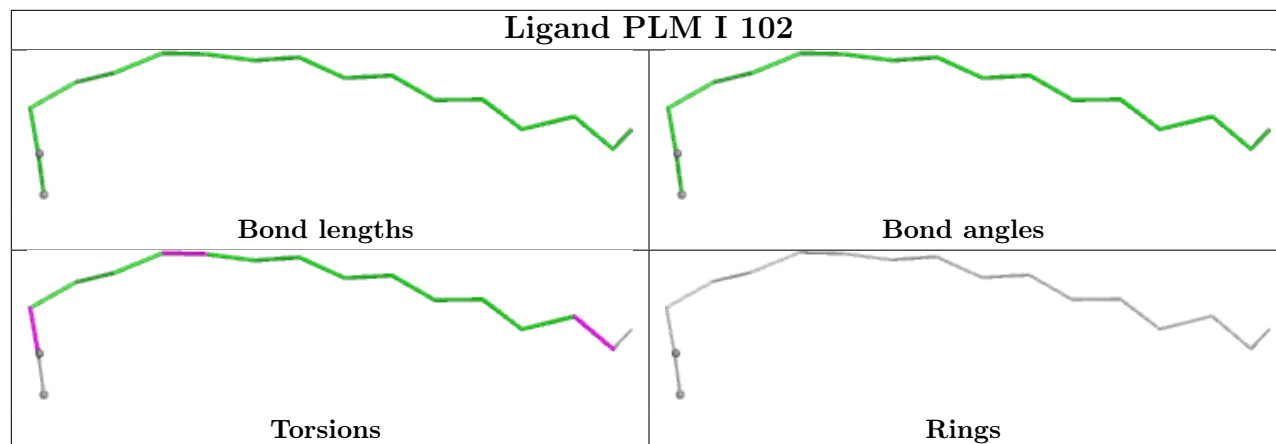
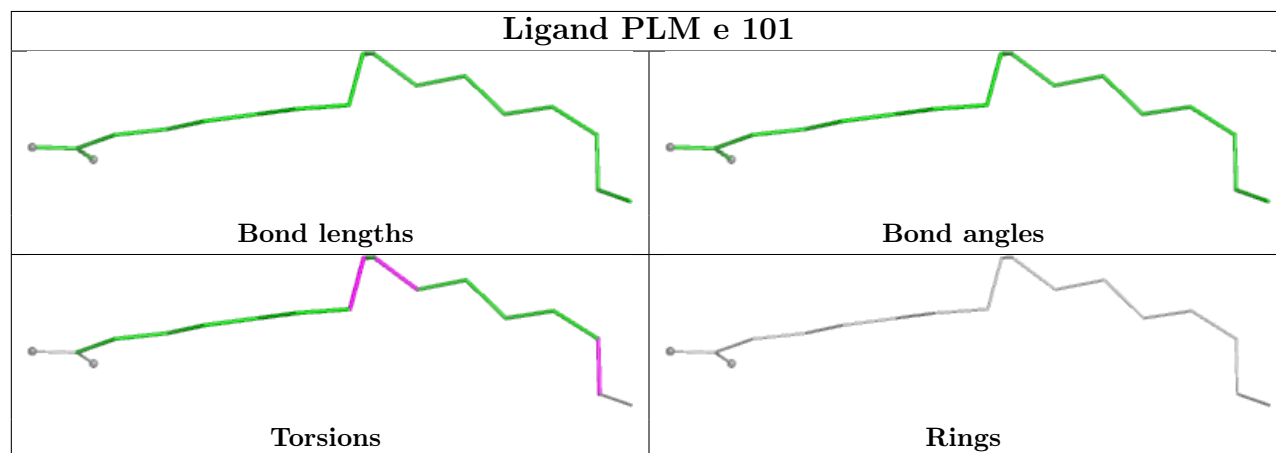
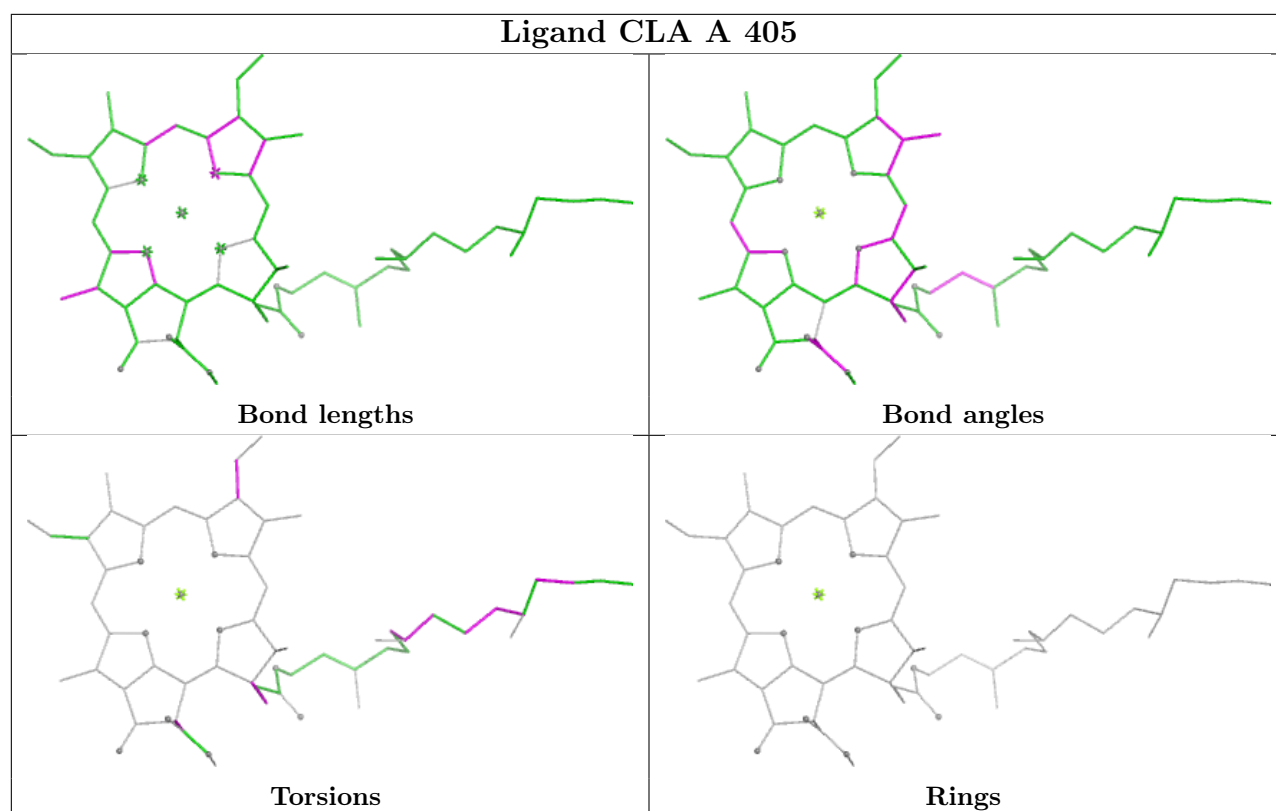


