



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 06:40 PM EDT

PDB ID : 5E79 / pdb\_00005e79  
Title : Macromolecular diffractive imaging using imperfect crystals  
Authors : Ayer, K.; Yefanov, O.; Oberthur, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffer, A.; Dorner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.  
Deposited on : 2015-10-12  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12

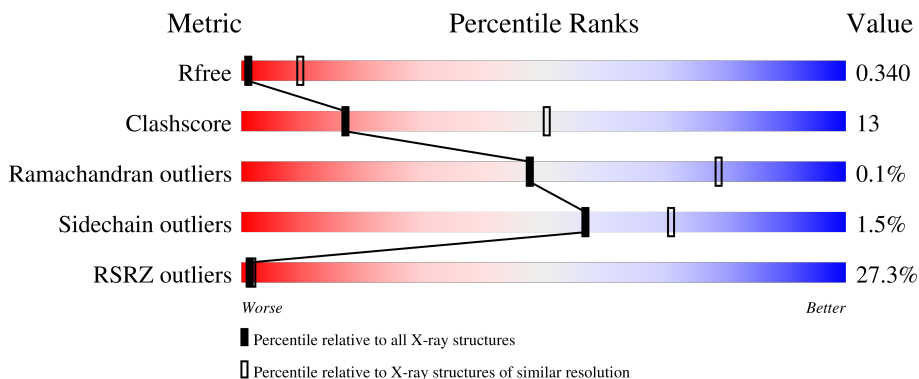
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CL	U	201	-	-	-	X
22	CL	a	604	-	-	-	X
22	CL	u	201	-	-	-	X
23	BCT	A	605	-	X	-	-
23	BCT	a	605	-	X	-	-
24	CLA	A	606	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	609	X	-	-	-
24	CLA	B	602	X	-	-	-

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Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607[A]	X	-	-	-
24	CLA	B	607[B]	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	606	X	-	-	-
24	CLA	a	607	X	-	-	-
24	CLA	a	609	X	-	-	-
24	CLA	a	615	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608[A]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	b	608[B]	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	A	610	-	X	-	-
26	BCR	B	618	-	X	X	-
26	BCR	B	619	-	X	-	-
26	BCR	B	620	-	X	-	-
26	BCR	C	514	-	X	-	-
26	BCR	F	101	-	X	-	-
26	BCR	H	101	-	X	-	-
26	BCR	I	101	-	X	-	-
26	BCR	K	101	-	X	-	-
26	BCR	K	102	-	X	-	-
26	BCR	T	101	-	X	X	-
26	BCR	a	610	-	X	-	-
26	BCR	b	619	-	X	X	-
26	BCR	b	620	-	X	-	-
26	BCR	b	621	-	X	-	-
26	BCR	c	514	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	BCR	c	515	-	X	-	-
26	BCR	c	521	-	X	-	-
26	BCR	f	101	-	X	X	-
26	BCR	h	101	-	X	-	-
26	BCR	k	101	-	X	-	-
26	BCR	t	101	-	X	X	-
27	PL9	D	405	-	X	-	-
27	PL9	a	611	-	-	-	X
27	PL9	d	404	-	X	-	-
29	LMG	Z	101	-	-	-	X
29	LMG	c	520	-	-	-	X
30	LHG	E	102	-	-	-	X
31	CA	b	602	-	-	-	X

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

## 2 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	250.80Å 250.80Å 250.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 29.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.98-3.50) 99.8 (29.98-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.324 , 0.331 0.344 , 0.340	Depositor DCC
$R_{free}$ test set	45921 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 21.7	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	50074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

### 3 Model quality

#### 3.1 Standard geometry

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

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	0.75	0/2734	0.99	1/3727 (0.0%)
1	a	0.64	0/2734	0.99	7/3727 (0.2%)
2	B	0.66	1/4194 (0.0%)	0.96	7/5713 (0.1%)
2	b	0.63	0/4194	0.96	13/5713 (0.2%)
3	C	0.64	0/3634	1.00	4/4947 (0.1%)
3	c	0.61	0/3634	0.95	5/4947 (0.1%)
4	D	0.67	0/2821	0.98	9/3844 (0.2%)
4	d	0.61	0/2821	0.93	6/3844 (0.2%)
5	E	0.62	0/693	0.94	0/944
5	e	0.60	0/693	0.93	0/944
6	F	0.76	1/284 (0.4%)	0.95	0/387
6	f	0.60	0/284	0.92	0/387
7	H	0.63	0/544	0.94	1/739 (0.1%)
7	h	0.64	0/544	0.91	1/739 (0.1%)
8	I	0.71	0/327	0.96	0/439
8	i	0.61	0/327	0.89	0/439
9	J	0.67	0/278	0.89	0/376
9	j	0.56	0/278	0.93	0/376
10	K	0.65	0/303	1.03	2/416 (0.5%)
10	k	0.77	0/303	1.41	4/416 (1.0%)
11	L	0.72	0/319	0.94	0/433
11	l	0.62	0/319	0.89	2/433 (0.5%)
12	M	0.69	0/278	1.18	1/378 (0.3%)
12	m	0.66	0/278	1.10	4/378 (1.1%)
13	O	0.59	0/1926	0.92	1/2611 (0.0%)
13	o	0.54	0/1926	0.88	2/2611 (0.1%)
14	T	0.81	0/282	0.90	0/382
14	t	0.65	0/282	0.92	0/382
15	U	0.63	0/785	0.87	0/1064
15	u	0.61	0/785	0.88	0/1064
16	V	0.64	0/1096	0.97	0/1487
16	v	0.56	0/1096	0.92	1/1487 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.61	0/216	0.96	1/289 (0.3%)
17	y	0.62	0/216	0.97	0/289
18	X	0.64	0/298	0.91	0/403
18	x	0.65	0/298	0.96	0/403
19	Z	0.61	0/490	1.00	0/669
19	z	0.68	1/490 (0.2%)	1.01	1/669 (0.1%)
All	All	0.64	3/43004 (0.0%)	0.96	73/58496 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	z	23	VAL	CA-CB	6.75	1.57	1.54
6	F	28	VAL	CA-CB	5.67	1.57	1.54
2	B	381	ILE	CA-CB	-5.42	1.48	1.53

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	k	11	LEU	CA-C-N	-8.17	109.63	119.84
10	k	11	LEU	C-N-CA	-8.17	109.63	119.84
4	d	170	ALA	CA-C-N	-8.03	111.73	119.76
4	d	170	ALA	C-N-CA	-8.03	111.73	119.76
4	D	170	ALA	CA-C-N	-7.58	112.18	119.76

There are no chirality outliers.

There are no planarity outliers.

### 3.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2637	0	2551	68	0
1	a	2637	0	2551	59	0
2	B	4024	0	3901	100	0
2	b	4024	0	3901	99	0
3	C	3506	0	3439	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3506	0	3439	61	0
4	D	2726	0	2627	76	0
4	d	2726	0	2627	65	0
5	E	668	0	658	16	0
5	e	668	0	658	7	0
6	F	275	0	282	17	0
6	f	275	0	282	11	0
7	H	525	0	558	20	0
7	h	525	0	558	18	0
8	I	320	0	339	7	0
8	i	320	0	339	4	0
9	J	272	0	279	2	0
9	j	272	0	279	5	0
10	K	293	0	305	10	0
10	k	293	0	305	15	0
11	L	309	0	327	14	0
11	l	309	0	327	13	0
12	M	272	0	300	10	0
12	m	272	0	300	11	0
13	O	1883	0	1865	28	0
13	o	1883	0	1865	26	0
14	T	270	0	278	15	0
14	t	270	0	278	13	0
15	U	774	0	773	9	0
15	u	774	0	773	8	0
16	V	1072	0	1088	13	0
16	v	1072	0	1088	9	0
17	Y	215	0	246	2	0
17	y	215	0	246	6	0
18	X	292	0	328	8	0
18	x	292	0	328	9	0
19	Z	479	0	516	2	0
19	z	479	0	516	2	0
20	A	10	0	0	0	0
20	a	10	0	0	1	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	1	0
22	U	1	0	0	0	0
22	a	2	0	0	0	0
22	u	1	0	0	0	0
23	A	4	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	4	0	1	0	0
24	A	195	0	216	19	0
24	B	1105	0	1224	67	0
24	C	845	0	936	53	0
24	D	195	0	216	13	0
24	a	260	0	288	16	0
24	b	1105	0	1224	59	0
24	c	845	0	936	40	0
24	d	130	0	144	7	0
25	A	64	0	74	3	0
25	D	64	0	74	10	0
25	a	64	0	74	2	0
25	d	64	0	74	4	0
26	A	40	0	55	14	0
26	B	120	0	165	58	0
26	C	40	0	55	14	0
26	F	40	0	55	20	0
26	H	40	0	55	16	0
26	I	40	0	55	18	0
26	K	80	0	110	29	0
26	T	40	0	55	22	0
26	a	40	0	55	13	0
26	b	120	0	166	59	0
26	c	120	0	165	53	0
26	f	40	0	55	21	0
26	h	40	0	55	17	0
26	k	40	0	55	18	0
26	t	40	0	55	23	0
27	A	55	0	80	11	0
27	D	55	0	80	13	0
27	a	55	0	80	12	0
27	d	55	0	80	7	0
28	A	108	0	156	7	0
28	B	54	0	30	8	0
28	L	54	0	26	12	0
28	X	43	0	53	3	0
28	a	108	0	156	3	0
28	b	54	0	30	12	0
28	l	54	0	29	5	0
28	x	43	0	53	4	0
29	A	51	0	72	2	0
29	B	51	0	72	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C	102	0	144	4	0
29	D	51	0	72	7	0
29	Z	37	0	44	0	0
29	a	51	0	72	1	0
29	b	51	0	72	4	0
29	c	102	0	144	2	0
29	j	51	0	72	6	0
29	z	37	0	44	1	0
30	A	49	0	74	10	0
30	D	98	0	148	8	0
30	E	42	0	57	0	0
30	L	49	0	74	6	0
30	a	49	0	74	10	0
30	d	98	0	148	4	0
30	e	42	0	57	2	0
30	l	49	0	74	6	0
31	B	1	0	0	0	0
31	F	1	0	0	0	0
31	O	1	0	0	0	0
31	b	1	0	0	0	0
31	f	1	0	0	0	0
31	o	1	0	0	0	0
32	C	186	0	246	5	0
32	E	62	0	82	1	0
32	H	62	0	82	6	0
32	c	186	0	246	8	0
32	d	62	0	82	4	0
32	h	62	0	82	6	0
33	E	43	0	30	6	0
33	V	43	0	30	7	0
33	e	43	0	30	2	0
33	v	43	0	30	4	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	50074	0	51320	1280	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 13.

The worst 5 of 1280 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)
26:T:101:BCR:C22	26:T:101:BCR:C37	1.74	1.65
26:B:619:BCR:C19	26:B:619:BCR:C20	1.76	1.64
26:B:620:BCR:C37	26:B:620:BCR:C22	1.76	1.64
26:c:514:BCR:C20	26:c:514:BCR:C19	1.74	1.62
26:b:619:BCR:C22	26:b:619:BCR:C37	1.75	1.62

There are no symmetry-related clashes.

### 3.3 Torsion angles [\(i\)](#)

#### 3.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	36	67
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	36	67
2	B	512/504 (102%)	506 (99%)	6 (1%)	0	100	100
2	b	512/504 (102%)	505 (99%)	7 (1%)	0	100	100
3	C	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	30	62
3	c	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	30	62
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	3	26
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	62
13	o	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	62
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5139 (98%)	104 (2%)	9 (0%)	48	74

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	412/402 (102%)	406 (98%)	6 (2%)	57	71
2	b	412/402 (102%)	406 (98%)	6 (2%)	57	71
3	C	357/352 (101%)	349 (98%)	8 (2%)	45	65
3	c	357/352 (101%)	352 (99%)	5 (1%)	59	71
4	D	277/277 (100%)	275 (99%)	2 (1%)	76	78
4	d	277/277 (100%)	275 (99%)	2 (1%)	76	78
5	E	74/72 (103%)	73 (99%)	1 (1%)	59	71
5	e	74/72 (103%)	73 (99%)	1 (1%)	59	71
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	57
6	f	28/28 (100%)	27 (96%)	1 (4%)	31	57
7	H	56/54 (104%)	53 (95%)	3 (5%)	20	46
7	h	56/54 (104%)	53 (95%)	3 (5%)	20	46
8	I	36/35 (103%)	36 (100%)	0	100	100
8	i	36/35 (103%)	36 (100%)	0	100	100
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	41
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	28
11	L	36/35 (103%)	35 (97%)	1 (3%)	38	61
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	61
12	M	32/31 (103%)	31 (97%)	1 (3%)	35	59
12	m	32/31 (103%)	30 (94%)	2 (6%)	16	42
13	O	210/206 (102%)	206 (98%)	4 (2%)	50	68
13	o	210/206 (102%)	206 (98%)	4 (2%)	50	68

*Continued on next page...*

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	63	73
15	u	84/84 (100%)	83 (99%)	1 (1%)	63	73
16	V	118/117 (101%)	117 (99%)	1 (1%)	73	77
16	v	118/117 (101%)	117 (99%)	1 (1%)	73	77
17	Y	22/22 (100%)	21 (96%)	1 (4%)	24	50
17	y	22/22 (100%)	21 (96%)	1 (4%)	24	50
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	33 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	55
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	55
All	All	4370/4302 (102%)	4303 (98%)	67 (2%)	57	71

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	m	20	VAL
13	o	62	GLU
19	z	4	LEU
12	M	9	ILE
11	L	1	MET

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

Mol	Chain	Res	Type
1	a	198	HIS
19	z	58	ASN
2	b	26	HIS
4	d	197	HIS
1	a	338	ASN

### 3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 3.6 Ligand geometry [i](#)

Of 168 ligands modelled in this entry, 168 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

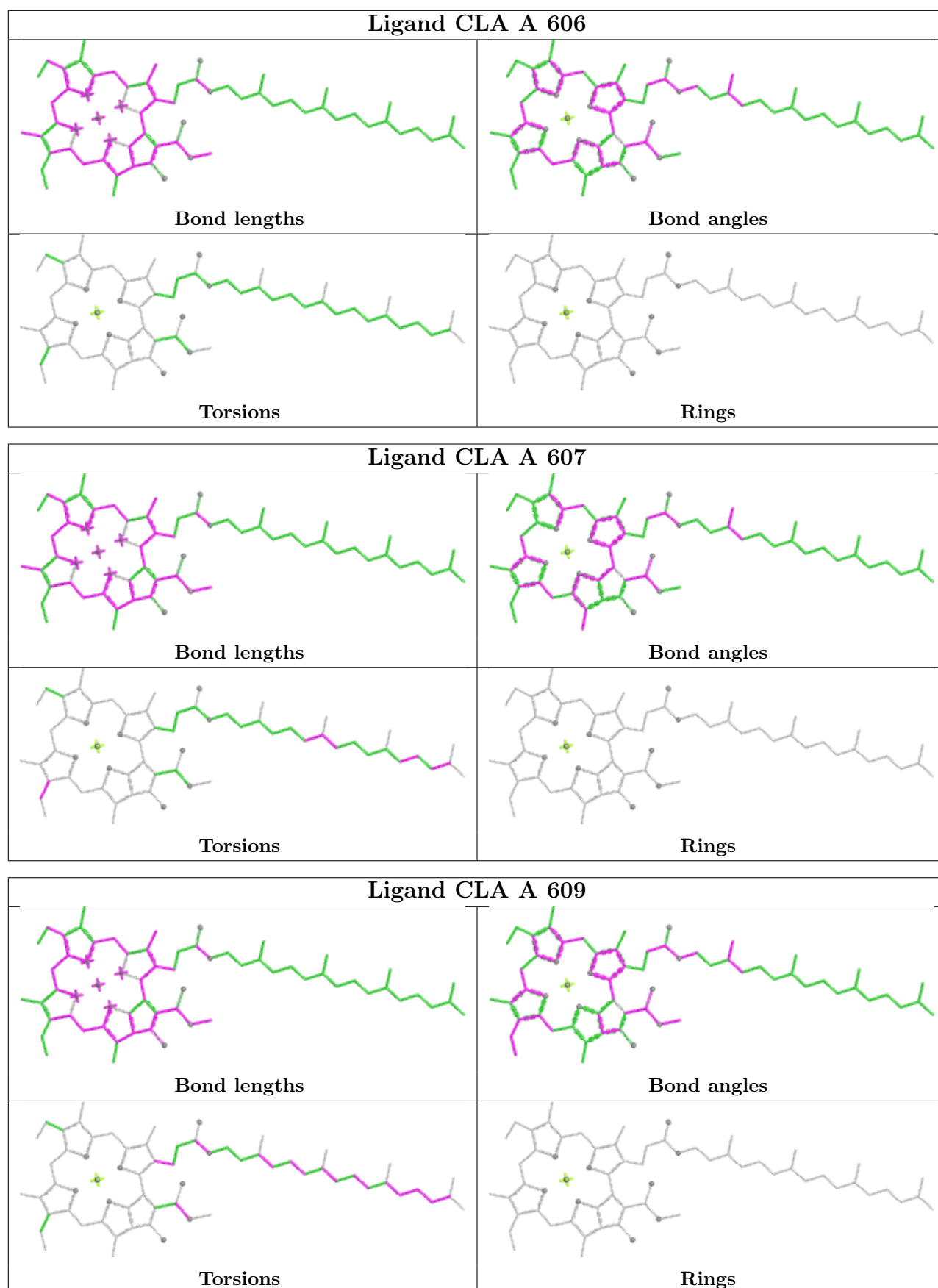
There are no chirality outliers.

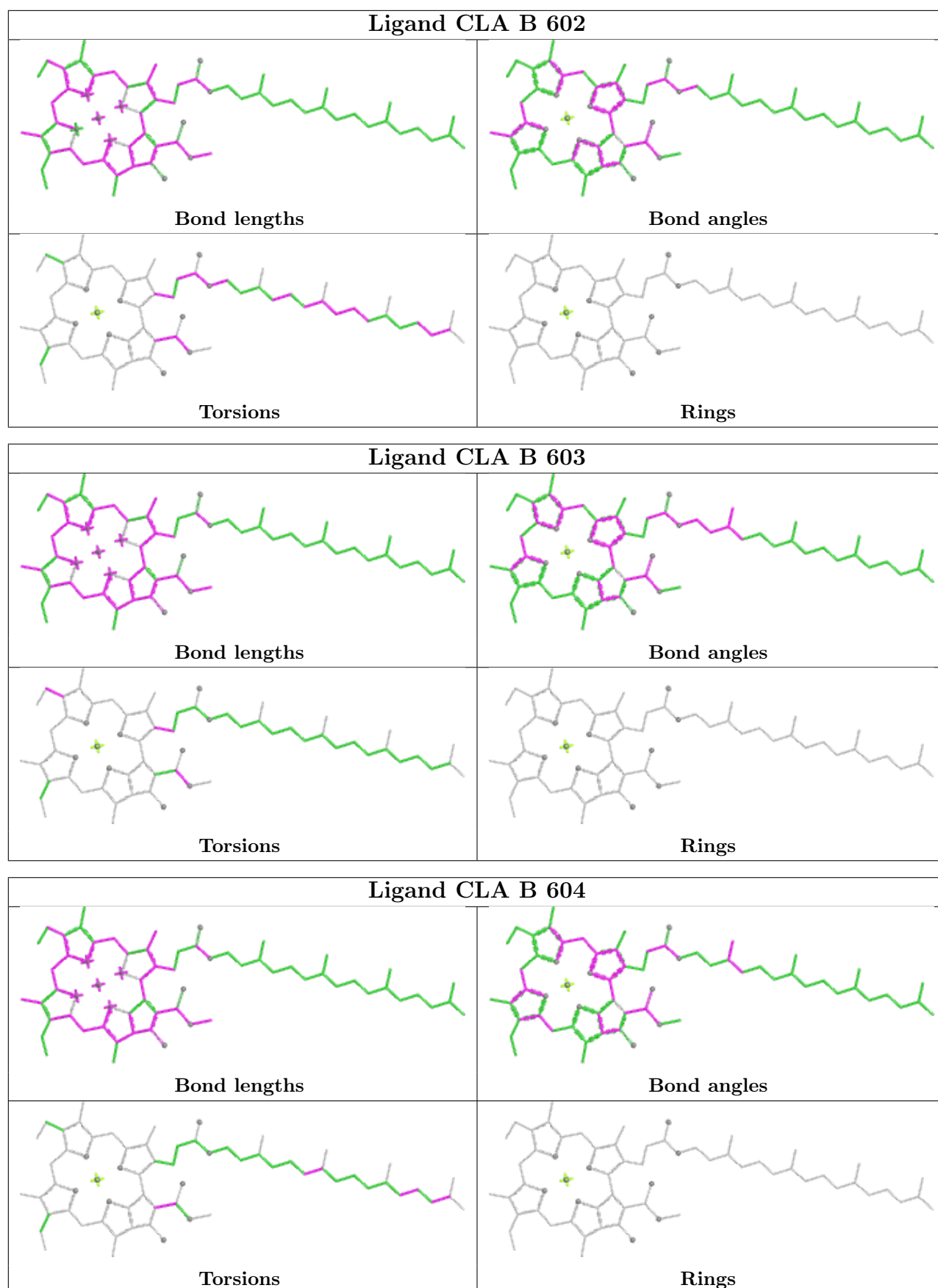
There are no torsion outliers.

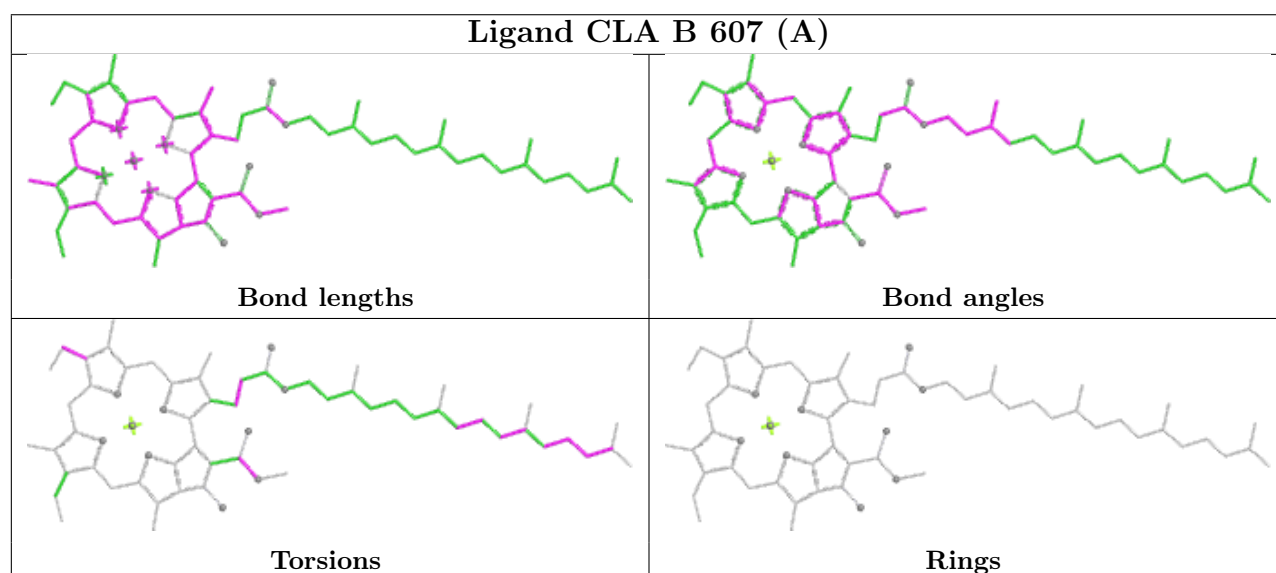
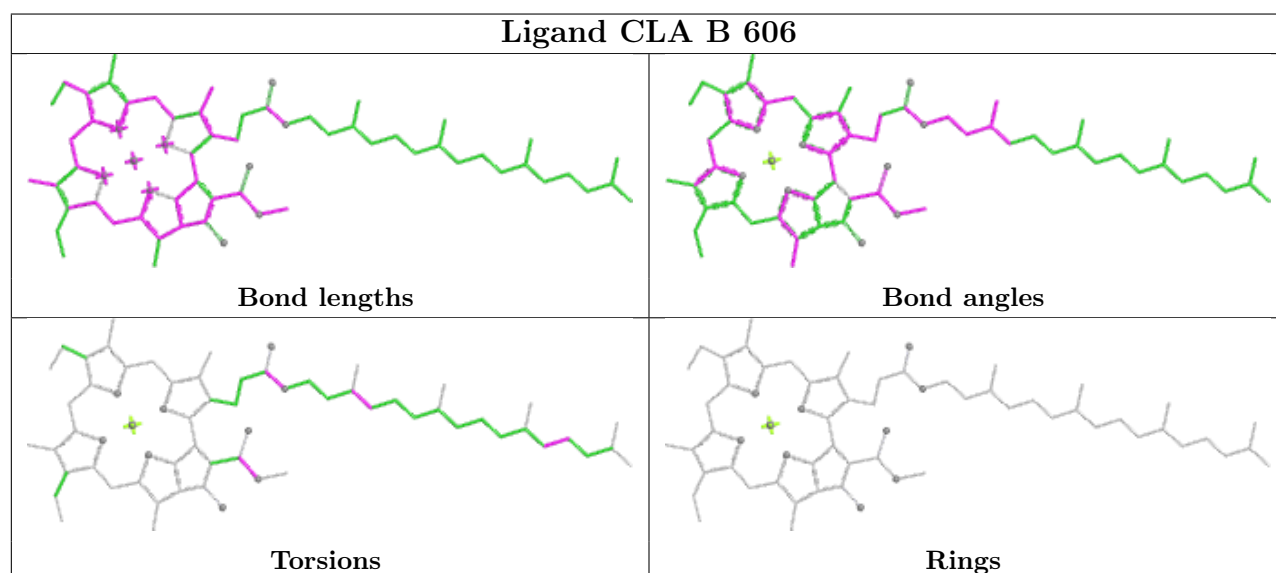
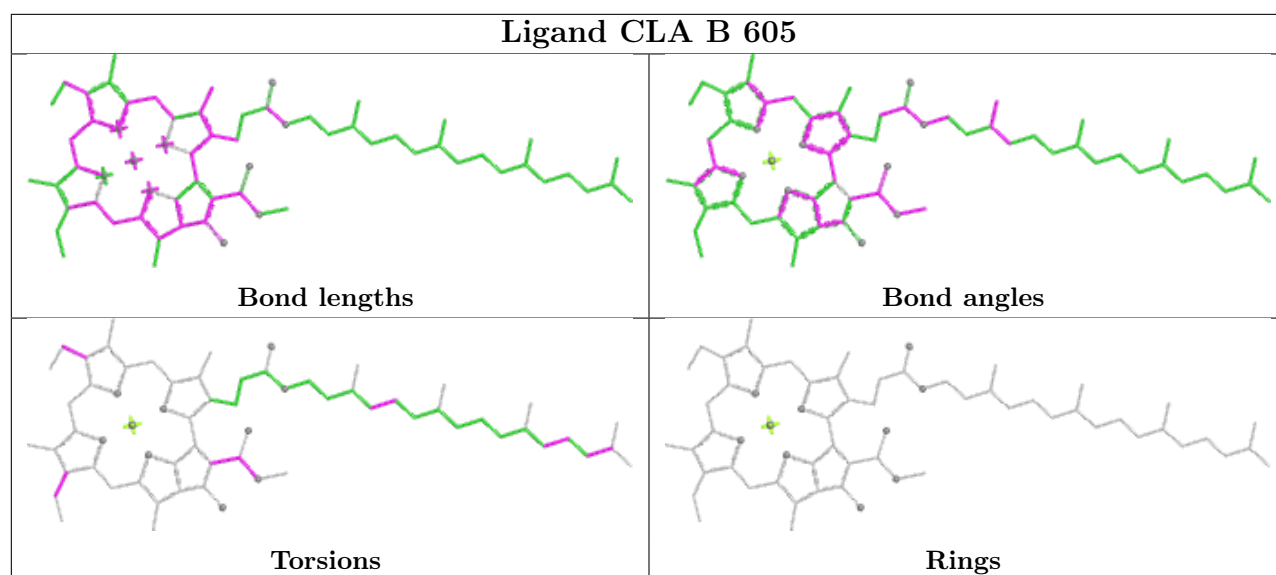
There are no ring outliers.

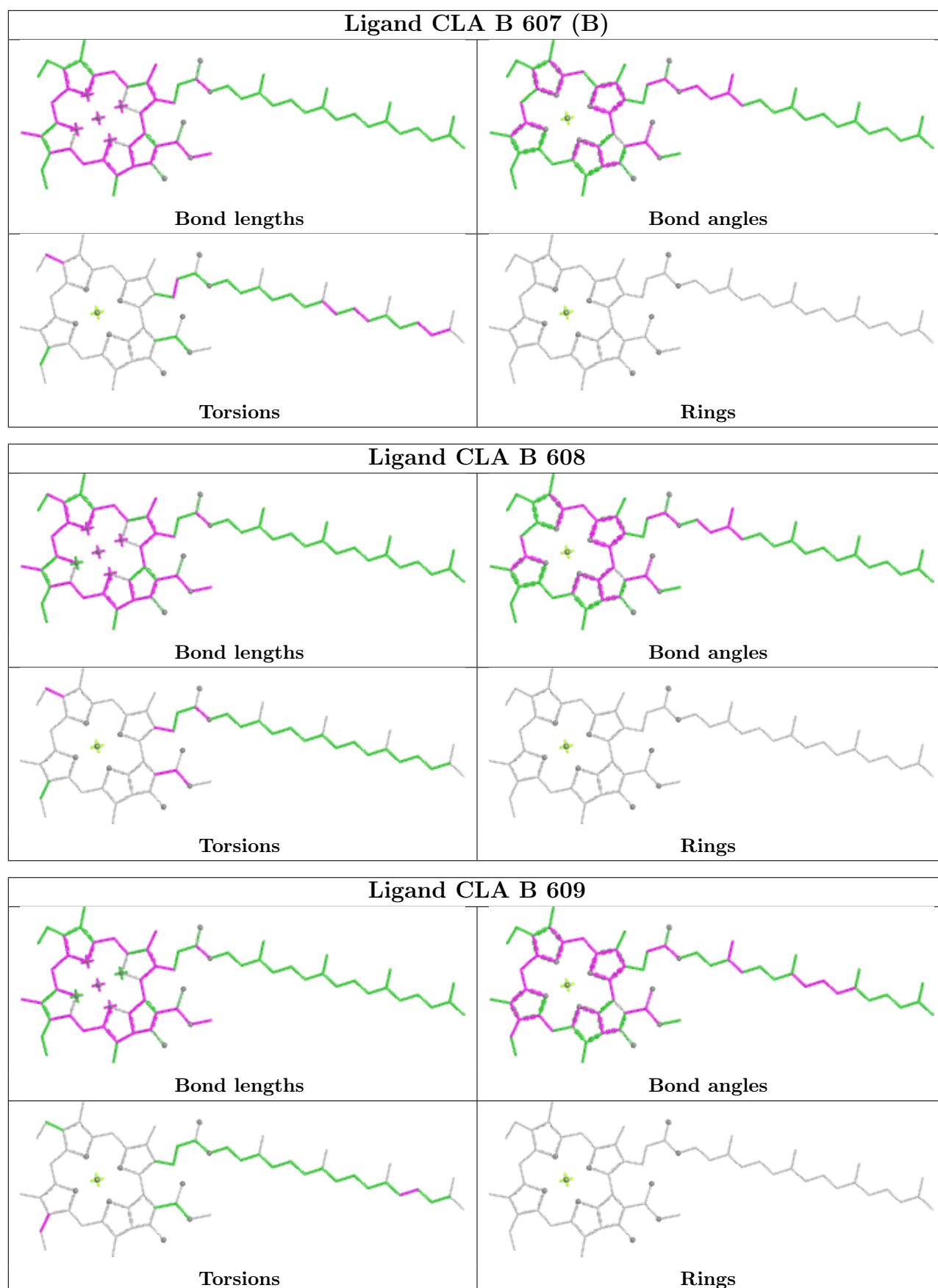
No monomer is involved in short contacts.

