



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 02:15 pm BST

PDB ID : 7PIW  
EMDB ID : EMD-13455  
Title : Stacked stretched Dunaliella PSII  
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.  
Deposited on : 2021-08-23  
Resolution : 4.00 Å(reported)  
Based on initial model : 6KAC

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

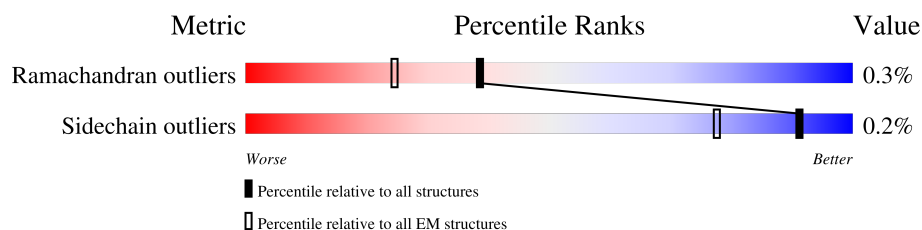
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	336	<div> <div>31%</div> <div>99%</div> </div>
1	A1	336	<div> <div>16%</div> <div>100%</div> </div>
1	a	336	<div> <div>37%</div> <div>99%</div> </div>
1	a1	336	<div> <div>42%</div> <div>99%</div> </div>
2	B	484	<div> <div>53%</div> <div>99%</div> </div>
2	B1	484	<div> <div>16%</div> <div>100%</div> </div>
2	b	484	<div> <div>56%</div> <div>100%</div> </div>
2	b1	484	<div> <div>33%</div> <div>100%</div> </div>
3	V	32	<div> <div>59%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	V1	32	28% 100%
3	v	32	84% 100%
3	v1	32	66% 100%
4	C	449	28% 99%
4	C1	449	11% 100%
4	c	449	46% 99%
4	c1	449	36% 99%
5	D	348	41% 99%
5	D1	348	18% 100%
5	d	348	41% 99%
5	d1	348	43% 99%
6	E	76	58% 100%
6	E1	76	12% 100%
6	e	76	75% 100%
6	e1	76	45% 100%
7	F	31	45% 100%
7	F1	31	• 100%
7	f	31	65% 100%
7	f1	31	29% 100%
8	H	67	70% 97%
8	H1	67	34% 100%
8	h	67	78% 99%
8	h1	67	46% 99%
9	I	35	40% 100%
9	I1	35	20% 100%

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Mol	Chain	Length	Quality of chain	
9	i	35	37%	100%
9	i1	35	46%	100%
10	J	36	39%	100%
10	J1	36	36%	100%
10	j	36	72%	100%
10	j1	36	47%	100%
11	K	37	51%	97%
11	K1	37	19%	97%
11	k	37	57%	100%
11	k1	37	46%	100%
12	L	38	53%	97%
12	L1	38	39%	100%
12	l	38	50%	100%
13	M	32	62%	97%
13	m	32	84%	97%
14	O	238	79%	98%
14	O1	238	24%	98%
14	o	238	82%	98%
14	o1	238	33%	98%
15	P	187	100%	99%
15	P1	187	94%	99%
15	p	187	100%	100%
15	p1	187	93%	100%
16	T	30	53%	97%
16	T1	30	40%	97%

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Mol	Chain	Length	Quality of chain
16	t	30	53% 97% .
16	t1	30	63% 100%
17	W	44	68% 98% .
17	W1	44	14% 98% .
17	w	44	59% 100%
17	w1	44	41% 100%
18	X	30	73% 100%
18	X1	30	20% 100%
18	x	30	73% 100%
18	x1	30	60% 100%
19	Z	61	75% 100%
19	Z1	61	15% 100%
19	z	61	92% 100%
19	z1	61	46% 100%
20	N	222	65% 99% .
20	N1	222	9% 100%
20	n	222	88% 98% .
20	n1	222	26% 100%
21	G	221	83% 99% .
21	G1	221	10% 100%
21	g	221	89% 99% .
21	g1	221	23% 100%
22	R	202	97% 100%
22	r	202	94% 100%
23	S	243	77% 98% .

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Mol	Chain	Length	Quality of chain
23	S1	243	
23	s	243	
23	s1	243	
24	Y	222	
24	Y1	222	
24	y	222	
24	y1	222	
25	U	27	
25	U1	27	
25	u	27	
25	u1	27	
26	M1	31	
26	m1	31	
27	R1	202	
27	r1	202	

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
31	CLA	A	405	X	-	-	-
31	CLA	A	406	X	-	-	-
31	CLA	A	407	X	-	-	-
31	CLA	A	410	X	-	-	-
31	CLA	A1	405	X	-	-	-
31	CLA	A1	406	X	-	-	-
31	CLA	A1	407	X	-	-	-
31	CLA	A1	410	X	-	-	-
31	CLA	B	602	X	-	-	-
31	CLA	B	603	X	-	-	-
31	CLA	B	604	X	-	-	-
31	CLA	B	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	B	606	X	-	-	-
31	CLA	B	607	X	-	-	-
31	CLA	B	608	X	-	-	-
31	CLA	B	609	X	-	-	-
31	CLA	B	610	X	-	-	-
31	CLA	B	611	X	-	-	-
31	CLA	B	612	X	-	-	-
31	CLA	B	613	X	-	-	-
31	CLA	B	614	X	-	-	-
31	CLA	B	615	X	-	-	-
31	CLA	B	616	X	-	-	-
31	CLA	B	617	X	-	-	-
31	CLA	B1	602	X	-	-	-
31	CLA	B1	603	X	-	-	-
31	CLA	B1	604	X	-	-	-
31	CLA	B1	605	X	-	-	-
31	CLA	B1	606	X	-	-	-
31	CLA	B1	607	X	-	-	-
31	CLA	B1	608	X	-	-	-
31	CLA	B1	609	X	-	-	-
31	CLA	B1	610	X	-	-	-
31	CLA	B1	611	X	-	-	-
31	CLA	B1	612	X	-	-	-
31	CLA	B1	613	X	-	-	-
31	CLA	B1	614	X	-	-	-
31	CLA	B1	615	X	-	-	-
31	CLA	B1	616	X	-	-	-
31	CLA	B1	617	X	-	-	-
31	CLA	C	501	X	-	-	-
31	CLA	C	502	X	-	-	-
31	CLA	C	503	X	-	-	-
31	CLA	C	504	X	-	-	-
31	CLA	C	505	X	-	-	-
31	CLA	C	506	X	-	-	-
31	CLA	C	507	X	-	-	-
31	CLA	C	508	X	-	-	-
31	CLA	C	509	X	-	-	-
31	CLA	C	510	X	-	-	-
31	CLA	C	511	X	-	-	-
31	CLA	C	512	X	-	-	-
31	CLA	C	513	X	-	-	-
31	CLA	C1	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	C1	502	X	-	-	-
31	CLA	C1	503	X	-	-	-
31	CLA	C1	504	X	-	-	-
31	CLA	C1	505	X	-	-	-
31	CLA	C1	506	X	-	-	-
31	CLA	C1	507	X	-	-	-
31	CLA	C1	508	X	-	-	-
31	CLA	C1	509	X	-	-	-
31	CLA	C1	510	X	-	-	-
31	CLA	C1	511	X	-	-	-
31	CLA	C1	512	X	-	-	-
31	CLA	C1	513	X	-	-	-
31	CLA	D	402	X	-	-	-
31	CLA	D	403	X	-	-	-
31	CLA	D1	402	X	-	-	-
31	CLA	D1	403	X	-	-	-
31	CLA	G	602	X	-	-	-
31	CLA	G	603	X	-	-	-
31	CLA	G	604	X	-	-	-
31	CLA	G	610	X	-	-	-
31	CLA	G	611	X	-	-	-
31	CLA	G	612	X	-	-	-
31	CLA	G	613	X	-	-	-
31	CLA	G	614	X	-	-	-
31	CLA	G1	602	X	-	-	-
31	CLA	G1	603	X	-	-	-
31	CLA	G1	604	X	-	-	-
31	CLA	G1	610	X	-	-	-
31	CLA	G1	611	X	-	-	-
31	CLA	G1	612	X	-	-	-
31	CLA	G1	613	X	-	-	-
31	CLA	G1	614	X	-	-	-
31	CLA	N	602	X	-	-	-
31	CLA	N	603	X	-	-	-
31	CLA	N	604	X	-	-	-
31	CLA	N	610	X	-	-	-
31	CLA	N	611	X	-	-	-
31	CLA	N	612	X	-	-	-
31	CLA	N	613	X	-	-	-
31	CLA	N	614	X	-	-	-
31	CLA	N1	602	X	-	-	-
31	CLA	N1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	N1	604	X	-	-	-
31	CLA	N1	610	X	-	-	-
31	CLA	N1	611	X	-	-	-
31	CLA	N1	612	X	-	-	-
31	CLA	N1	613	X	-	-	-
31	CLA	N1	614	X	-	-	-
31	CLA	R	602	X	-	-	-
31	CLA	R	603	X	-	-	-
31	CLA	R	604	X	-	-	-
31	CLA	R	608	X	-	-	-
31	CLA	R	609	X	-	-	-
31	CLA	R	610	X	-	-	-
31	CLA	R	611	X	-	-	-
31	CLA	R	612	X	-	-	-
31	CLA	R	613	X	-	-	-
31	CLA	R1	602	X	-	-	-
31	CLA	R1	603	X	-	-	-
31	CLA	R1	604	X	-	-	-
31	CLA	R1	608	X	-	-	-
31	CLA	R1	609	X	-	-	-
31	CLA	R1	610	X	-	-	-
31	CLA	R1	612	X	-	-	-
31	CLA	S	602	X	-	-	-
31	CLA	S	603	X	-	-	-
31	CLA	S	604	X	-	-	-
31	CLA	S	605	X	-	-	-
31	CLA	S	609	X	-	-	-
31	CLA	S	610	X	-	-	-
31	CLA	S	611	X	-	-	-
31	CLA	S	612	X	-	-	-
31	CLA	S	613	X	-	-	-
31	CLA	S	614	X	-	-	-
31	CLA	S	617	X	-	-	-
31	CLA	S1	602	X	-	-	-
31	CLA	S1	603	X	-	-	-
31	CLA	S1	604	X	-	-	-
31	CLA	S1	605	X	-	-	-
31	CLA	S1	609	X	-	-	-
31	CLA	S1	610	X	-	-	-
31	CLA	S1	611	X	-	-	-
31	CLA	S1	612	X	-	-	-
31	CLA	S1	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	S1	614	X	-	-	-
31	CLA	S1	617	X	-	-	-
31	CLA	Y	602	X	-	-	-
31	CLA	Y	603	X	-	-	-
31	CLA	Y	604	X	-	-	-
31	CLA	Y	608	X	-	-	-
31	CLA	Y	610	X	-	-	-
31	CLA	Y	611	X	-	-	-
31	CLA	Y	612	X	-	-	-
31	CLA	Y	613	X	-	-	-
31	CLA	Y	614	X	-	-	-
31	CLA	Y1	602	X	-	-	-
31	CLA	Y1	603	X	-	-	-
31	CLA	Y1	604	X	-	-	-
31	CLA	Y1	608	X	-	-	-
31	CLA	Y1	610	X	-	-	-
31	CLA	Y1	611	X	-	-	-
31	CLA	Y1	612	X	-	-	-
31	CLA	Y1	613	X	-	-	-
31	CLA	Y1	614	X	-	-	-
31	CLA	a	405	X	-	-	-
31	CLA	a	406	X	-	-	-
31	CLA	a	407	X	-	-	-
31	CLA	a	410	X	-	-	-
31	CLA	a1	405	X	-	-	-
31	CLA	a1	406	X	-	-	-
31	CLA	a1	407	X	-	-	-
31	CLA	a1	410	X	-	-	-
31	CLA	b	602	X	-	-	-
31	CLA	b	603	X	-	-	-
31	CLA	b	604	X	-	-	-
31	CLA	b	605	X	-	-	-
31	CLA	b	606	X	-	-	-
31	CLA	b	607	X	-	-	-
31	CLA	b	608	X	-	-	-
31	CLA	b	609	X	-	-	-
31	CLA	b	610	X	-	-	-
31	CLA	b	611	X	-	-	-
31	CLA	b	612	X	-	-	-
31	CLA	b	613	X	-	-	-
31	CLA	b	614	X	-	-	-
31	CLA	b	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	b	616	X	-	-	-
31	CLA	b	617	X	-	-	-
31	CLA	b1	602	X	-	-	-
31	CLA	b1	603	X	-	-	-
31	CLA	b1	604	X	-	-	-
31	CLA	b1	605	X	-	-	-
31	CLA	b1	606	X	-	-	-
31	CLA	b1	607	X	-	-	-
31	CLA	b1	608	X	-	-	-
31	CLA	b1	609	X	-	-	-
31	CLA	b1	610	X	-	-	-
31	CLA	b1	611	X	-	-	-
31	CLA	b1	612	X	-	-	-
31	CLA	b1	613	X	-	-	-
31	CLA	b1	614	X	-	-	-
31	CLA	b1	615	X	-	-	-
31	CLA	b1	616	X	-	-	-
31	CLA	b1	617	X	-	-	-
31	CLA	c	501	X	-	-	-
31	CLA	c	502	X	-	-	-
31	CLA	c	503	X	-	-	-
31	CLA	c	504	X	-	-	-
31	CLA	c	505	X	-	-	-
31	CLA	c	506	X	-	-	-
31	CLA	c	507	X	-	-	-
31	CLA	c	508	X	-	-	-
31	CLA	c	509	X	-	-	-
31	CLA	c	510	X	-	-	-
31	CLA	c	511	X	-	-	-
31	CLA	c	512	X	-	-	-
31	CLA	c	513	X	-	-	-
31	CLA	c1	501	X	-	-	-
31	CLA	c1	502	X	-	-	-
31	CLA	c1	503	X	-	-	-
31	CLA	c1	504	X	-	-	-
31	CLA	c1	505	X	-	-	-
31	CLA	c1	506	X	-	-	-
31	CLA	c1	507	X	-	-	-
31	CLA	c1	508	X	-	-	-
31	CLA	c1	509	X	-	-	-
31	CLA	c1	510	X	-	-	-
31	CLA	c1	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	c1	512	X	-	-	-
31	CLA	c1	513	X	-	-	-
31	CLA	d	402	X	-	-	-
31	CLA	d	403	X	-	-	-
31	CLA	d1	402	X	-	-	-
31	CLA	d1	403	X	-	-	-
31	CLA	g	602	X	-	-	-
31	CLA	g	603	X	-	-	-
31	CLA	g	604	X	-	-	-
31	CLA	g	610	X	-	-	-
31	CLA	g	611	X	-	-	-
31	CLA	g	612	X	-	-	-
31	CLA	g	613	X	-	-	-
31	CLA	g	614	X	-	-	-
31	CLA	g1	602	X	-	-	-
31	CLA	g1	603	X	-	-	-
31	CLA	g1	604	X	-	-	-
31	CLA	g1	610	X	-	-	-
31	CLA	g1	611	X	-	-	-
31	CLA	g1	612	X	-	-	-
31	CLA	g1	613	X	-	-	-
31	CLA	g1	614	X	-	-	-
31	CLA	n	602	X	-	-	-
31	CLA	n	603	X	-	-	-
31	CLA	n	604	X	-	-	-
31	CLA	n	610	X	-	-	-
31	CLA	n	611	X	-	-	-
31	CLA	n	612	X	-	-	-
31	CLA	n	613	X	-	-	-
31	CLA	n	614	X	-	-	-
31	CLA	n1	602	X	-	-	-
31	CLA	n1	603	X	-	-	-
31	CLA	n1	604	X	-	-	-
31	CLA	n1	610	X	-	-	-
31	CLA	n1	611	X	-	-	-
31	CLA	n1	612	X	-	-	-
31	CLA	n1	613	X	-	-	-
31	CLA	n1	614	X	-	-	-
31	CLA	r	602	X	-	-	-
31	CLA	r	603	X	-	-	-
31	CLA	r	604	X	-	-	-
31	CLA	r	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	r	609	X	-	-	-
31	CLA	r	610	X	-	-	-
31	CLA	r	611	X	-	-	-
31	CLA	r	612	X	-	-	-
31	CLA	r	613	X	-	-	-
31	CLA	r1	602	X	-	-	-
31	CLA	r1	603	X	-	-	-
31	CLA	r1	604	X	-	-	-
31	CLA	r1	608	X	-	-	-
31	CLA	r1	609	X	-	-	-
31	CLA	r1	610	X	-	-	-
31	CLA	r1	612	X	-	-	-
31	CLA	s	602	X	-	-	-
31	CLA	s	603	X	-	-	-
31	CLA	s	604	X	-	-	-
31	CLA	s	605	X	-	-	-
31	CLA	s	609	X	-	-	-
31	CLA	s	610	X	-	-	-
31	CLA	s	611	X	-	-	-
31	CLA	s	612	X	-	-	-
31	CLA	s	613	X	-	-	-
31	CLA	s	614	X	-	-	-
31	CLA	s	617	X	-	-	-
31	CLA	s1	602	X	-	-	-
31	CLA	s1	603	X	-	-	-
31	CLA	s1	604	X	-	-	-
31	CLA	s1	605	X	-	-	-
31	CLA	s1	609	X	-	-	-
31	CLA	s1	610	X	-	-	-
31	CLA	s1	611	X	-	-	-
31	CLA	s1	612	X	-	-	-
31	CLA	s1	613	X	-	-	-
31	CLA	s1	614	X	-	-	-
31	CLA	s1	617	X	-	-	-
31	CLA	y	602	X	-	-	-
31	CLA	y	603	X	-	-	-
31	CLA	y	604	X	-	-	-
31	CLA	y	608	X	-	-	-
31	CLA	y	610	X	-	-	-
31	CLA	y	611	X	-	-	-
31	CLA	y	612	X	-	-	-
31	CLA	y	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	y	614	X	-	-	-
31	CLA	y1	602	X	-	-	-
31	CLA	y1	603	X	-	-	-
31	CLA	y1	604	X	-	-	-
31	CLA	y1	608	X	-	-	-
31	CLA	y1	610	X	-	-	-
31	CLA	y1	611	X	-	-	-
31	CLA	y1	612	X	-	-	-
31	CLA	y1	613	X	-	-	-
31	CLA	y1	614	X	-	-	-
37	C7Z	B	620	X	-	-	-
37	C7Z	B1	620	X	-	-	-
37	C7Z	b	620	X	-	-	-
37	C7Z	b1	620	X	-	-	-
42	LMK	C	527	X	-	-	-
42	LMK	C1	527	X	-	-	-
42	LMK	c	627	X	-	-	-
42	LMK	c1	527	X	-	-	-
46	RRX	H	101	X	-	-	-
46	RRX	H1	101	X	-	-	-
46	RRX	h	101	X	-	-	-
46	RRX	h1	101	X	-	-	-
47	CHL	G	601	X	-	-	-
47	CHL	G	605	X	-	-	-
47	CHL	G	606	X	-	-	-
47	CHL	G	607	X	-	-	-
47	CHL	G	608	X	-	-	-
47	CHL	G	609	X	-	-	-
47	CHL	G1	601	X	-	-	-
47	CHL	G1	605	X	-	-	-
47	CHL	G1	606	X	-	-	-
47	CHL	G1	607	X	-	-	-
47	CHL	G1	608	X	-	-	-
47	CHL	G1	609	X	-	-	-
47	CHL	N	601	X	-	-	-
47	CHL	N	605	X	-	-	-
47	CHL	N	606	X	-	-	-
47	CHL	N	607	X	-	-	-
47	CHL	N	608	X	-	-	-
47	CHL	N	609	X	-	-	-
47	CHL	N1	601	X	-	-	-
47	CHL	N1	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	CHL	N1	606	X	-	-	-
47	CHL	N1	607	X	-	-	-
47	CHL	N1	608	X	-	-	-
47	CHL	N1	609	X	-	-	-
47	CHL	R	606	X	-	-	-
47	CHL	R	607	X	-	-	-
47	CHL	R1	606	X	-	-	-
47	CHL	R1	607	X	-	-	-
47	CHL	S	601	X	-	-	-
47	CHL	S	606	X	-	-	-
47	CHL	S	607	X	-	-	-
47	CHL	S	608	X	-	-	-
47	CHL	S1	601	X	-	-	-
47	CHL	S1	606	X	-	-	-
47	CHL	S1	607	X	-	-	-
47	CHL	S1	608	X	-	-	-
47	CHL	Y	601	X	-	-	-
47	CHL	Y	605	X	-	-	-
47	CHL	Y	606	X	-	-	-
47	CHL	Y	607	X	-	-	-
47	CHL	Y	609	X	-	-	-
47	CHL	Y1	601	X	-	-	-
47	CHL	Y1	605	X	-	-	-
47	CHL	Y1	606	X	-	-	-
47	CHL	Y1	607	X	-	-	-
47	CHL	Y1	609	X	-	-	-
47	CHL	g	601	X	-	-	-
47	CHL	g	605	X	-	-	-
47	CHL	g	606	X	-	-	-
47	CHL	g	607	X	-	-	-
47	CHL	g	608	X	-	-	-
47	CHL	g	609	X	-	-	-
47	CHL	g1	601	X	-	-	-
47	CHL	g1	605	X	-	-	-
47	CHL	g1	606	X	-	-	-
47	CHL	g1	607	X	-	-	-
47	CHL	g1	608	X	-	-	-
47	CHL	g1	609	X	-	-	-
47	CHL	n	601	X	-	-	-
47	CHL	n	605	X	-	-	-
47	CHL	n	606	X	-	-	-
47	CHL	n	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	CHL	n	608	X	-	-	-
47	CHL	n	609	X	-	-	-
47	CHL	n1	601	X	-	-	-
47	CHL	n1	605	X	-	-	-
47	CHL	n1	606	X	-	-	-
47	CHL	n1	607	X	-	-	-
47	CHL	n1	608	X	-	-	-
47	CHL	n1	609	X	-	-	-
47	CHL	r	606	X	-	-	-
47	CHL	r	607	X	-	-	-
47	CHL	r1	606	X	-	-	-
47	CHL	r1	607	X	-	-	-
47	CHL	s	601	X	-	-	-
47	CHL	s	606	X	-	-	-
47	CHL	s	607	X	-	-	-
47	CHL	s	608	X	-	-	-
47	CHL	s1	601	X	-	-	-
47	CHL	s1	606	X	-	-	-
47	CHL	s1	607	X	-	-	-
47	CHL	s1	608	X	-	-	-
47	CHL	y	601	X	-	-	-
47	CHL	y	605	X	-	-	-
47	CHL	y	606	X	-	-	-
47	CHL	y	607	X	-	-	-
47	CHL	y	609	X	-	-	-
47	CHL	y1	601	X	-	-	-
47	CHL	y1	605	X	-	-	-
47	CHL	y1	606	X	-	-	-
47	CHL	y1	607	X	-	-	-
47	CHL	y1	609	X	-	-	-
48	LUT	G	621	X	-	-	-
48	LUT	R1	620	X	-	-	-
48	LUT	S	620	X	-	-	-
48	LUT	Y	621	X	-	-	-
48	LUT	g1	621	X	-	-	-
48	LUT	n	621	X	-	-	-
48	LUT	s	620	X	-	-	-
49	XAT	G	622	X	-	-	-
49	XAT	G1	622	X	-	-	-
49	XAT	N	622	X	-	-	-
49	XAT	N1	622	X	-	-	-
49	XAT	R	621	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
49	XAT	Y	622	X	-	-	-
49	XAT	Y1	622	X	-	-	-
49	XAT	g	622	X	-	-	-
49	XAT	g1	622	X	-	-	-
49	XAT	n1	622	X	-	-	-
49	XAT	r	622	X	-	-	-
49	XAT	r1	621	X	-	-	-
56	ERG	R1	626	X	-	-	-
56	ERG	r1	626	X	-	-	-

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 151508 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	A1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	B1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	298	VAL	LEU	variant	UNP D0FY05
B	415	SER	LEU	variant	UNP D0FY05
b	298	VAL	LEU	variant	UNP D0FY05
b	415	SER	LEU	variant	UNP D0FY05
B1	298	VAL	LEU	variant	UNP D0FY05
B1	415	SER	LEU	variant	UNP D0FY05
b1	298	VAL	LEU	variant	UNP D0FY05
b1	415	SER	LEU	variant	UNP D0FY05

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		
3	V1	32	Total	C	N	O	0	0
			227	152	37	38		
3	v1	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	C1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	D1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	319	ILE	LEU	variant	UNP D0FXW8
d	319	ILE	LEU	variant	UNP D0FXW8
D1	319	ILE	LEU	variant	UNP D0FXW8
d1	319	ILE	LEU	variant	UNP D0FXW8

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		
6	e	76	Total	C	N	O	0	0
			621	404	102	115		
6	E1	76	Total	C	N	O	0	0
			621	404	102	115		
6	e1	76	Total	C	N	O	0	0
			621	404	102	115		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	F1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	H1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	85	ALA	SER	variant	UNP D0FY02
h	85	ALA	SER	variant	UNP D0FY02
H1	85	ALA	SER	variant	UNP D0FY02
h1	85	ALA	SER	variant	UNP D0FY02

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	I1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	36	Total	C	N	O		0	0
			266	183	40	43			
10	j	36	Total	C	N	O		0	0
			266	183	40	43			
10	J1	36	Total	C	N	O		0	0
			266	183	40	43			
10	j1	36	Total	C	N	O		0	0
			266	183	40	43			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	7	ILE	THR	variant	UNP D0FXW2
J	28	ALA	GLY	variant	UNP D0FXW2
J	42	LEU	GLN	variant	UNP D0FXW2
j	7	ILE	THR	variant	UNP D0FXW2
j	28	ALA	GLY	variant	UNP D0FXW2
j	42	LEU	GLN	variant	UNP D0FXW2
J1	7	ILE	THR	variant	UNP D0FXW2
J1	28	ALA	GLY	variant	UNP D0FXW2
J1	42	LEU	GLN	variant	UNP D0FXW2
j1	7	ILE	THR	variant	UNP D0FXW2
j1	28	ALA	GLY	variant	UNP D0FXW2
j1	42	LEU	GLN	variant	UNP D0FXW2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O		0	0
			297	207	43	47			

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Mol	Chain	Residues	Atoms				AltConf	Trace
11	k	37	Total	C	N	O	0	0
			297	207	43	47		
11	K1	37	Total	C	N	O	0	0
			297	207	43	47		
11	k1	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	L1	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	32	Total	C	N	O	0	0
			243	164	34	45		
13	m	32	Total	C	N	O	0	0
			243	164	34	45		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	9	THR	ILE	variant	UNP D0FXZ3
m	9	THR	ILE	variant	UNP D0FXZ3

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	O1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	P1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	T1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	W1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	30	Total	C	N	O	0	0
			201	132	32	37		
18	x	30	Total	C	N	O	0	0
			201	132	32	37		
18	X1	30	Total	C	N	O	0	0
			201	132	32	37		

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Mol	Chain	Residues	Atoms				AltConf	Trace
18	x1	30	Total	C	N	O	0	0
			201	132	32	37		

- Molecule 19 is a protein called PsbZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	Z1	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z1	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	n	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	N1	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	n1	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		

- Molecule 21 is a protein called LHCII M2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	G1	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g1	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		
22	r	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	242	Total	C	N	O	S	0	0
			1849	1195	297	354	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	S1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	Y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	U1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 26 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	M1	31	Total	C	N	O	0	0
			234	159	33	42		
26	m1	31	Total	C	N	O	0	0
			234	159	33	42		

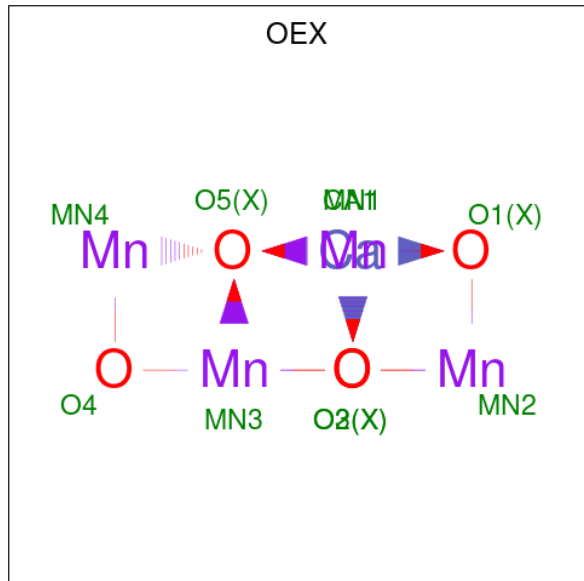
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M1	9	THR	ILE	variant	UNP D0FXZ3
m1	9	THR	ILE	variant	UNP D0FXZ3

- Molecule 27 is a protein called CP29.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	R1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
27	r1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

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Mol	Chain	Residues	Atoms				AltConf
28	A1	1	Total	Ca	Mn	O	0
			10	1	4	5	
28	a1	1	Total	Ca	Mn	O	0
			10	1	4	5	

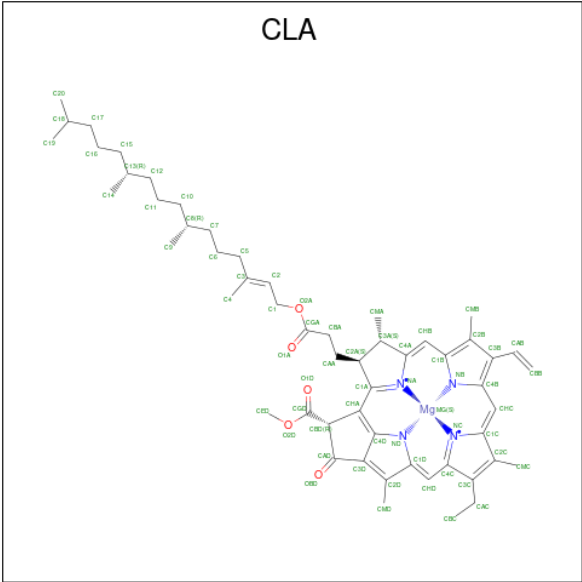
- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	Fe	0
			1	1	
29	a	1	Total	Fe	0
			1	1	
29	A1	1	Total	Fe	0
			1	1	
29	a1	1	Total	Fe	0
			1	1	

- Molecule 30 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
30	A	2	Total	Cl	0
			2	2	
30	a	2	Total	Cl	0
			2	2	
30	A1	2	Total	Cl	0
			2	2	
30	a1	2	Total	Cl	0
			2	2	

- Molecule 31 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
31	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	A1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	D1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	D1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	N1	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N1	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G1	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	G1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	S1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	S1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	S1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	S1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	S1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S1	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	S1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	a1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	n1	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	n1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g1	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
31	g1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r1	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	s1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	s1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	s1	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	s1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s1	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	s1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s1	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	y1	1	Total 65	C 55	Mg 1	N 4	O 5	0

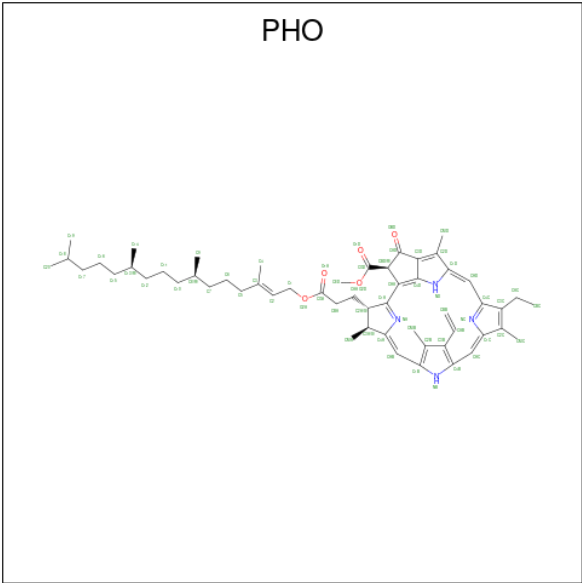
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Mol	Chain	Residues	Atoms					AltConf
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 32 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



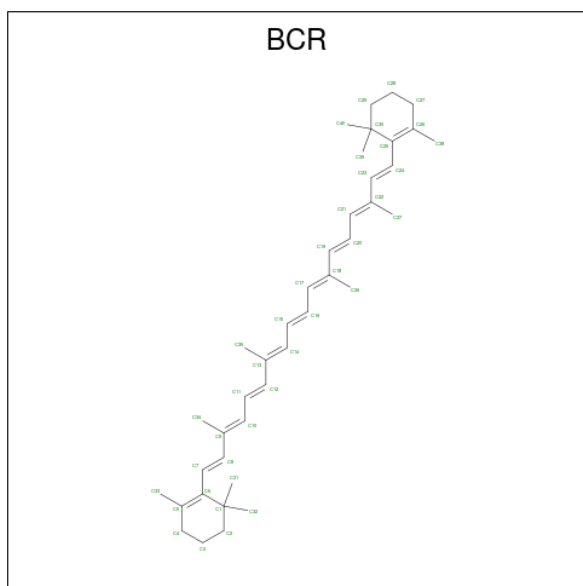
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	N	O	0
			64	55	4	5	
32	A	1	Total	C	N	O	0
			64	55	4	5	
32	a	1	Total	C	N	O	0
			64	55	4	5	

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Mol	Chain	Residues	Atoms				AltConf
32	a	1	Total	C	N	O	0
			64	55	4	5	
32	A1	1	Total	C	N	O	0
			64	55	4	5	
32	A1	1	Total	C	N	O	0
			64	55	4	5	
32	a1	1	Total	C	N	O	0
			64	55	4	5	
32	a1	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 33 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	C	1	Total	C	0
			40	40	
33	C	1	Total	C	0
			40	40	
33	C	1	Total	C	0
			40	40	

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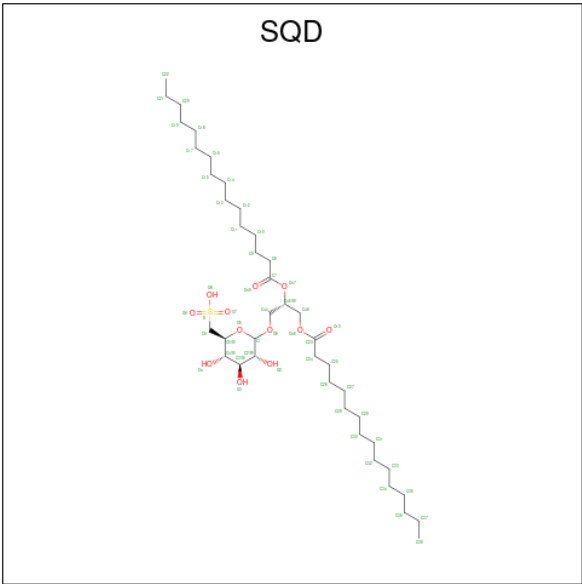
Mol	Chain	Residues	Atoms	AltConf
33	C	1	Total C 40 40	0
33	D	1	Total C 40 40	0
33	a	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	d	1	Total C 40 40	0
33	A1	1	Total C 40 40	0
33	B1	1	Total C 40 40	0
33	B1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	D1	1	Total C 40 40	0
33	a1	1	Total C 40 40	0
33	b1	1	Total C 40 40	0
33	b1	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
33	c1	1	Total	C	0
			40	40	
33	c1	1	Total	C	0
			40	40	
33	c1	1	Total	C	0
			40	40	
33	c1	1	Total	C	0
			40	40	
33	d1	1	Total	C	0
			40	40	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



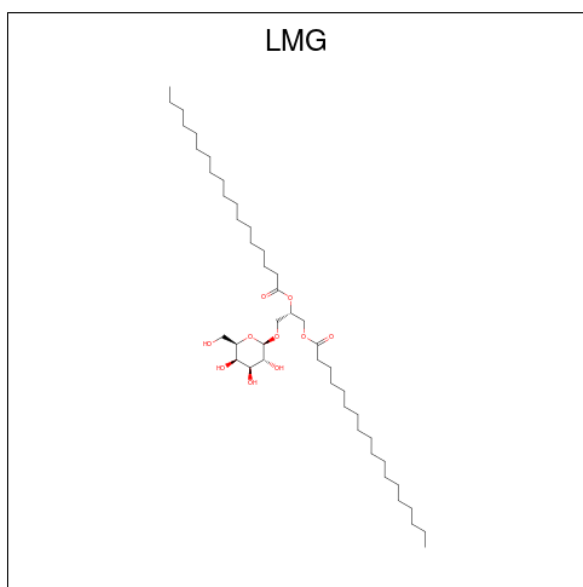
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	S	0
			51	38	12	1	
34	B	1	Total	C	O	S	0
			54	41	12	1	
34	C	1	Total	C	O	S	0
			54	41	12	1	
34	a	1	Total	C	O	S	0
			51	38	12	1	
34	b	1	Total	C	O	S	0
			54	41	12	1	
34	c	1	Total	C	O	S	0
			54	41	12	1	

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Mol	Chain	Residues	Atoms				AltConf
34	A1	1	Total	C	O	S	0
			51	38	12	1	
34	B1	1	Total	C	O	S	0
			42	29	12	1	
34	B1	1	Total	C	O	S	0
			54	41	12	1	
34	C1	1	Total	C	O	S	0
			54	41	12	1	
34	M1	1	Total	C	O	S	0
			42	29	12	1	
34	a1	1	Total	C	O	S	0
			51	38	12	1	
34	b1	1	Total	C	O	S	0
			42	29	12	1	
34	b1	1	Total	C	O	S	0
			54	41	12	1	
34	c1	1	Total	C	O	S	0
			54	41	12	1	
34	m1	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			48	38	10	

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Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			44	34	10	
35	C	1	Total	C	O	0
			51	41	10	
35	D	1	Total	C	O	0
			46	36	10	
35	H	1	Total	C	O	0
			48	38	10	
35	J	1	Total	C	O	0
			45	35	10	
35	a	1	Total	C	O	0
			48	38	10	
35	b	1	Total	C	O	0
			44	34	10	
35	c	1	Total	C	O	0
			51	41	10	
35	d	1	Total	C	O	0
			46	36	10	
35	h	1	Total	C	O	0
			48	38	10	
35	j	1	Total	C	O	0
			45	35	10	
35	A1	1	Total	C	O	0
			48	38	10	
35	B1	1	Total	C	O	0
			44	34	10	
35	C1	1	Total	C	O	0
			51	41	10	
35	C1	1	Total	C	O	0
			55	45	10	
35	D1	1	Total	C	O	0
			46	36	10	
35	H1	1	Total	C	O	0
			48	38	10	
35	W1	1	Total	C	O	0
			39	29	10	
35	a1	1	Total	C	O	0
			48	38	10	
35	b1	1	Total	C	O	0
			44	34	10	
35	c1	1	Total	C	O	0
			51	41	10	

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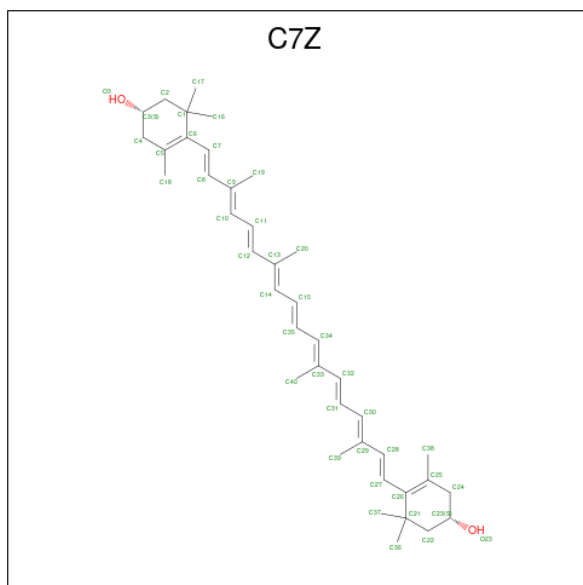
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Mol	Chain	Residues	Atoms			AltConf
35	c1	1	Total	C	O	0
			55	45	10	
35	d1	1	Total	C	O	0
			46	36	10	
35	h1	1	Total	C	O	0
			48	38	10	
35	w1	1	Total	C	O	0
			39	29	10	

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

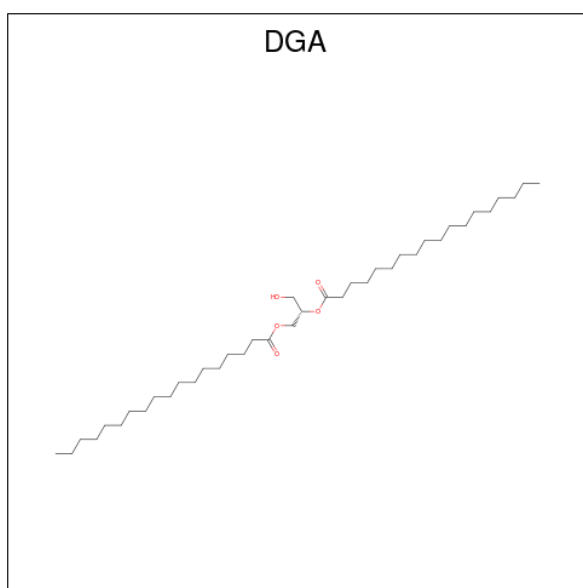
Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Na	0
			1	1	
36	a	1	Total	Na	0
			1	1	
36	A1	1	Total	Na	0
			1	1	
36	a1	1	Total	Na	0
			1	1	

- Molecule 37 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			42	40	2	
37	b	1	Total	C	O	0
			42	40	2	
37	B1	1	Total	C	O	0
			42	40	2	
37	b1	1	Total	C	O	0
			42	40	2	

- Molecule 38 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ).



Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			44	39	5	
38	C	1	Total	C	O	0
			44	39	5	
38	b	1	Total	C	O	0
			44	39	5	
38	c	1	Total	C	O	0
			44	39	5	
38	B1	1	Total	C	O	0
			44	39	5	
38	C1	1	Total	C	O	0
			44	39	5	
38	J1	1	Total	C	O	0
			29	24	5	
38	b1	1	Total	C	O	0
			44	39	5	

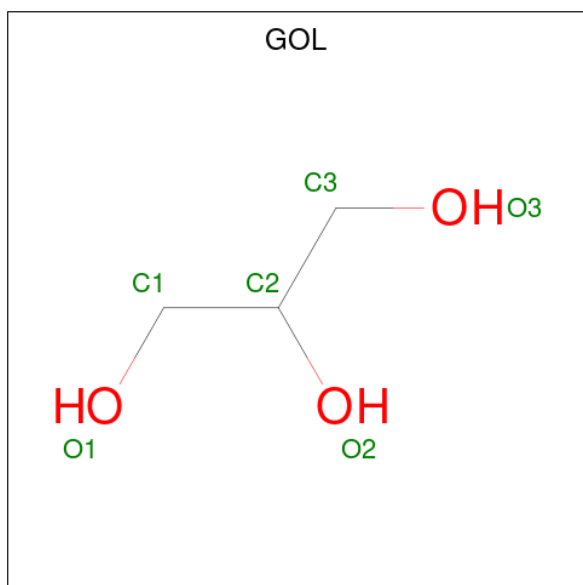
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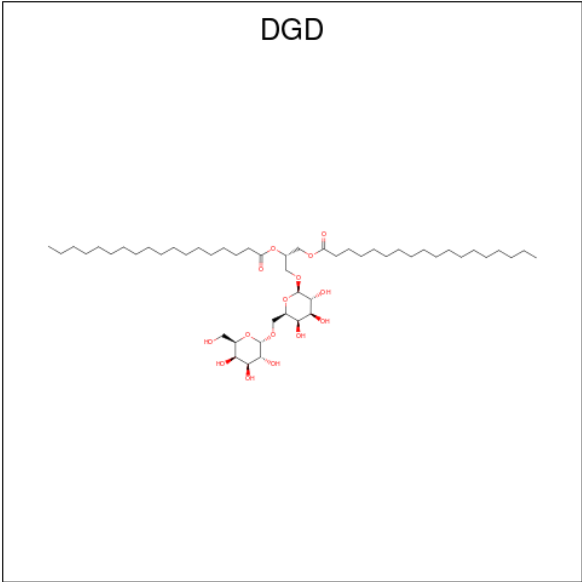
Mol	Chain	Residues	Atoms			AltConf
38	c1	1	Total	C	O	0
			44	39	5	
38	j1	1	Total	C	O	0
			29	24	5	

- Molecule 39 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			6	3	3	
39	b	1	Total	C	O	0
			6	3	3	
39	b	1	Total	C	O	0
			6	3	3	
39	y	1	Total	C	O	0
			6	3	3	
39	I1	1	Total	C	O	0
			6	3	3	

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



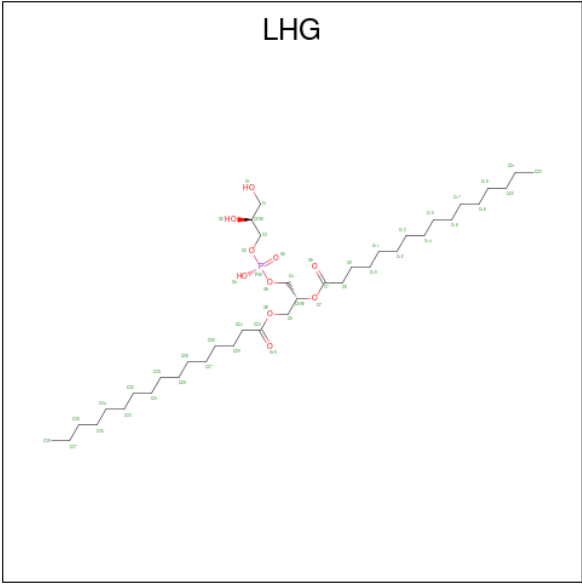
Mol	Chain	Residues	Atoms			AltConf
40	C	1	Total	C	O	0
			55	40	15	
40	C	1	Total	C	O	0
			62	47	15	
40	C	1	Total	C	O	0
			59	44	15	
40	C	1	Total	C	O	0
			66	51	15	
40	c	1	Total	C	O	0
			55	40	15	
40	c	1	Total	C	O	0
			62	47	15	
40	c	1	Total	C	O	0
			59	44	15	
40	c	1	Total	C	O	0
			66	51	15	
40	B1	1	Total	C	O	0
			43	28	15	
40	C1	1	Total	C	O	0
			55	40	15	
40	C1	1	Total	C	O	0
			62	47	15	
40	C1	1	Total	C	O	0
			59	44	15	
40	b1	1	Total	C	O	0
			43	28	15	
40	c1	1	Total	C	O	0
			55	40	15	

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Mol	Chain	Residues	Atoms			AltConf
40	c1	1	Total	C	O	0
			62	47	15	
40	c1	1	Total	C	O	0
			59	44	15	

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
41	C	1	Total	C	O	P	0
			47	36	10	1	
41	D	1	Total	C	O	P	0
			44	33	10	1	
41	D	1	Total	C	O	P	0
			49	38	10	1	
41	D	1	Total	C	O	P	0
			39	28	10	1	
41	L	1	Total	C	O	P	0
			49	38	10	1	
41	N	1	Total	C	O	P	0
			49	38	10	1	
41	G	1	Total	C	O	P	0
			49	38	10	1	
41	S	1	Total	C	O	P	0
			45	34	10	1	
41	Y	1	Total	C	O	P	0
			49	38	10	1	

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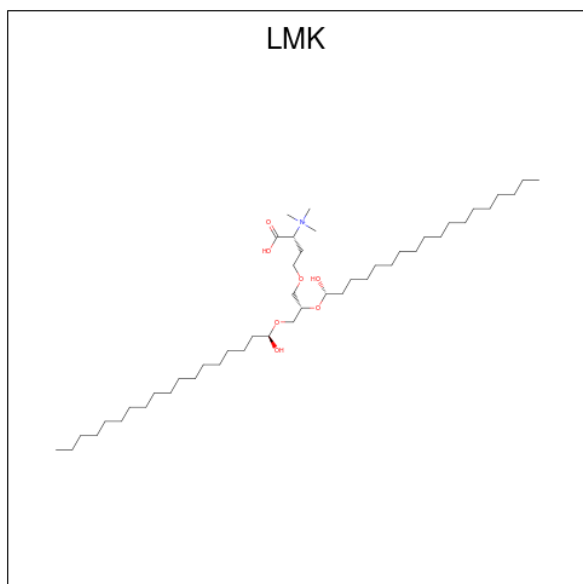
Mol	Chain	Residues	Atoms				AltConf
41	c	1	Total 47	C 36	O 10	P 1	0
41	d	1	Total 44	C 33	O 10	P 1	0
41	d	1	Total 49	C 38	O 10	P 1	0
41	d	1	Total 39	C 28	O 10	P 1	0
41	l	1	Total 49	C 38	O 10	P 1	0
41	n	1	Total 49	C 38	O 10	P 1	0
41	g	1	Total 49	C 38	O 10	P 1	0
41	s	1	Total 45	C 34	O 10	P 1	0
41	y	1	Total 49	C 38	O 10	P 1	0
41	C1	1	Total 47	C 36	O 10	P 1	0
41	D1	1	Total 44	C 33	O 10	P 1	0
41	D1	1	Total 49	C 38	O 10	P 1	0
41	D1	1	Total 39	C 28	O 10	P 1	0
41	L1	1	Total 49	C 38	O 10	P 1	0
41	N1	1	Total 49	C 38	O 10	P 1	0
41	G1	1	Total 49	C 38	O 10	P 1	0
41	S1	1	Total 45	C 34	O 10	P 1	0
41	Y1	1	Total 49	C 38	O 10	P 1	0
41	c1	1	Total 47	C 36	O 10	P 1	0
41	d1	1	Total 44	C 33	O 10	P 1	0
41	d1	1	Total 49	C 38	O 10	P 1	0

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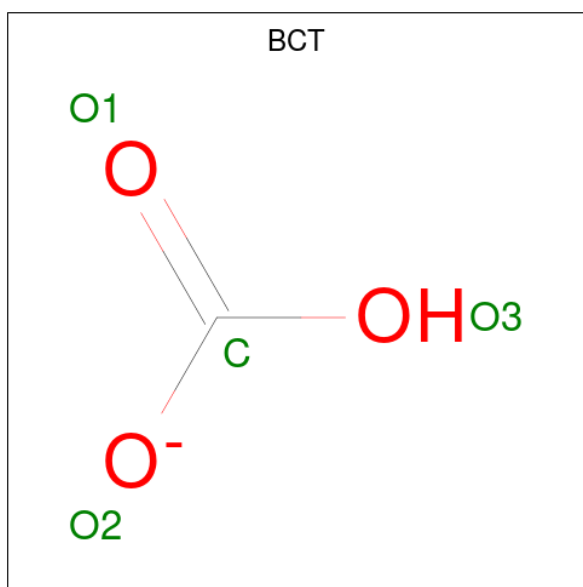
Mol	Chain	Residues	Atoms				AltConf
41	d1	1	Total	C	O	P	0
			39	28	10	1	
41	n1	1	Total	C	O	P	0
			49	38	10	1	
41	g1	1	Total	C	O	P	0
			49	38	10	1	
41	s1	1	Total	C	O	P	0
			45	34	10	1	
41	y1	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 42 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidan-nyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (three-letter code: LMK) (formula:  $C_{46}H_{94}NO_7$ ).



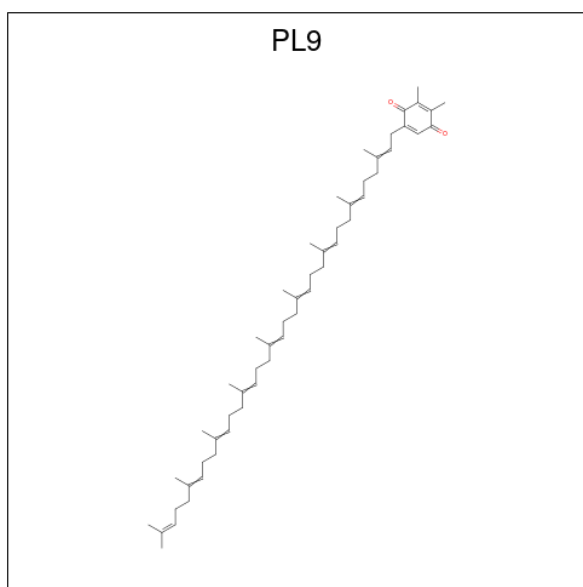
Mol	Chain	Residues	Atoms				AltConf
42	C	1	Total	C	N	O	0
			40	32	1	7	
42	c	1	Total	C	N	O	0
			40	32	1	7	
42	C1	1	Total	C	N	O	0
			40	32	1	7	
42	c1	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 43 is BICARBONATE ION (three-letter code: BCT) (formula:  $CHO_3$ ).



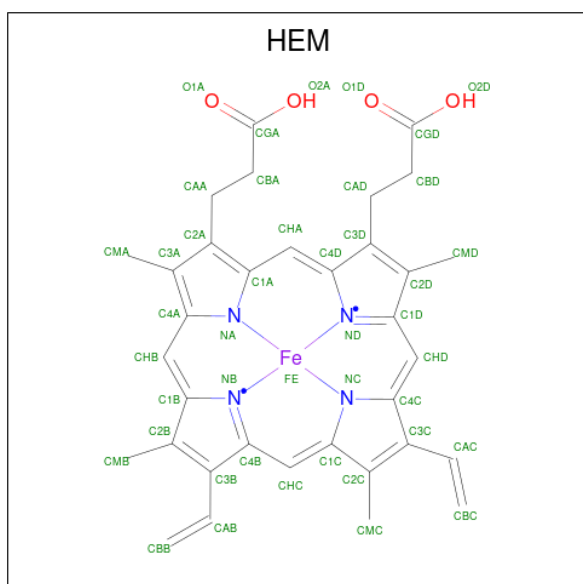
Mol	Chain	Residues	Atoms			AltConf
43	D	1	Total	C	O	0
			4	1	3	
43	d	1	Total	C	O	0
			4	1	3	
43	D1	1	Total	C	O	0
			4	1	3	
43	d1	1	Total	C	O	0
			4	1	3	

- Molecule 44 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 (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



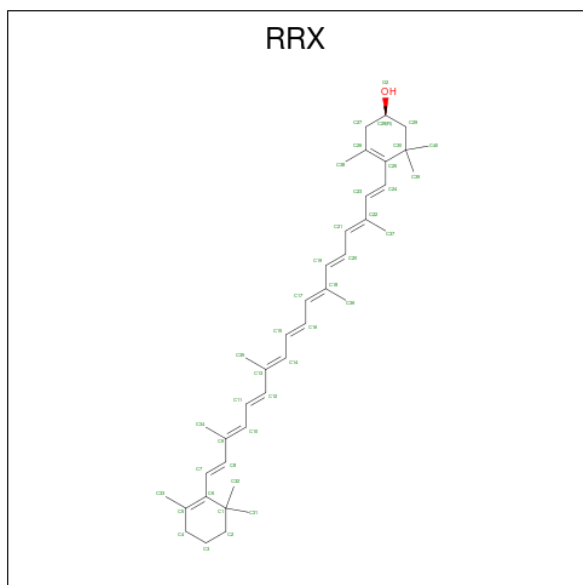
Mol	Chain	Residues	Atoms			AltConf
44	D	1	Total	C	O	0
			55	53	2	
44	d	1	Total	C	O	0
			55	53	2	
44	D1	1	Total	C	O	0
			55	53	2	
44	d1	1	Total	C	O	0
			55	53	2	

- Molecule 45 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					AltConf
45	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
45	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
45	F1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
45	f1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

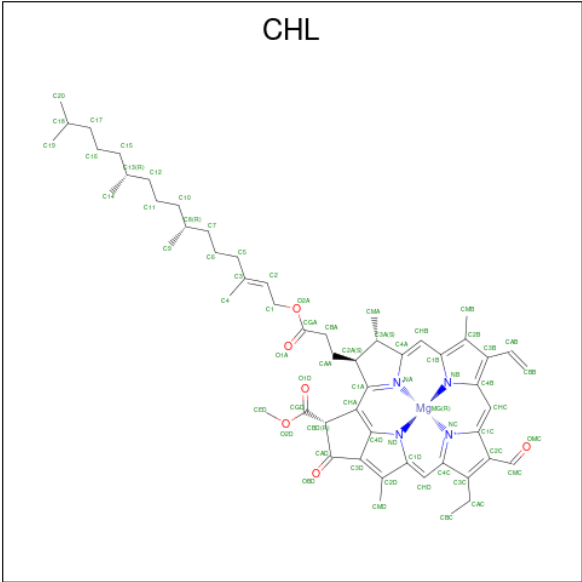
- Molecule 46 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula:  $C_{40}H_{56}O$ ).



Mol	Chain	Residues	Atoms			AltConf
46	H	1	Total	C	O	0
			41	40	1	
46	h	1	Total	C	O	0
			41	40	1	
46	H1	1	Total	C	O	0
			41	40	1	
46	h1	1	Total	C	O	0
			41	40	1	

- Molecule 47 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).





Mol	Chain	Residues	Atoms						AltConf
47	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
47	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
47	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
47	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
47	N	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
47	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
47	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
47	G	1	Total	C	Mg	N	O		0
			48	37	1	4	6		
47	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
47	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
47	G	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
47	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
47	R	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
47	R	1	Total	C	Mg	N	O		0
			50	39	1	4	6		

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Mol	Chain	Residues	Atoms					AltConf
47	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
47	S	1	Total 61	C 50	Mg 1	N 4	O 6	0
47	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
47	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	g	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	g	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
47	r	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	s	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	s	1	Total 43	C 34	Mg 1	N 4	O 4	0
47	s	1	Total 61	C 50	Mg 1	N 4	O 6	0
47	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	N1	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	N1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	G1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	G1	1	Total 48	C 37	Mg 1	N 4	O 6	0
47	G1	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	G1	1	Total 66	C 55	Mg 1	N 4	O 6	0

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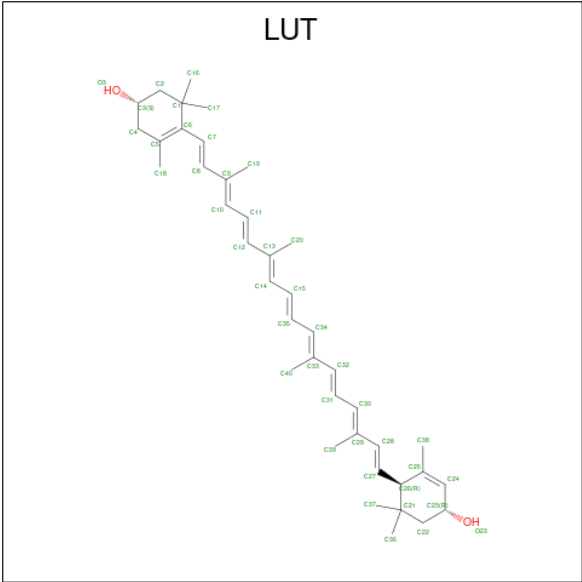
Mol	Chain	Residues	Atoms					AltConf
47	G1	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	G1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	R1	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	R1	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	S1	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	S1	1	Total 44	C 35	Mg 1	N 4	O 4	0
47	S1	1	Total 43	C 34	Mg 1	N 4	O 4	0
47	S1	1	Total 61	C 50	Mg 1	N 4	O 6	0
47	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y1	1	Total 46	C 35	Mg 1	N 4	O 6	0
47	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	Y1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	n1	1	Total 50	C 39	Mg 1	N 4	O 6	0
47	n1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	g1	1	Total 66	C 55	Mg 1	N 4	O 6	0
47	g1	1	Total 48	C 37	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
47	g1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	g1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	g1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	g1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	r1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	r1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	s1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
47	s1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	s1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
47	s1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 48 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			42	40	2	
48	N	1	Total	C	O	0
			42	40	2	
48	G	1	Total	C	O	0
			42	40	2	
48	G	1	Total	C	O	0
			42	40	2	
48	R	1	Total	C	O	0
			42	40	2	
48	S	1	Total	C	O	0
			42	40	2	
48	S	1	Total	C	O	0
			42	40	2	
48	Y	1	Total	C	O	0
			42	40	2	
48	Y	1	Total	C	O	0
			42	40	2	
48	n	1	Total	C	O	0
			42	40	2	
48	n	1	Total	C	O	0
			42	40	2	
48	g	1	Total	C	O	0
			42	40	2	
48	g	1	Total	C	O	0
			42	40	2	
48	r	1	Total	C	O	0
			42	40	2	

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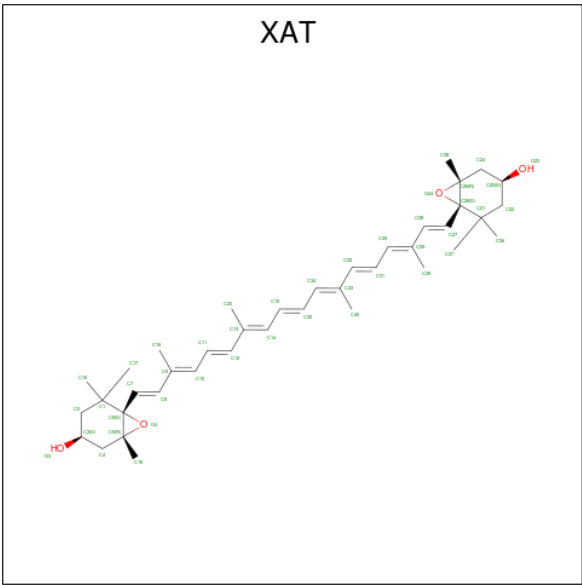
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	s	1	42	40	2	0
48	s	1	42	40	2	0
48	y	1	42	40	2	0
48	y	1	42	40	2	0
48	N1	1	42	40	2	0
48	N1	1	42	40	2	0
48	G1	1	42	40	2	0
48	G1	1	42	40	2	0
48	R1	1	42	40	2	0
48	S1	1	42	40	2	0
48	S1	1	42	40	2	0
48	Y1	1	42	40	2	0
48	Y1	1	42	40	2	0
48	n1	1	42	40	2	0
48	n1	1	42	40	2	0
48	g1	1	42	40	2	0
48	g1	1	42	40	2	0
48	r1	1	42	40	2	0
48	s1	1	42	40	2	0
48	s1	1	42	40	2	0
48	y1	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
48	y1	1	Total	C	O	0
			42	40	2	

- Molecule 49 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	R	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	
49	n	1	Total	C	O	0
			44	40	4	
49	g	1	Total	C	O	0
			44	40	4	
49	r	1	Total	C	O	0
			44	40	4	
49	y	1	Total	C	O	0
			44	40	4	
49	N1	1	Total	C	O	0
			44	40	4	
49	G1	1	Total	C	O	0
			44	40	4	

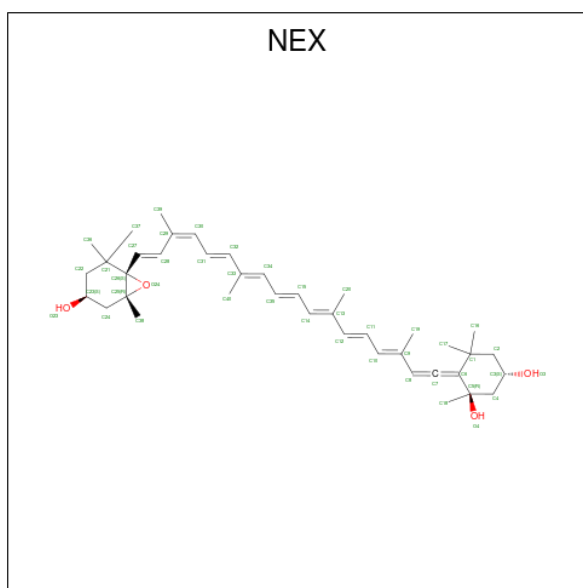
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Mol	Chain	Residues	Atoms			AltConf
49	R1	1	Total	C	O	0
			44	40	4	
49	Y1	1	Total	C	O	0
			44	40	4	
49	n1	1	Total	C	O	0
			44	40	4	
49	g1	1	Total	C	O	0
			44	40	4	
49	r1	1	Total	C	O	0
			44	40	4	
49	y1	1	Total	C	O	0
			44	40	4	

- Molecule 50 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA-DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



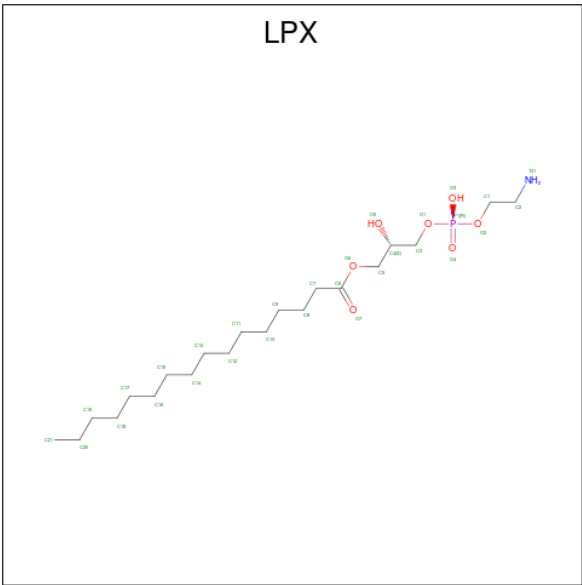
Mol	Chain	Residues	Atoms			AltConf
50	N	1	Total	C	O	0
			44	40	4	
50	G	1	Total	C	O	0
			44	40	4	
50	R	1	Total	C	O	0
			44	40	4	
50	S	1	Total	C	O	0
			44	40	4	

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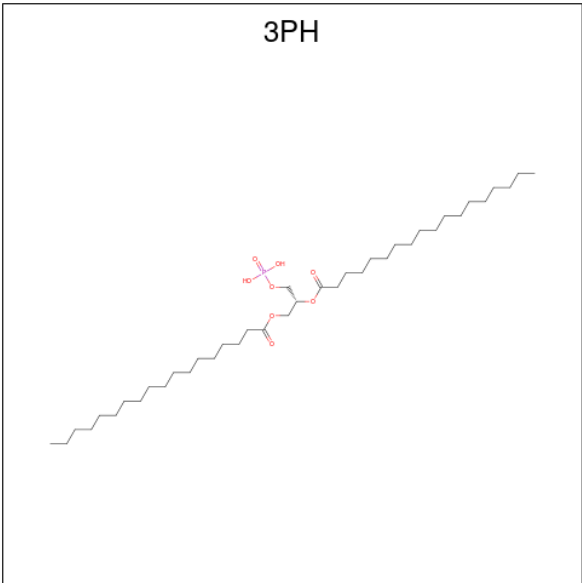
Mol	Chain	Residues	Atoms			AltConf
50	Y	1	Total	C	O	0
			44	40	4	
50	n	1	Total	C	O	0
			44	40	4	
50	g	1	Total	C	O	0
			44	40	4	
50	r	1	Total	C	O	0
			44	40	4	
50	s	1	Total	C	O	0
			44	40	4	
50	y	1	Total	C	O	0
			44	40	4	
50	N1	1	Total	C	O	0
			44	40	4	
50	G1	1	Total	C	O	0
			44	40	4	
50	R1	1	Total	C	O	0
			44	40	4	
50	S1	1	Total	C	O	0
			44	40	4	
50	Y1	1	Total	C	O	0
			44	40	4	
50	n1	1	Total	C	O	0
			44	40	4	
50	g1	1	Total	C	O	0
			44	40	4	
50	r1	1	Total	C	O	0
			44	40	4	
50	s1	1	Total	C	O	0
			44	40	4	
50	y1	1	Total	C	O	0
			44	40	4	

- Molecule 51 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C<sub>21</sub>H<sub>44</sub>NO<sub>7</sub>P).



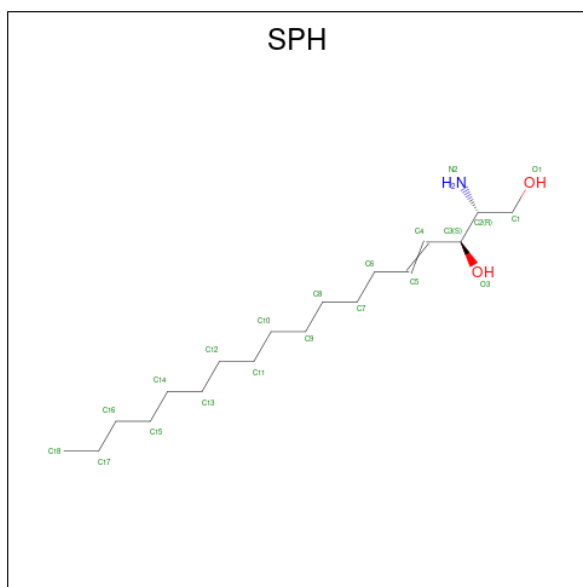
Mol	Chain	Residues	Atoms					AltConf
51	S	1	Total	C	N	O	P	0
			30	21	1	7	1	
51	s	1	Total	C	N	O	P	0
			30	21	1	7	1	
51	S1	1	Total	C	N	O	P	0
			30	21	1	7	1	
51	s1	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 52 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				AltConf
52	S	1	Total	C	O	P	0
			48	39	8	1	
52	i	1	Total	C	O	P	0
			48	39	8	1	
52	s	1	Total	C	O	P	0
			48	39	8	1	
52	B1	1	Total	C	O	P	0
			48	39	8	1	
52	T1	1	Total	C	O	P	0
			48	39	8	1	
52	S1	1	Total	C	O	P	0
			48	39	8	1	
52	b1	1	Total	C	O	P	0
			48	39	8	1	
52	t1	1	Total	C	O	P	0
			48	39	8	1	
52	s1	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 53 is SPHINGOSINE (three-letter code: SPH) (formula:  $C_{18}H_{37}NO_2$ ).



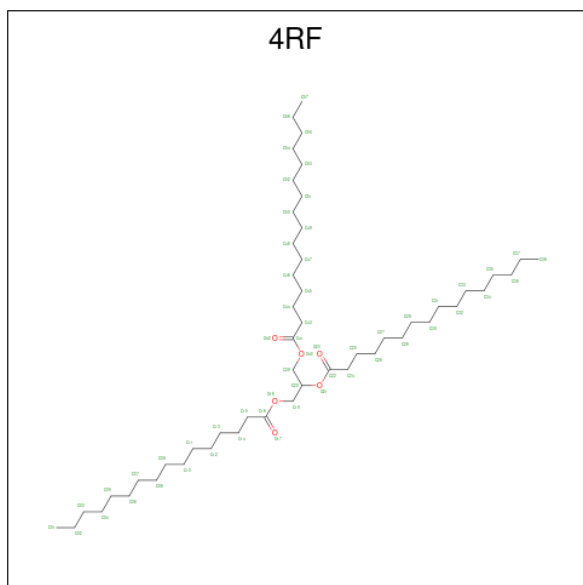
Mol	Chain	Residues	Atoms				AltConf
53	Y	1	Total	C	N	O	0
			21	18	1	2	
53	y	1	Total	C	N	O	0
			21	18	1	2	
53	A1	1	Total	C	N	O	0
			21	18	1	2	

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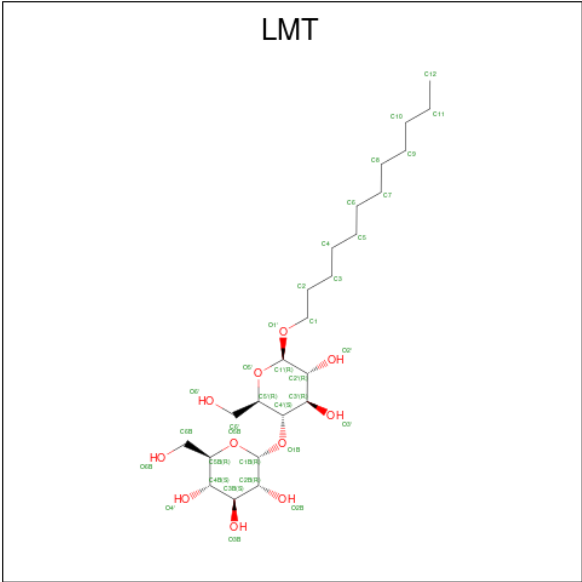
Mol	Chain	Residues	Atoms				AltConf
53	Y1	1	Total	C	N	O	0
			21	18	1	2	
53	a1	1	Total	C	N	O	0
			21	18	1	2	
53	y1	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 54 is Tripalmitoylglycerol (three-letter code: 4RF) (formula:  $C_{51}H_{98}O_6$ ).



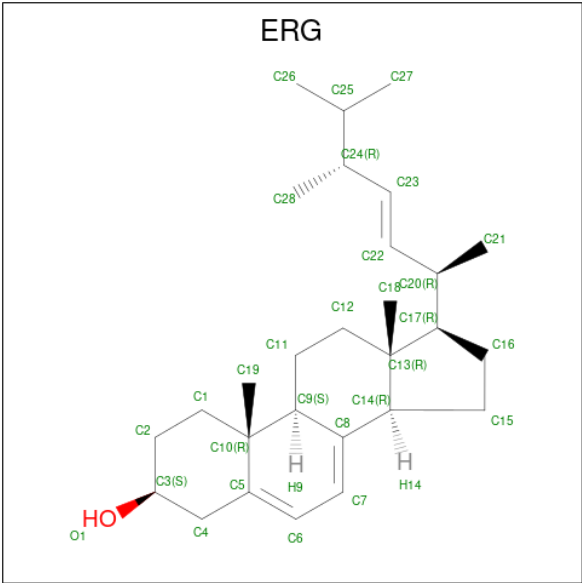
Mol	Chain	Residues	Atoms			AltConf
54	I1	1	Total	C	O	0
			57	51	6	
54	K1	1	Total	C	O	0
			57	51	6	
54	i1	1	Total	C	O	0
			57	51	6	
54	k1	1	Total	C	O	0
			57	51	6	

- Molecule 55 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



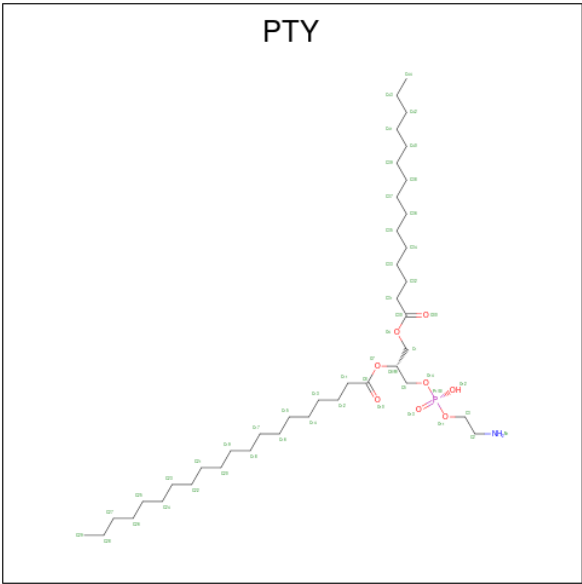
Mol	Chain	Residues	Atoms			AltConf
55	R1	1	Total	C	O	0
			35	24	11	
55	r1	1	Total	C	O	0
			35	24	11	

- Molecule 56 is ERGOSTEROL (three-letter code: ERG) (formula: C<sub>28</sub>H<sub>44</sub>O).



Mol	Chain	Residues	Atoms			AltConf
56	R1	1	Total	C	O	0
			29	28	1	
56	r1	1	Total	C	O	0
			29	28	1	

- Molecule 57 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).

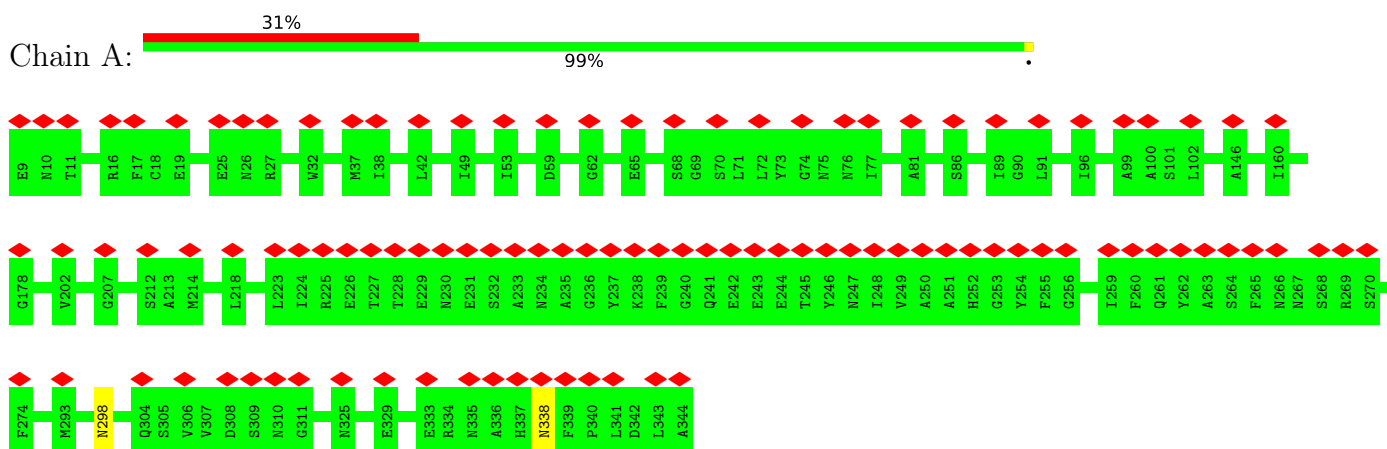


Mol	Chain	Residues	Atoms					AltConf
57	Y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
57	Y1	1	Total	C	N	O	P	0
			19	9	1	8	1	
57	y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
57	y1	1	Total	C	N	O	P	0
			19	9	1	8	1	

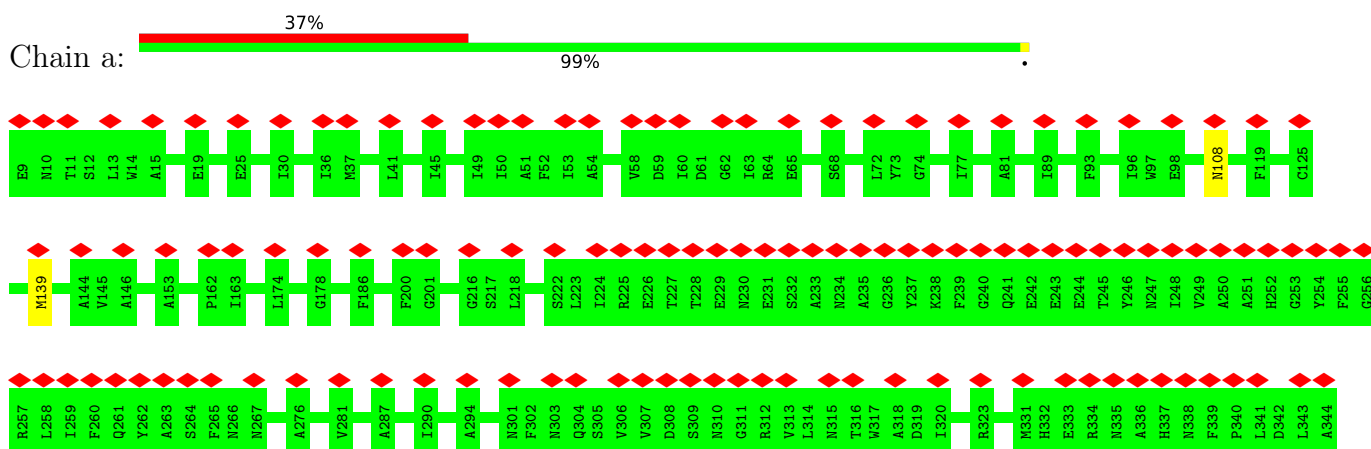
### 3 Residue-property plots [i](#)

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.

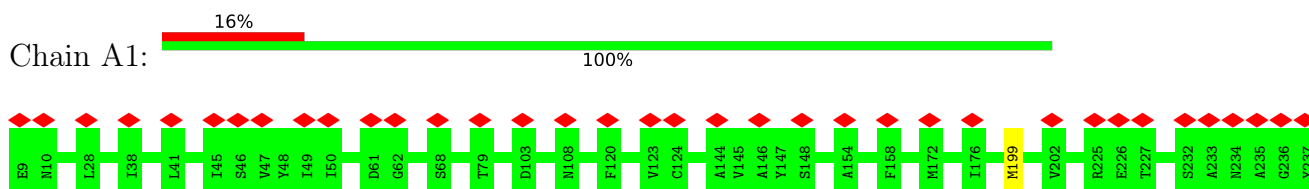
#### • Molecule 1: Photosystem II protein D1



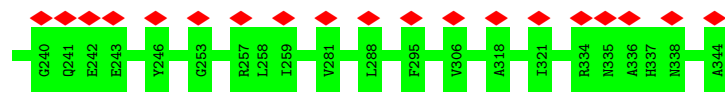
#### • Molecule 1: Photosystem II protein D1



#### • Molecule 1: Photosystem II protein D1

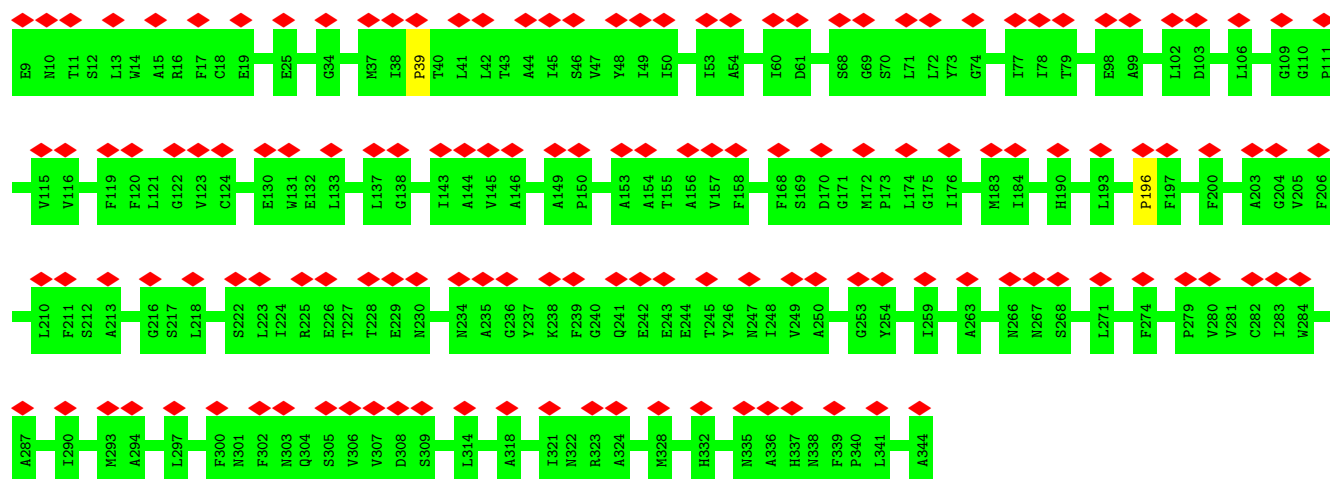






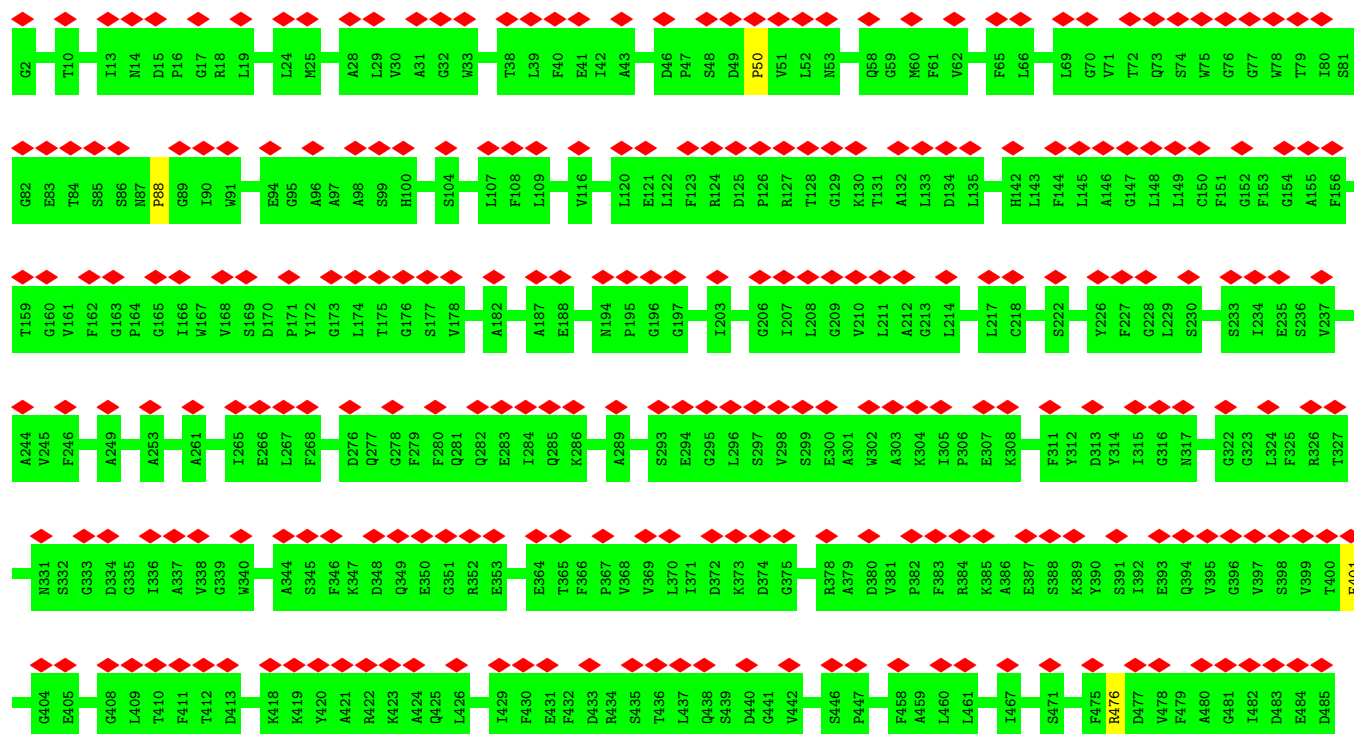
• Molecule 1: Photosystem II protein D1

Chain a1: 42% 99%

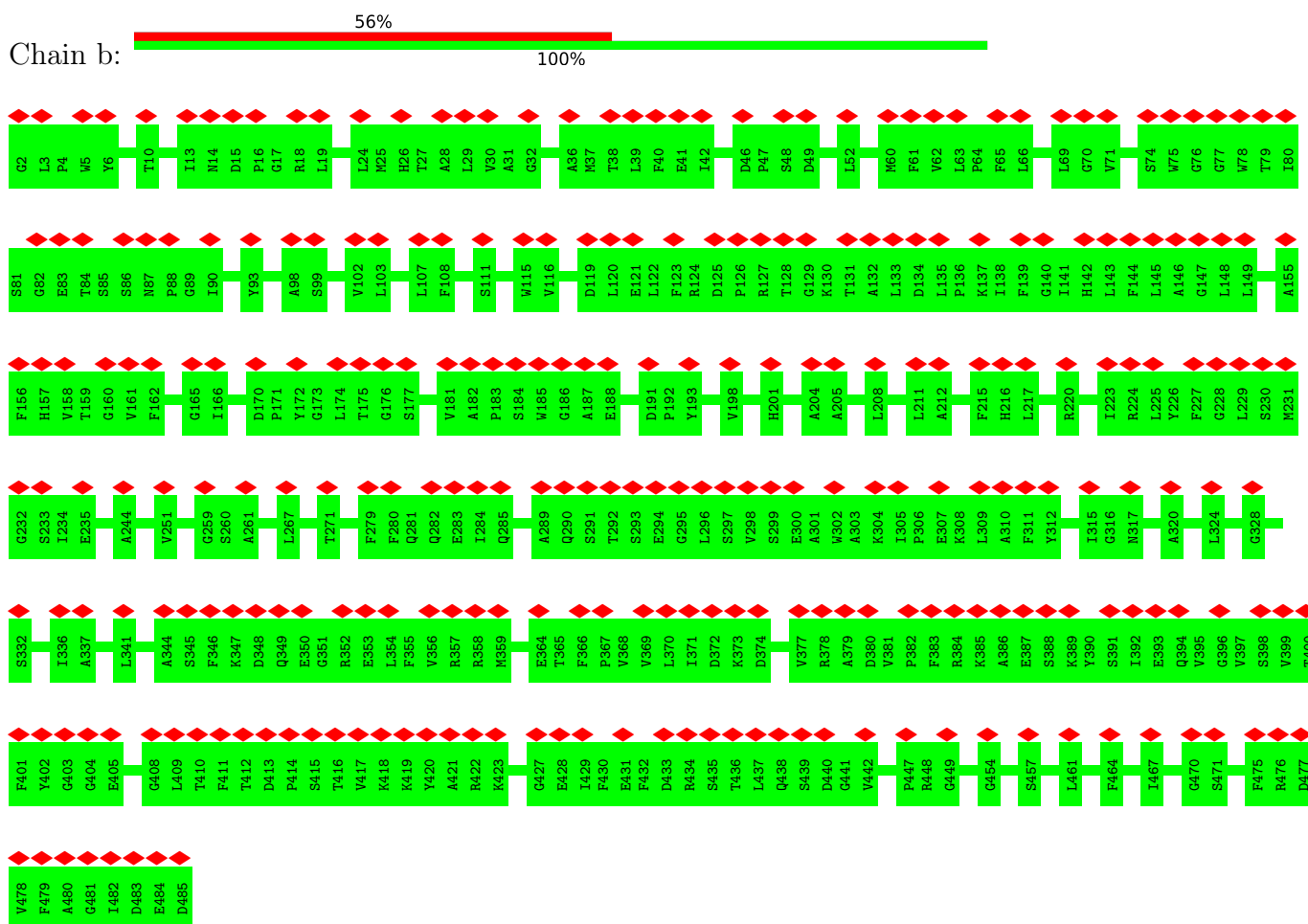


• Molecule 2: Photosystem II CP47 reaction center protein

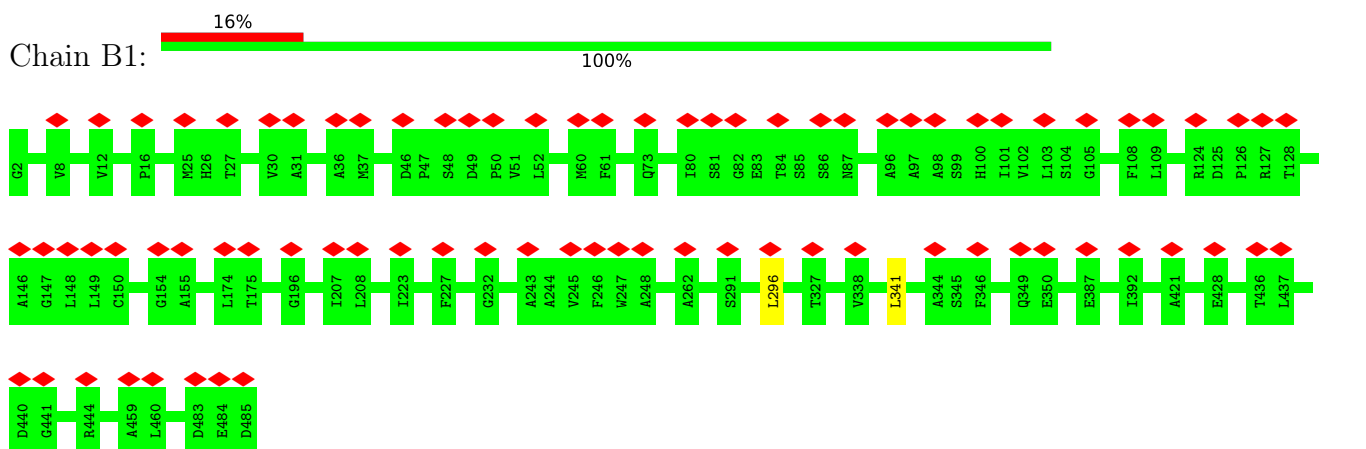
Chain B: 53% 99%



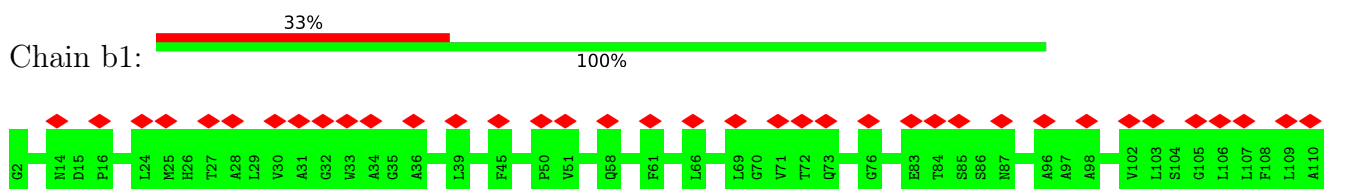
• Molecule 2: Photosystem II CP47 reaction center protein

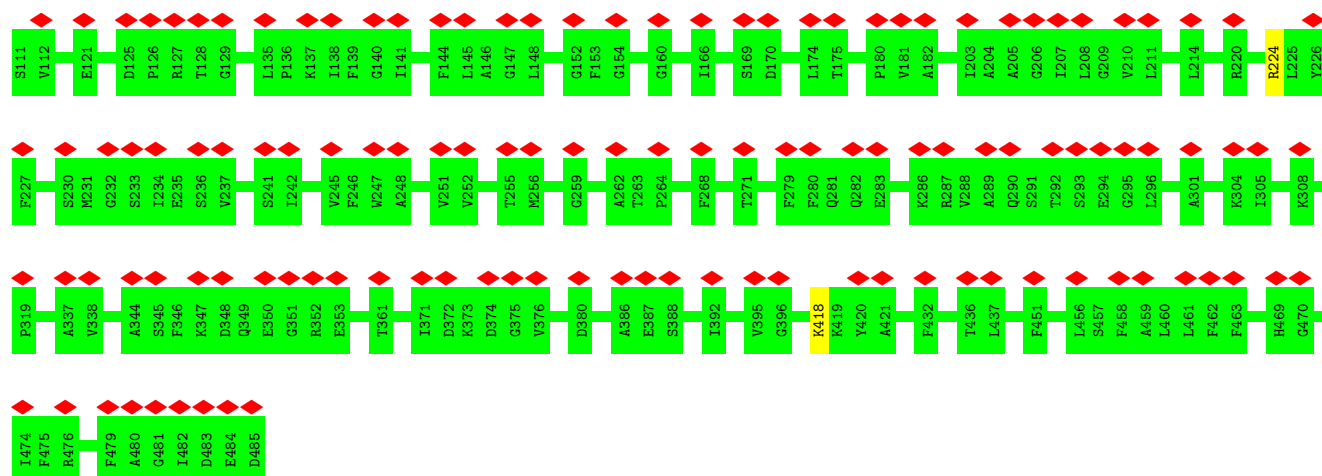


• Molecule 2: Photosystem II CP47 reaction center protein

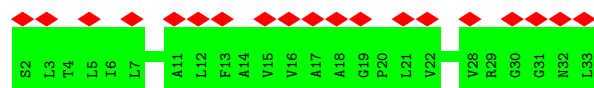


• Molecule 2: Photosystem II CP47 reaction center protein

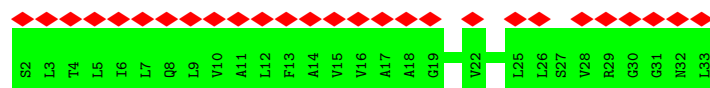
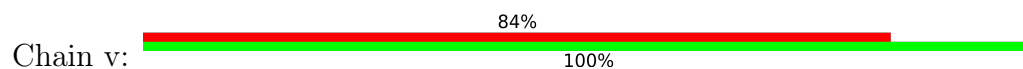




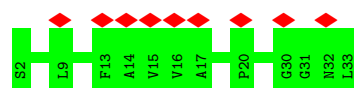
- Molecule 3: Photosystem II reaction center protein Ycf12



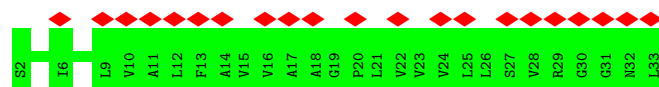
- Molecule 3: Photosystem II reaction center protein Ycf12



- Molecule 3: Photosystem II reaction center protein Ycf12

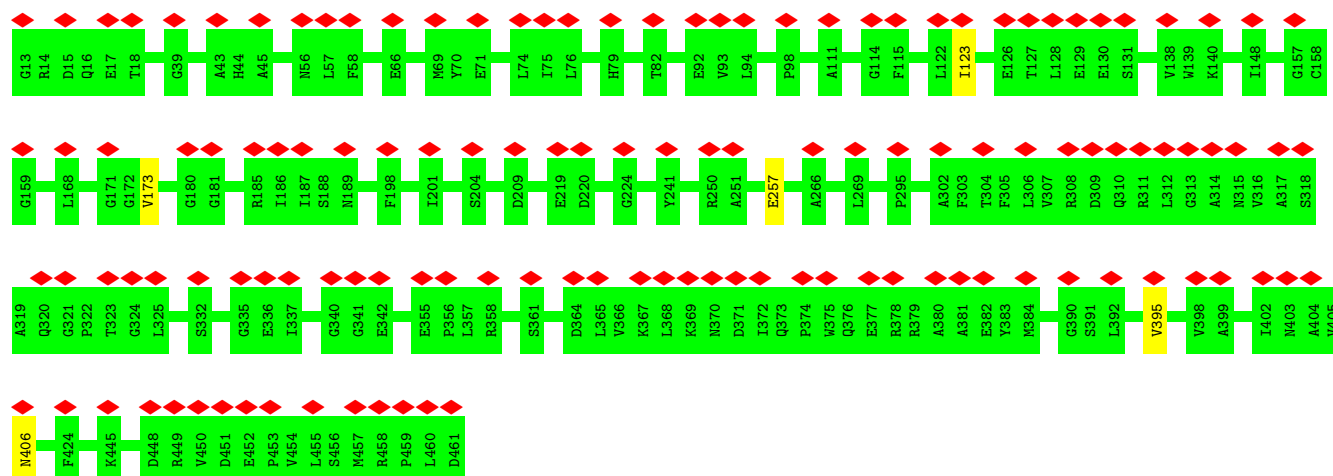


- Molecule 3: Photosystem II reaction center protein Ycf12



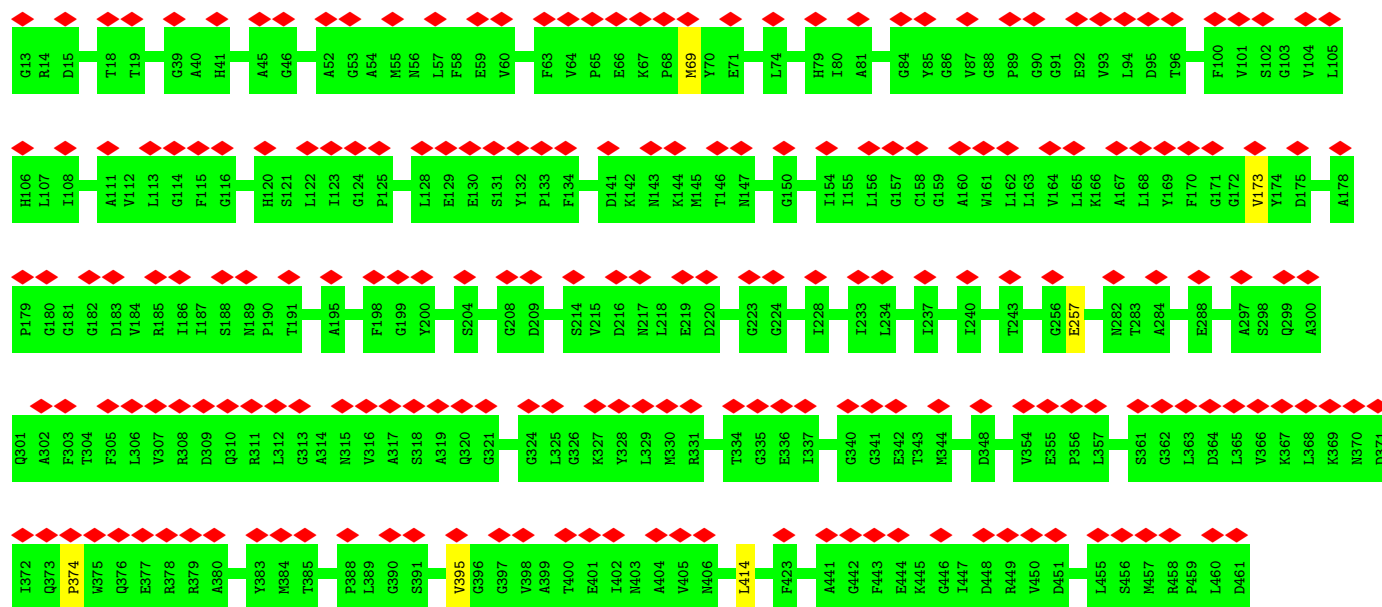
- Molecule 4: Photosystem II CP43 reaction center protein





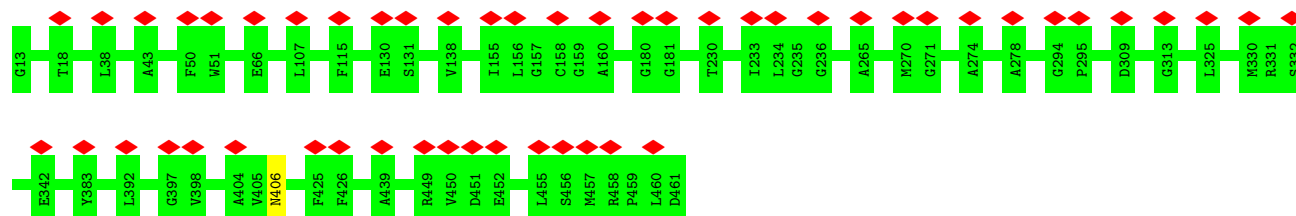
• Molecule 4: Photosystem II CP43 reaction center protein

Chain c: 46% 99% .



• Molecule 4: Photosystem II CP43 reaction center protein

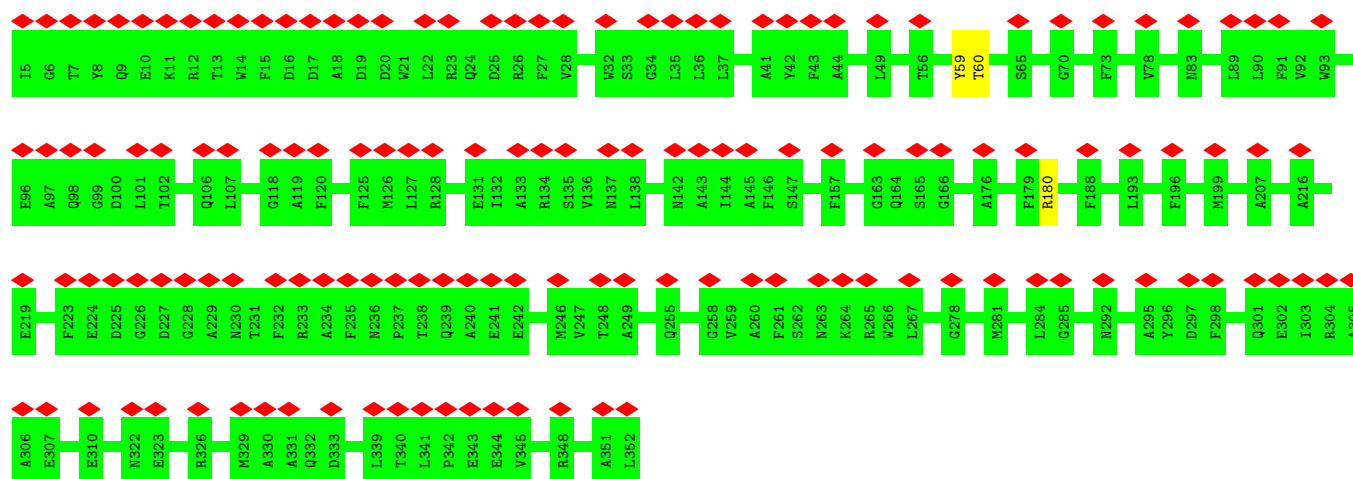
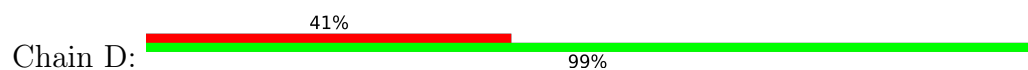
Chain C1: 11% 100%



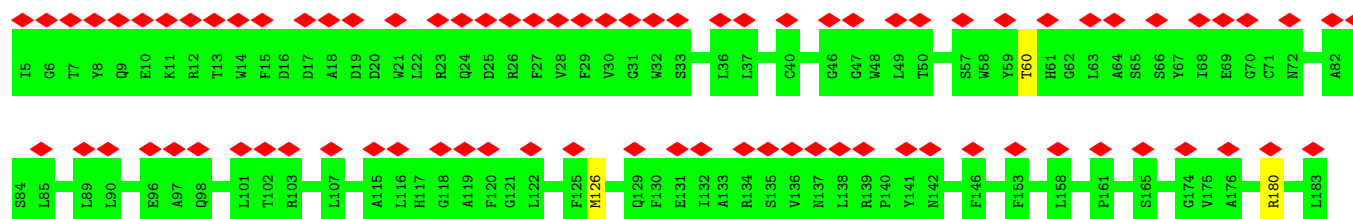
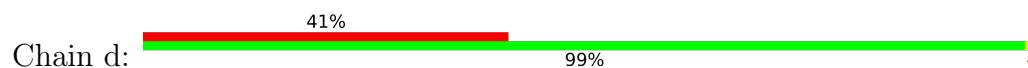
• Molecule 4: Photosystem II CP43 reaction center protein

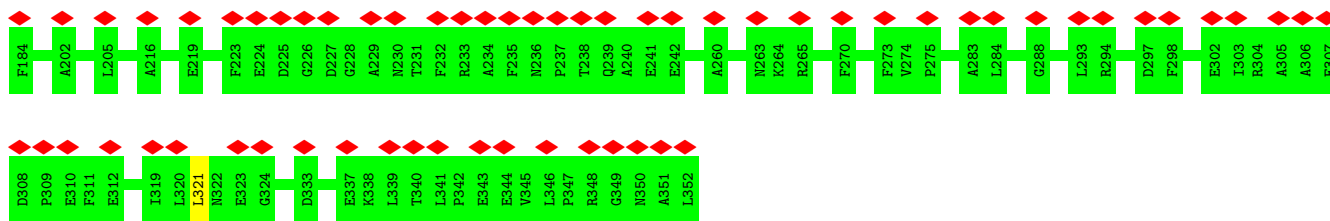


• Molecule 5: Photosystem II D2 protein

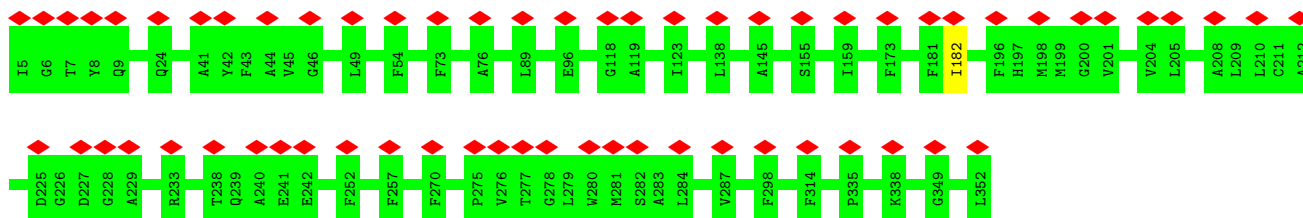


• Molecule 5: Photosystem II D2 protein

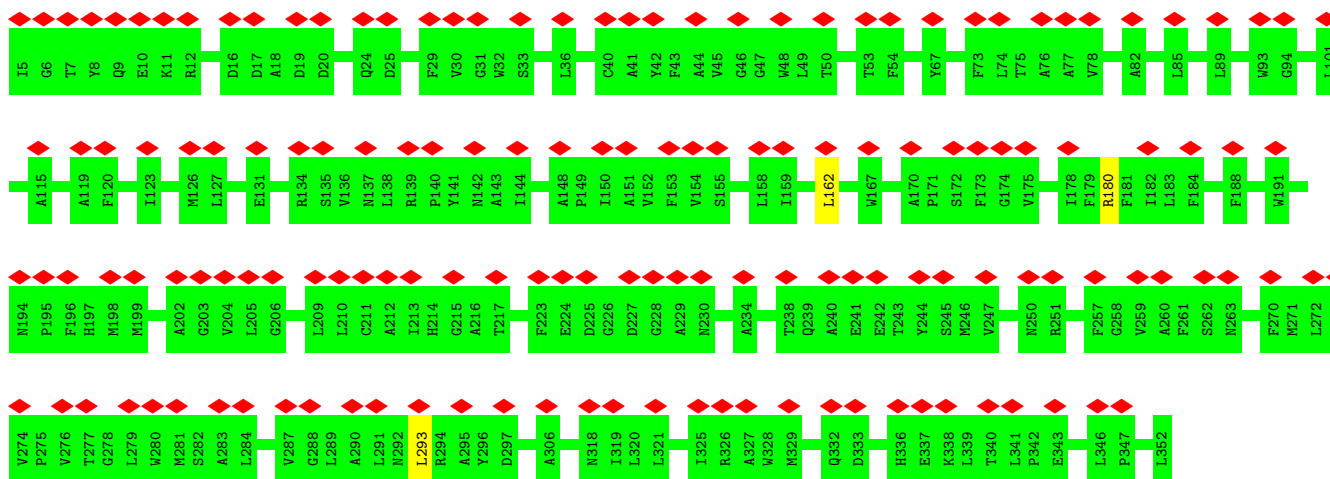
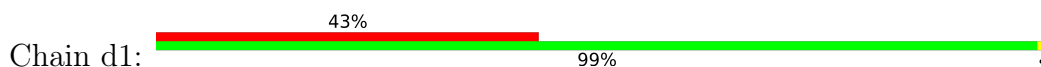




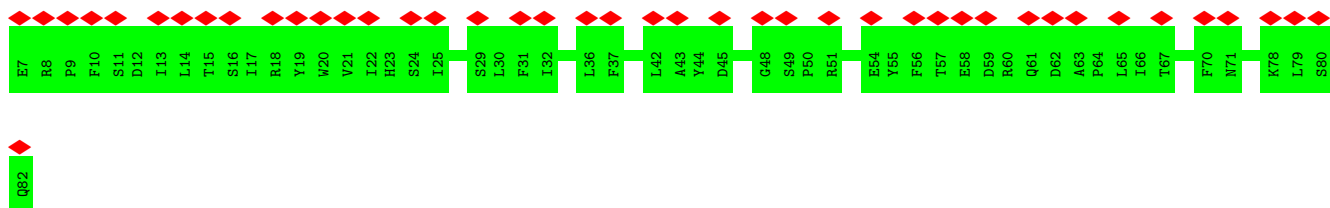
• Molecule 5: Photosystem II D2 protein



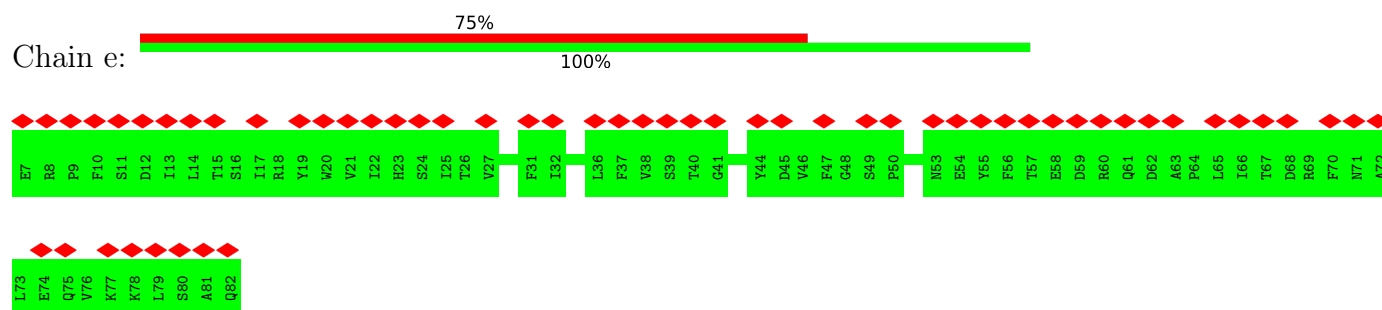
• Molecule 5: Photosystem II D2 protein



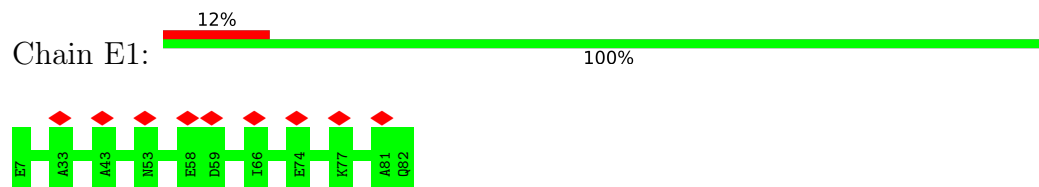
• Molecule 6: Cytochrome b559 subunit alpha



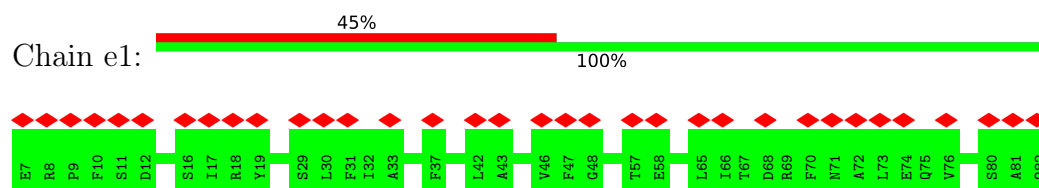
• Molecule 6: Cytochrome b559 subunit alpha



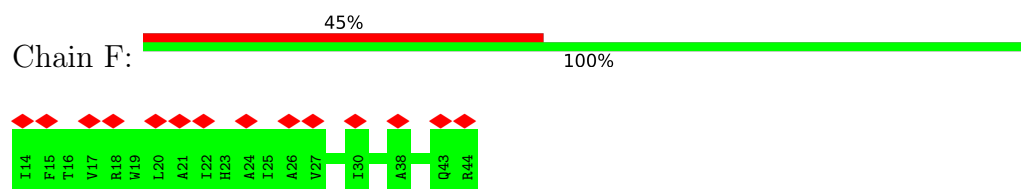
- Molecule 6: Cytochrome b559 subunit alpha



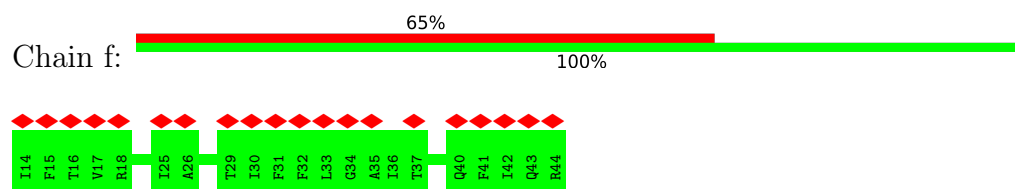
- Molecule 6: Cytochrome b559 subunit alpha



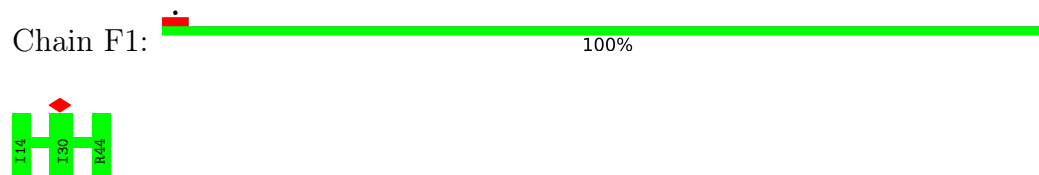
- Molecule 7: Cytochrome b559 subunit beta



- Molecule 7: Cytochrome b559 subunit beta

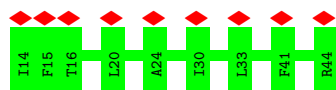


- Molecule 7: Cytochrome b559 subunit beta

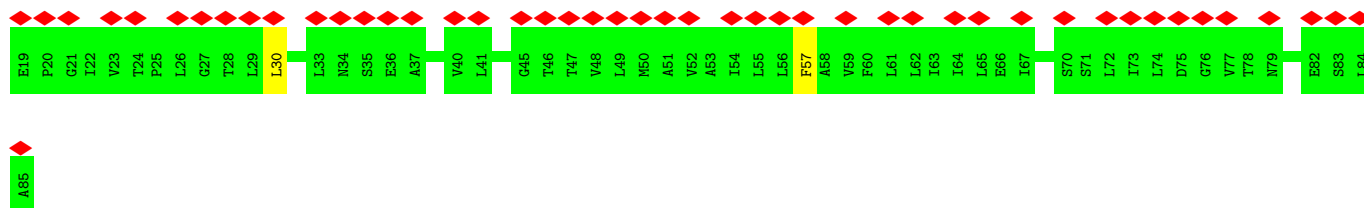


- Molecule 7: Cytochrome b559 subunit beta

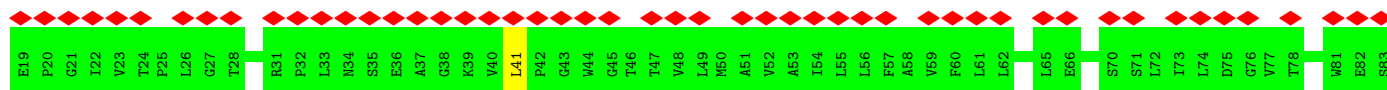
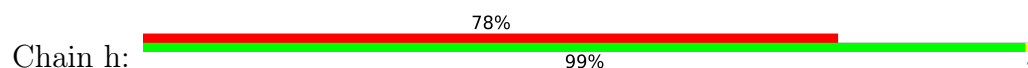




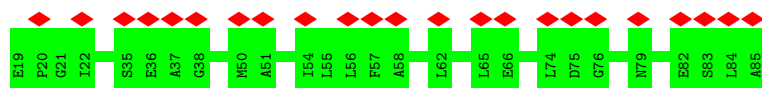
- Molecule 8: Photosystem II reaction center protein H



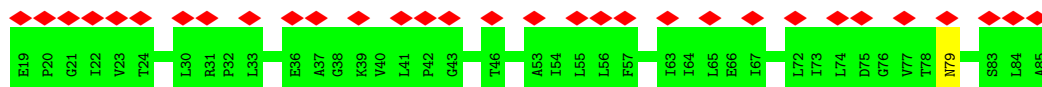
- Molecule 8: Photosystem II reaction center protein H



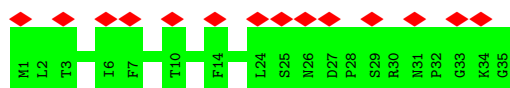
- Molecule 8: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein H

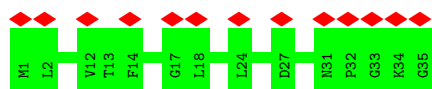


- Molecule 9: Photosystem II reaction center protein I

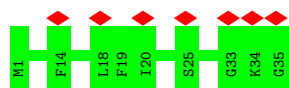


- Molecule 9: Photosystem II reaction center protein I

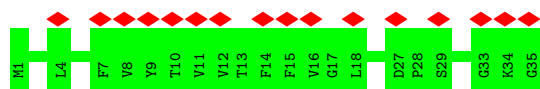




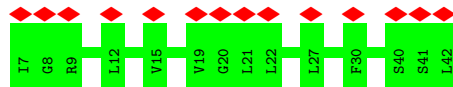
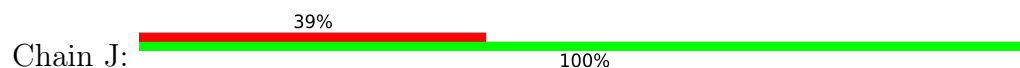
- Molecule 9: Photosystem II reaction center protein I



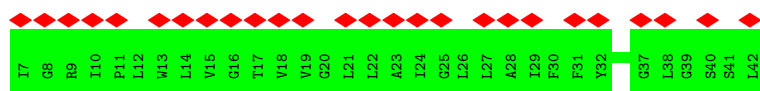
- Molecule 9: Photosystem II reaction center protein I



- Molecule 10: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein J

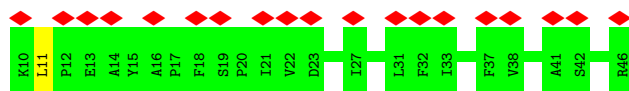


- Molecule 10: Photosystem II reaction center protein J





- Molecule 11: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein K



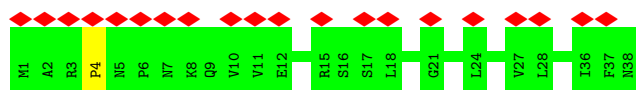
- Molecule 11: Photosystem II reaction center protein K



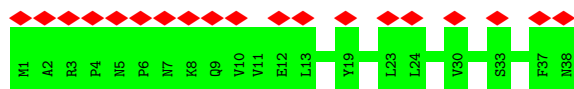
- Molecule 11: Photosystem II reaction center protein K



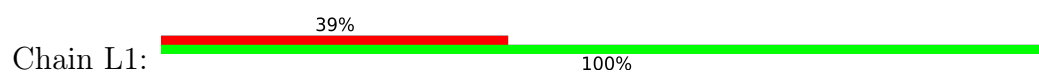
- Molecule 12: Photosystem II reaction center protein L



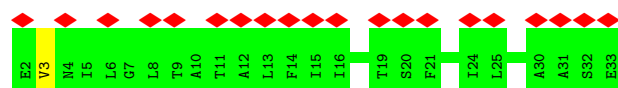
- Molecule 12: Photosystem II reaction center protein L



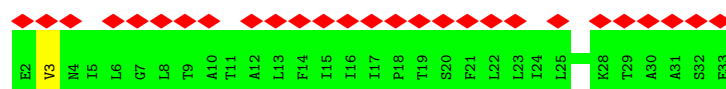
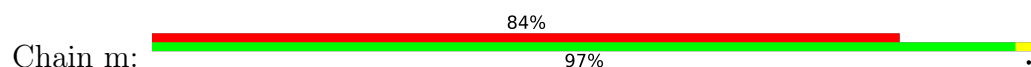
- Molecule 12: Photosystem II reaction center protein L



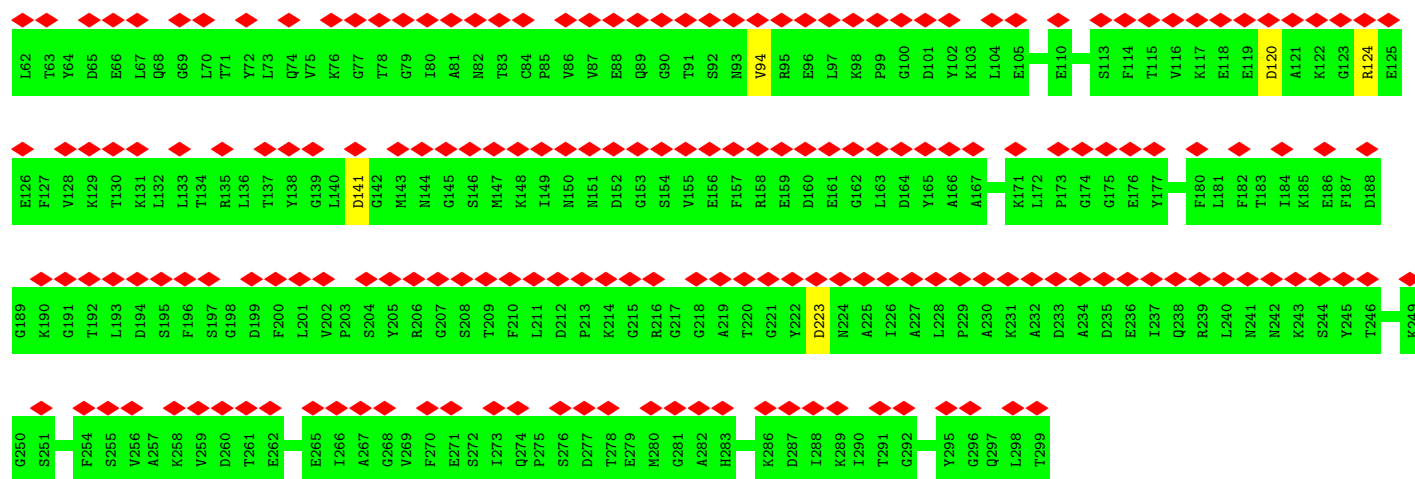
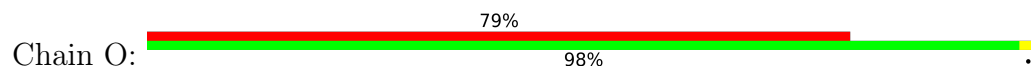
- Molecule 13: Photosystem II reaction center protein M



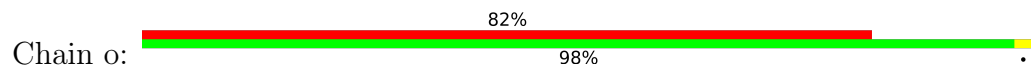
- Molecule 13: Photosystem II reaction center protein M

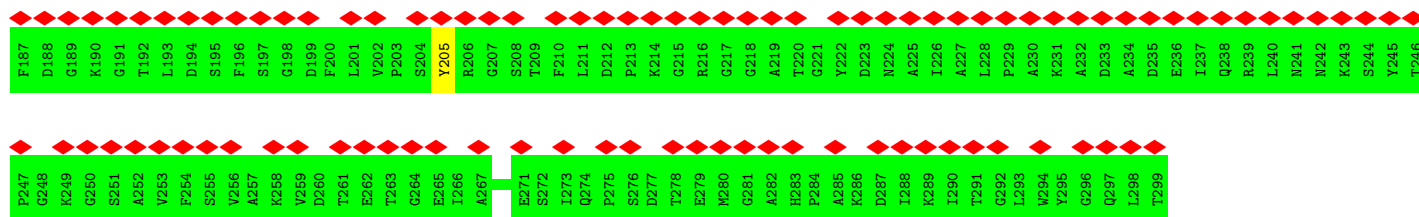


- Molecule 14: PsbO

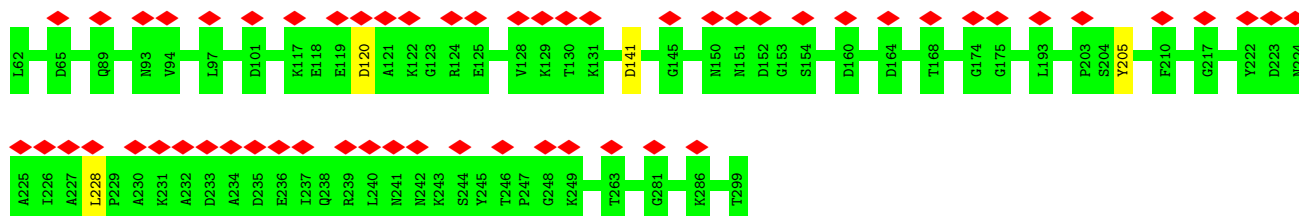


- Molecule 14: PsbO

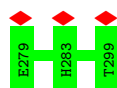
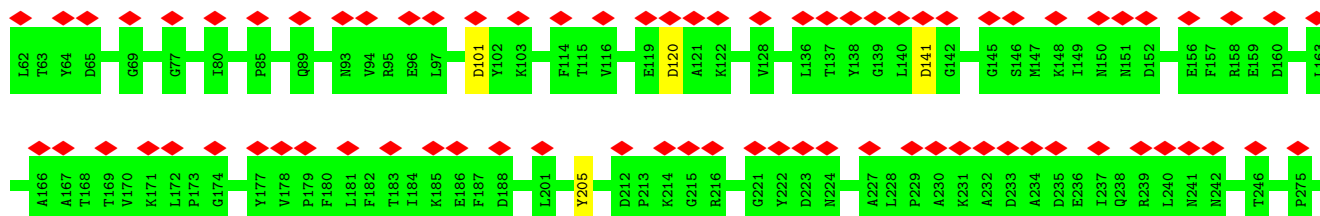




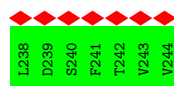
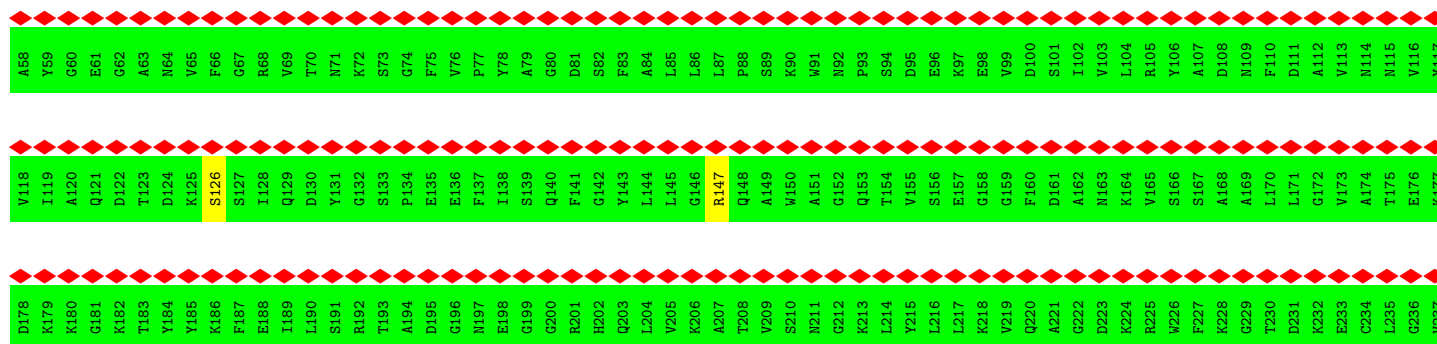
• Molecule 14: PsbO



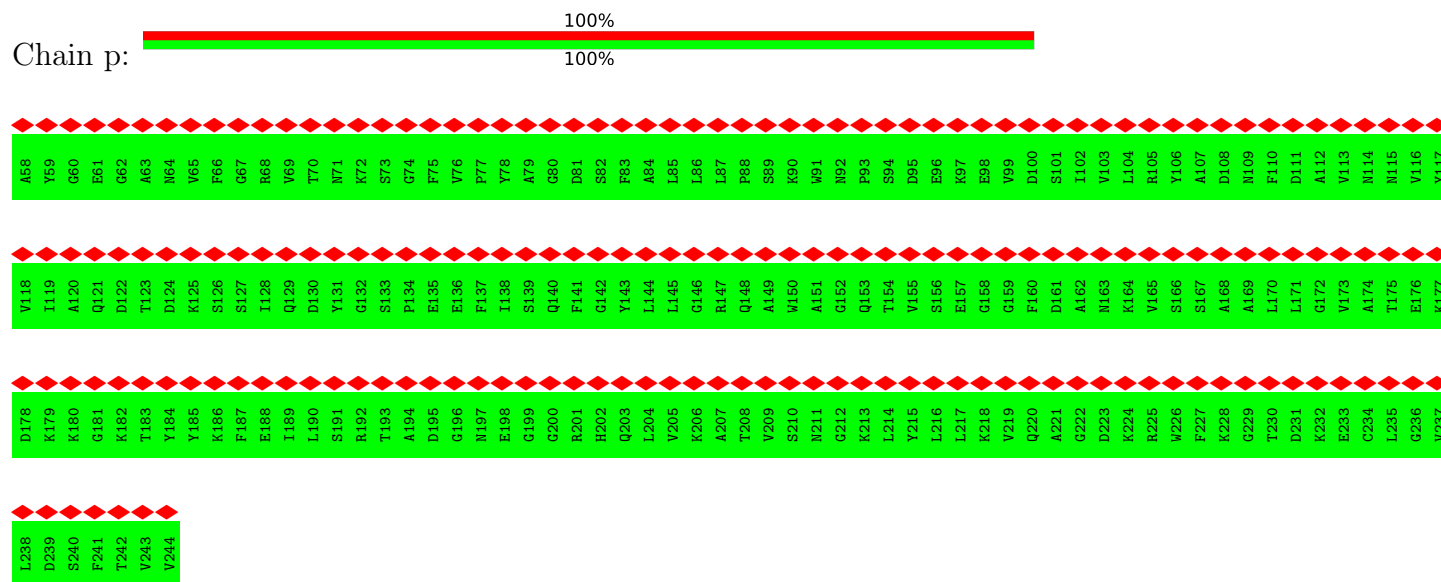
• Molecule 14: PsbO



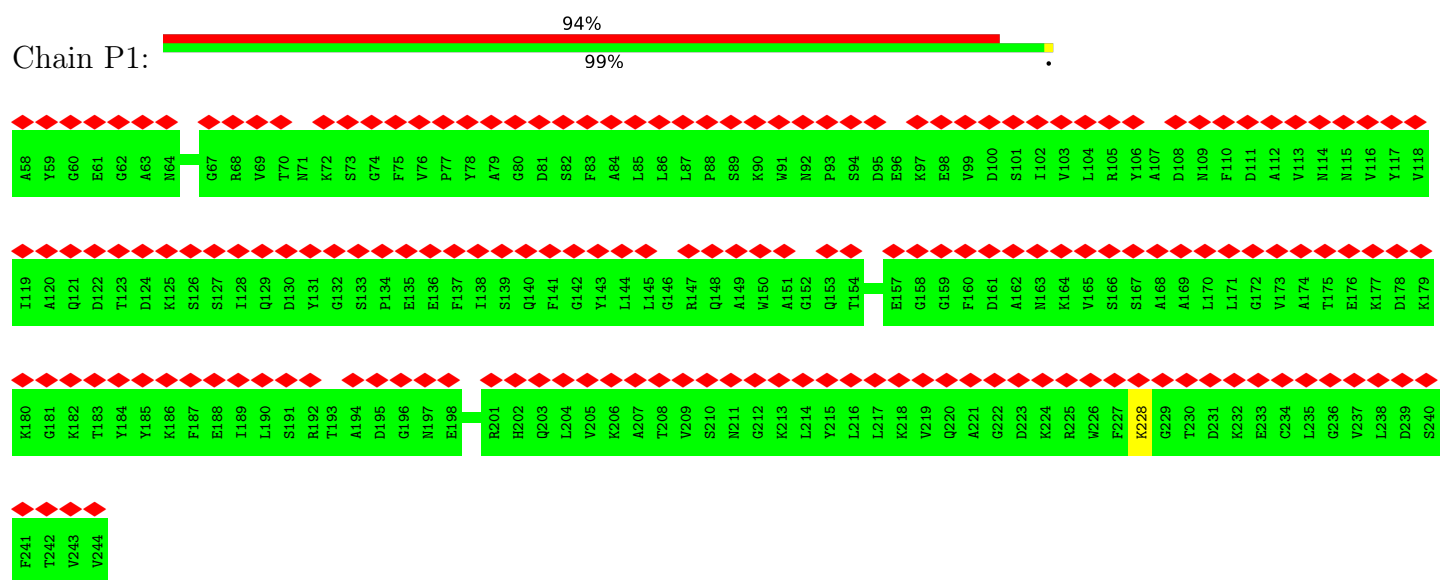
• Molecule 15: PsbP



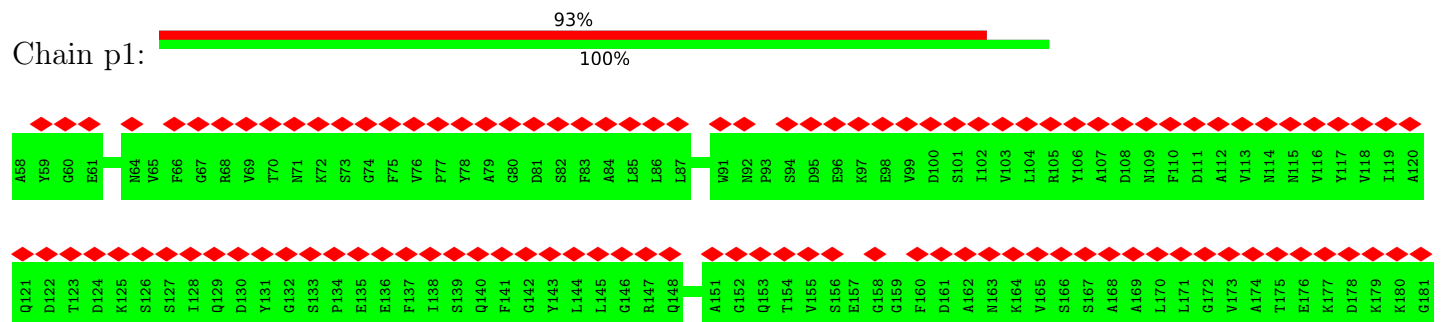
## ● Molecule 15: PsbP

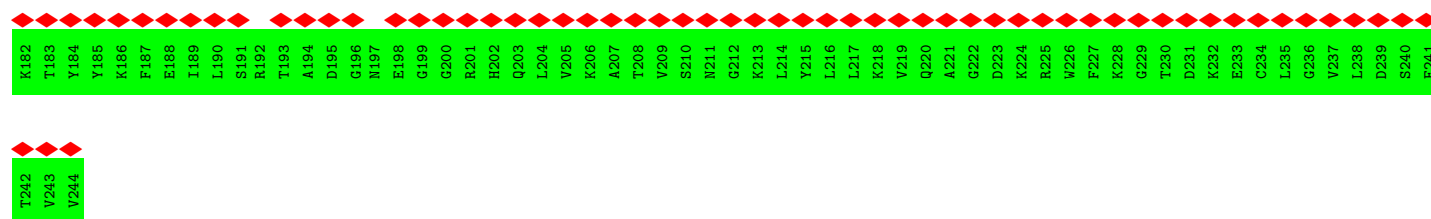


## ● Molecule 15: PsbP

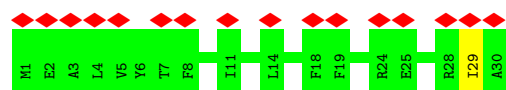


## ● Molecule 15: PsbP

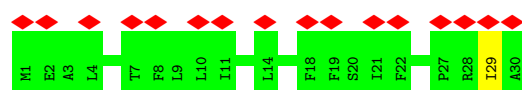




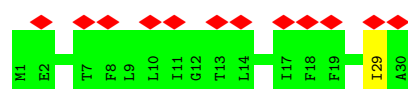
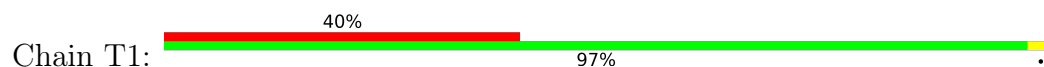
- Molecule 16: Photosystem II reaction center protein T



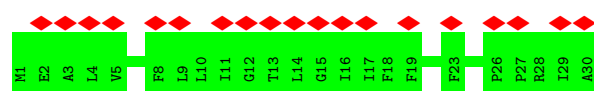
- Molecule 16: Photosystem II reaction center protein T



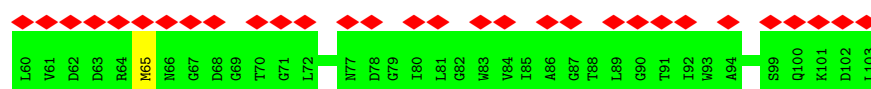
- Molecule 16: Photosystem II reaction center protein T



- Molecule 16: Photosystem II reaction center protein T

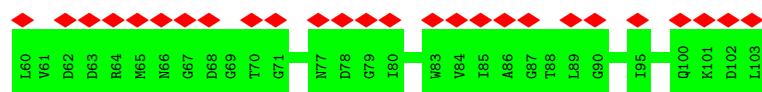


- Molecule 17: PsbW

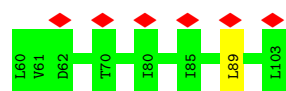


- Molecule 17: PsbW

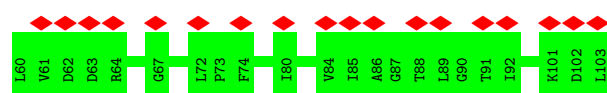
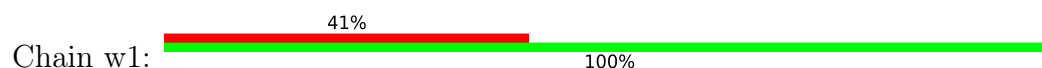




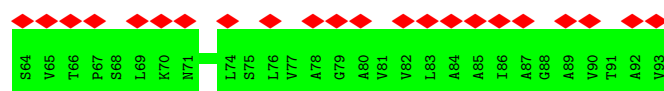
- Molecule 17: PsbW



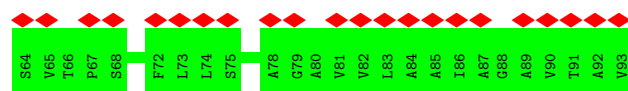
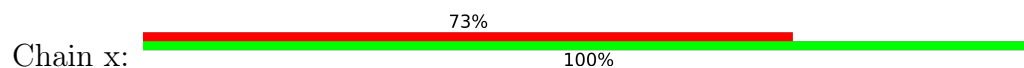
- Molecule 17: PsbW



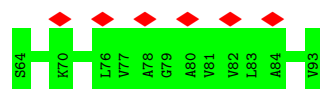
- Molecule 18: PsbX



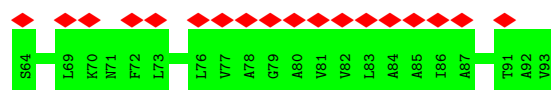
- Molecule 18: PsbX



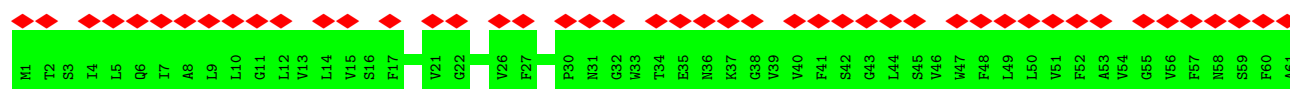
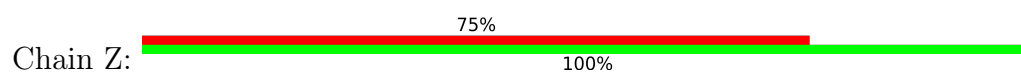
- Molecule 18: PsbX



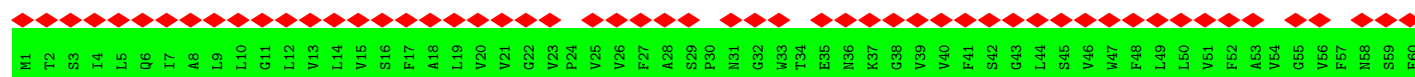
- Molecule 18: PsbX



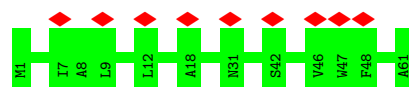
- Molecule 19: PsbZ



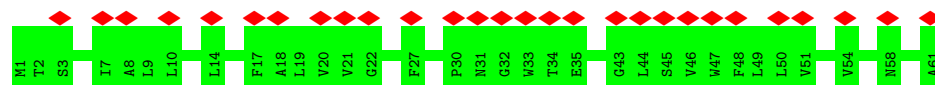
- Molecule 19: PsbZ



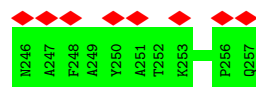
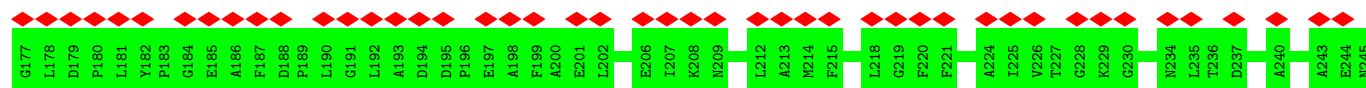
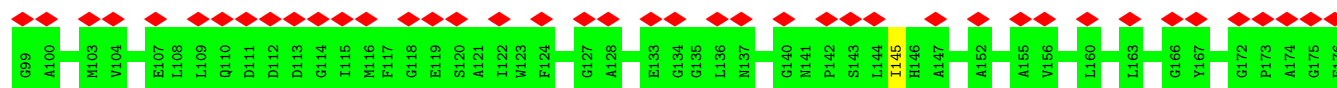
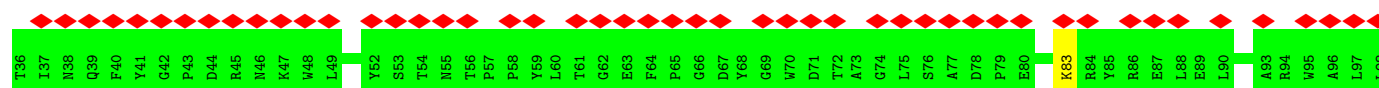
- Molecule 19: PsbZ



- Molecule 19: PsbZ

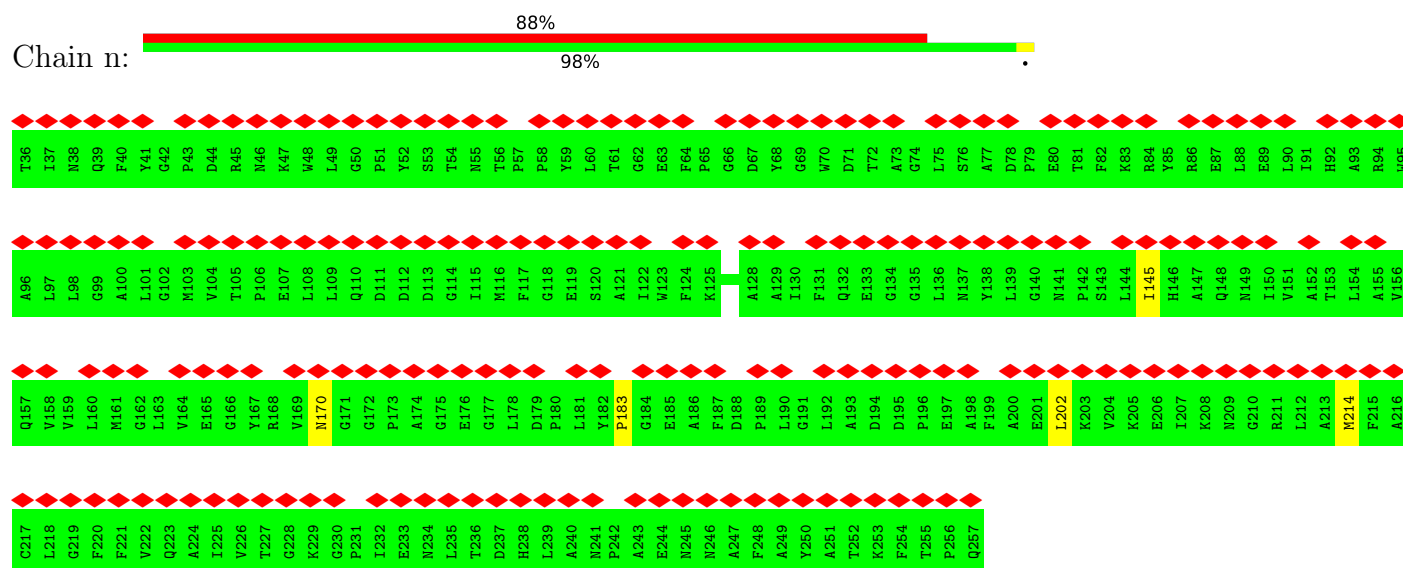


- Molecule 20: LHCII M3

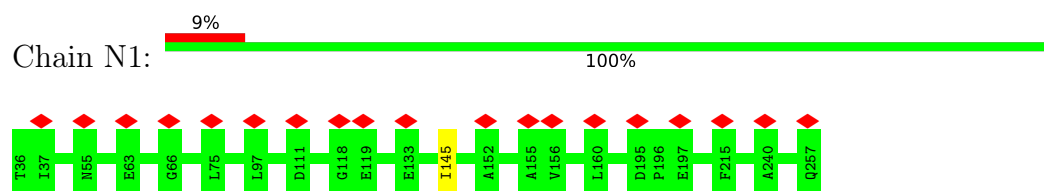


- Molecule 20: LHCII M3

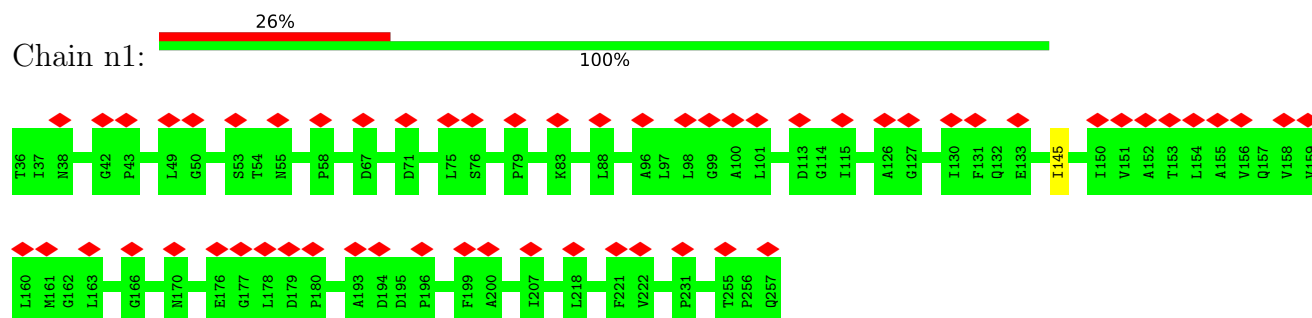




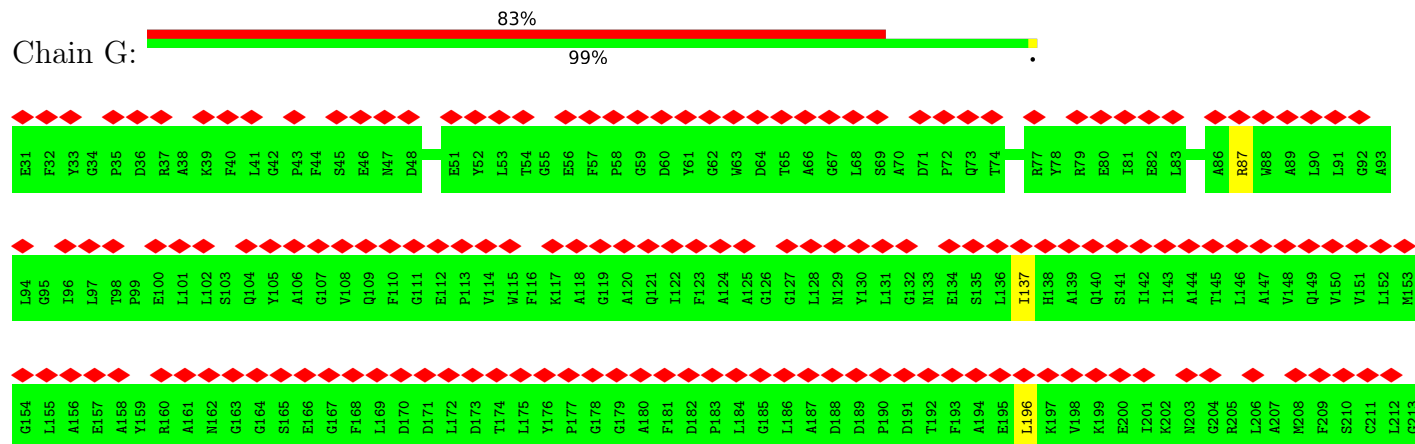
• Molecule 20: LHCII M3

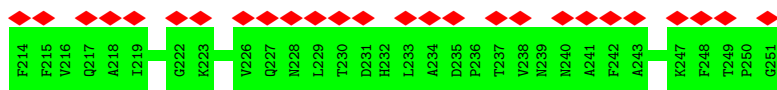


• Molecule 20: LHCII M3

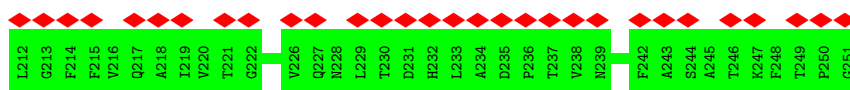
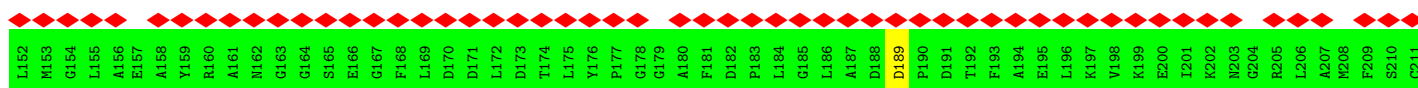
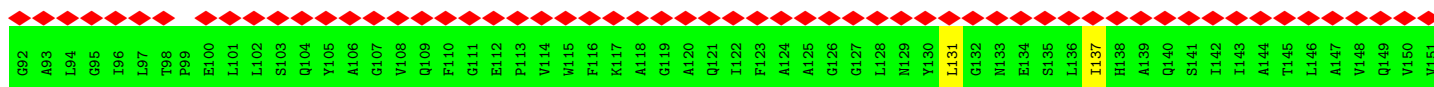
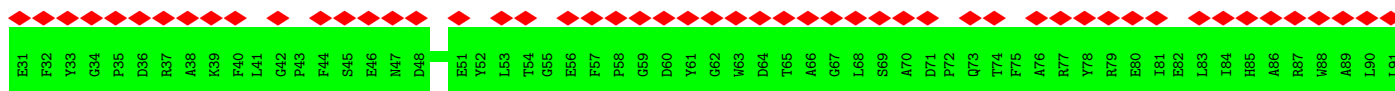
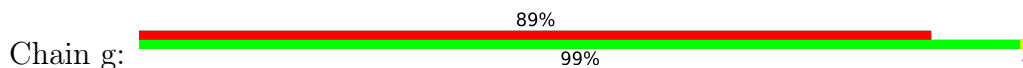


• Molecule 21: LHCII M2

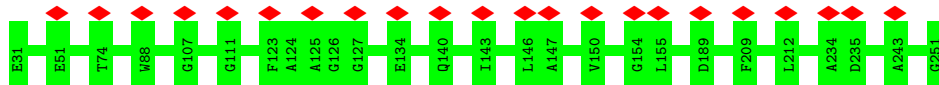




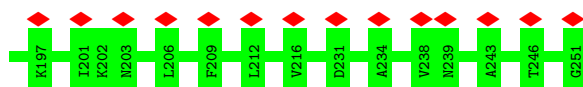
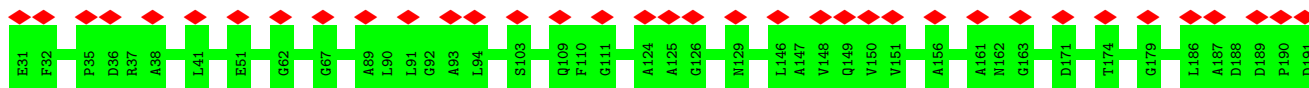
• Molecule 21: LHCII M2



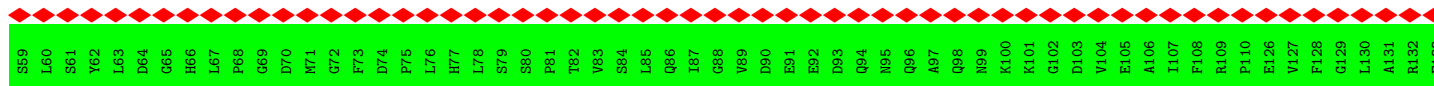
• Molecule 21: LHCII M2

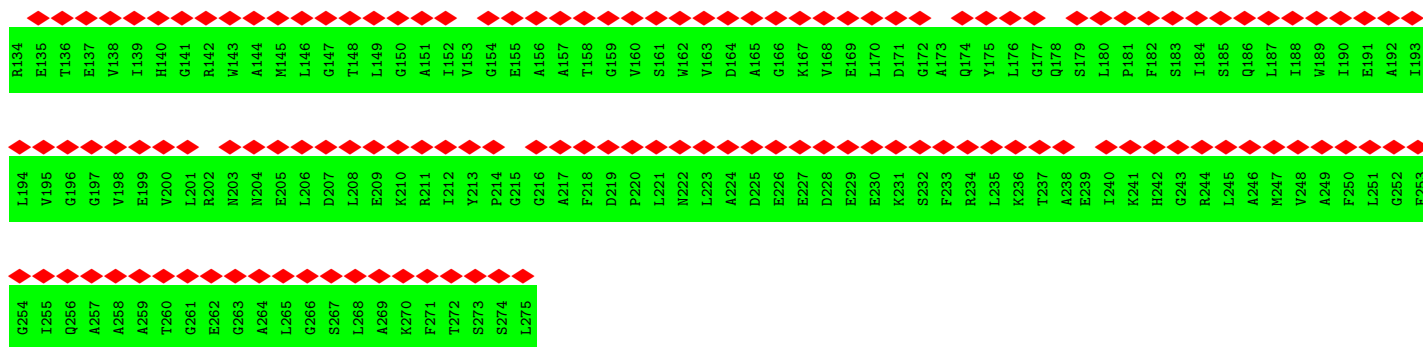


• Molecule 21: LHCII M2

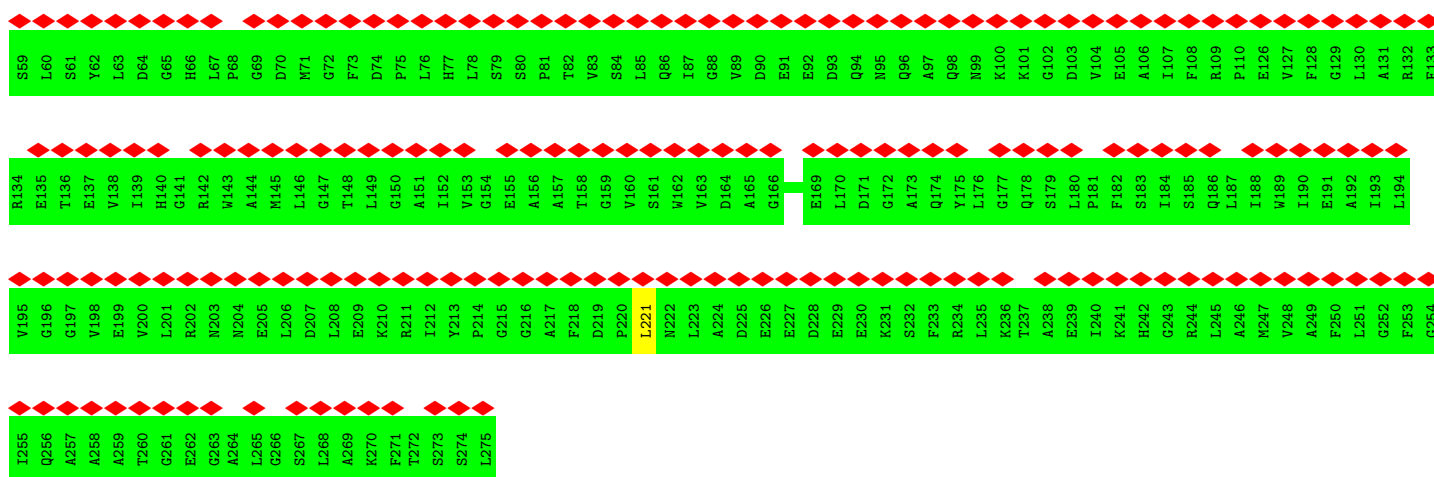
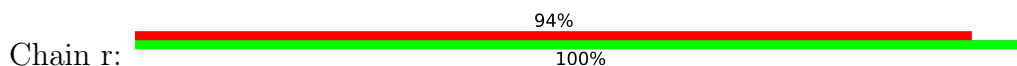


• Molecule 22: CP29

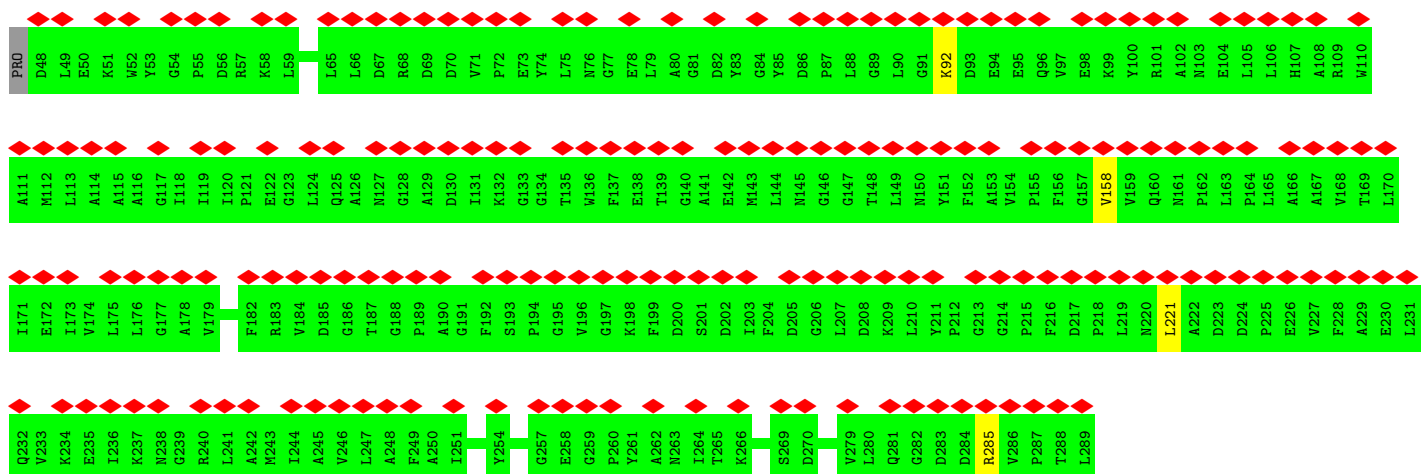
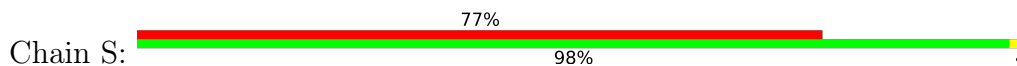




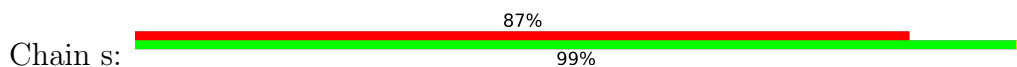
• Molecule 22: CP29

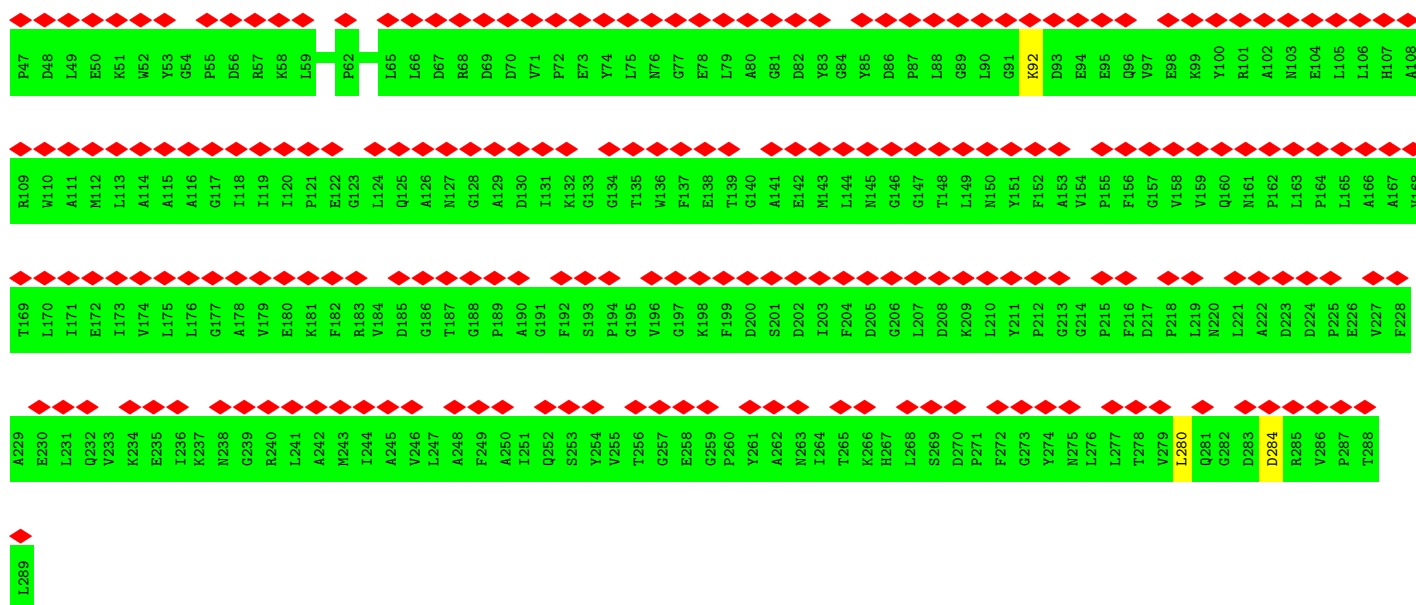


• Molecule 23: CP26

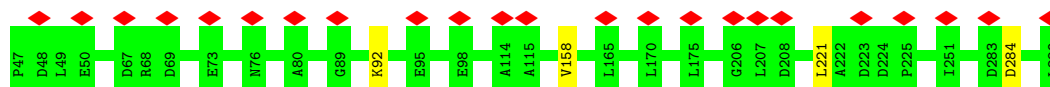


• Molecule 23: CP26

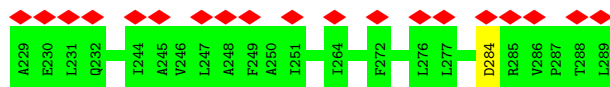
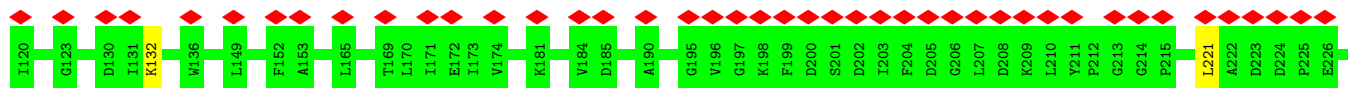
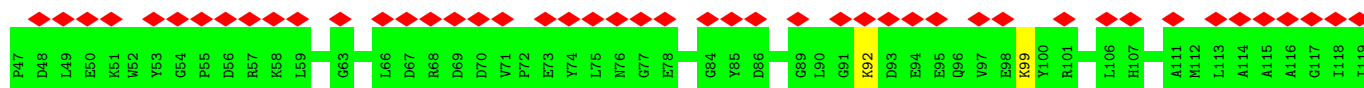
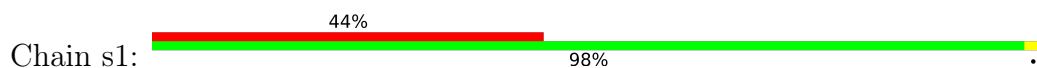




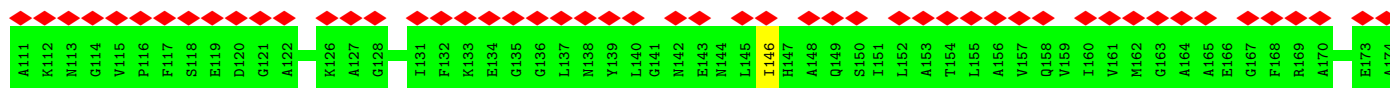
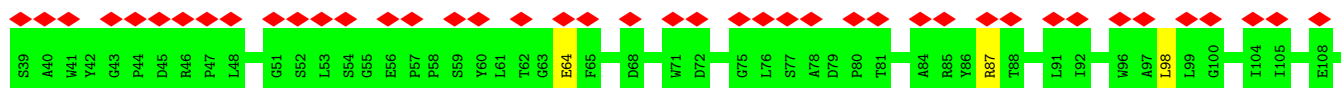
• Molecule 23: CP26

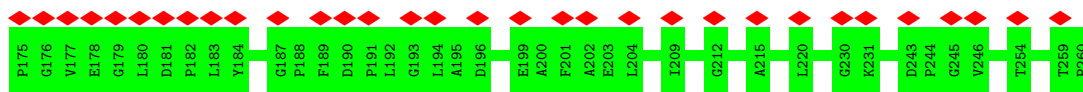


• Molecule 23: CP26



• Molecule 24: LHCII M1

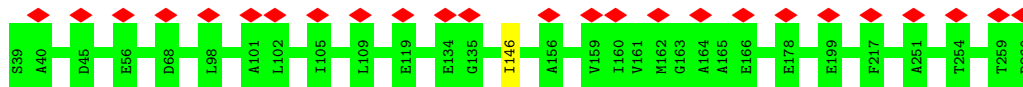




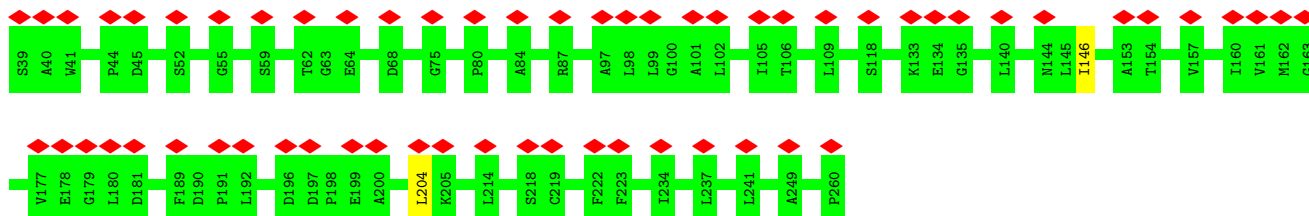
- Molecule 24: LHCII M1



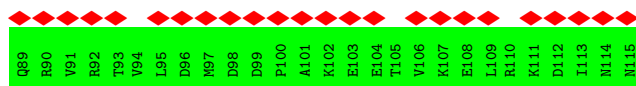
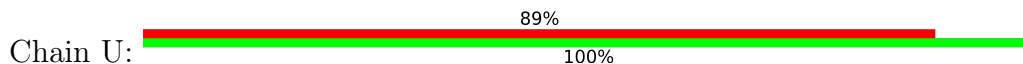
- Molecule 24: LHCII M1



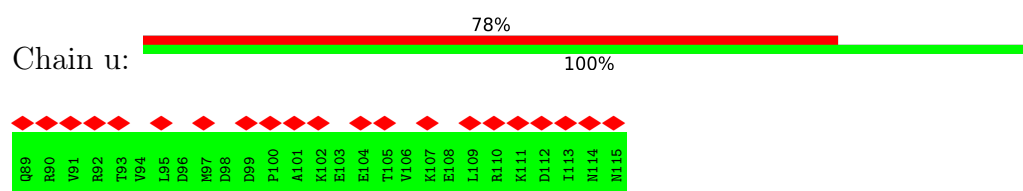
- Molecule 24: LHCII M1



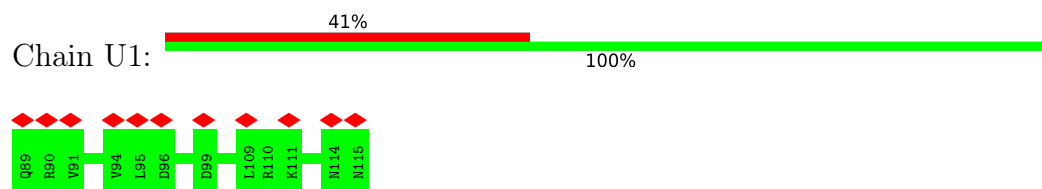
- Molecule 25: PsbU



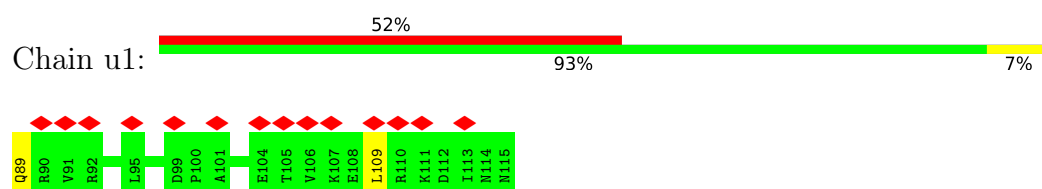
- Molecule 25: PsbU



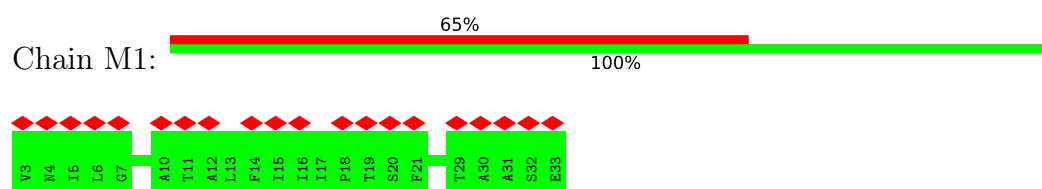
- Molecule 25: PsbU



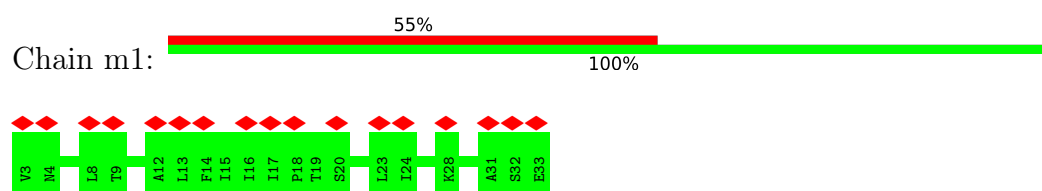
- Molecule 25: PsbU



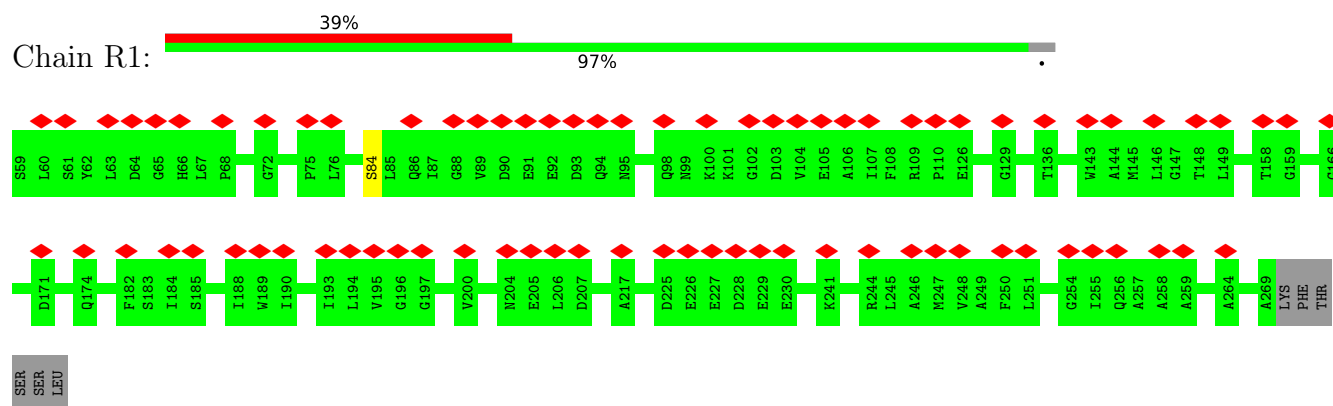
- Molecule 26: Photosystem II reaction center protein M



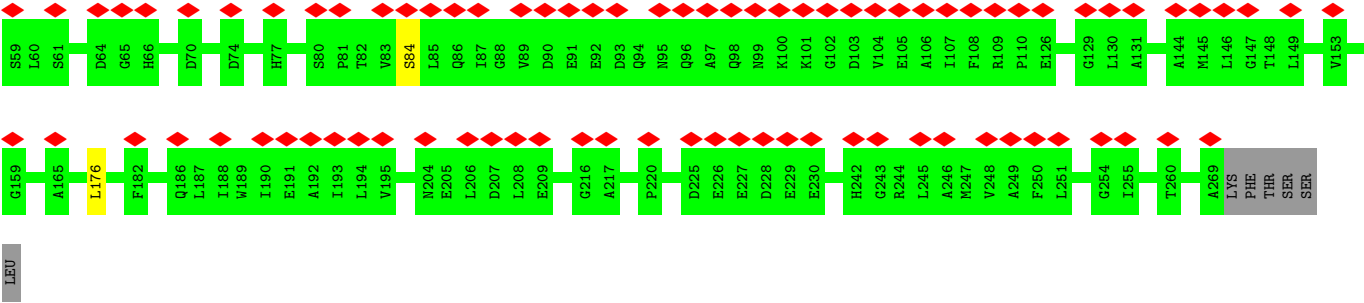
- Molecule 26: Photosystem II reaction center protein M



- Molecule 27: CP29



- Molecule 27: CP29



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14307	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0175	Depositor
Map size ( $\text{\AA}$ )	460.8, 460.8, 460.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.96, 0.96, 0.96	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SPH, DGA, RRX, C7Z, LHG, SEP, NA, PTY, CLA, OEX, NEX, LUT, LMK, BCR, 4RF, HEM, LMG, PL9, PHO, LPX, GOL, LMT, DGD, XAT, CL, ERG, CHL, SQD, FE2, BCT, 3PH

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	0.33	0/2723	0.61	1/3715 (0.0%)
1	A1	0.31	0/2723	0.59	1/3715 (0.0%)
1	a	0.35	0/2723	0.63	1/3715 (0.0%)
1	a1	0.31	1/2723 (0.0%)	0.59	3/3715 (0.1%)
2	B	0.40	2/3912 (0.1%)	0.66	6/5327 (0.1%)
2	B1	0.29	0/3912	0.56	2/5327 (0.0%)
2	b	0.31	0/3912	0.59	0/5327
2	b1	0.29	0/3912	0.56	0/5327
3	V	0.26	0/228	0.58	0/311
3	V1	0.25	0/228	0.65	0/311
3	v	0.28	0/228	0.57	0/311
3	v1	0.24	0/228	0.58	0/311
4	C	0.32	0/3602	0.59	1/4913 (0.0%)
4	C1	0.29	0/3602	0.55	0/4913
4	c	0.43	1/3602 (0.0%)	0.74	6/4913 (0.1%)
4	c1	0.32	0/3602	0.57	1/4913 (0.0%)
5	D	0.32	0/2860	0.62	1/3899 (0.0%)
5	D1	0.30	0/2860	0.59	1/3899 (0.0%)
5	d	0.33	0/2860	0.62	3/3899 (0.1%)
5	d1	0.30	0/2860	0.58	2/3899 (0.1%)
6	E	0.30	0/639	0.57	0/870
6	E1	0.27	0/639	0.53	0/870
6	e	0.30	0/639	0.59	0/870
6	e1	0.26	0/639	0.51	0/870
7	F	0.28	0/259	0.59	0/351
7	F1	0.29	0/259	0.53	0/351
7	f	0.27	0/259	0.54	0/351
7	f1	0.25	0/259	0.49	0/351
8	H	6.04	6/513 (1.2%)	0.91	5/703 (0.7%)
8	H1	0.26	0/513	0.60	0/703
8	h	0.31	0/513	0.66	1/703 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	h1	0.28	0/513	0.56	0/703
9	I	0.31	0/287	0.60	0/386
9	I1	0.35	0/287	0.66	0/386
9	i	0.32	0/287	0.65	0/386
9	i1	0.27	0/287	0.50	0/386
10	J	0.26	0/272	0.54	0/369
10	J1	0.26	0/272	0.55	0/369
10	j	0.26	0/272	0.50	0/369
10	j1	0.27	0/272	0.56	0/369
11	K	0.36	0/308	0.69	1/423 (0.2%)
11	K1	0.32	0/308	0.65	1/423 (0.2%)
11	k	0.36	0/308	0.66	0/423
11	k1	0.37	0/308	0.63	0/423
12	L	0.43	0/321	0.73	1/435 (0.2%)
12	L1	0.29	0/321	0.64	0/435
12	l	0.31	0/321	0.55	0/435
13	M	0.29	0/246	0.55	0/335
13	m	0.29	0/246	0.66	0/335
14	O	0.30	0/1855	0.64	3/2505 (0.1%)
14	O1	0.28	0/1855	0.64	3/2505 (0.1%)
14	o	0.29	0/1855	0.61	2/2505 (0.1%)
14	o1	0.29	0/1855	0.66	3/2505 (0.1%)
15	P	0.28	0/1473	0.56	0/1988
15	P1	0.27	0/1473	0.57	0/1988
15	p	0.26	0/1473	0.51	0/1988
15	p1	0.26	0/1473	0.54	0/1988
16	T	0.30	0/254	0.57	0/342
16	T1	0.29	0/254	0.56	0/342
16	t	0.32	0/254	0.62	0/342
16	t1	0.29	0/254	0.65	0/342
17	W	0.29	0/339	0.54	0/460
17	W1	0.26	0/339	0.60	1/460 (0.2%)
17	w	0.28	0/339	0.52	0/460
17	w1	0.25	0/339	0.52	0/460
18	X	0.25	0/202	0.53	0/276
18	X1	0.28	0/202	0.49	0/276
18	x	0.28	0/202	0.58	0/276
18	x1	0.28	0/202	0.42	0/276
19	Z	0.29	0/469	0.58	0/641
19	Z1	0.26	0/469	0.48	0/641
19	z	0.27	0/469	0.46	0/641
19	z1	0.28	0/469	0.48	0/641
20	N	0.31	0/1751	0.60	0/2386

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	N1	0.30	0/1751	0.55	0/2386
20	n	0.33	0/1751	0.67	2/2386 (0.1%)
20	n1	0.27	0/1750	0.52	0/2382
21	G	0.31	0/1725	0.62	1/2348 (0.0%)
21	G1	0.28	0/1725	0.54	0/2348
21	g	0.31	0/1725	0.59	2/2348 (0.1%)
21	g1	0.28	0/1725	0.54	0/2348
22	R	0.27	0/1561	0.57	0/2110
22	r	0.28	0/1561	0.59	1/2110 (0.0%)
23	S	0.30	0/1895	0.59	1/2579 (0.0%)
23	S1	0.27	0/1903	0.56	1/2590 (0.0%)
23	s	0.28	0/1902	0.57	1/2587 (0.0%)
23	s1	0.27	0/1903	0.54	1/2590 (0.0%)
24	Y	0.38	0/1715	0.71	3/2338 (0.1%)
24	Y1	0.32	0/1715	0.56	0/2338
24	y	0.45	2/1715 (0.1%)	0.75	4/2338 (0.2%)
24	y1	0.28	0/1715	0.54	1/2338 (0.0%)
25	U	0.25	0/224	0.66	0/298
25	U1	0.30	0/224	0.61	0/298
25	u	0.32	0/224	0.79	0/298
25	u1	0.30	0/224	0.70	1/298 (0.3%)
26	M1	0.27	0/237	0.57	0/323
26	m1	0.27	0/237	0.48	0/323
27	R1	0.26	0/1506	0.52	0/2035
27	r1	0.27	0/1506	0.59	1/2035 (0.0%)
All	All	0.50	12/118105 (0.0%)	0.60	70/160649 (0.0%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	57	PHE	CE2-CZ	63.39	2.57	1.37
8	H	57	PHE	CD2-CE2	62.87	2.65	1.39
8	H	57	PHE	CE1-CZ	62.87	2.56	1.37
8	H	57	PHE	CD1-CE1	61.06	2.61	1.39
8	H	57	PHE	CG-CD2	38.86	1.97	1.38

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	185	PRO	N-CD-CG	-17.70	76.65	103.20
4	c	374	PRO	N-CD-CG	-16.63	78.26	103.20
2	B	88	PRO	N-CD-CG	-13.67	82.69	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	185	PRO	CA-CB-CG	-11.49	82.17	104.00
2	B	50	PRO	CA-N-CD	-10.86	96.29	111.50

There are no chirality outliers.

There are no planarity outliers.

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/336 (100%)	304 (91%)	30 (9%)	1 (0%)	37	71
1	A1	335/336 (100%)	313 (93%)	22 (7%)	0	100	100
1	a	335/336 (100%)	313 (93%)	22 (7%)	0	100	100
1	a1	335/336 (100%)	316 (94%)	19 (6%)	0	100	100
2	B	482/484 (100%)	460 (95%)	21 (4%)	1 (0%)	44	76
2	B1	482/484 (100%)	459 (95%)	23 (5%)	0	100	100
2	b	482/484 (100%)	454 (94%)	28 (6%)	0	100	100
2	b1	482/484 (100%)	462 (96%)	20 (4%)	0	100	100
3	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	V1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	v	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	410 (92%)	34 (8%)	3 (1%)	19	55
4	C1	447/449 (100%)	427 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	c	447/449 (100%)	413 (92%)	31 (7%)	3 (1%)	19	55
4	c1	447/449 (100%)	425 (95%)	22 (5%)	0	100	100
5	D	346/348 (99%)	330 (95%)	15 (4%)	1 (0%)	37	71
5	D1	346/348 (99%)	332 (96%)	14 (4%)	0	100	100
5	d	346/348 (99%)	332 (96%)	13 (4%)	1 (0%)	37	71
5	d1	346/348 (99%)	331 (96%)	15 (4%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	E1	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
6	e	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
6	e1	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	F1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
7	f1	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	H1	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	h	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
8	h1	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	I1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
9	i1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
10	J	34/36 (94%)	34 (100%)	0	0	100	100
10	J1	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
10	j1	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
11	K1	35/37 (95%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	k1	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L1	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	30/32 (94%)	29 (97%)	0	1 (3%)	3	25
13	m	30/32 (94%)	28 (93%)	1 (3%)	1 (3%)	3	25
14	O	236/238 (99%)	210 (89%)	25 (11%)	1 (0%)	30	66
14	O1	236/238 (99%)	214 (91%)	21 (9%)	1 (0%)	30	66
14	o	236/238 (99%)	215 (91%)	20 (8%)	1 (0%)	30	66
14	o1	236/238 (99%)	217 (92%)	18 (8%)	1 (0%)	30	66
15	P	185/187 (99%)	167 (90%)	17 (9%)	1 (0%)	25	61
15	P1	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
15	p1	185/187 (99%)	171 (92%)	14 (8%)	0	100	100
16	T	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	3	24
16	T1	28/30 (93%)	27 (96%)	0	1 (4%)	3	24
16	t	28/30 (93%)	27 (96%)	0	1 (4%)	3	24
16	t1	28/30 (93%)	28 (100%)	0	0	100	100
17	W	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
17	W1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	X1	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
18	x1	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	Z1	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
19	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
19	z1	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	25	61
20	N1	220/222 (99%)	201 (91%)	18 (8%)	1 (0%)	25	61
20	n	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	n1	218/222 (98%)	198 (91%)	19 (9%)	1 (0%)	25	61
21	G	219/221 (99%)	203 (93%)	15 (7%)	1 (0%)	25	61
21	G1	219/221 (99%)	201 (92%)	18 (8%)	0	100	100
21	g	219/221 (99%)	209 (95%)	9 (4%)	1 (0%)	25	61
21	g1	219/221 (99%)	202 (92%)	17 (8%)	0	100	100
22	R	198/202 (98%)	188 (95%)	10 (5%)	0	100	100
22	r	198/202 (98%)	181 (91%)	17 (9%)	0	100	100
23	S	240/243 (99%)	218 (91%)	20 (8%)	2 (1%)	16	53
23	S1	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	11	43
23	s	239/243 (98%)	219 (92%)	18 (8%)	2 (1%)	16	53
23	s1	241/243 (99%)	219 (91%)	20 (8%)	2 (1%)	16	53
24	Y	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	25	61
24	Y1	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	25	61
24	y	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	25	61
24	y1	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	25	61
25	U	25/27 (93%)	25 (100%)	0	0	100	100
25	U1	25/27 (93%)	25 (100%)	0	0	100	100
25	u	25/27 (93%)	25 (100%)	0	0	100	100
25	u1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
26	M1	29/31 (94%)	29 (100%)	0	0	100	100
26	m1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
27	R1	191/202 (95%)	183 (96%)	8 (4%)	0	100	100
27	r1	191/202 (95%)	181 (95%)	10 (5%)	0	100	100
All	All	14651/14872 (98%)	13772 (94%)	839 (6%)	40 (0%)	38	71

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	257	GLU
4	C	395	VAL
14	O	94	VAL
4	c	257	GLU
4	c	395	VAL

### 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	276/275 (100%)	276 (100%)	0	100	100
1	A1	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	275 (100%)	1 (0%)	89	91
1	a1	276/275 (100%)	276 (100%)	0	100	100
2	B	388/388 (100%)	387 (100%)	1 (0%)	91	92
2	B1	388/388 (100%)	388 (100%)	0	100	100
2	b	388/388 (100%)	388 (100%)	0	100	100
2	b1	388/388 (100%)	386 (100%)	2 (0%)	86	89
3	V	25/25 (100%)	25 (100%)	0	100	100
3	V1	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
3	v1	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	349 (100%)	1 (0%)	91	92
4	C1	350/350 (100%)	349 (100%)	1 (0%)	91	92
4	c	350/350 (100%)	350 (100%)	0	100	100
4	c1	350/350 (100%)	348 (99%)	2 (1%)	84	88
5	D	279/279 (100%)	278 (100%)	1 (0%)	89	91
5	D1	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	278 (100%)	1 (0%)	89	91
5	d1	279/279 (100%)	278 (100%)	1 (0%)	89	91
6	E	68/68 (100%)	68 (100%)	0	100	100
6	E1	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
6	e1	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	F1	25/25 (100%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	f	25/25 (100%)	25 (100%)	0	100	100
7	f1	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	H1	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
8	h1	56/56 (100%)	55 (98%)	1 (2%)	54	71
9	I	31/31 (100%)	31 (100%)	0	100	100
9	I1	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
9	i1	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	J1	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
10	j1	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	K1	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
11	k1	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	L1	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	27/27 (100%)	27 (100%)	0	100	100
13	m	27/27 (100%)	27 (100%)	0	100	100
14	O	195/195 (100%)	194 (100%)	1 (0%)	86	89
14	O1	195/195 (100%)	195 (100%)	0	100	100
14	o	195/195 (100%)	194 (100%)	1 (0%)	86	89
14	o1	195/195 (100%)	195 (100%)	0	100	100
15	P	151/151 (100%)	150 (99%)	1 (1%)	81	86
15	P1	151/151 (100%)	150 (99%)	1 (1%)	81	86
15	p	151/151 (100%)	151 (100%)	0	100	100
15	p1	151/151 (100%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	T	26/26 (100%)	26 (100%)	0	100	100
16	T1	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
16	t1	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	33 (97%)	1 (3%)	37	58
17	W1	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
17	w1	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	X1	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
18	x1	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	Z1	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
19	z1	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	170 (99%)	1 (1%)	84	88
20	N1	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	170 (99%)	1 (1%)	84	88
20	n1	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	167 (99%)	1 (1%)	84	88
21	G1	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
21	g1	168/168 (100%)	168 (100%)	0	100	100
22	R	158/158 (100%)	158 (100%)	0	100	100
22	r	158/158 (100%)	158 (100%)	0	100	100
23	S	189/190 (100%)	188 (100%)	1 (0%)	86	89
23	S1	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
23	s1	190/190 (100%)	188 (99%)	2 (1%)	70	80
24	Y	167/167 (100%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Y1	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
24	y1	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	U1	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
25	u1	26/26 (100%)	25 (96%)	1 (4%)	28	51
26	M1	26/26 (100%)	26 (100%)	0	100	100
26	m1	26/26 (100%)	26 (100%)	0	100	100
27	R1	151/157 (96%)	151 (100%)	0	100	100
27	r1	151/157 (96%)	151 (100%)	0	100	100
All	All	11856/11865 (100%)	11832 (100%)	24 (0%)	91	93

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	P1	228	LYS
4	c1	384	MET
2	b1	418	LYS
4	c1	406	ASN
20	N	83	LYS

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

Mol	Chain	Res	Type
1	a1	26	ASN
4	c1	429	HIS
1	a1	181	ASN
3	v1	8	GLN
5	d1	336	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
27	SEP	R1	84	27	8,9,10	1.56	1 (12%)	8,12,14	1.86	2 (25%)
27	SEP	r1	84	27	8,9,10	1.55	1 (12%)	8,12,14	1.26	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SEP	R1	84	27	-	3/5/8/10	-
27	SEP	r1	84	27	-	3/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	r1	84	SEP	P-O1P	3.40	1.61	1.50
27	R1	84	SEP	P-O1P	3.37	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R1	84	SEP	OG-CB-CA	3.54	111.59	108.14
27	R1	84	SEP	P-OG-CB	-3.40	108.92	118.30
27	r1	84	SEP	P-OG-CB	-2.20	112.25	118.30

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	R1	84	SEP	CB-OG-P-O1P
27	R1	84	SEP	CB-OG-P-O2P
27	R1	84	SEP	CB-OG-P-O3P
27	r1	84	SEP	CB-OG-P-O2P
27	r1	84	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 703 ligands modelled in this entry, 16 are monoatomic - leaving 687 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	$\# Z  > 2$
31	CLA	C	509	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	17 (22%)
31	CLA	N1	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.07	19 (25%)
41	LHG	D	410	-	38,38,48	0.44	0	41,44,54	1.03	2 (4%)
48	LUT	y	621	-	42,43,43	2.30	1 (2%)	51,60,60	2.02	12 (23%)
31	CLA	G1	614	-	49,57,73	1.56	9 (18%)	55,93,113	2.26	15 (27%)
47	CHL	s	606	-	44,52,74	1.02	3 (6%)	46,87,114	1.42	9 (19%)
39	GOL	b	625	-	5,5,5	0.58	0	5,5,5	0.31	0
52	3PH	s1	626	-	47,47,47	0.88	4 (8%)	51,52,52	4.43	4 (7%)
49	XAT	g1	622	-	39,47,47	0.71	1 (2%)	54,74,74	1.80	13 (24%)
47	CHL	y	605	24	46,54,74	0.98	2 (4%)	49,90,114	1.37	11 (22%)
48	LUT	n	620	-	42,43,43	2.36	1 (2%)	51,60,60	2.11	13 (25%)
31	CLA	C1	503	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	17 (22%)
47	CHL	N1	608	-	50,58,74	0.94	3 (6%)	52,94,114	1.48	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	c	507	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	18 (23%)
49	XAT	n1	622	-	39,47,47	0.70	1 (2%)	54,74,74	1.88	14 (25%)
35	LMG	B1	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.12	3 (5%)
31	CLA	S1	610	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	20 (26%)
47	CHL	S1	601	23	46,54,74	1.01	3 (6%)	49,90,114	1.37	7 (14%)
33	BCR	A1	411	-	41,41,41	1.82	4 (9%)	56,56,56	4.39	15 (26%)
31	CLA	G	614	-	49,57,73	1.54	7 (14%)	55,93,113	2.30	18 (32%)
50	NEX	G	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.84	11 (22%)
31	CLA	b1	609	-	65,73,73	1.37	8 (12%)	76,113,113	2.07	18 (23%)
41	LHG	c	625	-	46,46,48	0.41	0	49,52,54	1.03	4 (8%)
31	CLA	y	614	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	16 (21%)
31	CLA	c1	508	-	65,73,73	1.32	7 (10%)	76,113,113	1.97	14 (18%)
47	CHL	g	609	-	66,74,74	0.87	3 (4%)	73,114,114	1.16	10 (13%)
49	XAT	g	622	-	39,47,47	0.68	1 (2%)	54,74,74	1.96	14 (25%)
49	XAT	r1	621	-	39,47,47	0.67	1 (2%)	54,74,74	1.92	16 (29%)
31	CLA	Y1	614	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	18 (23%)
31	CLA	y	610	-	65,73,73	1.36	8 (12%)	76,113,113	2.04	19 (25%)
31	CLA	d	403	-	65,73,73	1.38	7 (10%)	76,113,113	1.99	15 (19%)
31	CLA	s1	613	-	55,63,73	1.50	9 (16%)	64,101,113	2.13	15 (23%)
43	BCT	D1	401	-	2,3,3	1.24	0	2,3,3	4.24	2 (100%)
35	LMG	w1	201	-	39,39,55	0.86	2 (5%)	47,47,63	1.20	3 (6%)
38	DGA	b1	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.47	3 (6%)
47	CHL	n1	606	-	66,74,74	0.85	3 (4%)	73,114,114	1.17	9 (12%)
47	CHL	g	608	-	44,52,74	0.99	3 (6%)	46,87,114	1.51	10 (21%)
34	SQD	C	526	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
31	CLA	c	510	-	65,73,73	1.34	9 (13%)	76,113,113	2.04	18 (23%)
31	CLA	C	503	-	65,73,73	1.37	9 (13%)	76,113,113	1.99	17 (22%)
31	CLA	c	501	-	65,73,73	1.35	9 (13%)	76,113,113	2.01	17 (22%)
31	CLA	S1	609	-	60,68,73	1.41	10 (16%)	70,107,113	2.09	18 (25%)
31	CLA	r	611	-	46,54,73	1.62	10 (21%)	53,90,113	2.14	14 (26%)
31	CLA	R1	602	-	60,68,73	1.40	8 (13%)	70,107,113	2.13	18 (25%)
33	BCR	d	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.14	17 (30%)
31	CLA	G1	602	-	65,73,73	1.34	7 (10%)	76,113,113	2.04	17 (22%)
31	CLA	G1	604	-	49,57,73	1.56	9 (18%)	55,93,113	2.22	18 (32%)
31	CLA	s1	604	-	55,63,73	1.49	10 (18%)	64,101,113	2.17	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	B1	605	-	65,73,73	1.32	7 (10%)	76,113,113	2.10	19 (25%)
31	CLA	R1	609	-	60,68,73	1.39	8 (13%)	70,107,113	4.52	21 (30%)
34	SQD	b	621	-	53,54,54	0.80	0	62,65,65	0.89	2 (3%)
31	CLA	C1	506	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	18 (23%)
47	CHL	r	606	-	44,52,74	1.04	3 (6%)	46,87,114	1.32	7 (15%)
31	CLA	a	406	-	65,73,73	1.32	6 (9%)	76,113,113	2.05	16 (21%)
41	LHG	s	624	-	44,44,48	0.41	0	47,50,54	1.11	3 (6%)
52	3PH	b1	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.16	2 (3%)
31	CLA	R1	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.33	13 (23%)
31	CLA	S1	612	-	45,53,73	1.60	7 (15%)	52,89,113	2.22	14 (26%)
31	CLA	B1	611	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	18 (23%)
35	LMG	C	521	-	51,51,55	1.06	6 (11%)	59,59,63	1.08	4 (6%)
31	CLA	c	509	-	65,73,73	1.37	7 (10%)	76,113,113	1.99	15 (19%)
31	CLA	B1	604	-	65,73,73	1.38	9 (13%)	76,113,113	1.90	16 (21%)
41	LHG	C	525	-	46,46,48	0.39	0	49,52,54	1.07	2 (4%)
31	CLA	n1	610	-	65,73,73	1.34	7 (10%)	76,113,113	2.03	19 (25%)
44	PL9	D	405	-	55,55,55	1.27	4 (7%)	68,69,69	1.56	13 (19%)
47	CHL	R	607	-	50,58,74	0.94	2 (4%)	52,94,114	1.37	8 (15%)
52	3PH	t1	101	-	47,47,47	0.87	4 (8%)	51,52,52	1.11	2 (3%)
48	LUT	y	620	-	42,43,43	2.33	1 (2%)	51,60,60	2.14	15 (29%)
44	PL9	d1	405	-	55,55,55	1.07	2 (3%)	68,69,69	1.57	12 (17%)
41	LHG	s1	624	-	44,44,48	0.41	0	47,50,54	1.02	3 (6%)
31	CLA	y1	612	-	65,73,73	1.35	9 (13%)	76,113,113	1.97	16 (21%)
33	BCR	b	619	-	41,41,41	1.87	4 (9%)	56,56,56	4.43	19 (33%)
31	CLA	y1	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.96	16 (21%)
40	DGD	C	520	-	60,60,67	1.07	6 (10%)	74,74,81	0.99	2 (2%)
41	LHG	N1	624	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
42	LMK	C	527	-	38,39,53	1.49	2 (5%)	41,46,60	1.27	2 (4%)
31	CLA	c1	512	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	18 (23%)
31	CLA	r1	603	-	60,68,73	1.43	8 (13%)	70,107,113	2.00	15 (21%)
41	LHG	c1	525	-	46,46,48	0.39	0	49,52,54	1.02	3 (6%)
47	CHL	Y	601	-	66,74,74	0.83	2 (3%)	73,114,114	1.20	10 (13%)
31	CLA	S	613	-	55,63,73	1.49	8 (14%)	64,101,113	2.34	18 (28%)
33	BCR	D1	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	16 (28%)
49	XAT	Y1	622	-	39,47,47	0.69	1 (2%)	54,74,74	3.76	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	CHL	n	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.37	8 (15%)
31	CLA	b	609	-	65,73,73	1.41	9 (13%)	76,113,113	2.09	18 (23%)
47	CHL	g1	609	-	66,74,74	0.85	2 (3%)	73,114,114	1.14	10 (13%)
31	CLA	r	612	-	60,68,73	1.43	9 (15%)	70,107,113	1.98	15 (21%)
31	CLA	g	611	-	45,53,73	1.62	8 (17%)	52,89,113	2.26	15 (28%)
41	LHG	D	409	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
33	BCR	c1	516	-	41,41,41	1.85	4 (9%)	56,56,56	4.44	16 (28%)
35	LMG	H	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.08	2 (3%)
44	PL9	D1	405	-	55,55,55	0.99	5 (9%)	68,69,69	1.60	10 (14%)
52	3PH	s	626	-	47,47,47	0.86	4 (8%)	51,52,52	1.12	2 (3%)
31	CLA	S	612	-	45,53,73	1.63	8 (17%)	52,89,113	2.14	13 (25%)
34	SQD	b1	621	-	41,42,54	0.88	0	50,53,65	0.96	2 (4%)
31	CLA	y1	614	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	17 (22%)
31	CLA	y	613	-	65,73,73	1.34	8 (12%)	76,113,113	2.02	17 (22%)
47	CHL	G	608	-	44,52,74	1.01	3 (6%)	46,87,114	1.46	9 (19%)
31	CLA	y	602	-	65,73,73	1.32	8 (12%)	76,113,113	2.12	20 (26%)
50	NEX	y1	623	-	38,46,46	3.30	9 (23%)	50,70,70	1.97	13 (26%)
31	CLA	c1	503	-	65,73,73	1.37	8 (12%)	76,113,113	2.06	20 (26%)
49	XAT	G1	622	-	39,47,47	0.71	1 (2%)	54,74,74	1.88	14 (25%)
31	CLA	b	612	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	18 (23%)
44	PL9	d	405	-	55,55,55	1.26	6 (10%)	68,69,69	1.50	11 (16%)
31	CLA	B	612	-	65,73,73	1.36	7 (10%)	76,113,113	1.94	15 (19%)
31	CLA	B	611	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	17 (22%)
31	CLA	C1	510	-	65,73,73	1.36	7 (10%)	76,113,113	1.94	16 (21%)
45	HEM	F	101	7,6	41,50,50	1.51	3 (7%)	45,82,82	1.55	8 (17%)
47	CHL	g1	608	-	44,52,74	1.02	3 (6%)	46,87,114	1.37	9 (19%)
31	CLA	C1	504	-	65,73,73	1.34	7 (10%)	76,113,113	2.06	15 (19%)
31	CLA	B1	613	-	65,73,73	1.34	8 (12%)	76,113,113	1.94	15 (19%)
31	CLA	s1	611	-	65,73,73	1.39	8 (12%)	76,113,113	1.99	19 (25%)
31	CLA	c1	509	-	65,73,73	1.34	6 (9%)	76,113,113	1.94	16 (21%)
31	CLA	y1	604	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	17 (22%)
40	DGD	c1	519	-	63,63,67	1.12	7 (11%)	77,77,81	0.98	5 (6%)
34	SQD	a1	412	-	50,51,54	0.81	0	59,62,65	0.91	2 (3%)
31	CLA	s	614	-	55,63,73	1.47	7 (12%)	64,101,113	2.22	16 (25%)
49	XAT	y	622	-	39,47,47	0.67	1 (2%)	54,74,74	3.73	19 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	Y	610	-	65,73,73	1.36	9 (13%)	76,113,113	2.03	18 (23%)
49	XAT	Y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.73	17 (31%)
31	CLA	B	604	-	65,73,73	1.38	9 (13%)	76,113,113	1.96	18 (23%)
31	CLA	C1	508	-	65,73,73	1.32	7 (10%)	76,113,113	1.99	18 (23%)
31	CLA	b1	602	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	16 (21%)
37	C7Z	b	620	-	43,43,43	5.42	26 (60%)	58,60,60	2.17	18 (31%)
47	CHL	s	601	23	46,54,74	1.02	4 (8%)	49,90,114	1.40	7 (14%)
41	LHG	L	101	-	48,48,48	0.40	0	51,54,54	0.96	2 (3%)
47	CHL	S1	608	-	61,69,74	0.88	3 (4%)	67,108,114	1.33	11 (16%)
31	CLA	C1	502	-	65,73,73	1.39	8 (12%)	76,113,113	1.94	15 (19%)
31	CLA	b	606	-	65,73,73	1.34	8 (12%)	76,113,113	2.05	14 (18%)
31	CLA	N1	612	-	45,53,73	1.62	8 (17%)	52,89,113	2.15	13 (25%)
31	CLA	G	604	-	49,57,73	1.58	9 (18%)	55,93,113	2.29	15 (27%)
31	CLA	N1	611	-	49,57,73	1.57	8 (16%)	55,93,113	2.20	14 (25%)
47	CHL	Y1	609	-	66,74,74	0.85	3 (4%)	73,114,114	1.28	13 (17%)
47	CHL	R1	606	-	44,52,74	1.04	2 (4%)	46,87,114	1.27	5 (10%)
47	CHL	G1	606	-	50,58,74	0.95	3 (6%)	52,94,114	1.38	8 (15%)
48	LUT	g1	621	-	42,43,43	2.38	1 (2%)	51,60,60	1.90	12 (23%)
31	CLA	g	612	-	43,51,73	1.68	9 (20%)	49,86,113	2.25	15 (30%)
47	CHL	G1	607	-	66,74,74	0.80	2 (3%)	73,114,114	1.18	9 (12%)
48	LUT	r1	620	-	42,43,43	2.37	1 (2%)	51,60,60	2.13	15 (29%)
40	DGD	C	523	-	67,67,67	1.18	7 (10%)	81,81,81	1.07	3 (3%)
47	CHL	y	606	-	66,74,74	0.87	3 (4%)	73,114,114	1.19	11 (15%)
50	NEX	r1	622	-	38,46,46	3.39	10 (26%)	50,70,70	1.74	11 (22%)
48	LUT	y1	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.08	13 (25%)
31	CLA	G	610	-	65,73,73	1.34	8 (12%)	76,113,113	2.07	18 (23%)
31	CLA	g1	614	-	49,57,73	1.57	9 (18%)	55,93,113	2.27	15 (27%)
31	CLA	d1	403	-	65,73,73	1.35	8 (12%)	76,113,113	2.06	18 (23%)
49	XAT	R1	621	-	39,47,47	0.64	1 (2%)	54,74,74	1.91	14 (25%)
47	CHL	g1	601	-	66,74,74	0.83	3 (4%)	73,114,114	1.21	9 (12%)
31	CLA	b1	607	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	17 (22%)
34	SQD	A	412	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)
47	CHL	G	606	-	50,58,74	0.99	3 (6%)	52,94,114	1.38	9 (17%)
31	CLA	c	504	-	65,73,73	1.31	6 (9%)	76,113,113	2.20	20 (26%)
31	CLA	S	609	-	60,68,73	1.42	10 (16%)	70,107,113	1.99	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	SQD	c1	526	-	53,54,54	0.79	0	62,65,65	0.90	3 (4%)
47	CHL	G	607	-	50,58,74	0.89	2 (4%)	52,94,114	1.45	10 (19%)
47	CHL	Y	609	-	66,74,74	0.83	3 (4%)	73,114,114	1.22	12 (16%)
48	LUT	g	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.09	12 (23%)
41	LHG	D1	408	-	43,43,48	0.41	0	46,49,54	1.07	4 (8%)
38	DGA	b	623	-	43,43,43	1.13	2 (4%)	45,45,45	1.52	3 (6%)
47	CHL	g	605	-	48,56,74	0.95	2 (4%)	51,92,114	1.39	11 (21%)
31	CLA	B	613	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	15 (19%)
31	CLA	s1	605	23	50,58,73	1.58	8 (16%)	58,95,113	2.28	17 (29%)
50	NEX	R1	622	-	38,46,46	3.29	9 (23%)	50,70,70	1.82	11 (22%)
47	CHL	N1	605	20	66,74,74	0.85	2 (3%)	73,114,114	1.25	11 (15%)
31	CLA	B1	615	-	65,73,73	1.37	10 (15%)	76,113,113	1.96	15 (19%)
52	3PH	T1	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.10	2 (3%)
33	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.22	12 (21%)
31	CLA	B1	609	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	18 (23%)
34	SQD	c	626	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
40	DGD	c1	518	-	56,56,67	1.01	4 (7%)	70,70,81	0.97	3 (4%)
31	CLA	y1	610	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
31	CLA	R	613	-	46,54,73	1.61	9 (19%)	53,90,113	2.22	15 (28%)
34	SQD	M1	101	-	41,42,54	0.89	0	50,53,65	0.96	2 (4%)
31	CLA	n1	612	-	45,53,73	1.64	9 (20%)	52,89,113	2.09	14 (26%)
33	BCR	C	515	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	16 (28%)
41	LHG	D1	409	-	48,48,48	0.39	0	51,54,54	1.10	5 (9%)
32	PHO	a	408	-	51,69,69	1.02	4 (7%)	47,99,99	1.18	5 (10%)
47	CHL	Y1	606	-	66,74,74	0.86	3 (4%)	73,114,114	1.16	7 (9%)
31	CLA	B1	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.96	15 (19%)
47	CHL	R1	607	-	50,58,74	0.94	2 (4%)	52,94,114	1.39	10 (19%)
31	CLA	Y1	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	18 (23%)
48	LUT	G	621	-	42,43,43	2.38	1 (2%)	51,60,60	2.07	16 (31%)
31	CLA	s1	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.08	17 (22%)
41	LHG	S1	624	-	44,44,48	0.41	0	47,50,54	1.11	4 (8%)
31	CLA	S1	603	-	65,73,73	1.37	8 (12%)	76,113,113	2.10	19 (25%)
31	CLA	n	611	-	49,57,73	1.59	9 (18%)	55,93,113	2.31	16 (29%)
31	CLA	r1	604	-	49,57,73	1.54	8 (16%)	55,93,113	2.31	16 (29%)
31	CLA	n	604	-	65,73,73	1.32	6 (9%)	76,113,113	2.14	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	BCR	c1	515	-	41,41,41	1.88	5 (12%)	56,56,56	4.30	16 (28%)
48	LUT	N1	620	-	42,43,43	2.40	1 (2%)	51,60,60	1.89	10 (19%)
31	CLA	N1	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.05	17 (22%)
31	CLA	c1	505	-	65,73,73	1.39	9 (13%)	76,113,113	1.92	15 (19%)
38	DGA	j1	101	-	28,28,43	1.29	3 (10%)	30,30,45	1.30	2 (6%)
41	LHG	y	624	-	48,48,48	0.38	0	51,54,54	1.08	3 (5%)
47	CHL	y	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.25	9 (12%)
52	3PH	i	101	-	47,47,47	0.86	4 (8%)	51,52,52	1.18	2 (3%)
32	PHO	A1	408	-	51,69,69	0.99	4 (7%)	47,99,99	1.12	5 (10%)
31	CLA	S1	604	-	55,63,73	1.47	7 (12%)	64,101,113	2.26	18 (28%)
31	CLA	A1	405	-	65,73,73	1.40	8 (12%)	76,113,113	2.15	23 (30%)
31	CLA	Y1	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	16 (21%)
40	DGD	C	519	-	63,63,67	1.12	6 (9%)	77,77,81	1.09	5 (6%)
48	LUT	n1	620	-	42,43,43	2.43	1 (2%)	51,60,60	1.80	13 (25%)
31	CLA	r	609	-	60,68,73	1.41	7 (11%)	70,107,113	2.03	17 (24%)
47	CHL	y1	609	-	66,74,74	0.83	3 (4%)	73,114,114	1.22	10 (13%)
28	OEX	A	401	4,1	0,15,15	-	-	-	-	-
31	CLA	C	507	-	65,73,73	1.37	8 (12%)	76,113,113	1.94	18 (23%)
48	LUT	G1	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.14	12 (23%)
31	CLA	g	614	-	49,57,73	1.56	8 (16%)	55,93,113	2.28	17 (30%)
31	CLA	c1	504	-	65,73,73	1.35	7 (10%)	76,113,113	2.04	17 (22%)
33	BCR	B1	618	-	41,41,41	1.88	4 (9%)	56,56,56	4.50	18 (32%)
48	LUT	G1	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.05	10 (19%)
31	CLA	n	602	-	65,73,73	1.34	7 (10%)	76,113,113	2.07	21 (27%)
38	DGA	C	524	-	43,43,43	1.12	3 (6%)	45,45,45	1.51	3 (6%)
47	CHL	G1	601	21	66,74,74	0.83	3 (4%)	73,114,114	1.30	14 (19%)
31	CLA	R	610	-	60,68,73	1.39	7 (11%)	70,107,113	2.12	21 (30%)
31	CLA	b	608	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	17 (22%)
35	LMG	b1	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.16	3 (5%)
35	LMG	c	521	-	51,51,55	1.08	5 (9%)	59,59,63	1.19	3 (5%)
31	CLA	g1	613	-	65,73,73	1.34	8 (12%)	76,113,113	2.03	18 (23%)
31	CLA	S1	605	-	50,58,73	1.56	9 (18%)	58,95,113	2.29	18 (31%)
52	3PH	S1	626	-	47,47,47	0.85	4 (8%)	51,52,52	4.44	4 (7%)
31	CLA	B	602	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	16 (21%)
48	LUT	g	620	-	42,43,43	2.38	1 (2%)	51,60,60	2.09	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	n1	611	-	49,57,73	1.56	9 (18%)	55,93,113	2.26	15 (27%)
31	CLA	n1	613	-	65,73,73	1.36	8 (12%)	76,113,113	2.09	18 (23%)
41	LHG	N	624	-	48,48,48	0.37	0	51,54,54	1.16	3 (5%)
47	CHL	N	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.33	11 (15%)
49	XAT	R	621	-	39,47,47	0.70	1 (2%)	54,74,74	2.03	14 (25%)
31	CLA	g1	612	-	43,51,73	1.67	8 (18%)	49,86,113	2.21	13 (26%)
31	CLA	B	609	-	65,73,73	1.38	8 (12%)	76,113,113	2.09	21 (27%)
31	CLA	N	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	18 (23%)
40	DGD	c	520	-	60,60,67	1.06	5 (8%)	74,74,81	1.02	2 (2%)
40	DGD	B1	623	-	44,44,67	0.84	1 (2%)	58,58,81	1.26	5 (8%)
31	CLA	C	501	-	65,73,73	1.35	9 (13%)	76,113,113	2.08	18 (23%)
46	RRX	h	101	-	42,42,42	4.90	24 (57%)	57,58,58	1.94	17 (29%)
31	CLA	c	506	-	65,73,73	1.38	8 (12%)	76,113,113	2.03	19 (25%)
31	CLA	Y	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	17 (22%)
31	CLA	g1	604	-	49,57,73	1.57	8 (16%)	55,93,113	2.22	19 (34%)
48	LUT	s1	620	-	42,43,43	2.38	1 (2%)	51,60,60	2.05	14 (27%)
47	CHL	s1	606	-	44,52,74	0.95	2 (4%)	46,87,114	1.44	9 (19%)
48	LUT	n	621	-	42,43,43	2.39	1 (2%)	51,60,60	2.00	12 (23%)
31	CLA	Y	611	-	65,73,73	1.36	7 (10%)	76,113,113	1.90	14 (18%)
34	SQD	B1	621	-	41,42,54	0.87	0	50,53,65	0.95	3 (6%)
31	CLA	C	505	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	16 (21%)
38	DGA	J1	101	-	28,28,43	1.30	3 (10%)	30,30,45	1.26	2 (6%)
41	LHG	d1	410	-	38,38,48	0.42	0	41,44,54	1.16	3 (7%)
35	LMG	a	413	-	48,48,55	1.01	5 (10%)	56,56,63	1.20	4 (7%)
47	CHL	y1	606	-	66,74,74	0.85	3 (4%)	73,114,114	1.17	11 (15%)
31	CLA	S1	614	-	55,63,73	1.47	7 (12%)	64,101,113	2.10	16 (25%)
43	BCT	d	401	29	2,3,3	1.26	0	2,3,3	4.15	2 (100%)
52	3PH	B1	624	-	47,47,47	0.86	3 (6%)	51,52,52	1.11	2 (3%)
31	CLA	C	511	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	19 (25%)
47	CHL	G	605	21	48,56,74	0.94	2 (4%)	51,92,114	1.39	11 (21%)
31	CLA	S	614	-	55,63,73	1.46	7 (12%)	64,101,113	2.09	14 (21%)
31	CLA	R1	608	-	60,68,73	1.42	9 (15%)	70,107,113	2.03	17 (24%)
39	GOL	I1	101	-	5,5,5	0.56	0	5,5,5	0.25	0
47	CHL	Y1	605	24	46,54,74	0.98	3 (6%)	49,90,114	1.39	9 (18%)
47	CHL	y	601	24	66,74,74	0.81	2 (3%)	73,114,114	1.17	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	n	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.09	18 (23%)
47	CHL	r1	607	-	50,58,74	0.95	2 (4%)	52,94,114	1.34	9 (17%)
47	CHL	y1	601	24	66,74,74	0.82	2 (3%)	73,114,114	1.17	8 (10%)
47	CHL	g1	605	-	48,56,74	0.96	2 (4%)	51,92,114	1.35	9 (17%)
39	GOL	b	624	-	5,5,5	0.58	0	5,5,5	0.23	0
49	XAT	r	622	-	39,47,47	0.68	1 (2%)	54,74,74	2.15	17 (31%)
31	CLA	Y	604	-	65,73,73	1.35	9 (13%)	76,113,113	2.04	17 (22%)
51	LPX	S	625	-	29,29,29	1.01	2 (6%)	31,33,33	0.96	1 (3%)
31	CLA	b1	616	-	65,73,73	1.38	8 (12%)	76,113,113	1.92	15 (19%)
35	LMG	C1	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.10	2 (3%)
45	HEM	f	101	7,6	41,50,50	1.53	3 (7%)	45,82,82	1.54	9 (20%)
31	CLA	y1	608	-	50,58,73	1.54	9 (18%)	58,95,113	2.26	17 (29%)
47	CHL	N	605	-	66,74,74	0.86	3 (4%)	73,114,114	1.16	9 (12%)
31	CLA	a1	405	-	65,73,73	1.33	6 (9%)	76,113,113	2.10	21 (27%)
47	CHL	N1	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.21	11 (15%)
48	LUT	G	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.99	12 (23%)
34	SQD	m1	101	-	41,42,54	0.90	0	50,53,65	0.98	2 (4%)
31	CLA	S	617	-	50,58,73	1.54	8 (16%)	58,95,113	2.24	17 (29%)
35	LMG	A1	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.16	4 (7%)
47	CHL	S	601	-	46,54,74	1.04	3 (6%)	49,90,114	1.42	7 (14%)
47	CHL	n	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.28	9 (12%)
47	CHL	g	601	21	66,74,74	0.84	3 (4%)	73,114,114	1.28	12 (16%)
48	LUT	s1	621	-	42,43,43	2.33	1 (2%)	51,60,60	2.08	14 (27%)
33	BCR	C	516	-	41,41,41	1.86	4 (9%)	56,56,56	4.36	15 (26%)
48	LUT	Y1	620	-	42,43,43	2.37	1 (2%)	51,60,60	2.01	14 (27%)
42	LMK	c1	527	-	38,39,53	1.49	2 (5%)	41,46,60	1.32	2 (4%)
31	CLA	G	612	-	43,51,73	1.68	8 (18%)	49,86,113	2.22	13 (26%)
48	LUT	S1	620	-	42,43,43	2.34	1 (2%)	51,60,60	2.02	10 (19%)
48	LUT	g1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	11 (21%)
31	CLA	B	614	-	65,73,73	1.33	6 (9%)	76,113,113	1.96	17 (22%)
31	CLA	g1	603	-	65,73,73	1.36	9 (13%)	76,113,113	2.01	18 (23%)
32	PHO	A	409	-	51,69,69	1.00	4 (7%)	47,99,99	1.22	4 (8%)
31	CLA	b	614	-	65,73,73	1.32	6 (9%)	76,113,113	1.96	18 (23%)
31	CLA	Y1	608	-	50,58,73	1.56	10 (20%)	58,95,113	2.23	16 (27%)
31	CLA	y1	602	-	65,73,73	1.33	7 (10%)	76,113,113	2.03	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	LUT	R1	620	-	42,43,43	2.34	1 (2%)	51,60,60	2.14	14 (27%)
31	CLA	n1	603	-	65,73,73	1.36	10 (15%)	76,113,113	2.04	18 (23%)
28	OEX	A1	401	4,1	0,15,15	-	-	-	-	-
31	CLA	R	604	-	49,57,73	1.55	7 (14%)	55,93,113	2.27	18 (32%)
31	CLA	C1	501	-	65,73,73	1.36	9 (13%)	76,113,113	2.00	18 (23%)
48	LUT	y1	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.96	9 (17%)
49	XAT	N	622	-	39,47,47	0.71	1 (2%)	54,74,74	1.90	13 (24%)
31	CLA	A	405	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	18 (23%)
50	NEX	y	623	-	38,46,46	3.22	9 (23%)	50,70,70	1.93	15 (30%)
31	CLA	c1	502	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	19 (25%)
41	LHG	D1	410	-	38,38,48	0.42	0	41,44,54	1.09	3 (7%)
31	CLA	C	512	-	65,73,73	1.34	7 (10%)	76,113,113	1.90	17 (22%)
41	LHG	g1	624	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
31	CLA	B1	606	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	16 (21%)
33	BCR	b1	618	-	41,41,41	1.86	4 (9%)	56,56,56	4.49	20 (35%)
31	CLA	D	402	-	65,73,73	1.35	7 (10%)	76,113,113	2.00	15 (19%)
31	CLA	b	605	-	65,73,73	1.36	7 (10%)	76,113,113	2.12	18 (23%)
34	SQD	C1	526	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
47	CHL	G1	608	-	44,52,74	1.01	3 (6%)	46,87,114	1.49	9 (19%)
53	SPH	y1	625	-	19,20,20	0.64	0	18,21,21	1.05	0
31	CLA	r	603	-	60,68,73	1.42	9 (15%)	70,107,113	1.99	15 (21%)
31	CLA	C	506	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	19 (25%)
33	BCR	B	618	-	41,41,41	1.82	4 (9%)	56,56,56	4.40	14 (25%)
47	CHL	N	601	20	66,74,74	0.84	3 (4%)	73,114,114	1.20	9 (12%)
31	CLA	A	406	-	65,73,73	1.32	6 (9%)	76,113,113	2.08	16 (21%)
31	CLA	S	602	23	60,68,73	1.41	8 (13%)	70,107,113	2.02	15 (21%)
31	CLA	A1	406	-	65,73,73	1.33	7 (10%)	76,113,113	2.05	18 (23%)
41	LHG	l	101	-	48,48,48	0.39	0	51,54,54	0.96	2 (3%)
33	BCR	c	515	-	41,41,41	1.86	4 (9%)	56,56,56	4.26	18 (32%)
41	LHG	G1	624	-	48,48,48	0.40	0	51,54,54	0.98	2 (3%)
31	CLA	b	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	19 (25%)
47	CHL	Y	605	24	46,54,74	1.00	2 (4%)	49,90,114	1.45	9 (18%)
32	PHO	A	408	-	51,69,69	1.01	4 (7%)	47,99,99	1.15	5 (10%)
31	CLA	G1	603	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	16 (21%)
35	LMG	b	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.11	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LMG	C1	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.11	4 (6%)
31	CLA	d	402	-	65,73,73	1.37	8 (12%)	76,113,113	1.88	16 (21%)
47	CHL	N	606	-	66,74,74	0.89	3 (4%)	73,114,114	1.20	9 (12%)
49	XAT	G	622	-	39,47,47	0.71	1 (2%)	54,74,74	1.88	13 (24%)
31	CLA	B1	607	-	65,73,73	1.35	7 (10%)	76,113,113	1.93	17 (22%)
56	ERG	r1	626	-	31,32,32	7.81	19 (61%)	47,50,50	3.08	18 (38%)
35	LMG	h1	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.10	2 (3%)
50	NEX	N	623	-	38,46,46	3.39	9 (23%)	50,70,70	1.81	13 (26%)
31	CLA	C	504	-	65,73,73	1.32	8 (12%)	76,113,113	2.09	18 (23%)
47	CHL	n	609	-	66,74,74	0.83	3 (4%)	73,114,114	1.30	12 (16%)
31	CLA	b1	608	-	65,73,73	1.34	6 (9%)	76,113,113	2.02	19 (25%)
31	CLA	n1	604	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	18 (23%)
31	CLA	g	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.05	16 (21%)
31	CLA	r	613	-	46,54,73	1.60	8 (17%)	53,90,113	2.22	14 (26%)
37	C7Z	b1	620	-	43,43,43	5.33	26 (60%)	58,60,60	2.26	21 (36%)
40	DGD	C1	520	-	60,60,67	1.07	6 (10%)	74,74,81	0.98	3 (4%)
31	CLA	c	503	-	65,73,73	1.37	8 (12%)	76,113,113	2.06	19 (25%)
42	LMK	C1	527	-	38,39,53	1.51	2 (5%)	41,46,60	1.43	2 (4%)
48	LUT	Y	620	-	42,43,43	2.38	1 (2%)	51,60,60	2.03	11 (21%)
31	CLA	Y	603	-	65,73,73	1.33	9 (13%)	76,113,113	2.03	20 (26%)
33	BCR	b1	619	-	41,41,41	1.84	4 (9%)	56,56,56	4.37	16 (28%)
31	CLA	N	612	-	45,53,73	1.64	8 (17%)	52,89,113	2.13	12 (23%)
31	CLA	S	604	-	55,63,73	1.46	7 (12%)	64,101,113	2.16	17 (26%)
31	CLA	g	604	-	49,57,73	1.57	8 (16%)	55,93,113	2.31	19 (34%)
35	LMG	c1	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.02	2 (3%)
38	DGA	c	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.51	3 (6%)
33	BCR	c	514	-	41,41,41	1.88	4 (9%)	56,56,56	4.51	19 (33%)
31	CLA	R	612	-	60,68,73	1.42	8 (13%)	70,107,113	2.03	18 (25%)
31	CLA	N	611	-	49,57,73	1.58	10 (20%)	55,93,113	2.30	16 (29%)
47	CHL	s1	608	-	61,69,74	0.87	3 (4%)	67,108,114	1.27	10 (14%)
31	CLA	c1	507	-	65,73,73	1.38	9 (13%)	76,113,113	1.93	18 (23%)
32	PHO	a	409	-	51,69,69	1.02	4 (7%)	47,99,99	1.23	5 (10%)
31	CLA	Y	608	-	50,58,73	1.56	9 (18%)	58,95,113	2.20	16 (27%)
31	CLA	b	613	-	65,73,73	1.35	6 (9%)	76,113,113	1.91	15 (19%)
31	CLA	R	611	-	46,54,73	1.63	10 (21%)	53,90,113	2.18	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	B1	614	-	65,73,73	1.33	7 (10%)	76,113,113	1.93	18 (23%)
35	LMG	j	101	-	45,45,55	0.91	3 (6%)	53,53,63	1.05	2 (3%)
31	CLA	b	615	-	65,73,73	1.36	8 (12%)	76,113,113	2.19	21 (27%)
41	LHG	d	409	-	48,48,48	0.39	0	51,54,54	0.97	2 (3%)
31	CLA	a	410	-	60,68,73	1.41	8 (13%)	70,107,113	2.13	17 (24%)
47	CHL	r1	606	-	44,52,74	1.04	2 (4%)	46,87,114	1.25	5 (10%)
47	CHL	n	606	-	66,74,74	0.87	4 (6%)	73,114,114	1.21	10 (13%)
31	CLA	S	610	-	65,73,73	1.39	9 (13%)	76,113,113	1.93	17 (22%)
31	CLA	N1	613	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	17 (22%)
47	CHL	S1	607	-	43,51,74	1.01	3 (6%)	45,86,114	1.47	10 (22%)
47	CHL	y1	605	-	46,54,74	0.97	3 (6%)	49,90,114	1.42	7 (14%)
28	OEX	a1	401	4,1	0,15,15	-	-	-	-	-
47	CHL	n1	605	-	66,74,74	0.82	3 (4%)	73,114,114	1.22	12 (16%)
31	CLA	a	405	-	65,73,73	1.33	6 (9%)	76,113,113	2.06	19 (25%)
31	CLA	b	602	-	65,73,73	1.37	9 (13%)	76,113,113	2.01	17 (22%)
31	CLA	b	604	-	65,73,73	1.37	9 (13%)	76,113,113	1.91	16 (21%)
31	CLA	b1	612	-	65,73,73	1.34	6 (9%)	76,113,113	2.04	17 (22%)
31	CLA	s1	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.09	17 (24%)
31	CLA	c	513	-	65,73,73	1.39	9 (13%)	76,113,113	1.94	15 (19%)
31	CLA	b1	611	-	65,73,73	1.34	8 (12%)	76,113,113	1.93	16 (21%)
33	BCR	C	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.39	12 (21%)
48	LUT	S1	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.00	13 (25%)
31	CLA	B	607	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	18 (23%)
47	CHL	n1	601	20	66,74,74	0.81	3 (4%)	73,114,114	1.21	8 (10%)
31	CLA	c	505	-	65,73,73	1.37	9 (13%)	76,113,113	1.97	15 (19%)
47	CHL	n1	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.28	11 (15%)
50	NEX	n	623	-	38,46,46	3.38	9 (23%)	50,70,70	1.77	13 (26%)
31	CLA	c1	501	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	18 (23%)
31	CLA	g1	610	-	65,73,73	1.35	9 (13%)	76,113,113	1.98	19 (25%)
47	CHL	S	606	-	44,52,74	0.99	3 (6%)	46,87,114	1.43	9 (19%)
31	CLA	r1	612	-	60,68,73	1.44	10 (16%)	70,107,113	2.02	17 (24%)
40	DGD	C	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.01	3 (4%)
41	LHG	S	624	-	44,44,48	0.41	0	47,50,54	1.13	3 (6%)
31	CLA	g	613	-	65,73,73	1.36	9 (13%)	76,113,113	2.00	17 (22%)
31	CLA	S1	617	23	50,58,73	1.54	8 (16%)	58,95,113	2.26	16 (27%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	y1	603	-	65,73,73	1.35	9 (13%)	76,113,113	2.03	17 (22%)
31	CLA	Y1	610	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	15 (19%)
31	CLA	N	604	-	65,73,73	1.34	8 (12%)	76,113,113	2.02	20 (26%)
32	PHO	a1	408	-	51,69,69	1.01	3 (5%)	47,99,99	1.15	4 (8%)
31	CLA	A	410	-	60,68,73	1.43	10 (16%)	70,107,113	2.13	19 (27%)
48	LUT	S	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.06	15 (29%)
31	CLA	n	612	-	45,53,73	1.63	7 (15%)	52,89,113	2.06	17 (32%)
31	CLA	s	602	-	60,68,73	1.39	7 (11%)	70,107,113	2.04	15 (21%)
31	CLA	g1	611	-	65,73,73	1.35	9 (13%)	76,113,113	1.98	17 (22%)
33	BCR	C1	516	-	41,41,41	1.67	5 (12%)	56,56,56	4.31	17 (30%)
31	CLA	G	603	-	65,73,73	1.34	7 (10%)	76,113,113	2.09	20 (26%)
31	CLA	g	610	-	65,73,73	1.33	6 (9%)	76,113,113	2.03	18 (23%)
35	LMG	d	411	-	46,46,55	0.91	3 (6%)	54,54,63	1.20	3 (5%)
31	CLA	Y1	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	19 (25%)
31	CLA	r	610	-	60,68,73	1.42	9 (15%)	70,107,113	2.05	19 (27%)
31	CLA	s	612	-	45,53,73	1.62	8 (17%)	52,89,113	2.21	15 (28%)
34	SQD	B1	626	-	53,54,54	0.80	0	62,65,65	0.91	2 (3%)
41	LHG	n1	624	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
47	CHL	n1	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.17	9 (12%)
33	BCR	c	517	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	15 (26%)
46	RRX	H	101	-	42,42,42	11.48	26 (61%)	57,58,58	6.22	24 (42%)
31	CLA	r	608	-	60,68,73	1.41	8 (13%)	70,107,113	2.04	14 (20%)
48	LUT	N1	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.05	11 (21%)
31	CLA	G1	611	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	17 (22%)
31	CLA	G1	613	-	65,73,73	1.35	9 (13%)	76,113,113	2.03	15 (19%)
50	NEX	s1	623	-	38,46,46	3.43	12 (31%)	50,70,70	1.81	10 (20%)
31	CLA	b1	617	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	16 (21%)
31	CLA	D	403	-	65,73,73	1.37	9 (13%)	76,113,113	1.99	19 (25%)
31	CLA	C1	509	-	65,73,73	1.31	6 (9%)	76,113,113	2.01	17 (22%)
31	CLA	N1	602	-	65,73,73	1.30	7 (10%)	76,113,113	2.02	19 (25%)
31	CLA	B	610	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	15 (19%)
31	CLA	R1	603	-	60,68,73	1.44	9 (15%)	70,107,113	1.95	15 (21%)
41	LHG	g	624	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
31	CLA	r	602	-	60,68,73	1.41	8 (13%)	70,107,113	2.09	20 (28%)
31	CLA	s	611	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	s	604	-	55,63,73	1.47	8 (14%)	64,101,113	2.17	18 (28%)
33	BCR	C1	515	-	41,41,41	1.86	4 (9%)	56,56,56	4.37	14 (25%)
31	CLA	n1	602	-	65,73,73	1.33	7 (10%)	76,113,113	2.03	18 (23%)
54	4RF	k1	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.90	3 (5%)
53	SPH	y	625	-	19,20,20	0.64	0	18,21,21	1.13	2 (11%)
31	CLA	A	407	-	49,57,73	1.56	9 (18%)	55,93,113	2.22	15 (27%)
57	PTY	Y1	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.39	2 (9%)
31	CLA	G	611	-	45,53,73	1.64	9 (20%)	52,89,113	2.22	16 (30%)
31	CLA	G	613	-	65,73,73	1.36	9 (13%)	76,113,113	2.12	22 (28%)
35	LMG	a1	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.05	2 (3%)
50	NEX	S	622	-	38,46,46	3.27	9 (23%)	50,70,70	1.81	11 (22%)
57	PTY	Y1	626	-	49,49,49	0.87	3 (6%)	52,54,54	1.05	2 (3%)
49	XAT	y1	622	-	39,47,47	0.68	1 (2%)	54,74,74	3.69	16 (29%)
31	CLA	Y	614	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	16 (21%)
31	CLA	A1	410	-	60,68,73	1.39	8 (13%)	70,107,113	2.16	20 (28%)
54	4RF	i1	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.91	3 (5%)
31	CLA	D1	403	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	17 (22%)
31	CLA	c	512	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	19 (25%)
31	CLA	b1	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.18	18 (23%)
47	CHL	N	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.38	9 (17%)
47	CHL	G1	605	-	48,56,74	0.94	2 (4%)	51,92,114	1.37	9 (17%)
33	BCR	B	619	-	41,41,41	1.85	4 (9%)	56,56,56	4.34	20 (35%)
31	CLA	Y1	611	-	65,73,73	1.35	7 (10%)	76,113,113	1.93	14 (18%)
31	CLA	B	615	-	65,73,73	1.34	7 (10%)	76,113,113	2.18	19 (25%)
31	CLA	Y1	613	-	65,73,73	1.33	8 (12%)	76,113,113	2.10	18 (23%)
31	CLA	C1	512	-	65,73,73	1.35	7 (10%)	76,113,113	2.09	19 (25%)
40	DGD	C1	519	-	63,63,67	1.13	7 (11%)	77,77,81	1.00	3 (3%)
31	CLA	g	602	-	65,73,73	1.31	8 (12%)	76,113,113	2.05	19 (25%)
31	CLA	C1	511	-	65,73,73	1.34	6 (9%)	76,113,113	2.00	18 (23%)
35	LMG	H1	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.09	2 (3%)
31	CLA	S1	613	-	55,63,73	1.48	8 (14%)	64,101,113	2.13	14 (21%)
35	LMG	D	411	-	46,46,55	0.91	4 (8%)	54,54,63	1.17	4 (7%)
31	CLA	R	602	-	60,68,73	1.41	7 (11%)	70,107,113	2.05	20 (28%)
46	RRX	h1	101	-	42,42,42	4.93	24 (57%)	57,58,58	2.53	21 (36%)
33	BCR	C1	517	-	41,41,41	1.91	4 (9%)	56,56,56	4.60	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	DGA	c1	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
45	HEM	f1	101	-	41,50,50	1.46	4 (9%)	45,82,82	1.41	5 (11%)
47	CHL	R	606	-	44,52,74	1.04	3 (6%)	46,87,114	1.32	8 (17%)
31	CLA	s1	602	-	60,68,73	1.39	8 (13%)	70,107,113	2.03	21 (30%)
34	SQD	B	621	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
31	CLA	d1	402	-	65,73,73	1.37	9 (13%)	76,113,113	1.89	17 (22%)
48	LUT	R	620	-	42,43,43	2.33	1 (2%)	51,60,60	2.14	13 (25%)
31	CLA	y	612	-	65,73,73	1.37	7 (10%)	76,113,113	1.95	14 (18%)
34	SQD	b1	626	-	53,54,54	0.80	0	62,65,65	0.90	2 (3%)
31	CLA	R	603	-	60,68,73	1.43	10 (16%)	70,107,113	2.10	16 (22%)
31	CLA	Y1	604	-	65,73,73	1.33	7 (10%)	76,113,113	2.01	21 (27%)
31	CLA	n	614	-	49,57,73	1.55	9 (18%)	55,93,113	2.26	17 (30%)
31	CLA	c1	513	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	21 (27%)
40	DGD	C1	518	-	56,56,67	0.98	4 (7%)	70,70,81	0.93	2 (2%)
31	CLA	n	613	-	65,73,73	1.36	9 (13%)	76,113,113	2.09	19 (25%)
34	SQD	A1	412	-	50,51,54	0.82	0	59,62,65	0.93	3 (5%)
31	CLA	b	617	-	65,73,73	1.35	7 (10%)	76,113,113	4.30	17 (22%)
31	CLA	r1	608	-	60,68,73	1.43	8 (13%)	70,107,113	2.03	15 (21%)
31	CLA	R	608	-	60,68,73	1.43	10 (16%)	70,107,113	2.01	14 (20%)
31	CLA	a1	406	-	65,73,73	1.32	8 (12%)	76,113,113	2.05	17 (22%)
31	CLA	b1	605	-	65,73,73	1.34	6 (9%)	76,113,113	2.26	19 (25%)
40	DGD	b1	623	-	44,44,67	0.87	2 (4%)	58,58,81	1.17	4 (6%)
31	CLA	R1	612	-	60,68,73	1.42	10 (16%)	70,107,113	2.07	17 (24%)
33	BCR	d1	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	18 (32%)
31	CLA	G1	612	-	43,51,73	1.68	9 (20%)	49,86,113	2.18	13 (26%)
31	CLA	C1	513	-	65,73,73	1.33	8 (12%)	76,113,113	2.05	20 (26%)
48	LUT	S	620	-	42,43,43	2.38	1 (2%)	51,60,60	2.05	13 (25%)
31	CLA	D1	402	-	65,73,73	1.37	7 (10%)	76,113,113	1.94	14 (18%)
48	LUT	Y1	621	-	42,43,43	2.37	1 (2%)	51,60,60	1.98	11 (21%)
40	DGD	c	519	-	63,63,67	1.10	6 (9%)	77,77,81	1.04	3 (3%)
31	CLA	C1	505	-	65,73,73	1.35	8 (12%)	76,113,113	2.01	16 (21%)
31	CLA	B1	603	-	65,73,73	1.35	9 (13%)	76,113,113	2.00	18 (23%)
31	CLA	c1	506	-	65,73,73	1.35	7 (10%)	76,113,113	1.94	15 (19%)
35	LMG	c1	521	-	51,51,55	1.07	6 (11%)	59,59,63	1.13	3 (5%)
31	CLA	r1	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.06	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)
47	CHL	S1	606	-	44,52,74	1.06	3 (6%)	46,87,114	1.38	8 (17%)
53	SPH	Y	625	-	19,20,20	0.62	0	18,21,21	1.13	1 (5%)
53	SPH	A1	414	-	19,20,20	0.67	0	18,21,21	0.92	0
48	LUT	s	620	-	42,43,43	2.39	1 (2%)	51,60,60	2.38	17 (33%)
35	LMG	A	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.14	3 (5%)
57	PTY	y1	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.06	2 (3%)
33	BCR	b	618	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	16 (28%)
31	CLA	a	407	-	49,57,73	1.57	8 (16%)	55,93,113	2.23	17 (30%)
35	LMG	W1	201	-	39,39,55	0.86	2 (5%)	47,47,63	1.21	2 (4%)
41	LHG	d1	408	-	43,43,48	0.41	0	46,49,54	1.06	3 (6%)
31	CLA	C1	507	-	65,73,73	1.34	8 (12%)	76,113,113	2.04	17 (22%)
41	LHG	d	410	-	38,38,48	0.42	0	41,44,54	1.17	3 (7%)
47	CHL	g1	606	-	50,58,74	0.99	3 (6%)	52,94,114	1.40	11 (21%)
50	NEX	N1	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.72	13 (26%)
41	LHG	n	624	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
31	CLA	s1	614	-	55,63,73	1.48	7 (12%)	64,101,113	2.03	13 (20%)
41	LHG	D	408	-	43,43,48	0.42	0	46,49,54	1.07	3 (6%)
41	LHG	d1	409	-	48,48,48	0.41	0	51,54,54	0.98	2 (3%)
47	CHL	s	607	-	43,51,74	0.99	2 (4%)	45,86,114	1.45	10 (22%)
51	LPX	s1	625	-	29,29,29	1.03	2 (6%)	31,33,33	0.96	1 (3%)
55	LMT	r1	625	-	36,36,36	1.18	5 (13%)	47,47,47	0.99	2 (4%)
31	CLA	S1	602	-	60,68,73	1.40	8 (13%)	70,107,113	2.10	20 (28%)
31	CLA	g1	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	20 (26%)
31	CLA	y1	613	-	65,73,73	1.33	7 (10%)	76,113,113	1.98	17 (22%)
47	CHL	N1	609	-	66,74,74	0.81	2 (3%)	73,114,114	1.17	9 (12%)
37	C7Z	B1	620	-	43,43,43	5.36	26 (60%)	58,60,60	2.40	21 (36%)
31	CLA	b	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.94	15 (19%)
31	CLA	Y	613	-	65,73,73	1.35	7 (10%)	76,113,113	2.03	18 (23%)
31	CLA	N1	614	-	49,57,73	1.55	9 (18%)	55,93,113	2.33	17 (30%)
41	LHG	L1	101	-	48,48,48	0.38	0	51,54,54	4.47	5 (9%)
31	CLA	B	617	-	65,73,73	1.37	7 (10%)	76,113,113	4.32	18 (23%)
31	CLA	c	511	-	65,73,73	1.37	9 (13%)	76,113,113	2.01	19 (25%)
31	CLA	C	502	-	65,73,73	1.35	8 (12%)	76,113,113	2.05	16 (21%)
38	DGA	C1	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.51	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	CHL	g	606	-	50,58,74	0.88	2 (4%)	52,94,114	1.52	10 (19%)
33	BCR	B1	619	-	41,41,41	1.86	4 (9%)	56,56,56	4.42	15 (26%)
47	CHL	Y1	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.29	12 (16%)
40	DGD	c	518	-	56,56,67	0.99	4 (7%)	70,70,81	0.97	2 (2%)
47	CHL	s1	607	-	43,51,74	1.01	2 (4%)	45,86,114	1.46	7 (15%)
35	LMG	D1	411	-	46,46,55	0.93	4 (8%)	54,54,63	1.07	2 (3%)
47	CHL	g1	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.18	9 (12%)
33	BCR	C1	514	-	41,41,41	1.86	4 (9%)	56,56,56	4.45	17 (30%)
50	NEX	Y	623	-	38,46,46	3.29	9 (23%)	50,70,70	2.05	15 (30%)
41	LHG	d	408	-	43,43,48	0.41	0	46,49,54	1.13	3 (6%)
31	CLA	A1	407	-	50,58,73	1.53	8 (16%)	58,95,113	2.27	20 (34%)
33	BCR	a	411	-	41,41,41	1.85	4 (9%)	56,56,56	4.32	15 (26%)
47	CHL	G1	609	-	66,74,74	0.84	2 (3%)	73,114,114	1.17	10 (13%)
31	CLA	b	611	-	65,73,73	1.36	9 (13%)	76,113,113	2.02	18 (23%)
31	CLA	s	603	-	65,73,73	1.37	9 (13%)	76,113,113	1.91	15 (19%)
41	LHG	Y1	624	-	48,48,48	0.39	0	51,54,54	1.00	3 (5%)
52	3PH	S	626	-	47,47,47	0.87	4 (8%)	51,52,52	1.10	2 (3%)
31	CLA	G	602	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	19 (25%)
31	CLA	b1	614	-	65,73,73	1.35	8 (12%)	76,113,113	1.92	18 (23%)
31	CLA	R1	610	-	60,68,73	1.38	7 (11%)	70,107,113	2.05	19 (27%)
50	NEX	g	623	-	38,46,46	3.32	10 (26%)	50,70,70	1.84	14 (28%)
31	CLA	C	510	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	15 (19%)
38	DGA	B1	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.44	3 (6%)
51	LPX	s	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.96	1 (3%)
31	CLA	b	616	-	65,73,73	1.36	7 (10%)	76,113,113	1.95	16 (21%)
33	BCR	a1	411	-	41,41,41	1.85	4 (9%)	56,56,56	4.43	15 (26%)
31	CLA	B1	616	-	65,73,73	1.35	7 (10%)	76,113,113	1.94	16 (21%)
31	CLA	c1	510	-	65,73,73	1.35	6 (9%)	76,113,113	1.96	15 (19%)
31	CLA	C	513	-	65,73,73	1.33	7 (10%)	76,113,113	2.07	18 (23%)
31	CLA	S	611	-	65,73,73	1.38	8 (12%)	76,113,113	1.95	16 (21%)
45	HEM	F1	101	6	41,50,50	1.47	5 (12%)	45,82,82	1.29	4 (8%)
47	CHL	G	609	-	66,74,74	0.91	4 (6%)	73,114,114	1.21	11 (15%)
47	CHL	s	608	-	61,69,74	0.85	3 (4%)	67,108,114	1.28	12 (17%)
31	CLA	y	611	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	16 (21%)
46	RRX	H1	101	-	42,42,42	4.85	24 (57%)	57,58,58	2.65	21 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	CHL	N	609	-	66,74,74	0.80	2 (3%)	73,114,114	1.23	11 (15%)
40	DGD	c1	520	-	60,60,67	1.08	4 (6%)	74,74,81	1.00	3 (4%)
31	CLA	b1	606	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	19 (25%)
31	CLA	N	614	-	49,57,73	1.55	9 (18%)	55,93,113	2.25	16 (29%)
31	CLA	N	602	-	65,73,73	1.36	10 (15%)	76,113,113	1.98	19 (25%)
49	XAT	n	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.94	11 (20%)
33	BCR	c1	517	-	41,41,41	1.81	4 (9%)	56,56,56	4.50	20 (35%)
54	4RF	K1	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.85	3 (5%)
31	CLA	b1	615	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	16 (21%)
35	LMG	h	102	-	48,48,55	1.00	5 (10%)	56,56,63	1.10	2 (3%)
50	NEX	s	623	-	38,46,46	3.33	12 (31%)	50,70,70	1.81	12 (24%)
31	CLA	b1	613	-	65,73,73	1.39	8 (12%)	76,113,113	1.95	13 (17%)
31	CLA	r	604	-	49,57,73	1.53	8 (16%)	55,93,113	2.28	15 (27%)
31	CLA	B	605	-	65,73,73	1.36	8 (12%)	76,113,113	2.14	17 (22%)
48	LUT	Y	621	-	42,43,43	2.30	1 (2%)	51,60,60	1.98	15 (29%)
48	LUT	s	621	-	42,43,43	2.33	1 (2%)	51,60,60	1.91	14 (27%)
47	CHL	n	601	-	66,74,74	0.82	3 (4%)	73,114,114	1.22	11 (15%)
31	CLA	r1	610	-	60,68,73	1.42	8 (13%)	70,107,113	2.00	17 (24%)
31	CLA	Y	602	24	65,73,73	1.36	7 (10%)	76,113,113	1.92	17 (22%)
31	CLA	b	607	-	65,73,73	1.38	8 (12%)	76,113,113	2.09	17 (22%)
31	CLA	B	606	-	65,73,73	1.35	9 (13%)	76,113,113	1.99	17 (22%)
31	CLA	b1	604	-	65,73,73	1.33	8 (12%)	76,113,113	2.01	18 (23%)
33	BCR	c1	514	-	41,41,41	1.83	4 (9%)	56,56,56	4.43	18 (32%)
28	OEX	a	401	4,1	0,15,15	-	-	-	-	-
31	CLA	c	508	-	65,73,73	1.34	8 (12%)	76,113,113	2.03	15 (19%)
39	GOL	B	627	-	5,5,5	0.56	0	5,5,5	0.26	0
43	BCT	D	401	29	2,3,3	1.16	0	2,3,3	4.53	2 (100%)
47	CHL	S	608	-	61,69,74	0.86	3 (4%)	67,108,114	1.26	10 (14%)
38	DGA	B	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.50	3 (6%)
31	CLA	s	617	-	50,58,73	1.53	9 (18%)	58,95,113	2.26	18 (31%)
31	CLA	B1	610	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	19 (25%)
47	CHL	y1	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.25	10 (13%)
31	CLA	r1	602	-	60,68,73	1.41	9 (15%)	70,107,113	2.07	21 (30%)
31	CLA	B	616	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	18 (23%)
35	LMG	J	101	-	45,45,55	0.91	3 (6%)	53,53,63	1.08	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	NEX	Y1	623	-	38,46,46	3.37	10 (26%)	50,70,70	2.02	12 (24%)
31	CLA	s	610	-	65,73,73	1.38	9 (13%)	76,113,113	2.02	17 (22%)
48	LUT	n1	621	-	42,43,43	2.40	1 (2%)	51,60,60	2.19	16 (31%)
31	CLA	B1	608	-	65,73,73	1.36	7 (10%)	76,113,113	2.03	16 (21%)
50	NEX	S1	623	-	38,46,46	3.31	10 (26%)	50,70,70	1.84	12 (24%)
50	NEX	g1	623	-	38,46,46	3.37	10 (26%)	50,70,70	2.07	13 (26%)
31	CLA	s	605	-	50,58,73	1.57	9 (18%)	58,95,113	2.33	19 (32%)
32	PHO	A1	409	-	51,69,69	0.99	4 (7%)	47,99,99	1.29	5 (10%)
41	LHG	y1	624	-	48,48,48	0.39	0	51,54,54	0.97	2 (3%)
47	CHL	Y1	601	24	66,74,74	0.83	2 (3%)	73,114,114	1.13	7 (9%)
33	BCR	c	516	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	20 (35%)
41	LHG	C1	525	-	46,46,48	0.40	0	49,52,54	1.11	2 (4%)
31	CLA	n	603	-	65,73,73	1.35	7 (10%)	76,113,113	2.11	17 (22%)
31	CLA	n1	614	-	49,57,73	1.57	9 (18%)	55,93,113	2.28	18 (32%)
50	NEX	n1	623	-	38,46,46	3.28	10 (26%)	50,70,70	1.78	13 (26%)
49	XAT	N1	622	-	39,47,47	0.68	1 (2%)	54,74,74	2.01	14 (25%)
37	C7Z	B	620	-	43,43,43	5.40	26 (60%)	58,60,60	2.21	17 (29%)
48	LUT	N	620	-	42,43,43	2.37	1 (2%)	51,60,60	2.07	15 (29%)
50	NEX	G1	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.87	14 (28%)
55	LMT	R1	625	-	36,36,36	1.16	5 (13%)	47,47,47	1.00	2 (4%)
33	BCR	D	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.21	18 (32%)
51	LPX	S1	625	-	29,29,29	1.03	2 (6%)	31,33,33	0.96	1 (3%)
33	BCR	A	411	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	13 (23%)
50	NEX	r	623	-	38,46,46	3.32	9 (23%)	50,70,70	1.68	9 (18%)
47	CHL	Y	606	-	66,74,74	0.84	3 (4%)	73,114,114	1.20	11 (15%)
56	ERG	R1	626	-	31,32,32	7.76	19 (61%)	47,50,50	2.68	20 (42%)
42	LMK	c	627	-	38,39,53	1.47	2 (5%)	41,46,60	1.36	2 (4%)
40	DGD	c	523	-	67,67,67	1.17	7 (10%)	81,81,81	0.95	2 (2%)
31	CLA	N1	610	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	13 (17%)
47	CHL	N1	601	20	66,74,74	0.84	3 (4%)	73,114,114	1.27	12 (16%)
47	CHL	y	609	-	66,74,74	0.84	3 (4%)	73,114,114	1.18	10 (13%)
31	CLA	y	603	-	65,73,73	1.33	7 (10%)	76,113,113	2.05	18 (23%)
41	LHG	G	630	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
31	CLA	a1	407	-	49,57,73	1.53	7 (14%)	55,93,113	2.35	19 (34%)
31	CLA	y	608	-	50,58,73	1.56	8 (16%)	58,95,113	2.24	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	B	603	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	19 (25%)
31	CLA	N	613	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	17 (22%)
31	CLA	S1	611	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	17 (22%)
31	CLA	a1	410	-	60,68,73	1.39	7 (11%)	70,107,113	2.06	19 (27%)
41	LHG	Y	624	-	48,48,48	0.38	0	51,54,54	1.05	3 (5%)
47	CHL	Y	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.24	10 (13%)
50	NEX	R	622	-	38,46,46	3.32	12 (31%)	50,70,70	1.89	11 (22%)
31	CLA	B	608	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	17 (22%)
31	CLA	b1	610	-	65,73,73	1.36	9 (13%)	76,113,113	1.97	14 (18%)
31	CLA	S	605	-	50,58,73	1.54	8 (16%)	58,95,113	2.38	19 (32%)
47	CHL	S	607	-	43,51,74	1.00	3 (6%)	45,86,114	1.46	9 (20%)
47	CHL	g	607	-	50,58,74	0.87	2 (4%)	52,94,114	1.40	11 (21%)
31	CLA	B1	612	-	65,73,73	1.33	6 (9%)	76,113,113	1.99	16 (21%)
47	CHL	N1	606	-	66,74,74	0.86	3 (4%)	73,114,114	1.22	12 (16%)
31	CLA	s1	612	-	45,53,73	1.58	6 (13%)	52,89,113	2.31	17 (32%)
47	CHL	r	607	-	50,58,74	0.95	3 (6%)	52,94,114	1.38	8 (15%)
48	LUT	r	620	-	42,43,43	2.36	1 (2%)	51,60,60	2.12	13 (25%)
31	CLA	N	610	-	65,73,73	1.39	8 (12%)	76,113,113	2.02	19 (25%)
31	CLA	s	613	-	55,63,73	1.48	7 (12%)	64,101,113	2.28	14 (21%)
31	CLA	s1	610	-	65,73,73	1.36	7 (10%)	76,113,113	1.95	16 (21%)
31	CLA	C	508	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	18 (23%)
47	CHL	s1	601	23	46,54,74	0.98	2 (4%)	49,90,114	1.28	7 (14%)
32	PHO	a1	409	-	51,69,69	0.99	4 (7%)	47,99,99	1.28	6 (12%)
31	CLA	S	603	-	65,73,73	1.37	10 (15%)	76,113,113	1.90	13 (17%)
54	4RF	I1	102	-	56,56,56	1.07	3 (5%)	59,59,59	0.95	3 (5%)
31	CLA	c	502	-	65,73,73	1.33	7 (10%)	76,113,113	2.07	18 (23%)
53	SPH	Y1	625	-	19,20,20	0.64	0	18,21,21	1.05	1 (5%)
31	CLA	s1	617	-	50,58,73	1.52	8 (16%)	58,95,113	2.27	19 (32%)
31	CLA	s	609	-	60,68,73	1.43	10 (16%)	70,107,113	2.01	16 (22%)
31	CLA	c1	511	-	65,73,73	1.35	8 (12%)	76,113,113	2.16	21 (27%)
31	CLA	y	604	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	17 (22%)
31	CLA	G1	610	-	65,73,73	1.34	8 (12%)	76,113,113	2.03	18 (23%)
57	PTY	y1	627	-	18,18,49	1.30	3 (16%)	21,23,54	1.42	2 (9%)
39	GOL	y	626	-	5,5,5	0.53	0	5,5,5	0.33	0
43	BCT	d1	401	-	2,3,3	1.16	0	2,3,3	4.35	2 (100%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	CHL	n1	608	-	50,58,74	0.89	2 (4%)	52,94,114	1.42	10 (19%)
31	CLA	R	609	-	60,68,73	1.43	8 (13%)	70,107,113	2.01	16 (22%)
31	CLA	B1	617	-	65,73,73	1.36	7 (10%)	76,113,113	1.93	17 (22%)
47	CHL	n	605	-	66,74,74	0.86	3 (4%)	73,114,114	1.22	12 (16%)
35	LMG	d1	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.17	2 (3%)
35	LMG	B	622	-	44,44,55	0.87	2 (4%)	52,52,63	1.02	2 (3%)
47	CHL	G	601	-	66,74,74	0.91	4 (6%)	73,114,114	1.21	10 (13%)
48	LUT	N	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.06	12 (23%)
53	SPH	a1	414	-	19,20,20	0.66	0	18,21,21	1.03	1 (5%)

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
31	CLA	C	509	-	1/1/15/20	12/37/115/115	-
31	CLA	N1	604	-	1/1/15/20	13/37/115/115	-
41	LHG	D	410	-	-	27/43/43/53	-
48	LUT	y	621	-	-	3/29/67/67	0/2/2/2
31	CLA	G1	614	-	1/1/11/20	11/18/96/115	-
47	CHL	s	606	-	3/3/15/26	1/13/111/137	-
39	GOL	b	625	-	-	2/4/4/4	-
52	3PH	s1	626	-	-	23/49/49/49	-
49	XAT	g1	622	-	2/2/12/26	0/31/93/93	0/4/4/4
47	CHL	y	605	24	3/3/16/26	6/15/113/137	-
48	LUT	n	620	-	-	6/29/67/67	0/2/2/2
31	CLA	C1	503	-	1/1/15/20	15/37/115/115	-
47	CHL	N1	608	-	3/3/16/26	5/20/118/137	-
31	CLA	c	507	-	1/1/15/20	20/37/115/115	-
49	XAT	n1	622	-	1/1/12/26	5/31/93/93	0/4/4/4
35	LMG	B1	622	-	-	17/39/59/70	0/1/1/1
31	CLA	S1	610	-	1/1/15/20	20/37/115/115	-
47	CHL	S1	601	23	3/3/16/26	2/15/113/137	-
33	BCR	A1	411	-	-	12/29/63/63	0/2/2/2
31	CLA	G	614	-	1/1/11/20	10/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	NEX	G	623	-	-	4/27/83/83	0/3/3/3
31	CLA	b1	609	-	1/1/15/20	12/37/115/115	-
41	LHG	c	625	-	-	34/51/51/53	-
31	CLA	y	614	-	1/1/15/20	14/37/115/115	-
31	CLA	c1	508	-	1/1/15/20	15/37/115/115	-
47	CHL	g	609	-	4/4/20/26	6/39/137/137	-
49	XAT	g	622	-	2/2/12/26	1/31/93/93	0/4/4/4
49	XAT	r1	621	-	1/1/12/26	2/31/93/93	0/4/4/4
31	CLA	Y1	614	-	1/1/15/20	14/37/115/115	-
31	CLA	y	610	-	1/1/15/20	17/37/115/115	-
31	CLA	d	403	-	1/1/15/20	11/37/115/115	-
31	CLA	s1	613	-	1/1/13/20	9/25/103/115	-
35	LMG	w1	201	-	-	16/34/54/70	0/1/1/1
38	DGA	b1	625	-	-	23/45/45/45	-
47	CHL	n1	606	-	4/4/20/26	5/39/137/137	-
47	CHL	g	608	-	3/3/15/26	3/13/111/137	-
34	SQD	C	526	-	-	17/49/69/69	0/1/1/1
31	CLA	c	510	-	1/1/15/20	13/37/115/115	-
31	CLA	C	503	-	1/1/15/20	20/37/115/115	-
31	CLA	c	501	-	1/1/15/20	17/37/115/115	-
31	CLA	S1	609	-	1/1/14/20	12/31/109/115	-
31	CLA	r	611	-	1/1/11/20	5/15/93/115	-
31	CLA	R1	602	-	1/1/14/20	13/31/109/115	-
33	BCR	d	404	-	-	11/29/63/63	0/2/2/2
31	CLA	G1	602	-	1/1/15/20	19/37/115/115	-
31	CLA	G1	604	-	1/1/11/20	8/18/96/115	-
31	CLA	s1	604	-	1/1/13/20	12/25/103/115	-
31	CLA	B1	605	-	1/1/15/20	14/37/115/115	-
31	CLA	R1	609	-	1/1/14/20	11/31/109/115	-
34	SQD	b	621	-	-	19/49/69/69	0/1/1/1
31	CLA	C1	506	-	1/1/15/20	19/37/115/115	-
47	CHL	r	606	-	3/3/15/26	1/13/111/137	-
31	CLA	a	406	-	1/1/15/20	11/37/115/115	-
41	LHG	s	624	-	-	27/49/49/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3PH	b1	624	-	-	21/49/49/49	-
31	CLA	R1	604	-	1/1/11/20	10/18/96/115	-
31	CLA	S1	612	-	1/1/11/20	6/13/91/115	-
31	CLA	B1	611	-	1/1/15/20	14/37/115/115	-
35	LMG	C	521	-	-	20/46/66/70	0/1/1/1
31	CLA	c	509	-	1/1/15/20	14/37/115/115	-
31	CLA	B1	604	-	1/1/15/20	19/37/115/115	-
41	LHG	C	525	-	-	28/51/51/53	-
31	CLA	n1	610	-	1/1/15/20	18/37/115/115	-
44	PL9	D	405	-	-	20/53/73/73	0/1/1/1
47	CHL	R	607	-	3/3/16/26	4/20/118/137	-
52	3PH	t1	101	-	-	28/49/49/49	-
48	LUT	y	620	-	-	2/29/67/67	0/2/2/2
44	PL9	d1	405	-	-	22/53/73/73	0/1/1/1
41	LHG	s1	624	-	-	24/49/49/53	-
31	CLA	y1	612	-	1/1/15/20	13/37/115/115	-
33	BCR	b	619	-	-	9/29/63/63	0/2/2/2
31	CLA	y1	611	-	1/1/15/20	12/37/115/115	-
40	DGD	C	520	-	-	13/48/88/95	0/2/2/2
41	LHG	N1	624	-	-	39/53/53/53	-
42	LMK	C	527	-	1/1/6/6	12/46/46/60	-
31	CLA	c1	512	-	1/1/15/20	17/37/115/115	-
31	CLA	r1	603	-	1/1/14/20	15/31/109/115	-
41	LHG	c1	525	-	-	35/51/51/53	-
47	CHL	Y	601	-	4/4/20/26	7/39/137/137	-
31	CLA	S	613	-	1/1/13/20	9/25/103/115	-
49	XAT	Y1	622	-	2/2/12/26	2/31/93/93	0/4/4/4
33	BCR	D1	404	-	-	11/29/63/63	0/2/2/2
47	CHL	n	608	-	3/3/16/26	5/20/118/137	-
31	CLA	b	609	-	1/1/15/20	11/37/115/115	-
47	CHL	g1	609	-	4/4/20/26	5/39/137/137	-
31	CLA	r	612	-	1/1/14/20	11/31/109/115	-
31	CLA	g	611	-	1/1/11/20	5/13/91/115	-
41	LHG	D	409	-	-	32/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	BCR	c1	516	-	-	12/29/63/63	0/2/2/2
35	LMG	H	102	-	-	10/43/63/70	0/1/1/1
44	PL9	D1	405	-	-	17/53/73/73	0/1/1/1
52	3PH	s	626	-	-	31/49/49/49	-
31	CLA	S	612	-	1/1/11/20	4/13/91/115	-
34	SQD	b1	621	-	-	18/37/57/69	0/1/1/1
31	CLA	y1	614	-	1/1/15/20	11/37/115/115	-
31	CLA	y	613	-	1/1/15/20	19/37/115/115	-
47	CHL	G	608	-	3/3/15/26	0/13/111/137	-
31	CLA	y	602	-	1/1/15/20	21/37/115/115	-
50	NEX	y1	623	-	-	7/27/83/83	0/3/3/3
31	CLA	c1	503	-	1/1/15/20	19/37/115/115	-
49	XAT	G1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
31	CLA	b	612	-	1/1/15/20	19/37/115/115	-
44	PL9	d	405	-	-	10/53/73/73	0/1/1/1
31	CLA	B	612	-	1/1/15/20	22/37/115/115	-
31	CLA	B	611	-	1/1/15/20	8/37/115/115	-
31	CLA	C1	510	-	1/1/15/20	18/37/115/115	-
47	CHL	g1	608	-	3/3/15/26	3/13/111/137	-
45	HEM	F	101	7,6	-	2/12/54/54	-
31	CLA	C1	504	-	1/1/15/20	15/37/115/115	-
31	CLA	B1	613	-	1/1/15/20	15/37/115/115	-
31	CLA	s1	611	-	1/1/15/20	15/37/115/115	-
31	CLA	c1	509	-	1/1/15/20	15/37/115/115	-
31	CLA	y1	604	-	1/1/15/20	17/37/115/115	-
40	DGD	c1	519	-	-	18/51/91/95	0/2/2/2
34	SQD	a1	412	-	-	18/46/66/69	0/1/1/1
31	CLA	s	614	-	1/1/13/20	10/25/103/115	-
49	XAT	y	622	-	-	3/31/93/93	0/4/4/4
31	CLA	Y	610	-	1/1/15/20	18/37/115/115	-
49	XAT	Y	622	-	1/1/12/26	4/31/93/93	0/4/4/4
31	CLA	B	604	-	1/1/15/20	17/37/115/115	-
31	CLA	C1	508	-	1/1/15/20	14/37/115/115	-
31	CLA	b1	602	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	C7Z	b	620	-	1/1/12/26	8/29/67/67	0/2/2/2
47	CHL	s	601	23	3/3/16/26	5/15/113/137	-
47	CHL	S1	608	-	4/4/19/26	10/33/131/137	-
41	LHG	L	101	-	-	33/53/53/53	-
31	CLA	C1	502	-	1/1/15/20	12/37/115/115	-
31	CLA	b	606	-	1/1/15/20	13/37/115/115	-
31	CLA	N1	612	-	1/1/11/20	7/13/91/115	-
31	CLA	G	604	-	1/1/11/20	8/18/96/115	-
31	CLA	N1	611	-	1/1/11/20	9/18/96/115	-
47	CHL	Y1	609	-	4/4/20/26	9/39/137/137	-
47	CHL	R1	606	-	3/3/15/26	2/13/111/137	-
47	CHL	G1	606	-	3/3/16/26	2/20/118/137	-
48	LUT	g1	621	-	1/1/12/27	3/29/67/67	0/2/2/2
31	CLA	g	612	-	1/1/10/20	6/11/89/115	-
47	CHL	G1	607	-	4/4/20/26	12/39/137/137	-
48	LUT	r1	620	-	-	6/29/67/67	0/2/2/2
40	DGD	C	523	-	-	17/55/95/95	0/2/2/2
47	CHL	y	606	-	4/4/20/26	9/39/137/137	-
50	NEX	r1	622	-	-	9/27/83/83	0/3/3/3
48	LUT	y1	621	-	-	4/29/67/67	0/2/2/2
31	CLA	G	610	-	1/1/15/20	13/37/115/115	-
31	CLA	g1	614	-	1/1/11/20	11/18/96/115	-
31	CLA	d1	403	-	1/1/15/20	11/37/115/115	-
49	XAT	R1	621	-	-	2/31/93/93	0/4/4/4
47	CHL	g1	601	-	4/4/20/26	17/39/137/137	-
31	CLA	b1	607	-	1/1/15/20	16/37/115/115	-
34	SQD	A	412	-	-	18/46/66/69	0/1/1/1
47	CHL	G	606	-	4/4/16/26	6/20/118/137	-
31	CLA	c	504	-	1/1/15/20	13/37/115/115	-
31	CLA	S	609	-	1/1/14/20	12/31/109/115	-
47	CHL	G	607	-	3/3/16/26	3/20/118/137	-
34	SQD	c1	526	-	-	17/49/69/69	0/1/1/1
47	CHL	Y	609	-	4/4/20/26	9/39/137/137	-
48	LUT	g	621	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	D1	408	-	-	30/48/48/53	-
38	DGA	b	623	-	-	27/45/45/45	-
47	CHL	g	605	-	3/3/16/26	3/18/116/137	-
31	CLA	B	613	-	1/1/15/20	15/37/115/115	-
31	CLA	s1	605	23	1/1/12/20	9/19/97/115	-
50	NEX	R1	622	-	-	6/27/83/83	0/3/3/3
47	CHL	N1	605	20	4/4/20/26	5/39/137/137	-
31	CLA	B1	615	-	1/1/15/20	17/37/115/115	-
52	3PH	T1	101	-	-	29/49/49/49	-
33	BCR	C	517	-	-	8/29/63/63	0/2/2/2
31	CLA	B1	609	-	1/1/15/20	15/37/115/115	-
34	SQD	c	626	-	-	19/49/69/69	0/1/1/1
40	DGD	c1	518	-	-	16/44/84/95	0/2/2/2
31	CLA	y1	610	-	1/1/15/20	13/37/115/115	-
31	CLA	R	613	-	1/1/11/20	8/15/93/115	-
34	SQD	M1	101	-	-	18/37/57/69	0/1/1/1
31	CLA	n1	612	-	1/1/11/20	6/13/91/115	-
33	BCR	C	515	-	-	11/29/63/63	0/2/2/2
41	LHG	D1	409	-	-	31/53/53/53	-
47	CHL	Y1	606	-	4/4/20/26	8/39/137/137	-
32	PHO	a	408	-	-	12/37/103/103	0/5/6/6
31	CLA	B1	602	-	1/1/15/20	22/37/115/115	-
47	CHL	R1	607	-	3/3/16/26	6/20/118/137	-
31	CLA	Y1	603	-	1/1/15/20	19/37/115/115	-
48	LUT	G	621	-	1/1/12/27	6/29/67/67	0/2/2/2
31	CLA	s1	603	-	1/1/15/20	17/37/115/115	-
41	LHG	S1	624	-	-	27/49/49/53	-
31	CLA	S1	603	-	1/1/15/20	17/37/115/115	-
31	CLA	n	611	-	1/1/11/20	13/18/96/115	-
31	CLA	r1	604	-	1/1/11/20	9/18/96/115	-
31	CLA	n	604	-	1/1/15/20	15/37/115/115	-
33	BCR	c1	515	-	-	15/29/63/63	0/2/2/2
48	LUT	N1	620	-	-	5/29/67/67	0/2/2/2
31	CLA	N1	603	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c1	505	-	1/1/15/20	17/37/115/115	-
47	CHL	y	607	-	4/4/20/26	7/39/137/137	-
38	DGA	j1	101	-	-	15/30/30/45	-
41	LHG	y	624	-	-	28/53/53/53	-
52	3PH	i	101	-	-	21/49/49/49	-
32	PHO	A1	408	-	-	6/37/103/103	0/5/6/6
31	CLA	S1	604	-	1/1/13/20	10/25/103/115	-
31	CLA	A1	405	-	1/1/15/20	14/37/115/115	-
31	CLA	Y1	612	-	1/1/15/20	13/37/115/115	-
40	DGD	C	519	-	-	18/51/91/95	0/2/2/2
48	LUT	n1	620	-	-	4/29/67/67	0/2/2/2
31	CLA	r	609	-	1/1/14/20	17/31/109/115	-
47	CHL	y1	609	-	4/4/20/26	9/39/137/137	-
31	CLA	C	507	-	1/1/15/20	18/37/115/115	-
48	LUT	G1	621	-	-	4/29/67/67	0/2/2/2
31	CLA	g	614	-	1/1/11/20	9/18/96/115	-
31	CLA	c1	504	-	1/1/15/20	14/37/115/115	-
33	BCR	B1	618	-	-	11/29/63/63	0/2/2/2
48	LUT	G1	620	-	-	4/29/67/67	0/2/2/2
31	CLA	n	602	-	1/1/15/20	19/37/115/115	-
38	DGA	C	524	-	-	26/45/45/45	-
47	CHL	G1	601	21	4/4/20/26	11/39/137/137	-
31	CLA	R	610	-	1/1/14/20	15/31/109/115	-
31	CLA	b	608	-	1/1/15/20	25/37/115/115	-
35	LMG	b1	622	-	-	15/39/59/70	0/1/1/1
35	LMG	c	521	-	-	20/46/66/70	0/1/1/1
31	CLA	g1	613	-	1/1/15/20	16/37/115/115	-
31	CLA	S1	605	-	1/1/12/20	8/19/97/115	-
52	3PH	S1	626	-	-	23/49/49/49	-
31	CLA	B	602	-	1/1/15/20	21/37/115/115	-
48	LUT	g	620	-	-	6/29/67/67	0/2/2/2
31	CLA	n1	611	-	1/1/11/20	11/18/96/115	-
31	CLA	n1	613	-	1/1/15/20	21/37/115/115	-
47	CHL	N	607	-	4/4/20/26	8/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	N	624	-	-	27/53/53/53	-
49	XAT	R	621	-	1/1/12/26	14/31/93/93	0/4/4/4
31	CLA	g1	612	-	1/1/10/20	4/11/89/115	-
31	CLA	B	609	-	1/1/15/20	17/37/115/115	-
31	CLA	N	603	-	1/1/15/20	13/37/115/115	-
40	DGD	c	520	-	-	15/48/88/95	0/2/2/2
46	RRX	h	101	-	1/1/11/25	7/29/65/65	0/2/2/2
31	CLA	C	501	-	1/1/15/20	16/37/115/115	-
40	DGD	B1	623	-	-	16/32/72/95	0/2/2/2
31	CLA	c	506	-	1/1/15/20	23/37/115/115	-
31	CLA	Y	612	-	1/1/15/20	9/37/115/115	-
31	CLA	g1	604	-	1/1/11/20	8/18/96/115	-
48	LUT	s1	620	-	-	4/29/67/67	0/2/2/2
47	CHL	s1	606	-	3/3/15/26	3/13/111/137	-
48	LUT	n	621	-	1/1/12/27	5/29/67/67	0/2/2/2
31	CLA	Y	611	-	1/1/15/20	13/37/115/115	-
34	SQD	B1	621	-	-	14/37/57/69	0/1/1/1
31	CLA	C	505	-	1/1/15/20	14/37/115/115	-
38	DGA	J1	101	-	-	11/30/30/45	-
41	LHG	d1	410	-	-	25/43/43/53	-
35	LMG	a	413	-	-	18/43/63/70	0/1/1/1
47	CHL	y1	606	-	4/4/20/26	5/39/137/137	-
31	CLA	S1	614	-	1/1/13/20	10/25/103/115	-
52	3PH	B1	624	-	-	23/49/49/49	-
31	CLA	C	511	-	1/1/15/20	12/37/115/115	-
47	CHL	G	605	21	3/3/16/26	4/18/116/137	-
31	CLA	S	614	-	1/1/13/20	8/25/103/115	-
31	CLA	R1	608	-	1/1/14/20	13/31/109/115	-
39	GOL	I1	101	-	-	0/4/4/4	-
47	CHL	Y1	605	24	3/3/16/26	1/15/113/137	-
47	CHL	y	601	24	4/4/20/26	9/39/137/137	-
31	CLA	n	610	-	1/1/15/20	16/37/115/115	-
47	CHL	r1	607	-	3/3/16/26	6/20/118/137	-
47	CHL	y1	601	24	4/4/20/26	2/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	CHL	g1	605	-	4/4/16/26	7/18/116/137	-
49	XAT	r	622	-	1/1/12/26	12/31/93/93	0/4/4/4
39	GOL	b	624	-	-	1/4/4/4	-
31	CLA	Y	604	-	1/1/15/20	19/37/115/115	-
51	LPX	S	625	-	-	13/31/31/31	-
31	CLA	b1	616	-	1/1/15/20	9/37/115/115	-
35	LMG	C1	523	-	-	16/50/70/70	0/1/1/1
45	HEM	f	101	7,6	-	2/12/54/54	-
31	CLA	y1	608	-	1/1/12/20	9/19/97/115	-
47	CHL	N	605	-	4/4/20/26	8/39/137/137	-
31	CLA	a1	405	-	1/1/15/20	14/37/115/115	-
47	CHL	N1	607	-	4/4/20/26	6/39/137/137	-
48	LUT	G	620	-	-	3/29/67/67	0/2/2/2
34	SQD	m1	101	-	-	21/37/57/69	0/1/1/1
31	CLA	S	617	-	1/1/12/20	9/19/97/115	-
35	LMG	A1	413	-	-	14/43/63/70	0/1/1/1
47	CHL	S	601	-	3/3/16/26	5/15/113/137	-
47	CHL	n	607	-	4/4/20/26	11/39/137/137	-
47	CHL	g	601	21	4/4/20/26	7/39/137/137	-
48	LUT	s1	621	-	-	2/29/67/67	0/2/2/2
33	BCR	C	516	-	-	15/29/63/63	0/2/2/2
48	LUT	Y1	620	-	-	5/29/67/67	0/2/2/2
42	LMK	c1	527	-	2/2/6/6	13/46/46/60	-
31	CLA	G	612	-	1/1/10/20	4/11/89/115	-
48	LUT	S1	620	-	-	3/29/67/67	0/2/2/2
48	LUT	g1	620	-	-	5/29/67/67	0/2/2/2
31	CLA	B	614	-	1/1/15/20	13/37/115/115	-
31	CLA	g1	603	-	1/1/15/20	20/37/115/115	-
32	PHO	A	409	-	-	8/37/103/103	0/5/6/6
31	CLA	b	614	-	1/1/15/20	17/37/115/115	-
31	CLA	Y1	608	-	1/1/12/20	9/19/97/115	-
31	CLA	y1	602	-	1/1/15/20	16/37/115/115	-
48	LUT	R1	620	-	1/1/12/27	5/29/67/67	0/2/2/2
31	CLA	n1	603	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	R	604	-	1/1/11/20	10/18/96/115	-
31	CLA	C1	501	-	1/1/15/20	12/37/115/115	-
48	LUT	y1	620	-	-	4/29/67/67	0/2/2/2
49	XAT	N	622	-	1/1/12/26	3/31/93/93	0/4/4/4
31	CLA	A	405	-	1/1/15/20	12/37/115/115	-
50	NEX	y	623	-	-	5/27/83/83	0/3/3/3
31	CLA	c1	502	-	1/1/15/20	14/37/115/115	-
41	LHG	D1	410	-	-	22/43/43/53	-
31	CLA	C	512	-	1/1/15/20	18/37/115/115	-
41	LHG	g1	624	-	-	30/53/53/53	-
31	CLA	B1	606	-	1/1/15/20	7/37/115/115	-
33	BCR	b1	618	-	-	8/29/63/63	0/2/2/2
31	CLA	D	402	-	1/1/15/20	18/37/115/115	-
31	CLA	b	605	-	1/1/15/20	18/37/115/115	-
47	CHL	G1	608	-	3/3/15/26	1/13/111/137	-
34	SQD	C1	526	-	-	24/49/69/69	0/1/1/1
53	SPH	y1	625	-	-	11/21/21/21	-
31	CLA	r	603	-	1/1/14/20	14/31/109/115	-
31	CLA	C	506	-	1/1/15/20	23/37/115/115	-
47	CHL	N	601	20	4/4/20/26	5/39/137/137	-
33	BCR	B	618	-	-	12/29/63/63	0/2/2/2
31	CLA	A	406	-	1/1/15/20	16/37/115/115	-
31	CLA	S	602	23	1/1/14/20	13/31/109/115	-
31	CLA	A1	406	-	1/1/15/20	16/37/115/115	-
41	LHG	l	101	-	-	28/53/53/53	-
33	BCR	c	515	-	-	11/29/63/63	0/2/2/2
41	LHG	G1	624	-	-	30/53/53/53	-
31	CLA	b	603	-	1/1/15/20	19/37/115/115	-
47	CHL	Y	605	24	3/3/16/26	1/15/113/137	-
32	PHO	A	408	-	-	6/37/103/103	0/5/6/6
31	CLA	G1	603	-	1/1/15/20	17/37/115/115	-
35	LMG	b	622	-	-	12/39/59/70	0/1/1/1
35	LMG	C1	521	-	-	12/46/66/70	0/1/1/1
31	CLA	d	402	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	CHL	N	606	-	4/4/20/26	5/39/137/137	-
49	XAT	G	622	-	2/2/12/26	0/31/93/93	0/4/4/4
31	CLA	B1	607	-	1/1/15/20	17/37/115/115	-
56	ERG	r1	626	-	5/5/11/15	8/13/71/71	0/4/4/4
35	LMG	h1	102	-	-	14/43/63/70	0/1/1/1
50	NEX	N	623	-	-	7/27/83/83	0/3/3/3
31	CLA	C	504	-	1/1/15/20	15/37/115/115	-
47	CHL	n	609	-	4/4/20/26	10/39/137/137	-
31	CLA	b1	608	-	1/1/15/20	24/37/115/115	-
31	CLA	n1	604	-	1/1/15/20	14/37/115/115	-
31	CLA	g	603	-	1/1/15/20	16/37/115/115	-
31	CLA	r	613	-	1/1/11/20	8/15/93/115	-
37	C7Z	b1	620	-	1/1/12/26	15/29/67/67	0/2/2/2
40	DGD	C1	520	-	-	14/48/88/95	0/2/2/2
31	CLA	c	503	-	1/1/15/20	18/37/115/115	-
42	LMK	C1	527	-	2/2/6/6	14/46/46/60	-
48	LUT	Y	620	-	-	6/29/67/67	0/2/2/2
31	CLA	Y	603	-	1/1/15/20	17/37/115/115	-
33	BCR	b1	619	-	-	7/29/63/63	0/2/2/2
31	CLA	N	612	-	1/1/11/20	6/13/91/115	-
31	CLA	S	604	-	1/1/13/20	11/25/103/115	-
31	CLA	g	604	-	1/1/11/20	8/18/96/115	-
35	LMG	c1	523	-	-	14/50/70/70	0/1/1/1
47	CHL	s1	608	-	4/4/19/26	5/33/131/137	-
33	BCR	c	514	-	-	12/29/63/63	0/2/2/2
31	CLA	R	612	-	1/1/14/20	13/31/109/115	-
31	CLA	N	611	-	1/1/11/20	10/18/96/115	-
38	DGA	c	524	-	-	22/45/45/45	-
31	CLA	c1	507	-	1/1/15/20	19/37/115/115	-
32	PHO	a	409	-	-	11/37/103/103	0/5/6/6
31	CLA	Y	608	-	1/1/12/20	6/19/97/115	-
31	CLA	b	613	-	1/1/15/20	18/37/115/115	-
31	CLA	R	611	-	1/1/11/20	4/15/93/115	-
31	CLA	B1	614	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	j	101	-	-	14/40/60/70	0/1/1/1
31	CLA	b	615	-	1/1/15/20	11/37/115/115	-
41	LHG	d	409	-	-	29/53/53/53	-
31	CLA	a	410	-	1/1/14/20	9/31/109/115	-
47	CHL	r1	606	-	3/3/15/26	2/13/111/137	-
47	CHL	n	606	-	4/4/20/26	5/39/137/137	-
31	CLA	S	610	-	1/1/15/20	14/37/115/115	-
31	CLA	N1	613	-	1/1/15/20	18/37/115/115	-
47	CHL	S1	607	-	3/3/15/26	3/12/110/137	-
47	CHL	y1	605	-	3/3/16/26	1/15/113/137	-
47	CHL	n1	605	-	4/4/20/26	11/39/137/137	-
31	CLA	a	405	-	1/1/15/20	15/37/115/115	-
31	CLA	b	602	-	1/1/15/20	23/37/115/115	-
31	CLA	b	604	-	1/1/15/20	18/37/115/115	-
31	CLA	b1	612	-	1/1/15/20	12/37/115/115	-
31	CLA	s1	609	-	1/1/14/20	14/31/109/115	-
31	CLA	c	513	-	1/1/15/20	21/37/115/115	-
31	CLA	b1	611	-	1/1/15/20	12/37/115/115	-
33	BCR	C	514	-	-	10/29/63/63	0/2/2/2
48	LUT	S1	621	-	-	3/29/67/67	0/2/2/2
31	CLA	B	607	-	1/1/15/20	19/37/115/115	-
47	CHL	n1	601	20	4/4/20/26	10/39/137/137	-
31	CLA	c	505	-	1/1/15/20	19/37/115/115	-
47	CHL	n1	609	-	4/4/20/26	6/39/137/137	-
50	NEX	n	623	-	-	4/27/83/83	0/3/3/3
31	CLA	c1	501	-	1/1/15/20	18/37/115/115	-
31	CLA	g1	610	-	1/1/15/20	17/37/115/115	-
47	CHL	S	606	-	3/3/15/26	1/13/111/137	-
31	CLA	r1	612	-	1/1/14/20	16/31/109/115	-
40	DGD	C	518	-	-	12/44/84/95	0/2/2/2
41	LHG	S	624	-	-	28/49/49/53	-
31	CLA	g	613	-	1/1/15/20	18/37/115/115	-
31	CLA	S1	617	23	1/1/12/20	7/19/97/115	-
31	CLA	y1	603	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	Y1	610	-	1/1/15/20	15/37/115/115	-
31	CLA	N	604	-	1/1/15/20	17/37/115/115	-
32	PHO	a1	408	-	-	5/37/103/103	0/5/6/6
31	CLA	A	410	-	1/1/14/20	10/31/109/115	-
48	LUT	S	621	-	-	1/29/67/67	0/2/2/2
31	CLA	n	612	-	1/1/11/20	3/13/91/115	-
31	CLA	s	602	-	1/1/14/20	14/31/109/115	-
31	CLA	g1	611	-	1/1/15/20	16/37/115/115	-
33	BCR	C1	516	-	-	15/29/63/63	0/2/2/2
31	CLA	G	603	-	1/1/15/20	22/37/115/115	-
31	CLA	g	610	-	1/1/15/20	13/37/115/115	-
35	LMG	d	411	-	-	9/41/61/70	0/1/1/1
31	CLA	Y1	602	-	1/1/15/20	20/37/115/115	-
31	CLA	r	610	-	1/1/14/20	15/31/109/115	-
31	CLA	s	612	-	1/1/11/20	8/13/91/115	-
34	SQD	B1	626	-	-	24/49/69/69	0/1/1/1
47	CHL	n1	607	-	4/4/20/26	5/39/137/137	-
41	LHG	n1	624	-	-	35/53/53/53	-
33	BCR	c	517	-	-	11/29/63/63	0/2/2/2
46	RRX	H	101	-	1/1/11/25	10/29/65/65	0/2/2/2
31	CLA	r	608	-	1/1/14/20	15/31/109/115	-
48	LUT	N1	621	-	-	4/29/67/67	0/2/2/2
31	CLA	G1	611	-	1/1/15/20	15/37/115/115	-
31	CLA	G1	613	-	1/1/15/20	11/37/115/115	-
50	NEX	s1	623	-	-	3/27/83/83	0/3/3/3
31	CLA	b1	617	-	1/1/15/20	17/37/115/115	-
31	CLA	D	403	-	1/1/15/20	15/37/115/115	-
31	CLA	C1	509	-	1/1/15/20	15/37/115/115	-
31	CLA	N1	602	-	1/1/15/20	12/37/115/115	-
31	CLA	B	610	-	1/1/15/20	19/37/115/115	-
31	CLA	R1	603	-	1/1/14/20	12/31/109/115	-
41	LHG	g	624	-	-	28/53/53/53	-
31	CLA	r	602	-	1/1/14/20	6/31/109/115	-
31	CLA	s	611	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	s	604	-	1/1/13/20	11/25/103/115	-
33	BCR	C1	515	-	-	11/29/63/63	0/2/2/2
31	CLA	n1	602	-	1/1/15/20	18/37/115/115	-
54	4RF	k1	101	-	-	35/59/59/59	-
53	SPH	y	625	-	-	13/21/21/21	-
31	CLA	A	407	-	1/1/11/20	4/18/96/115	-
57	PTY	Y1	627	-	-	12/20/20/53	-
31	CLA	G	611	-	1/1/11/20	4/13/91/115	-
31	CLA	G	613	-	1/1/15/20	18/37/115/115	-
35	LMG	a1	413	-	-	14/43/63/70	0/1/1/1
50	NEX	S	622	-	-	12/27/83/83	0/3/3/3
57	PTY	Y1	626	-	-	19/53/53/53	-
49	XAT	y1	622	-	-	4/31/93/93	0/4/4/4
31	CLA	Y	614	-	1/1/15/20	11/37/115/115	-
31	CLA	A1	410	-	1/1/14/20	8/31/109/115	-
54	4RF	i1	101	-	-	27/59/59/59	-
31	CLA	D1	403	-	1/1/15/20	17/37/115/115	-
31	CLA	c	512	-	1/1/15/20	21/37/115/115	-
31	CLA	b1	603	-	1/1/15/20	15/37/115/115	-
47	CHL	N	608	-	3/3/16/26	7/20/118/137	-
47	CHL	G1	605	-	4/4/16/26	5/18/116/137	-
33	BCR	B	619	-	-	3/29/63/63	0/2/2/2
31	CLA	Y1	611	-	1/1/15/20	14/37/115/115	-
31	CLA	B	615	-	1/1/15/20	10/37/115/115	-
31	CLA	Y1	613	-	1/1/15/20	21/37/115/115	-
31	CLA	C1	512	-	1/1/15/20	19/37/115/115	-
40	DGD	C1	519	-	-	21/51/91/95	0/2/2/2
31	CLA	g	602	-	1/1/15/20	22/37/115/115	-
31	CLA	C1	511	-	1/1/15/20	12/37/115/115	-
35	LMG	H1	102	-	-	14/43/63/70	0/1/1/1
31	CLA	S1	613	-	1/1/13/20	8/25/103/115	-
35	LMG	D	411	-	-	9/41/61/70	0/1/1/1
31	CLA	R	602	-	1/1/14/20	12/31/109/115	-
46	RRX	h1	101	-	1/1/11/25	9/29/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	CHL	R	606	-	3/3/15/26	5/13/111/137	-
33	BCR	C1	517	-	-	12/29/63/63	0/2/2/2
38	DGA	c1	524	-	-	23/45/45/45	-
45	HEM	f1	101	-	-	0/12/54/54	-
31	CLA	s1	602	-	1/1/14/20	11/31/109/115	-
34	SQD	B	621	-	-	18/49/69/69	0/1/1/1
31	CLA	d1	402	-	1/1/15/20	17/37/115/115	-
48	LUT	R	620	-	-	9/29/67/67	0/2/2/2
31	CLA	y	612	-	1/1/15/20	12/37/115/115	-
34	SQD	b1	626	-	-	23/49/69/69	0/1/1/1
31	CLA	R	603	-	1/1/14/20	16/31/109/115	-
31	CLA	Y1	604	-	1/1/15/20	18/37/115/115	-
31	CLA	n	614	-	1/1/11/20	5/18/96/115	-
31	CLA	c1	513	-	1/1/15/20	20/37/115/115	-
40	DGD	C1	518	-	-	14/44/84/95	0/2/2/2
31	CLA	n	613	-	1/1/15/20	16/37/115/115	-
34	SQD	A1	412	-	-	15/46/66/69	0/1/1/1
31	CLA	b	617	-	1/1/15/20	14/37/115/115	-
31	CLA	r1	608	-	1/1/14/20	22/31/109/115	-
31	CLA	R	608	-	1/1/14/20	17/31/109/115	-
31	CLA	a1	406	-	1/1/15/20	16/37/115/115	-
31	CLA	b1	605	-	1/1/15/20	19/37/115/115	-
40	DGD	b1	623	-	-	11/32/72/95	0/2/2/2
31	CLA	R1	612	-	1/1/14/20	14/31/109/115	-
33	BCR	d1	404	-	-	12/29/63/63	0/2/2/2
31	CLA	G1	612	-	1/1/10/20	5/11/89/115	-
31	CLA	C1	513	-	1/1/15/20	19/37/115/115	-
48	LUT	S	620	-	1/1/12/27	3/29/67/67	0/2/2/2
31	CLA	D1	402	-	1/1/15/20	22/37/115/115	-
48	LUT	Y1	621	-	-	2/29/67/67	0/2/2/2
40	DGD	c	519	-	-	22/51/91/95	0/2/2/2
31	CLA	C1	505	-	1/1/15/20	19/37/115/115	-
31	CLA	B1	603	-	1/1/15/20	18/37/115/115	-
31	CLA	c1	506	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	c1	521	-	-	12/46/66/70	0/1/1/1
31	CLA	r1	609	-	1/1/14/20	13/31/109/115	-
47	CHL	S1	606	-	3/3/15/26	2/13/111/137	-
34	SQD	a	412	-	-	13/46/66/69	0/1/1/1
53	SPH	Y	625	-	-	12/21/21/21	-
53	SPH	A1	414	-	-	13/21/21/21	-
48	LUT	s	620	-	1/1/12/27	3/29/67/67	0/2/2/2
35	LMG	A	413	-	-	12/43/63/70	0/1/1/1
57	PTY	y1	626	-	-	24/53/53/53	-
33	BCR	b	618	-	-	10/29/63/63	0/2/2/2
31	CLA	a	407	-	1/1/11/20	5/18/96/115	-
35	LMG	W1	201	-	-	16/34/54/70	0/1/1/1
41	LHG	d1	408	-	-	29/48/48/53	-
31	CLA	C1	507	-	1/1/15/20	16/37/115/115	-
41	LHG	d	410	-	-	32/43/43/53	-
47	CHL	g1	606	-	3/3/16/26	4/20/118/137	-
50	NEX	N1	623	-	-	5/27/83/83	0/3/3/3
41	LHG	n	624	-	-	31/53/53/53	-
31	CLA	s1	614	-	1/1/13/20	9/25/103/115	-
47	CHL	s	607	-	4/4/15/26	1/12/110/137	-
41	LHG	D	408	-	-	31/48/48/53	-
41	LHG	d1	409	-	-	32/53/53/53	-
51	LPX	s1	625	-	-	15/31/31/31	-
55	LMT	r1	625	-	-	9/21/61/61	0/2/2/2
31	CLA	S1	602	-	1/1/14/20	17/31/109/115	-
31	CLA	g1	602	-	1/1/15/20	19/37/115/115	-
31	CLA	y1	613	-	1/1/15/20	24/37/115/115	-
47	CHL	N1	609	-	4/4/20/26	8/39/137/137	-
37	C7Z	B1	620	-	1/1/12/26	11/29/67/67	0/2/2/2
31	CLA	b	610	-	1/1/15/20	16/37/115/115	-
31	CLA	Y	613	-	1/1/15/20	21/37/115/115	-
31	CLA	N1	614	-	1/1/11/20	5/18/96/115	-
41	LHG	L1	101	-	-	35/53/53/53	-
31	CLA	B	617	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	511	-	1/1/15/20	14/37/115/115	-
31	CLA	C	502	-	1/1/15/20	18/37/115/115	-
38	DGA	C1	524	-	-	34/45/45/45	-
47	CHL	g	606	-	3/3/16/26	6/20/118/137	-
47	CHL	Y1	607	-	4/4/20/26	8/39/137/137	-
33	BCR	B1	619	-	-	7/29/63/63	0/2/2/2
40	DGD	c	518	-	-	8/44/84/95	0/2/2/2
47	CHL	s1	607	-	3/3/15/26	1/12/110/137	-
35	LMG	D1	411	-	-	11/41/61/70	0/1/1/1
47	CHL	g1	607	-	4/4/20/26	9/39/137/137	-
33	BCR	C1	514	-	-	16/29/63/63	0/2/2/2
50	NEX	Y	623	-	-	3/27/83/83	0/3/3/3
41	LHG	d	408	-	-	30/48/48/53	-
31	CLA	A1	407	-	1/1/12/20	9/19/97/115	-
33	BCR	a	411	-	-	10/29/63/63	0/2/2/2
47	CHL	G1	609	-	4/4/20/26	9/39/137/137	-
31	CLA	b	611	-	1/1/15/20	10/37/115/115	-
31	CLA	s	603	-	1/1/15/20	18/37/115/115	-
41	LHG	Y1	624	-	-	26/53/53/53	-
52	3PH	S	626	-	-	19/49/49/49	-
31	CLA	G	602	-	1/1/15/20	22/37/115/115	-
31	CLA	b1	614	-	1/1/15/20	13/37/115/115	-
31	CLA	R1	610	-	1/1/14/20	13/31/109/115	-
50	NEX	g	623	-	-	4/27/83/83	0/3/3/3
31	CLA	C	510	-	1/1/15/20	17/37/115/115	-
38	DGA	B1	625	-	-	24/45/45/45	-
51	LPX	s	625	-	-	13/31/31/31	-
31	CLA	b	616	-	1/1/15/20	11/37/115/115	-
33	BCR	a1	411	-	-	13/29/63/63	0/2/2/2
31	CLA	B1	616	-	1/1/15/20	12/37/115/115	-
31	CLA	c1	510	-	1/1/15/20	17/37/115/115	-
31	CLA	C	513	-	1/1/15/20	21/37/115/115	-
31	CLA	S	611	-	1/1/15/20	16/37/115/115	-
47	CHL	G	609	-	4/4/20/26	12/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	HEM	F1	101	6	-	1/12/54/54	-
47	CHL	s	608	-	4/4/19/26	3/33/131/137	-
31	CLA	y	611	-	1/1/15/20	18/37/115/115	-
46	RRX	H1	101	-	1/1/11/25	5/29/65/65	0/2/2/2
47	CHL	N	609	-	4/4/20/26	8/39/137/137	-
40	DGD	c1	520	-	-	12/48/88/95	0/2/2/2
31	CLA	b1	606	-	1/1/15/20	12/37/115/115	-
31	CLA	N	614	-	1/1/11/20	6/18/96/115	-
31	CLA	N	602	-	1/1/15/20	15/37/115/115	-
49	XAT	n	622	-	-	2/31/93/93	0/4/4/4
33	BCR	c1	517	-	-	8/29/63/63	0/2/2/2
54	4RF	K1	101	-	-	31/59/59/59	-
31	CLA	b1	615	-	1/1/15/20	21/37/115/115	-
35	LMG	h	102	-	-	13/43/63/70	0/1/1/1
50	NEX	s	623	-	-	7/27/83/83	0/3/3/3
31	CLA	b1	613	-	1/1/15/20	20/37/115/115	-
31	CLA	r	604	-	1/1/11/20	9/18/96/115	-
31	CLA	B	605	-	1/1/15/20	18/37/115/115	-
48	LUT	Y	621	-	1/1/12/27	2/29/67/67	0/2/2/2
48	LUT	s	621	-	-	1/29/67/67	0/2/2/2
47	CHL	n	601	-	4/4/20/26	6/39/137/137	-
31	CLA	r1	610	-	1/1/14/20	17/31/109/115	-
31	CLA	Y	602	24	1/1/15/20	21/37/115/115	-
31	CLA	b	607	-	1/1/15/20	16/37/115/115	-
31	CLA	B	606	-	1/1/15/20	14/37/115/115	-
31	CLA	b1	604	-	1/1/15/20	16/37/115/115	-
33	BCR	c1	514	-	-	14/29/63/63	0/2/2/2
31	CLA	c	508	-	1/1/15/20	13/37/115/115	-
39	GOL	B	627	-	-	0/4/4/4	-
47	CHL	S	608	-	4/4/19/26	3/33/131/137	-
38	DGA	B	625	-	-	28/45/45/45	-
31	CLA	s	617	-	1/1/12/20	9/19/97/115	-
31	CLA	B1	610	-	1/1/15/20	14/37/115/115	-
47	CHL	y1	607	-	4/4/20/26	9/39/137/137	-
31	CLA	r1	602	-	1/1/14/20	13/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	616	-	1/1/15/20	13/37/115/115	-
35	LMG	J	101	-	-	15/40/60/70	0/1/1/1
50	NEX	Y1	623	-	-	8/27/83/83	0/3/3/3
31	CLA	s	610	-	1/1/15/20	22/37/115/115	-
48	LUT	n1	621	-	-	3/29/67/67	0/2/2/2
31	CLA	B1	608	-	1/1/15/20	24/37/115/115	-
50	NEX	S1	623	-	-	3/27/83/83	0/3/3/3
50	NEX	g1	623	-	-	3/27/83/83	0/3/3/3
31	CLA	s	605	-	1/1/12/20	8/19/97/115	-
32	PHO	A1	409	-	-	14/37/103/103	0/5/6/6
41	LHG	y1	624	-	-	27/53/53/53	-
47	CHL	Y1	601	24	4/4/20/26	2/39/137/137	-
33	BCR	c	516	-	-	12/29/63/63	0/2/2/2
41	LHG	C1	525	-	-	32/51/51/53	-
31	CLA	n	603	-	1/1/15/20	26/37/115/115	-
31	CLA	n1	614	-	1/1/11/20	7/18/96/115	-
50	NEX	n1	623	-	-	4/27/83/83	1/3/3/3
49	XAT	N1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
37	C7Z	B	620	-	1/1/12/26	11/29/67/67	0/2/2/2
48	LUT	N	620	-	-	6/29/67/67	0/2/2/2
50	NEX	G1	623	-	-	2/27/83/83	0/3/3/3
55	LMT	R1	625	-	-	9/21/61/61	0/2/2/2
33	BCR	D	404	-	-	13/29/63/63	0/2/2/2
51	LPX	S1	625	-	-	10/31/31/31	-
33	BCR	A	411	-	-	13/29/63/63	0/2/2/2
50	NEX	r	623	-	-	8/27/83/83	0/3/3/3
47	CHL	Y	606	-	4/4/20/26	6/39/137/137	-
56	ERG	R1	626	-	5/5/11/15	7/13/71/71	0/4/4/4
42	LMK	c	627	-	1/1/6/6	11/46/46/60	-
40	DGD	c	523	-	-	16/55/95/95	0/2/2/2
31	CLA	N1	610	-	1/1/15/20	18/37/115/115	-
47	CHL	N1	601	20	4/4/20/26	3/39/137/137	-
47	CHL	y	609	-	4/4/20/26	6/39/137/137	-
31	CLA	y	603	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	G	630	-	-	30/53/53/53	-
31	CLA	a1	407	-	1/1/11/20	7/18/96/115	-
31	CLA	y	608	-	1/1/12/20	6/19/97/115	-
31	CLA	B	603	-	1/1/15/20	19/37/115/115	-
31	CLA	N	613	-	1/1/15/20	18/37/115/115	-
31	CLA	S1	611	-	1/1/15/20	18/37/115/115	-
31	CLA	a1	410	-	1/1/14/20	9/31/109/115	-
47	CHL	Y	607	-	4/4/20/26	8/39/137/137	-
41	LHG	Y	624	-	-	32/53/53/53	-
50	NEX	R	622	-	-	11/27/83/83	0/3/3/3
31	CLA	B	608	-	1/1/15/20	21/37/115/115	-
31	CLA	b1	610	-	1/1/15/20	15/37/115/115	-
31	CLA	S	605	-	1/1/12/20	10/19/97/115	-
47	CHL	S	607	-	4/4/15/26	1/12/110/137	-
47	CHL	g	607	-	3/3/16/26	3/20/118/137	-
31	CLA	B1	612	-	1/1/15/20	11/37/115/115	-
47	CHL	N1	606	-	4/4/20/26	12/39/137/137	-
31	CLA	s1	612	-	1/1/11/20	6/13/91/115	-
47	CHL	r	607	-	3/3/16/26	6/20/118/137	-
48	LUT	r	620	-	-	8/29/67/67	0/2/2/2
31	CLA	N	610	-	1/1/15/20	9/37/115/115	-
31	CLA	s	613	-	1/1/13/20	10/25/103/115	-
31	CLA	s1	610	-	1/1/15/20	17/37/115/115	-
31	CLA	C	508	-	1/1/15/20	15/37/115/115	-
47	CHL	s1	601	23	3/3/16/26	3/15/113/137	-
32	PHO	a1	409	-	-	11/37/103/103	0/5/6/6
31	CLA	S	603	-	1/1/15/20	10/37/115/115	-
54	4RF	I1	102	-	-	35/59/59/59	-
31	CLA	c	502	-	1/1/15/20	13/37/115/115	-
53	SPH	Y1	625	-	-	11/21/21/21	-
31	CLA	s1	617	-	1/1/12/20	7/19/97/115	-
31	CLA	s	609	-	1/1/14/20	14/31/109/115	-
31	CLA	c1	511	-	1/1/15/20	13/37/115/115	-
31	CLA	y	604	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	G1	610	-	1/1/15/20	14/37/115/115	-
57	PTY	y1	627	-	-	14/20/20/53	-
39	GOL	y	626	-	-	0/4/4/4	-
47	CHL	n1	608	-	3/3/16/26	3/20/118/137	-
31	CLA	R	609	-	1/1/14/20	17/31/109/115	-
31	CLA	B1	617	-	1/1/15/20	15/37/115/115	-
47	CHL	n	605	-	4/4/20/26	5/39/137/137	-
35	LMG	d1	411	-	-	12/41/61/70	0/1/1/1
35	LMG	B	622	-	-	11/39/59/70	0/1/1/1
47	CHL	G	601	-	4/4/20/26	6/39/137/137	-
48	LUT	N	621	-	-	3/29/67/67	0/2/2/2
53	SPH	a1	414	-	-	12/21/21/21	-

The worst 5 of 3725 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H	101	RRX	C21-C22	66.78	2.24	1.35
56	R1	626	ERG	C1-C10	-23.16	1.10	1.54
56	r1	626	ERG	C1-C10	-22.95	1.10	1.54
56	r1	626	ERG	C10-C9	-20.09	1.28	1.55
56	R1	626	ERG	C10-C9	-19.60	1.29	1.55

The worst 5 of 8419 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	H	101	RRX	C37-C22-C23	-30.79	69.57	118.08
41	L1	101	LHG	O7-C7-C8	23.38	161.90	111.50
31	R1	609	CLA	C4-C3-C5	-22.81	76.90	115.27
52	S1	626	3PH	O21-C21-C22	22.50	160.00	111.50
31	B	617	CLA	C4-C3-C5	-22.49	77.43	115.27

5 of 694 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	A	405	CLA	ND
31	A	406	CLA	ND
31	A	407	CLA	ND
31	A	410	CLA	ND
31	B	602	CLA	ND

5 of 8670 torsion outliers are listed below:

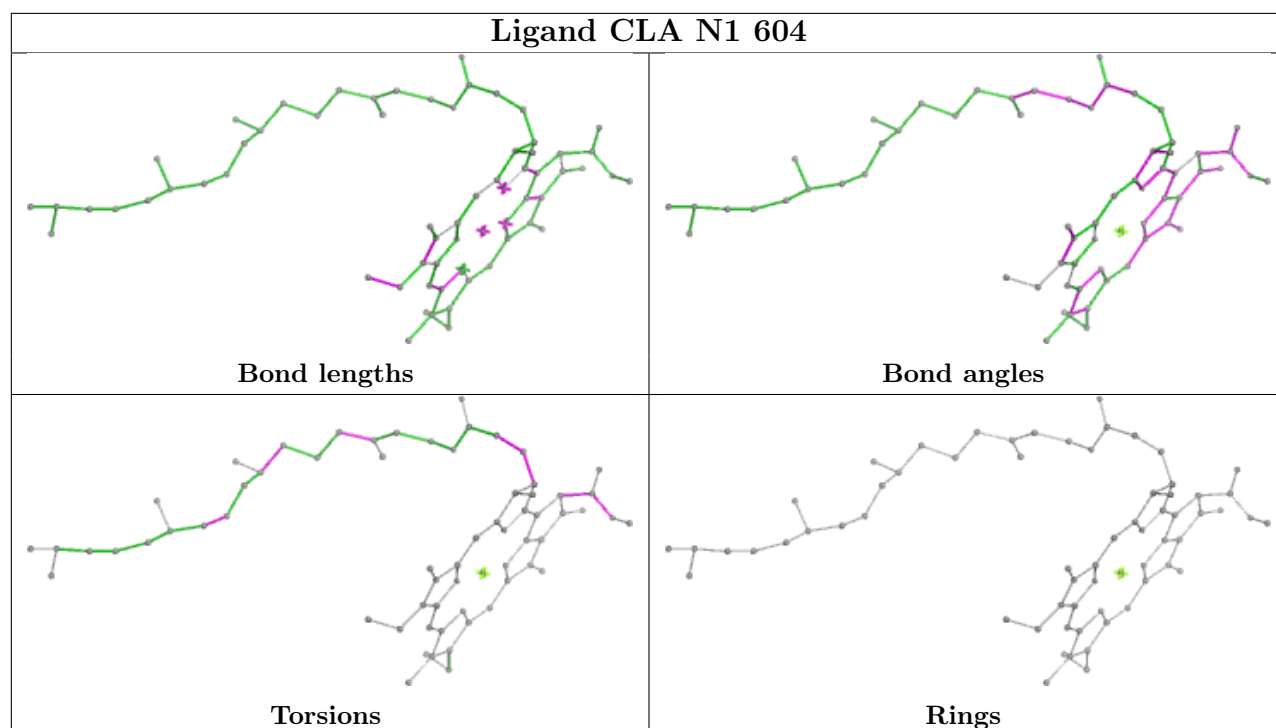
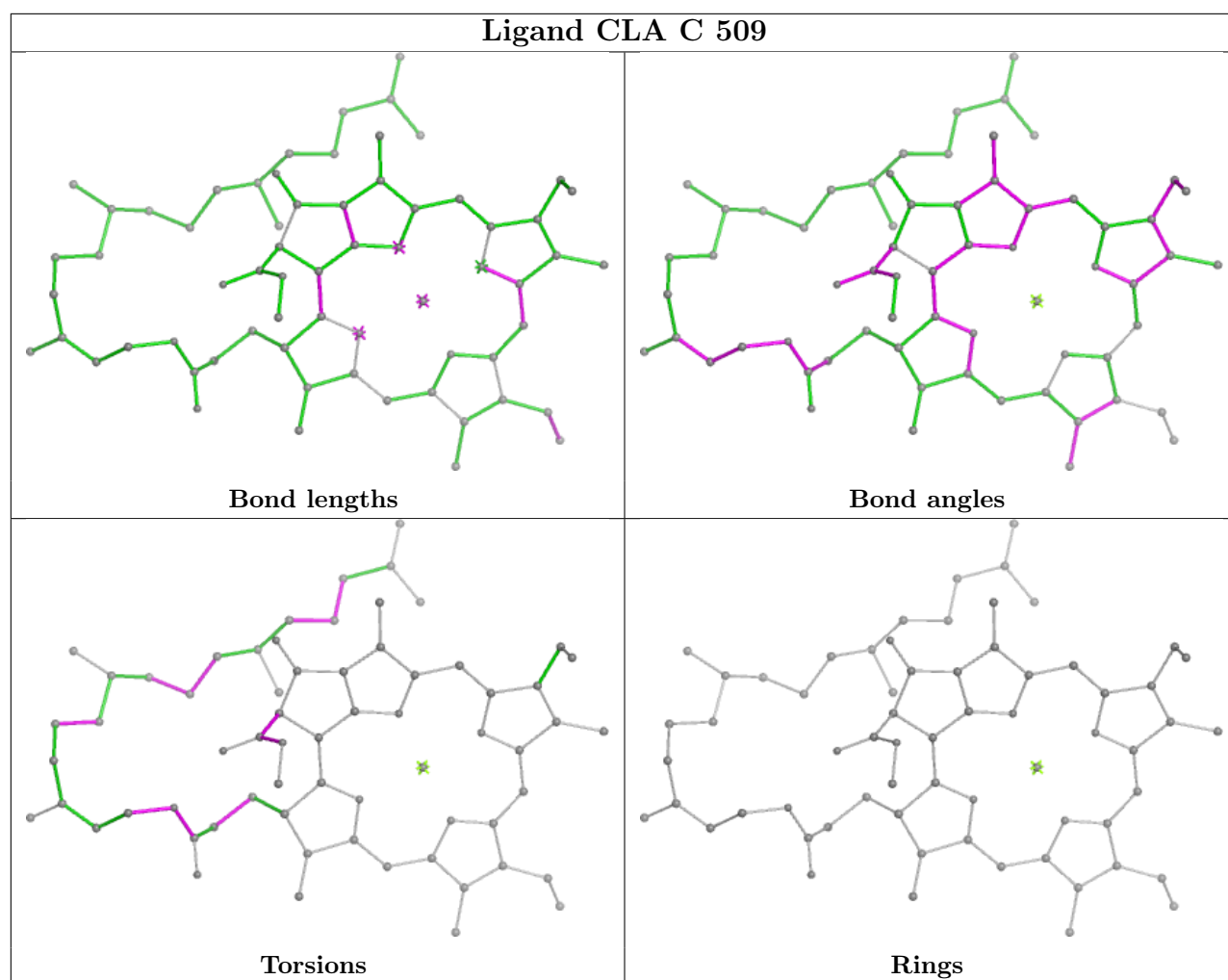
Mol	Chain	Res	Type	Atoms
31	A	405	CLA	CBD-CGD-O2D-CED
31	A	406	CLA	C1A-C2A-CAA-CBA
31	A	406	CLA	C3A-C2A-CAA-CBA
31	A	406	CLA	CHA-CBD-CGD-O1D
31	A	406	CLA	CHA-CBD-CGD-O2D

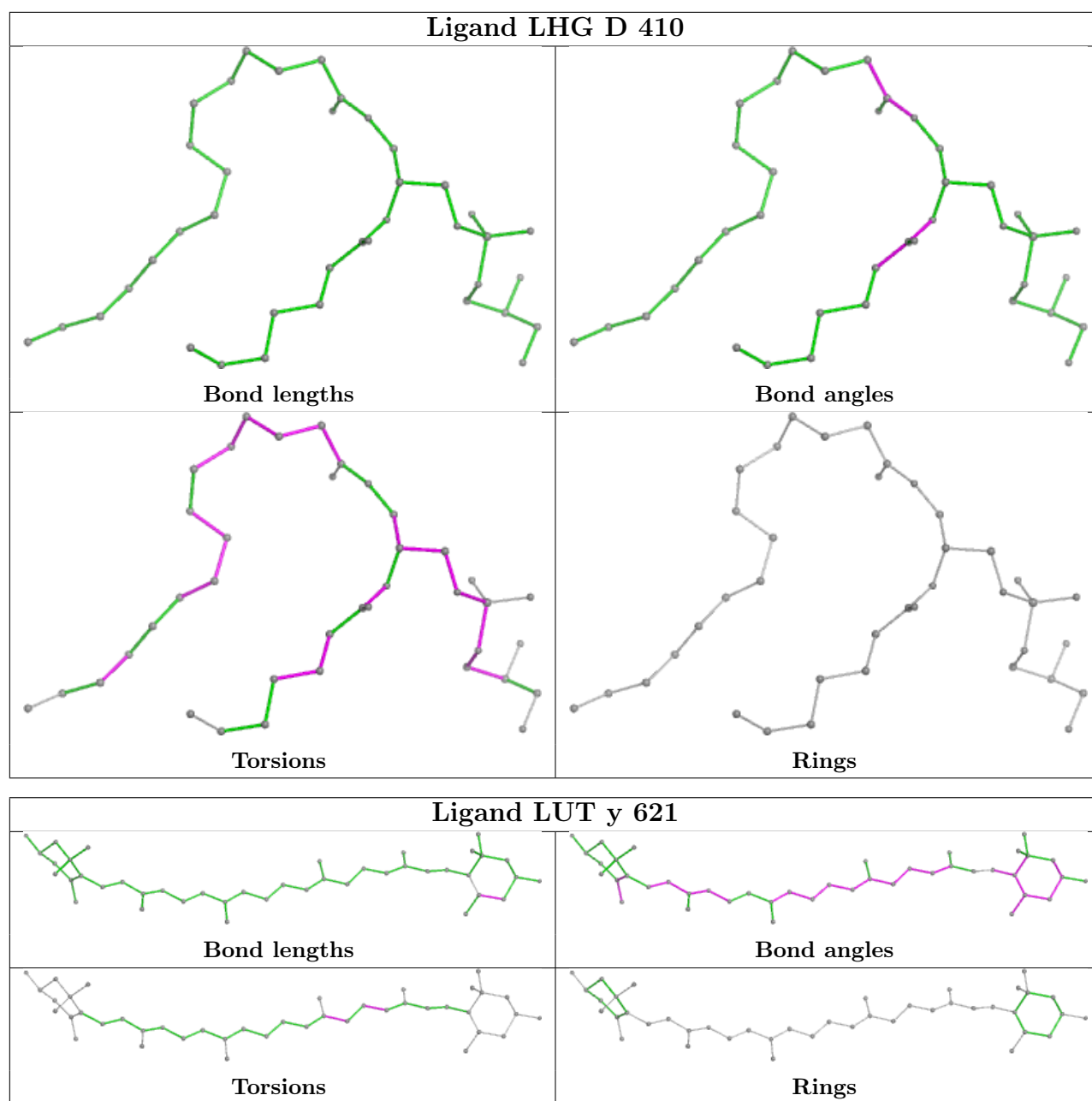
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	n1	623	NEX	C1-C2-C3-C4-C5-C6

No monomer is involved in short contacts.