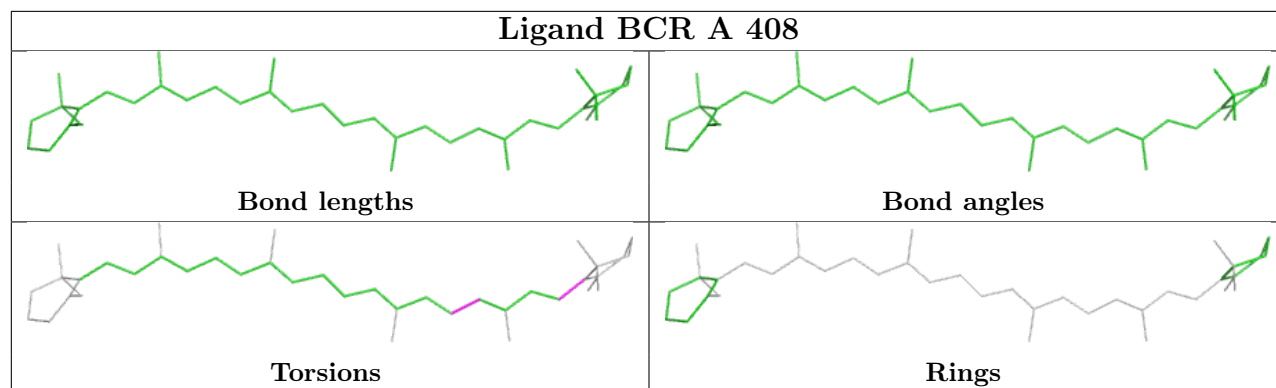
Rings











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.

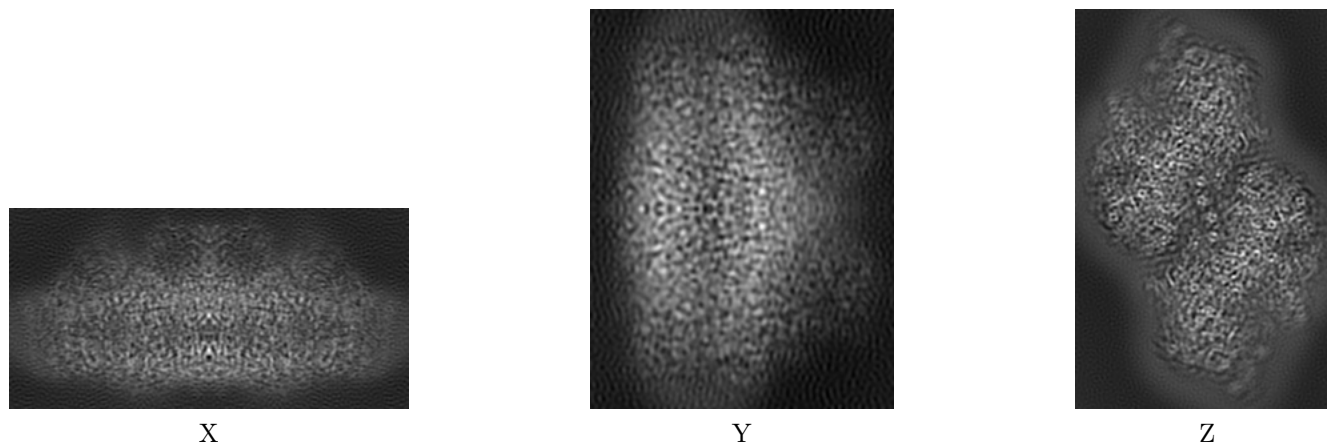
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51100. These allow visual inspection of the internal detail of the map and identification of artifacts.

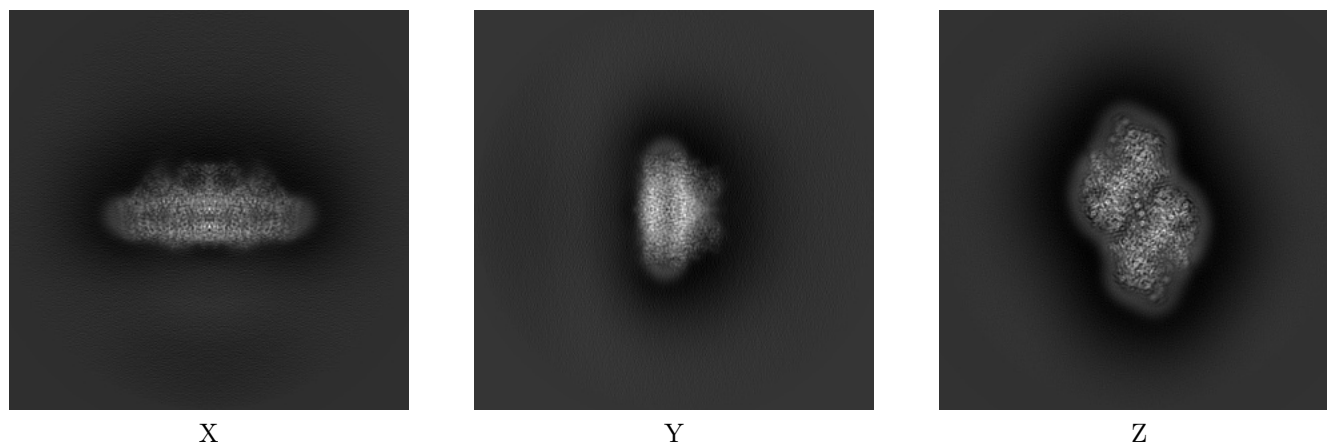
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