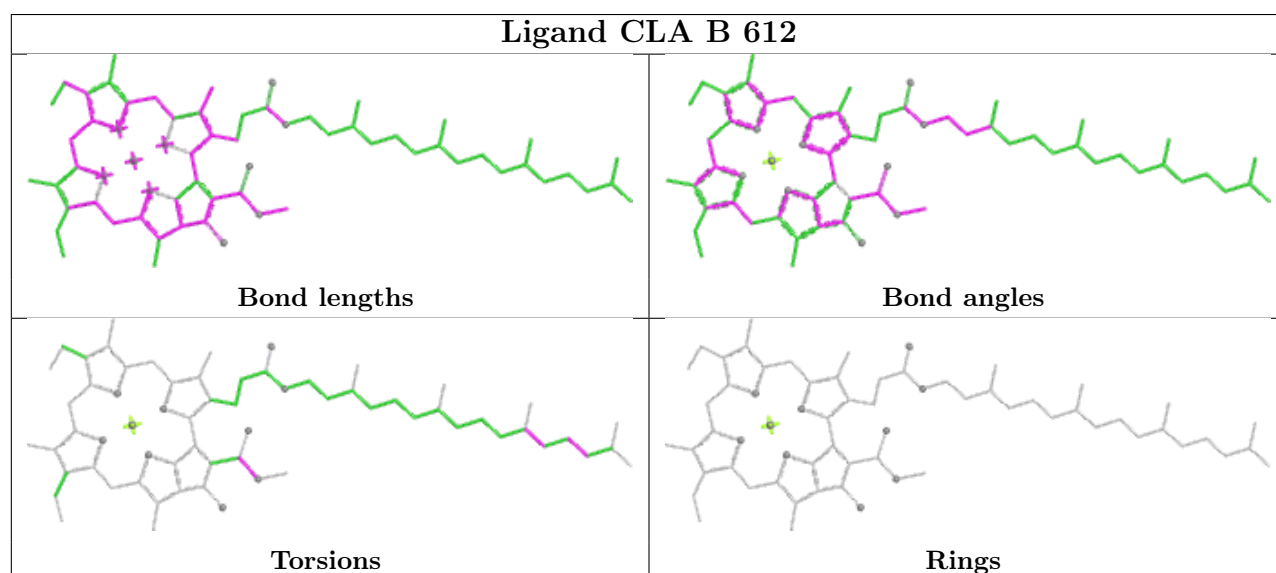
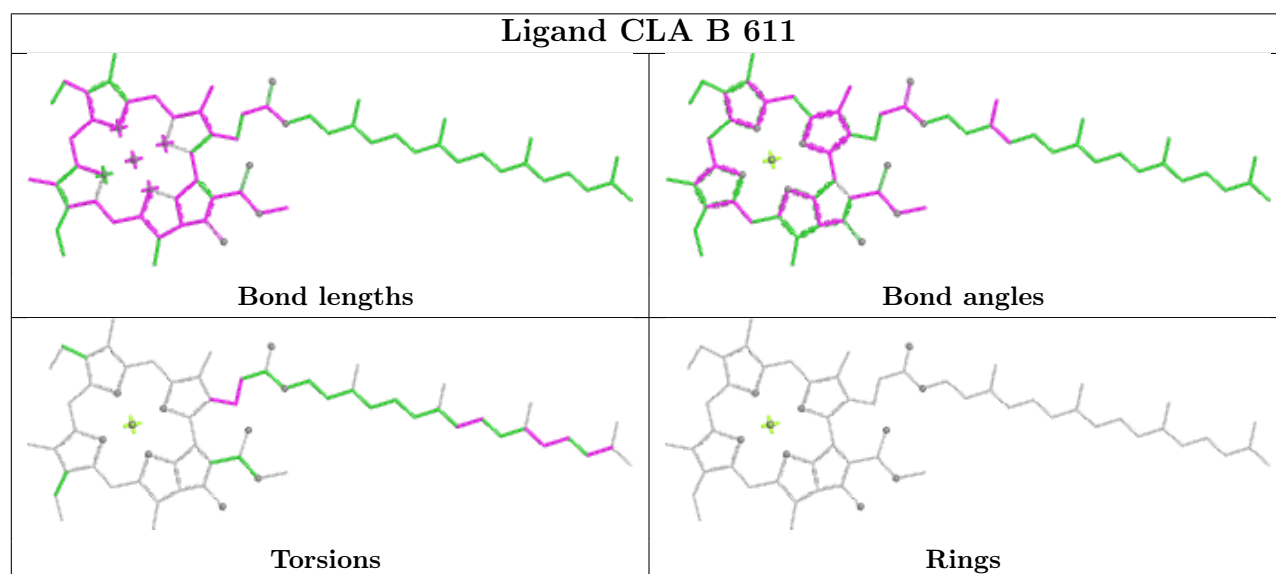
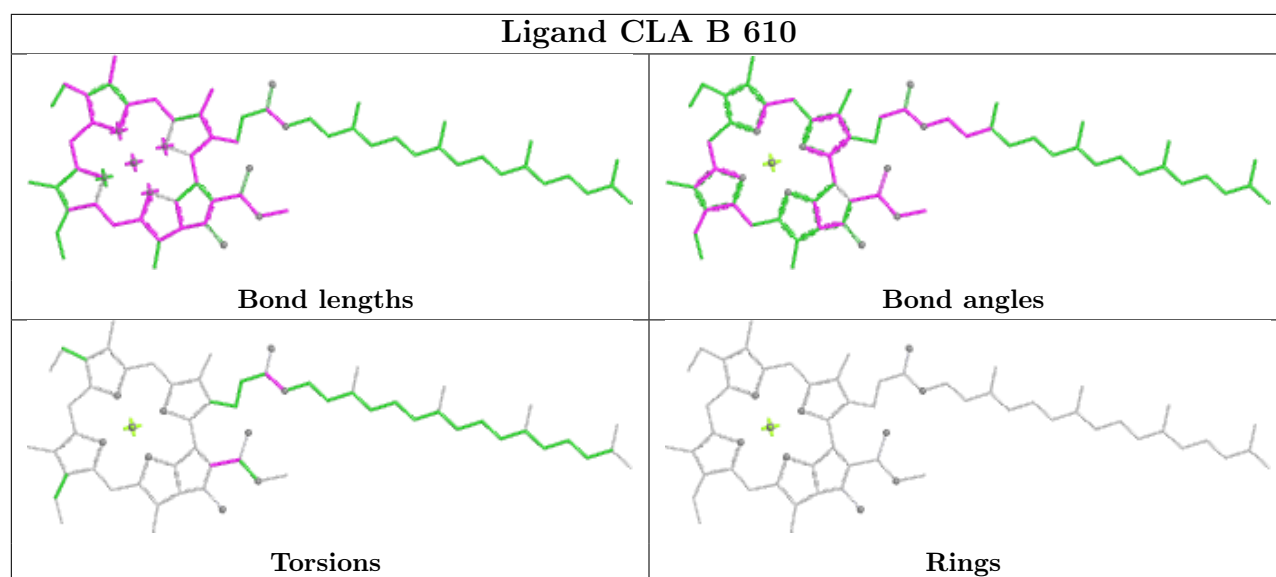
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

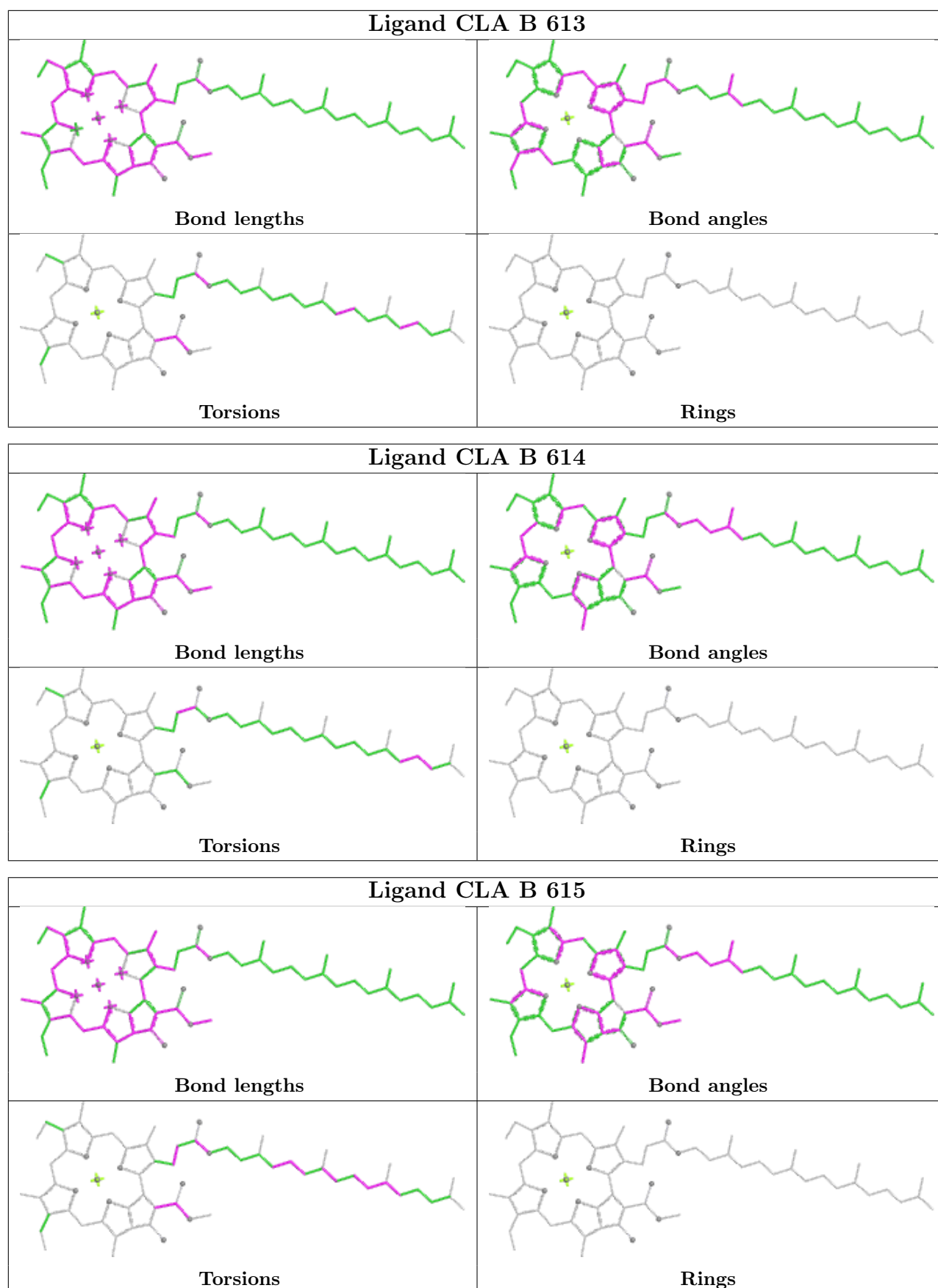


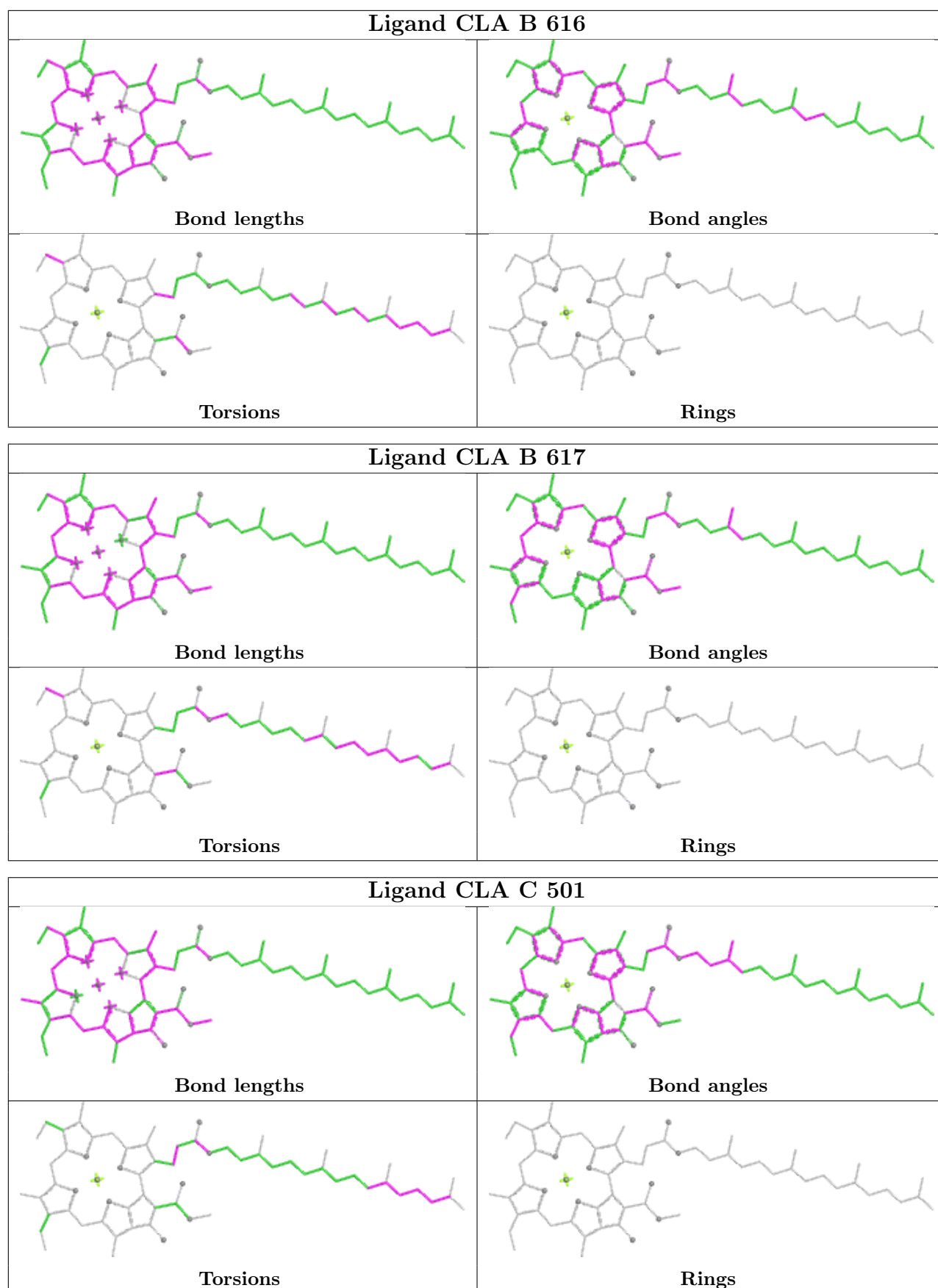


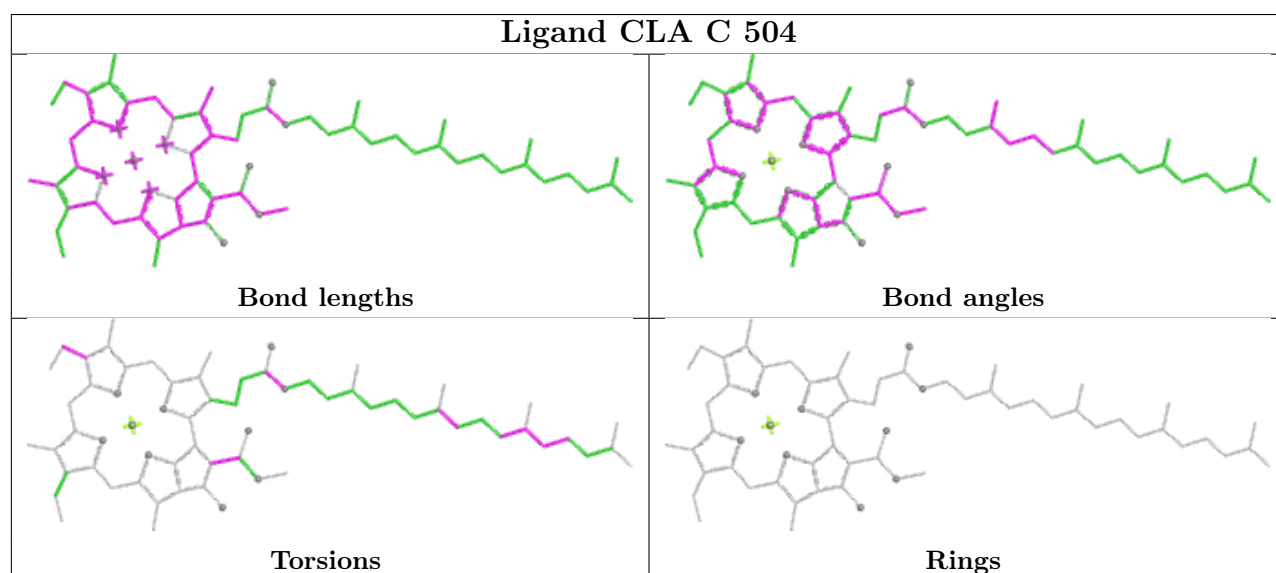
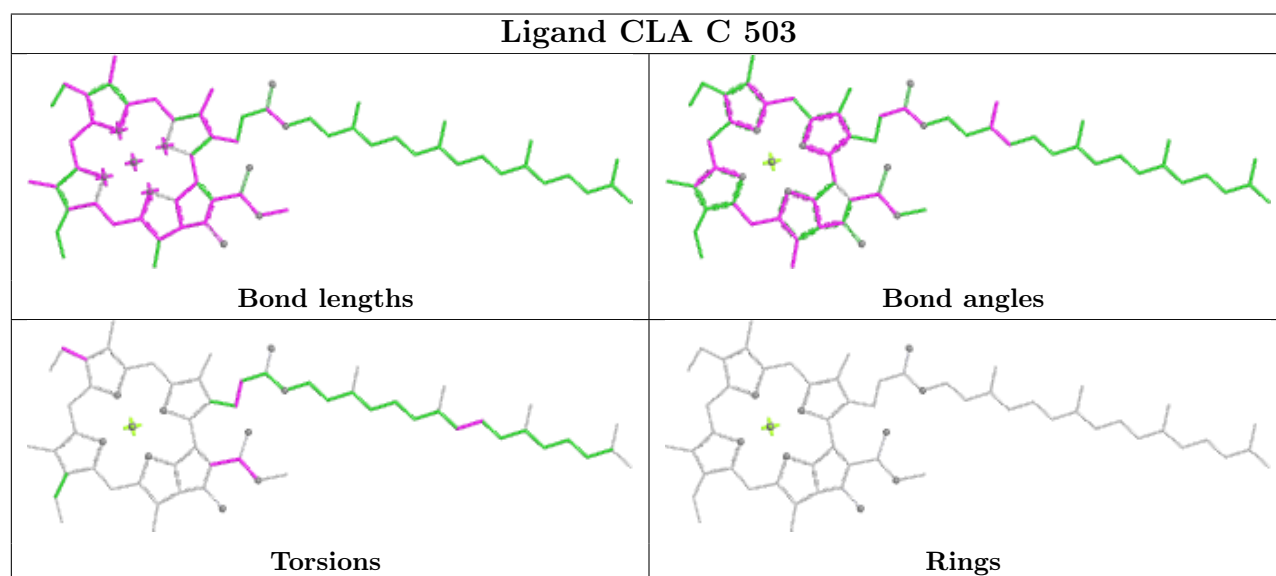
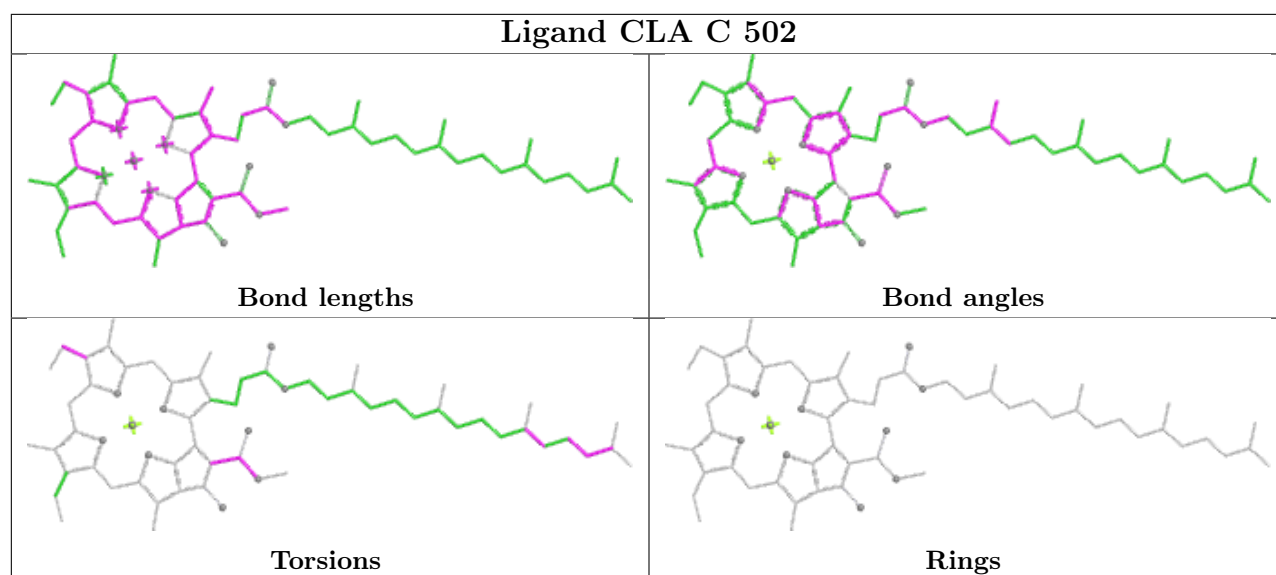


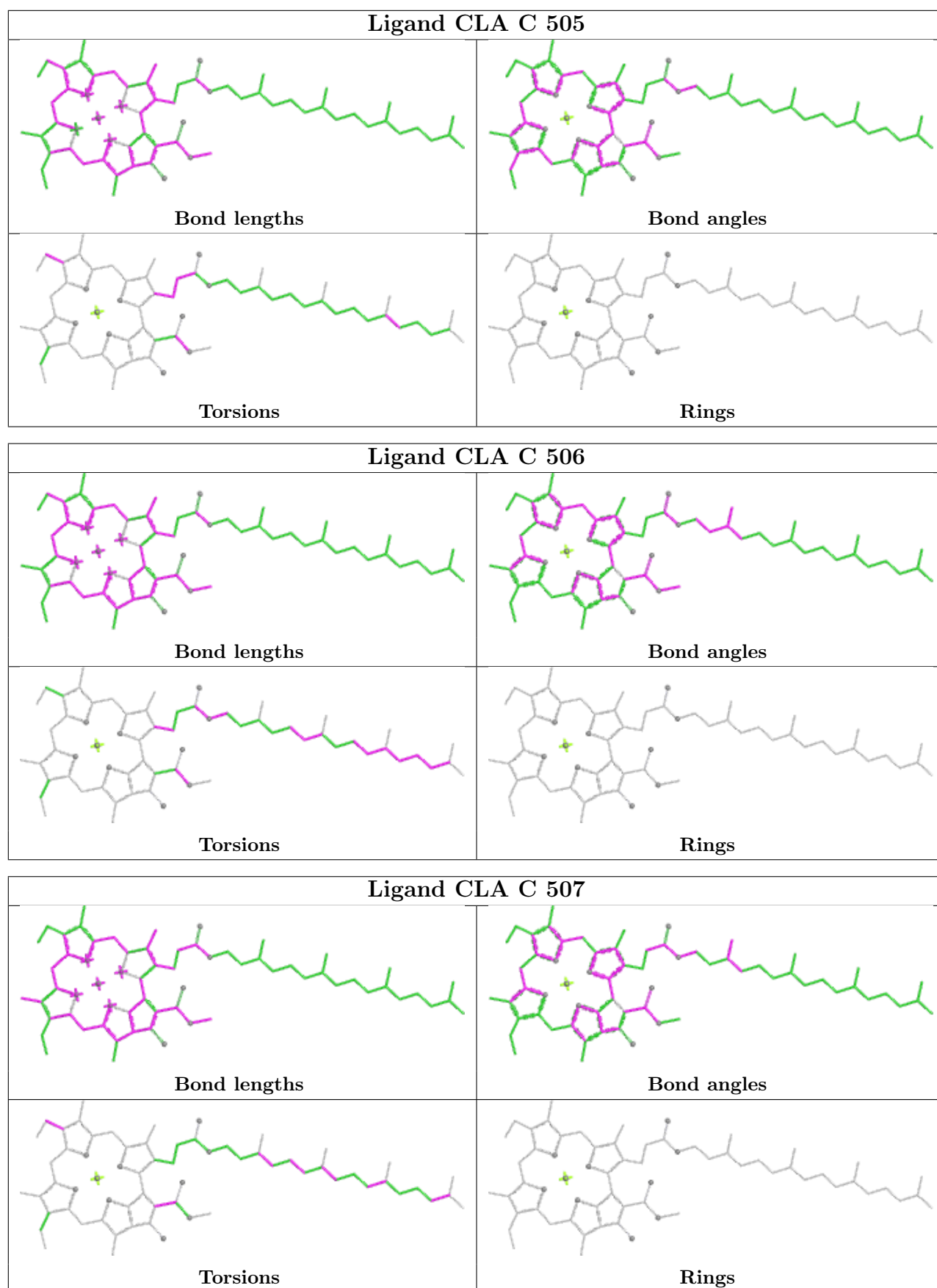


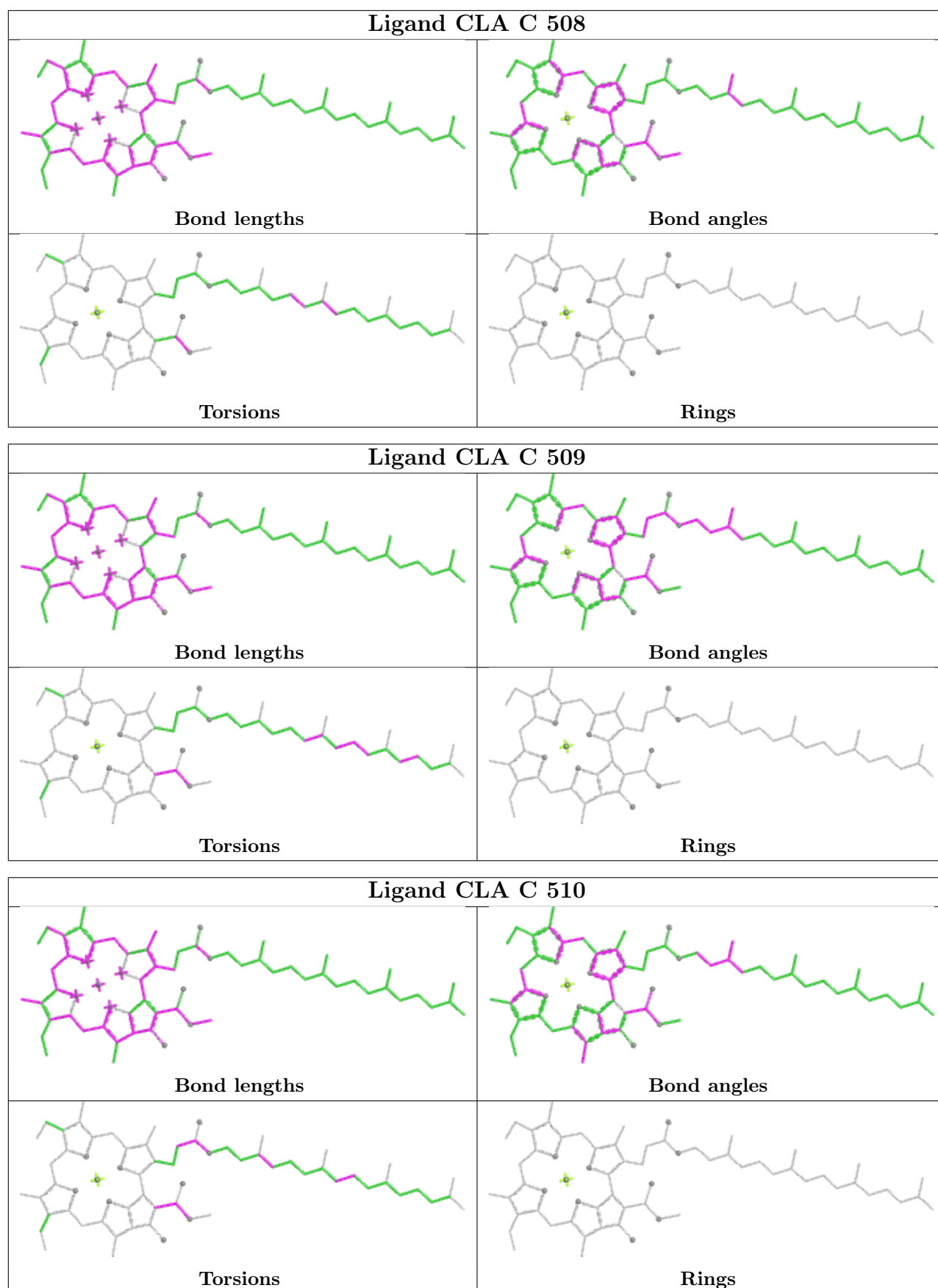


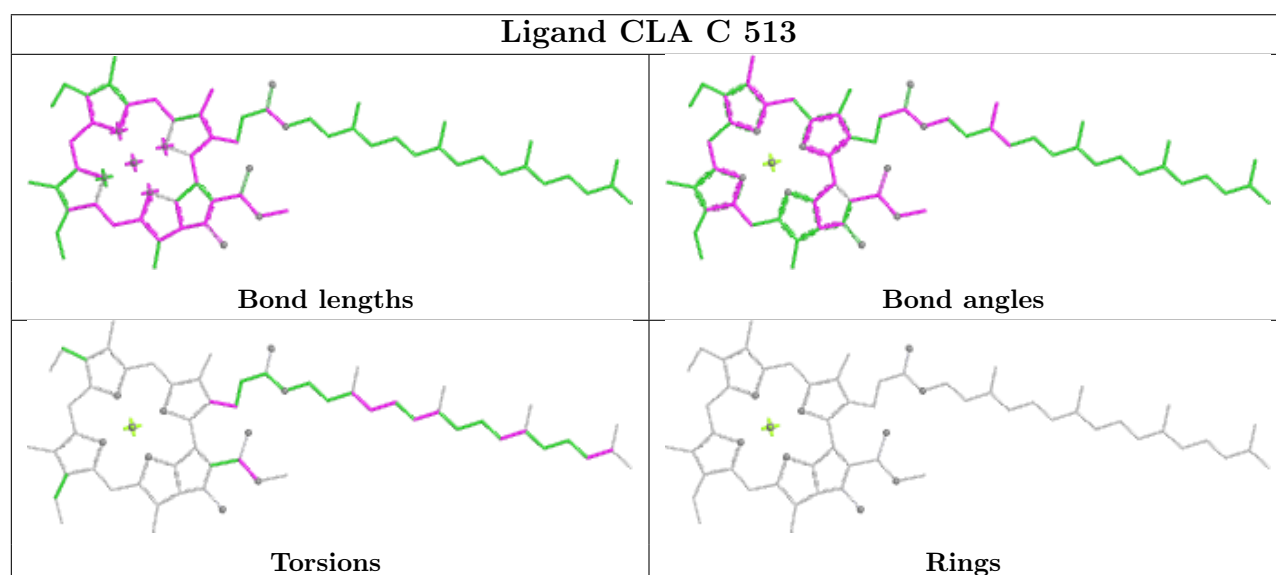
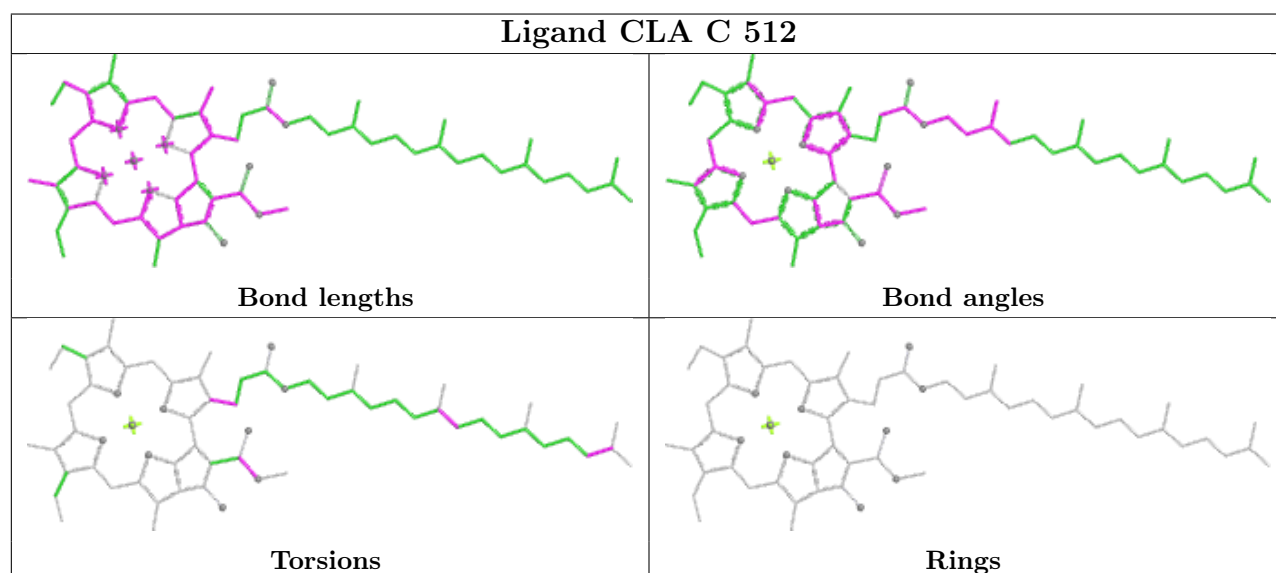
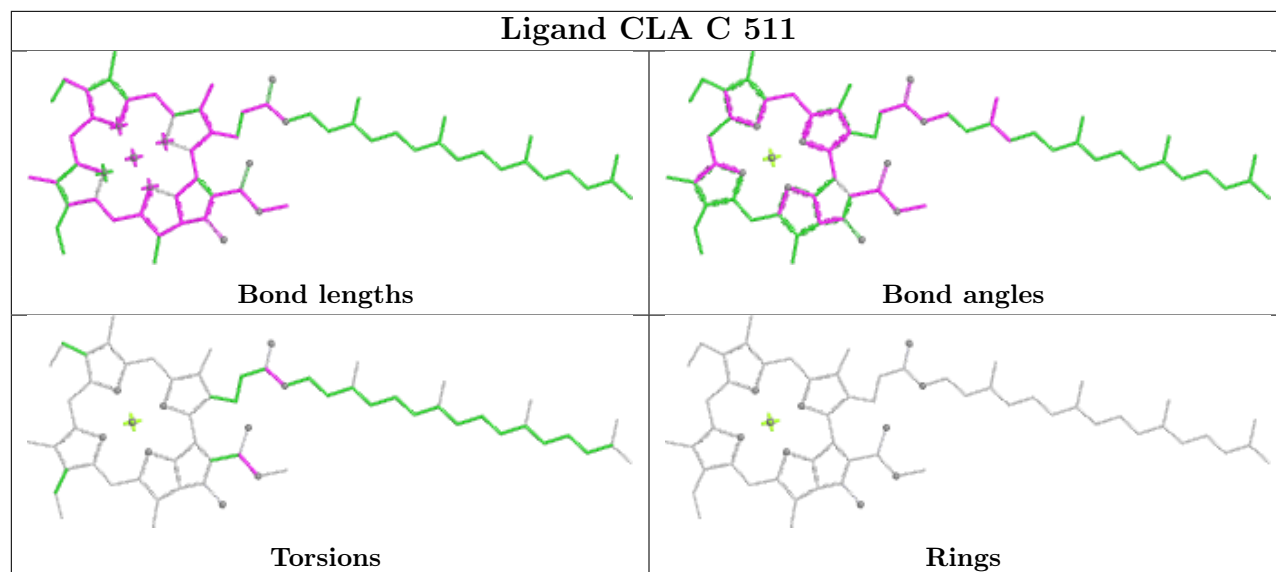