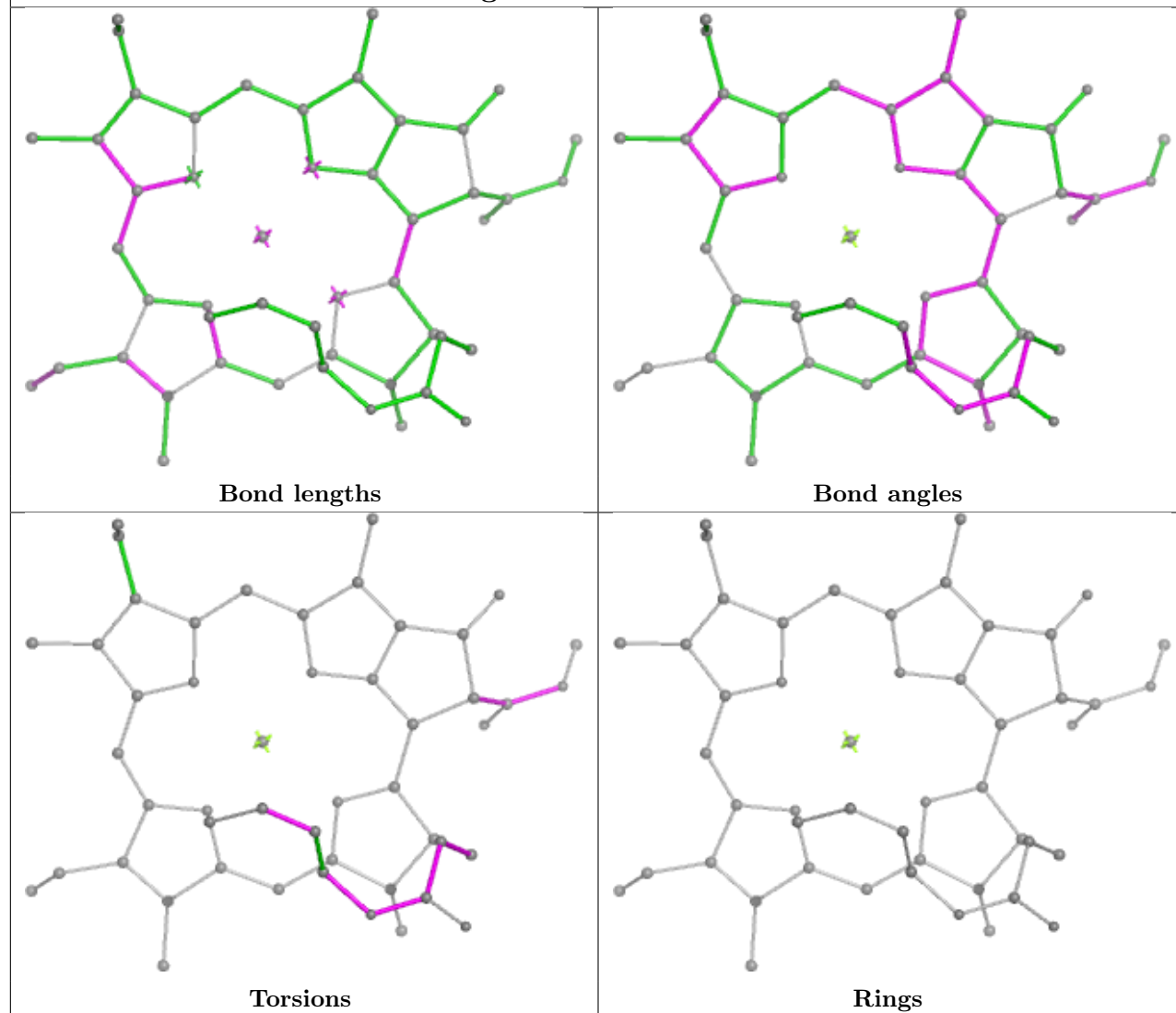
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



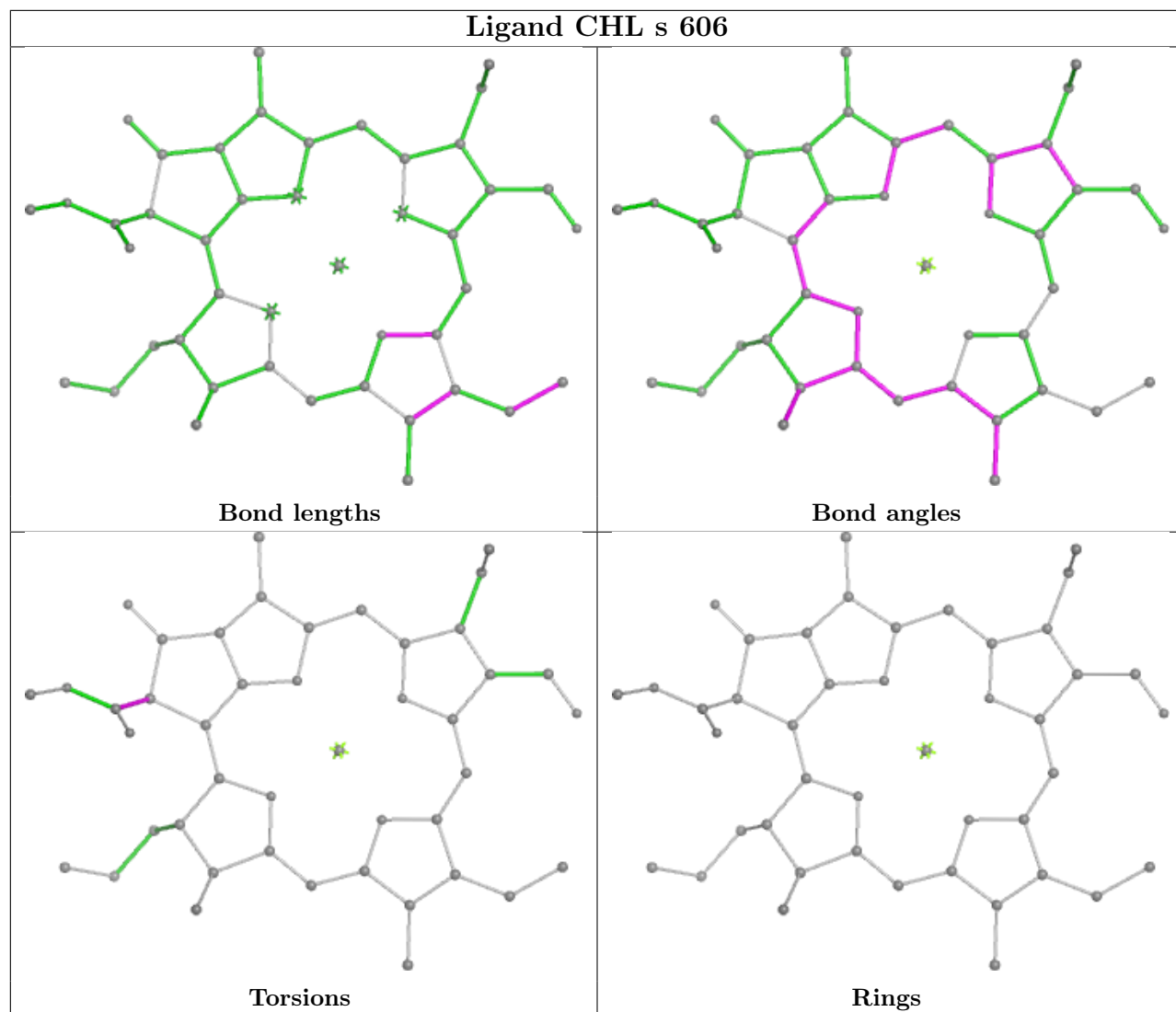


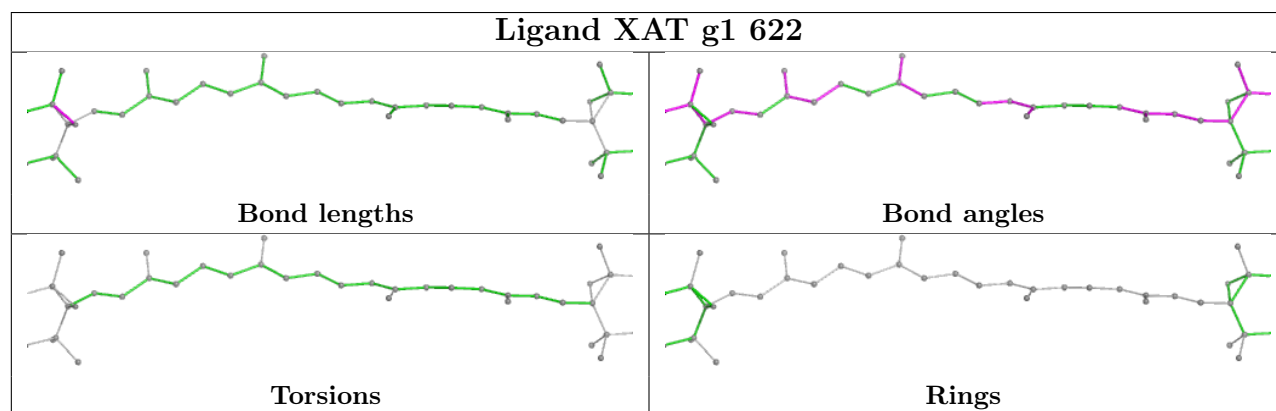
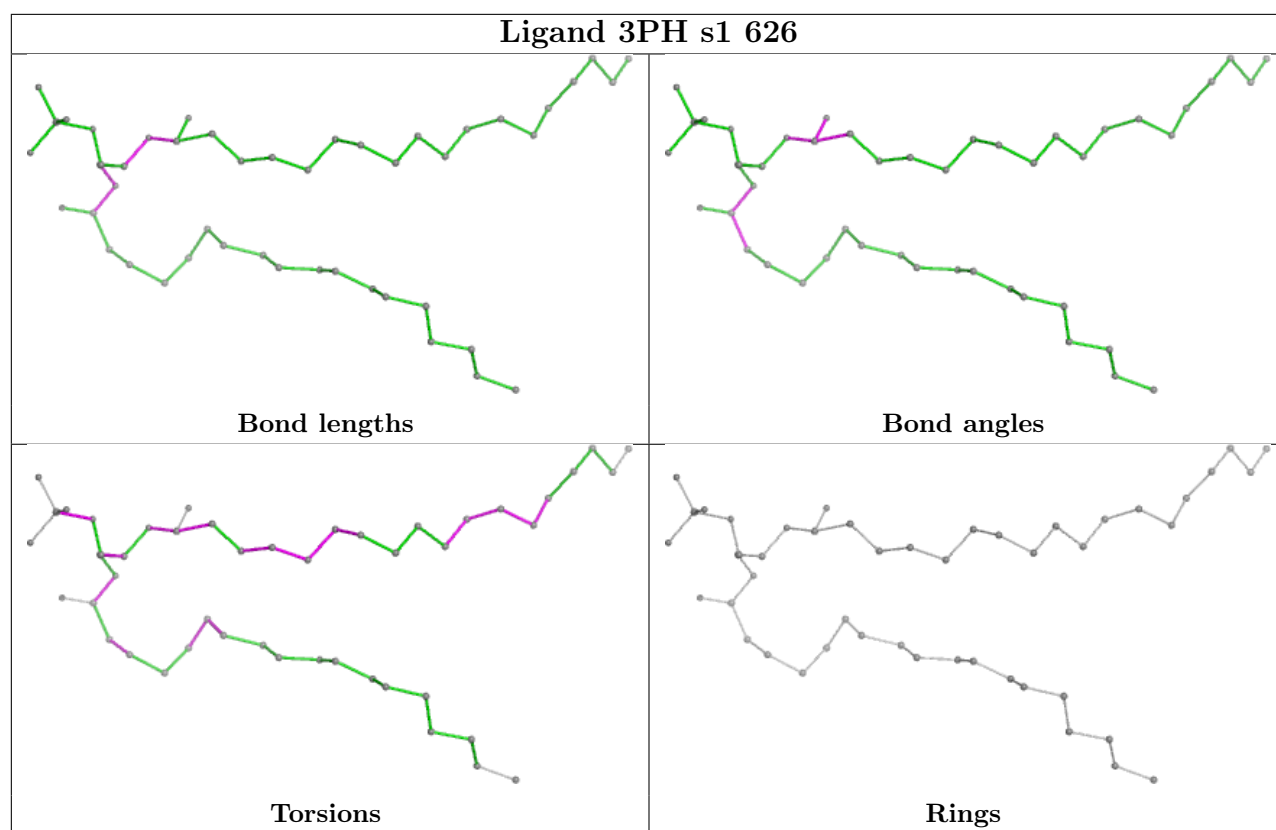


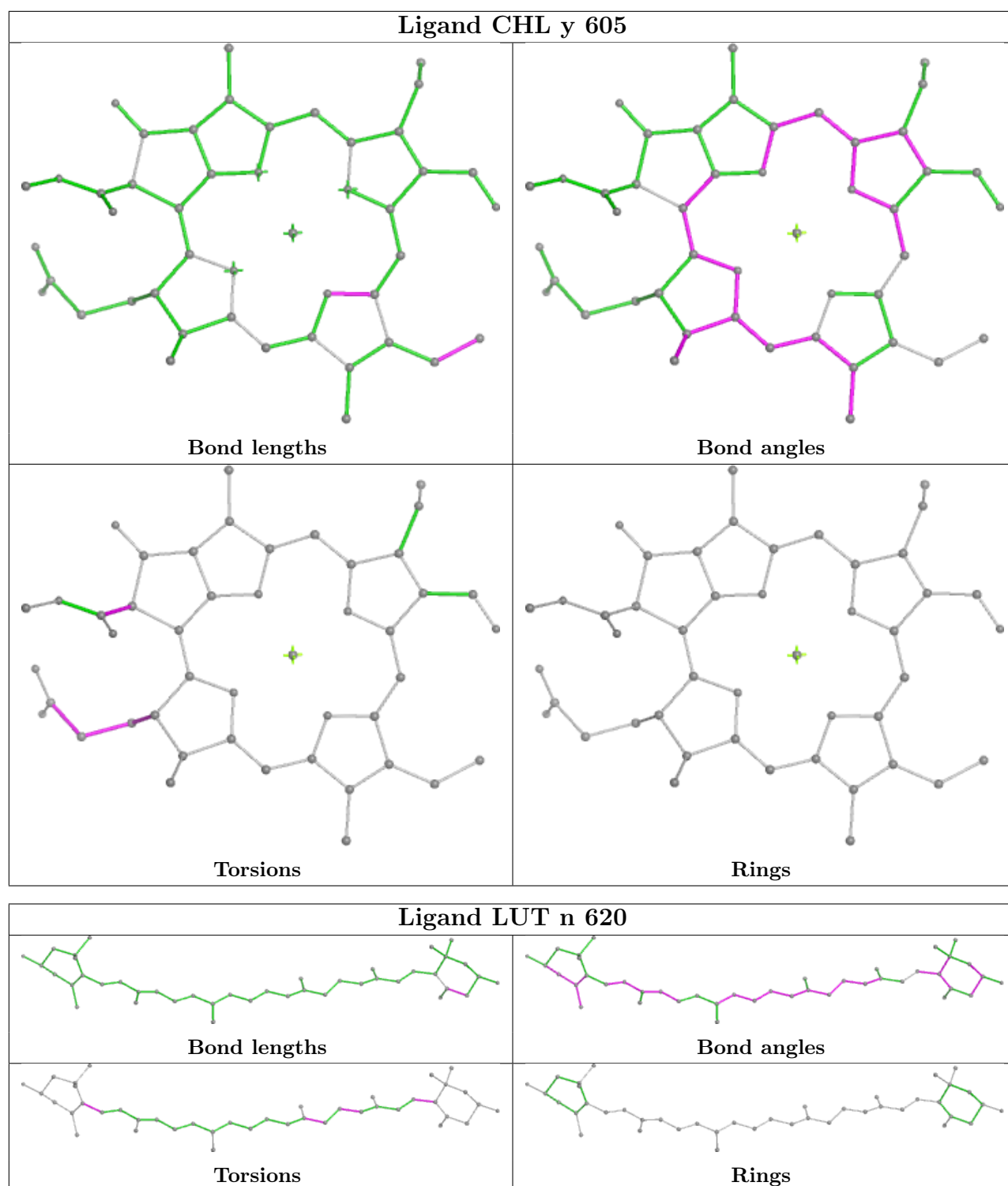
## Ligand CLA G1 614

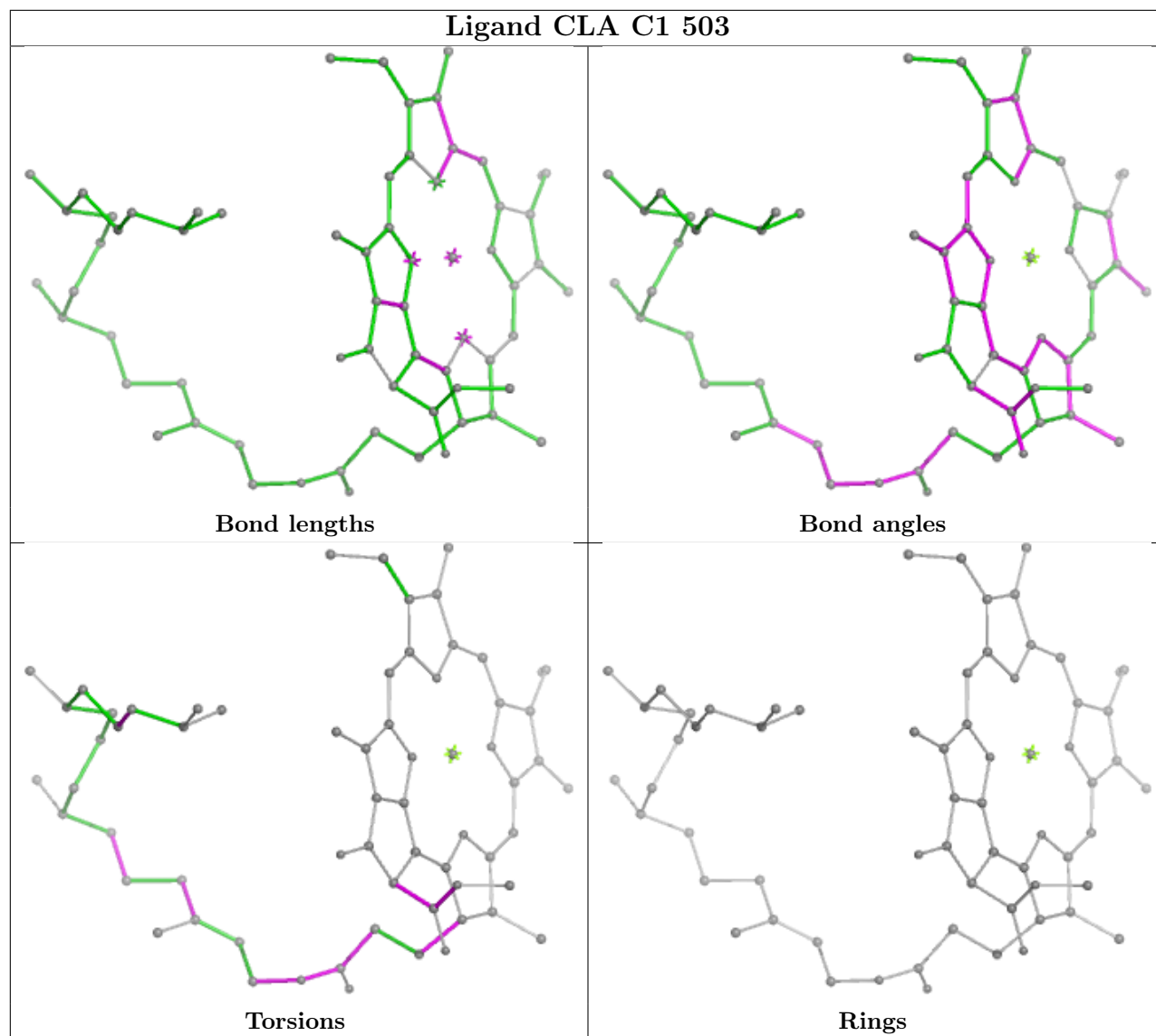


## Ligand CHL s 606

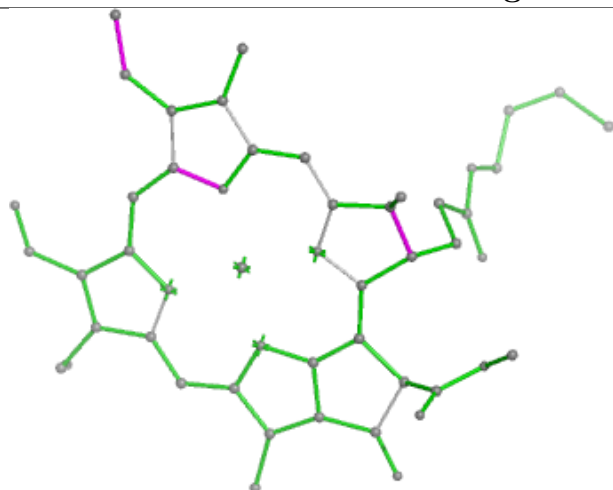




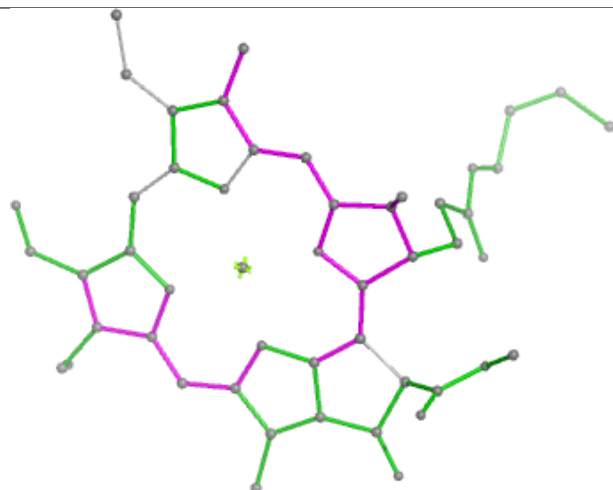




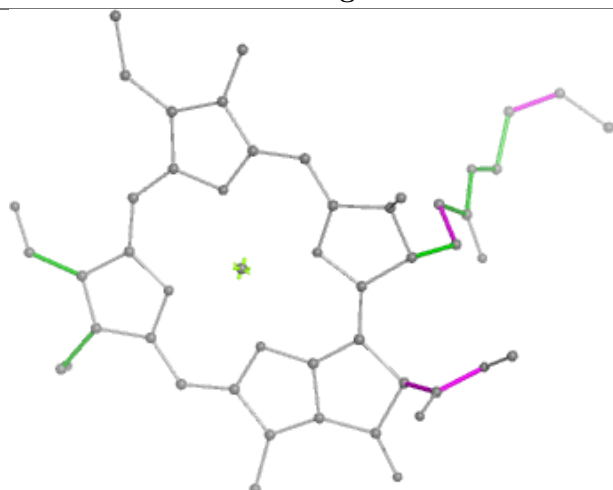
## Ligand CHL N1 608



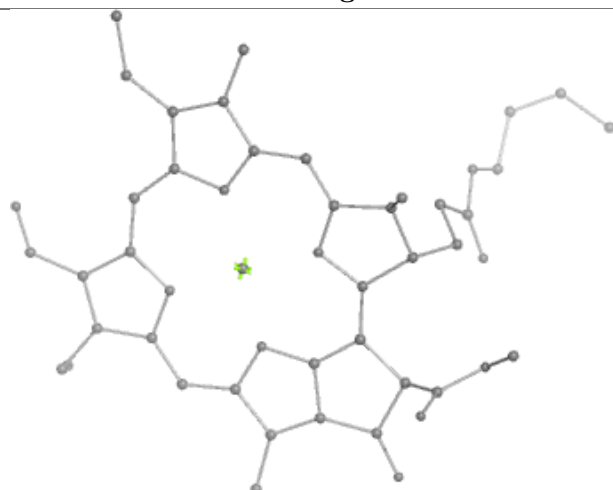
Bond lengths



Bond angles

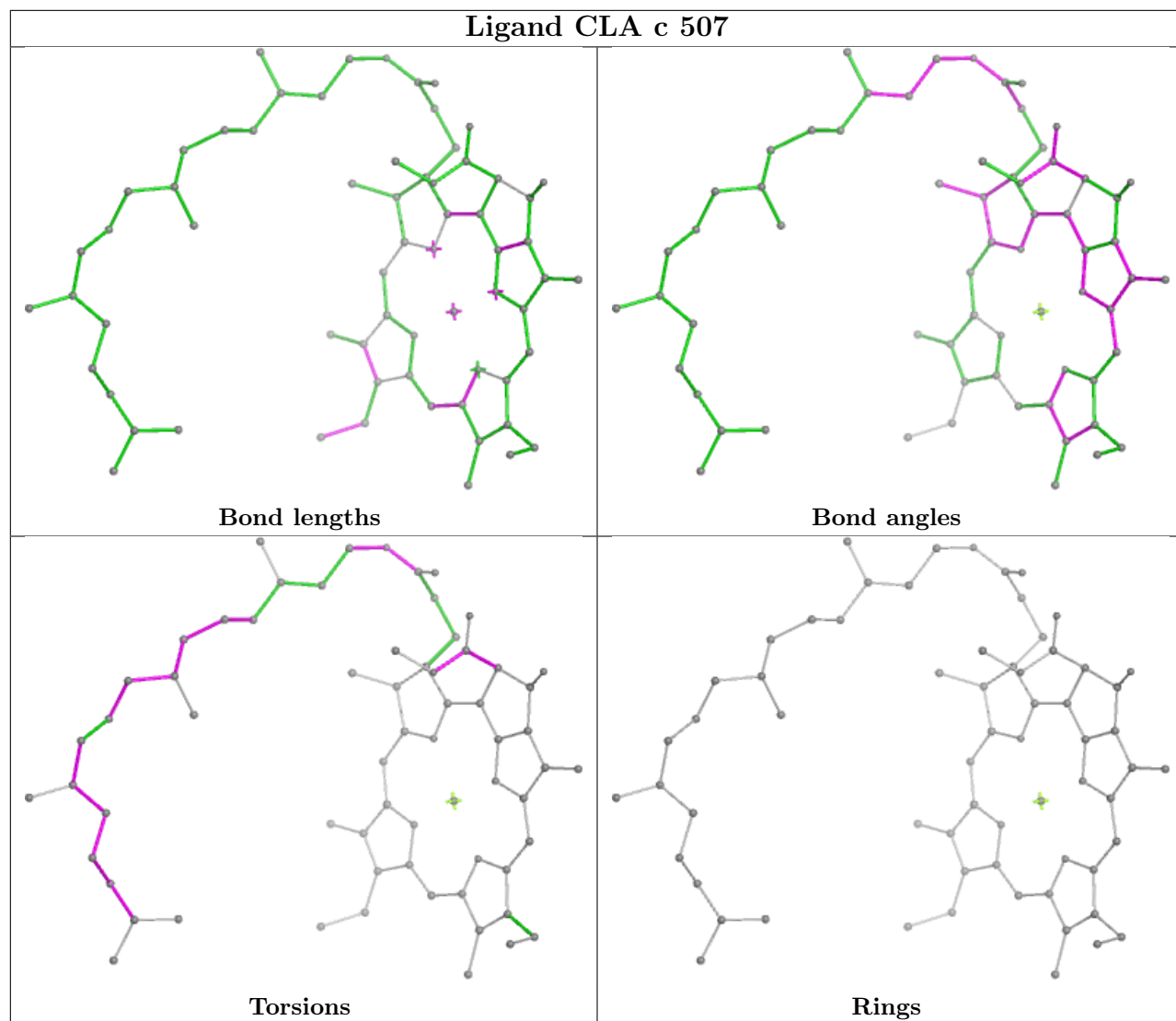


Torsions

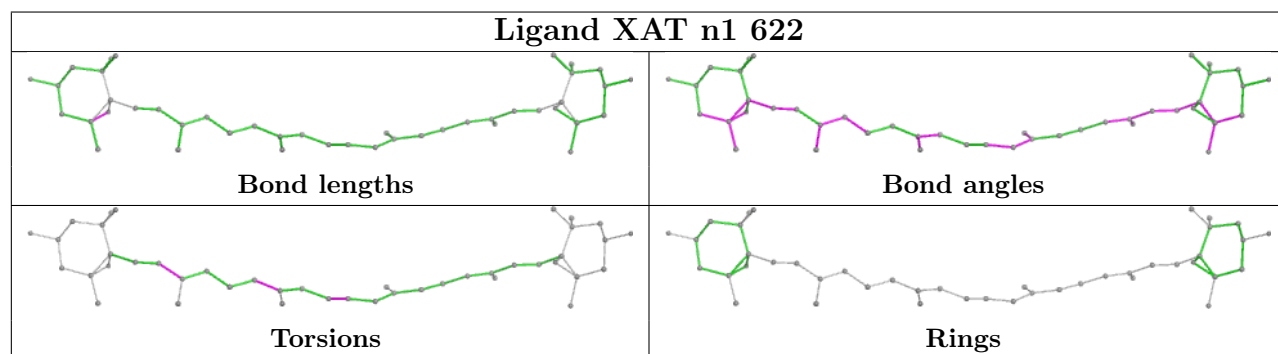


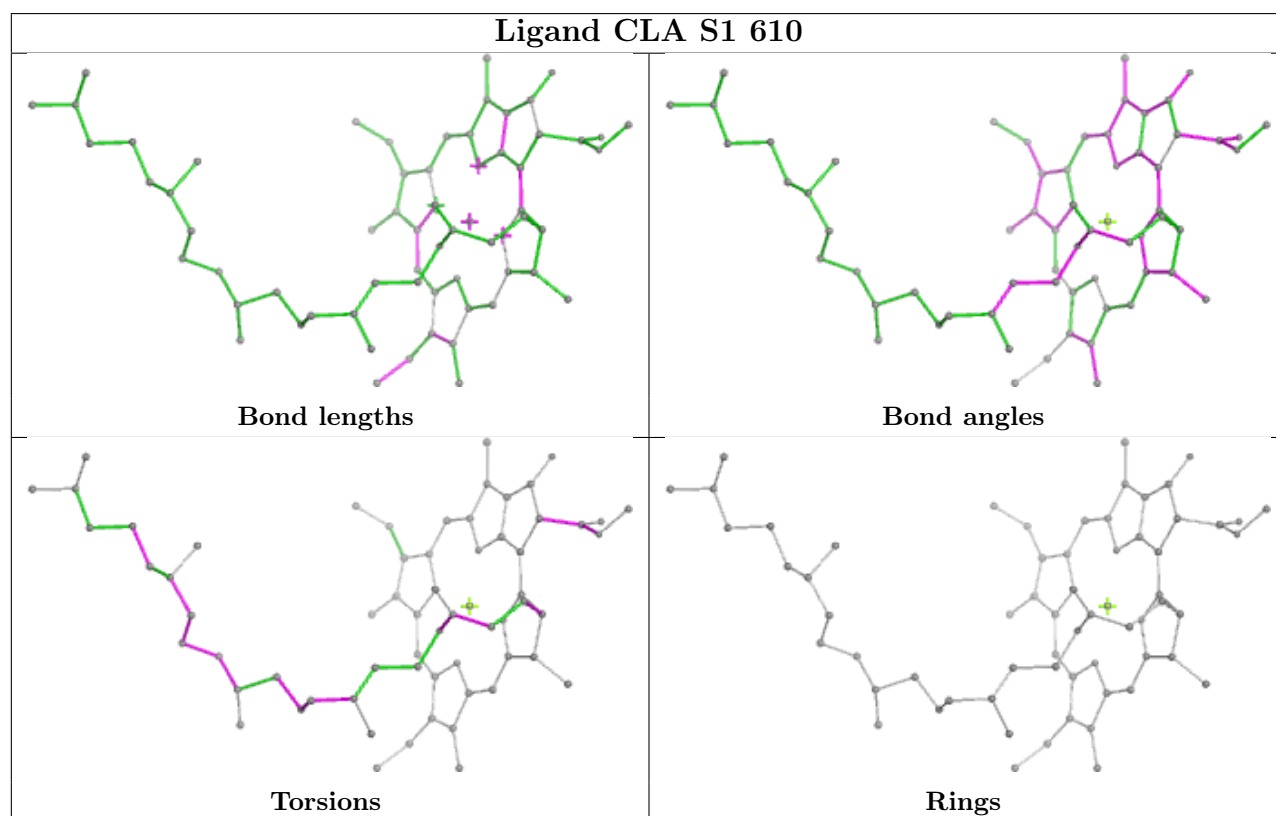
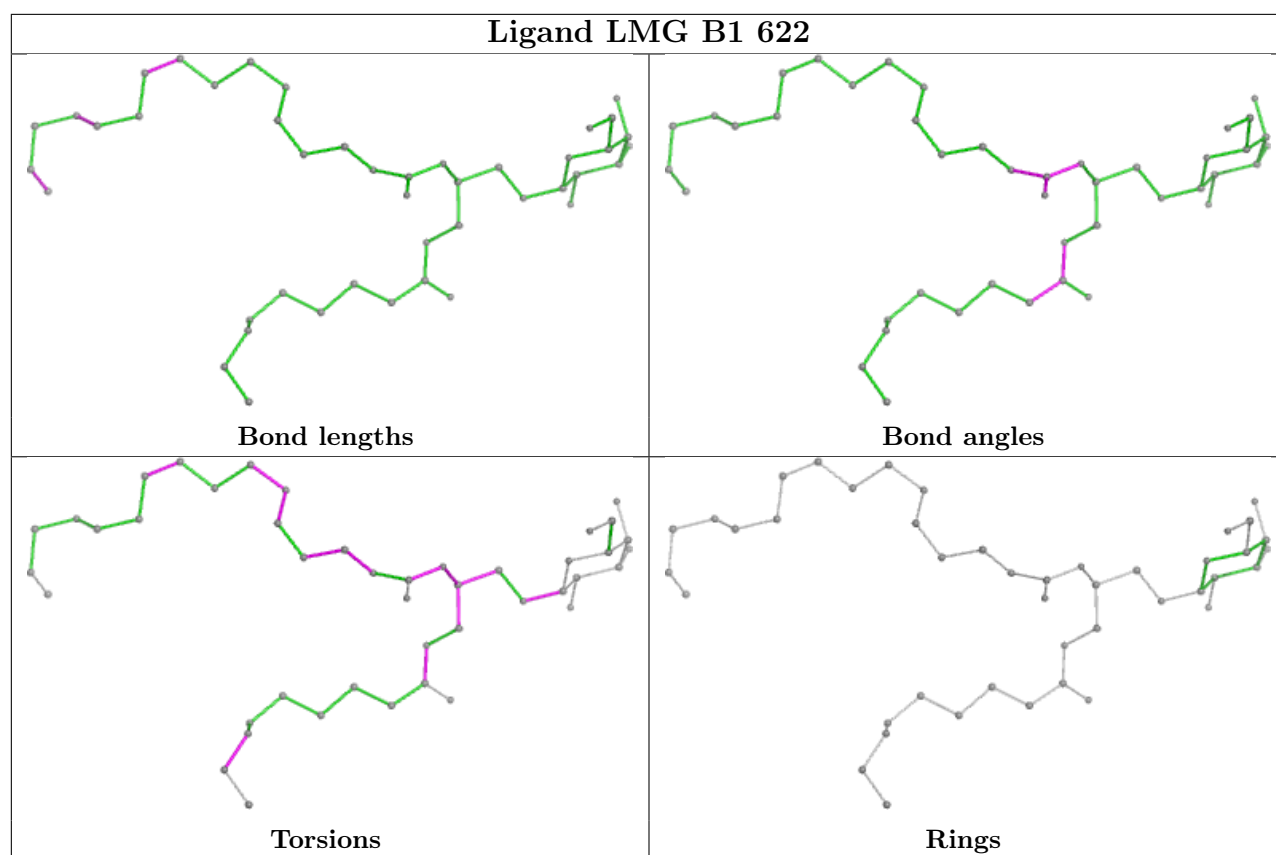
Rings

## Ligand CLA c 507

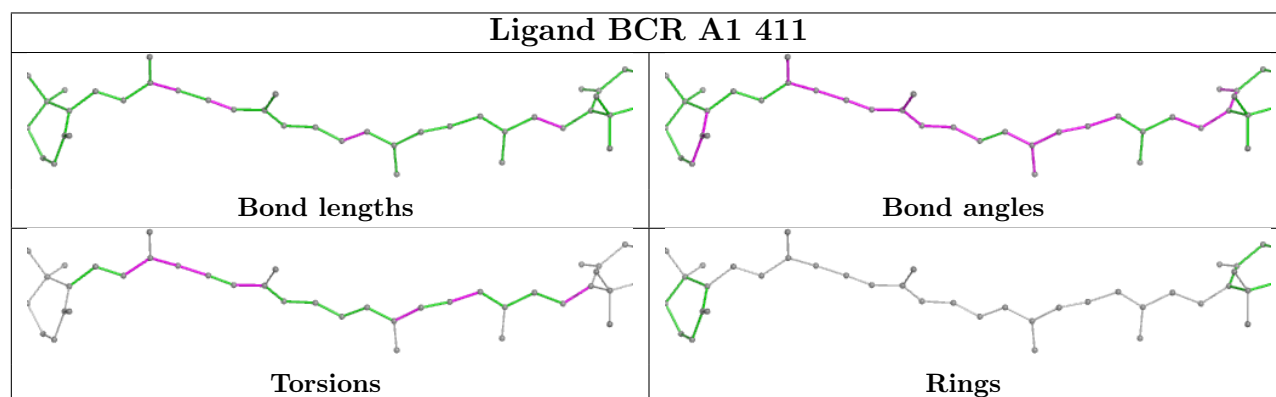
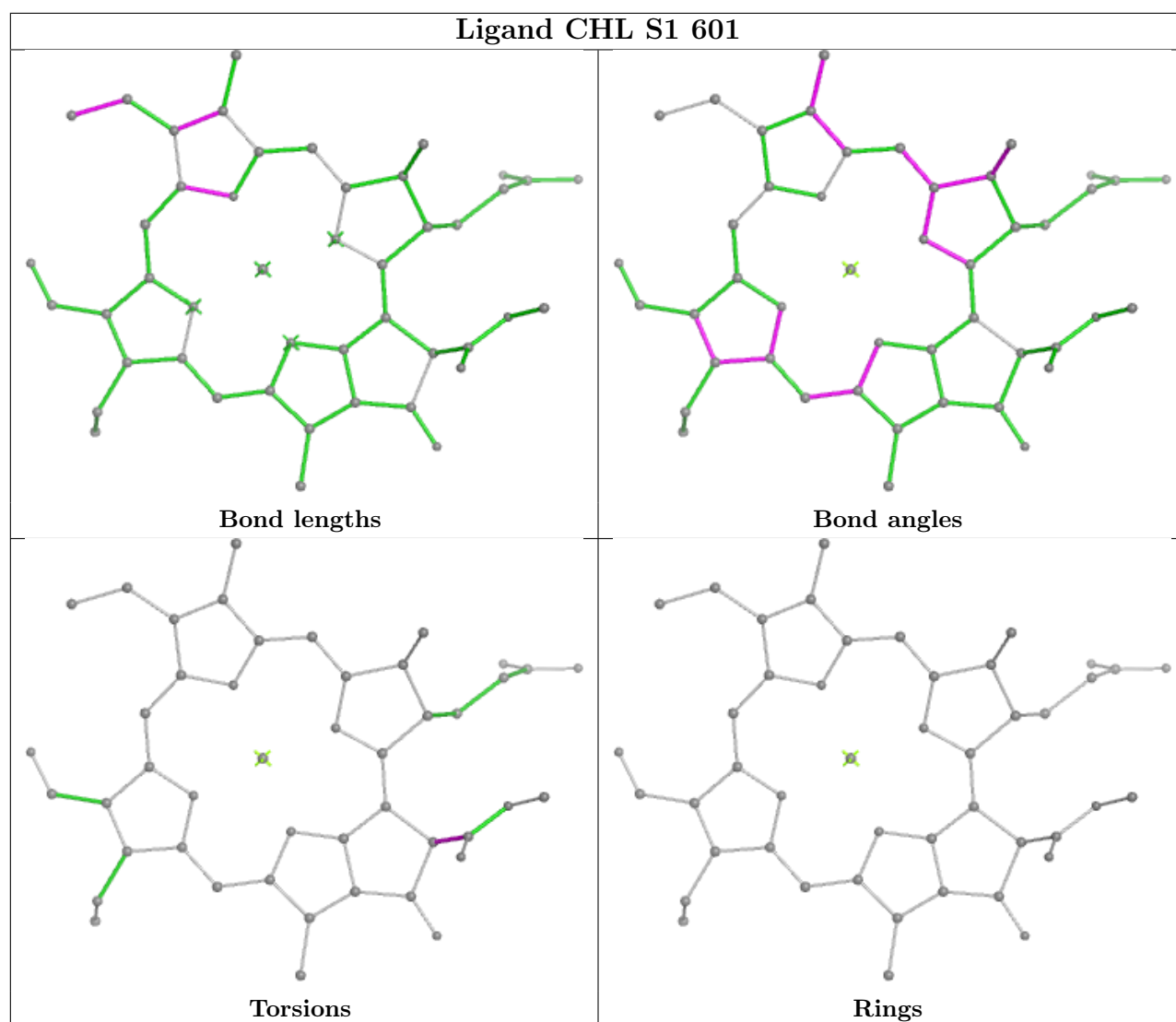


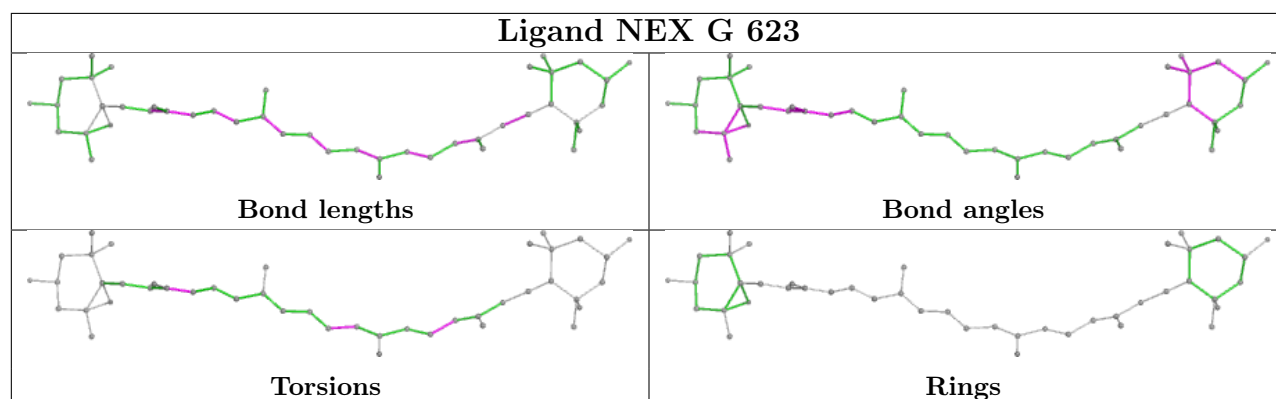
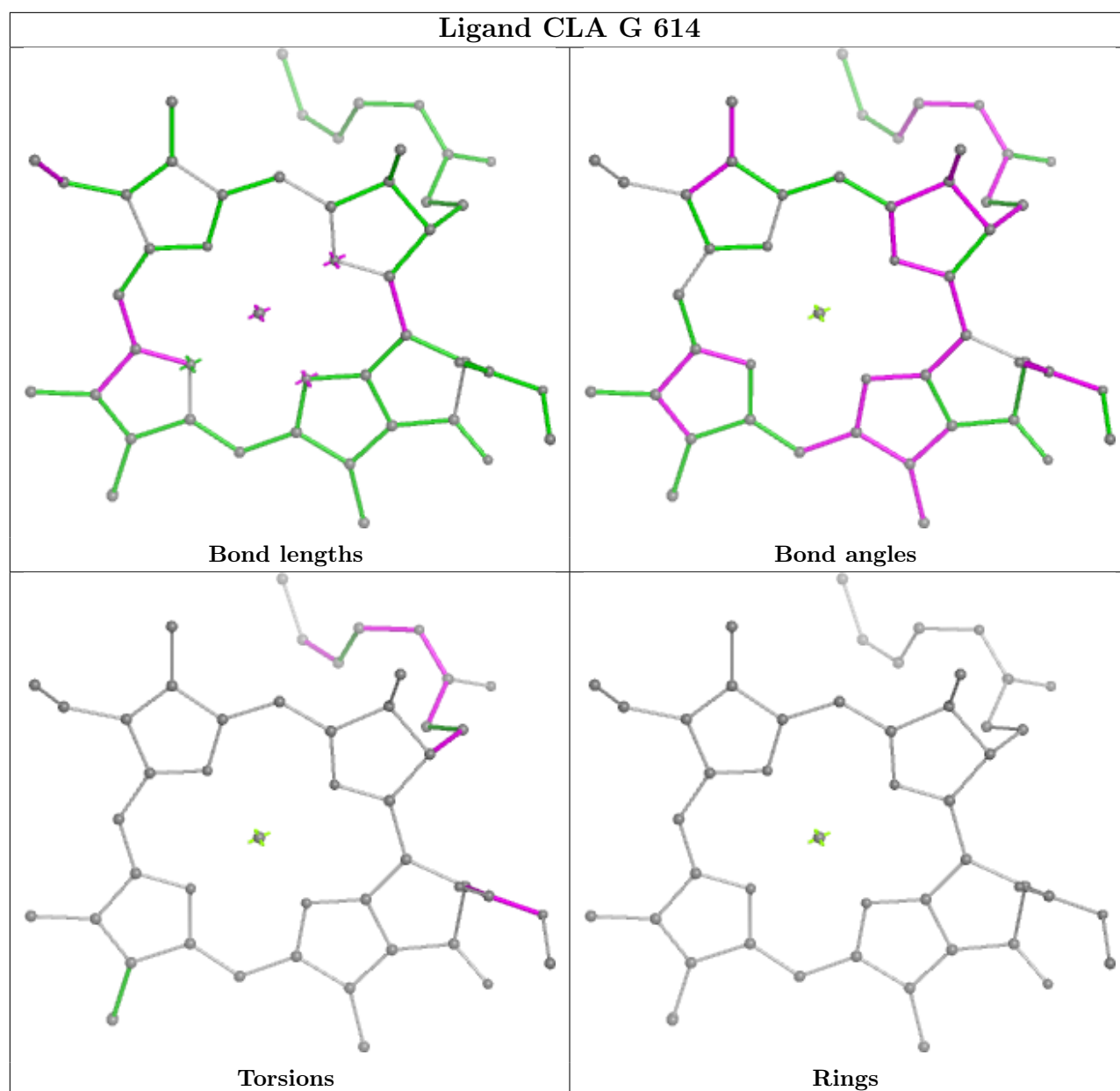
## Ligand XAT n1 622

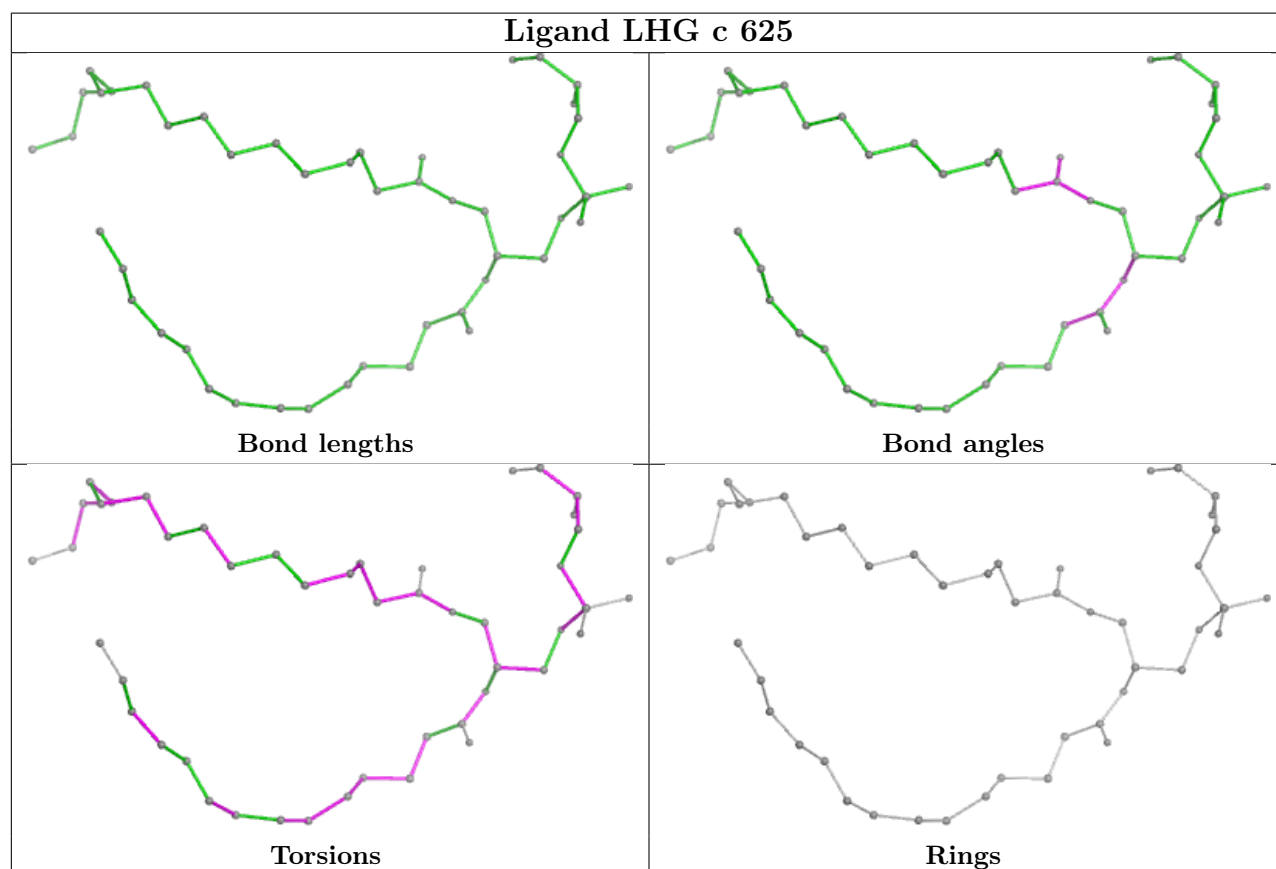
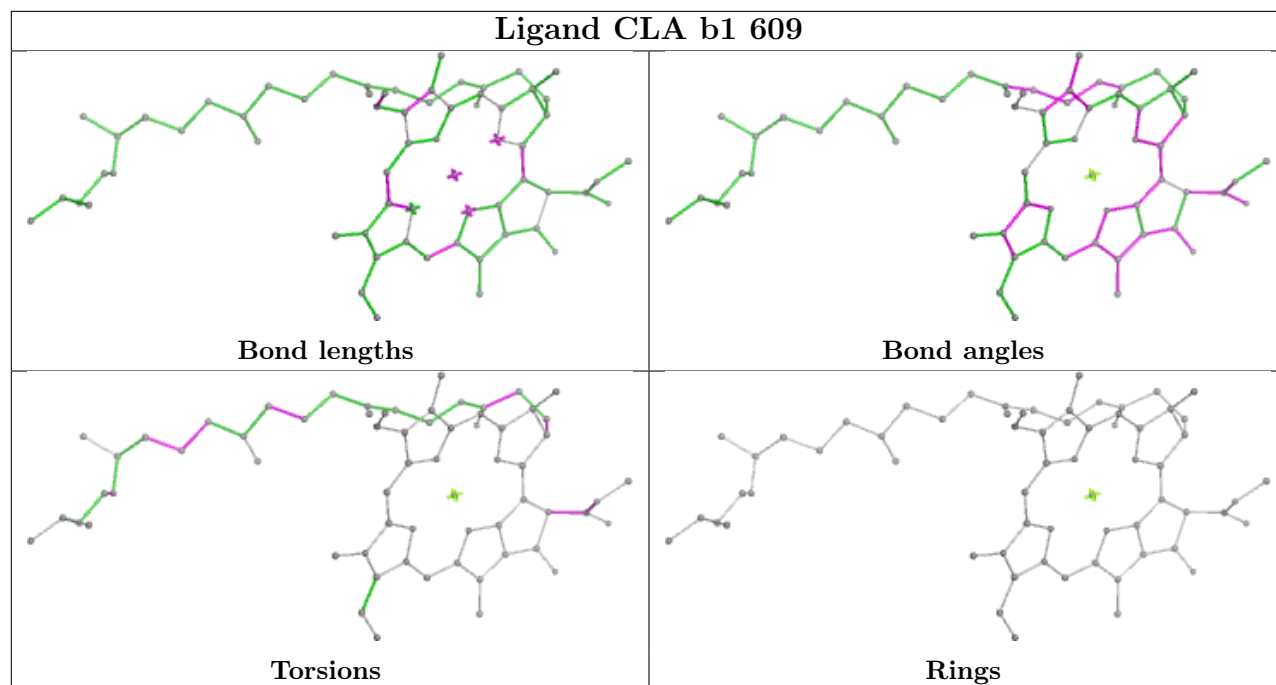


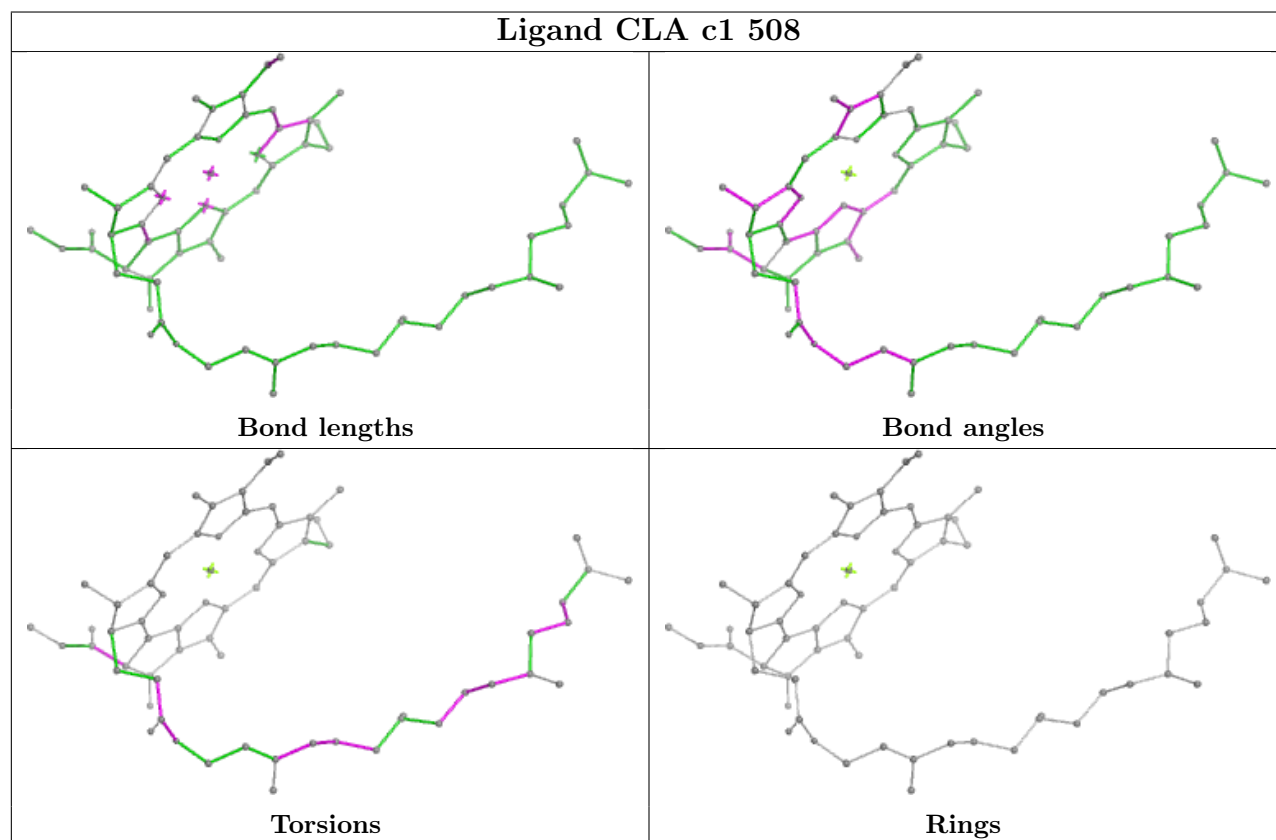
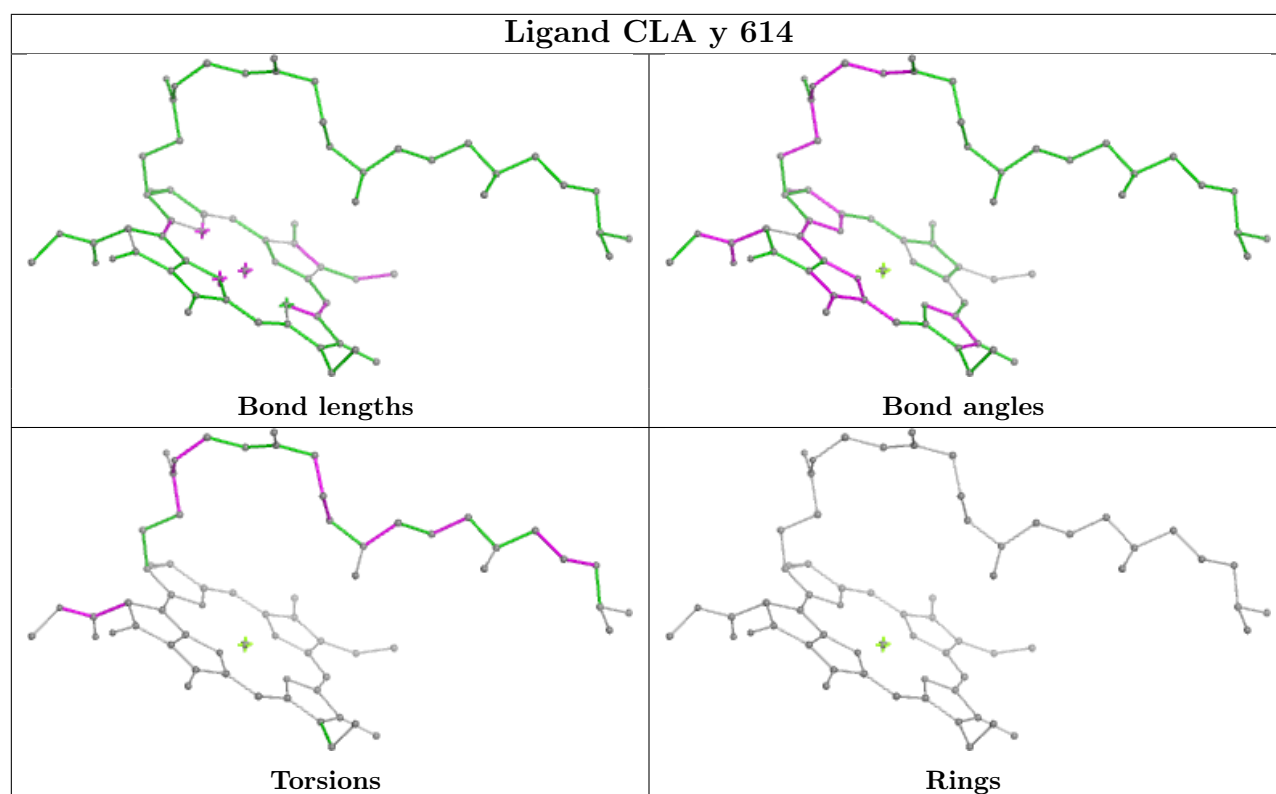


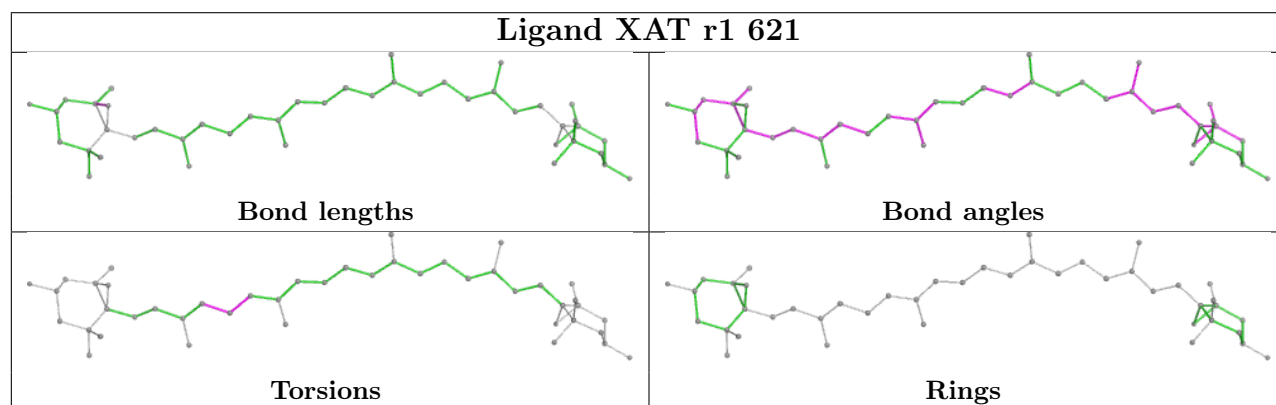
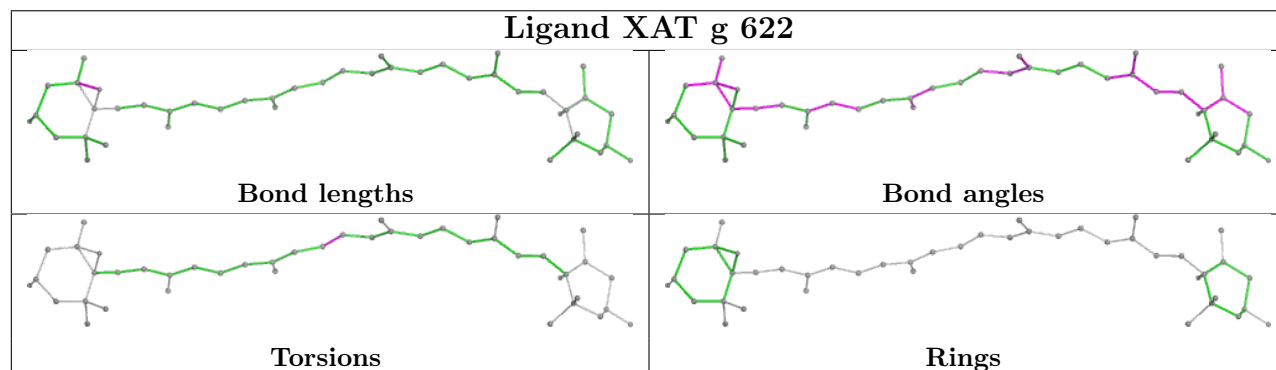
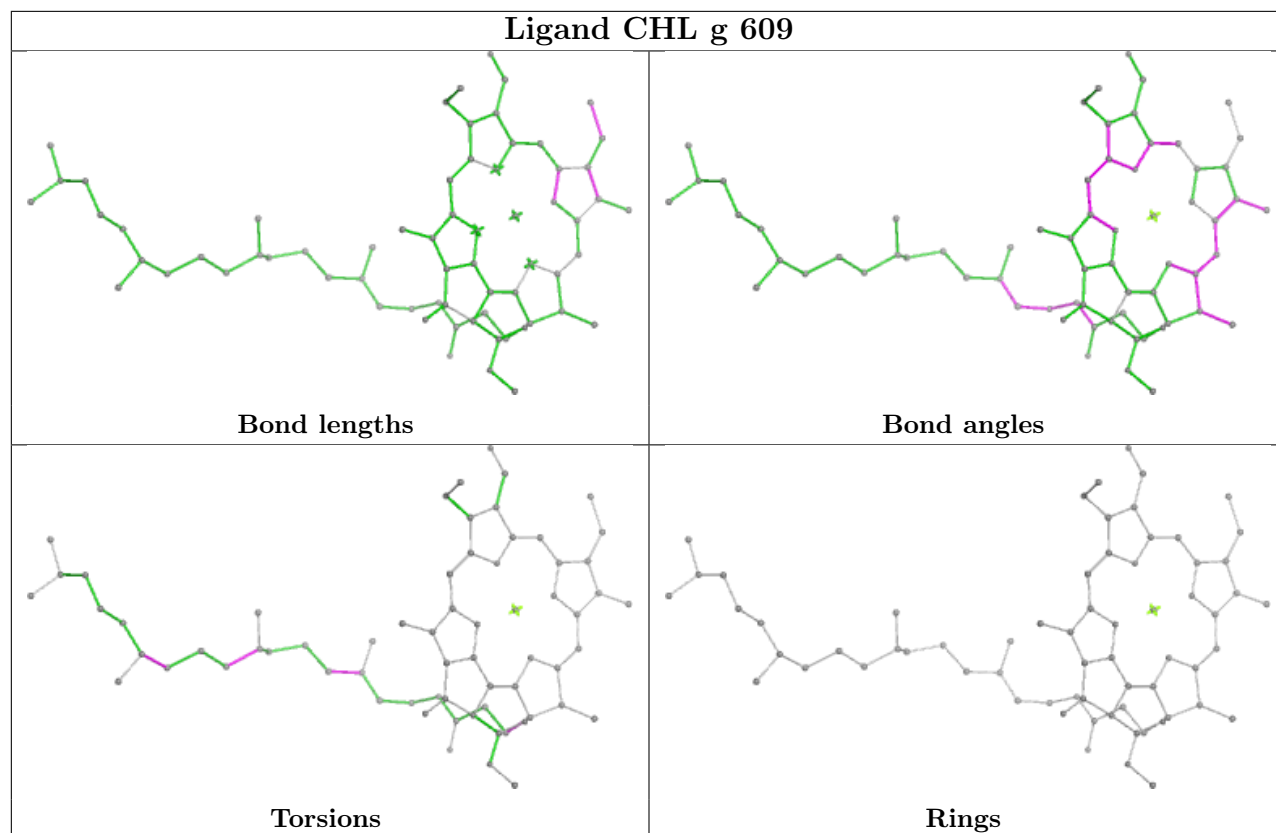


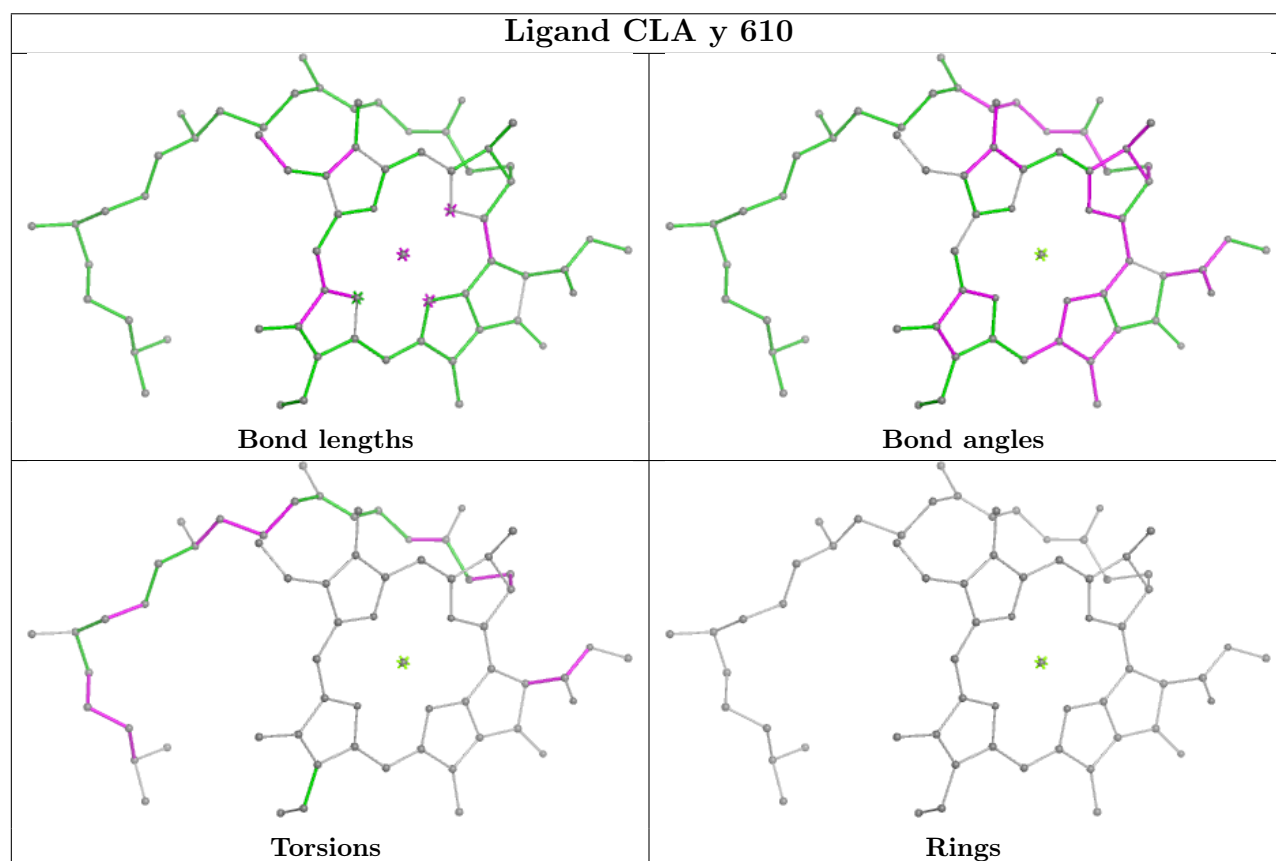
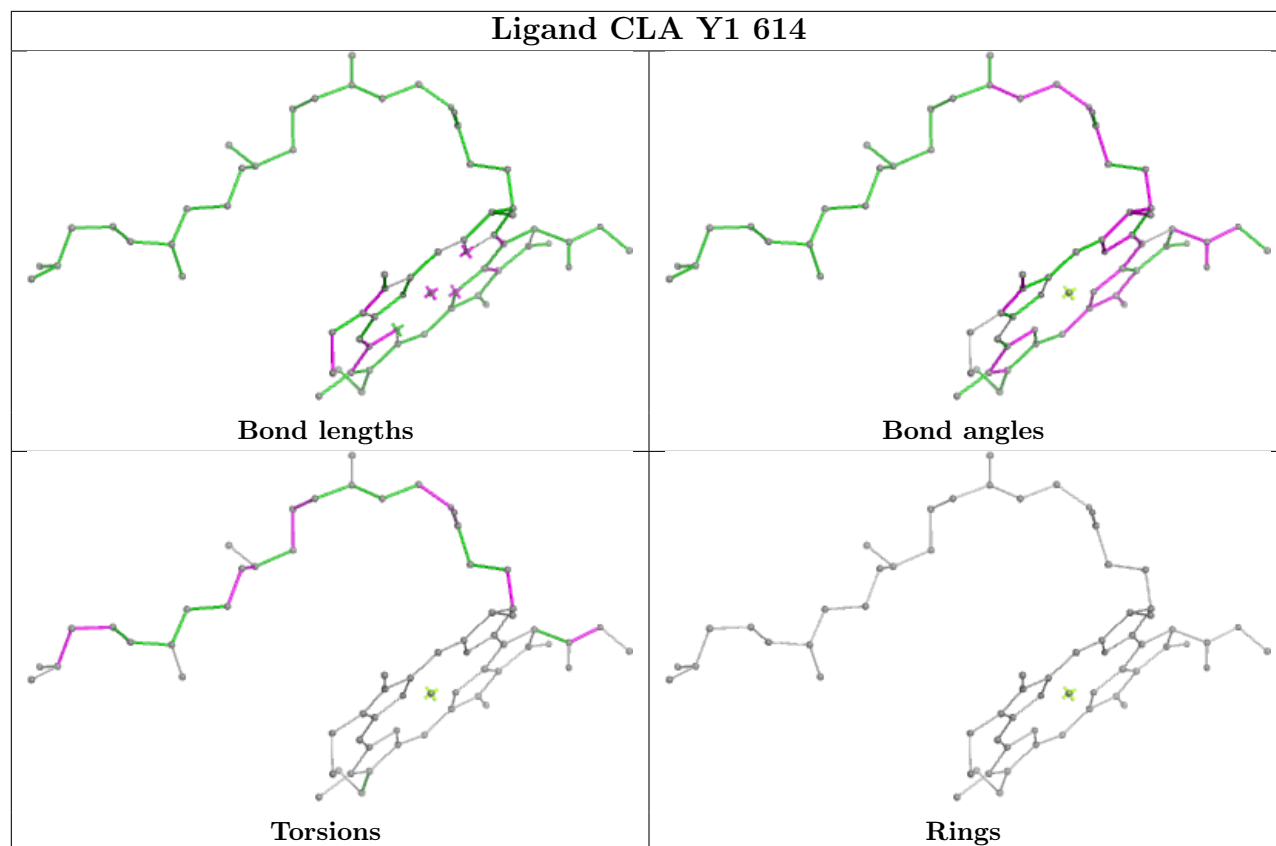


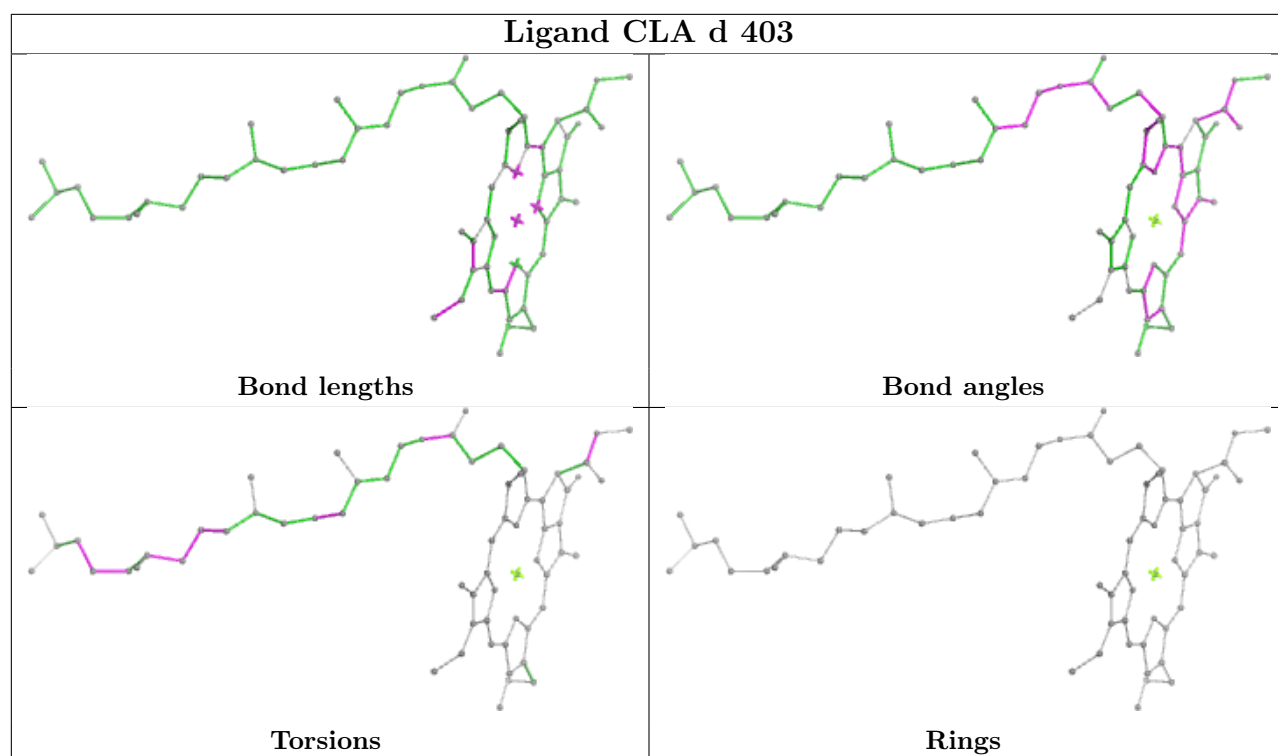


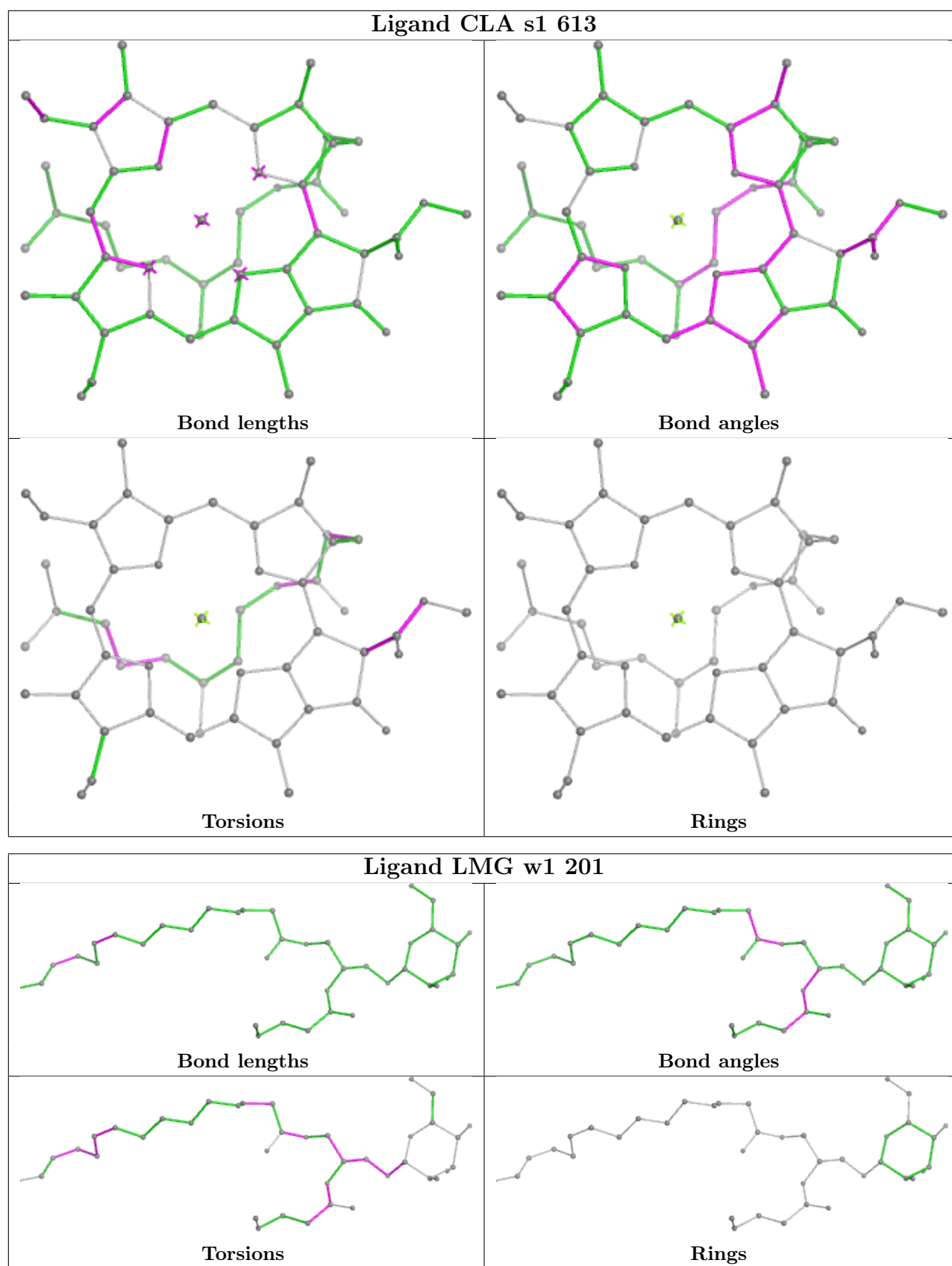




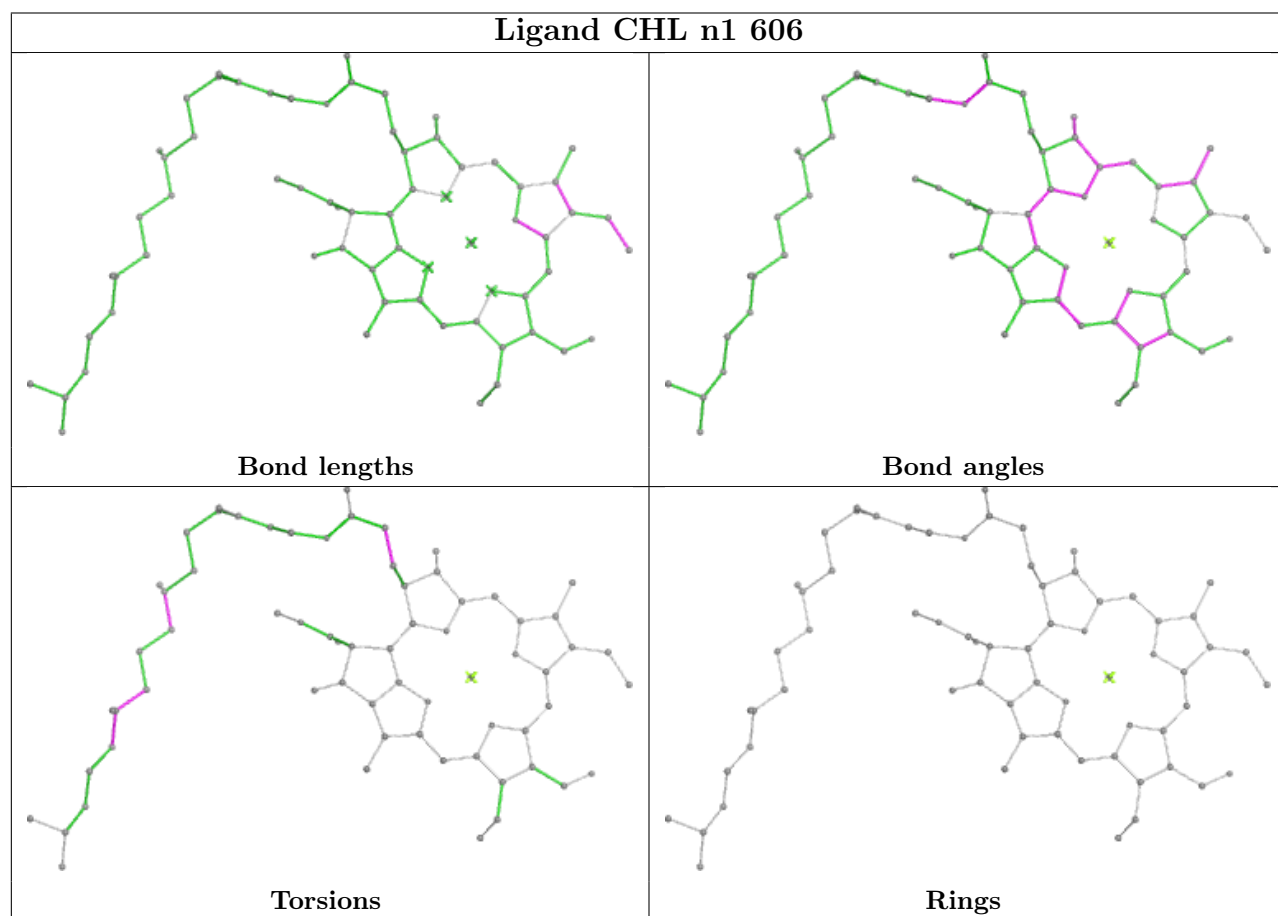
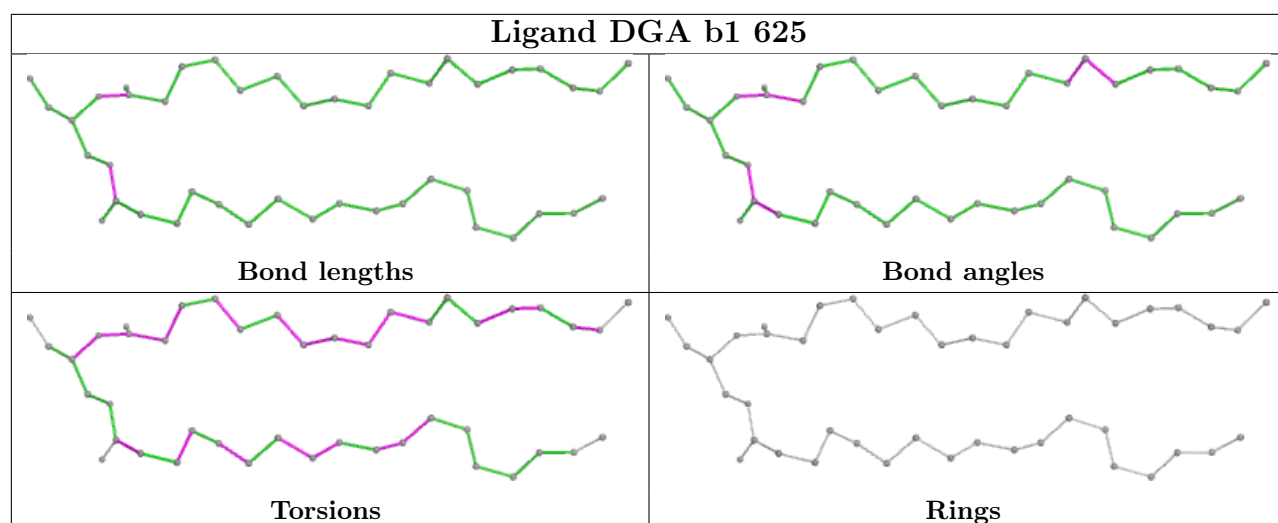




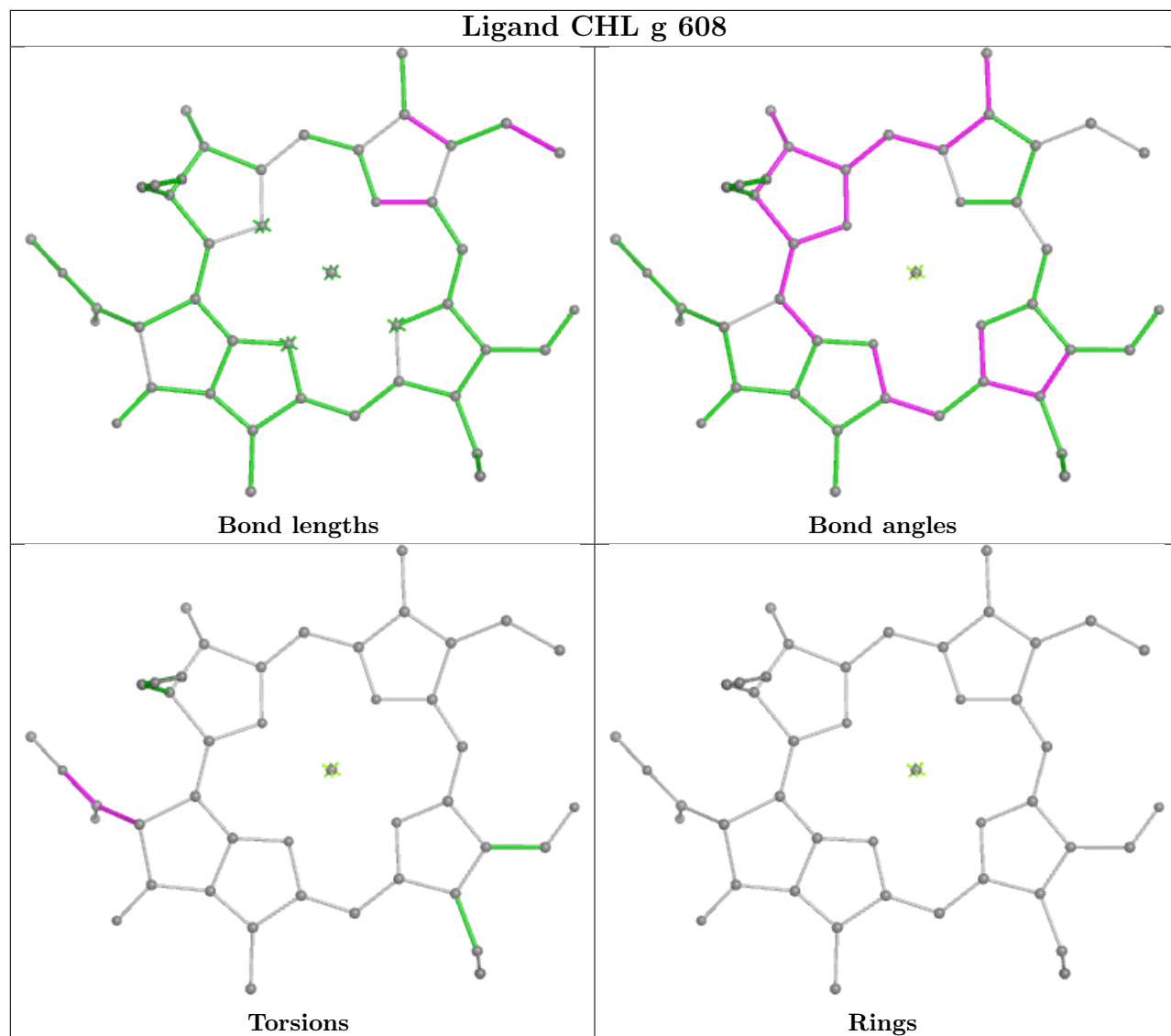


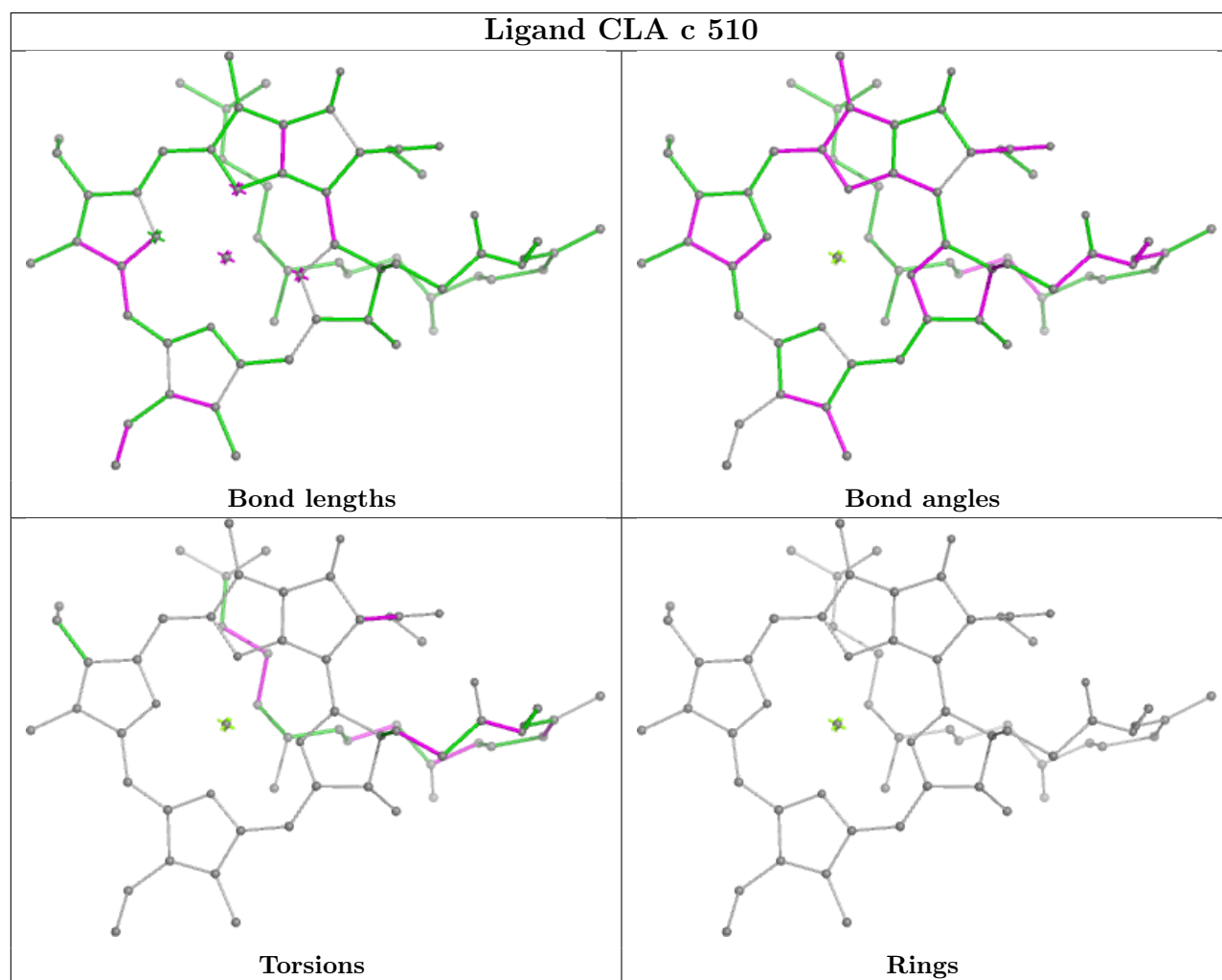
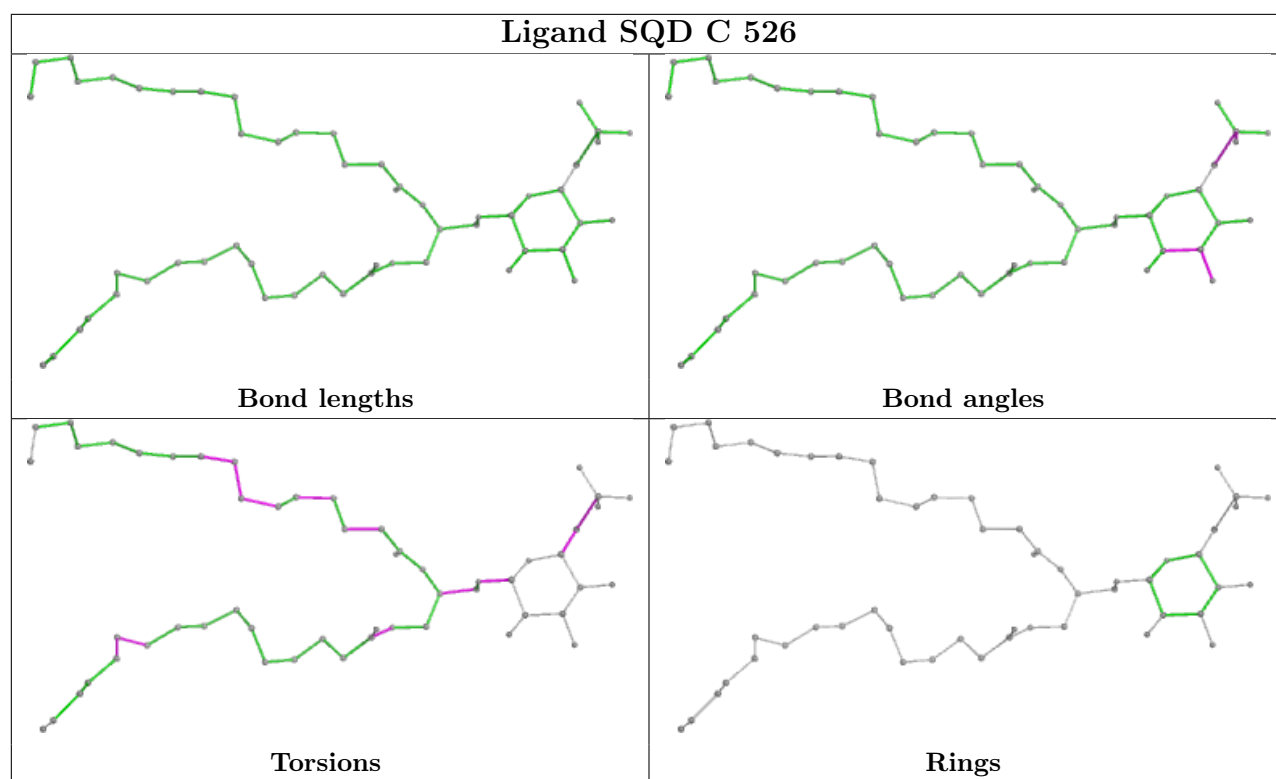




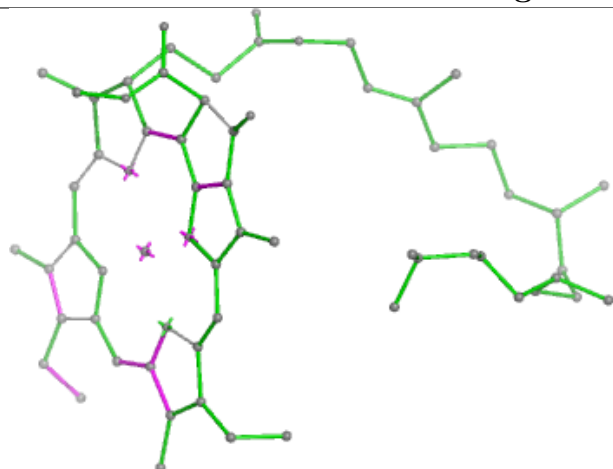


## Ligand CHL g 608

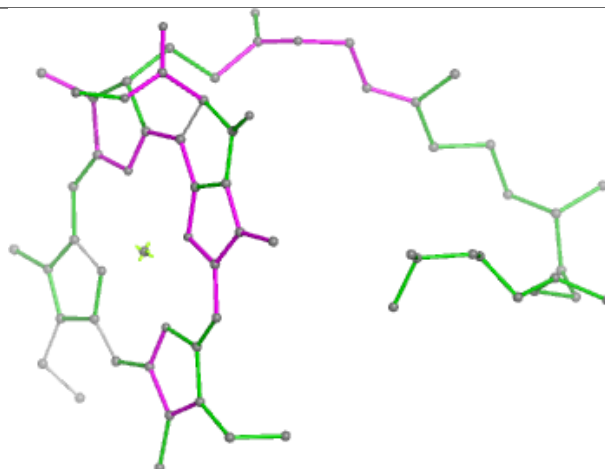




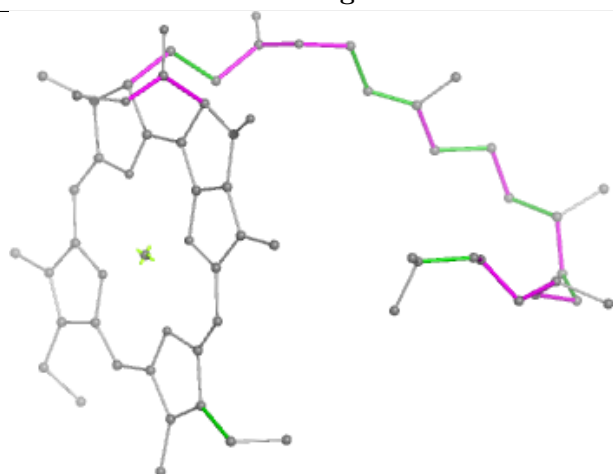
## Ligand CLA C 503



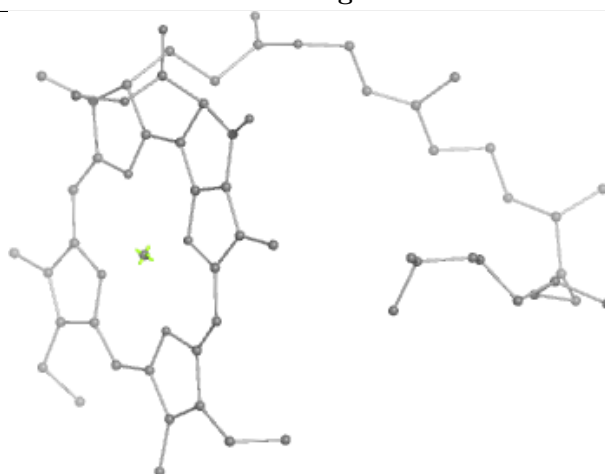
Bond lengths



Bond angles

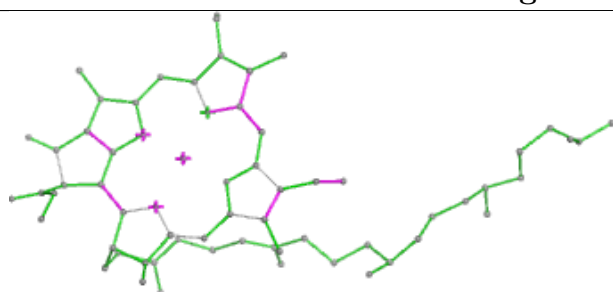


Torsions

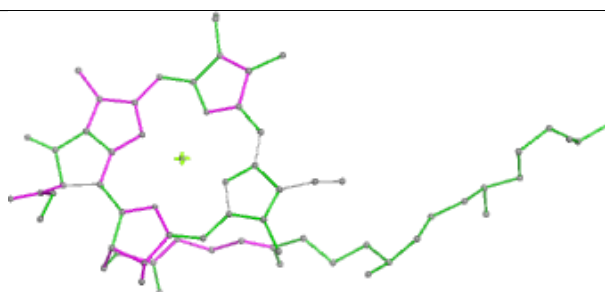


Rings

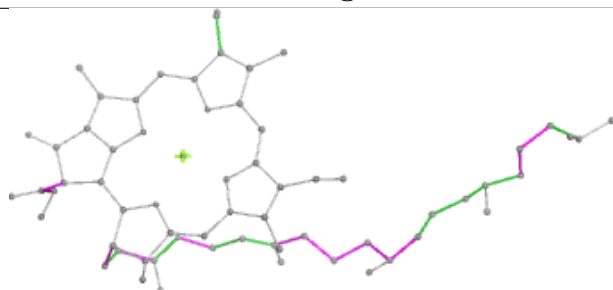
## Ligand CLA c 501



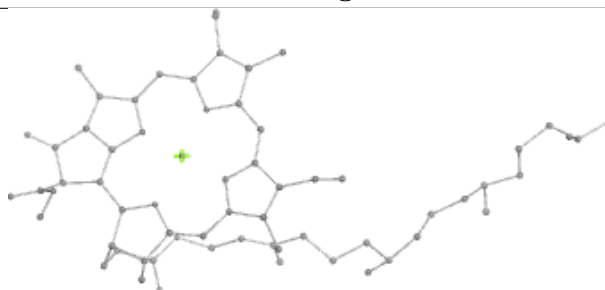
Bond lengths



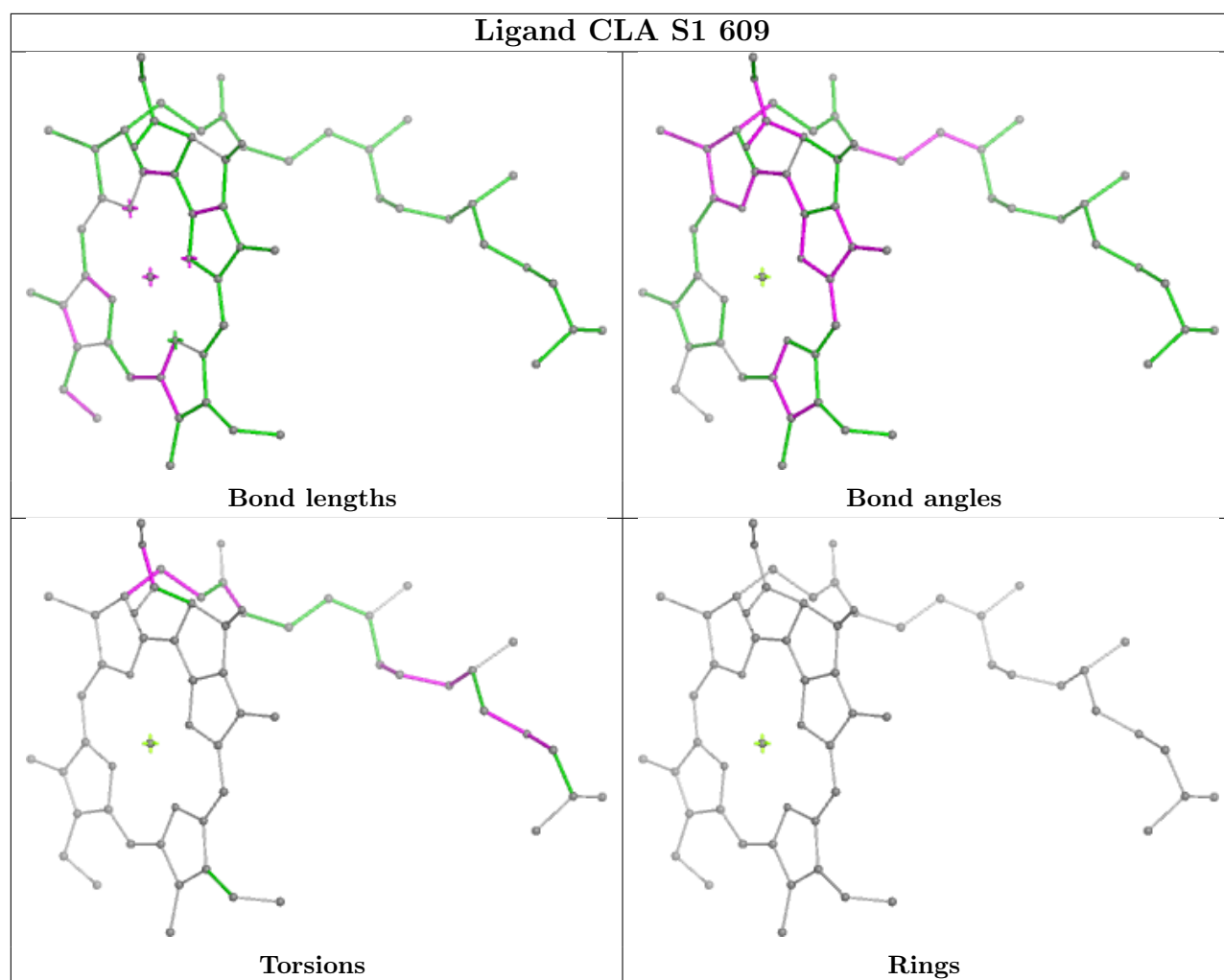
Bond angles



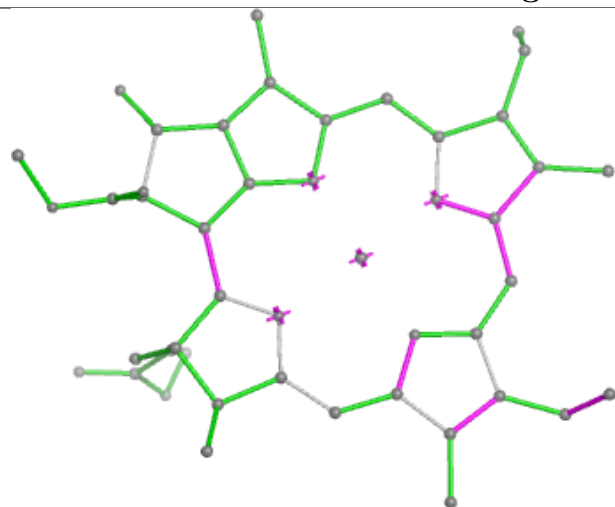
Torsions



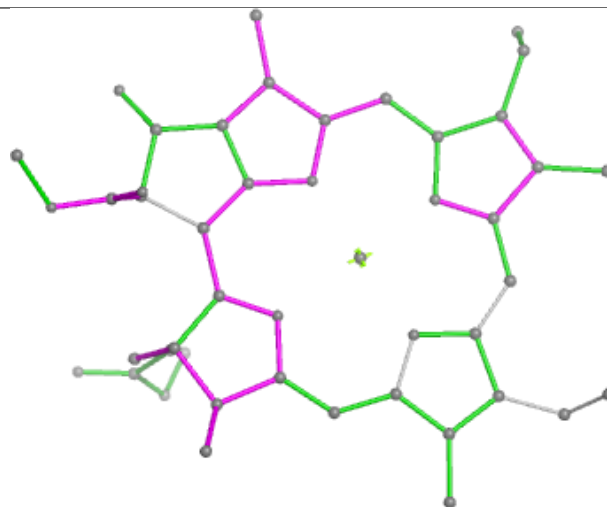
Rings



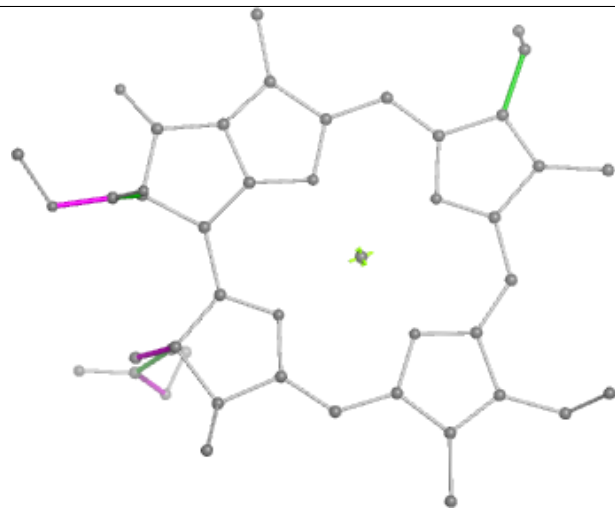
## Ligand CLA r 611



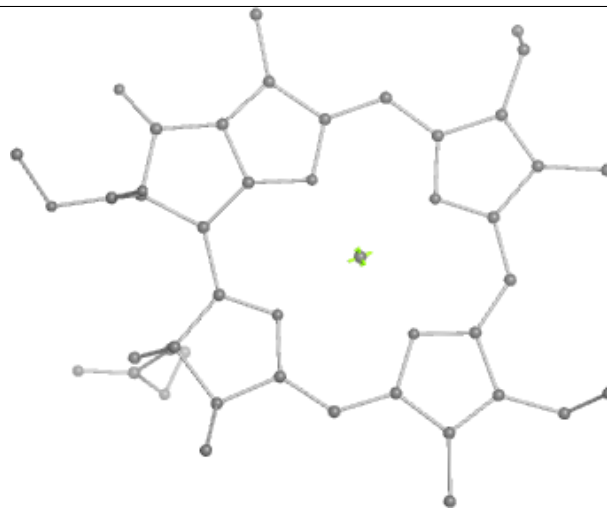
Bond lengths



Bond angles

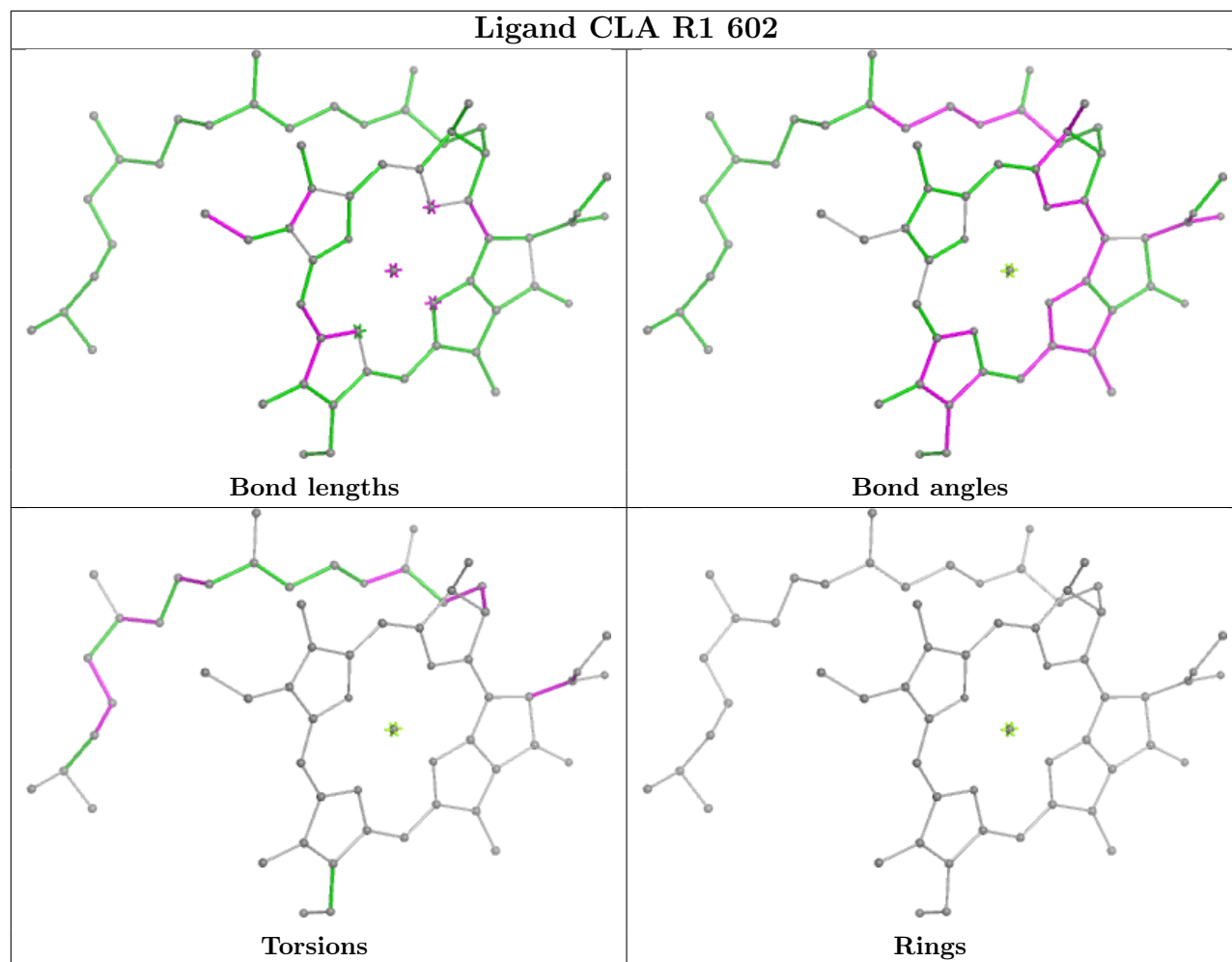


Torsions

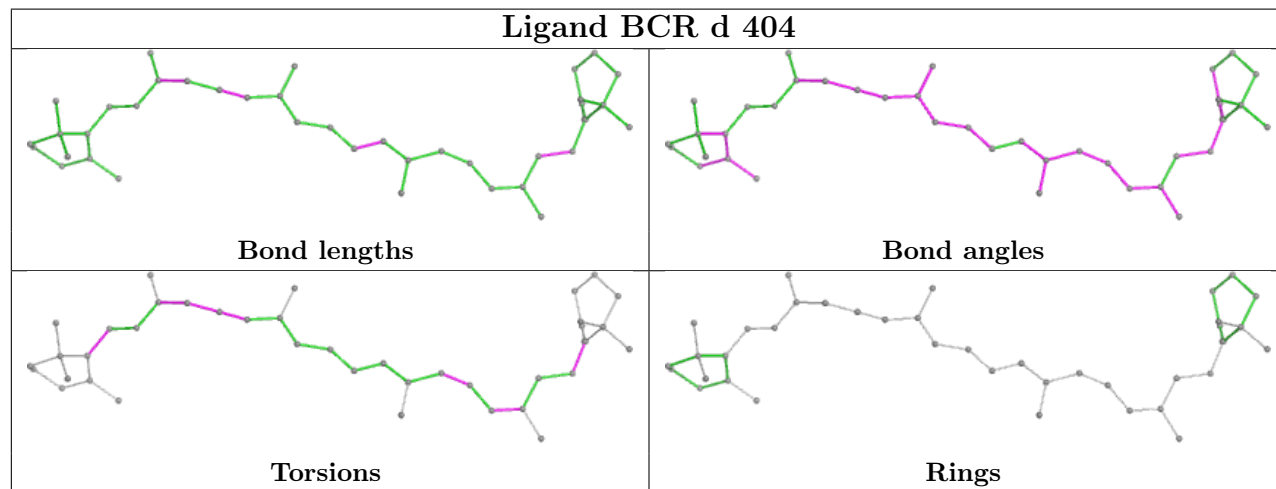


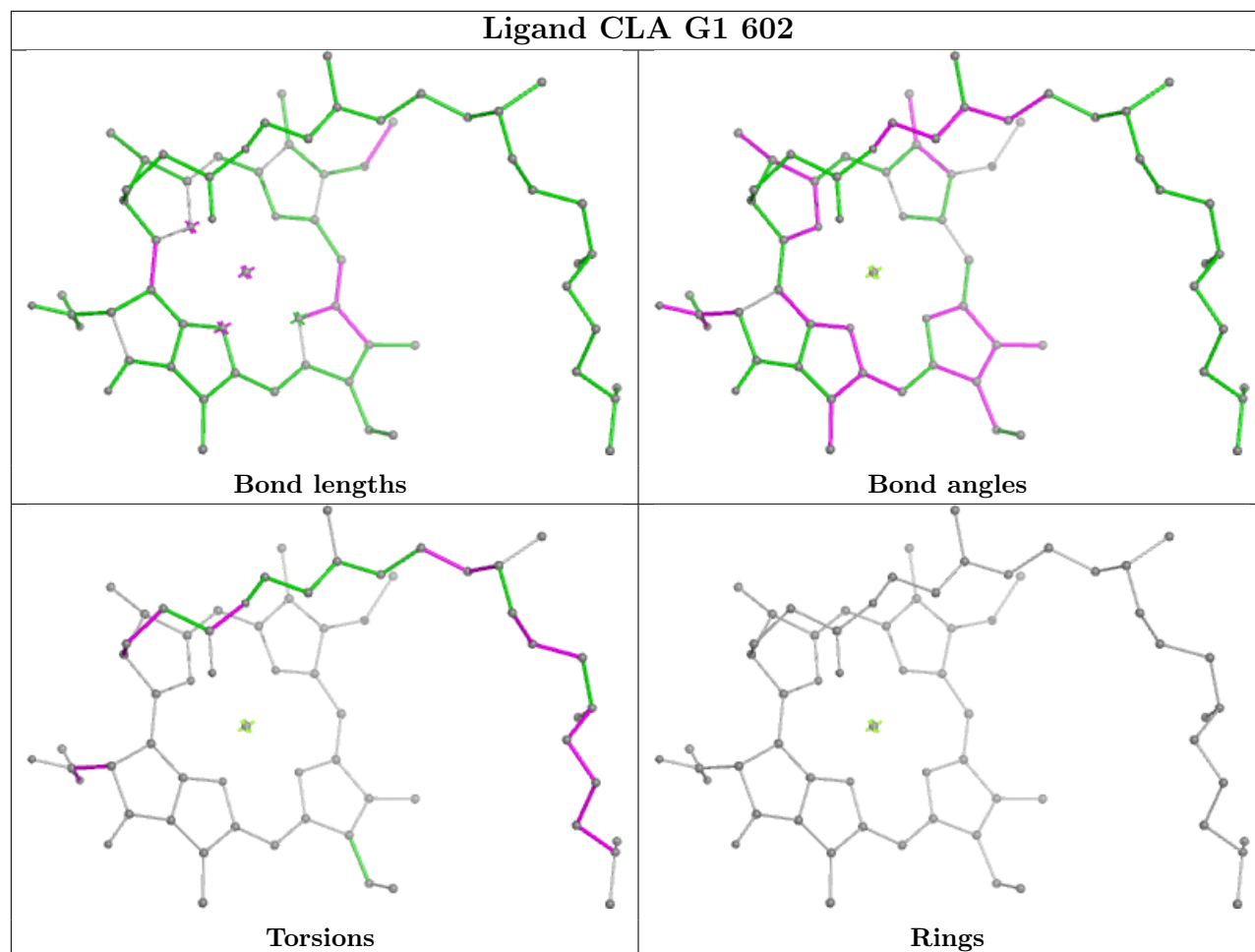
Rings

## Ligand CLA R1 602



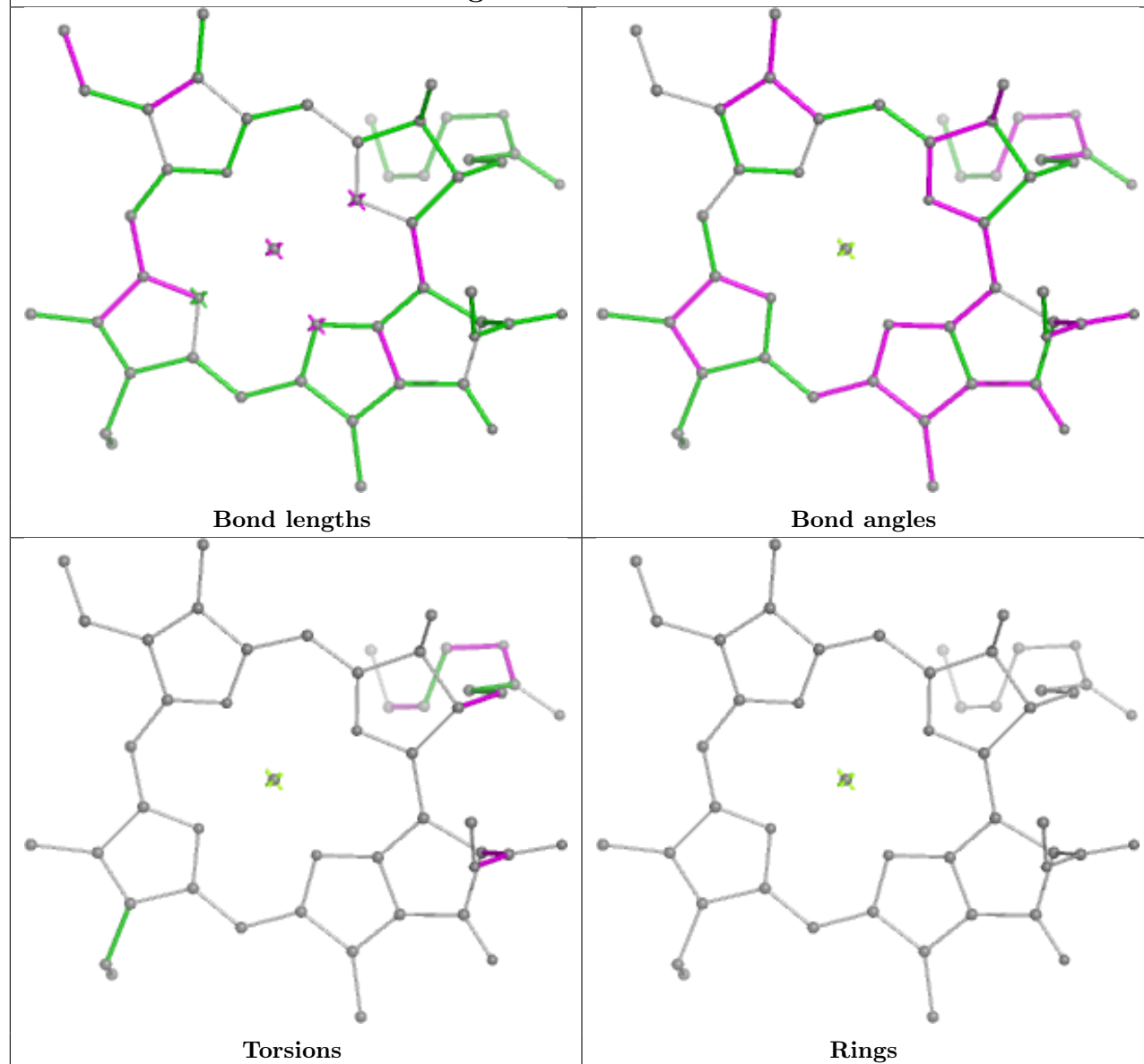
## Ligand BCR d 404

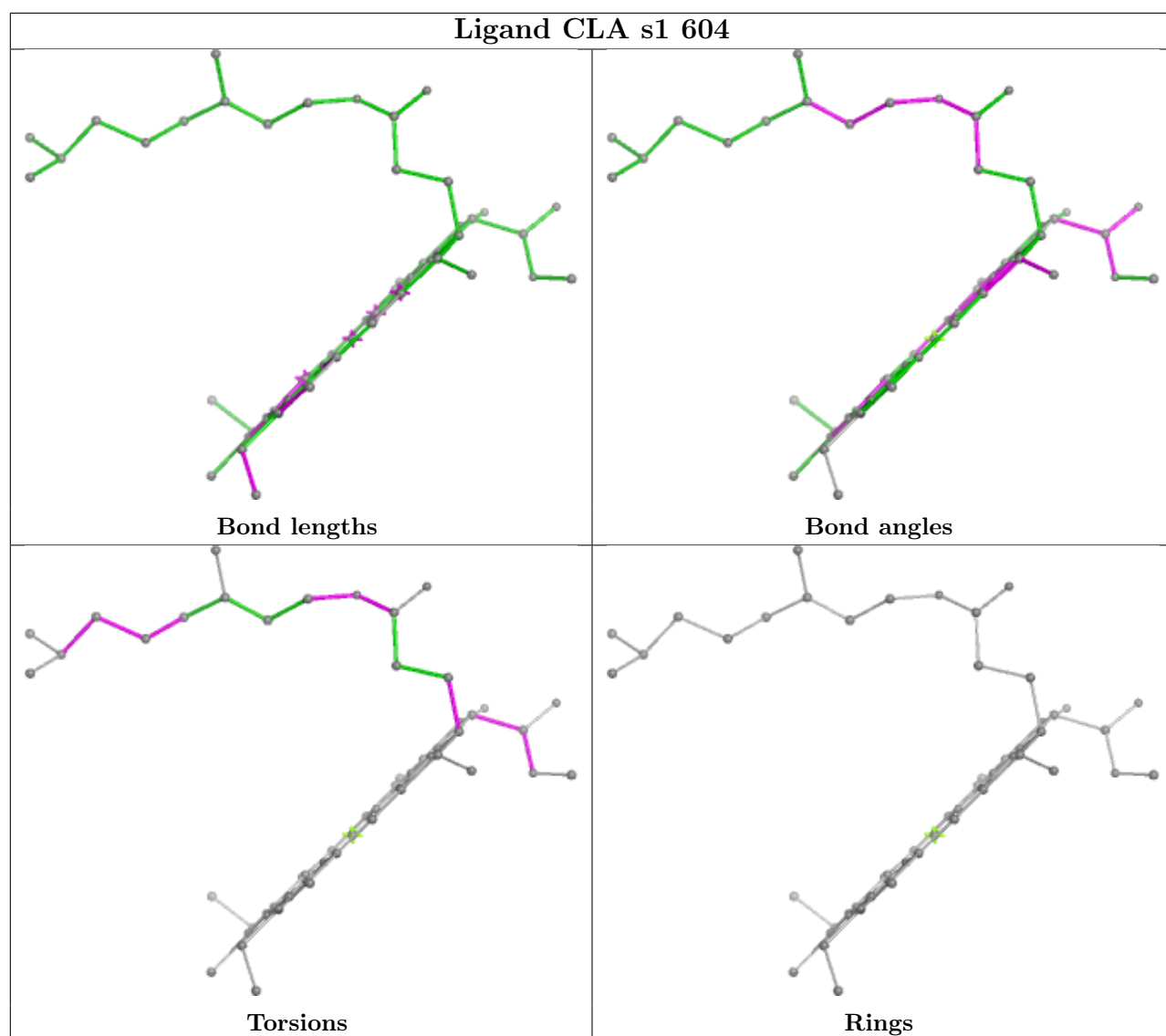


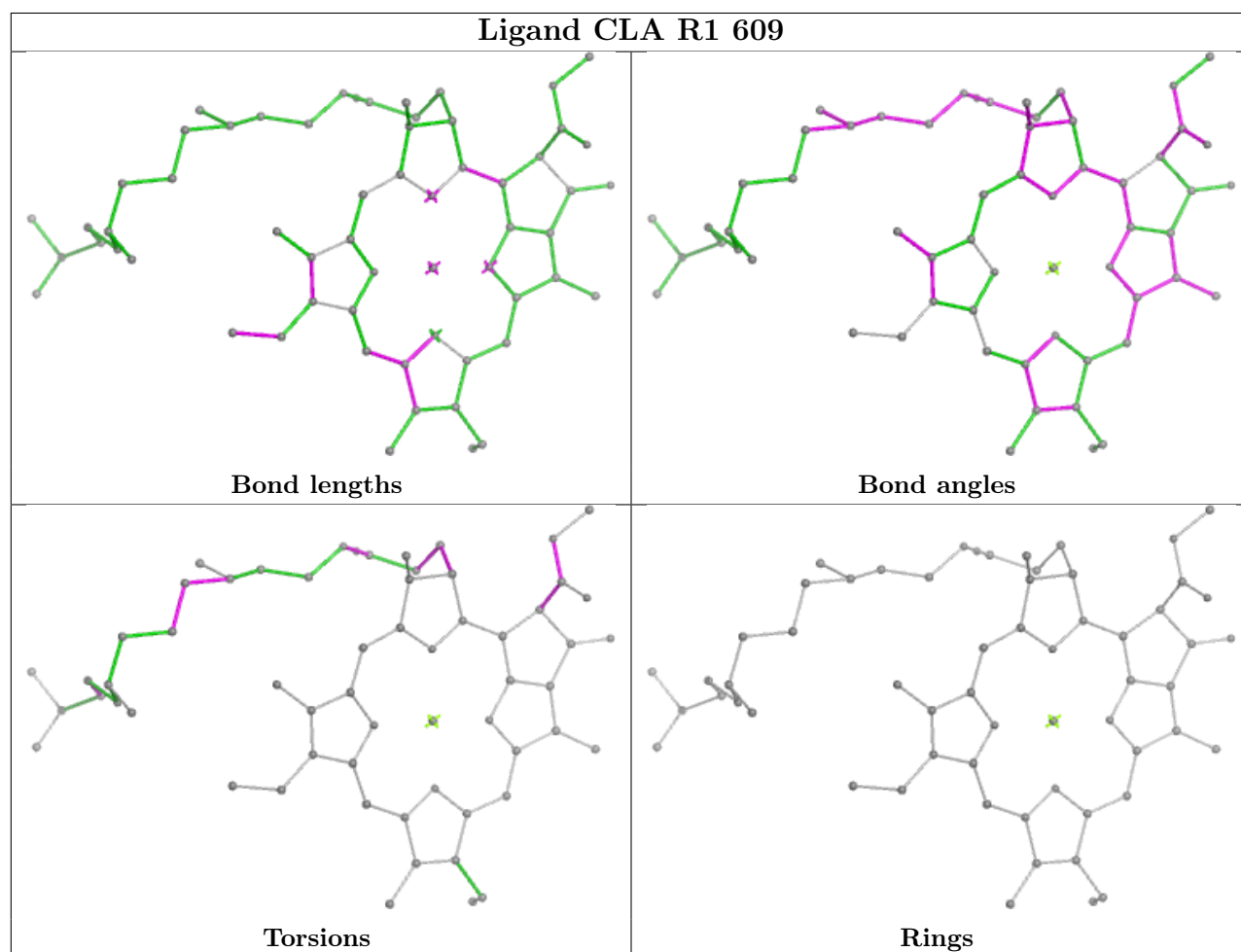
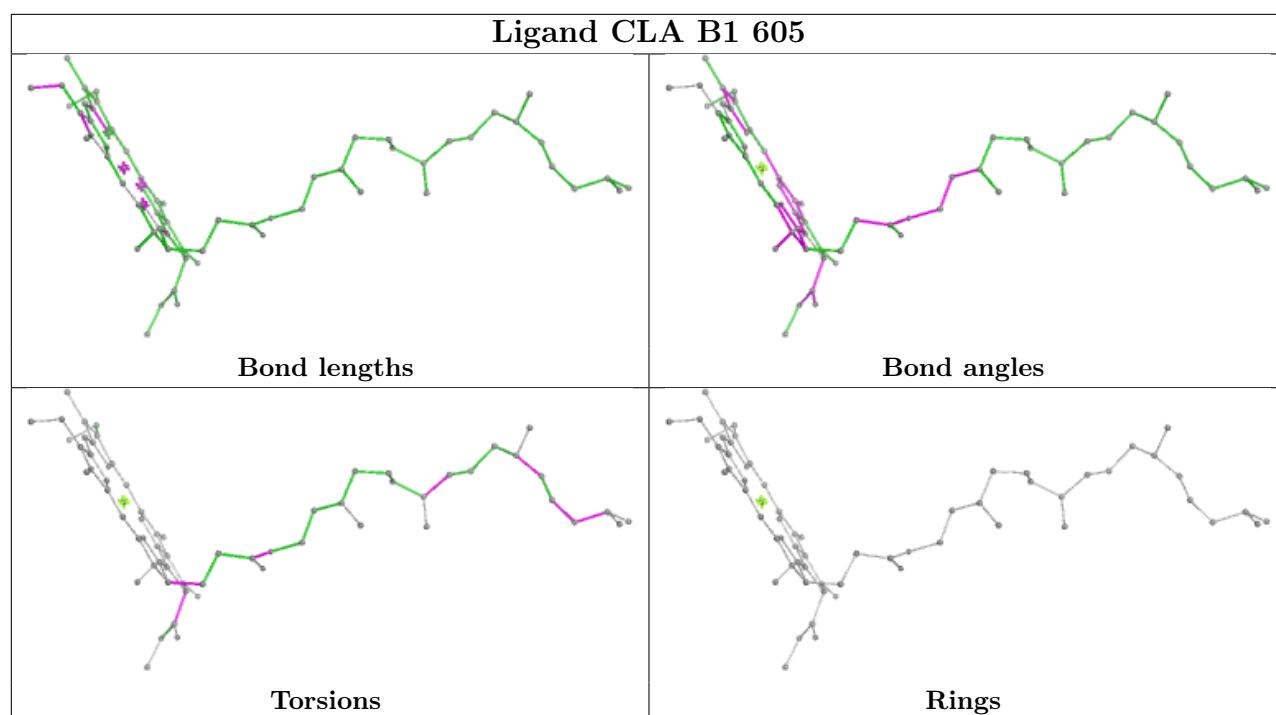


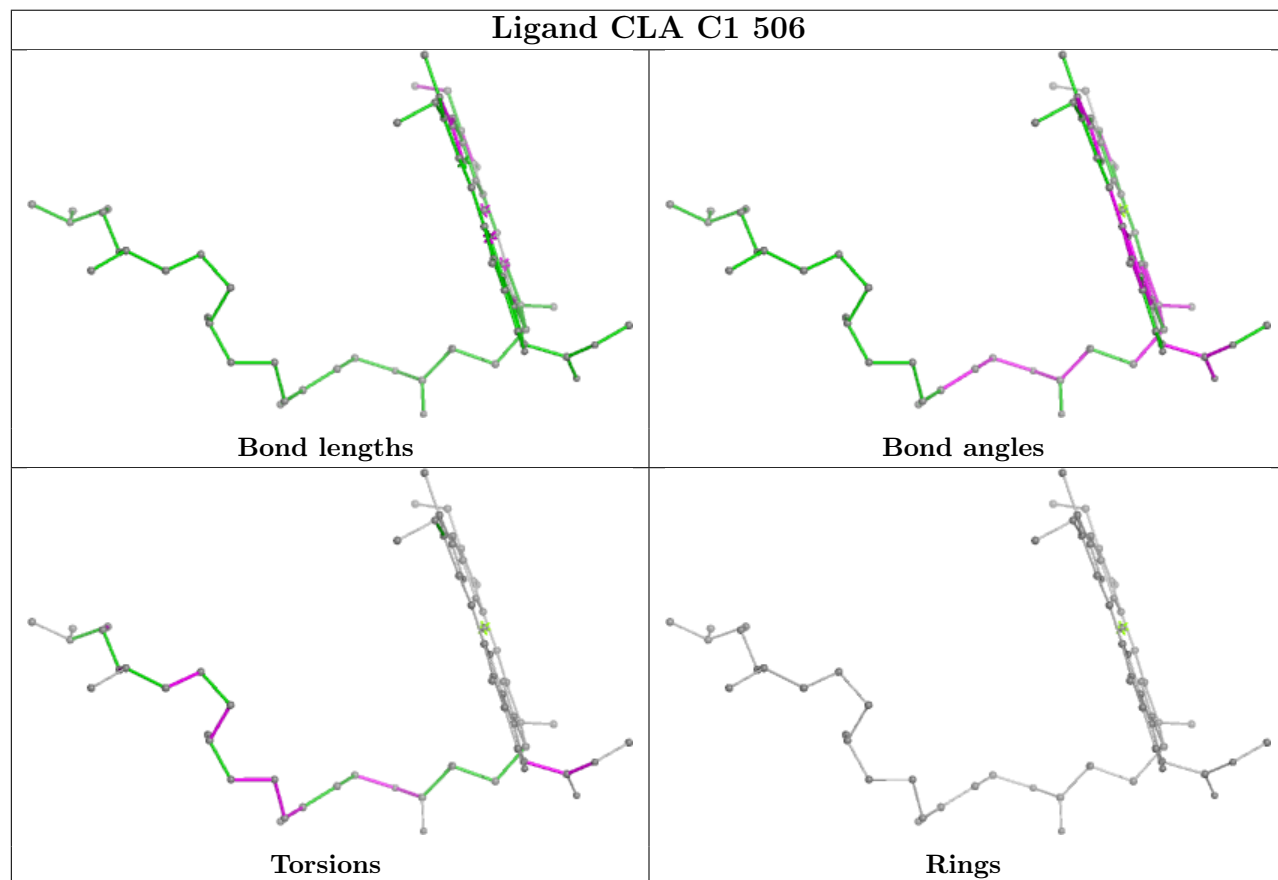
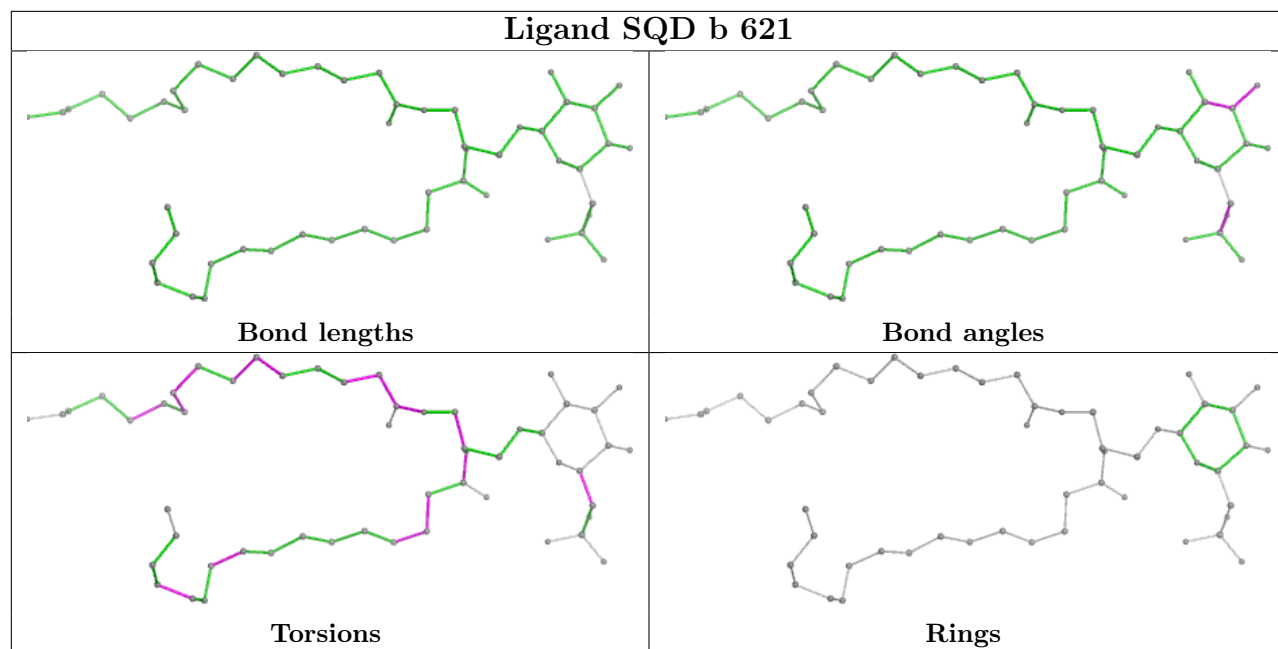


## Ligand CLA G1 604

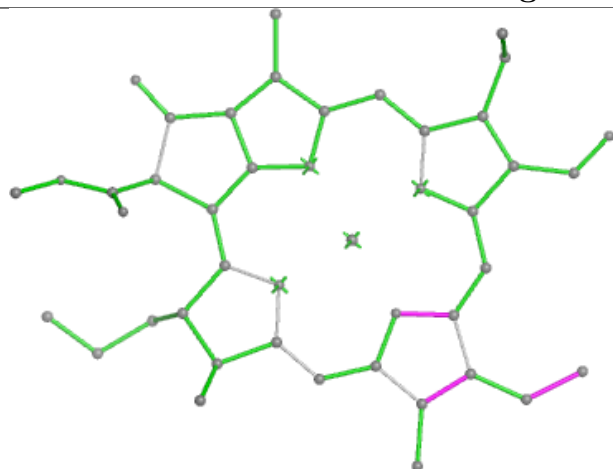




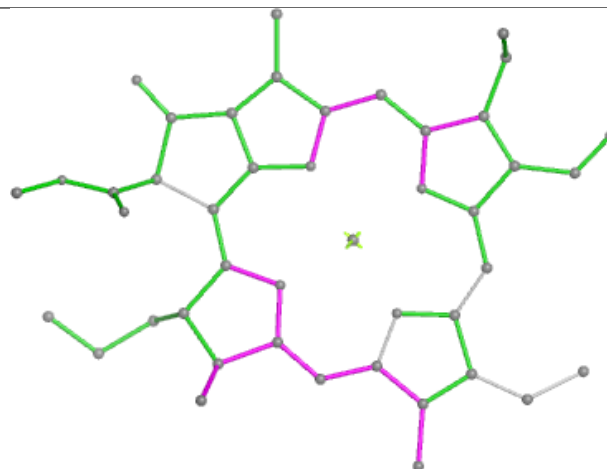




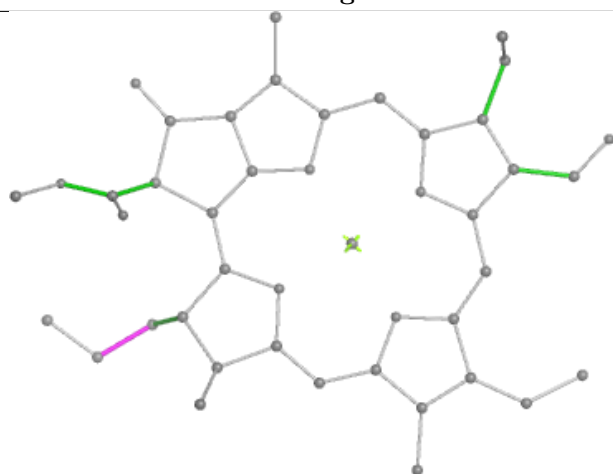
## Ligand CHL r 606



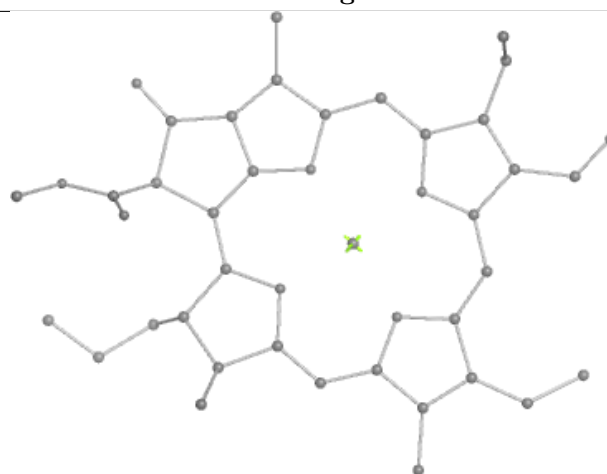
Bond lengths



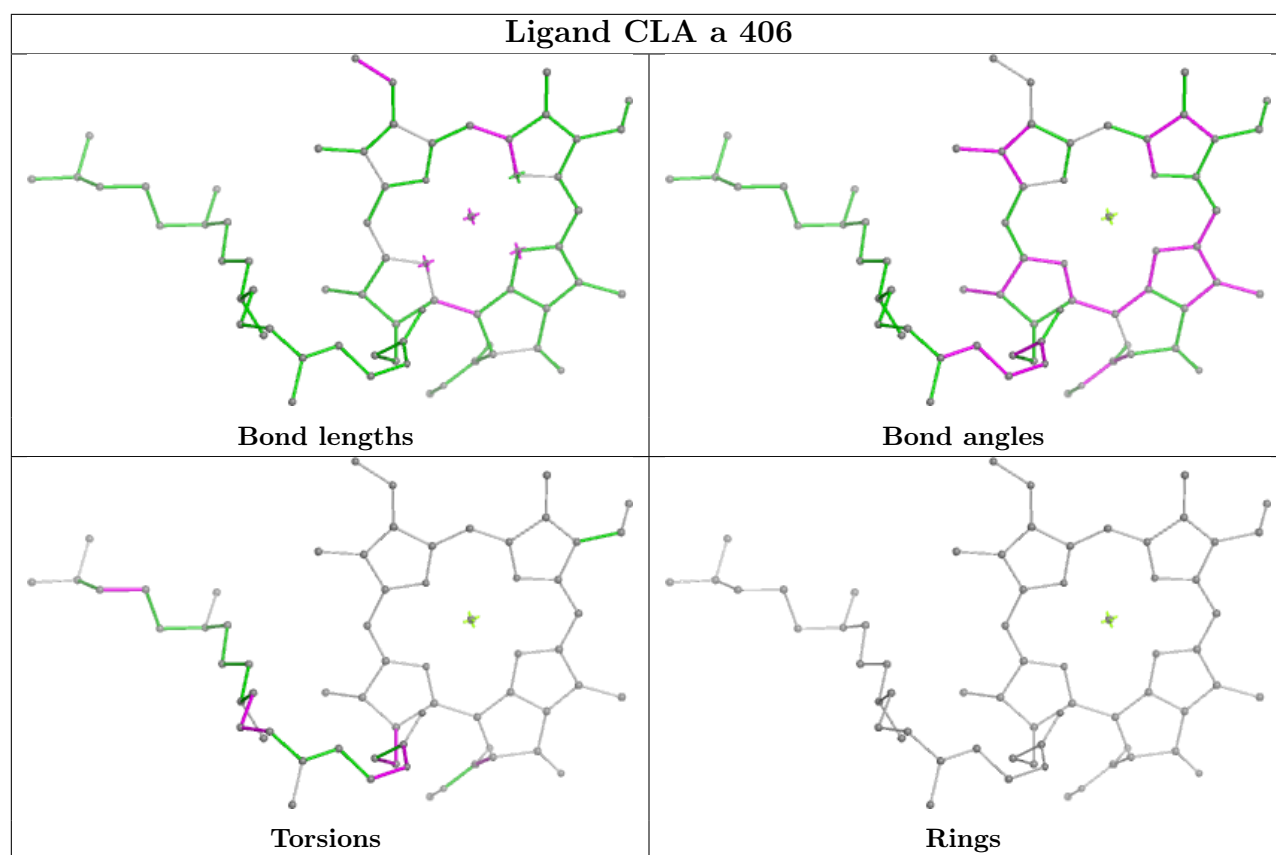
Bond angles

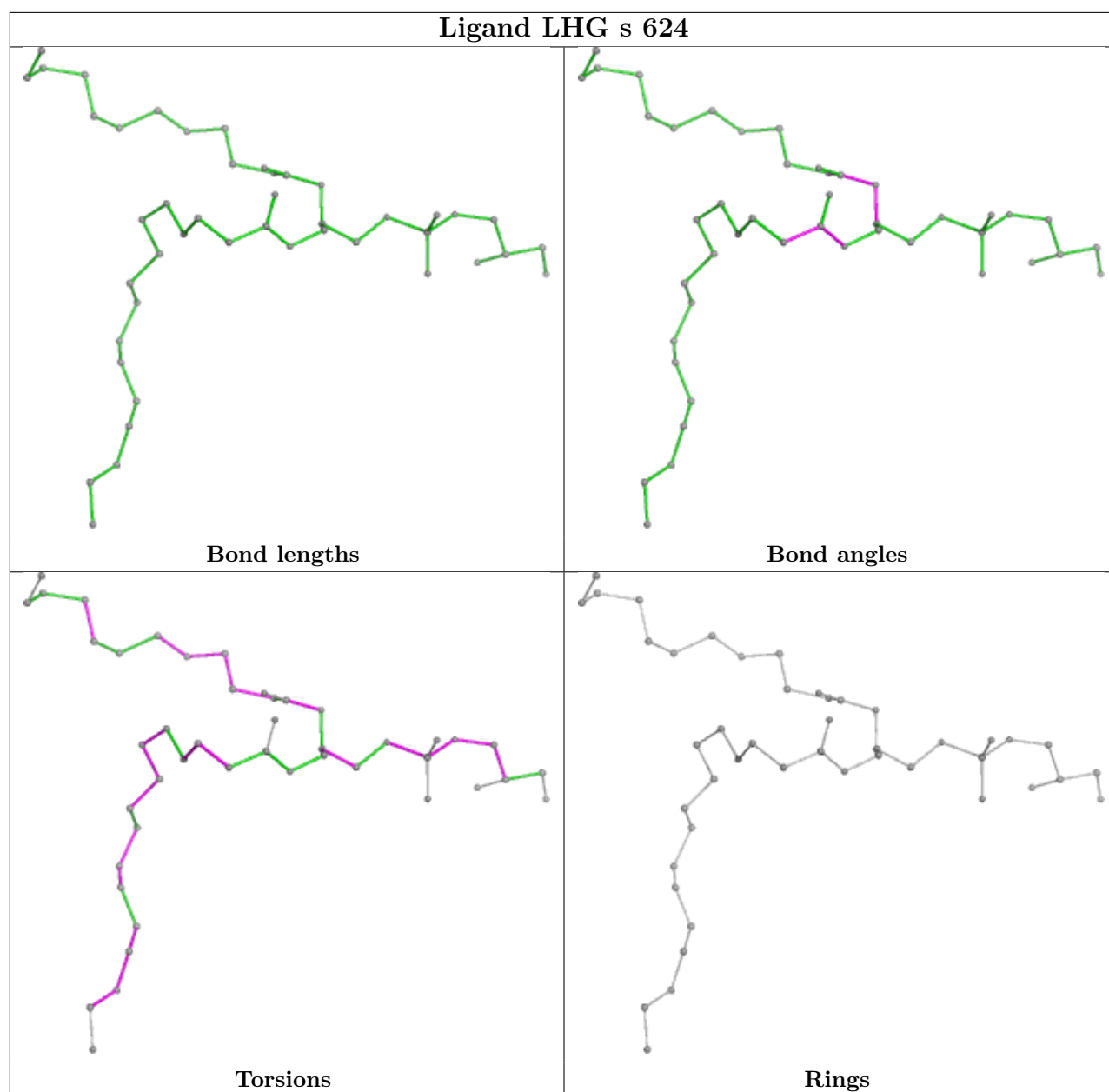


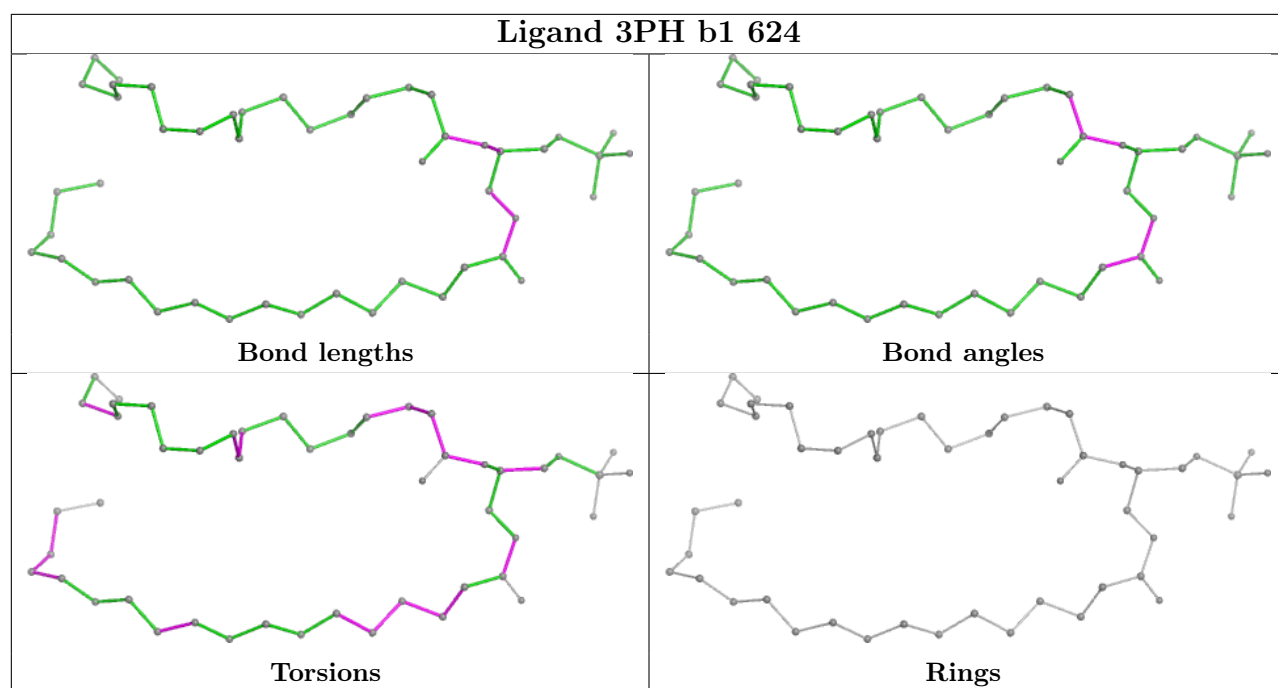
Torsions



Rings

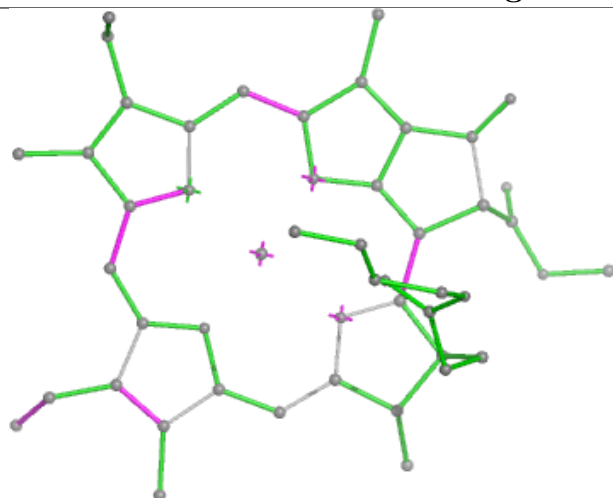




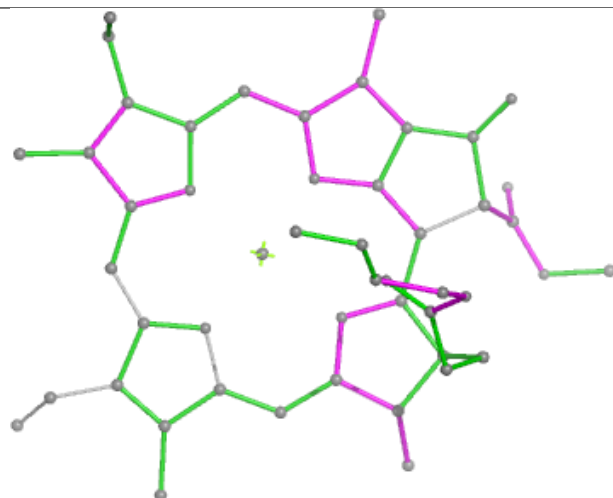




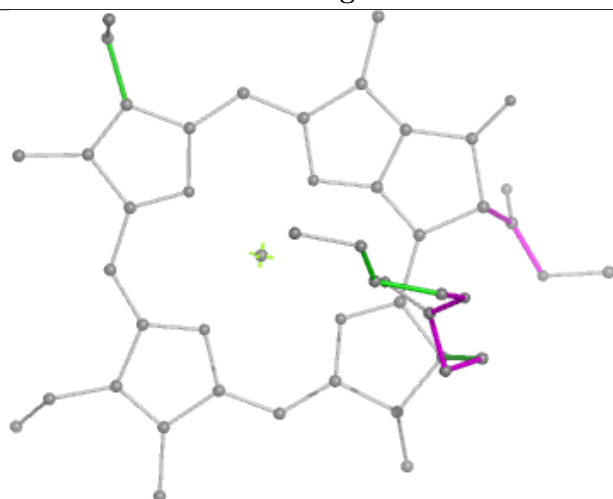
## Ligand CLA R1 604



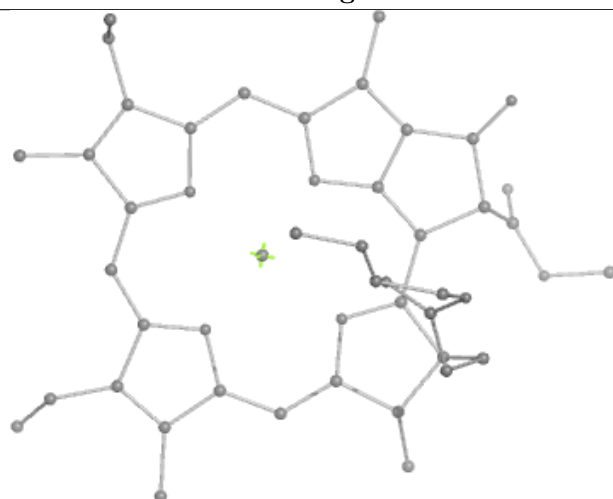
Bond lengths



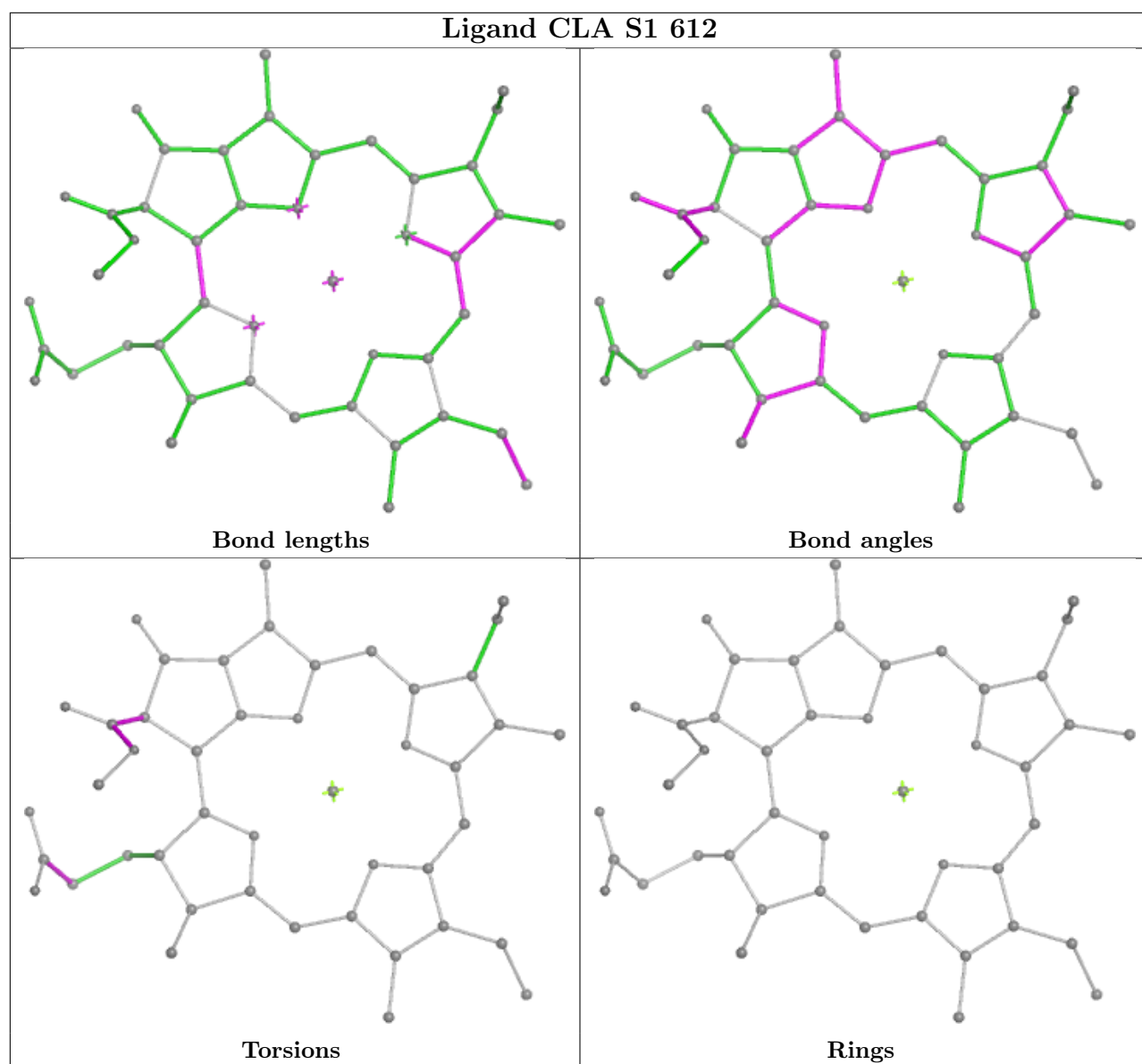
Bond angles

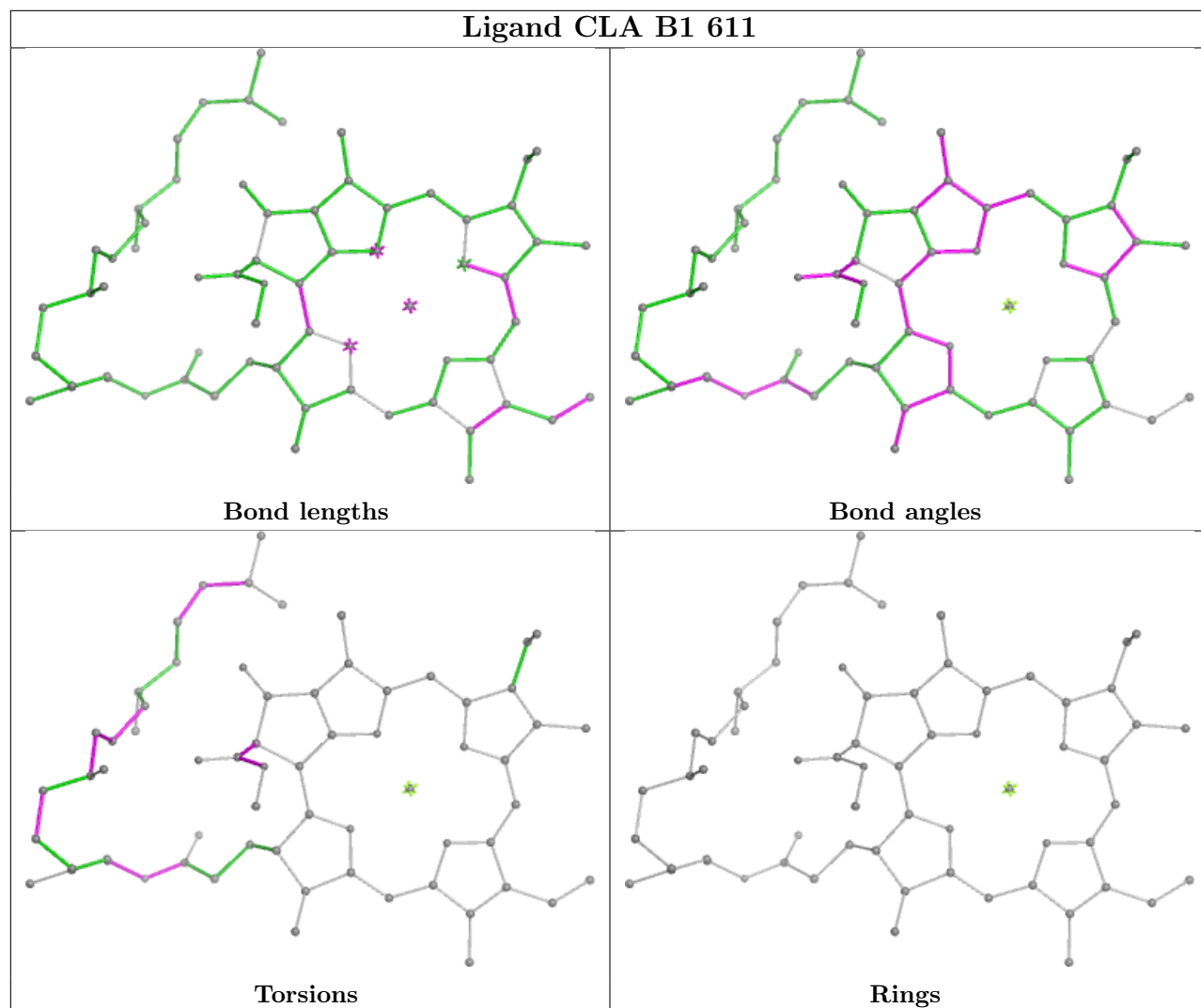


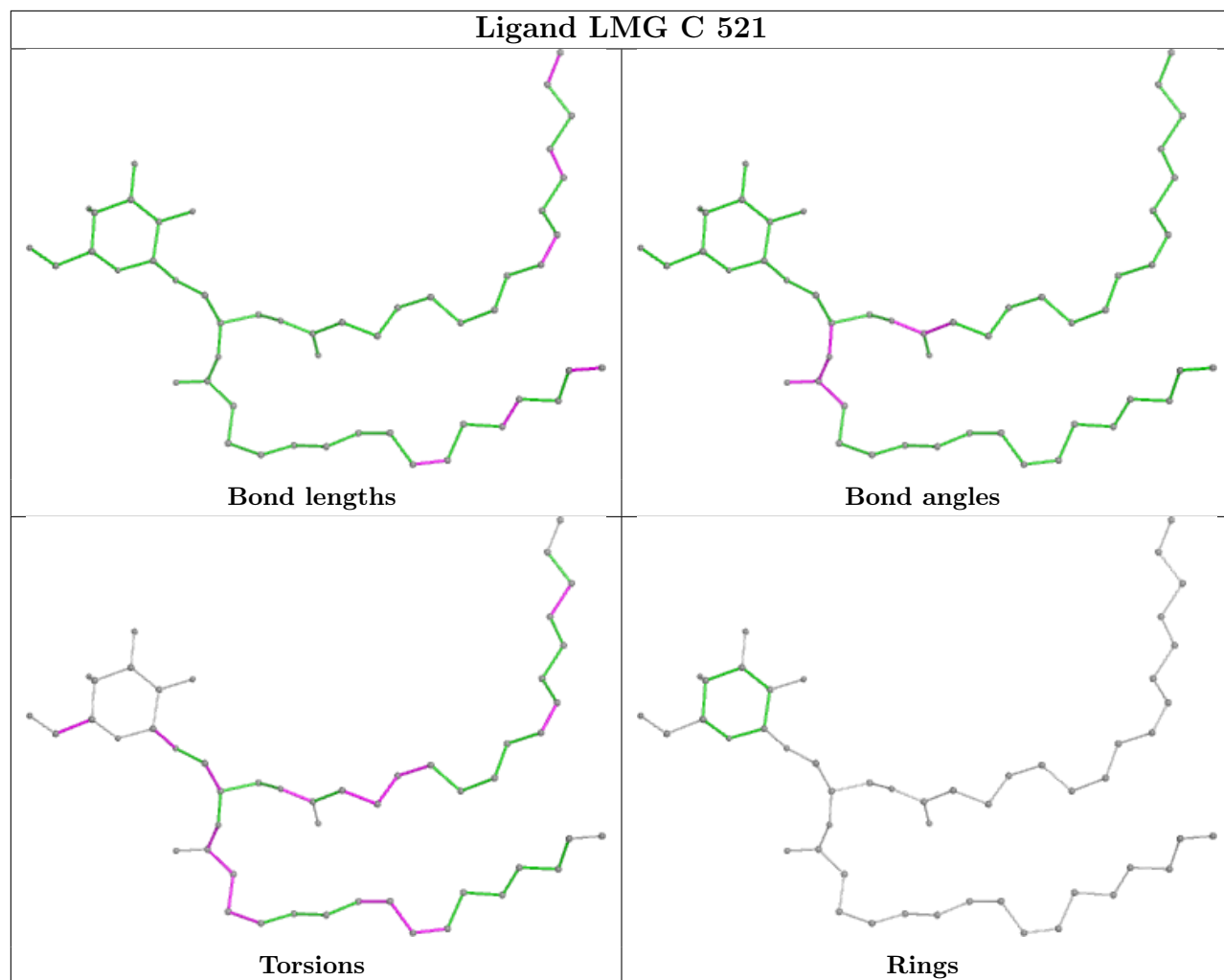
Torsions



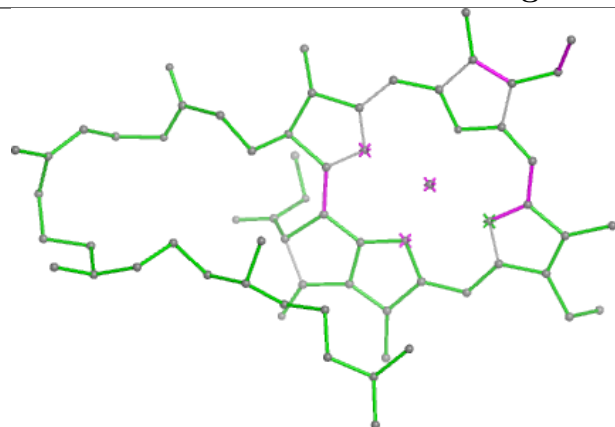
Rings



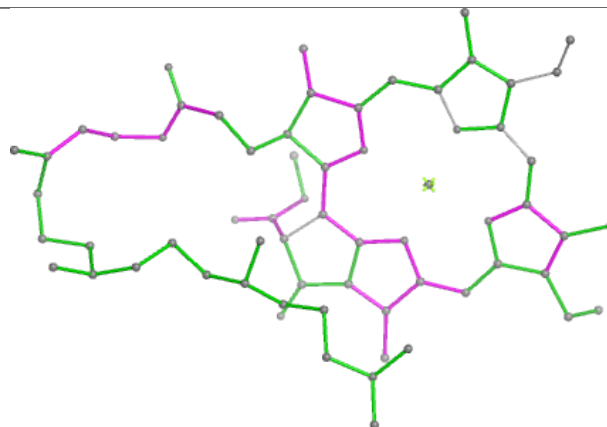




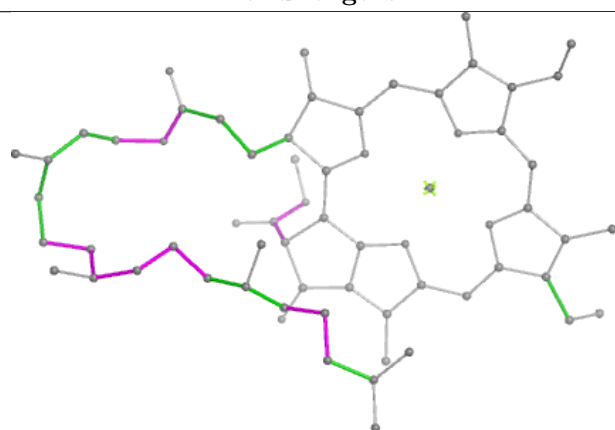
## Ligand CLA c 509



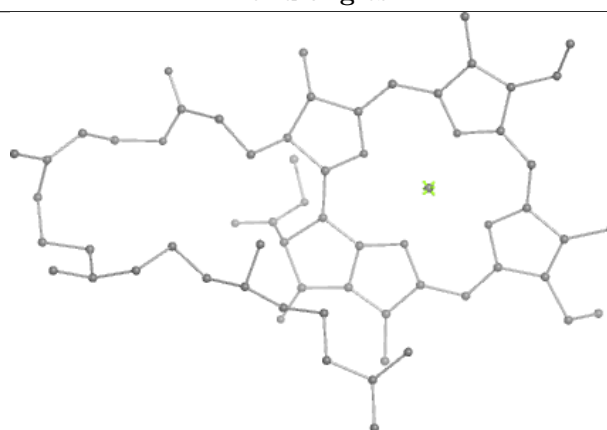
Bond lengths



Bond angles

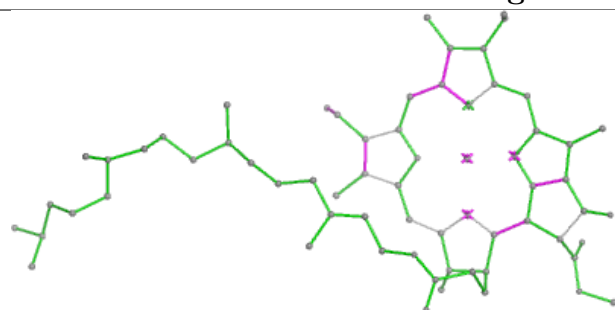


Torsions

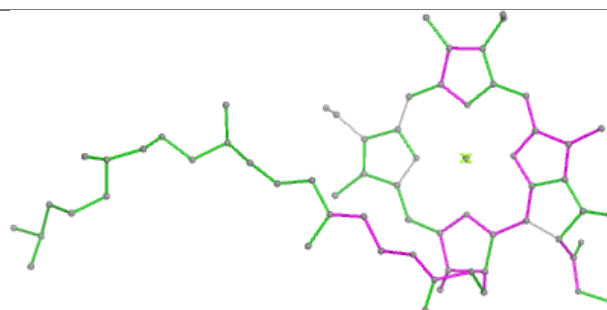


Rings

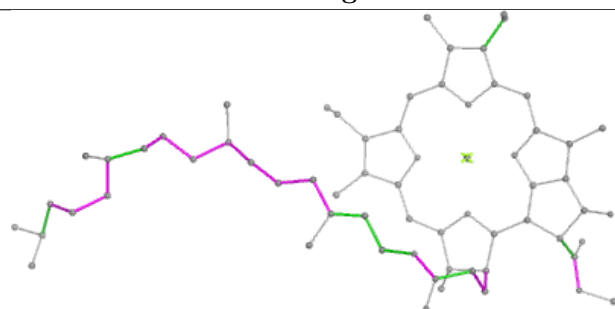
## Ligand CLA B1 604



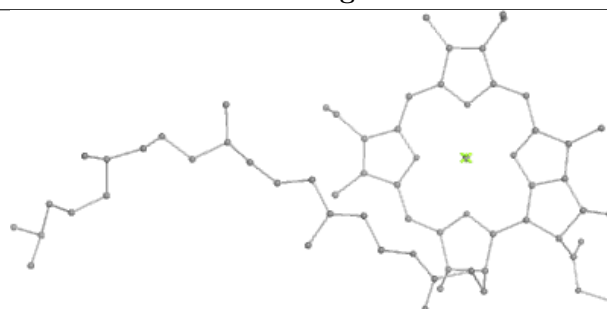
Bond lengths



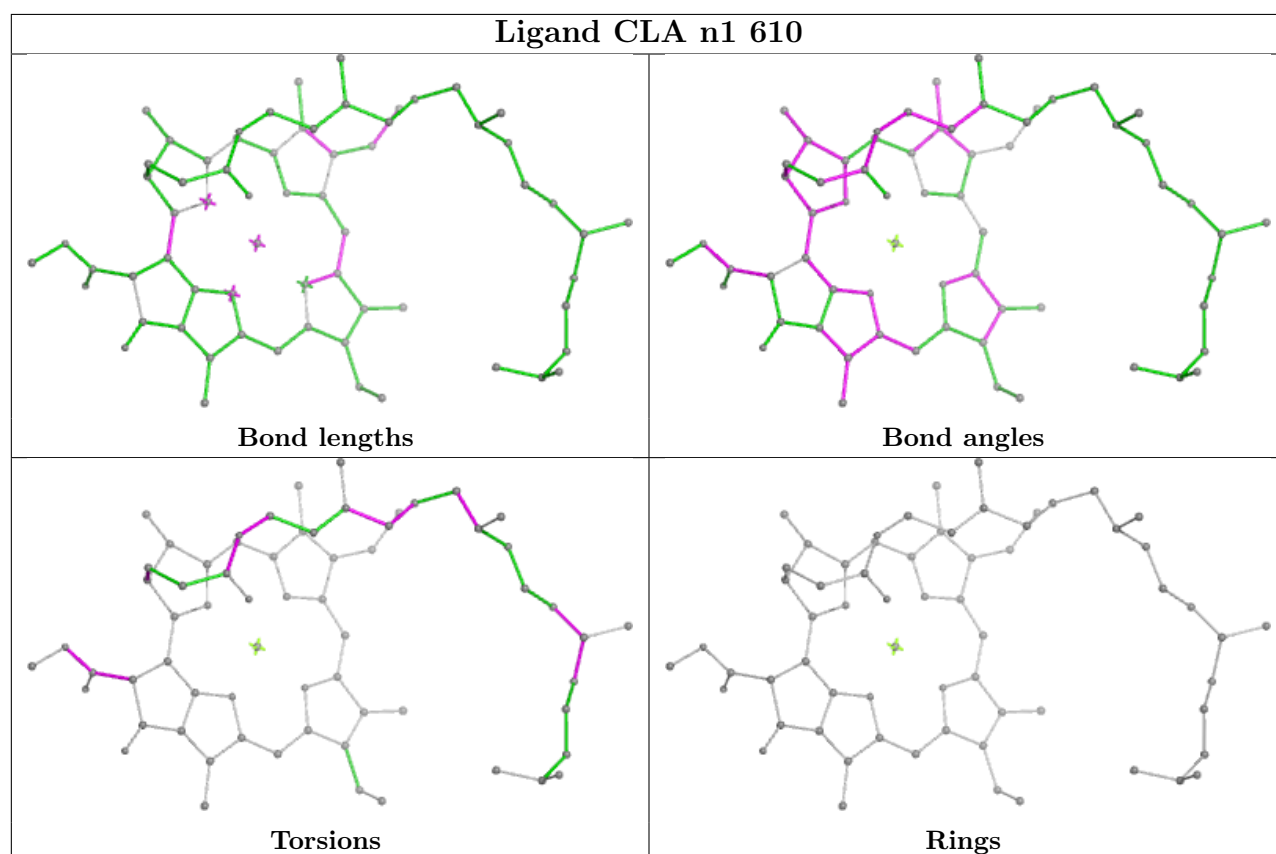
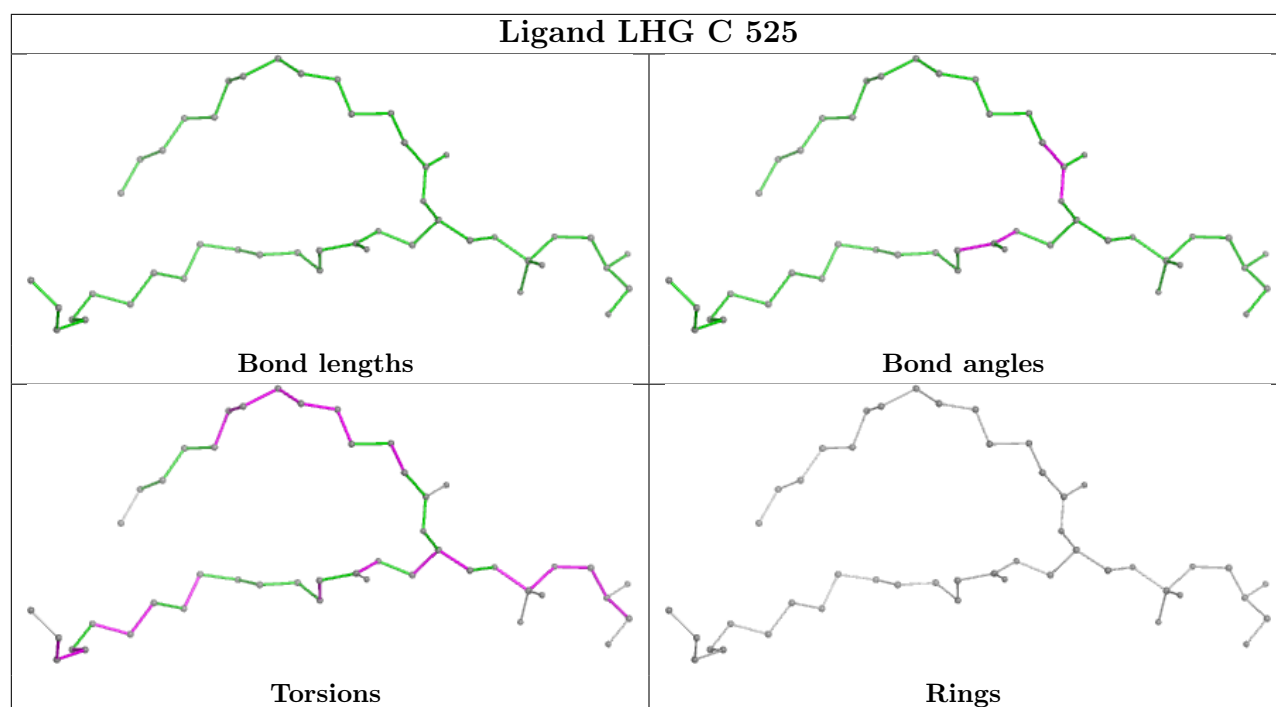
Bond angles

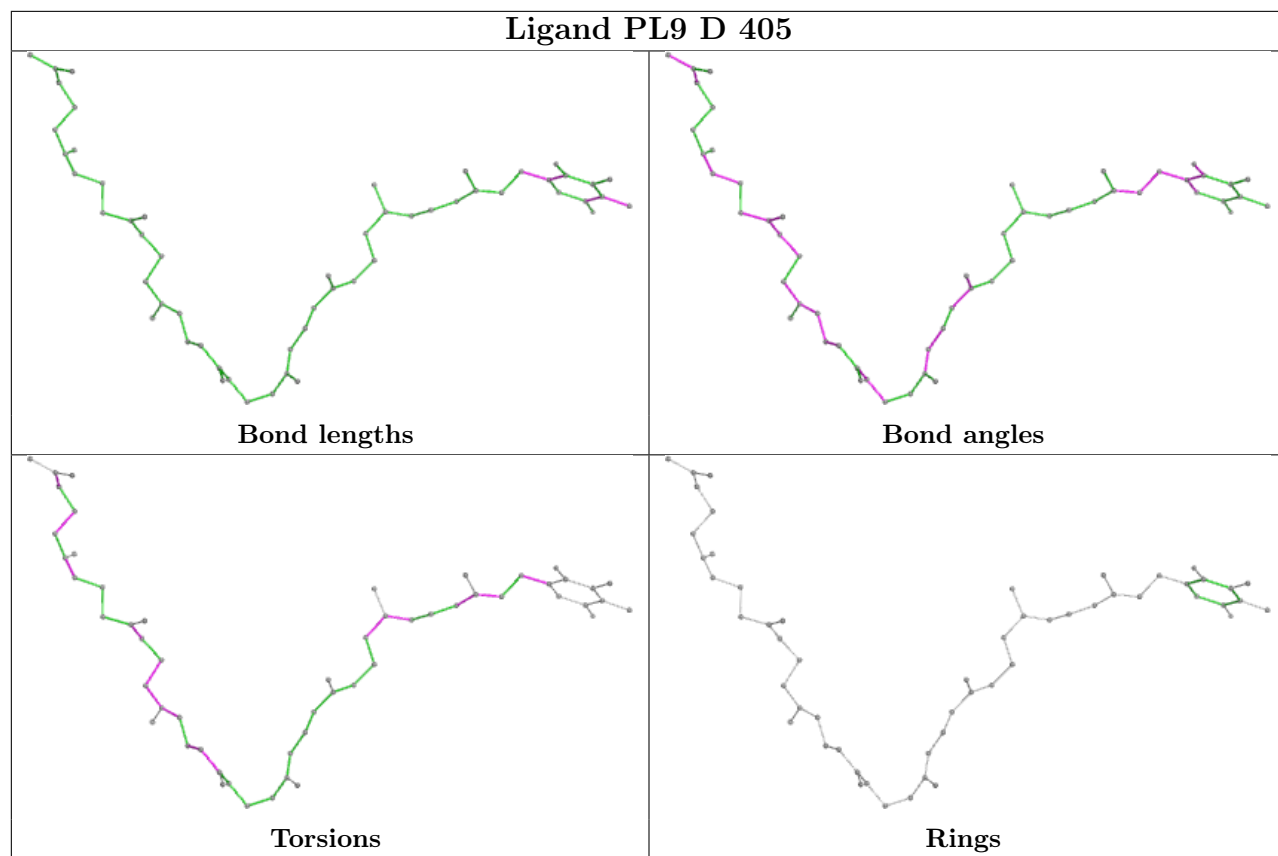


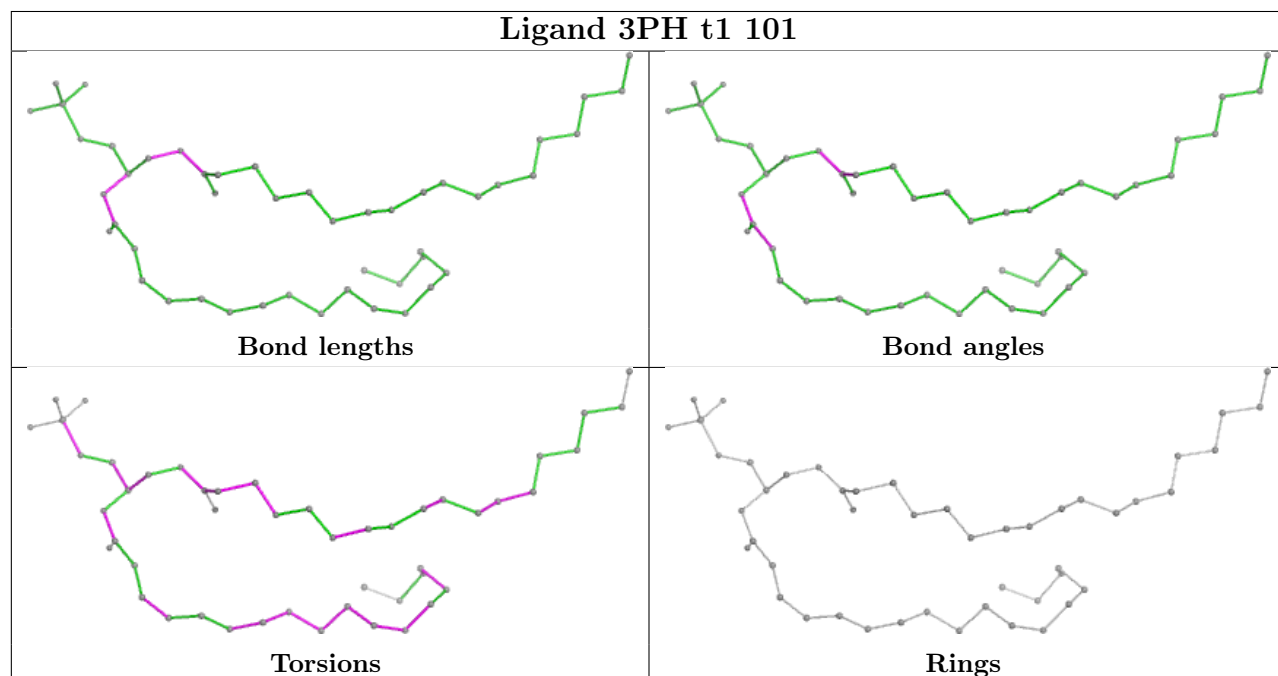
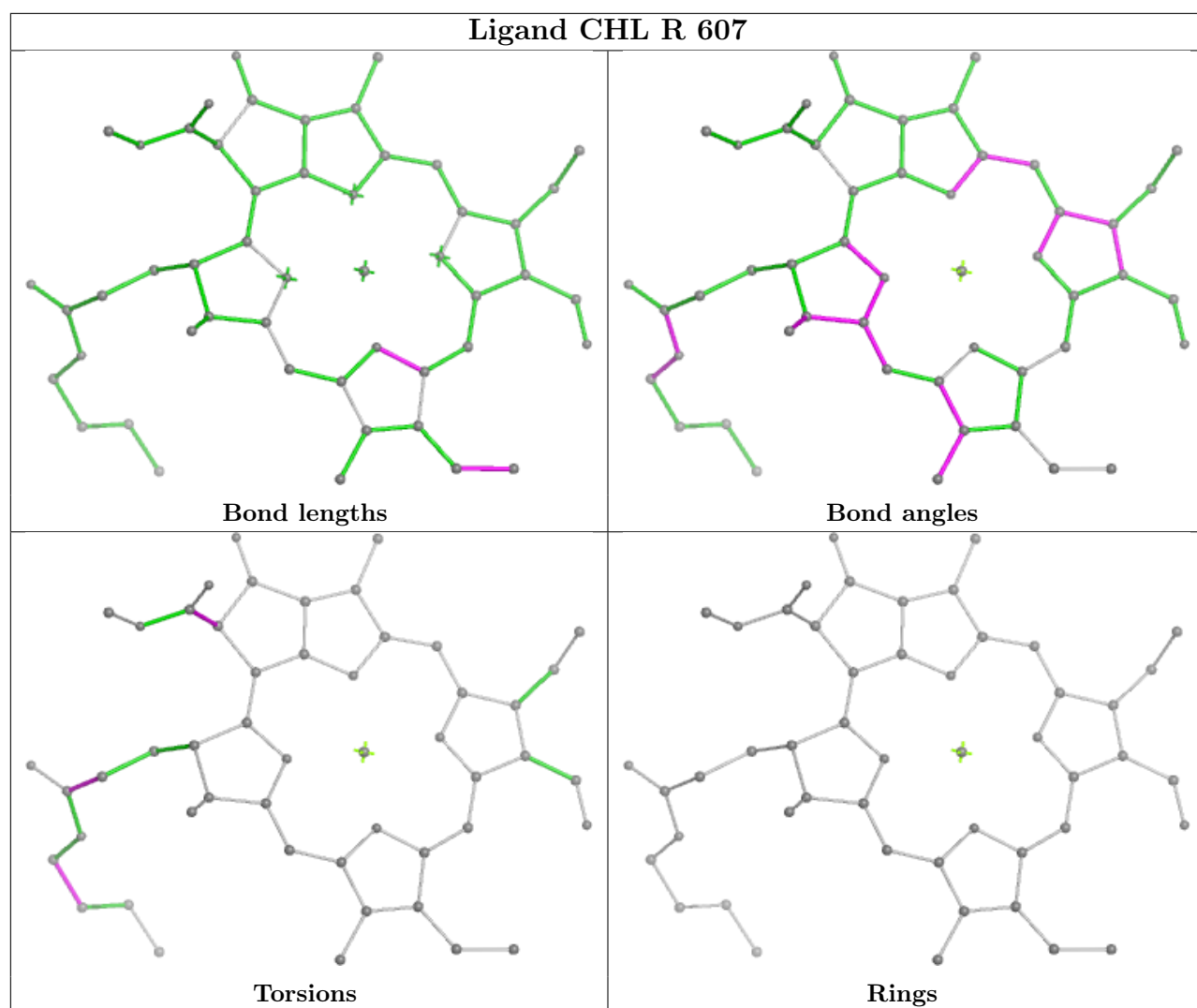
Torsions



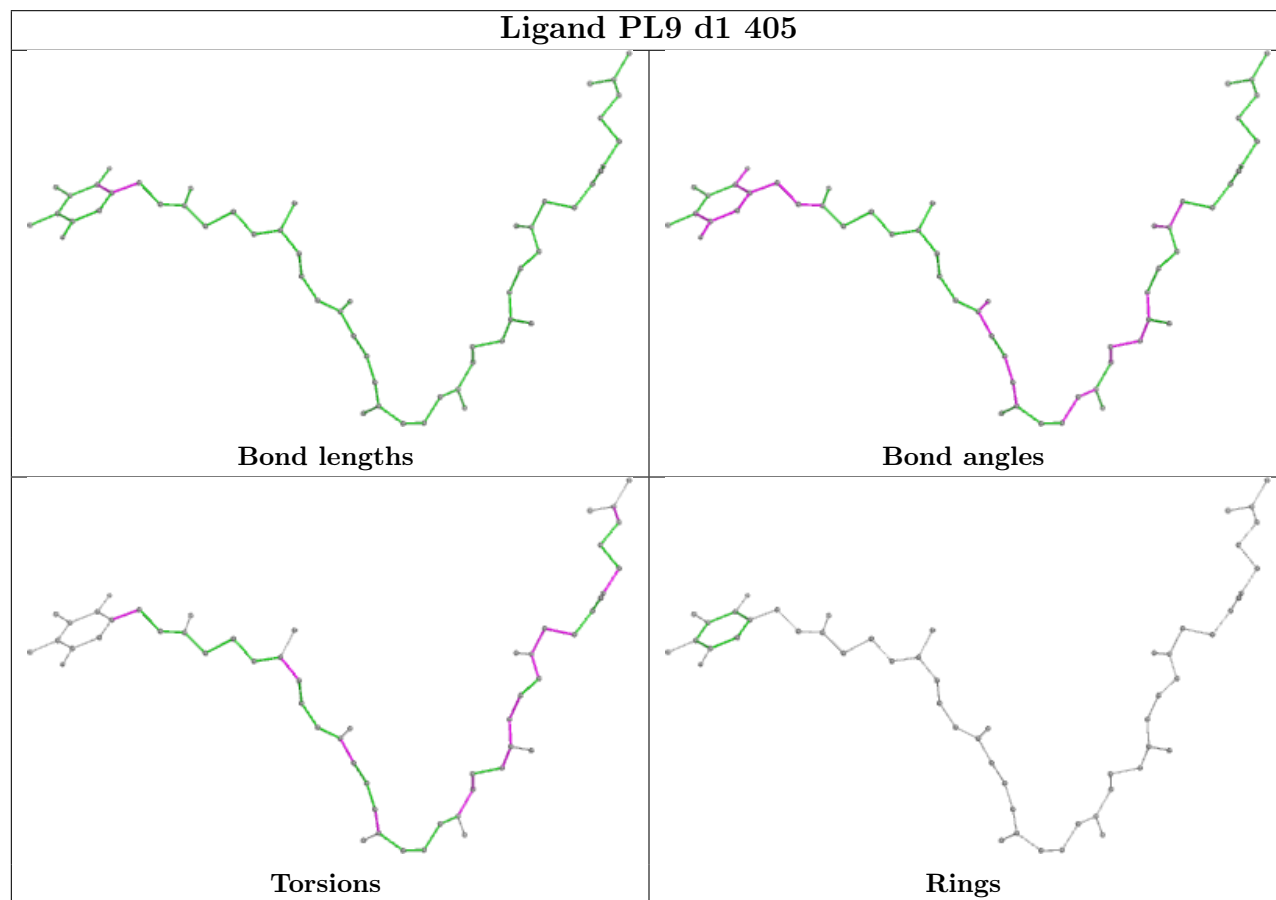
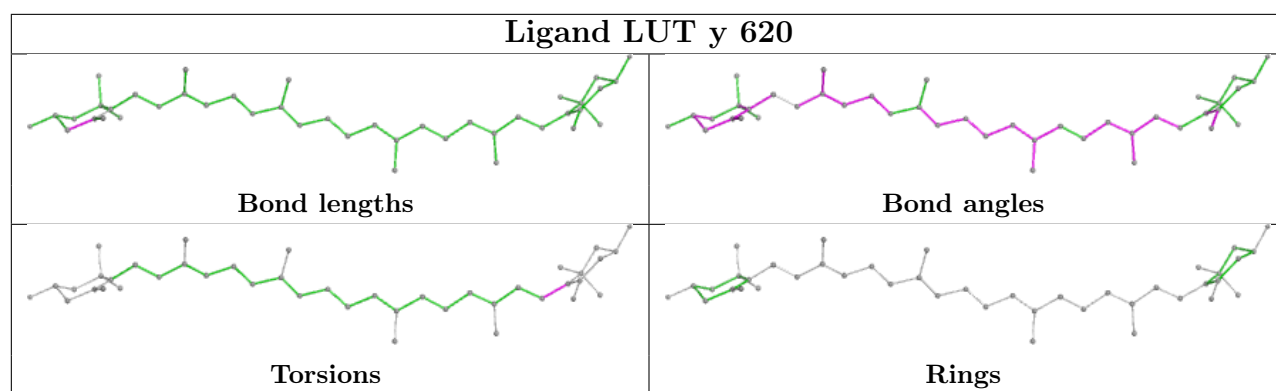
Rings

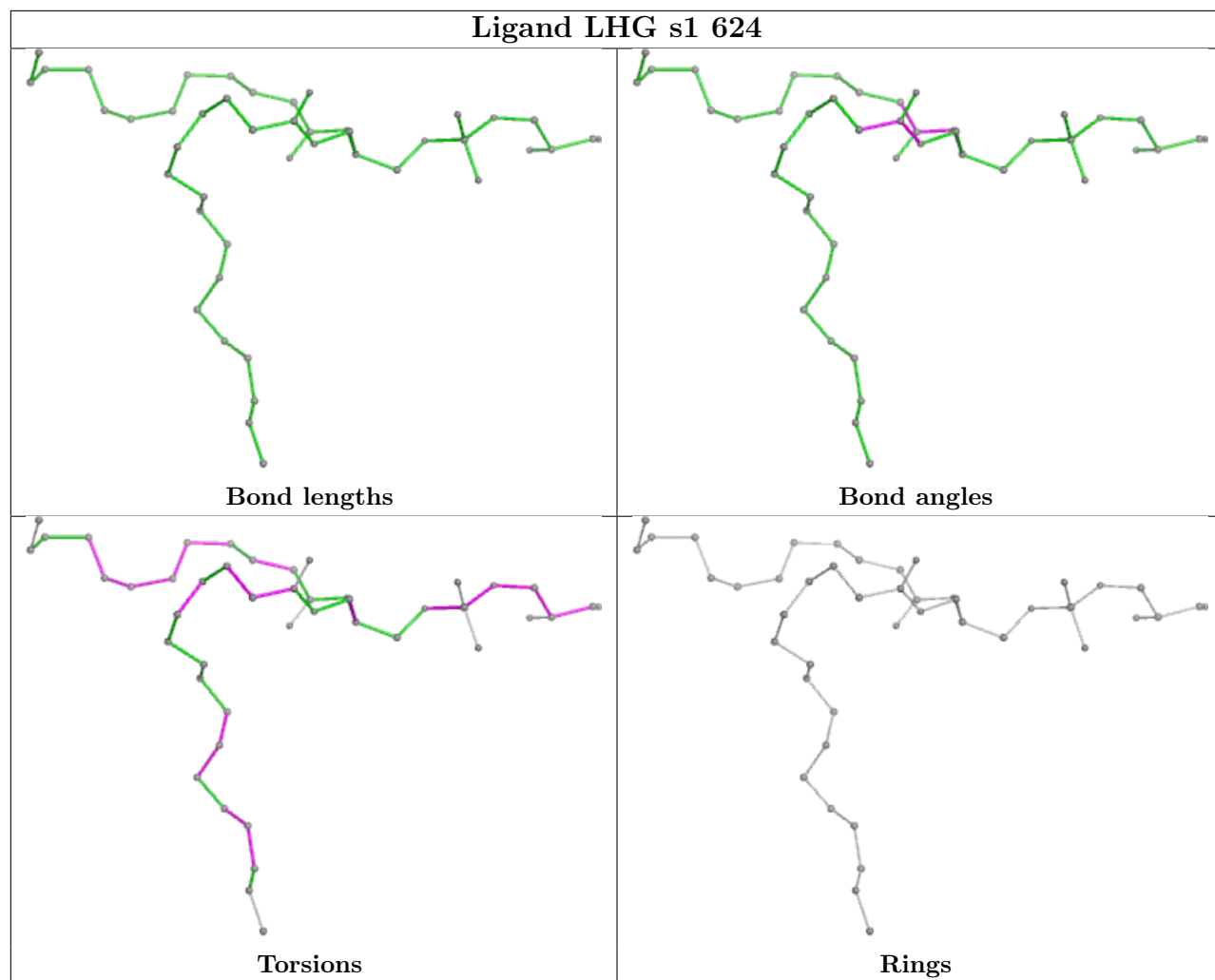


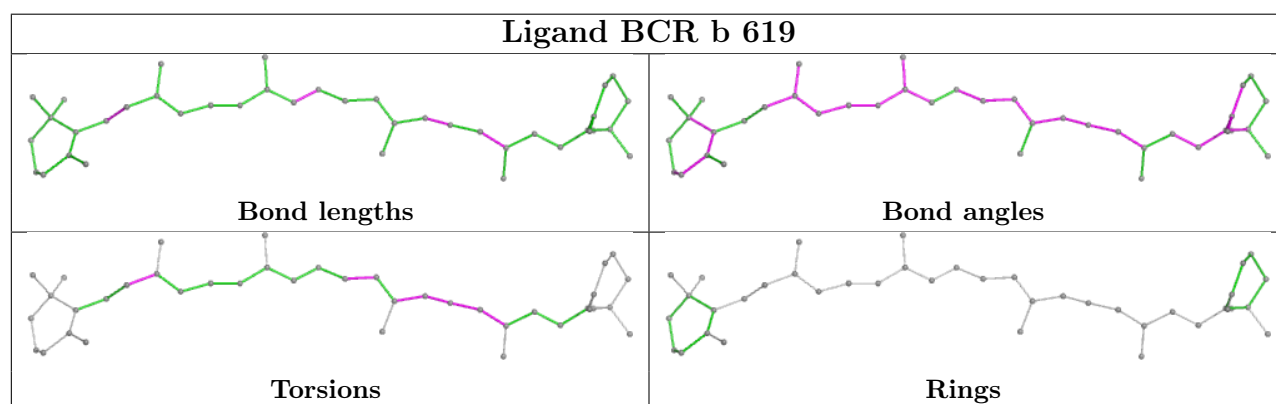
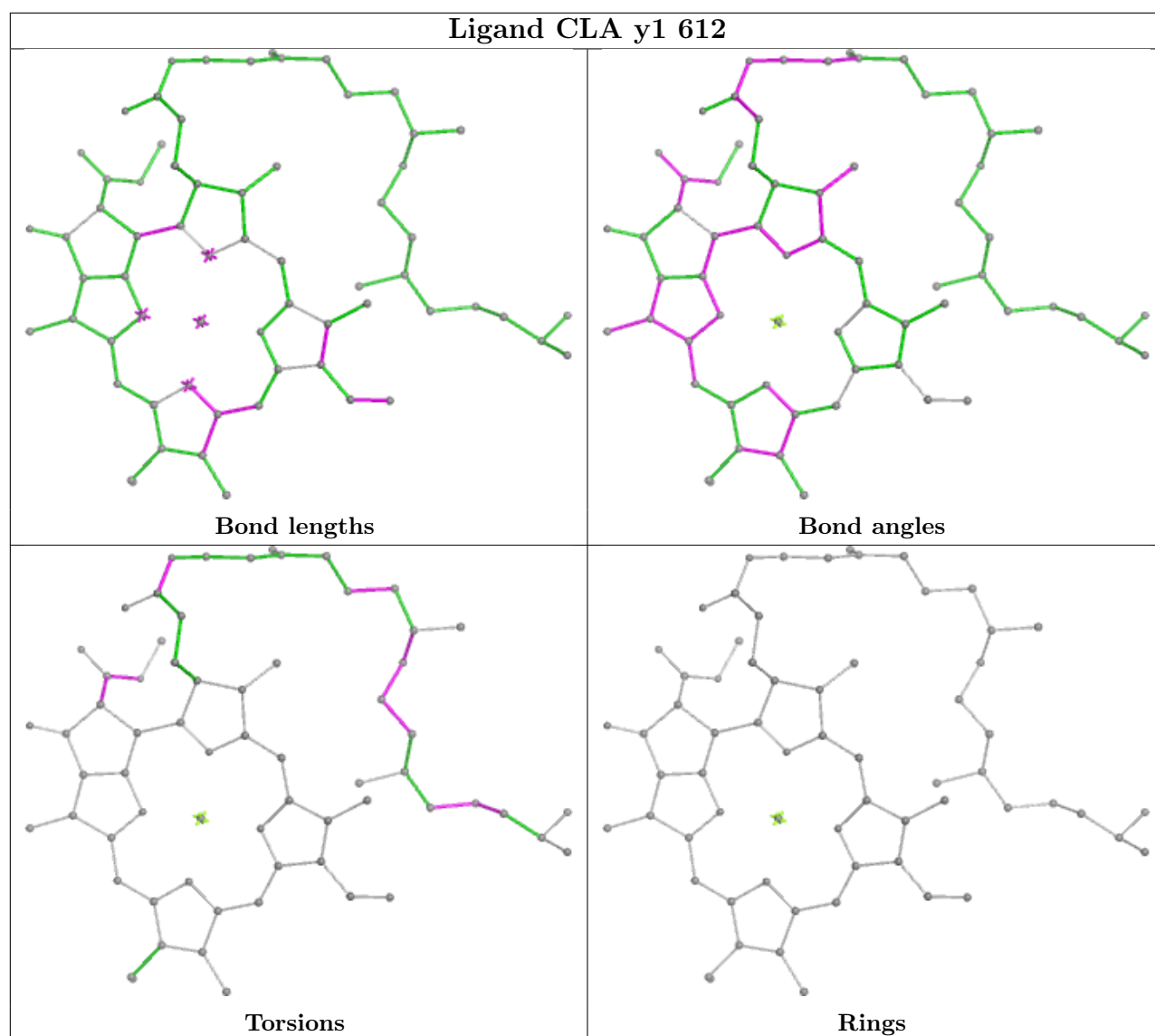


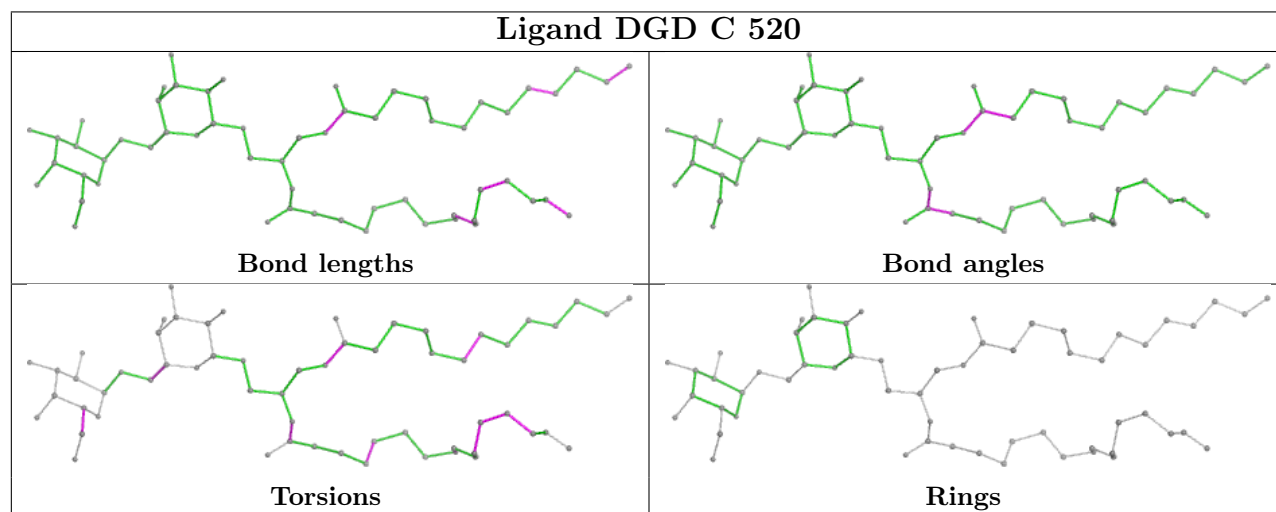
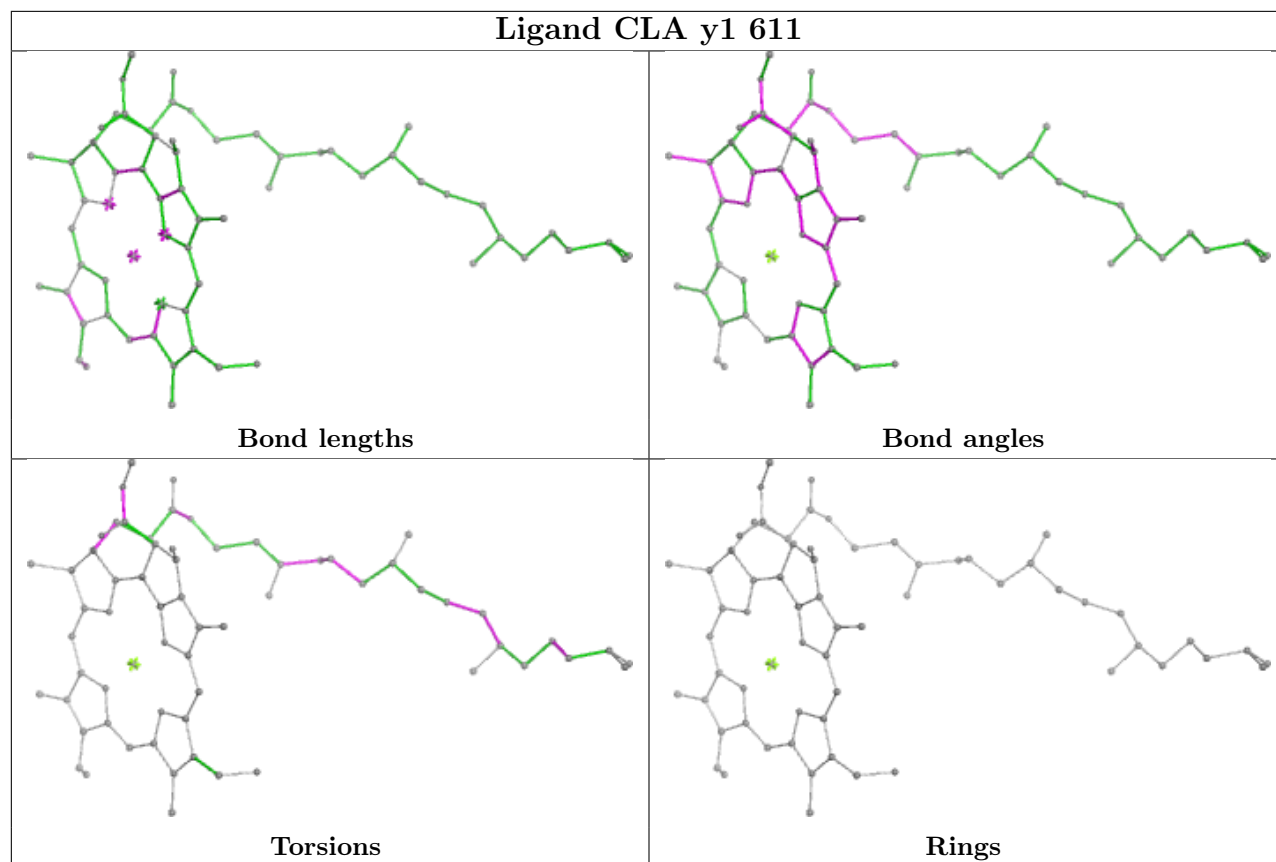


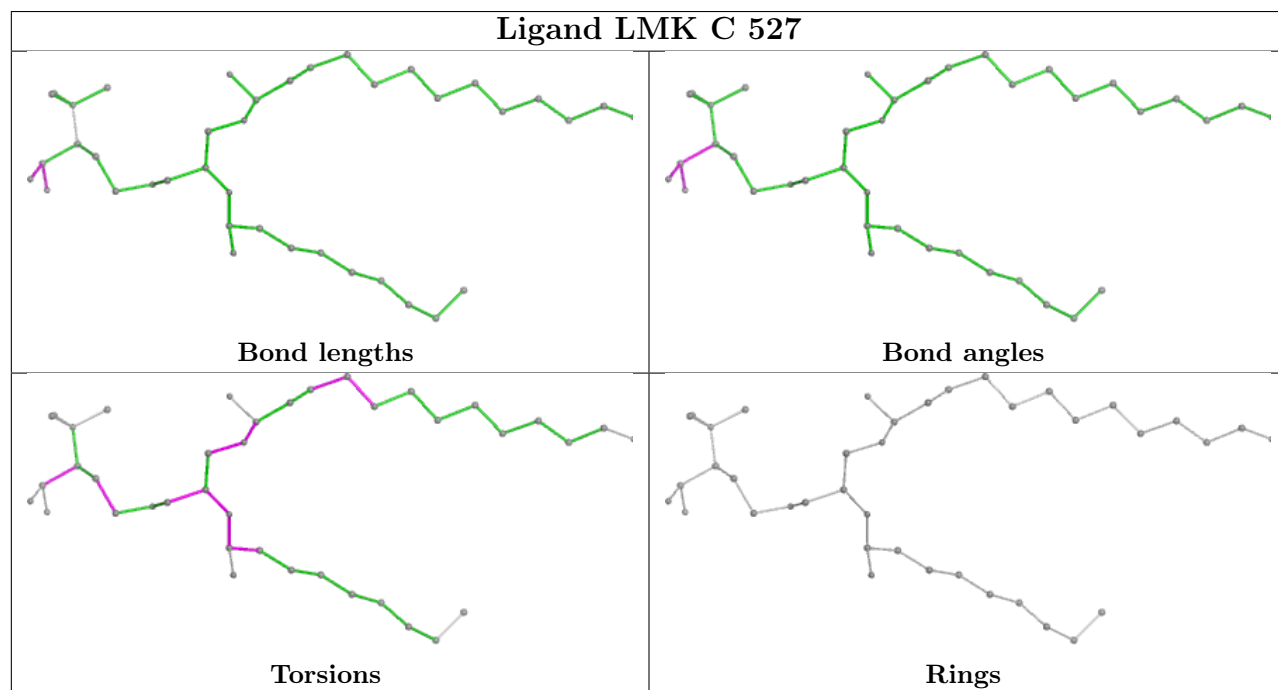
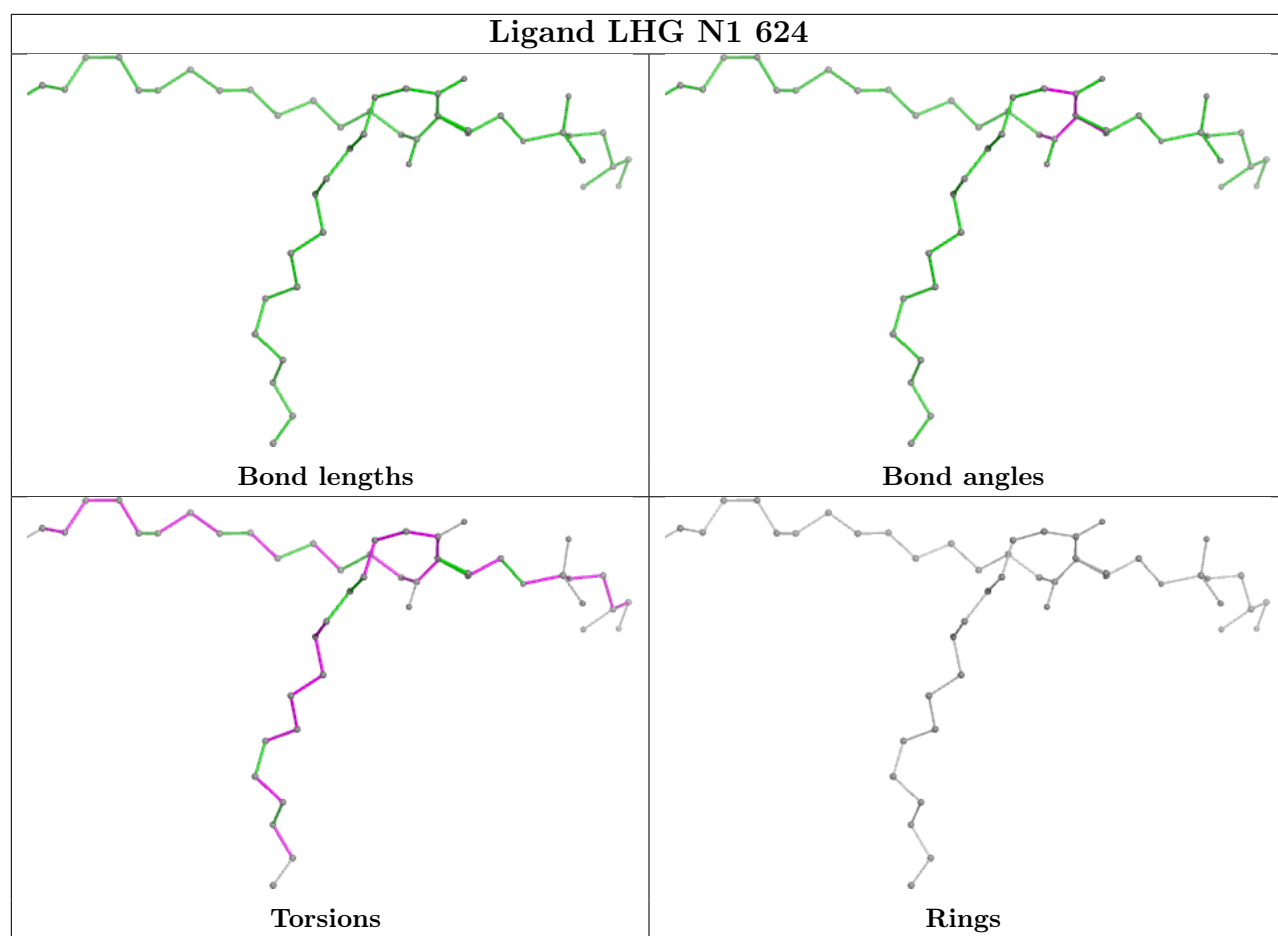


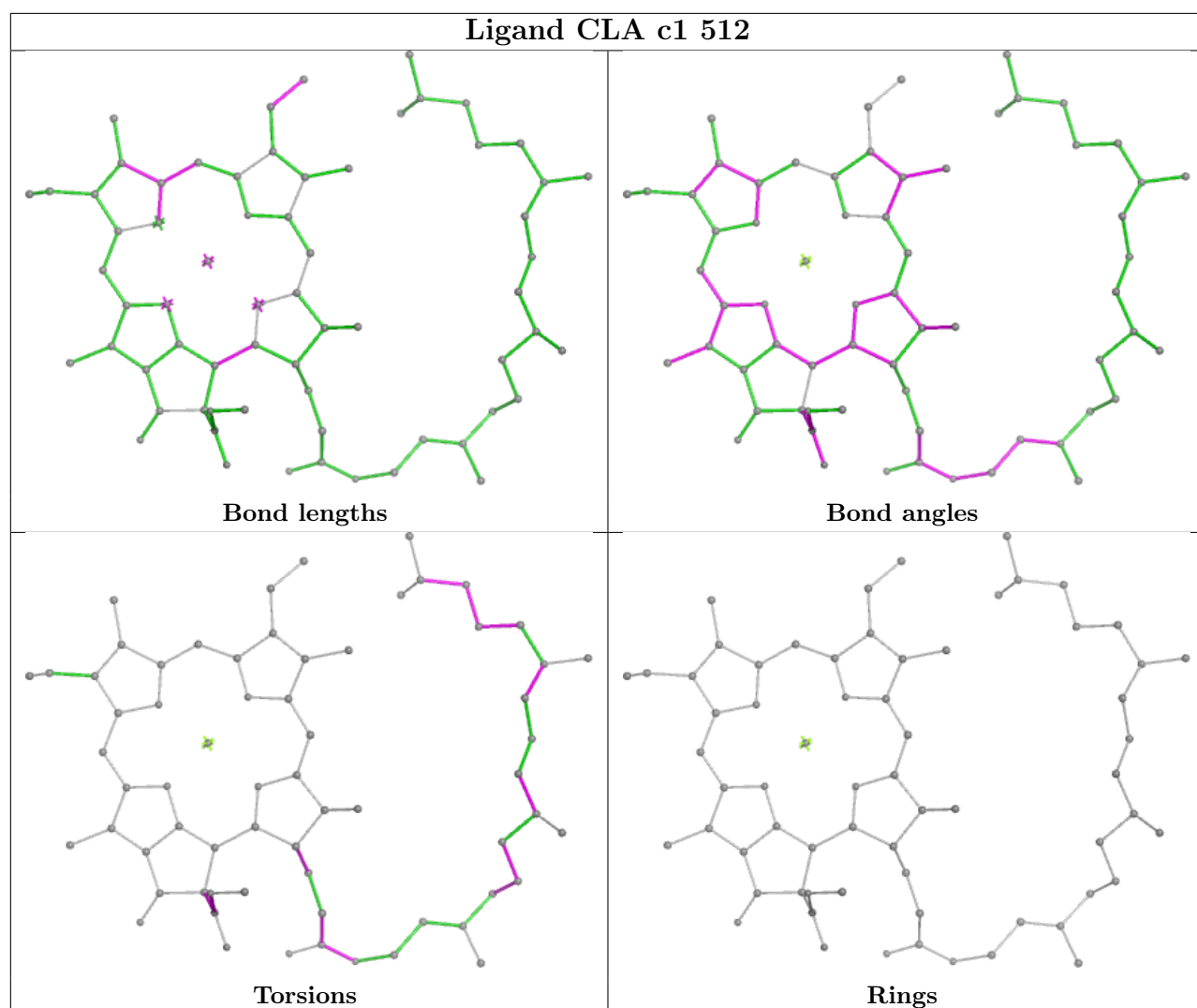


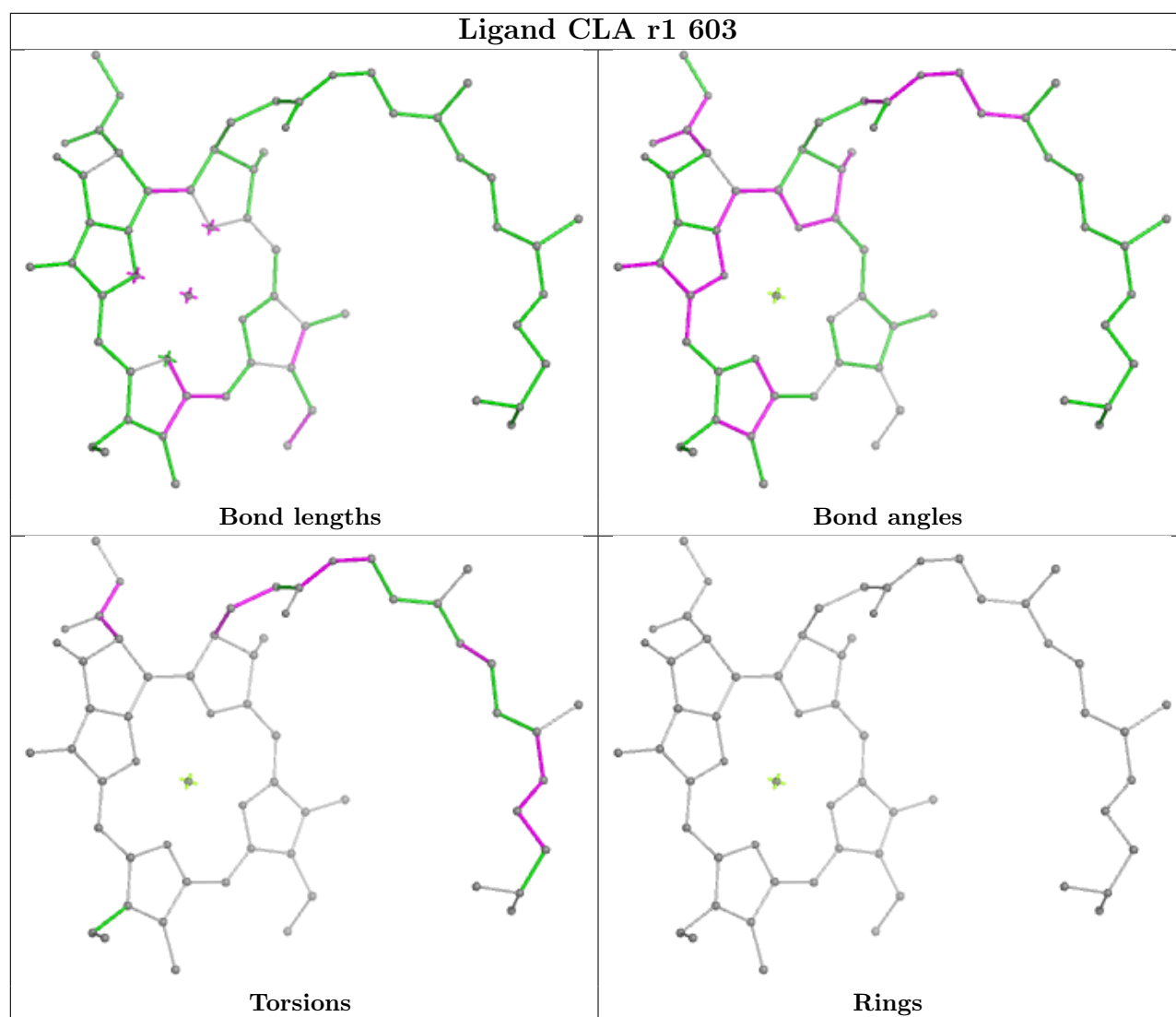


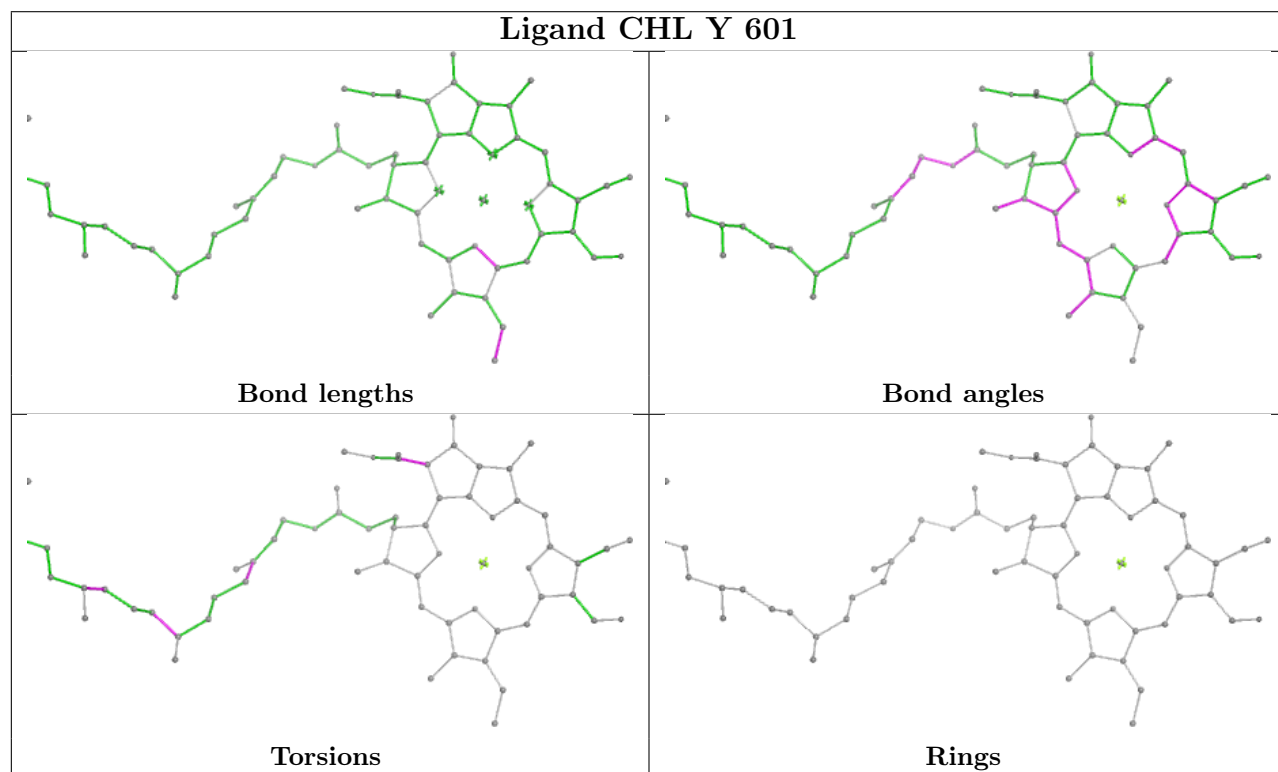
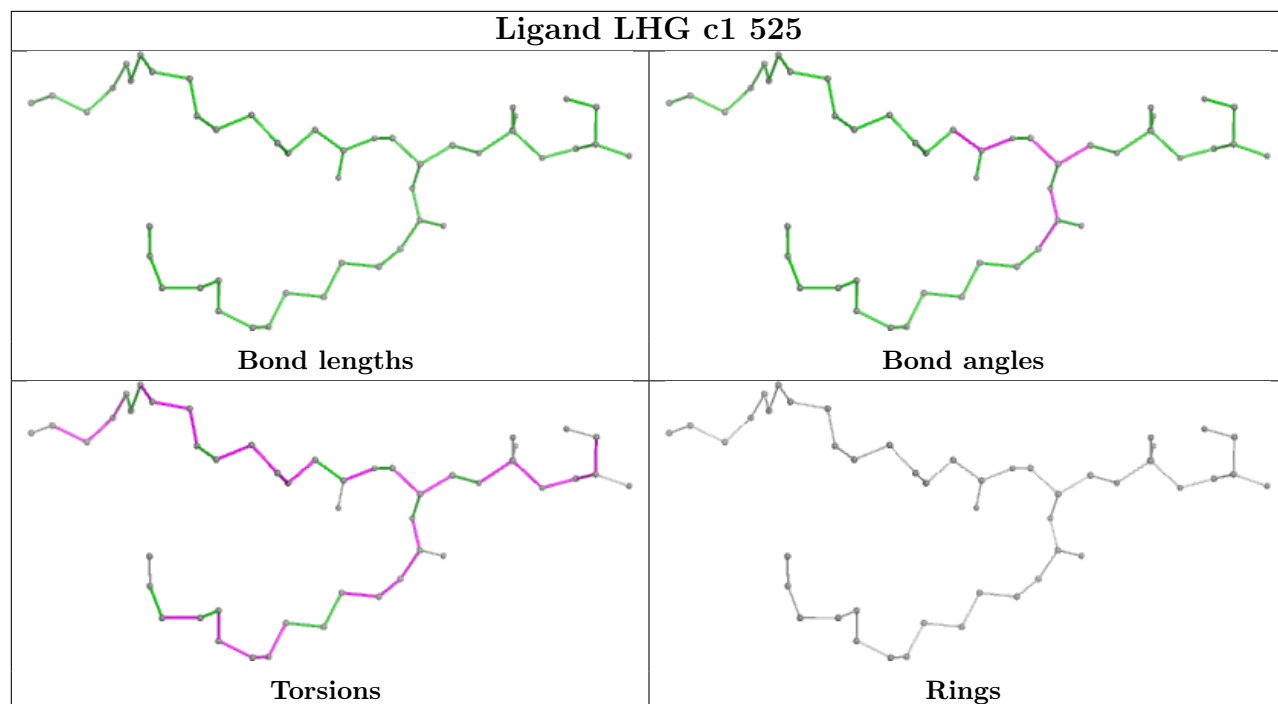






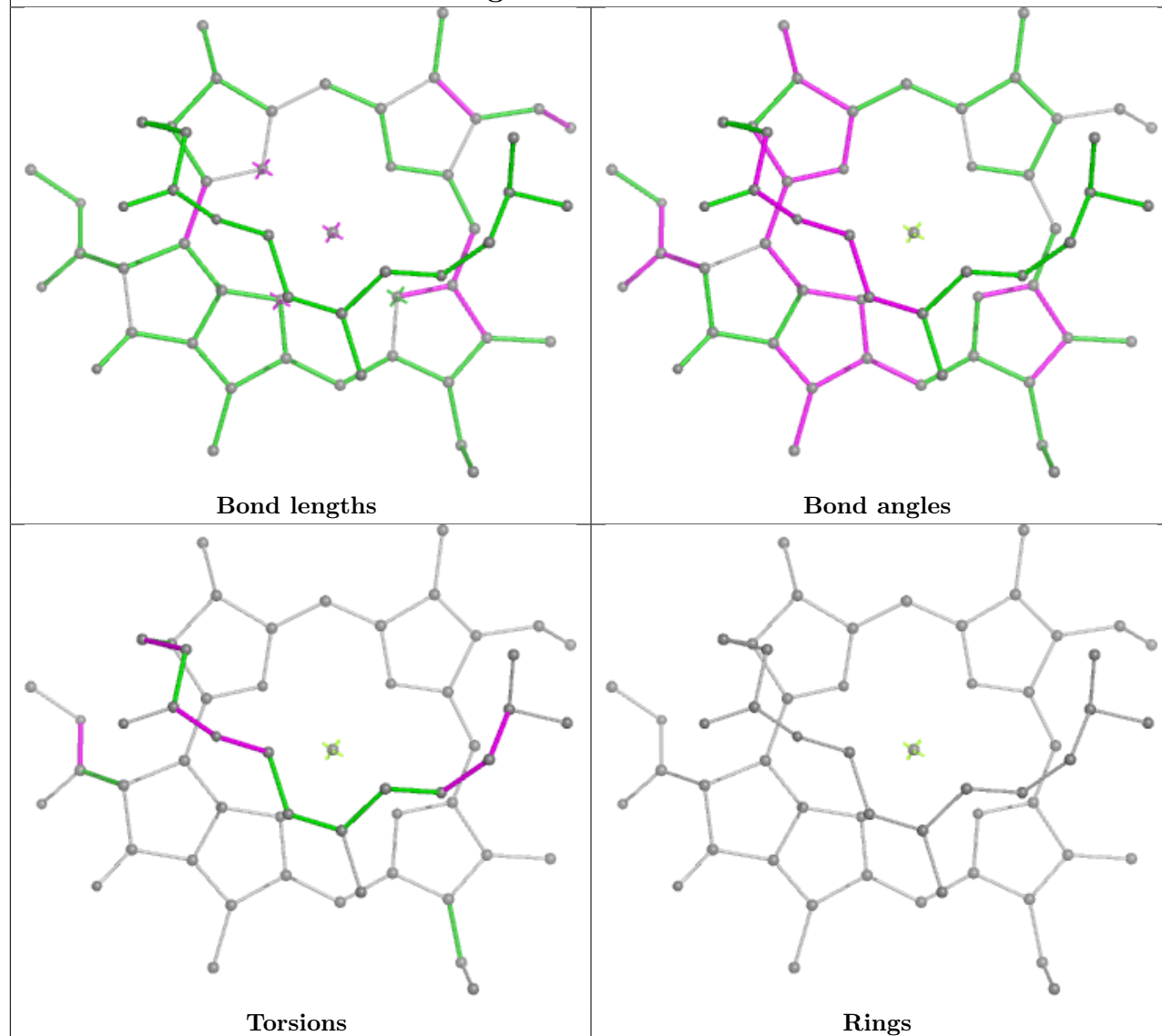




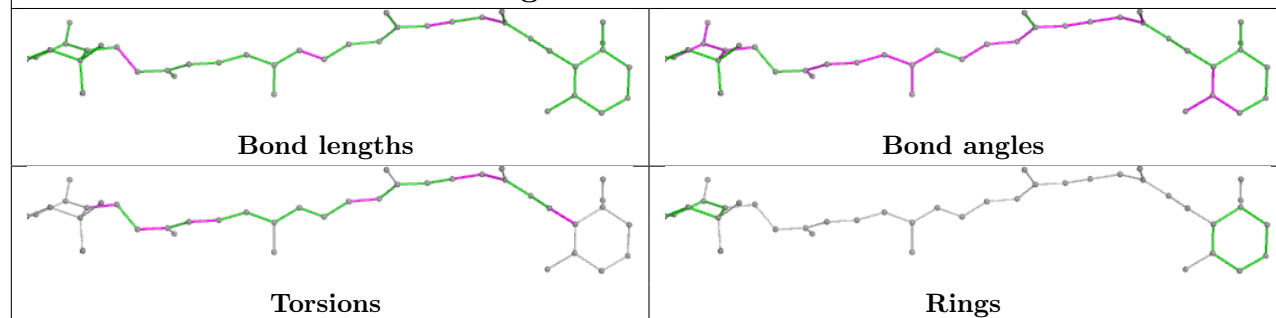


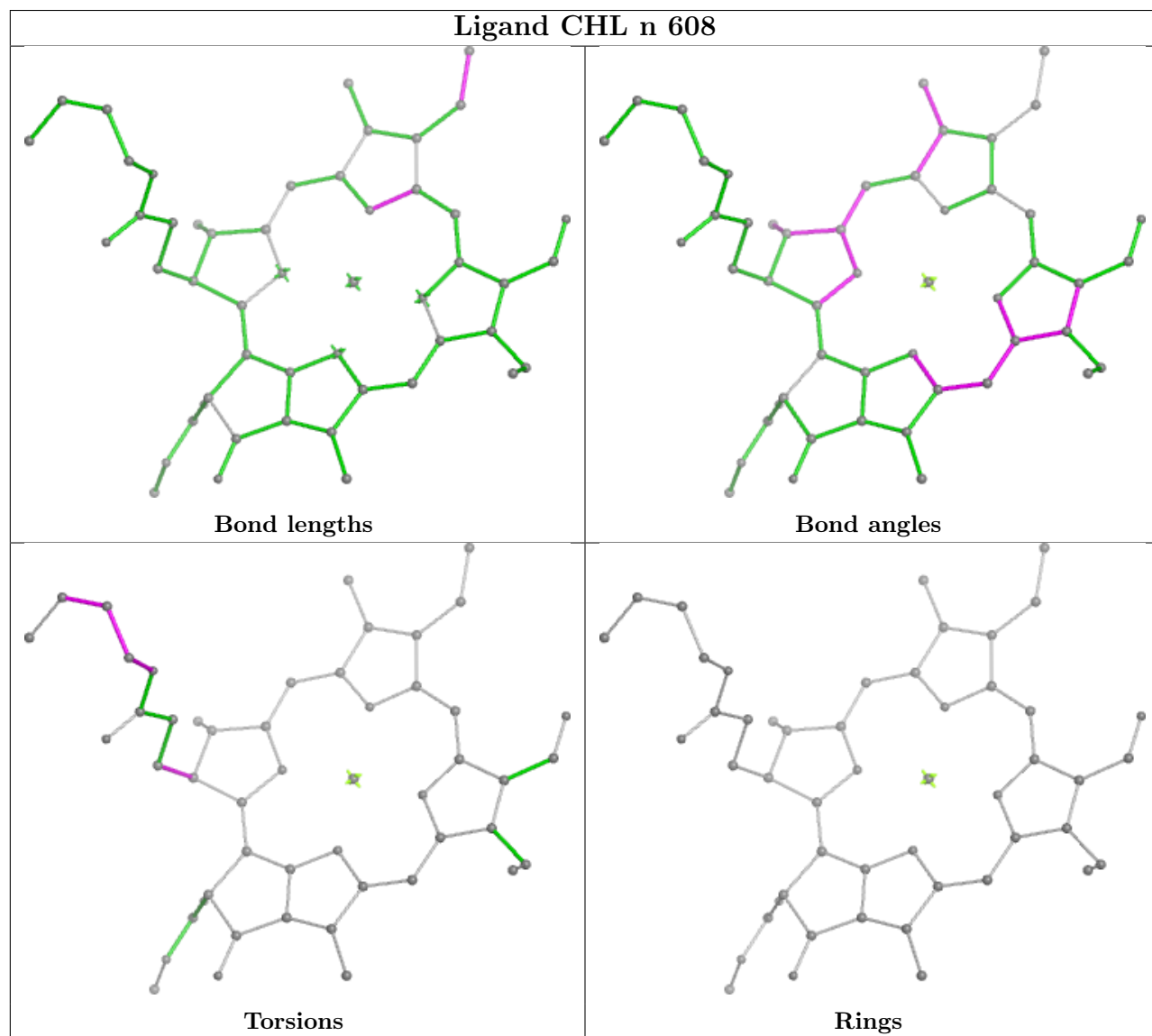
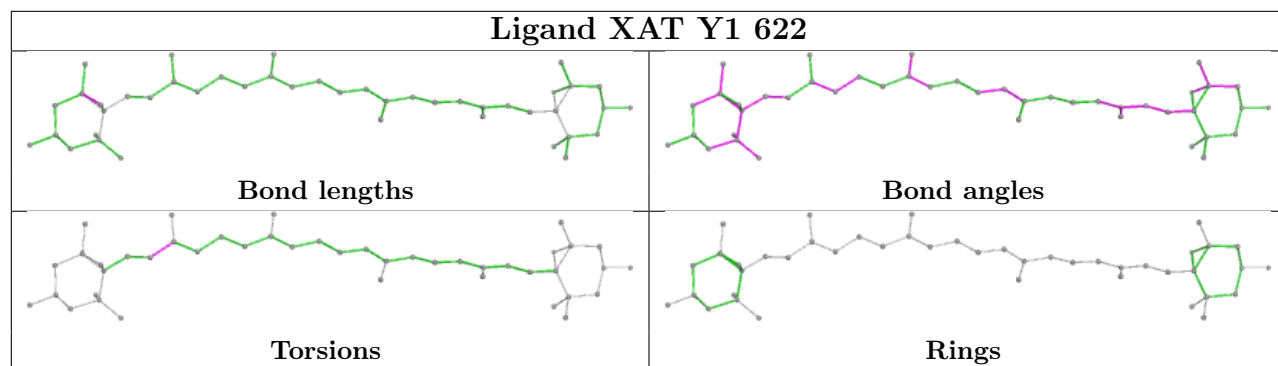


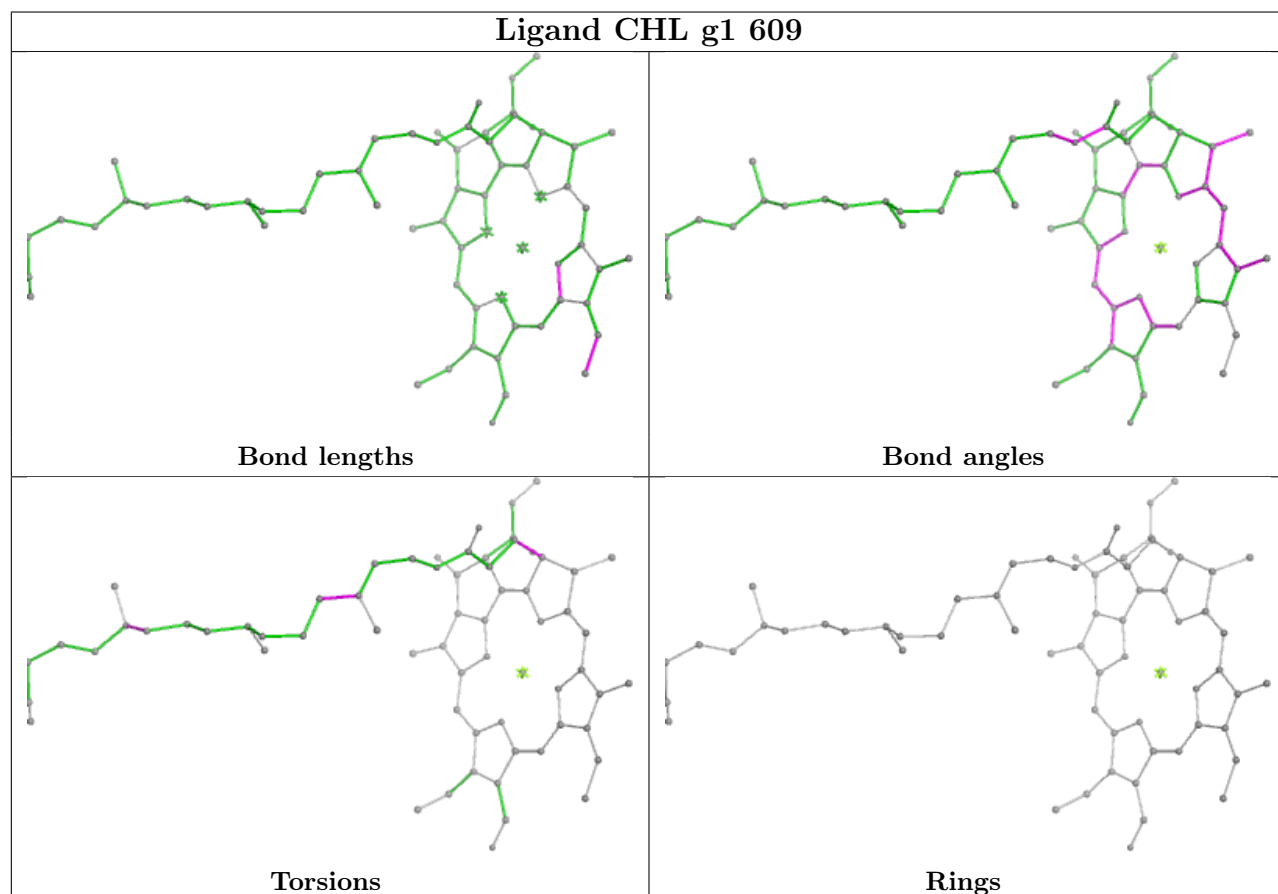
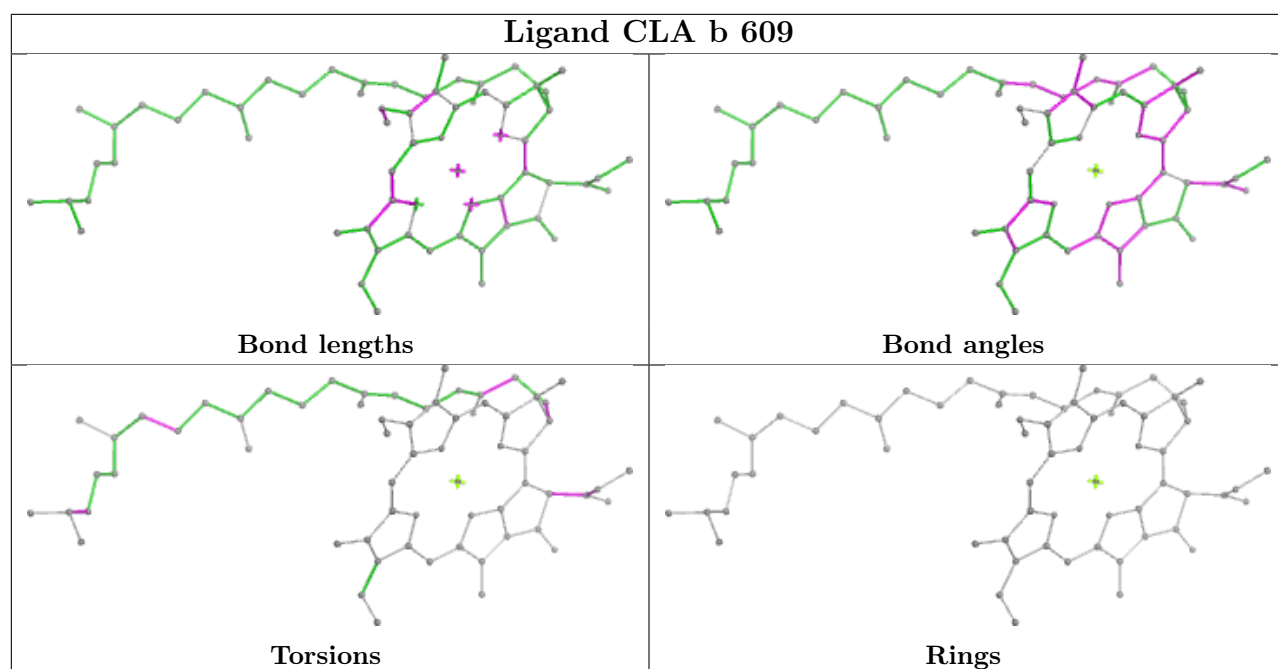
## Ligand CLA S 613

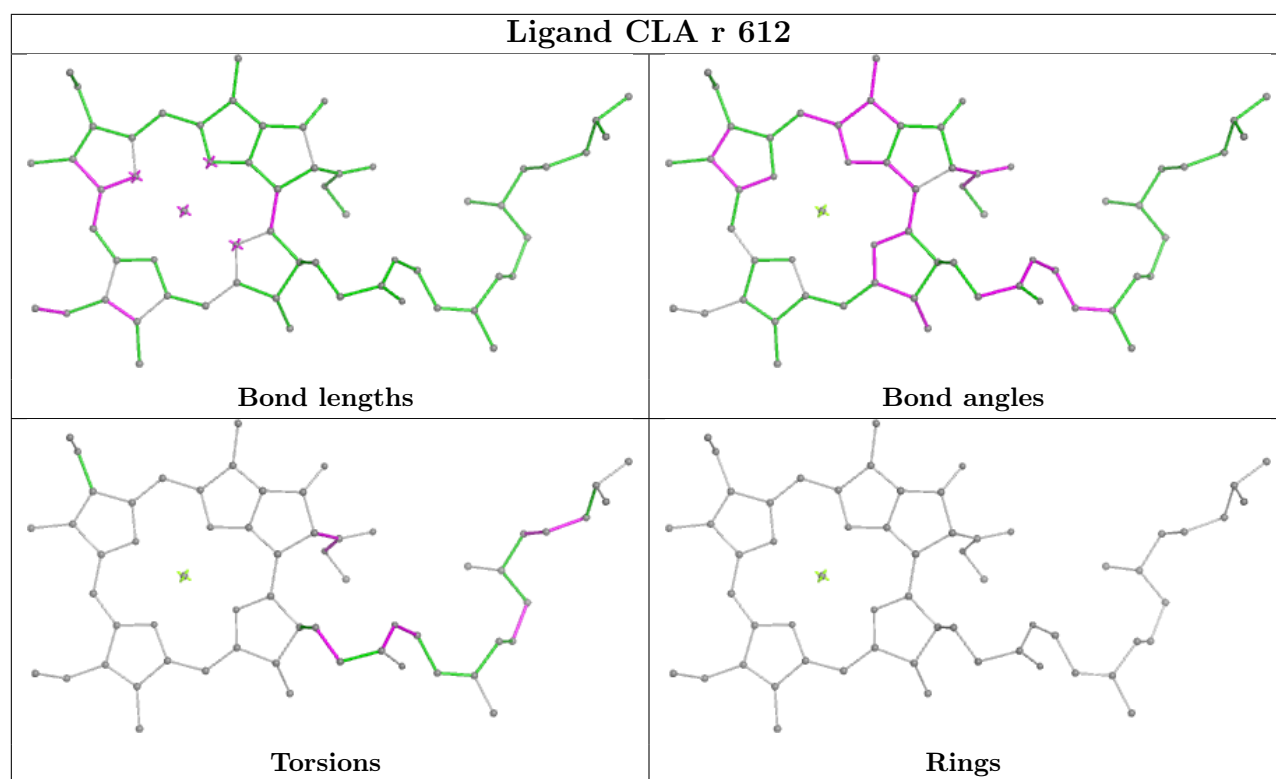


## Ligand BCR D1 404

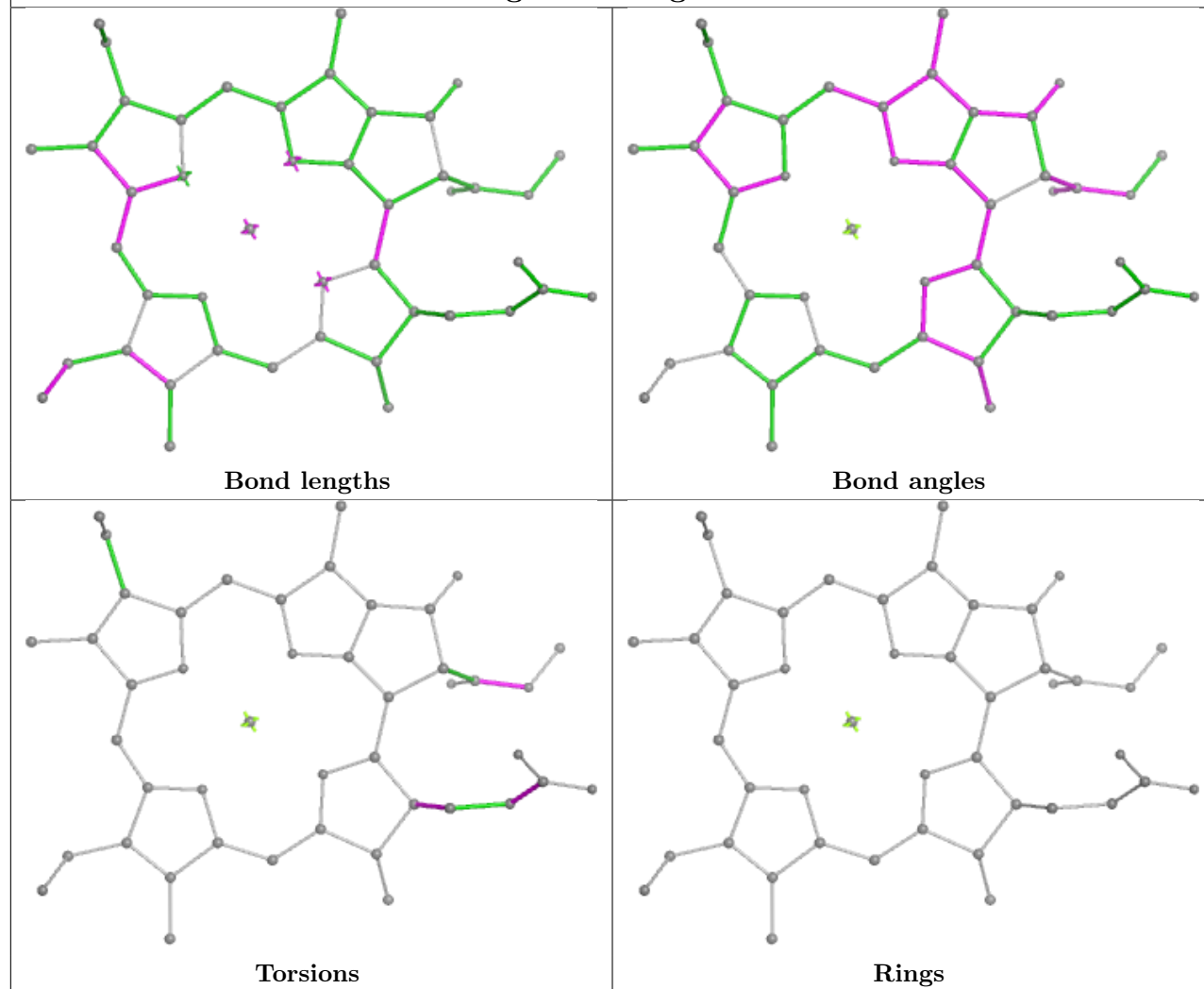


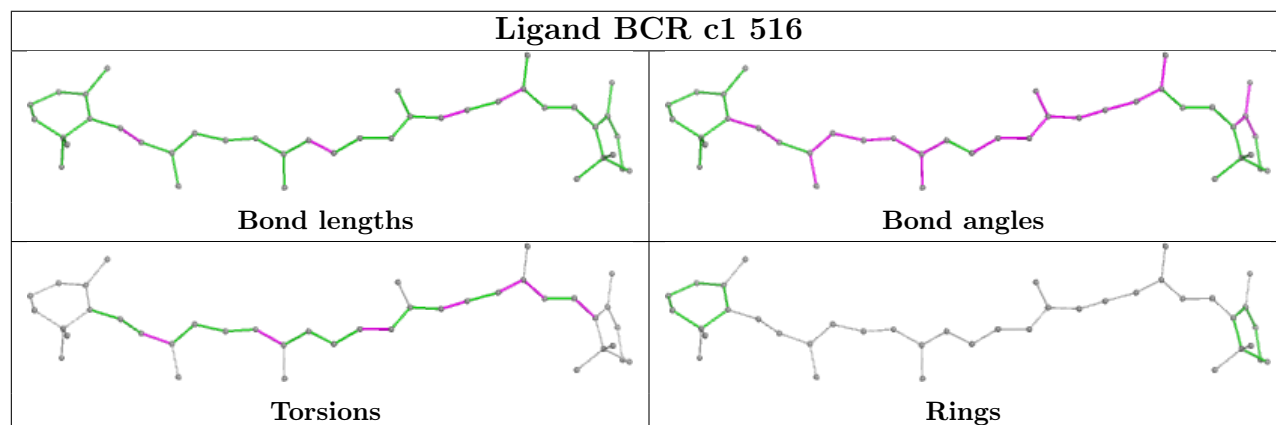
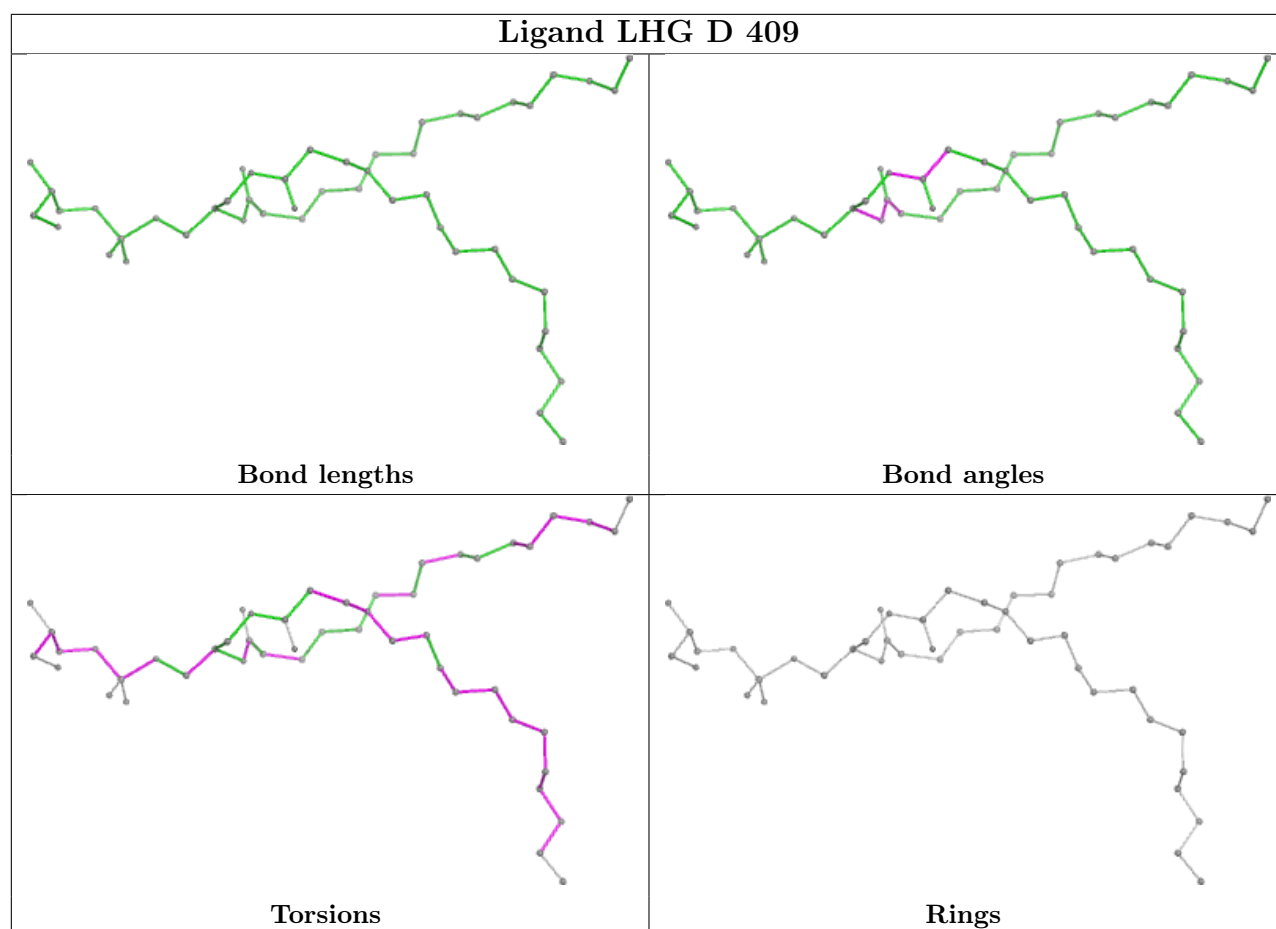


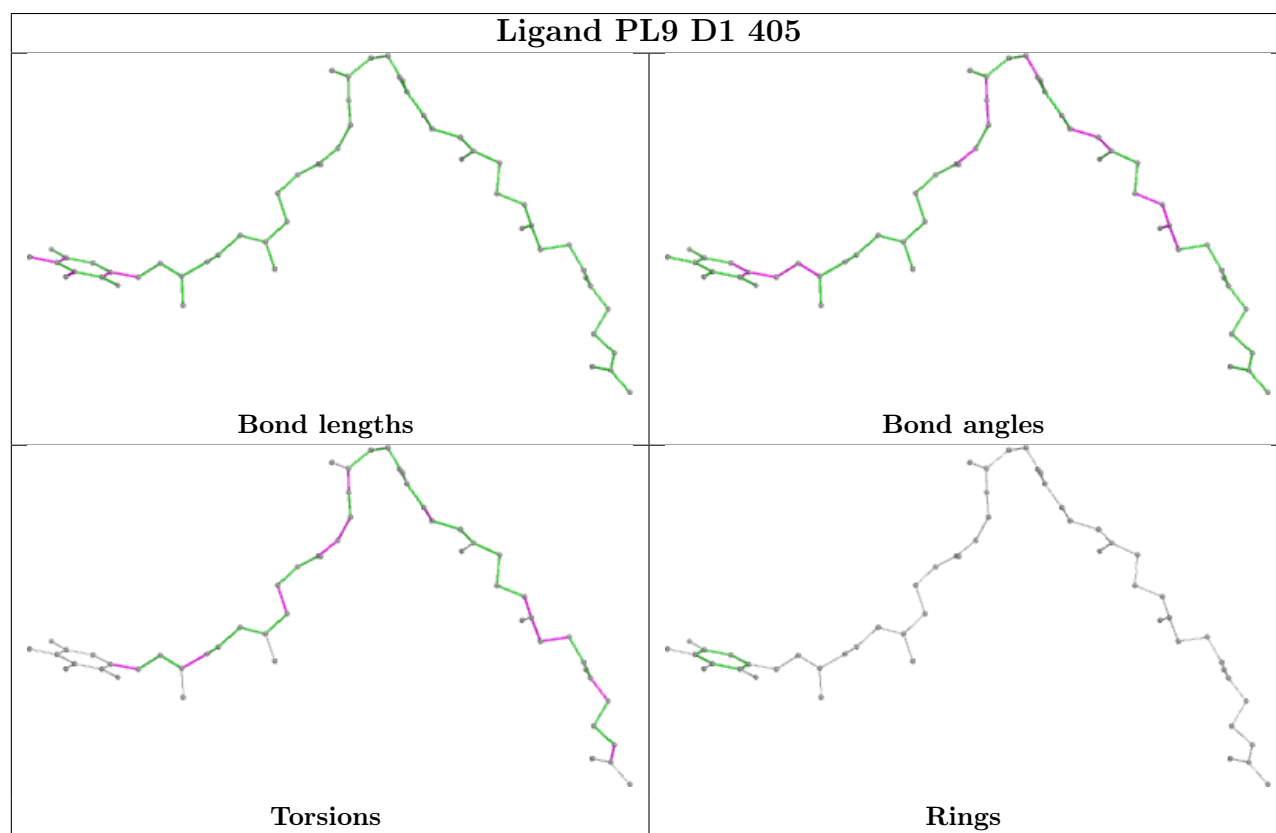
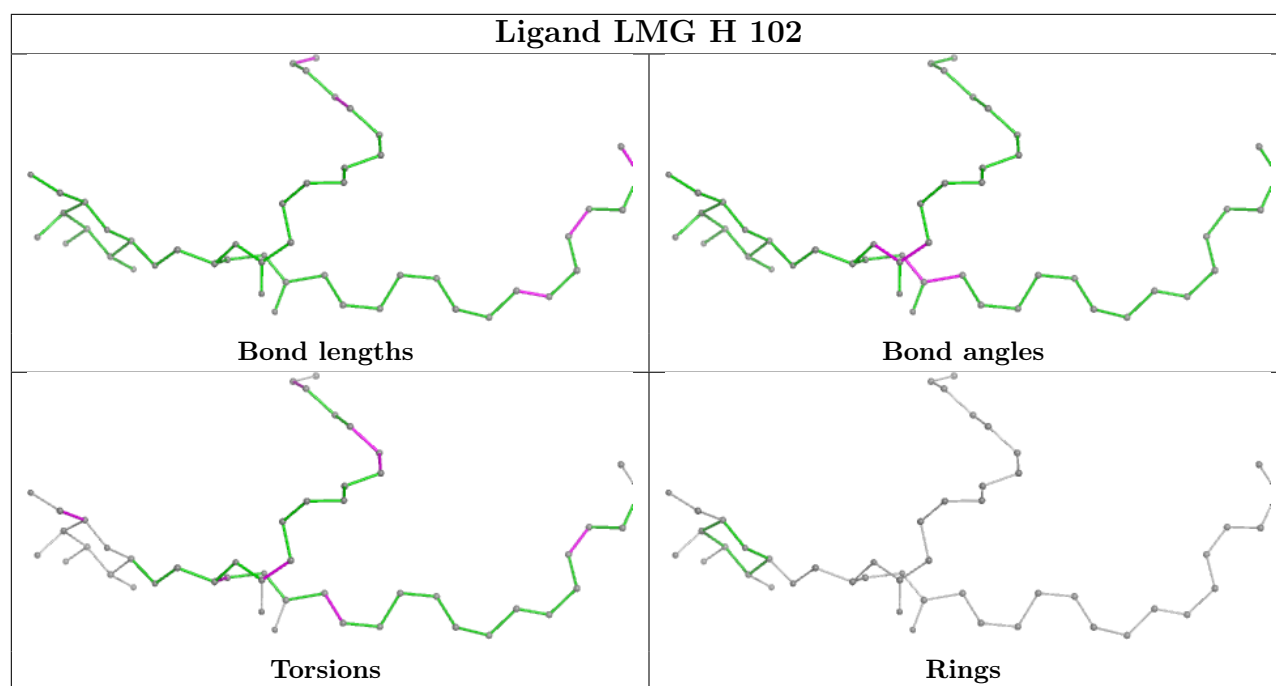