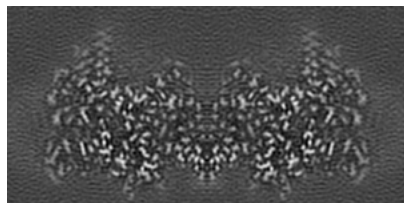
6.1.2 Raw map



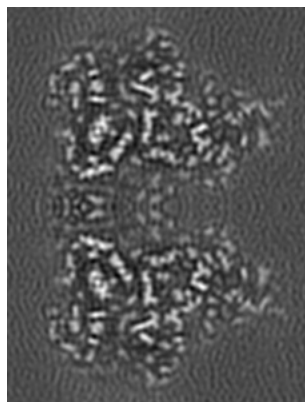
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

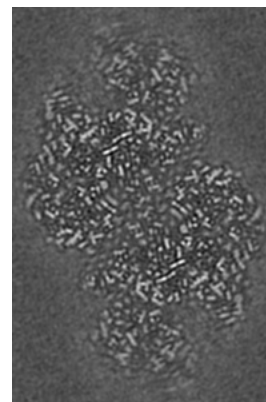
6.2.1 Primary map



X Index: 137

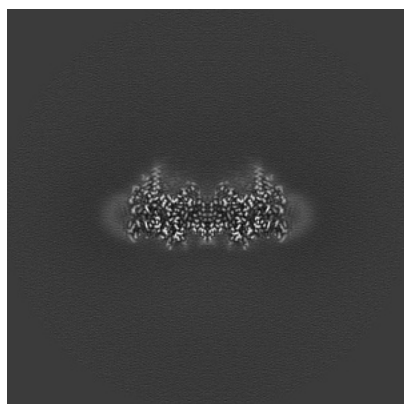


Y Index: 208

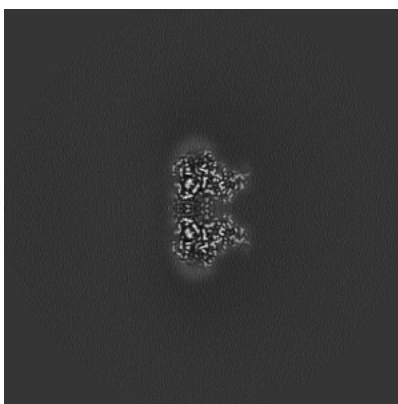


Z Index: 104

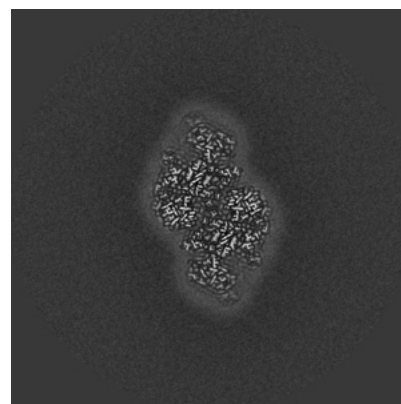
6.2.2 Raw map



X Index: 200



Y Index: 200

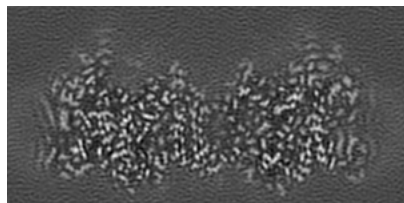


Z Index: 200

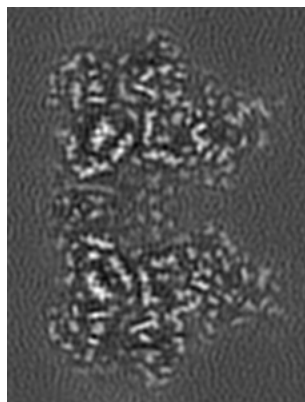
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