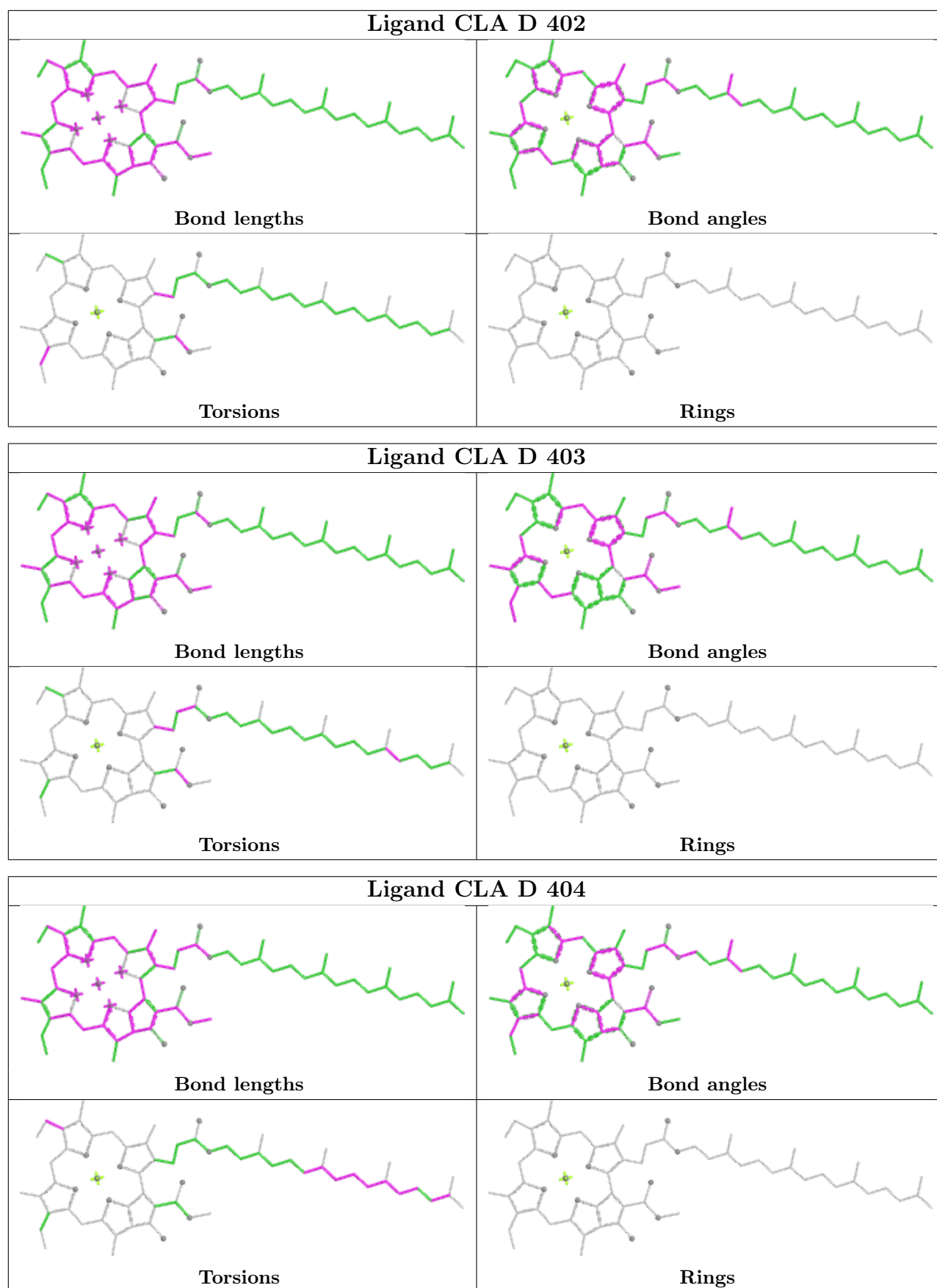


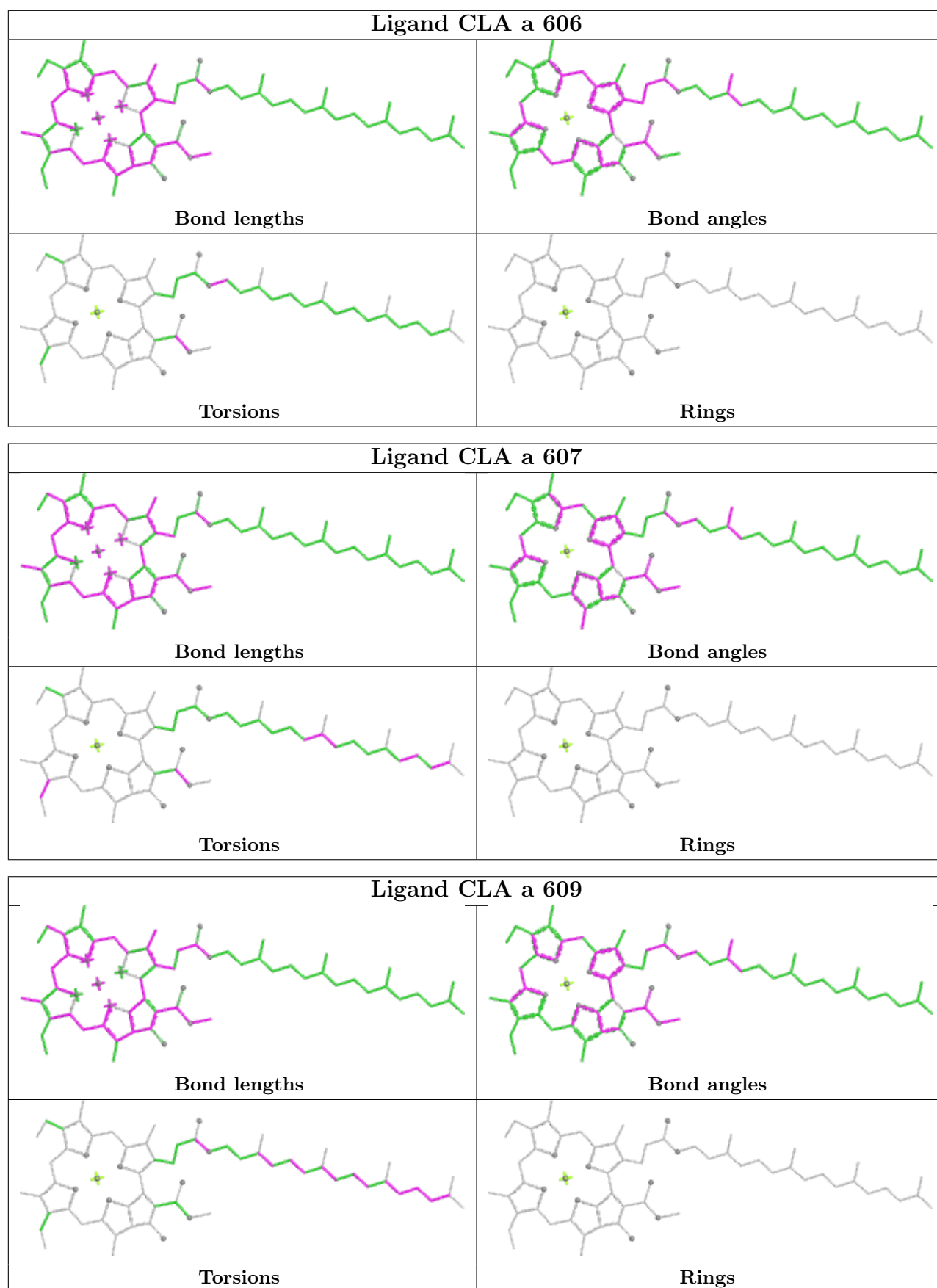


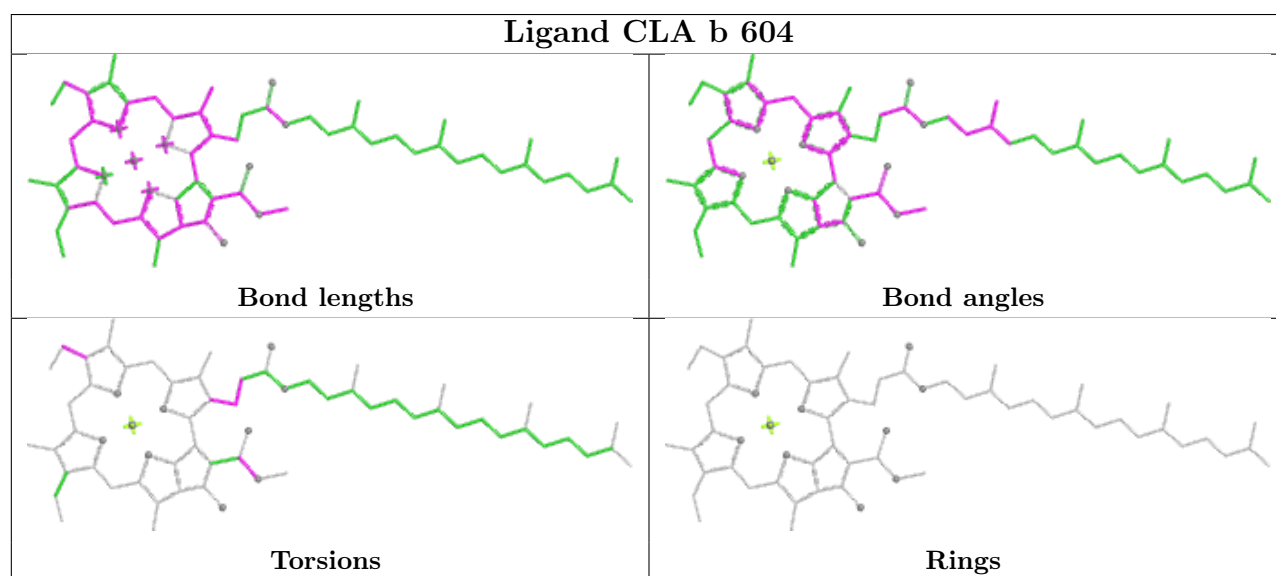
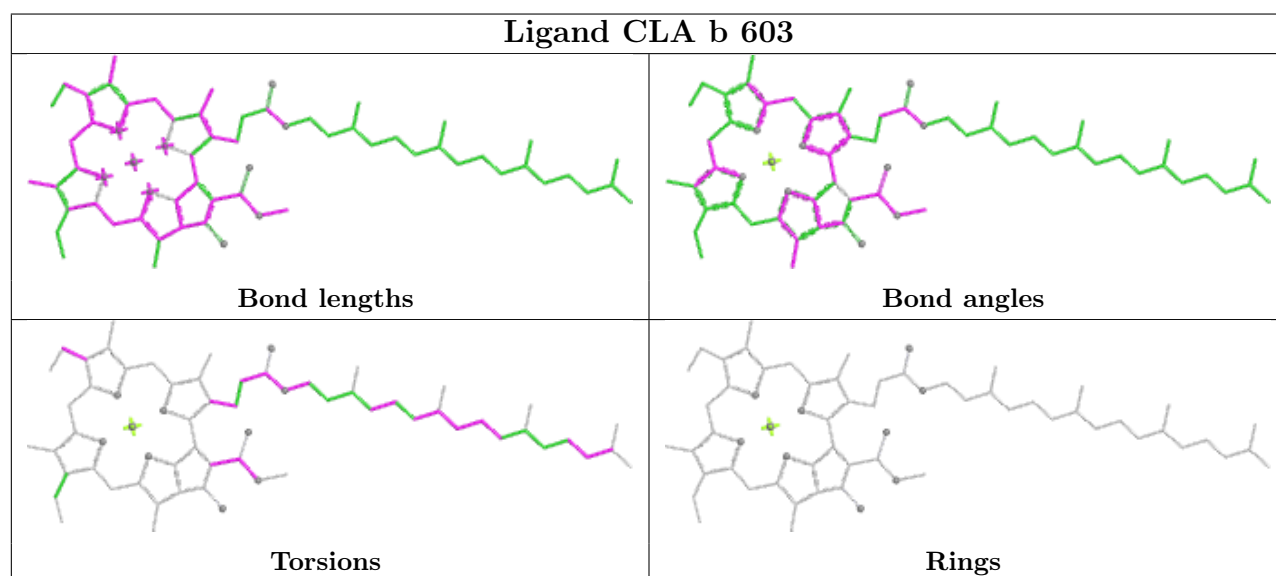
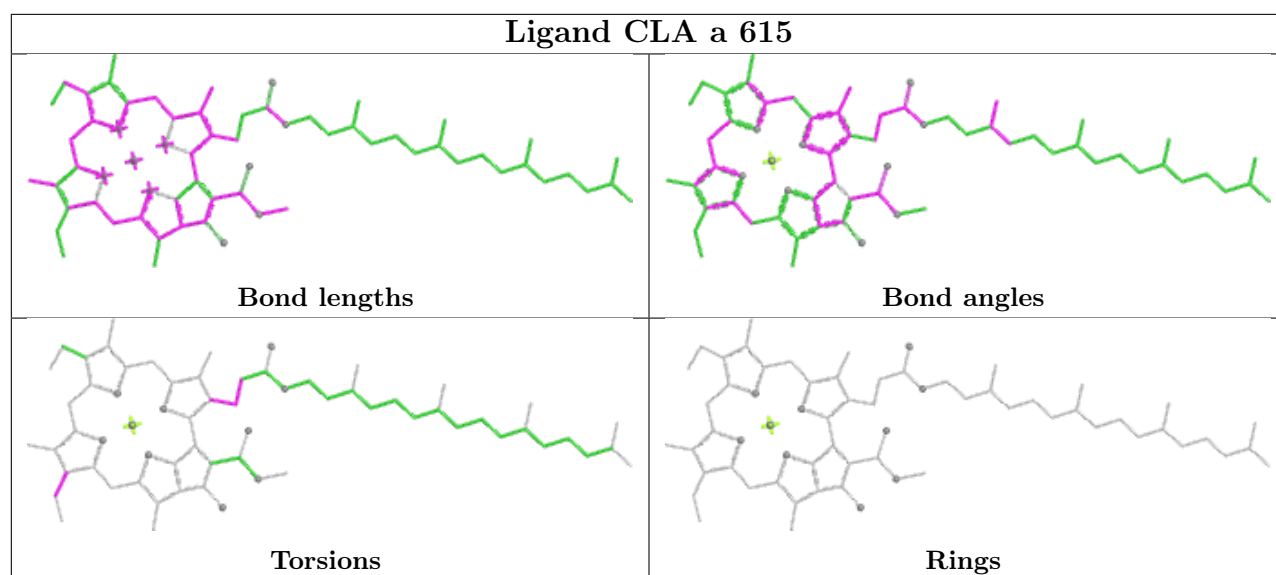


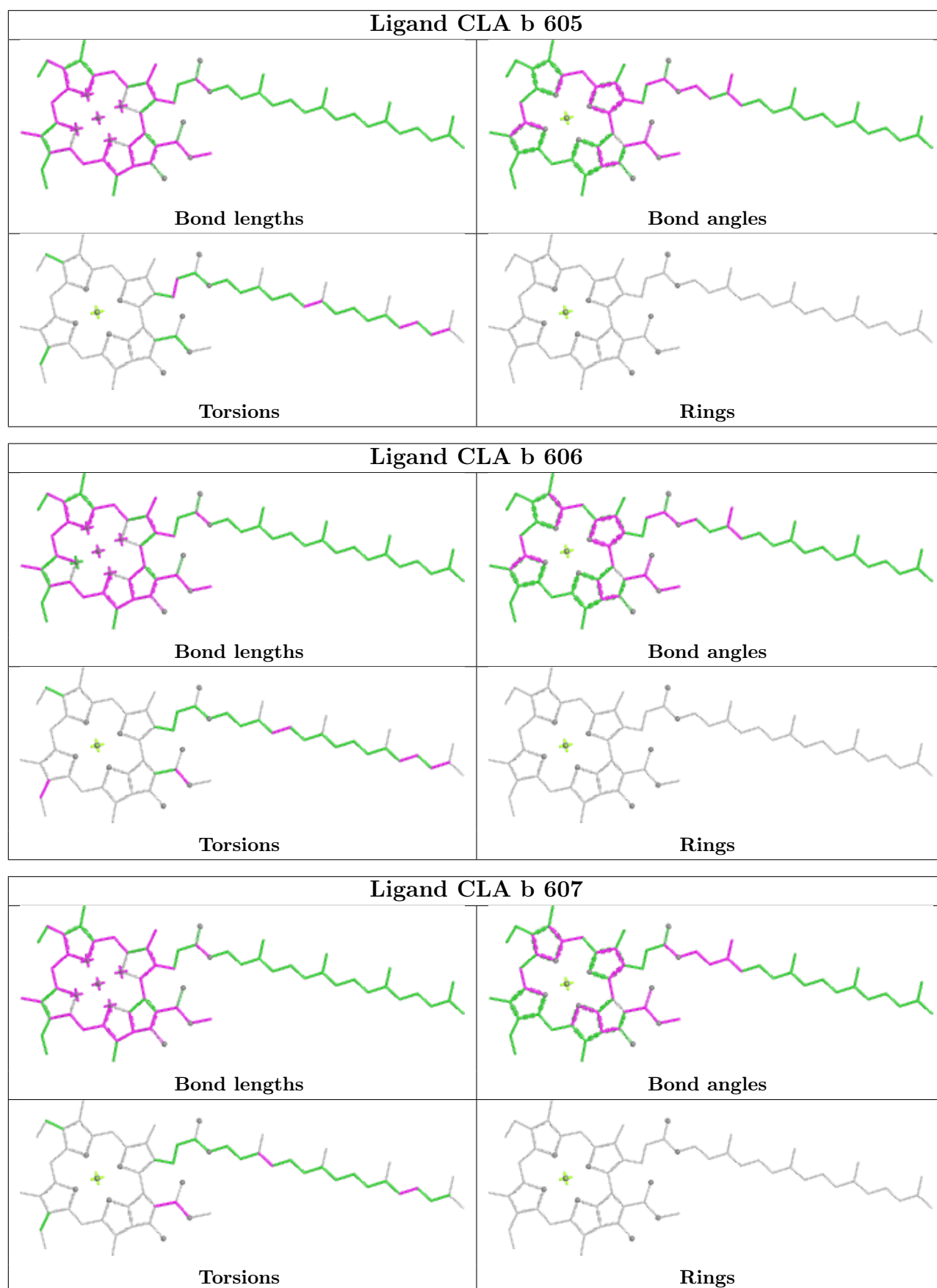


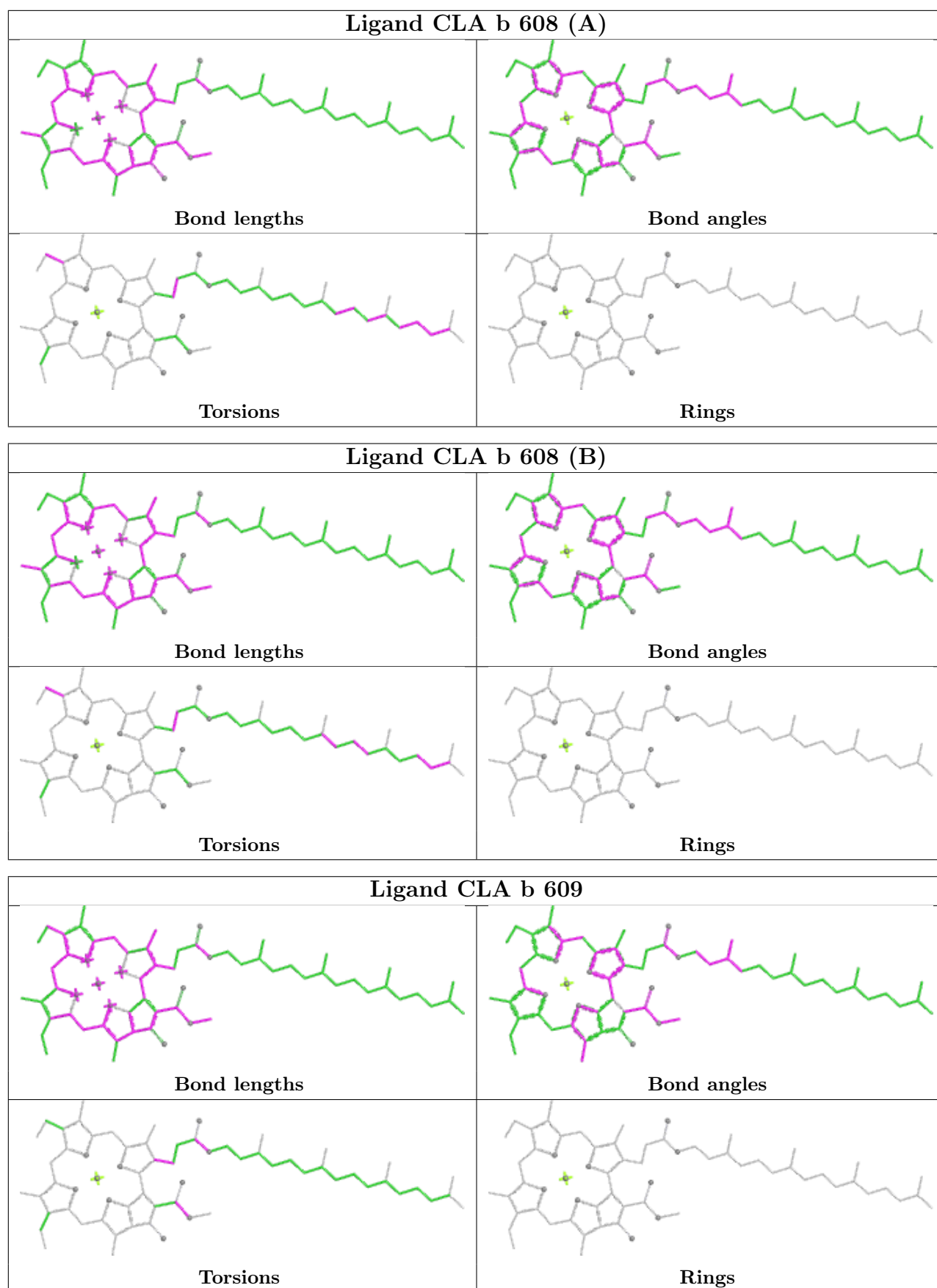


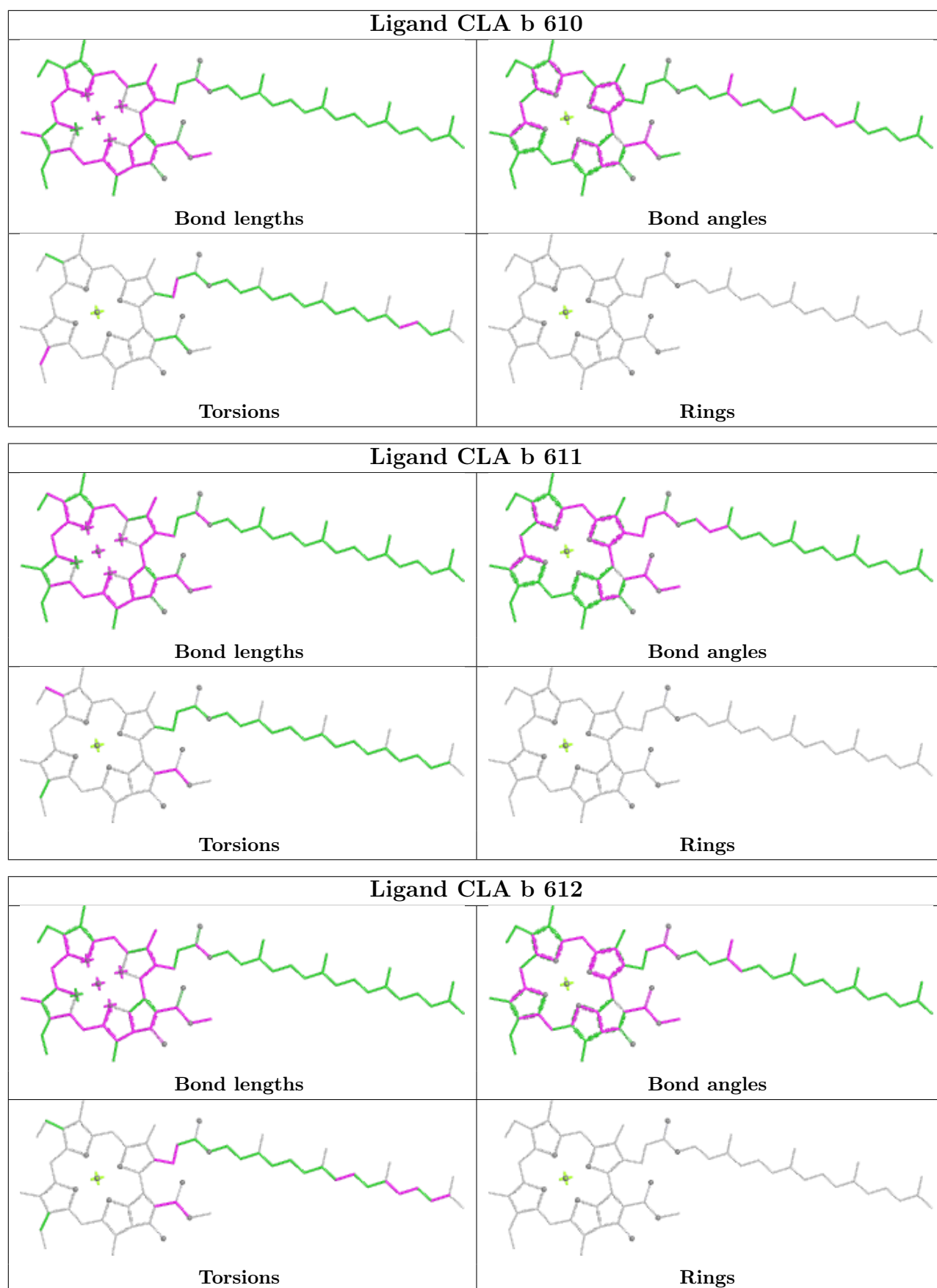


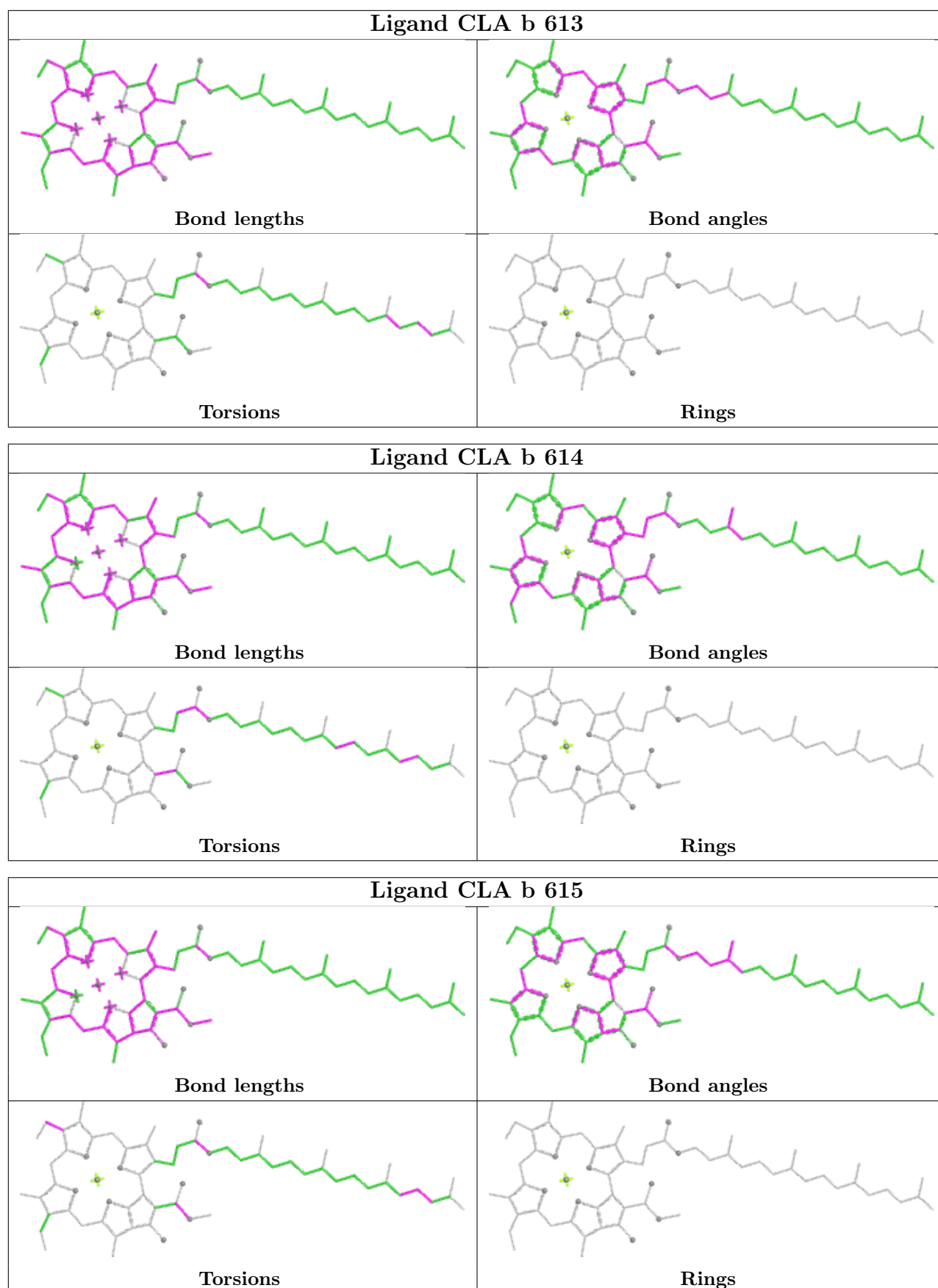


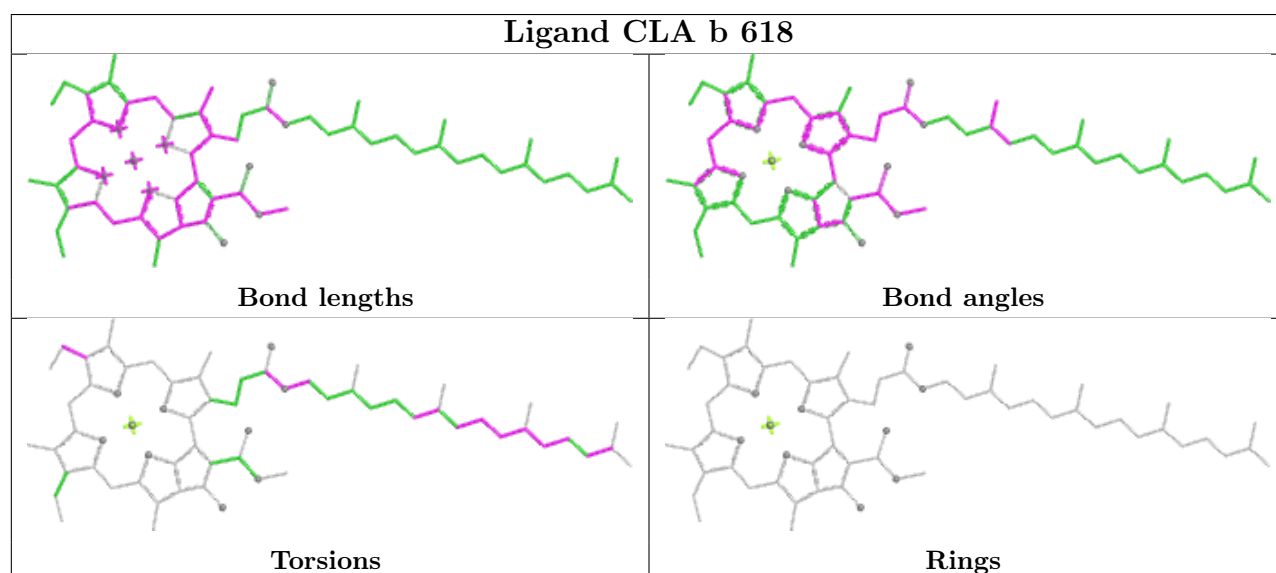
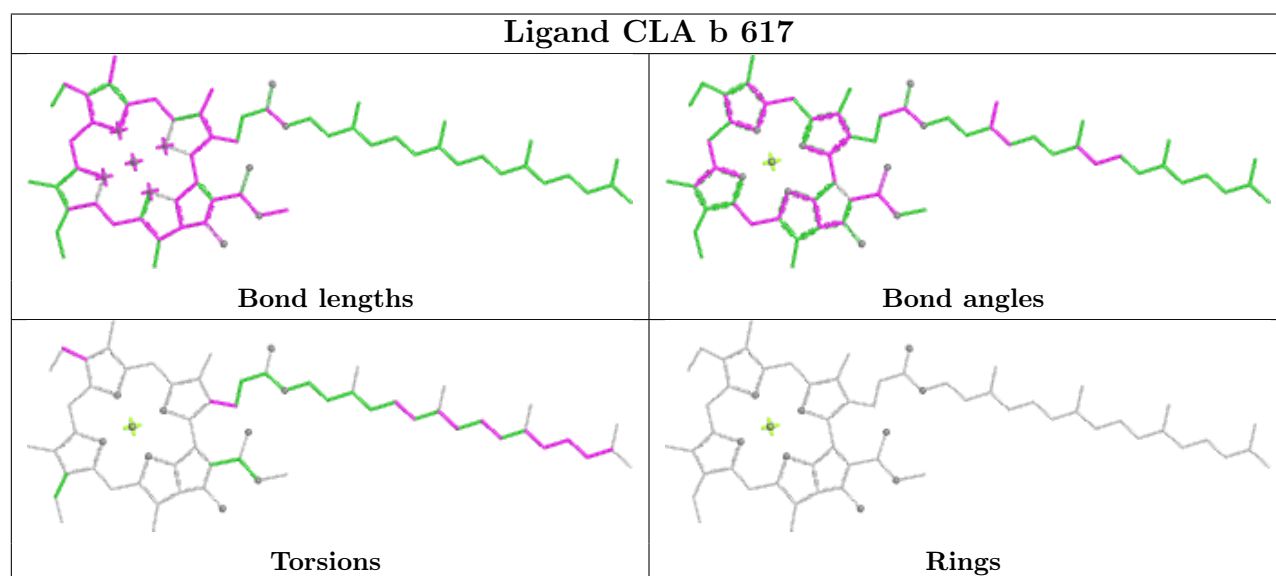
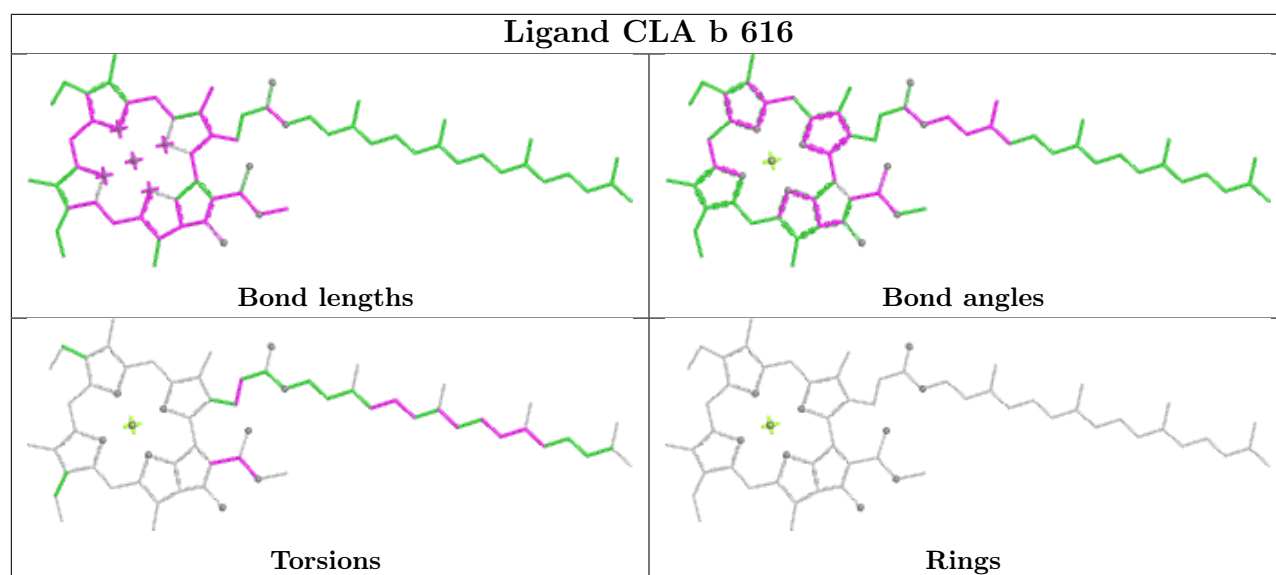


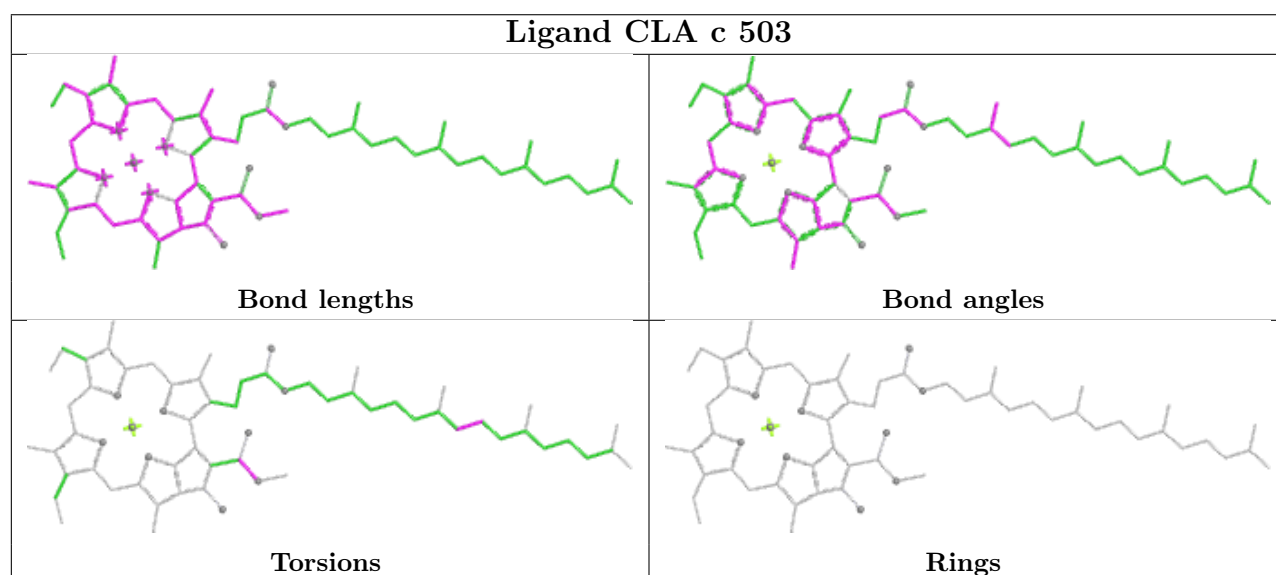
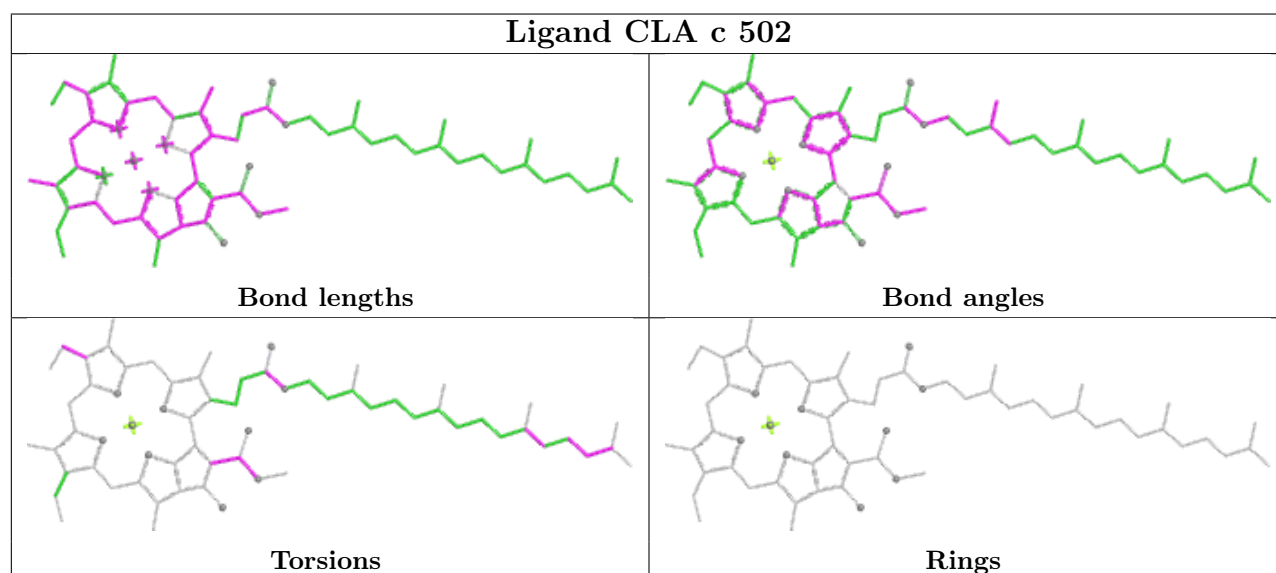
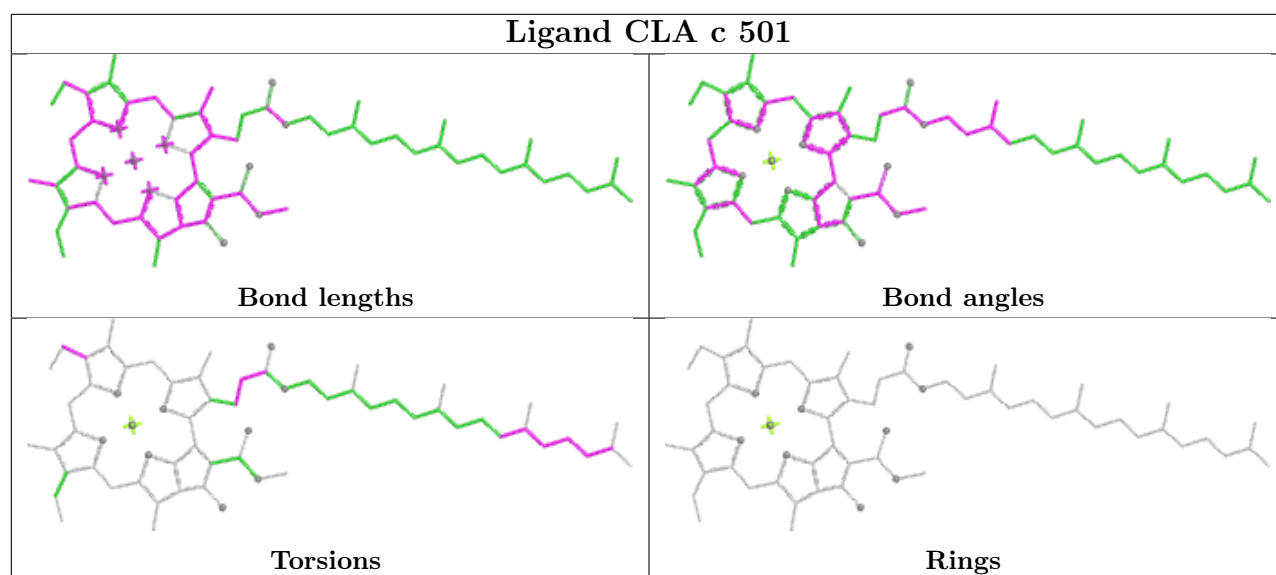