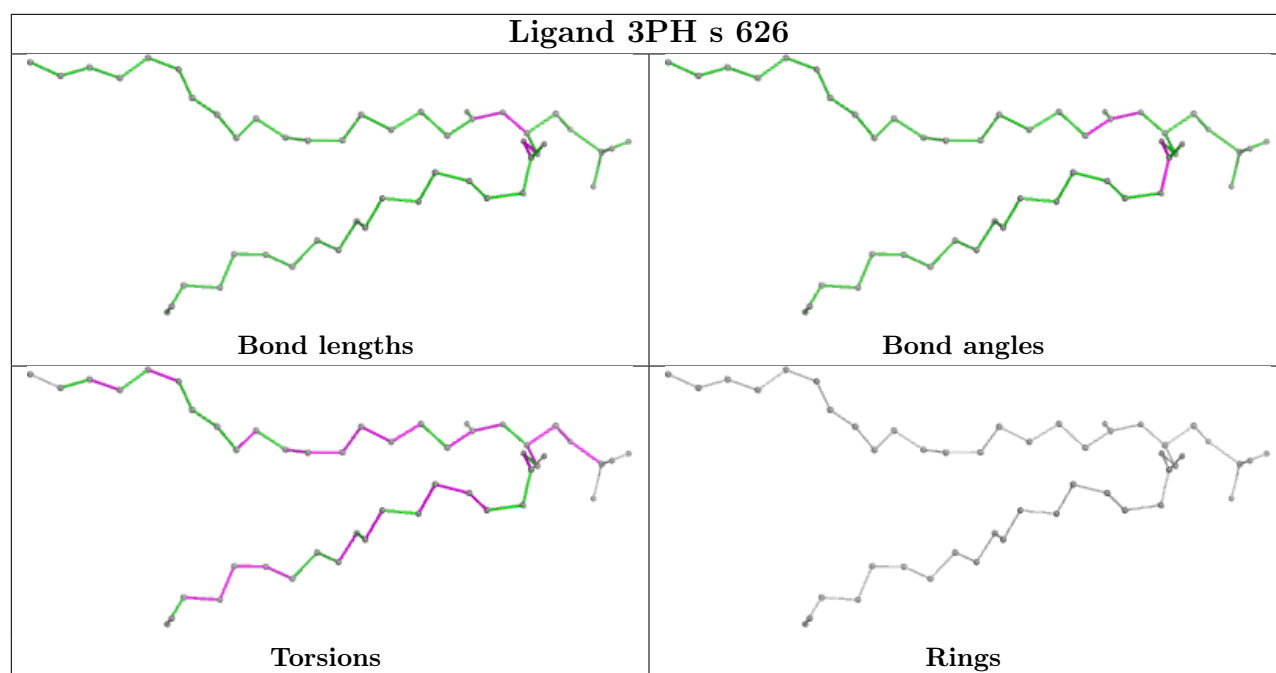


## Ligand CLA g 611



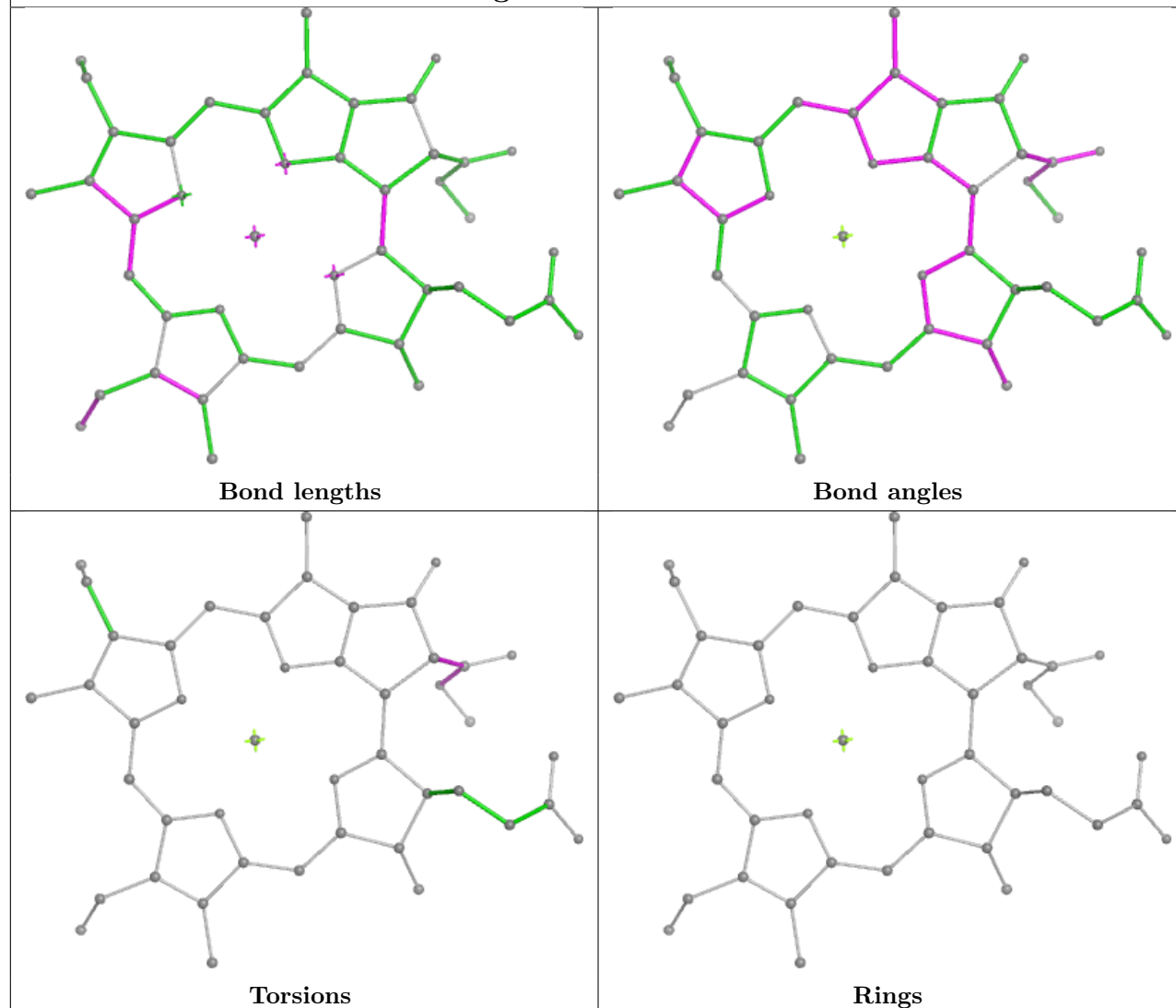




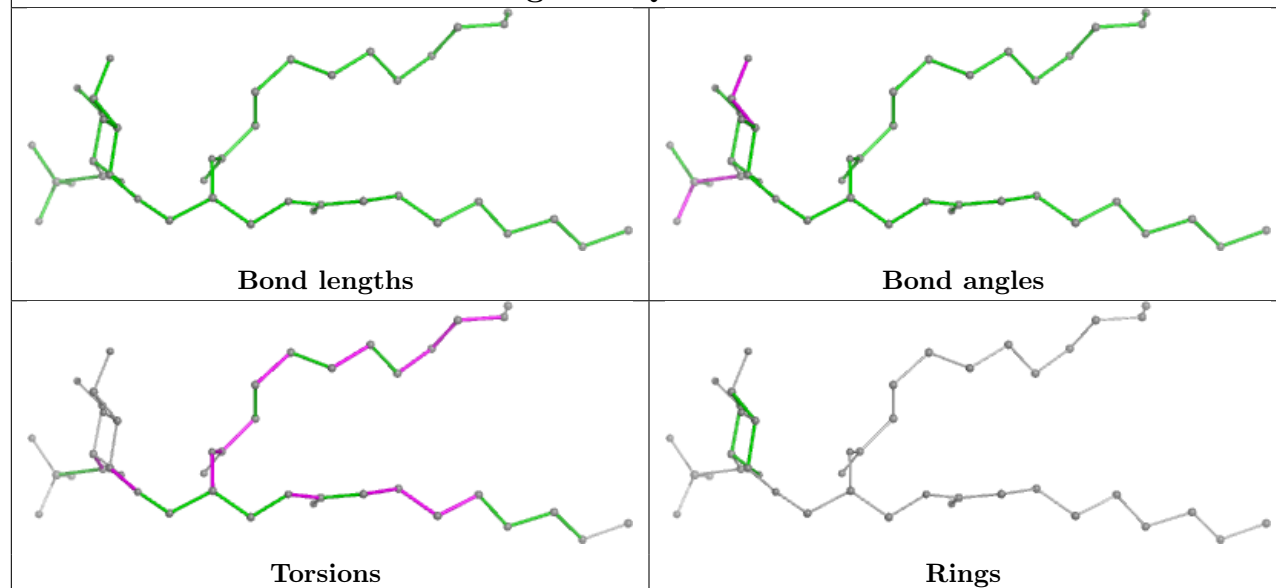


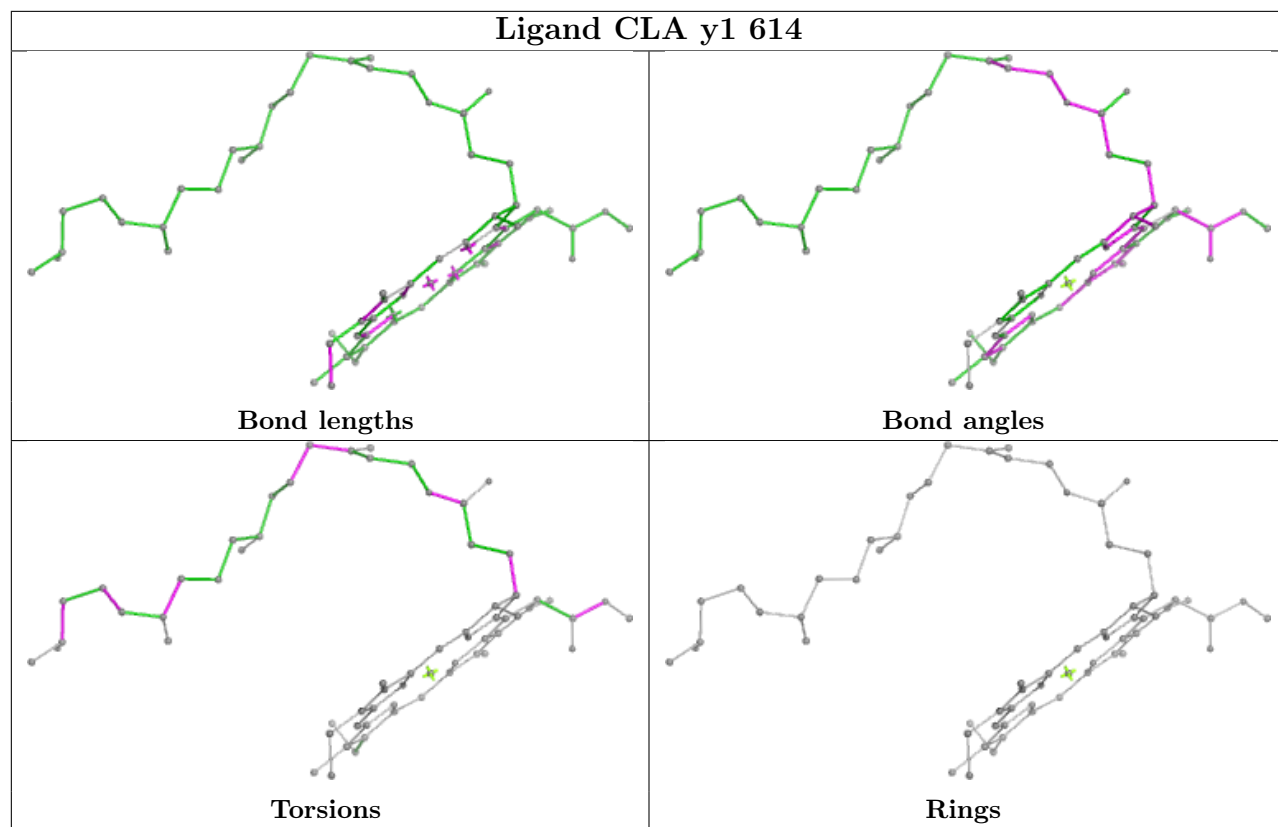


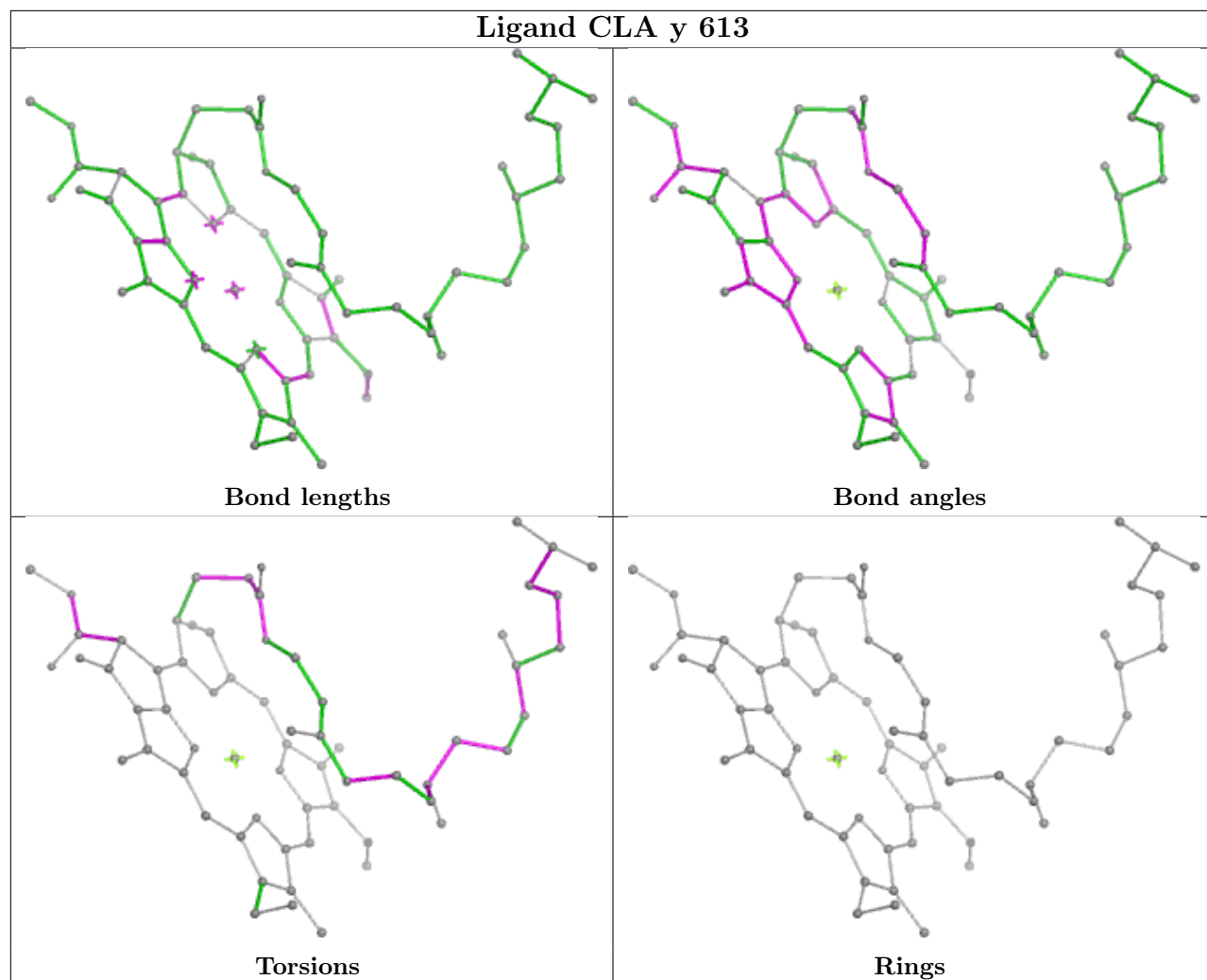
## Ligand CLA S 612

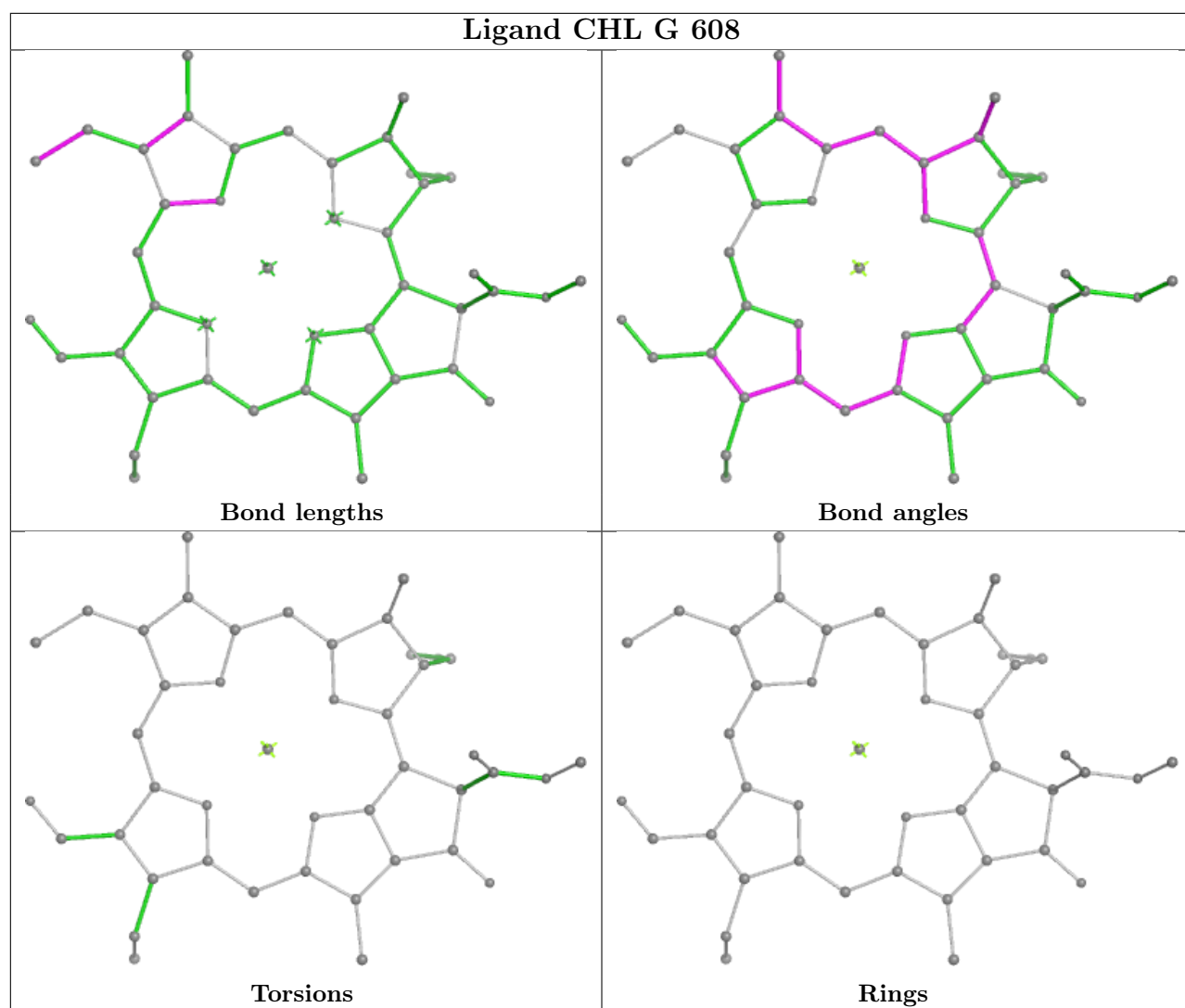


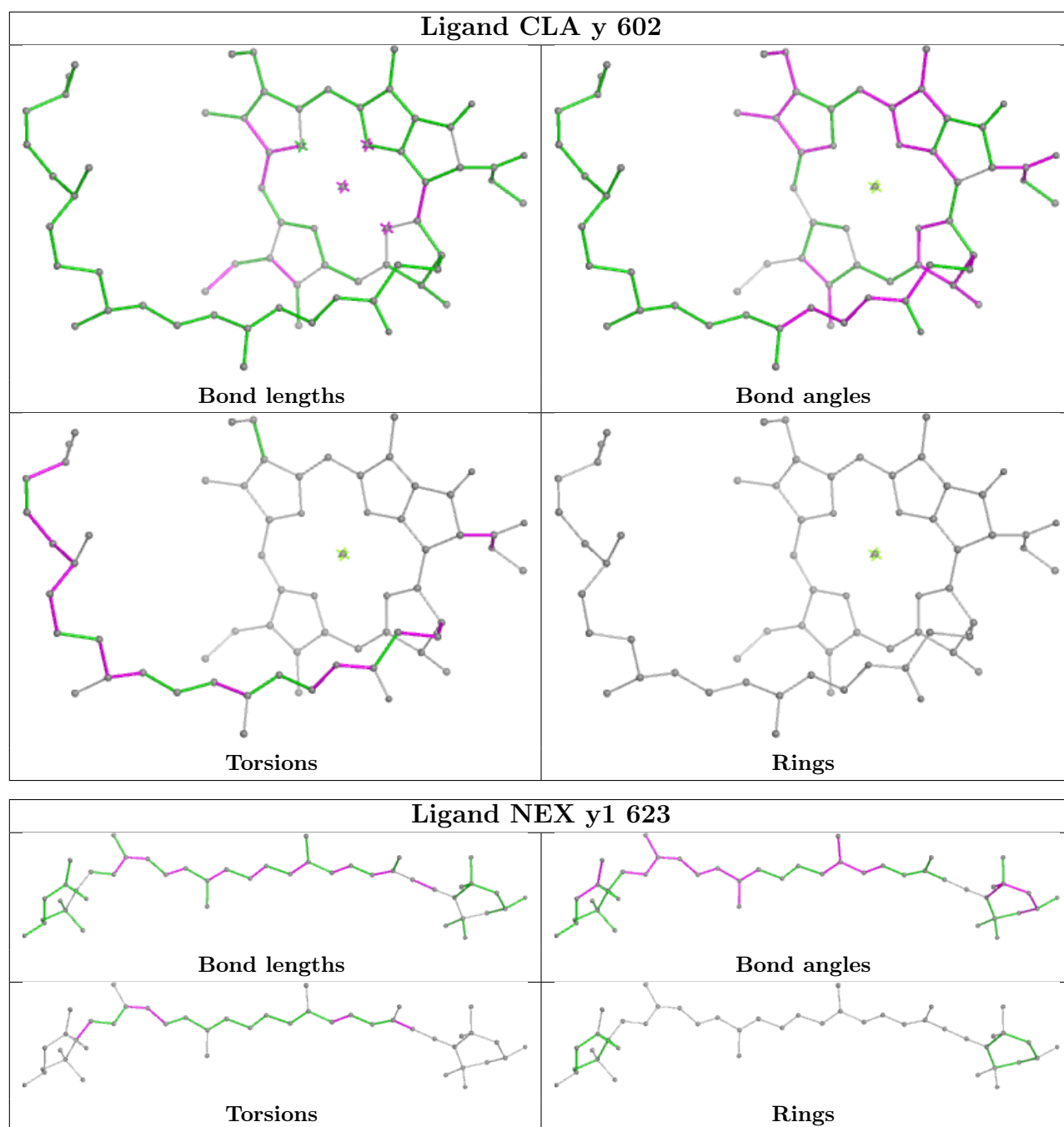
## Ligand SQD b1 621

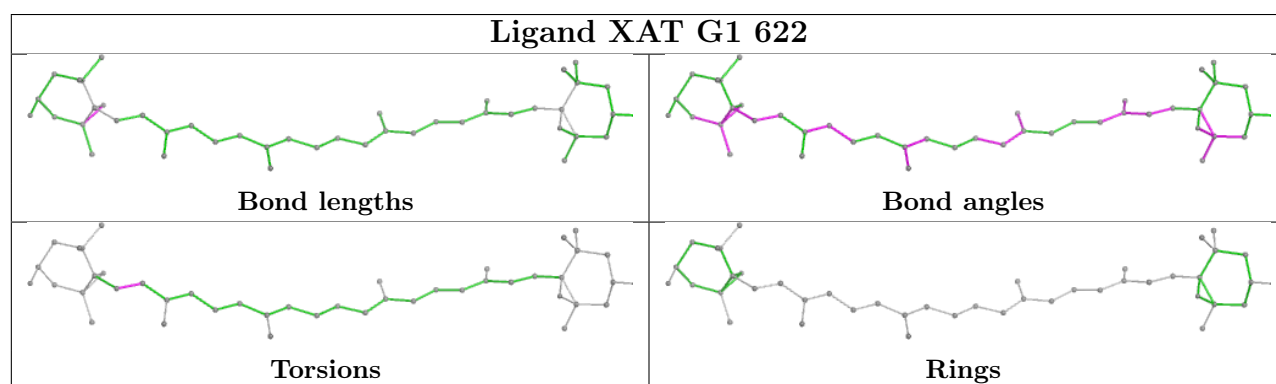
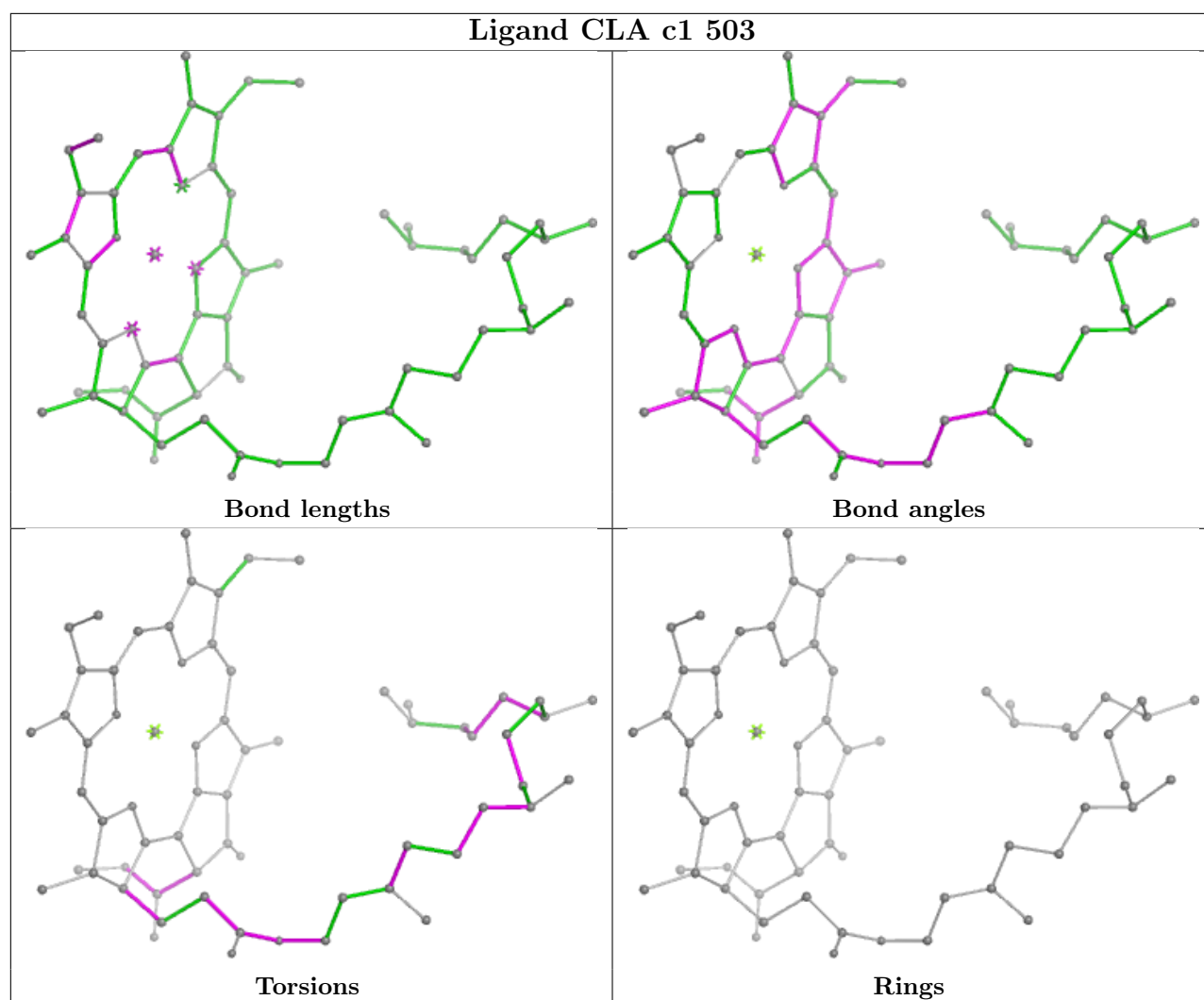


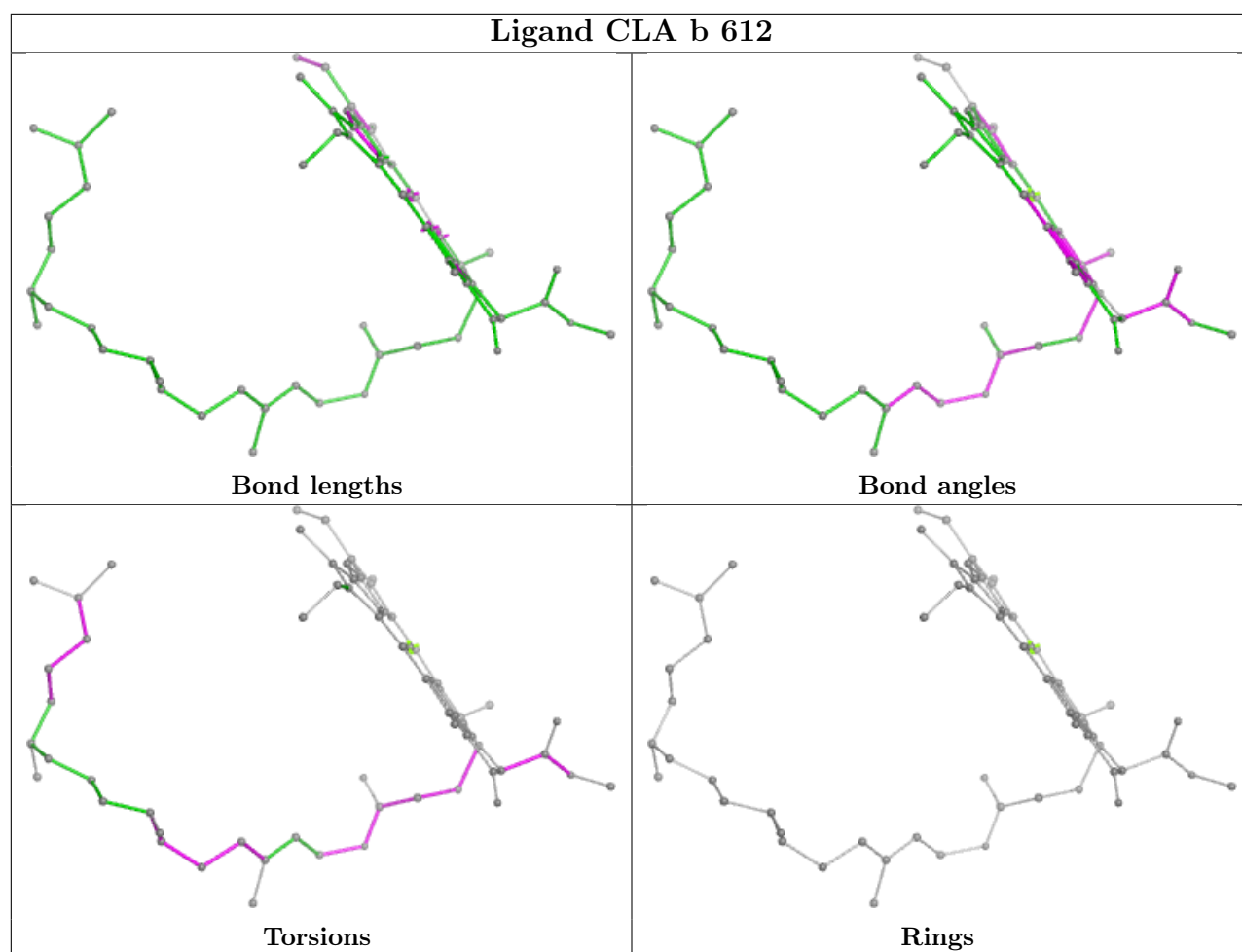


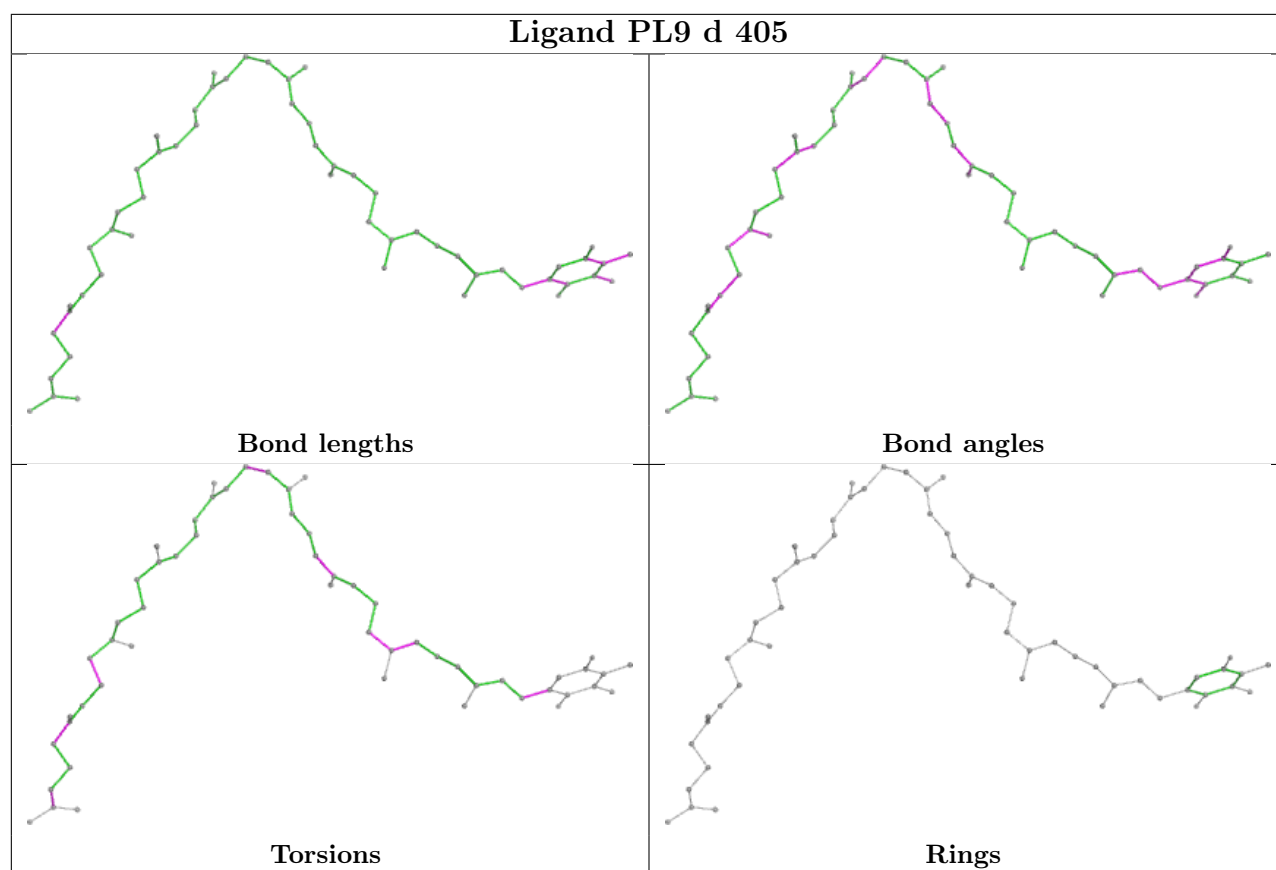




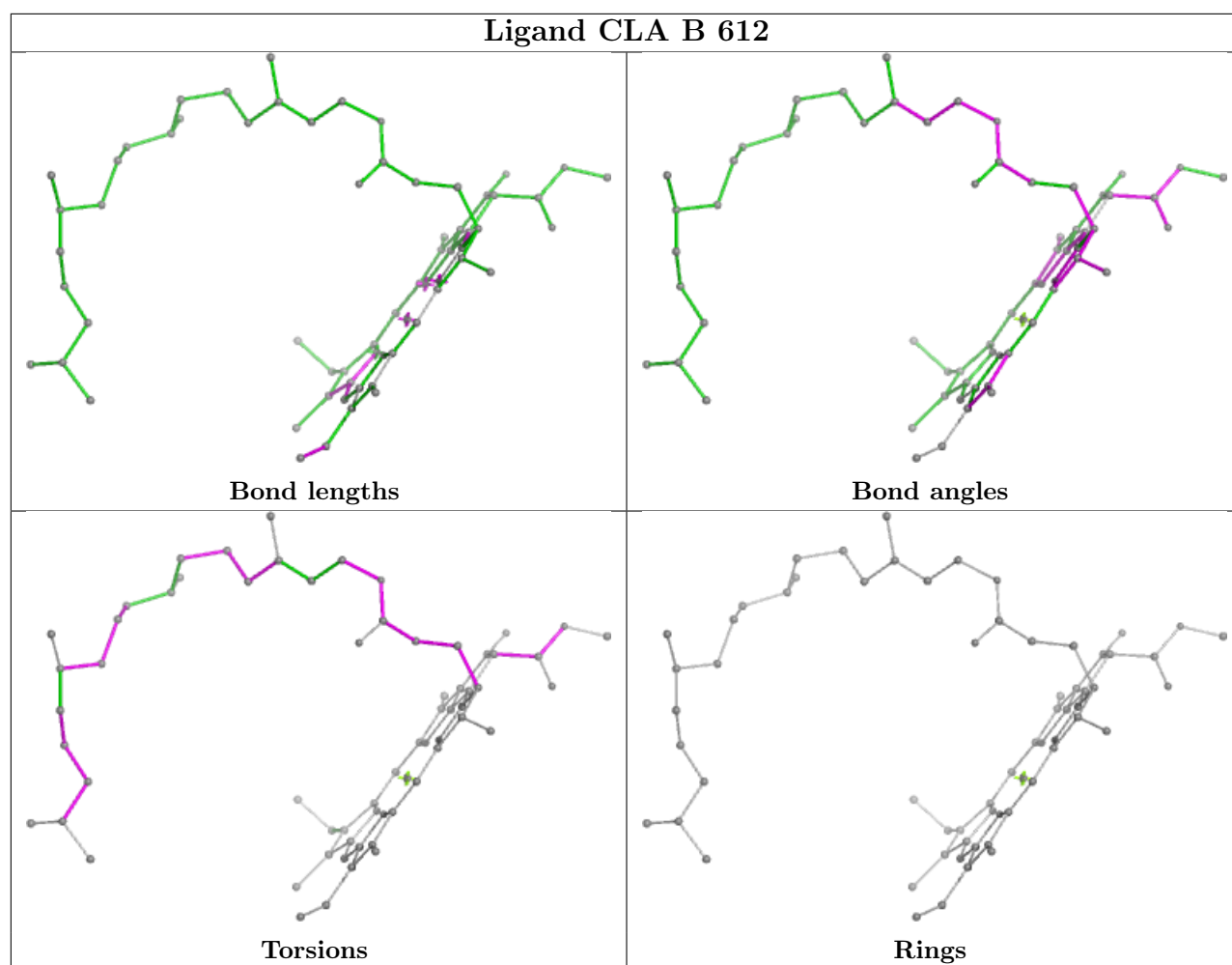




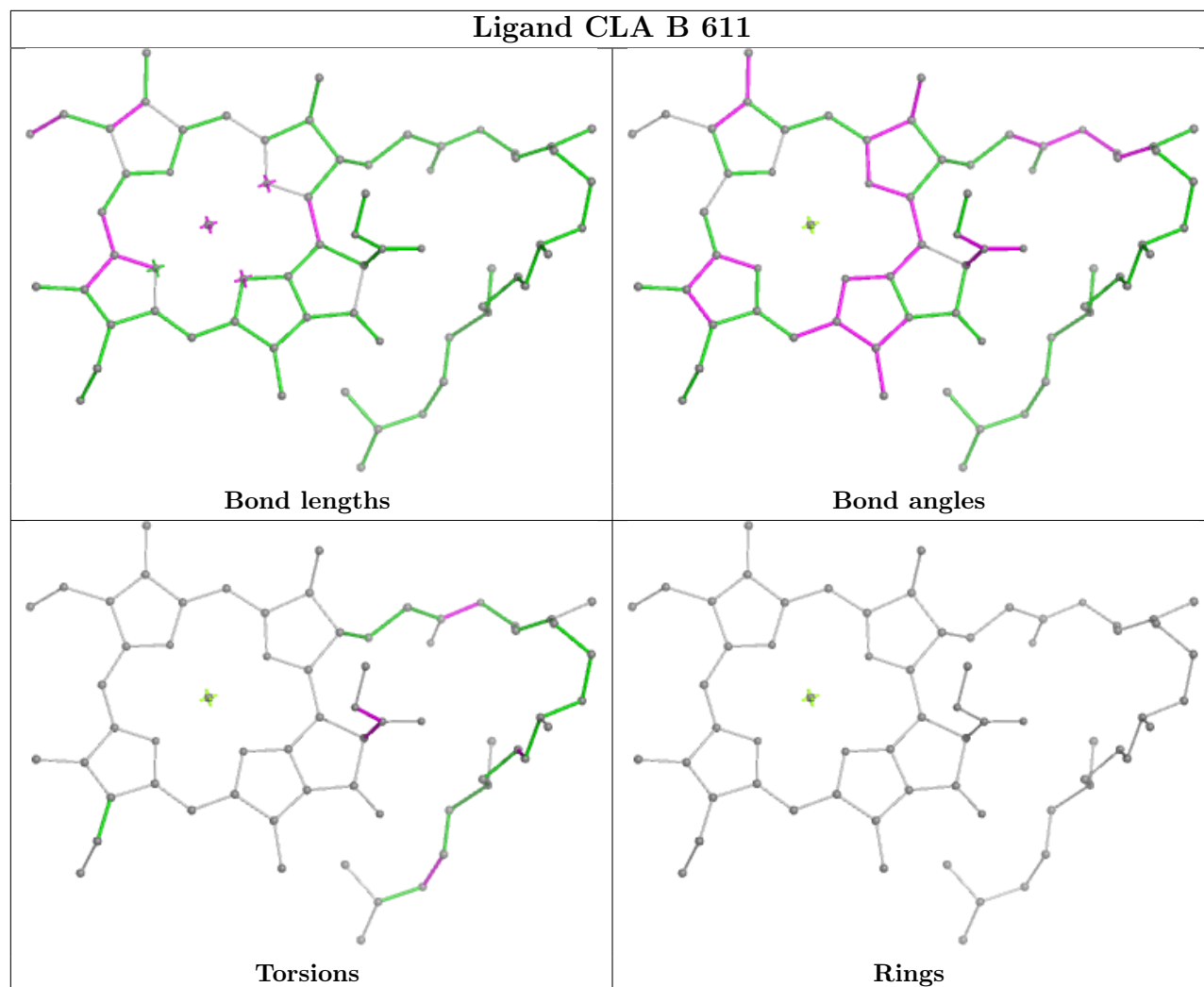


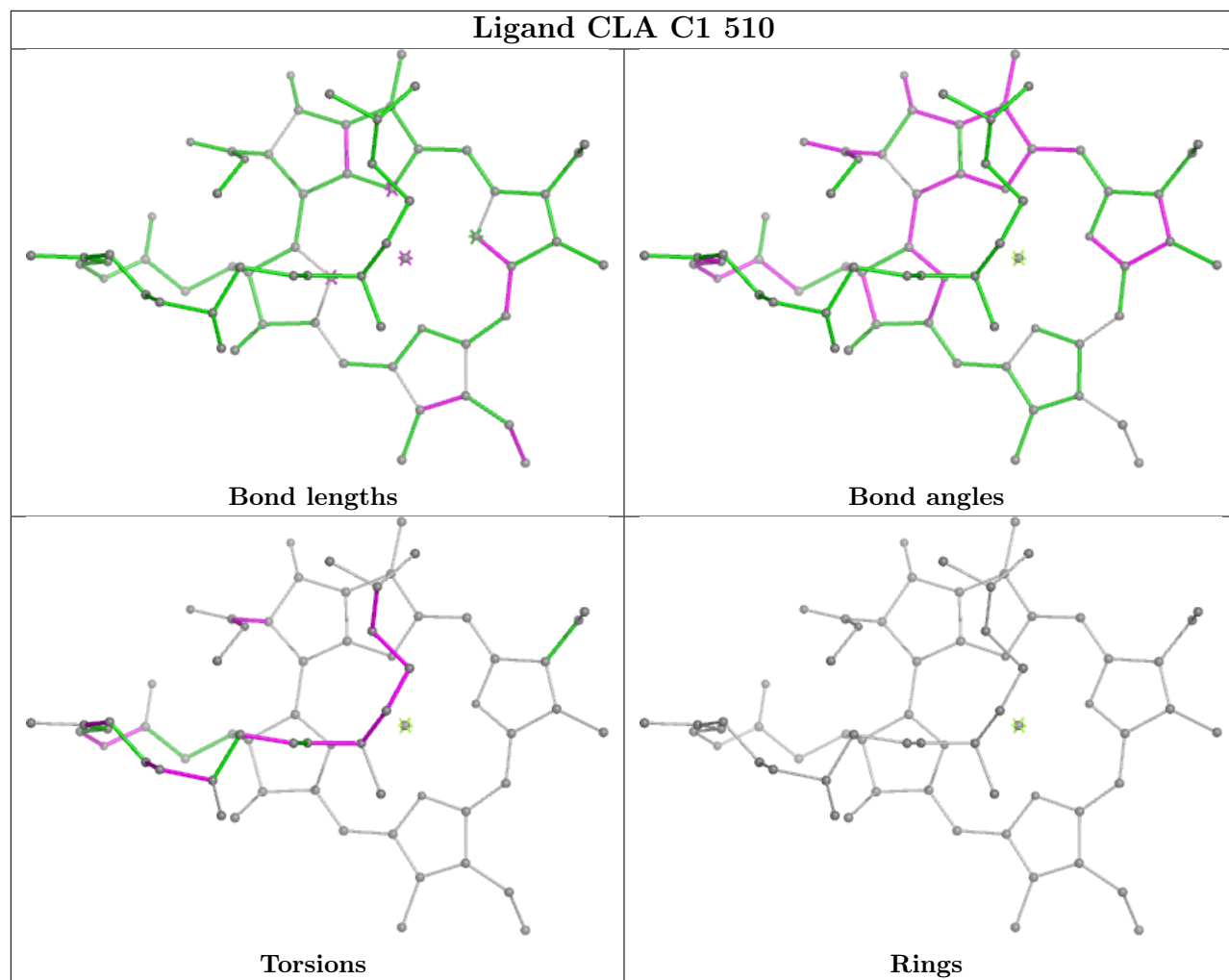


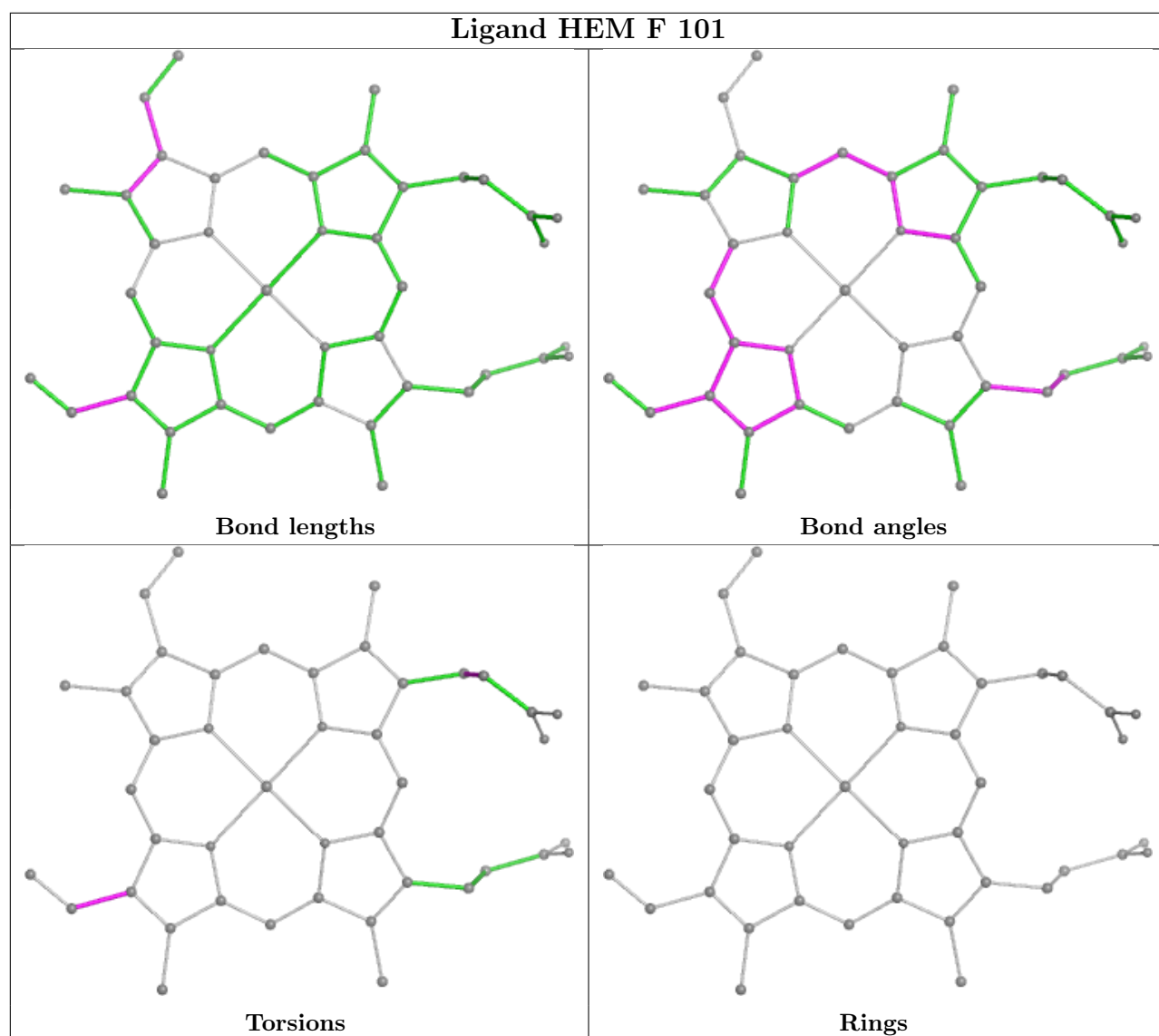


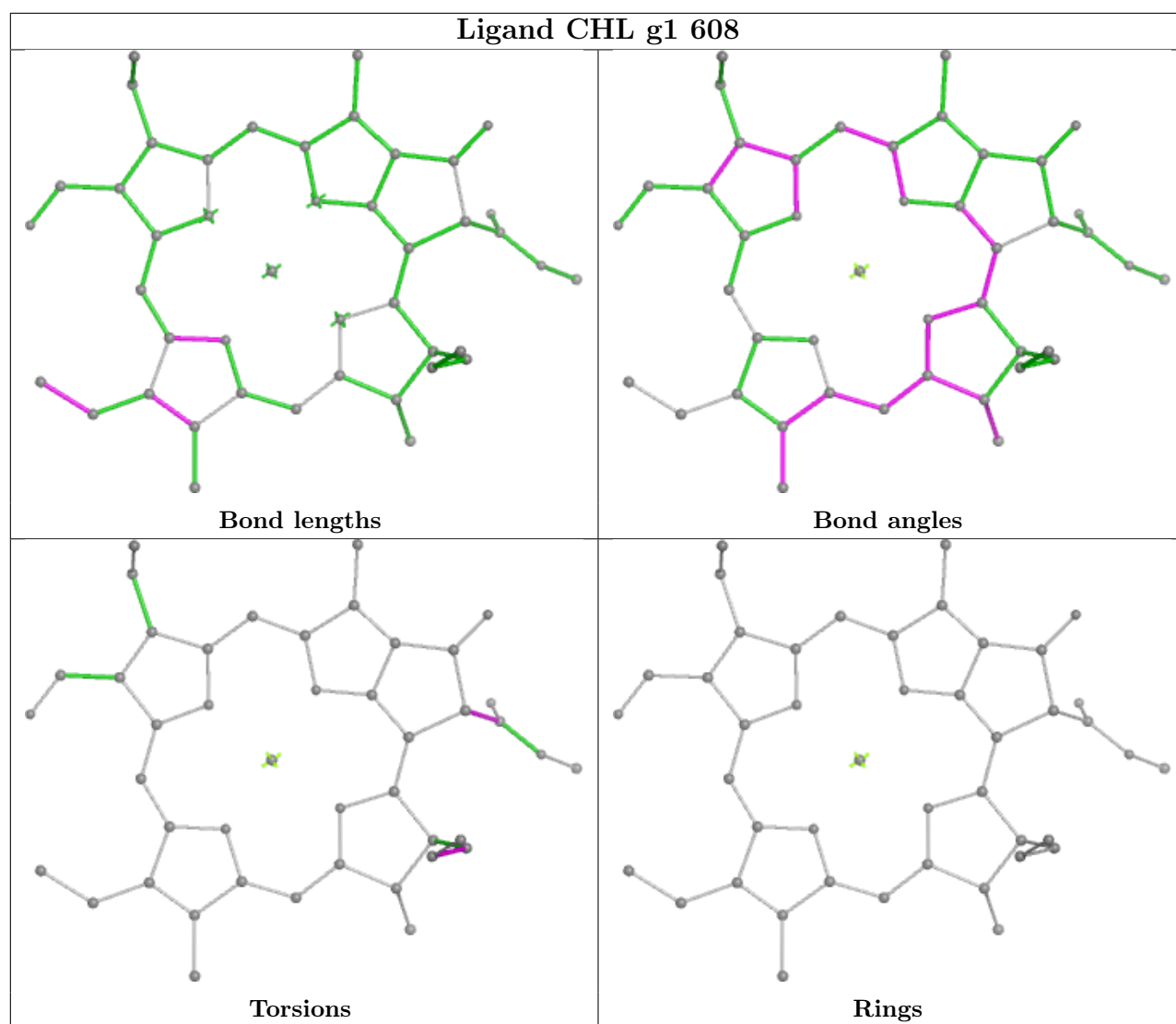


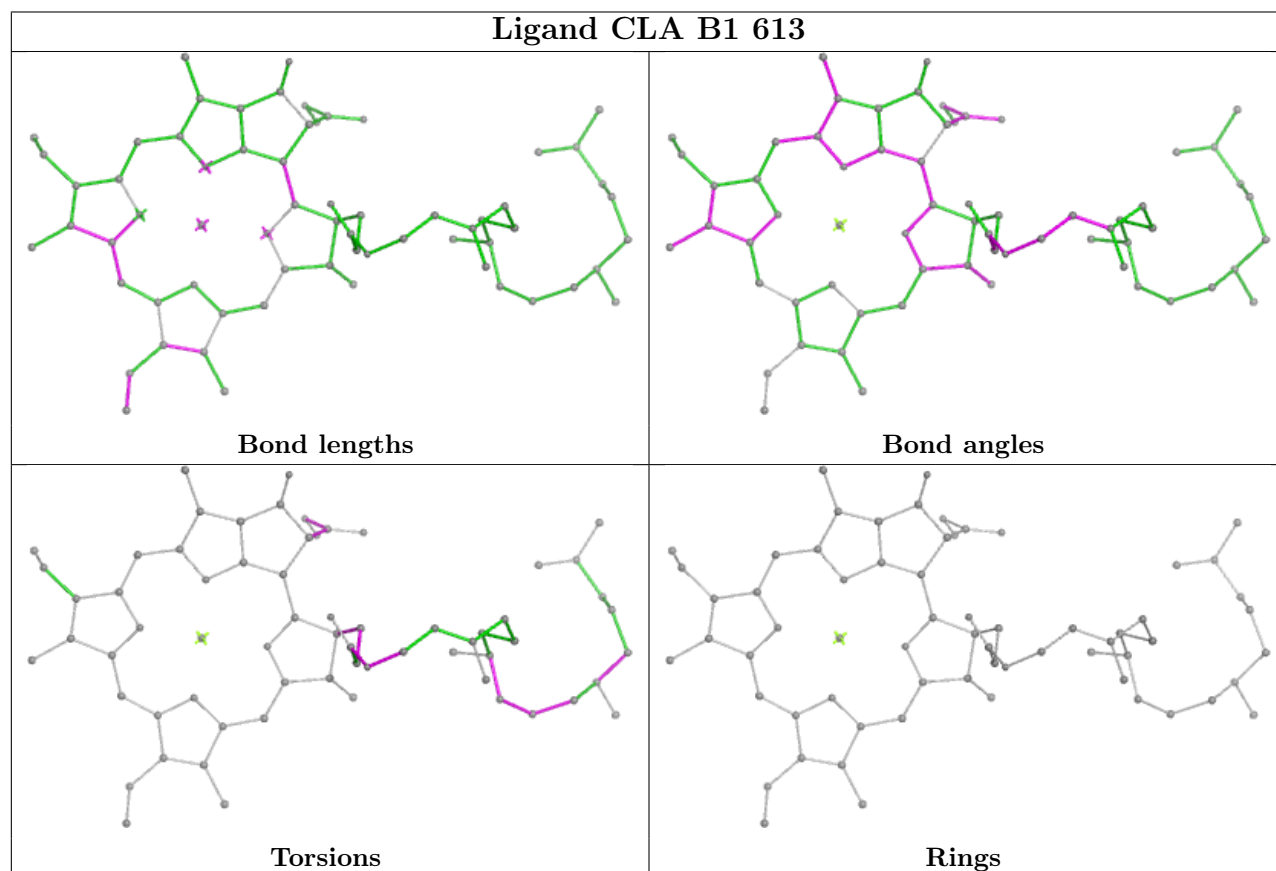
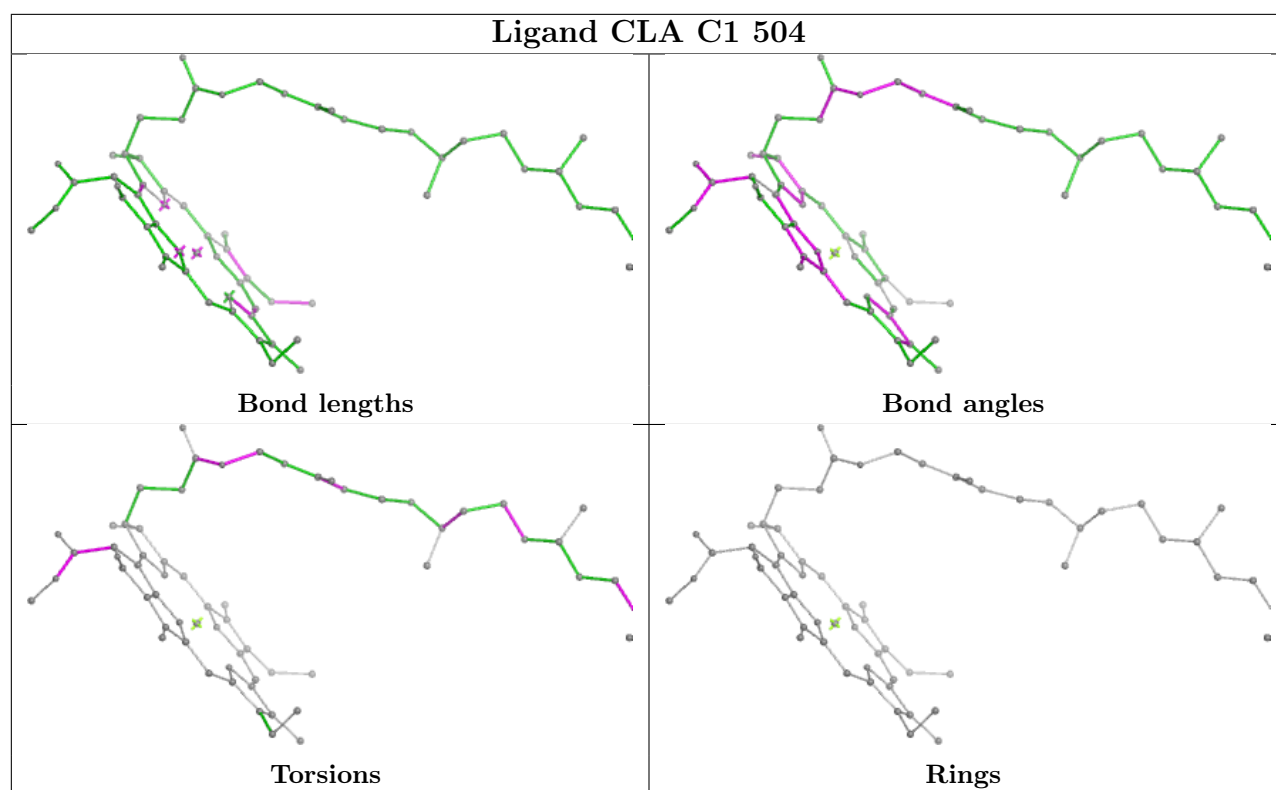
## Ligand CLA B 611

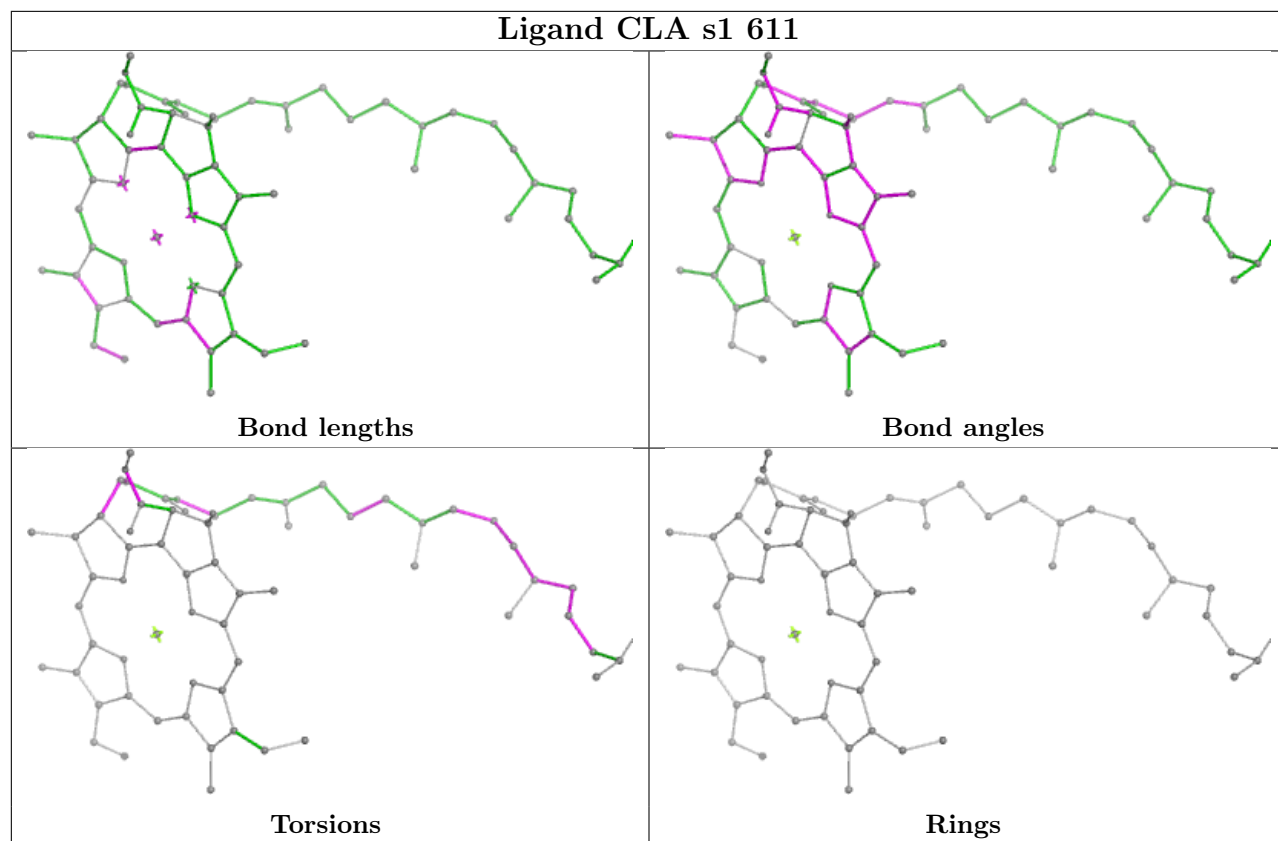


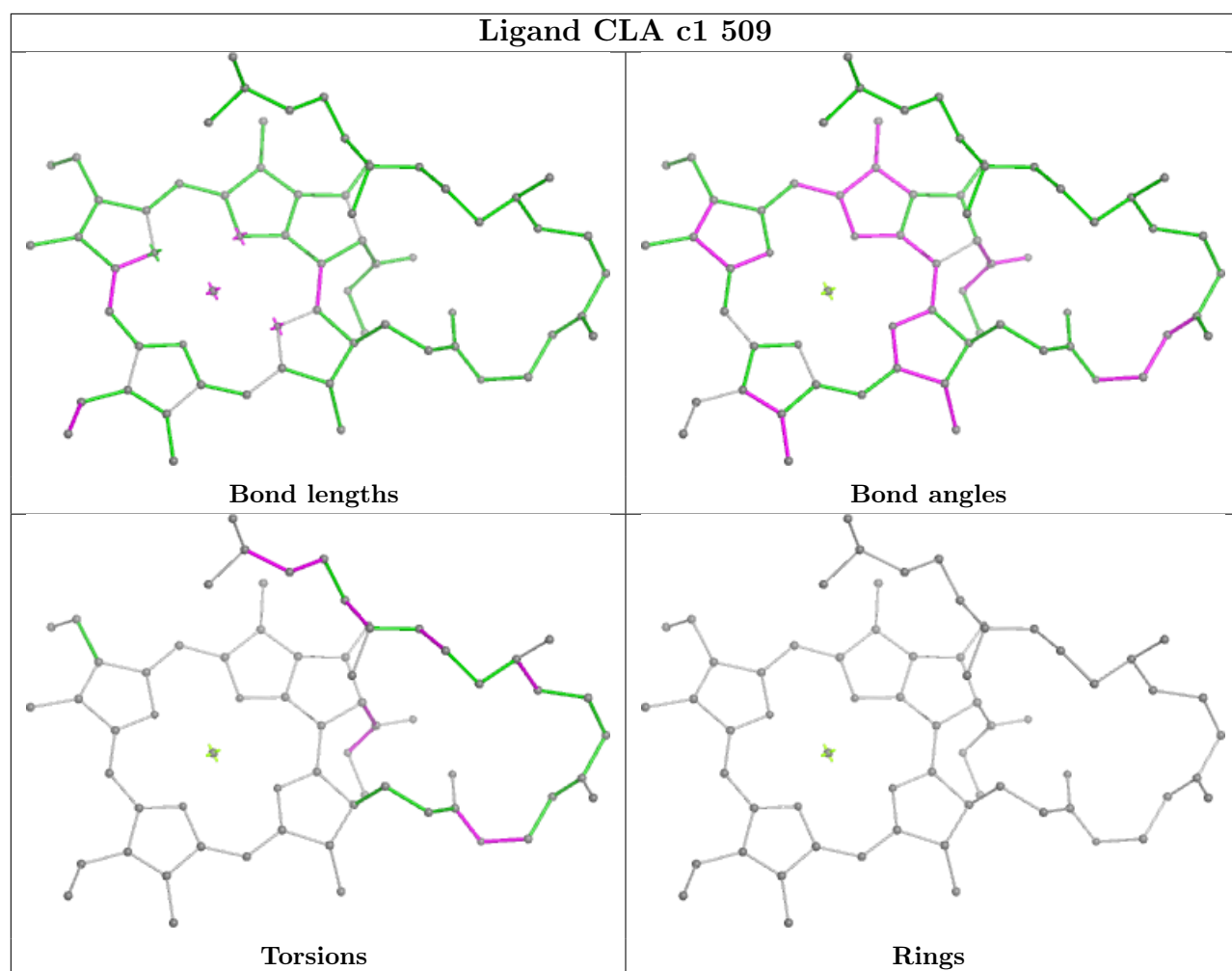




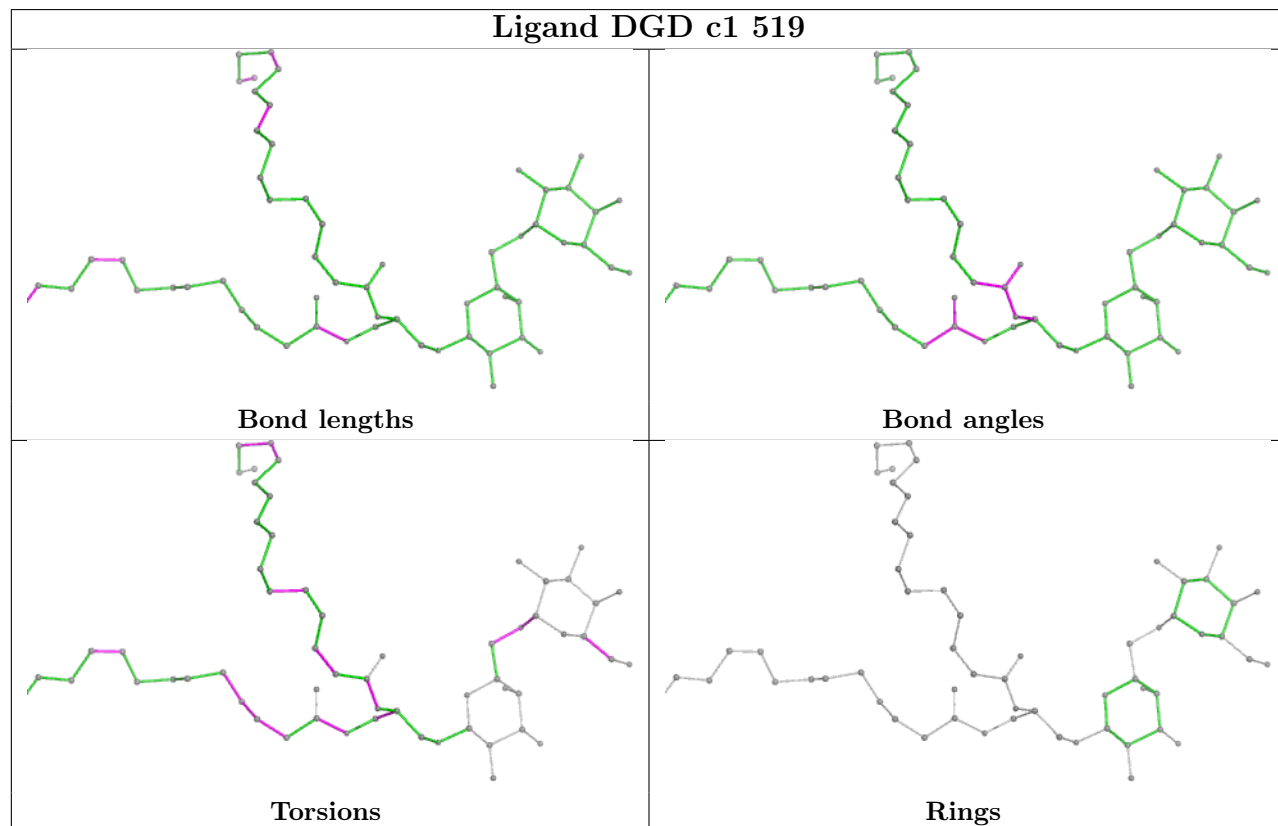
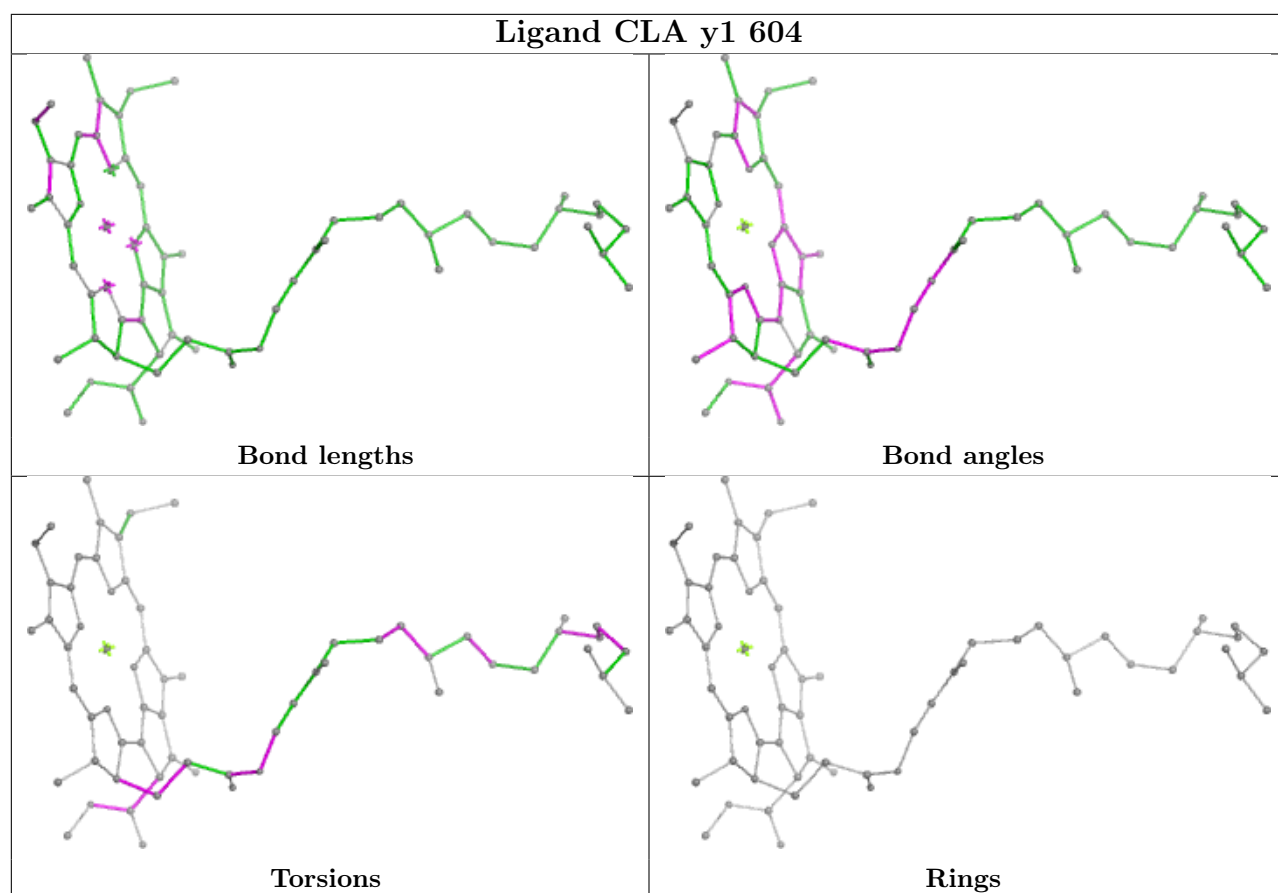


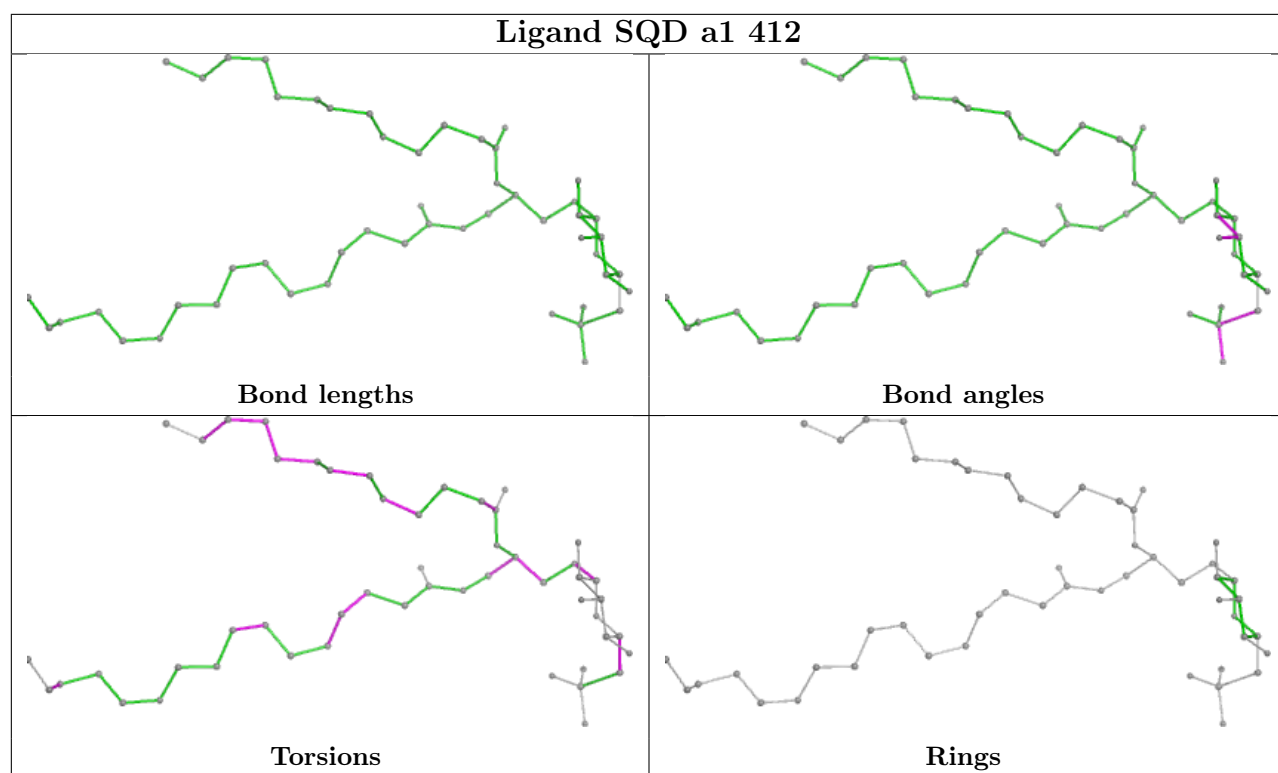


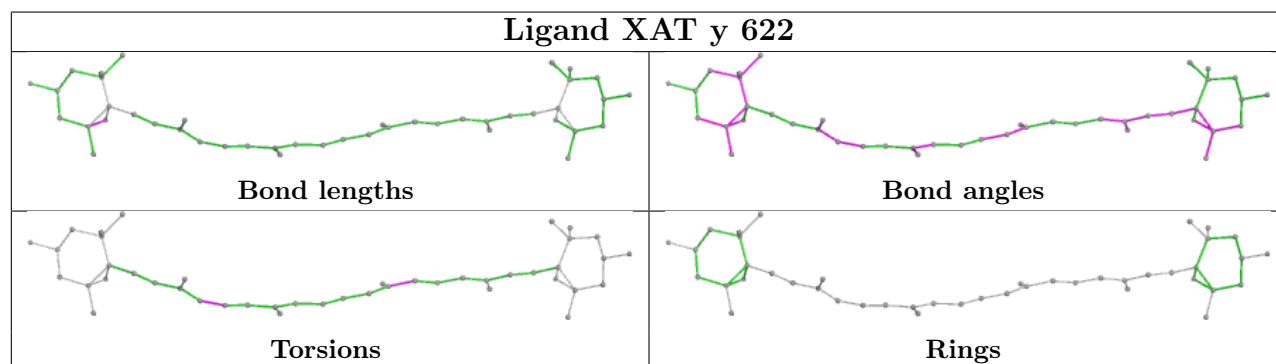
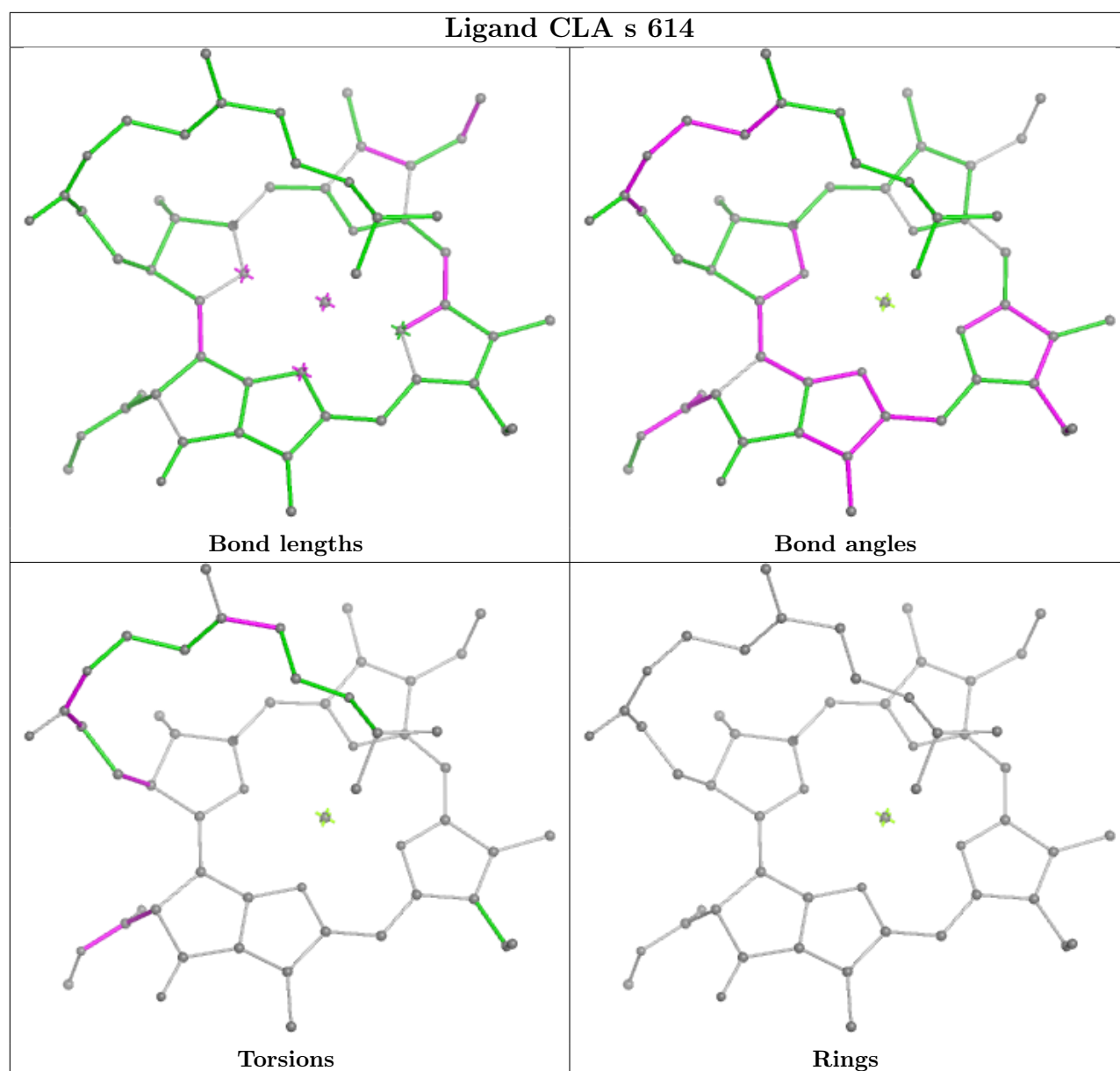


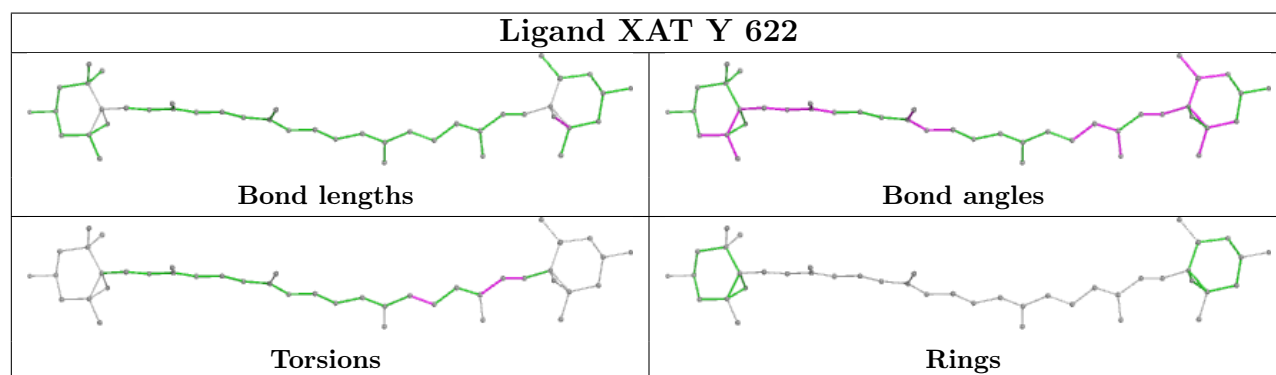
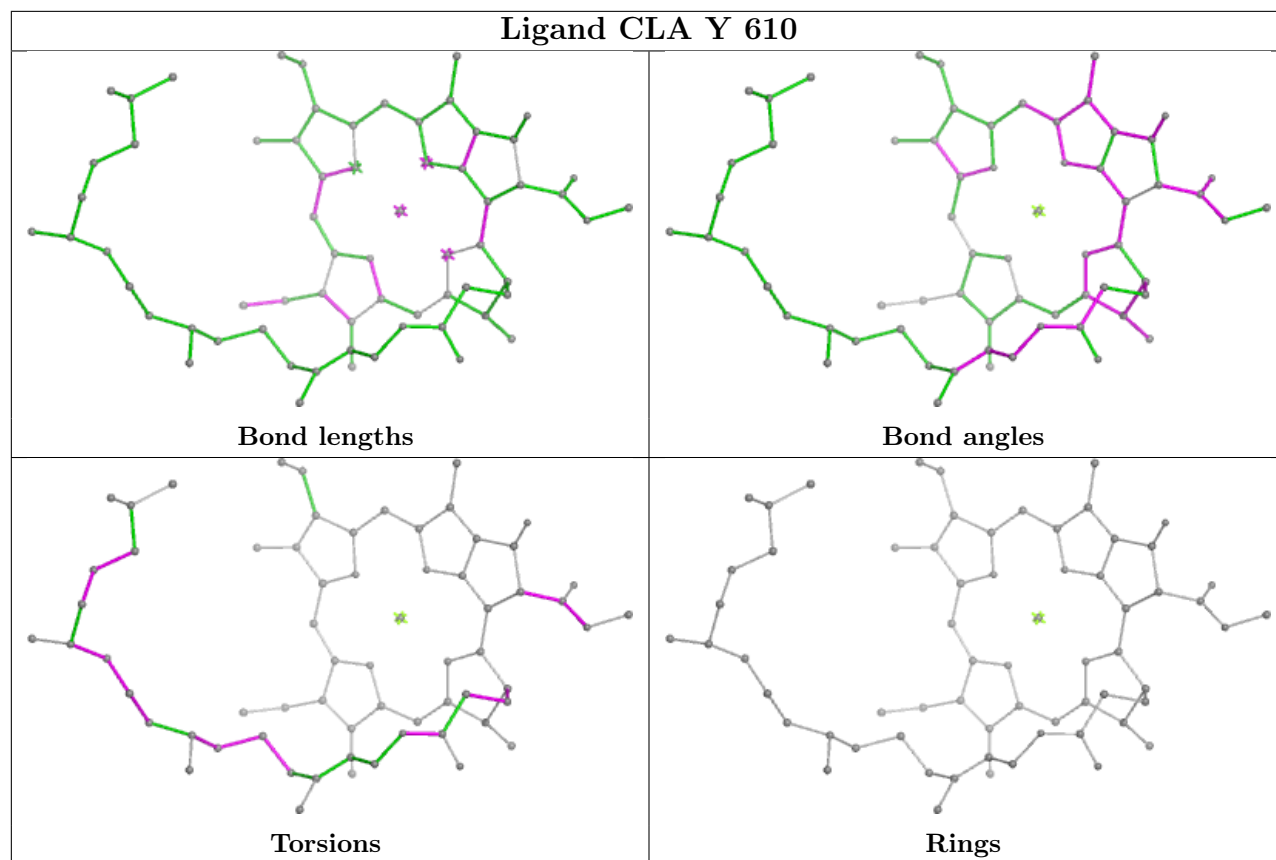


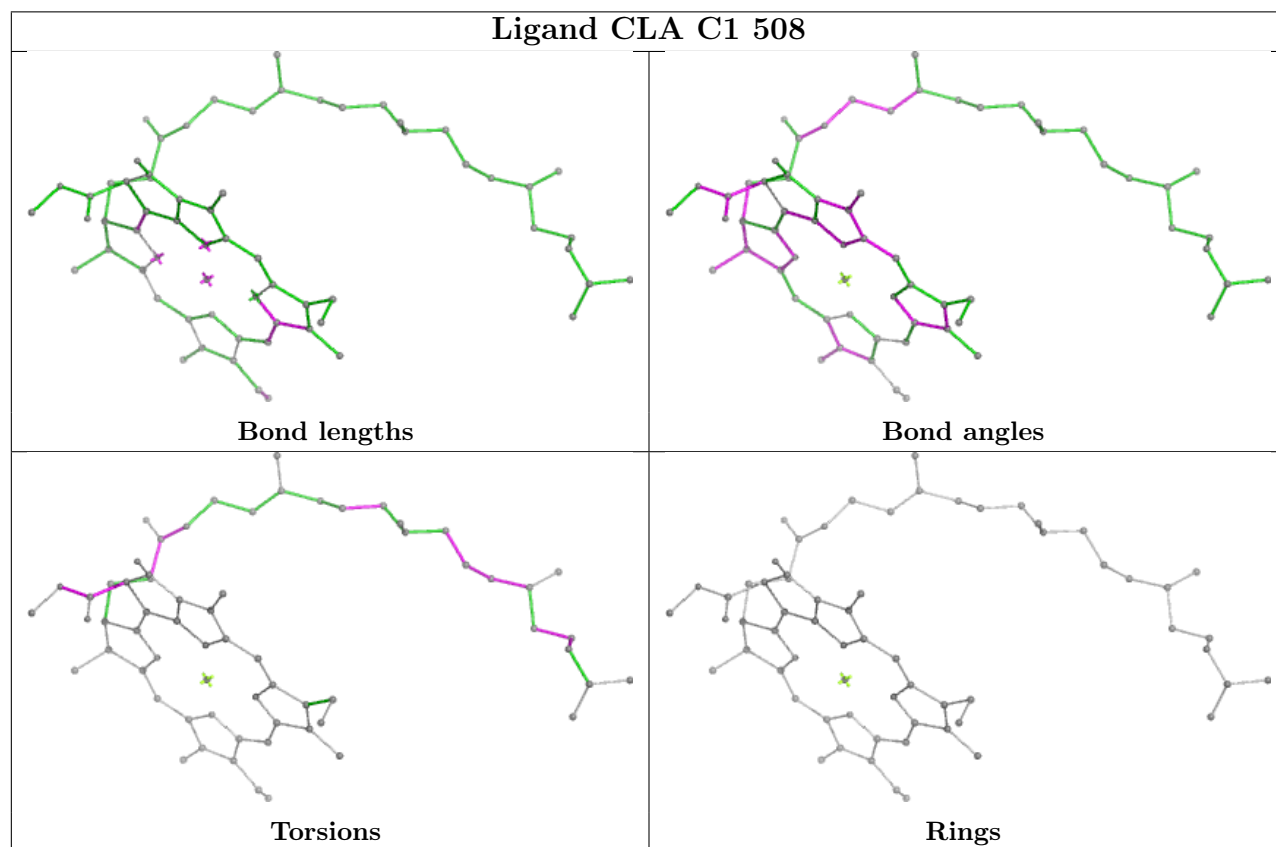
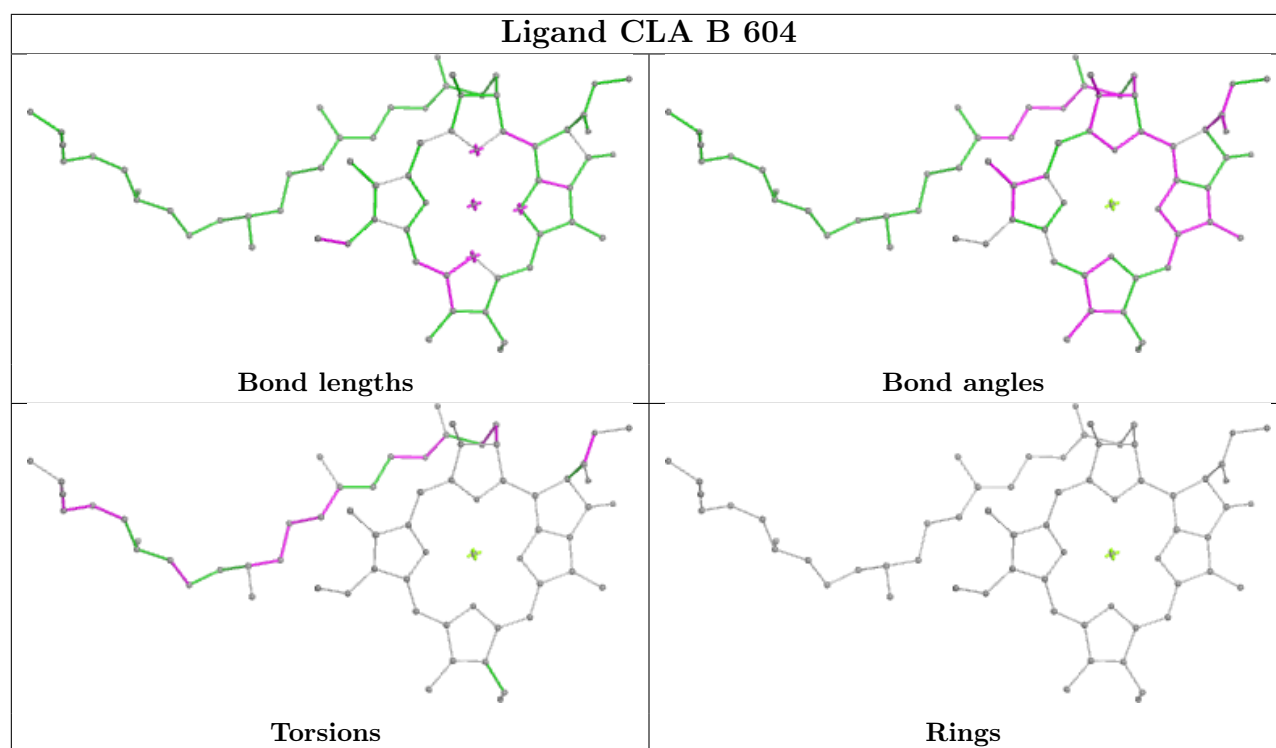


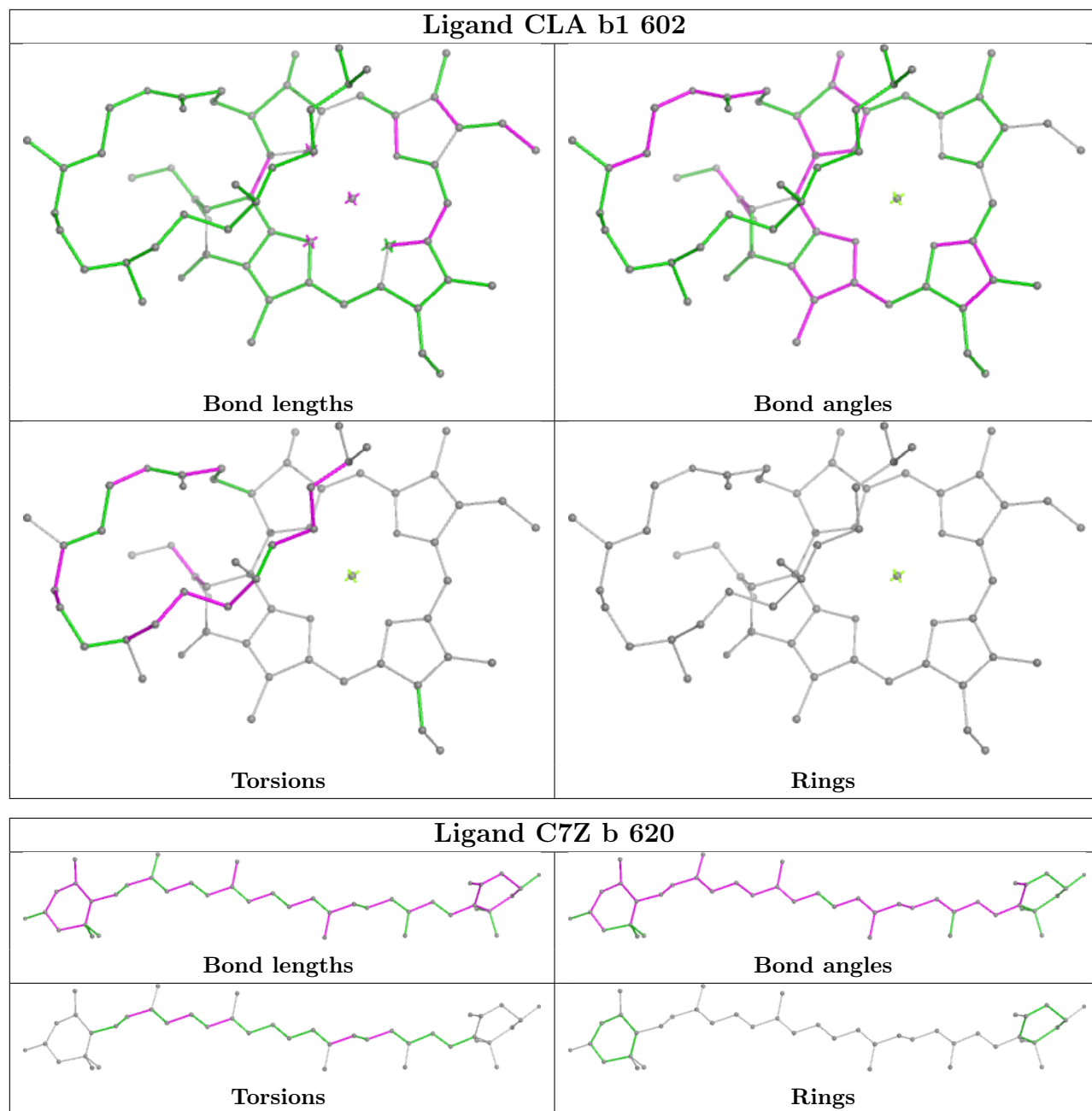




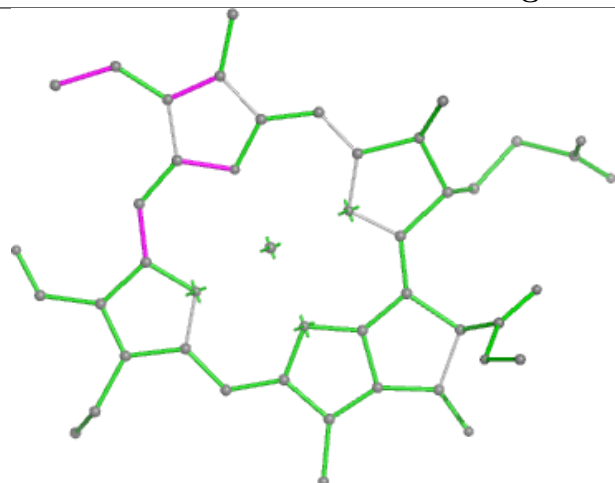




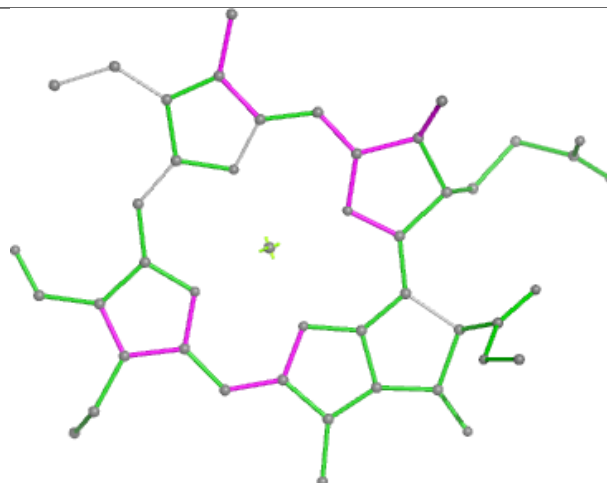




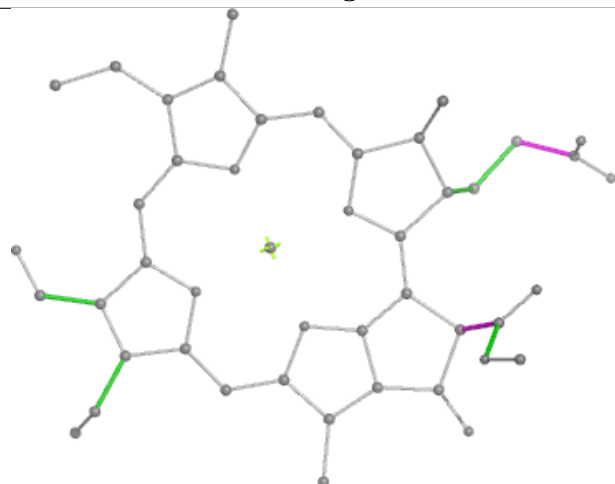
## Ligand CHL s 601



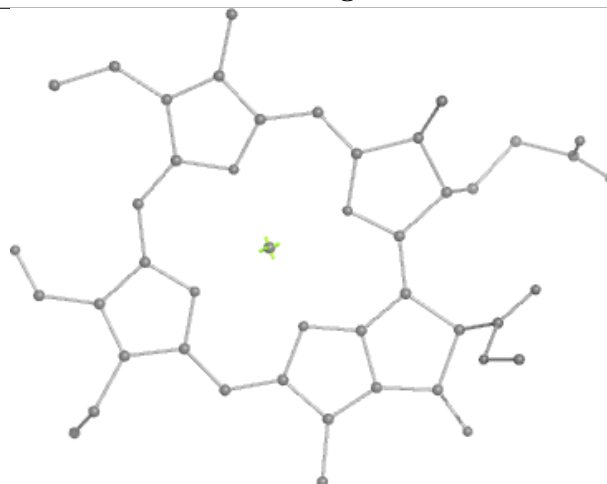
Bond lengths



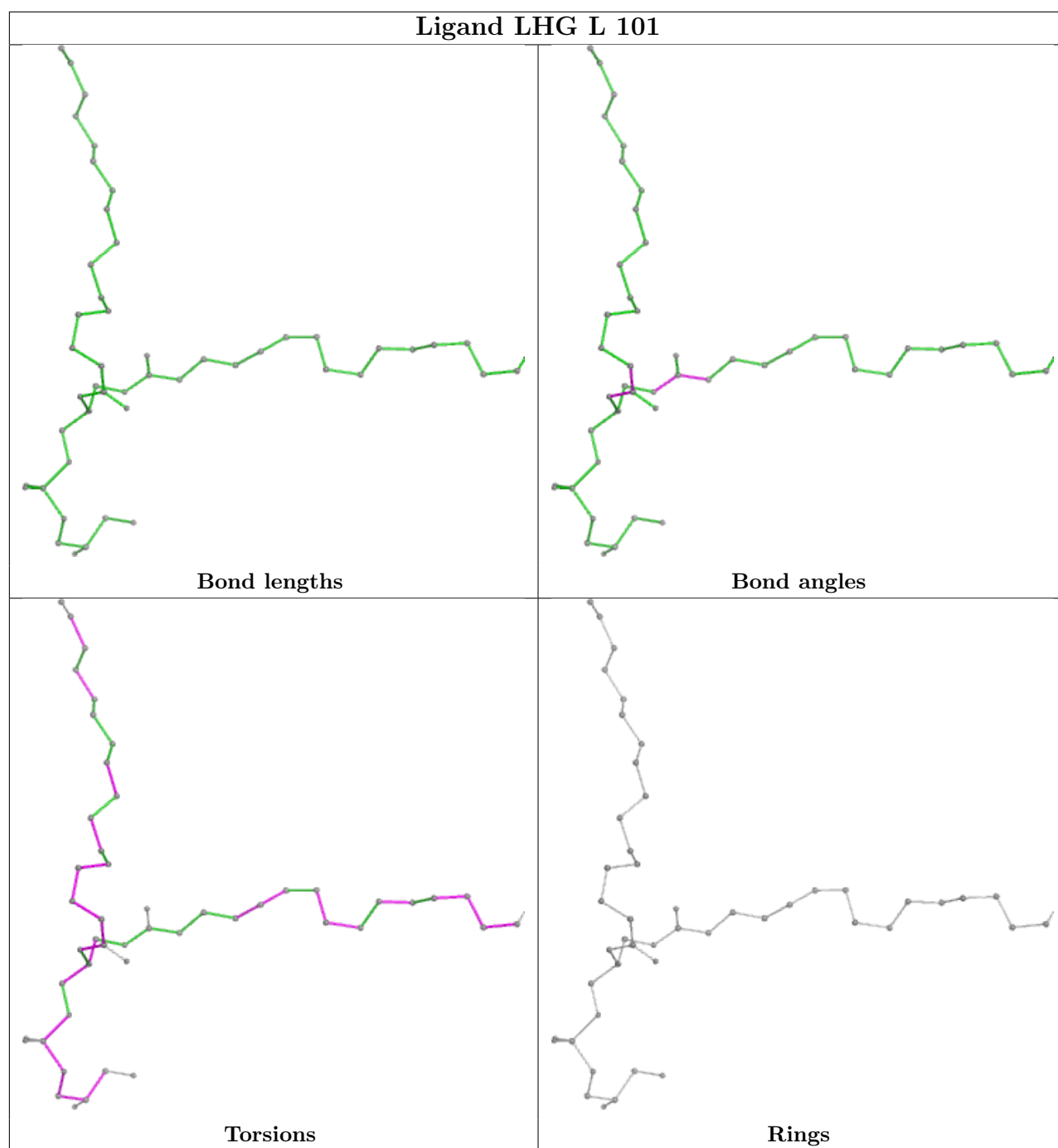
Bond angles



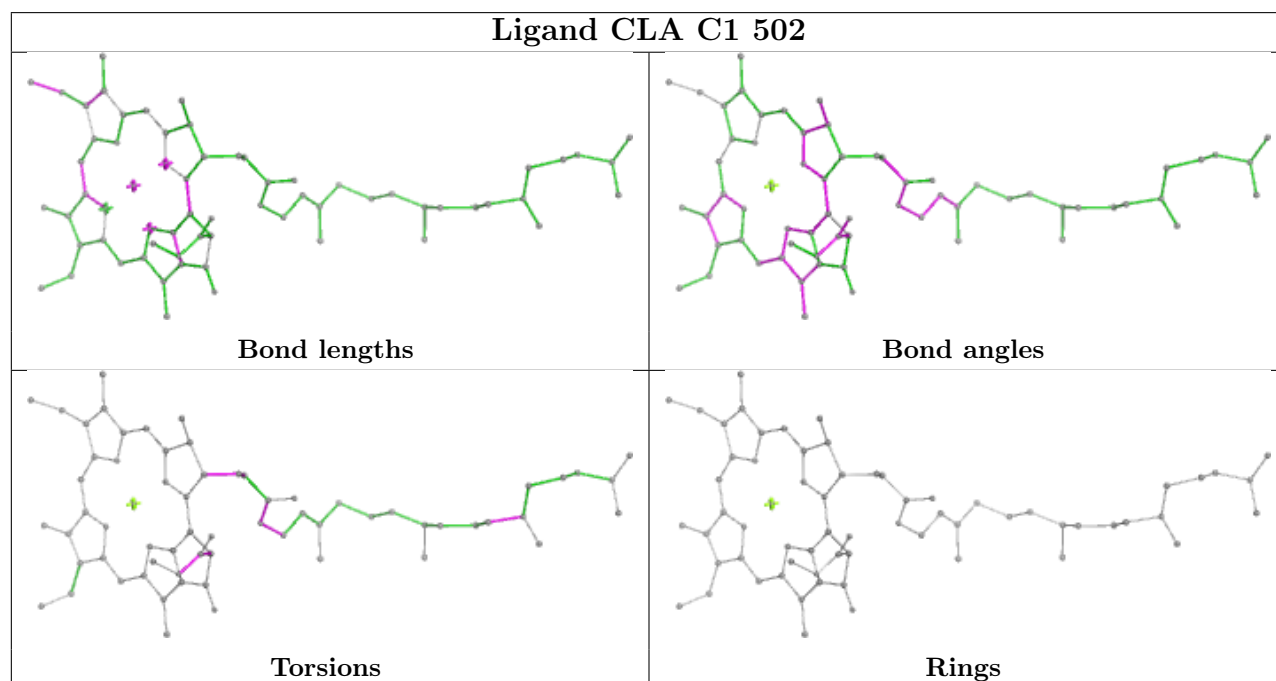
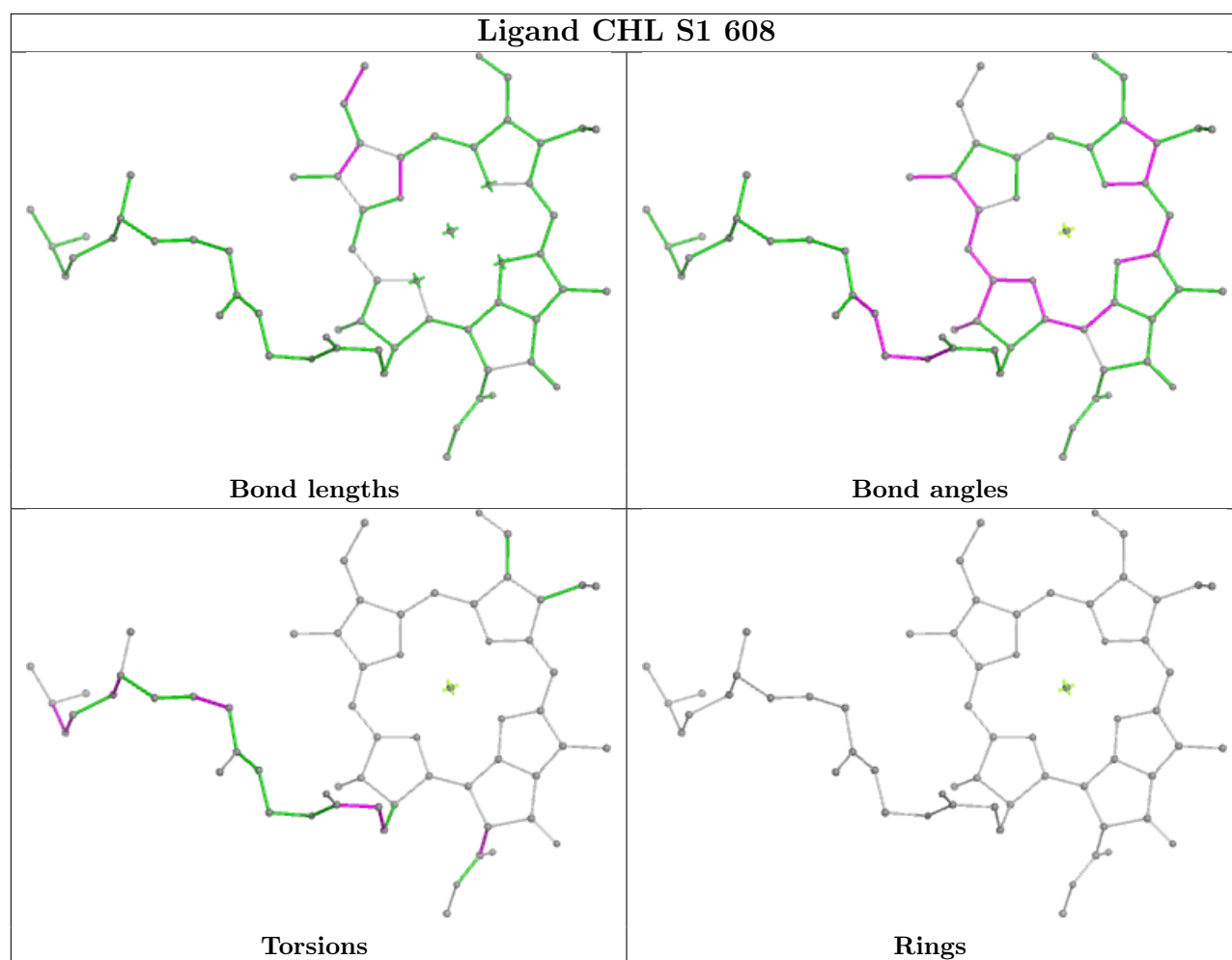
Torsions

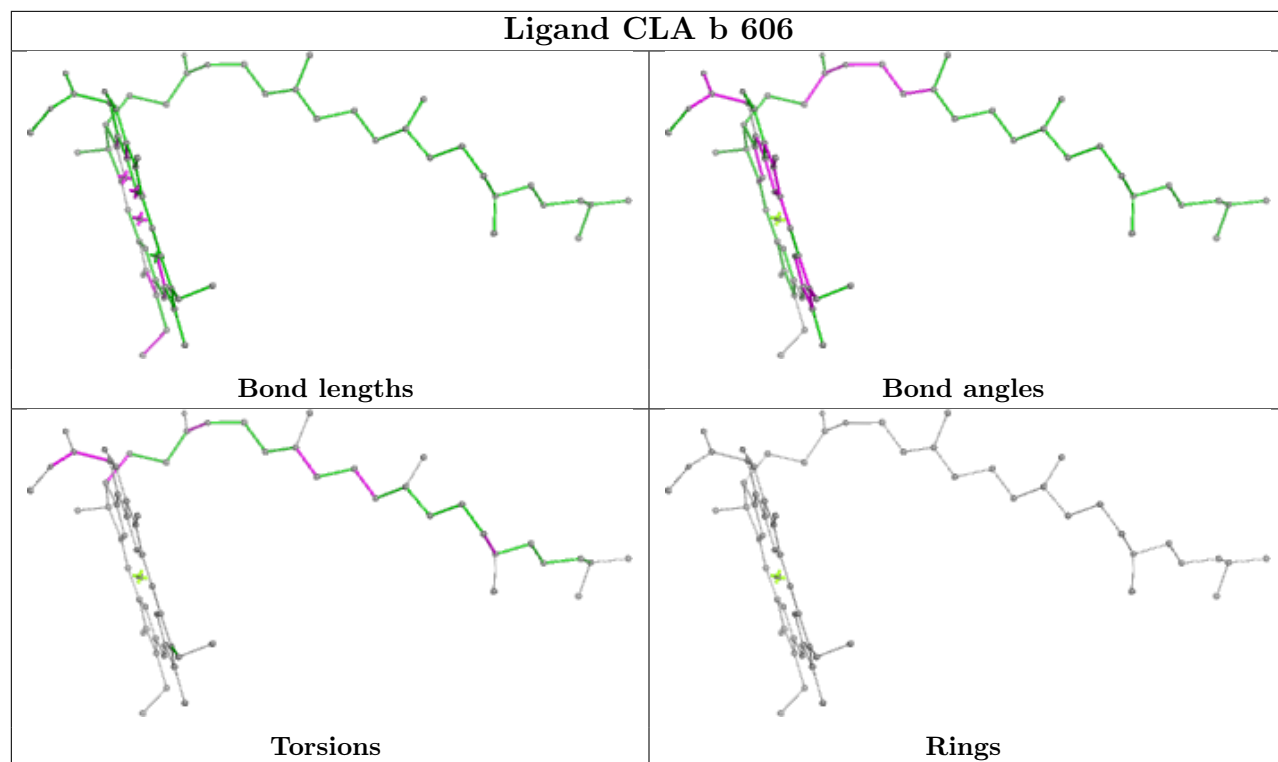


Rings

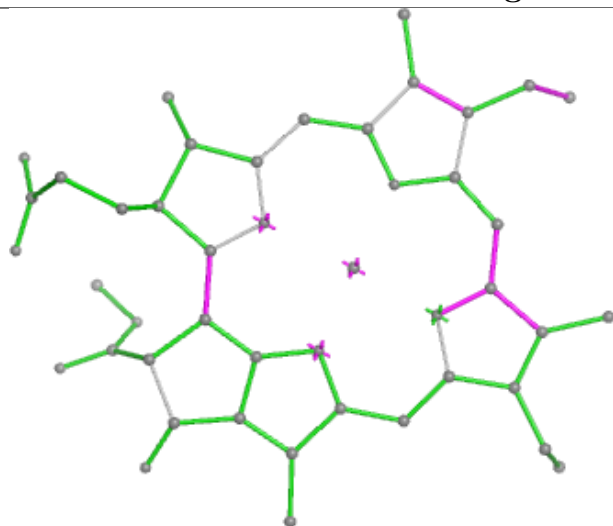




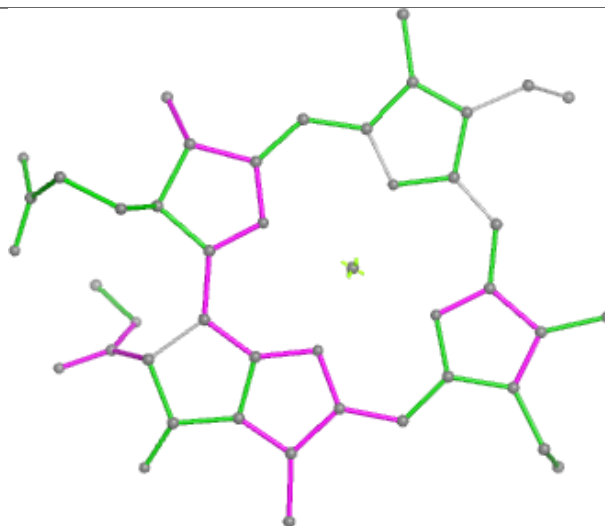




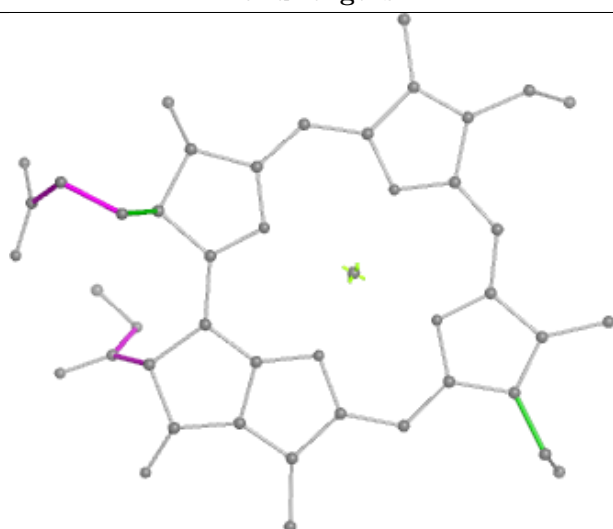
## Ligand CLA N1 612



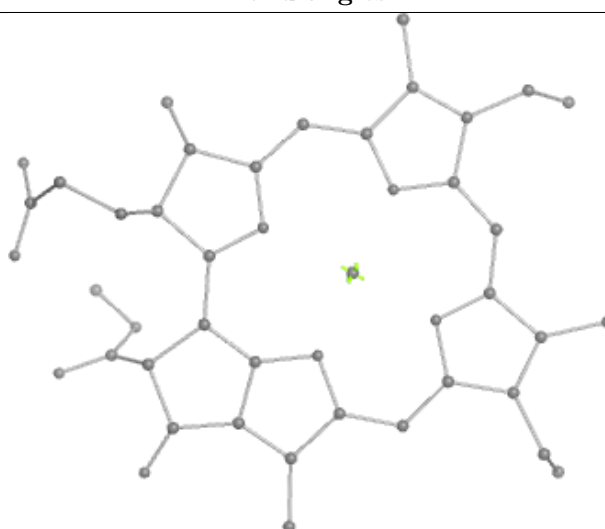
Bond lengths



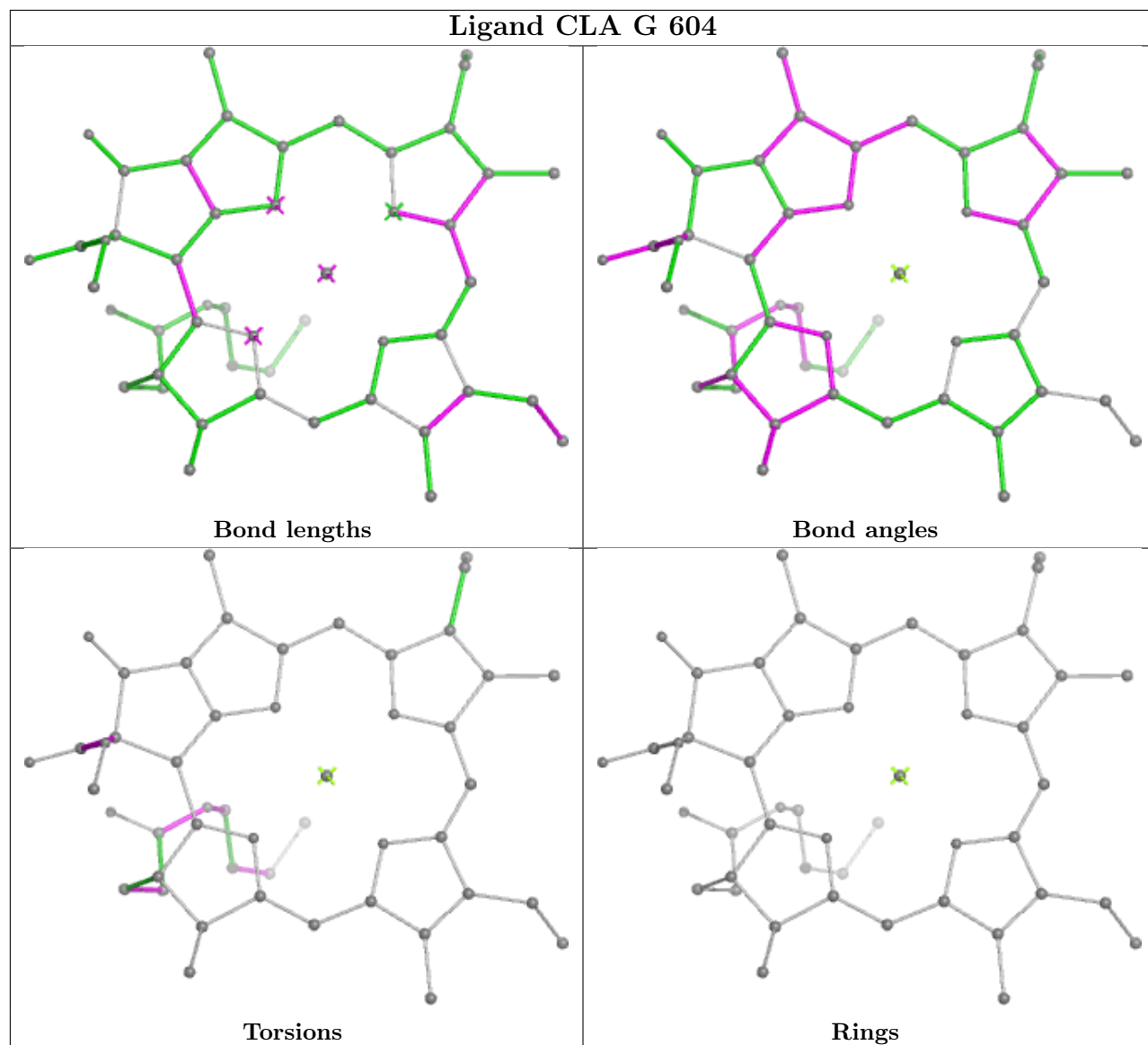
Bond angles



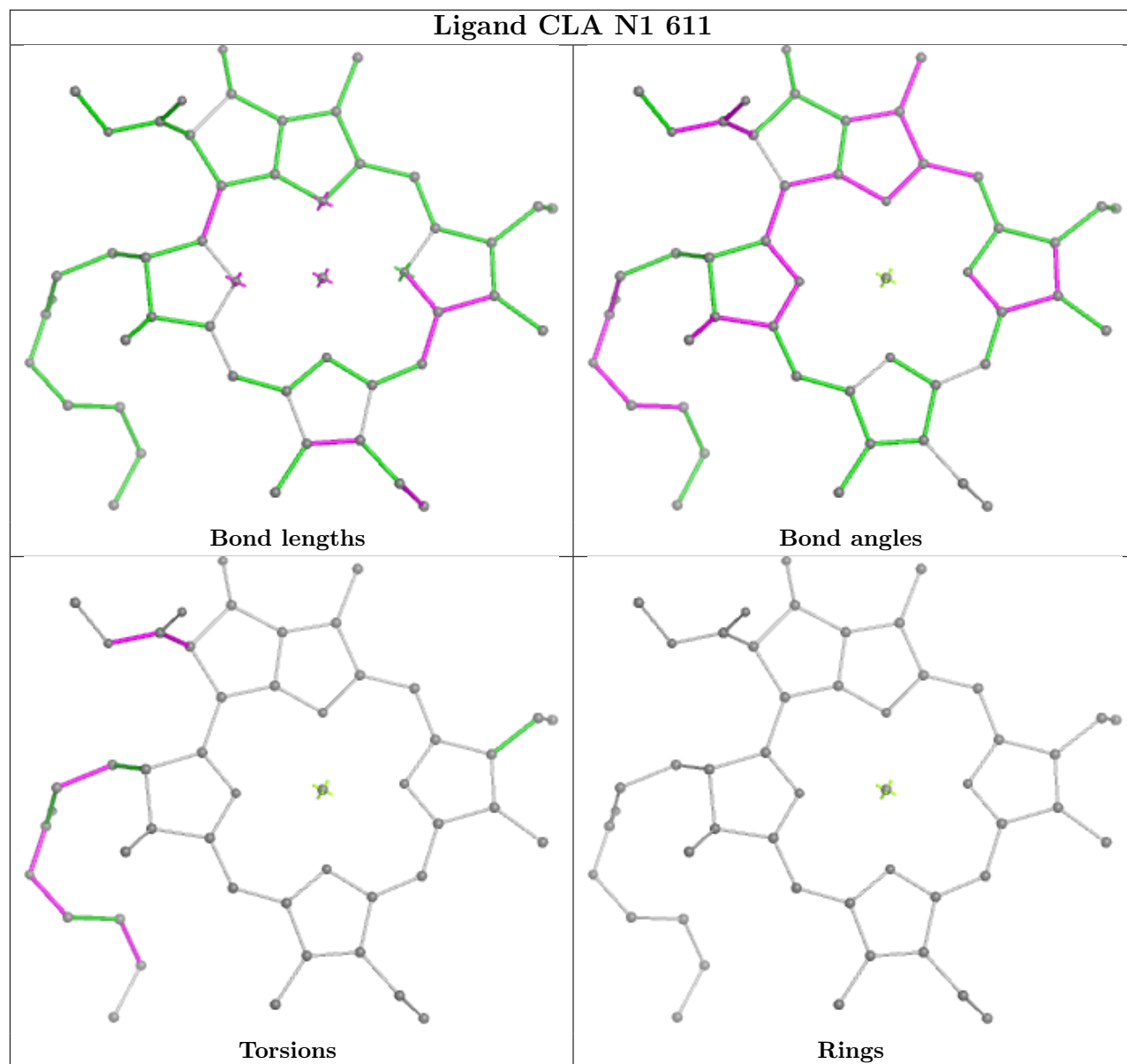
Torsions

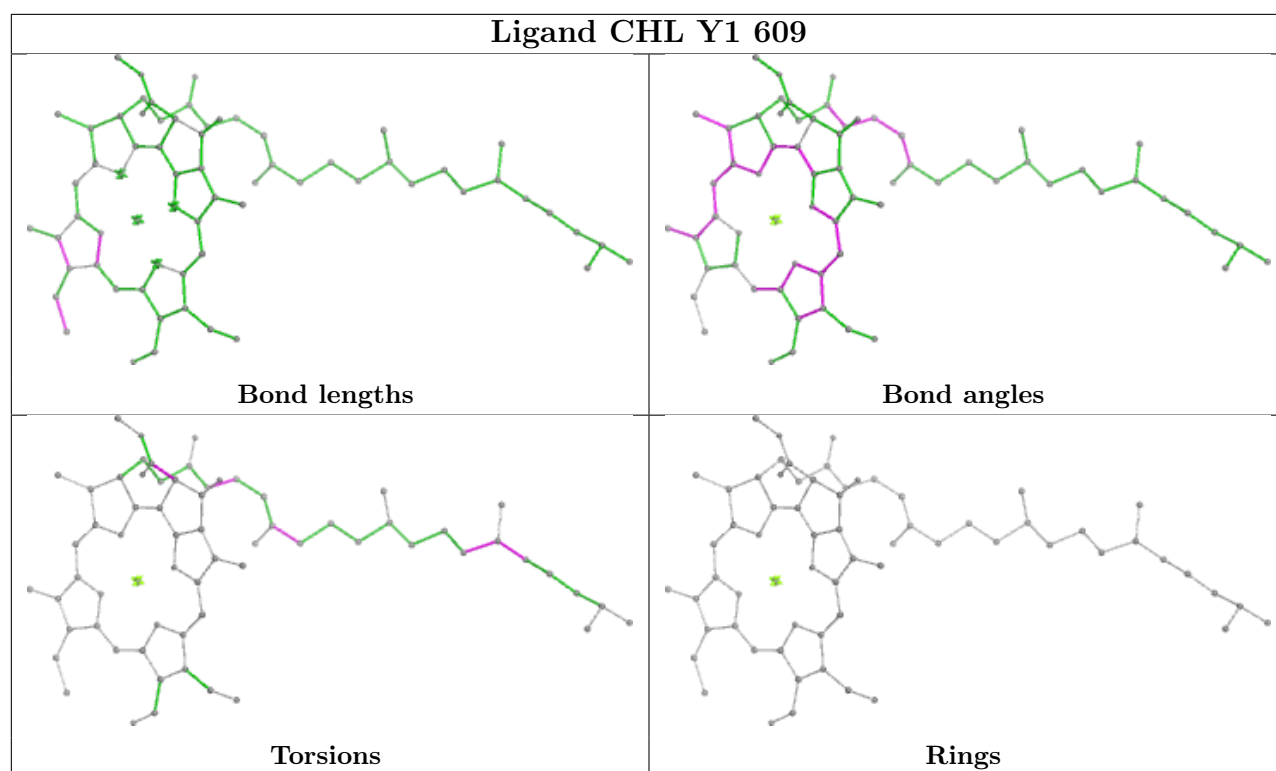


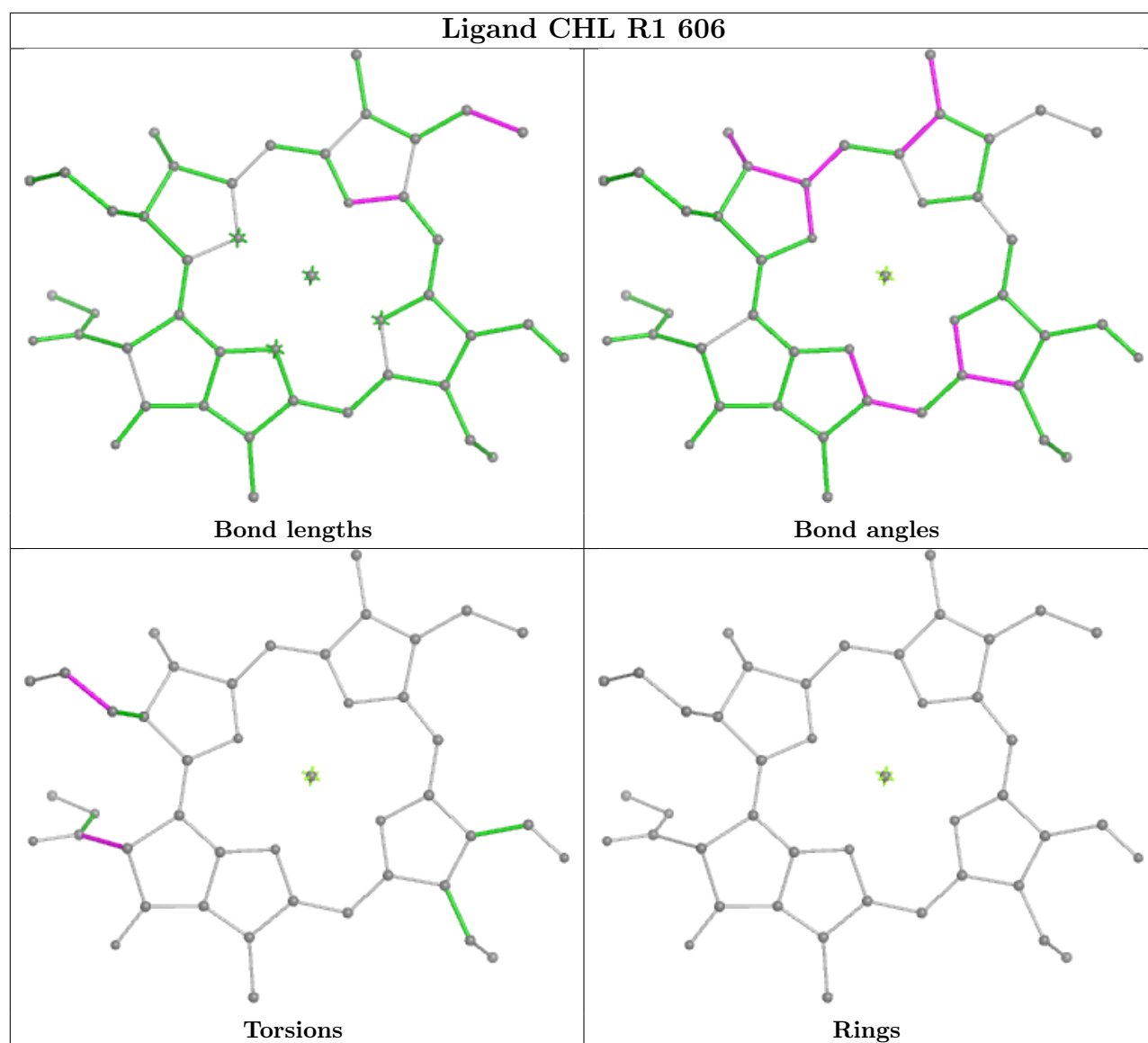
Rings

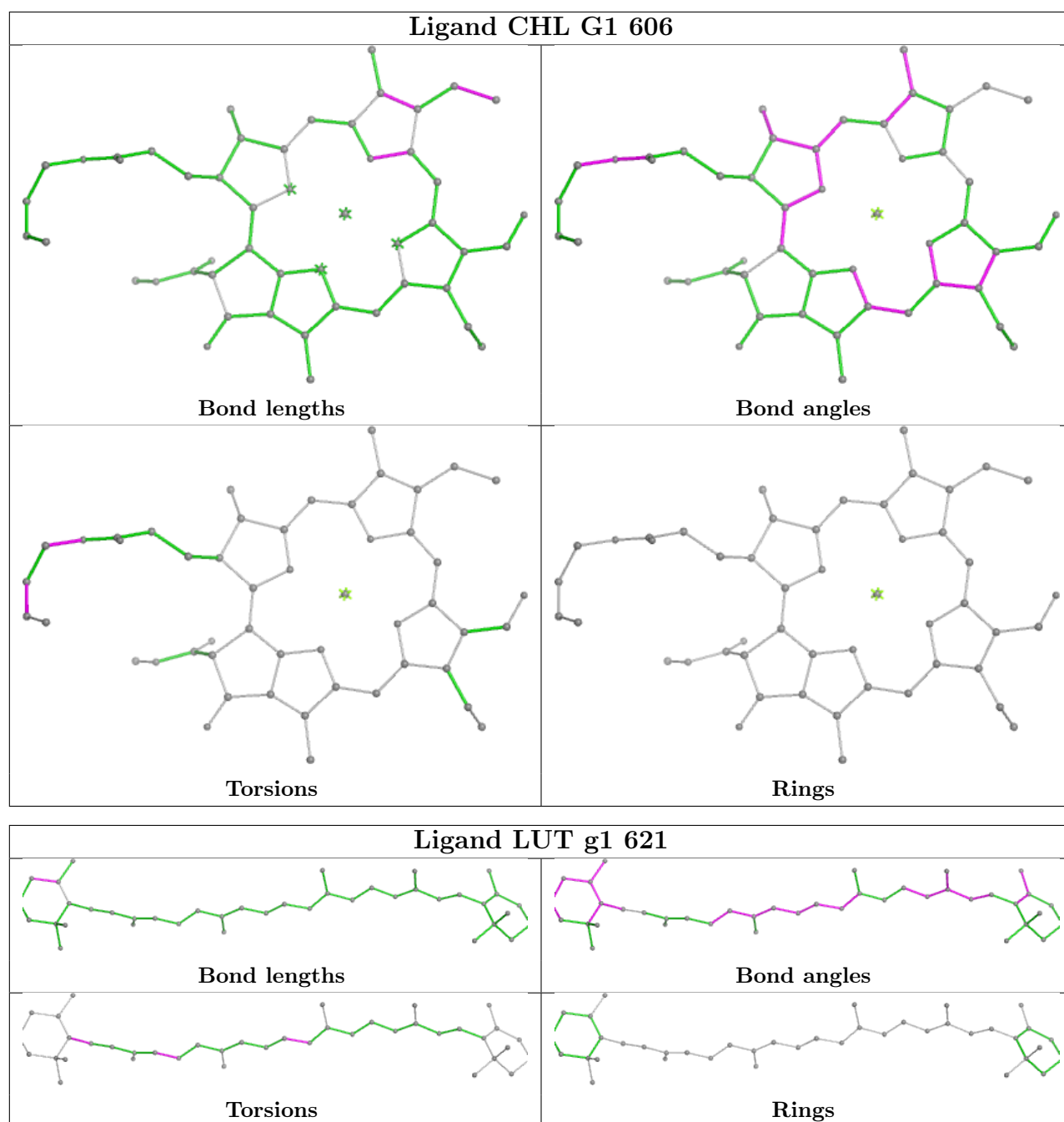


## Ligand CLA N1 611



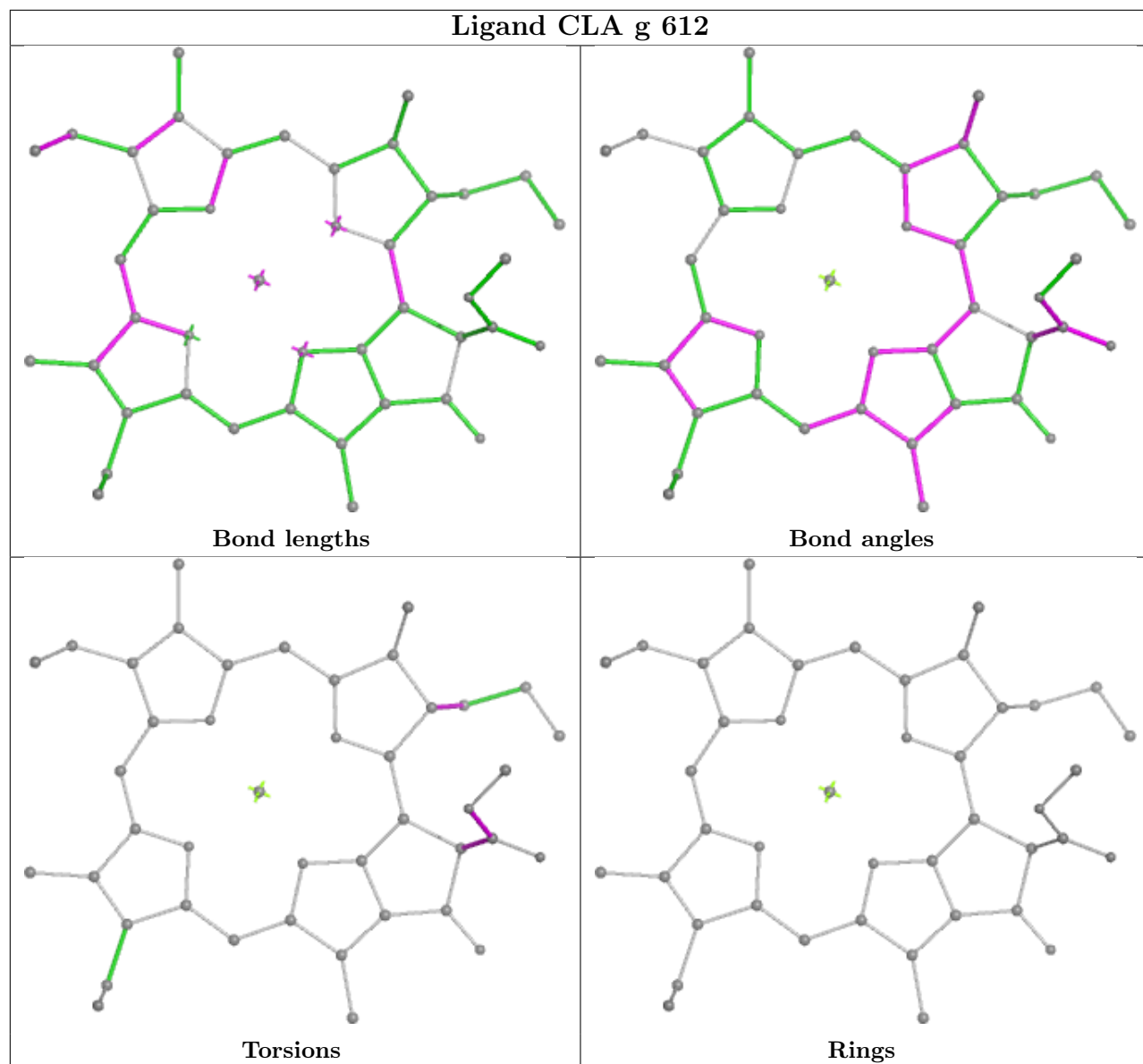


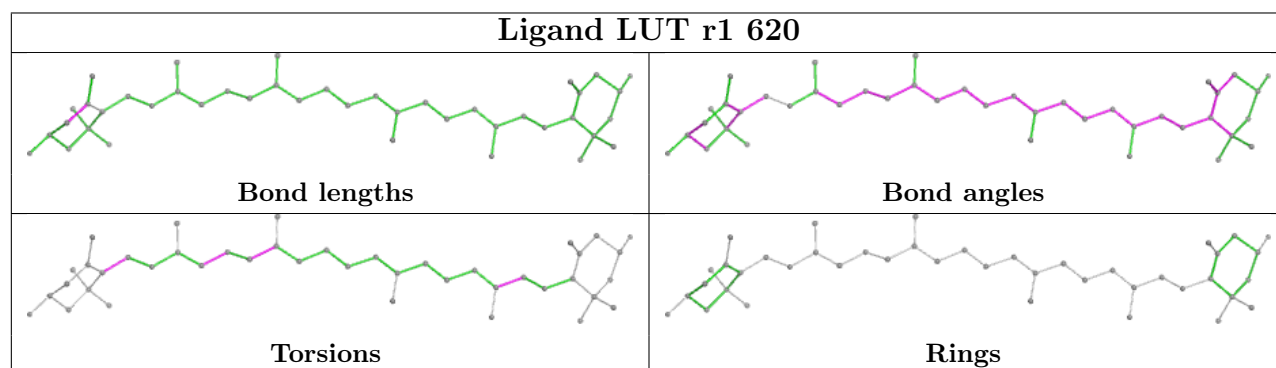
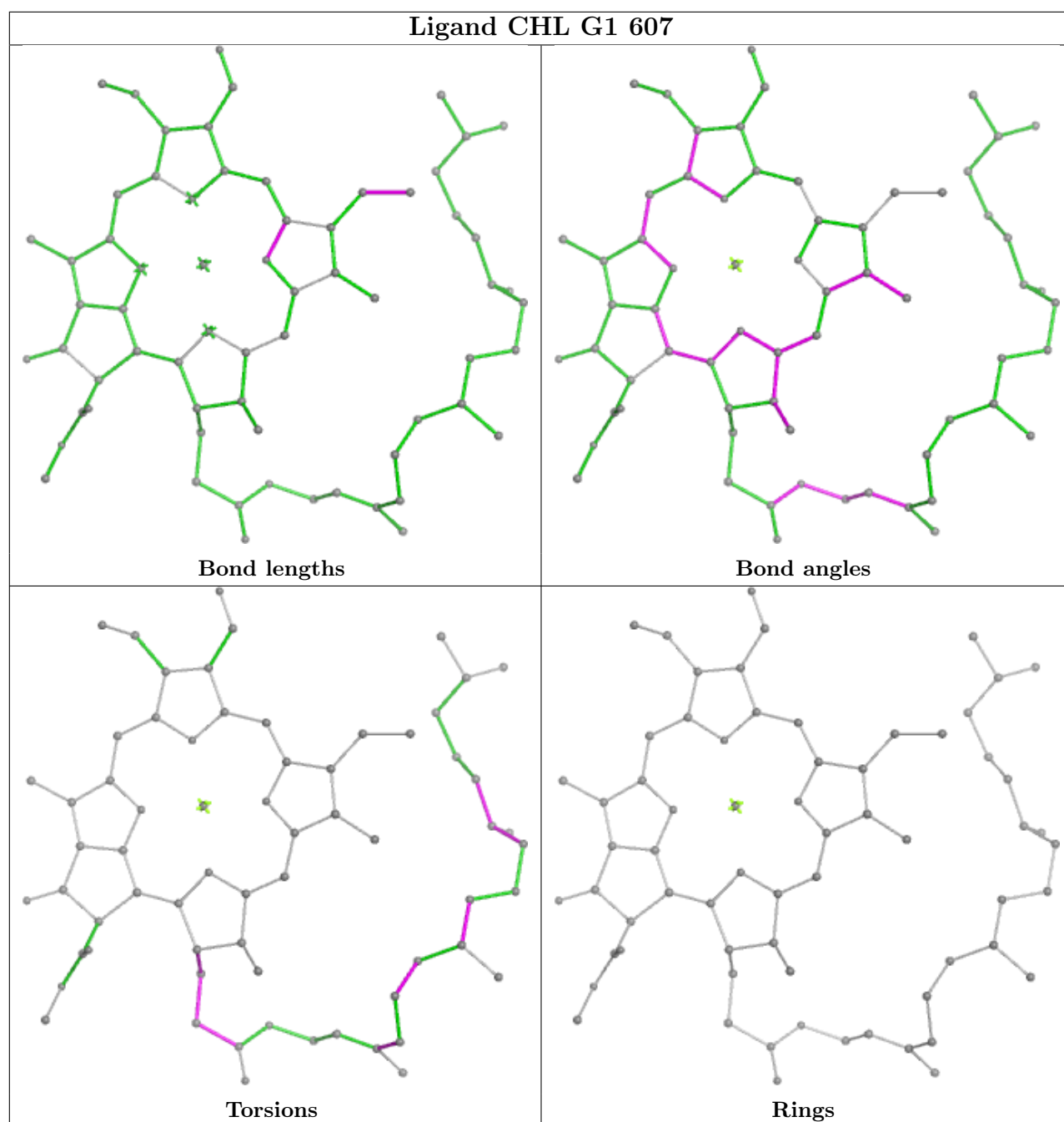


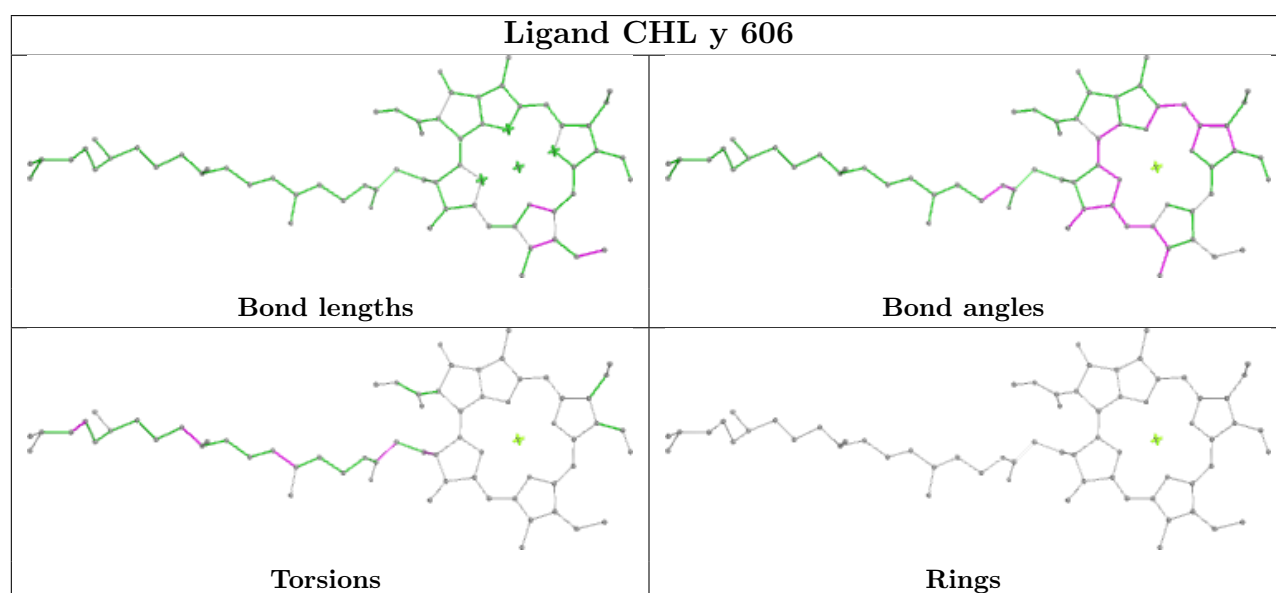
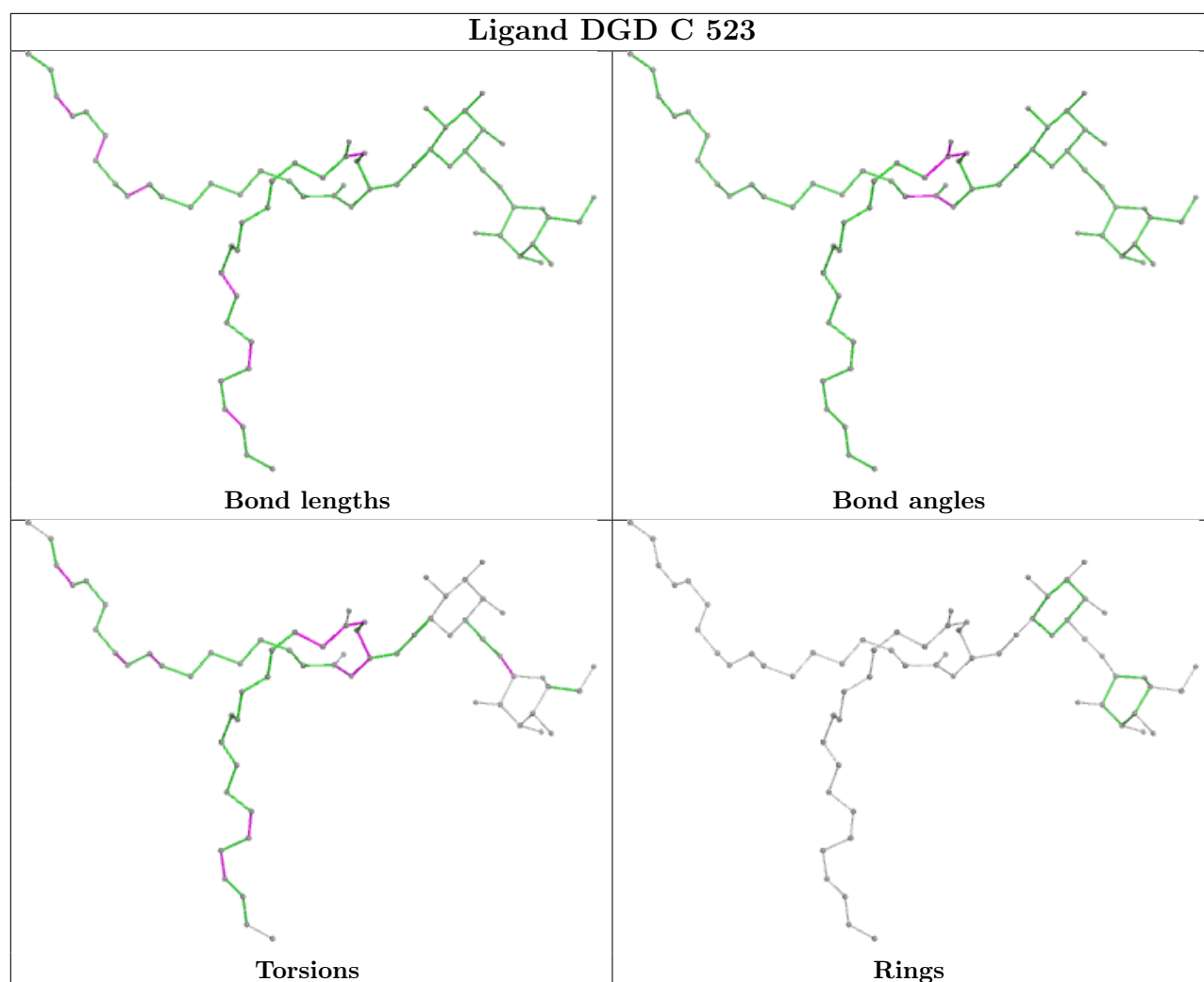


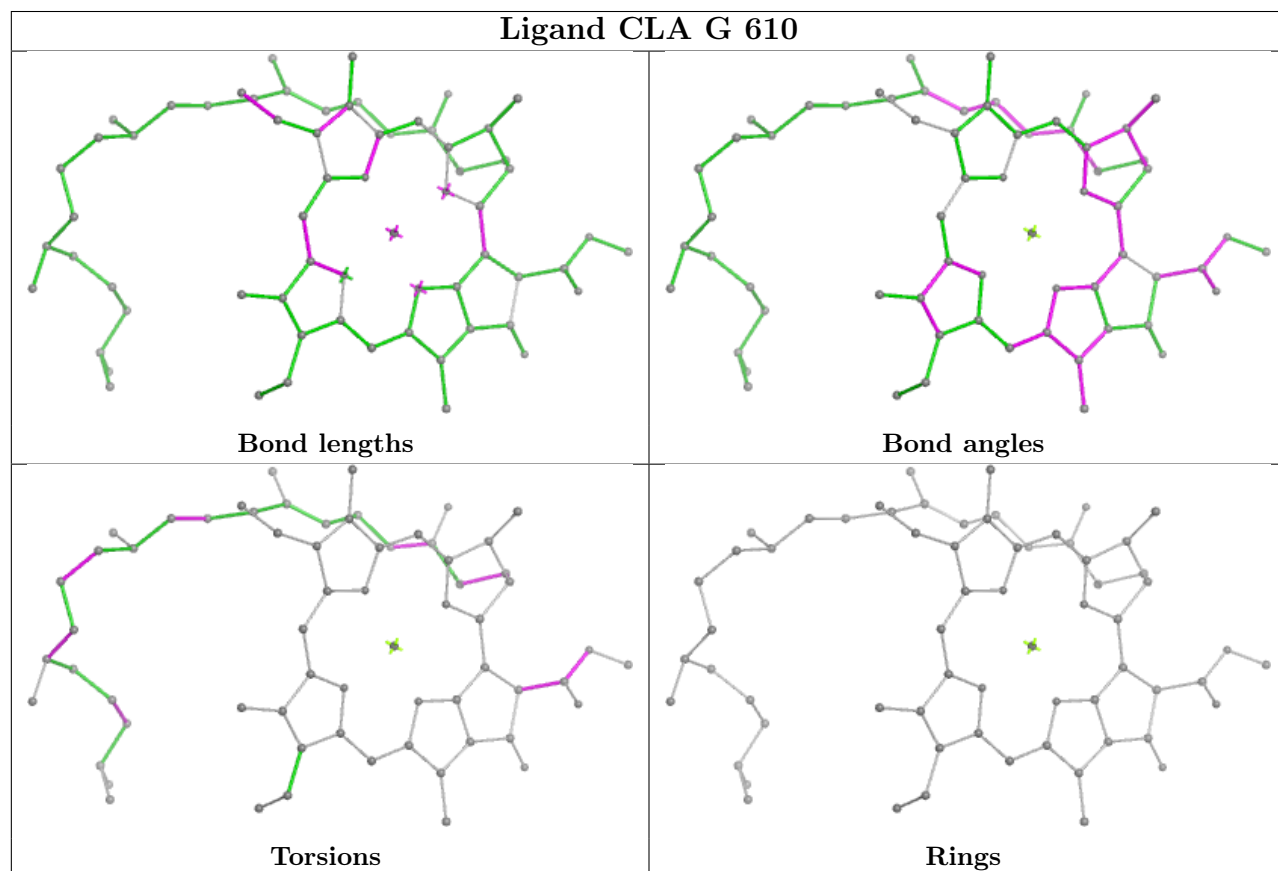
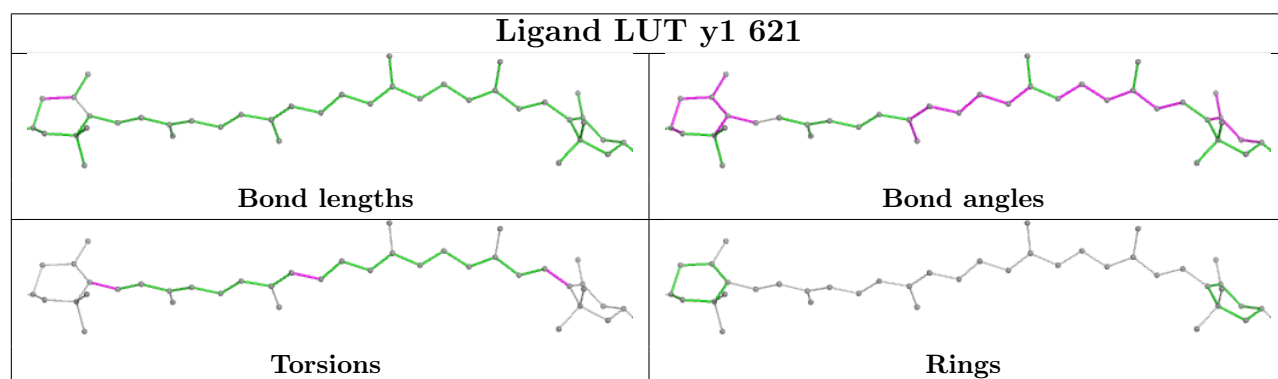
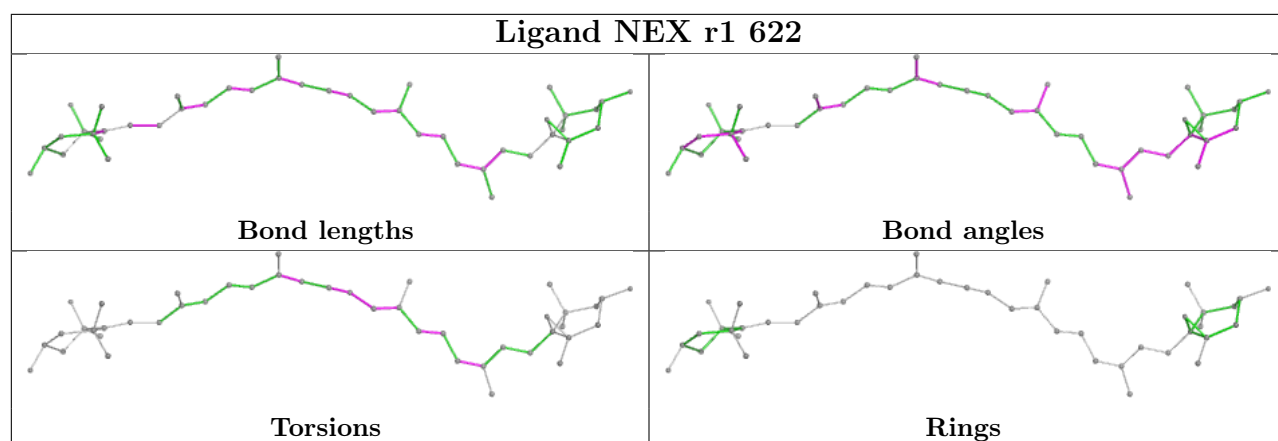


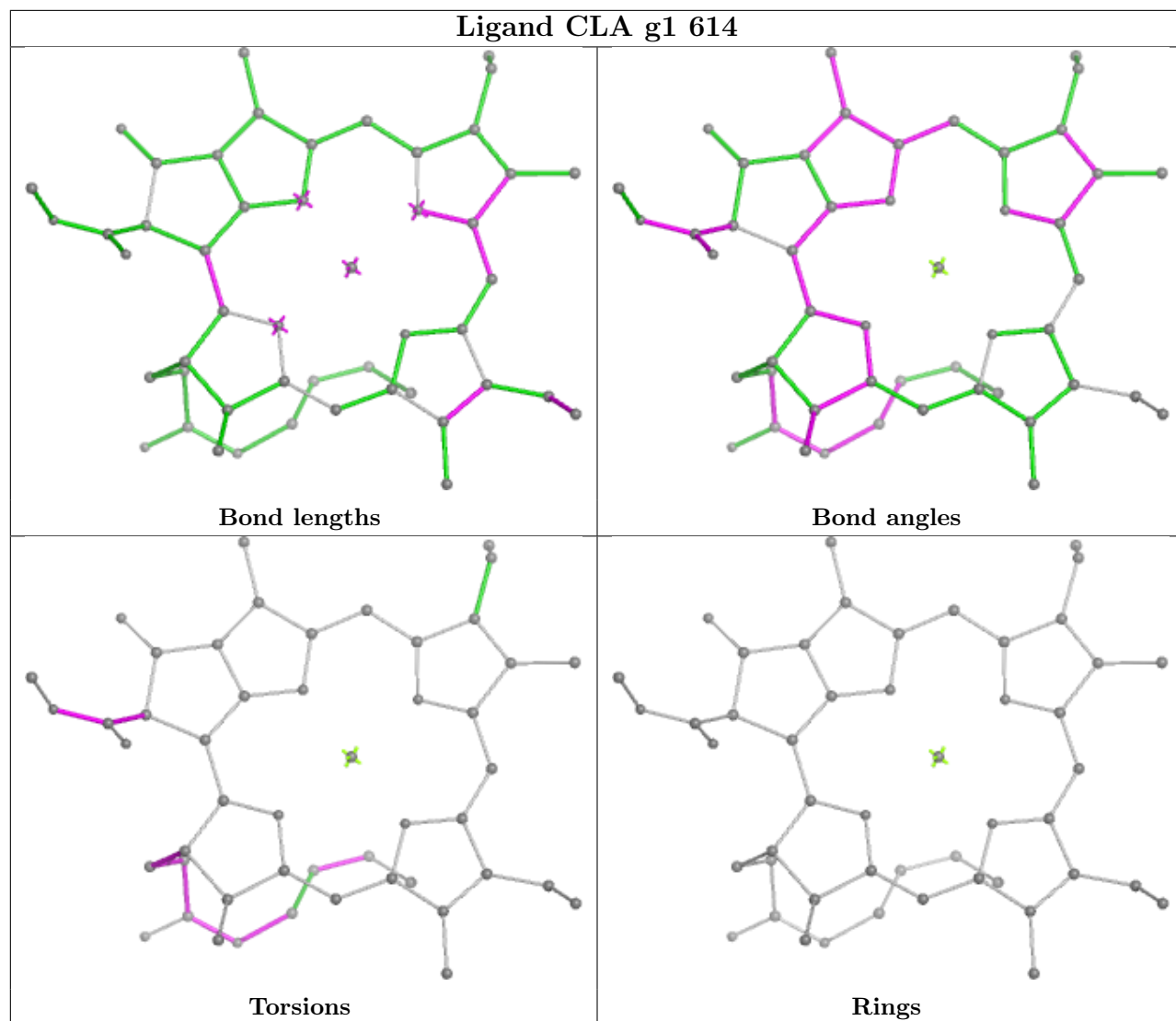
## Ligand CLA g 612

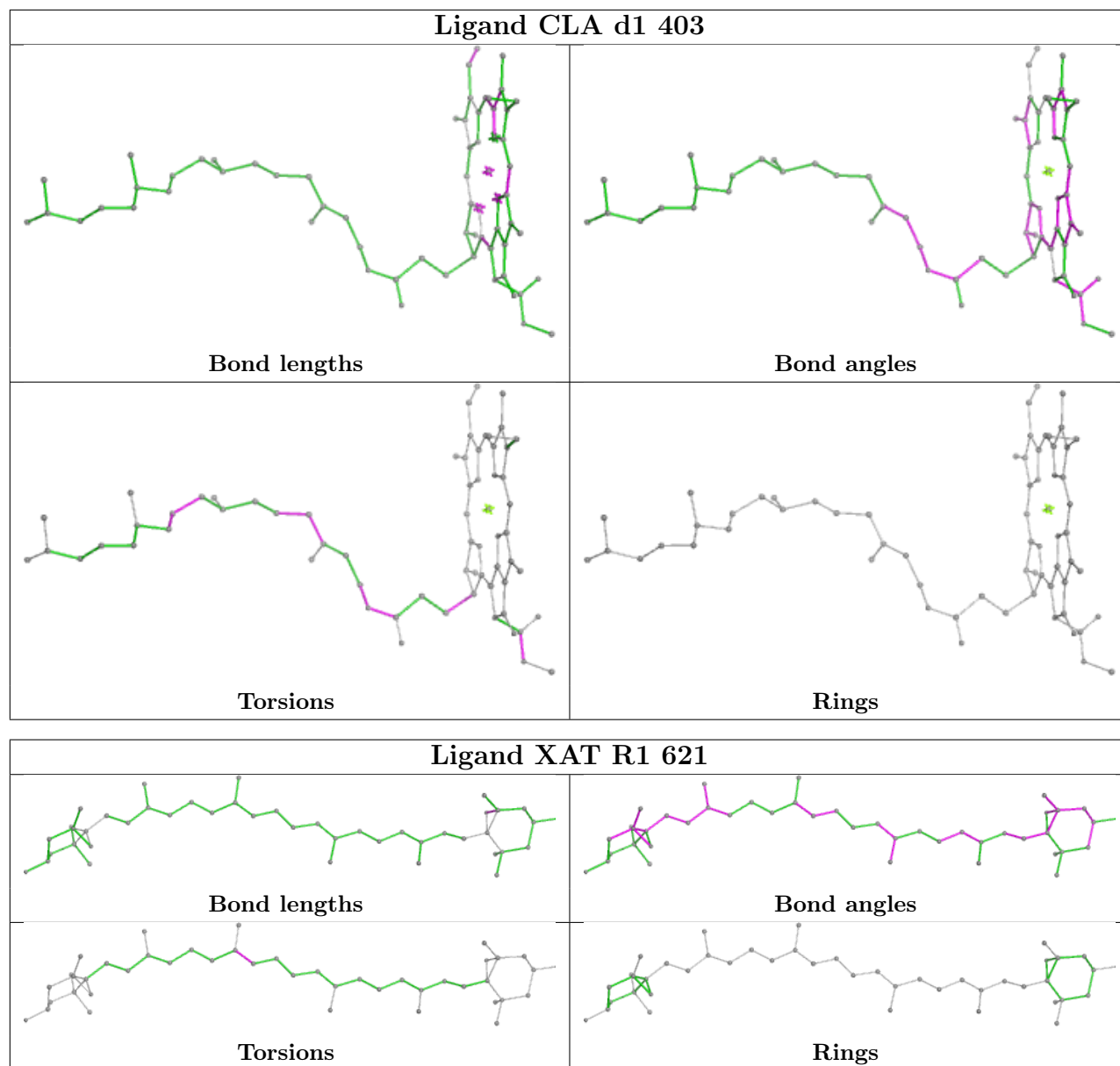


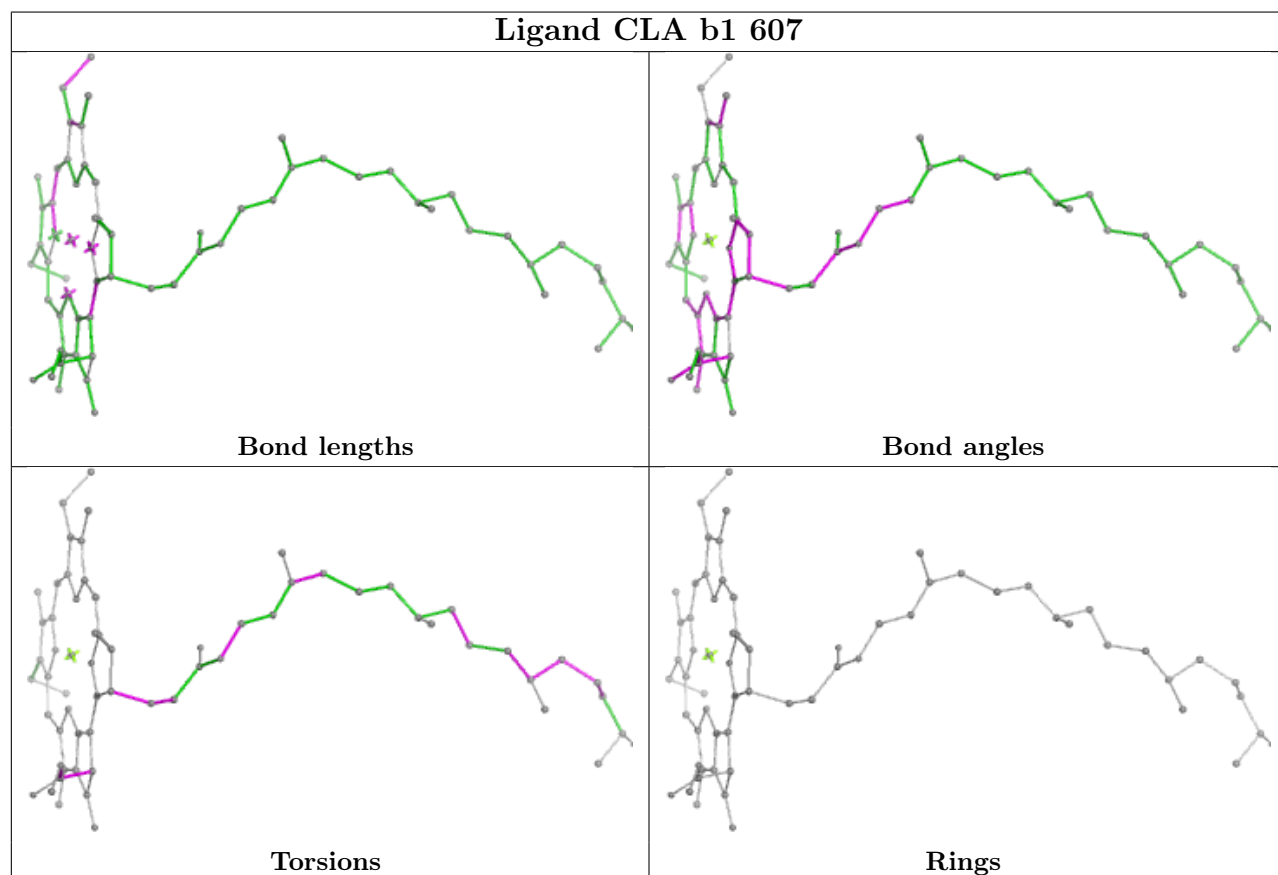
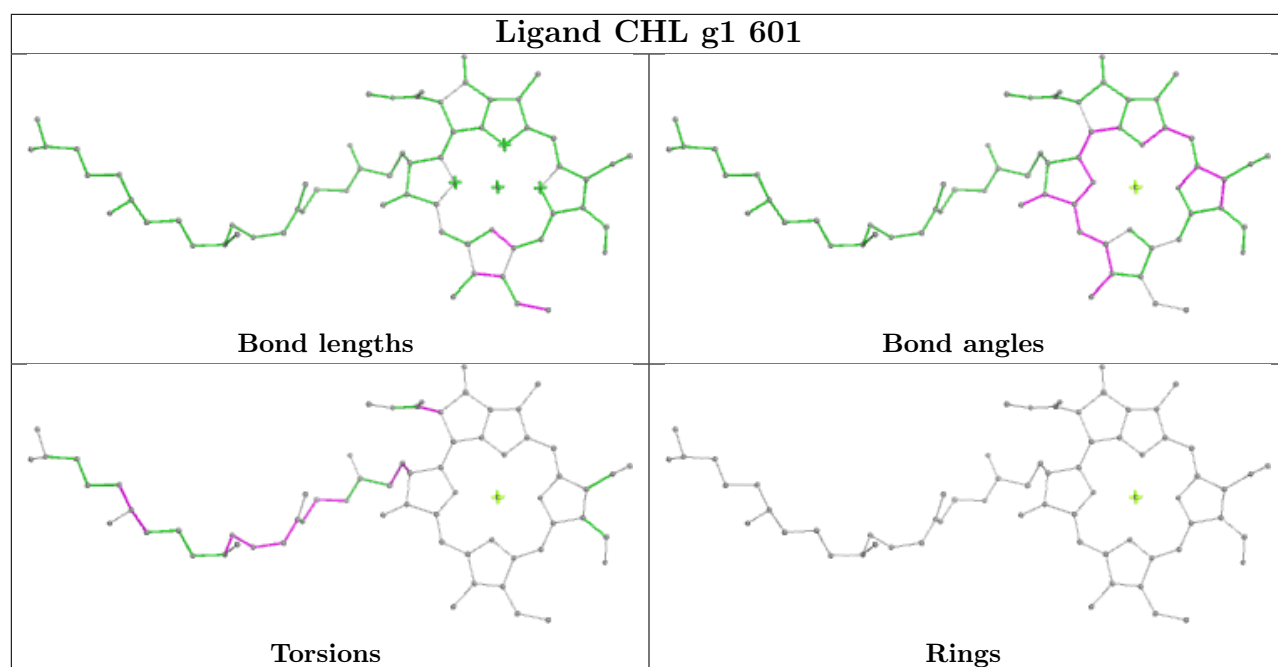


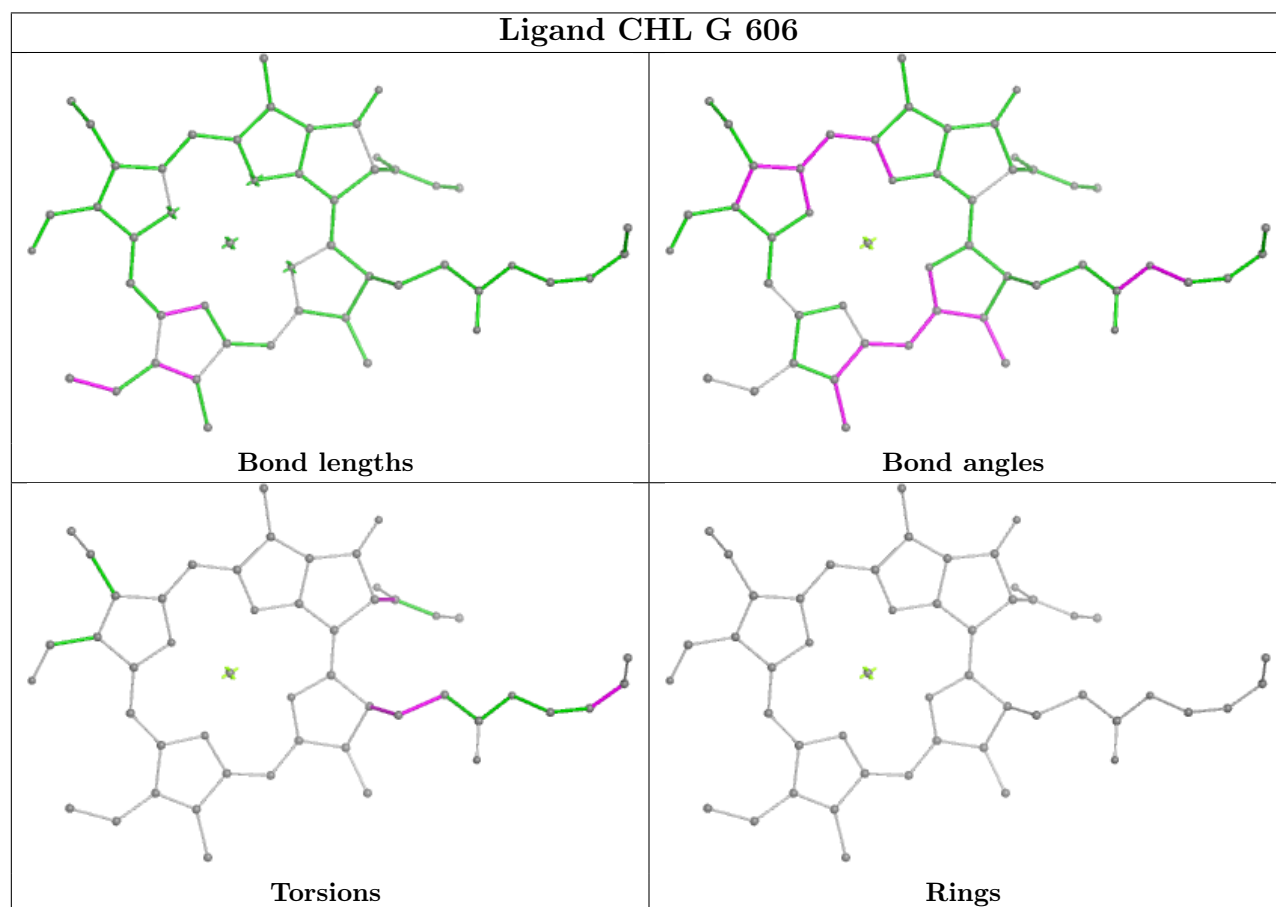
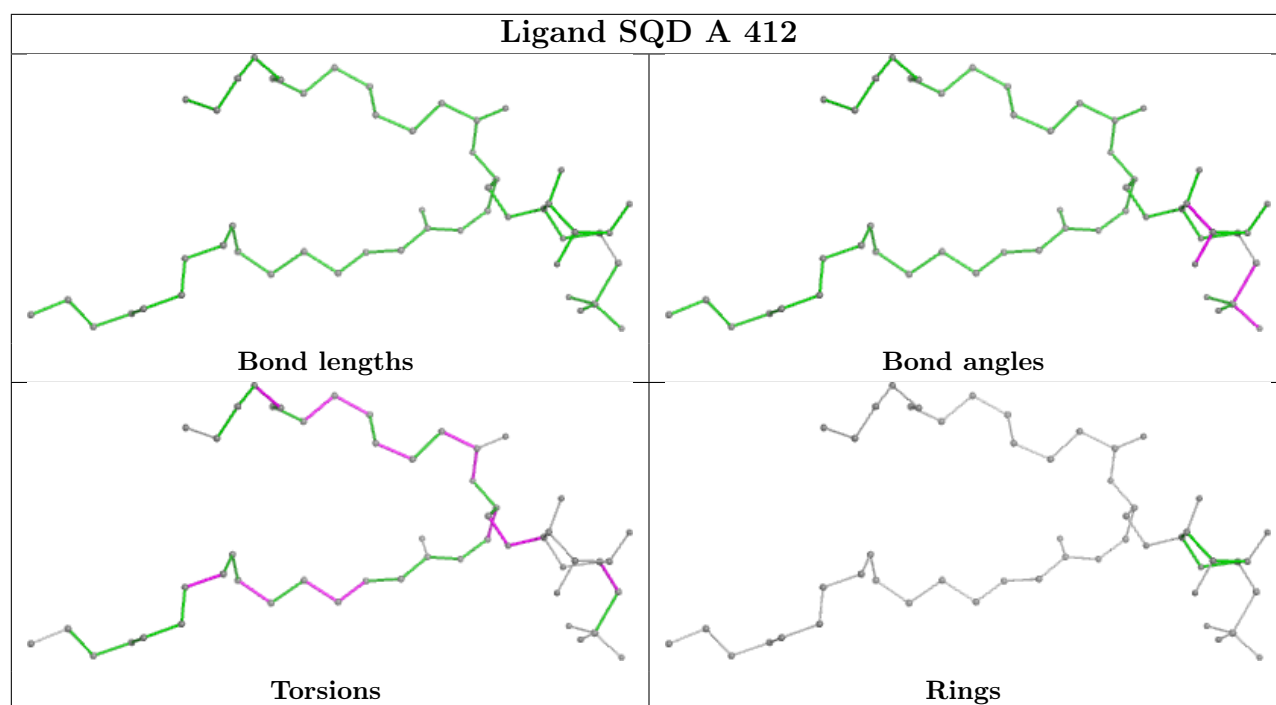




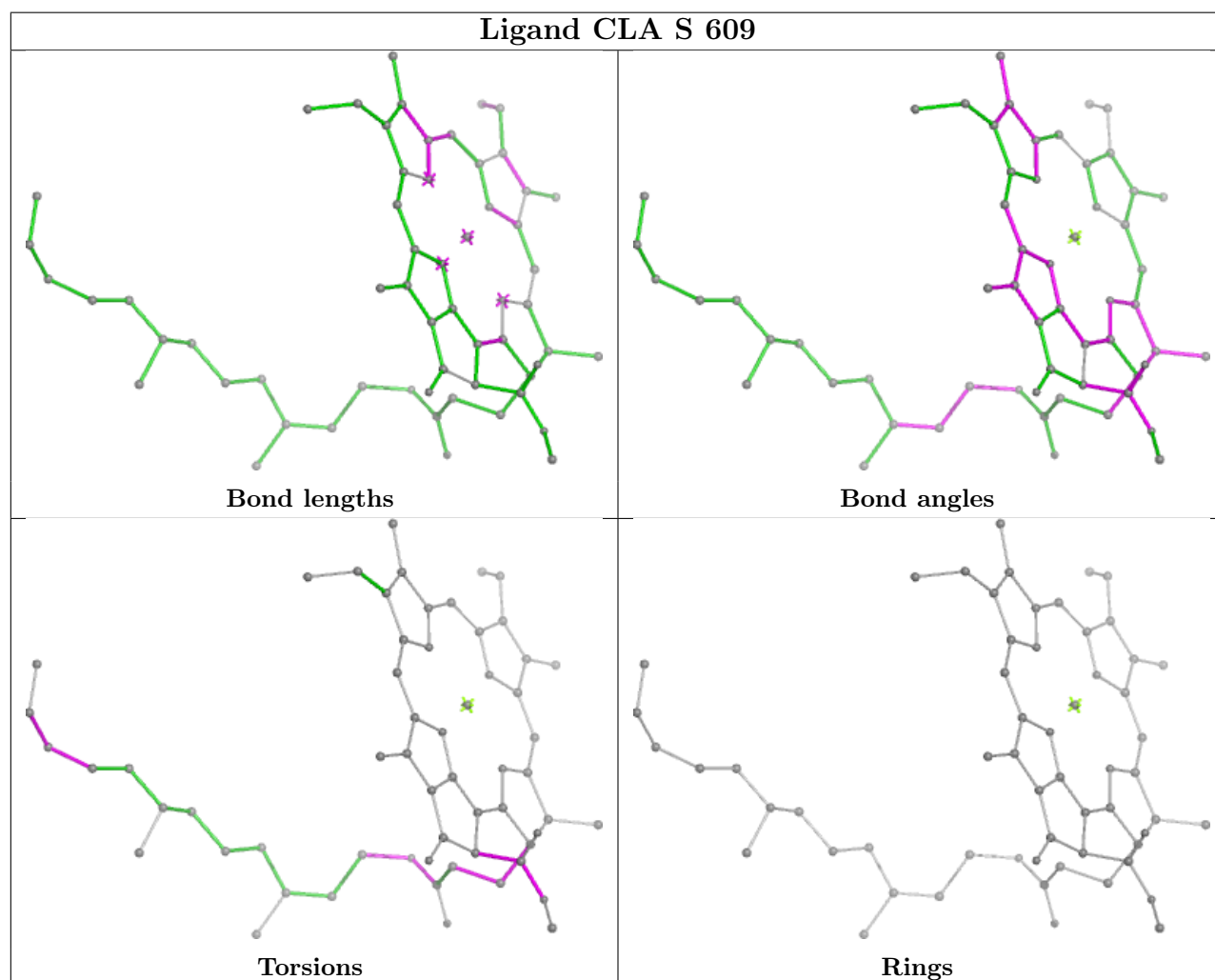
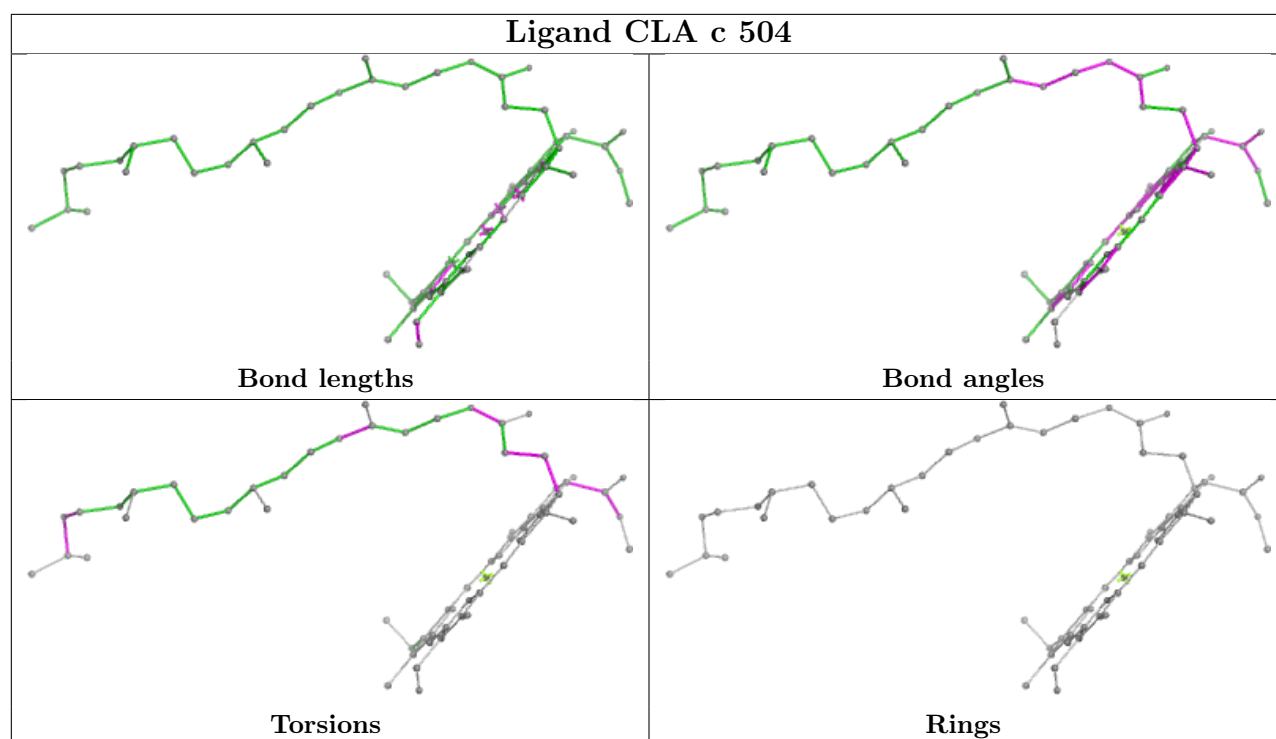


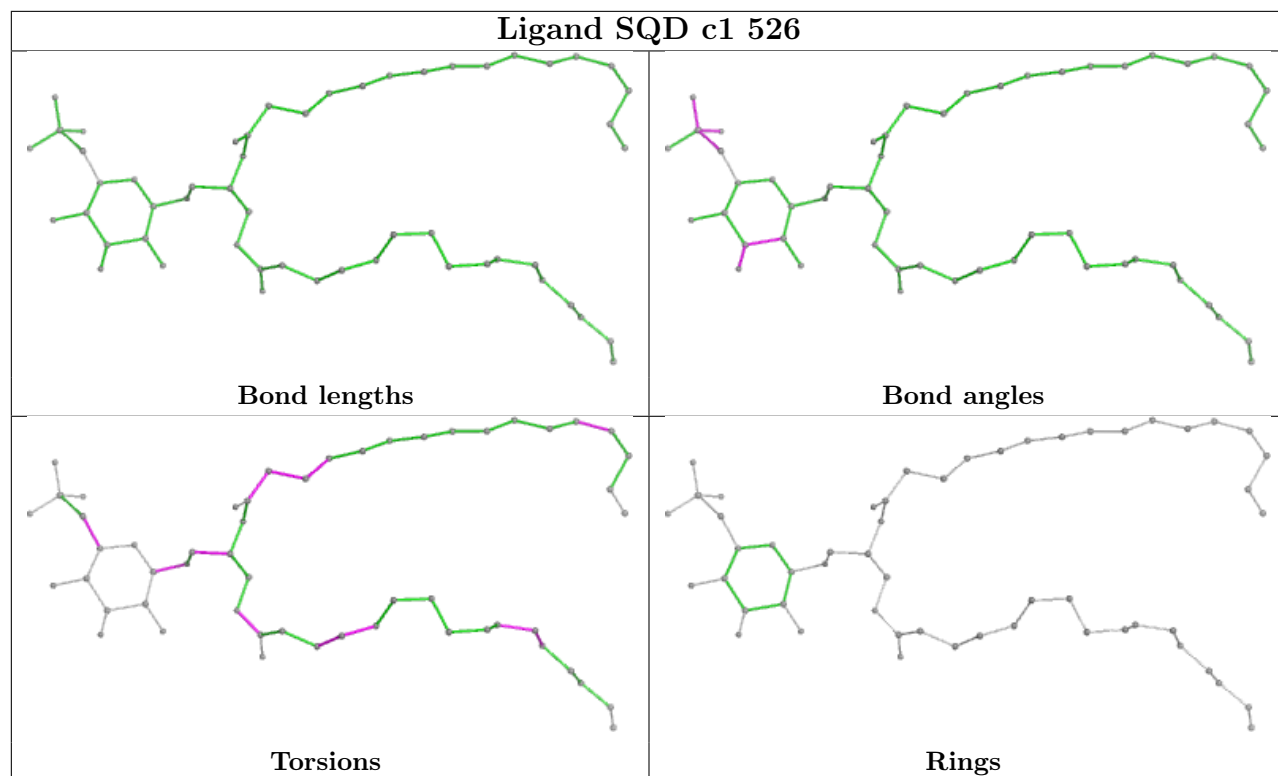


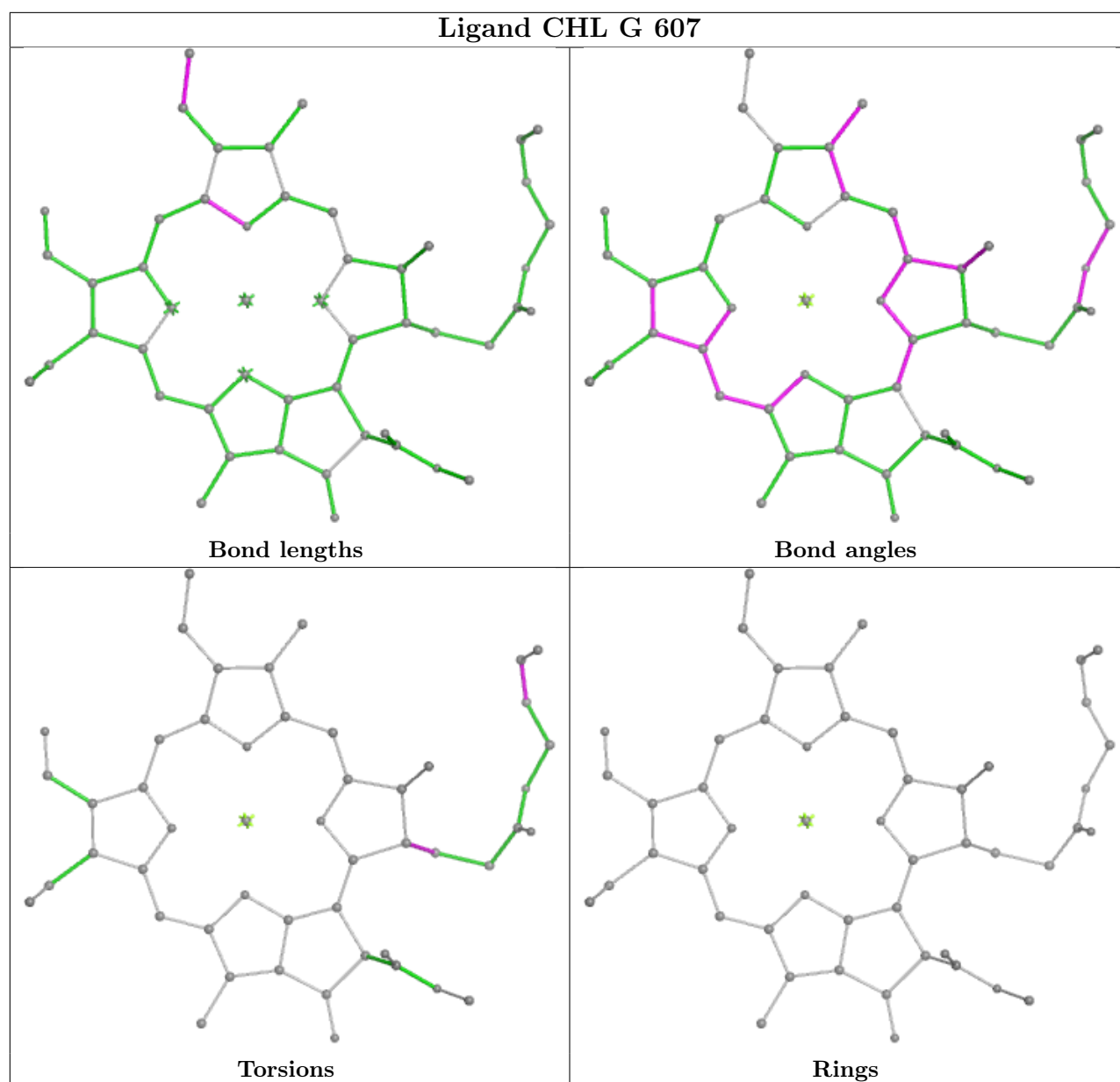


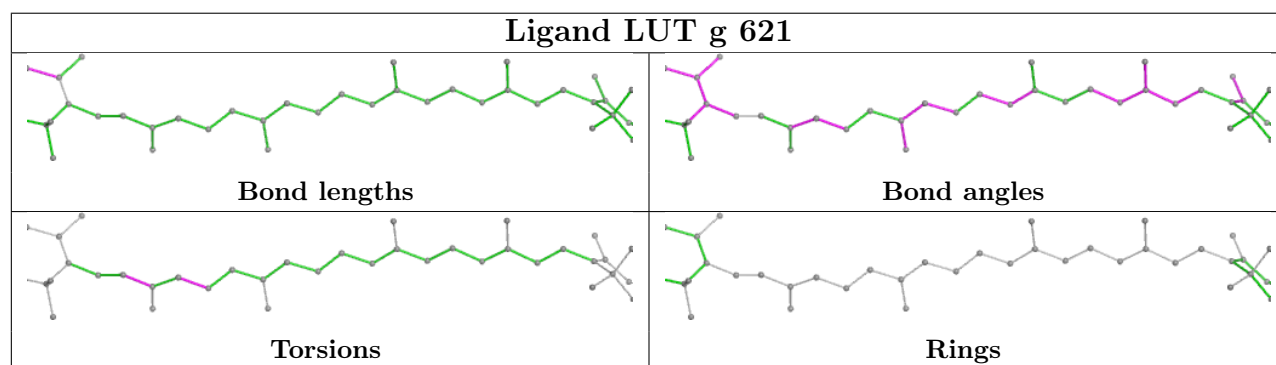
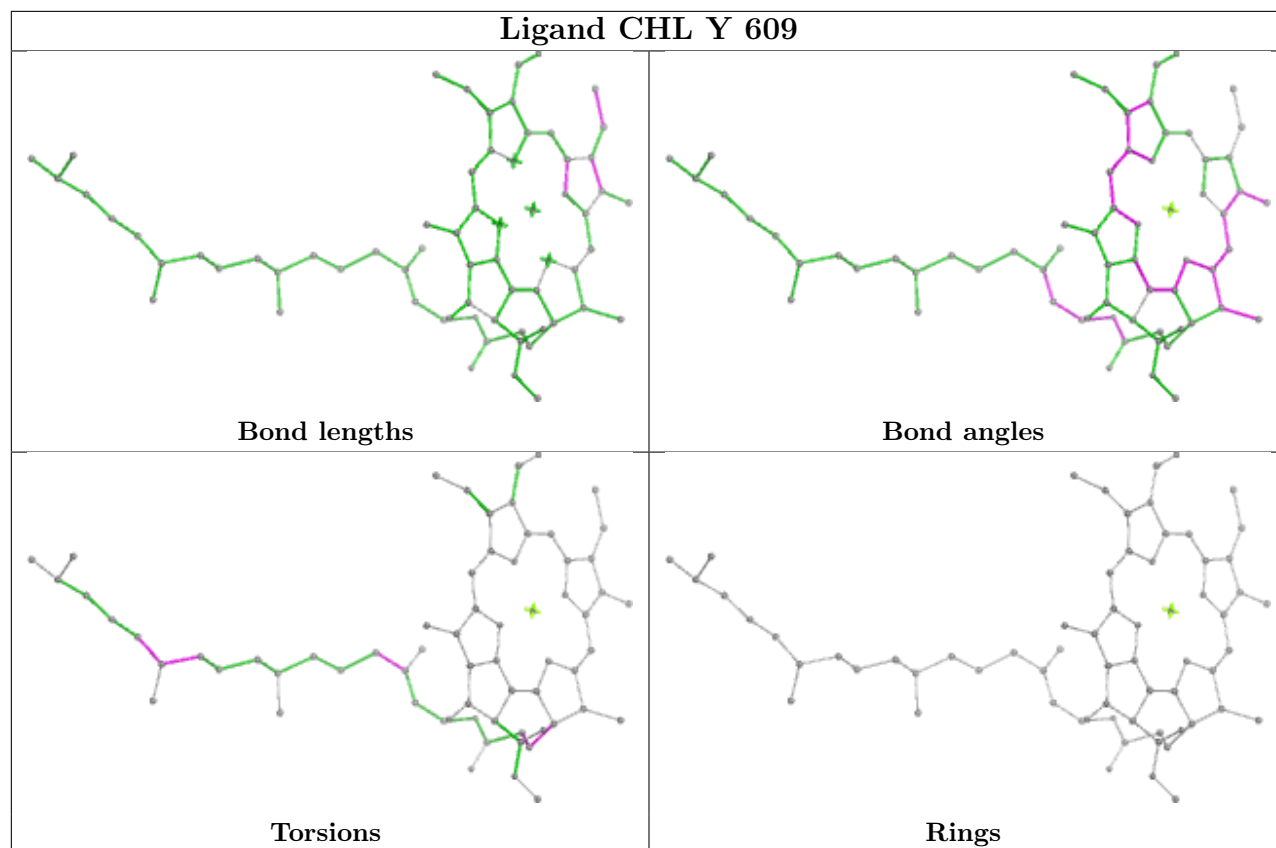


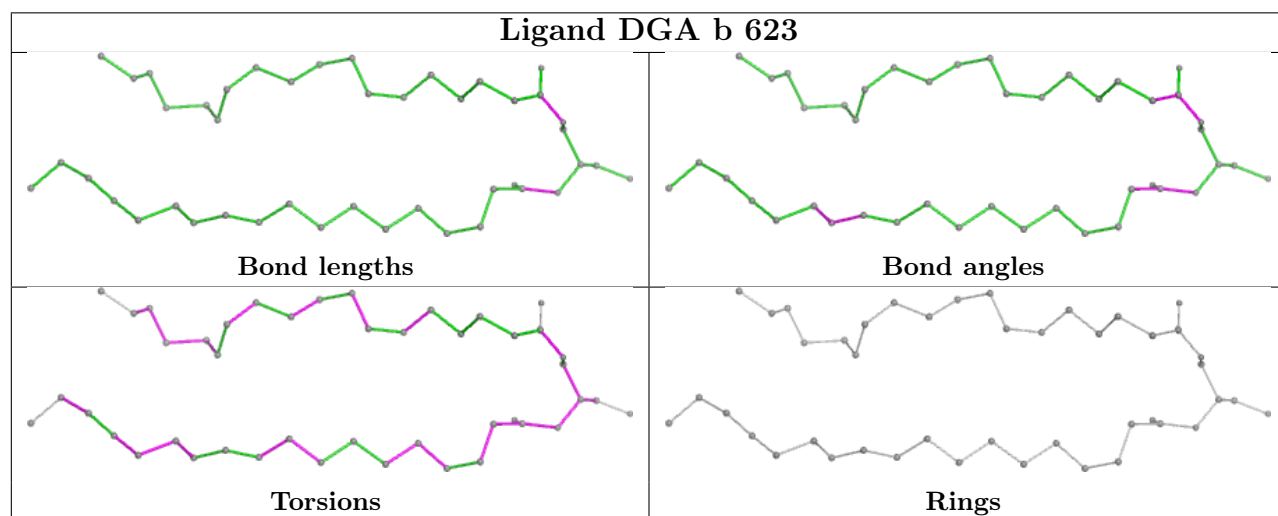
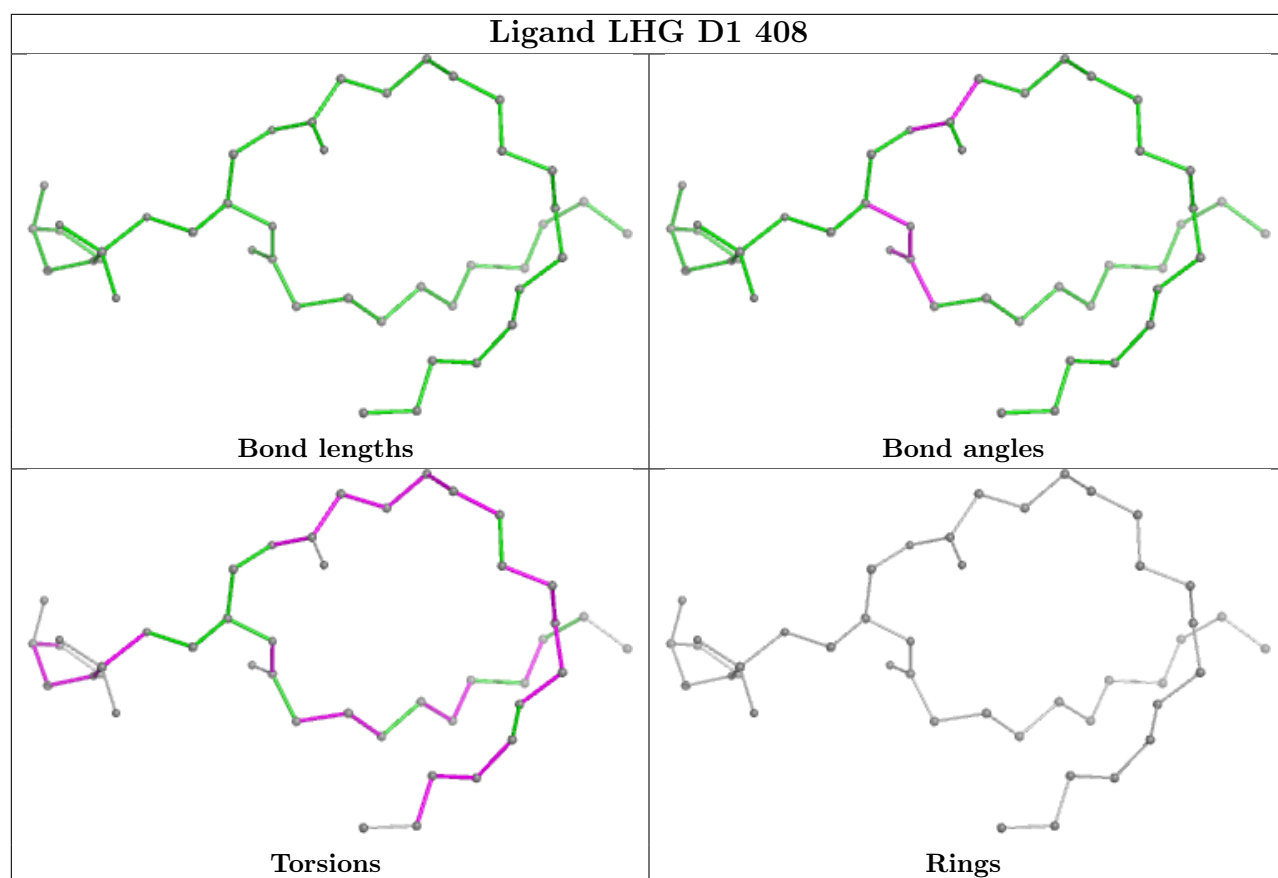




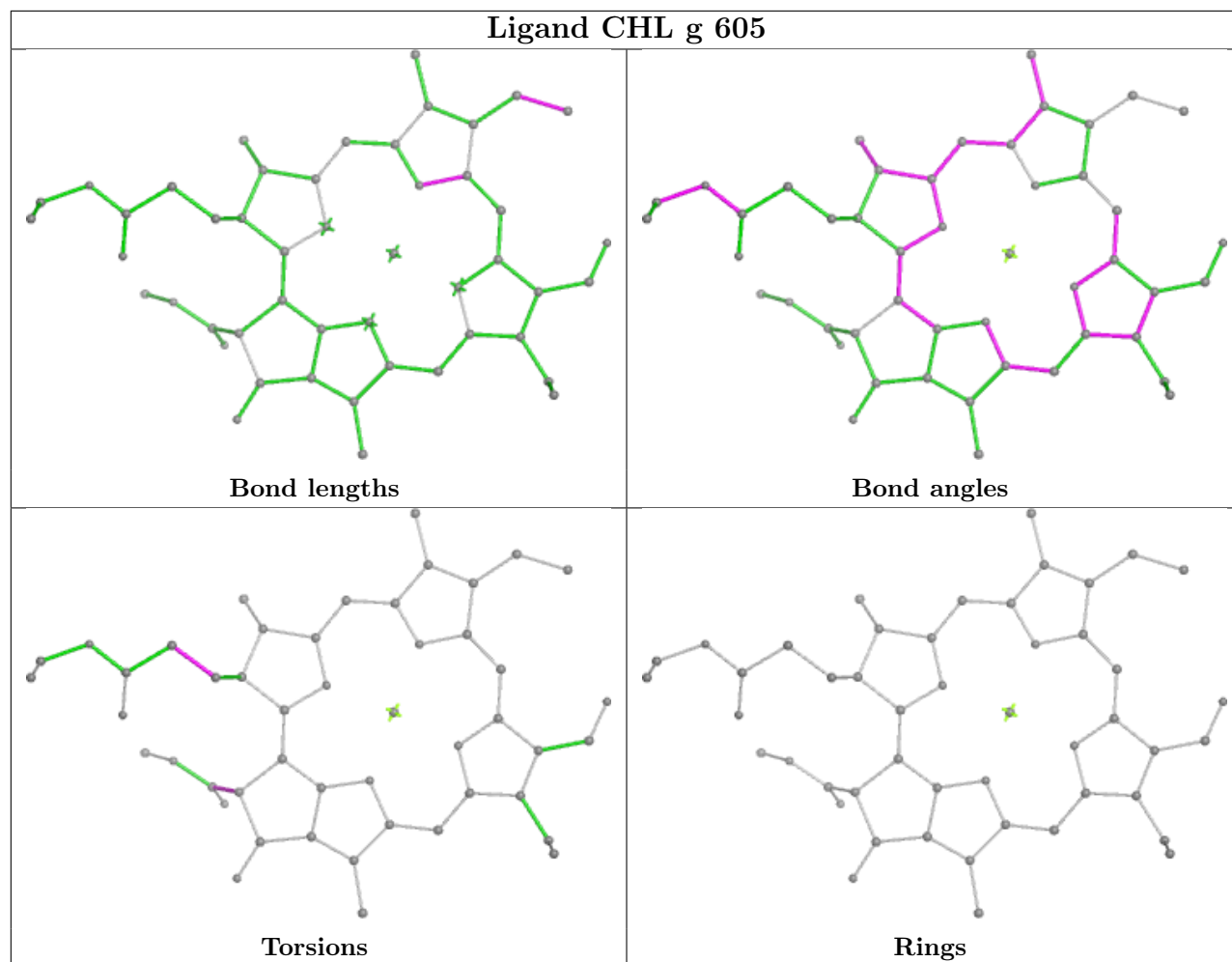


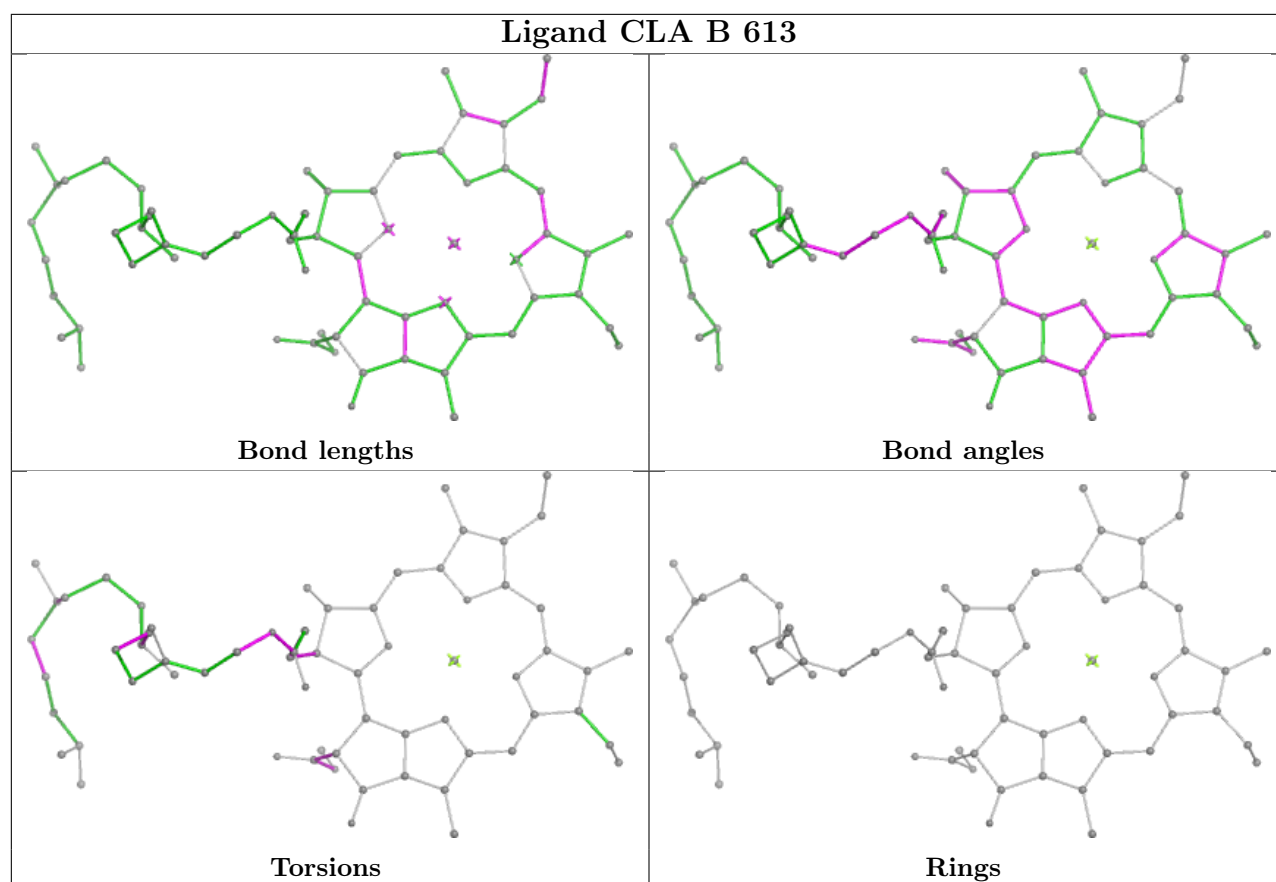


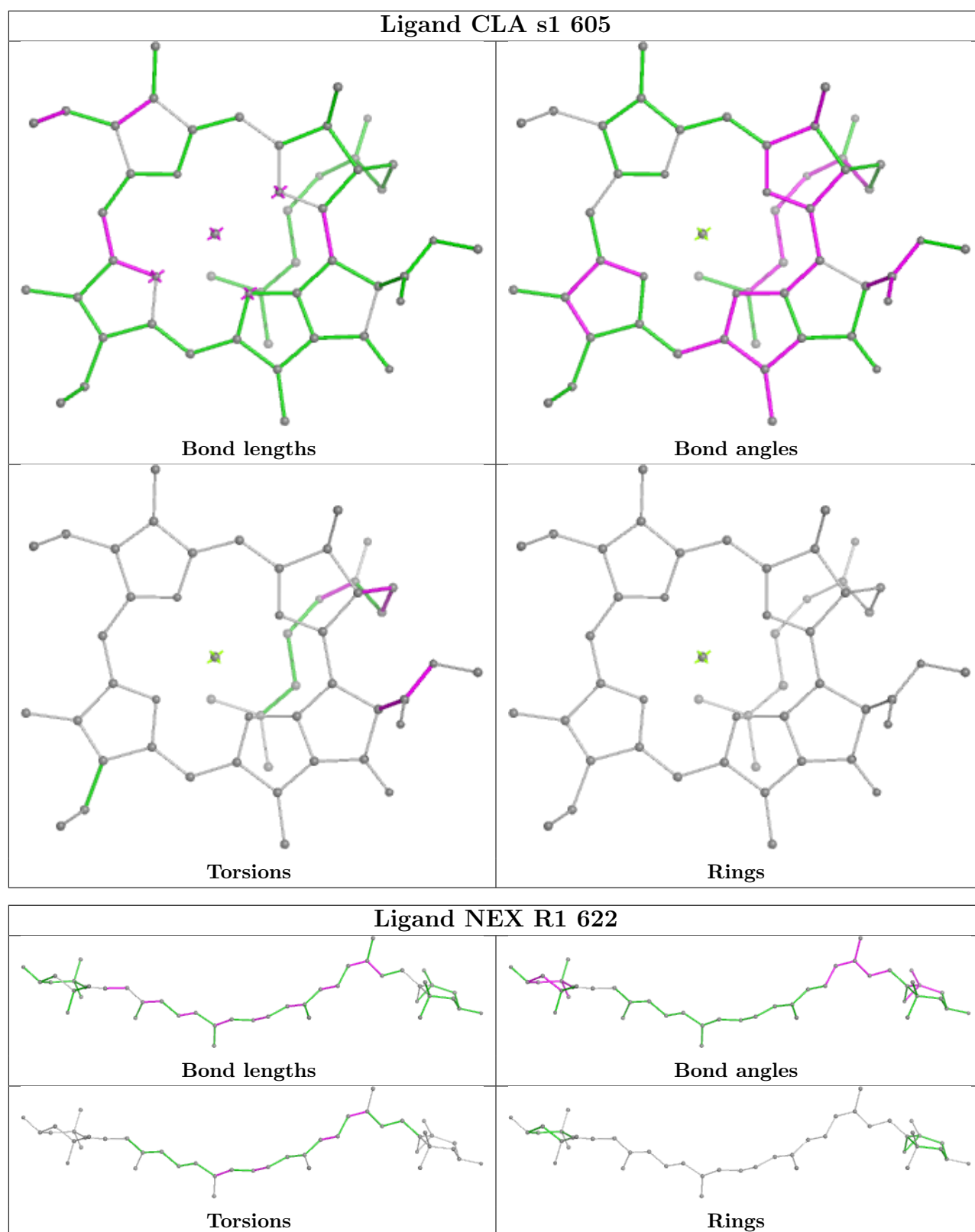




## Ligand CHL g 605

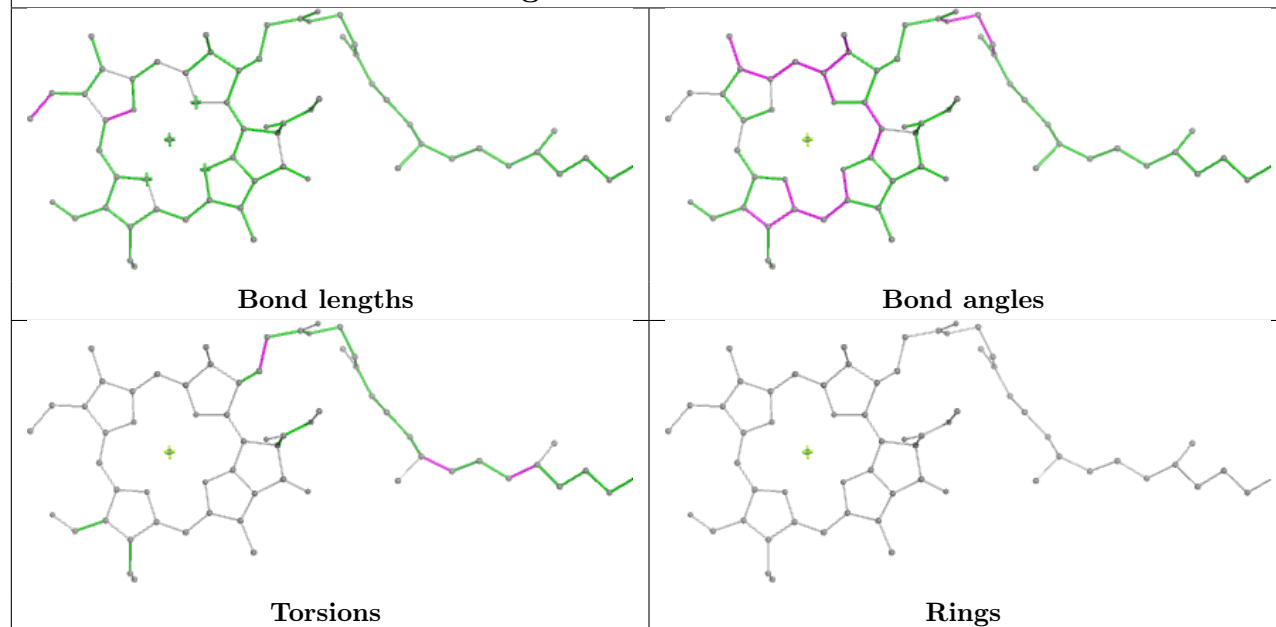




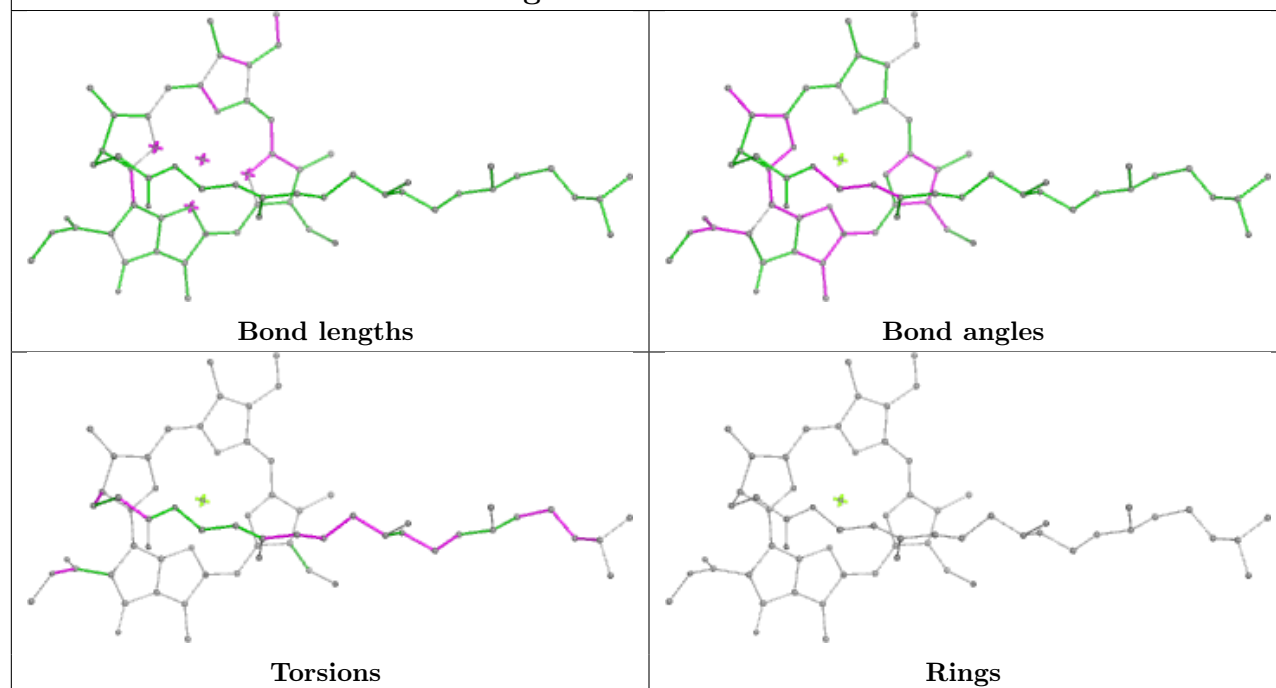


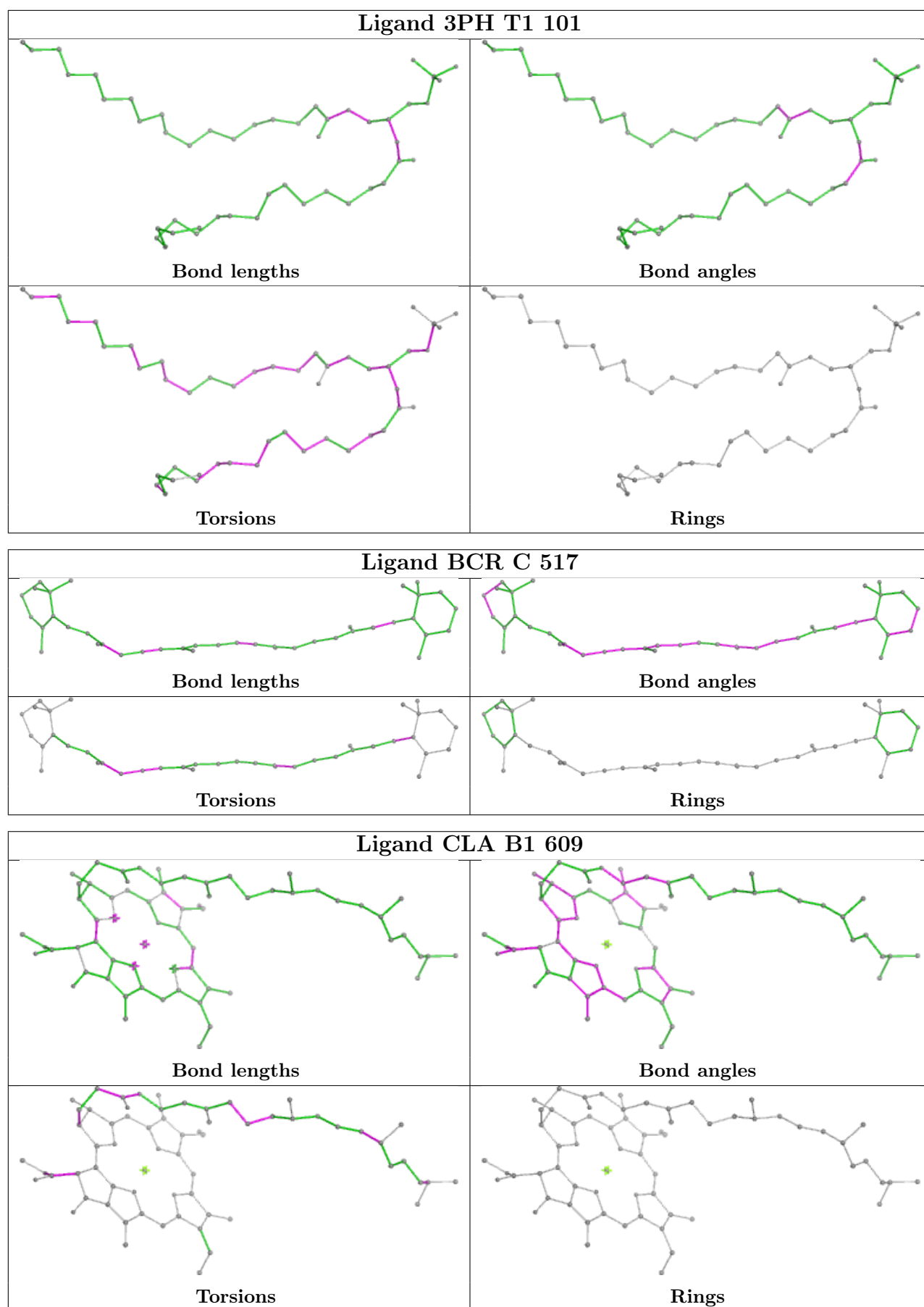


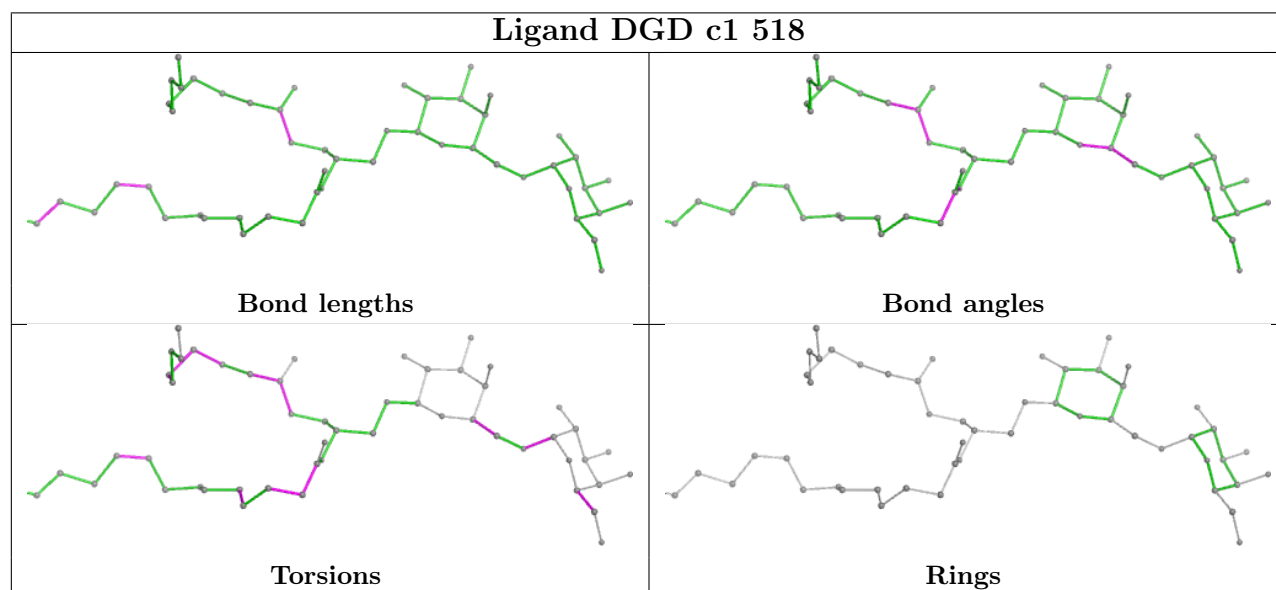
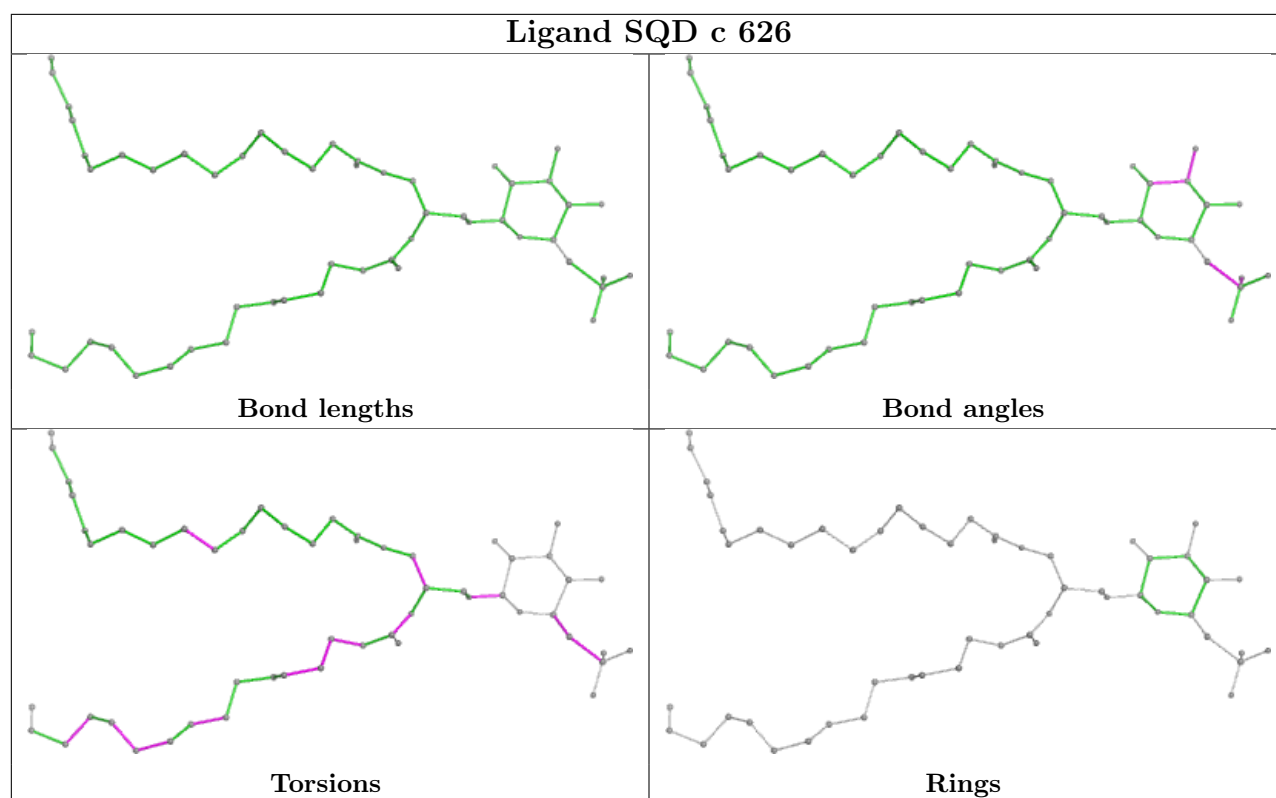
## Ligand CHL N1 605

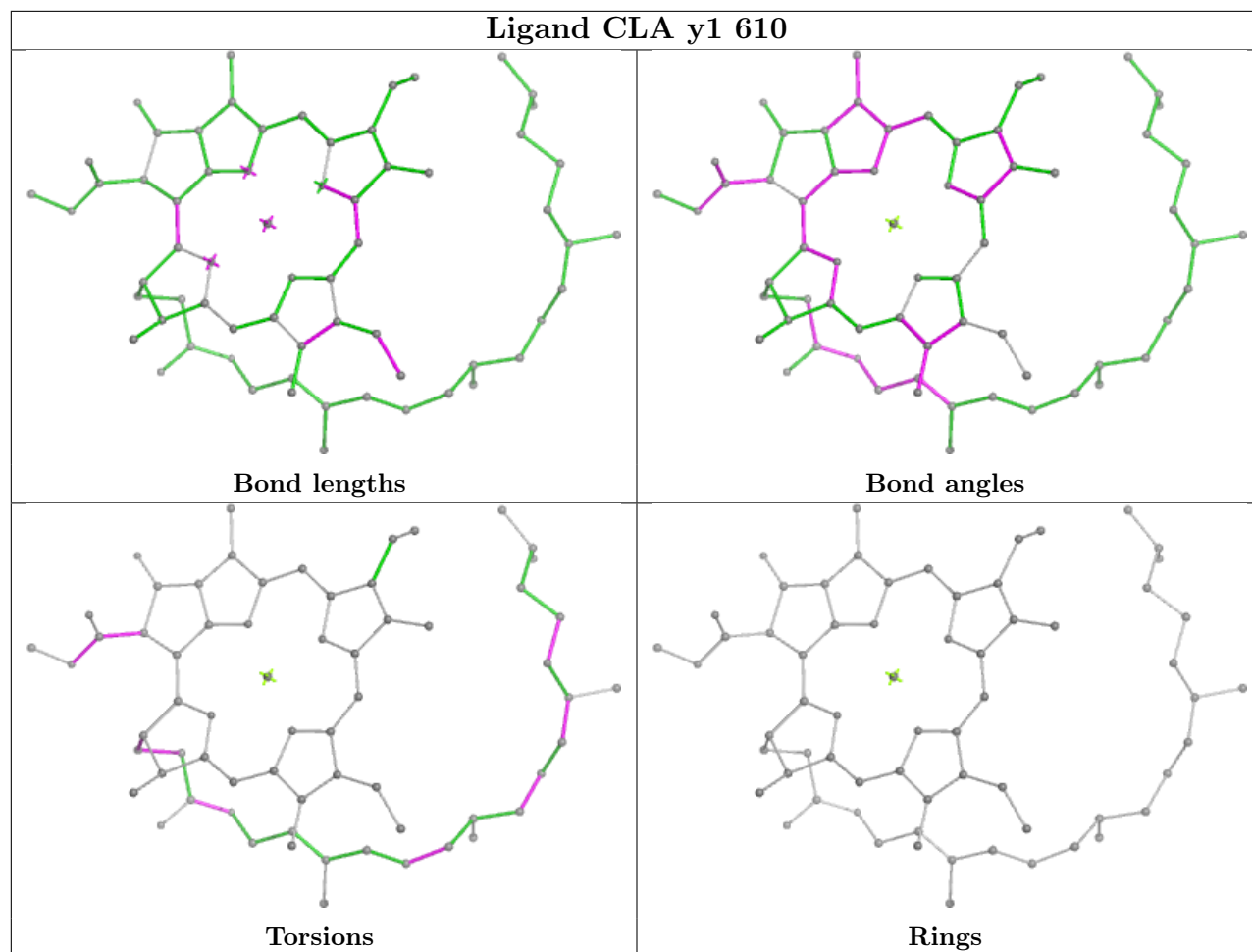


## Ligand CLA B1 615

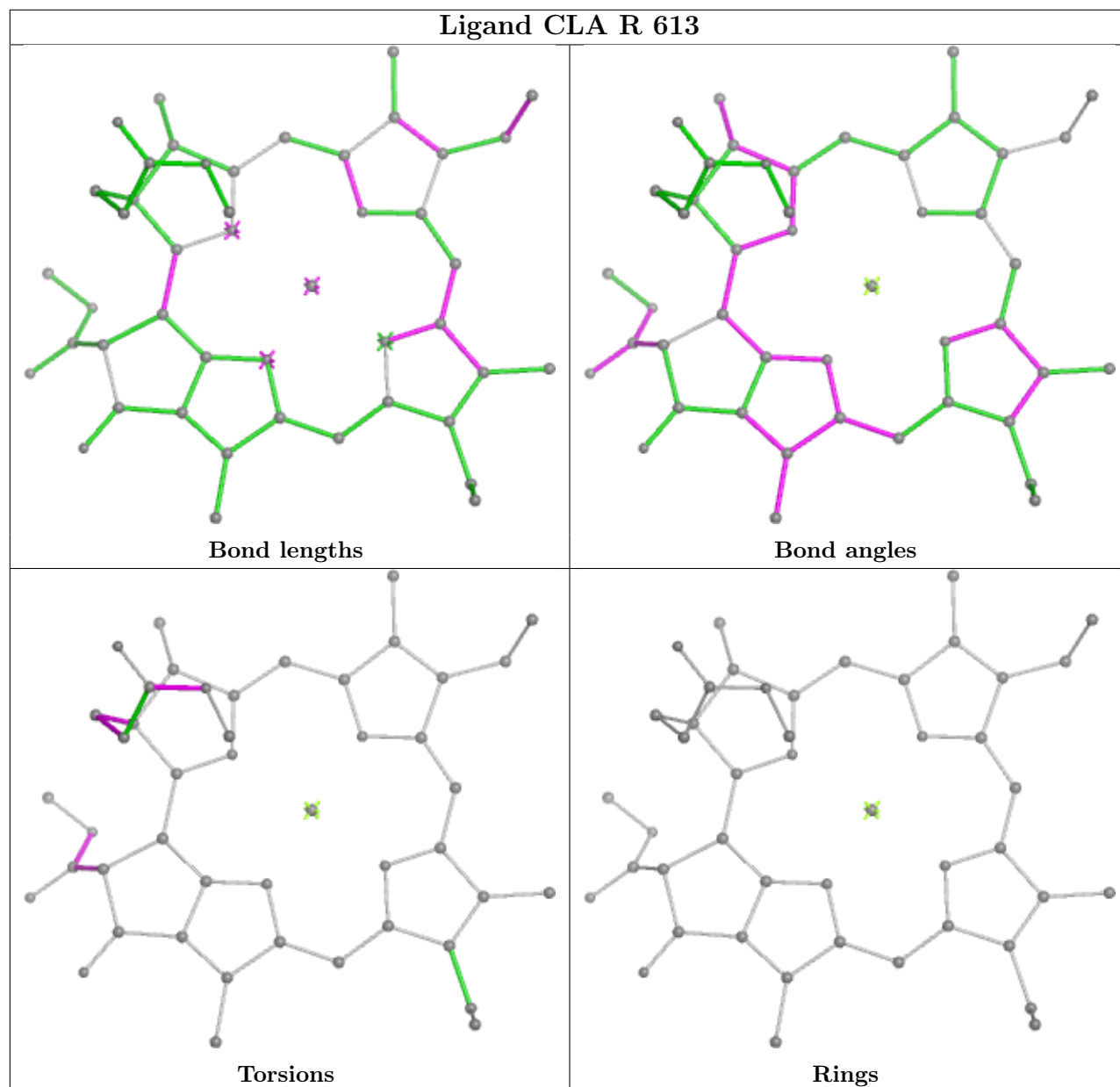


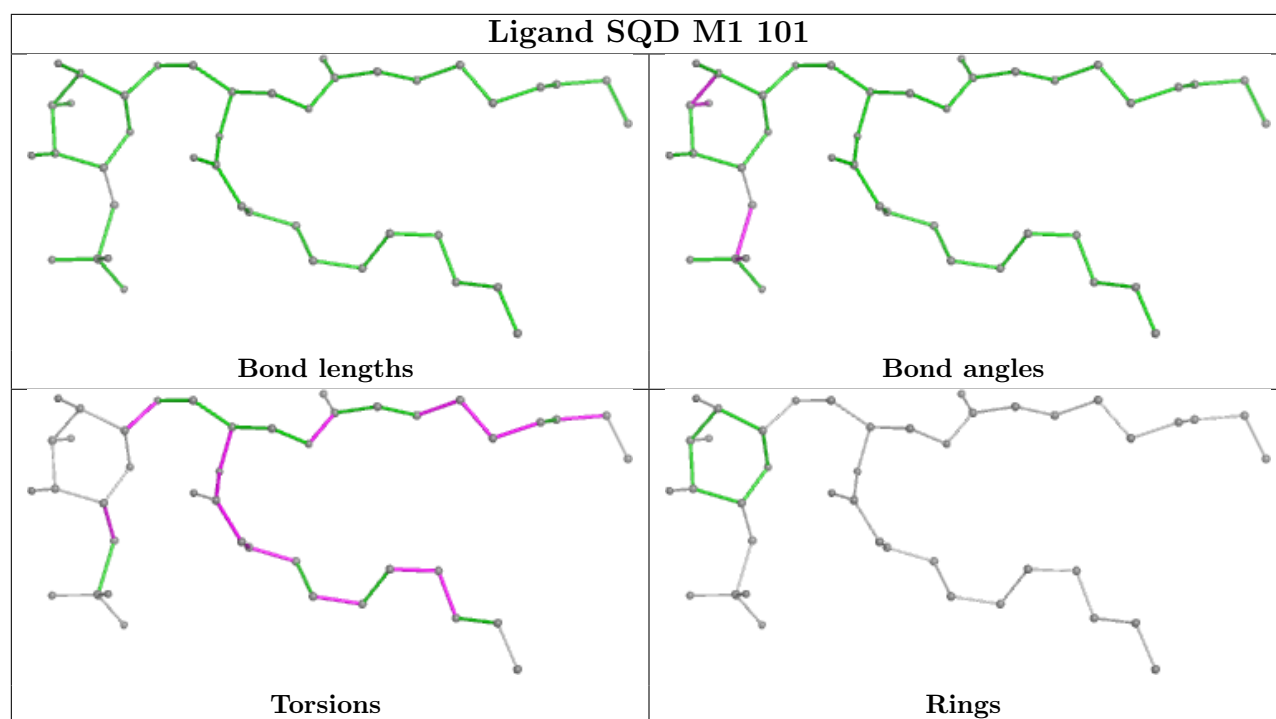


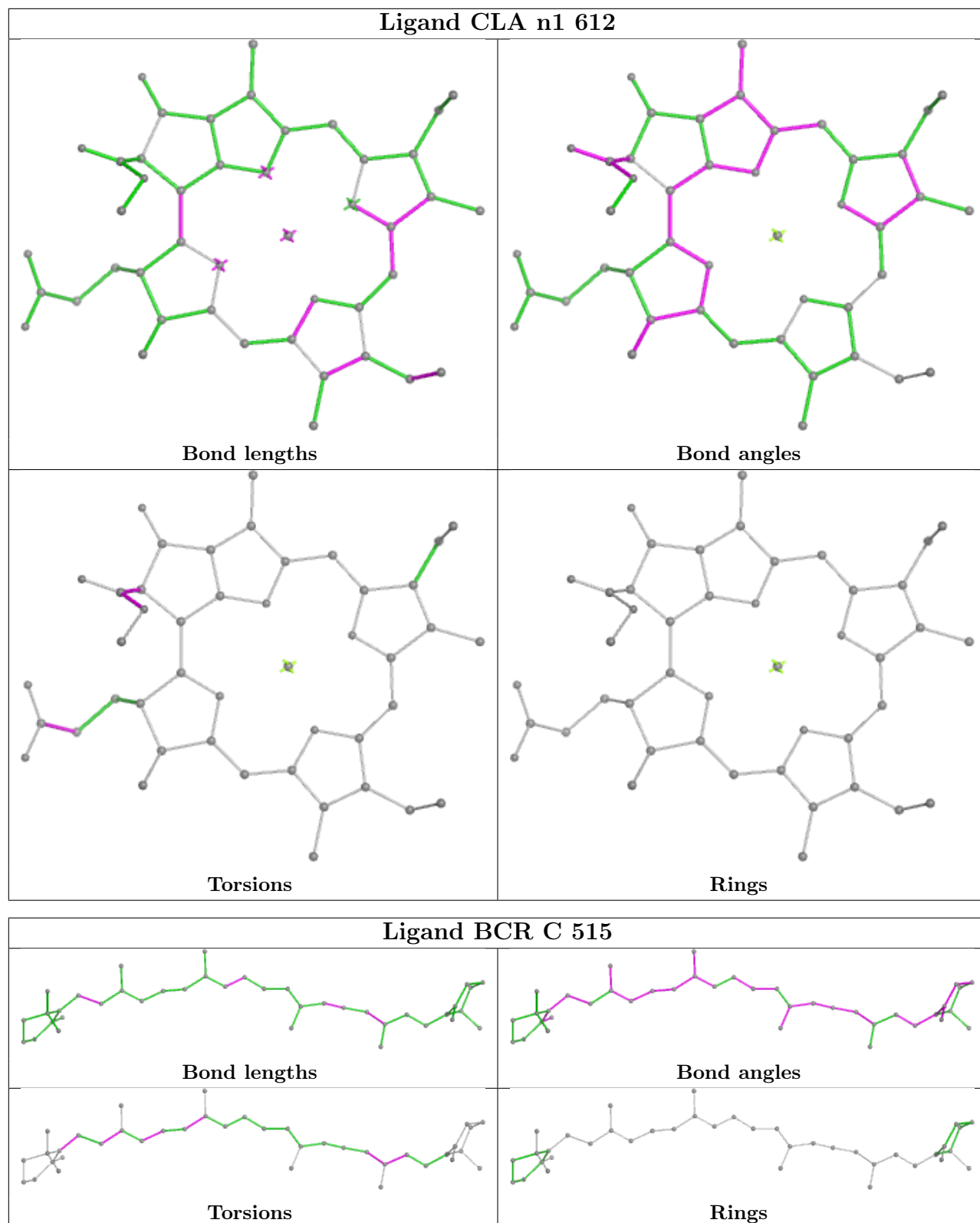


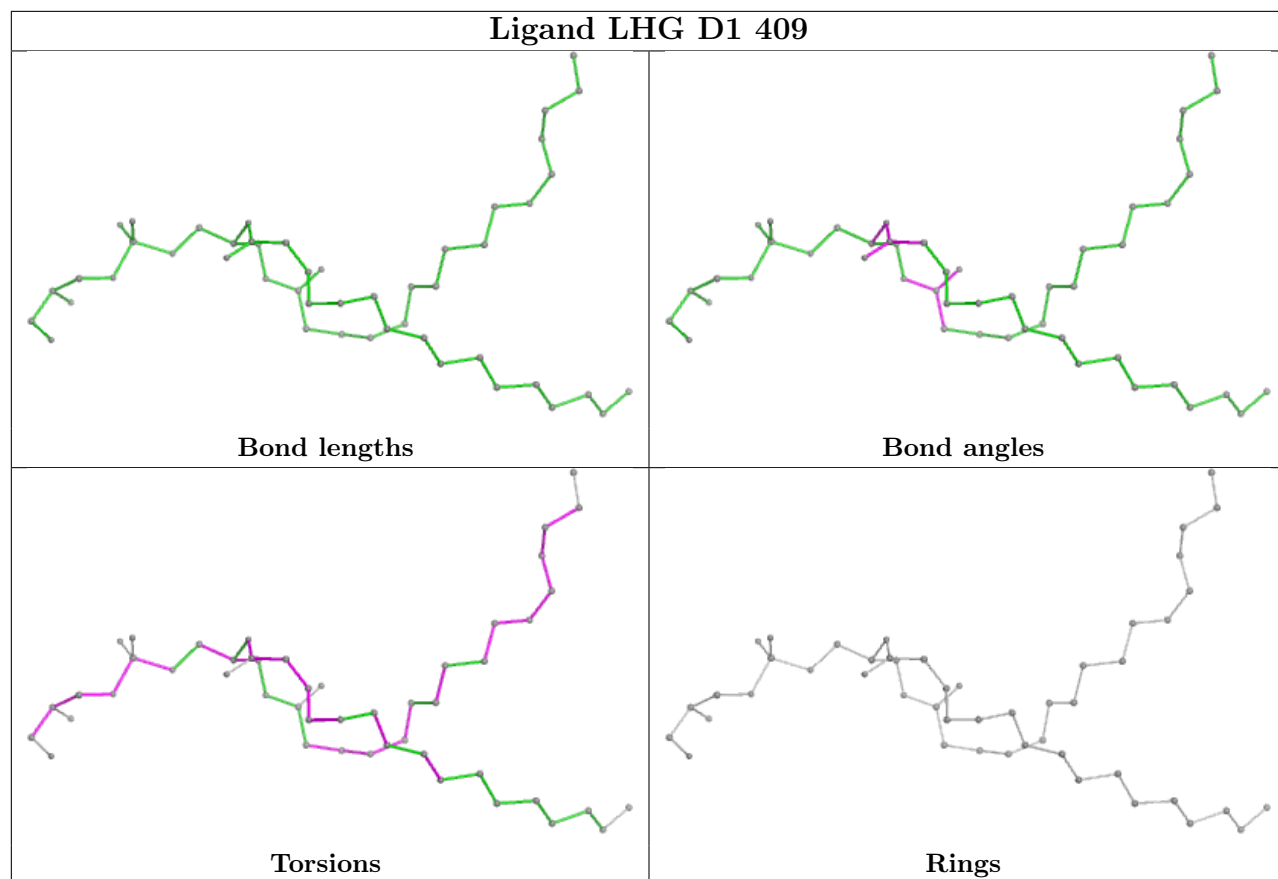


## Ligand CLA R 613

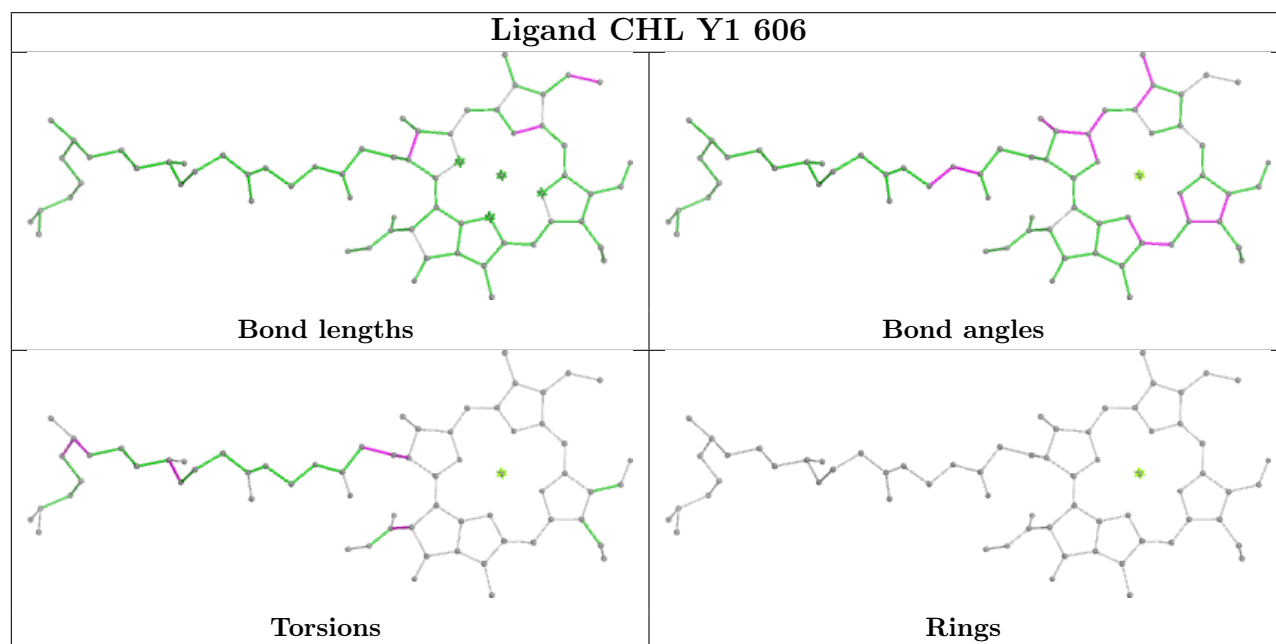
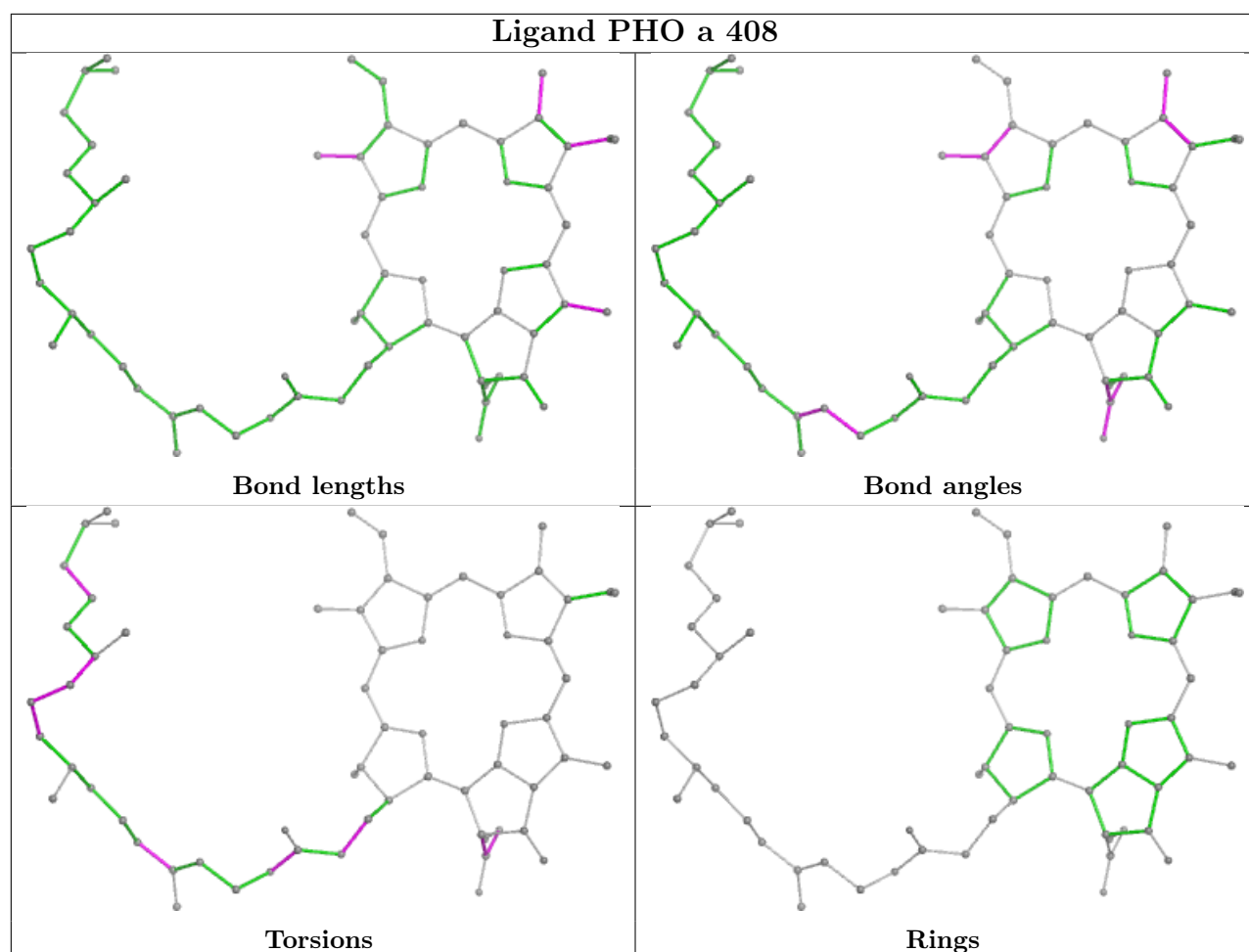


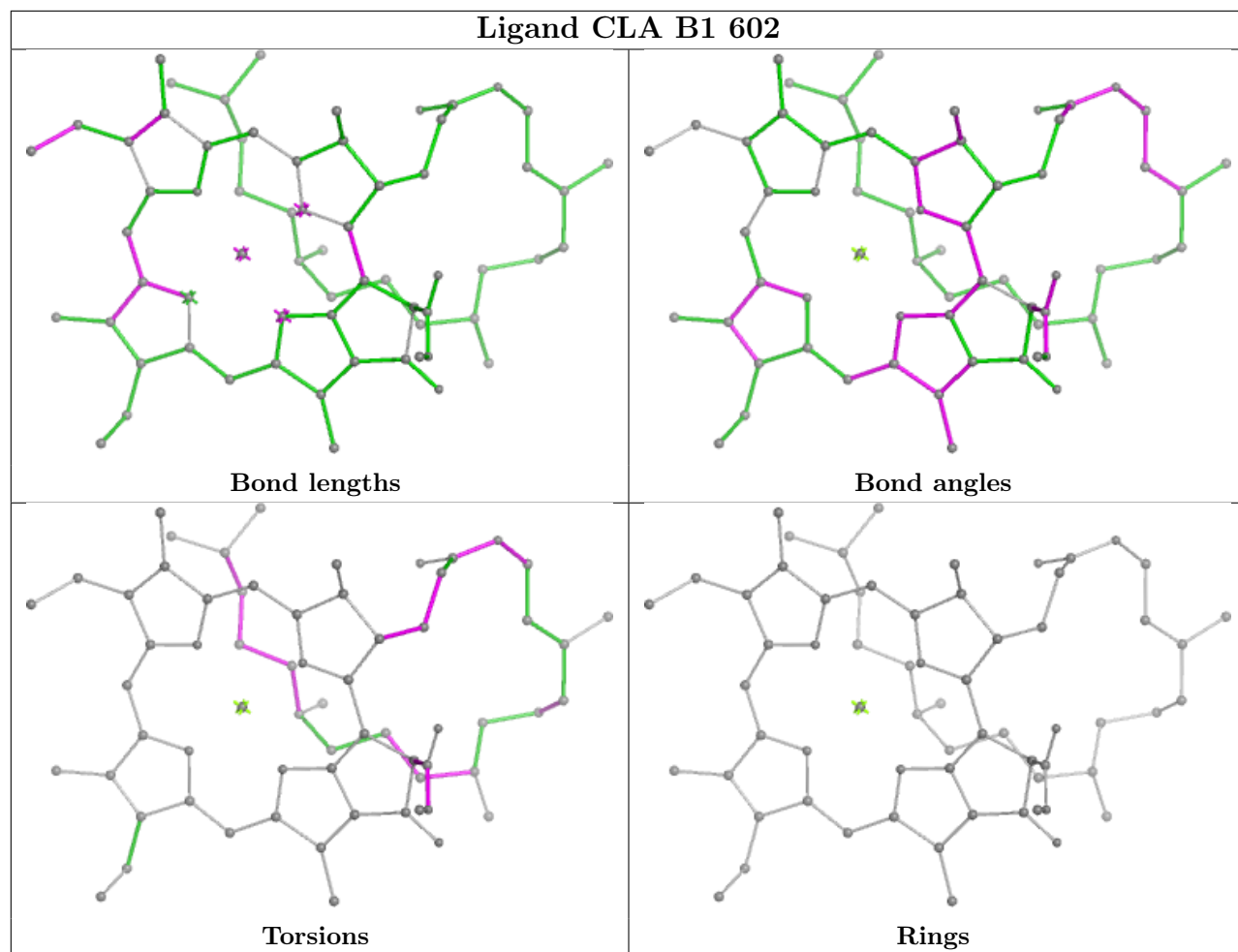




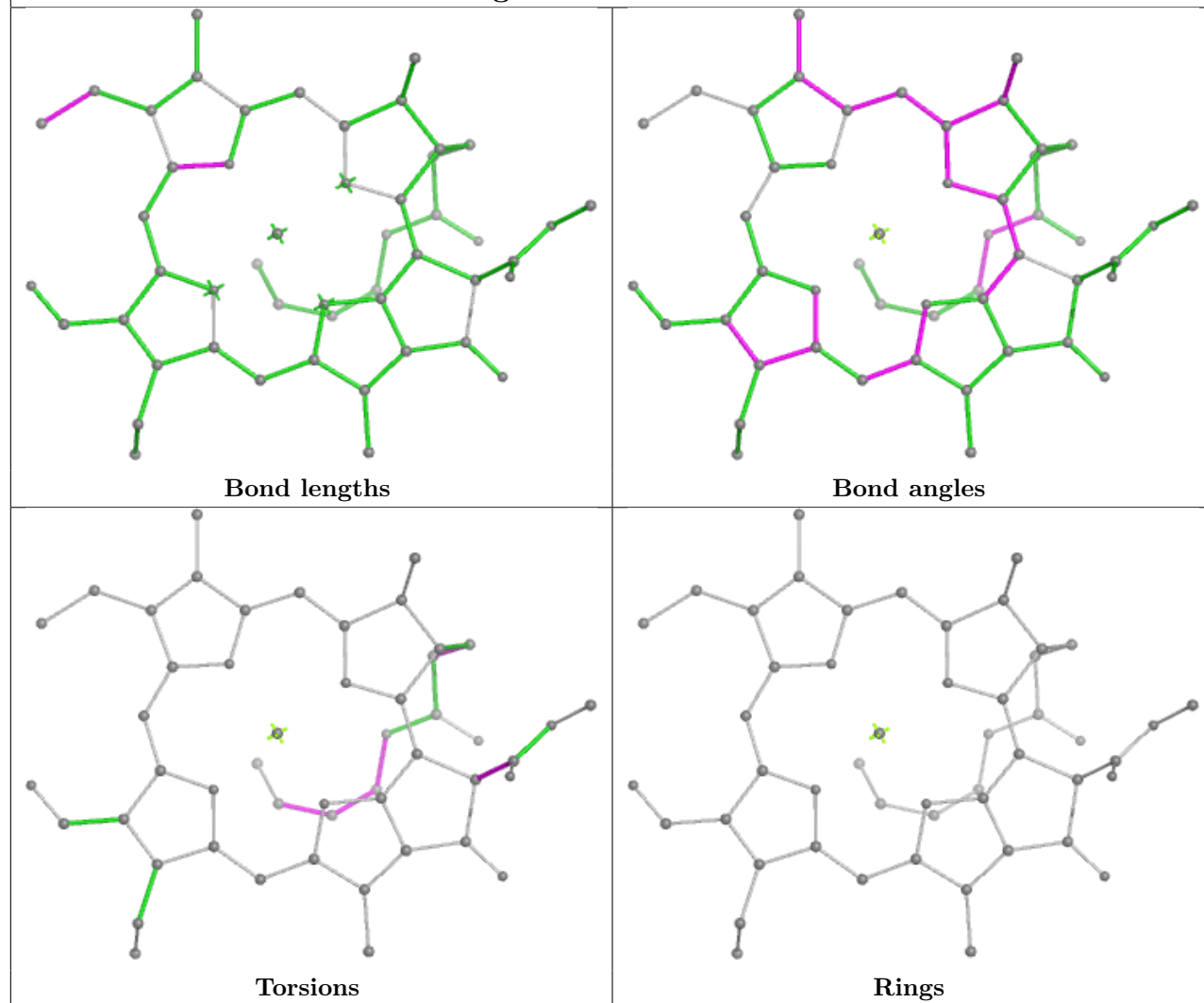


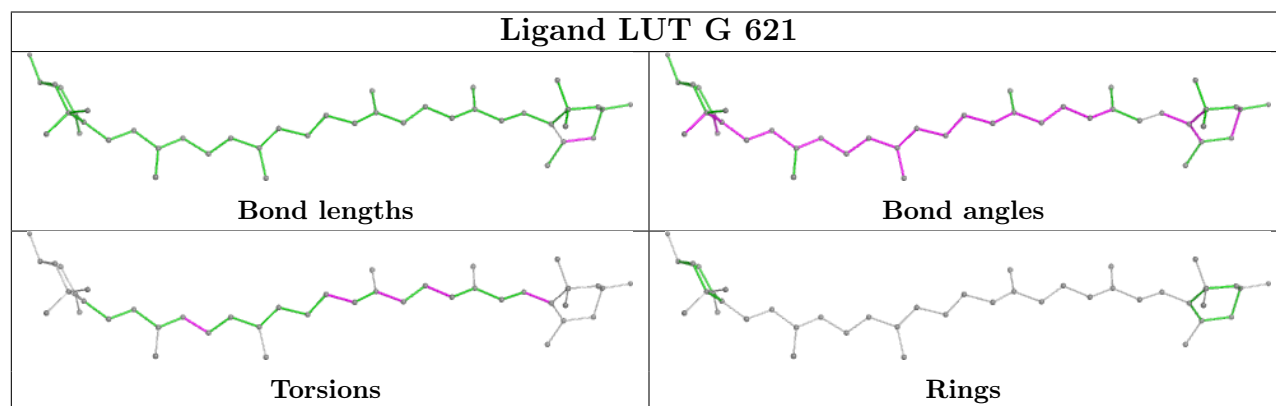
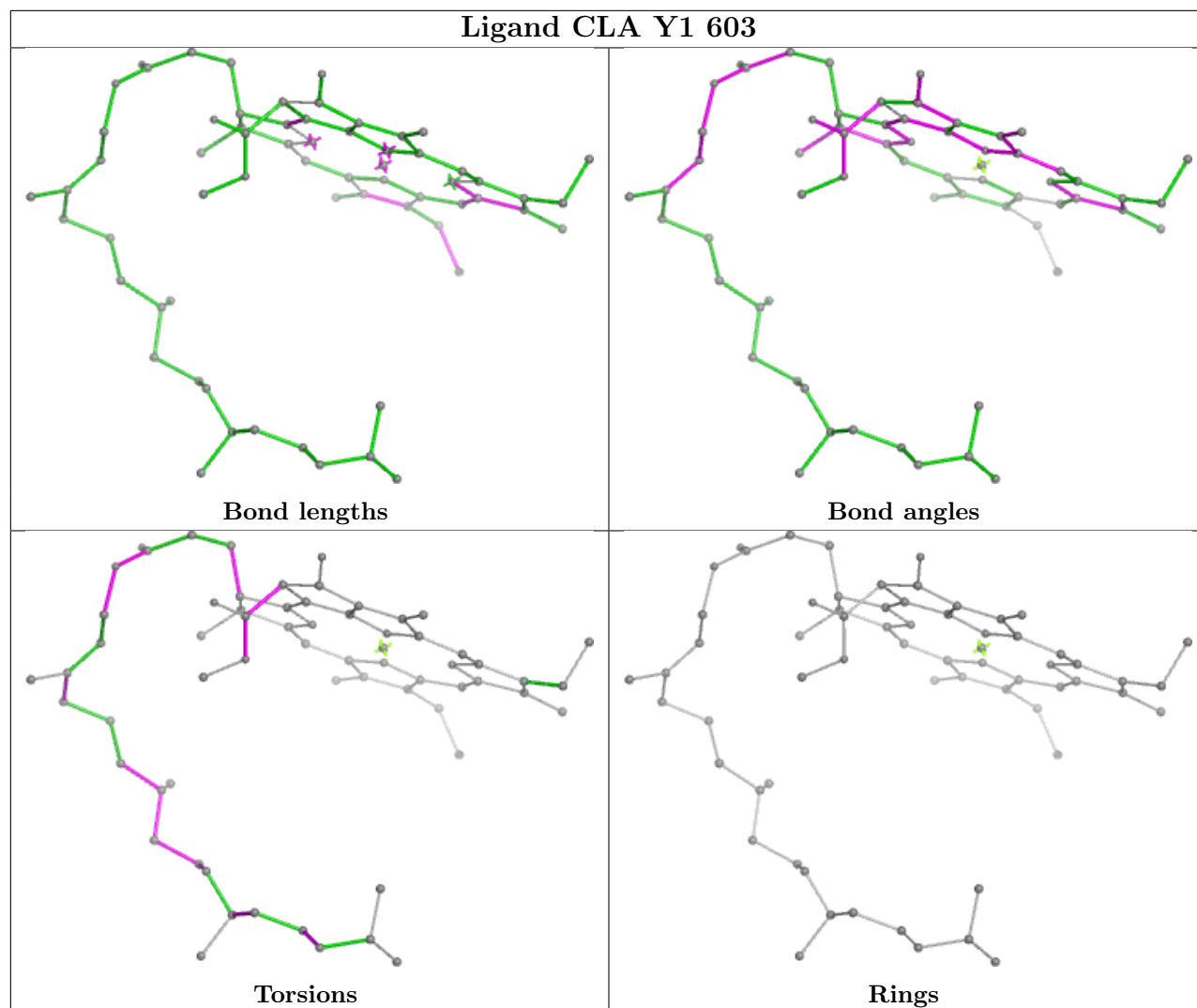


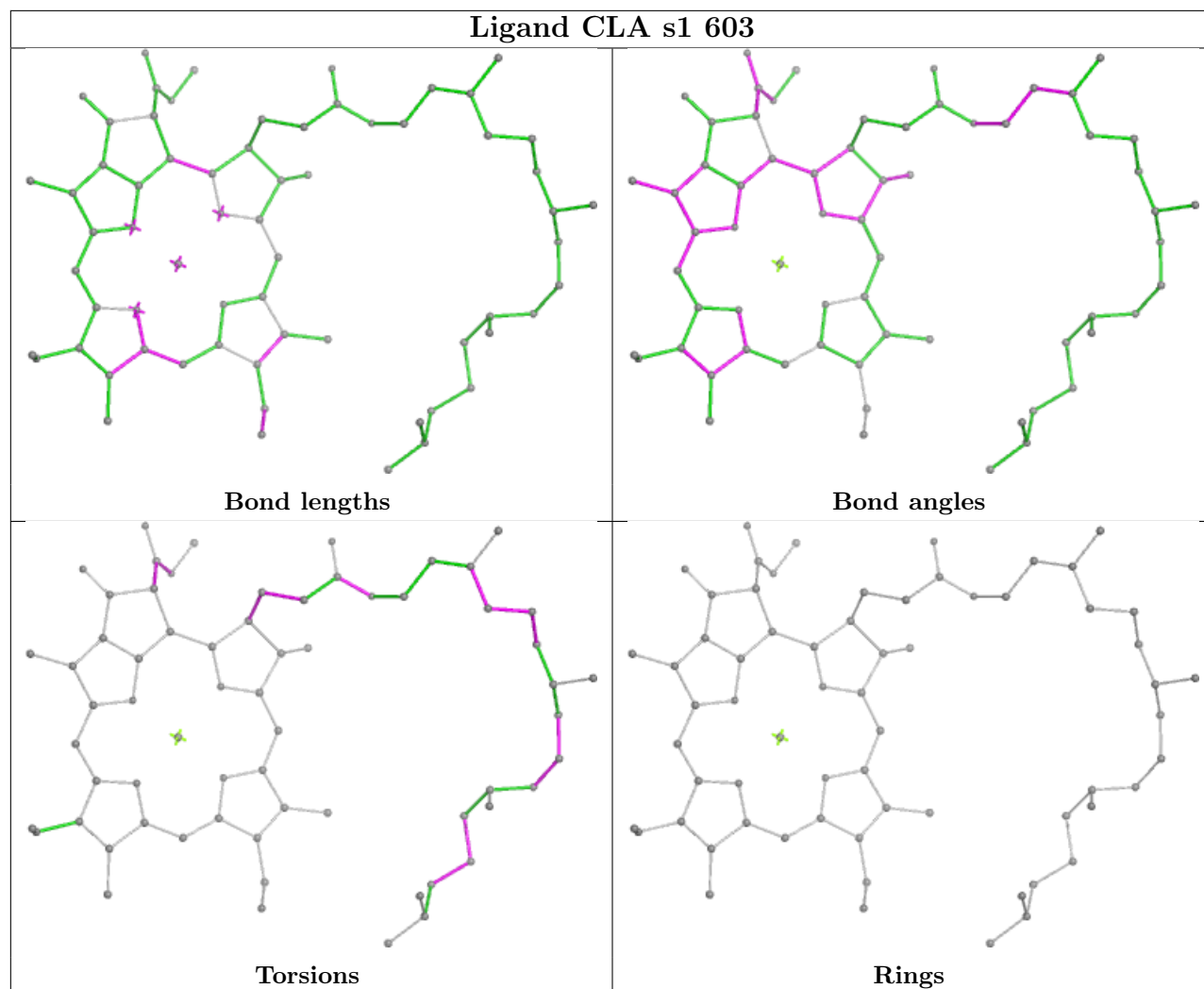


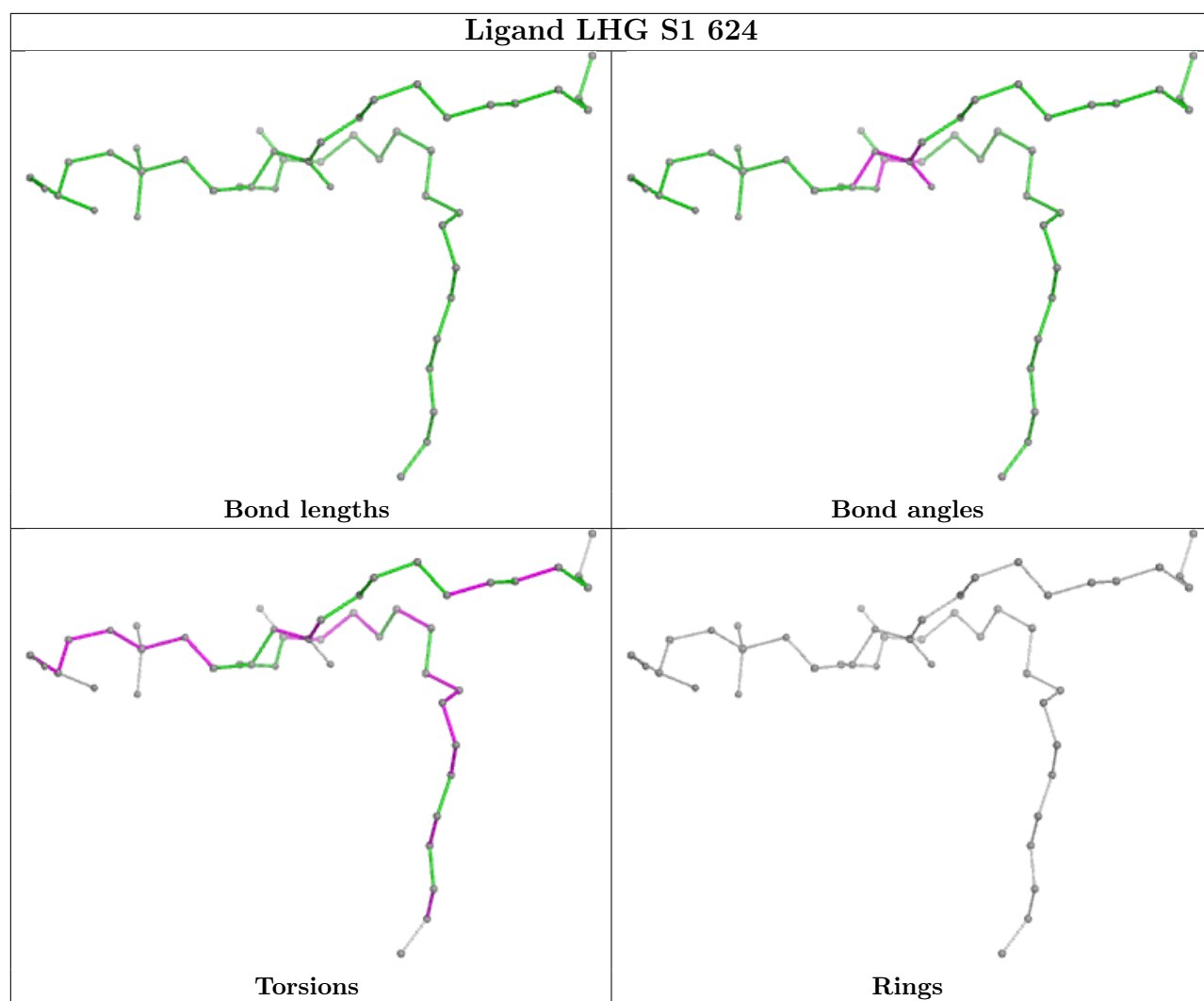


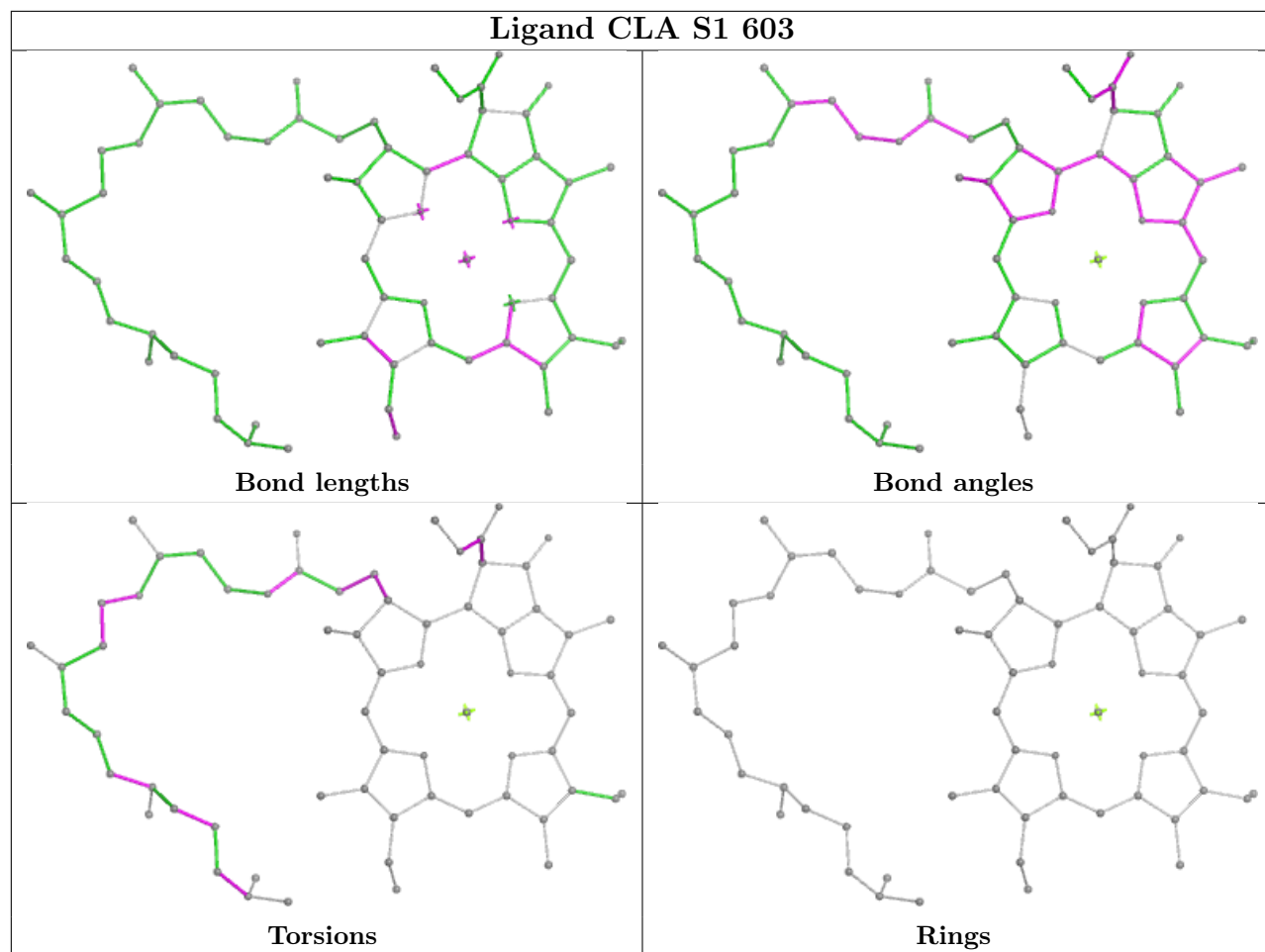
## Ligand CHL R1 607



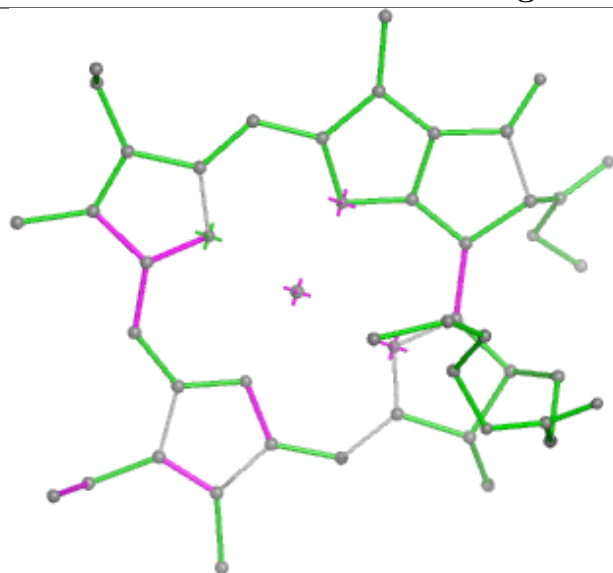




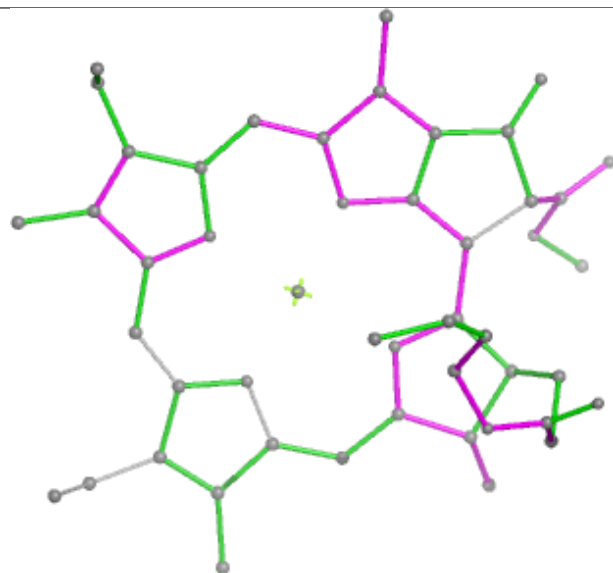




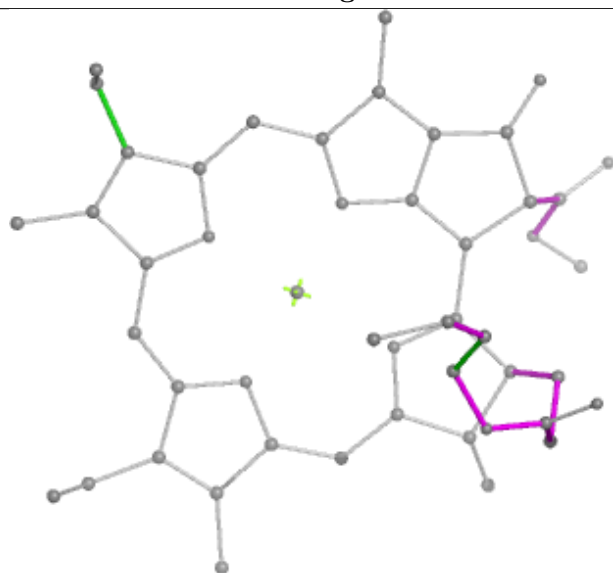
## Ligand CLA n 611



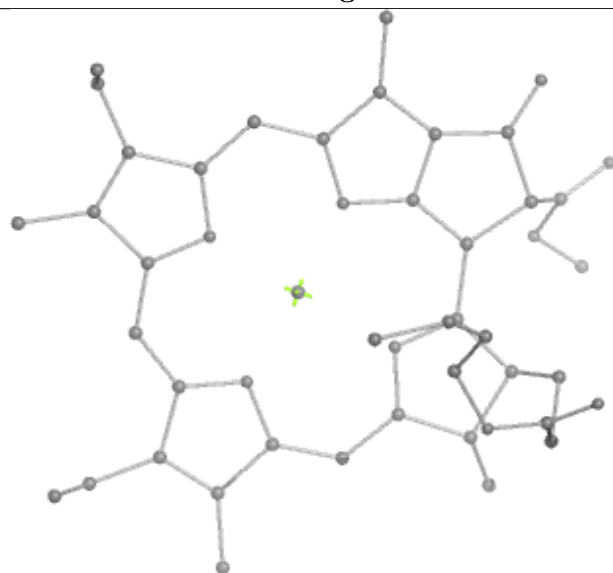
Bond lengths



Bond angles

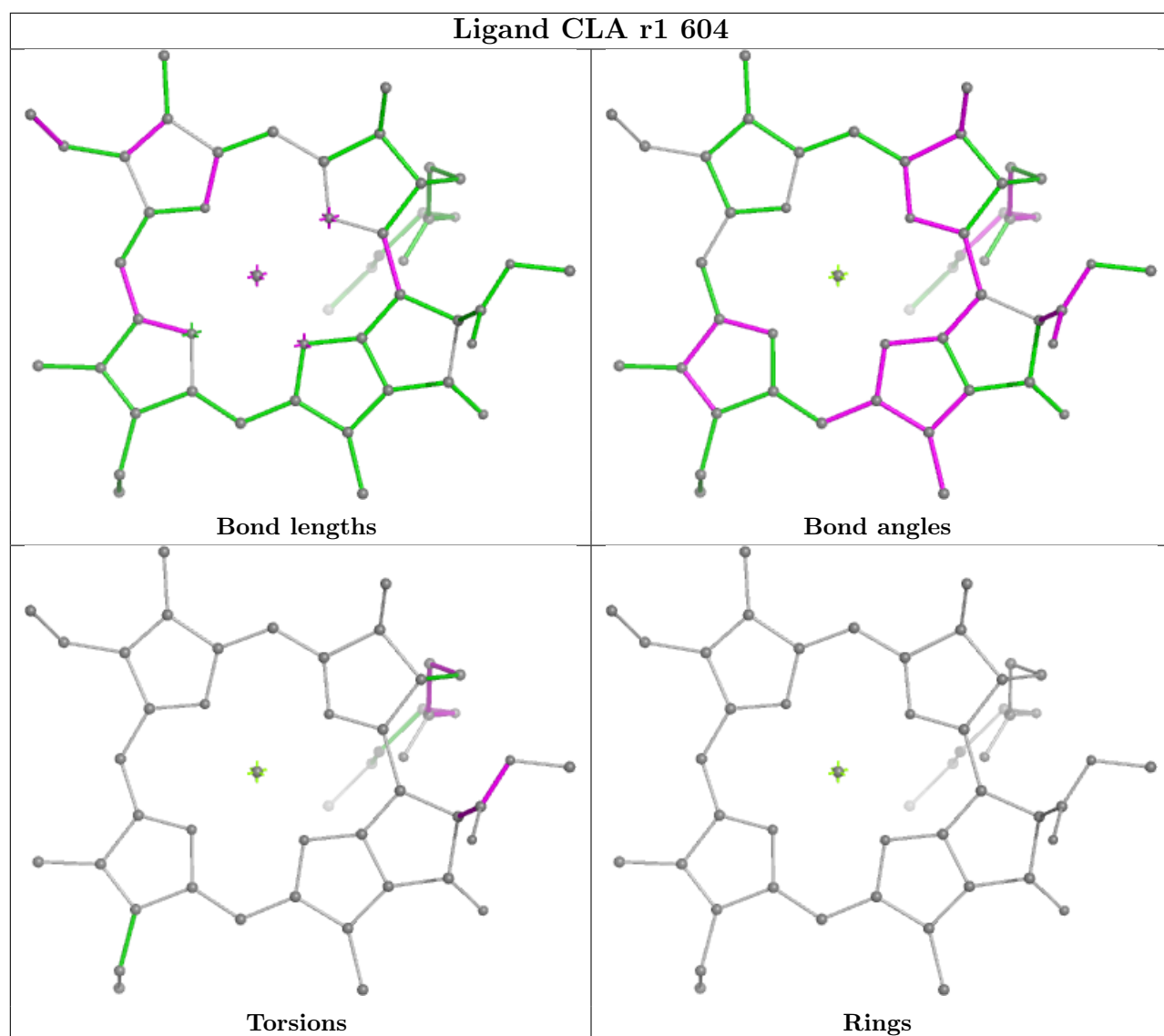


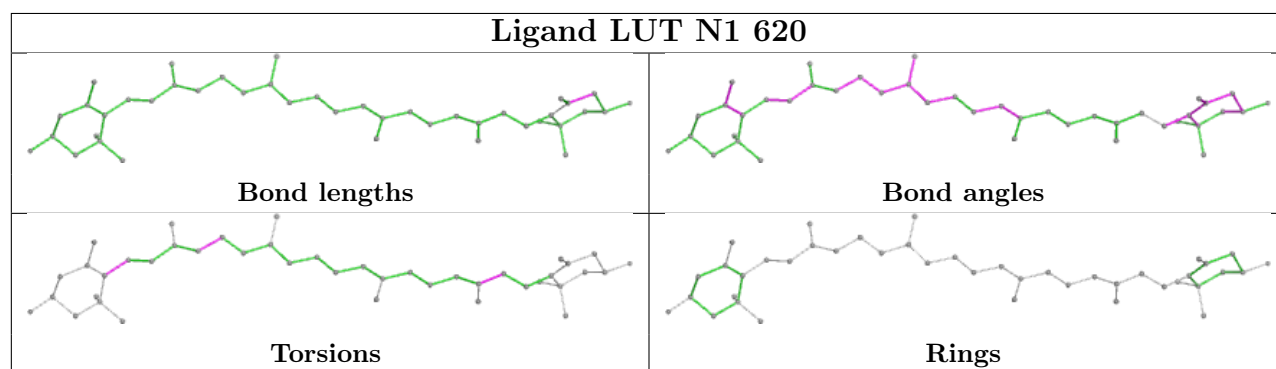
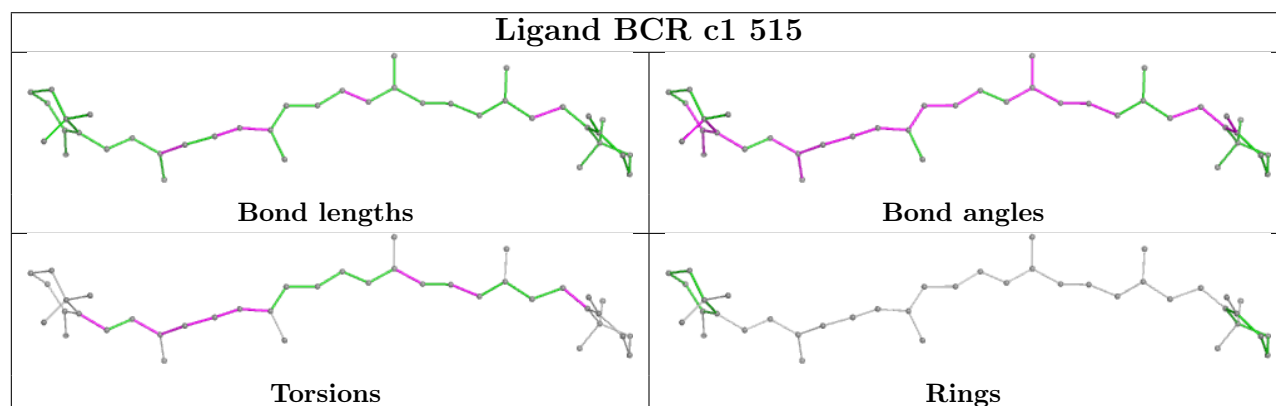
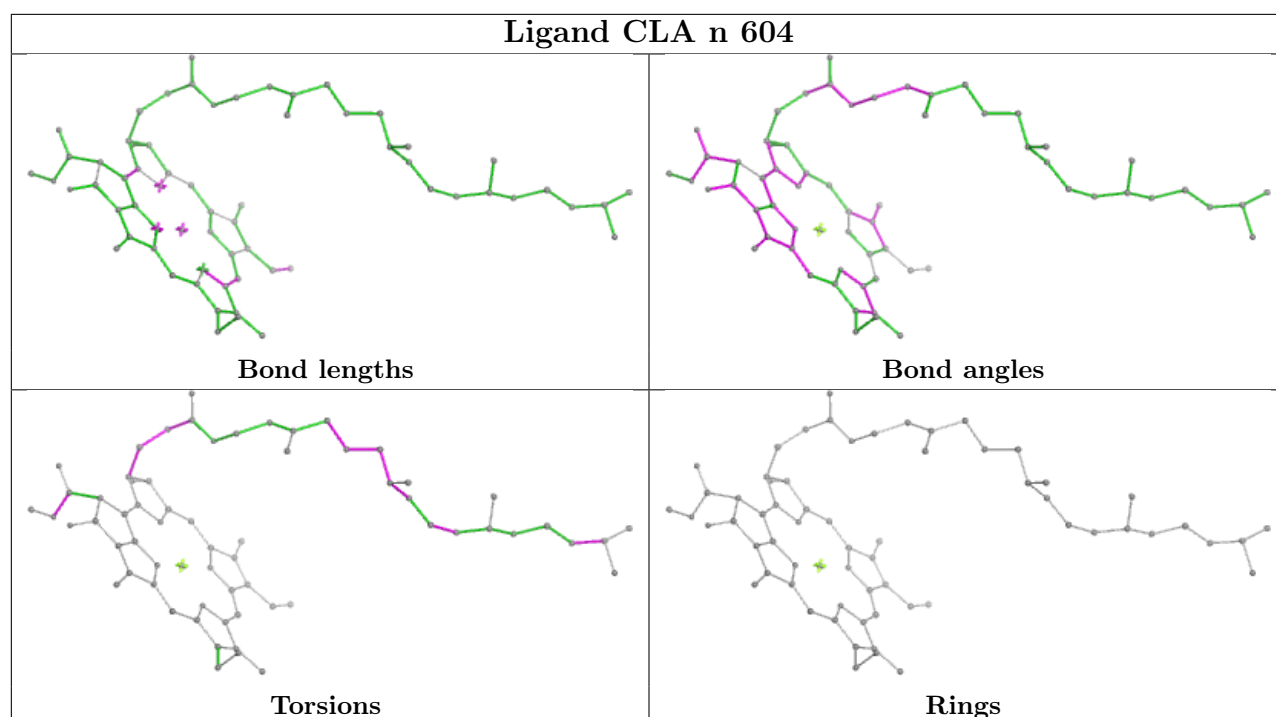
Torsions



