



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 04:15 pm GMT

PDB ID : 5MDX
EMDB ID : EMD-3491
Title : Cryo-EM structure of the PSII supercomplex from *Arabidopsis thaliana*
Authors : van Bezouwen, L.S.; Caffarri, S.; Kale, R.S.; Kouril, R.; Thunnissen, A.M.W.H.; Oostergetel, G.T.; Boekema, E.J.
Deposited on : 2016-11-13
Resolution : 5.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

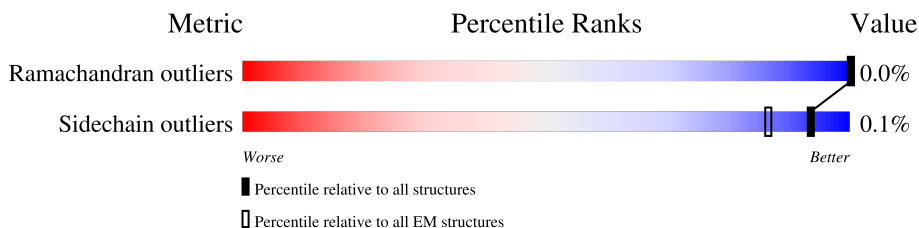
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.30 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	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	343	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin: 0;">14% 90% 10%</p>
1	a	343	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin: 0;">11% 96% .</p>
2	B	507	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin: 0;">8% 94% 6%</p>
2	b	507	<div style="display: flex; align-items: center;"> <div style="width: 30%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin: 0;">30% 94% 6%</p>
3	C	459	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin: 0;">6% 94% 6%</p>
3	c	459	<div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 93%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin: 0;">. 94% 6%</p>
4	D	352	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin: 0;">9% 95% . 5%</p>
4	d	352	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin: 0;">6% 95% . 5%</p>
5	E	83	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin: 0;">8% 87% 13%</p>

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Mol	Chain	Length	Quality of chain
5	e	83	7% 87% 13%
6	F	39	8% 74% 26%
6	f	39	8% 74% 26%
7	H	72	10% 72% 28%
7	h	72	10% 72% 28%
8	I	36	17% 97% 5%
8	i	36	11% 97% 5%
9	K	37	5% 97% 5%
9	k	37	11% 92% 5% 5%
10	L	38	11% 92% 5% 5%
10	l	38	6% 85% 15%
11	M	34	15% 82% 5% 15%
11	m	34	7% 77% 22%
12	O	247	7% 77% 22%
12	o	247	12% 88% 12%
13	T	33	18% 88% 12%
13	t	33	11% 85% 15%
14	W	54	7% 85% 15%
14	w	54	28% 72% 22%
15	X	116	8% 28% 72%
15	x	116	8% 28% 72%
16	Z	62	8% 98% 5%
16	z	62	6% 98% 5%
17	R	250	18% 75% 25%
17	r	250	18% 75% 25%

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Mol	Chain	Length	Quality of chain
18	S	232	
18	s	232	
19	1	224	
19	2	224	
19	3	224	
19	5	224	
19	6	224	
19	7	224	
19	G	224	
19	N	224	
19	Y	224	
19	g	224	
19	n	224	
19	y	224	
20	4	210	
20	8	210	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	2	602	X	-	-	-
22	CLA	2	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	604	X	-	-	-
22	CLA	2	609	X	-	-	-
22	CLA	2	610	X	-	-	-
22	CLA	2	611	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	2	613	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	-	-
22	CLA	3	313	X	-	-	-
22	CLA	3	314	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	613	X	-	-	-
22	CLA	5	614	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	613	X	-	-	-
22	CLA	7	303	X	-	-	-
22	CLA	7	304	X	-	-	-
22	CLA	7	305	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	7	314	X	-	-	-
22	CLA	8	302	X	-	-	-
22	CLA	8	303	X	-	-	-
22	CLA	8	304	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	G	602	X	-	-	-
22	CLA	G	603	X	-	-	-
22	CLA	G	604	X	-	-	-
22	CLA	G	610	X	-	-	-
22	CLA	G	611	X	-	-	-
22	CLA	G	612	X	-	-	-
22	CLA	G	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	G	614	X	-	-	-
22	CLA	N	602	X	-	-	-
22	CLA	N	603	X	-	-	-
22	CLA	N	604	X	-	-	-
22	CLA	N	610	X	-	-	-
22	CLA	N	611	X	-	-	-
22	CLA	N	612	X	-	-	-
22	CLA	N	613	X	-	-	-
22	CLA	N	614	X	-	-	-
22	CLA	R	301	X	-	-	-
22	CLA	R	302	X	-	-	-
22	CLA	R	303	X	-	-	-
22	CLA	R	307	X	-	-	-
22	CLA	R	308	X	-	-	-
22	CLA	R	309	X	-	-	-
22	CLA	R	310	X	-	-	-
22	CLA	R	311	X	-	-	-
22	CLA	R	312	X	-	-	-
22	CLA	S	301	X	-	-	-
22	CLA	S	303	X	-	-	-
22	CLA	S	304	X	-	-	-
22	CLA	S	305	X	-	-	-
22	CLA	S	309	X	-	-	-
22	CLA	S	310	X	-	-	-
22	CLA	S	311	X	-	-	-
22	CLA	S	312	X	-	-	-
22	CLA	S	313	X	-	-	-
22	CLA	S	314	X	-	-	-
22	CLA	Y	602	X	-	-	-
22	CLA	Y	603	X	-	-	-
22	CLA	Y	604	X	-	-	-
22	CLA	Y	610	X	-	-	-
22	CLA	Y	611	X	-	-	-
22	CLA	Y	612	X	-	-	-
22	CLA	Y	613	X	-	-	-
22	CLA	Y	614	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	g	602	X	-	-	-
22	CLA	g	603	X	-	-	-
22	CLA	g	604	X	-	-	-
22	CLA	g	610	X	-	-	-
22	CLA	g	611	X	-	-	-
22	CLA	g	612	X	-	-	-
22	CLA	g	613	X	-	-	-
22	CLA	g	614	X	-	-	-
22	CLA	n	602	X	-	-	-
22	CLA	n	603	X	-	-	-
22	CLA	n	604	X	-	-	-
22	CLA	n	610	X	-	-	-
22	CLA	n	611	X	-	-	-
22	CLA	n	612	X	-	-	-
22	CLA	n	613	X	-	-	-
22	CLA	n	614	X	-	-	-
22	CLA	r	301	X	-	-	-
22	CLA	r	302	X	-	-	-
22	CLA	r	303	X	-	-	-
22	CLA	r	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	r	308	X	-	-	-
22	CLA	r	309	X	-	-	-
22	CLA	r	310	X	-	-	-
22	CLA	r	311	X	-	-	-
22	CLA	r	312	X	-	-	-
22	CLA	s	301	X	-	-	-
22	CLA	s	303	X	-	-	-
22	CLA	s	304	X	-	-	-
22	CLA	s	305	X	-	-	-
22	CLA	s	309	X	-	-	-
22	CLA	s	310	X	-	-	-
22	CLA	s	311	X	-	-	-
22	CLA	s	312	X	-	-	-
22	CLA	s	313	X	-	-	-
22	CLA	s	314	X	-	-	-
22	CLA	y	602	X	-	-	-
22	CLA	y	603	X	-	-	-
22	CLA	y	604	X	-	-	-
22	CLA	y	610	X	-	-	-
22	CLA	y	611	X	-	-	-
22	CLA	y	612	X	-	-	-
22	CLA	y	613	X	-	-	-
22	CLA	y	614	X	-	-	-
25	CHL	1	601	X	-	-	-
25	CHL	1	605	X	-	-	-
25	CHL	1	606	X	-	-	-
25	CHL	1	607	X	-	-	-
25	CHL	1	608	X	-	-	-
25	CHL	1	609	X	-	-	-
25	CHL	1	615	X	-	-	-
25	CHL	2	601	X	-	-	-
25	CHL	2	605	X	-	-	-
25	CHL	2	606	X	-	-	-
25	CHL	2	607	X	-	-	-
25	CHL	2	608	X	-	-	-
25	CHL	3	301	X	-	-	-
25	CHL	3	302	X	-	-	-
25	CHL	3	306	X	-	-	-
25	CHL	3	307	X	-	-	-
25	CHL	3	308	X	-	-	-
25	CHL	3	309	X	-	-	-
25	CHL	4	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	4	305	X	-	-	-
25	CHL	4	306	X	-	-	-
25	CHL	4	307	X	-	-	-
25	CHL	4	308	X	-	-	-
25	CHL	5	601	X	-	-	-
25	CHL	5	605	X	-	-	-
25	CHL	5	606	X	-	-	-
25	CHL	5	607	X	-	-	-
25	CHL	5	608	X	-	-	-
25	CHL	5	609	X	-	-	-
25	CHL	5	615	X	-	-	-
25	CHL	6	601	X	-	-	-
25	CHL	6	605	X	-	-	-
25	CHL	6	606	X	-	-	-
25	CHL	6	607	X	-	-	-
25	CHL	6	608	X	-	-	-
25	CHL	7	301	X	-	-	-
25	CHL	7	302	X	-	-	-
25	CHL	7	306	X	-	-	-
25	CHL	7	307	X	-	-	-
25	CHL	7	308	X	-	-	-
25	CHL	7	309	X	-	-	-
25	CHL	8	301	X	-	-	-
25	CHL	8	305	X	-	-	-
25	CHL	8	306	X	-	-	-
25	CHL	8	307	X	-	-	-
25	CHL	8	308	X	-	-	-
25	CHL	G	601	X	-	-	-
25	CHL	G	605	X	-	-	-
25	CHL	G	606	X	-	-	-
25	CHL	G	607	X	-	-	-
25	CHL	G	608	X	-	-	-
25	CHL	G	609	X	-	-	-
25	CHL	N	601	X	-	-	-
25	CHL	N	605	X	-	-	-
25	CHL	N	606	X	-	-	-
25	CHL	N	607	X	-	-	-
25	CHL	N	608	X	-	-	-
25	CHL	N	609	X	-	-	-
25	CHL	R	304	X	-	-	-
25	CHL	R	305	X	-	-	-
25	CHL	R	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	S	302	X	-	-	-
25	CHL	S	306	X	-	-	-
25	CHL	S	307	X	-	-	-
25	CHL	S	308	X	-	-	-
25	CHL	Y	601	X	-	-	-
25	CHL	Y	605	X	-	-	-
25	CHL	Y	606	X	-	-	-
25	CHL	Y	607	X	-	-	-
25	CHL	Y	608	X	-	-	-
25	CHL	Y	609	X	-	-	-
25	CHL	g	601	X	-	-	-
25	CHL	g	605	X	-	-	-
25	CHL	g	606	X	-	-	-
25	CHL	g	607	X	-	-	-
25	CHL	g	608	X	-	-	-
25	CHL	g	609	X	-	-	-
25	CHL	n	601	X	-	-	-
25	CHL	n	605	X	-	-	-
25	CHL	n	606	X	-	-	-
25	CHL	n	607	X	-	-	-
25	CHL	n	608	X	-	-	-
25	CHL	n	609	X	-	-	-
25	CHL	r	304	X	-	-	-
25	CHL	r	305	X	-	-	-
25	CHL	r	306	X	-	-	-
25	CHL	s	302	X	-	-	-
25	CHL	s	306	X	-	-	-
25	CHL	s	307	X	-	-	-
25	CHL	s	308	X	-	-	-
25	CHL	y	601	X	-	-	-
25	CHL	y	605	X	-	-	-
25	CHL	y	606	X	-	-	-
25	CHL	y	607	X	-	-	-
25	CHL	y	608	X	-	-	-
25	CHL	y	609	X	-	-	-

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 78324 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
			Total	C	N	O	S		
1	A	308	Total	C	N	O	S	0	0
			2388	1558	392	426	12		
1	a	330	Total	C	N	O	S	0	0
			2584	1688	426	457	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	478	Total	C	N	O	S	0	0
			3752	2459	635	646	12		
2	b	478	Total	C	N	O	S	0	0
			3752	2459	635	646	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		
3	c	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	336	Total	C	N	O	S	0	0
			2675	1770	438	455	12		
4	d	336	Total	C	N	O	S	0	0
			2675	1770	438	455	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	72	Total	C	N	O	0	0
			586	386	93	107		
5	e	72	Total	C	N	O	0	0
			586	386	93	107		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	29	Total	C	N	O	S	0	0
			224	147	40	36	1		
6	f	29	Total	C	N	O	S	0	0
			224	147	40	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	52	Total	C	N	O	S	0	0
			389	257	61	69	2		
7	h	52	Total	C	N	O	S	0	0
			389	257	61	69	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			286	195	44	46	1		
8	i	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	36	Total	C	N	O	S	0	0
			290	205	40	44	1		
9	k	36	Total	C	N	O	S	0	0
			290	205	40	44	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	36	Total	C	N	O	0	0
			302	200	47	55		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	l	36	302	200	47	55	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	M	29	226	158	32	36	0	0
11	m	29	226	158	32	36	0	0

- Molecule 12 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	O	193	1487	951	235	297	4	0	0
12	o	193	1487	951	235	297	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	T	29	239	168	33	37	1	0	0
13	t	29	239	168	33	37	1	0	0

- Molecule 14 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	W	46	372	247	53	71	1	0	0
14	w	46	372	247	53	71	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	X	32	226	149	35	42	0	0
15	x	32	226	149	35	42	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Z	61	458	310	68	79	1	0	0
16	z	61	458	310	68	79	1	0	0

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	188	1459	953	238	265	3	0	0
17	r	188	1459	953	238	265	3	0	0

- Molecule 18 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	214	1653	1082	270	297	4	0	0
18	s	214	1653	1082	270	297	4	0	0

- Molecule 19 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	G	219	1666	1078	273	310	5	0	0
19	N	219	1666	1078	273	310	5	0	0
19	Y	219	1666	1078	273	310	5	0	0
19	g	219	1666	1078	273	310	5	0	0
19	n	219	1666	1078	273	310	5	0	0
19	y	219	1666	1078	273	310	5	0	0
19	1	219	1666	1078	273	310	5	0	0
19	2	219	1666	1078	273	310	5	0	0
19	3	219	1666	1078	273	310	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	5	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	6	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	7	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

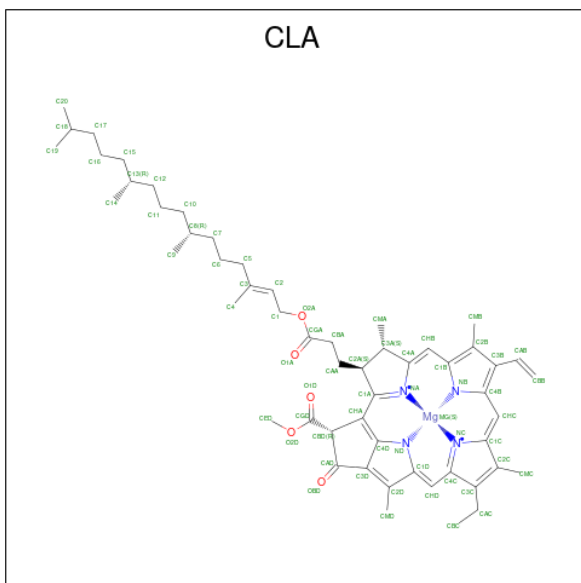
- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		
20	8	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	A	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	A	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	C	1	540	420	12	48	60	0
22	C	1	540	420	12	48	60	0
22	C	1	540	420	12	48	60	0
22	C	1	540	420	12	48	60	0
22	C	1	540	420	12	48	60	0
22	C	1	540	420	12	48	60	0
22	C	1	540	420	12	48	60	0
22	C	1	540	420	12	48	60	0
22	C	1	540	420	12	48	60	0
22	D	1	135	105	3	12	15	0
22	D	1	135	105	3	12	15	0
22	D	1	135	105	3	12	15	0
22	a	1	135	105	3	12	15	0
22	a	1	135	105	3	12	15	0
22	a	1	135	105	3	12	15	0
22	b	1	720	560	16	64	80	0
22	b	1	720	560	16	64	80	0
22	b	1	720	560	16	64	80	0
22	b	1	720	560	16	64	80	0
22	b	1	720	560	16	64	80	0
22	b	1	720	560	16	64	80	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	b	1	Total 720	C 560	Mg 16	N 64	O 80	0
22	d	1	Total 135	C 105	Mg 3	N 12	O 15	0
22	d	1	Total 135	C 105	Mg 3	N 12	O 15	0
22	d	1	Total 135	C 105	Mg 3	N 12	O 15	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	c	1	Total 540	C 420	Mg 12	N 48	O 60	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	R	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0

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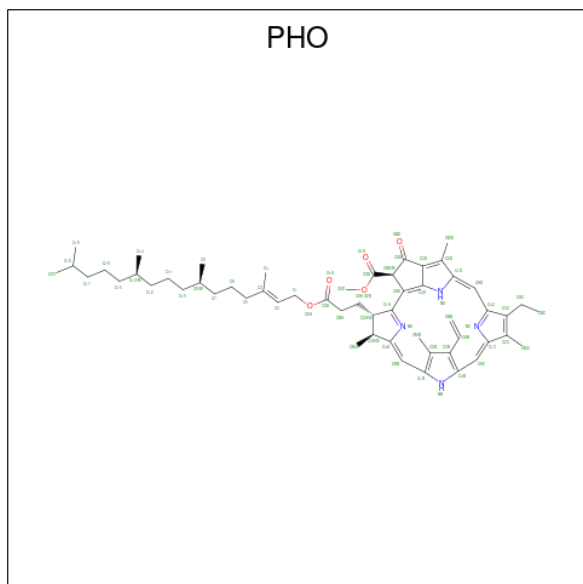
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	8	1	225	175	5	20	25	0

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



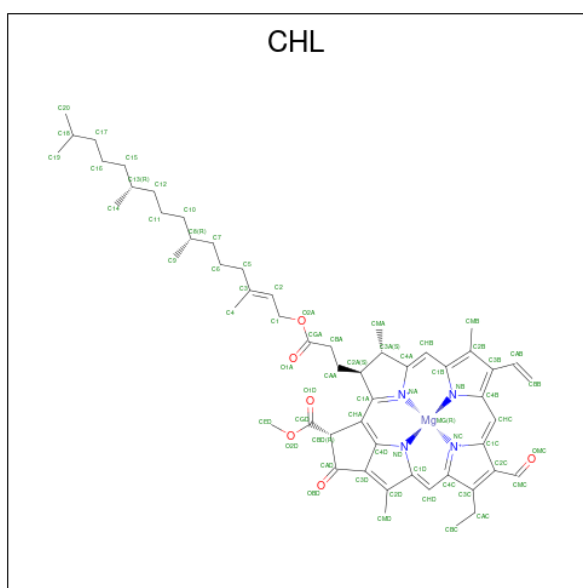
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
23	A	1	44	35	4	5	0
23	D	1	44	35	4	5	0
23	a	1	44	35	4	5	0
23	d	1	44	35	4	5	0

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
24	E	1	43	34	1	4	4	0
24	e	1	43	34	1	4	4	0

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
25	R	1	138	105	3	12	18	0
25	R	1	138	105	3	12	18	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	R	1	Total 138	C 105	Mg 3	N 12	O 18	0
25	S	1	Total 184	C 140	Mg 4	N 16	O 24	0
25	S	1	Total 184	C 140	Mg 4	N 16	O 24	0
25	S	1	Total 184	C 140	Mg 4	N 16	O 24	0
25	S	1	Total 184	C 140	Mg 4	N 16	O 24	0
25	G	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	G	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	G	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	G	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	G	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	G	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	N	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	N	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	N	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	N	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	N	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	N	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	N	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	Y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	Y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	Y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	Y	1	Total 272	C 208	Mg 6	N 24	O 34	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	Y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	Y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	r	1	Total 138	C 105	Mg 3	N 12	O 18	0
25	r	1	Total 138	C 105	Mg 3	N 12	O 18	0
25	r	1	Total 138	C 105	Mg 3	N 12	O 18	0
25	s	1	Total 184	C 140	Mg 4	N 16	O 24	0
25	s	1	Total 184	C 140	Mg 4	N 16	O 24	0
25	s	1	Total 184	C 140	Mg 4	N 16	O 24	0
25	s	1	Total 184	C 140	Mg 4	N 16	O 24	0
25	g	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	g	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	g	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	g	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	g	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	g	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	n	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	n	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	n	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	n	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	n	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	n	1	Total 272	C 208	Mg 6	N 24	O 34	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	y	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	1	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	2	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	2	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	2	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	2	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	2	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	3	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	3	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	3	1	Total 272	C 208	Mg 6	N 24	O 34	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	3	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	3	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	3	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	4	1	Total 230	C 175	Mg 5	N 20	O 30	0
25	4	1	Total 230	C 175	Mg 5	N 20	O 30	0
25	4	1	Total 230	C 175	Mg 5	N 20	O 30	0
25	4	1	Total 230	C 175	Mg 5	N 20	O 30	0
25	4	1	Total 230	C 175	Mg 5	N 20	O 30	0
25	5	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	5	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	5	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	5	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	5	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	5	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	5	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	5	1	Total 318	C 243	Mg 7	N 28	O 40	0
25	6	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	6	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	6	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	6	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	6	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	6	1	Total 226	C 173	Mg 5	N 20	O 28	0
25	7	1	Total 272	C 208	Mg 6	N 24	O 34	0

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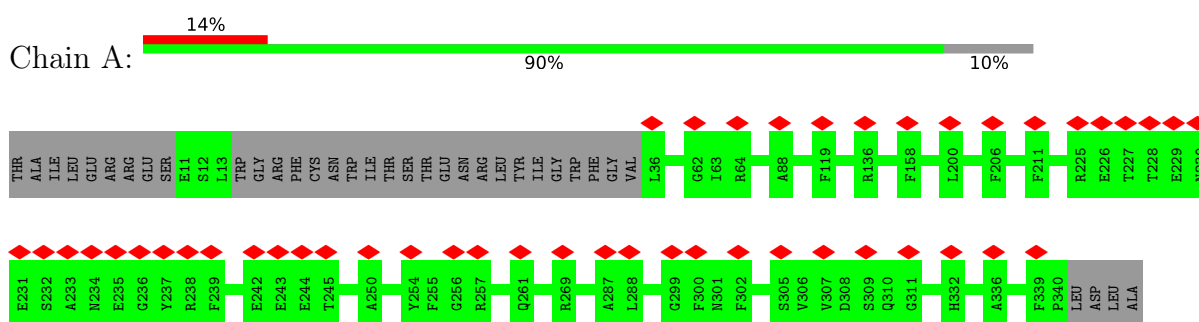
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
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25	7	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	7	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	7	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	7	1	Total 272	C 208	Mg 6	N 24	O 34	0
25	8	1	Total 230	C 175	Mg 5	N 20	O 30	0
25	8	1	Total 230	C 175	Mg 5	N 20	O 30	0
25	8	1	Total 230	C 175	Mg 5	N 20	O 30	0
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25	8	1	Total 230	C 175	Mg 5	N 20	O 30	0

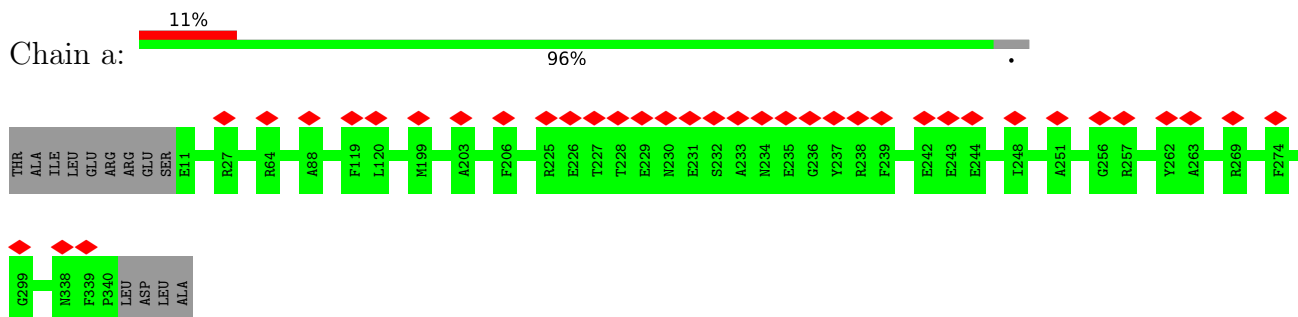
3 Residue-property plots [i](#)

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

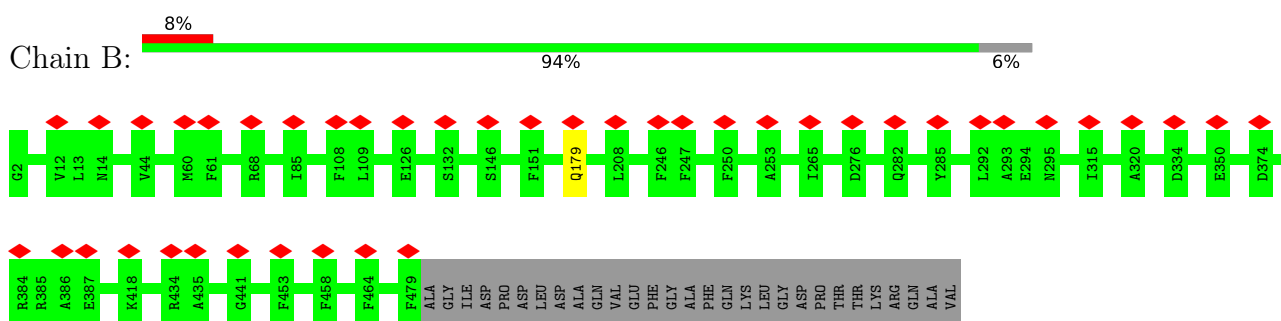
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

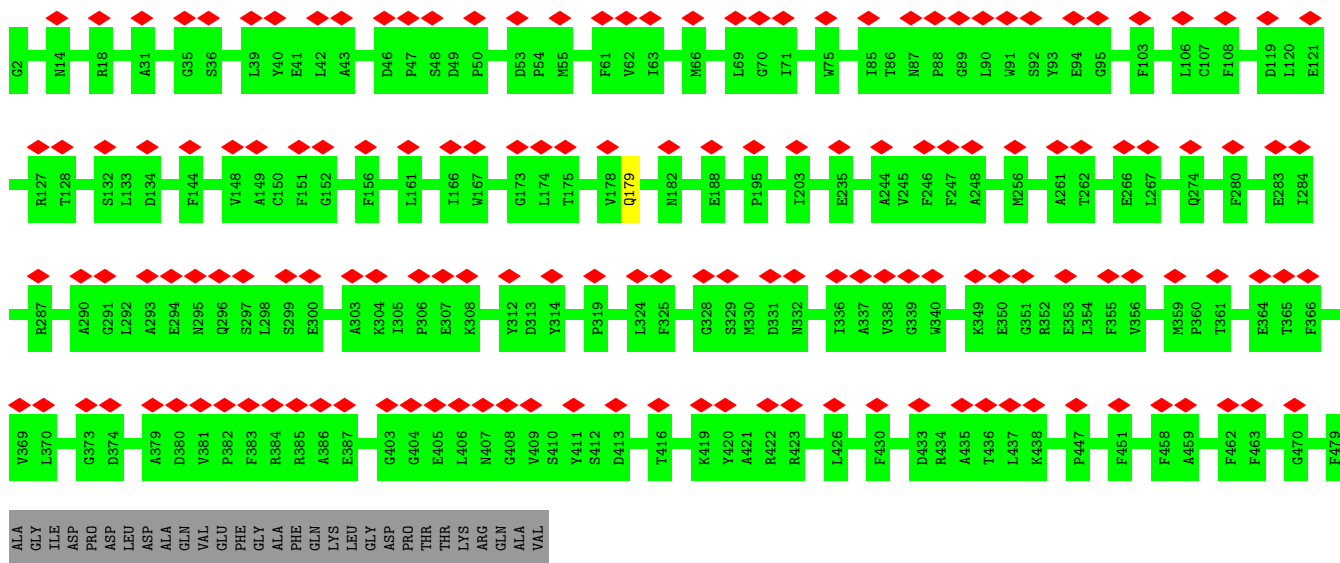


- Molecule 2: Photosystem II CP47 reaction center protein

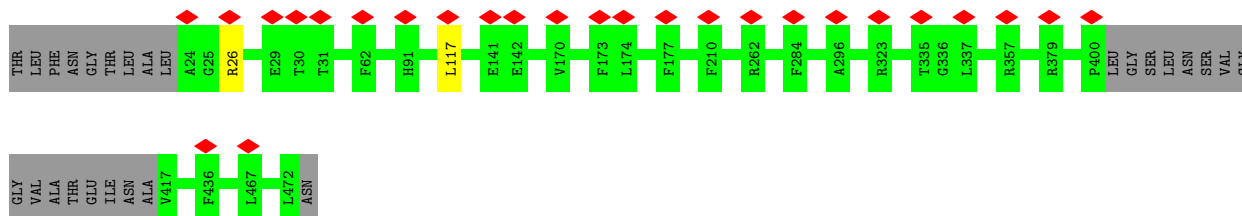


- Molecule 2: Photosystem II CP47 reaction center protein

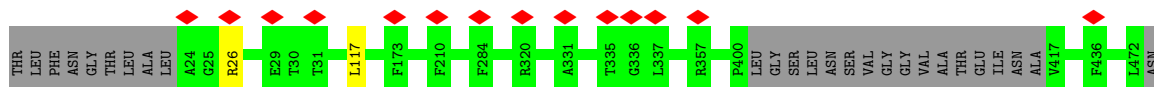




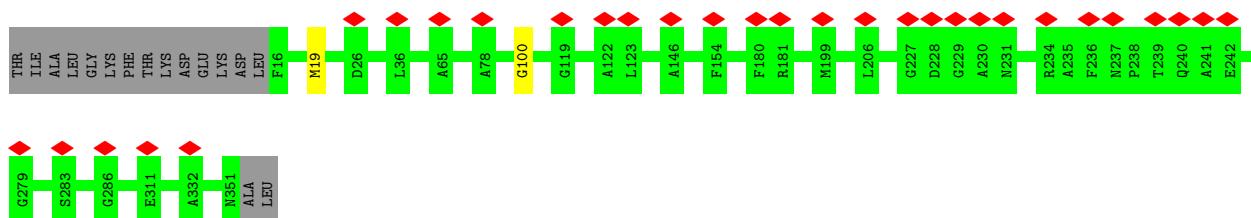
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

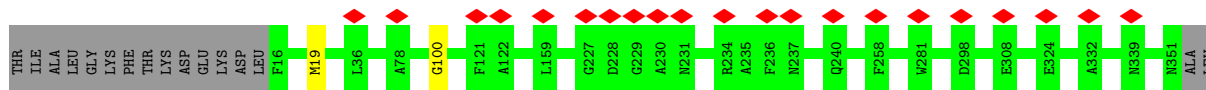


• Molecule 4: Photosystem II D2 protein

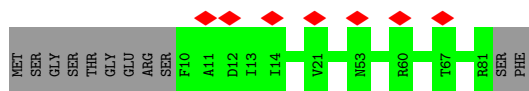
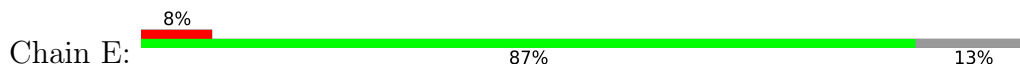


• Molecule 4: Photosystem II D2 protein

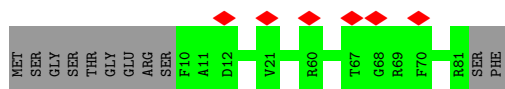
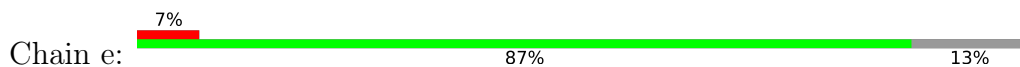




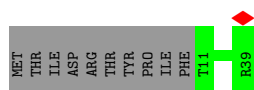
• Molecule 5: Cytochrome b559 subunit alpha



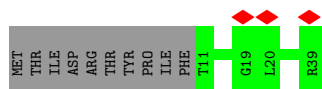
• Molecule 5: Cytochrome b559 subunit alpha



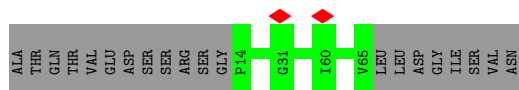
• Molecule 6: Cytochrome b559 subunit beta (PsbF)



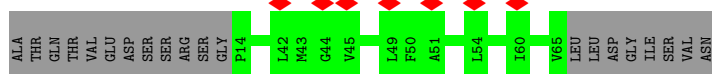
• Molecule 6: Cytochrome b559 subunit beta (PsbF)



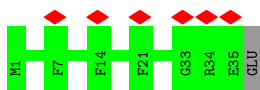
• Molecule 7: Photosystem II reaction center protein H



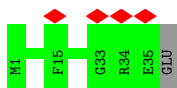
• Molecule 7: Photosystem II reaction center protein H



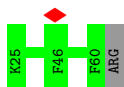
• Molecule 8: Photosystem II reaction center protein I



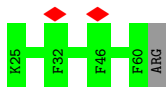
- Molecule 8: Photosystem II reaction center protein I



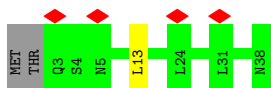
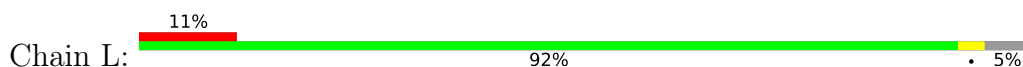
- Molecule 9: Photosystem II reaction center protein K



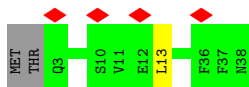
- Molecule 9: Photosystem II reaction center protein K



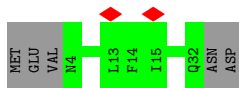
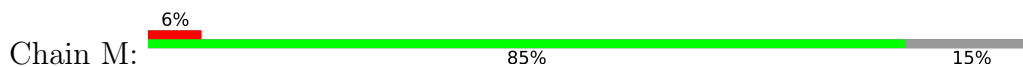
- Molecule 10: Photosystem II reaction center protein L



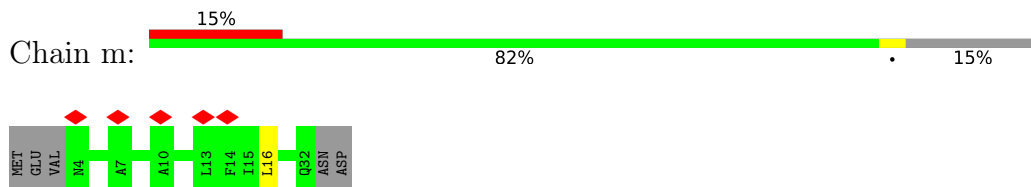
- Molecule 10: Photosystem II reaction center protein L



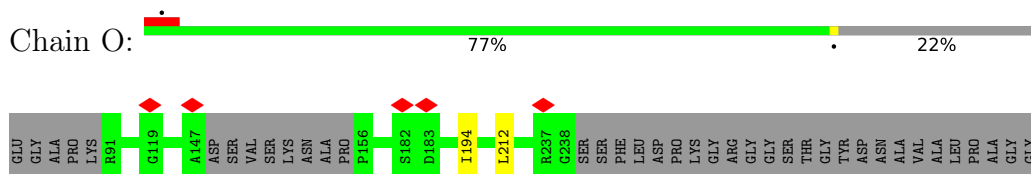
- Molecule 11: Photosystem II reaction center protein M



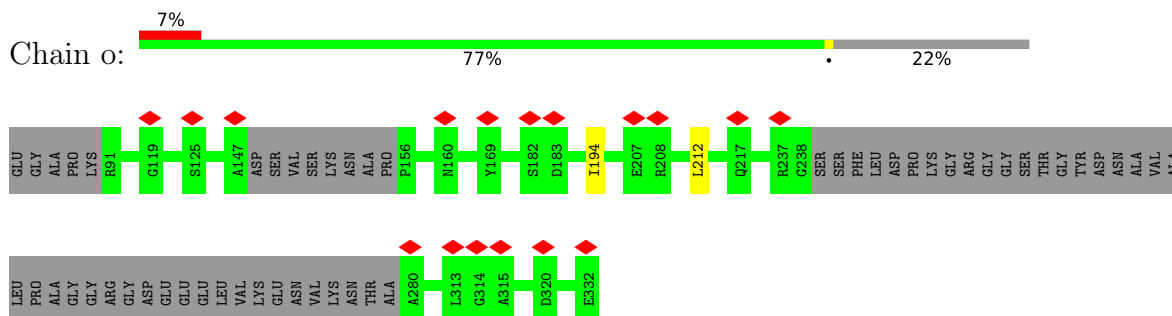
- Molecule 11: Photosystem II reaction center protein M



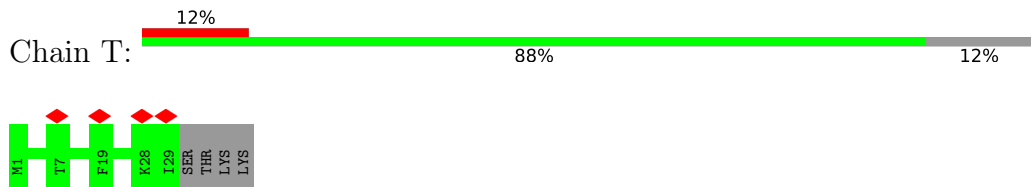
- Molecule 12: Oxygen-evolving enhancer protein 1-1, chloroplastic



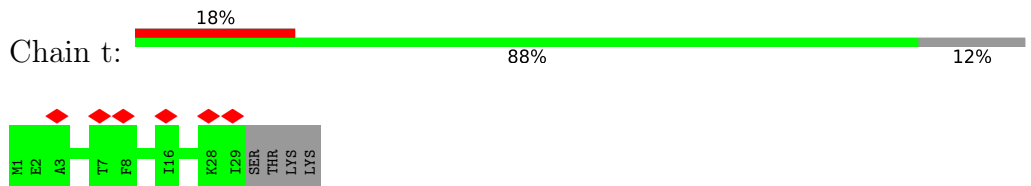
- Molecule 12: Oxygen-evolving enhancer protein 1-1, chloroplastic



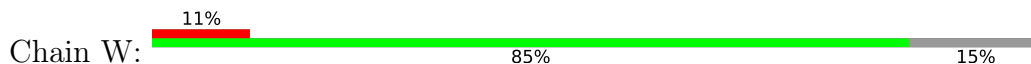
- Molecule 13: Photosystem II reaction center protein T

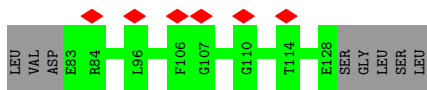


- Molecule 13: Photosystem II reaction center protein T

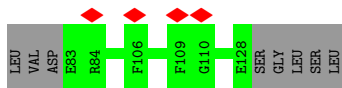
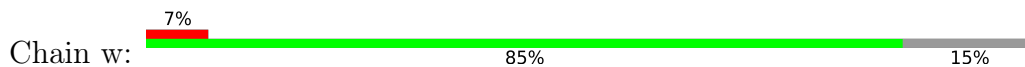


- Molecule 14: Photosystem II reaction center W protein, chloroplastic

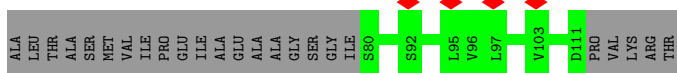
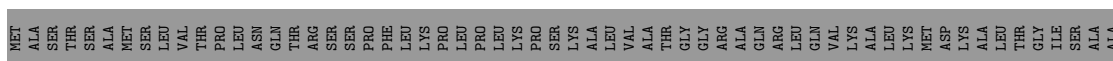




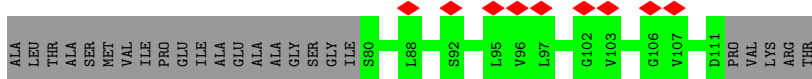
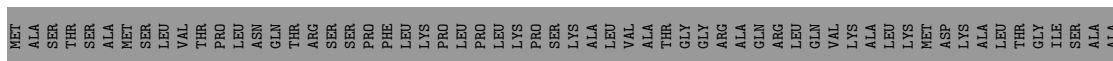
- Molecule 14: Photosystem II reaction center W protein, chloroplastic



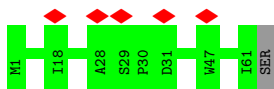
- Molecule 15: Photosystem II reaction center protein X



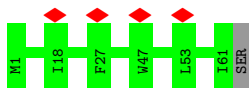
- Molecule 15: Photosystem II reaction center protein X



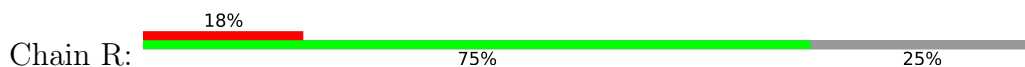
- Molecule 16: Photosystem II reaction center protein Z

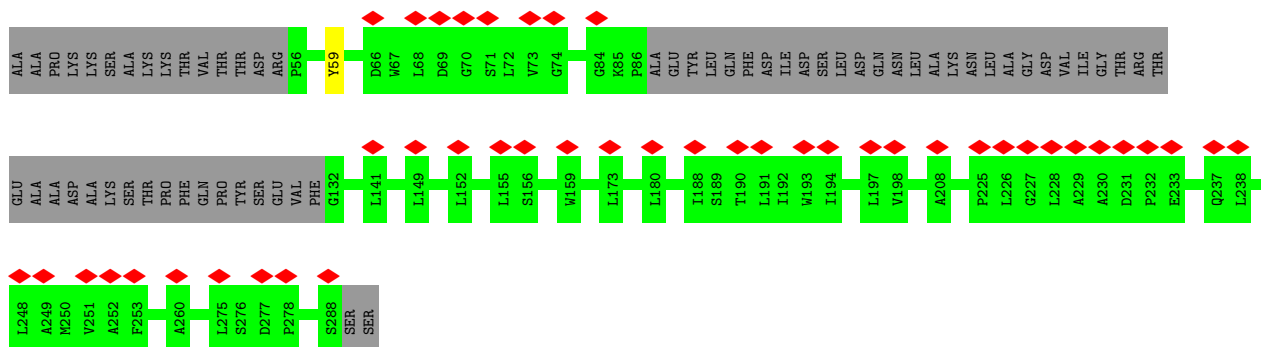


- Molecule 16: Photosystem II reaction center protein Z

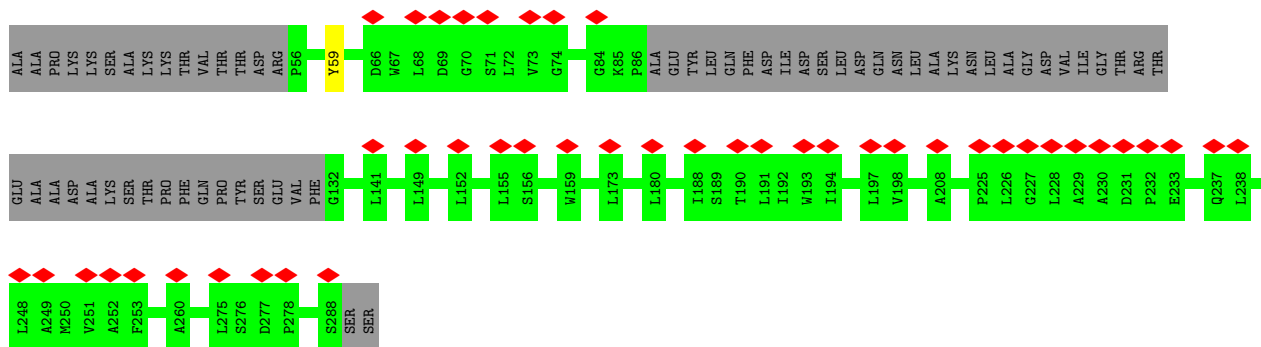


- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic

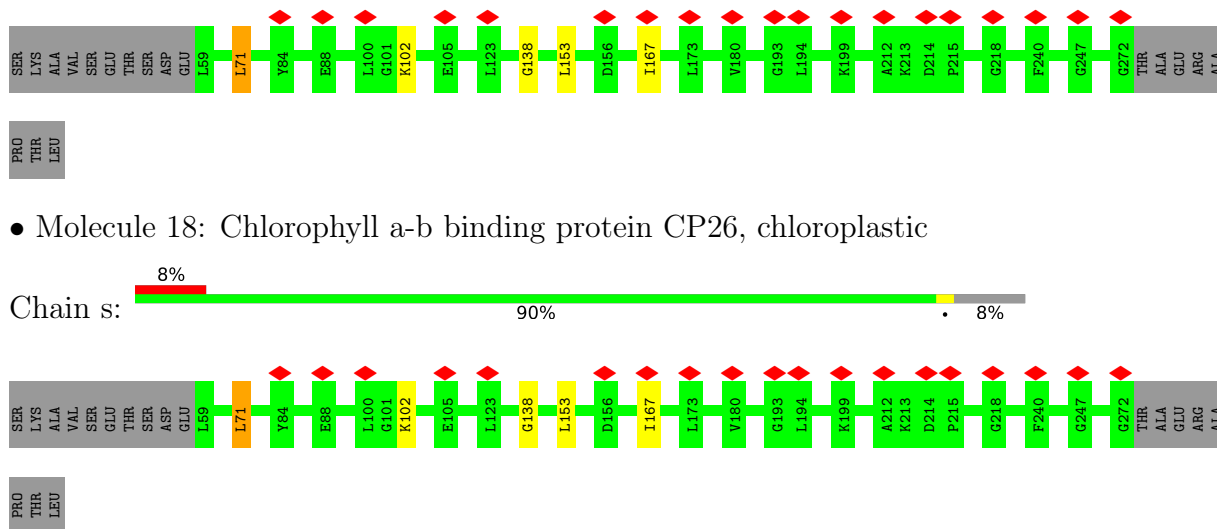




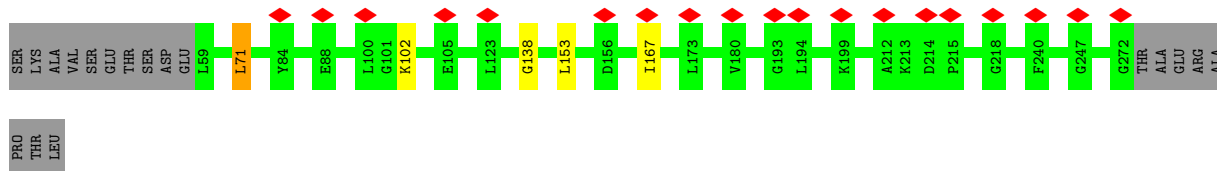
• Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic



• Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic

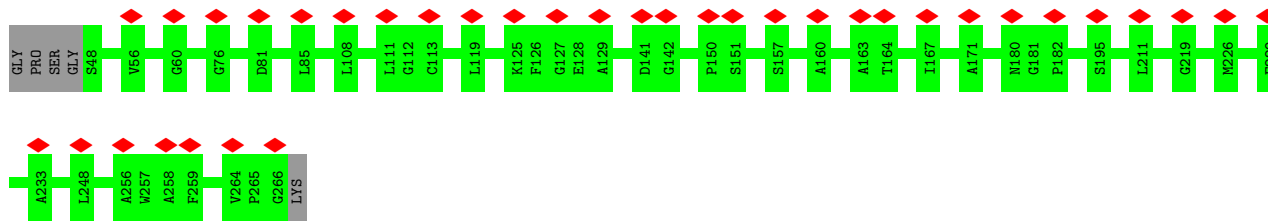


• Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic

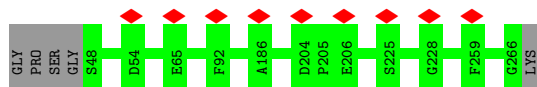


• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

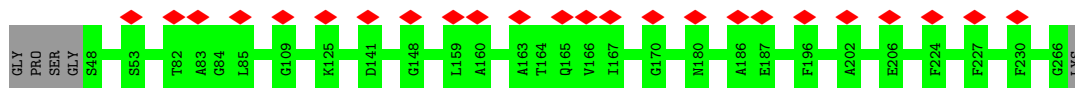




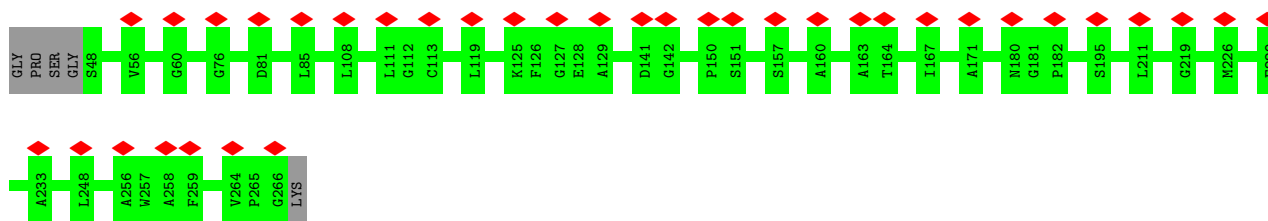
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



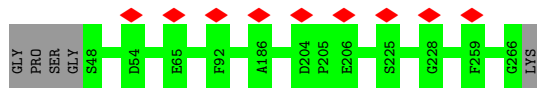
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



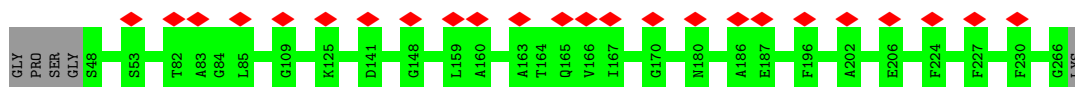
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



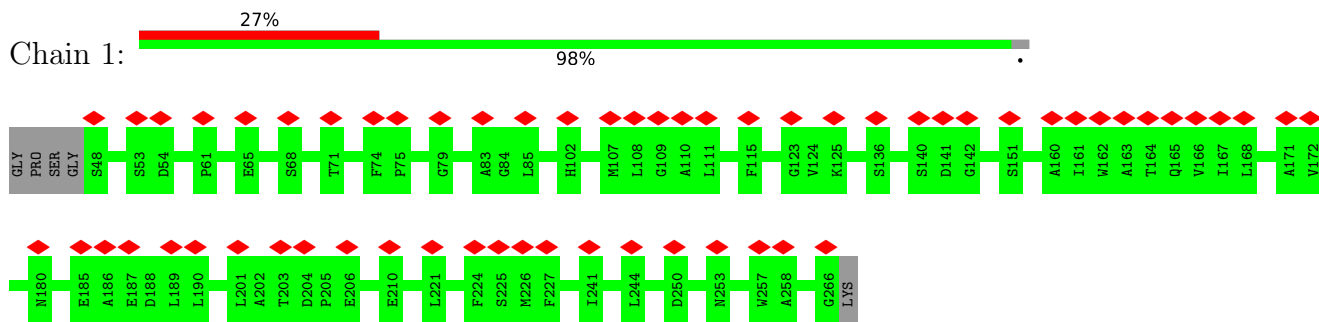
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



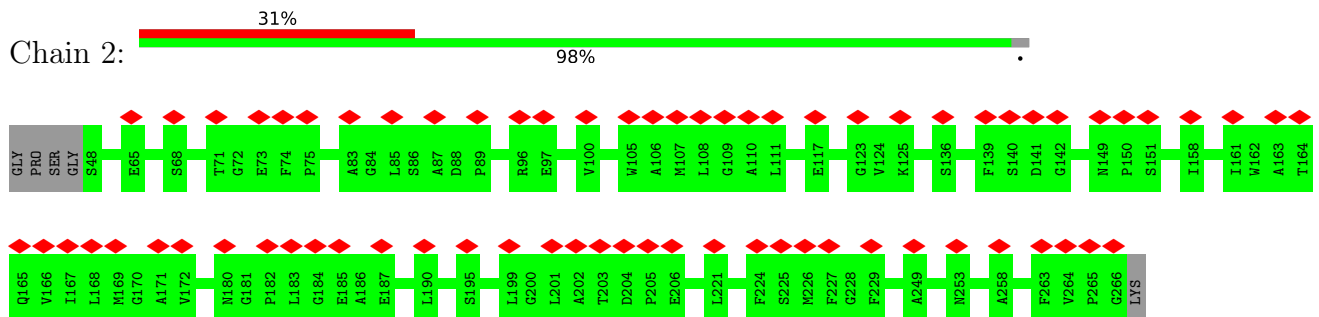
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



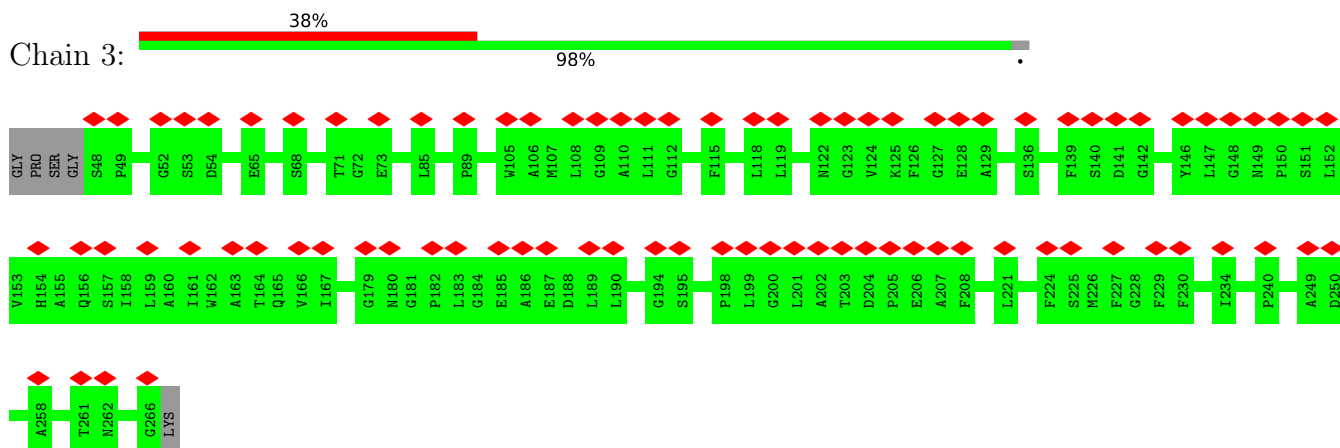
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



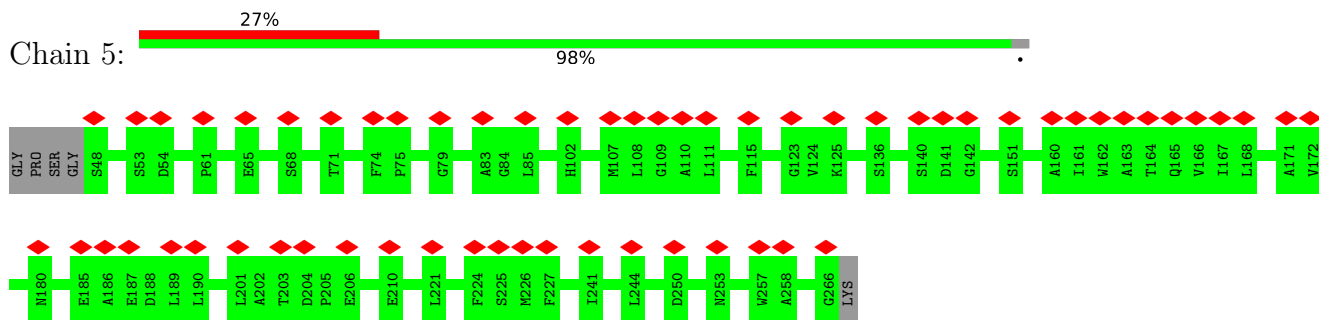
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

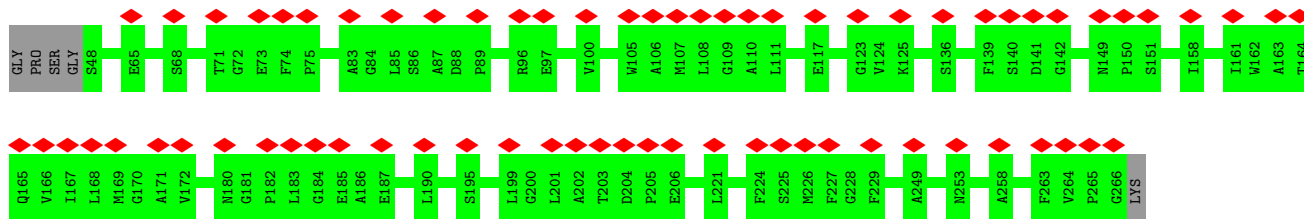


• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

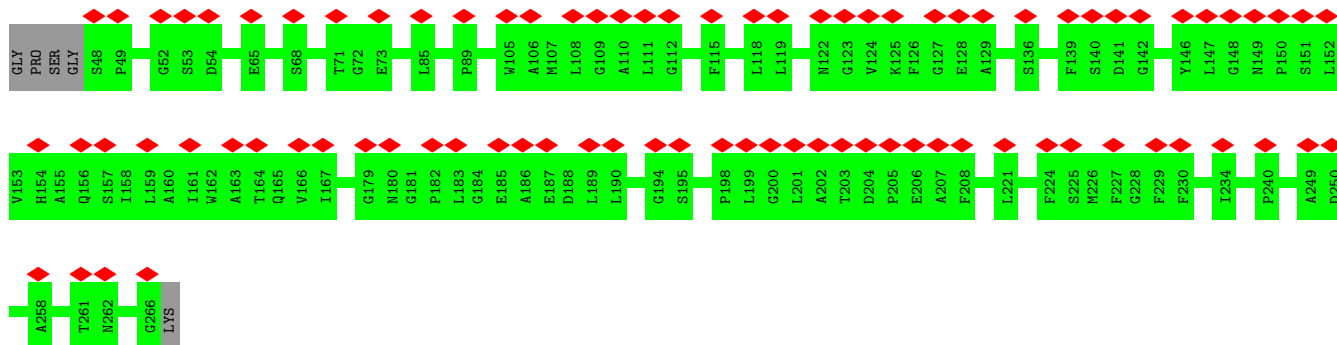


• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

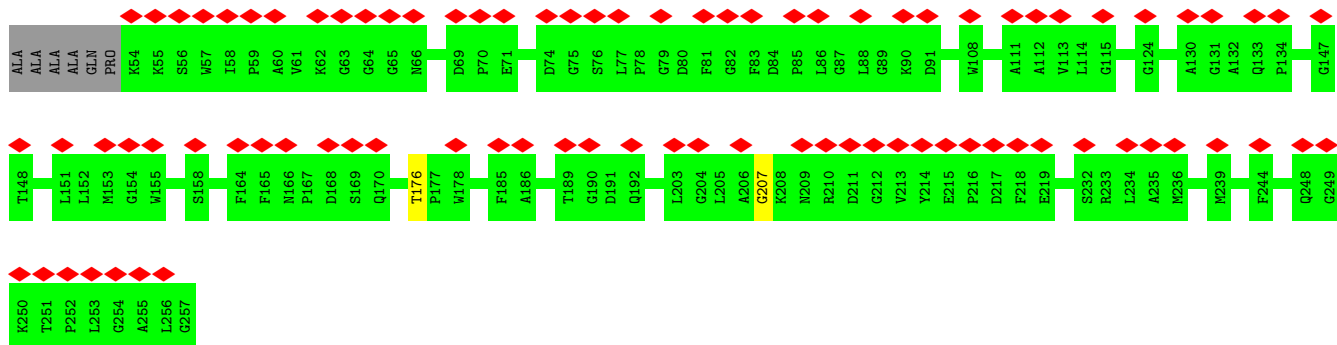
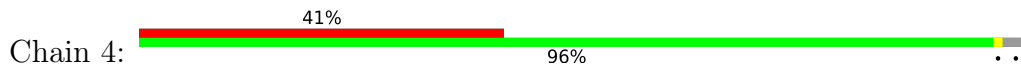




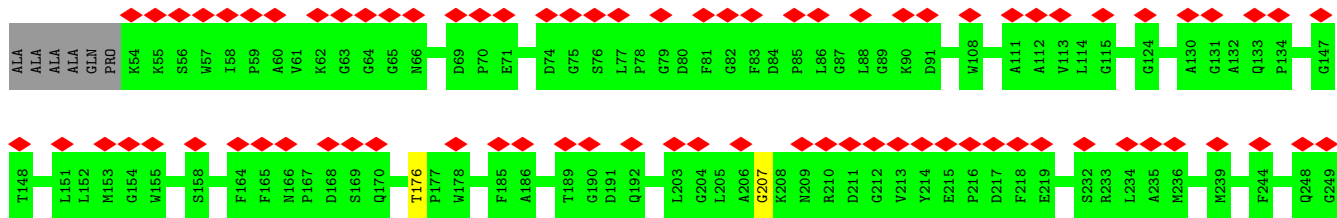
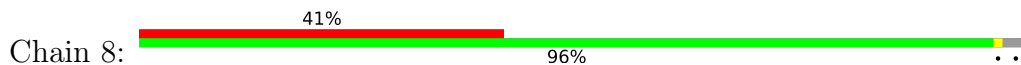
• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

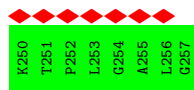


• Molecule 20: Chlorophyll a-b binding protein, chloroplastic



• Molecule 20: Chlorophyll a-b binding protein, chloroplastic





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	23434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.169	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	517.14, 517.14, 517.14	wwPDB
Map dimensions	468, 468, 468	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.105, 1.105, 1.105	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, FE2, CHL, HEM, PHO

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	0.36	0/2458	0.58	0/3348
1	a	0.36	0/2665	0.58	0/3634
2	B	0.35	0/3881	0.58	0/5286
2	b	0.35	0/3881	0.58	0/5286
3	C	0.37	0/3487	0.60	1/4750 (0.0%)
3	c	0.37	0/3487	0.60	1/4750 (0.0%)
4	D	0.38	0/2768	0.60	1/3774 (0.0%)
4	d	0.38	0/2768	0.60	1/3774 (0.0%)
5	E	0.37	0/603	0.65	0/819
5	e	0.37	0/603	0.65	0/819
6	F	0.36	0/229	0.62	0/311
6	f	0.36	0/229	0.62	0/311
7	H	0.34	0/398	0.55	0/541
7	h	0.34	0/398	0.56	0/541
8	I	0.46	0/294	0.69	0/397
8	i	0.46	0/294	0.69	0/397
9	K	0.40	0/301	0.66	0/414
9	k	0.40	0/301	0.66	0/414
10	L	0.41	0/310	0.77	1/421 (0.2%)
10	l	0.41	0/310	0.77	1/421 (0.2%)
11	M	0.42	0/230	0.65	0/315
11	m	0.42	0/230	0.65	0/315
12	O	0.35	0/1518	0.68	1/2049 (0.0%)
12	o	0.35	0/1518	0.68	1/2049 (0.0%)
13	T	0.39	0/246	0.61	0/333
13	t	0.39	0/246	0.61	0/333
14	W	0.37	0/383	0.65	0/519
14	w	0.37	0/383	0.66	0/519
15	X	0.37	0/228	0.46	0/310
15	x	0.37	0/228	0.46	0/310
16	Z	0.31	0/468	0.50	0/641
16	z	0.32	0/468	0.50	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.35	0/1502	0.52	0/2047
17	r	0.35	0/1502	0.52	0/2047
18	S	0.37	0/1698	0.78	4/2305 (0.2%)
18	s	0.37	0/1698	0.78	4/2305 (0.2%)
19	1	0.31	0/1716	0.53	0/2336
19	2	0.31	0/1716	0.53	0/2336
19	3	0.31	0/1716	0.53	0/2336
19	5	0.31	0/1716	0.53	0/2336
19	6	0.31	0/1716	0.53	0/2336
19	7	0.31	0/1716	0.53	0/2336
19	G	0.36	0/1716	0.57	0/2336
19	N	0.36	0/1716	0.56	0/2336
19	Y	0.36	0/1716	0.57	0/2336
19	g	0.36	0/1716	0.57	0/2336
19	n	0.36	0/1716	0.56	0/2336
19	y	0.36	0/1716	0.57	0/2336
20	4	0.36	0/1652	0.97	3/2242 (0.1%)
20	8	0.36	0/1652	0.97	3/2242 (0.1%)
All	All	0.36	0/66107	0.62	22/89962 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	b	0	1
17	R	0	1
17	r	0	1
18	S	0	1
18	s	0	1
20	4	0	1
20	8	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	207	GLY	CA-C-N	-23.99	64.42	117.20
20	8	207	GLY	CA-C-N	-23.99	64.42	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	207	GLY	O-C-N	-21.84	87.76	122.70
20	8	207	GLY	O-C-N	-21.84	87.76	122.70
20	4	207	GLY	CA-C-O	17.55	152.19	120.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	179	GLN	Peptide
17	R	59	TYR	Peptide
18	S	71	LEU	Peptide
2	b	179	GLN	Peptide
17	r	59	TYR	Peptide

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	303/343 (88%)	282 (93%)	21 (7%)	0	100	100
1	a	328/343 (96%)	306 (93%)	22 (7%)	0	100	100
2	B	476/507 (94%)	448 (94%)	28 (6%)	0	100	100
2	b	476/507 (94%)	448 (94%)	28 (6%)	0	100	100
3	C	429/459 (94%)	401 (94%)	28 (6%)	0	100	100
3	c	429/459 (94%)	402 (94%)	27 (6%)	0	100	100
4	D	334/352 (95%)	308 (92%)	26 (8%)	0	100	100
4	d	334/352 (95%)	307 (92%)	27 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	68/83 (82%)	59 (87%)	9 (13%)	0	100	100
5	e	68/83 (82%)	59 (87%)	9 (13%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	0	100	100
6	f	27/39 (69%)	27 (100%)	0	0	100	100
7	H	50/72 (69%)	44 (88%)	6 (12%)	0	100	100
7	h	50/72 (69%)	44 (88%)	6 (12%)	0	100	100
8	I	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
8	i	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
9	K	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
9	k	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
10	L	34/38 (90%)	28 (82%)	6 (18%)	0	100	100
10	l	34/38 (90%)	28 (82%)	6 (18%)	0	100	100
11	M	27/34 (79%)	27 (100%)	0	0	100	100
11	m	27/34 (79%)	27 (100%)	0	0	100	100
12	O	187/247 (76%)	162 (87%)	24 (13%)	1 (0%)	29	69
12	o	187/247 (76%)	163 (87%)	23 (12%)	1 (0%)	29	69
13	T	27/33 (82%)	27 (100%)	0	0	100	100
13	t	27/33 (82%)	27 (100%)	0	0	100	100
14	W	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
14	w	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
15	X	30/116 (26%)	29 (97%)	1 (3%)	0	100	100
15	x	30/116 (26%)	29 (97%)	1 (3%)	0	100	100
16	Z	59/62 (95%)	59 (100%)	0	0	100	100
16	z	59/62 (95%)	59 (100%)	0	0	100	100
17	R	184/250 (74%)	172 (94%)	12 (6%)	0	100	100
17	r	184/250 (74%)	172 (94%)	12 (6%)	0	100	100
18	S	212/232 (91%)	171 (81%)	41 (19%)	0	100	100
18	s	212/232 (91%)	171 (81%)	41 (19%)	0	100	100
19	1	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	2	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	3	217/224 (97%)	203 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	5	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	6	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	7	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	G	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	N	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	Y	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	g	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	n	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	y	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
20	4	202/210 (96%)	184 (91%)	18 (9%)	0	100	100
20	8	202/210 (96%)	184 (91%)	18 (9%)	0	100	100
All	All	8149/9096 (90%)	7521 (92%)	626 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	O	194	ILE
12	o	194	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	247/278 (89%)	247 (100%)	0	100	100
1	a	267/278 (96%)	267 (100%)	0	100	100
2	B	379/401 (94%)	379 (100%)	0	100	100
2	b	379/401 (94%)	379 (100%)	0	100	100
3	C	340/359 (95%)	339 (100%)	1 (0%)	92	95
3	c	340/359 (95%)	339 (100%)	1 (0%)	92	95
4	D	269/282 (95%)	268 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	269/282 (95%)	268 (100%)	1 (0%)	91	94
5	E	63/73 (86%)	63 (100%)	0	100	100
5	e	63/73 (86%)	63 (100%)	0	100	100
6	F	24/34 (71%)	24 (100%)	0	100	100
6	f	24/34 (71%)	24 (100%)	0	100	100
7	H	43/60 (72%)	43 (100%)	0	100	100
7	h	43/60 (72%)	43 (100%)	0	100	100
8	I	32/33 (97%)	32 (100%)	0	100	100
8	i	32/33 (97%)	32 (100%)	0	100	100
9	K	31/32 (97%)	31 (100%)	0	100	100
9	k	31/32 (97%)	31 (100%)	0	100	100
10	L	34/36 (94%)	34 (100%)	0	100	100
10	l	34/36 (94%)	34 (100%)	0	100	100
11	M	25/30 (83%)	25 (100%)	0	100	100
11	m	25/30 (83%)	24 (96%)	1 (4%)	31	55
12	O	164/204 (80%)	164 (100%)	0	100	100
12	o	164/204 (80%)	164 (100%)	0	100	100
13	T	26/30 (87%)	26 (100%)	0	100	100
13	t	26/30 (87%)	26 (100%)	0	100	100
14	W	40/47 (85%)	40 (100%)	0	100	100
14	w	40/47 (85%)	40 (100%)	0	100	100
15	X	27/92 (29%)	27 (100%)	0	100	100
15	x	27/92 (29%)	27 (100%)	0	100	100
16	Z	53/54 (98%)	53 (100%)	0	100	100
16	z	53/54 (98%)	53 (100%)	0	100	100
17	R	150/201 (75%)	150 (100%)	0	100	100
17	r	150/201 (75%)	150 (100%)	0	100	100
18	S	165/180 (92%)	164 (99%)	1 (1%)	86	91
18	s	165/180 (92%)	164 (99%)	1 (1%)	86	91
19	1	167/170 (98%)	167 (100%)	0	100	100
19	2	167/170 (98%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	3	167/170 (98%)	167 (100%)	0	100	100
19	5	167/170 (98%)	167 (100%)	0	100	100
19	6	167/170 (98%)	167 (100%)	0	100	100
19	7	167/170 (98%)	167 (100%)	0	100	100
19	G	167/170 (98%)	167 (100%)	0	100	100
19	N	167/170 (98%)	167 (100%)	0	100	100
19	Y	167/170 (98%)	167 (100%)	0	100	100
19	g	167/170 (98%)	167 (100%)	0	100	100
19	n	167/170 (98%)	167 (100%)	0	100	100
19	y	167/170 (98%)	167 (100%)	0	100	100
20	4	156/158 (99%)	156 (100%)	0	100	100
20	8	156/158 (99%)	156 (100%)	0	100	100
All	All	6560/7208 (91%)	6553 (100%)	7 (0%)	93	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	m	16	LEU
3	c	26	ARG
18	s	102	LYS
18	S	102	LYS
4	d	19	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
19	N	122	ASN
19	6	156	GLN
18	s	117	HIS
19	6	95	ASN
19	3	95	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 316 ligands modelled in this entry, 2 are monoatomic - leaving 314 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	y	608	-	46,54,74	1.80	10 (21%)	49,90,114	1.84	9 (18%)
22	CLA	C	506	-	45,53,73	2.17	16 (35%)	52,89,113	2.95	21 (40%)
22	CLA	N	613	19	45,53,73	2.16	16 (35%)	52,89,113	2.84	21 (40%)
22	CLA	7	303	19	45,53,73	2.19	17 (37%)	52,89,113	2.79	24 (46%)
25	CHL	2	607	-	46,54,74	1.82	11 (23%)	49,90,114	1.84	9 (18%)
25	CHL	G	605	19	42,50,74	1.69	10 (23%)	44,85,114	1.92	8 (18%)
25	CHL	Y	608	-	46,54,74	1.80	10 (21%)	49,90,114	1.84	9 (18%)
22	CLA	N	612	19	45,53,73	2.14	15 (33%)	52,89,113	2.83	24 (46%)
22	CLA	Y	614	-	45,53,73	2.19	14 (31%)	52,89,113	2.89	25 (48%)
22	CLA	c	507	-	45,53,73	2.11	13 (28%)	52,89,113	2.83	25 (48%)
25	CHL	Y	606	-	46,54,74	1.82	9 (19%)	49,90,114	1.90	11 (22%)
22	CLA	B	614	-	45,53,73	2.19	14 (31%)	52,89,113	2.83	25 (48%)
25	CHL	5	609	19	46,54,74	1.83	10 (21%)	49,90,114	2.14	10 (20%)
22	CLA	6	611	19	45,53,73	2.19	16 (35%)	52,89,113	2.74	21 (40%)
24	HEM	e	101	6,5	41,50,50	1.58	4 (9%)	45,82,82	1.63	8 (17%)
22	CLA	1	602	19	45,53,73	2.16	17 (37%)	52,89,113	2.78	22 (42%)
25	CHL	N	608	-	46,54,74	1.80	9 (19%)	49,90,114	1.80	10 (20%)
22	CLA	b	604	-	45,53,73	2.16	16 (35%)	52,89,113	2.81	21 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	1	609	19	46,54,74	1.83	10 (21%)	49,90,114	2.14	10 (20%)
22	CLA	G	612	19	45,53,73	2.19	15 (33%)	52,89,113	2.83	25 (48%)
22	CLA	6	613	-	45,53,73	2.23	18 (40%)	52,89,113	2.74	23 (44%)
22	CLA	b	603	-	45,53,73	2.23	17 (37%)	52,89,113	2.90	26 (50%)
25	CHL	g	607	-	46,54,74	1.82	11 (23%)	49,90,114	1.98	12 (24%)
22	CLA	n	604	-	45,53,73	2.22	14 (31%)	52,89,113	2.83	24 (46%)
25	CHL	5	601	19	46,54,74	1.80	11 (23%)	49,90,114	1.90	11 (22%)
22	CLA	r	311	17	45,53,73	2.19	16 (35%)	52,89,113	2.84	23 (44%)
22	CLA	N	602	19	45,53,73	2.17	15 (33%)	52,89,113	2.82	23 (44%)
22	CLA	n	614	-	45,53,73	2.23	18 (40%)	52,89,113	2.75	22 (42%)
25	CHL	6	608	19	46,54,74	1.79	10 (21%)	49,90,114	2.17	10 (20%)
25	CHL	y	601	19	46,54,74	1.73	10 (21%)	49,90,114	1.92	12 (24%)
22	CLA	8	304	-	45,53,73	2.21	18 (40%)	52,89,113	2.85	26 (50%)
22	CLA	5	610	19	45,53,73	2.18	15 (33%)	52,89,113	2.82	22 (42%)
22	CLA	B	609	-	45,53,73	2.17	15 (33%)	52,89,113	2.93	24 (46%)
22	CLA	S	301	-	45,53,73	2.19	15 (33%)	52,89,113	2.87	24 (46%)
22	CLA	C	508	-	45,53,73	2.20	16 (35%)	52,89,113	3.02	22 (42%)
25	CHL	n	607	-	46,54,74	1.80	9 (19%)	49,90,114	2.09	10 (20%)
25	CHL	6	607	-	46,54,74	1.82	11 (23%)	49,90,114	1.84	9 (18%)
25	CHL	8	305	20	46,54,74	1.80	11 (23%)	49,90,114	2.03	11 (22%)
22	CLA	4	309	20	45,53,73	2.16	15 (33%)	52,89,113	2.76	26 (50%)
22	CLA	y	610	19	45,53,73	2.16	14 (31%)	52,89,113	2.84	23 (44%)
22	CLA	1	603	-	45,53,73	2.16	17 (37%)	52,89,113	2.78	24 (46%)
22	CLA	2	610	-	45,53,73	2.19	16 (35%)	52,89,113	2.78	24 (46%)
22	CLA	1	610	19	45,53,73	2.18	15 (33%)	52,89,113	2.82	22 (42%)
22	CLA	7	310	19	45,53,73	2.20	15 (33%)	52,89,113	2.83	23 (44%)
22	CLA	s	313	18	45,53,73	2.19	15 (33%)	52,89,113	2.90	27 (51%)
25	CHL	2	606	-	46,54,74	1.85	10 (21%)	49,90,114	1.82	10 (20%)
25	CHL	7	307	-	46,54,74	1.84	11 (23%)	49,90,114	1.84	8 (16%)
22	CLA	c	503	-	45,53,73	2.16	14 (31%)	52,89,113	2.85	23 (44%)
22	CLA	Y	613	19	45,53,73	2.18	15 (33%)	52,89,113	2.90	24 (46%)
22	CLA	y	614	-	45,53,73	2.19	14 (31%)	52,89,113	2.89	25 (48%)
22	CLA	y	611	-	45,53,73	2.17	14 (31%)	52,89,113	2.93	23 (44%)
25	CHL	g	601	19	46,54,74	1.79	10 (21%)	49,90,114	2.03	13 (26%)
22	CLA	b	612	-	45,53,73	2.30	19 (42%)	52,89,113	2.83	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	1	604	-	45,53,73	2.21	17 (37%)	52,89,113	2.82	23 (44%)
22	CLA	y	604	-	45,53,73	2.22	14 (31%)	52,89,113	2.98	24 (46%)
22	CLA	3	310	19	45,53,73	2.20	15 (33%)	52,89,113	2.83	23 (44%)
25	CHL	4	301	-	46,54,74	1.82	11 (23%)	49,90,114	1.88	12 (24%)
22	CLA	7	314	-	45,53,73	2.25	18 (40%)	52,89,113	2.72	24 (46%)
22	CLA	R	308	17	45,53,73	2.19	15 (33%)	52,89,113	2.82	24 (46%)
25	CHL	2	601	19	46,54,74	1.81	11 (23%)	49,90,114	2.00	11 (22%)
25	CHL	g	608	-	46,54,74	1.83	10 (21%)	49,90,114	1.77	9 (18%)
25	CHL	n	609	19	46,54,74	1.79	10 (21%)	49,90,114	2.22	10 (20%)
22	CLA	4	303	-	45,53,73	2.18	17 (37%)	52,89,113	2.74	23 (44%)
22	CLA	b	601	-	45,53,73	2.17	15 (33%)	52,89,113	2.76	24 (46%)
22	CLA	S	310	18	45,53,73	2.16	15 (33%)	52,89,113	2.84	27 (51%)
23	PHO	a	404	-	31,49,69	1.84	7 (22%)	23,75,99	1.87	7 (30%)
22	CLA	d	403	-	45,53,73	2.25	15 (33%)	52,89,113	3.02	28 (53%)
22	CLA	b	606	-	45,53,73	2.31	18 (40%)	52,89,113	2.78	25 (48%)
25	CHL	Y	605	19	42,50,74	1.76	9 (21%)	44,85,114	2.01	9 (20%)
22	CLA	a	405	-	45,53,73	2.22	14 (31%)	52,89,113	2.94	25 (48%)
22	CLA	R	303	-	45,53,73	2.17	14 (31%)	52,89,113	3.00	27 (51%)
25	CHL	Y	607	-	46,54,74	1.81	10 (21%)	49,90,114	1.99	12 (24%)
22	CLA	R	301	17	45,53,73	2.18	15 (33%)	52,89,113	2.84	23 (44%)
22	CLA	4	304	-	45,53,73	2.21	18 (40%)	52,89,113	2.85	26 (50%)
25	CHL	r	305	-	46,54,74	1.84	10 (21%)	49,90,114	1.93	11 (22%)
22	CLA	b	605	-	45,53,73	2.25	16 (35%)	52,89,113	2.87	25 (48%)
22	CLA	3	304	-	45,53,73	2.19	18 (40%)	52,89,113	2.79	24 (46%)
22	CLA	G	603	-	45,53,73	2.16	18 (40%)	52,89,113	2.84	24 (46%)
22	CLA	s	303	18	45,53,73	2.18	14 (31%)	52,89,113	2.84	24 (46%)
25	CHL	7	308	-	46,54,74	1.84	10 (21%)	49,90,114	1.79	10 (20%)
25	CHL	3	302	19	46,54,74	1.84	11 (23%)	49,90,114	1.96	10 (20%)
22	CLA	C	507	-	45,53,73	2.14	15 (33%)	52,89,113	2.86	24 (46%)
25	CHL	R	306	-	46,54,74	1.81	11 (23%)	49,90,114	1.81	9 (18%)
22	CLA	A	402	-	45,53,73	2.18	14 (31%)	52,89,113	2.90	24 (46%)
22	CLA	7	305	-	45,53,73	2.21	18 (40%)	52,89,113	2.84	24 (46%)
22	CLA	c	508	-	45,53,73	2.22	16 (35%)	52,89,113	2.99	23 (44%)
22	CLA	B	616	-	45,53,73	2.19	16 (35%)	52,89,113	2.86	25 (48%)
22	CLA	C	509	-	45,53,73	2.22	18 (40%)	52,89,113	2.83	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	5	607	-	46,54,74	1.82	11 (23%)	49,90,114	1.96	9 (18%)
22	CLA	8	309	20	45,53,73	2.16	15 (33%)	52,89,113	2.76	26 (50%)
25	CHL	n	606	-	46,54,74	1.81	10 (21%)	49,90,114	1.87	10 (20%)
22	CLA	s	311	-	45,53,73	2.20	14 (31%)	52,89,113	2.88	24 (46%)
22	CLA	Y	603	-	45,53,73	2.12	14 (31%)	52,89,113	2.89	24 (46%)
22	CLA	D	401	-	45,53,73	2.20	15 (33%)	52,89,113	2.81	23 (44%)
25	CHL	S	307	-	46,54,74	1.82	10 (21%)	49,90,114	6.24	11 (22%)
22	CLA	d	404	-	45,53,73	2.20	16 (35%)	52,89,113	2.73	23 (44%)
25	CHL	5	605	19	42,50,74	1.75	10 (23%)	44,85,114	1.91	9 (20%)
25	CHL	G	606	-	46,54,74	1.85	10 (21%)	49,90,114	1.73	7 (14%)
22	CLA	d	401	-	45,53,73	2.18	15 (33%)	52,89,113	2.81	24 (46%)
22	CLA	3	312	19	45,53,73	2.18	17 (37%)	52,89,113	2.78	23 (44%)
25	CHL	8	306	-	46,54,74	1.84	11 (23%)	49,90,114	1.83	9 (18%)
25	CHL	R	305	-	46,54,74	1.84	10 (21%)	49,90,114	1.93	11 (22%)
22	CLA	R	312	20,17	45,53,73	2.20	17 (37%)	52,89,113	2.80	26 (50%)
22	CLA	5	604	-	45,53,73	2.21	17 (37%)	52,89,113	2.82	23 (44%)
25	CHL	3	301	-	46,54,74	1.84	11 (23%)	49,90,114	1.92	11 (22%)
23	PHO	A	404	-	31,49,69	1.93	7 (22%)	23,75,99	1.96	6 (26%)
22	CLA	n	612	19	45,53,73	2.14	15 (33%)	52,89,113	2.83	24 (46%)
22	CLA	s	312	18	45,53,73	2.22	16 (35%)	52,89,113	2.91	26 (50%)
25	CHL	G	601	19	46,54,74	1.79	10 (21%)	49,90,114	2.03	13 (26%)
22	CLA	B	613	-	45,53,73	2.19	16 (35%)	52,89,113	2.91	26 (50%)
22	CLA	G	604	-	45,53,73	2.20	17 (37%)	52,89,113	2.89	26 (50%)
22	CLA	G	610	19	45,53,73	2.16	14 (31%)	52,89,113	2.83	24 (46%)
22	CLA	2	609	19	45,53,73	2.18	14 (31%)	52,89,113	2.82	22 (42%)
22	CLA	G	614	-	45,53,73	2.21	16 (35%)	52,89,113	2.80	25 (48%)
25	CHL	r	306	-	46,54,74	1.81	11 (23%)	49,90,114	1.81	9 (18%)
22	CLA	S	305	-	45,53,73	2.21	15 (33%)	52,89,113	2.91	25 (48%)
22	CLA	3	305	-	45,53,73	2.21	18 (40%)	52,89,113	2.84	24 (46%)
25	CHL	s	307	-	46,54,74	1.82	10 (21%)	49,90,114	6.24	11 (22%)
22	CLA	S	312	18	45,53,73	2.22	16 (35%)	52,89,113	2.91	26 (50%)
22	CLA	1	613	19	45,53,73	2.20	17 (37%)	52,89,113	2.77	23 (44%)
25	CHL	4	307	-	46,54,74	1.83	11 (23%)	49,90,114	6.22	10 (20%)
22	CLA	8	310	-	45,53,73	2.21	17 (37%)	52,89,113	2.72	25 (48%)
22	CLA	c	502	-	45,53,73	2.14	16 (35%)	52,89,113	2.80	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	615	-	45,53,73	2.12	15 (33%)	52,89,113	3.07	24 (46%)
22	CLA	2	603	-	45,53,73	2.16	17 (37%)	52,89,113	2.76	25 (48%)
22	CLA	C	503	-	45,53,73	2.19	14 (31%)	52,89,113	2.79	25 (48%)
25	CHL	6	605	19	42,50,74	1.67	10 (23%)	44,85,114	1.97	8 (18%)
22	CLA	r	307	17	45,53,73	2.18	16 (35%)	52,89,113	2.79	24 (46%)
22	CLA	C	502	-	45,53,73	2.19	14 (31%)	52,89,113	2.68	24 (46%)
22	CLA	n	613	19	45,53,73	2.16	16 (35%)	52,89,113	2.84	21 (40%)
25	CHL	1	601	19	46,54,74	1.80	11 (23%)	49,90,114	1.90	11 (22%)
22	CLA	n	610	19	45,53,73	2.16	14 (31%)	52,89,113	2.83	22 (42%)
22	CLA	b	607	-	45,53,73	2.15	15 (33%)	52,89,113	2.82	25 (48%)
22	CLA	5	614	-	45,53,73	2.21	19 (42%)	52,89,113	2.94	25 (48%)
22	CLA	7	304	-	45,53,73	2.19	18 (40%)	52,89,113	2.79	24 (46%)
22	CLA	Y	602	19	45,53,73	2.19	16 (35%)	52,89,113	2.86	22 (42%)
24	HEM	E	101	6,5	41,50,50	1.53	3 (7%)	45,82,82	1.52	10 (22%)
22	CLA	g	613	19	45,53,73	2.17	14 (31%)	52,89,113	2.82	23 (44%)
22	CLA	7	311	-	45,53,73	2.20	17 (37%)	52,89,113	2.78	26 (50%)
25	CHL	7	302	19	46,54,74	1.84	11 (23%)	49,90,114	1.96	10 (20%)
22	CLA	6	612	19	45,53,73	2.18	16 (35%)	52,89,113	2.80	21 (40%)
22	CLA	B	608	-	45,53,73	2.19	16 (35%)	52,89,113	2.97	24 (46%)
25	CHL	2	608	19	46,54,74	1.79	10 (21%)	49,90,114	2.17	10 (20%)
25	CHL	1	607	-	46,54,74	1.82	11 (23%)	49,90,114	1.96	9 (18%)
22	CLA	R	307	17	45,53,73	2.18	16 (35%)	52,89,113	2.79	24 (46%)
22	CLA	B	606	-	45,53,73	2.10	13 (28%)	52,89,113	2.86	24 (46%)
25	CHL	n	608	-	46,54,74	1.80	9 (19%)	49,90,114	1.80	10 (20%)
25	CHL	8	307	-	46,54,74	1.83	11 (23%)	49,90,114	6.22	10 (20%)
25	CHL	1	605	19	42,50,74	1.75	10 (23%)	44,85,114	1.91	9 (20%)
25	CHL	y	605	19	42,50,74	1.76	9 (21%)	44,85,114	2.01	9 (20%)
25	CHL	g	605	19	42,50,74	1.69	10 (23%)	44,85,114	1.92	8 (18%)
25	CHL	5	608	-	46,54,74	1.85	11 (23%)	49,90,114	1.78	8 (16%)
22	CLA	S	313	18	45,53,73	2.19	15 (33%)	52,89,113	2.90	27 (51%)
22	CLA	Y	612	19	45,53,73	2.17	15 (33%)	52,89,113	2.86	25 (48%)
25	CHL	4	306	-	46,54,74	1.84	11 (23%)	49,90,114	1.83	9 (18%)
22	CLA	C	505	-	45,53,73	2.19	15 (33%)	52,89,113	2.87	24 (46%)
25	CHL	5	606	-	46,54,74	1.84	10 (21%)	49,90,114	1.81	10 (20%)
22	CLA	r	310	-	45,53,73	2.16	15 (33%)	52,89,113	2.80	23 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	6	603	-	45,53,73	2.16	17 (37%)	52,89,113	2.76	25 (48%)
25	CHL	3	306	19	42,50,74	1.69	10 (23%)	44,85,114	1.98	8 (18%)
22	CLA	G	611	-	45,53,73	2.16	13 (28%)	52,89,113	2.87	26 (50%)
22	CLA	R	302	-	45,53,73	2.20	15 (33%)	52,89,113	2.79	21 (40%)
22	CLA	B	603	-	45,53,73	2.23	14 (31%)	52,89,113	2.90	27 (51%)
22	CLA	R	311	17	45,53,73	2.19	16 (35%)	52,89,113	2.84	23 (44%)
25	CHL	1	608	-	46,54,74	1.85	11 (23%)	49,90,114	1.78	8 (16%)
25	CHL	G	607	-	46,54,74	1.82	11 (23%)	49,90,114	1.98	12 (24%)
25	CHL	s	306	18	46,54,74	1.77	10 (21%)	49,90,114	1.95	11 (22%)
22	CLA	S	303	18	45,53,73	2.18	14 (31%)	52,89,113	2.84	24 (46%)
25	CHL	N	607	-	46,54,74	1.80	9 (19%)	49,90,114	2.09	10 (20%)
25	CHL	1	606	-	46,54,74	1.84	10 (21%)	49,90,114	1.81	10 (20%)
22	CLA	A	403	-	45,53,73	2.27	17 (37%)	52,89,113	2.87	26 (50%)
25	CHL	n	605	19	42,50,74	1.69	9 (21%)	44,85,114	1.96	6 (13%)
22	CLA	B	607	-	45,53,73	2.18	15 (33%)	52,89,113	2.81	23 (44%)
22	CLA	5	602	19	45,53,73	2.16	17 (37%)	52,89,113	2.78	22 (42%)
25	CHL	s	308	-	46,54,74	1.79	11 (23%)	49,90,114	1.92	9 (18%)
22	CLA	g	610	19	45,53,73	2.16	14 (31%)	52,89,113	2.83	24 (46%)
25	CHL	3	309	19	46,54,74	1.82	10 (21%)	49,90,114	2.29	10 (20%)
22	CLA	Y	611	-	45,53,73	2.17	14 (31%)	52,89,113	2.93	23 (44%)
22	CLA	6	610	-	45,53,73	2.19	16 (35%)	52,89,113	2.78	24 (46%)
22	CLA	S	314	-	45,53,73	2.18	14 (31%)	52,89,113	2.88	24 (46%)
22	CLA	2	602	19	45,53,73	2.18	18 (40%)	52,89,113	2.78	22 (42%)
22	CLA	B	612	-	45,53,73	2.20	15 (33%)	52,89,113	2.90	24 (46%)
22	CLA	c	504	-	45,53,73	2.22	16 (35%)	52,89,113	2.80	25 (48%)
22	CLA	D	404	-	45,53,73	2.19	16 (35%)	52,89,113	2.80	25 (48%)
22	CLA	8	302	20	45,53,73	2.13	17 (37%)	52,89,113	2.97	25 (48%)
22	CLA	7	313	19	45,53,73	2.20	17 (37%)	52,89,113	2.77	21 (40%)
25	CHL	R	304	-	46,54,74	1.84	10 (21%)	49,90,114	1.90	11 (22%)
25	CHL	Y	609	19	46,54,74	1.77	9 (19%)	49,90,114	2.26	11 (22%)
25	CHL	S	306	18	46,54,74	1.77	10 (21%)	49,90,114	1.95	11 (22%)
25	CHL	7	301	-	46,54,74	1.84	11 (23%)	49,90,114	1.92	11 (22%)
23	PHO	D	402	-	31,49,69	1.77	7 (22%)	23,75,99	1.99	7 (30%)
22	CLA	b	608	-	45,53,73	2.25	16 (35%)	52,89,113	2.82	25 (48%)
22	CLA	5	611	-	45,53,73	2.19	17 (37%)	52,89,113	2.79	23 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	3	307	-	46,54,74	1.84	11 (23%)	49,90,114	1.84	8 (16%)
22	CLA	a	403	-	45,53,73	2.20	14 (31%)	52,89,113	2.93	24 (46%)
22	CLA	2	611	19	45,53,73	2.19	16 (35%)	52,89,113	2.74	21 (40%)
25	CHL	S	308	-	46,54,74	1.79	11 (23%)	49,90,114	1.92	9 (18%)
22	CLA	5	612	19	45,53,73	2.20	17 (37%)	52,89,113	2.76	25 (48%)
25	CHL	r	304	-	46,54,74	1.84	10 (21%)	49,90,114	1.90	11 (22%)
22	CLA	g	602	19	45,53,73	2.19	17 (37%)	52,89,113	2.82	23 (44%)
22	CLA	G	613	19	45,53,73	2.17	14 (31%)	52,89,113	2.82	23 (44%)
22	CLA	y	612	19	45,53,73	2.17	15 (33%)	52,89,113	2.86	25 (48%)
22	CLA	7	312	19	45,53,73	2.18	17 (37%)	52,89,113	2.78	23 (44%)
25	CHL	y	606	-	46,54,74	1.82	9 (19%)	49,90,114	1.90	11 (22%)
22	CLA	N	610	19	45,53,73	2.16	14 (31%)	52,89,113	2.83	22 (42%)
22	CLA	R	310	-	45,53,73	2.16	15 (33%)	52,89,113	2.80	23 (44%)
25	CHL	1	615	-	46,54,74	1.84	11 (23%)	49,90,114	1.90	11 (22%)
22	CLA	B	601	-	45,53,73	2.17	13 (28%)	52,89,113	2.75	22 (42%)
22	CLA	B	602	-	45,53,73	2.12	15 (33%)	52,89,113	2.78	22 (42%)
22	CLA	2	604	-	45,53,73	2.21	18 (40%)	52,89,113	2.85	25 (48%)
22	CLA	B	604	-	45,53,73	2.14	15 (33%)	52,89,113	2.97	23 (44%)
22	CLA	A	405	-	45,53,73	2.25	15 (33%)	52,89,113	2.93	24 (46%)
22	CLA	Y	610	19	45,53,73	2.16	14 (31%)	52,89,113	2.84	23 (44%)
22	CLA	2	613	-	45,53,73	2.23	18 (40%)	52,89,113	2.74	23 (44%)
22	CLA	r	309	-	45,53,73	2.16	15 (33%)	52,89,113	2.83	24 (46%)
22	CLA	c	509	-	45,53,73	2.20	14 (31%)	52,89,113	2.80	22 (42%)
22	CLA	g	614	-	45,53,73	2.21	16 (35%)	52,89,113	2.80	25 (48%)
22	CLA	g	611	-	45,53,73	2.16	13 (28%)	52,89,113	2.87	26 (50%)
22	CLA	C	511	3	45,53,73	2.21	18 (40%)	52,89,113	2.87	26 (50%)
25	CHL	N	605	19	42,50,74	1.69	9 (21%)	44,85,114	1.96	6 (13%)
22	CLA	r	312	20,17	45,53,73	2.20	17 (37%)	52,89,113	2.80	26 (50%)
25	CHL	N	601	19	46,54,74	1.79	10 (21%)	49,90,114	2.00	11 (22%)
25	CHL	N	606	-	46,54,74	1.81	10 (21%)	49,90,114	1.87	10 (20%)
22	CLA	3	311	-	45,53,73	2.20	17 (37%)	52,89,113	2.78	26 (50%)
22	CLA	4	310	-	45,53,73	2.21	17 (37%)	52,89,113	2.72	25 (48%)
22	CLA	B	611	-	45,53,73	2.20	15 (33%)	52,89,113	2.88	25 (48%)
22	CLA	N	604	-	45,53,73	2.22	14 (31%)	52,89,113	2.83	24 (46%)
25	CHL	6	606	-	46,54,74	1.85	10 (21%)	49,90,114	1.82	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	3	303	19	45,53,73	2.19	17 (37%)	52,89,113	2.79	24 (46%)
25	CHL	7	306	19	42,50,74	1.69	10 (23%)	44,85,114	1.98	8 (18%)
22	CLA	b	613	-	45,53,73	2.15	16 (35%)	52,89,113	3.01	28 (53%)
22	CLA	s	310	18	45,53,73	2.16	15 (33%)	52,89,113	2.84	27 (51%)
22	CLA	6	609	19	45,53,73	2.18	14 (31%)	52,89,113	2.82	22 (42%)
22	CLA	c	512	-	45,53,73	2.15	17 (37%)	52,89,113	2.89	24 (46%)
22	CLA	R	309	-	45,53,73	2.16	15 (33%)	52,89,113	2.83	24 (46%)
25	CHL	7	309	19	46,54,74	1.82	10 (21%)	49,90,114	2.29	10 (20%)
25	CHL	G	608	-	46,54,74	1.83	10 (21%)	49,90,114	1.77	9 (18%)
22	CLA	r	301	17	45,53,73	2.18	15 (33%)	52,89,113	2.84	23 (44%)
25	CHL	s	302	18	46,54,74	1.83	11 (23%)	49,90,114	1.74	8 (16%)
25	CHL	g	609	19	46,54,74	1.80	10 (21%)	49,90,114	2.29	11 (22%)
22	CLA	6	604	-	45,53,73	2.21	18 (40%)	52,89,113	2.85	25 (48%)
22	CLA	S	311	-	45,53,73	2.20	14 (31%)	52,89,113	2.88	24 (46%)
22	CLA	b	609	-	45,53,73	2.15	16 (35%)	52,89,113	2.94	26 (50%)
22	CLA	b	616	-	45,53,73	2.20	16 (35%)	52,89,113	3.14	26 (50%)
22	CLA	5	603	-	45,53,73	2.16	17 (37%)	52,89,113	2.78	24 (46%)
22	CLA	s	314	-	45,53,73	2.18	14 (31%)	52,89,113	2.88	24 (46%)
22	CLA	y	613	19	45,53,73	2.18	15 (33%)	52,89,113	2.90	24 (46%)
22	CLA	n	611	-	45,53,73	2.17	14 (31%)	52,89,113	2.88	26 (50%)
22	CLA	a	402	-	45,53,73	2.24	16 (35%)	52,89,113	2.81	25 (48%)
22	CLA	1	614	-	45,53,73	2.21	19 (42%)	52,89,113	2.94	25 (48%)
22	CLA	b	610	-	45,53,73	2.24	18 (40%)	52,89,113	2.80	23 (44%)
22	CLA	6	602	19	45,53,73	2.18	18 (40%)	52,89,113	2.78	22 (42%)
25	CHL	n	601	19	46,54,74	1.79	10 (21%)	49,90,114	2.00	11 (22%)
22	CLA	s	301	-	45,53,73	2.23	17 (37%)	52,89,113	2.76	25 (48%)
22	CLA	c	505	-	45,53,73	2.22	15 (33%)	52,89,113	2.89	25 (48%)
22	CLA	b	602	-	45,53,73	2.13	14 (31%)	52,89,113	2.81	24 (46%)
22	CLA	B	610	-	45,53,73	2.19	17 (37%)	52,89,113	2.78	23 (44%)
22	CLA	S	309	18	45,53,73	2.15	15 (33%)	52,89,113	2.74	24 (46%)
22	CLA	1	612	19	45,53,73	2.20	17 (37%)	52,89,113	2.76	25 (48%)
22	CLA	4	302	20	45,53,73	2.13	17 (37%)	52,89,113	2.97	25 (48%)
22	CLA	C	510	-	45,53,73	2.20	17 (37%)	52,89,113	2.94	24 (46%)
22	CLA	c	506	-	45,53,73	2.19	17 (37%)	52,89,113	2.93	22 (42%)
22	CLA	y	602	19	45,53,73	2.19	16 (35%)	52,89,113	2.86	22 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	y	609	19	46,54,74	1.77	9 (19%)	49,90,114	2.26	11 (22%)
22	CLA	N	614	-	45,53,73	2.23	18 (40%)	52,89,113	2.75	22 (42%)
22	CLA	2	612	19	45,53,73	2.18	16 (35%)	52,89,113	2.80	21 (40%)
22	CLA	D	403	-	45,53,73	2.23	13 (28%)	52,89,113	3.01	26 (50%)
25	CHL	5	615	-	46,54,74	1.84	11 (23%)	49,90,114	1.90	11 (22%)
22	CLA	B	605	-	45,53,73	2.16	15 (33%)	52,89,113	2.82	23 (44%)
22	CLA	c	511	3	45,53,73	2.19	17 (37%)	52,89,113	2.83	25 (48%)
23	PHO	d	402	-	31,49,69	1.81	7 (22%)	23,75,99	1.89	7 (30%)
25	CHL	g	606	-	46,54,74	1.85	10 (21%)	49,90,114	1.73	7 (14%)
22	CLA	3	313	19	45,53,73	2.20	17 (37%)	52,89,113	2.77	21 (40%)
22	CLA	s	309	18	45,53,73	2.15	15 (33%)	52,89,113	2.74	24 (46%)
25	CHL	8	301	-	46,54,74	1.82	11 (23%)	49,90,114	1.88	12 (24%)
22	CLA	g	604	-	45,53,73	2.20	17 (37%)	52,89,113	2.89	26 (50%)
25	CHL	6	601	19	46,54,74	1.81	11 (23%)	49,90,114	2.00	11 (22%)
22	CLA	N	611	-	45,53,73	2.17	14 (31%)	52,89,113	2.88	26 (50%)
22	CLA	n	602	19	45,53,73	2.17	15 (33%)	52,89,113	2.82	23 (44%)
22	CLA	g	603	-	45,53,73	2.16	18 (40%)	52,89,113	2.84	24 (46%)
25	CHL	y	607	-	46,54,74	1.81	10 (21%)	49,90,114	1.99	12 (24%)
22	CLA	8	303	-	45,53,73	2.18	17 (37%)	52,89,113	2.74	23 (44%)
22	CLA	s	305	-	45,53,73	2.21	15 (33%)	52,89,113	2.91	25 (48%)
25	CHL	4	305	20	46,54,74	1.80	11 (23%)	49,90,114	2.03	11 (22%)
22	CLA	b	614	-	45,53,73	2.18	16 (35%)	52,89,113	2.87	24 (46%)
25	CHL	N	609	19	46,54,74	1.79	10 (21%)	49,90,114	2.22	10 (20%)
22	CLA	S	304	-	45,53,73	2.10	14 (31%)	52,89,113	2.74	22 (42%)
22	CLA	g	612	19	45,53,73	2.19	15 (33%)	52,89,113	2.83	25 (48%)
22	CLA	y	603	-	45,53,73	2.12	14 (31%)	52,89,113	2.89	24 (46%)
22	CLA	b	615	-	45,53,73	2.23	17 (37%)	52,89,113	2.84	23 (44%)
25	CHL	S	302	18	46,54,74	1.83	11 (23%)	49,90,114	1.74	8 (16%)
22	CLA	C	501	-	45,53,73	2.23	16 (35%)	52,89,113	2.92	27 (51%)
22	CLA	G	602	19	45,53,73	2.19	17 (37%)	52,89,113	2.82	23 (44%)
22	CLA	Y	604	-	45,53,73	2.22	14 (31%)	52,89,113	2.98	24 (46%)
22	CLA	r	303	-	45,53,73	2.17	14 (31%)	52,89,113	3.00	27 (51%)
22	CLA	c	510	-	45,53,73	2.22	16 (35%)	52,89,113	2.83	24 (46%)
25	CHL	G	609	19	46,54,74	1.80	10 (21%)	49,90,114	2.29	11 (22%)
22	CLA	s	304	-	45,53,73	2.10	14 (31%)	52,89,113	2.74	22 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	501	-	45,53,73	2.22	14 (31%)	52,89,113	2.85	23 (44%)
22	CLA	C	512	-	45,53,73	2.22	17 (37%)	52,89,113	2.75	26 (50%)
22	CLA	5	613	19	45,53,73	2.20	17 (37%)	52,89,113	2.77	23 (44%)
22	CLA	1	611	-	45,53,73	2.19	17 (37%)	52,89,113	2.79	23 (44%)
22	CLA	C	504	-	45,53,73	2.17	16 (35%)	52,89,113	2.85	23 (44%)
22	CLA	b	611	-	45,53,73	2.17	15 (33%)	52,89,113	2.97	25 (48%)
22	CLA	n	603	-	45,53,73	2.15	14 (31%)	52,89,113	2.87	25 (48%)
25	CHL	4	308	20	46,54,74	1.81	10 (21%)	49,90,114	2.04	9 (18%)
22	CLA	r	308	17	45,53,73	2.19	15 (33%)	52,89,113	2.82	24 (46%)
22	CLA	3	314	-	45,53,73	2.25	18 (40%)	52,89,113	2.72	24 (46%)
22	CLA	r	302	-	45,53,73	2.20	15 (33%)	52,89,113	2.79	21 (40%)
25	CHL	2	605	19	42,50,74	1.67	10 (23%)	44,85,114	1.97	8 (18%)
25	CHL	3	308	-	46,54,74	1.84	10 (21%)	49,90,114	1.79	10 (20%)
25	CHL	8	308	20	46,54,74	1.81	10 (21%)	49,90,114	2.04	9 (18%)
22	CLA	N	603	-	45,53,73	2.15	14 (31%)	52,89,113	2.87	25 (48%)
25	CHL	Y	601	19	46,54,74	1.73	10 (21%)	49,90,114	1.92	12 (24%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	y	608	-	3/3/16/26	7/15/113/137	-
22	CLA	C	506	-	1/1/11/20	6/13/91/115	-
22	CLA	N	613	19	1/1/11/20	5/13/91/115	-
22	CLA	7	303	19	1/1/11/20	9/13/91/115	-
25	CHL	2	607	-	3/3/16/26	7/15/113/137	-
25	CHL	G	605	19	3/3/15/26	7/10/108/137	-
25	CHL	Y	608	-	3/3/16/26	7/15/113/137	-
22	CLA	N	612	19	1/1/11/20	8/13/91/115	-
22	CLA	Y	614	-	1/1/11/20	7/13/91/115	-
22	CLA	c	507	-	1/1/11/20	8/13/91/115	-
25	CHL	Y	606	-	3/3/16/26	8/15/113/137	-
22	CLA	B	614	-	1/1/11/20	8/13/91/115	-
25	CHL	5	609	19	3/3/16/26	12/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	611	19	1/1/11/20	8/13/91/115	-
24	HEM	e	101	6,5	-	5/12/54/54	-
22	CLA	1	602	19	1/1/11/20	8/13/91/115	-
25	CHL	N	608	-	3/3/16/26	8/15/113/137	-
22	CLA	b	604	-	1/1/11/20	9/13/91/115	-
25	CHL	1	609	19	3/3/16/26	12/15/113/137	-
22	CLA	G	612	19	1/1/11/20	8/13/91/115	-
22	CLA	6	613	-	1/1/11/20	6/13/91/115	-
22	CLA	b	603	-	1/1/11/20	5/13/91/115	-
25	CHL	g	607	-	3/3/16/26	5/15/113/137	-
22	CLA	n	604	-	1/1/11/20	8/13/91/115	-
25	CHL	5	601	19	3/3/16/26	7/15/113/137	-
22	CLA	r	311	17	1/1/11/20	5/13/91/115	-
22	CLA	N	602	19	1/1/11/20	9/13/91/115	-
22	CLA	n	614	-	1/1/11/20	7/13/91/115	-
25	CHL	6	608	19	3/3/16/26	12/15/113/137	-
25	CHL	y	601	19	3/3/16/26	7/15/113/137	-
22	CLA	8	304	-	1/1/11/20	7/13/91/115	-
22	CLA	5	610	19	1/1/11/20	6/13/91/115	-
22	CLA	B	609	-	-	4/13/91/115	-
22	CLA	S	301	-	1/1/11/20	2/13/91/115	-
22	CLA	C	508	-	1/1/11/20	5/13/91/115	-
25	CHL	n	607	-	3/3/16/26	5/15/113/137	-
25	CHL	6	607	-	3/3/16/26	7/15/113/137	-
25	CHL	8	305	20	3/3/16/26	7/15/113/137	-
22	CLA	4	309	20	1/1/11/20	6/13/91/115	-
22	CLA	y	610	19	1/1/11/20	6/13/91/115	-
22	CLA	1	603	-	1/1/11/20	5/13/91/115	-
22	CLA	2	610	-	1/1/11/20	3/13/91/115	-
22	CLA	1	610	19	1/1/11/20	6/13/91/115	-
22	CLA	7	310	19	1/1/11/20	7/13/91/115	-
22	CLA	s	313	18	1/1/11/20	5/13/91/115	-
25	CHL	2	606	-	3/3/16/26	7/15/113/137	-
25	CHL	7	307	-	3/3/16/26	6/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	503	-	1/1/11/20	9/13/91/115	-
22	CLA	Y	613	19	1/1/11/20	5/13/91/115	-
22	CLA	y	614	-	1/1/11/20	7/13/91/115	-
22	CLA	y	611	-	1/1/11/20	7/13/91/115	-
25	CHL	g	601	19	3/3/16/26	7/15/113/137	-
22	CLA	b	612	-	1/1/11/20	9/13/91/115	-
22	CLA	1	604	-	1/1/11/20	4/13/91/115	-
22	CLA	y	604	-	1/1/11/20	6/13/91/115	-
22	CLA	3	310	19	1/1/11/20	7/13/91/115	-
25	CHL	4	301	-	3/3/16/26	8/15/113/137	-
22	CLA	7	314	-	1/1/11/20	6/13/91/115	-
22	CLA	R	308	17	1/1/11/20	7/13/91/115	-
25	CHL	2	601	19	3/3/16/26	8/15/113/137	-
25	CHL	g	608	-	3/3/16/26	8/15/113/137	-
25	CHL	n	609	19	3/3/16/26	13/15/113/137	-
22	CLA	4	303	-	1/1/11/20	8/13/91/115	-
22	CLA	b	601	-	1/1/11/20	9/13/91/115	-
22	CLA	S	310	18	1/1/11/20	8/13/91/115	-
23	PHO	a	404	-	-	3/13/79/103	0/5/6/6
22	CLA	d	403	-	1/1/11/20	7/13/91/115	-
22	CLA	b	606	-	1/1/11/20	4/13/91/115	-
25	CHL	Y	605	19	3/3/15/26	7/10/108/137	-
22	CLA	a	405	-	1/1/11/20	4/13/91/115	-
22	CLA	R	303	-	1/1/11/20	4/13/91/115	-
25	CHL	Y	607	-	3/3/16/26	5/15/113/137	-
22	CLA	R	301	17	1/1/11/20	9/13/91/115	-
22	CLA	4	304	-	1/1/11/20	7/13/91/115	-
25	CHL	r	305	-	3/3/16/26	8/15/113/137	-
22	CLA	b	605	-	-	2/13/91/115	-
22	CLA	3	304	-	1/1/11/20	6/13/91/115	-
22	CLA	G	603	-	1/1/11/20	6/13/91/115	-
22	CLA	s	303	18	1/1/11/20	9/13/91/115	-
25	CHL	7	308	-	3/3/16/26	7/15/113/137	-
25	CHL	3	302	19	3/3/16/26	7/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	507	-	1/1/11/20	8/13/91/115	-
25	CHL	R	306	-	3/3/16/26	13/15/113/137	-
22	CLA	A	402	-	1/1/11/20	5/13/91/115	-
22	CLA	7	305	-	1/1/11/20	6/13/91/115	-
22	CLA	c	508	-	1/1/11/20	5/13/91/115	-
22	CLA	B	616	-	1/1/11/20	6/13/91/115	-
22	CLA	C	509	-	1/1/11/20	8/13/91/115	-
25	CHL	5	607	-	3/3/16/26	6/15/113/137	-
22	CLA	8	309	20	1/1/11/20	6/13/91/115	-
25	CHL	n	606	-	3/3/16/26	6/15/113/137	-
22	CLA	s	311	-	1/1/11/20	4/13/91/115	-
22	CLA	Y	603	-	1/1/11/20	8/13/91/115	-
22	CLA	D	401	-	1/1/11/20	6/13/91/115	-
25	CHL	S	307	-	3/3/16/26	7/15/113/137	-
22	CLA	d	404	-	1/1/11/20	6/13/91/115	-
25	CHL	5	605	19	3/3/15/26	7/10/108/137	-
25	CHL	G	606	-	3/3/16/26	8/15/113/137	-
22	CLA	d	401	-	1/1/11/20	6/13/91/115	-
22	CLA	3	312	19	1/1/11/20	7/13/91/115	-
25	CHL	8	306	-	3/3/16/26	12/15/113/137	-
25	CHL	R	305	-	3/3/16/26	8/15/113/137	-
22	CLA	R	312	20,17	1/1/11/20	5/13/91/115	-
22	CLA	5	604	-	1/1/11/20	4/13/91/115	-
25	CHL	3	301	-	3/3/16/26	7/15/113/137	-
23	PHO	A	404	-	-	4/13/79/103	0/5/6/6
22	CLA	n	612	19	1/1/11/20	8/13/91/115	-
22	CLA	s	312	18	1/1/11/20	6/13/91/115	-
25	CHL	G	601	19	3/3/16/26	7/15/113/137	-
22	CLA	B	613	-	1/1/11/20	5/13/91/115	-
22	CLA	G	604	-	1/1/11/20	8/13/91/115	-
22	CLA	G	610	19	1/1/11/20	7/13/91/115	-
22	CLA	2	609	19	1/1/11/20	6/13/91/115	-
22	CLA	G	614	-	1/1/11/20	6/13/91/115	-
22	CLA	S	305	-	1/1/11/20	9/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	305	-	1/1/11/20	6/13/91/115	-
25	CHL	r	306	-	3/3/16/26	13/15/113/137	-
25	CHL	s	307	-	3/3/16/26	7/15/113/137	-
22	CLA	S	312	18	1/1/11/20	6/13/91/115	-
22	CLA	1	613	19	1/1/11/20	4/13/91/115	-
25	CHL	4	307	-	3/3/16/26	10/15/113/137	-
22	CLA	8	310	-	1/1/11/20	4/13/91/115	-
22	CLA	c	502	-	1/1/11/20	6/13/91/115	-
22	CLA	B	615	-	1/1/11/20	10/13/91/115	-
22	CLA	2	603	-	1/1/11/20	6/13/91/115	-
22	CLA	C	503	-	1/1/11/20	9/13/91/115	-
25	CHL	6	605	19	3/3/15/26	6/10/108/137	-
22	CLA	r	307	17	1/1/11/20	9/13/91/115	-
22	CLA	C	502	-	1/1/11/20	7/13/91/115	-
22	CLA	n	613	19	1/1/11/20	5/13/91/115	-
25	CHL	1	601	19	3/3/16/26	7/15/113/137	-
22	CLA	n	610	19	1/1/11/20	7/13/91/115	-
22	CLA	b	607	-	1/1/11/20	6/13/91/115	-
22	CLA	5	614	-	1/1/11/20	6/13/91/115	-
22	CLA	7	304	-	1/1/11/20	6/13/91/115	-
22	CLA	Y	602	19	1/1/11/20	9/13/91/115	-
24	HEM	E	101	6,5	-	3/12/54/54	-
22	CLA	g	613	19	1/1/11/20	5/13/91/115	-
22	CLA	7	311	-	1/1/11/20	5/13/91/115	-
25	CHL	7	302	19	3/3/16/26	7/15/113/137	-
22	CLA	6	612	19	1/1/11/20	5/13/91/115	-
22	CLA	B	608	-	-	4/13/91/115	-
25	CHL	2	608	19	3/3/16/26	12/15/113/137	-
25	CHL	1	607	-	3/3/16/26	6/15/113/137	-
22	CLA	R	307	17	1/1/11/20	9/13/91/115	-
22	CLA	B	606	-	-	3/13/91/115	-
25	CHL	n	608	-	3/3/16/26	8/15/113/137	-
25	CHL	8	307	-	3/3/16/26	10/15/113/137	-
25	CHL	1	605	19	3/3/15/26	7/10/108/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	y	605	19	3/3/15/26	7/10/108/137	-
25	CHL	g	605	19	3/3/15/26	7/10/108/137	-
25	CHL	5	608	-	3/3/16/26	7/15/113/137	-
22	CLA	S	313	18	1/1/11/20	5/13/91/115	-
22	CLA	Y	612	19	1/1/11/20	9/13/91/115	-
25	CHL	4	306	-	3/3/16/26	12/15/113/137	-
22	CLA	C	505	-	1/1/11/20	8/13/91/115	-
25	CHL	5	606	-	3/3/16/26	6/15/113/137	-
22	CLA	r	310	-	1/1/11/20	7/13/91/115	-
22	CLA	6	603	-	1/1/11/20	6/13/91/115	-
25	CHL	3	306	19	3/3/15/26	7/10/108/137	-
22	CLA	G	611	-	1/1/11/20	5/13/91/115	-
22	CLA	R	302	-	1/1/11/20	9/13/91/115	-
22	CLA	B	603	-	1/1/11/20	6/13/91/115	-
22	CLA	R	311	17	1/1/11/20	5/13/91/115	-
25	CHL	1	608	-	3/3/16/26	7/15/113/137	-
25	CHL	G	607	-	3/3/16/26	5/15/113/137	-
25	CHL	s	306	18	3/3/16/26	9/15/113/137	-
22	CLA	S	303	18	1/1/11/20	9/13/91/115	-
25	CHL	N	607	-	3/3/16/26	5/15/113/137	-
25	CHL	1	606	-	3/3/16/26	6/15/113/137	-
22	CLA	A	403	-	1/1/11/20	8/13/91/115	-
25	CHL	n	605	19	3/3/15/26	7/10/108/137	-
22	CLA	B	607	-	1/1/11/20	4/13/91/115	-
22	CLA	5	602	19	1/1/11/20	8/13/91/115	-
25	CHL	s	308	-	3/3/16/26	7/15/113/137	-
22	CLA	g	610	19	1/1/11/20	7/13/91/115	-
25	CHL	3	309	19	3/3/16/26	12/15/113/137	-
22	CLA	Y	611	-	1/1/11/20	7/13/91/115	-
22	CLA	6	610	-	1/1/11/20	3/13/91/115	-
22	CLA	S	314	-	1/1/11/20	5/13/91/115	-
22	CLA	2	602	19	1/1/11/20	7/13/91/115	-
22	CLA	B	612	-	1/1/11/20	8/13/91/115	-
22	CLA	c	504	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	D	404	-	1/1/11/20	6/13/91/115	-
22	CLA	8	302	20	1/1/11/20	5/13/91/115	-
22	CLA	7	313	19	1/1/11/20	5/13/91/115	-
25	CHL	R	304	-	3/3/16/26	10/15/113/137	-
25	CHL	Y	609	19	3/3/16/26	13/15/113/137	-
25	CHL	S	306	18	3/3/16/26	9/15/113/137	-
25	CHL	7	301	-	3/3/16/26	7/15/113/137	-
23	PHO	D	402	-	-	4/13/79/103	0/5/6/6
22	CLA	b	608	-	1/1/11/20	4/13/91/115	-
22	CLA	5	611	-	1/1/11/20	5/13/91/115	-
25	CHL	3	307	-	3/3/16/26	6/15/113/137	-
22	CLA	a	403	-	1/1/11/20	8/13/91/115	-
22	CLA	2	611	19	1/1/11/20	8/13/91/115	-
25	CHL	S	308	-	3/3/16/26	7/15/113/137	-
22	CLA	5	612	19	1/1/11/20	7/13/91/115	-
25	CHL	r	304	-	3/3/16/26	10/15/113/137	-
22	CLA	g	602	19	1/1/11/20	9/13/91/115	-
22	CLA	G	613	19	1/1/11/20	5/13/91/115	-
22	CLA	y	612	19	1/1/11/20	9/13/91/115	-
22	CLA	7	312	19	1/1/11/20	7/13/91/115	-
25	CHL	y	606	-	3/3/16/26	8/15/113/137	-
22	CLA	N	610	19	1/1/11/20	7/13/91/115	-
22	CLA	R	310	-	1/1/11/20	7/13/91/115	-
25	CHL	1	615	-	3/3/16/26	9/15/113/137	-
22	CLA	B	601	-	-	9/13/91/115	-
22	CLA	B	602	-	1/1/11/20	7/13/91/115	-
22	CLA	2	604	-	1/1/11/20	8/13/91/115	-
22	CLA	B	604	-	1/1/11/20	7/13/91/115	-
22	CLA	A	405	-	1/1/11/20	4/13/91/115	-
22	CLA	Y	610	19	1/1/11/20	6/13/91/115	-
22	CLA	2	613	-	1/1/11/20	6/13/91/115	-
22	CLA	r	309	-	1/1/11/20	8/13/91/115	-
22	CLA	c	509	-	1/1/11/20	8/13/91/115	-
22	CLA	g	614	-	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	g	611	-	1/1/11/20	5/13/91/115	-
22	CLA	C	511	3	-	6/13/91/115	-
25	CHL	N	605	19	3/3/15/26	7/10/108/137	-
22	CLA	r	312	20,17	1/1/11/20	5/13/91/115	-
25	CHL	N	601	19	3/3/16/26	7/15/113/137	-
25	CHL	N	606	-	3/3/16/26	6/15/113/137	-
22	CLA	3	311	-	1/1/11/20	5/13/91/115	-
22	CLA	4	310	-	1/1/11/20	4/13/91/115	-
22	CLA	B	611	-	1/1/11/20	4/13/91/115	-
22	CLA	N	604	-	1/1/11/20	8/13/91/115	-
25	CHL	6	606	-	3/3/16/26	7/15/113/137	-
22	CLA	3	303	19	1/1/11/20	9/13/91/115	-
25	CHL	7	306	19	3/3/15/26	7/10/108/137	-
22	CLA	b	613	-	1/1/11/20	5/13/91/115	-
22	CLA	s	310	18	1/1/11/20	8/13/91/115	-
22	CLA	6	609	19	1/1/11/20	6/13/91/115	-
22	CLA	c	512	-	1/1/11/20	2/13/91/115	-
22	CLA	R	309	-	1/1/11/20	8/13/91/115	-
25	CHL	7	309	19	3/3/16/26	12/15/113/137	-
25	CHL	G	608	-	3/3/16/26	8/15/113/137	-
22	CLA	r	301	17	1/1/11/20	9/13/91/115	-
25	CHL	s	302	18	3/3/16/26	6/15/113/137	-
25	CHL	g	609	19	3/3/16/26	12/15/113/137	-
22	CLA	6	604	-	1/1/11/20	8/13/91/115	-
22	CLA	S	311	-	1/1/11/20	4/13/91/115	-
22	CLA	b	609	-	-	4/13/91/115	-
22	CLA	b	616	-	1/1/11/20	10/13/91/115	-
22	CLA	5	603	-	1/1/11/20	5/13/91/115	-
22	CLA	s	314	-	1/1/11/20	5/13/91/115	-
22	CLA	y	613	19	1/1/11/20	5/13/91/115	-
22	CLA	n	611	-	1/1/11/20	6/13/91/115	-
22	CLA	a	402	-	1/1/11/20	5/13/91/115	-
22	CLA	l	614	-	1/1/11/20	6/13/91/115	-
22	CLA	b	610	-	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	602	19	1/1/11/20	7/13/91/115	-
25	CHL	n	601	19	3/3/16/26	7/15/113/137	-
22	CLA	s	301	-	1/1/11/20	3/13/91/115	-
22	CLA	c	505	-	1/1/11/20	9/13/91/115	-
22	CLA	b	602	-	-	5/13/91/115	-
22	CLA	B	610	-	1/1/11/20	8/13/91/115	-
22	CLA	S	309	18	1/1/11/20	4/13/91/115	-
22	CLA	1	612	19	1/1/11/20	7/13/91/115	-
22	CLA	4	302	20	1/1/11/20	5/13/91/115	-
22	CLA	C	510	-	1/1/11/20	5/13/91/115	-
22	CLA	c	506	-	1/1/11/20	6/13/91/115	-
22	CLA	y	602	19	1/1/11/20	9/13/91/115	-
25	CHL	y	609	19	3/3/16/26	13/15/113/137	-
22	CLA	N	614	-	1/1/11/20	7/13/91/115	-
22	CLA	2	612	19	1/1/11/20	5/13/91/115	-
22	CLA	D	403	-	1/1/11/20	6/13/91/115	-
25	CHL	5	615	-	3/3/16/26	9/15/113/137	-
22	CLA	B	605	-	1/1/11/20	2/13/91/115	-
22	CLA	c	511	3	-	6/13/91/115	-
23	PHO	d	402	-	-	6/13/79/103	0/5/6/6
25	CHL	g	606	-	3/3/16/26	8/15/113/137	-
22	CLA	3	313	19	1/1/11/20	5/13/91/115	-
22	CLA	s	309	18	1/1/11/20	4/13/91/115	-
25	CHL	8	301	-	3/3/16/26	8/15/113/137	-
22	CLA	g	604	-	1/1/11/20	8/13/91/115	-
25	CHL	6	601	19	3/3/16/26	8/15/113/137	-
22	CLA	N	611	-	1/1/11/20	6/13/91/115	-
22	CLA	n	602	19	1/1/11/20	9/13/91/115	-
22	CLA	g	603	-	1/1/11/20	6/13/91/115	-
25	CHL	y	607	-	3/3/16/26	5/15/113/137	-
22	CLA	8	303	-	1/1/11/20	8/13/91/115	-
22	CLA	s	305	-	1/1/11/20	9/13/91/115	-
25	CHL	4	305	20	3/3/16/26	7/15/113/137	-
22	CLA	b	614	-	-	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	N	609	19	3/3/16/26	13/15/113/137	-
22	CLA	S	304	-	1/1/11/20	6/13/91/115	-
22	CLA	g	612	19	1/1/11/20	8/13/91/115	-
22	CLA	y	603	-	1/1/11/20	8/13/91/115	-
22	CLA	b	615	-	1/1/11/20	9/13/91/115	-
25	CHL	S	302	18	3/3/16/26	6/15/113/137	-
22	CLA	C	501	-	1/1/11/20	5/13/91/115	-
22	CLA	G	602	19	1/1/11/20	9/13/91/115	-
22	CLA	Y	604	-	1/1/11/20	6/13/91/115	-
22	CLA	r	303	-	1/1/11/20	4/13/91/115	-
22	CLA	c	510	-	1/1/11/20	5/13/91/115	-
25	CHL	G	609	19	3/3/16/26	12/15/113/137	-
22	CLA	s	304	-	1/1/11/20	6/13/91/115	-
22	CLA	c	501	-	1/1/11/20	4/13/91/115	-
22	CLA	C	512	-	1/1/11/20	3/13/91/115	-
22	CLA	5	613	19	1/1/11/20	4/13/91/115	-
22	CLA	1	611	-	1/1/11/20	5/13/91/115	-
22	CLA	C	504	-	1/1/11/20	8/13/91/115	-
22	CLA	b	611	-	-	3/13/91/115	-
22	CLA	n	603	-	1/1/11/20	5/13/91/115	-
25	CHL	4	308	20	3/3/16/26	8/15/113/137	-
22	CLA	r	308	17	1/1/11/20	7/13/91/115	-
22	CLA	3	314	-	1/1/11/20	6/13/91/115	-
22	CLA	r	302	-	1/1/11/20	9/13/91/115	-
25	CHL	2	605	19	3/3/15/26	6/10/108/137	-
25	CHL	3	308	-	3/3/16/26	7/15/113/137	-
25	CHL	8	308	20	3/3/16/26	8/15/113/137	-
22	CLA	N	603	-	1/1/11/20	5/13/91/115	-
25	CHL	Y	601	19	3/3/16/26	7/15/113/137	-