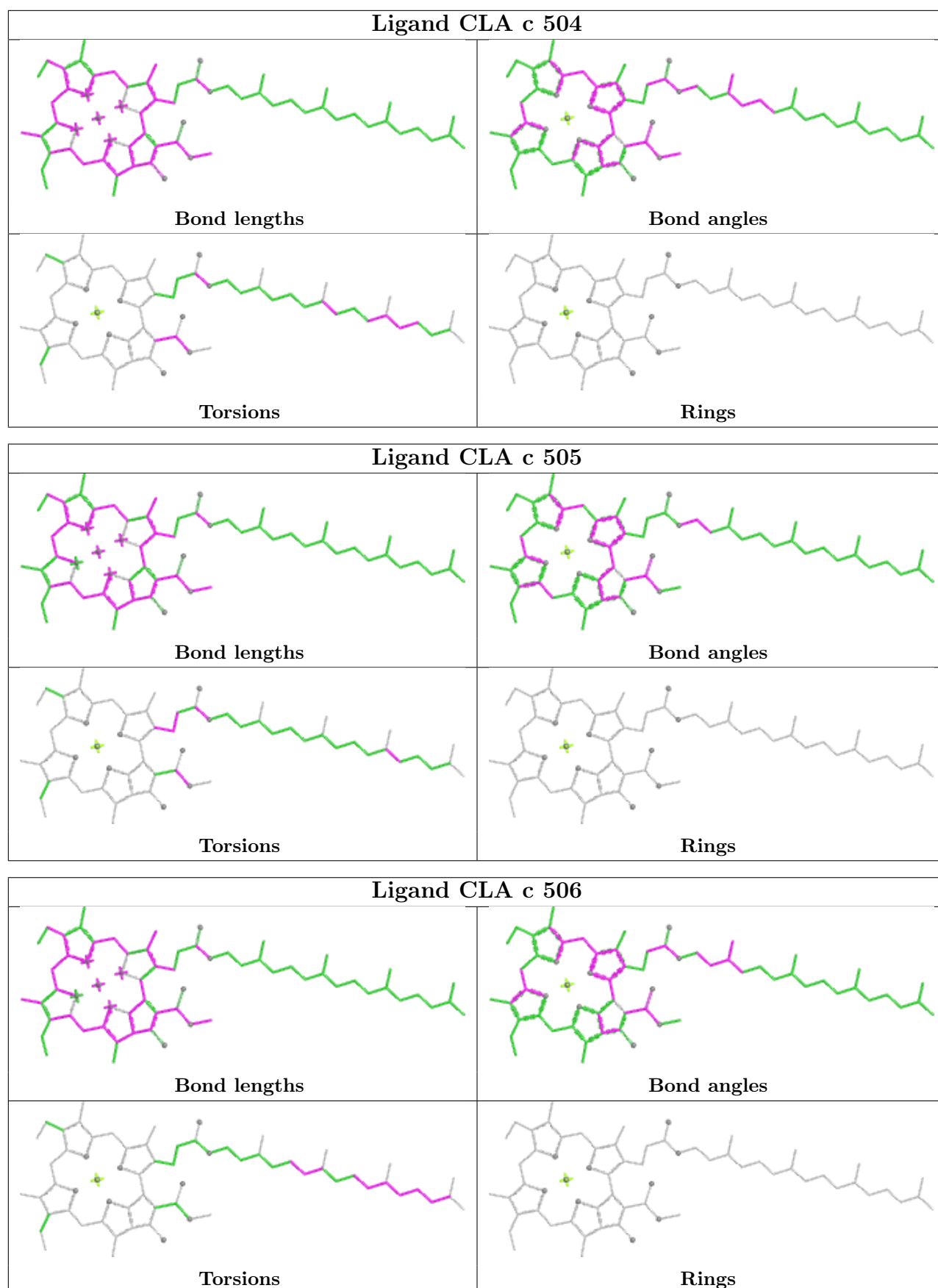


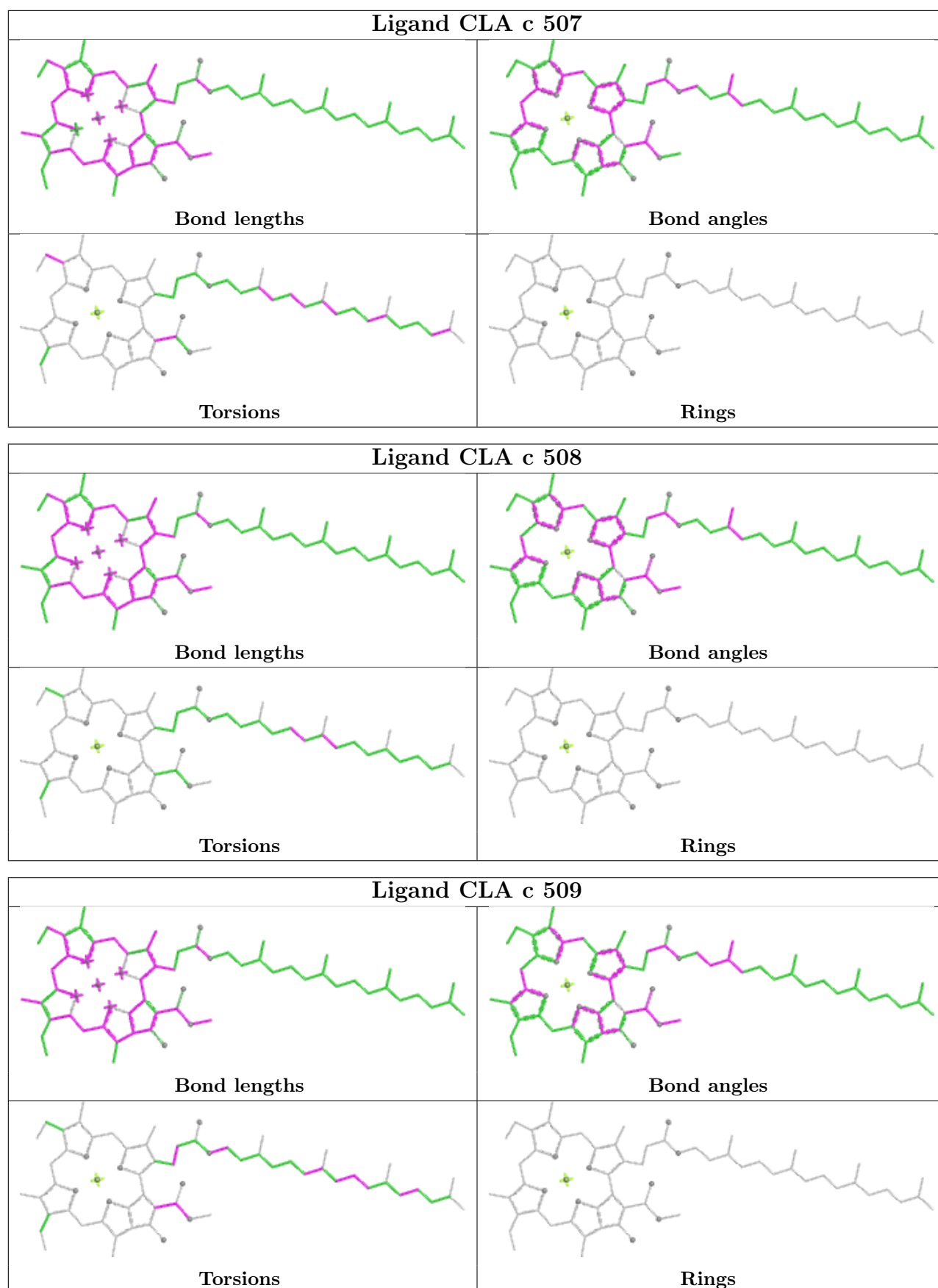


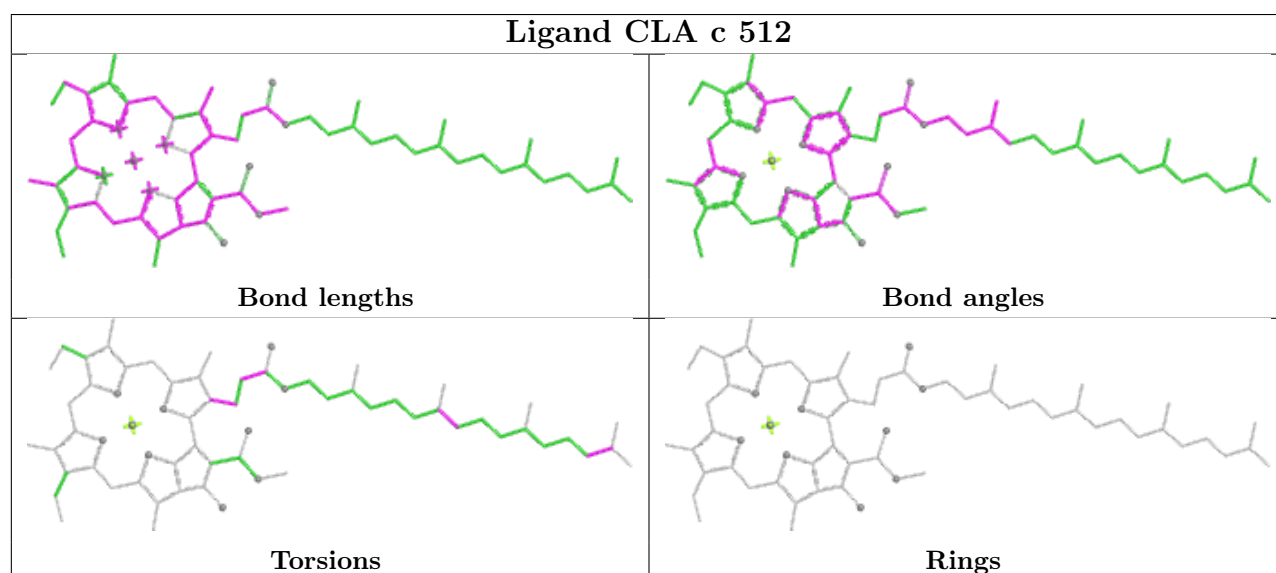
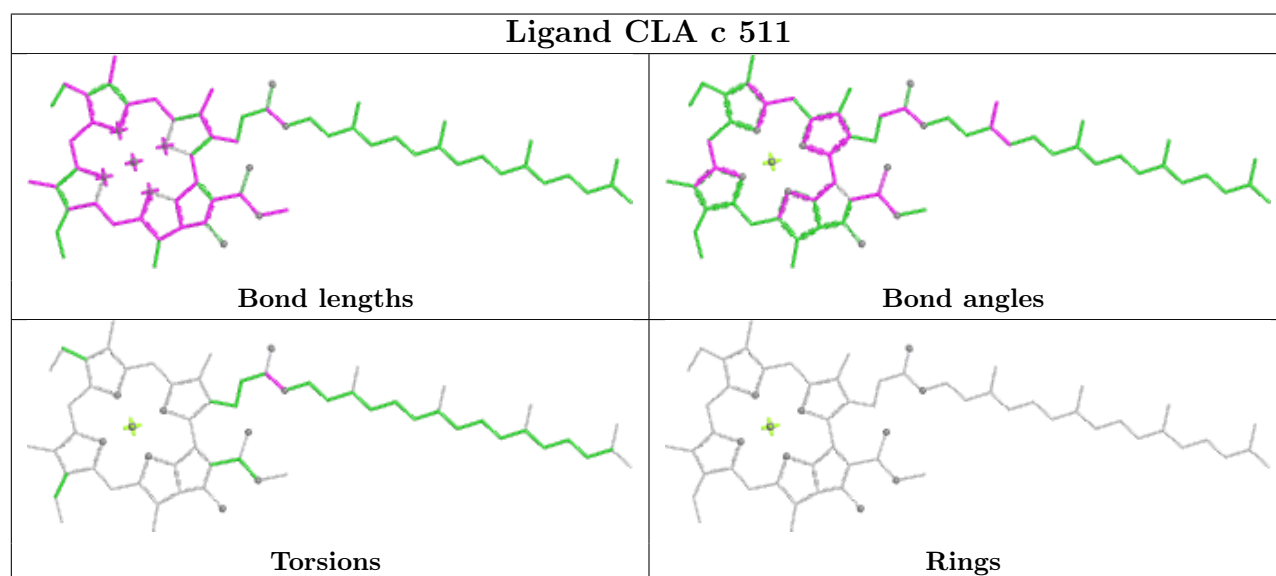
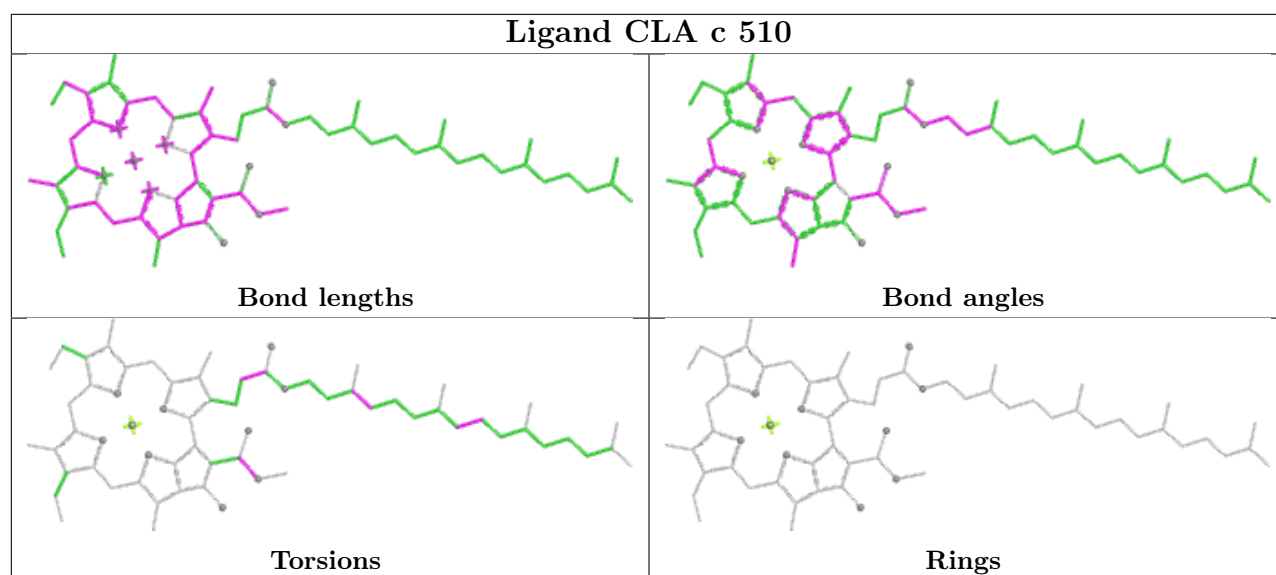


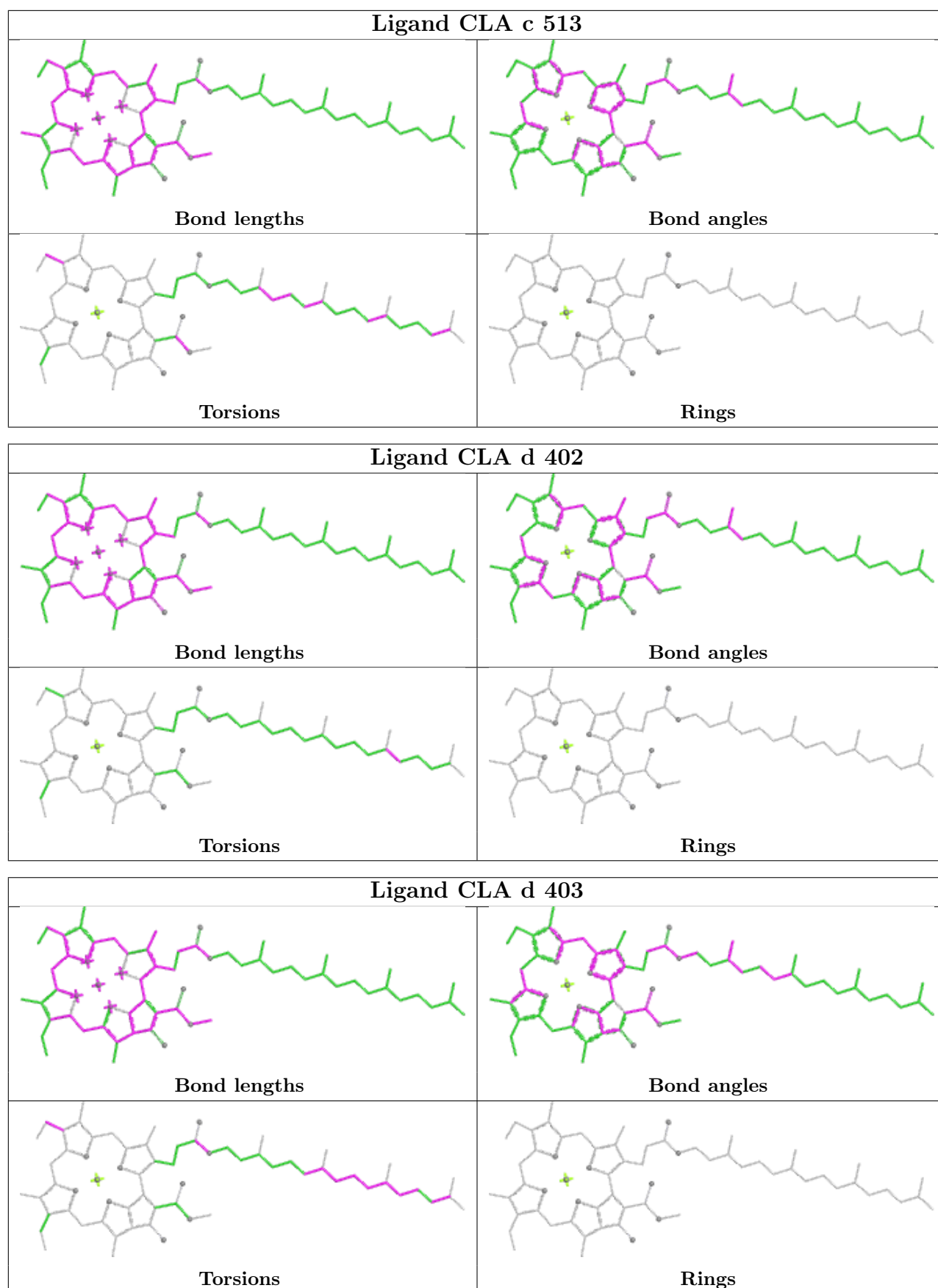


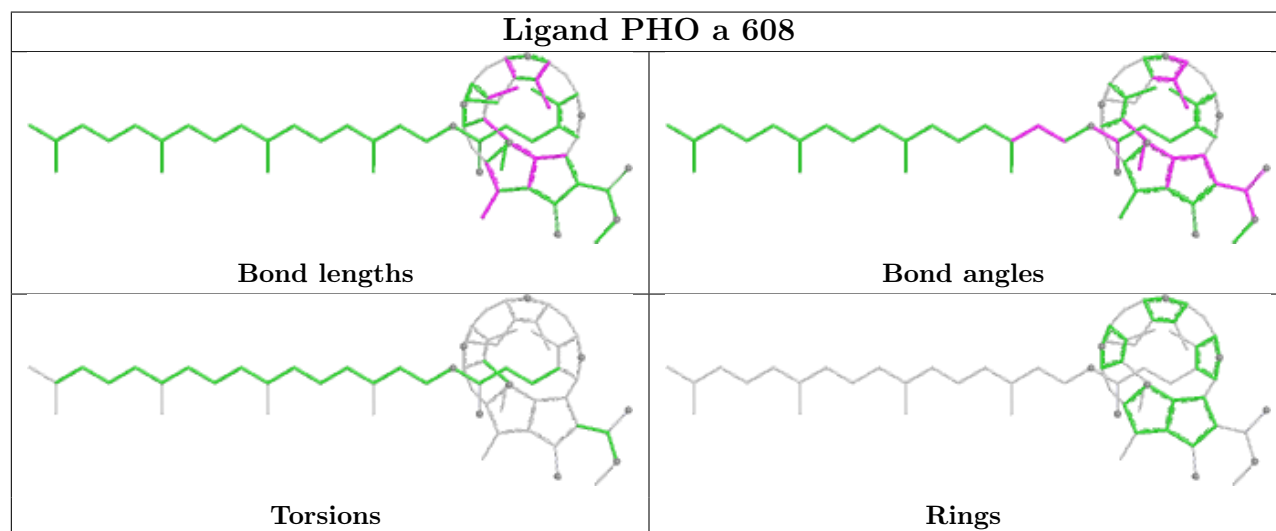
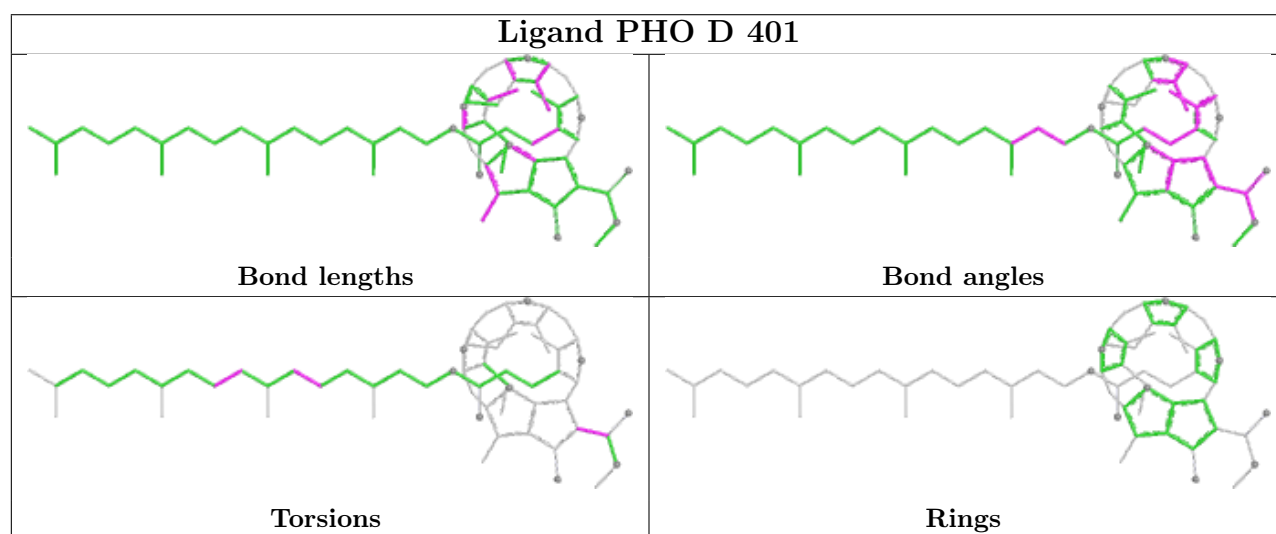
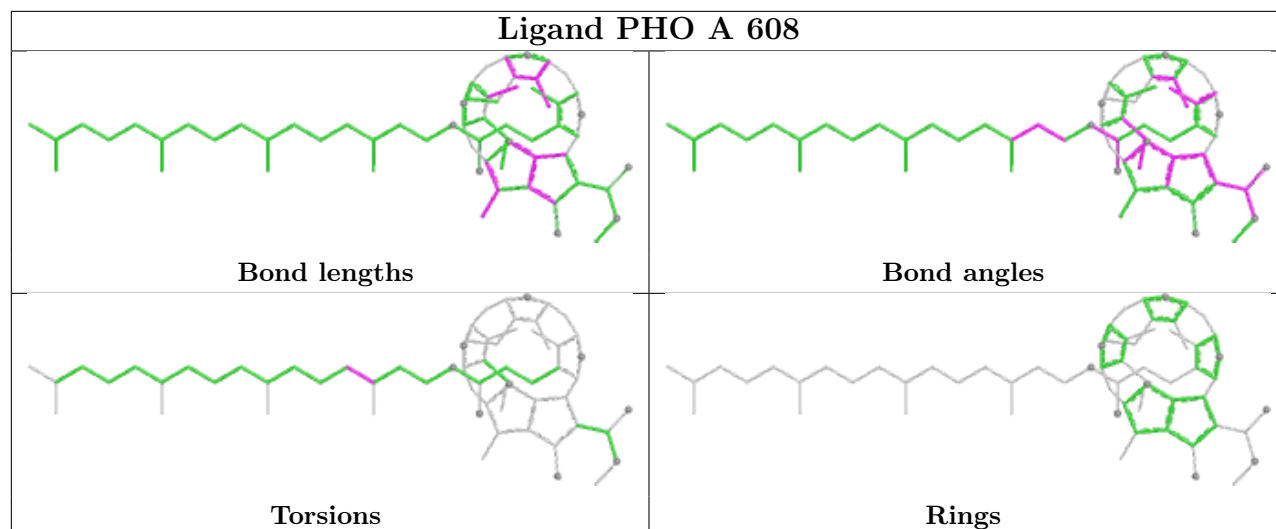


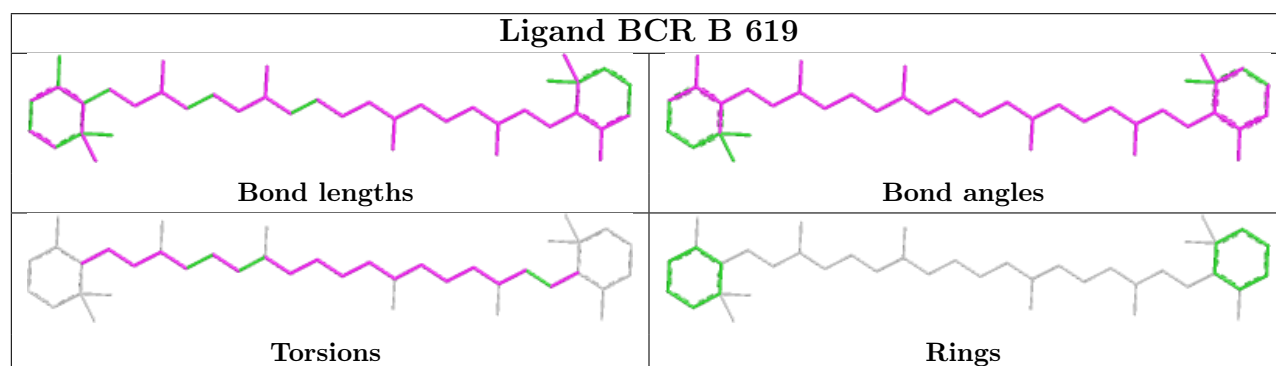
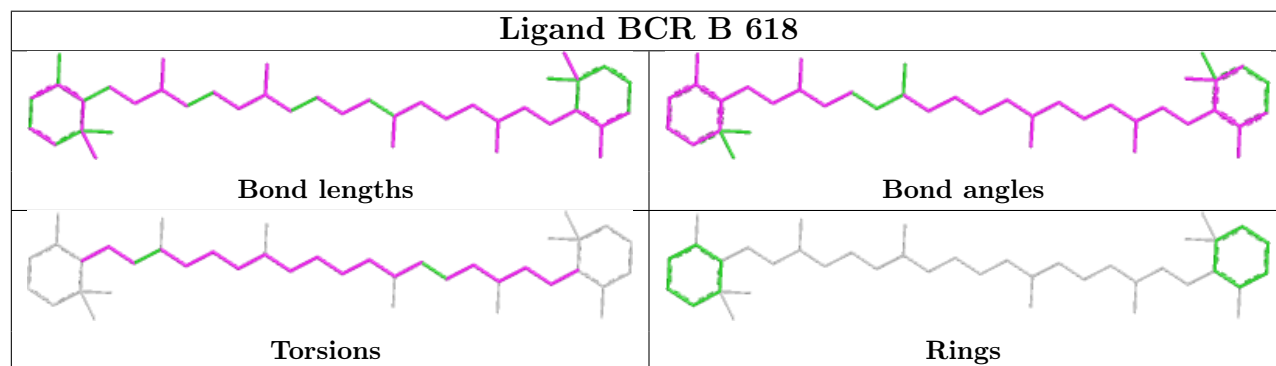
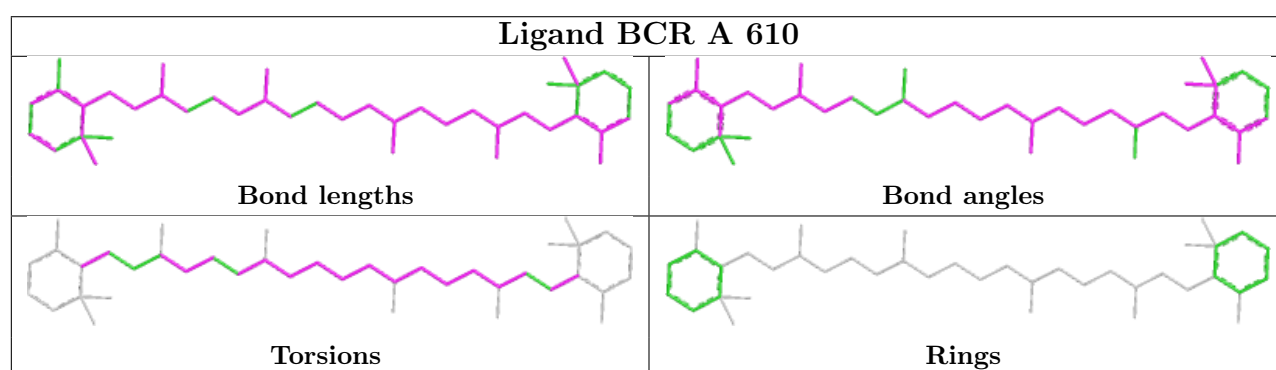
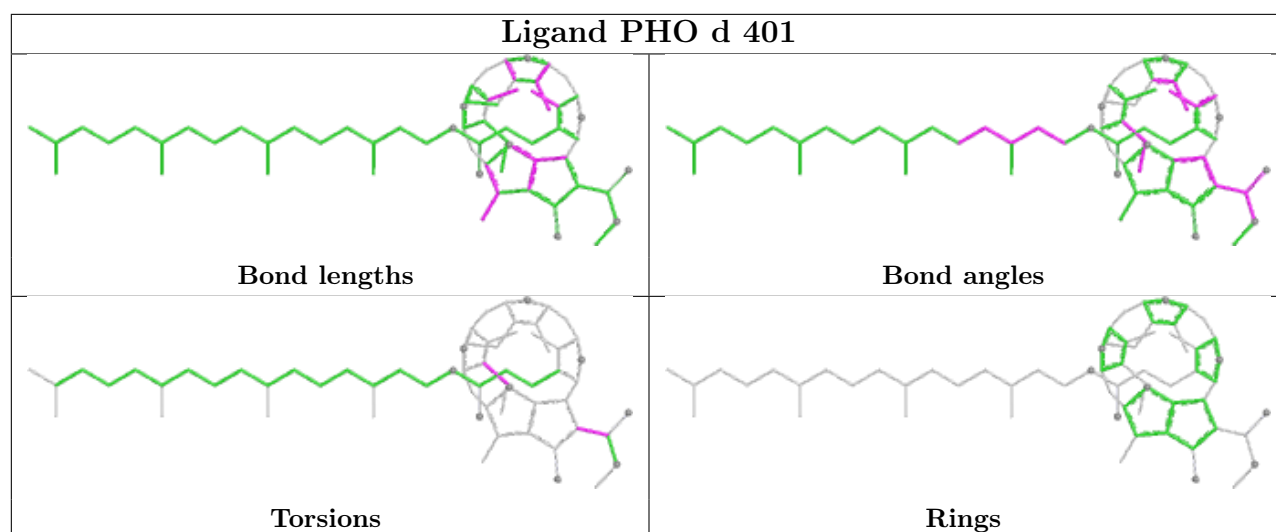