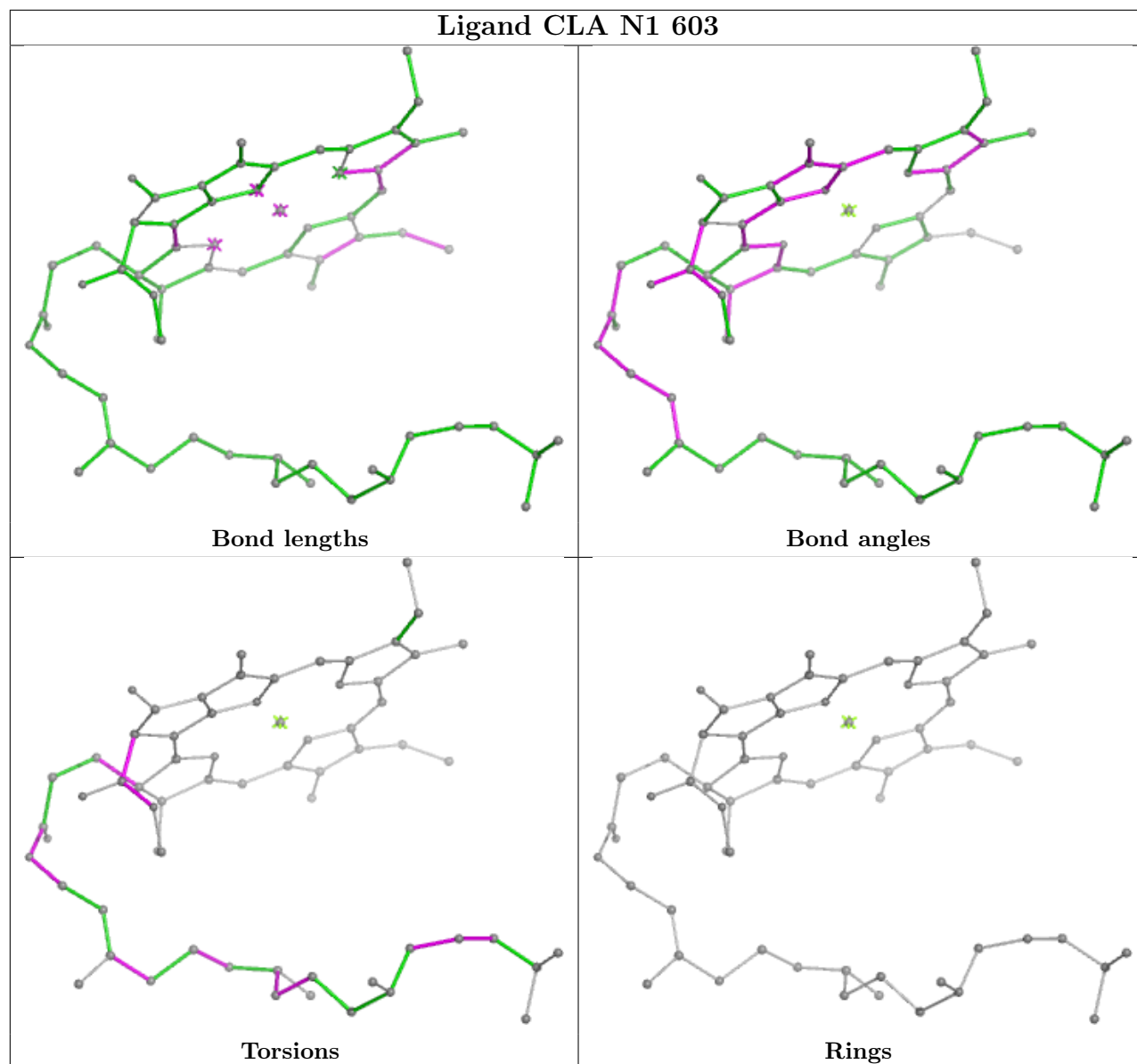
Rings

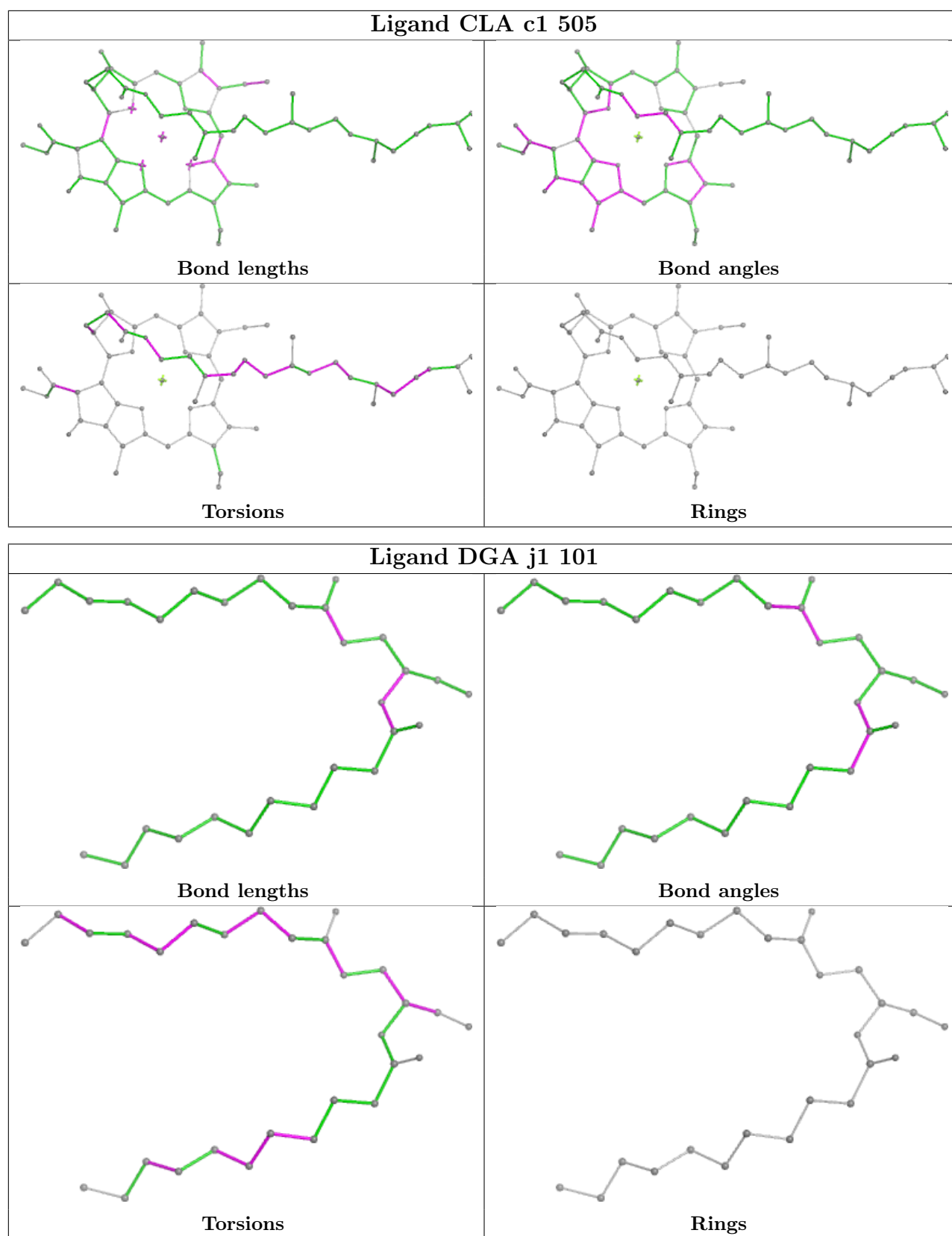


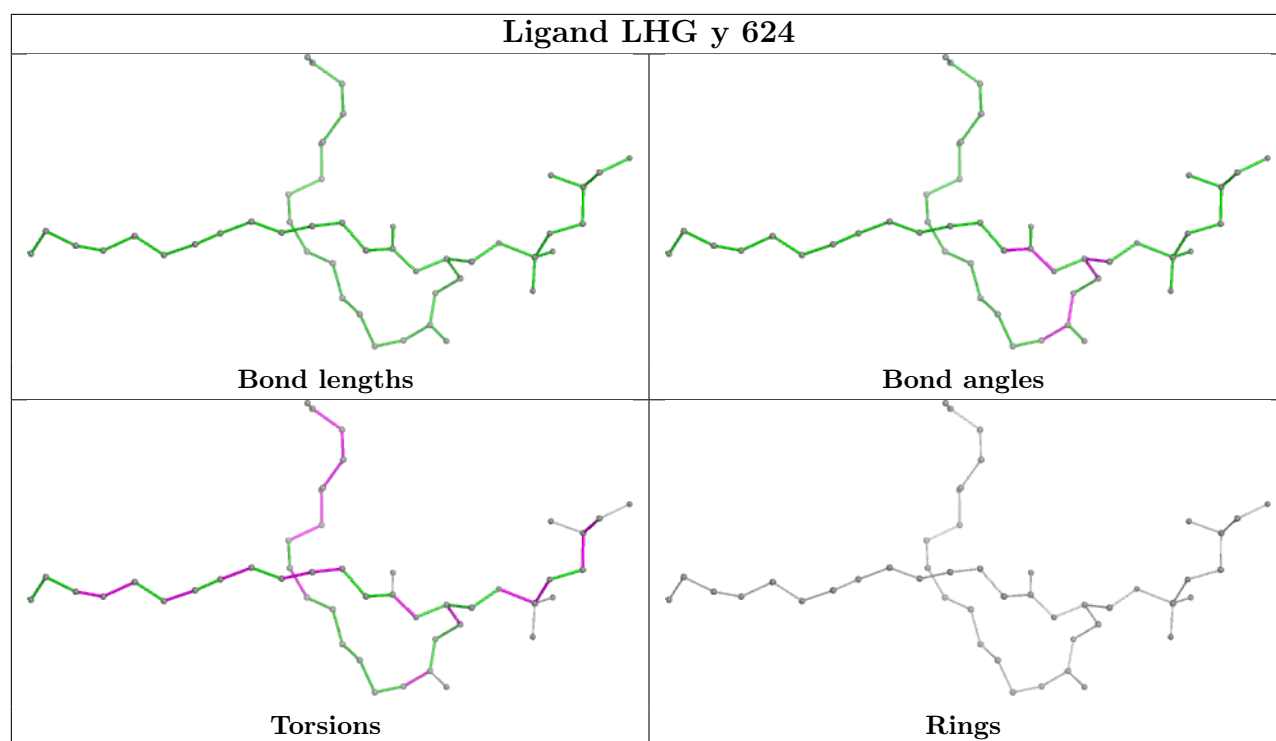


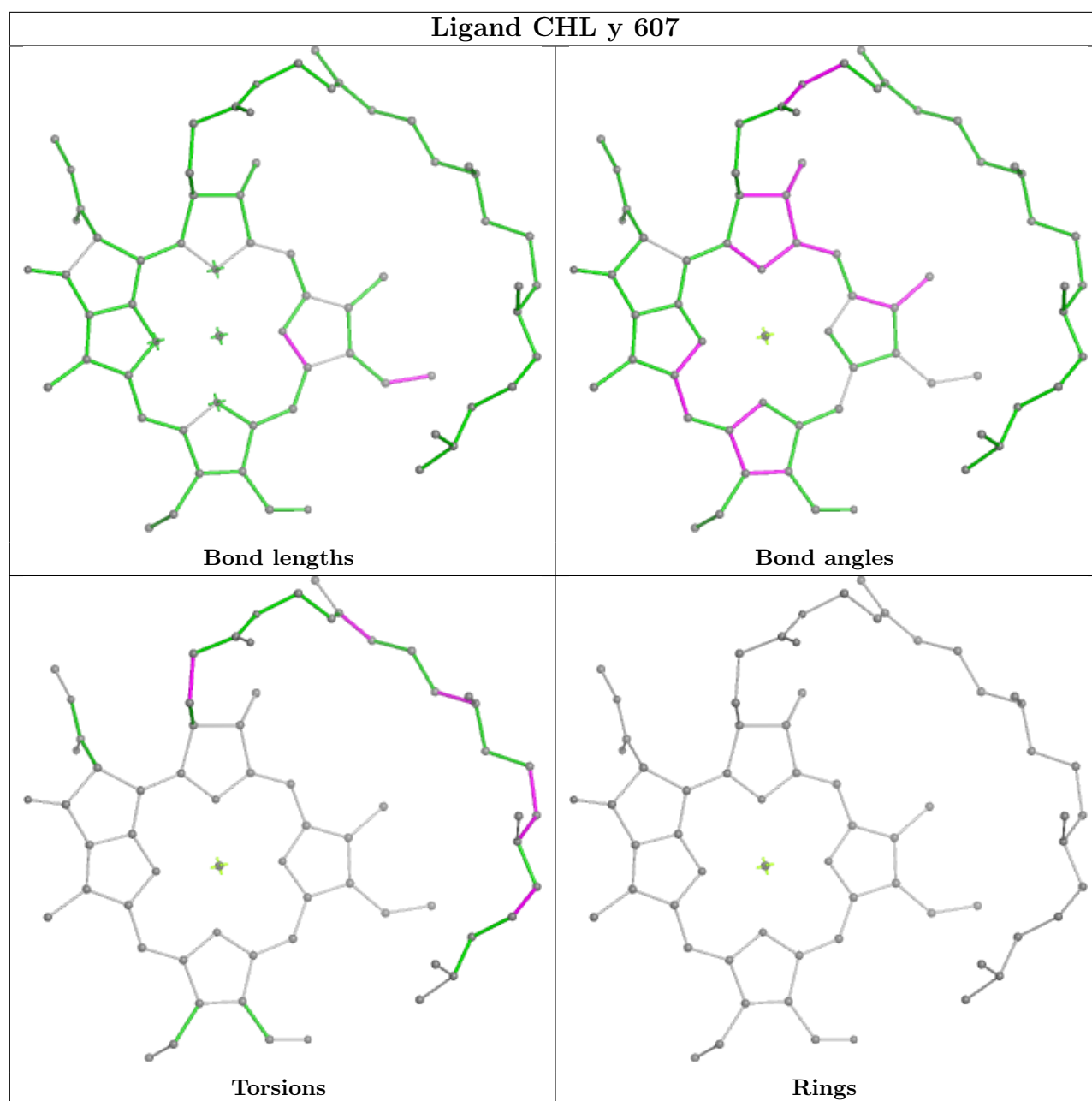


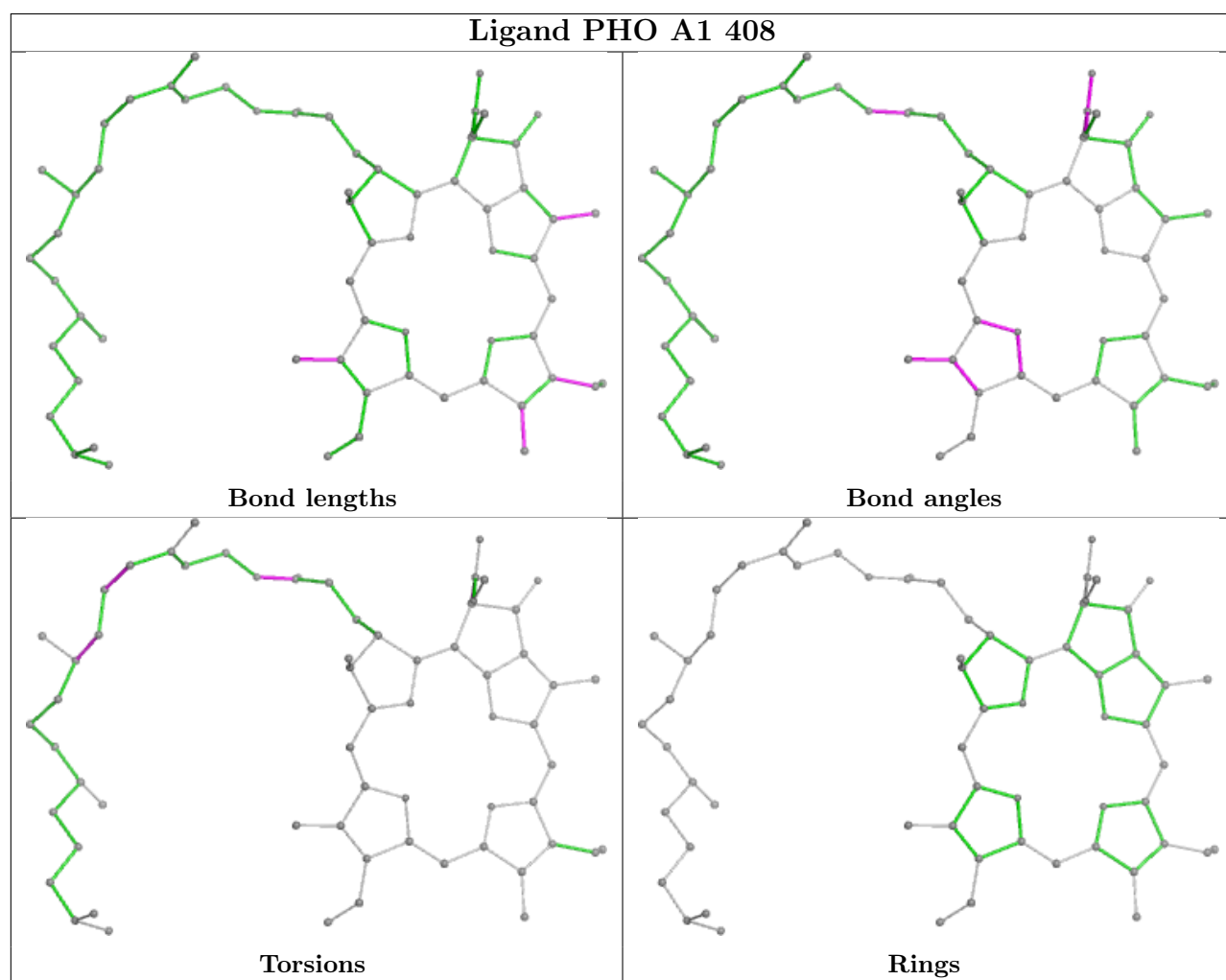
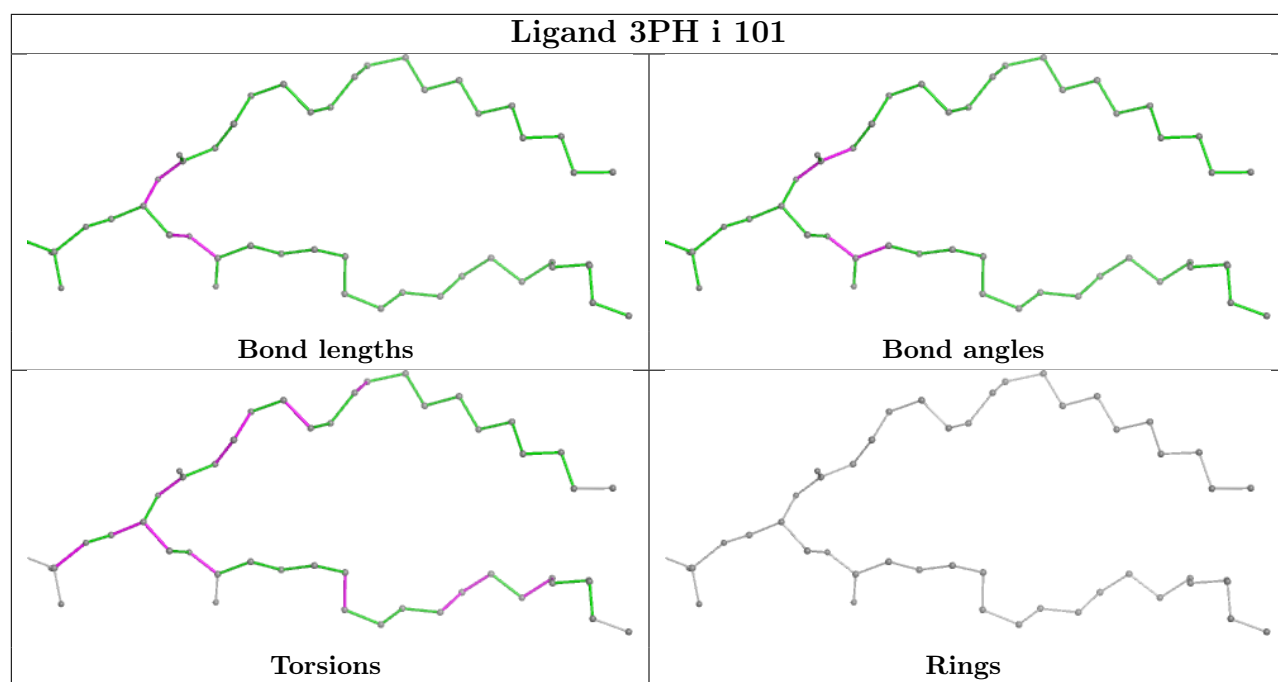
## Ligand CLA N1 603

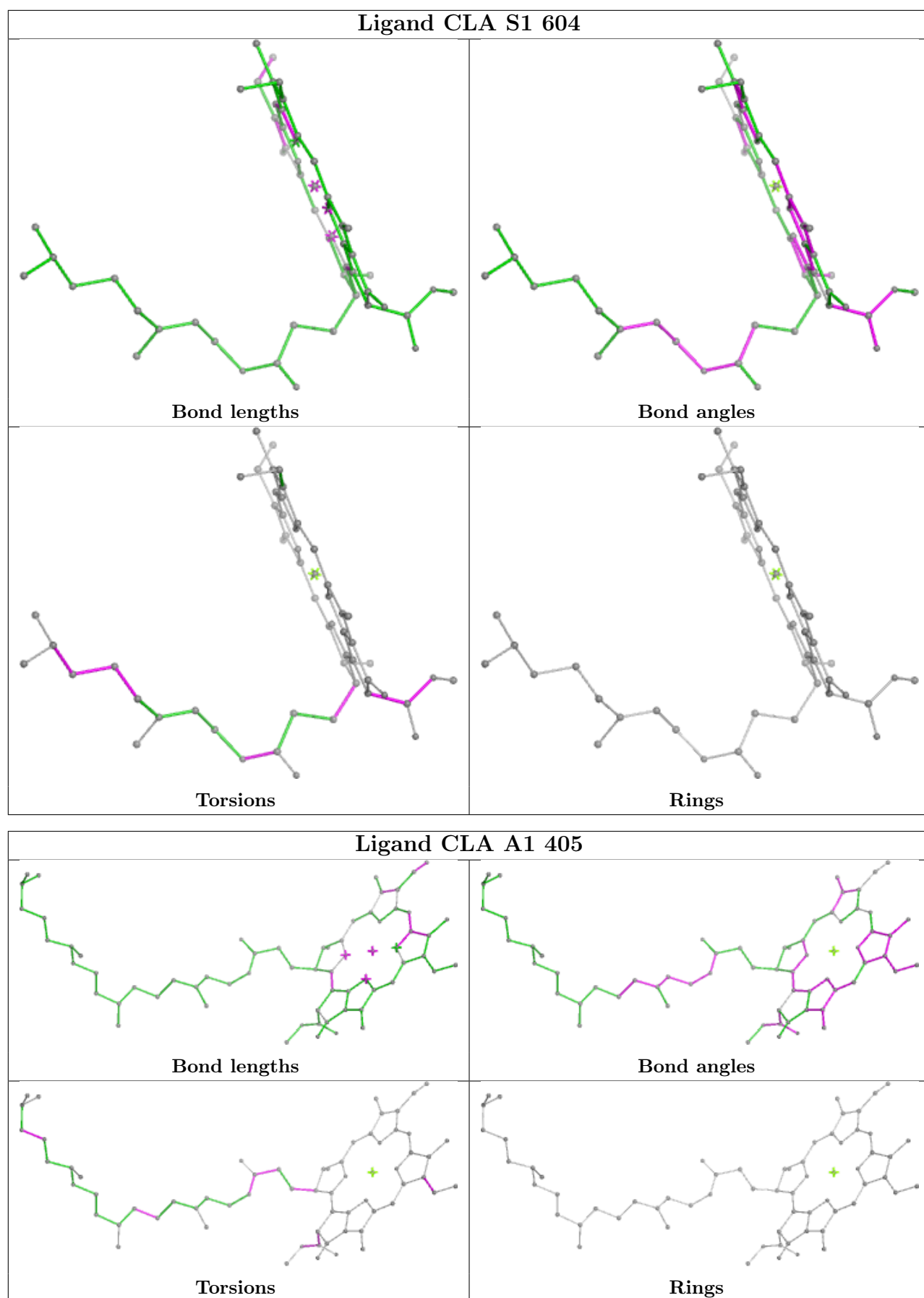






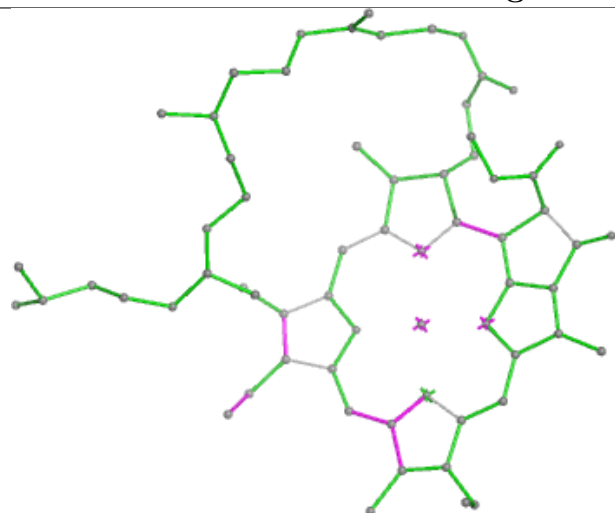




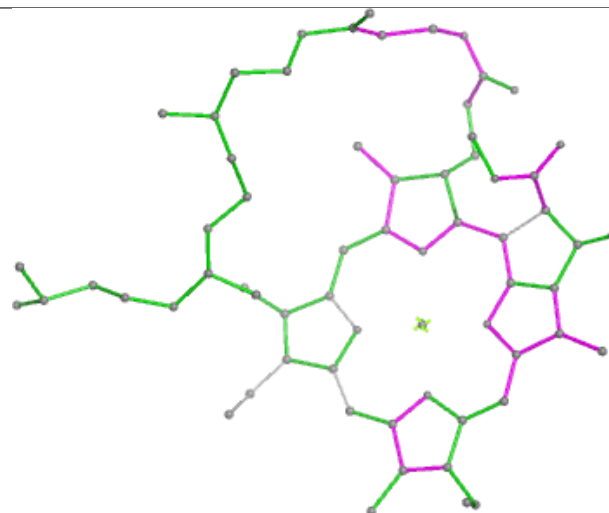




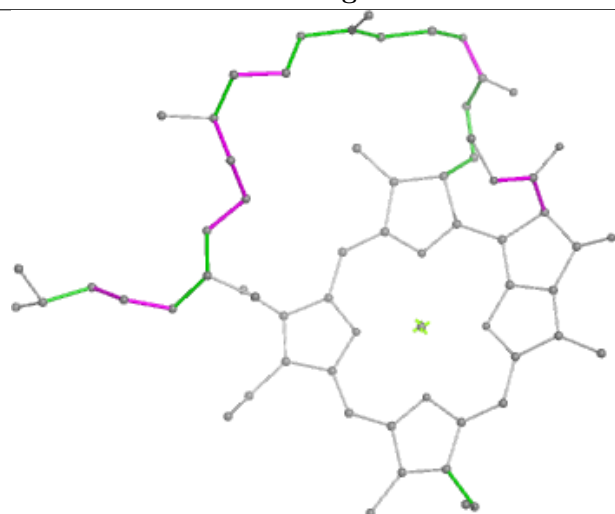
## Ligand CLA Y1 612



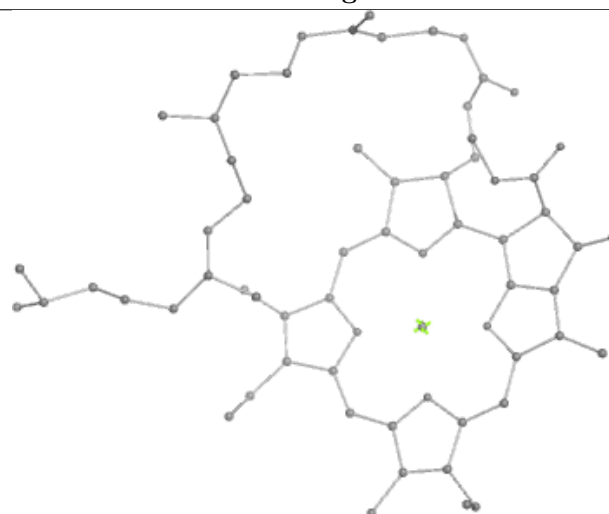
Bond lengths



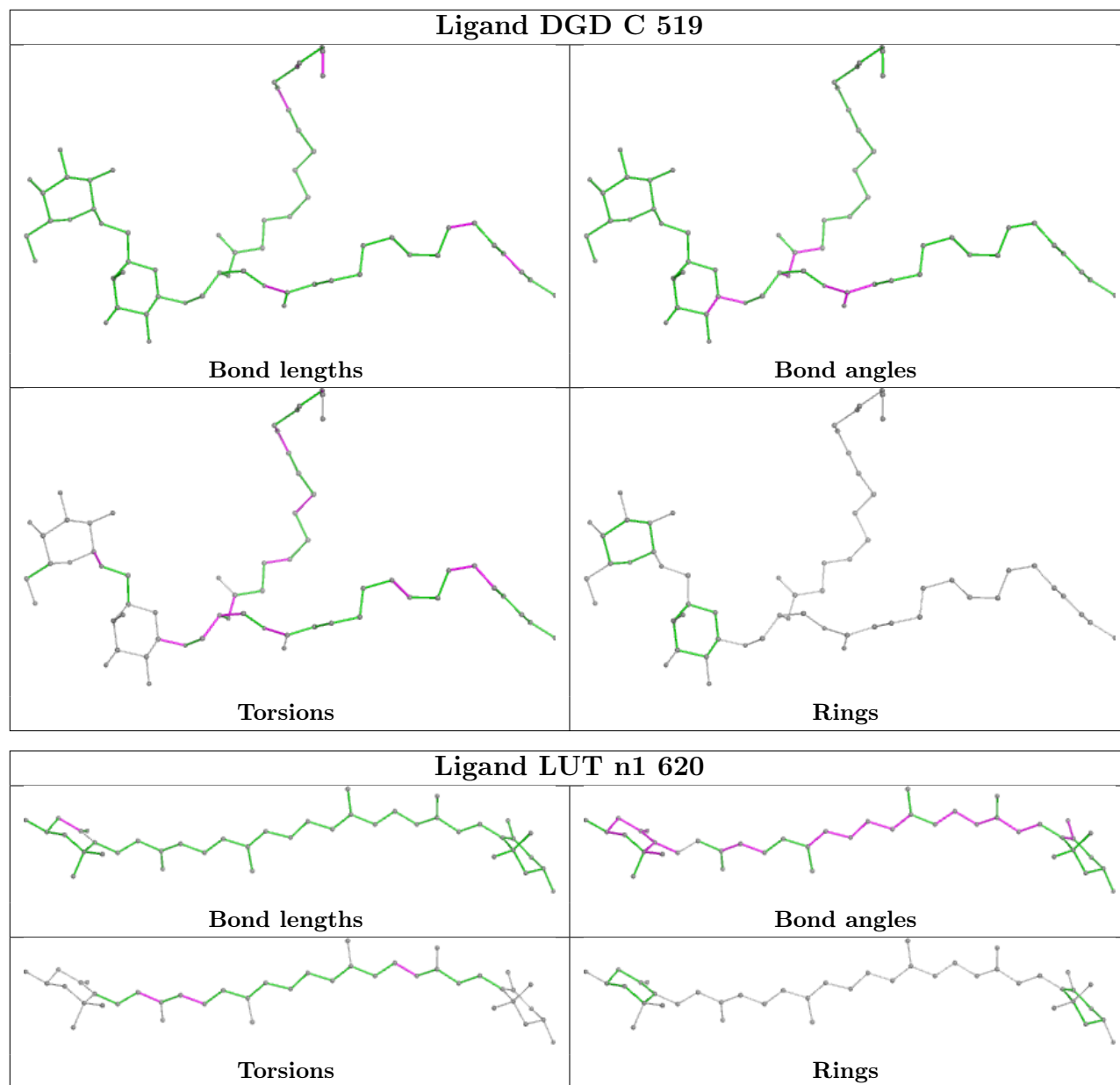
Bond angles



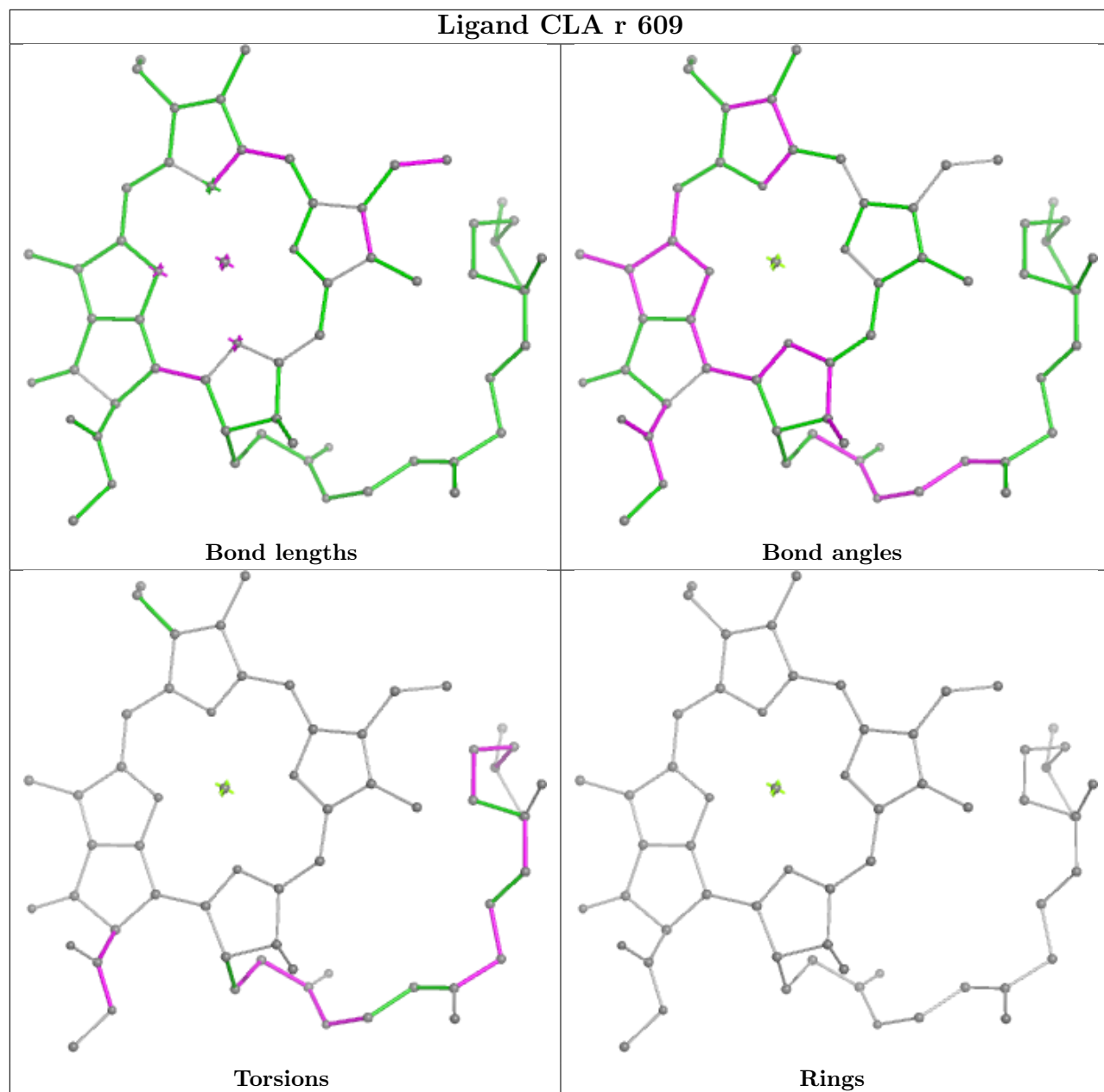
Torsions

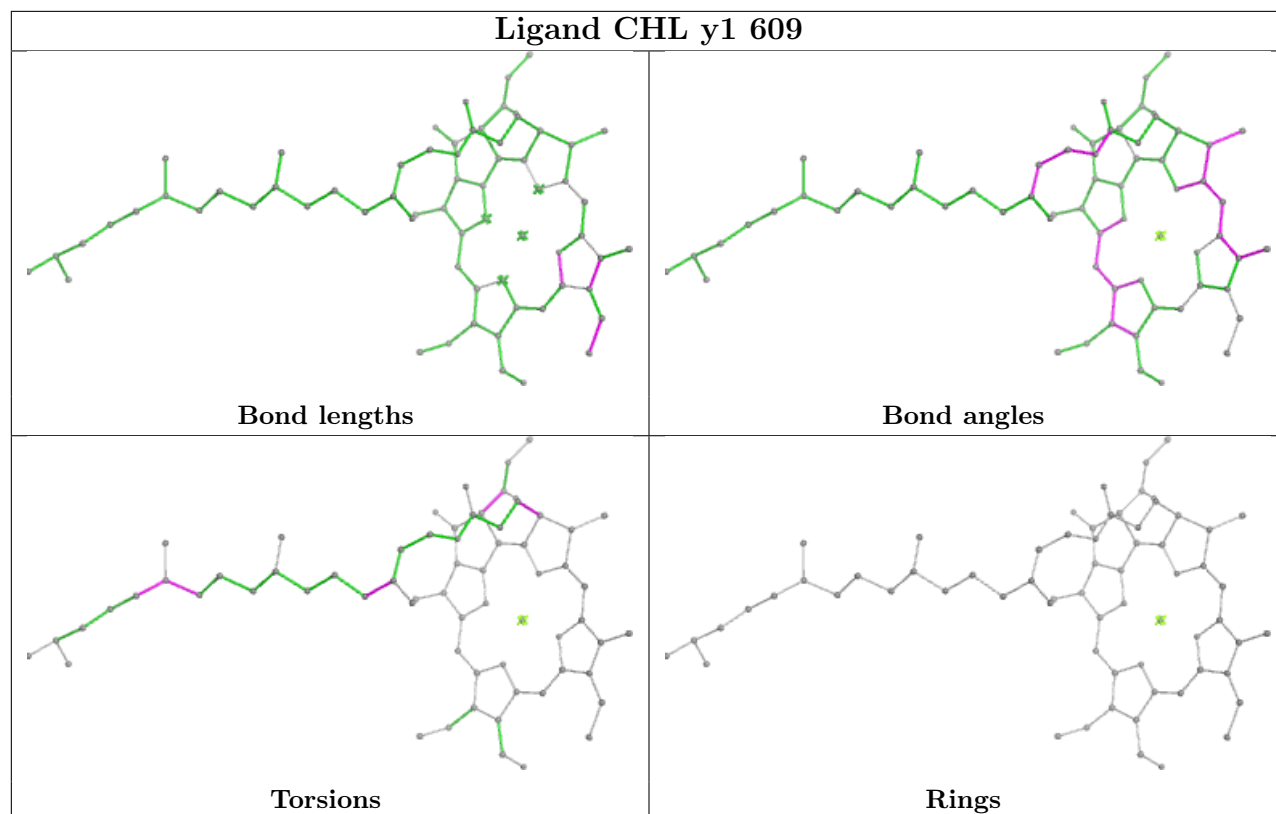


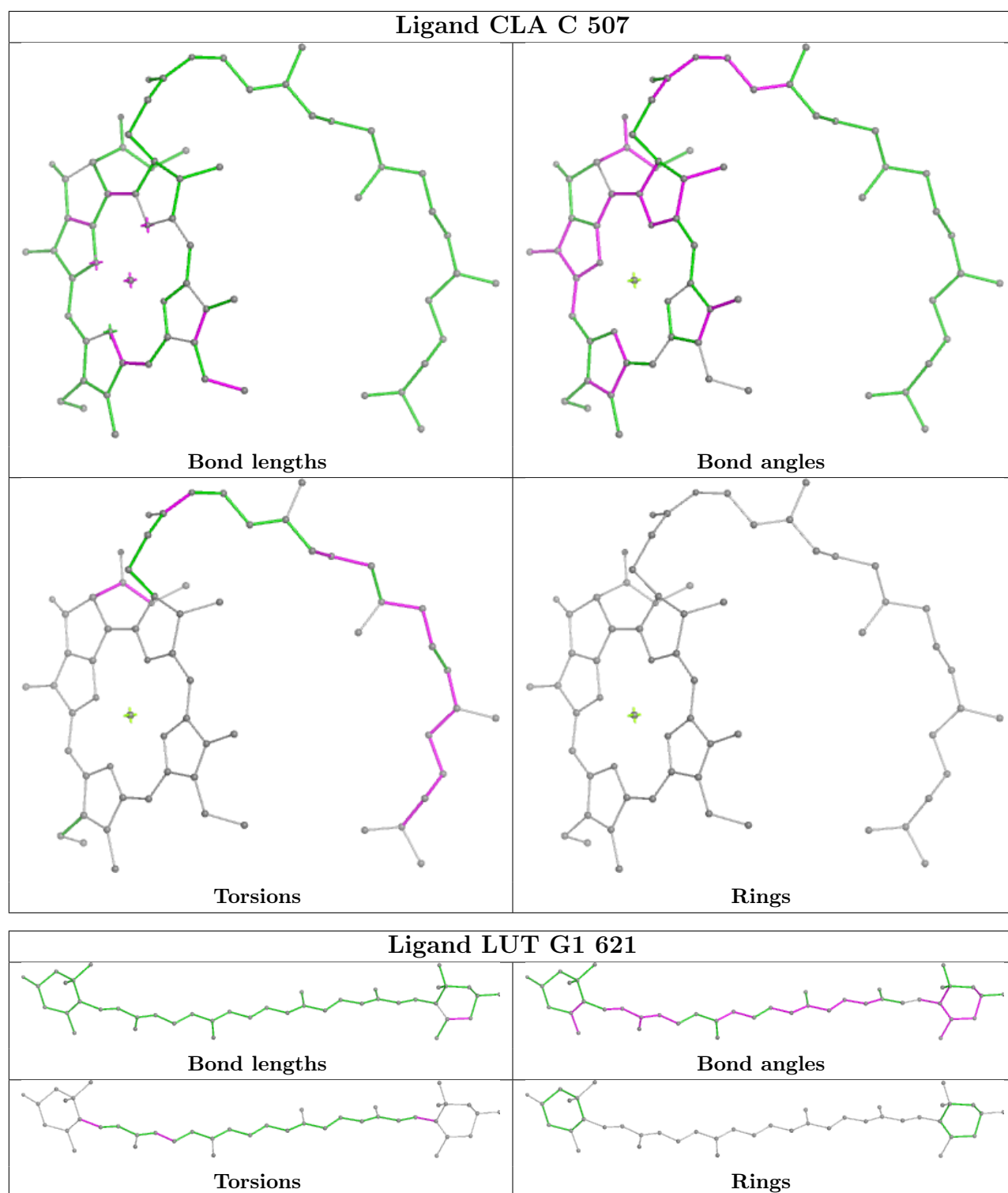
Rings



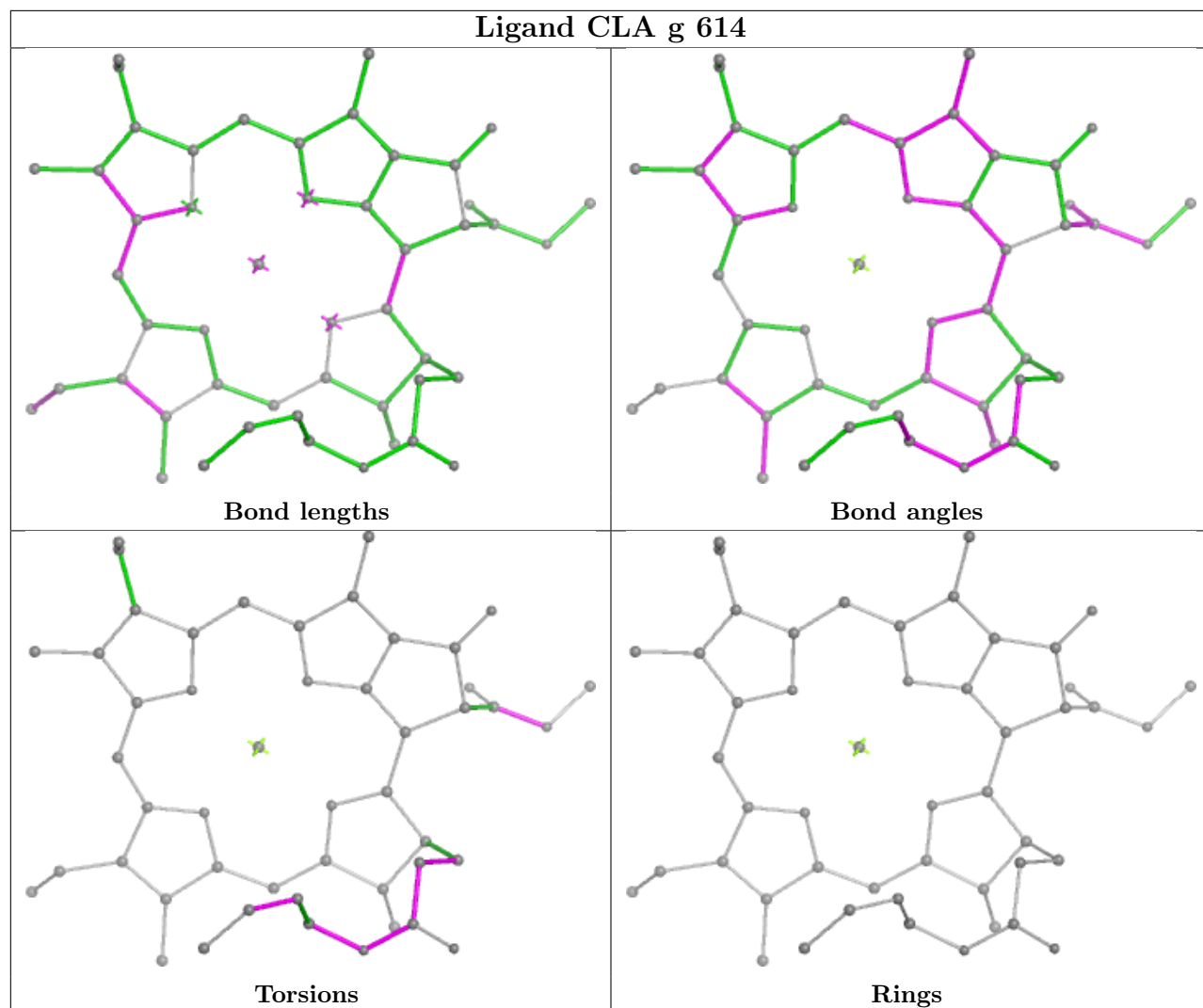
## Ligand CLA r 609

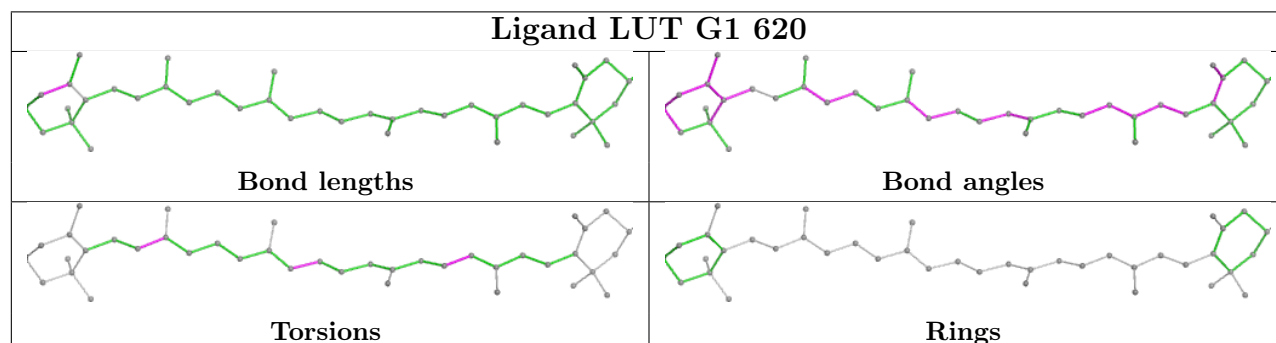
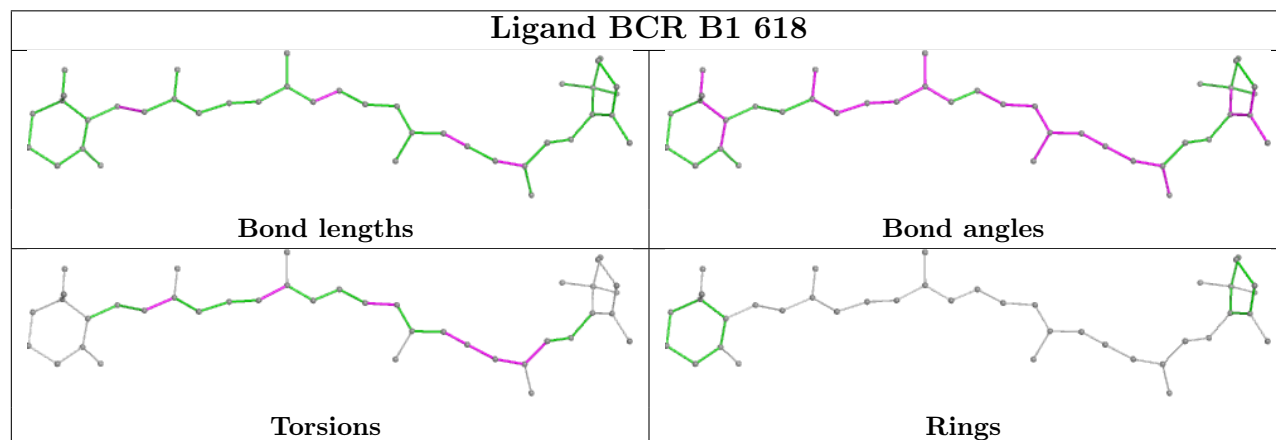
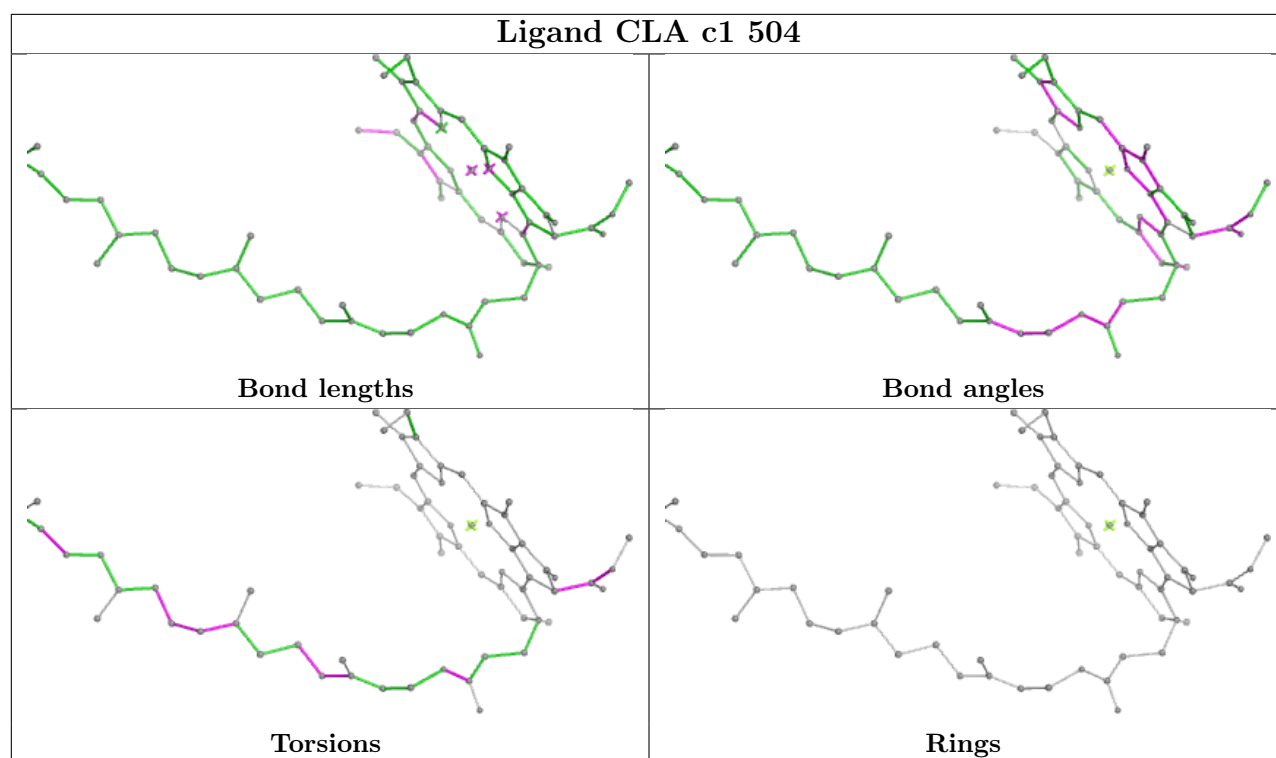


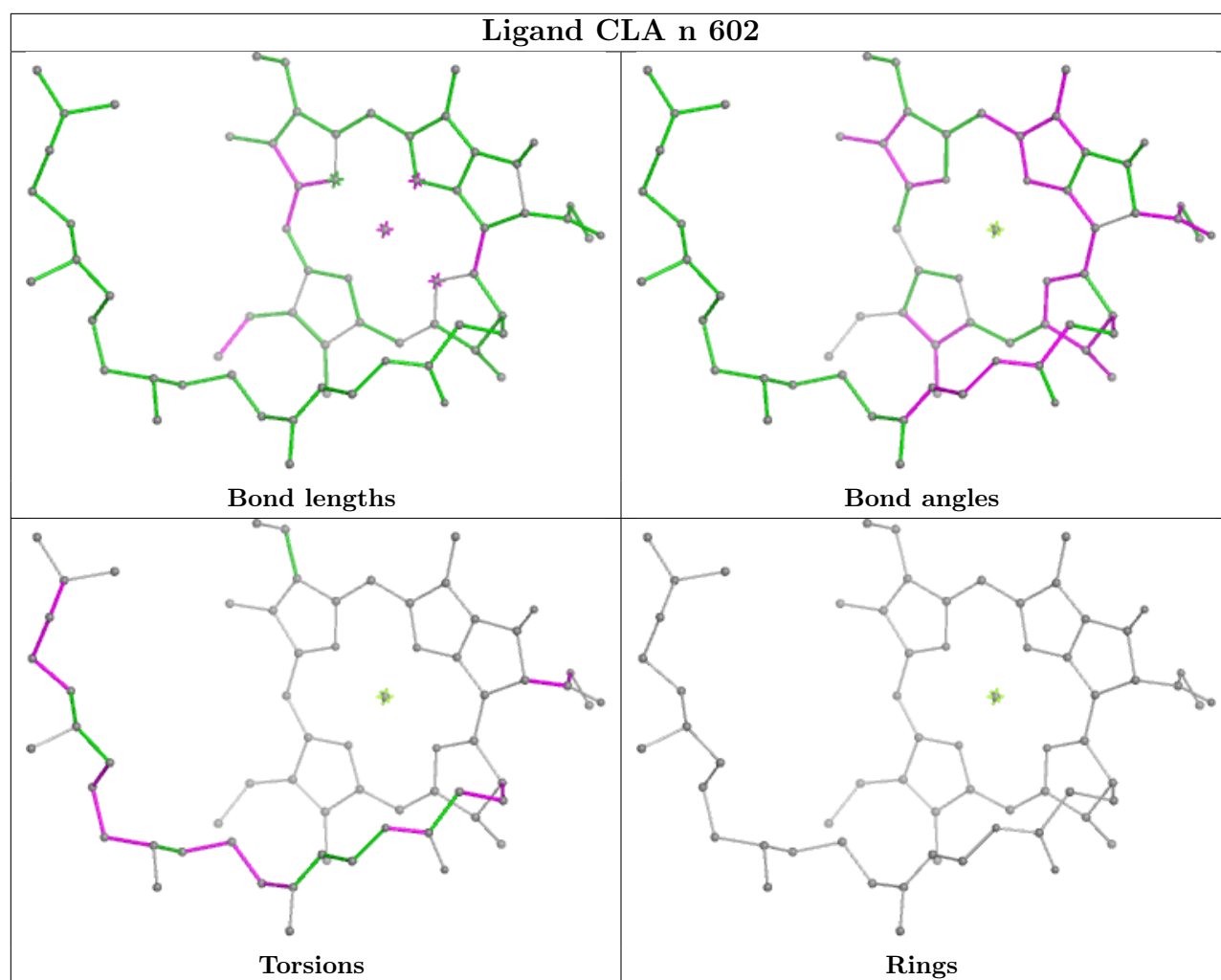




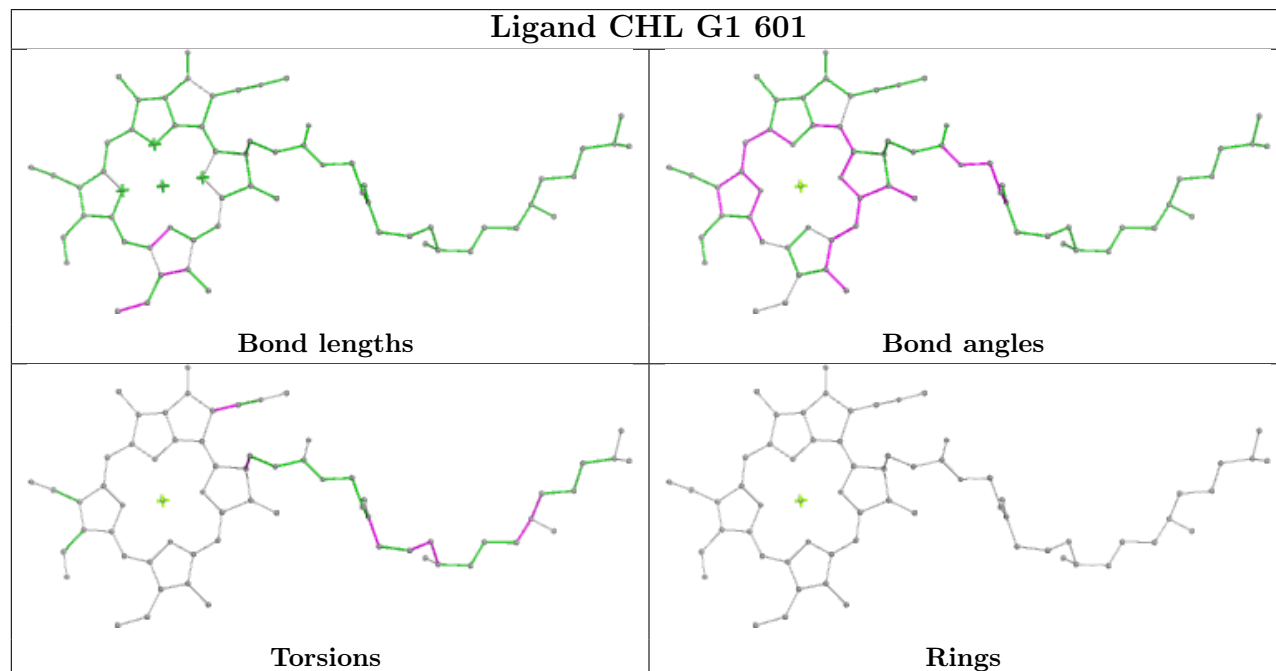
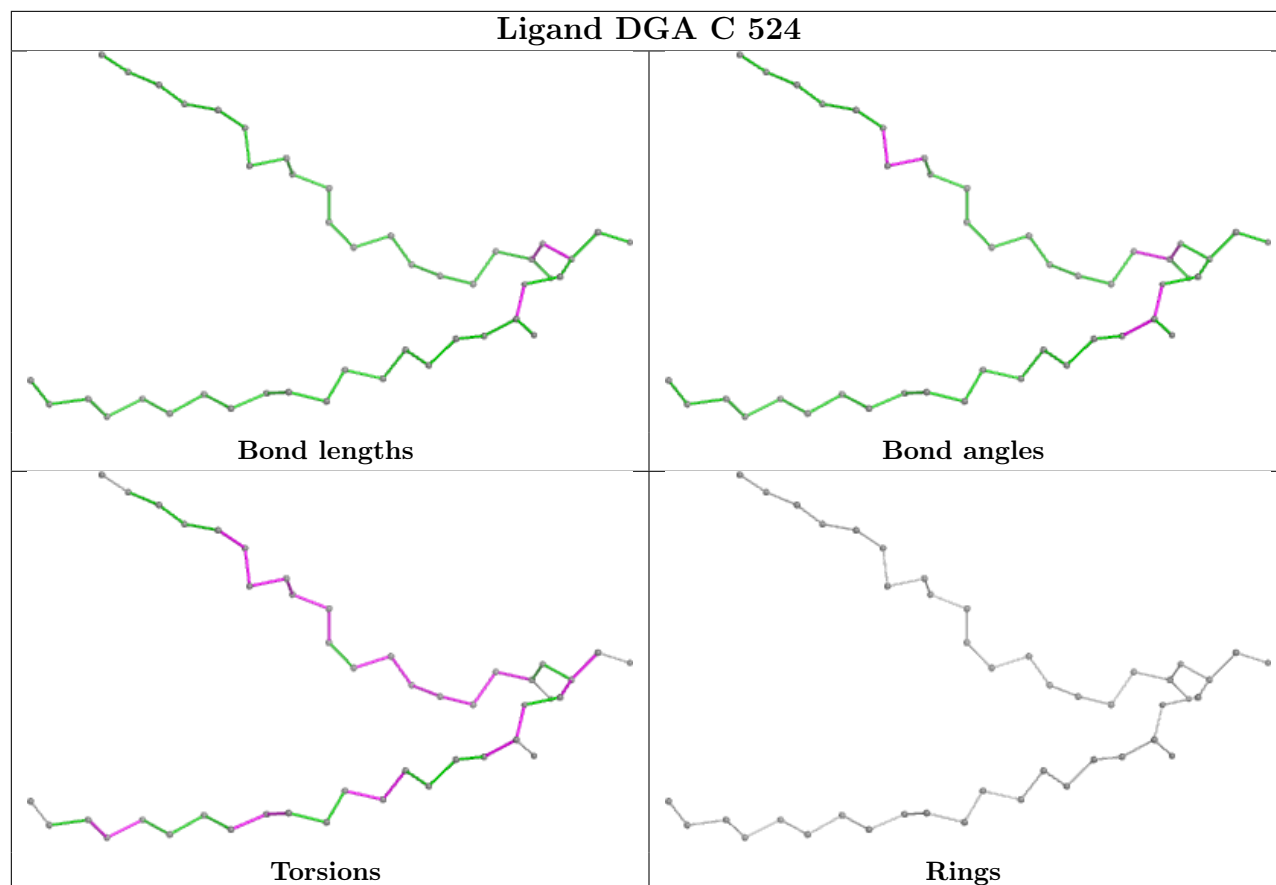
## Ligand CLA g 614

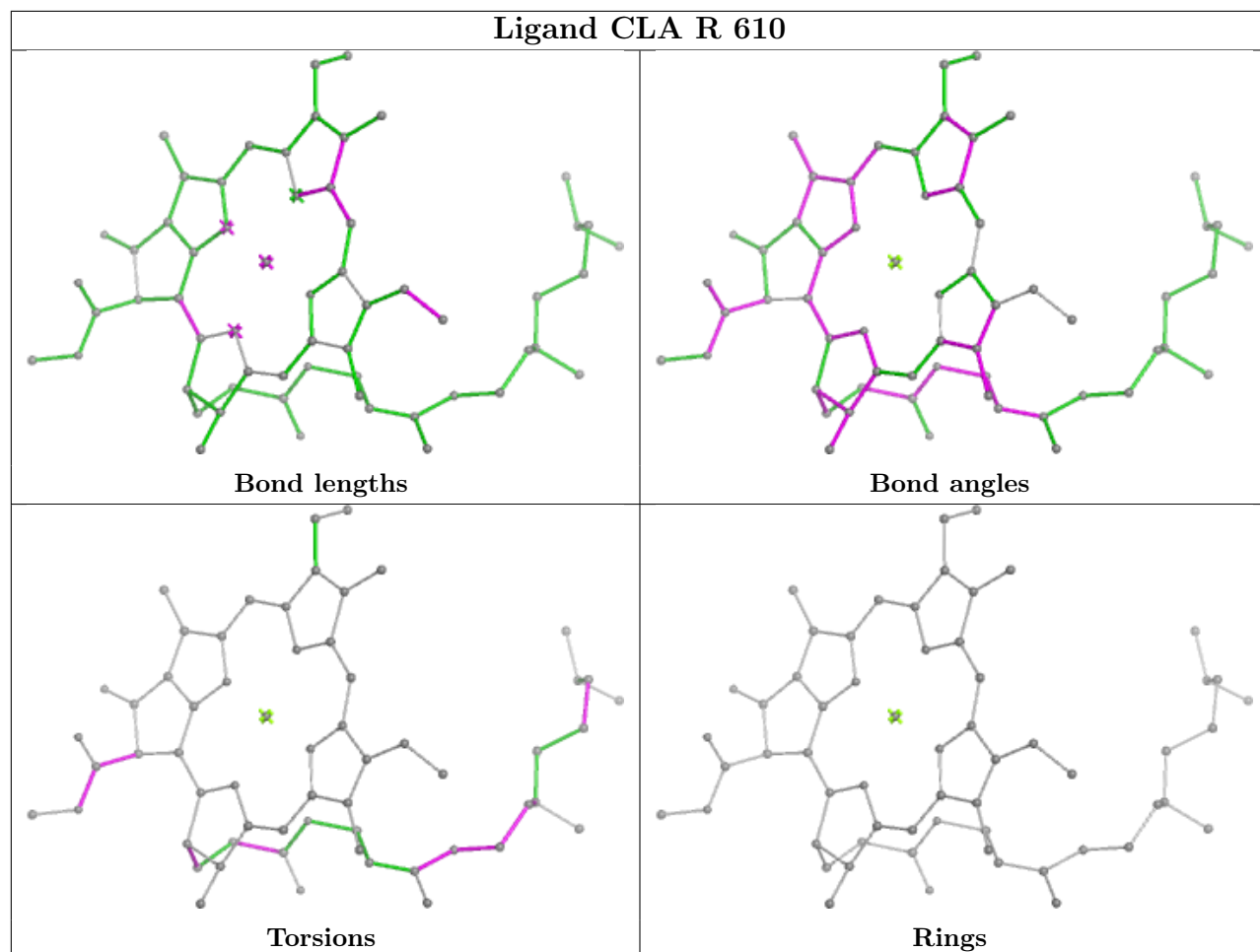


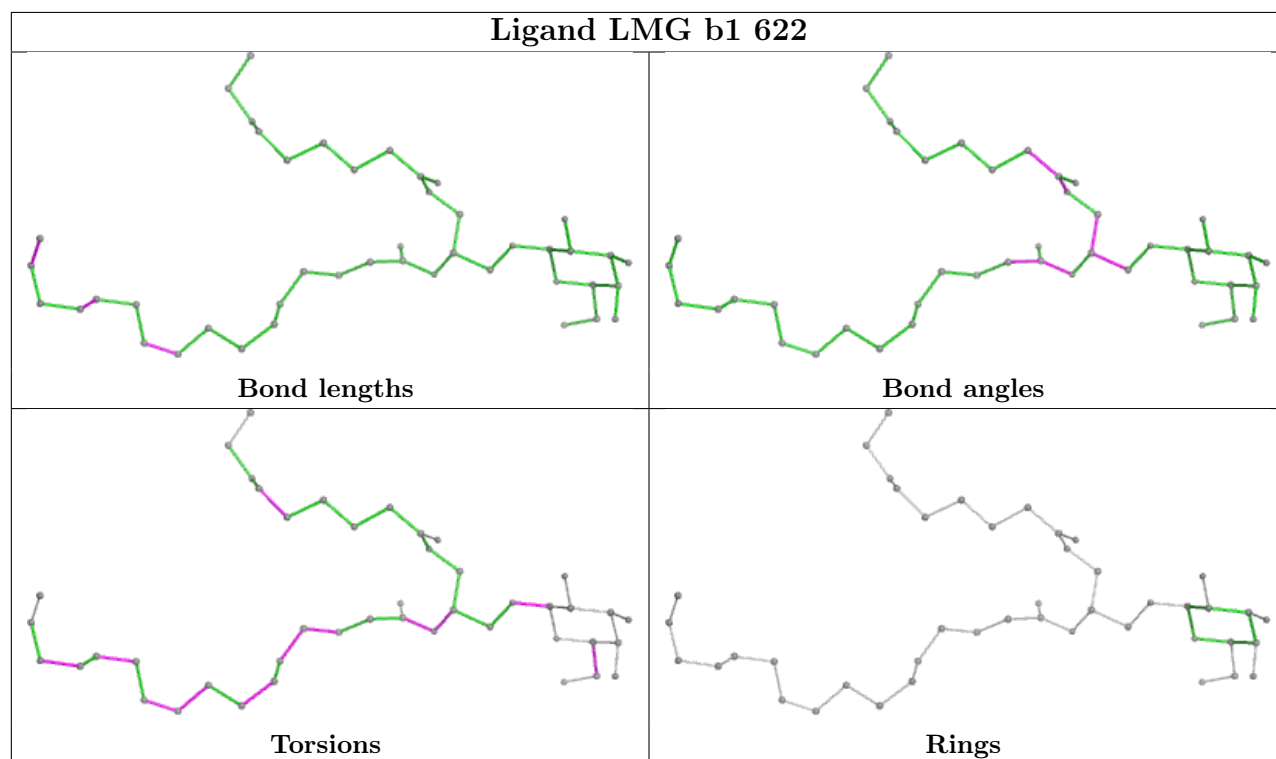
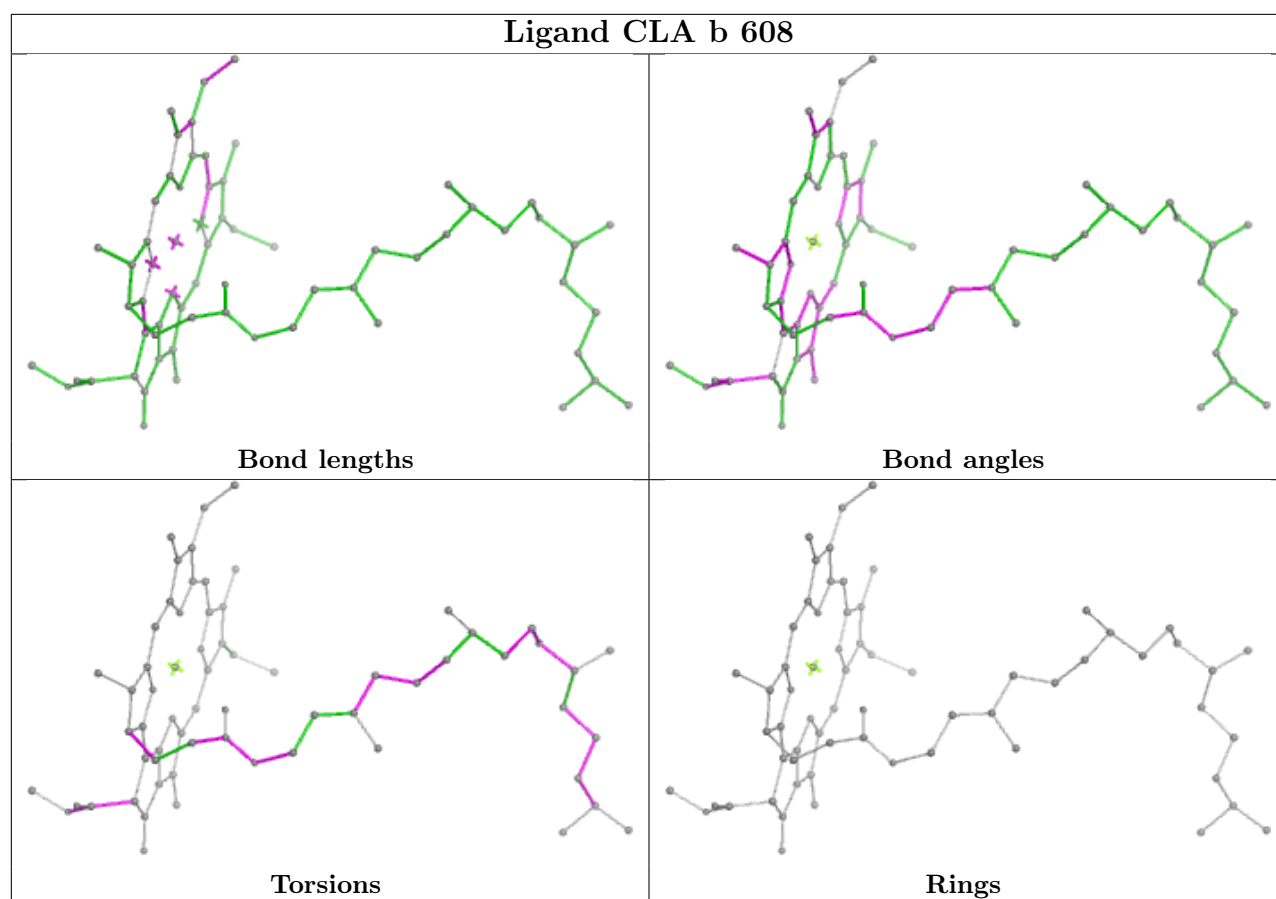


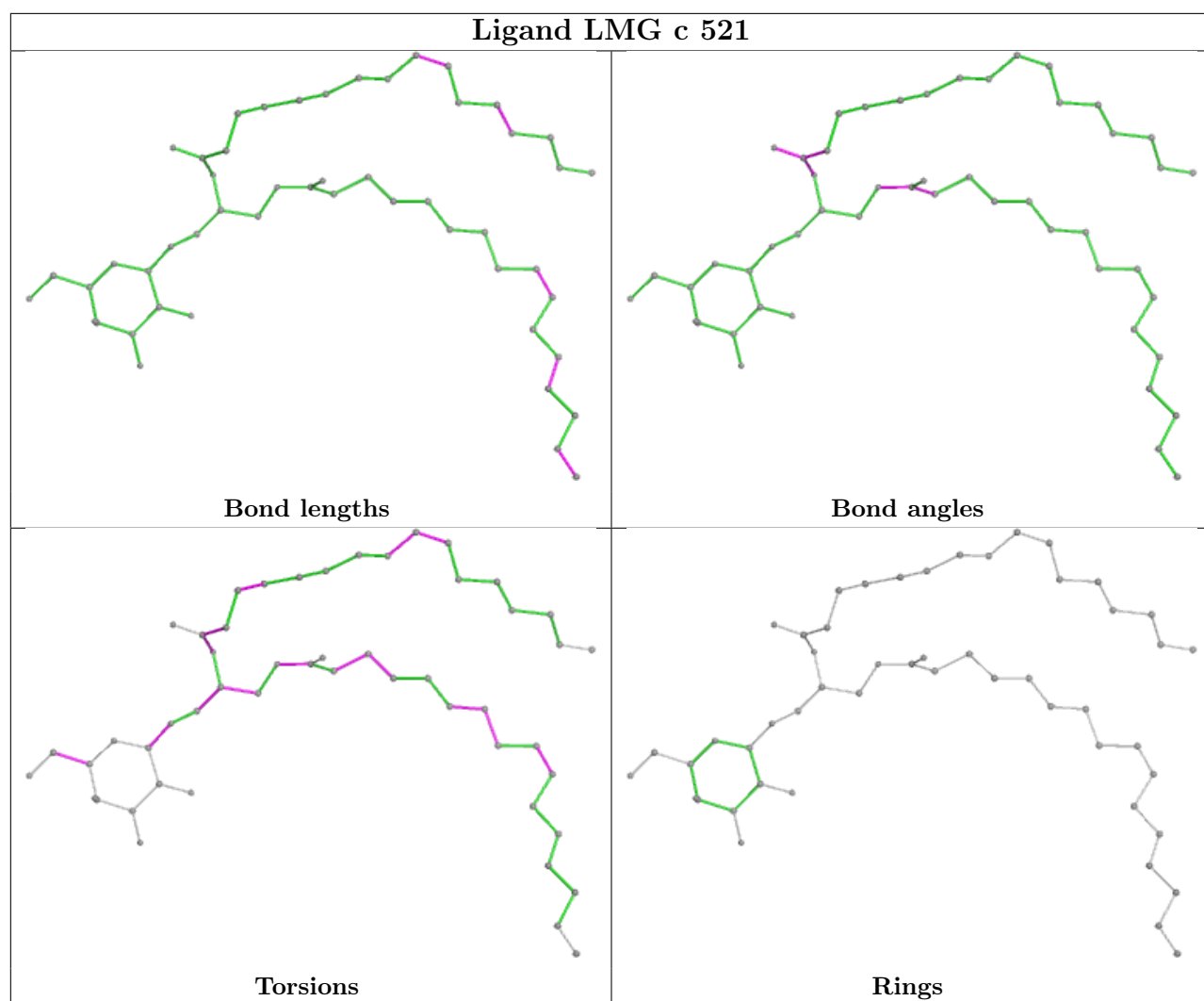


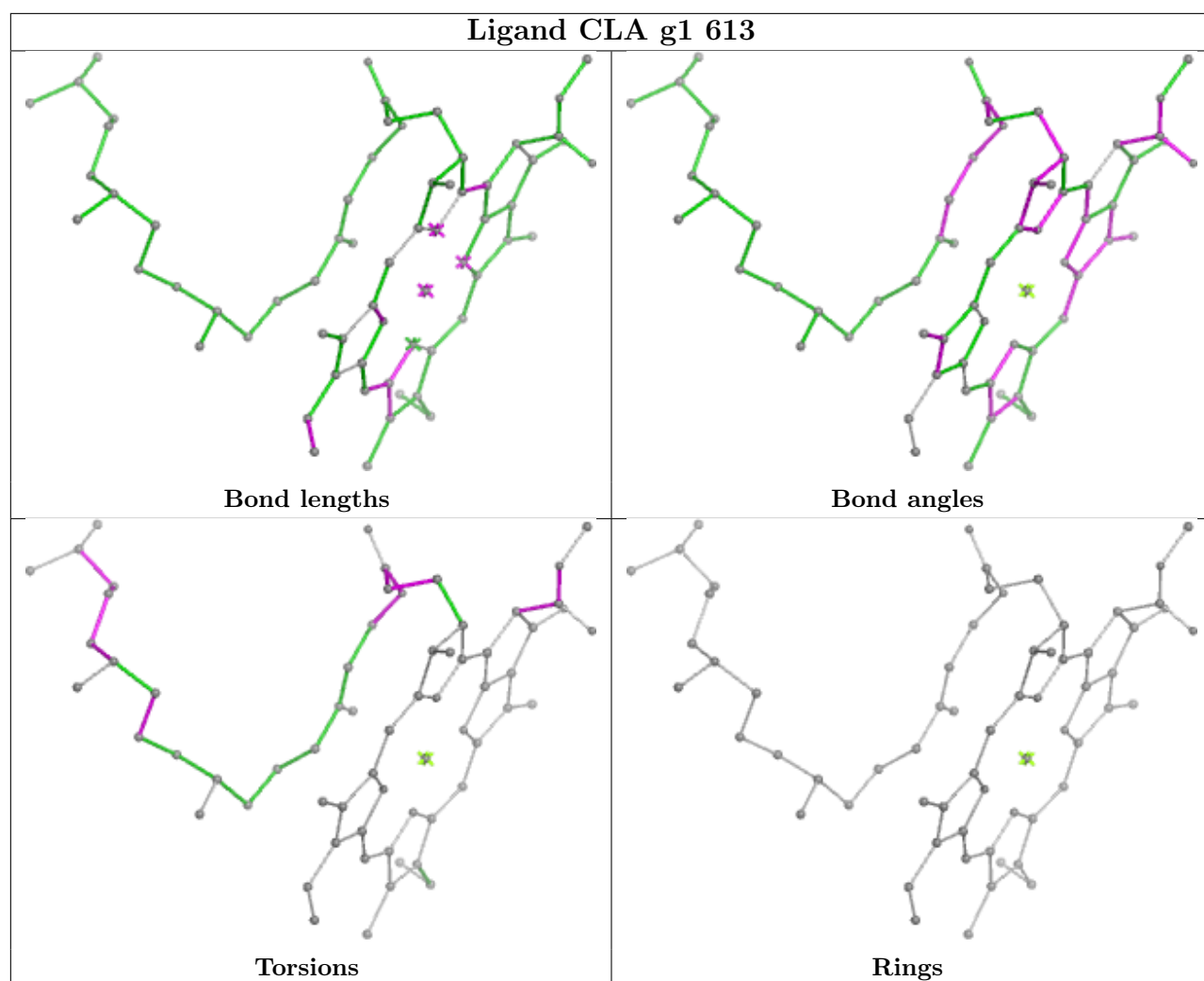


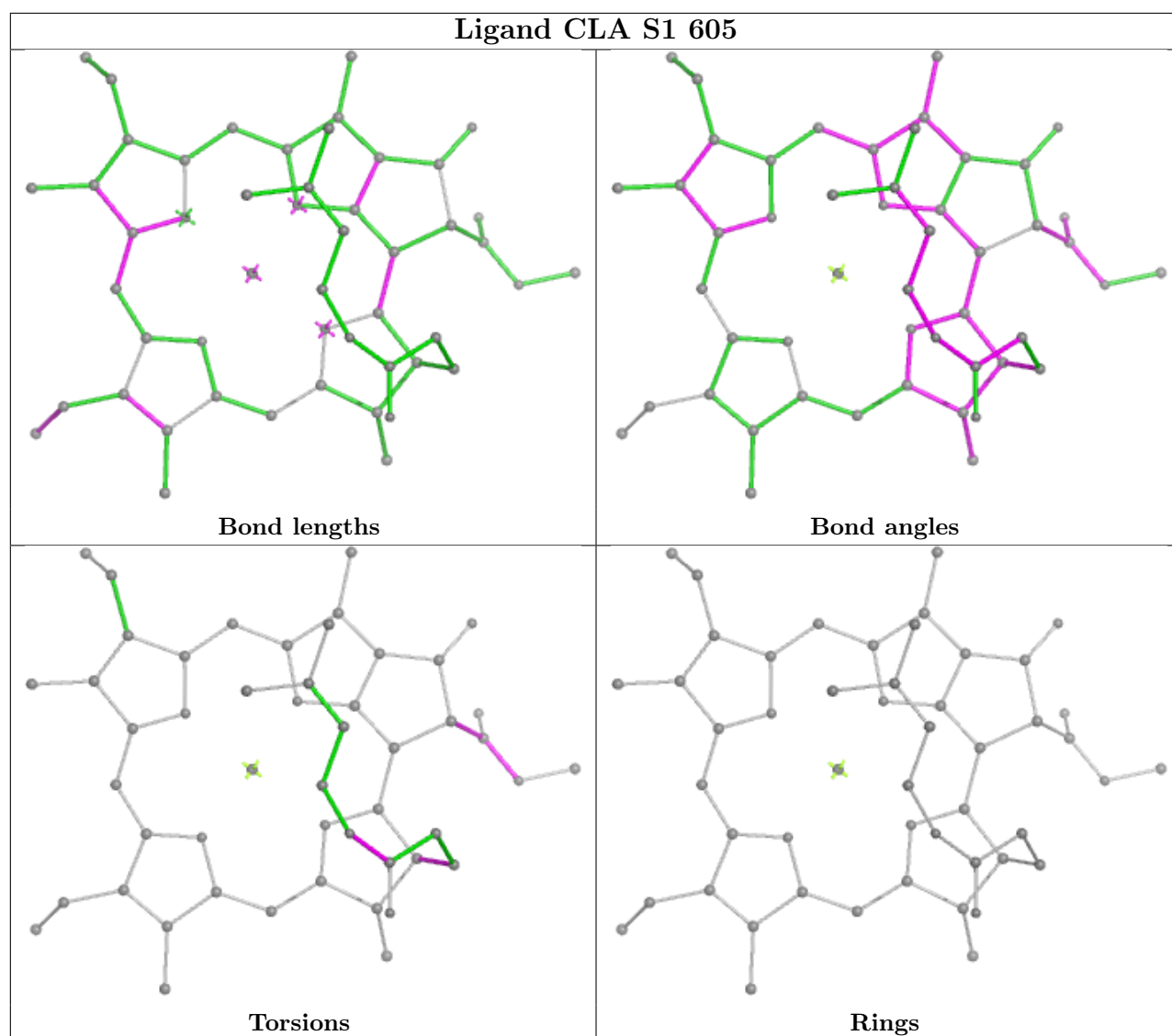


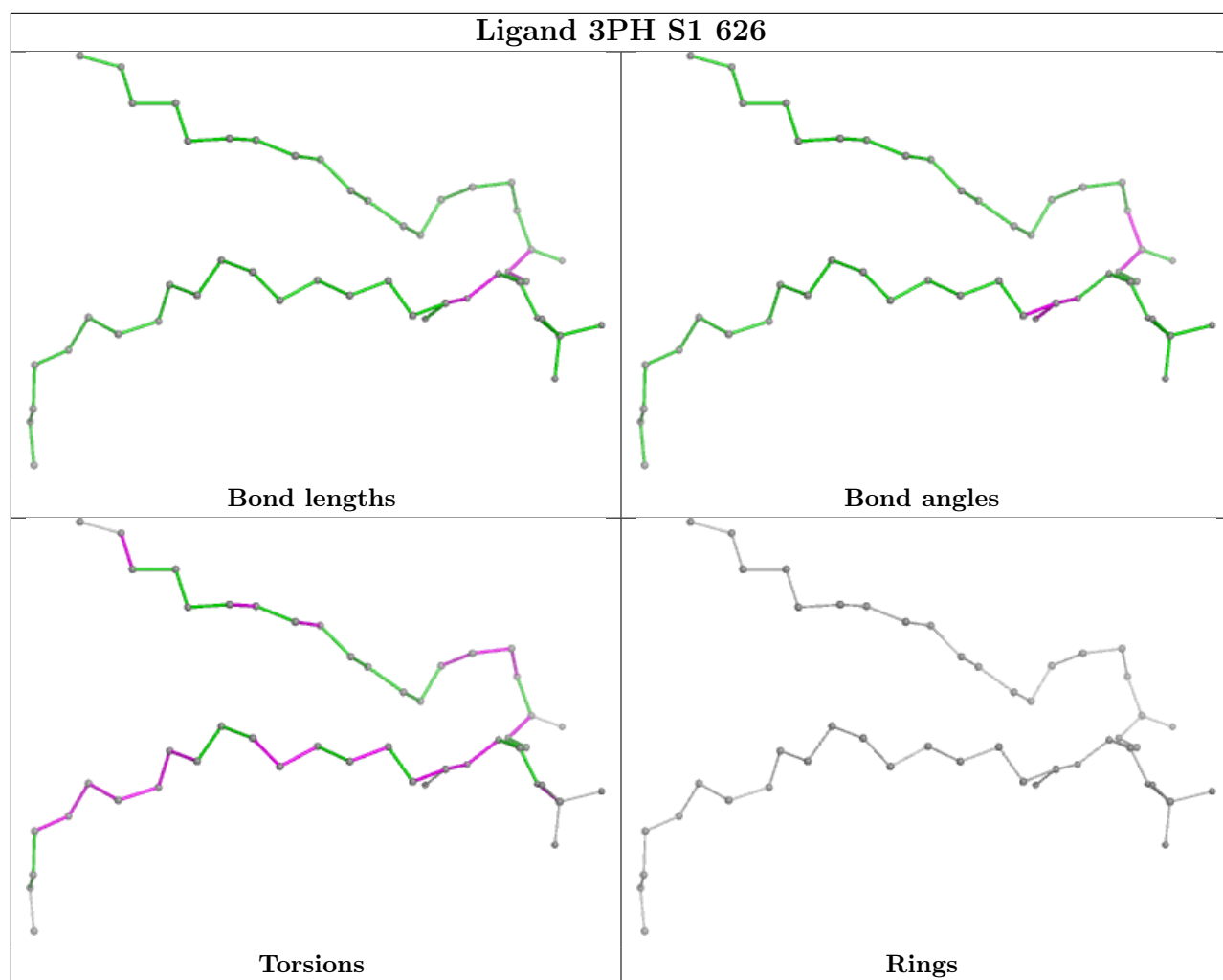




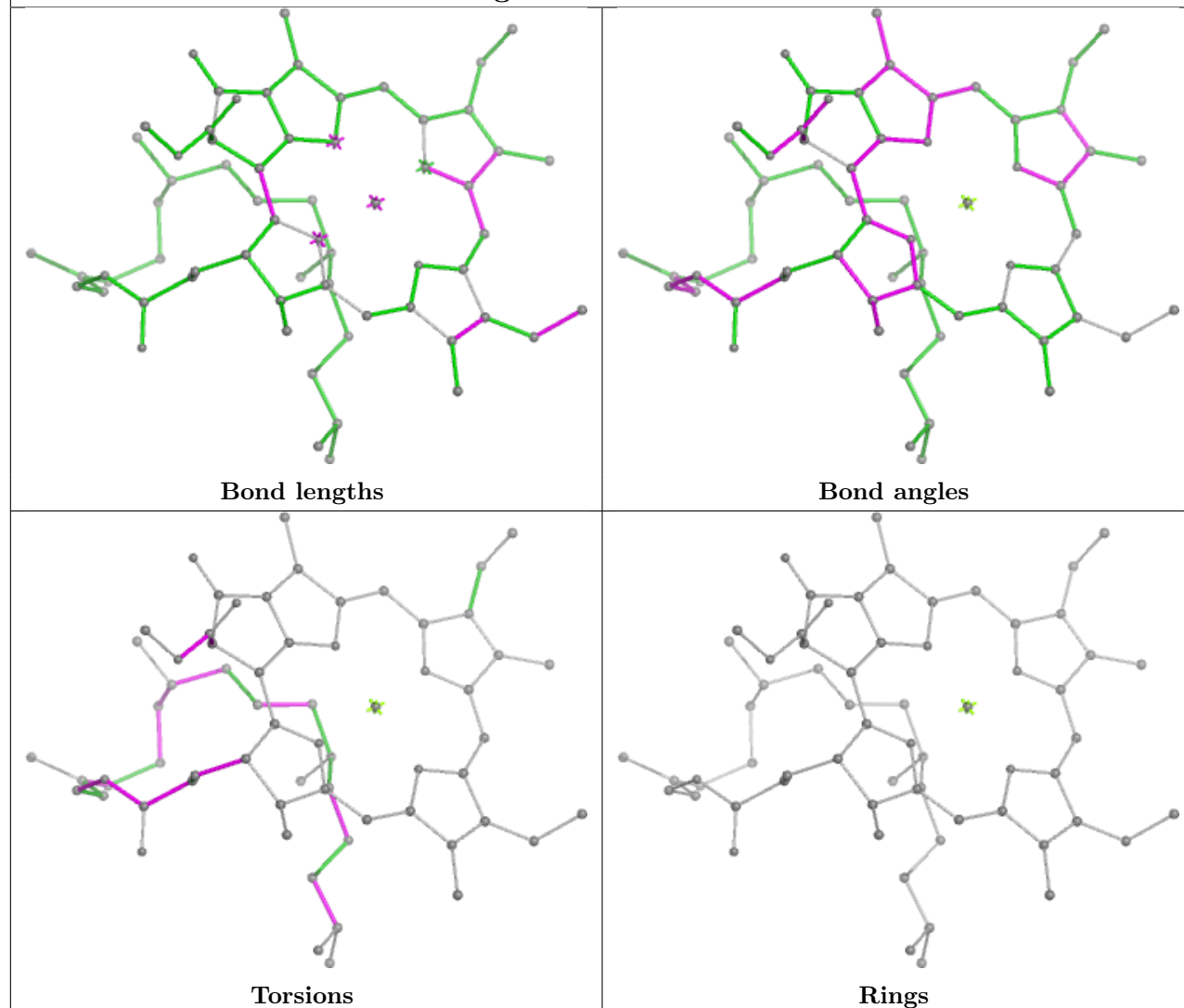




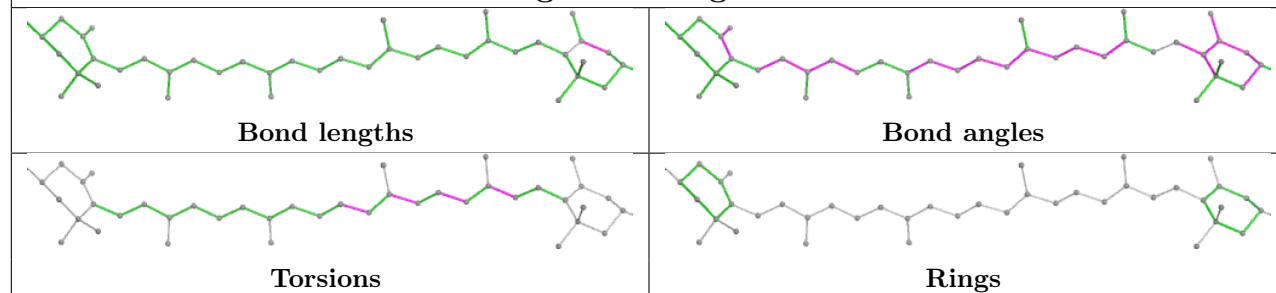




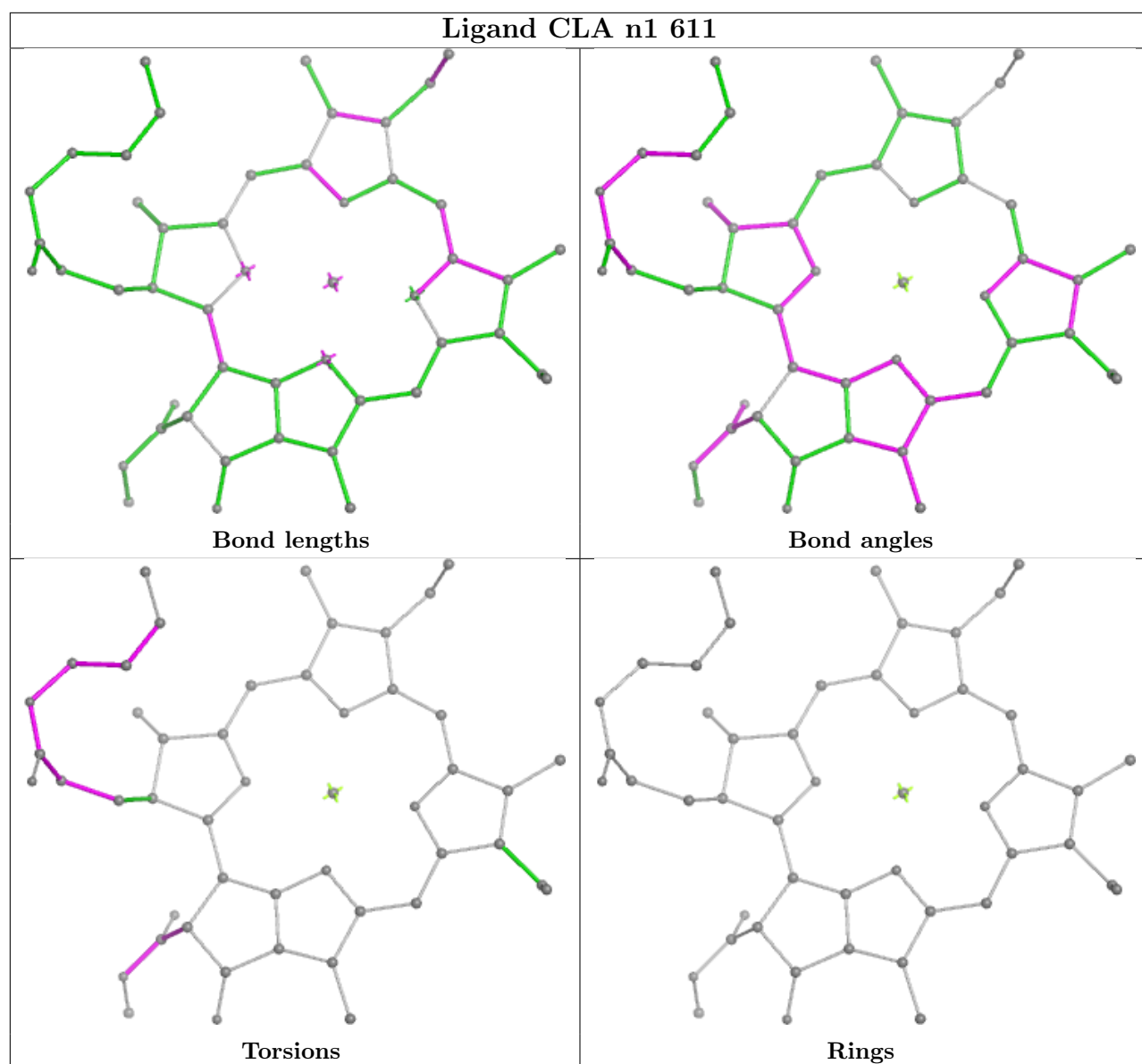
## Ligand CLA B 602

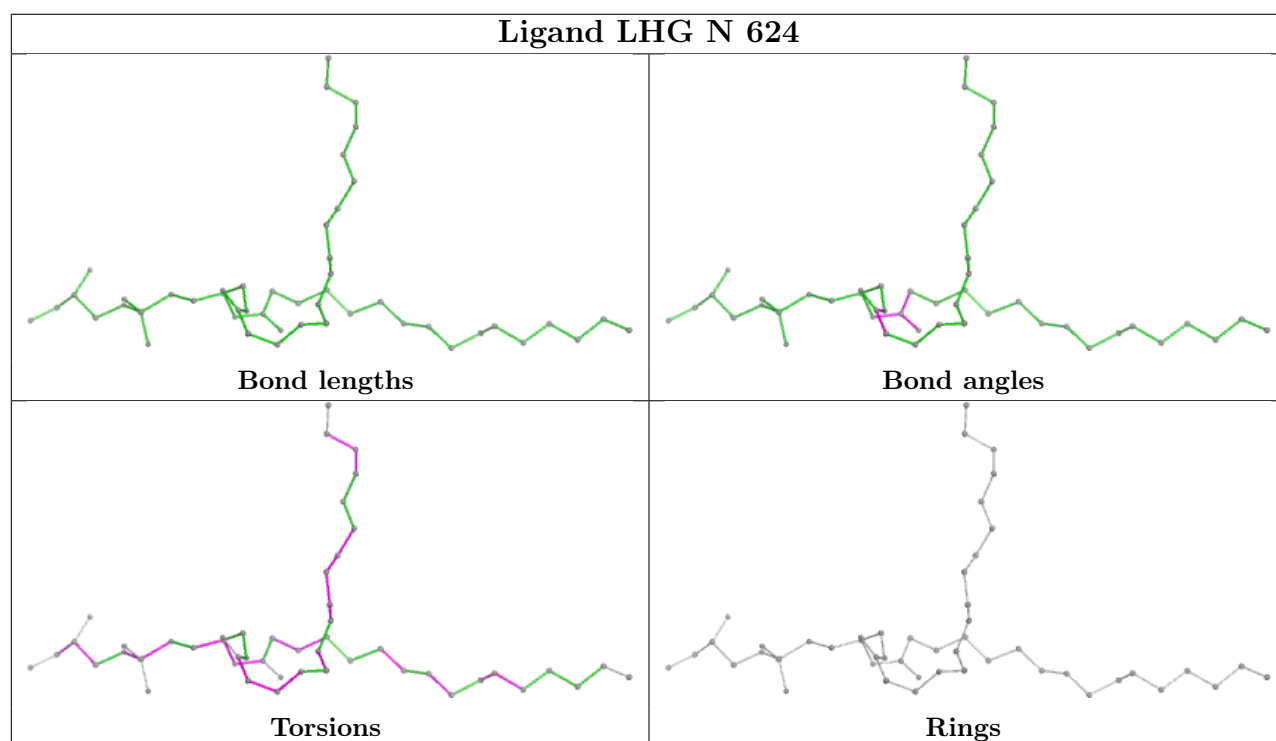
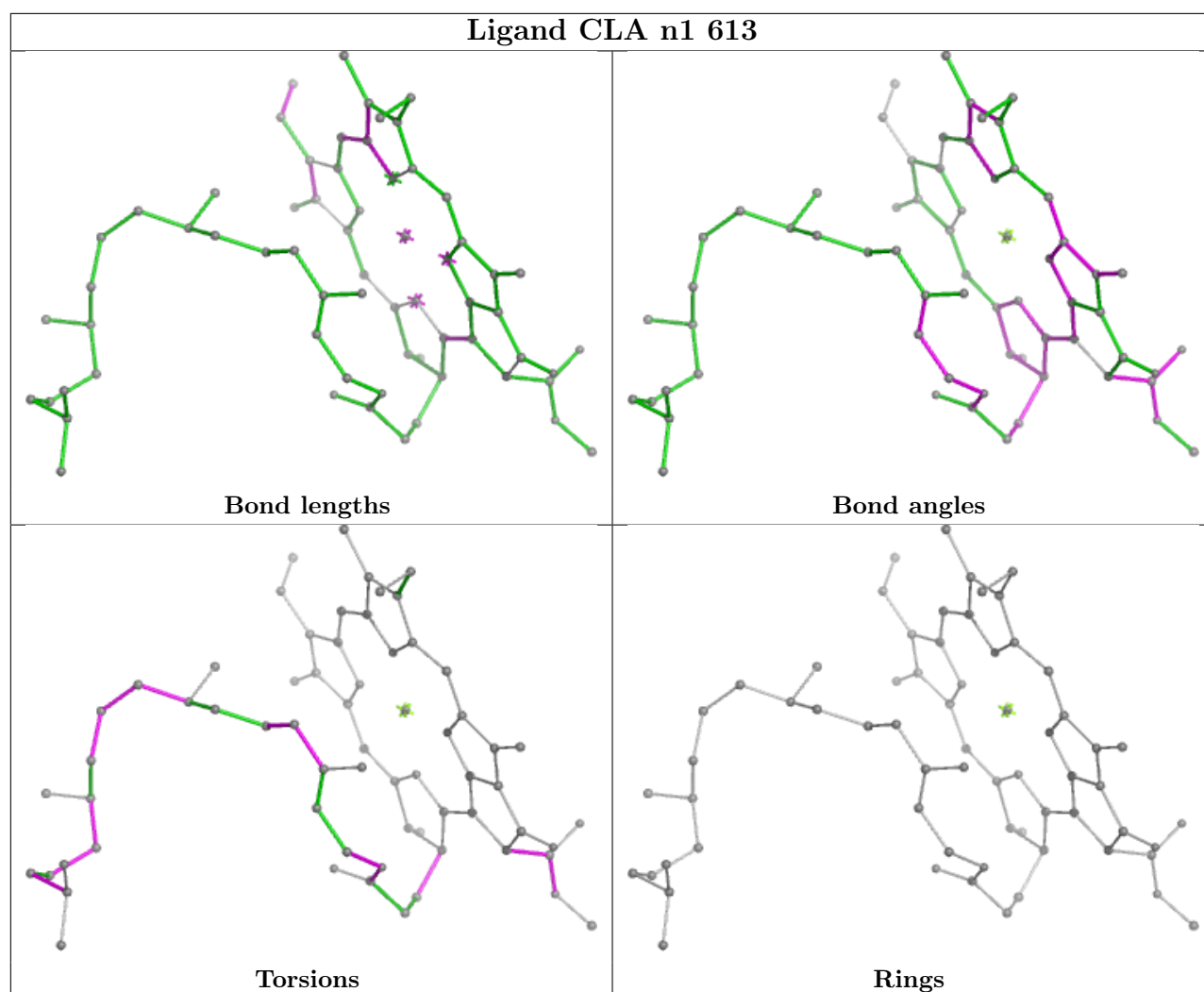


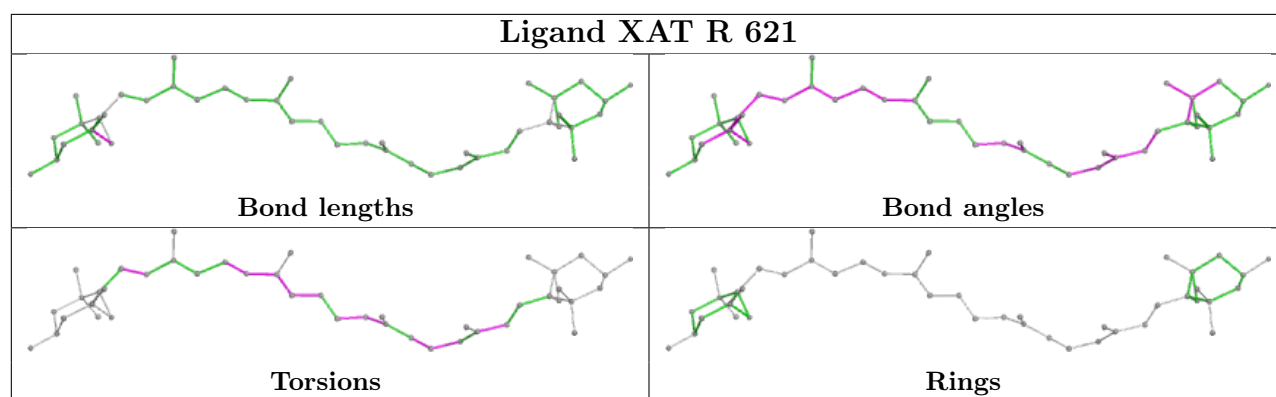
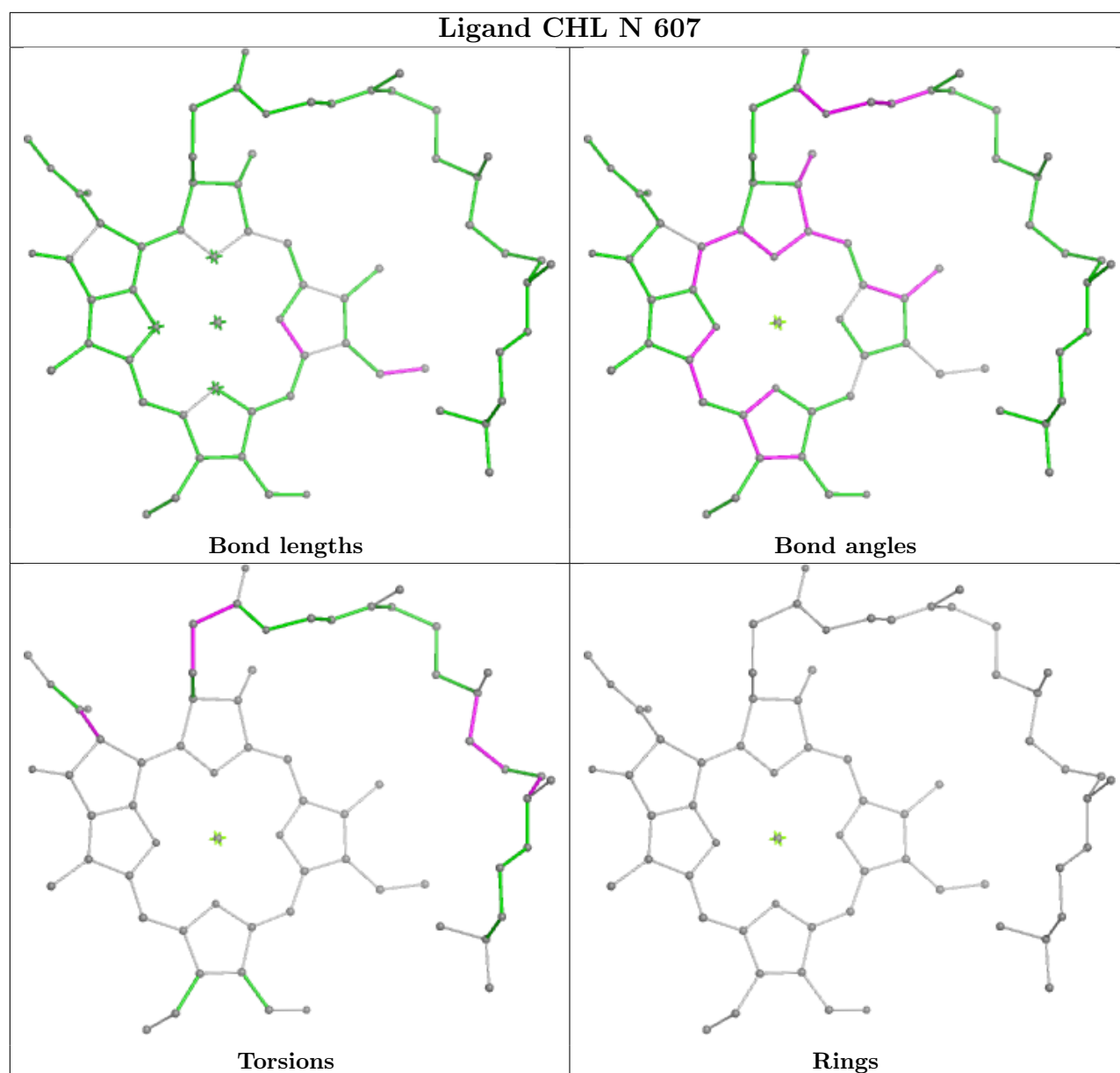
## Ligand LUT g 620

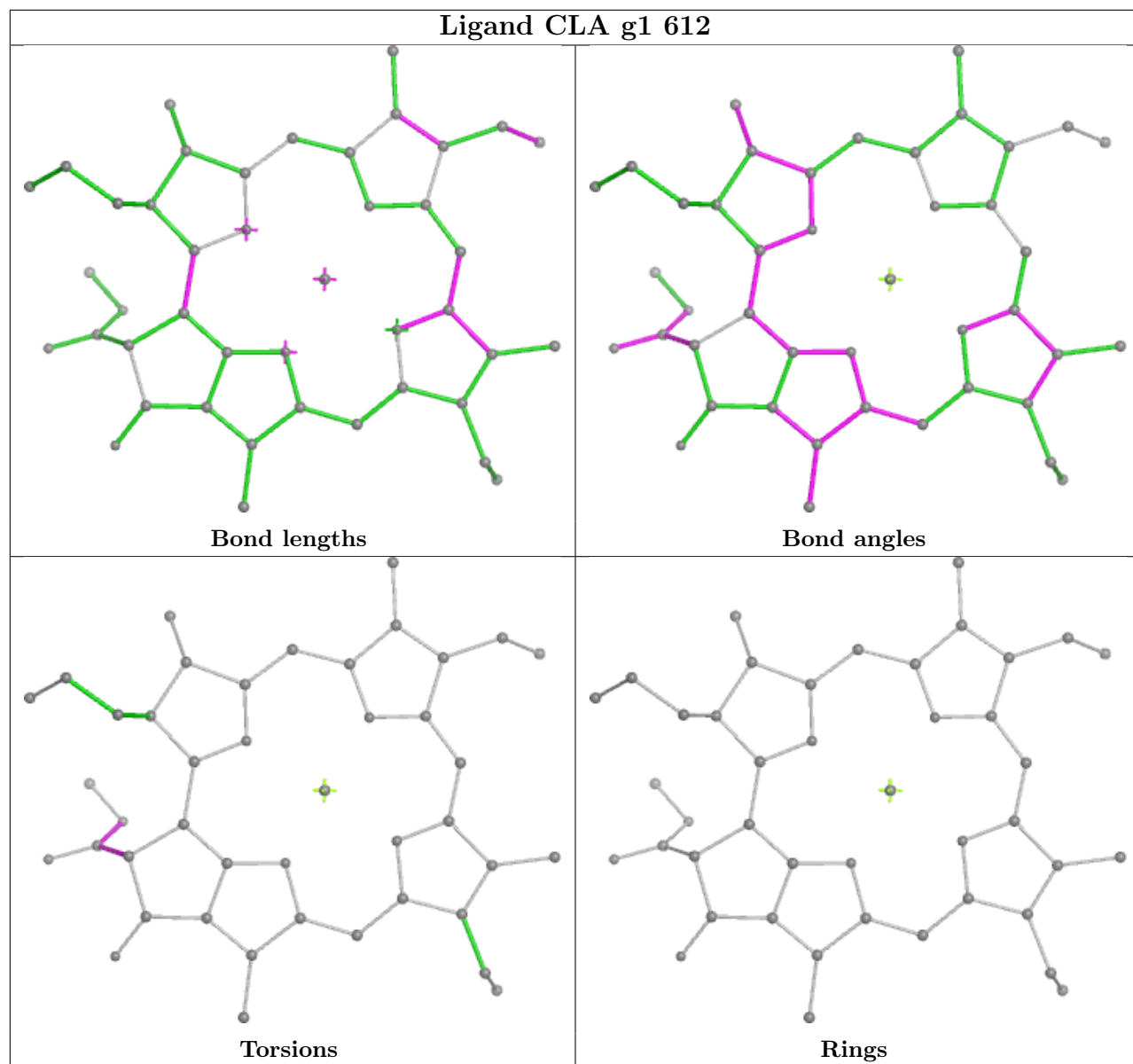


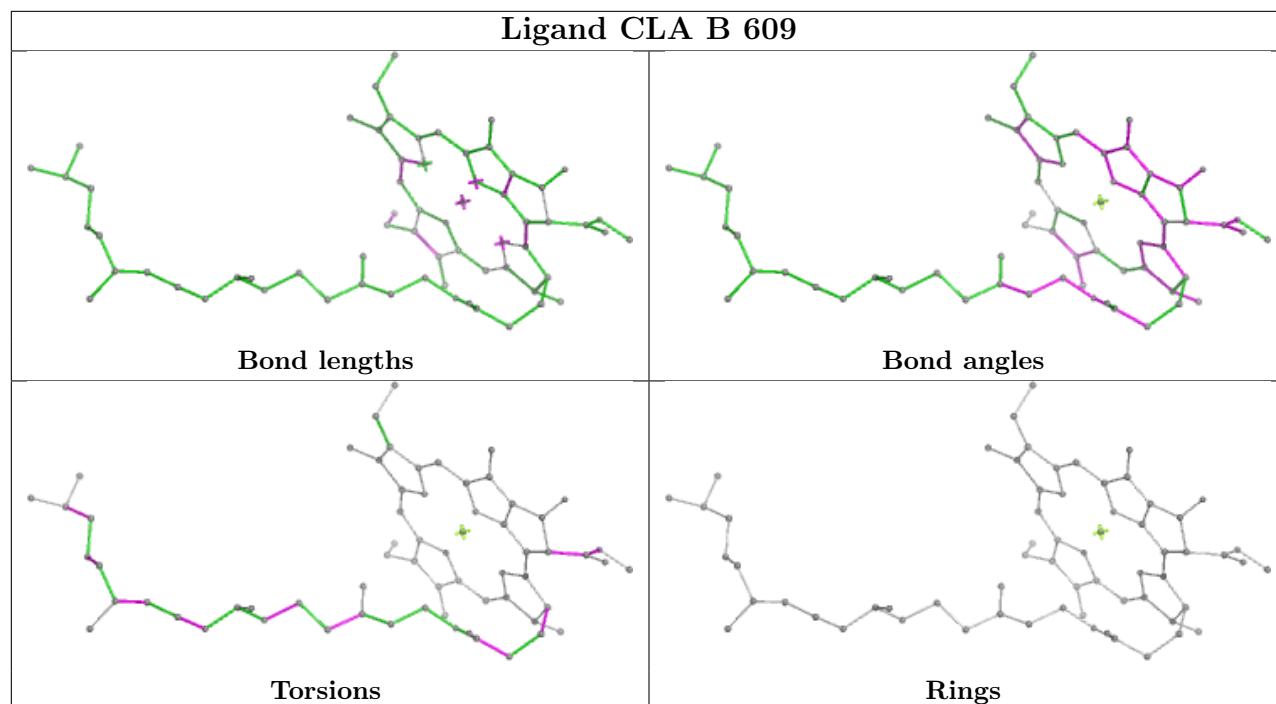
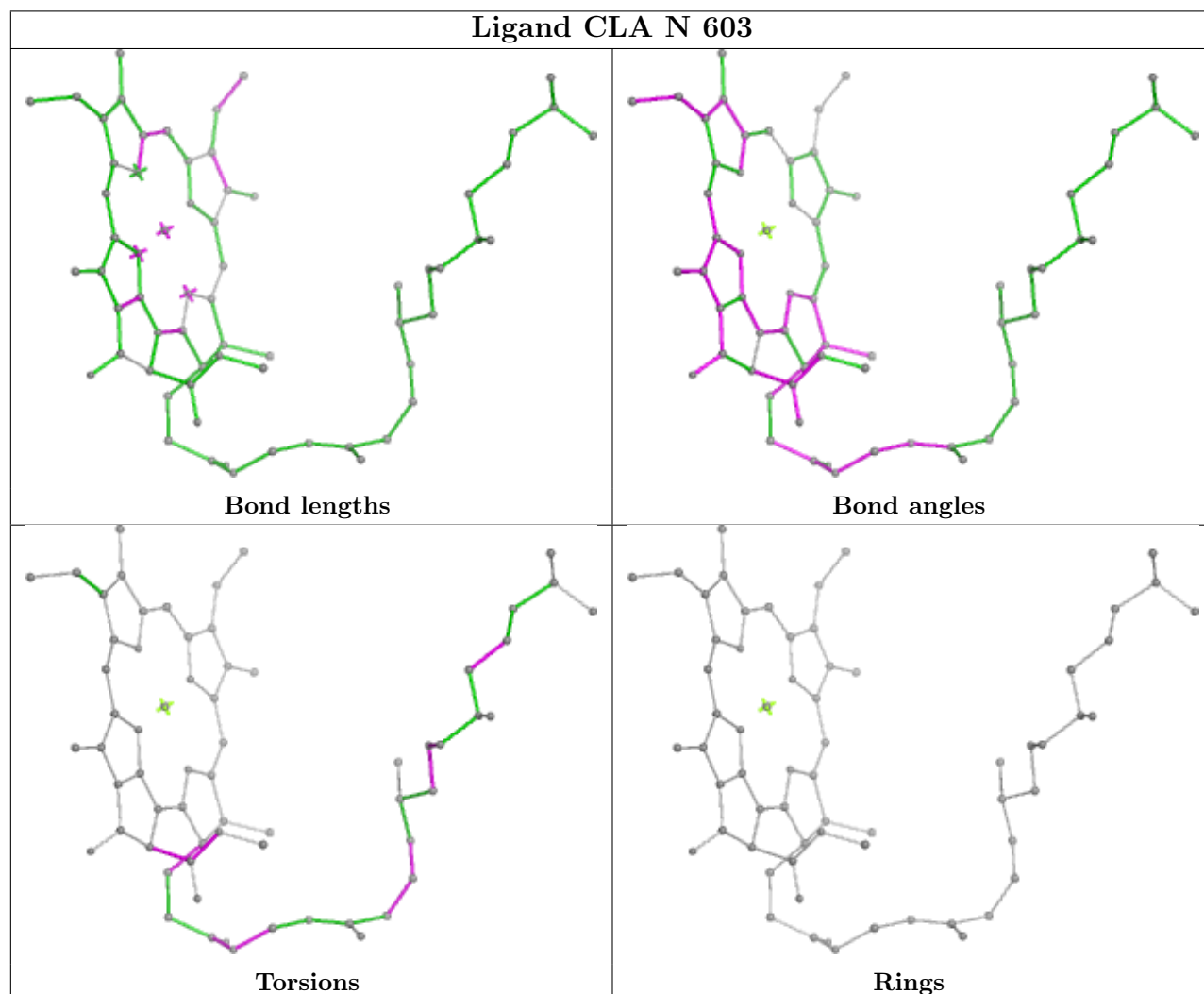


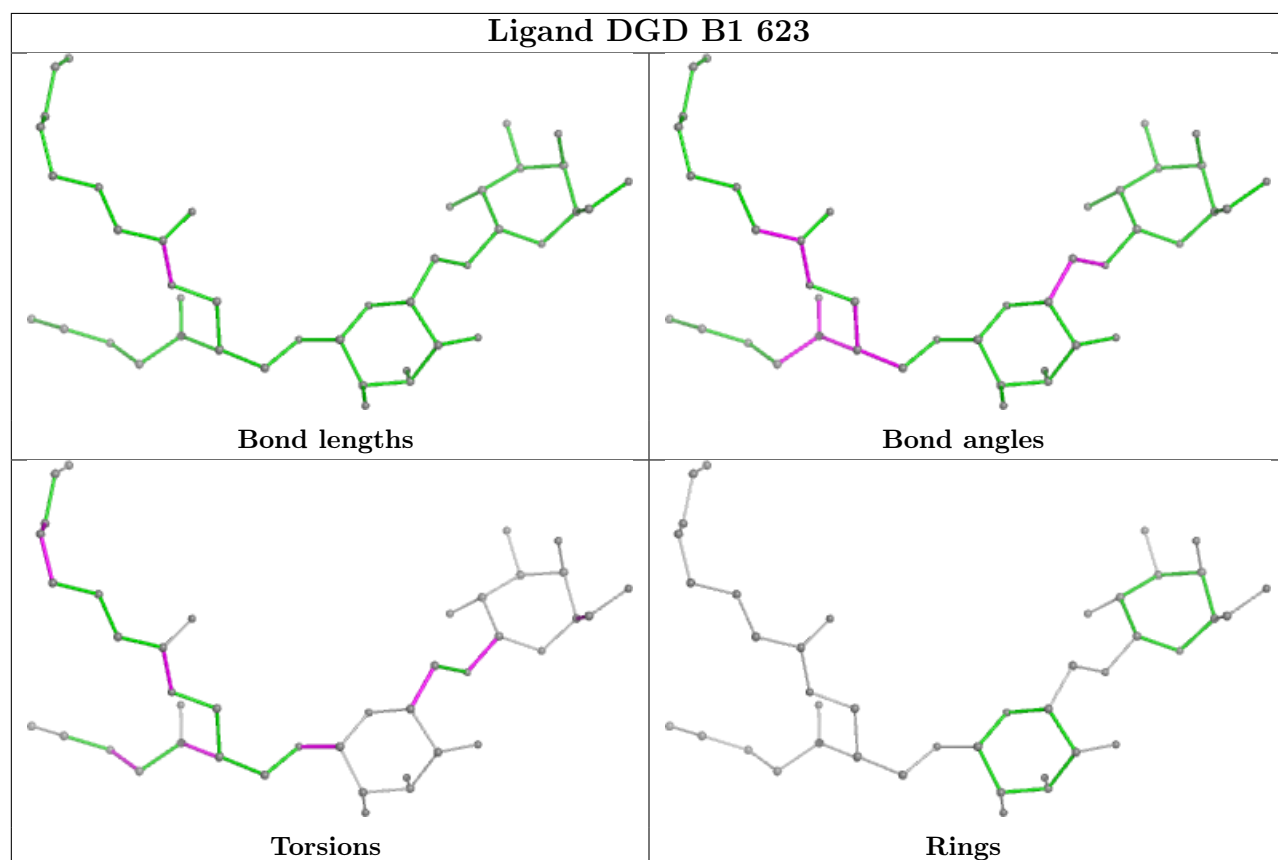
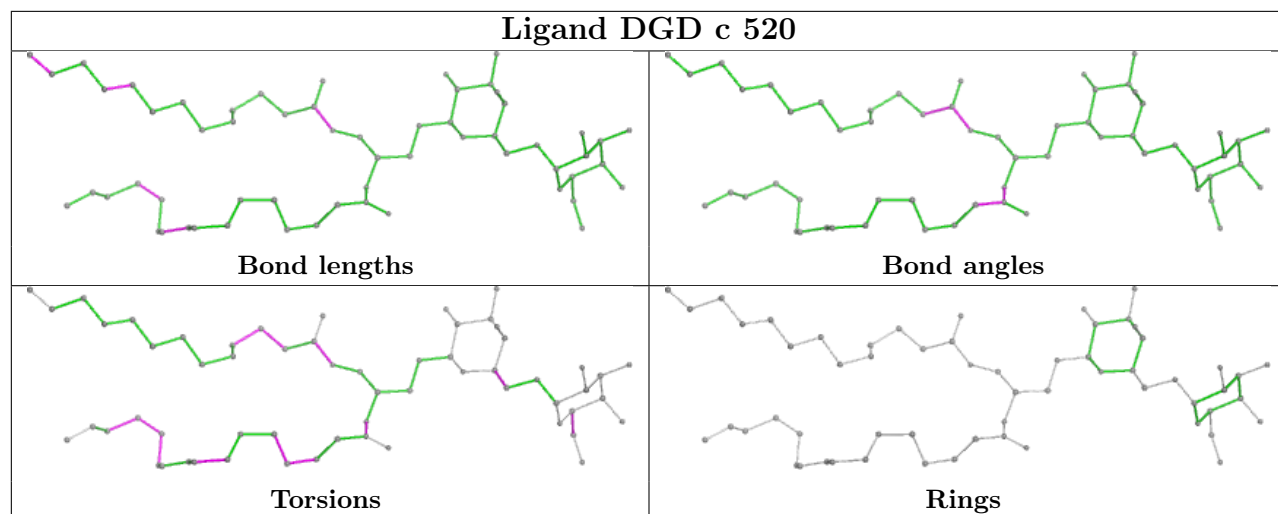


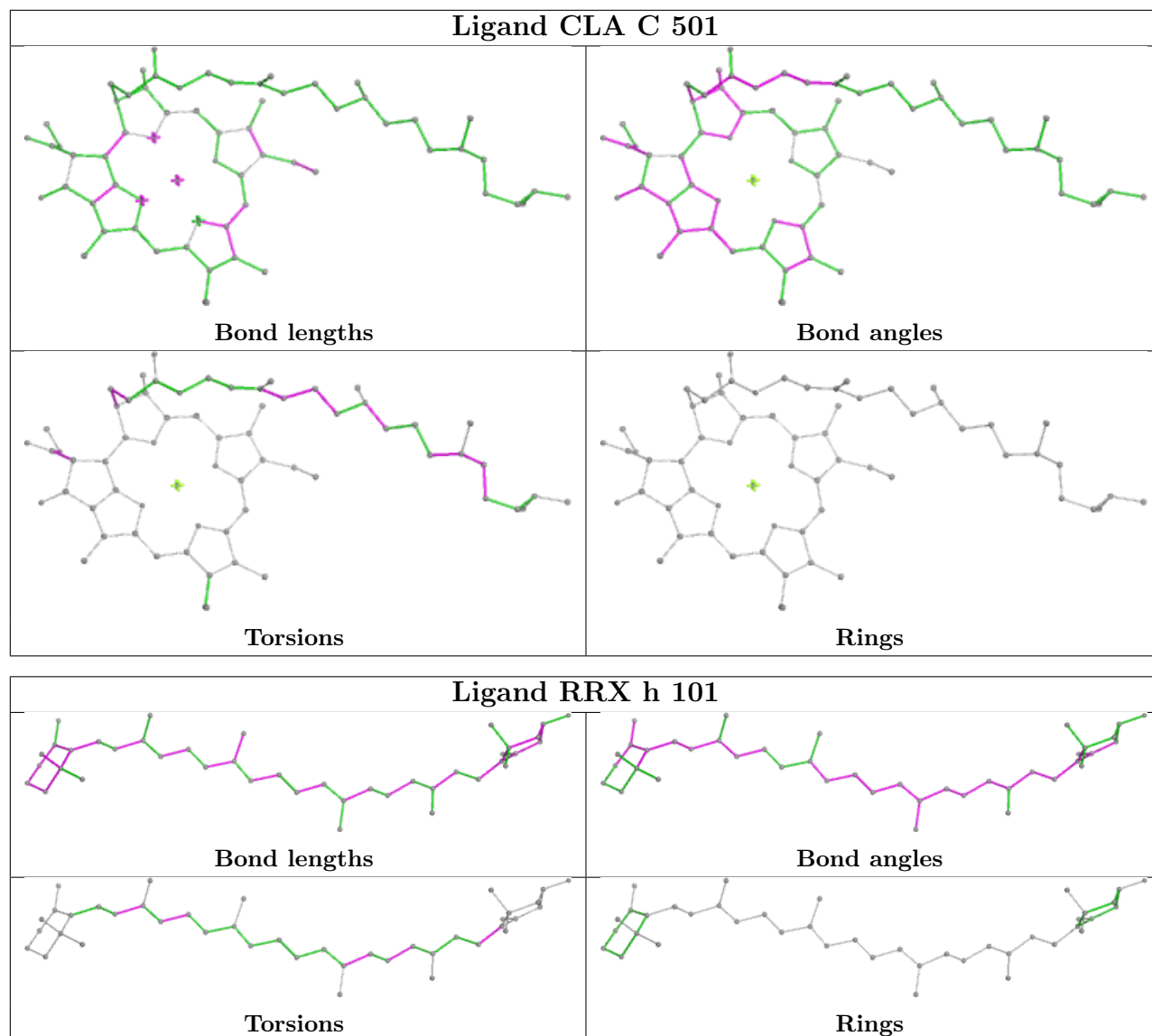




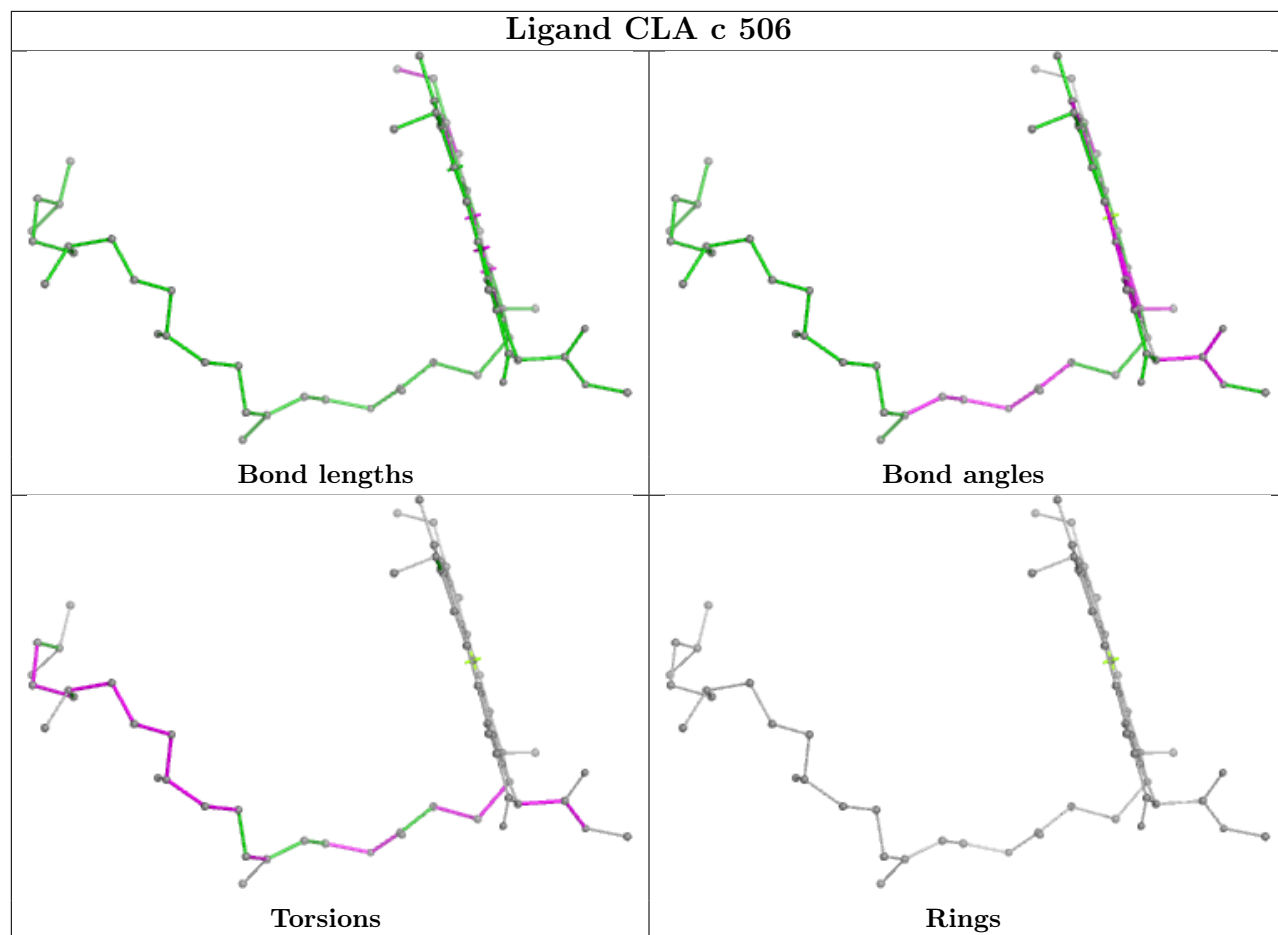


**Ligand CLA B 609****Ligand CLA N 603**



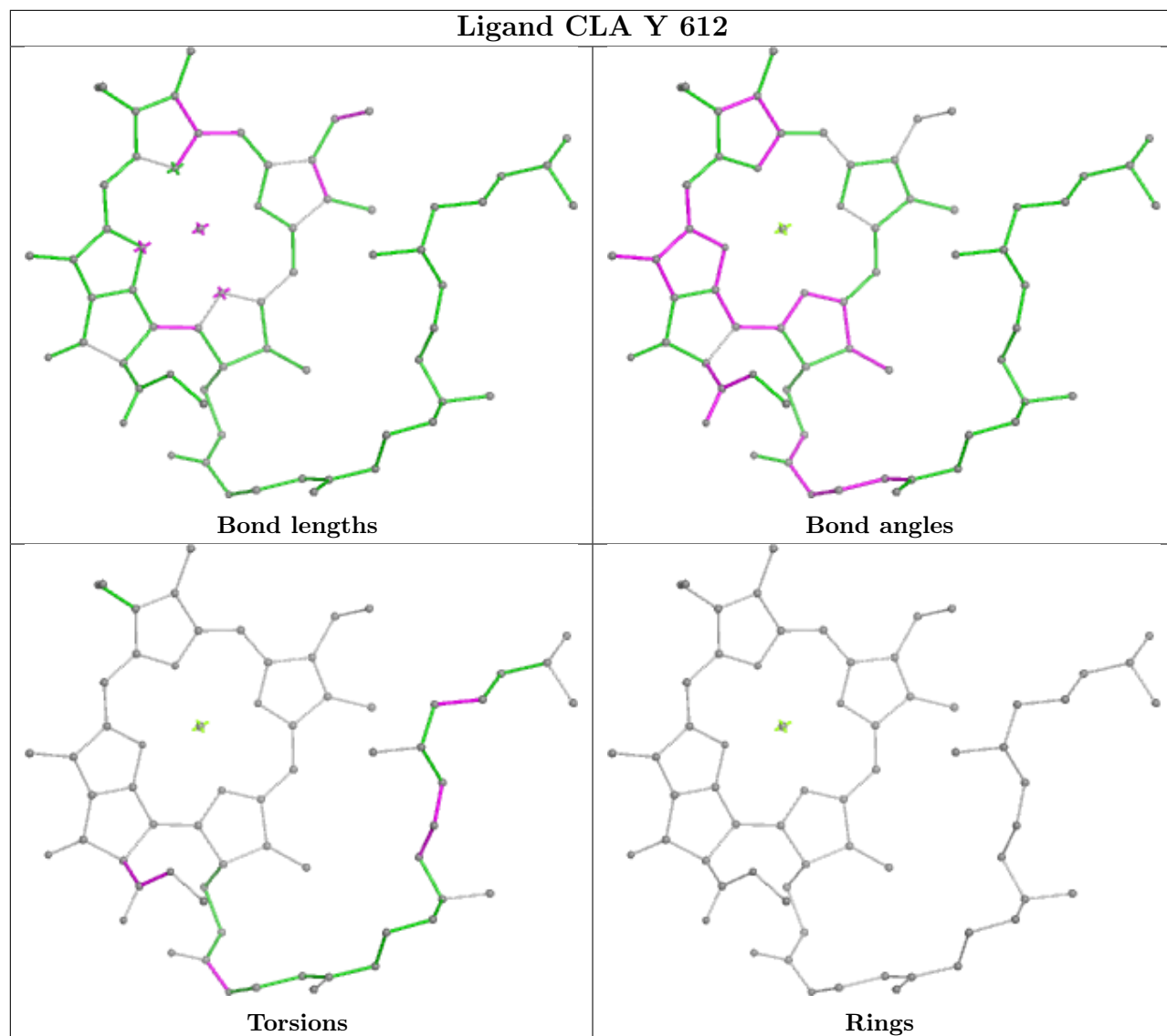


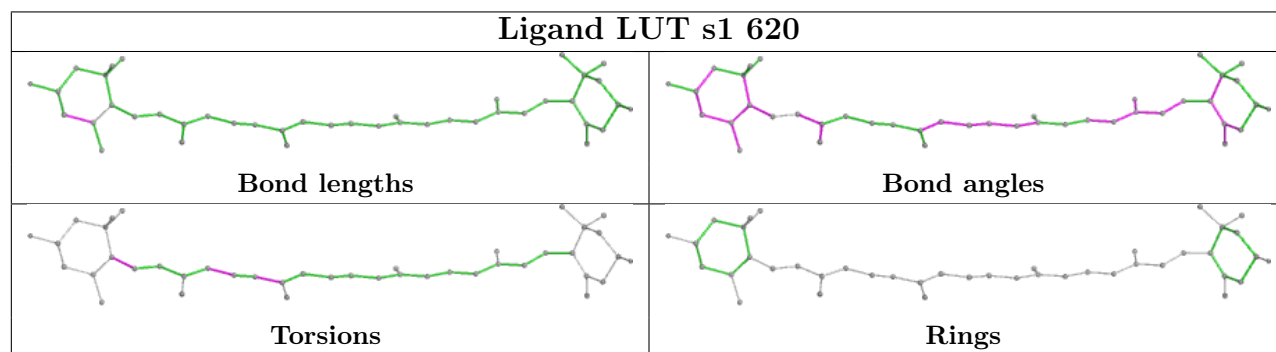
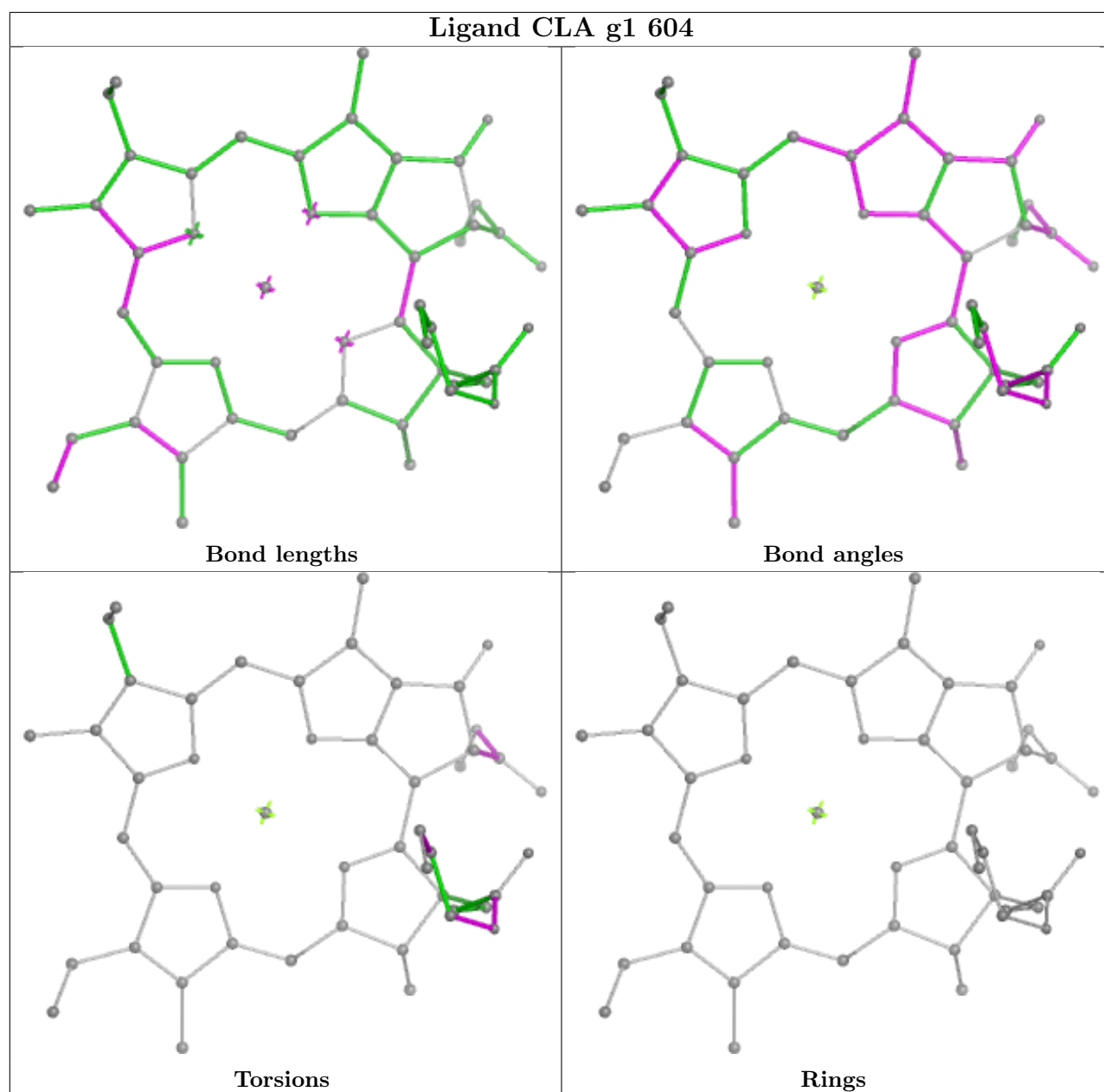
## Ligand CLA c 506

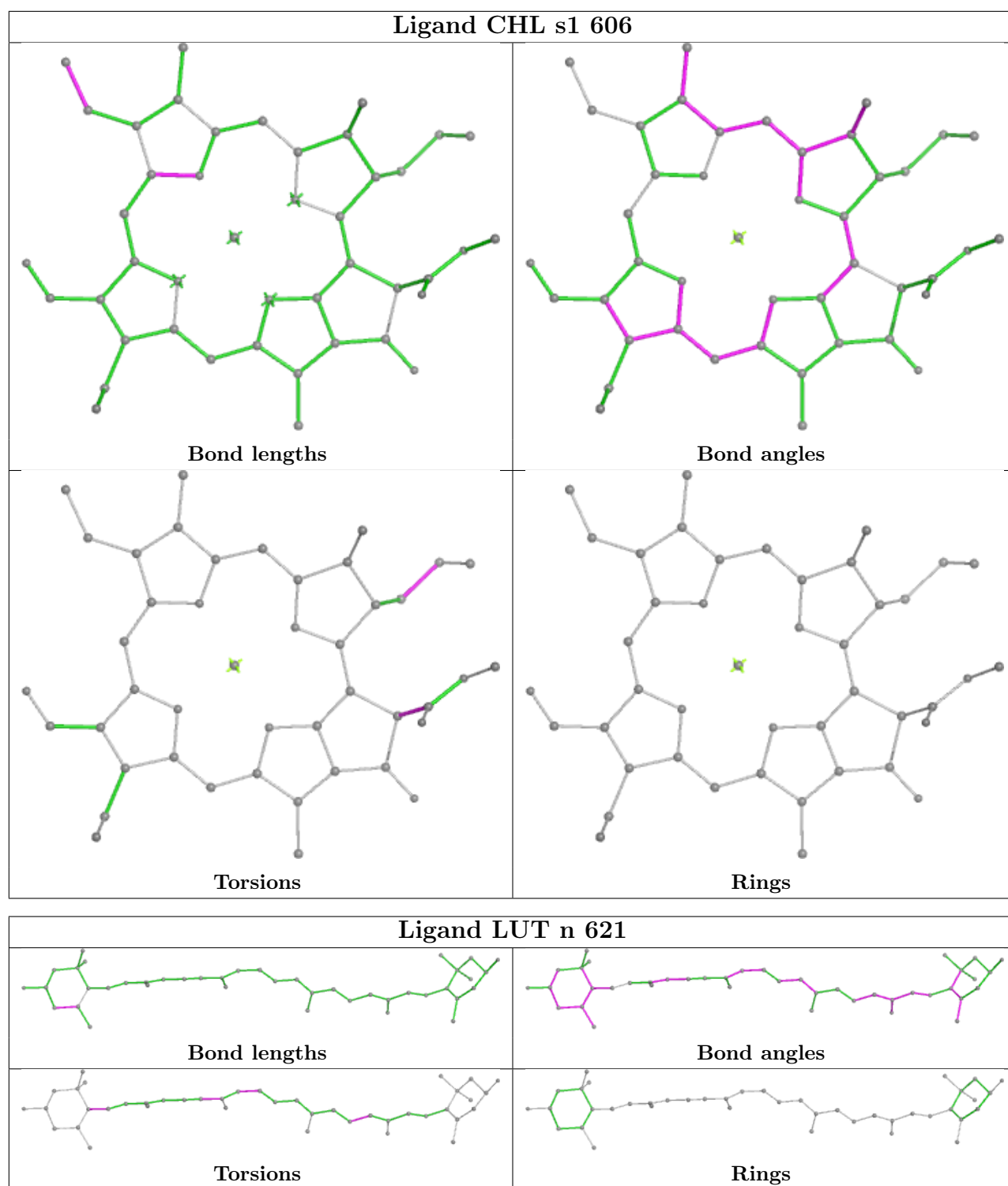


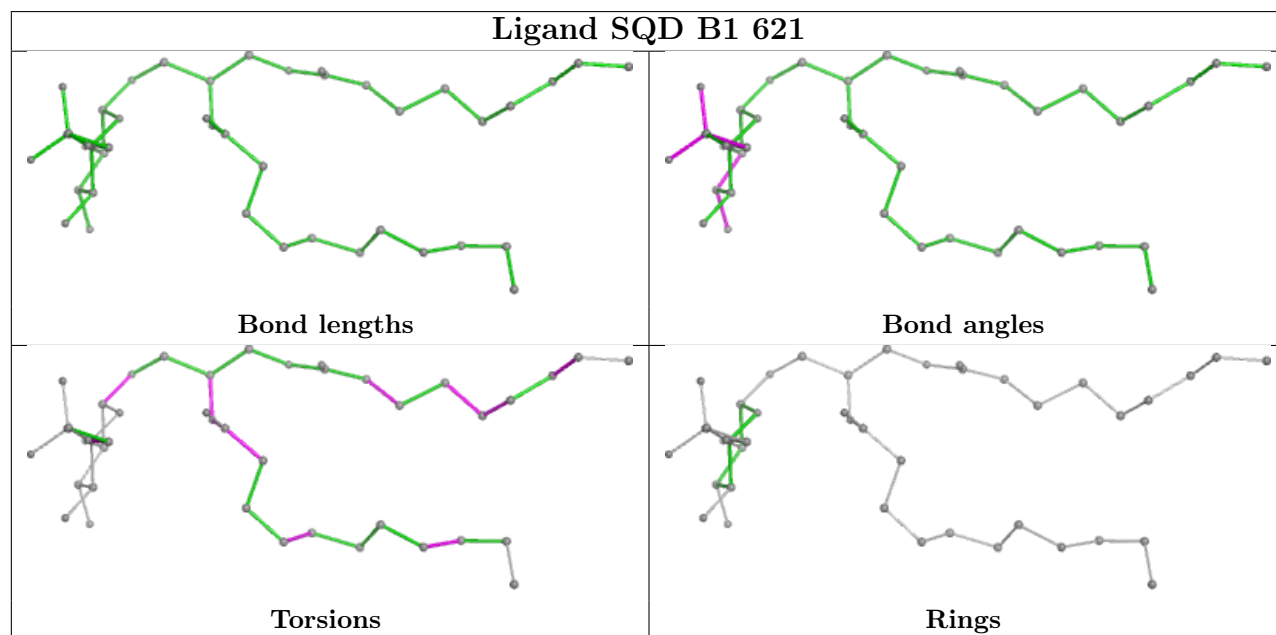
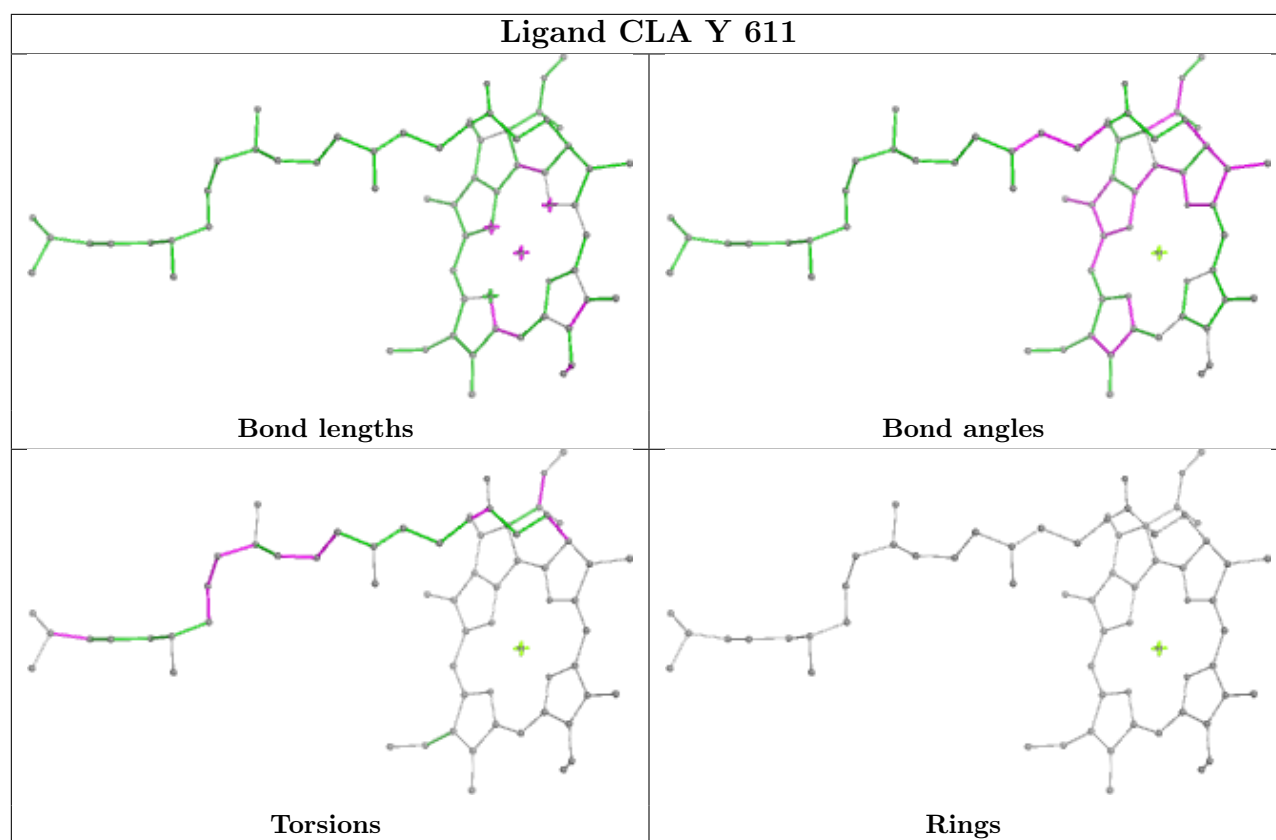


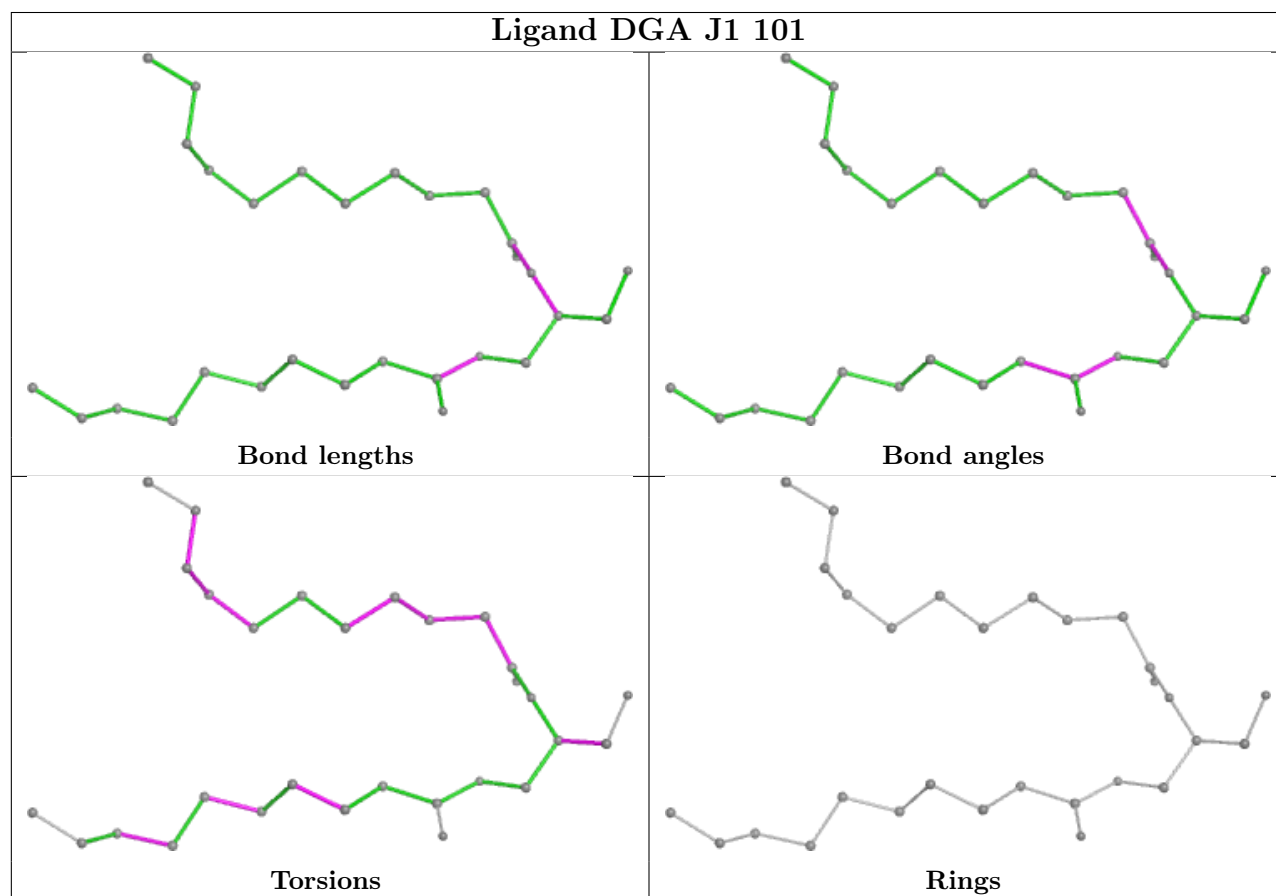
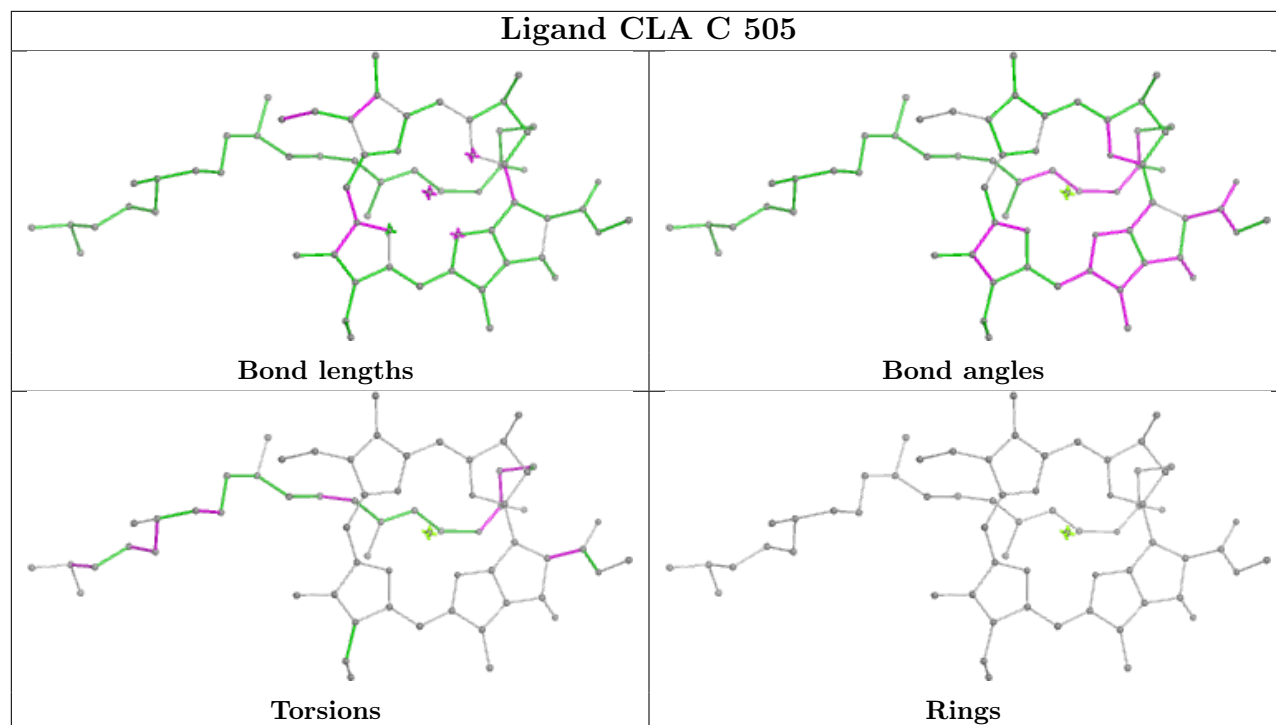
## Ligand CLA Y 612

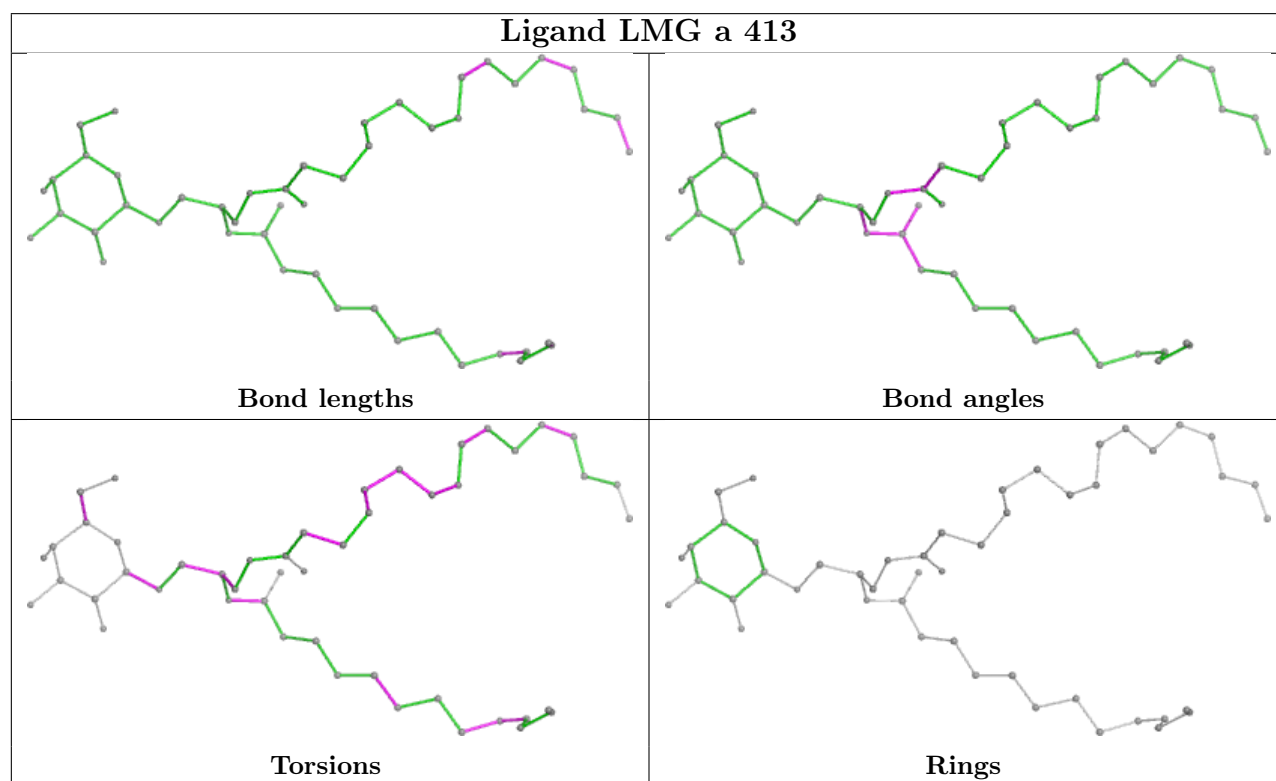
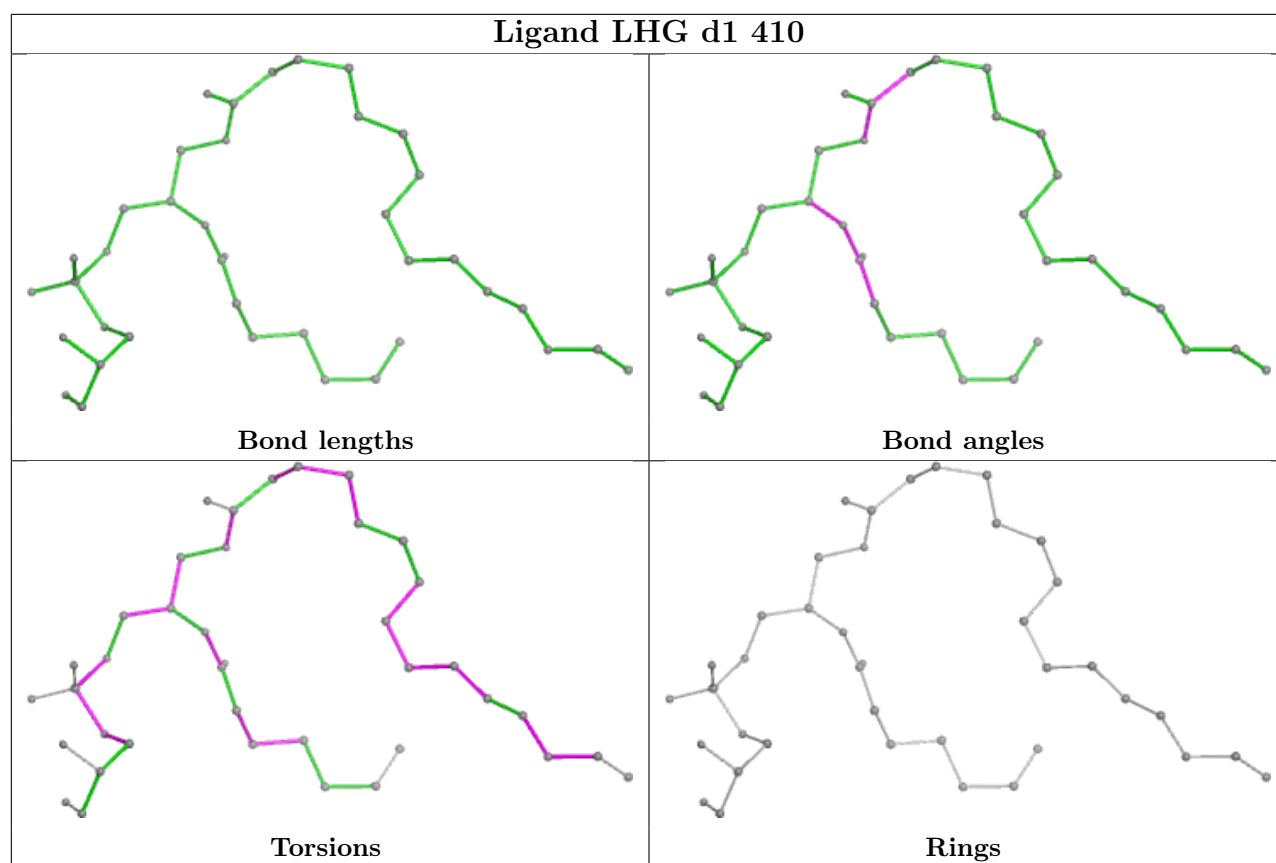


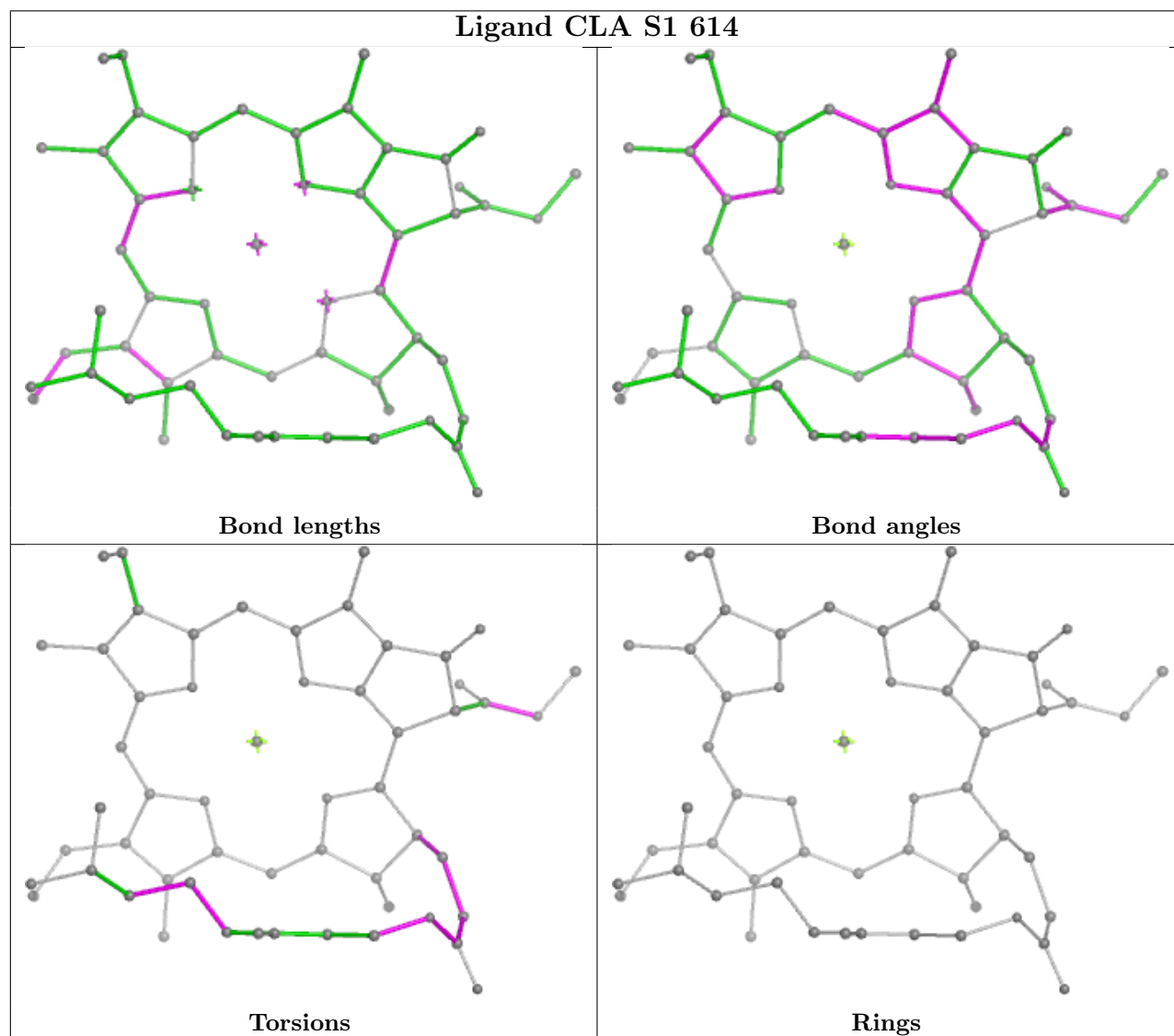
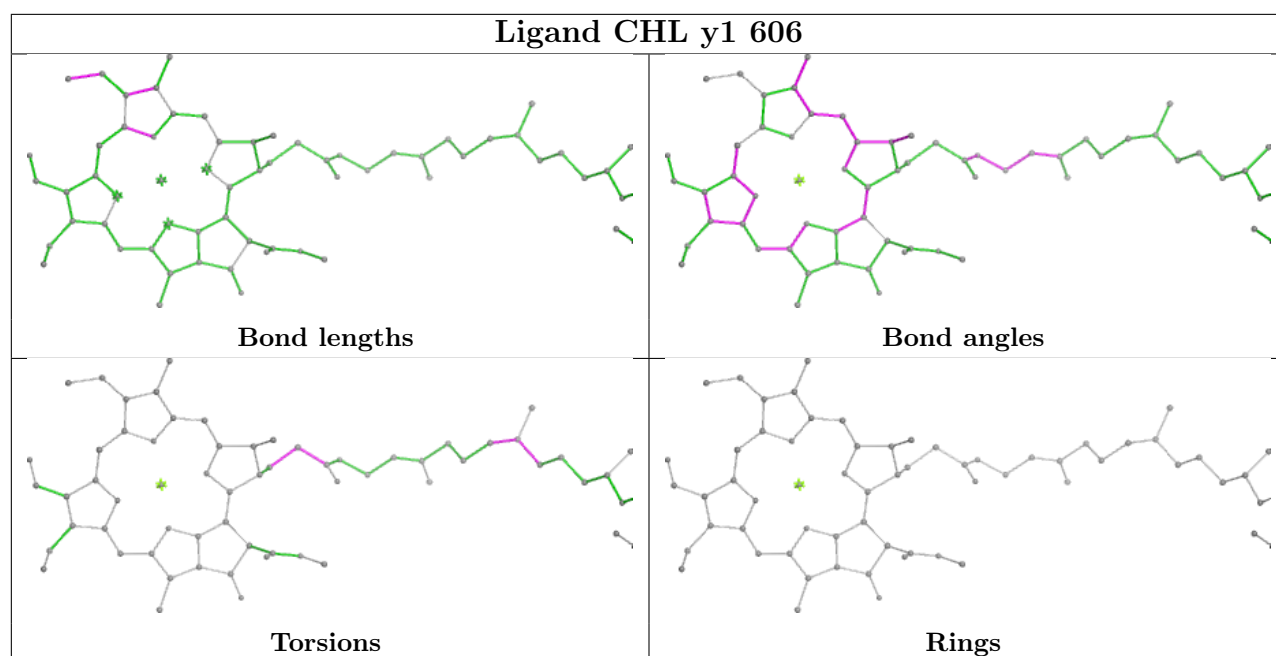


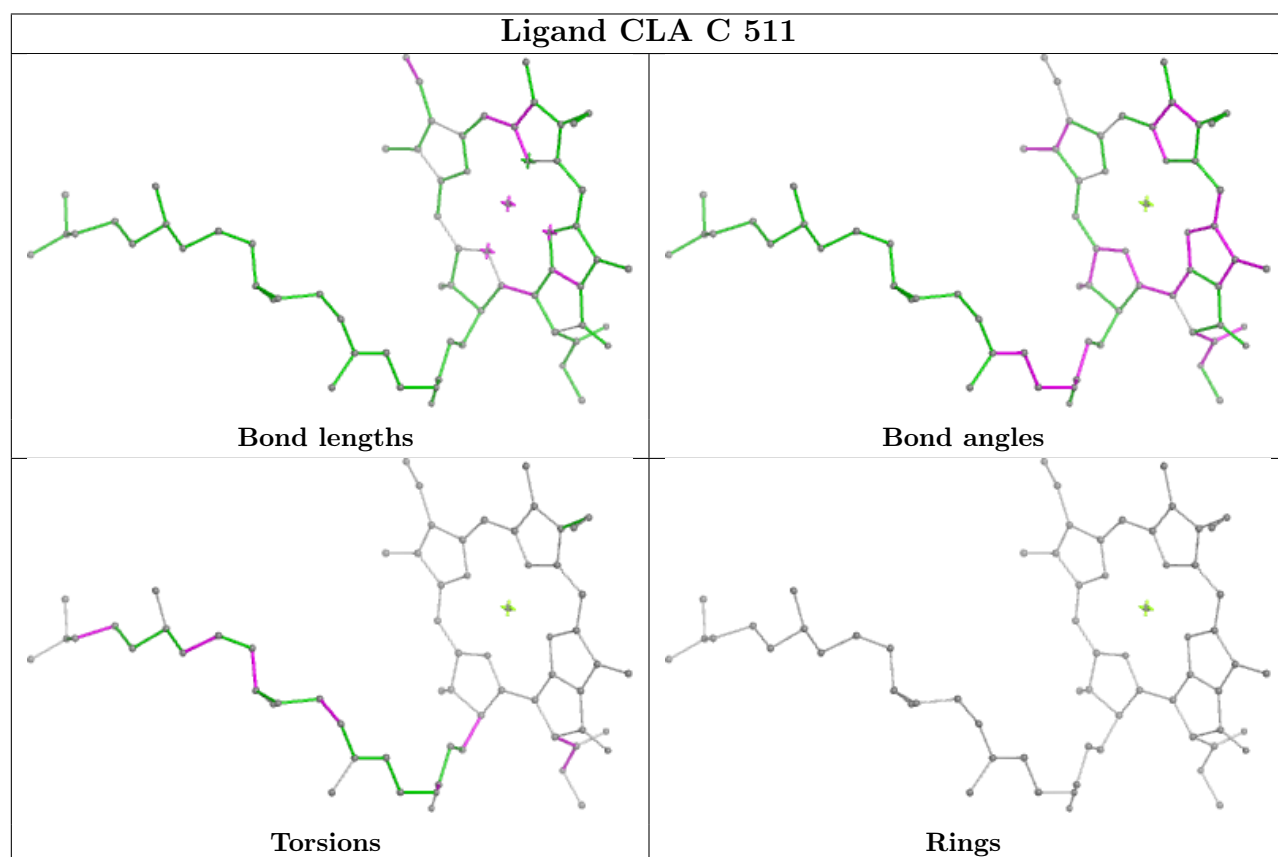
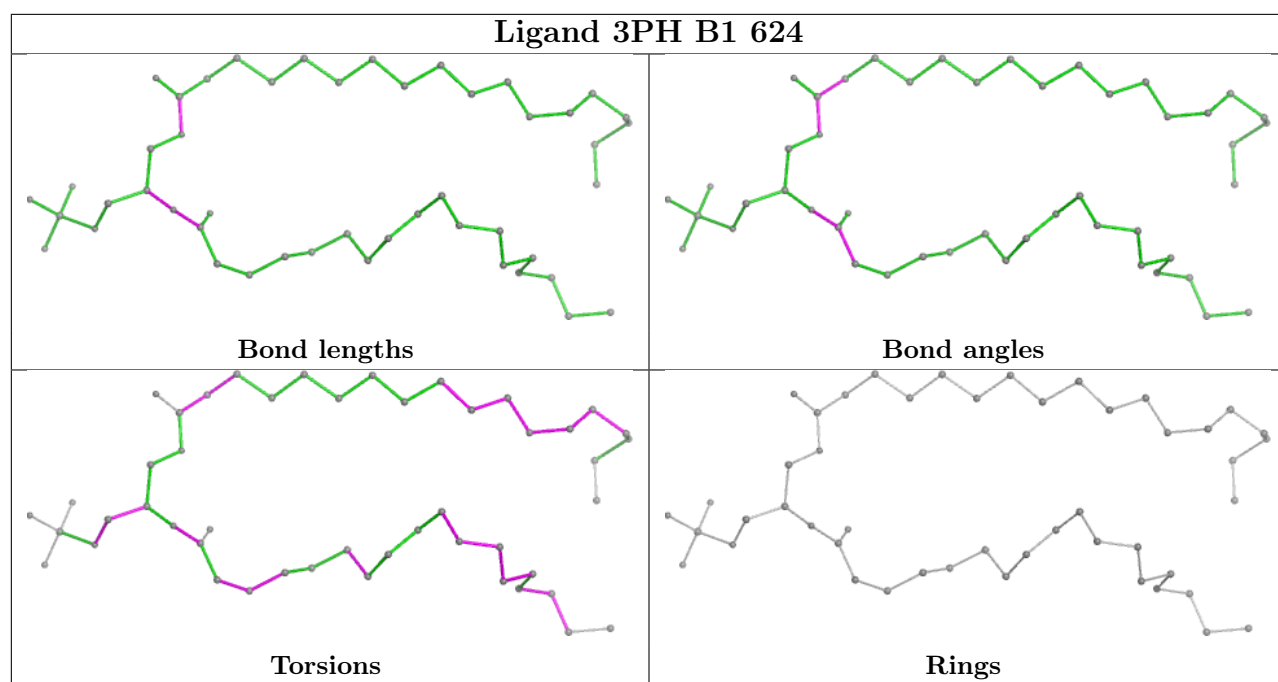




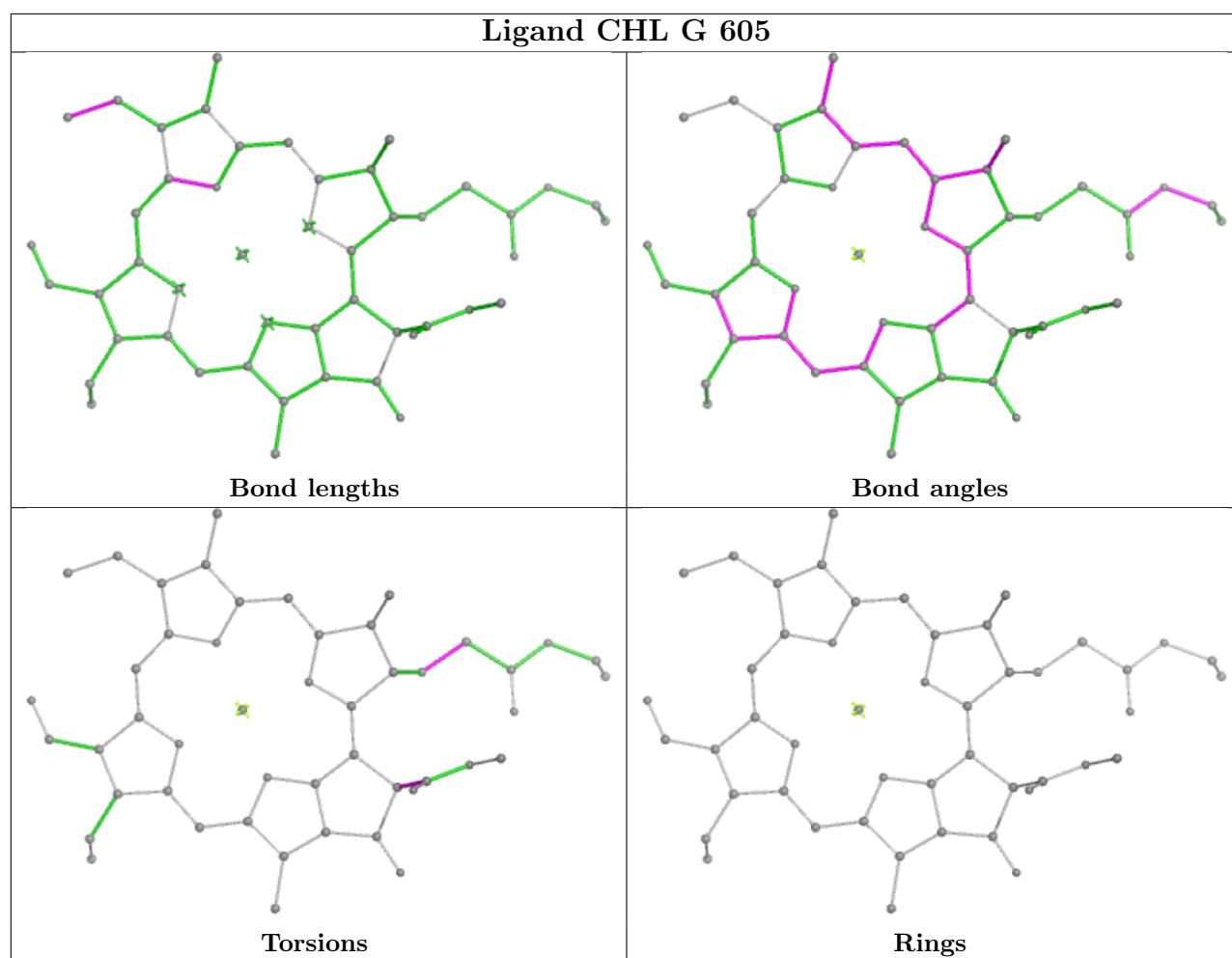




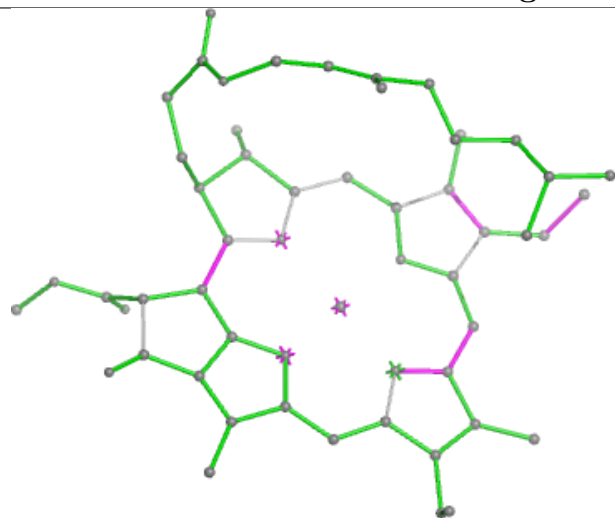




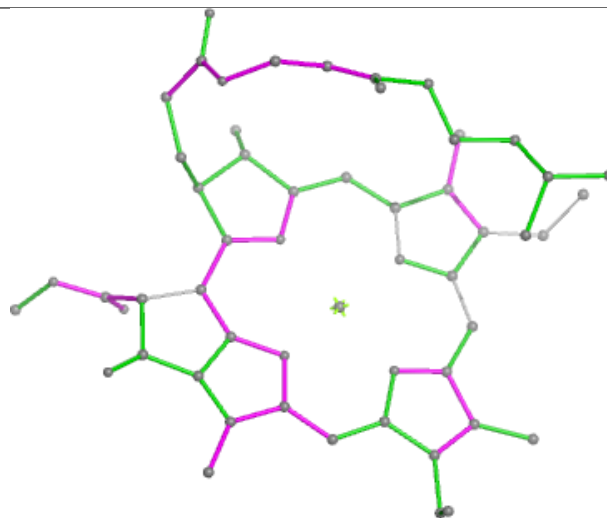




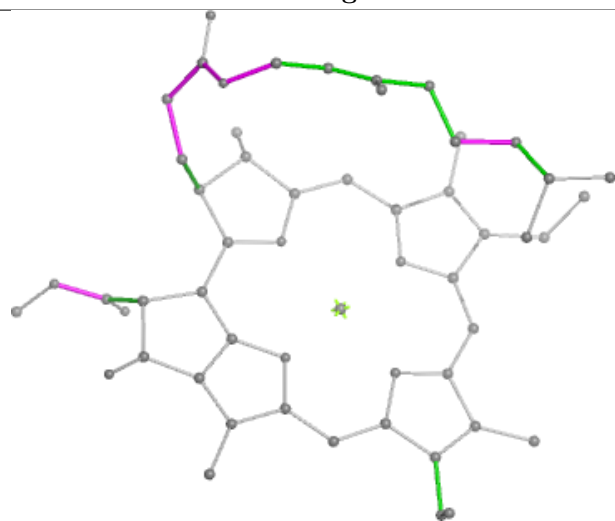
## Ligand CLA S 614



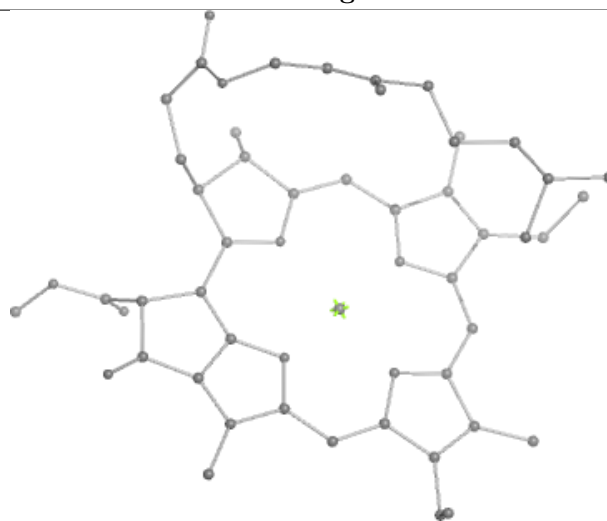
Bond lengths



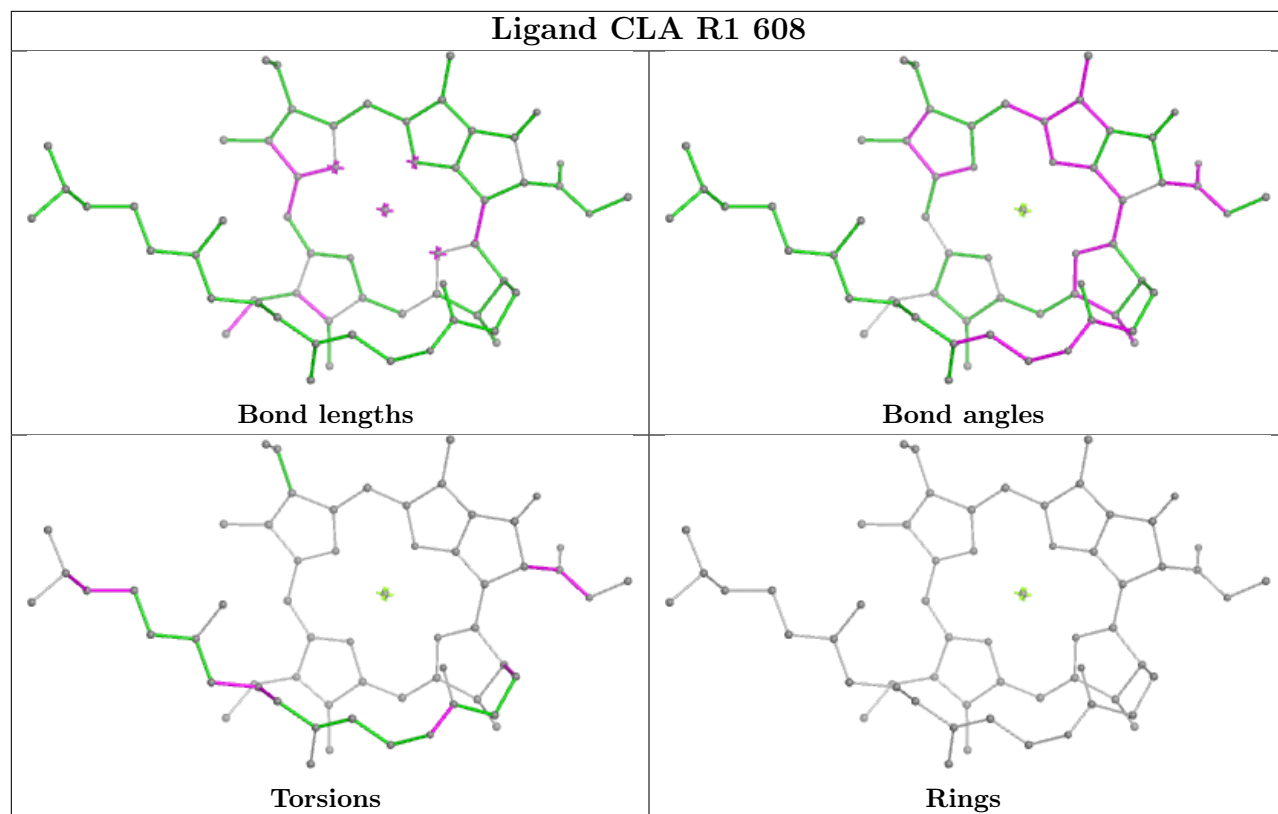
Bond angles



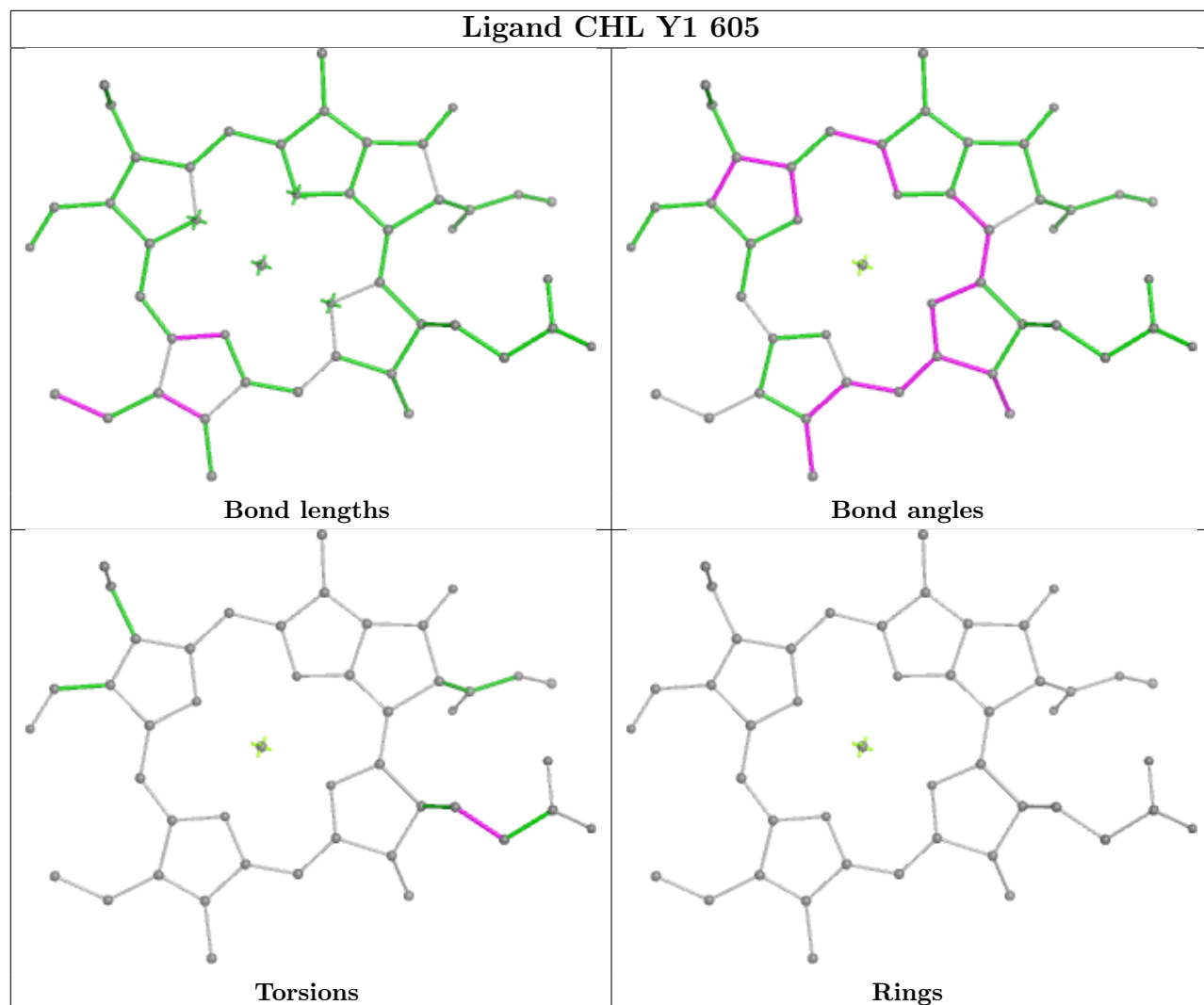
Torsions

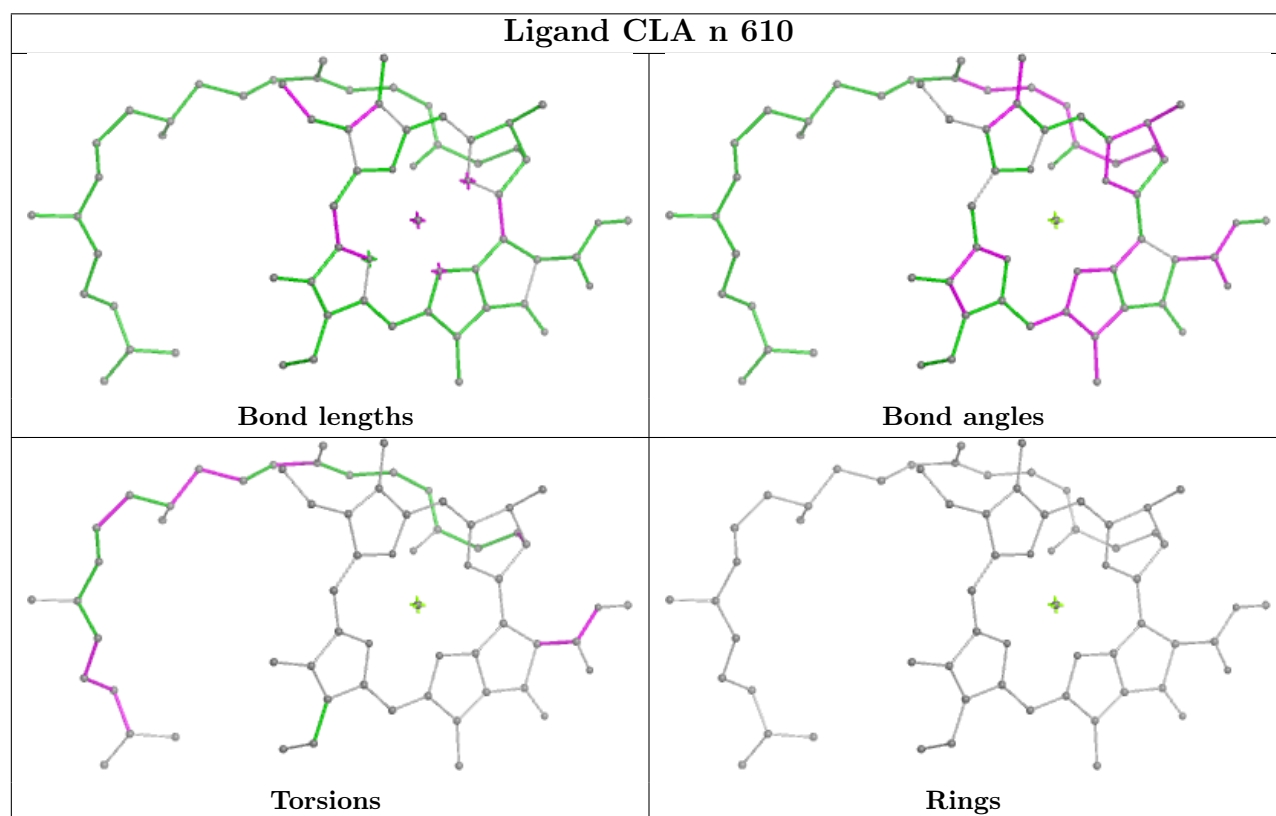
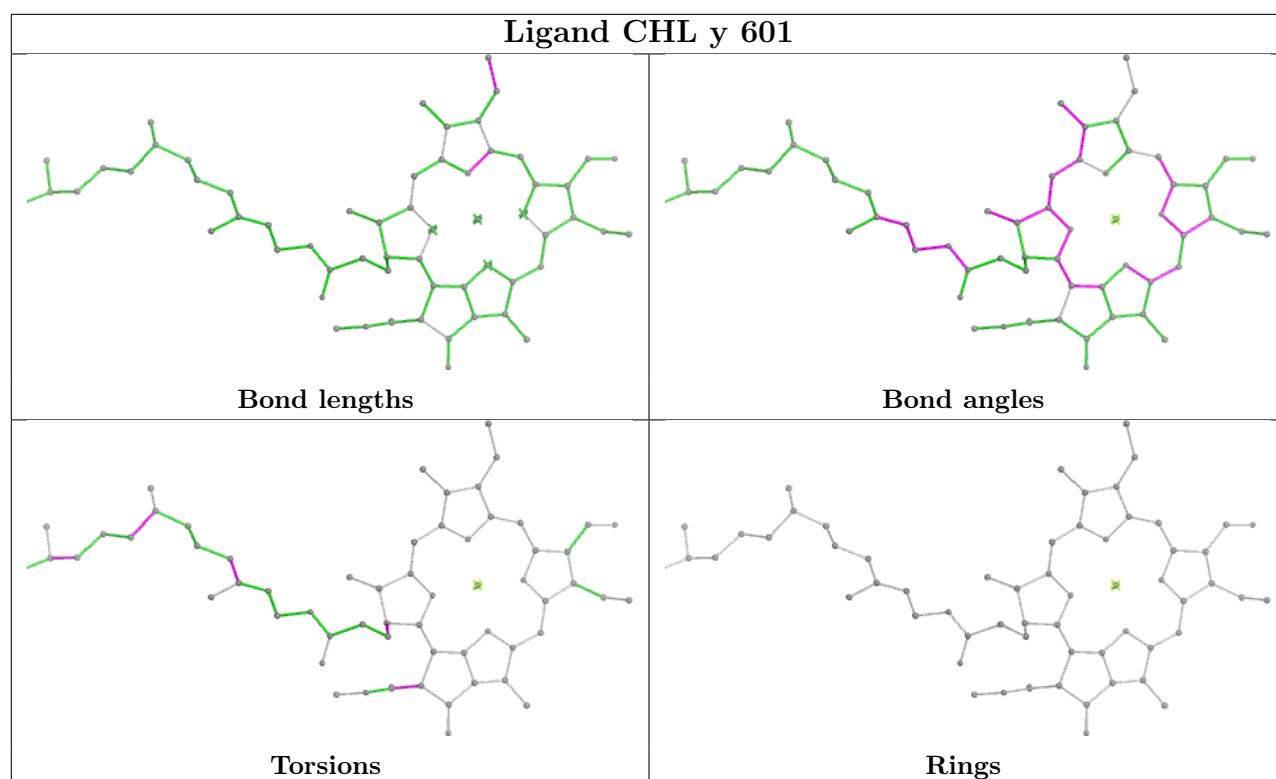


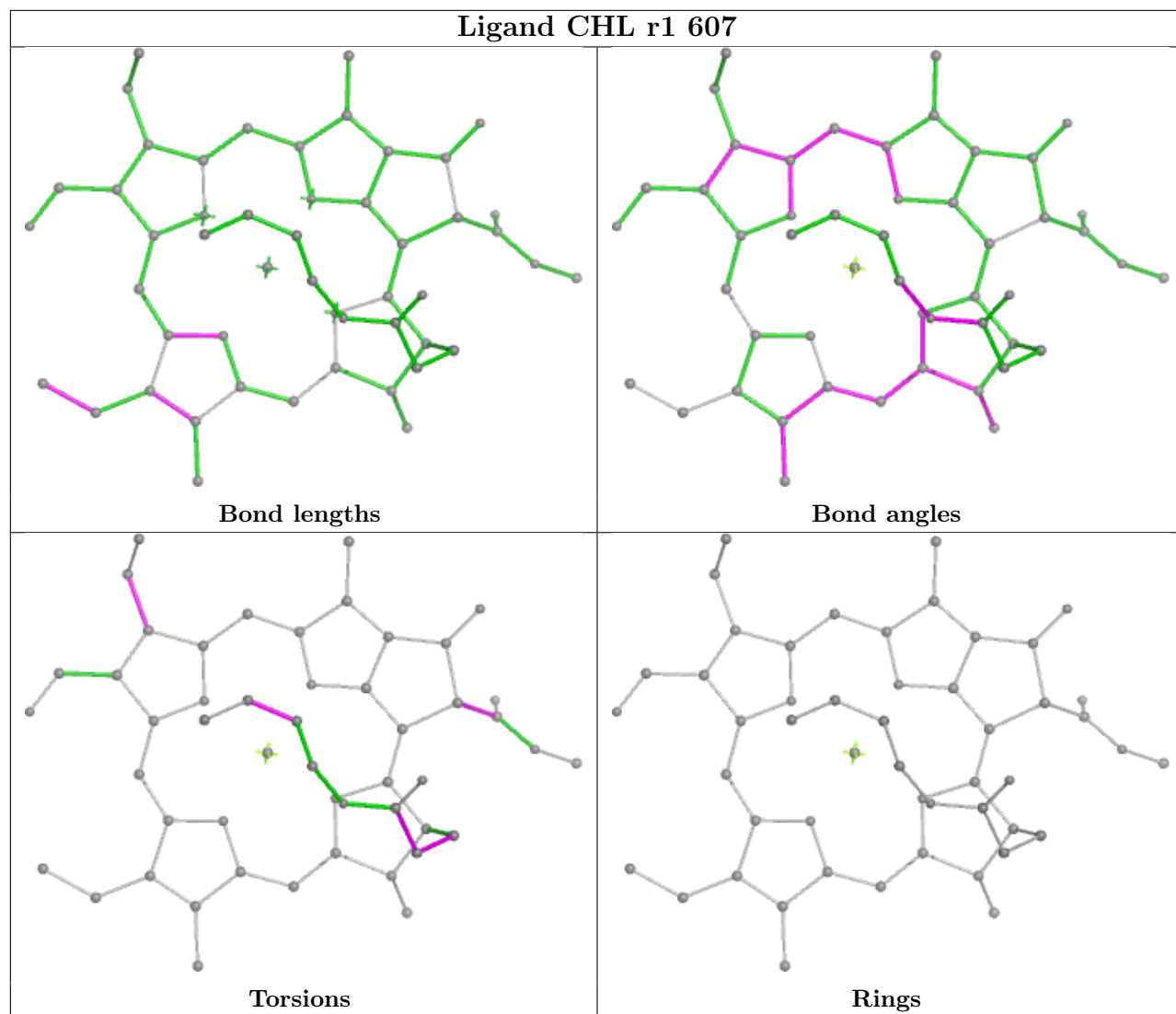
Rings

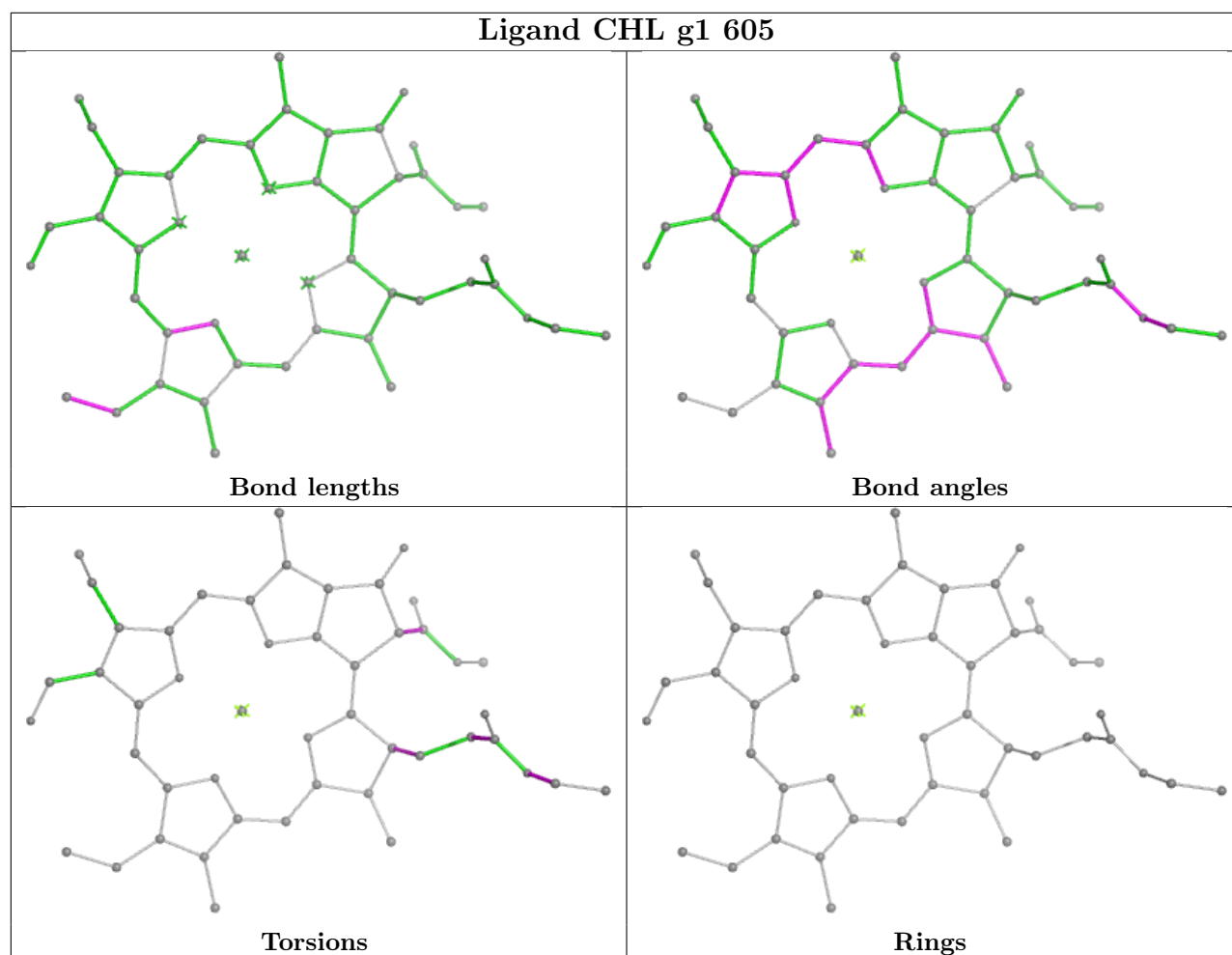
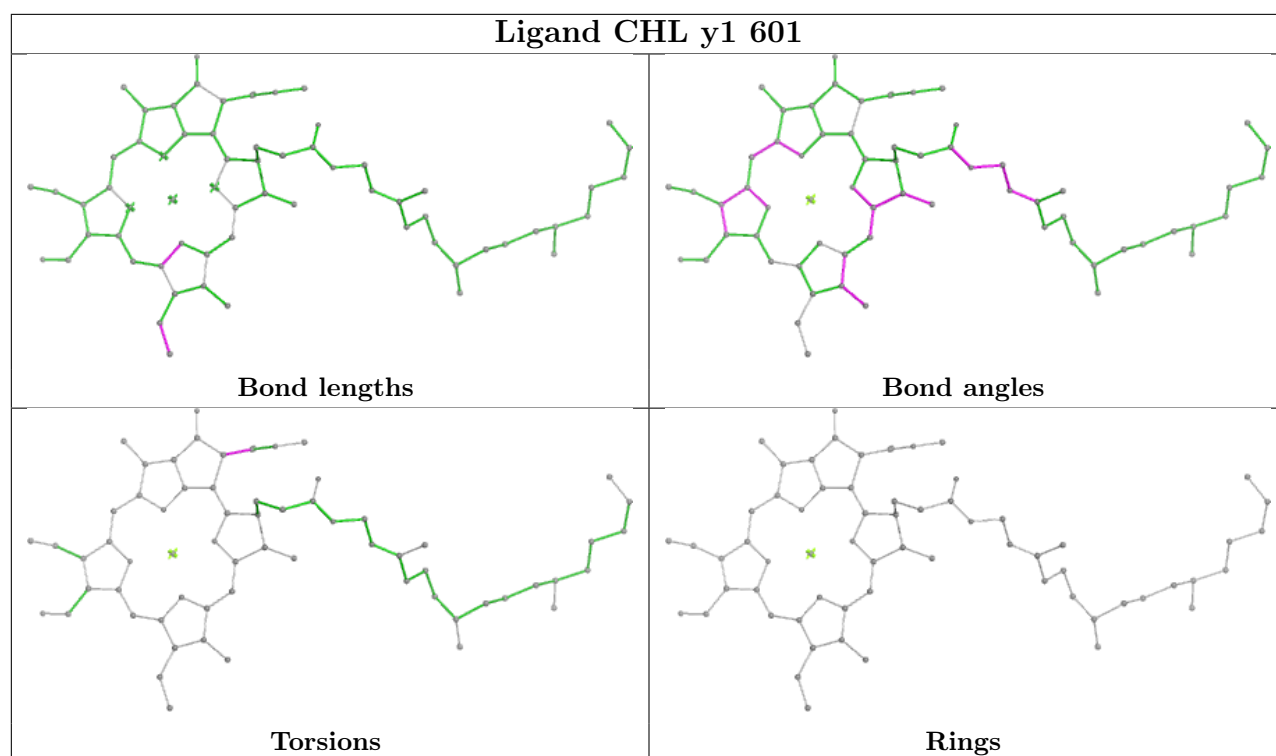


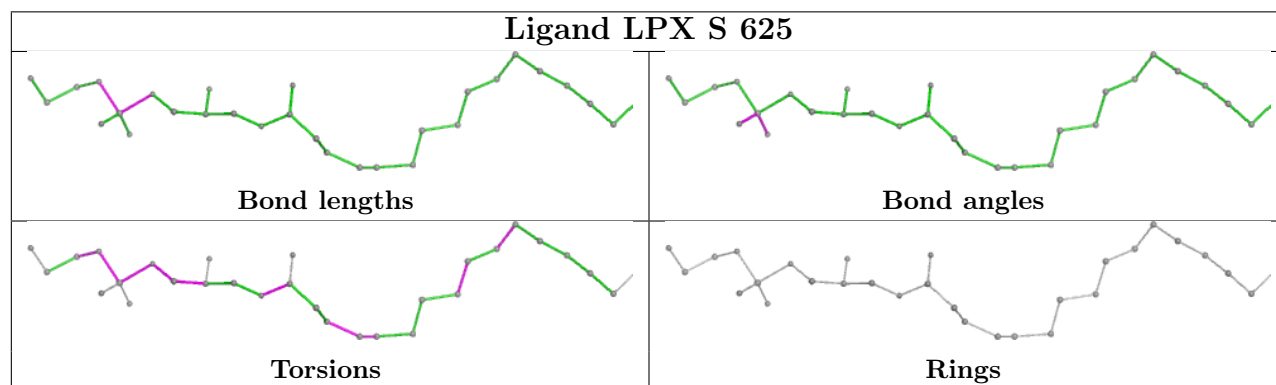
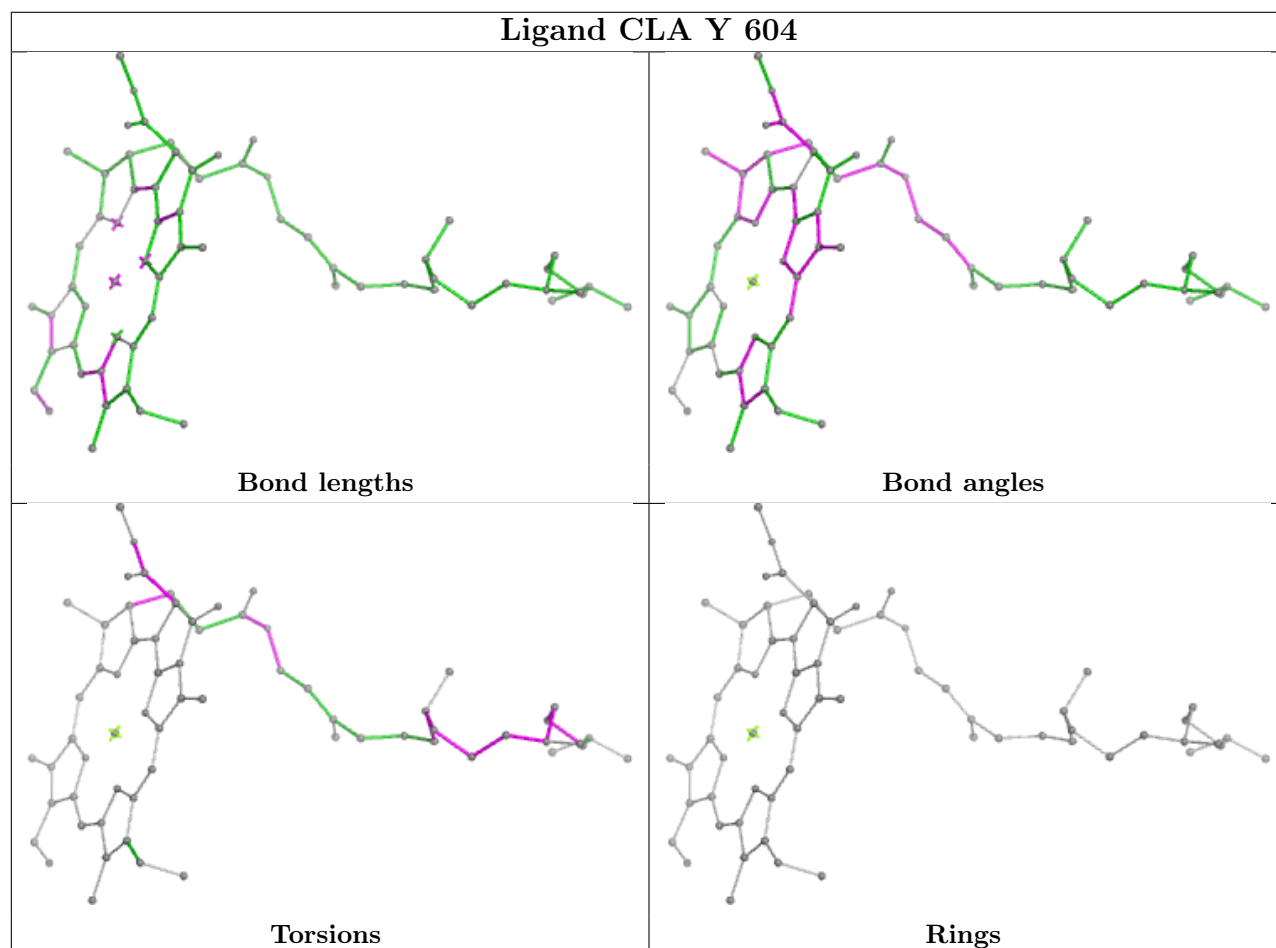
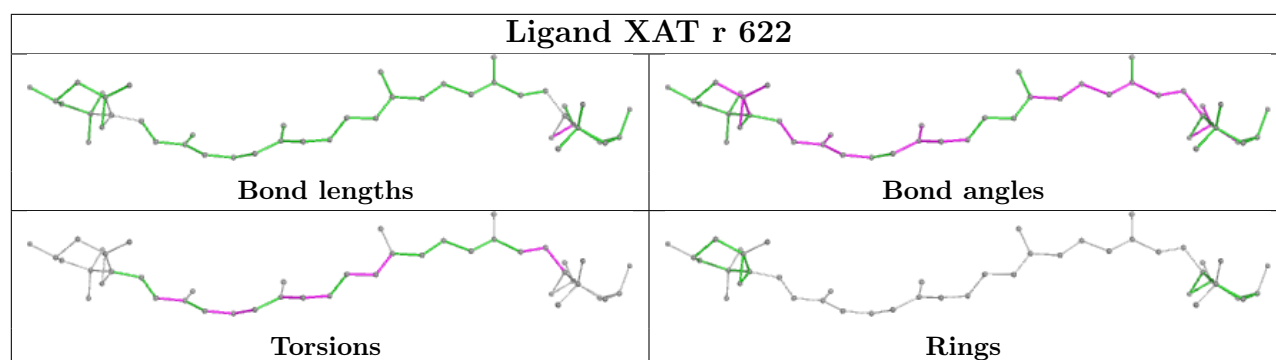
## Ligand CHL Y1 605



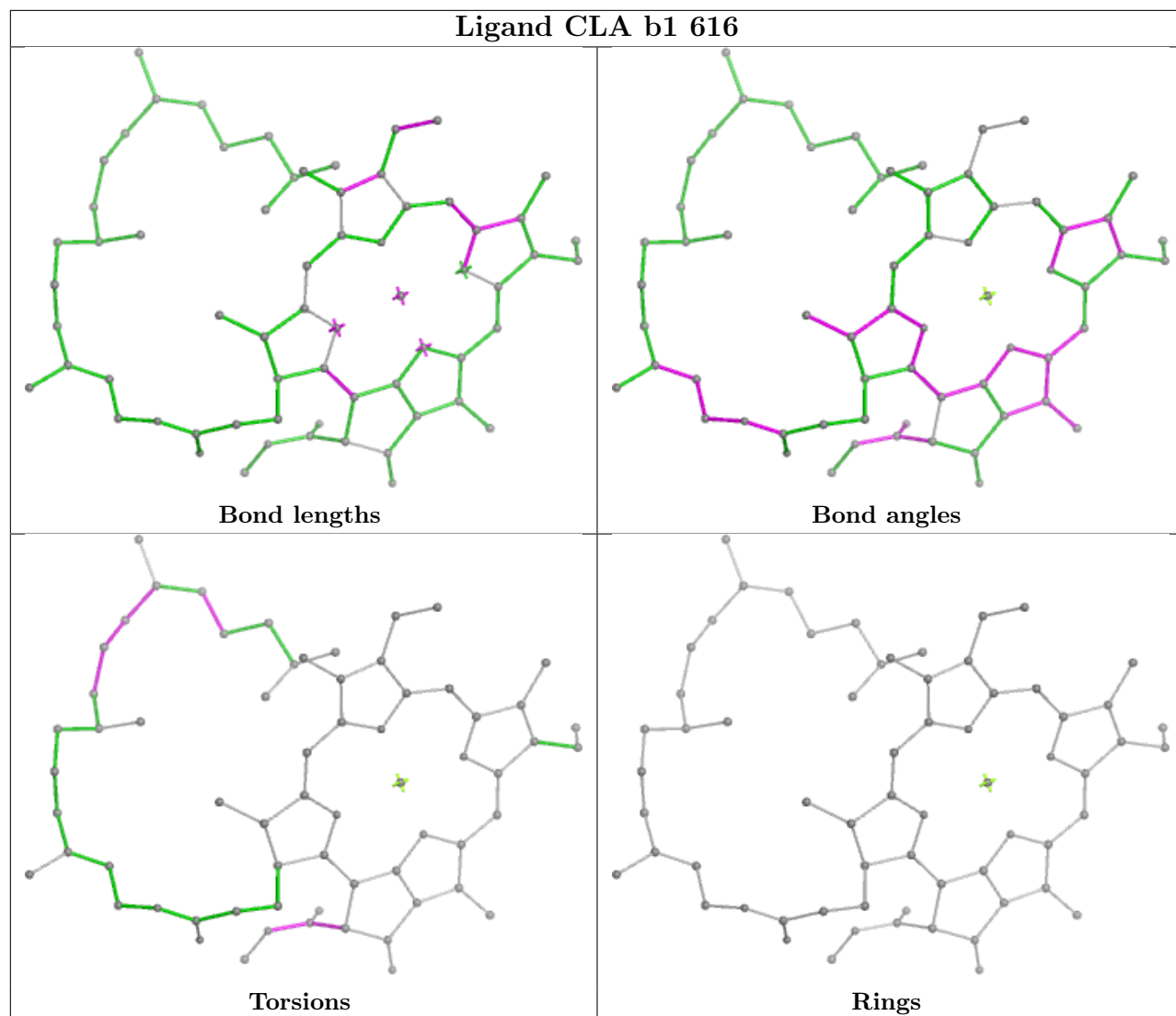


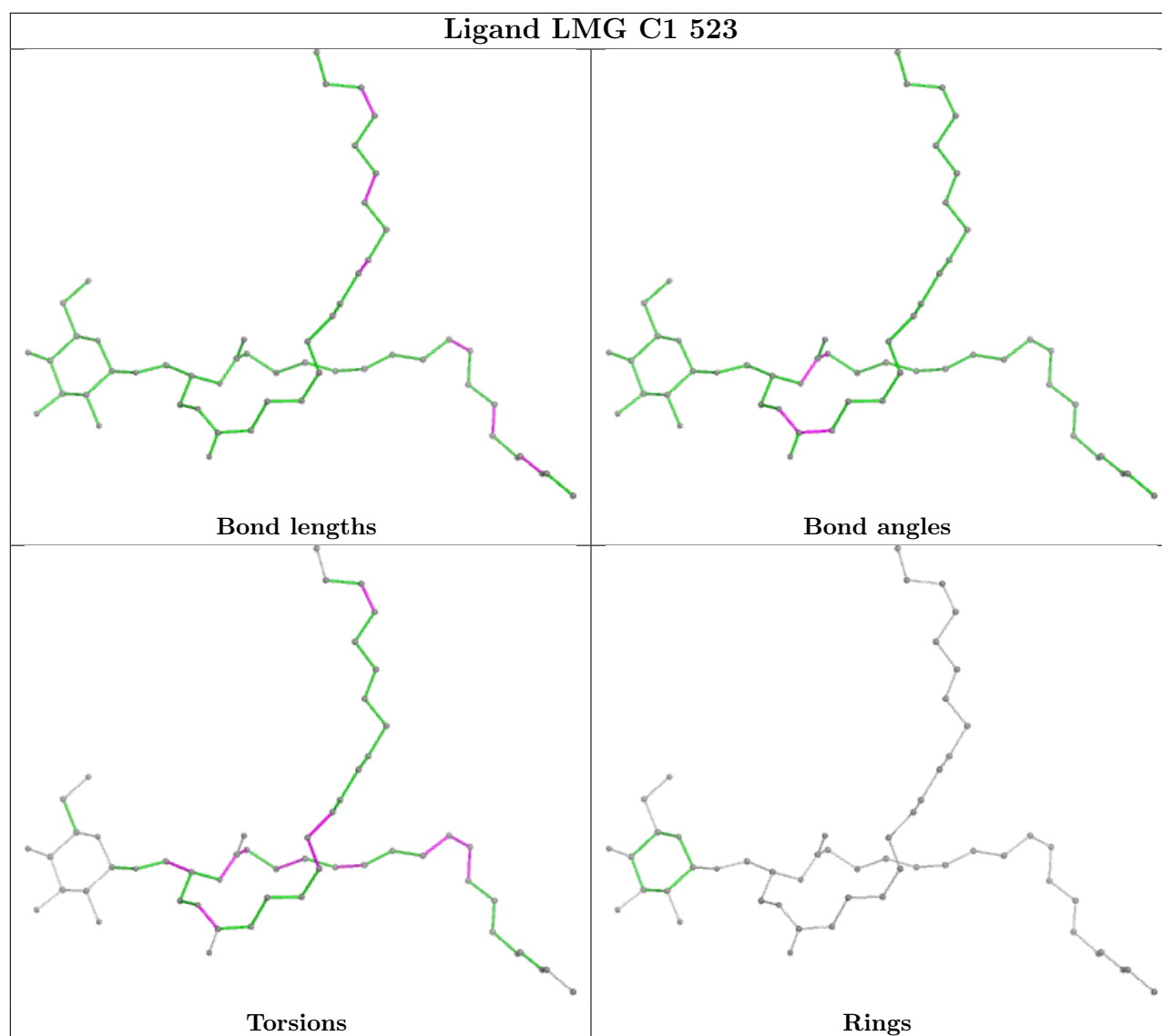




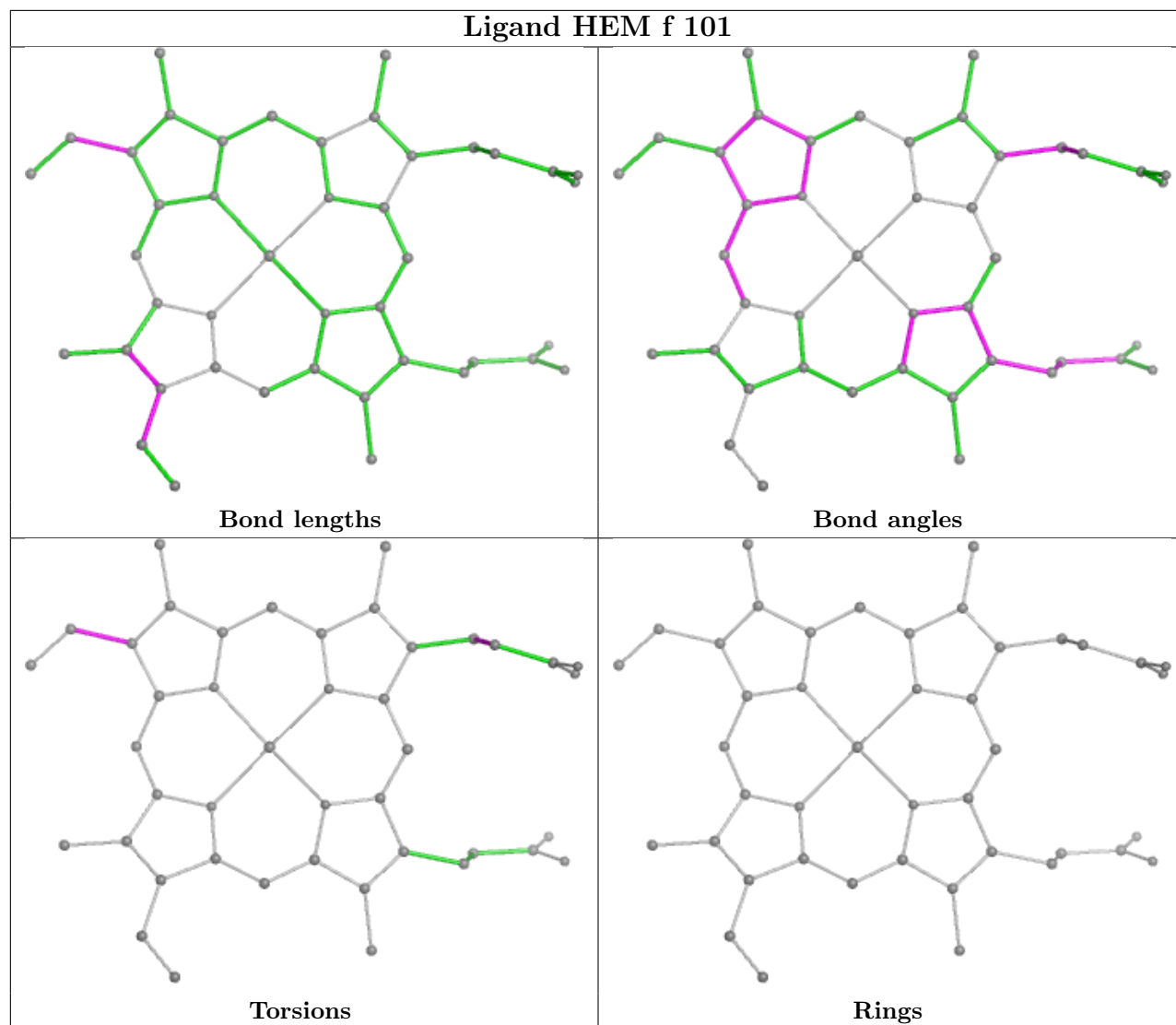


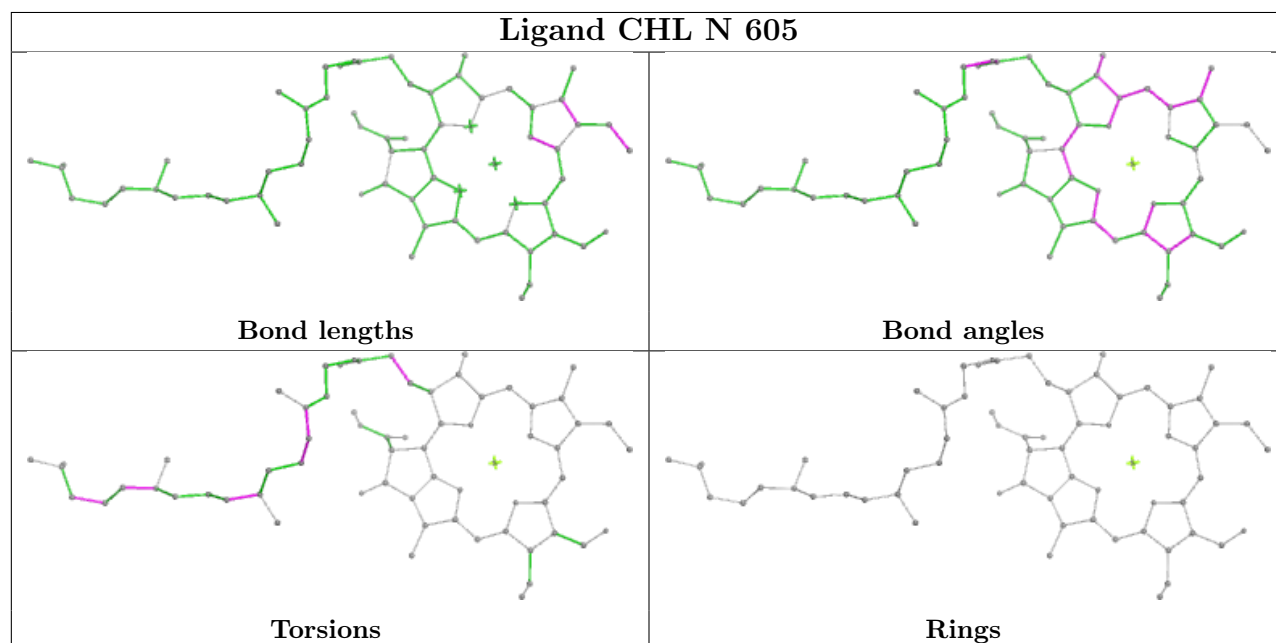
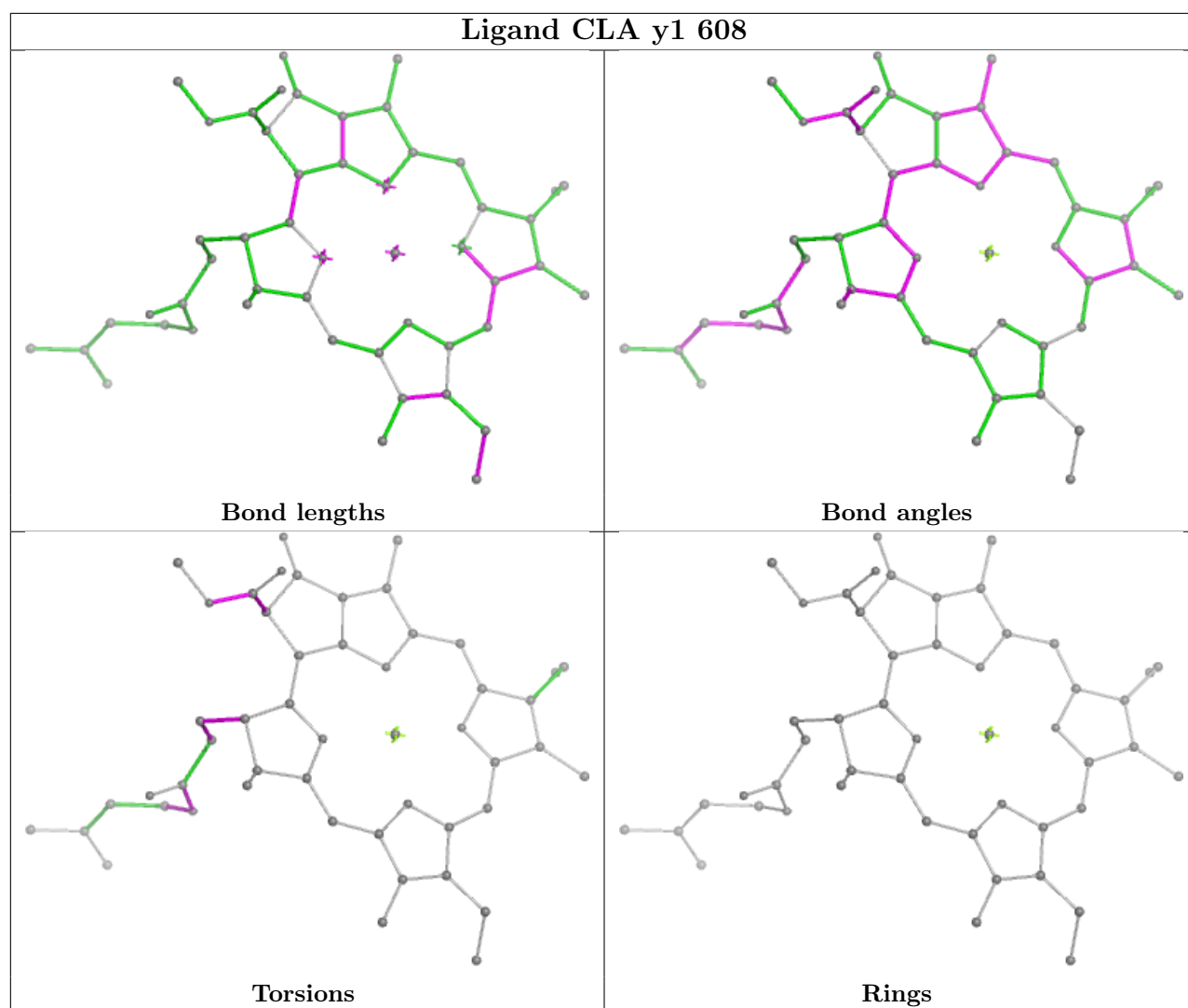


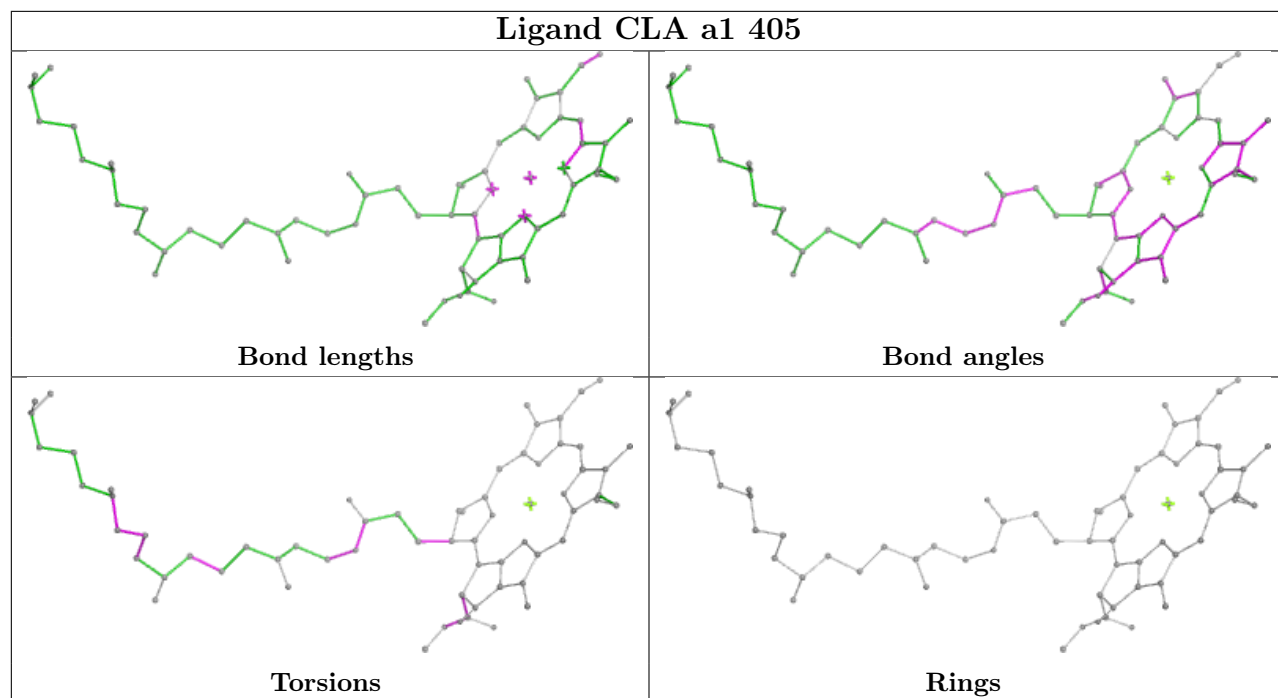


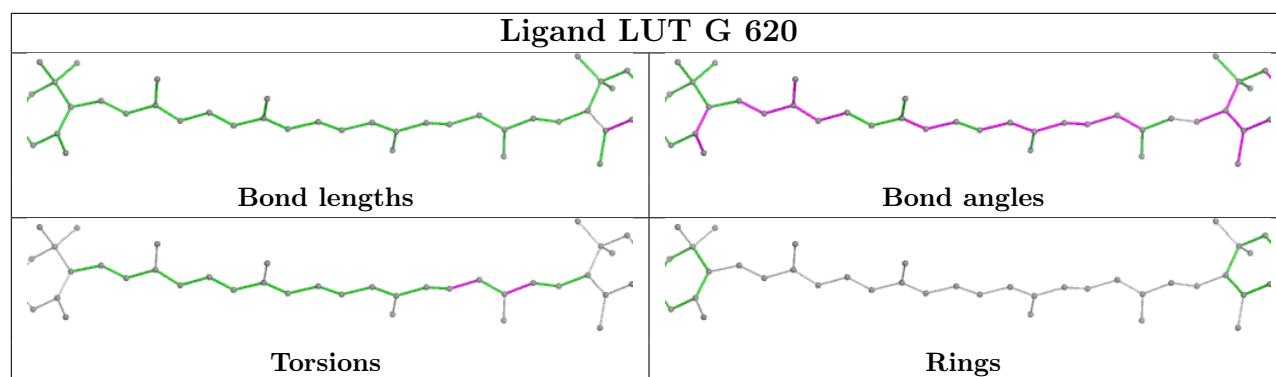
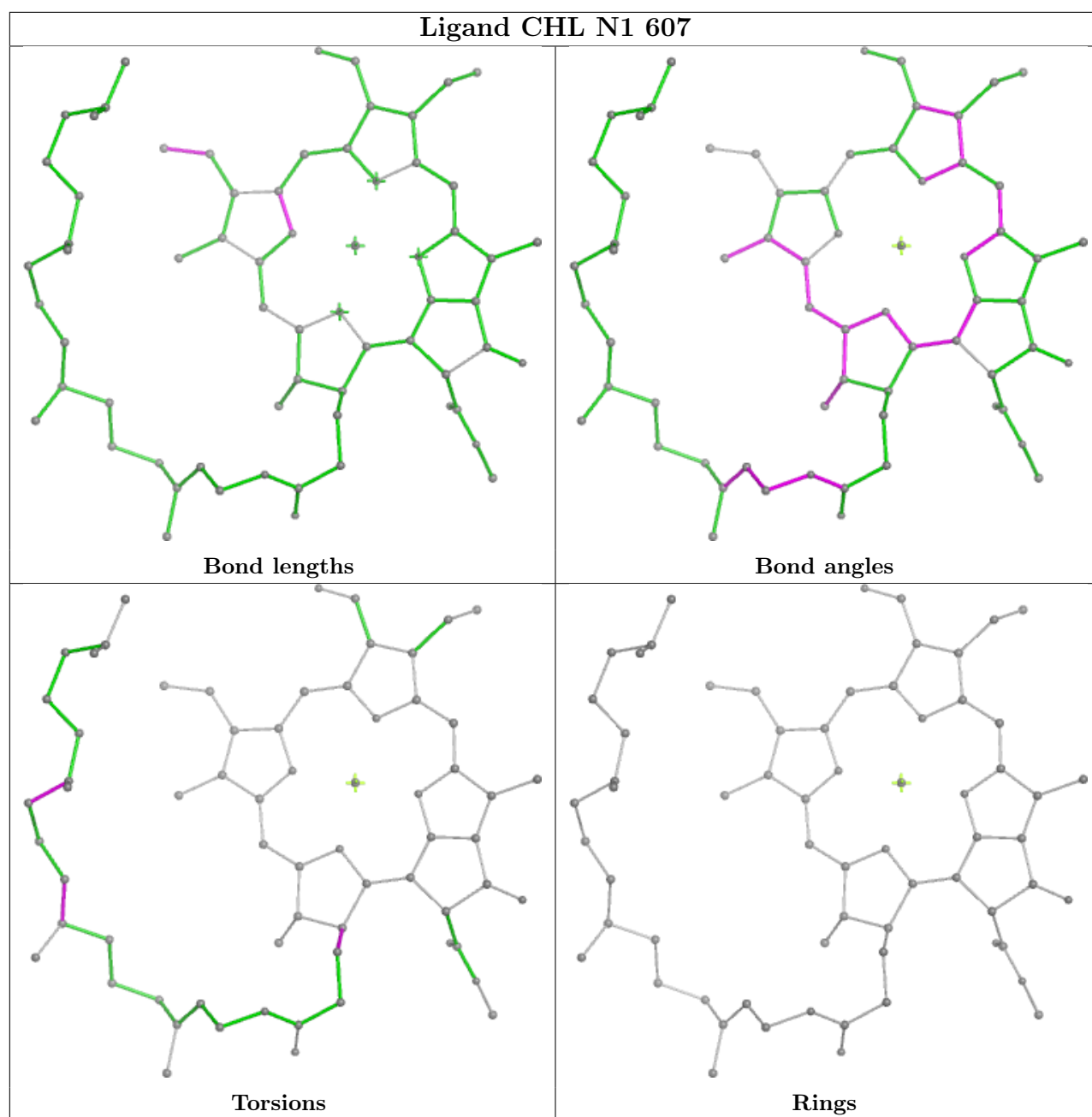


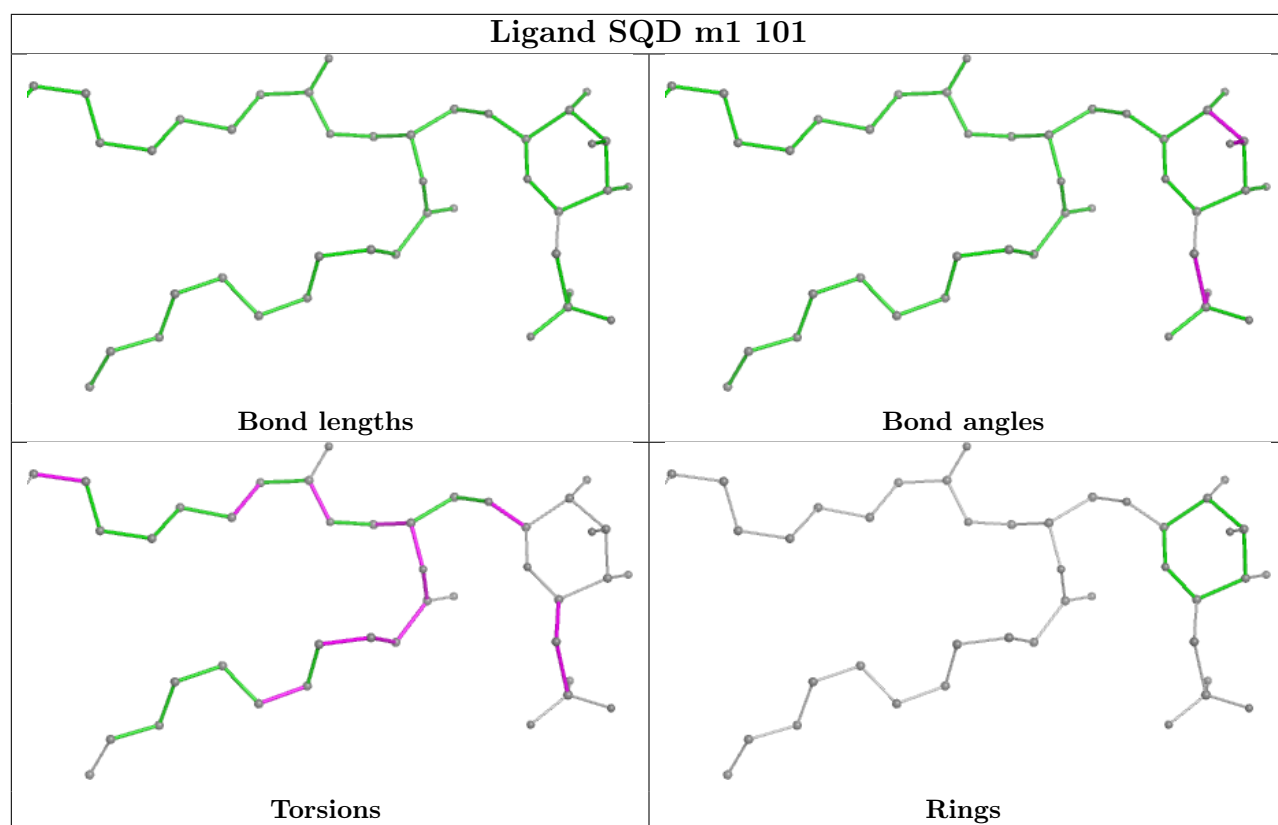
## Ligand HEM f 101



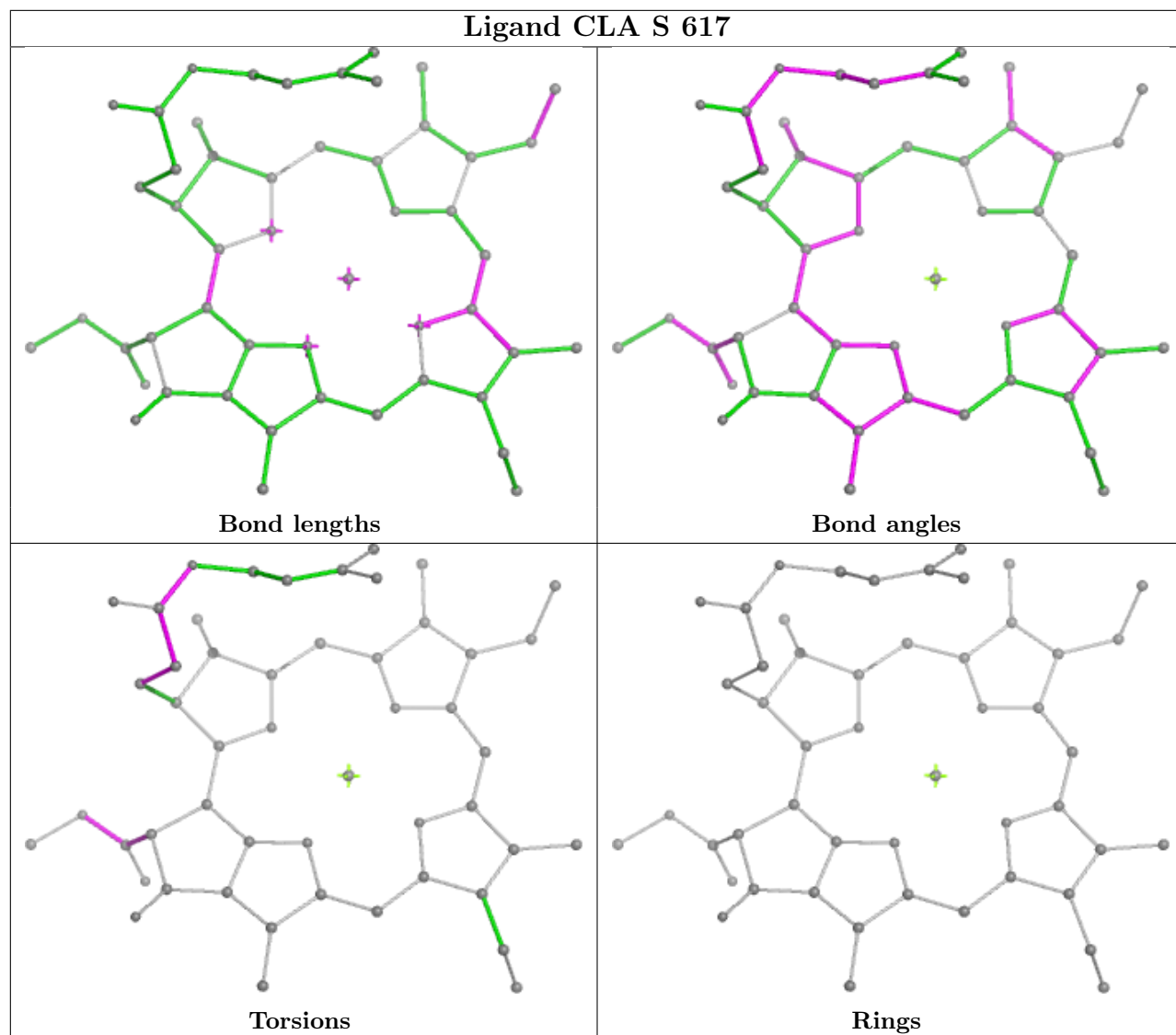




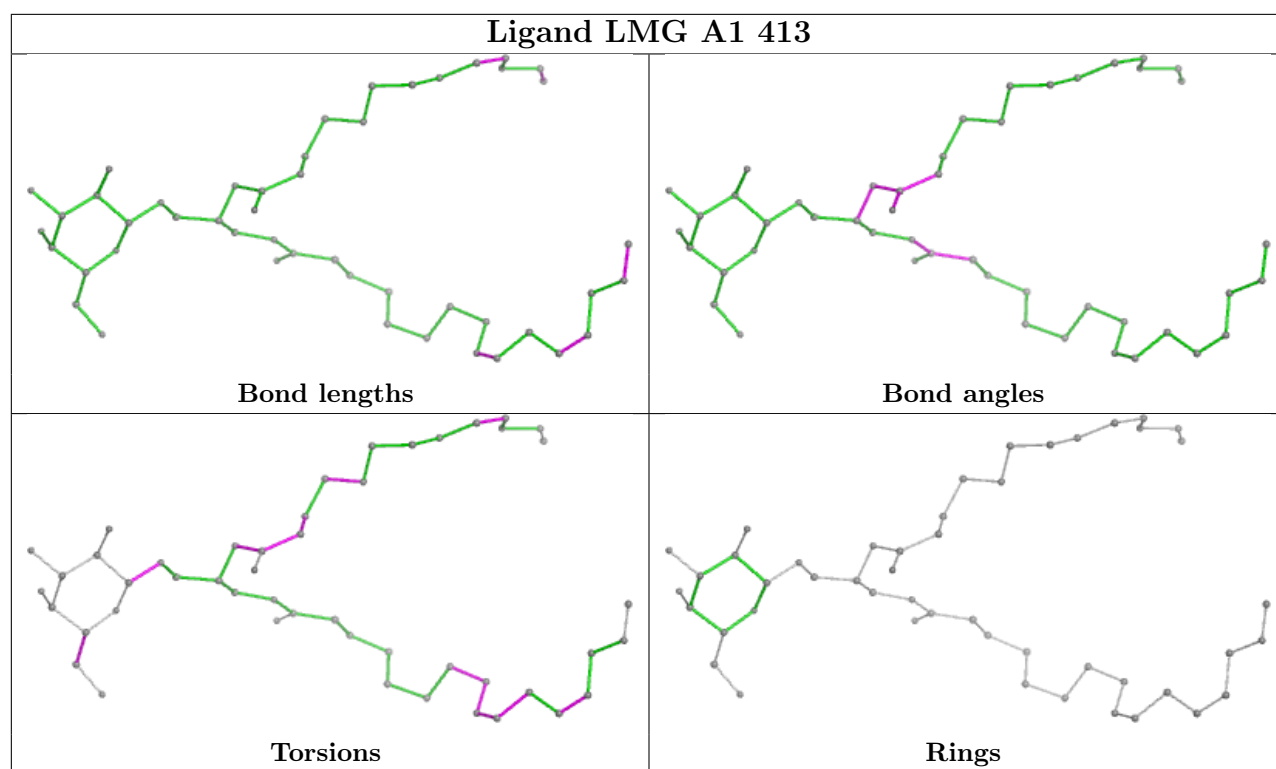




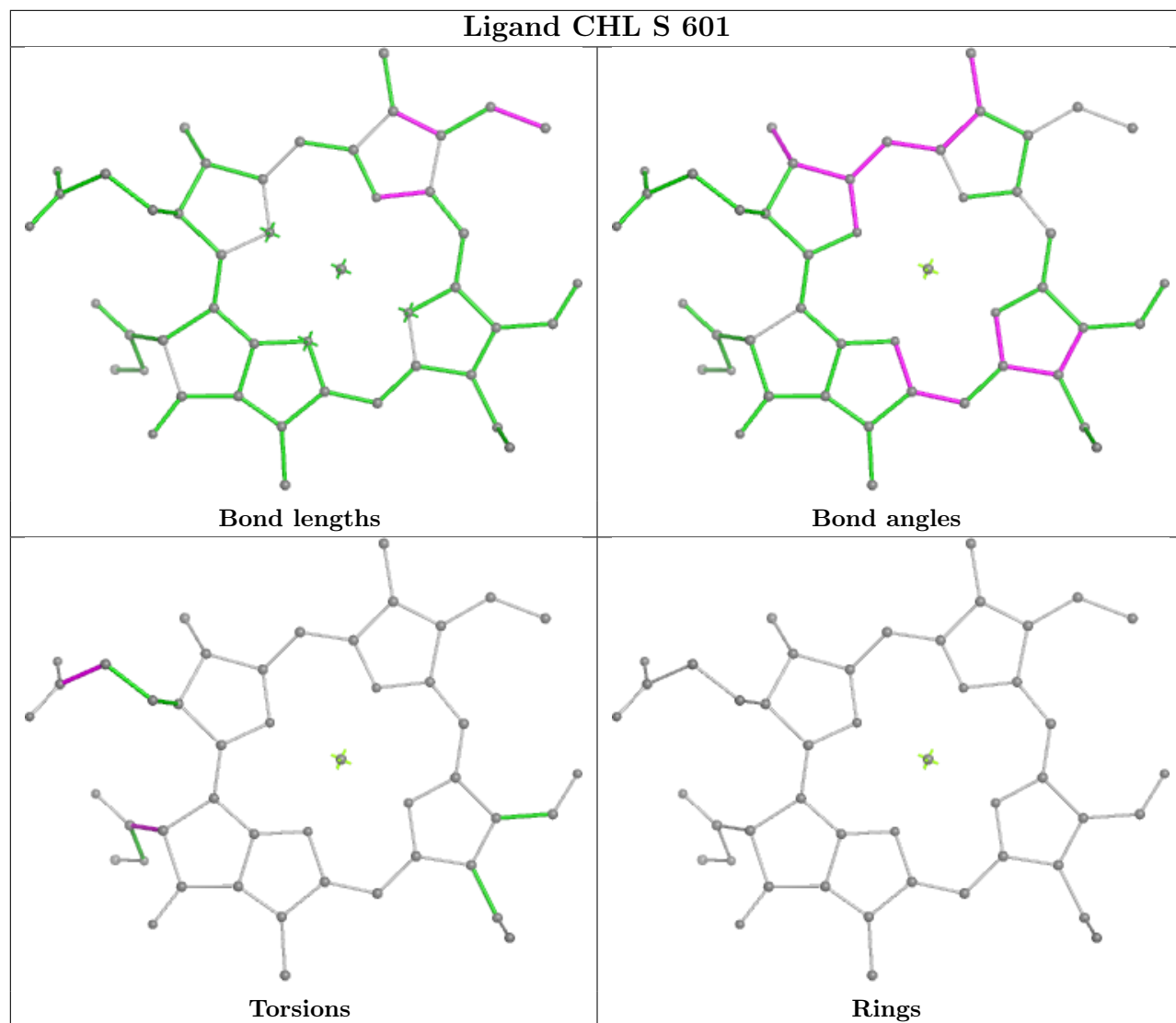
## Ligand CLA S 617



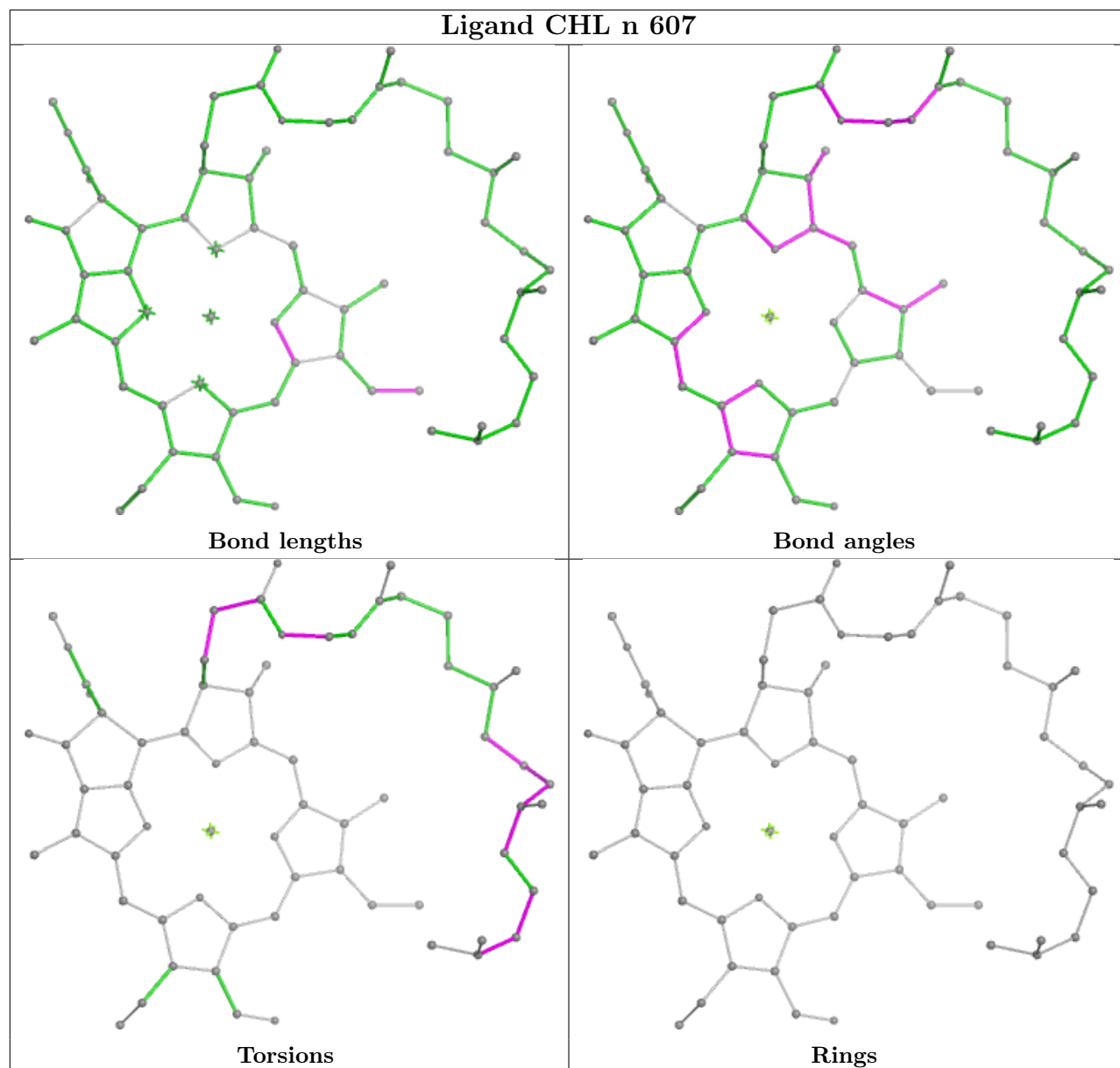


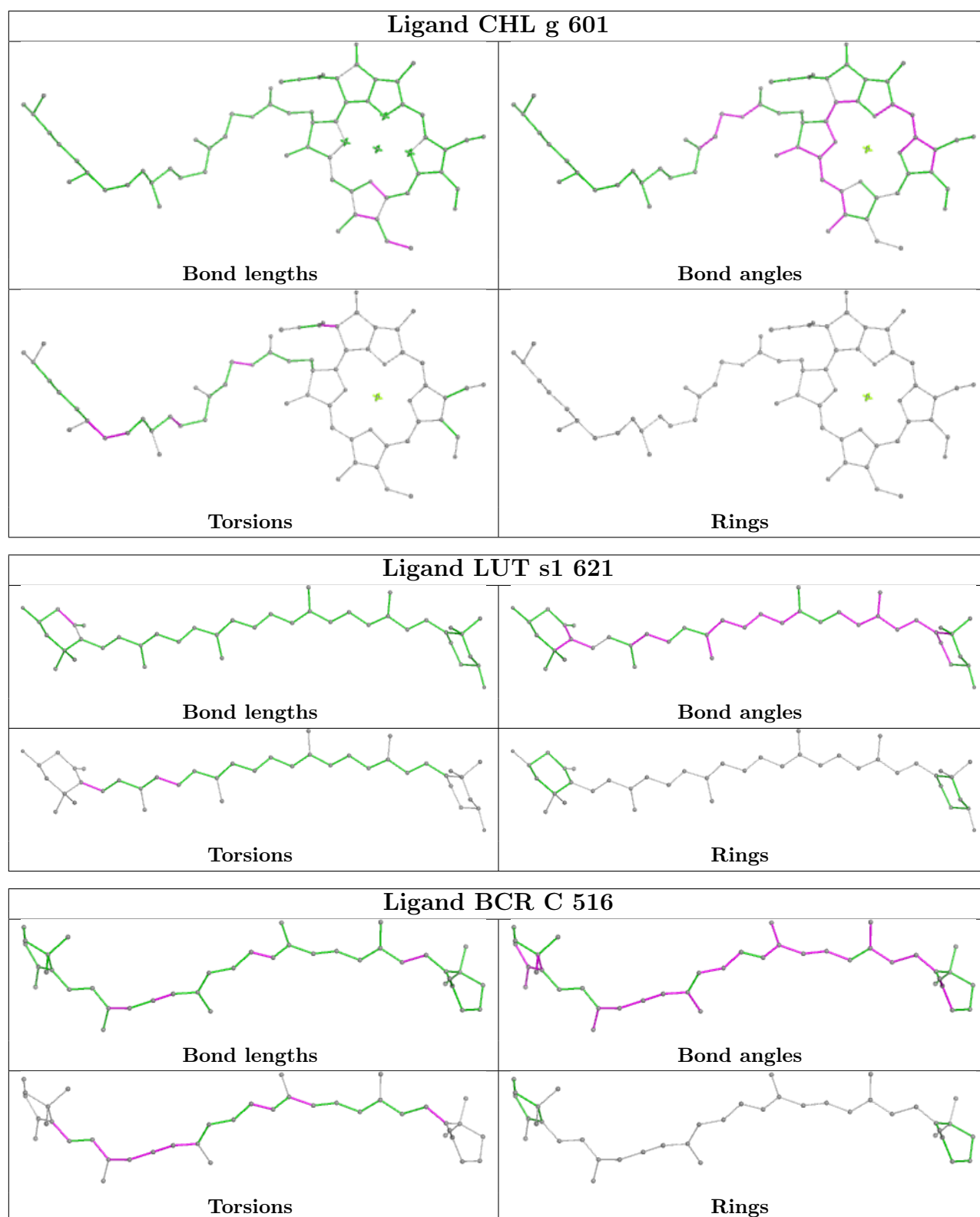


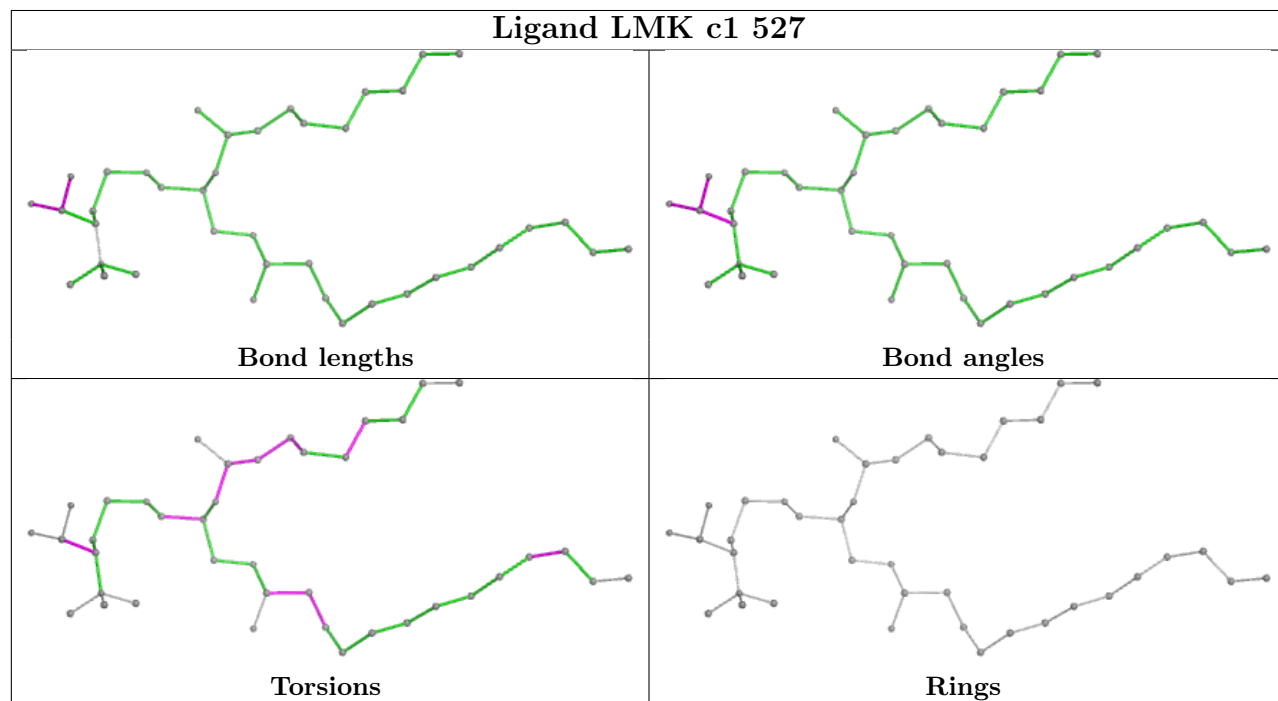
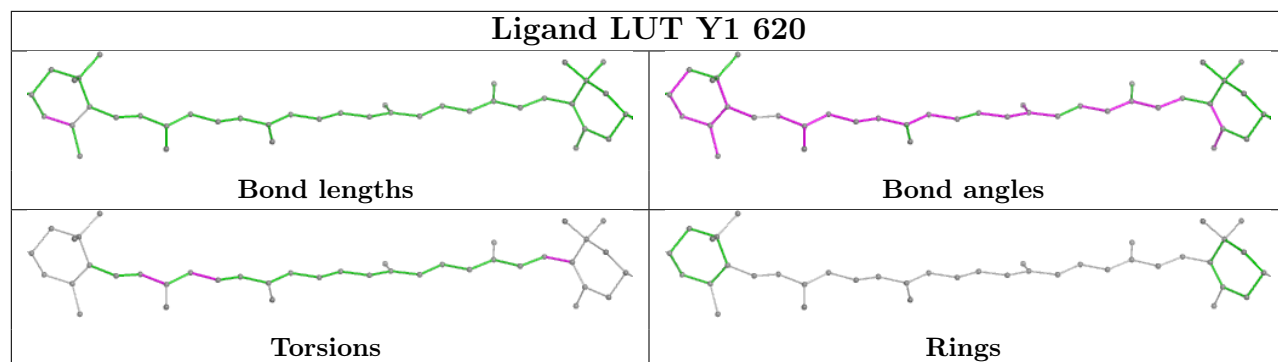
## Ligand CHL S 601

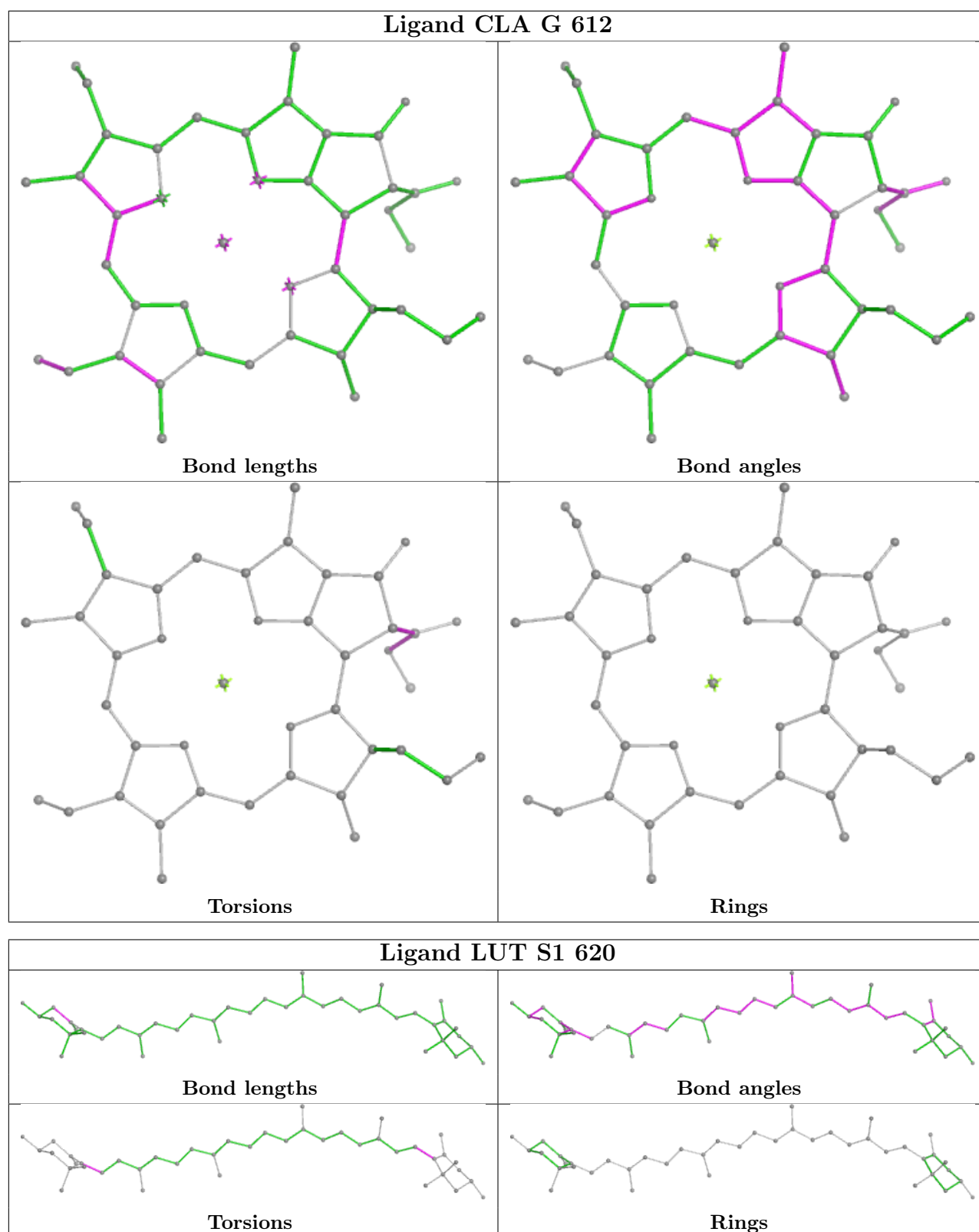


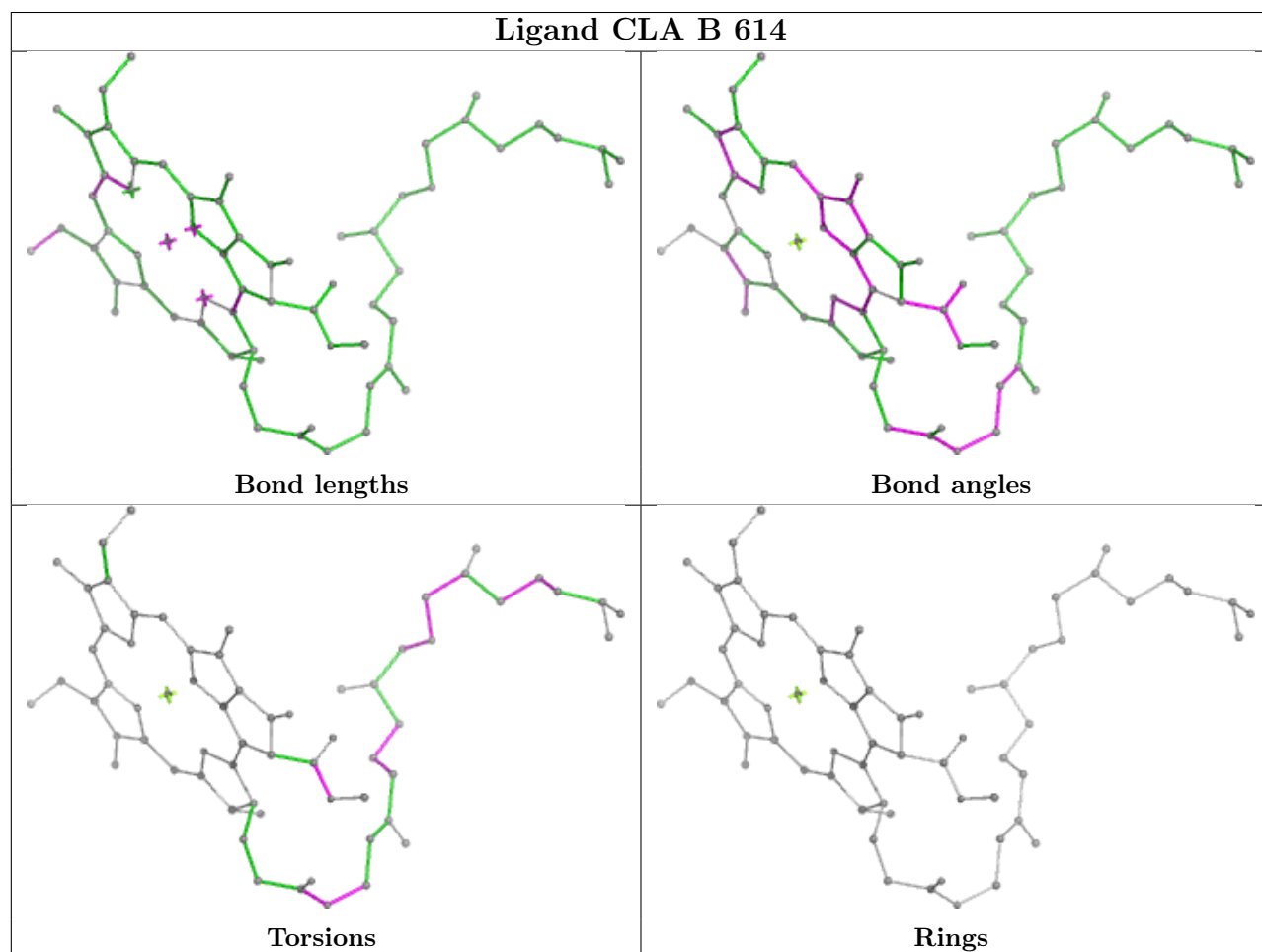
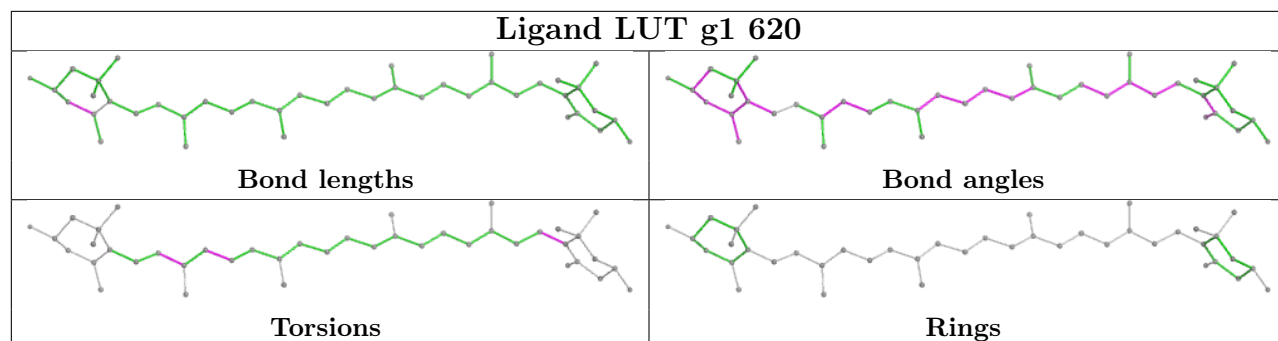
## Ligand CHL n 607

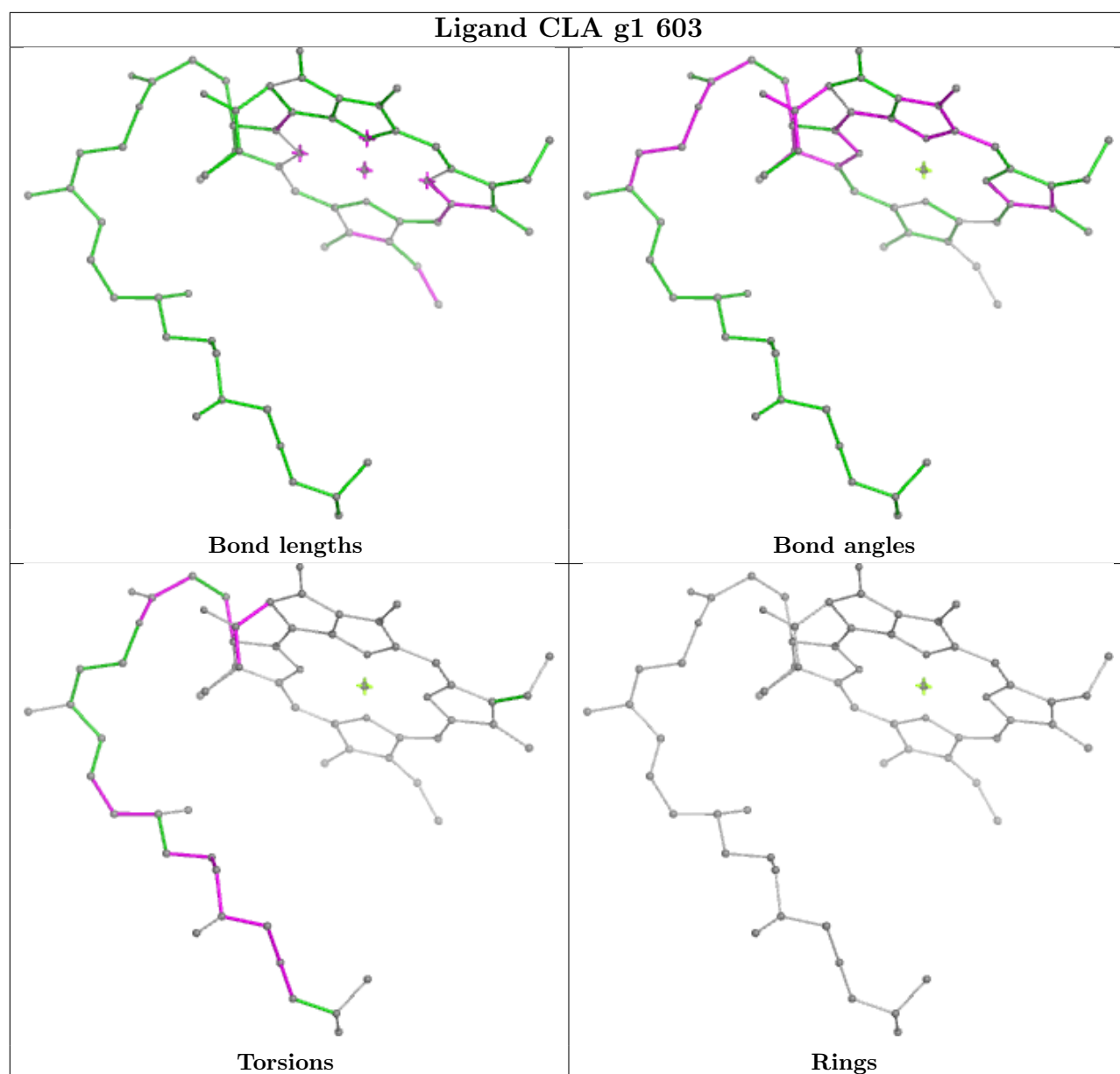




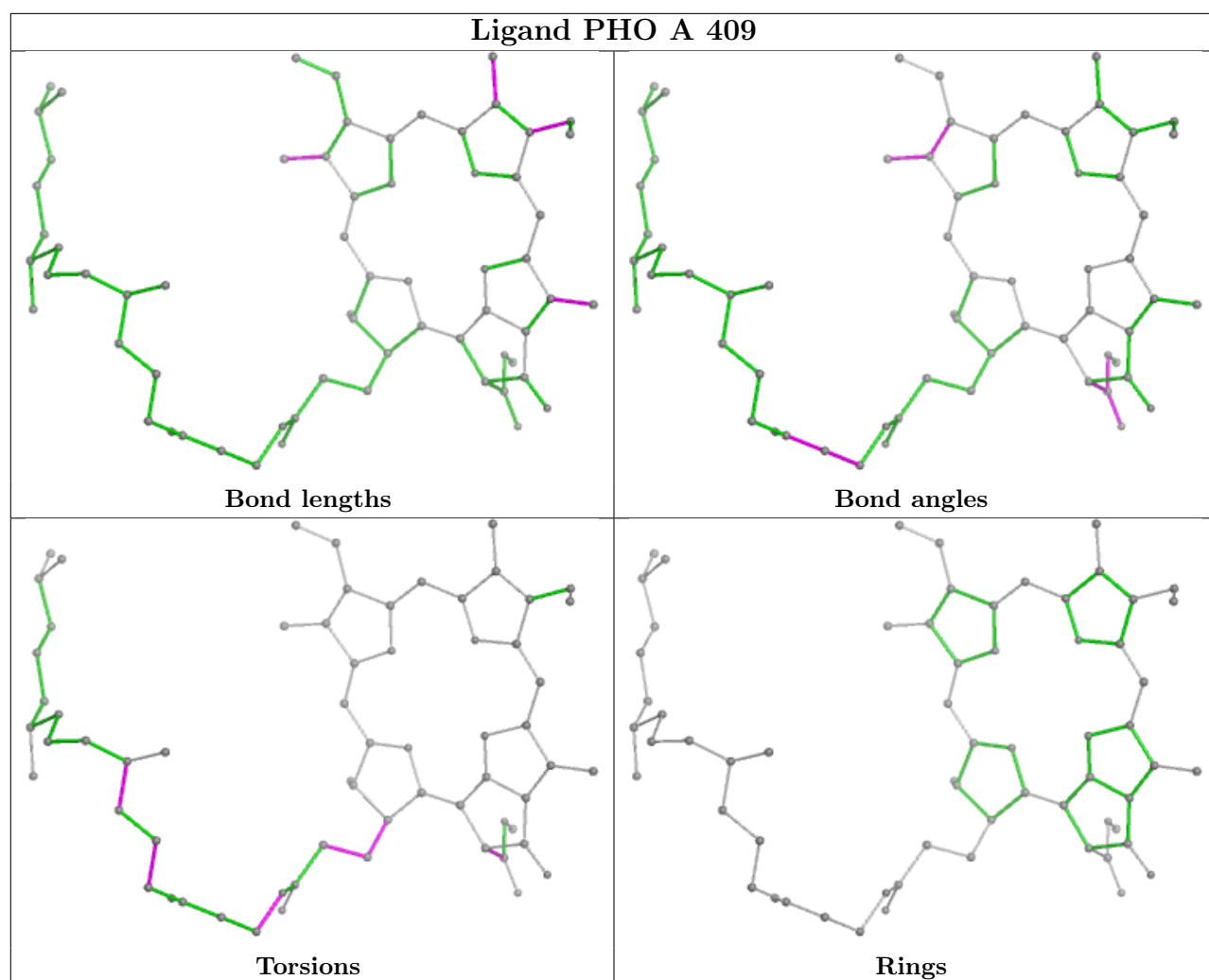


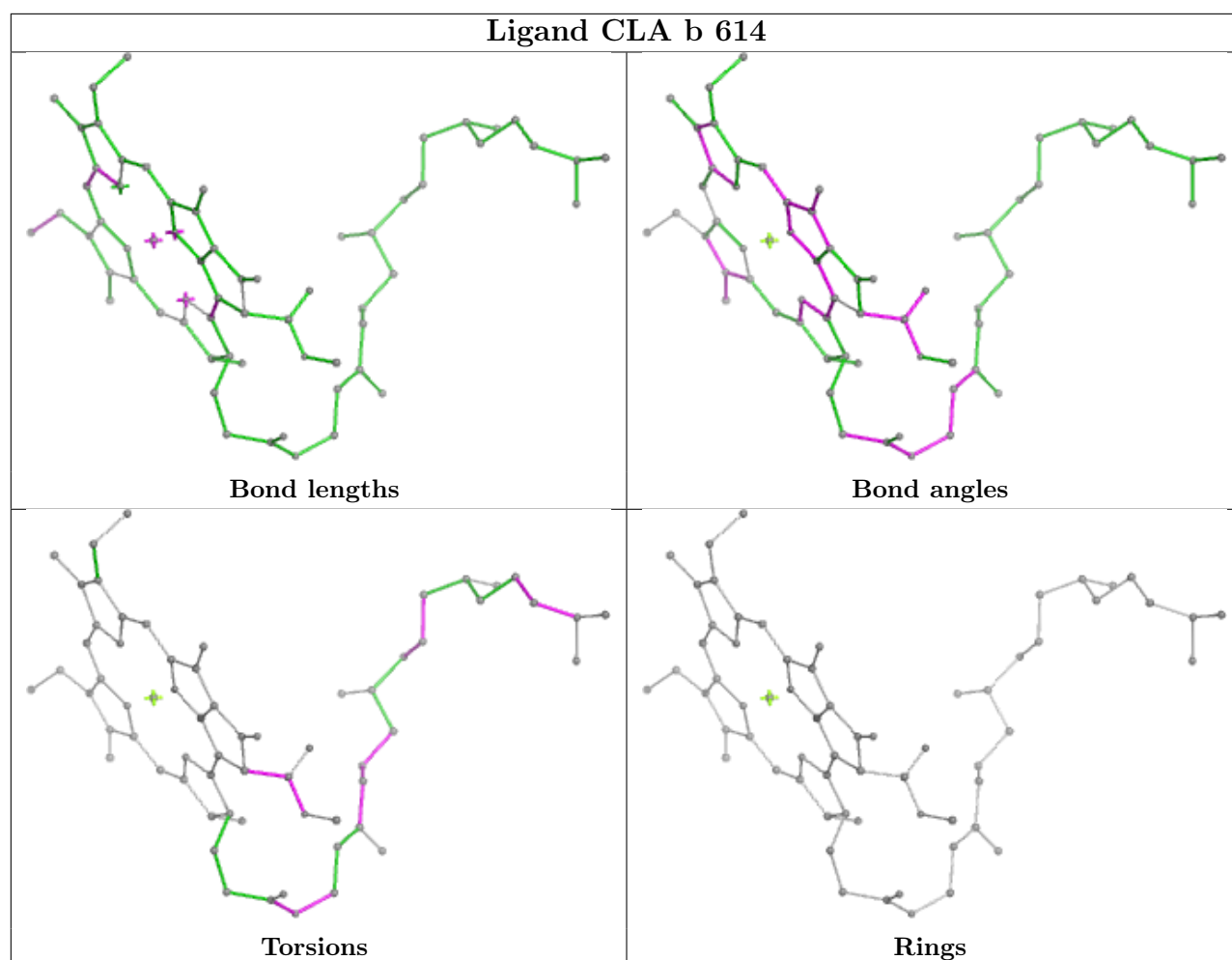


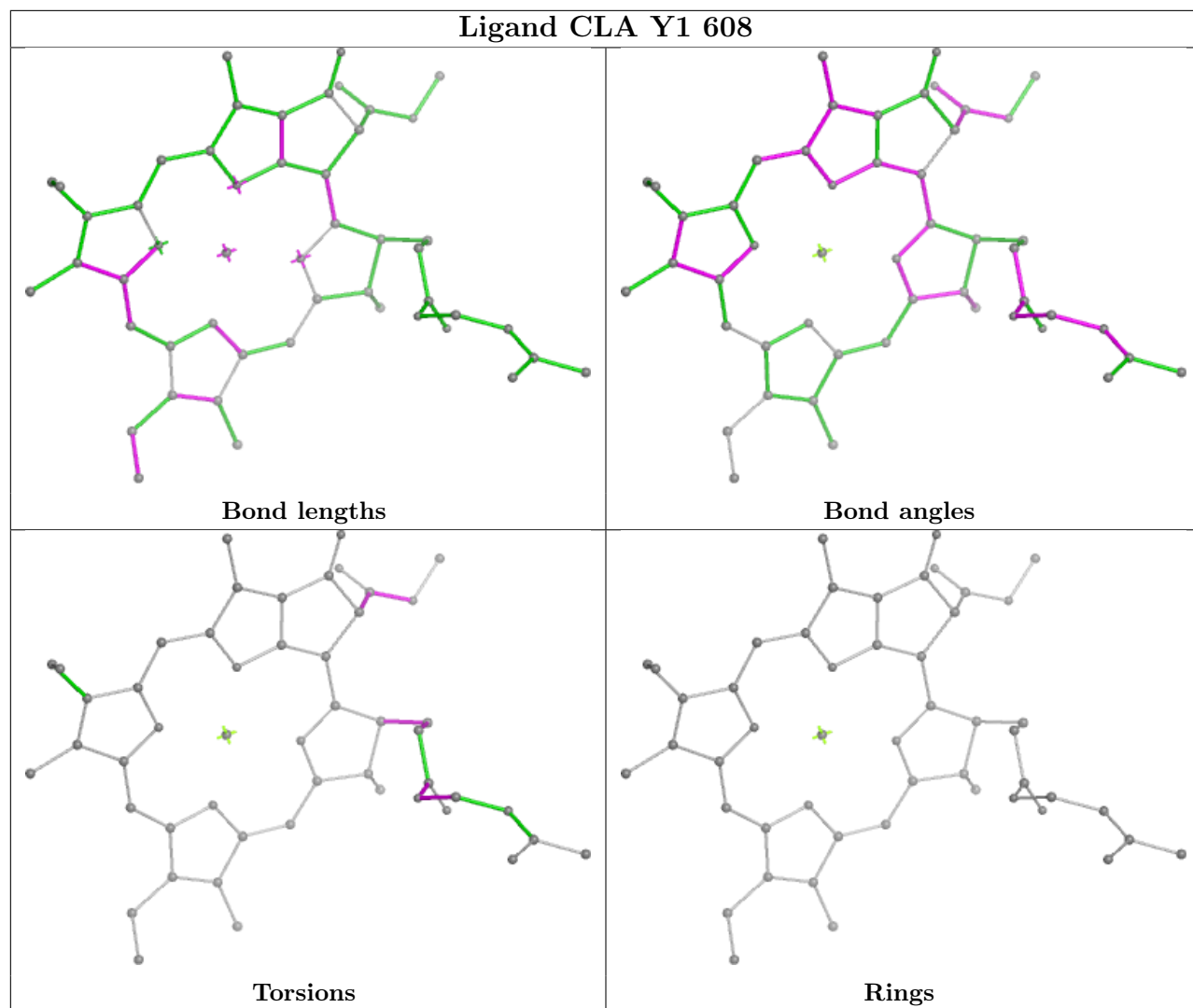


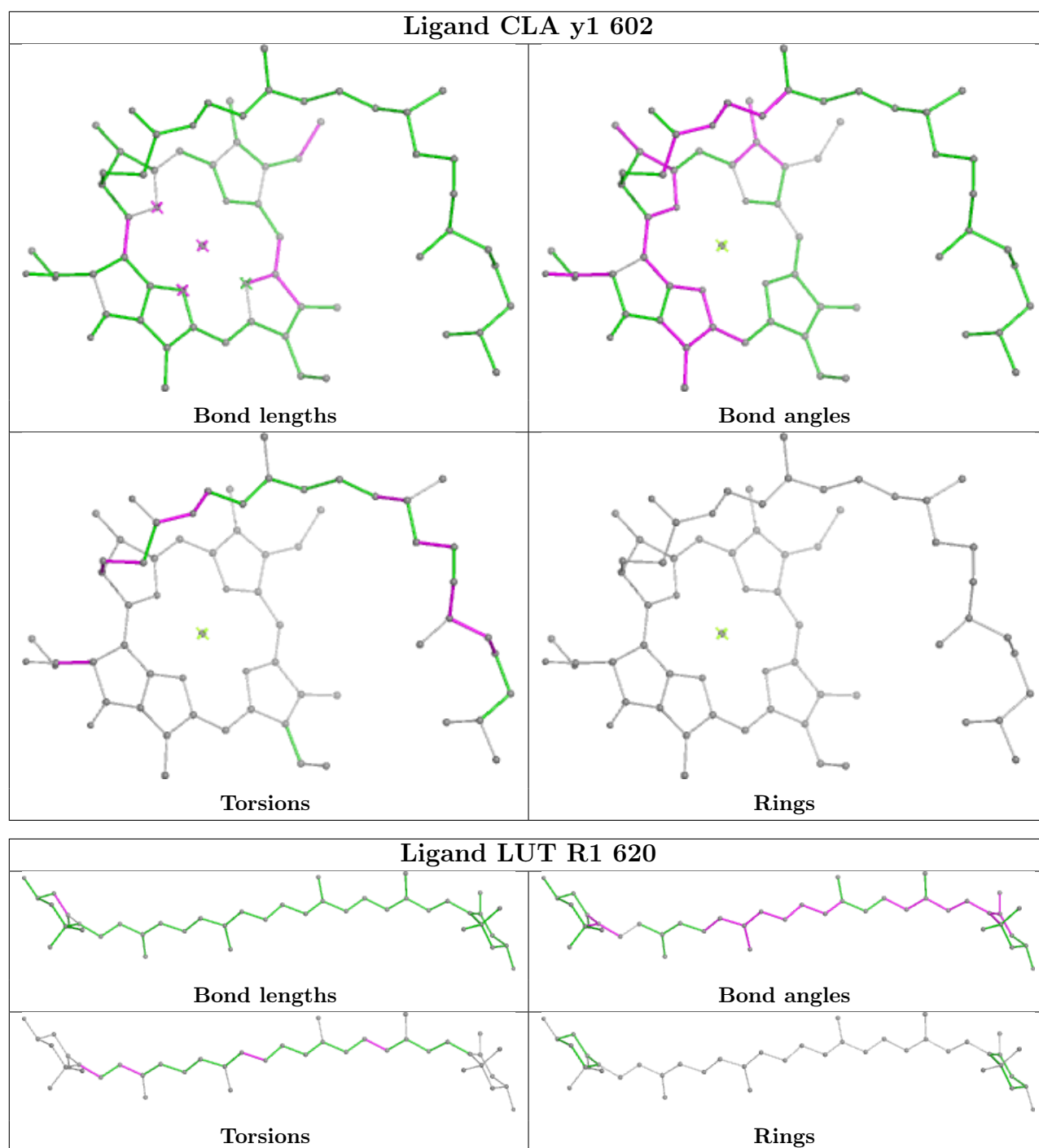


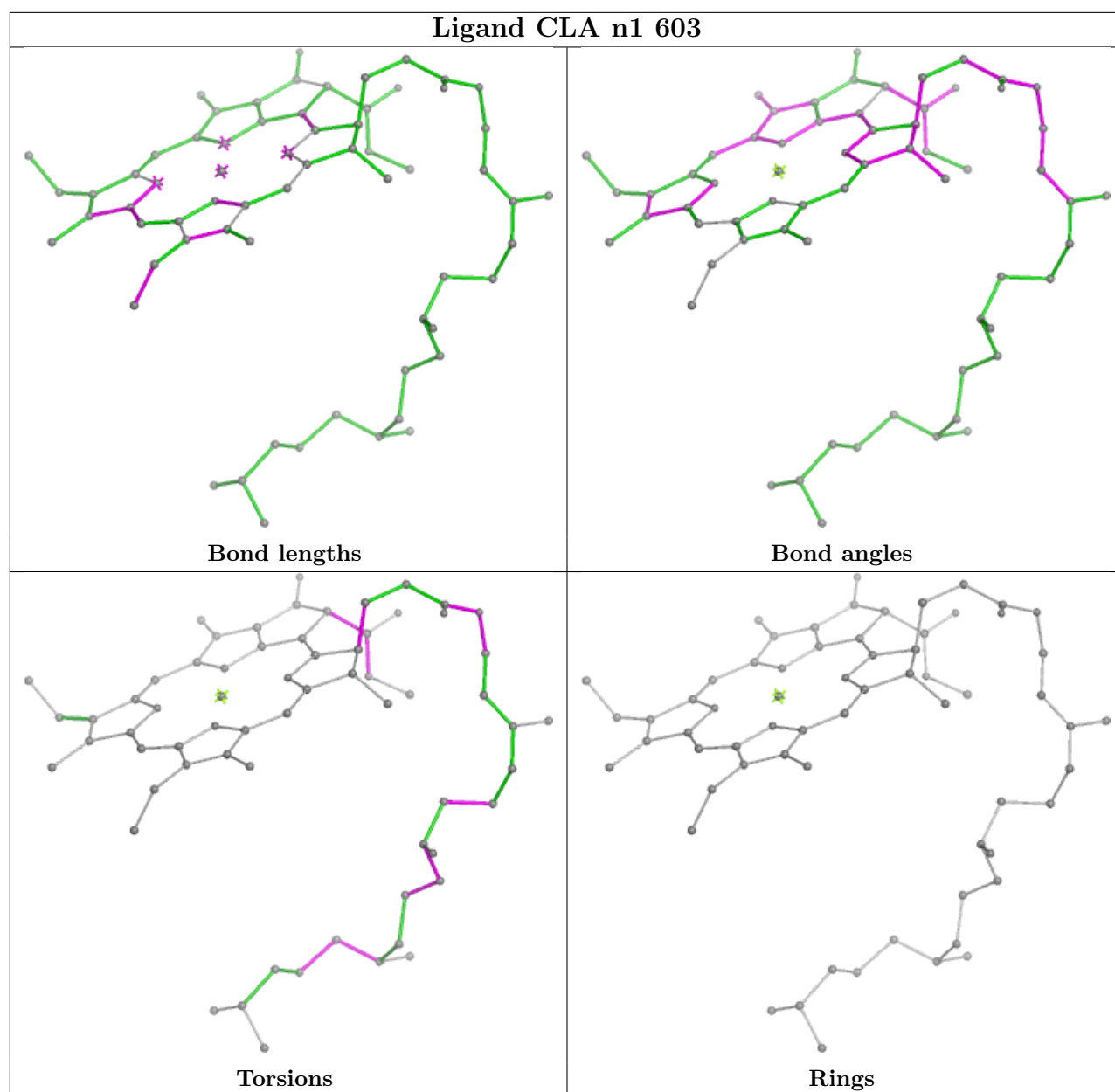




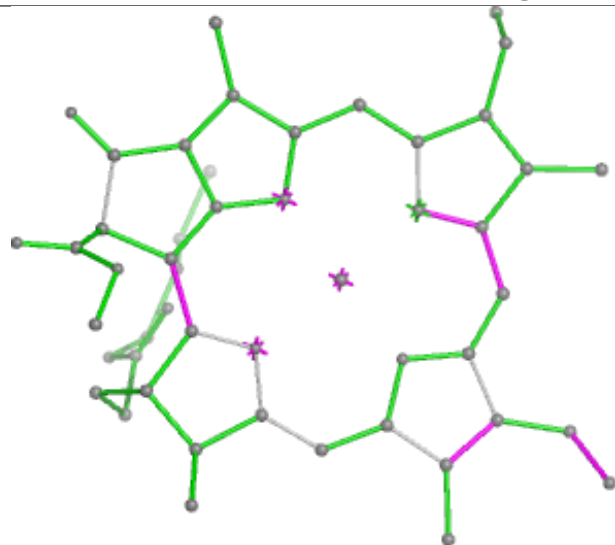




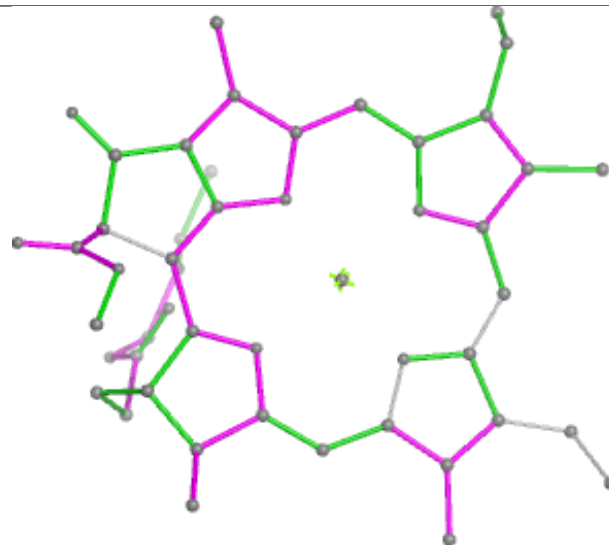




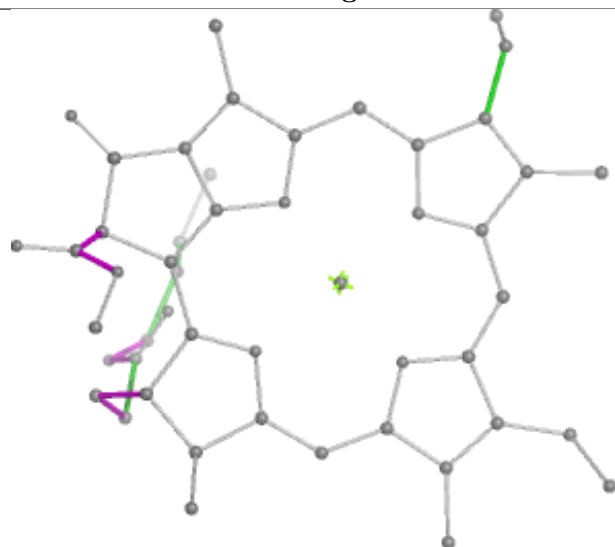
## Ligand CLA R 604



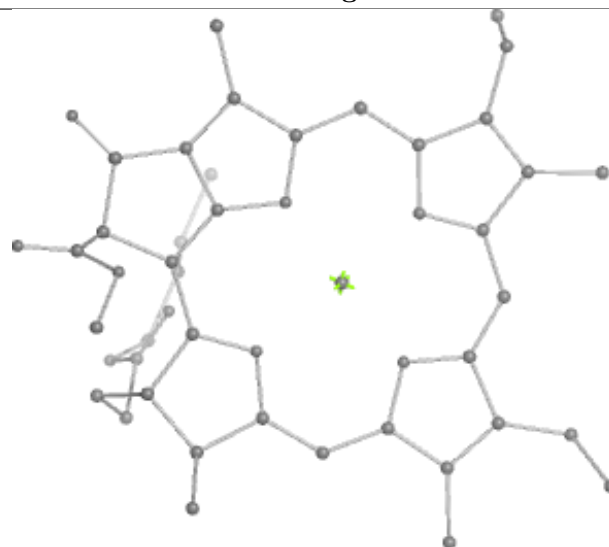
Bond lengths



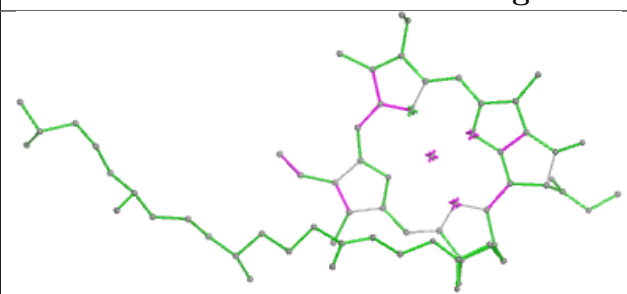
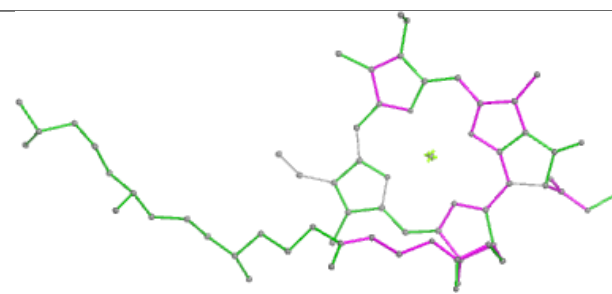
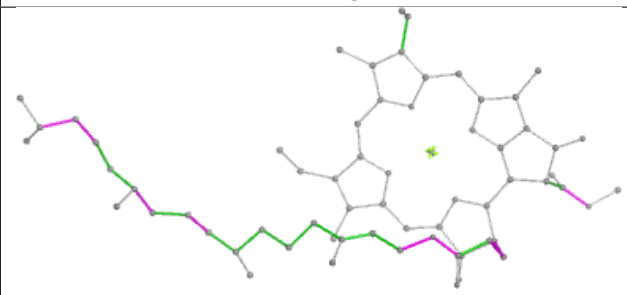
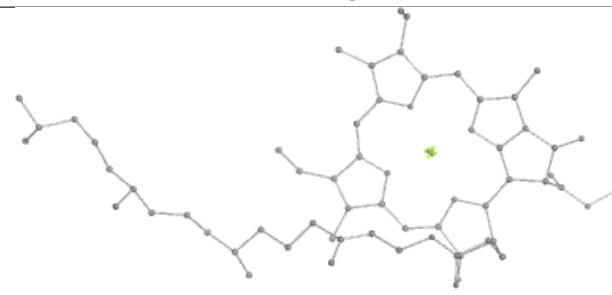
Bond angles