The worst 5 of 4345 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	609	CHL	O2A-CGA	6.01	1.51	1.30
25	g	609	CHL	O2A-CGA	6.01	1.51	1.30
25	N	609	CHL	O2A-CGA	6.00	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	609	CHL	O2A-CGA	6.00	1.50	1.30
25	3	309	CHL	O2A-CGA	5.97	1.50	1.30

The worst 5 of 6088 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	307	CHL	O2D-CGD-CBD	28.05	161.12	111.27
25	s	307	CHL	O2D-CGD-CBD	28.05	161.12	111.27
25	4	307	CHL	O2D-CGD-CBD	27.92	160.89	111.27
25	8	307	CHL	O2D-CGD-CBD	27.92	160.89	111.27
25	S	307	CHL	O2D-CGD-O1D	-23.93	77.05	123.84

5 of 489 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	405	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND

5 of 2132 torsion outliers are listed below:

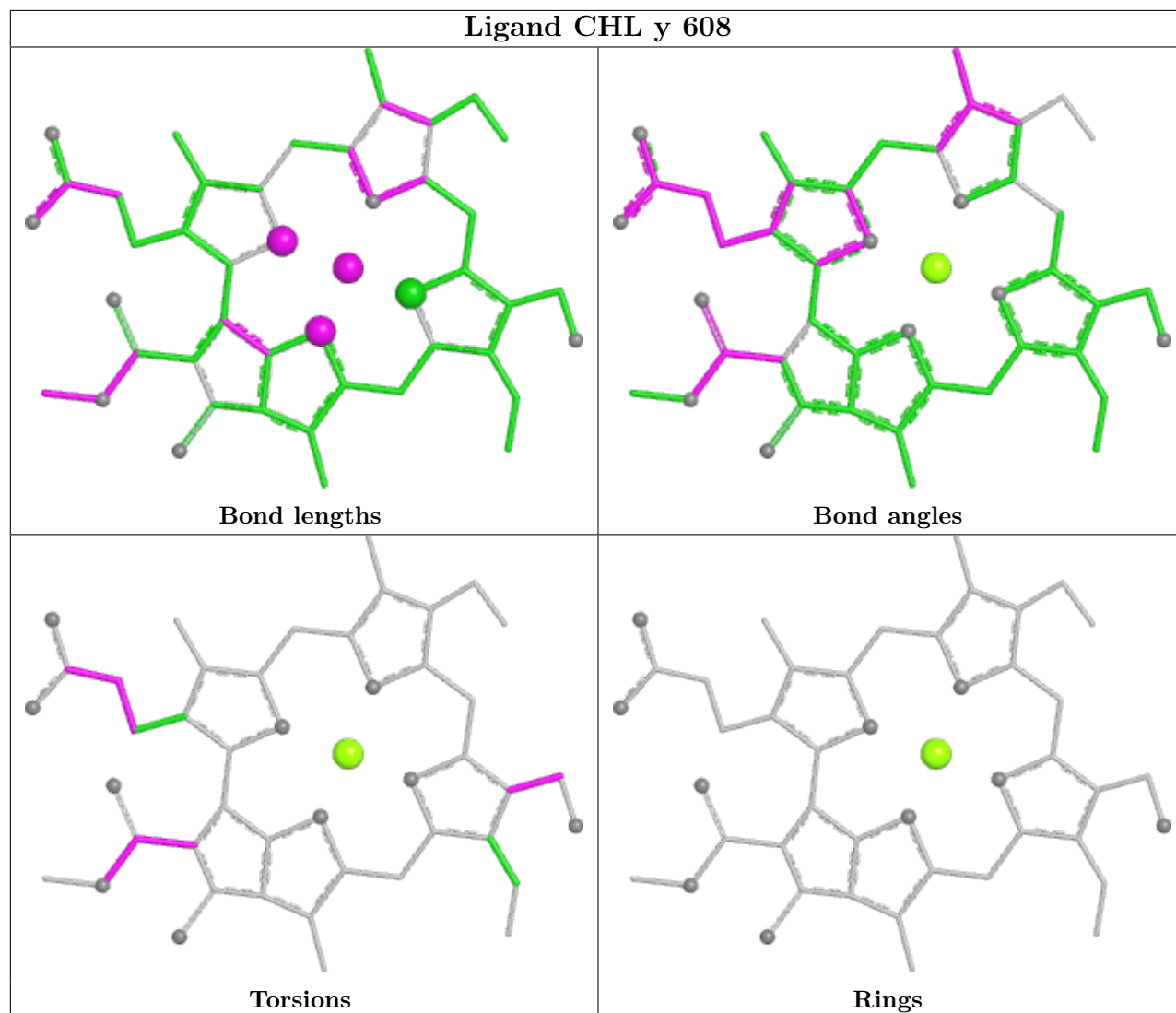
Mol	Chain	Res	Type	Atoms
22	A	402	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C1A-C2A-CAA-CBA
22	A	405	CLA	C3A-C2A-CAA-CBA
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CAD-CBD-CGD-O1D

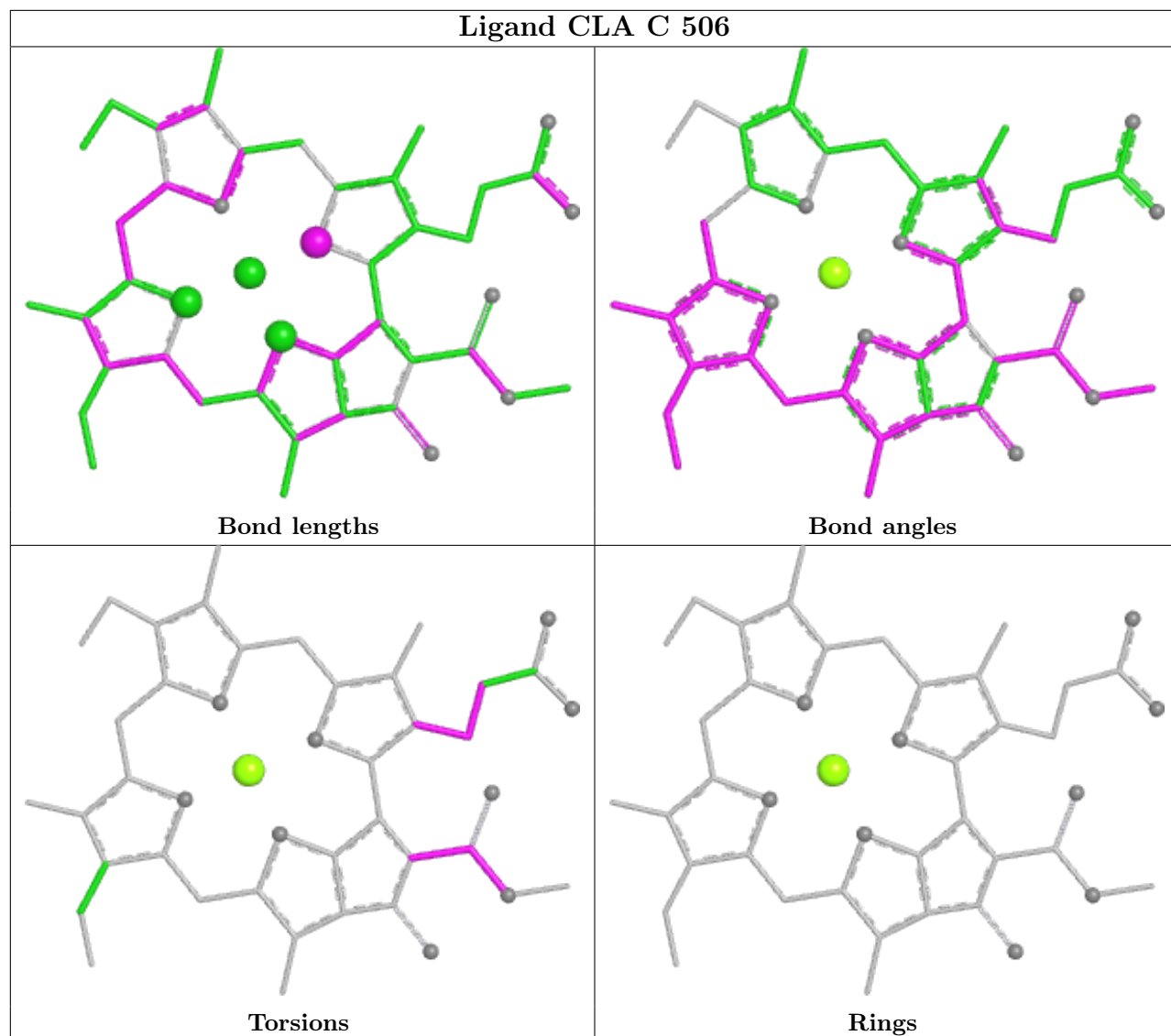
There are no ring outliers.

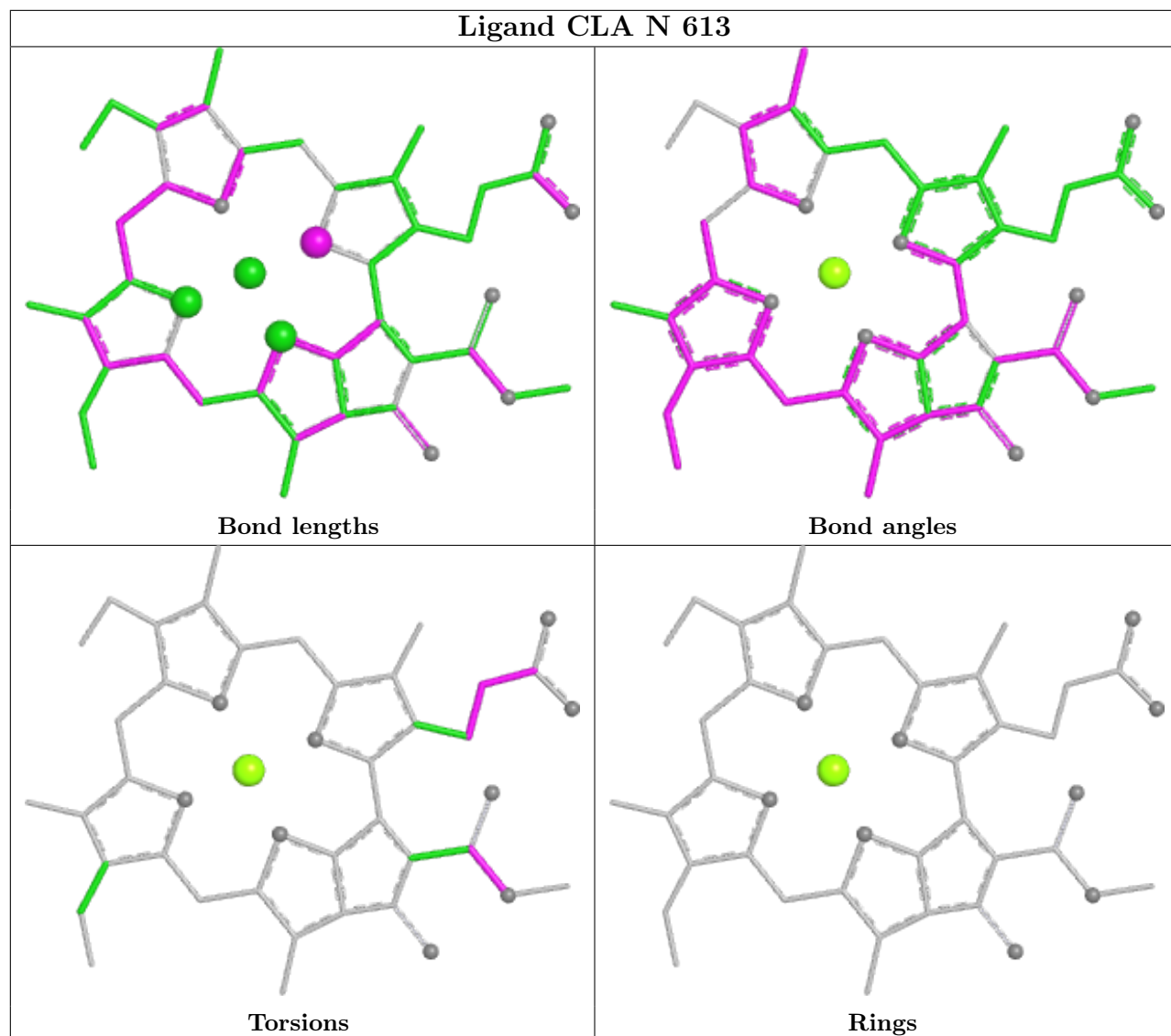
No monomer is involved in short contacts.

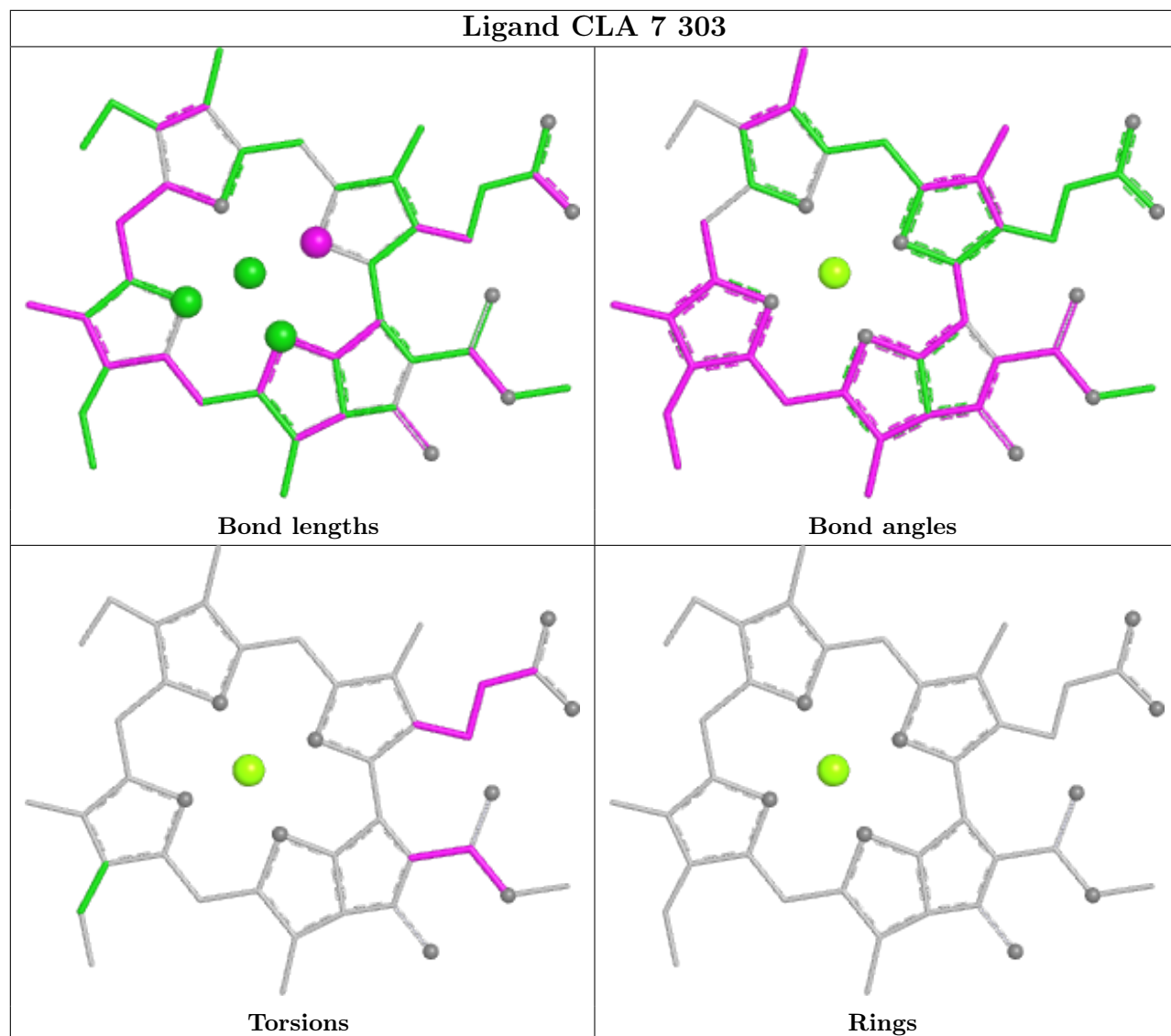
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

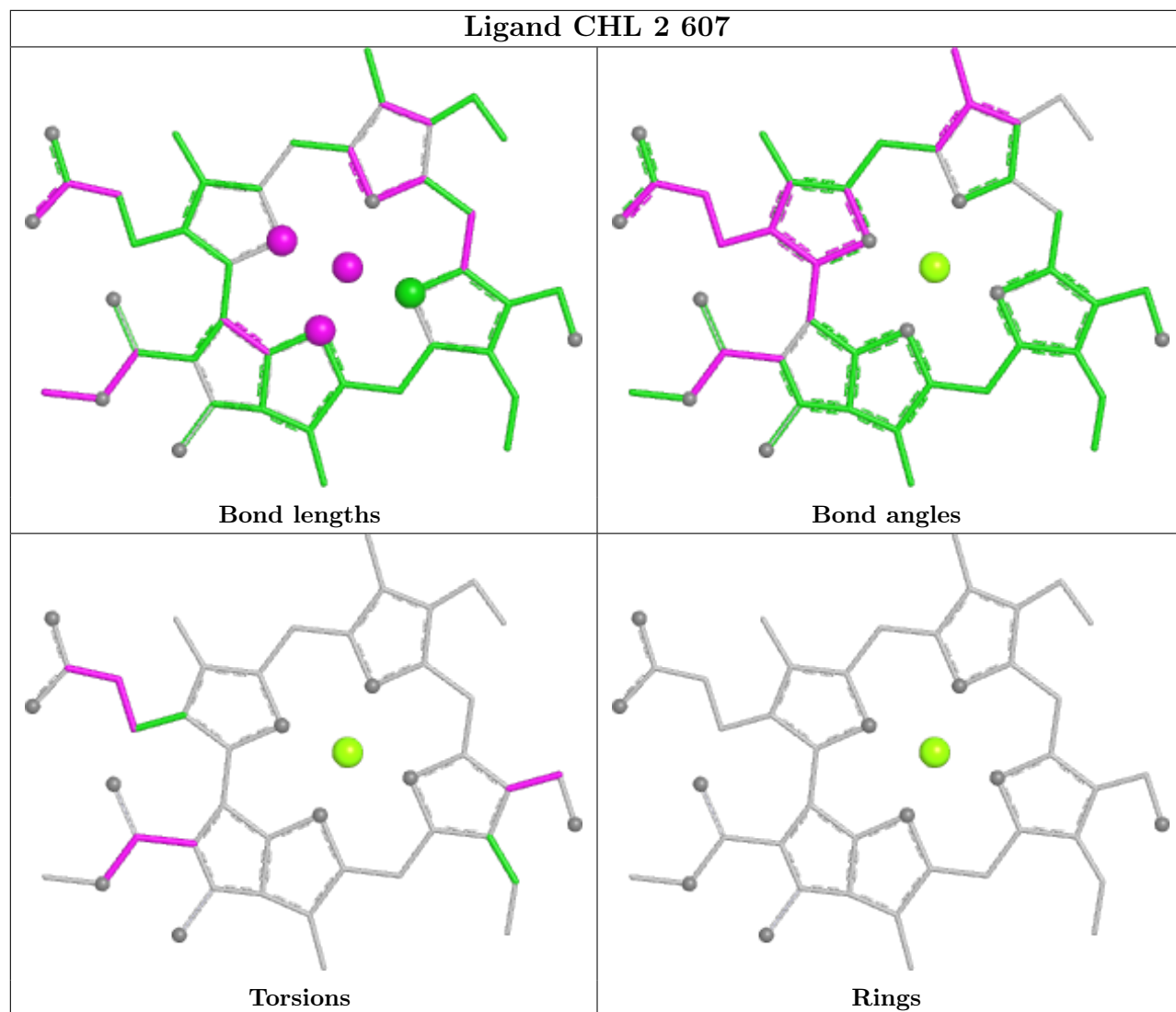
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