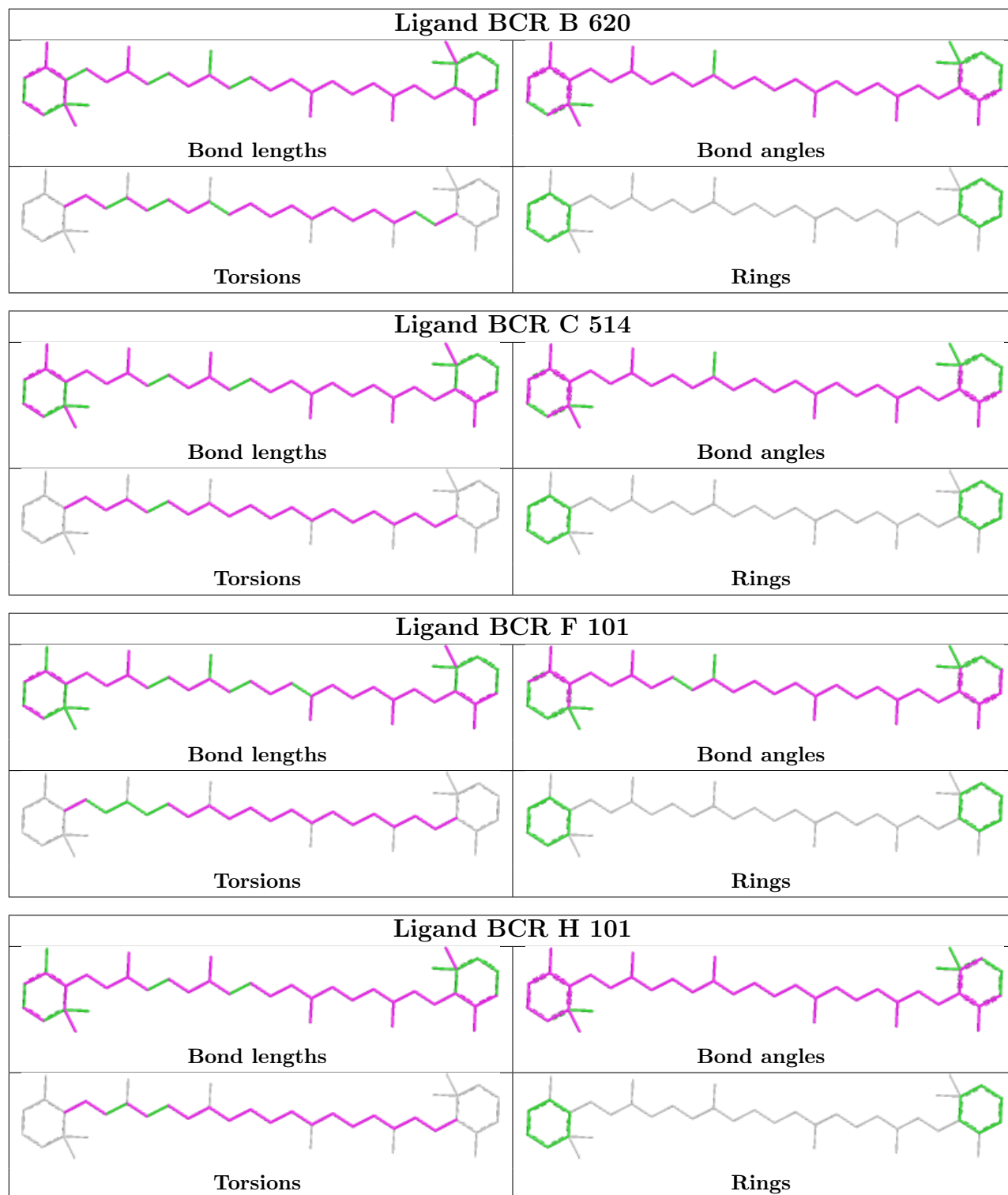


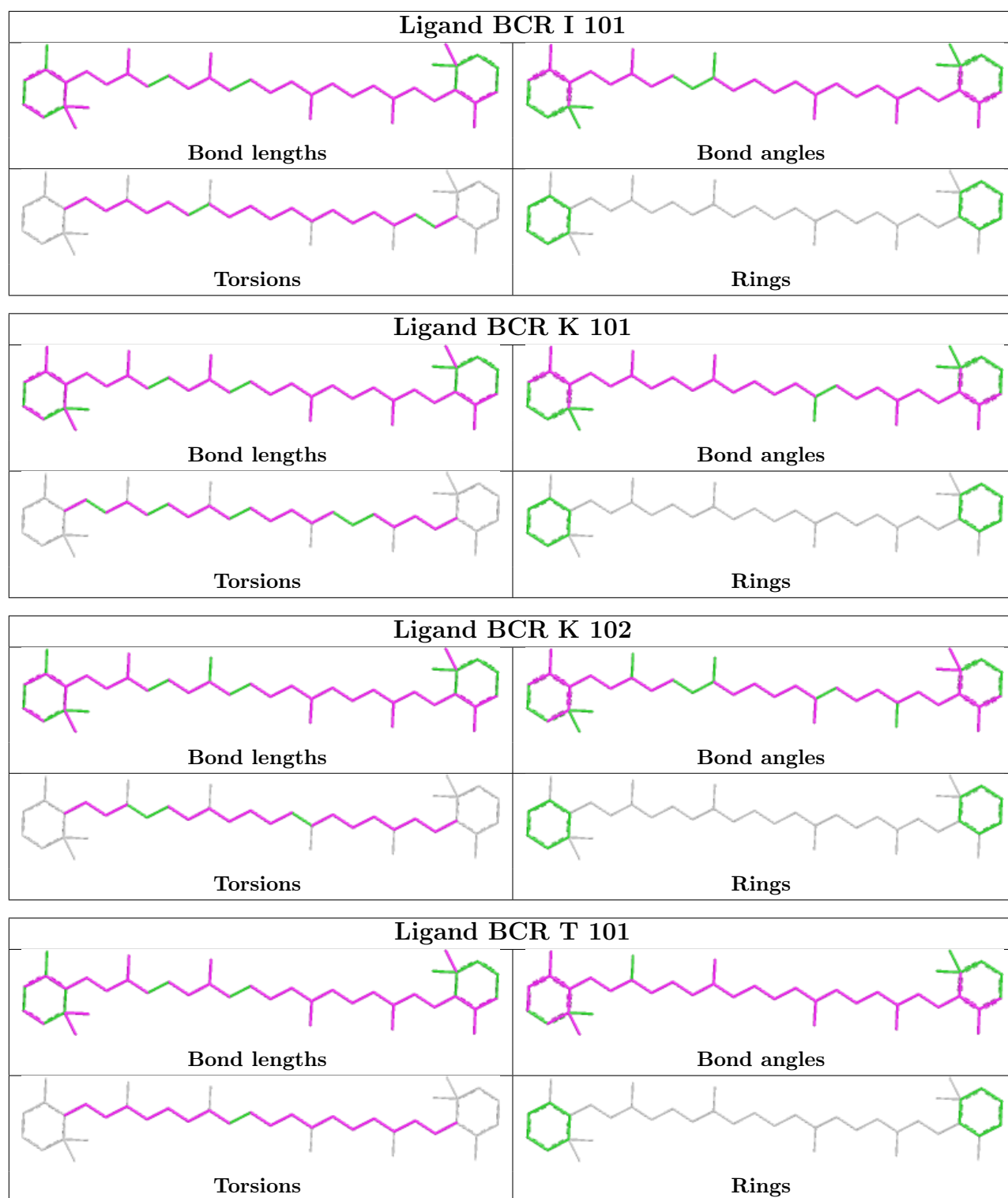


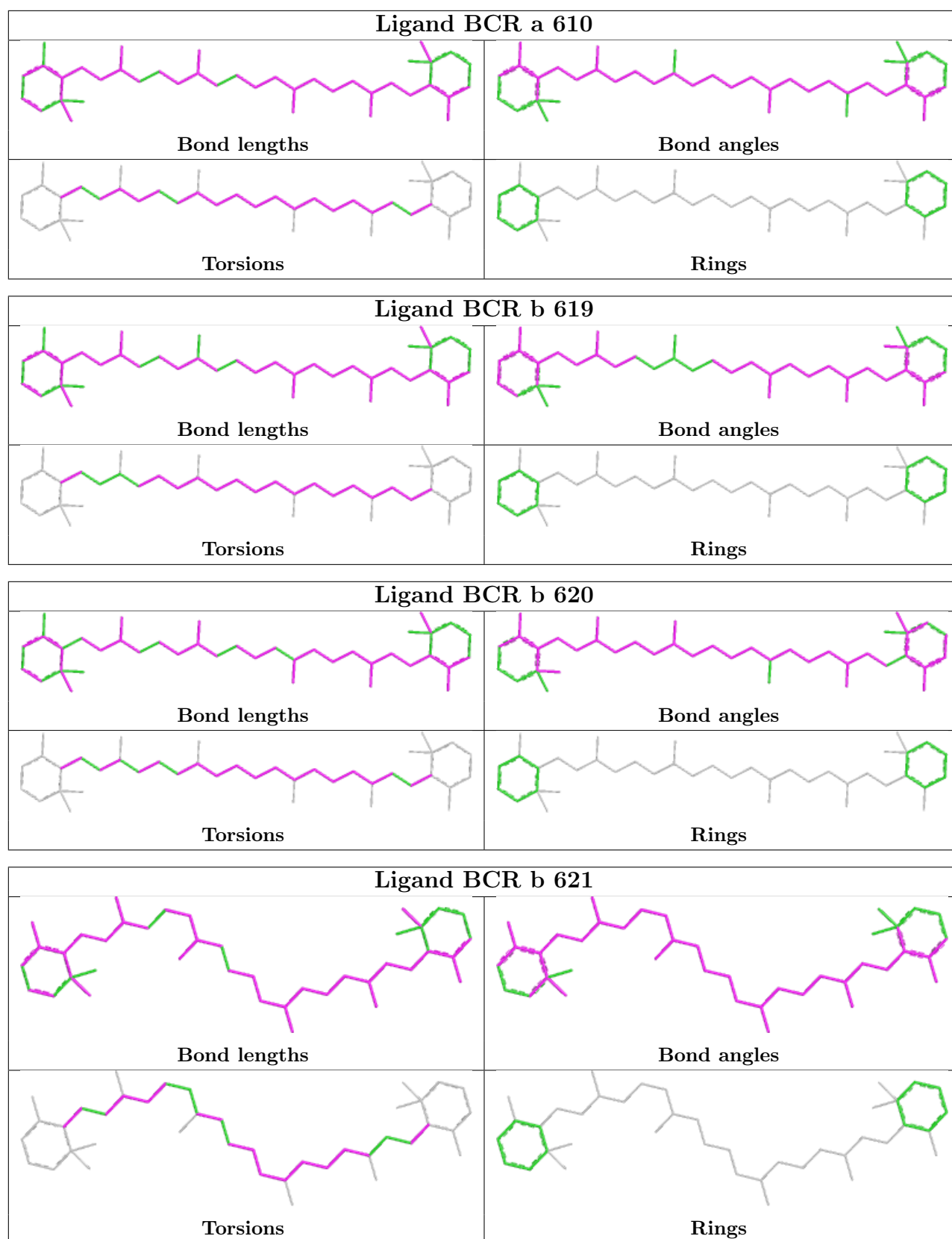


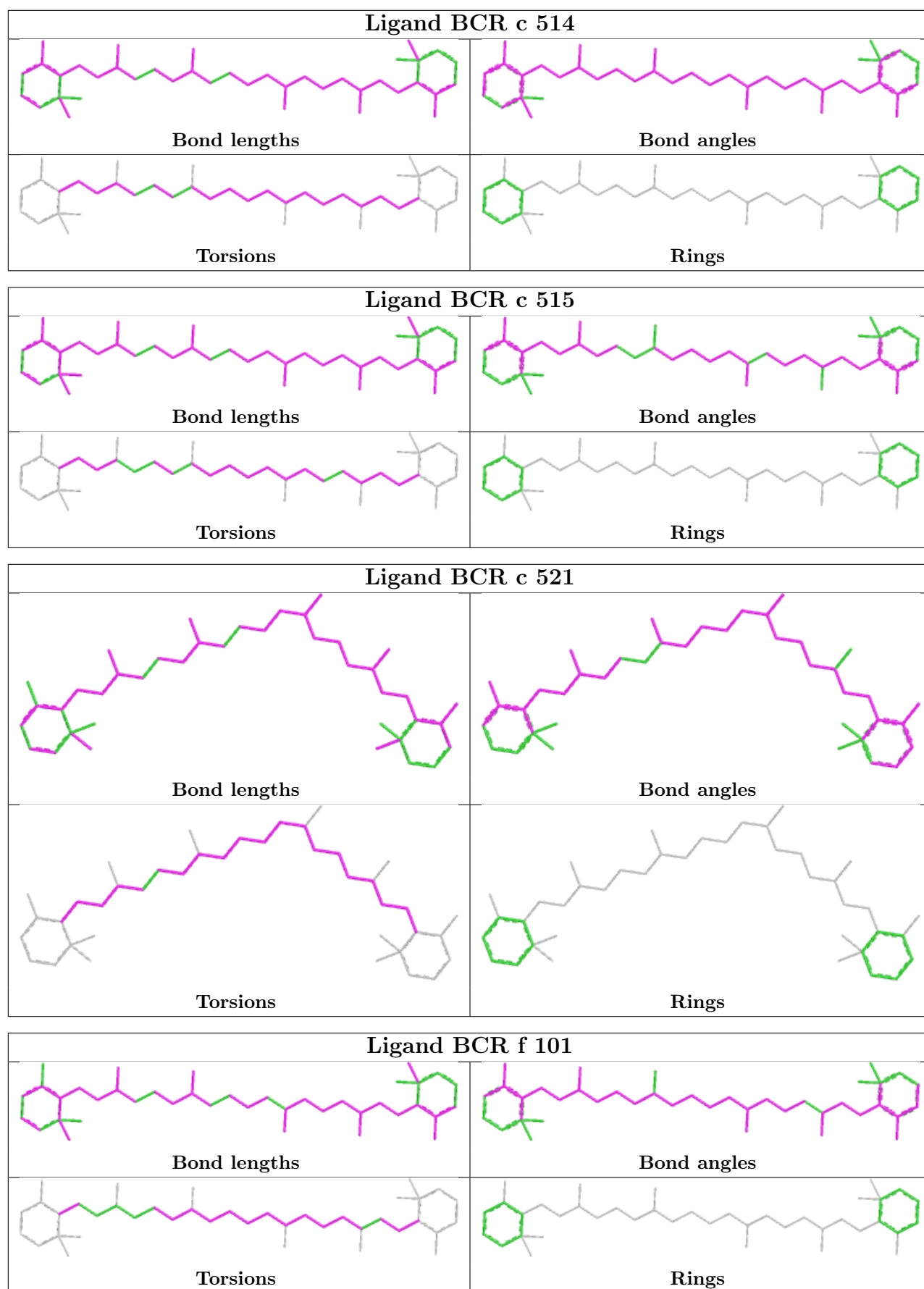


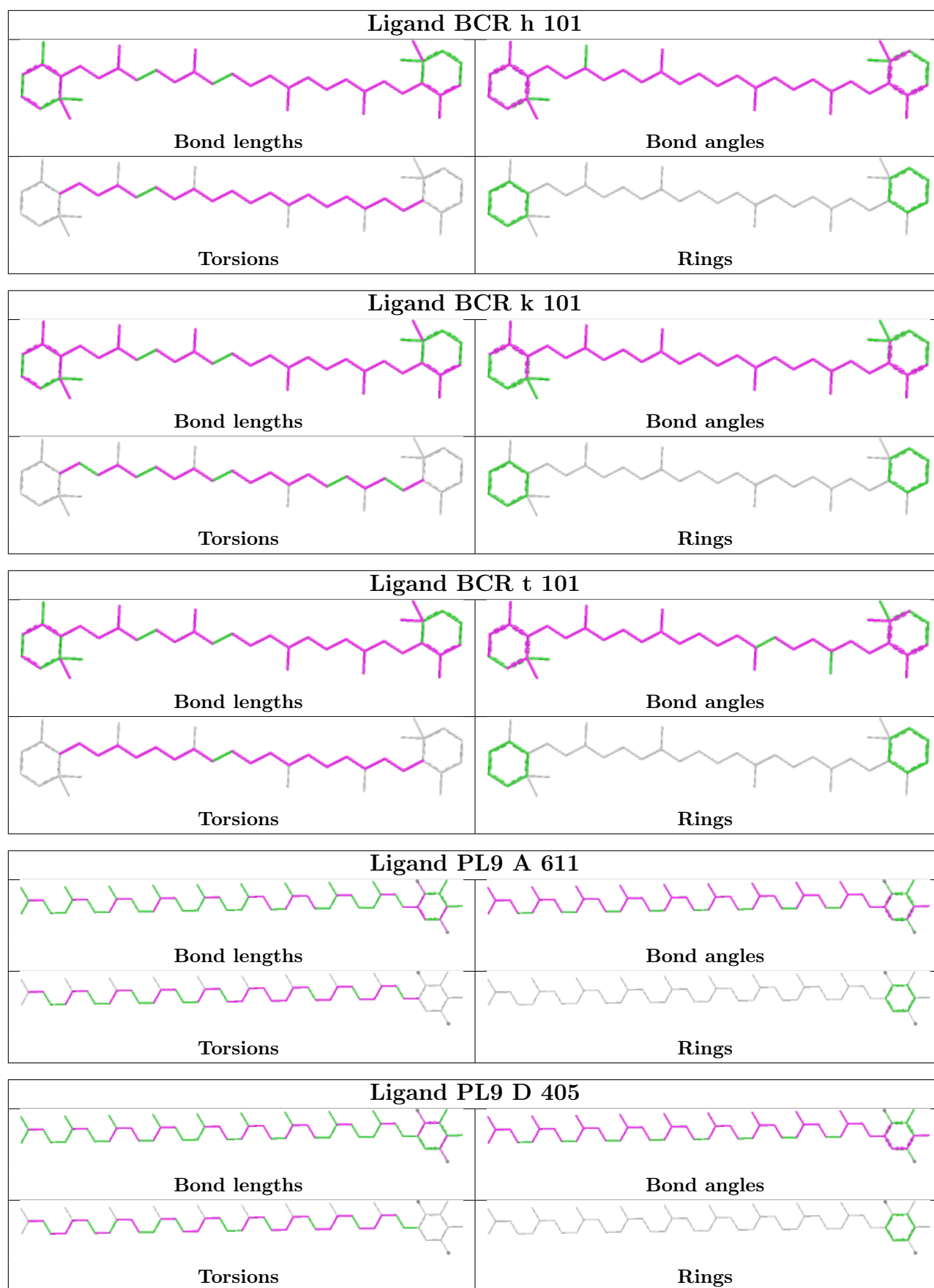


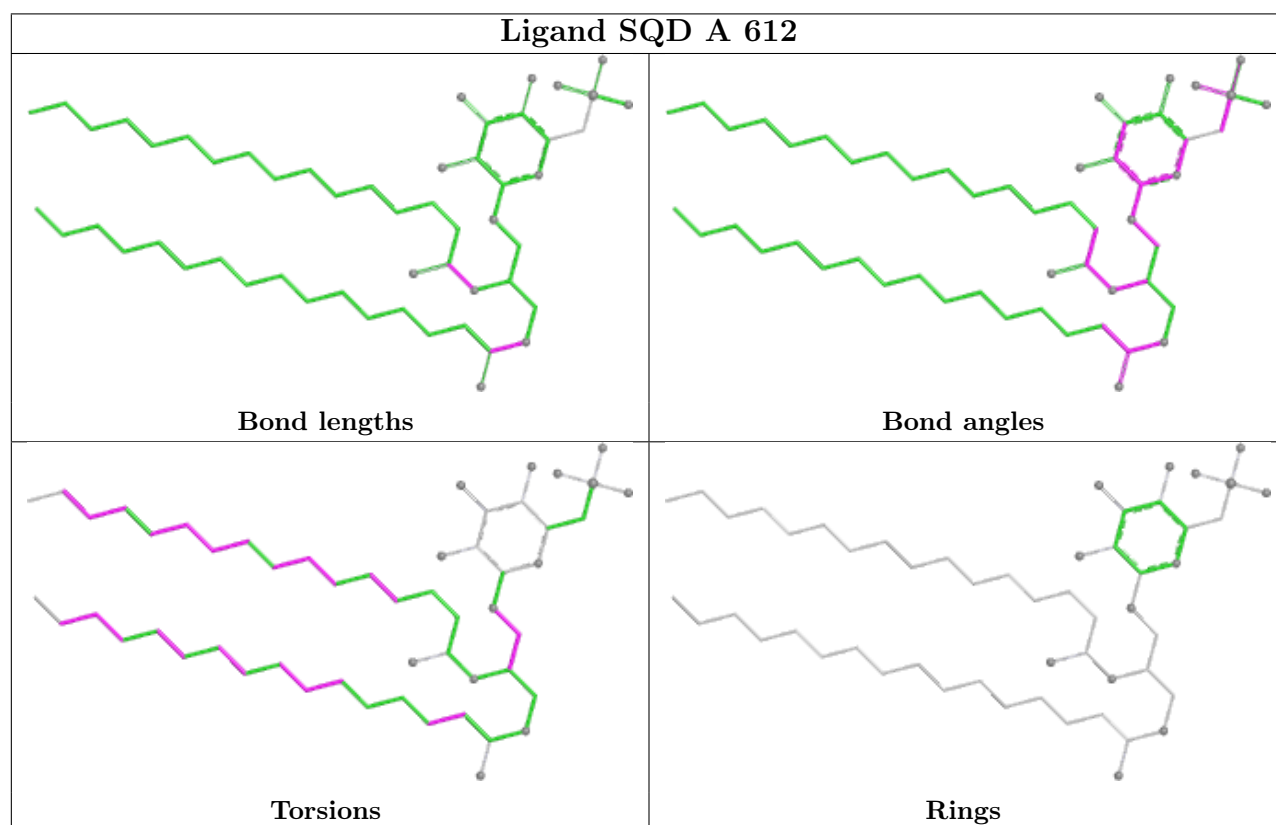
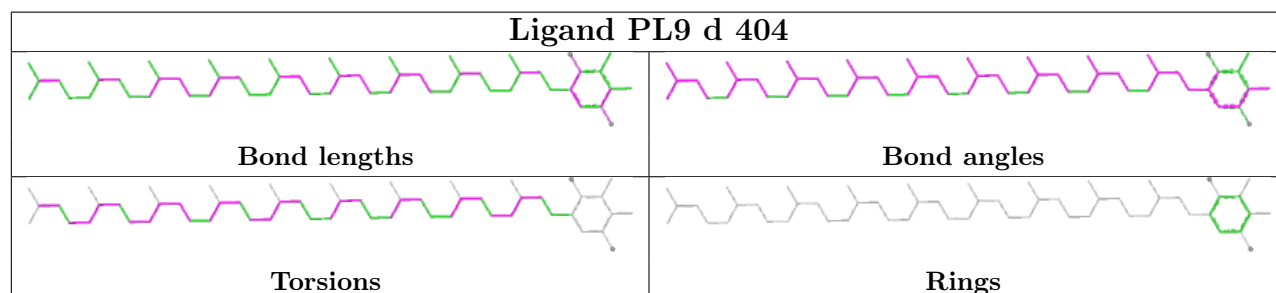
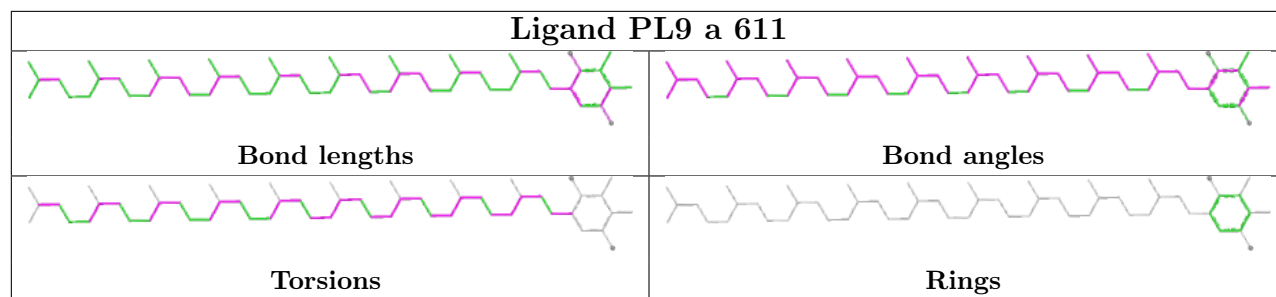


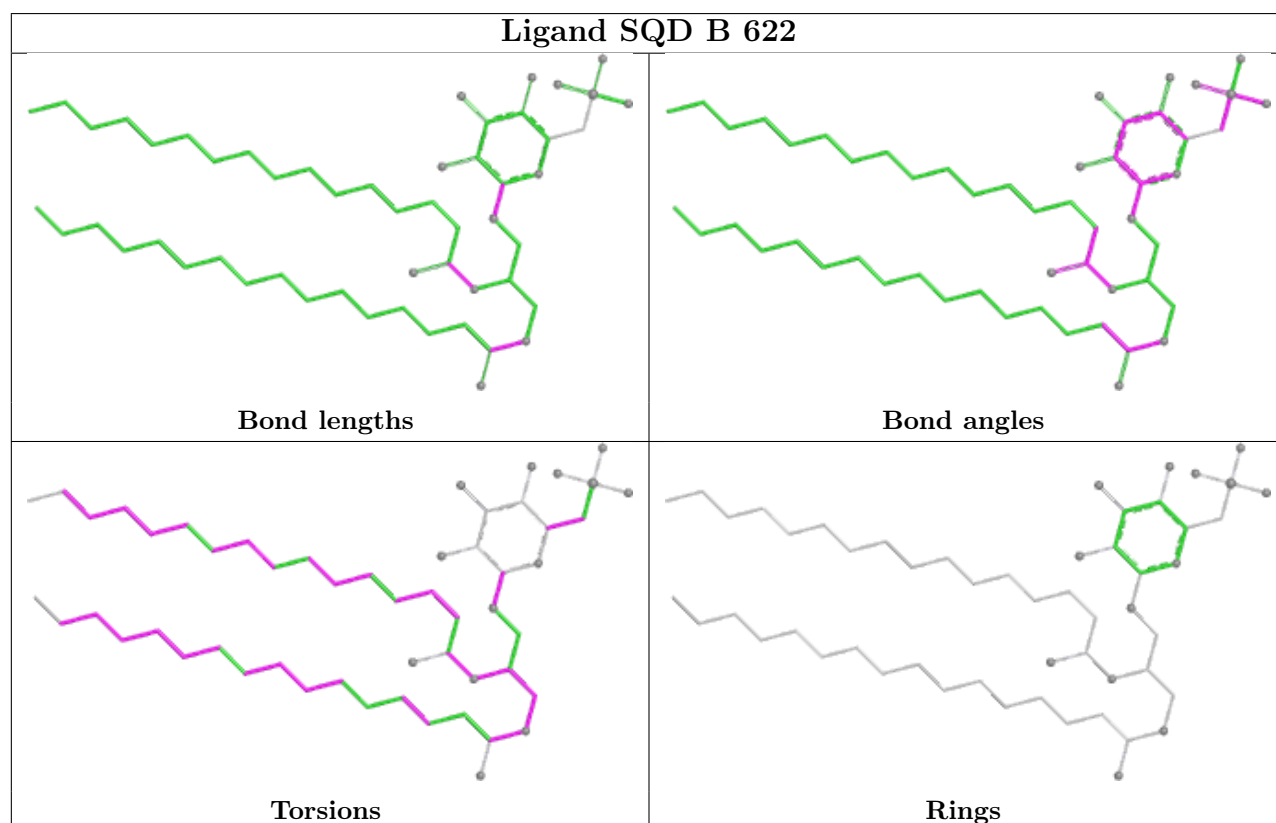
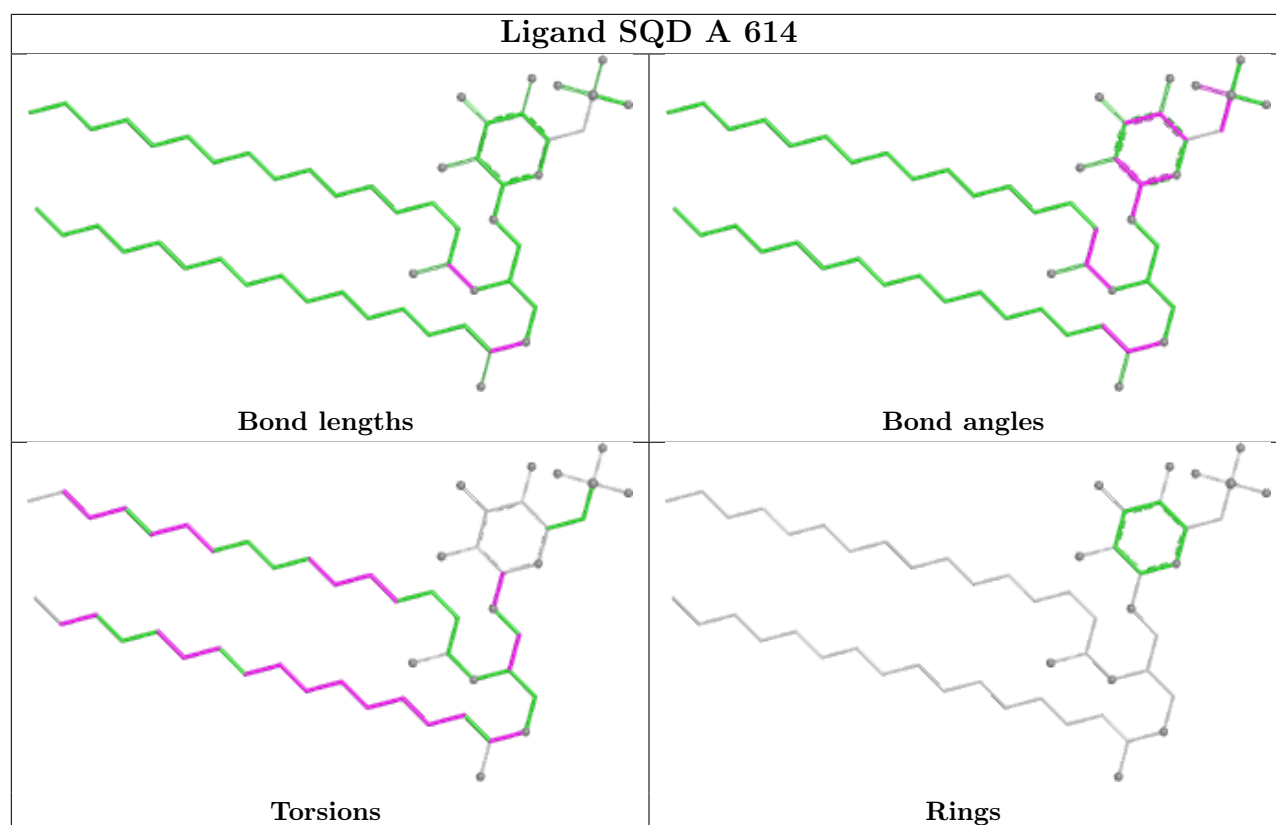


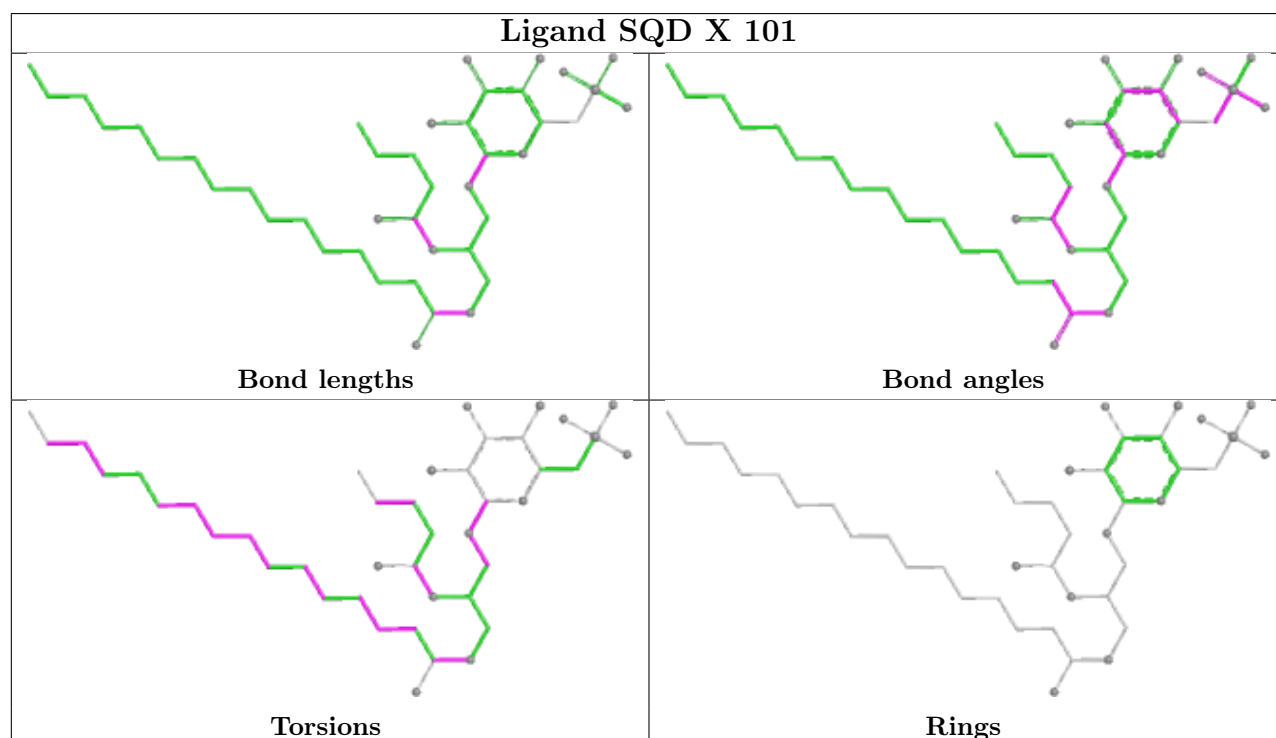
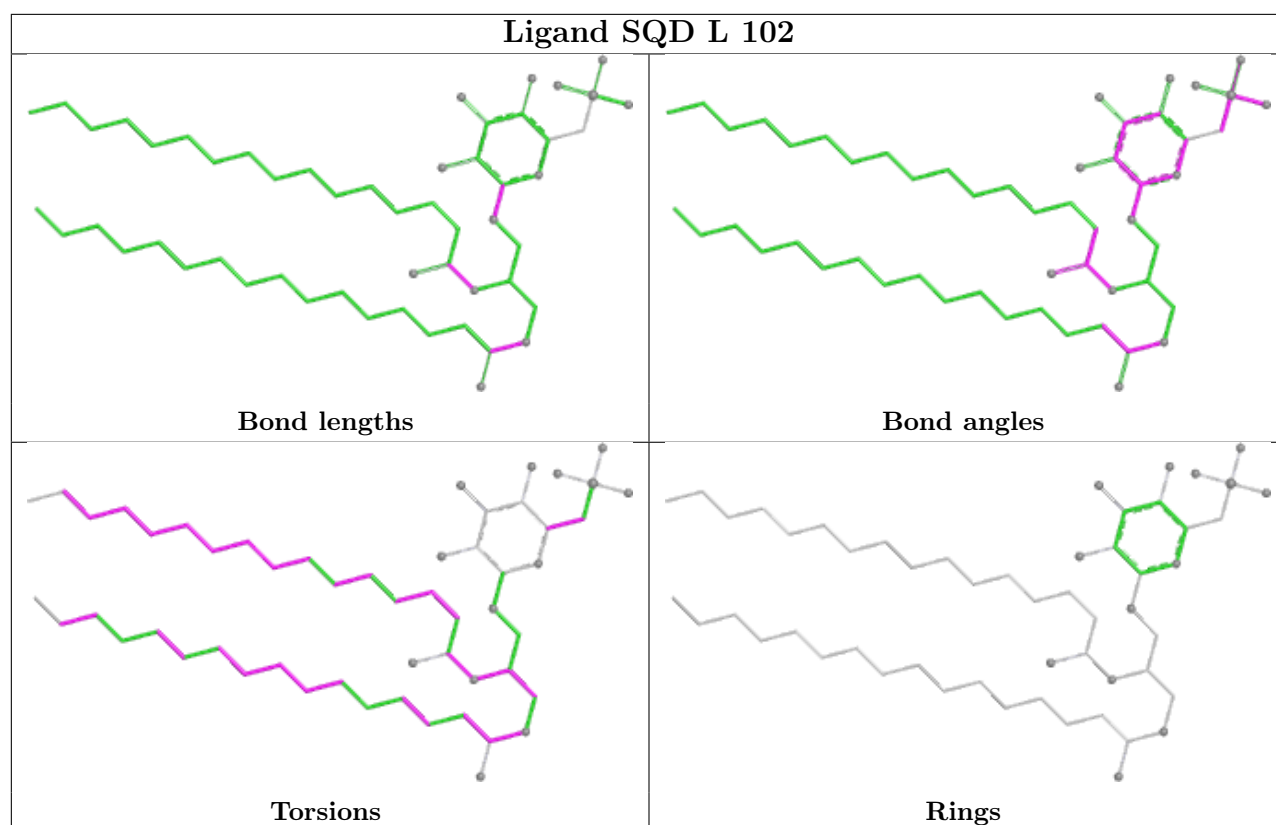