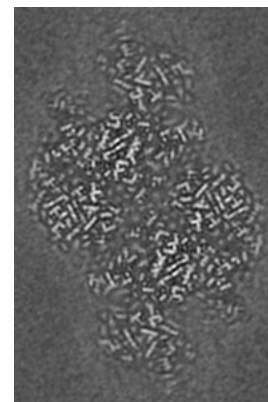
6.3.1 Primary map



X Index: 142

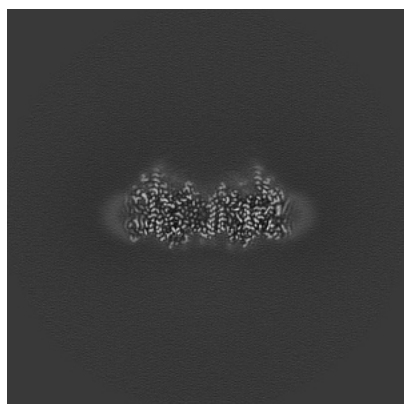


Y Index: 209

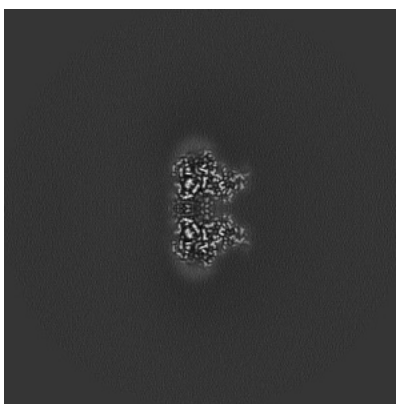


Z Index: 98

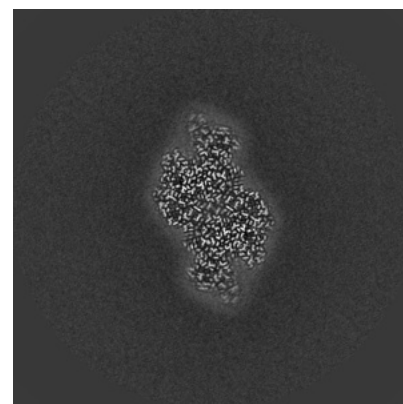
6.3.2 Raw map



X Index: 198



Y Index: 200

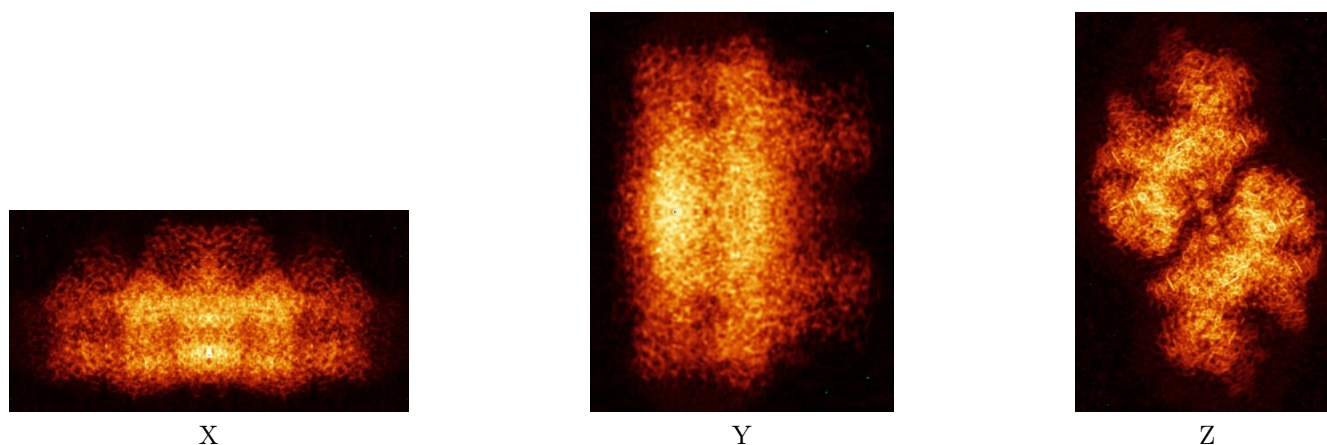


Z Index: 207

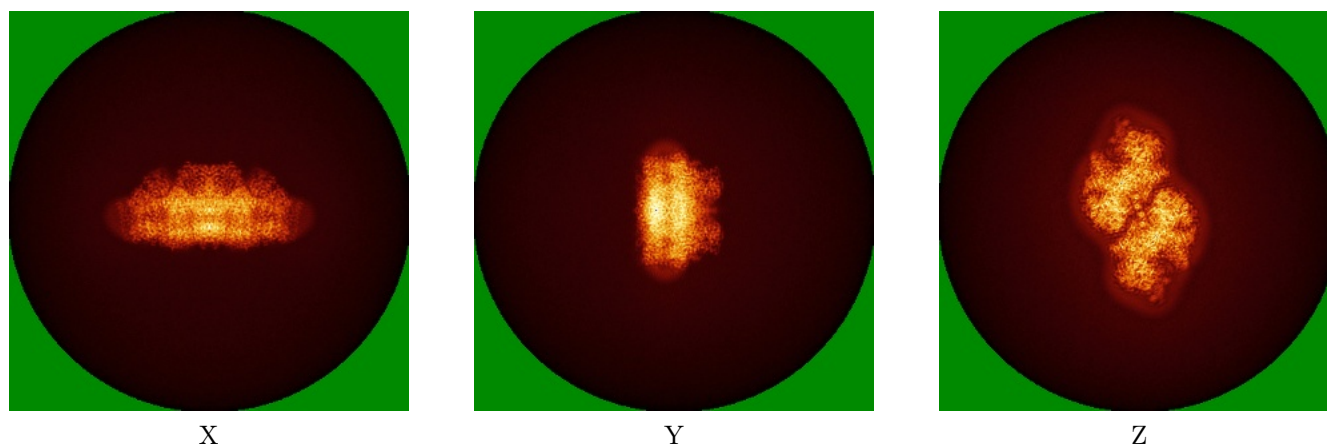
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



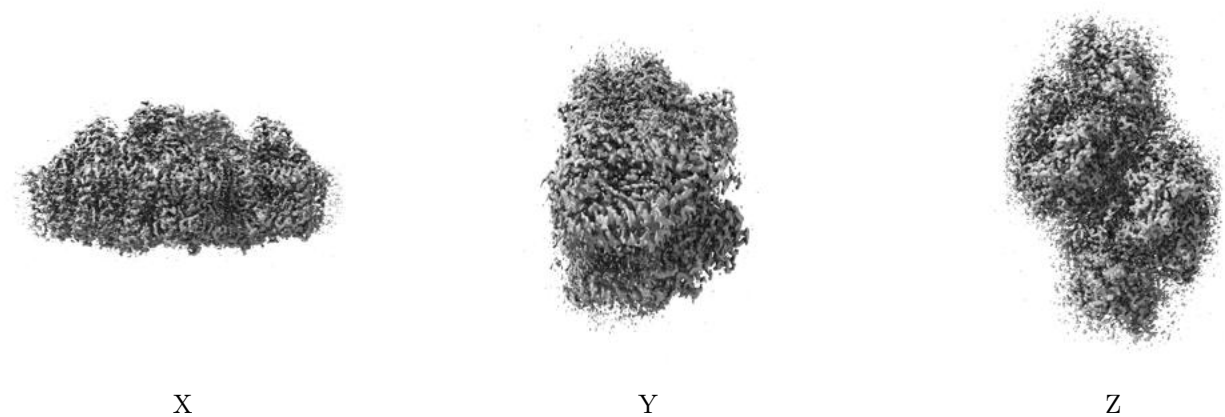
6.4.2 Raw map



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.