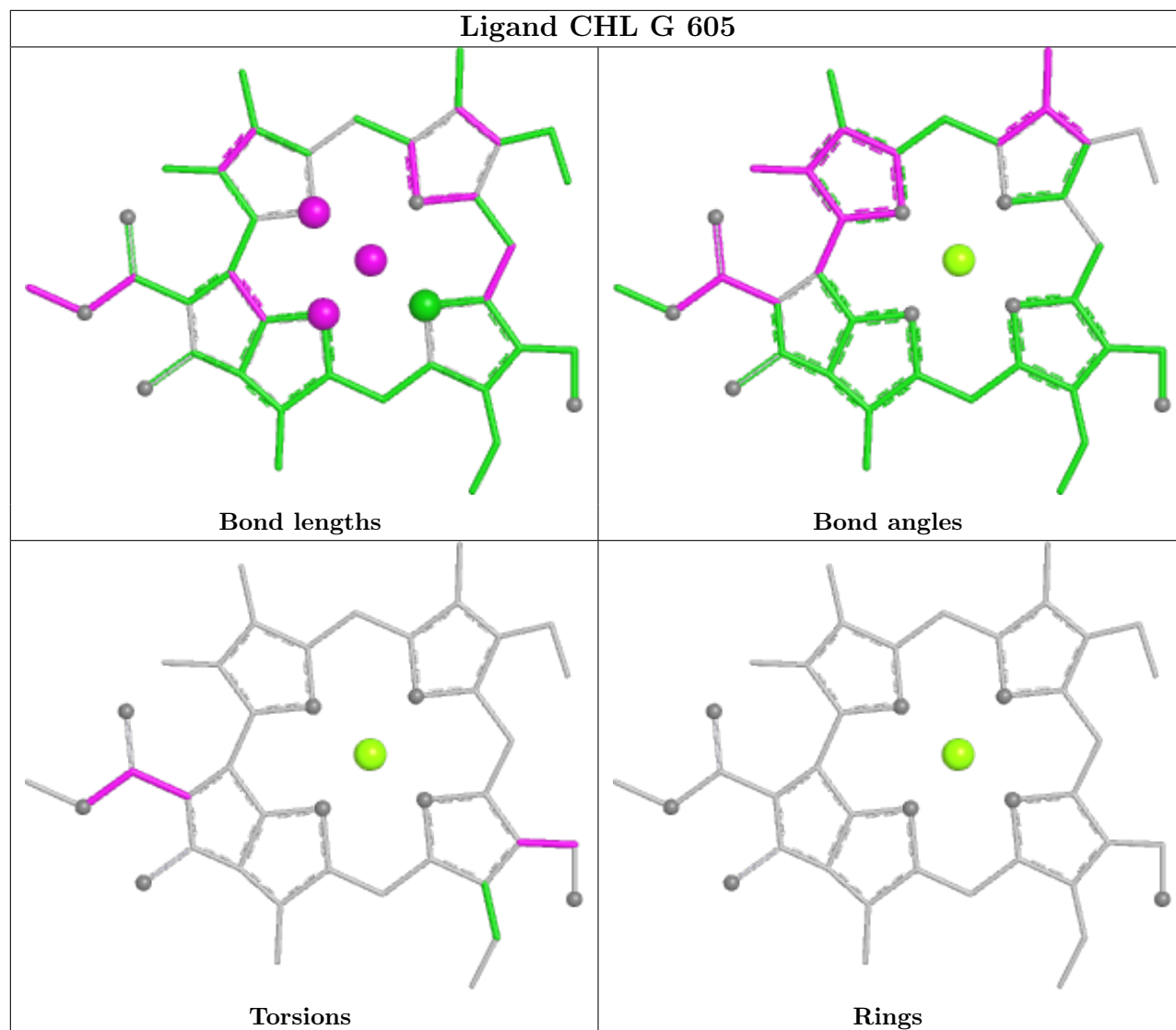


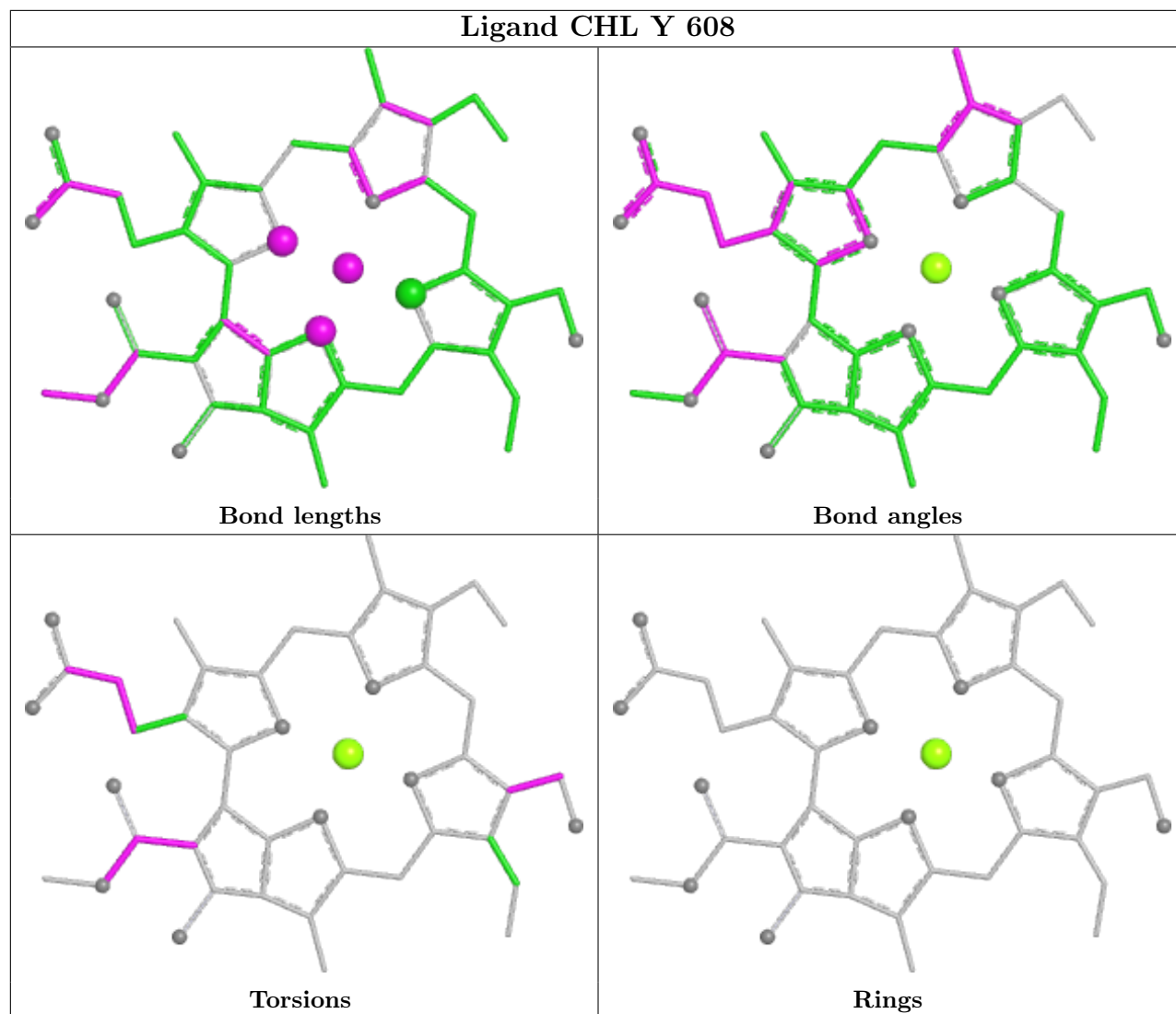


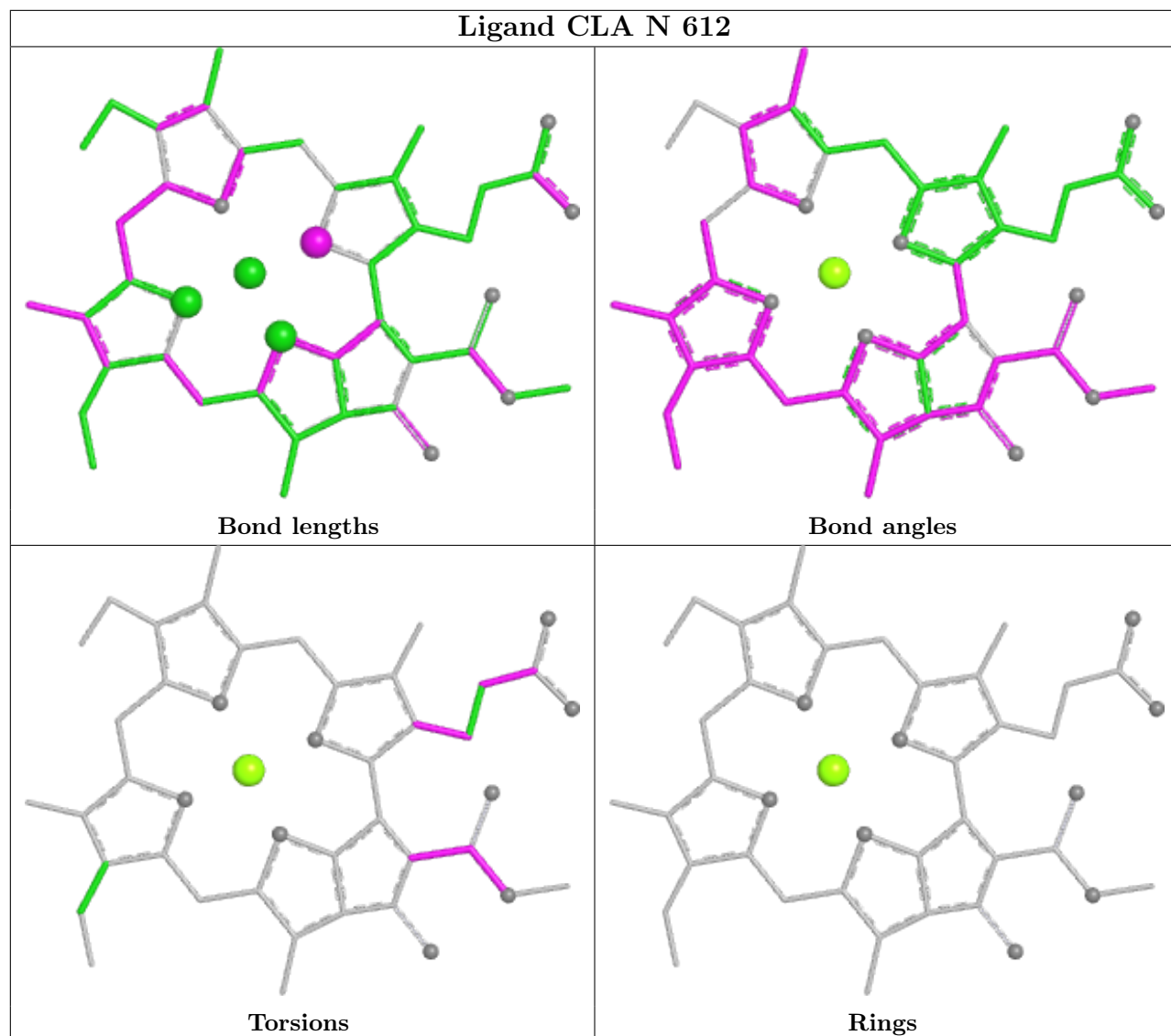


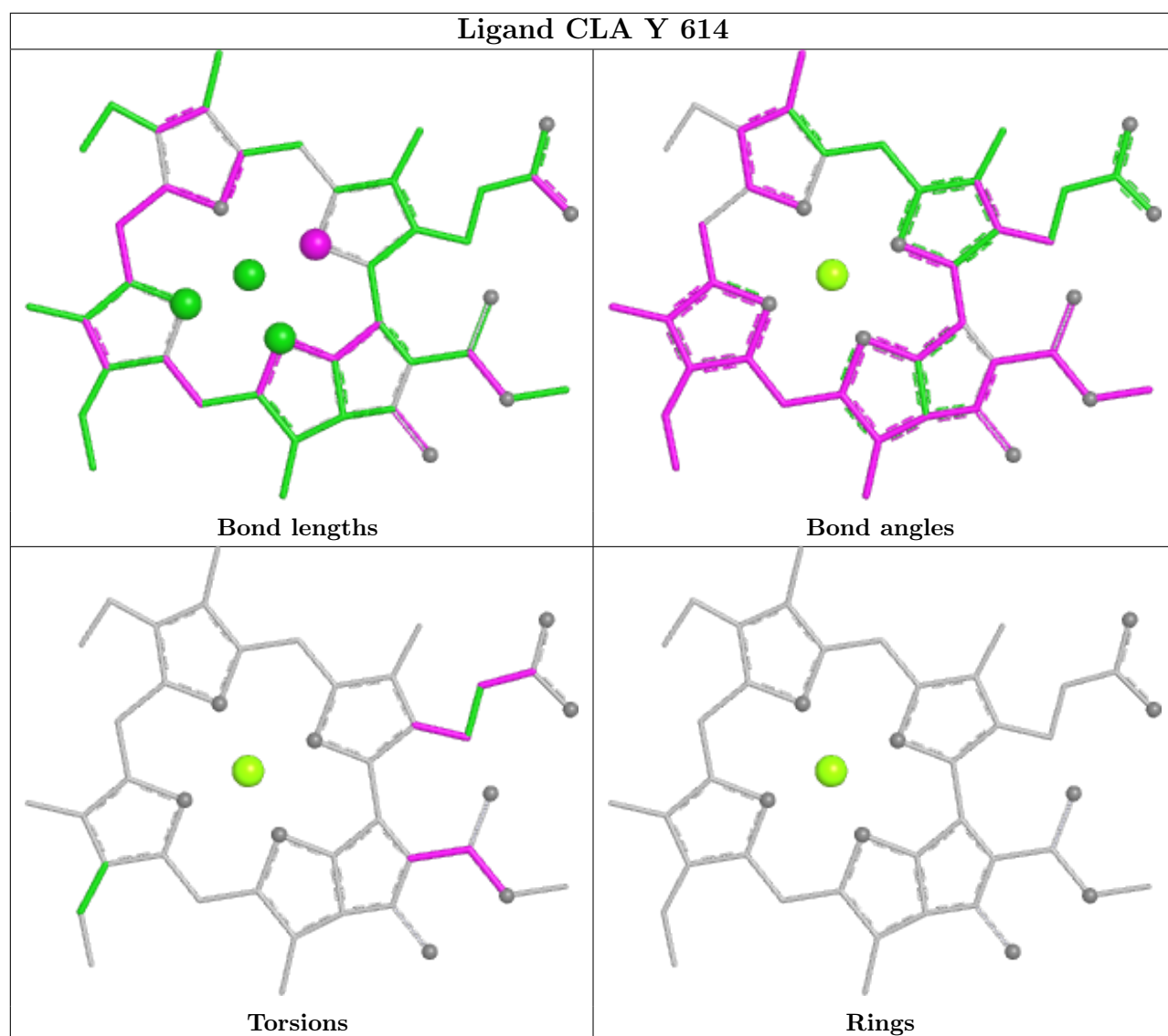


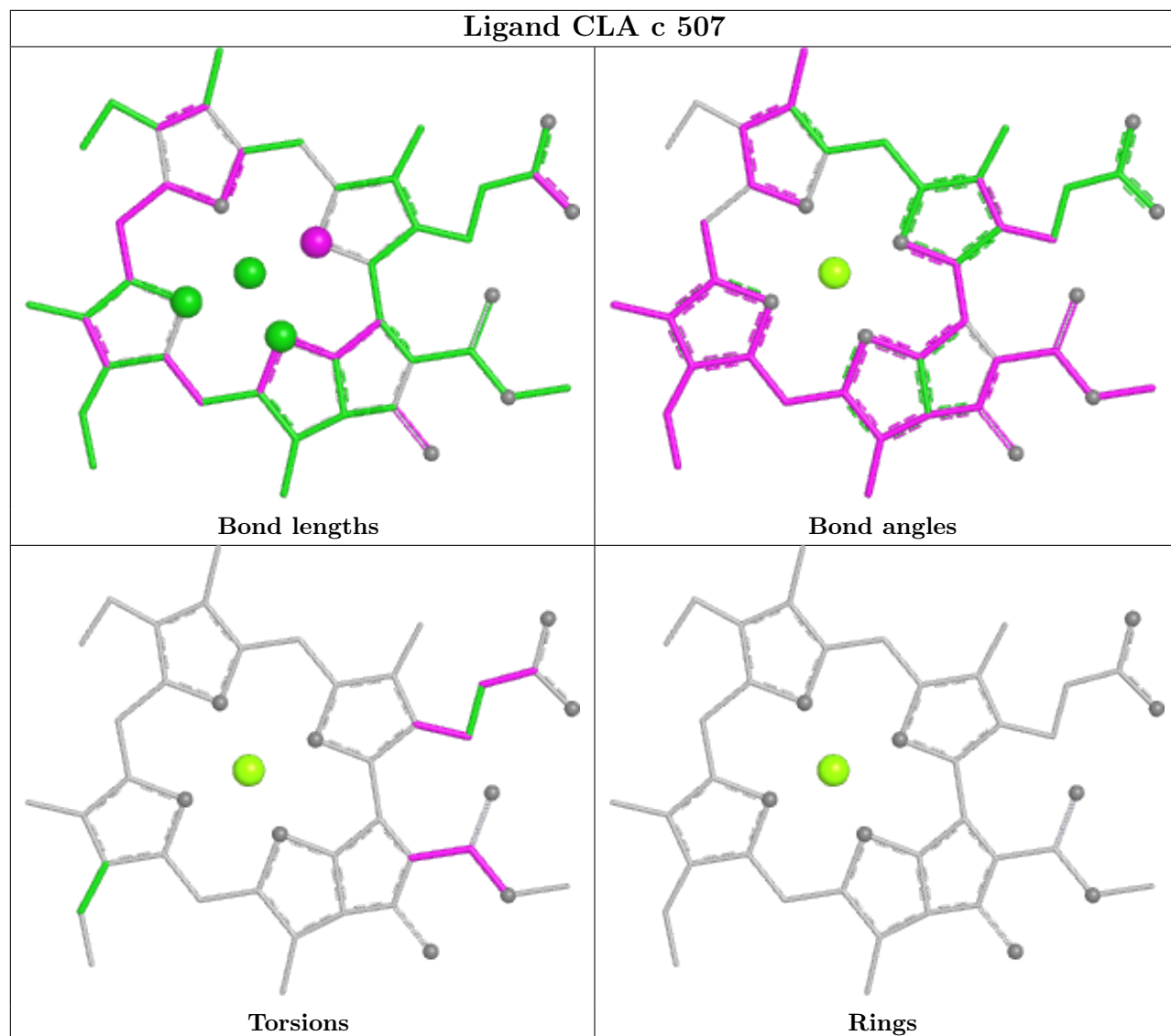


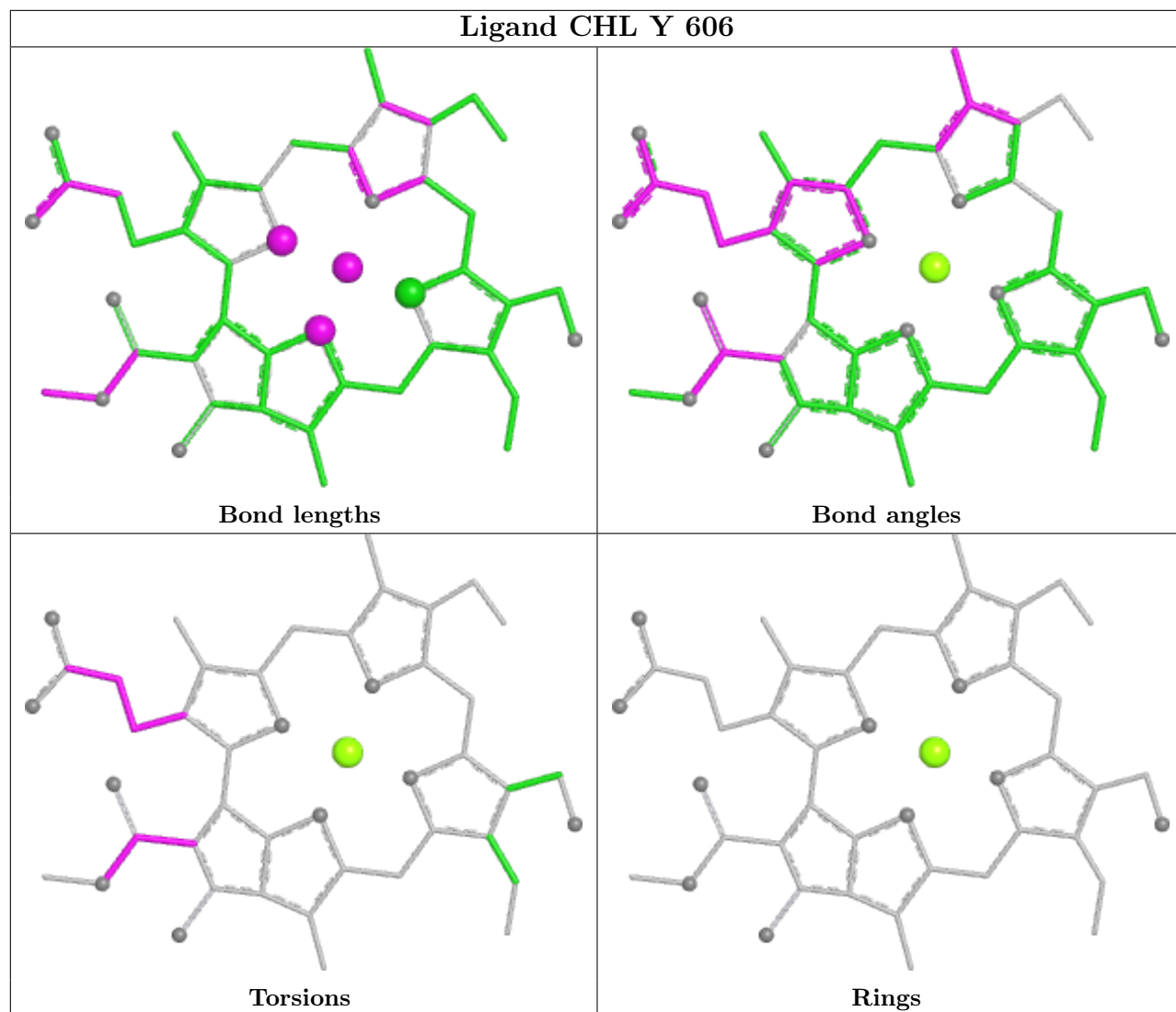


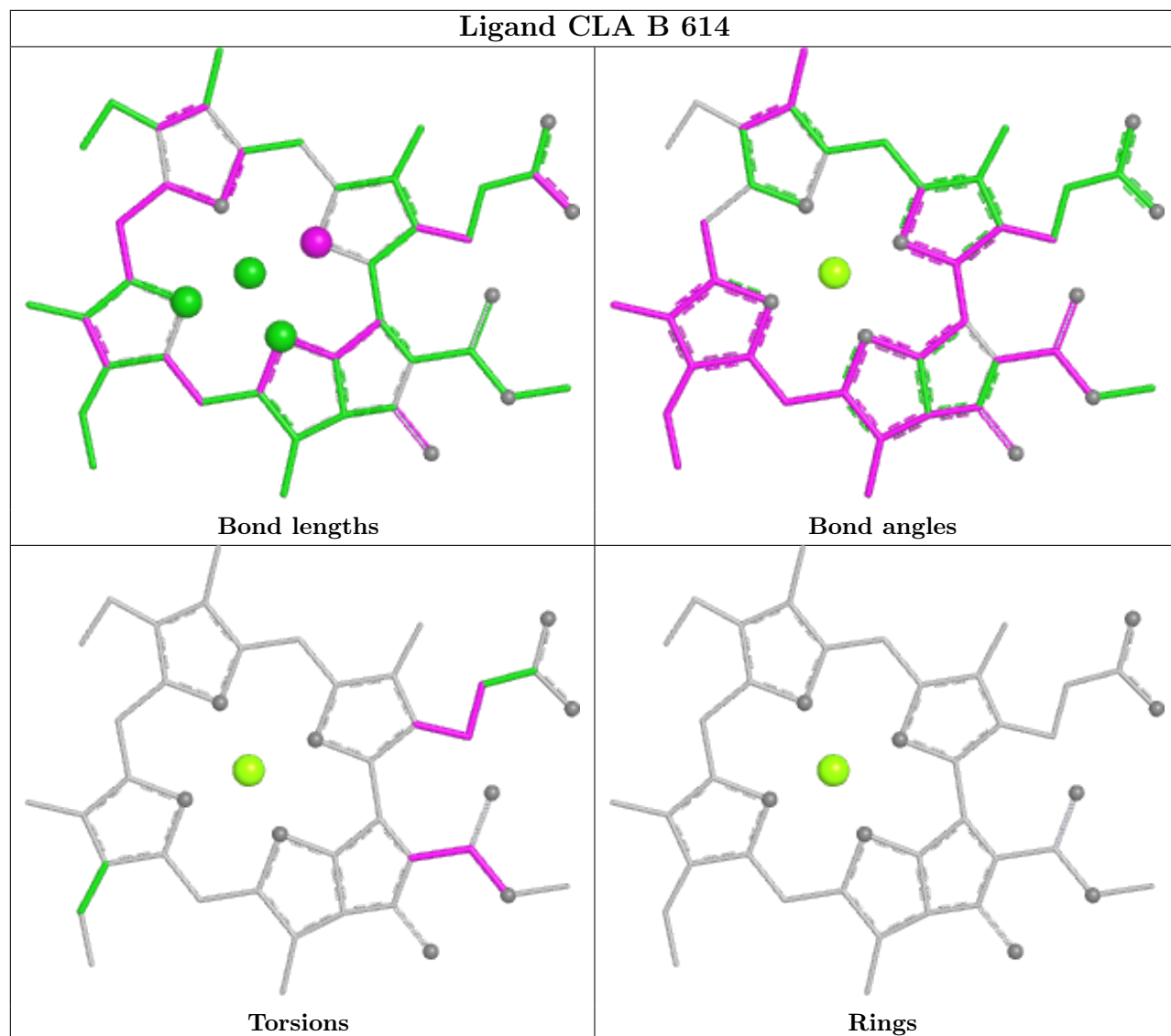


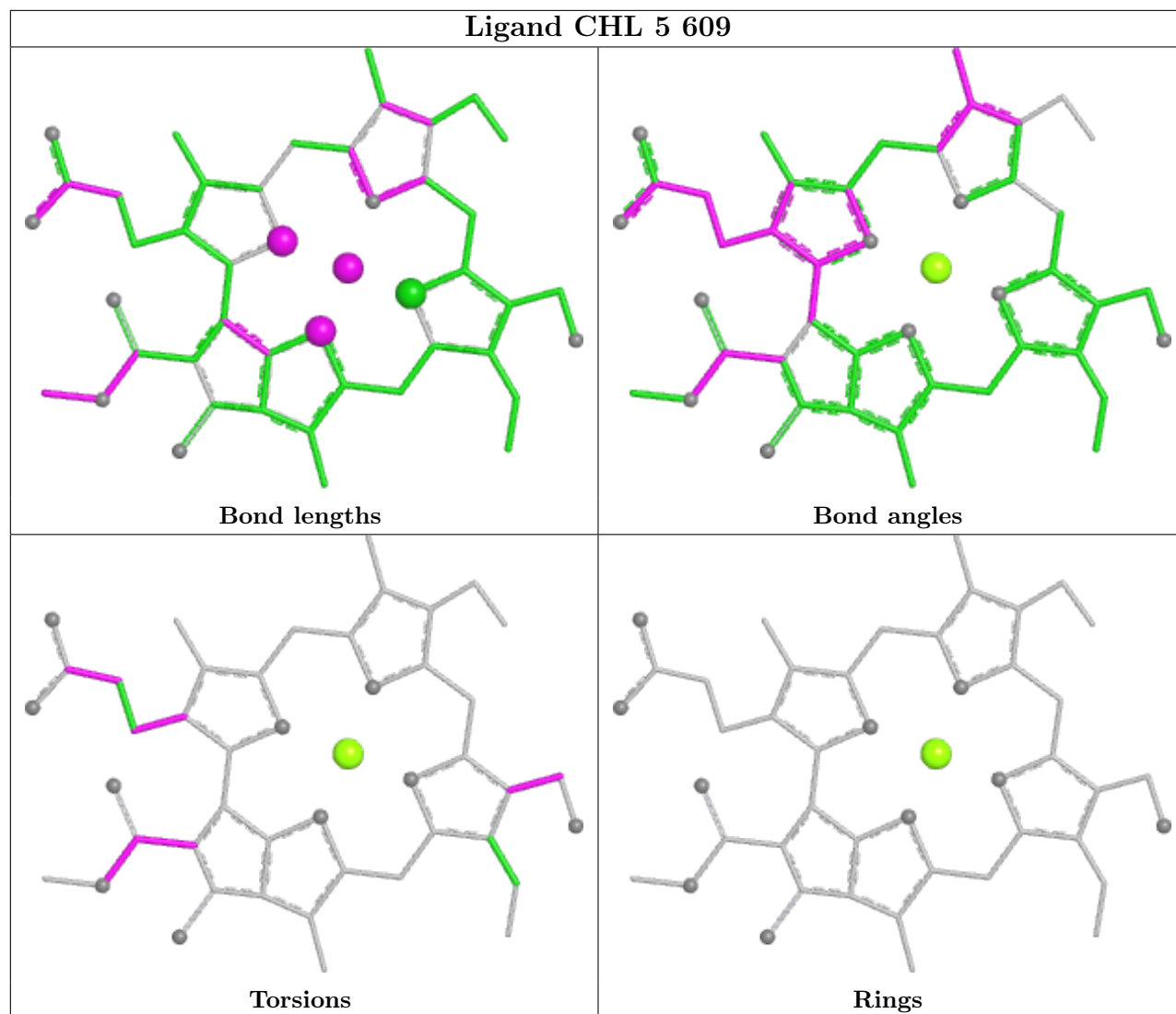


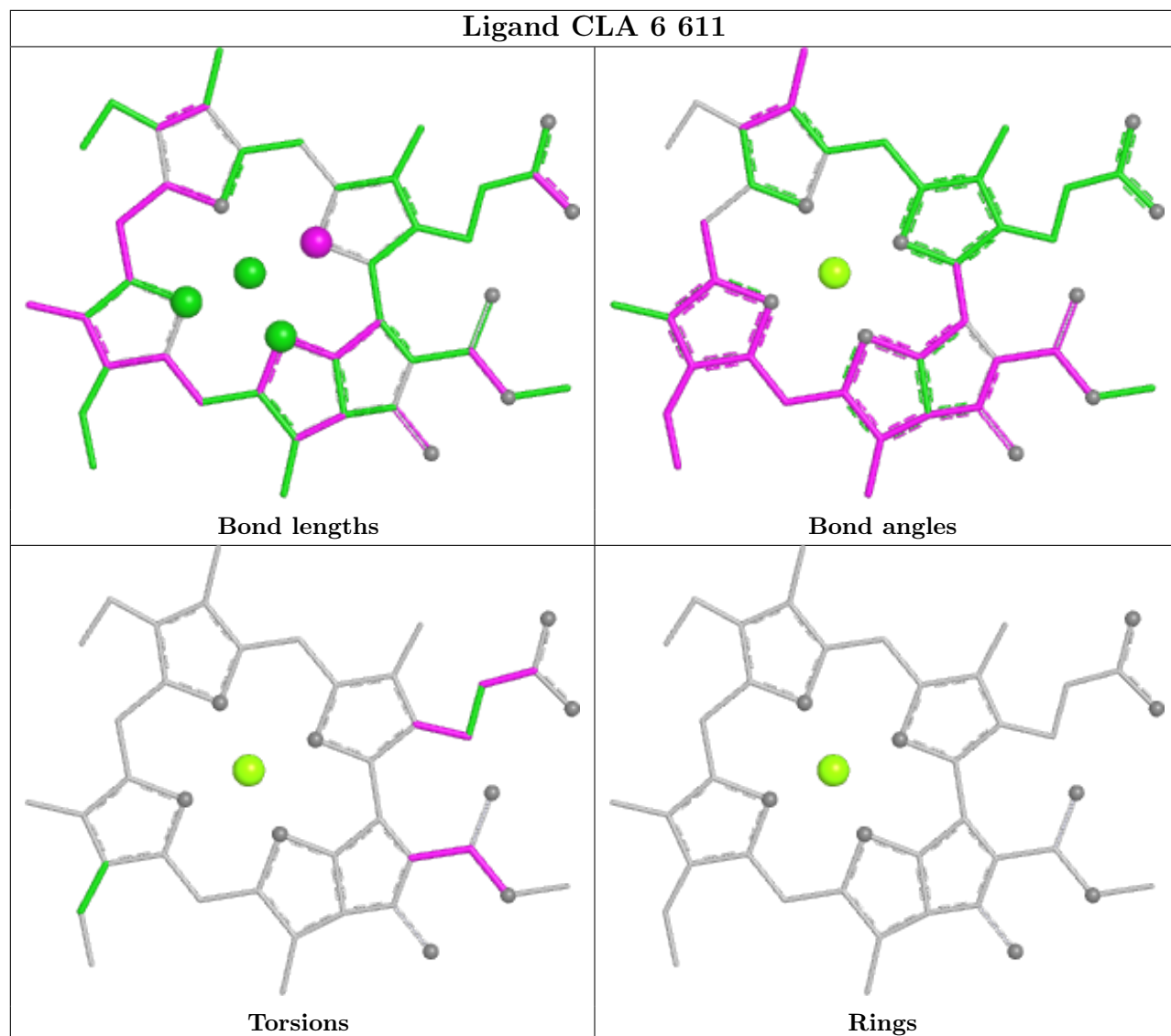


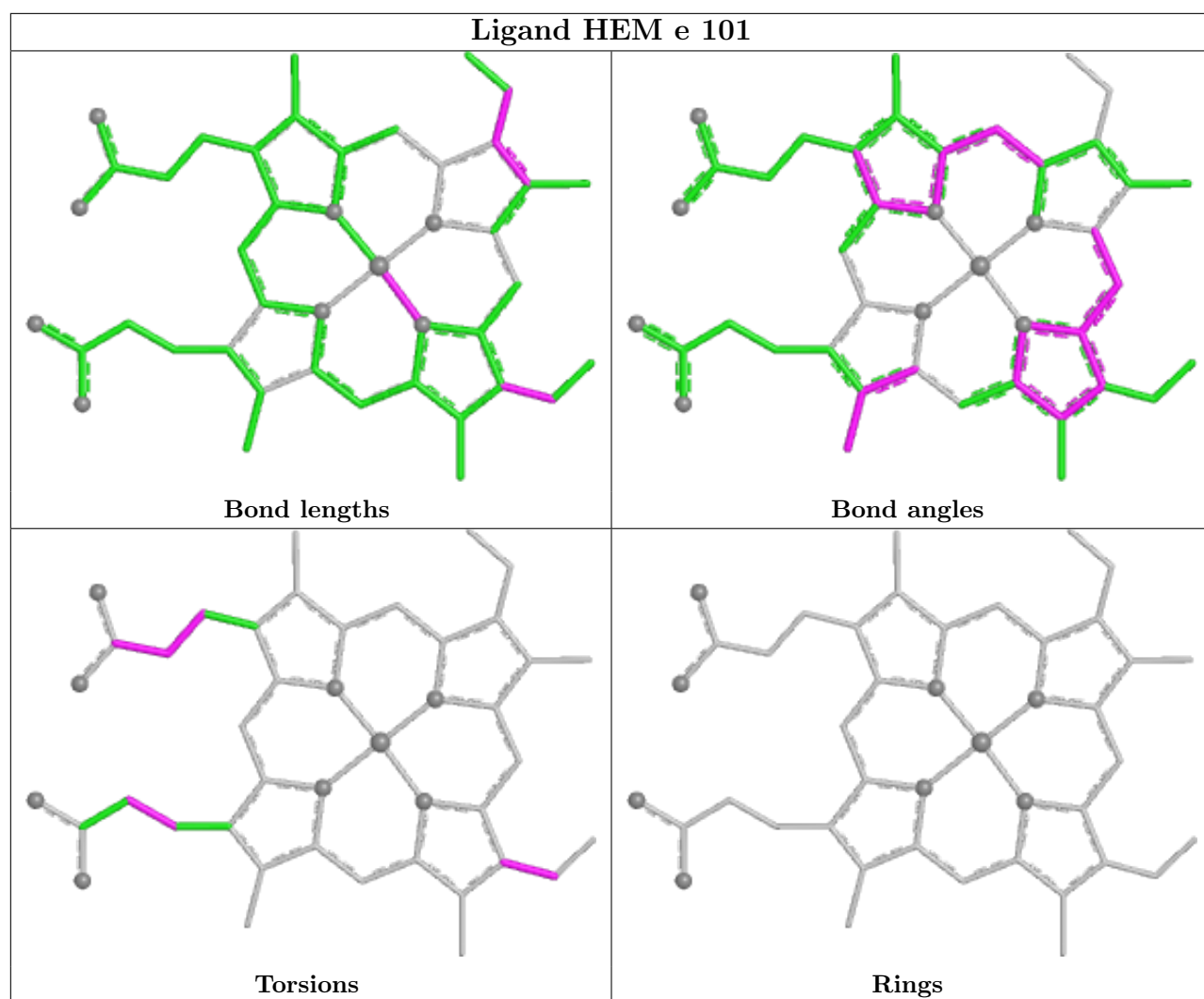


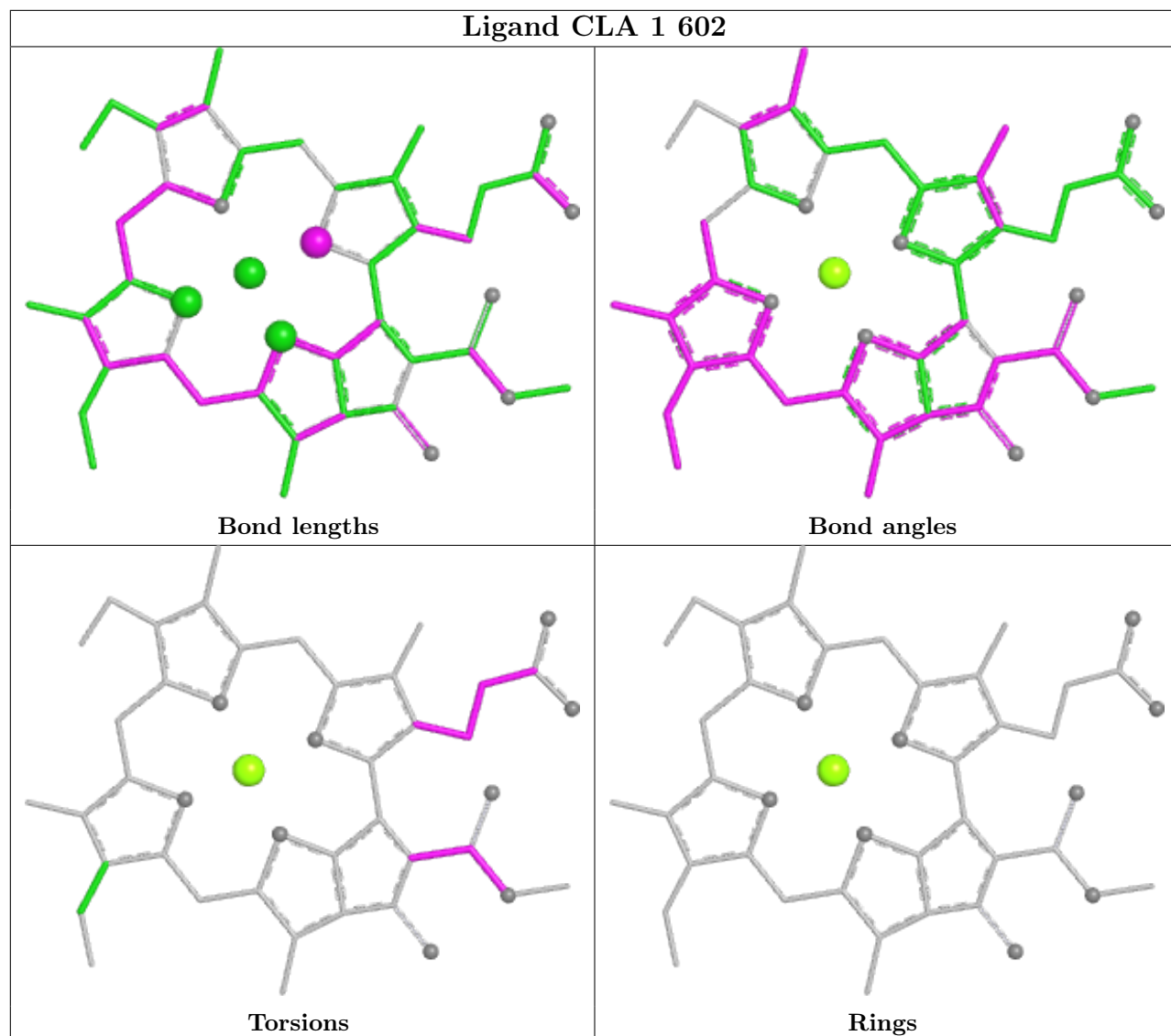


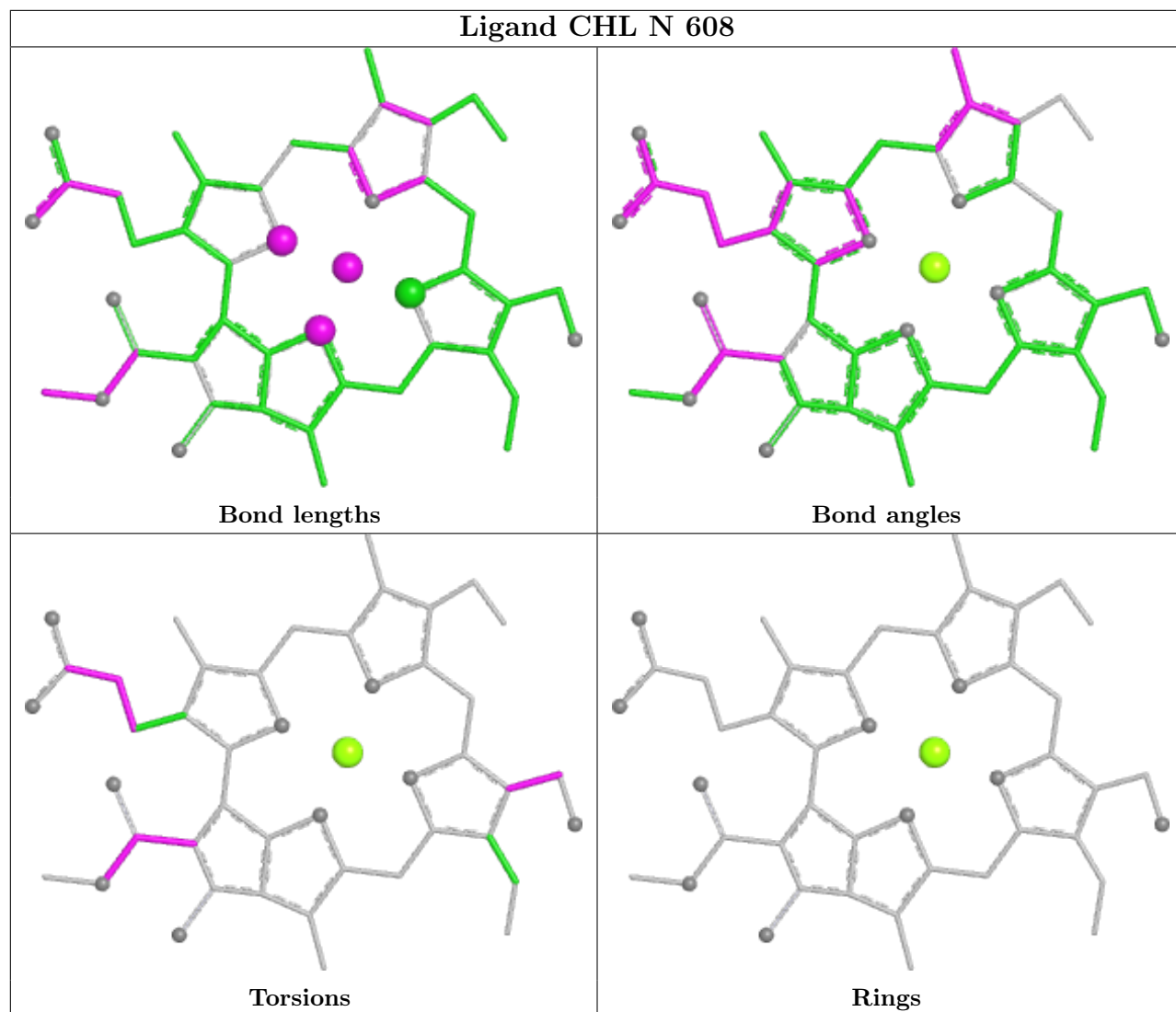


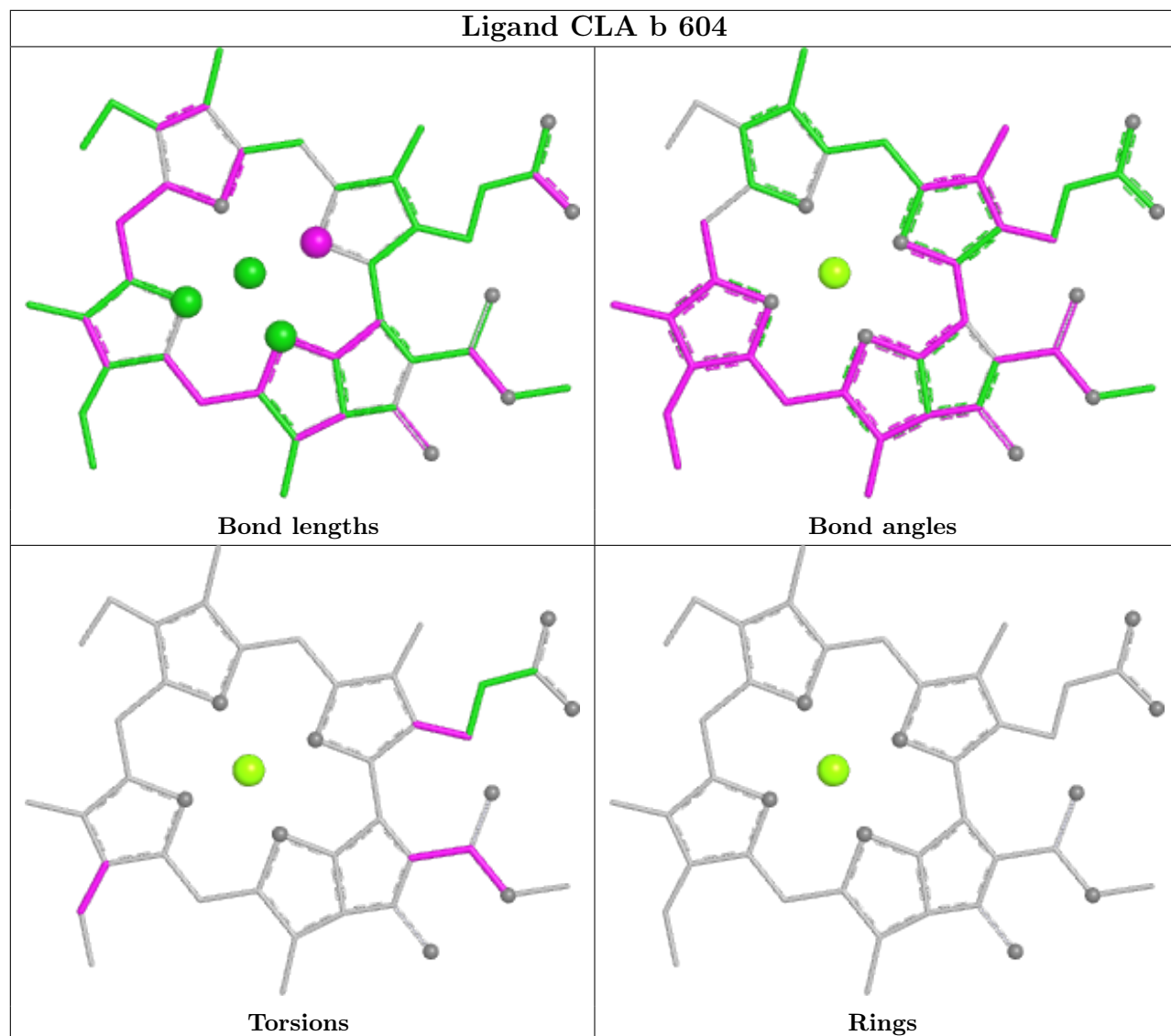


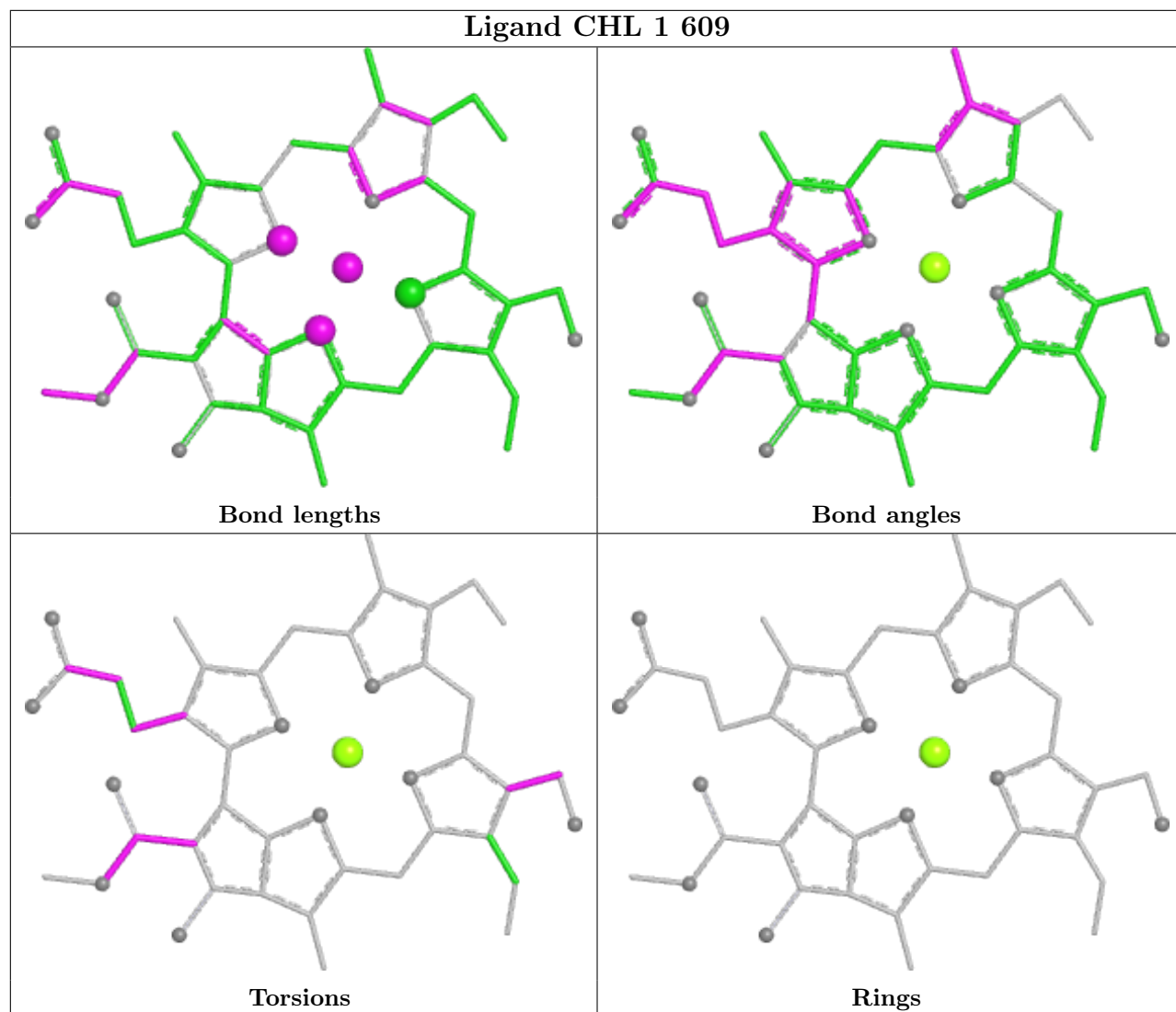


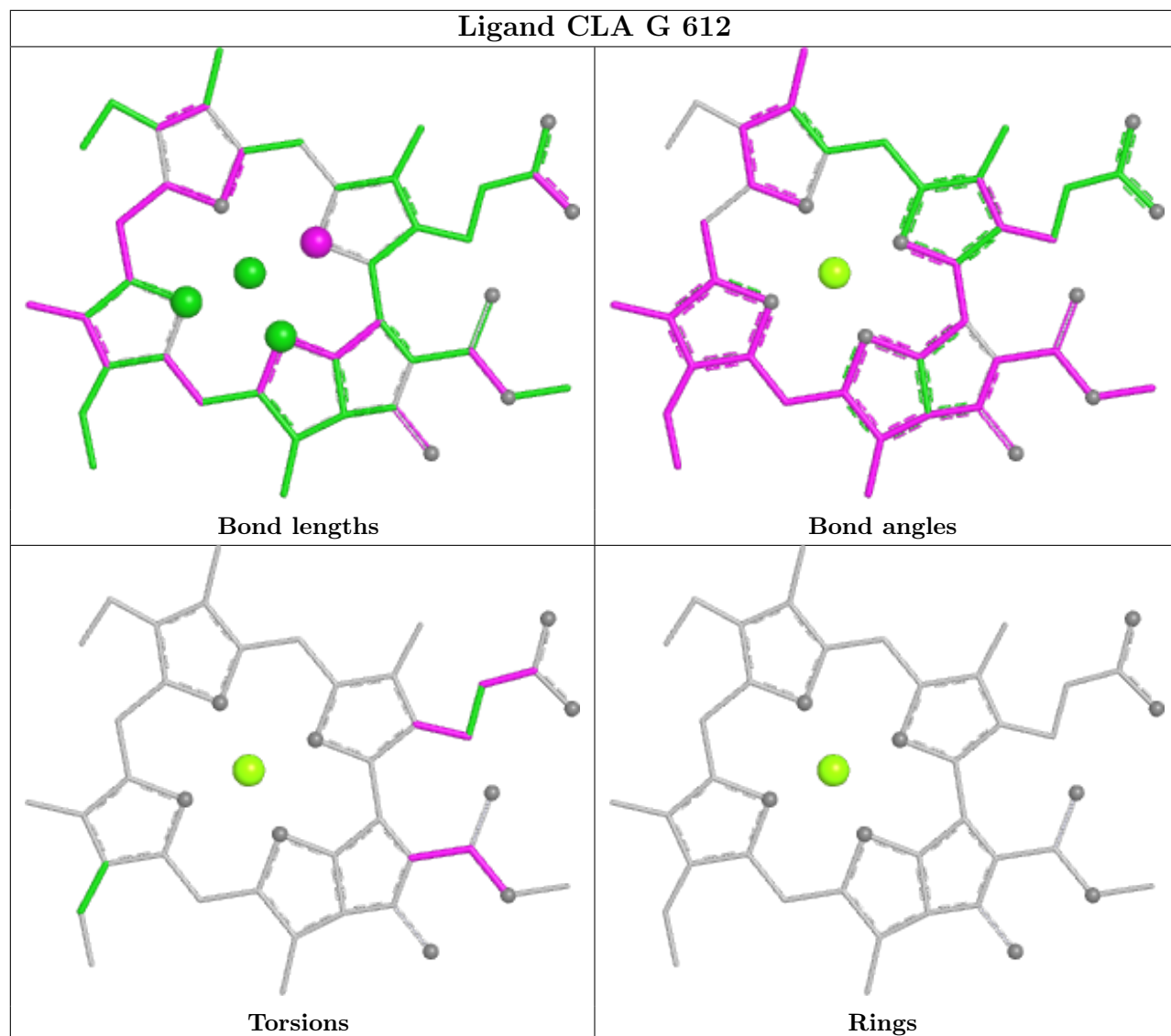


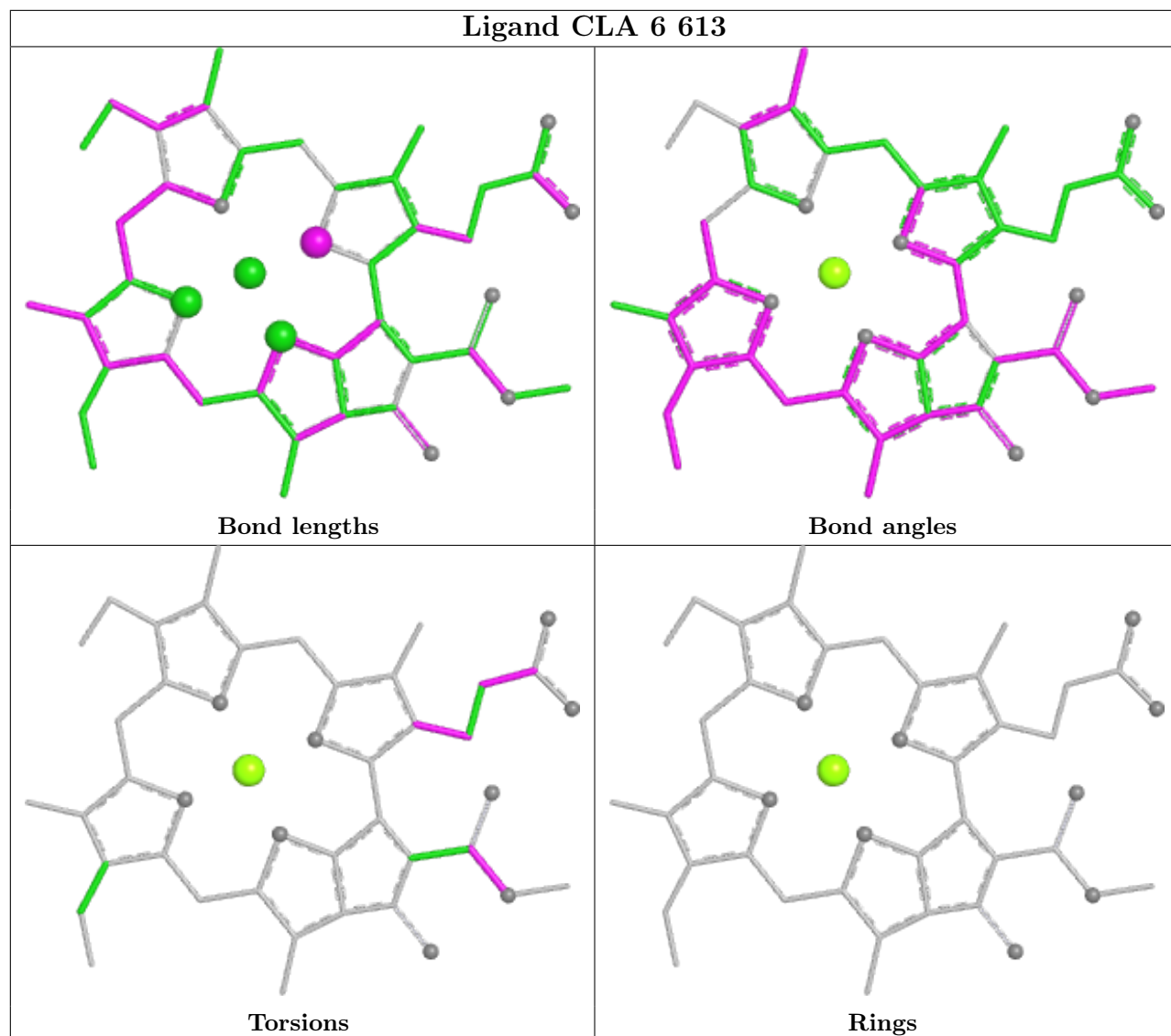


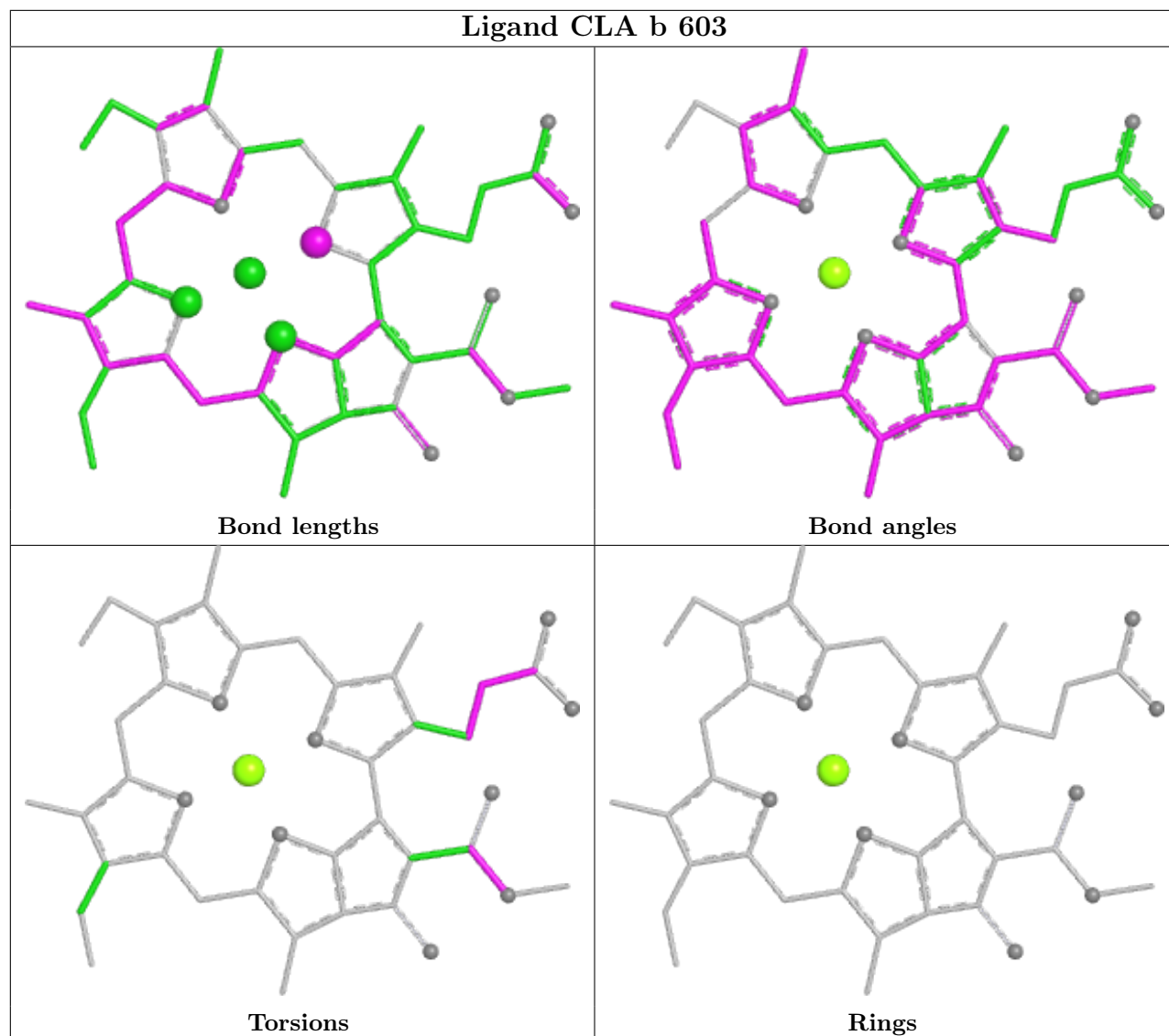


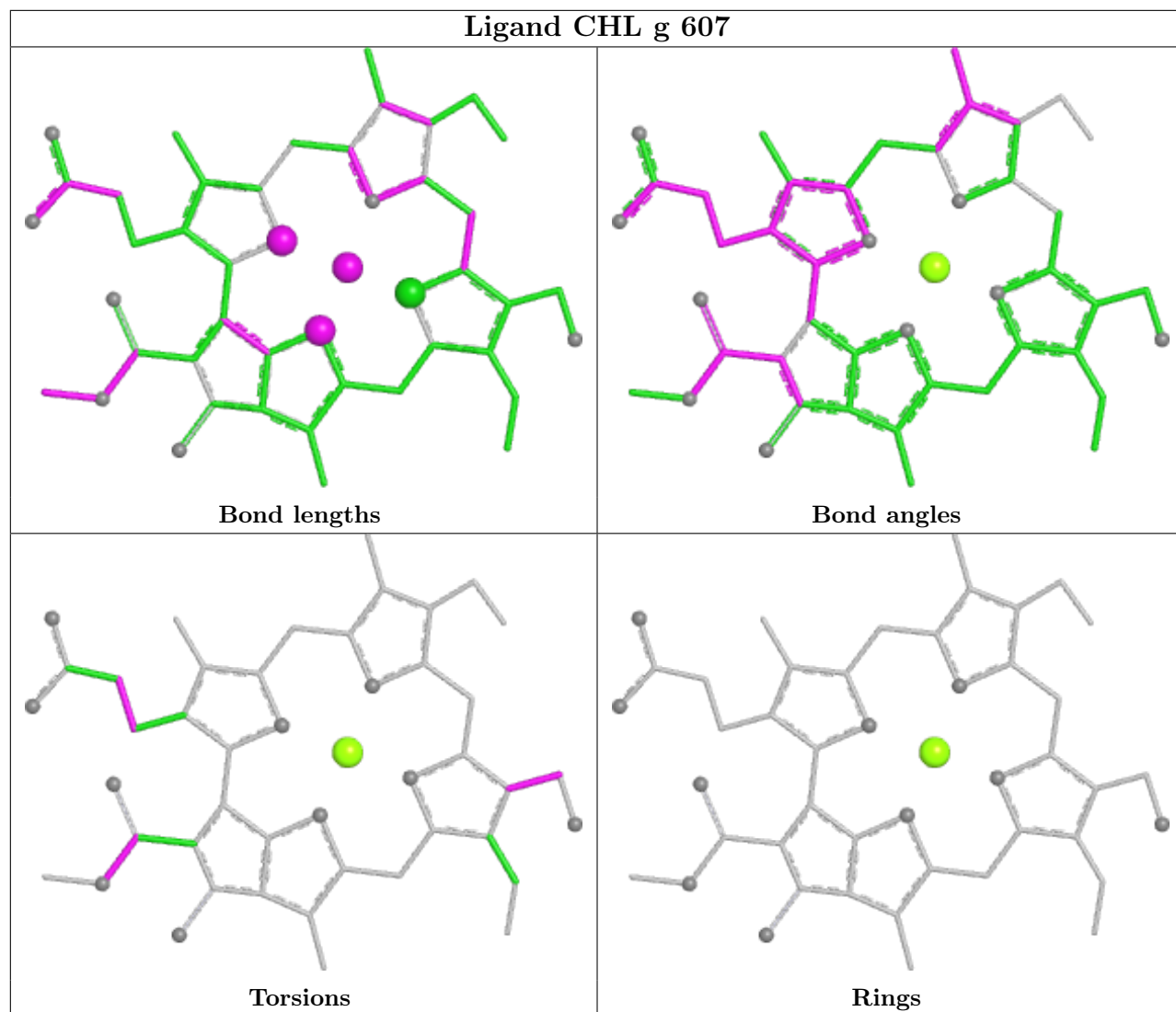


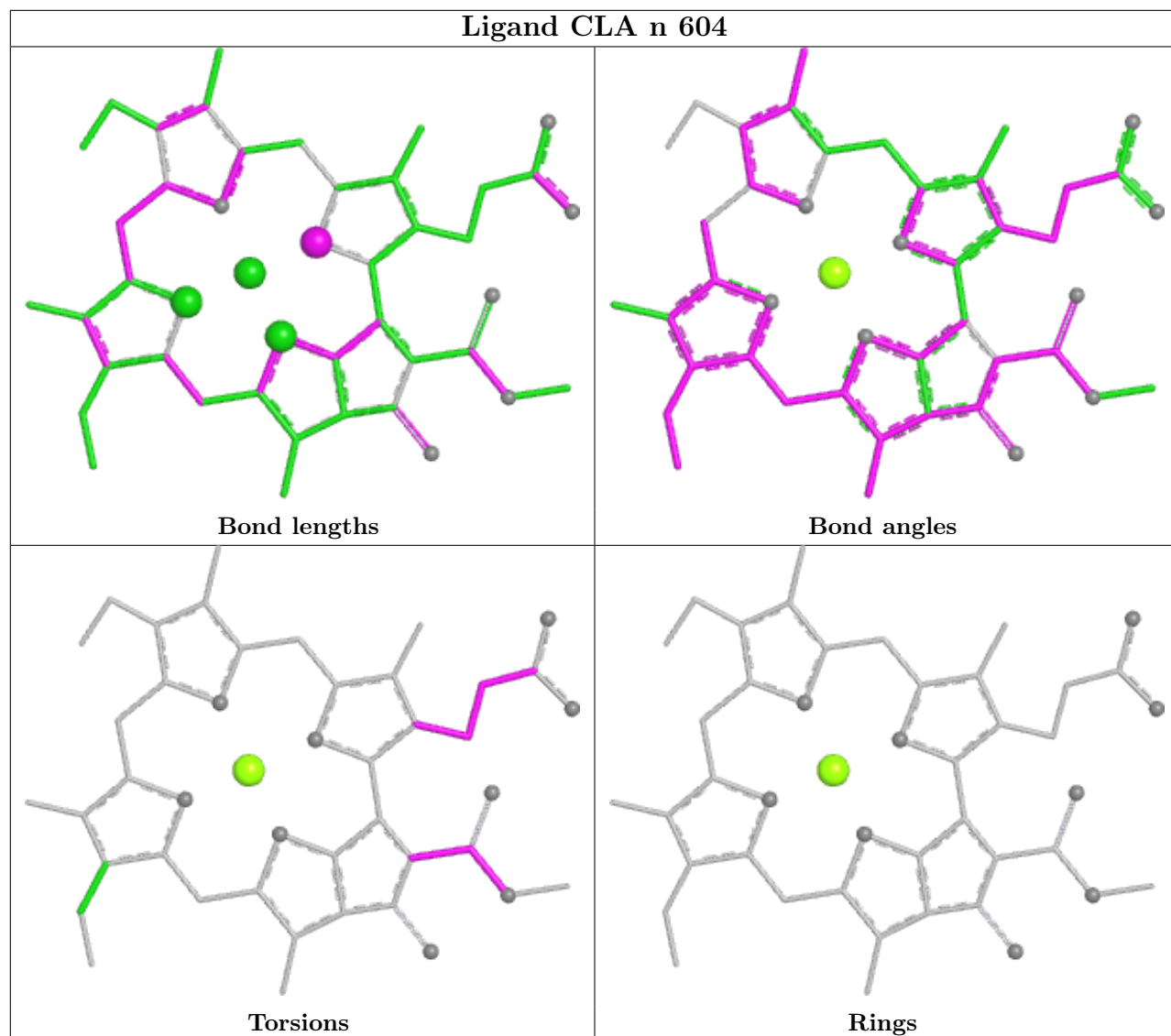


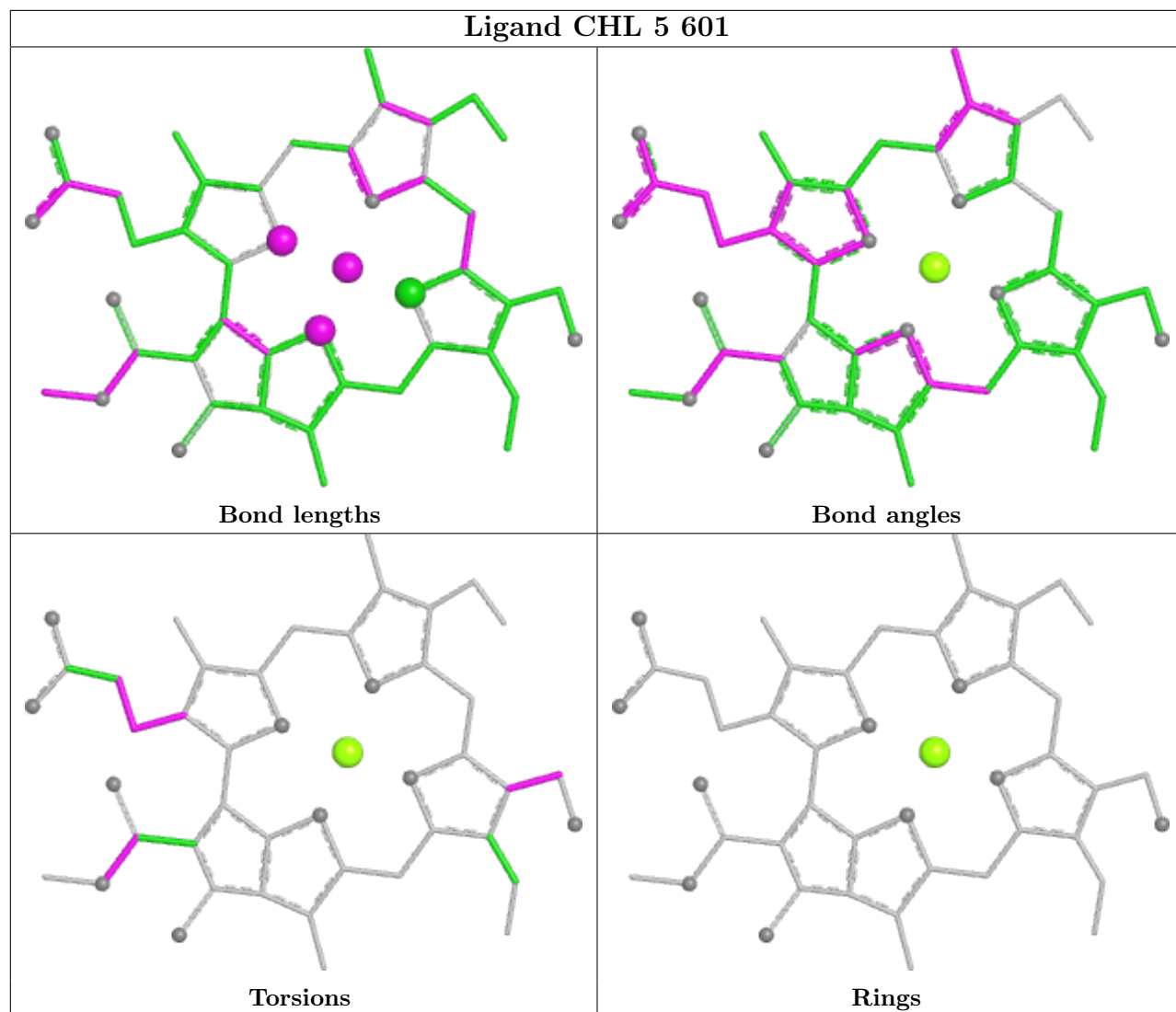


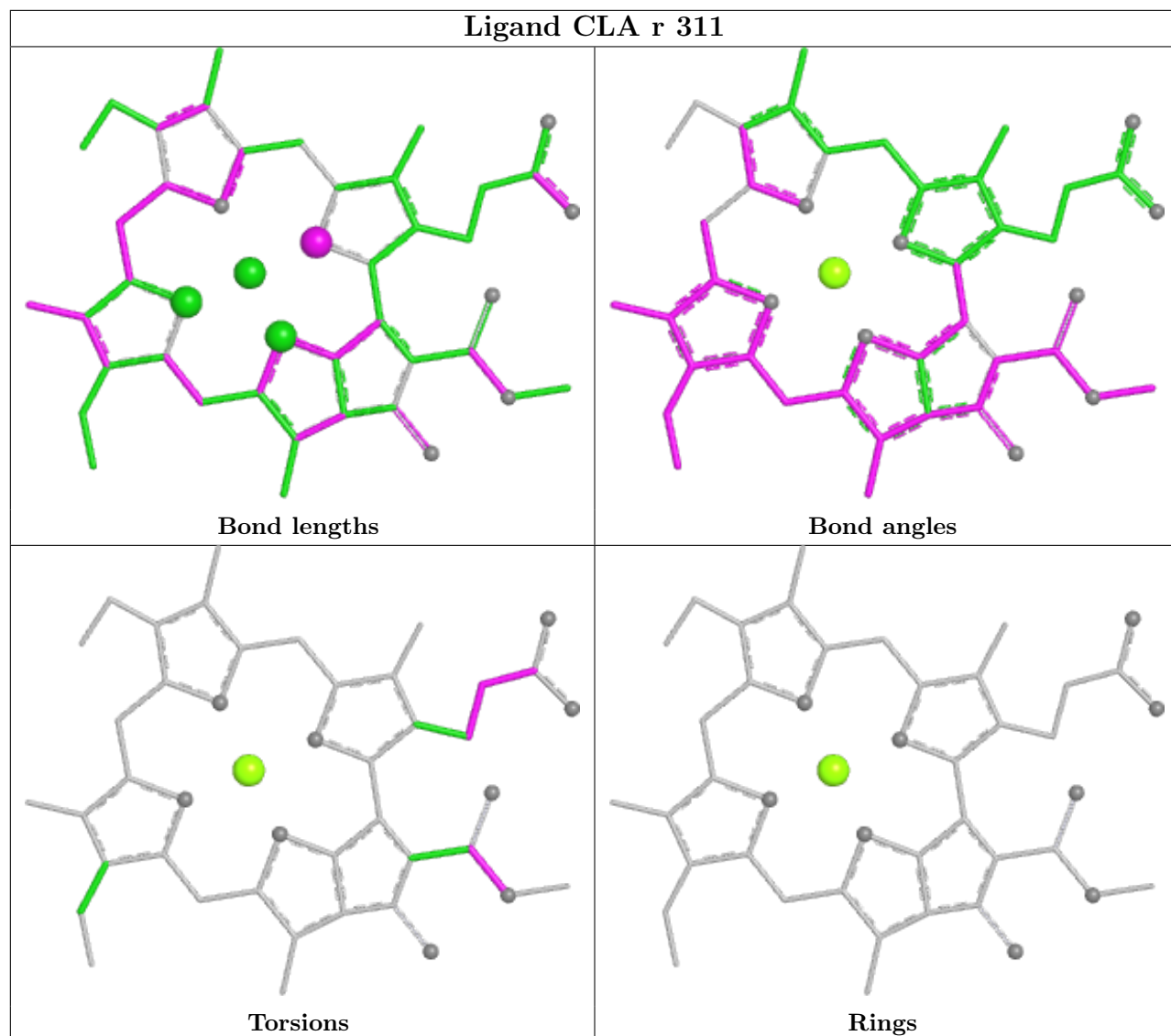


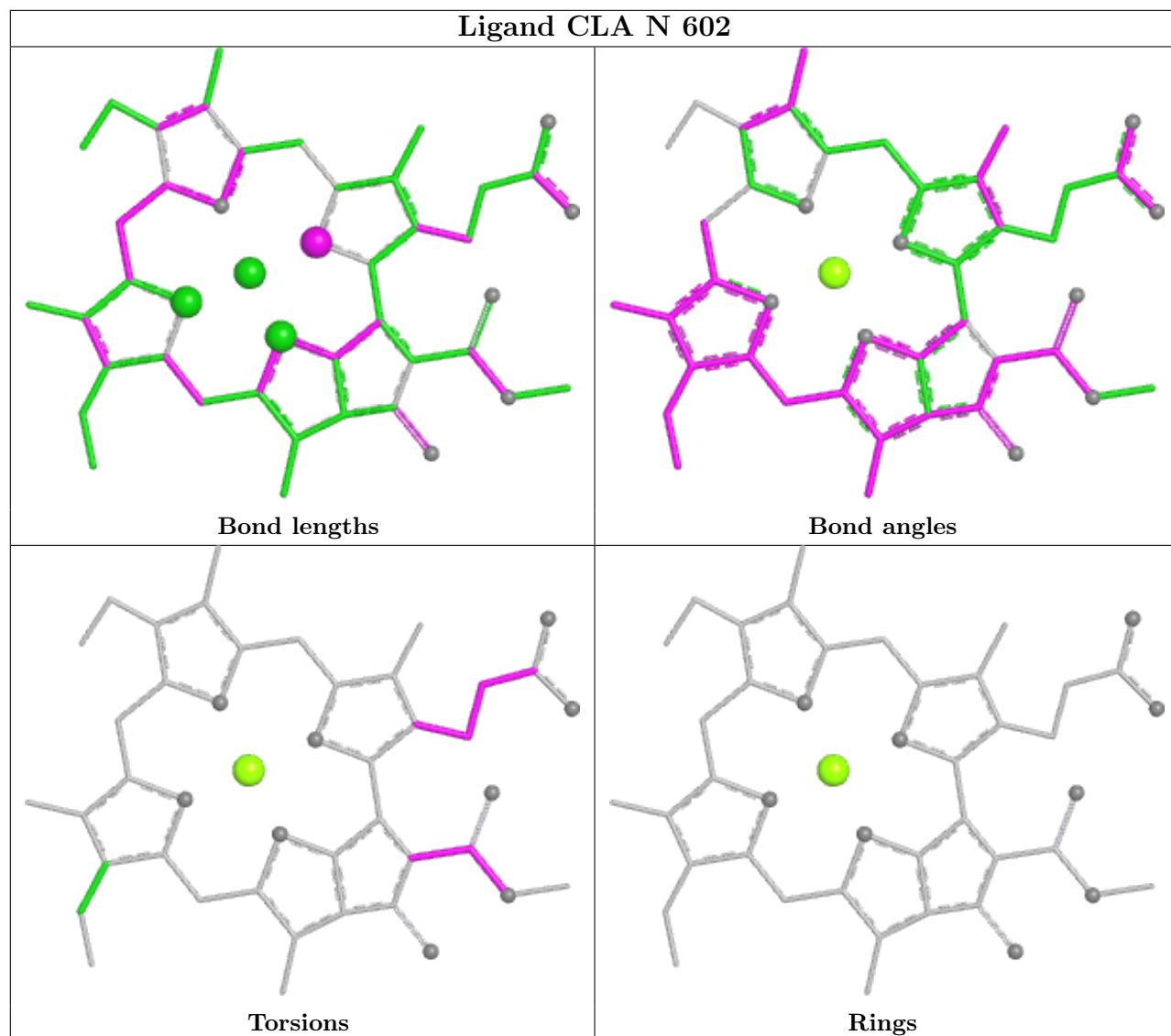


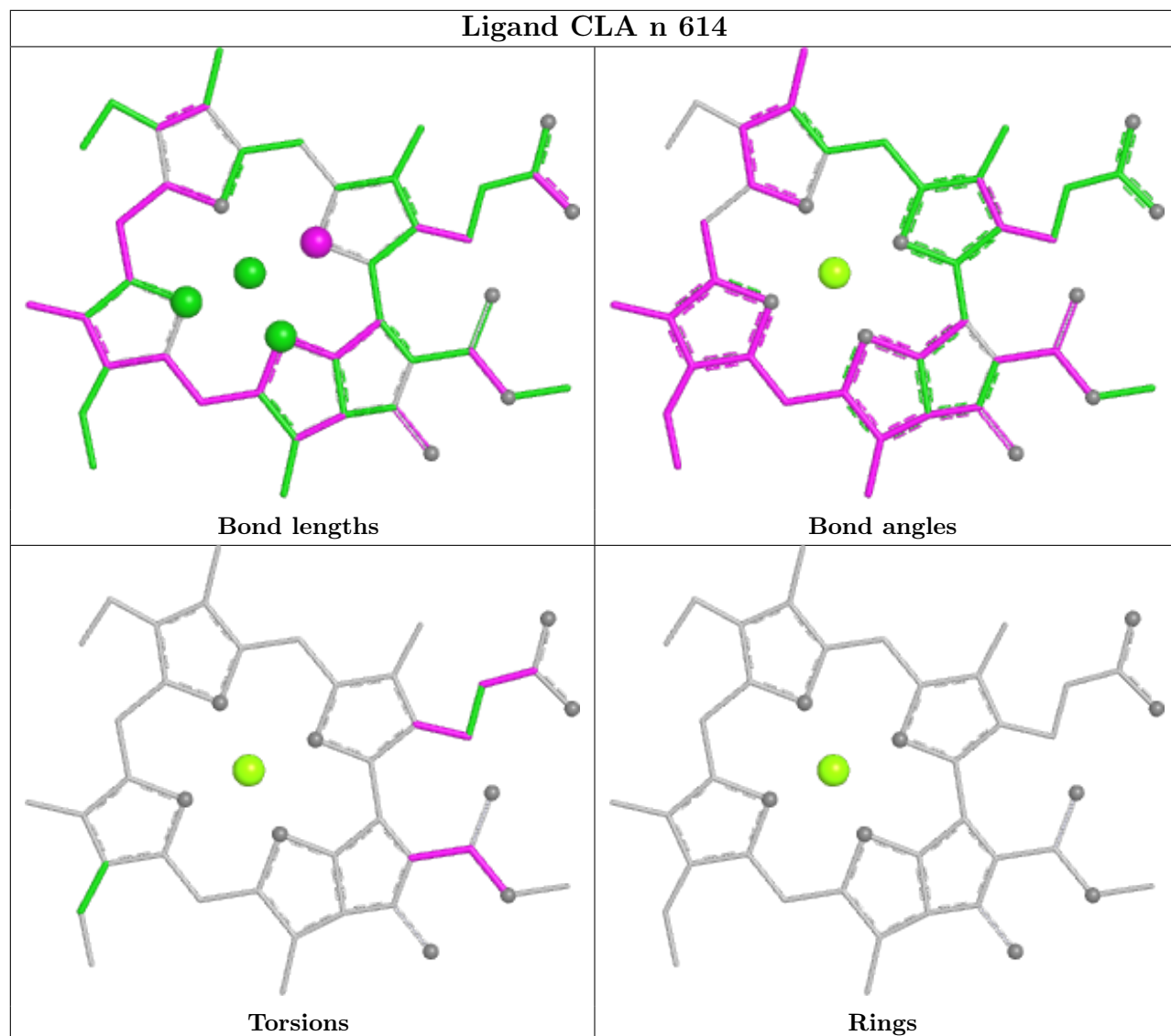


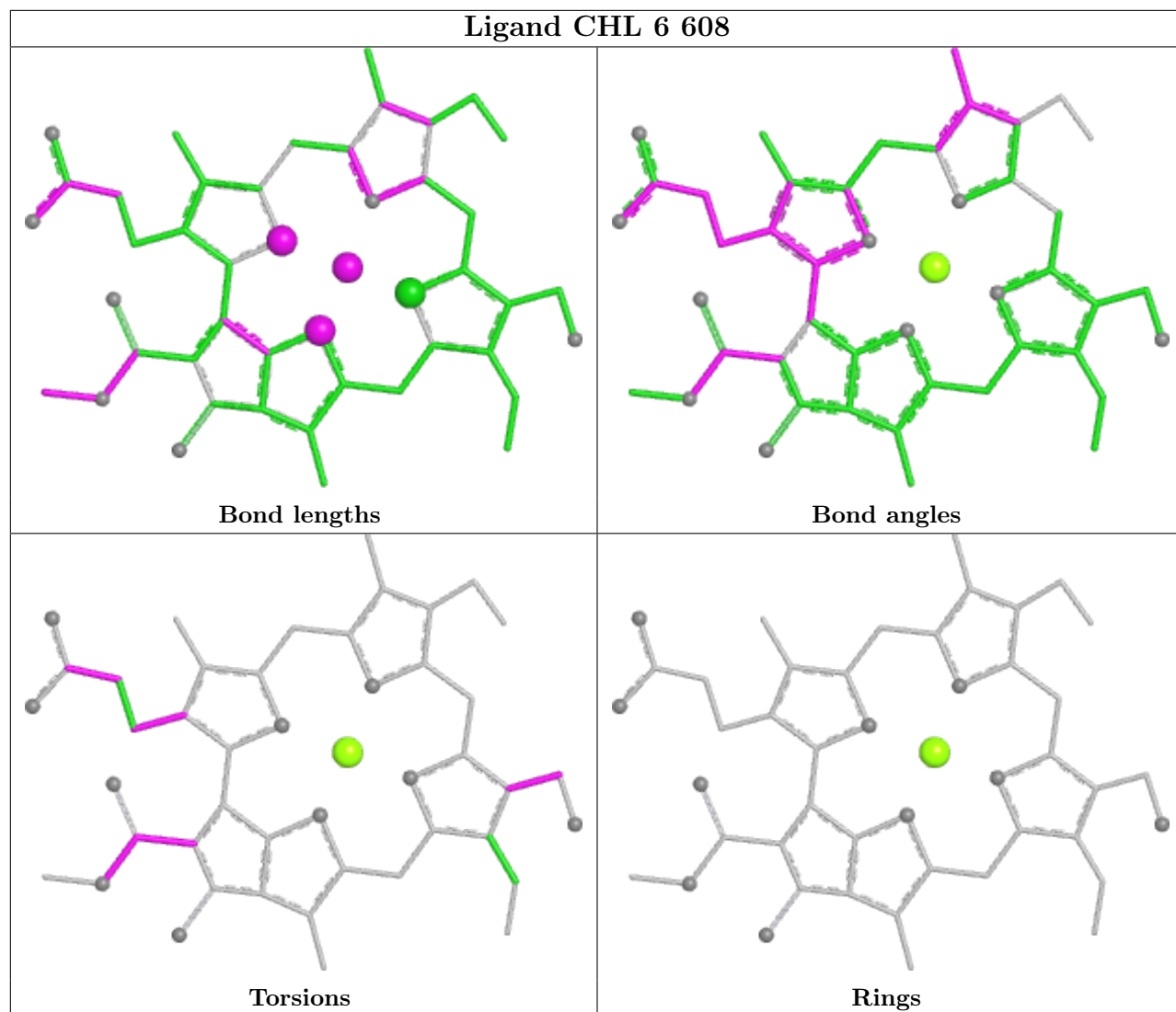


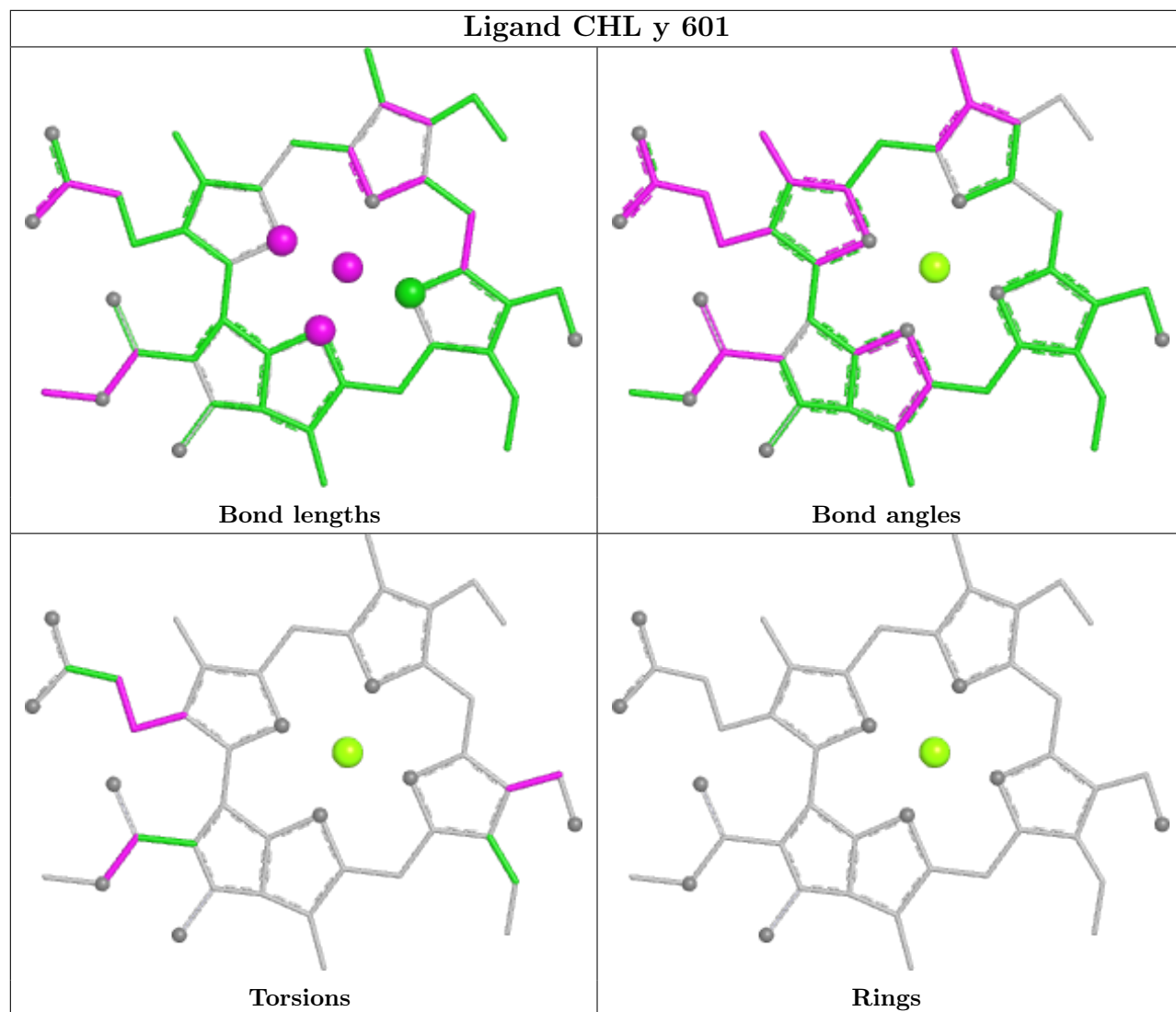


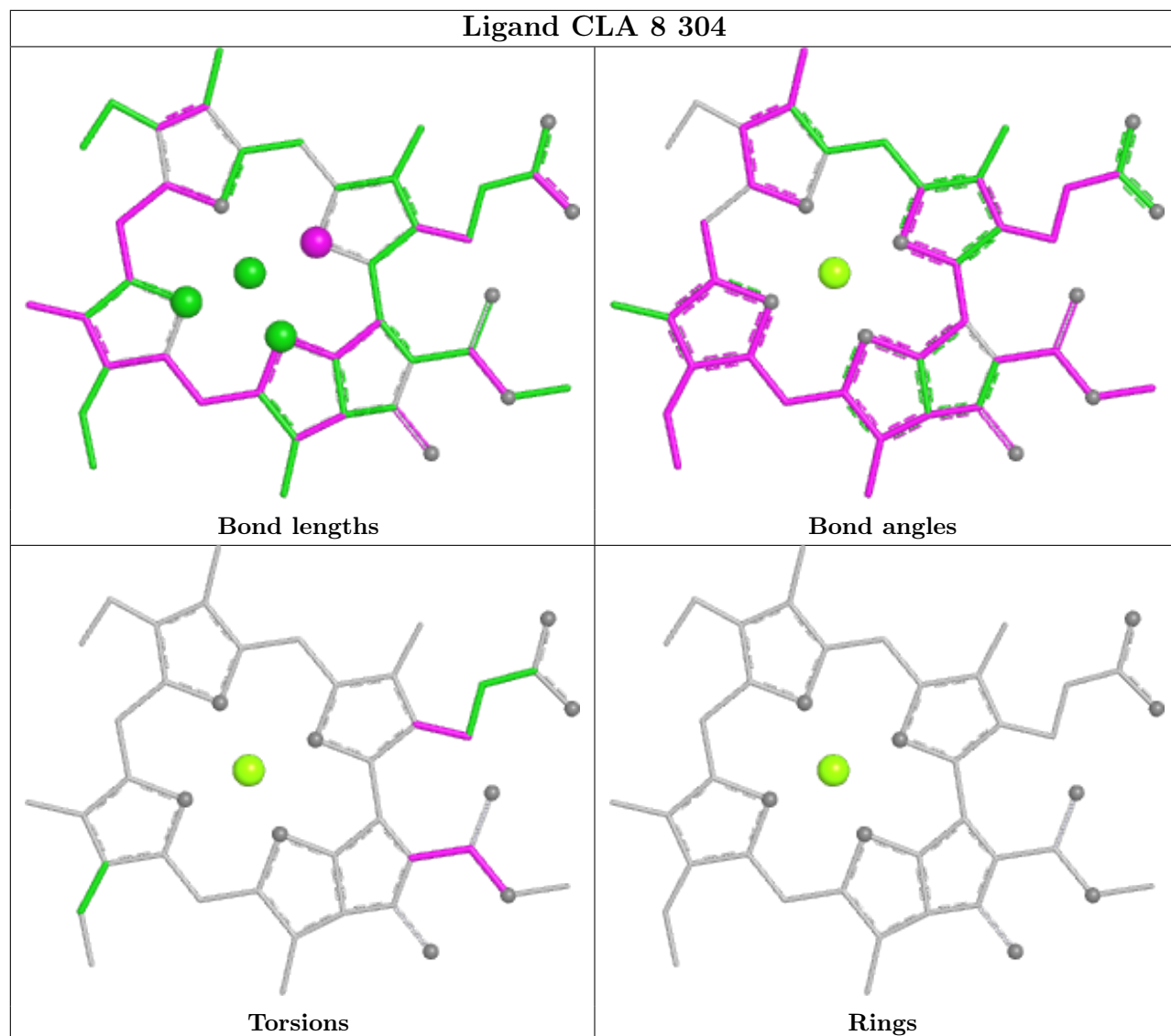


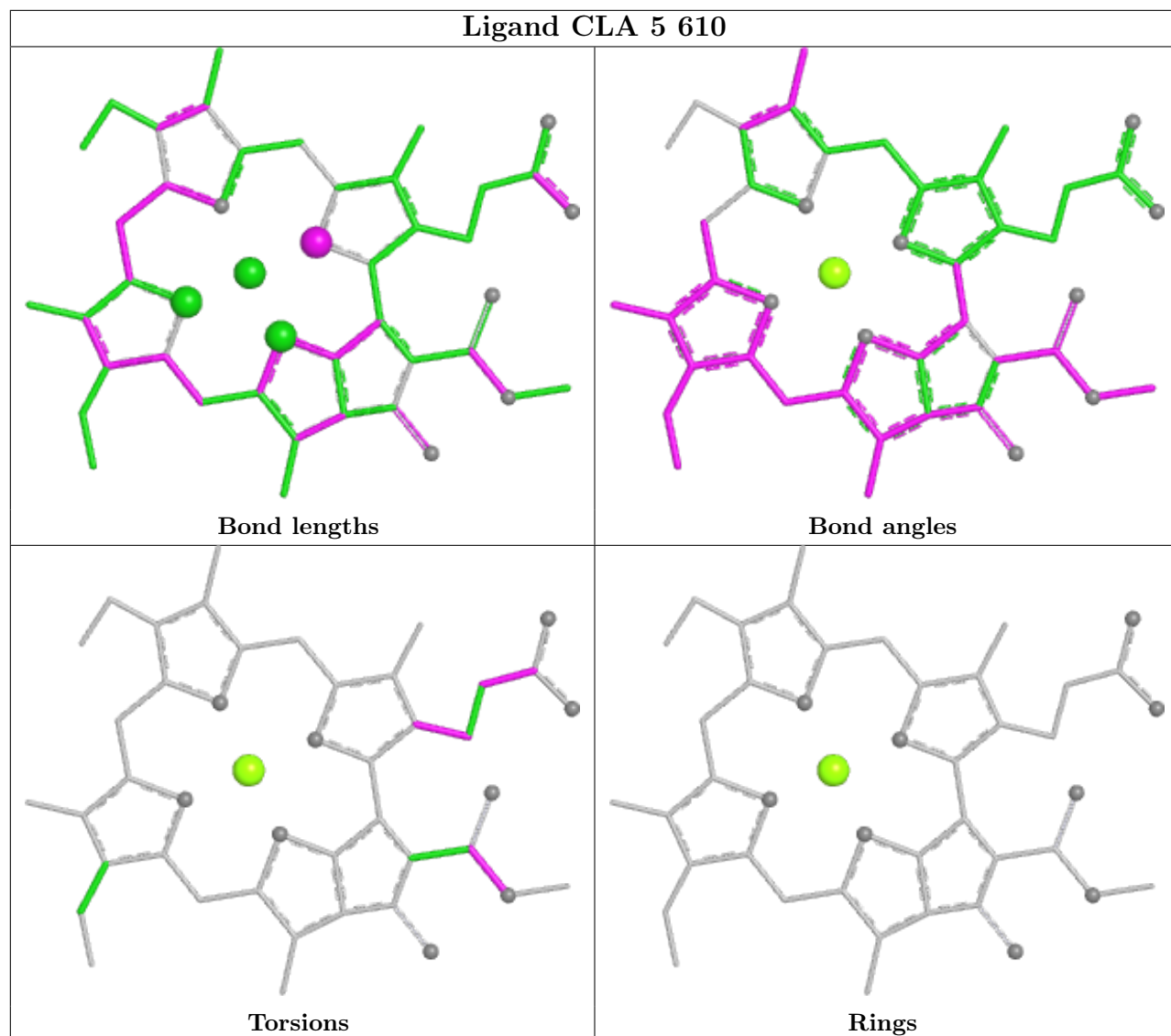


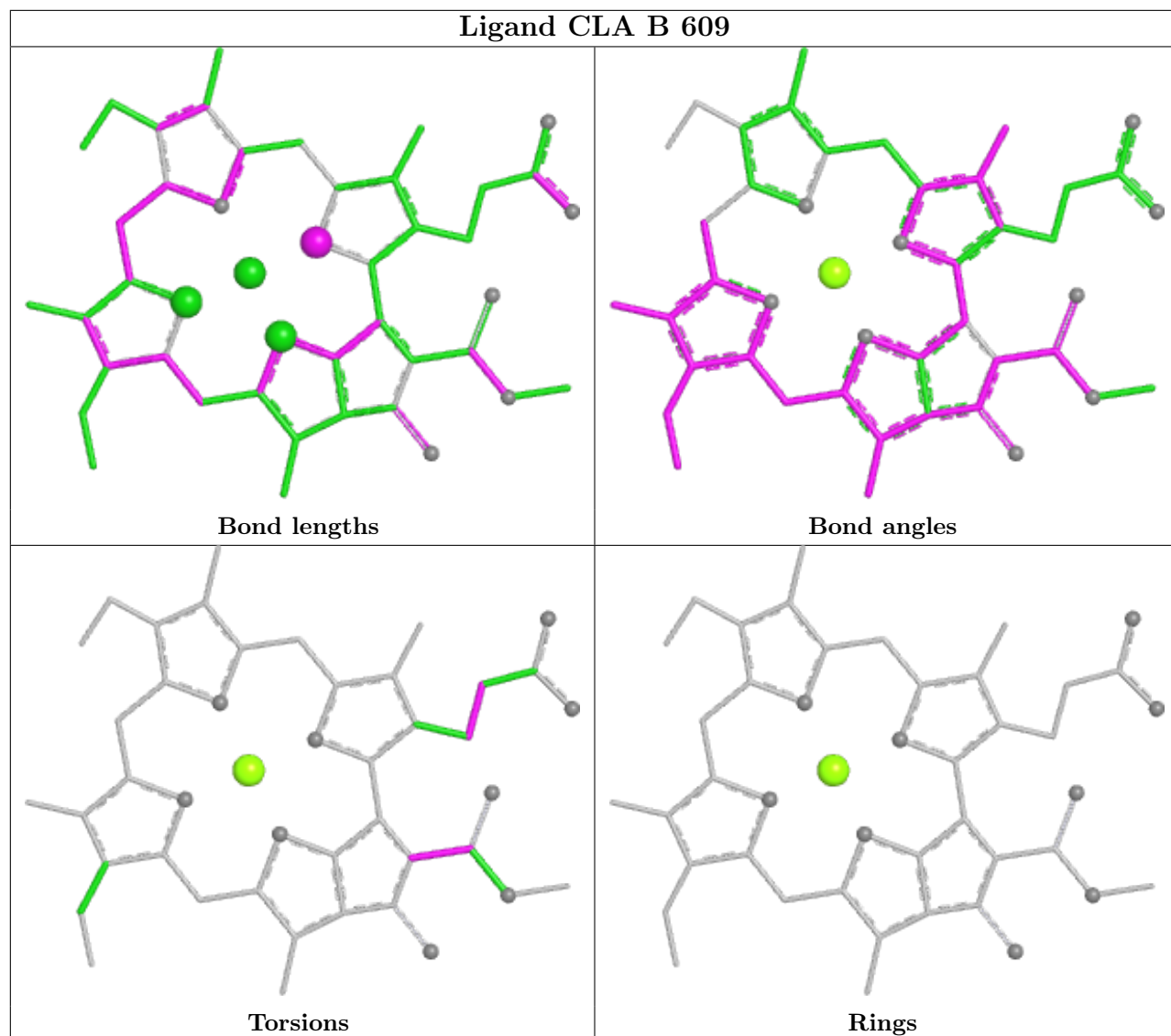


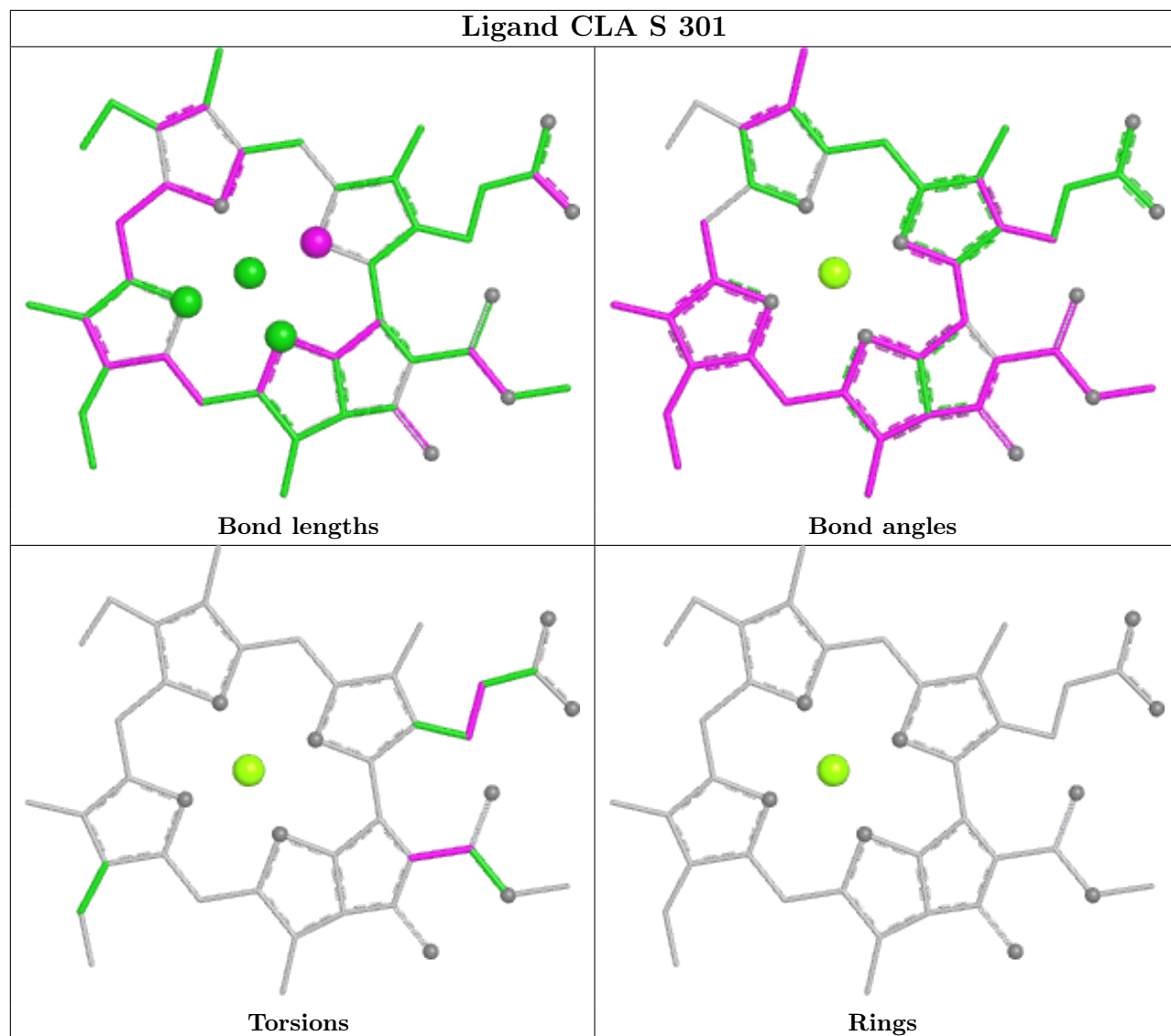


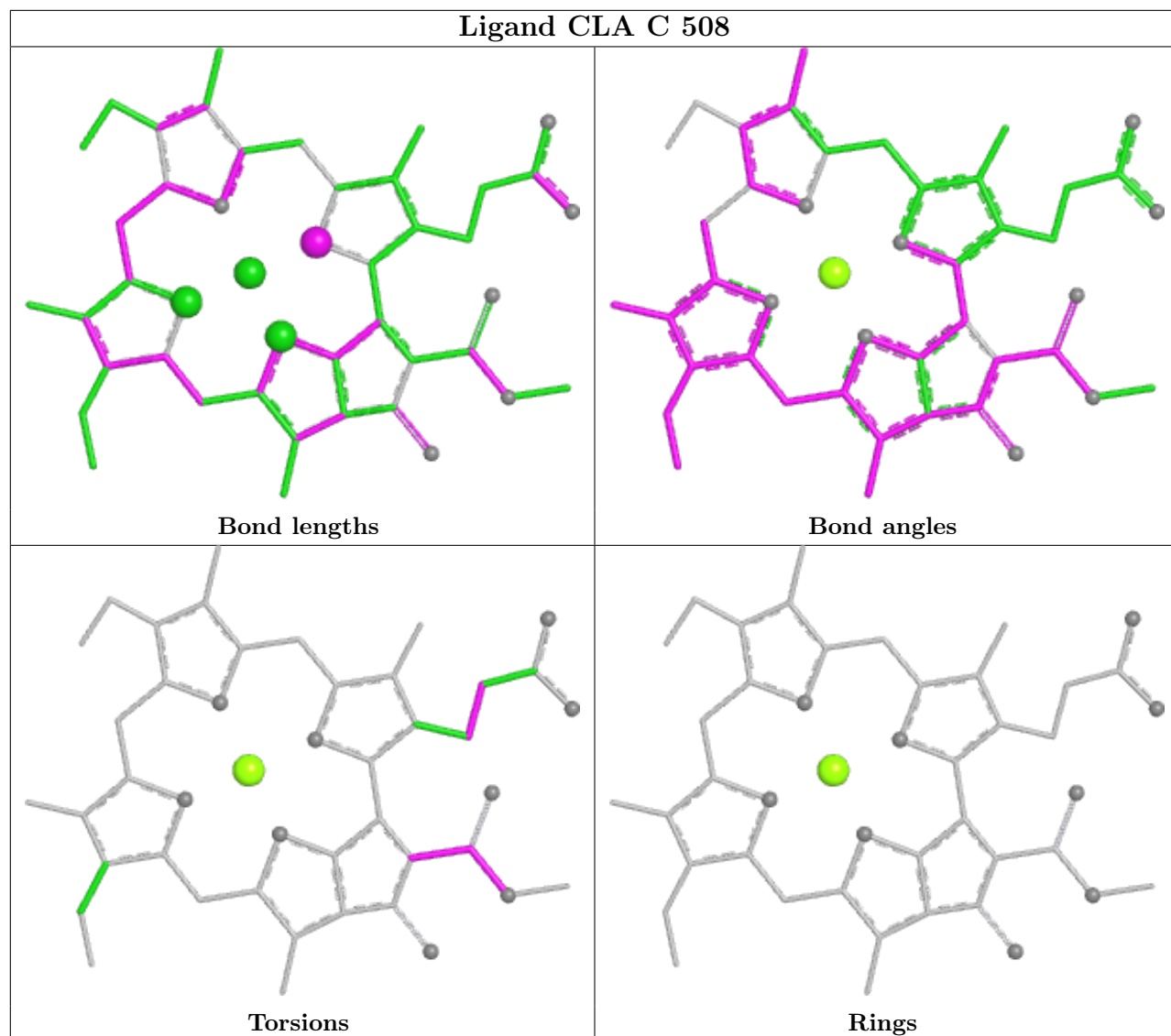


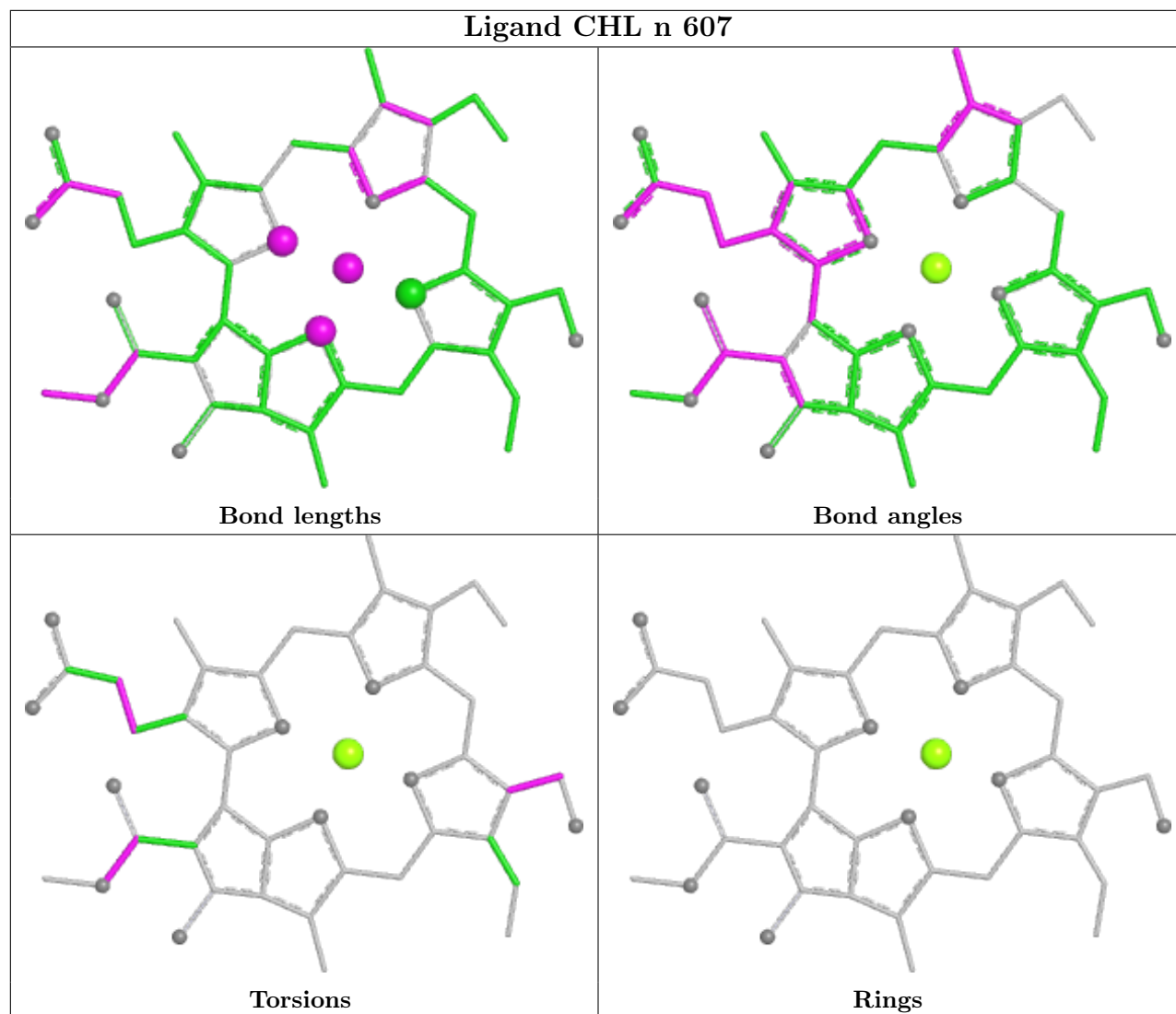