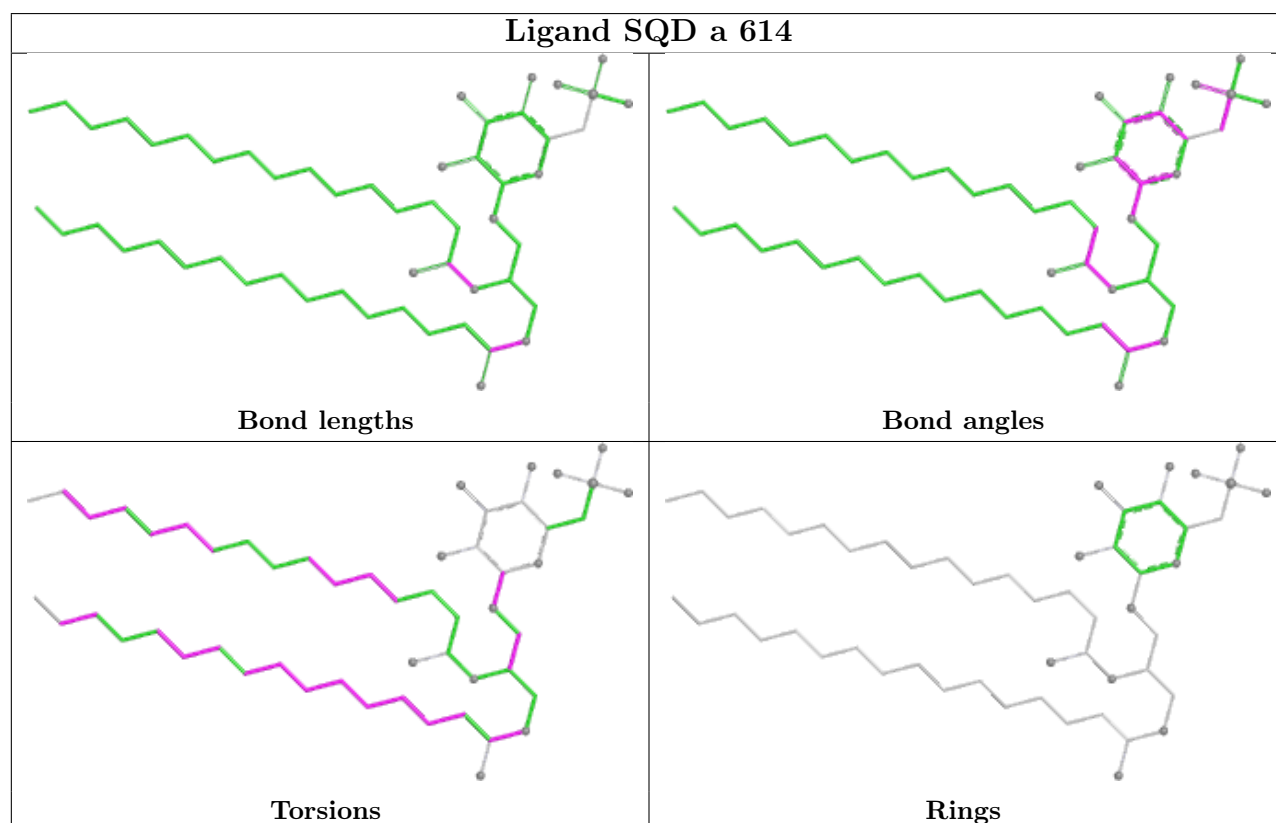
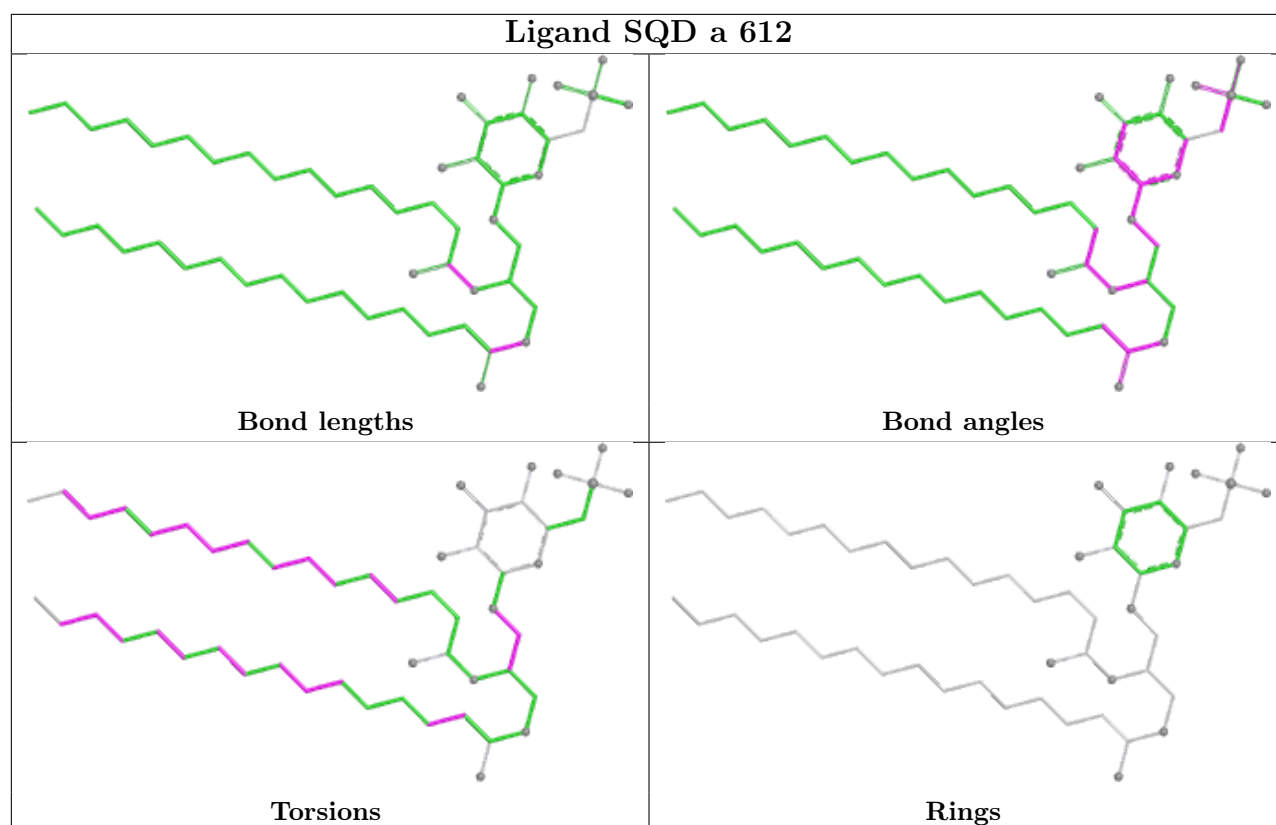


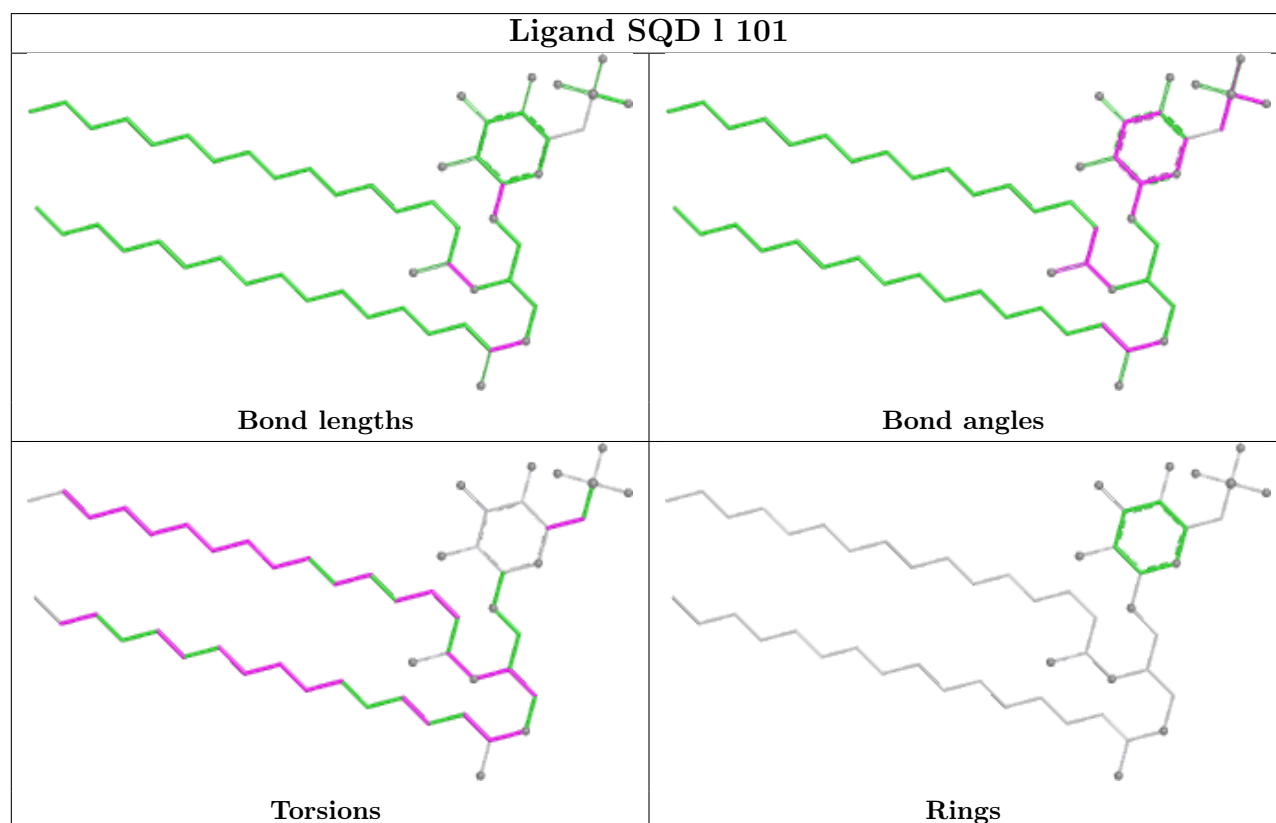
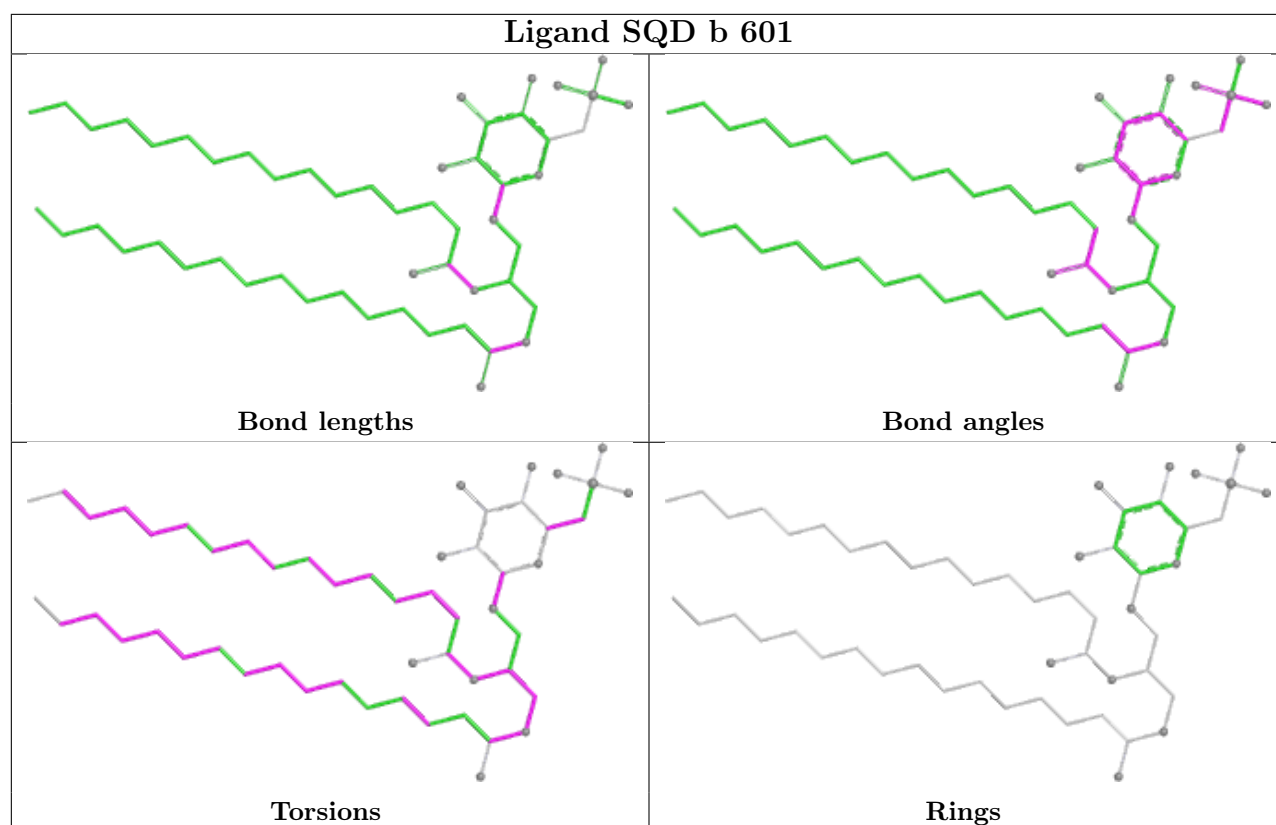


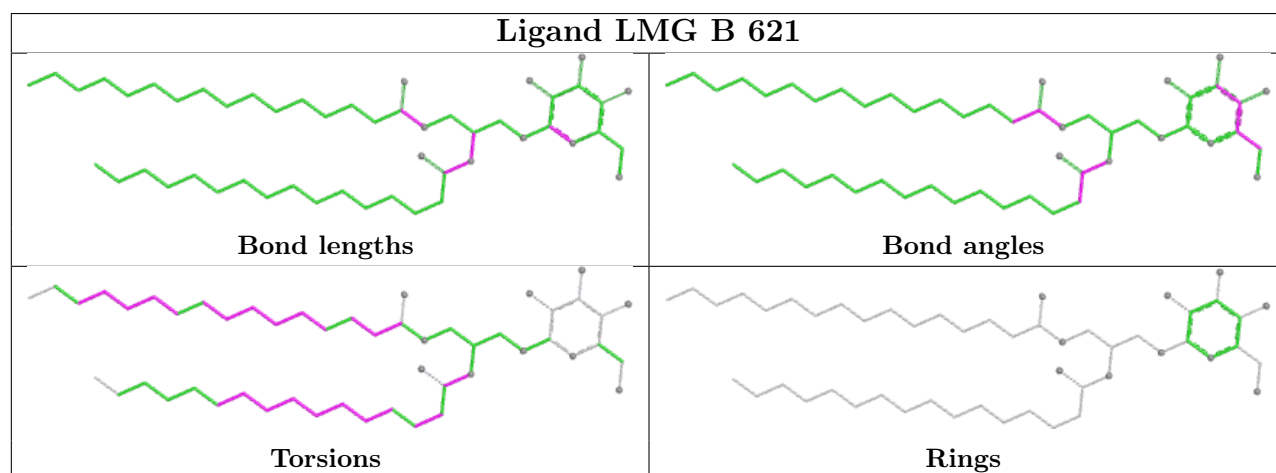
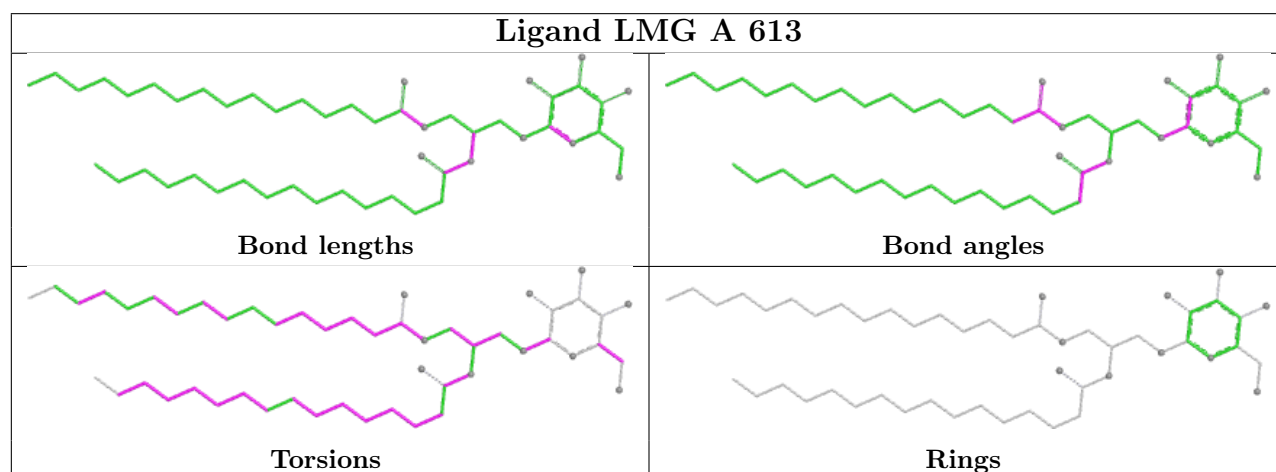
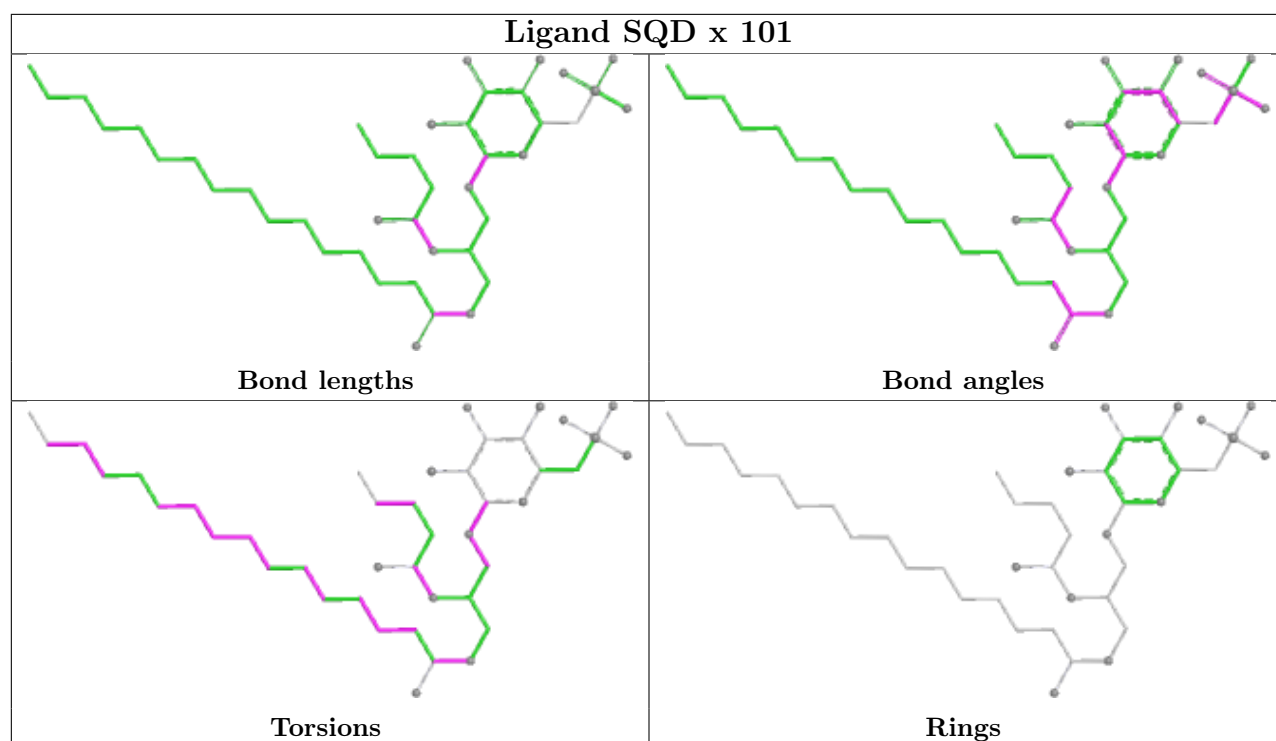


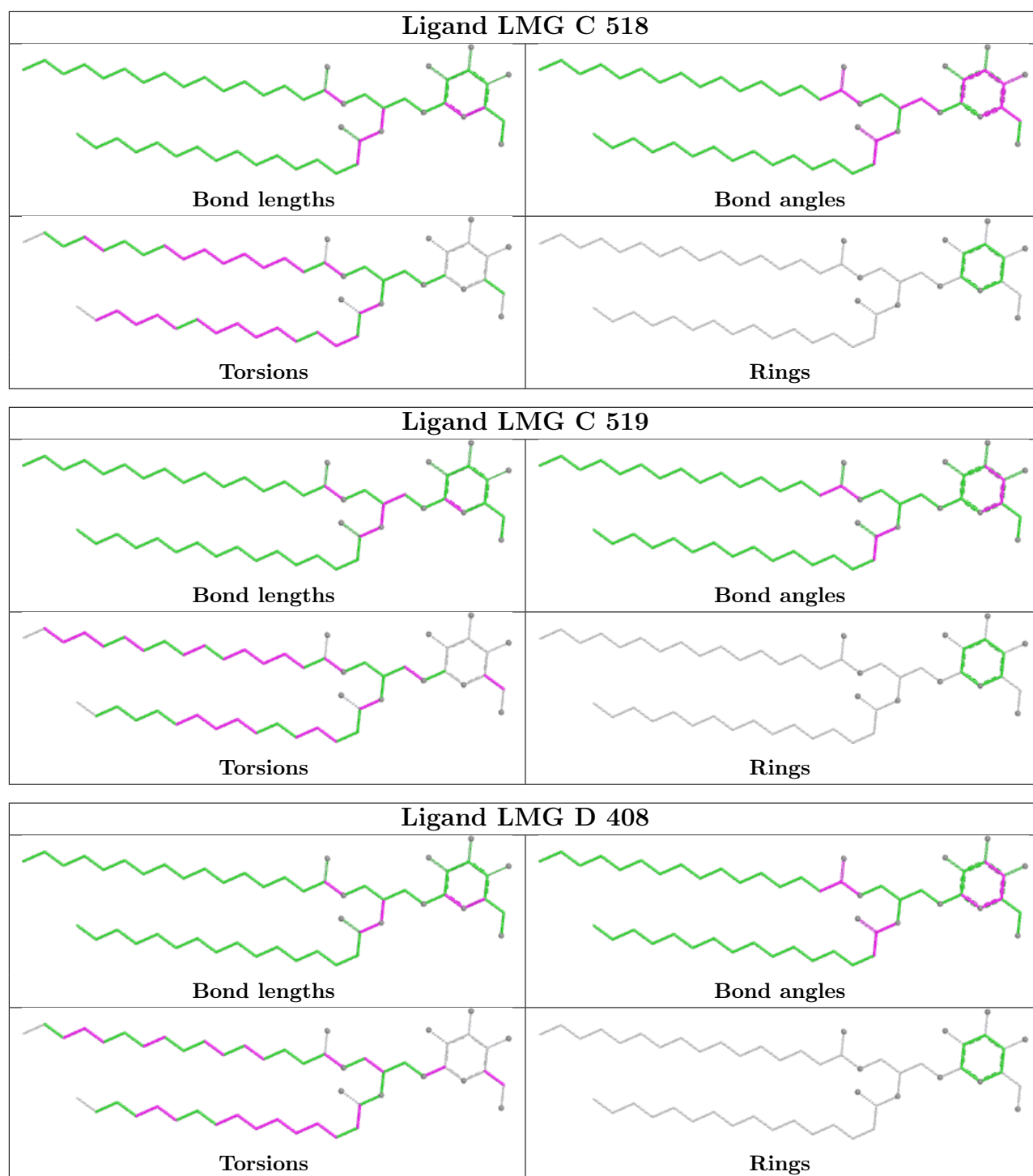


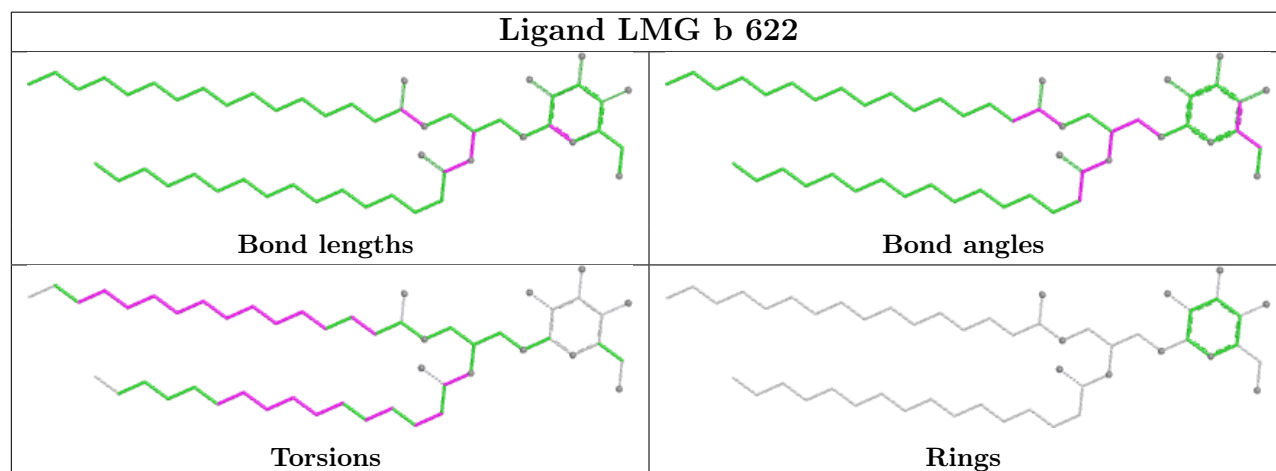
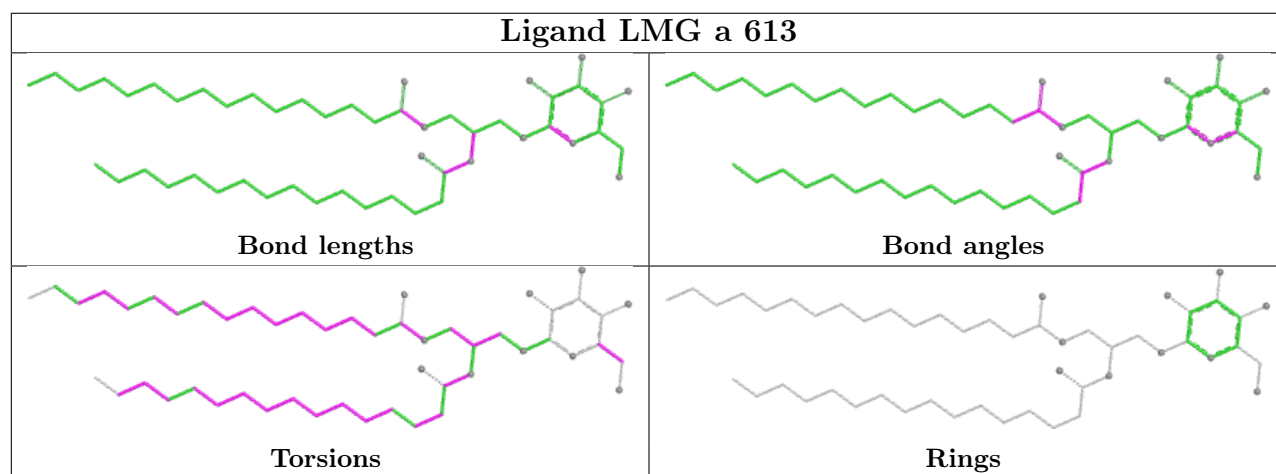
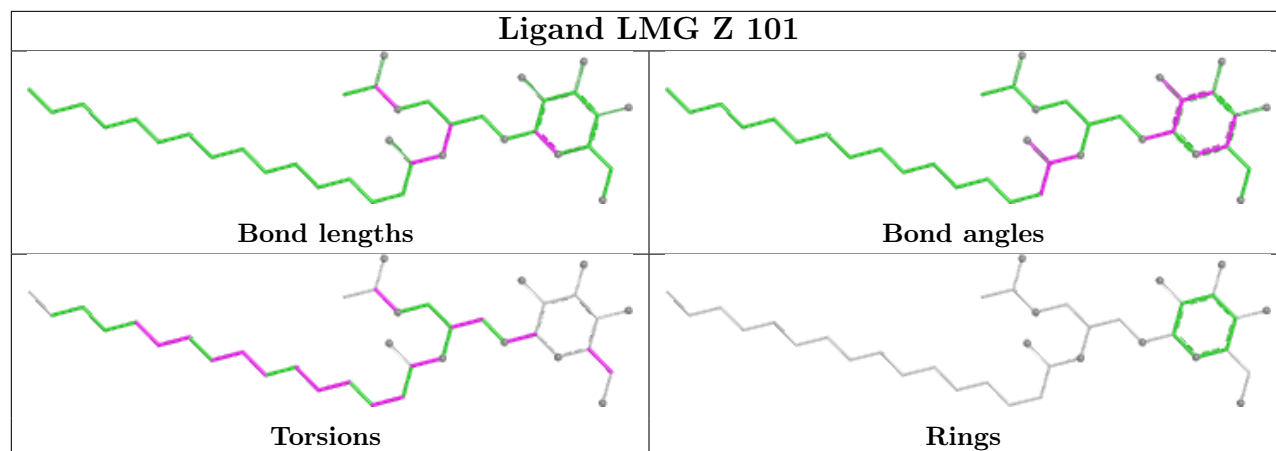


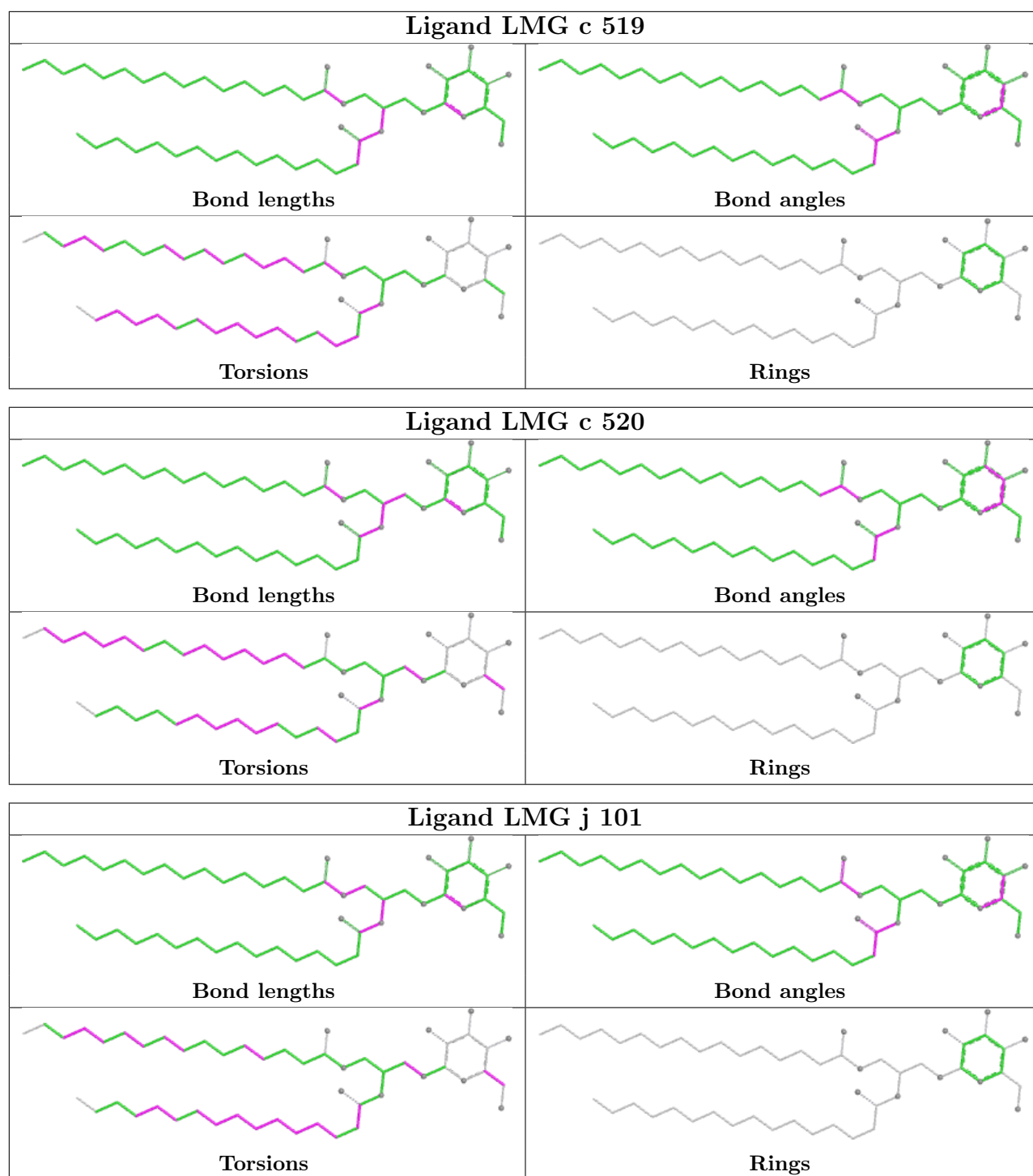


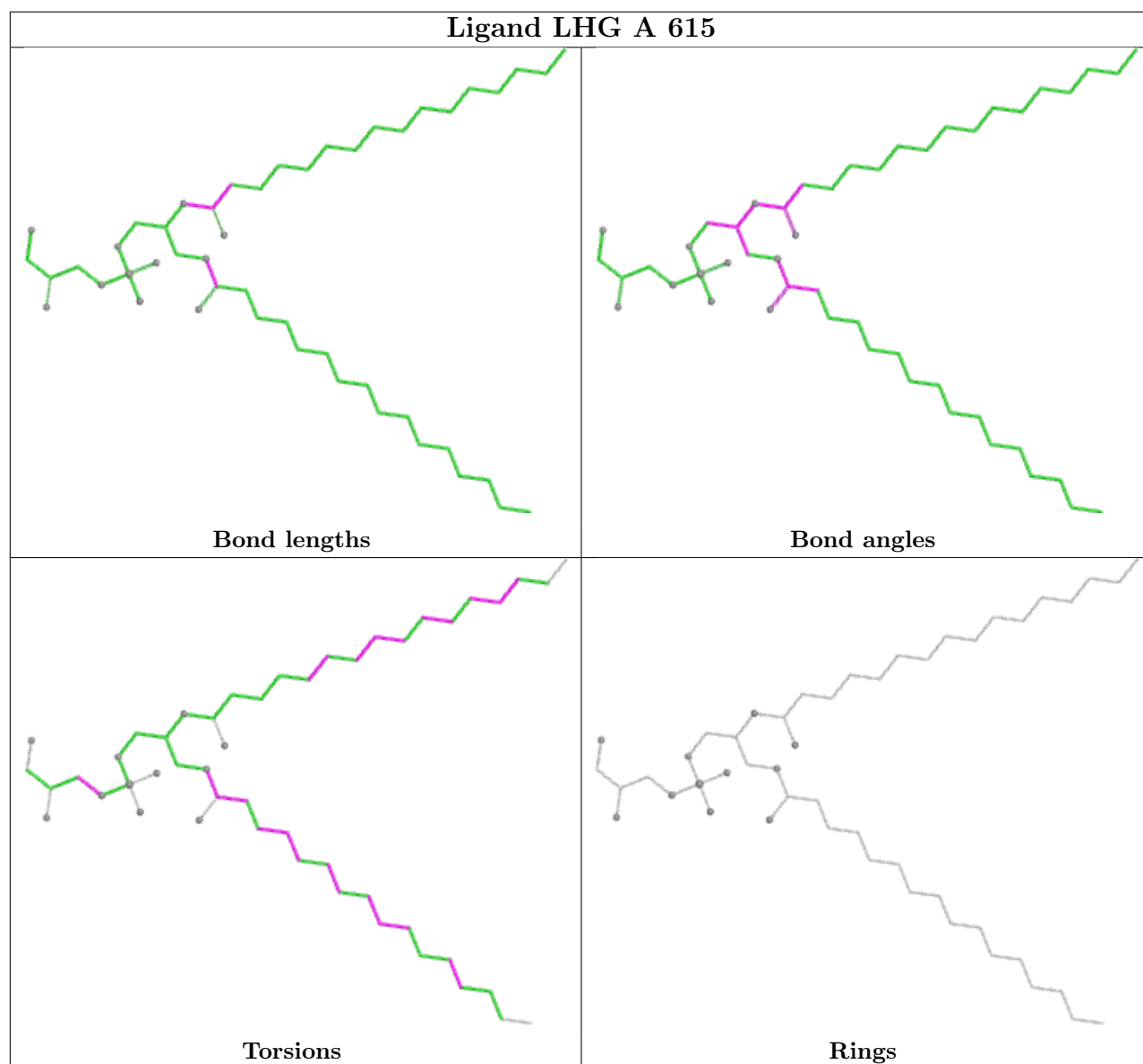
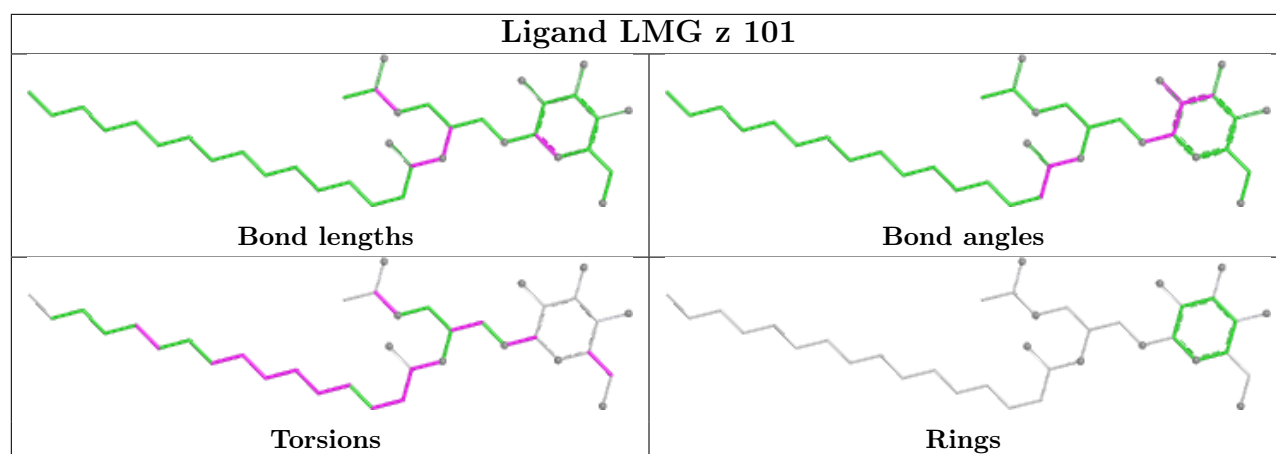