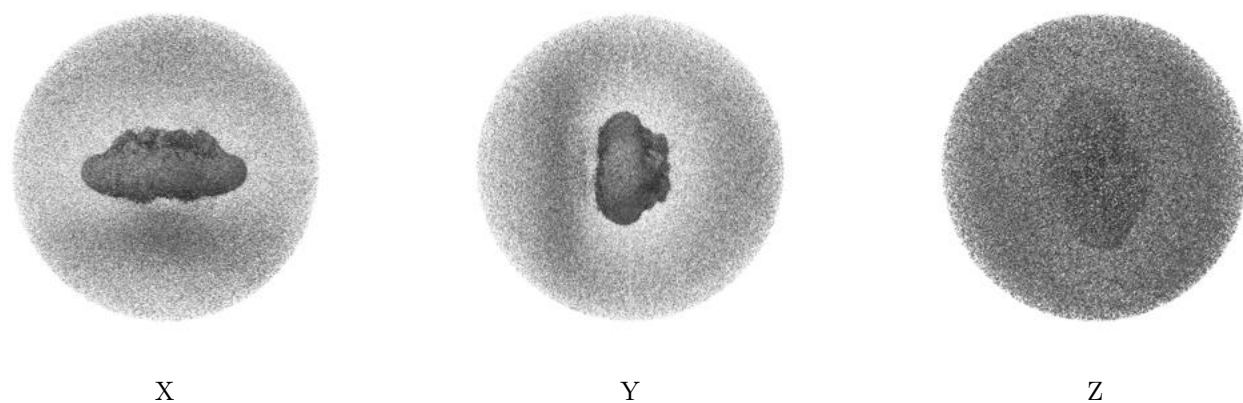
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.037. 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.

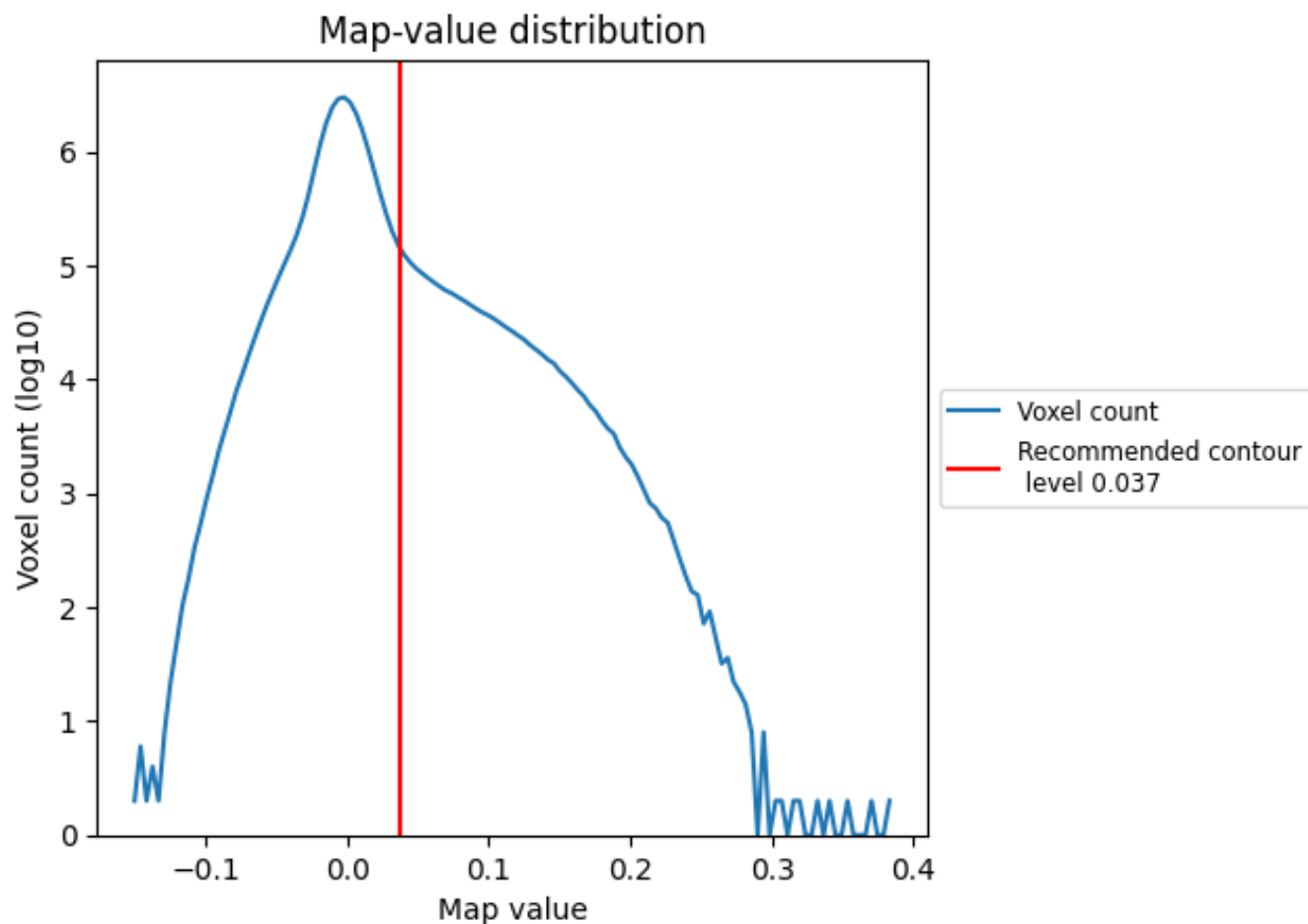
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