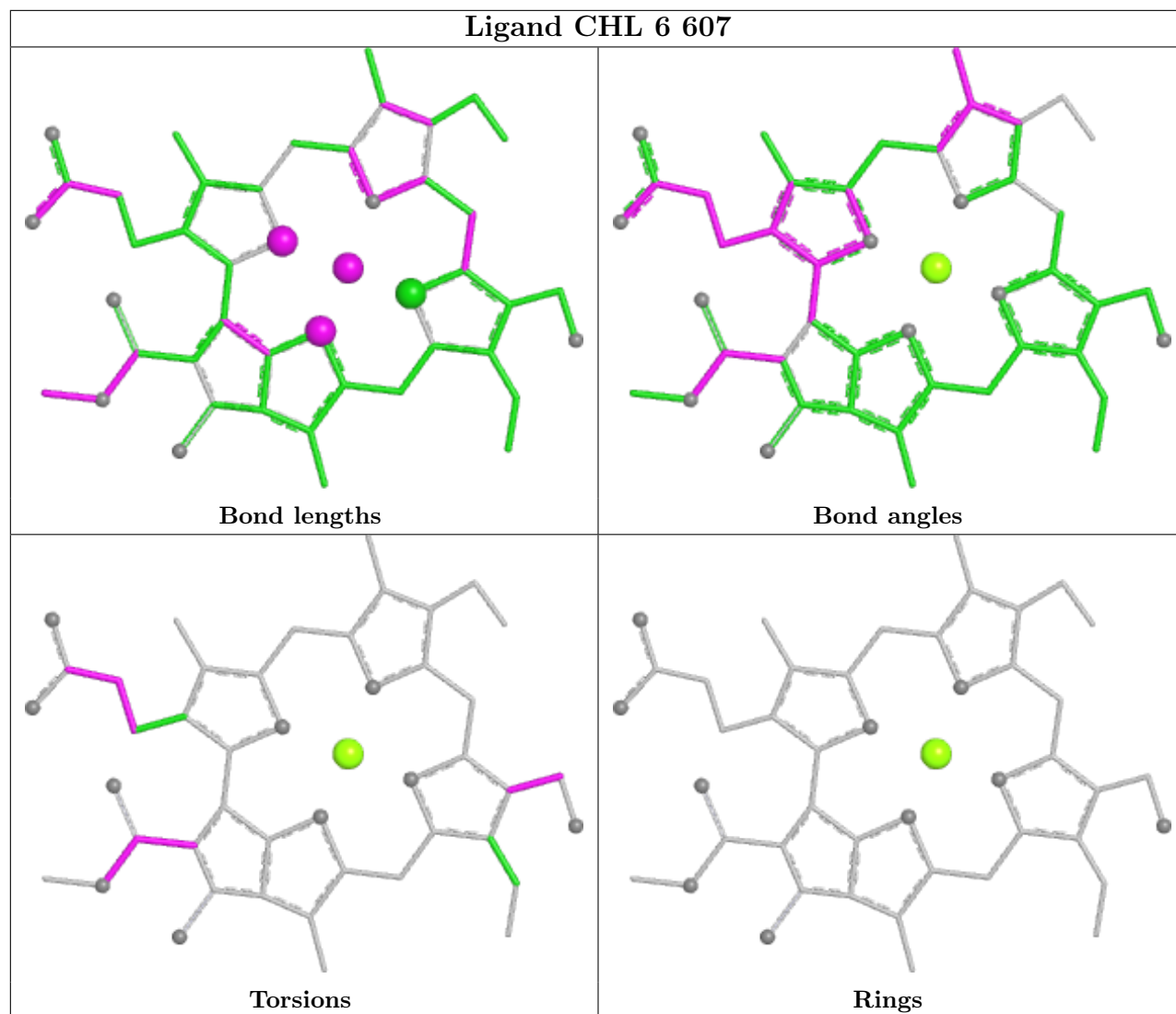


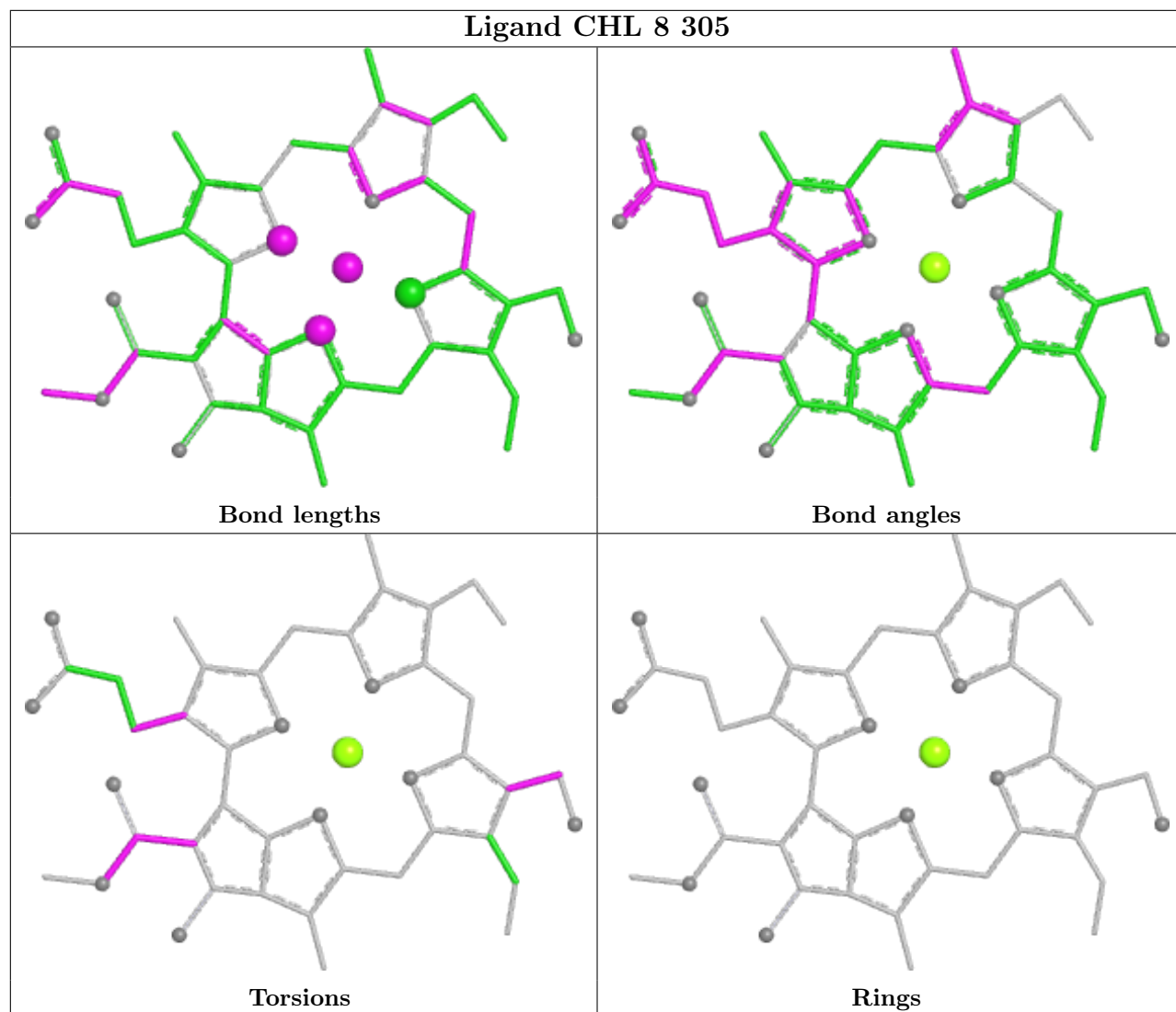


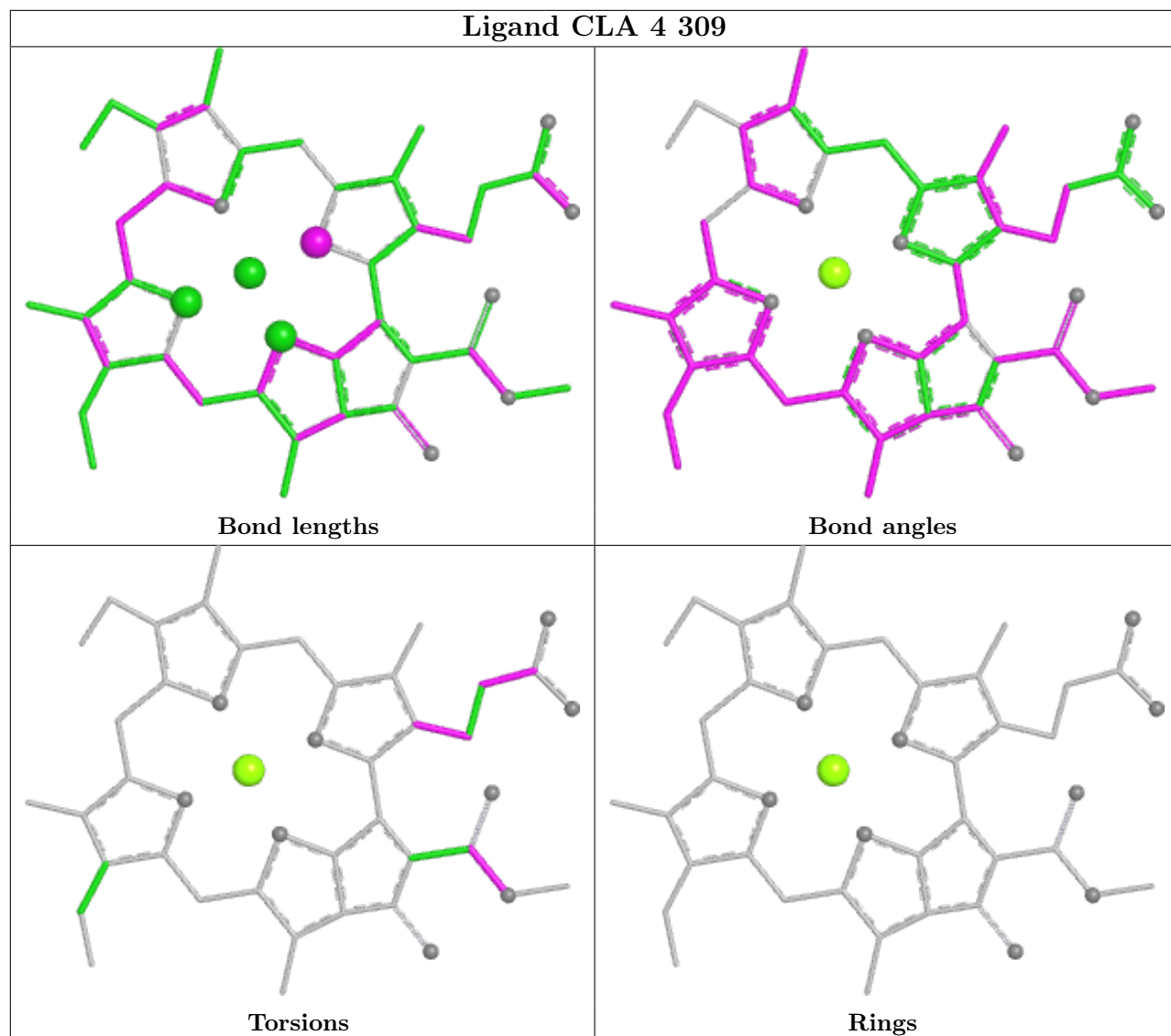


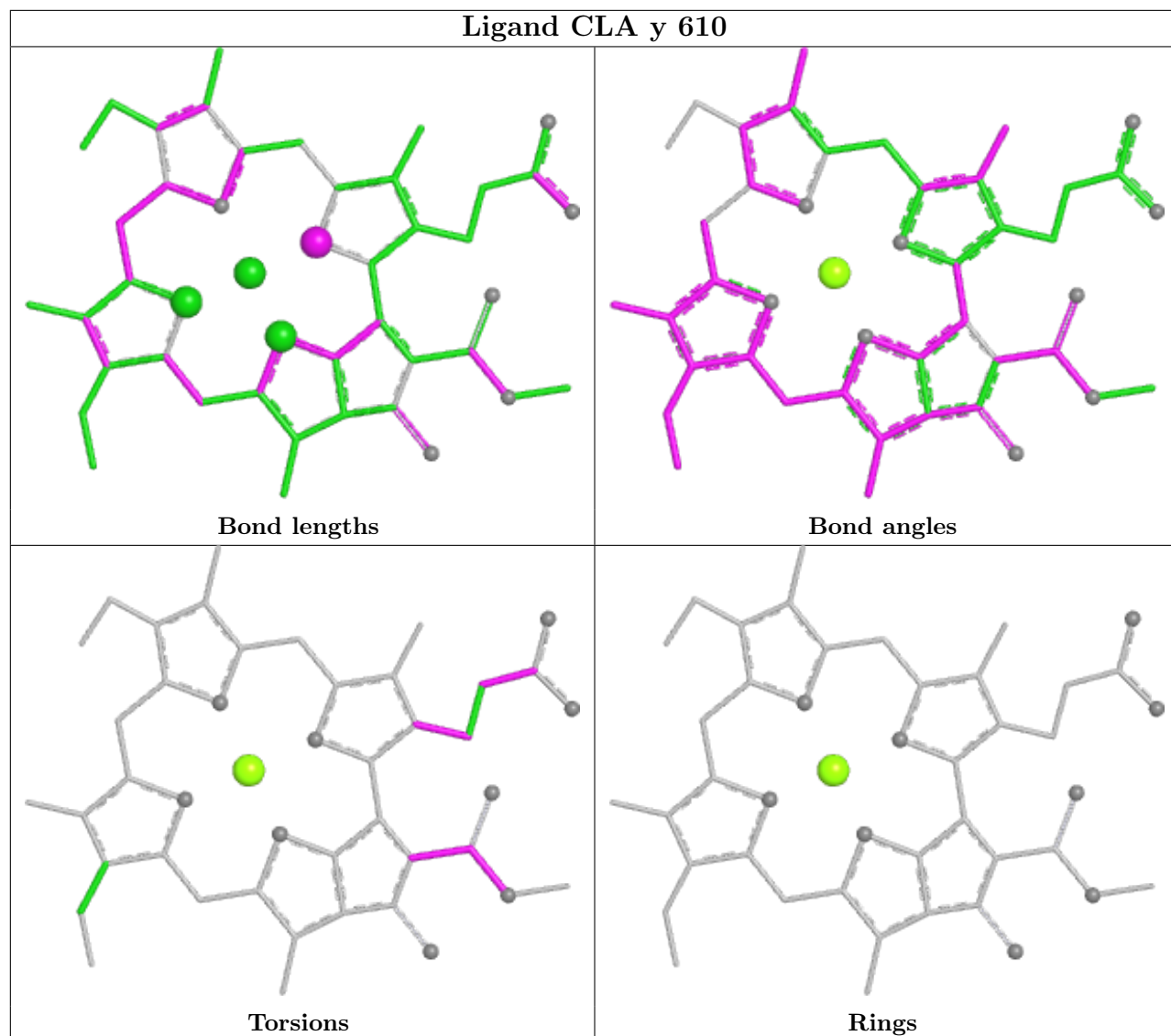


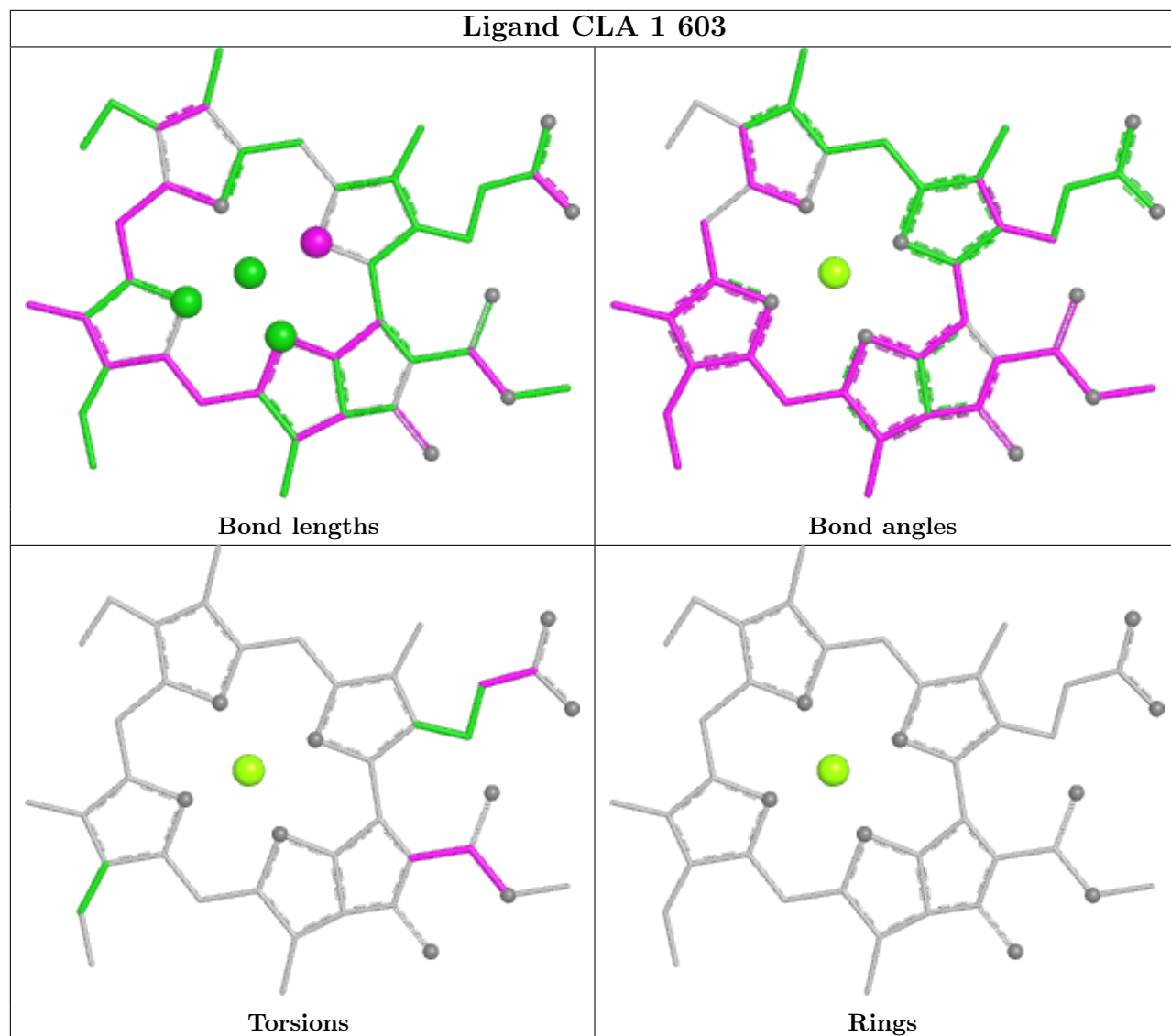


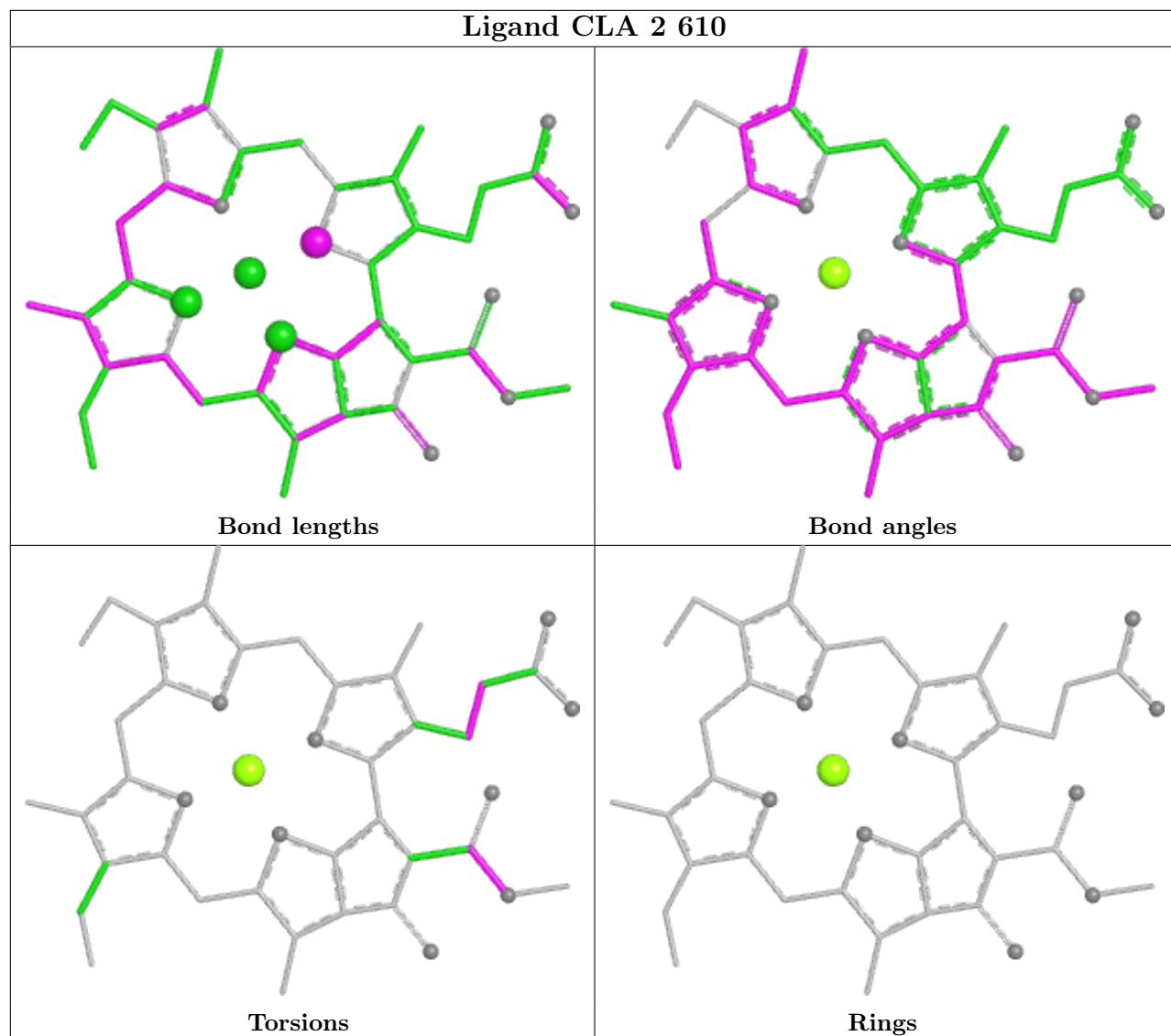


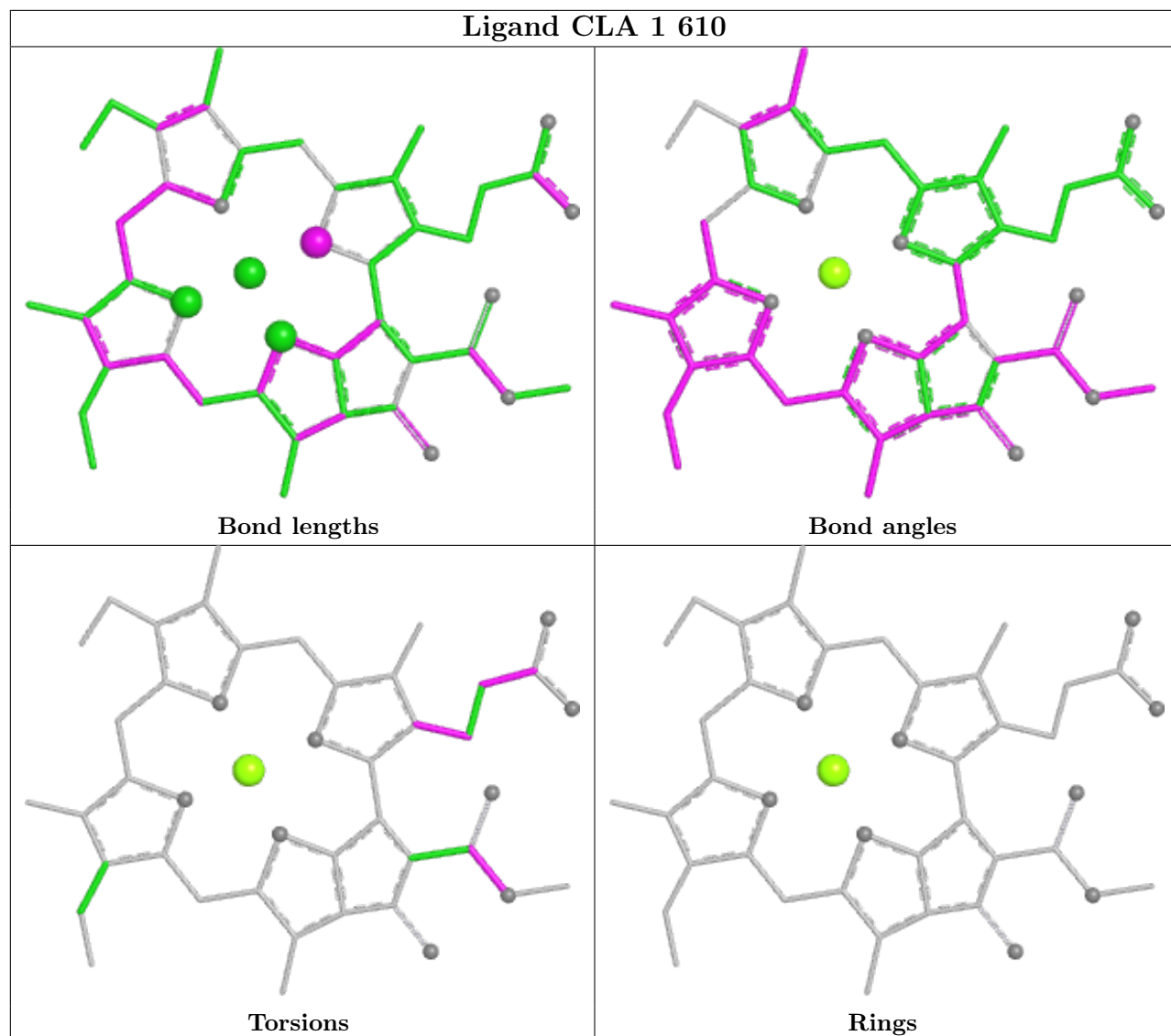


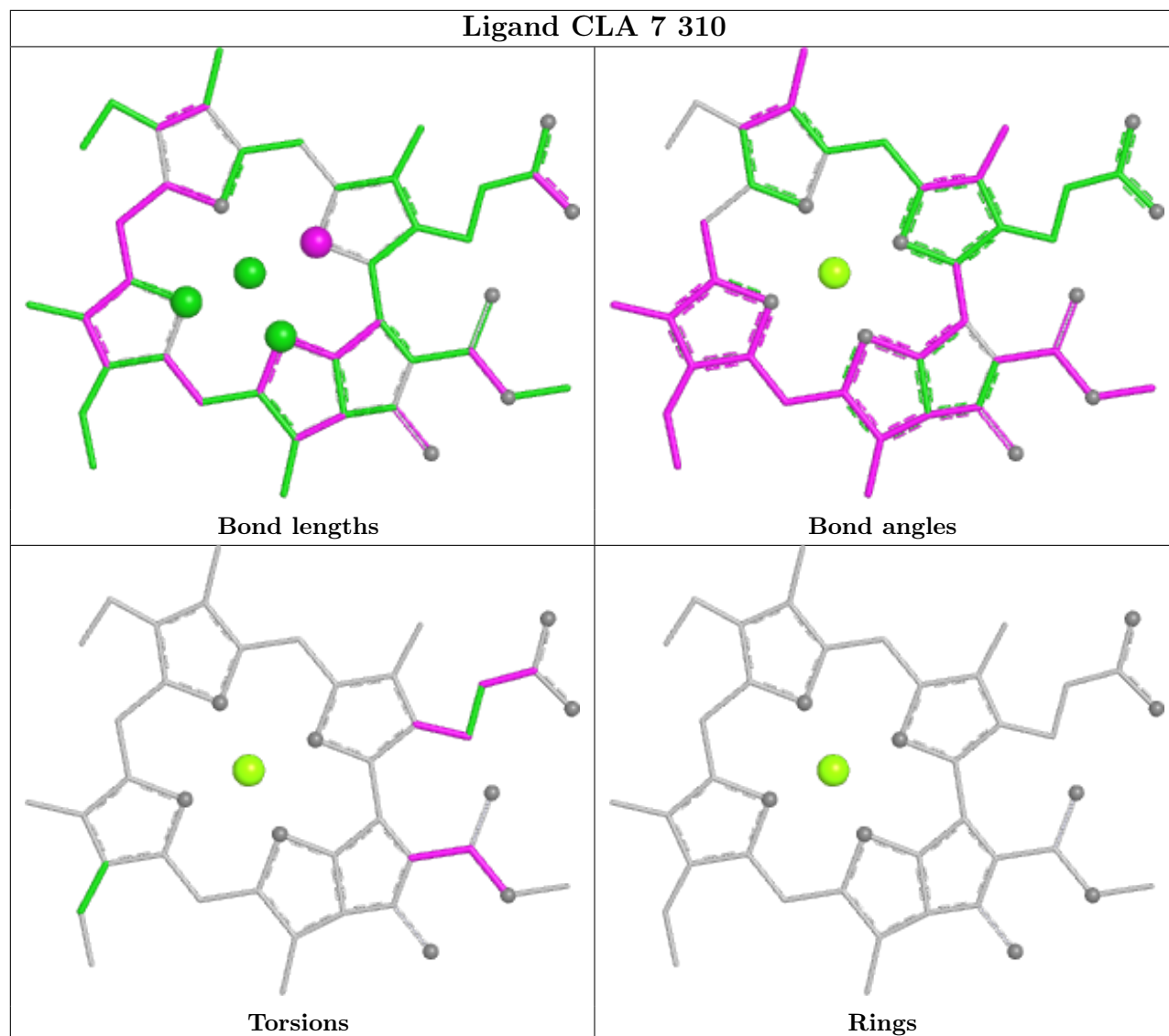


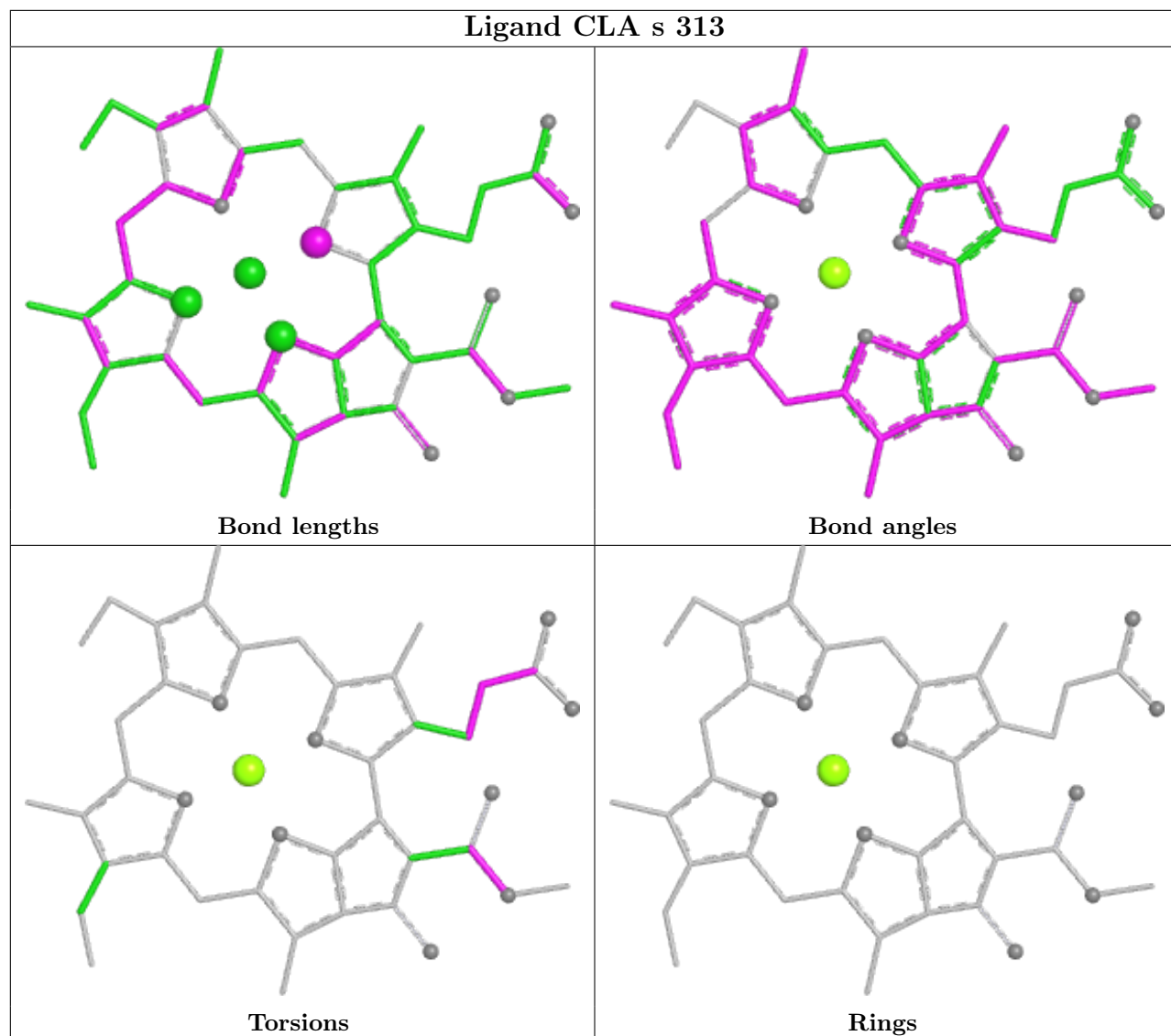


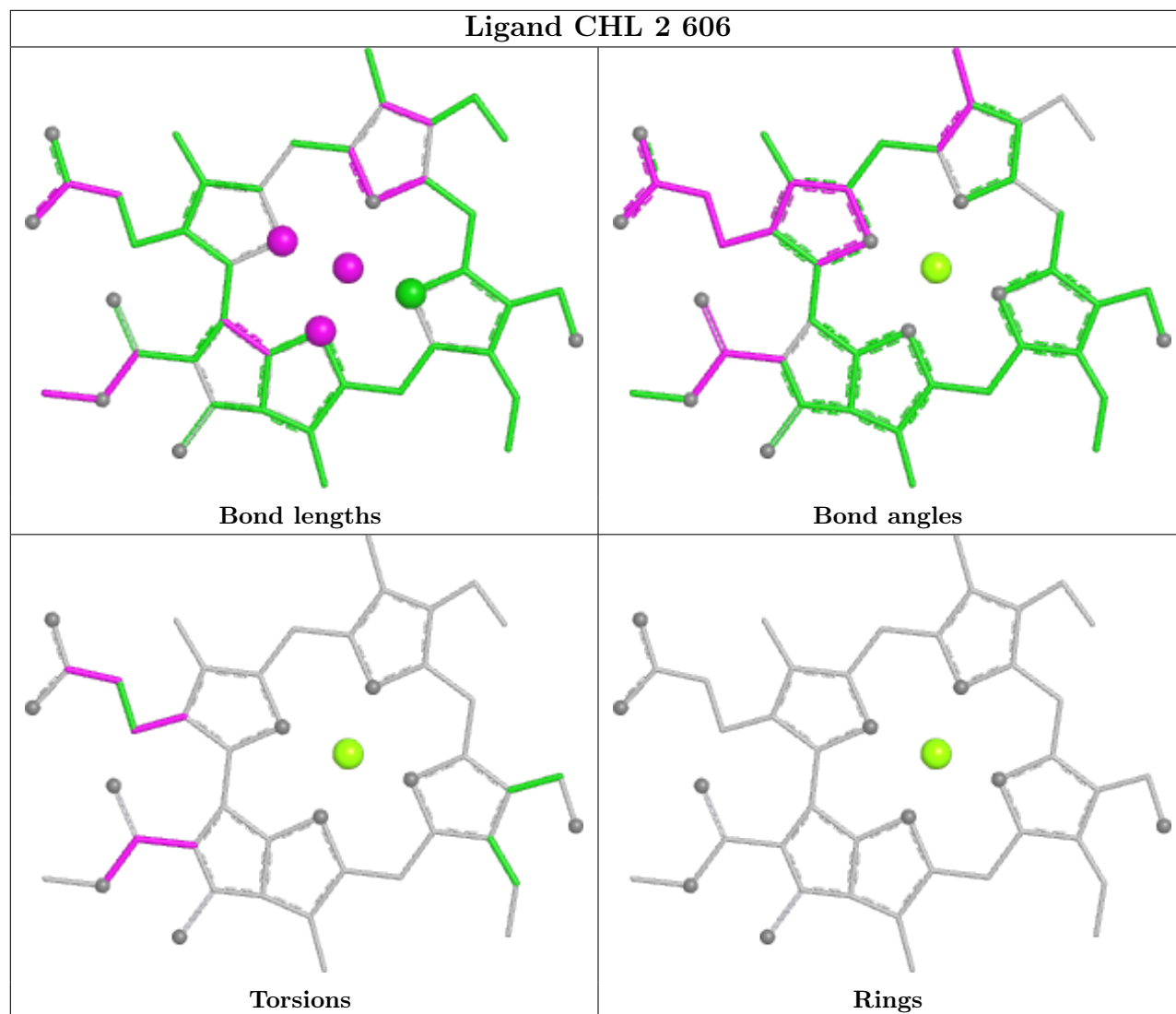


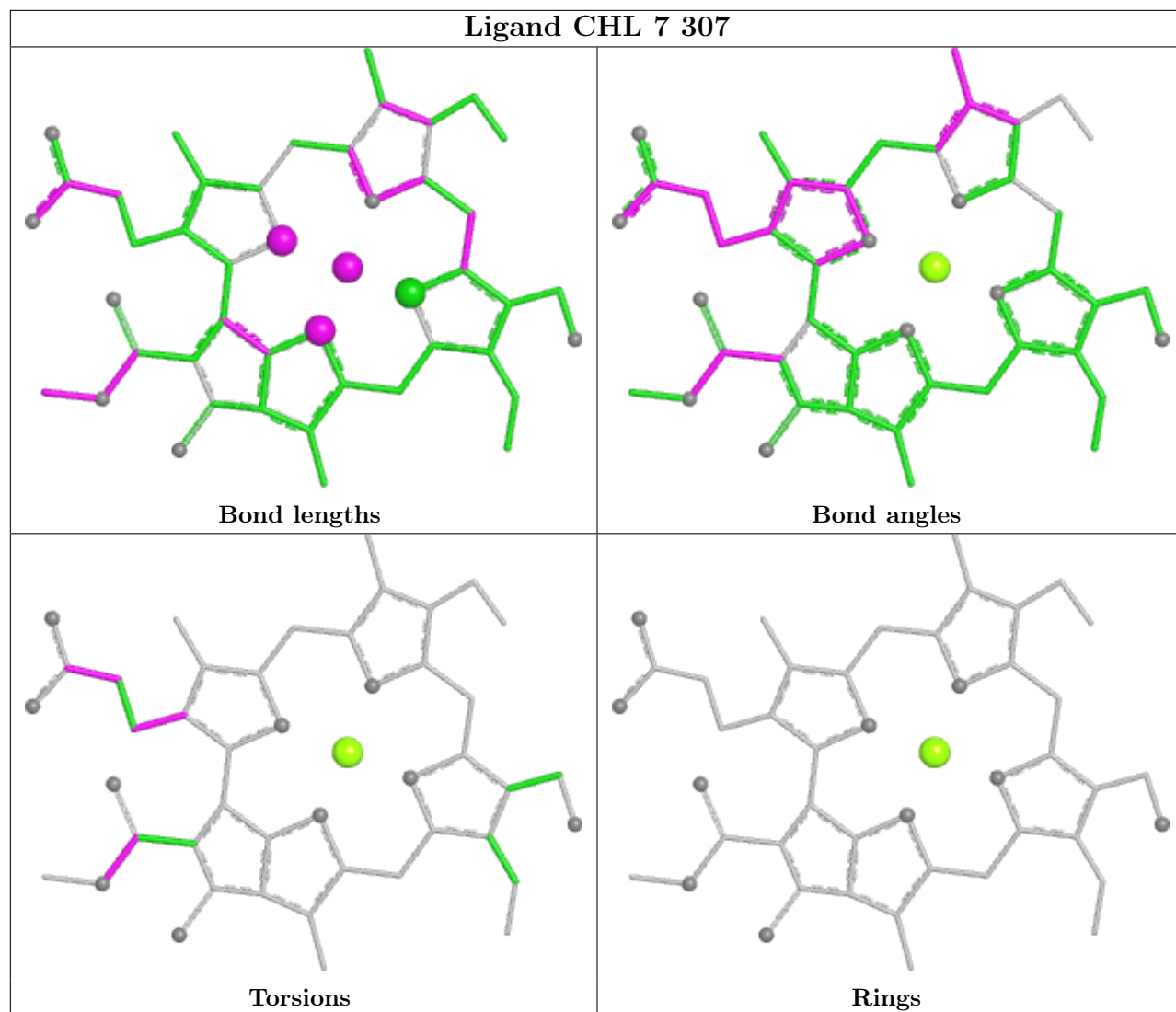


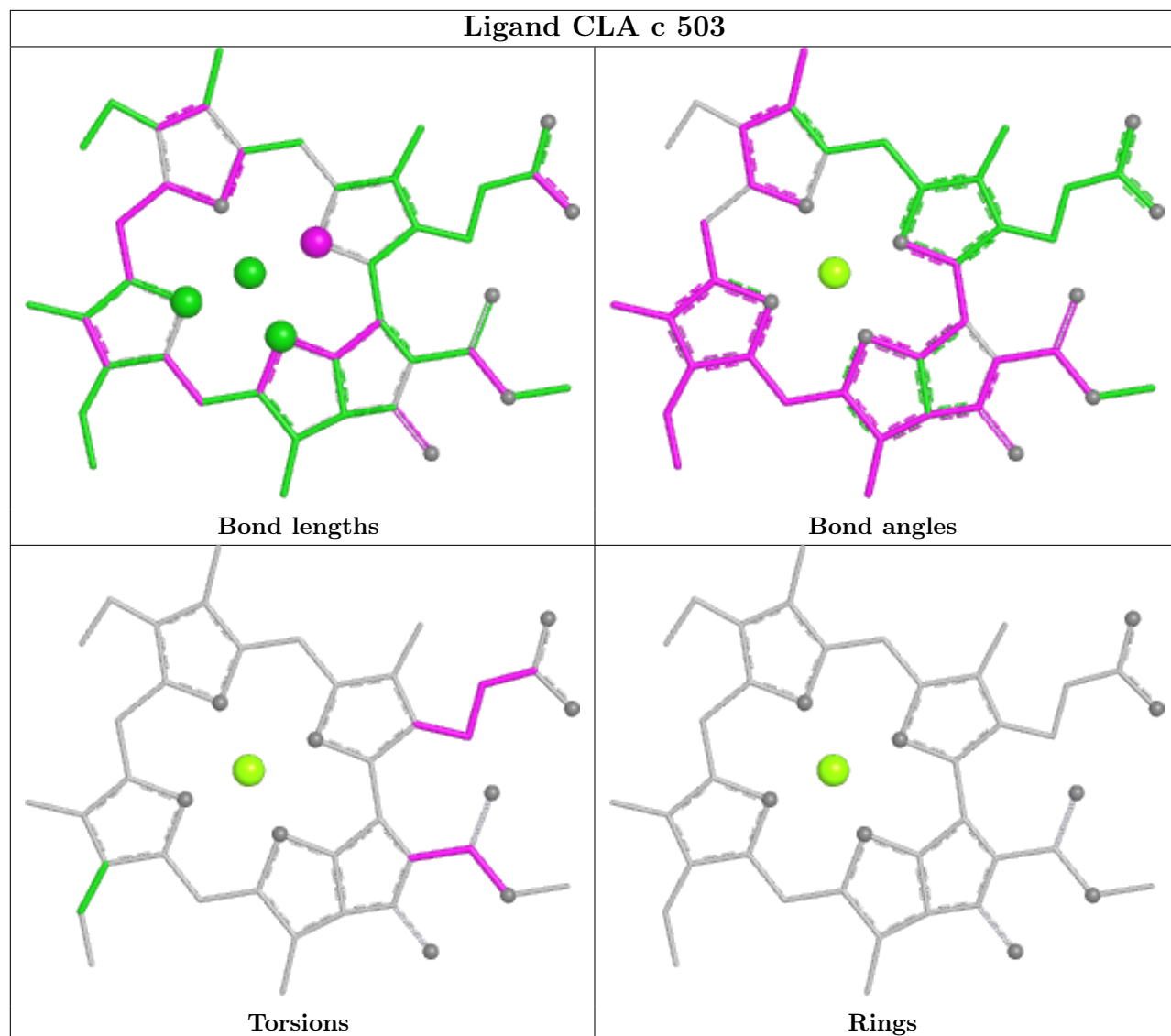


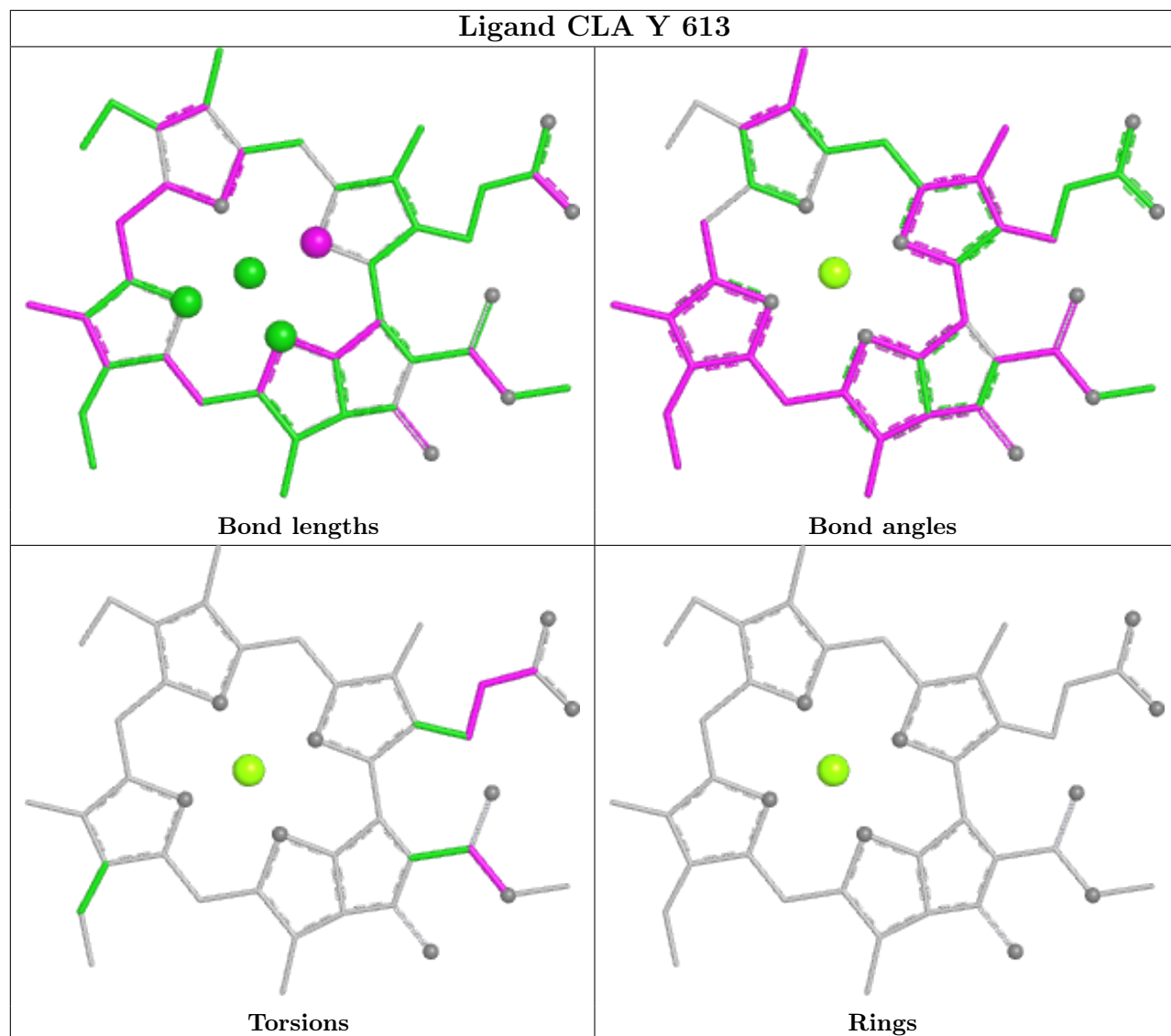


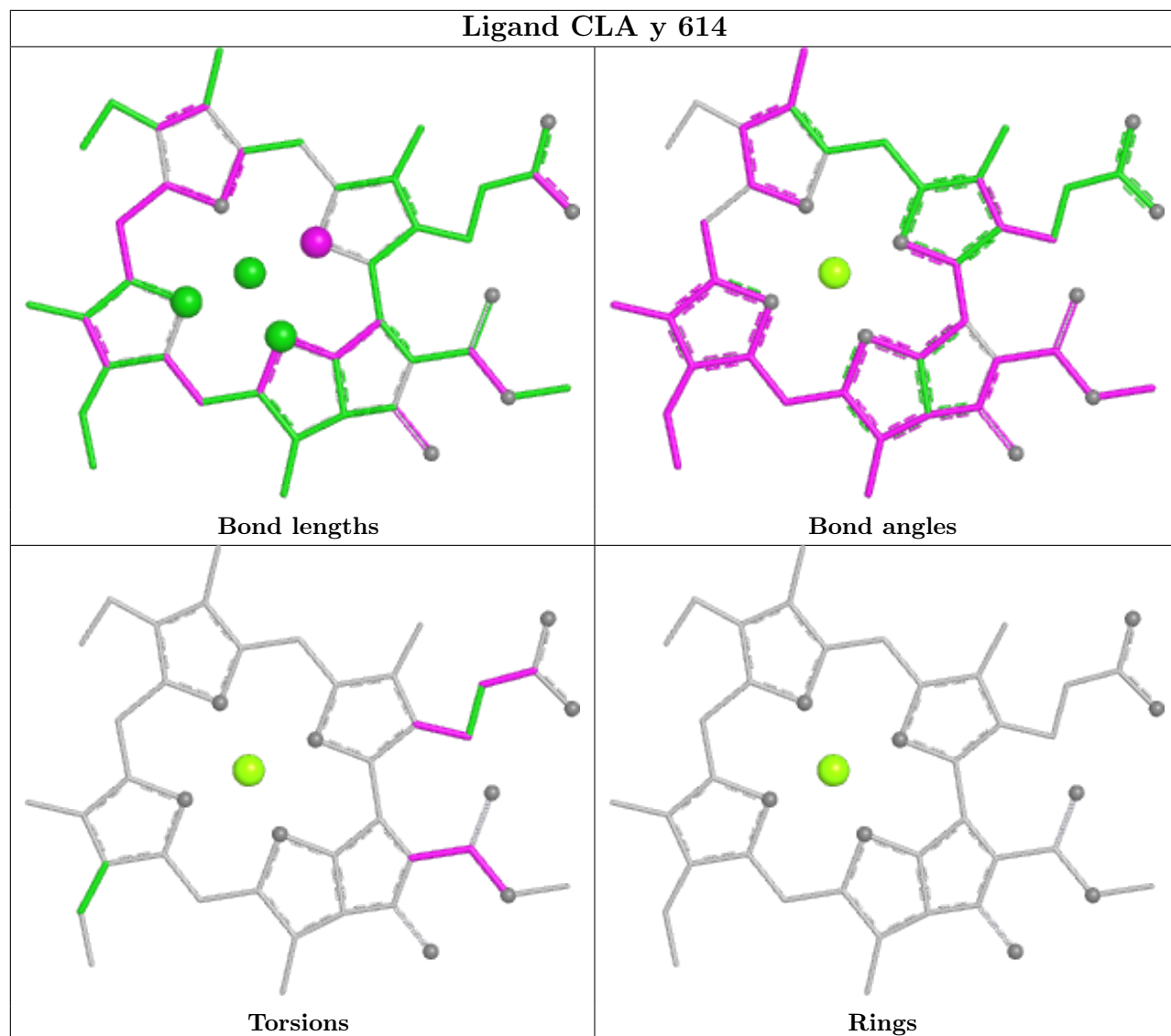


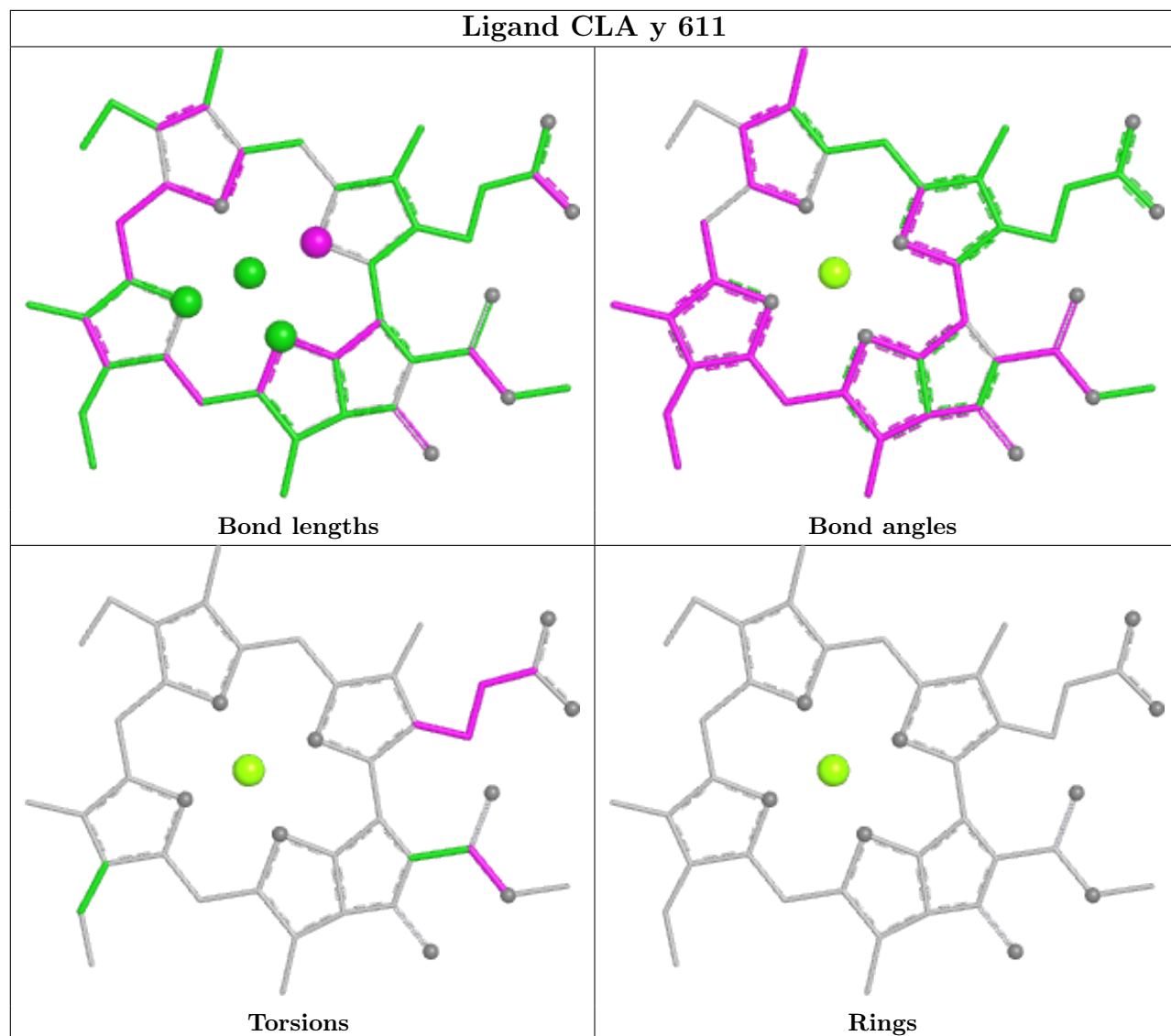


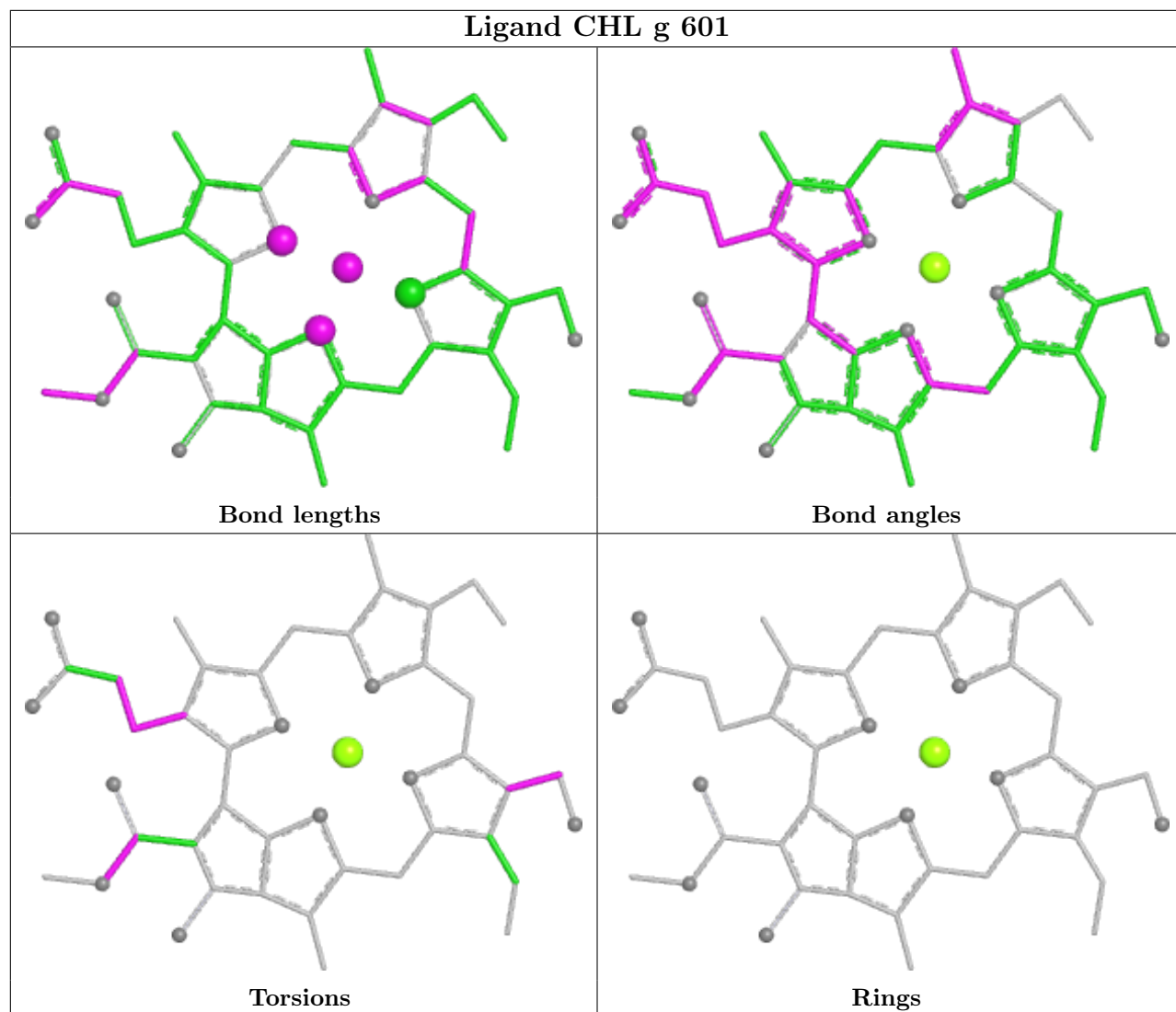


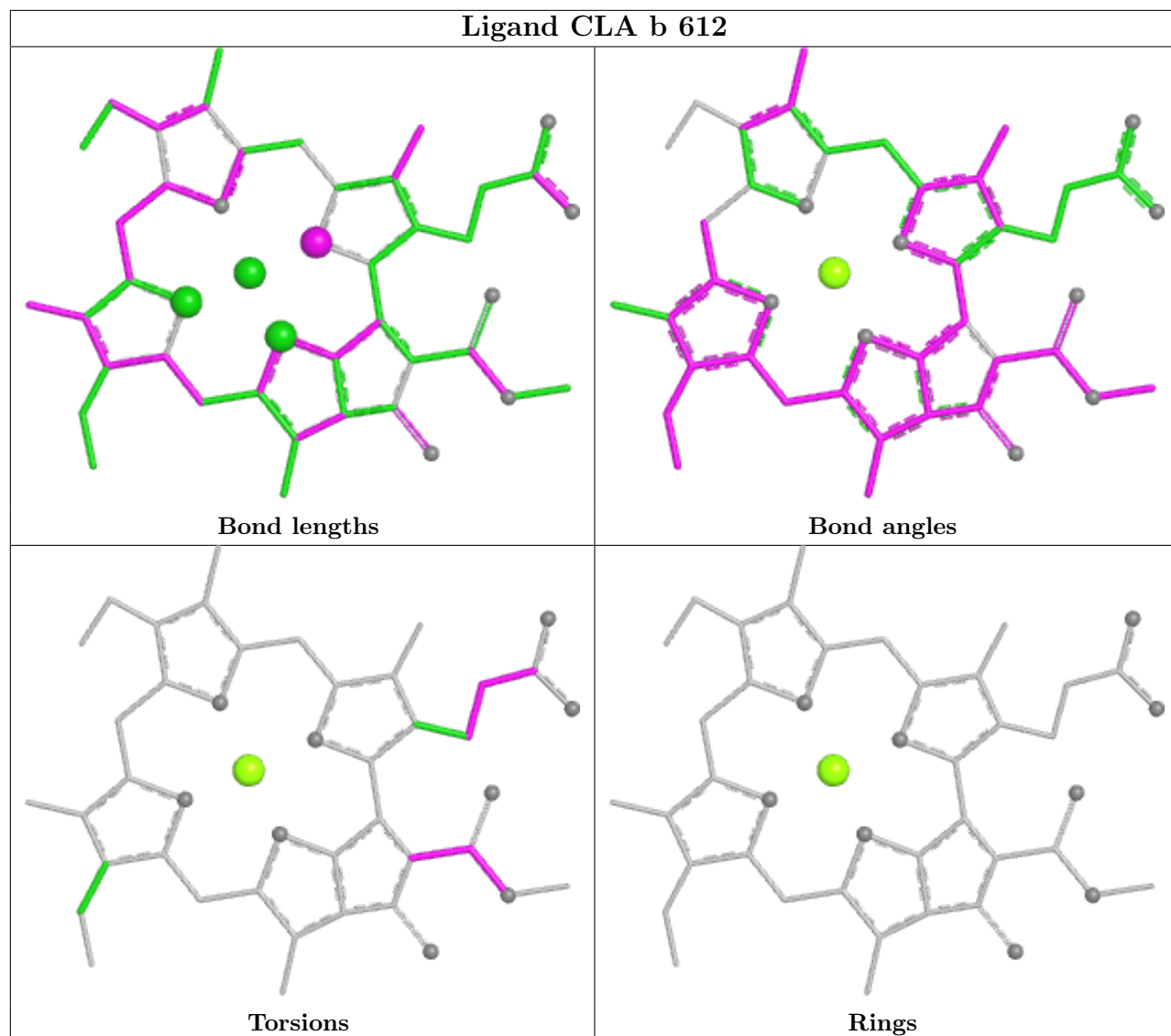


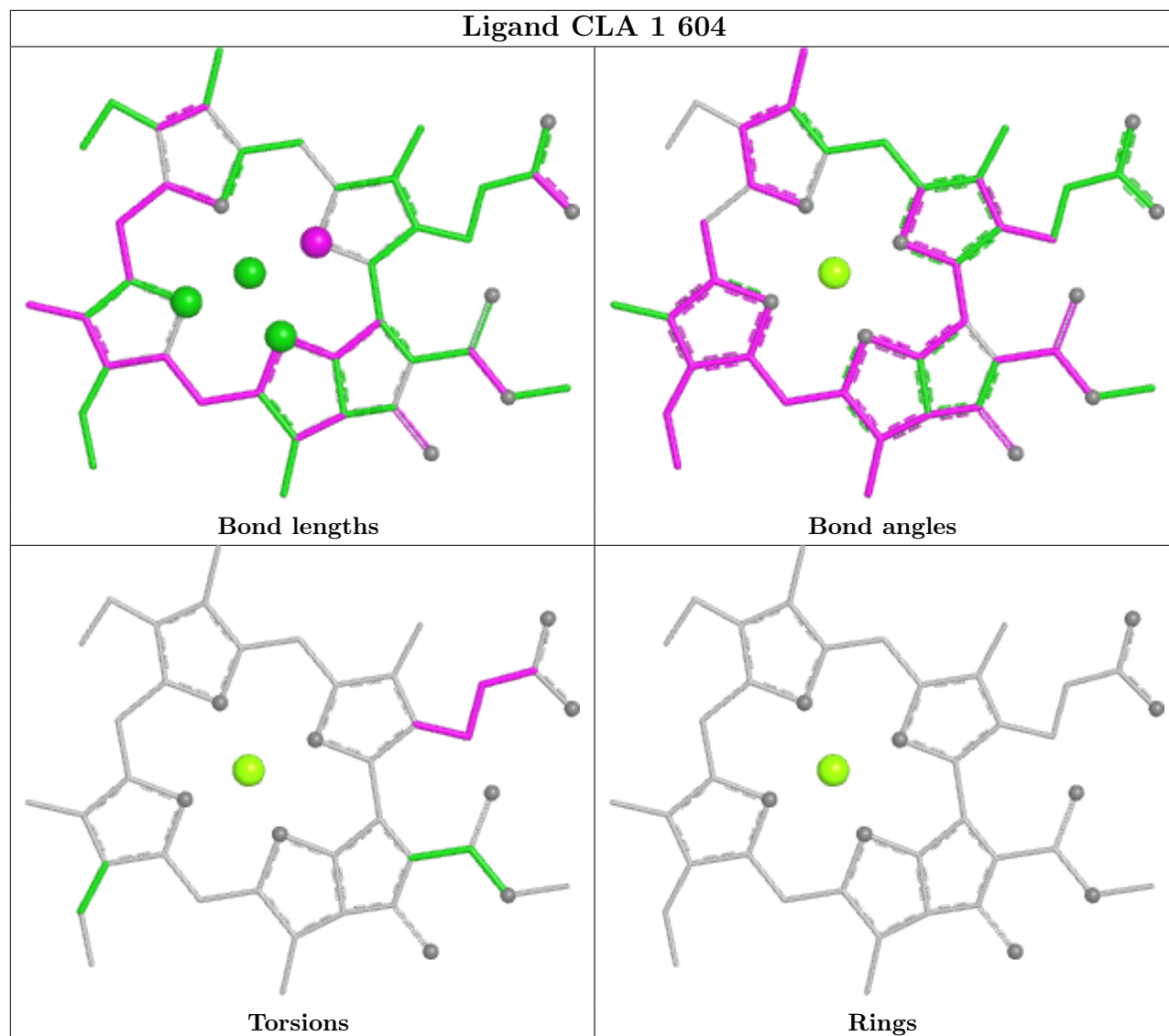


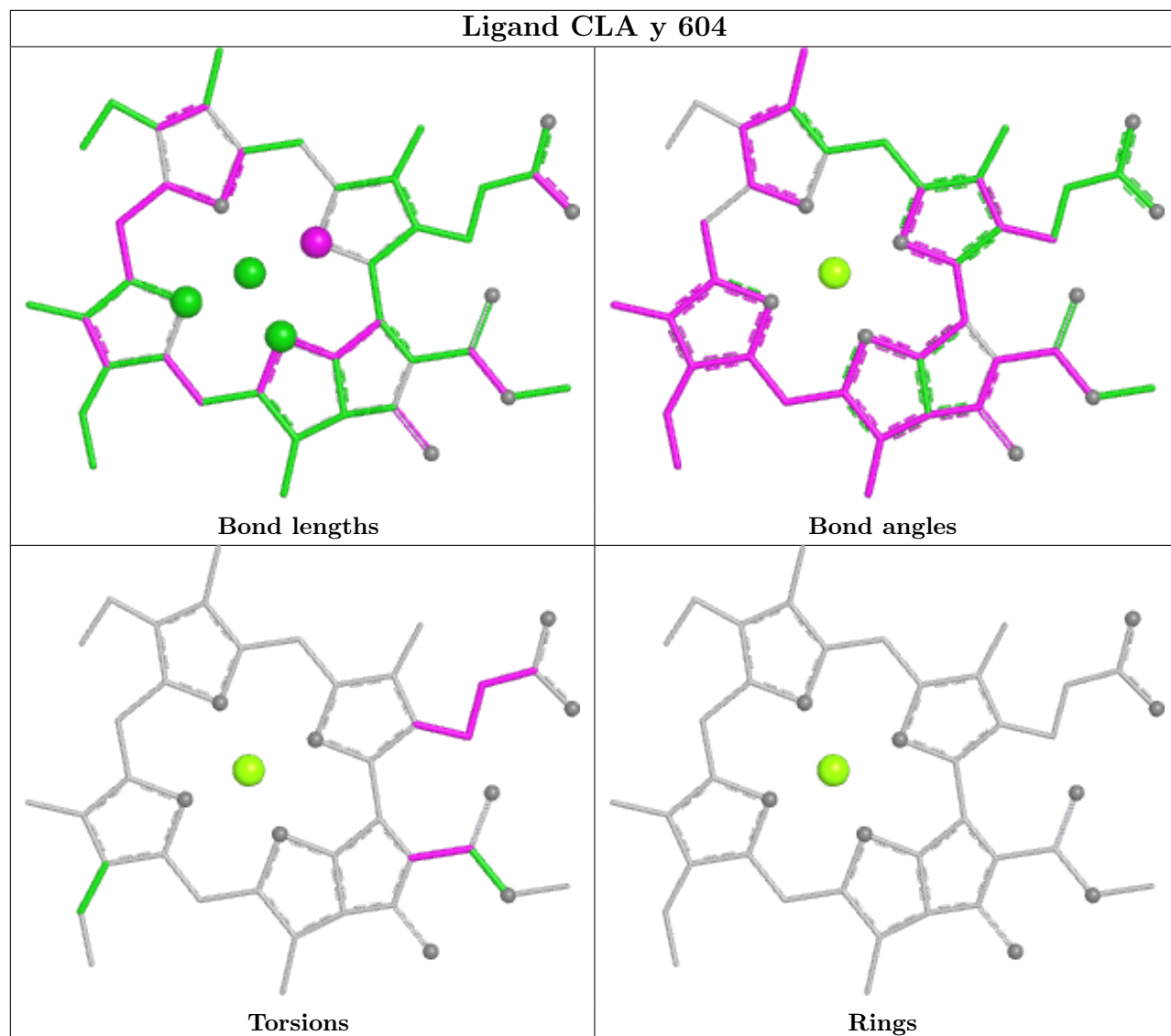


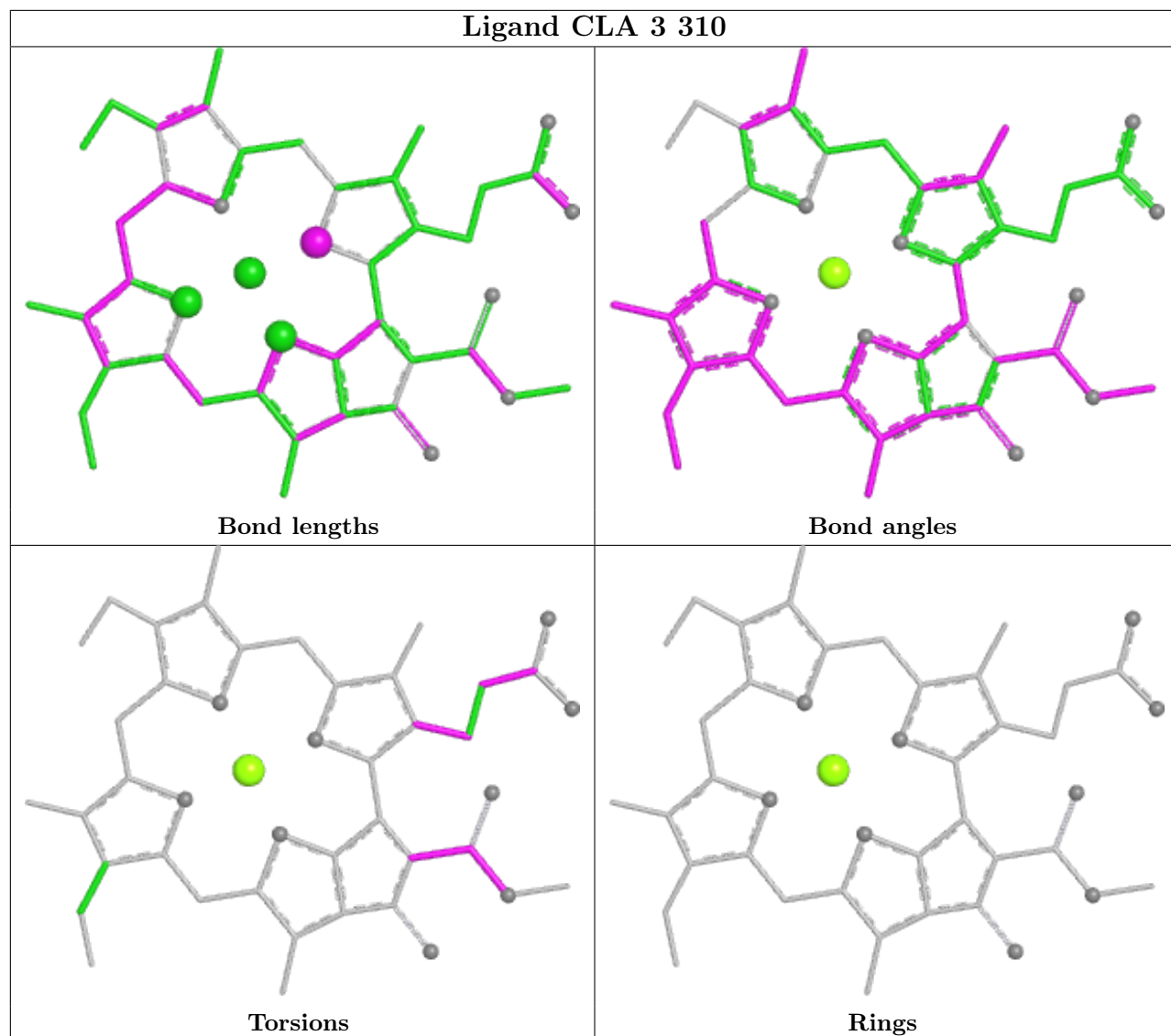


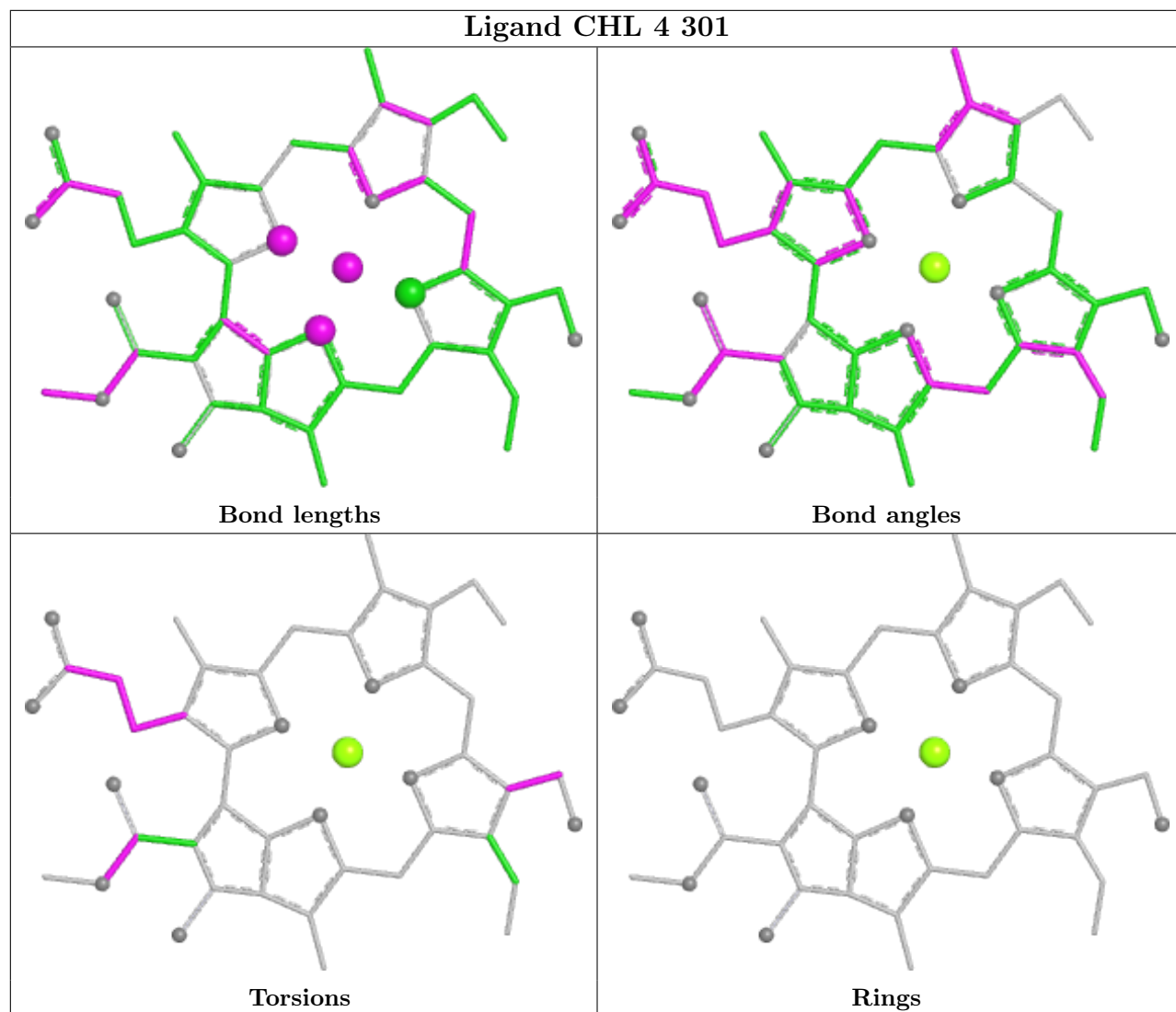


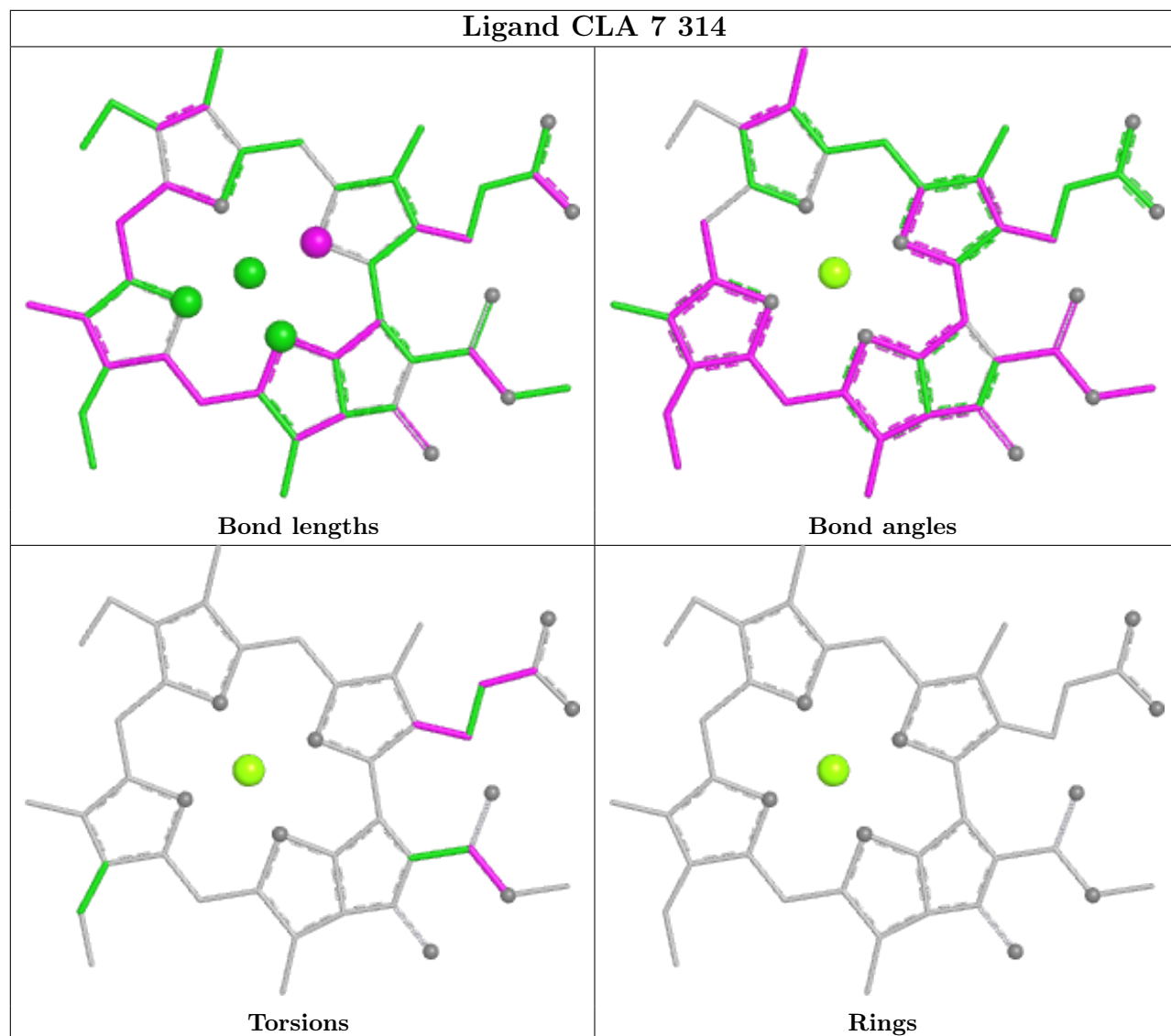


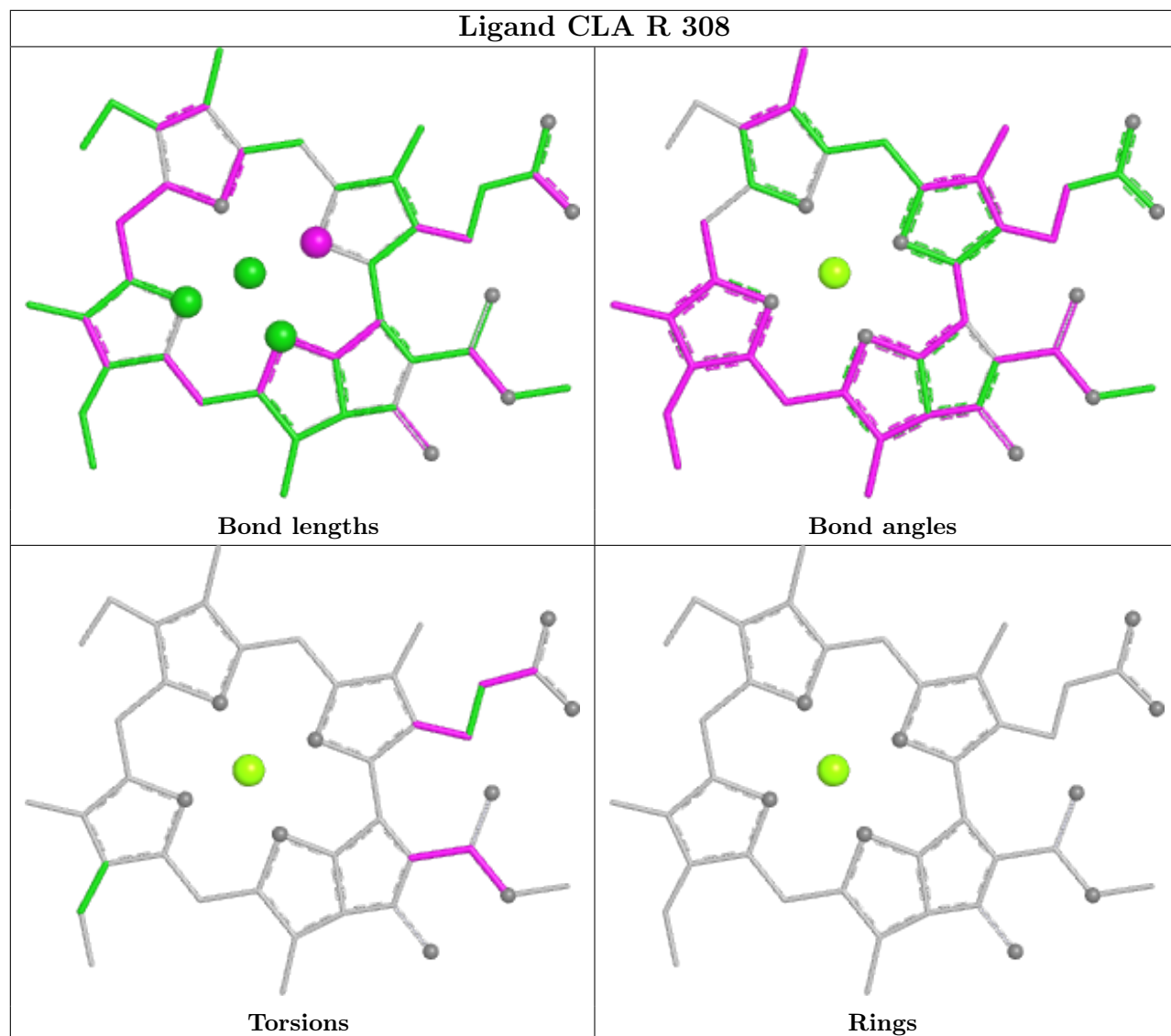


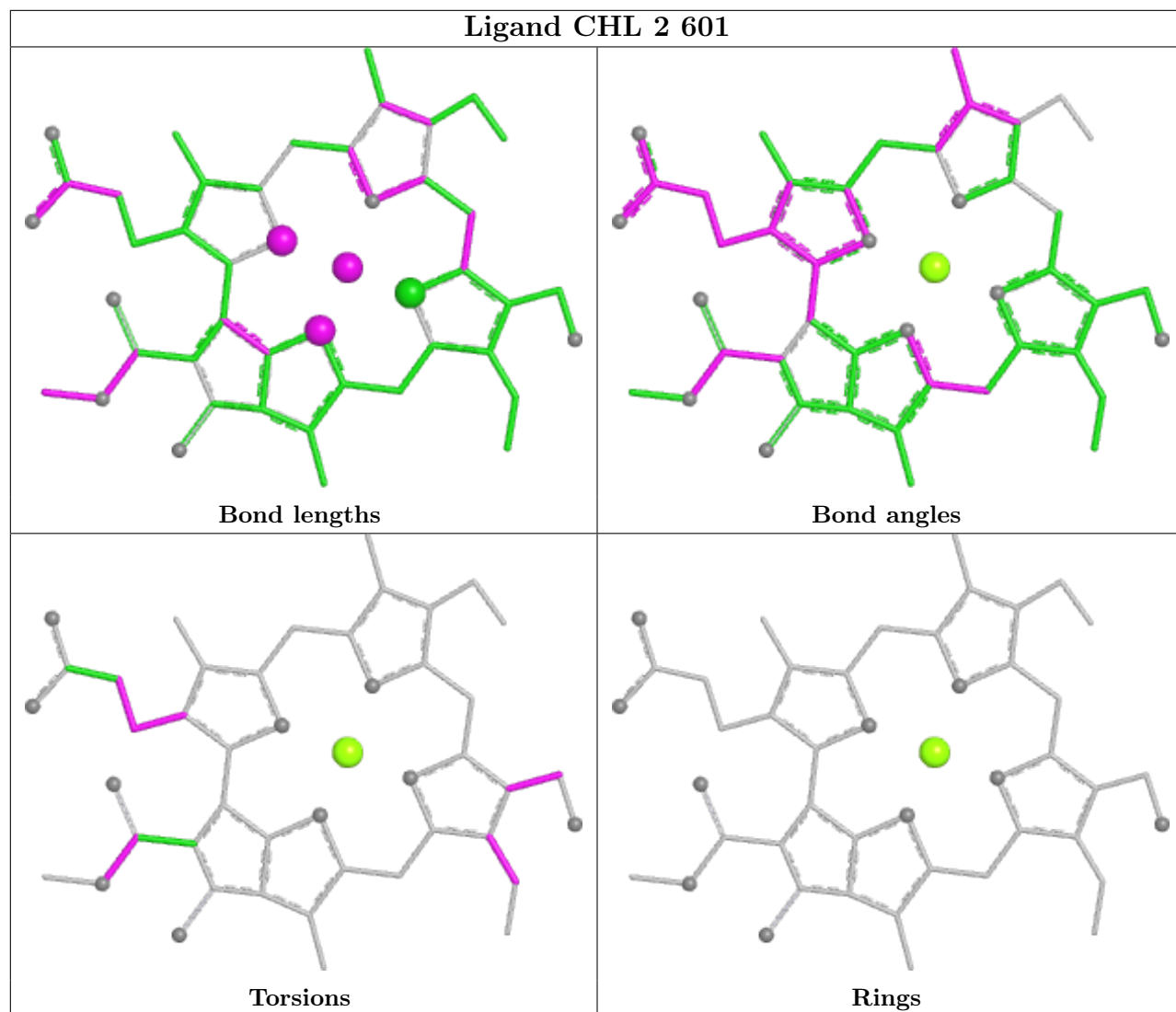


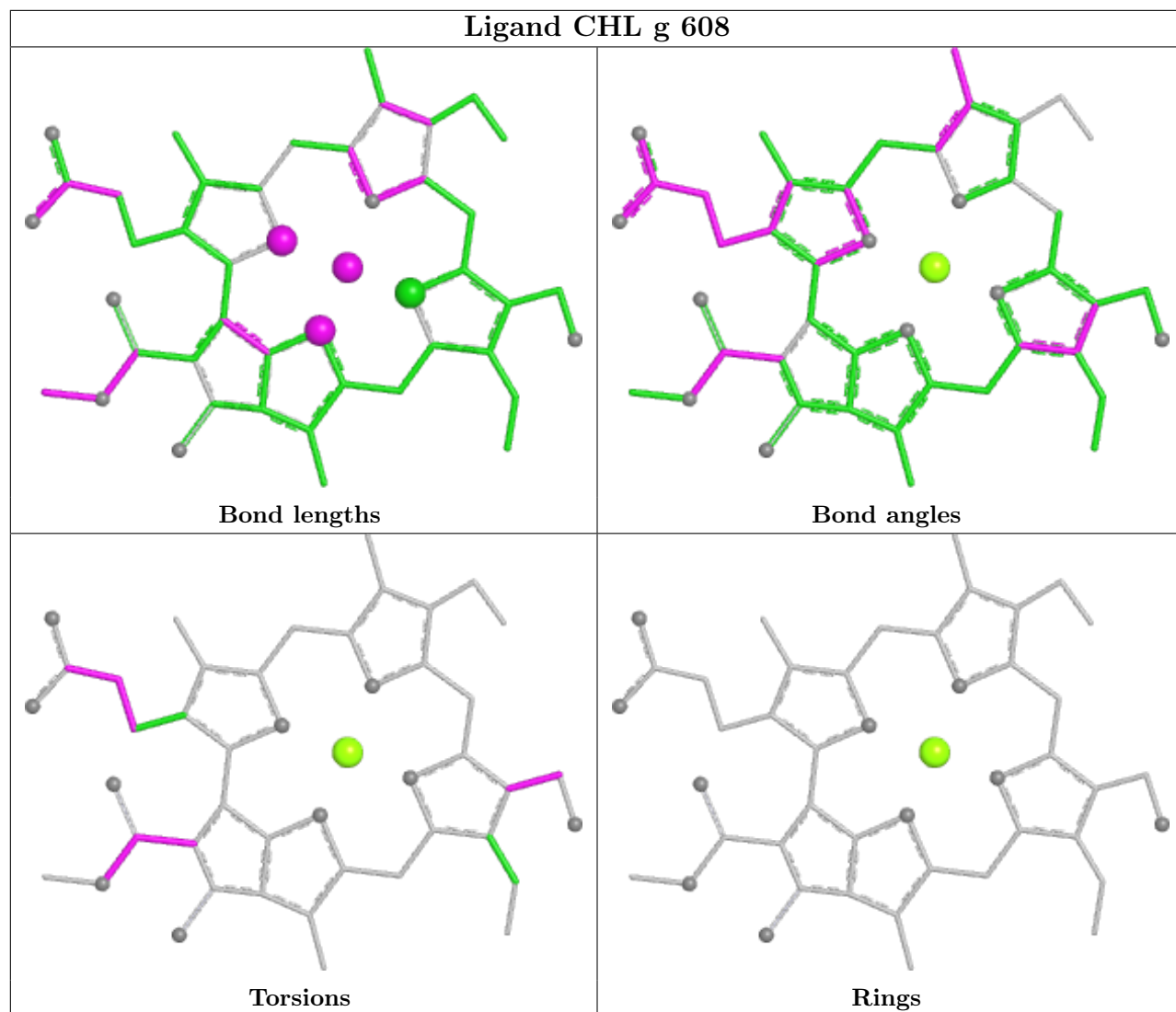


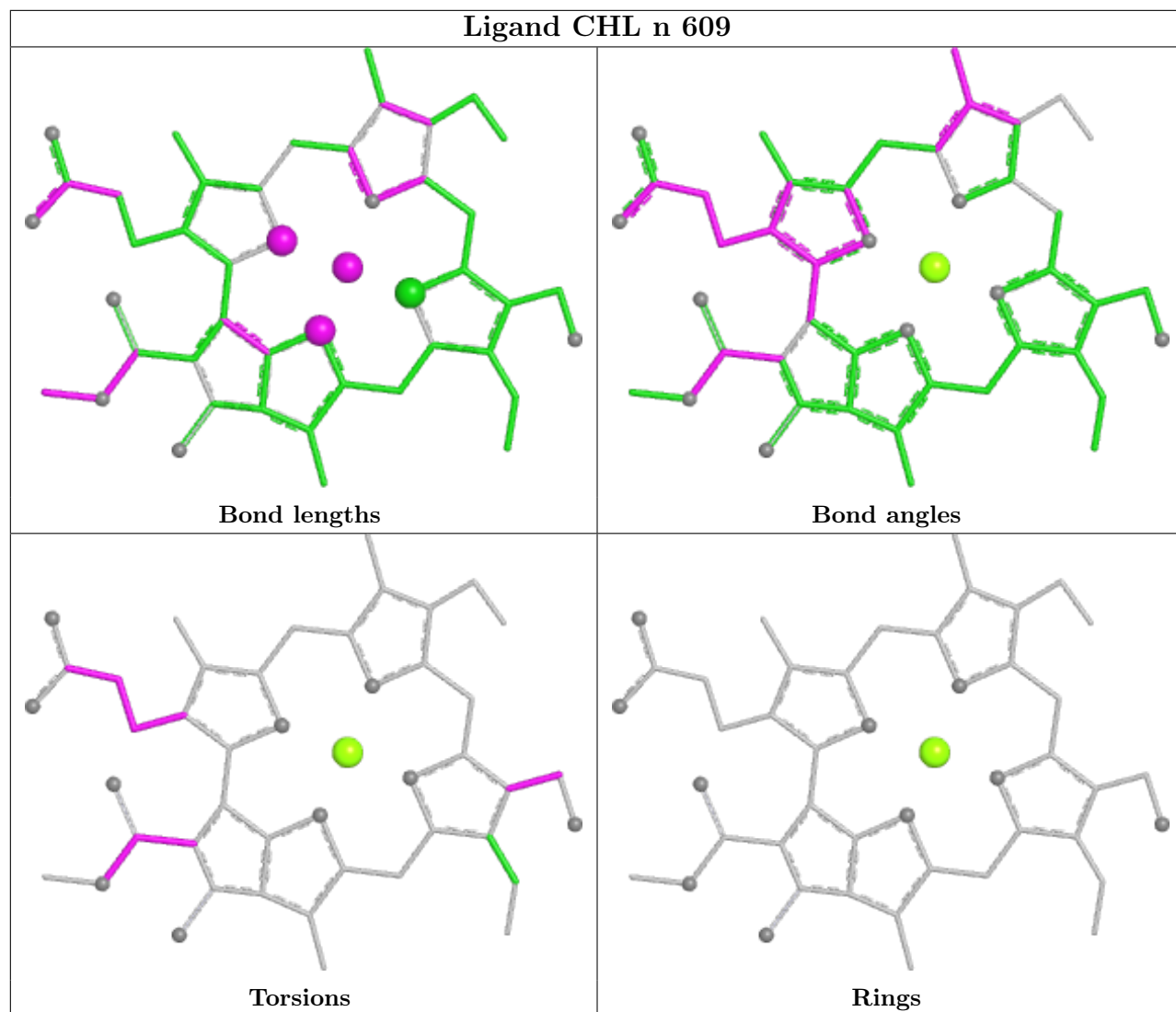


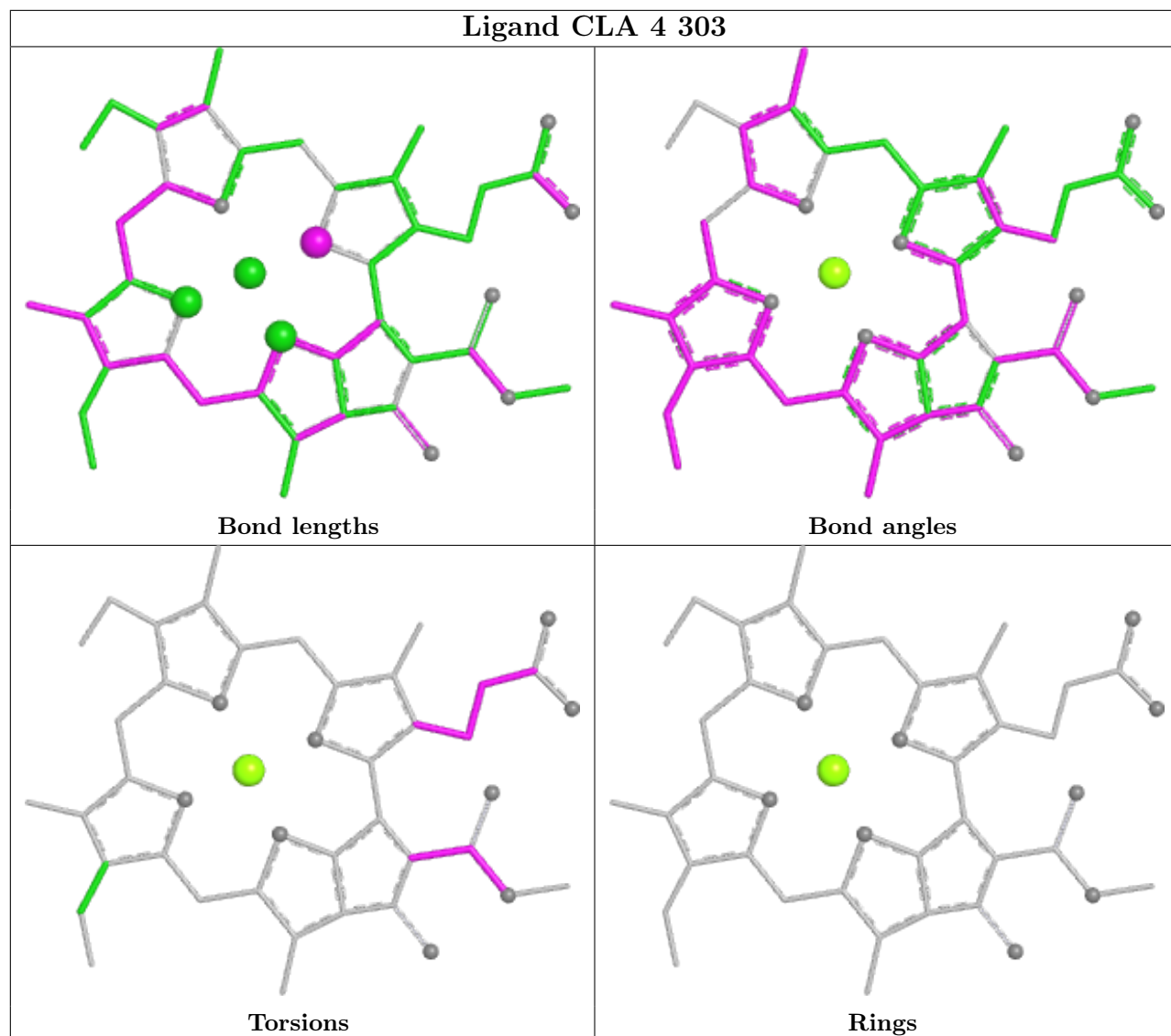


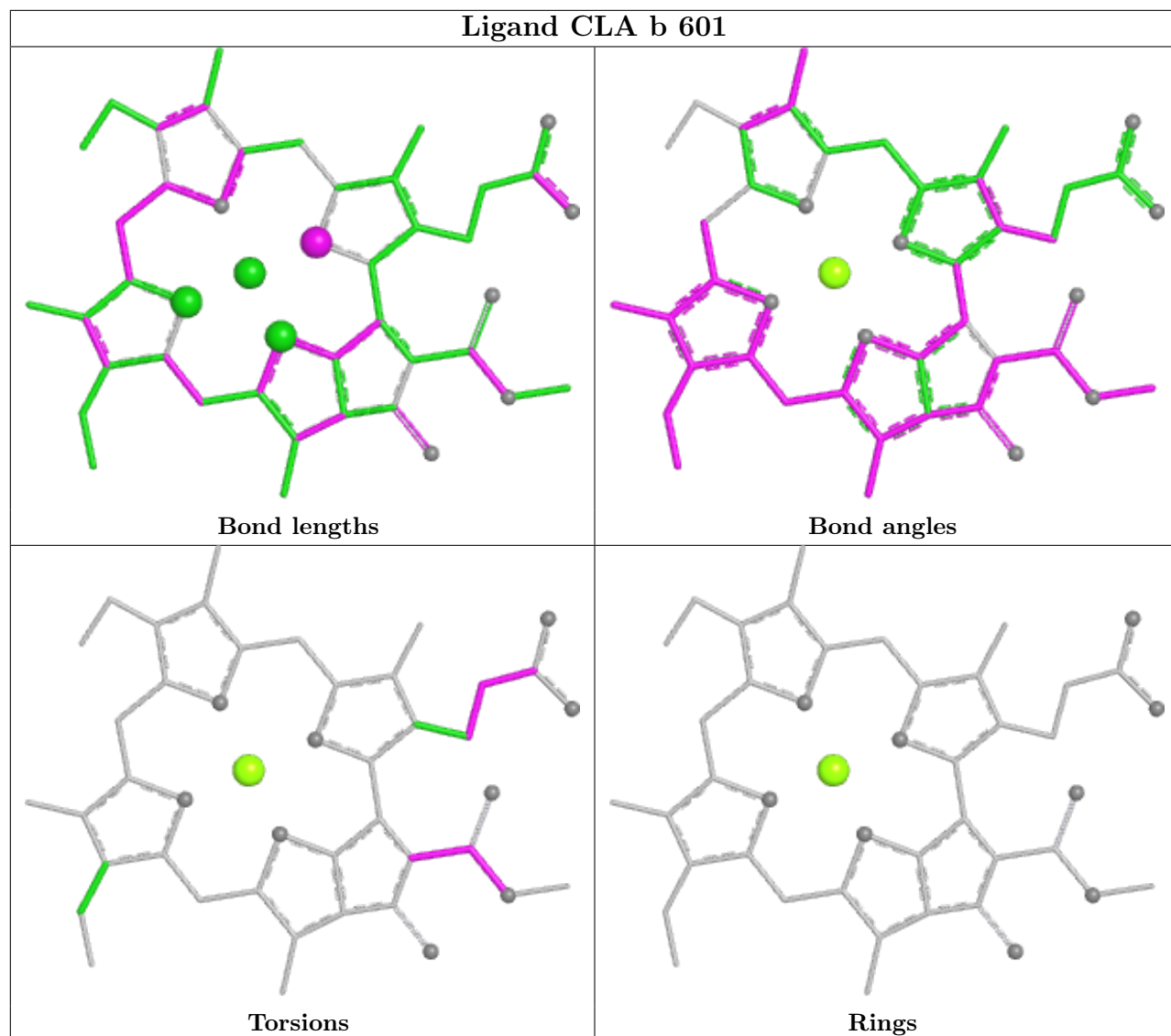


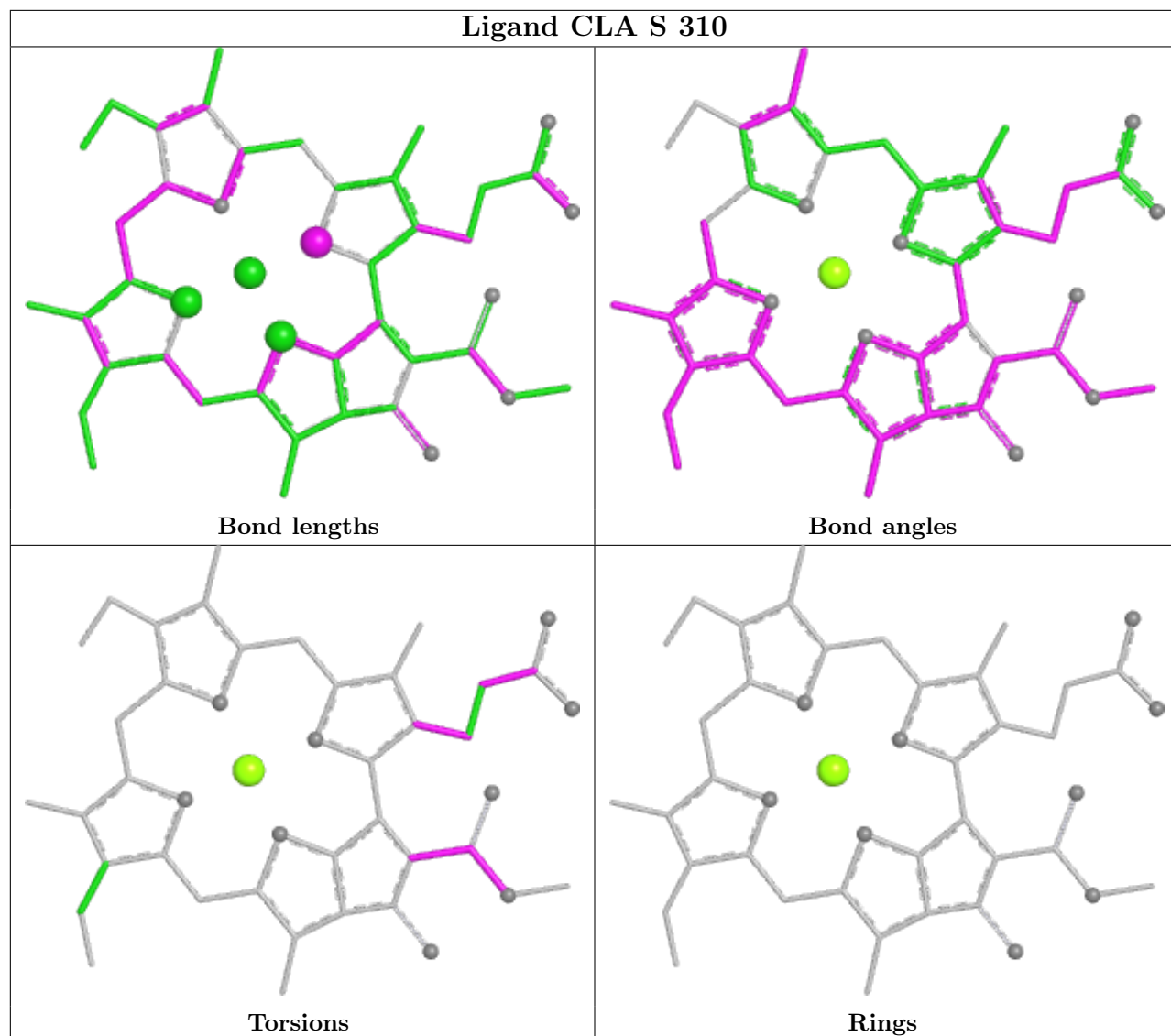


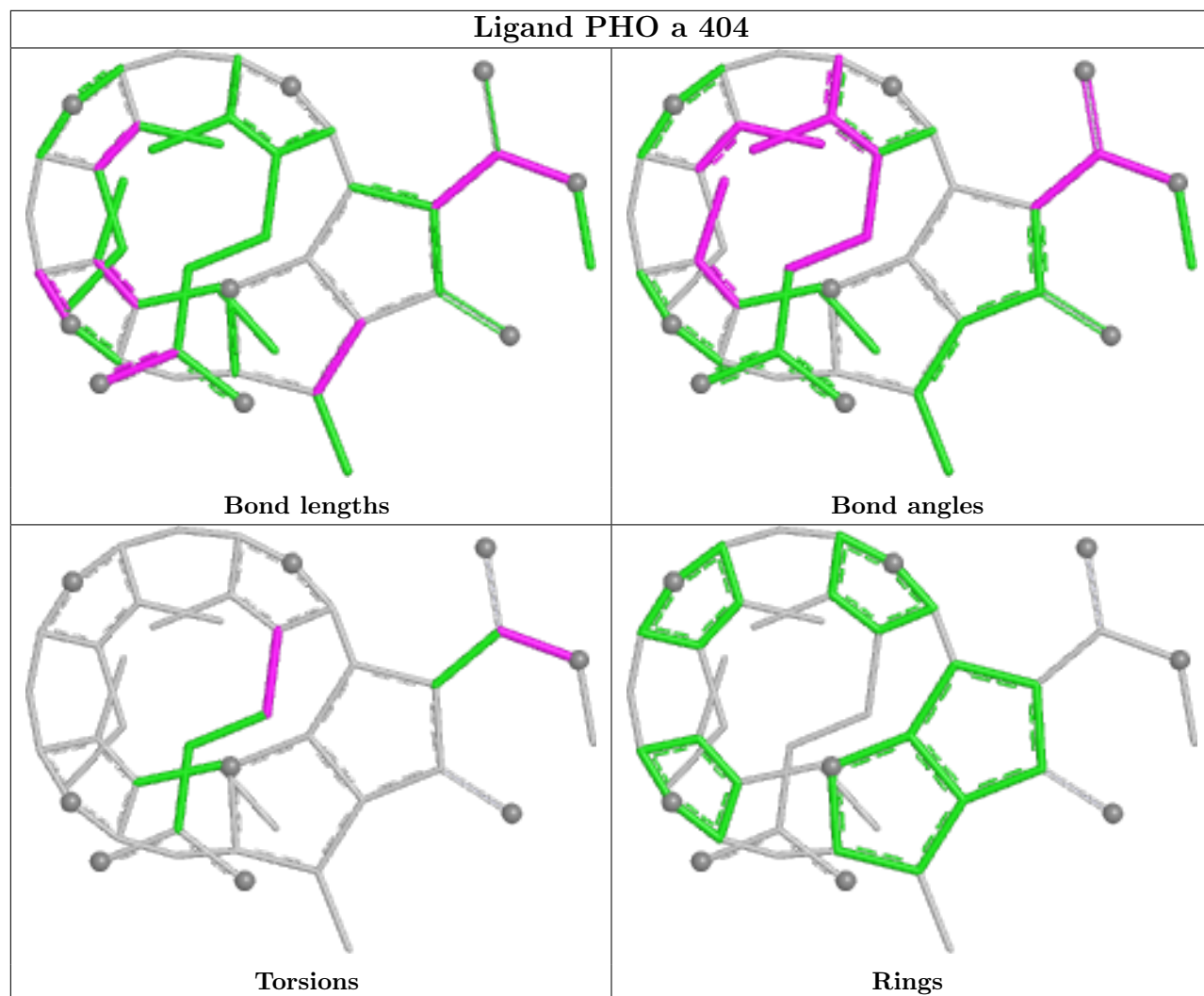


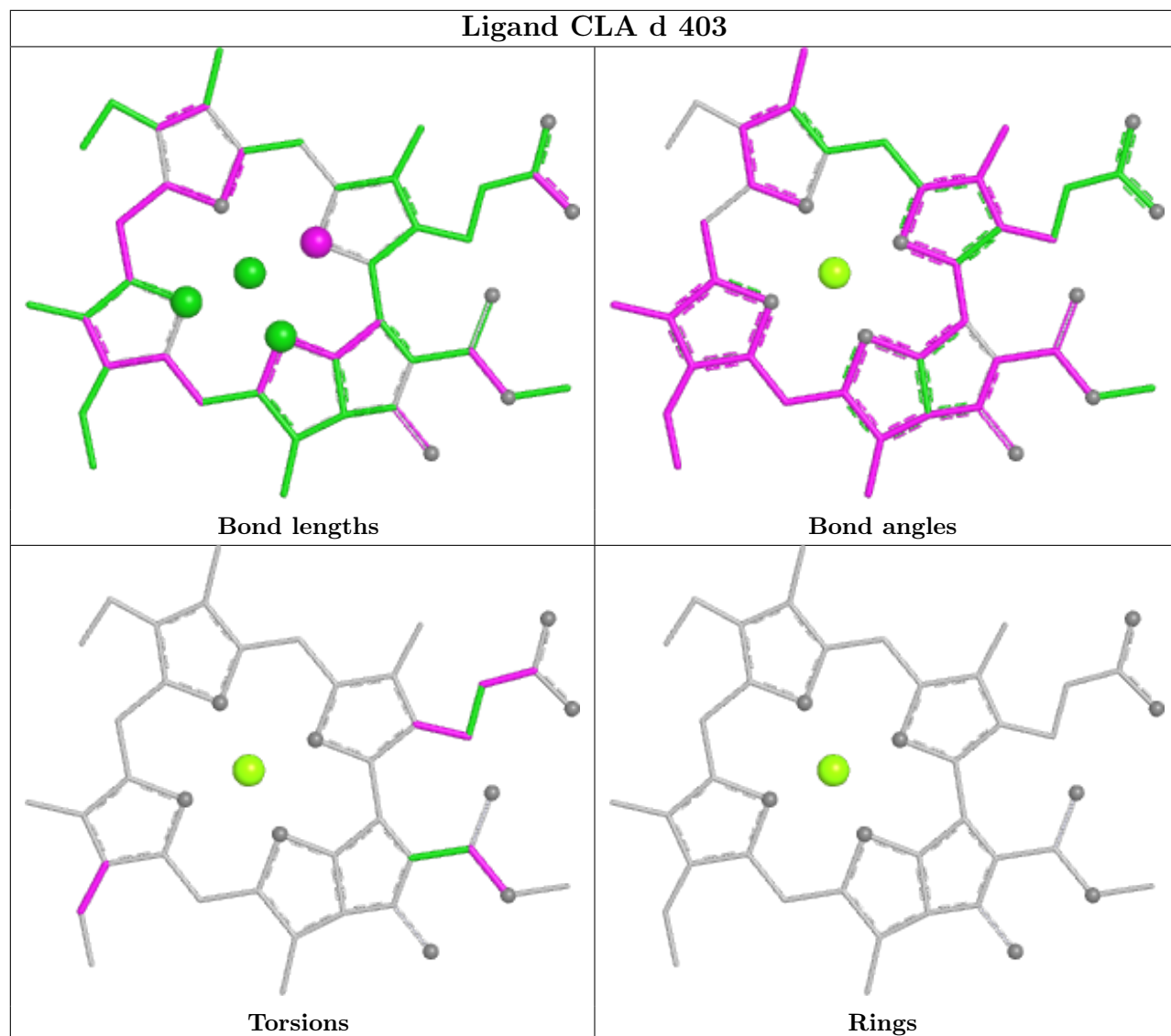