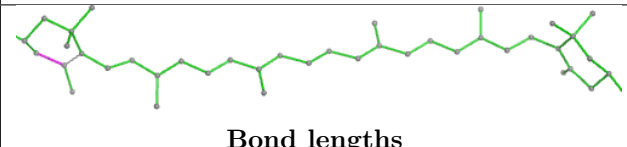
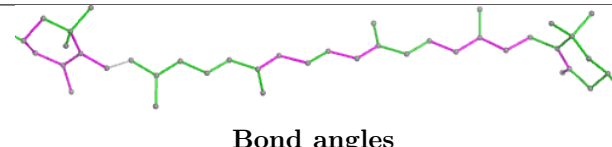
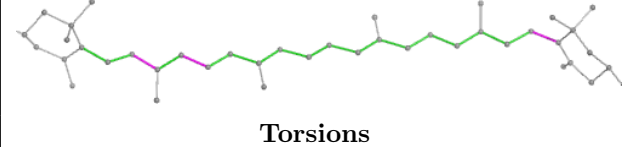
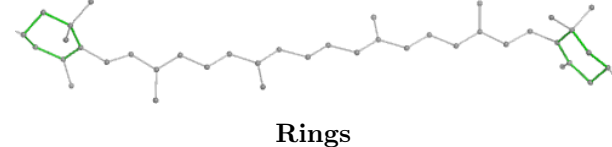


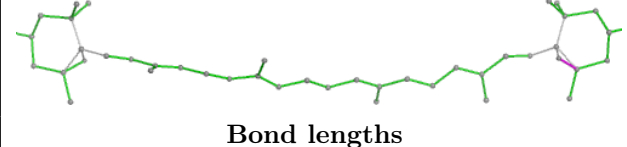
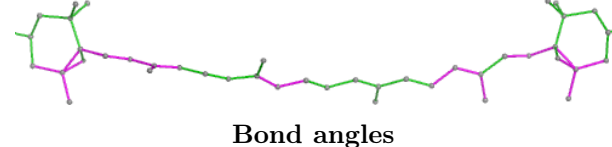
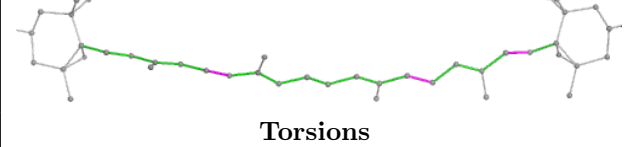

Torsions

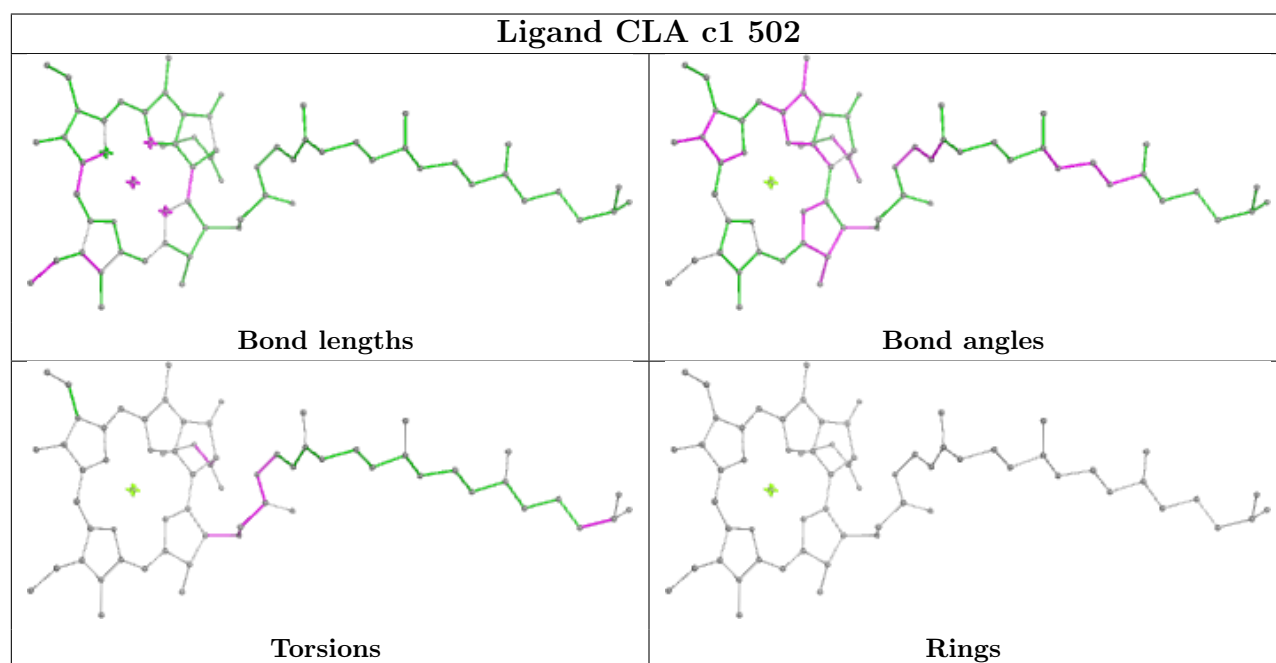
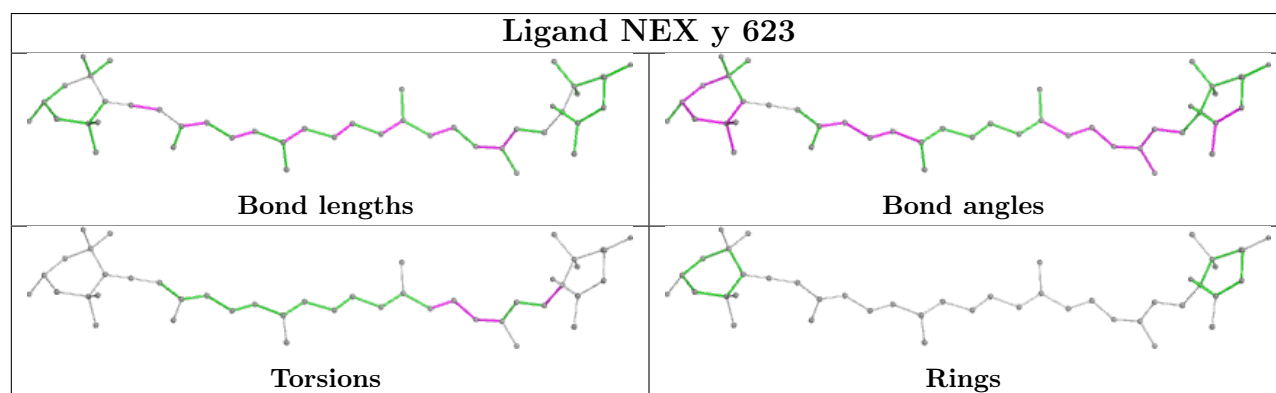
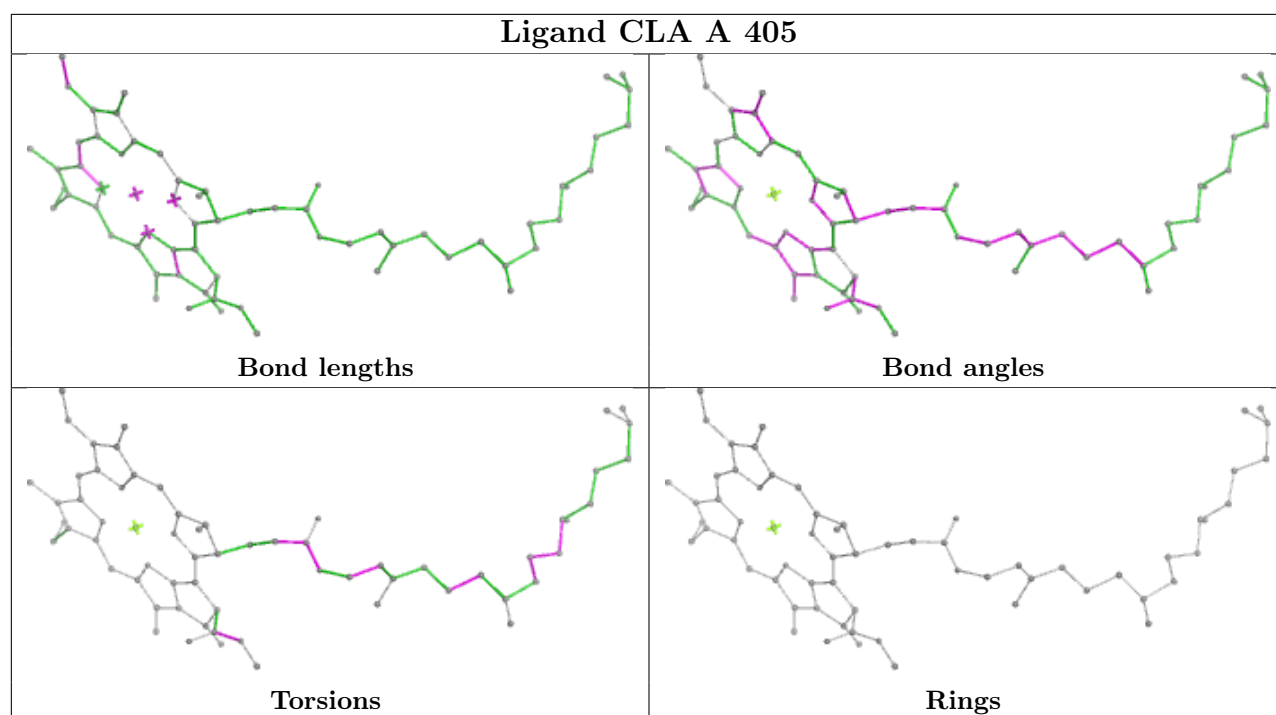


Rings

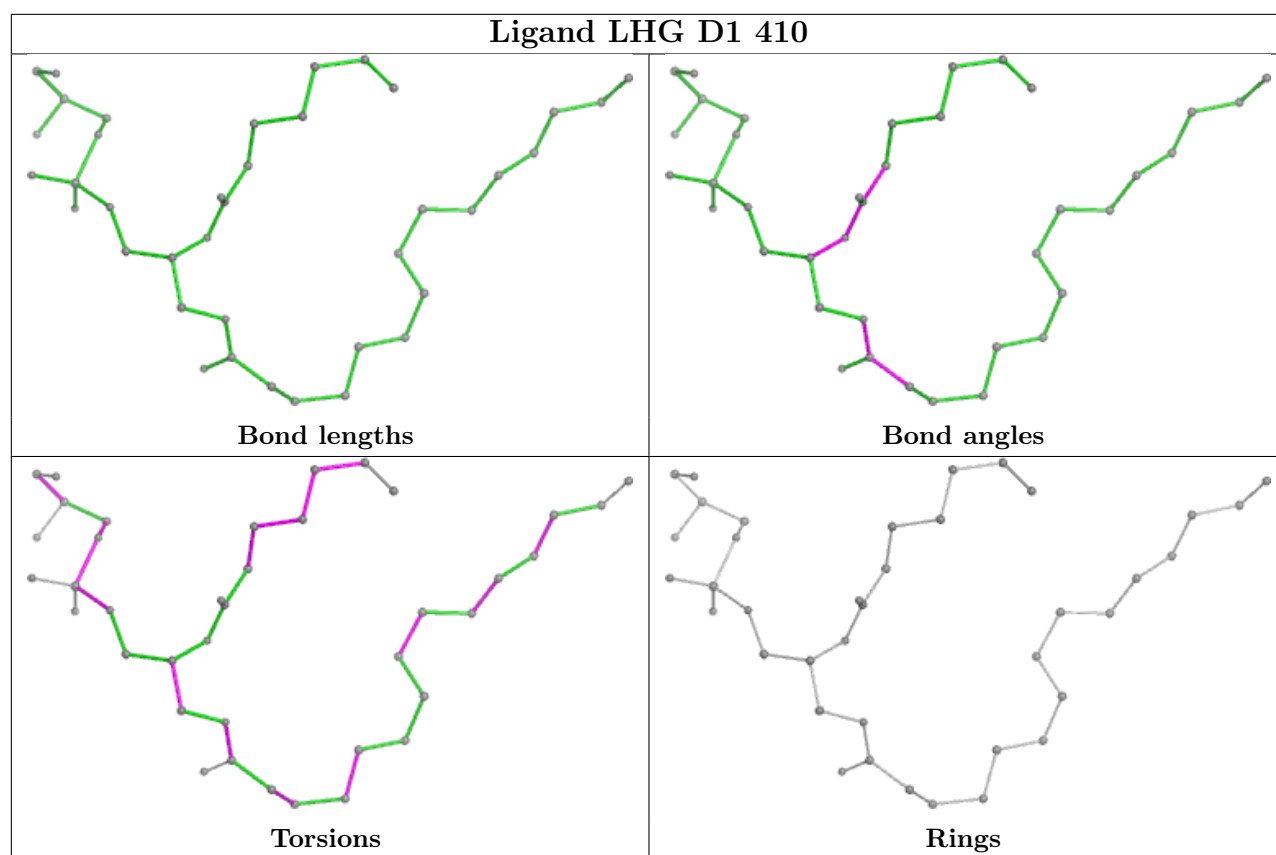
Ligand CLA C1 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

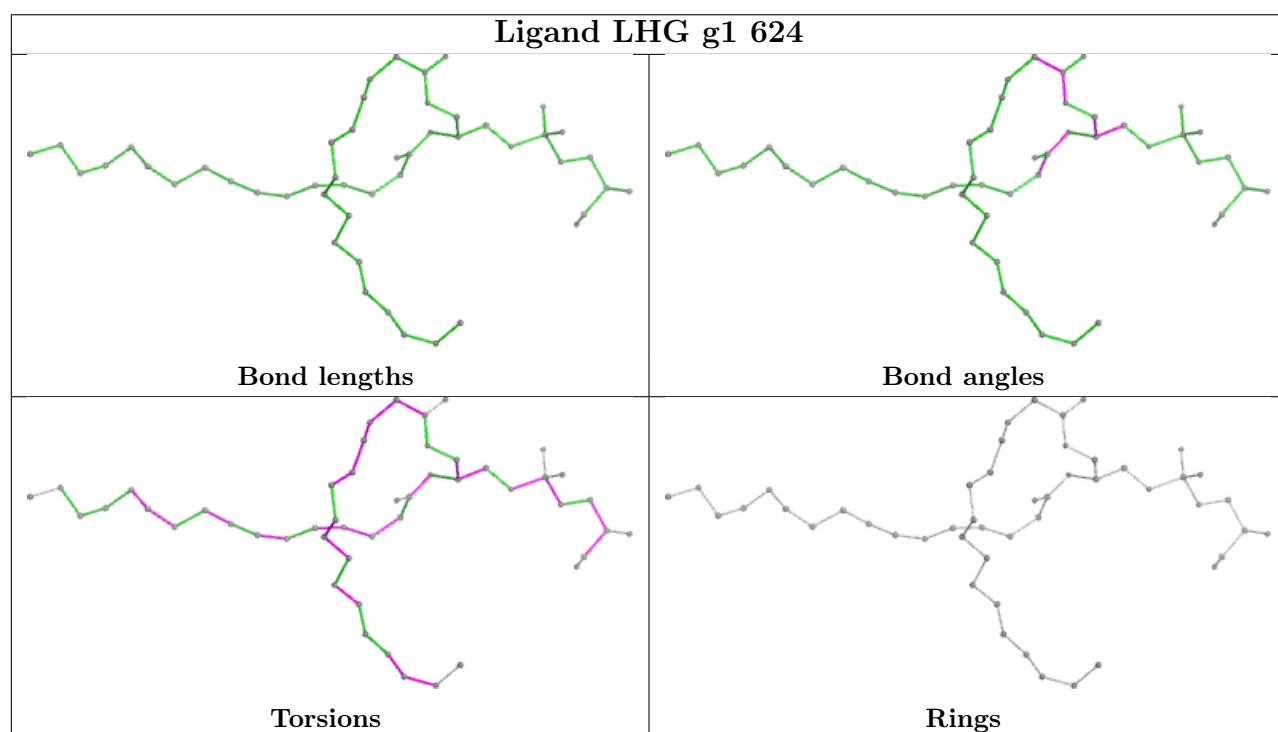
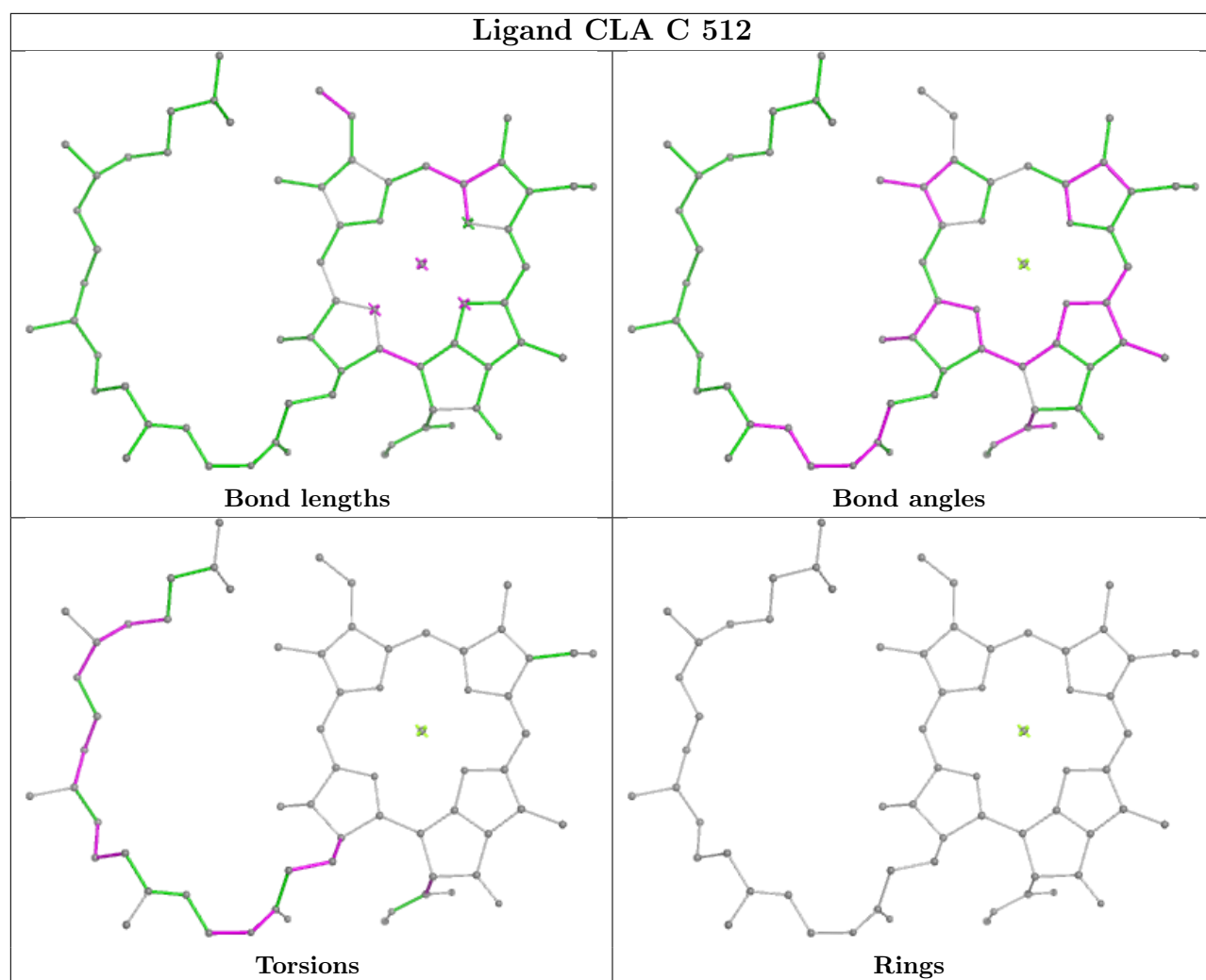
Ligand LUT y1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

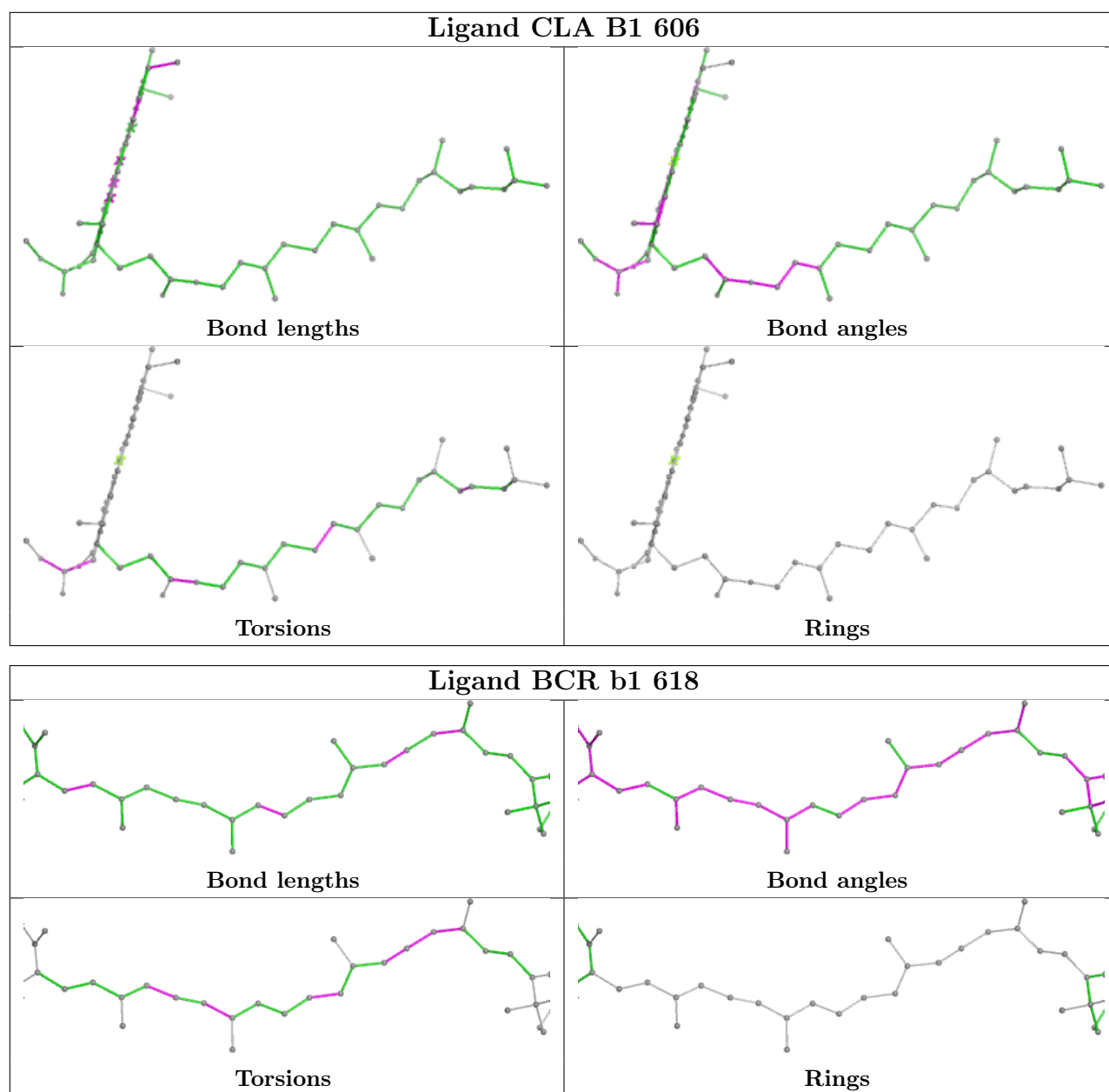
Ligand XAT N 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

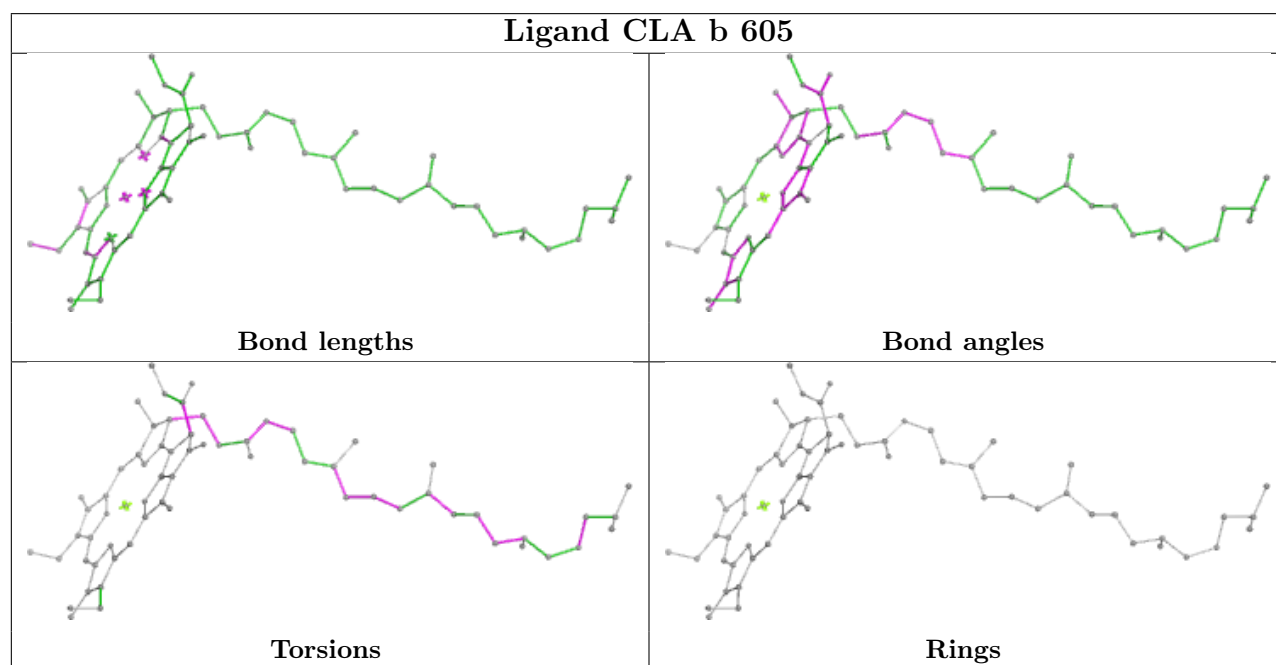
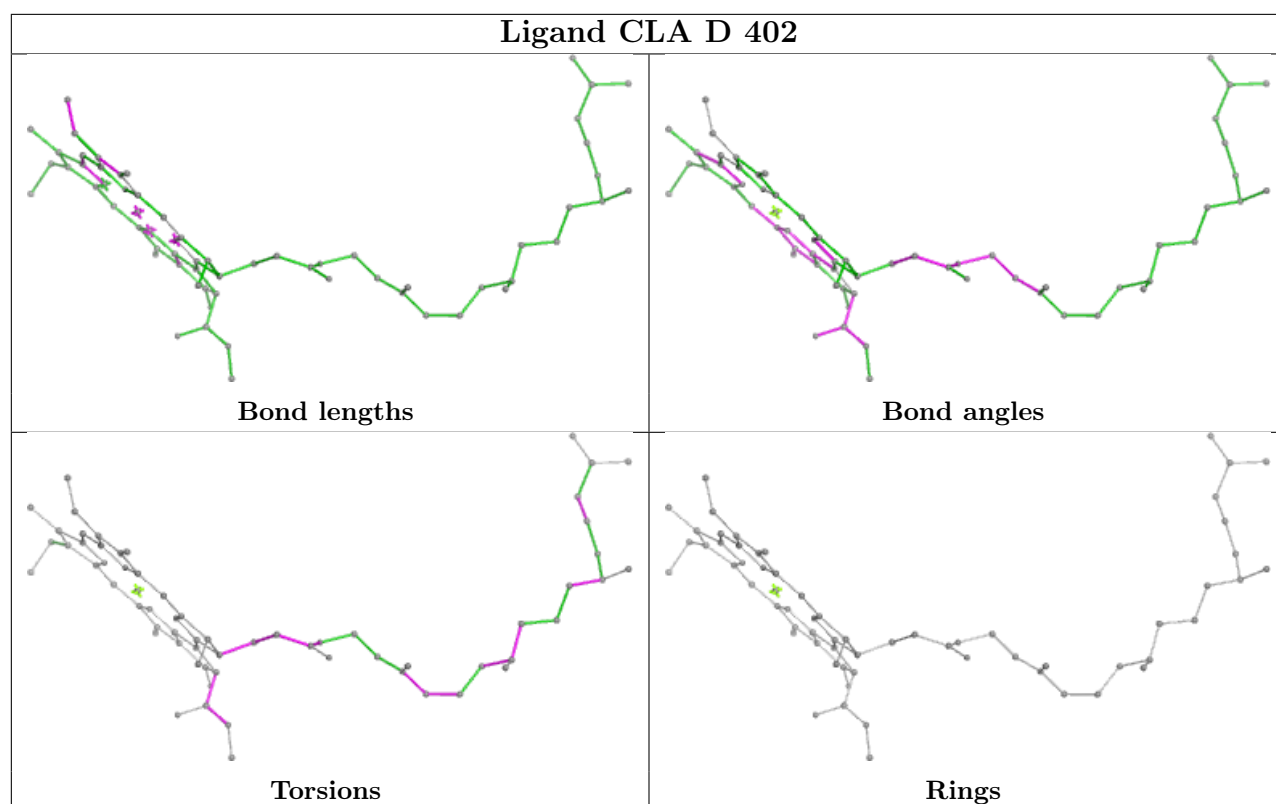


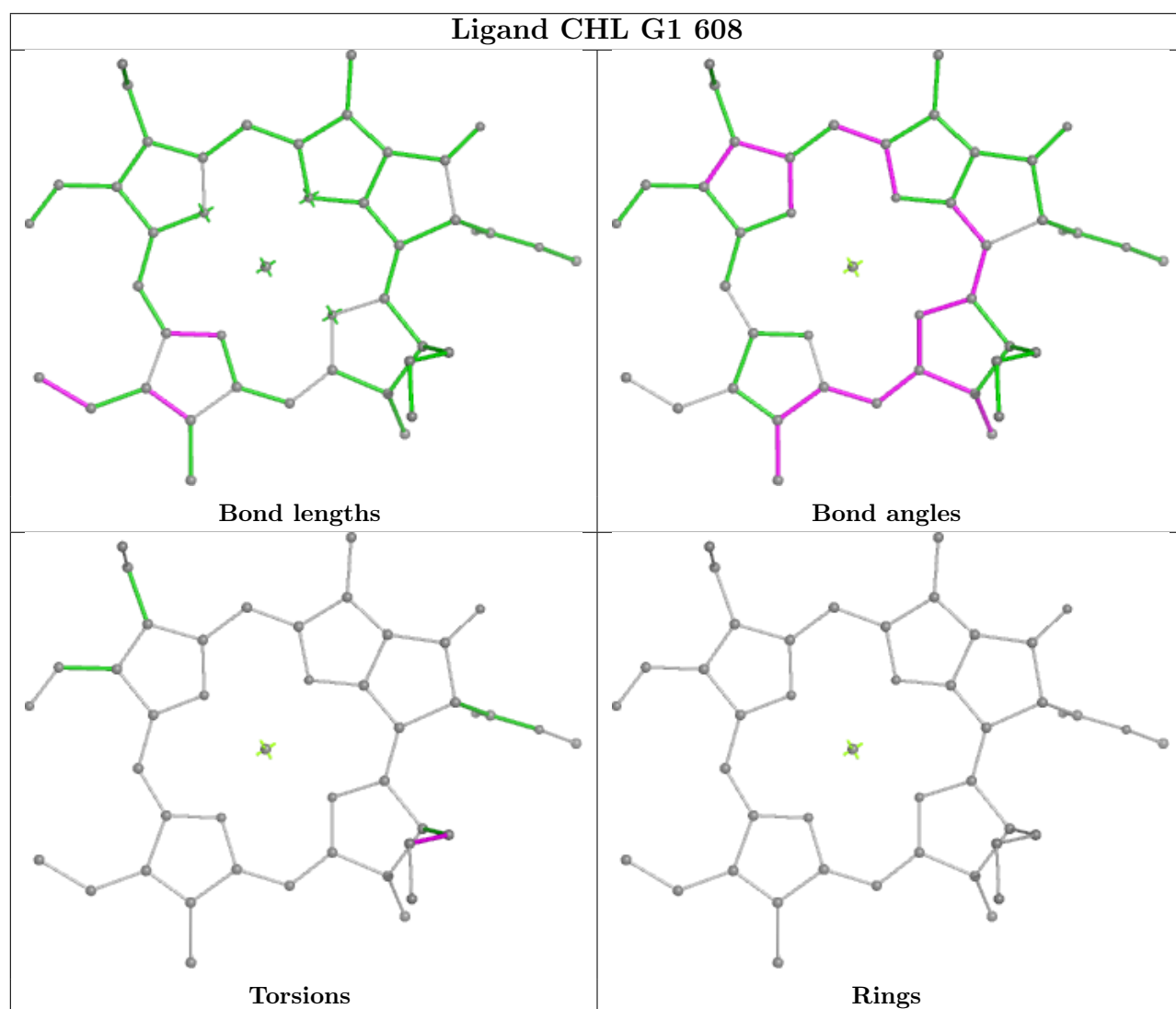
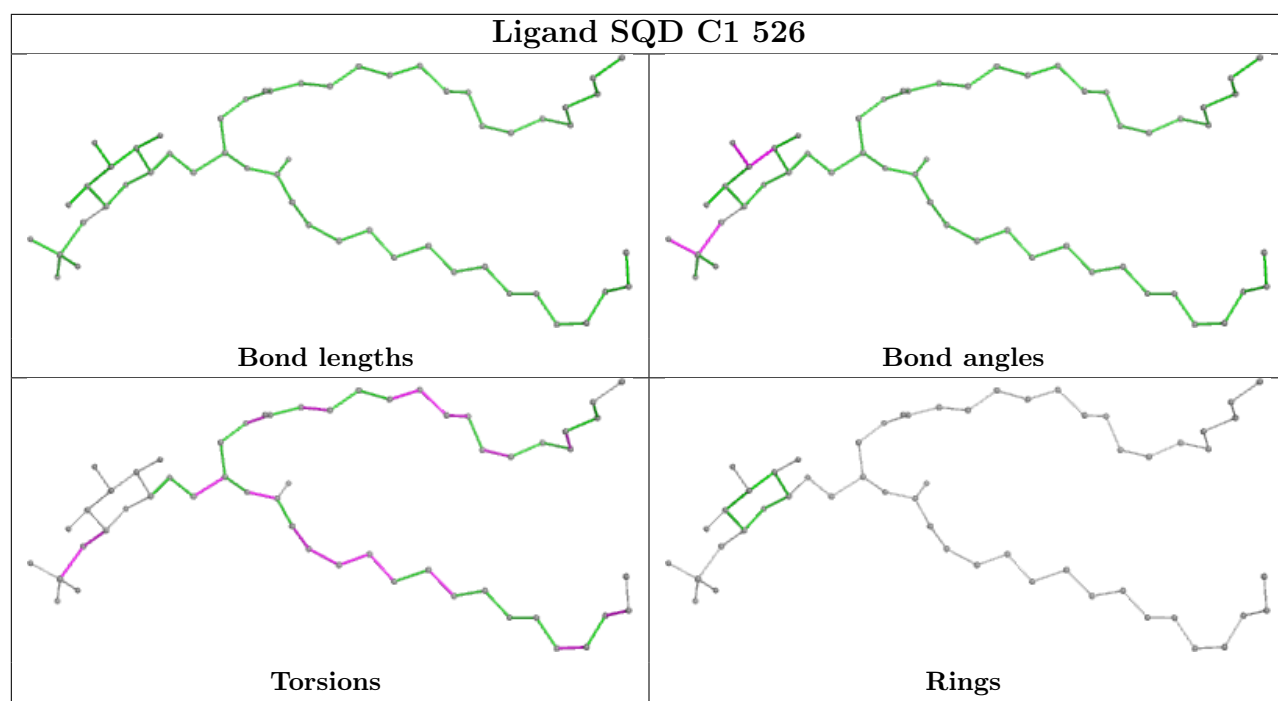


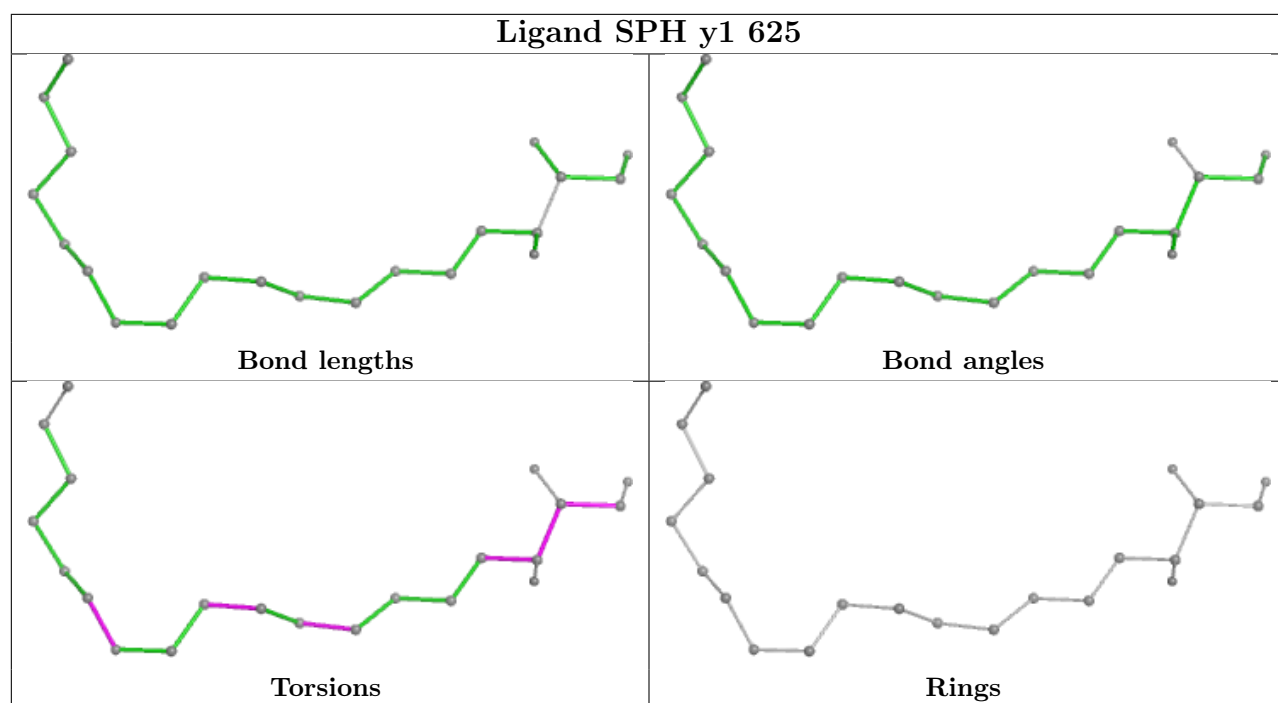




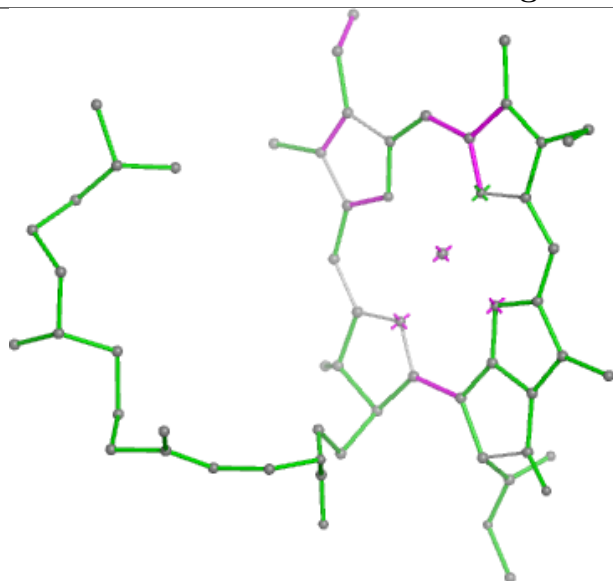




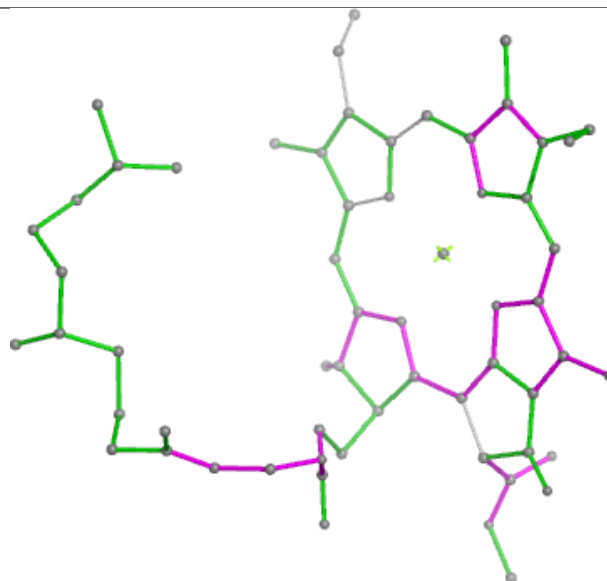




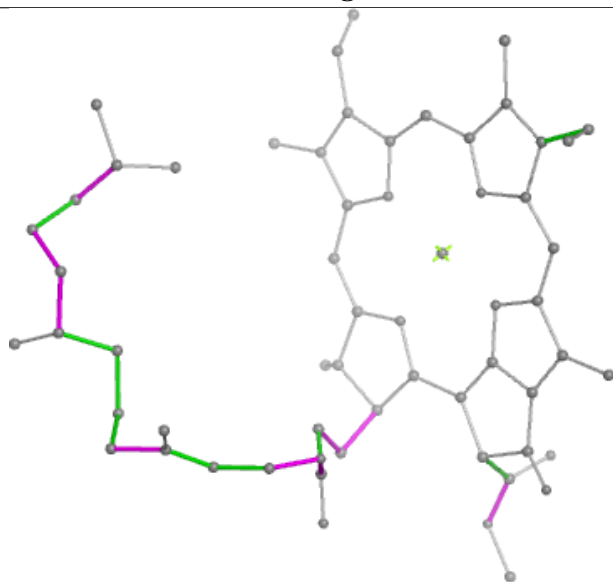
## Ligand CLA r 603



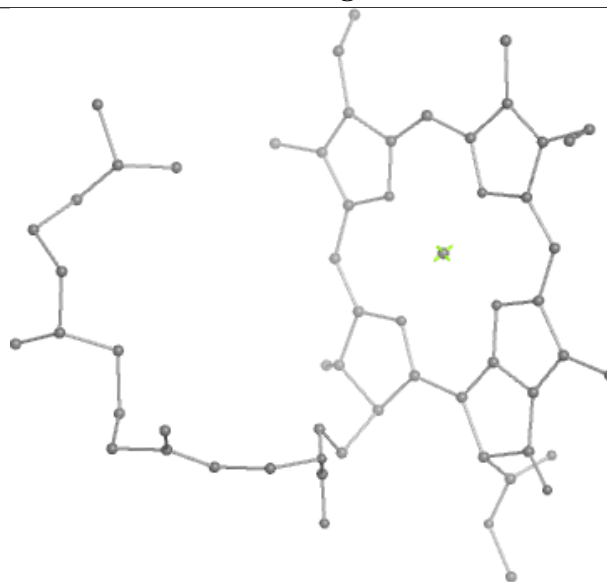
Bond lengths



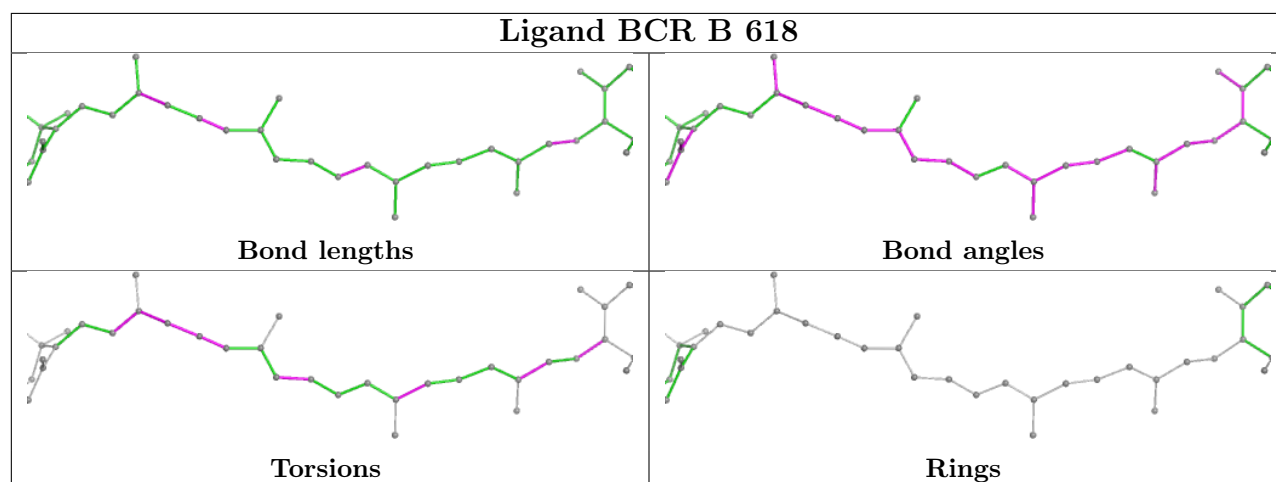
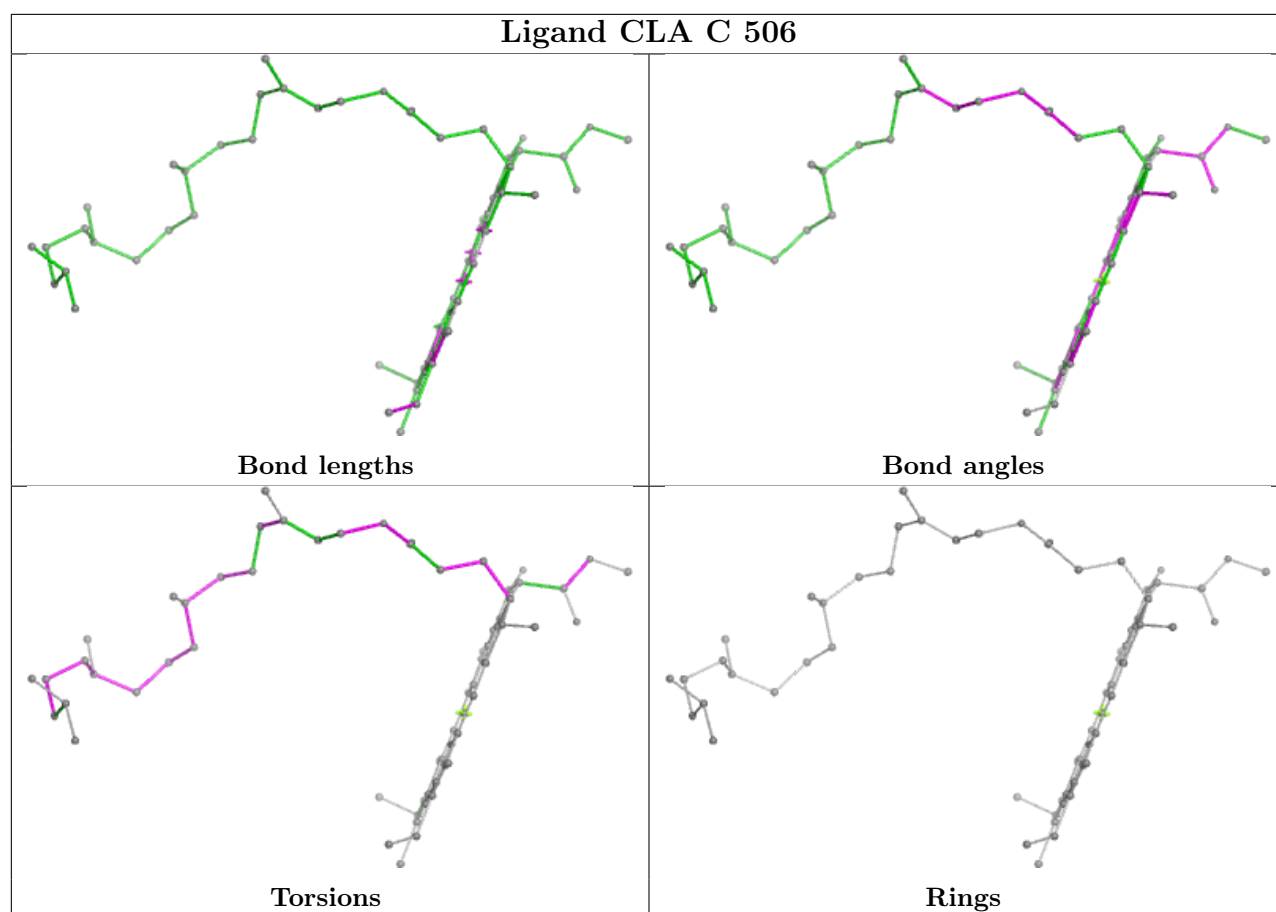
Bond angles



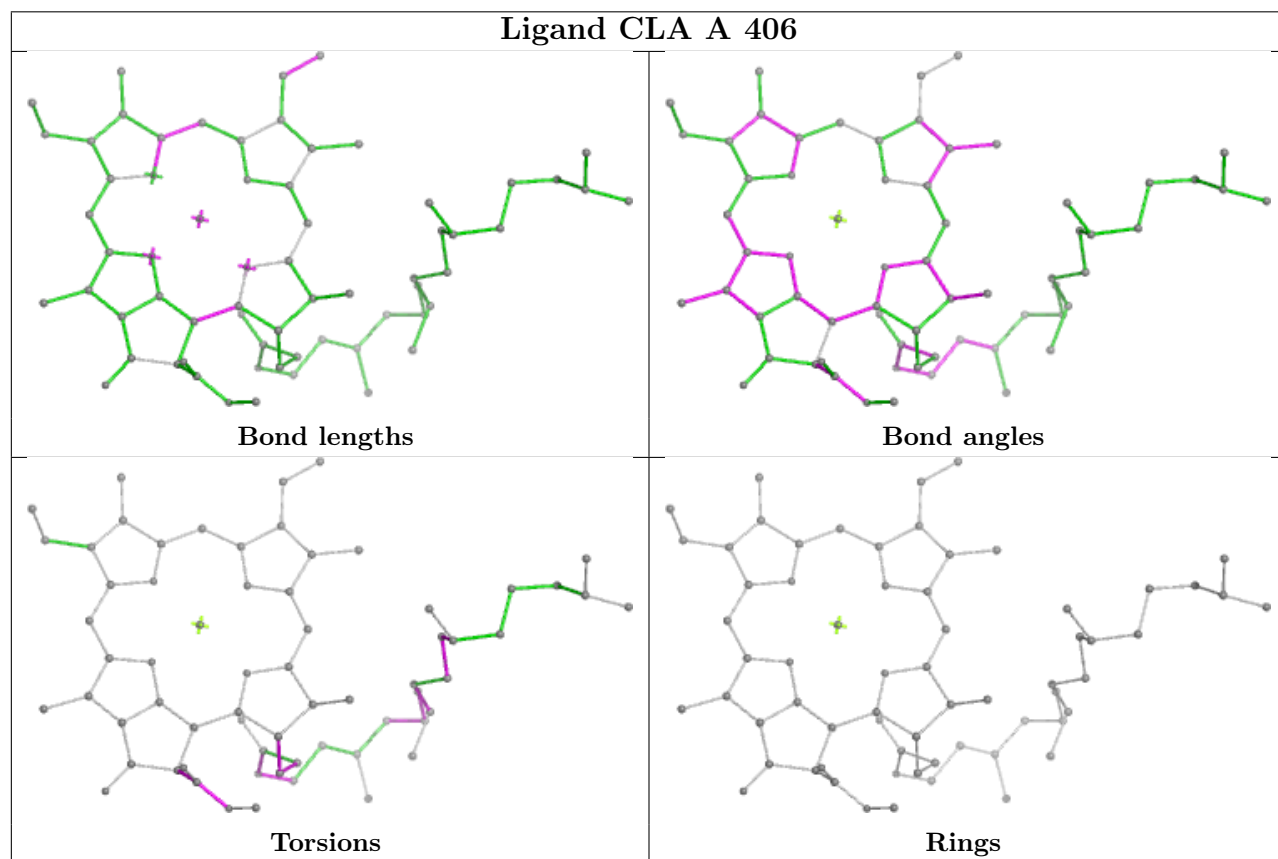
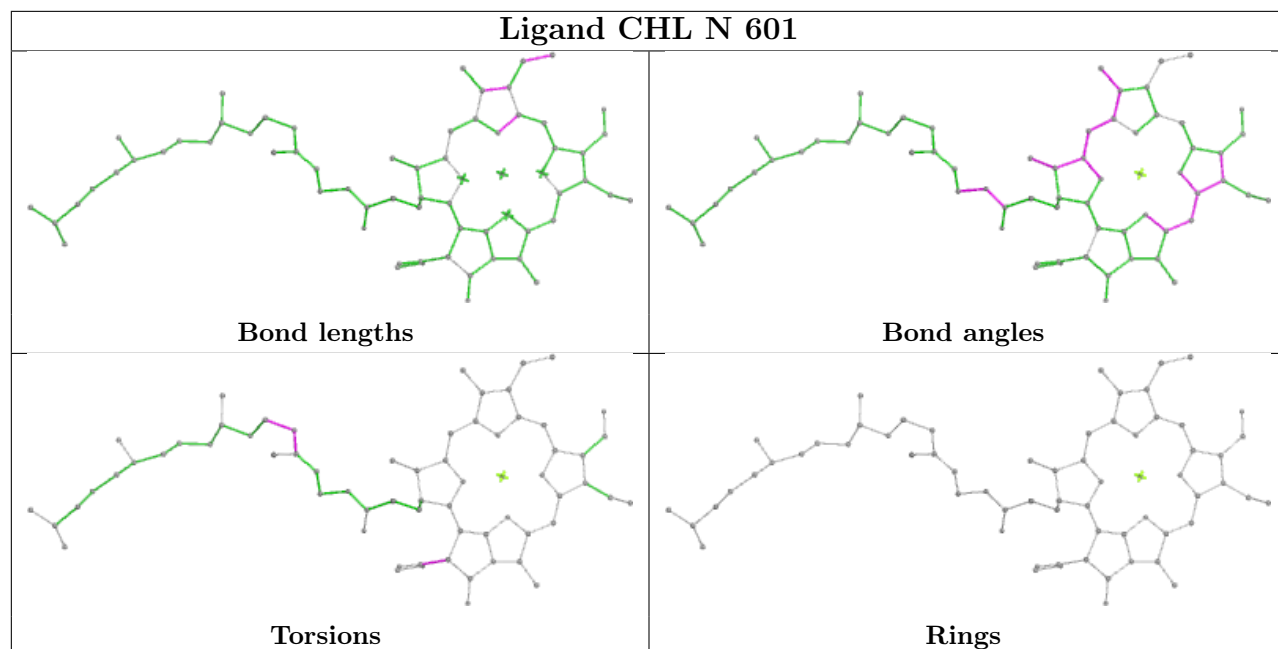
Torsions



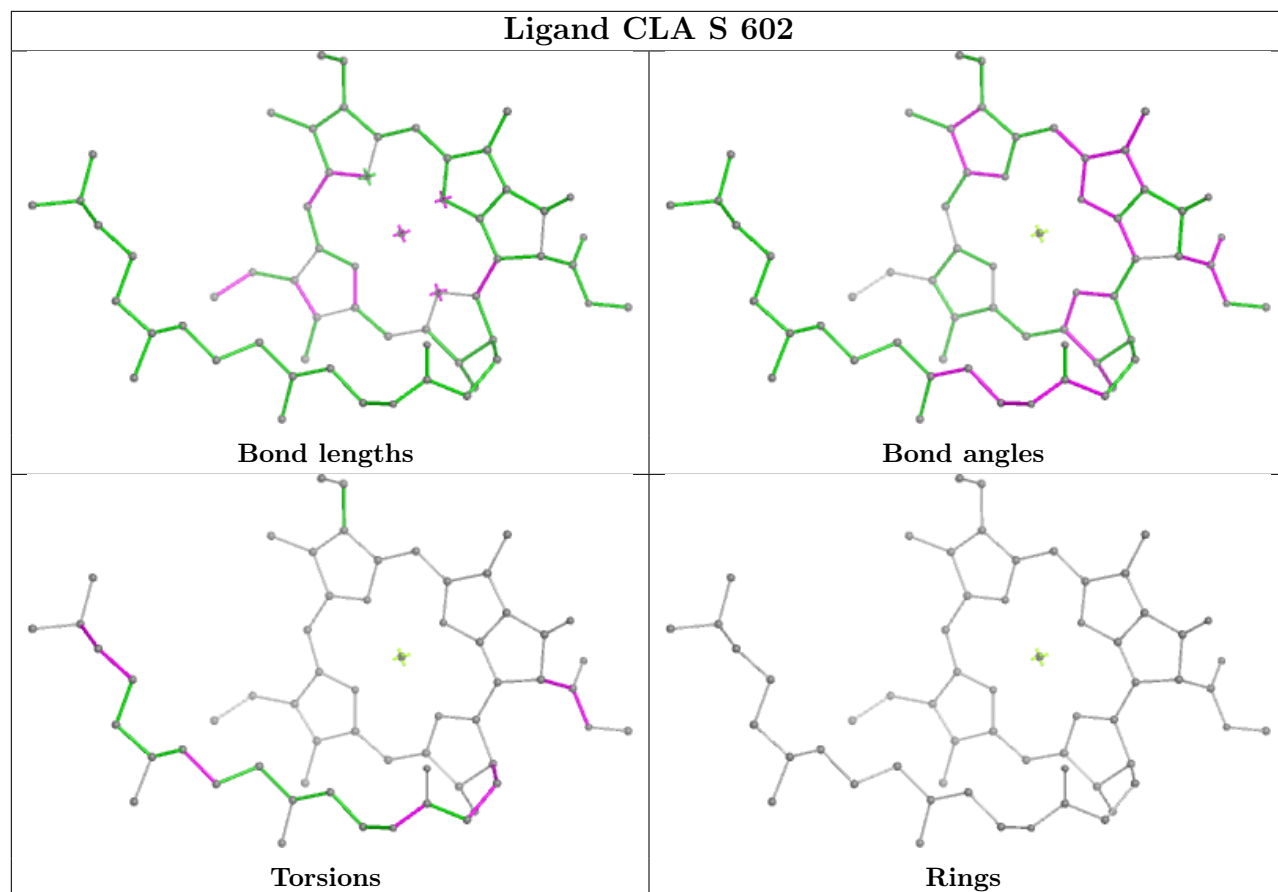
Rings



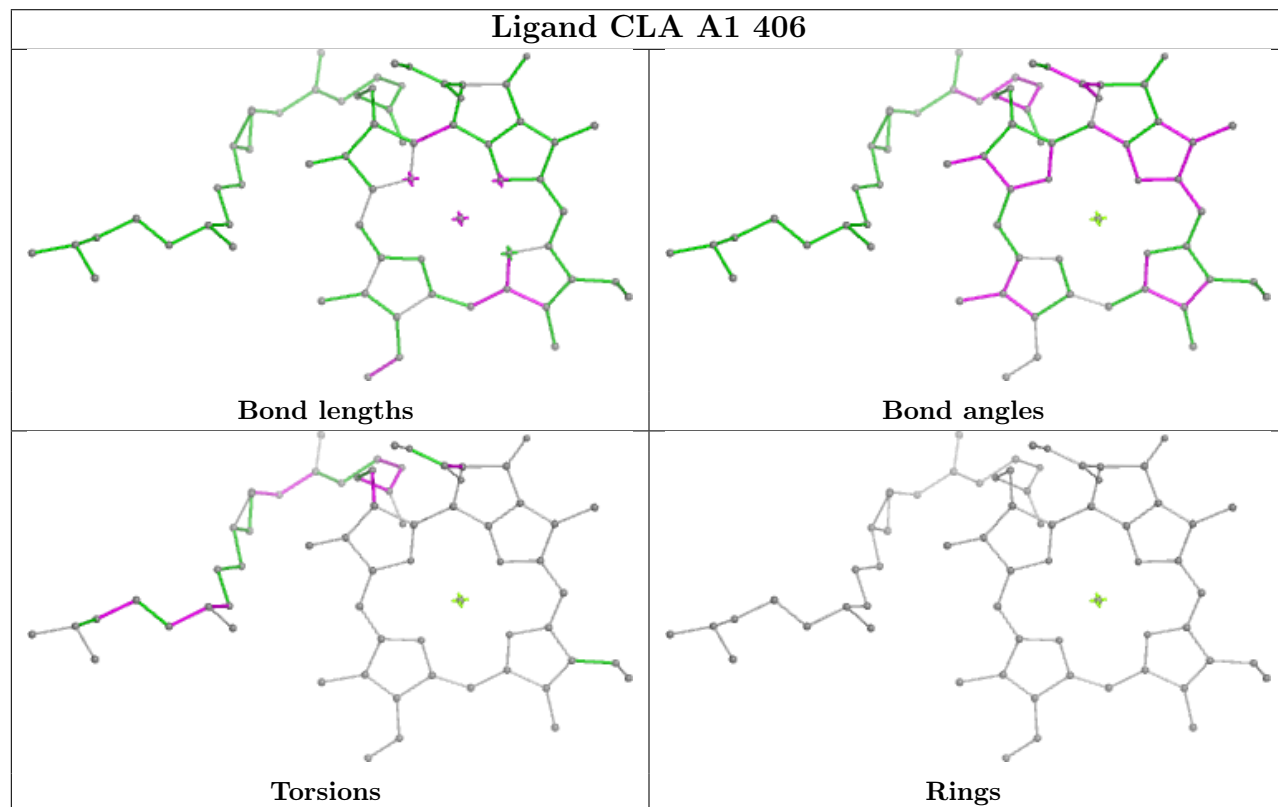


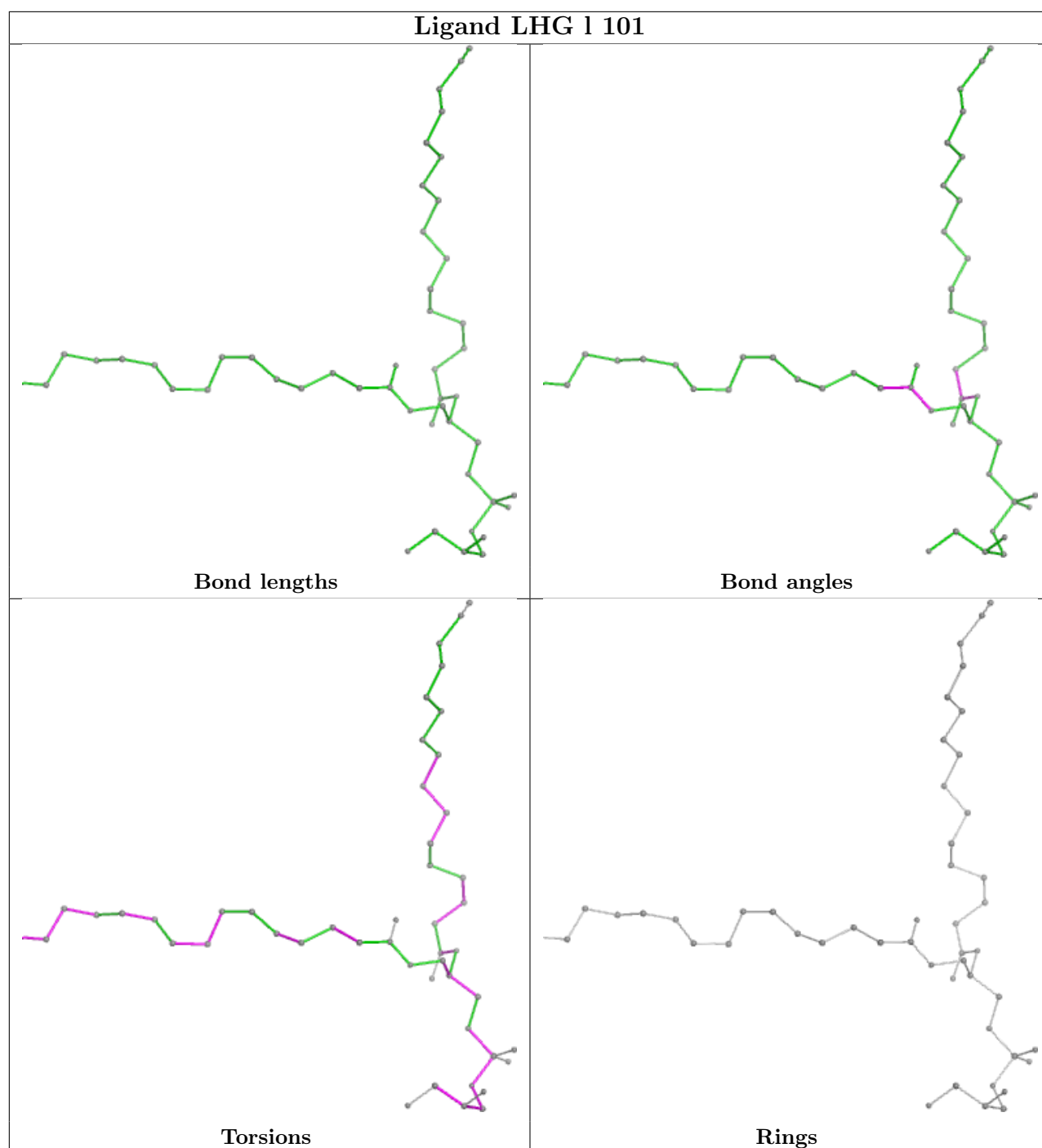


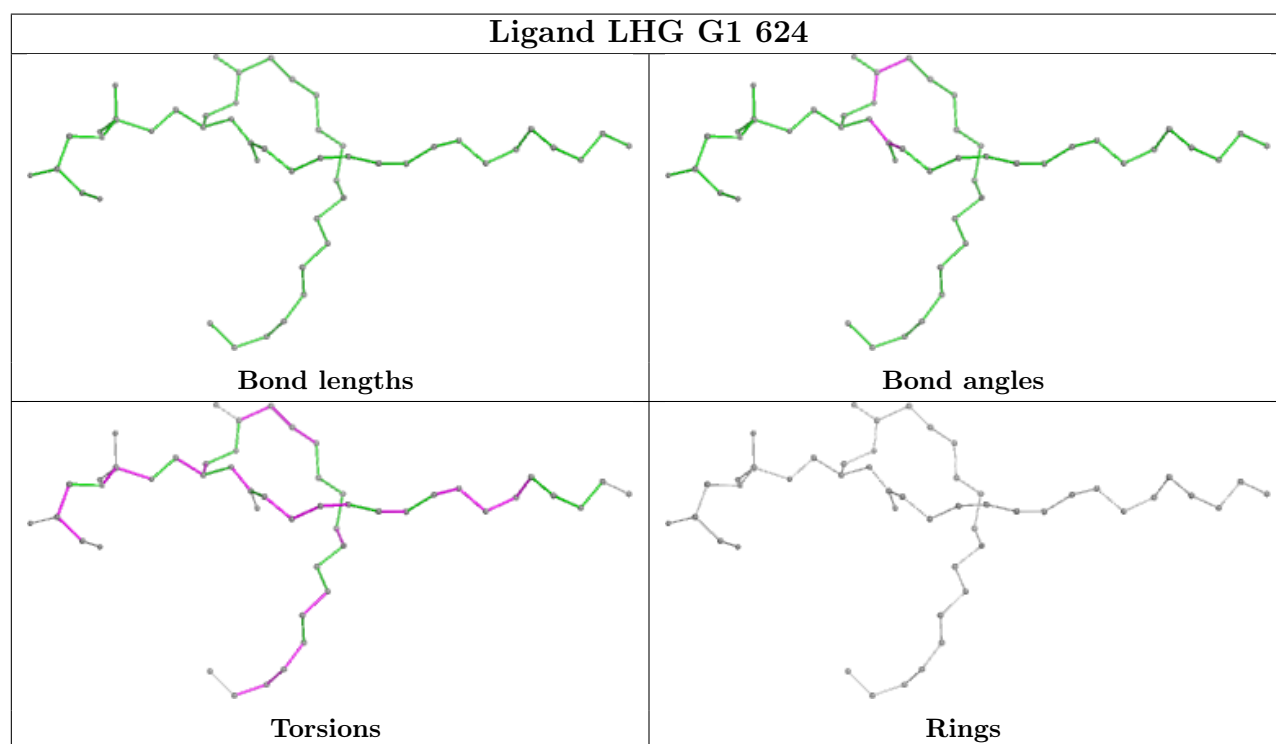
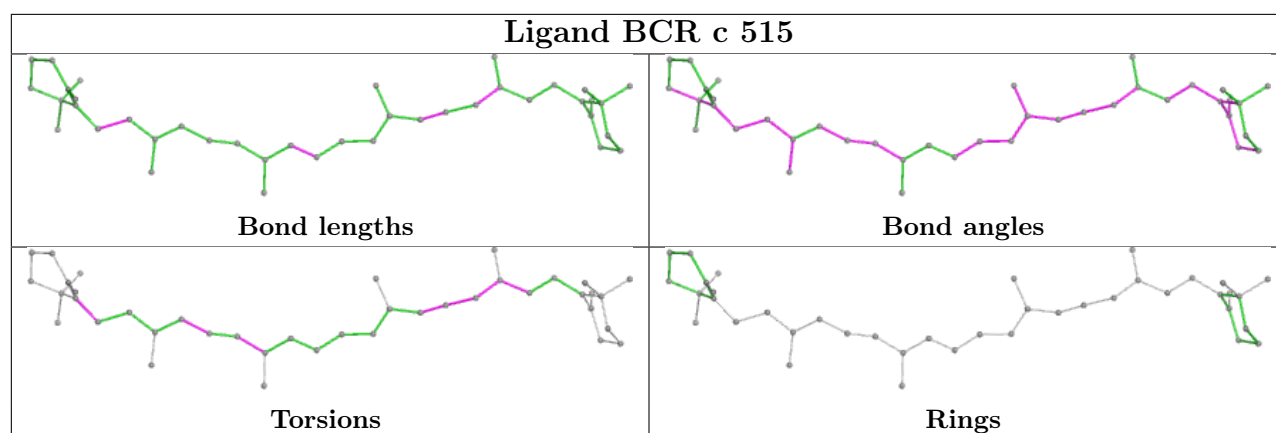
## Ligand CLA S 602

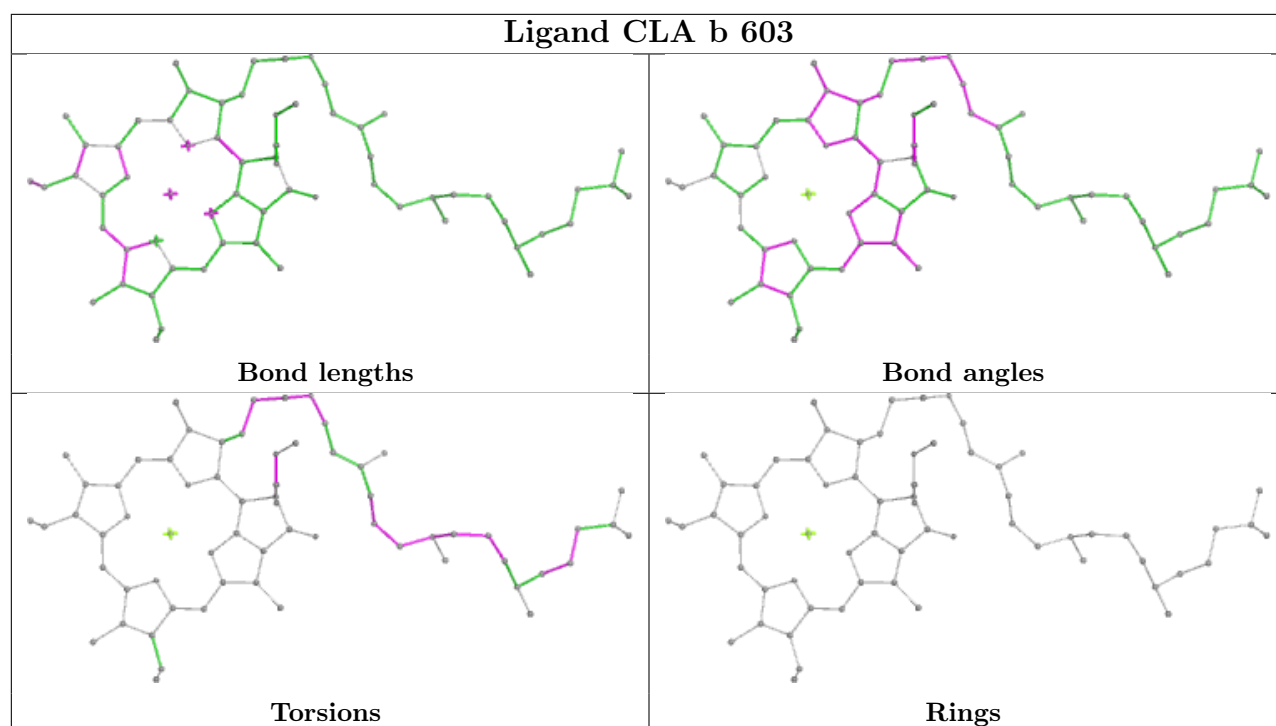


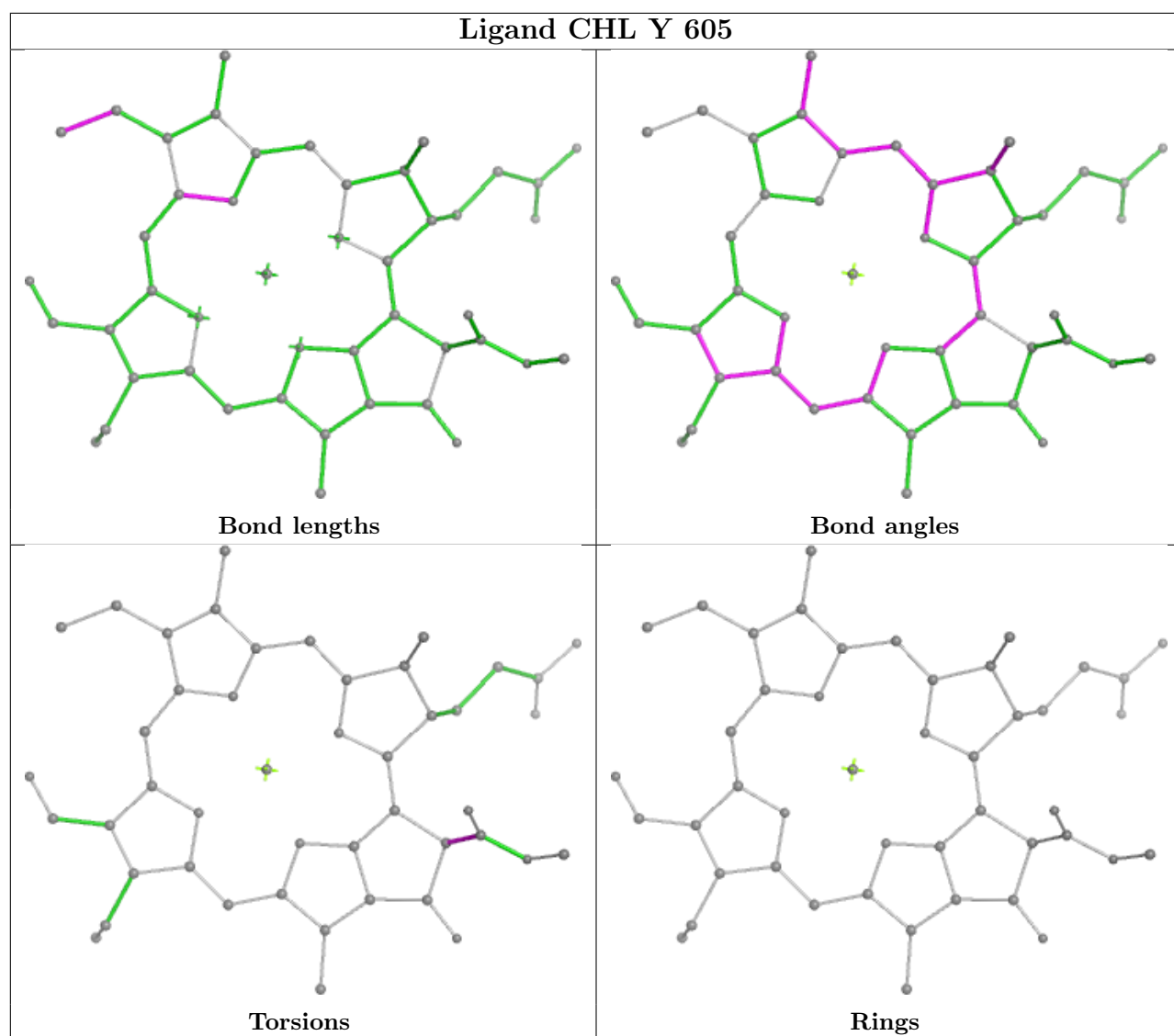
## Ligand CLA A1 406

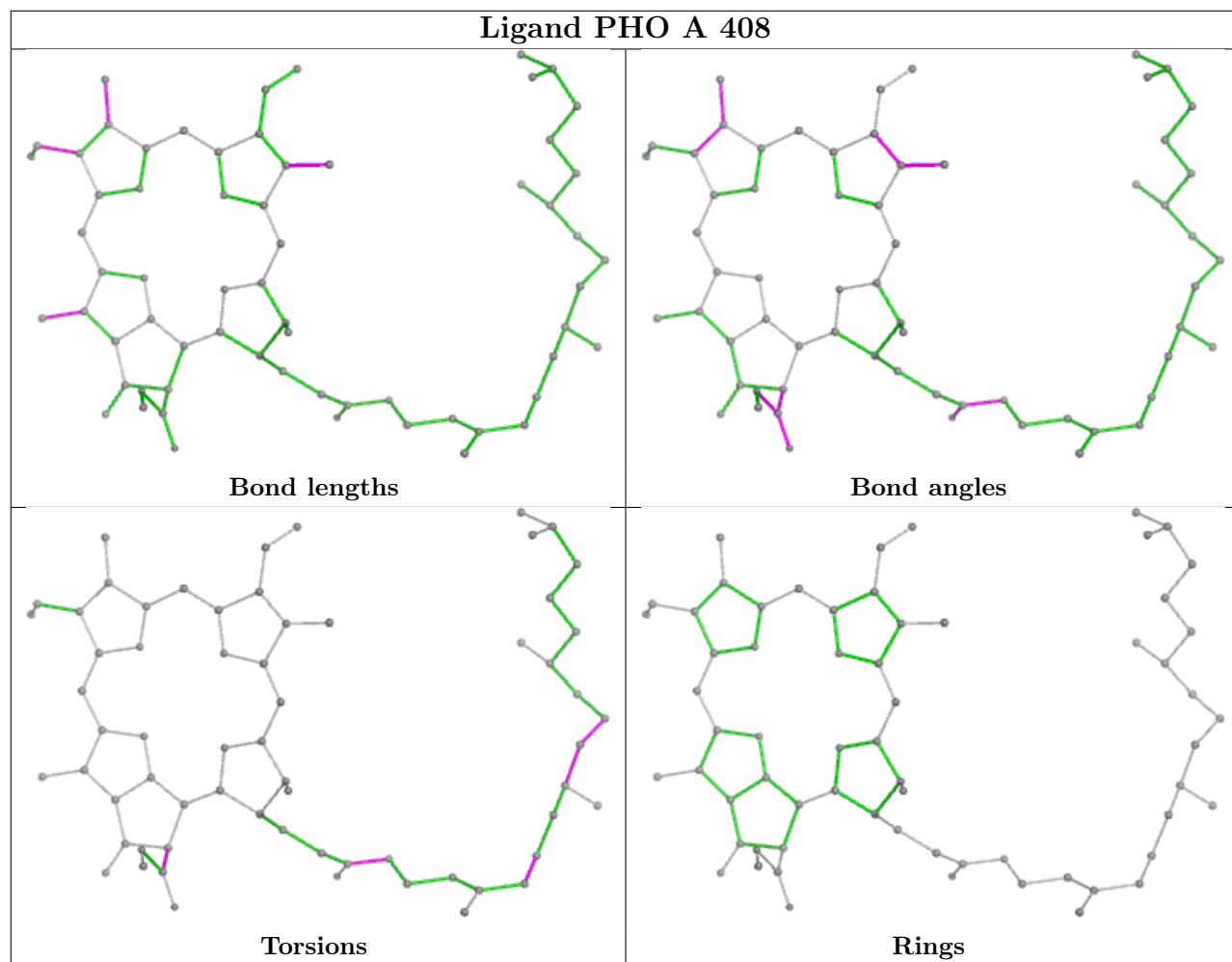




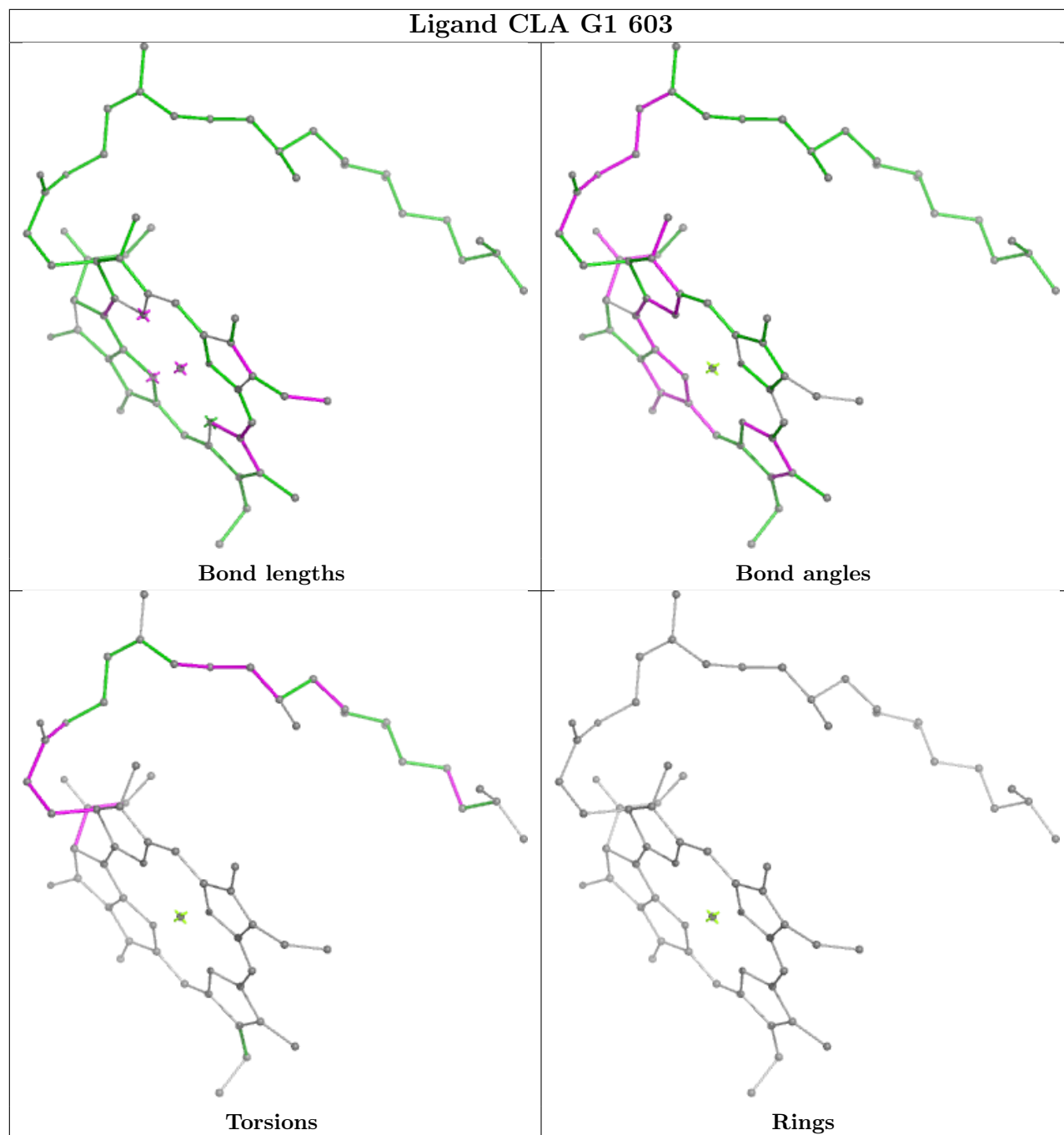




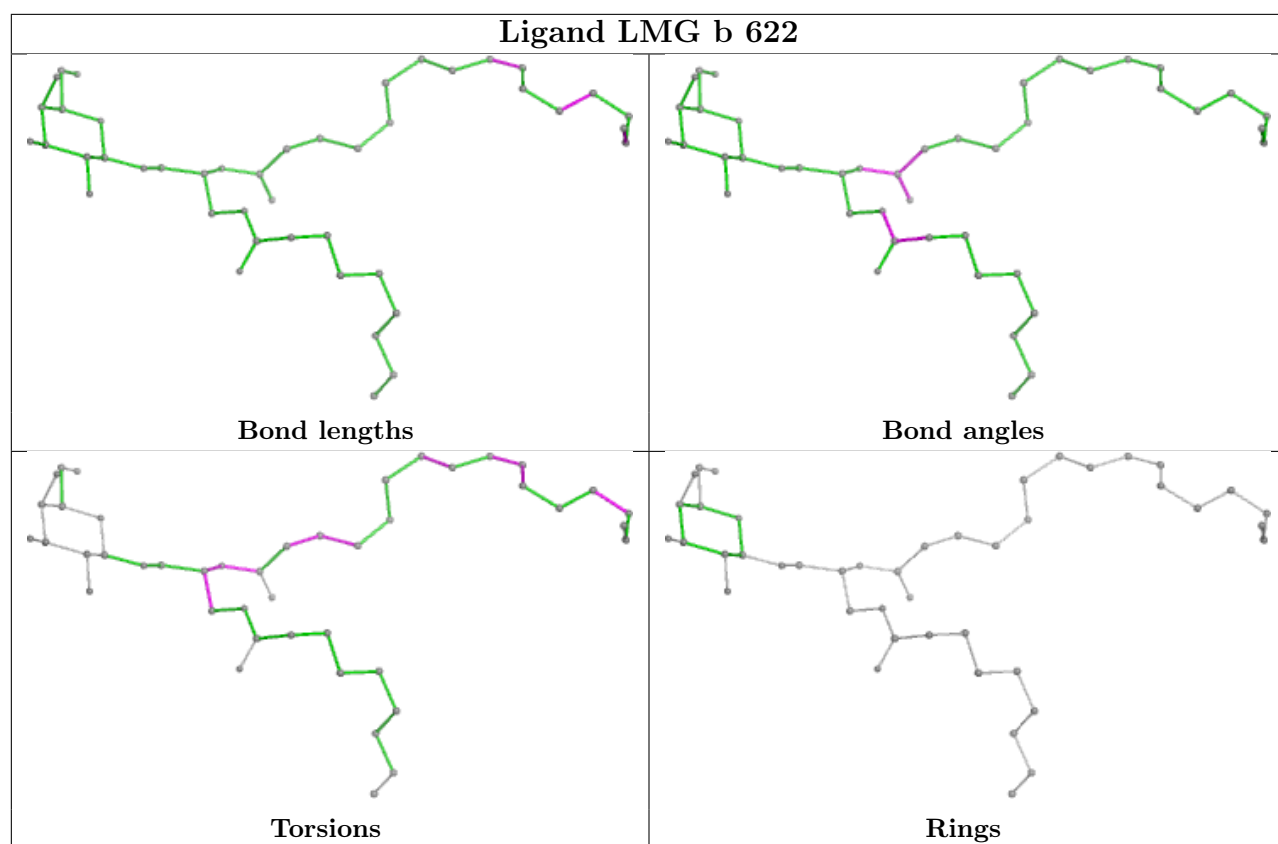


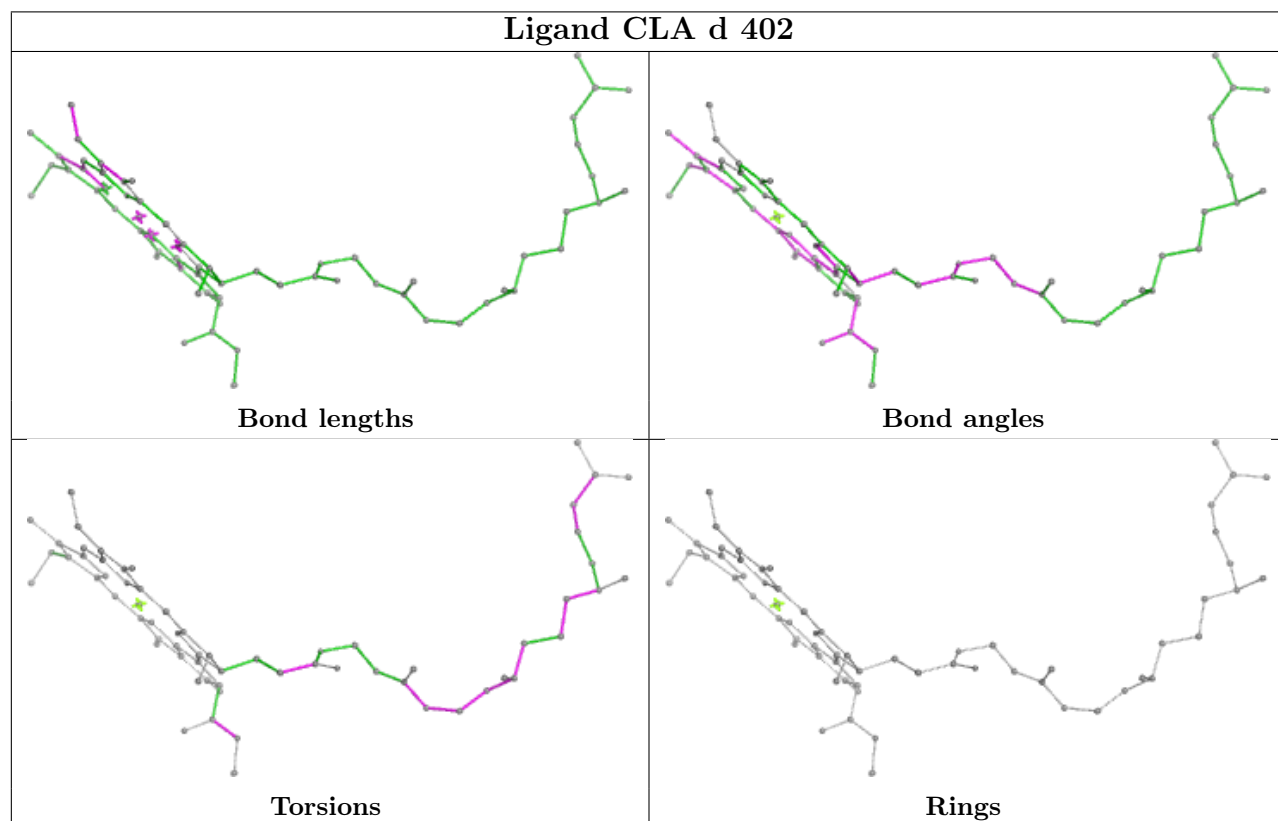
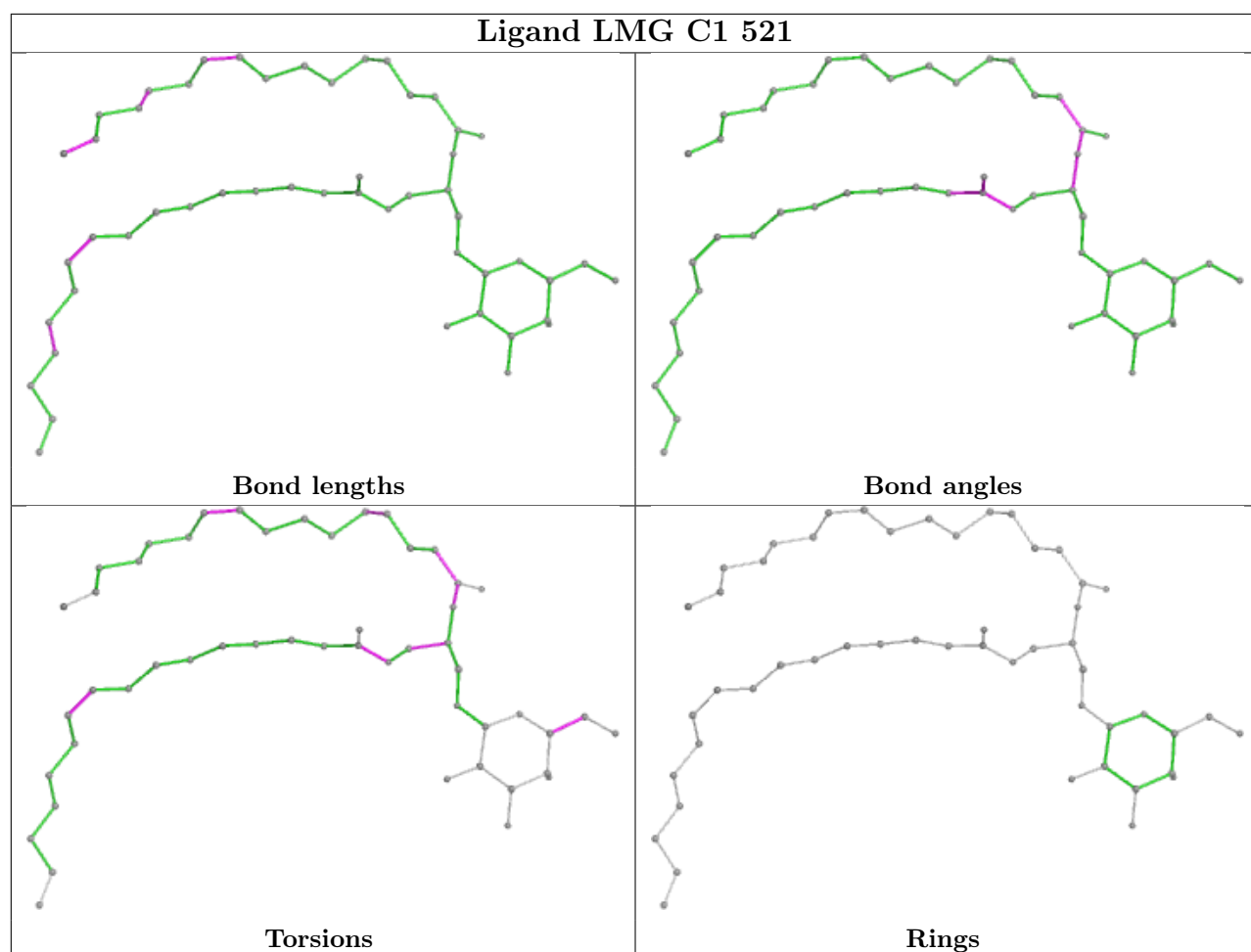


## Ligand CLA G1 603

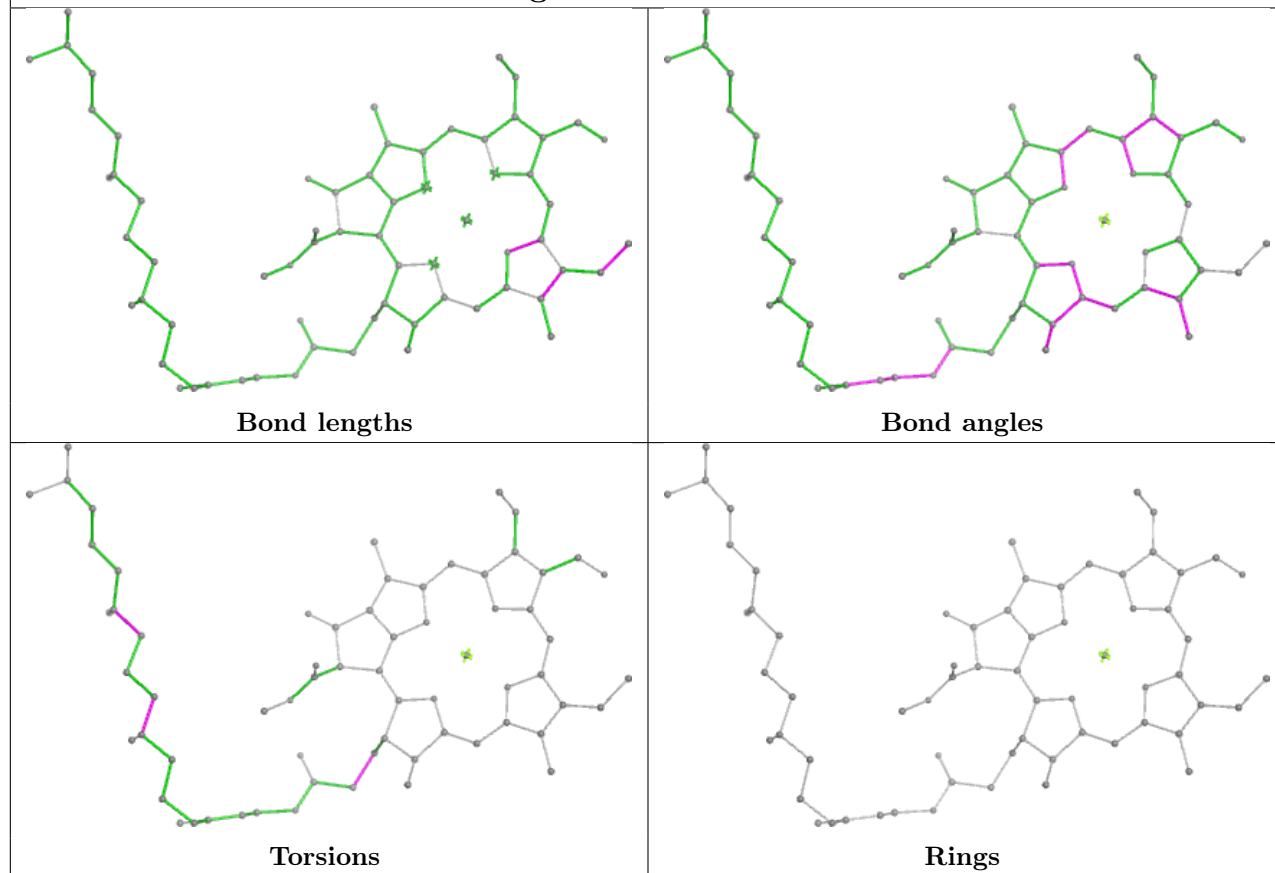




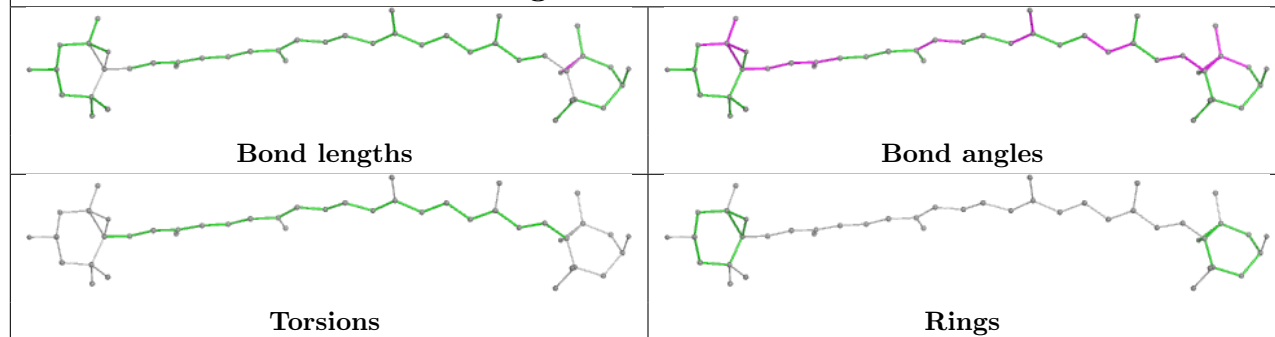


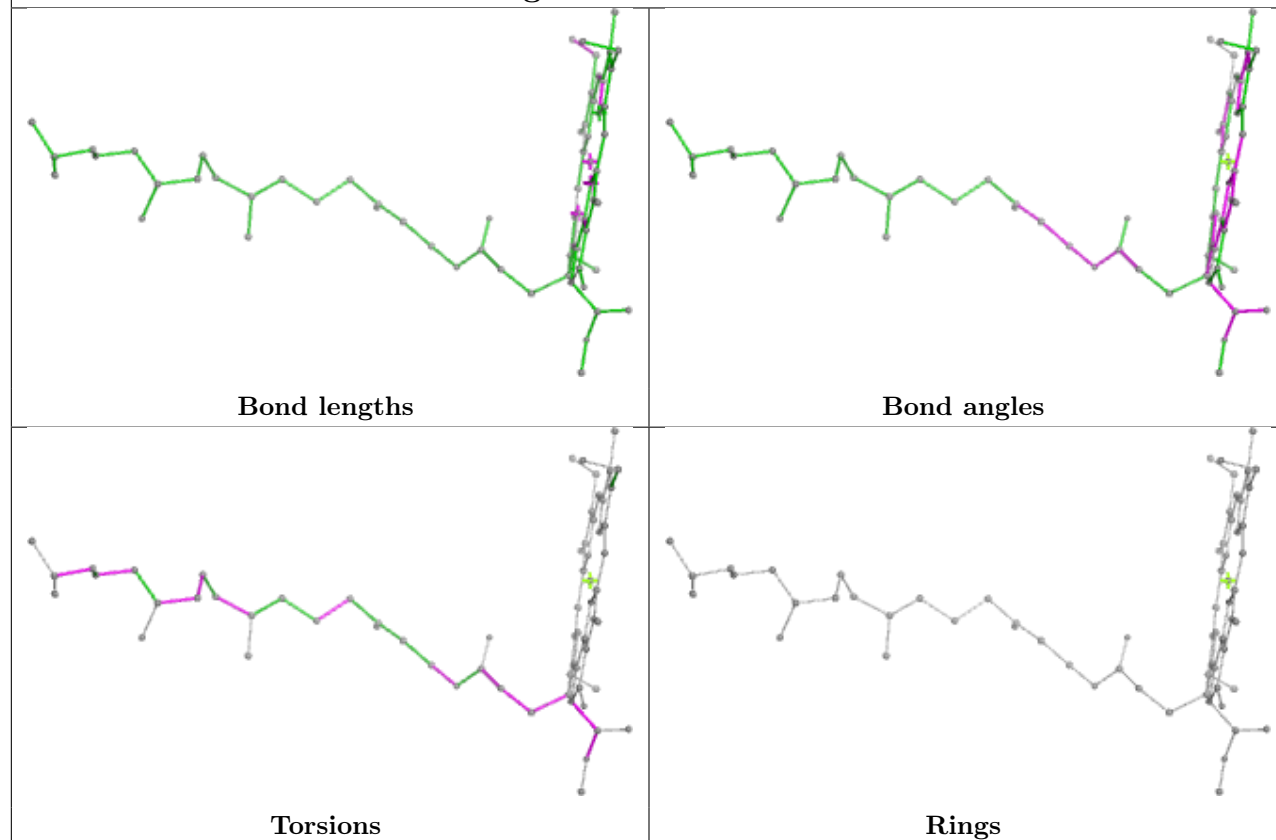
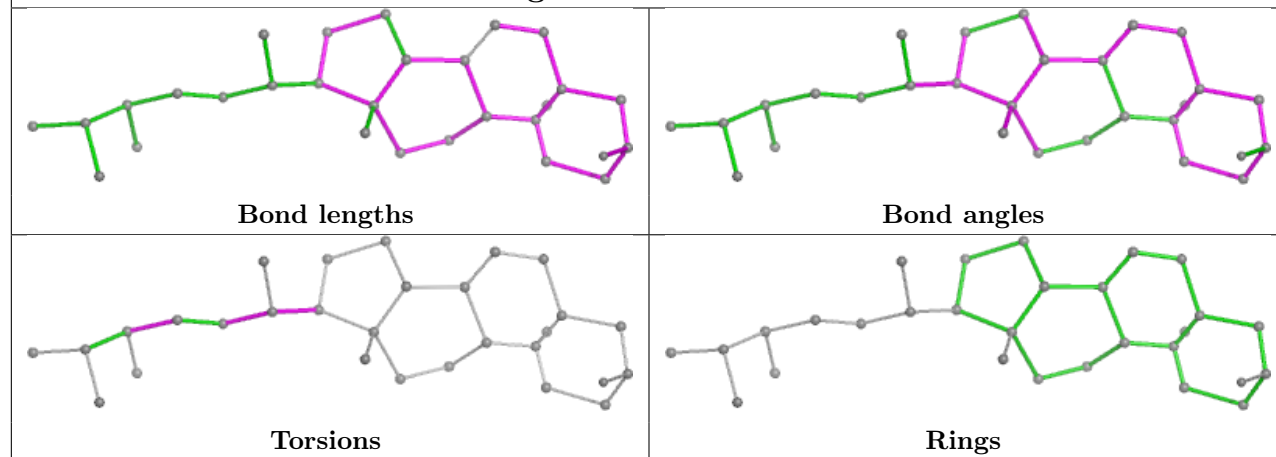


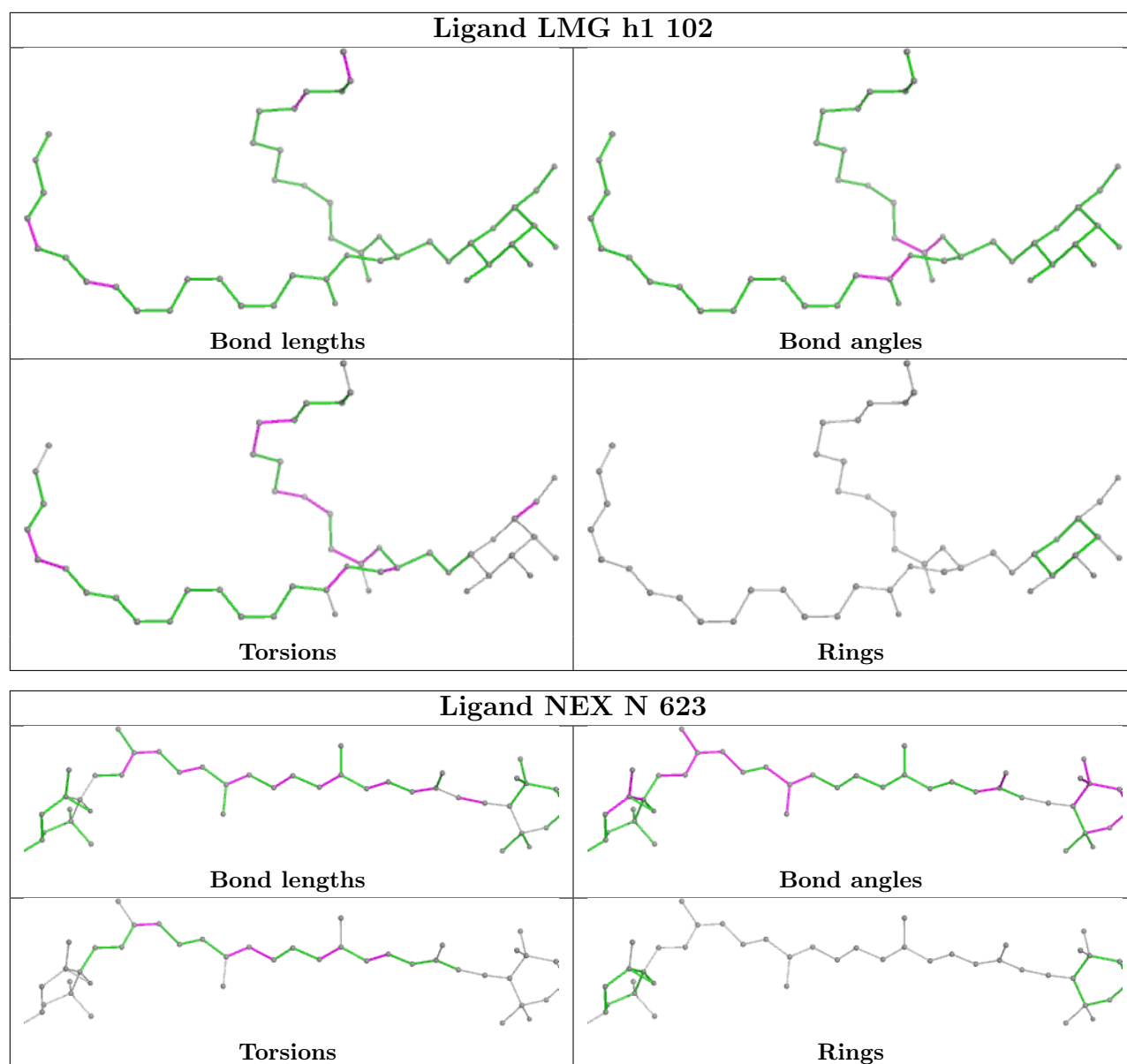
## Ligand CHL N 606

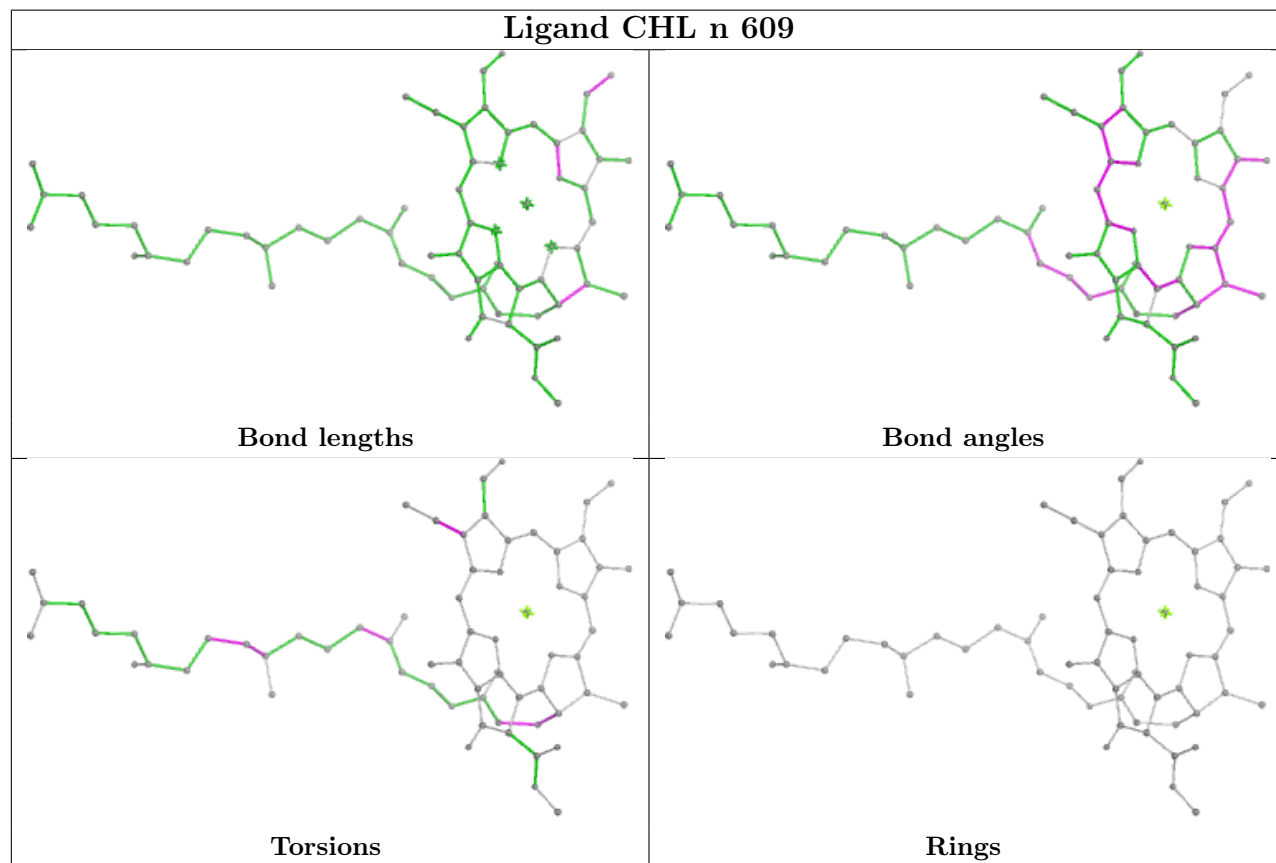
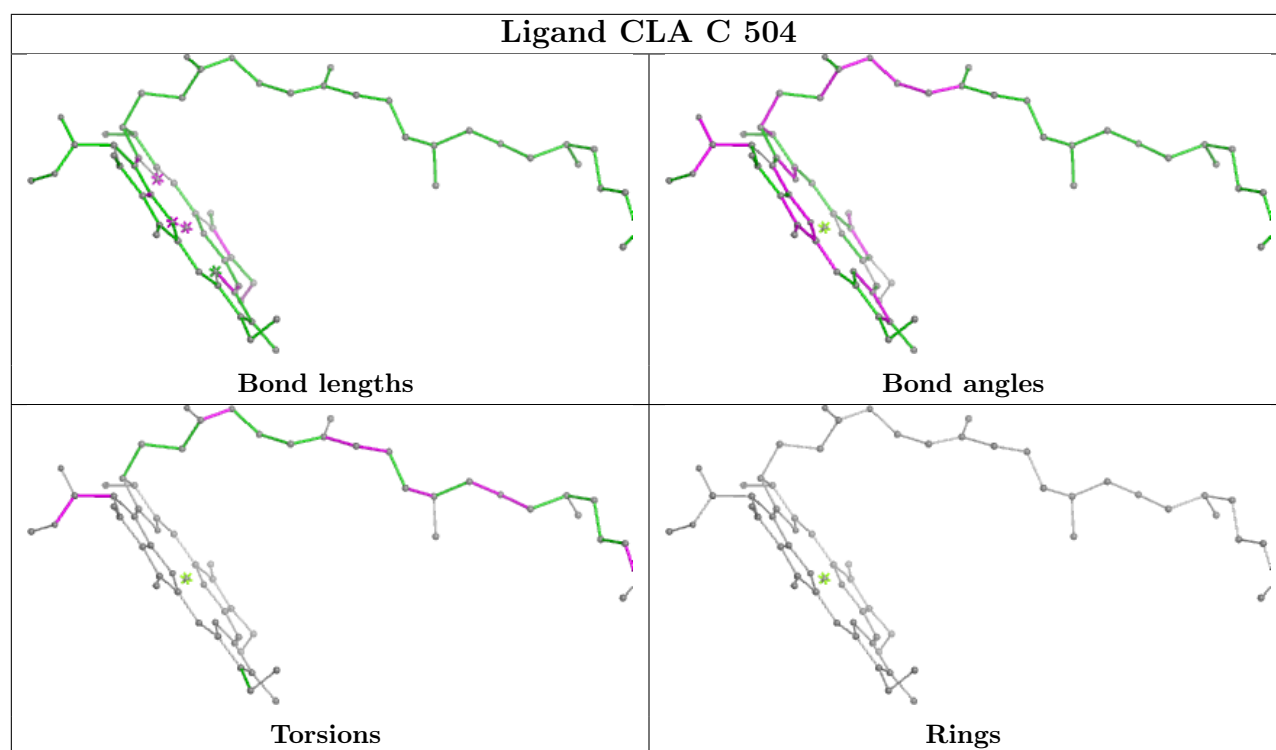


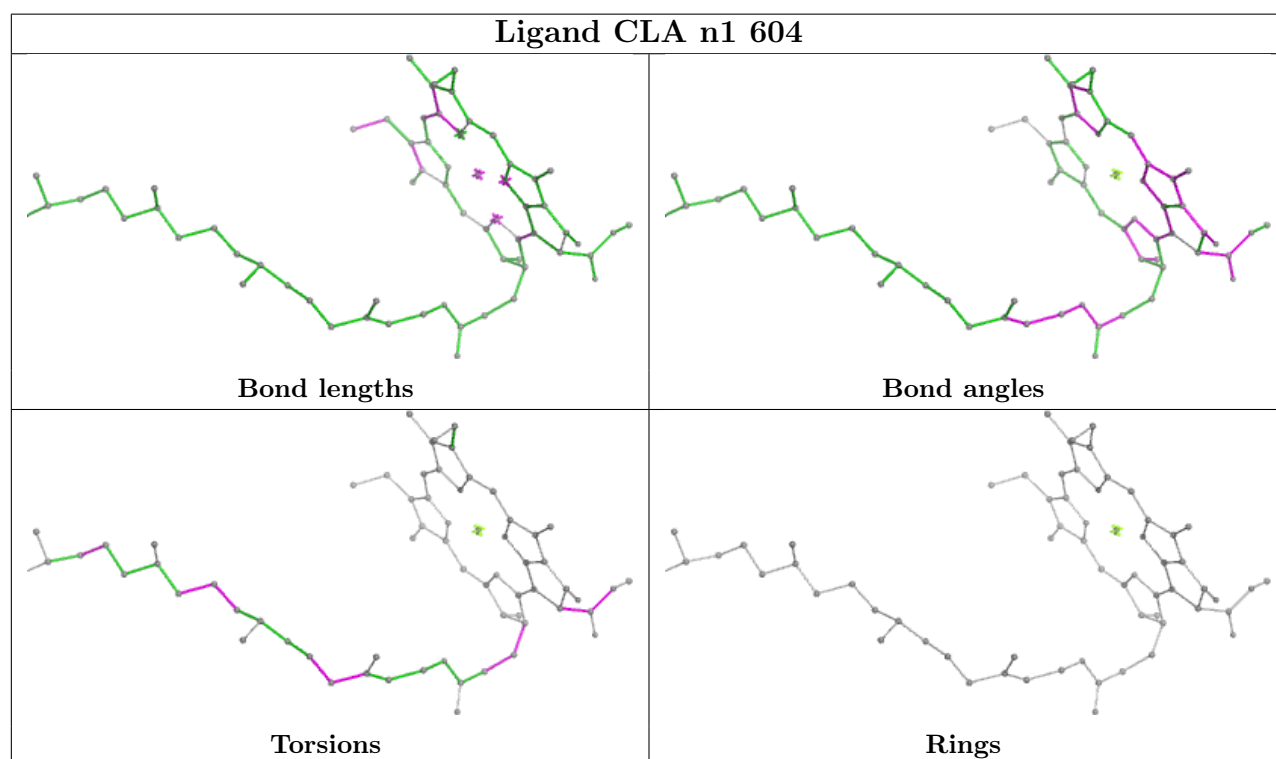
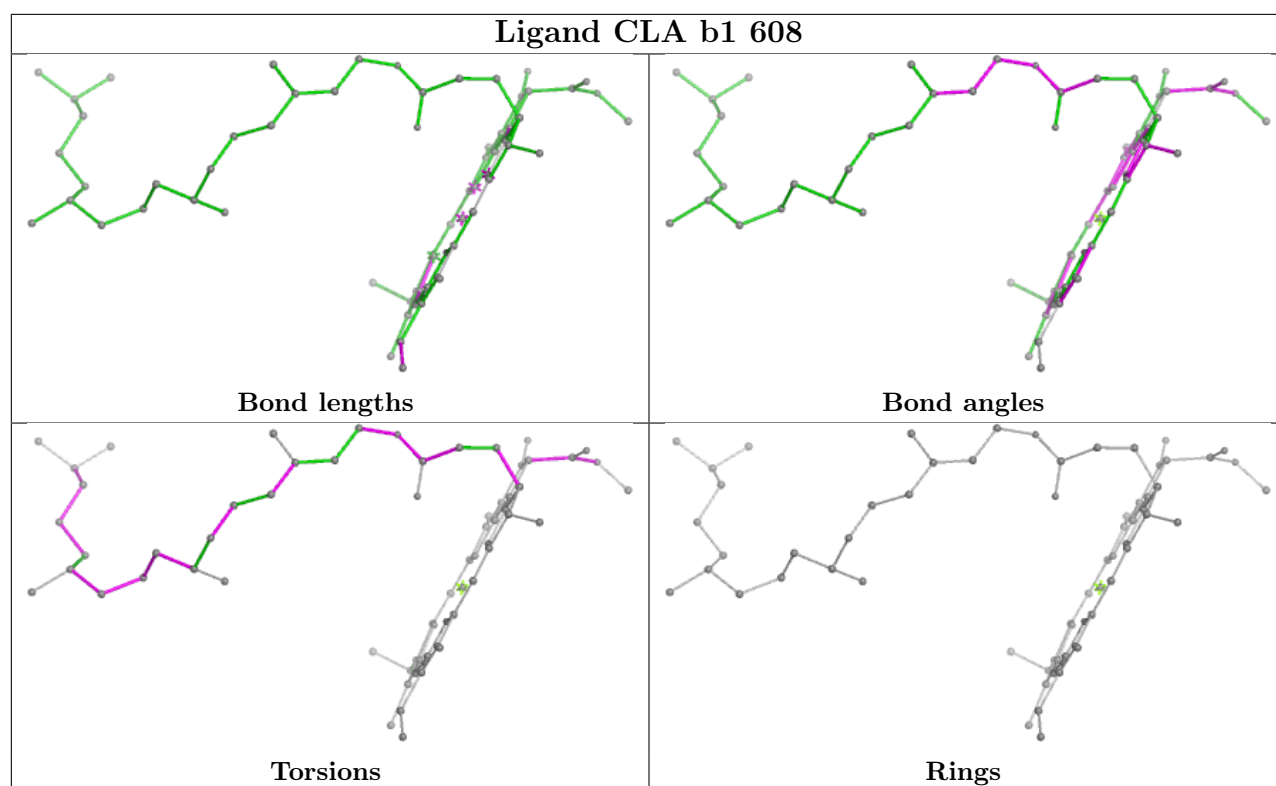
## Ligand XAT G 622



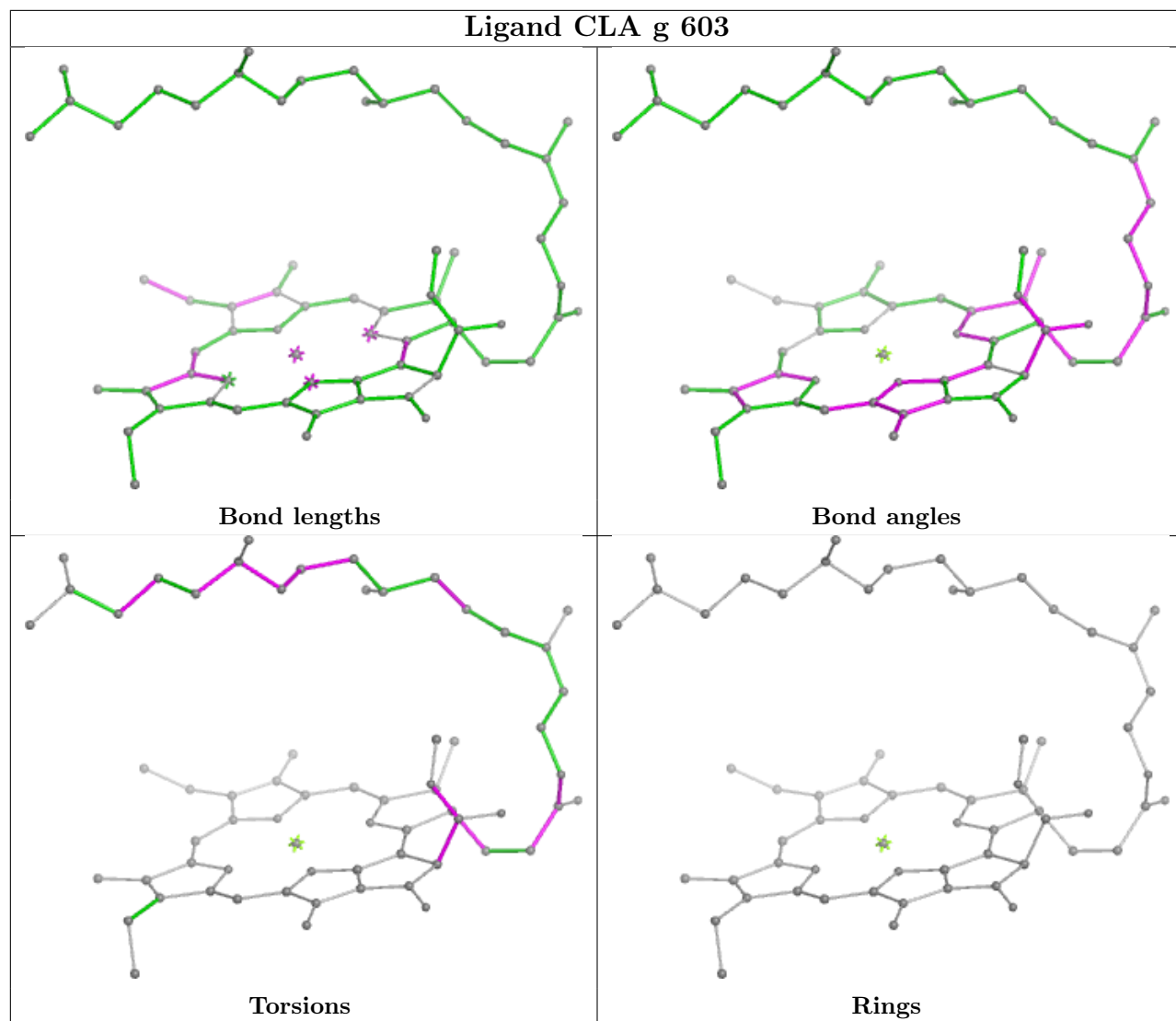
**Ligand CLA B1 607****Ligand ERG r1 626**



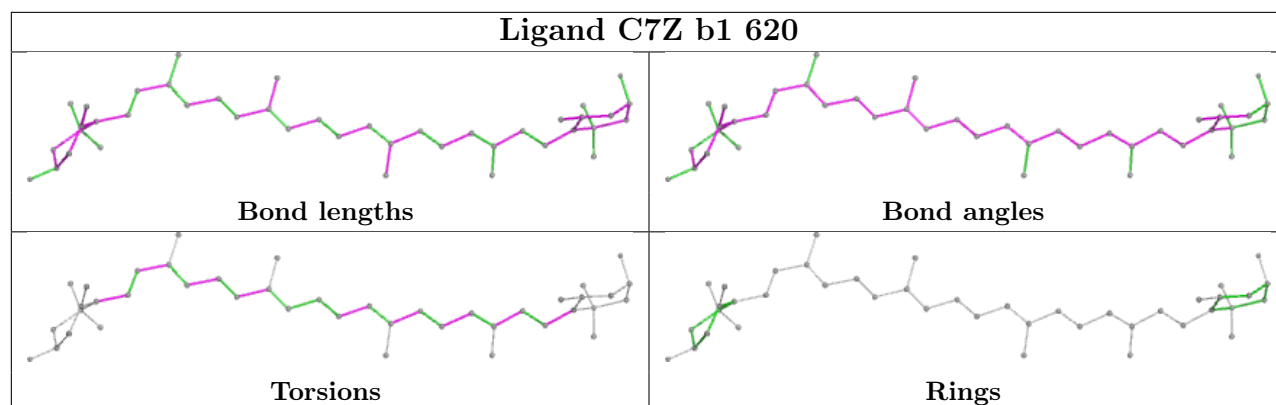
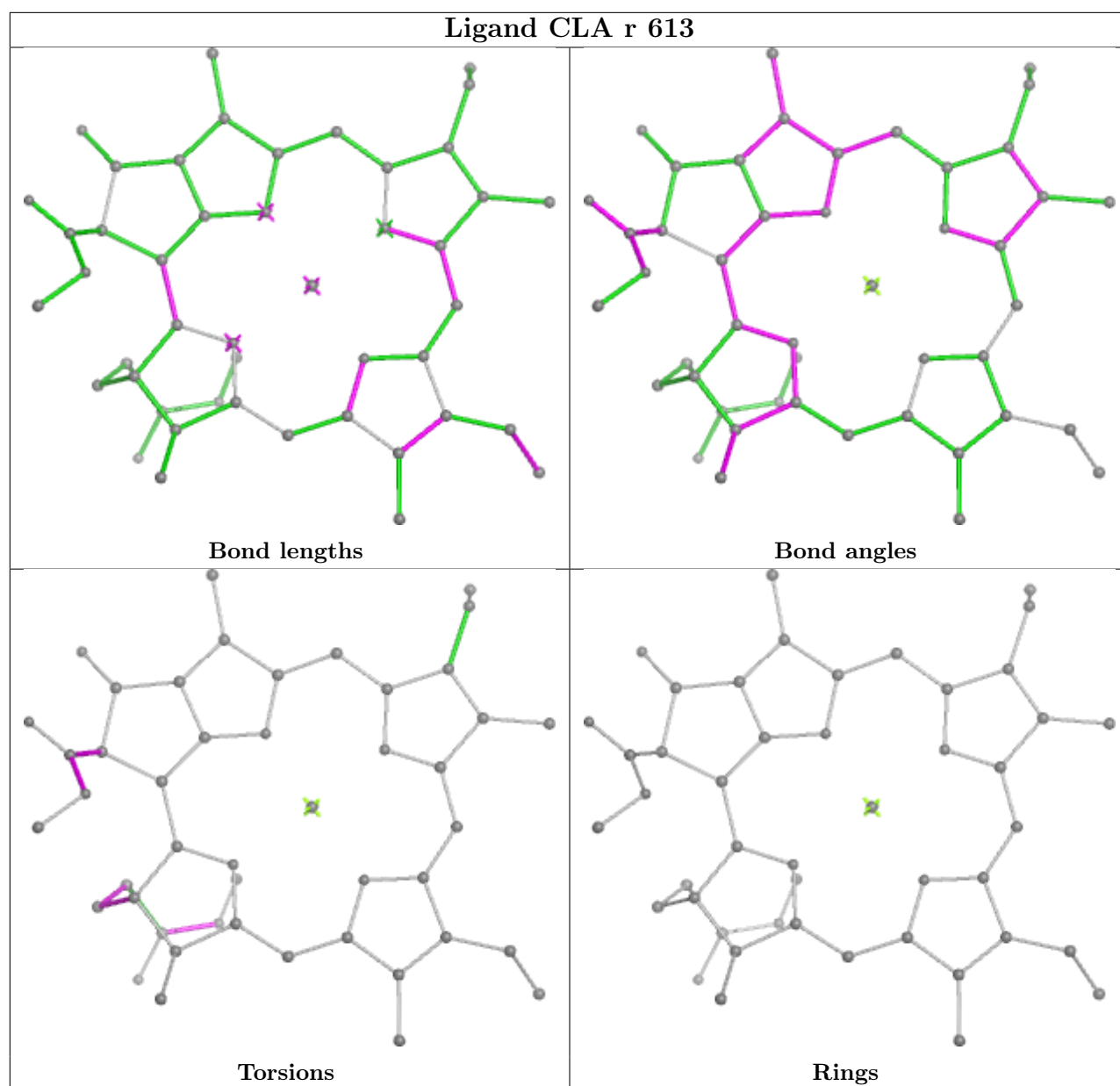


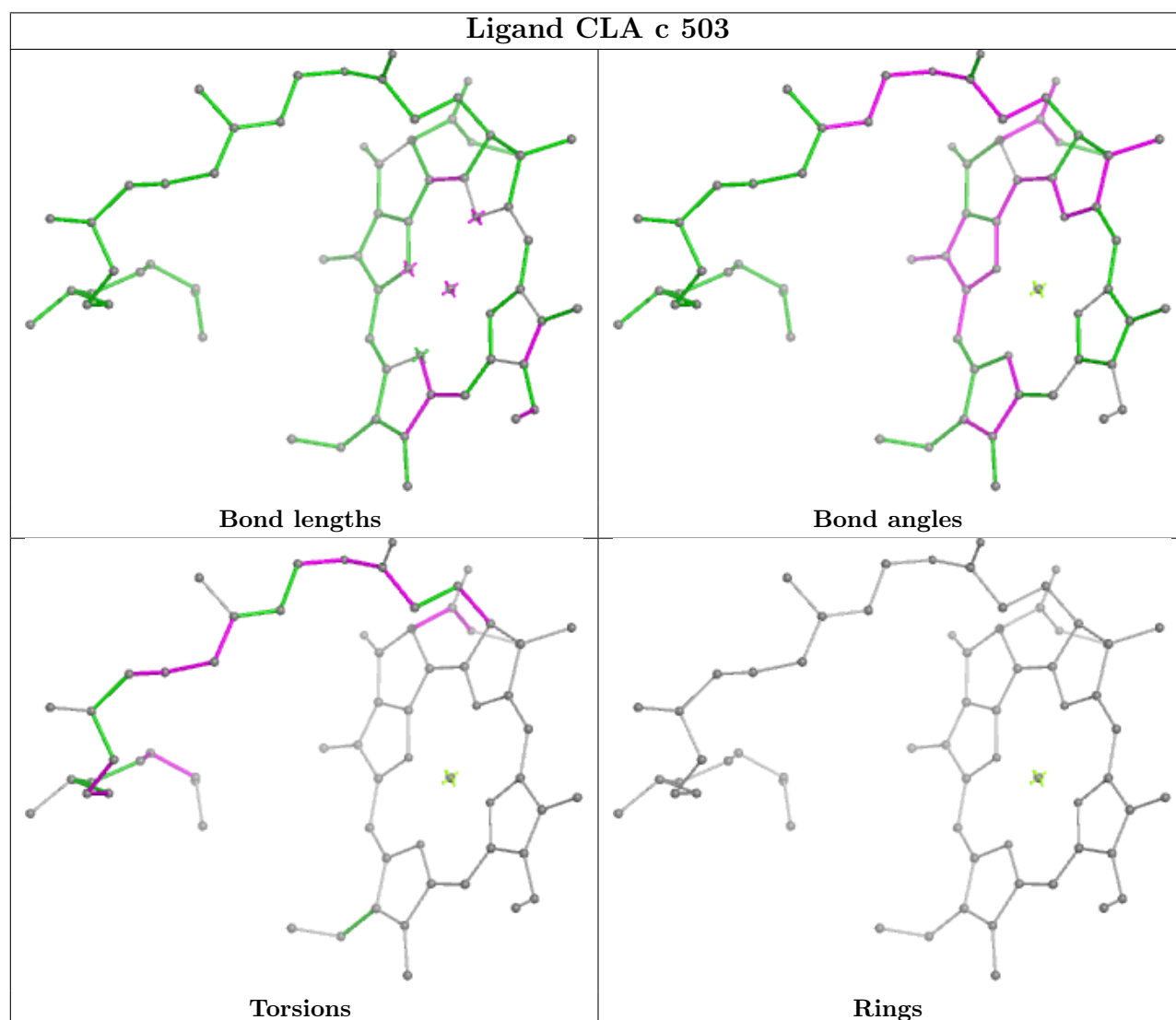
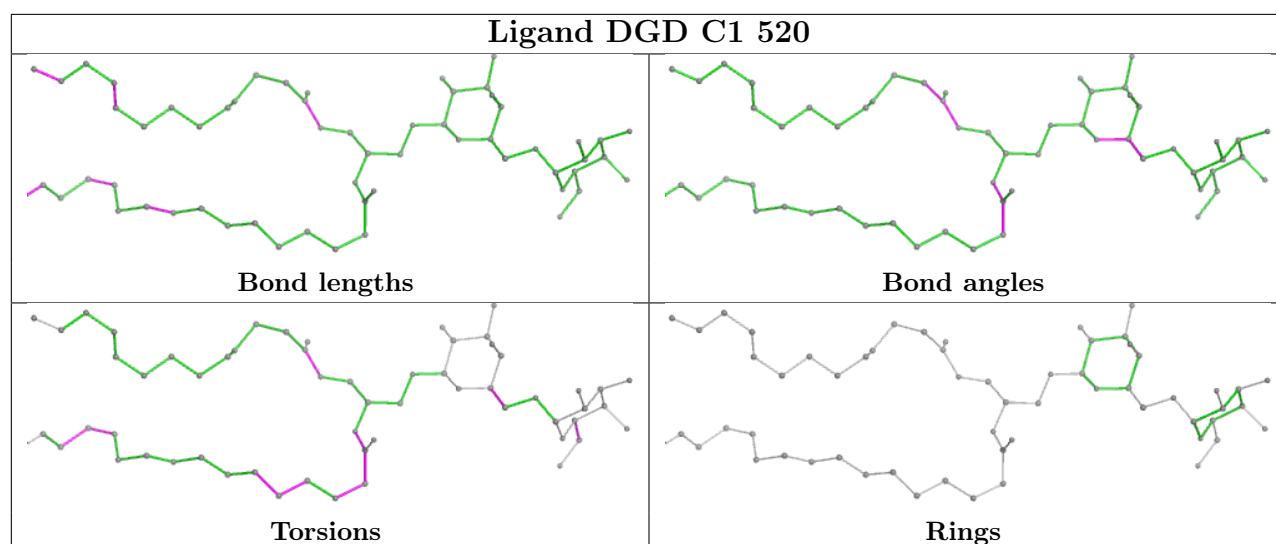


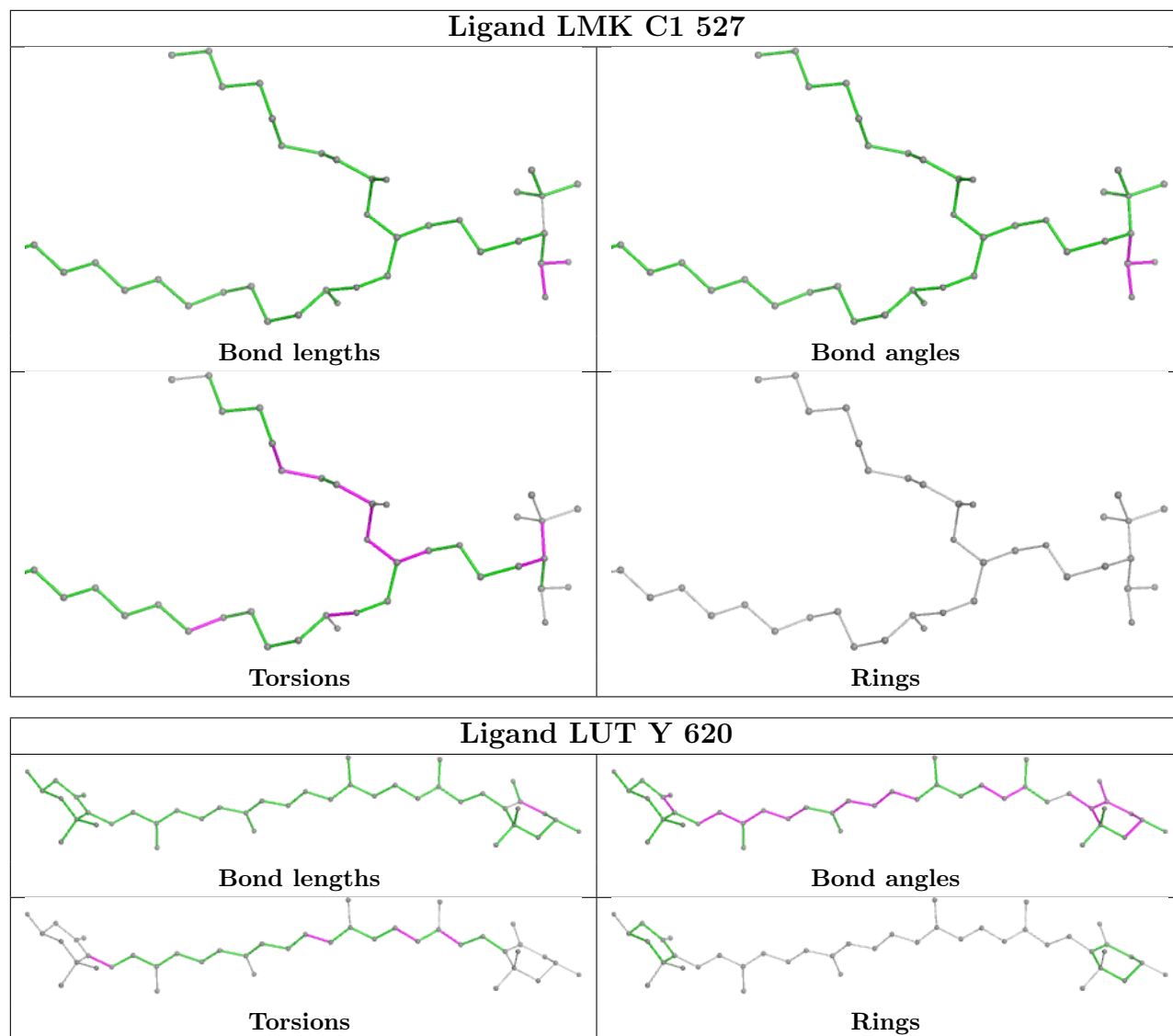
## Ligand CLA g 603



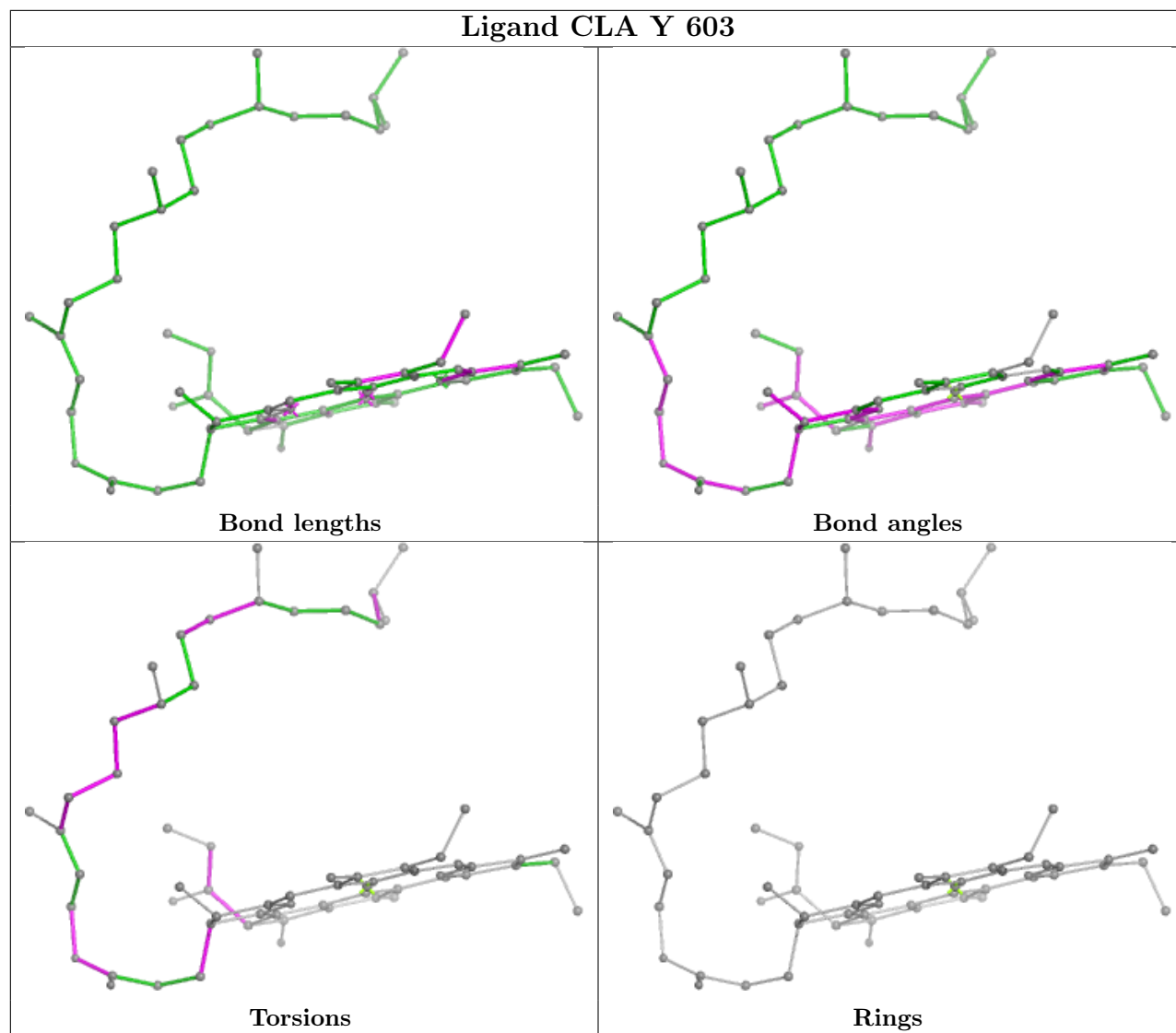




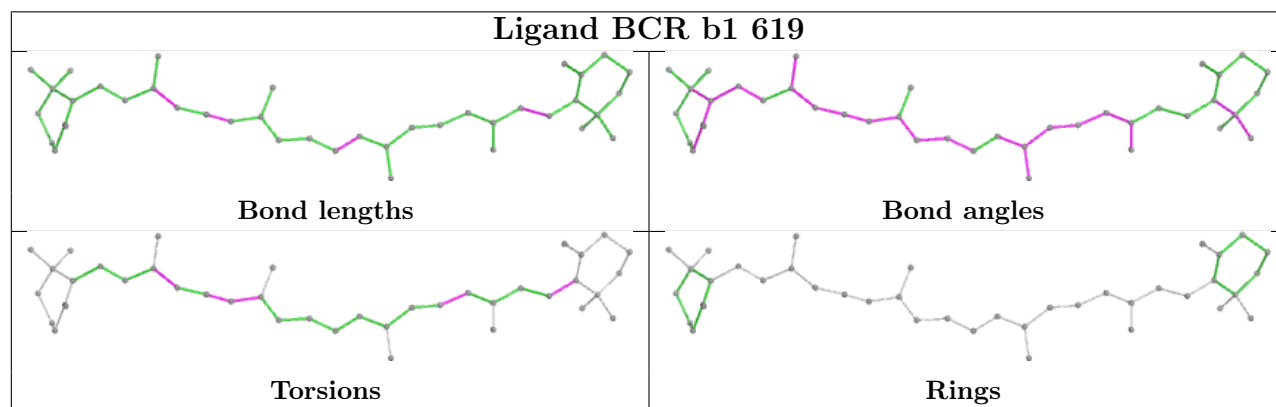




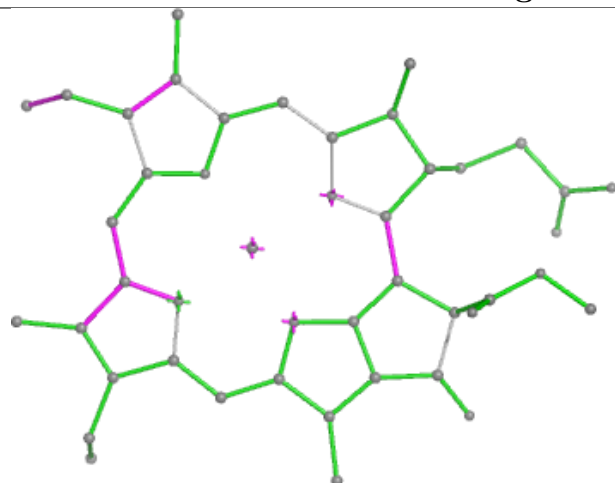
## Ligand CLA Y 603



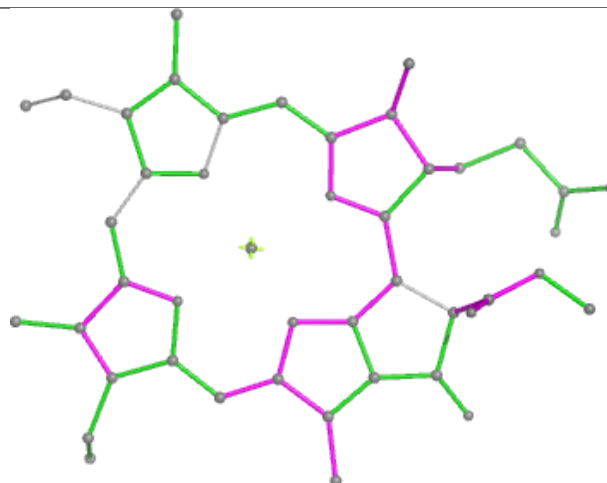
## Ligand BCR b1 619



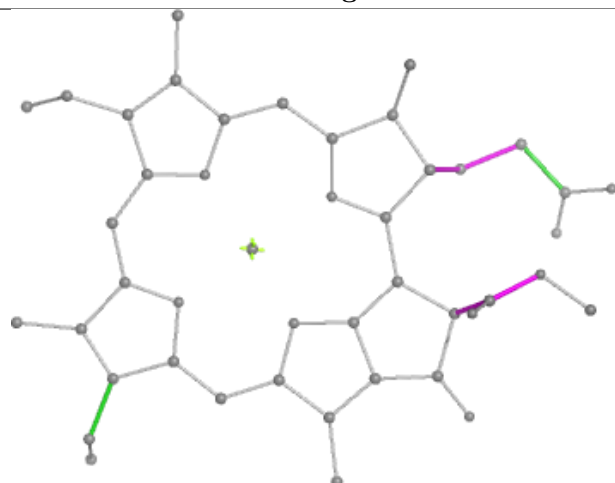
## Ligand CLA N 612



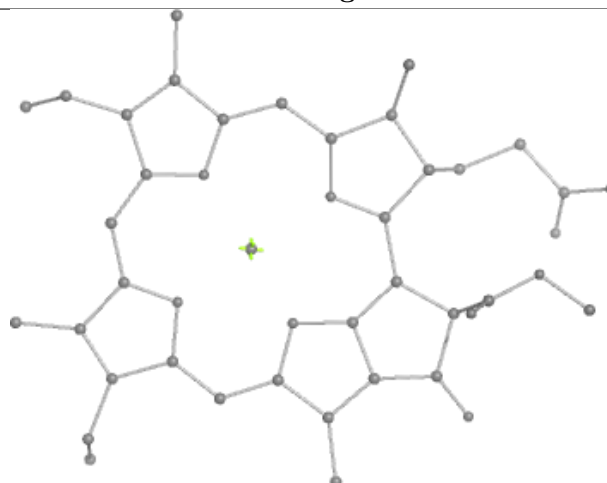
Bond lengths



Bond angles

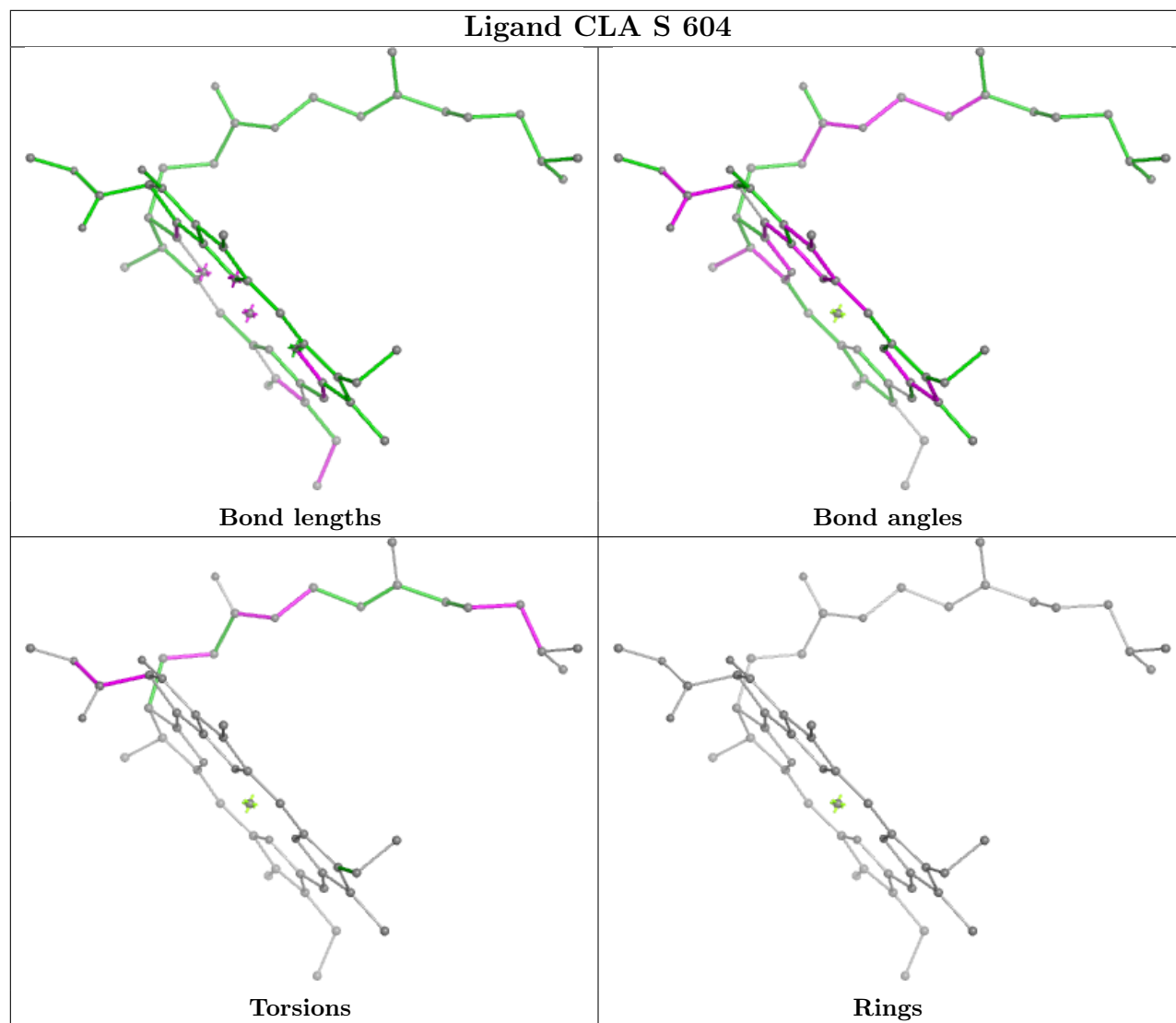


Torsions

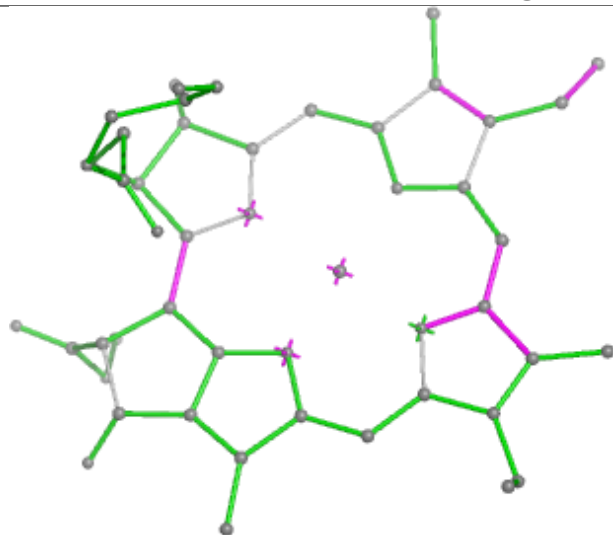


Rings

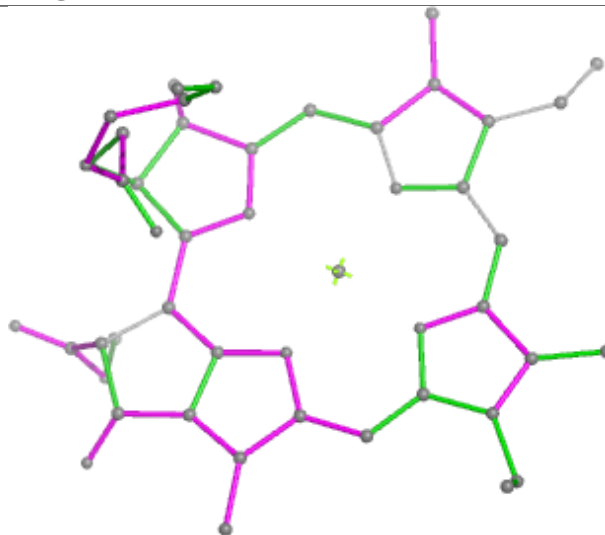
## Ligand CLA S 604



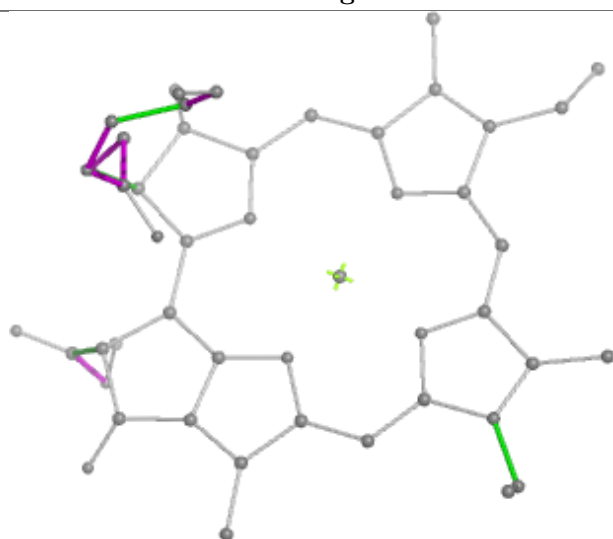
## Ligand CLA g 604



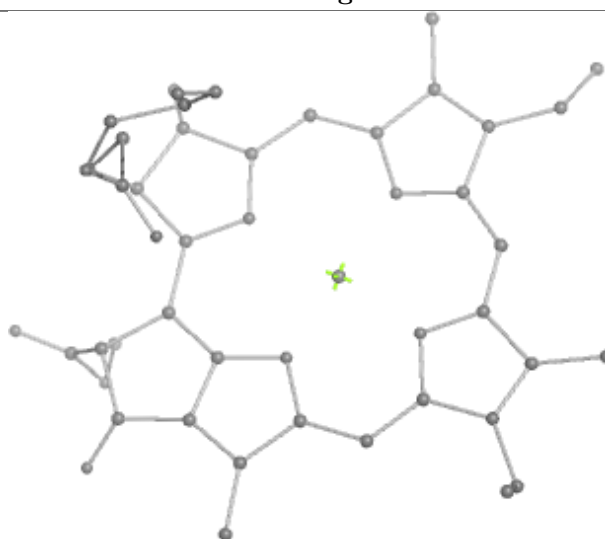
Bond lengths



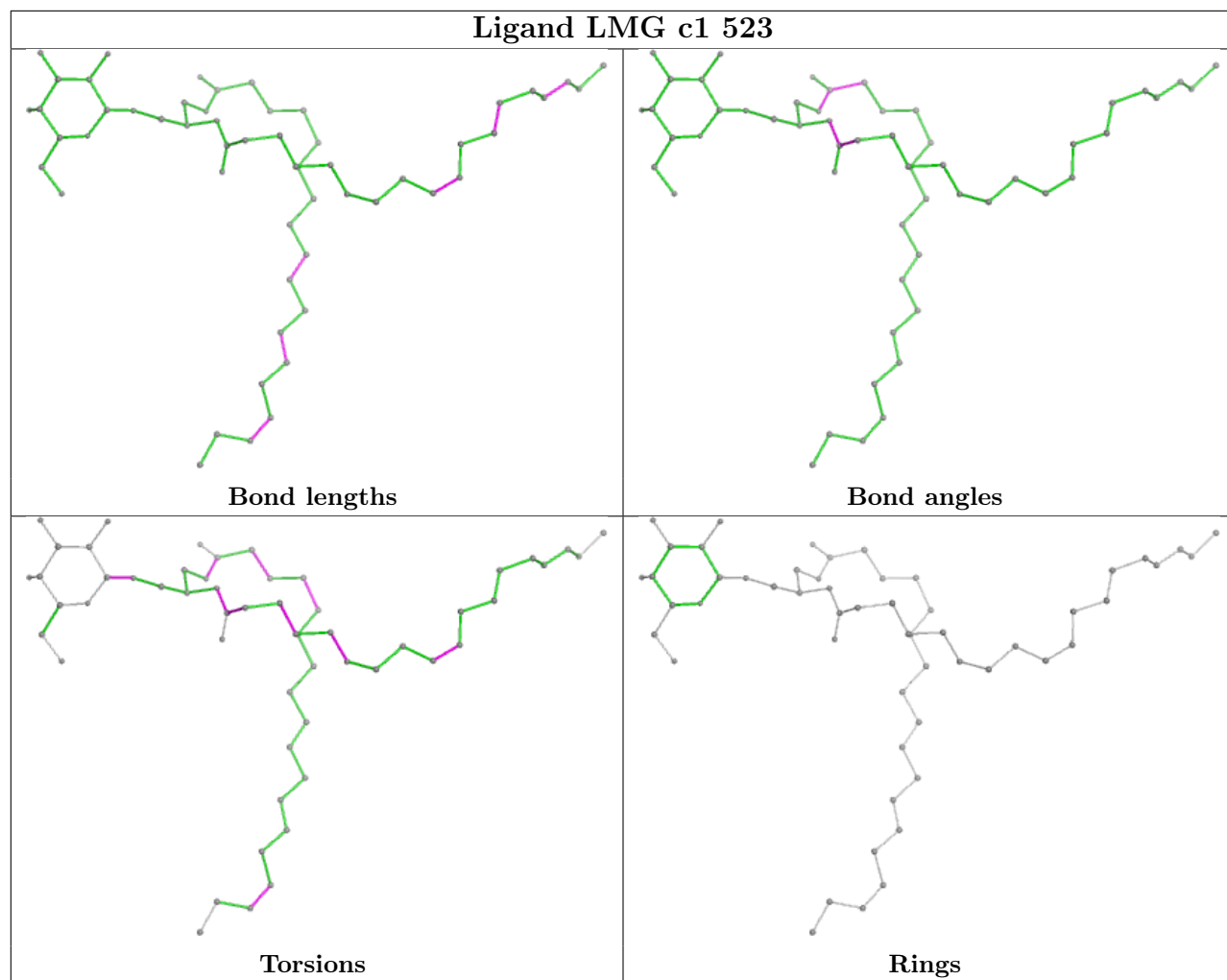
Bond angles



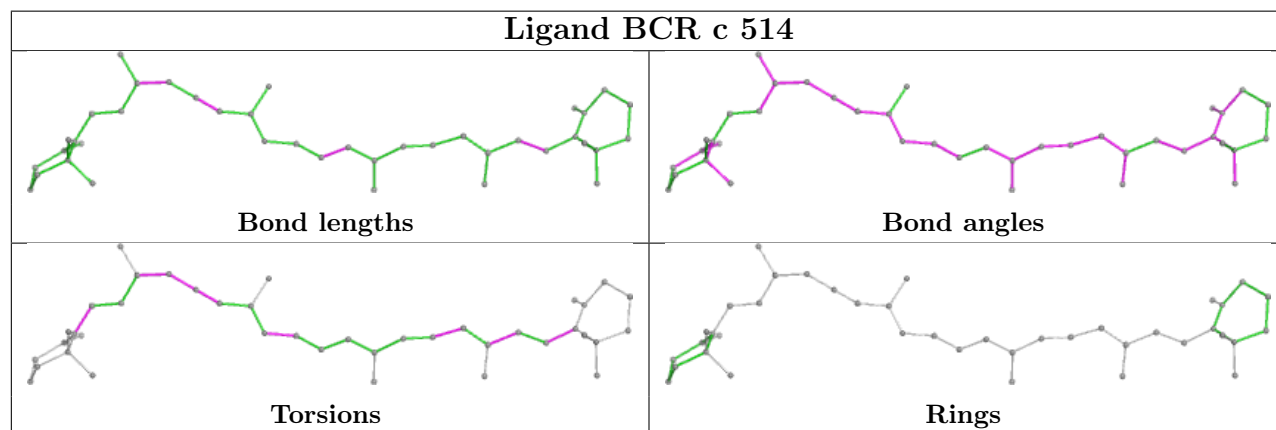
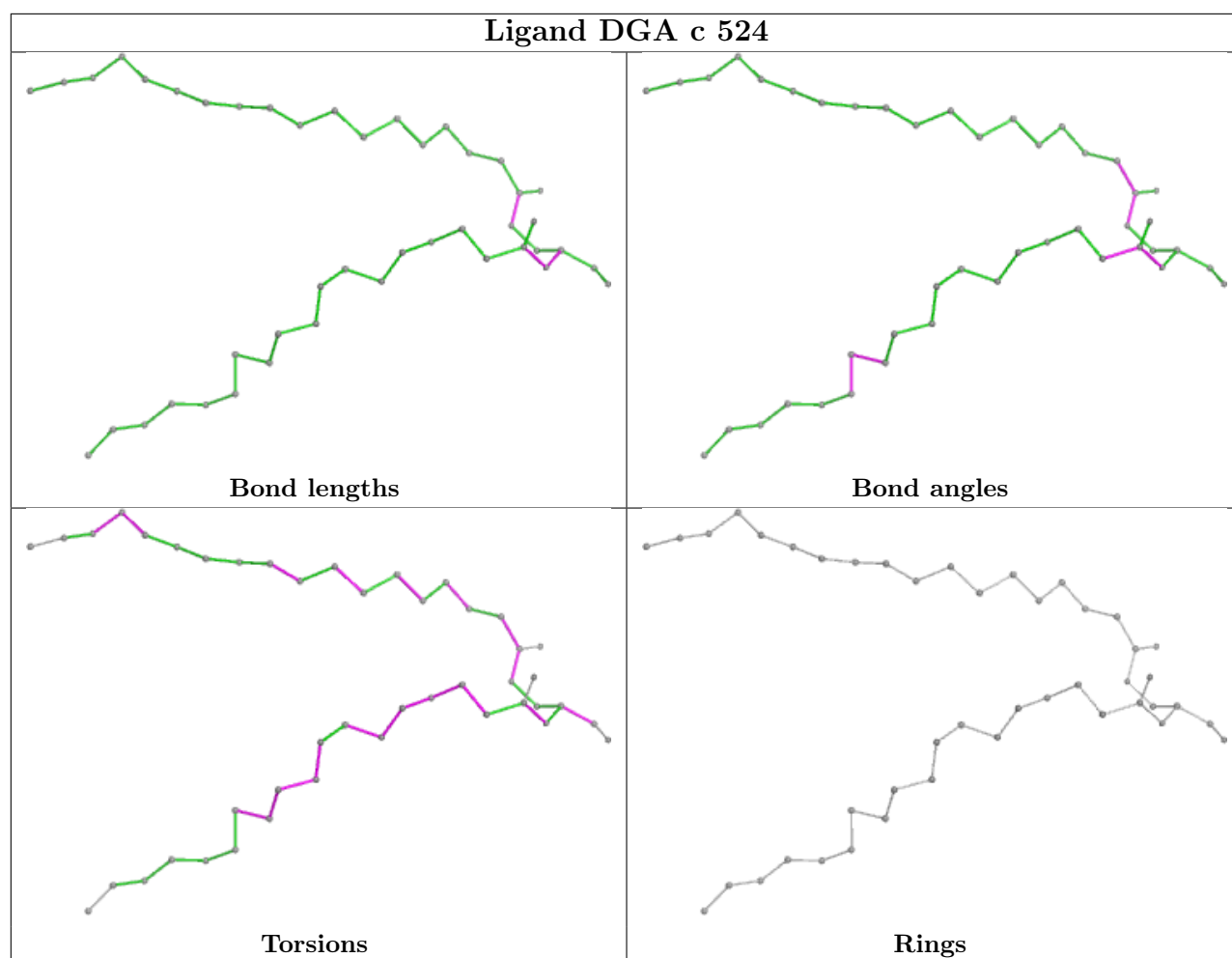
Torsions

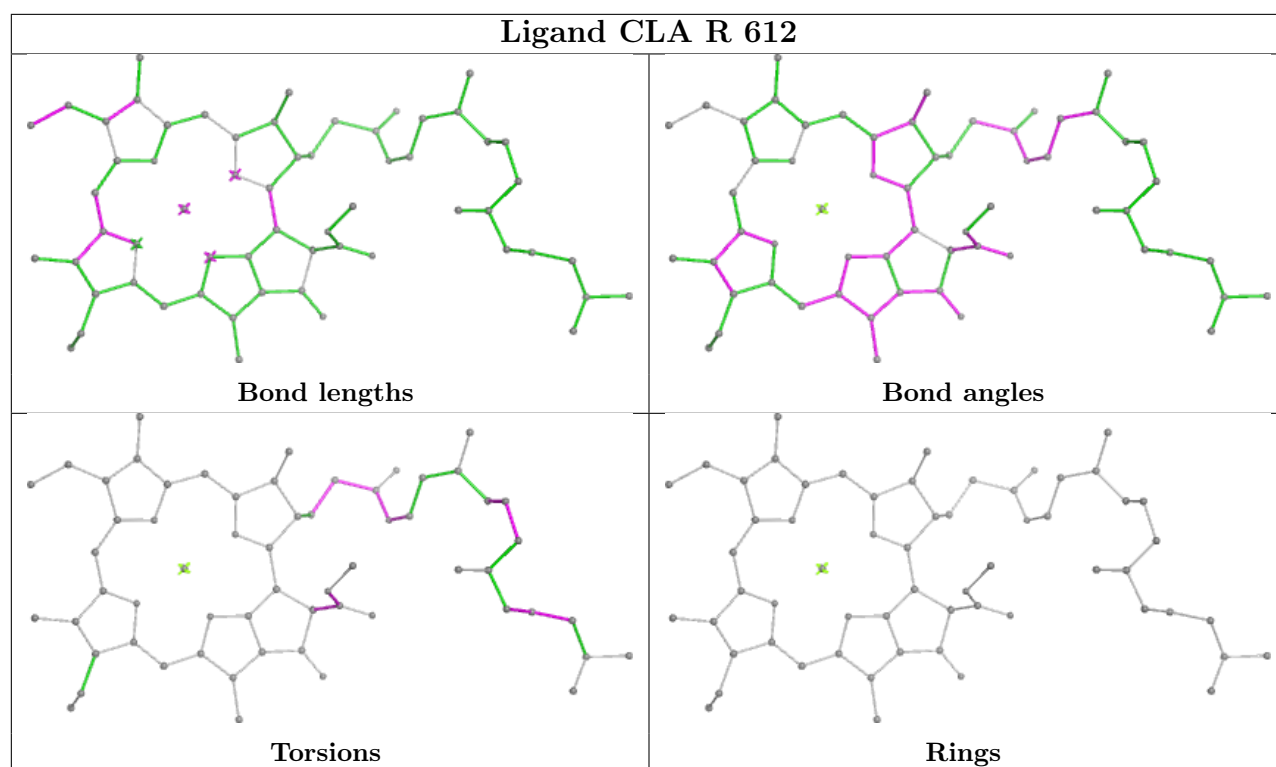


Rings

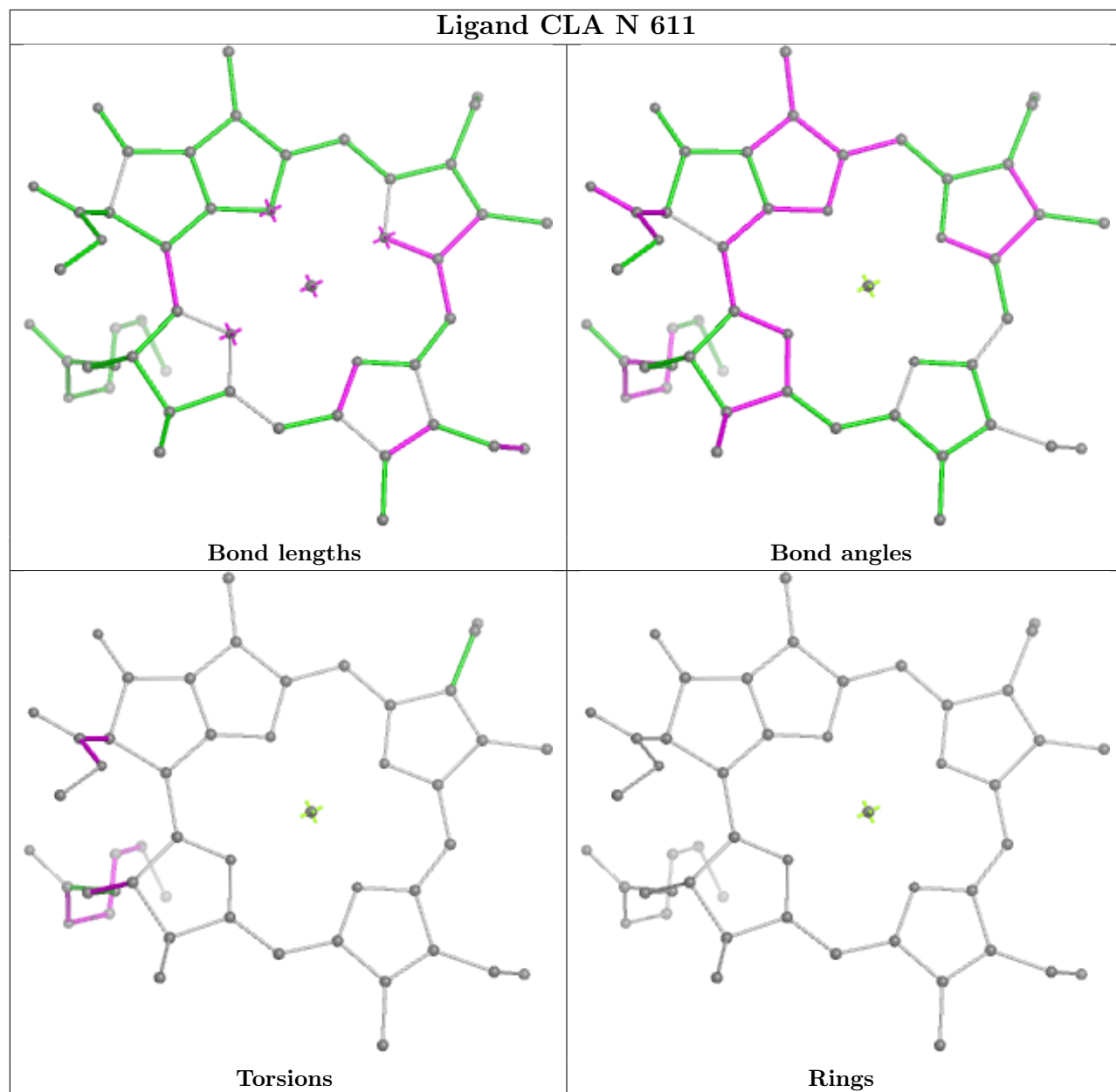


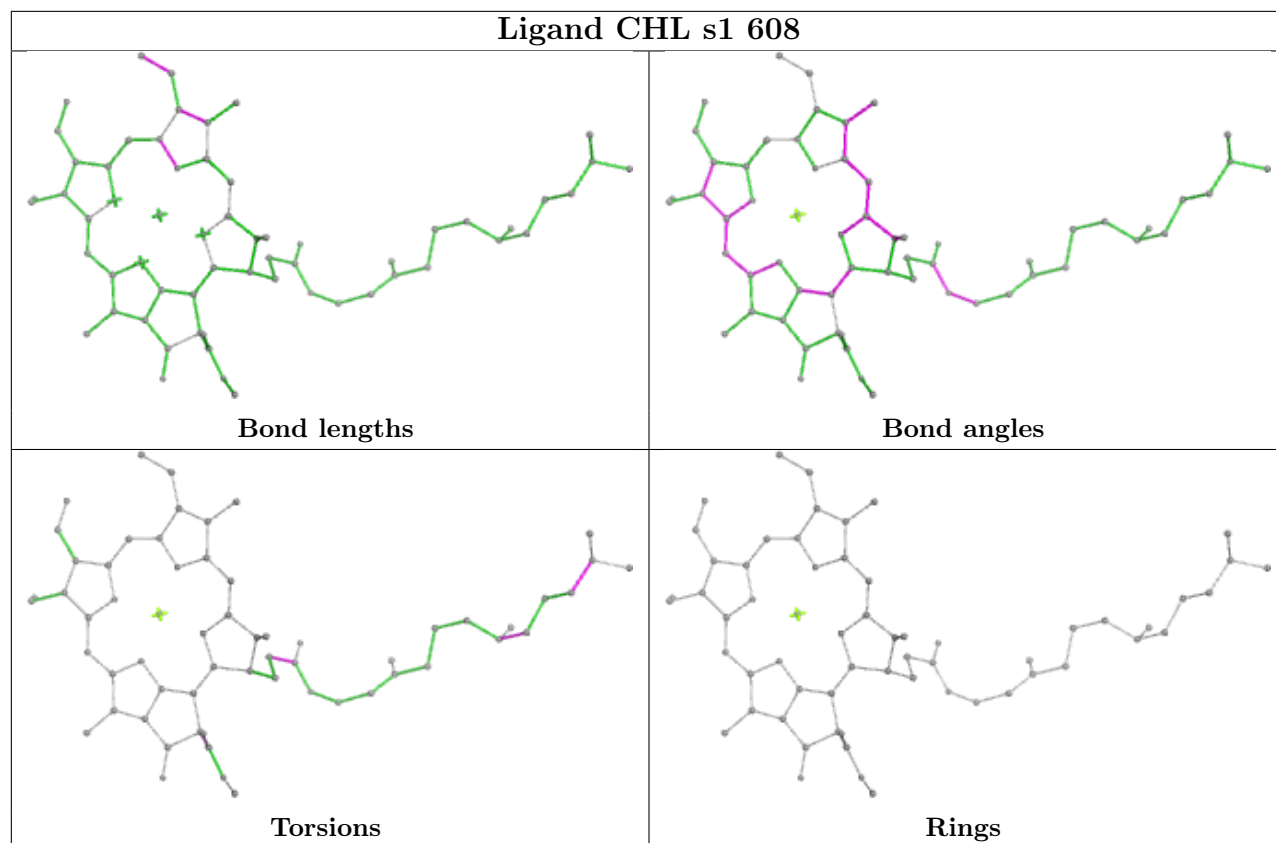


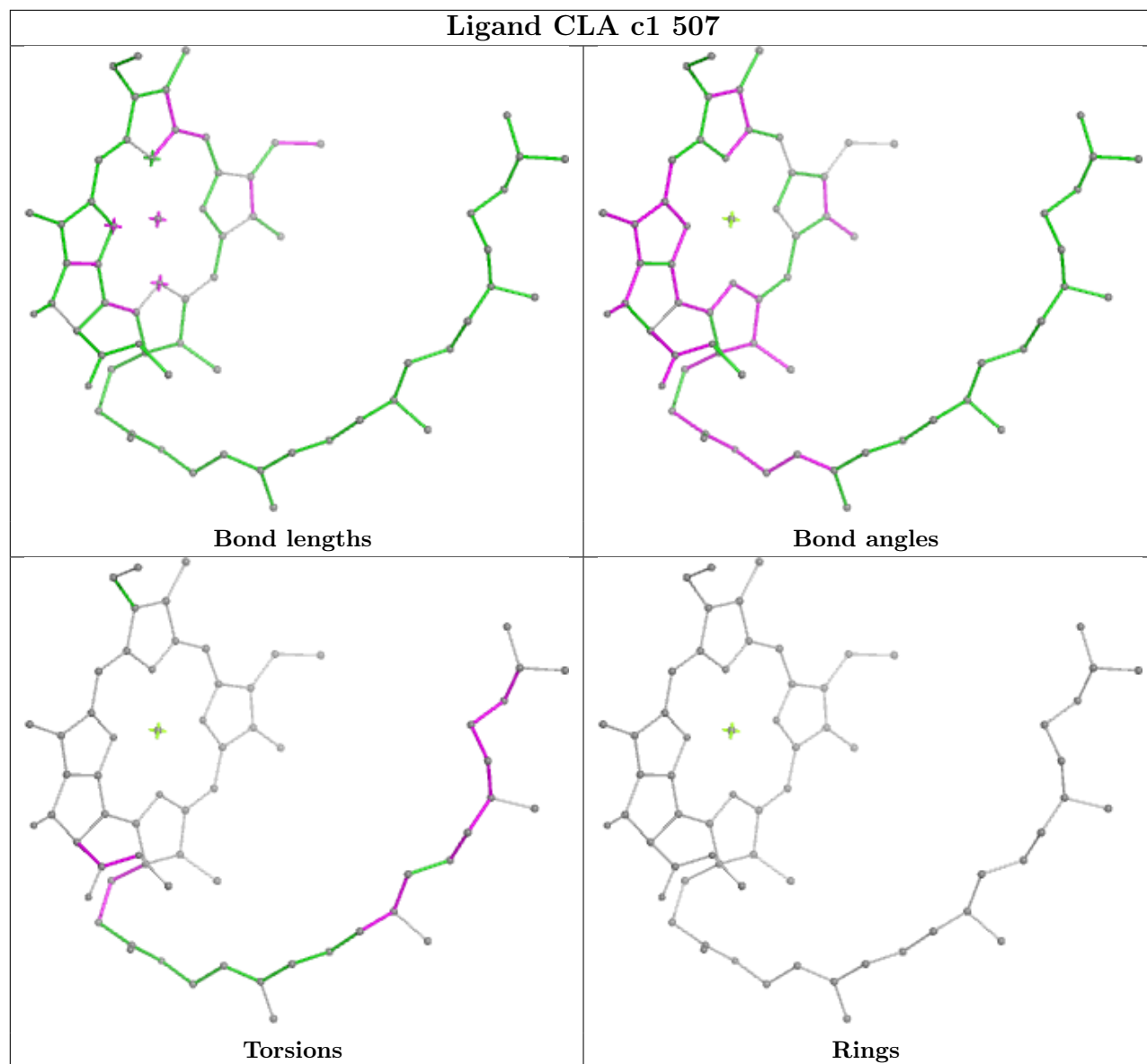


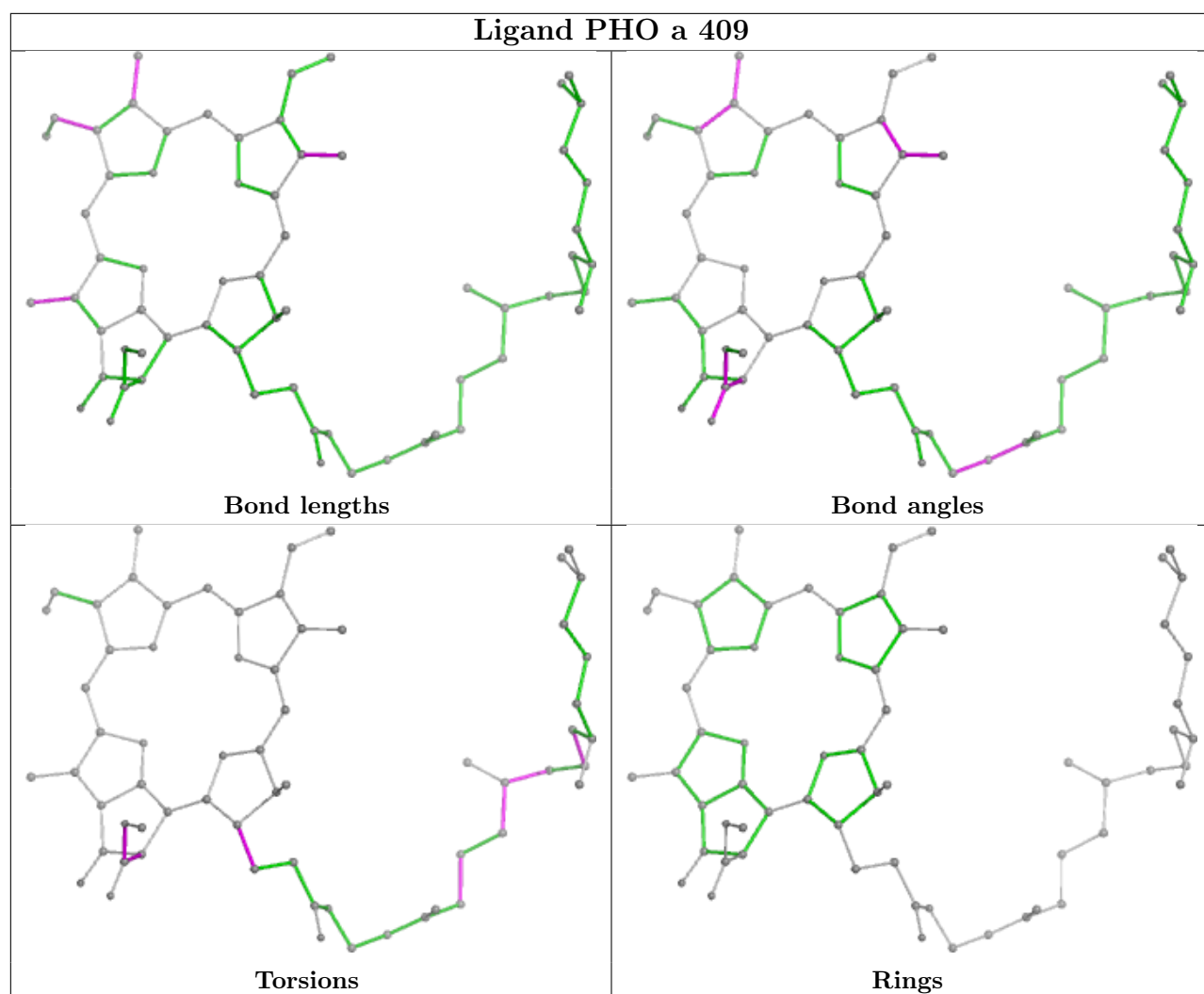


## Ligand CLA N 611

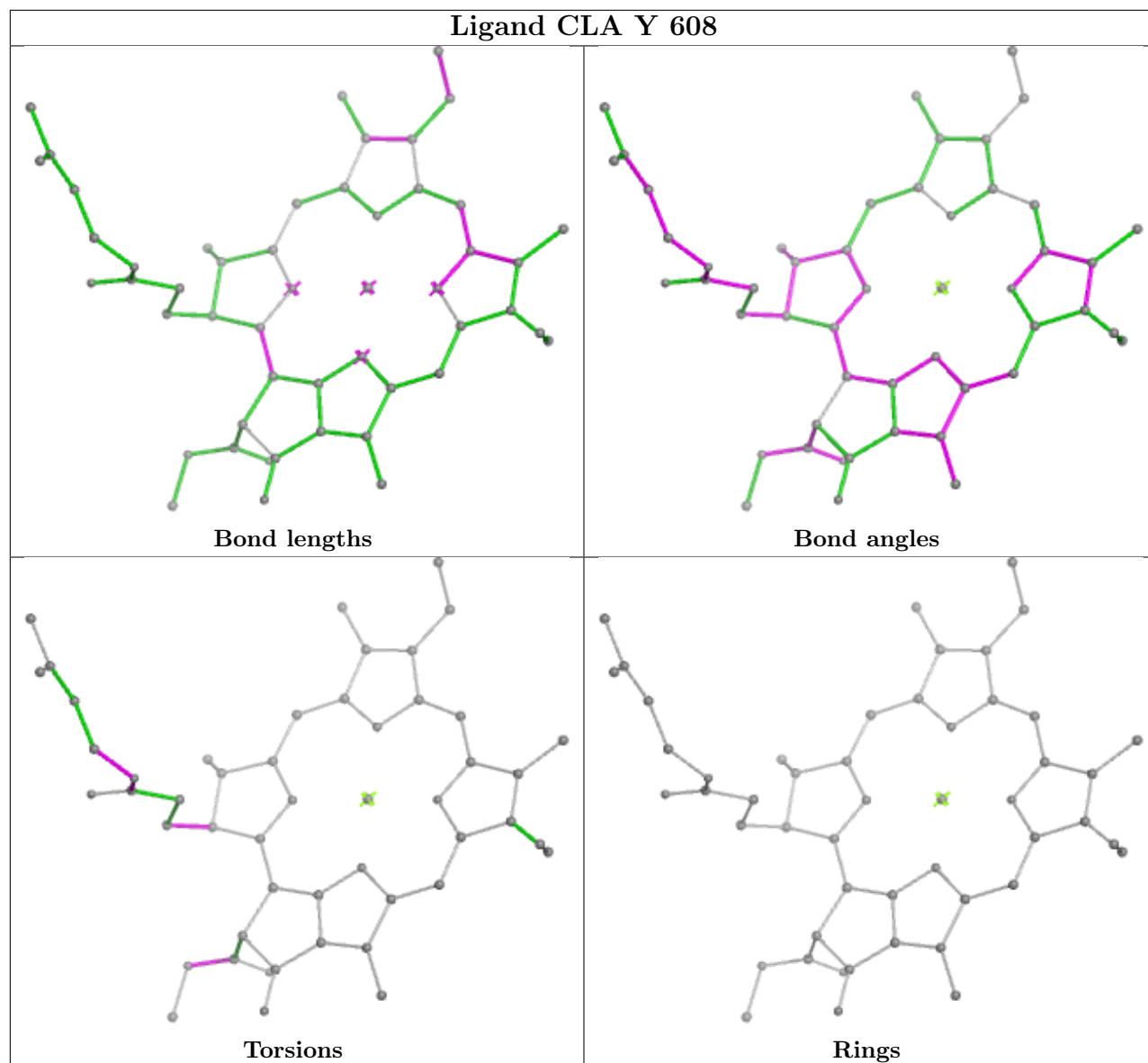




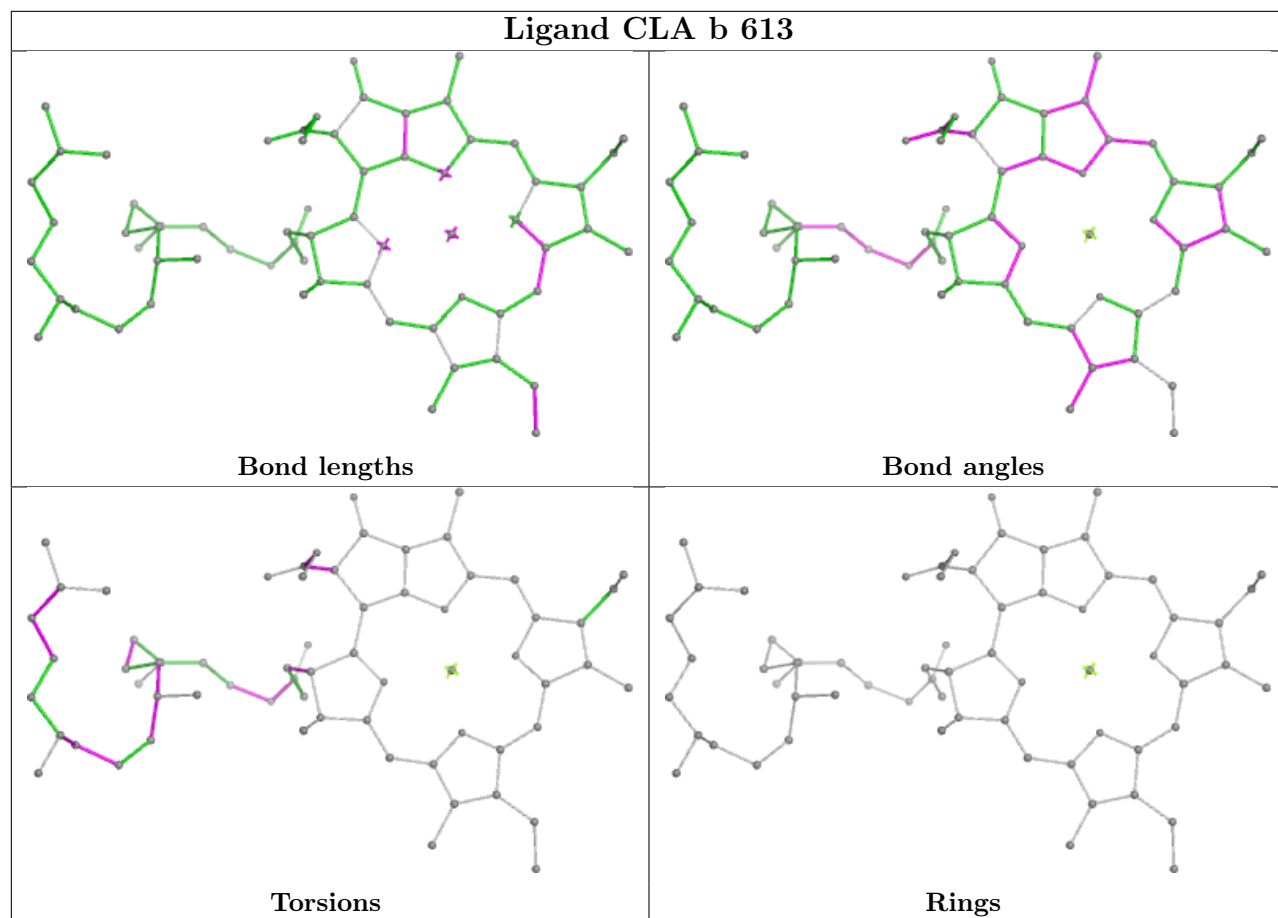




## Ligand CLA Y 608

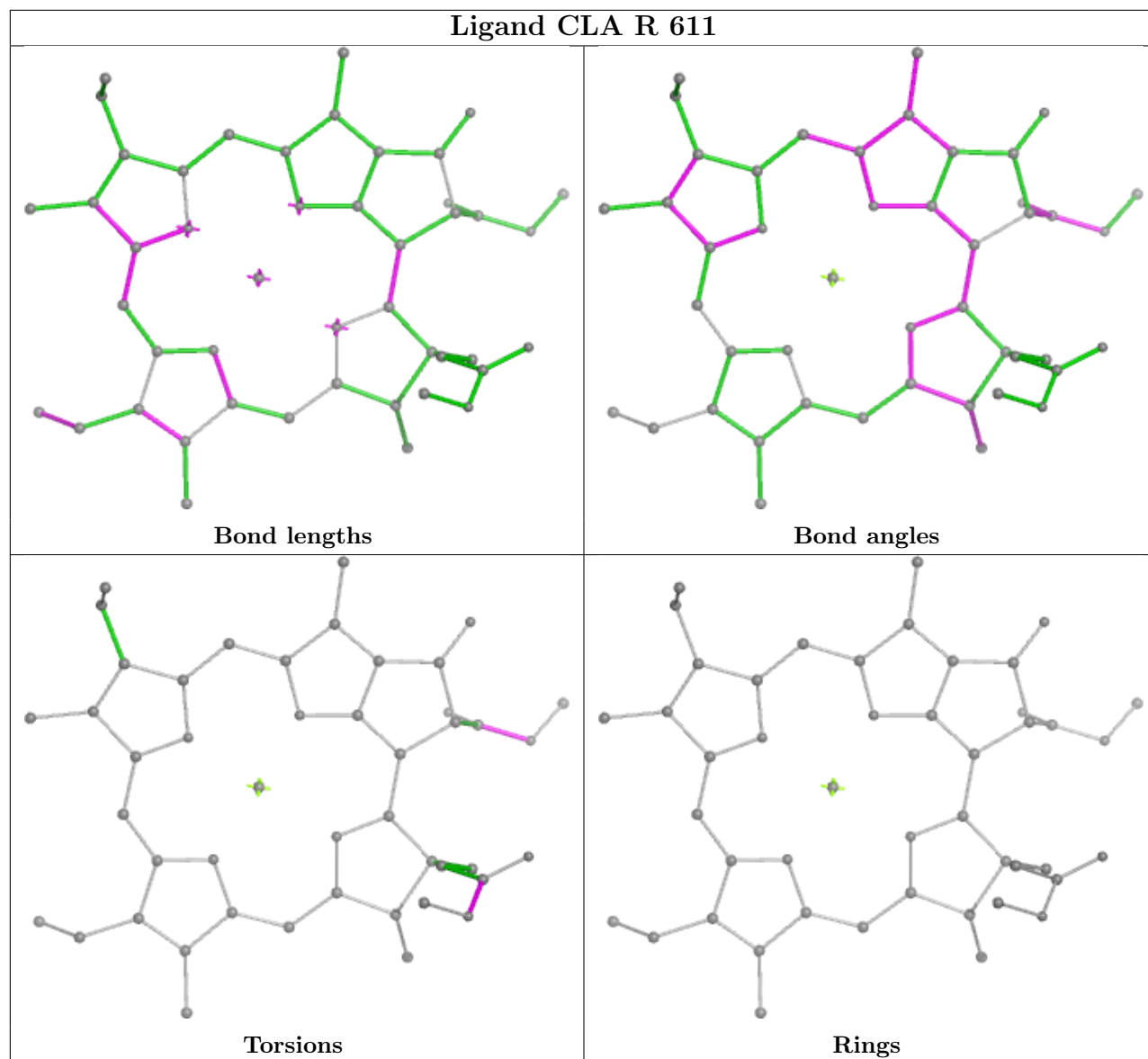


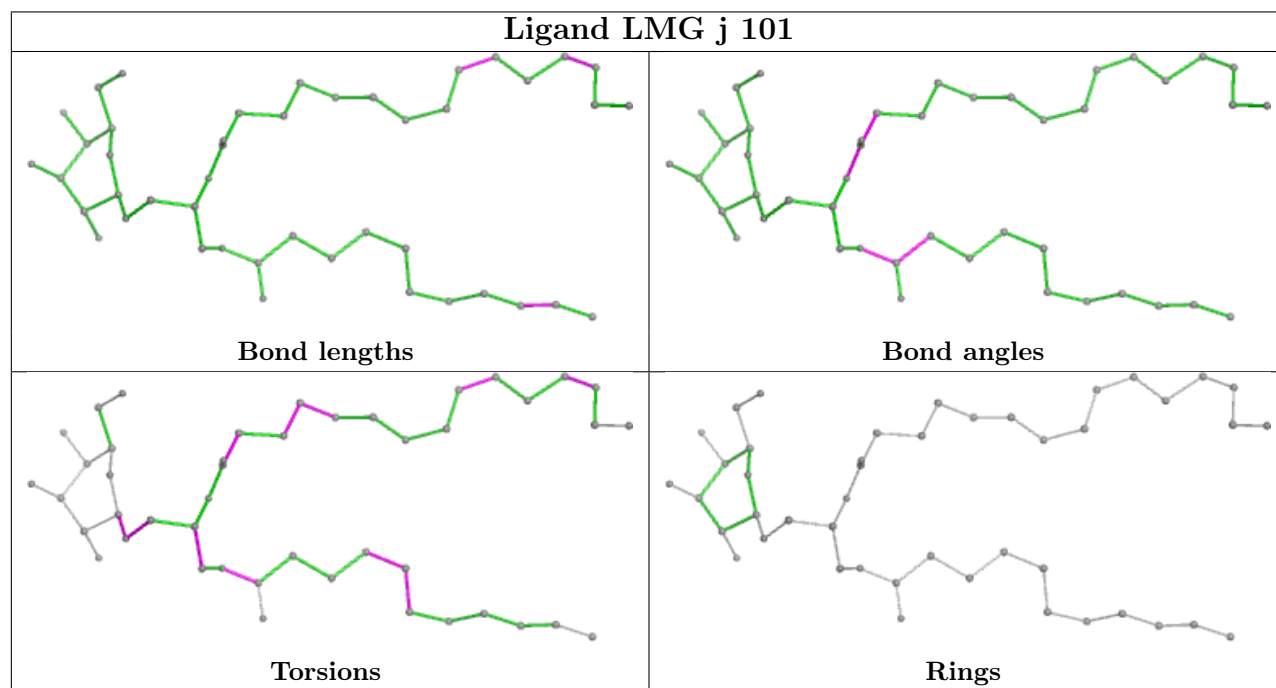
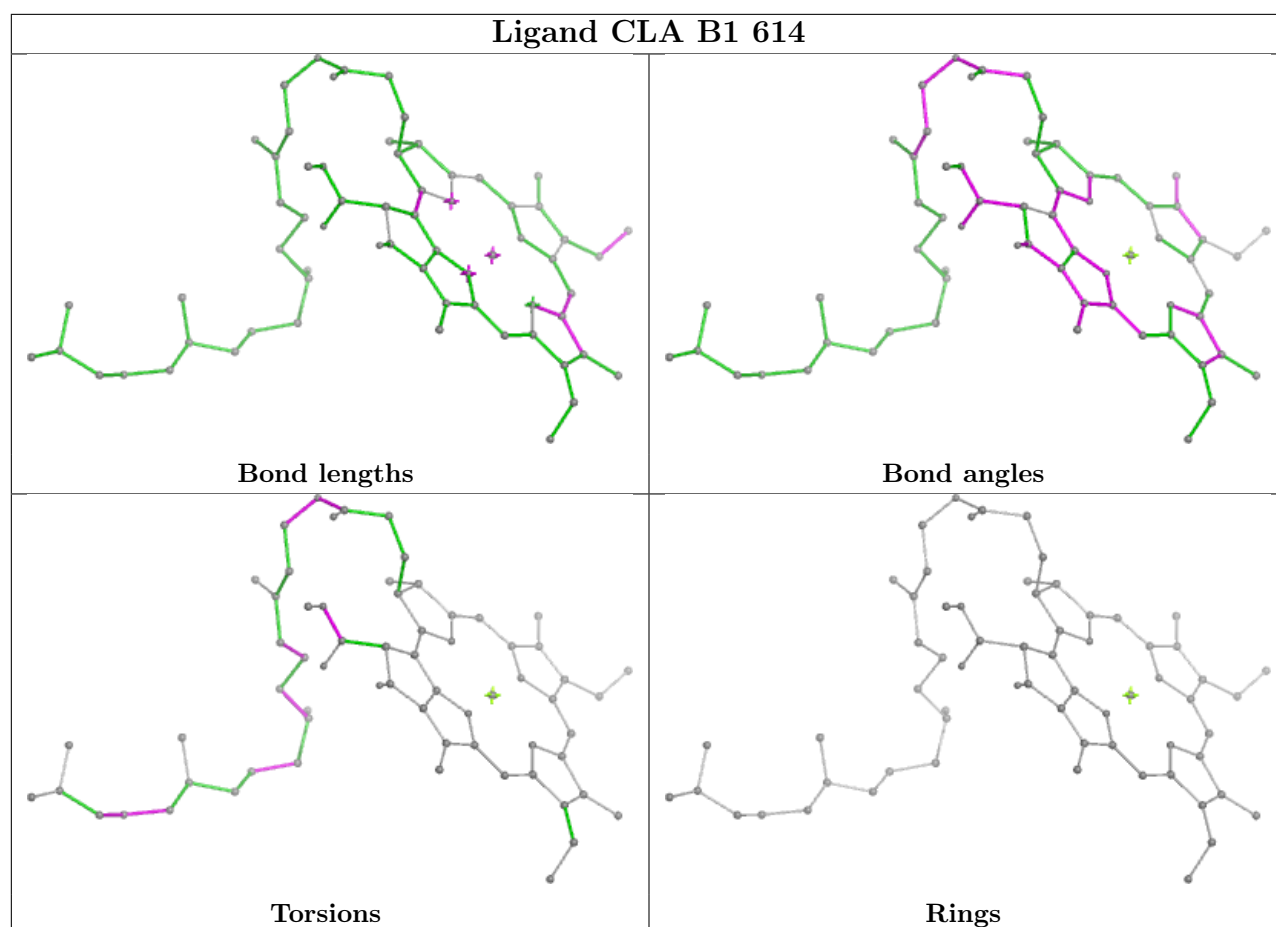
## Ligand CLA b 613

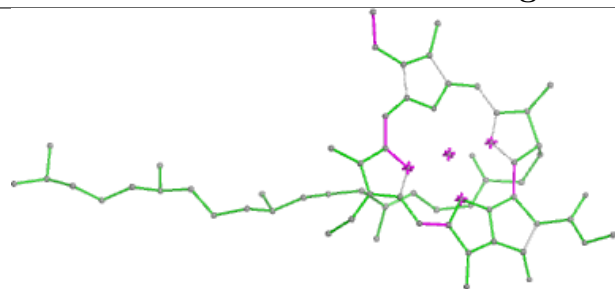
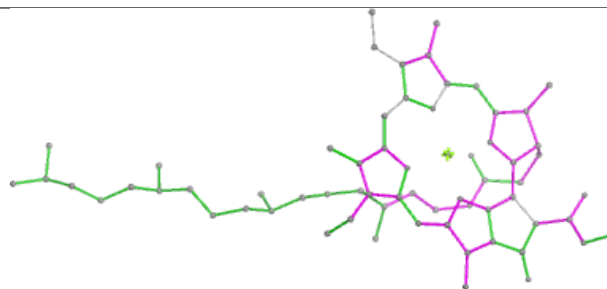
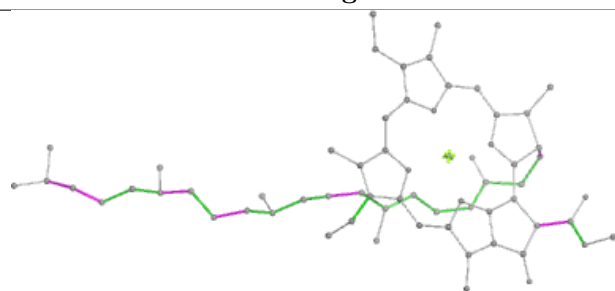
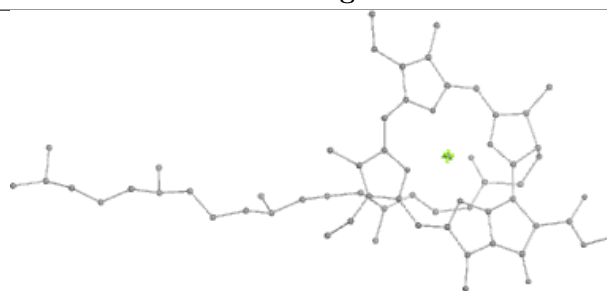
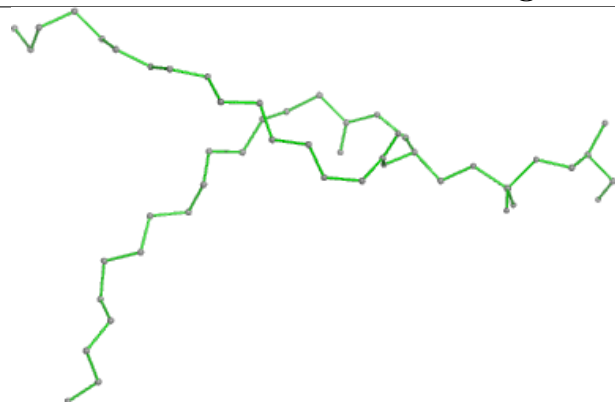
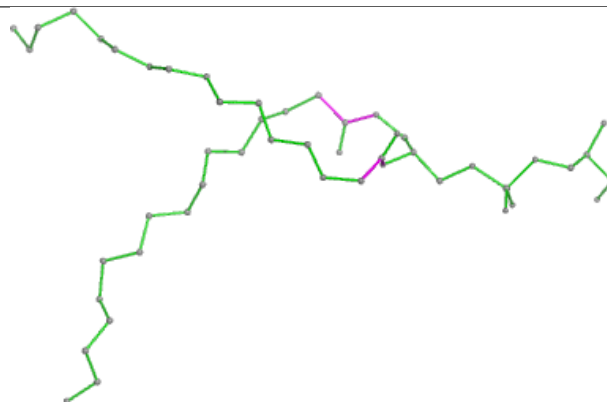
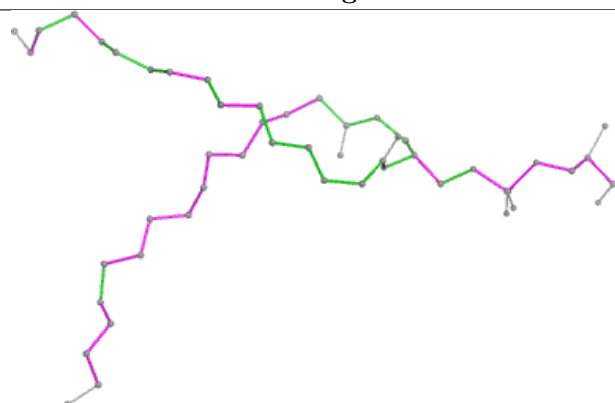
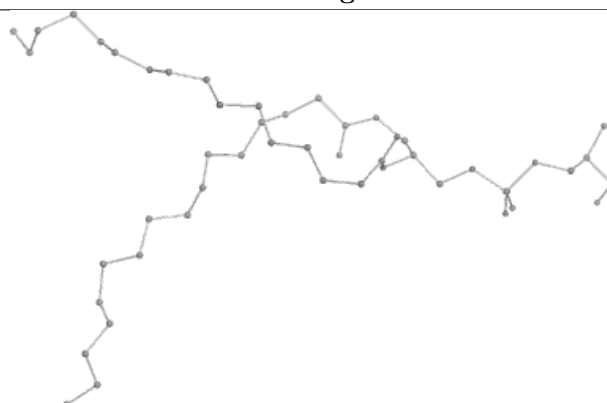




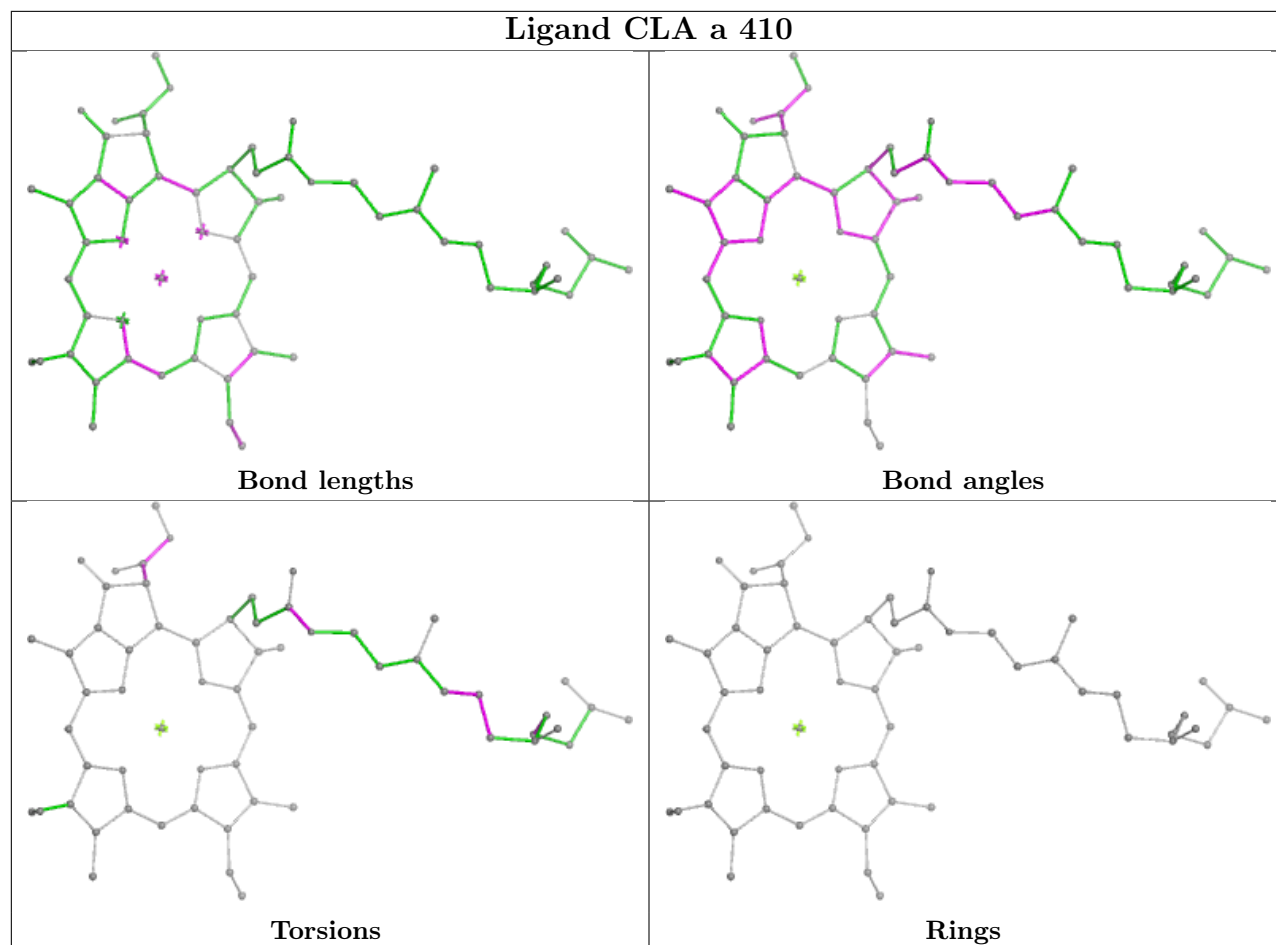
## Ligand CLA R 611

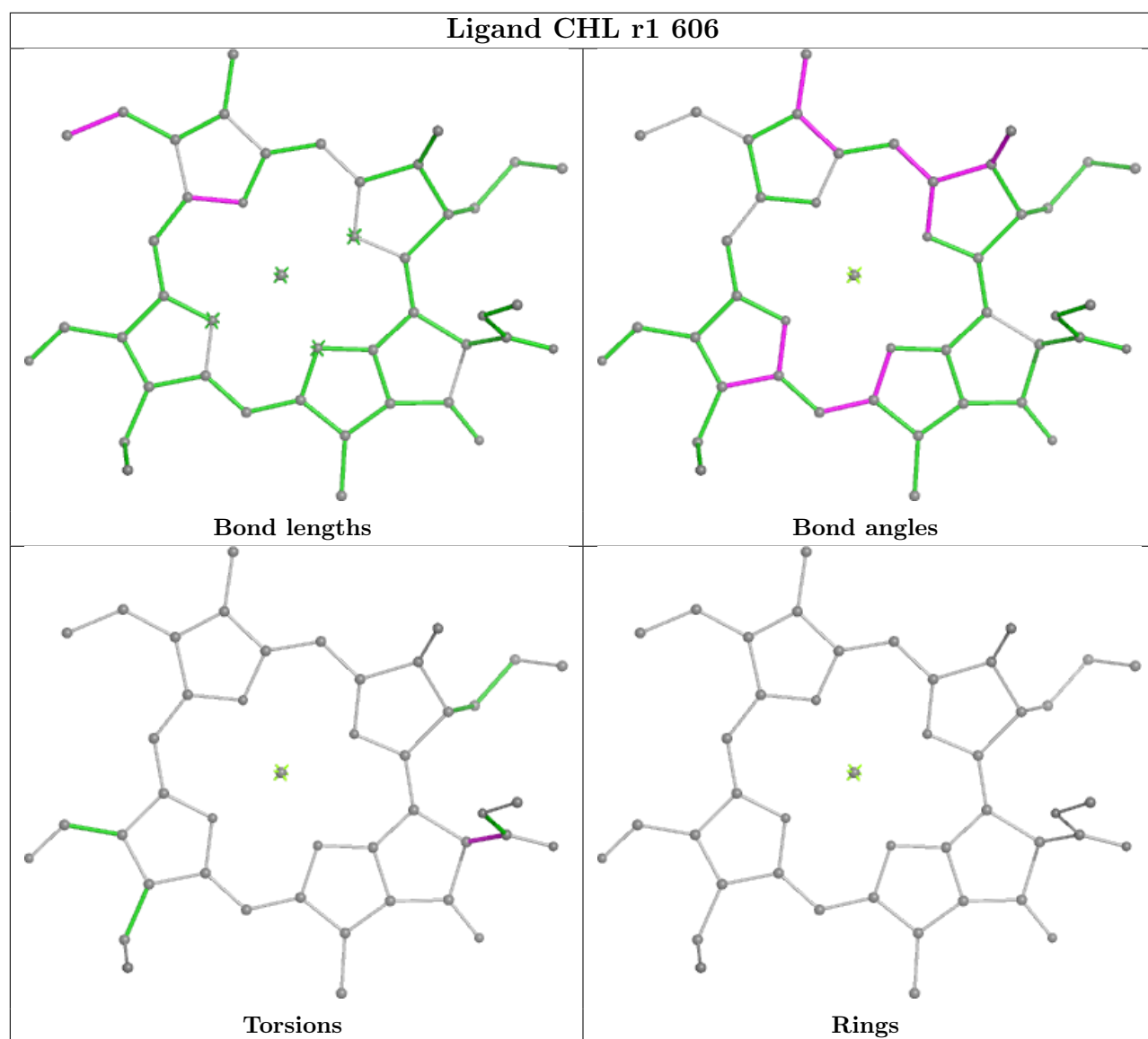




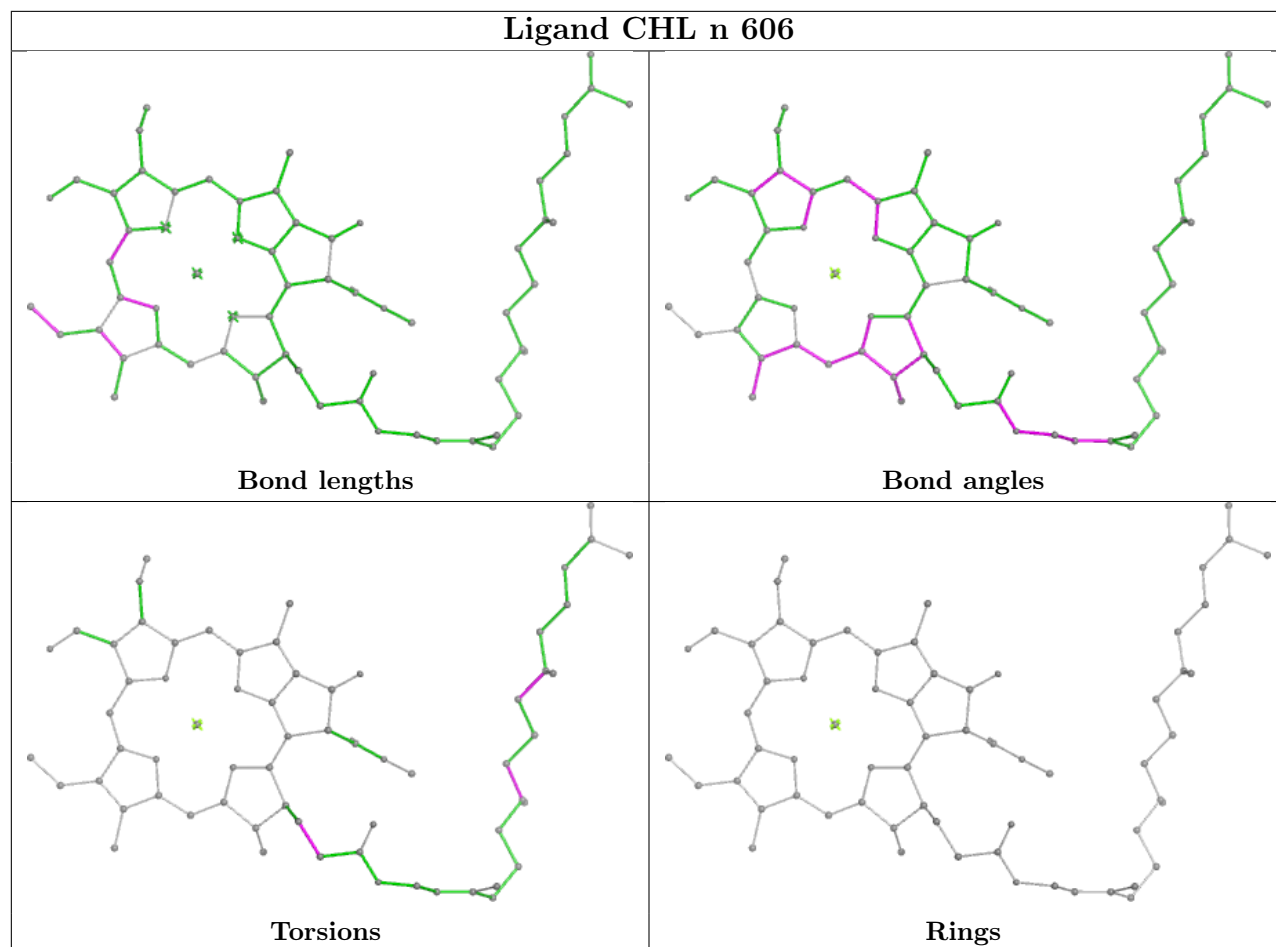
**Ligand CLA b 615****Bond lengths****Bond angles****Torsions****Rings****Ligand LHG d 409****Bond lengths****Bond angles****Torsions****Rings**

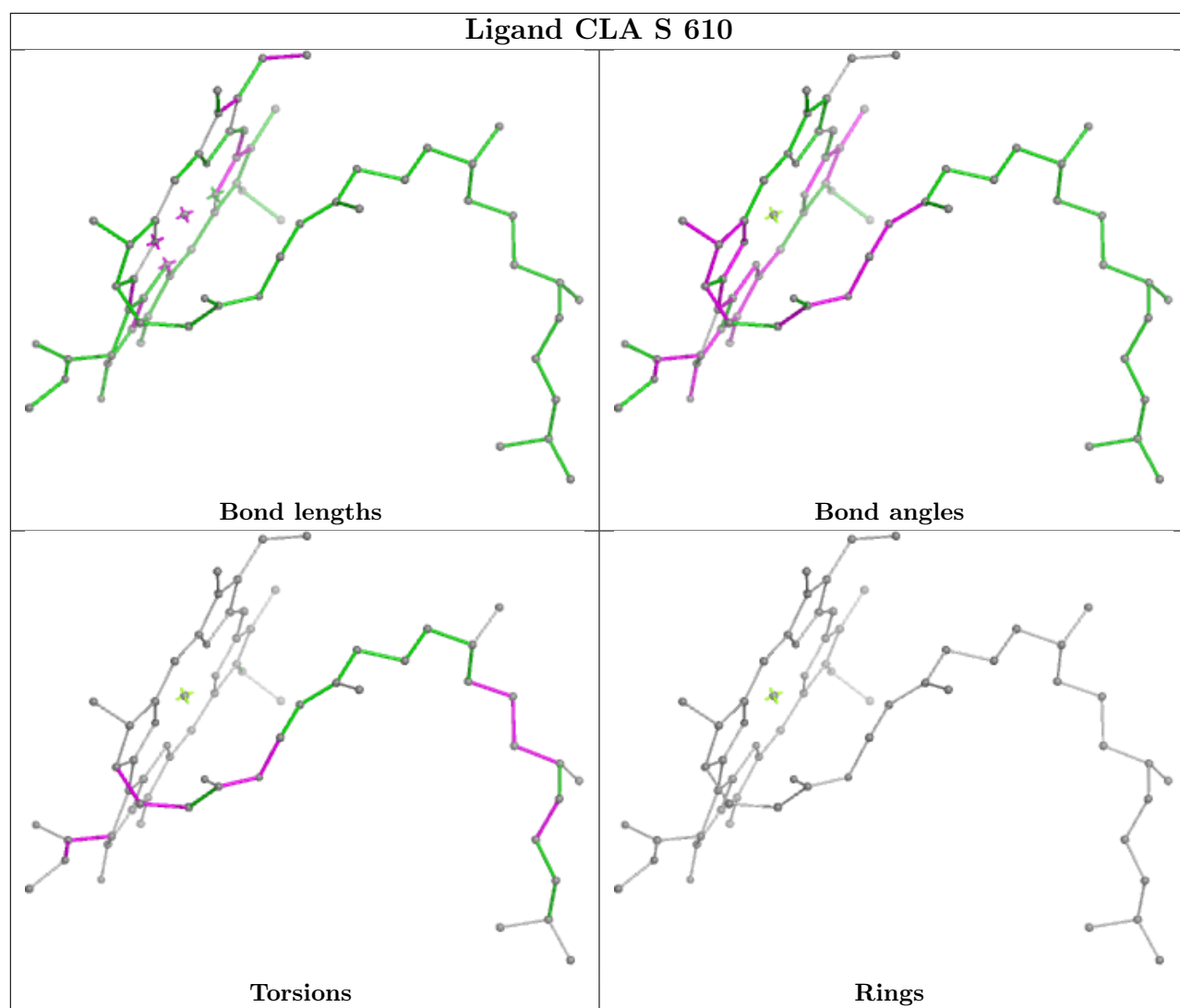
## Ligand CLA a 410

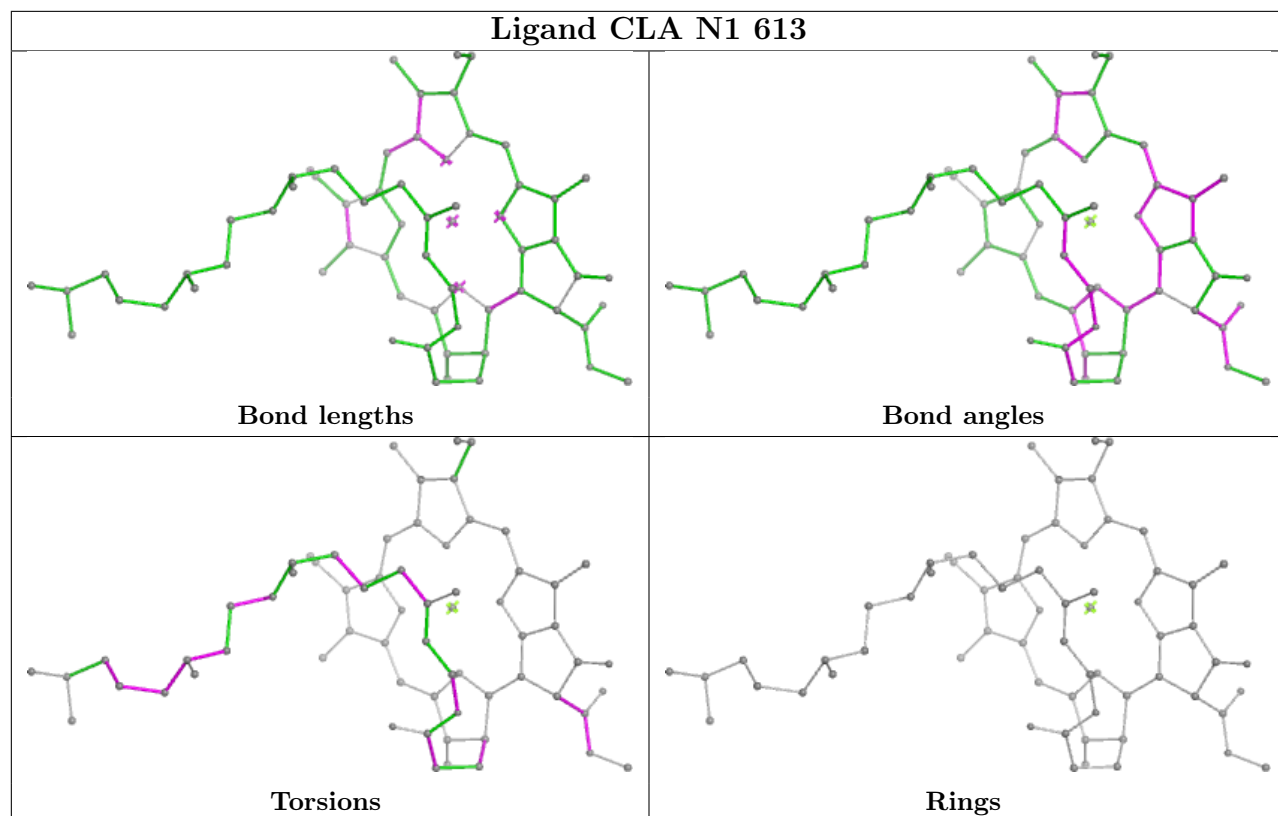




## Ligand CHL n 606

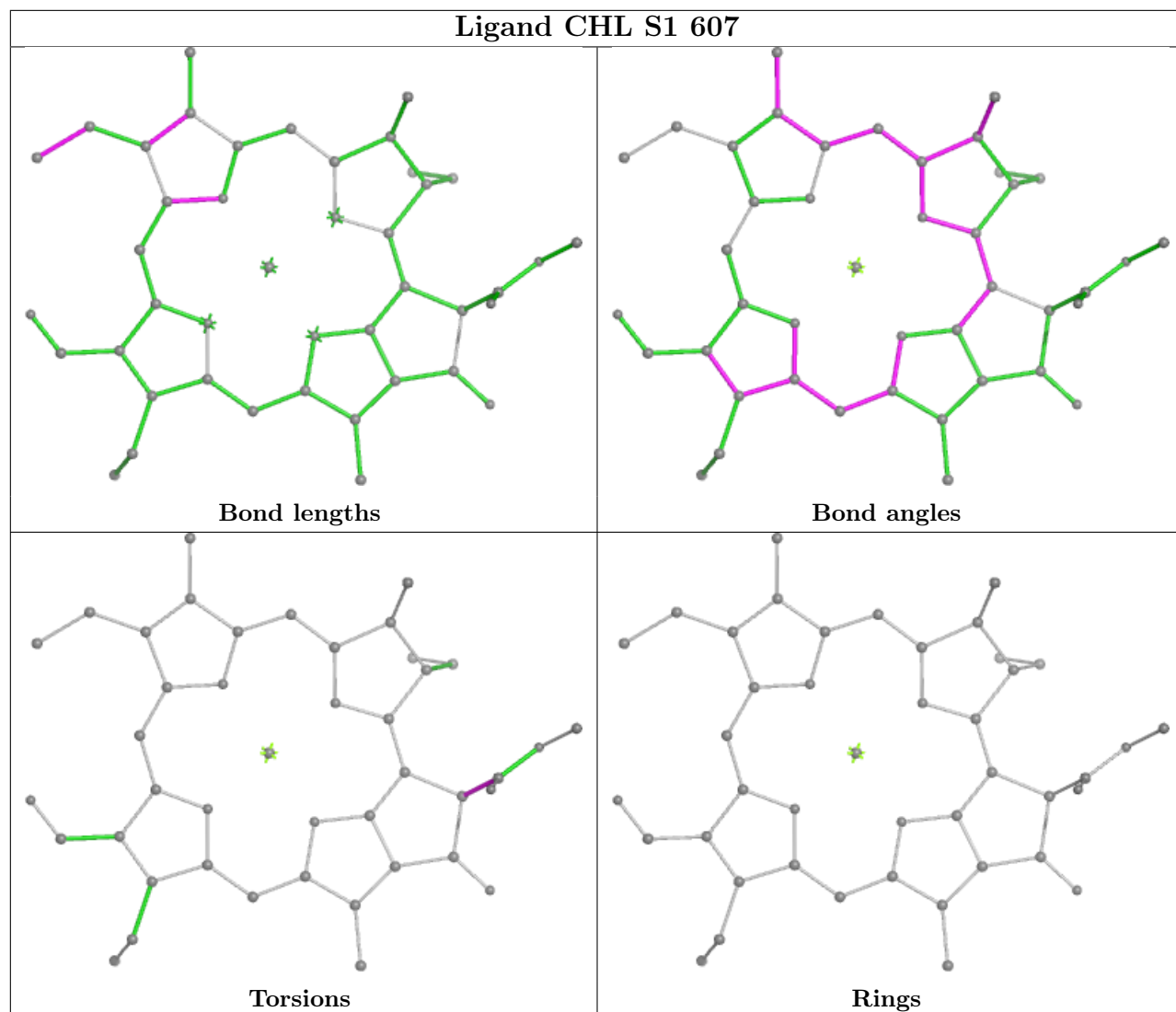


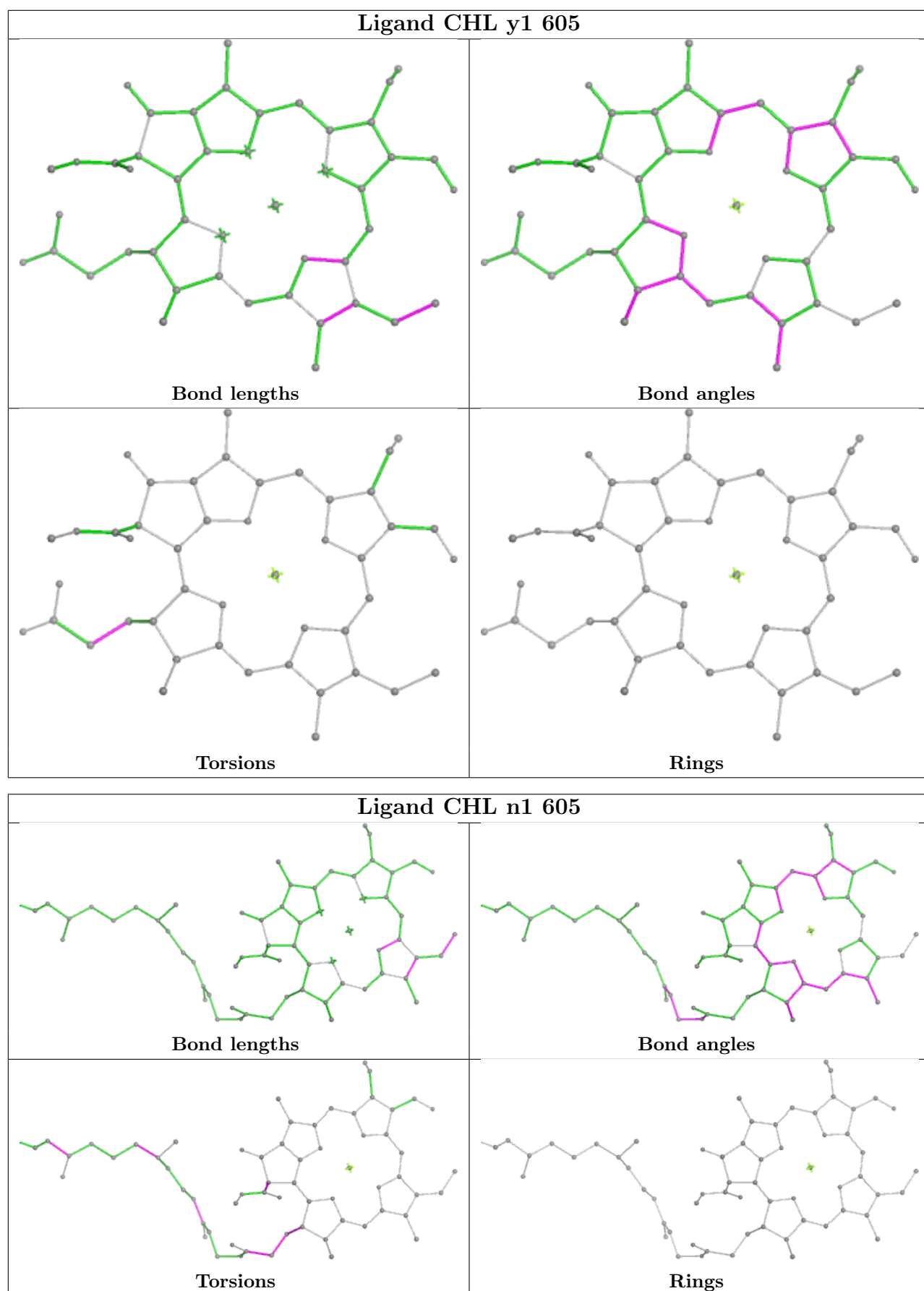


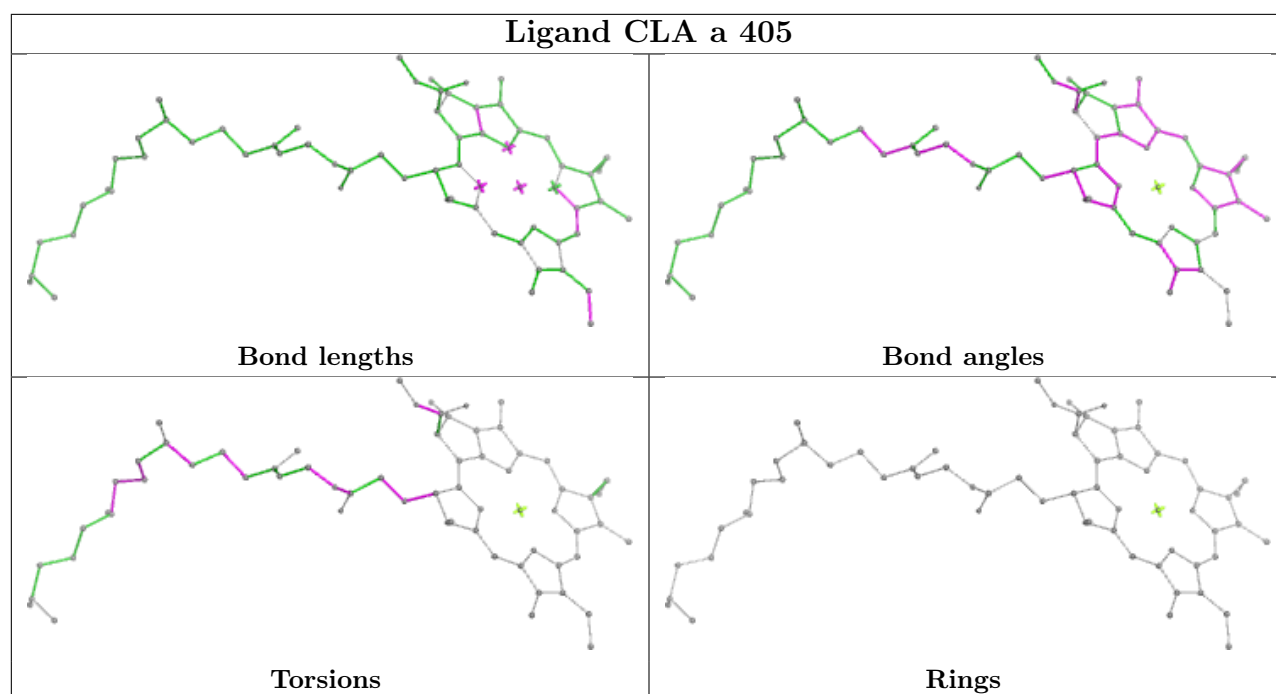




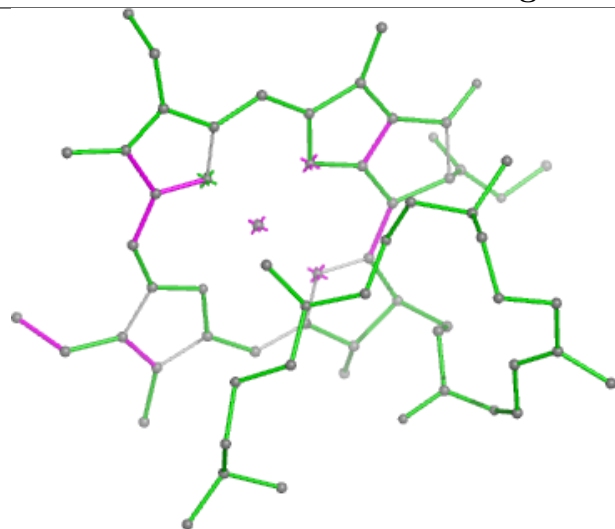
## Ligand CHL S1 607



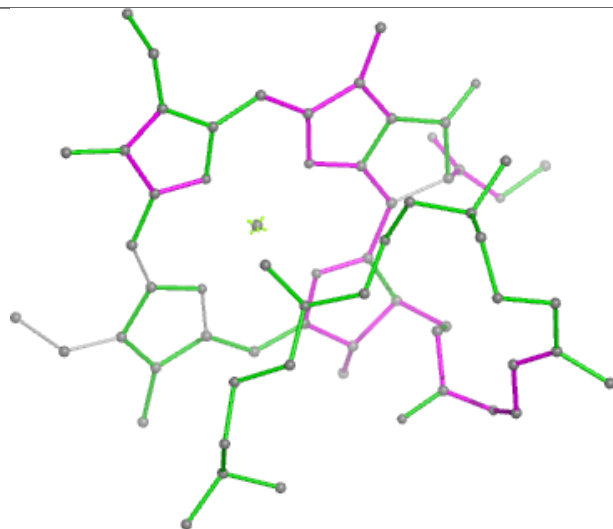




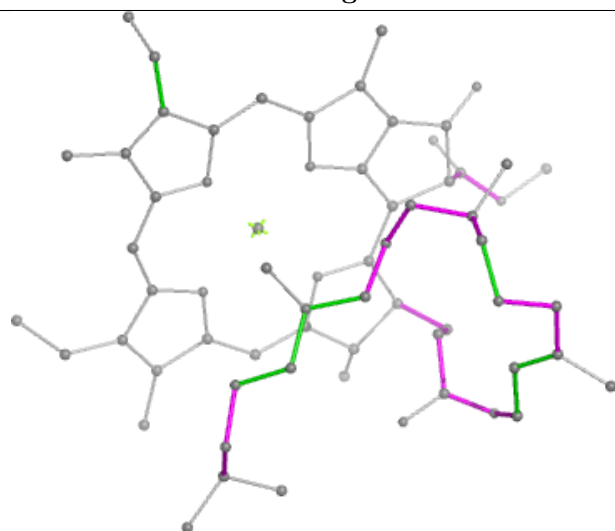
## Ligand CLA b 602



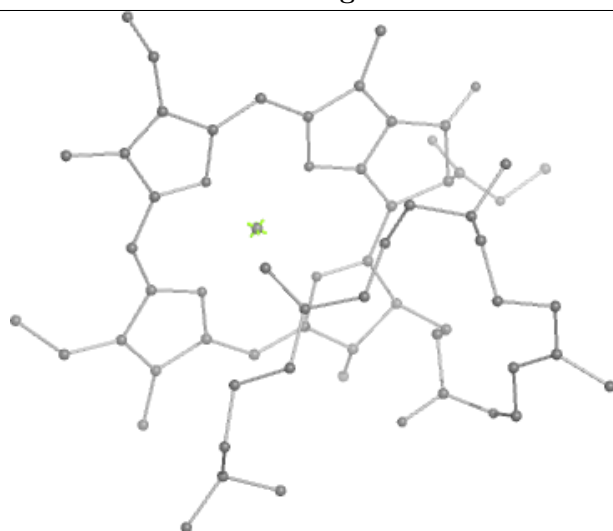
Bond lengths



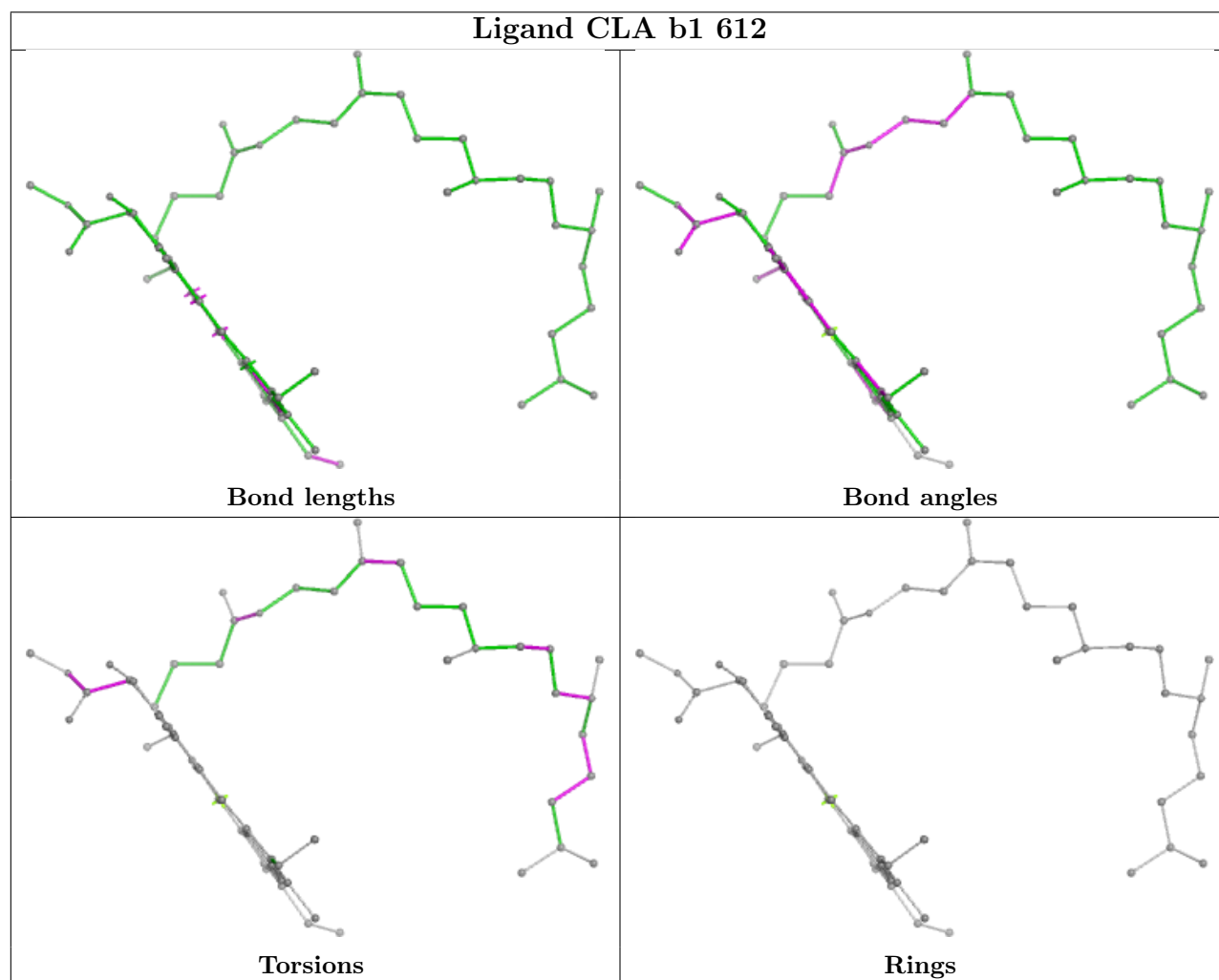
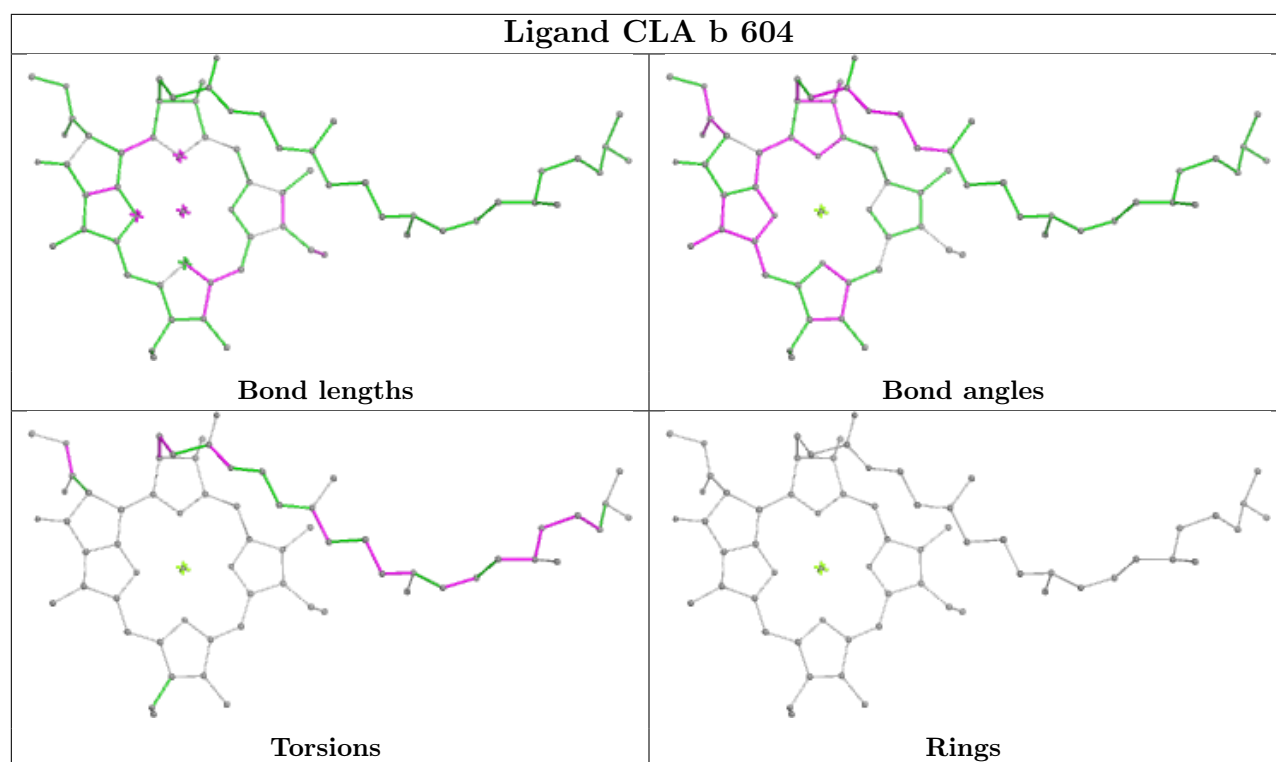
Bond angles

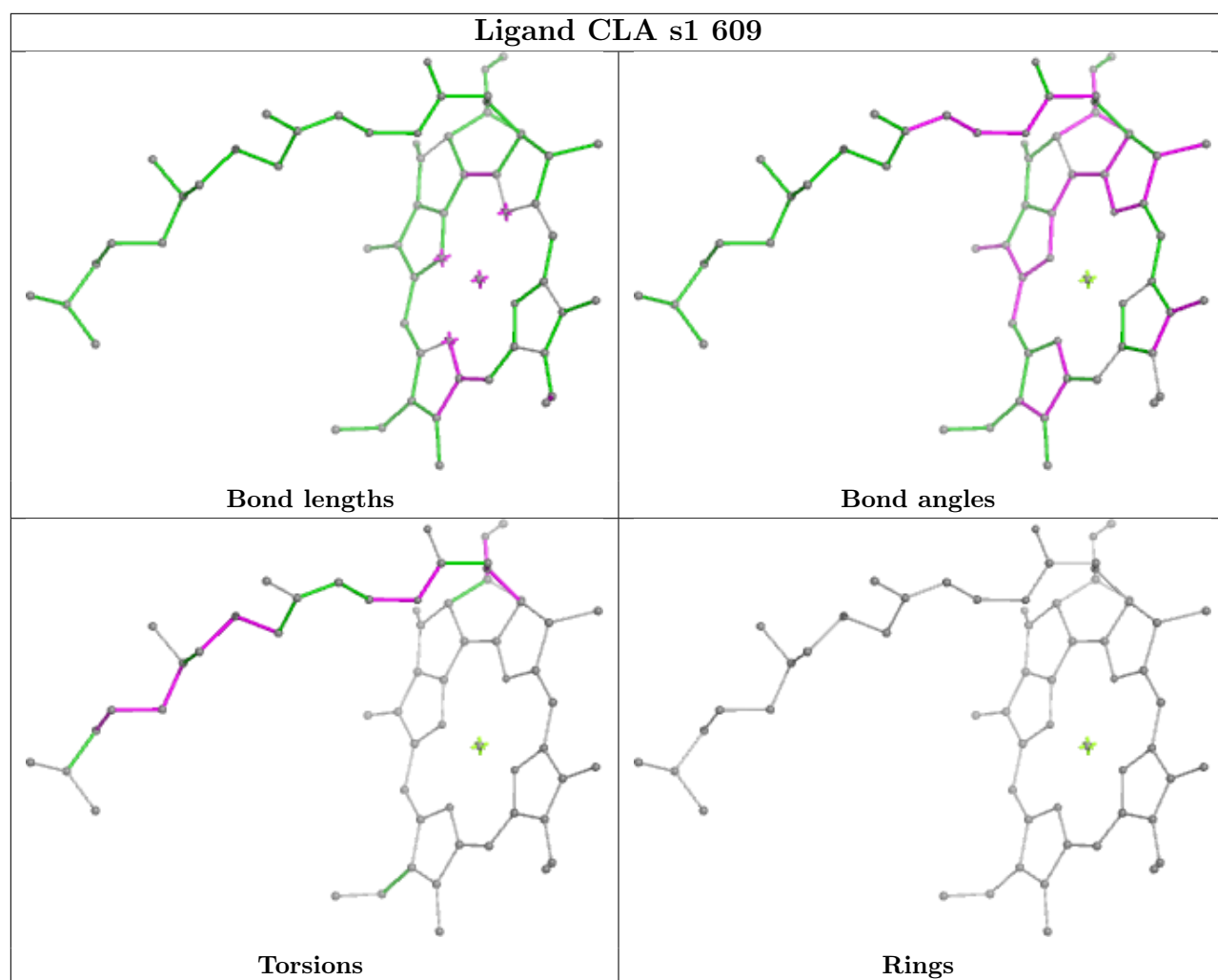


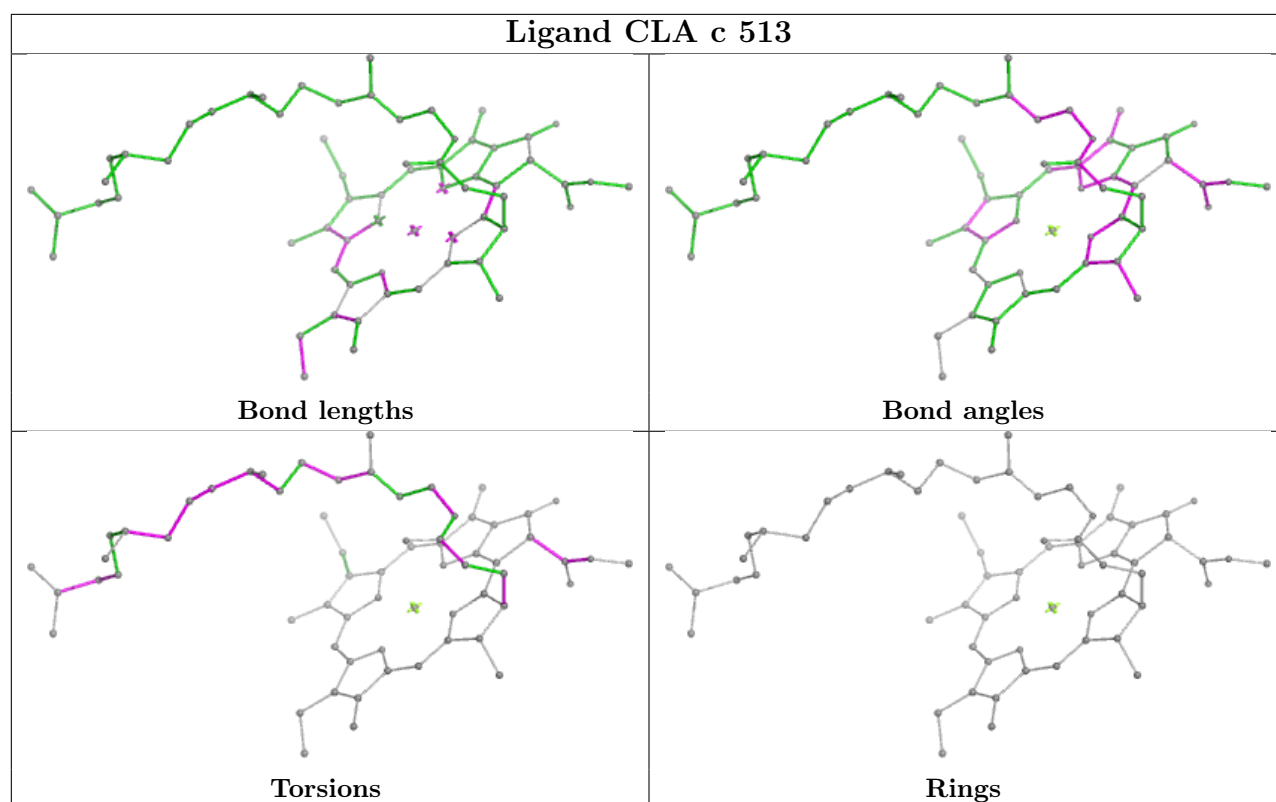
Torsions

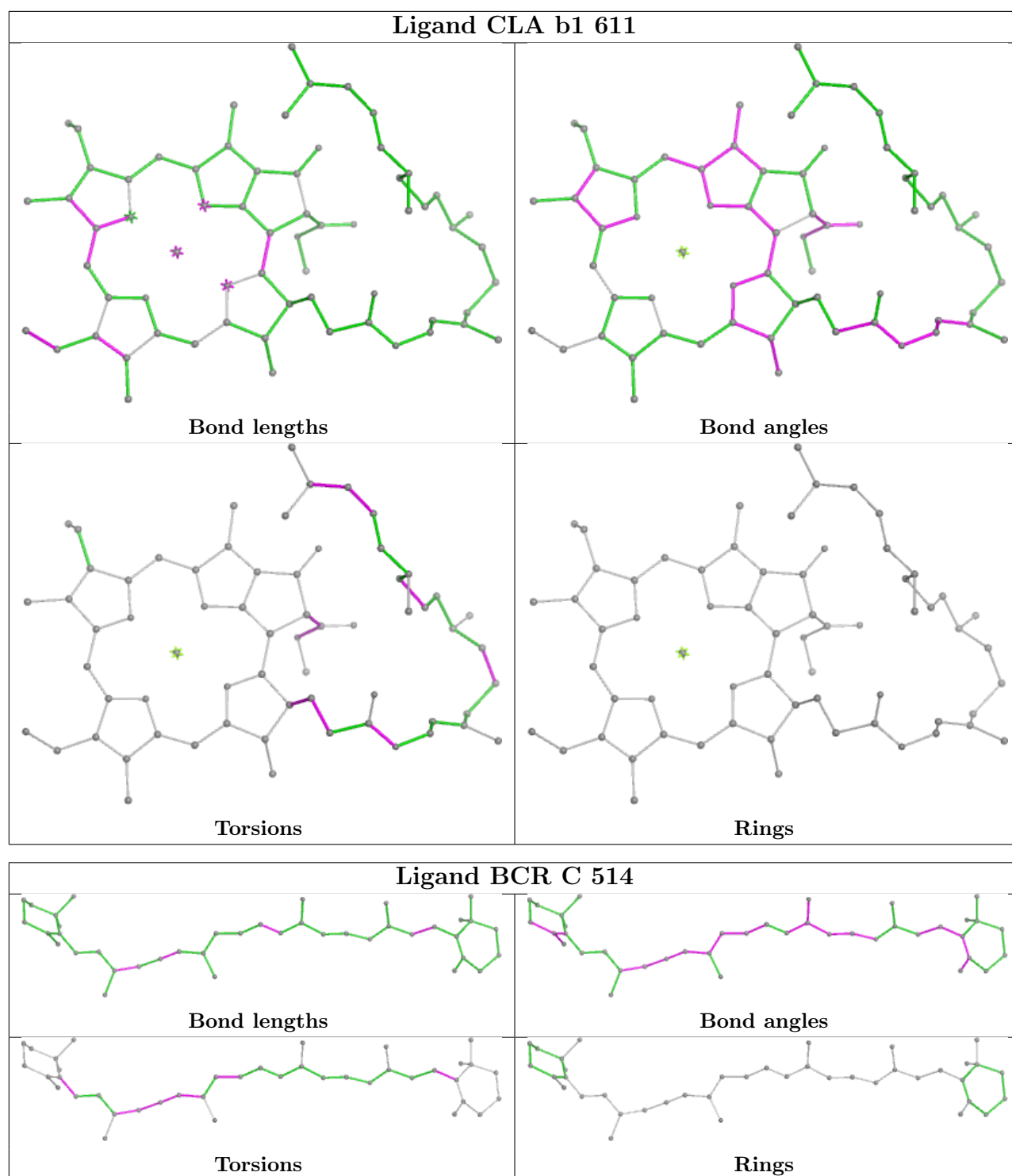


Rings

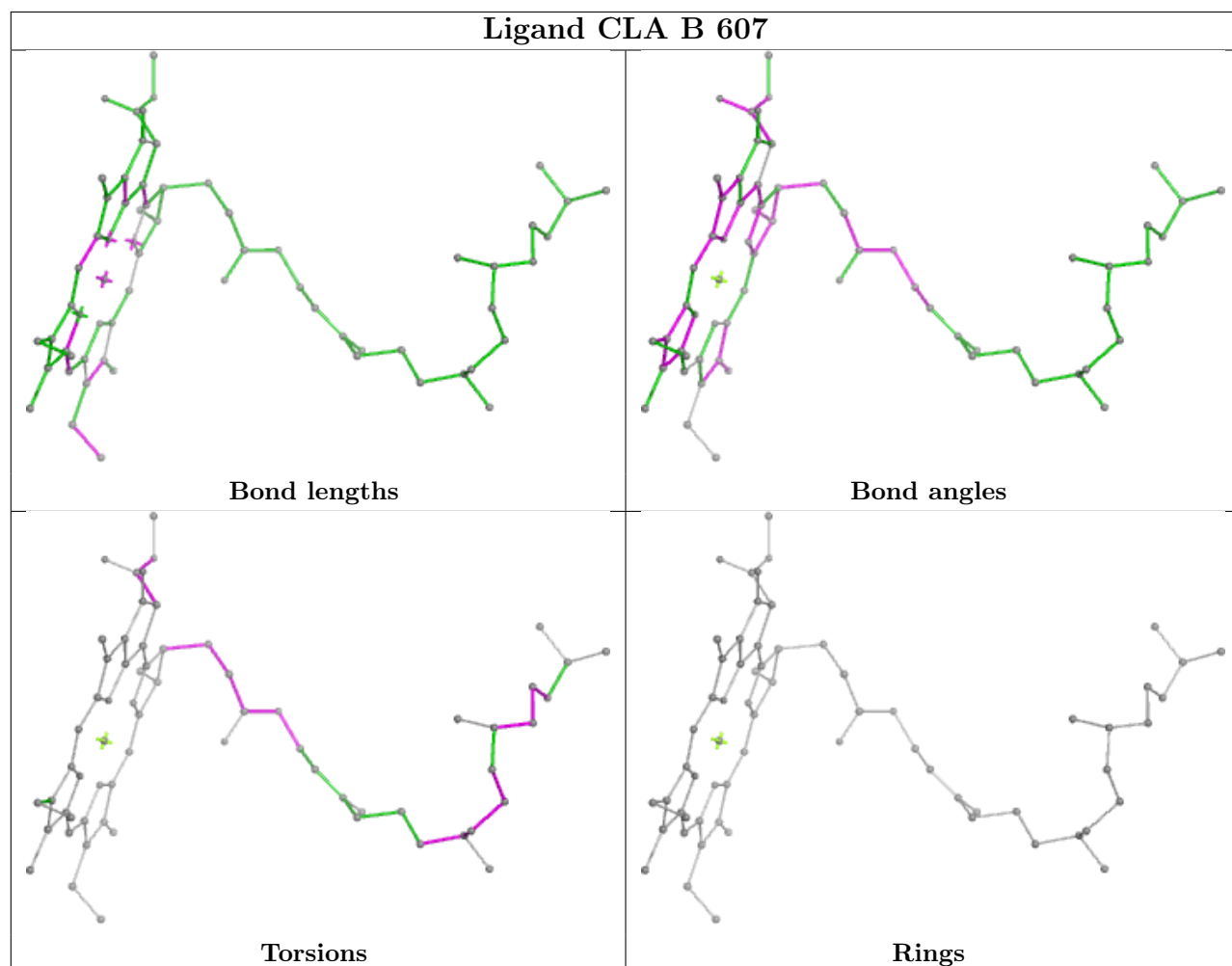
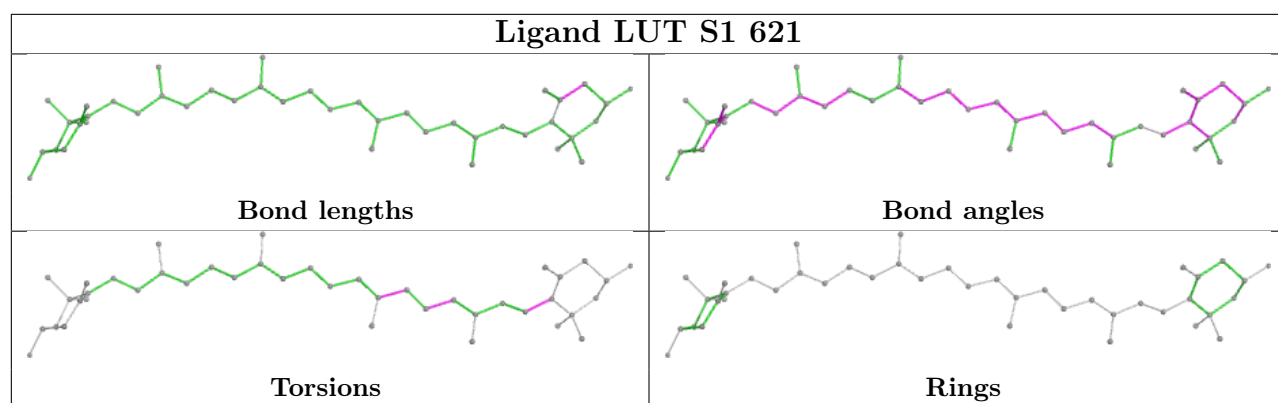


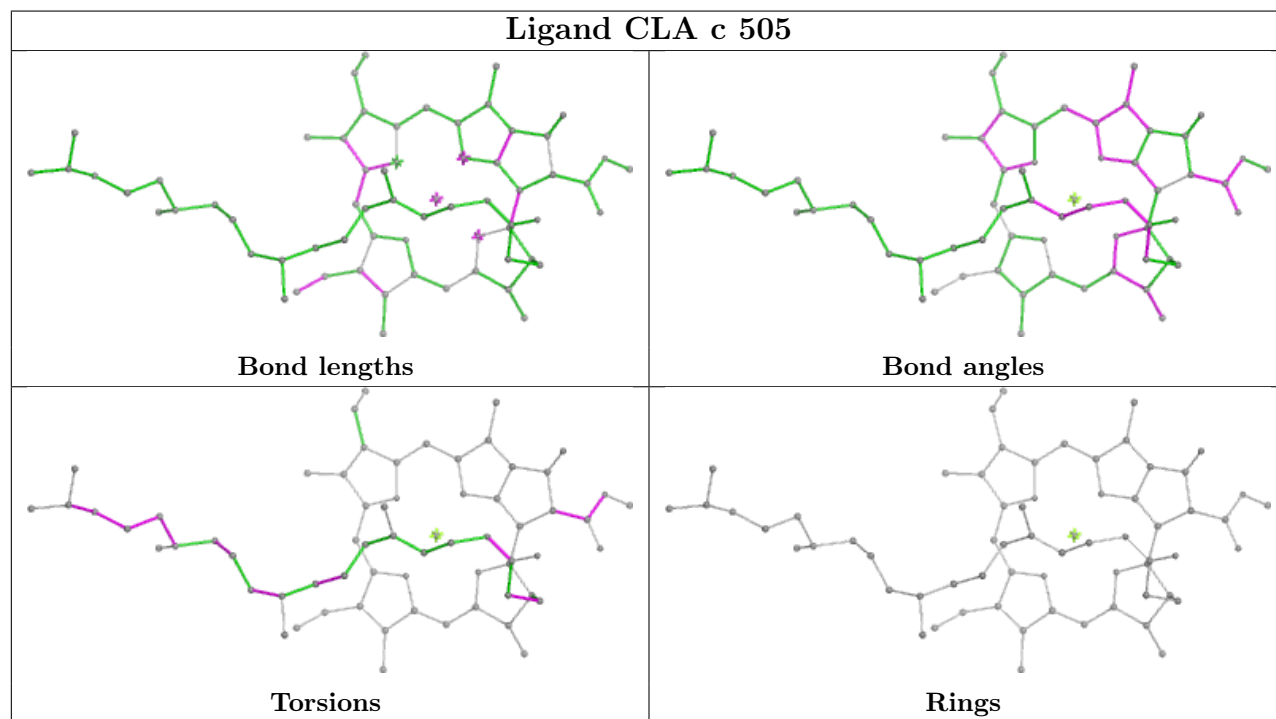
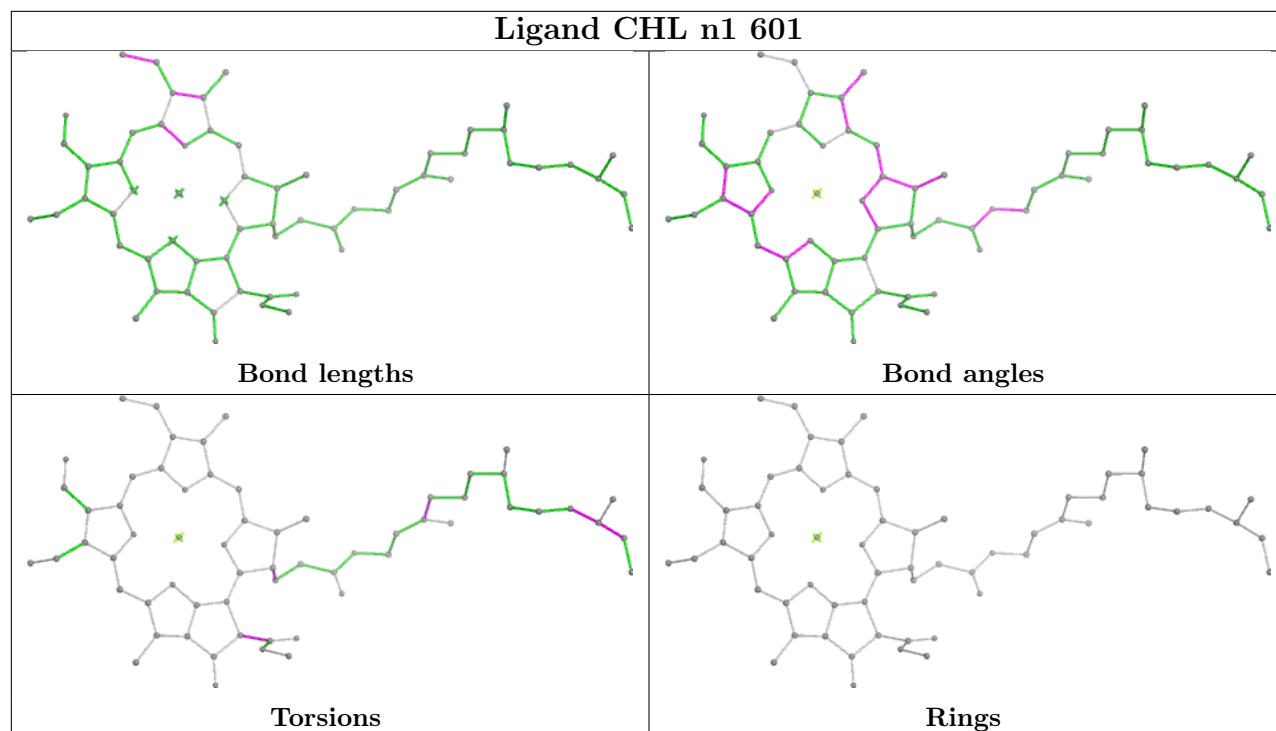


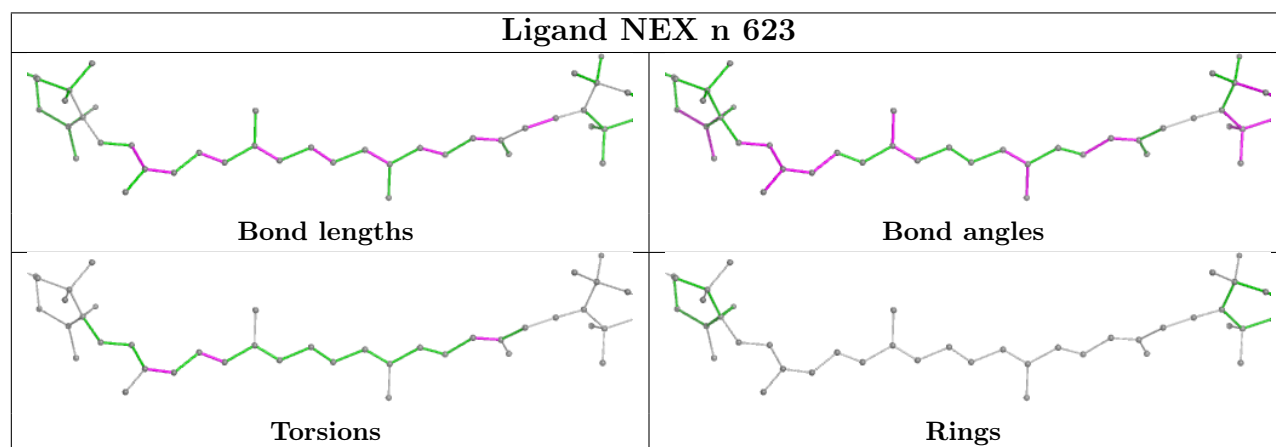
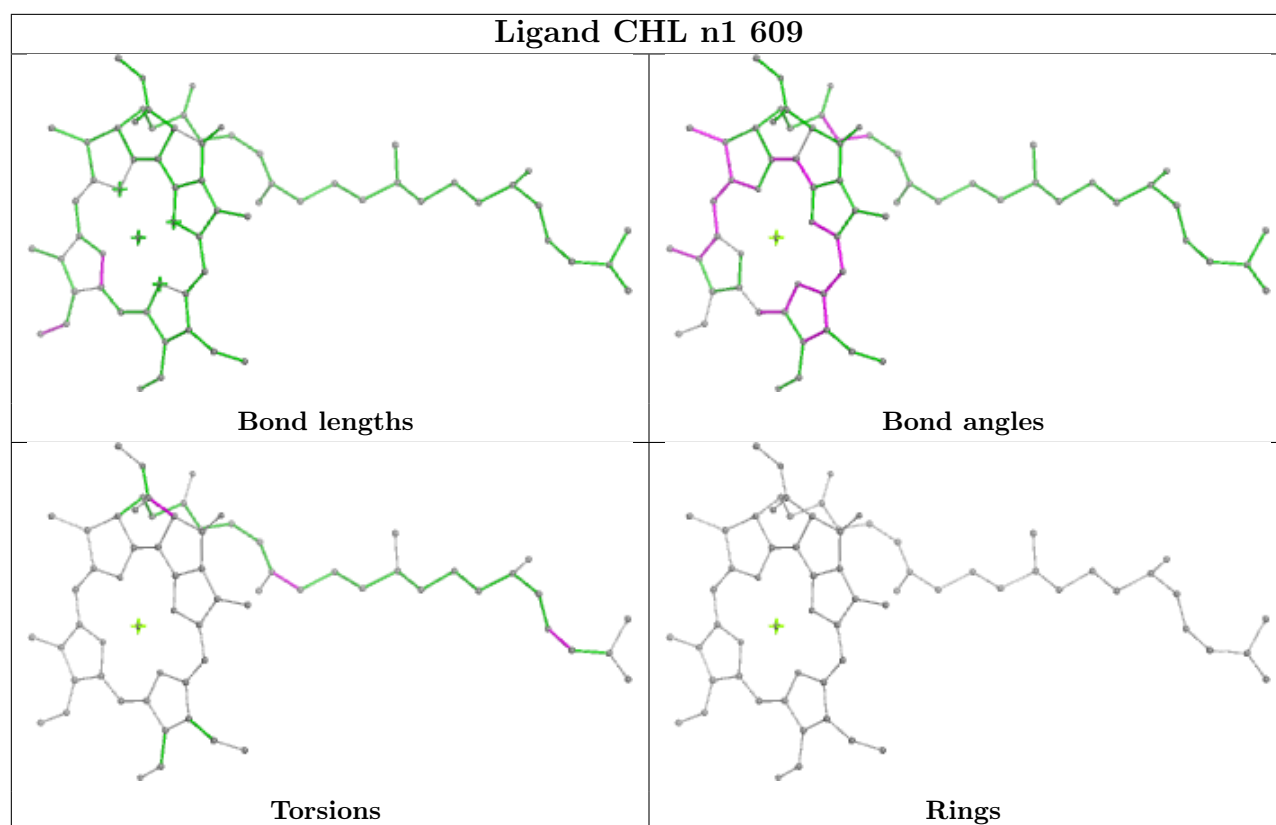


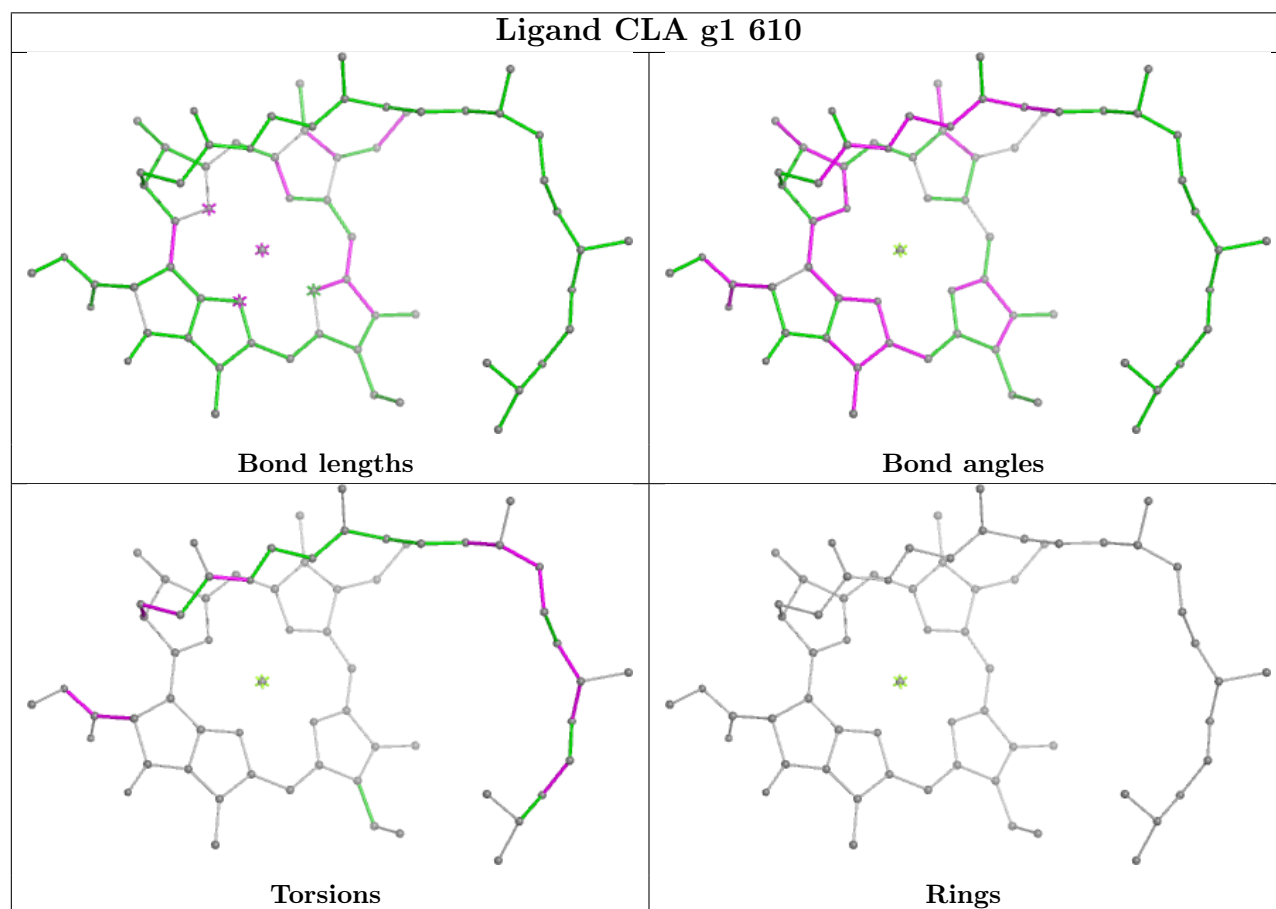
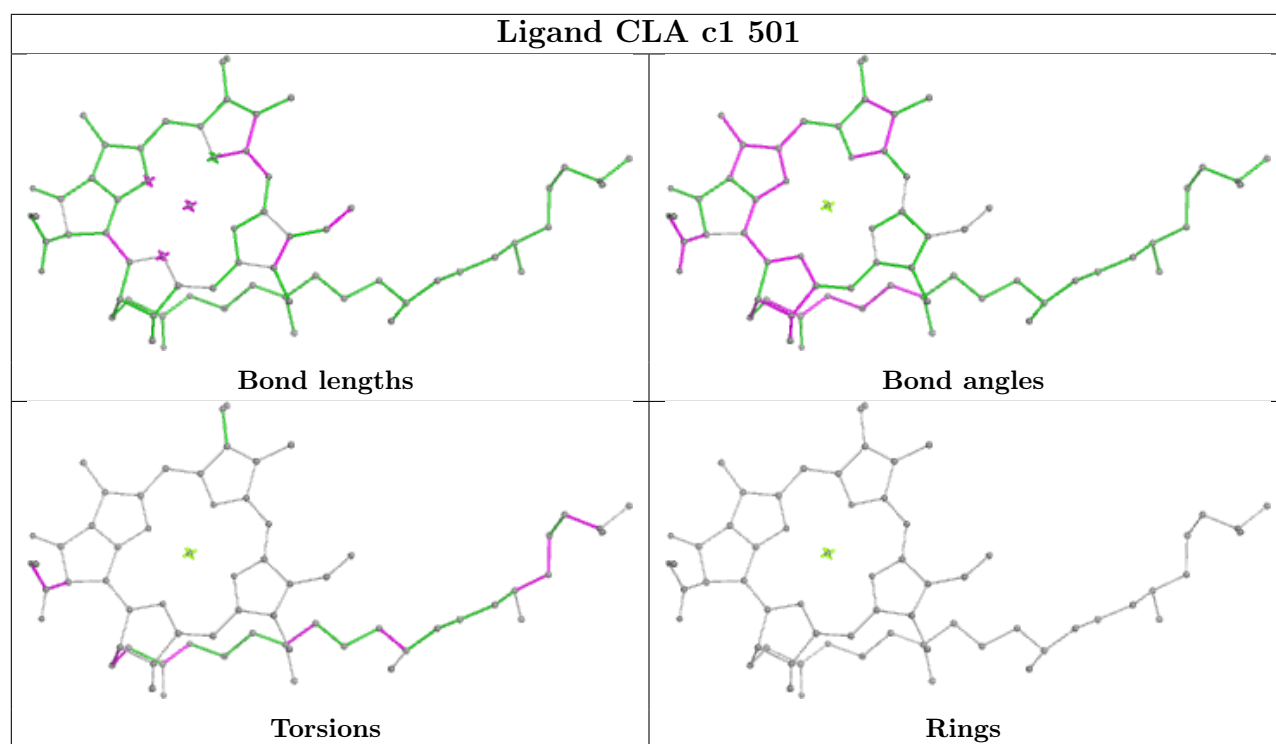