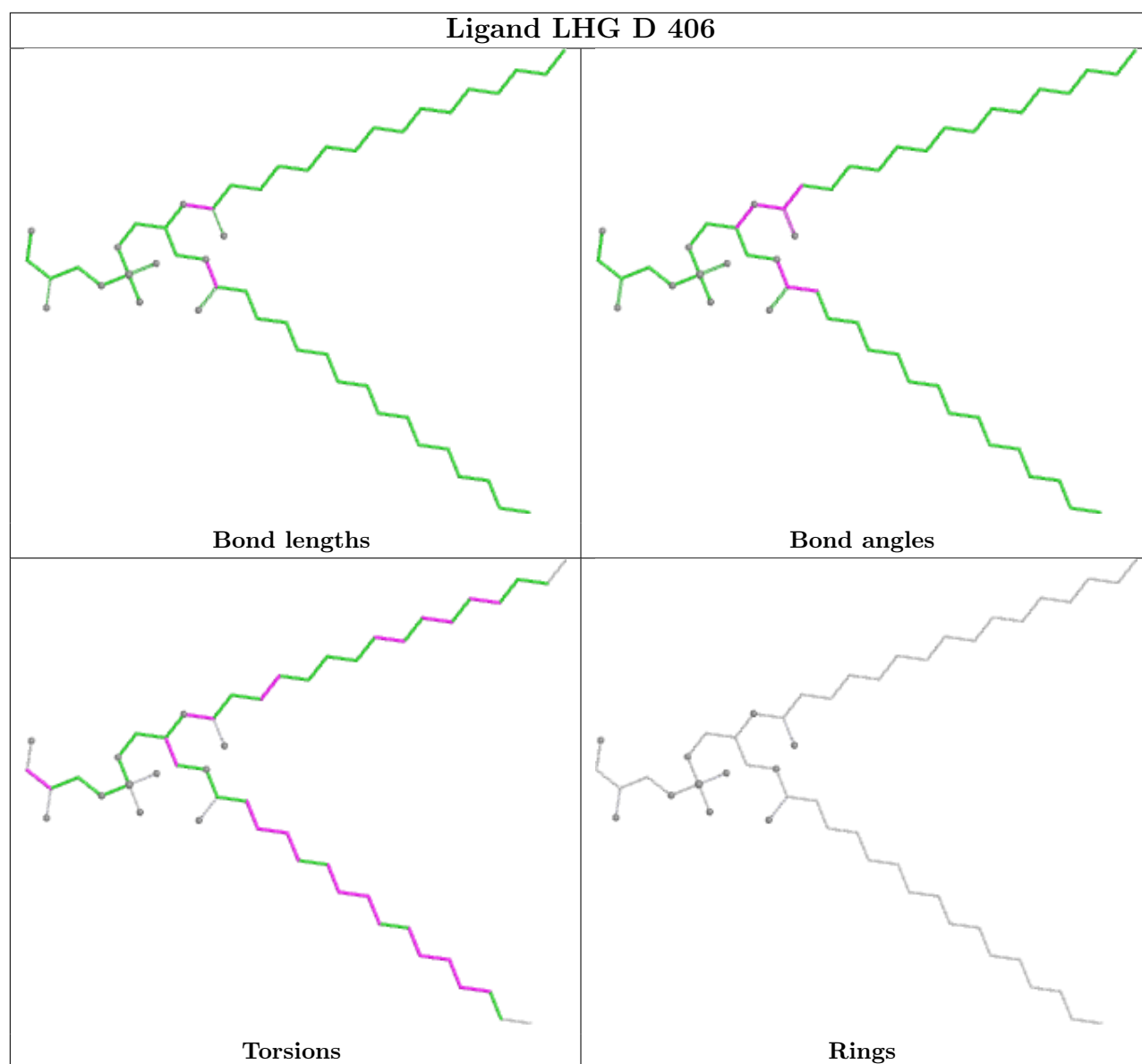


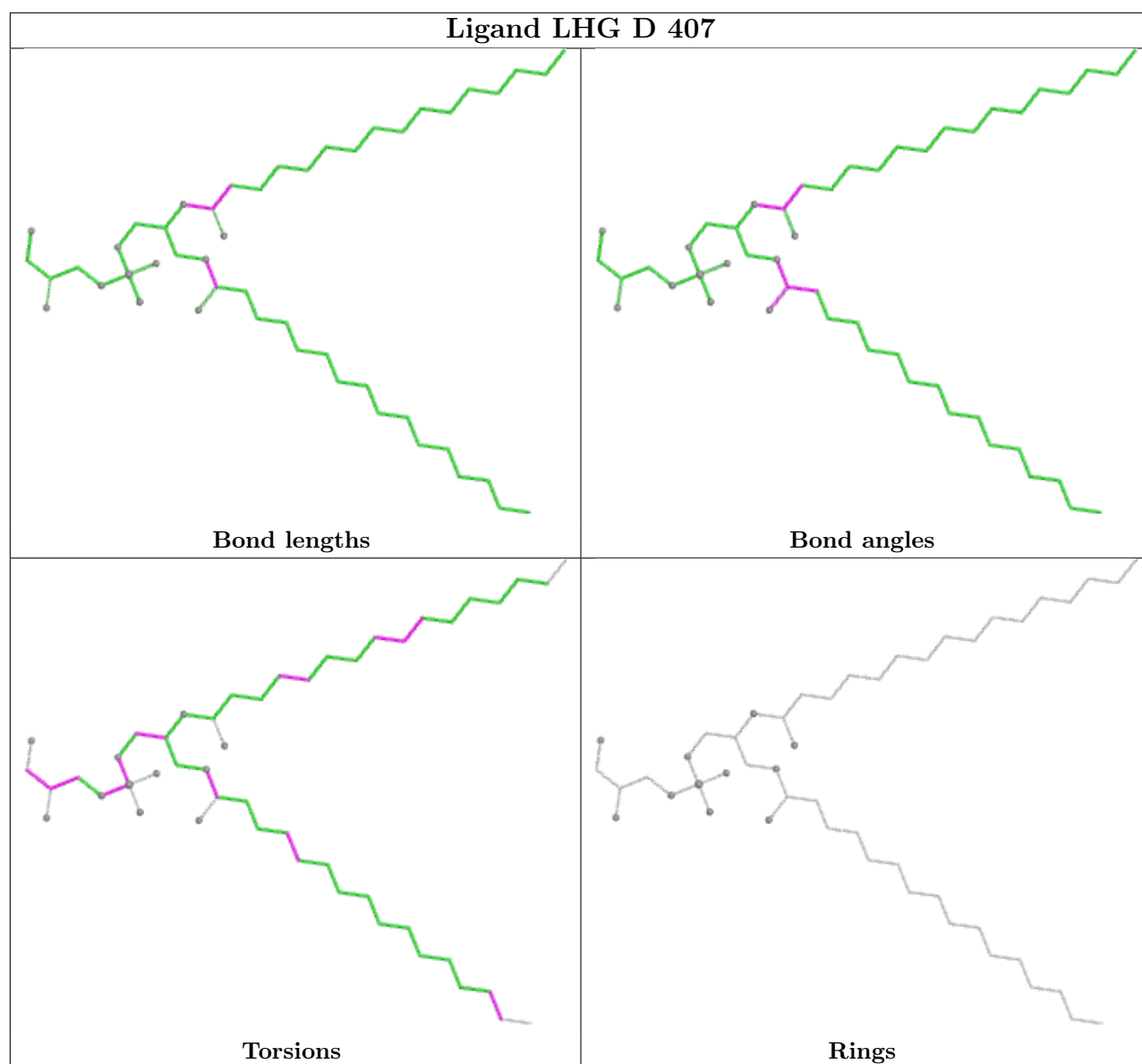


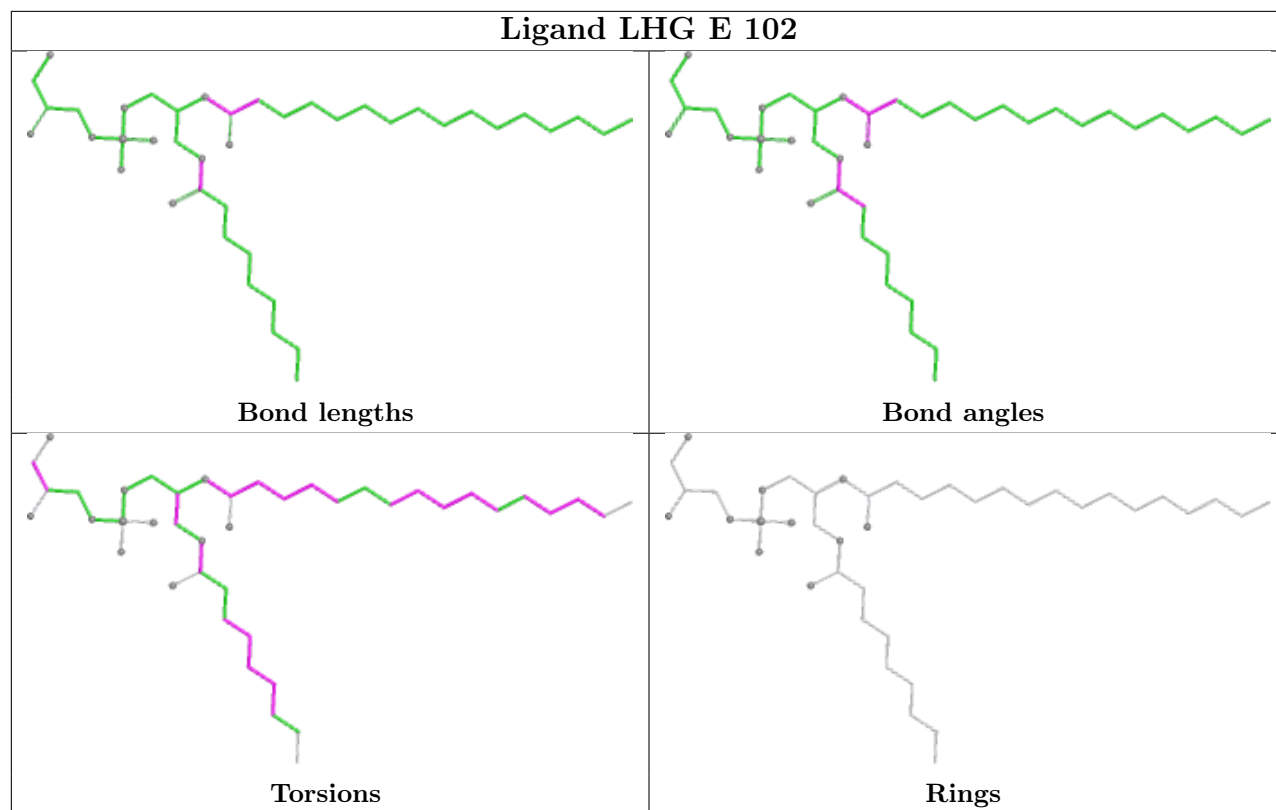


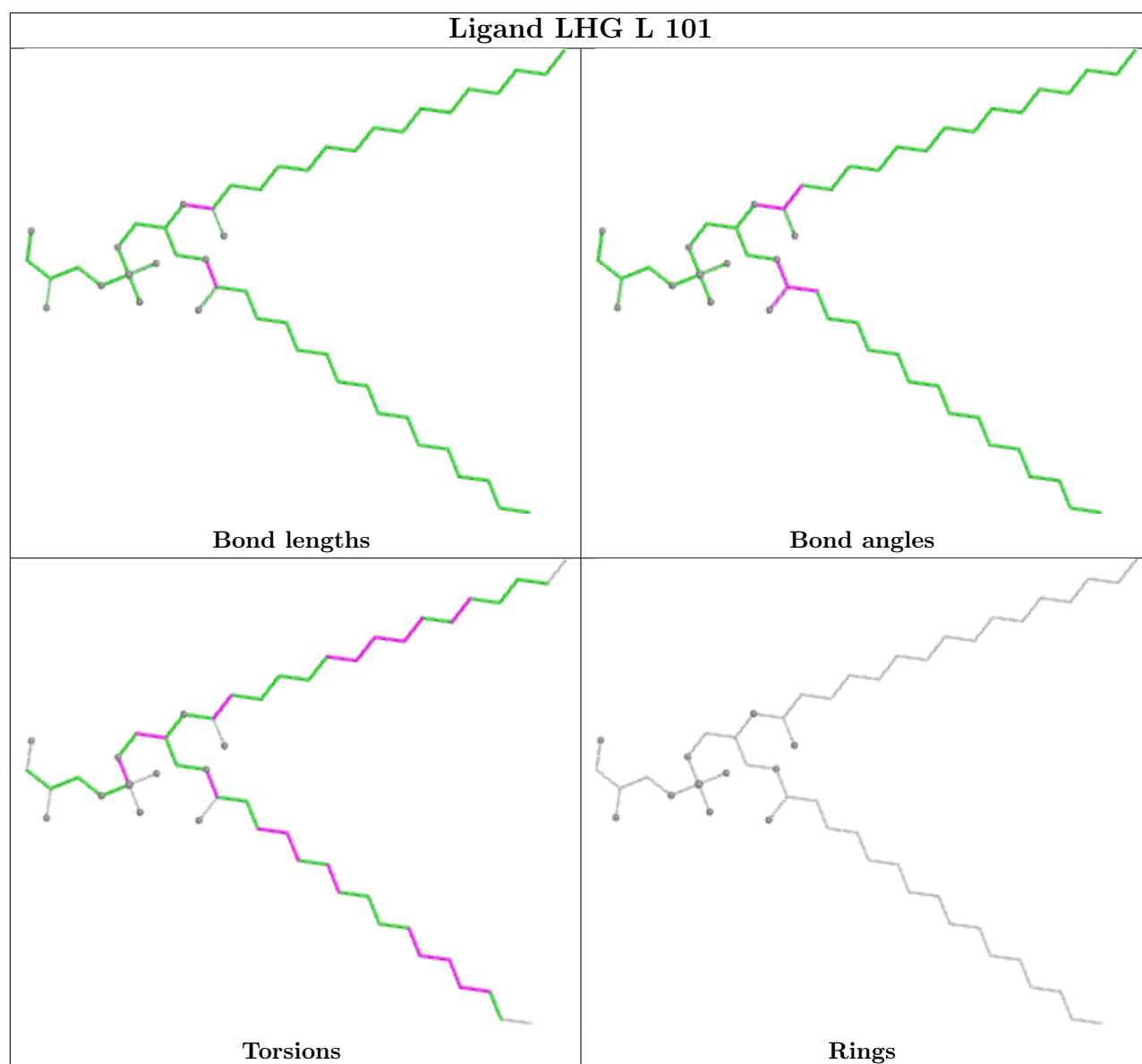


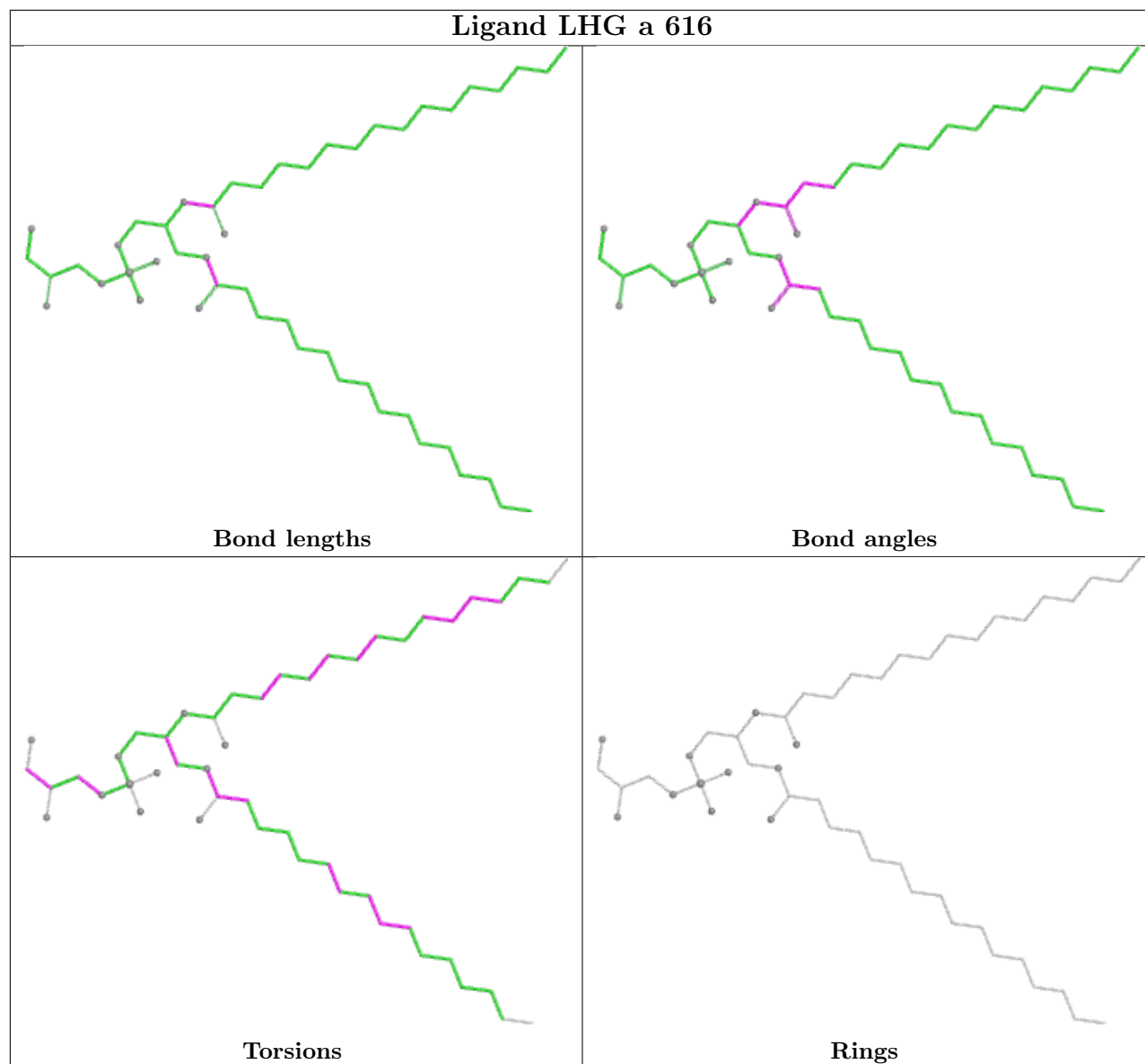


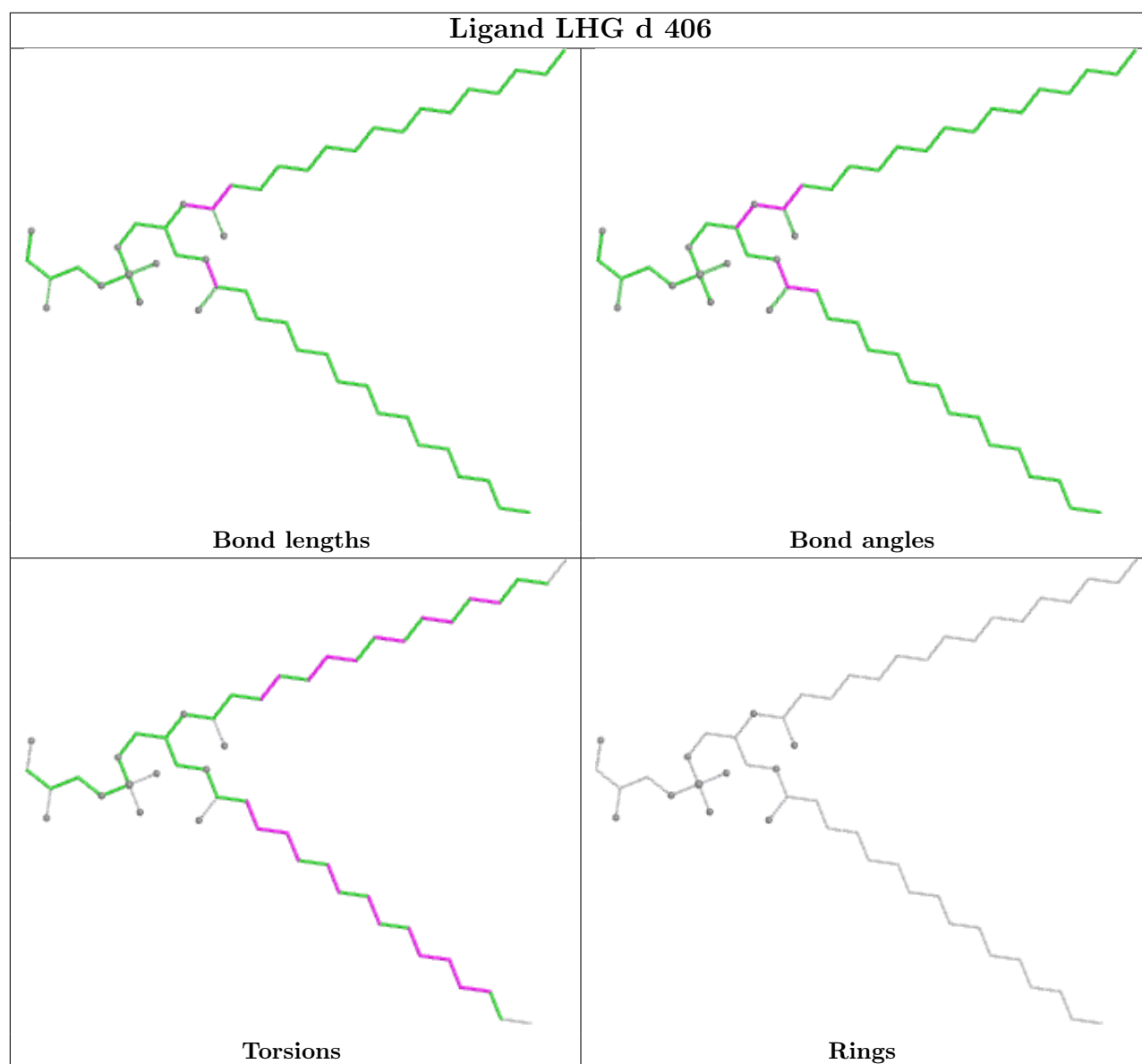


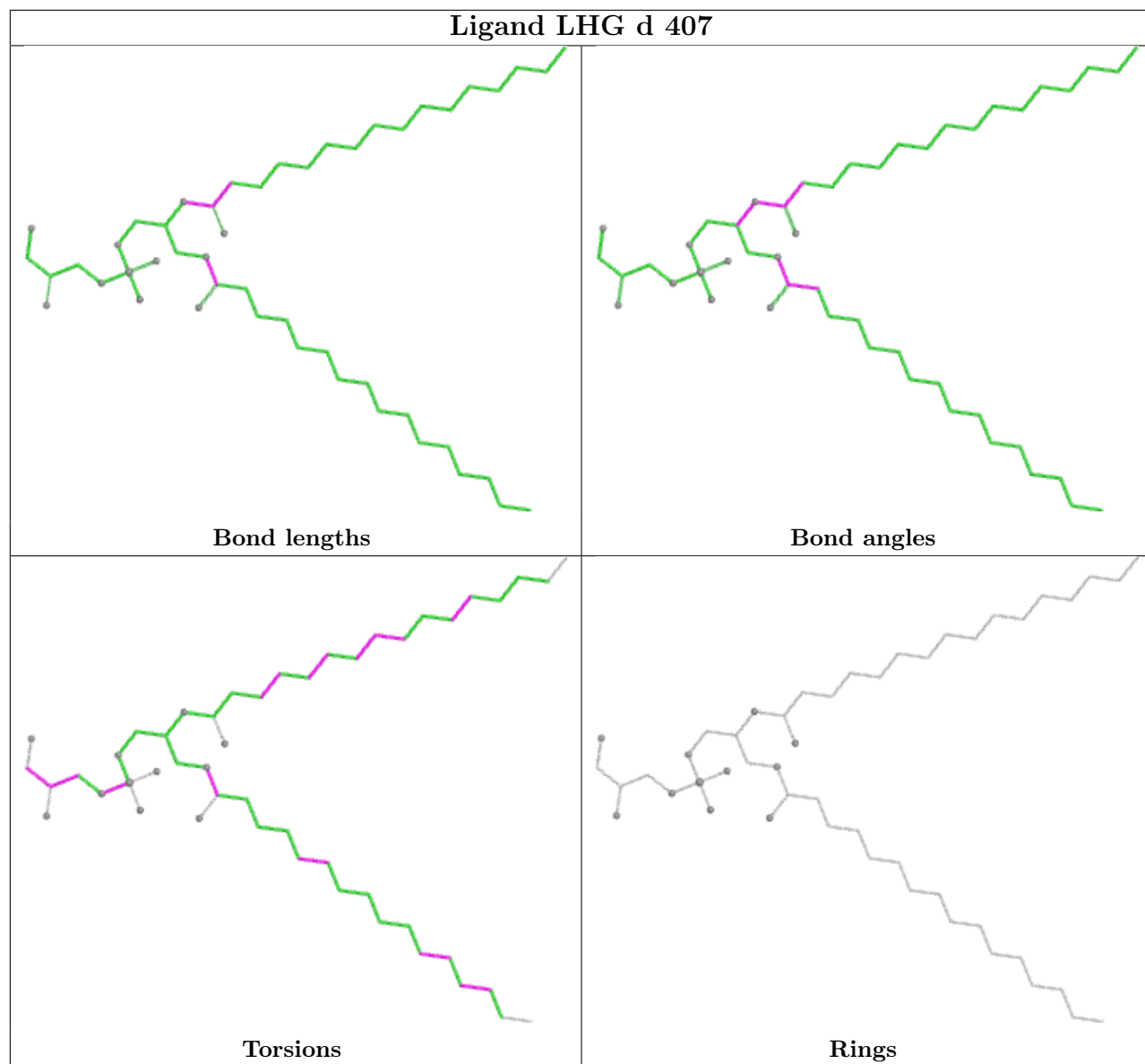


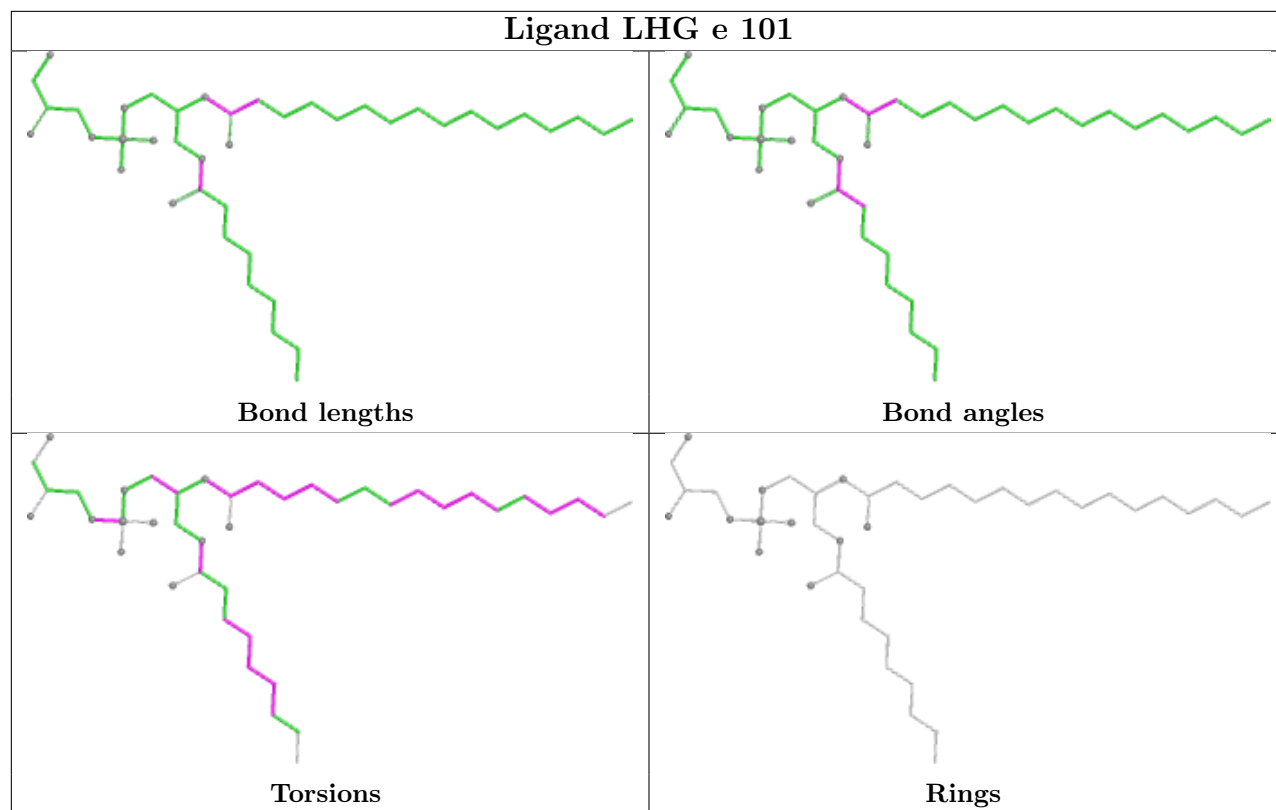


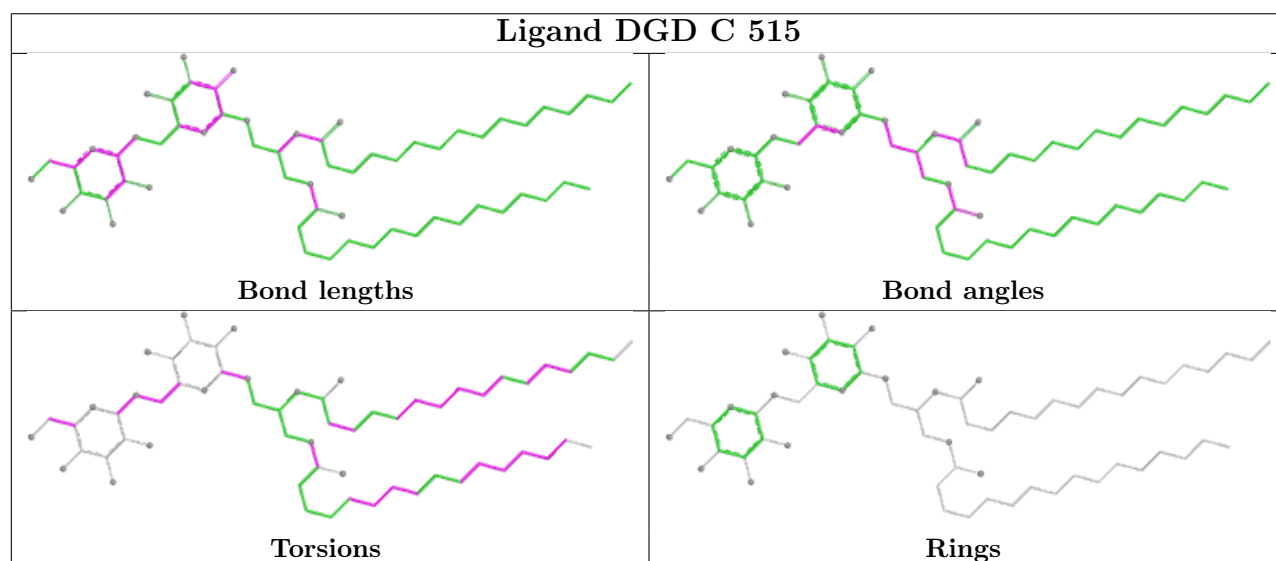
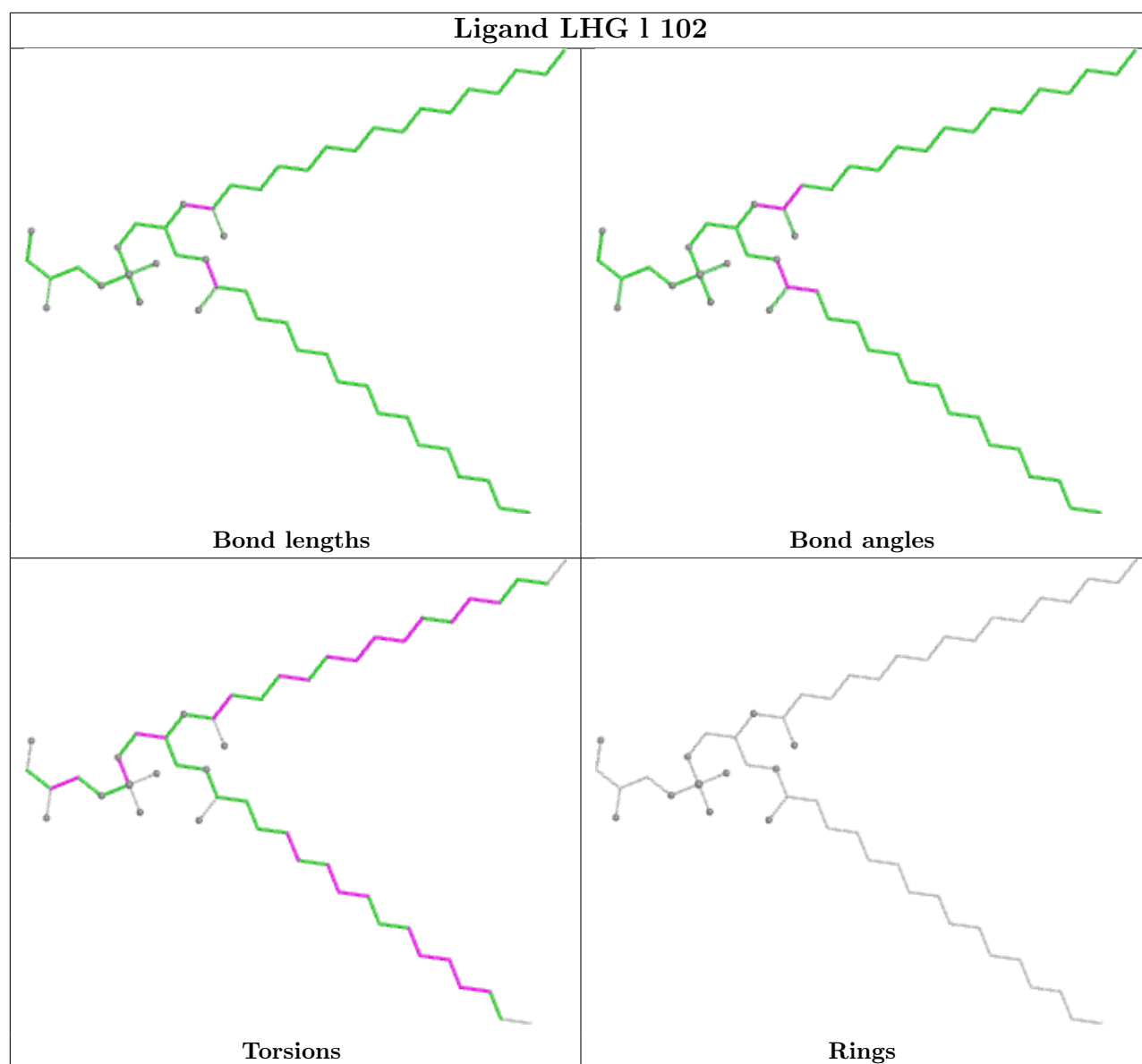