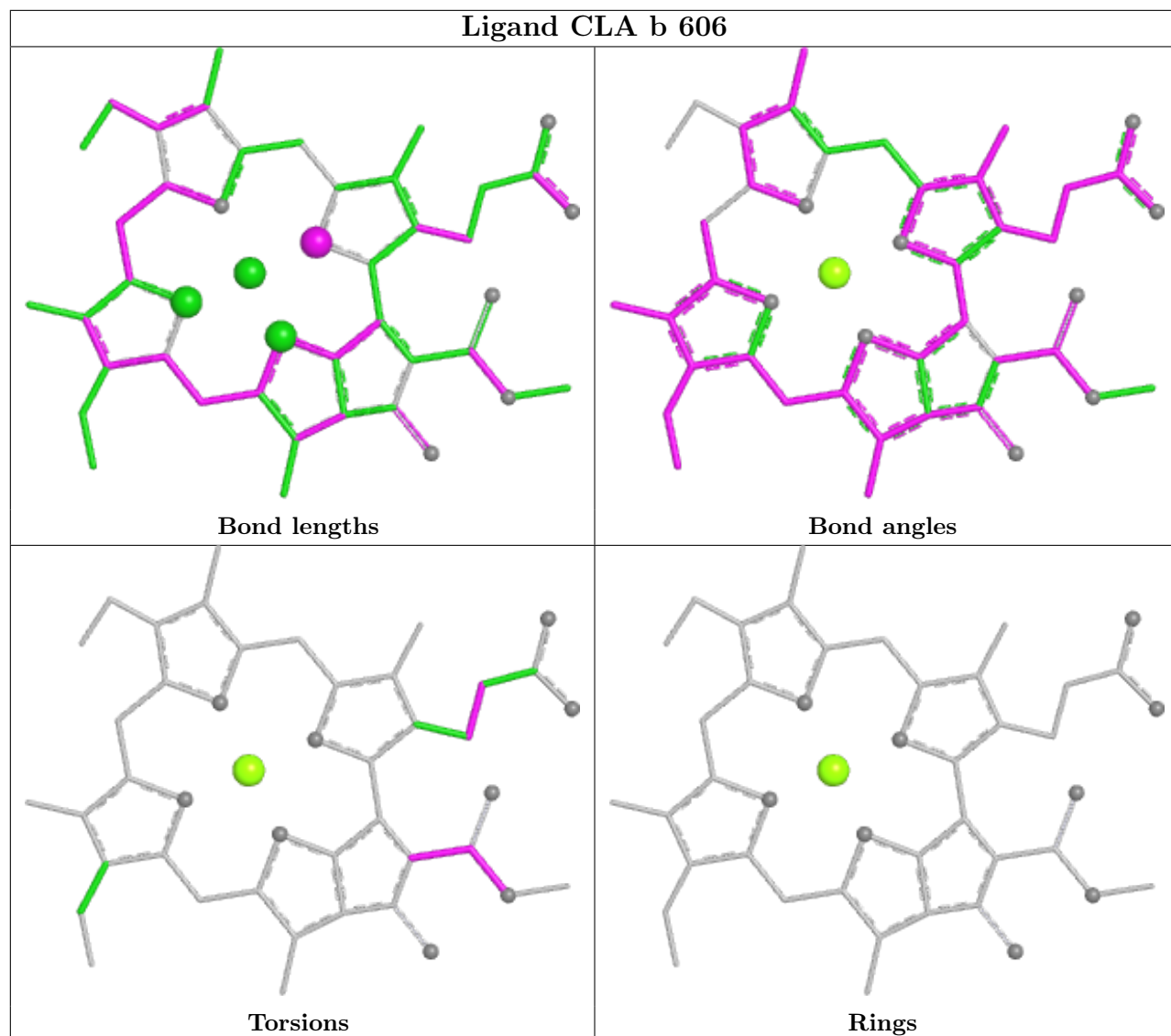


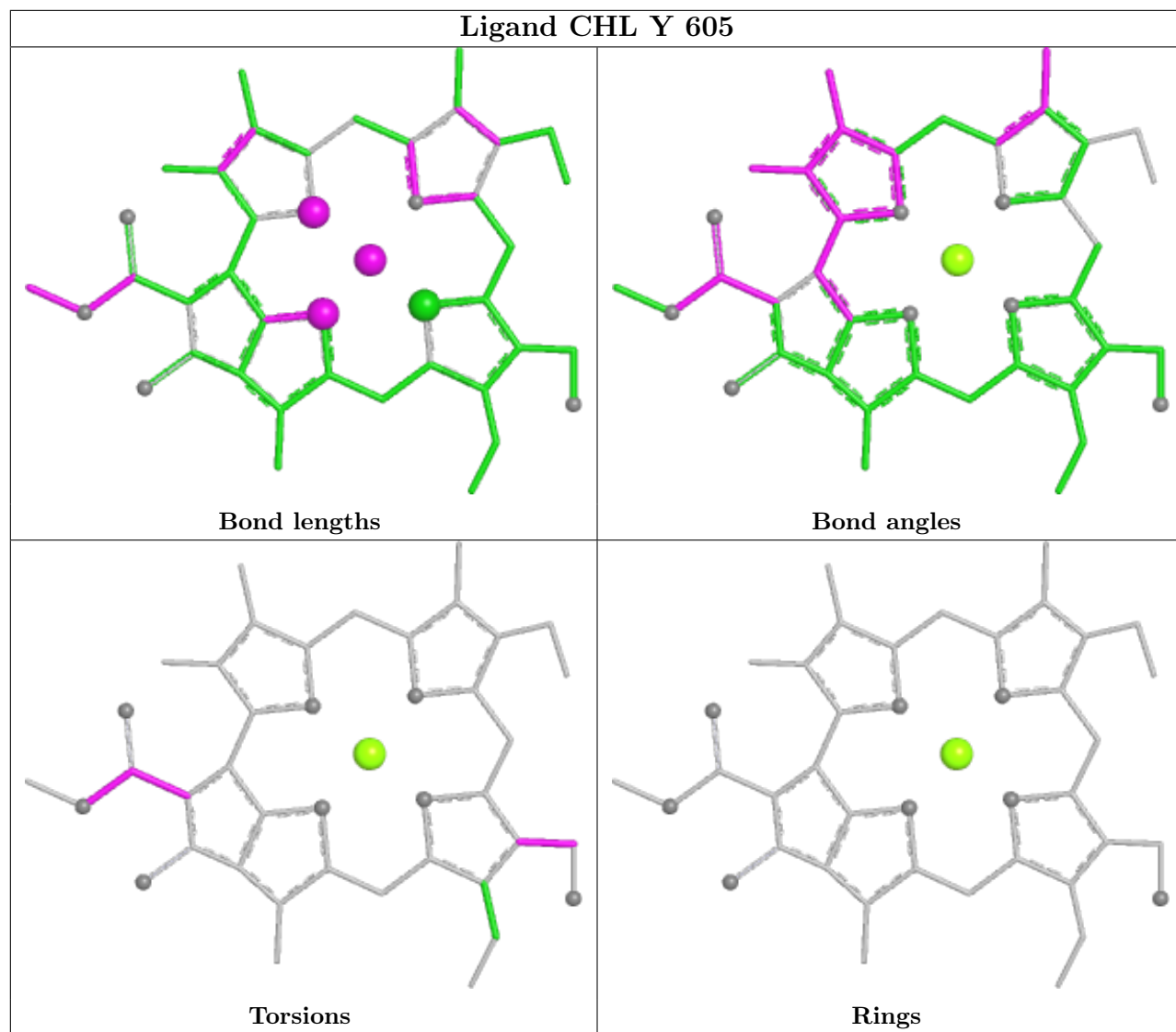


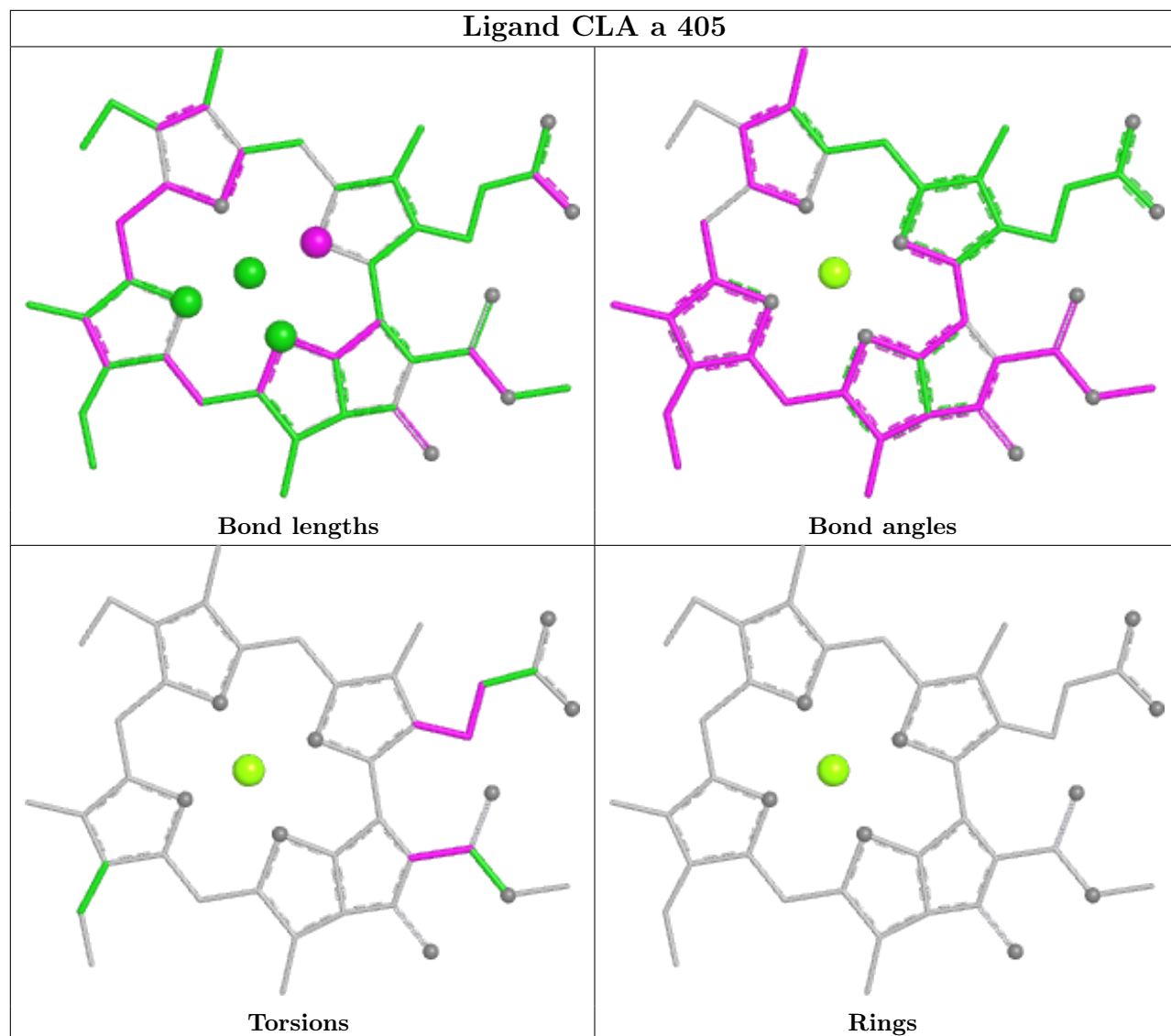


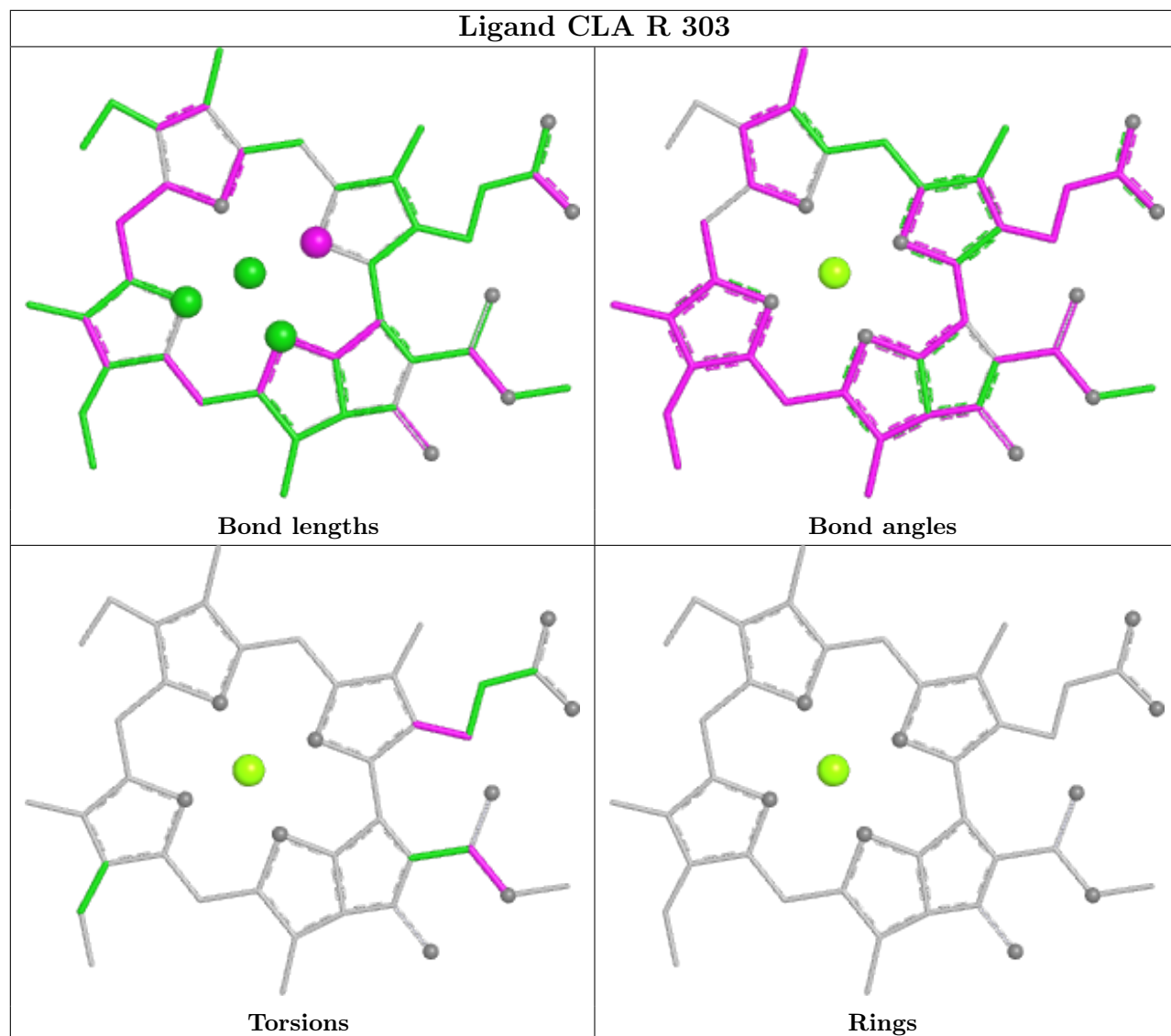


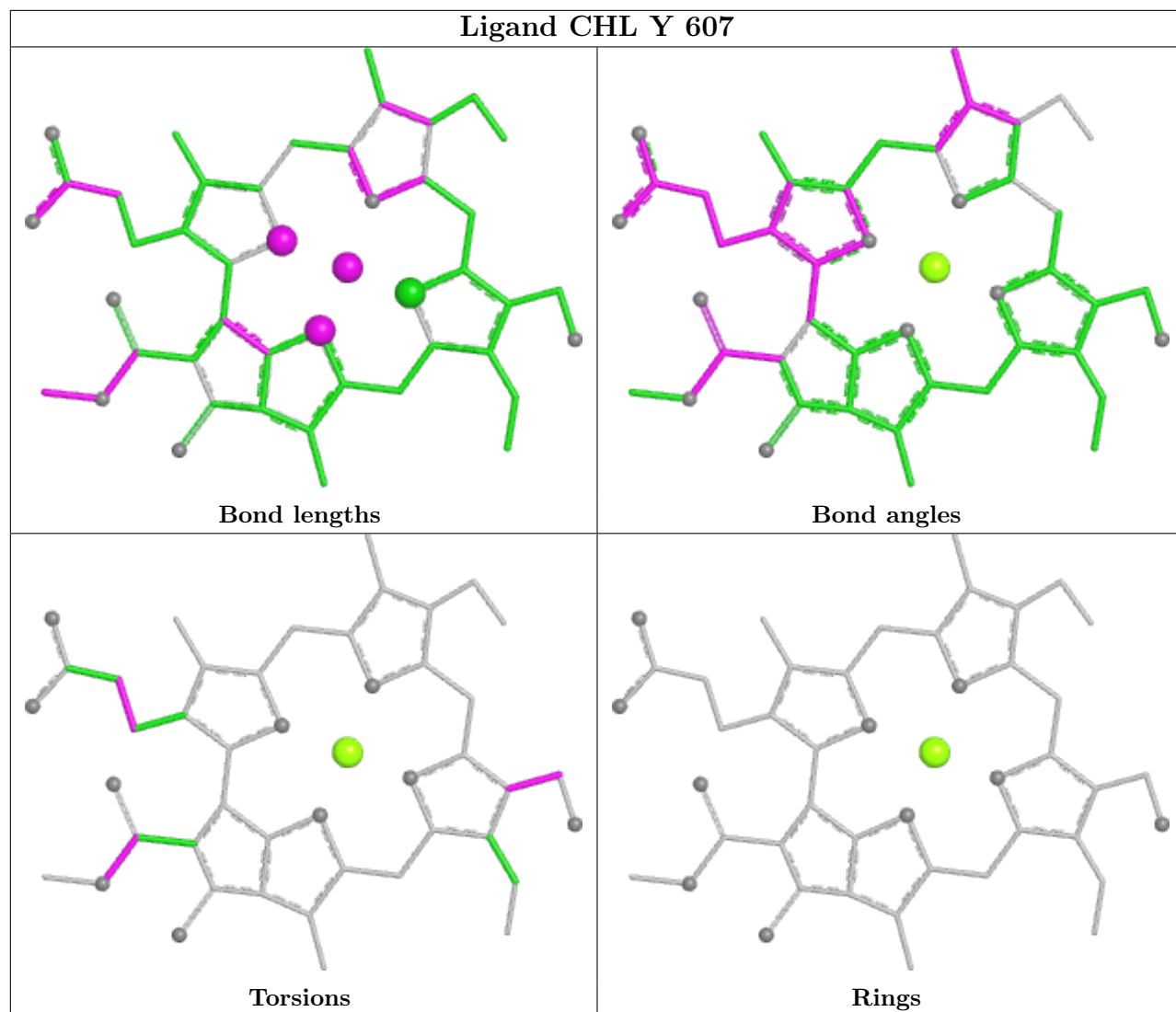


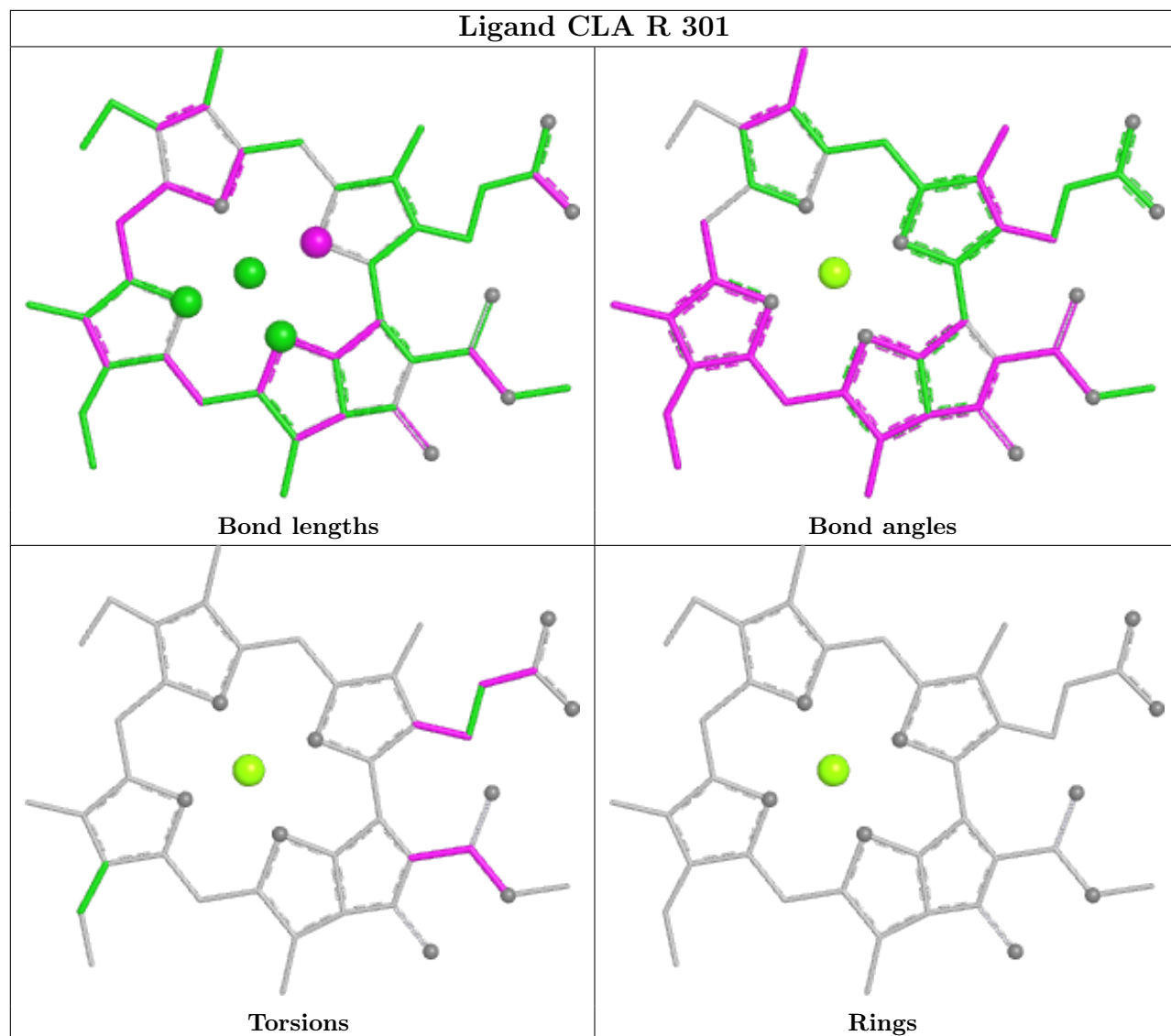


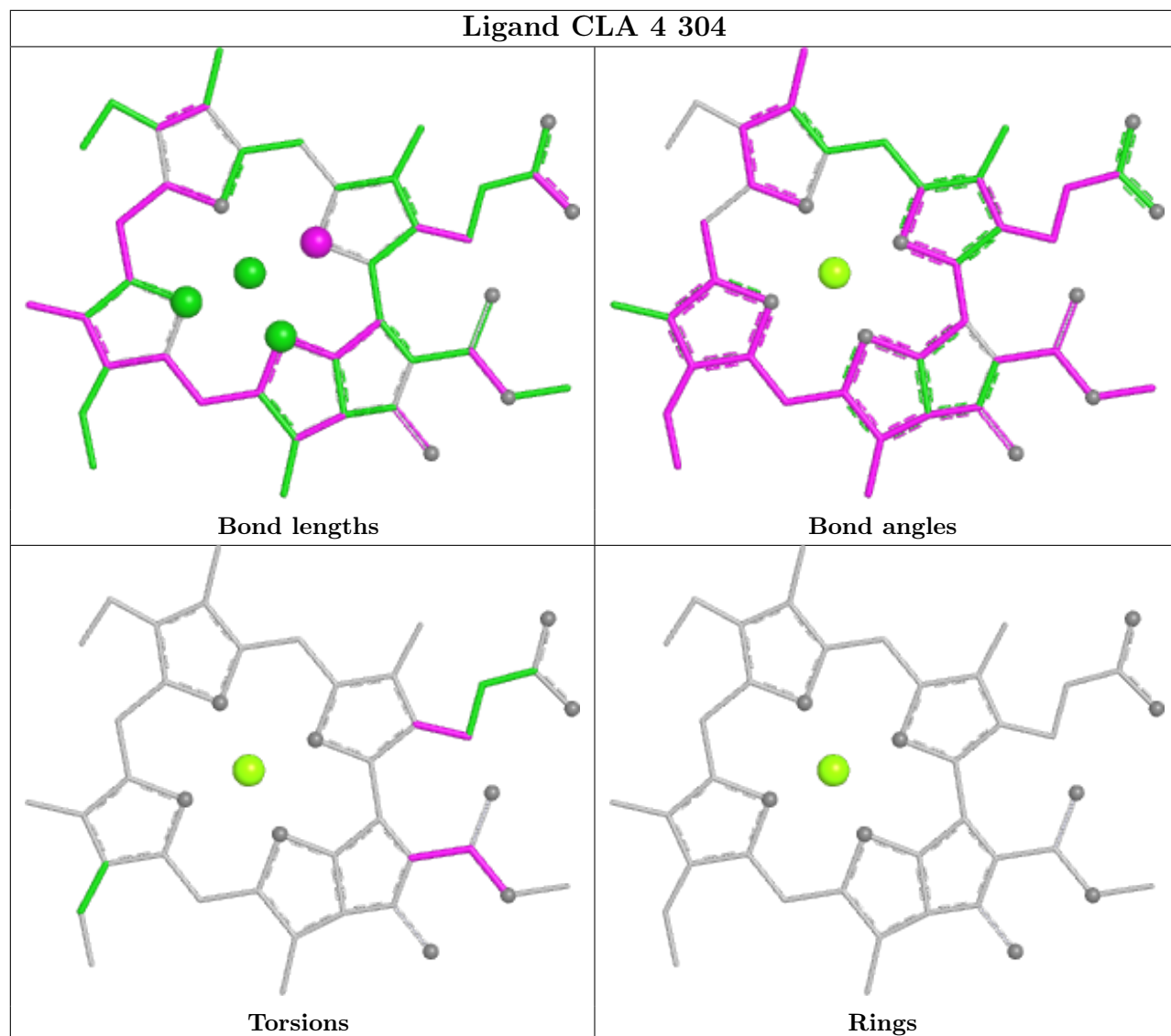


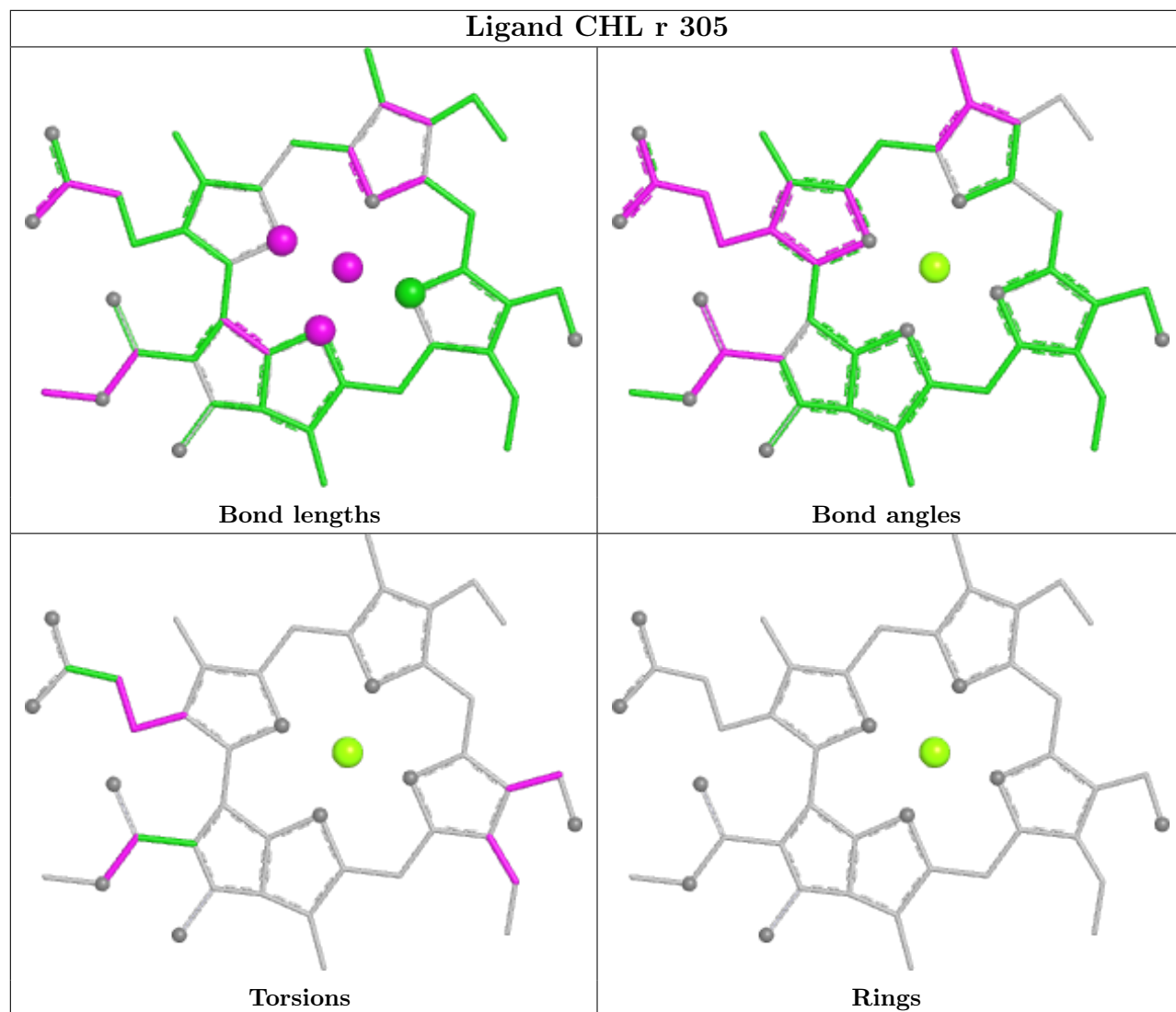


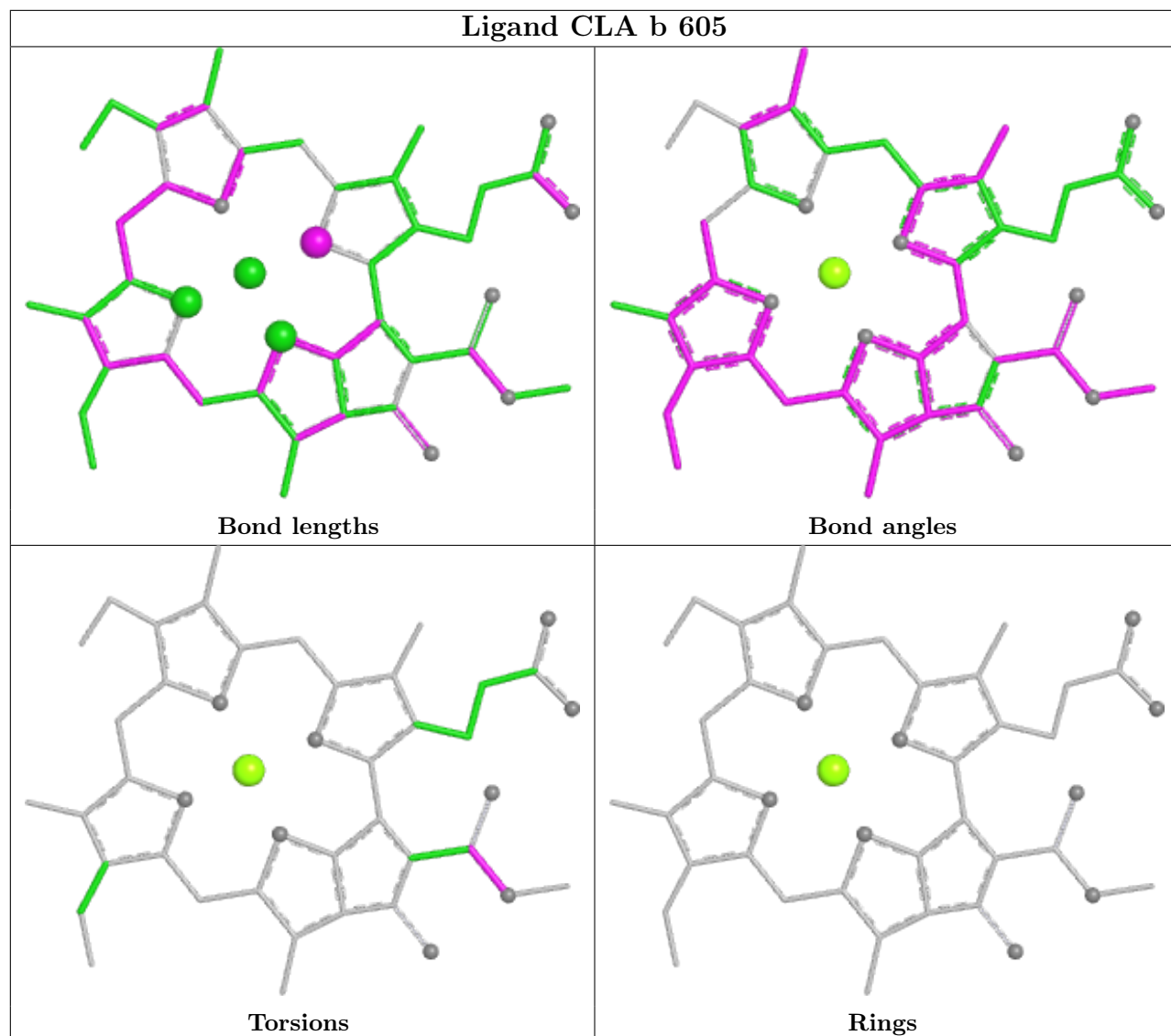


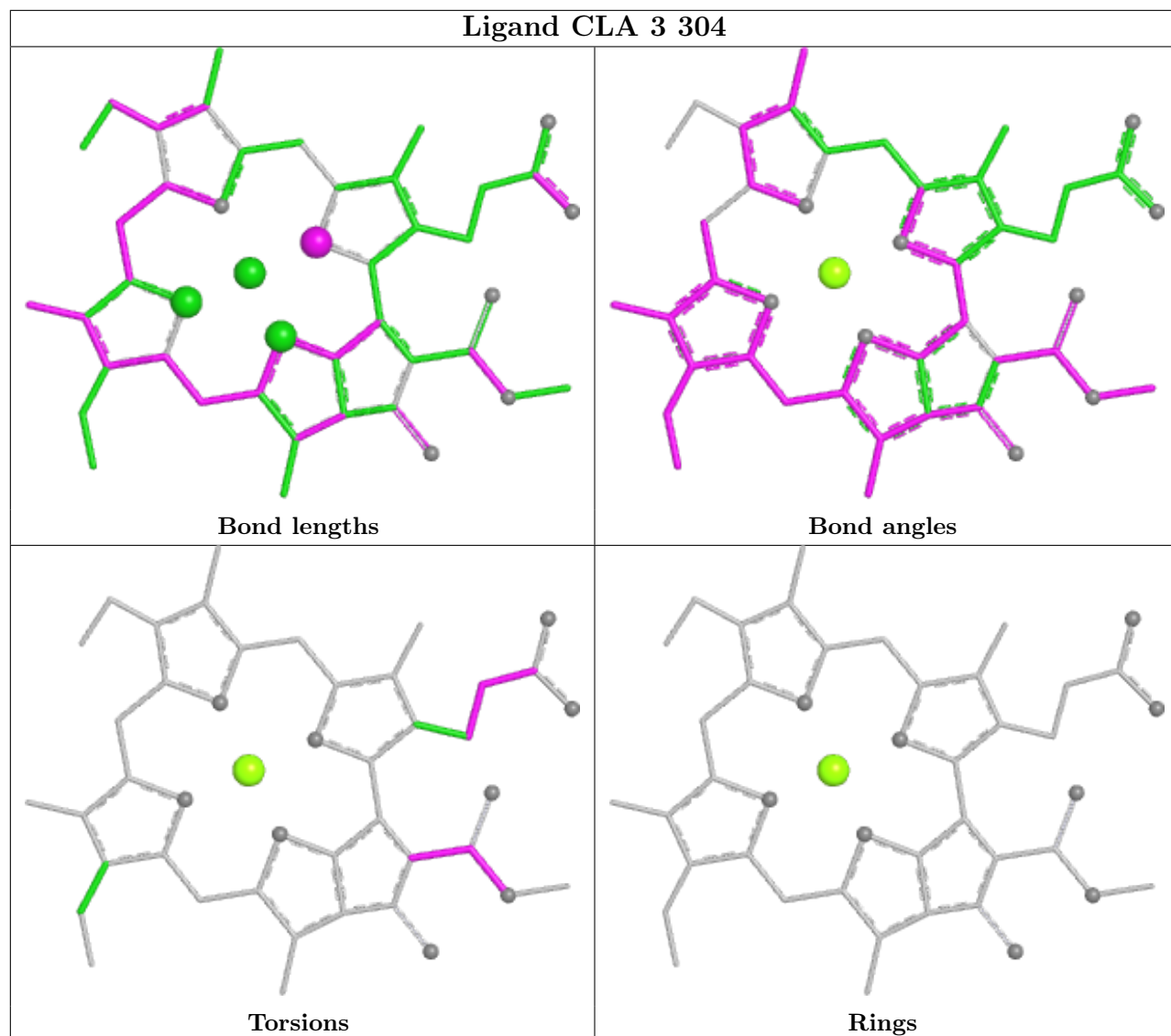


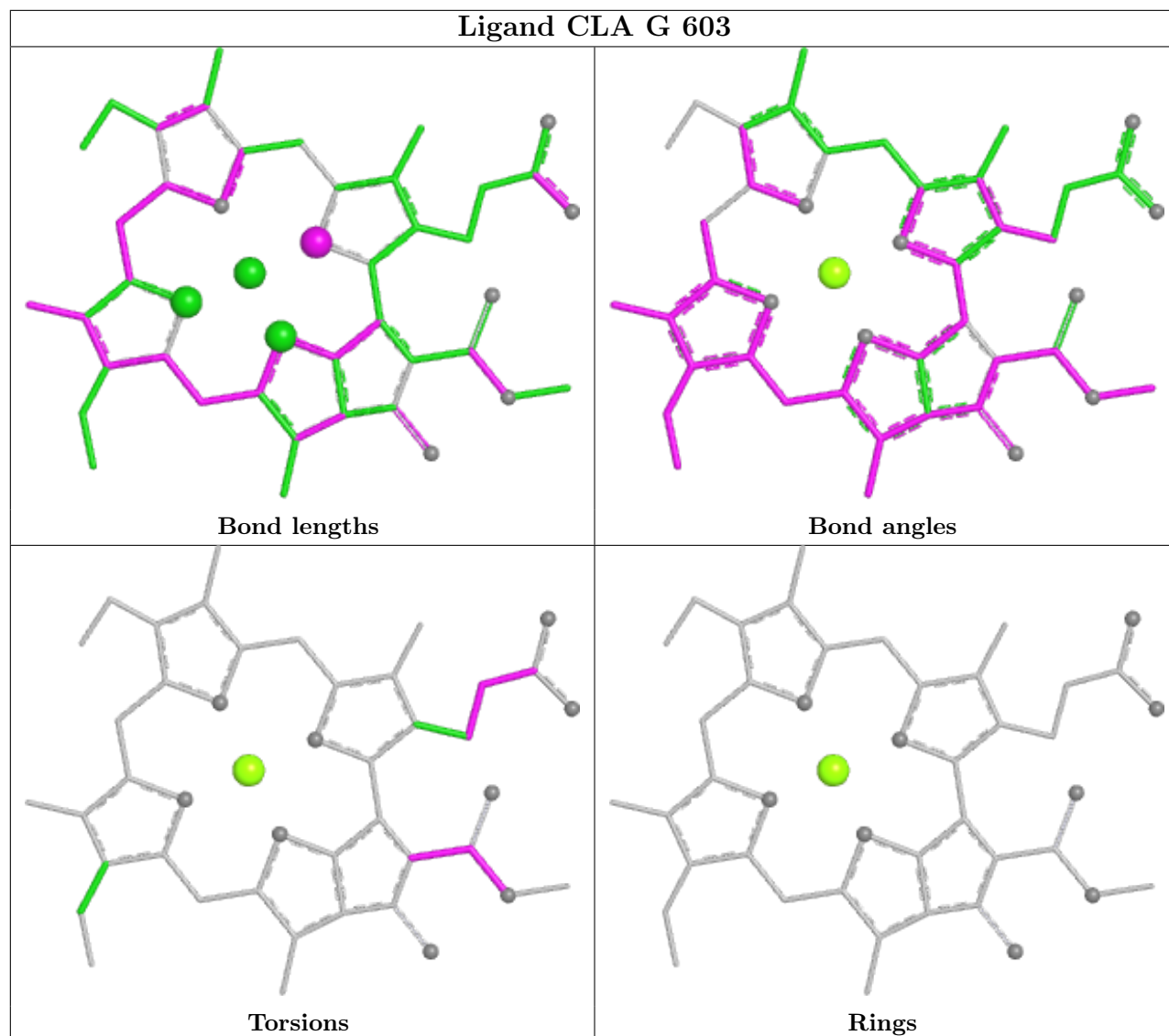


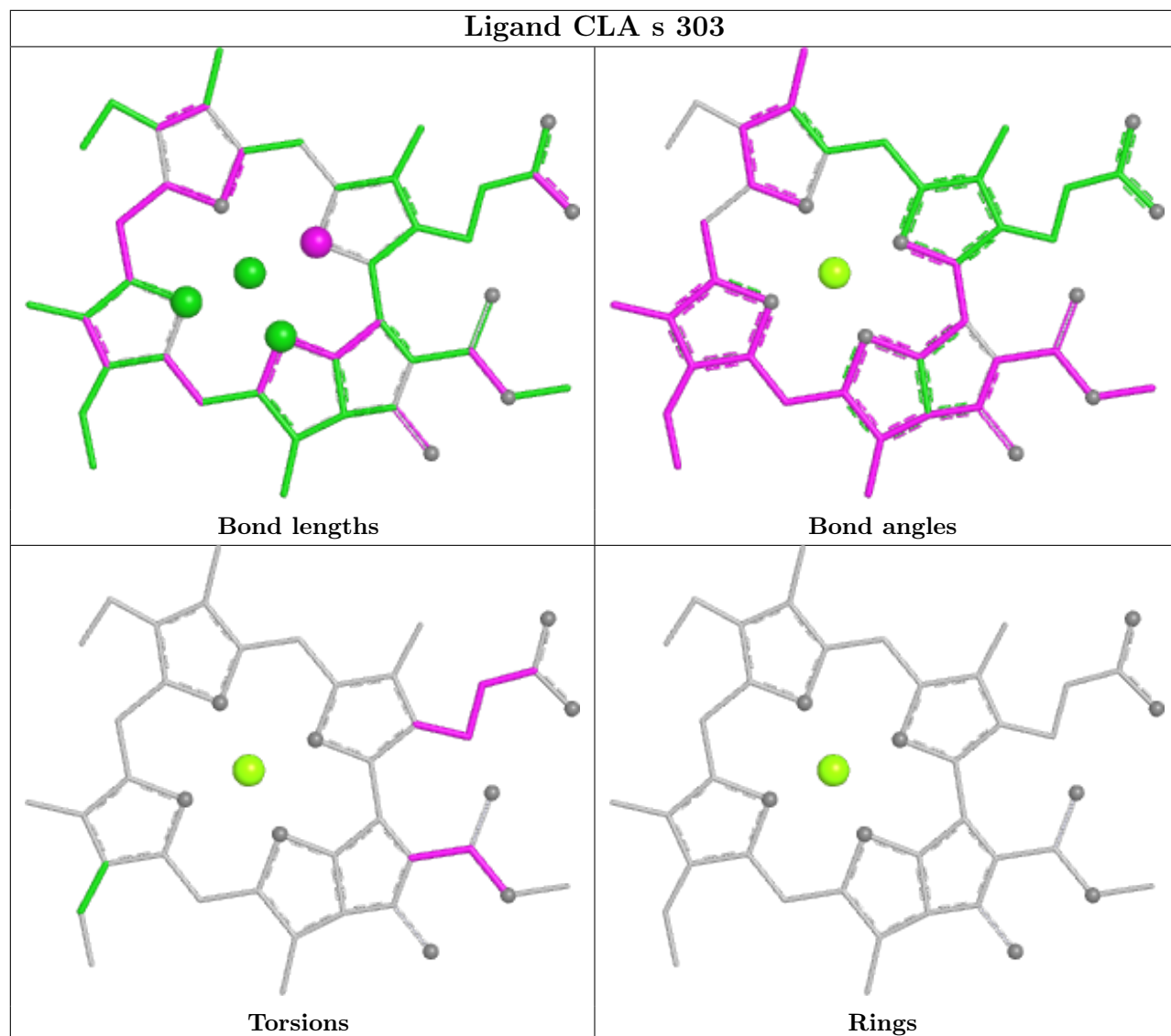


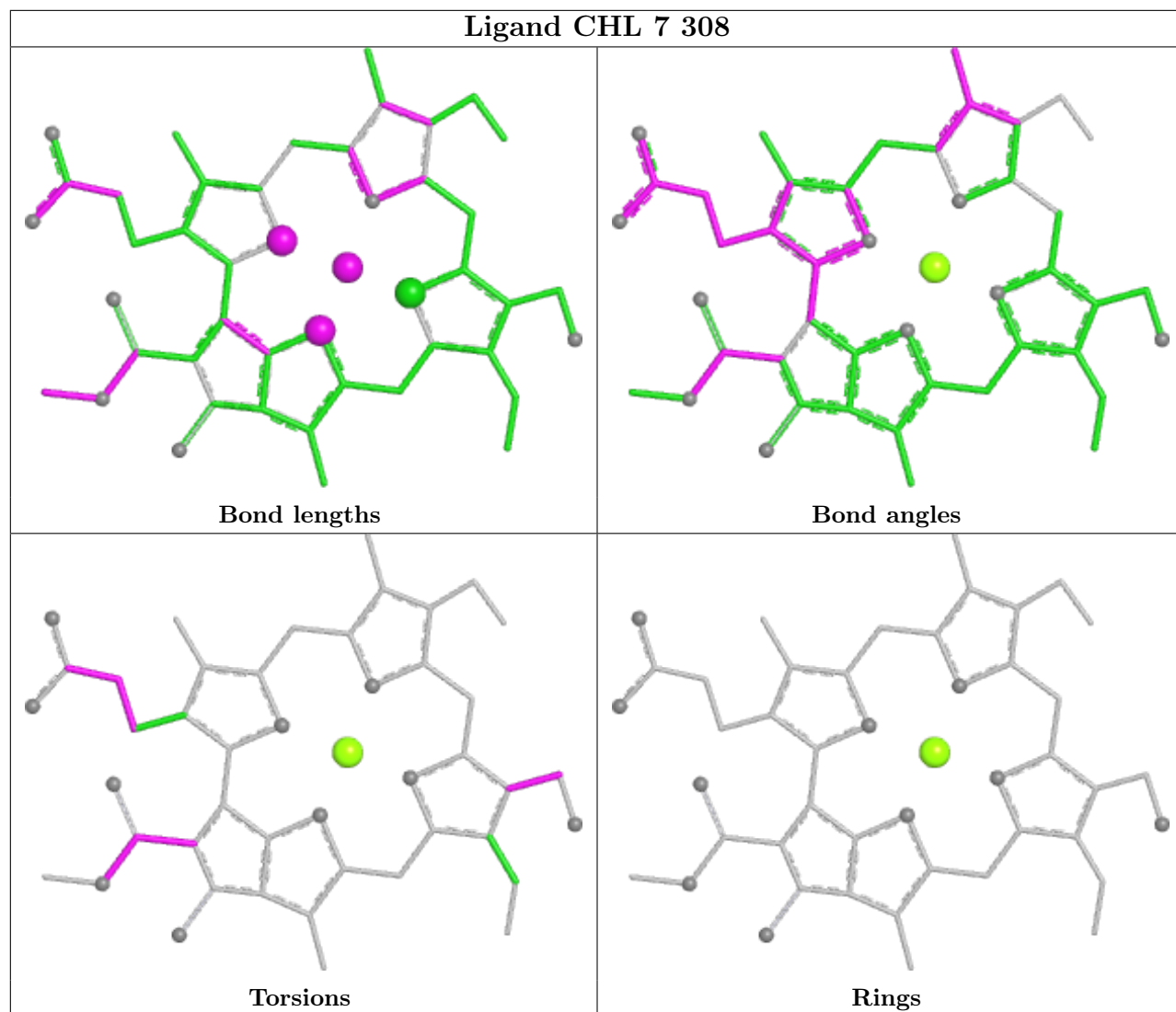


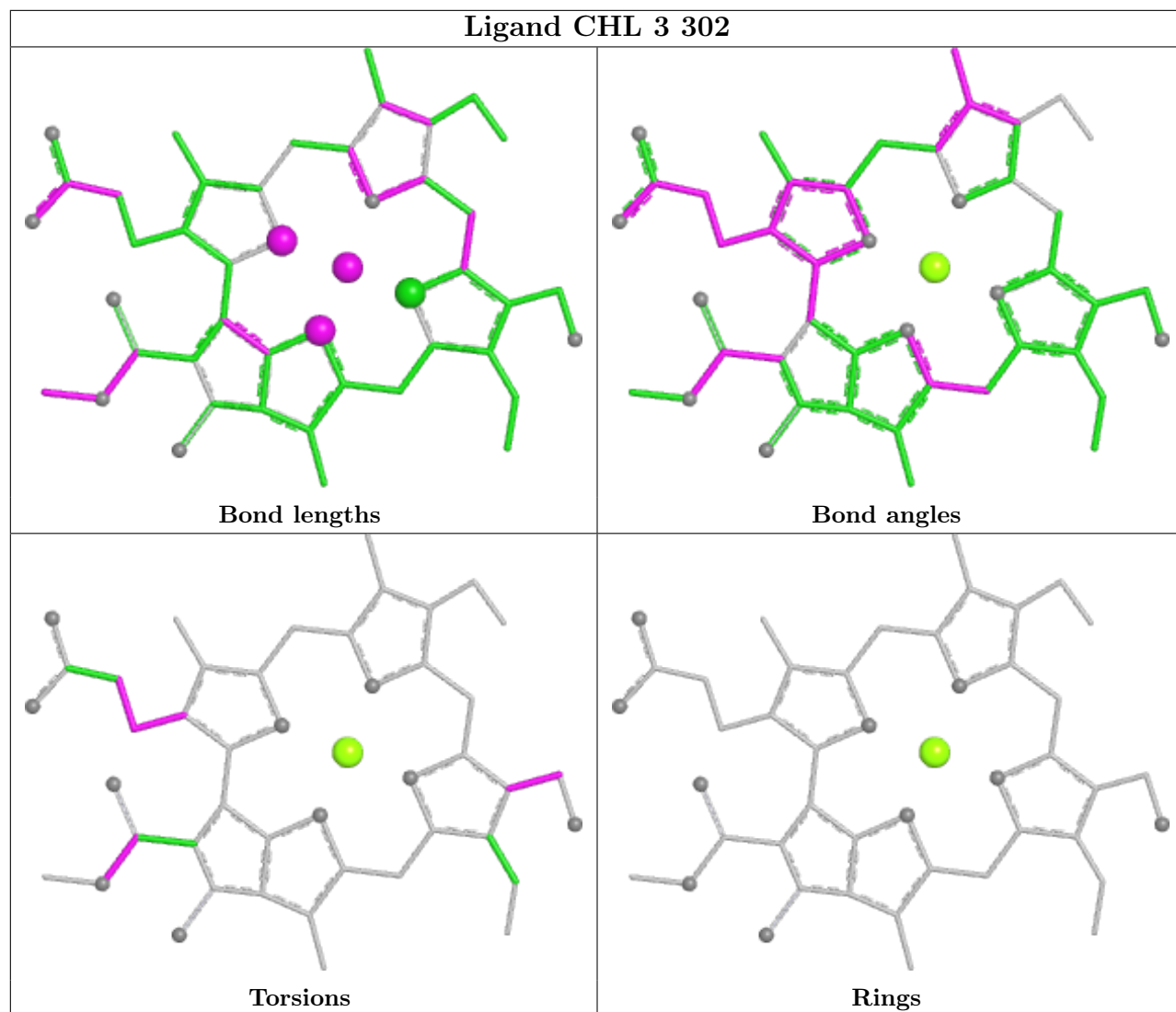


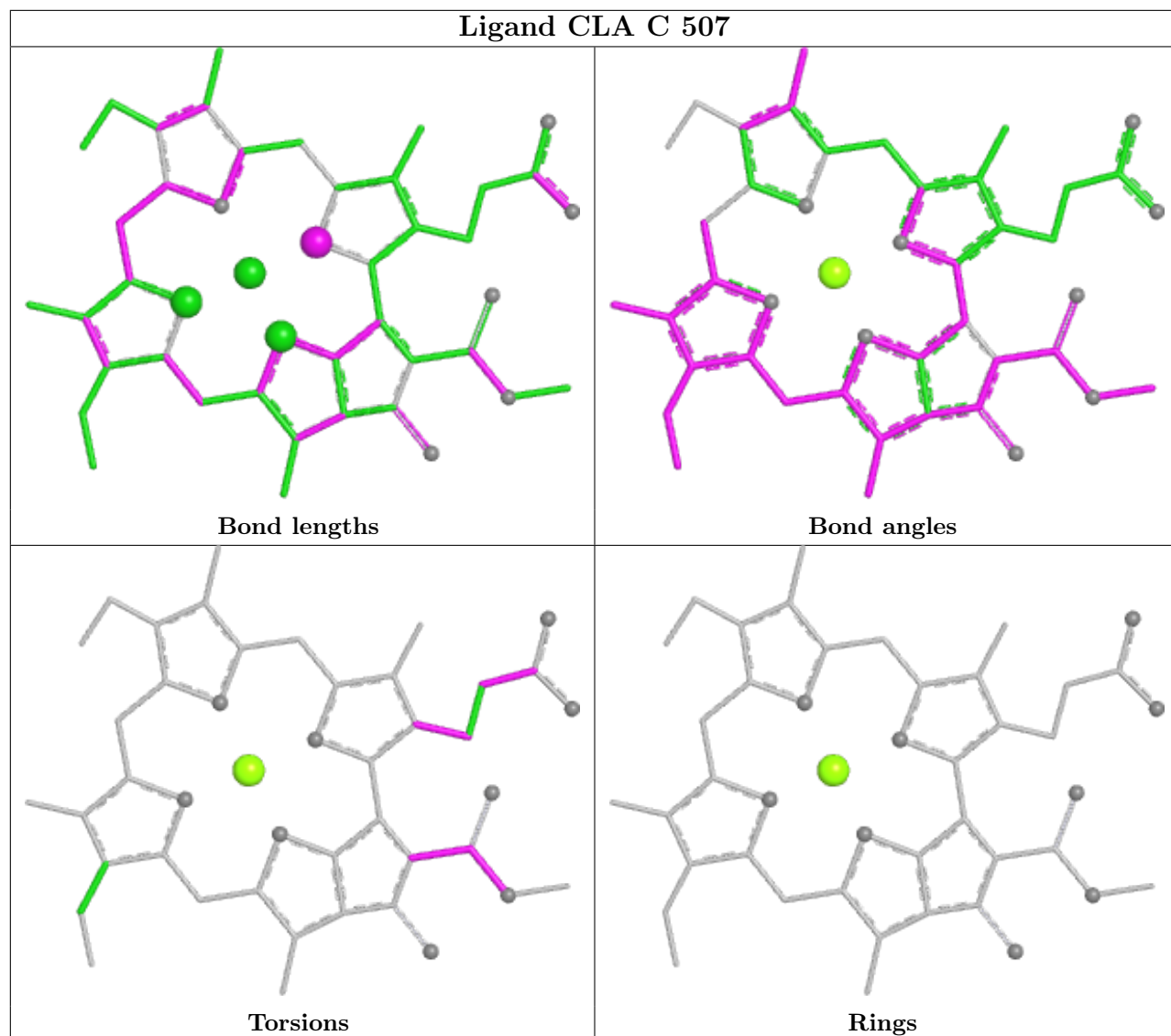


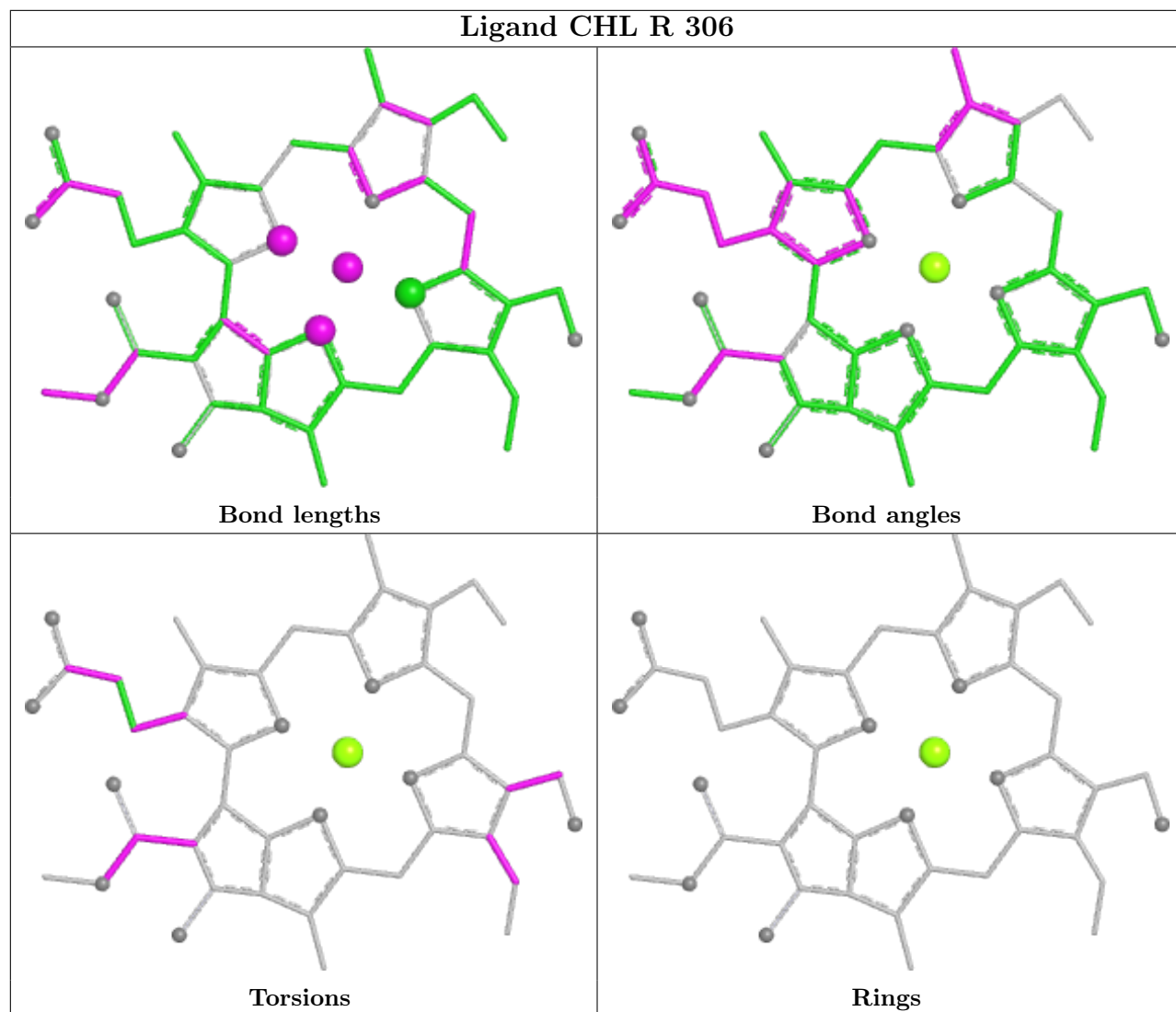


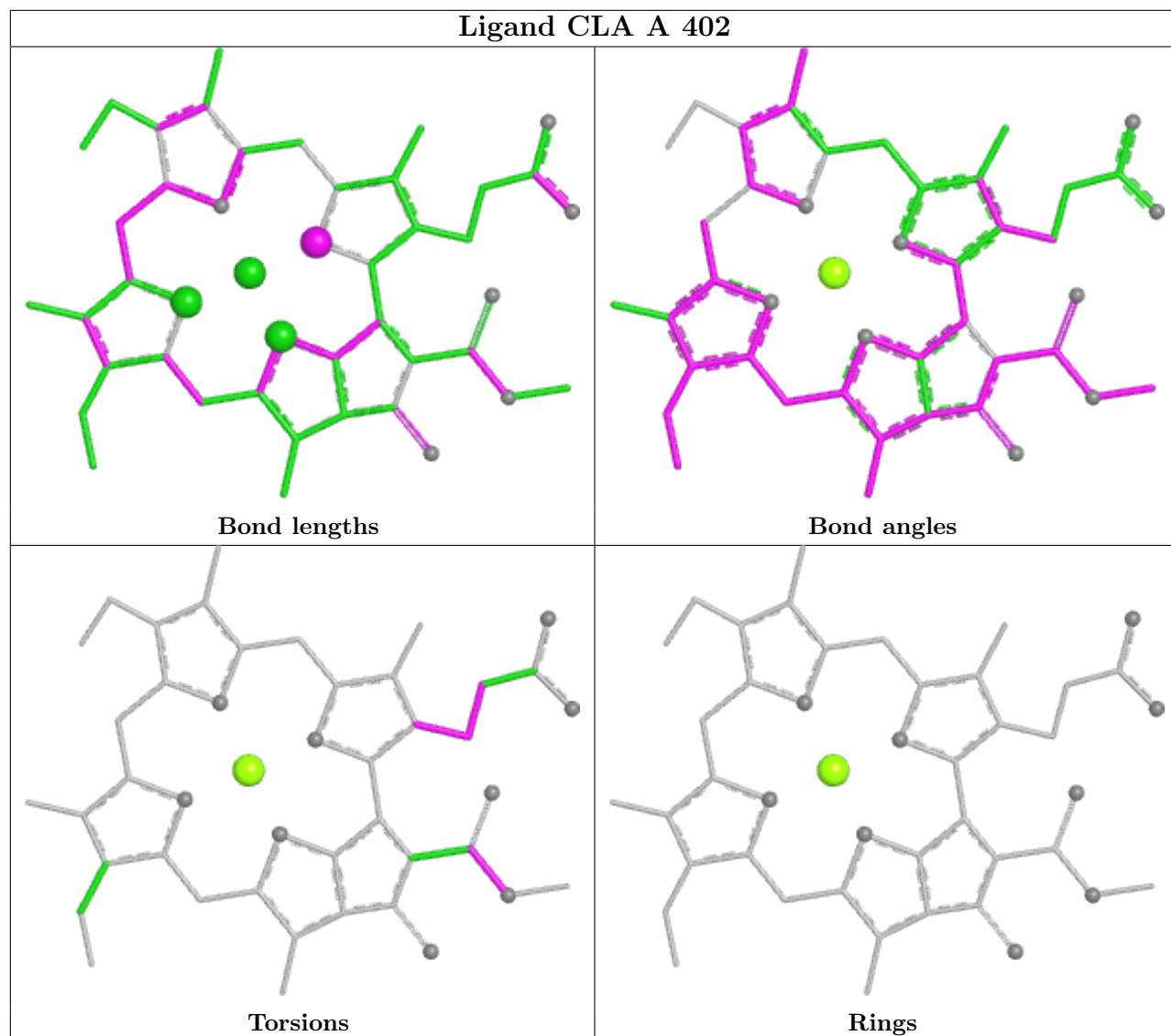


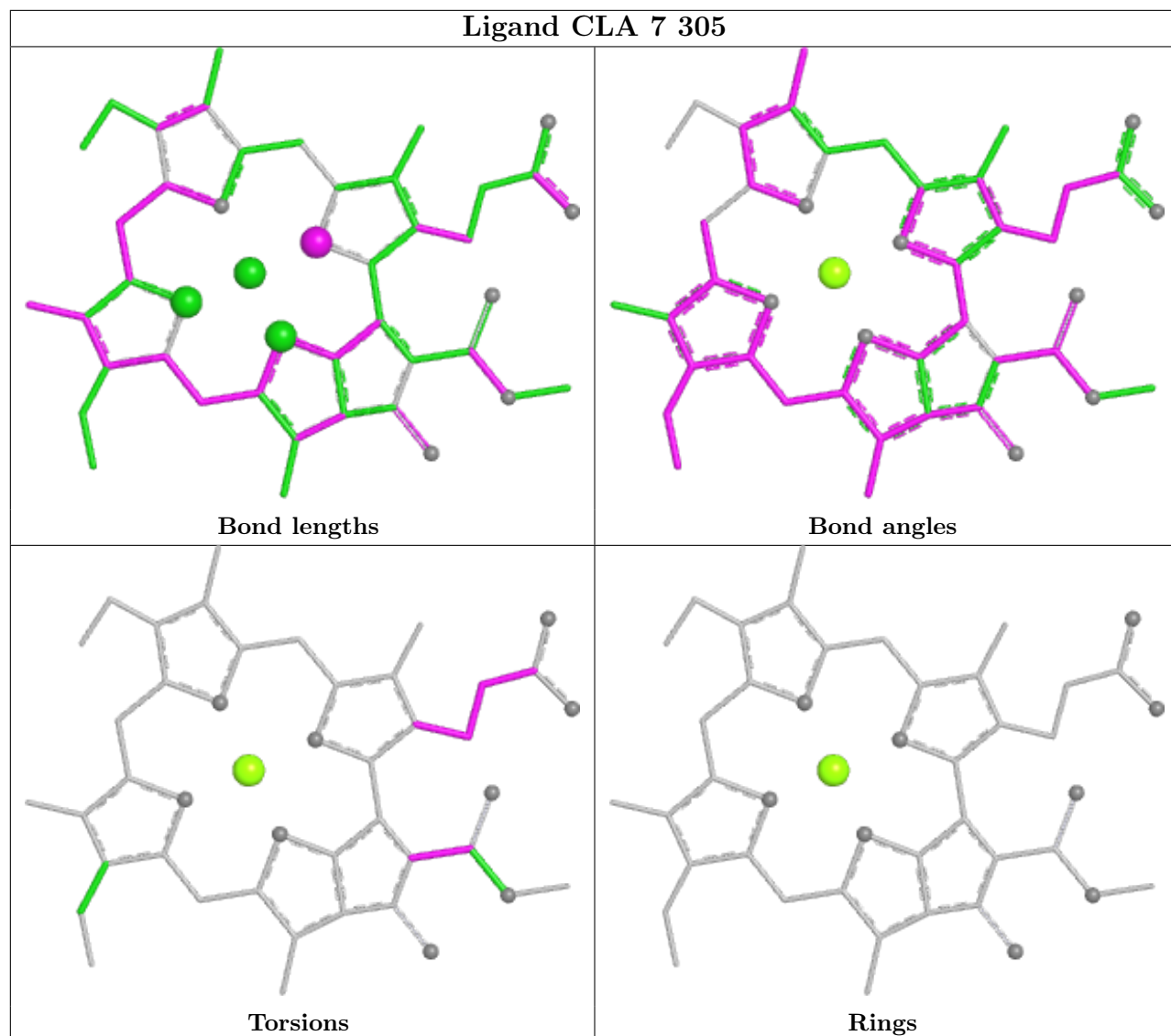


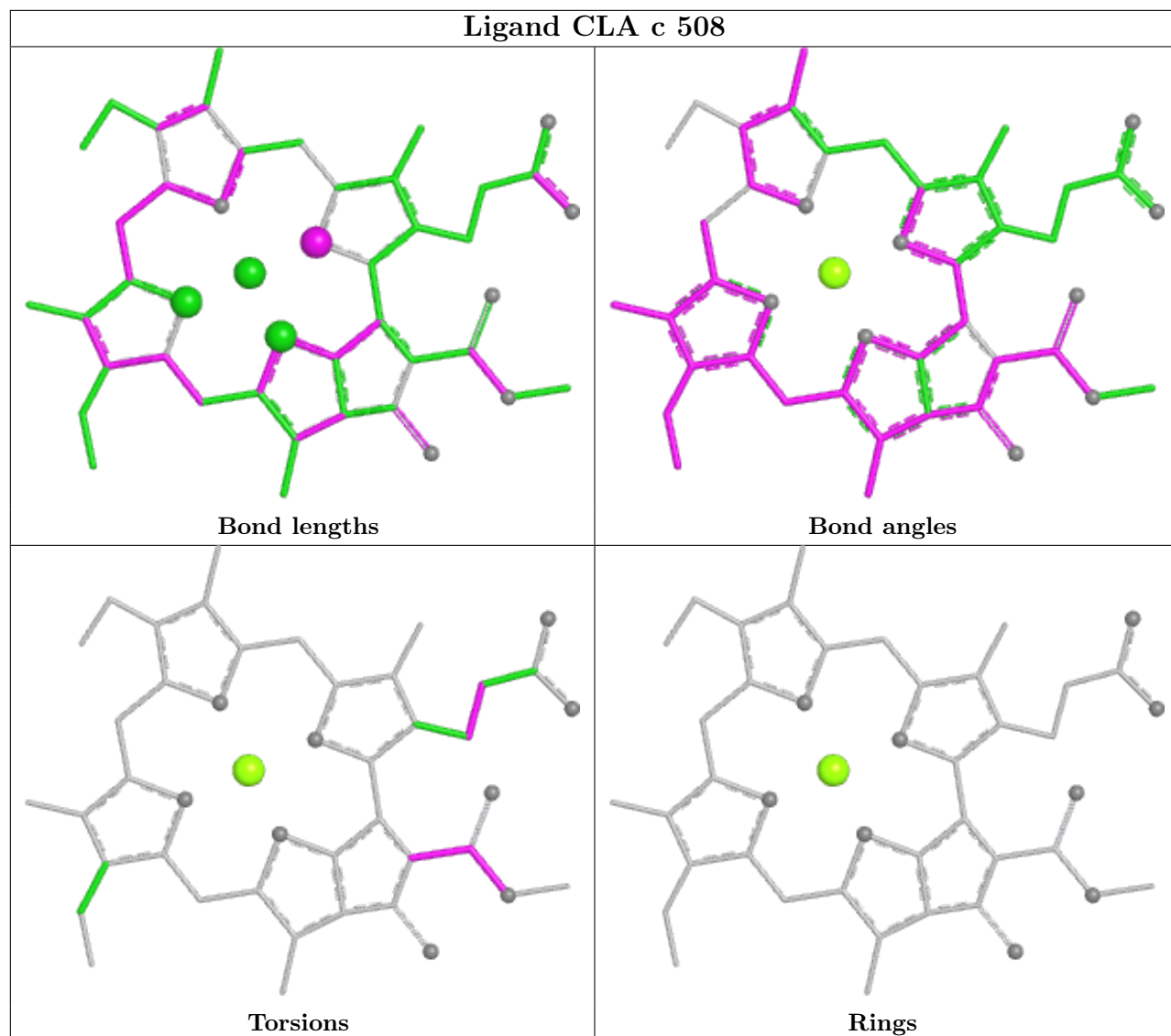


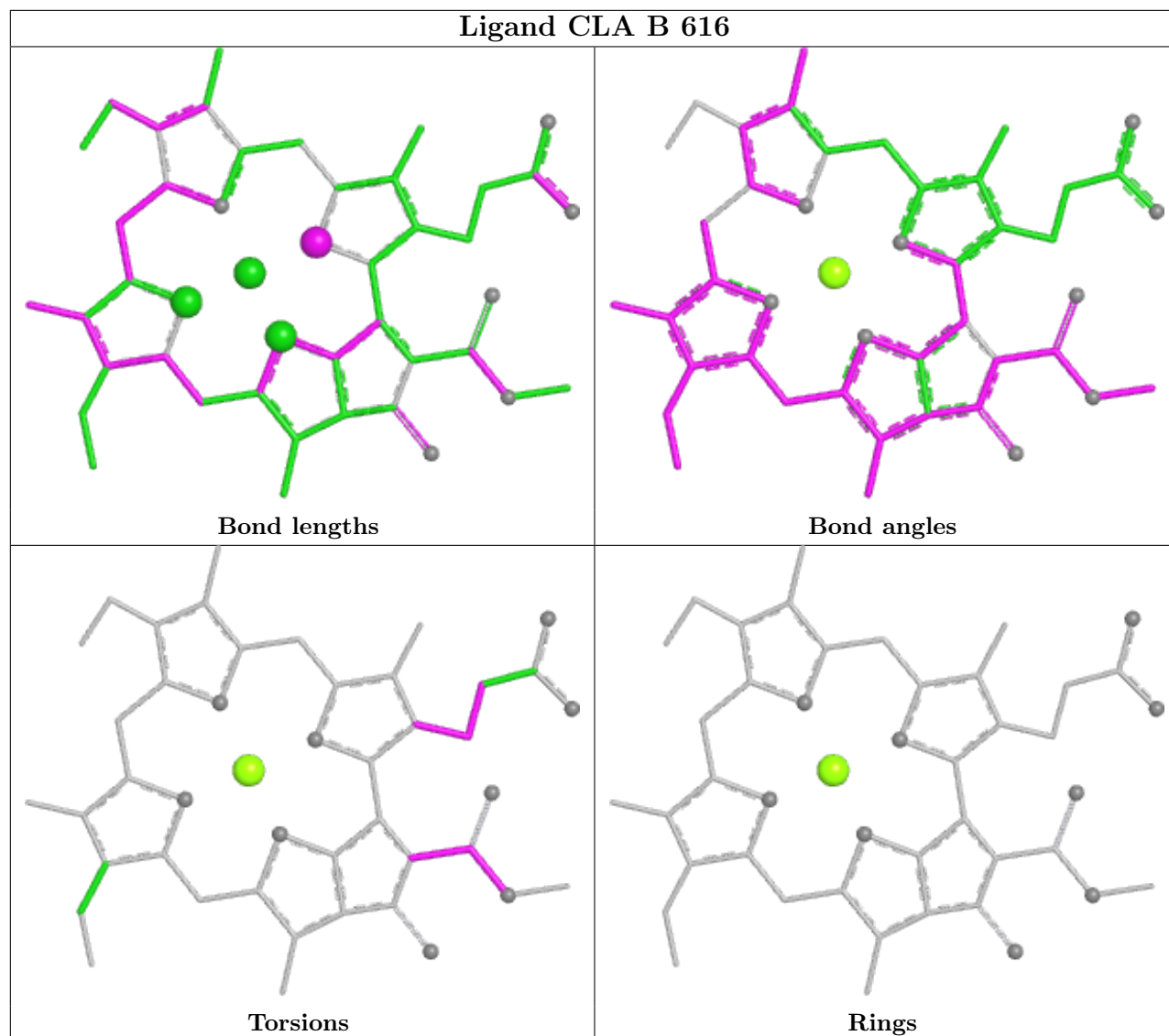


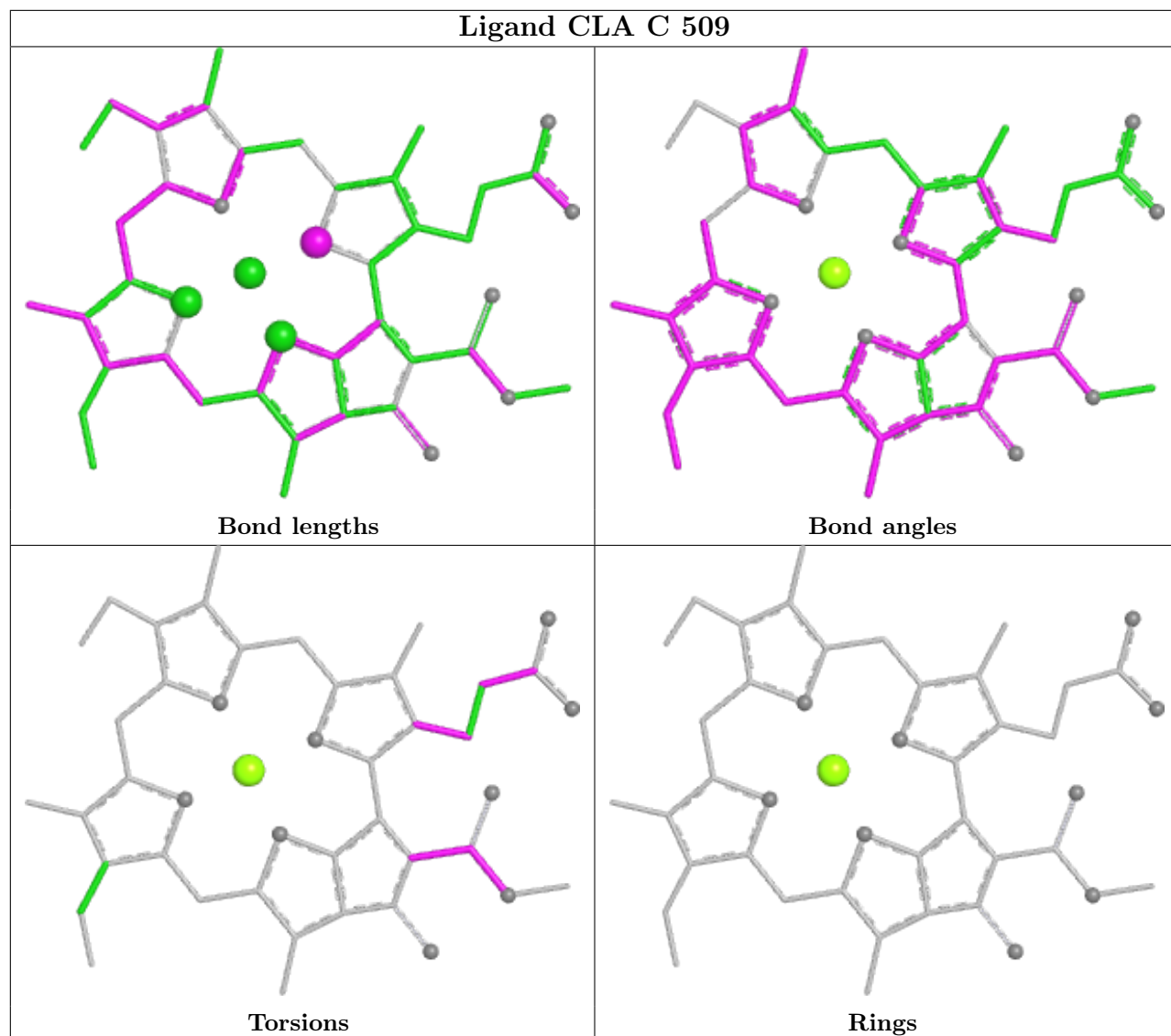


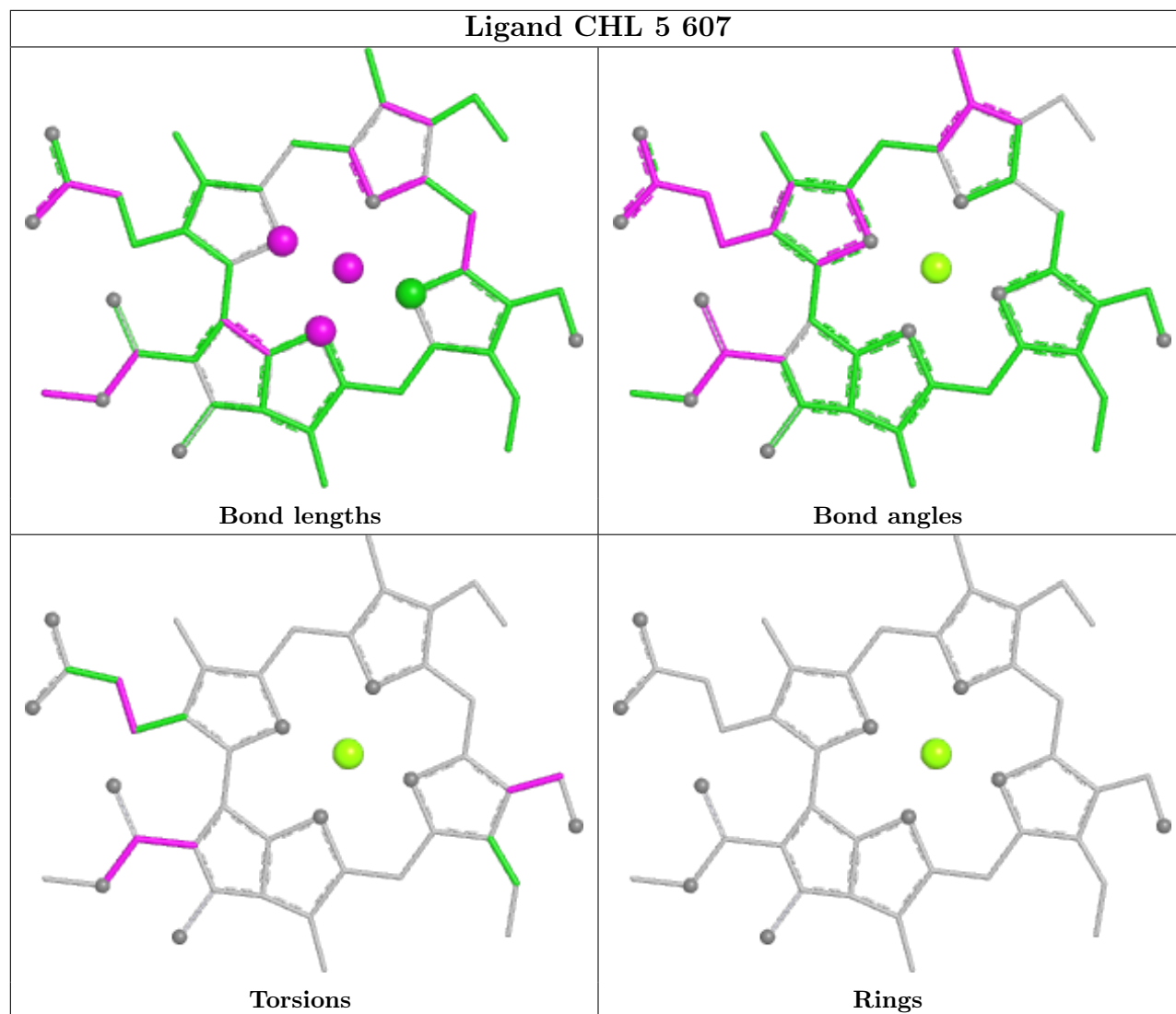


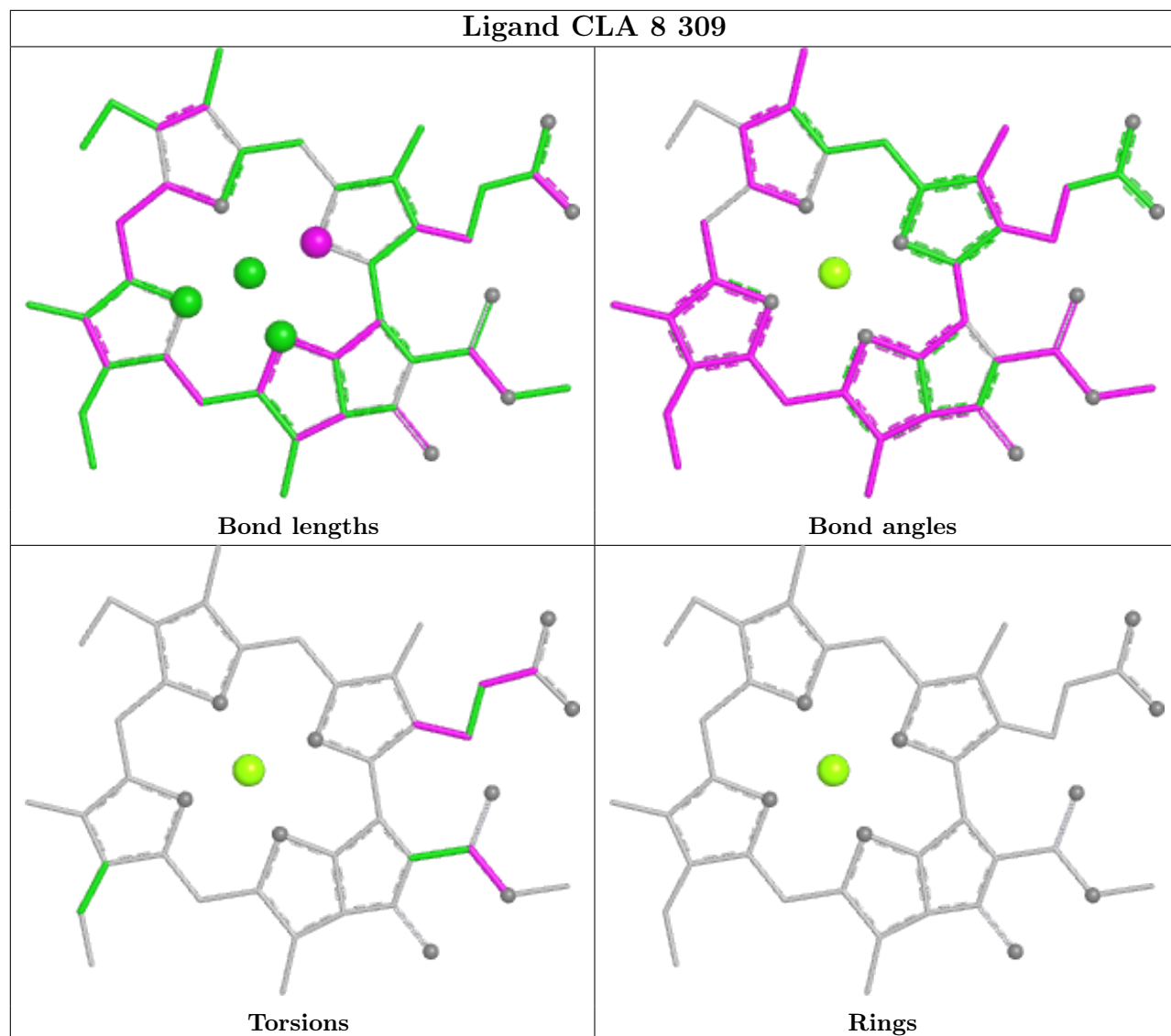


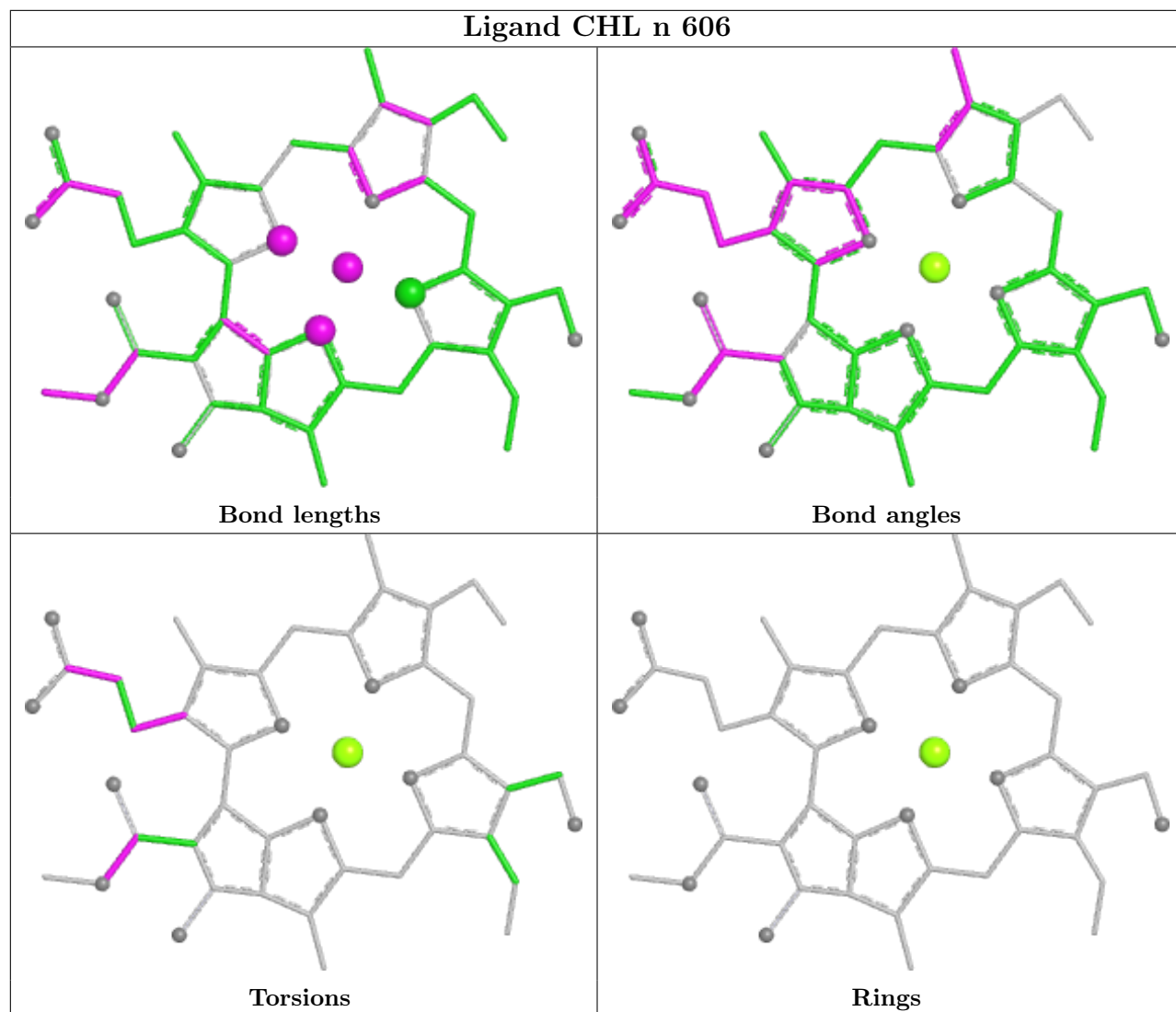


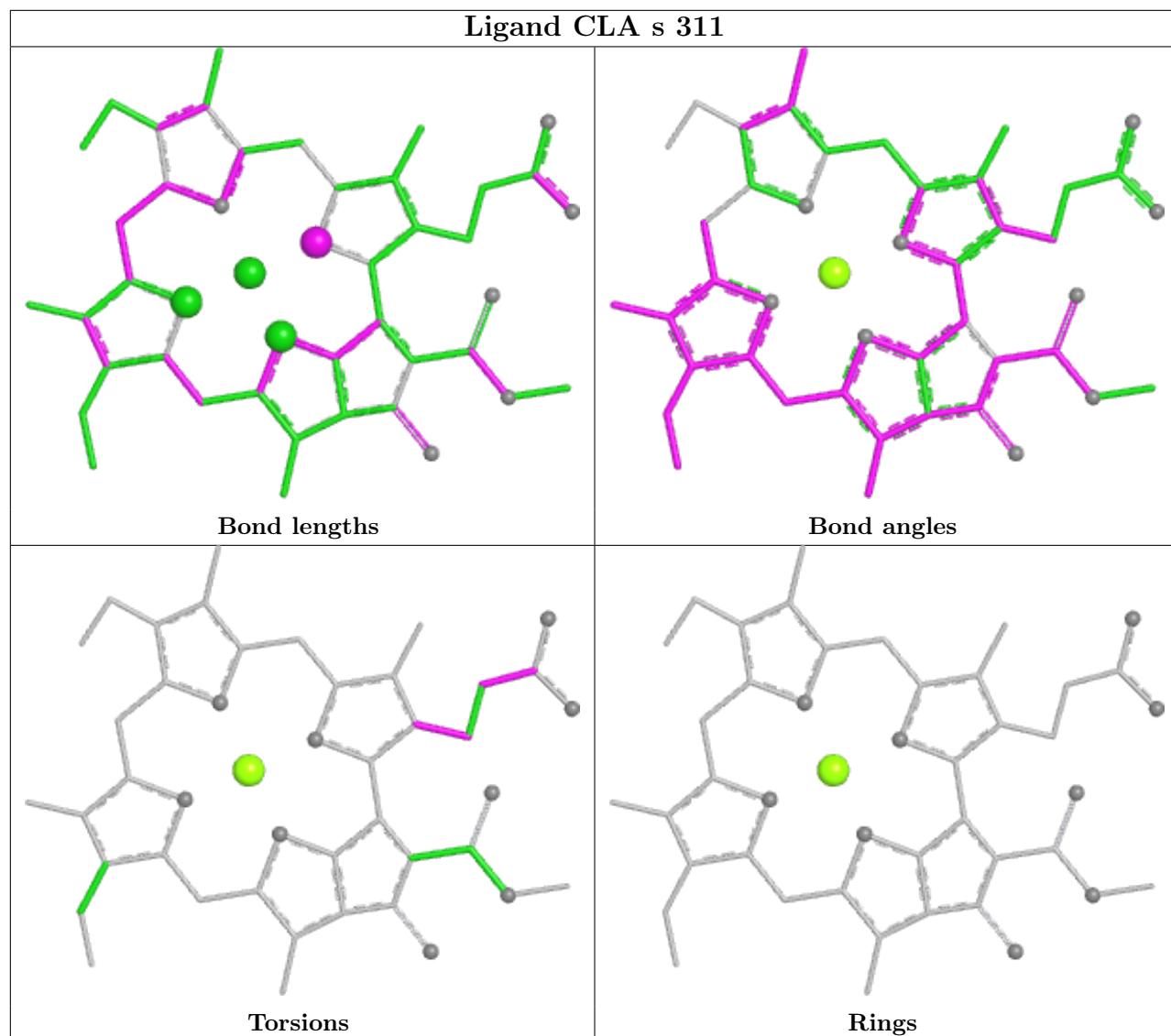


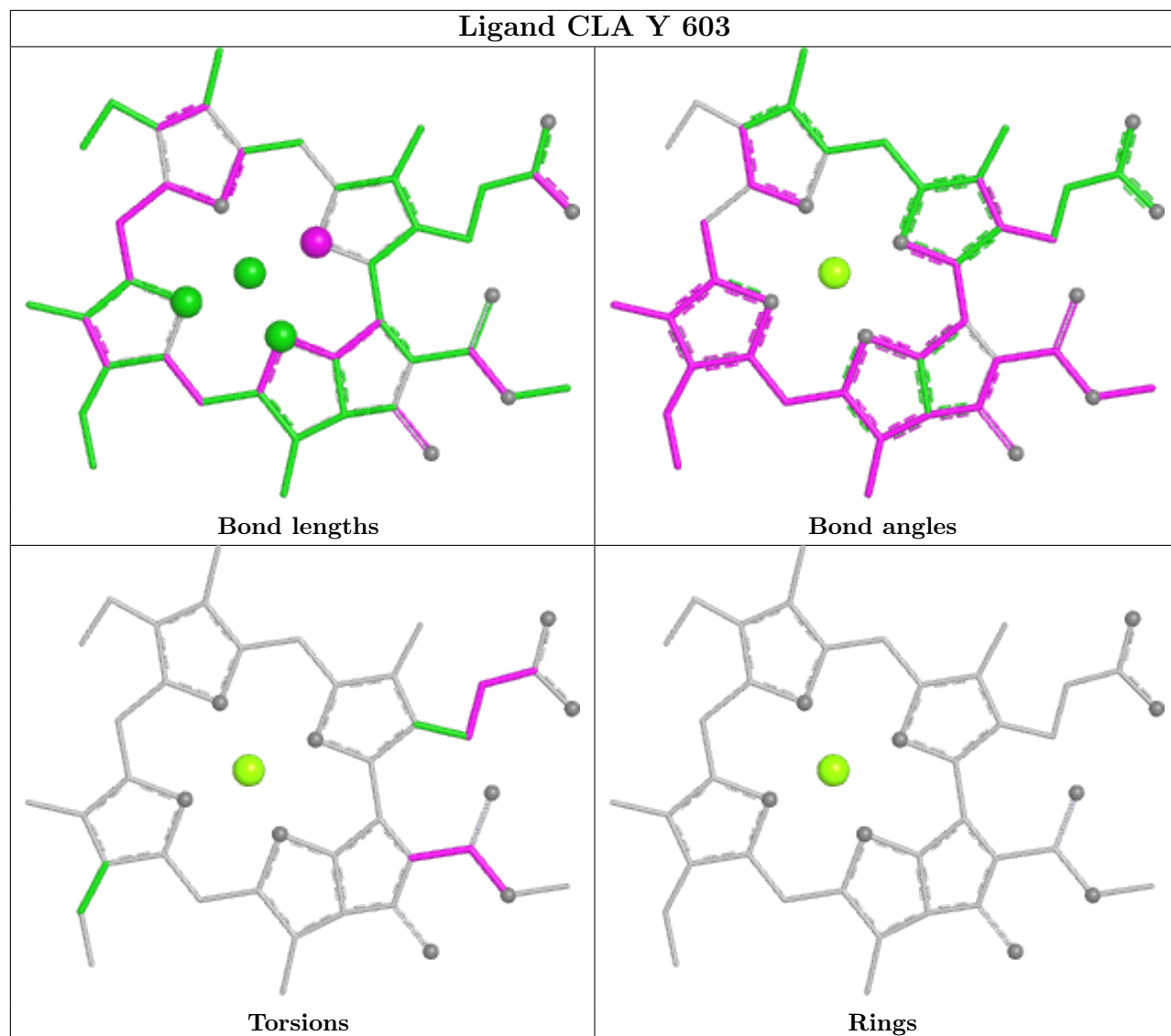


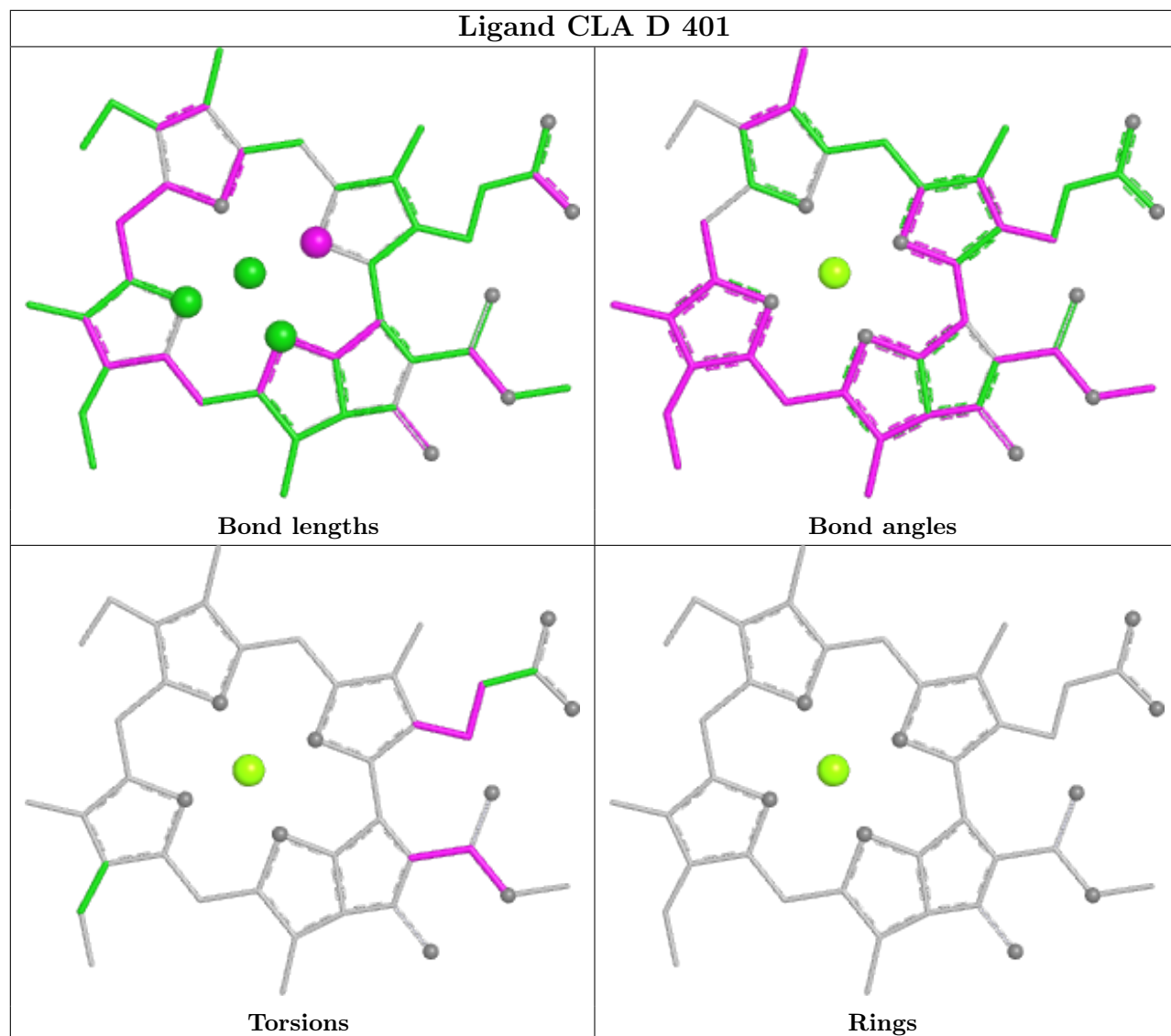


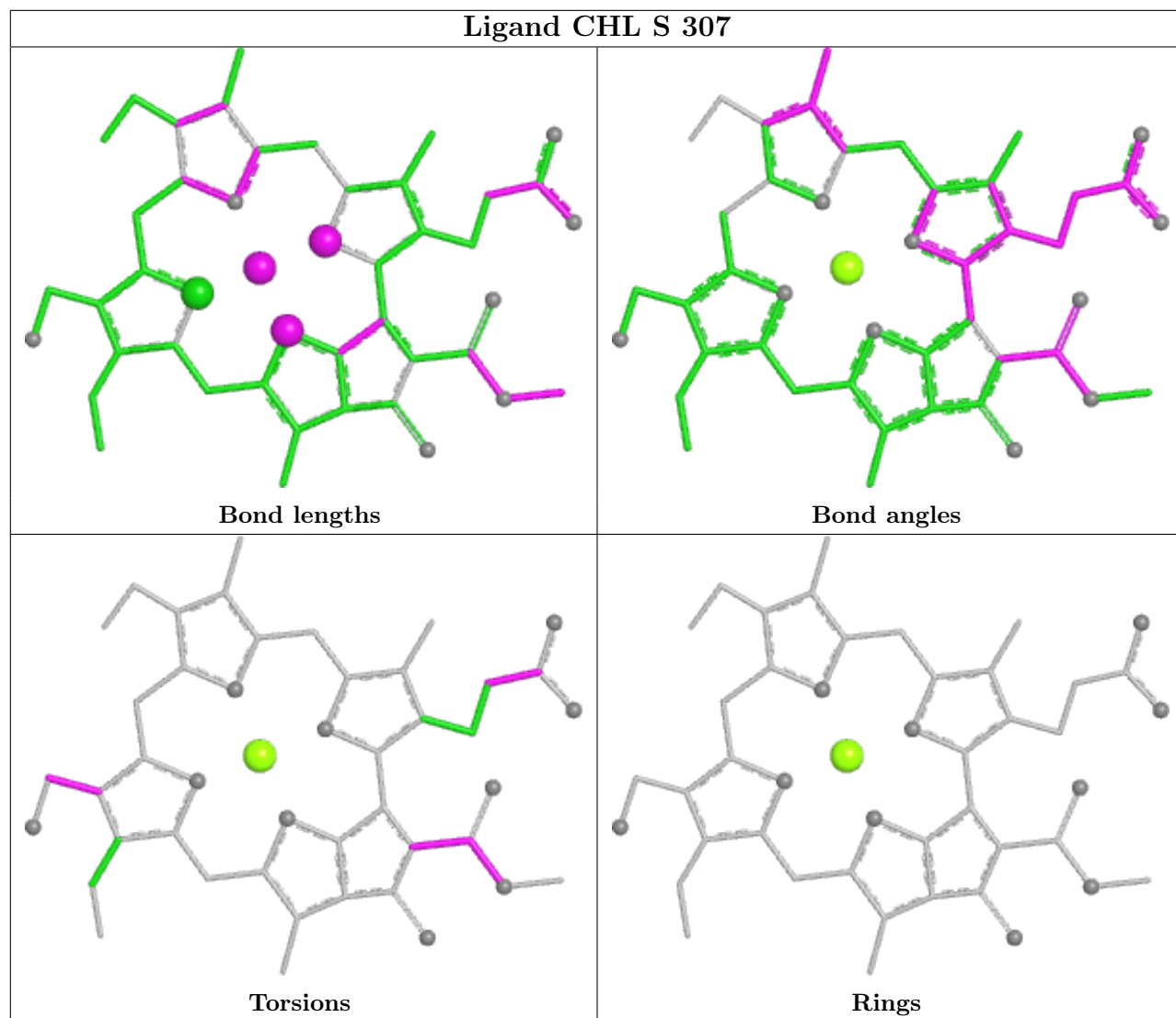


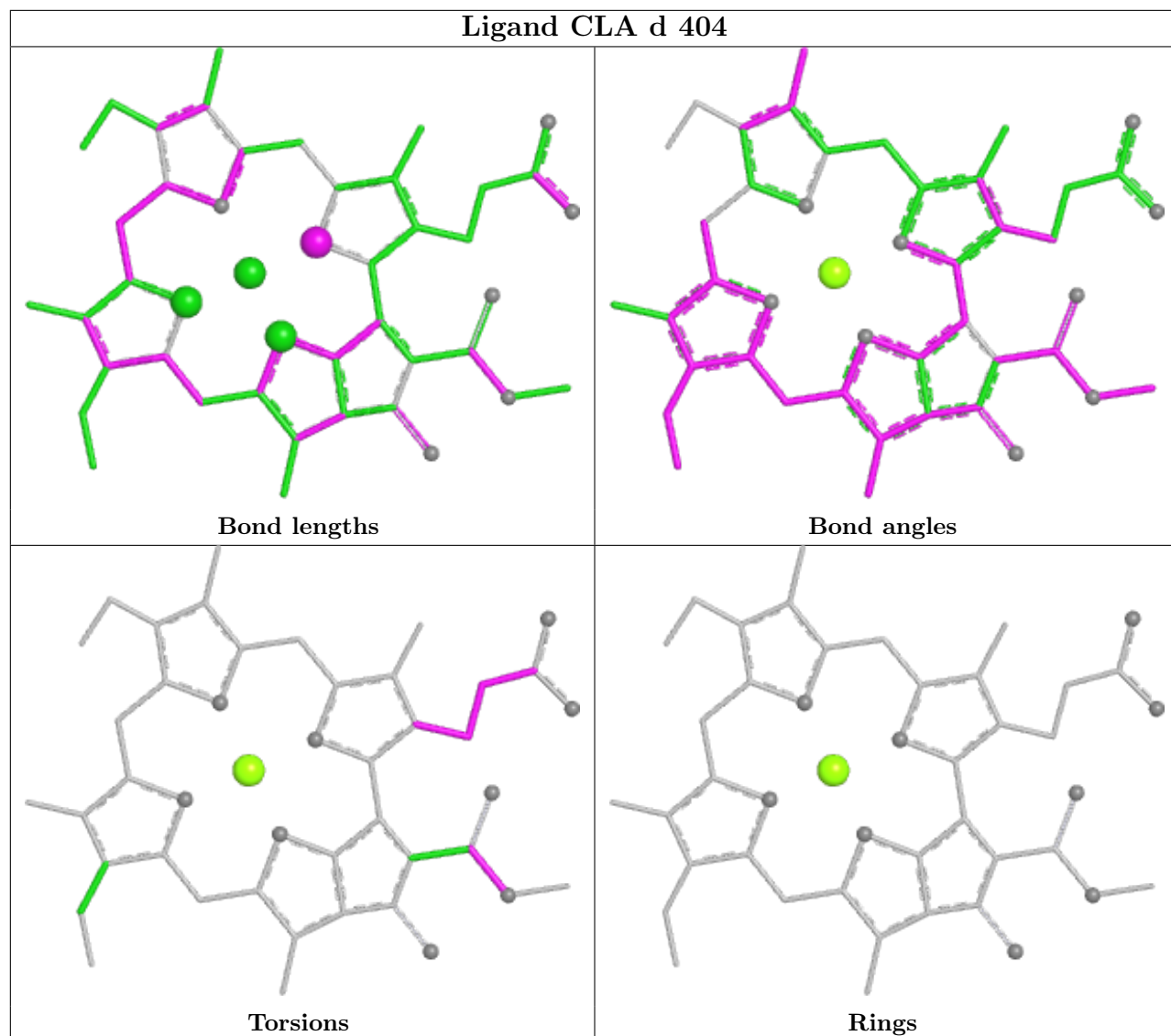


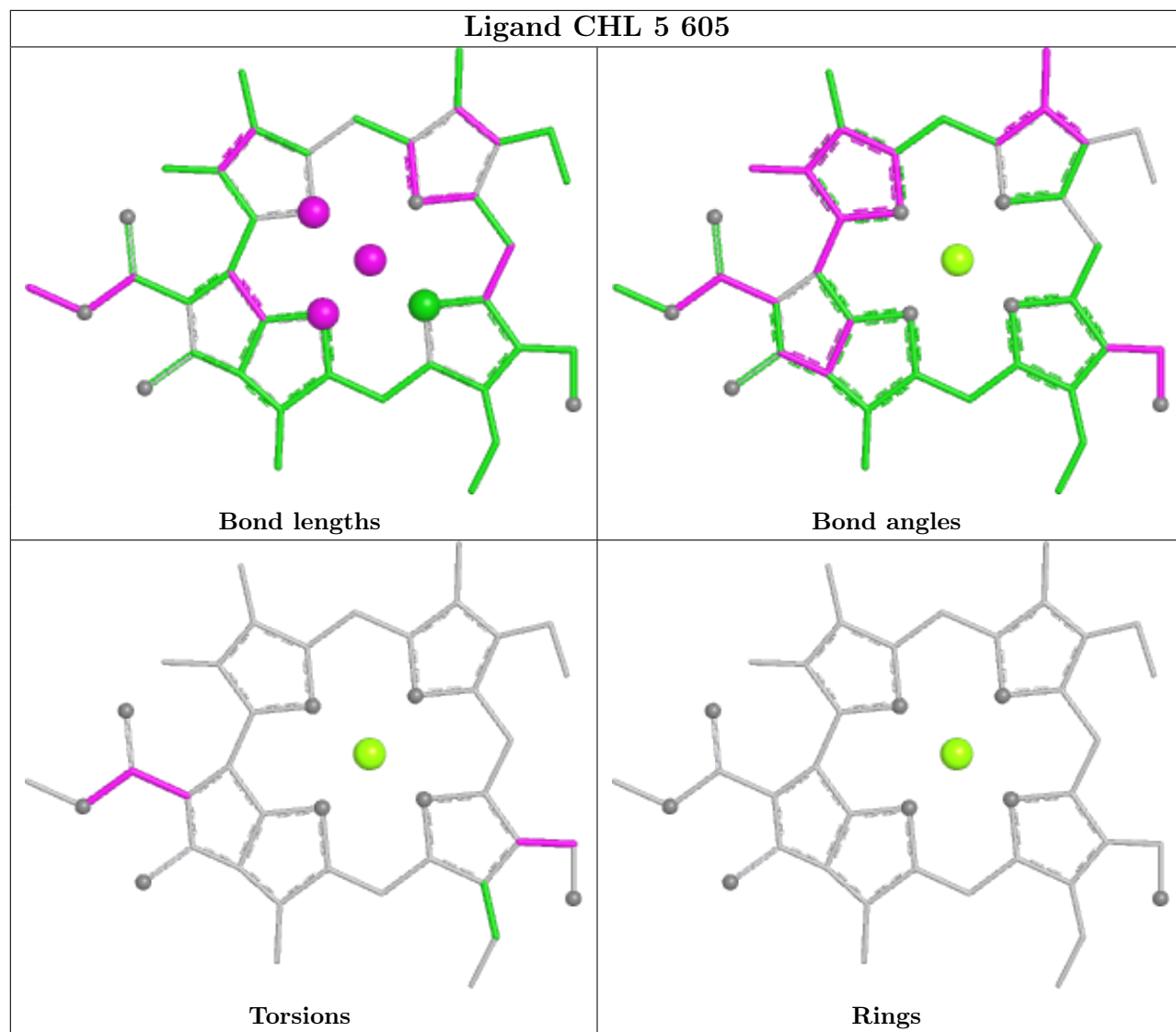