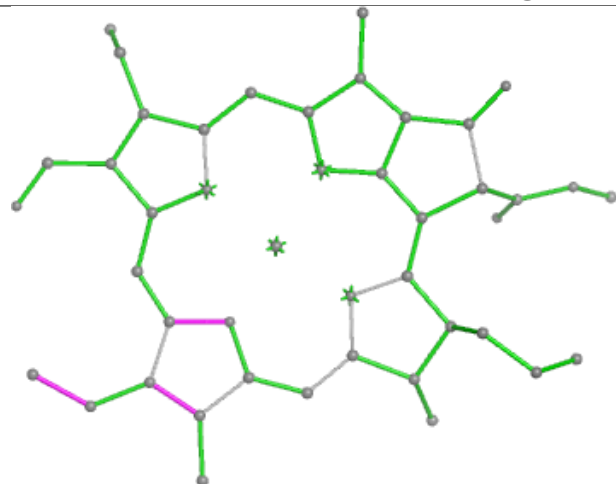




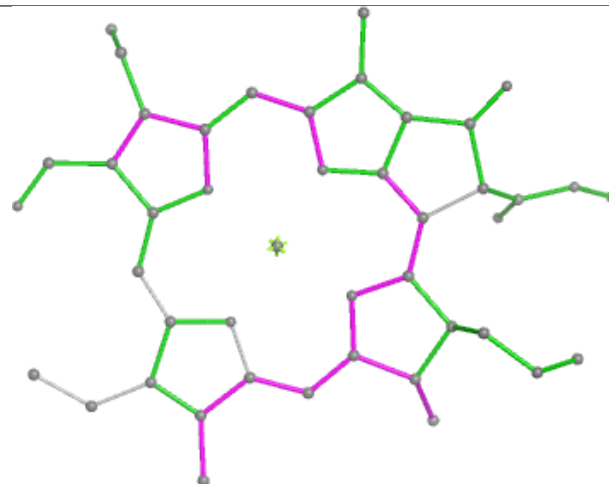




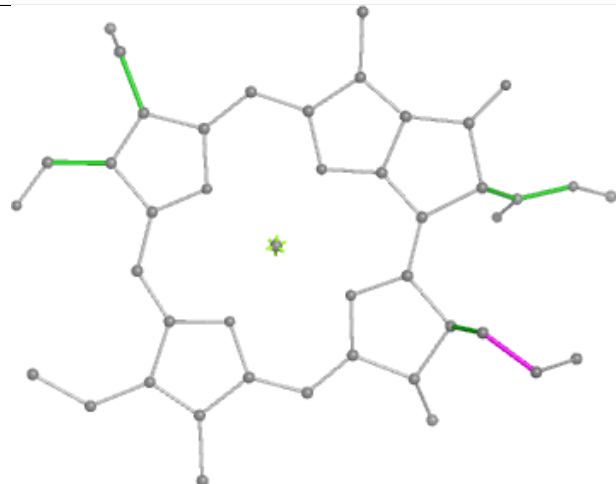
## Ligand CHL S 606



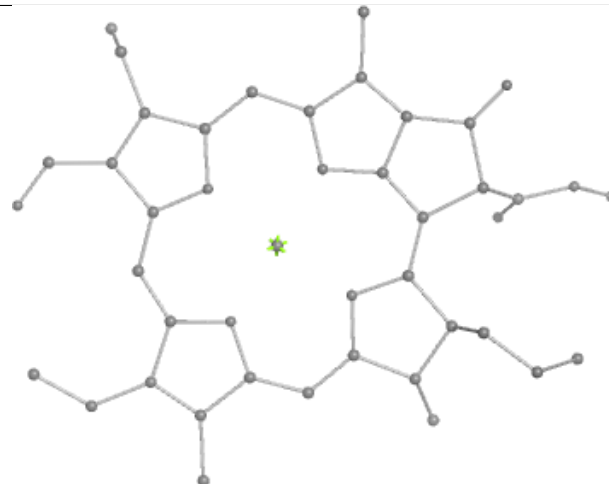
Bond lengths



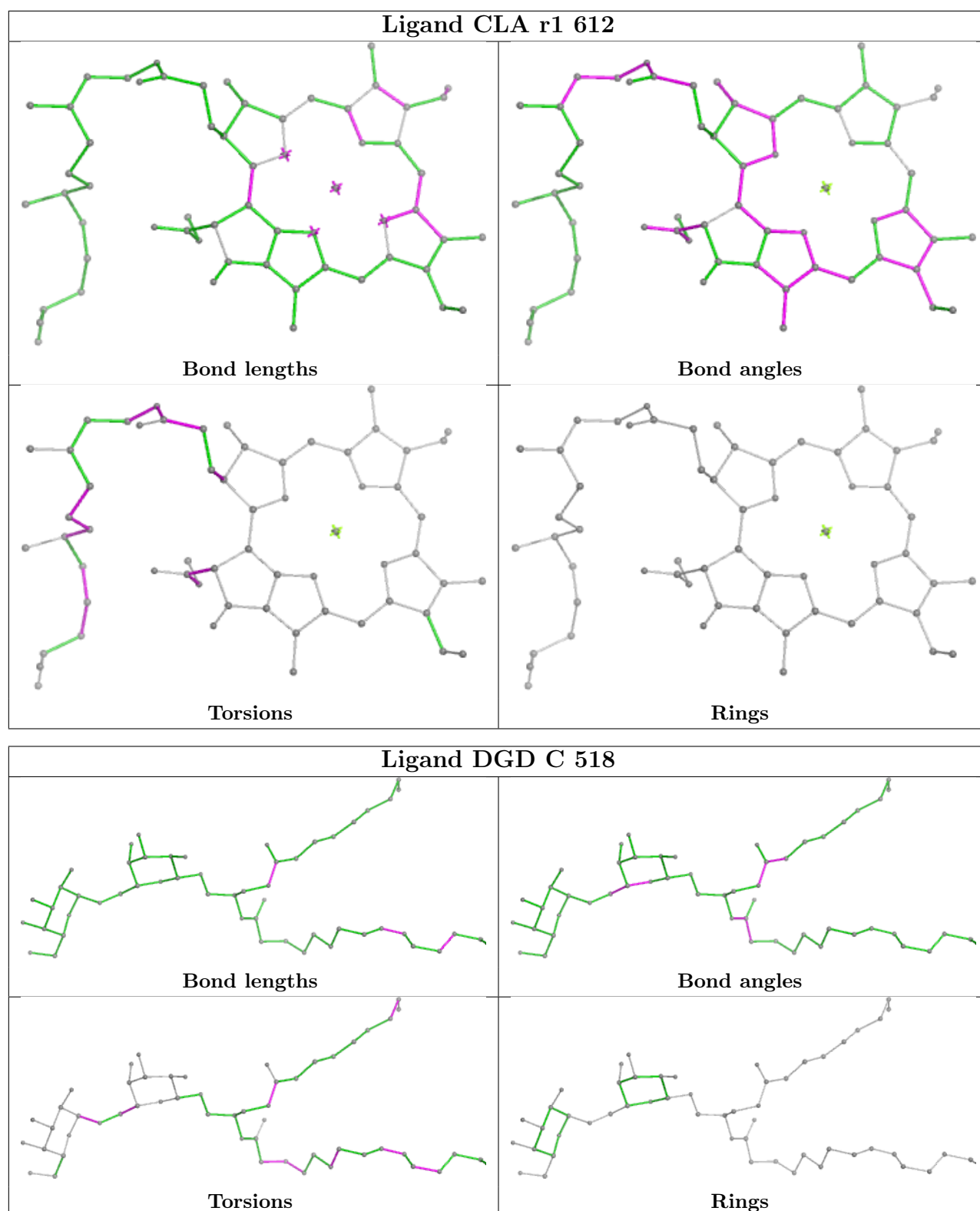
Bond angles

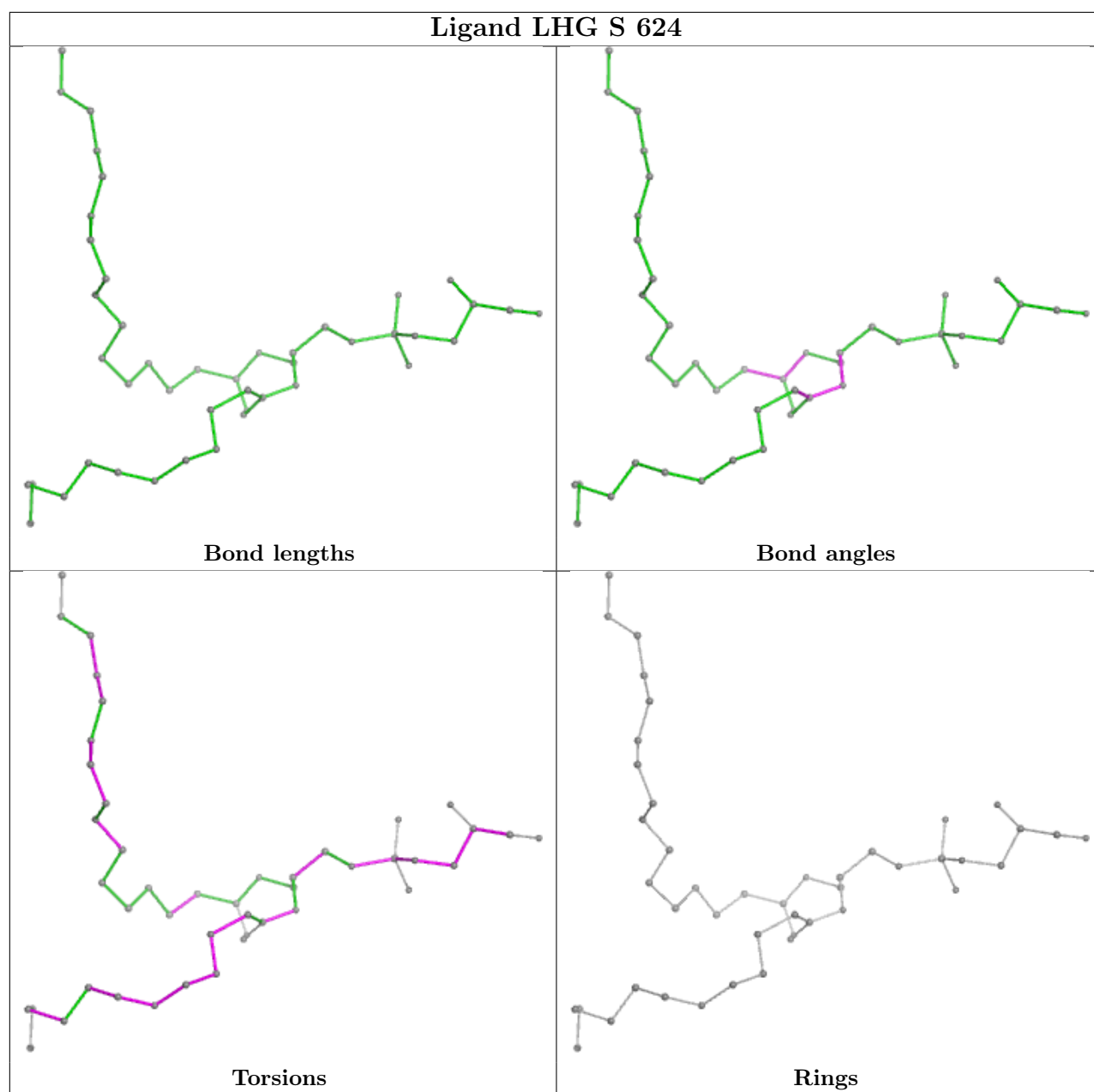


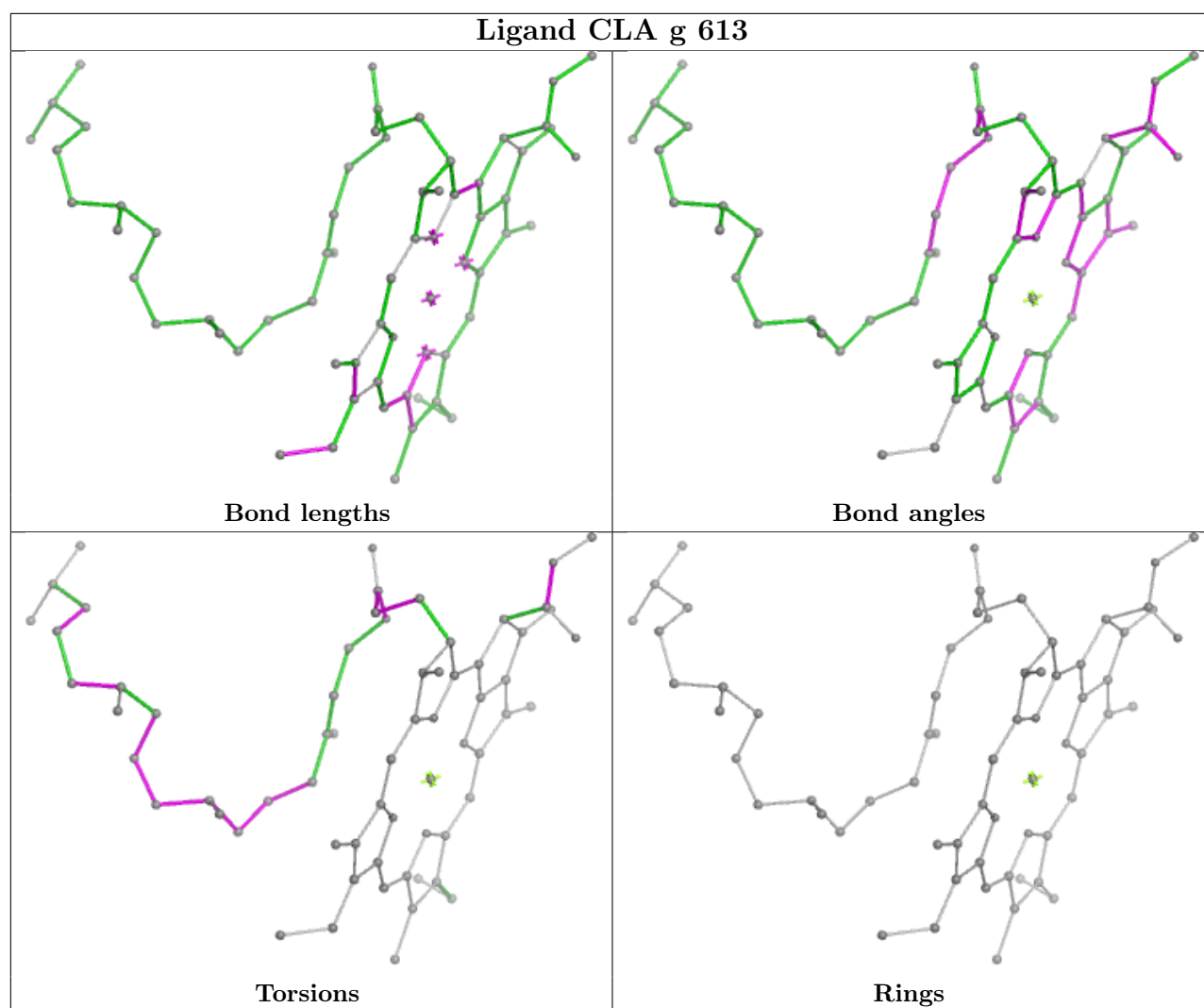
Torsions



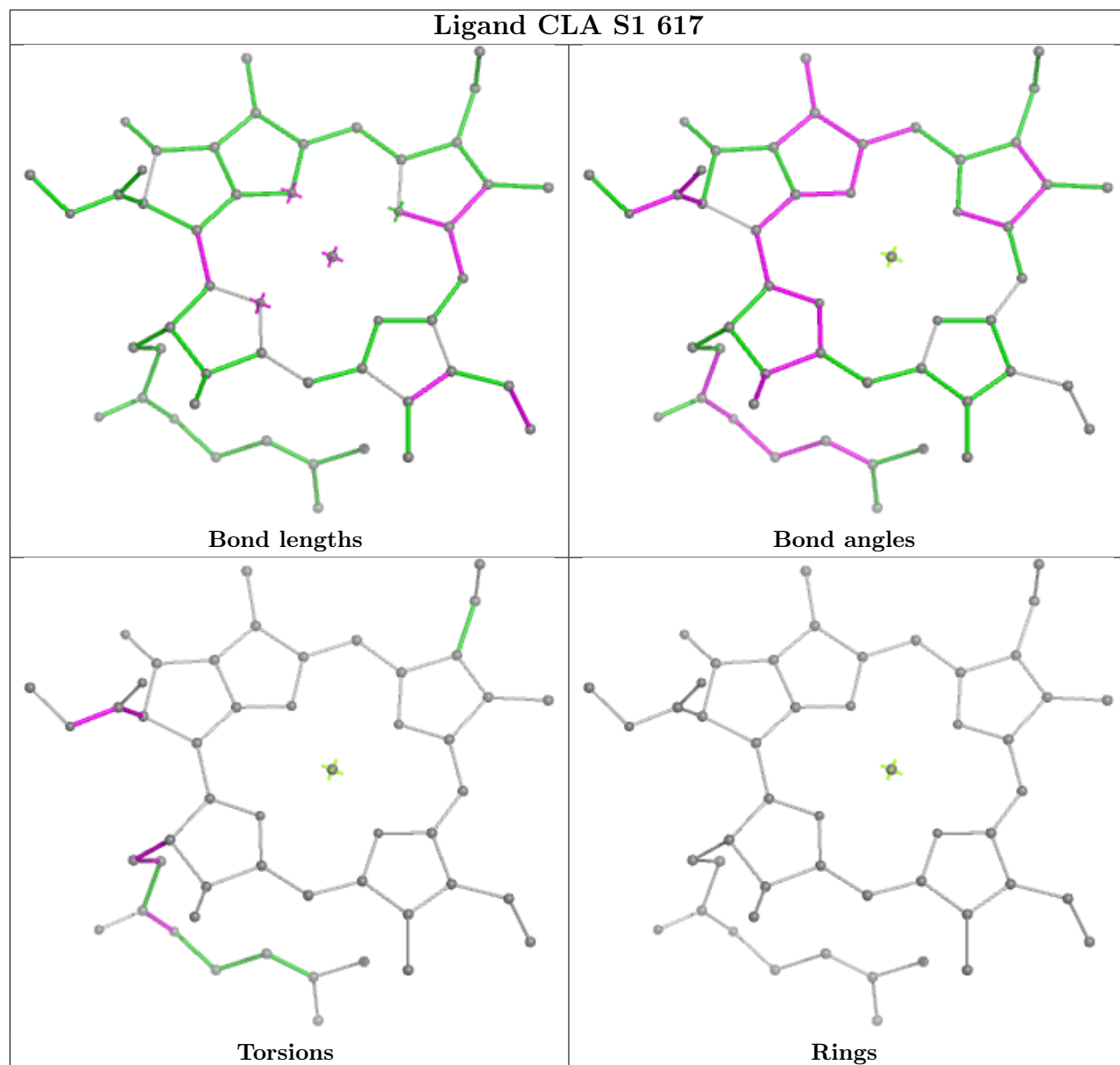
Rings

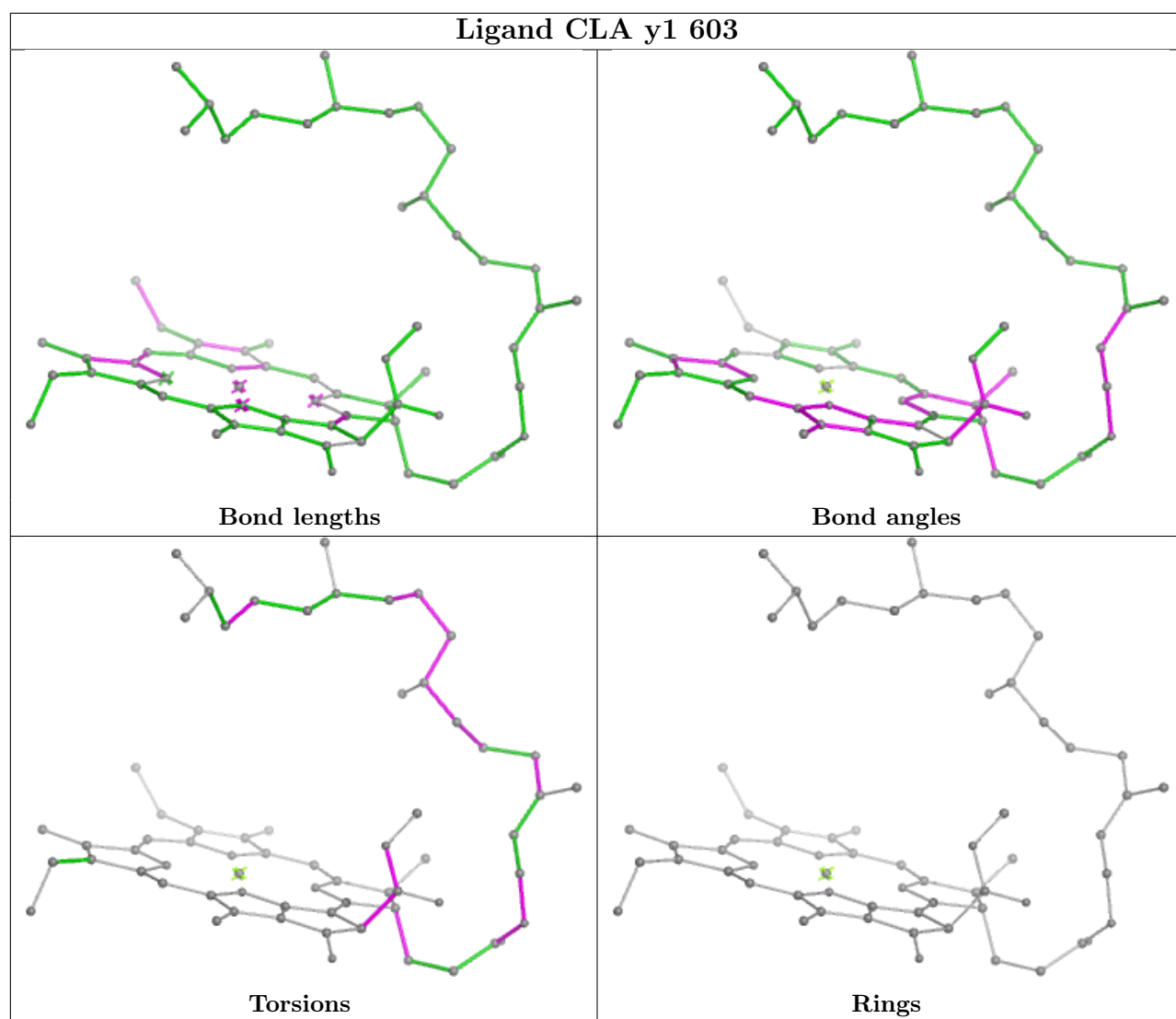




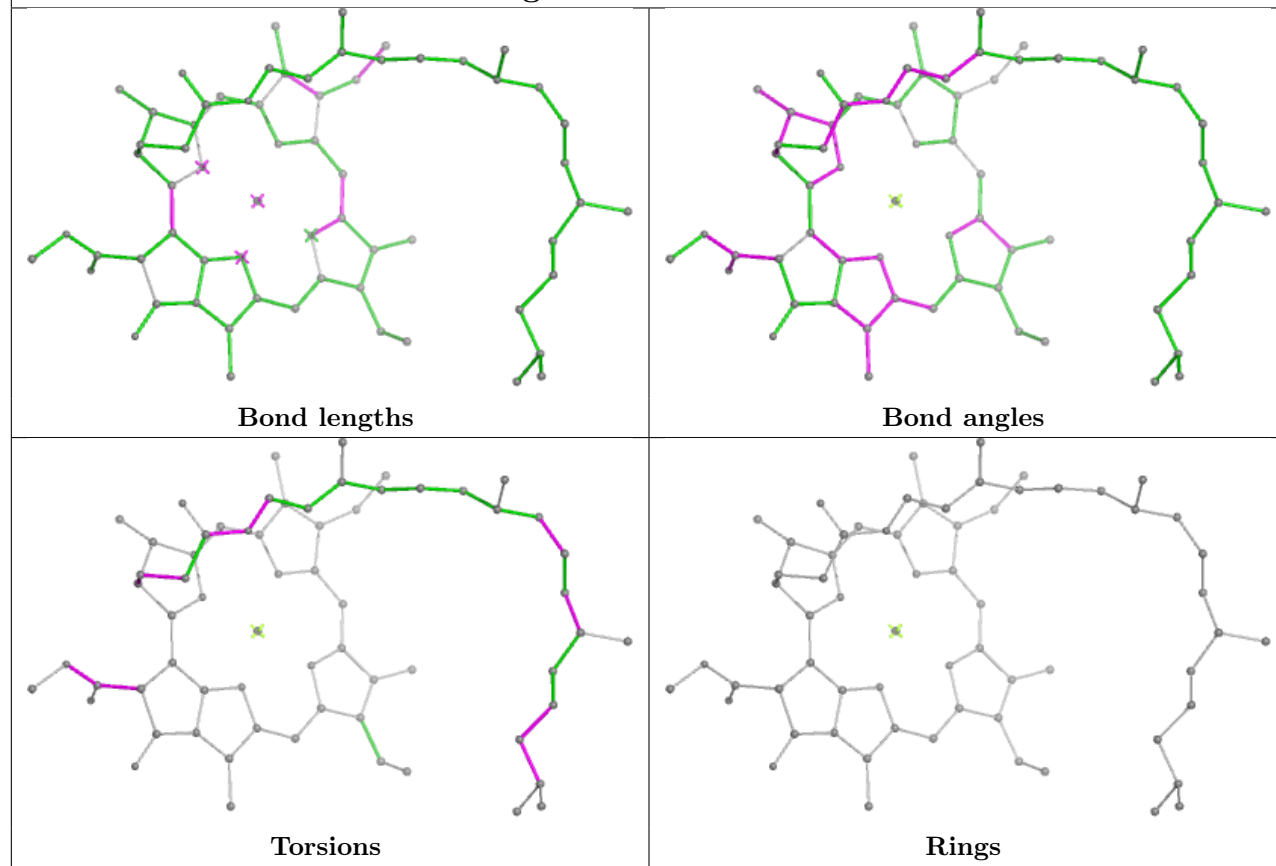




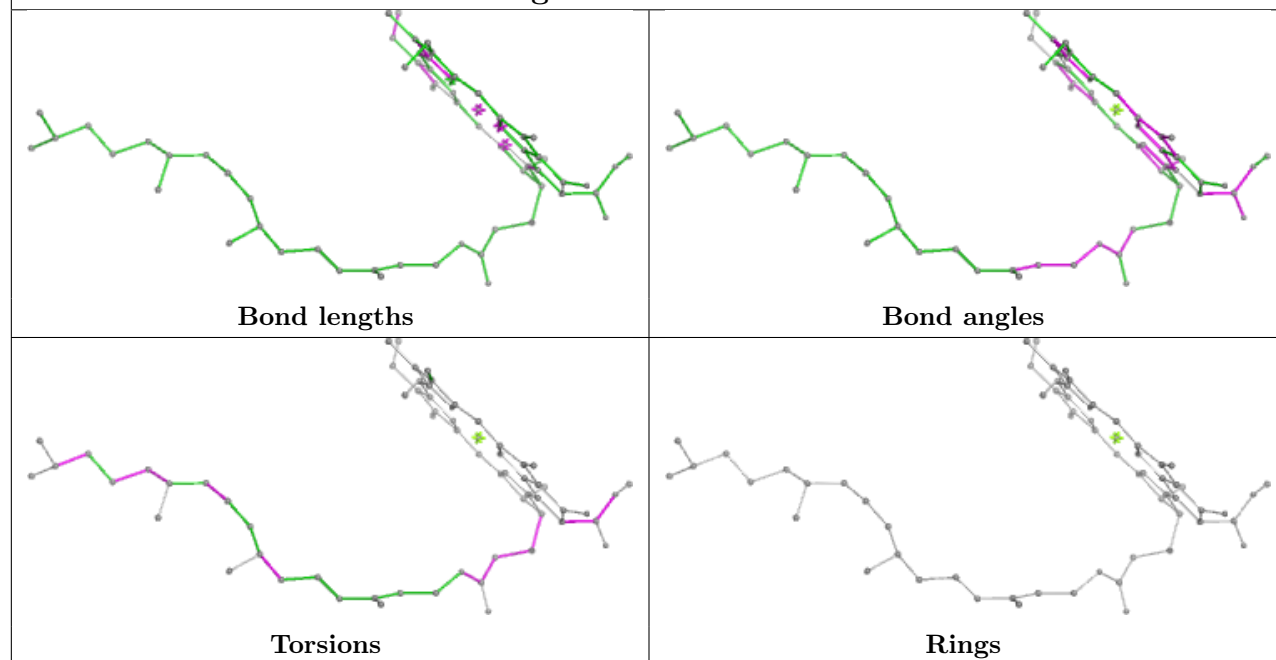


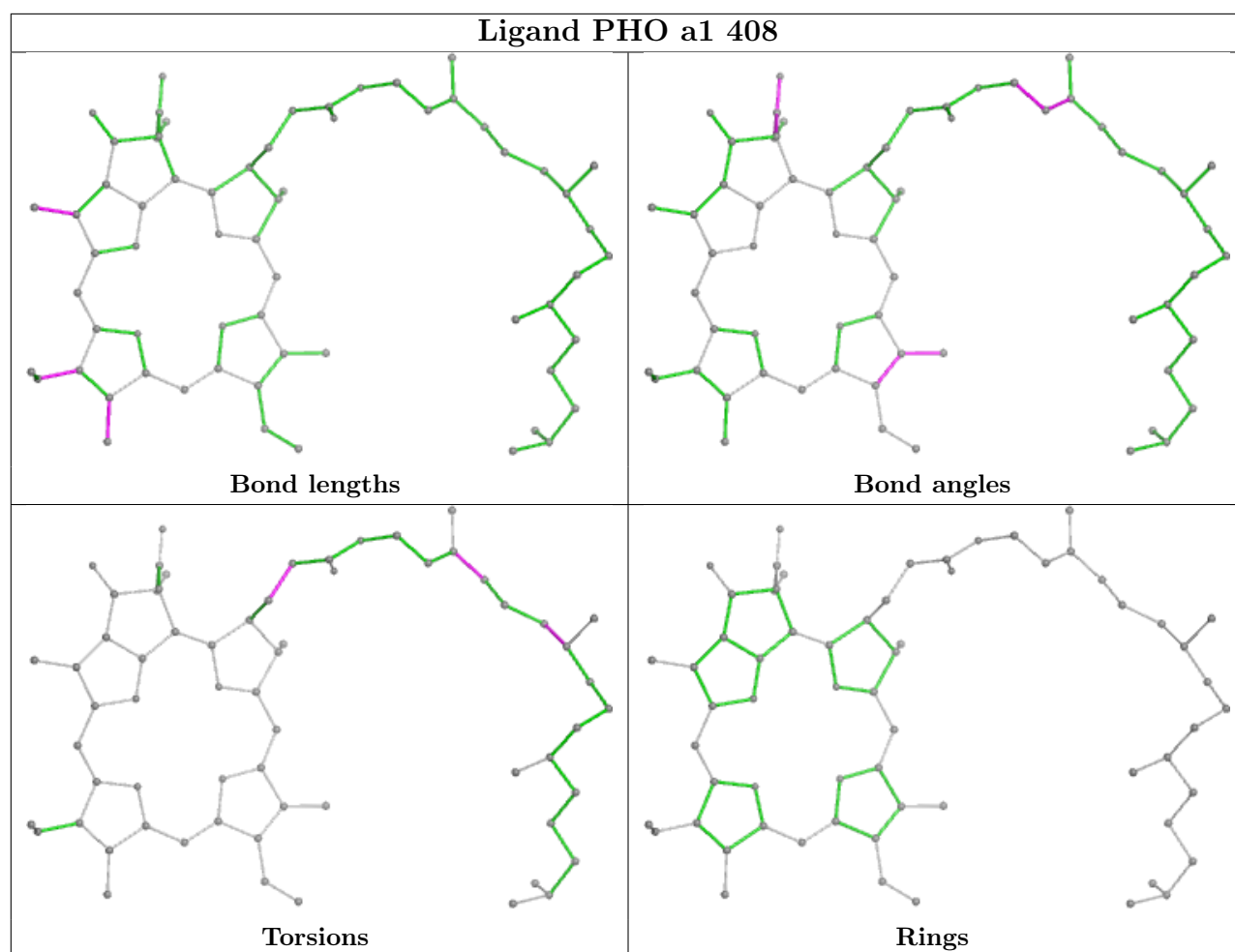


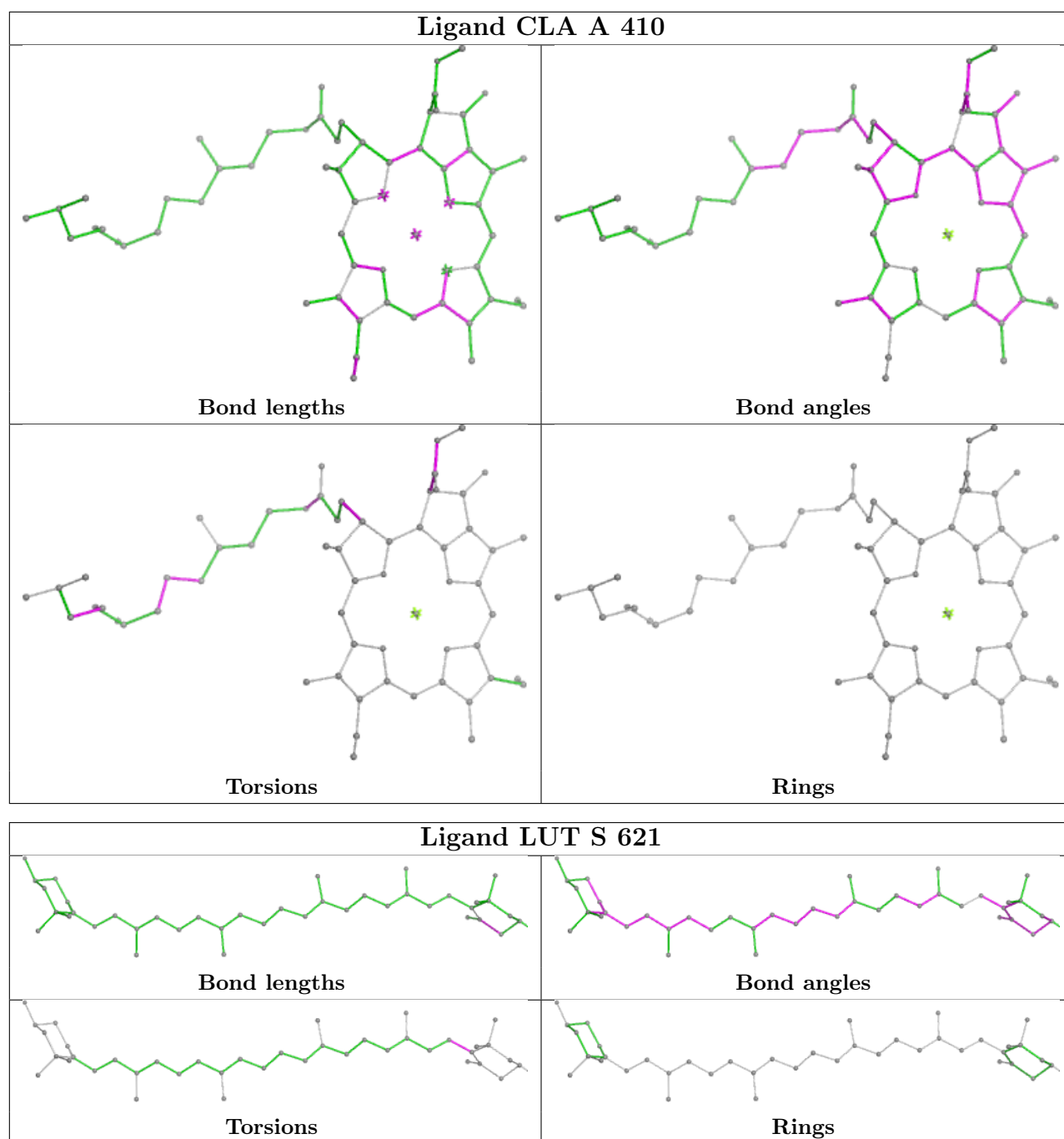
## Ligand CLA Y1 610



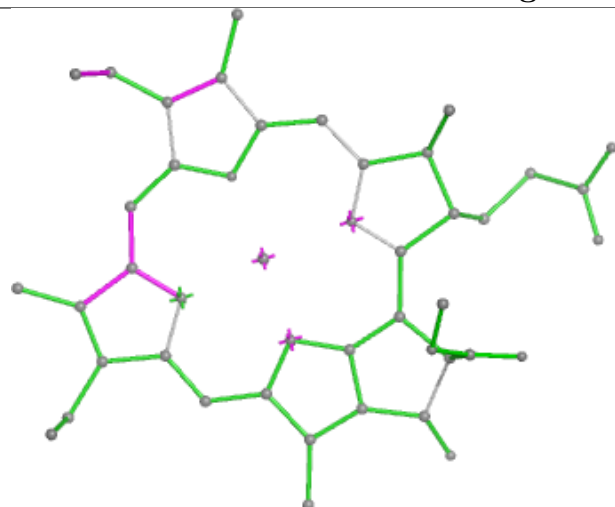
## Ligand CLA N 604



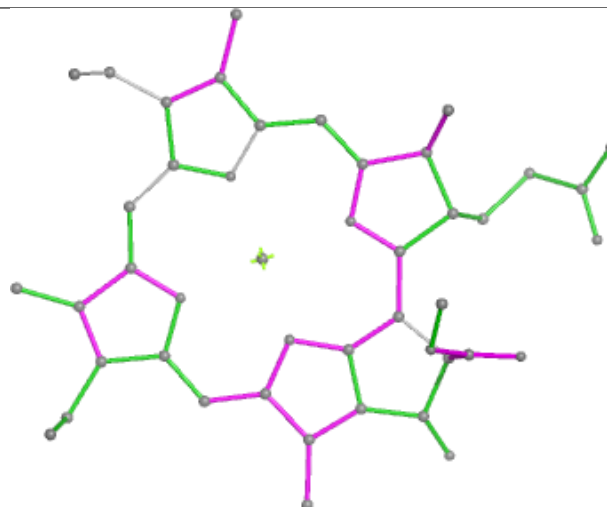




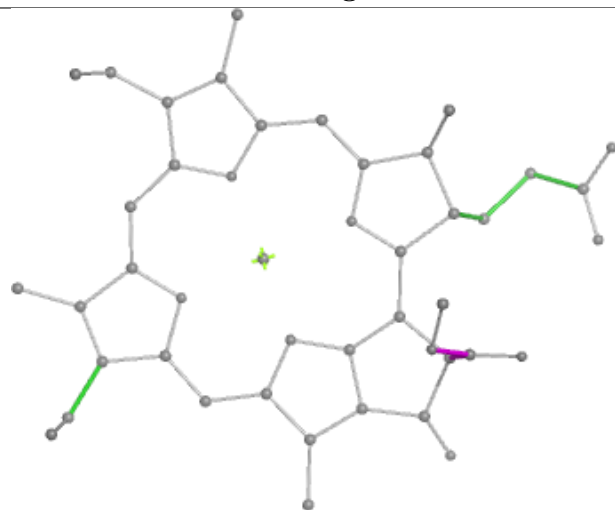
## Ligand CLA n 612



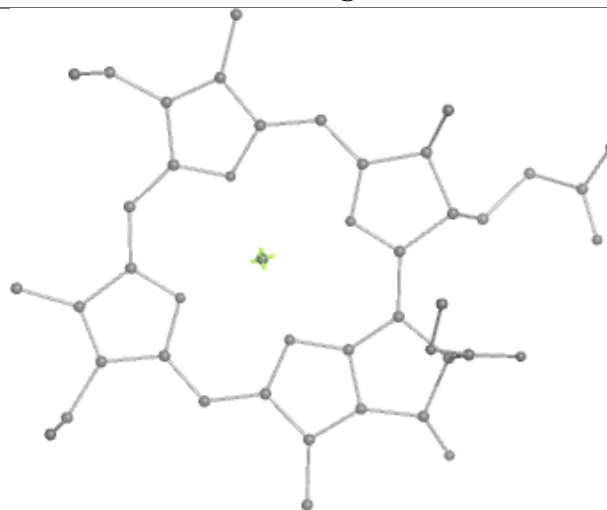
Bond lengths



Bond angles

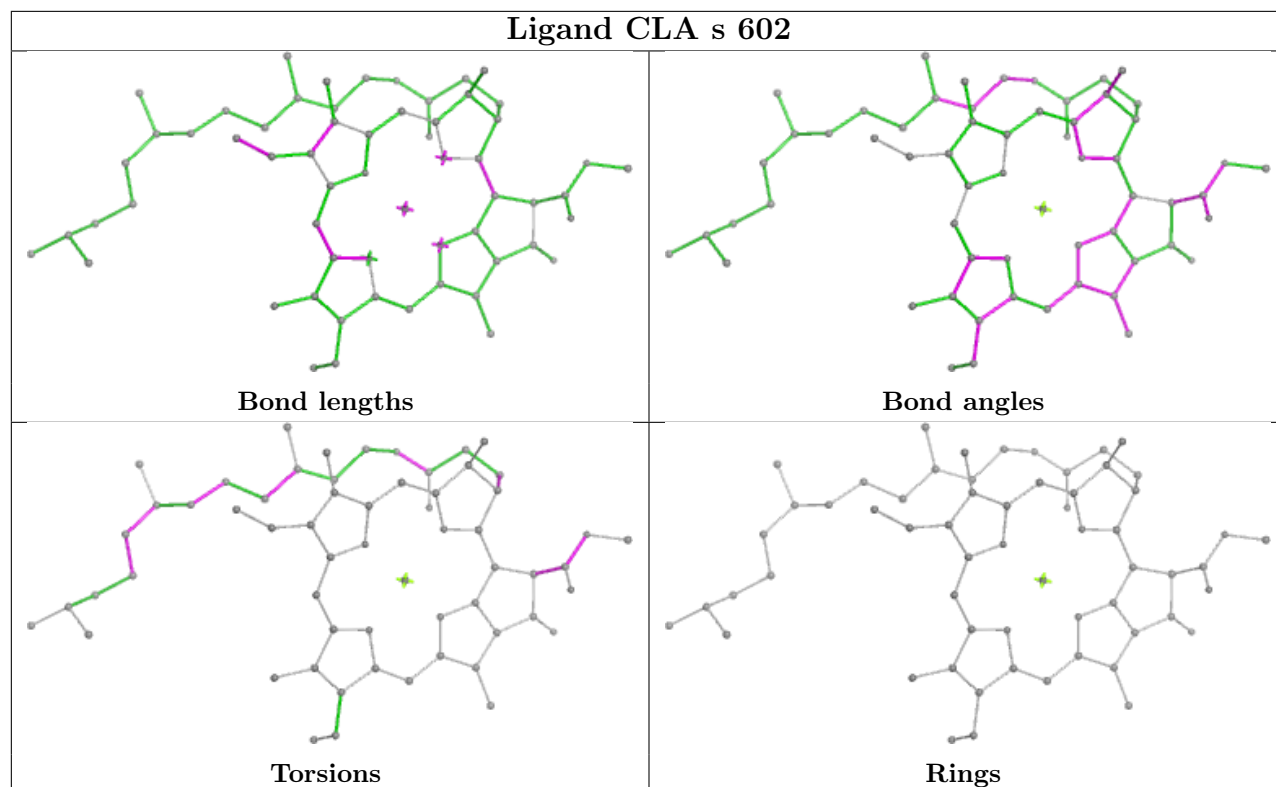


Torsions

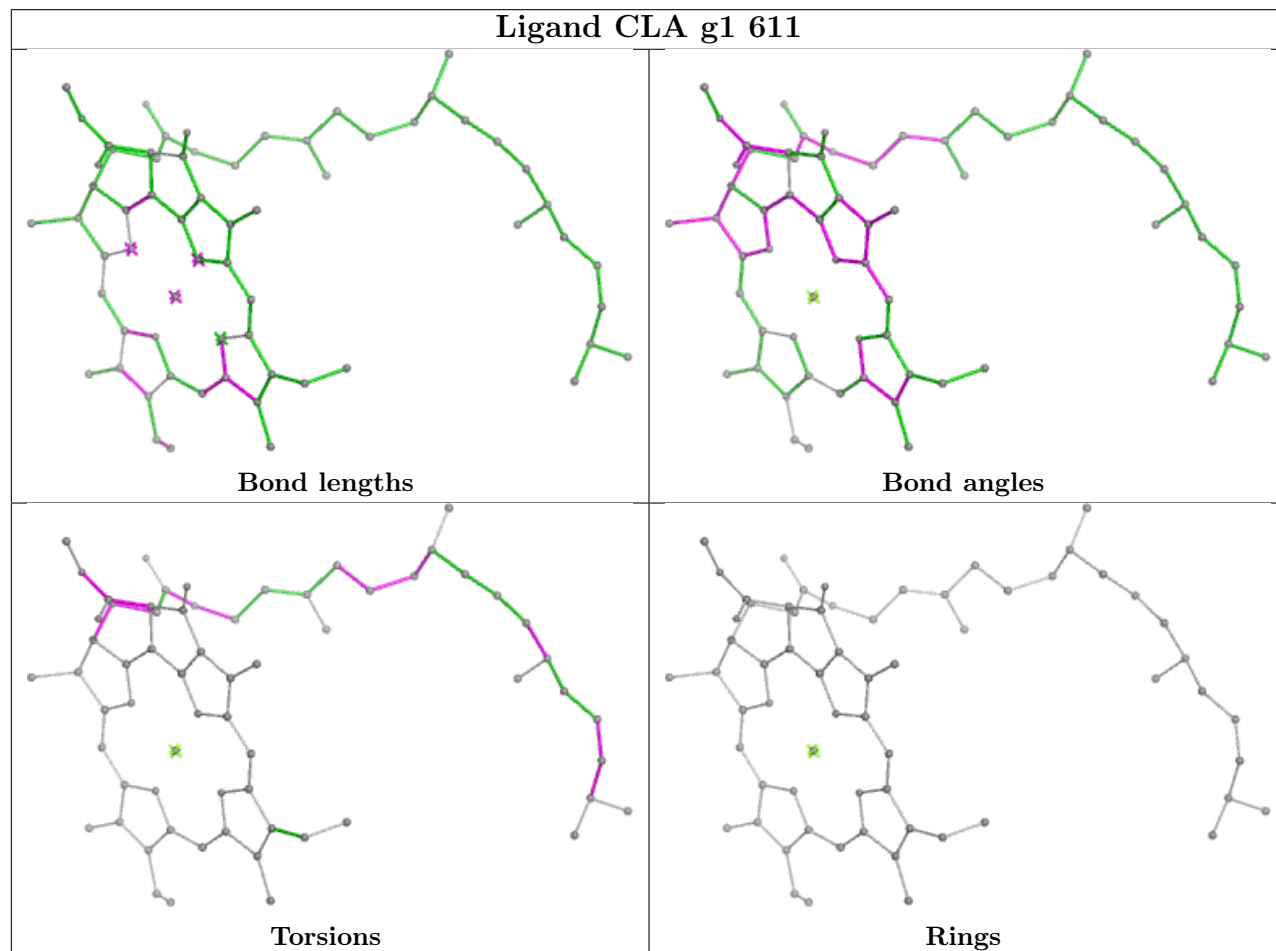


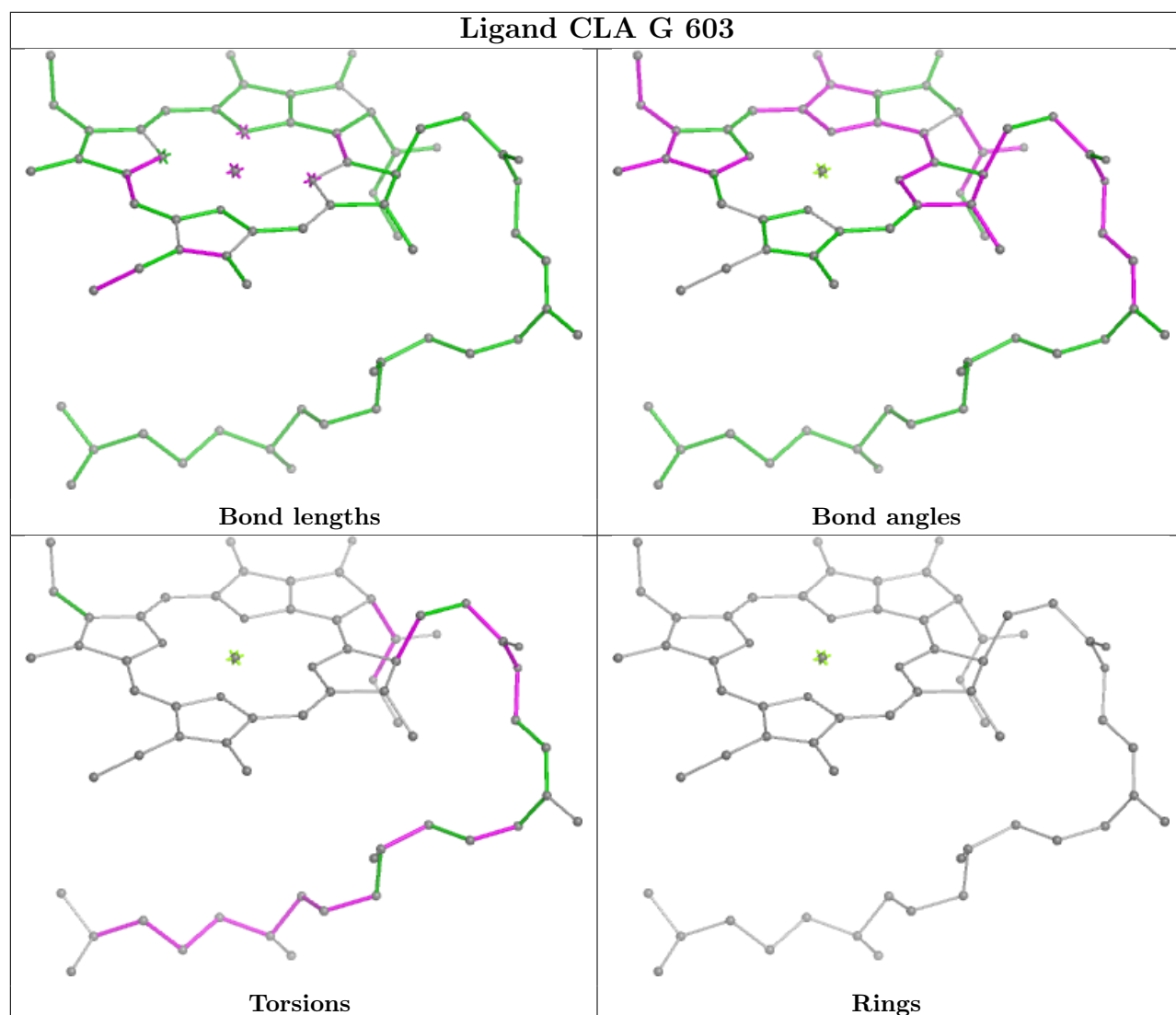
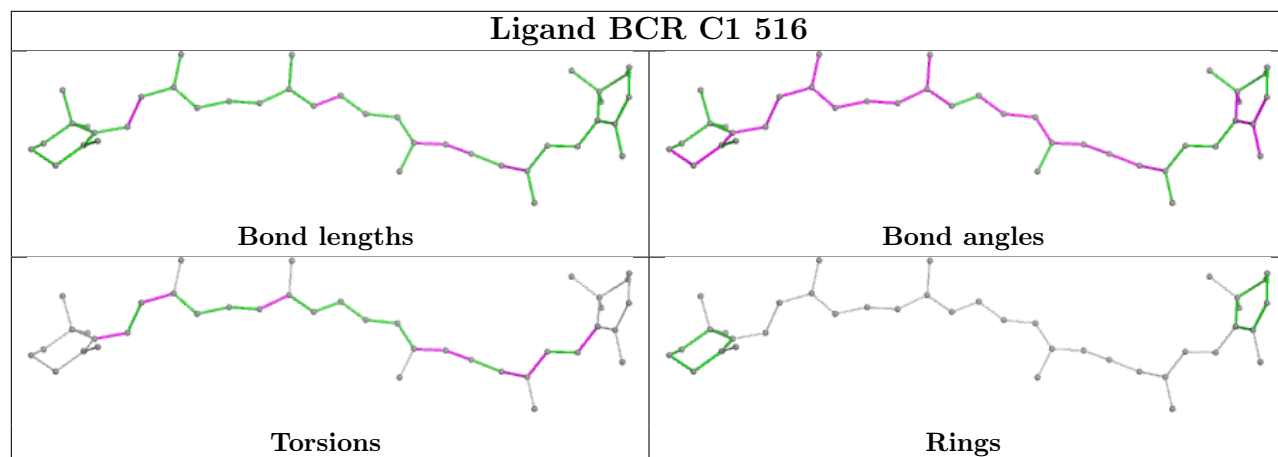
Rings

## Ligand CLA s 602



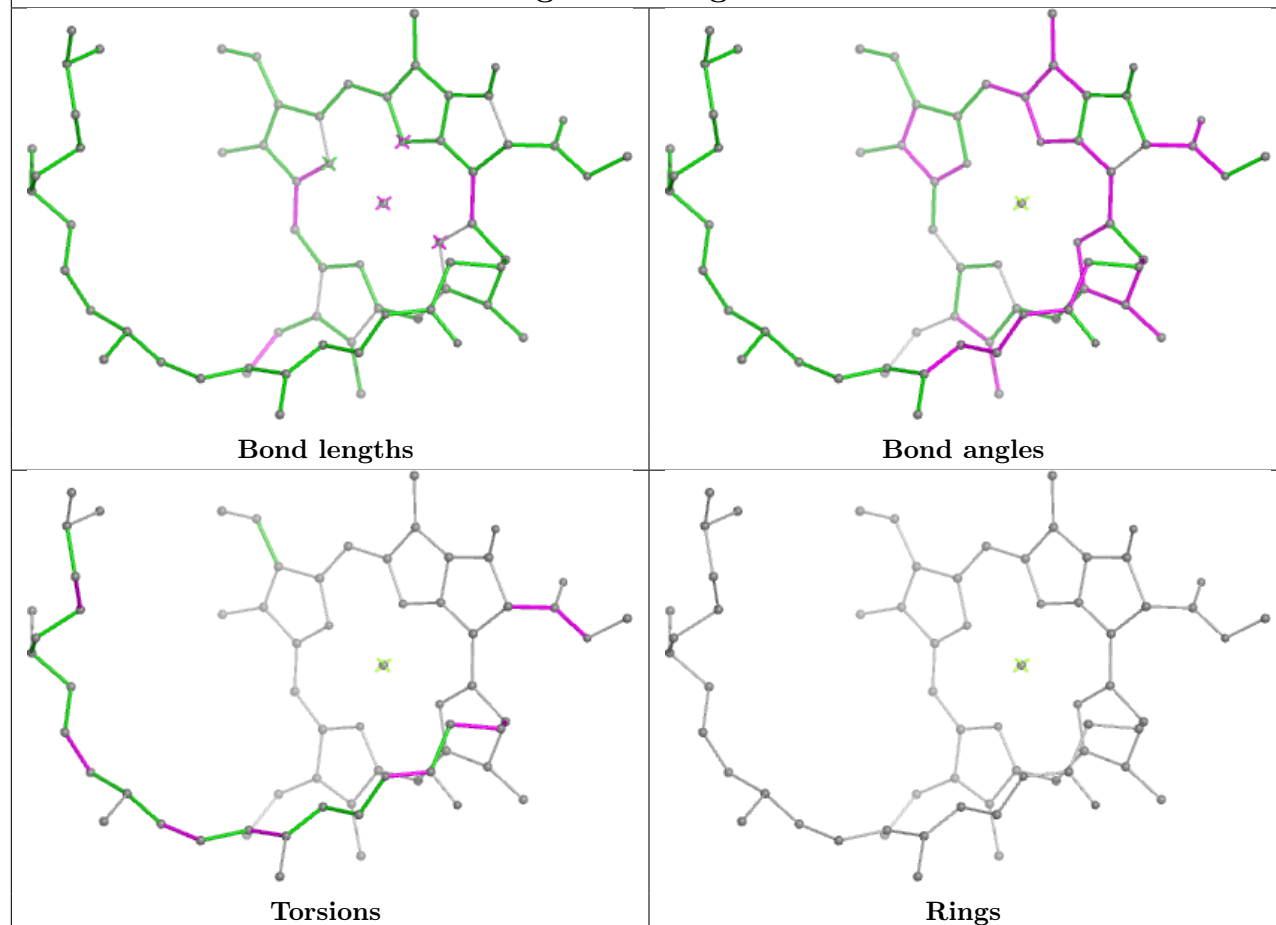
## Ligand CLA g1 611



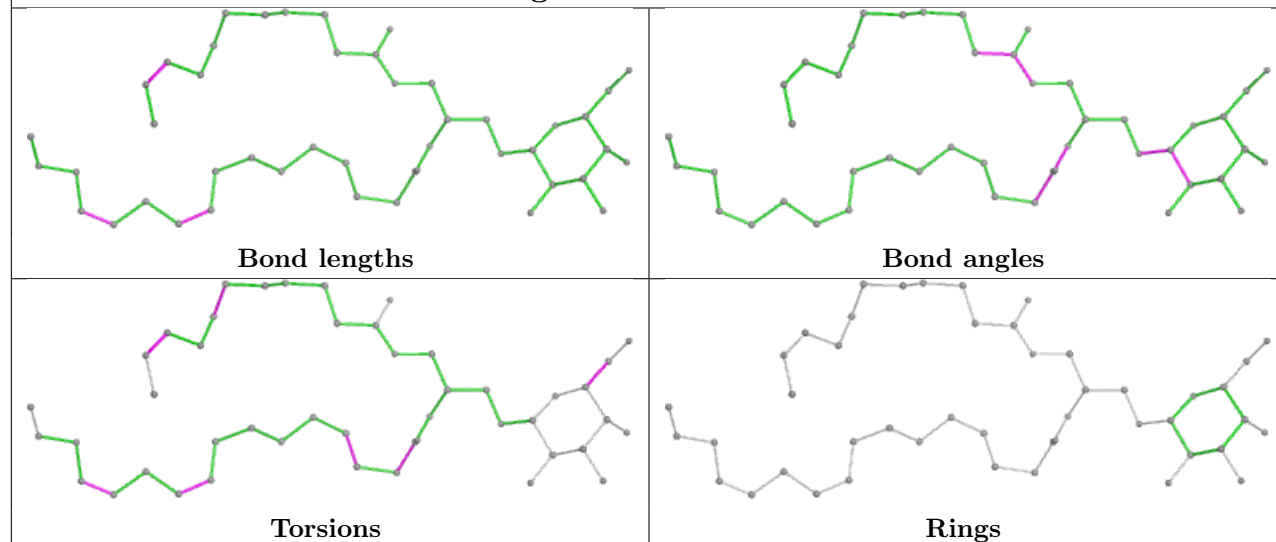


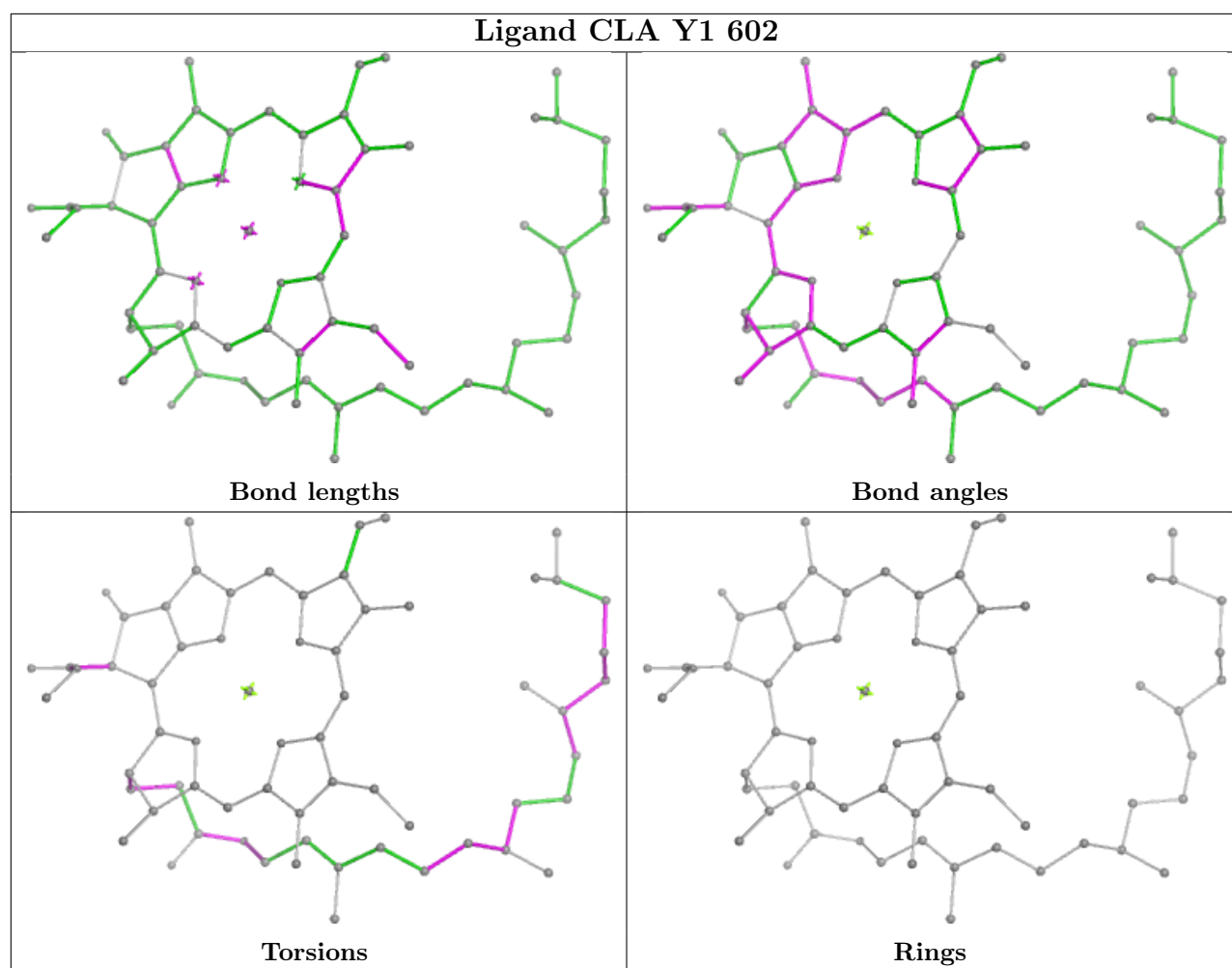


## Ligand CLA g 610

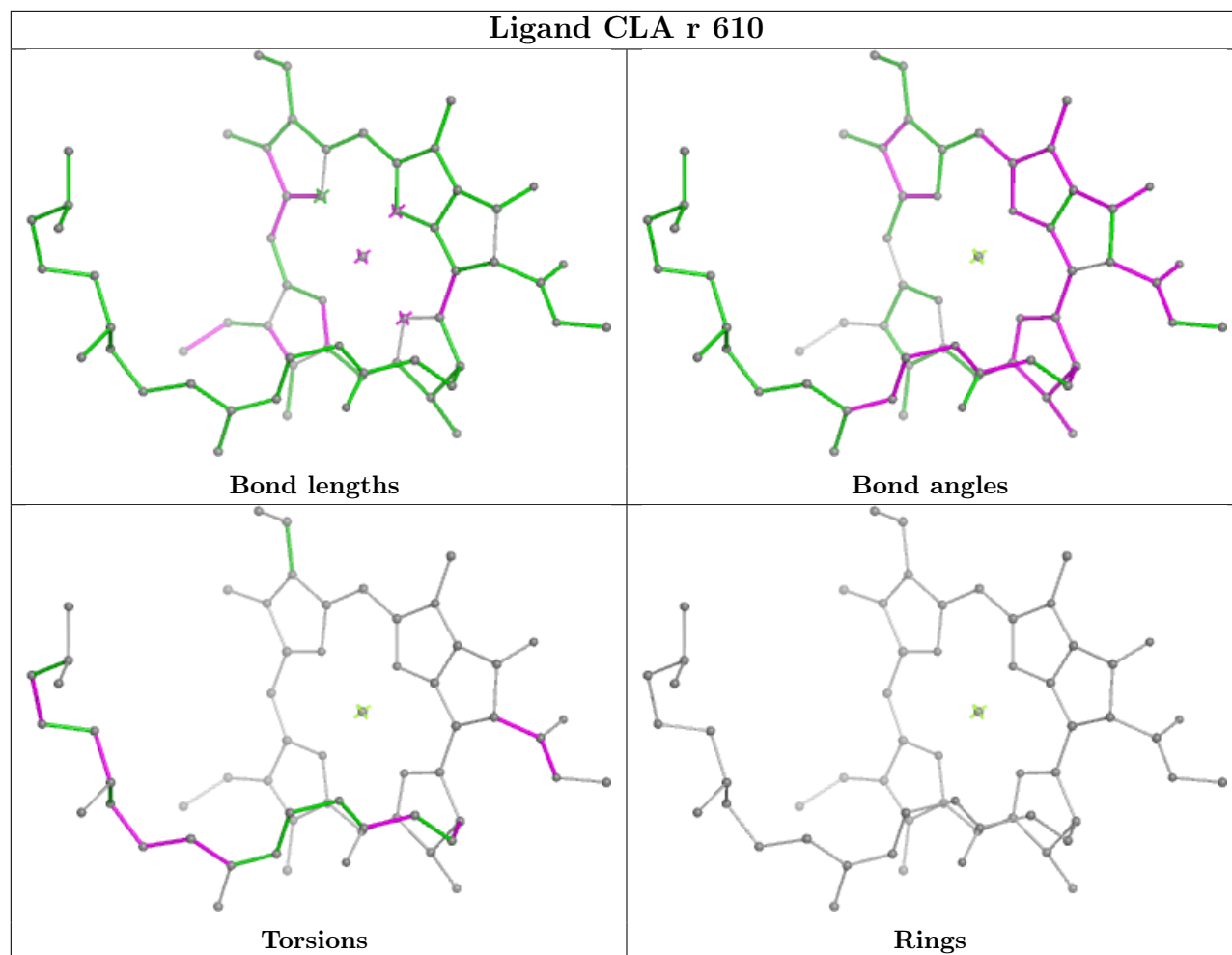


## Ligand LMG d 411

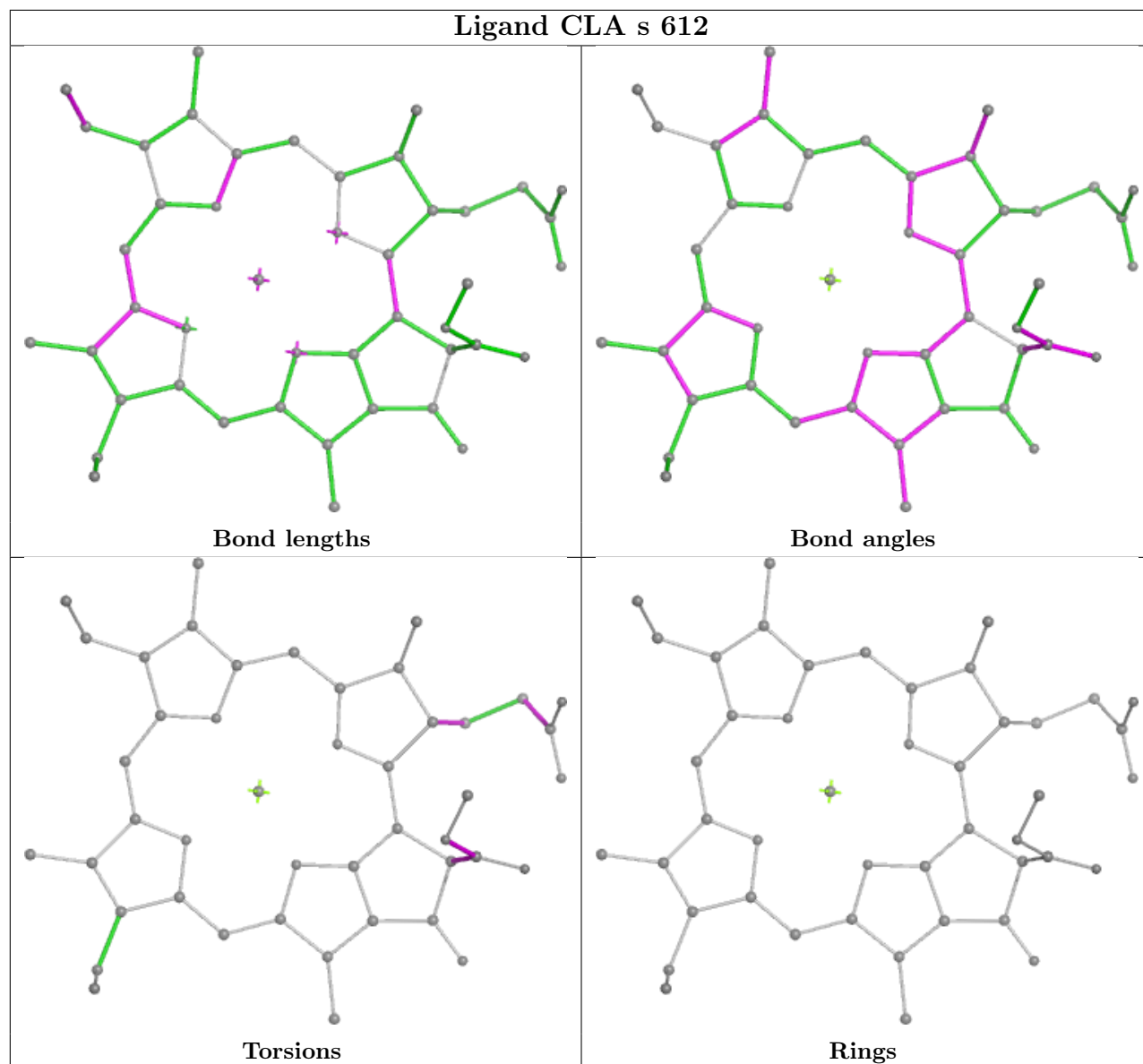




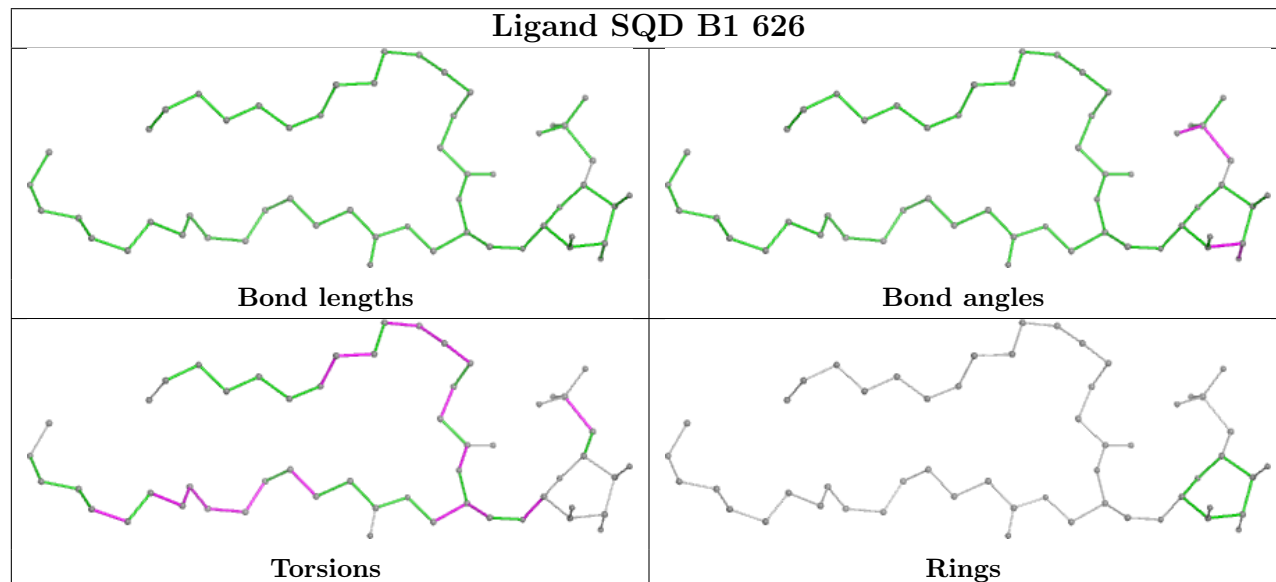
## Ligand CLA r 610

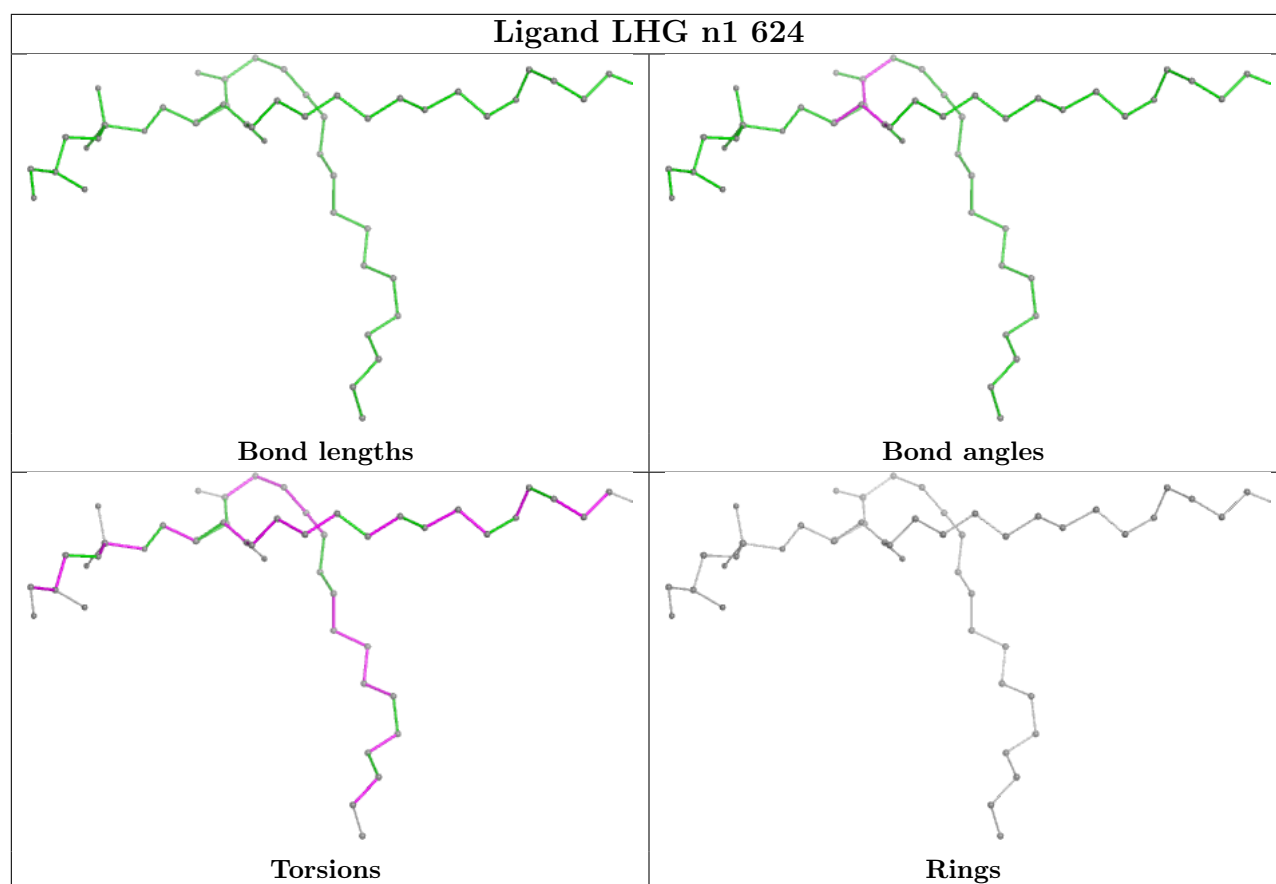


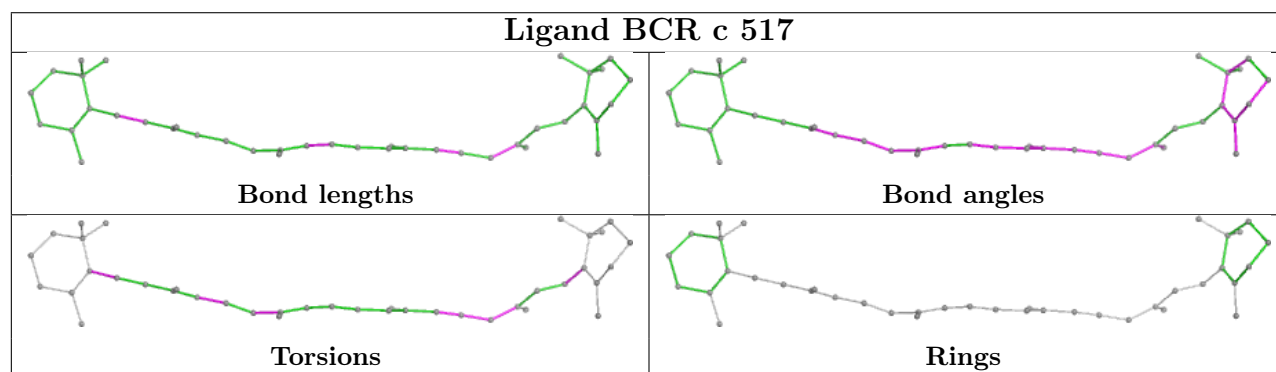
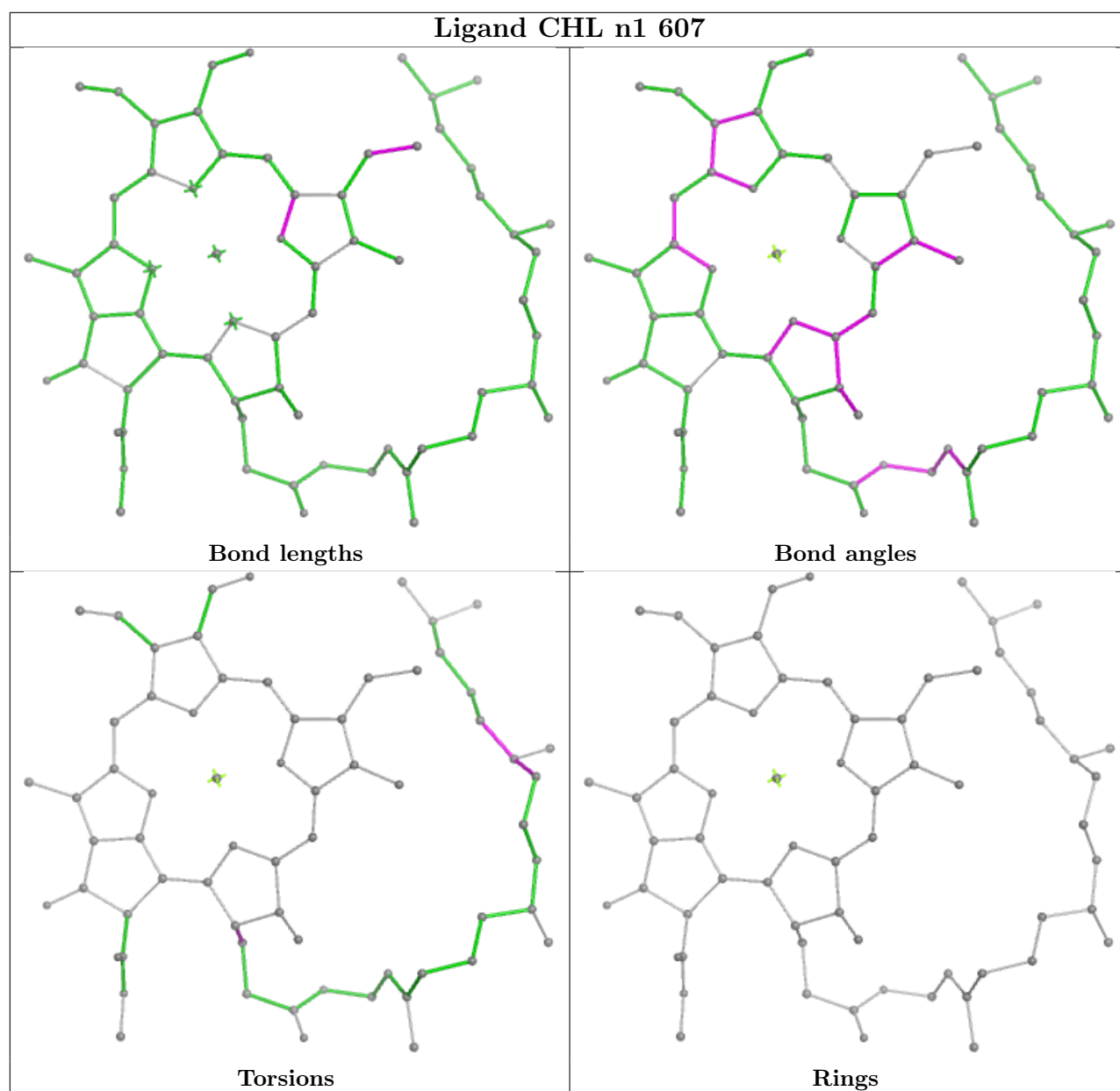
## Ligand CLA s 612

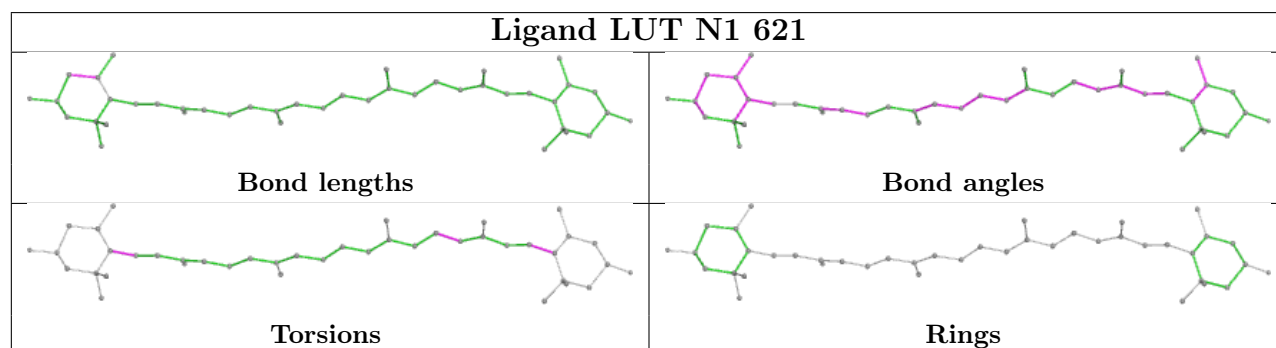
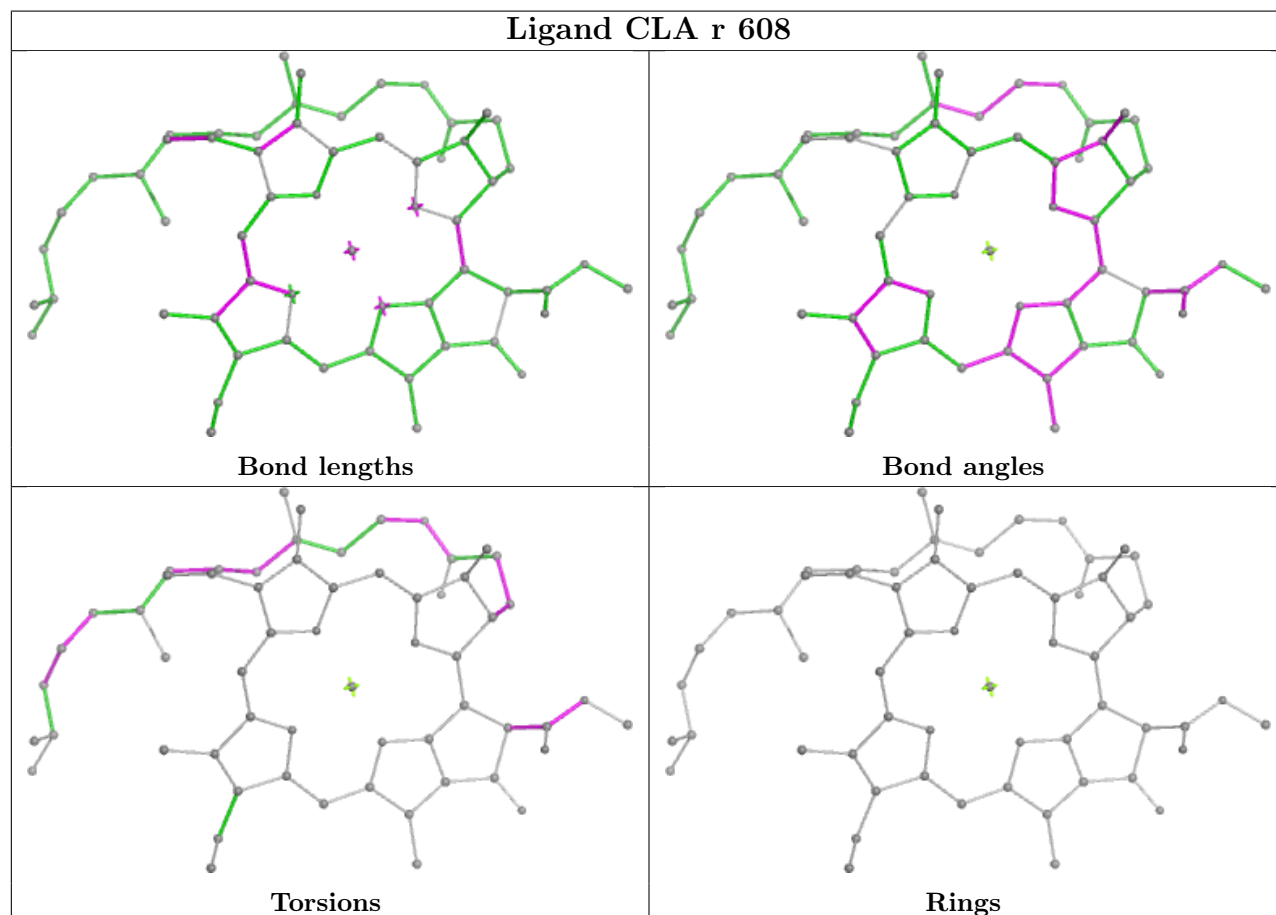
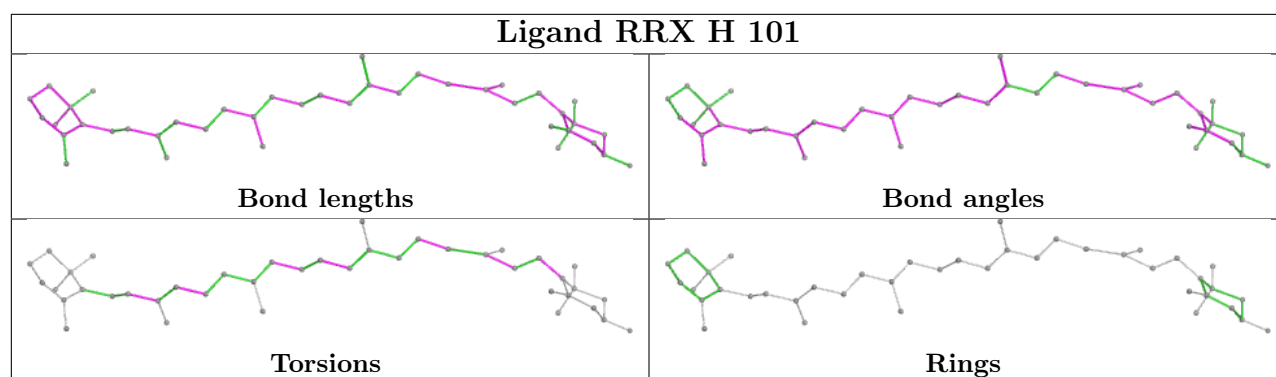


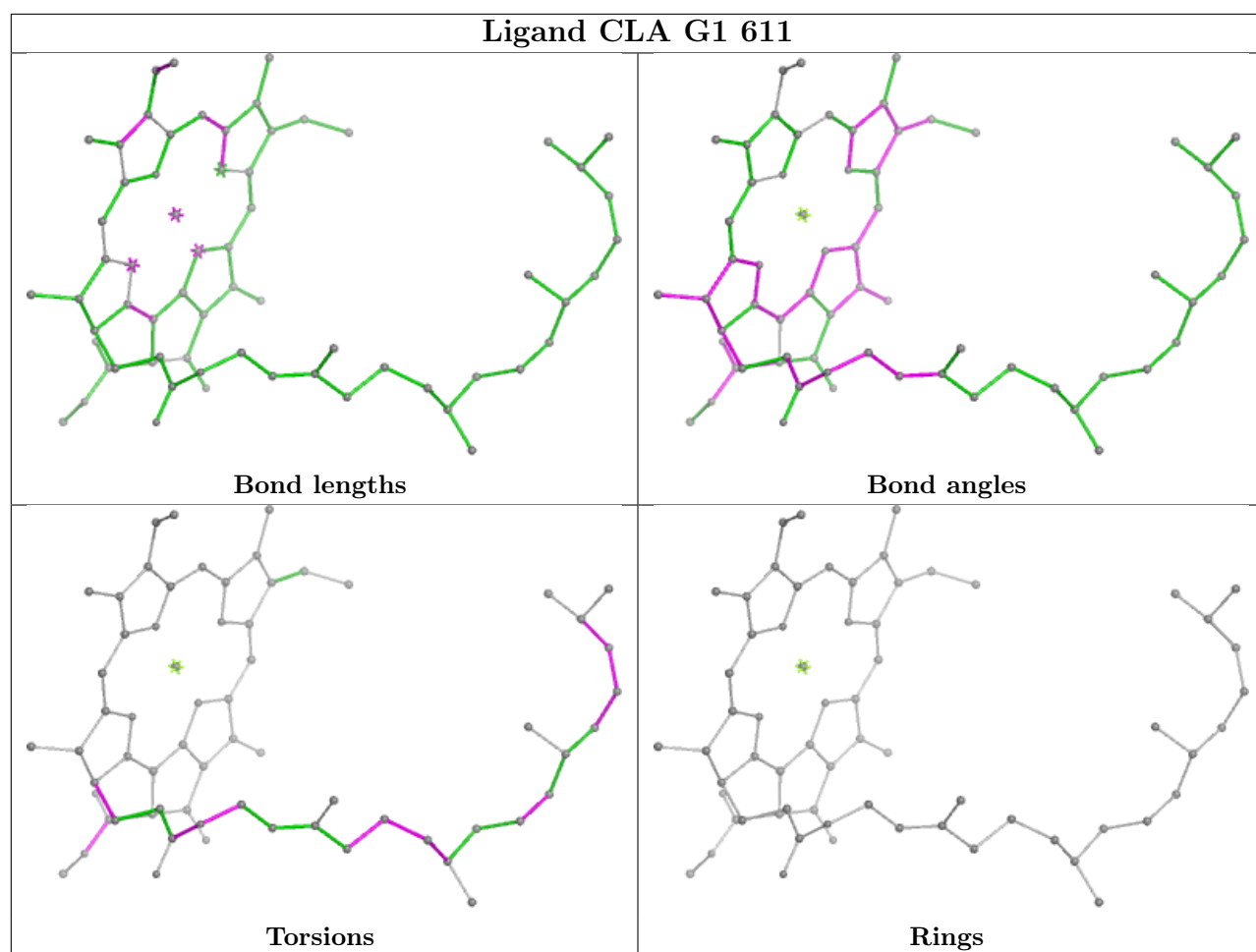
## Ligand SQD B1 626



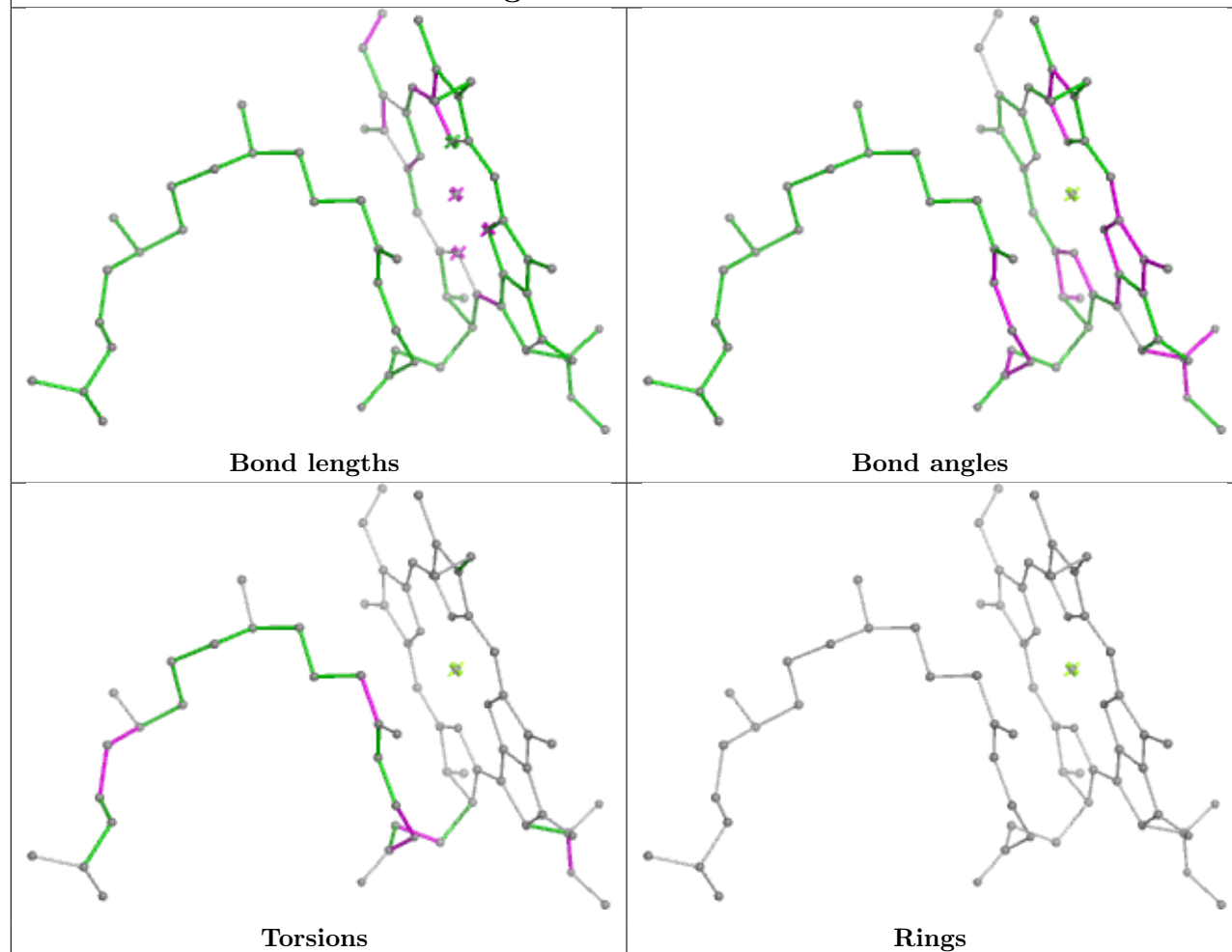
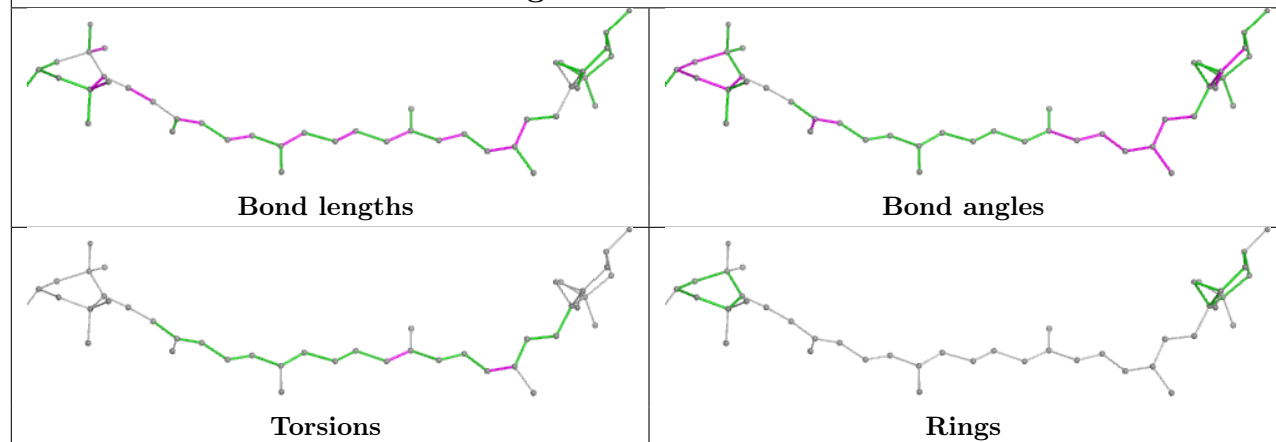


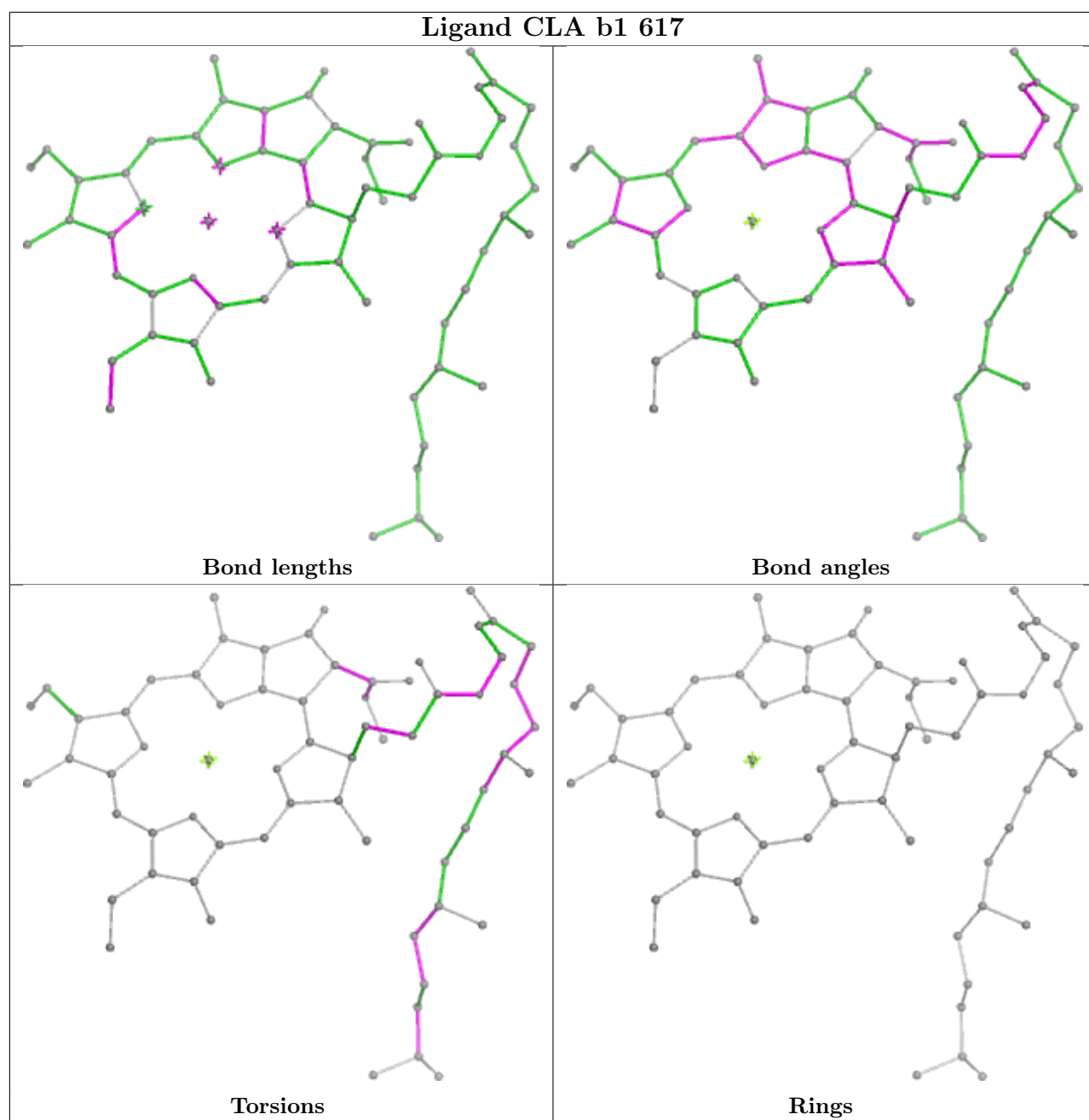


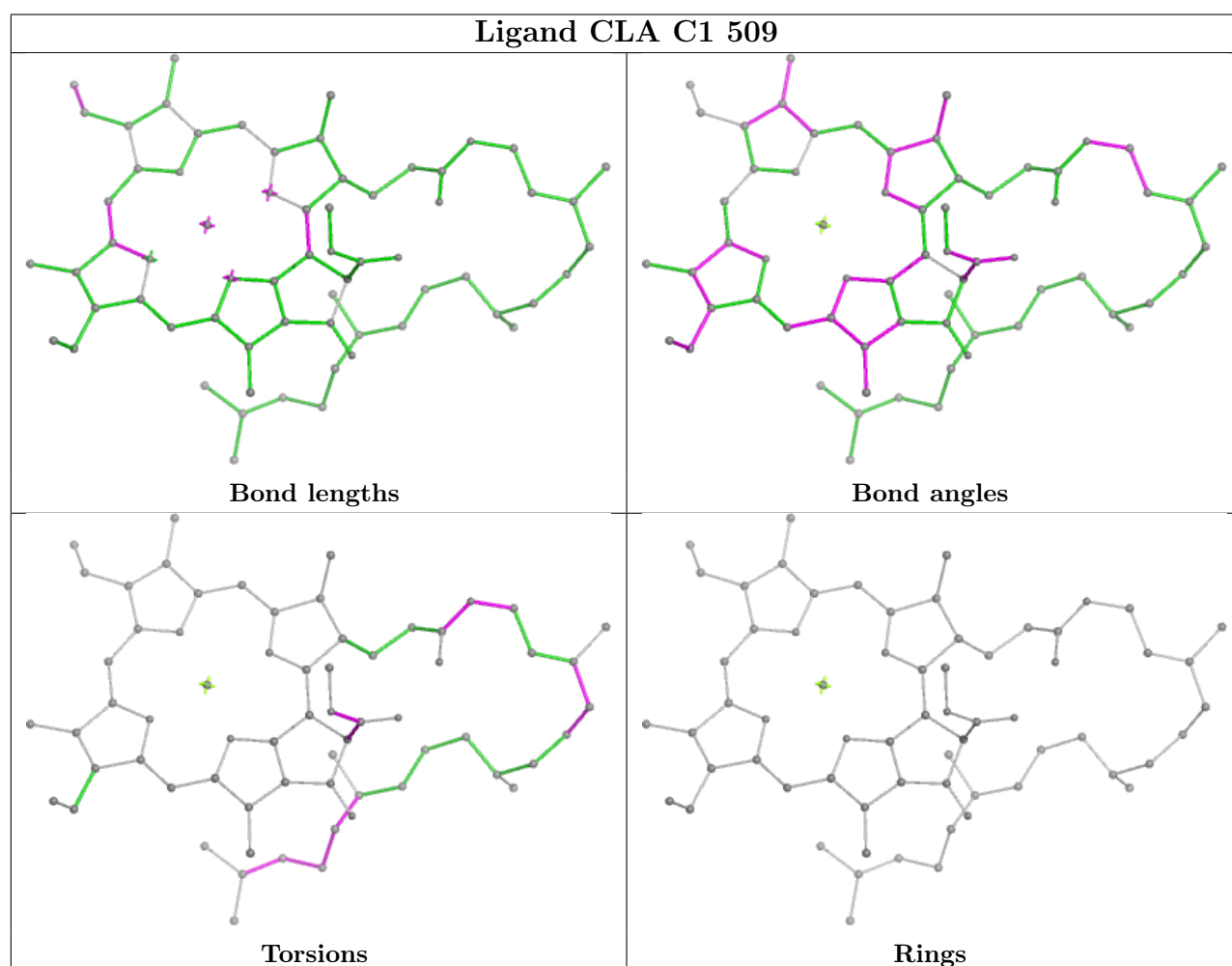
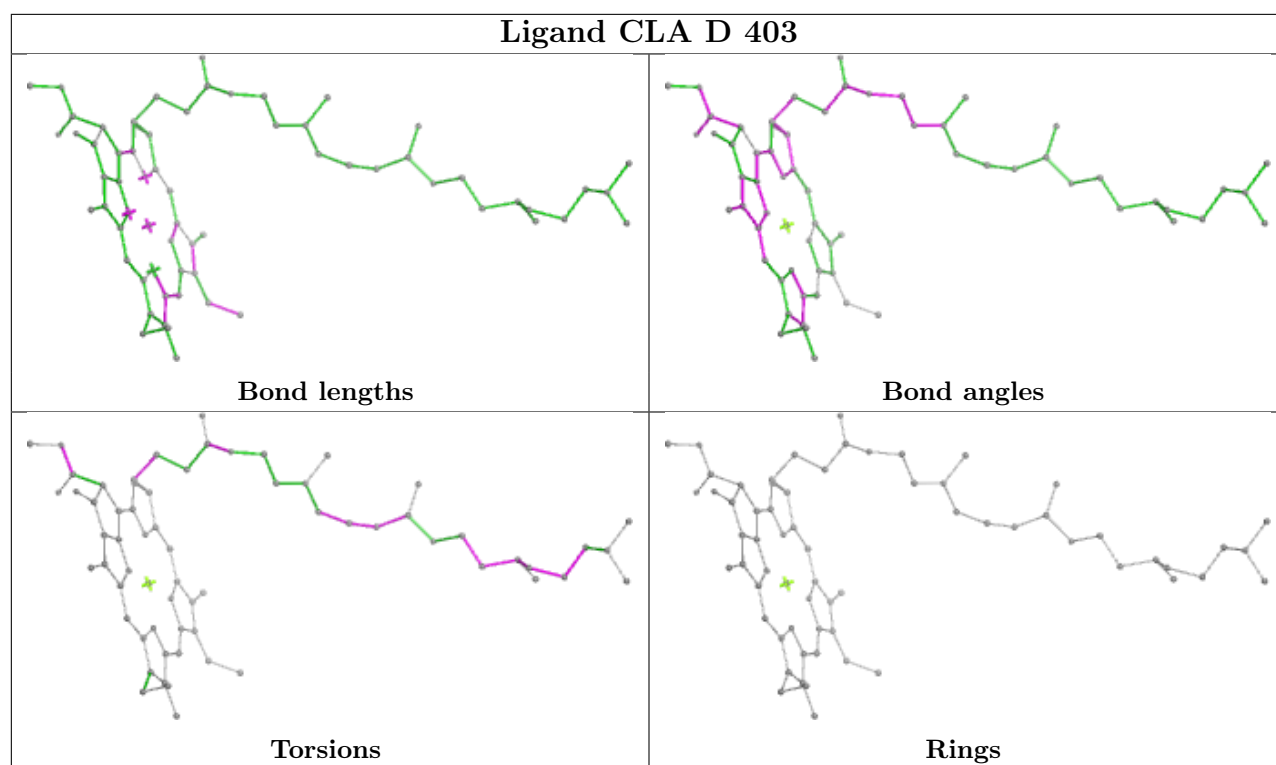




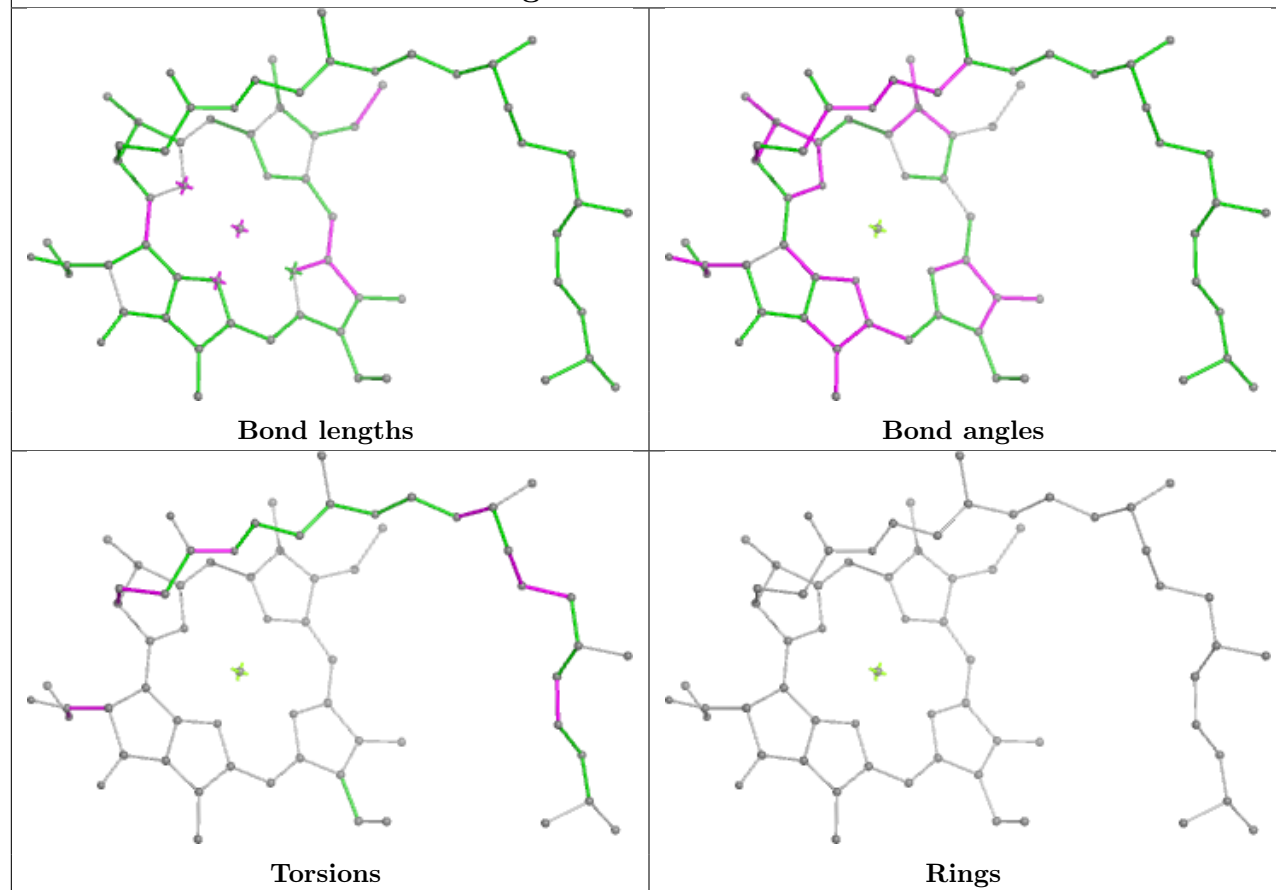


**Ligand CLA G1 613****Ligand NEX s1 623**

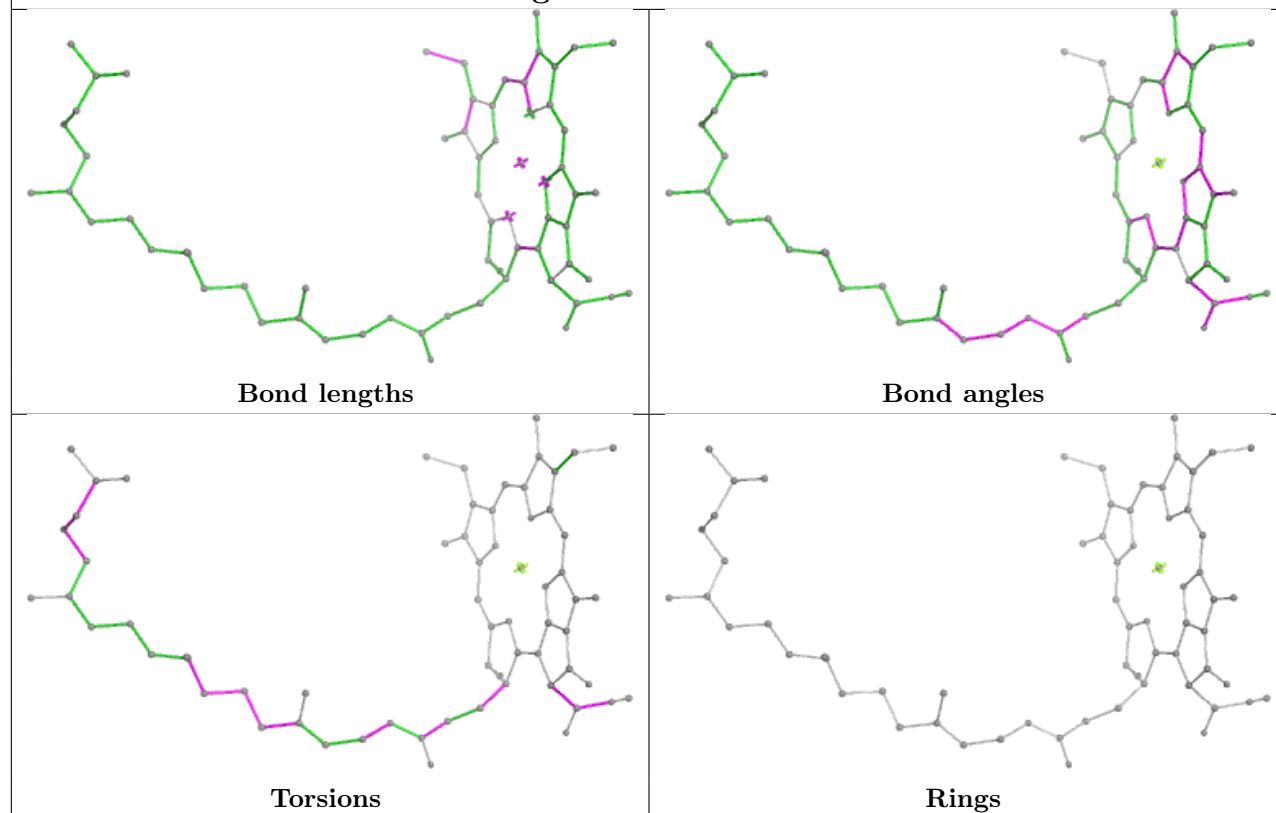


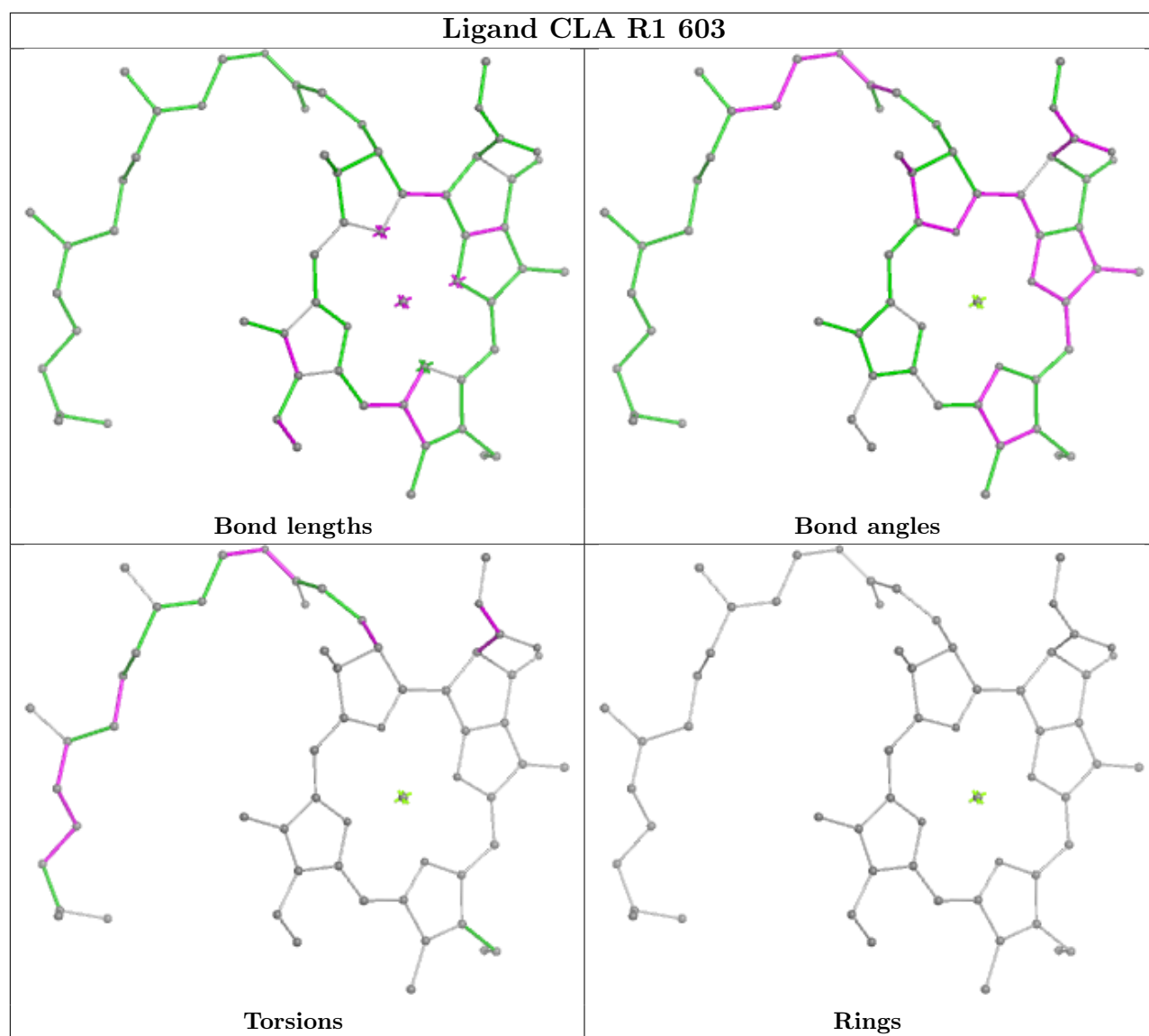


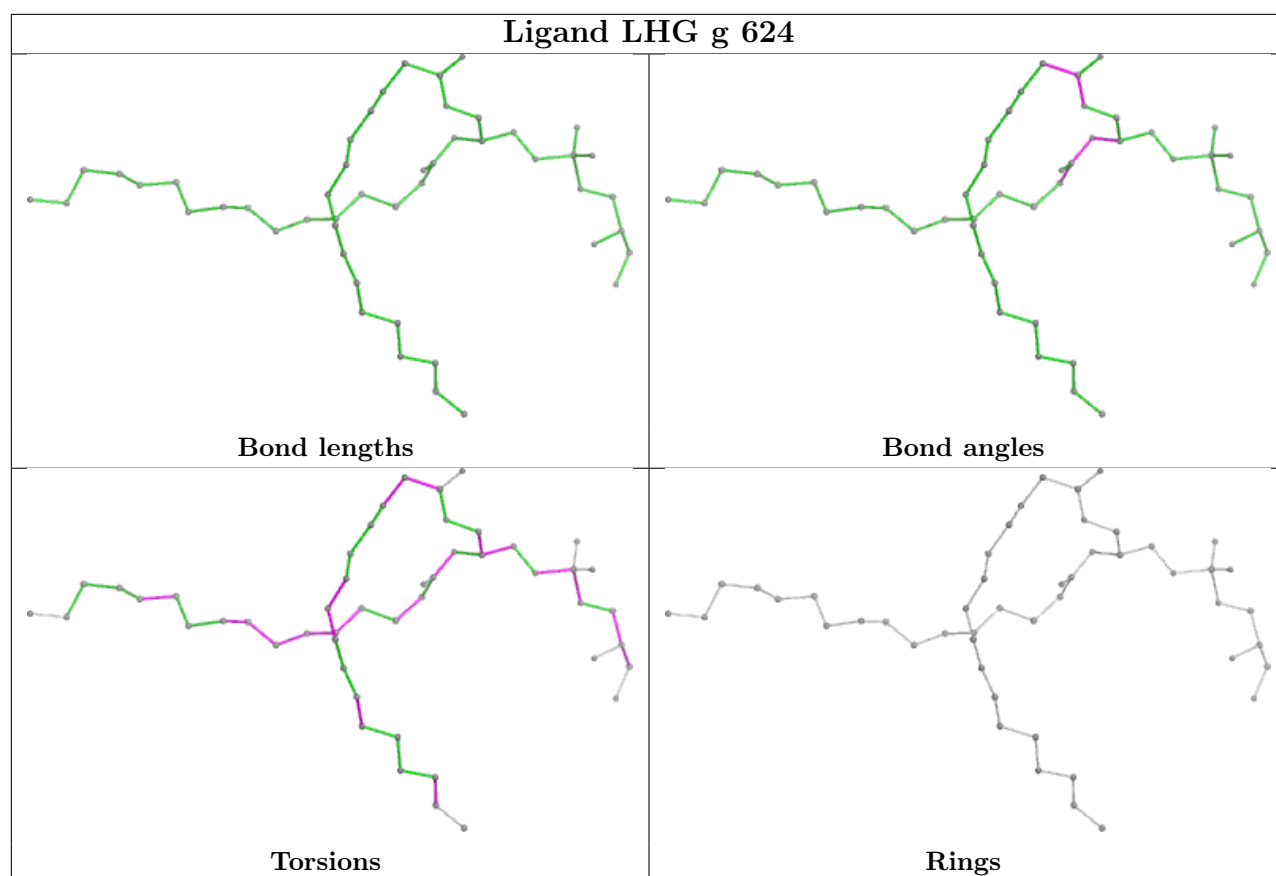
## Ligand CLA N1 602



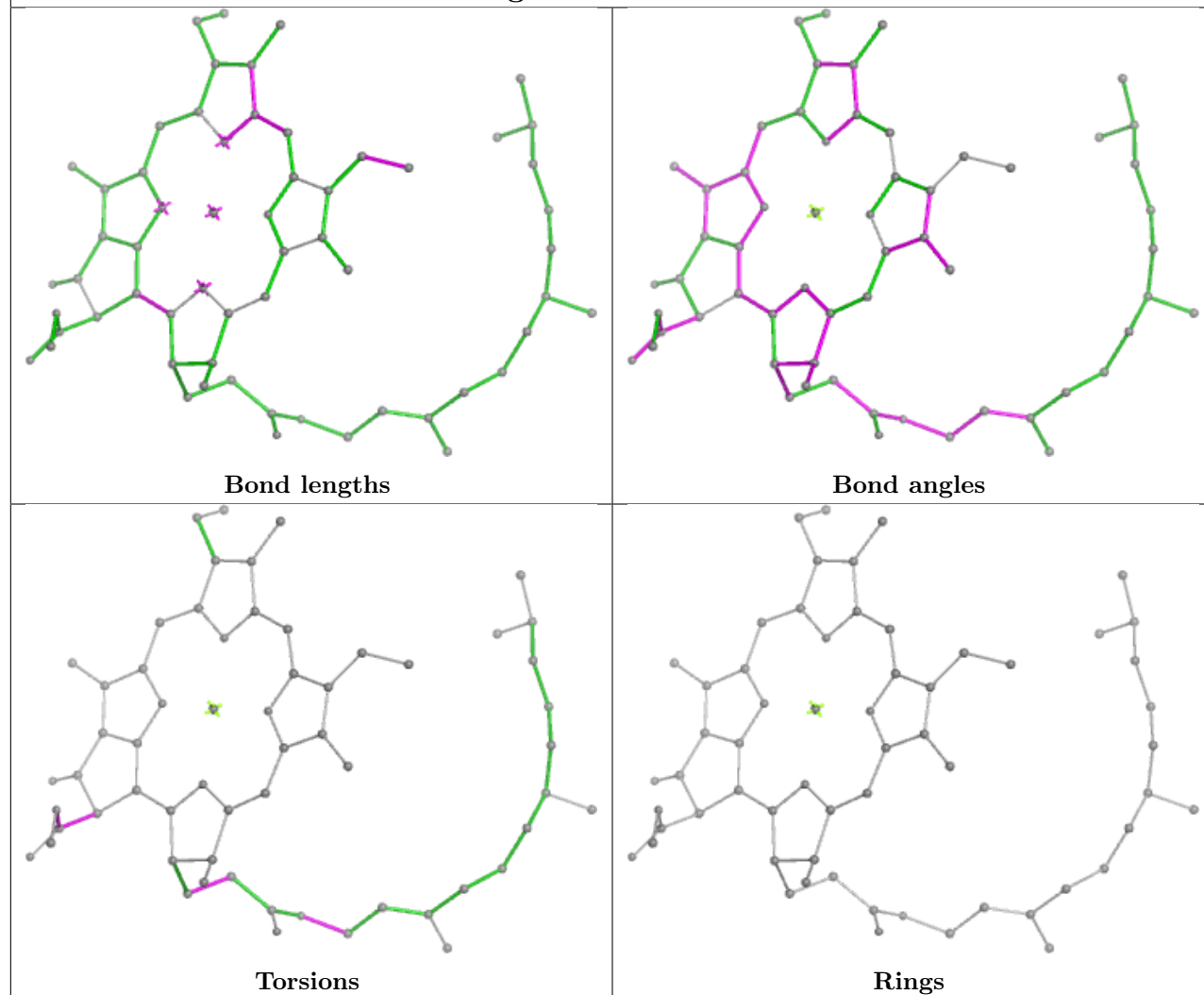
## Ligand CLA B 610

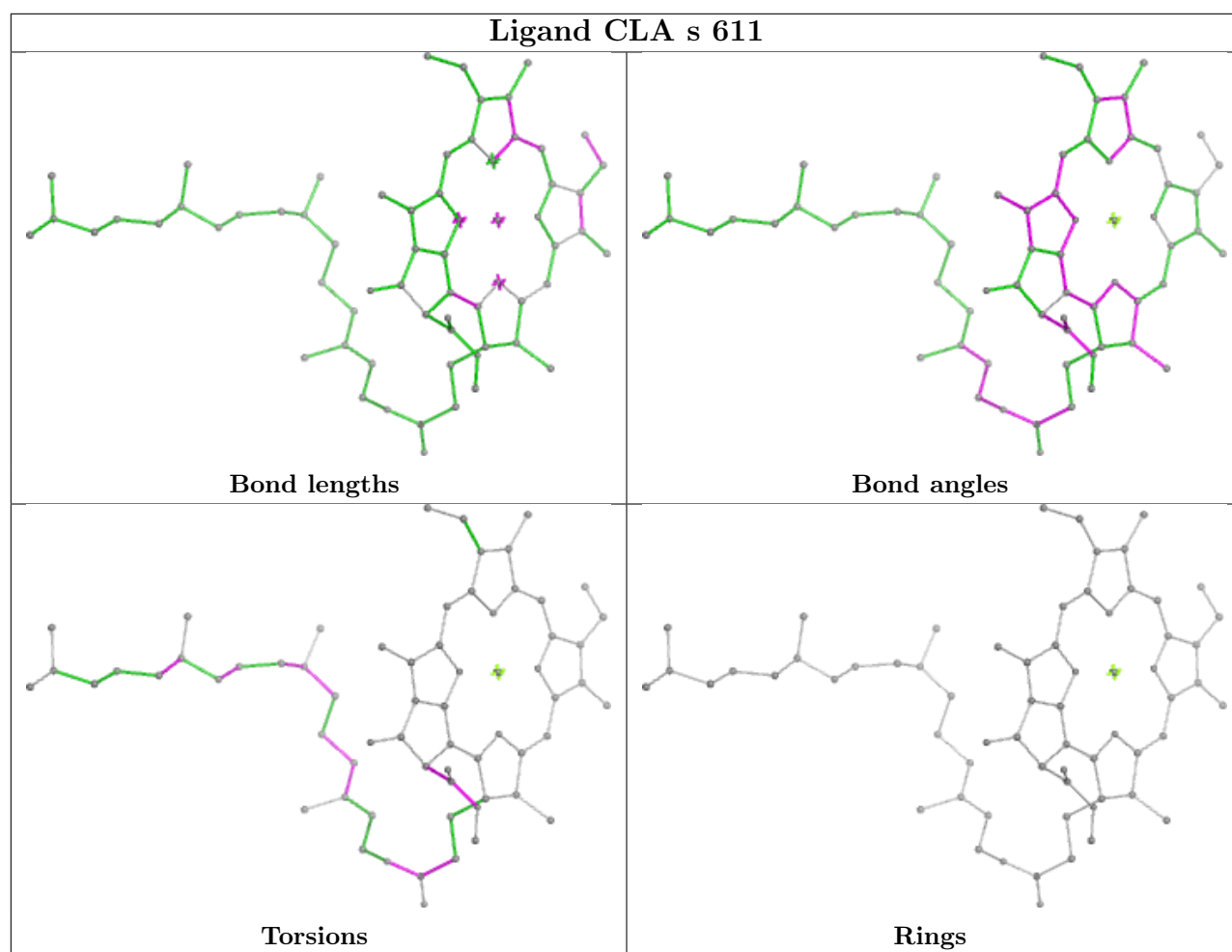






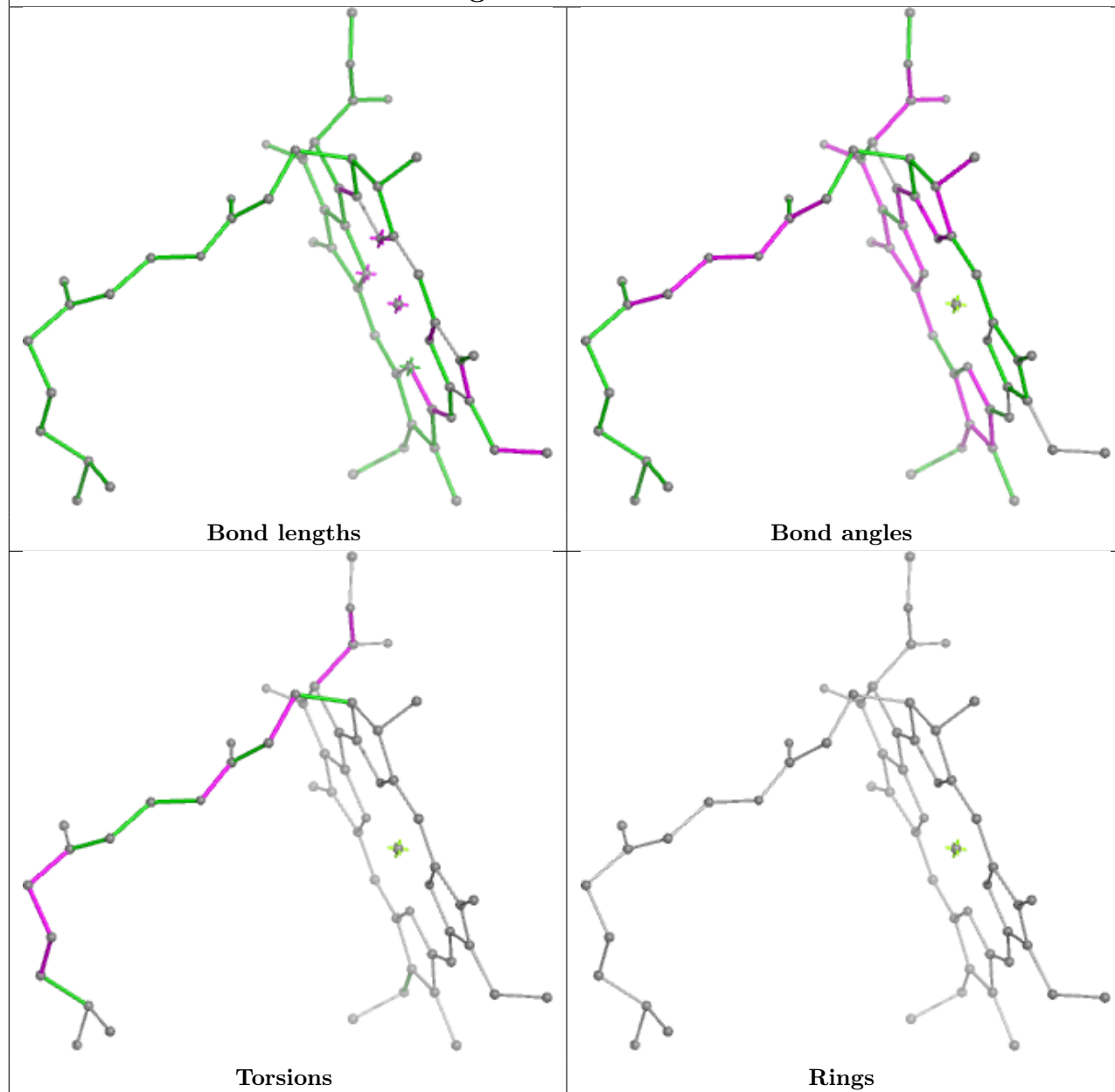
## Ligand CLA r 602



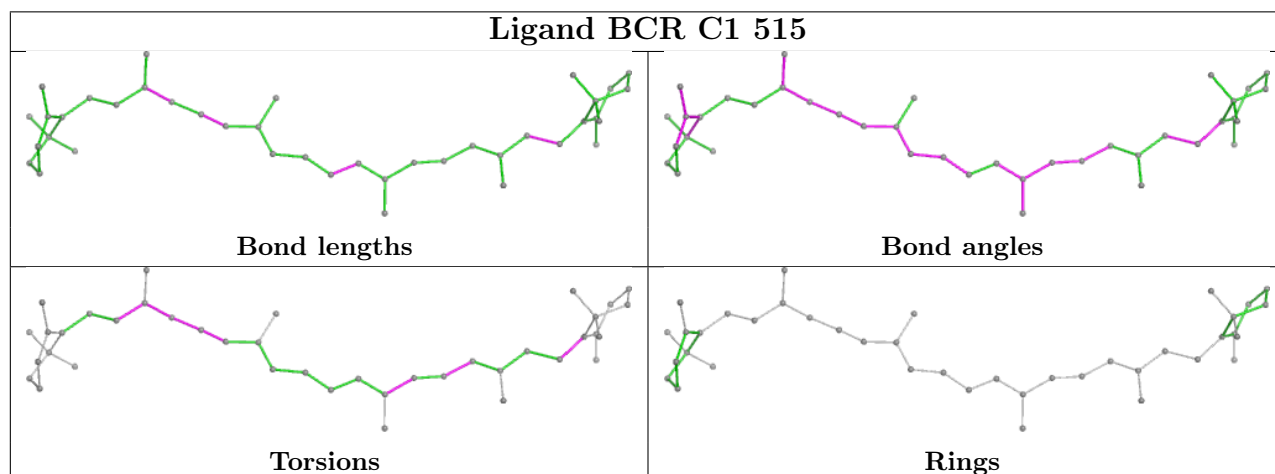


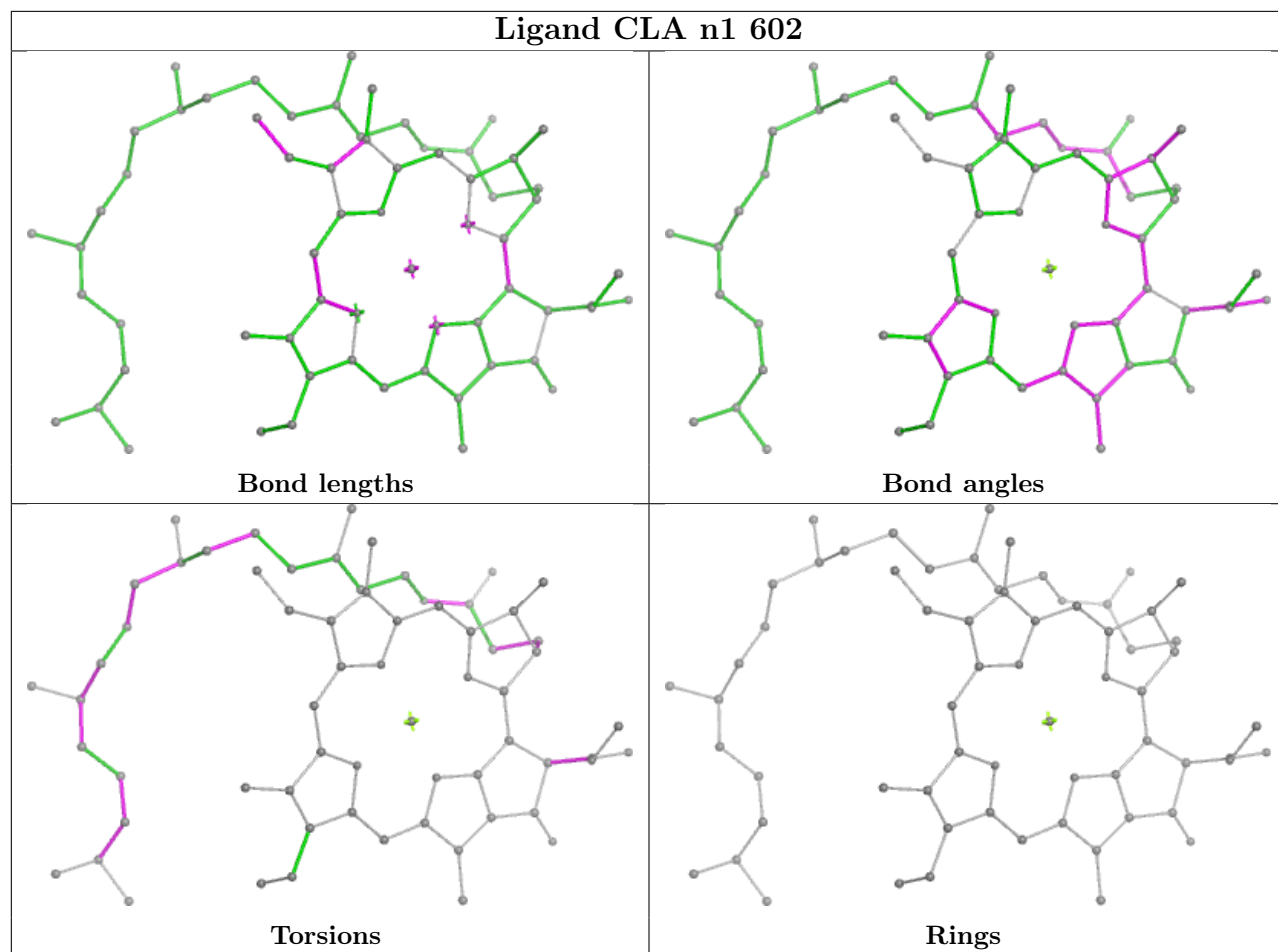


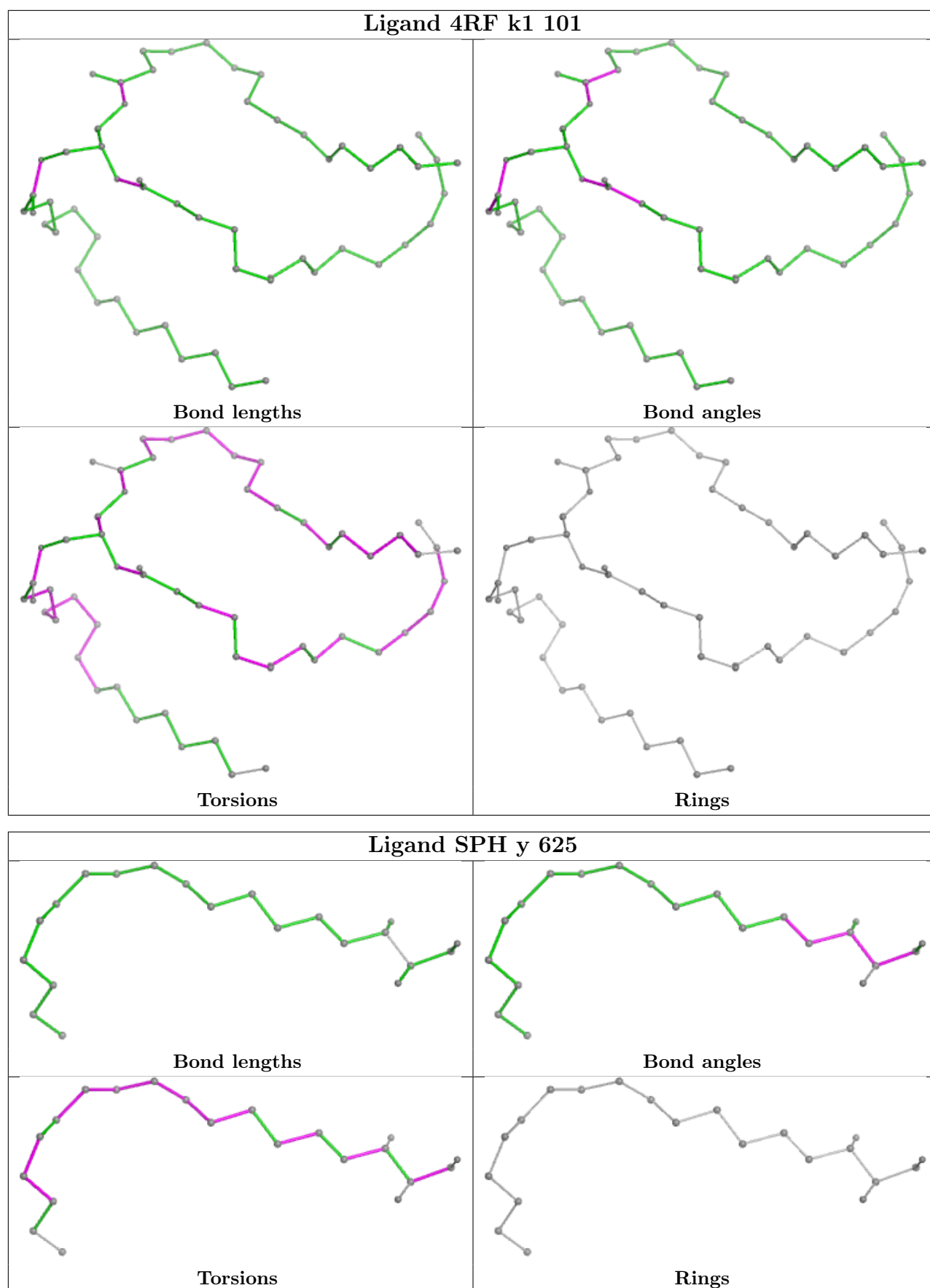
## Ligand CLA s 604



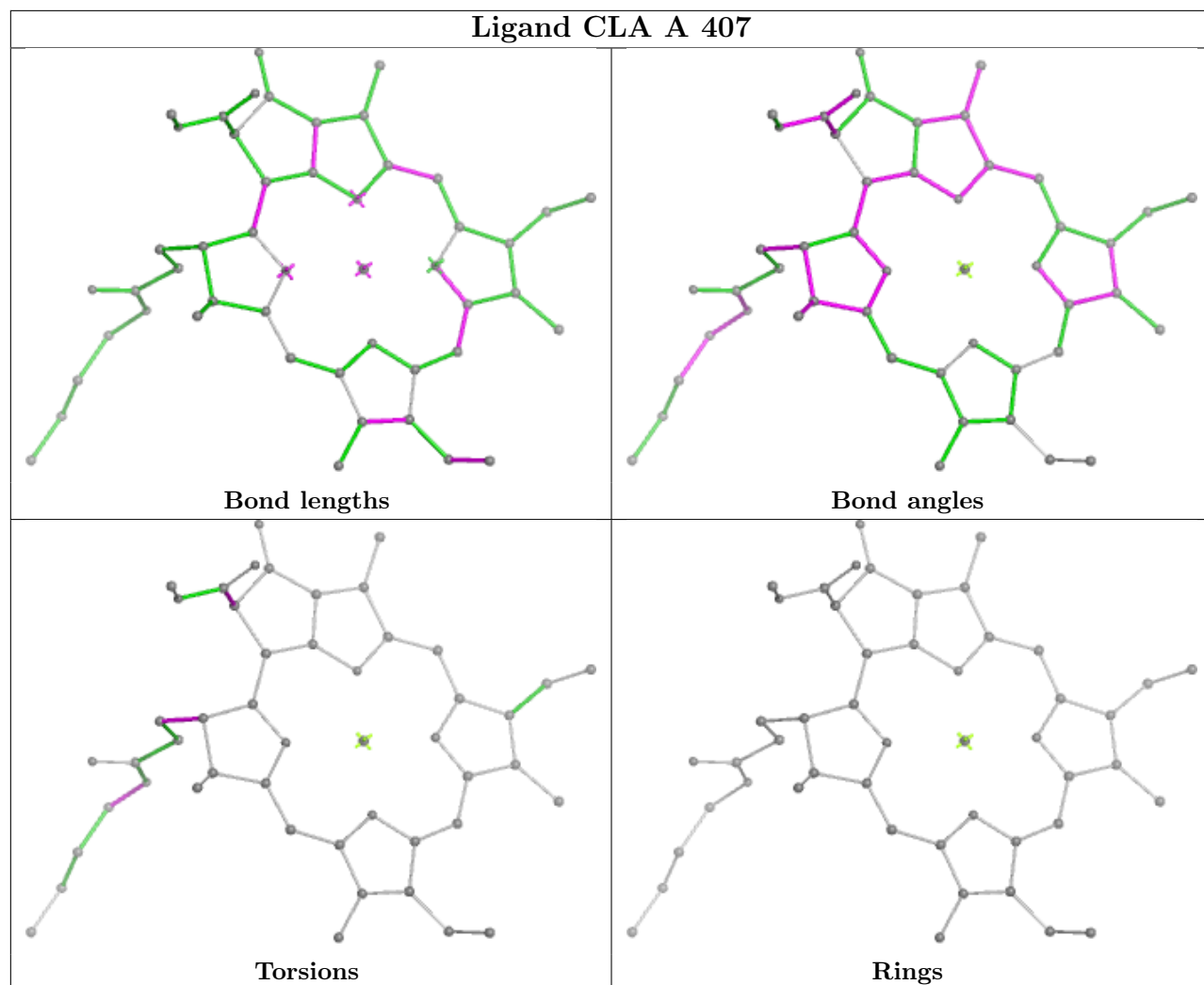
## Ligand BCR C1 515

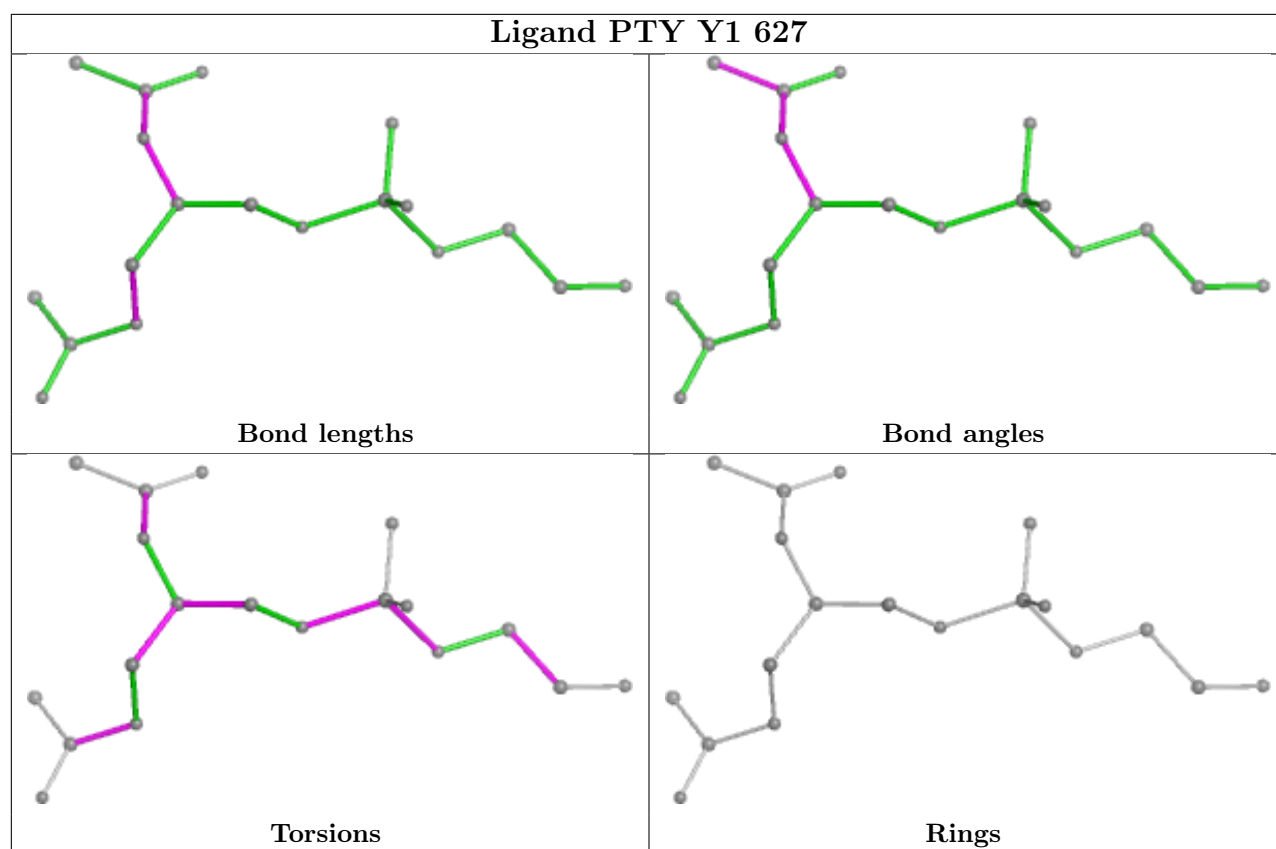


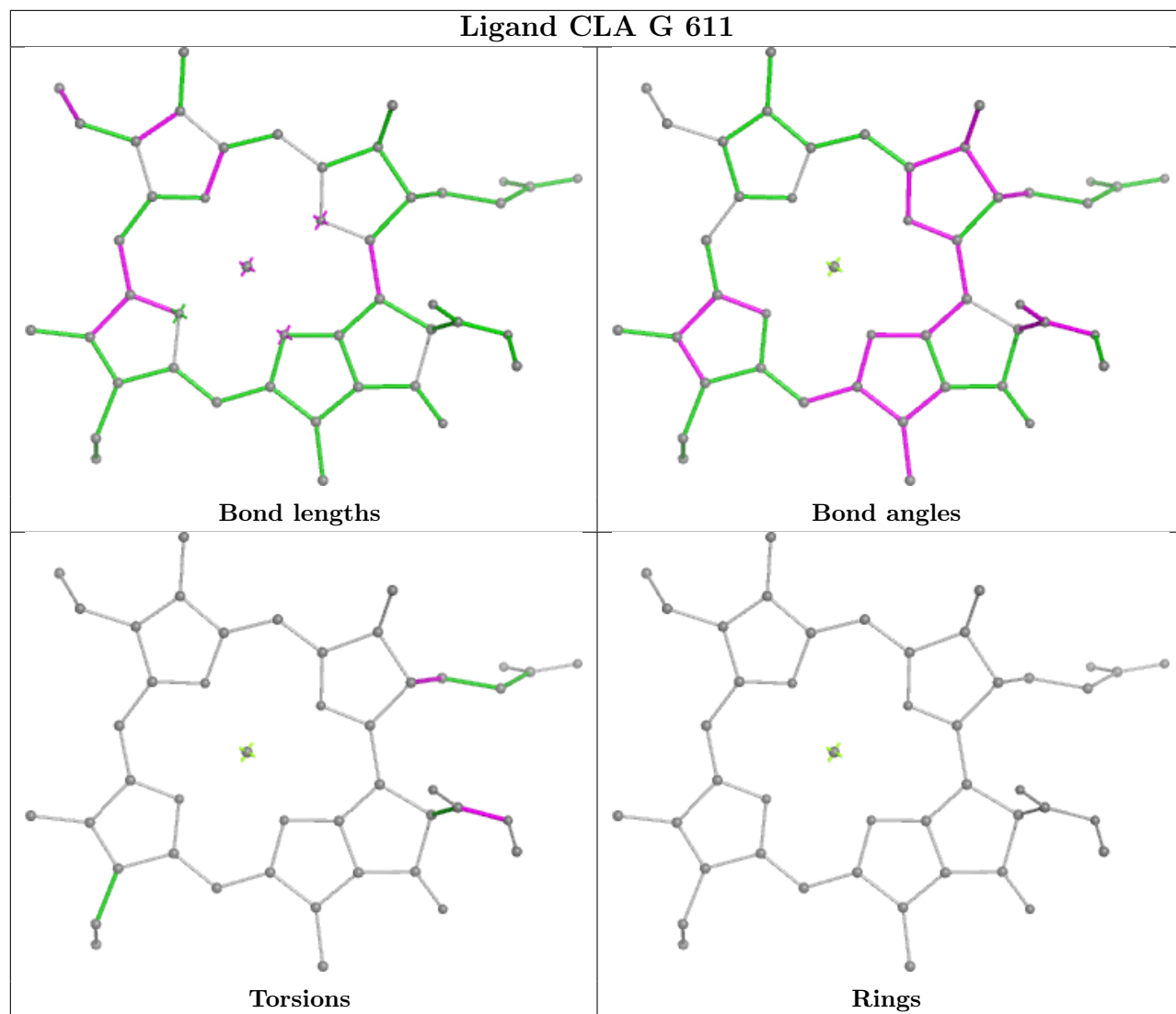


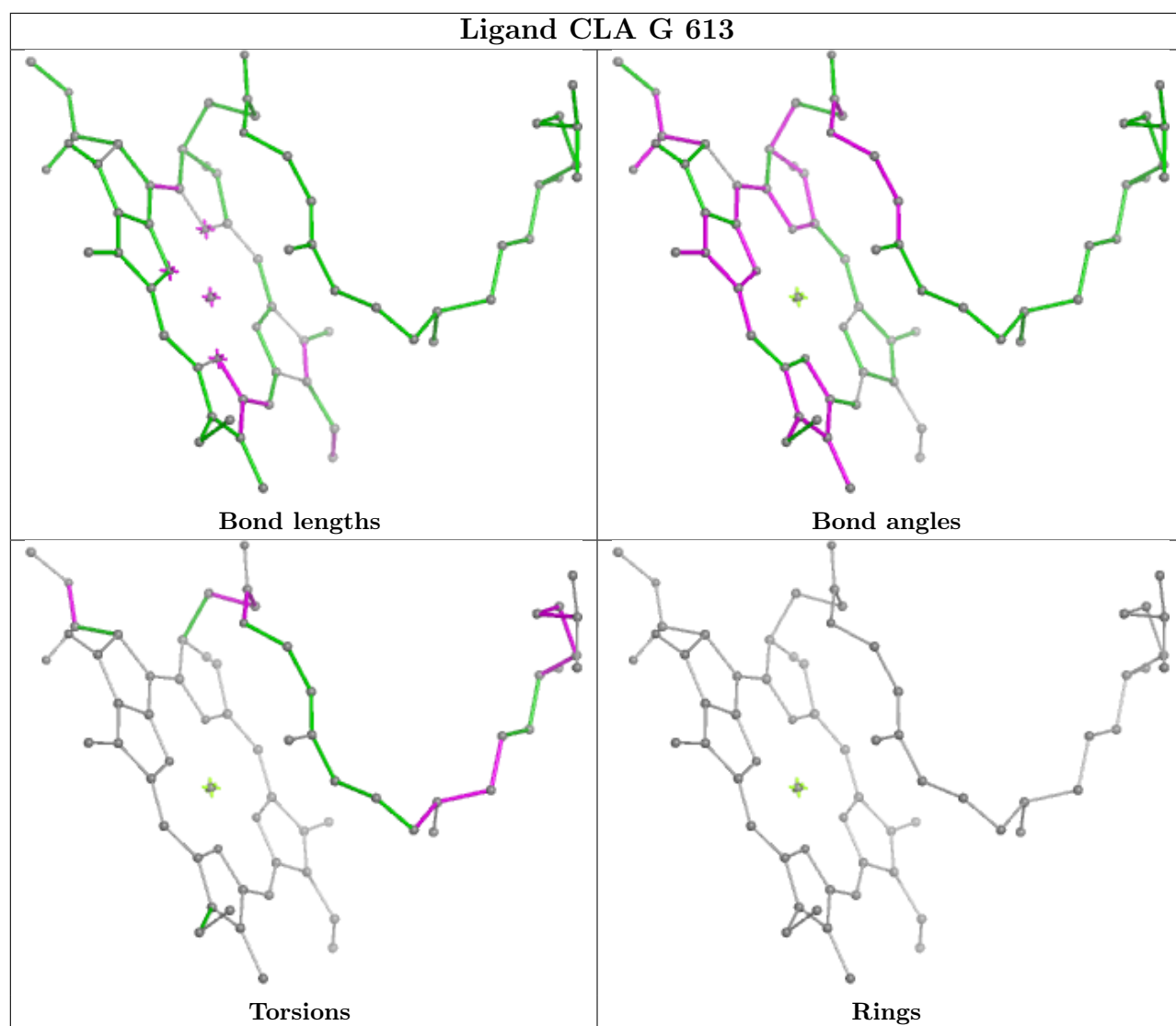


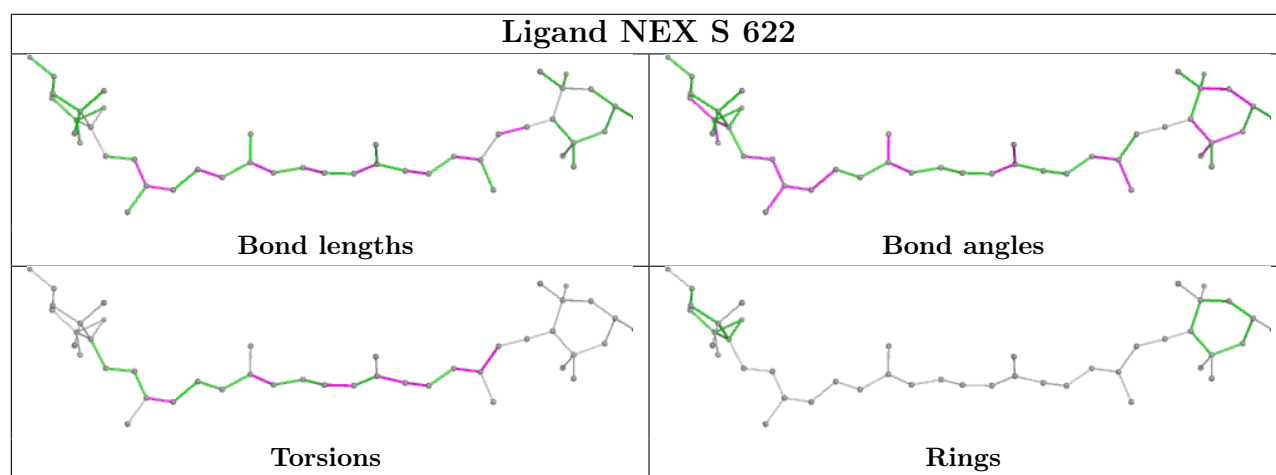
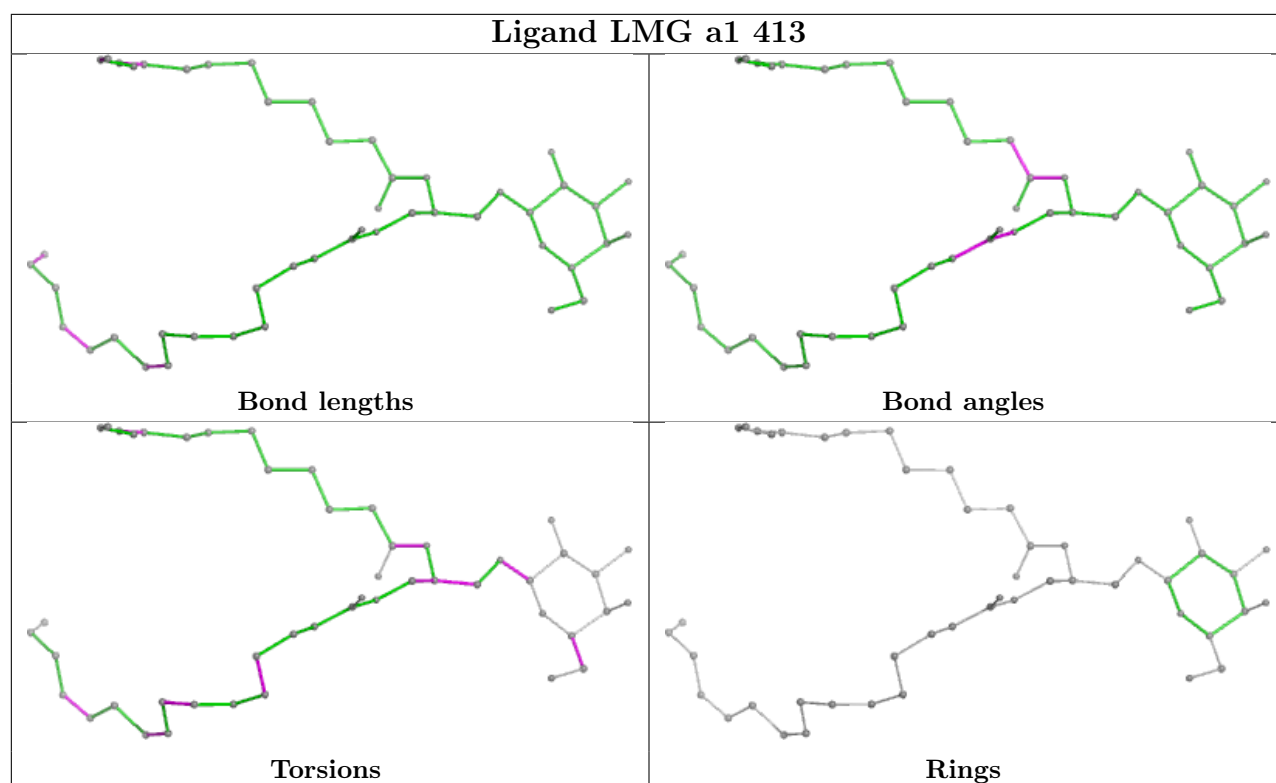
## Ligand CLA A 407



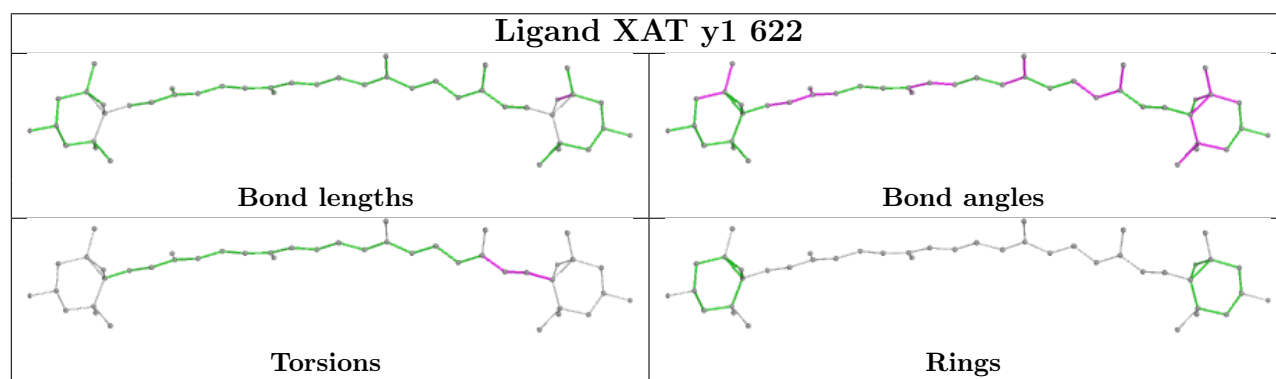
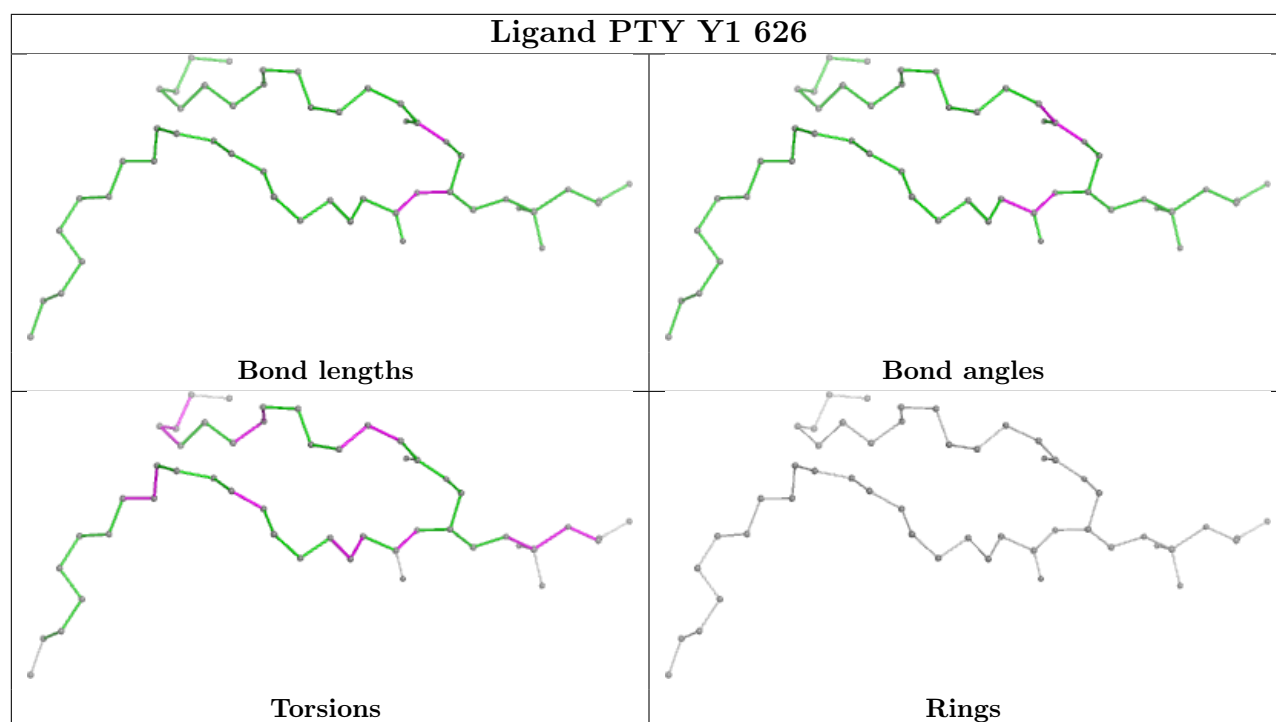


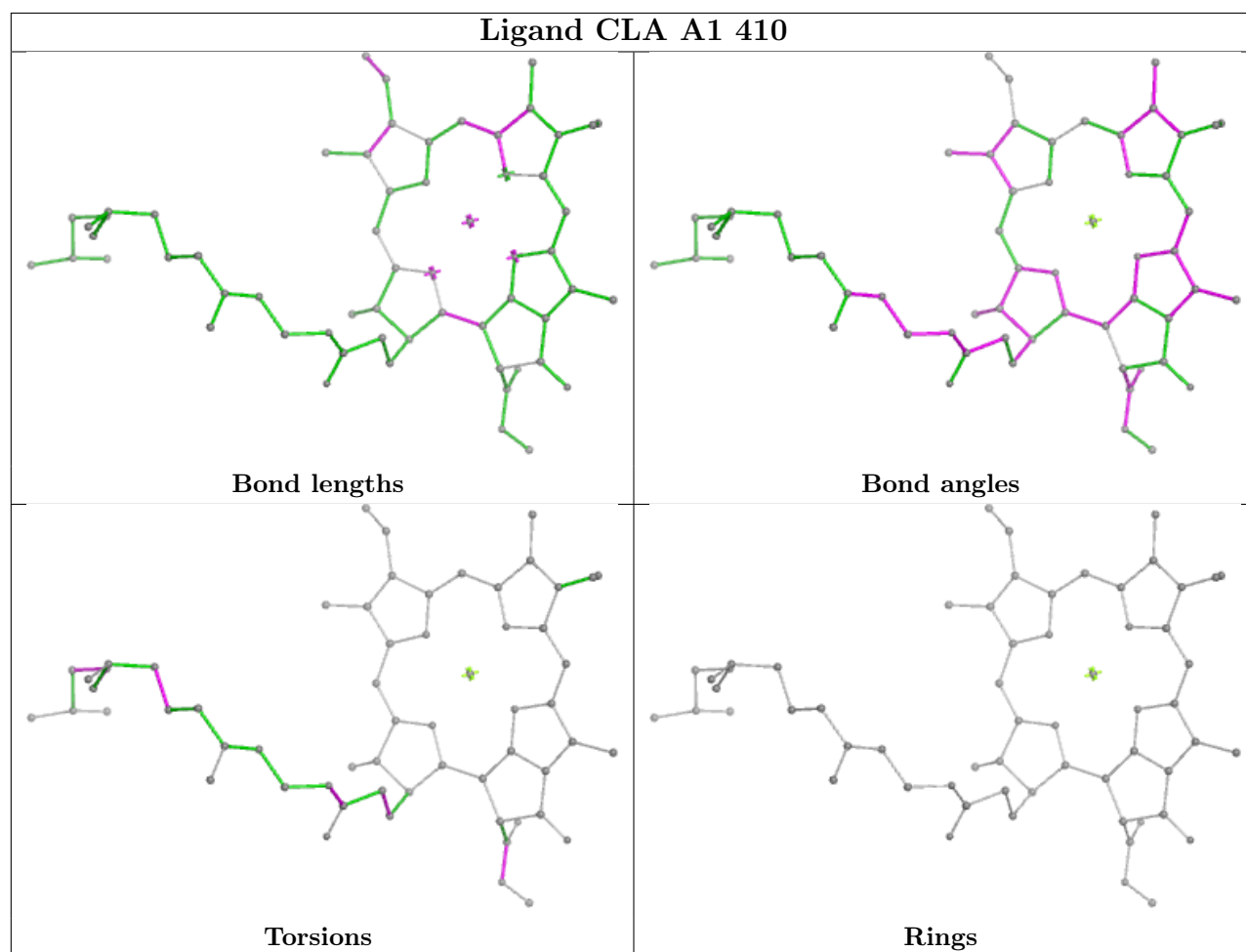
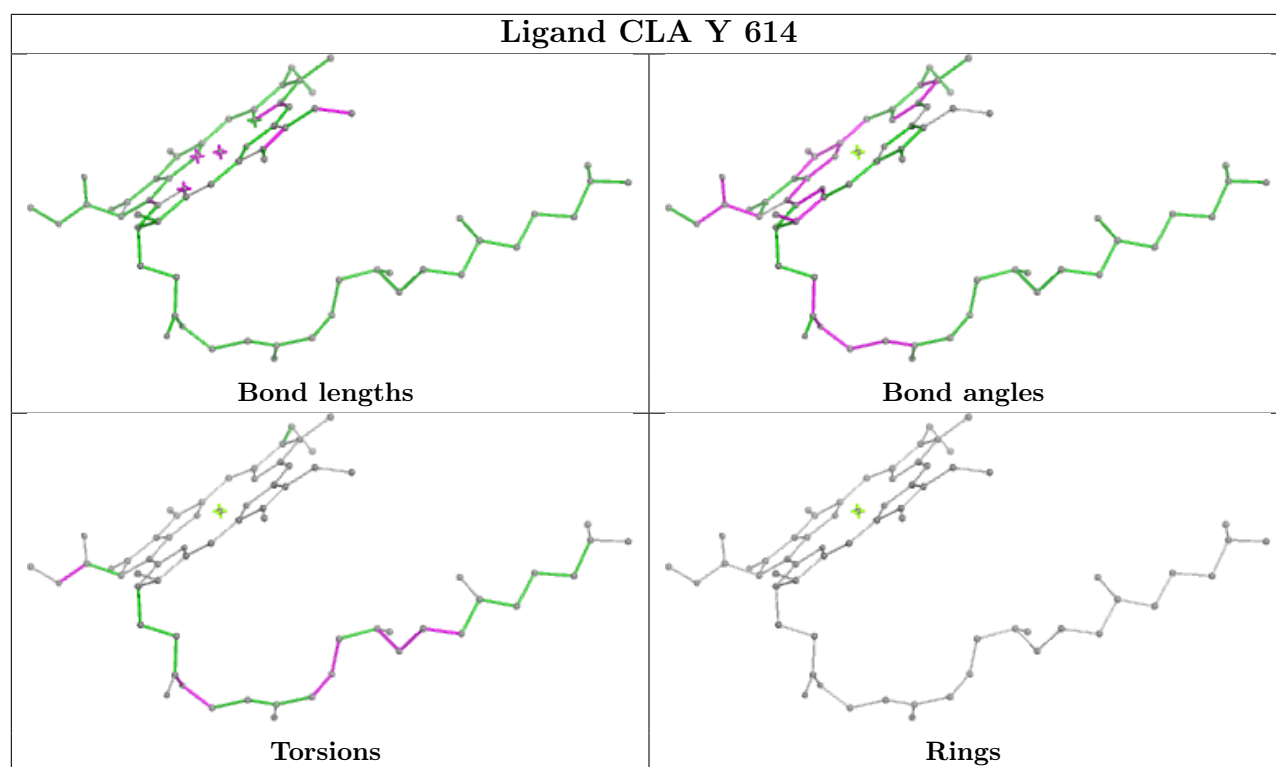


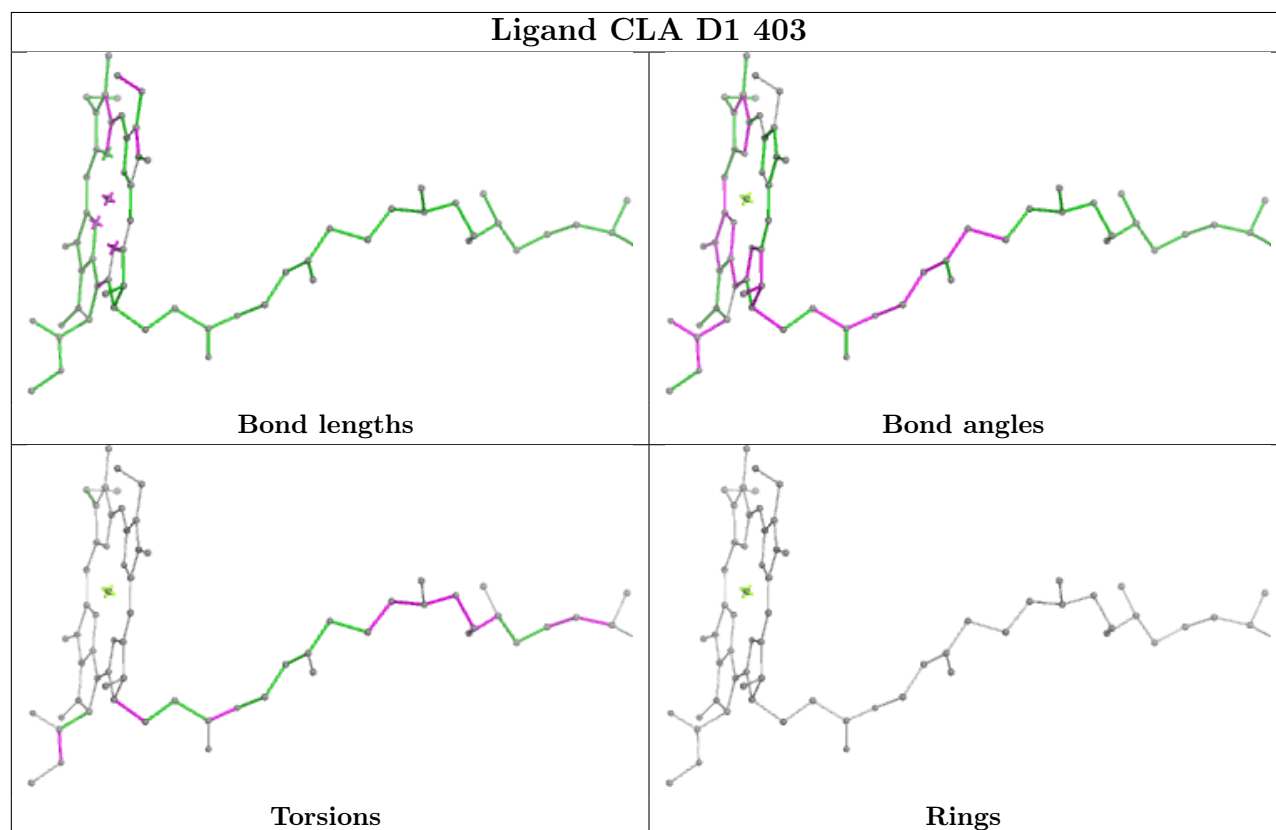
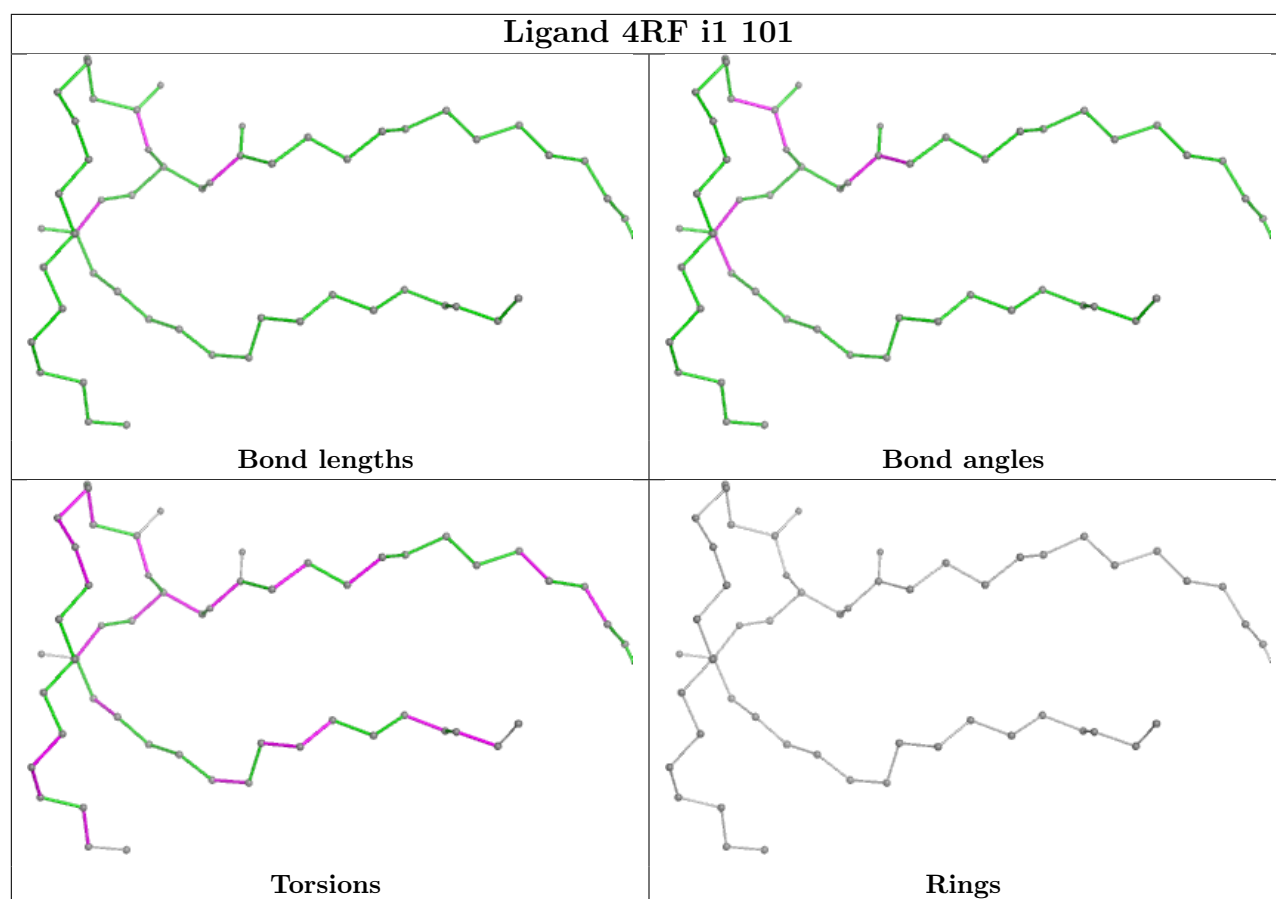


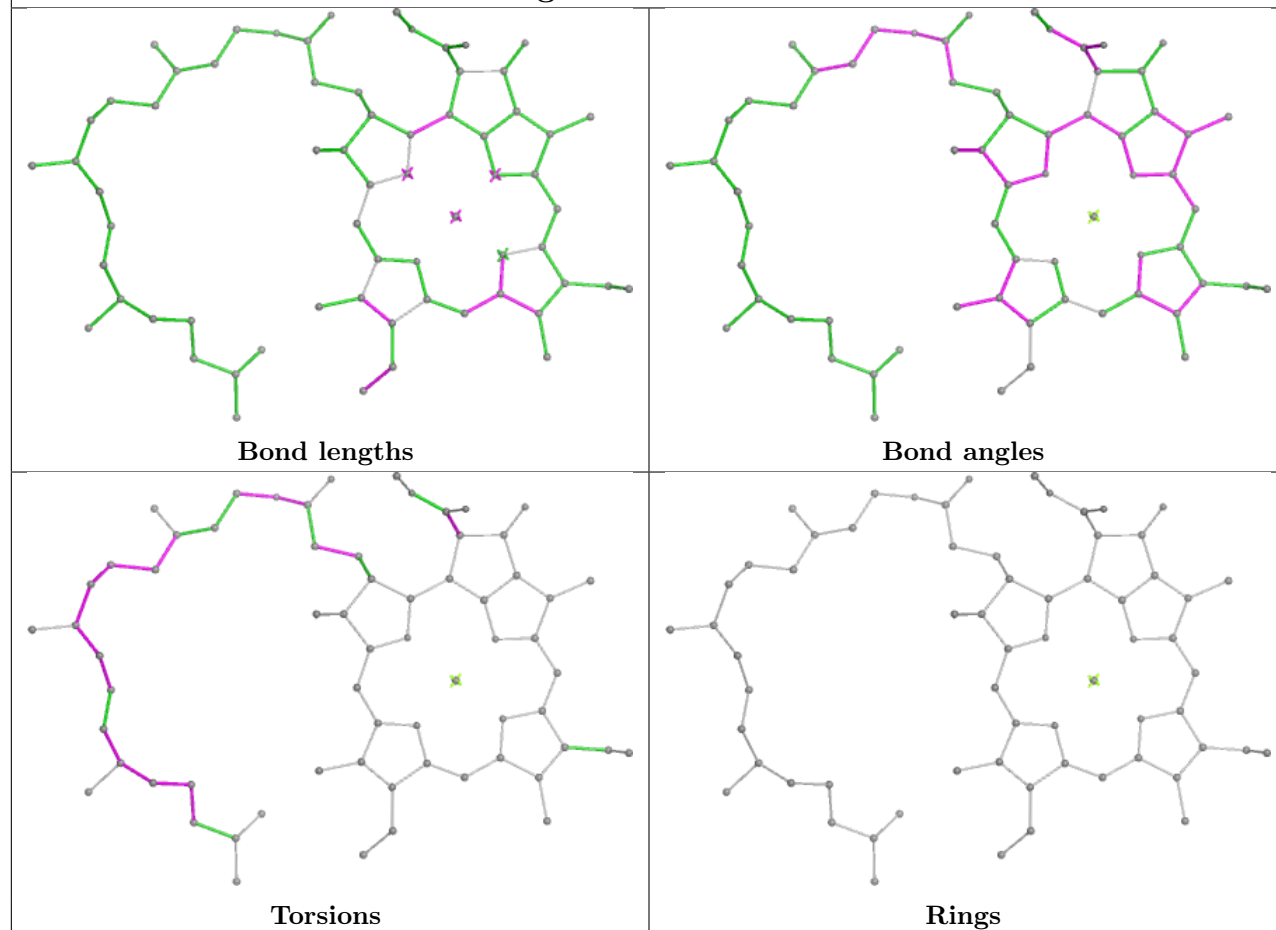
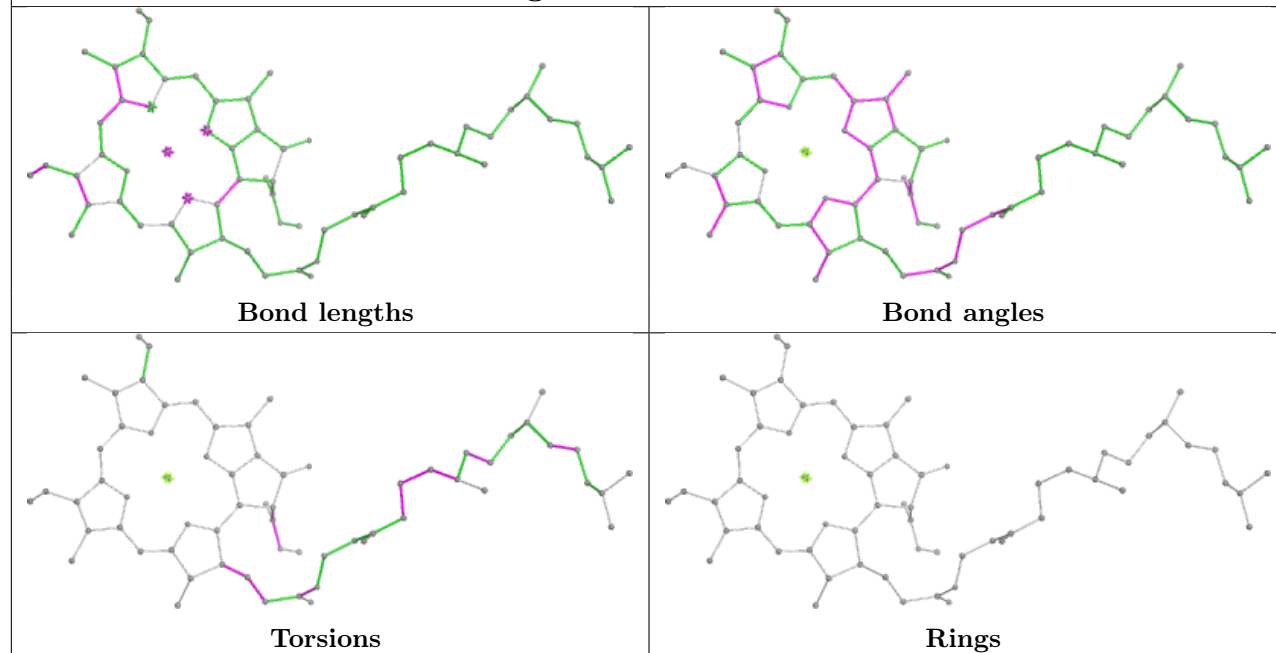




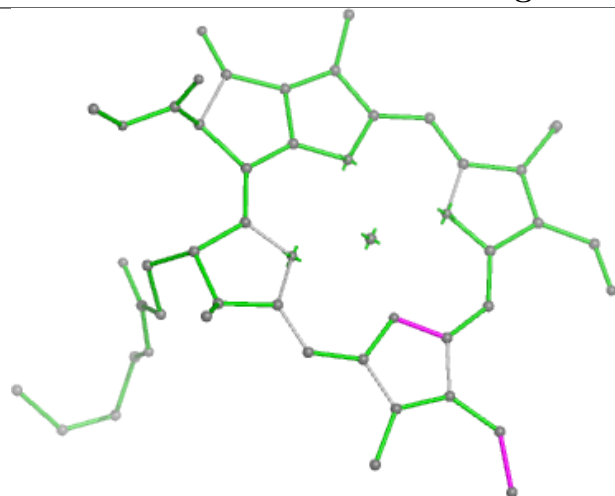




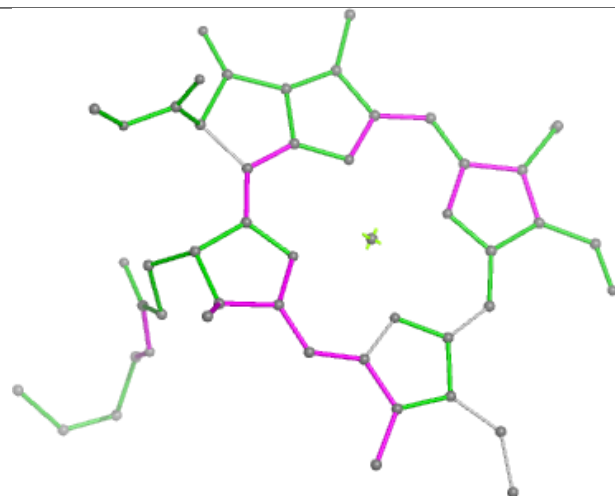


**Ligand CLA c 512****Ligand CLA b1 603**

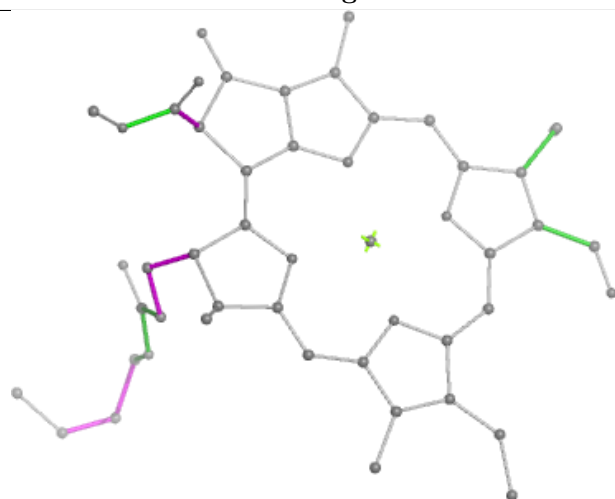
## Ligand CHL N 608



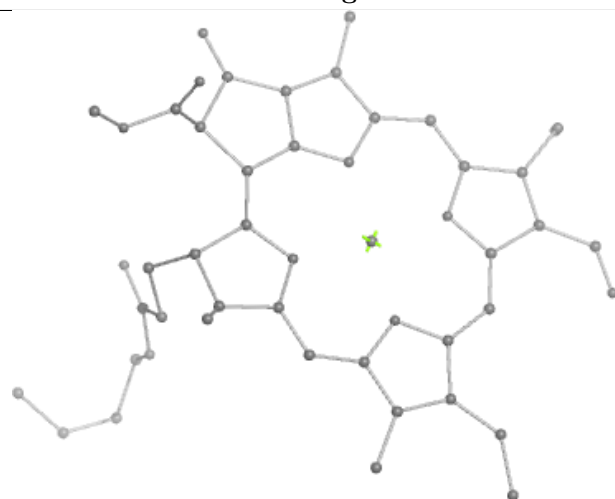
Bond lengths



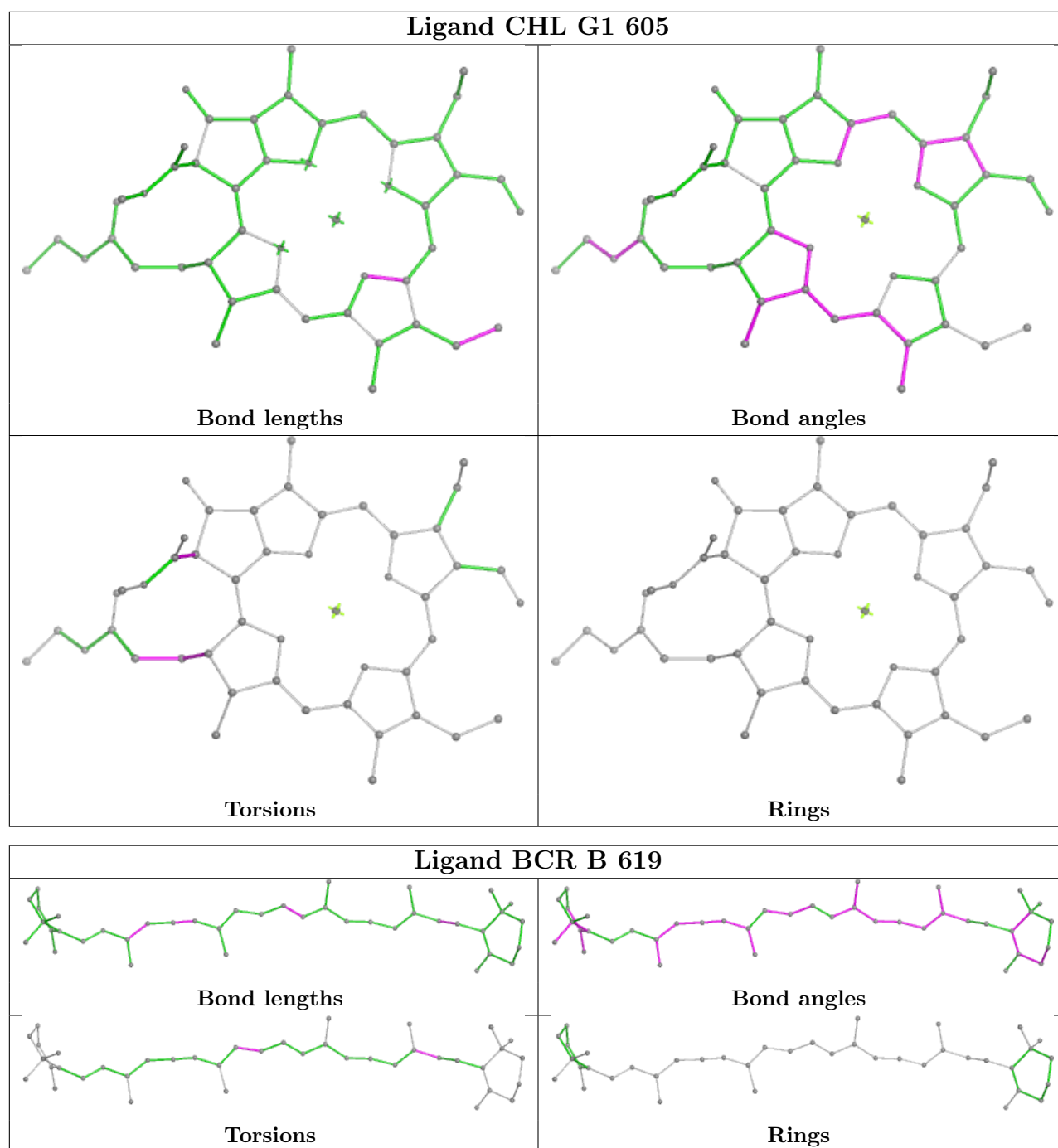
Bond angles

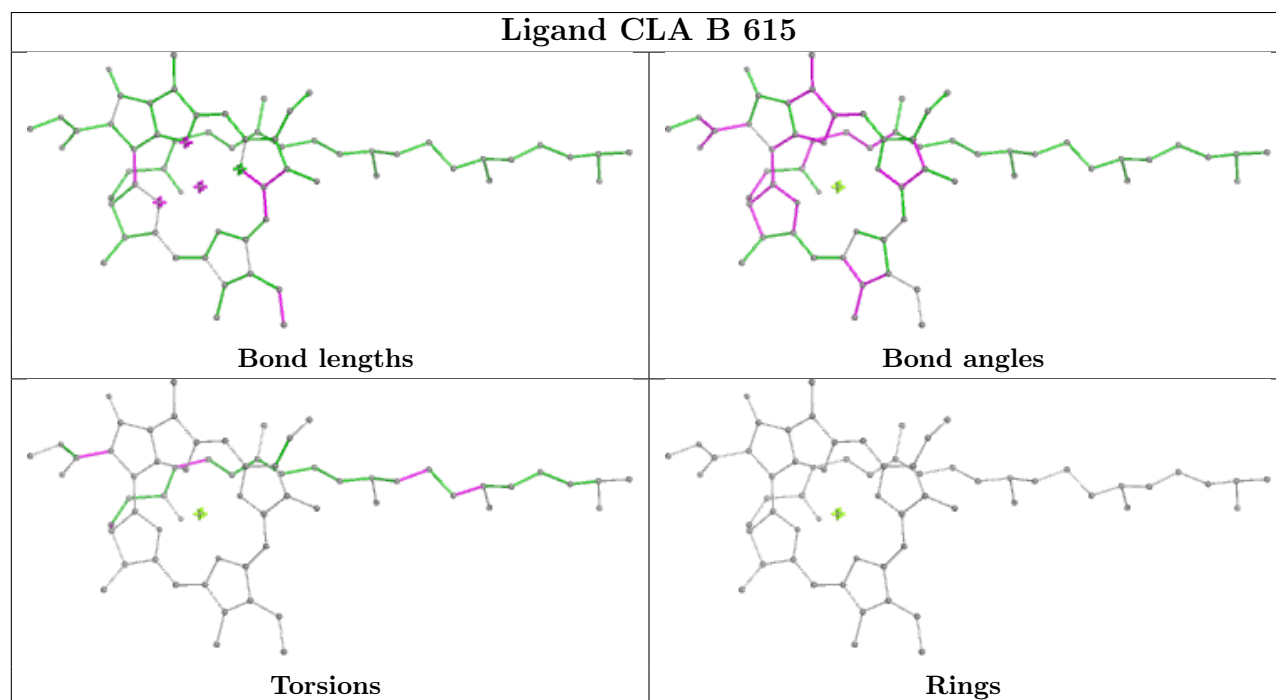
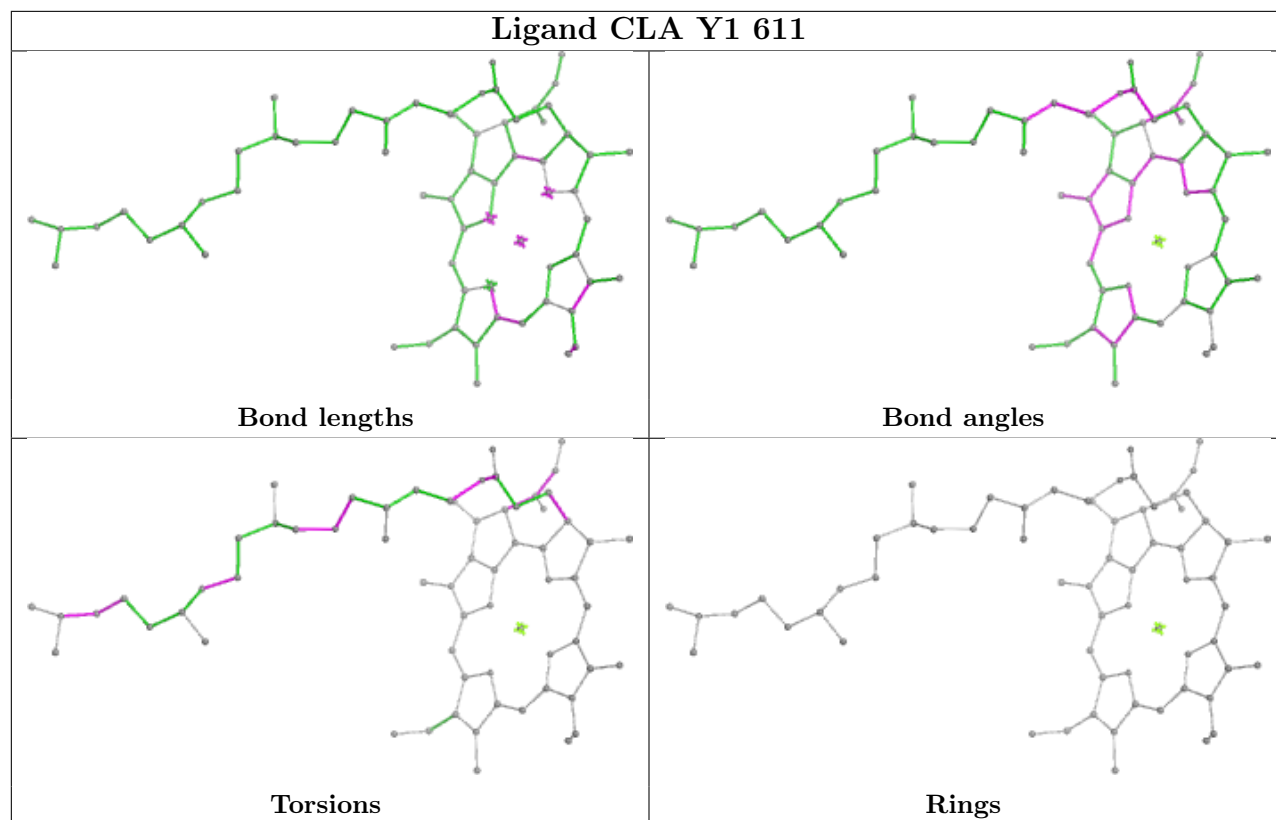


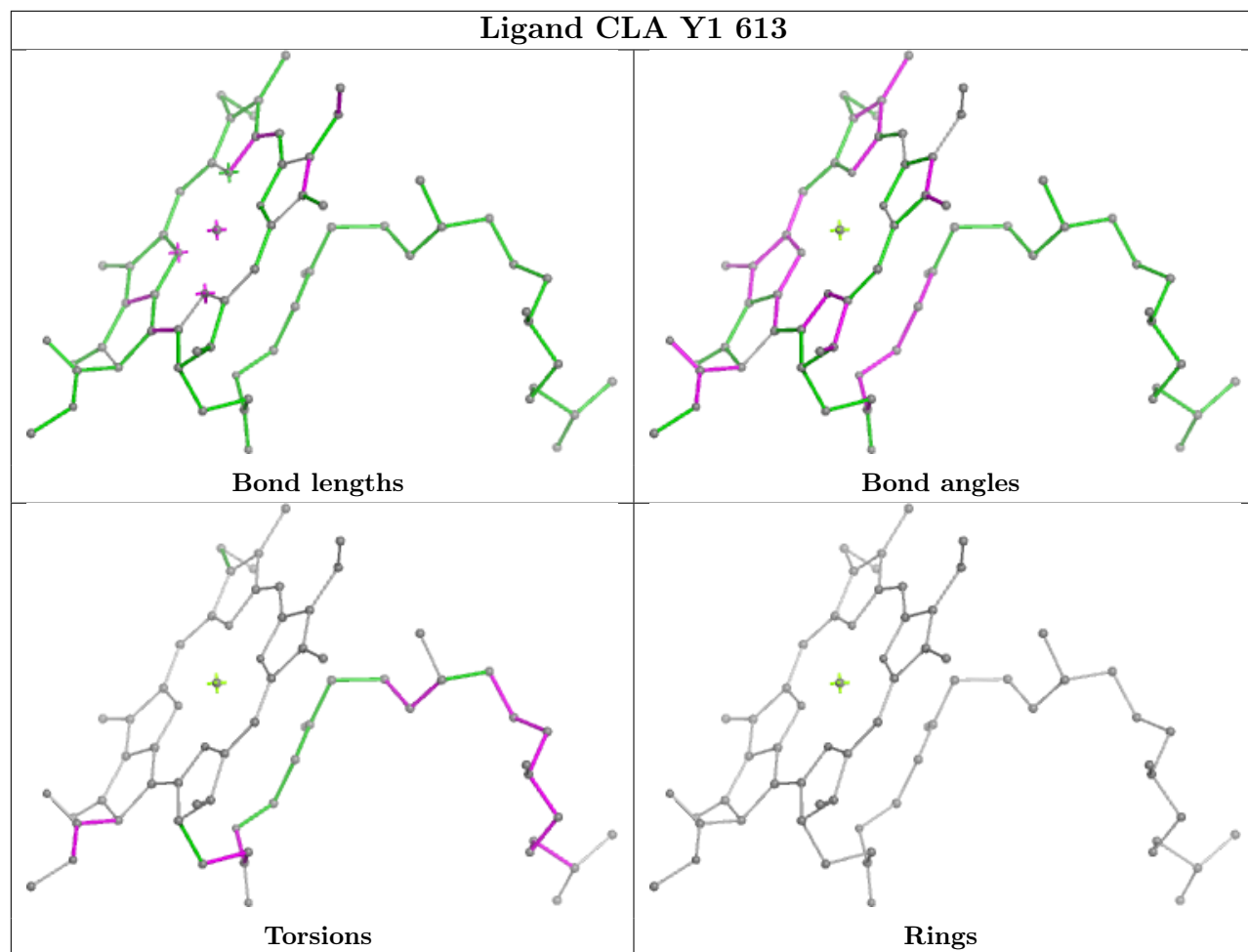
Torsions



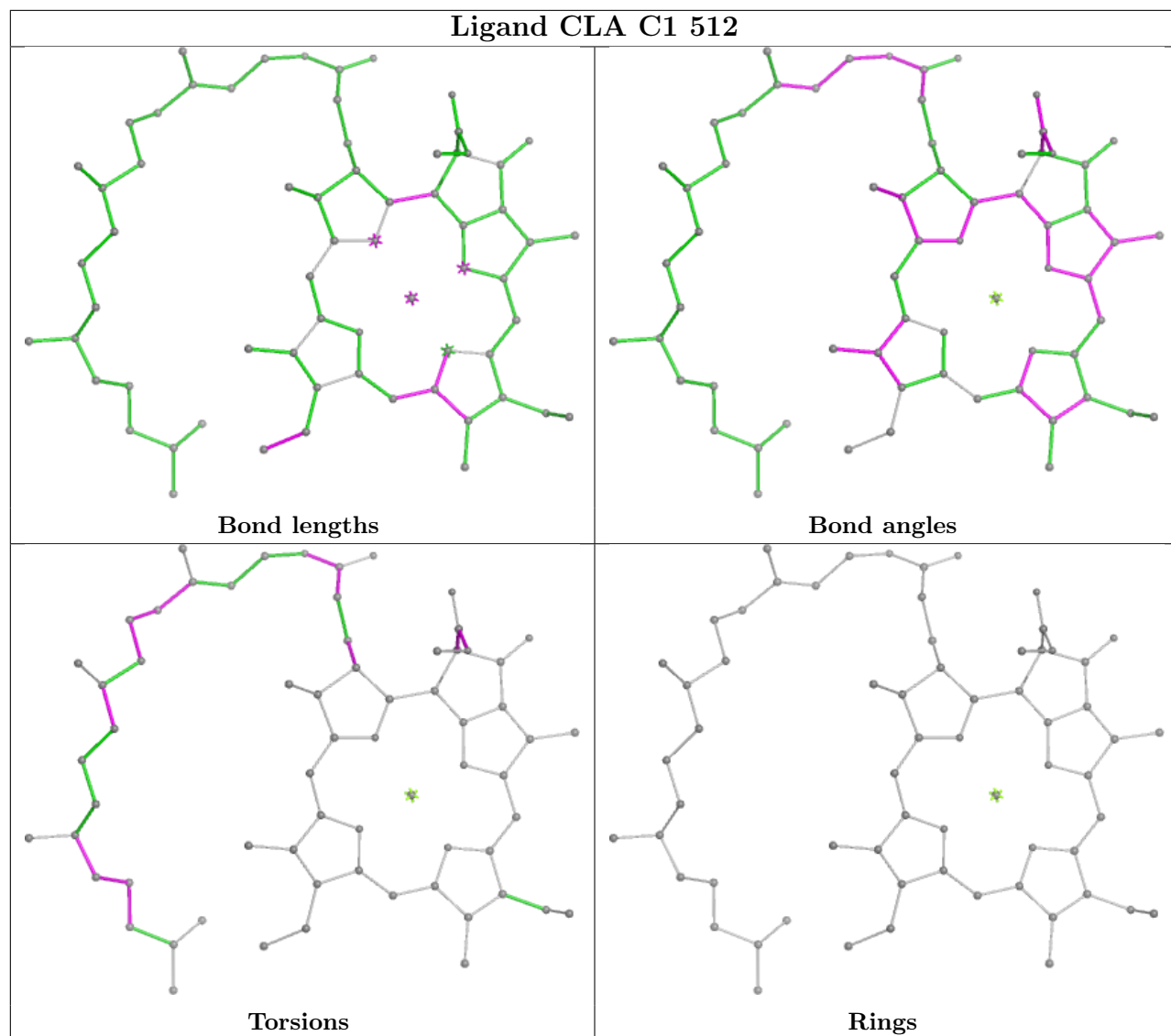
Rings

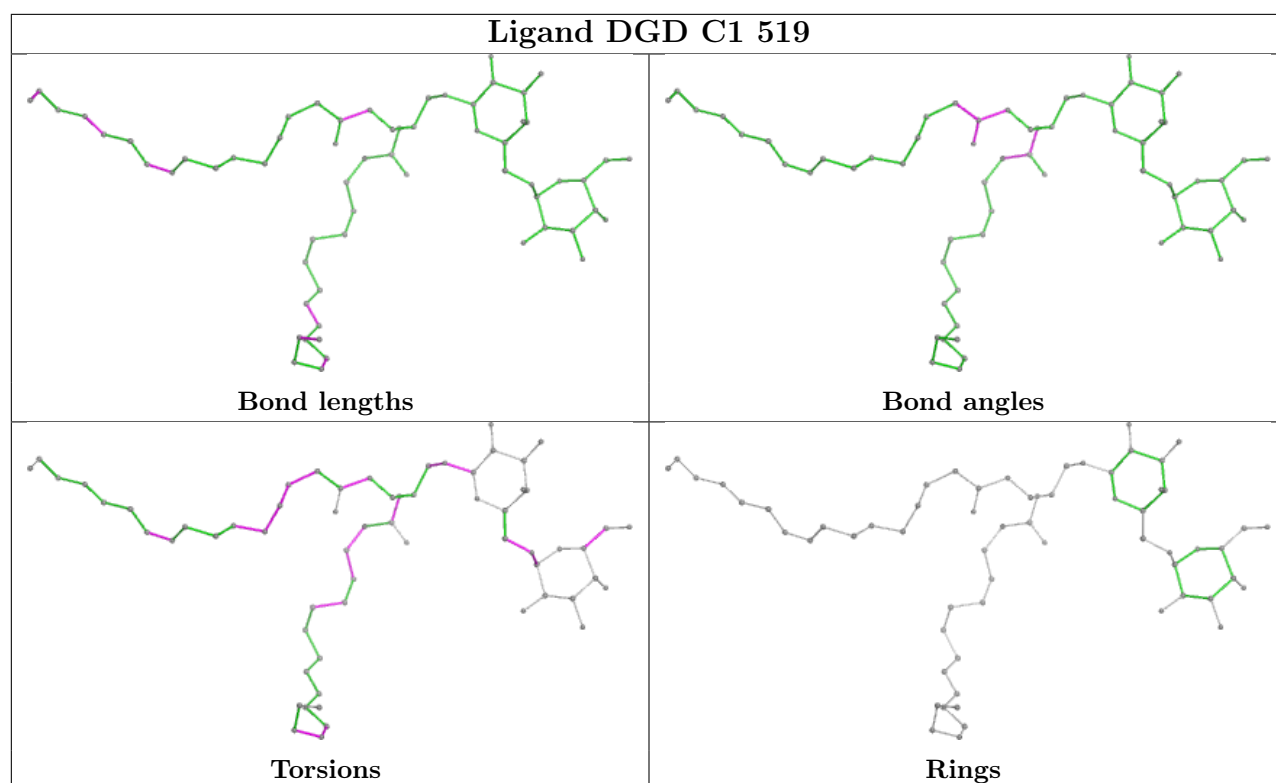




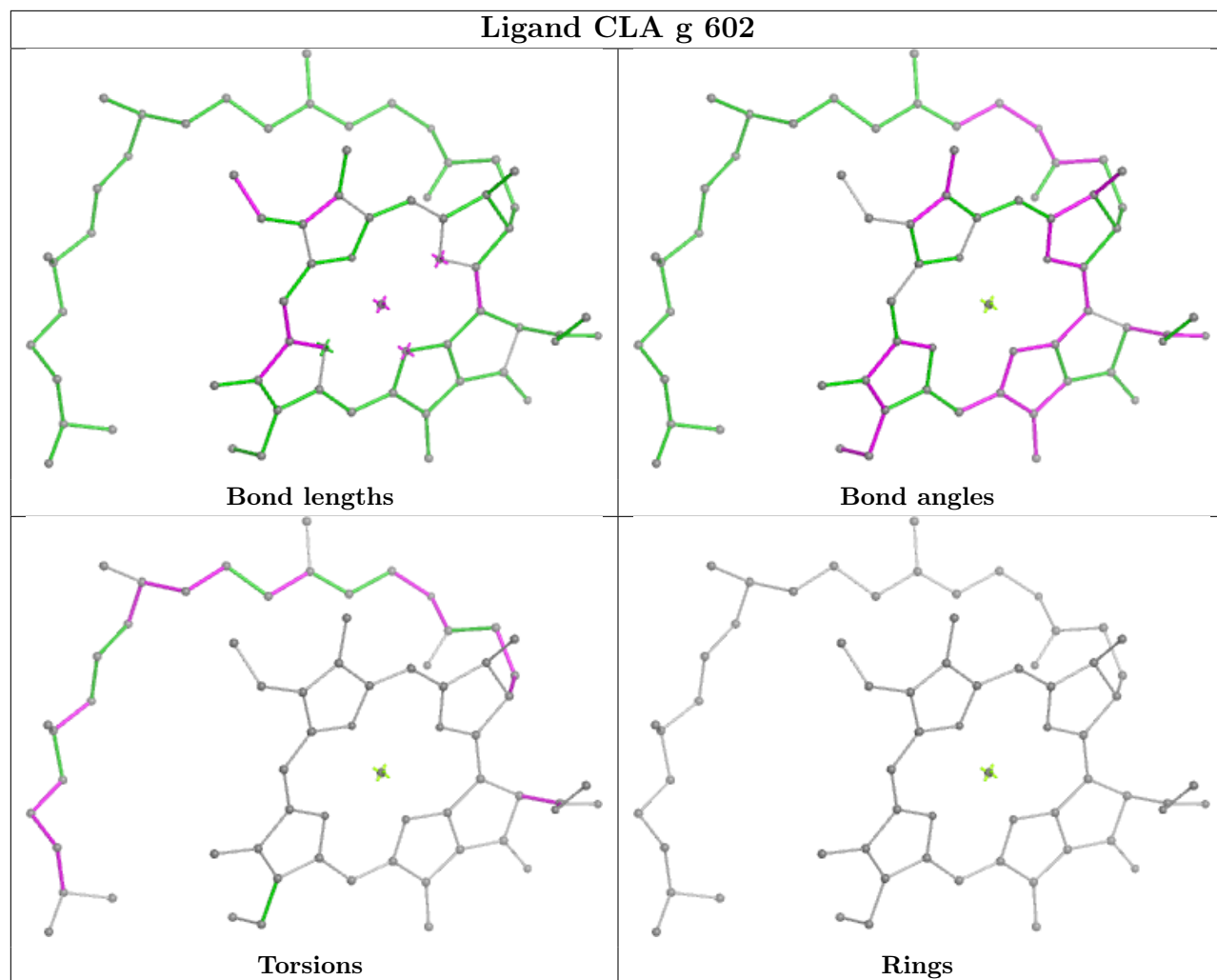


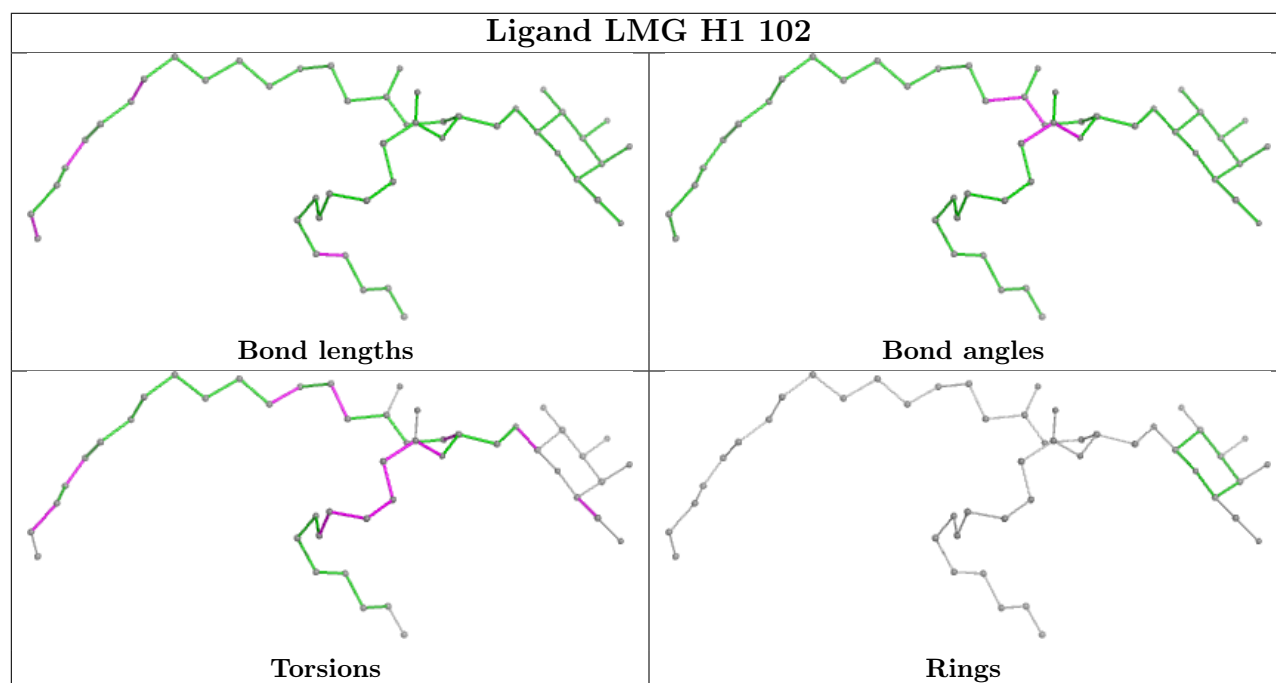
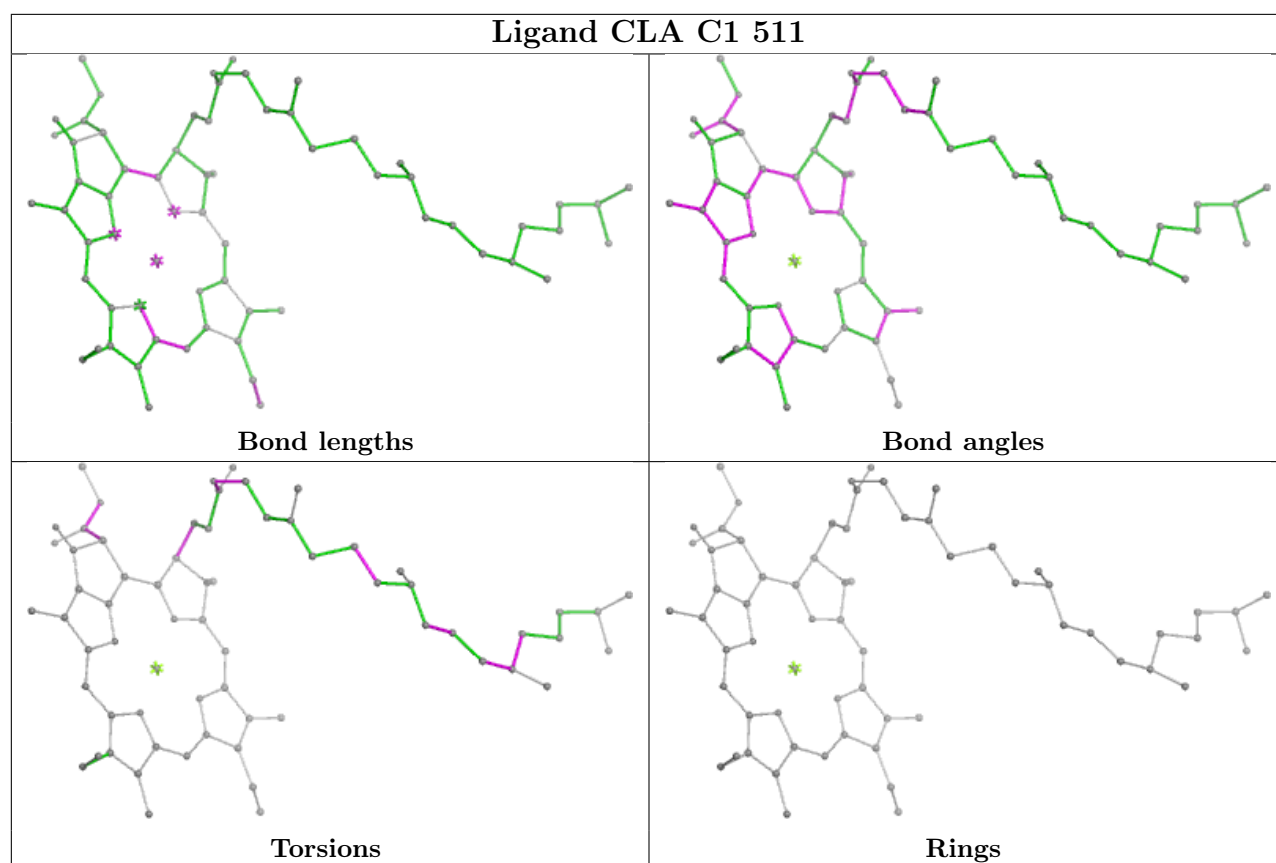


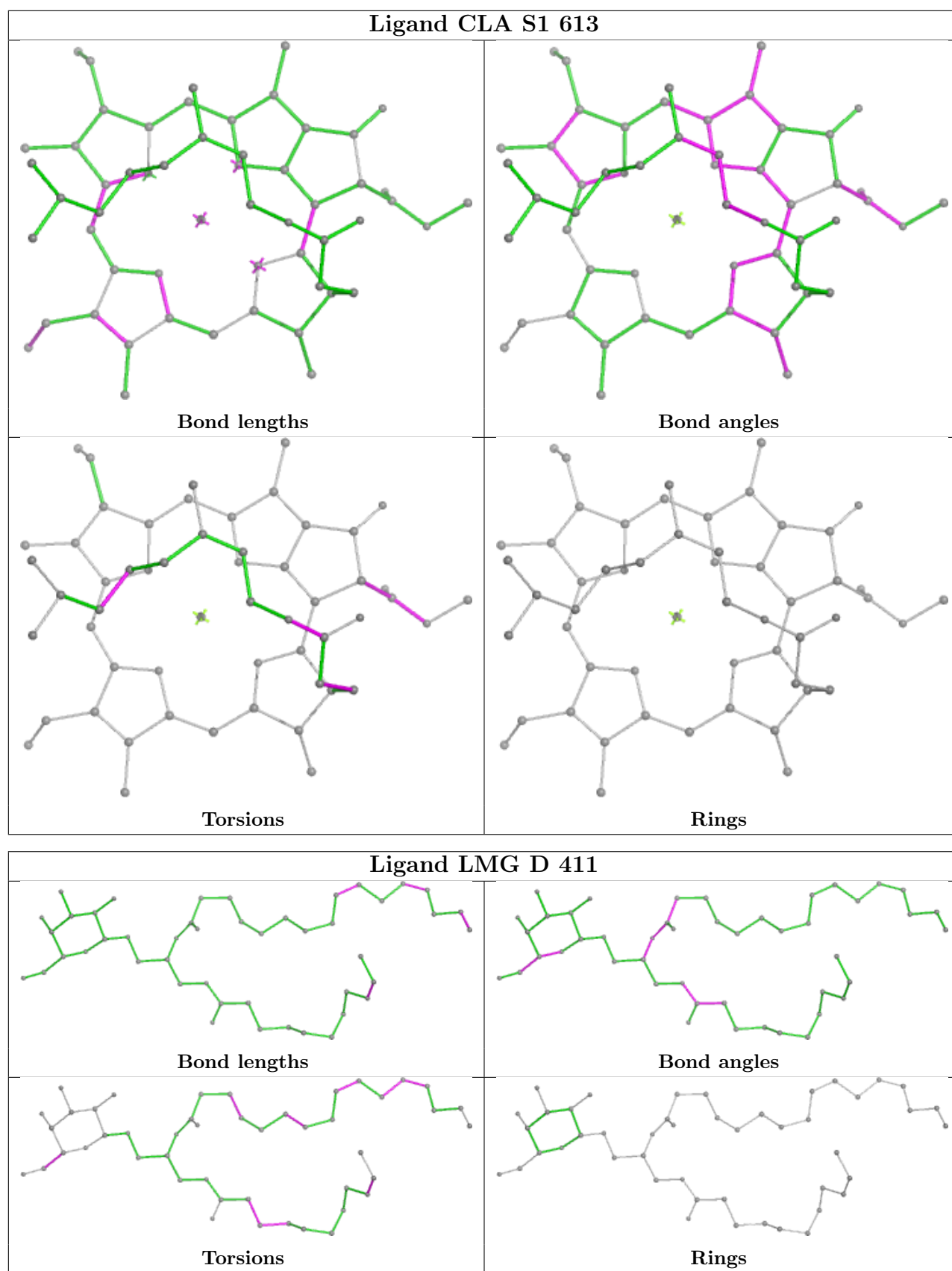




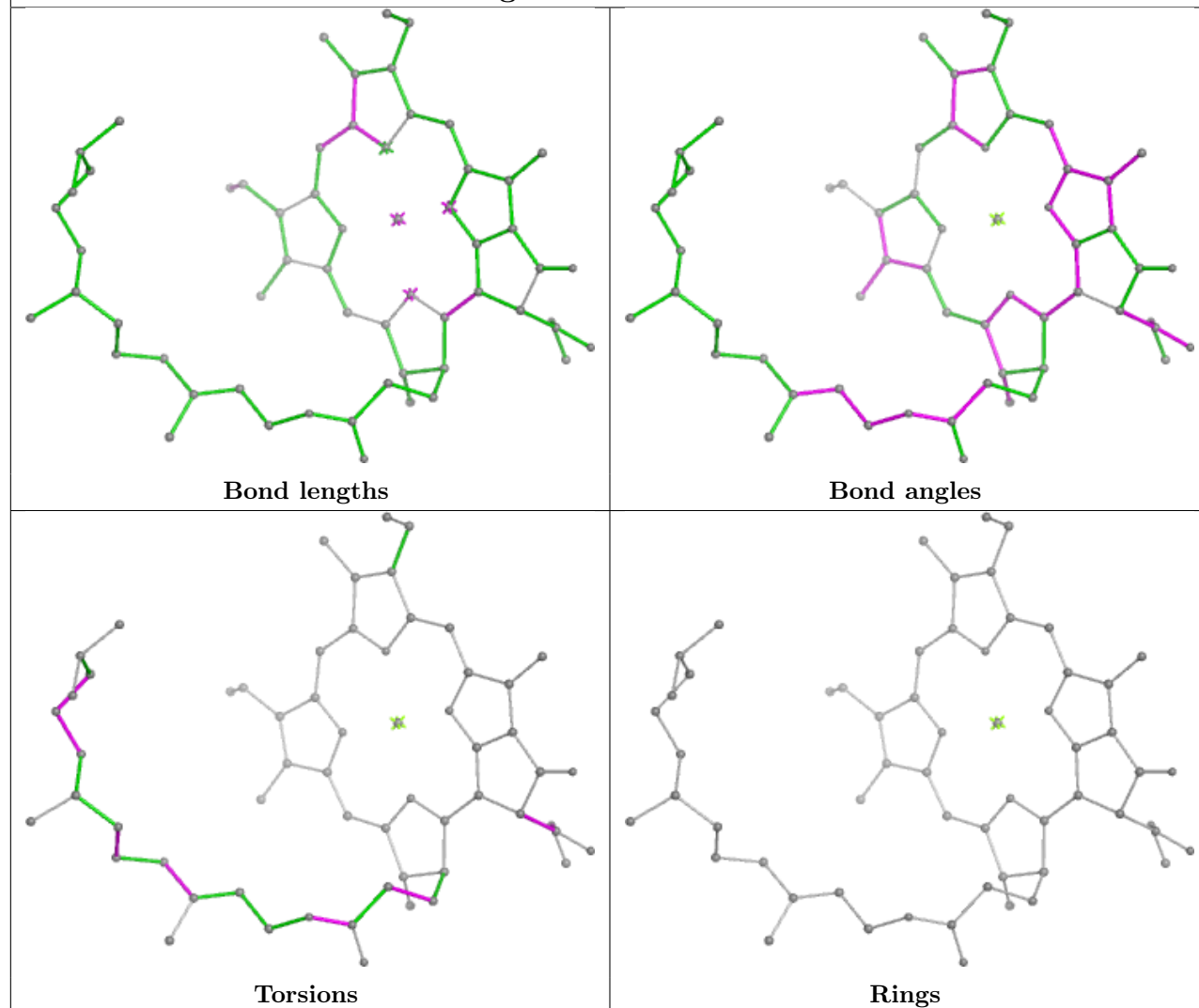
## Ligand CLA g 602



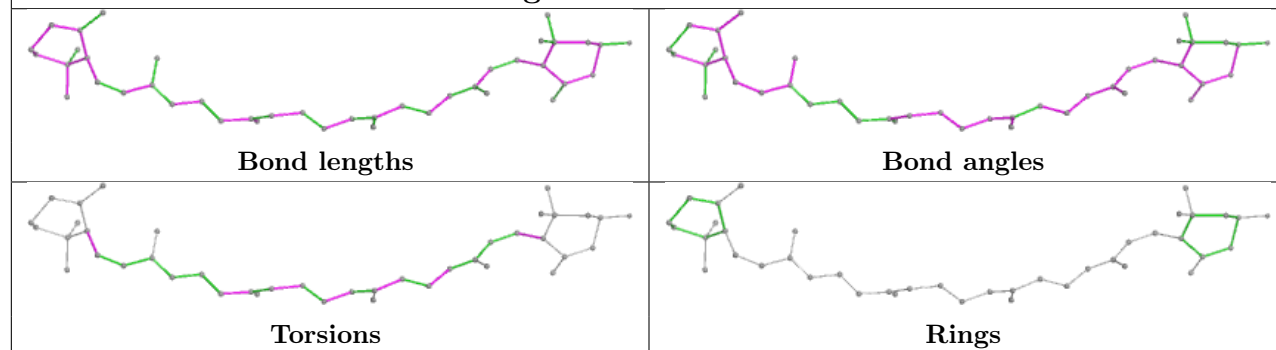


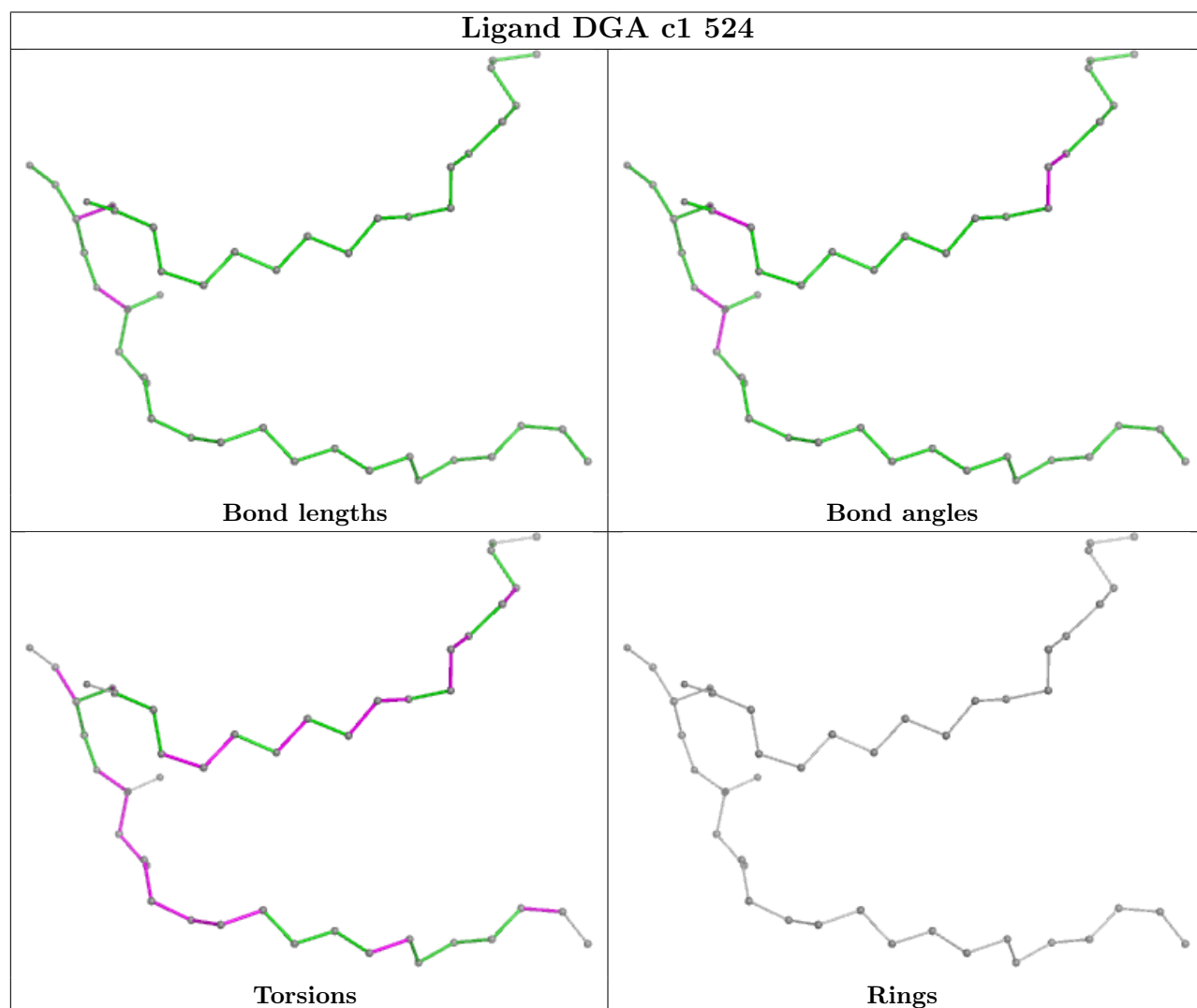
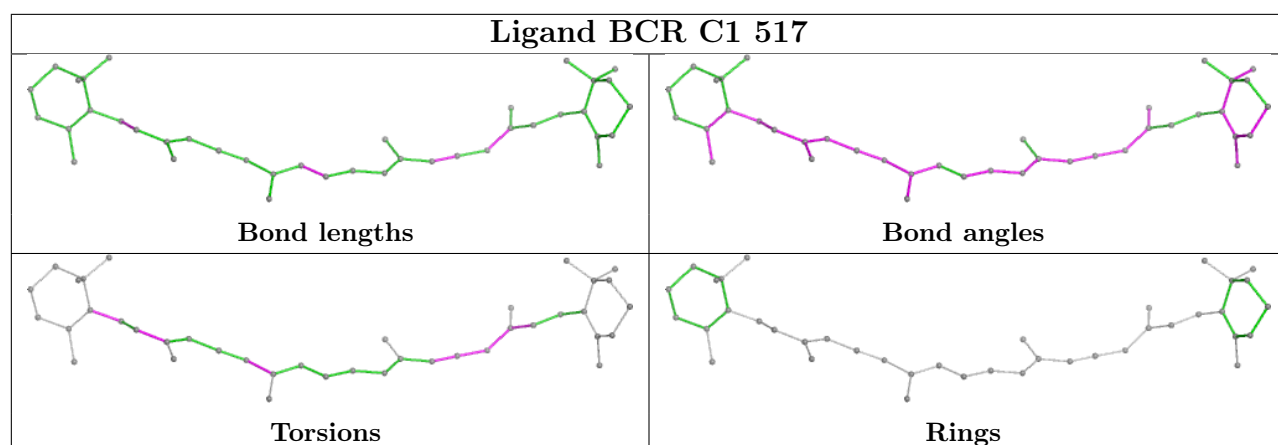


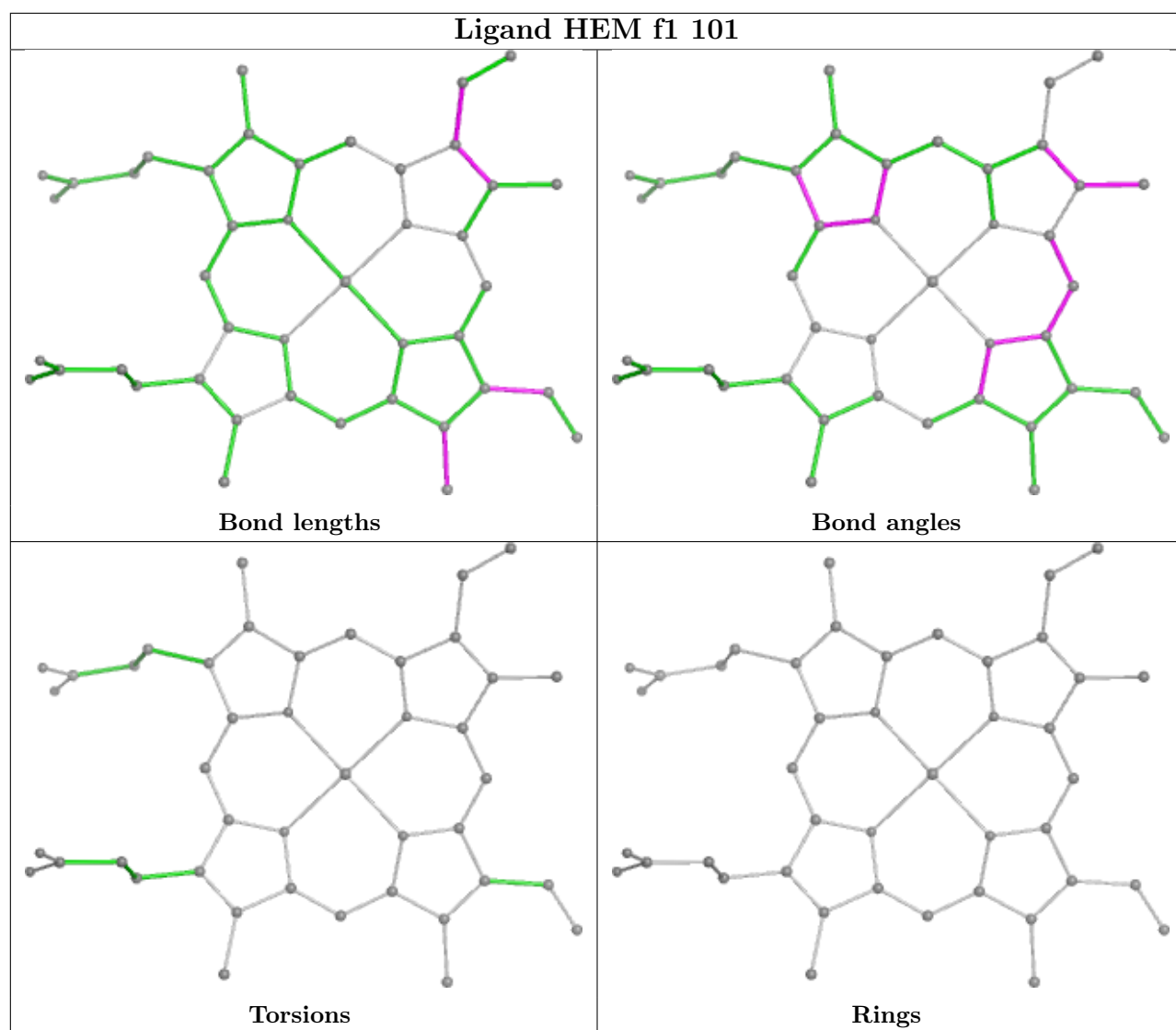
## Ligand CLA R 602



## Ligand RRX h1 101

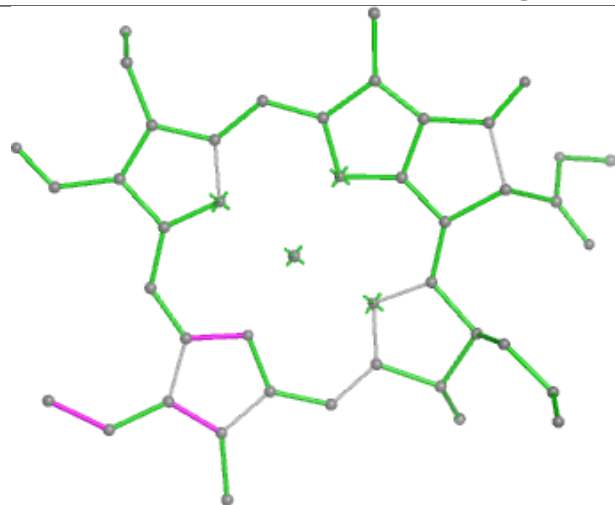




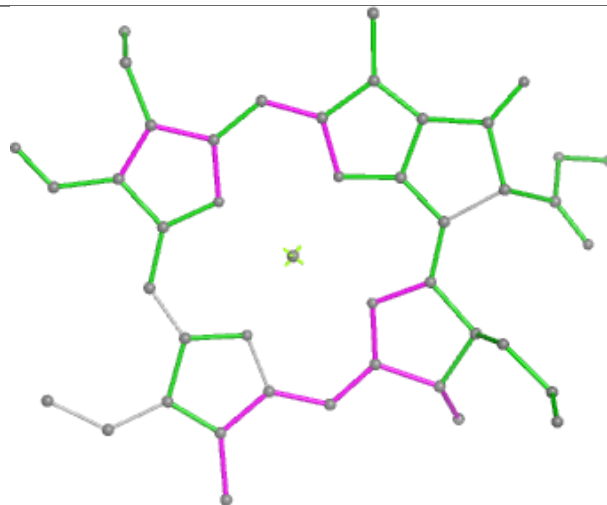




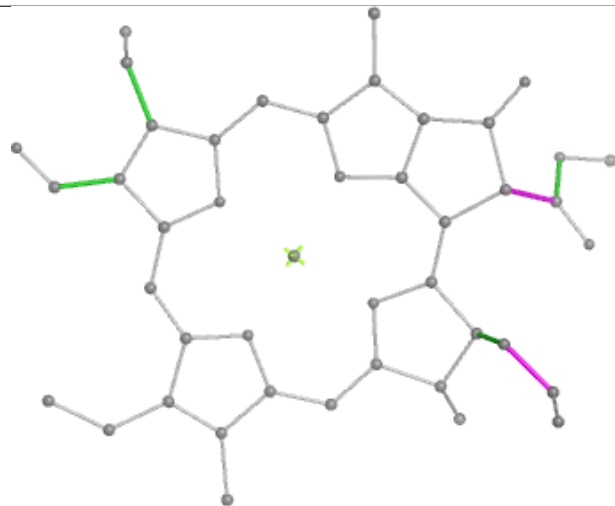
## Ligand CHL R 606



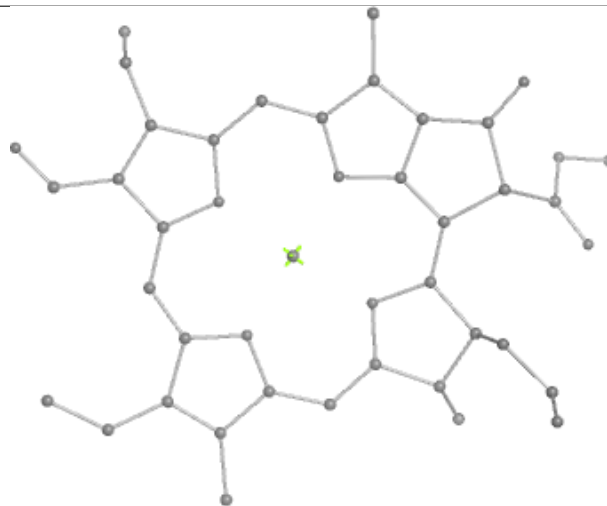
Bond lengths



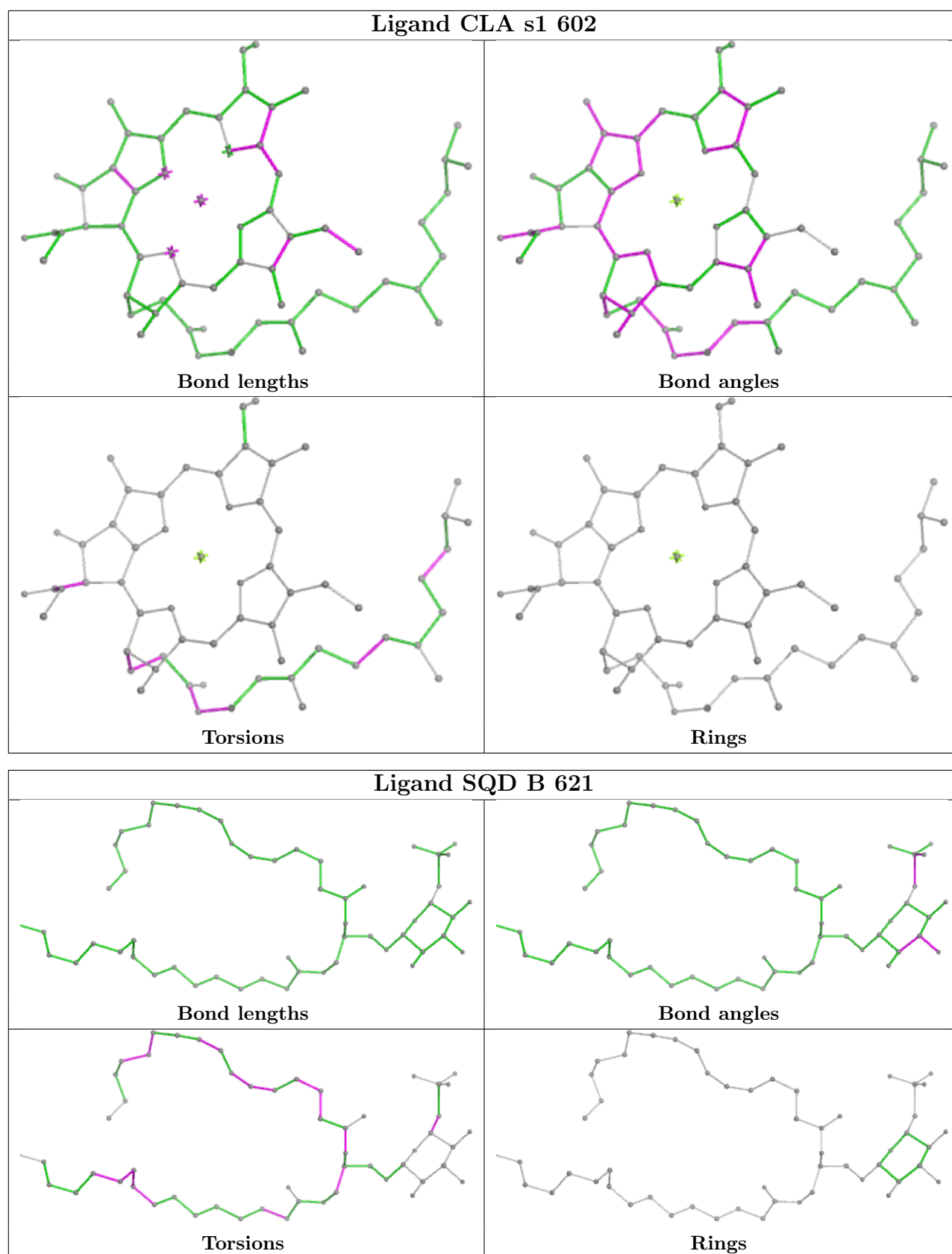
Bond angles

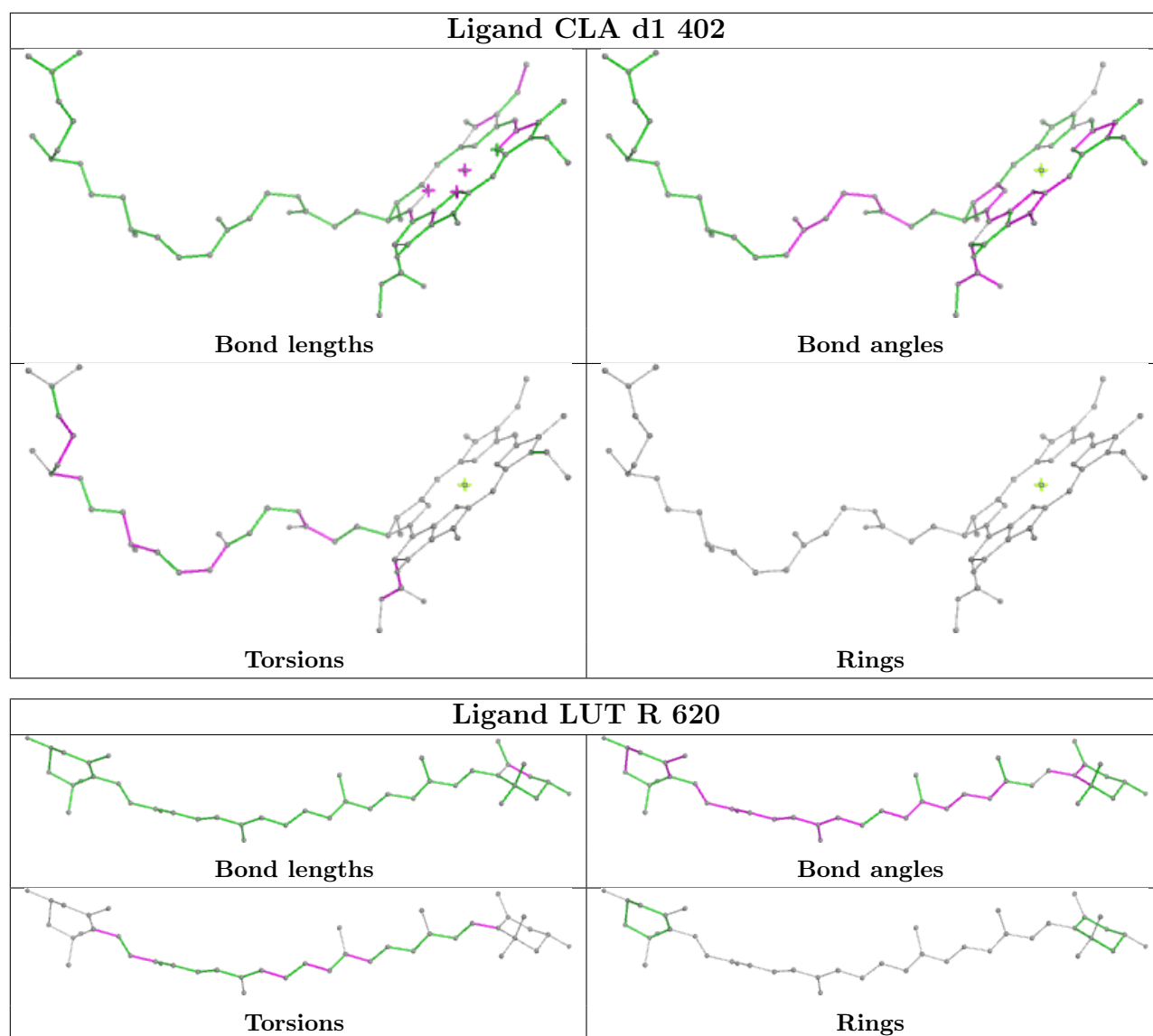


Torsions

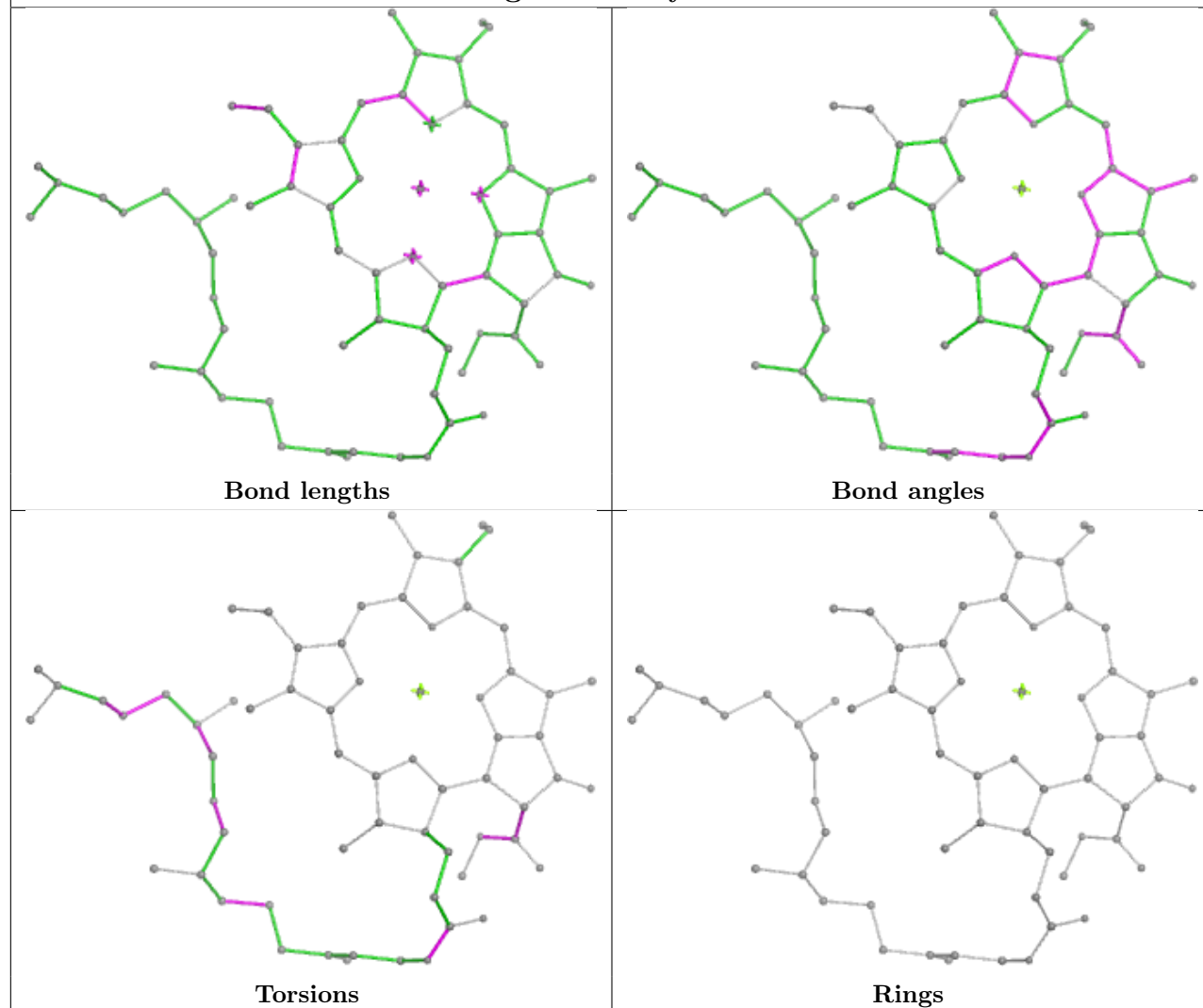


Rings

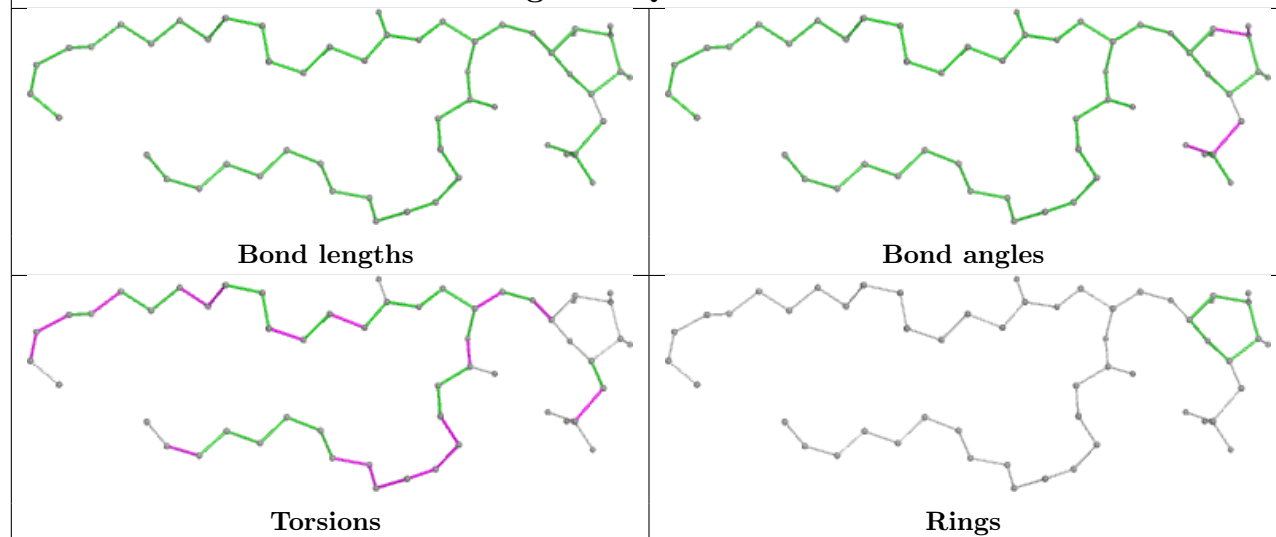


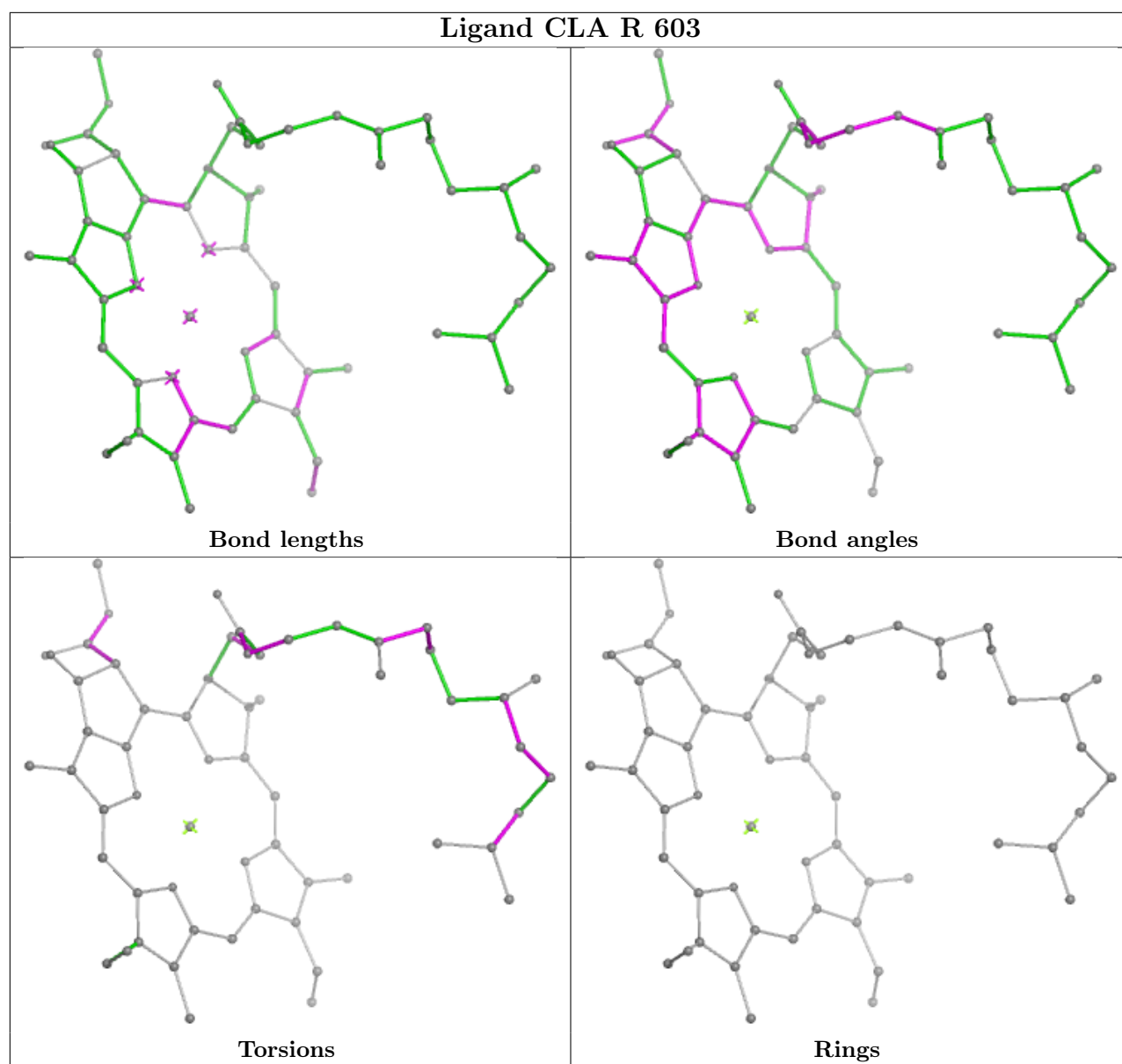


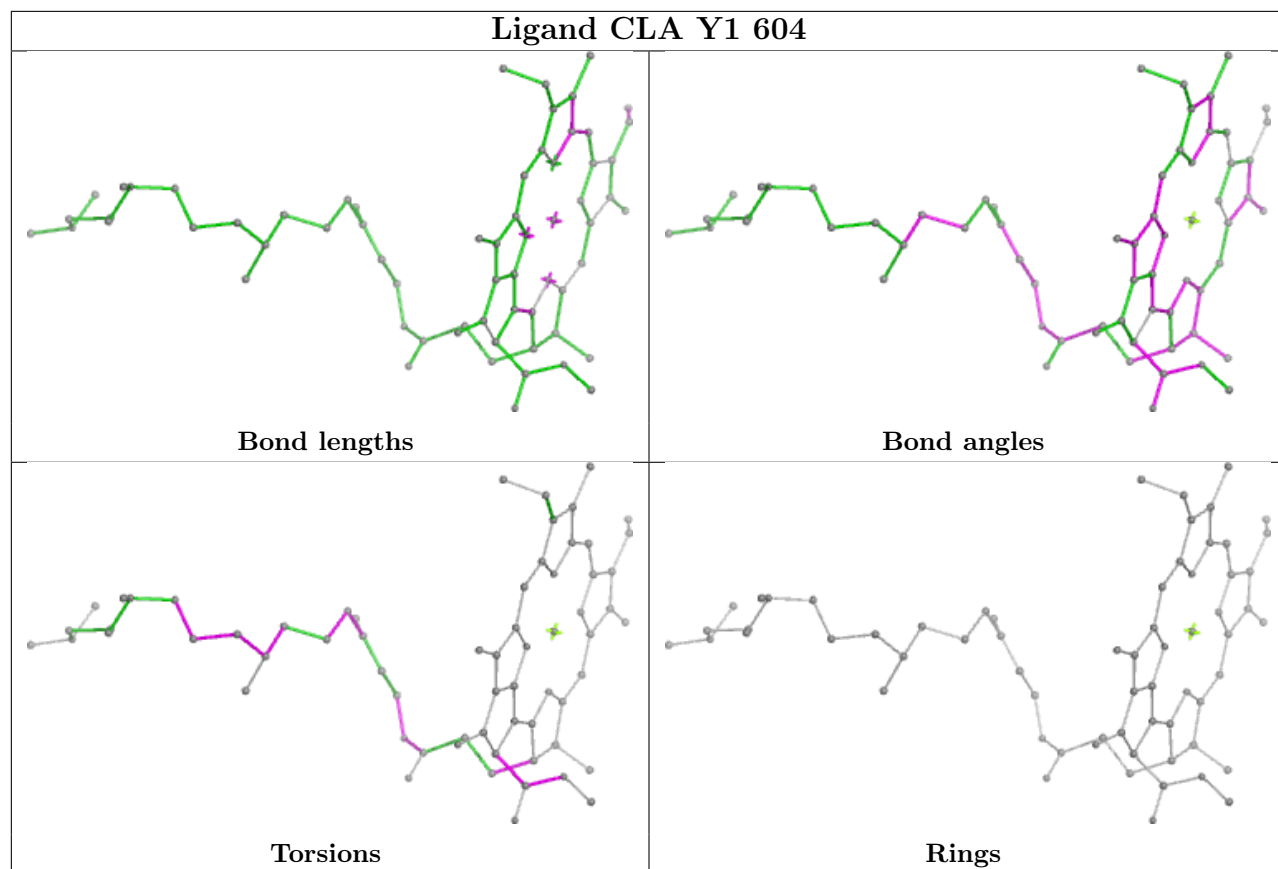
## Ligand CLA y 612

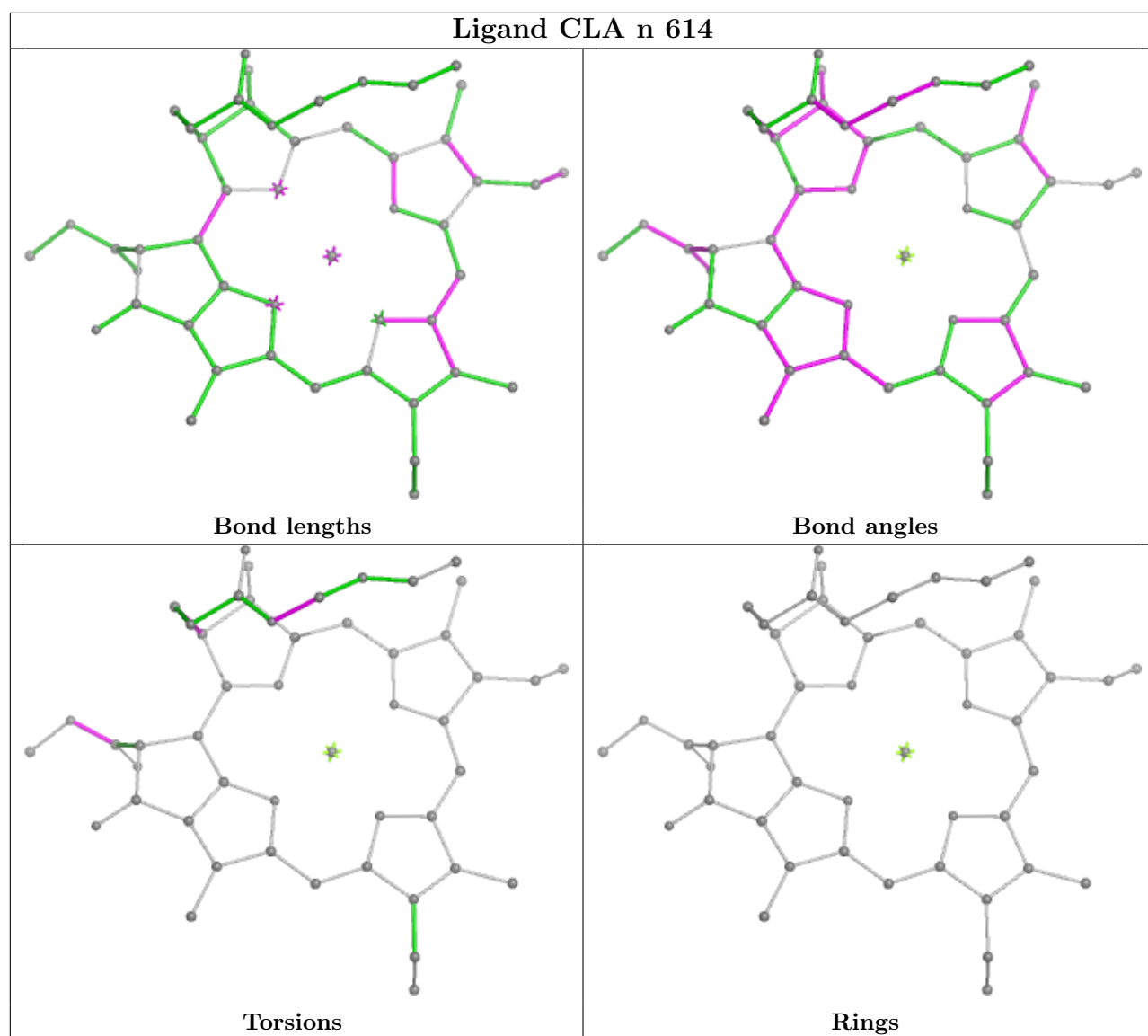


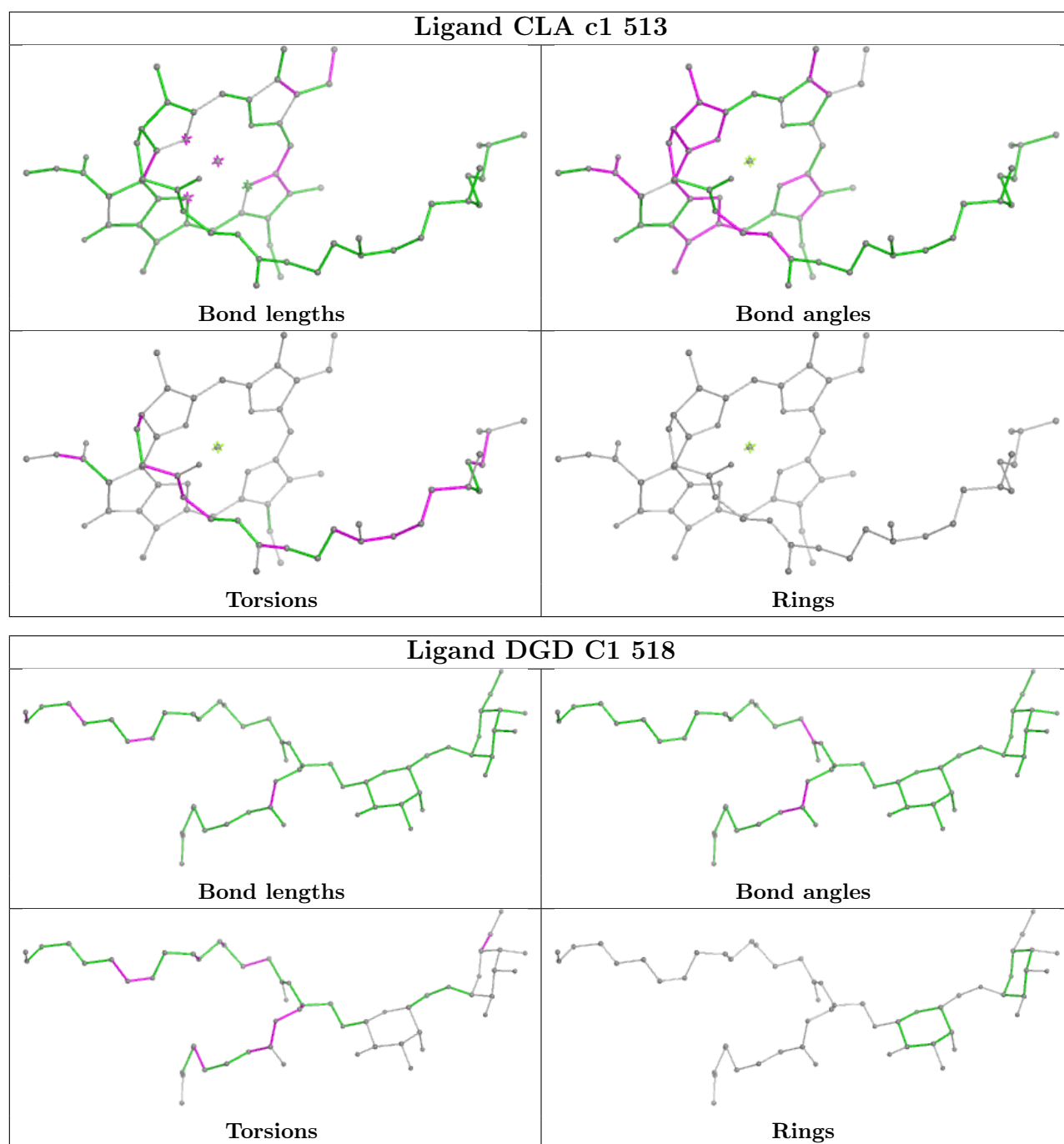
## Ligand SQD b1 626



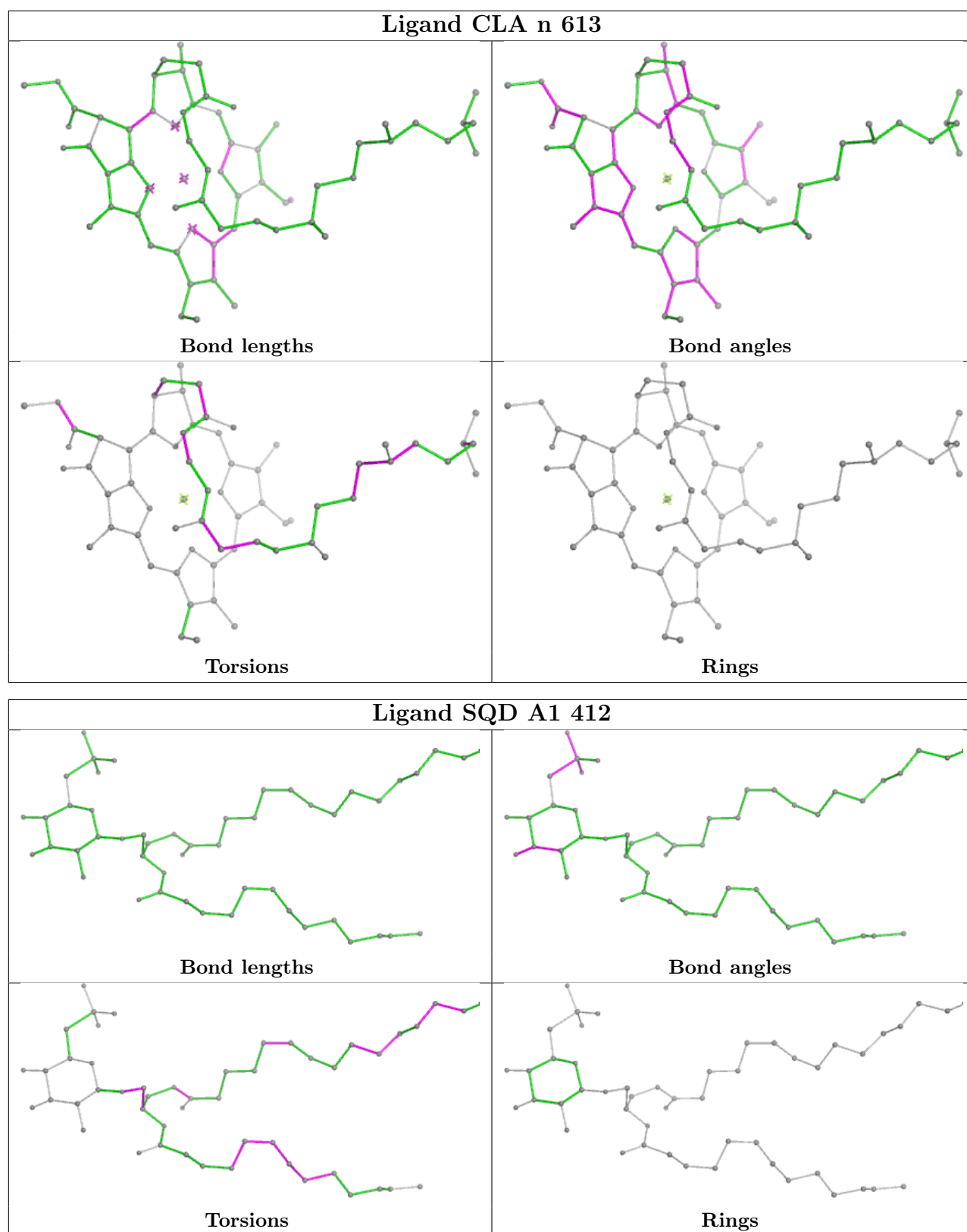




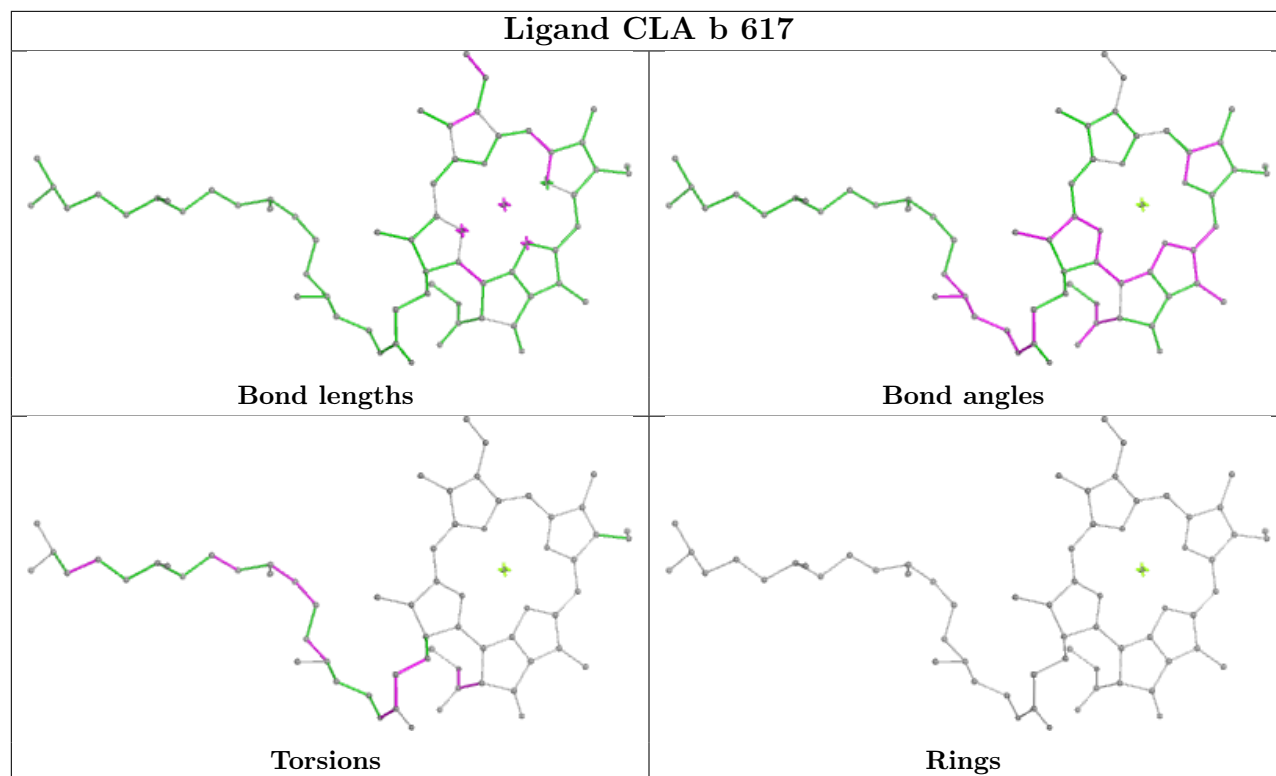




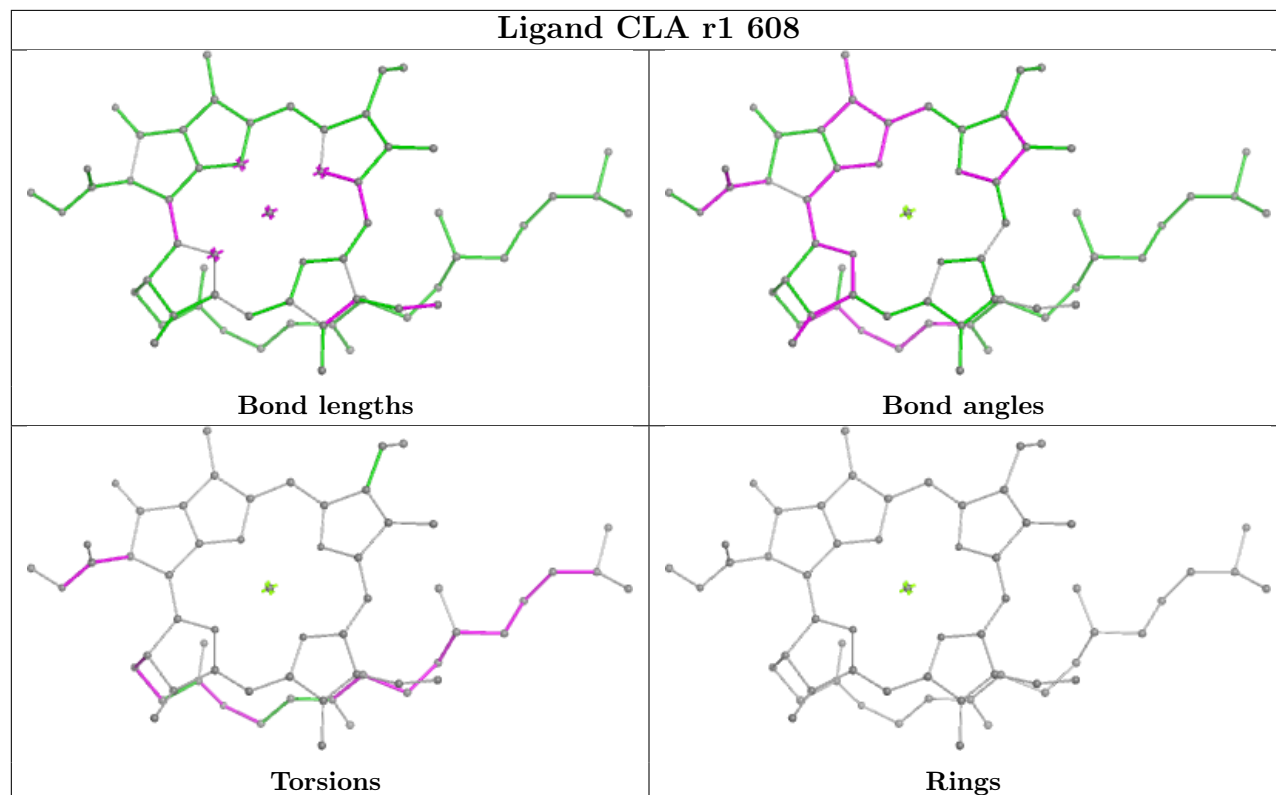




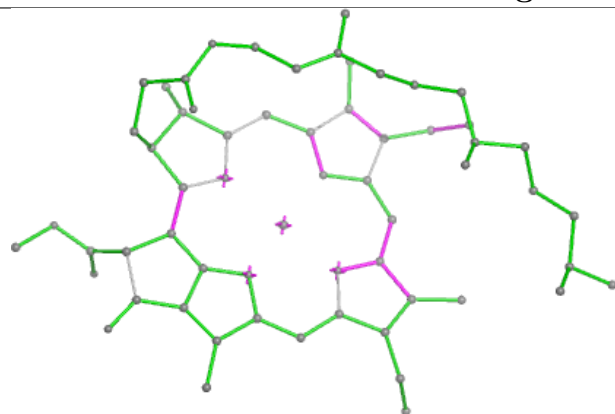
## Ligand CLA b 617



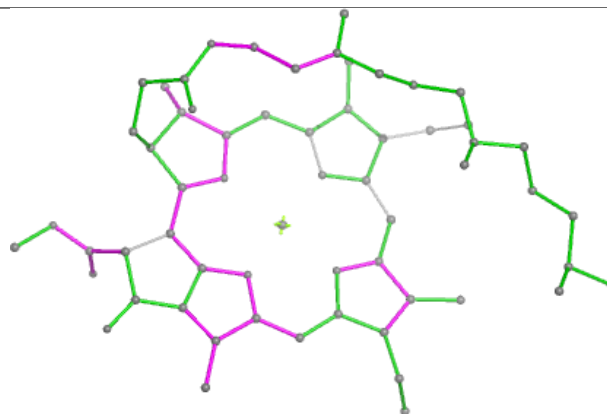
## Ligand CLA r1 608



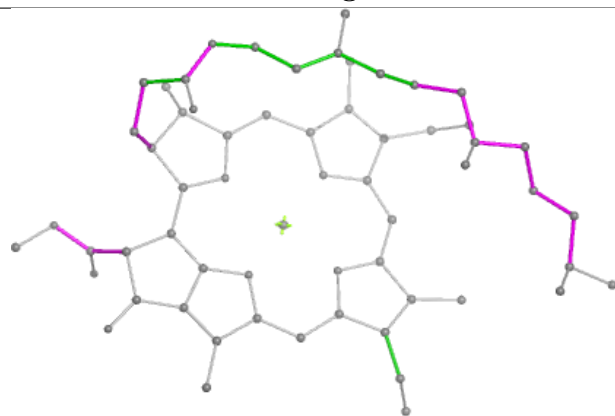
## Ligand CLA R 608



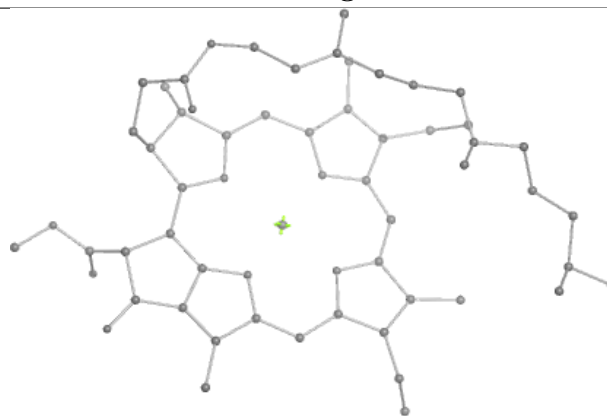
Bond lengths



Bond angles

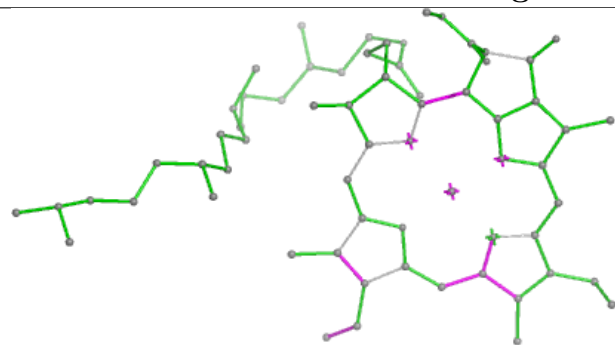


Torsions

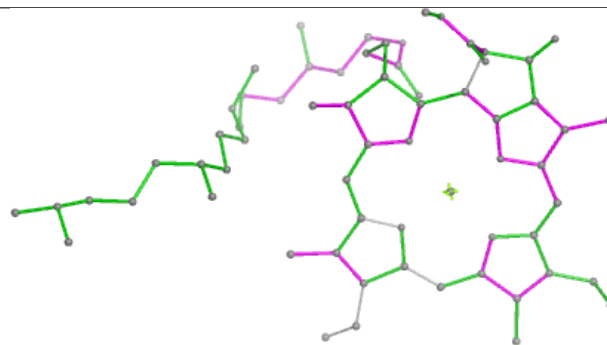


Rings

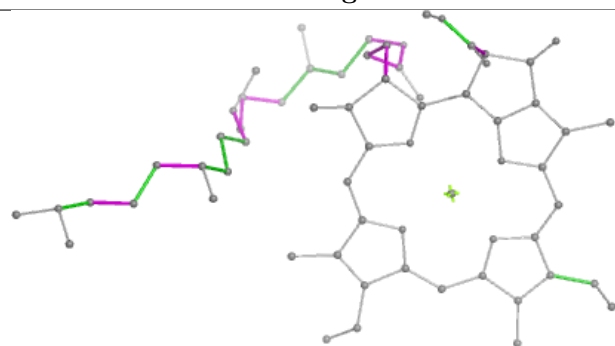
## Ligand CLA a1 406



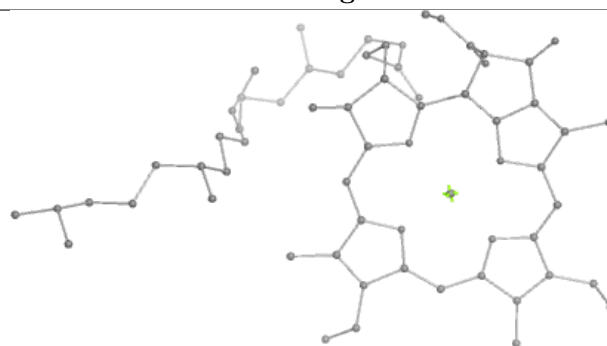
Bond lengths



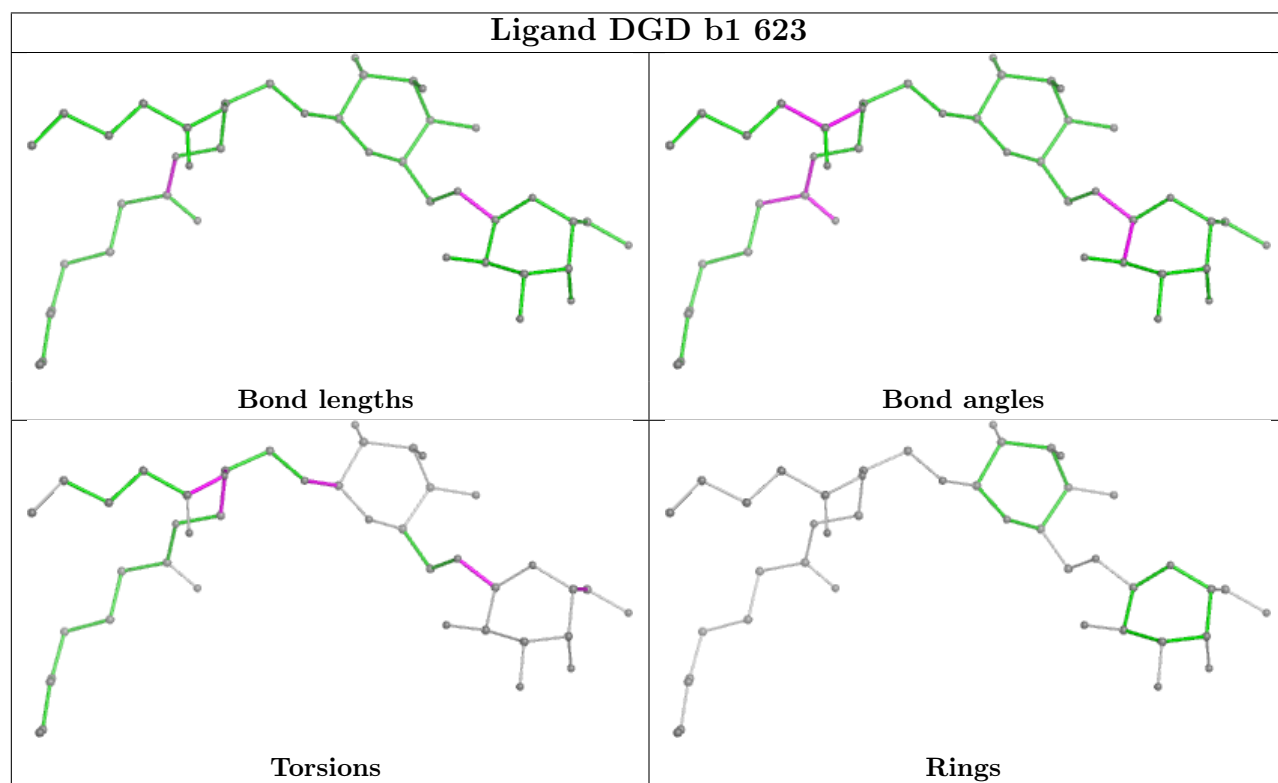
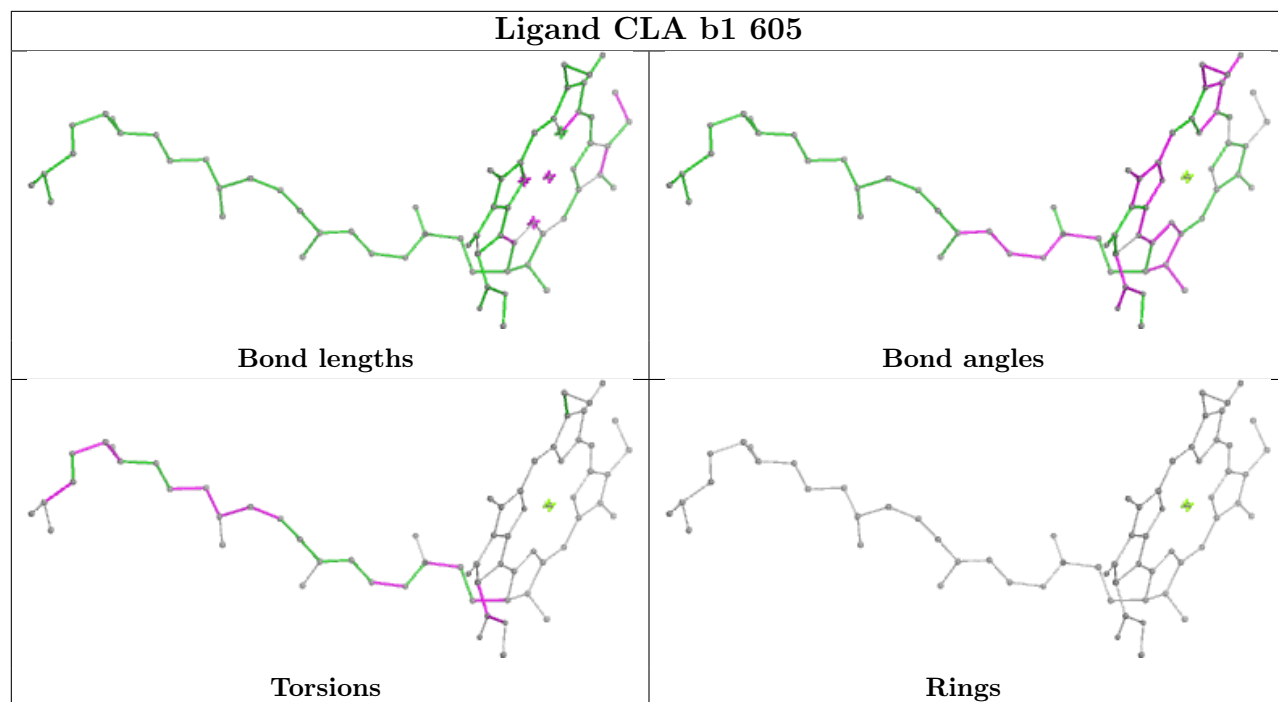
Bond angles