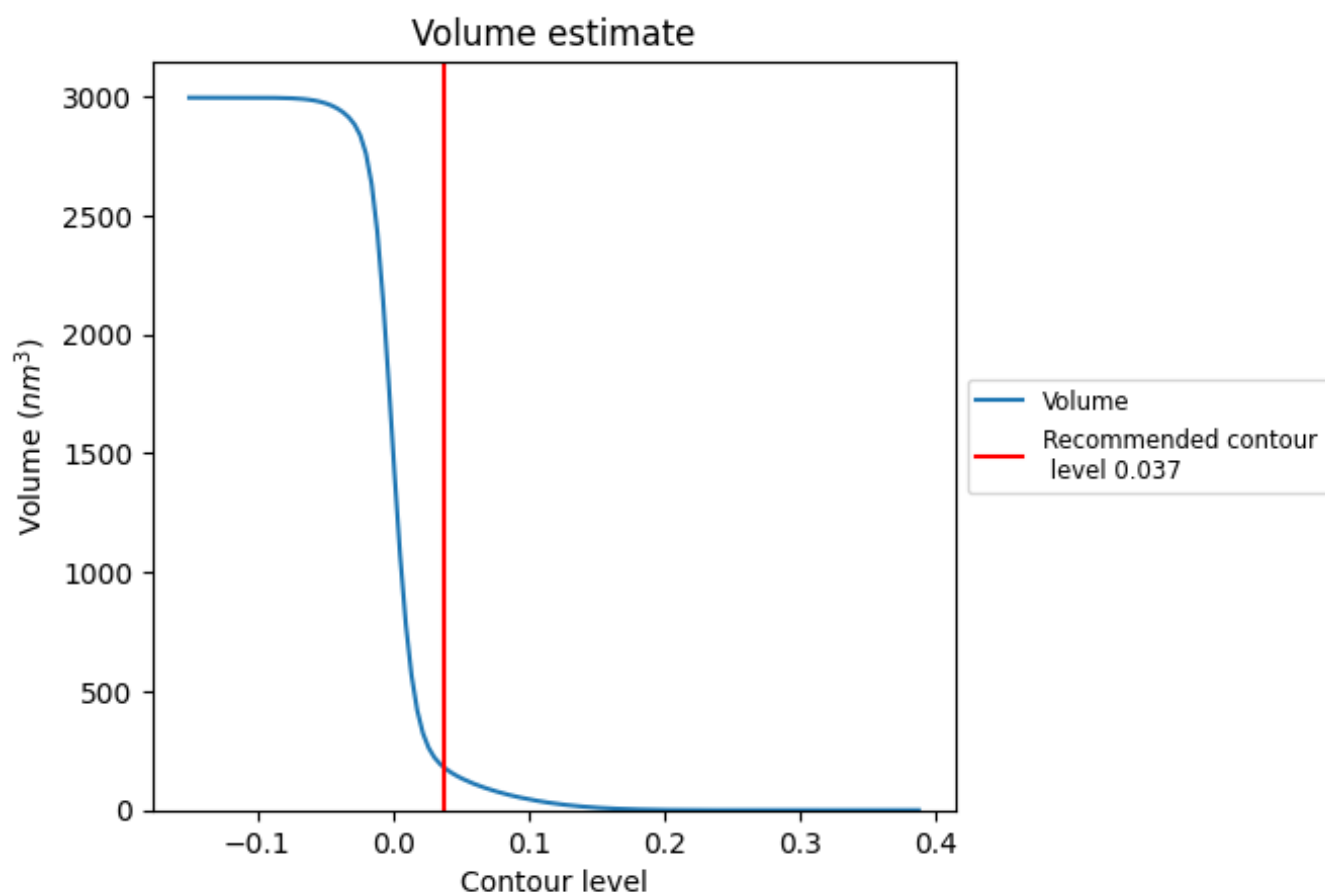
This section contains the results of statistical analysis of the map.

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 184 nm³; this corresponds to an approximate mass of 166 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.

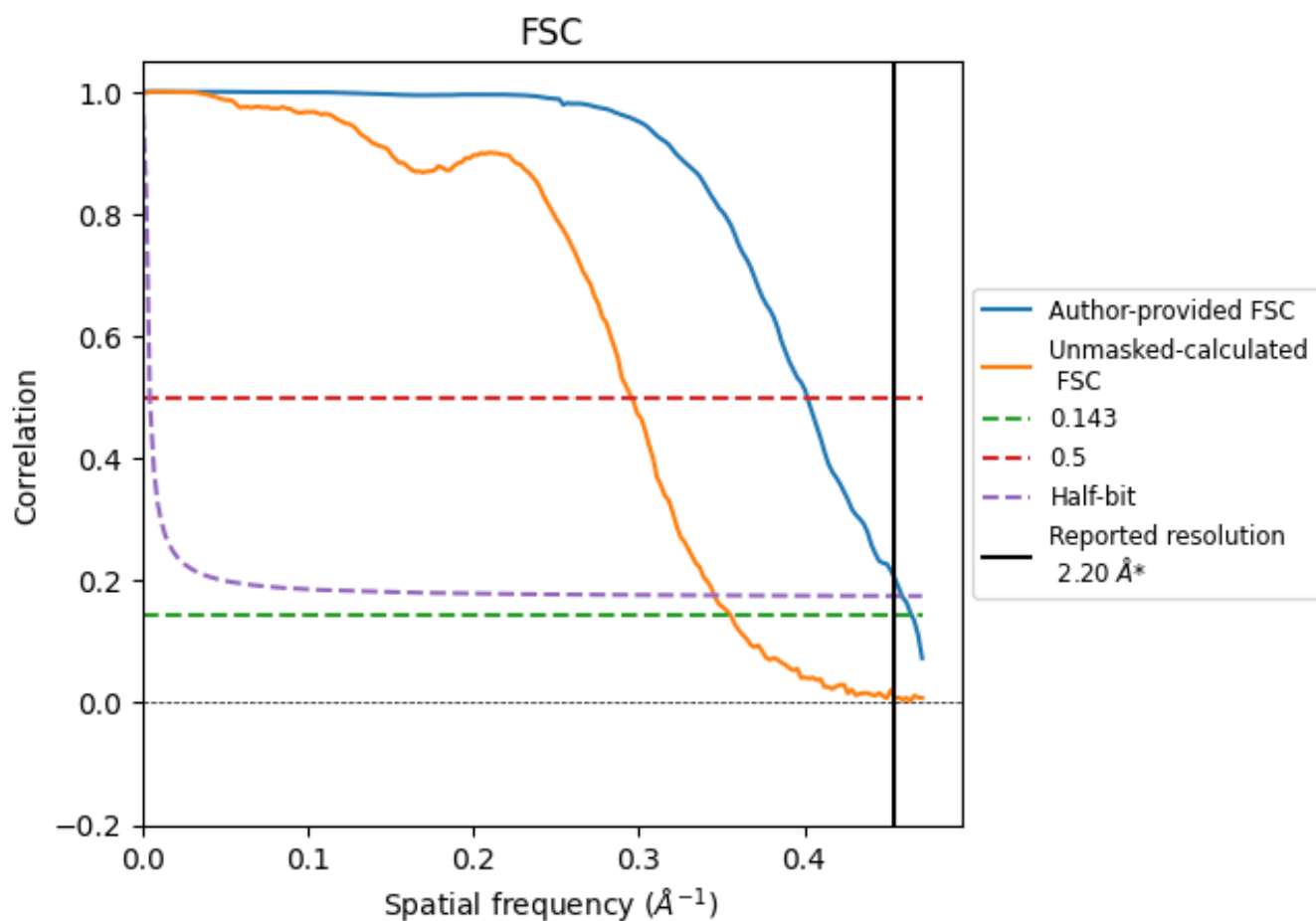
7.3 Rotationally averaged power spectrum [i](#)