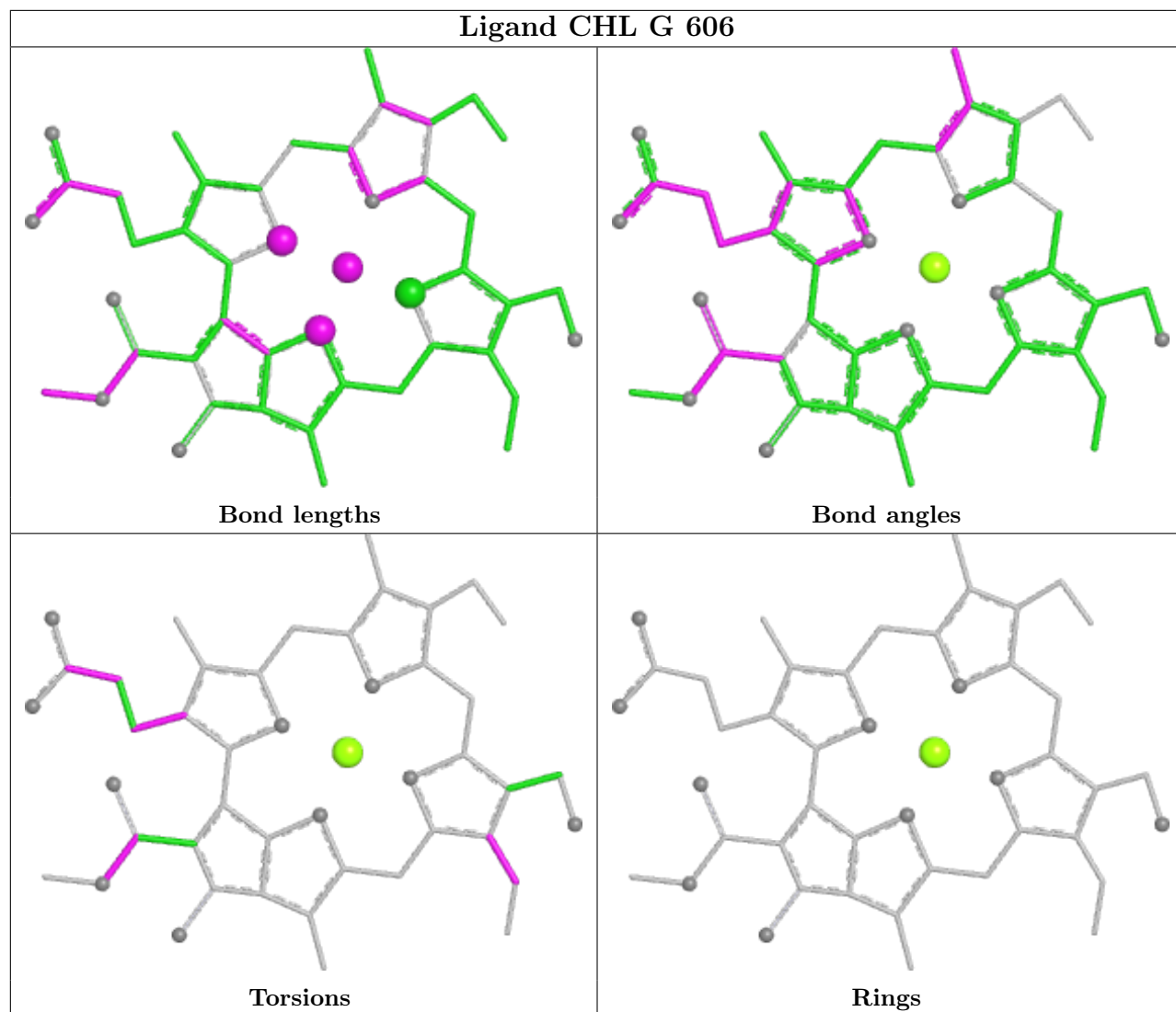


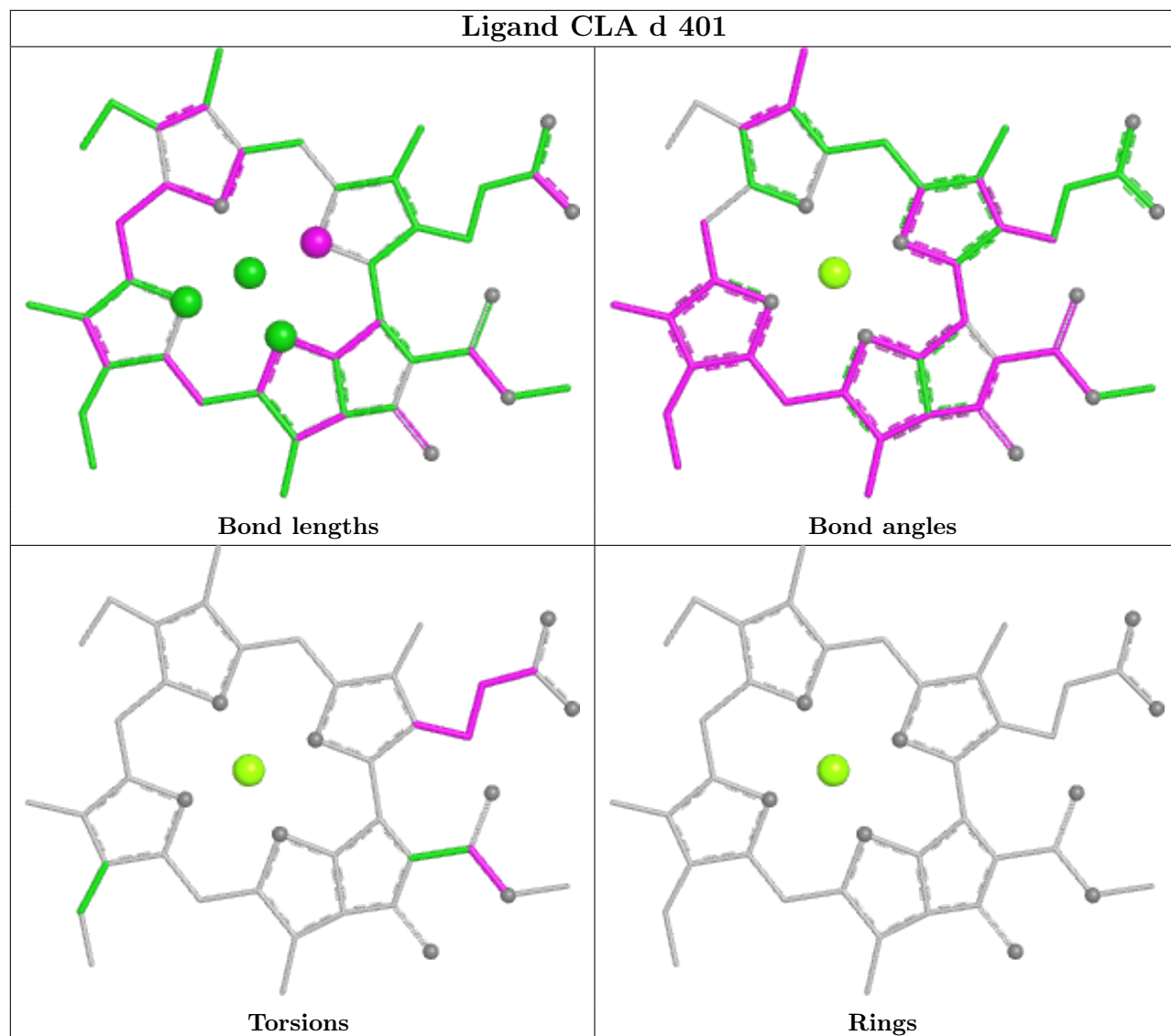


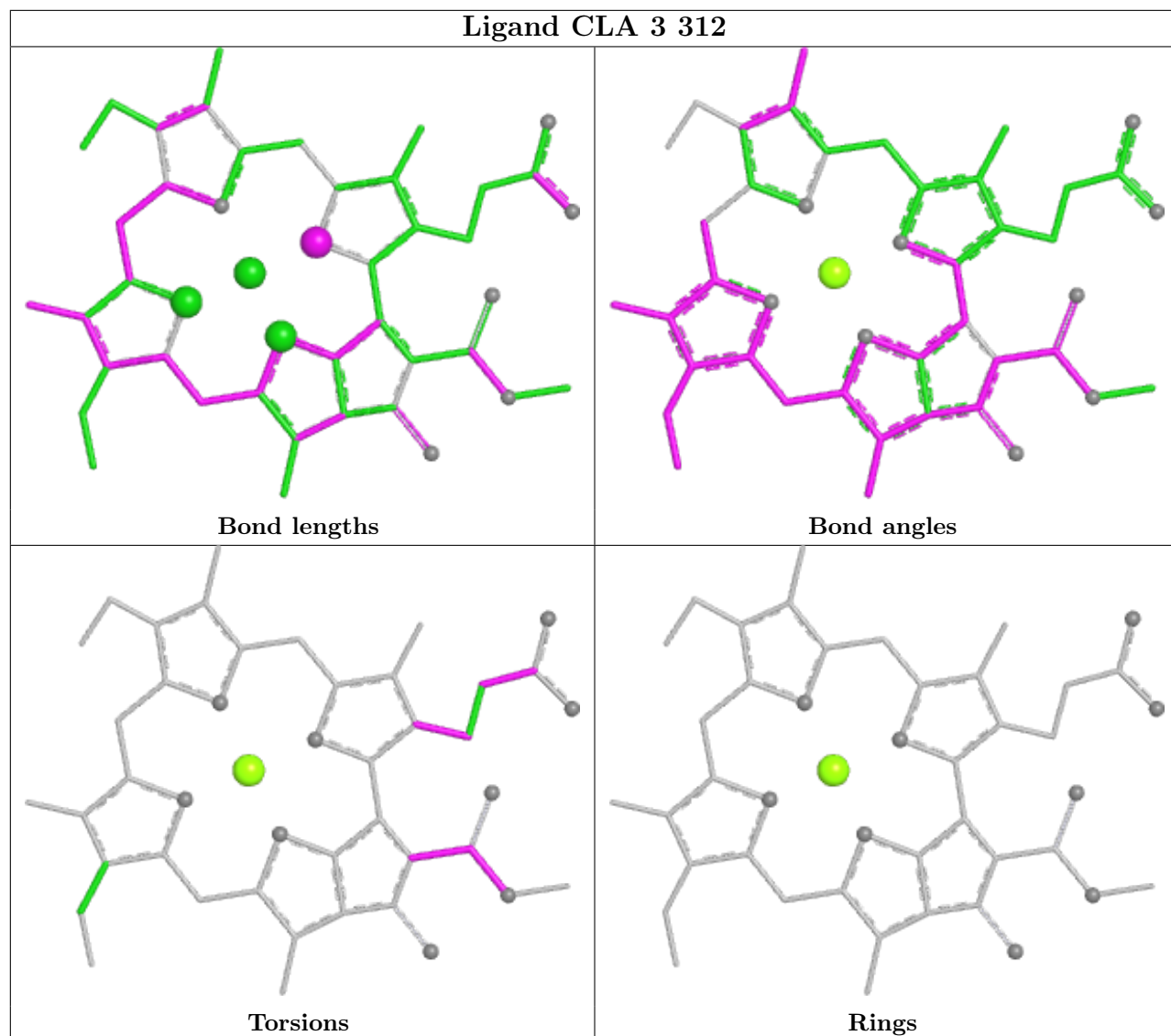


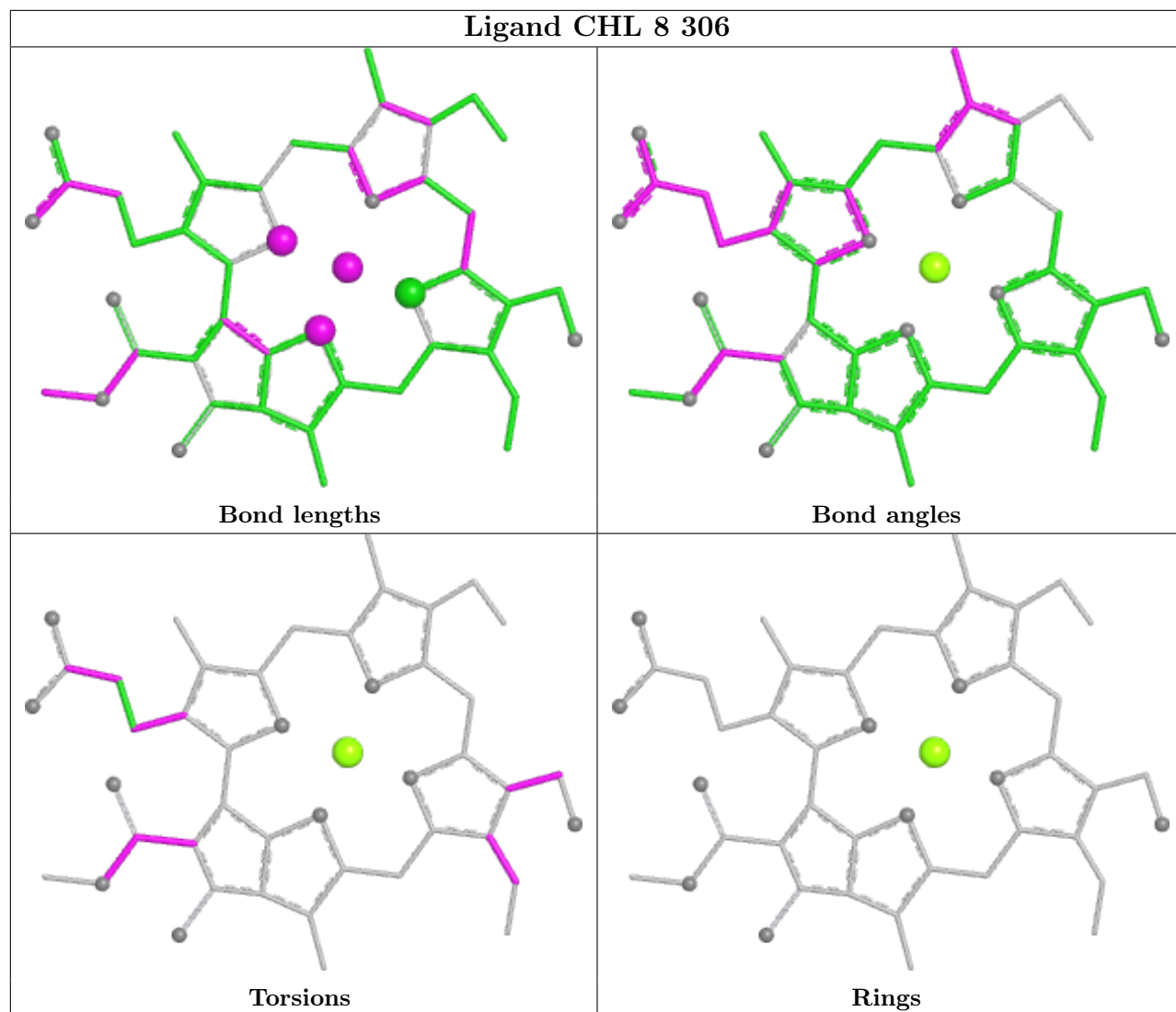


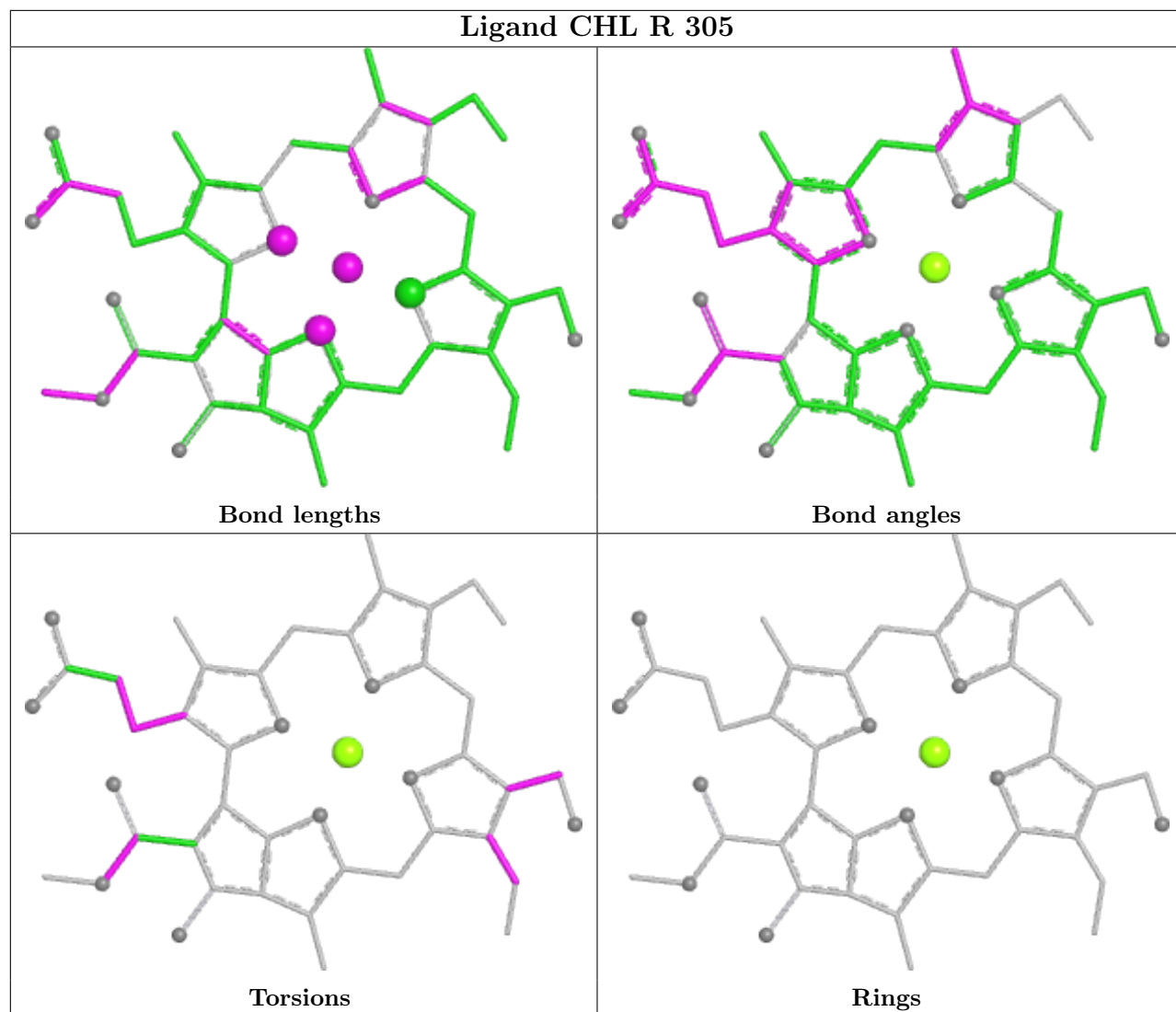


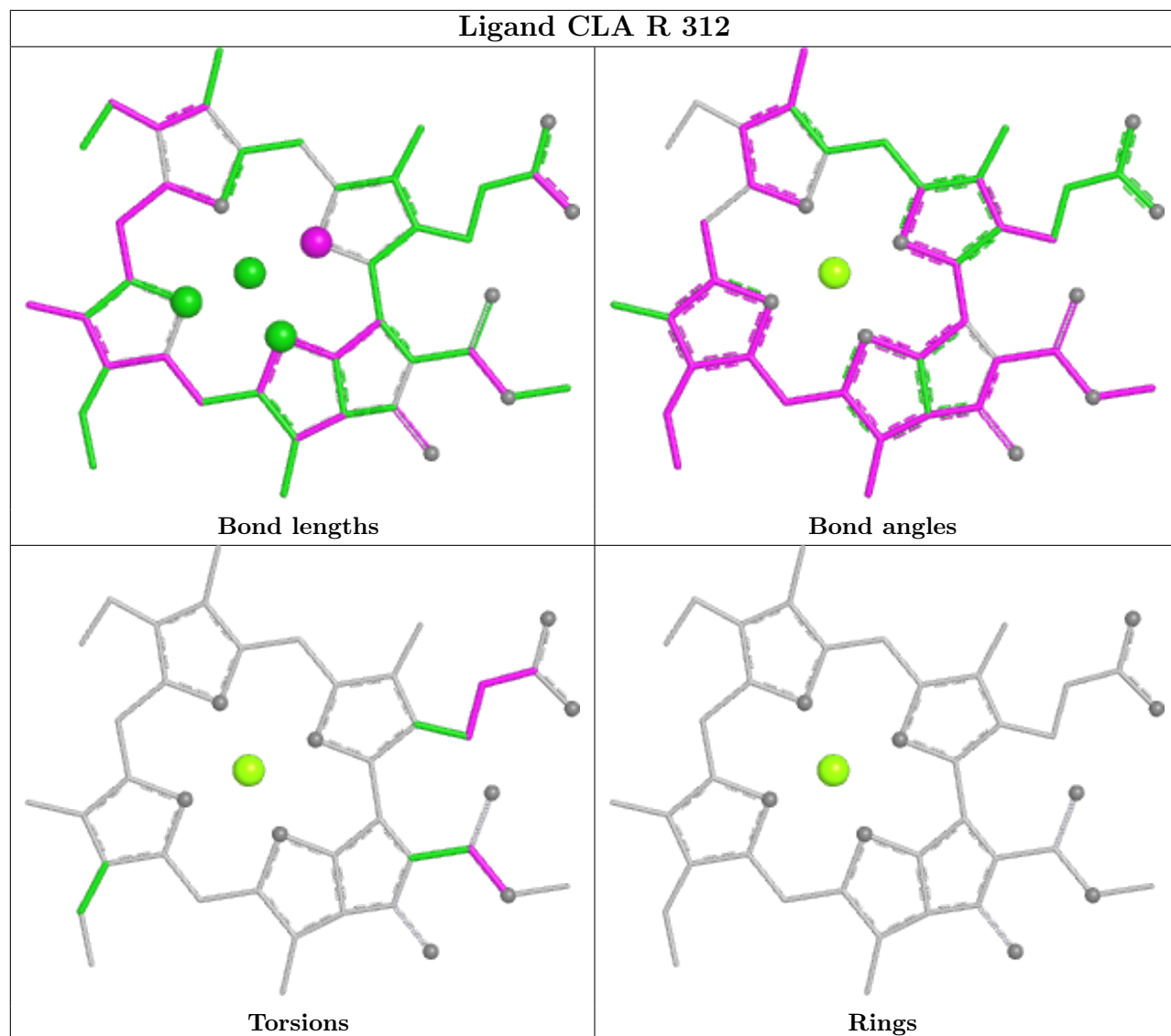


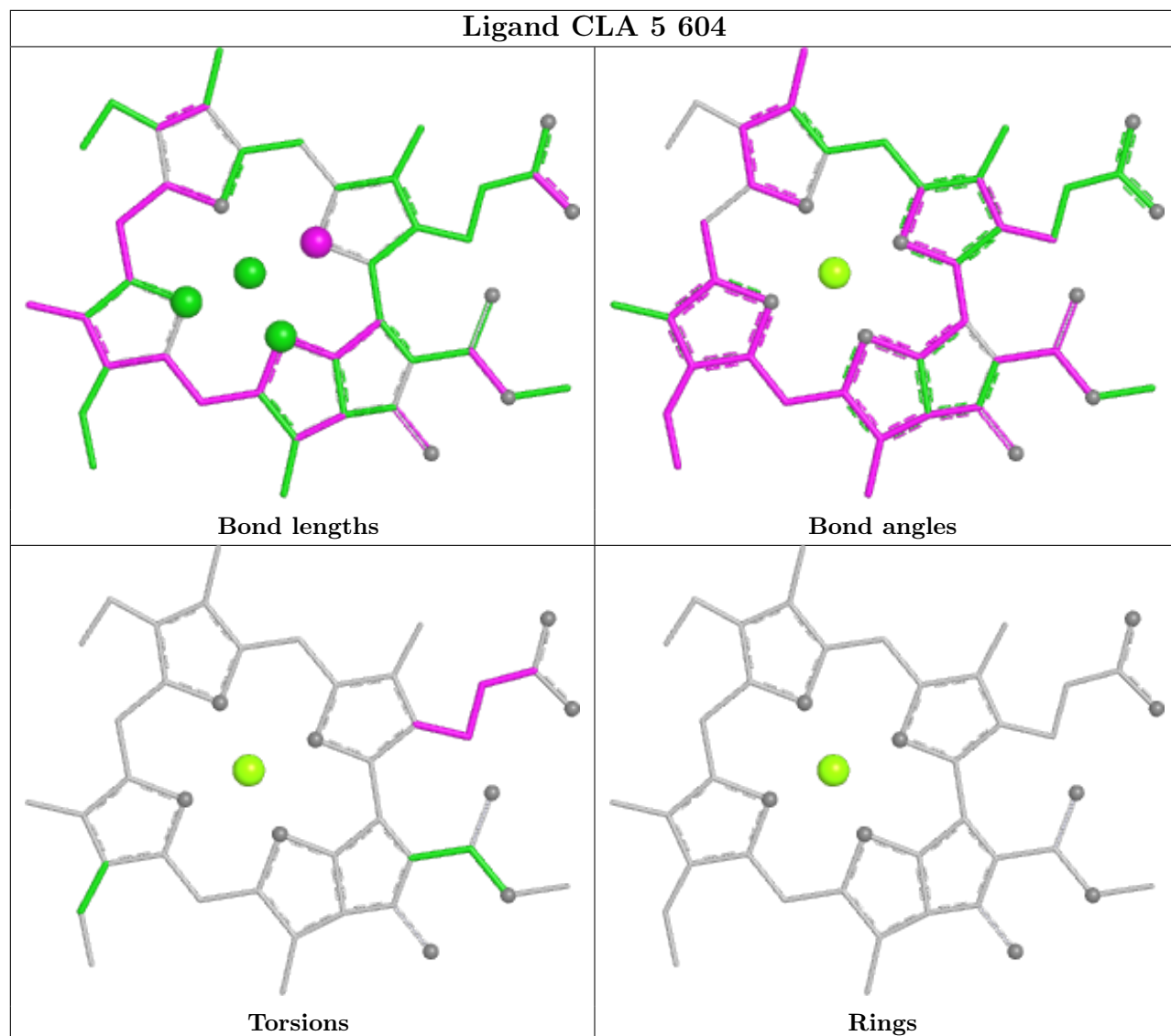


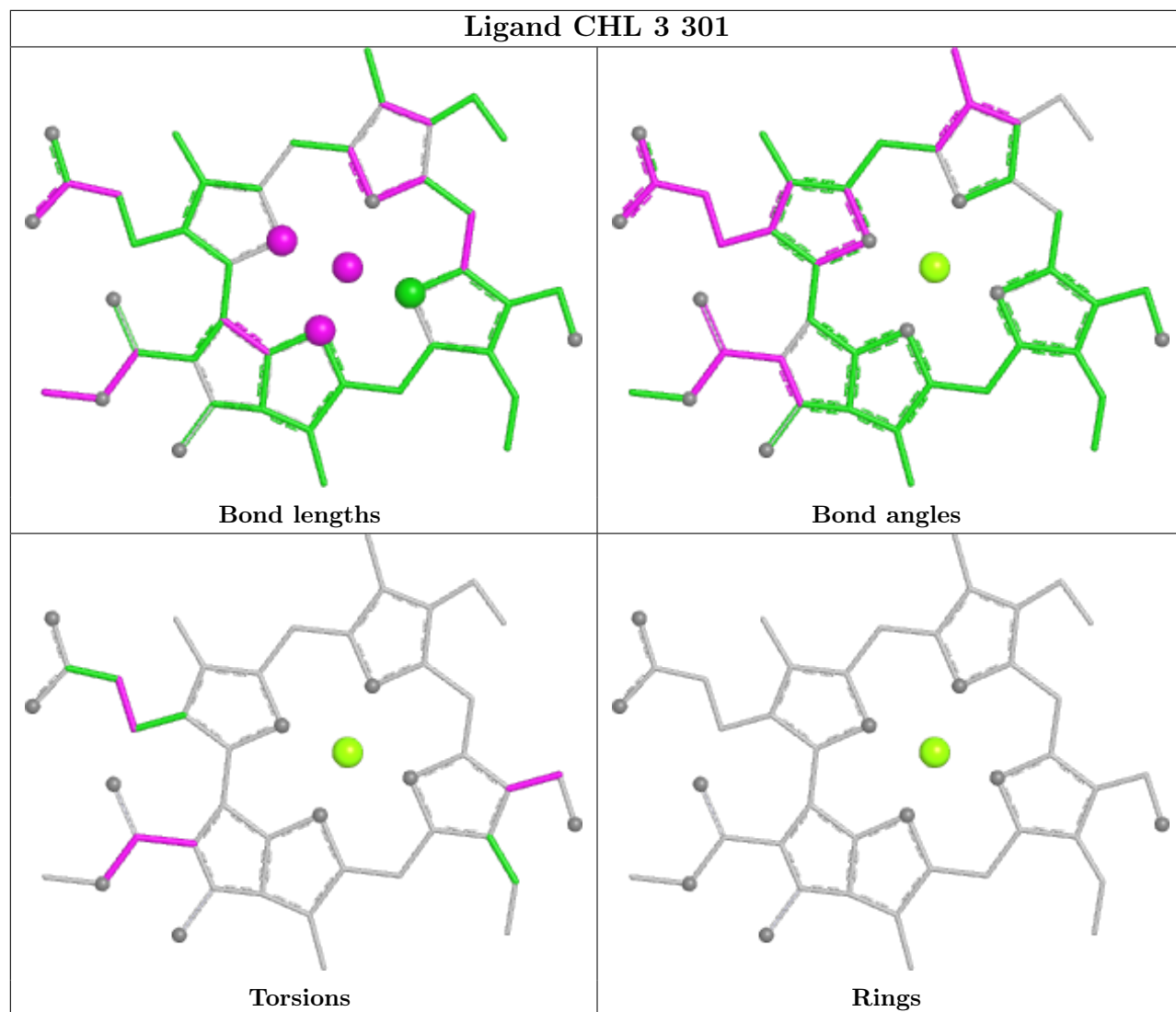


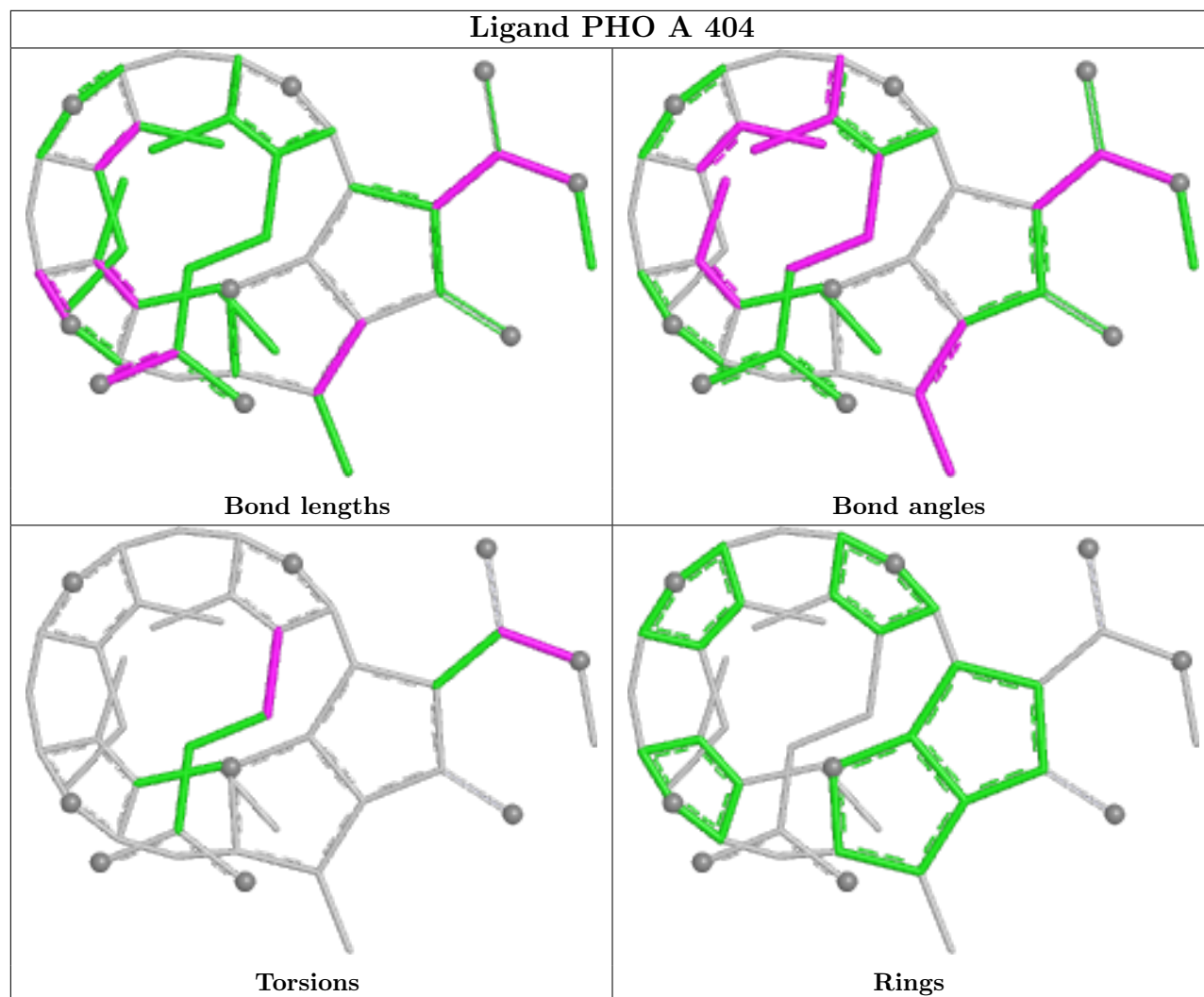


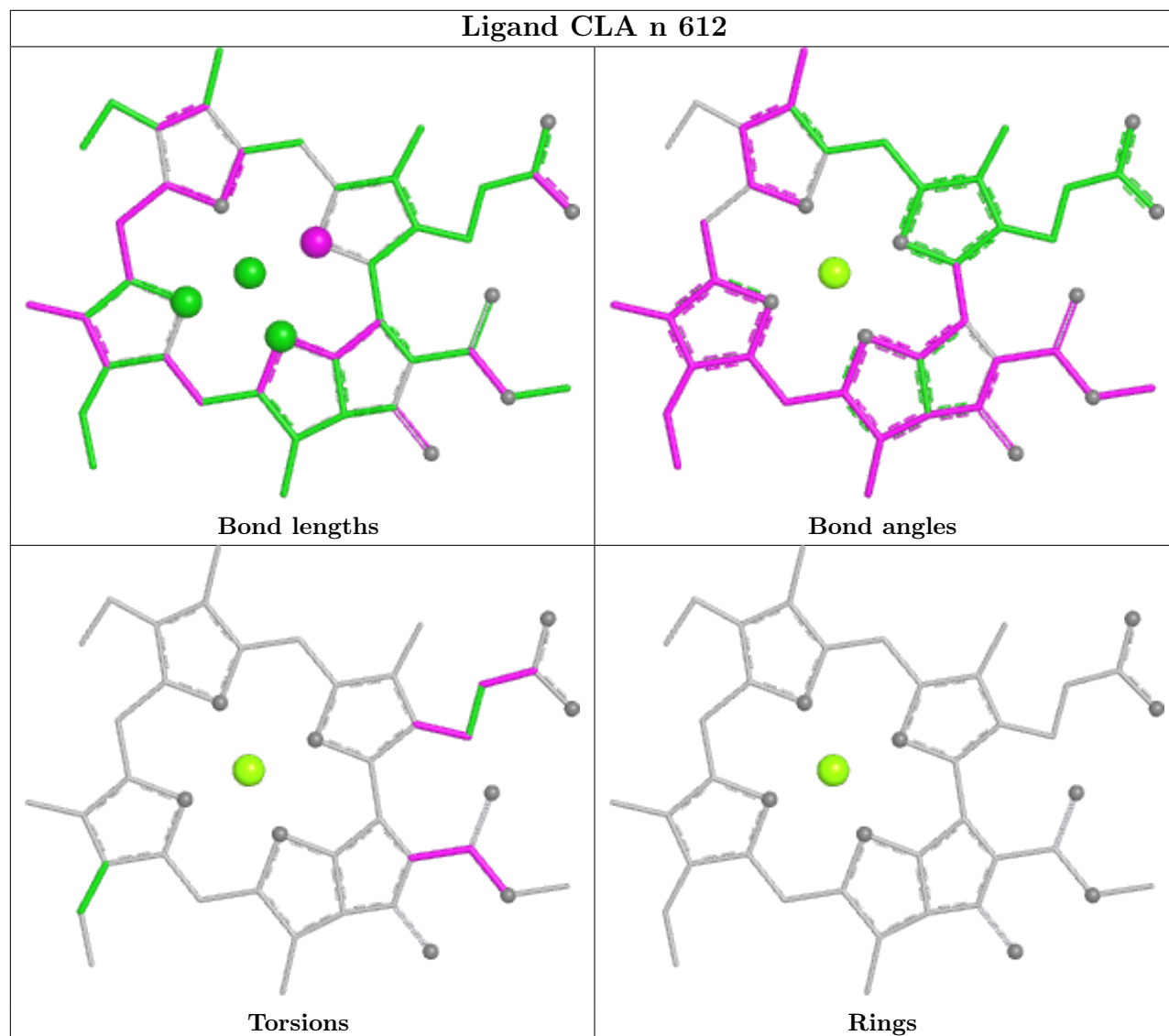


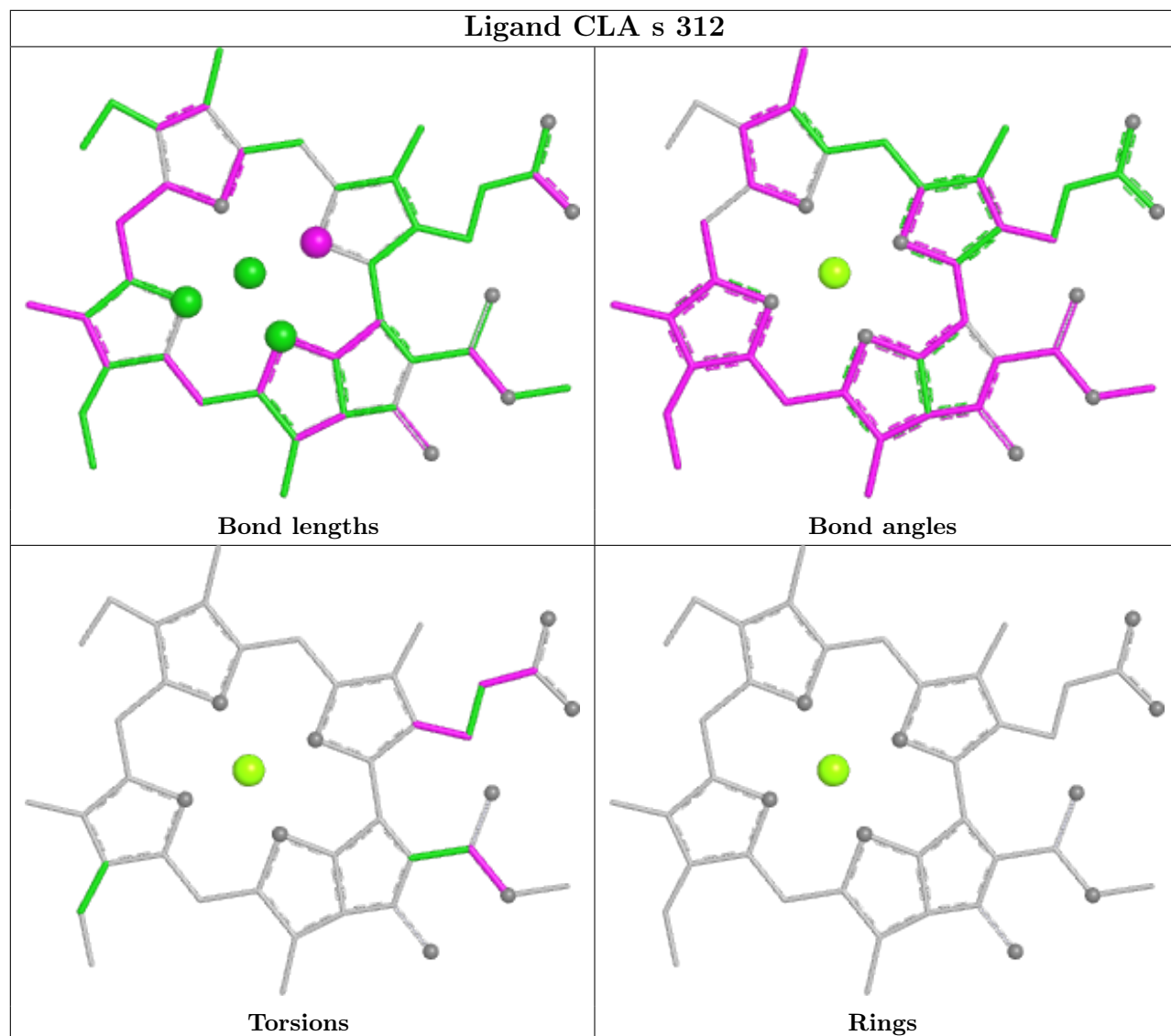


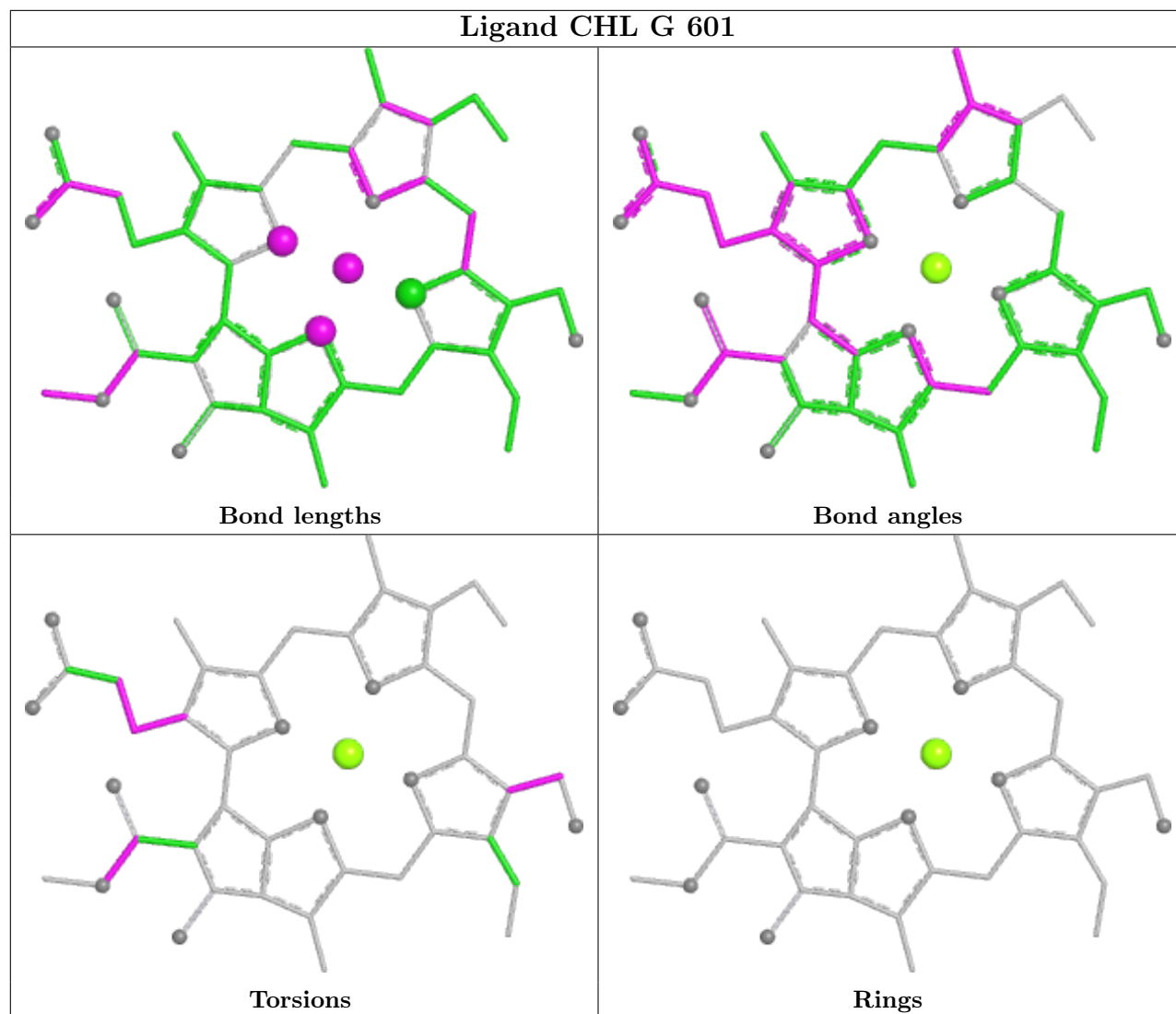


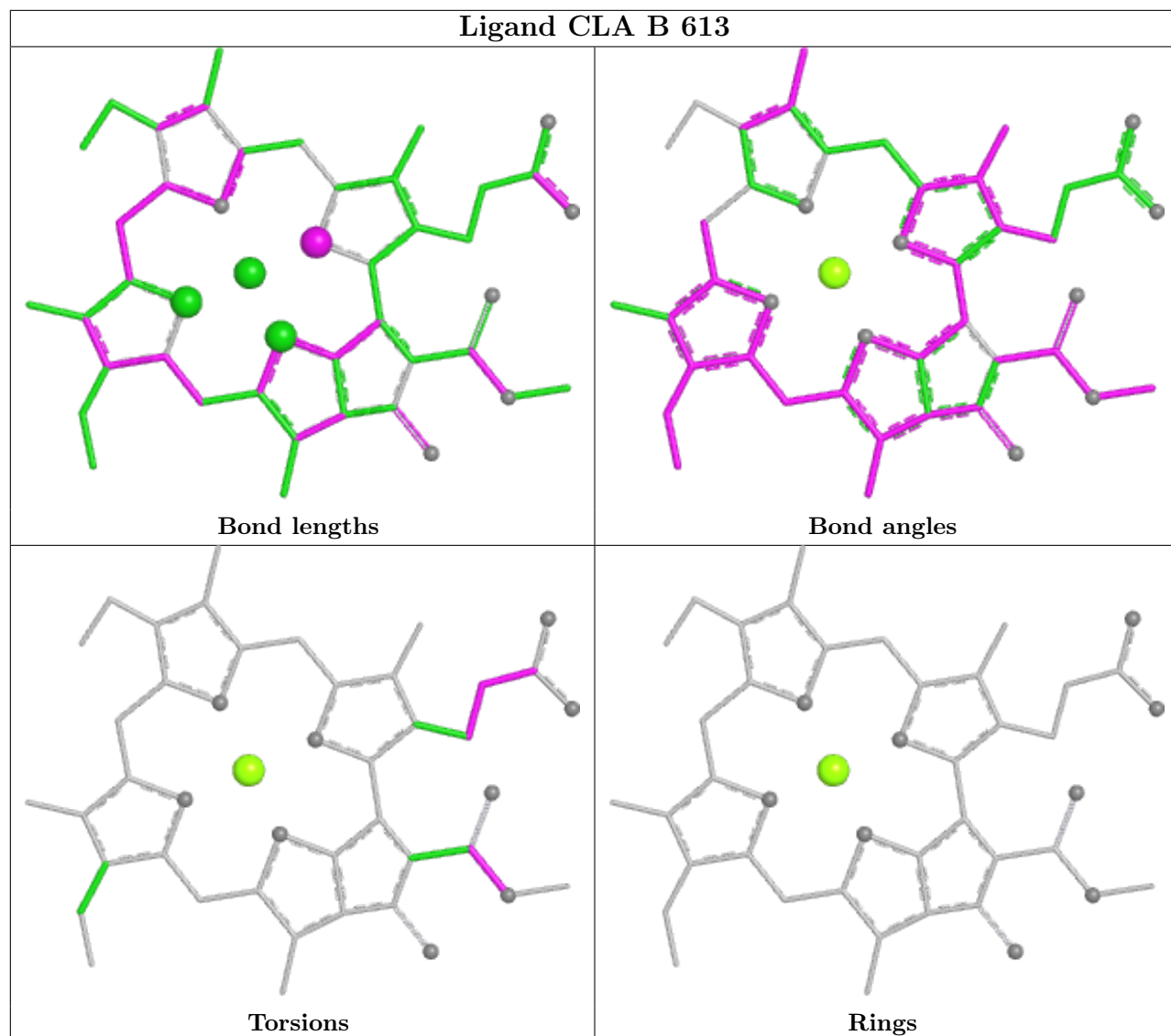


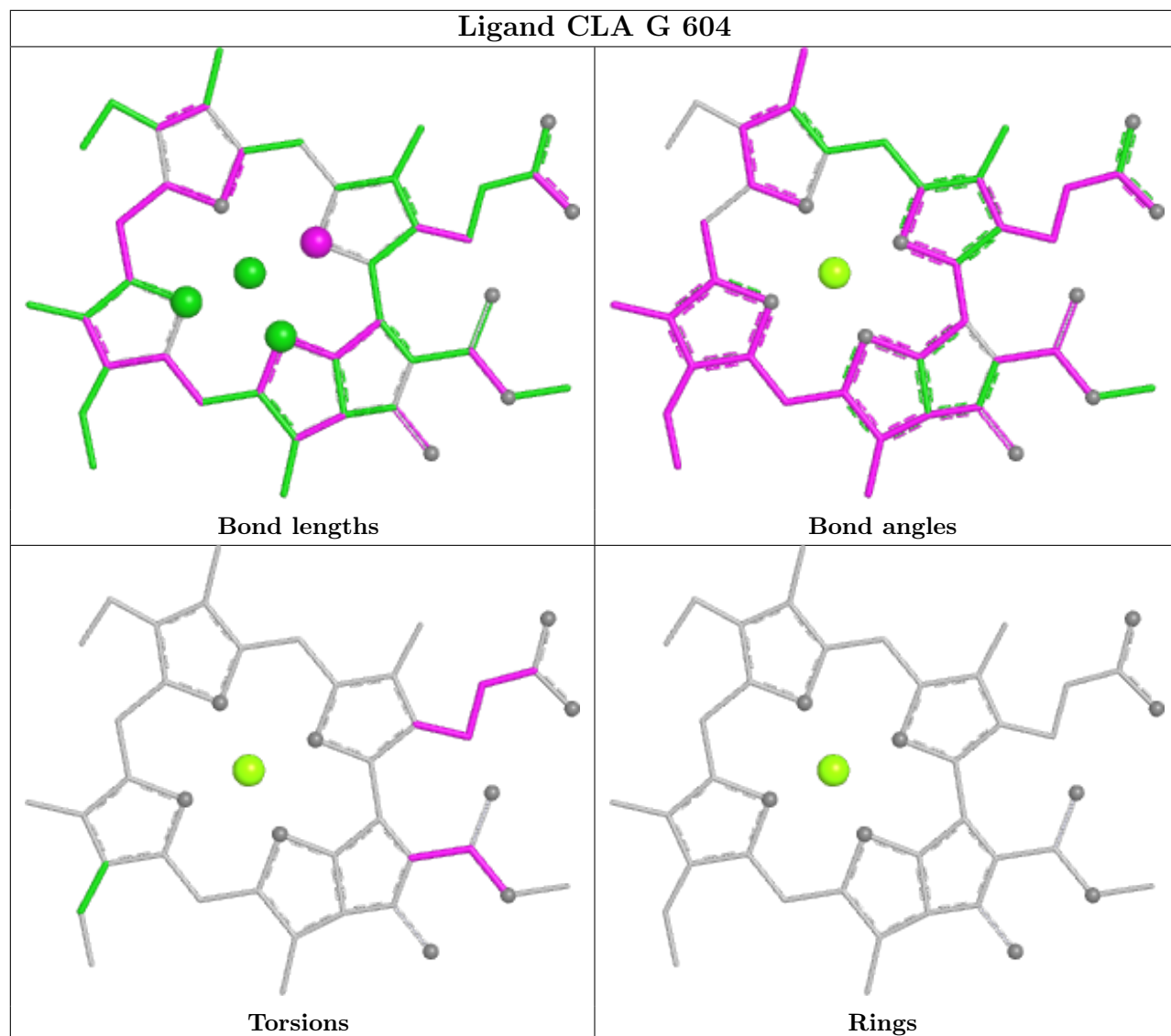


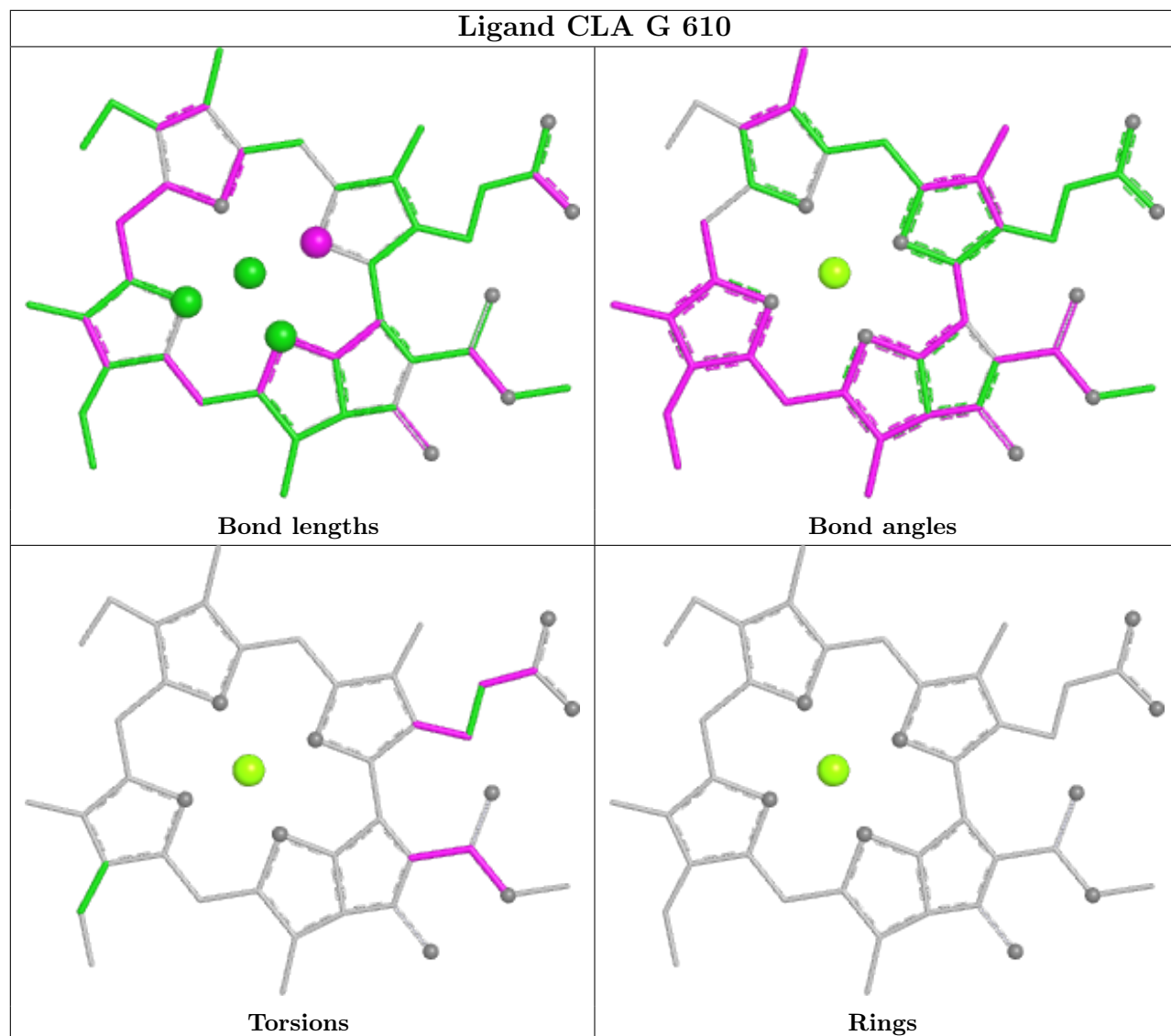


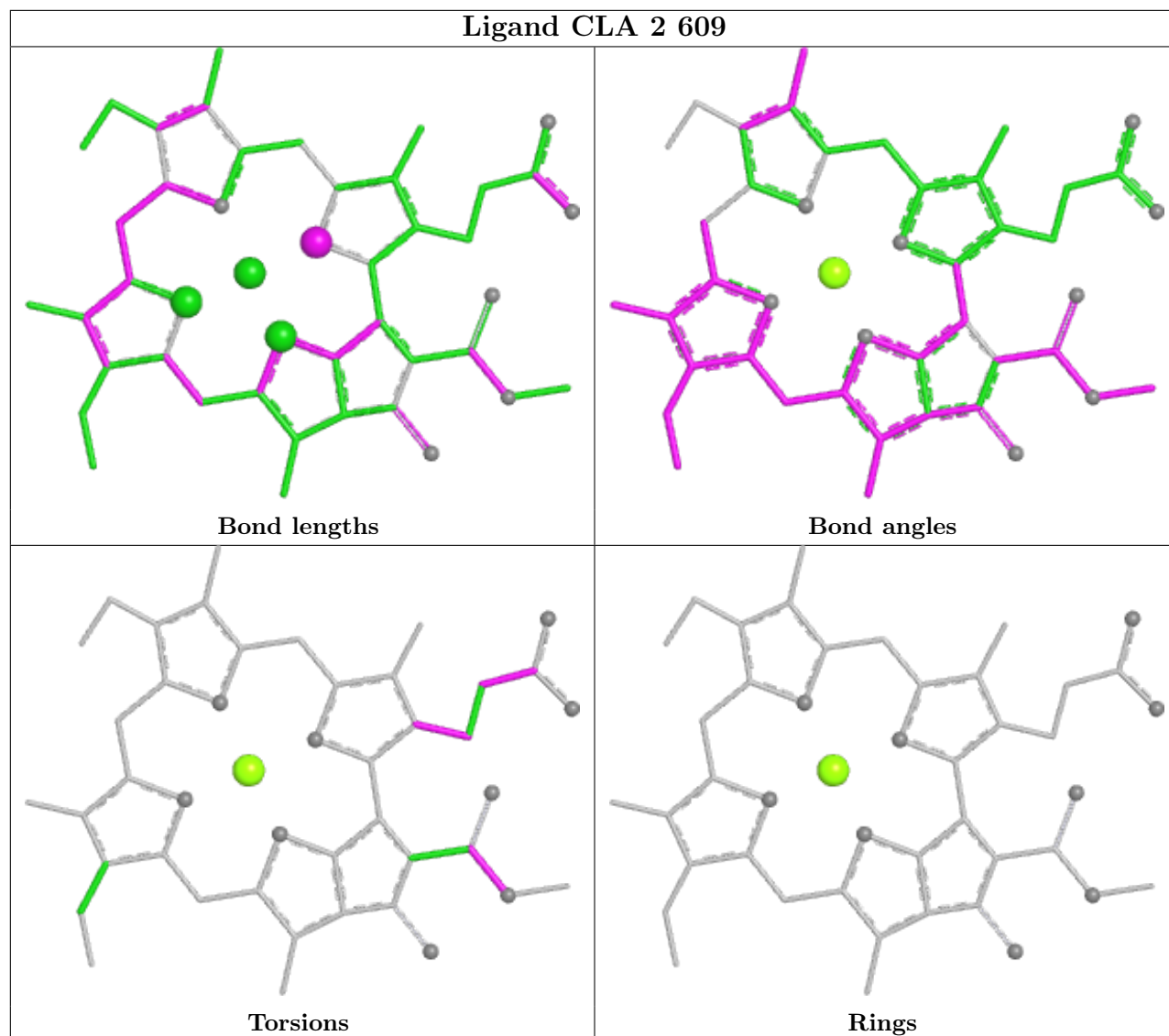


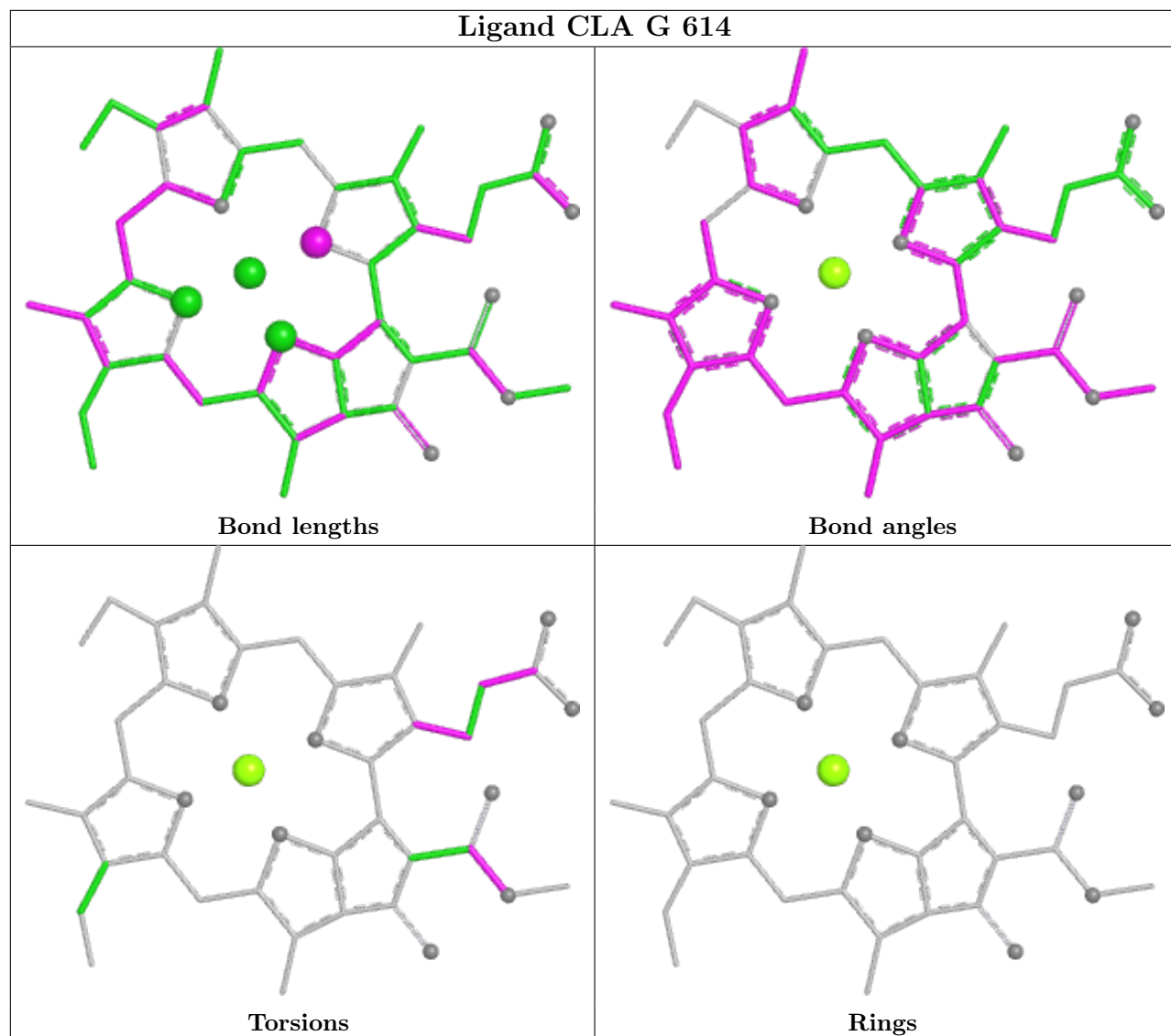


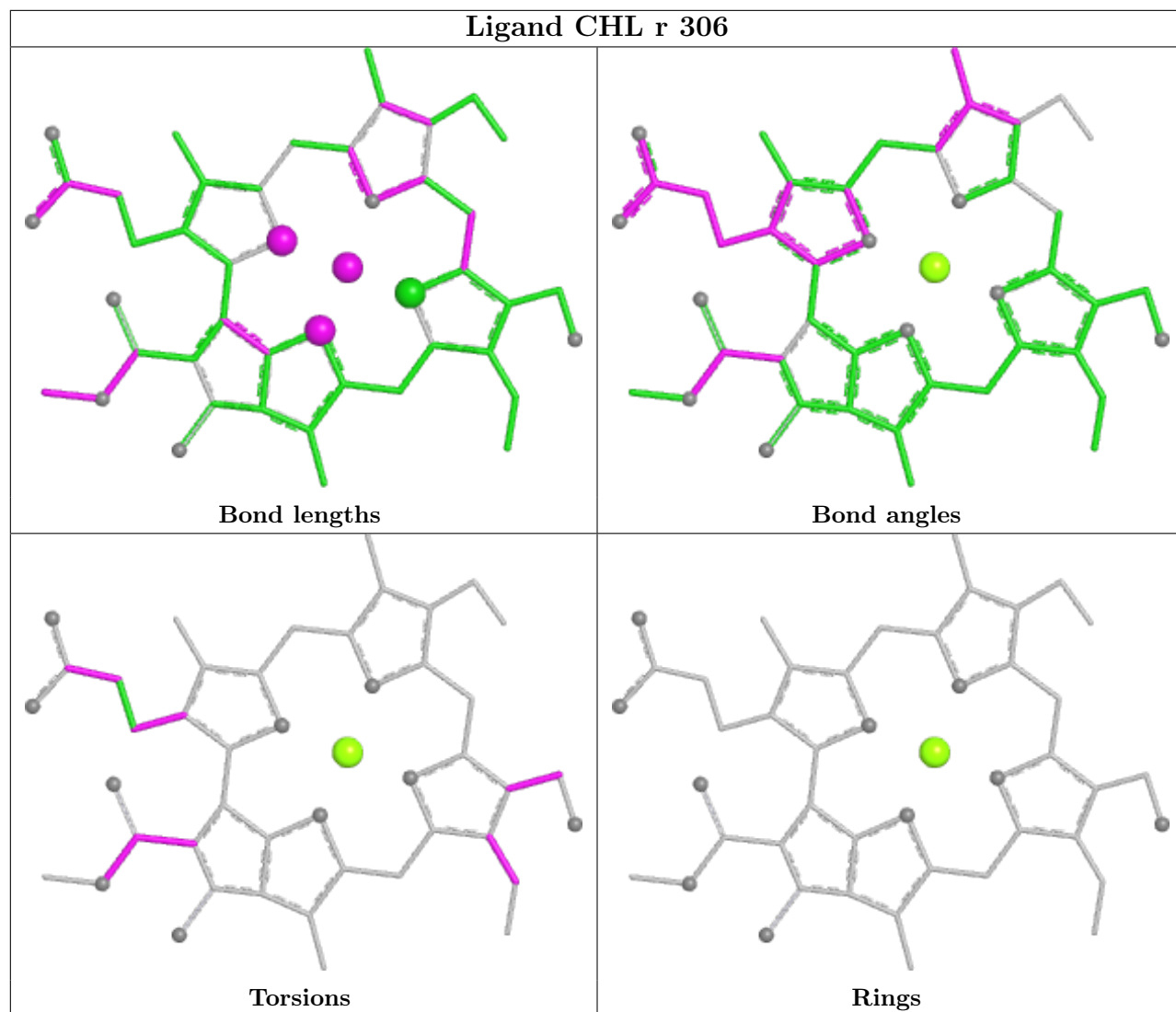


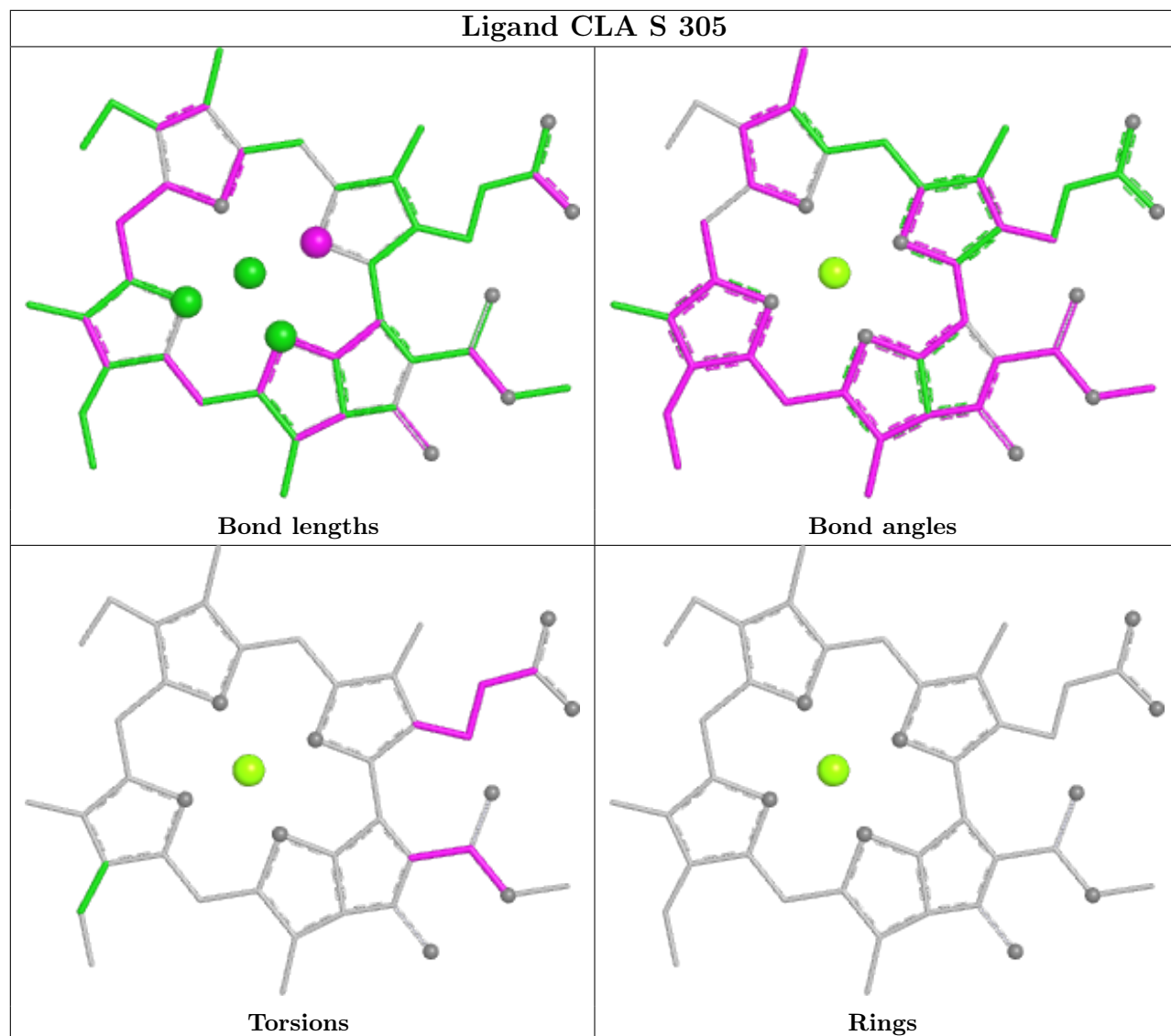


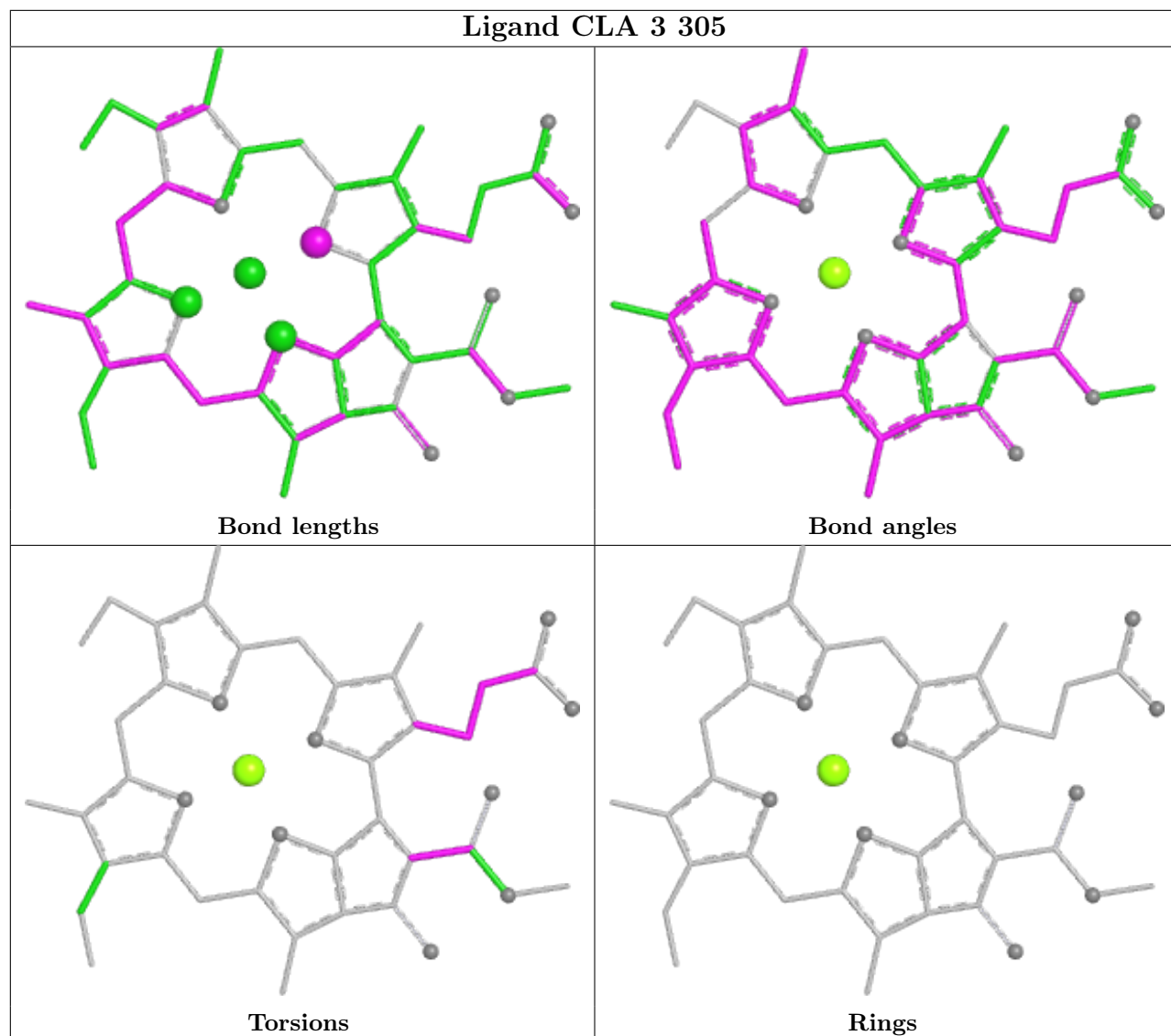


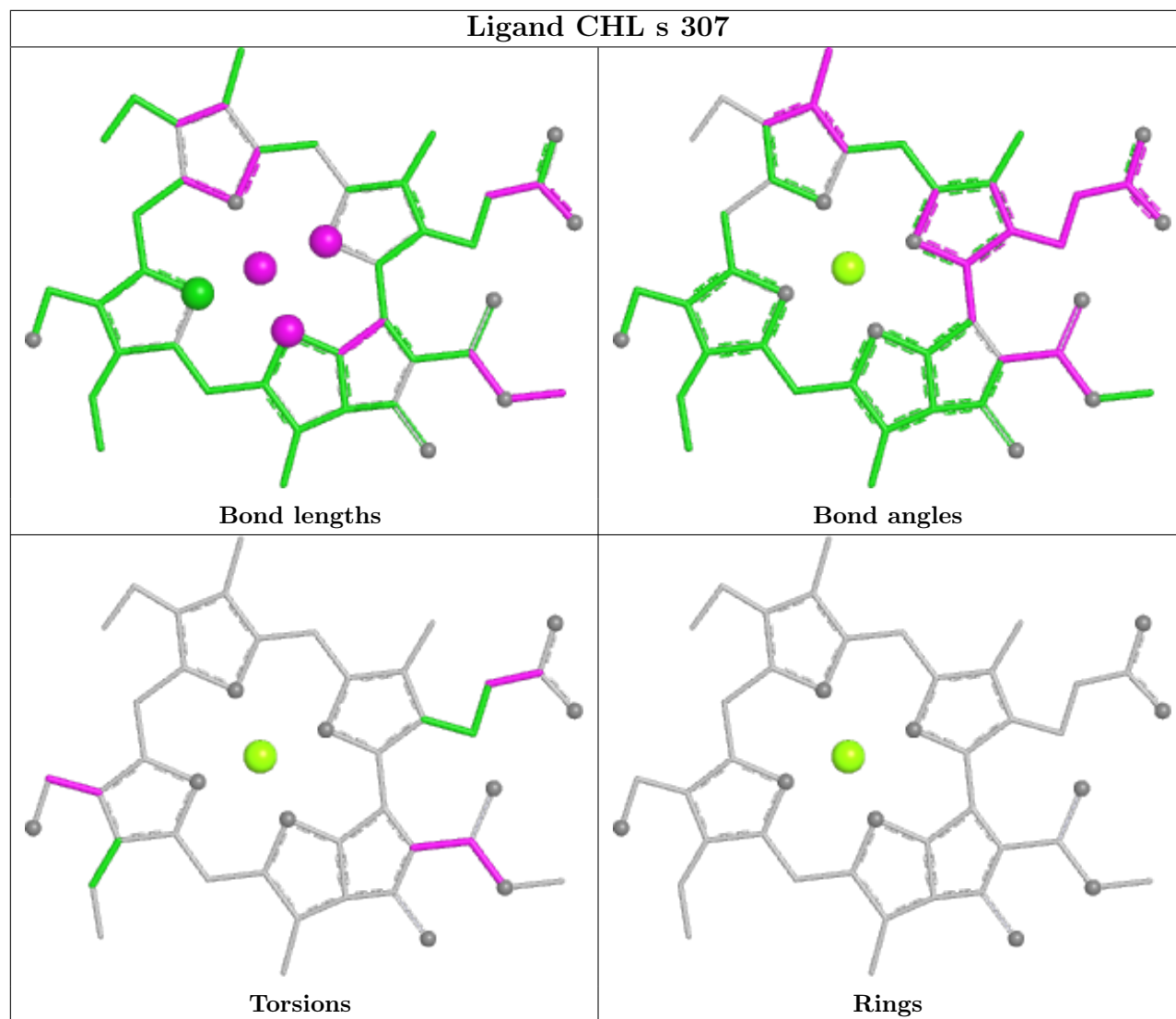


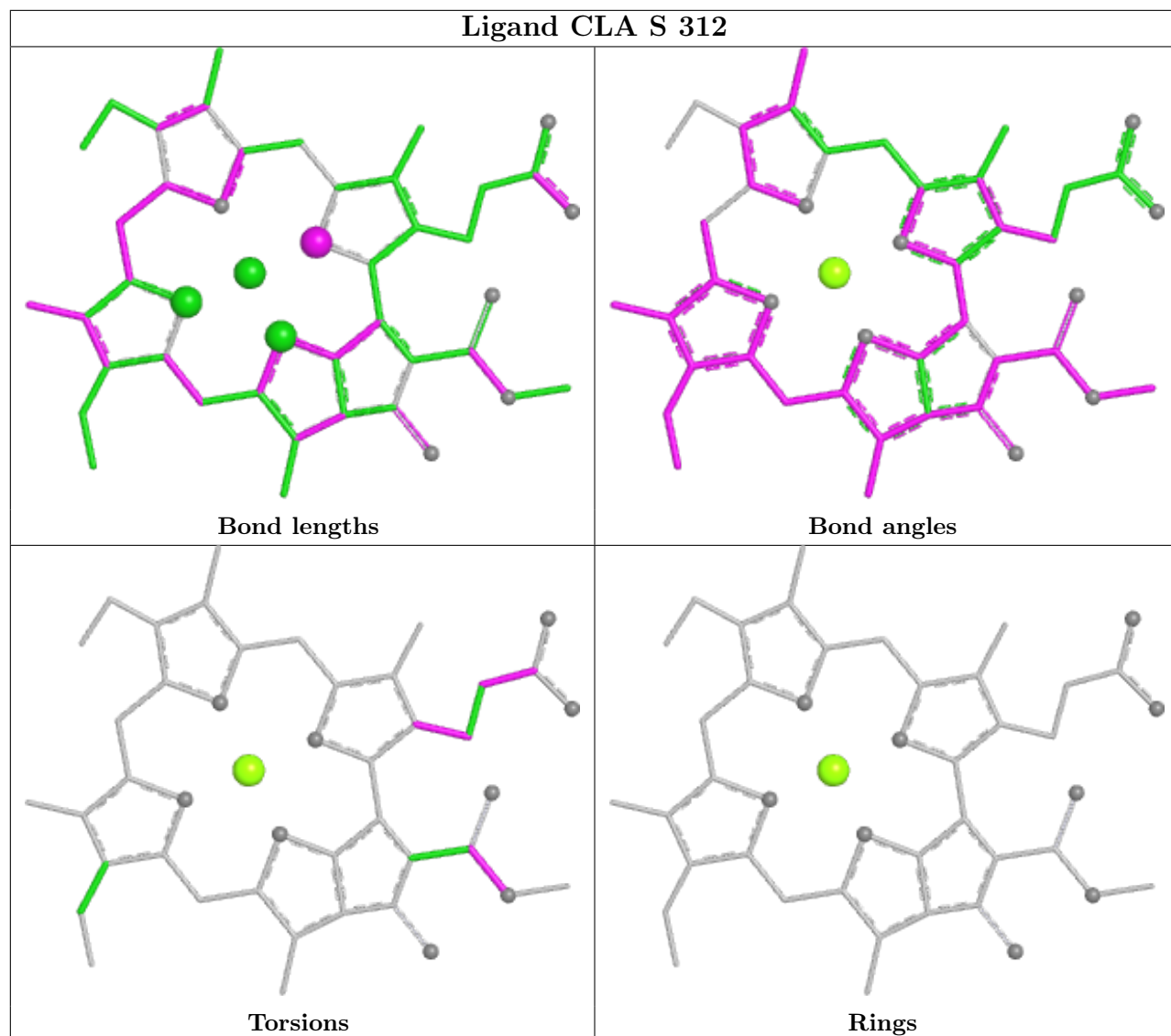


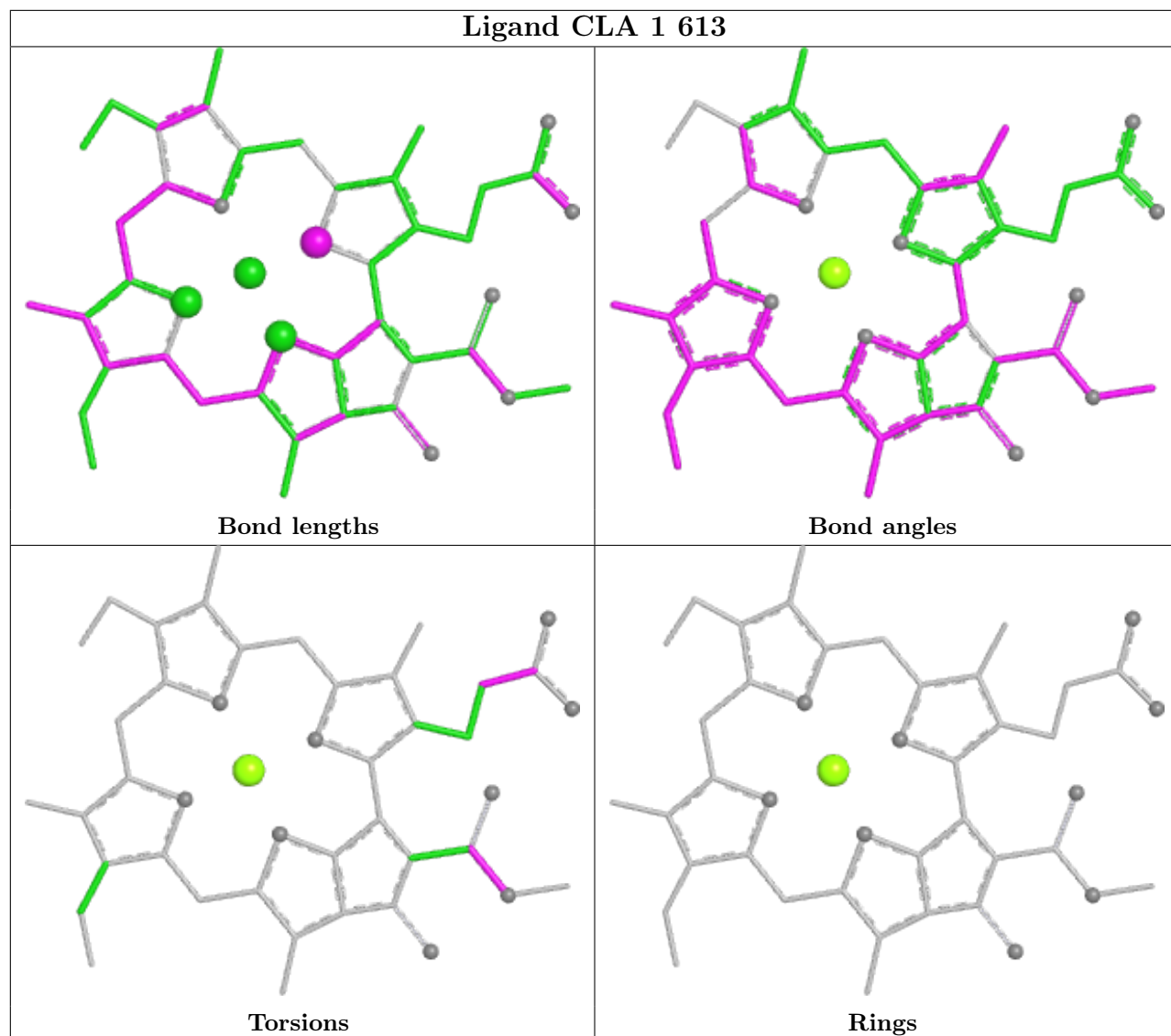


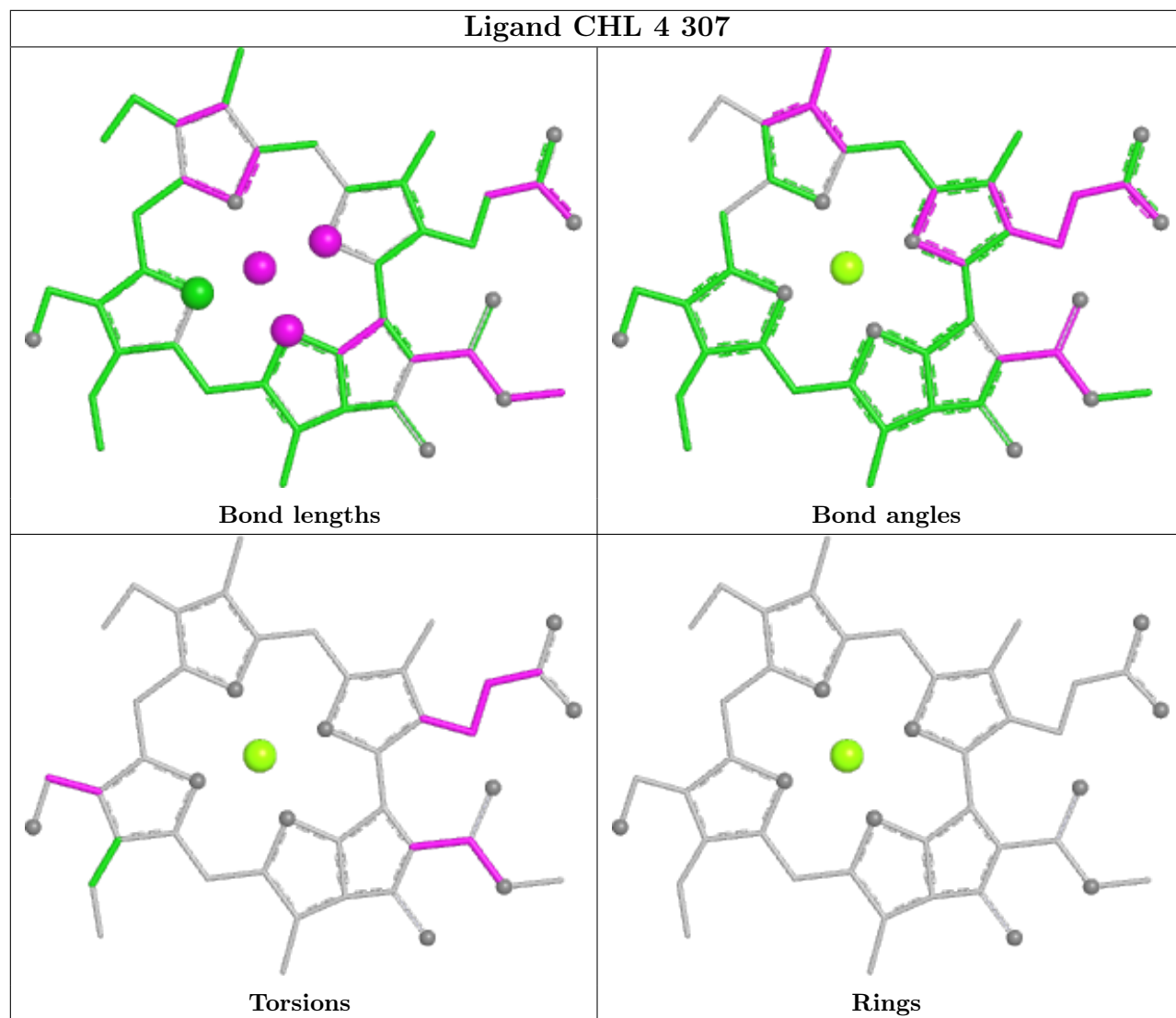


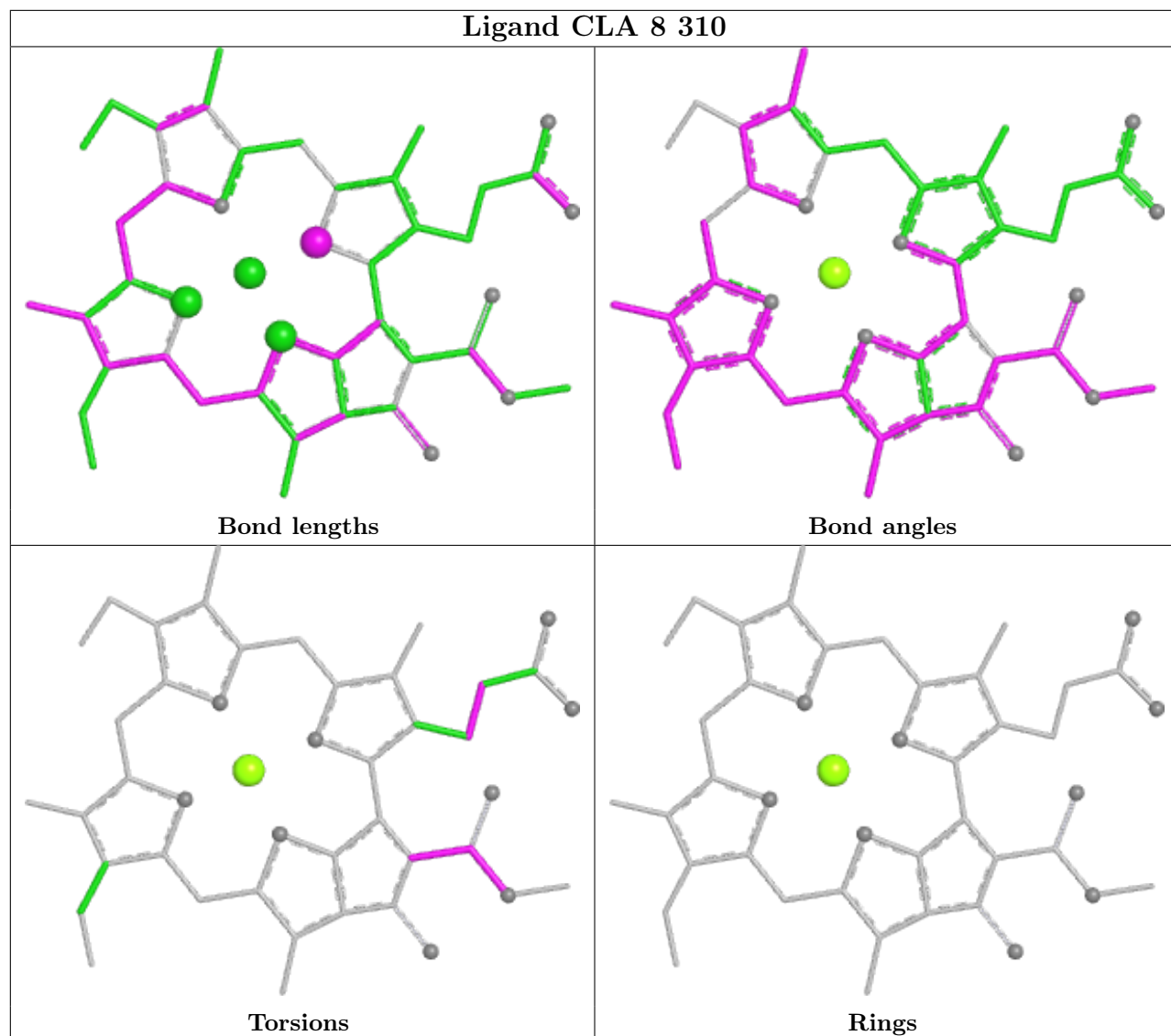


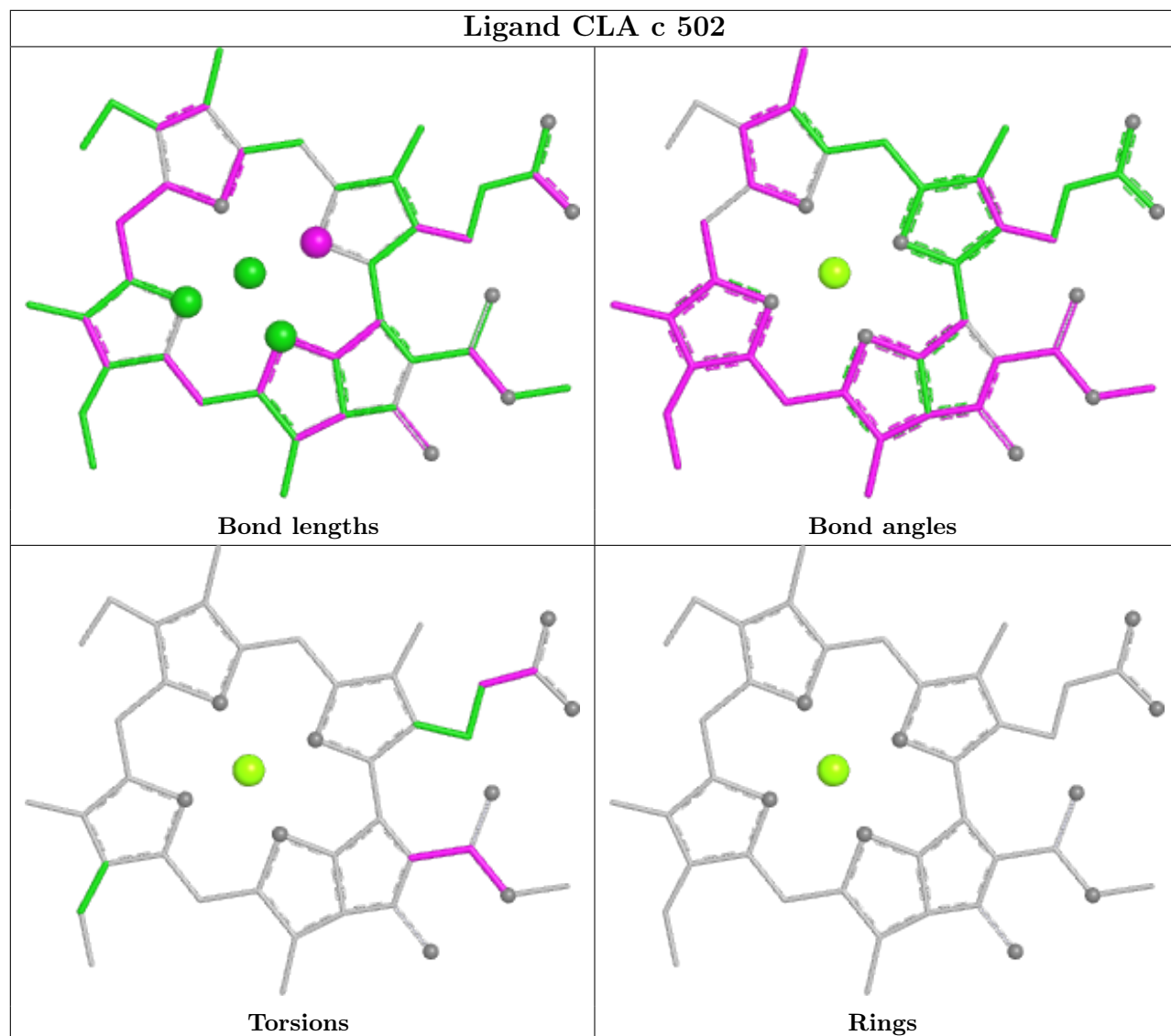


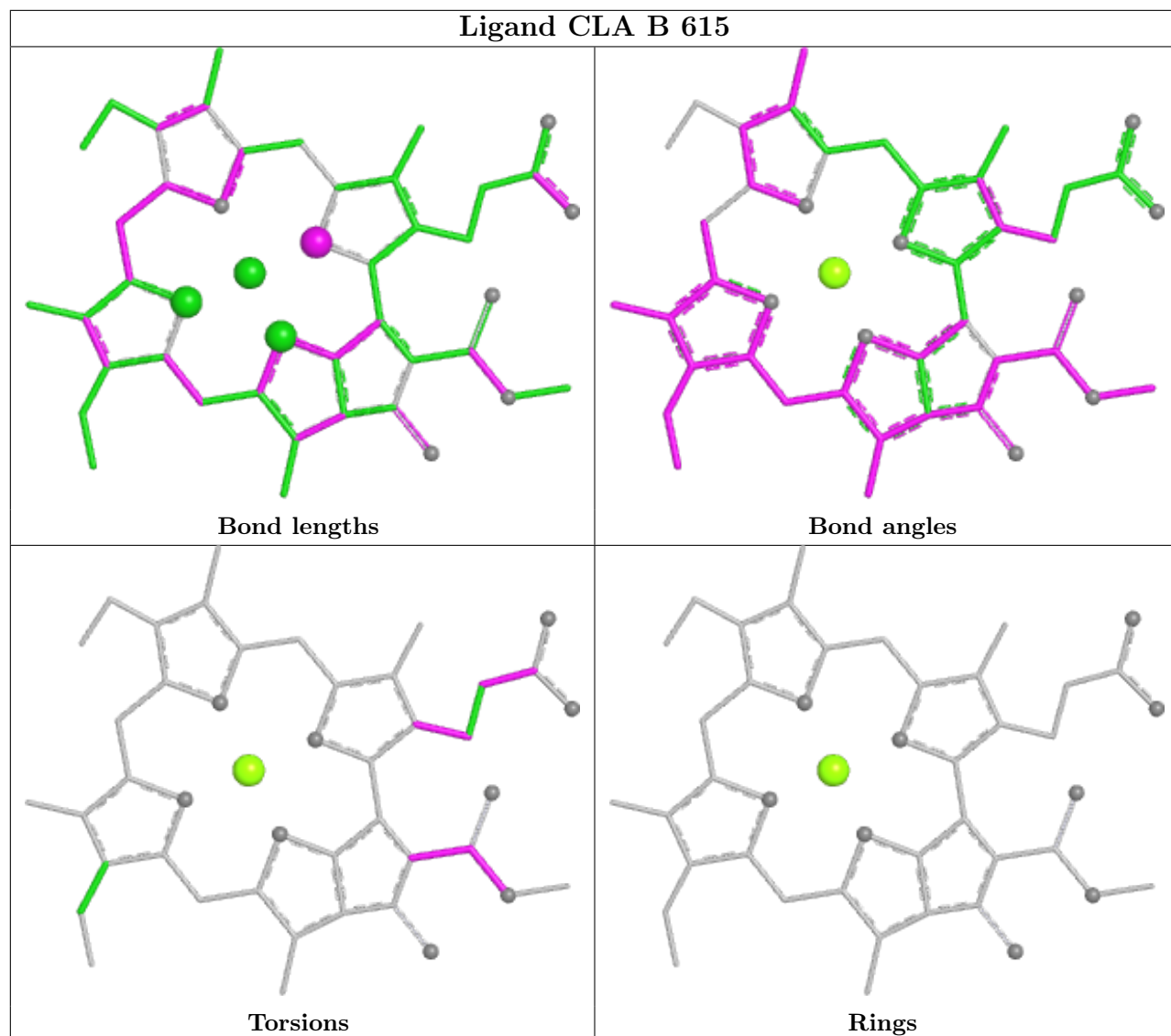


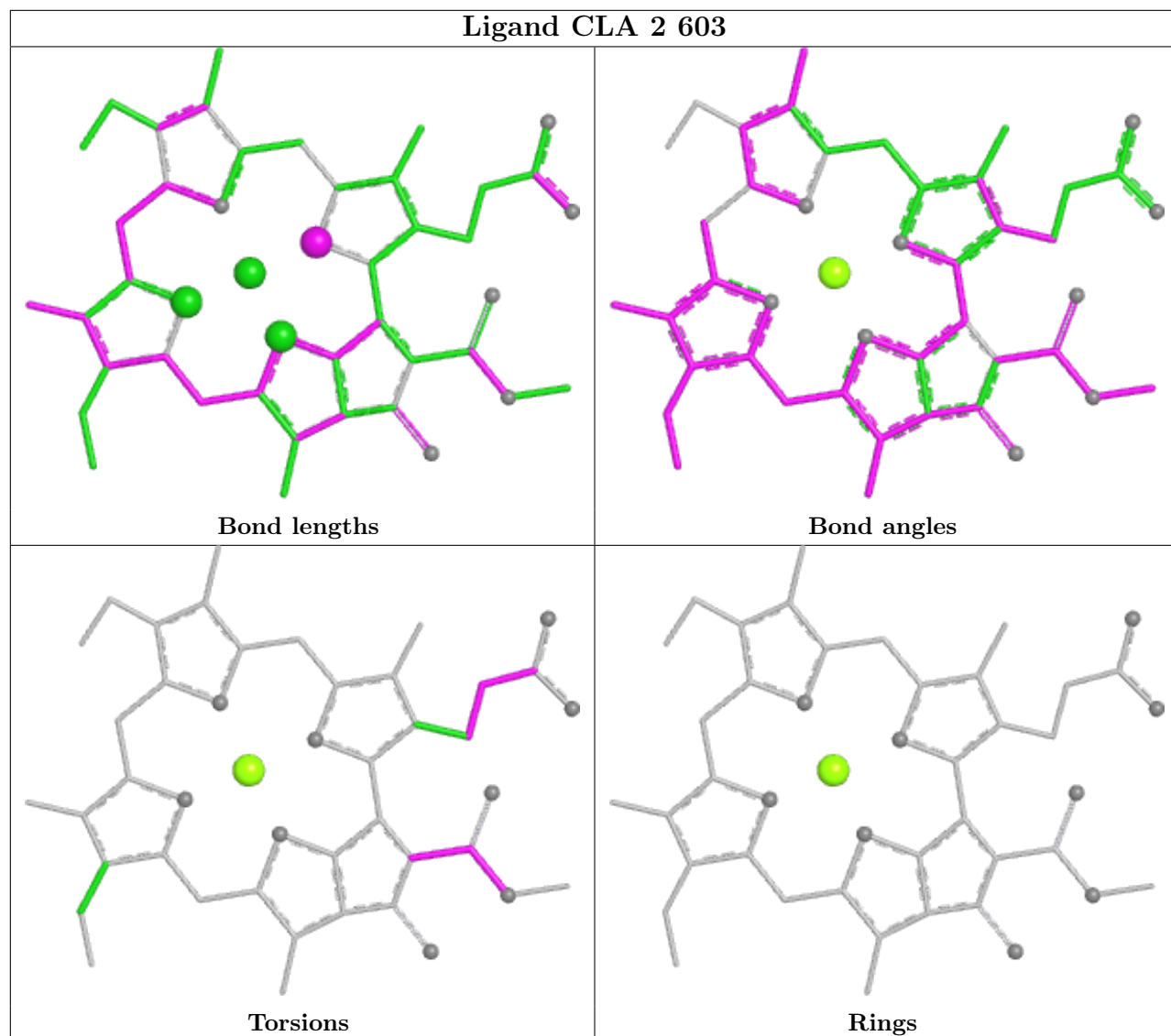


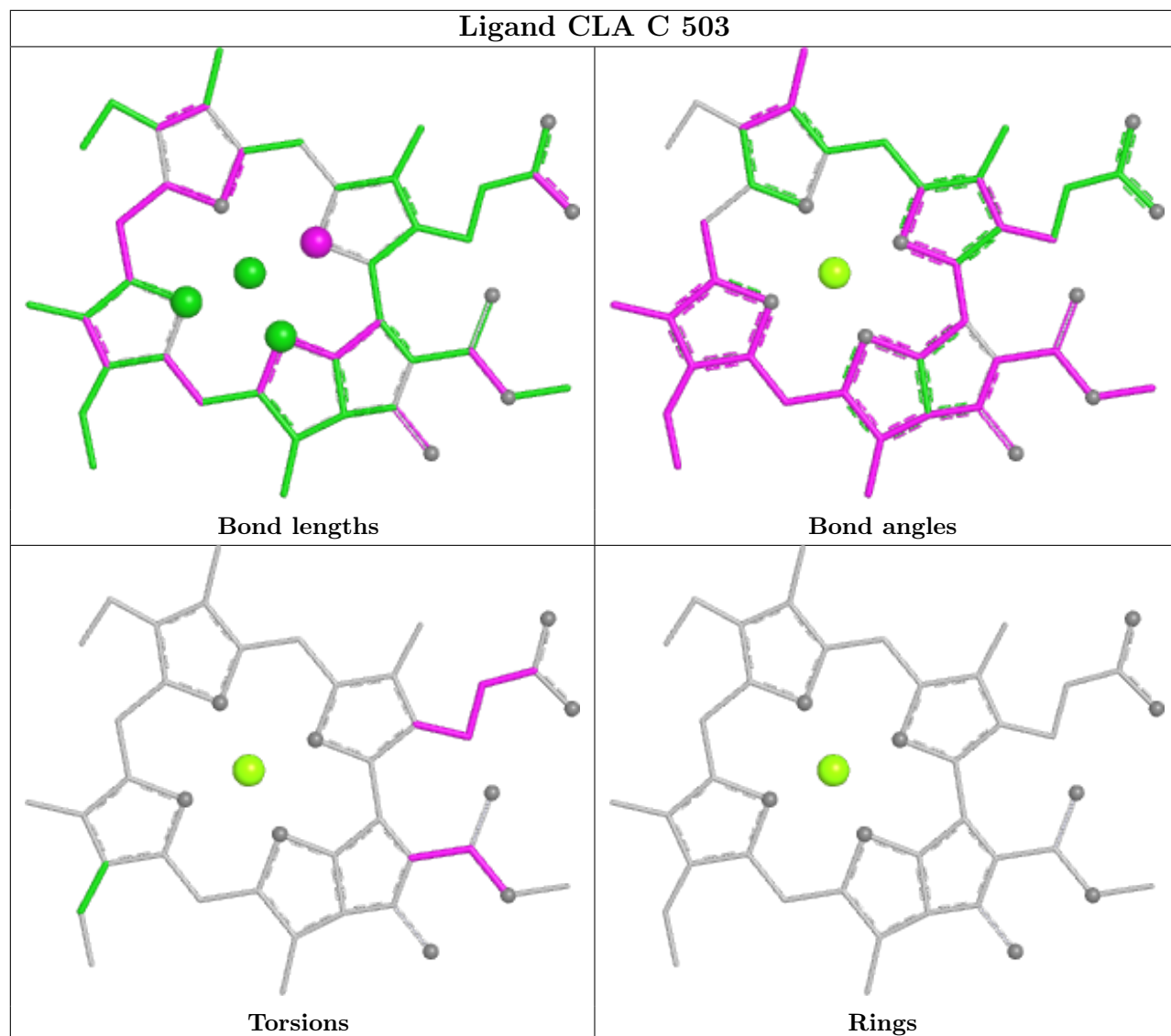


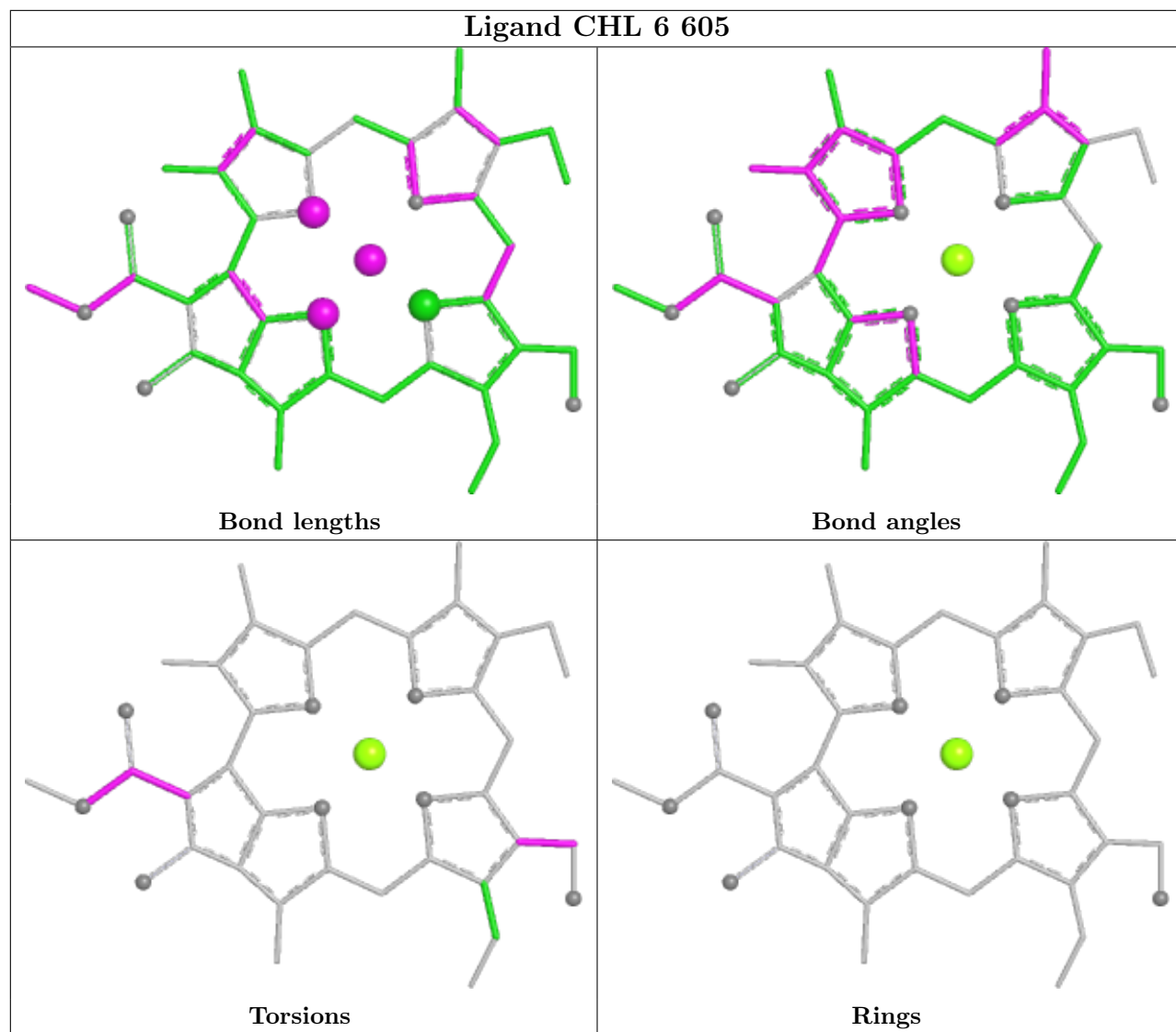


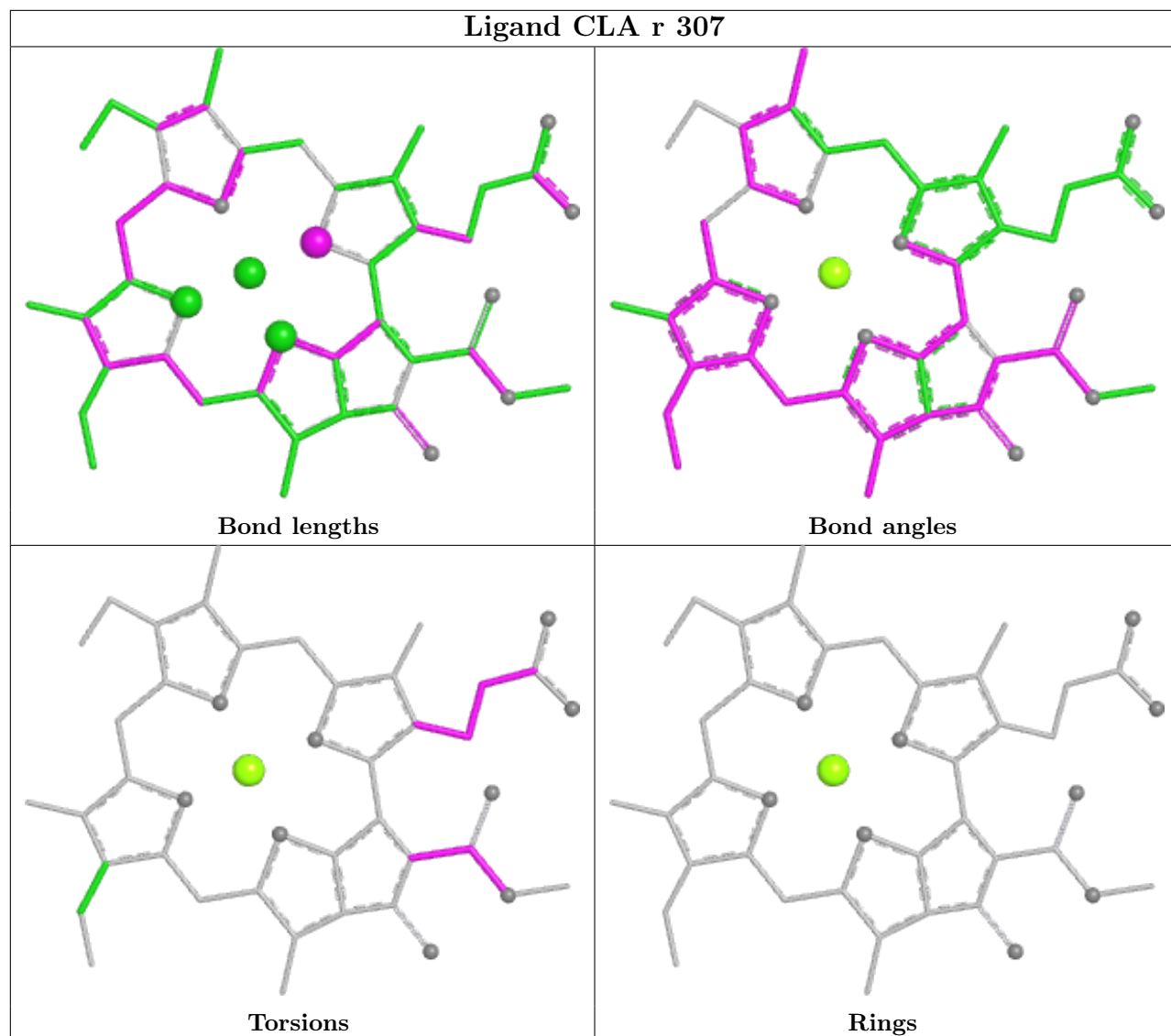