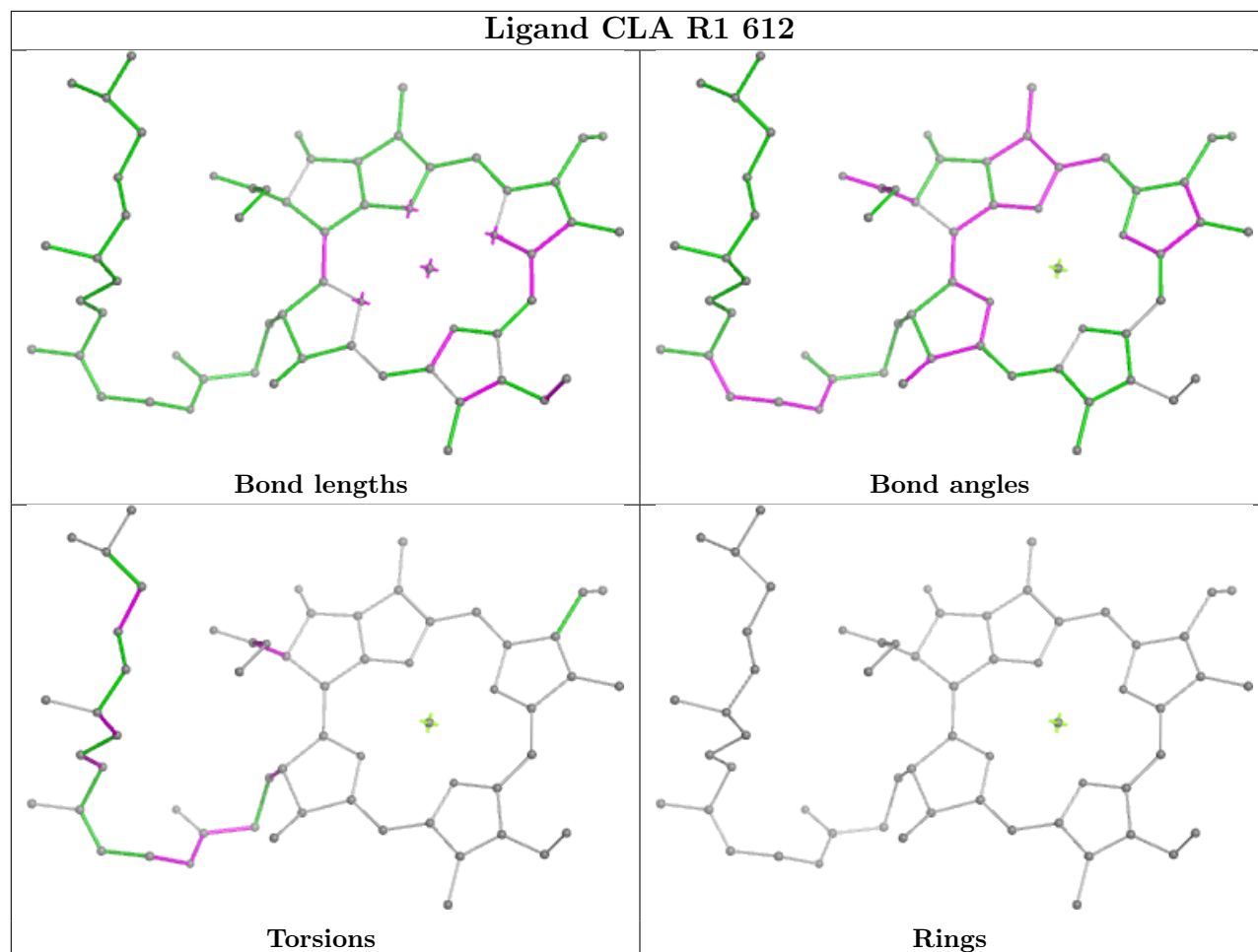
Torsions



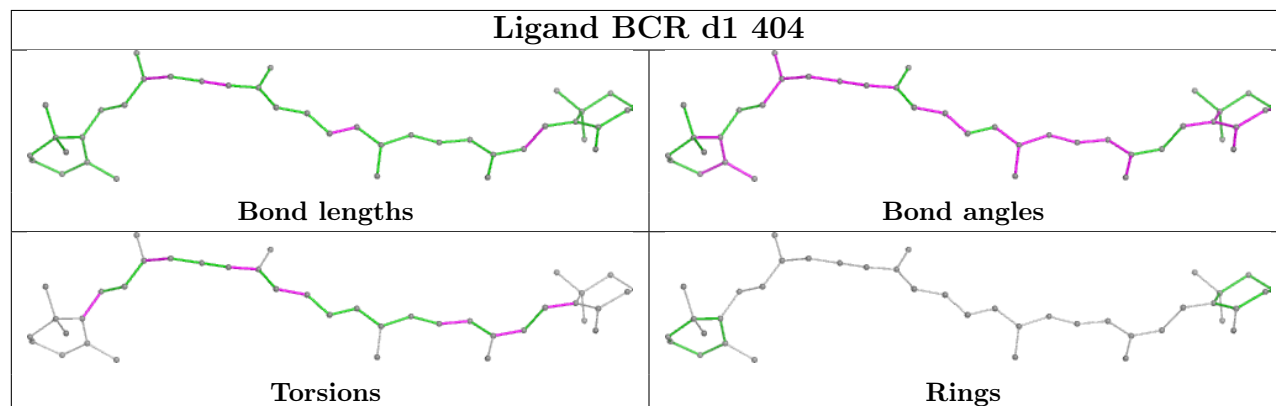
Rings

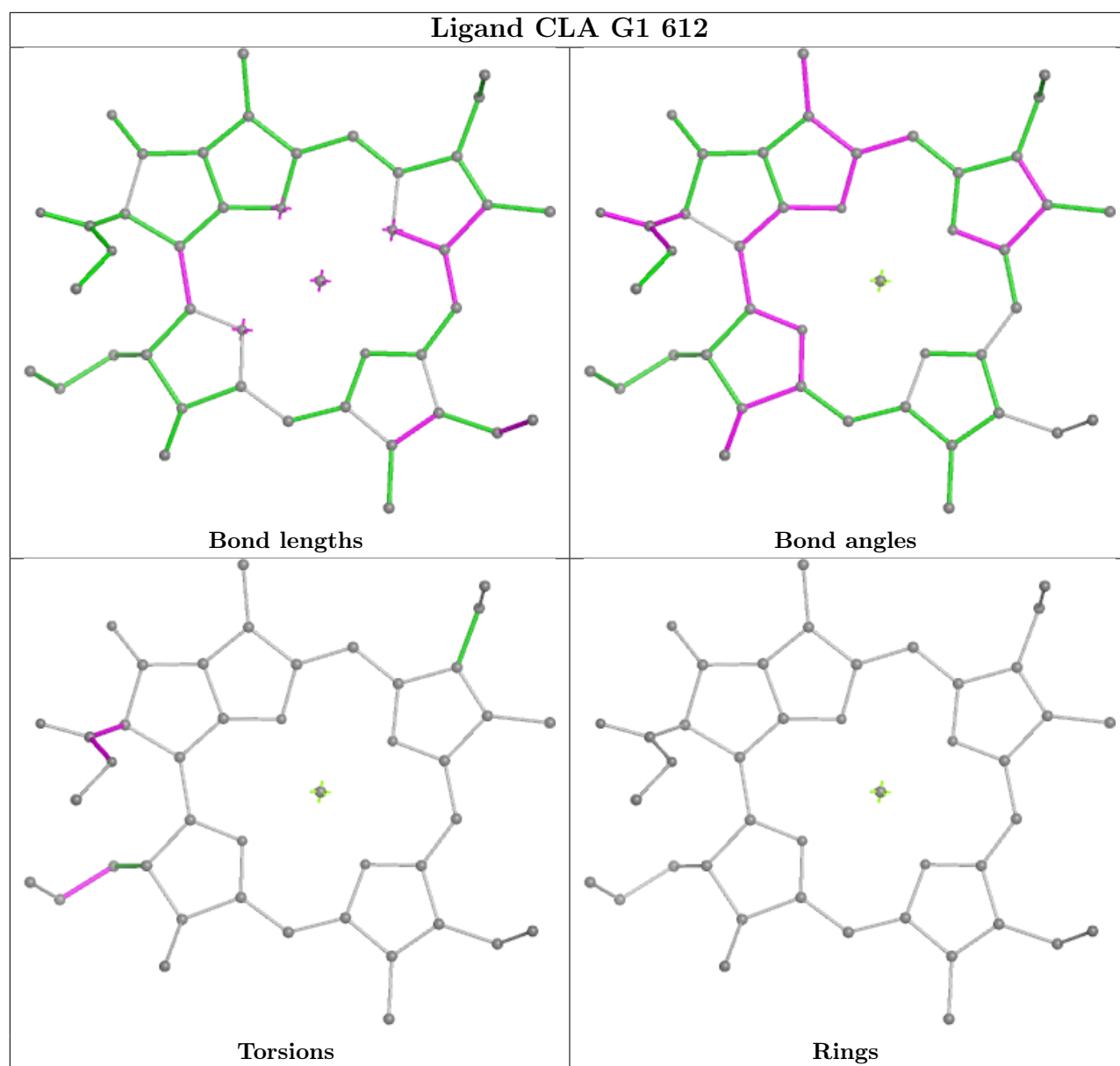


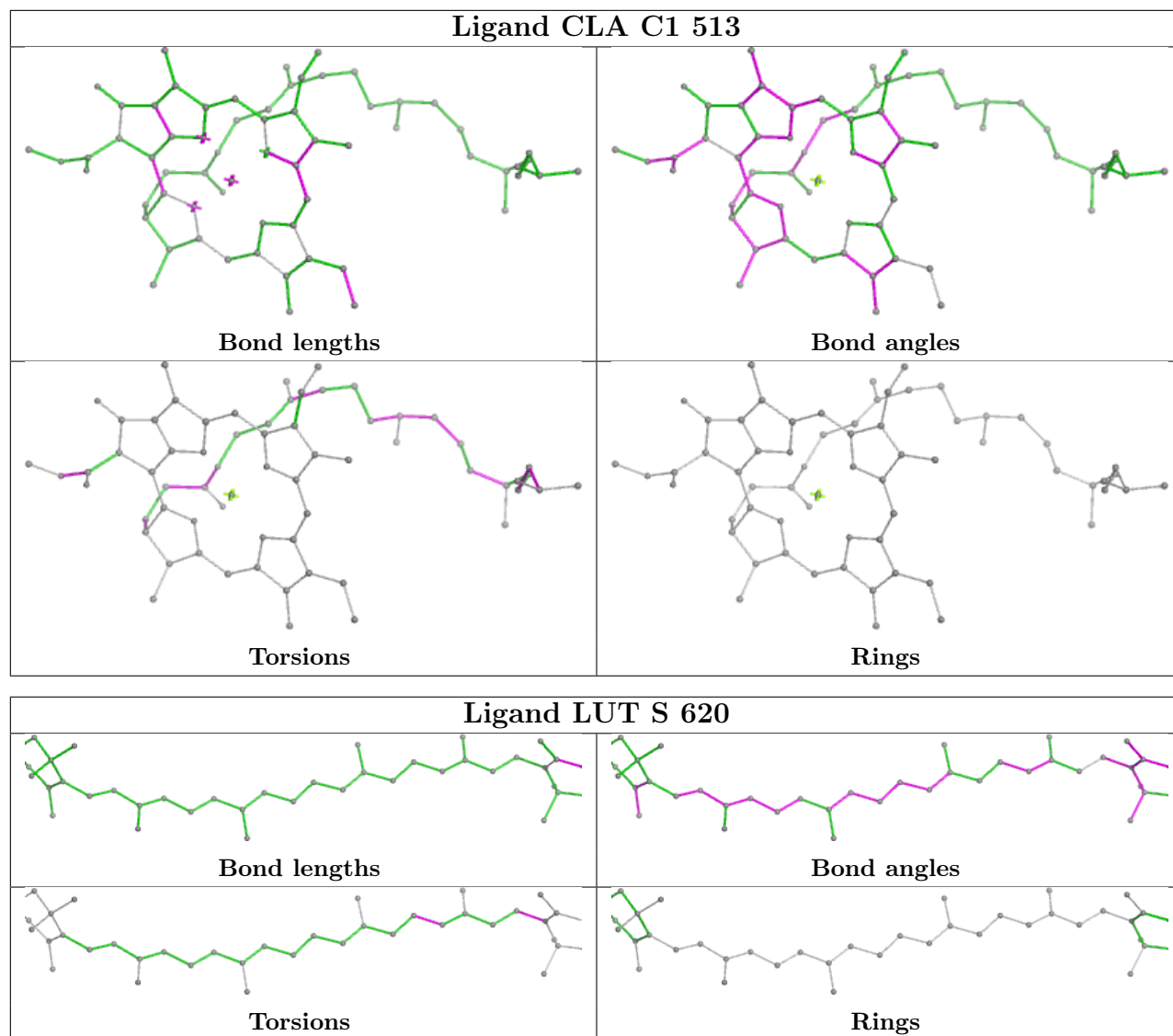
## Ligand CLA R1 612

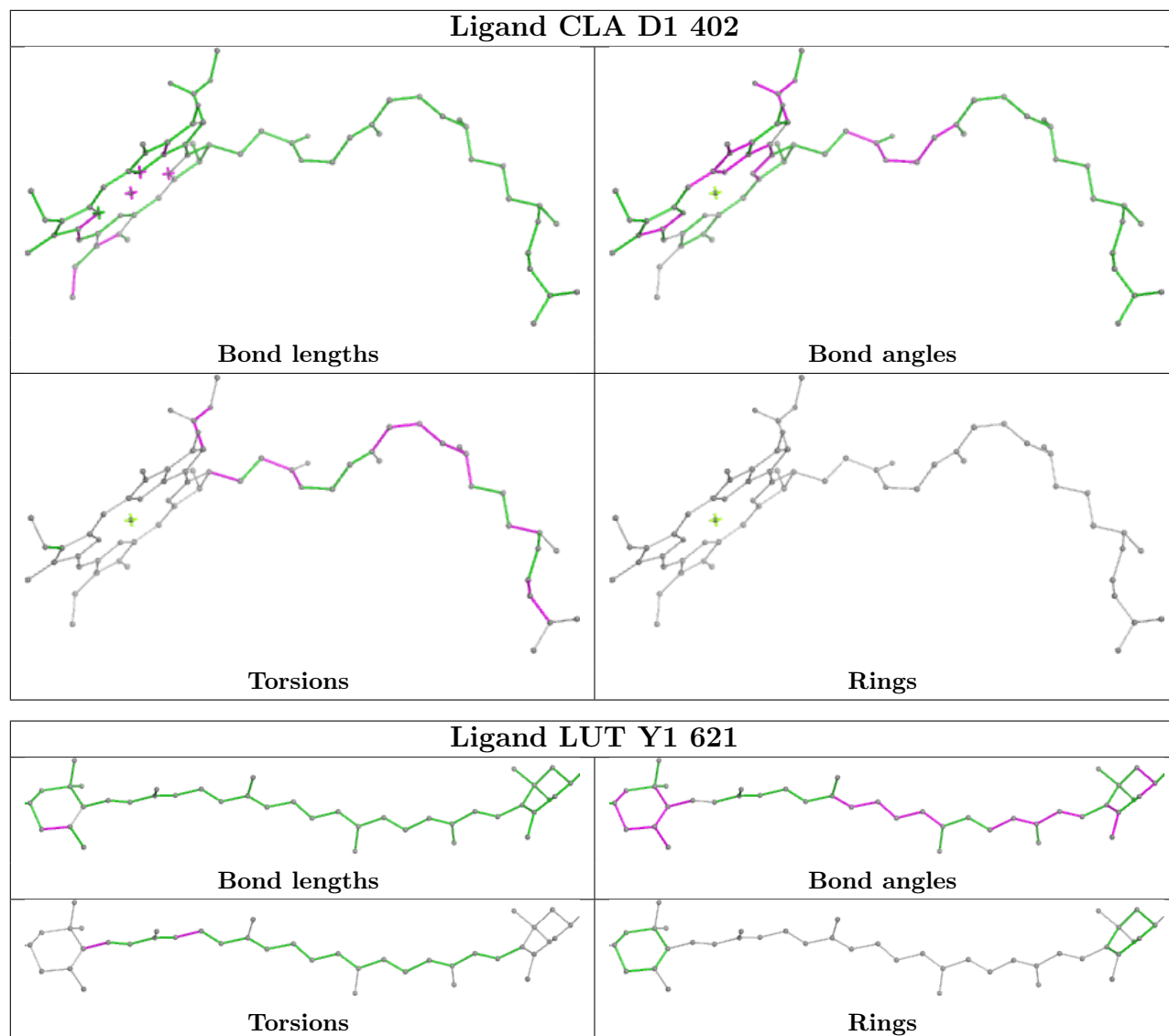


## Ligand BCR d1 404

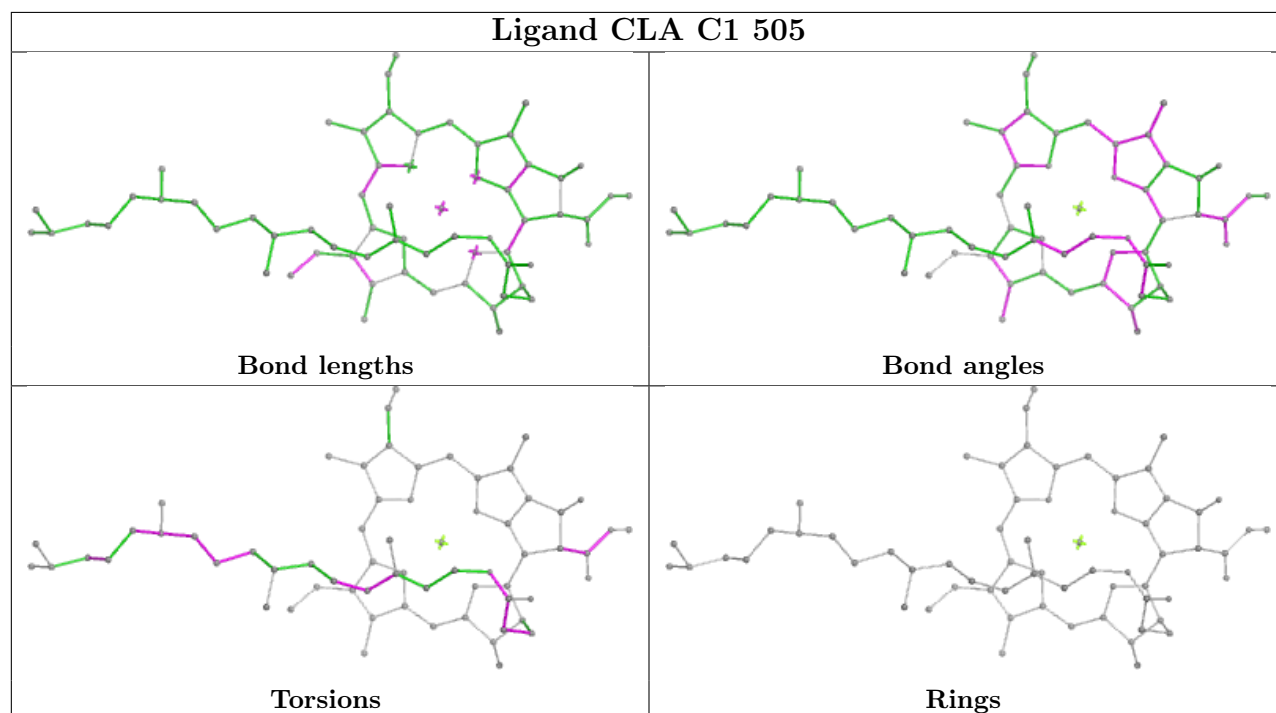
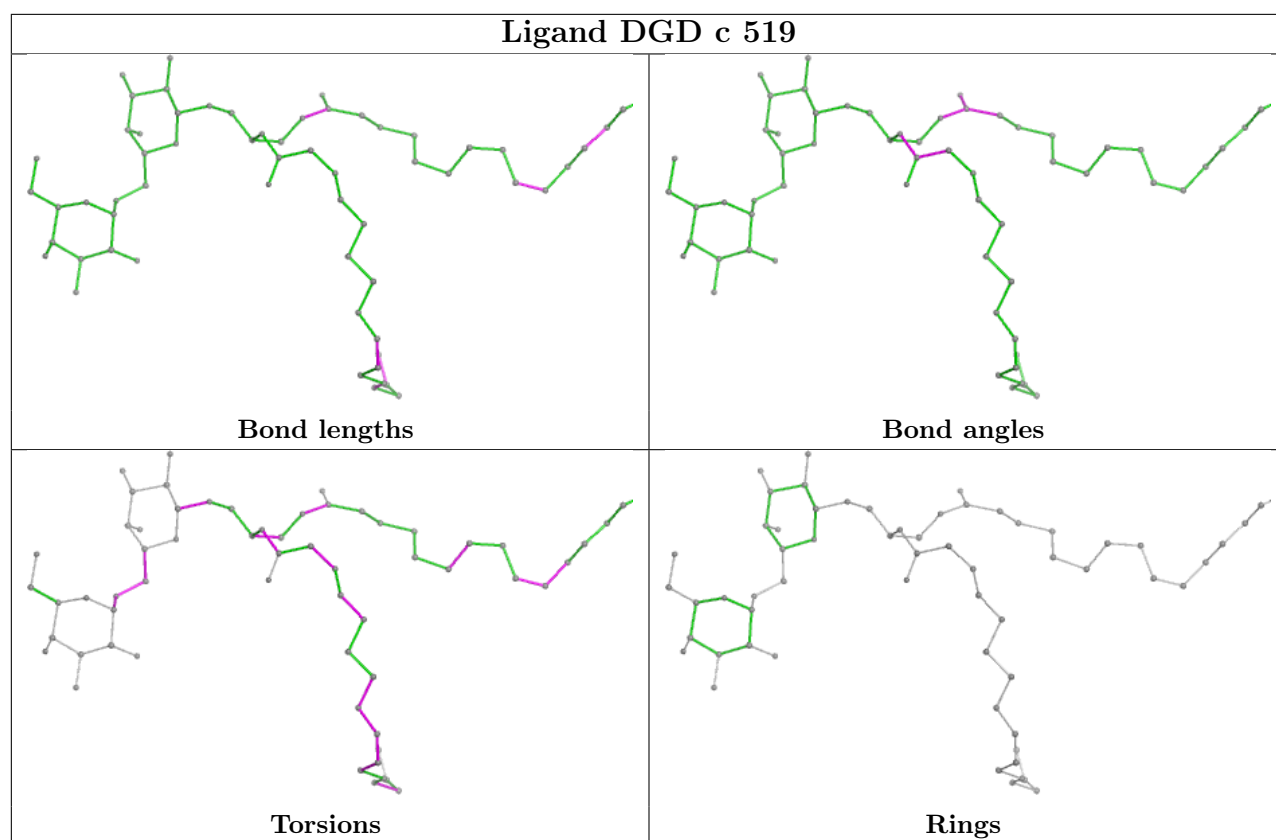


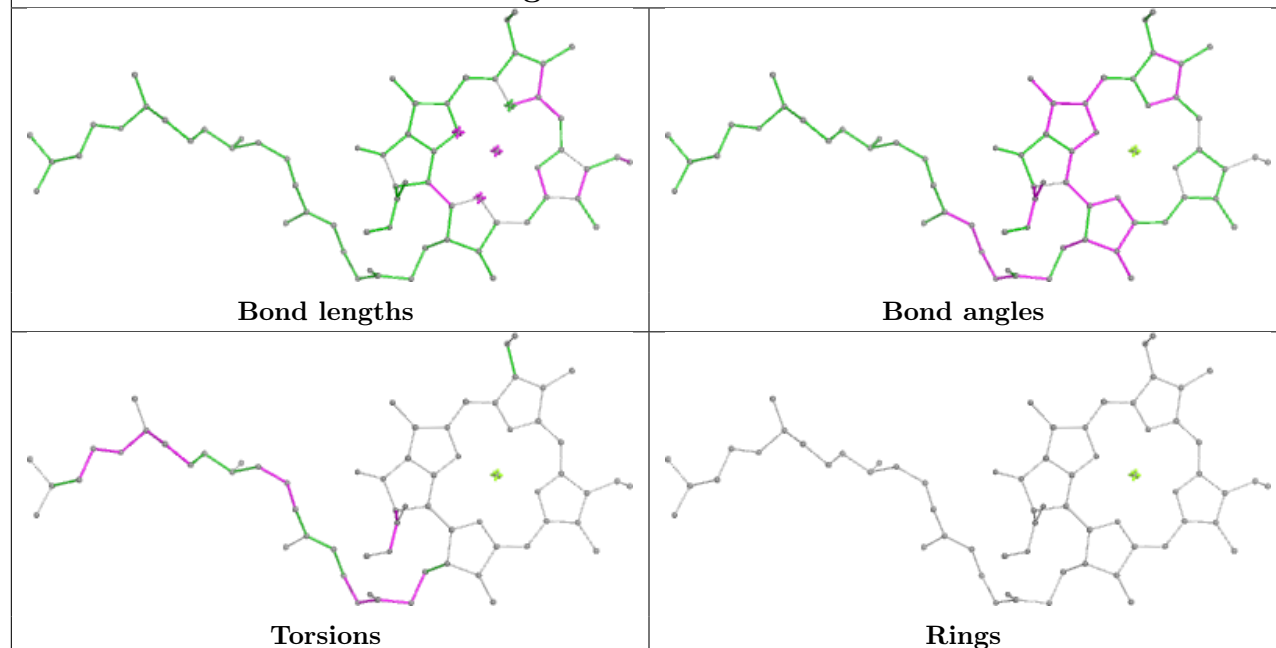
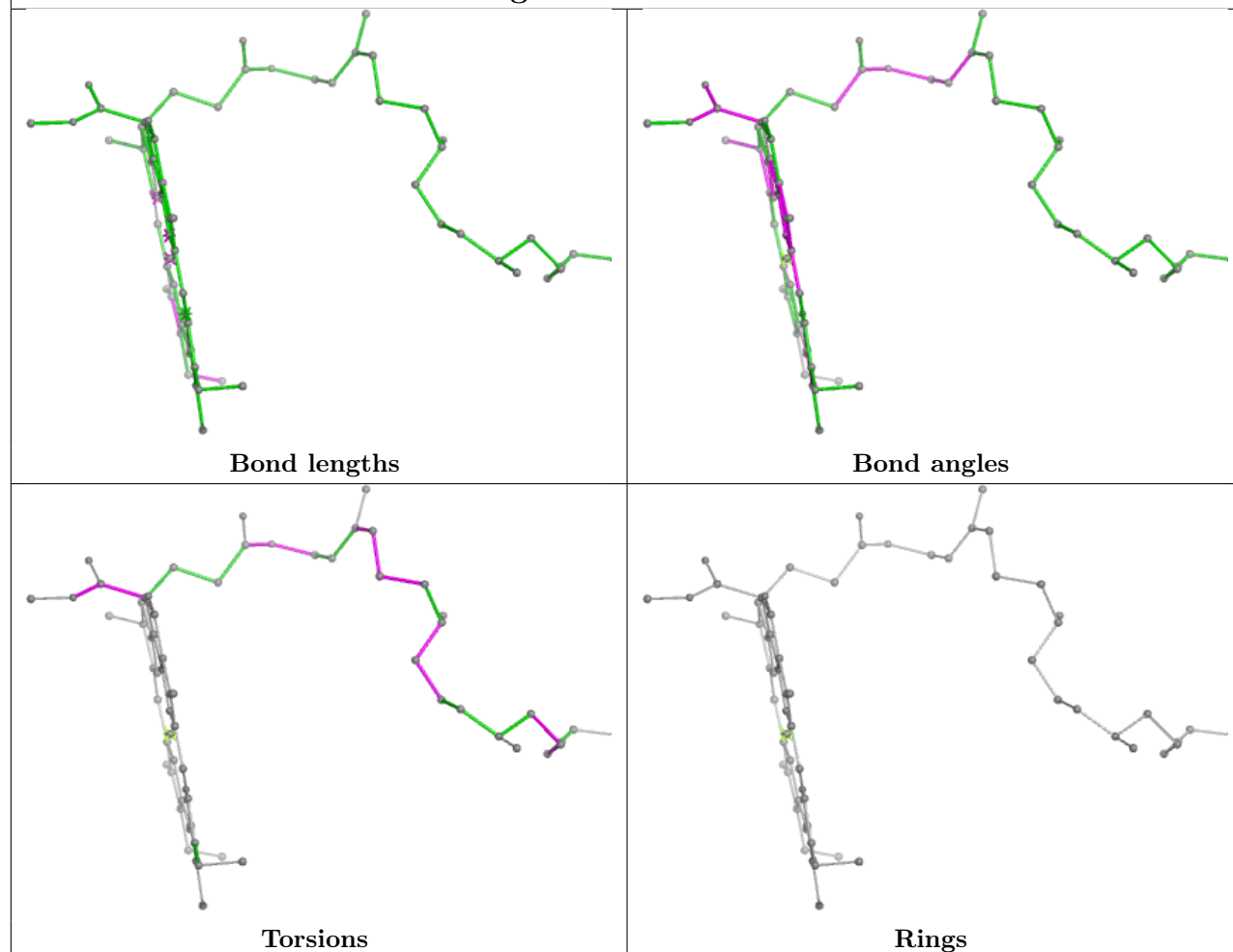


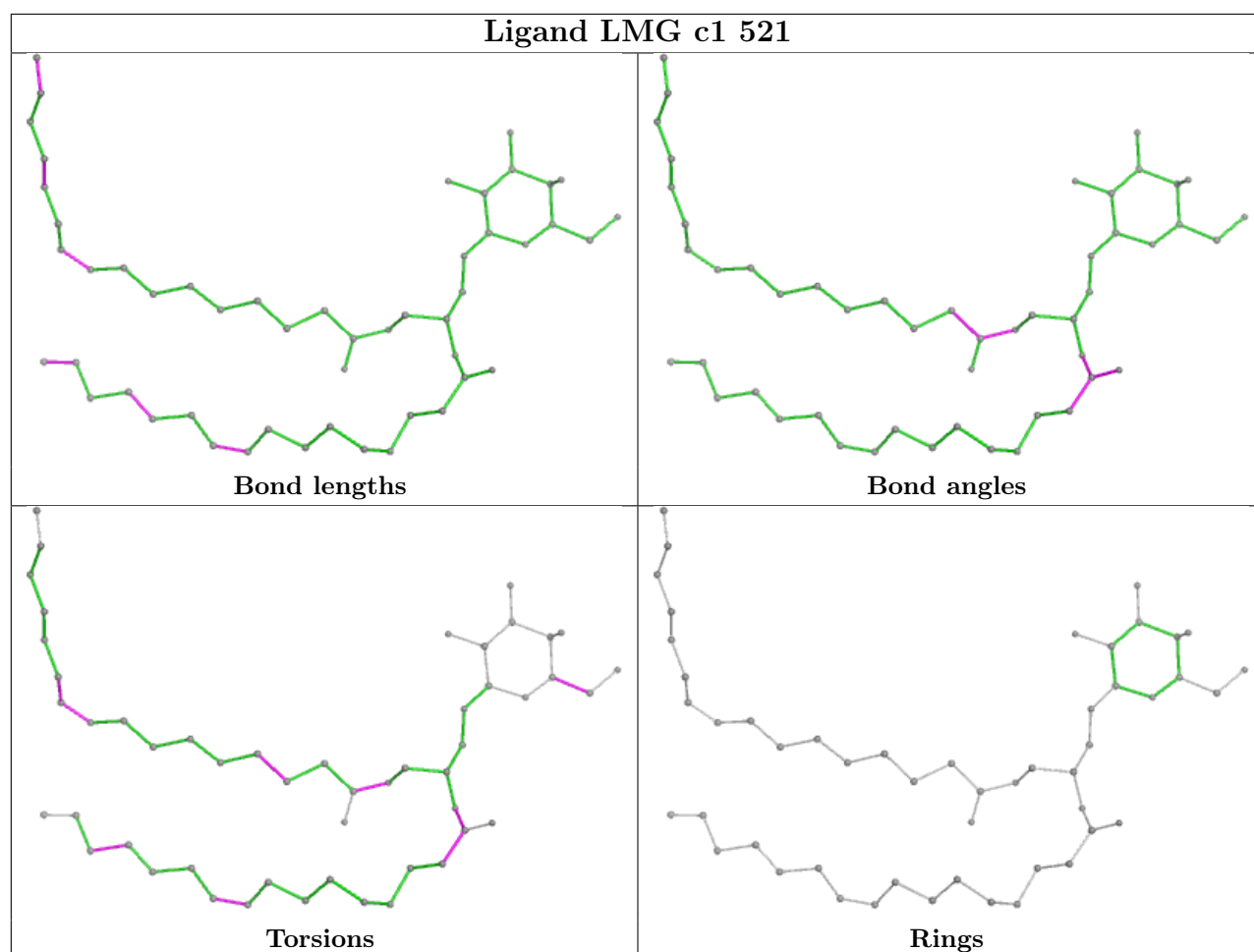


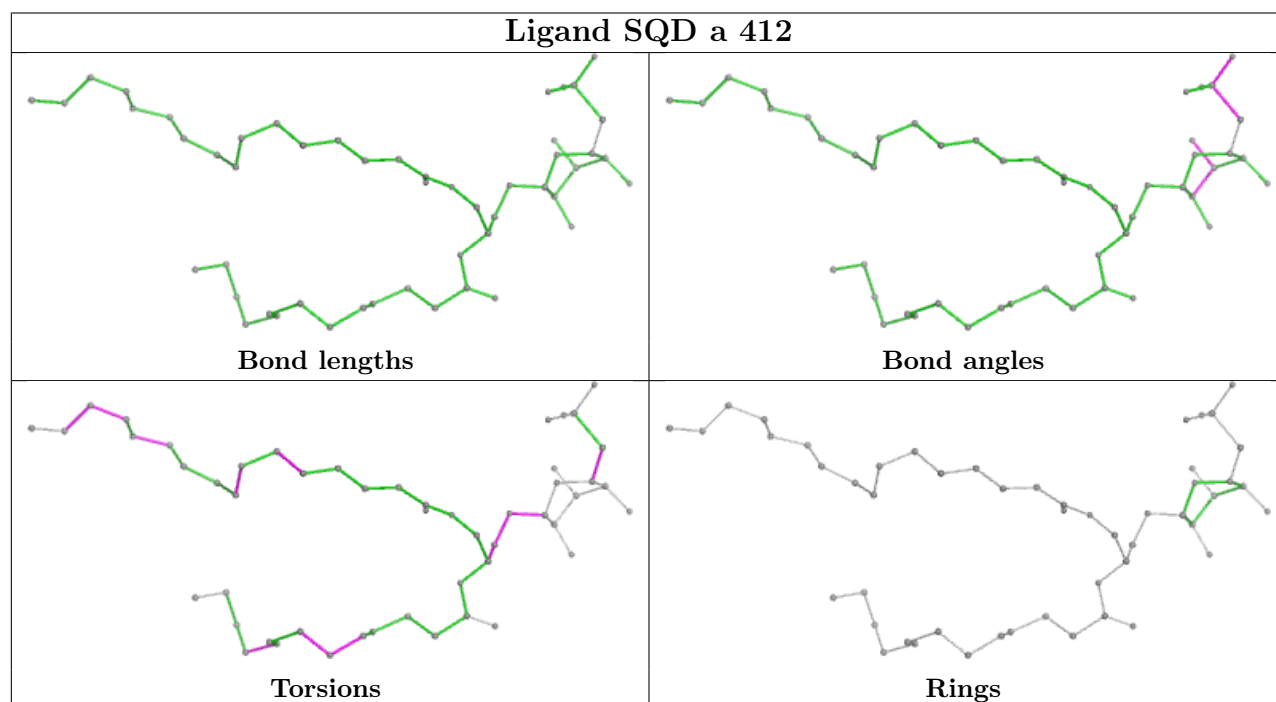
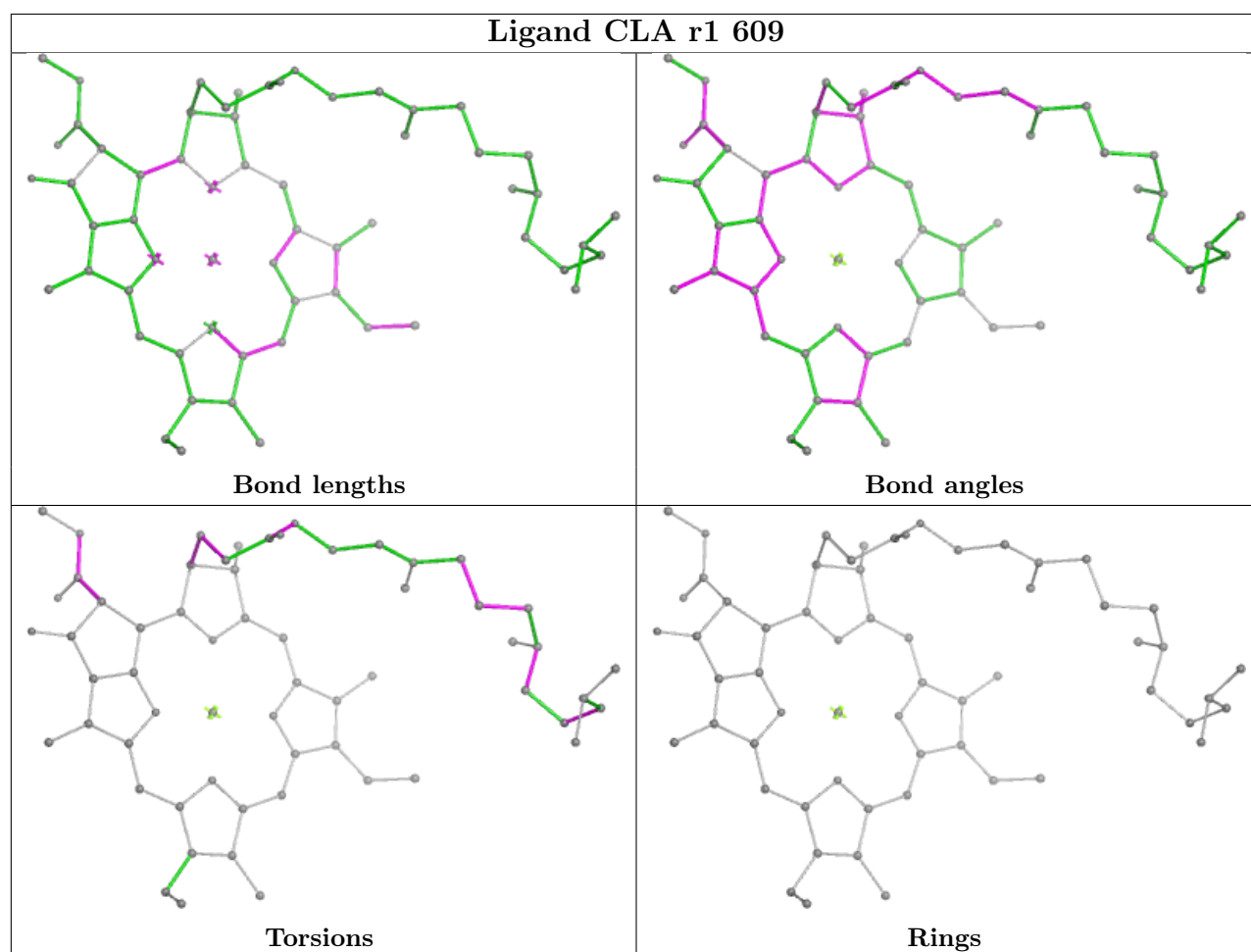


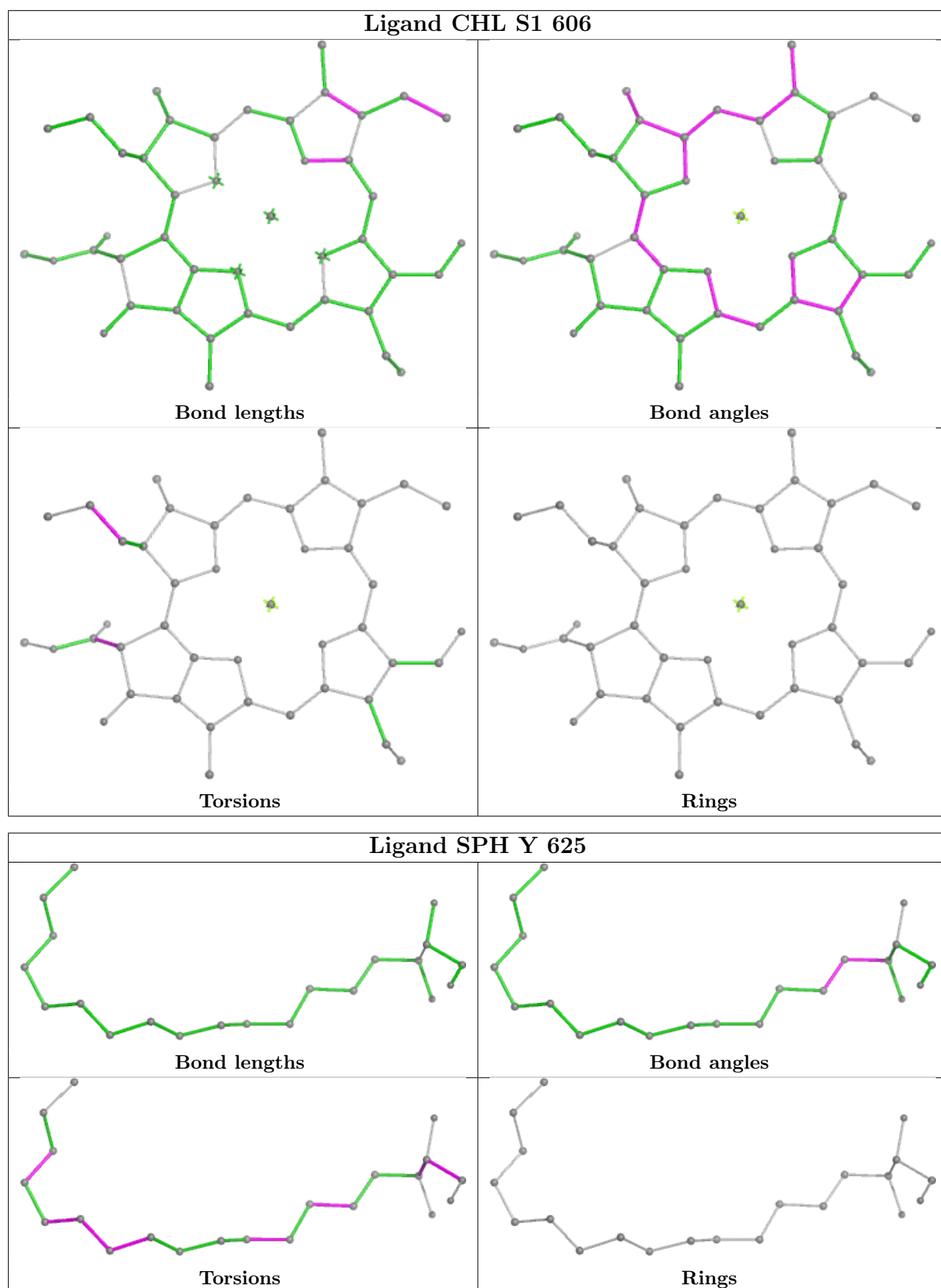


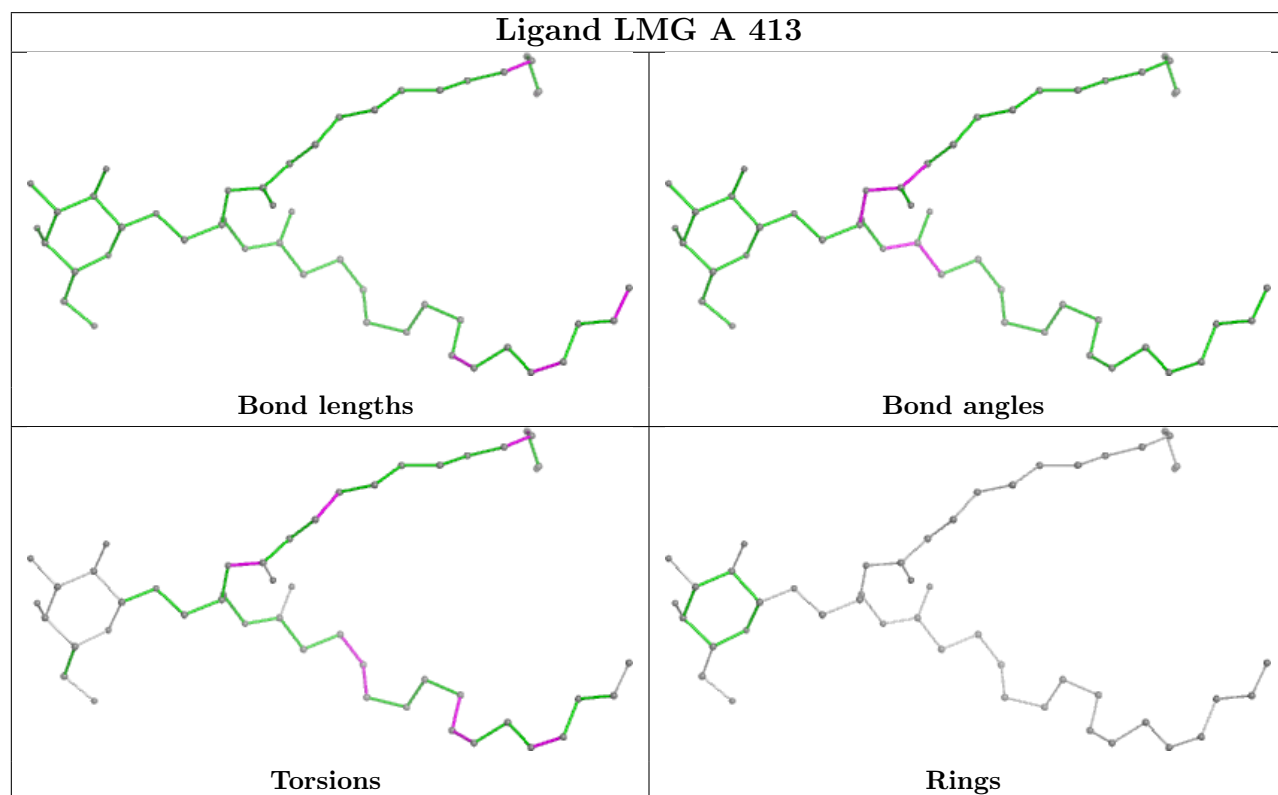
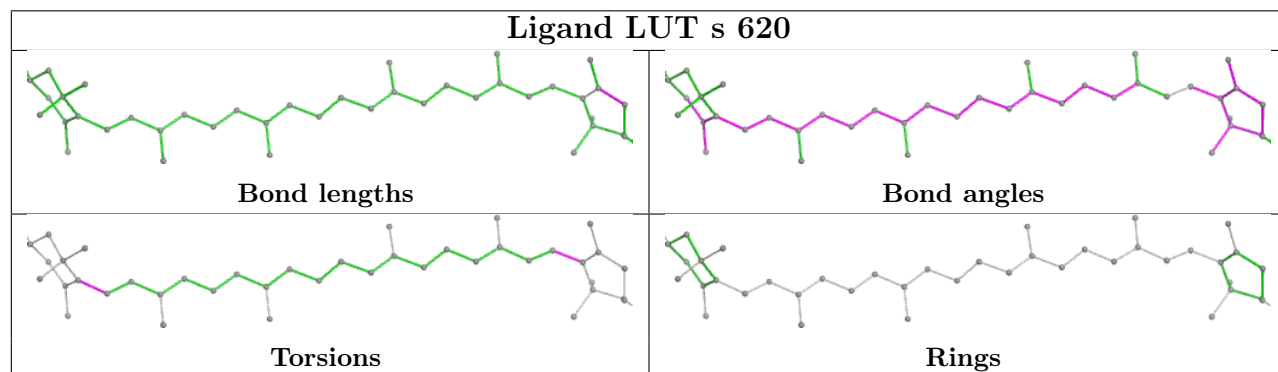
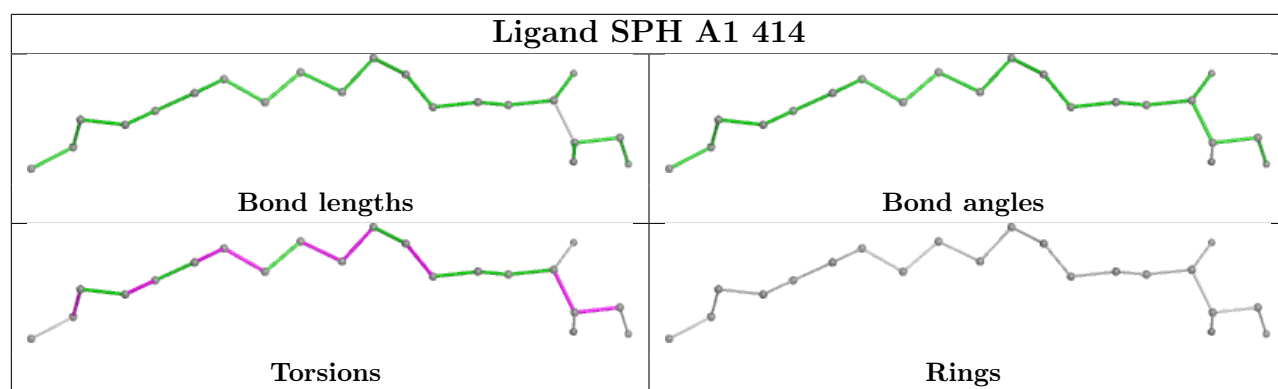


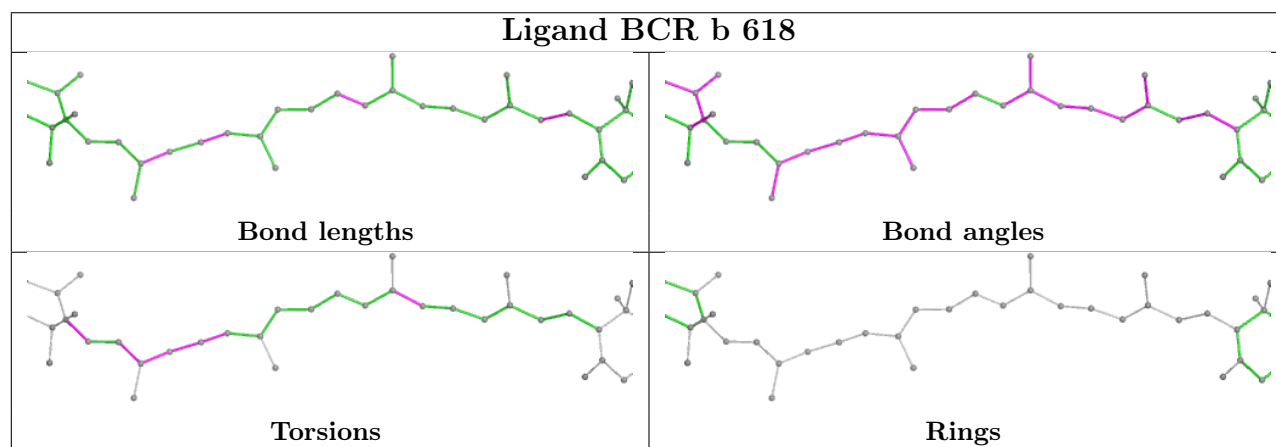
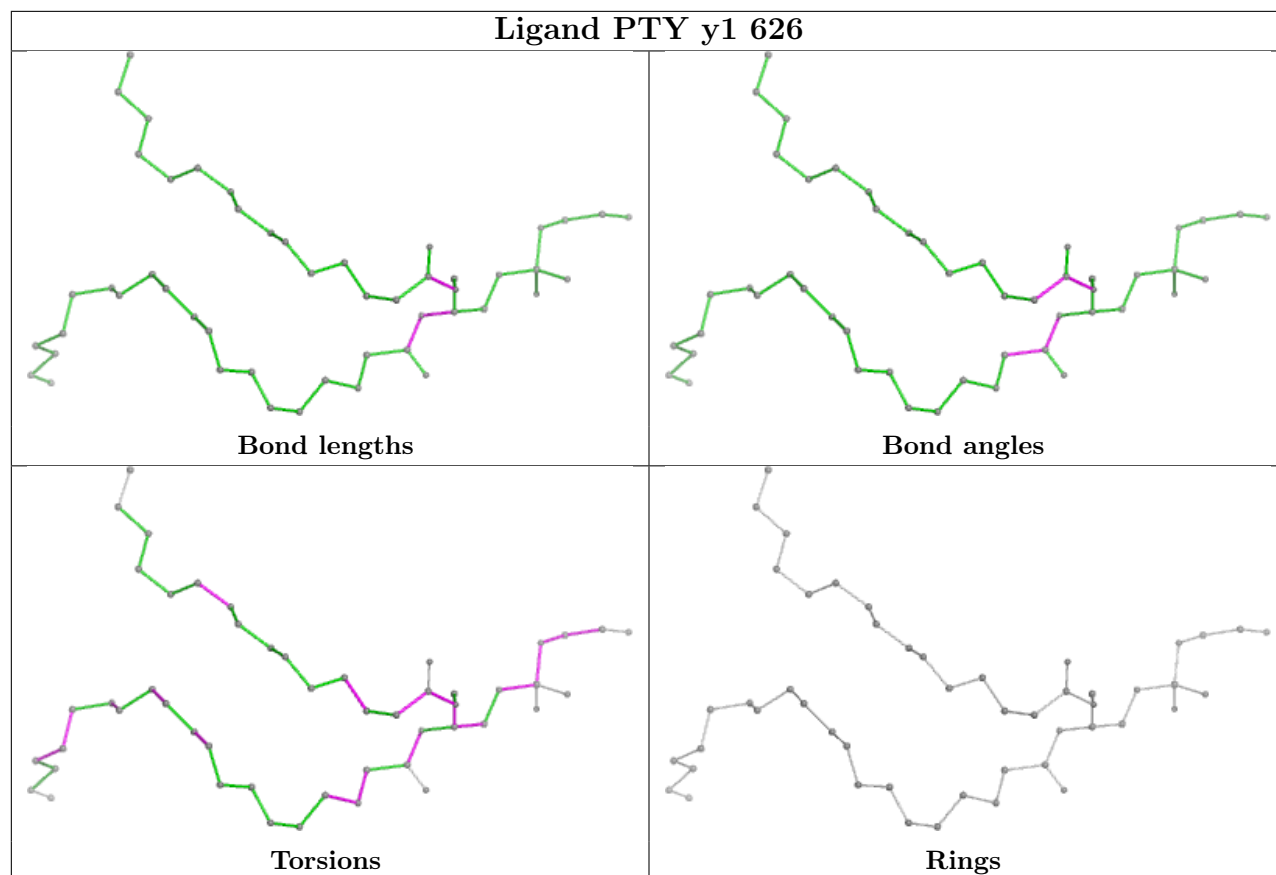
**Ligand CLA B1 603****Ligand CLA c1 506**



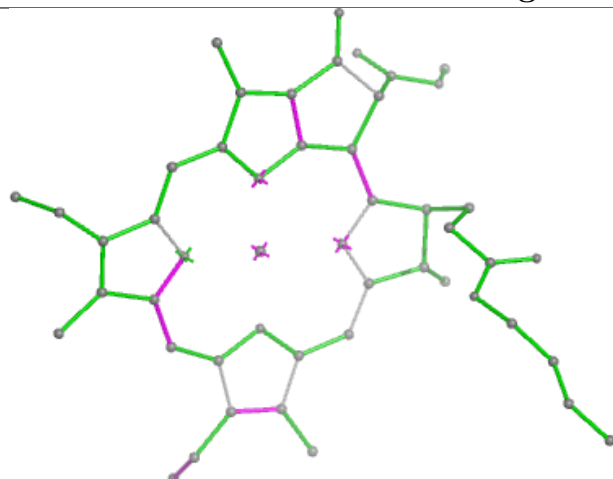




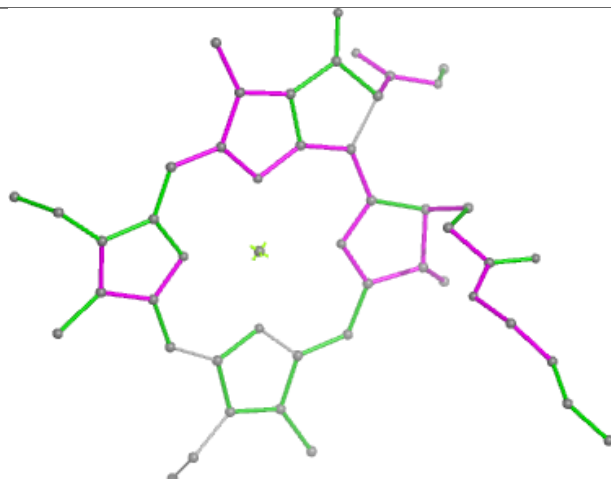




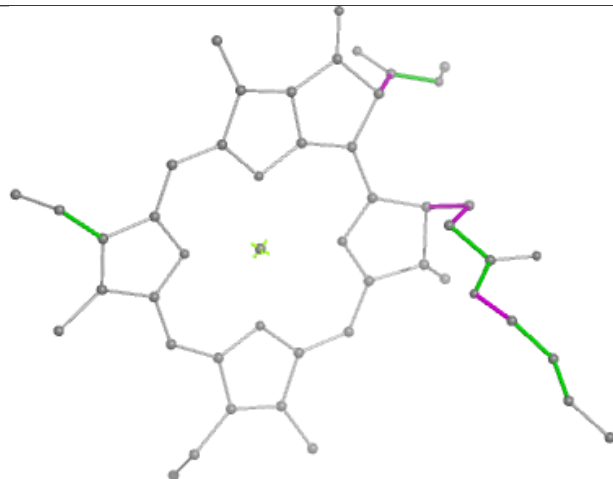
## Ligand CLA a 407



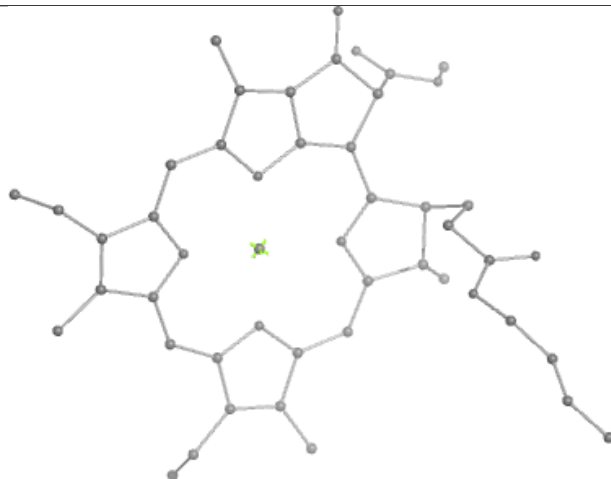
Bond lengths



Bond angles

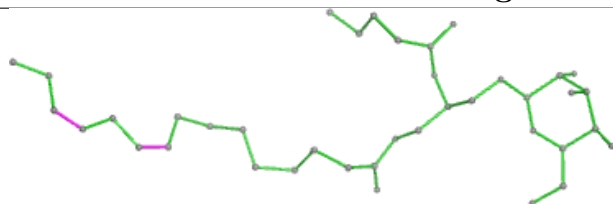


Torsions

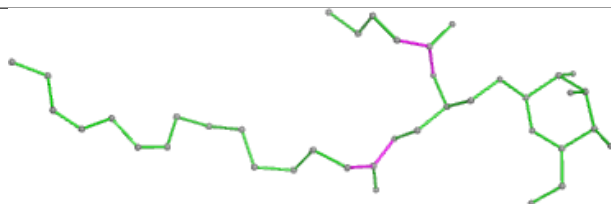


Rings

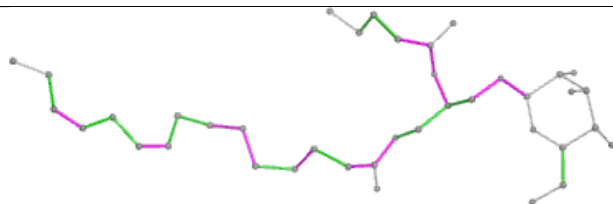
## Ligand LMG W1 201



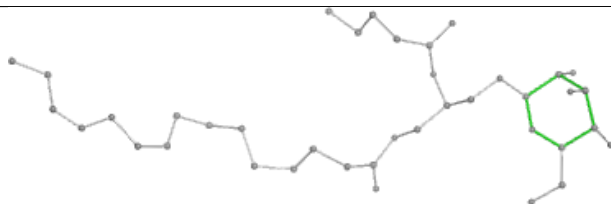
Bond lengths



Bond angles

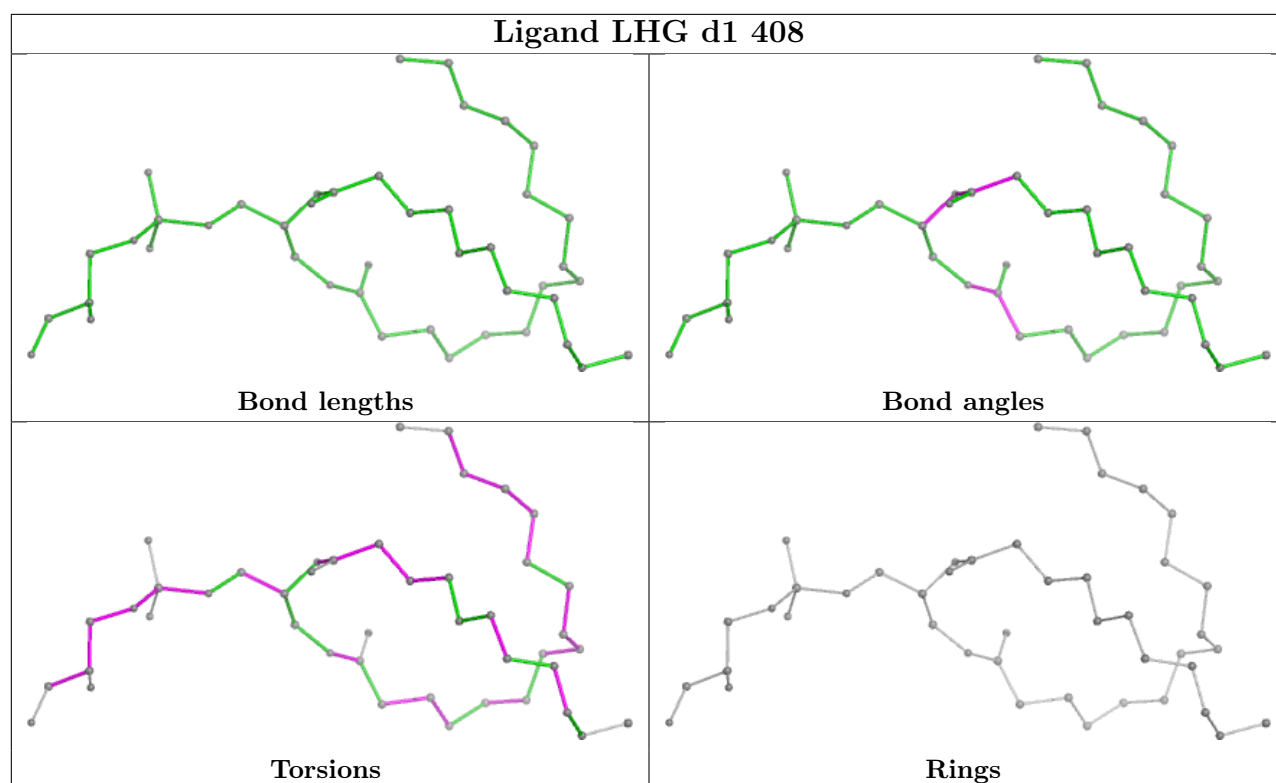


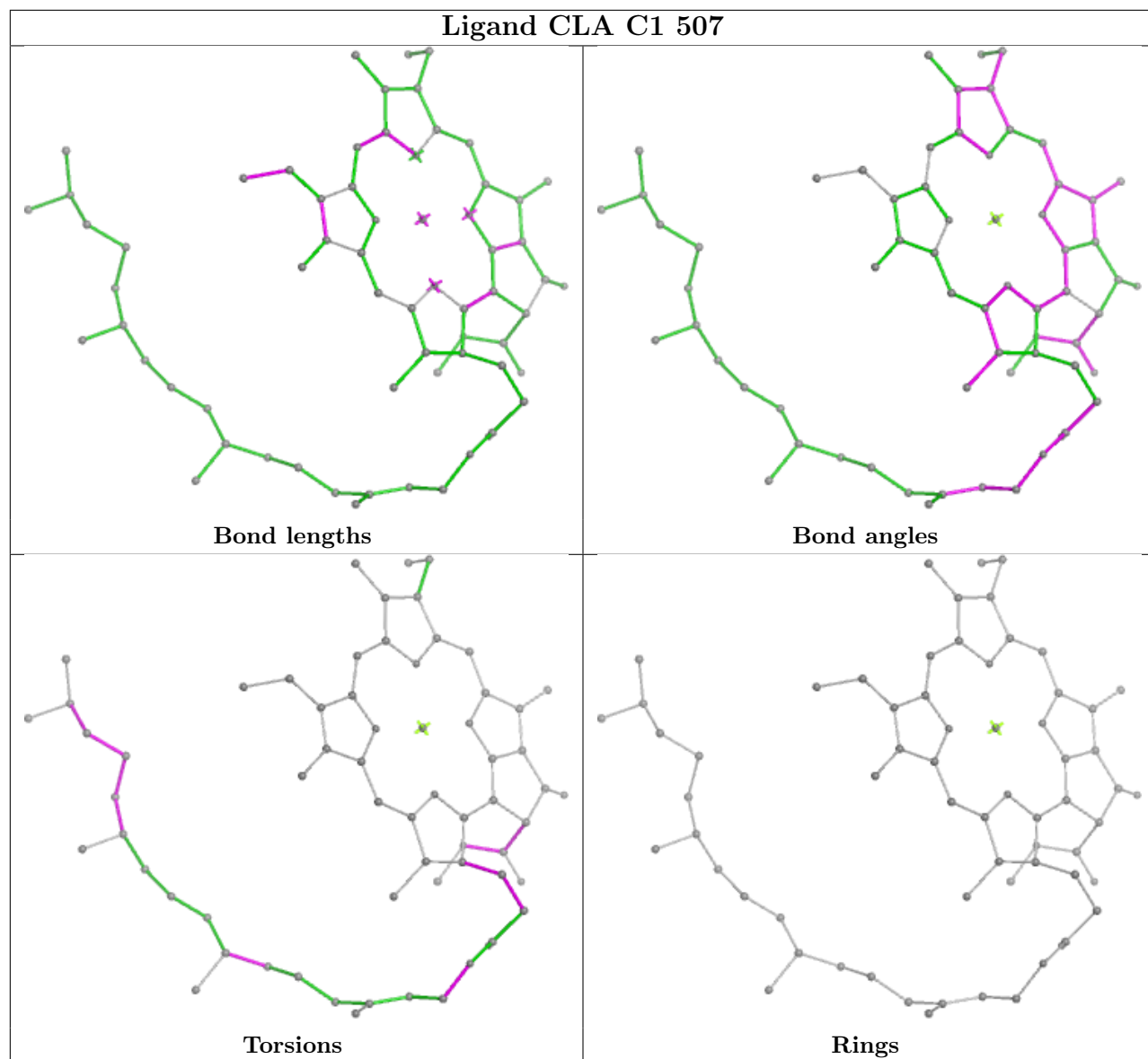
Torsions

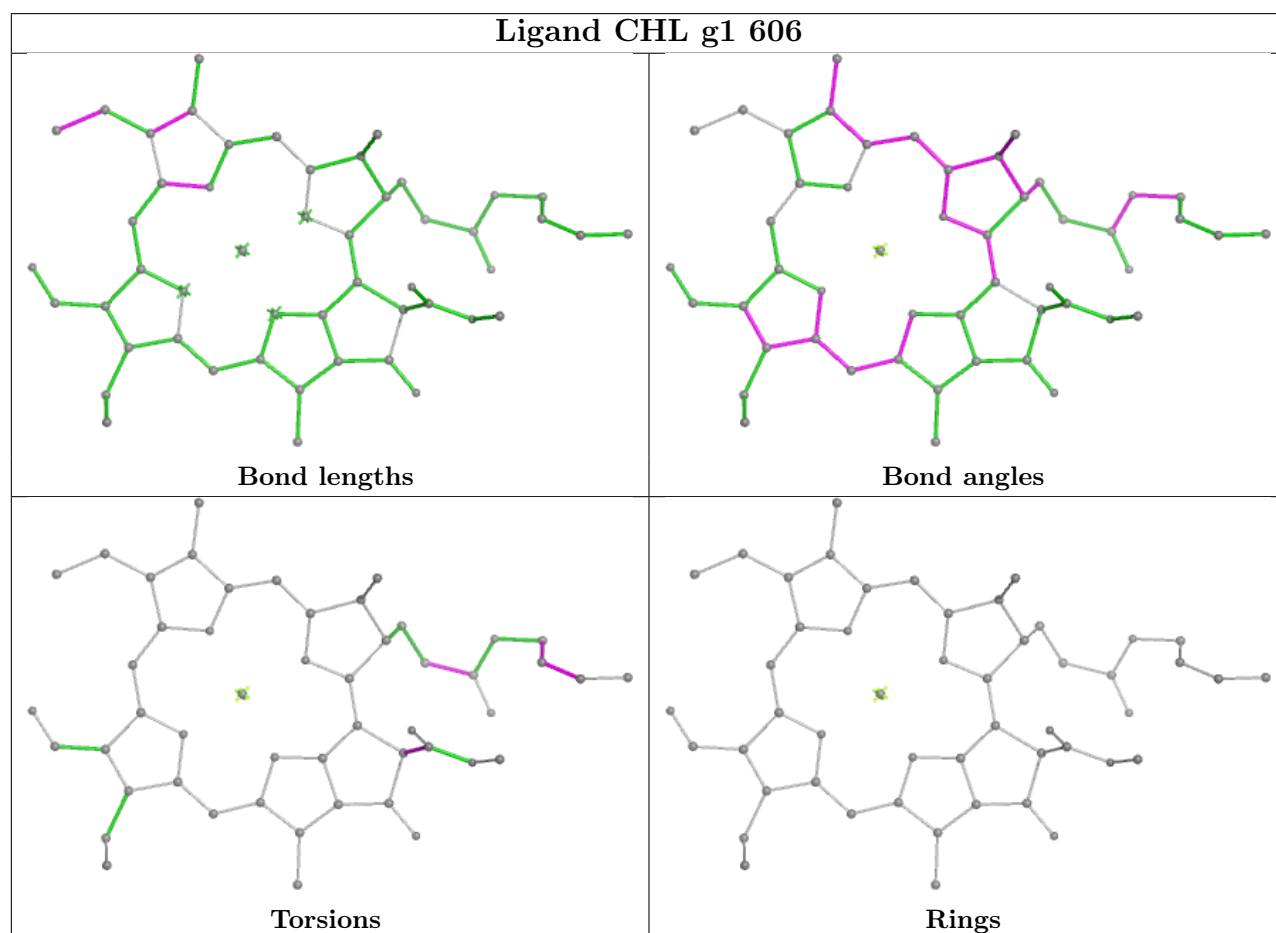
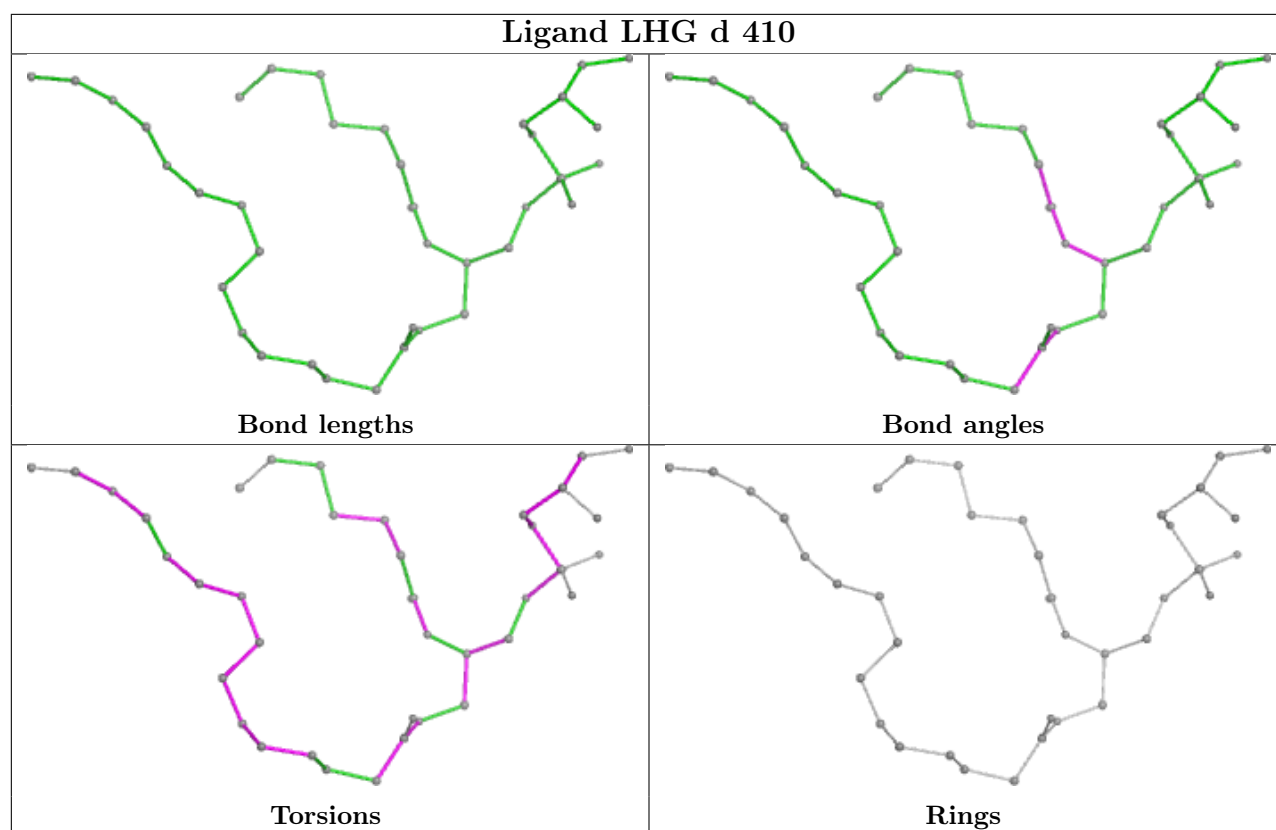


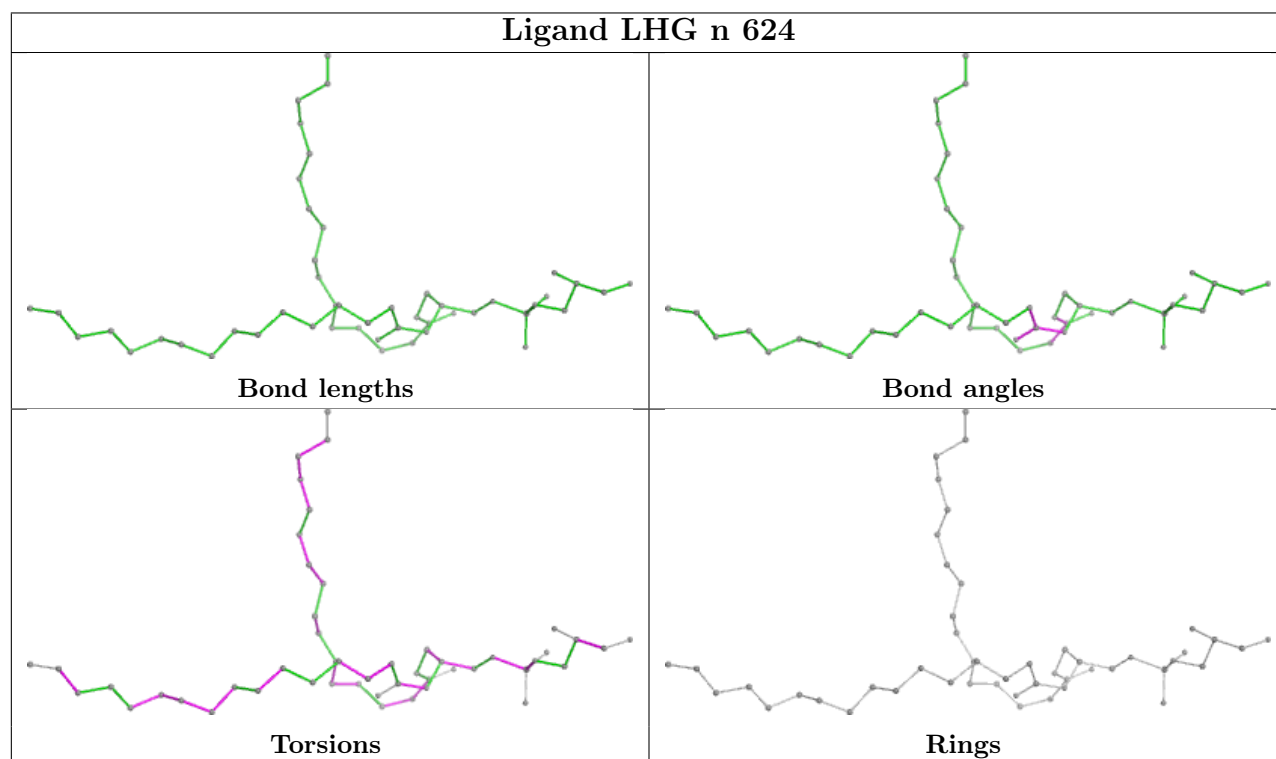
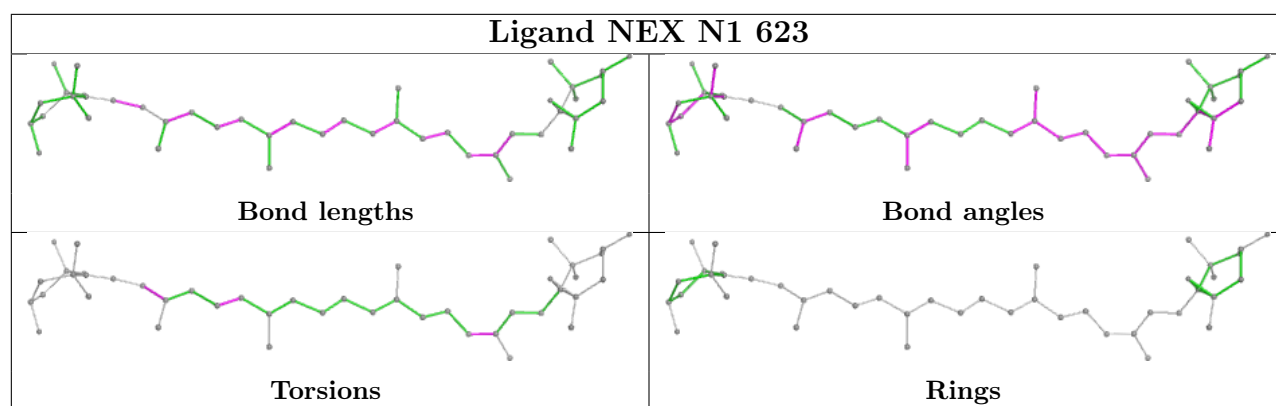
Rings

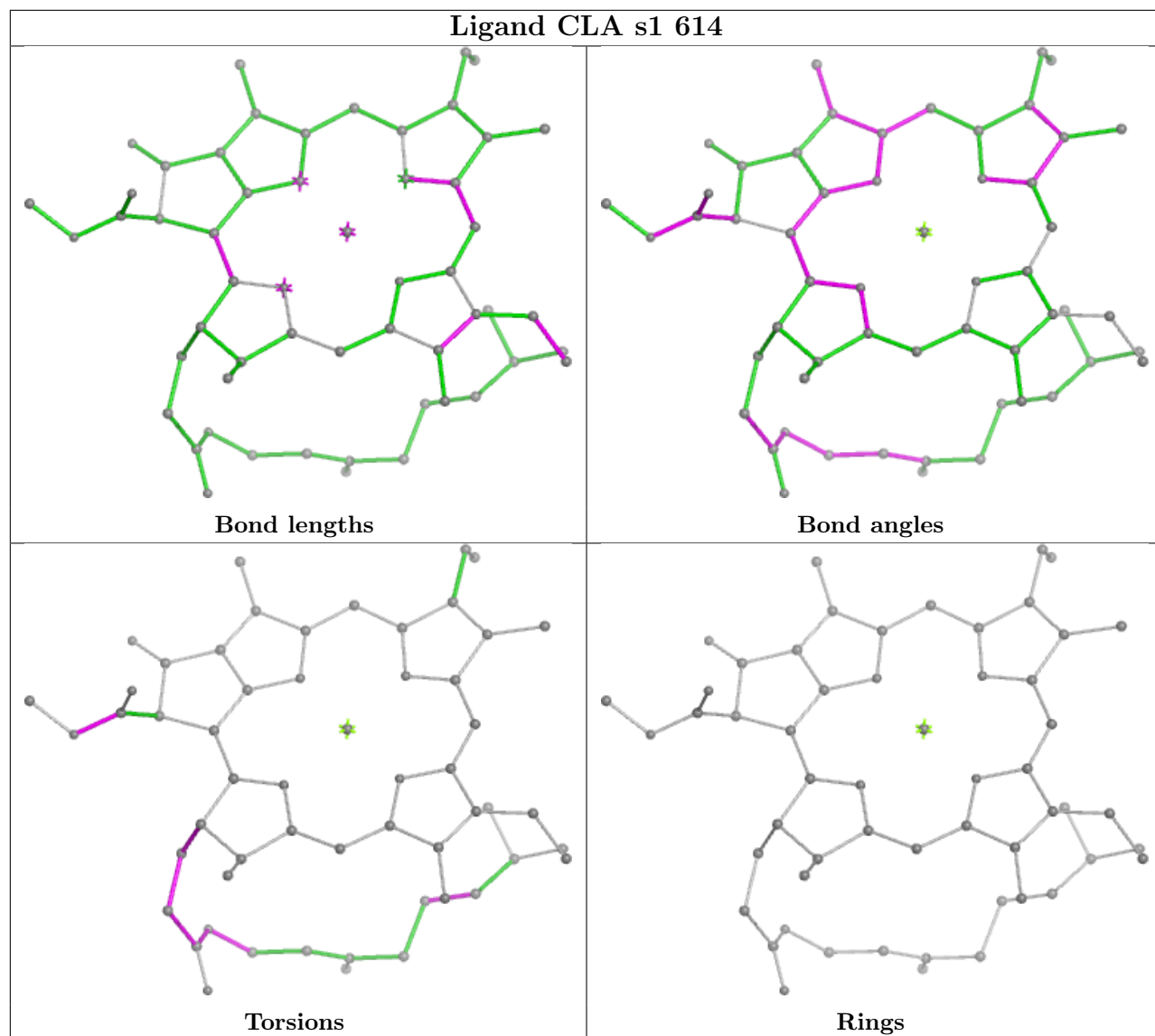


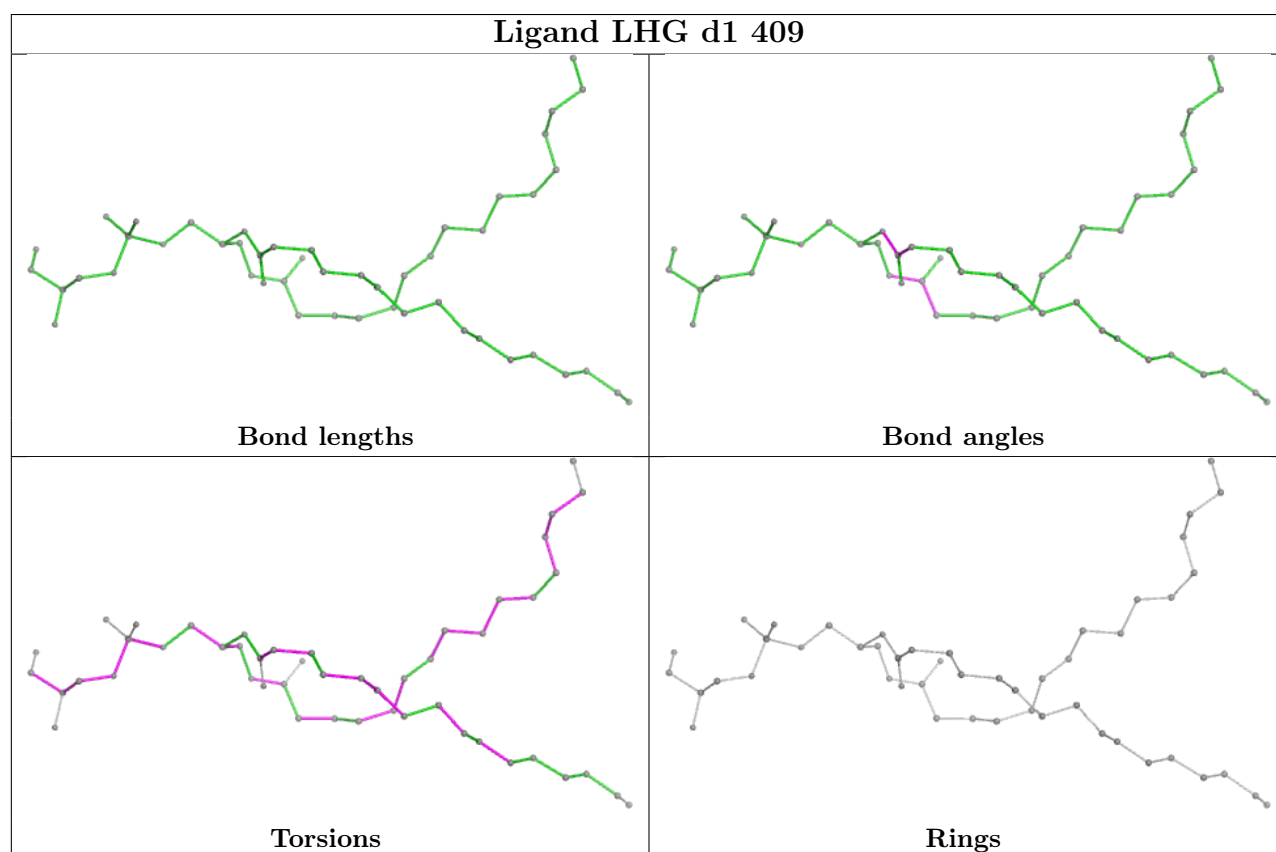
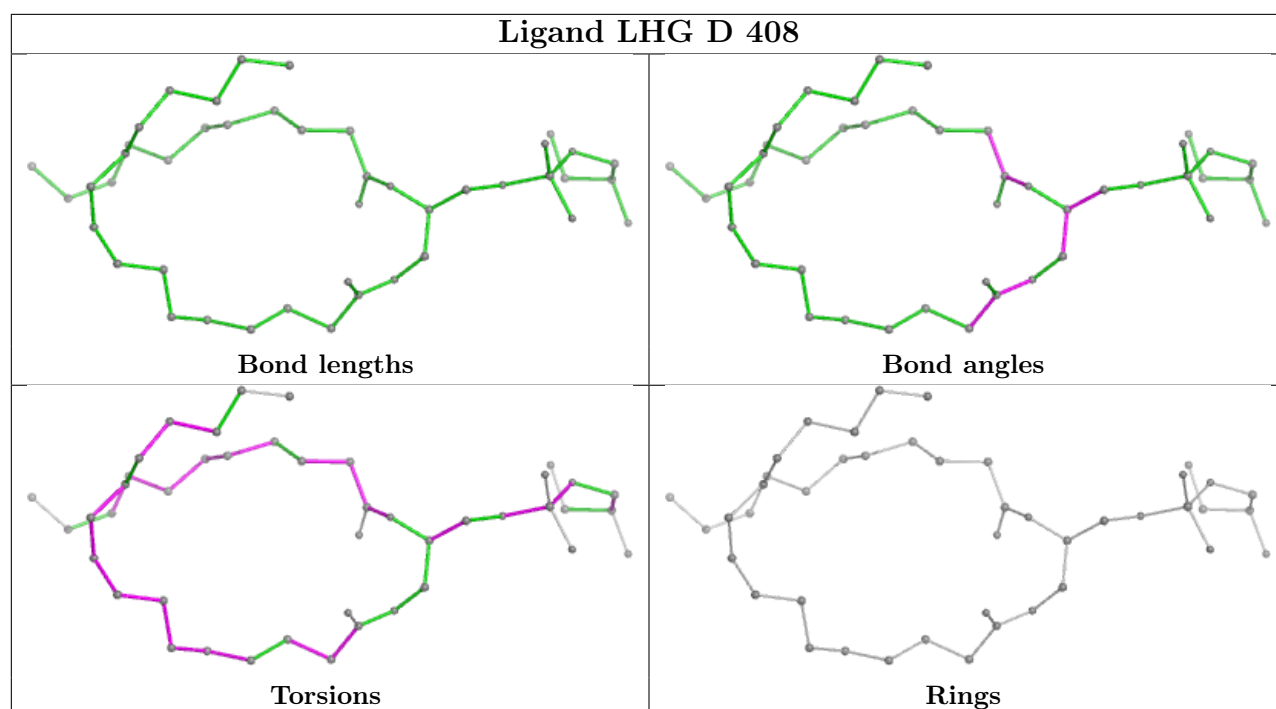




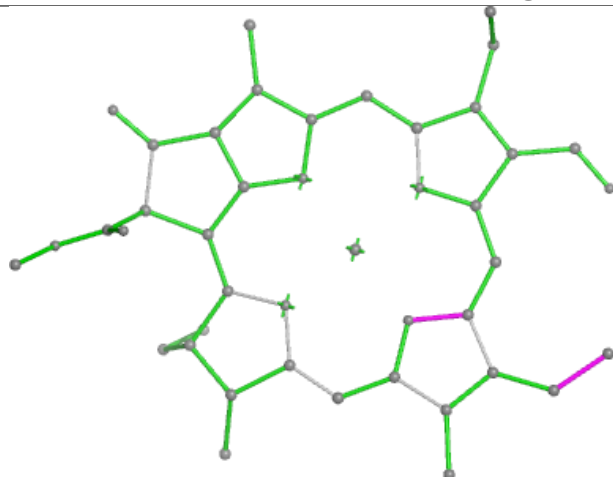




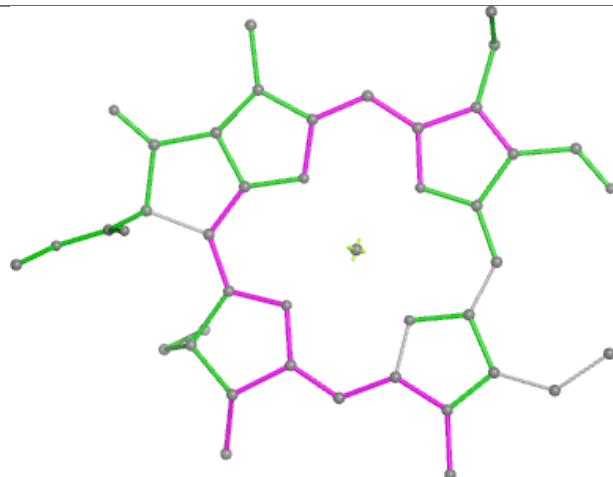




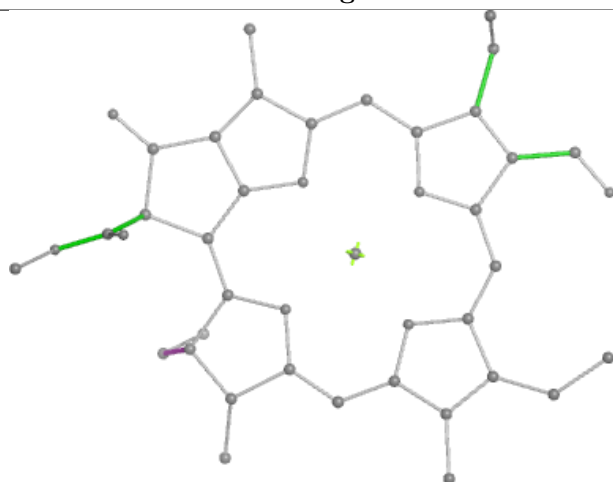
## Ligand CHL s 607



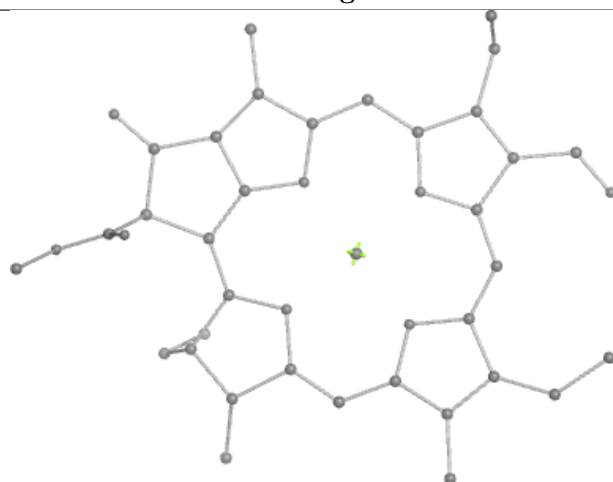
Bond lengths



Bond angles

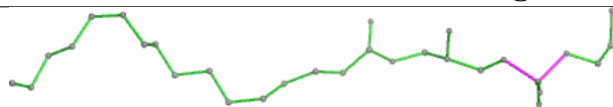


Torsions

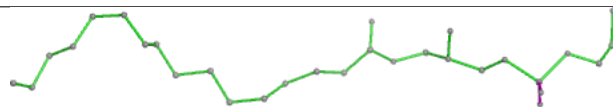


Rings

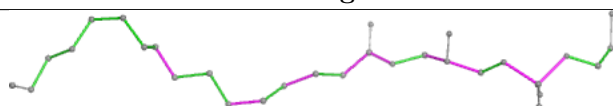
## Ligand LPX s1 625



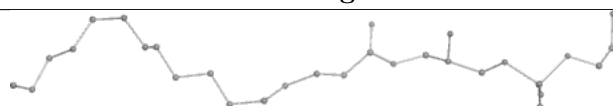
Bond lengths



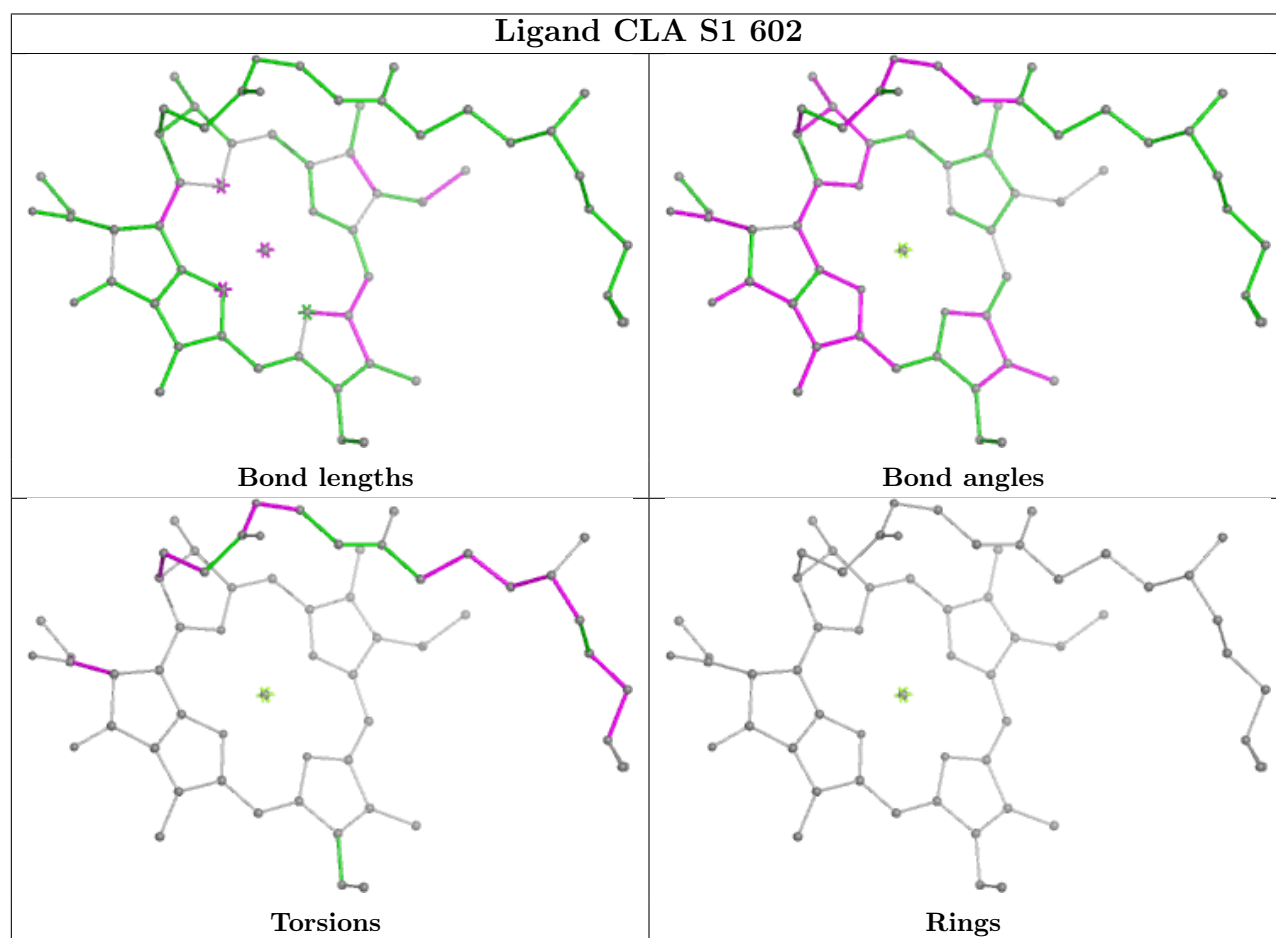
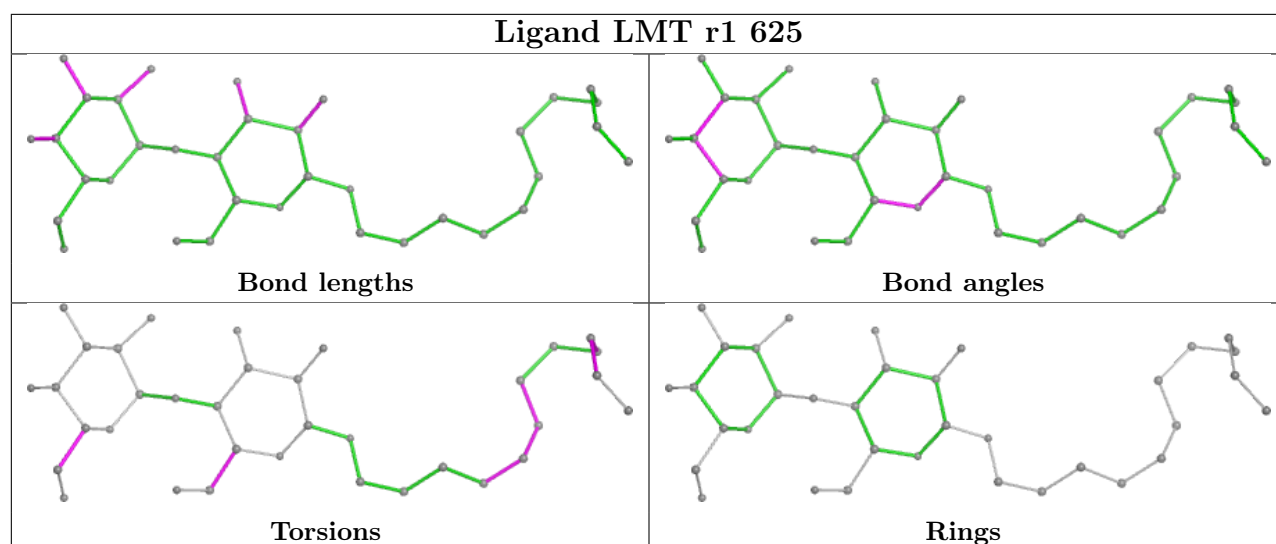
Bond angles



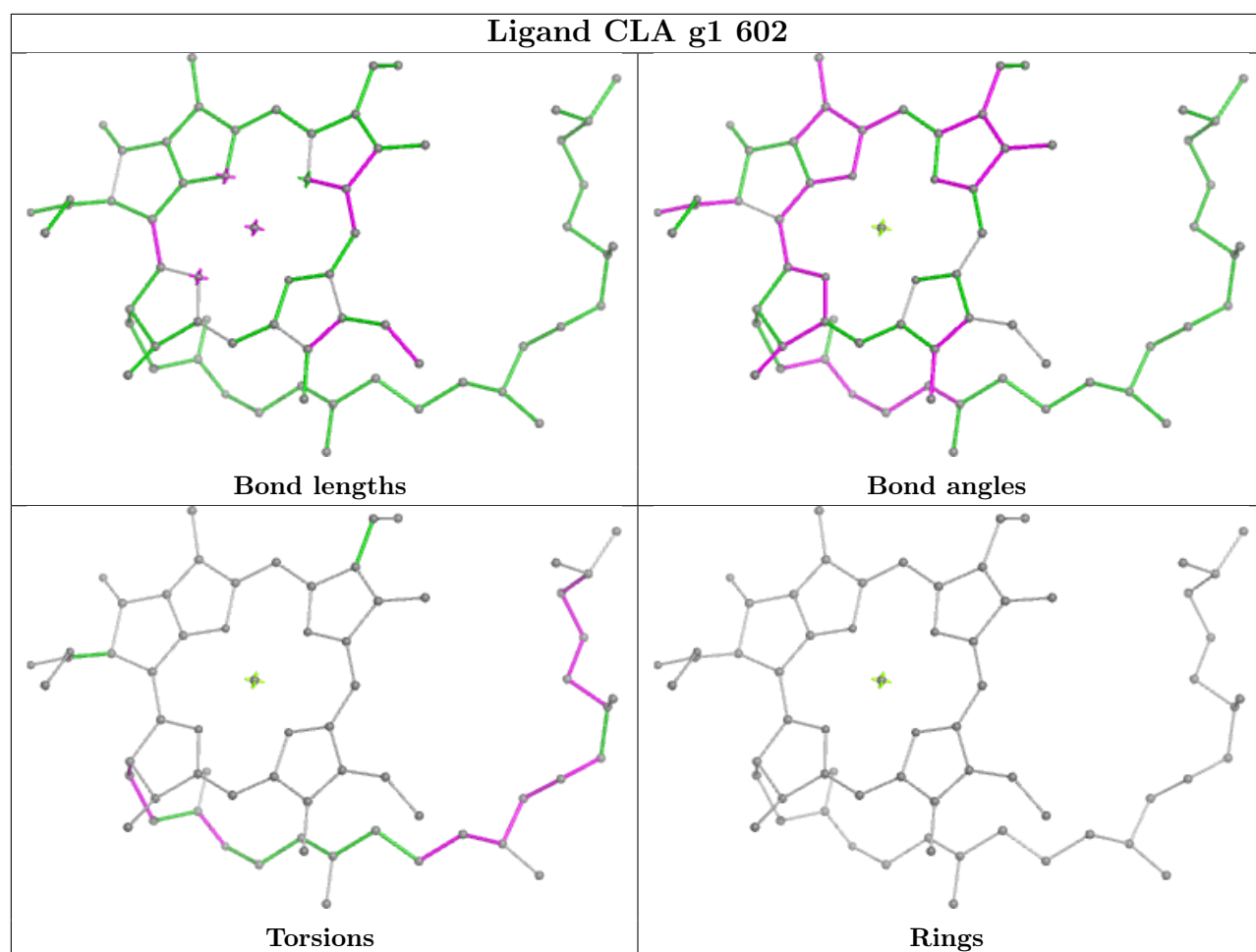
Torsions

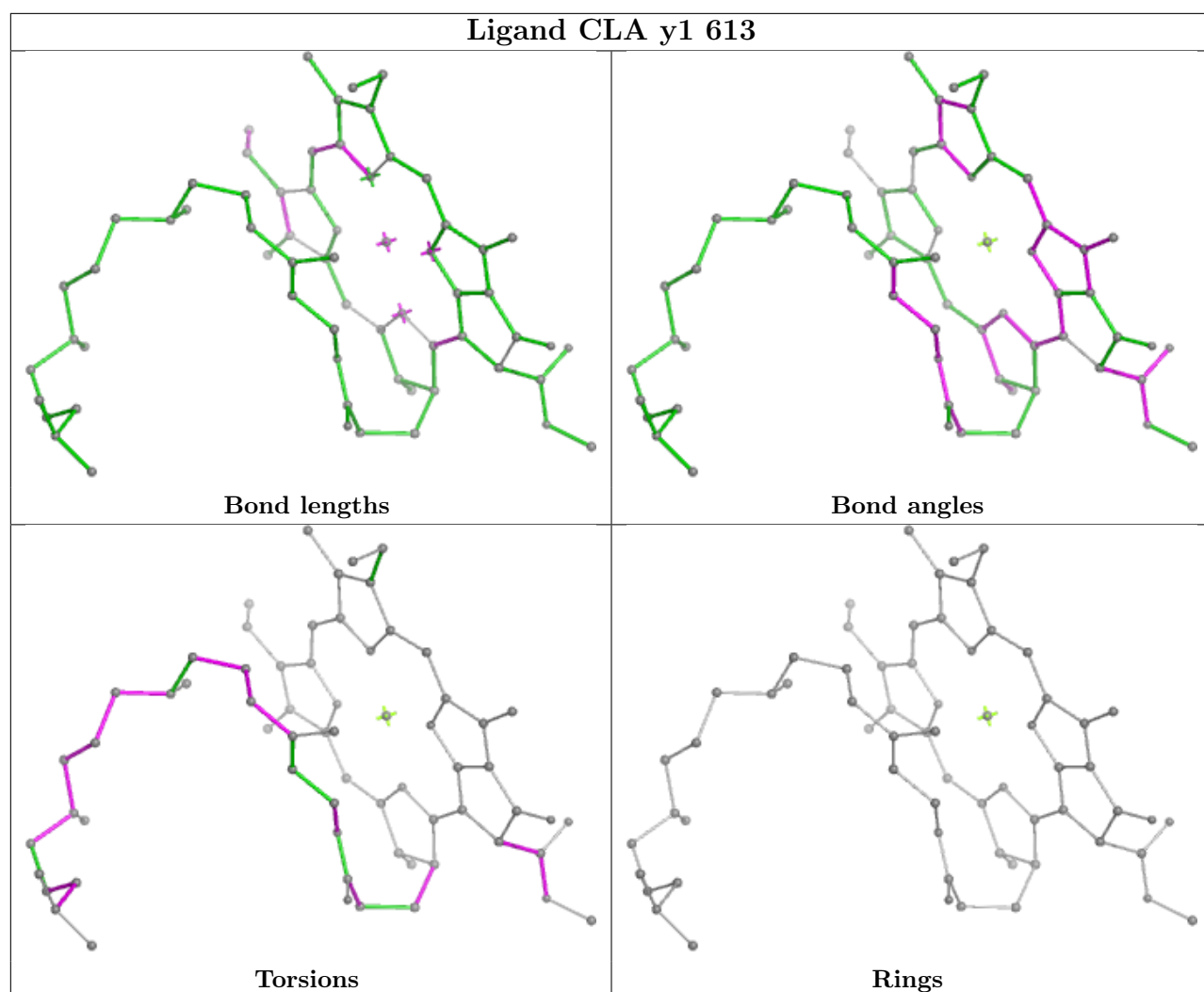


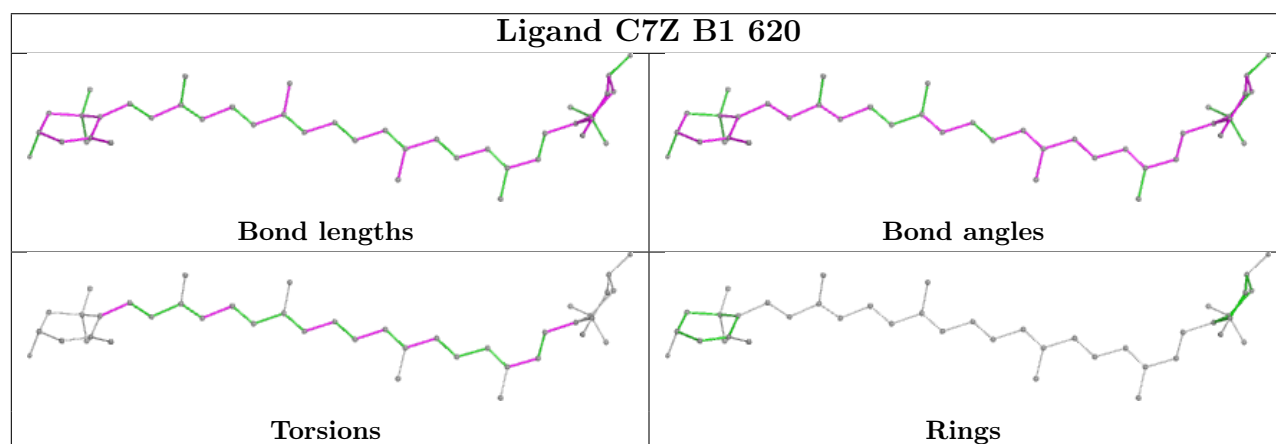
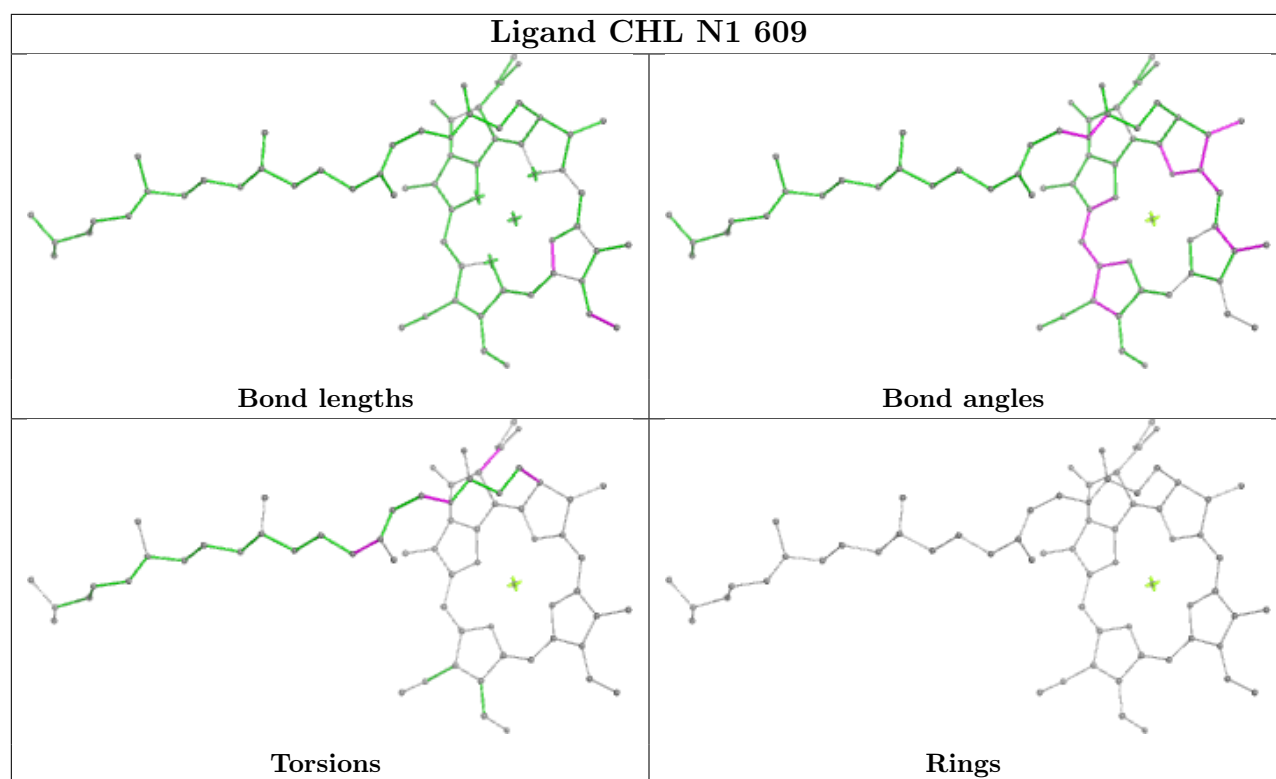
Rings

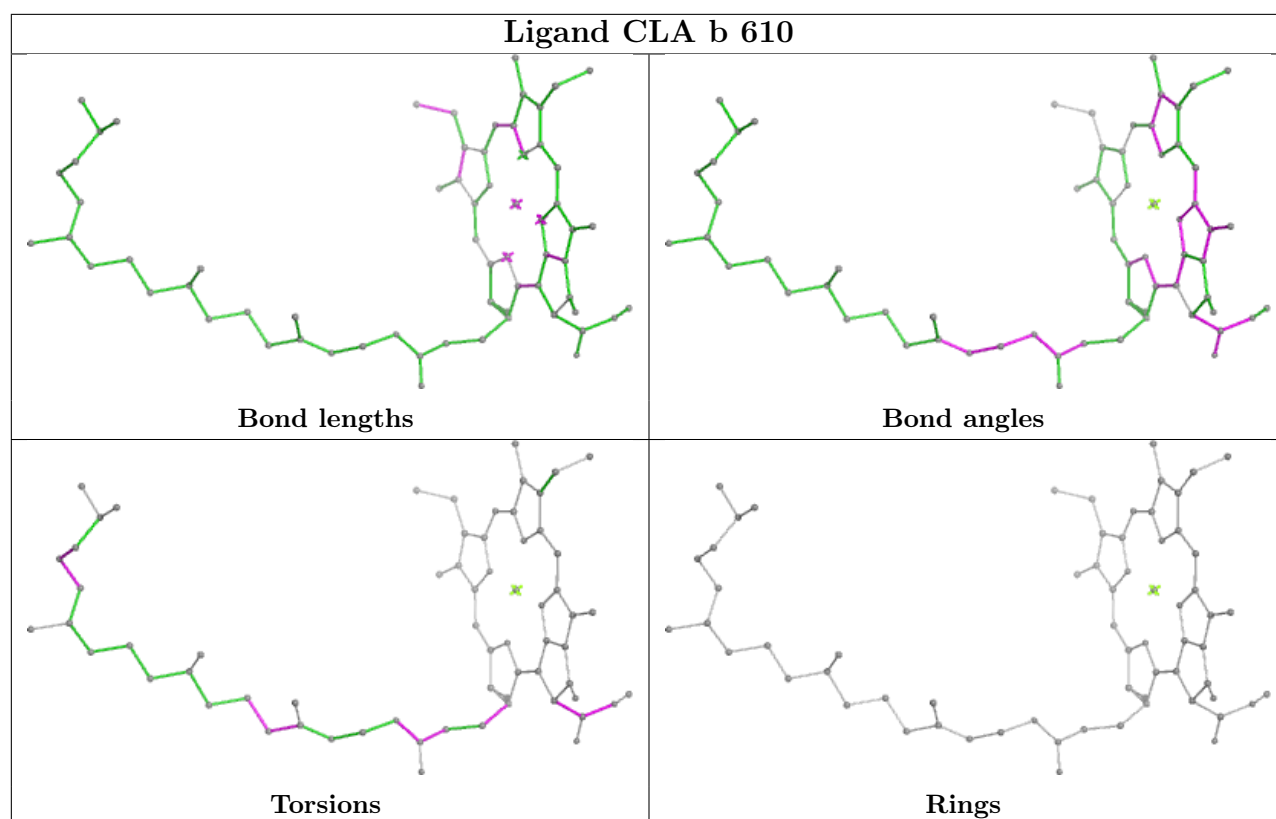


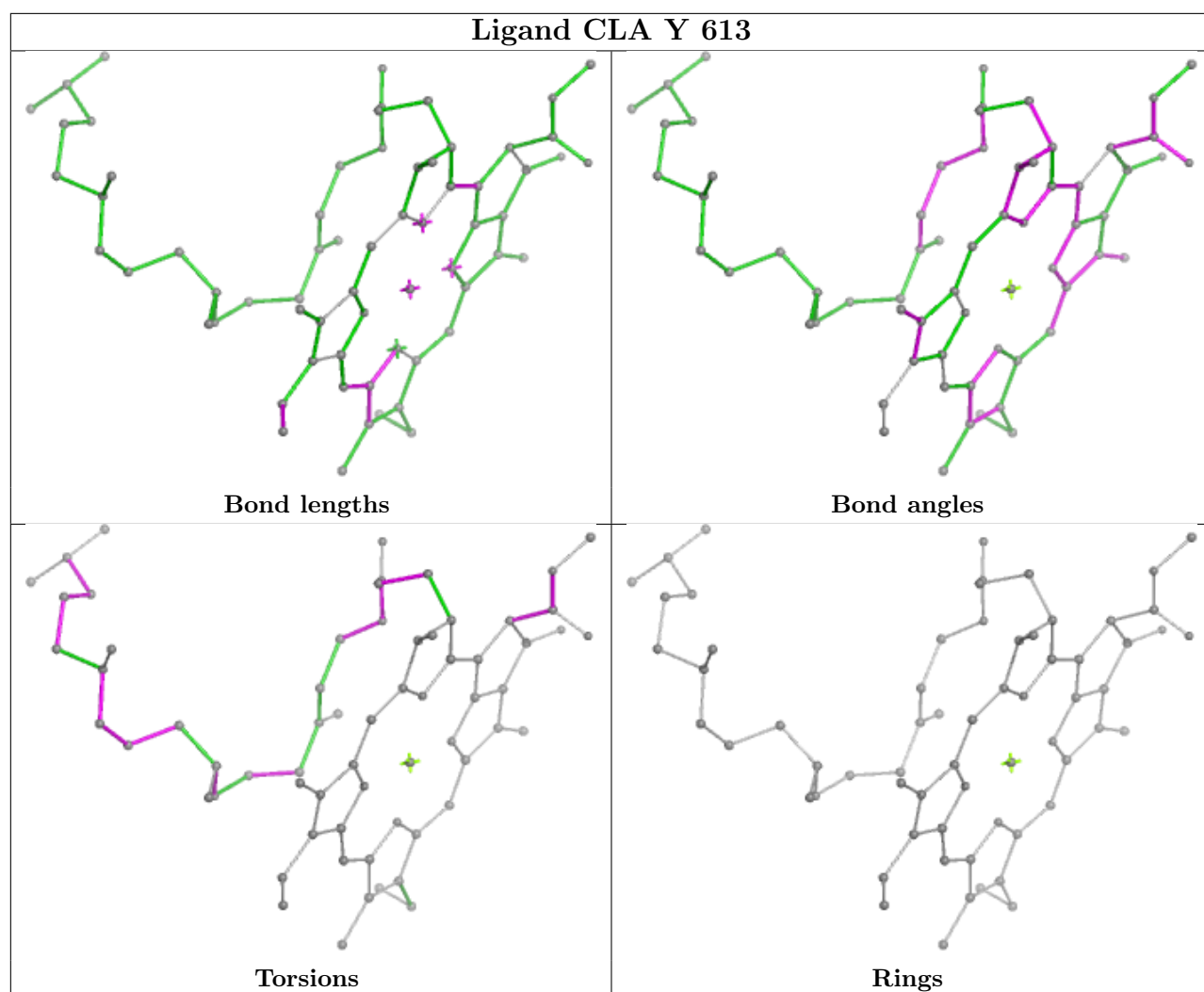




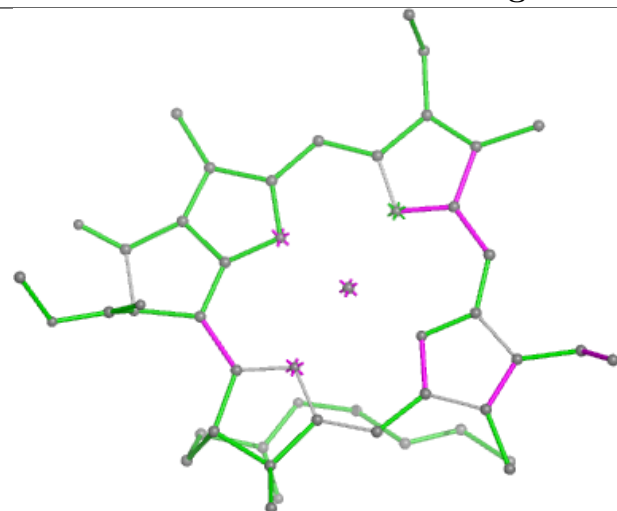




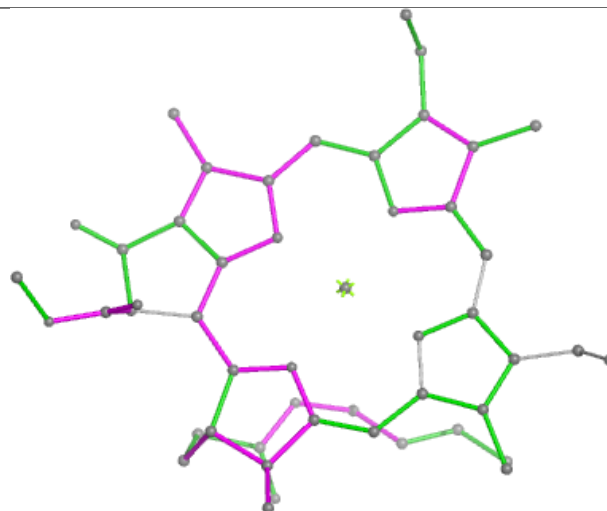




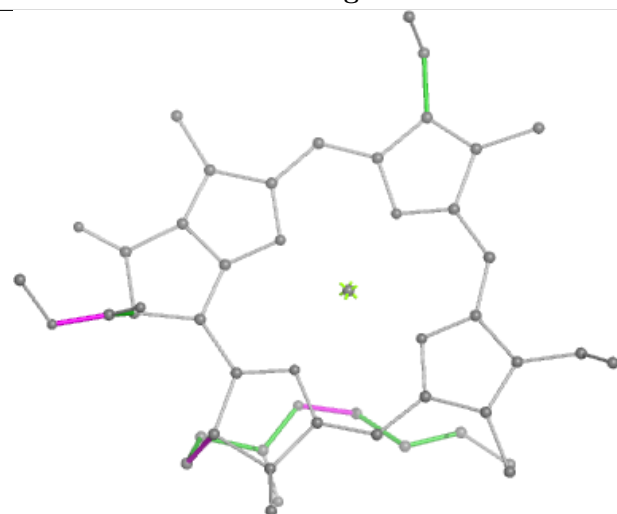
## Ligand CLA N1 614



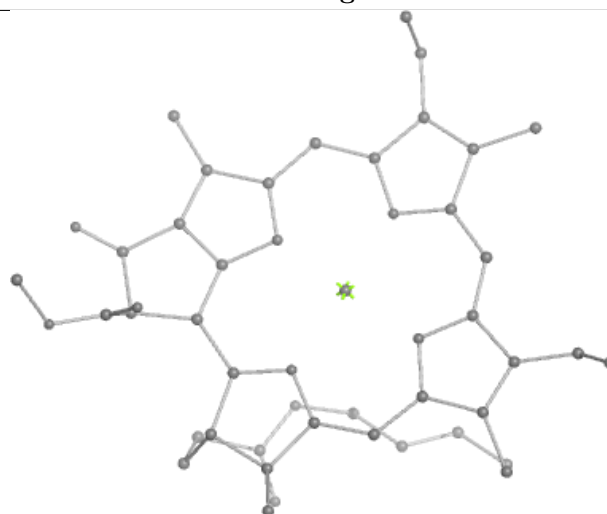
Bond lengths



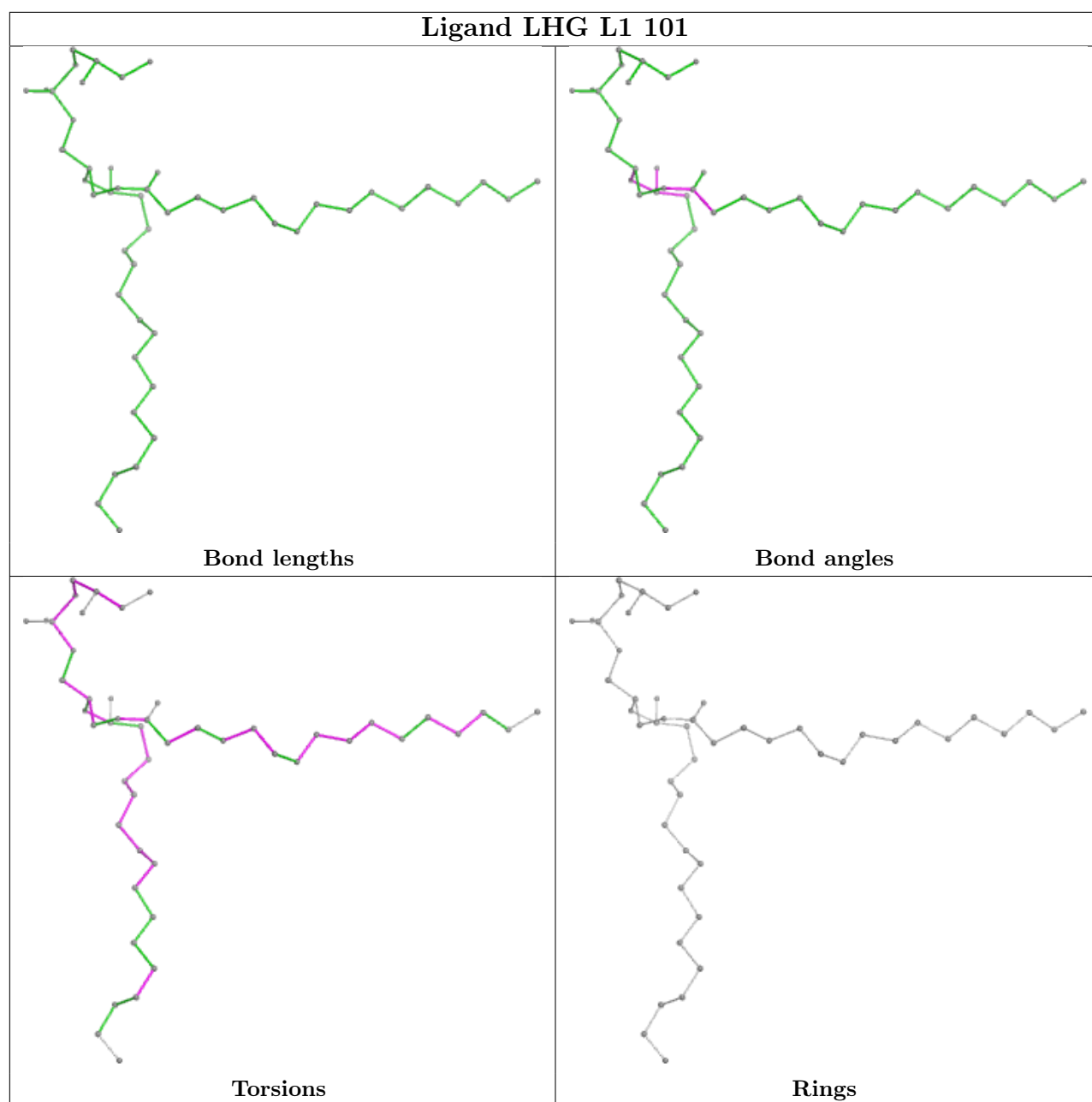
Bond angles

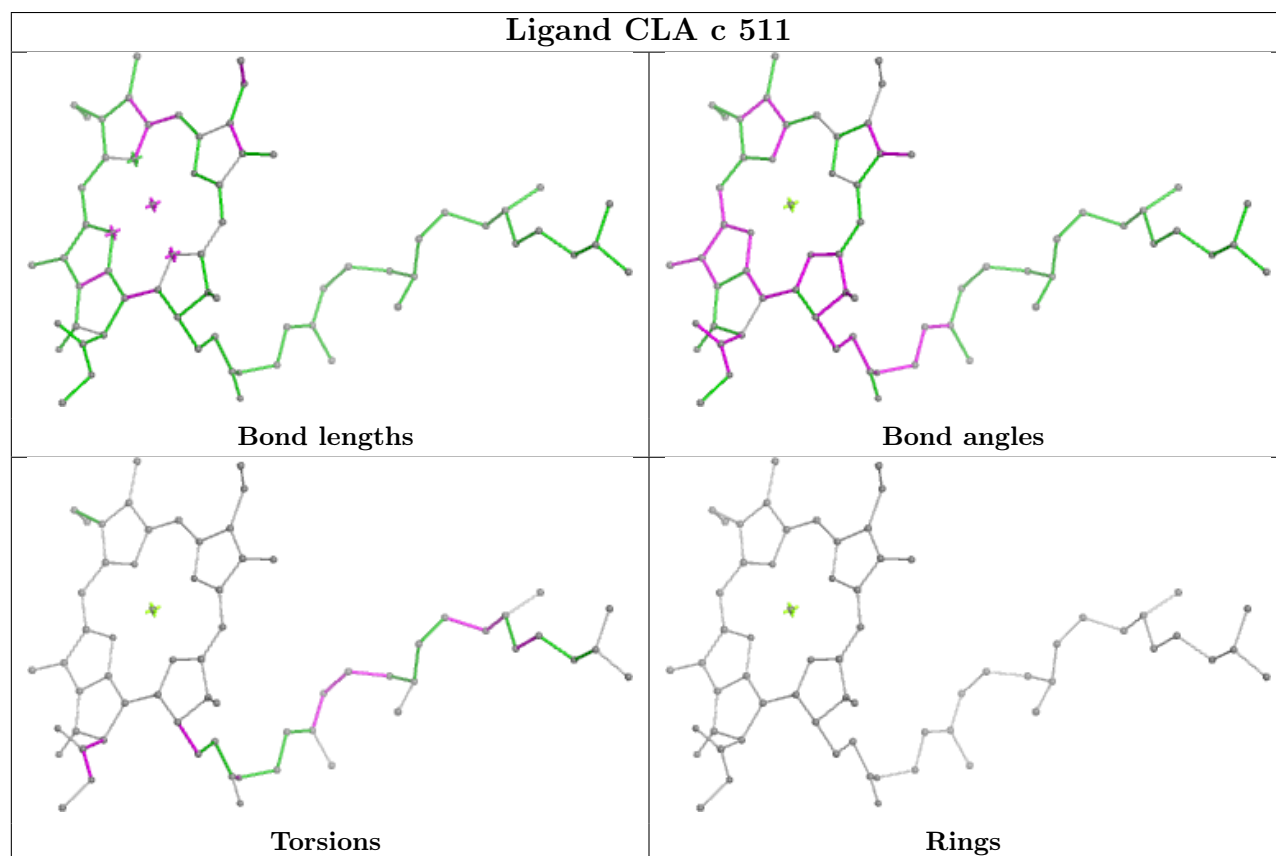
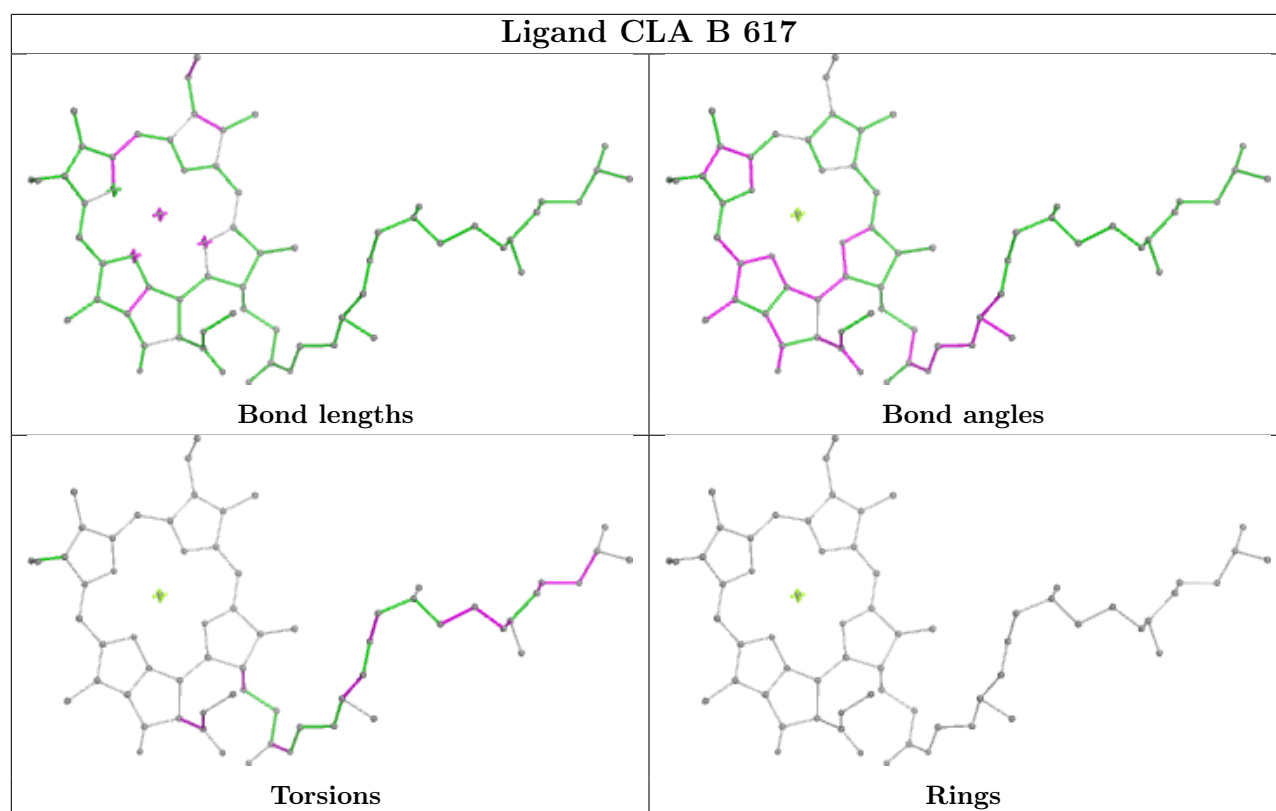


Torsions

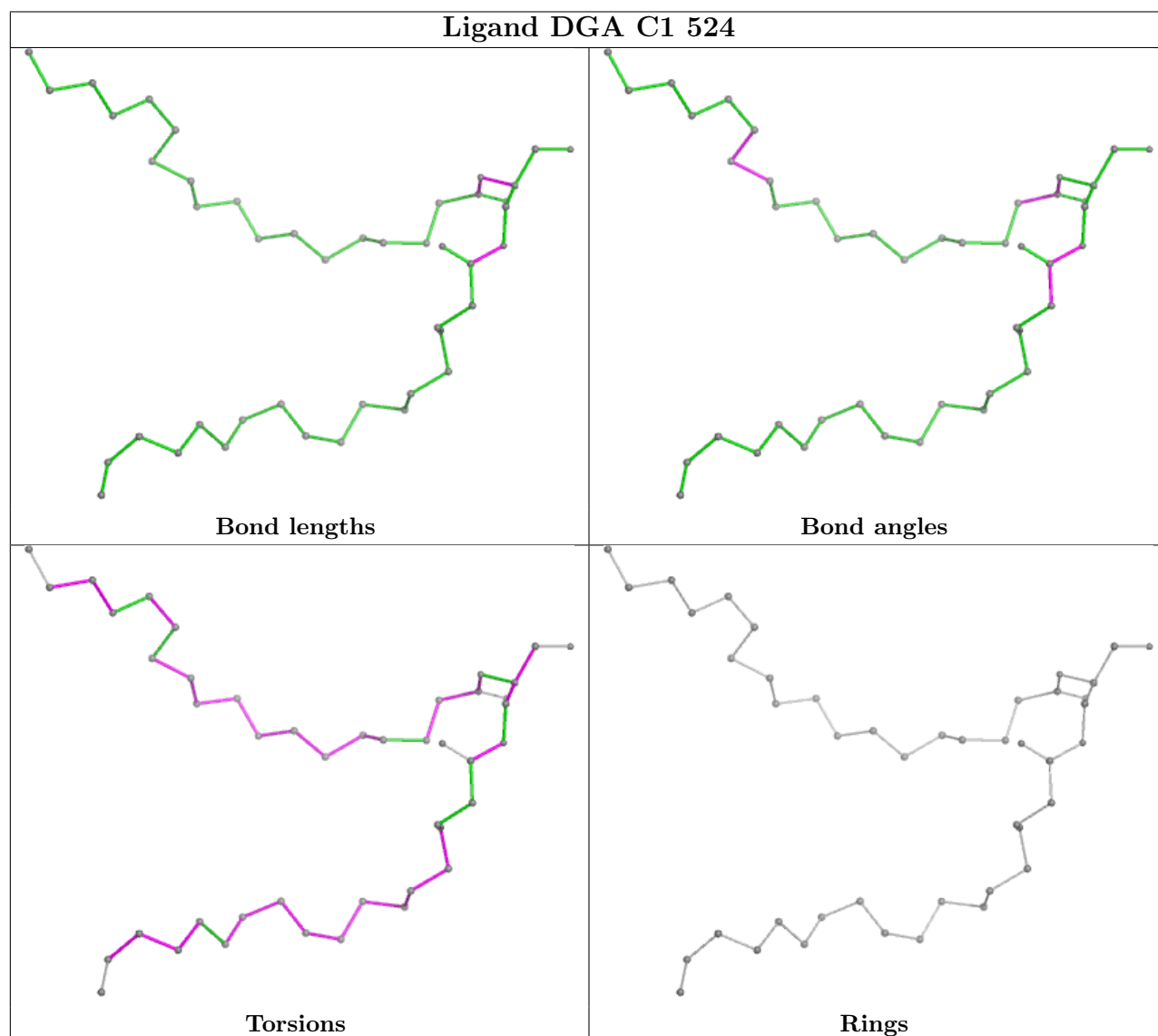
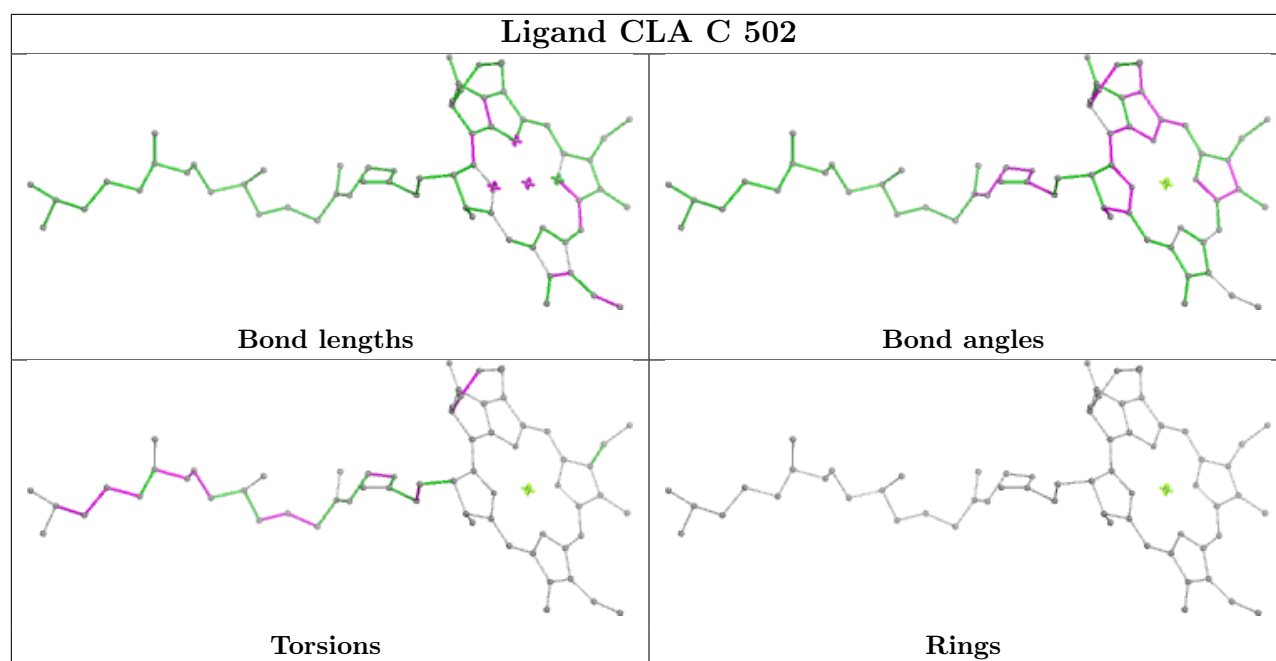


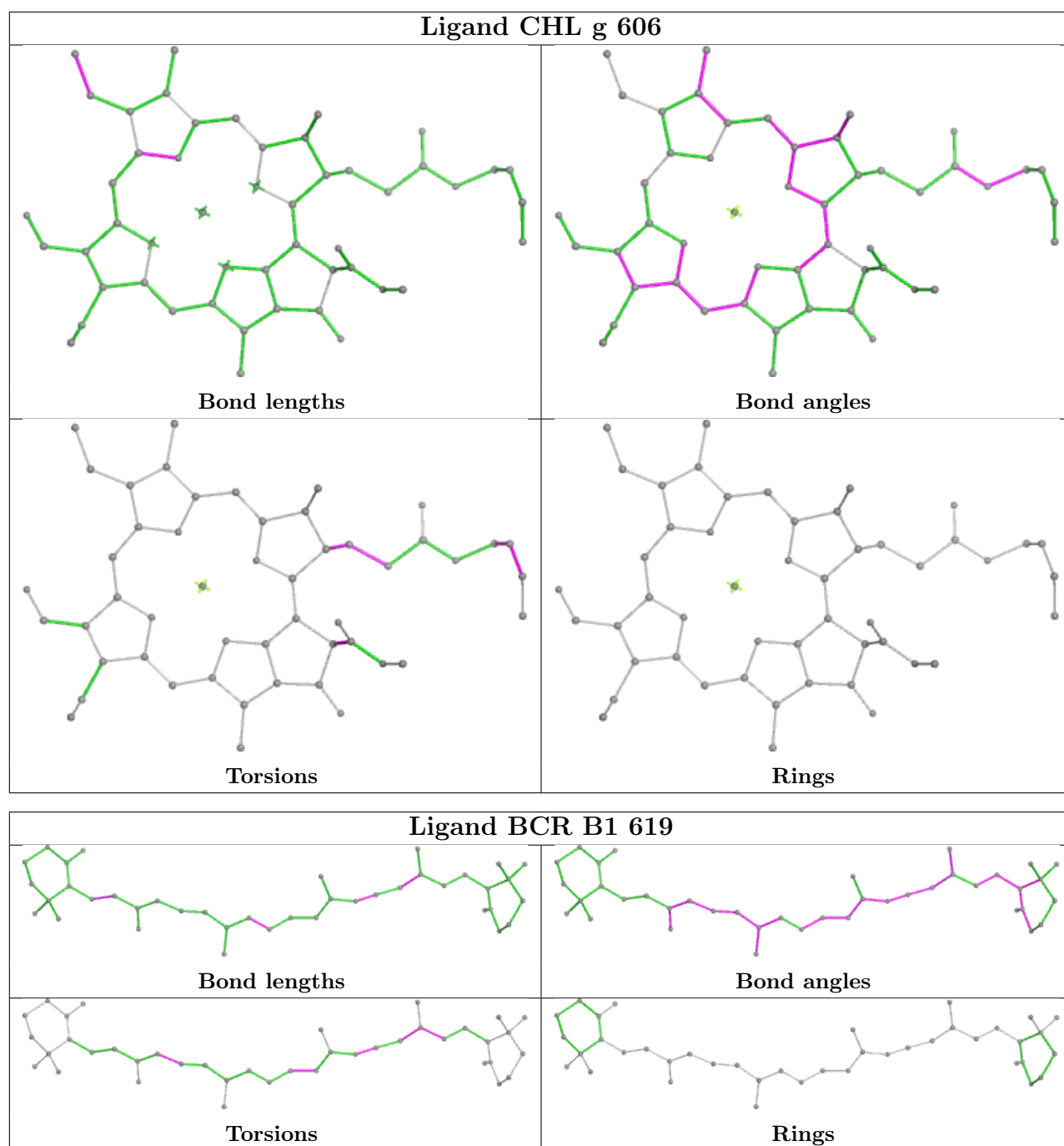
Rings

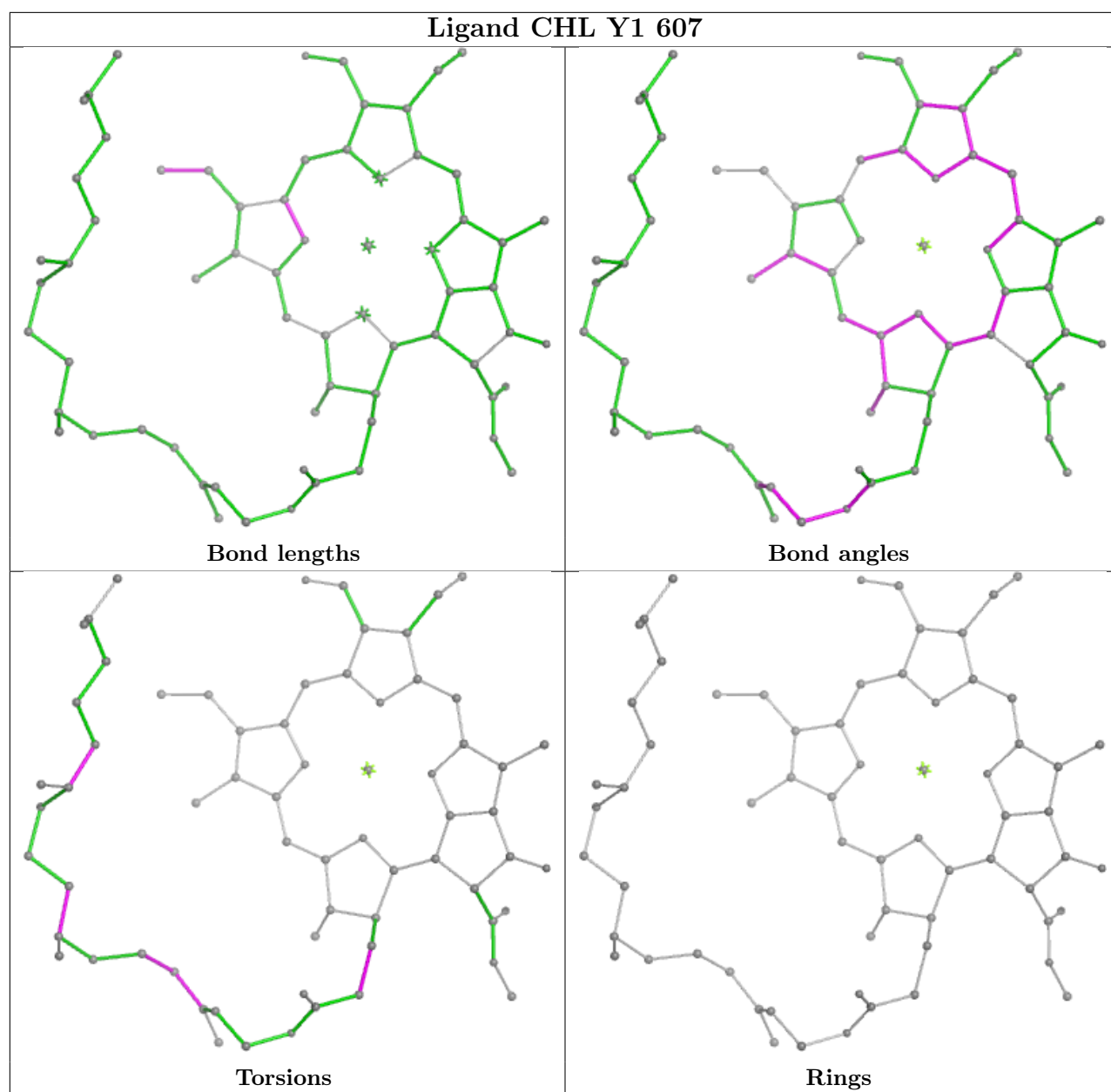


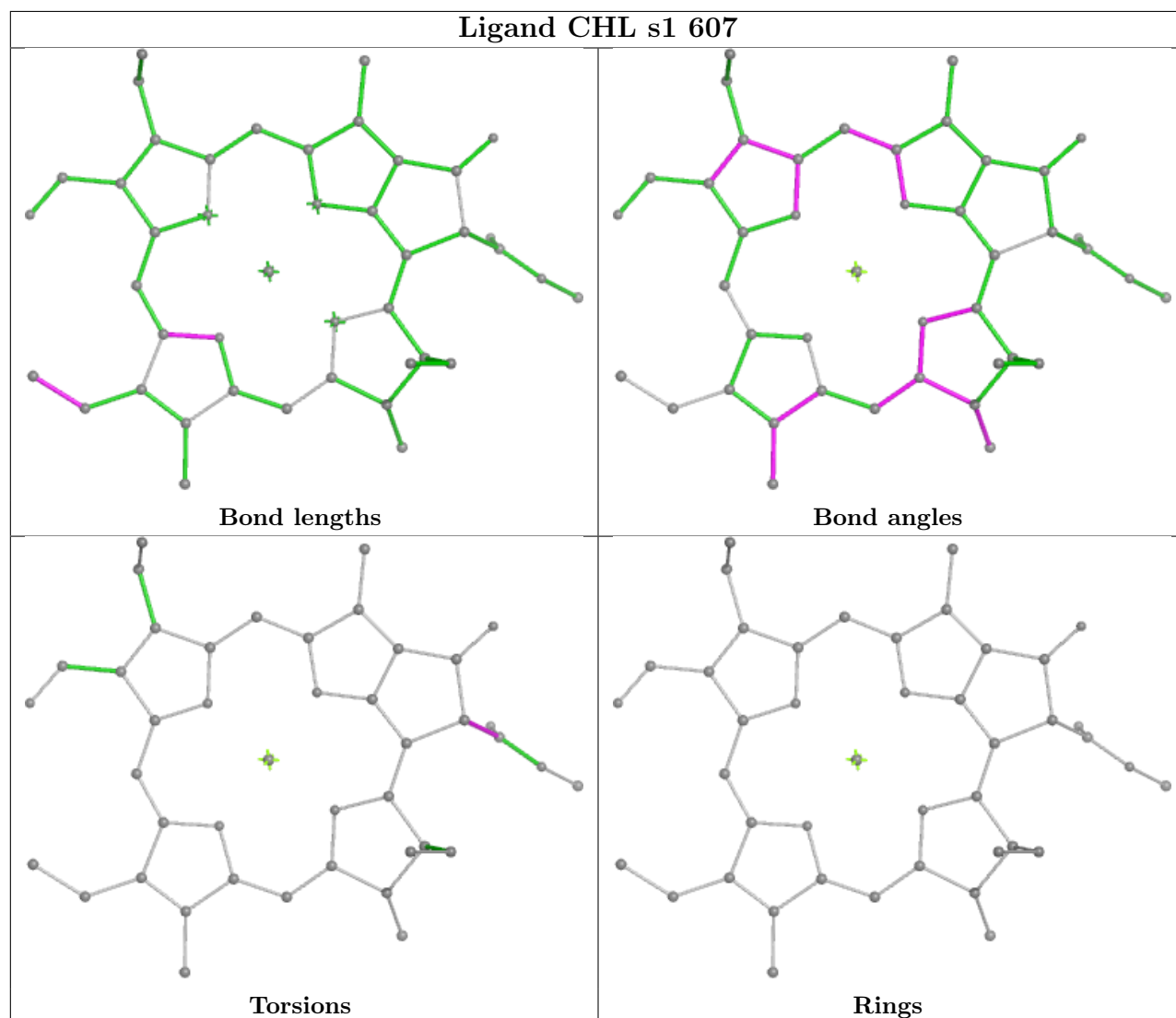
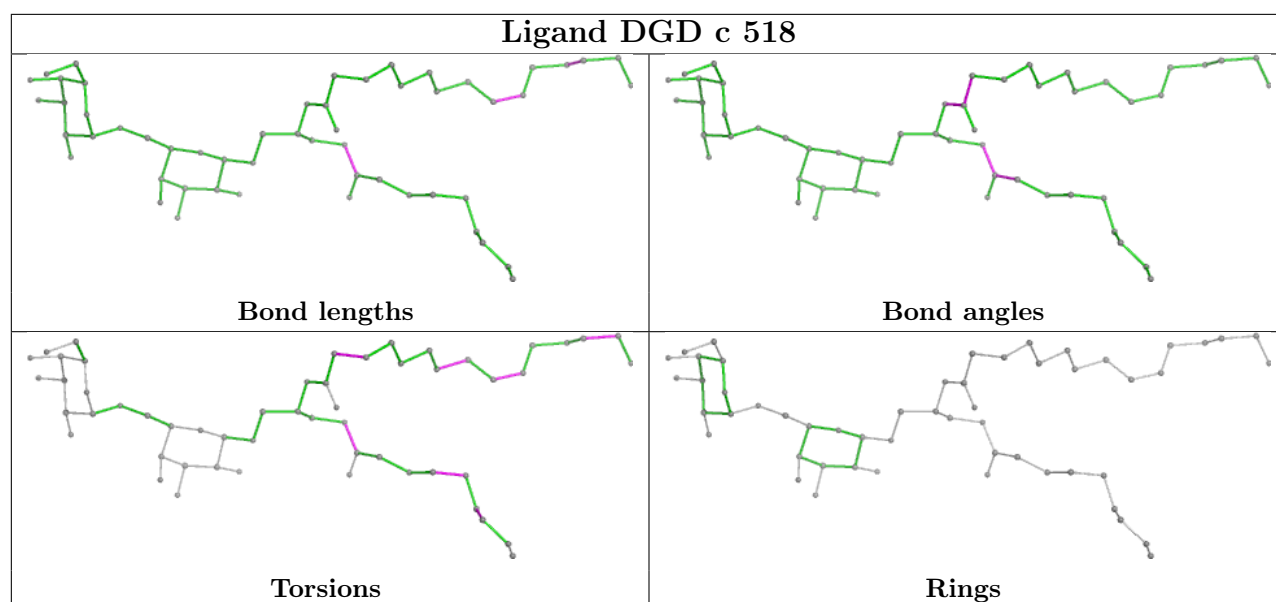


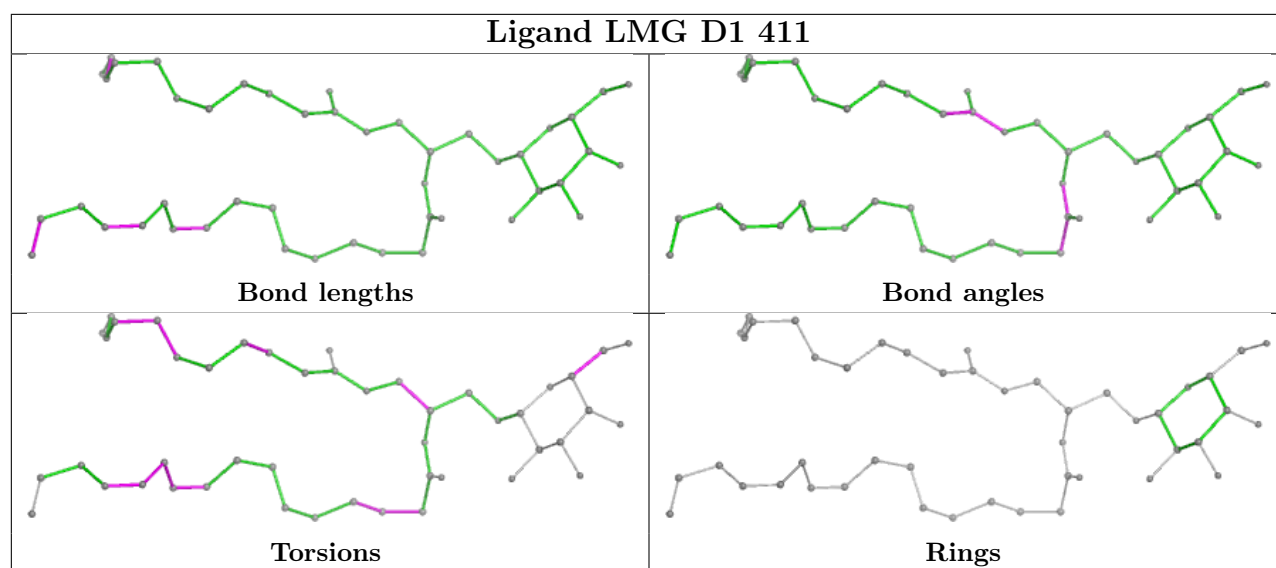


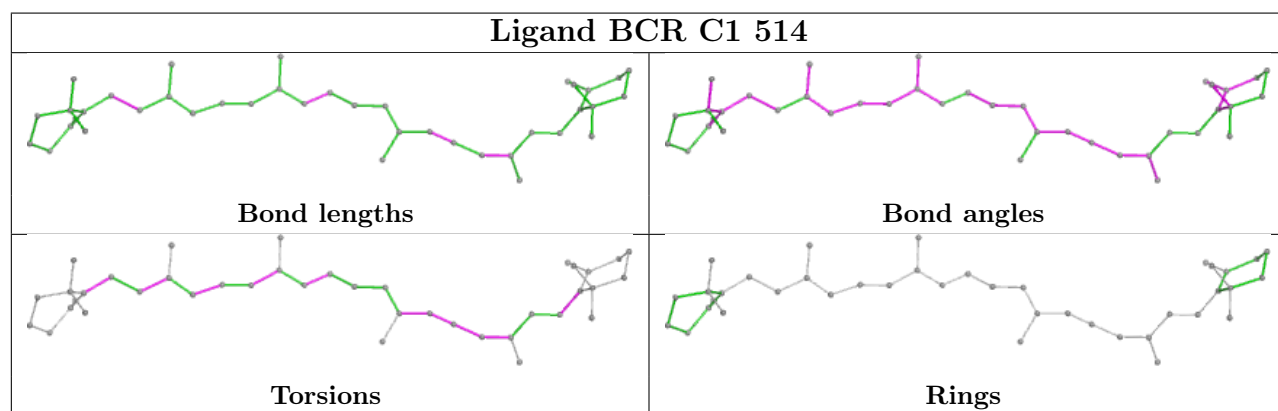
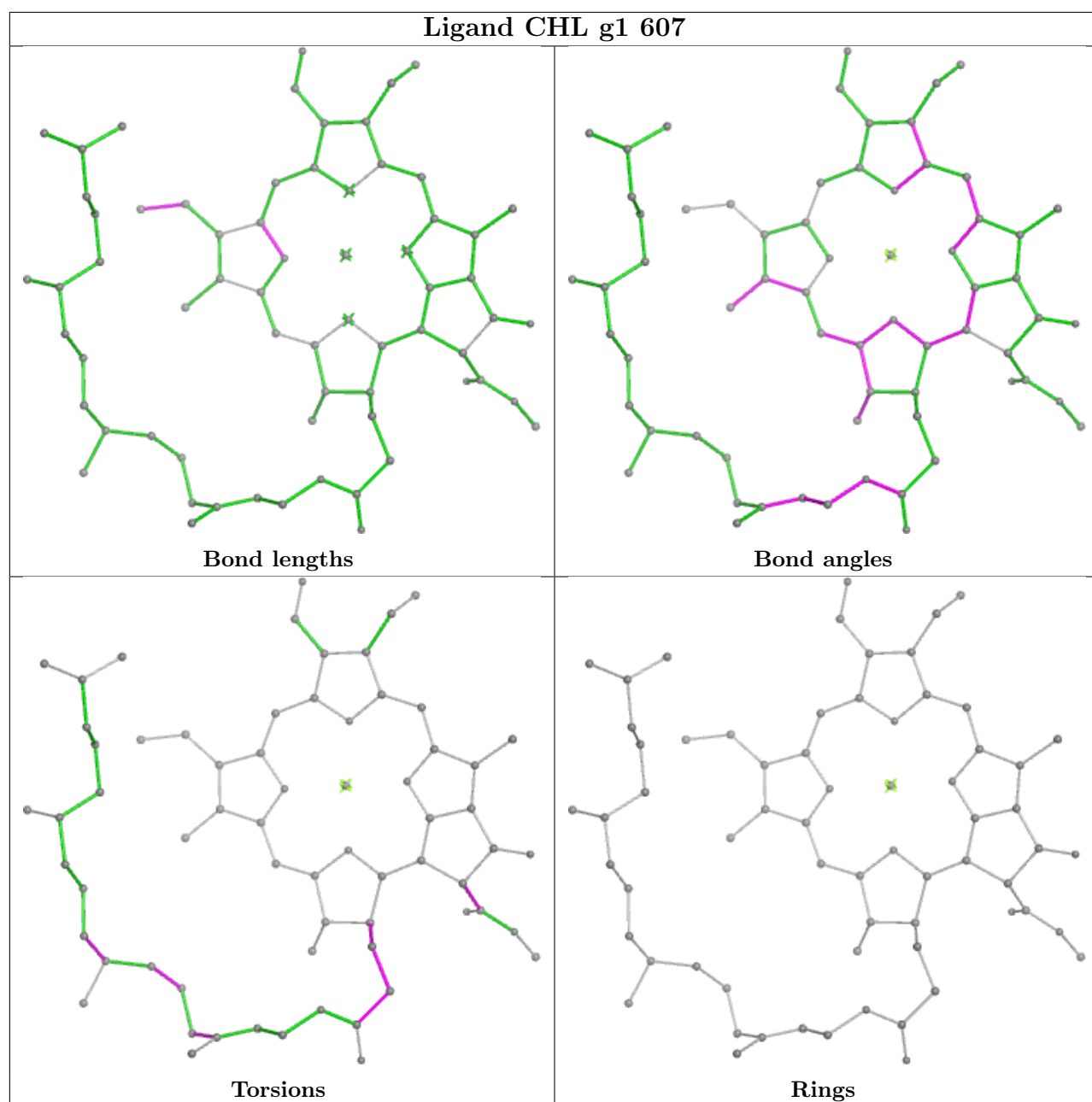


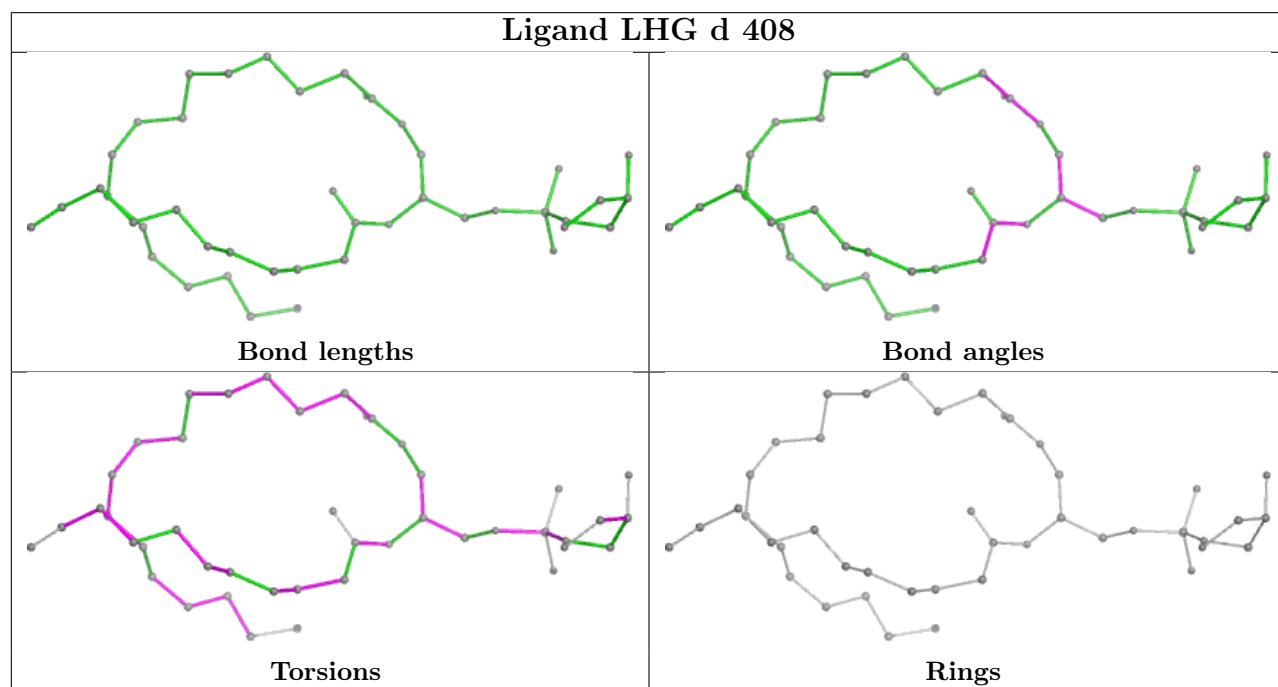
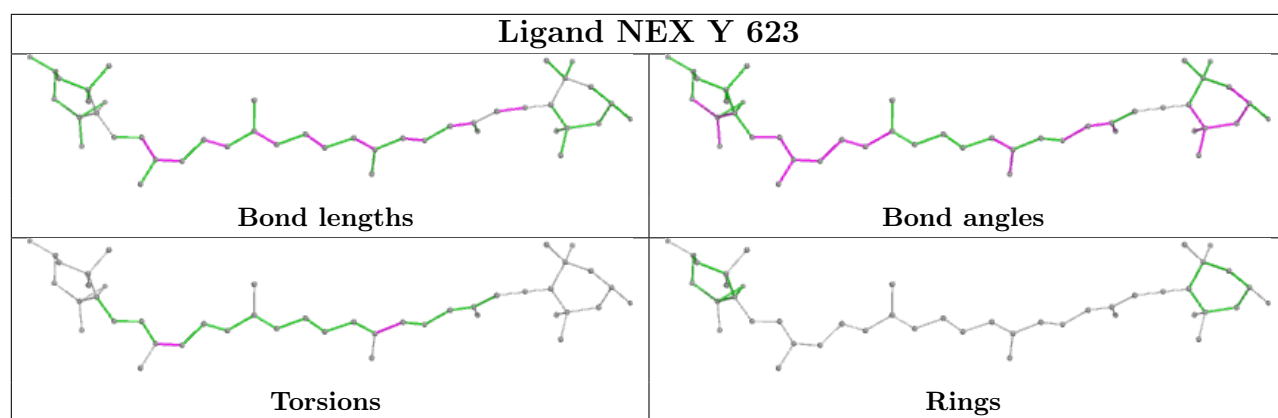




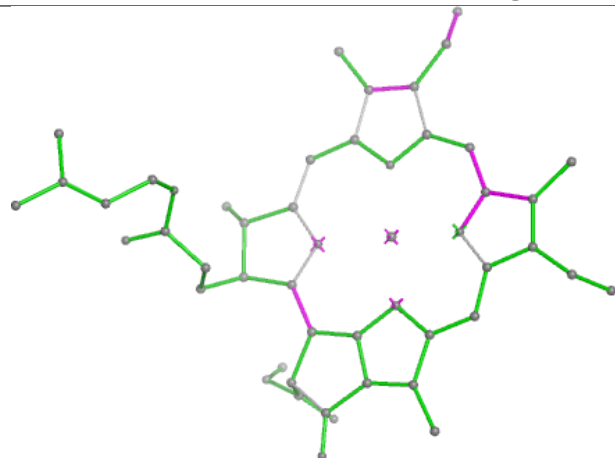




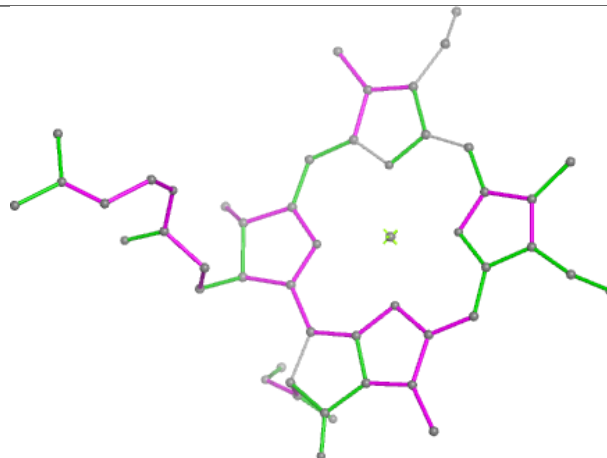




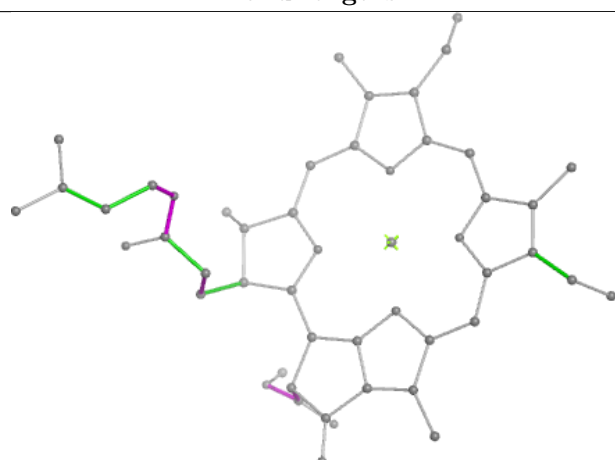
## Ligand CLA A1 407



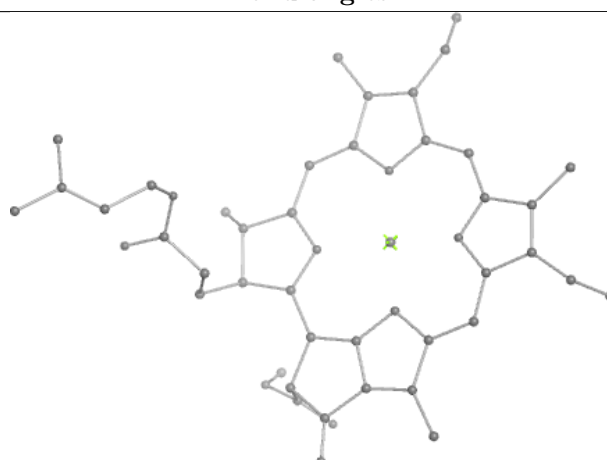
Bond lengths



Bond angles

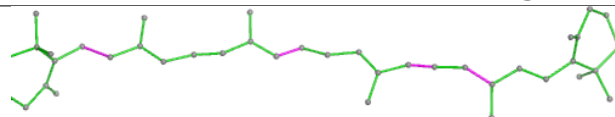


Torsions

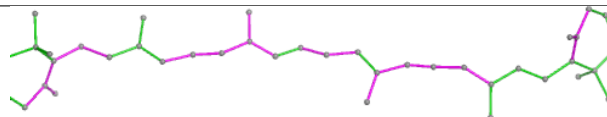


Rings

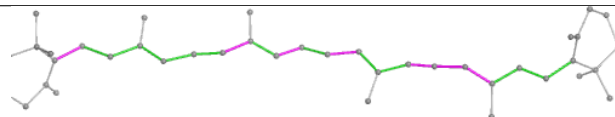
## Ligand BCR a 411



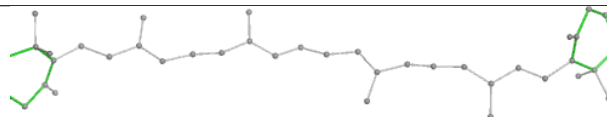
Bond lengths



Bond angles

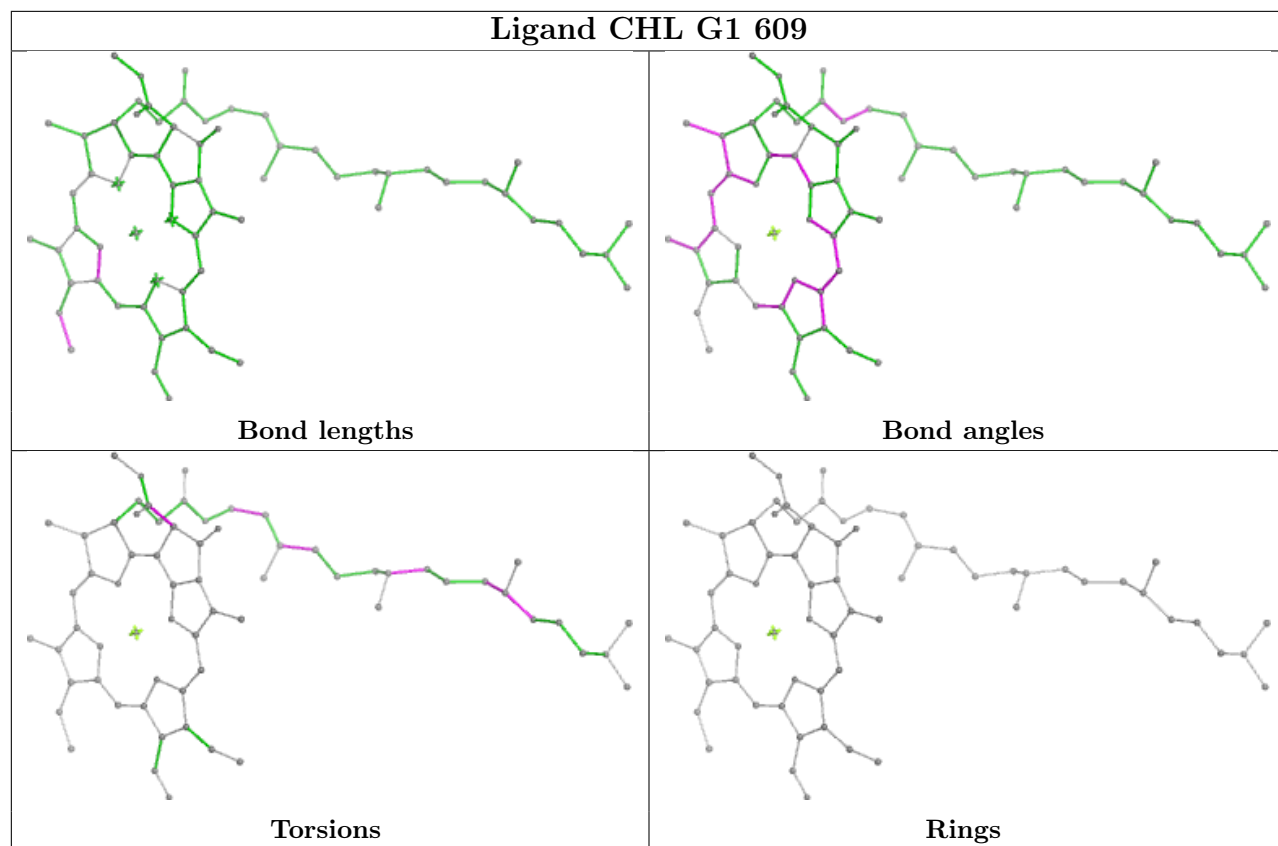


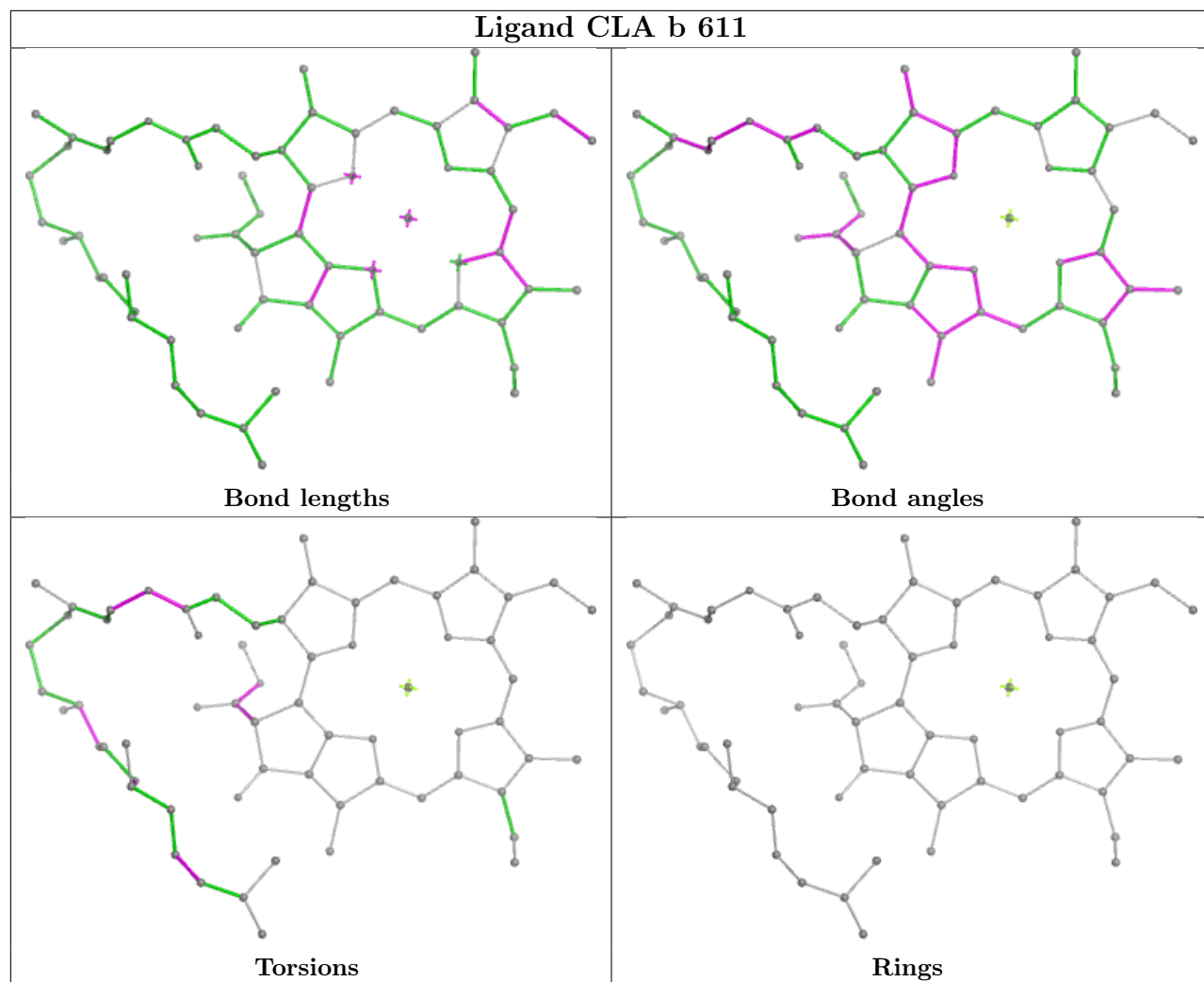
Torsions

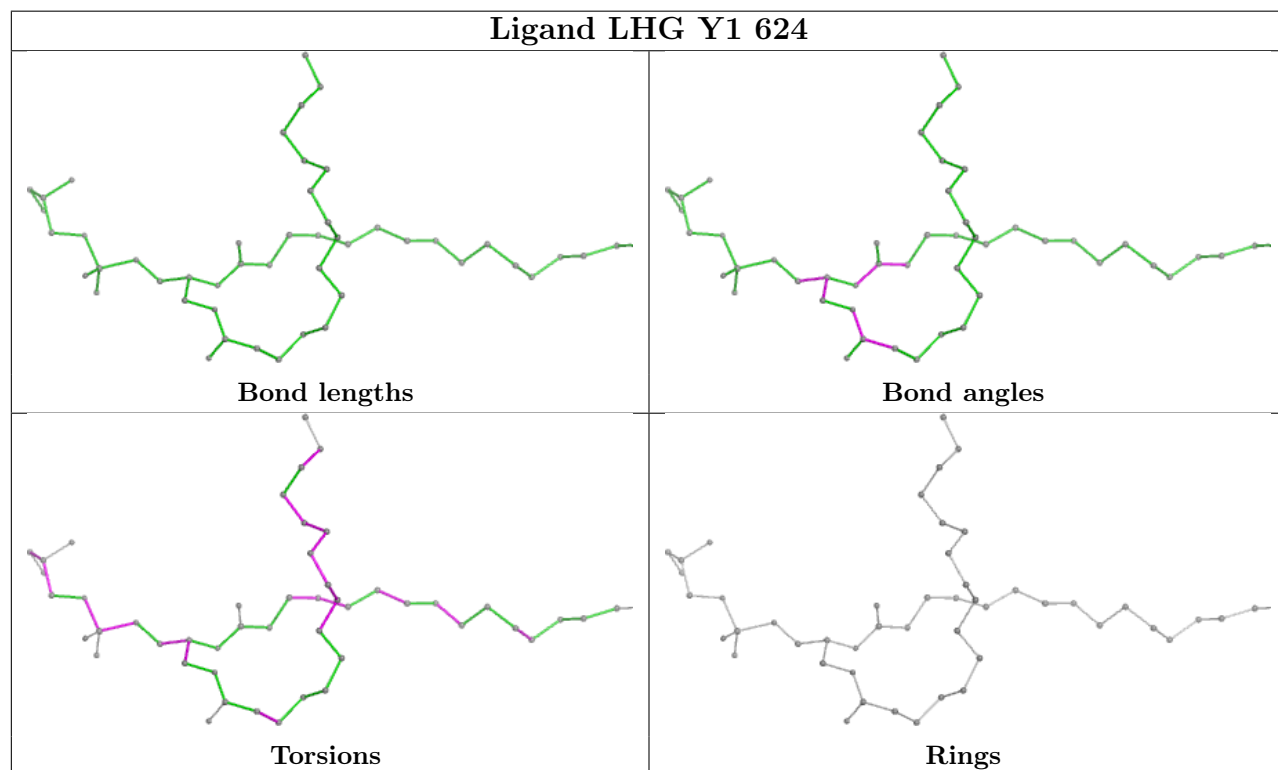
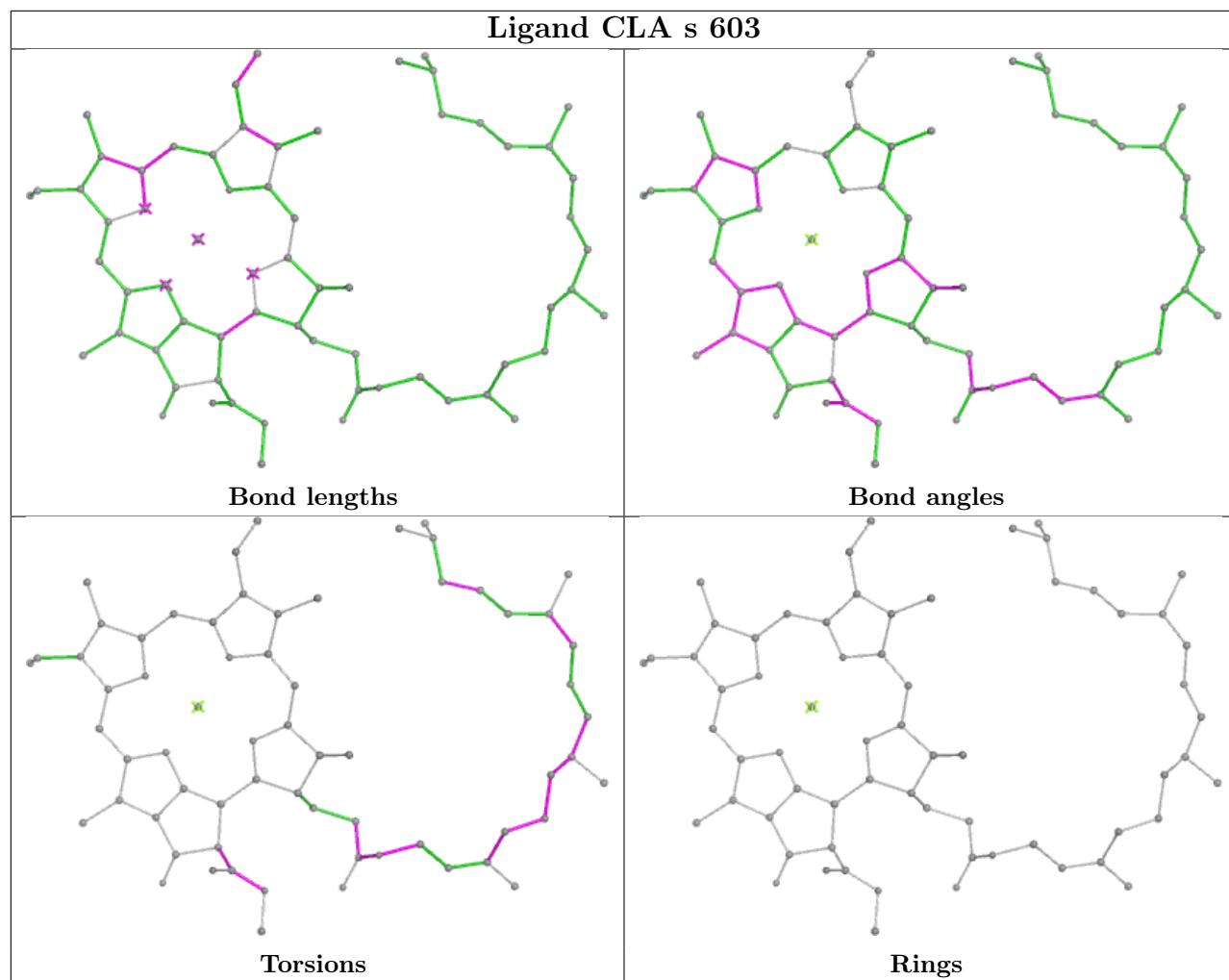


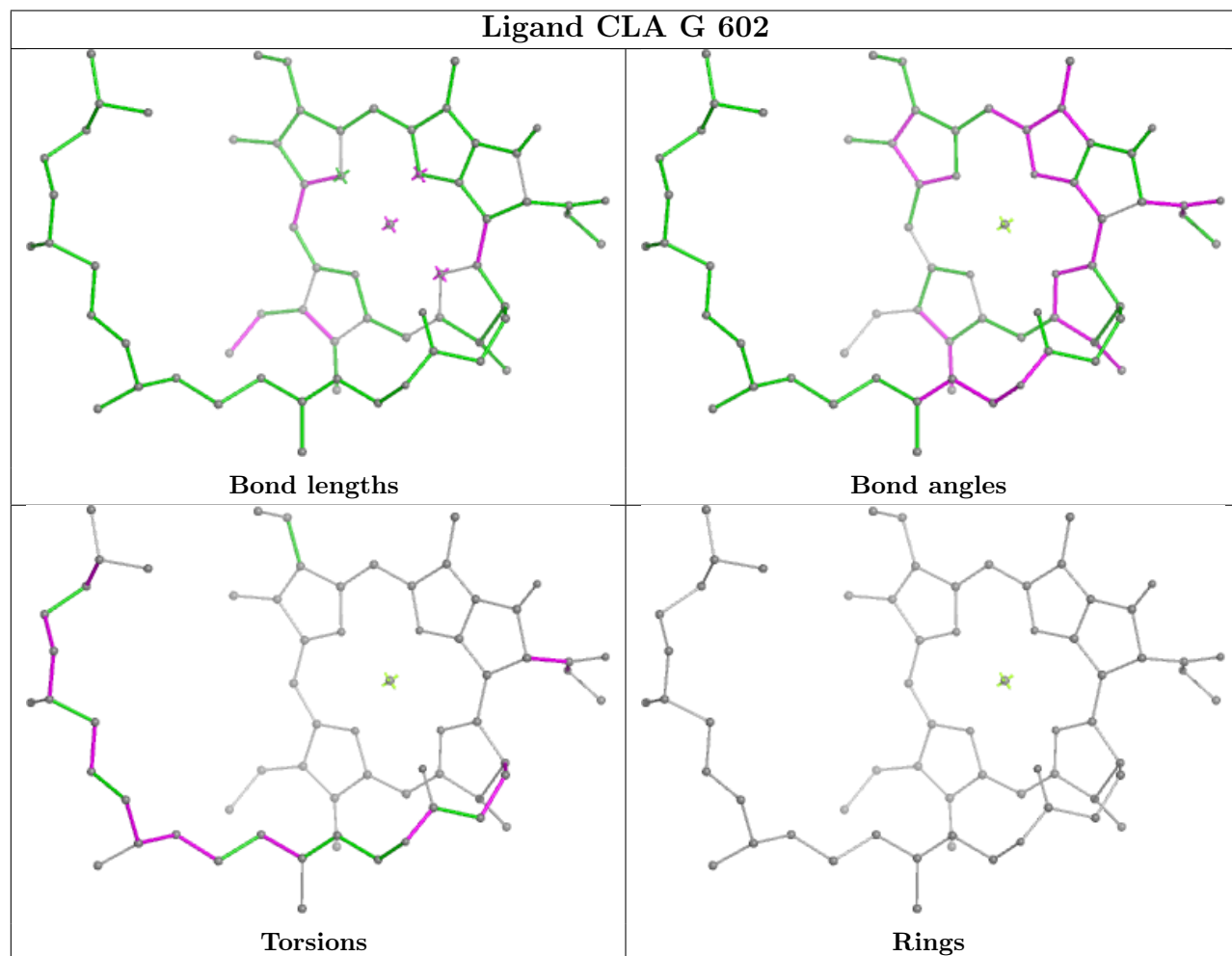
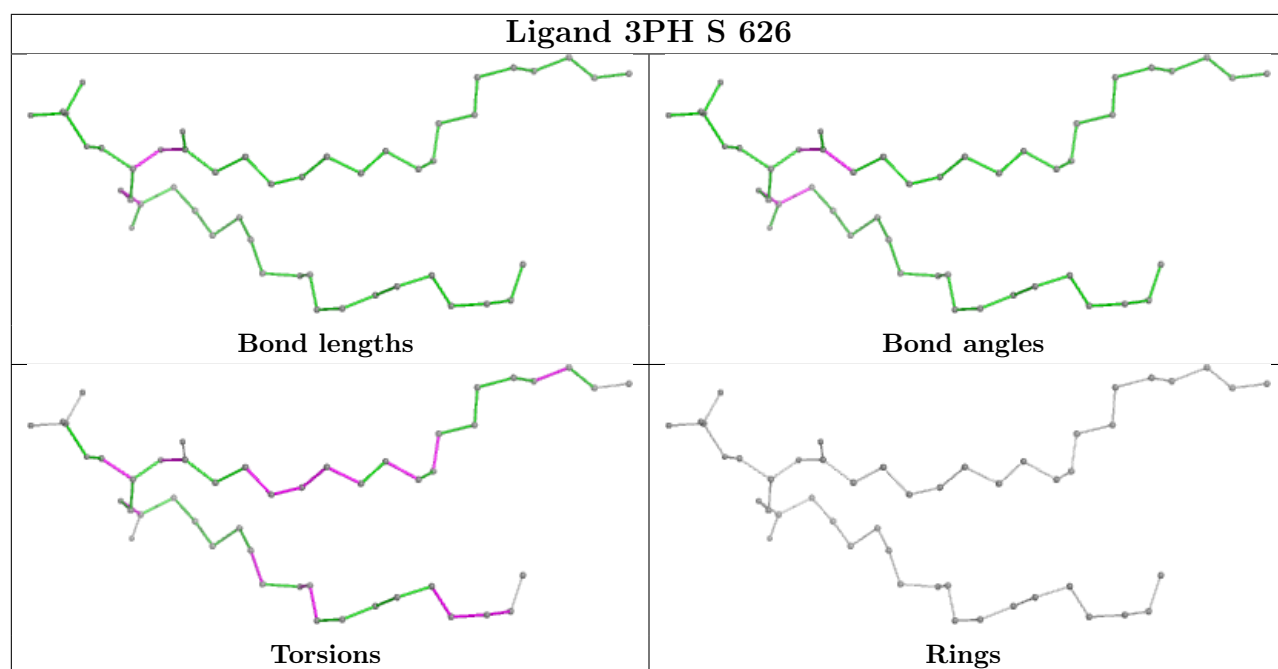
Rings

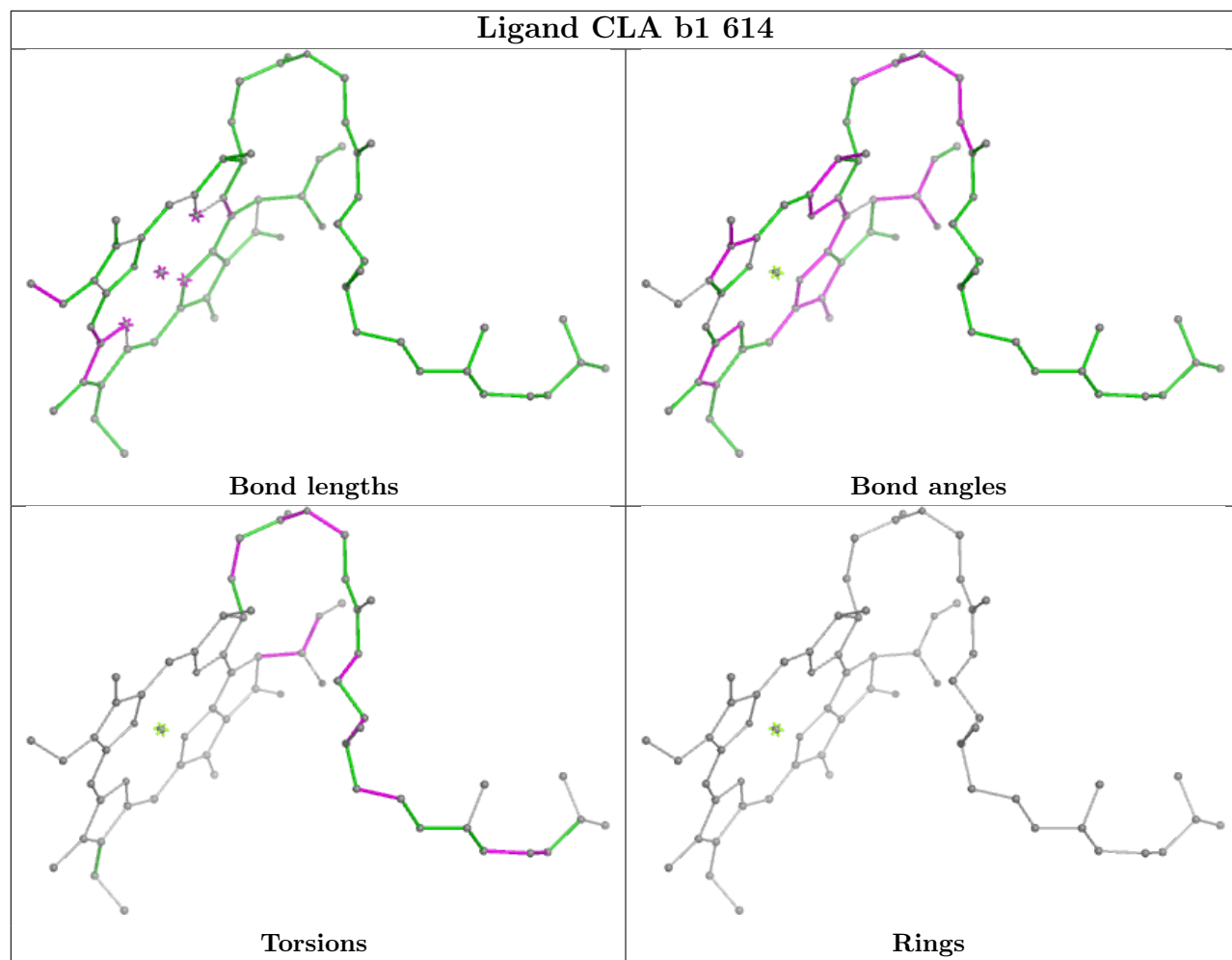


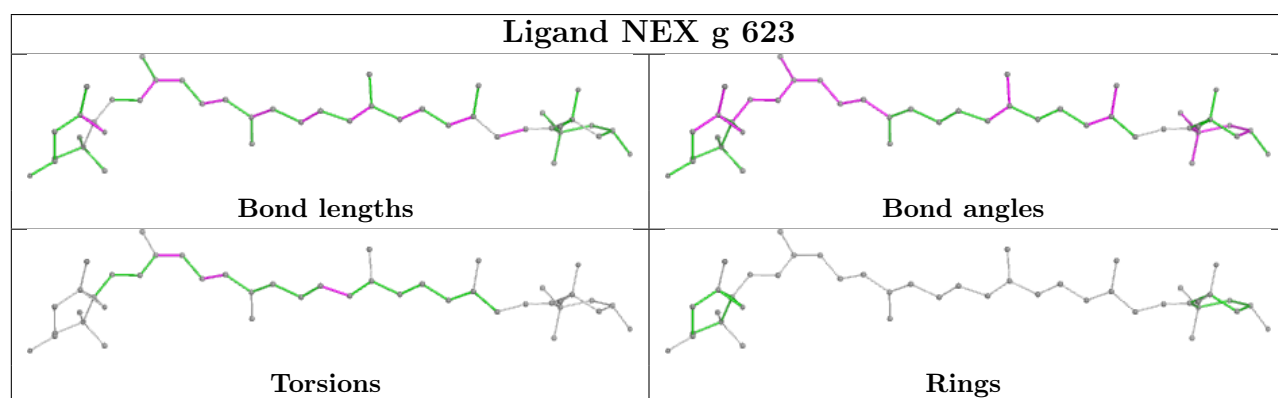
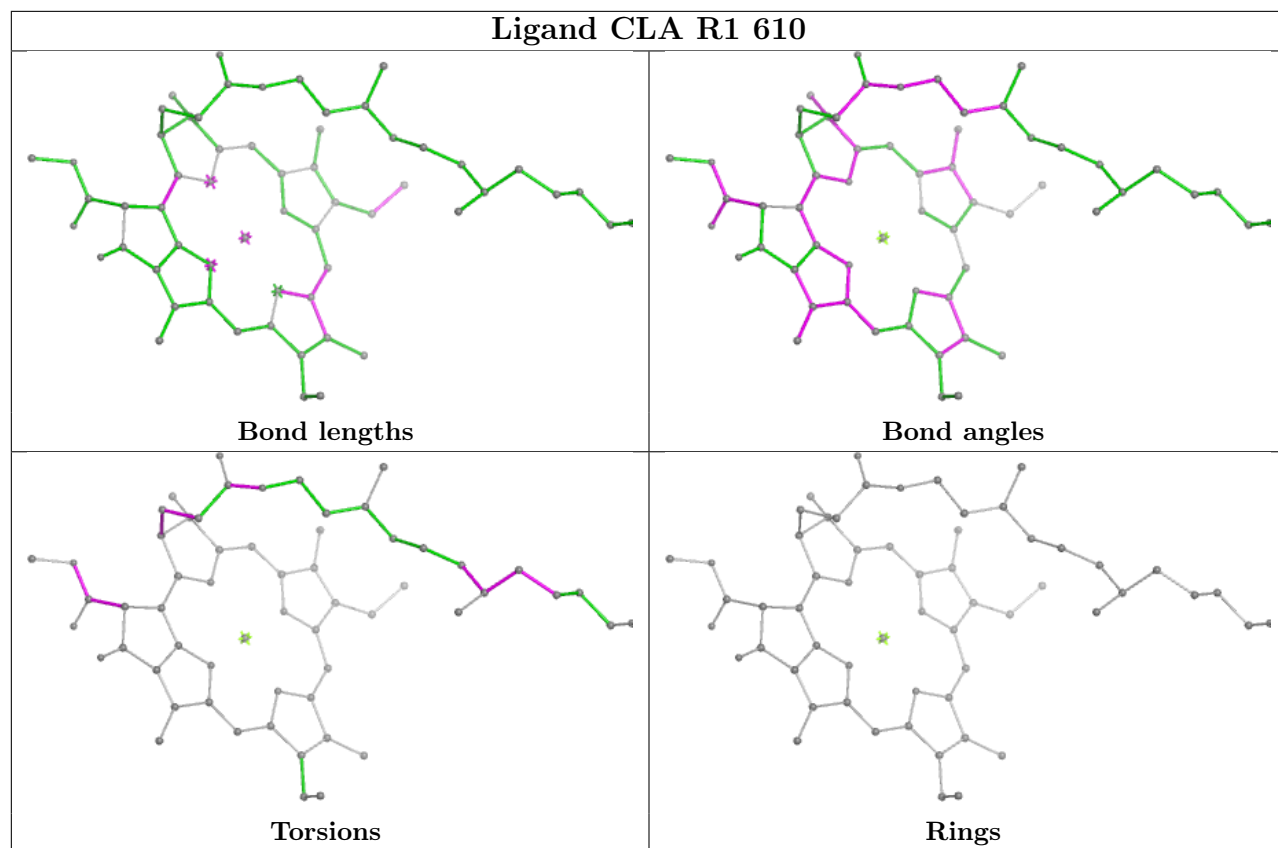




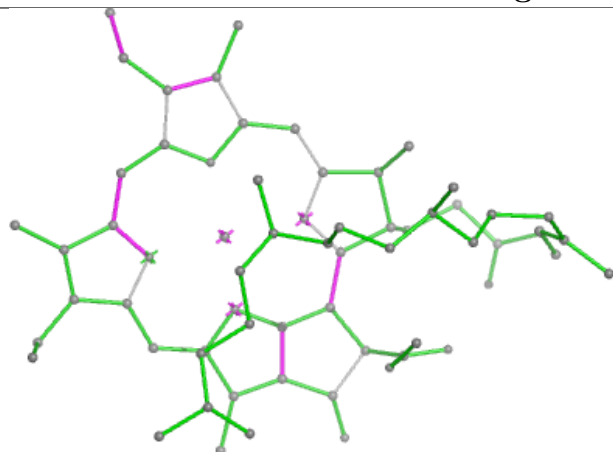




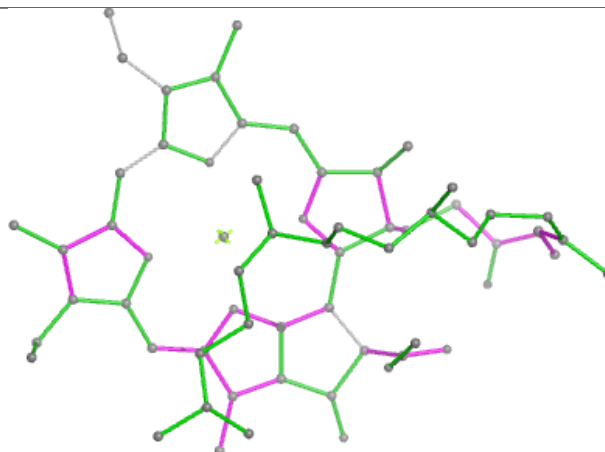




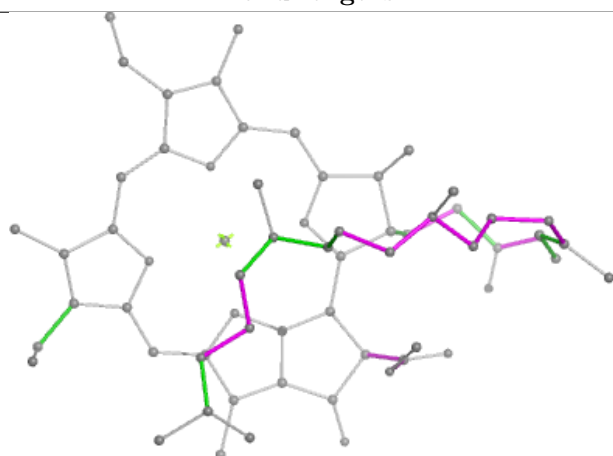
## Ligand CLA C 510



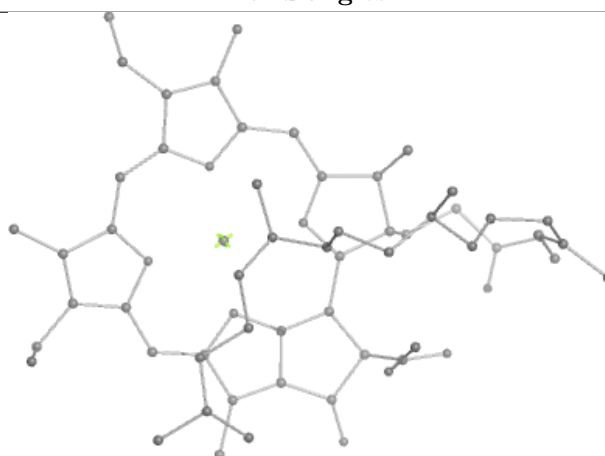
Bond lengths



Bond angles

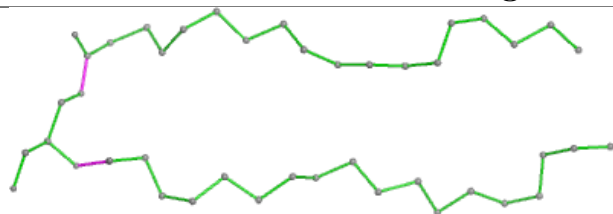


Torsions

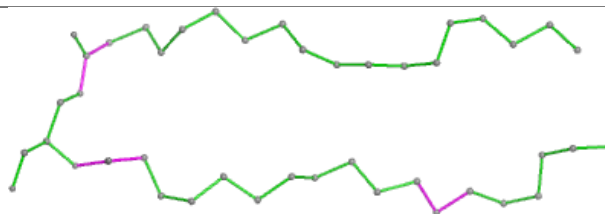


Rings

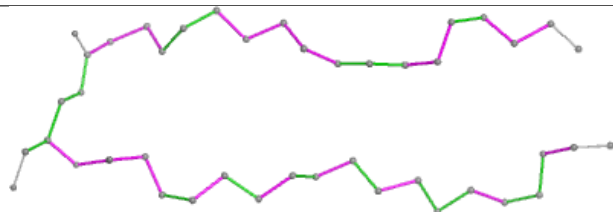
## Ligand DGA B1 625



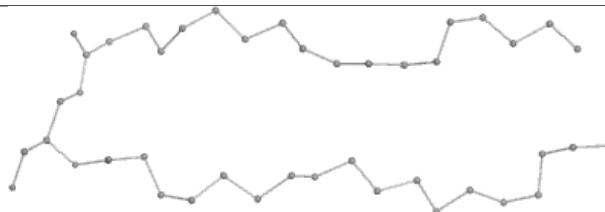
Bond lengths



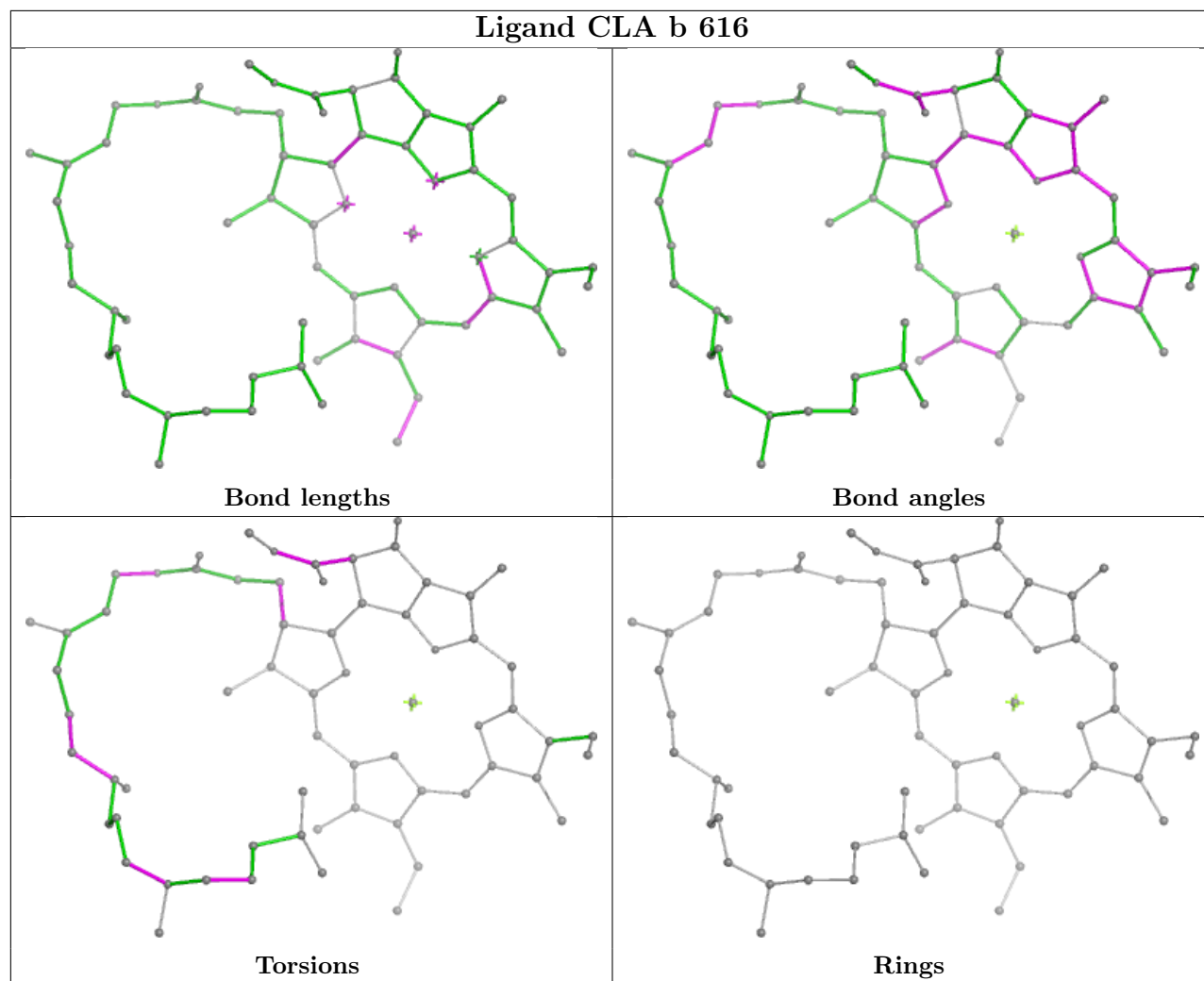
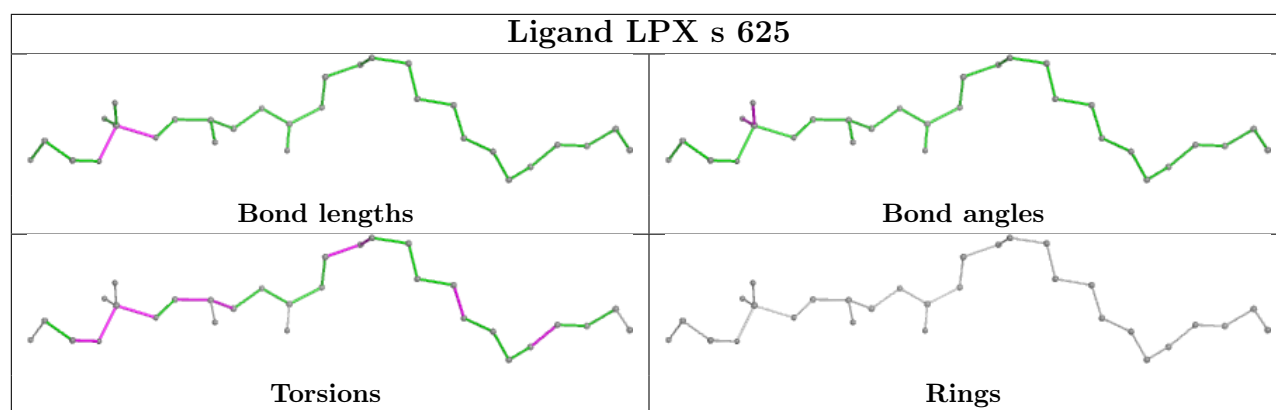
Bond angles



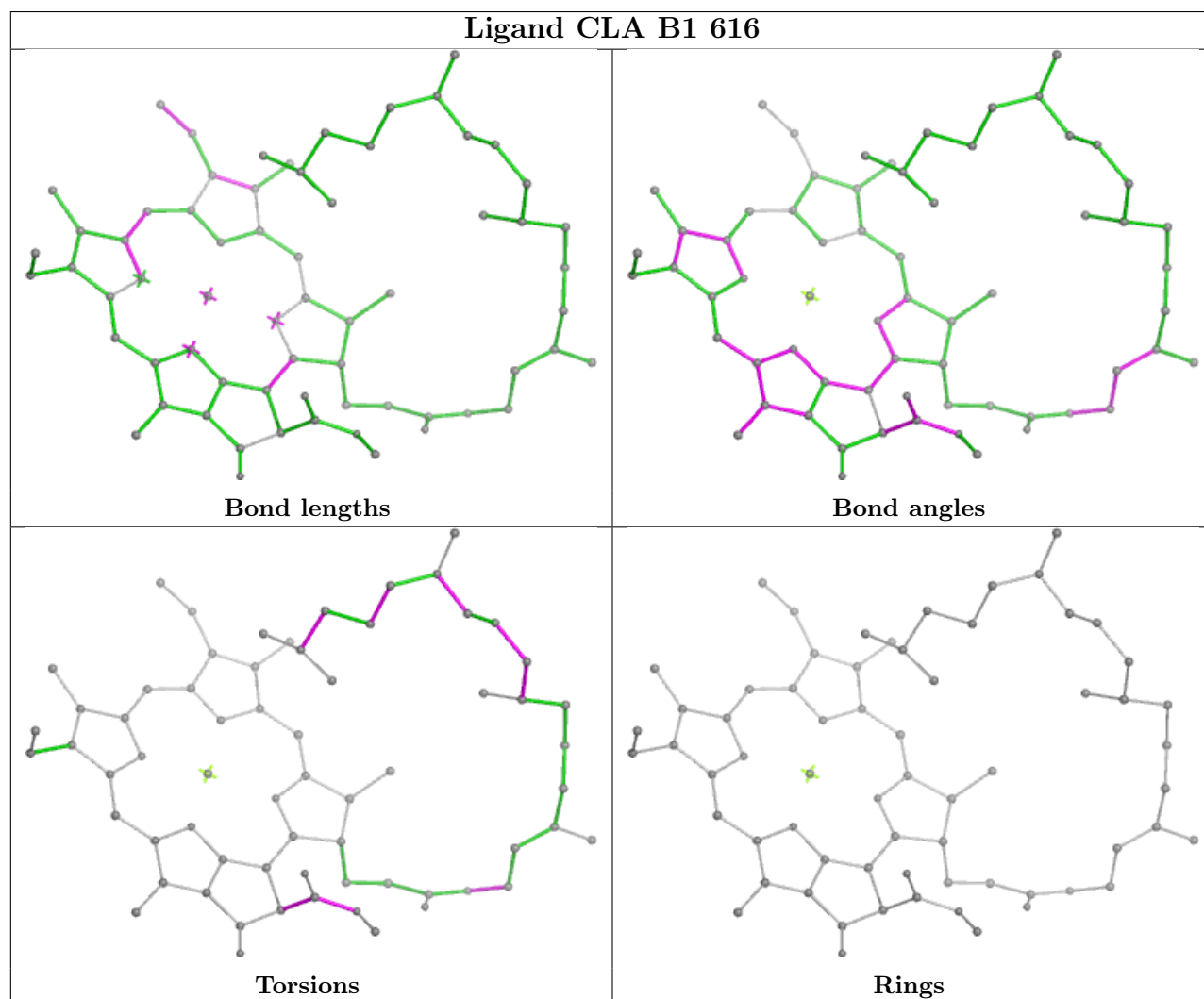
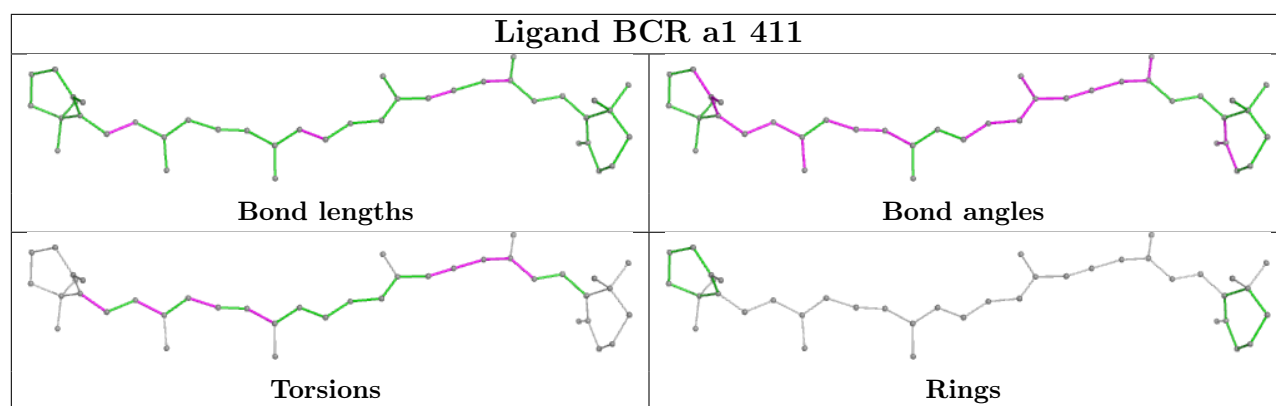
Torsions

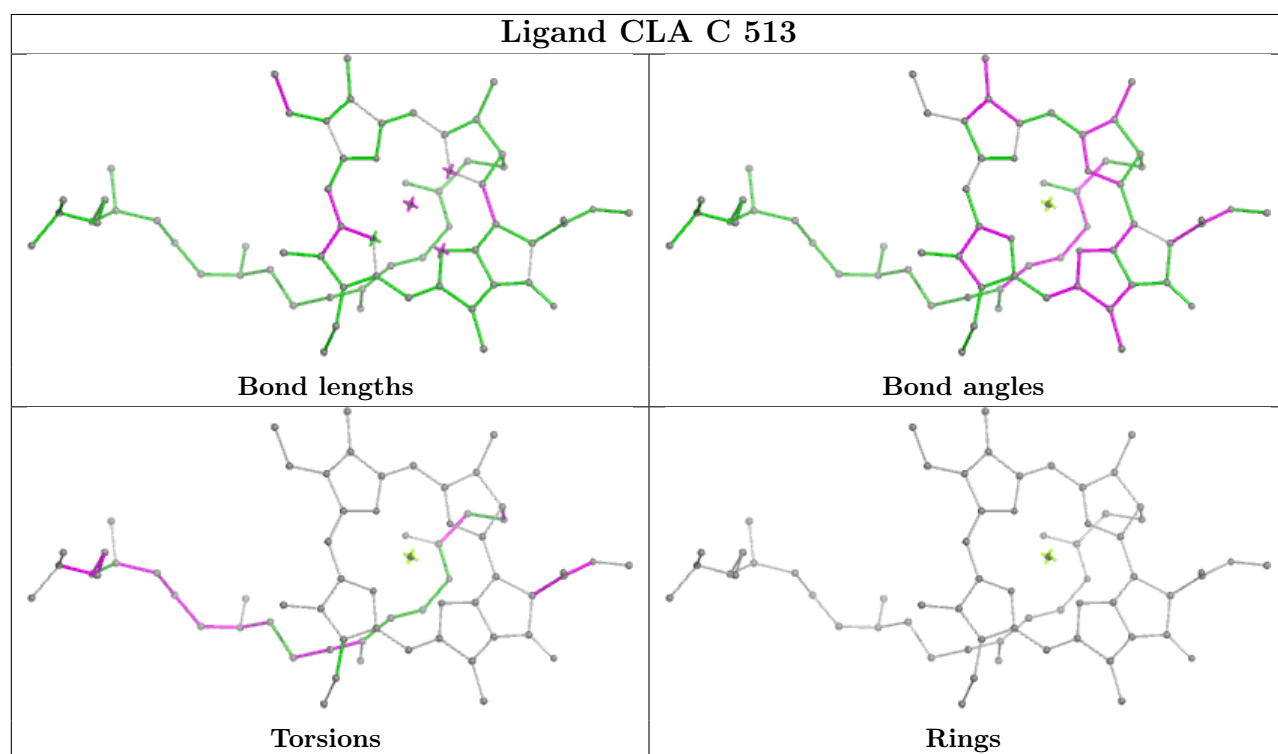
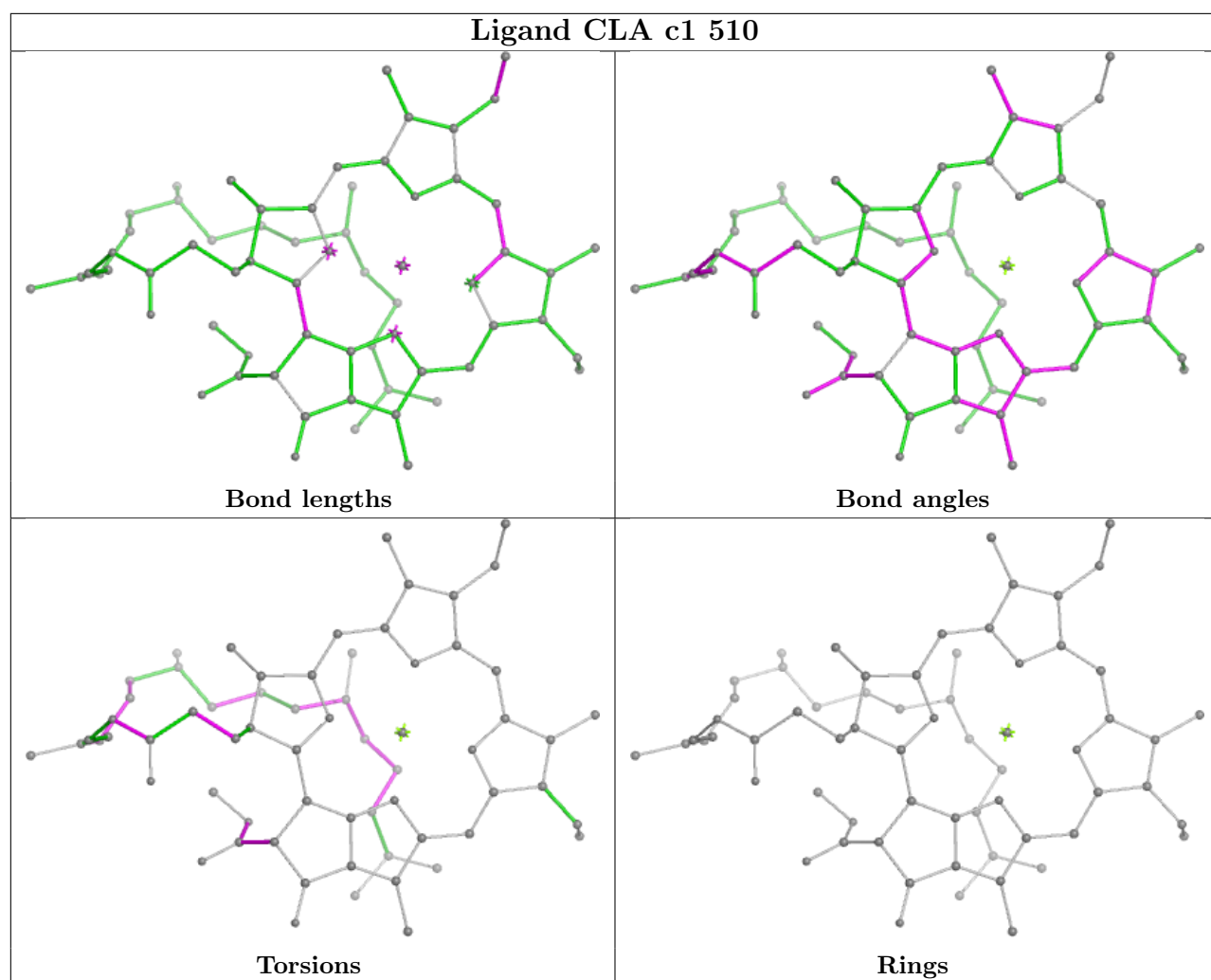


Rings

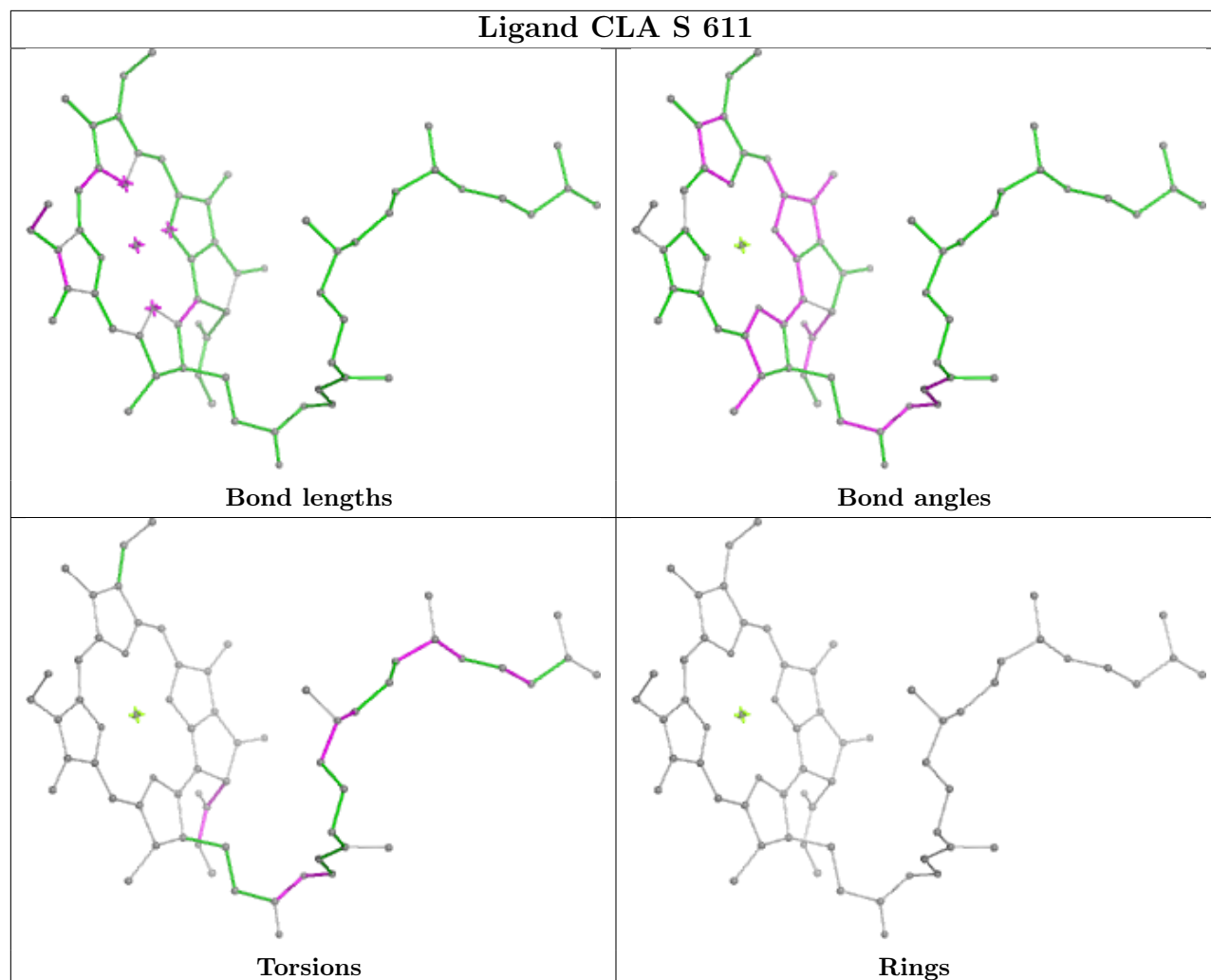


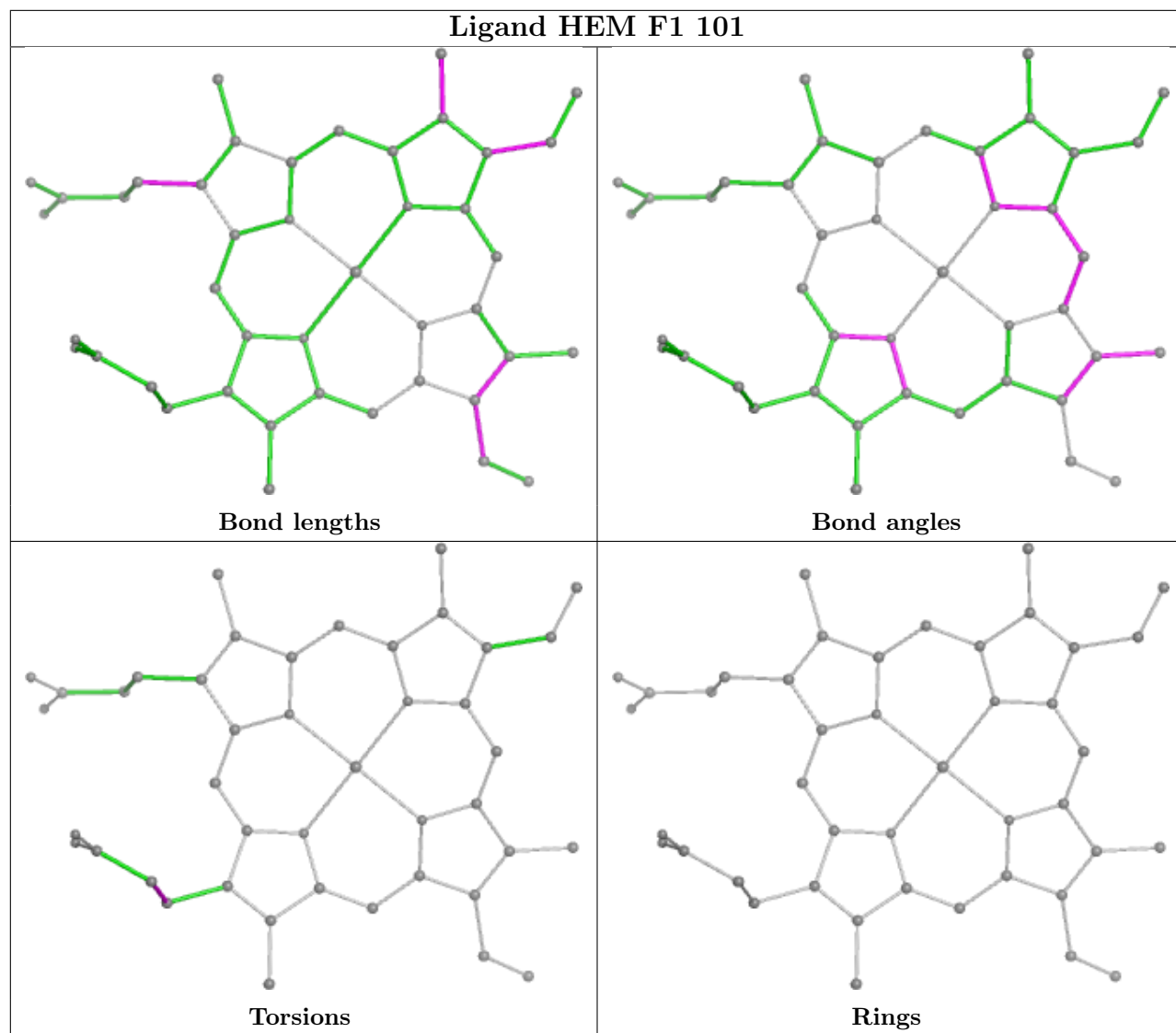


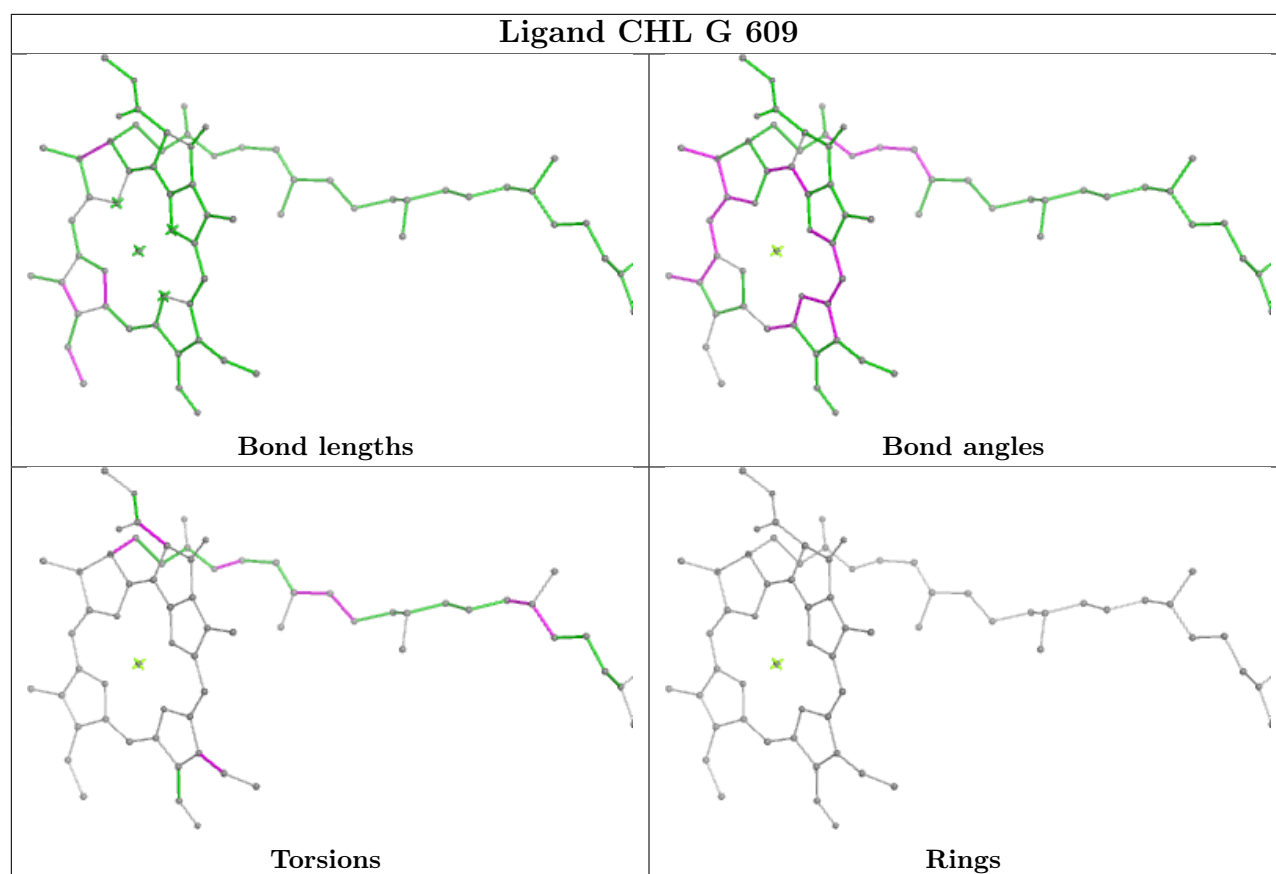




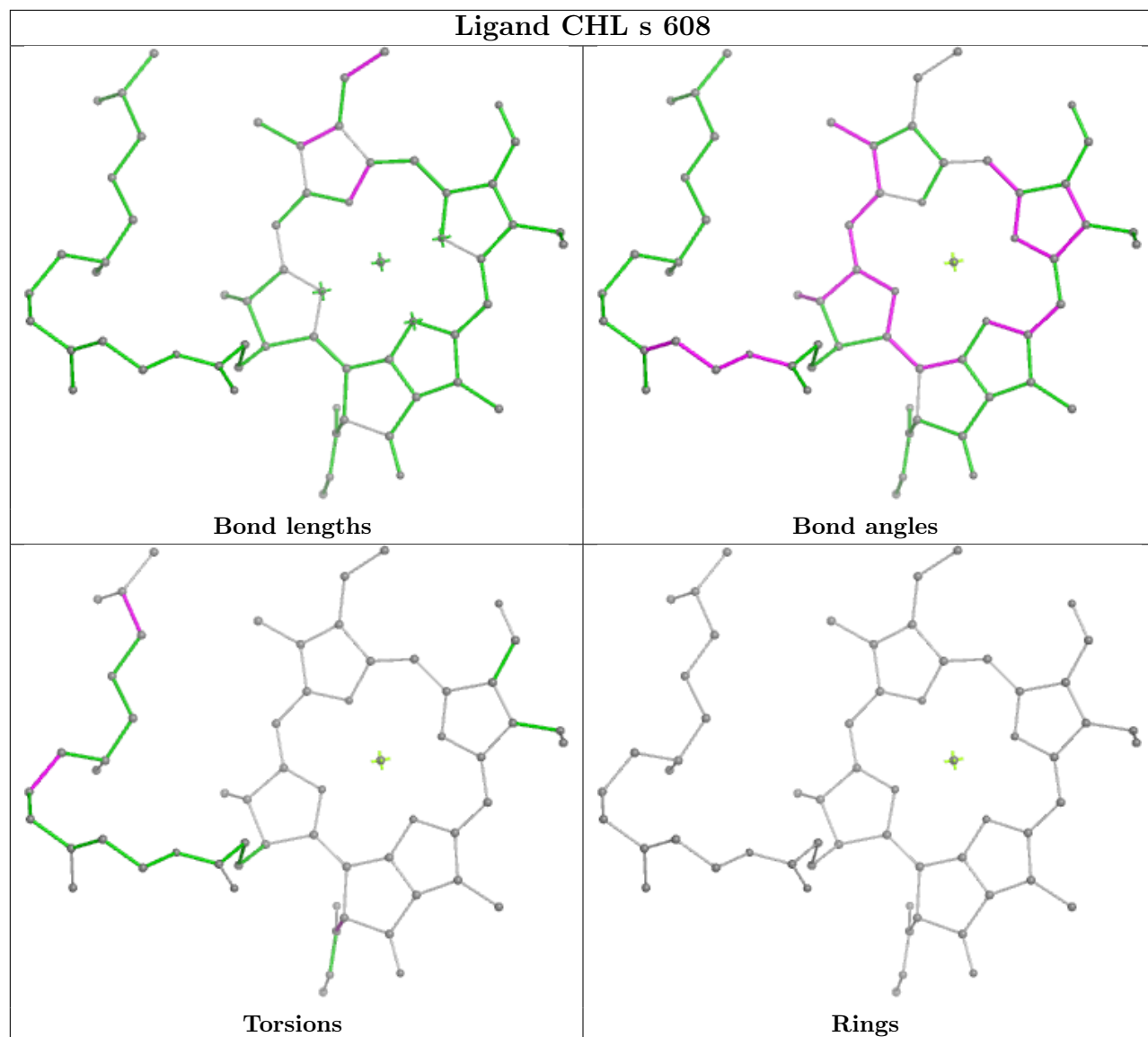
## Ligand CLA S 611

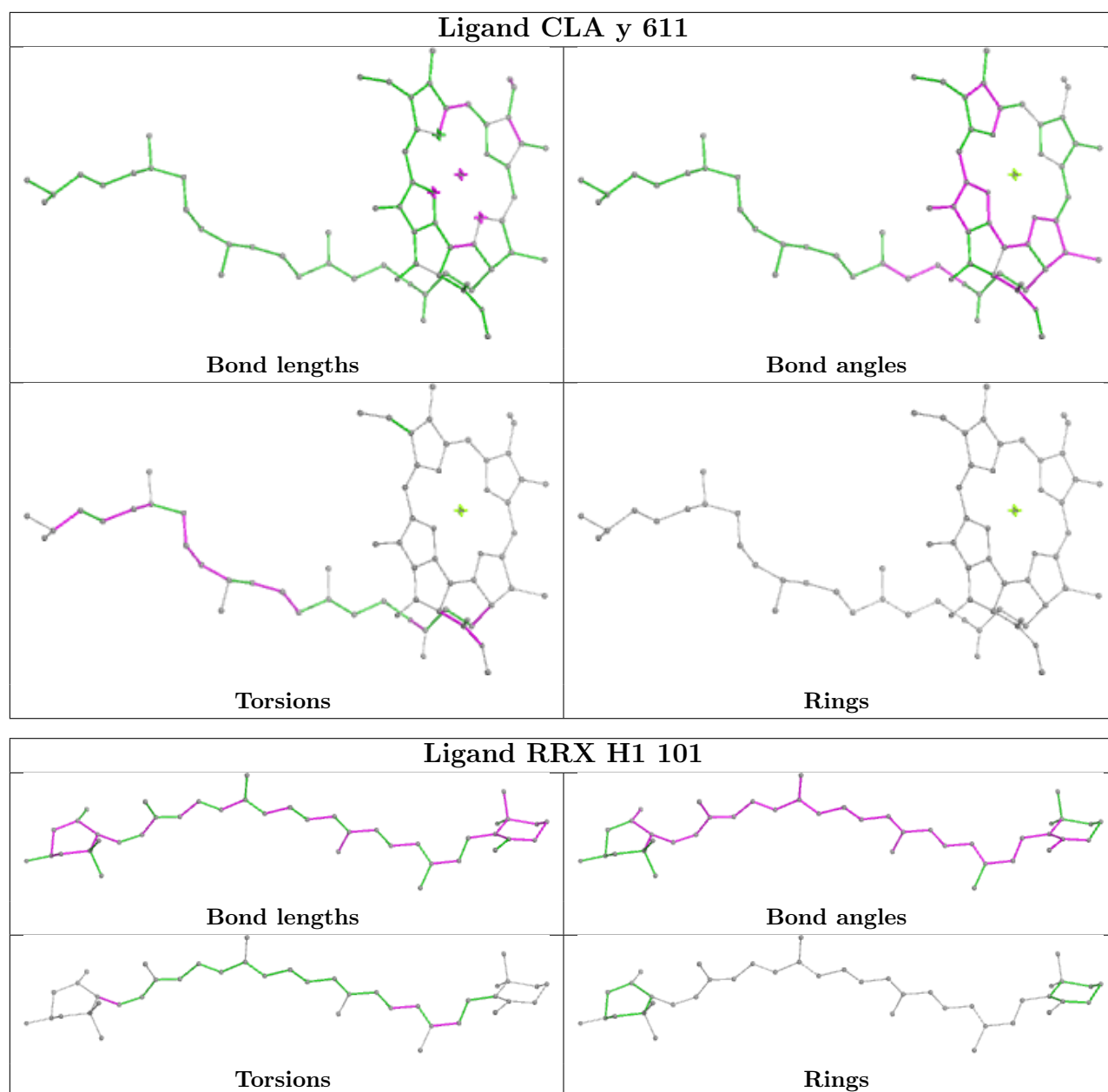


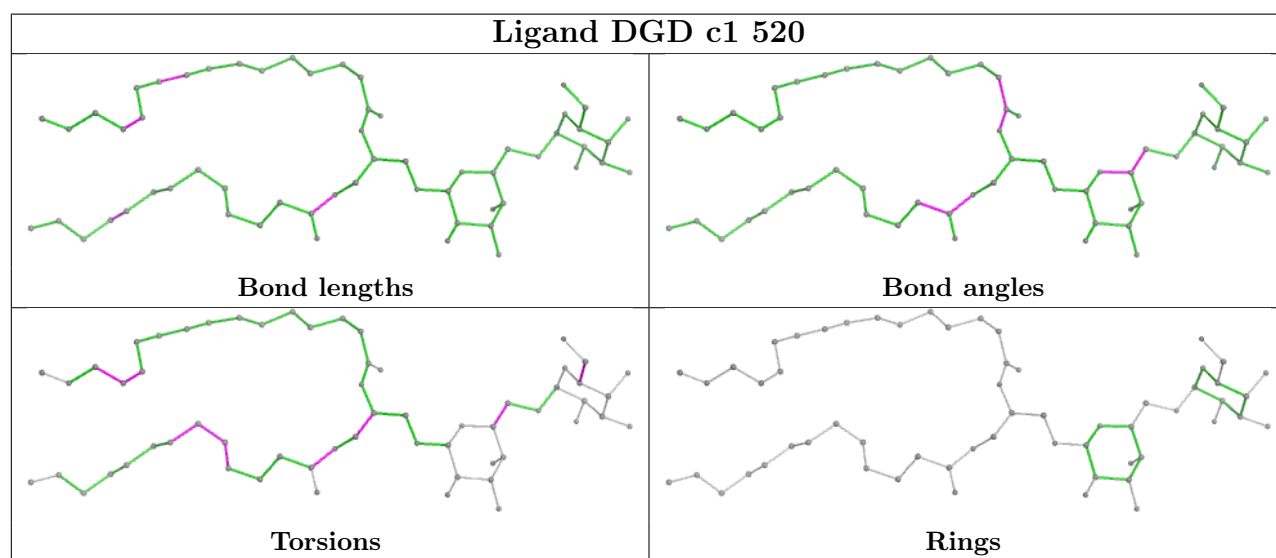
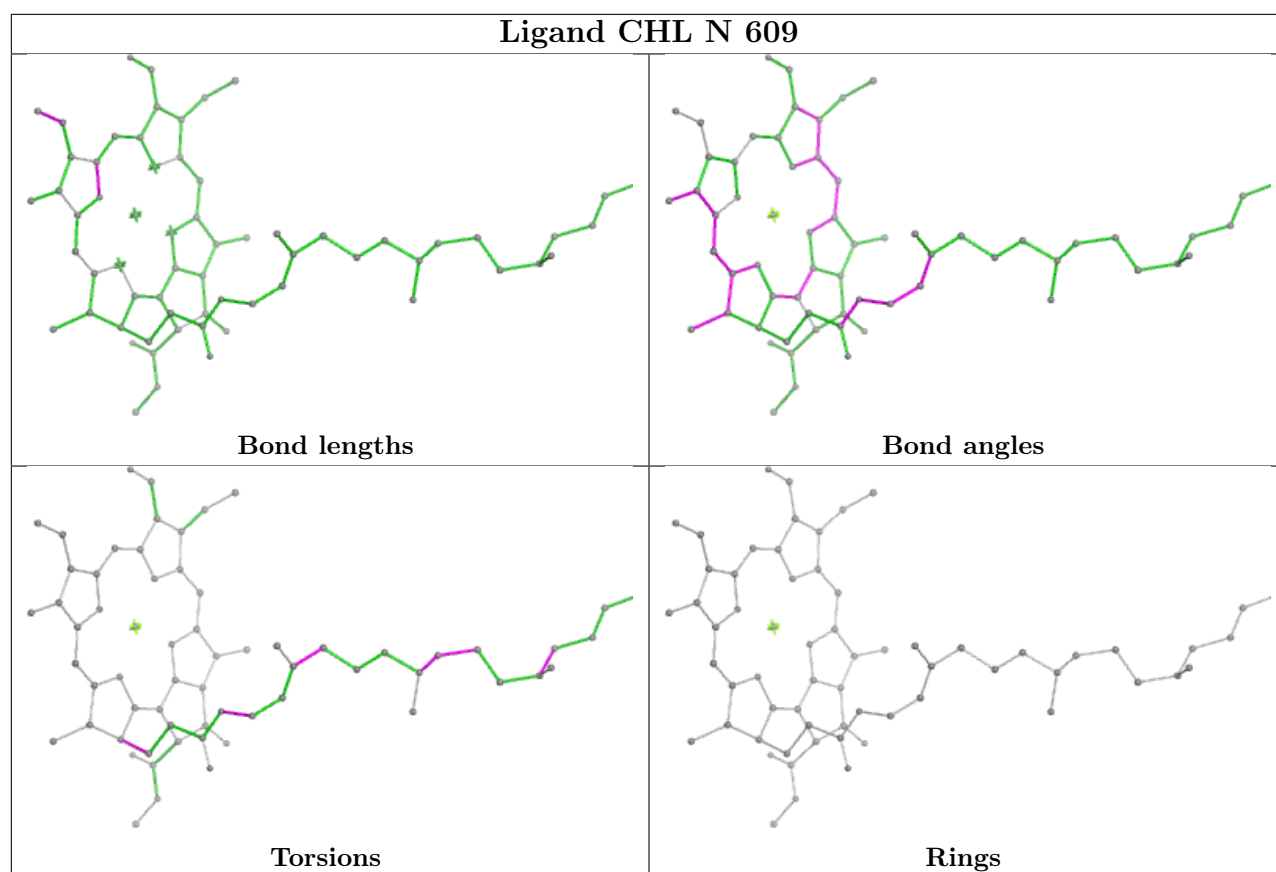




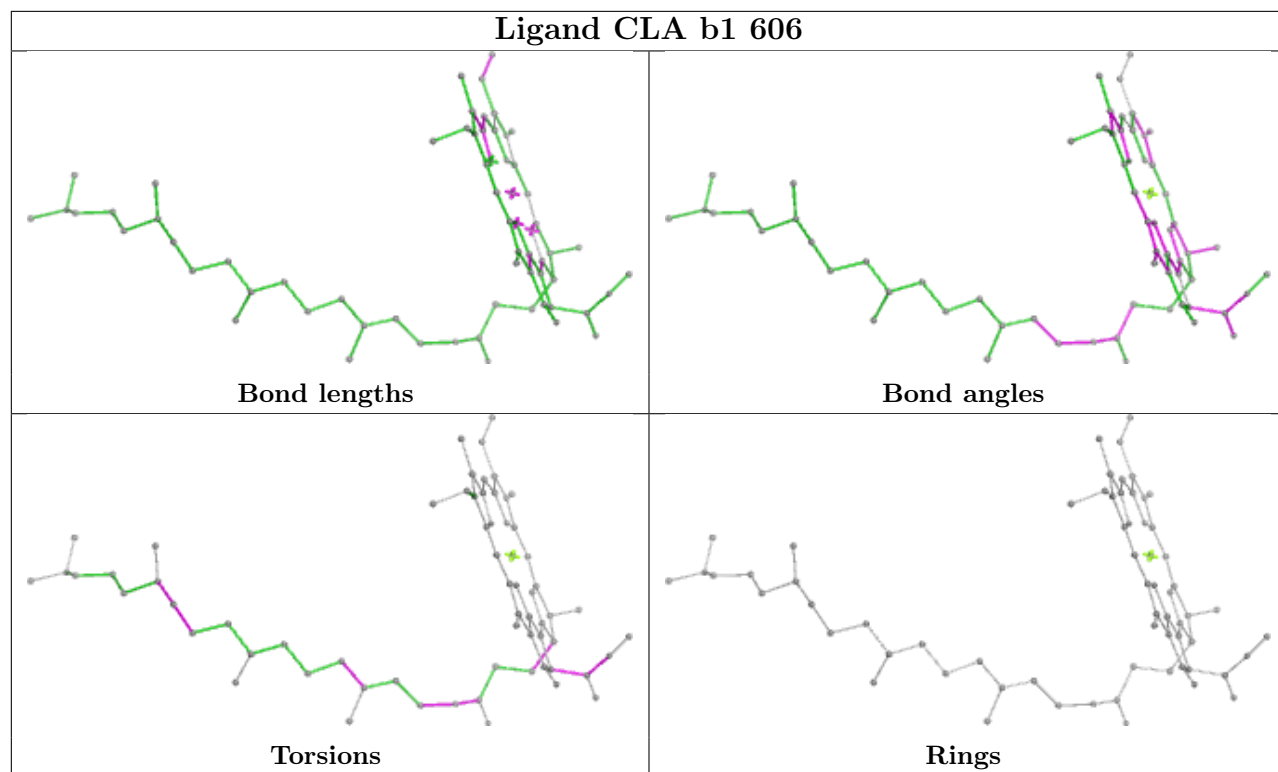
## Ligand CHL s 608

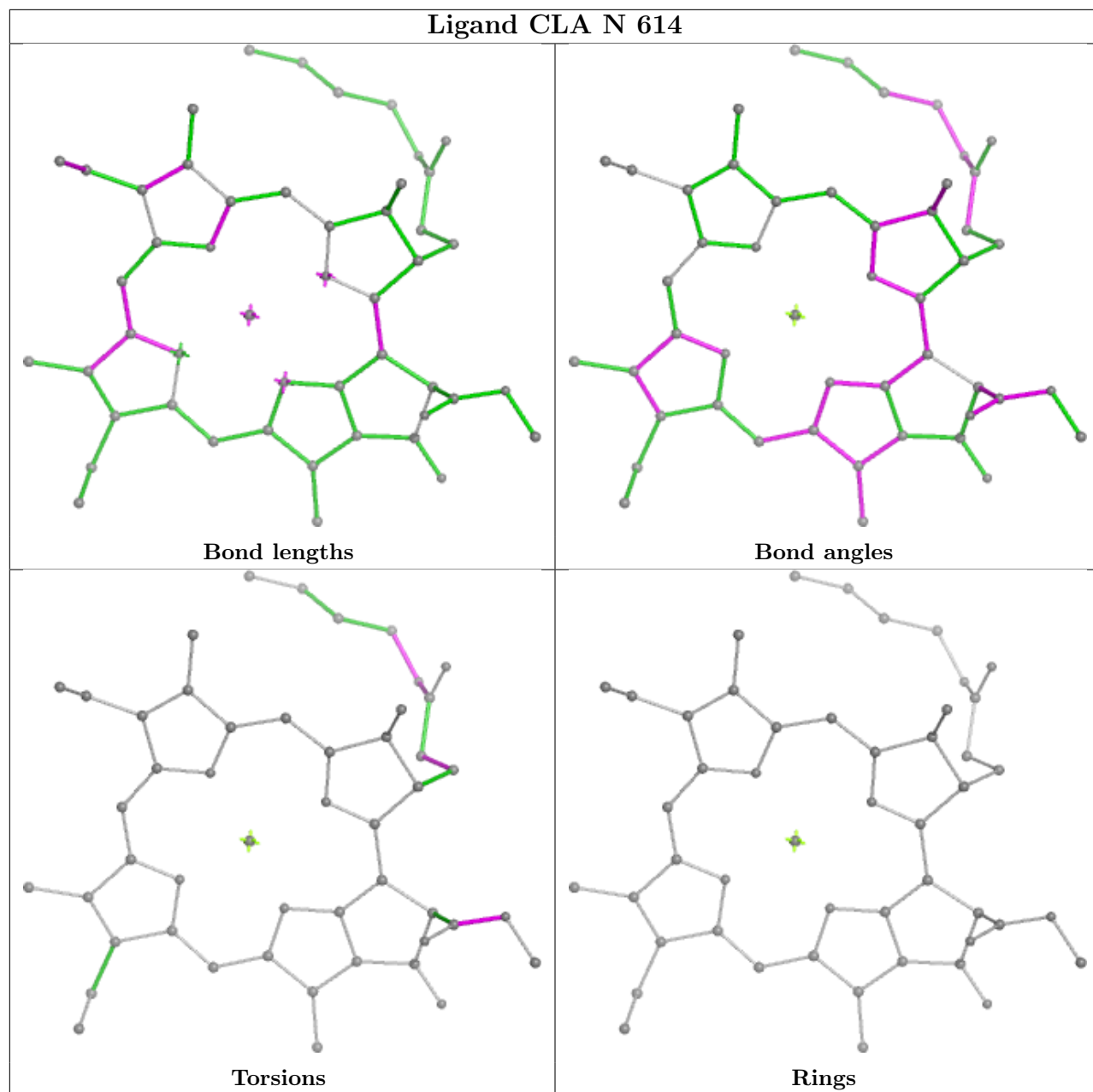


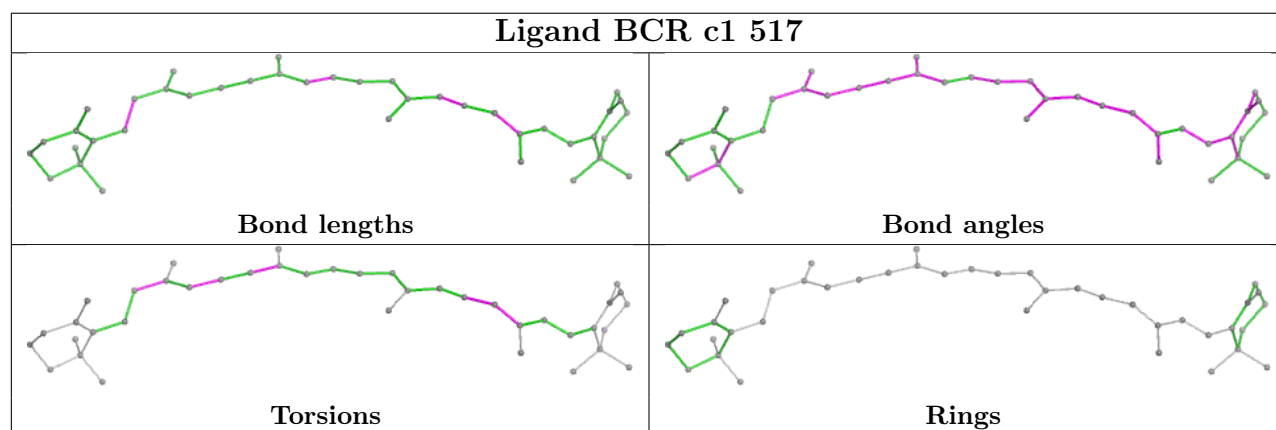
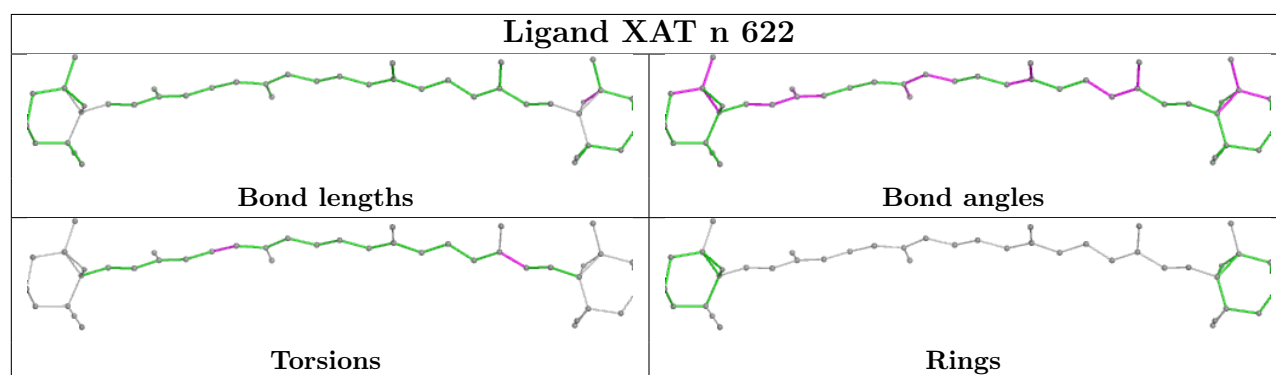
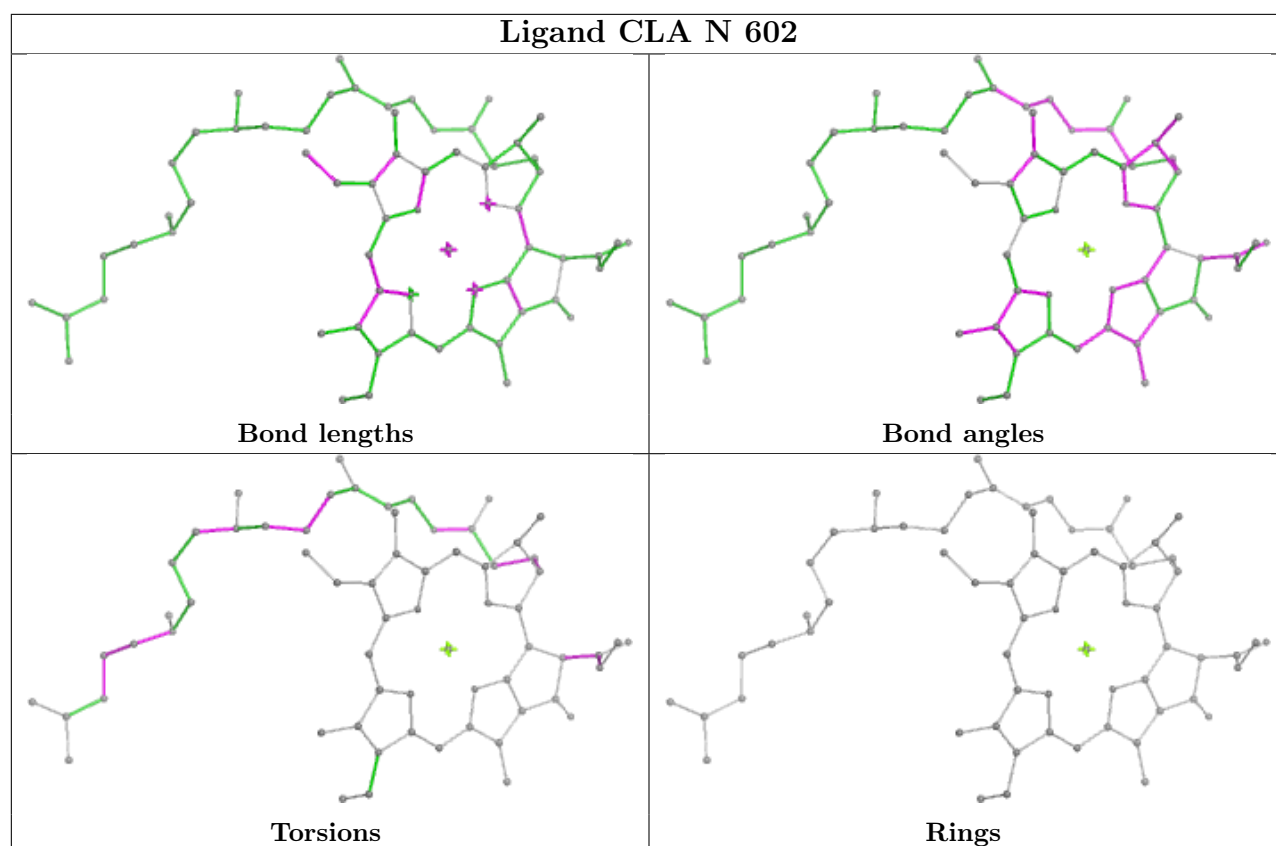


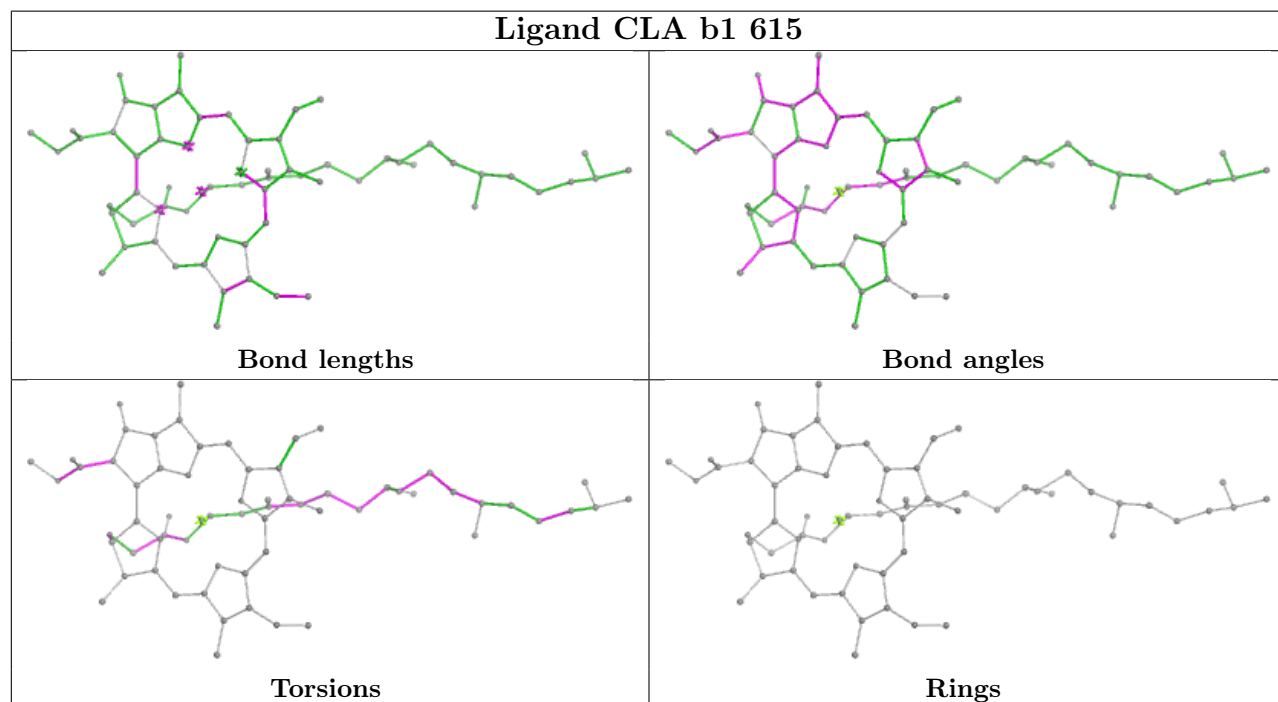
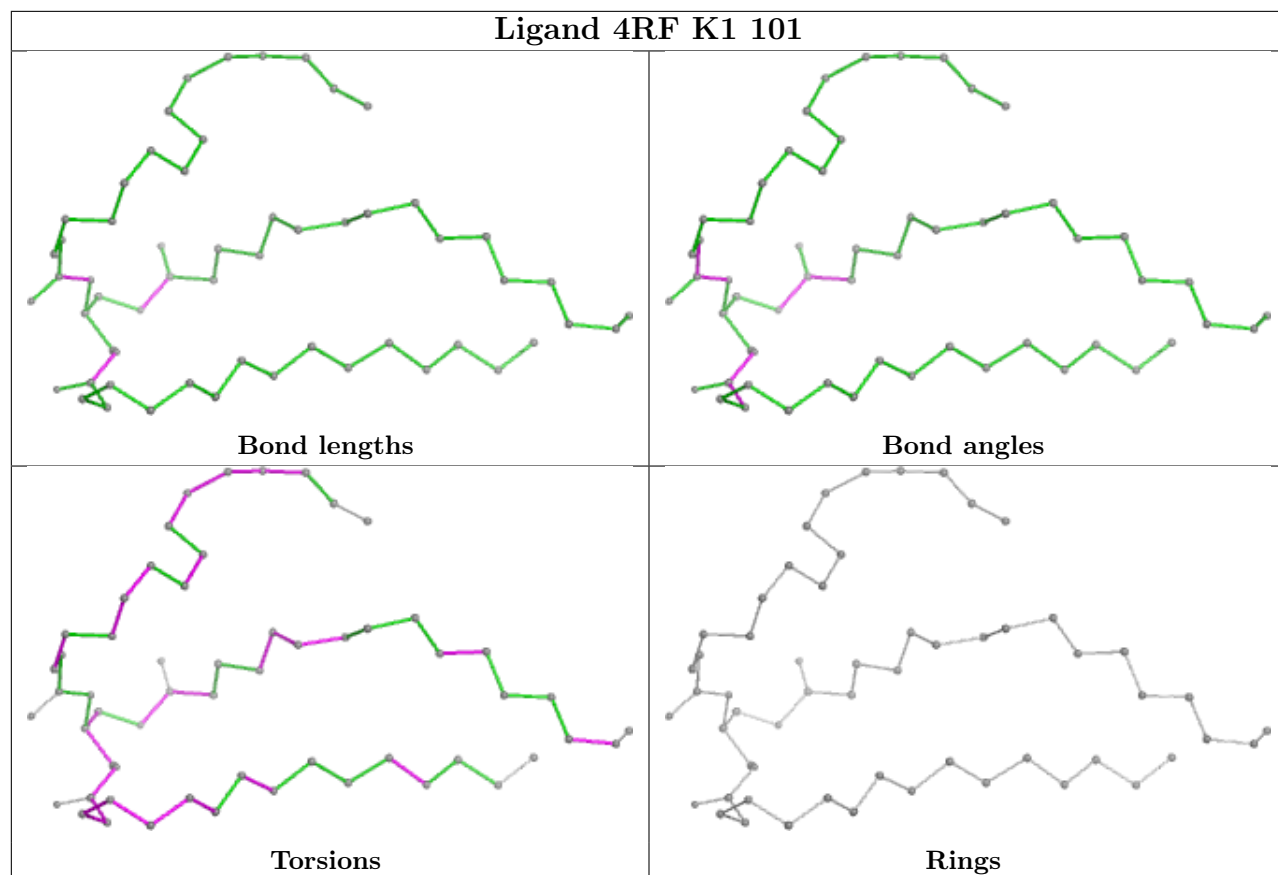


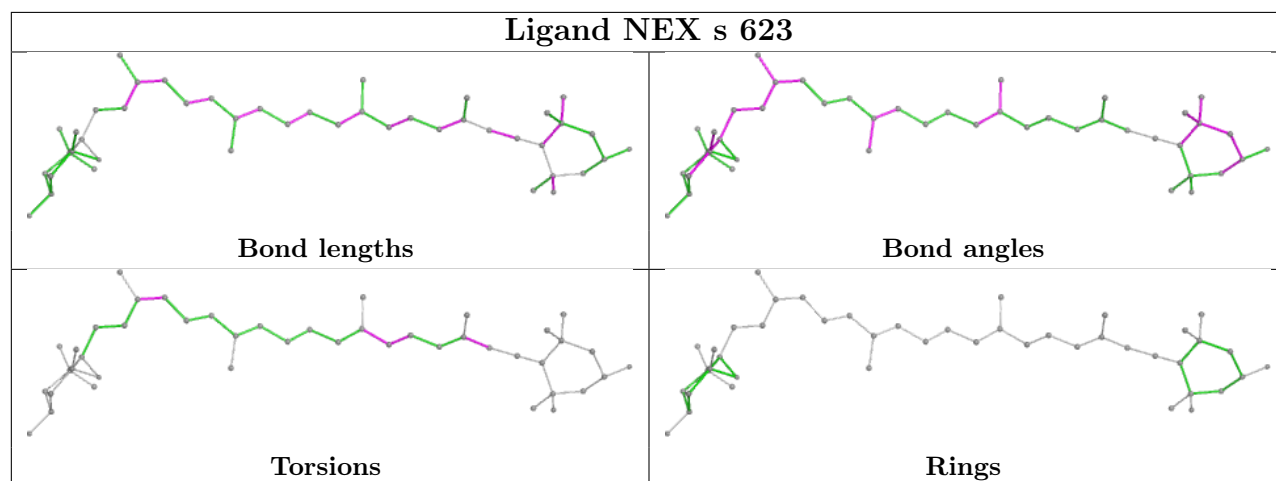
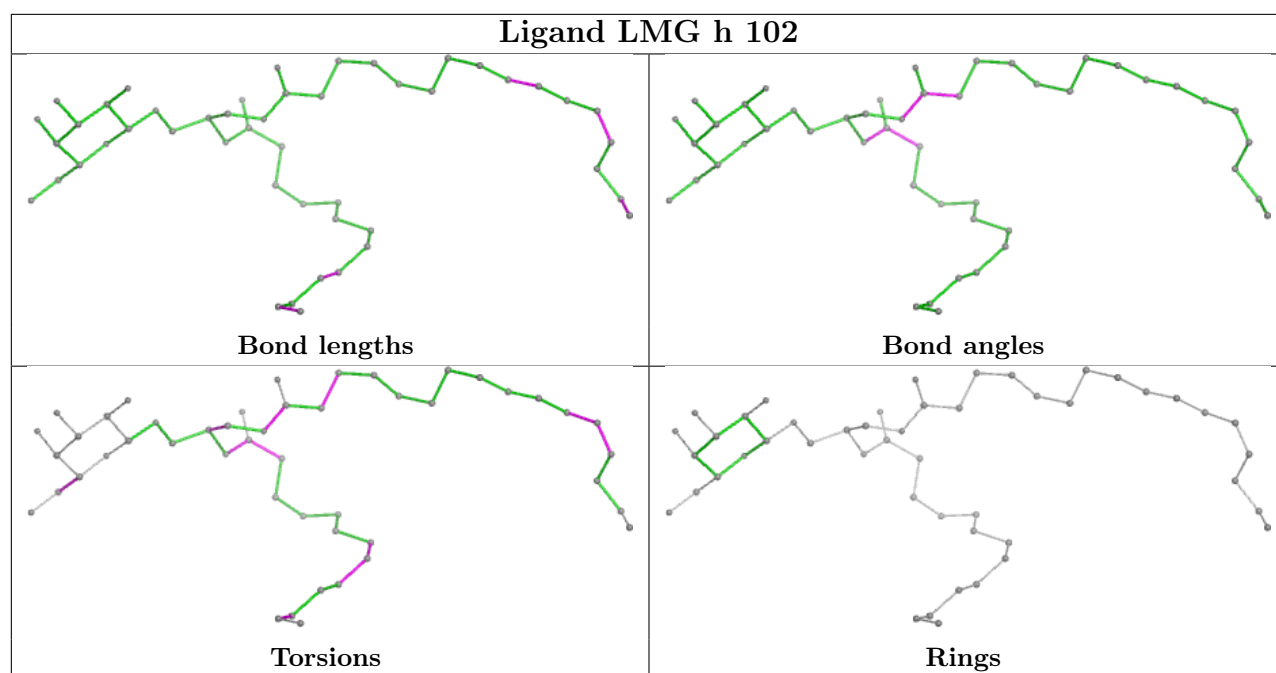


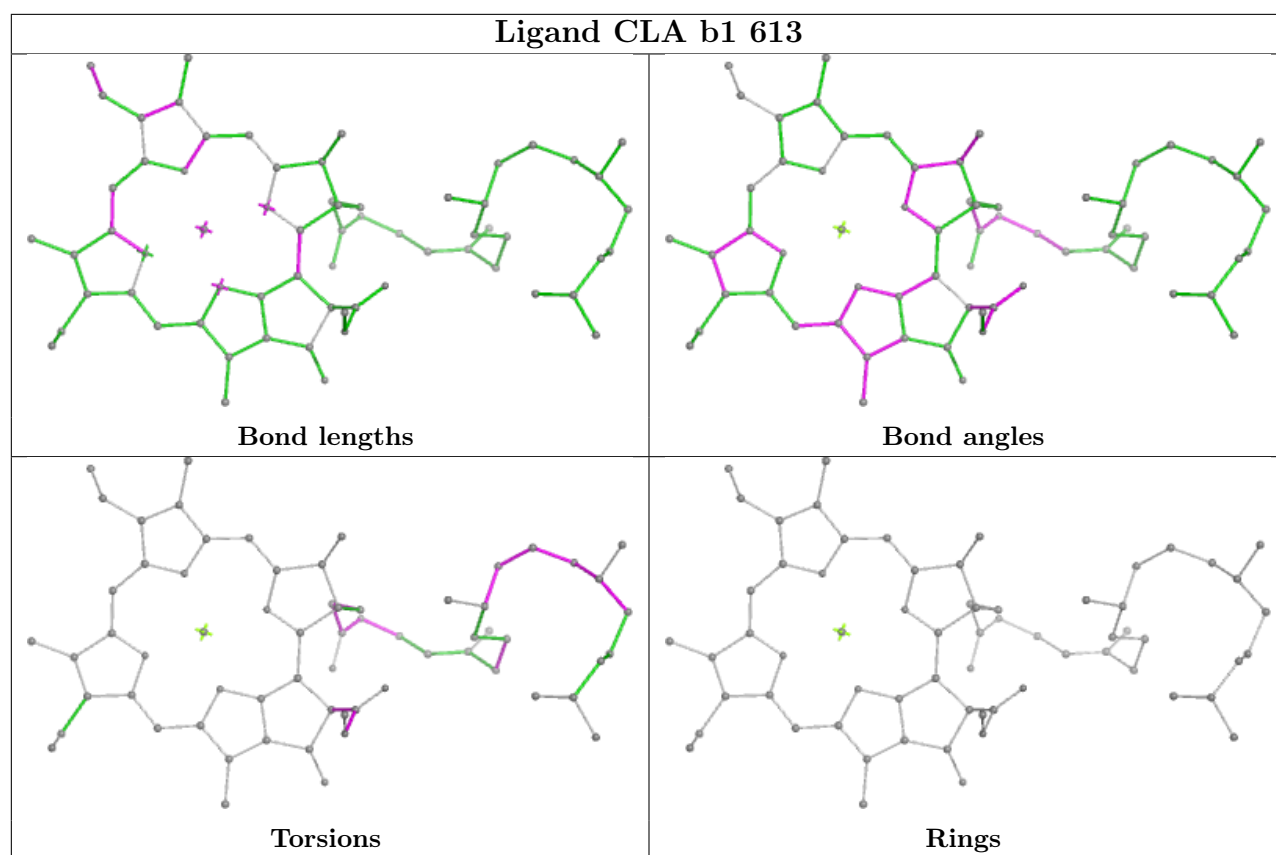




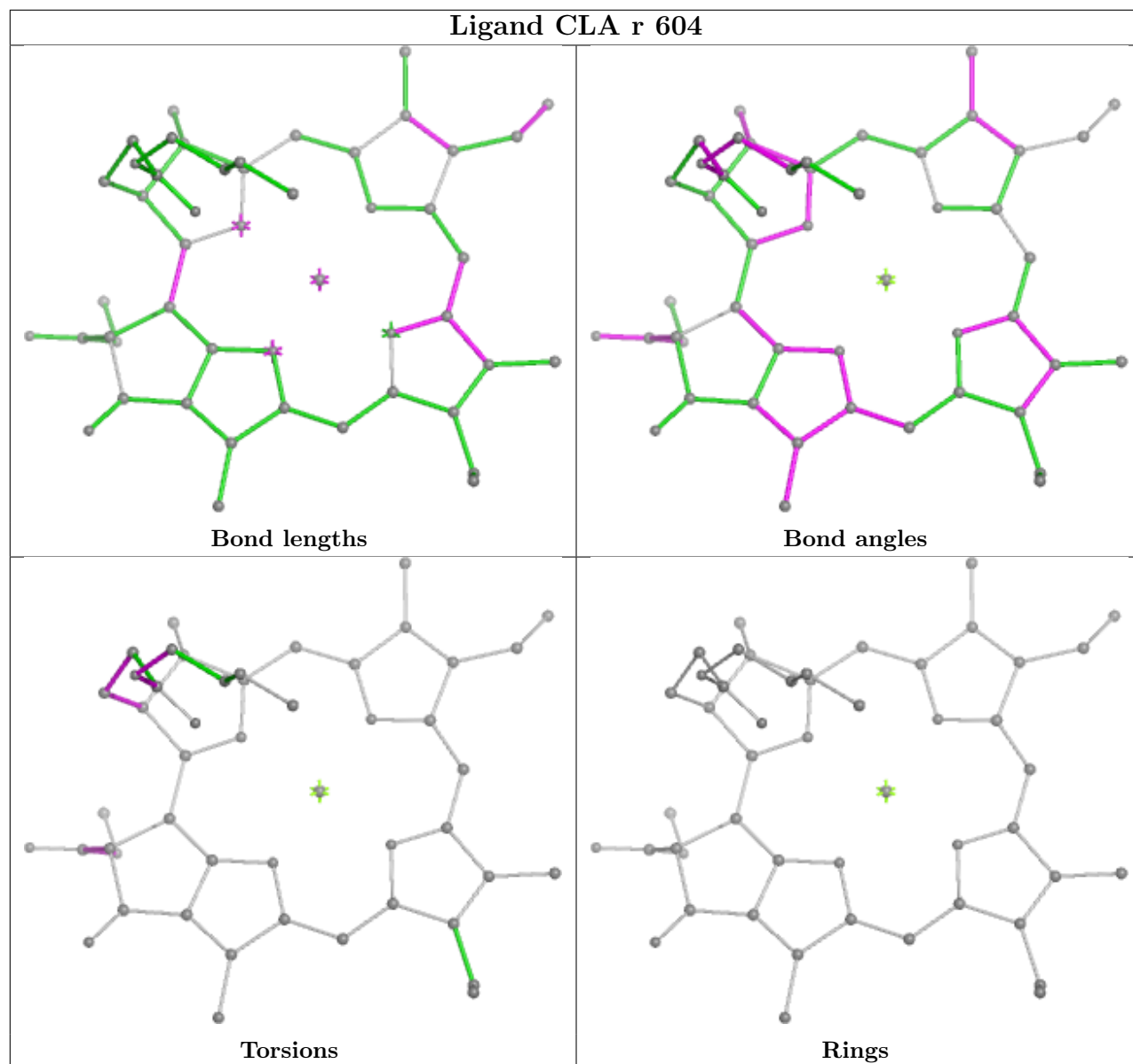


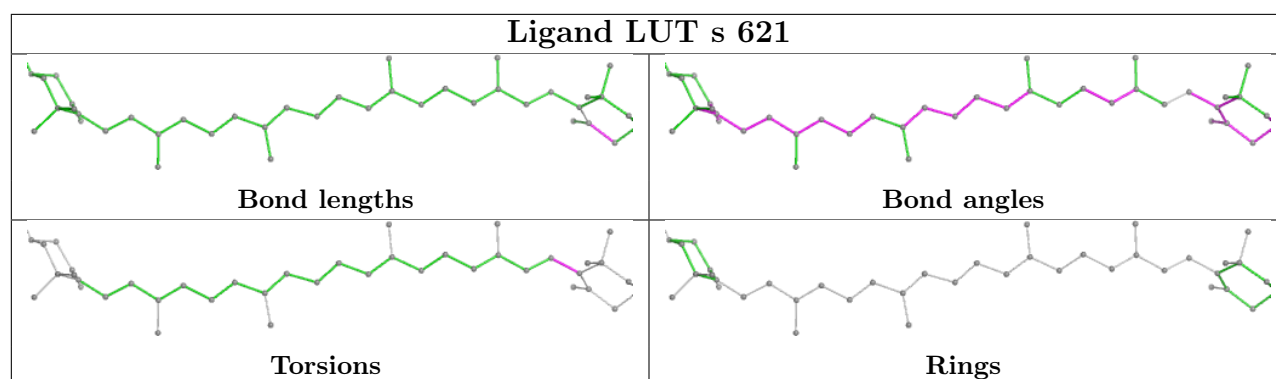
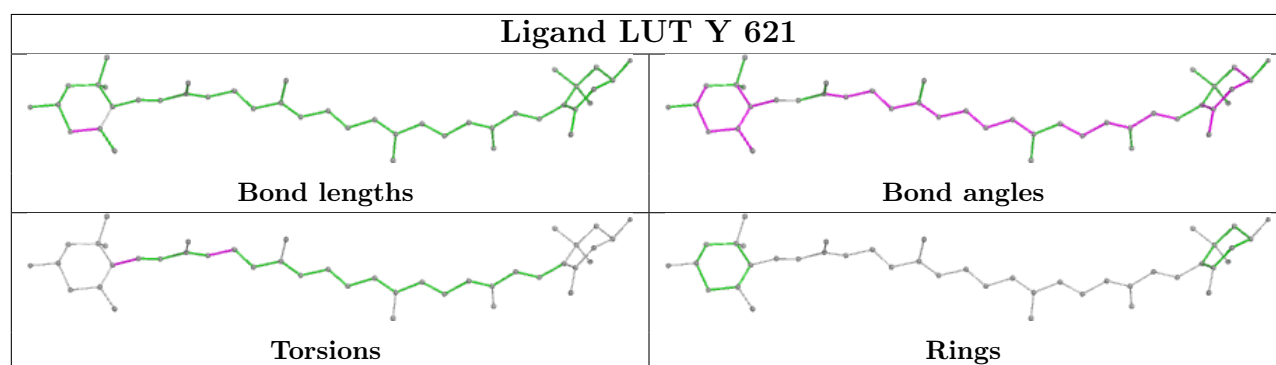
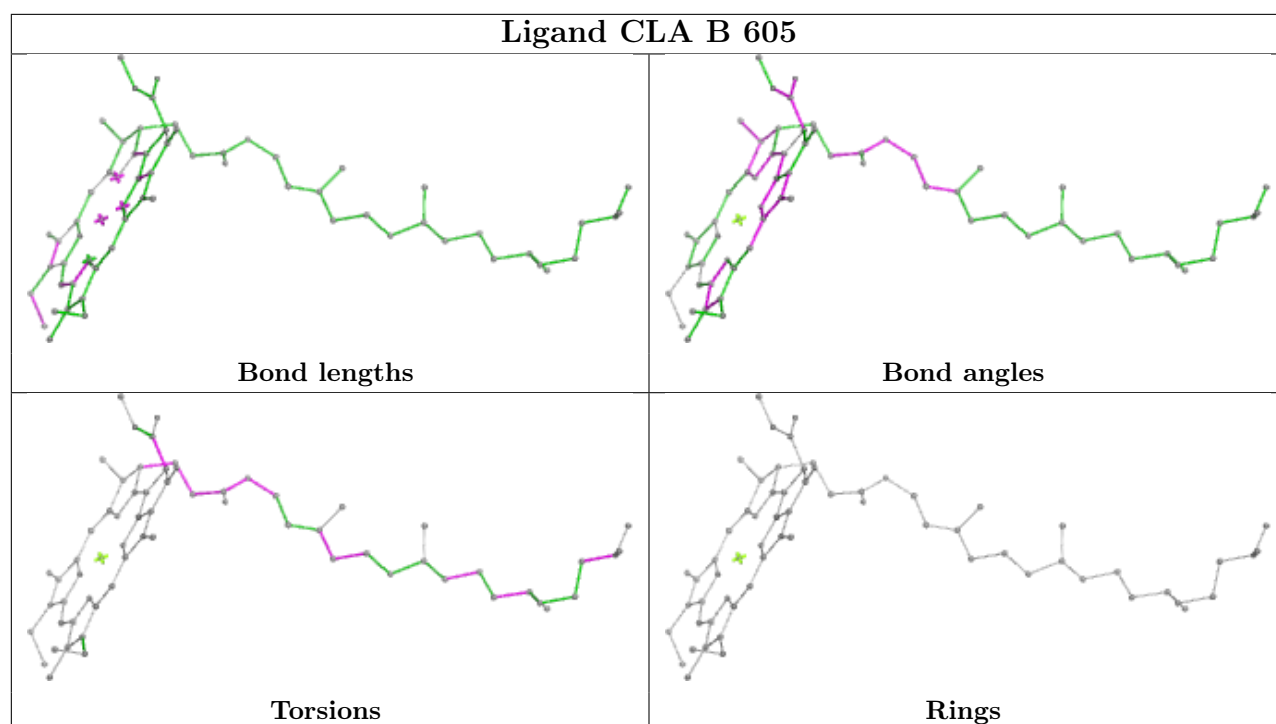