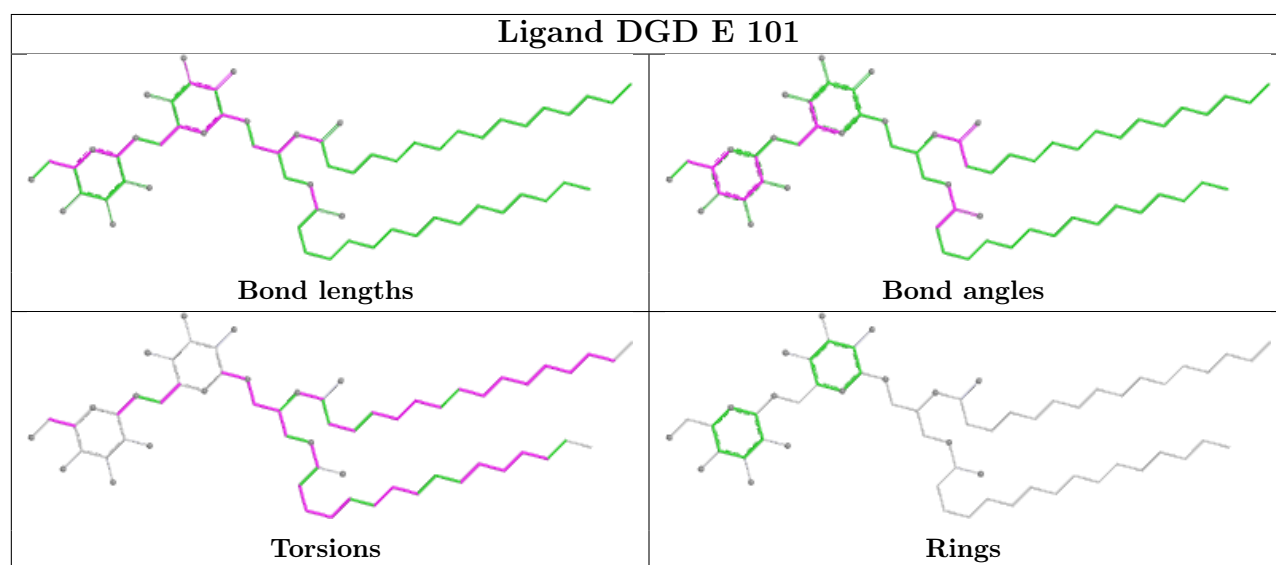
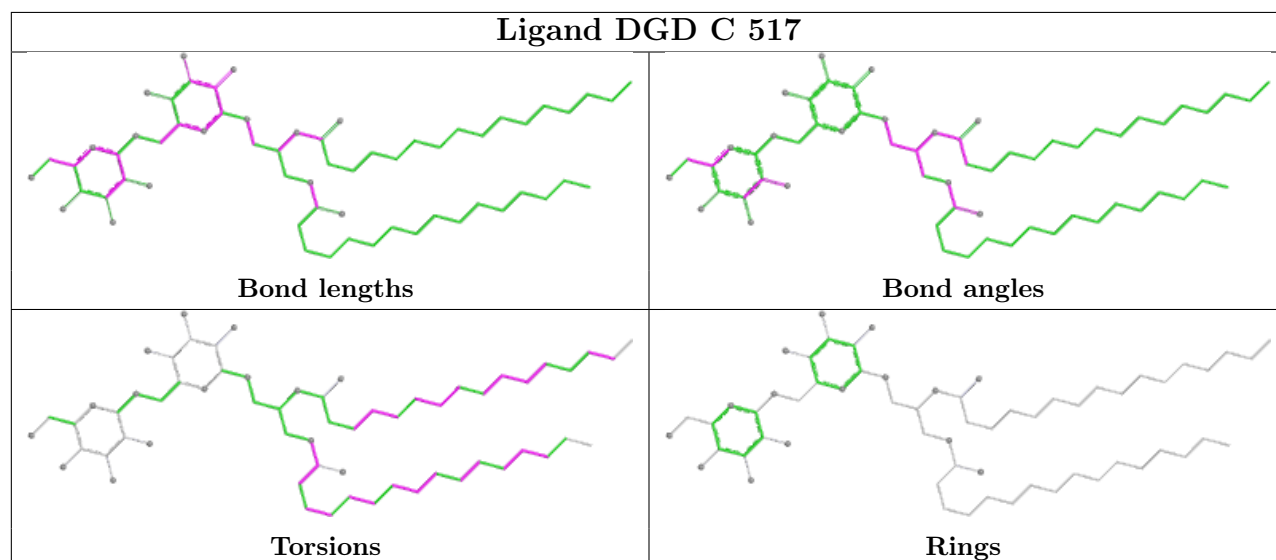
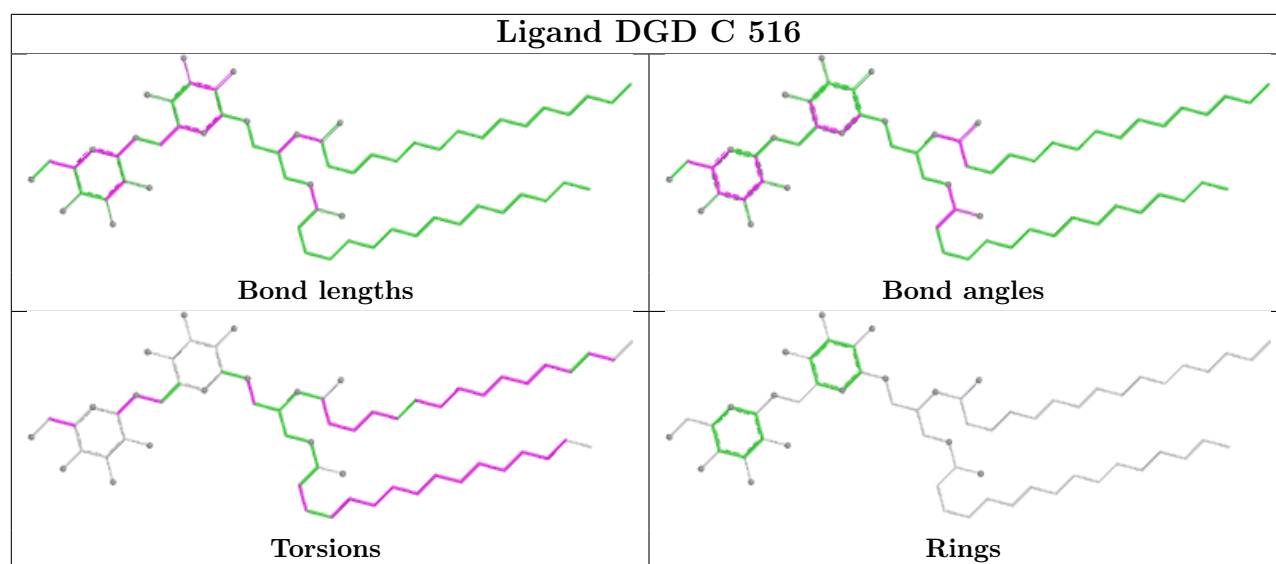


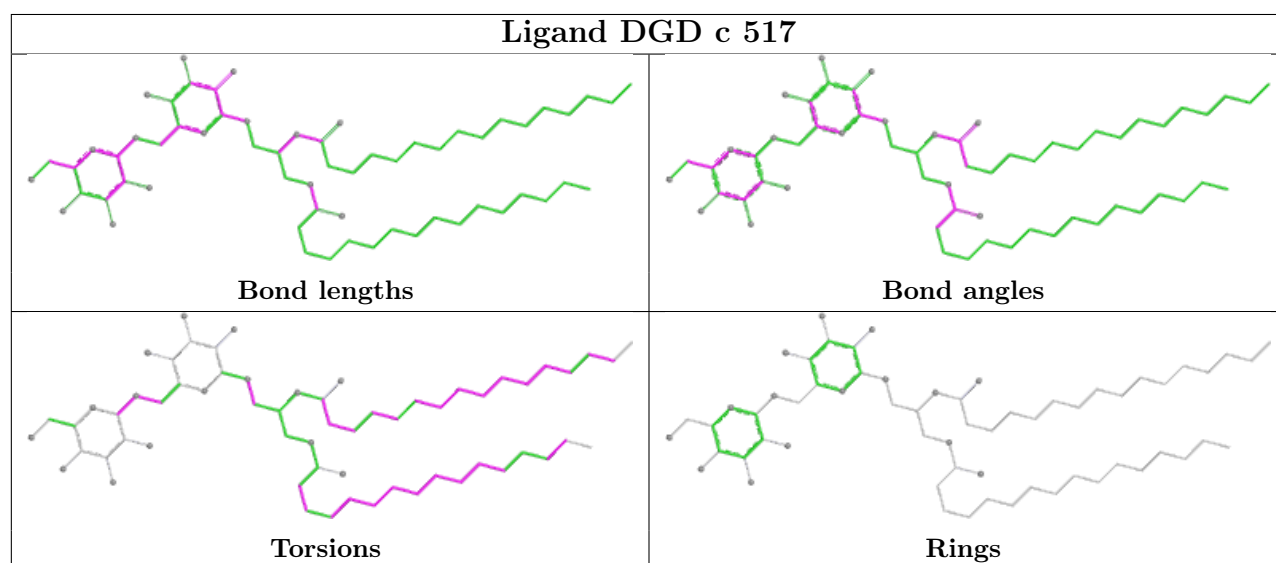
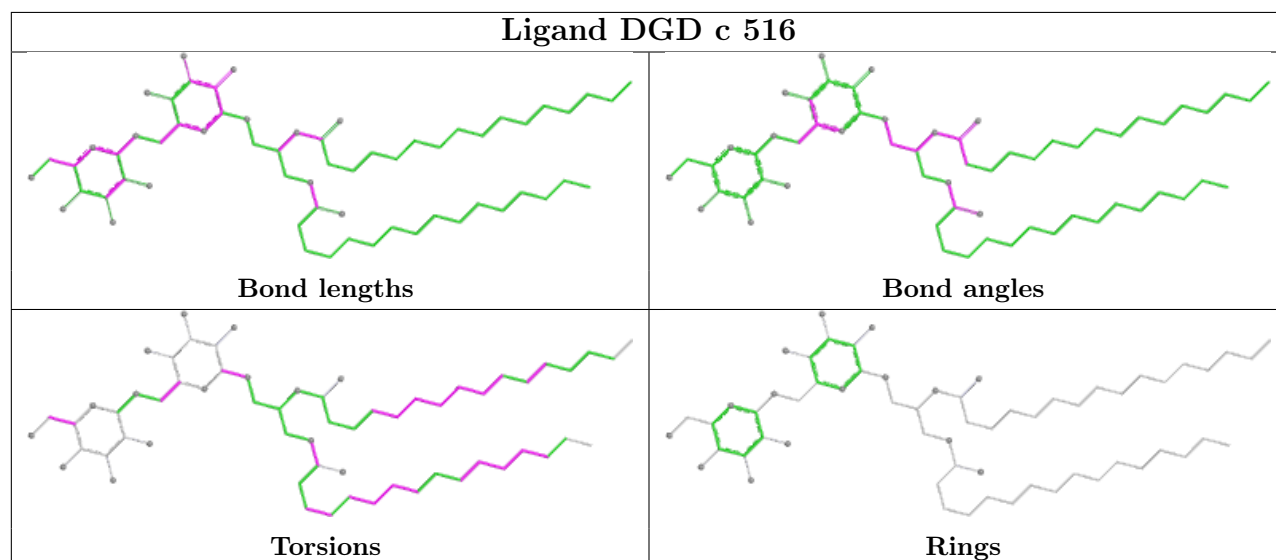
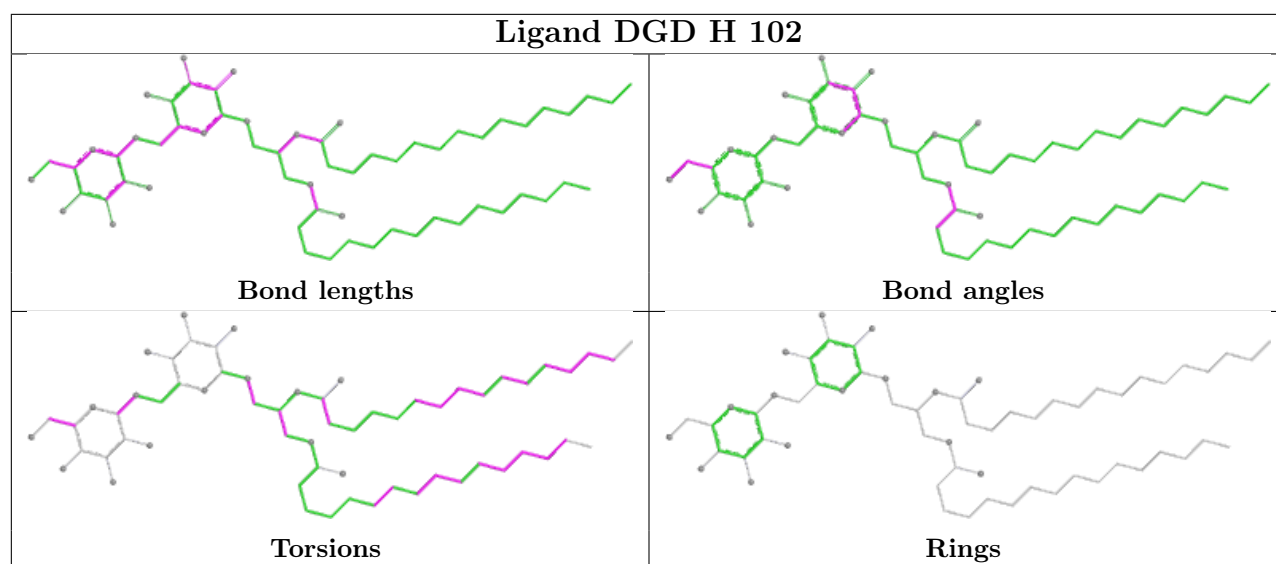


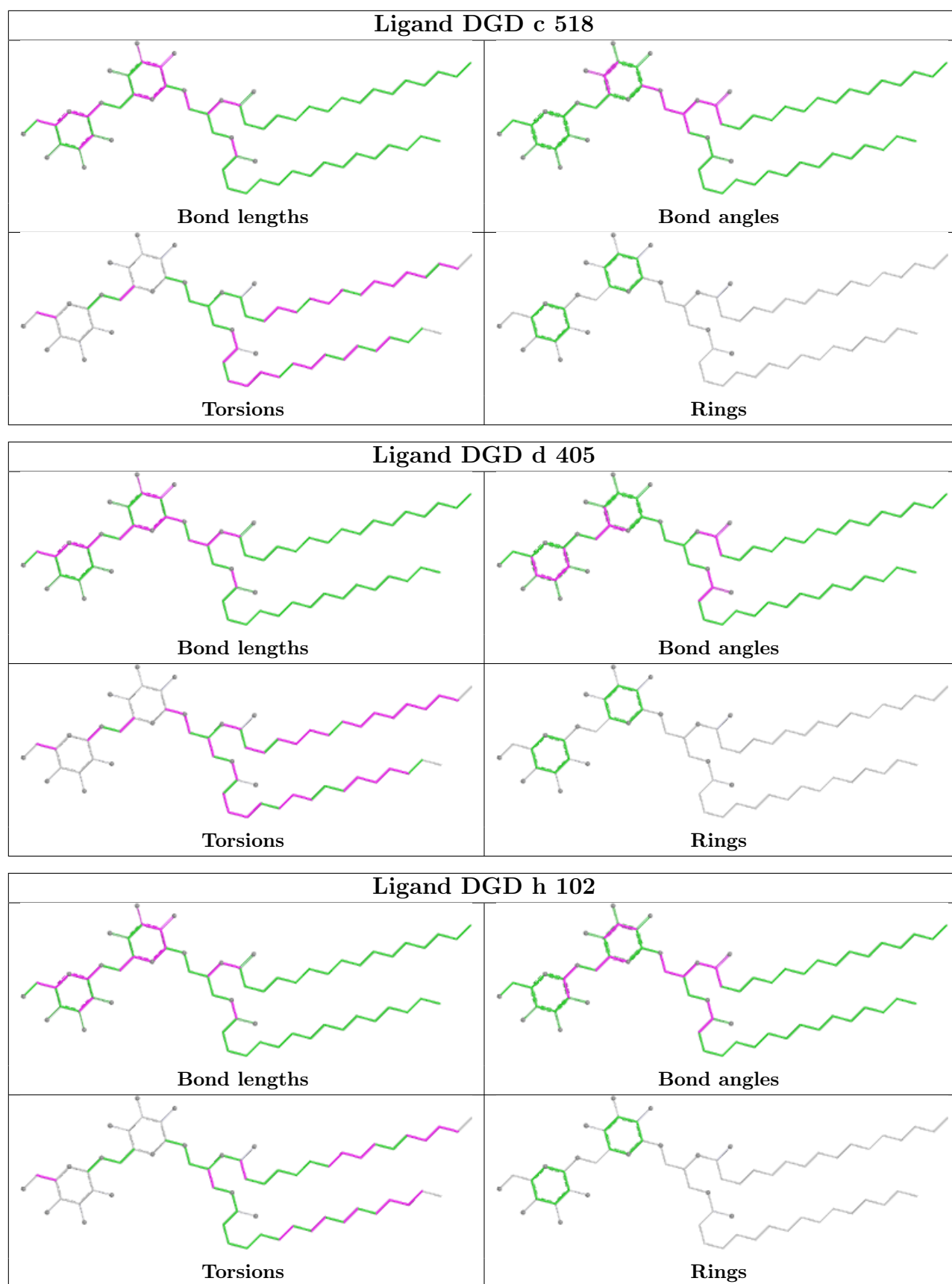


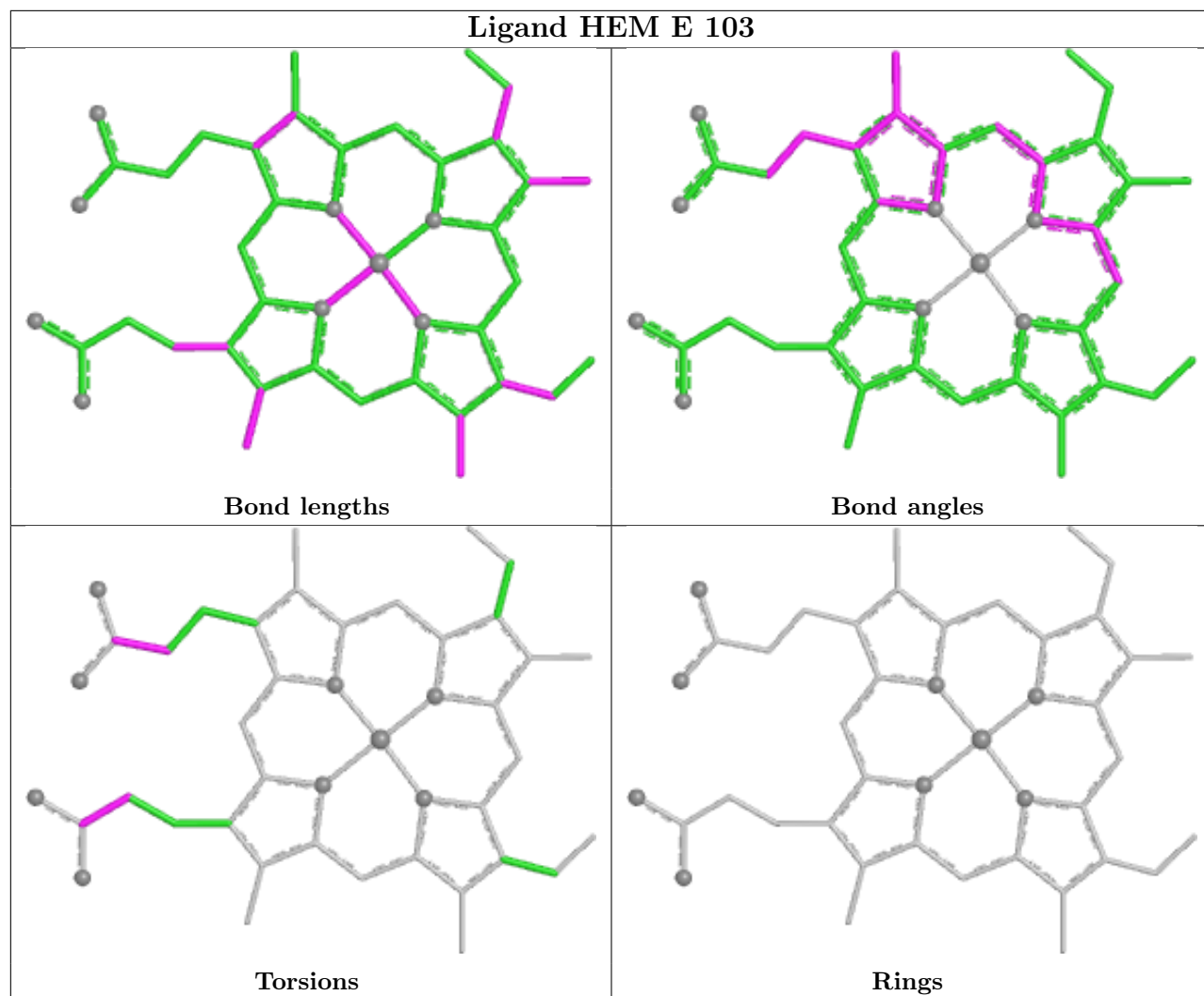


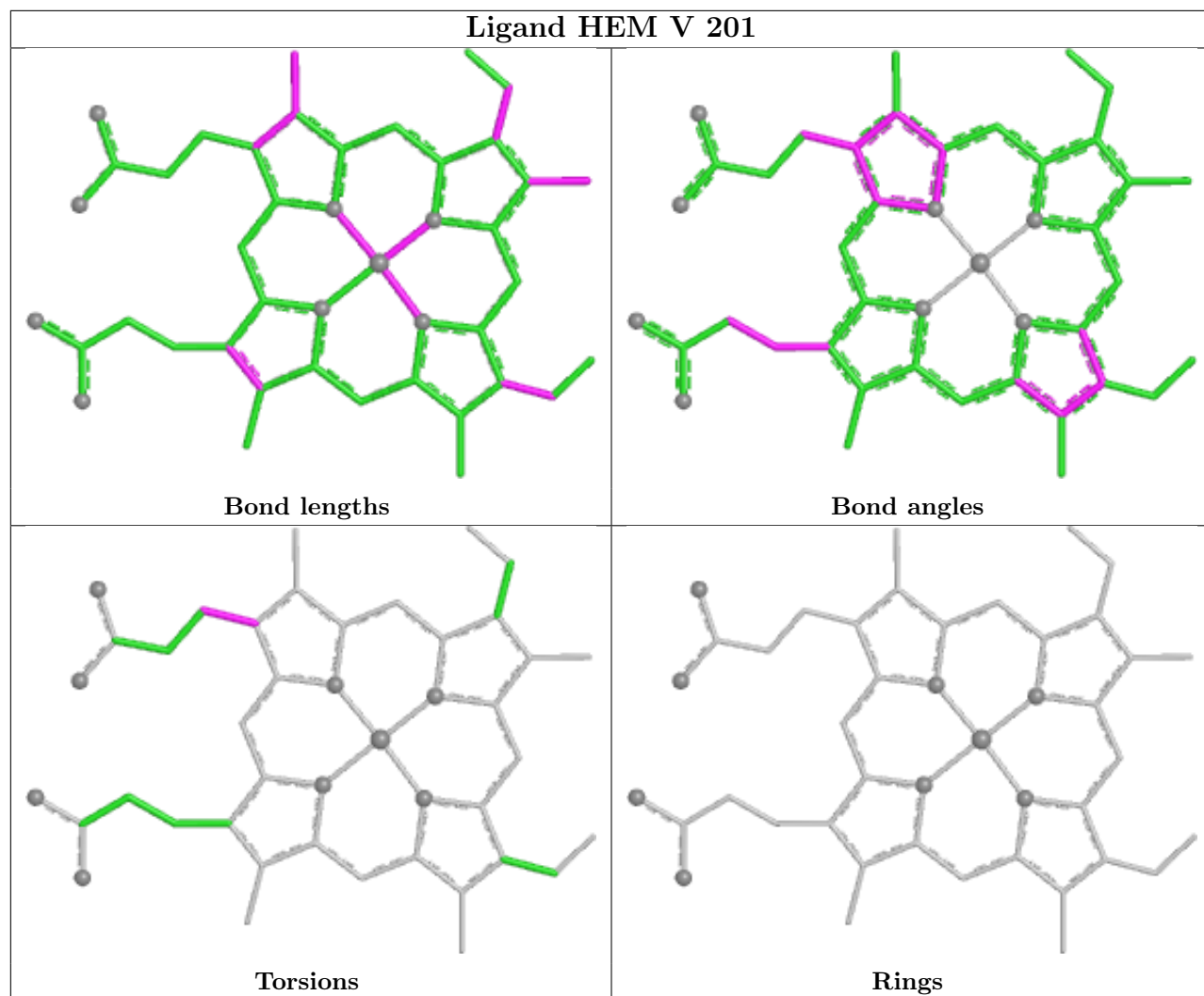


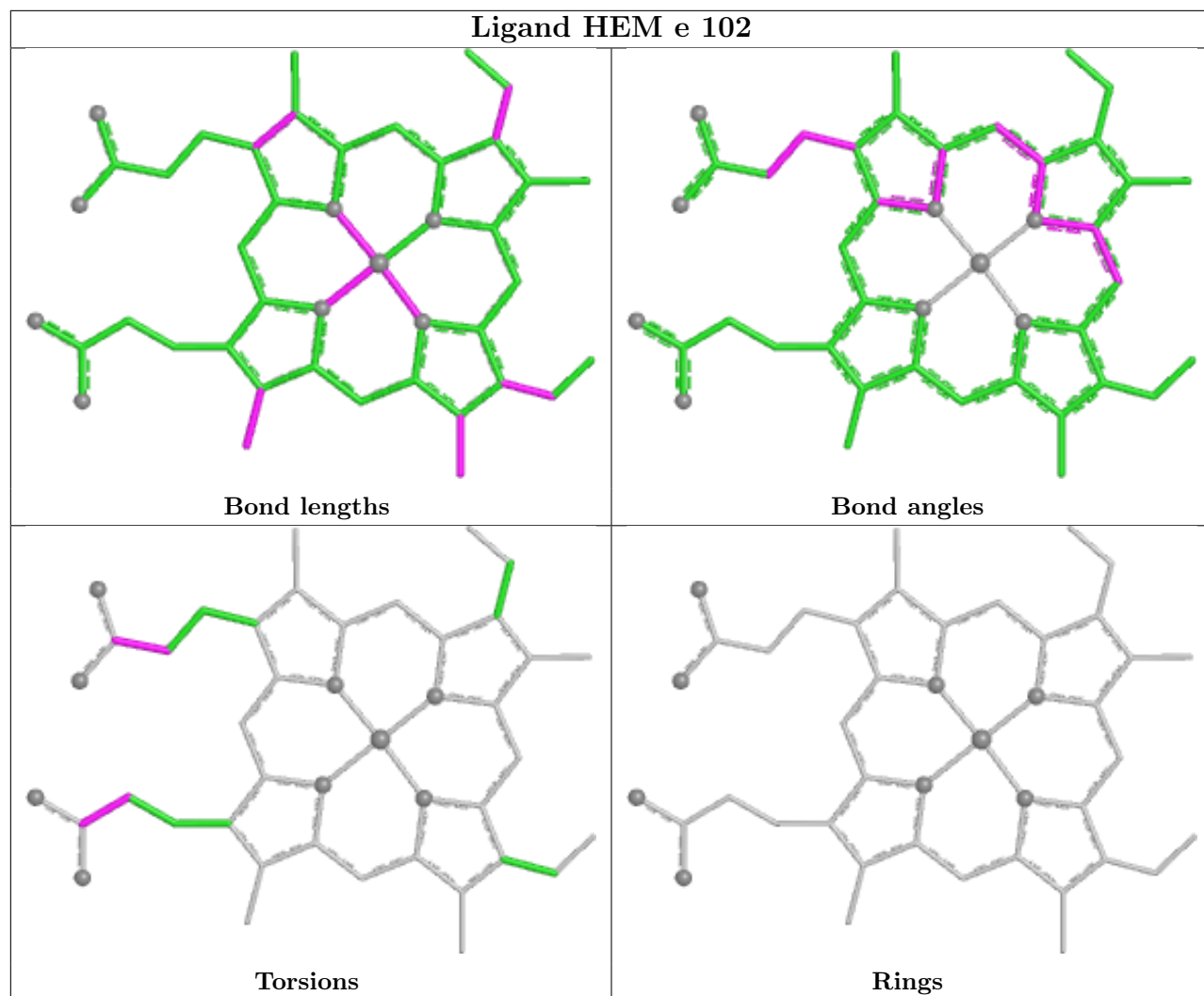


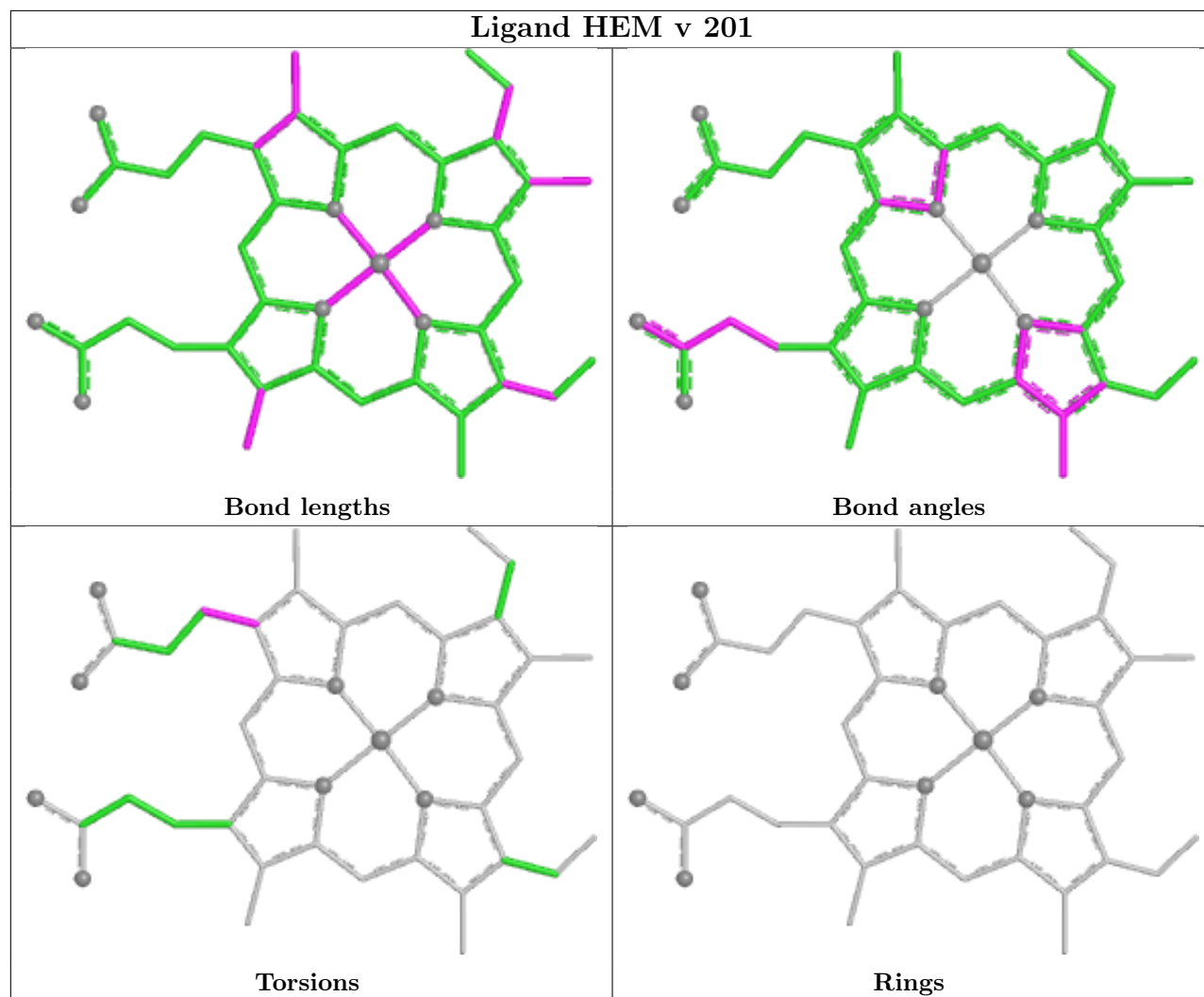












### 3.7 Other polymers [i](#)

There are no such residues in this entry.

### 3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/334 (100%)	1.45	69 (20%) 2 3	39, 63, 84, 93	4 (1%)
1	a	334/334 (100%)	1.74	110 (32%) 1 1	52, 84, 104, 114	4 (1%)
2	B	504/504 (100%)	1.29	96 (19%) 3 3	41, 68, 89, 111	10 (1%)
2	b	504/504 (100%)	1.73	160 (31%) 1 1	53, 88, 110, 131	10 (1%)
3	C	451/451 (100%)	1.31	89 (19%) 3 3	43, 72, 84, 97	5 (1%)
3	c	451/451 (100%)	1.74	154 (34%) 1 1	57, 92, 105, 118	5 (1%)
4	D	342/342 (100%)	1.32	71 (20%) 2 3	57, 64, 80, 102	0
4	d	342/342 (100%)	1.72	111 (32%) 1 1	78, 85, 101, 123	0
5	E	81/81 (100%)	1.53	20 (24%) 2 2	47, 80, 98, 104	2 (2%)
5	e	81/81 (100%)	1.93	37 (45%) 0 1	61, 101, 119, 125	2 (2%)
6	F	34/34 (100%)	1.39	6 (17%) 4 4	68, 74, 99, 102	0
6	f	34/34 (100%)	1.62	11 (32%) 1 1	89, 95, 120, 122	0
7	H	65/65 (100%)	1.43	16 (24%) 2 2	43, 74, 81, 99	2 (3%)
7	h	65/65 (100%)	1.99	25 (38%) 1 1	55, 95, 101, 120	2 (3%)
8	I	38/38 (100%)	1.76	13 (34%) 1 1	36, 74, 105, 109	1 (2%)
8	i	38/38 (100%)	2.13	16 (42%) 0 1	45, 95, 126, 130	1 (2%)
9	J	38/38 (100%)	1.65	9 (23%) 2 2	66, 78, 109, 112	0
9	j	38/38 (100%)	1.83	14 (36%) 1 1	87, 99, 129, 133	0
10	K	37/37 (100%)	1.06	3 (8%) 18 12	74, 79, 86, 88	0
10	k	37/37 (100%)	1.87	11 (29%) 1 1	94, 100, 107, 108	0
11	L	37/37 (100%)	1.34	8 (21%) 2 3	37, 62, 90, 99	1 (2%)
11	l	37/37 (100%)	1.76	12 (32%) 1 1	49, 83, 111, 120	1 (2%)
12	M	34/34 (100%)	1.66	10 (29%) 1 1	39, 64, 77, 93	1 (2%)
12	m	34/34 (100%)	2.36	12 (35%) 1 1	51, 84, 98, 114	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/243 (100%)	1.42	56 (23%) 2 2	40, 73, 95, 111	4 (1%)
13	o	243/243 (100%)	1.98	95 (39%) 1 1	53, 94, 116, 132	4 (1%)
14	T	30/30 (100%)	1.08	4 (13%) 7 6	32, 64, 85, 93	2 (6%)
14	t	30/30 (100%)	1.72	7 (23%) 2 2	43, 84, 105, 114	2 (6%)
15	U	97/97 (100%)	1.17	15 (15%) 5 5	64, 71, 89, 90	0
15	u	97/97 (100%)	1.64	30 (30%) 1 1	84, 92, 110, 111	0
16	V	137/137 (100%)	1.24	28 (20%) 3 3	39, 69, 80, 88	1 (0%)
16	v	137/137 (100%)	1.53	36 (26%) 1 2	51, 89, 101, 109	1 (0%)
17	Y	29/29 (100%)	1.43	7 (24%) 2 2	82, 89, 115, 118	0
17	y	29/29 (100%)	1.95	11 (37%) 1 1	103, 110, 136, 138	0
18	X	39/39 (100%)	1.32	6 (15%) 5 5	48, 80, 107, 108	1 (2%)
18	x	39/39 (100%)	1.71	11 (28%) 1 1	61, 101, 127, 129	1 (2%)
19	Z	62/62 (100%)	1.50	18 (29%) 1 1	80, 89, 109, 112	0
19	z	62/62 (100%)	2.04	29 (46%) 0 1	101, 110, 129, 133	0
All	All	5264/5264 (100%)	1.57	1436 (27%) 1 2	32, 83, 107, 138	68 (1%)

The worst 5 of 1436 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	d	11	GLU	12.1
12	m	5	GLN	11.3
8	i	38	GLU	10.2
2	b	485	GLU	10.0
9	j	3	SER	8.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 4.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

#### 4.4 Other polymers

There are no such residues in this entry.