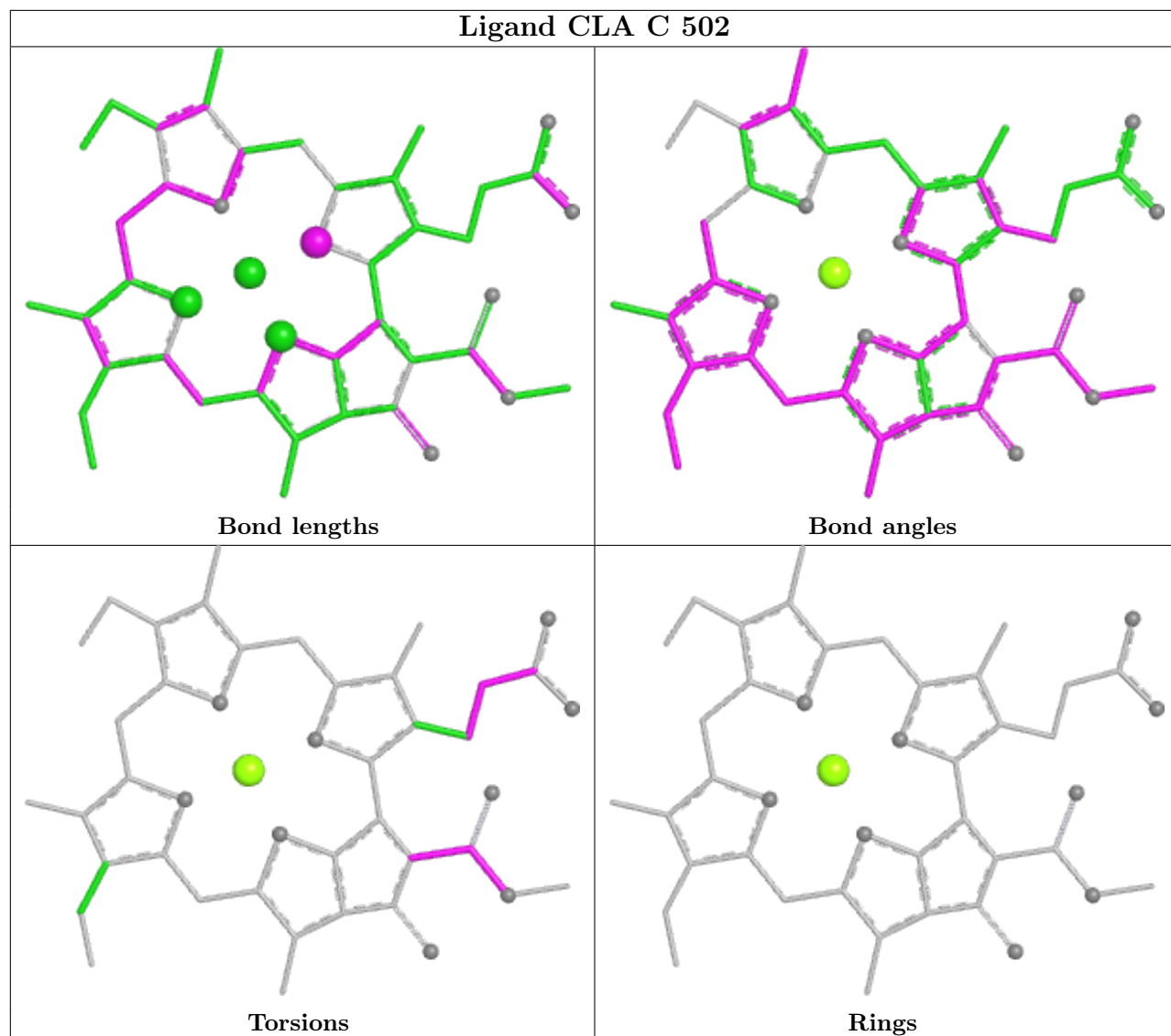


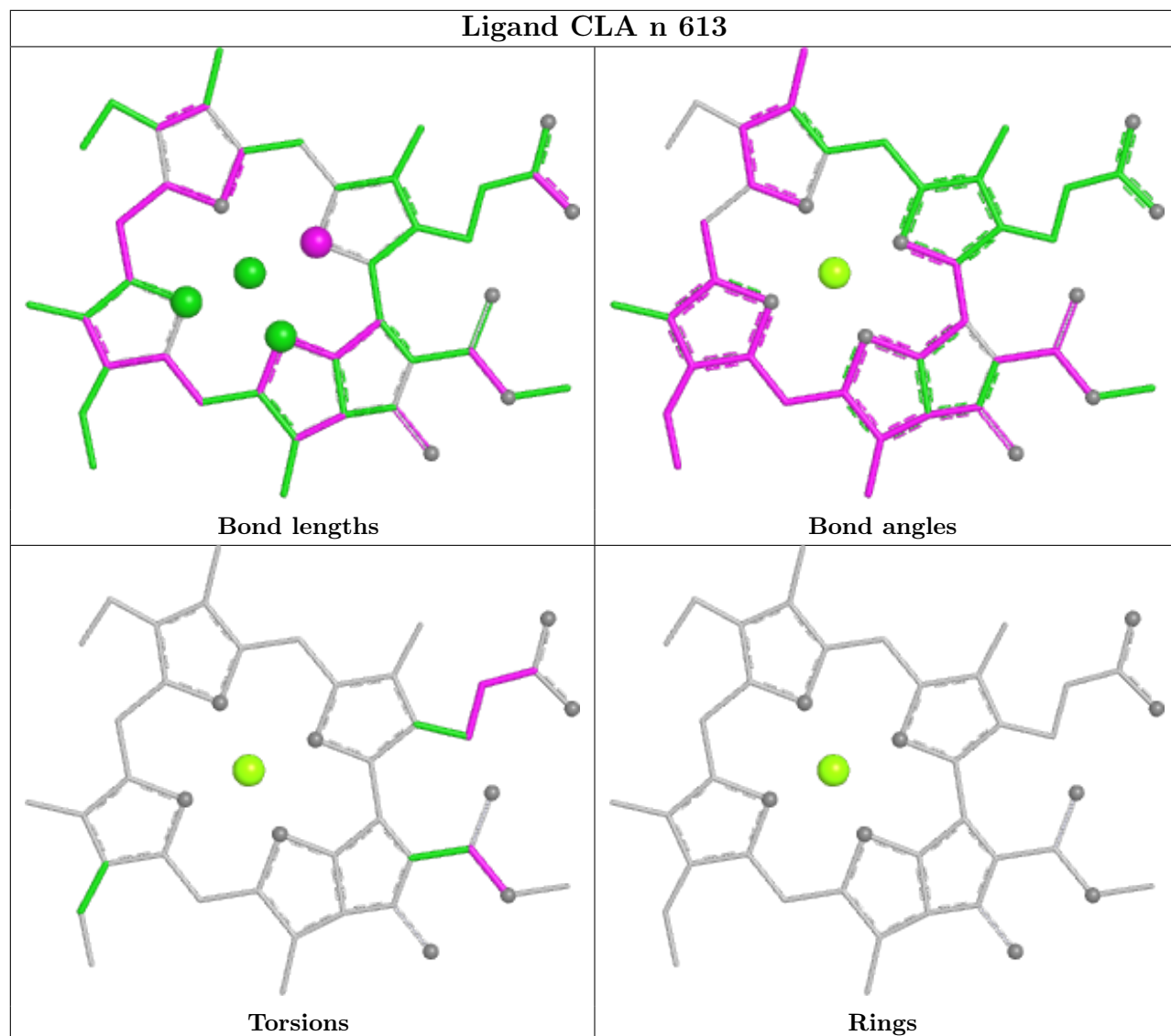


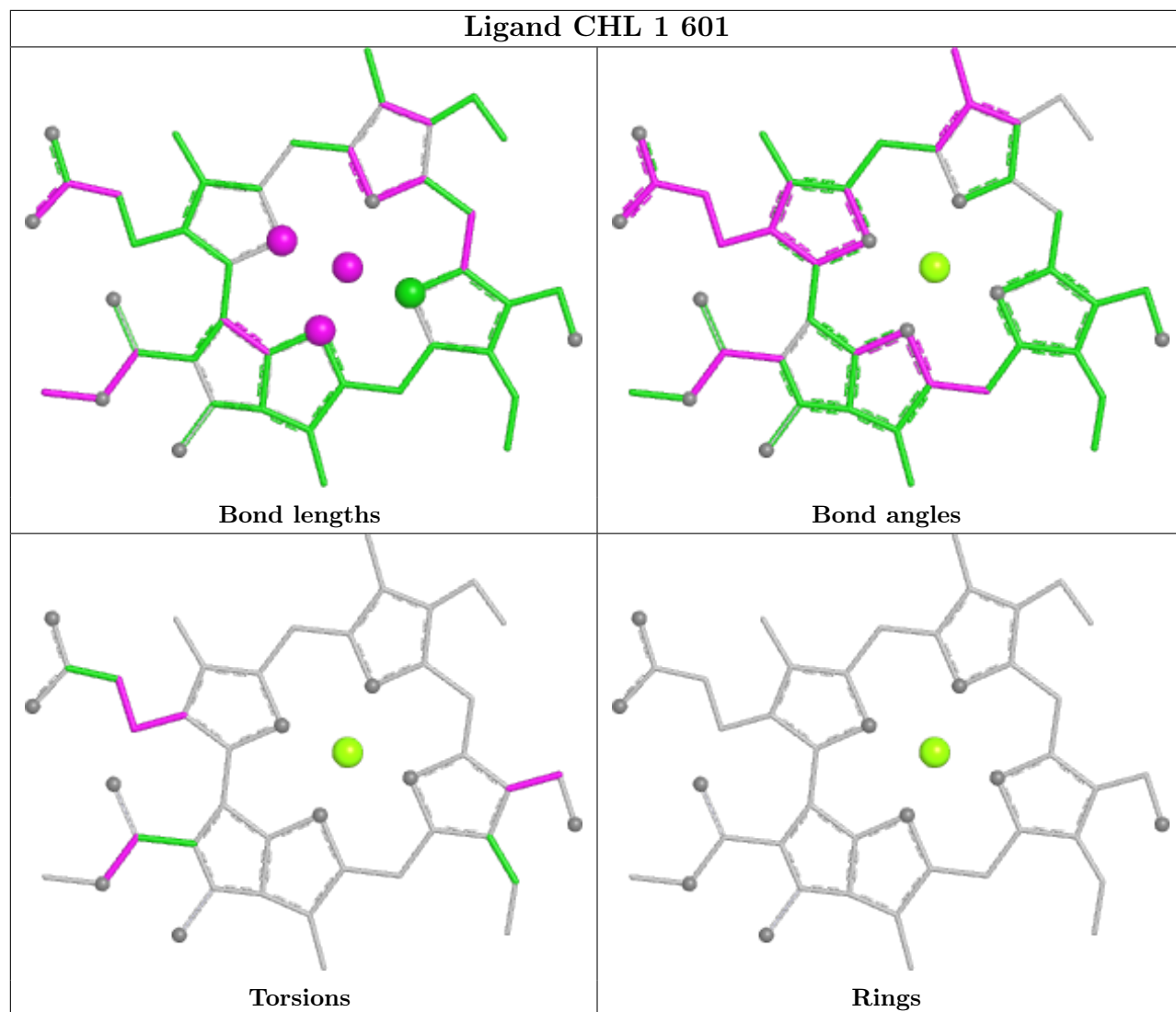


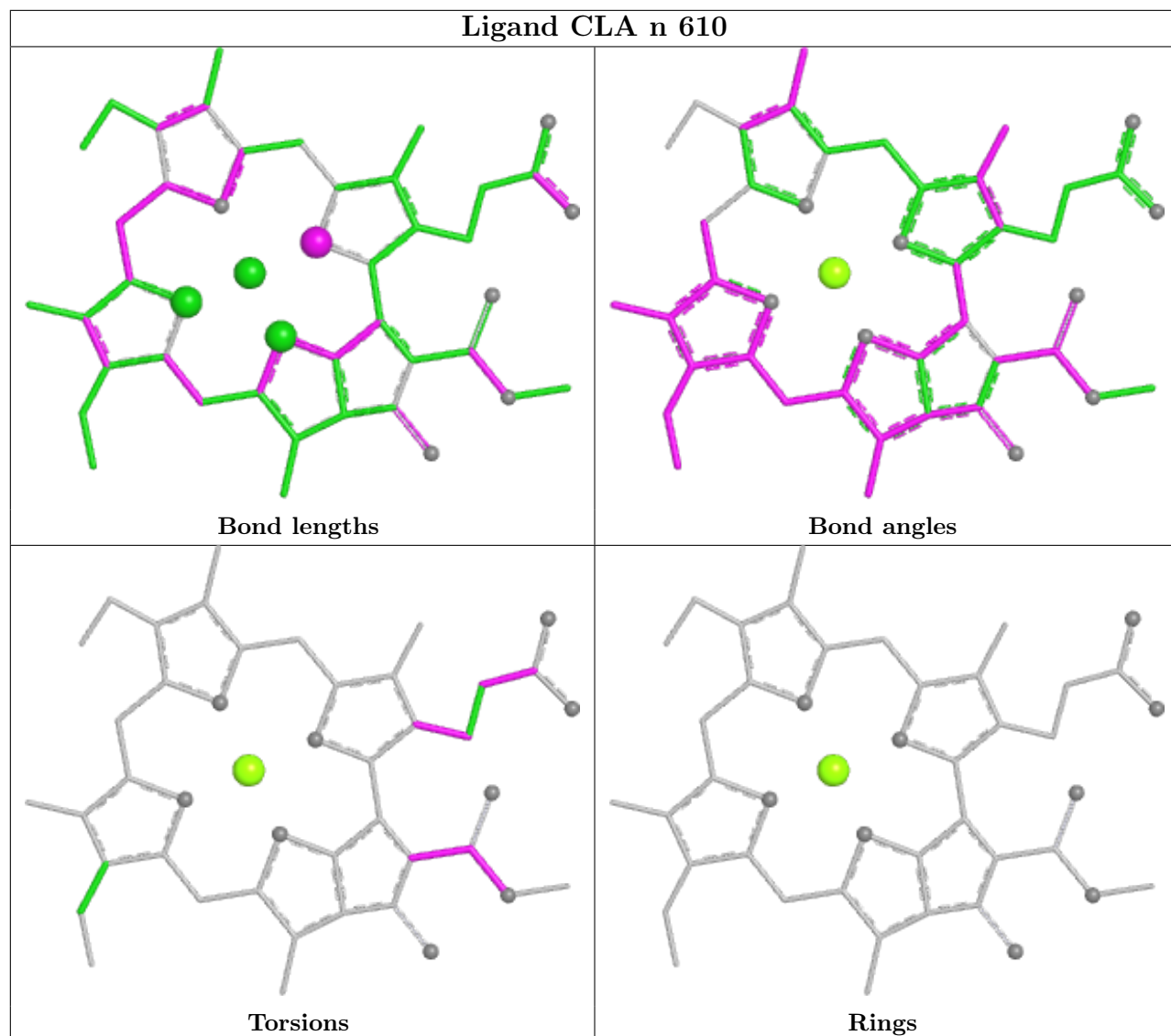


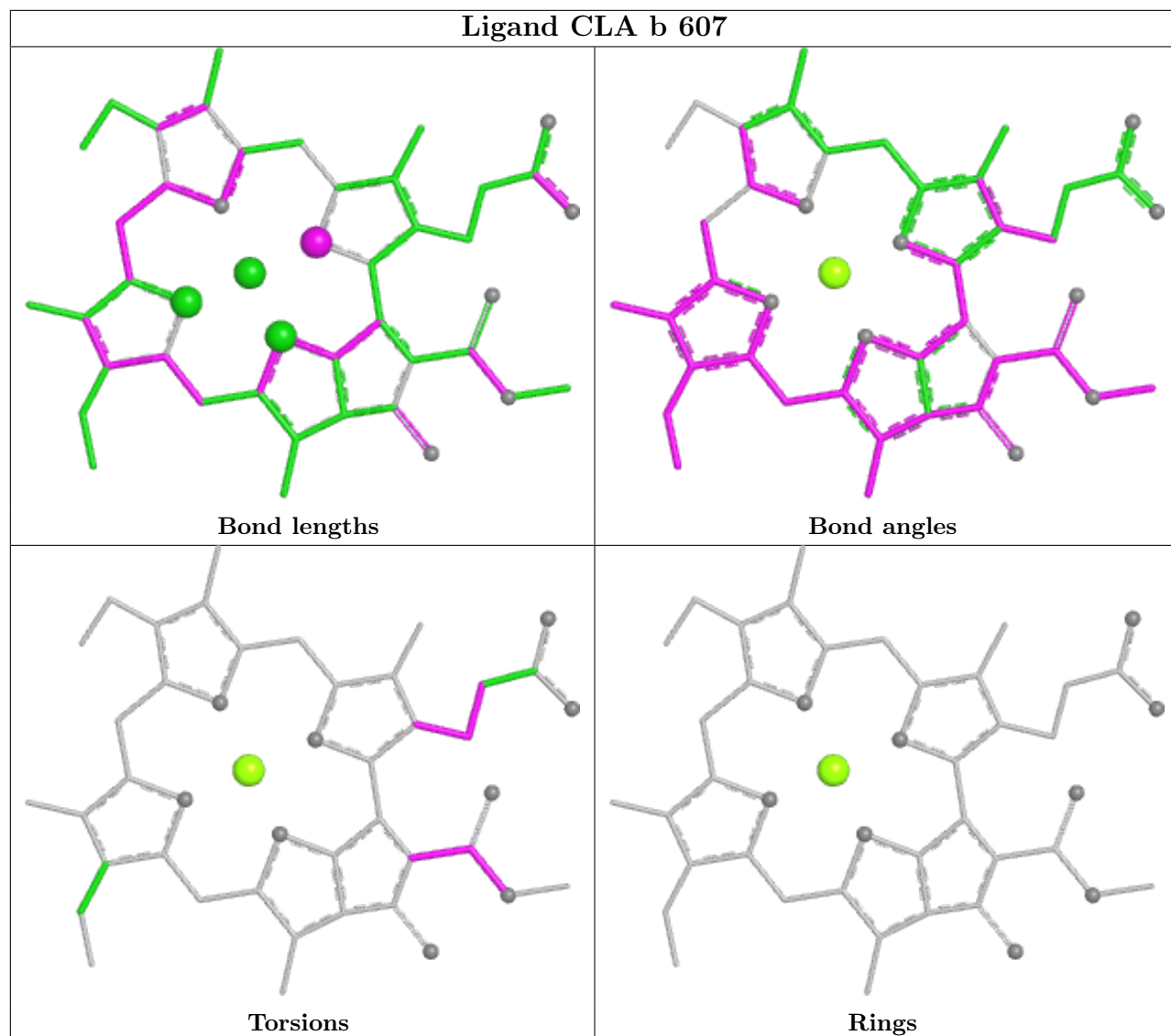


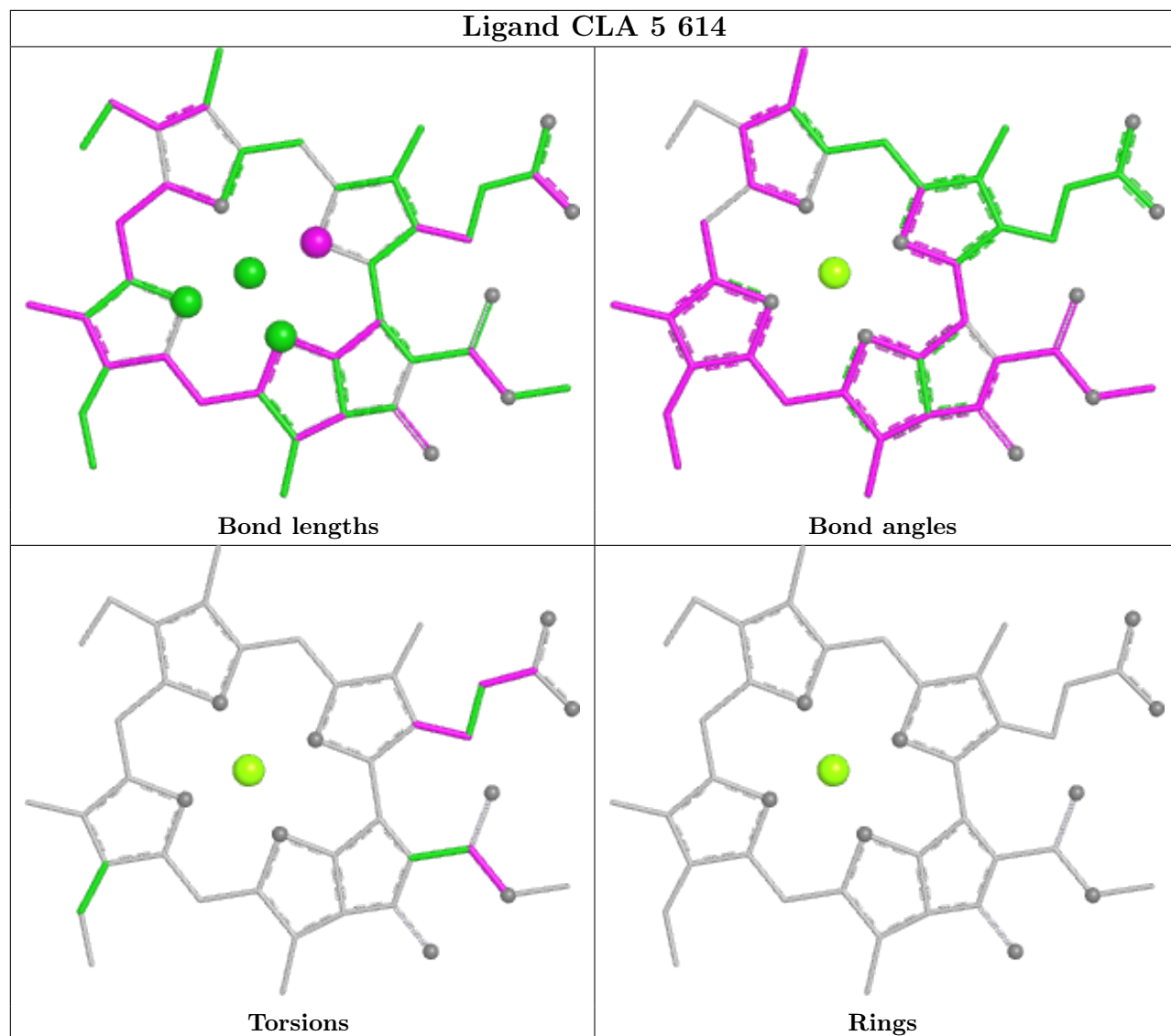


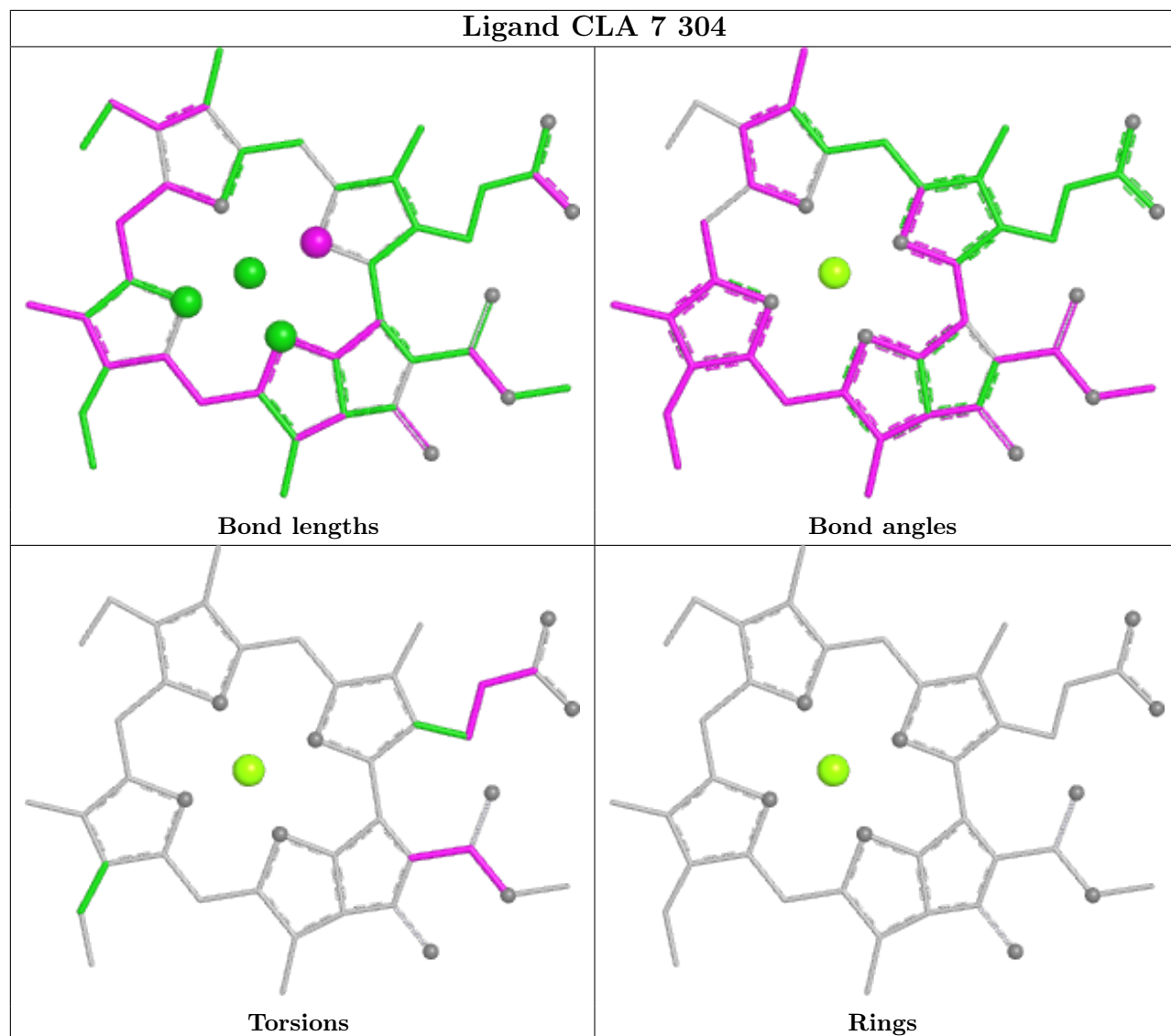


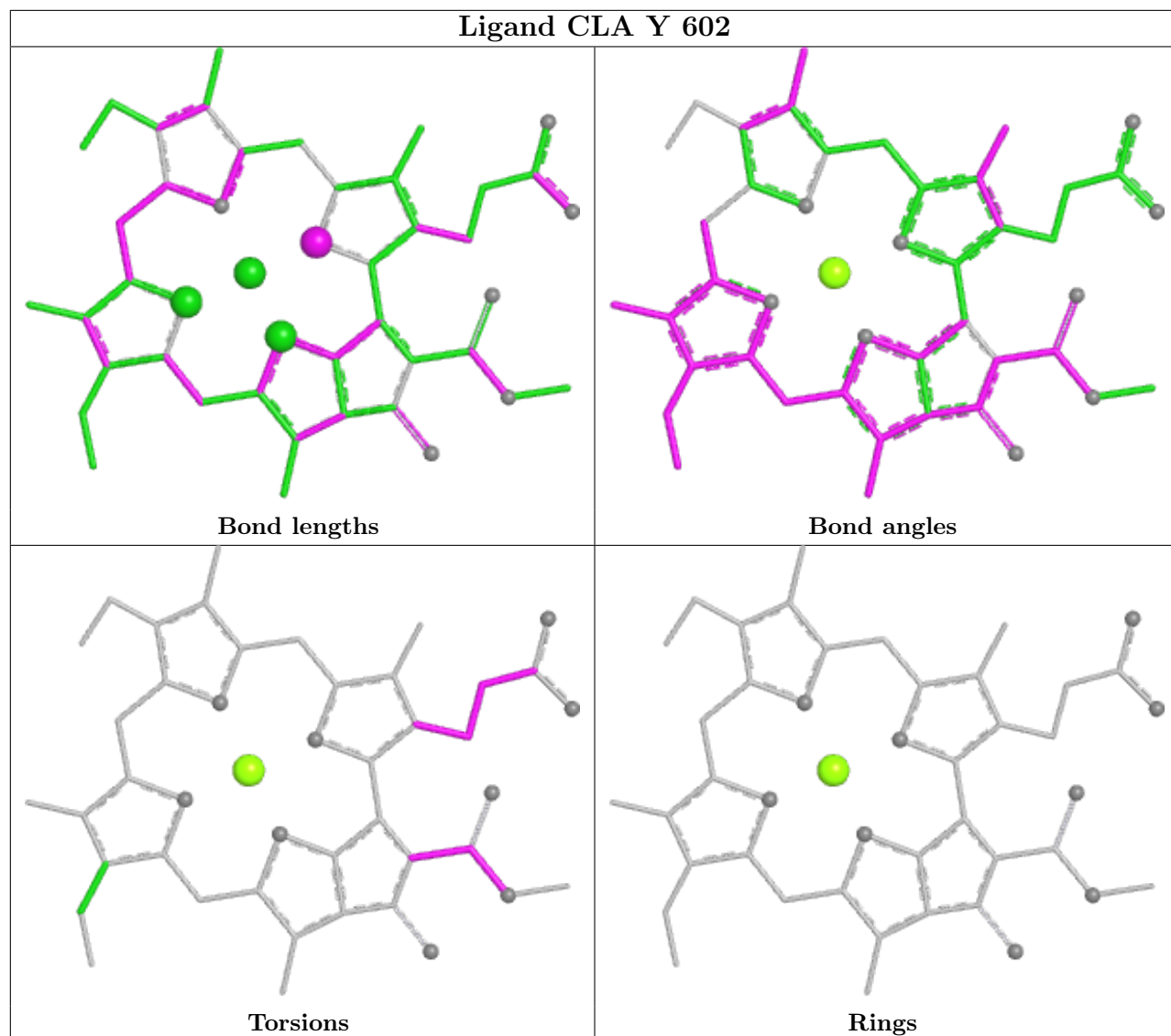


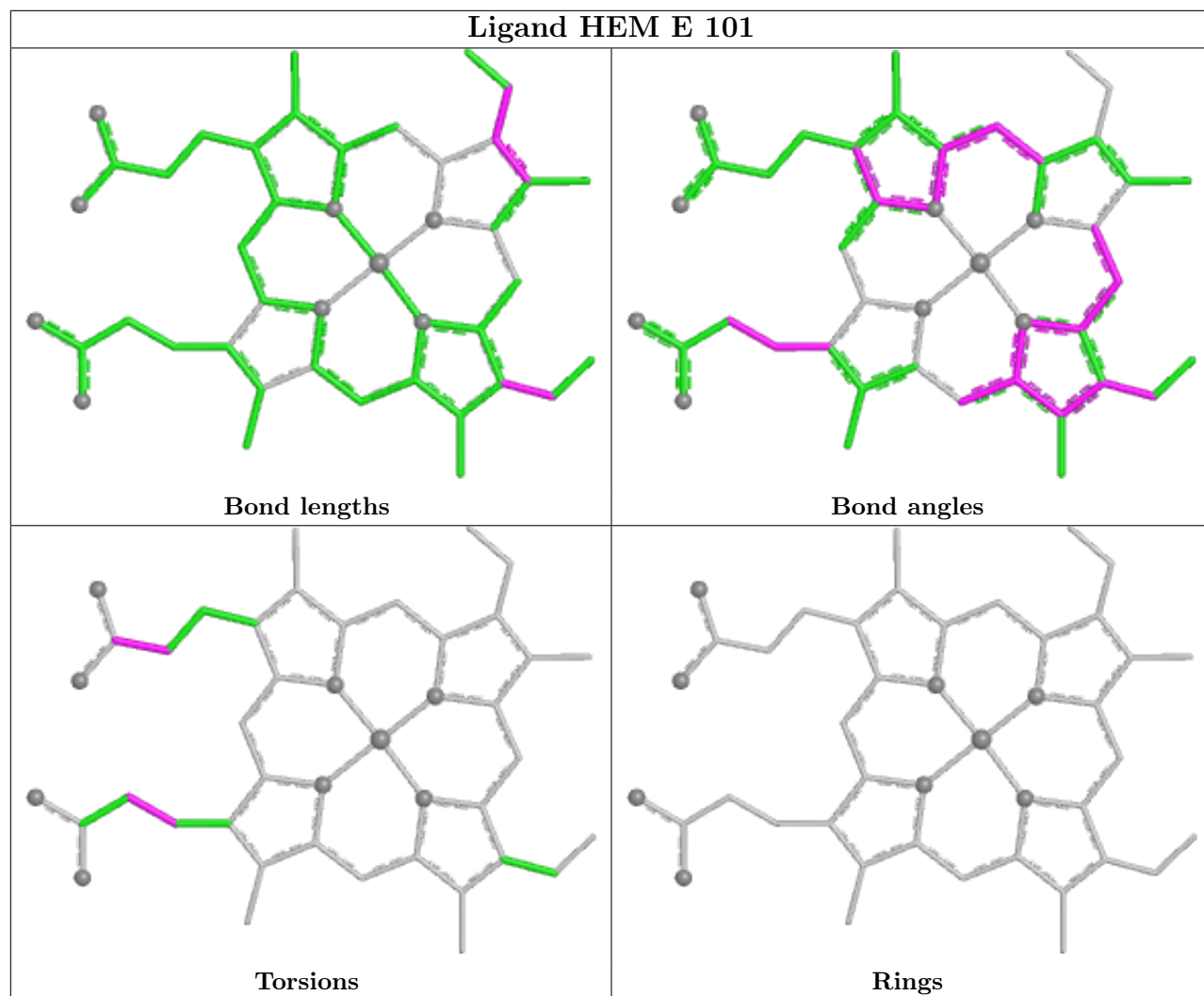


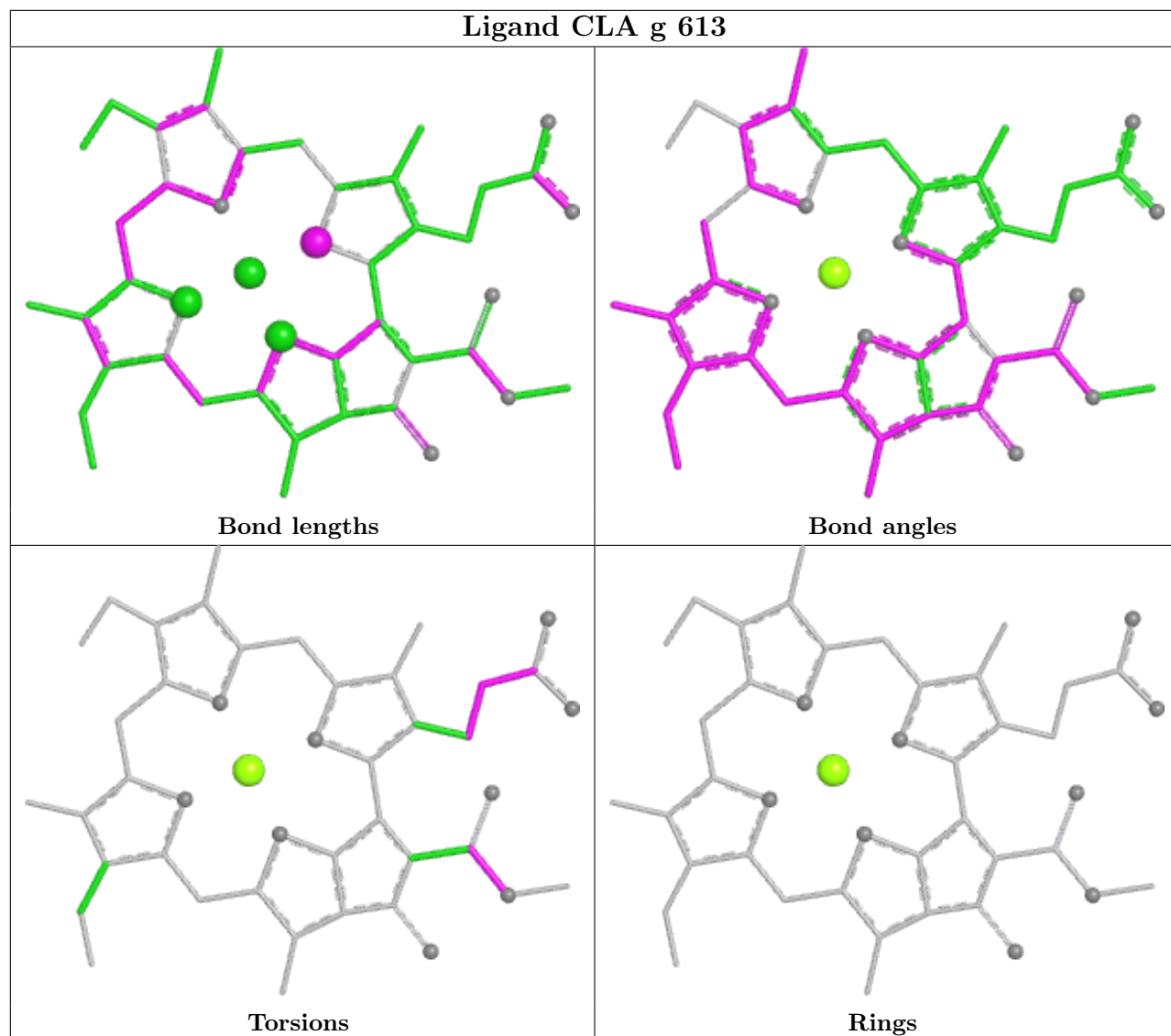


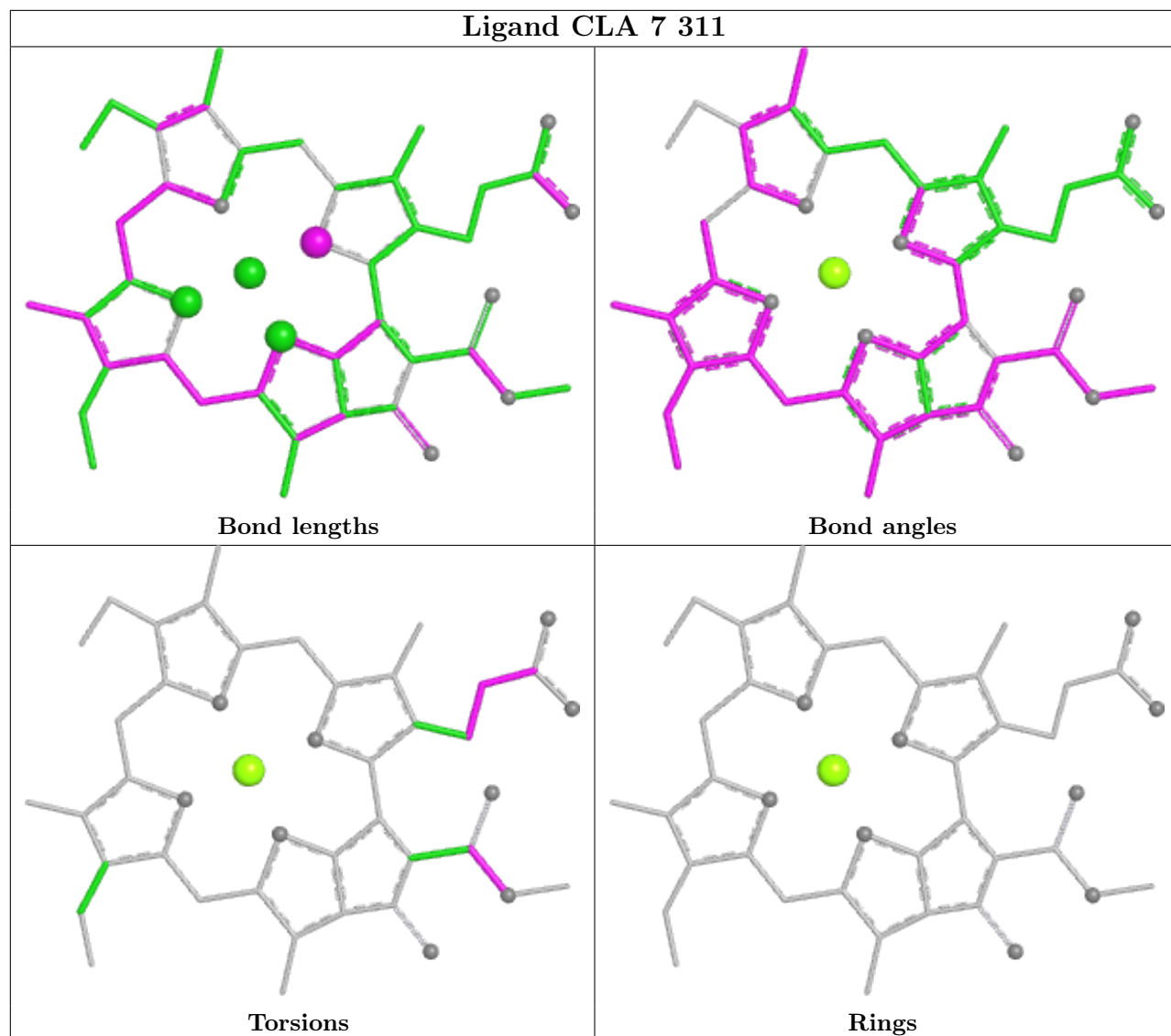


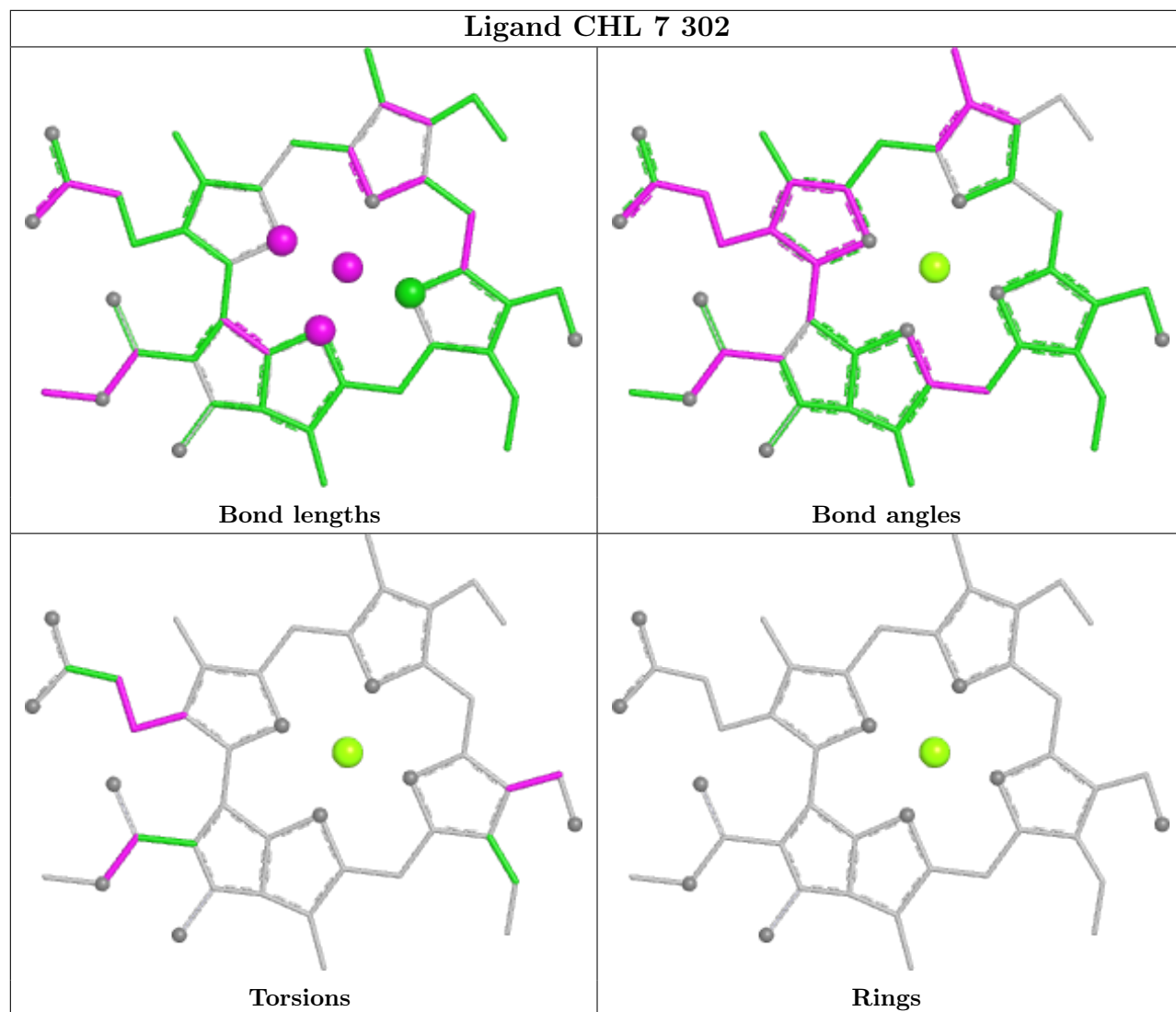


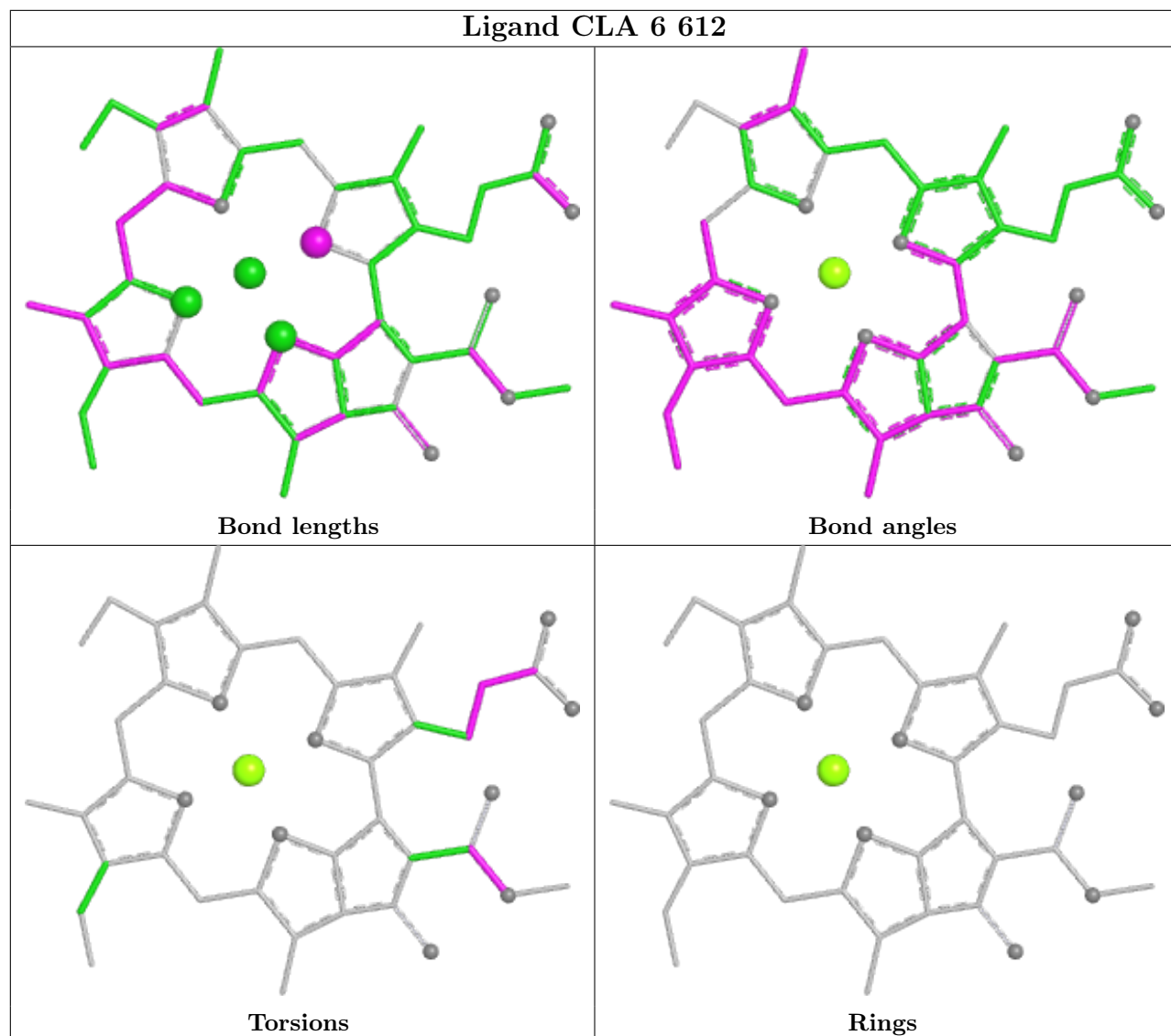


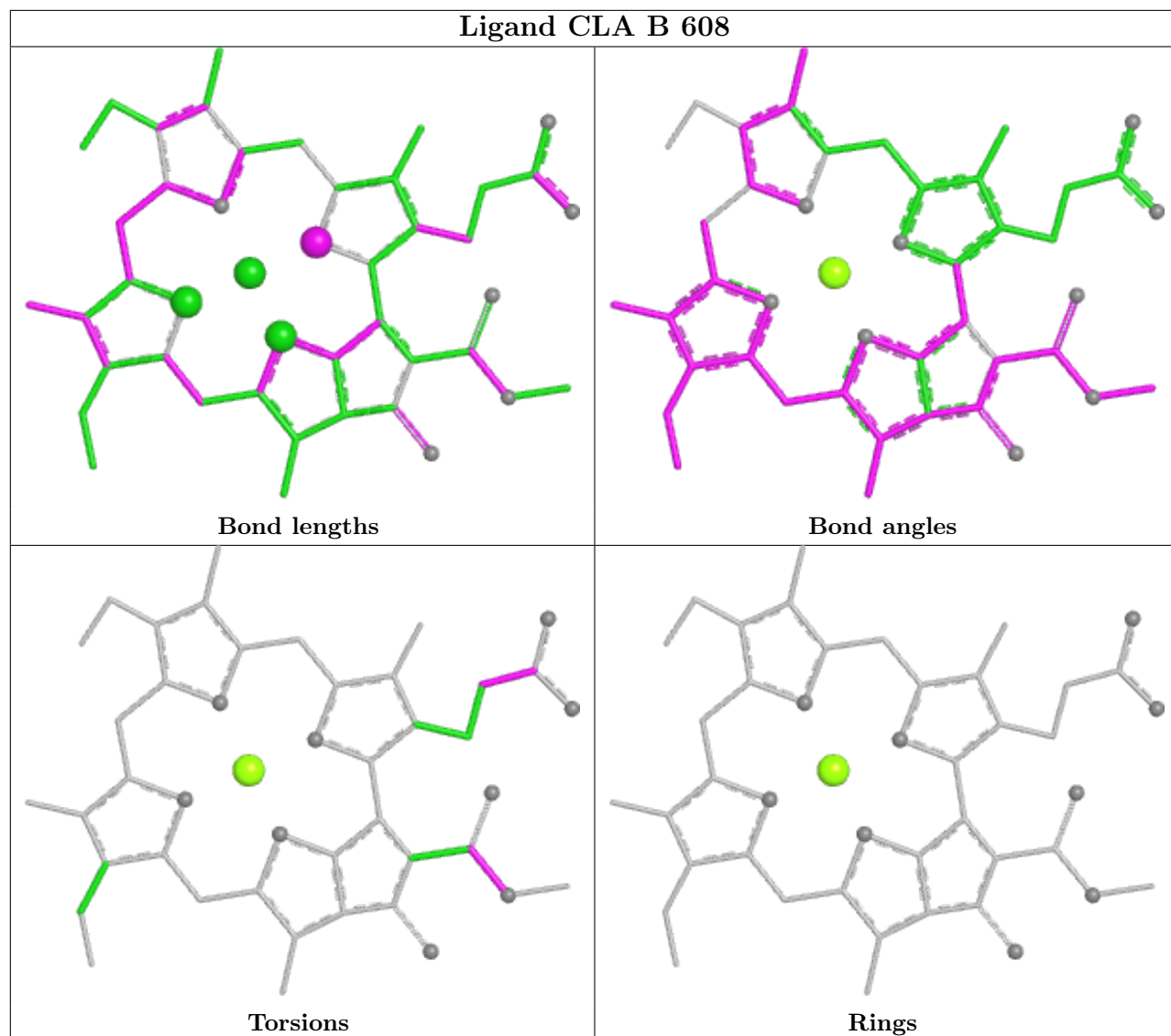


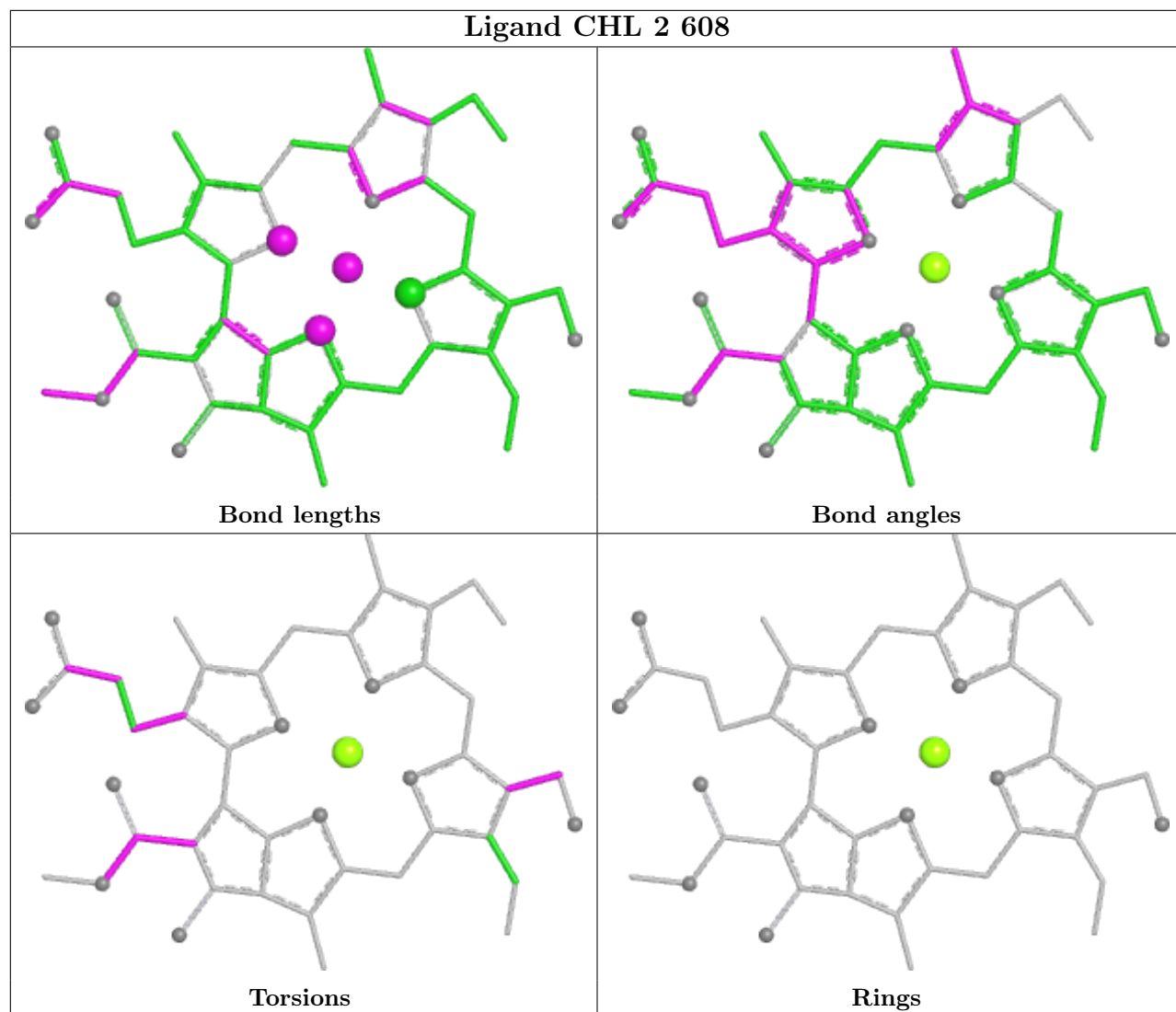


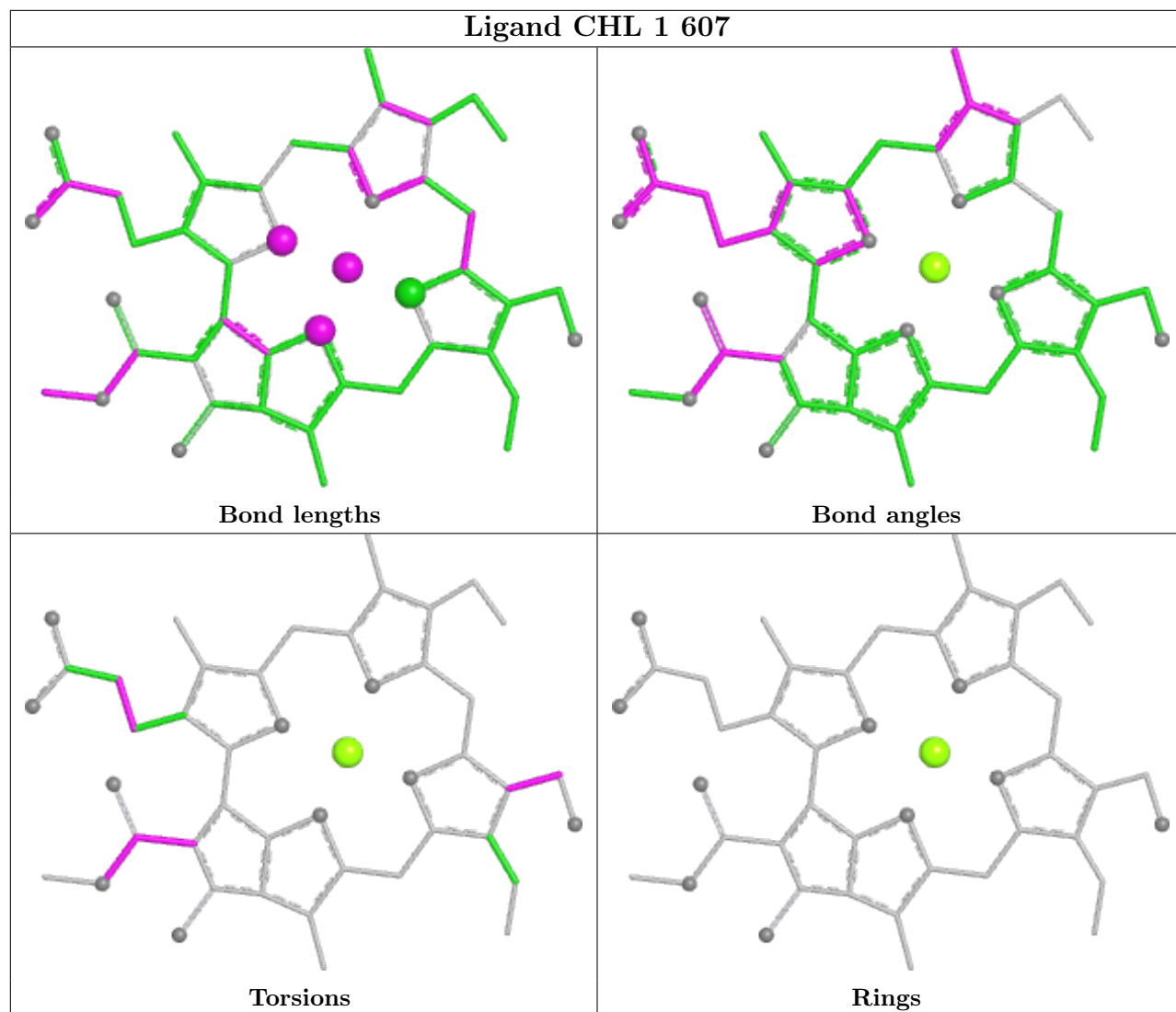


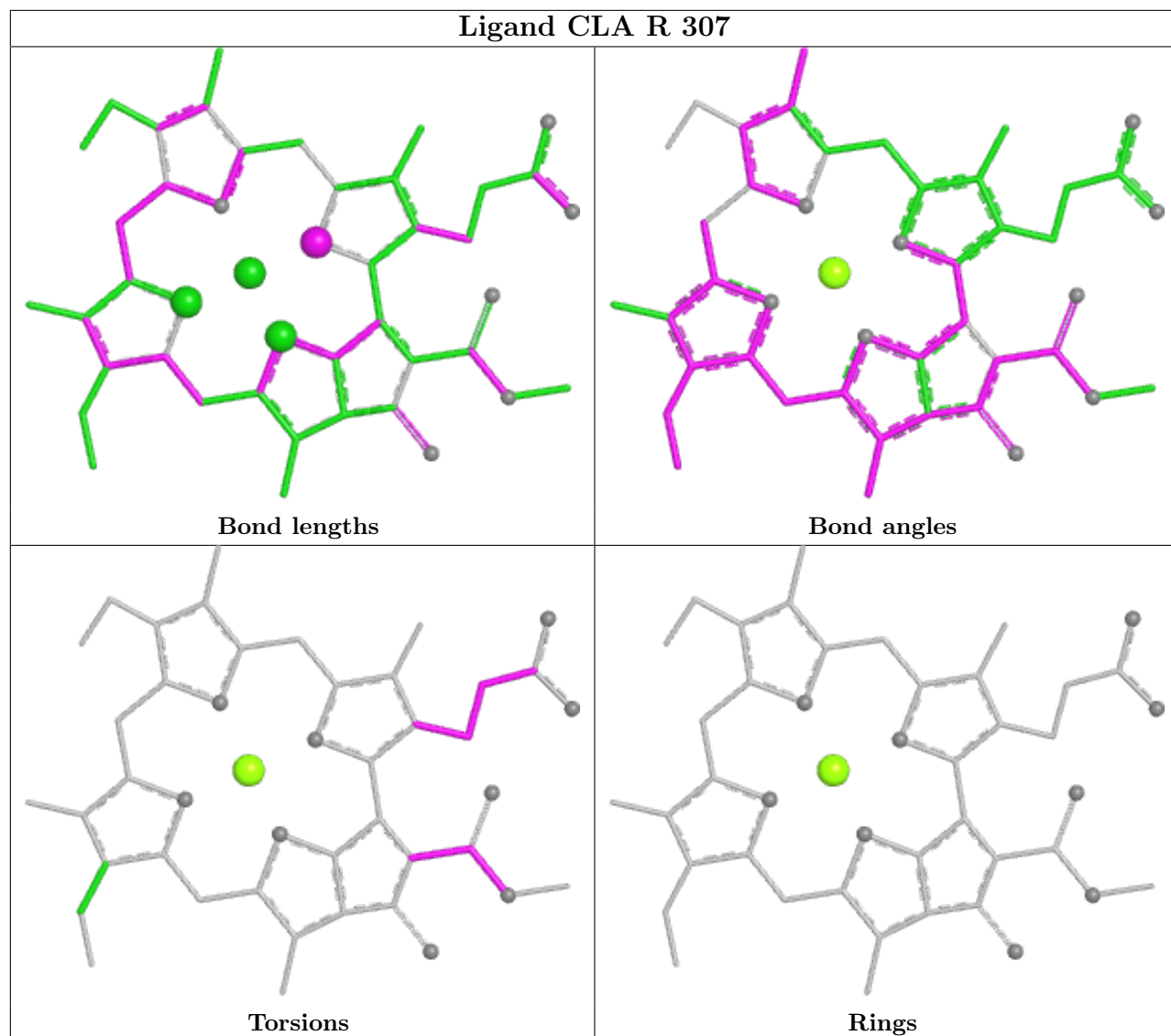


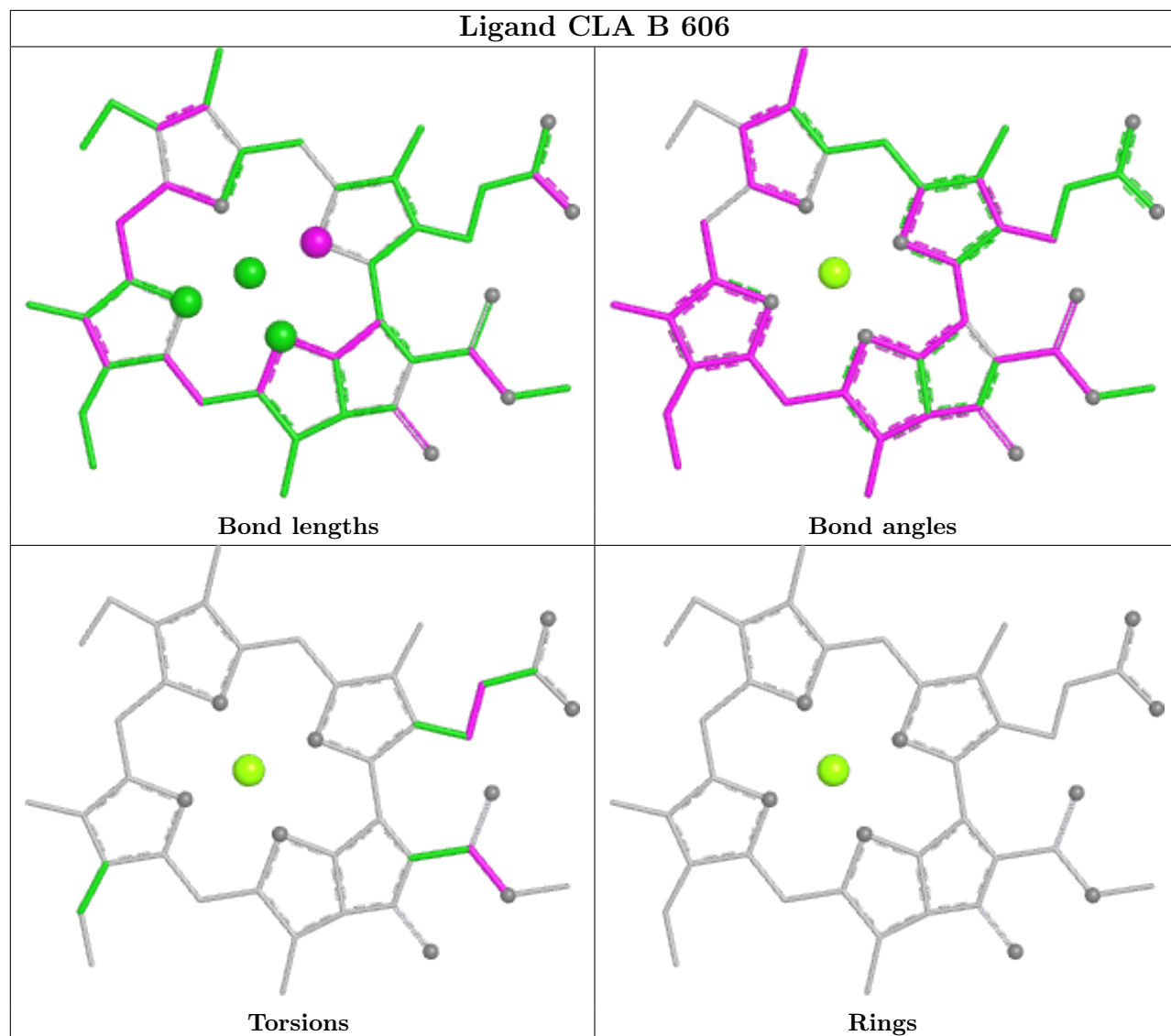


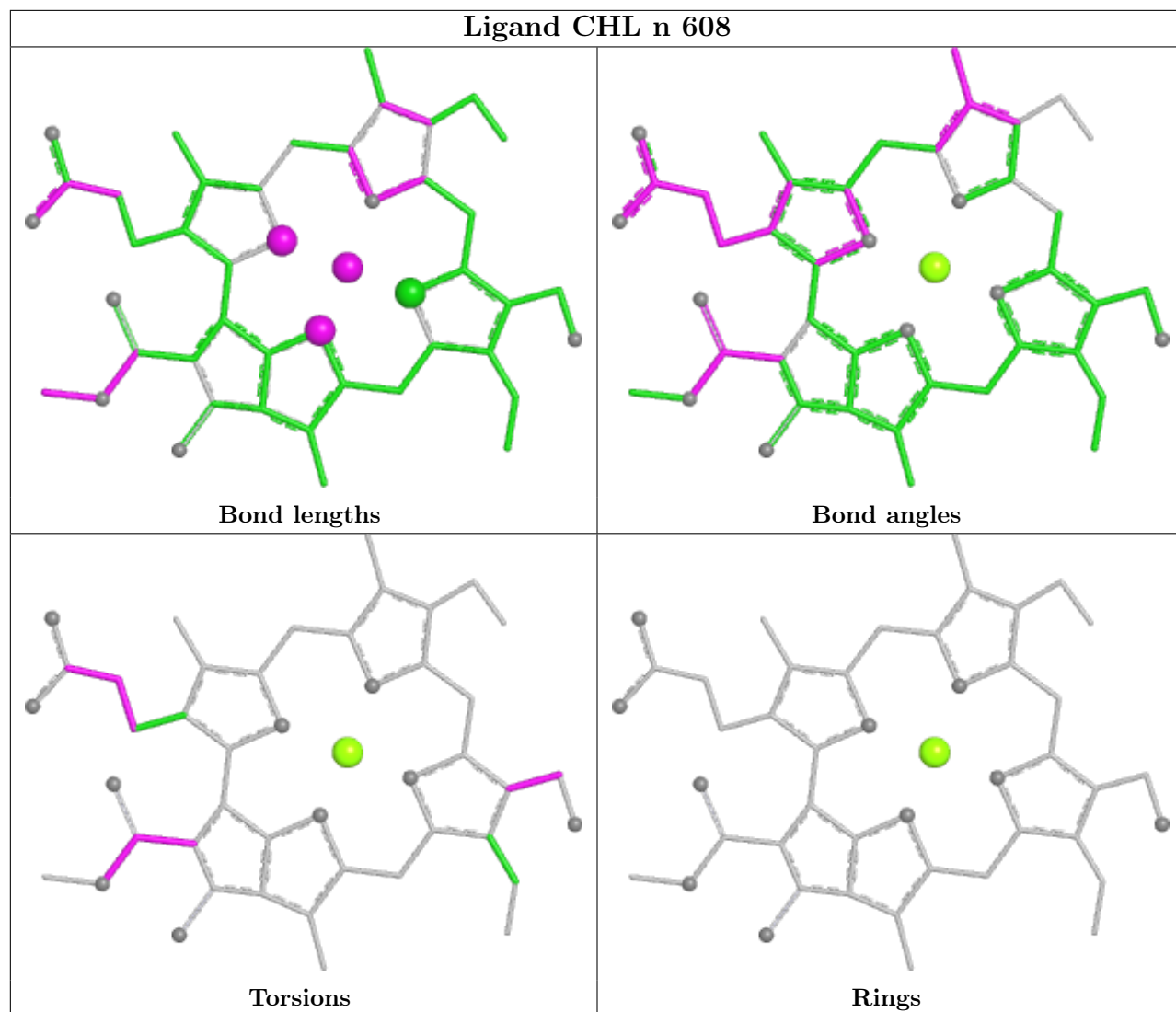


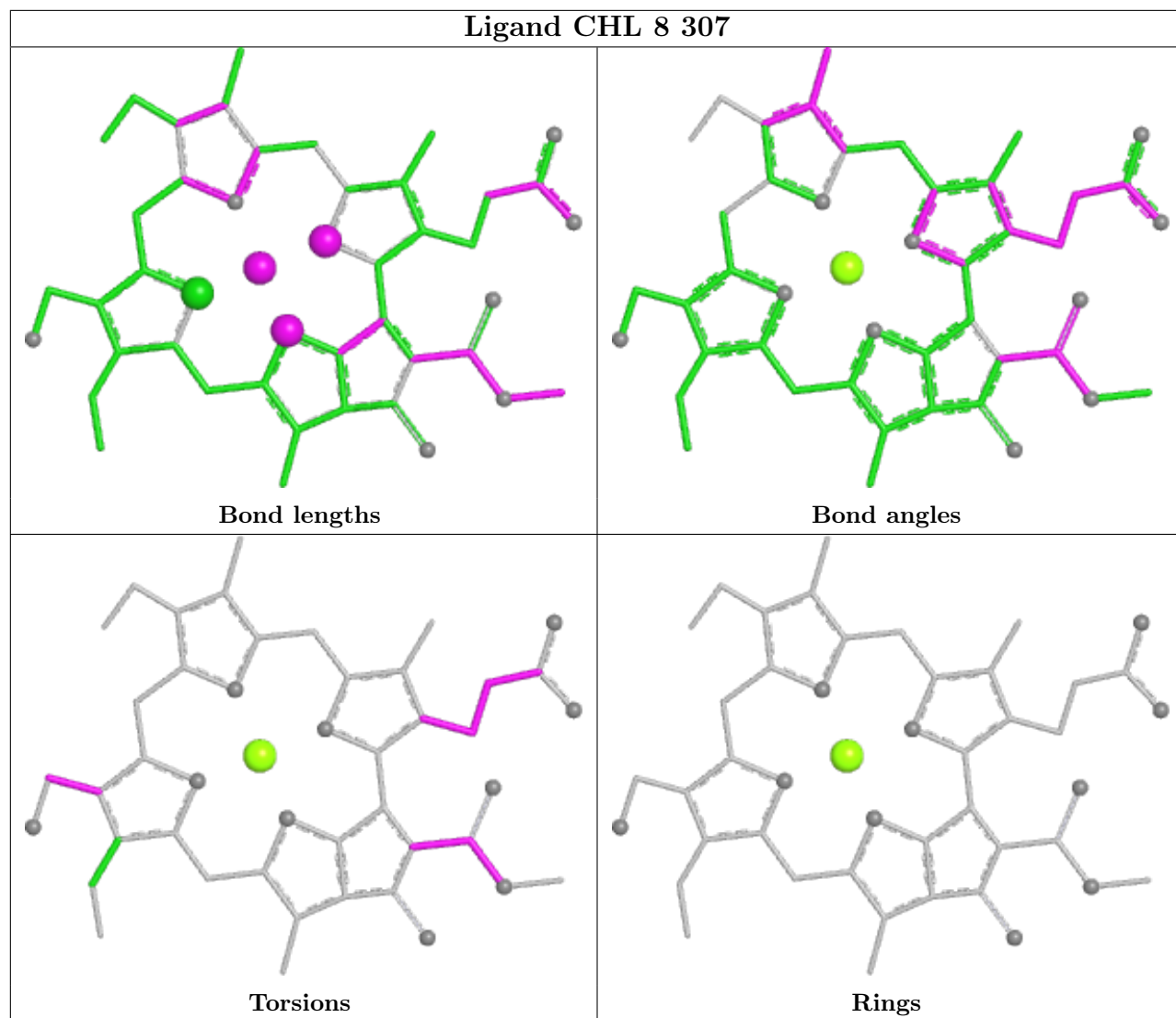


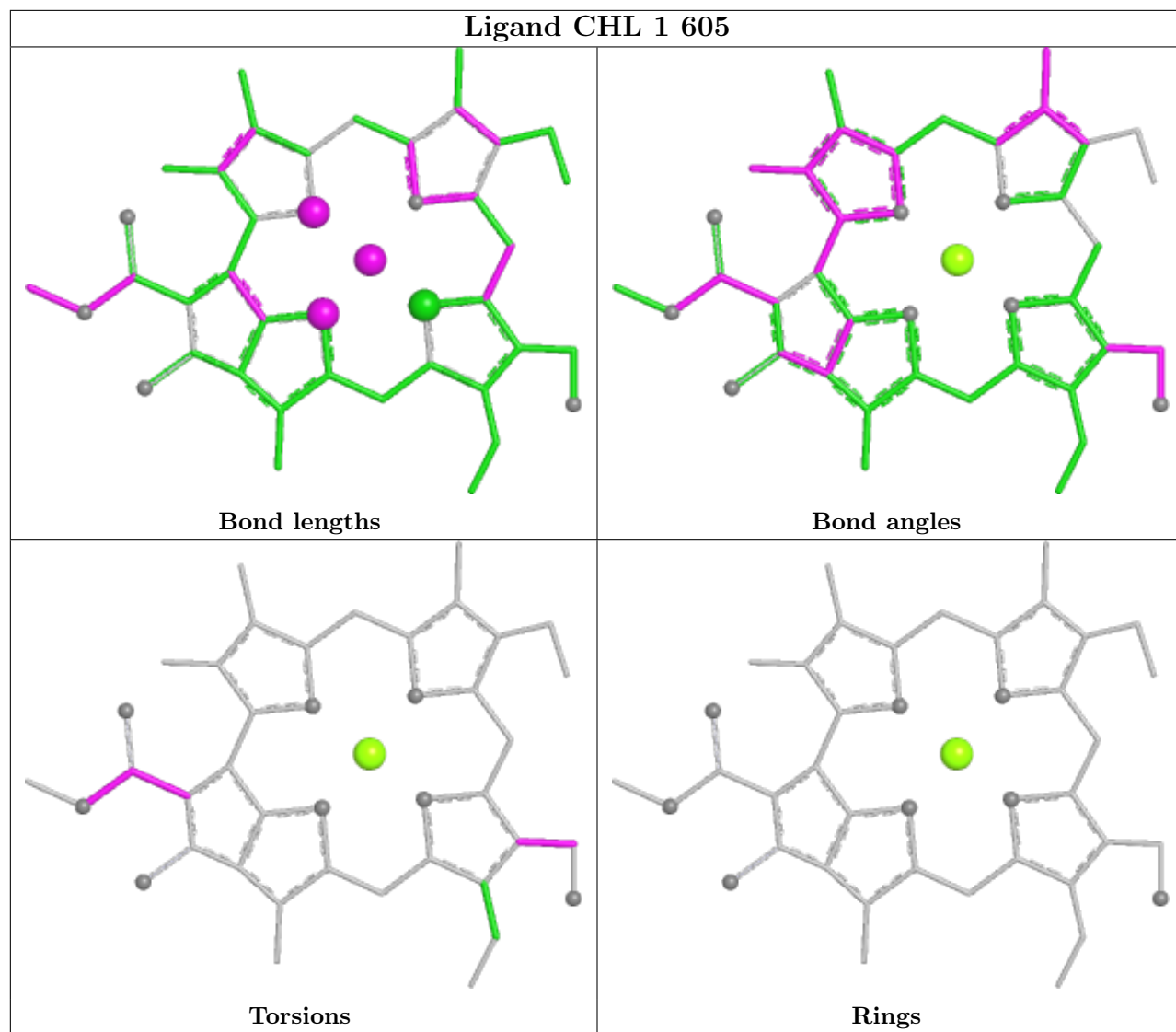


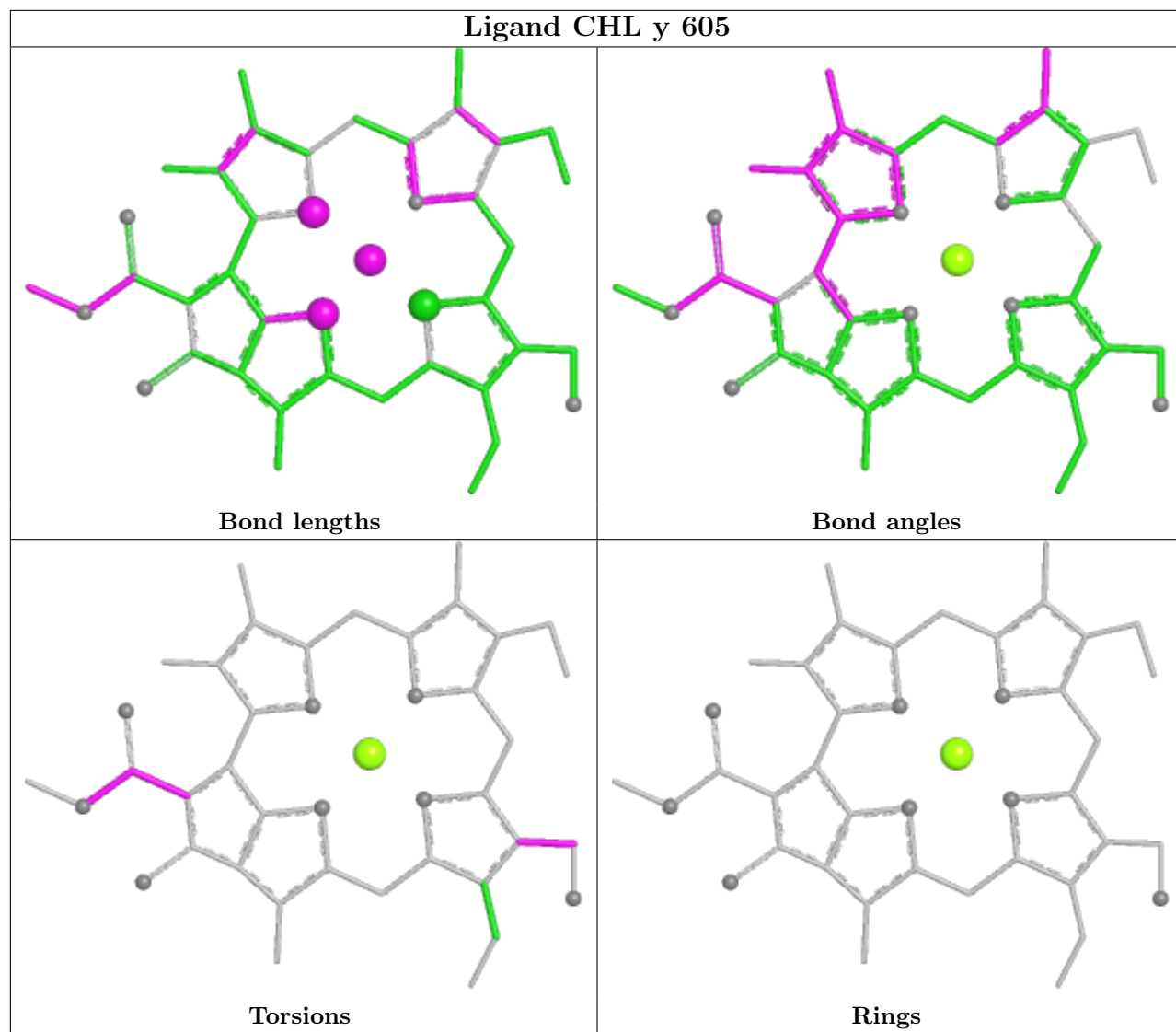


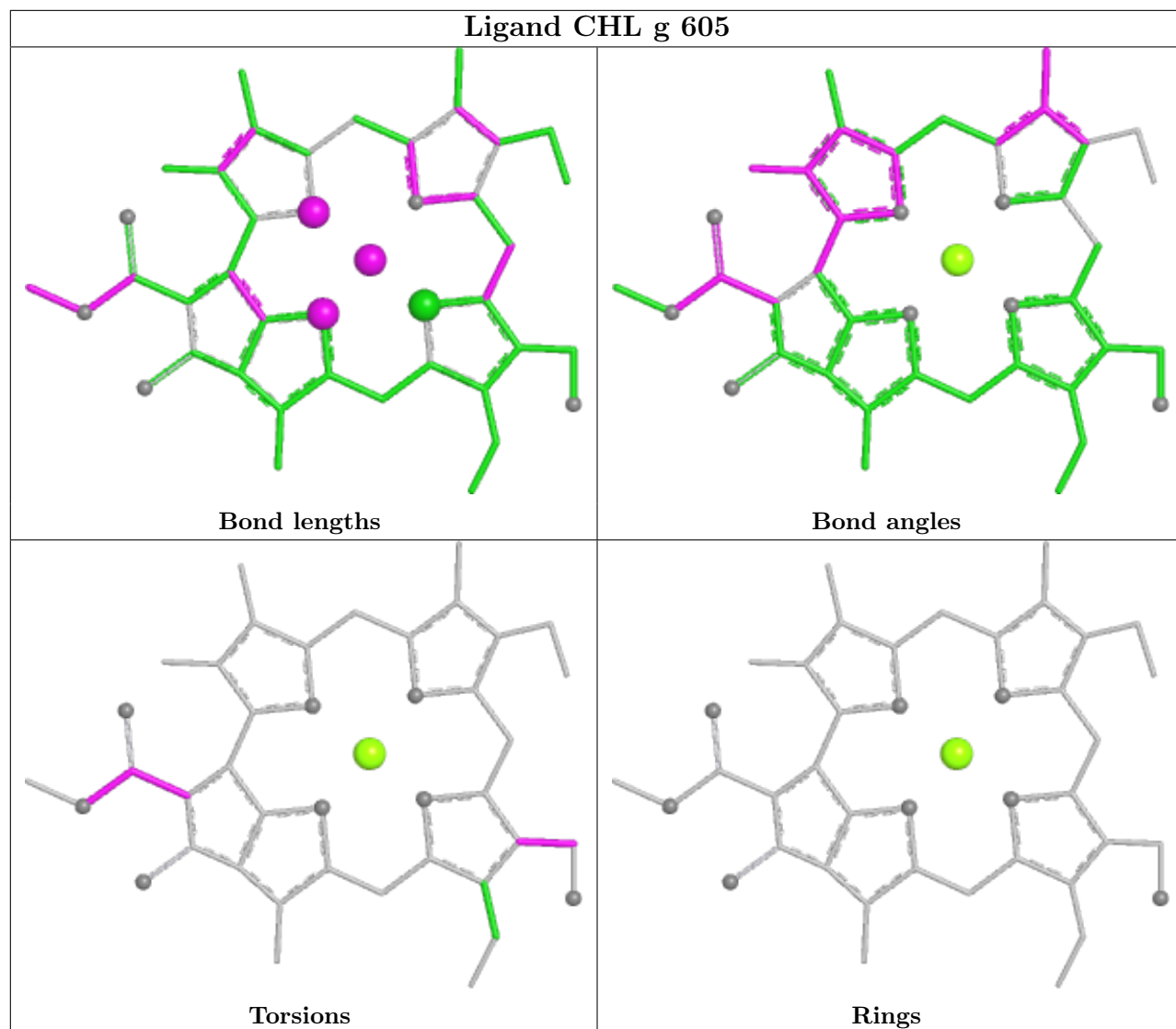


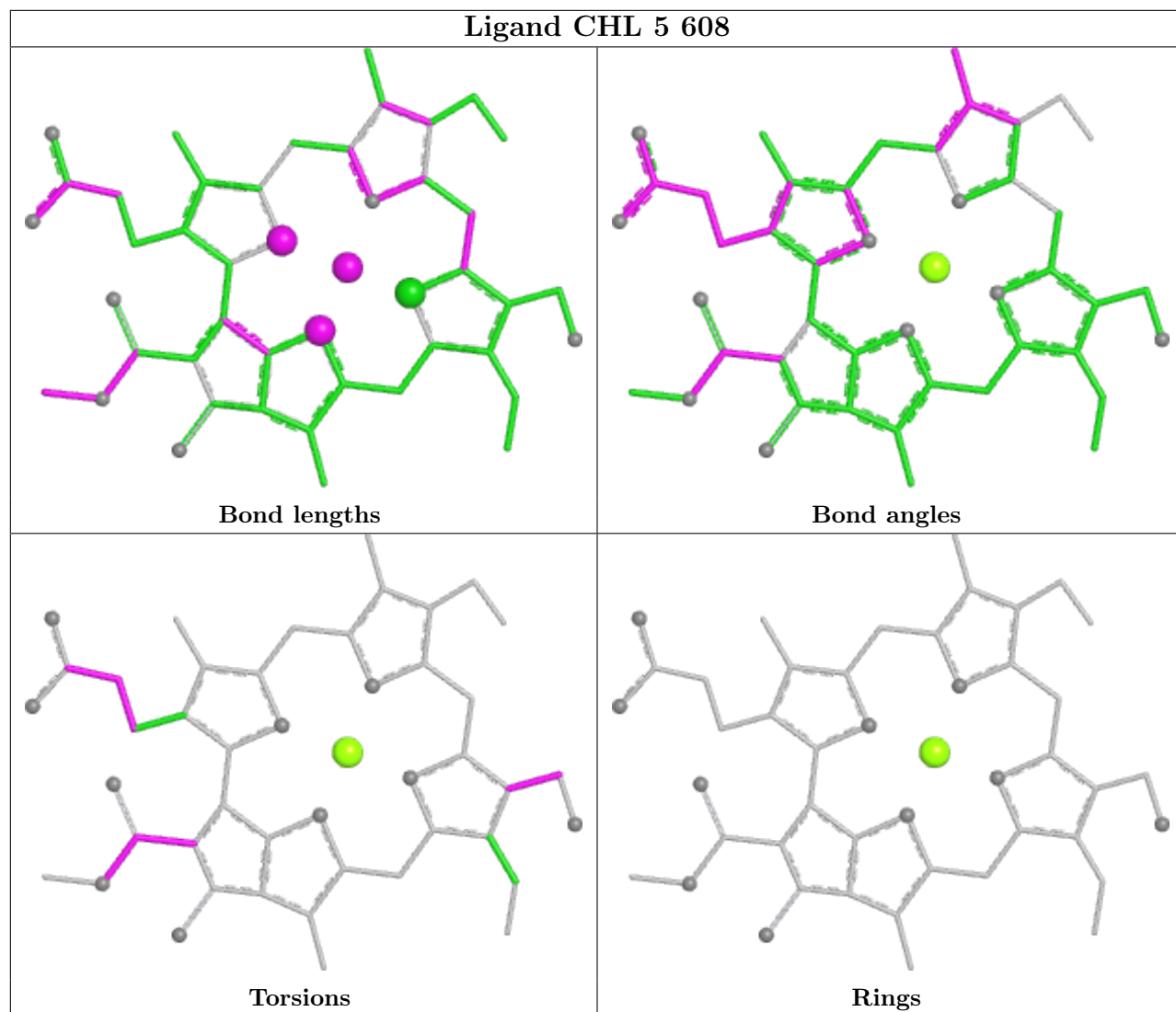


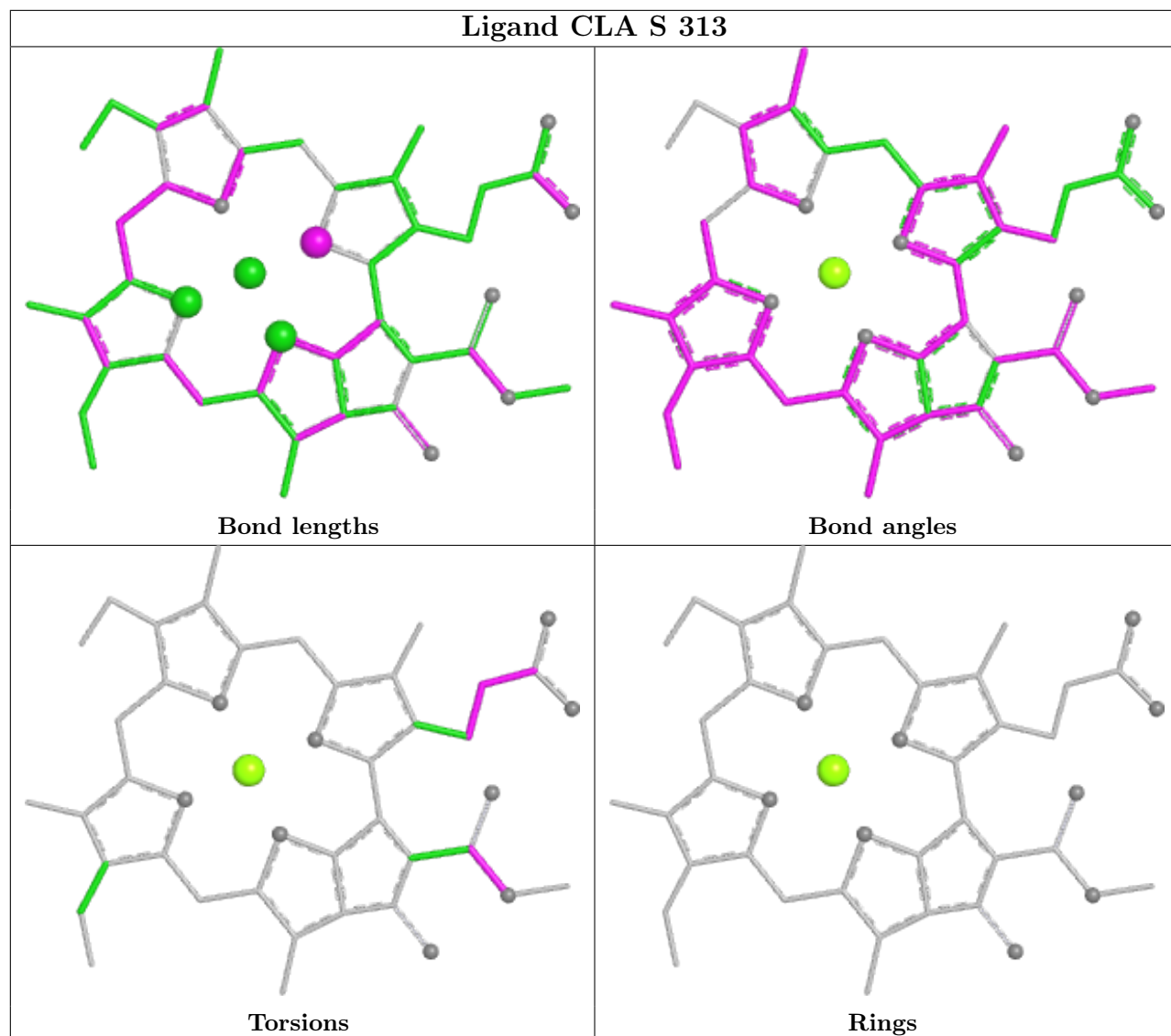


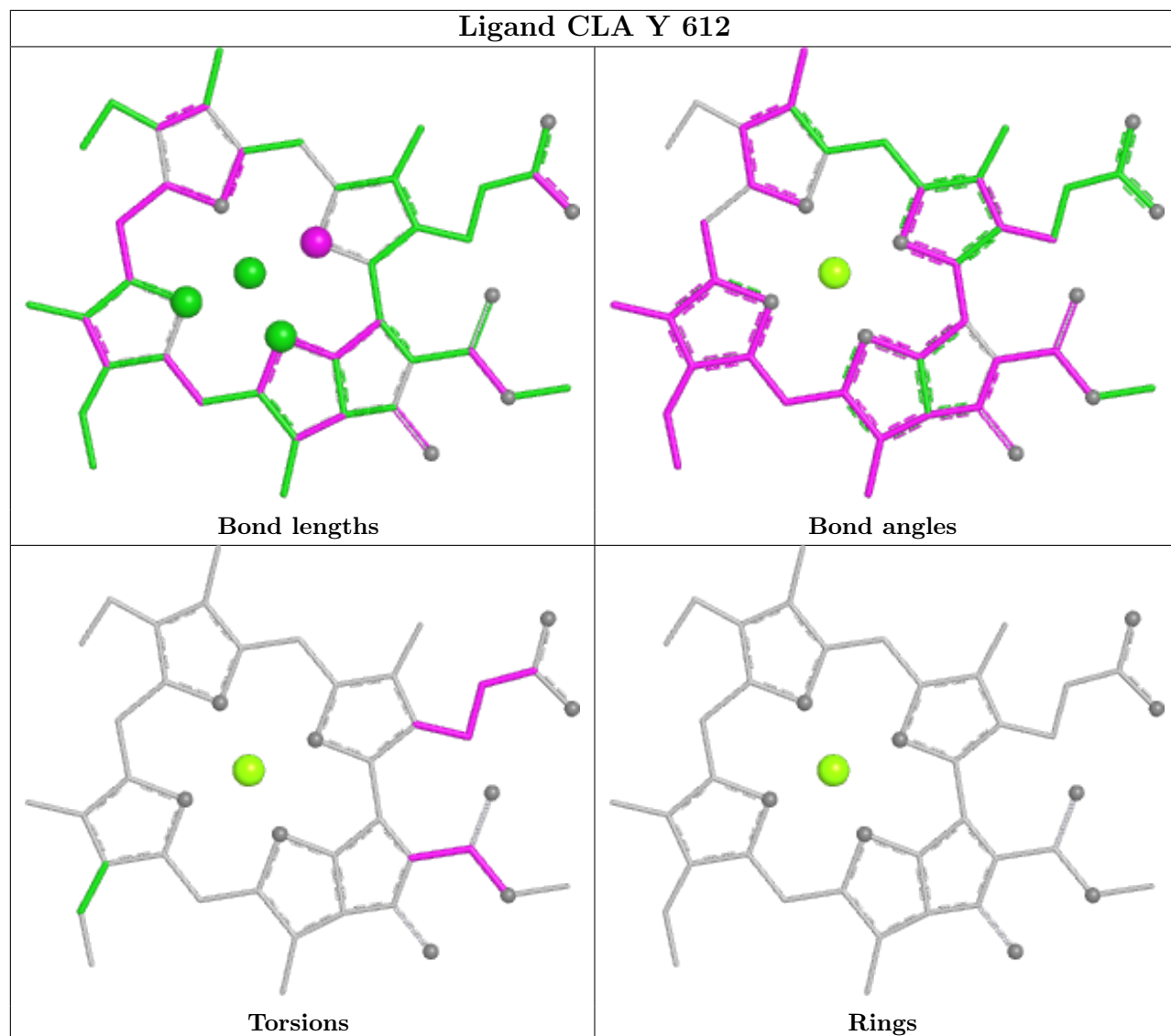


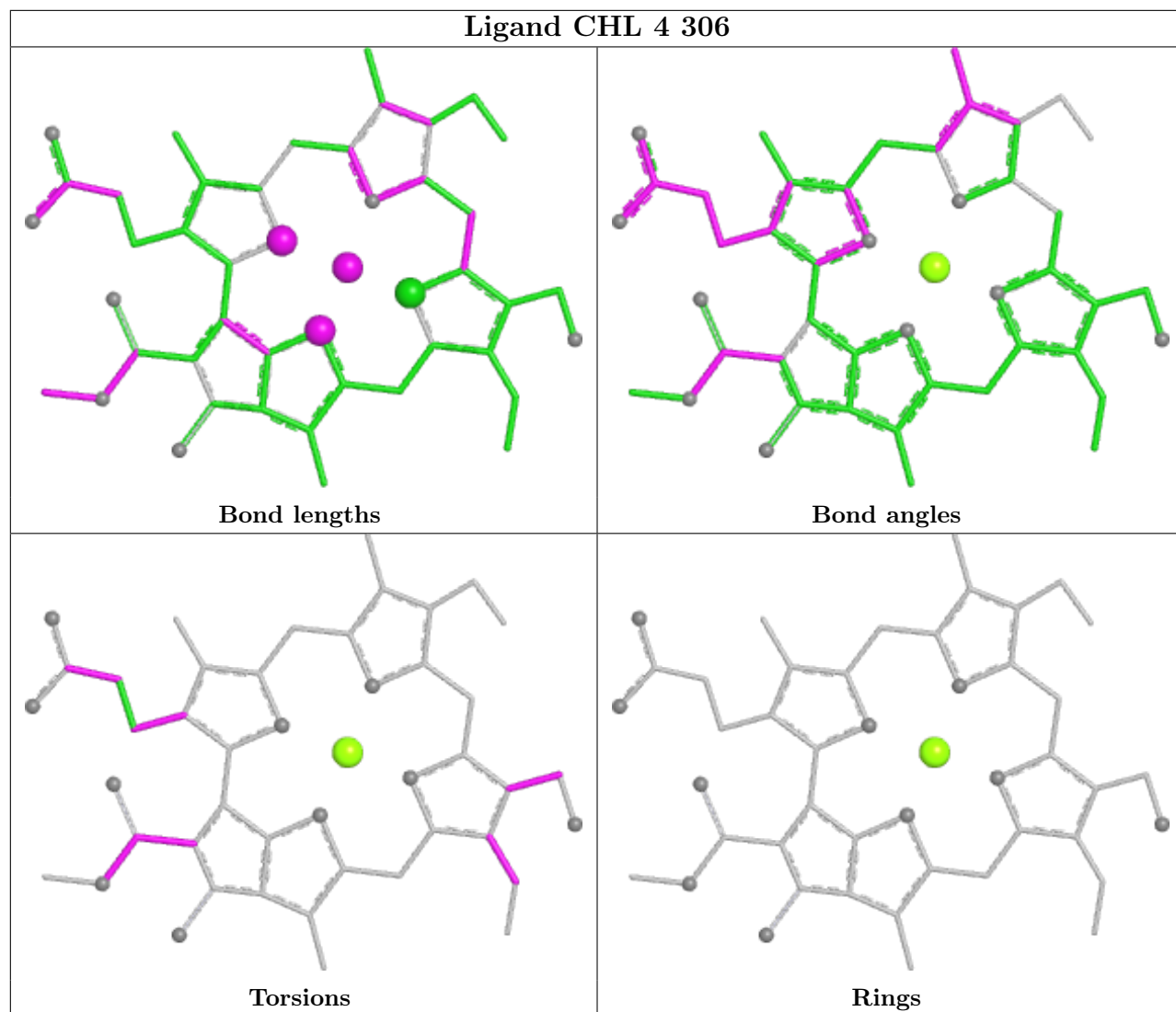


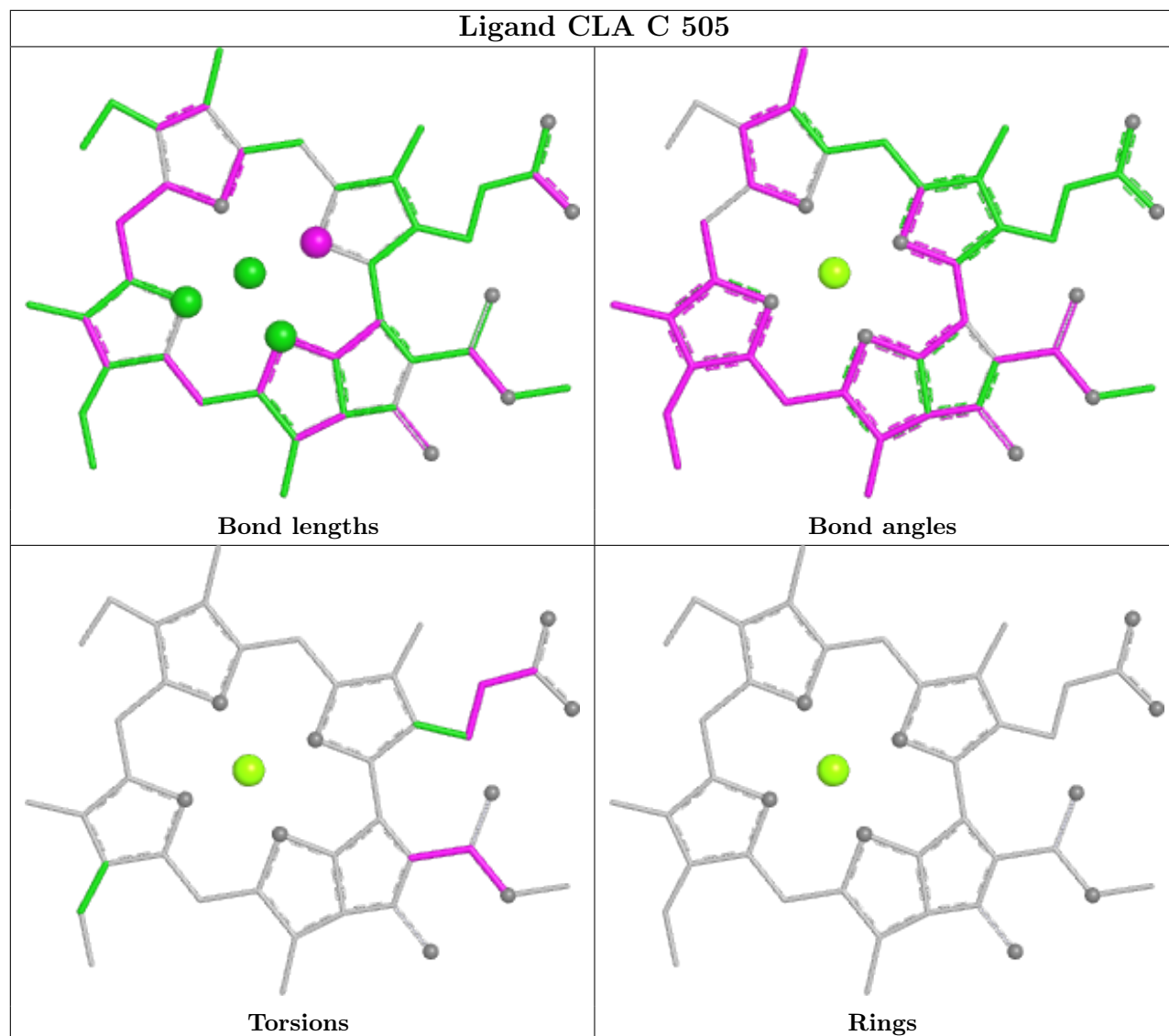


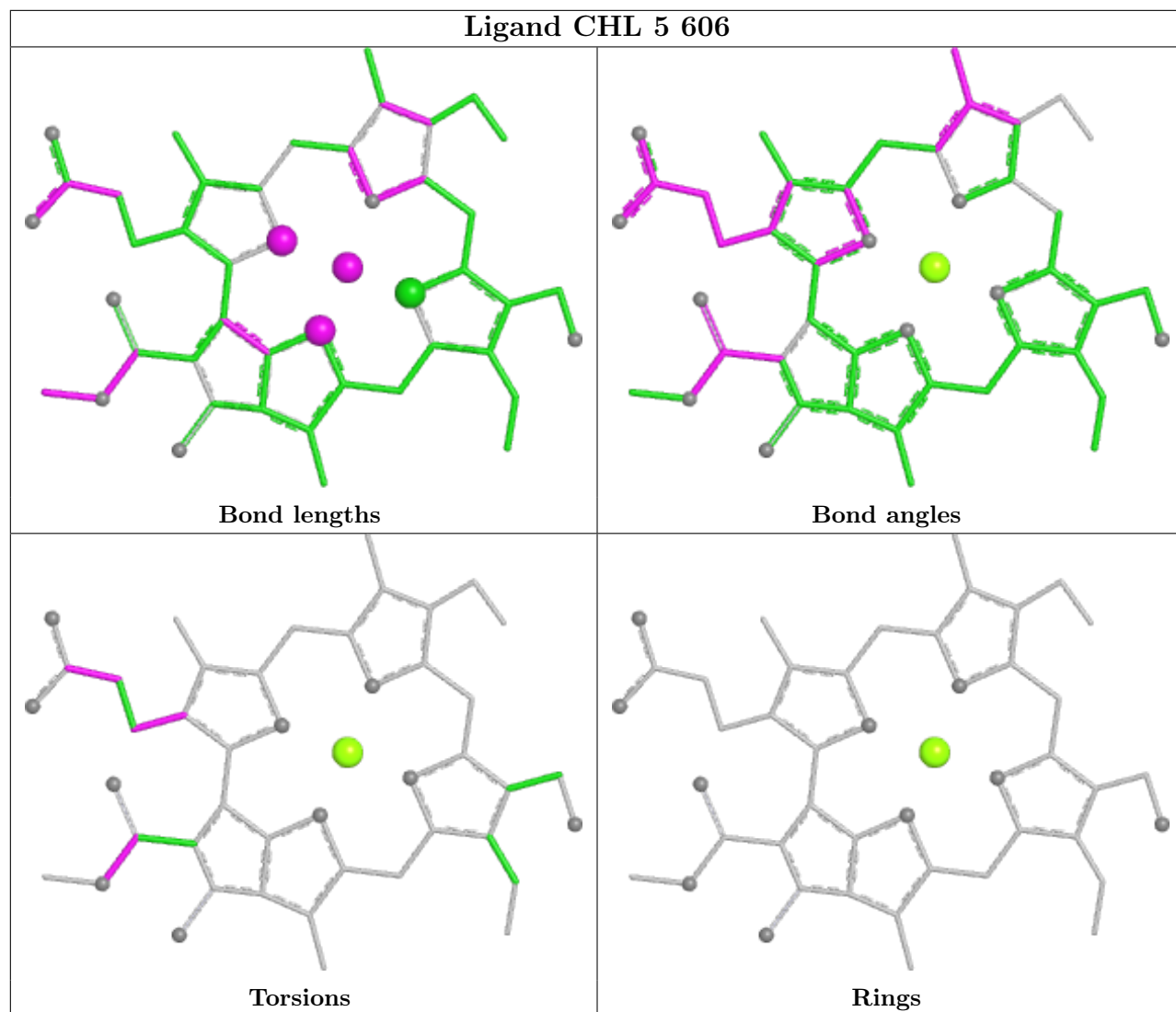


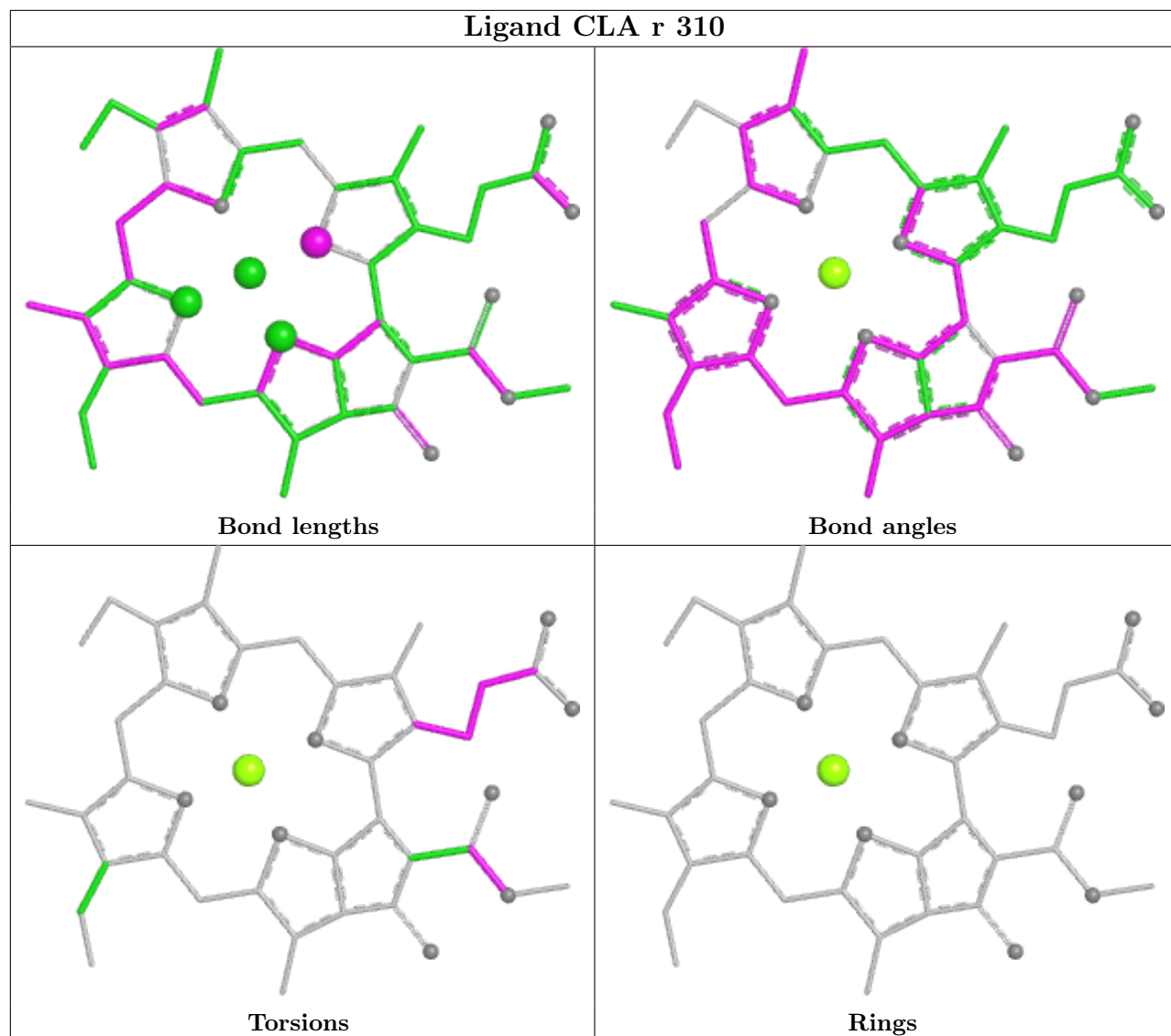


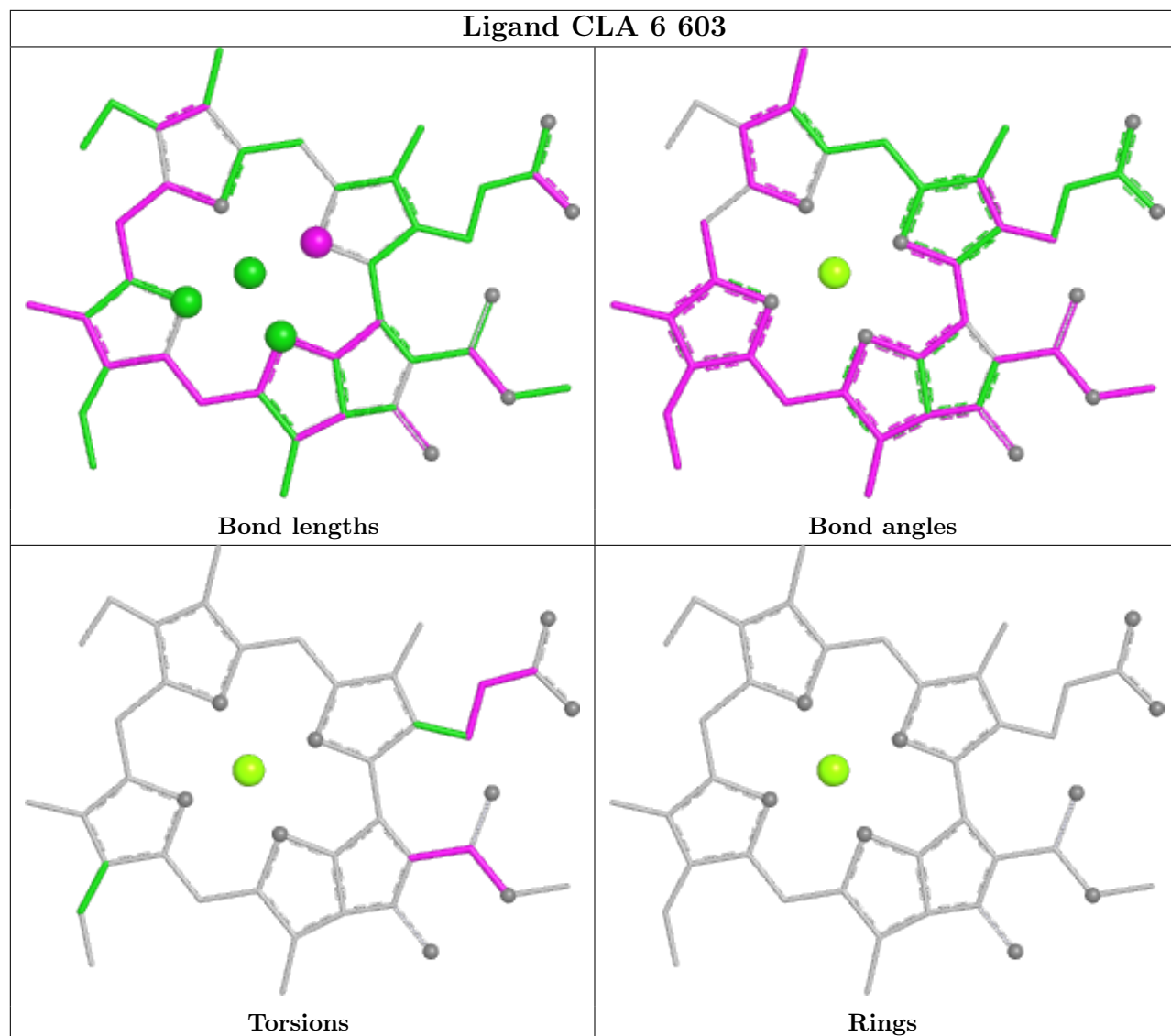