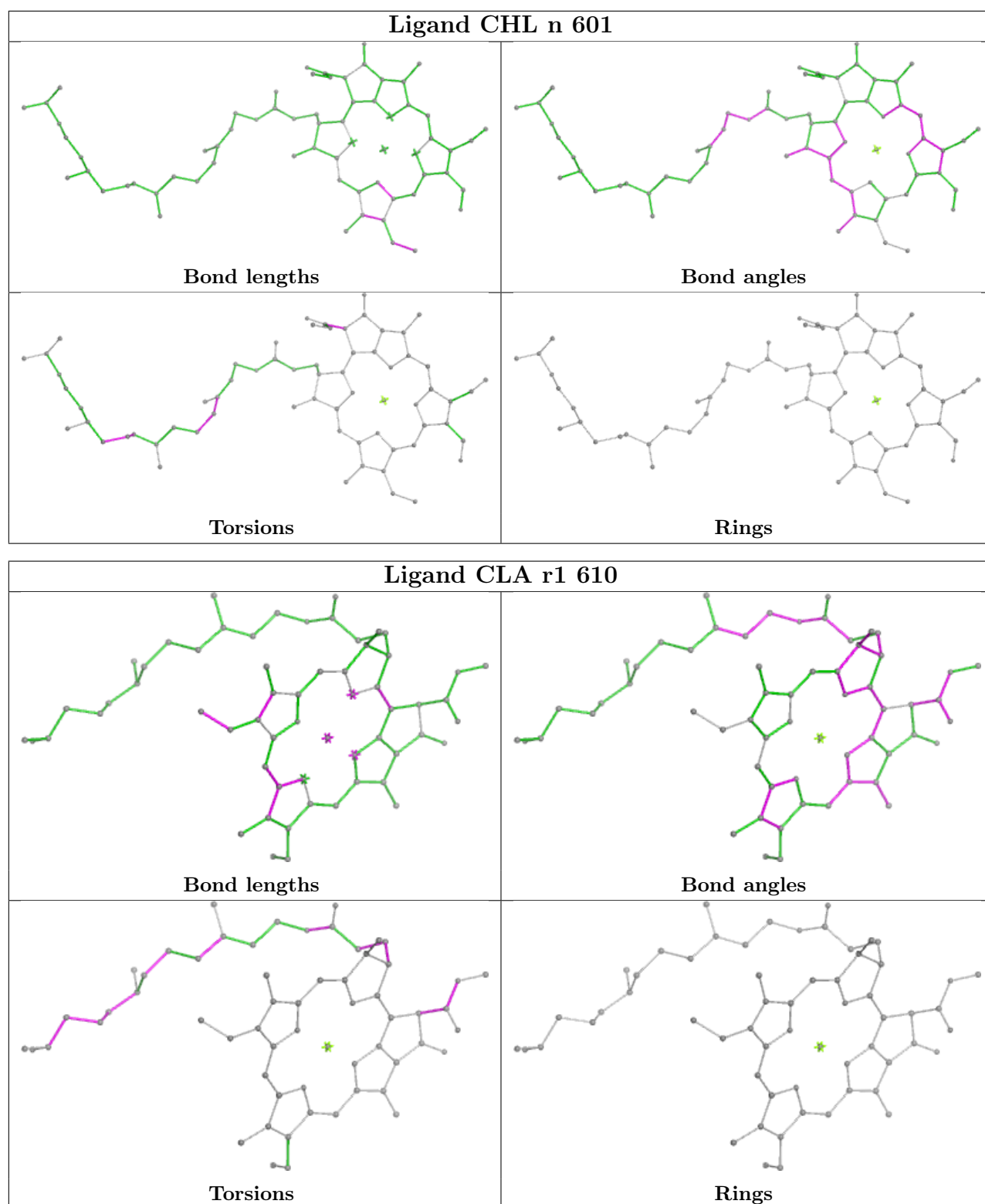


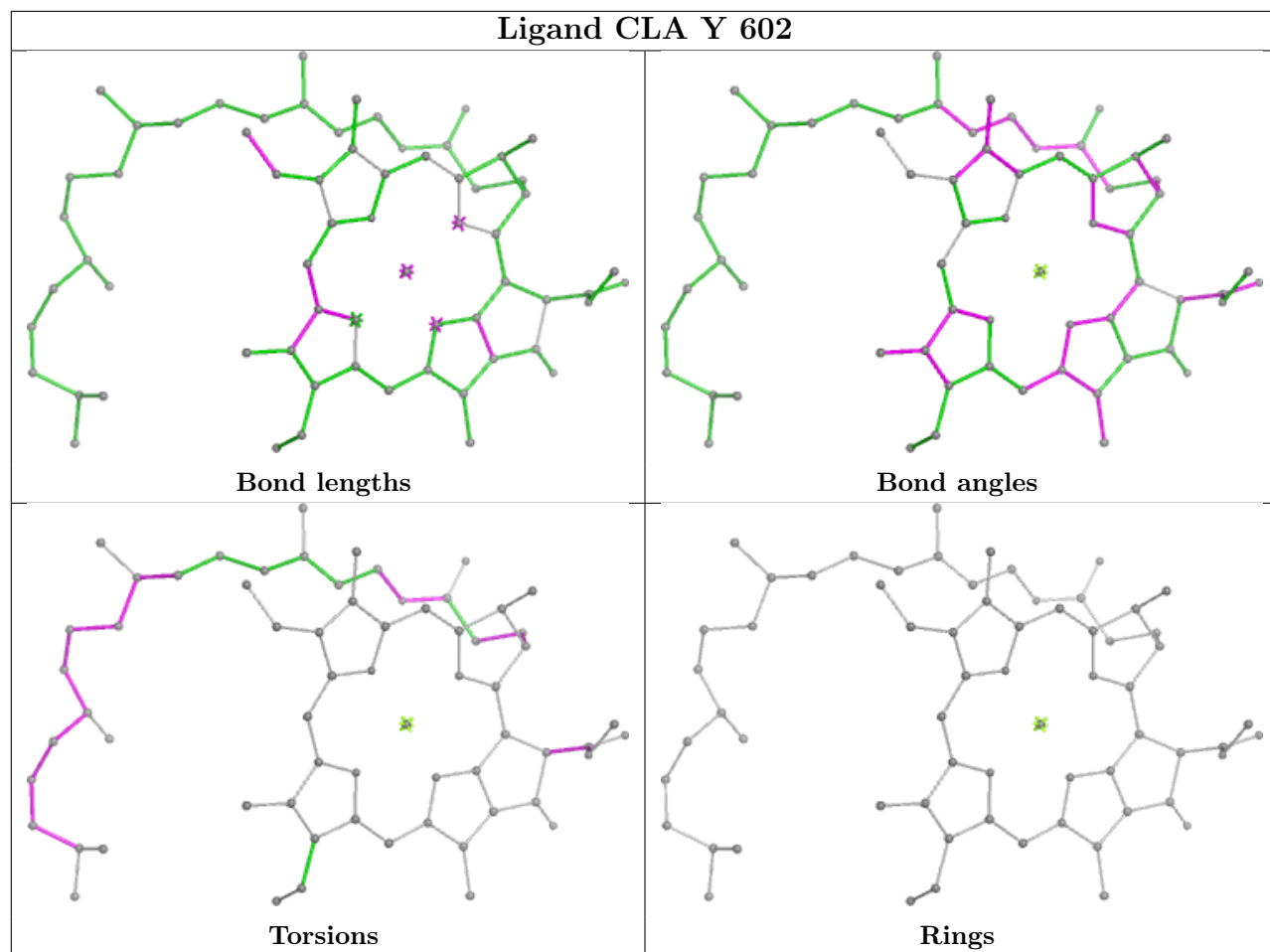
## Ligand CLA r 604



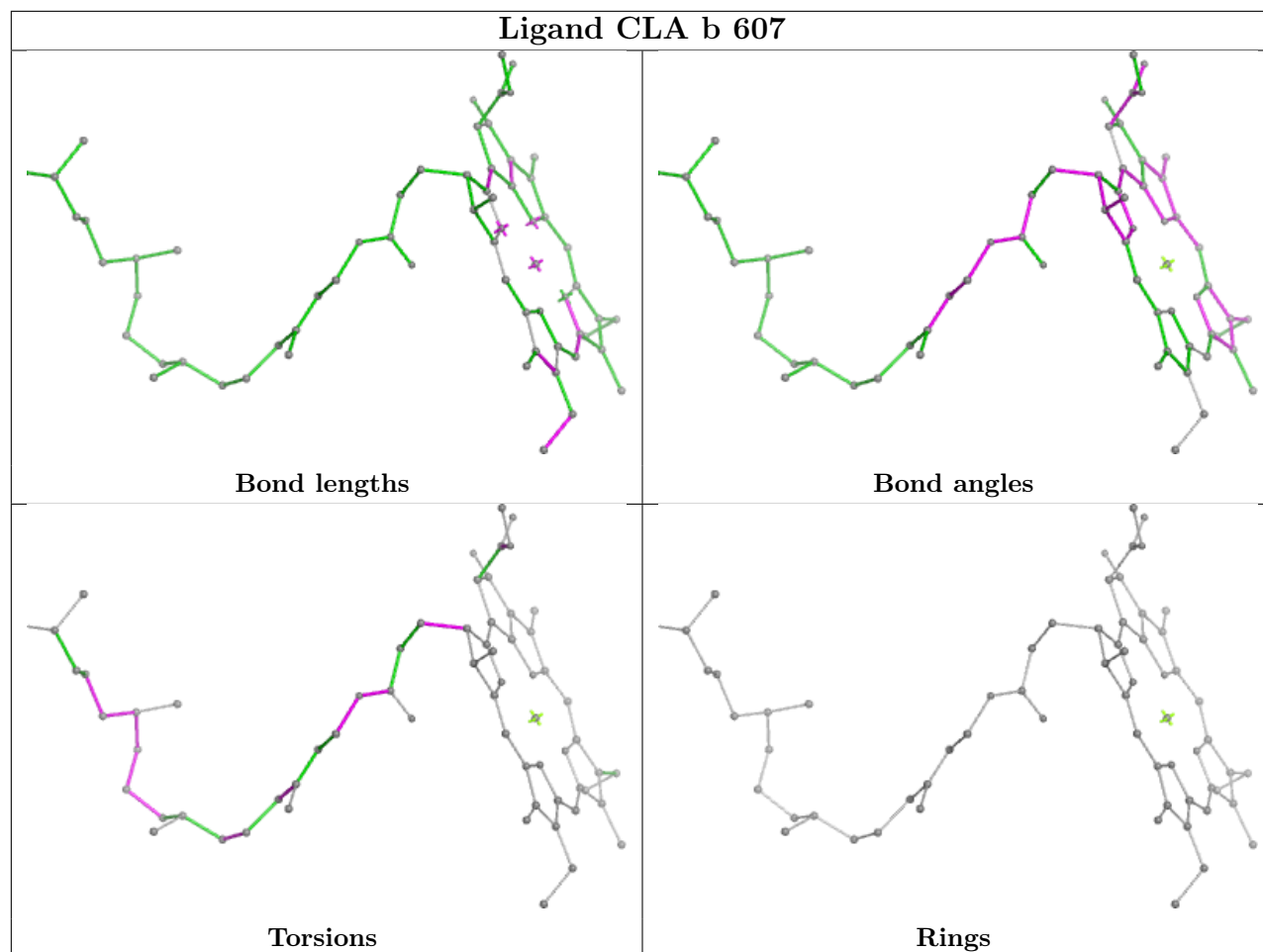




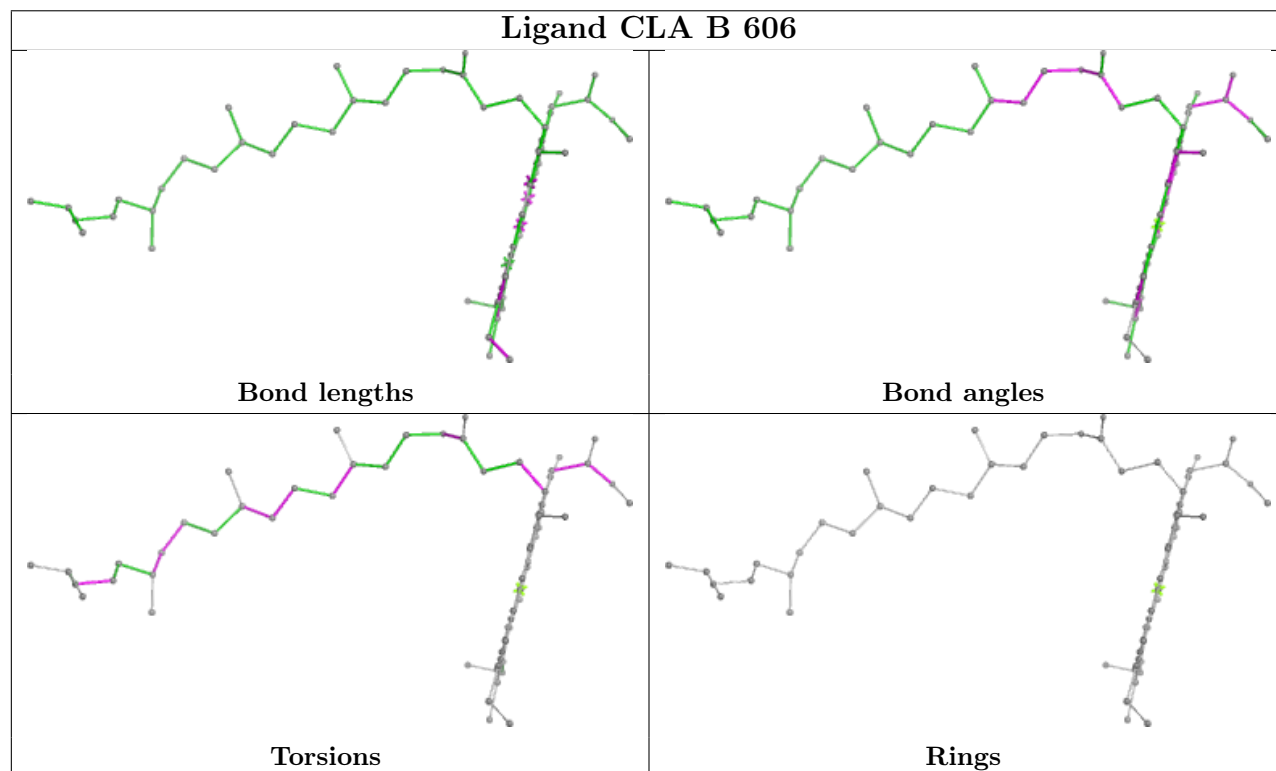


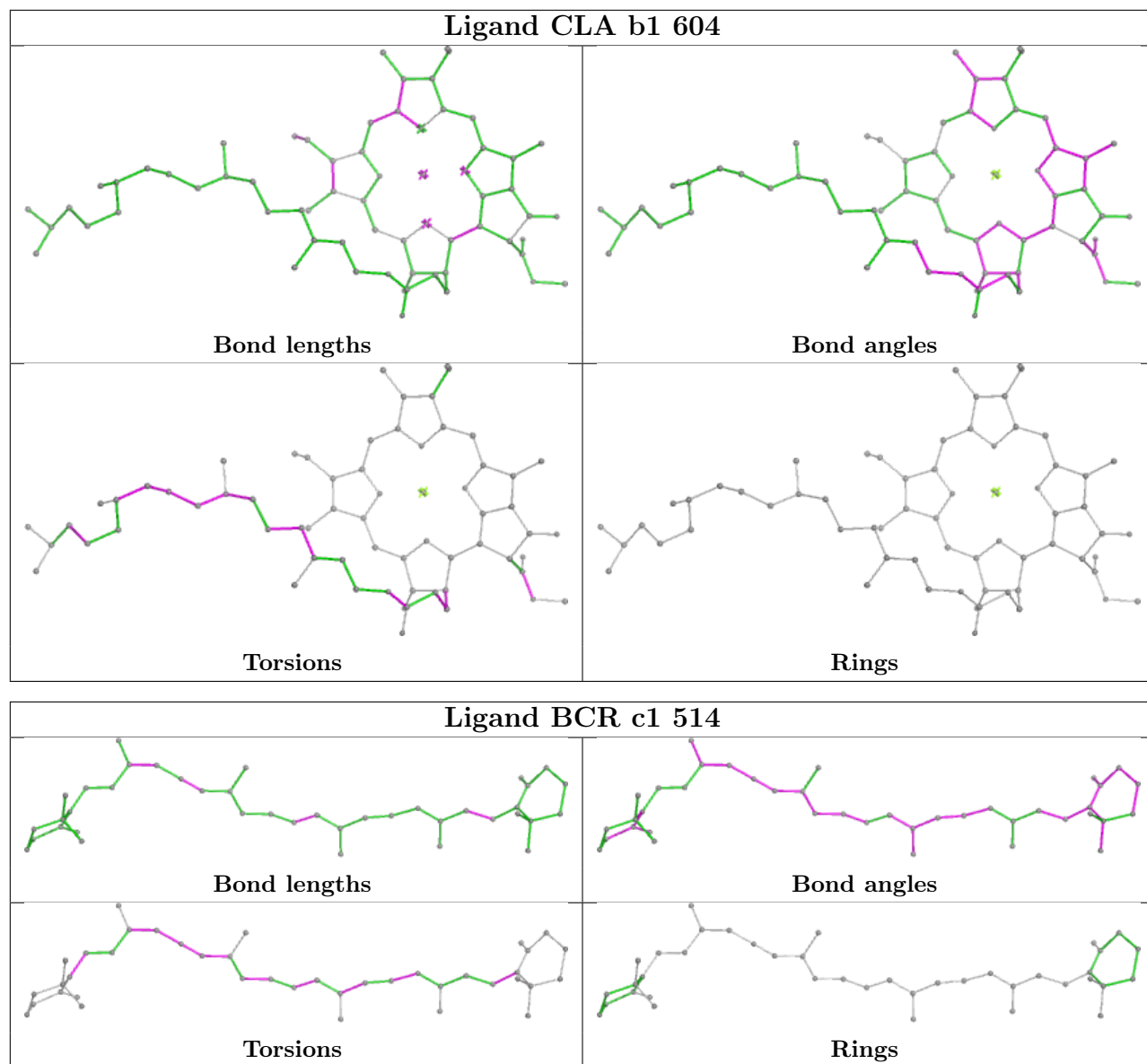


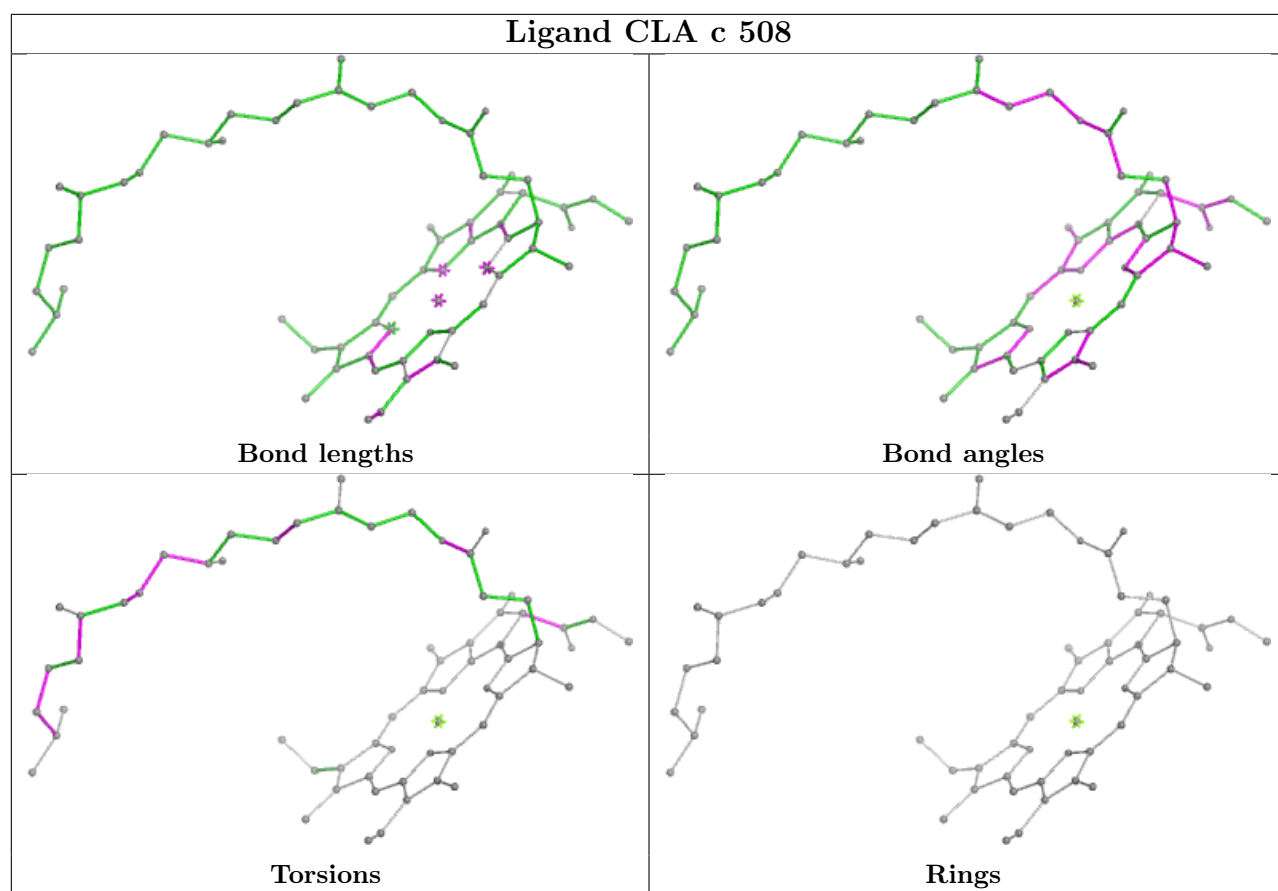
## Ligand CLA b 607



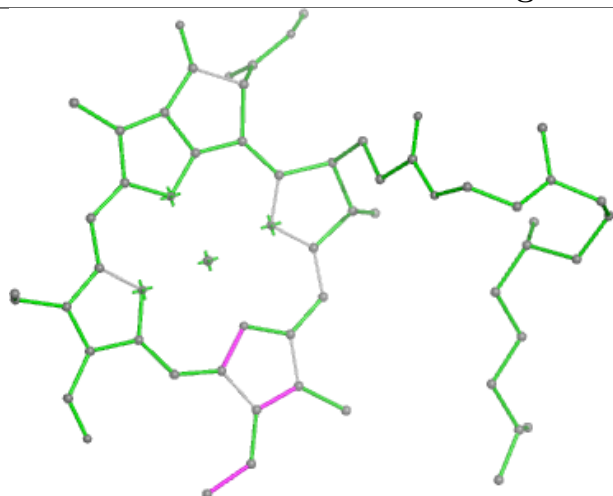
## Ligand CLA B 606



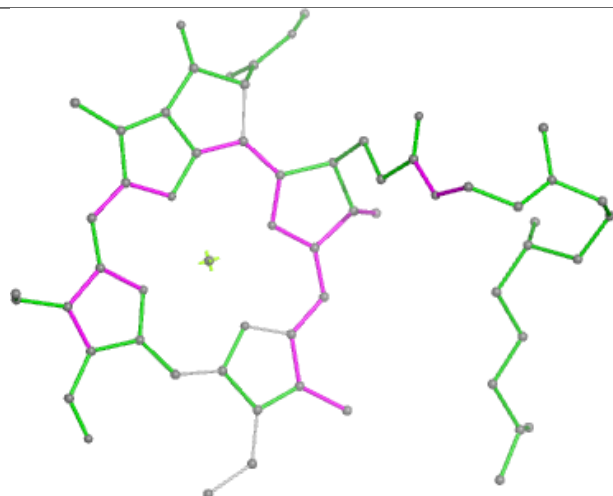




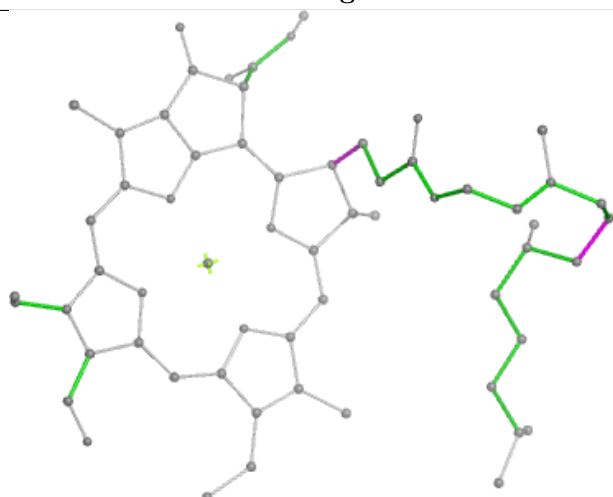
## Ligand CHL S 608



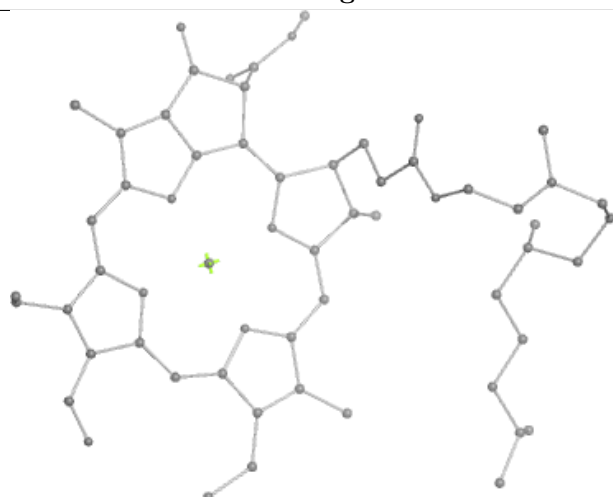
Bond lengths



Bond angles

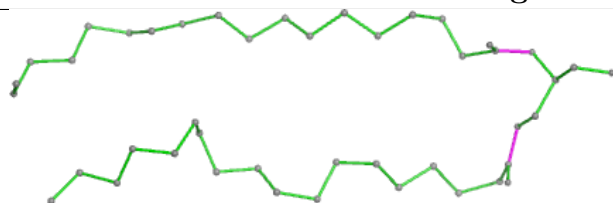


Torsions

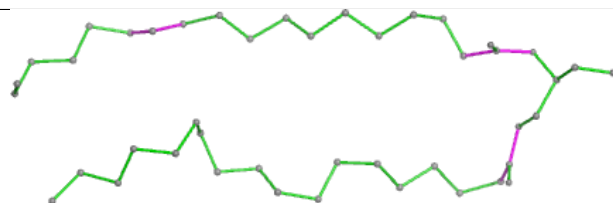


Rings

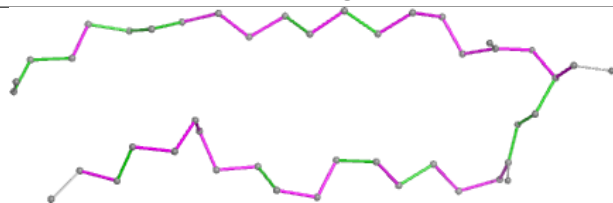
## Ligand DGA B 625



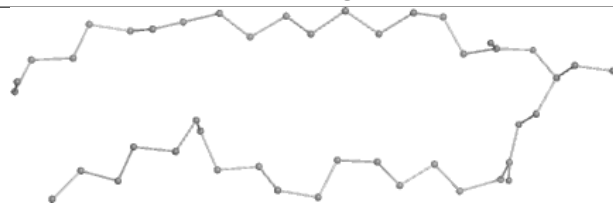
Bond lengths



Bond angles

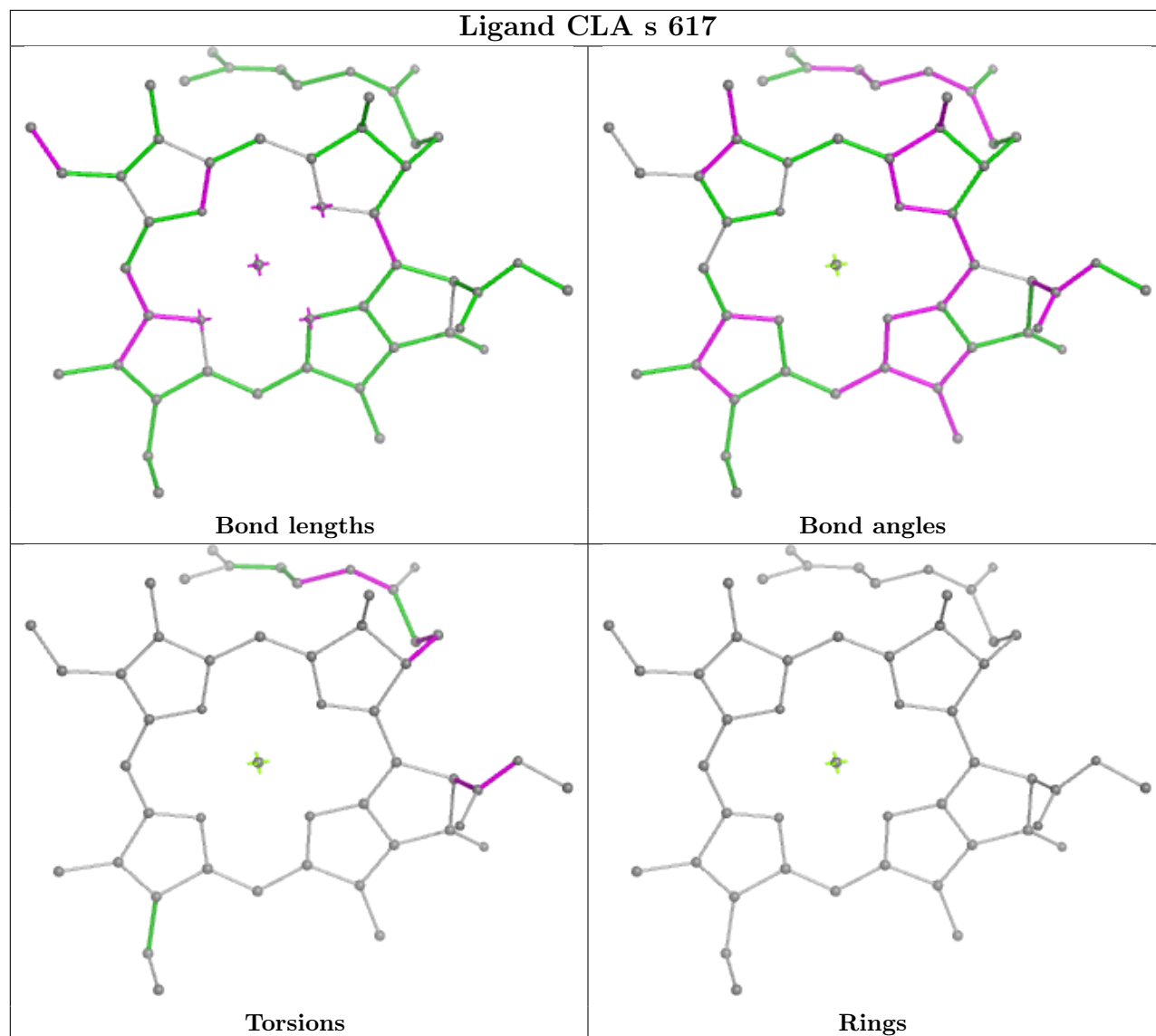


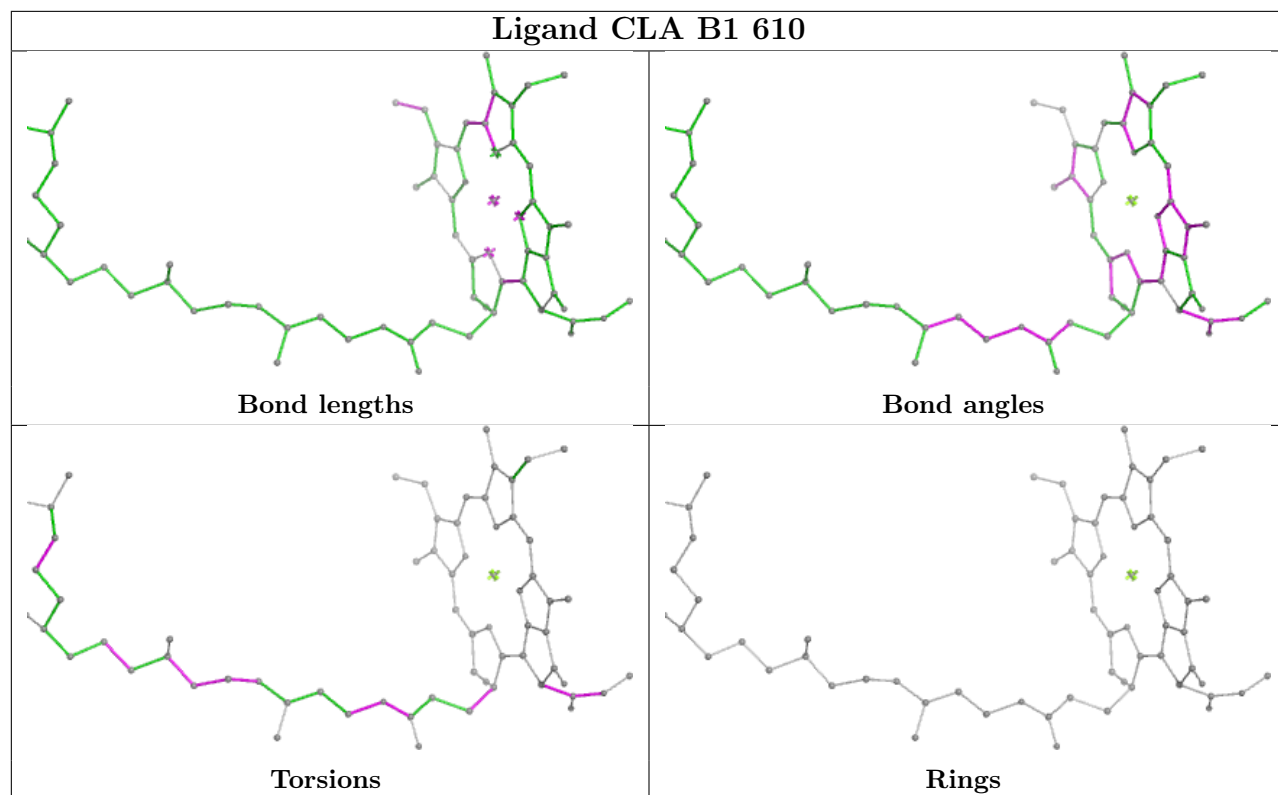
Torsions



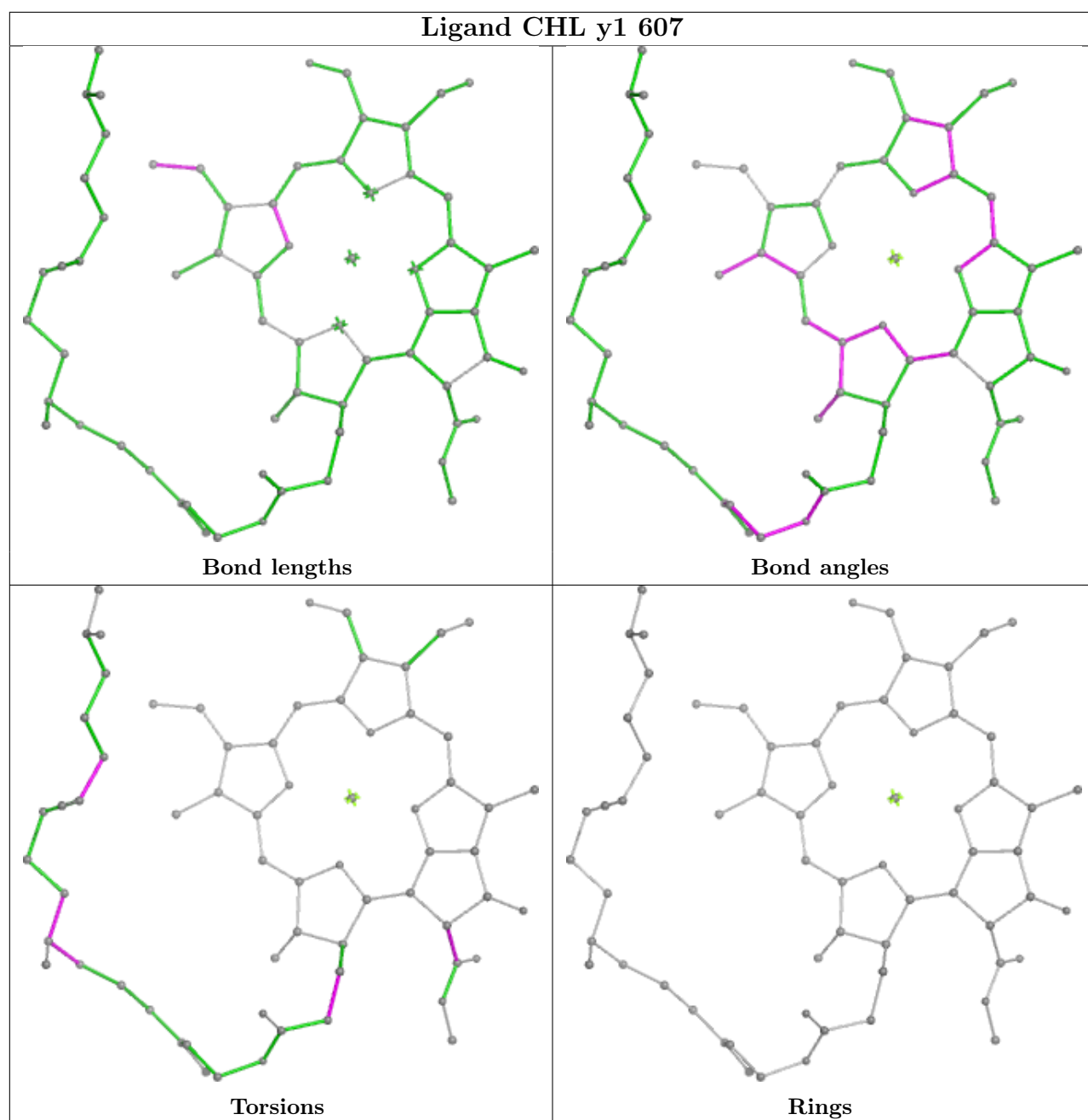
Rings

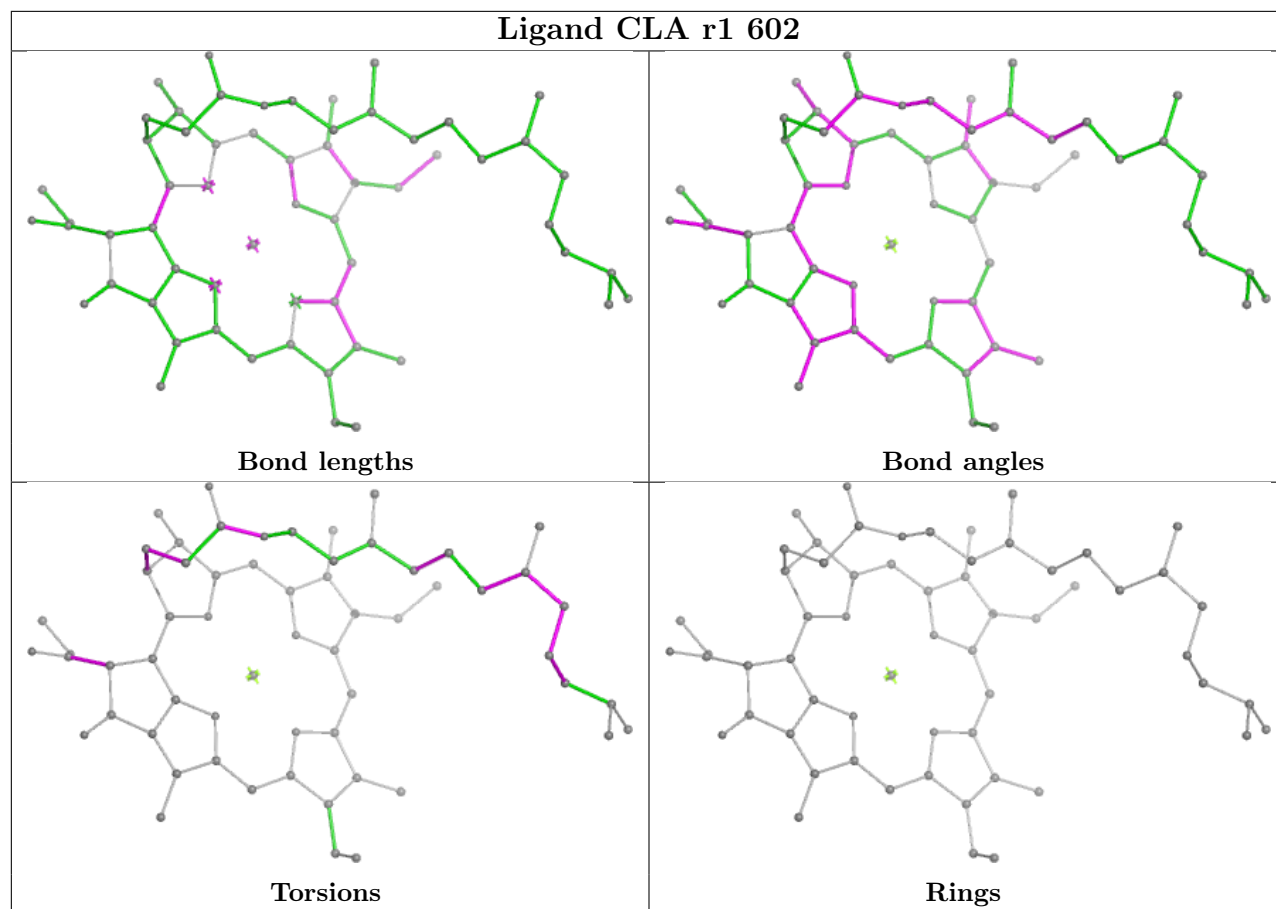
## Ligand CLA s 617



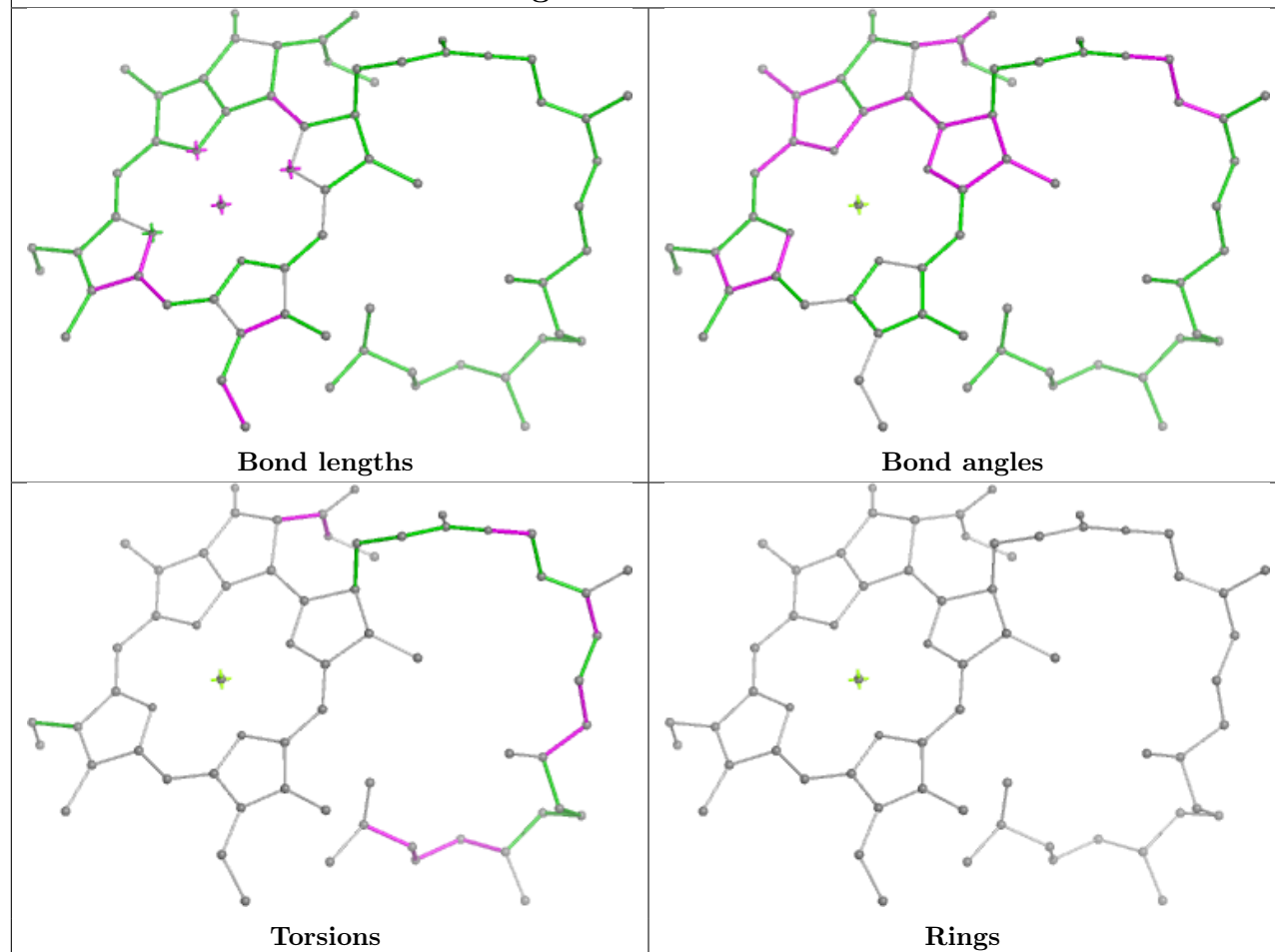




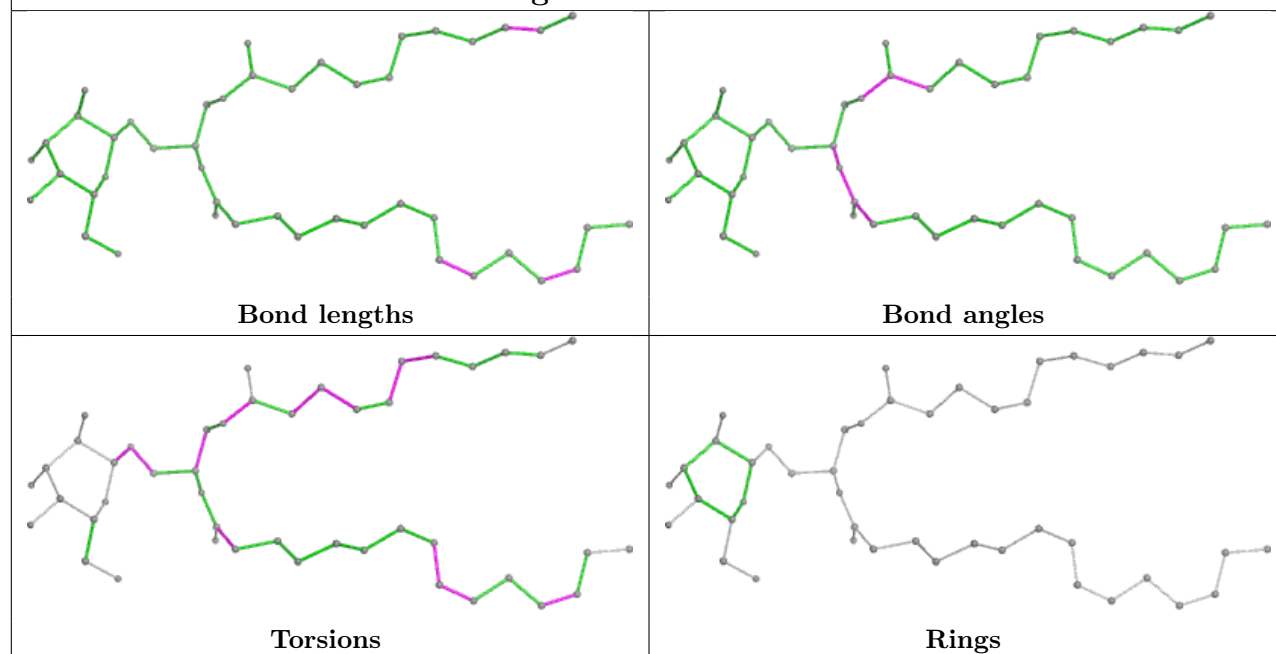


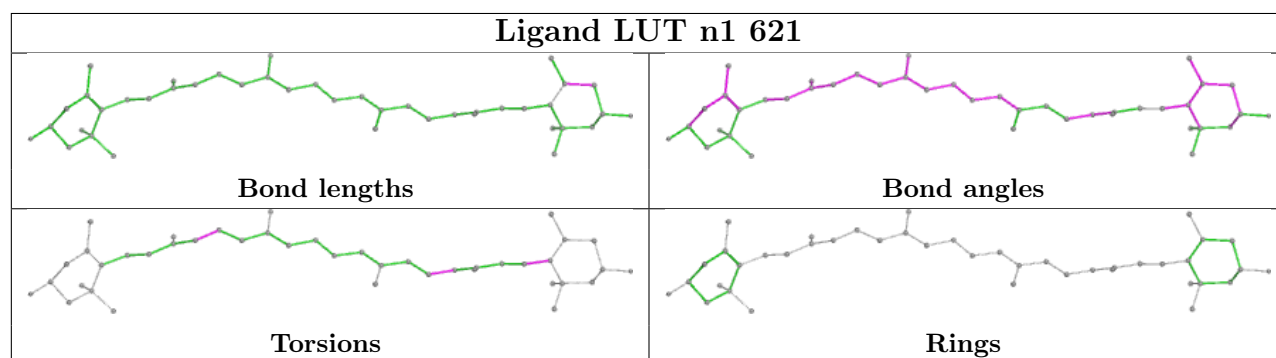
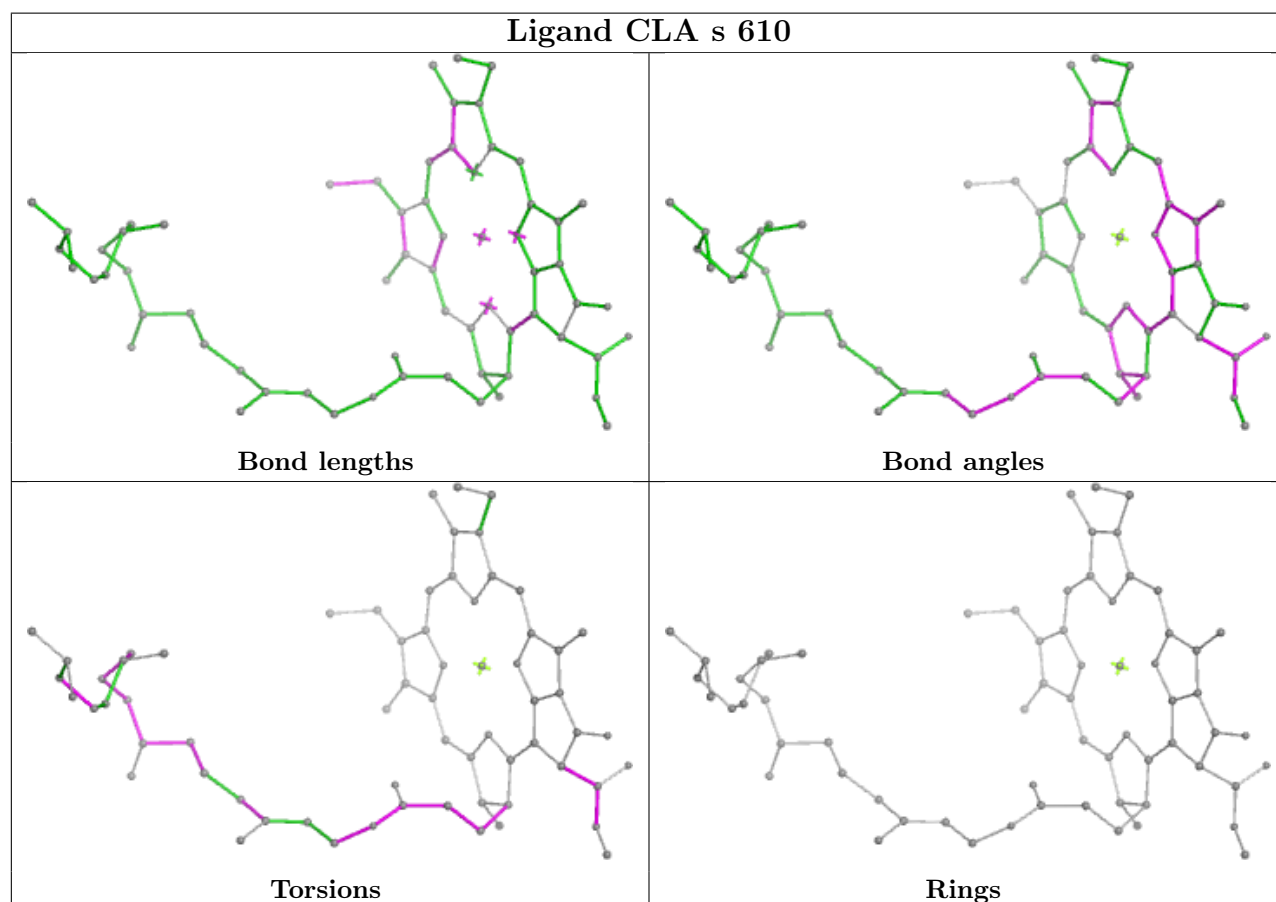
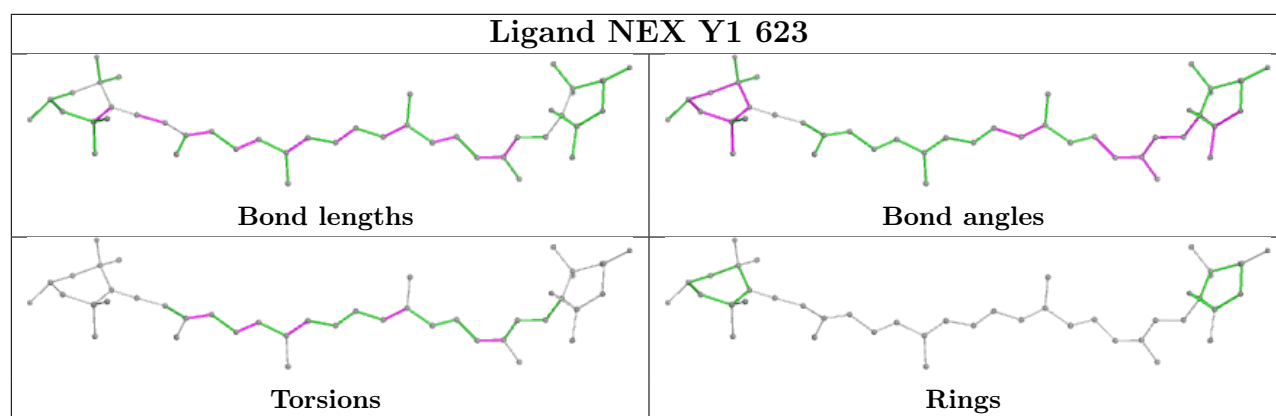


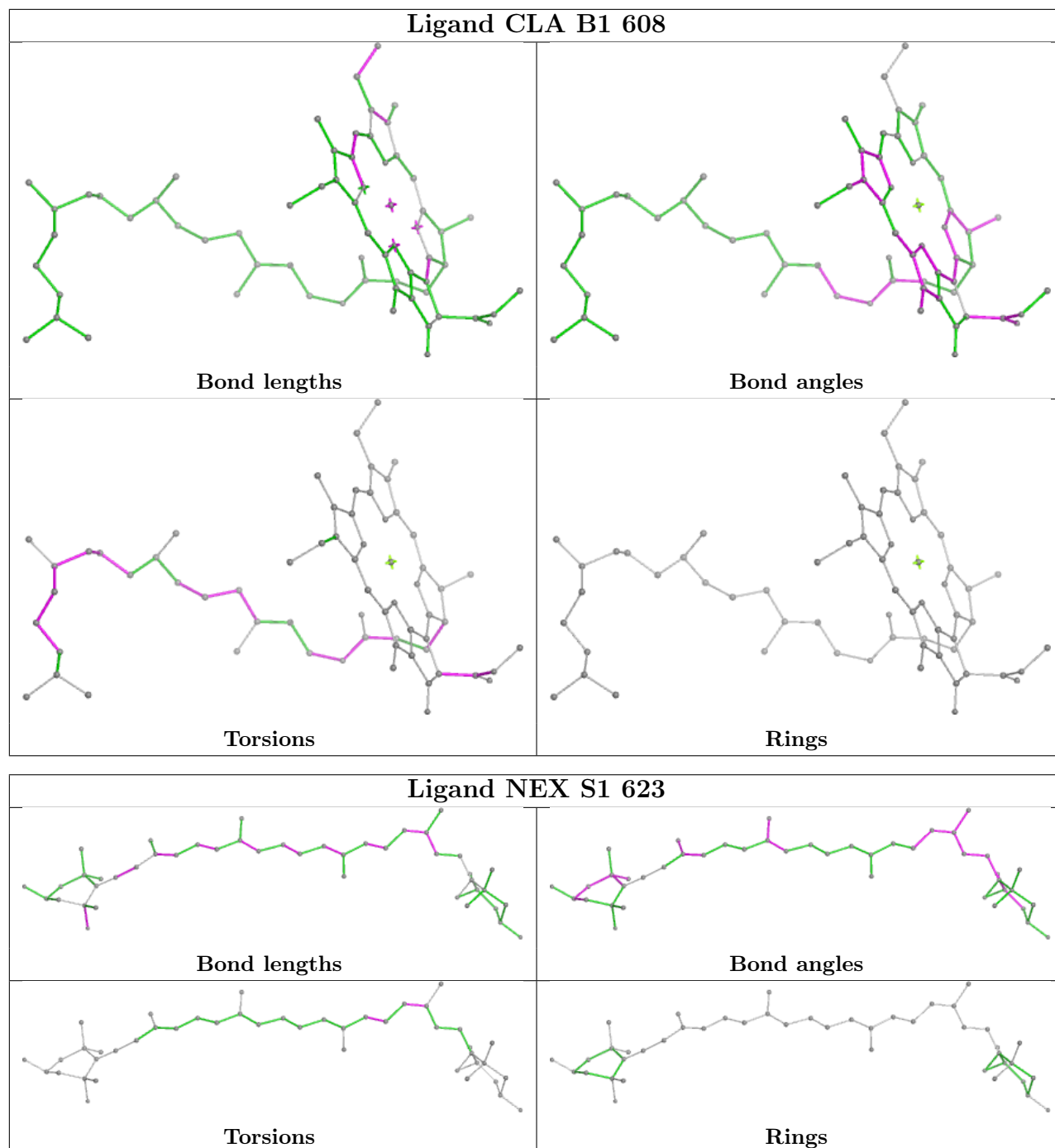
## Ligand CLA B 616

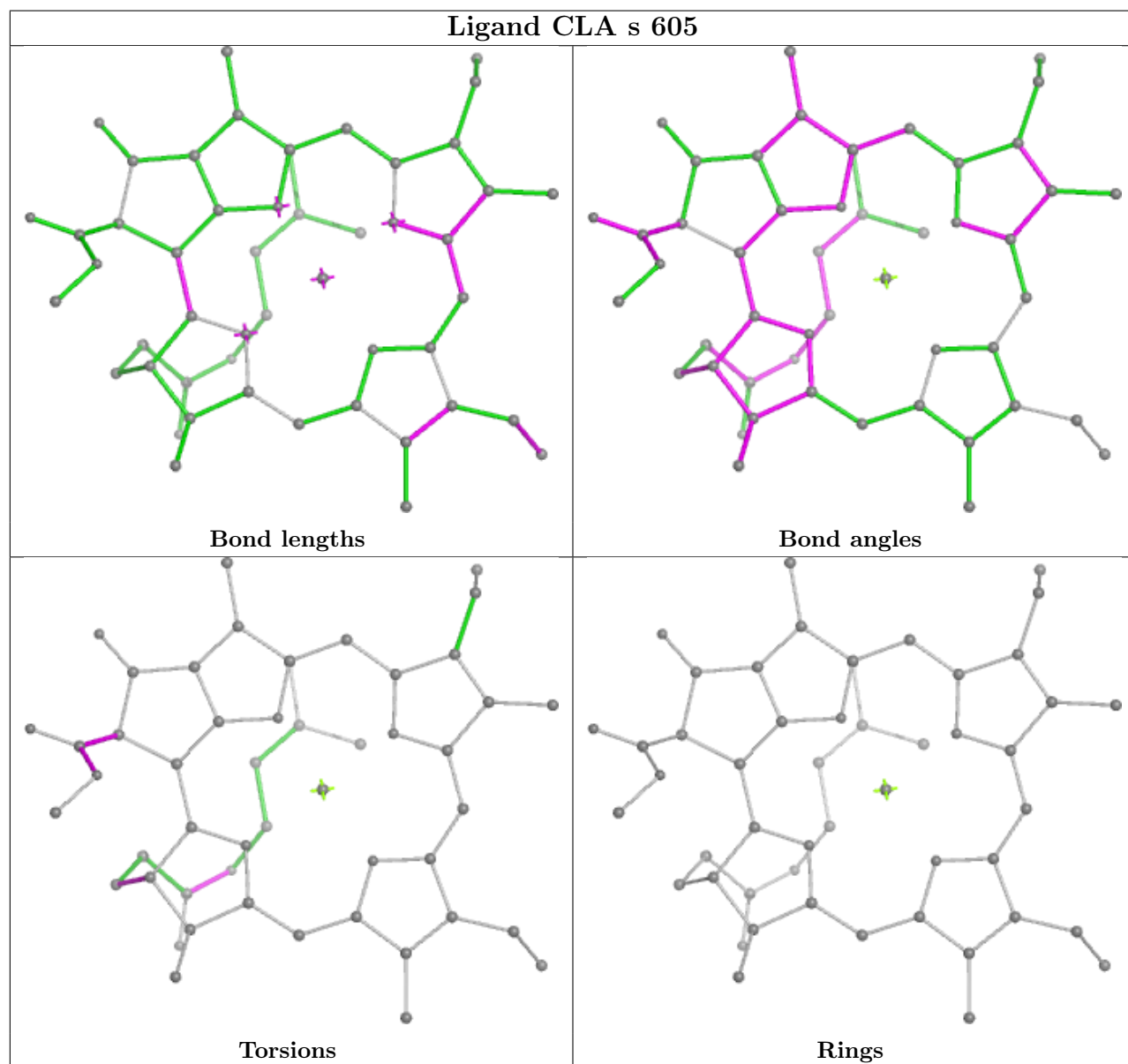
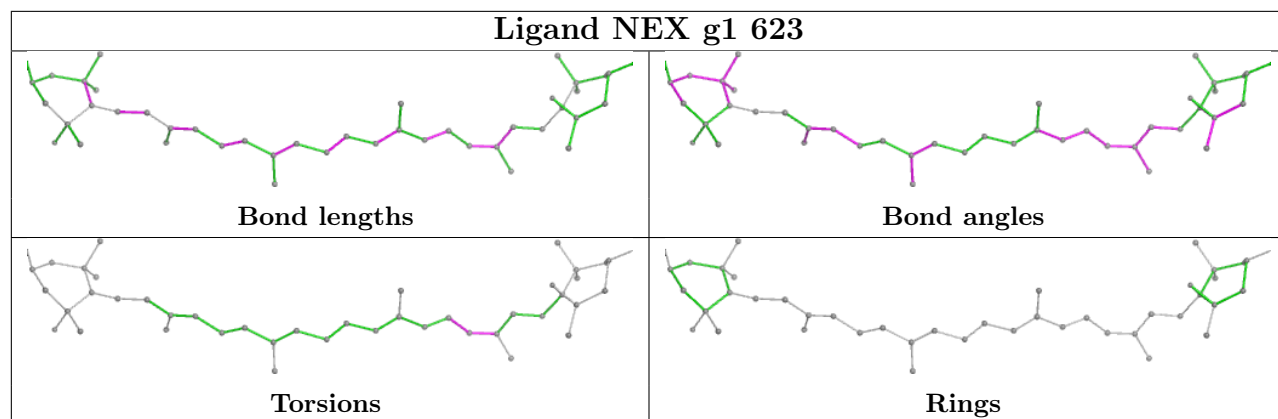


## Ligand LMG J 101

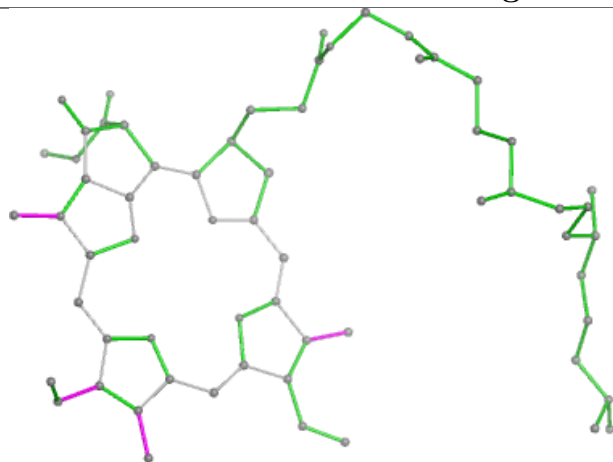




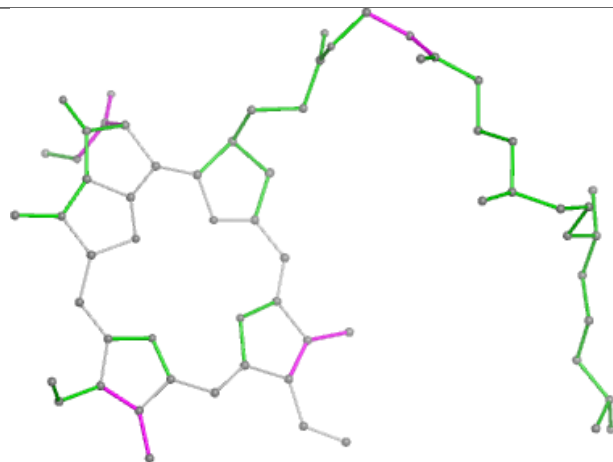




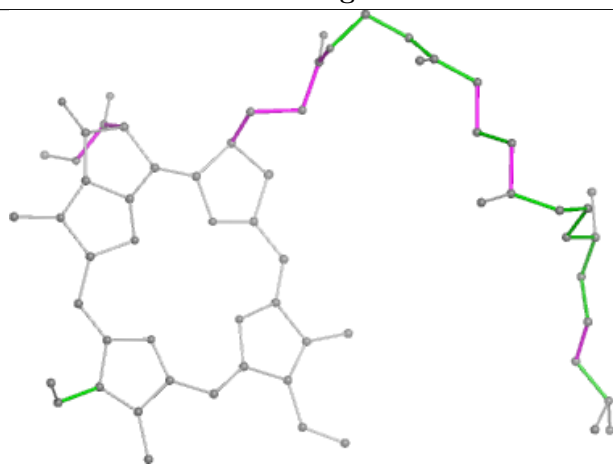
## Ligand PHO A1 409



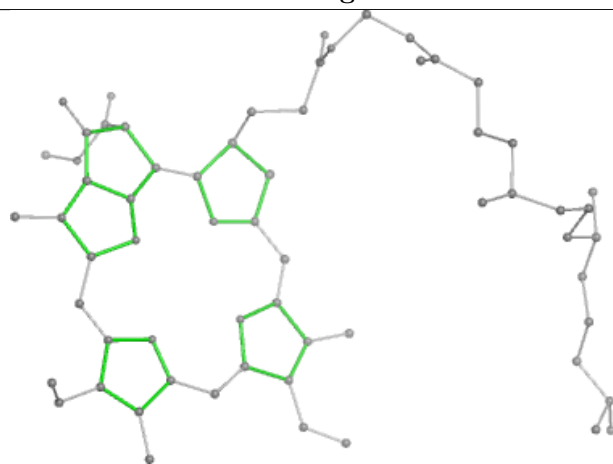
Bond lengths



Bond angles

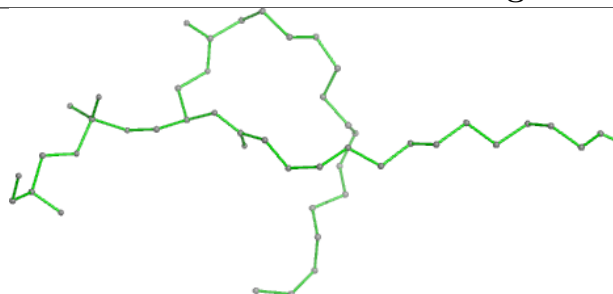


Torsions

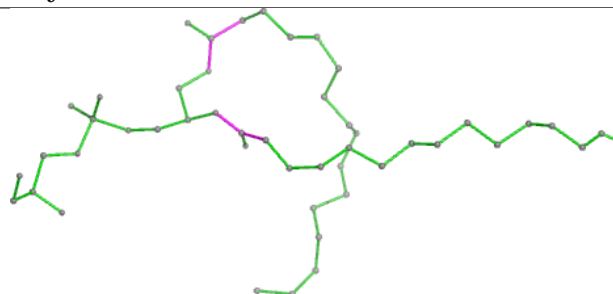


Rings

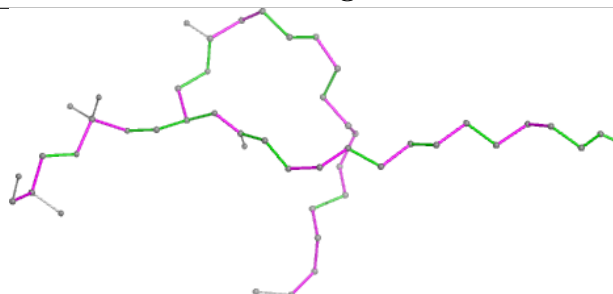
## Ligand LHG y1 624



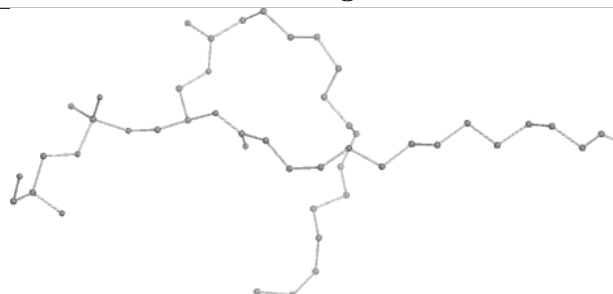
Bond lengths



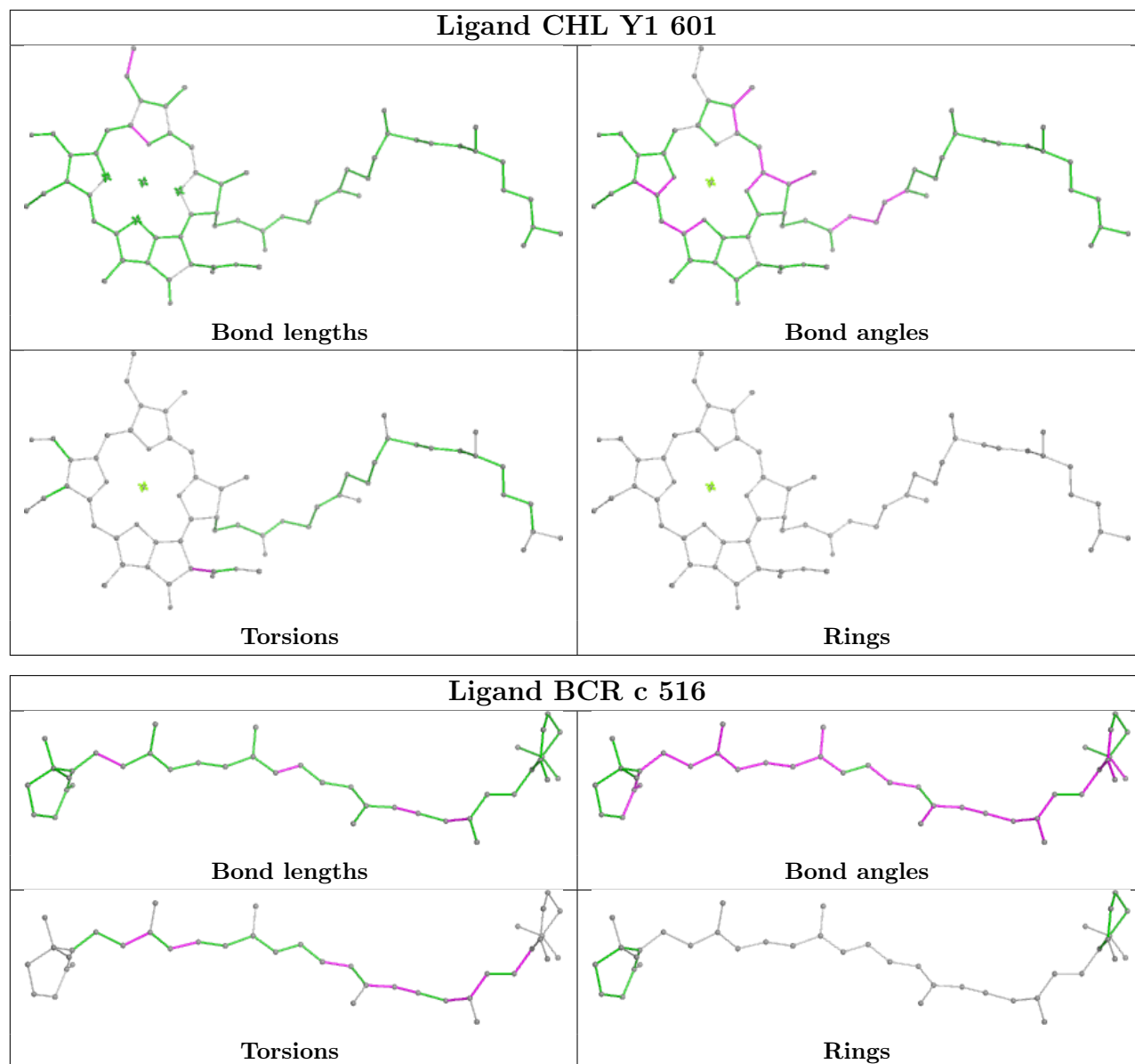
Bond angles



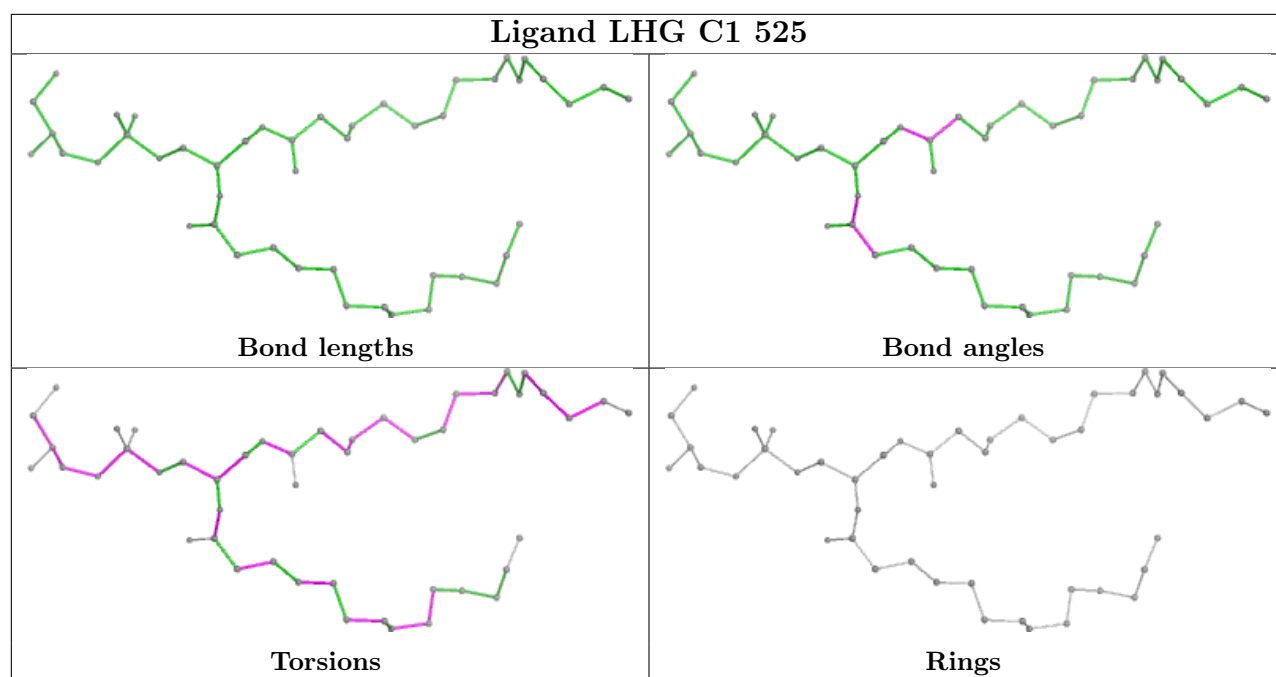
Torsions



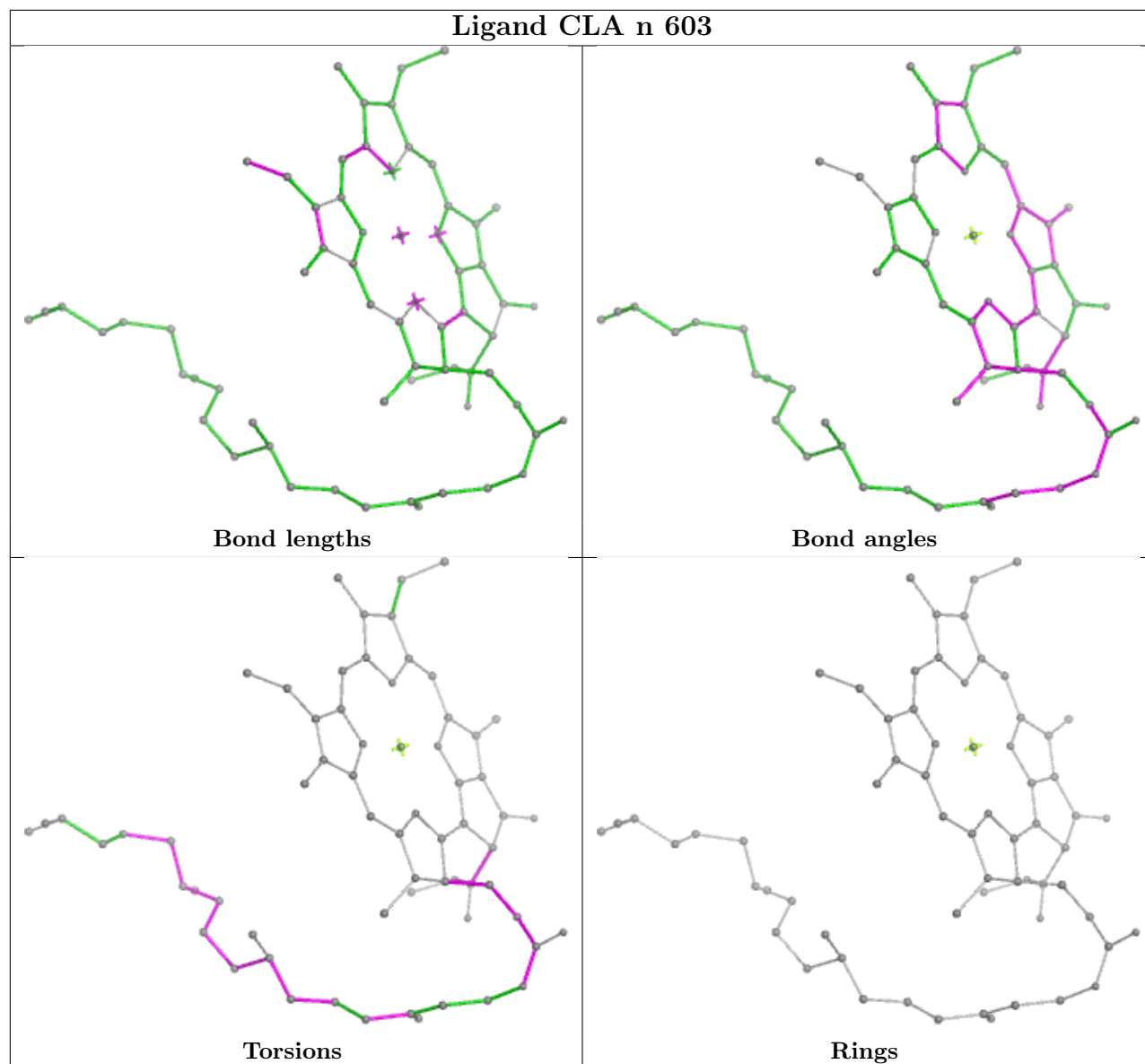
Rings

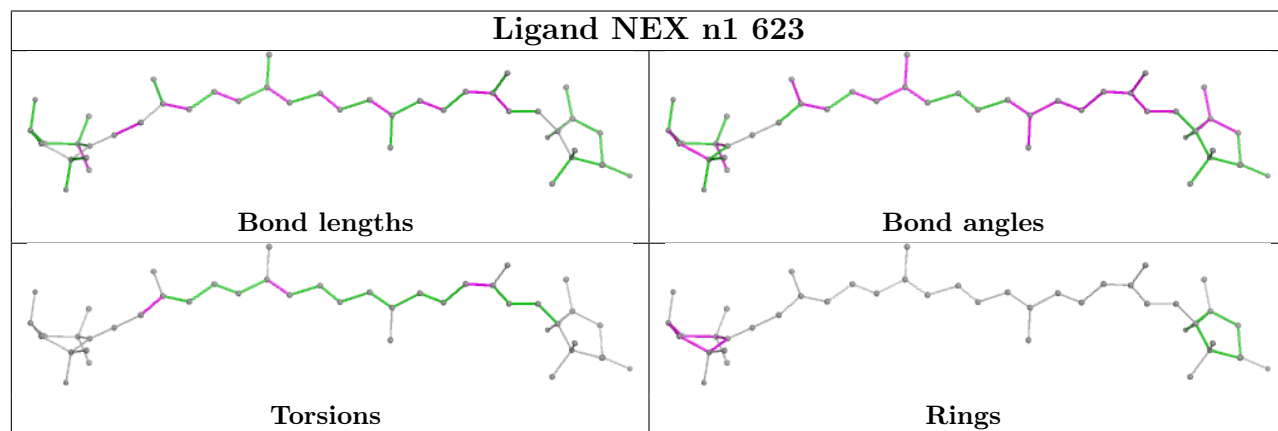
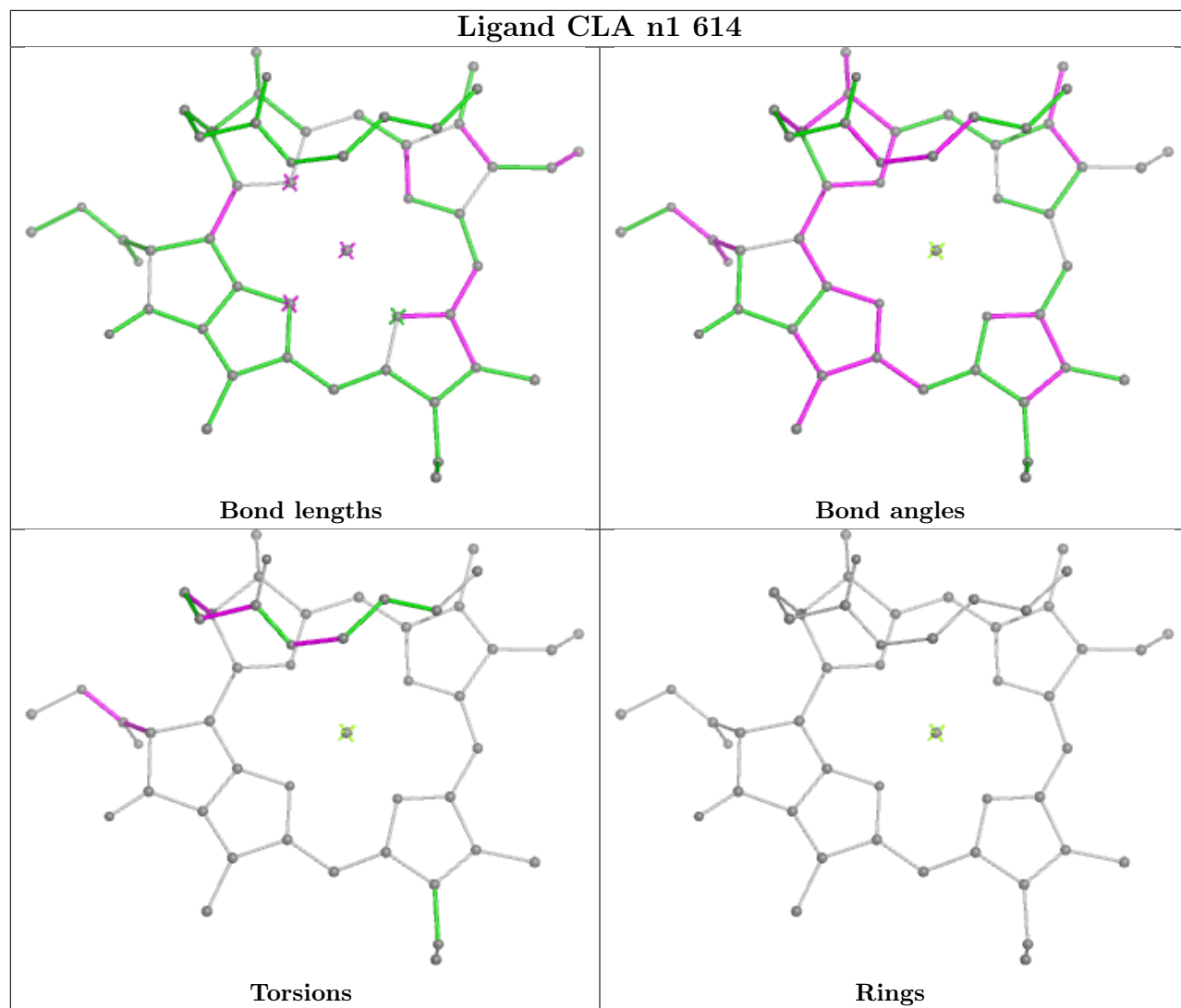


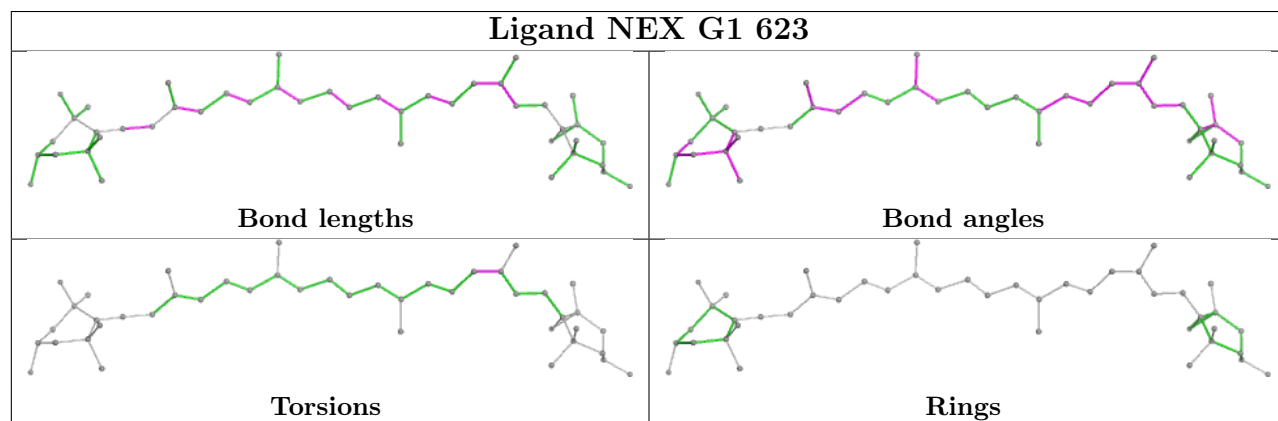
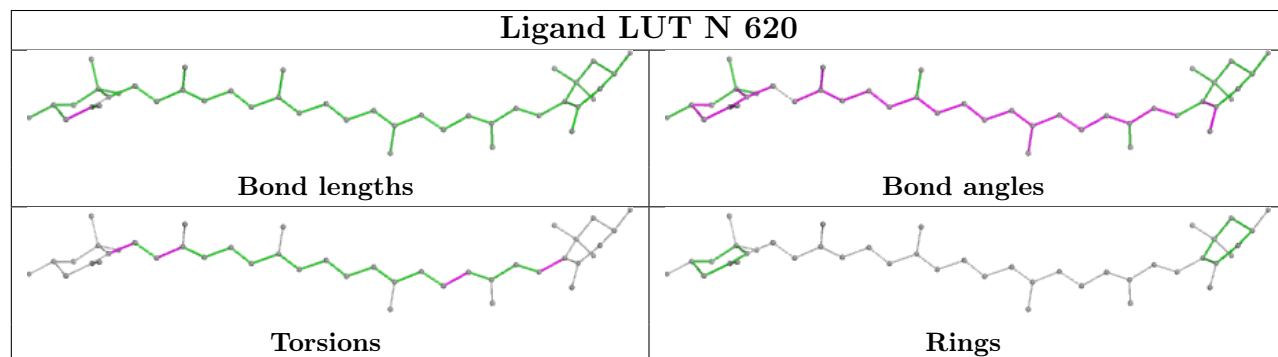
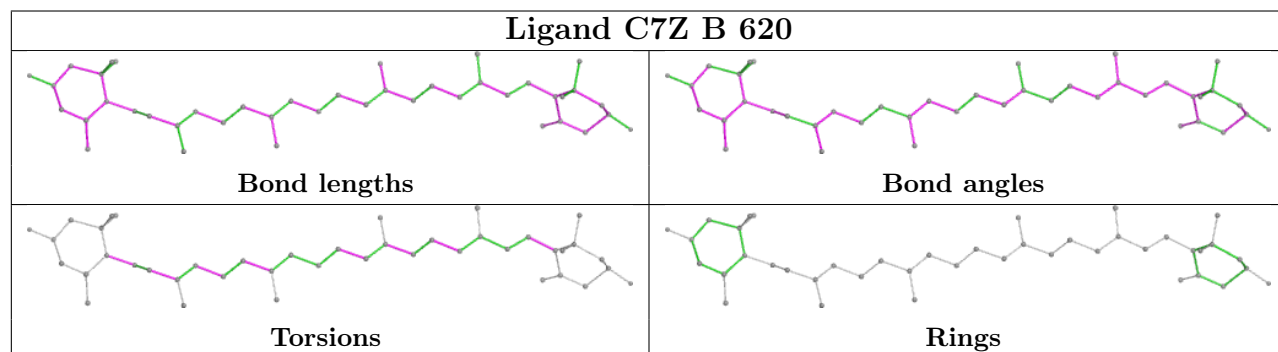
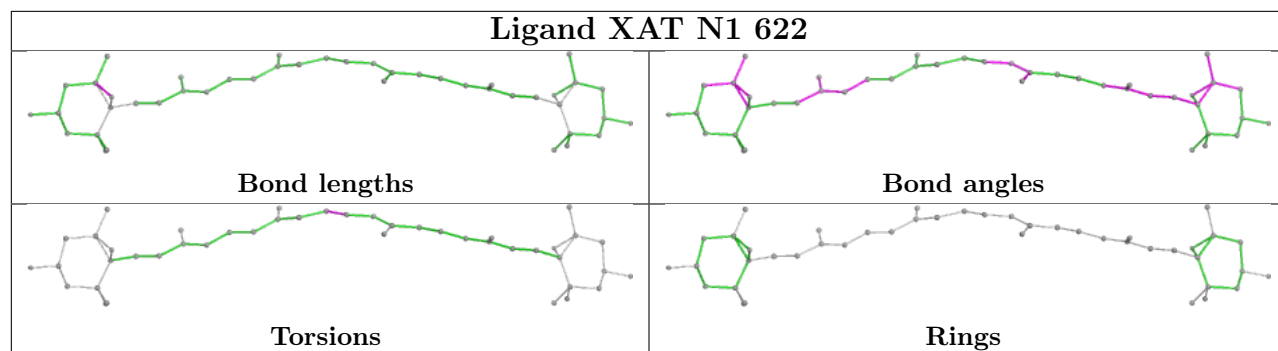


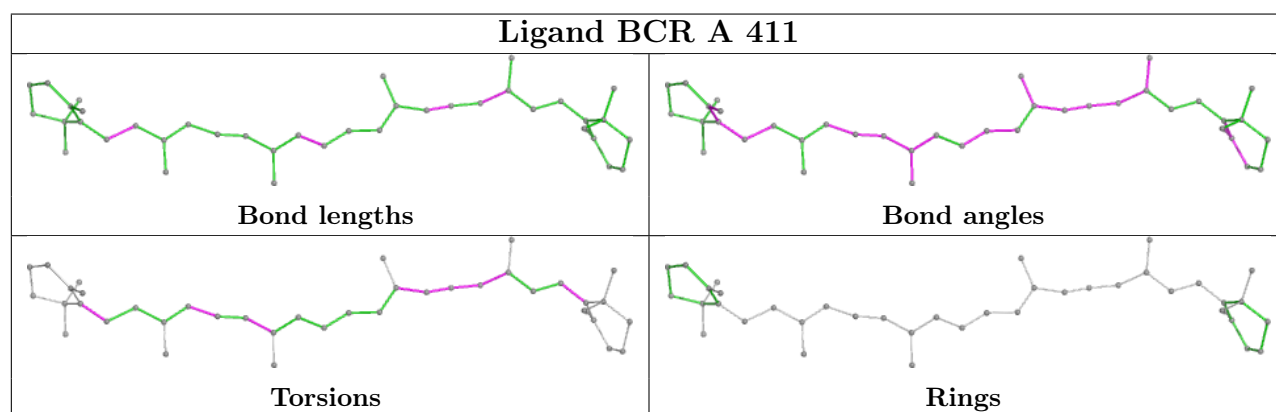
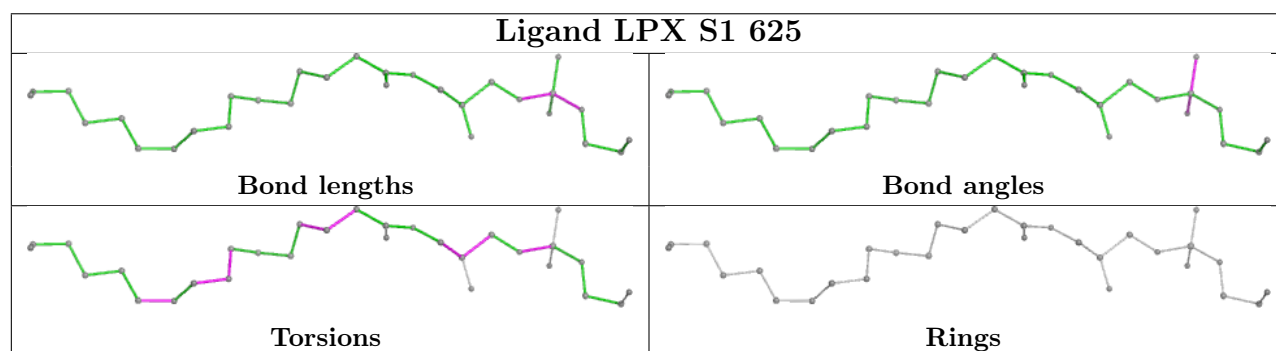
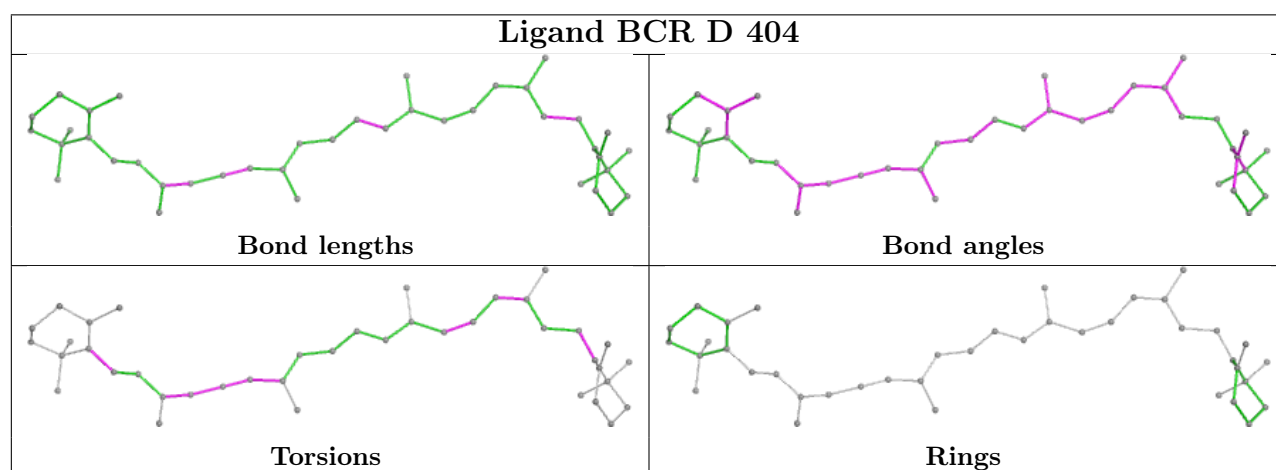
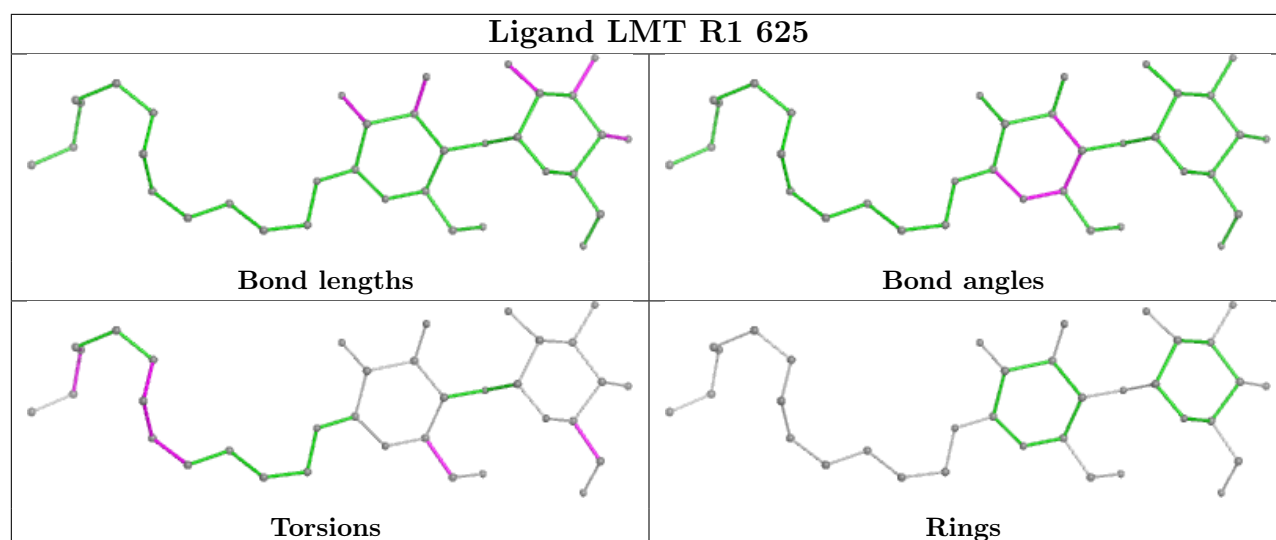


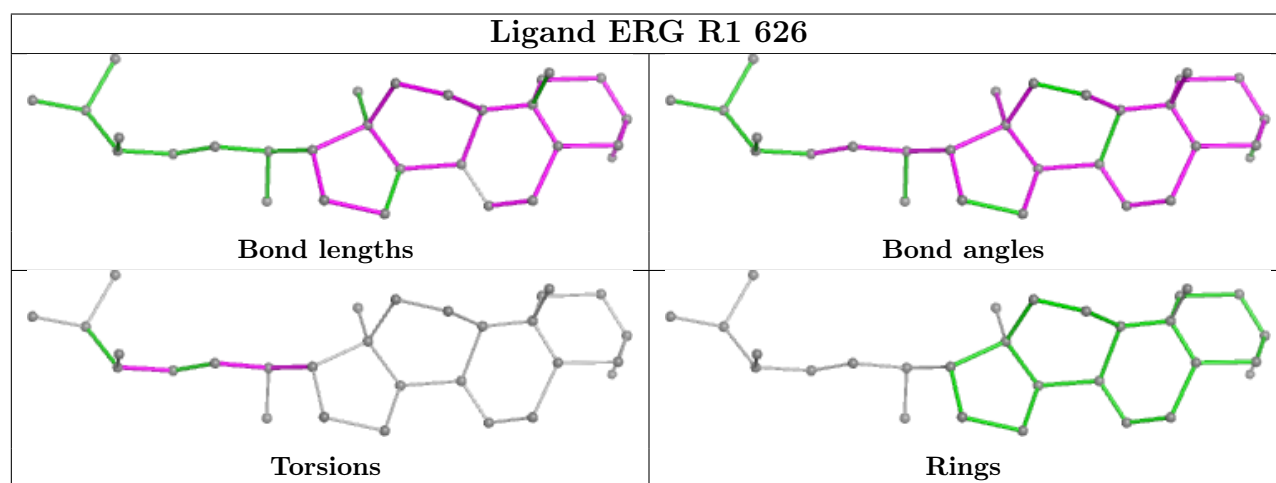
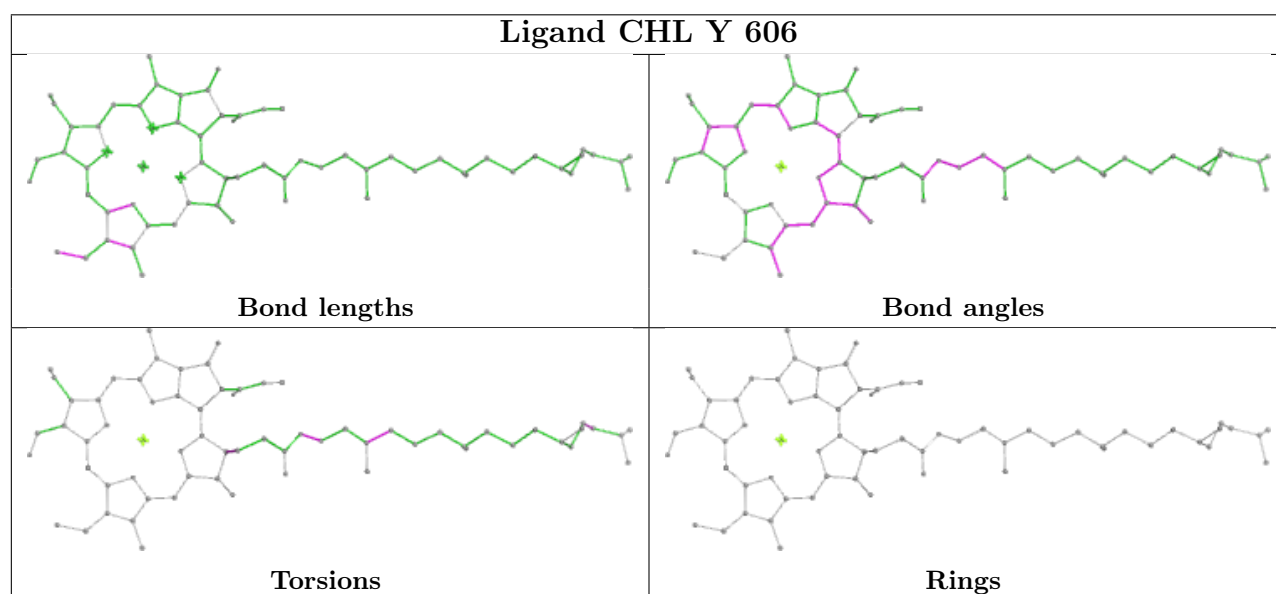
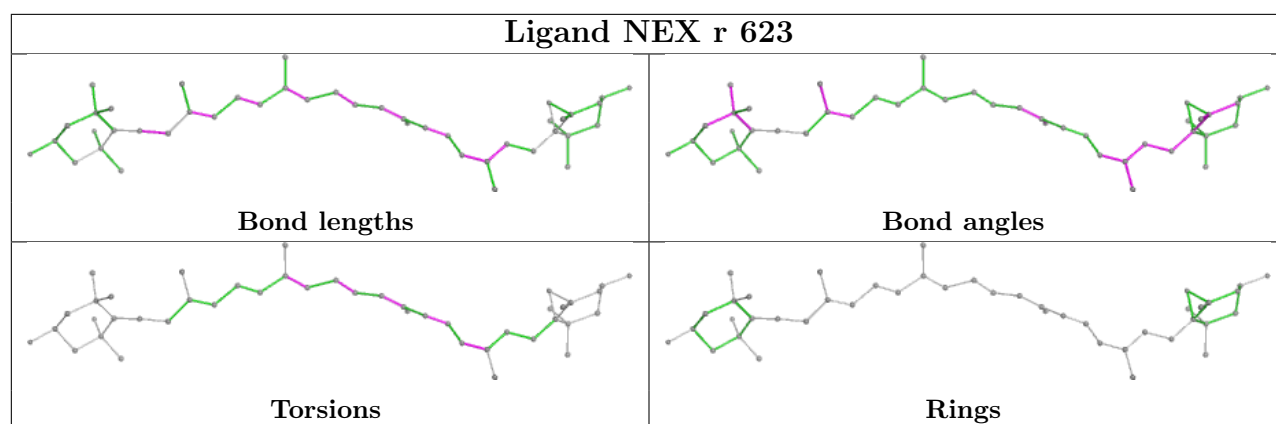
## Ligand CLA n 603

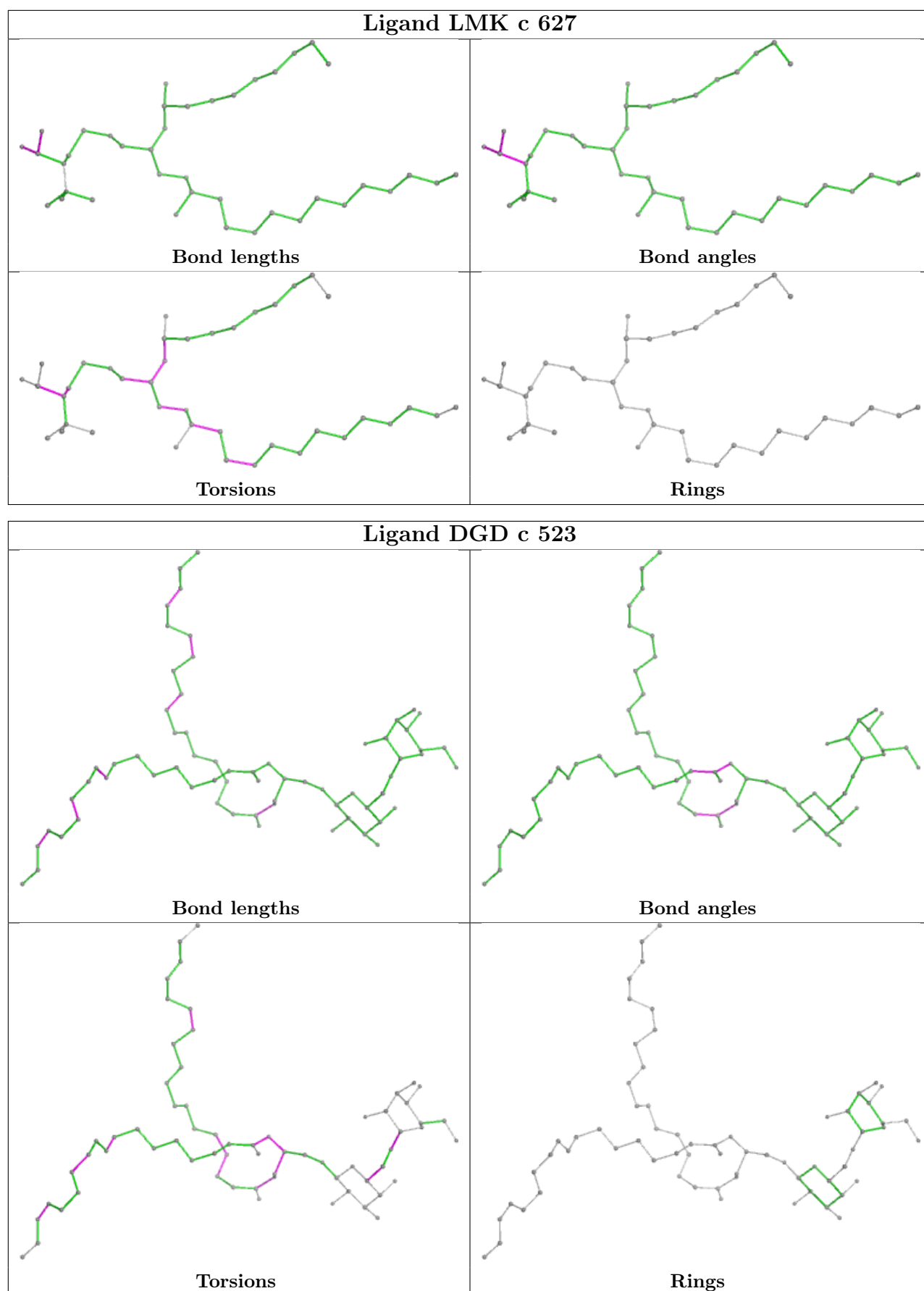


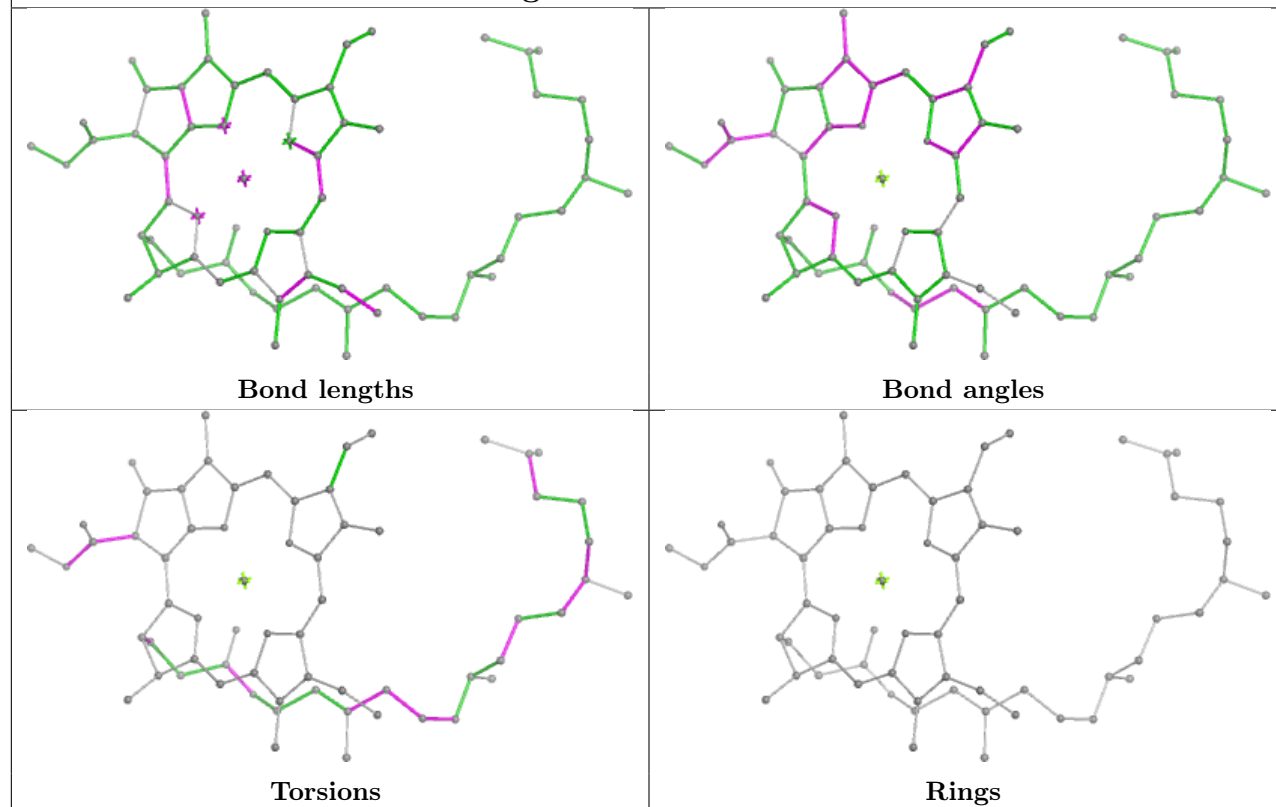
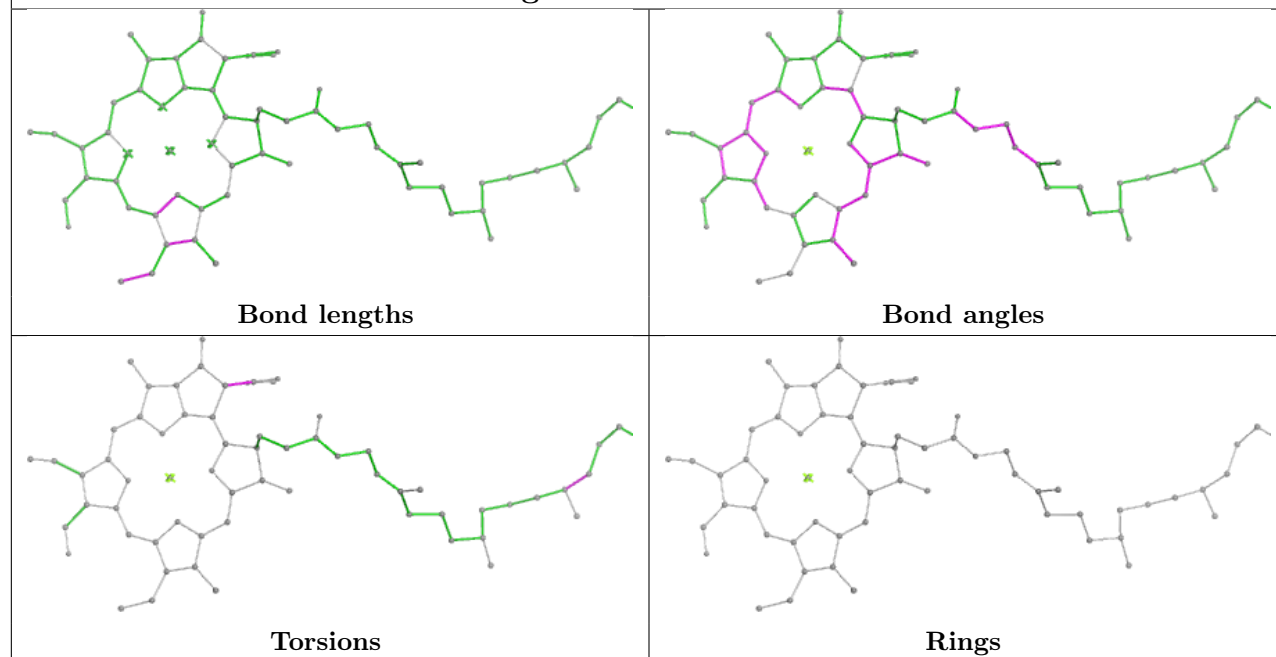




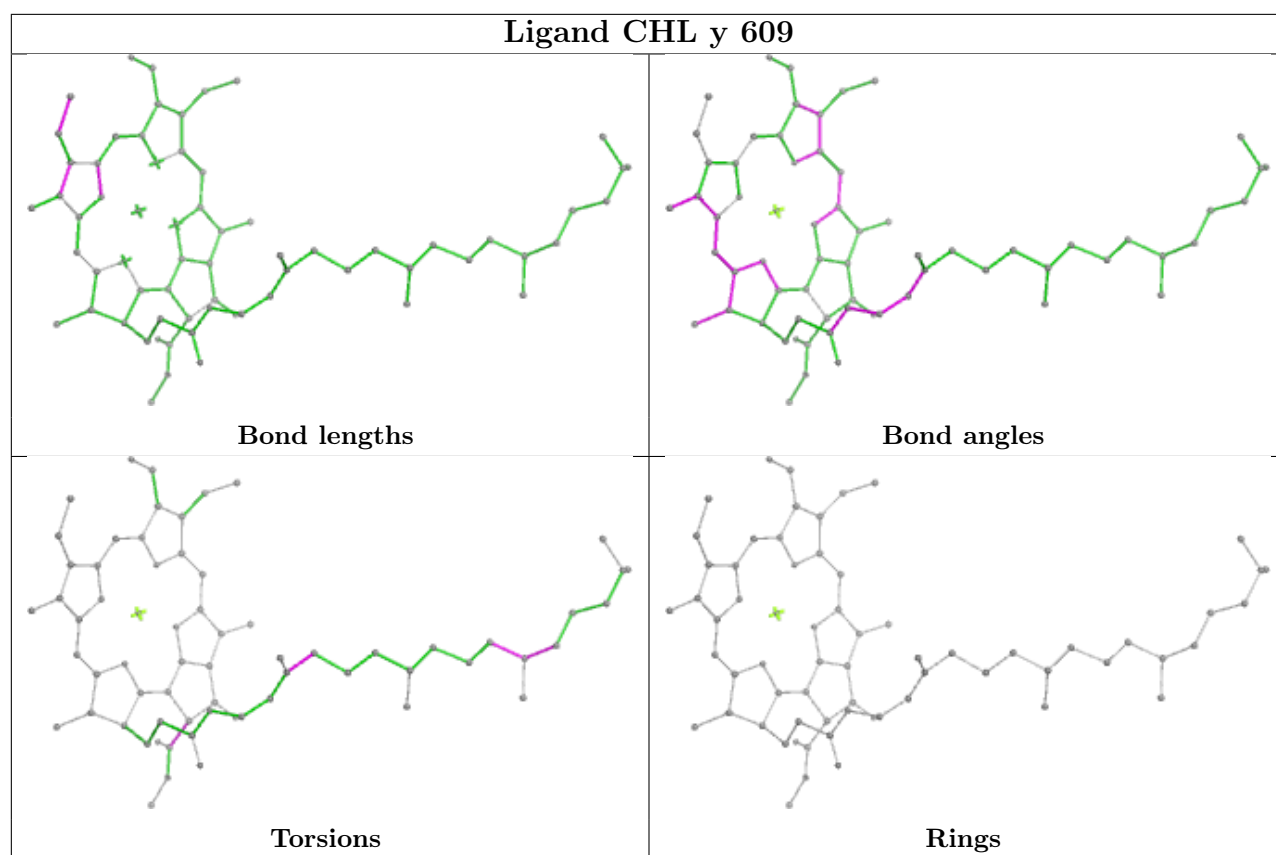


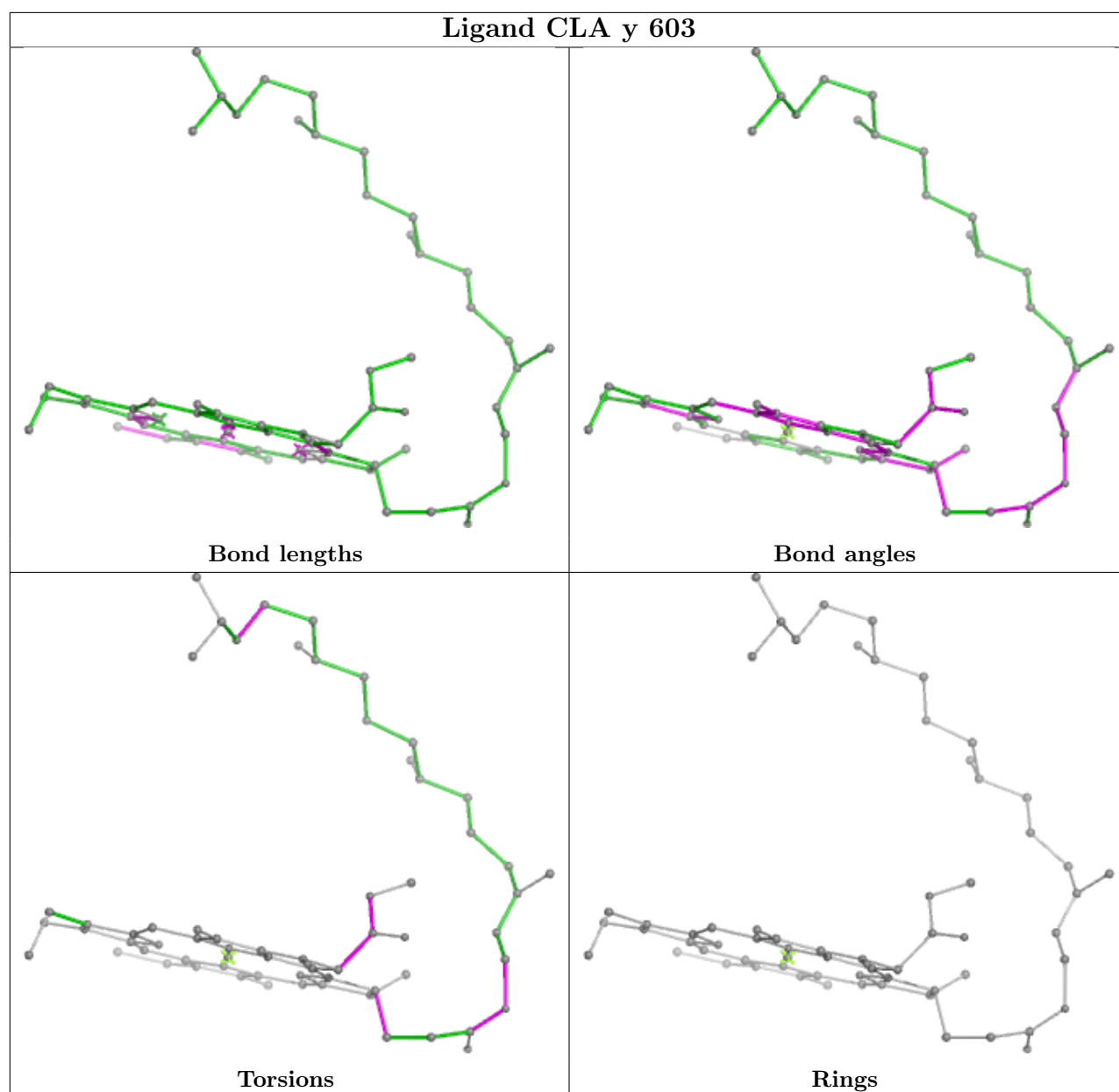


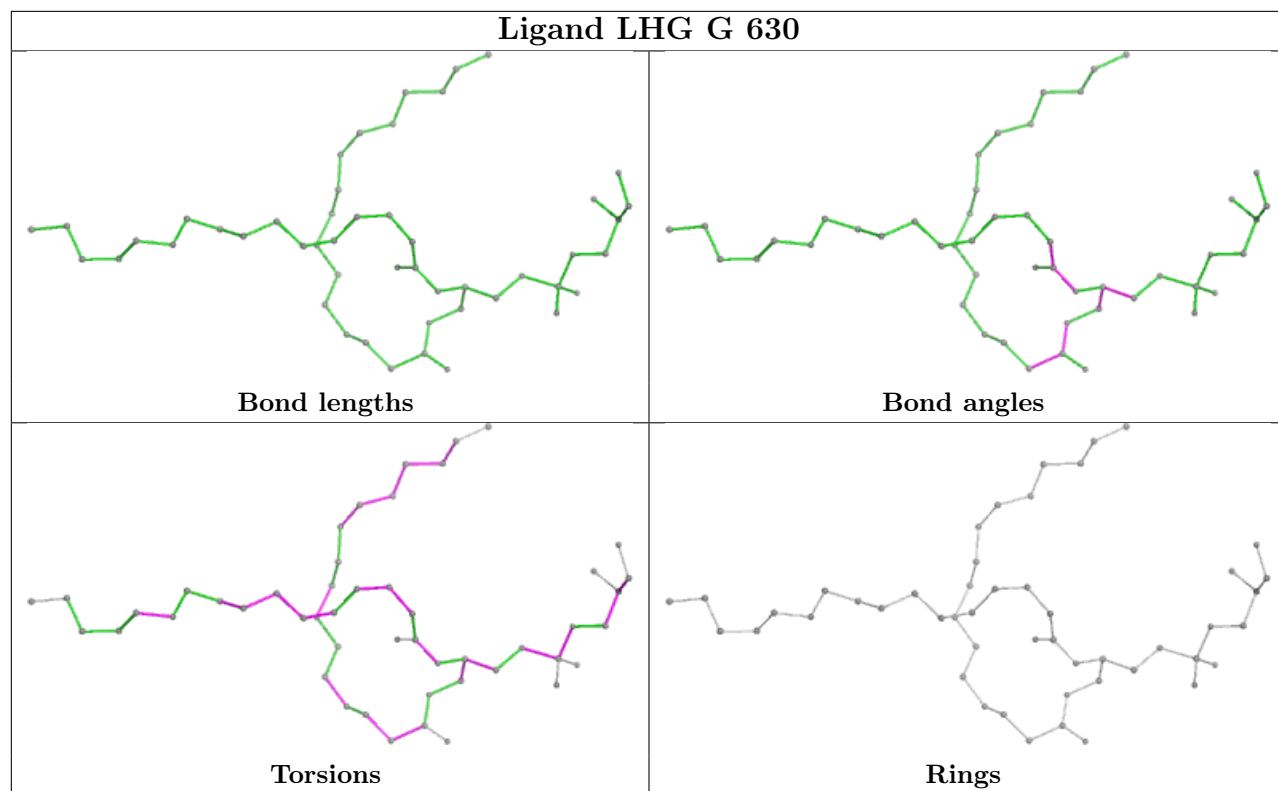


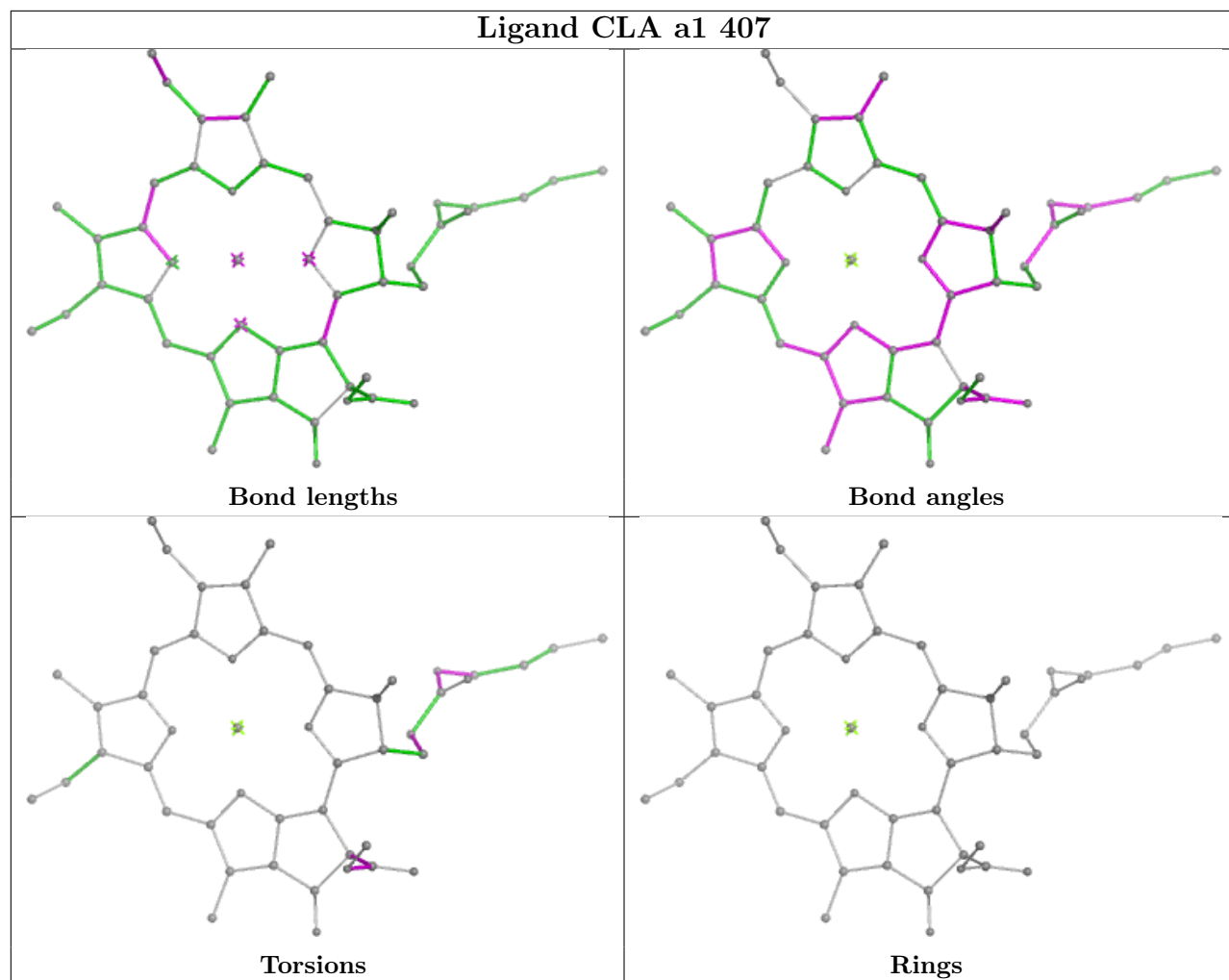
**Ligand CLA N1 610****Ligand CHL N1 601**



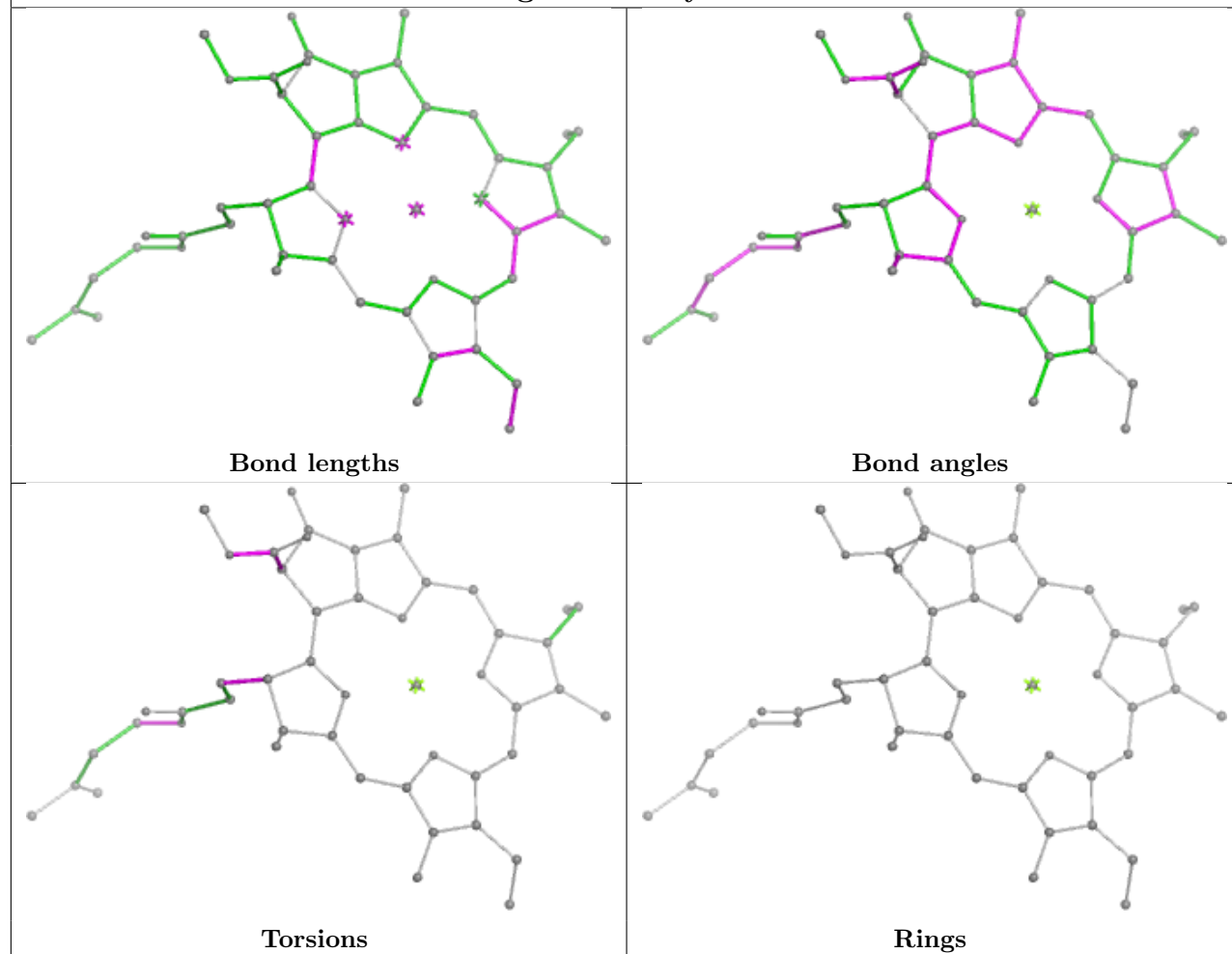




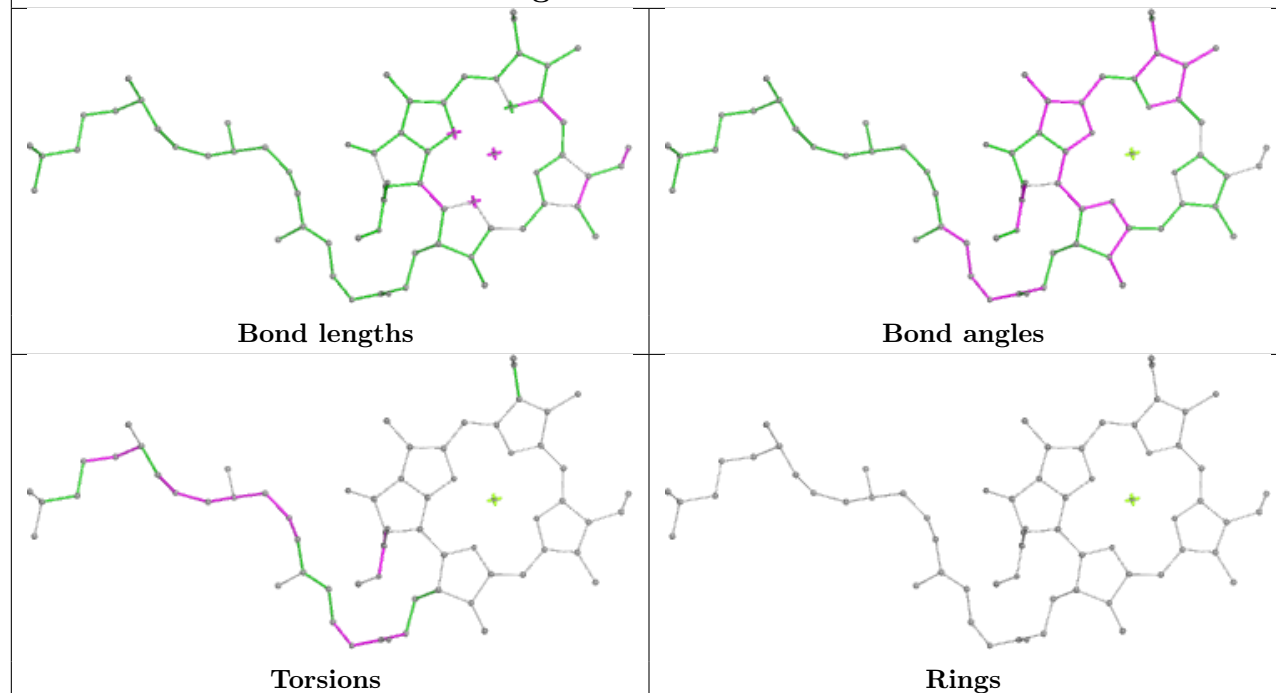


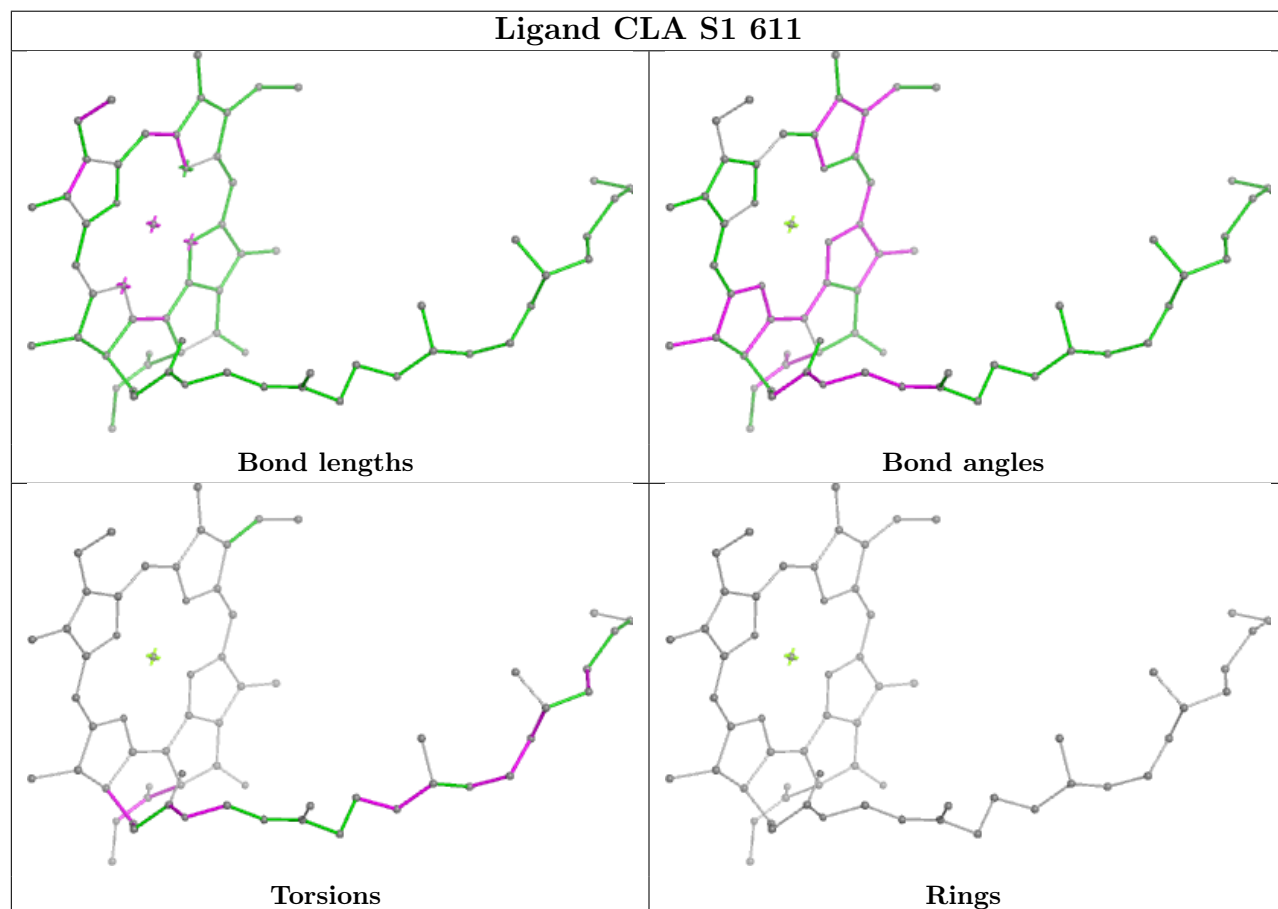
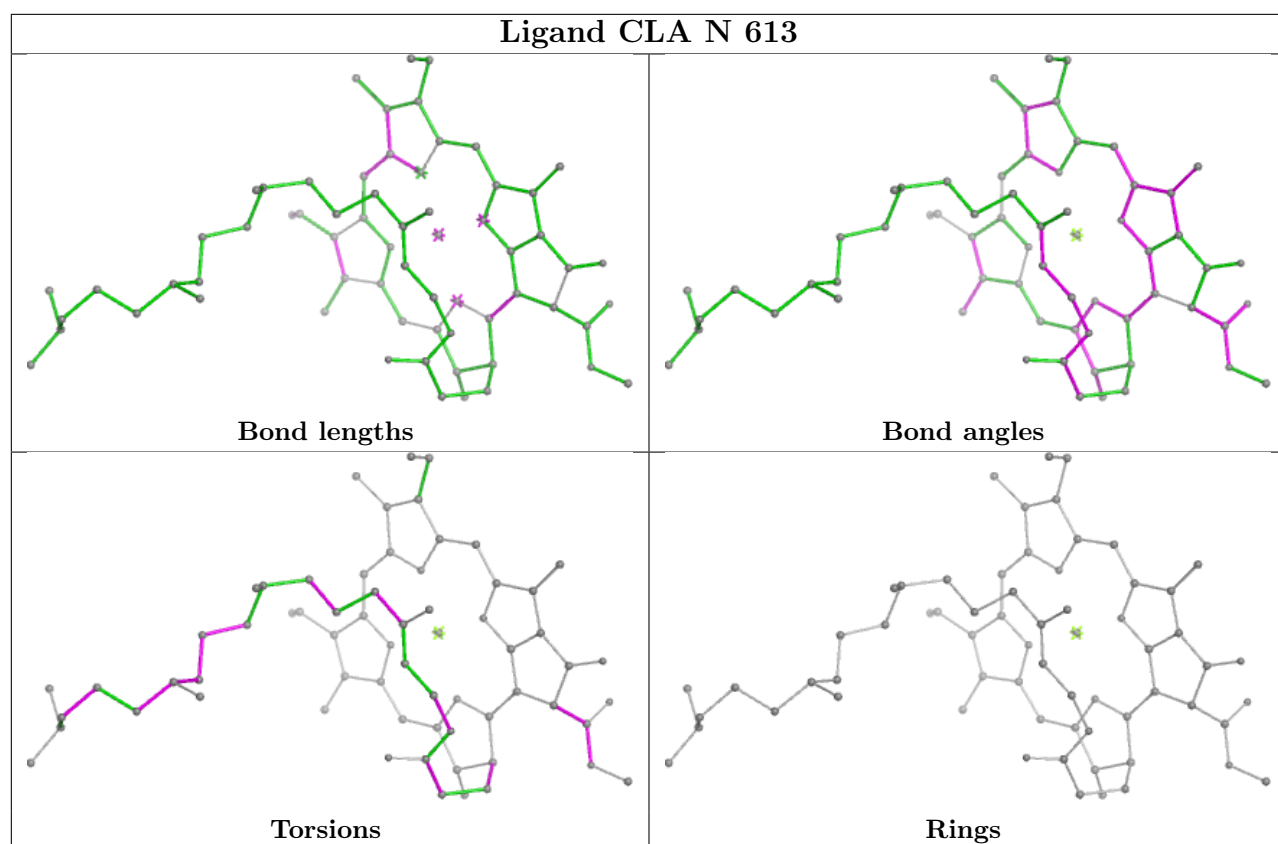


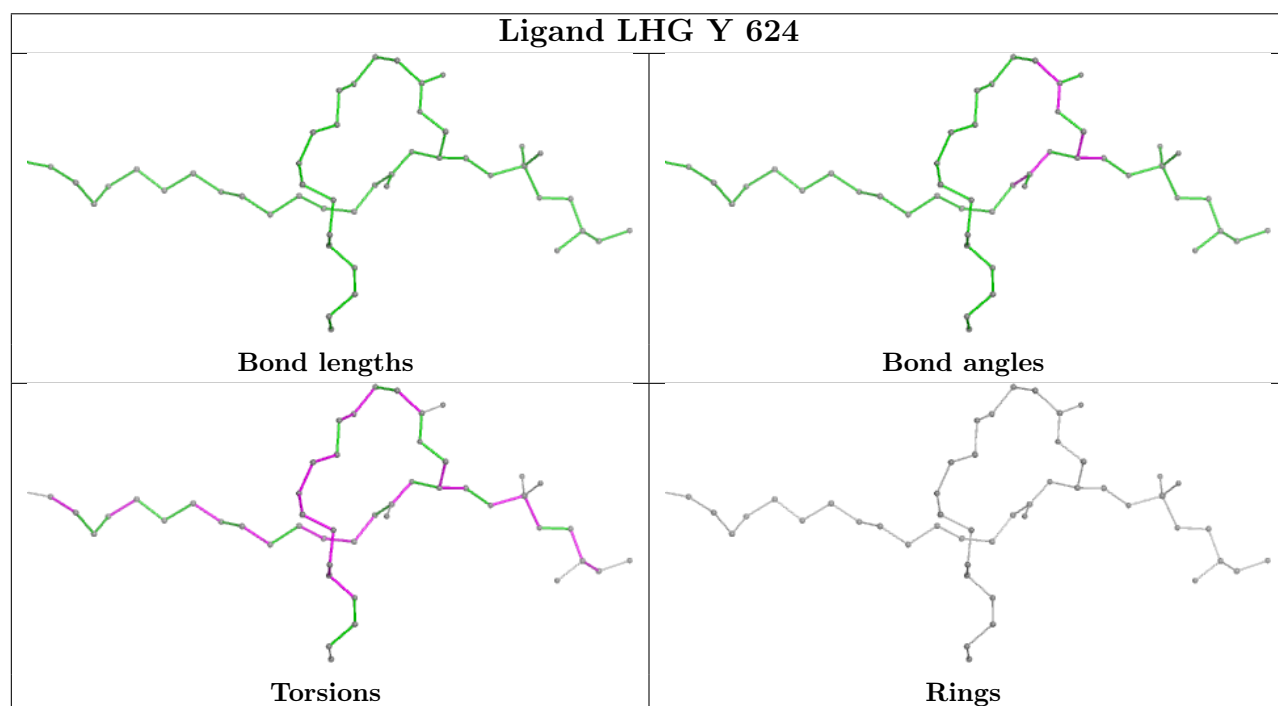
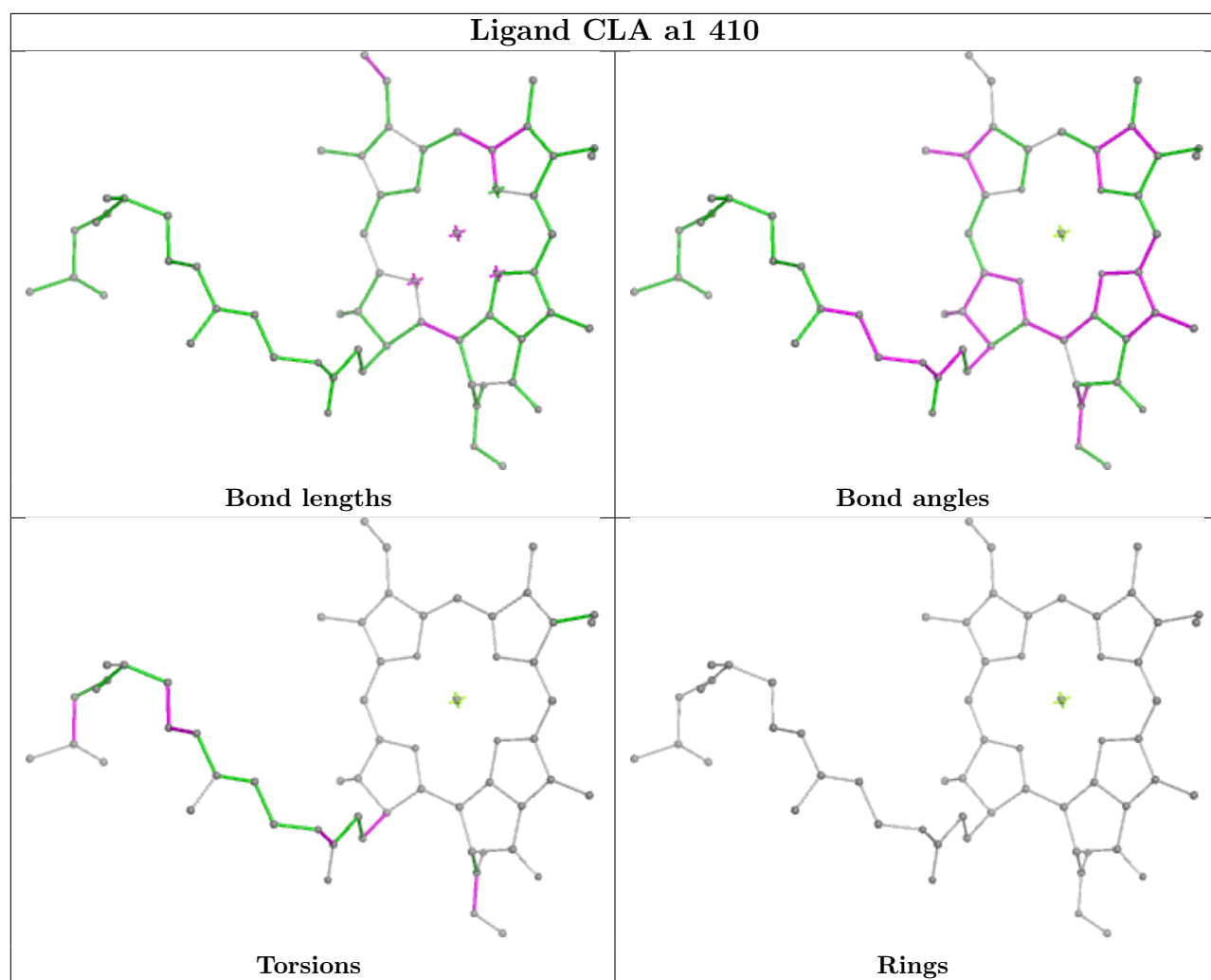
## Ligand CLA y 608

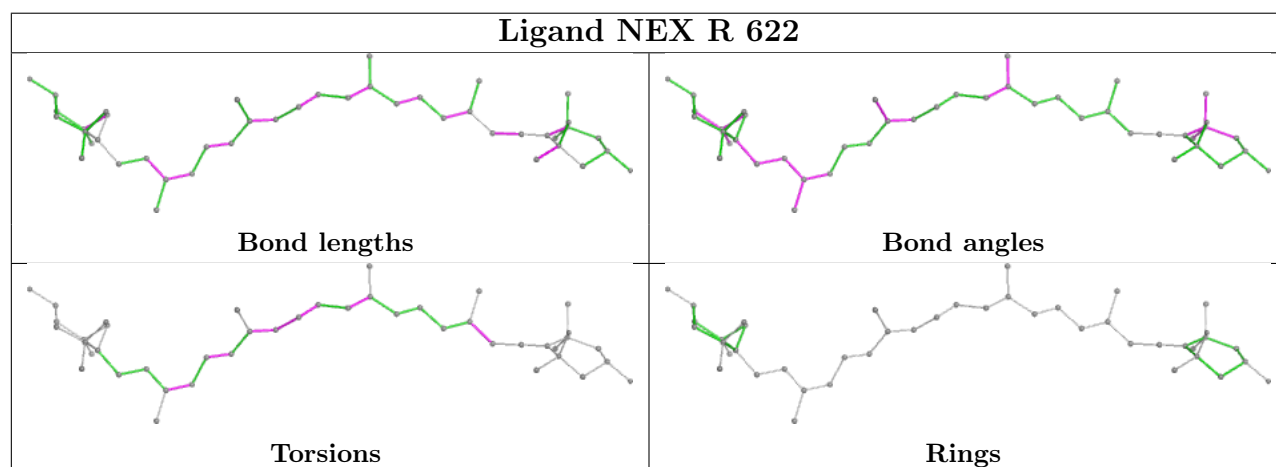
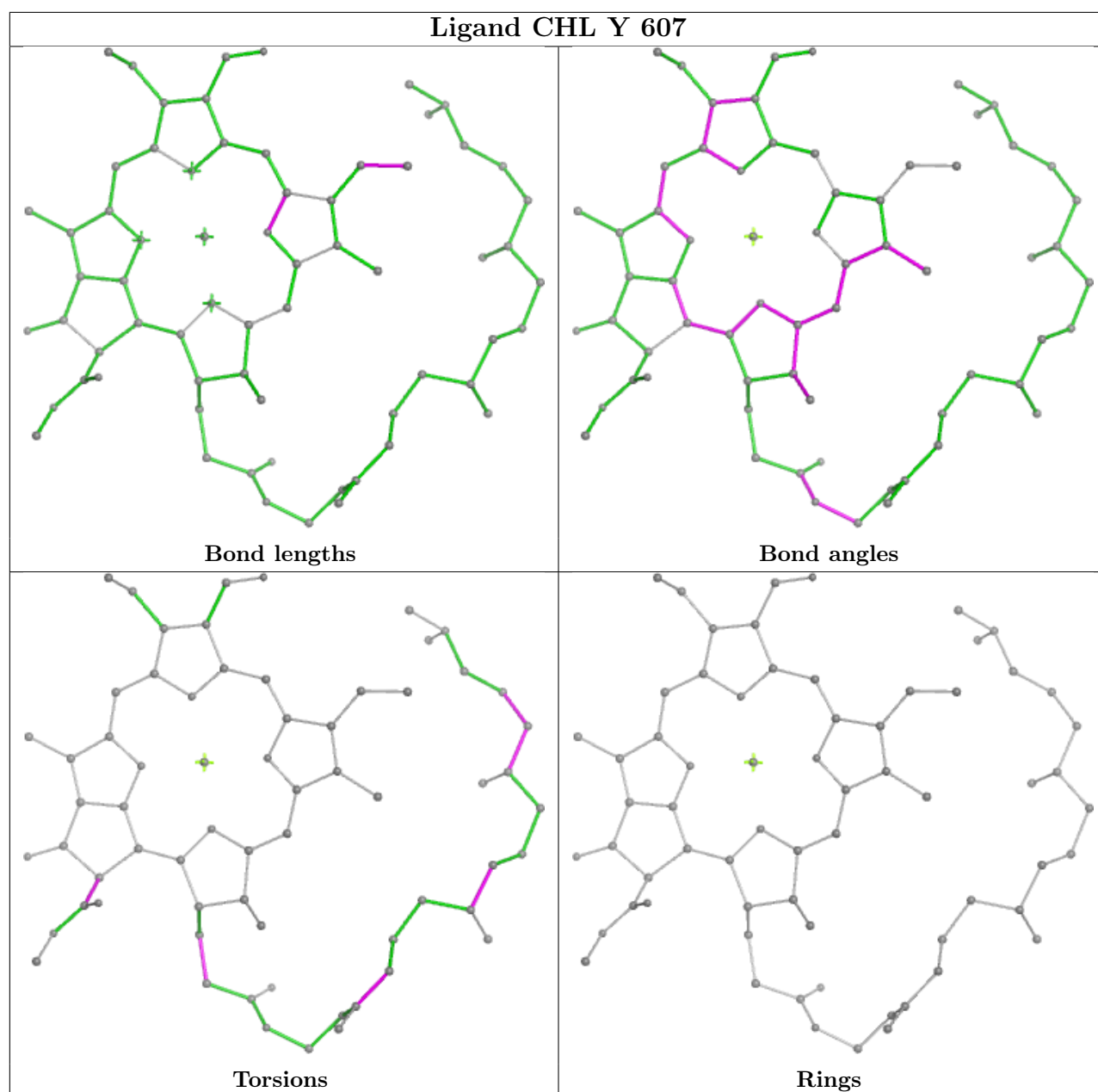


## Ligand CLA B 603

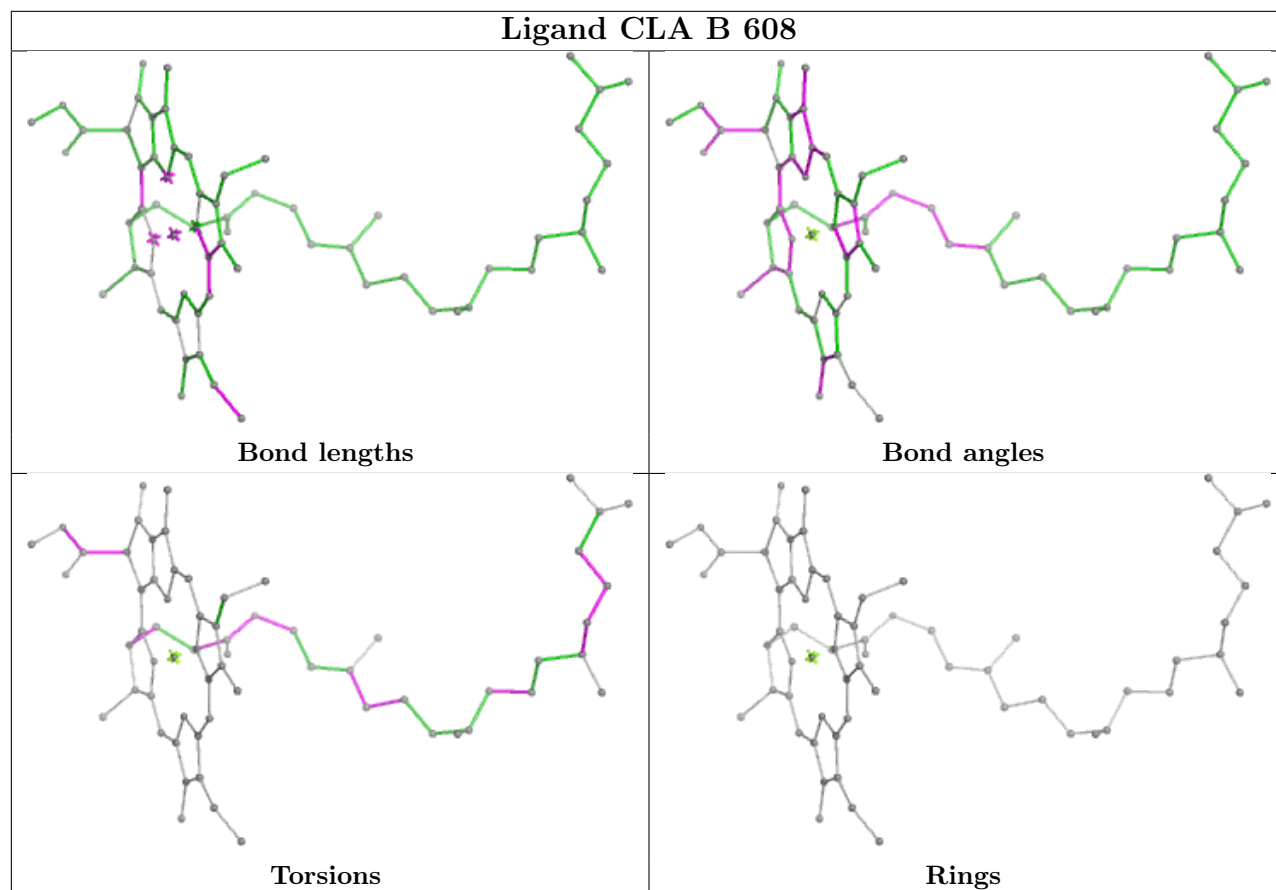
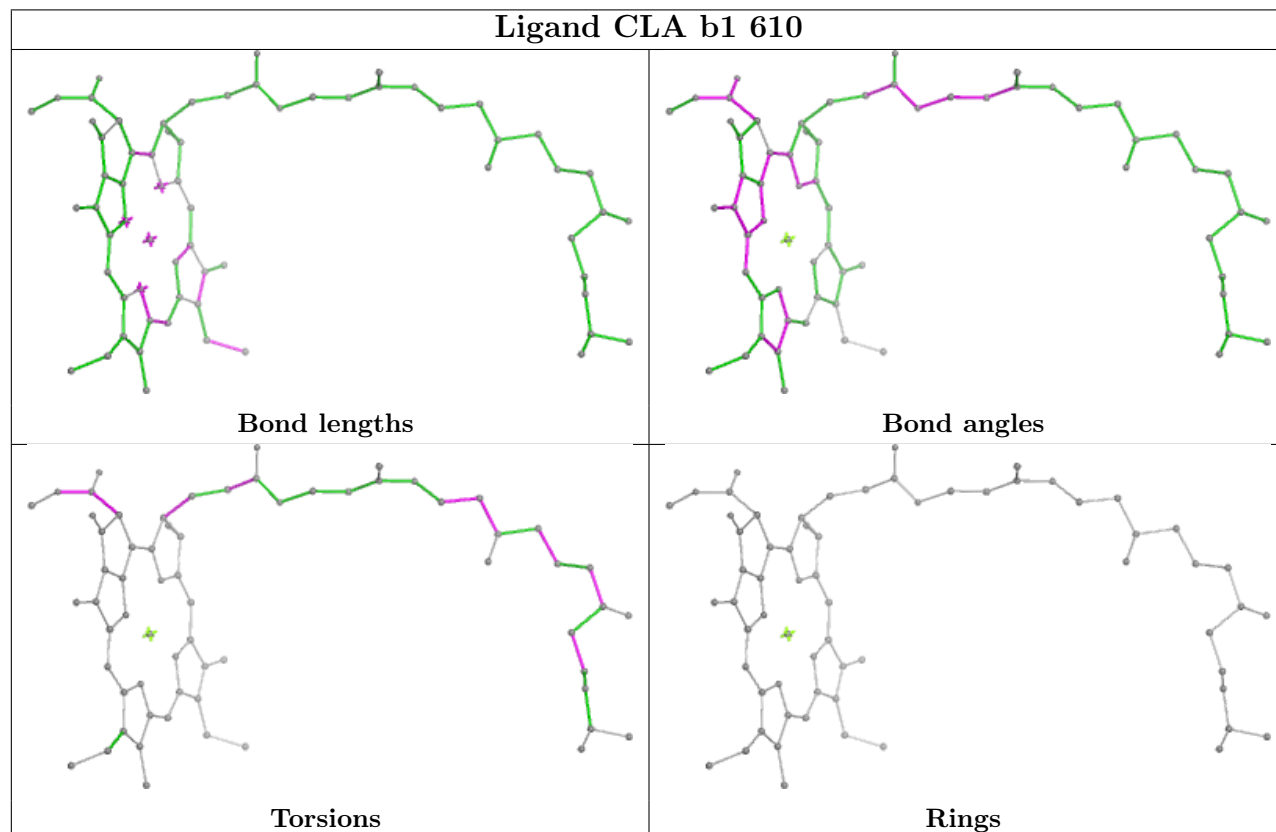




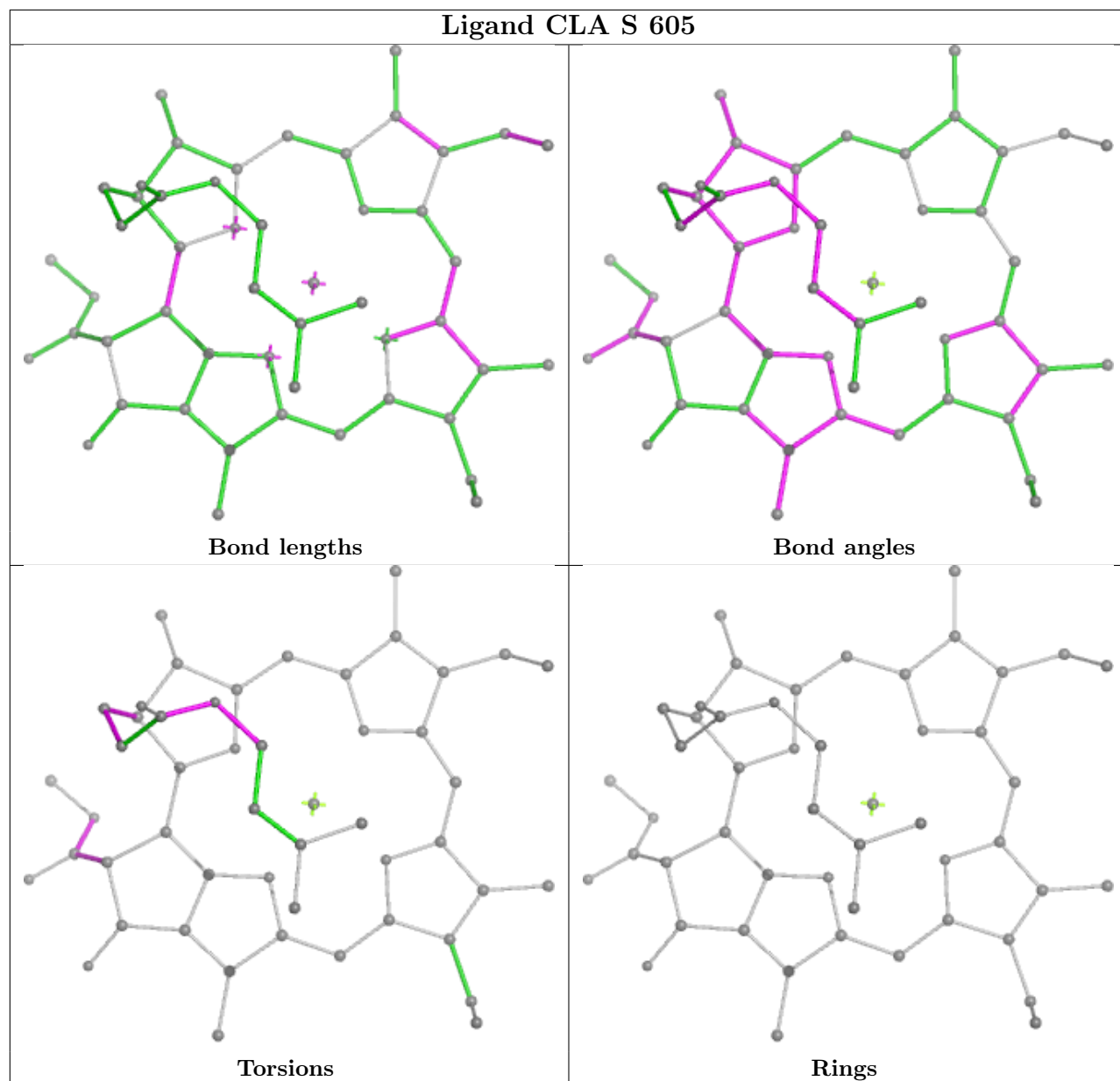




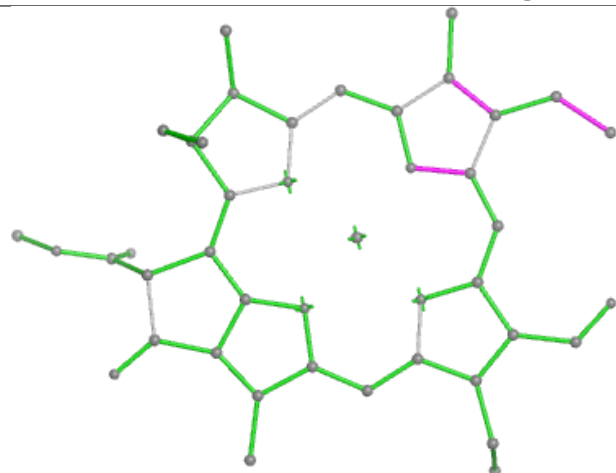


**Ligand CLA B 608****Ligand CLA b1 610**

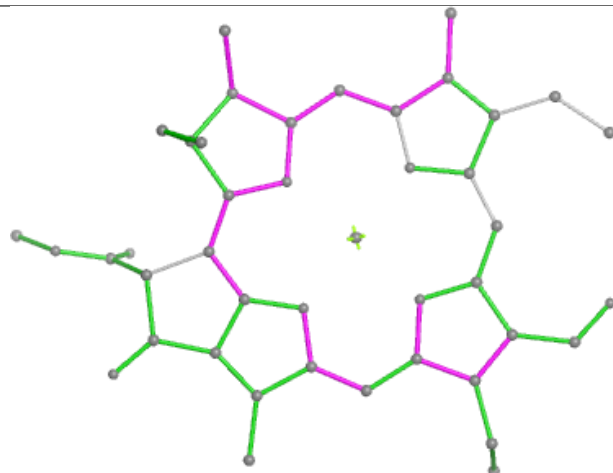
## Ligand CLA S 605



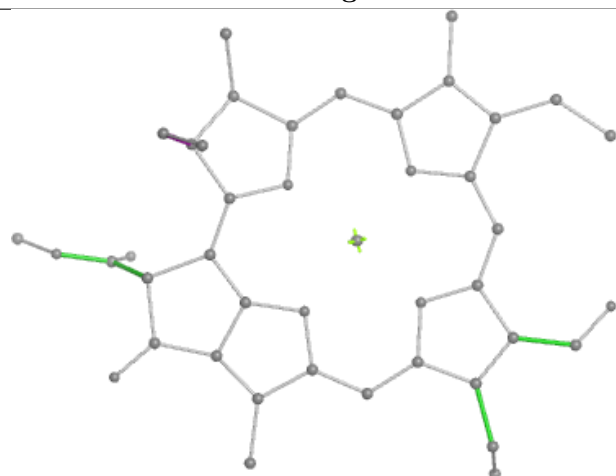
## Ligand CHL S 607



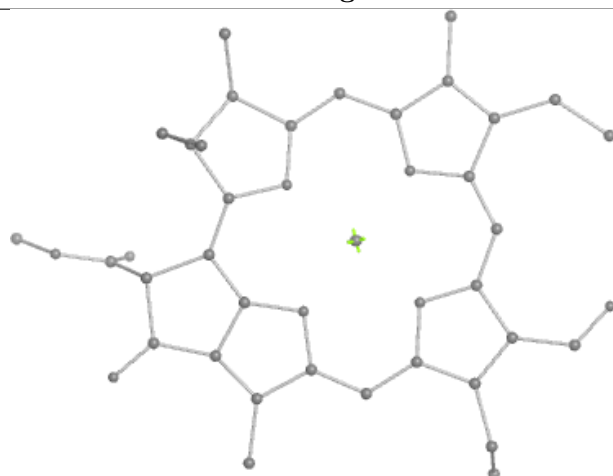
Bond lengths



Bond angles

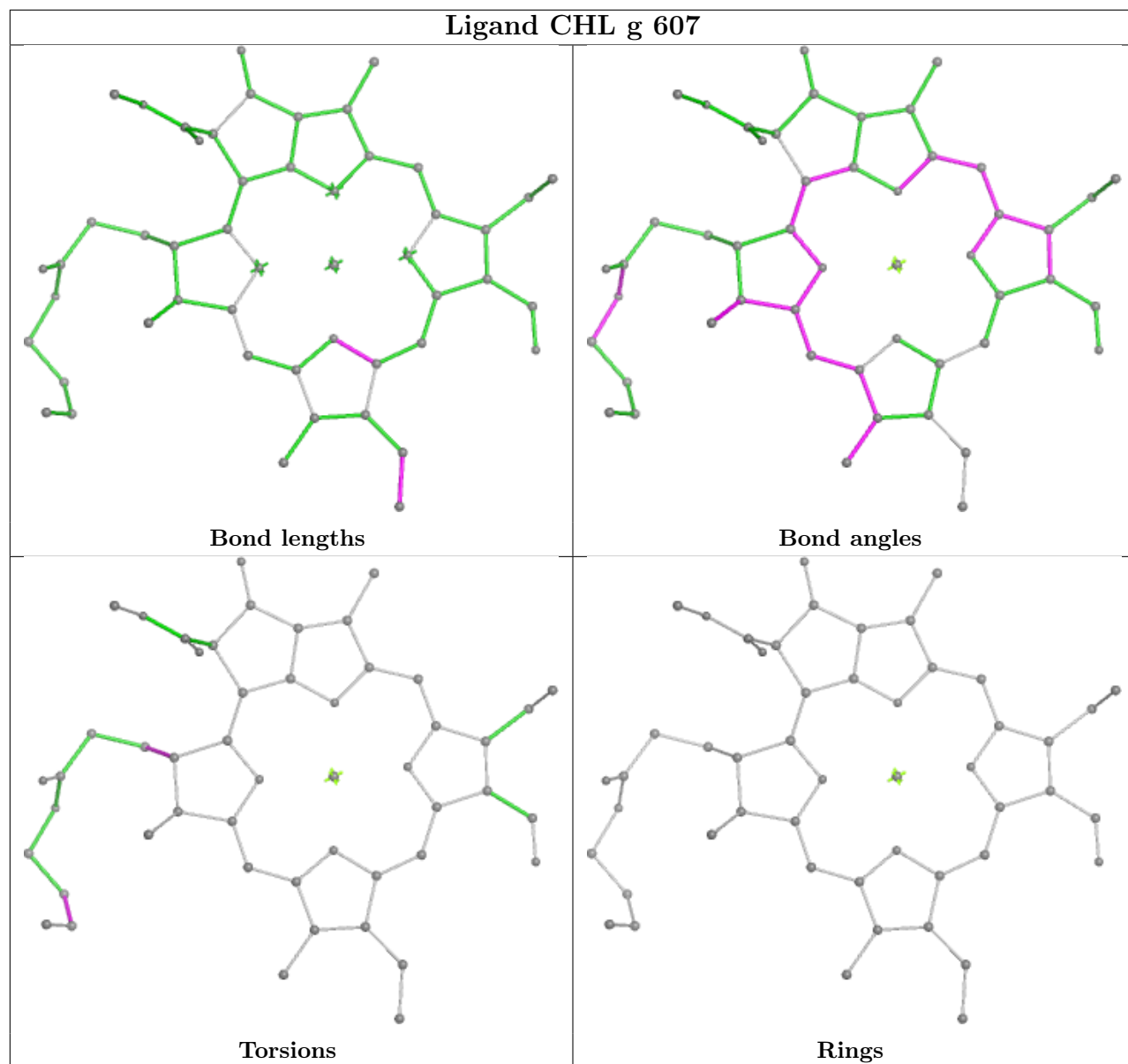


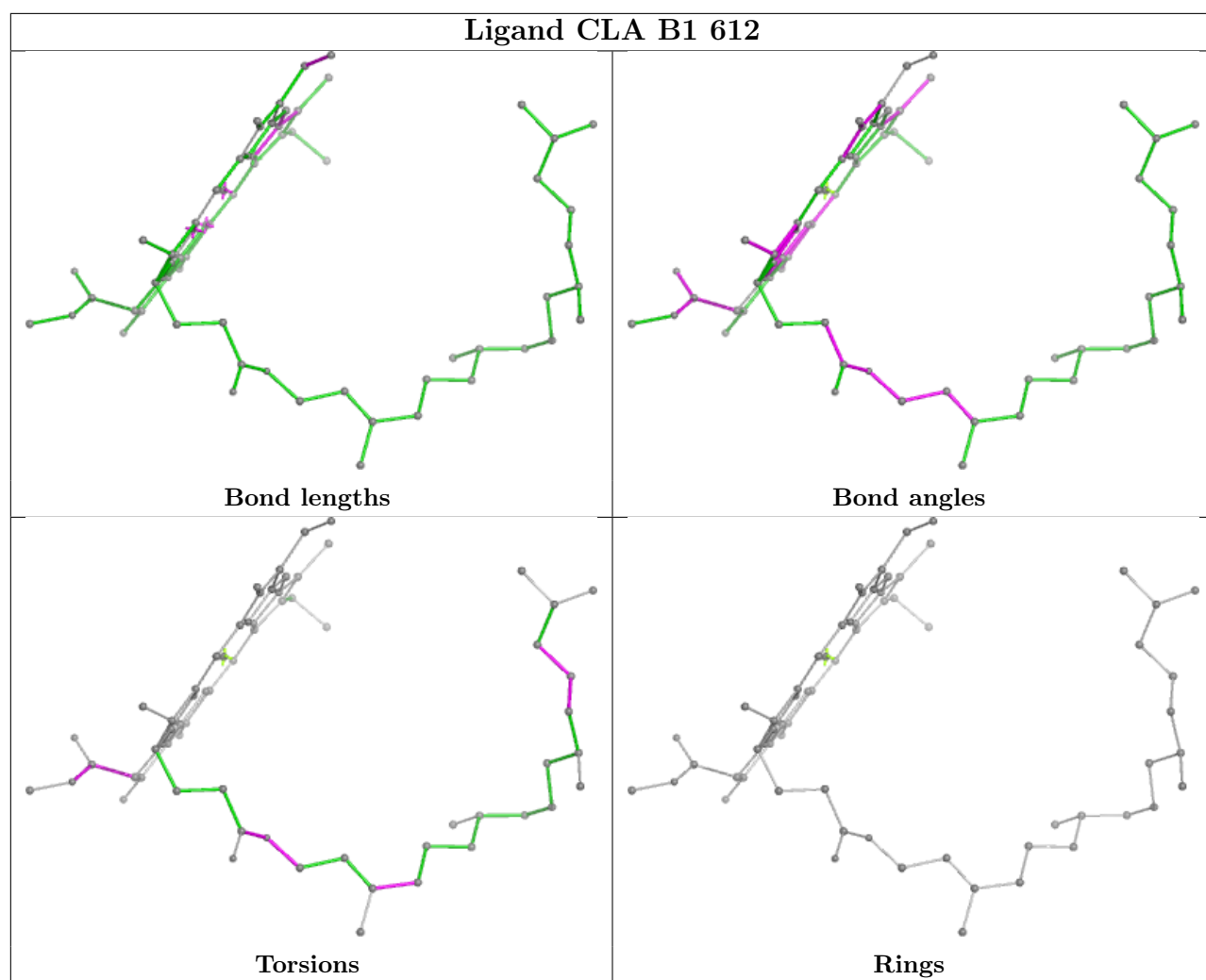
Torsions

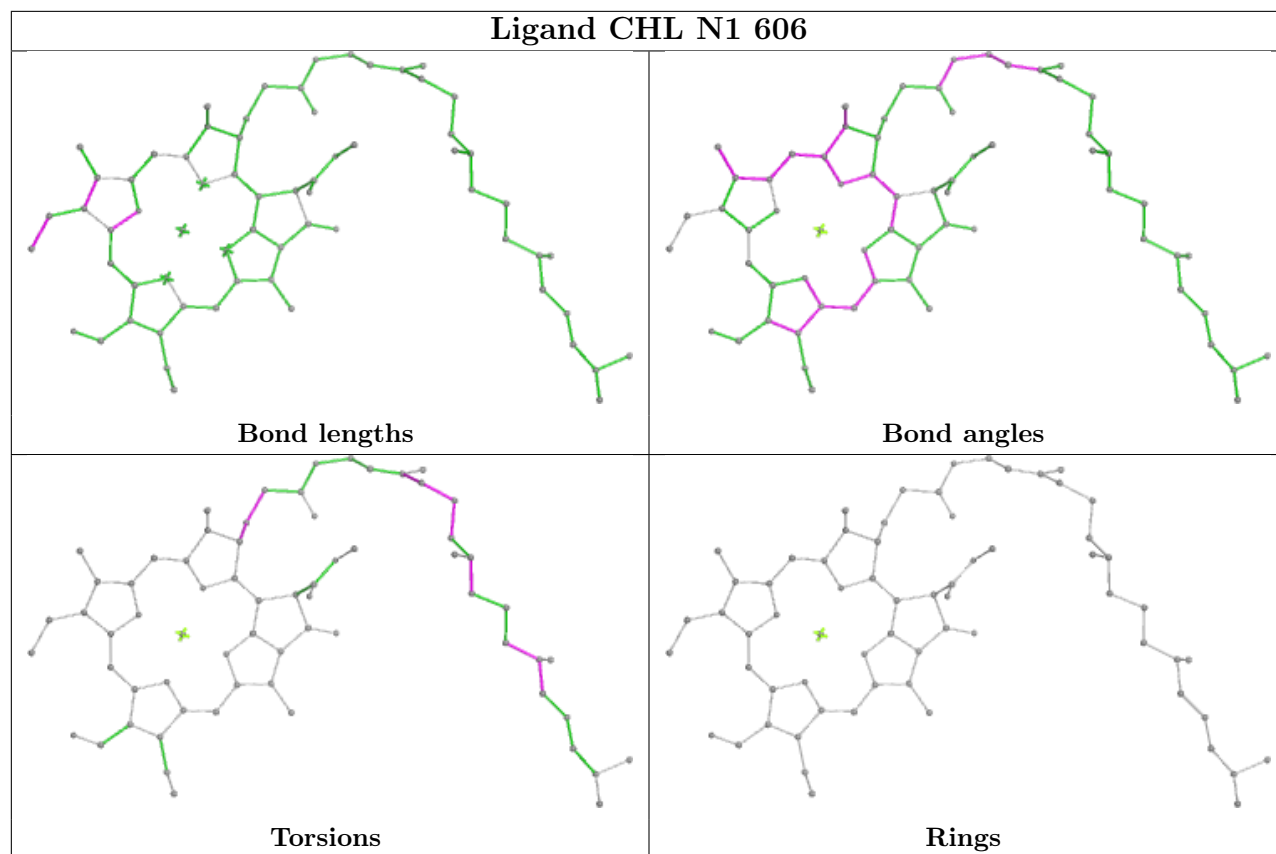


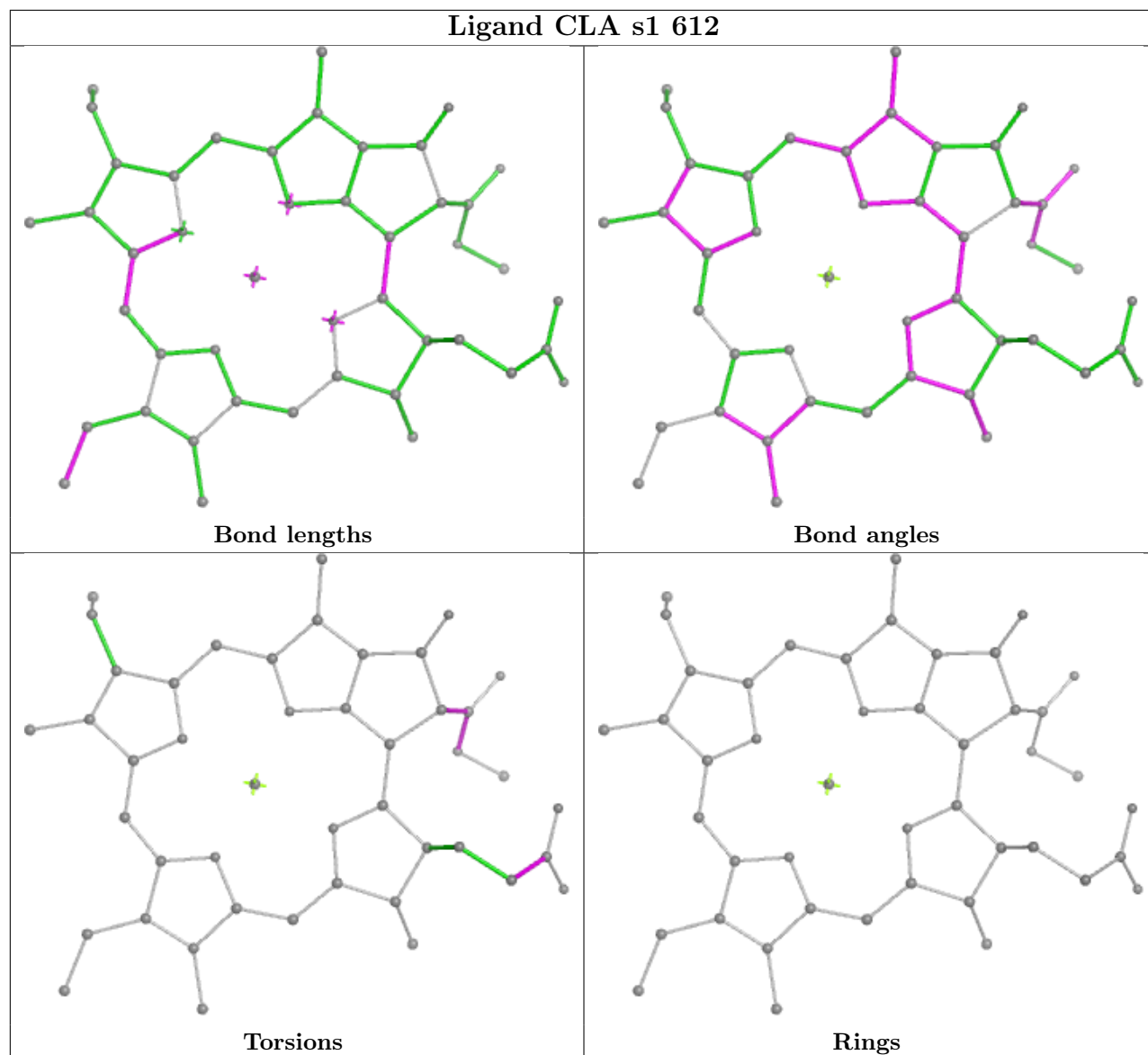
Rings

## Ligand CHL g 607

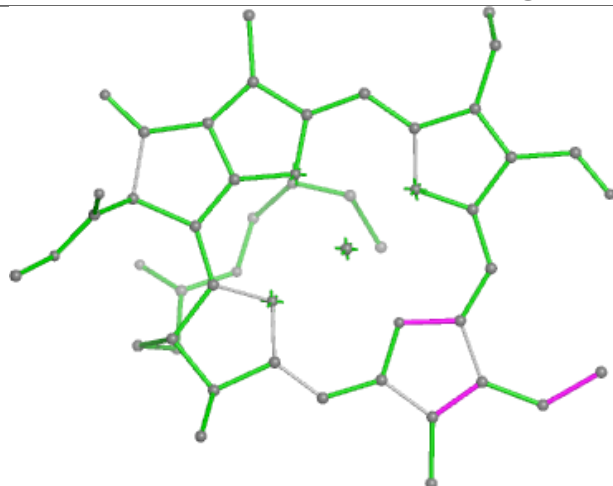




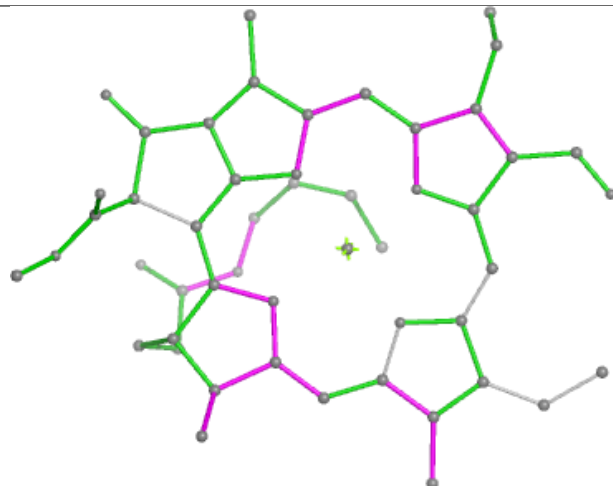




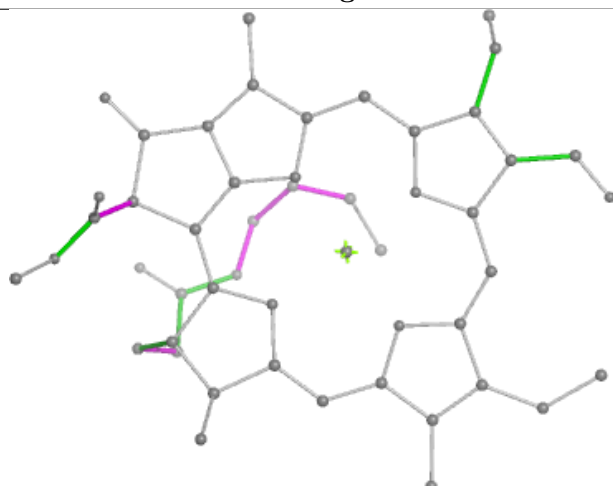
## Ligand CHL r 607



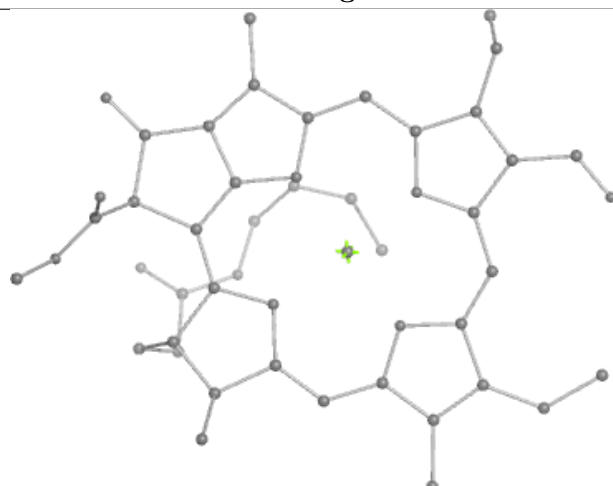
Bond lengths



Bond angles

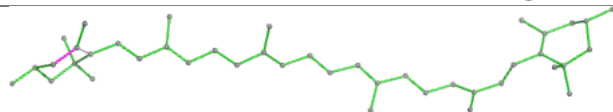


Torsions

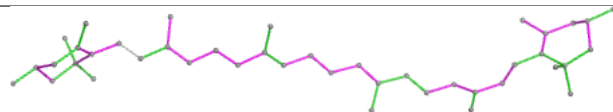


Rings

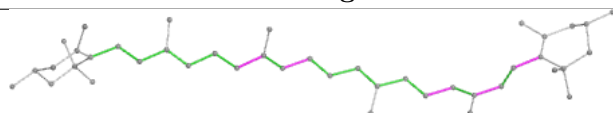
## Ligand LUT r 620



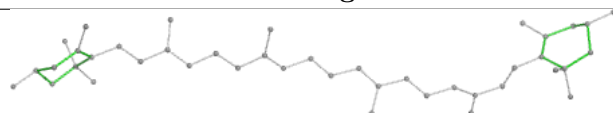
Bond lengths



Bond angles

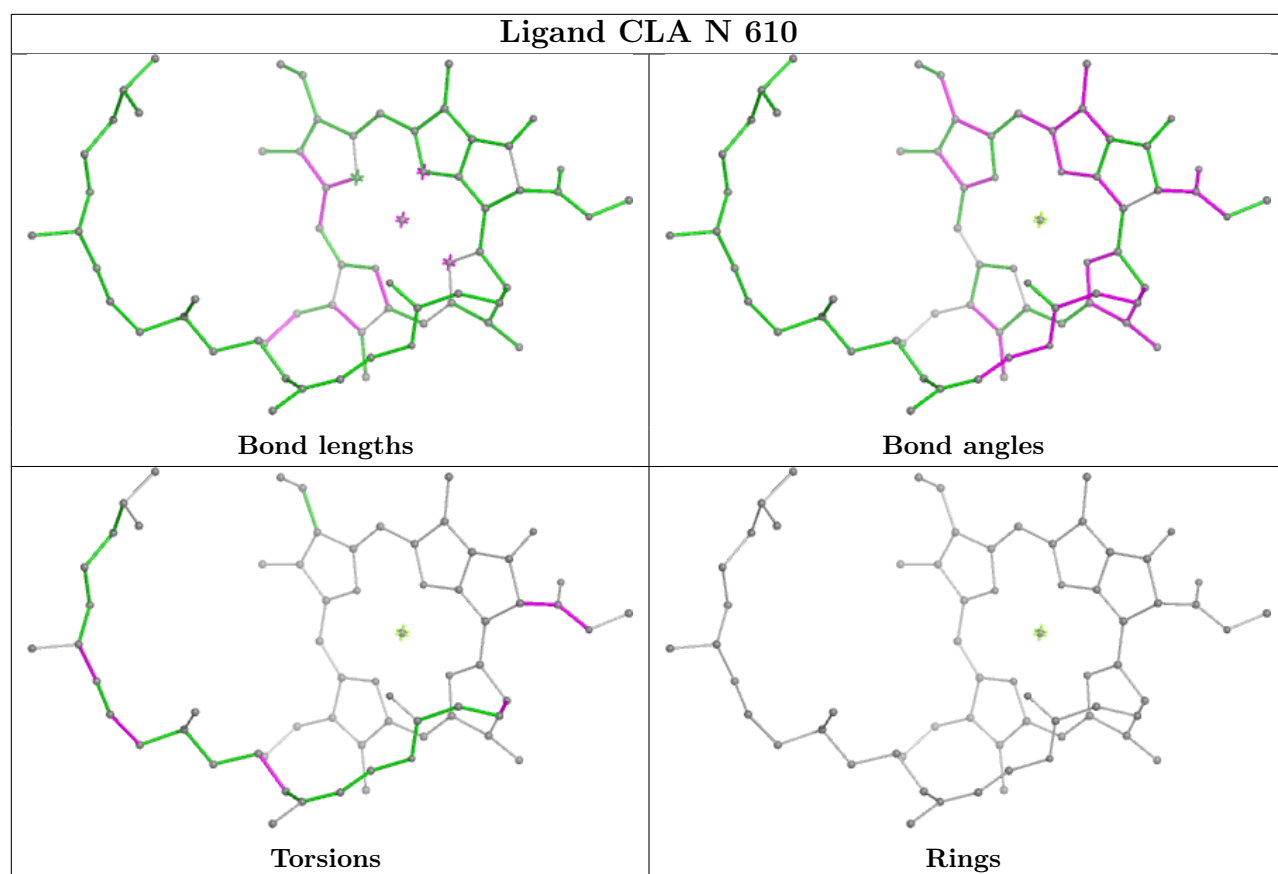


Torsions

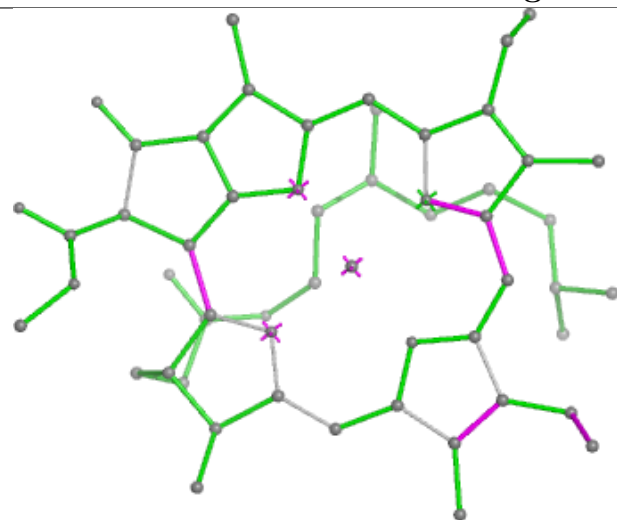


Rings

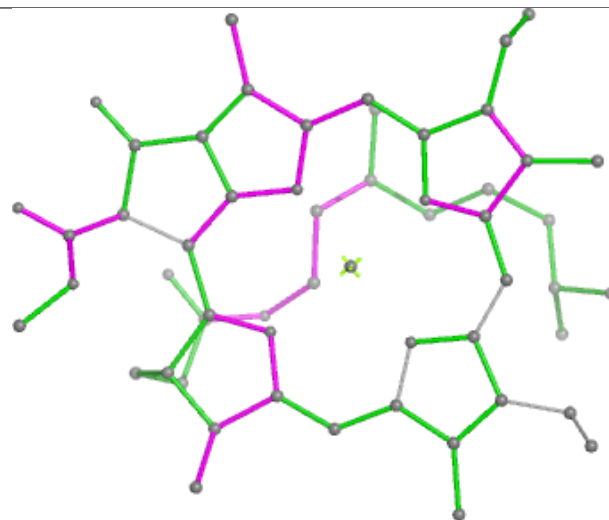




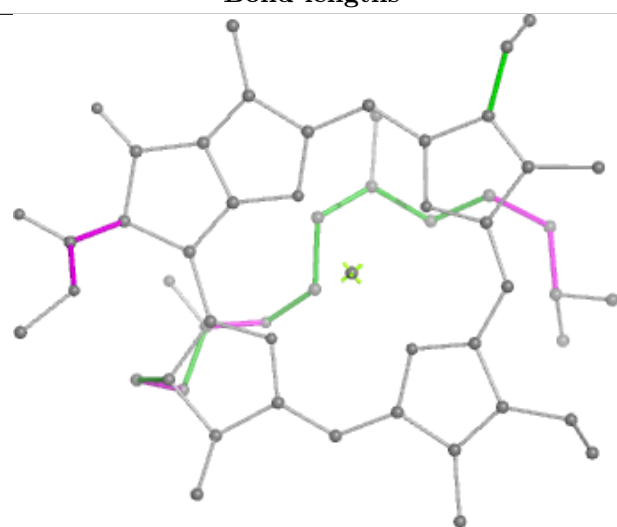
## Ligand CLA s 613



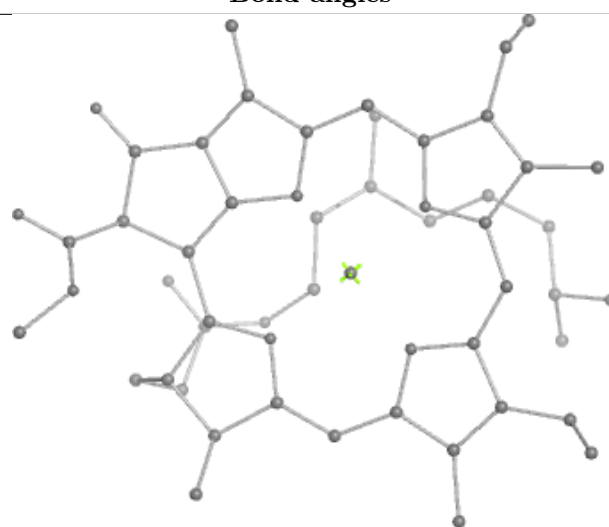
Bond lengths



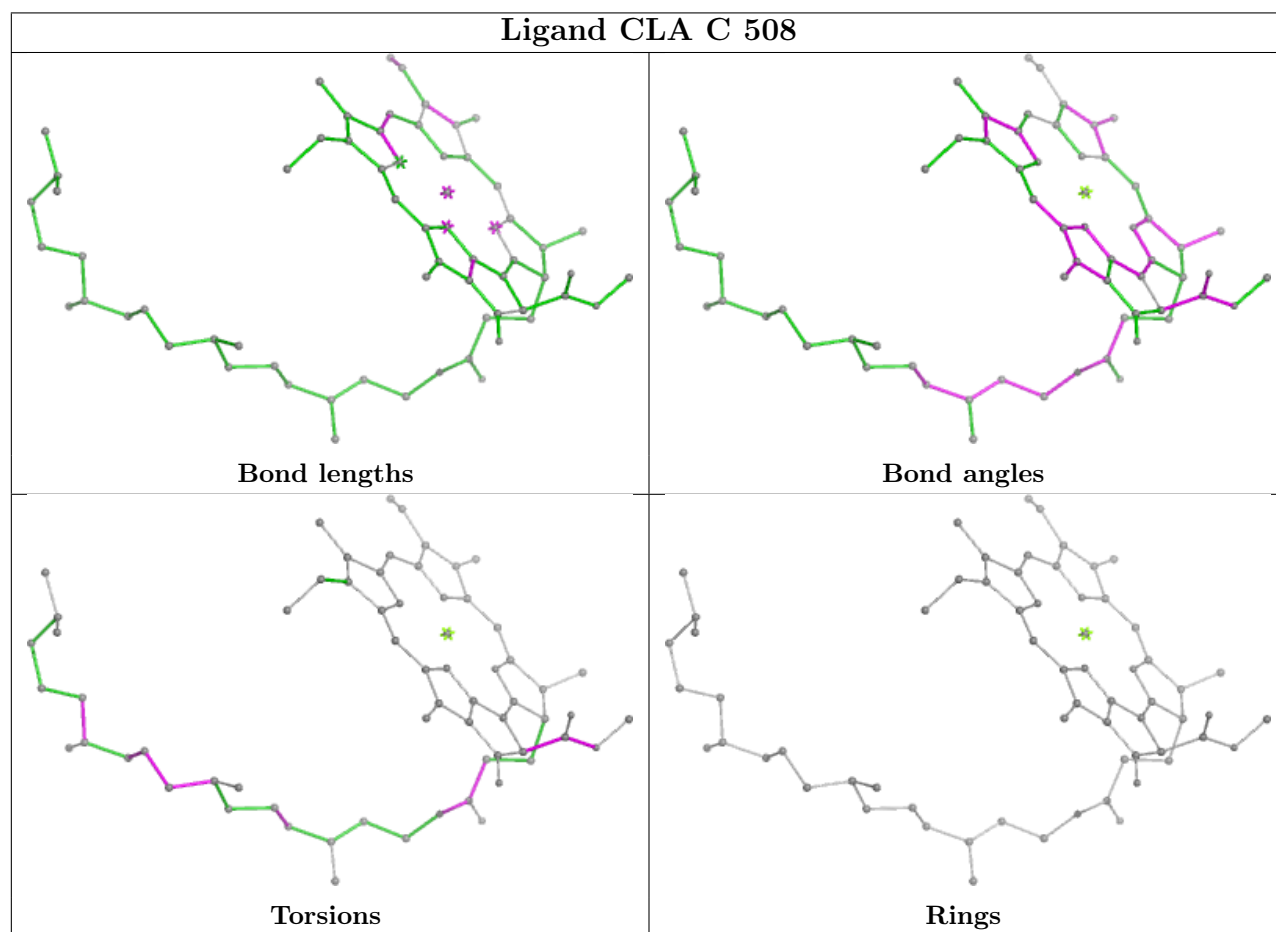
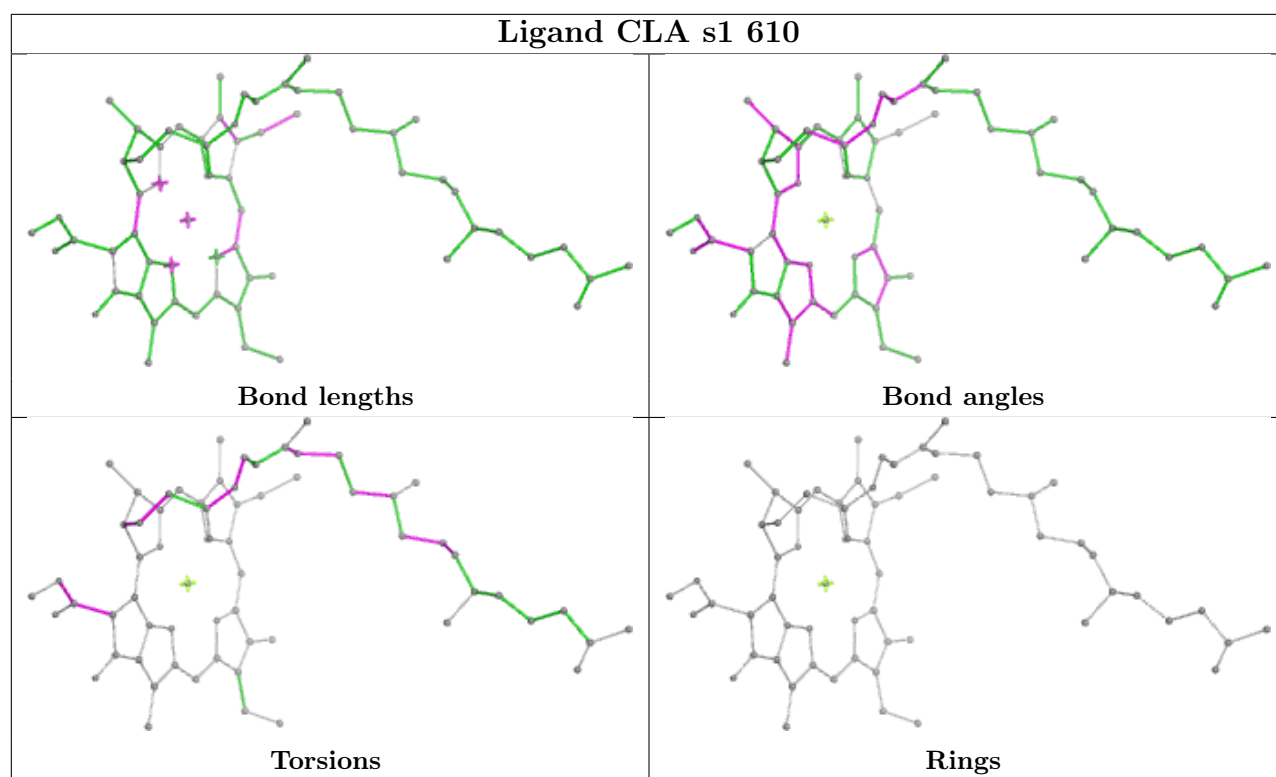
Bond angles

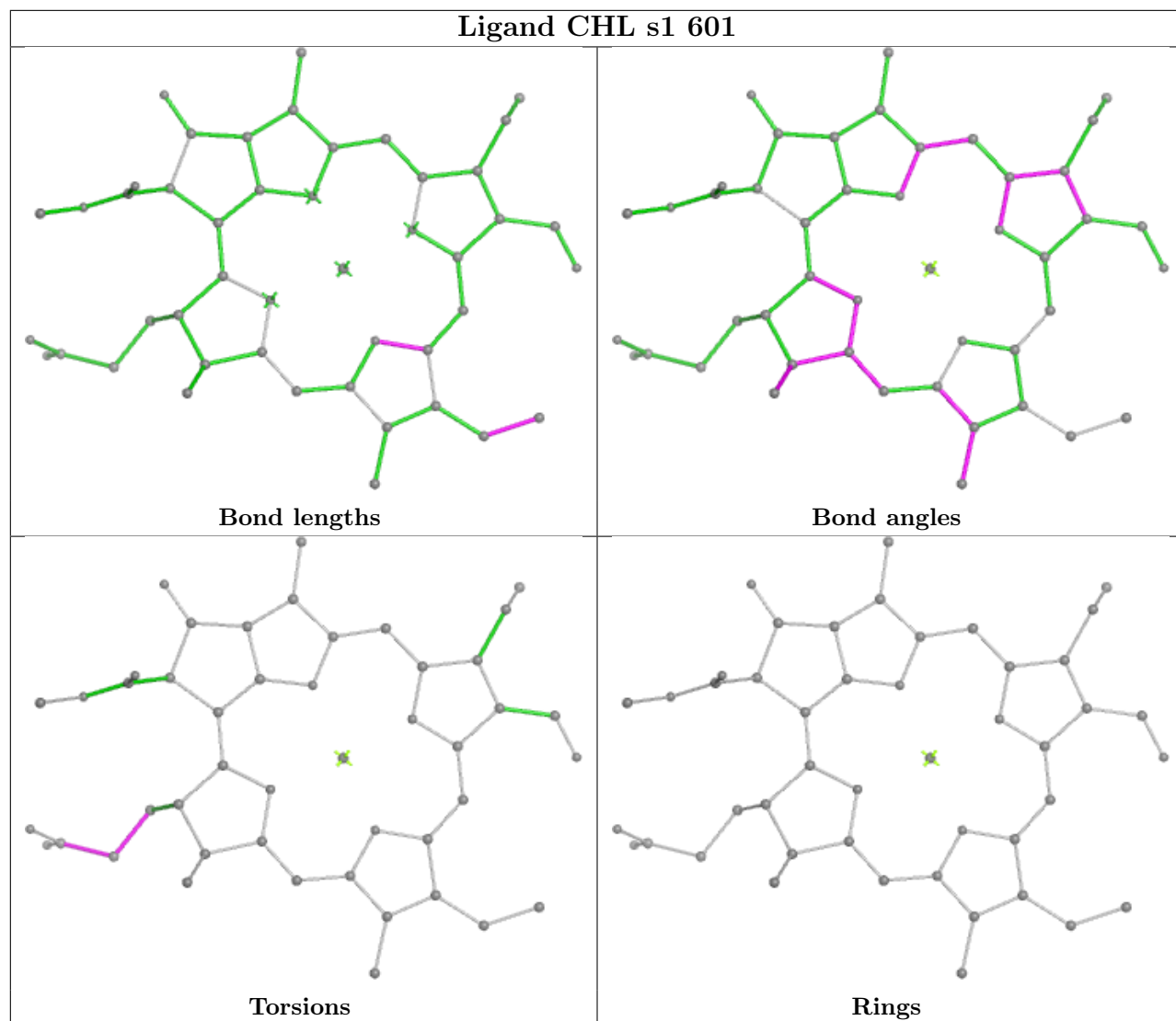


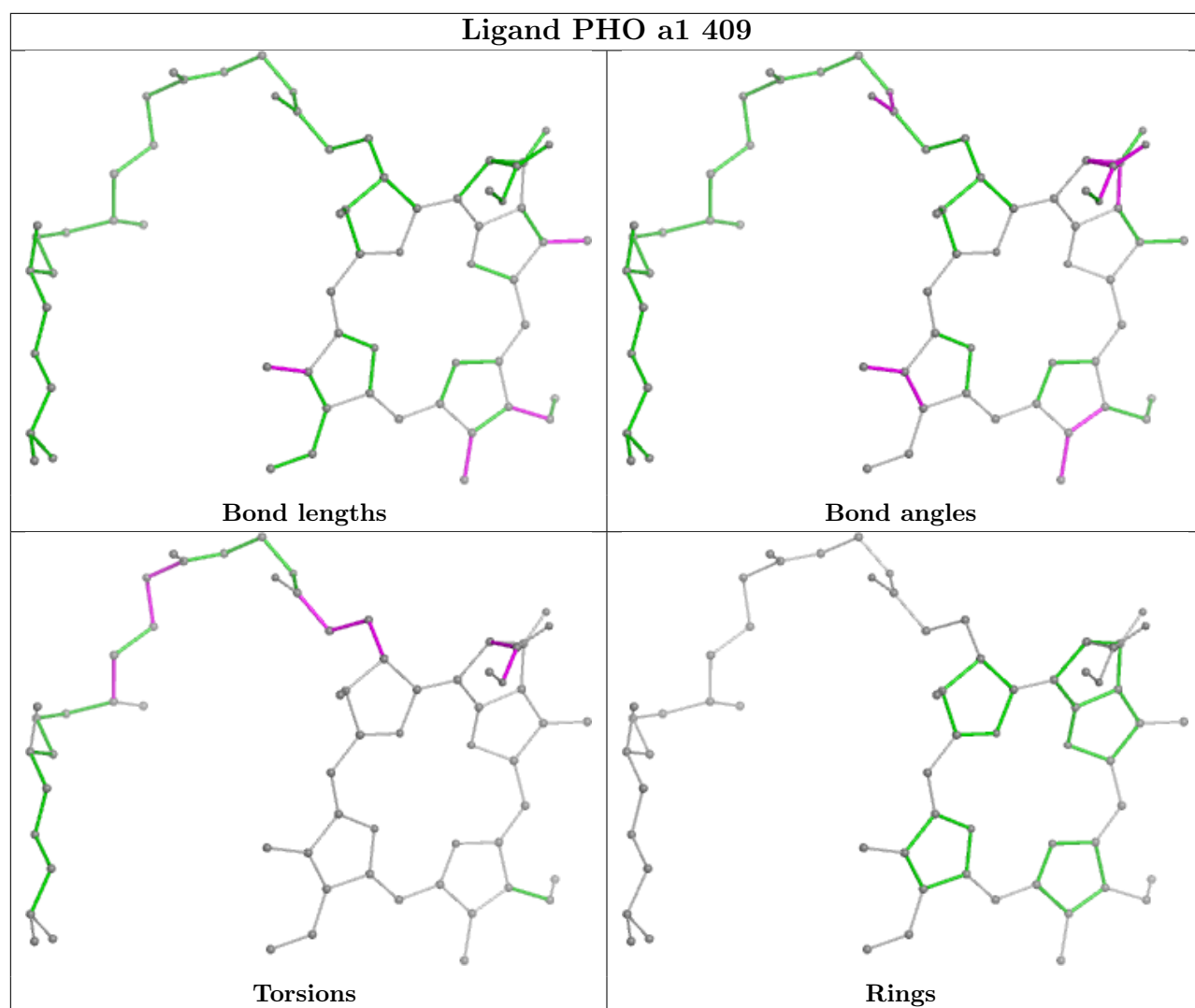
Torsions

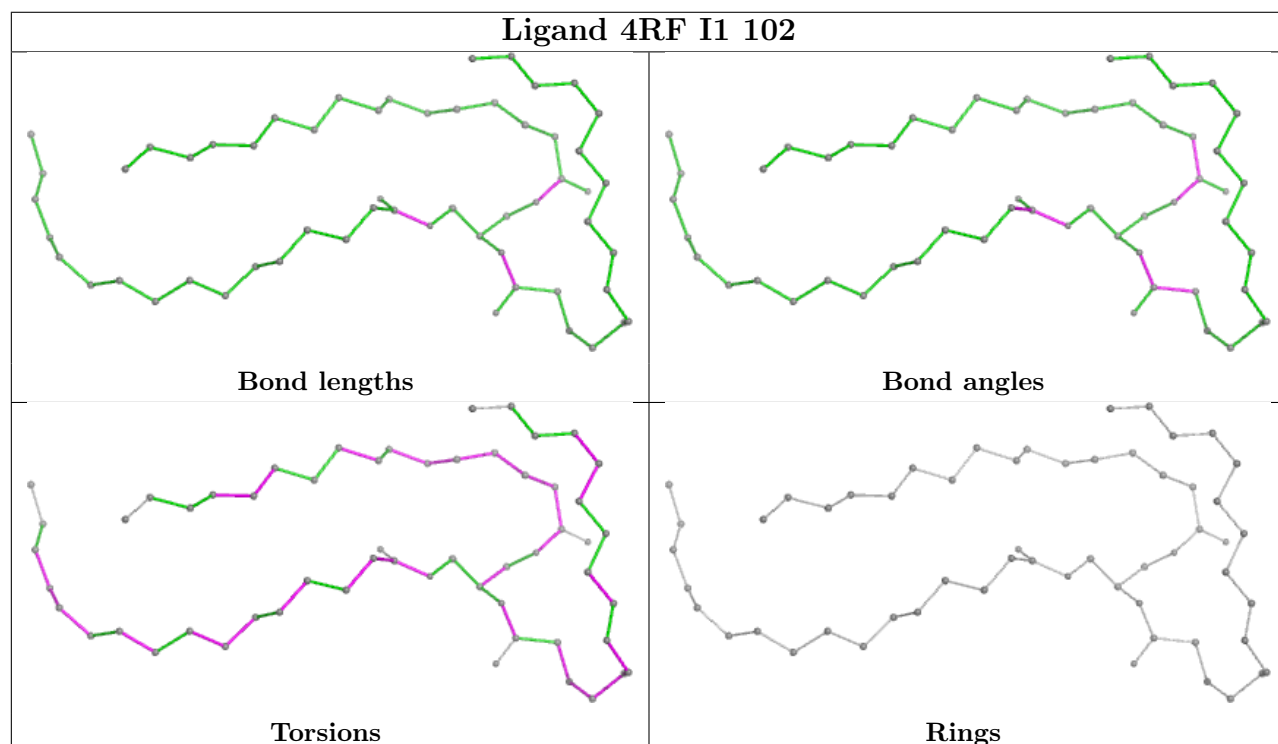
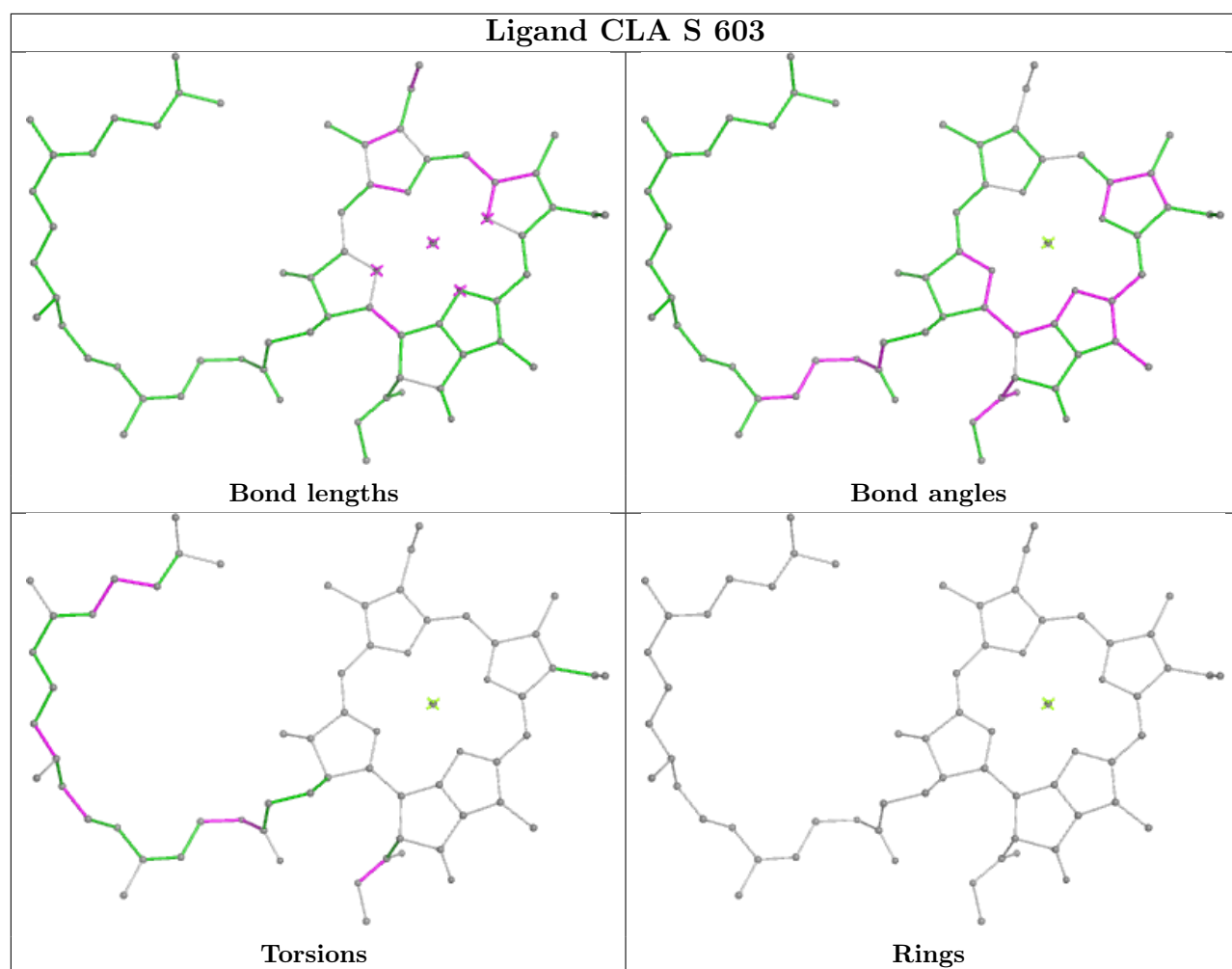


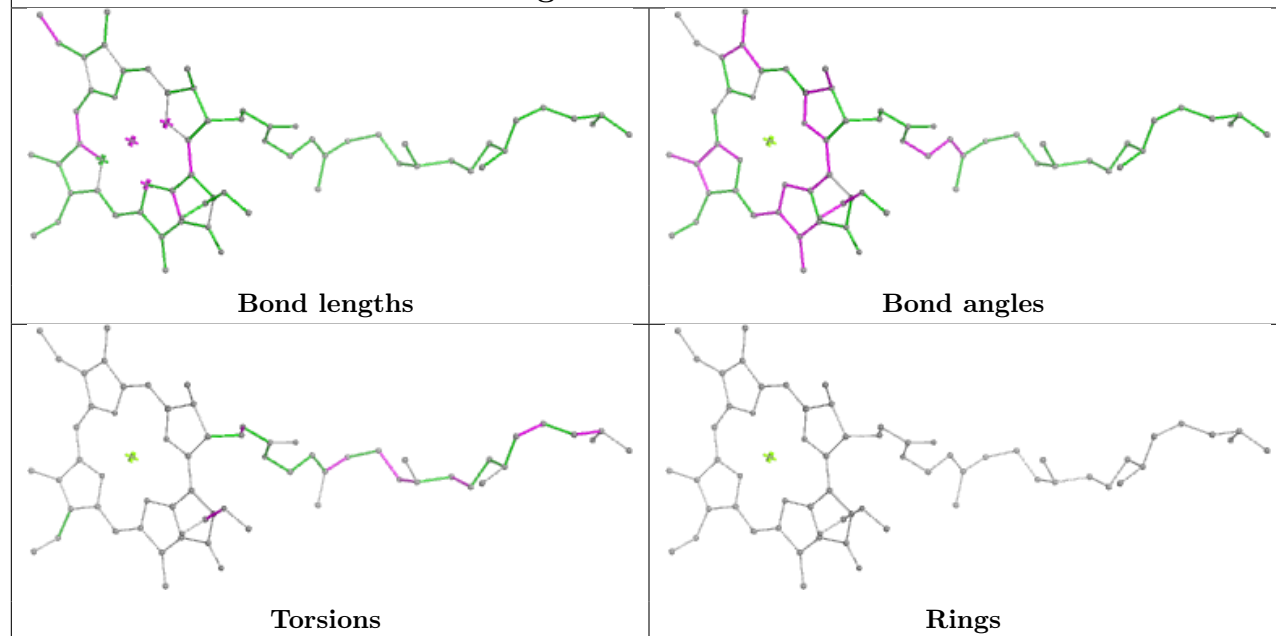
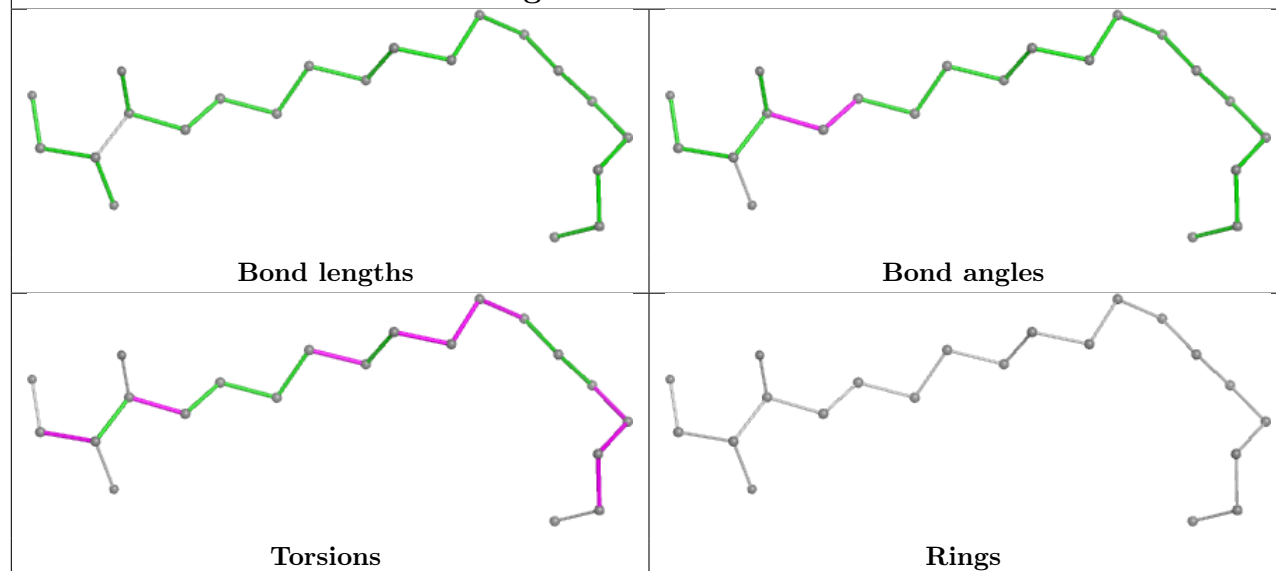
Rings

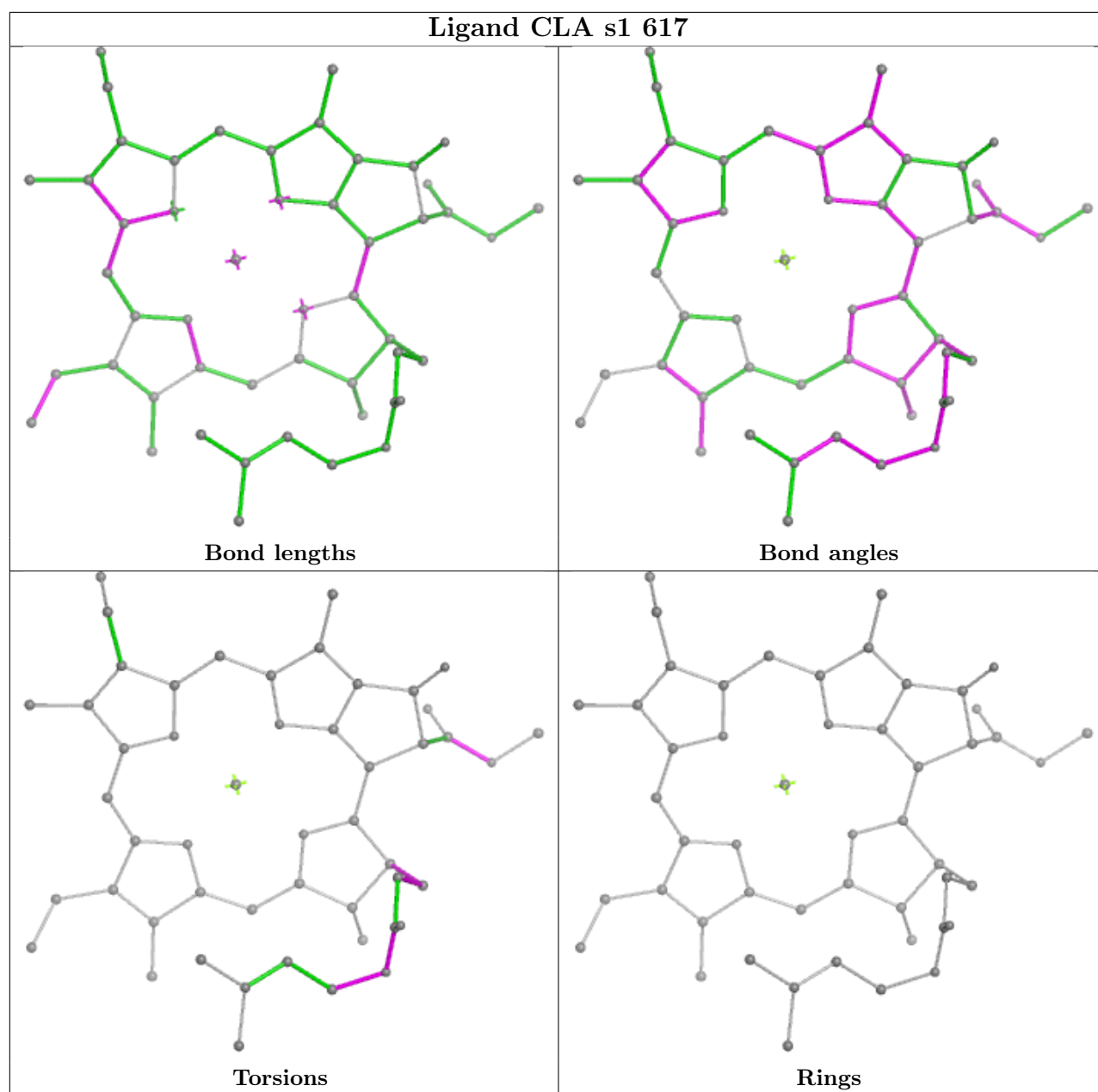






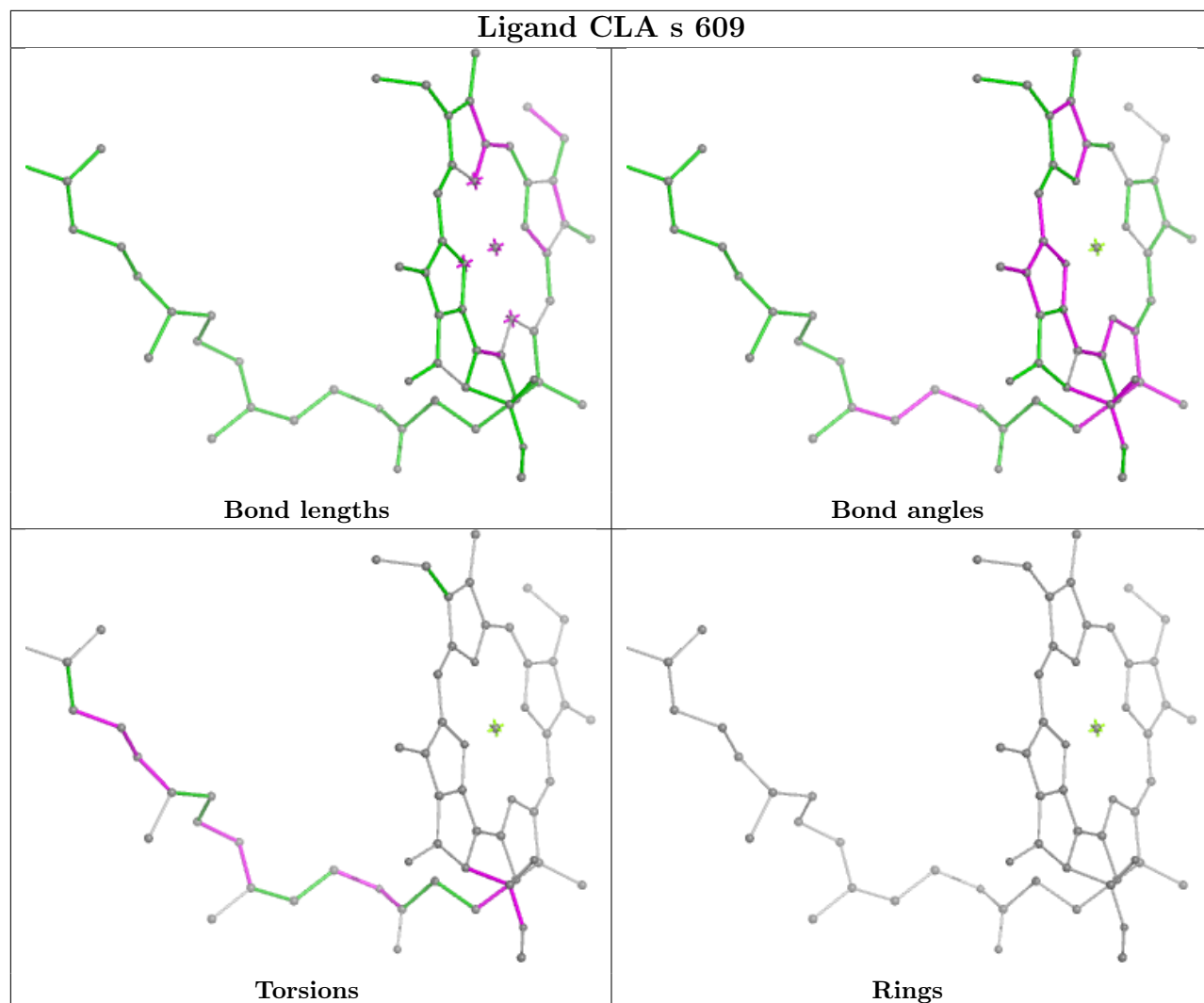


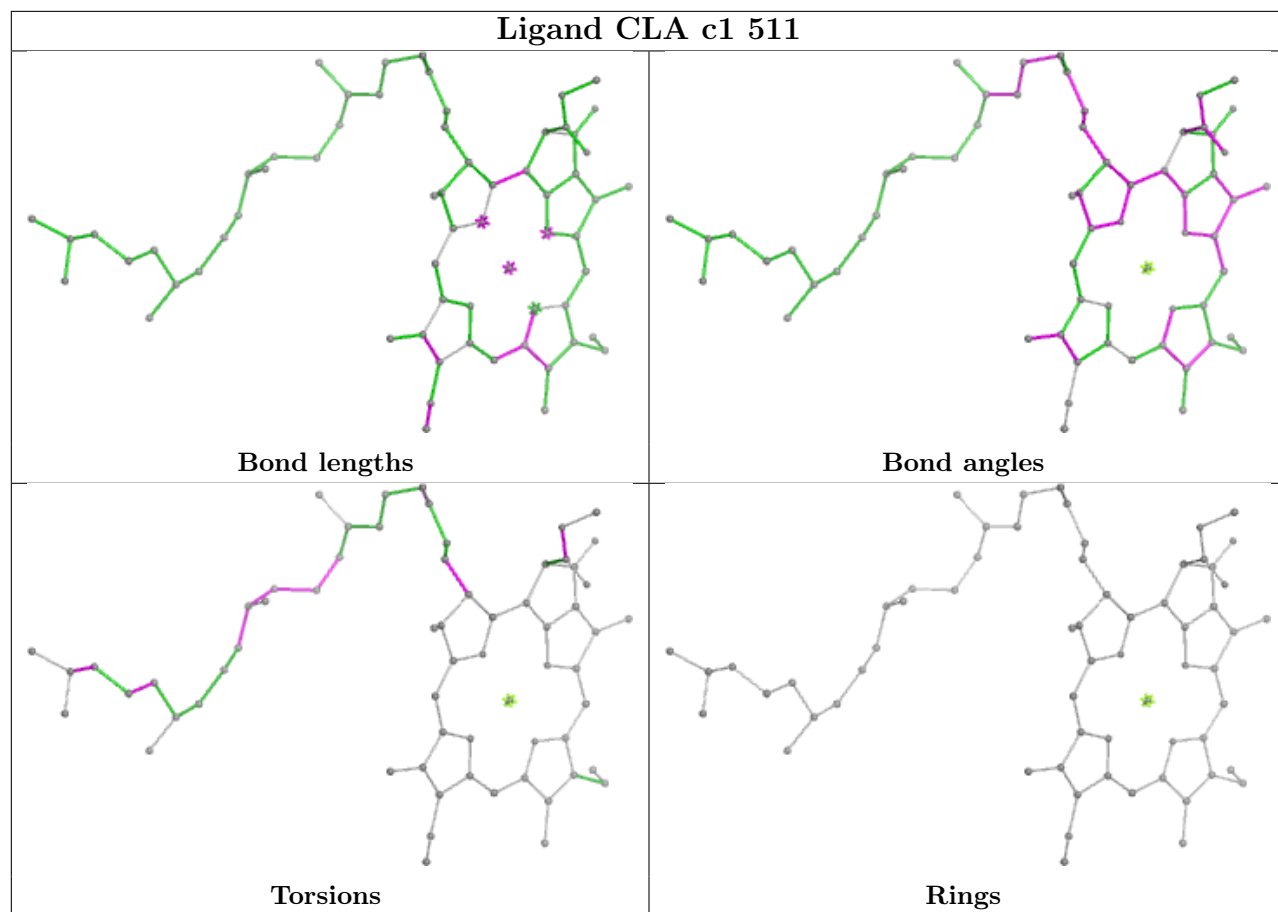
**Ligand CLA c 502****Ligand SPH Y1 625**

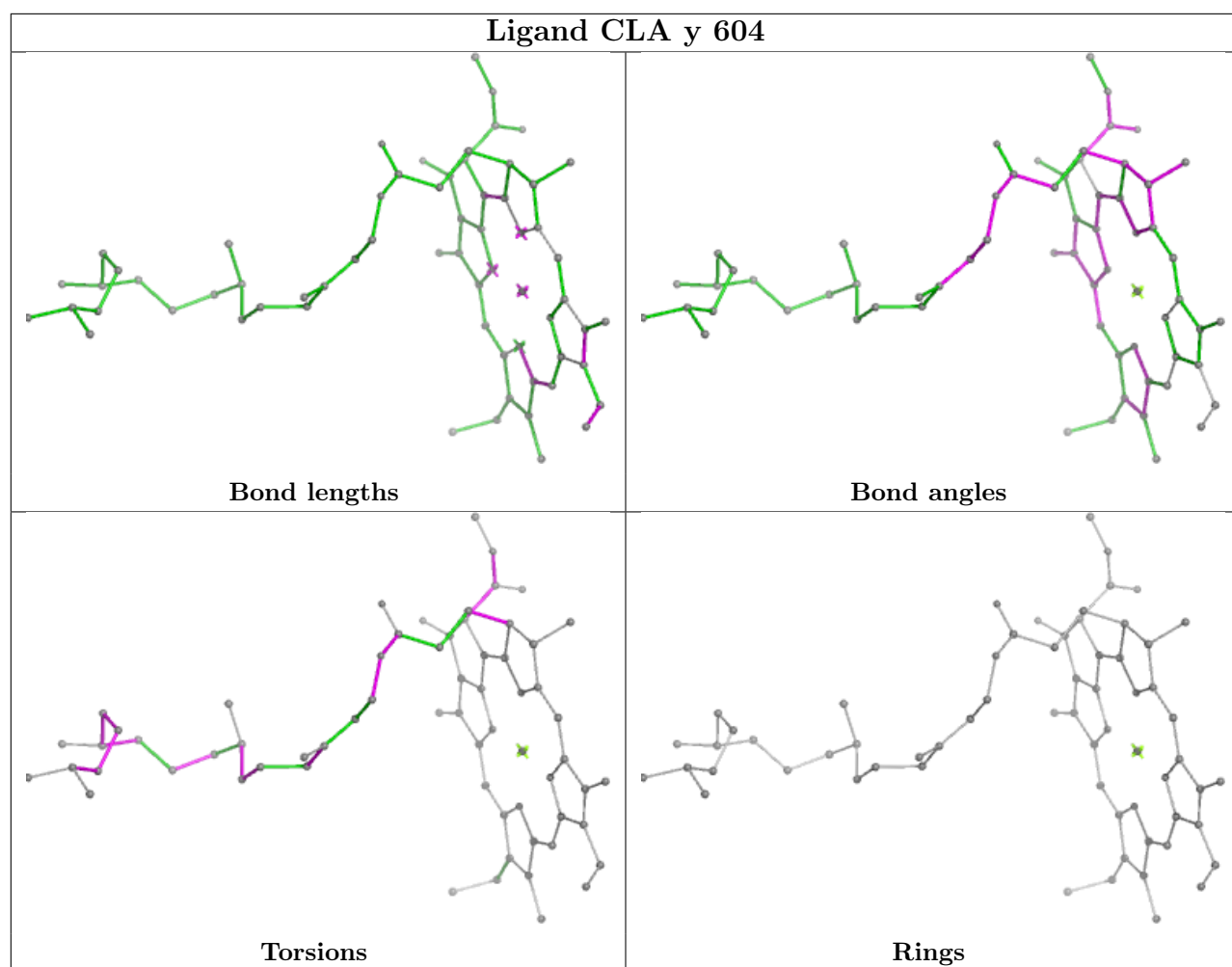




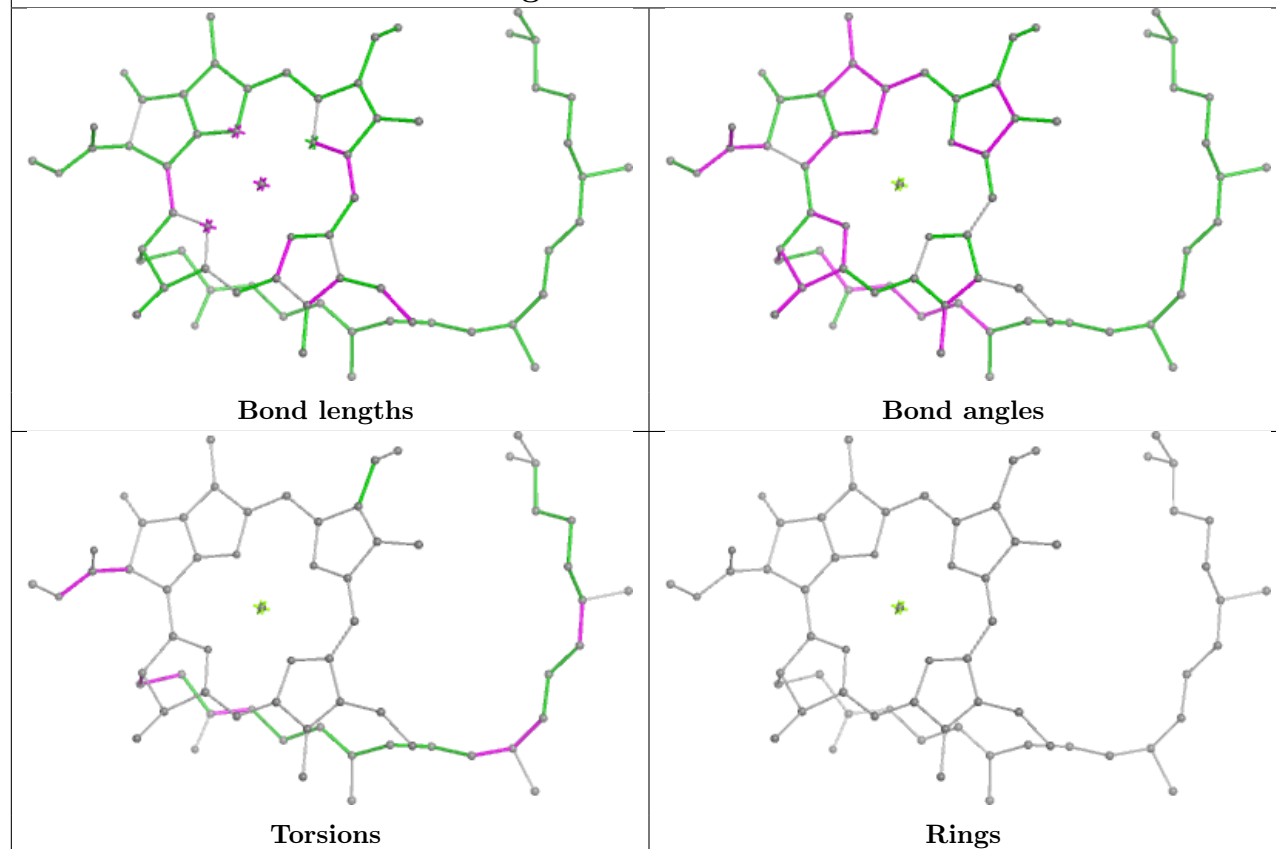
## Ligand CLA s 609



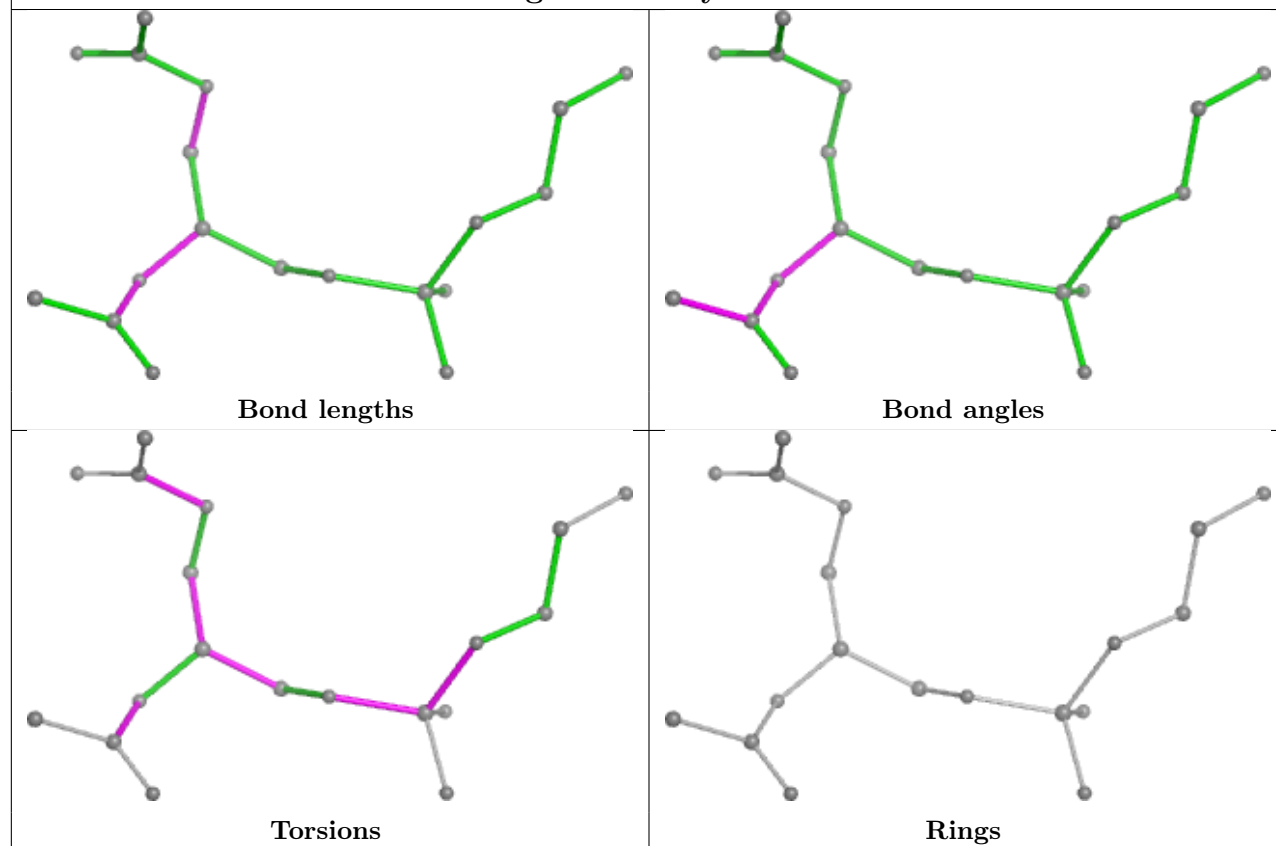


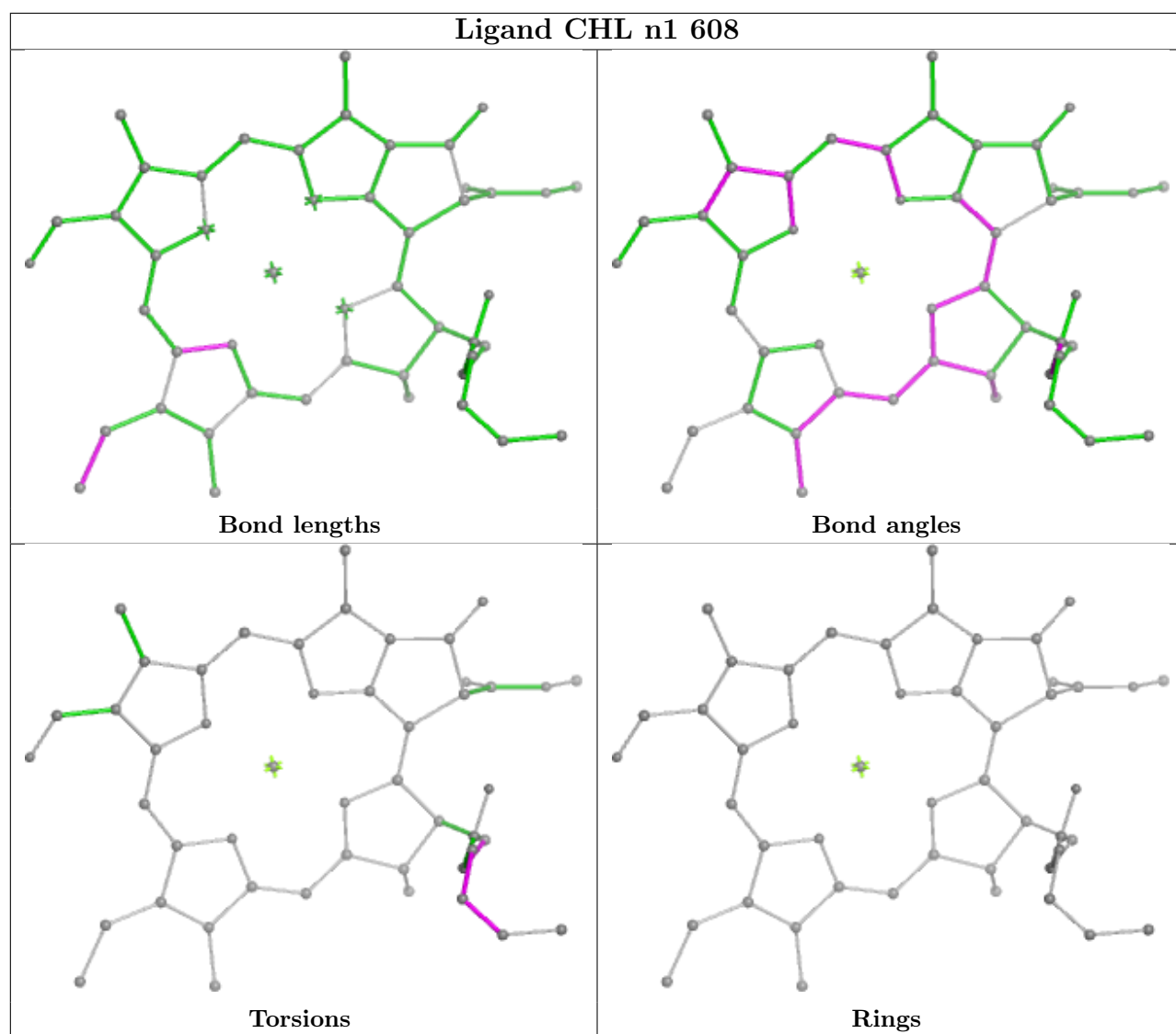


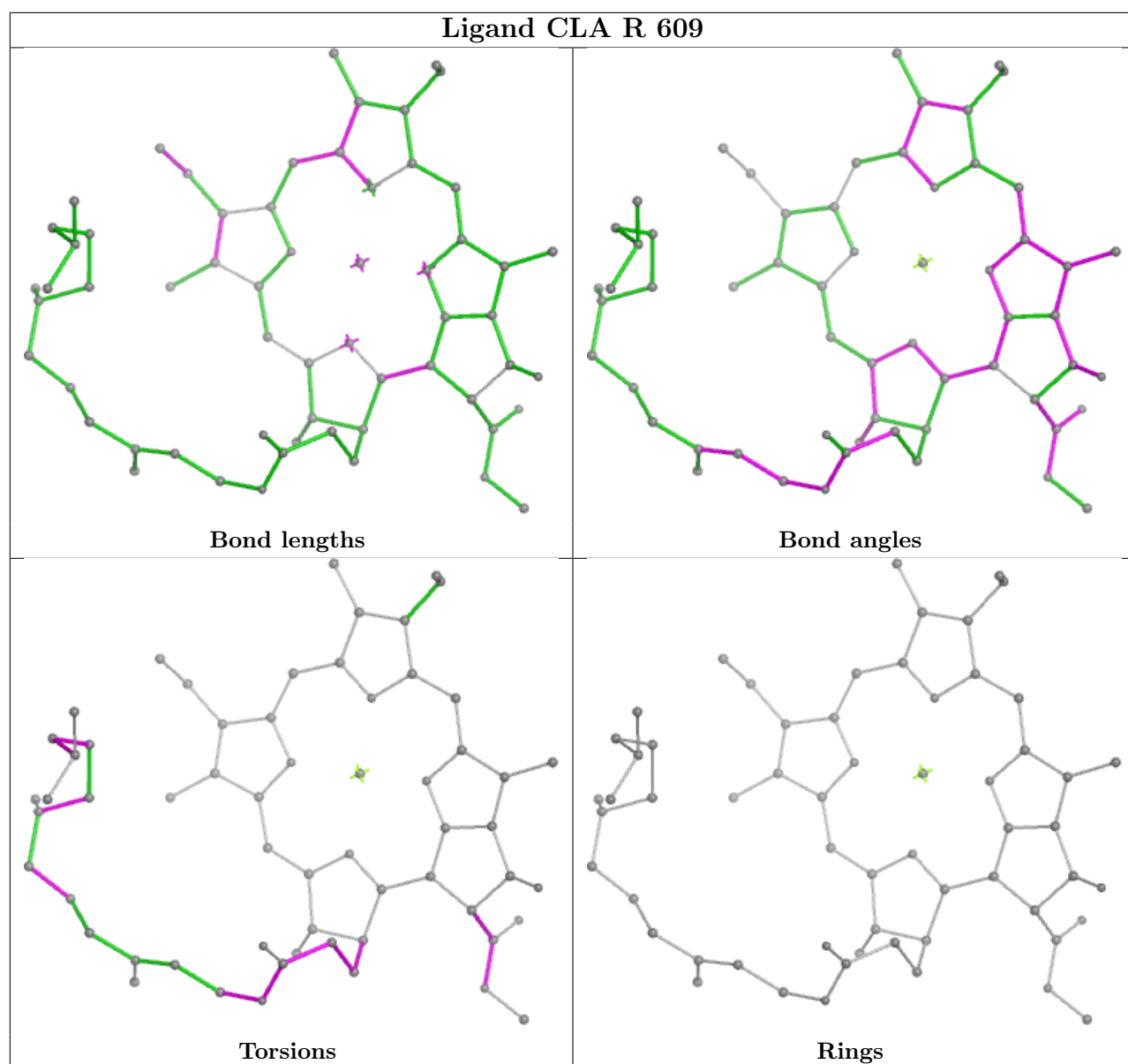
## Ligand CLA G1 610

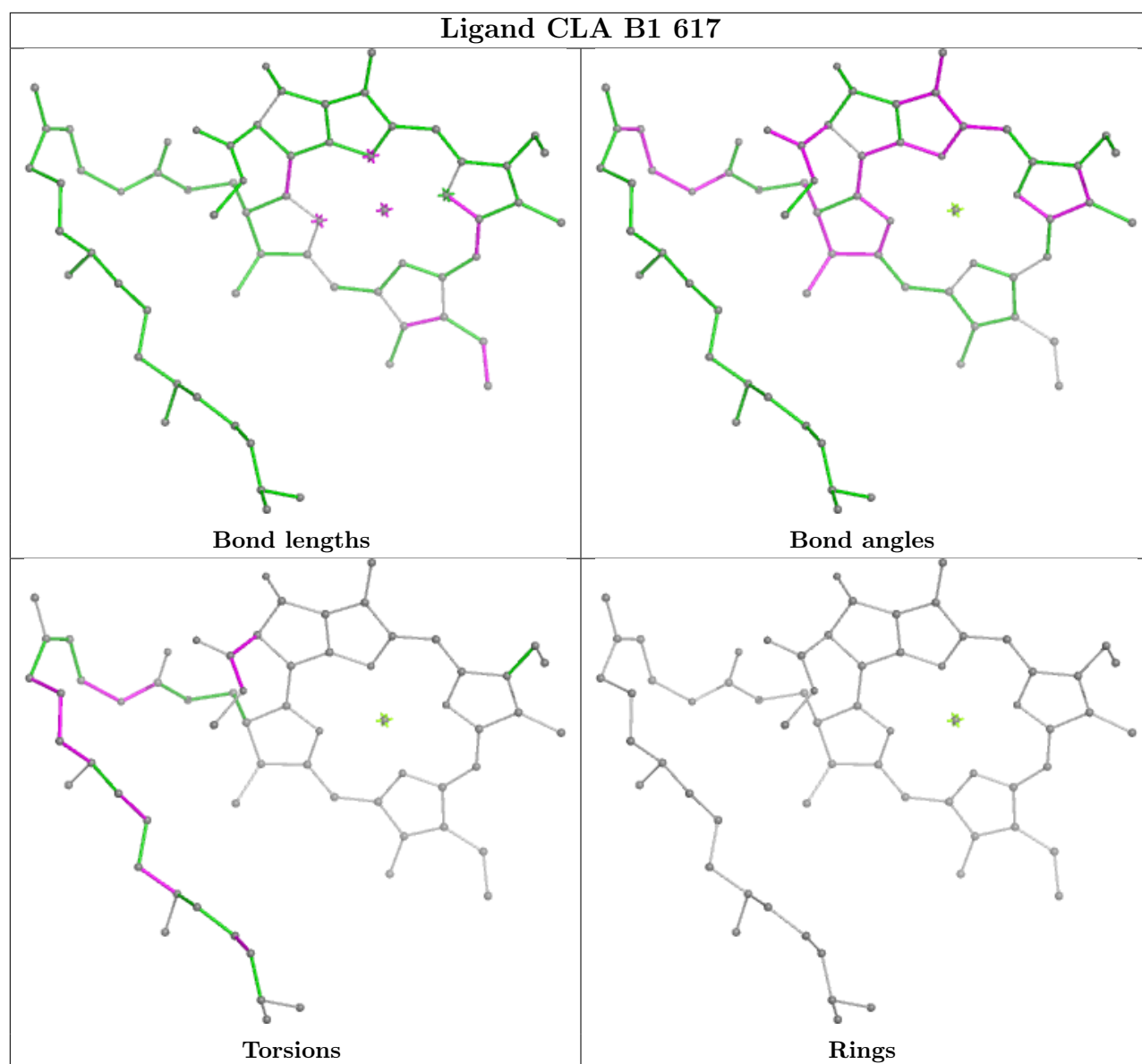


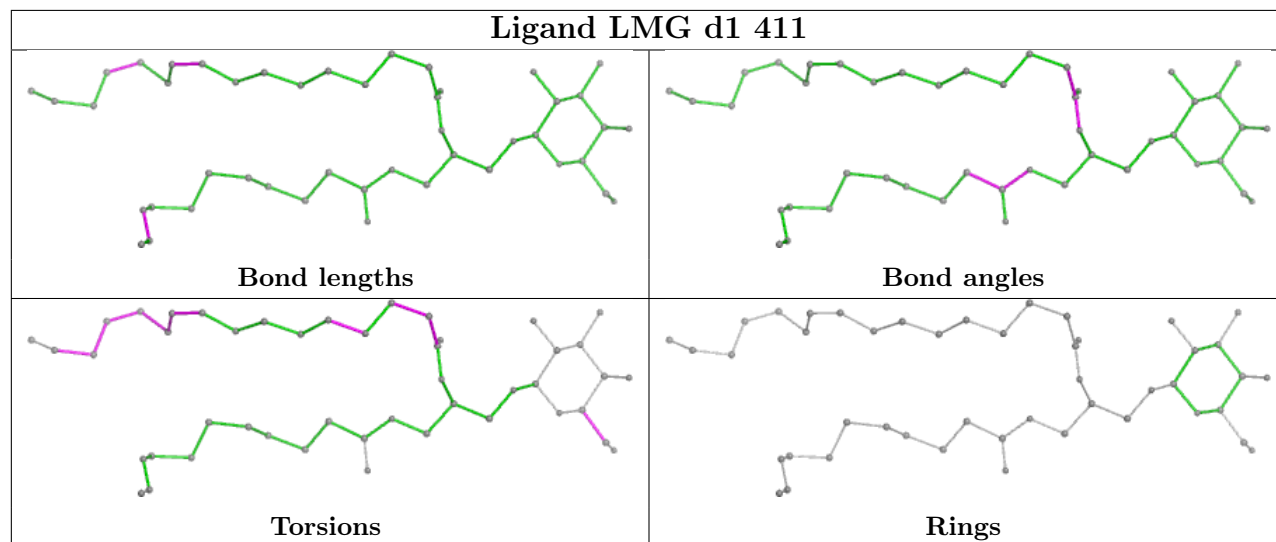
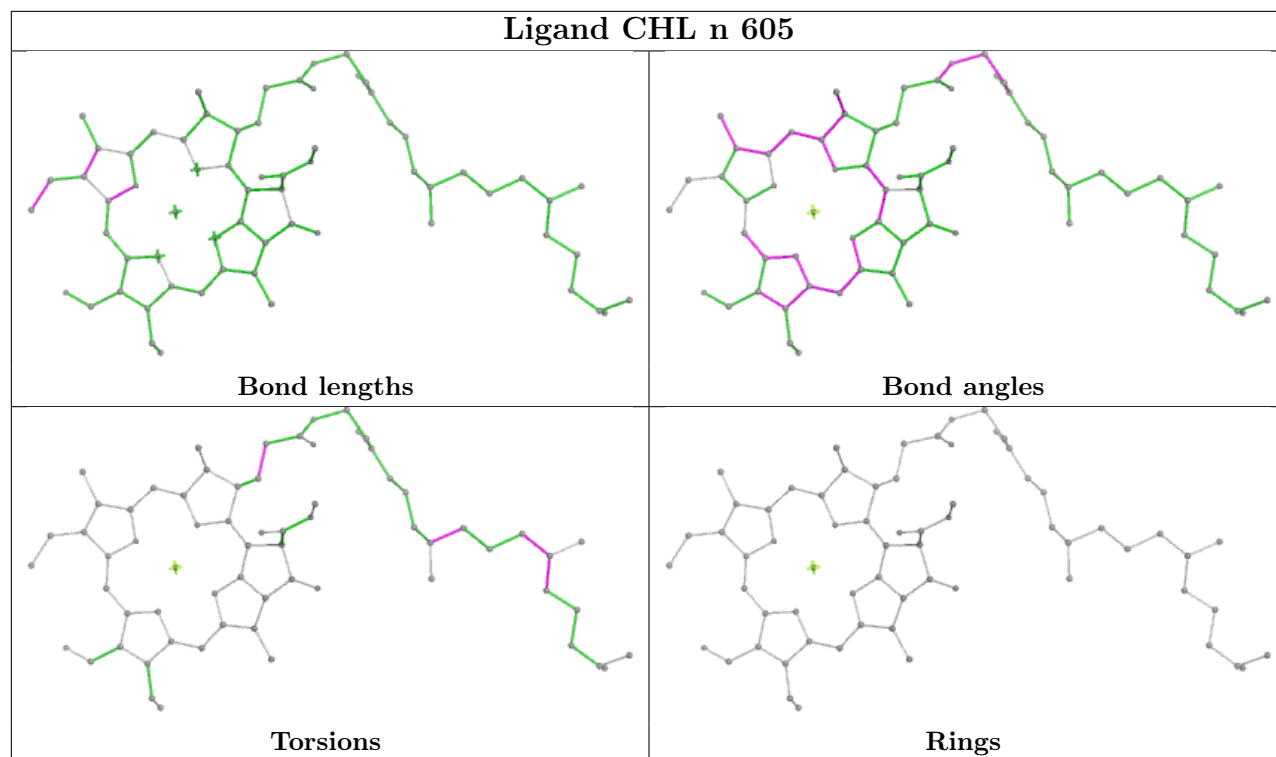
## Ligand PTY y1 627



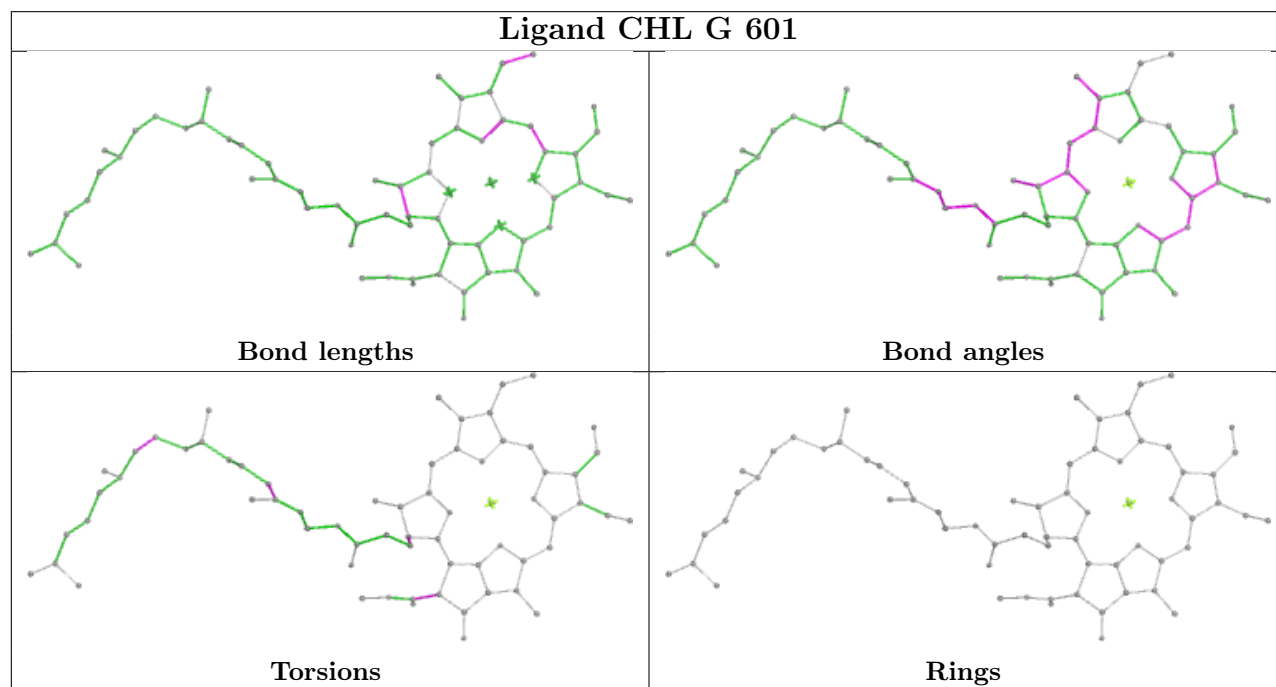
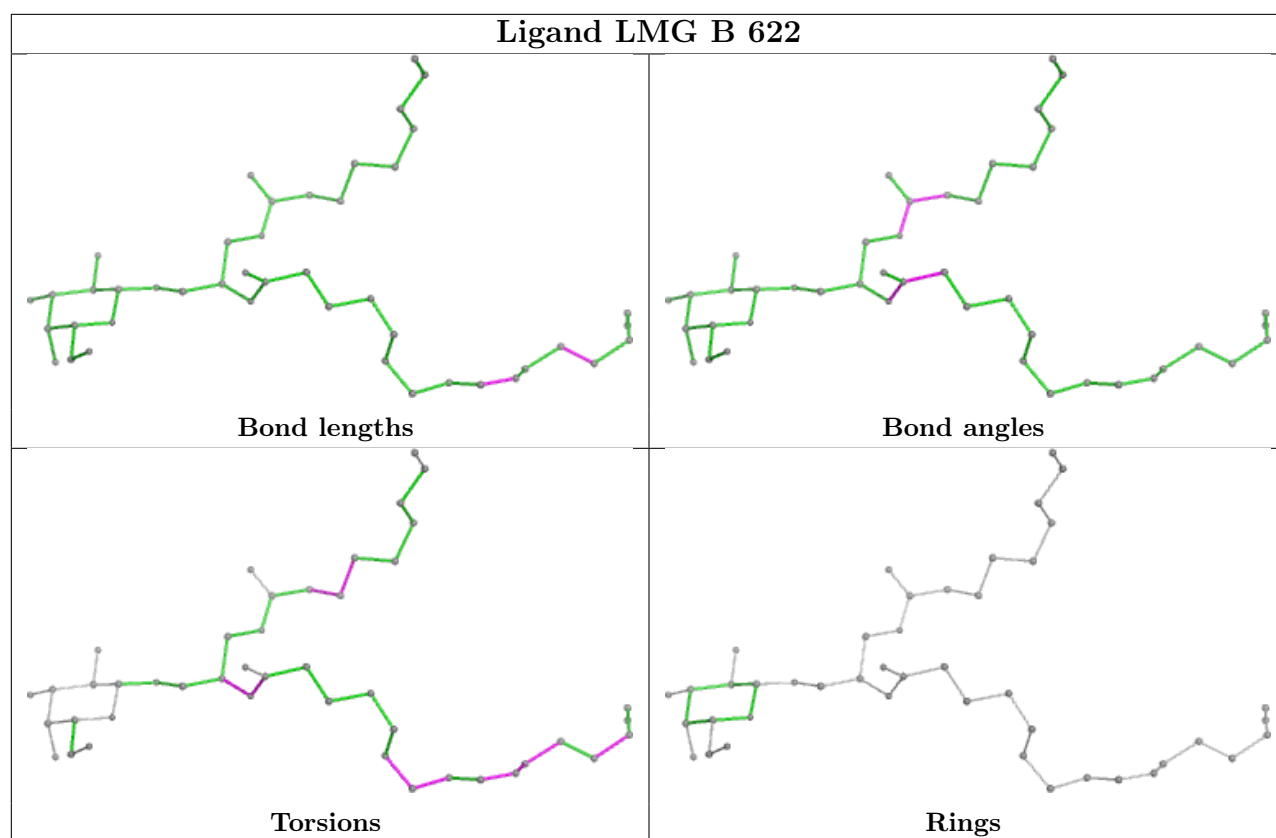


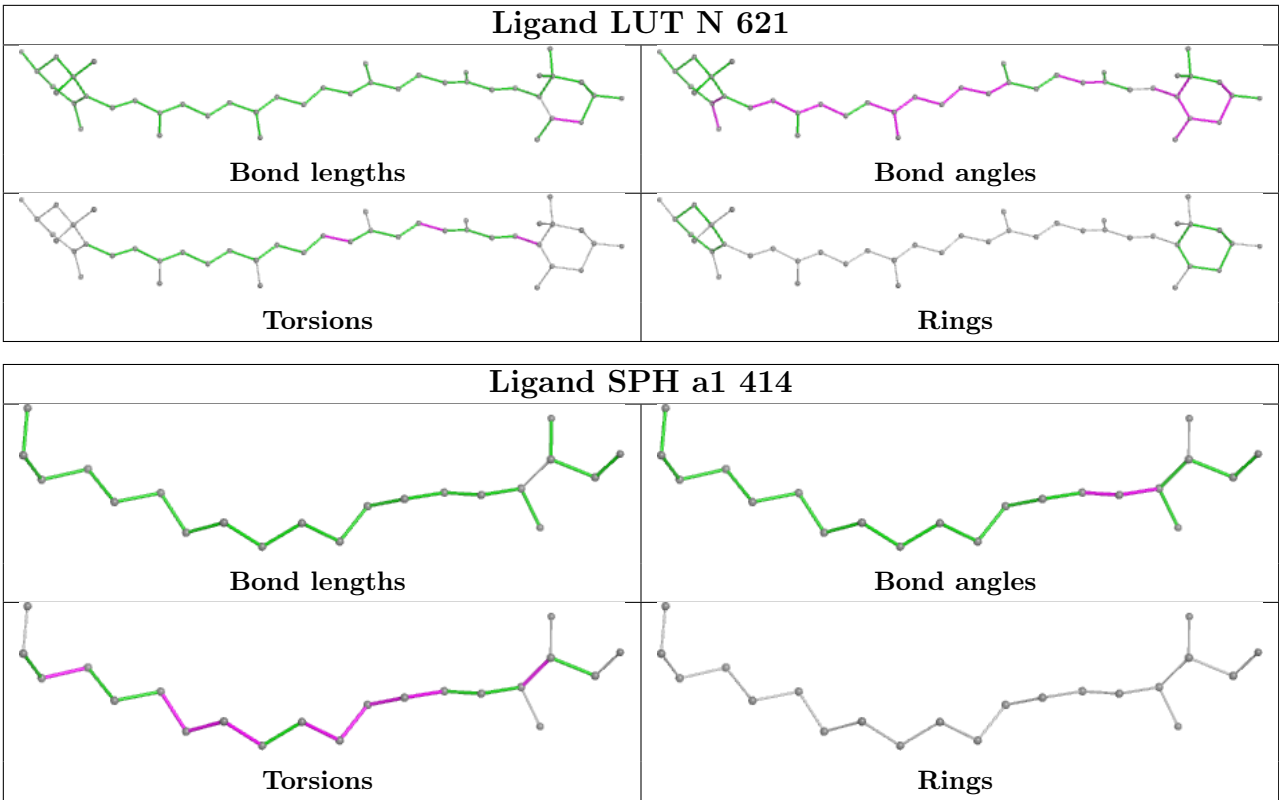












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	R	1
27	r1	1
27	R1	1
23	s	1
20	n1	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	18.97
1	R	110:PRO	C	126:GLU	N	18.01
1	r1	110:PRO	C	126:GLU	N	12.33

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R1	110:PRO	C	126:GLU	N	11.82
1	s	285:ARG	C	286:VAL	N	3.41

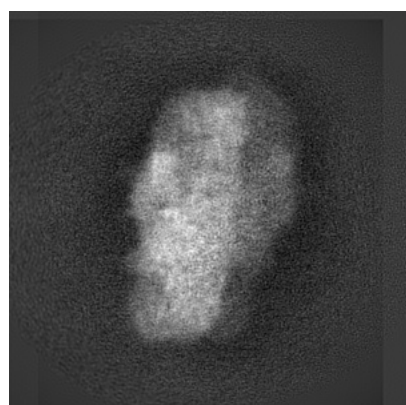
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13455. These allow visual inspection of the internal detail of the map and identification of artifacts.

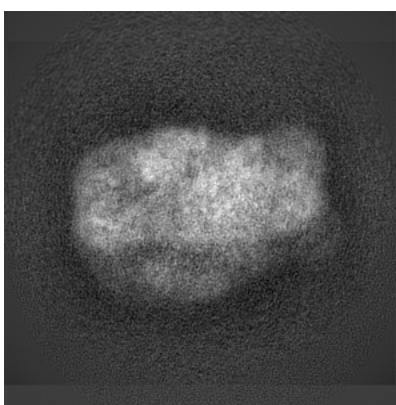
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

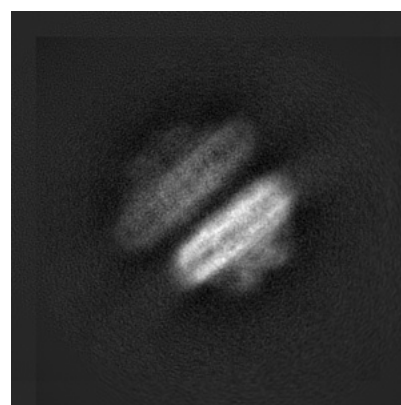
#### 6.1.1 Primary map



X



Y

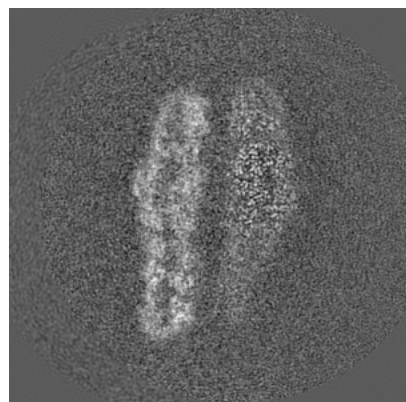


Z

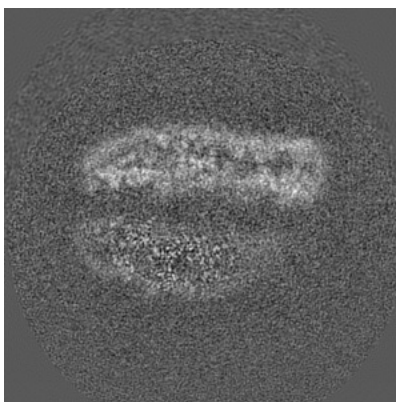
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

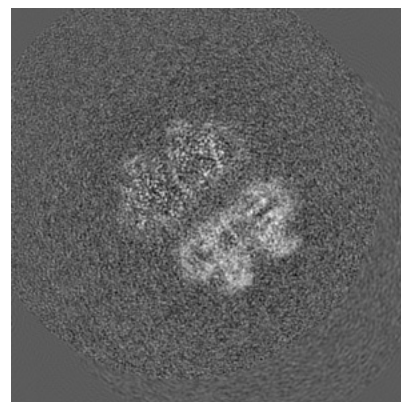
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

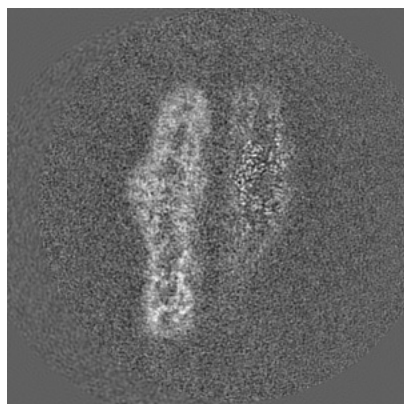


Z Index: 240

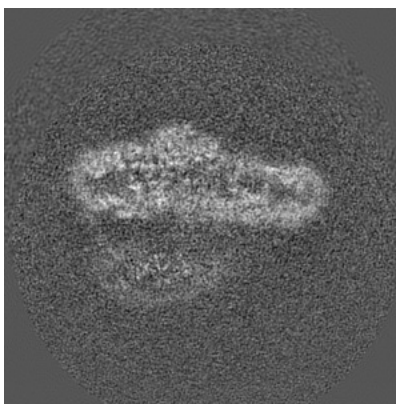
The images above show central slices of the map in three orthogonal directions.

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

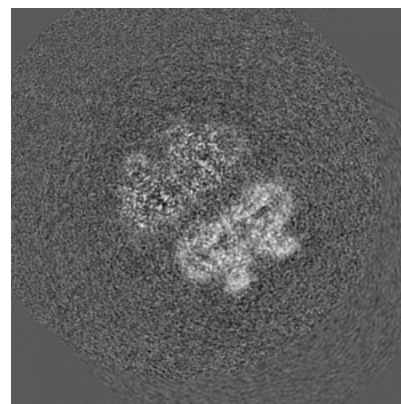
### 6.3.1 Primary map



X Index: 246



Y Index: 215

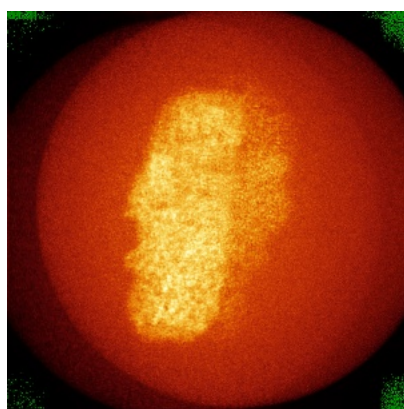


Z Index: 238

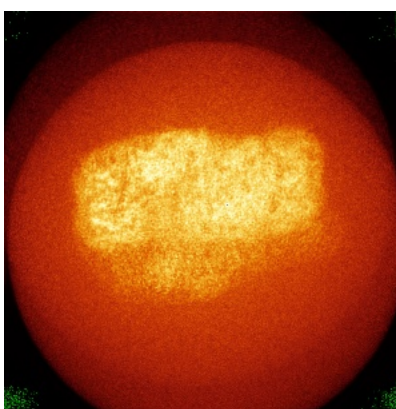
The images above show the largest variance slices of the map in three orthogonal directions.

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

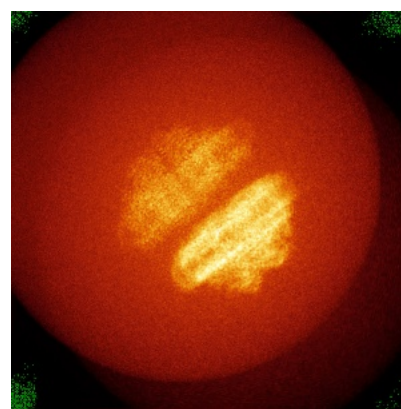
### 6.4.1 Primary map



X



Y

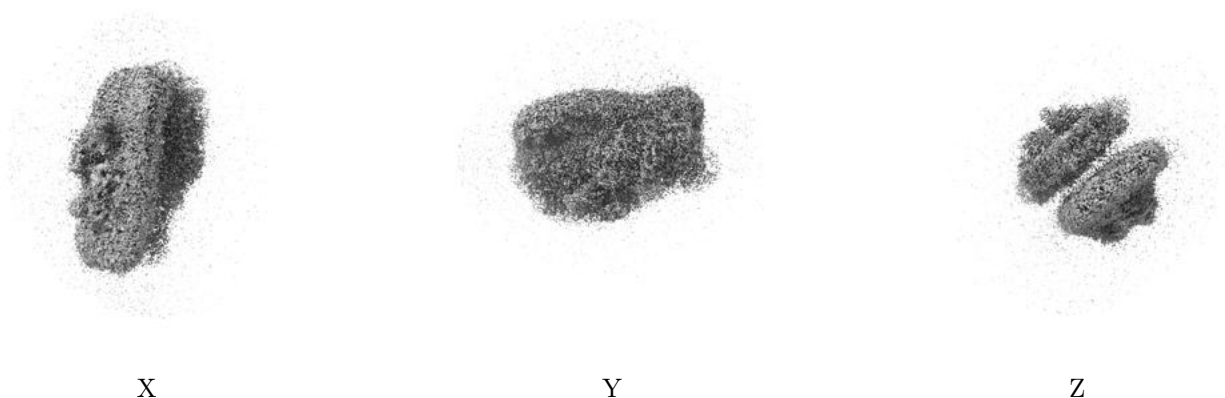


Z

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 0.0175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

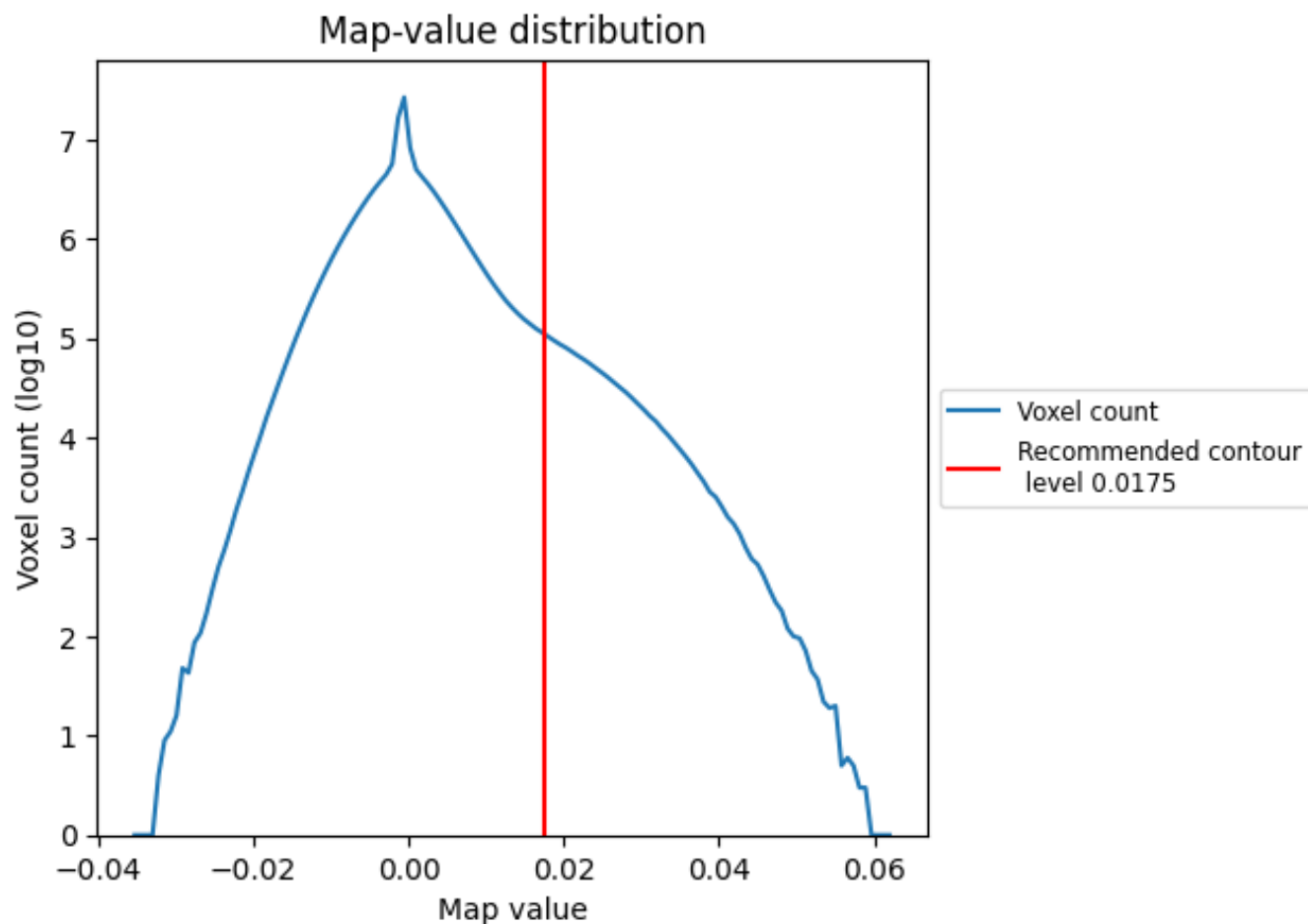
## 6.6 Mask visualisation [i](#)

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.

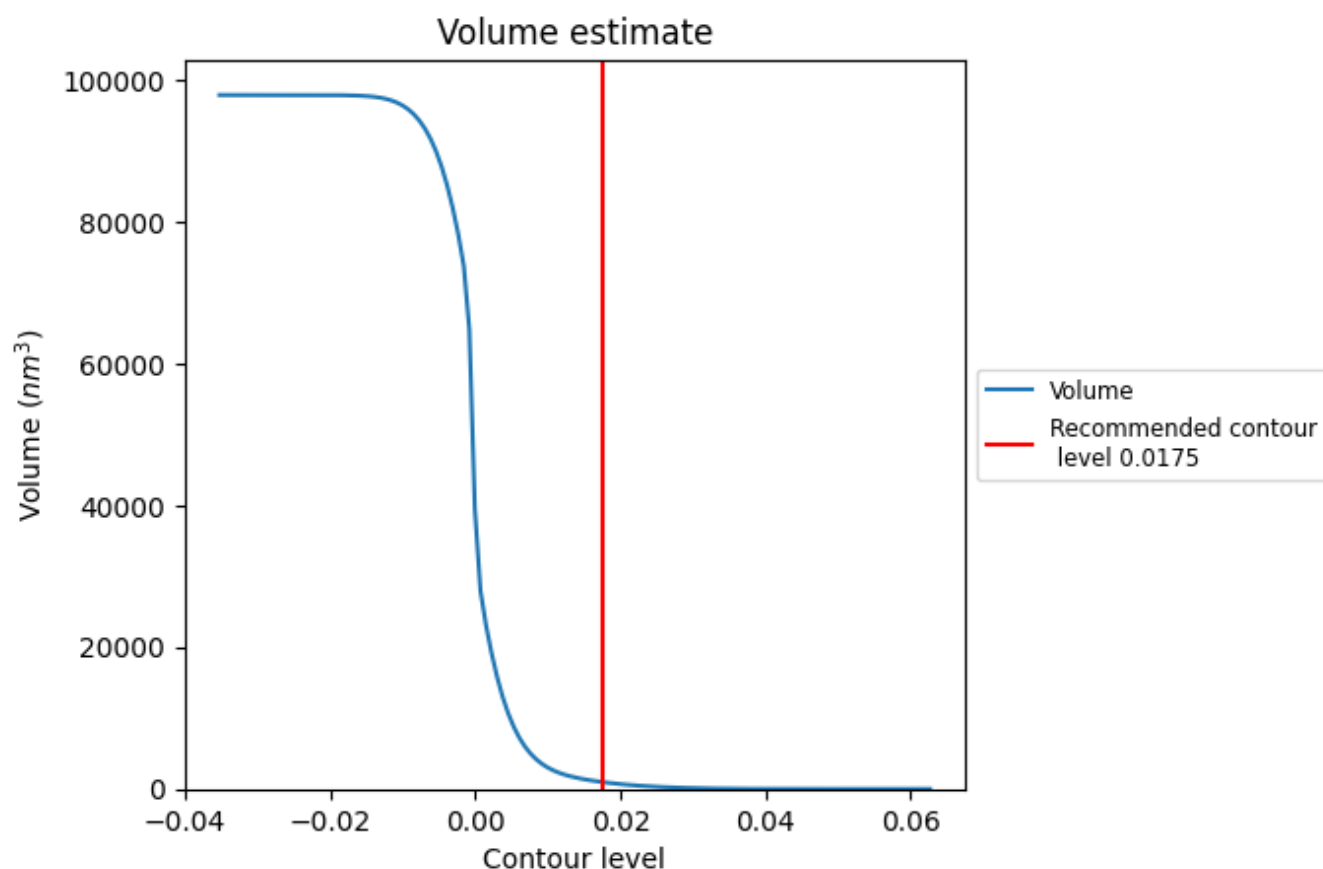
### 7.1 Map-value distribution [i](#)



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](#)

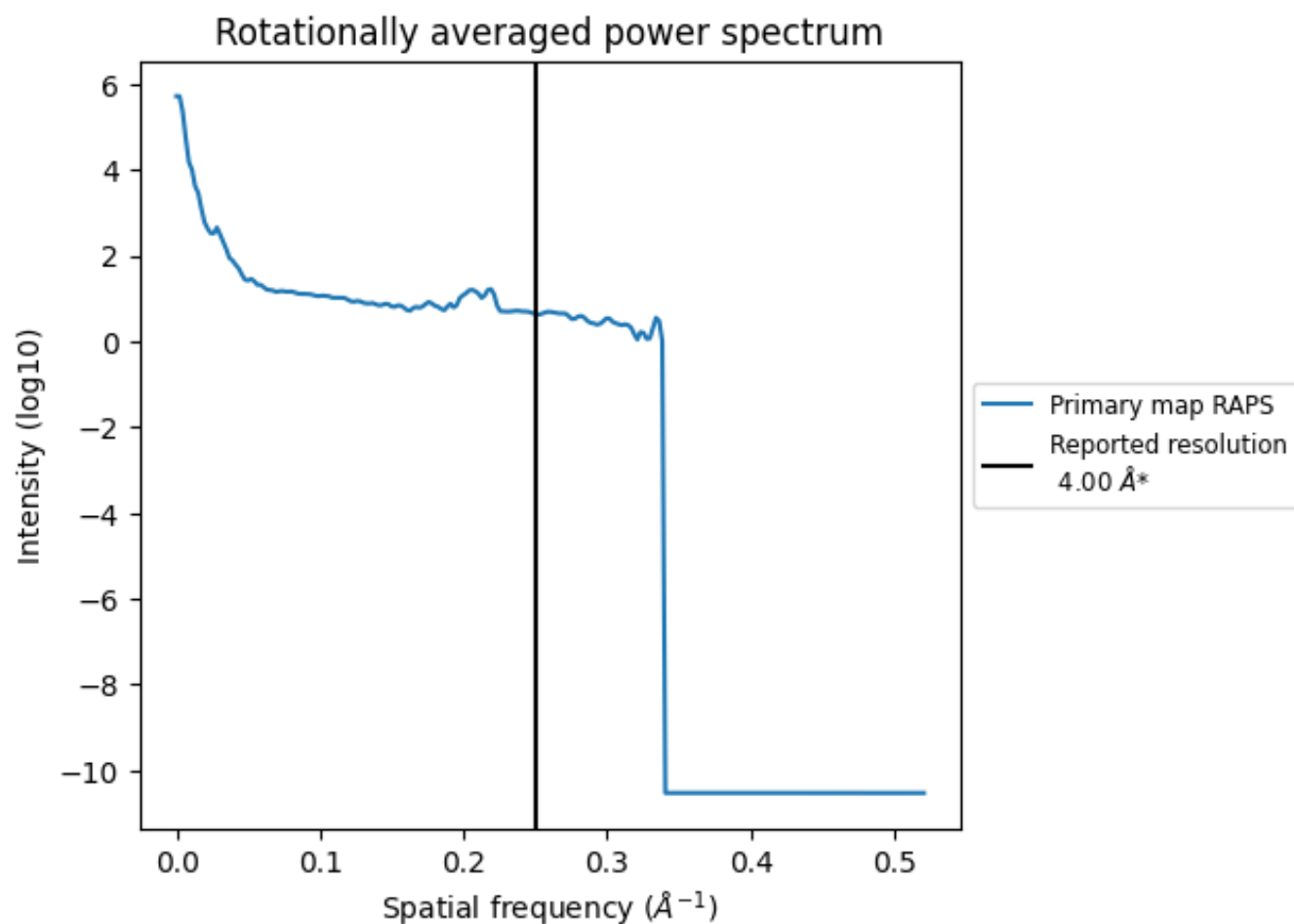


The volume at the recommended contour level is 976  $\text{nm}^3$ ; this corresponds to an approximate mass of 881 kDa.

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 ⓘ

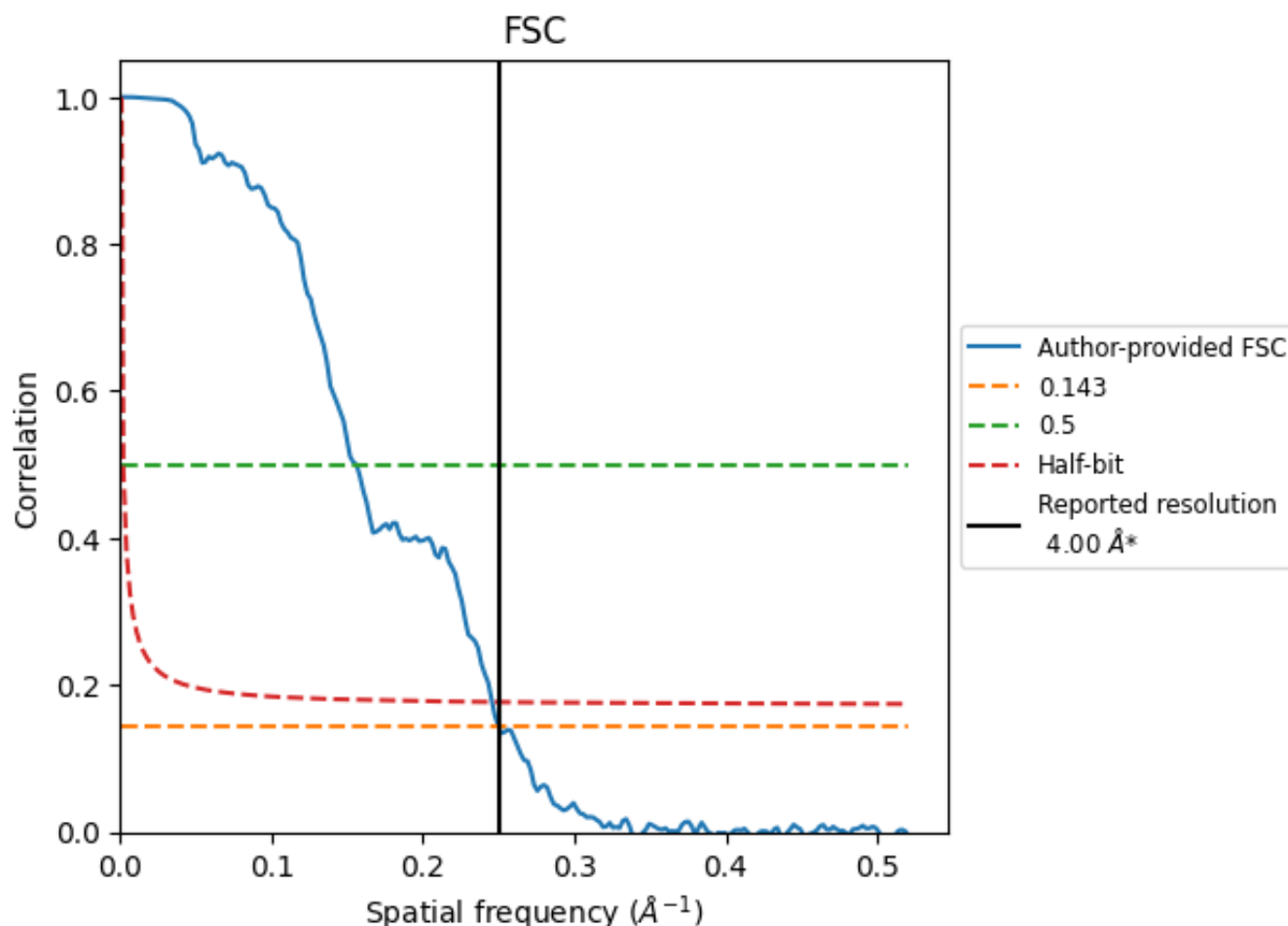


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

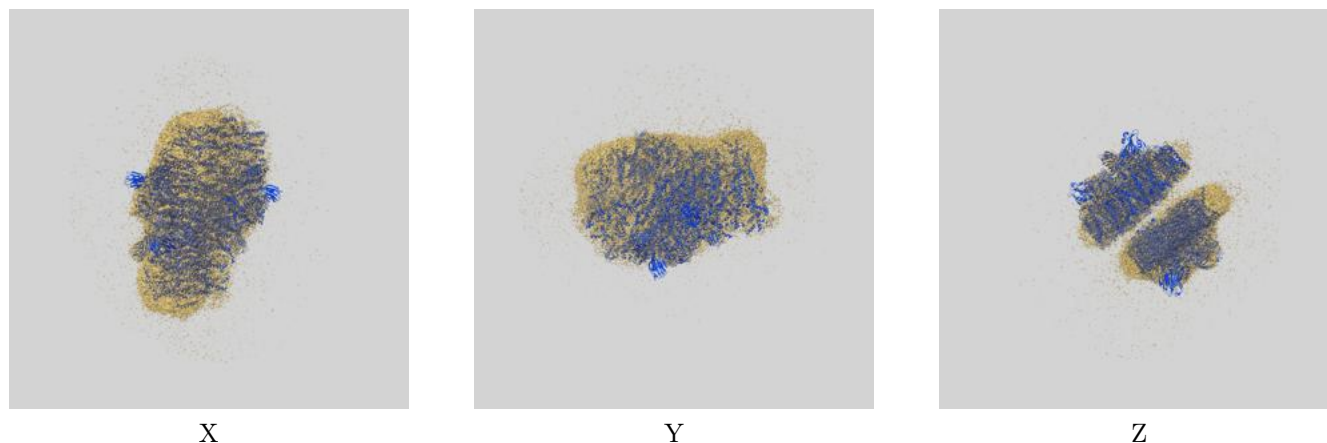
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	6.41	4.07
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

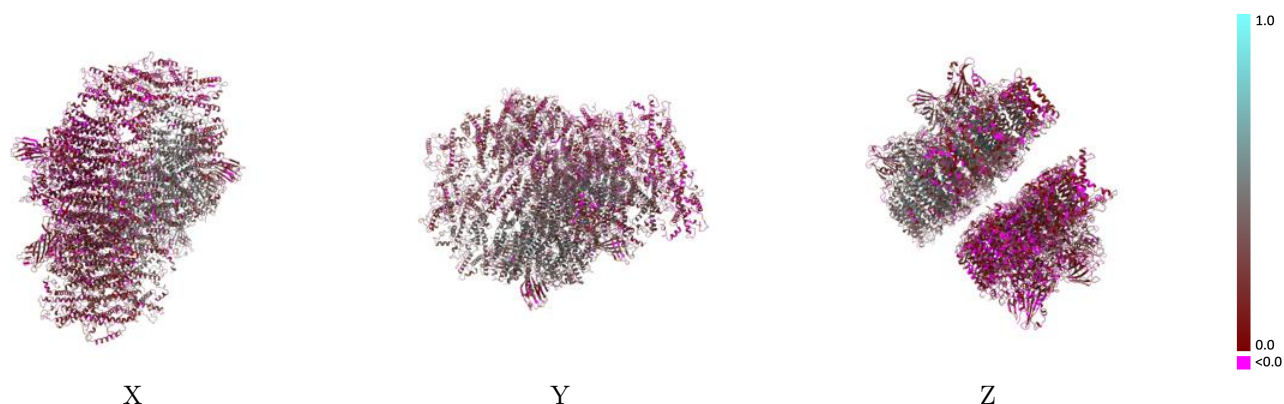
This section contains information regarding the fit between EMDB map EMD-13455 and PDB model 7PIW. Per-residue inclusion information can be found in section [3](#) on page [74](#).

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



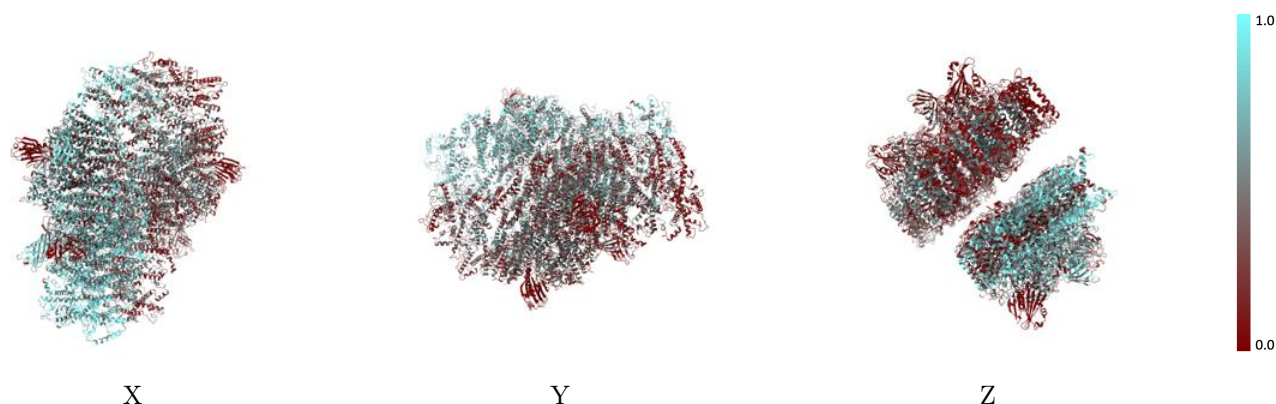
The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



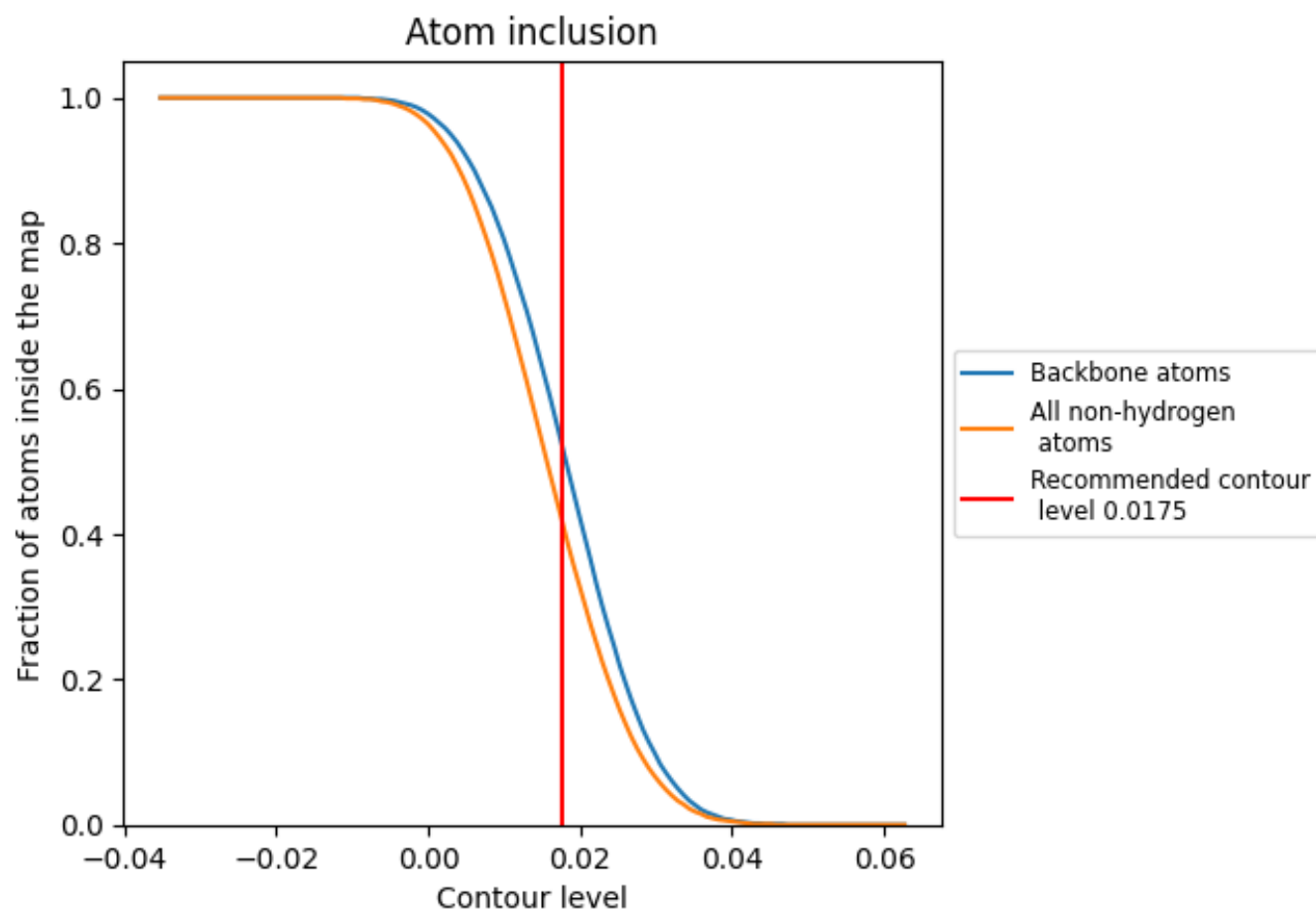
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0175).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 42% 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 (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4230	 0.2360
A	 0.4920	 0.4320
A1	 0.6120	 0.1910
B	 0.3740	 0.4030
B1	 0.5830	 0.1700
C	 0.4930	 0.4560
C1	 0.6260	 0.2020
D	 0.4420	 0.4380
D1	 0.5980	 0.1890
E	 0.3810	 0.3710
E1	 0.7460	 0.2080
F	 0.4090	 0.3800
F1	 0.7590	 0.2050
G	 0.1980	 0.2600
G1	 0.6690	 0.1600
H	 0.2980	 0.3500
H1	 0.5310	 0.1360
I	 0.4670	 0.4330
I1	 0.5400	 0.1970
J	 0.3820	 0.4050
J1	 0.5240	 0.1330
K	 0.4160	 0.4140
K1	 0.6510	 0.1960
L	 0.3520	 0.4110
L1	 0.4340	 0.1560
M	 0.3310	 0.3640
M1	 0.3820	 0.1470
N	 0.2960	 0.3340
N1	 0.6720	 0.1820
O	 0.2270	 0.3310
O1	 0.6070	 0.1800
P	 0.0180	 0.2020
P1	 0.0950	 0.1420
R	 0.1040	 0.1750
R1	 0.4660	 0.1110



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Chain	Atom inclusion	Q-score
S	 0.2680	 0.3030
S1	 0.6810	 0.1710
T	 0.3590	 0.4290
T1	 0.3960	 0.2160
U	 0.2200	 0.3330
U1	 0.5410	 0.2320
V	 0.3600	 0.3860
V1	 0.6090	 0.1950
W	 0.3150	 0.3650
W1	 0.6040	 0.2360
X	 0.2690	 0.2770
X1	 0.6270	 0.1450
Y	 0.3620	 0.3620
Y1	 0.6270	 0.1880
Z	 0.2730	 0.3710
Z1	 0.6530	 0.1750
a	 0.4670	 0.4160
a1	 0.4720	 0.1010
b	 0.3610	 0.3830
b1	 0.4930	 0.1120
c	 0.4000	 0.3630
c1	 0.4770	 0.0910
d	 0.4390	 0.4230
d1	 0.4440	 0.1090
e	 0.2430	 0.2560
e1	 0.4650	 0.1240
f	 0.3670	 0.3420
f1	 0.5450	 0.1770
g	 0.1420	 0.1520
g1	 0.5720	 0.0970
h	 0.2440	 0.3270
h1	 0.4570	 0.1090
i	 0.4500	 0.4350
i1	 0.4140	 0.1420
j	 0.2450	 0.3000
j1	 0.4380	 0.1210
k	 0.3480	 0.3170
k1	 0.4060	 0.0940
l	 0.3920	 0.4300
m	 0.2480	 0.3610
m1	 0.3740	 0.1220
n	 0.1660	 0.1610

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Chain	Atom inclusion	Q-score
n1	 0.5480	 0.1050
o	 0.2180	 0.2800
o1	 0.5320	 0.1330
p	 0.0080	 0.1570
p1	 0.0860	 0.0850
r	 0.1200	 0.1900
r1	 0.4780	 0.1150
s	 0.1610	 0.1410
s1	 0.4600	 0.0870
t	 0.3590	 0.3890
t1	 0.3090	 0.1070
u	 0.2060	 0.3570
u1	 0.4130	 0.1420
v	 0.2090	 0.2760
v1	 0.3330	 0.1020
w	 0.3360	 0.3470
w1	 0.4700	 0.1230
x	 0.2590	 0.2950
x1	 0.3830	 0.0660
y	 0.3310	 0.3270
y1	 0.5280	 0.1190
z	 0.1600	 0.1980
z1	 0.4240	 0.1280