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

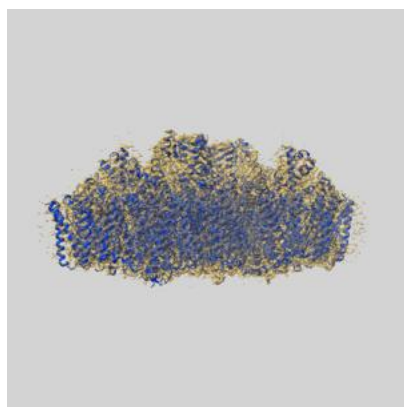
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.15	2.49	2.18
Unmasked-calculated*	2.81	3.38	2.89

*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 2.81 differs from the reported value 2.2 by more than 10 %

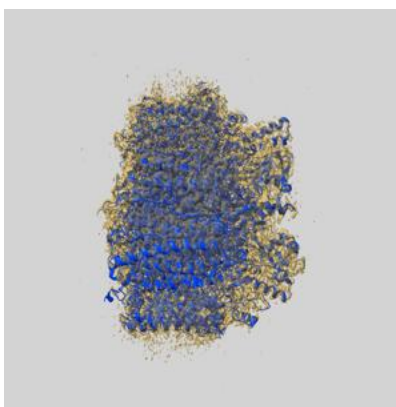
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51100 and PDB model 9G6F. Per-residue inclusion information can be found in section [3](#) on page [27](#).

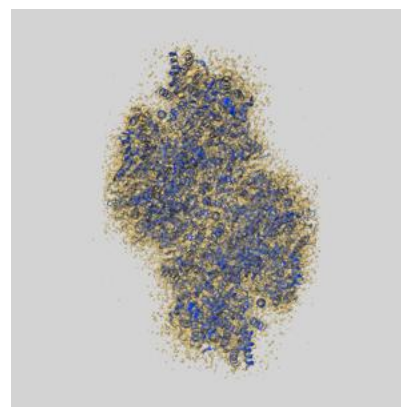
9.1 Map-model overlay [i](#)



X



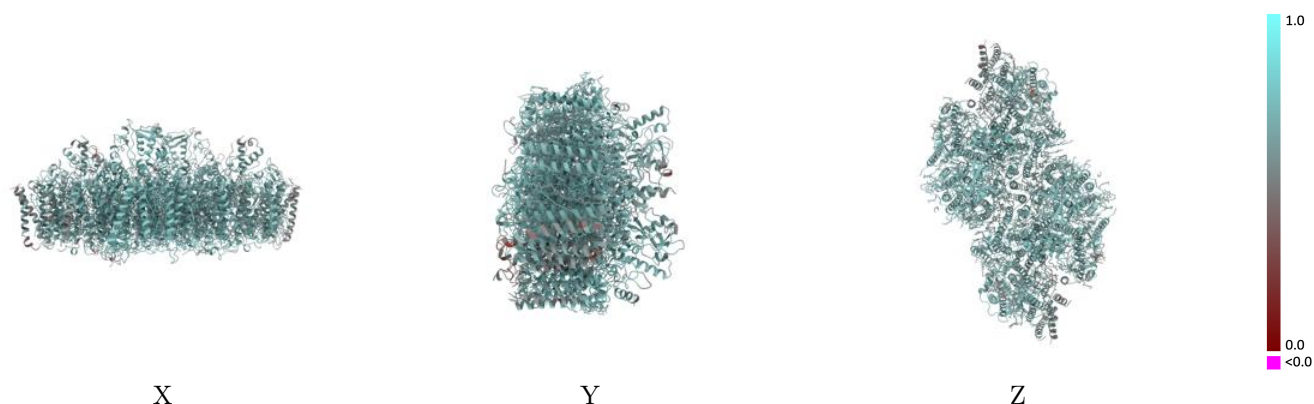
Y



Z

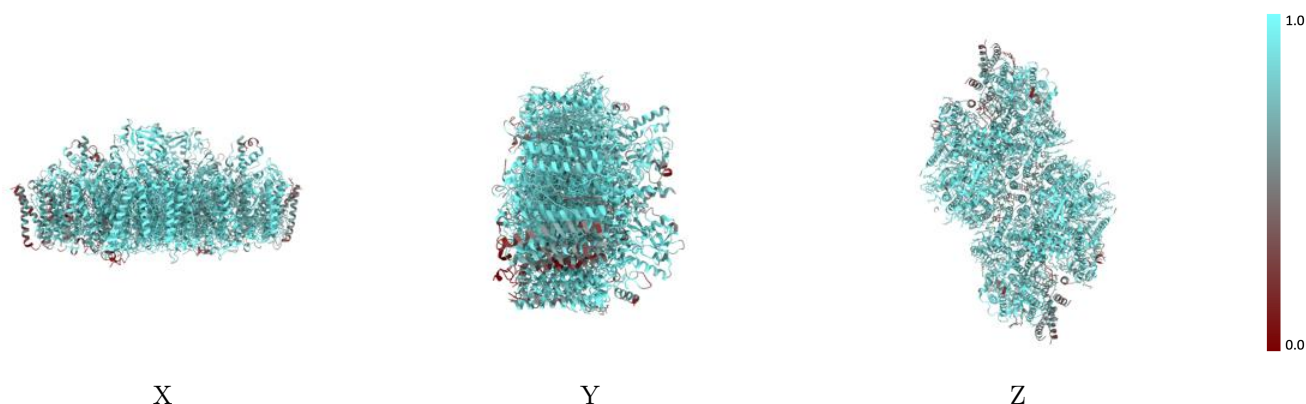
The images above show the 3D surface view of the map at the recommended contour level 0.037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



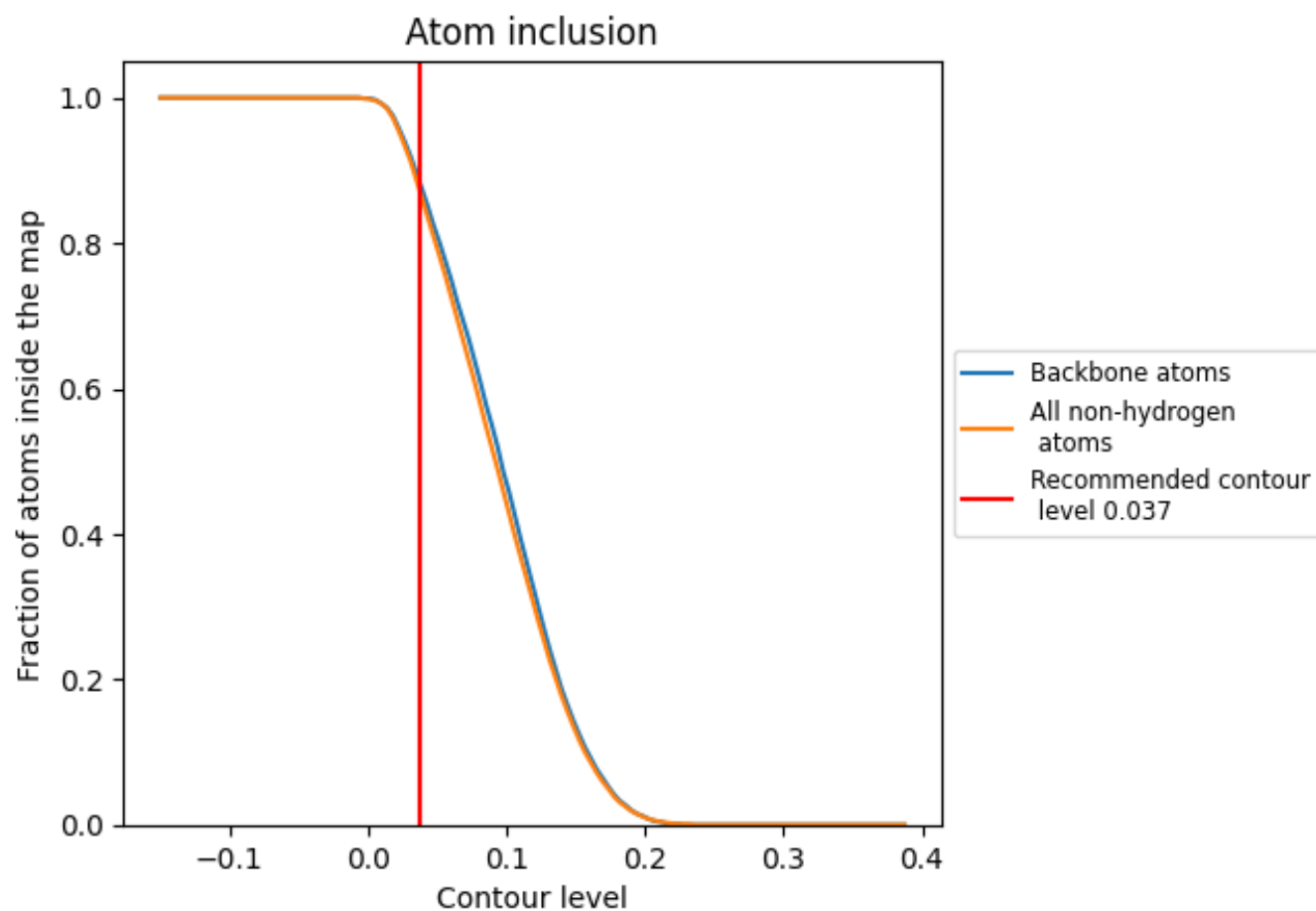
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.037).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.6690
A	 0.9290	 0.7000
B	 0.9110	 0.6820
C	 0.8770	 0.6630
D	 0.9410	 0.7010
E	 0.6890	 0.5760
F	 0.7370	 0.6100
H	 0.9250	 0.6760
I	 0.8870	 0.6710
J	 0.4120	 0.5200
K	 0.8350	 0.6350
L	 0.9010	 0.6850
M	 0.8520	 0.6610
T	 0.9250	 0.7070
X	 0.8610	 0.6600
Y	 0.5310	 0.5490
Z	 0.5040	 0.5240
a	 0.9150	 0.6910
b	 0.9120	 0.6900
c	 0.8530	 0.6460
d	 0.9430	 0.7060
e	 0.7130	 0.5940
f	 0.7000	 0.6030
h	 0.9460	 0.6910
i	 0.8380	 0.6470
j	 0.3790	 0.5080
k	 0.8510	 0.6250
l	 0.9040	 0.6820
m	 0.8600	 0.6680
t	 0.9020	 0.6800
x	 0.9120	 0.6730
y	 0.5590	 0.5650
z	 0.4920	 0.4990