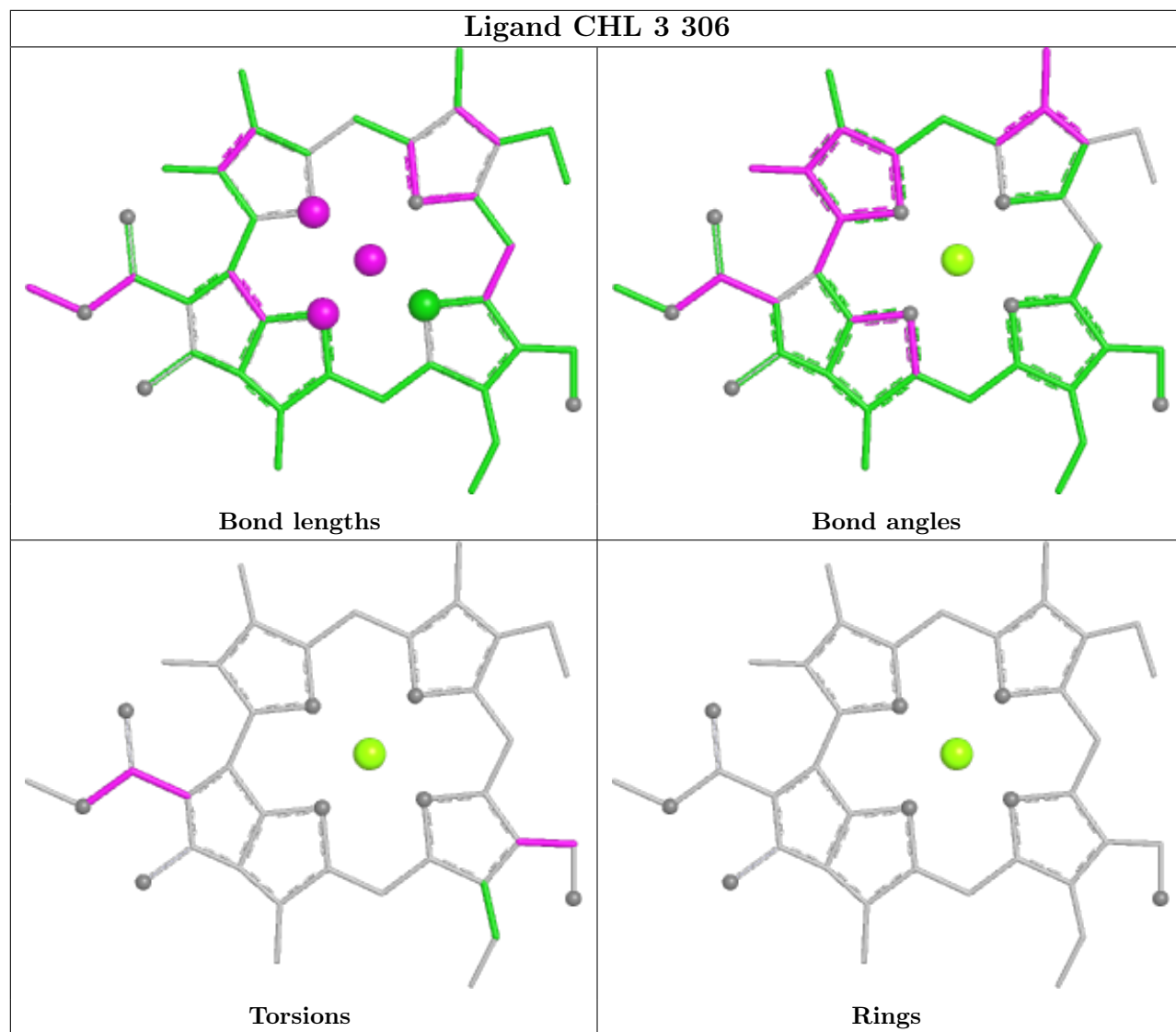


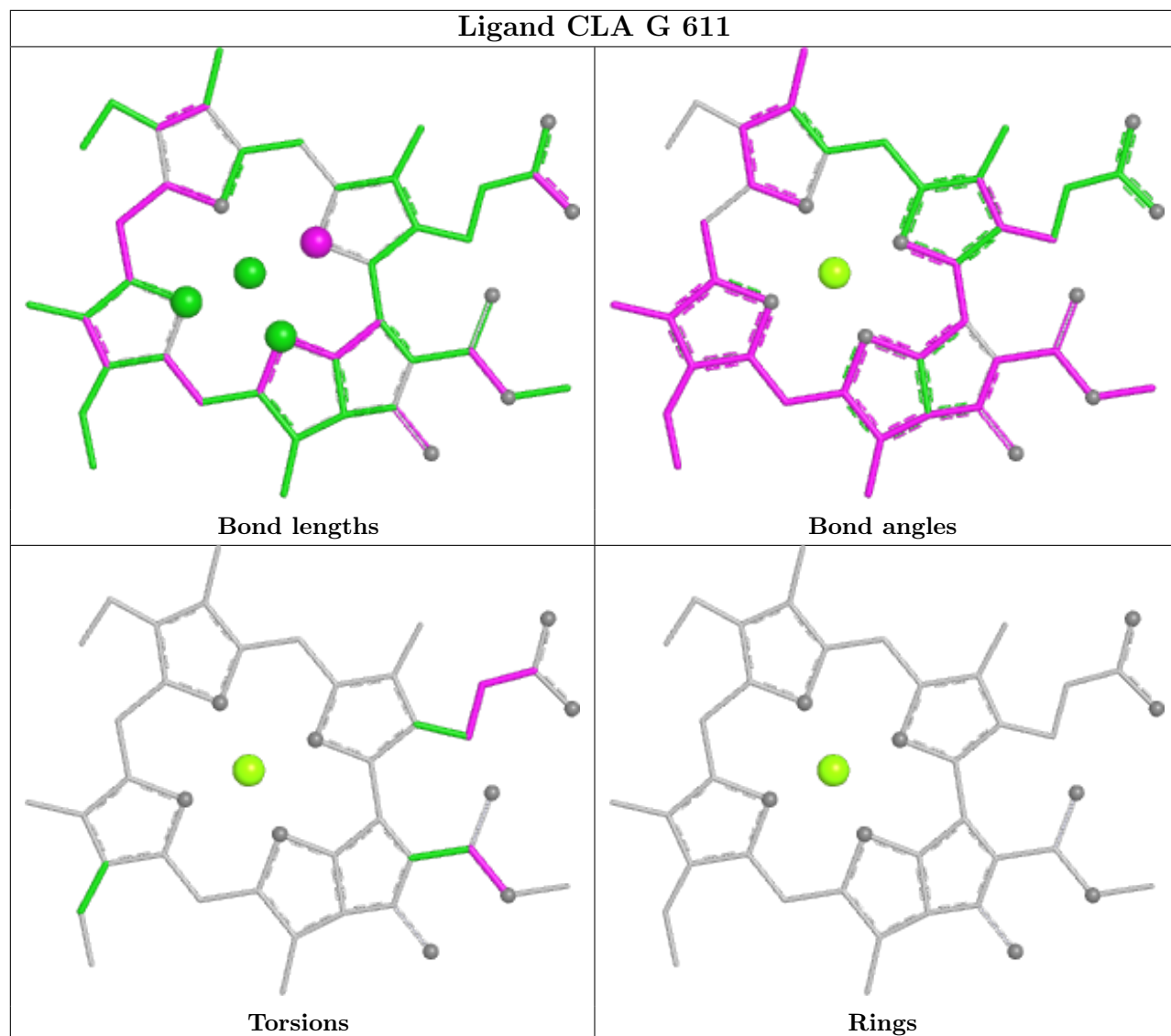


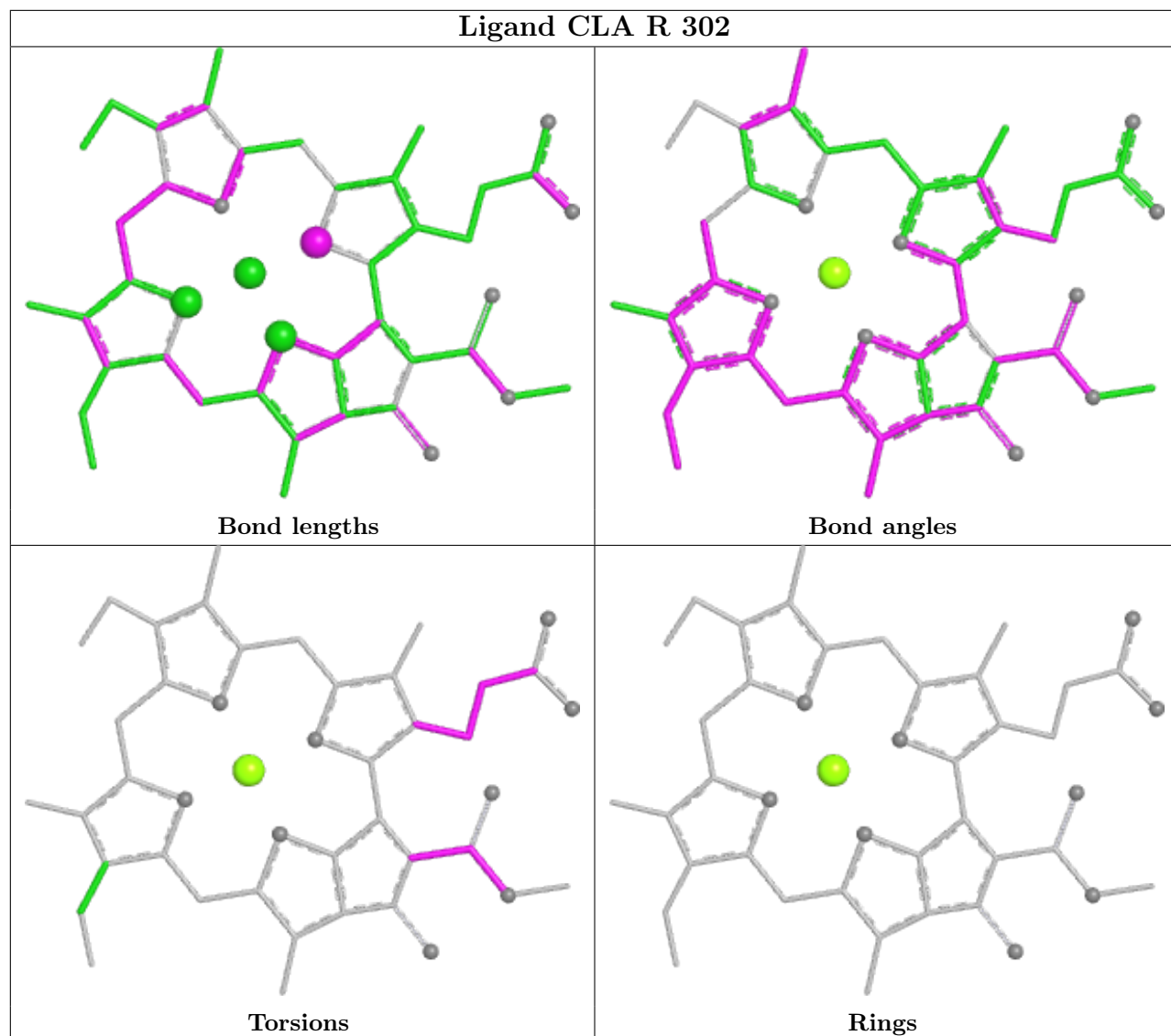


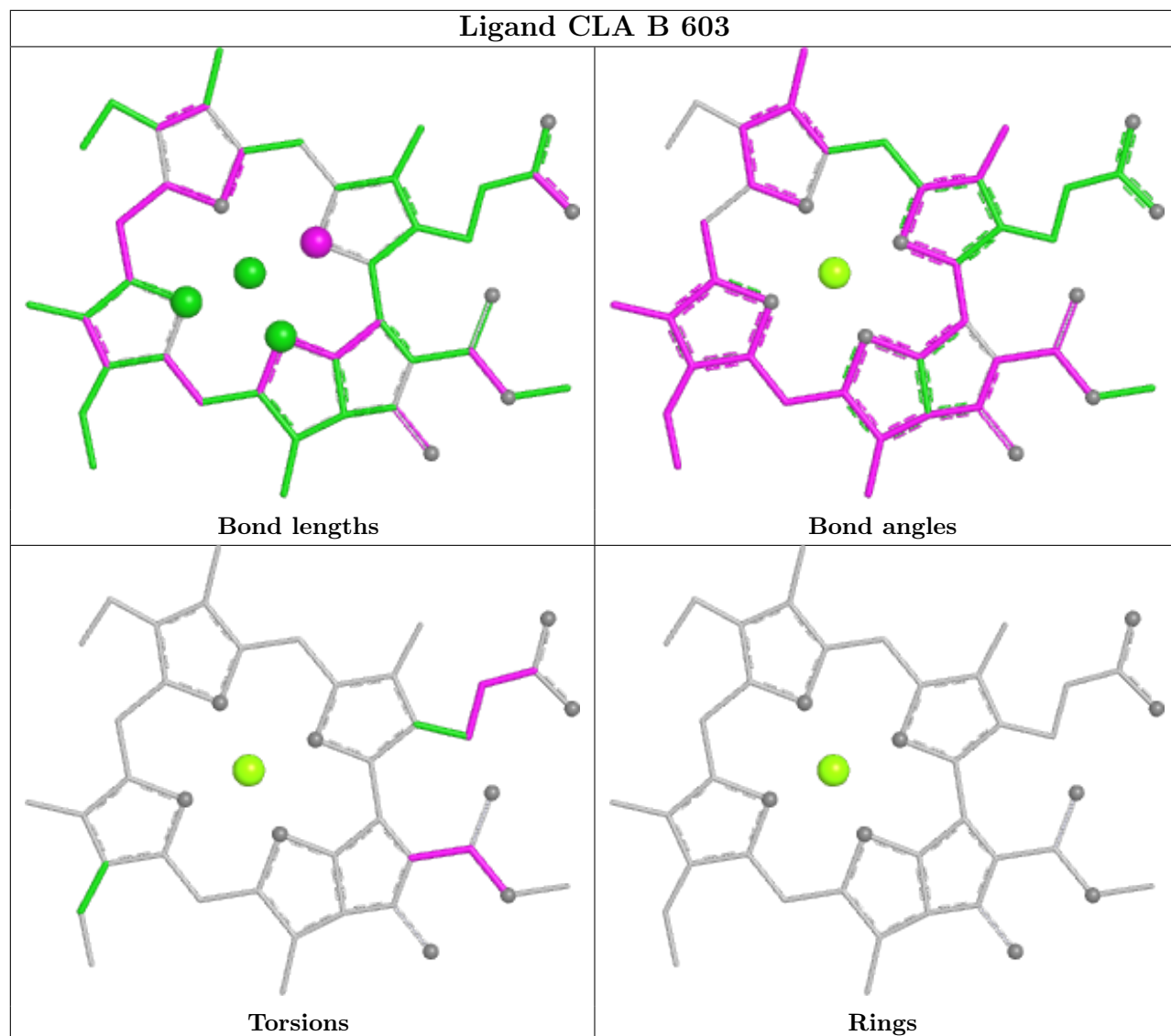


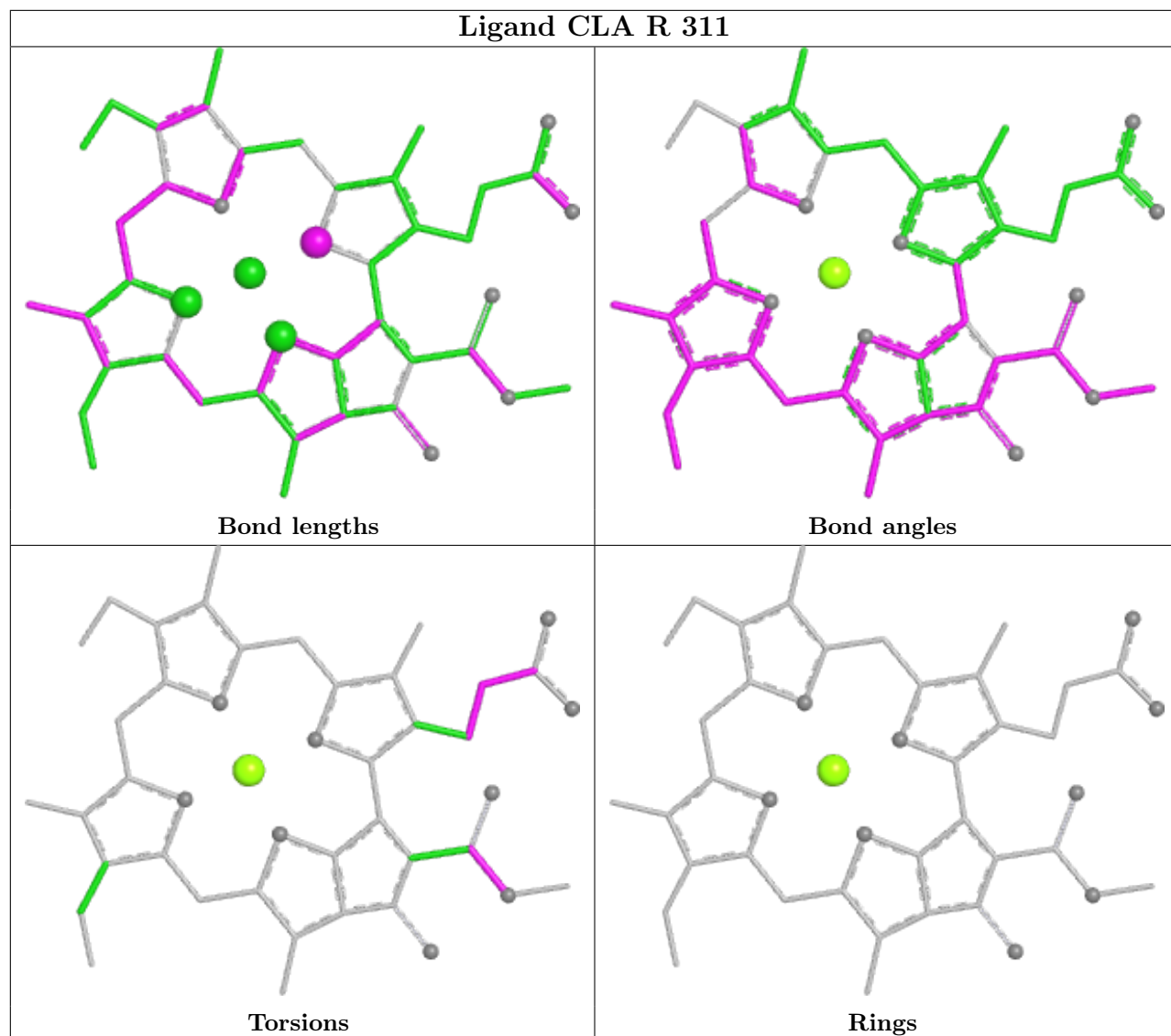


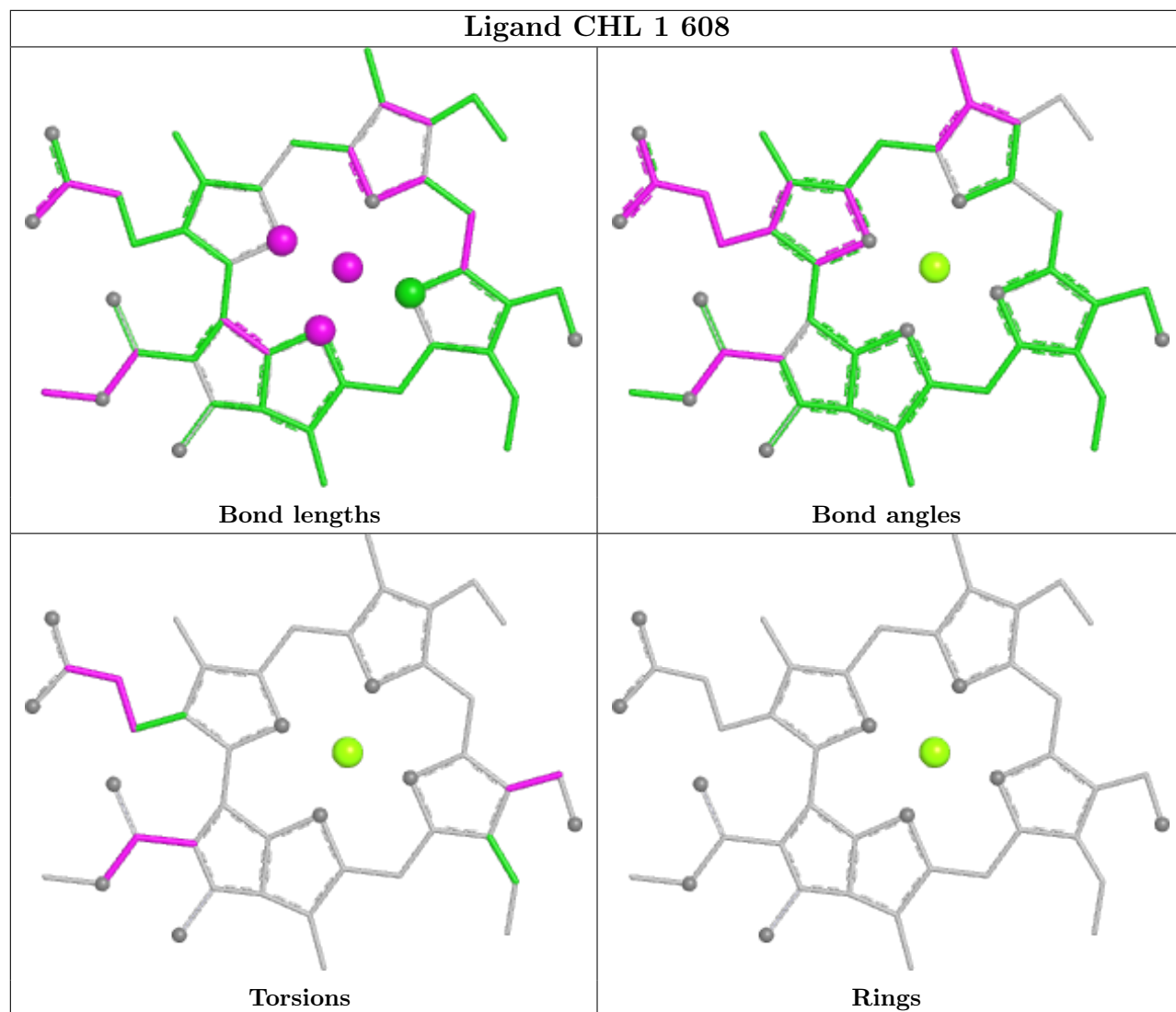


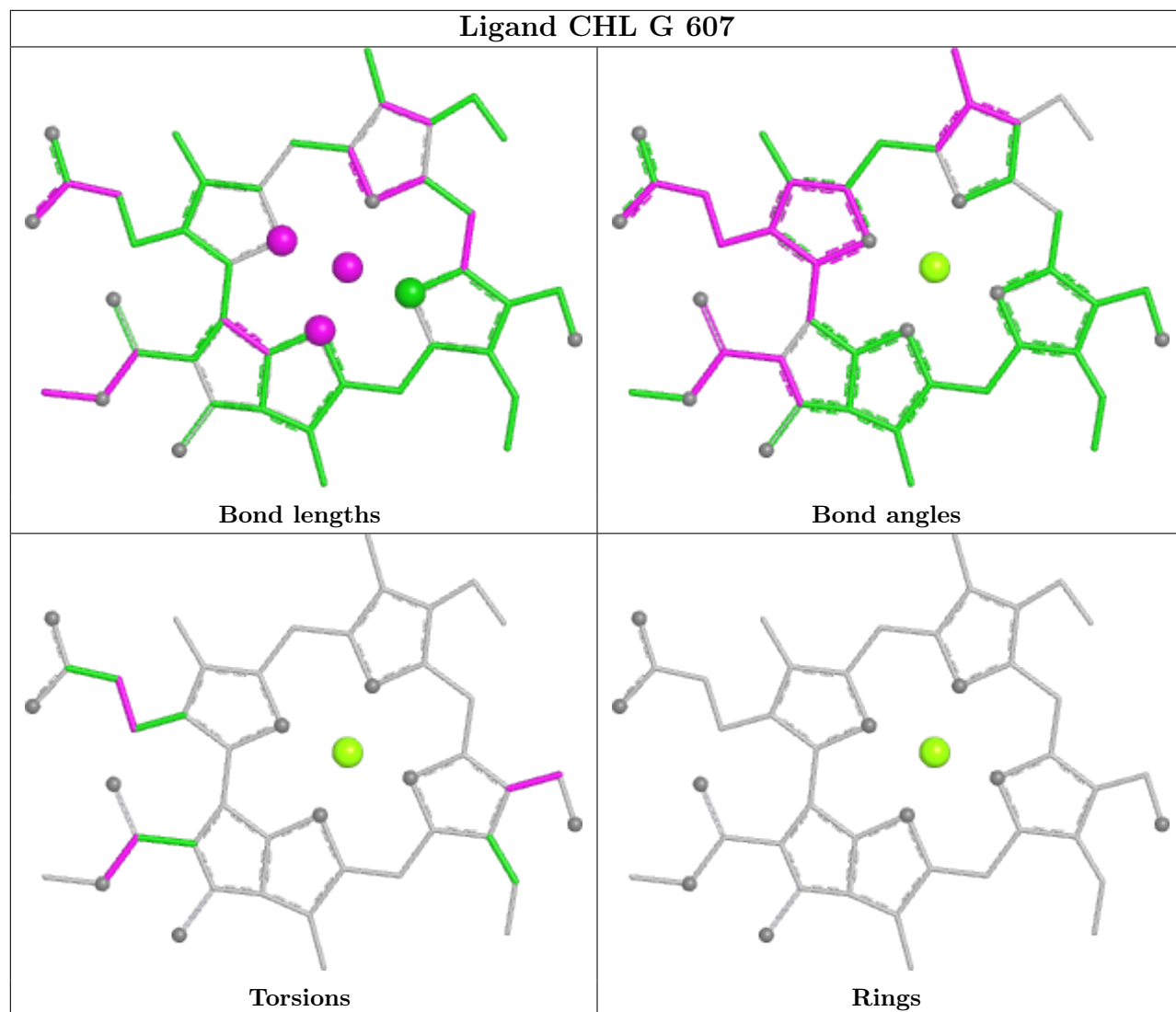


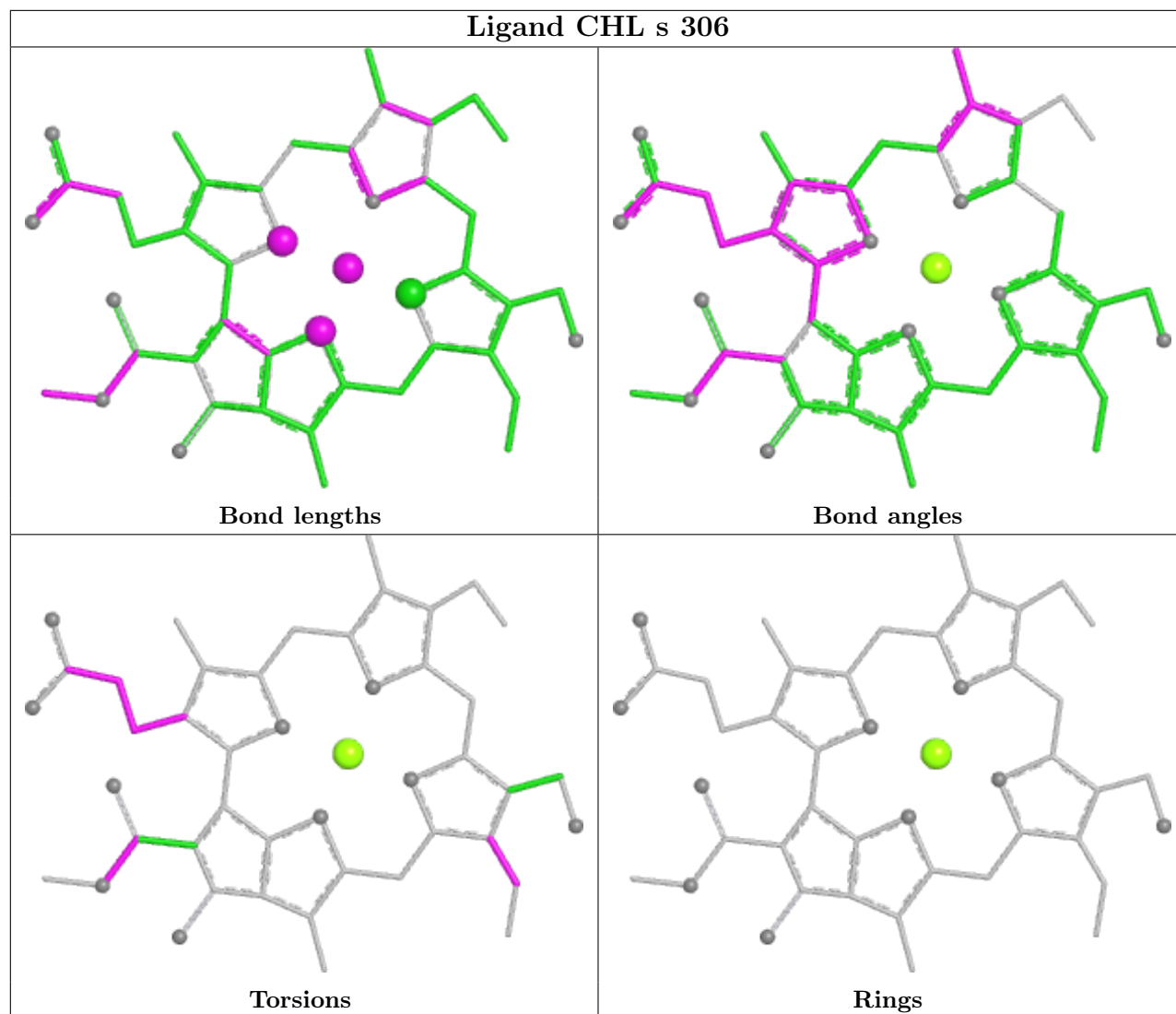


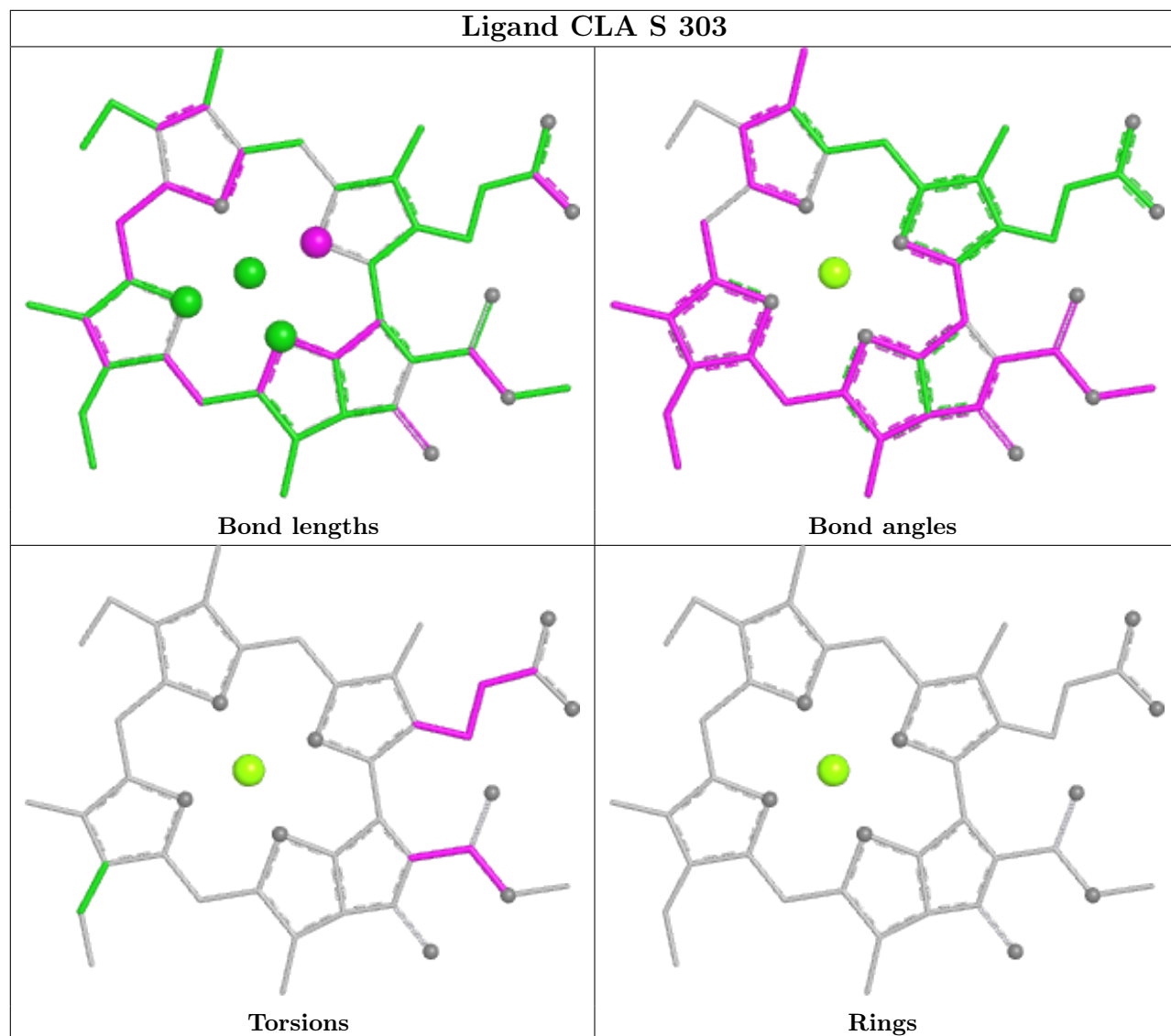


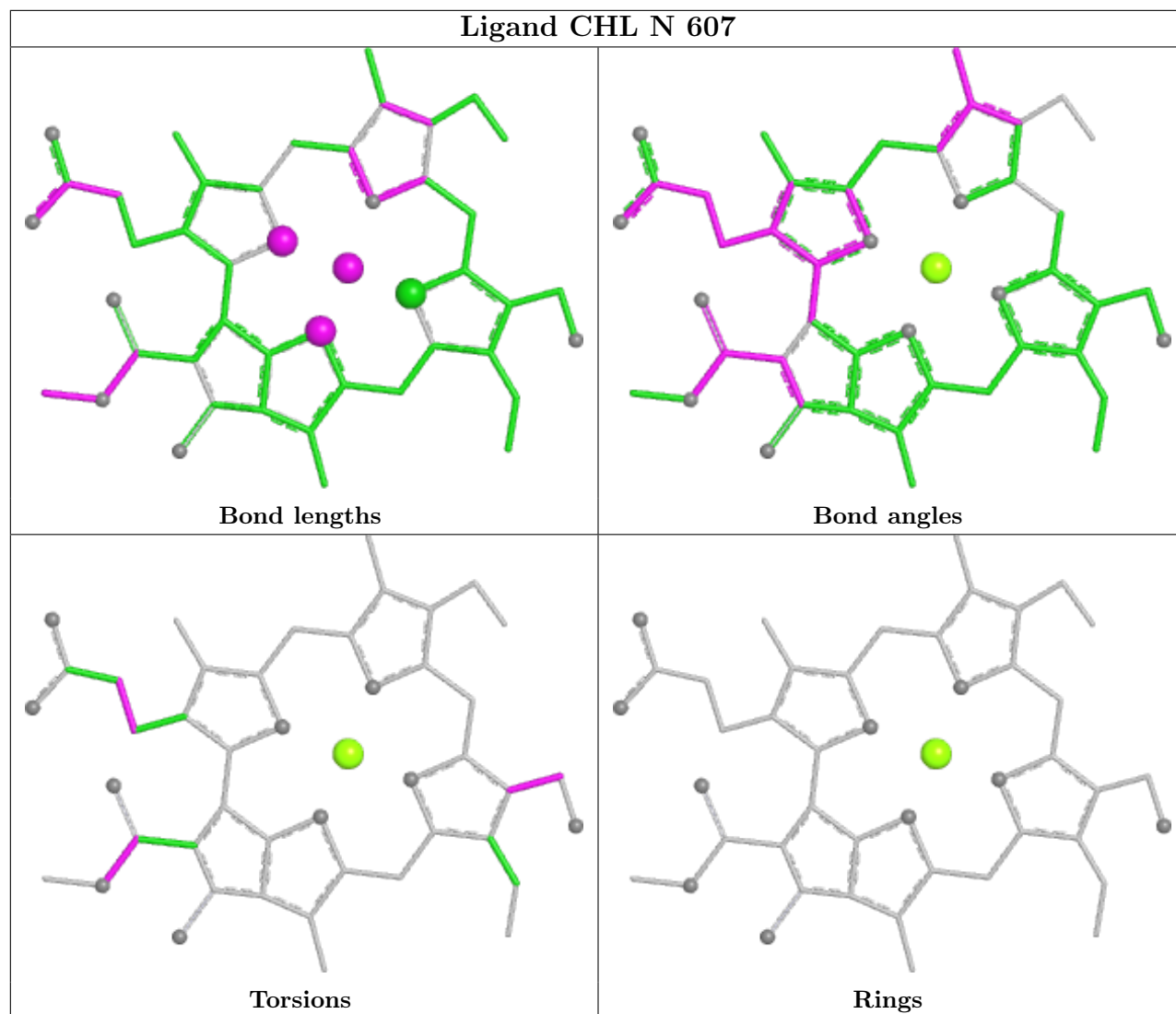


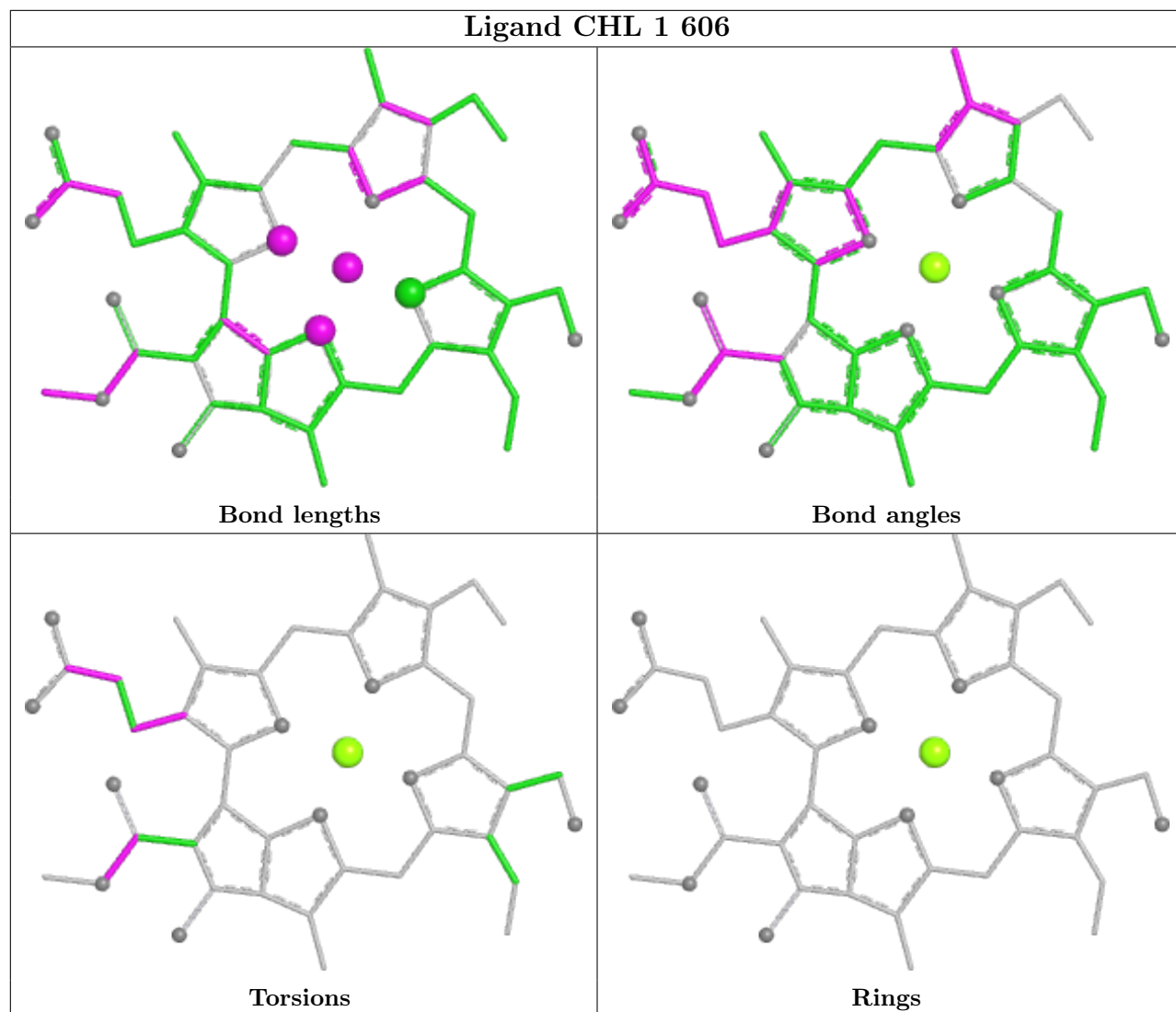


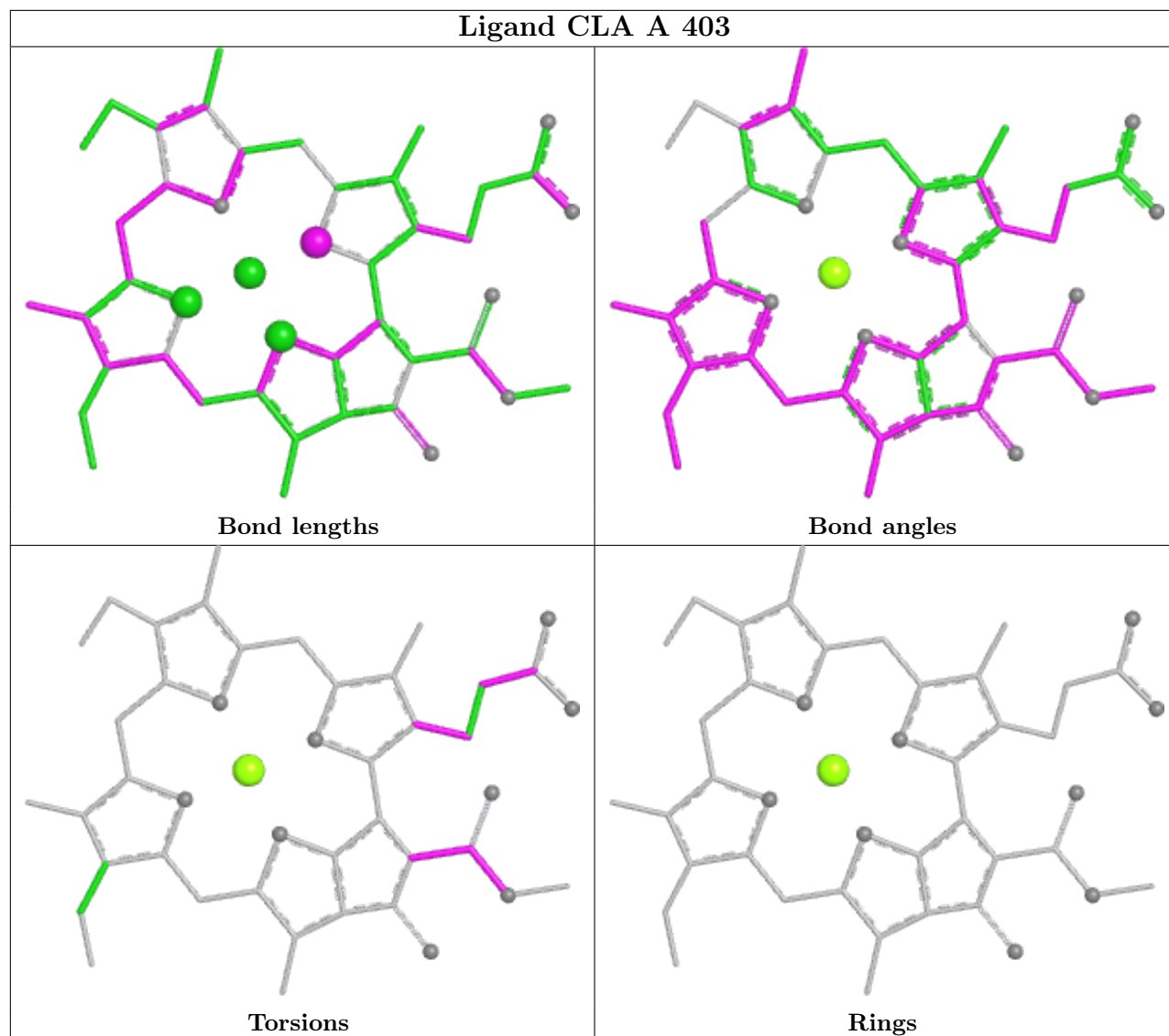


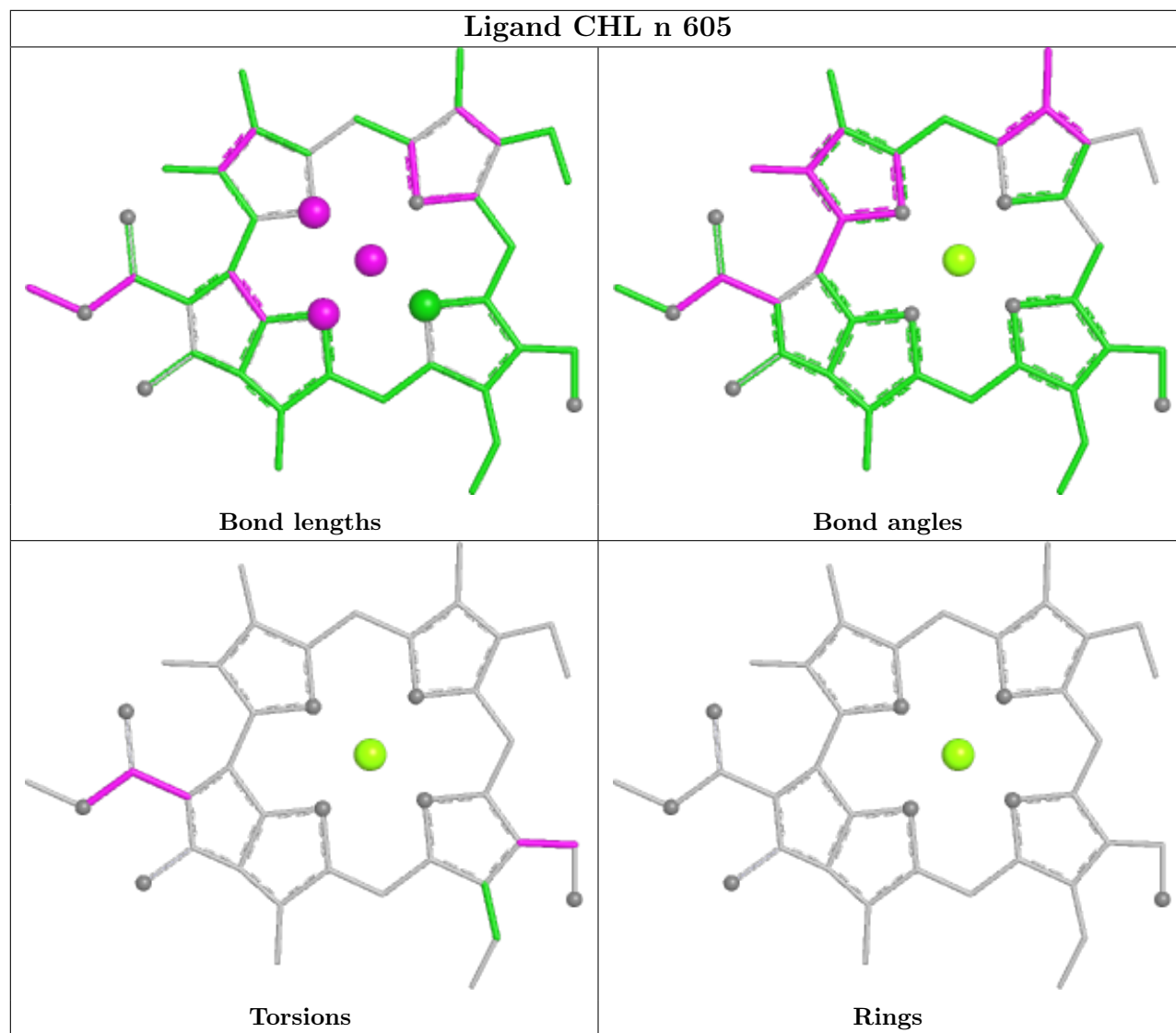


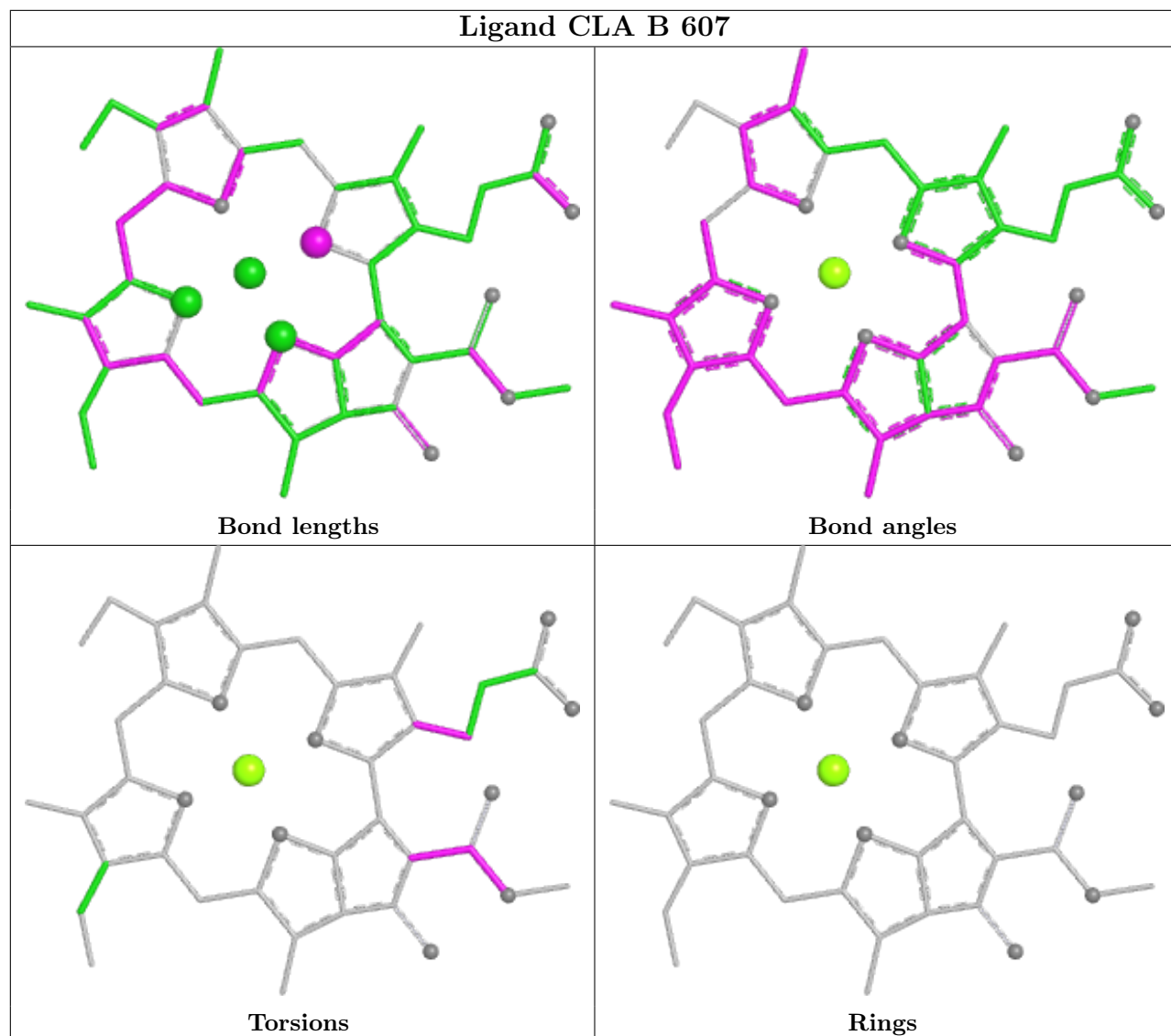


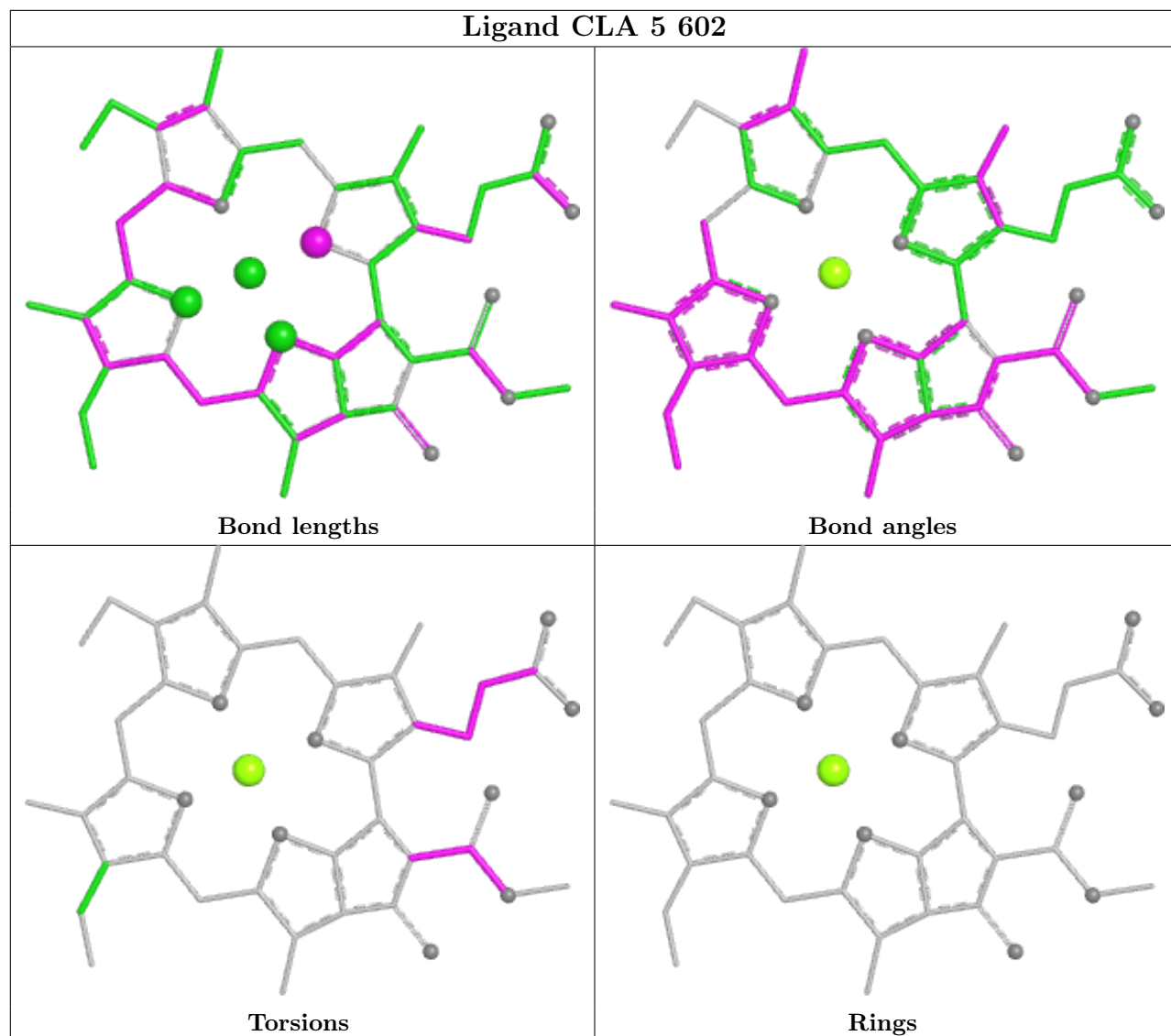


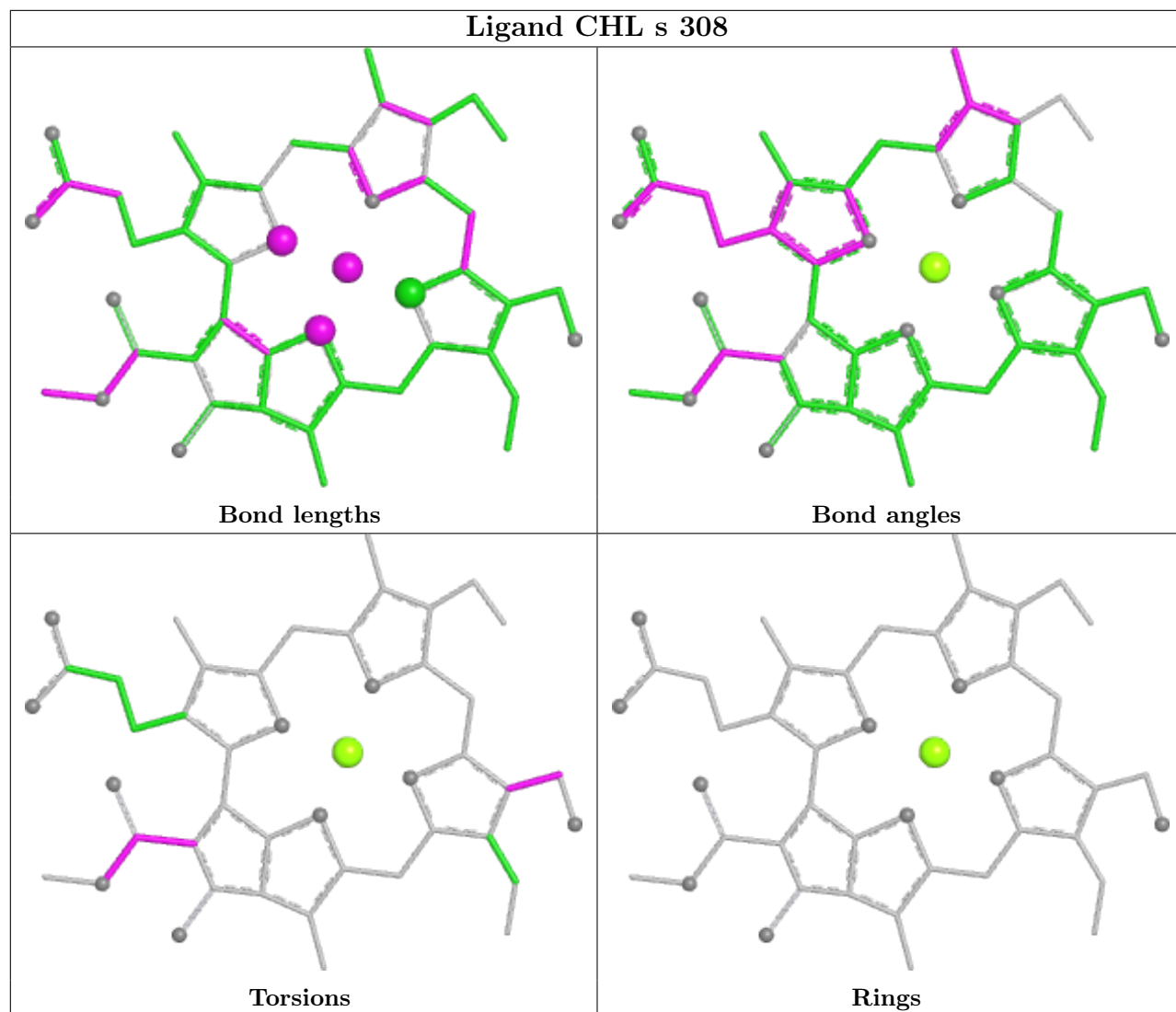


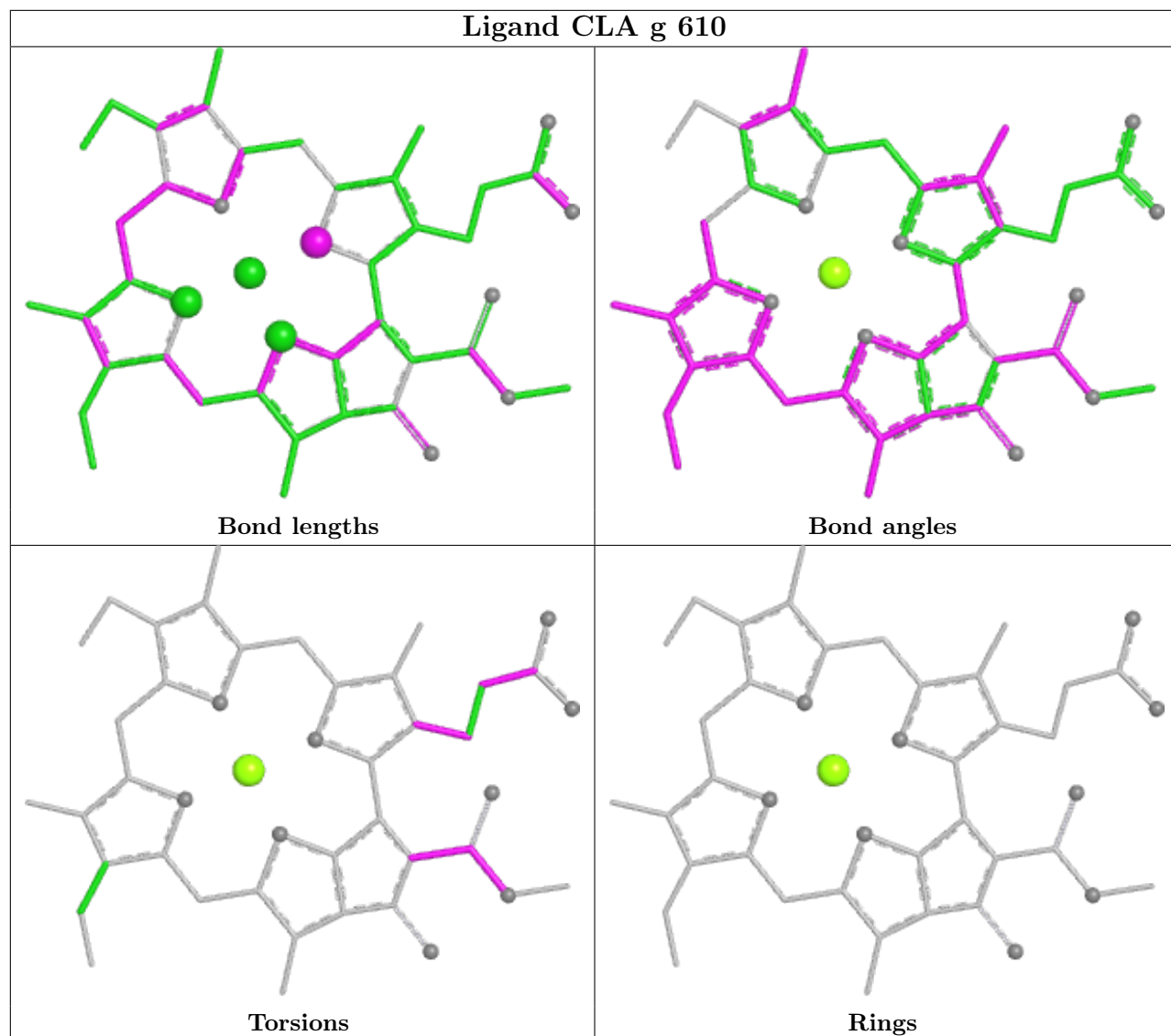


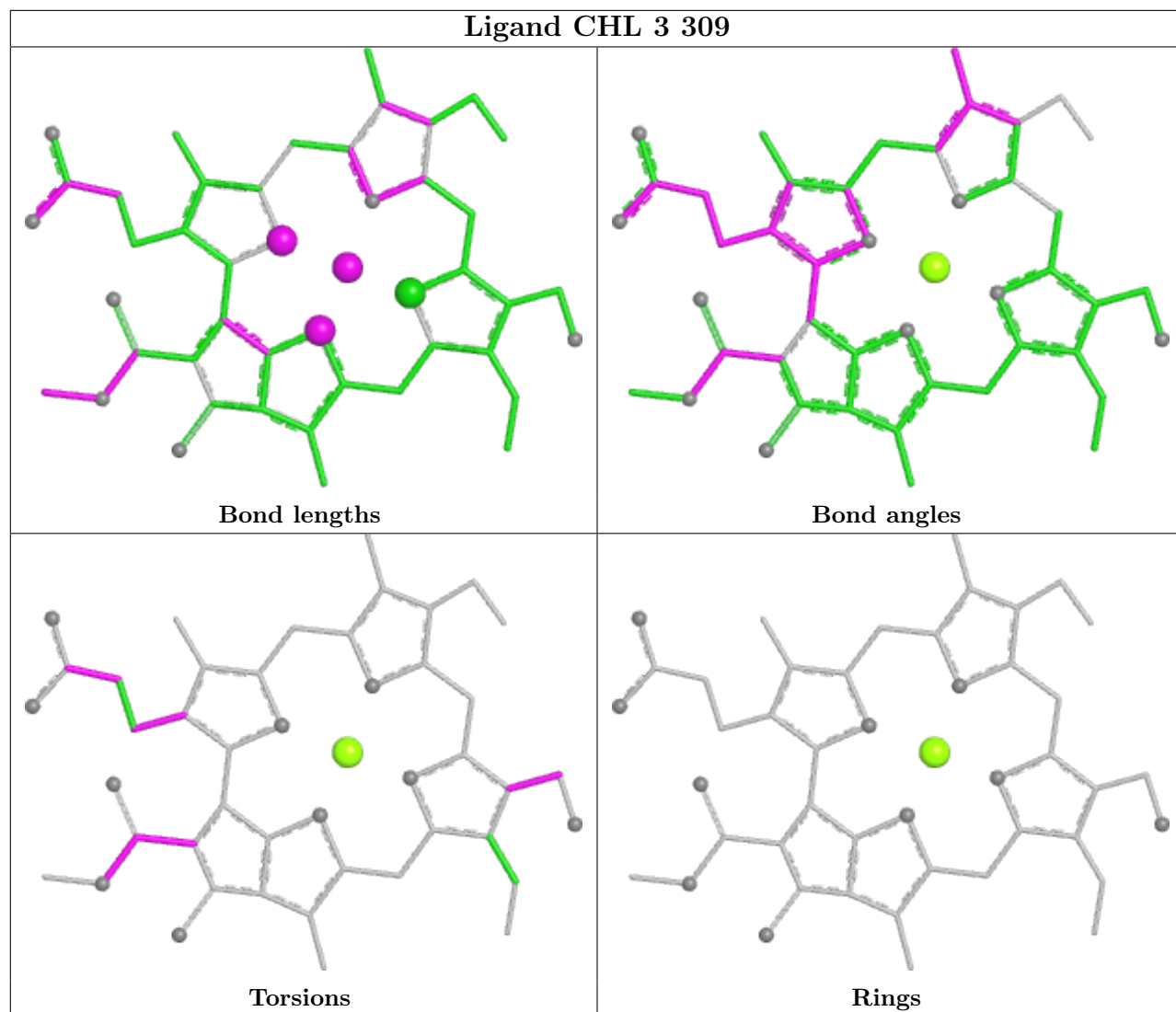


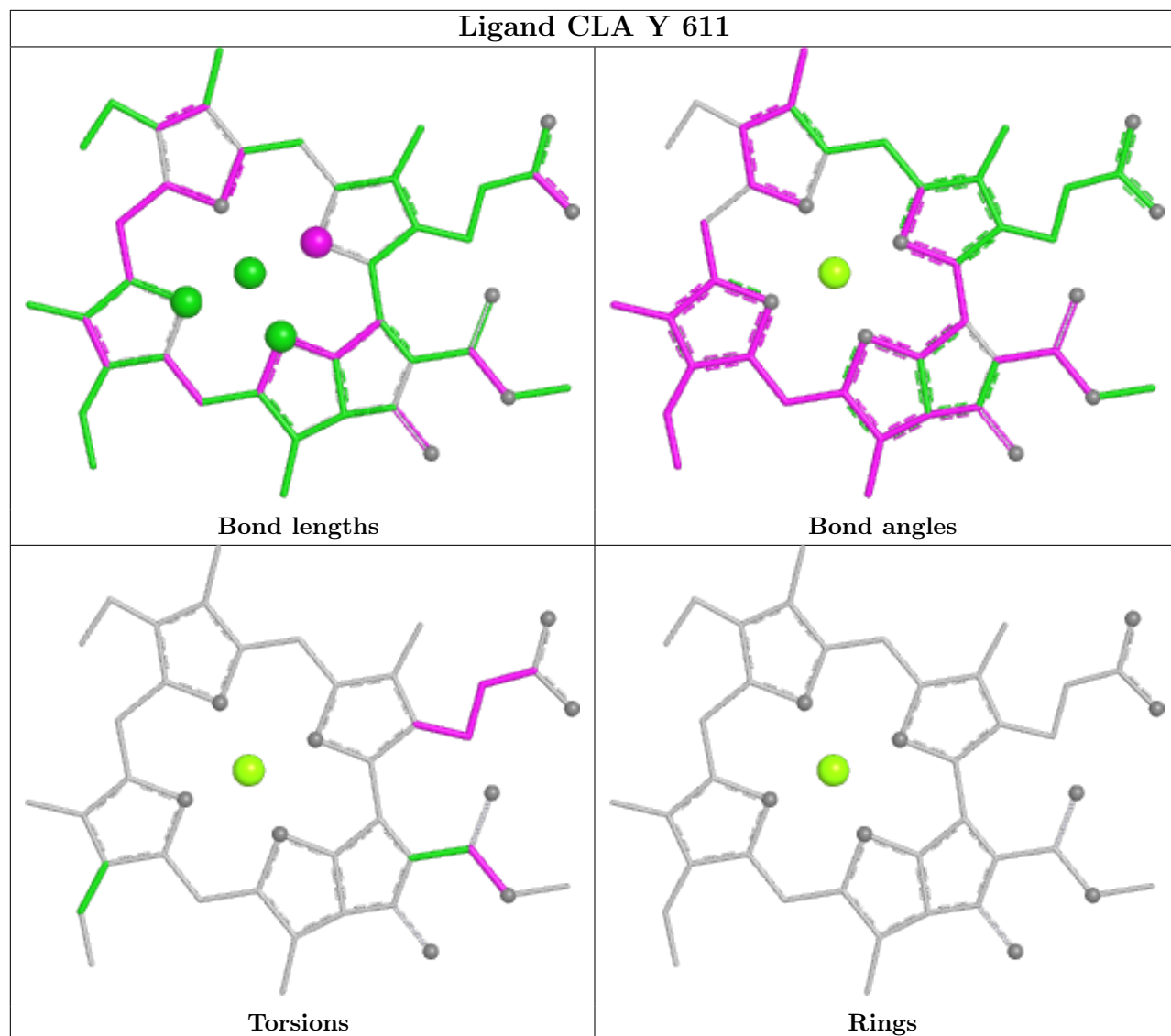


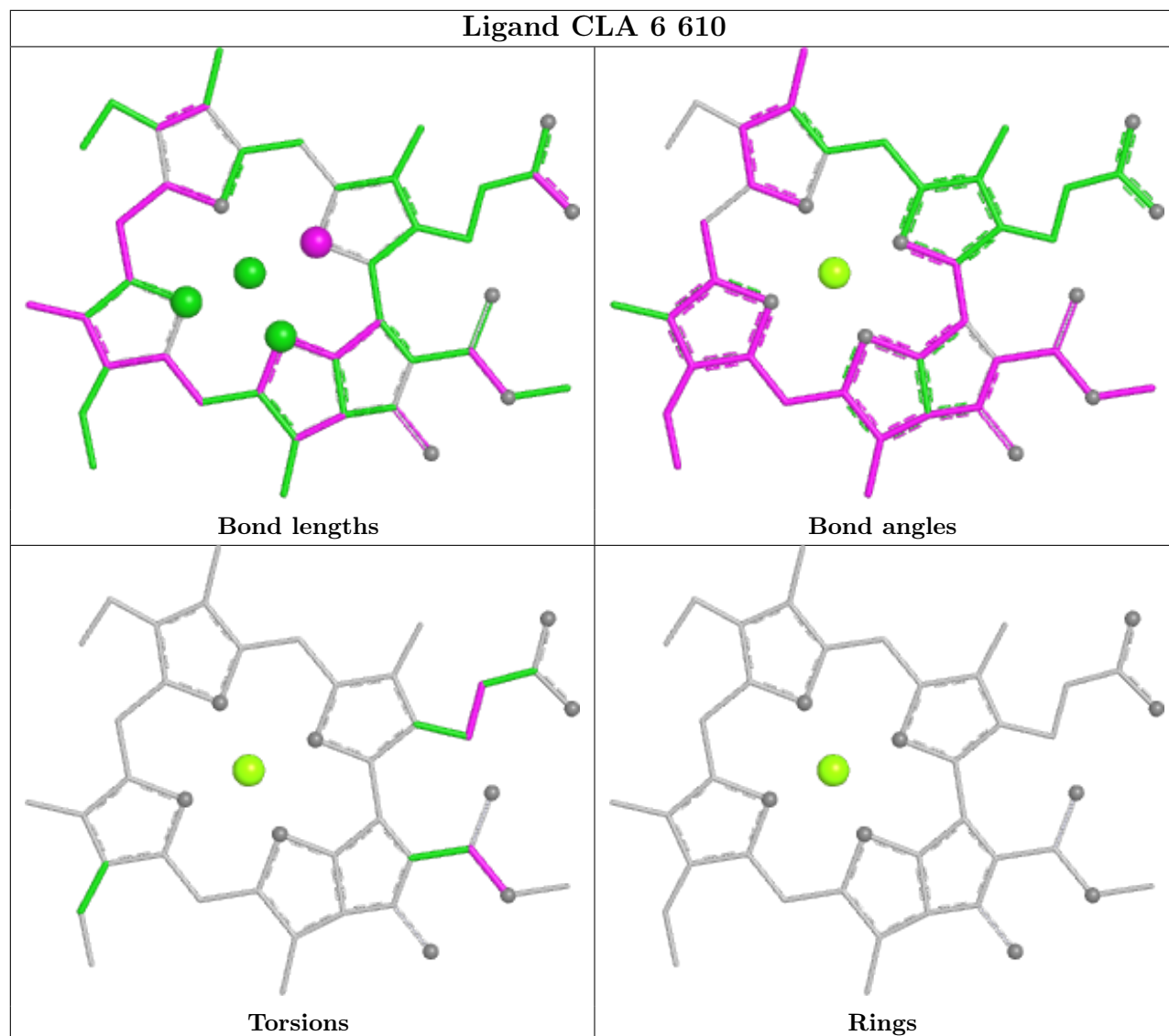


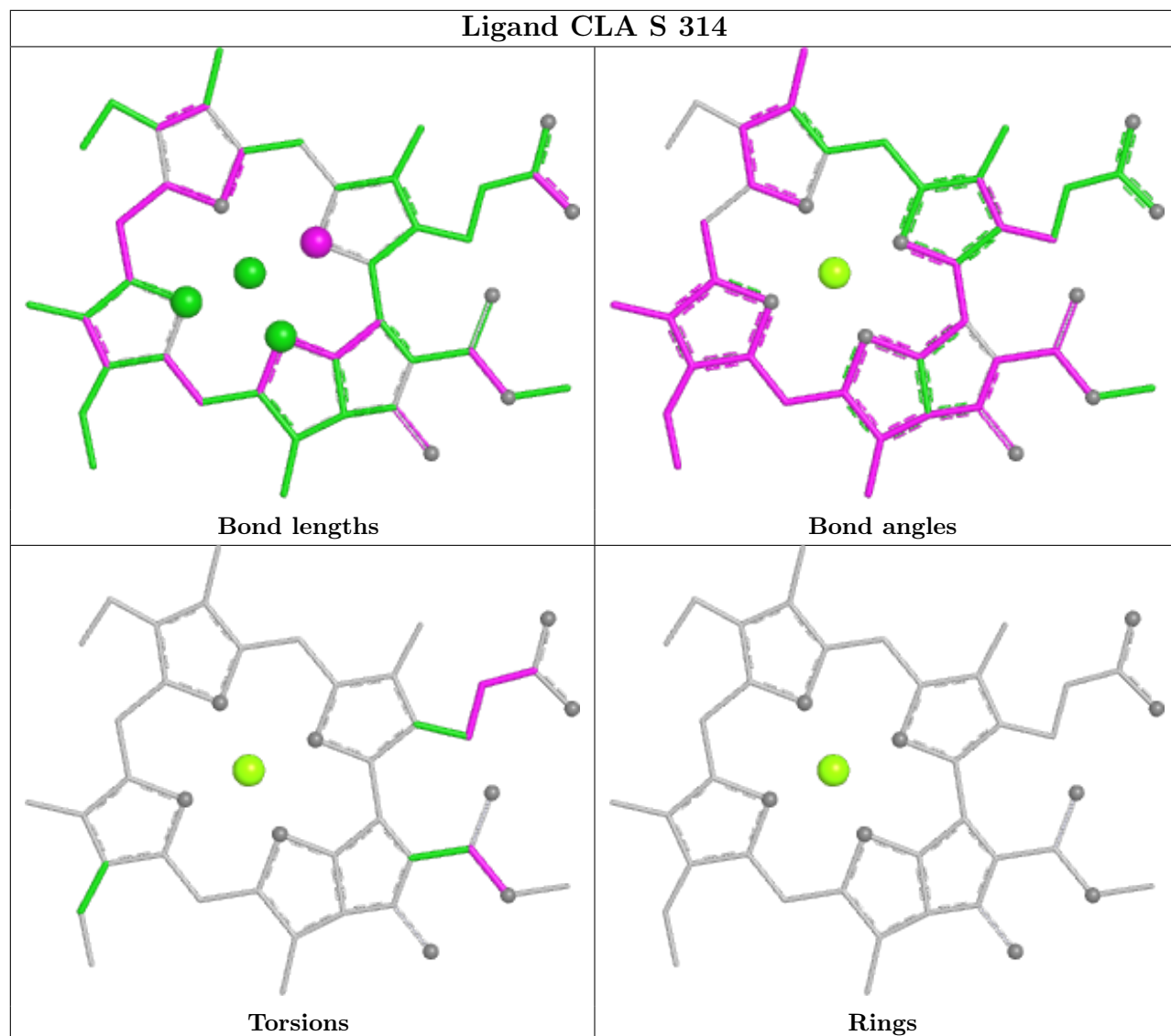


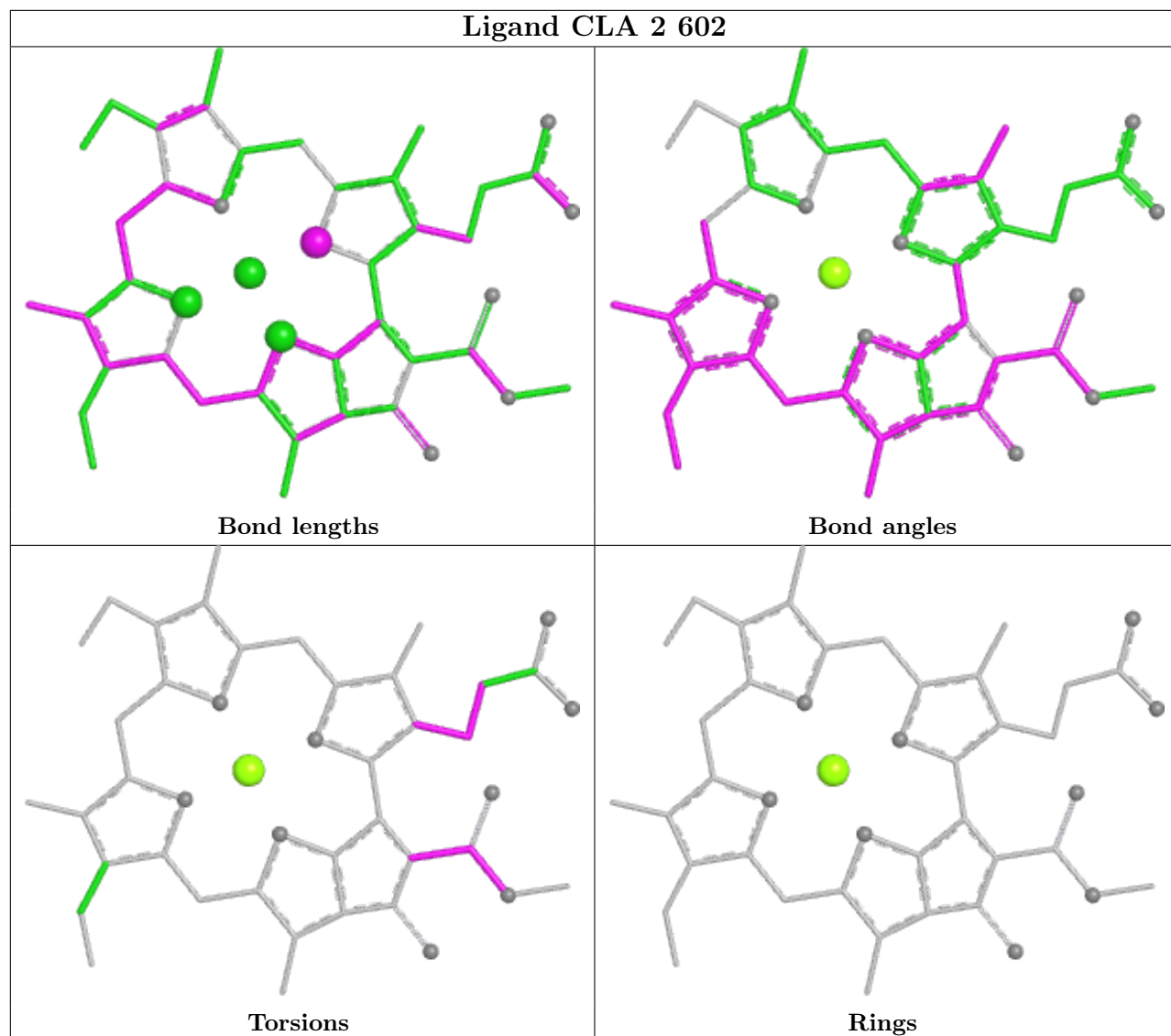


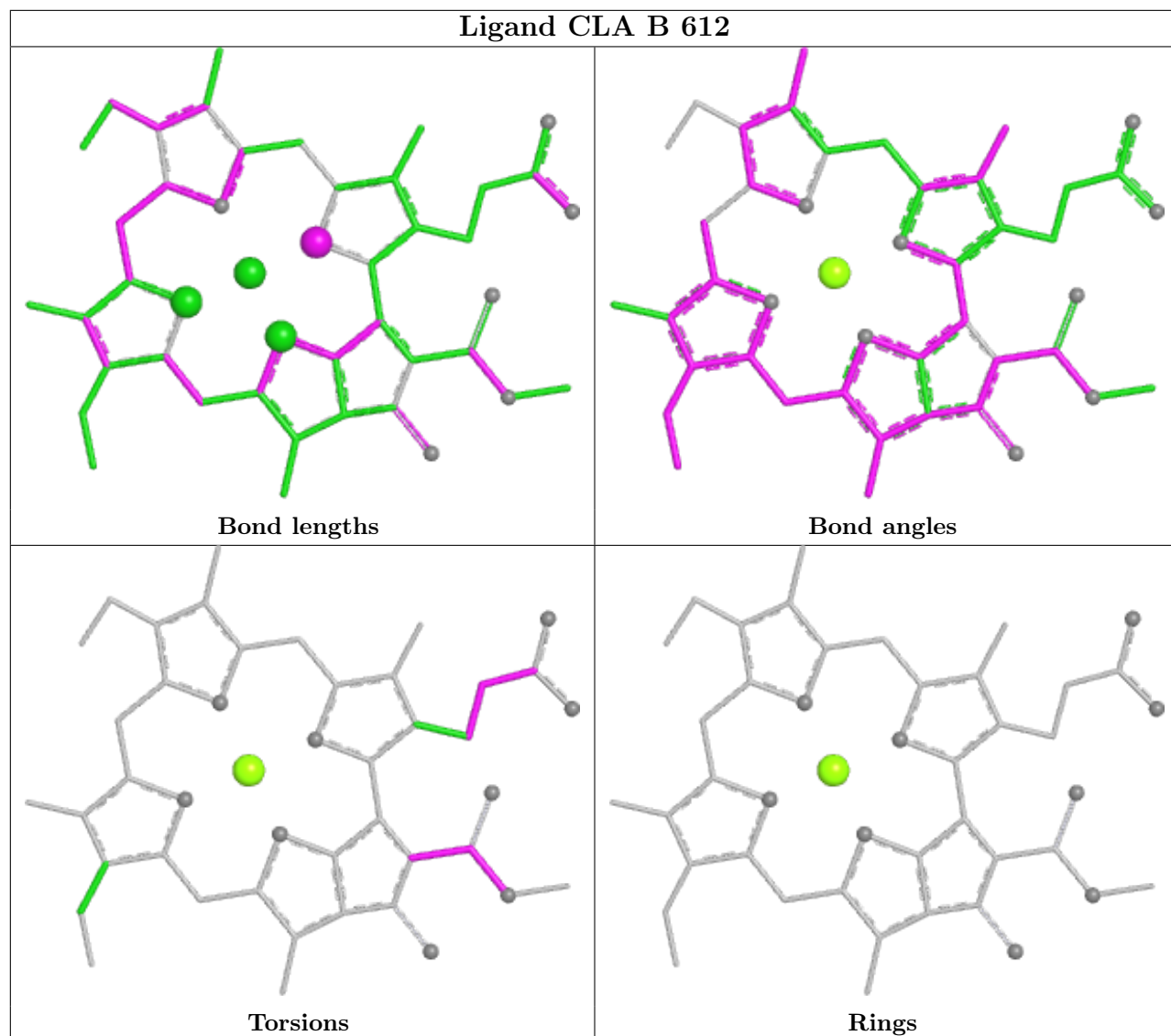


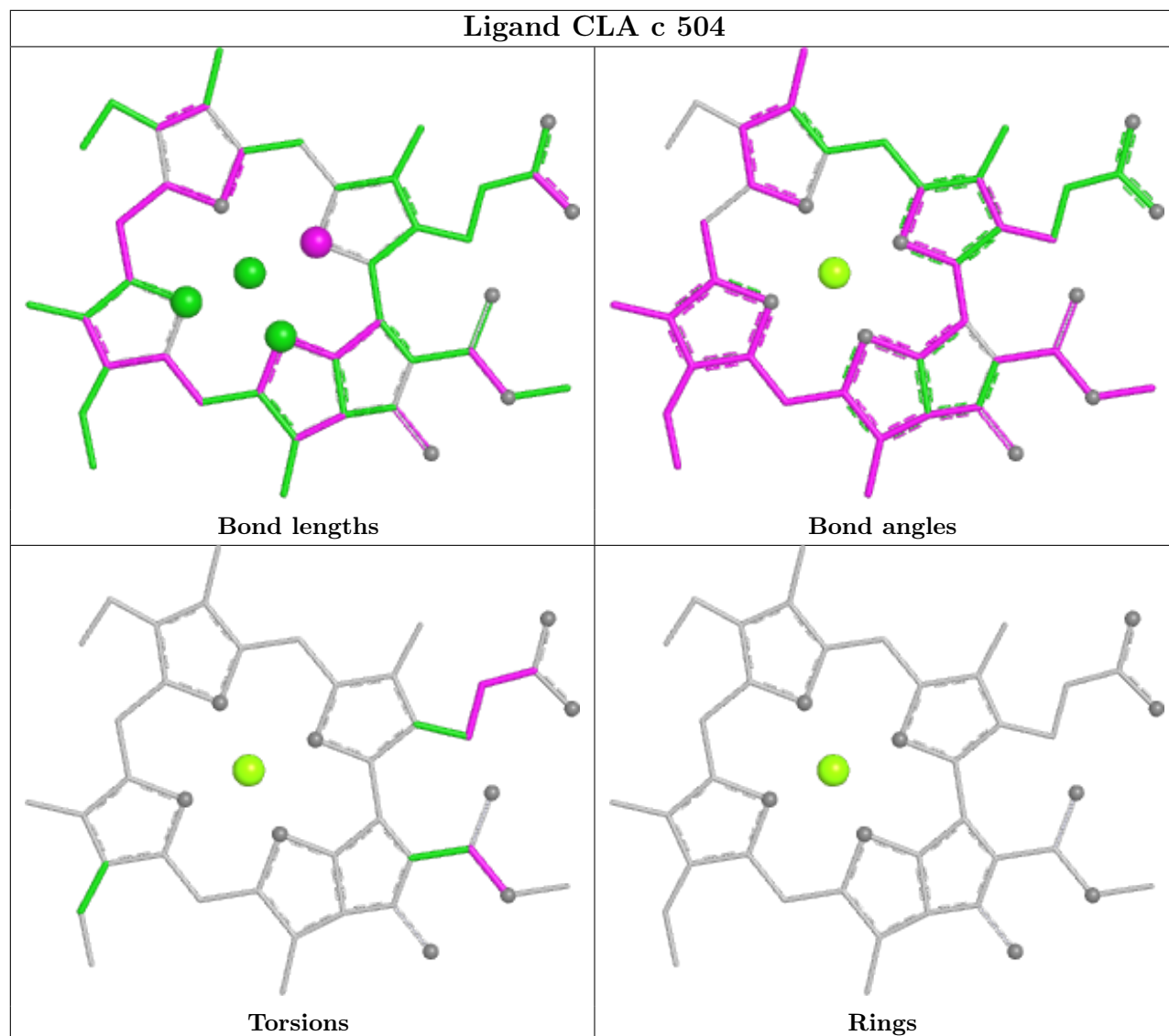


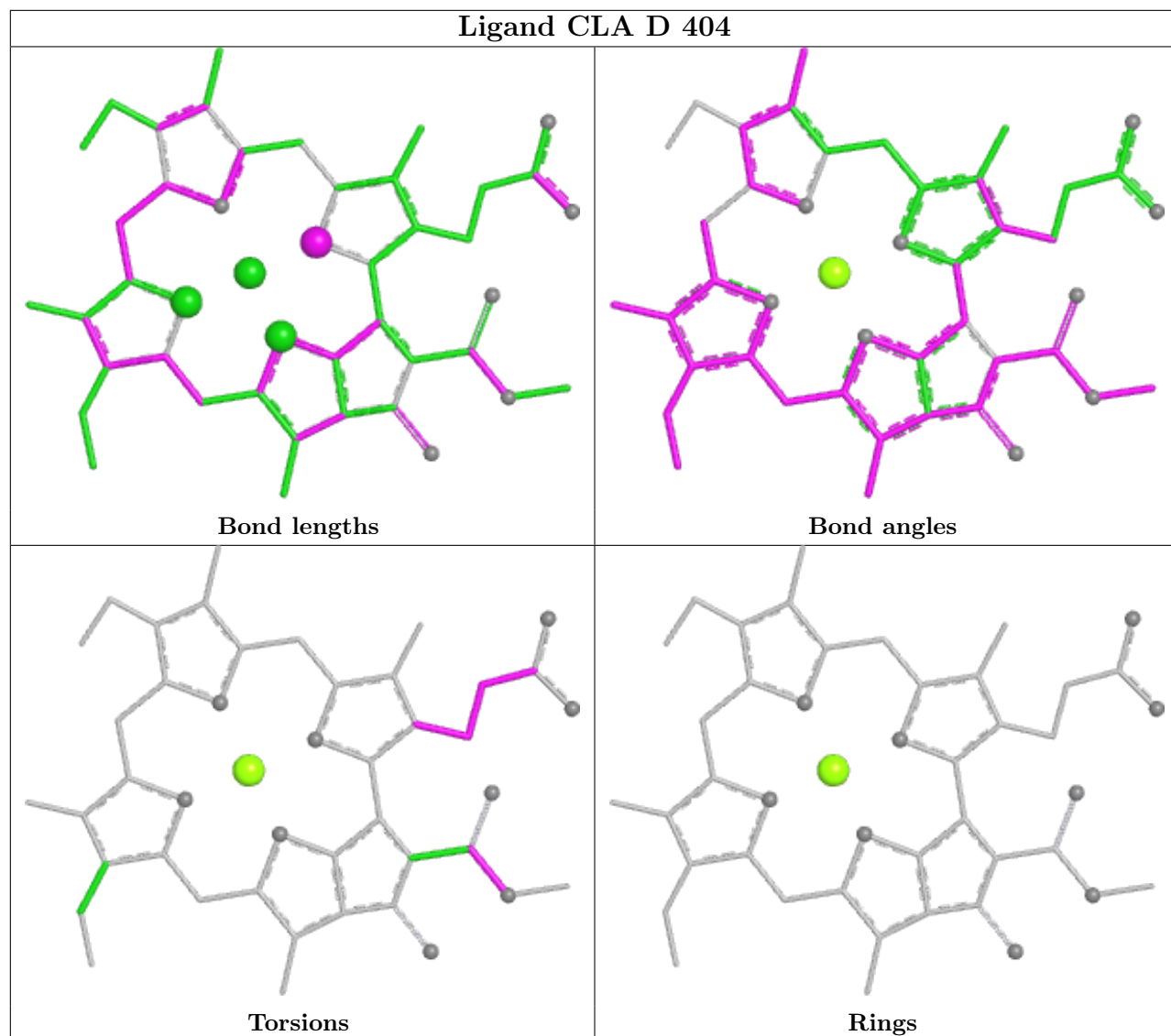


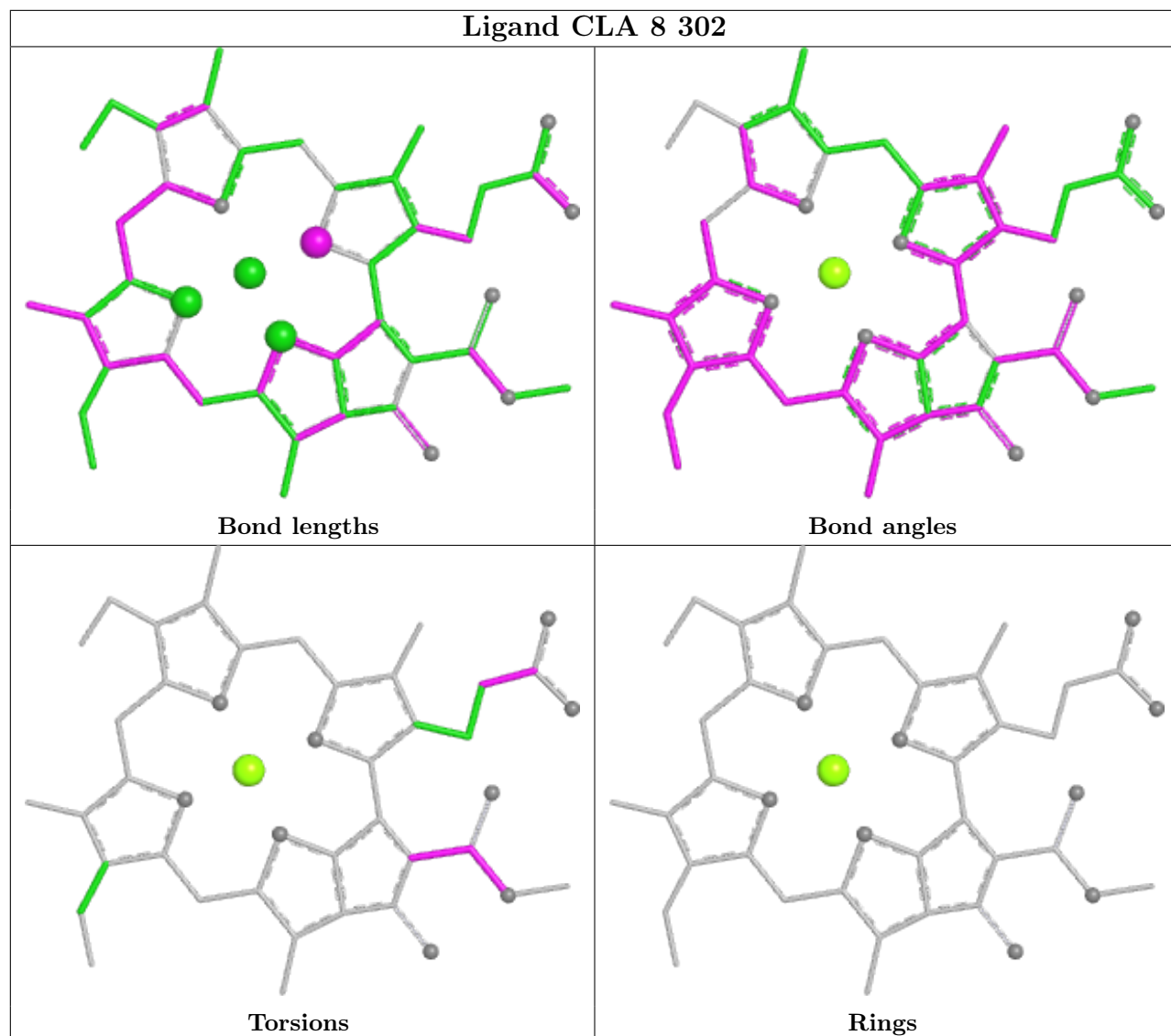


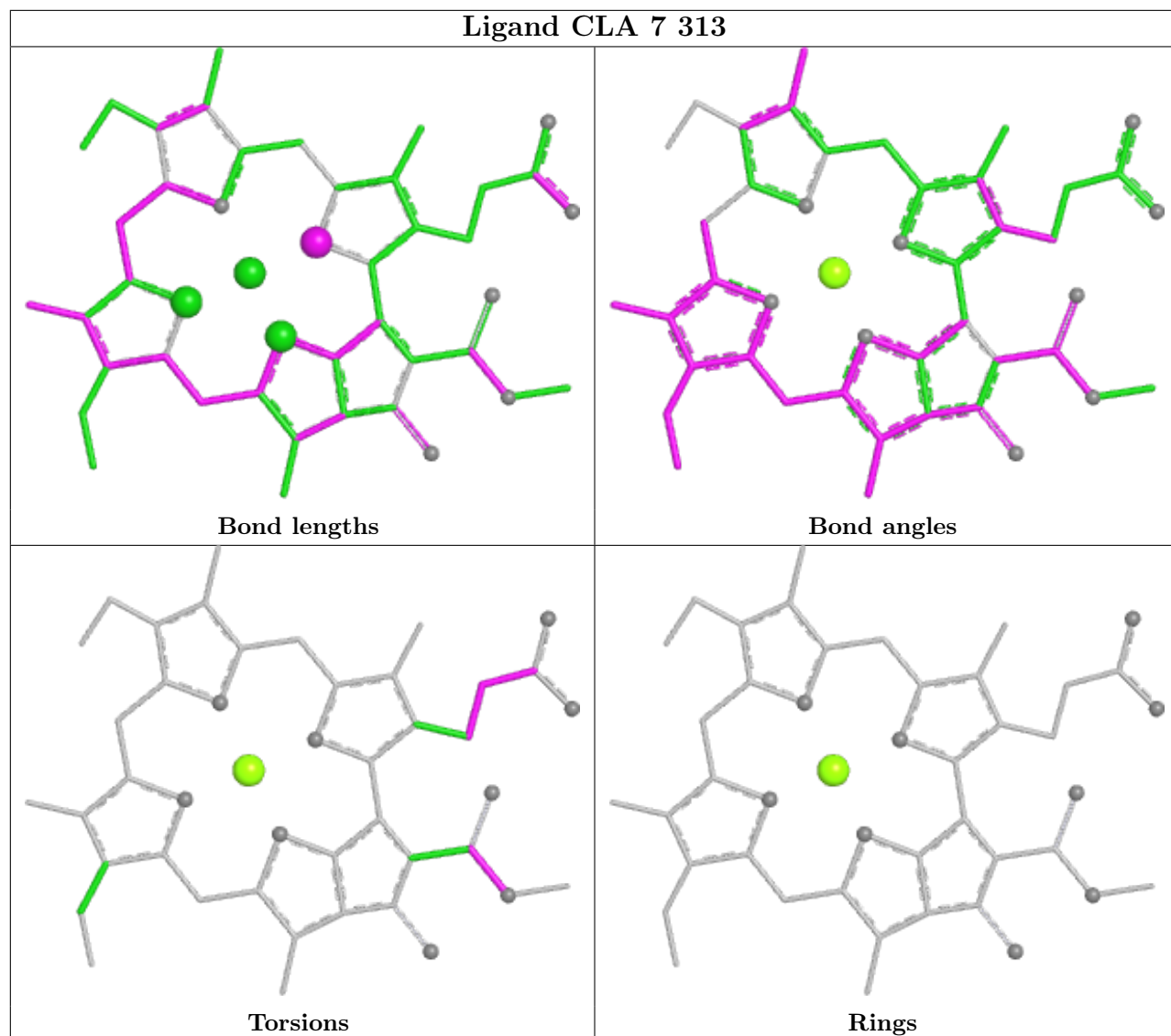


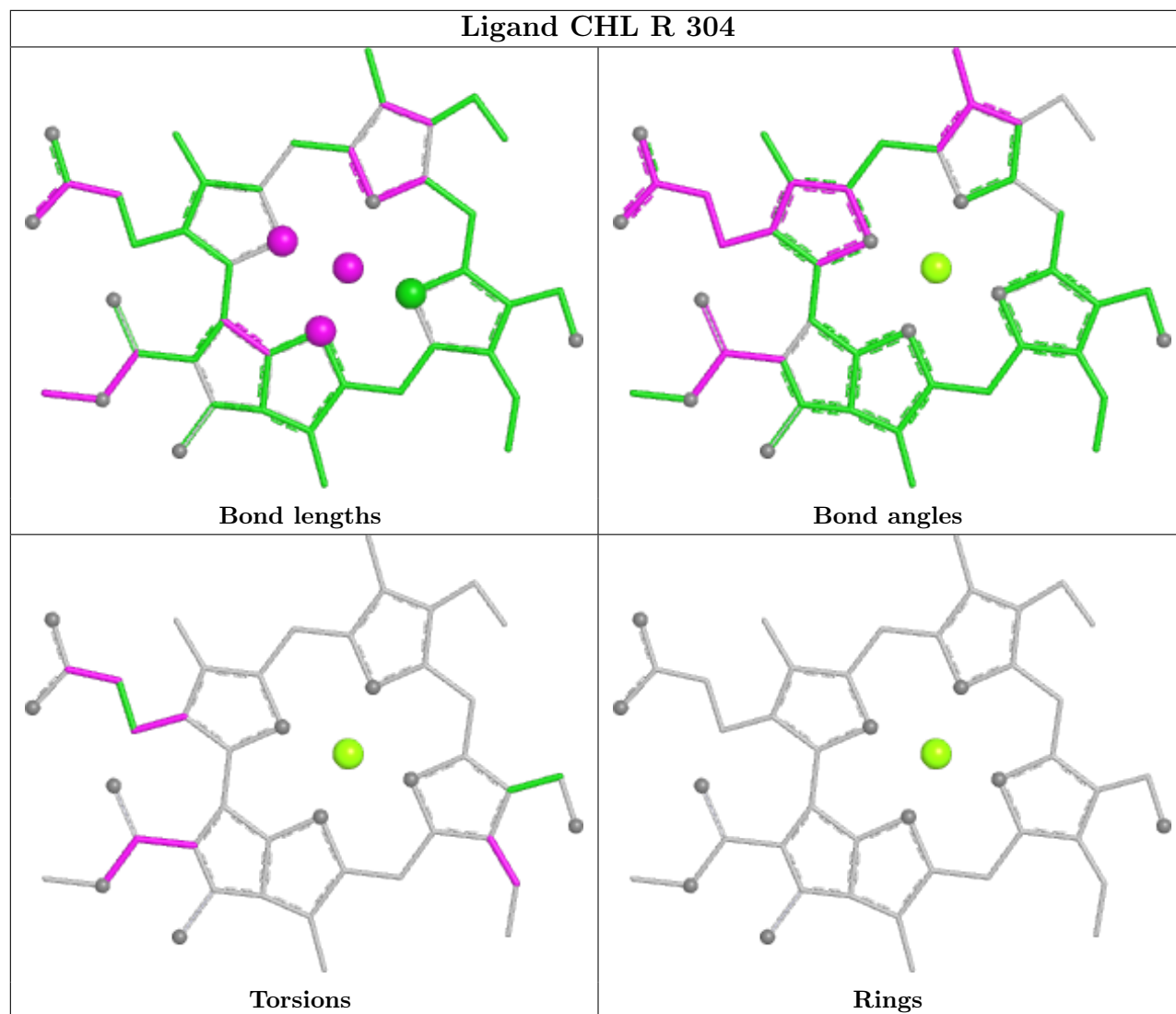


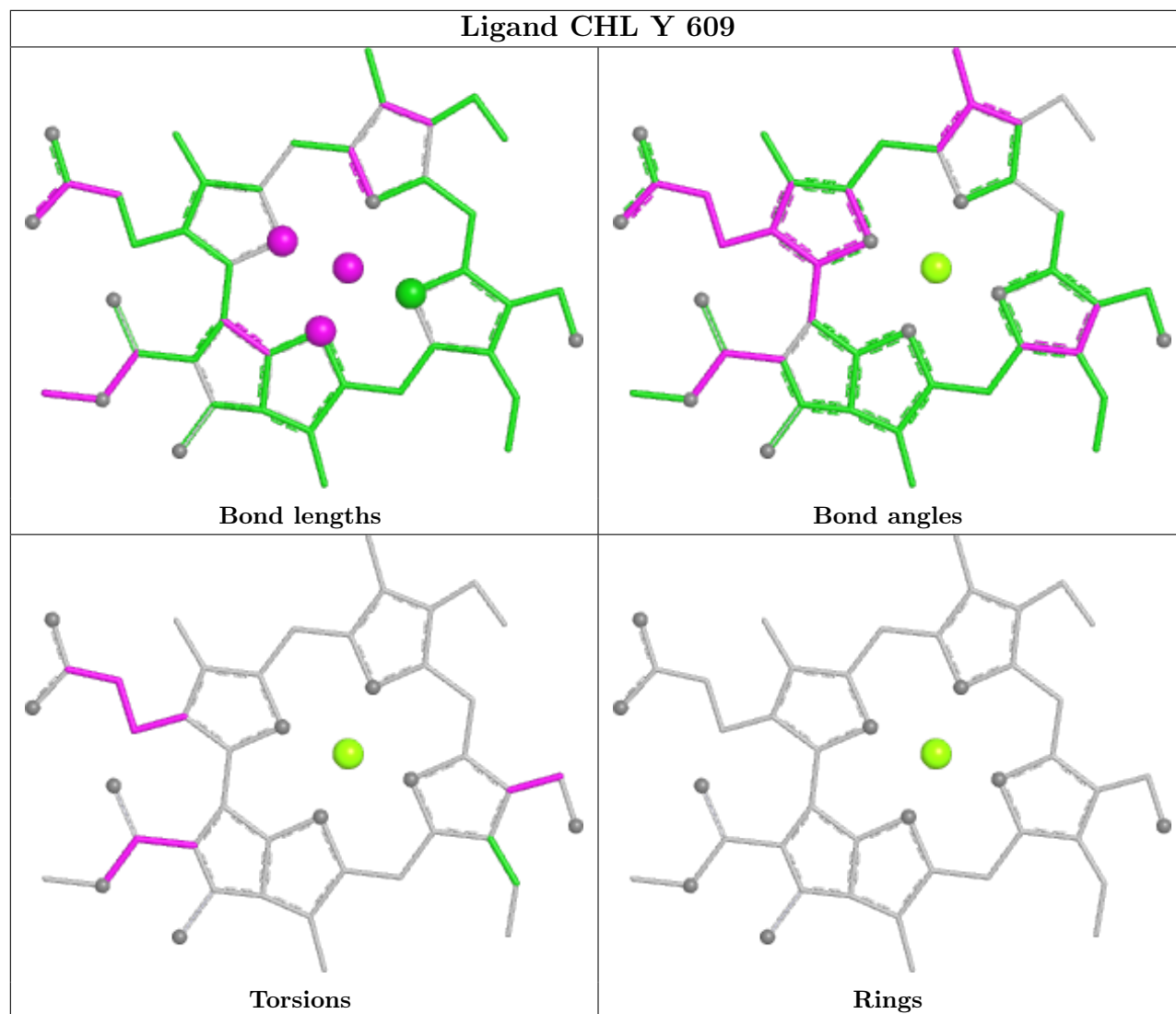


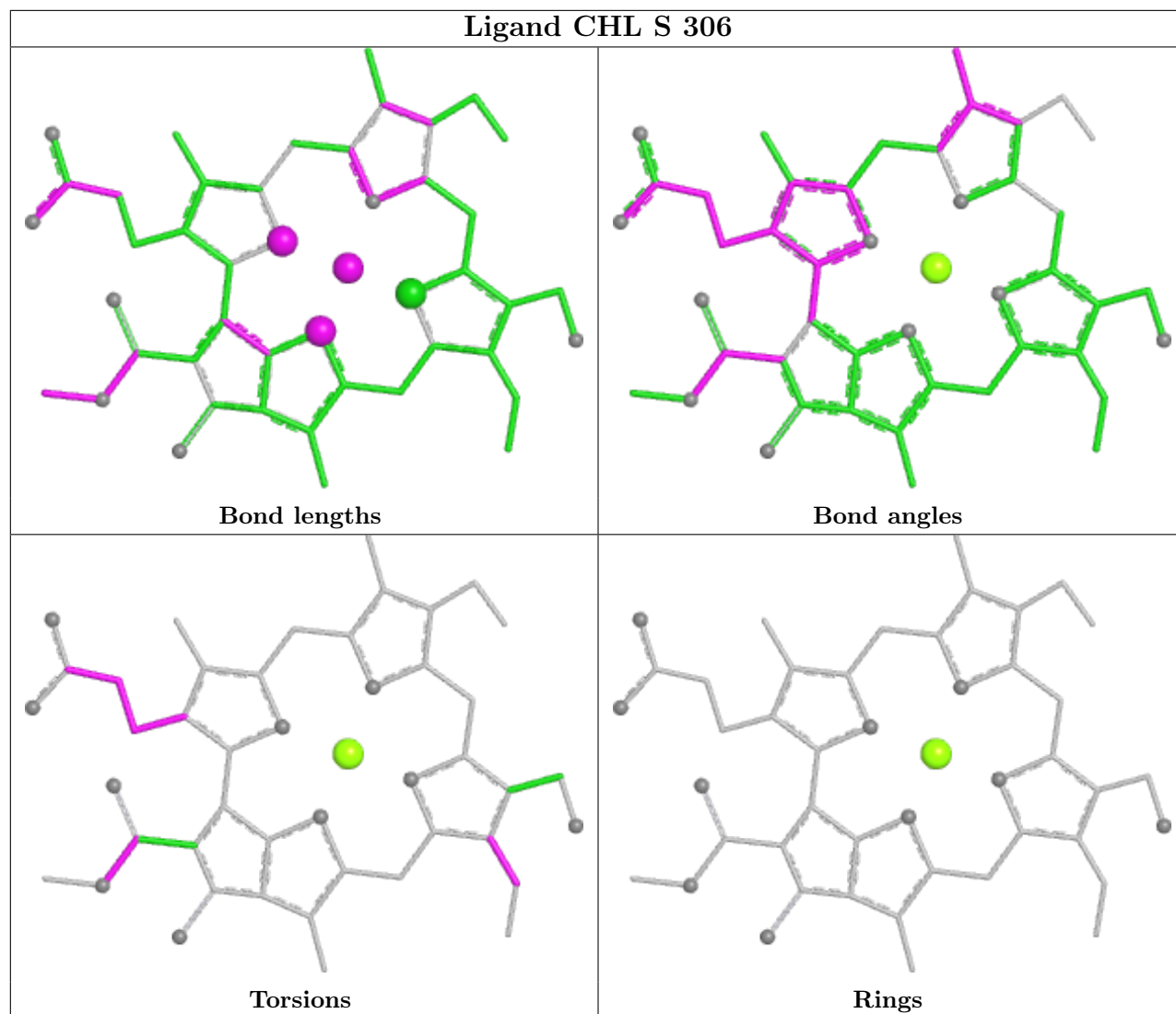


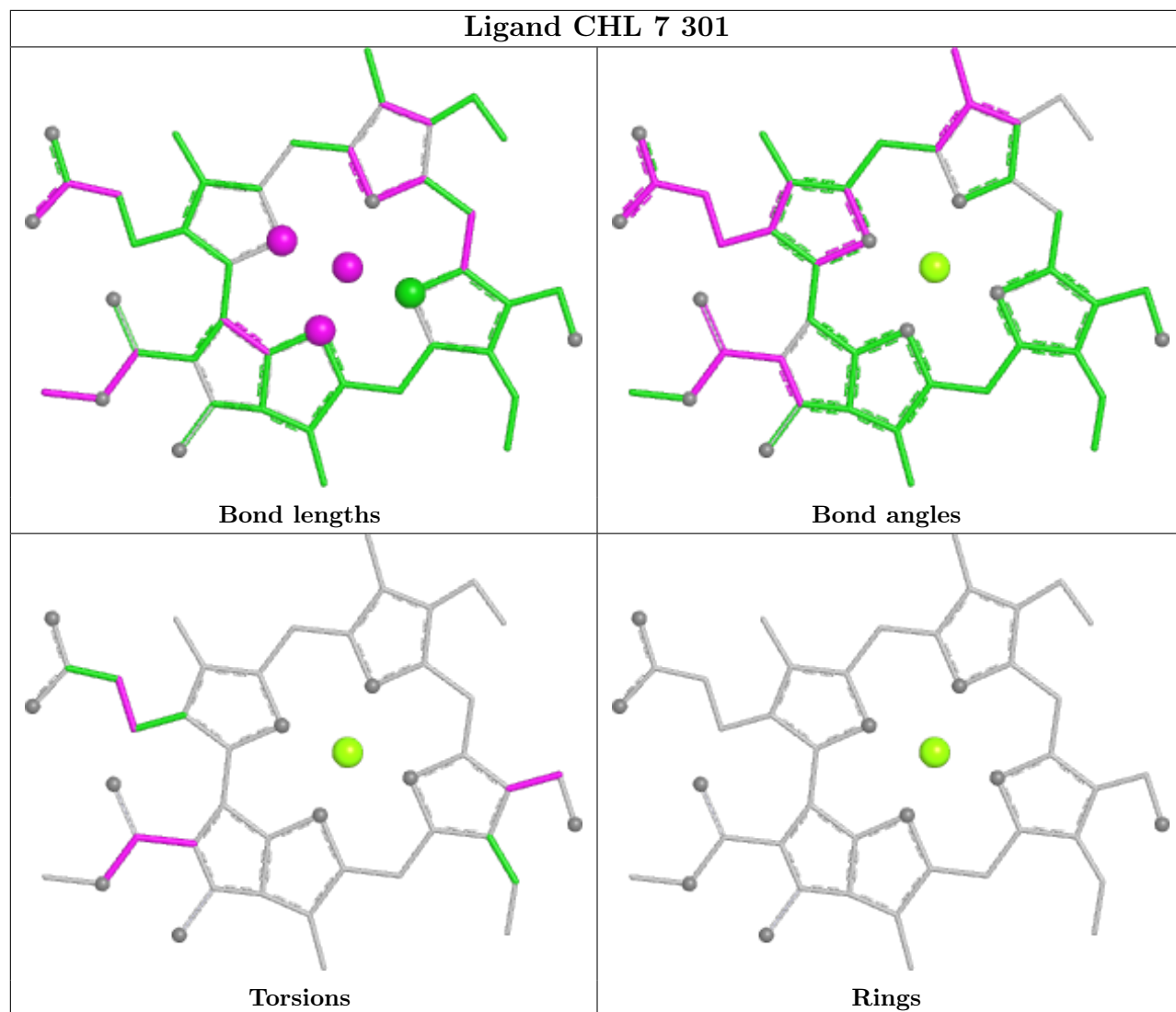


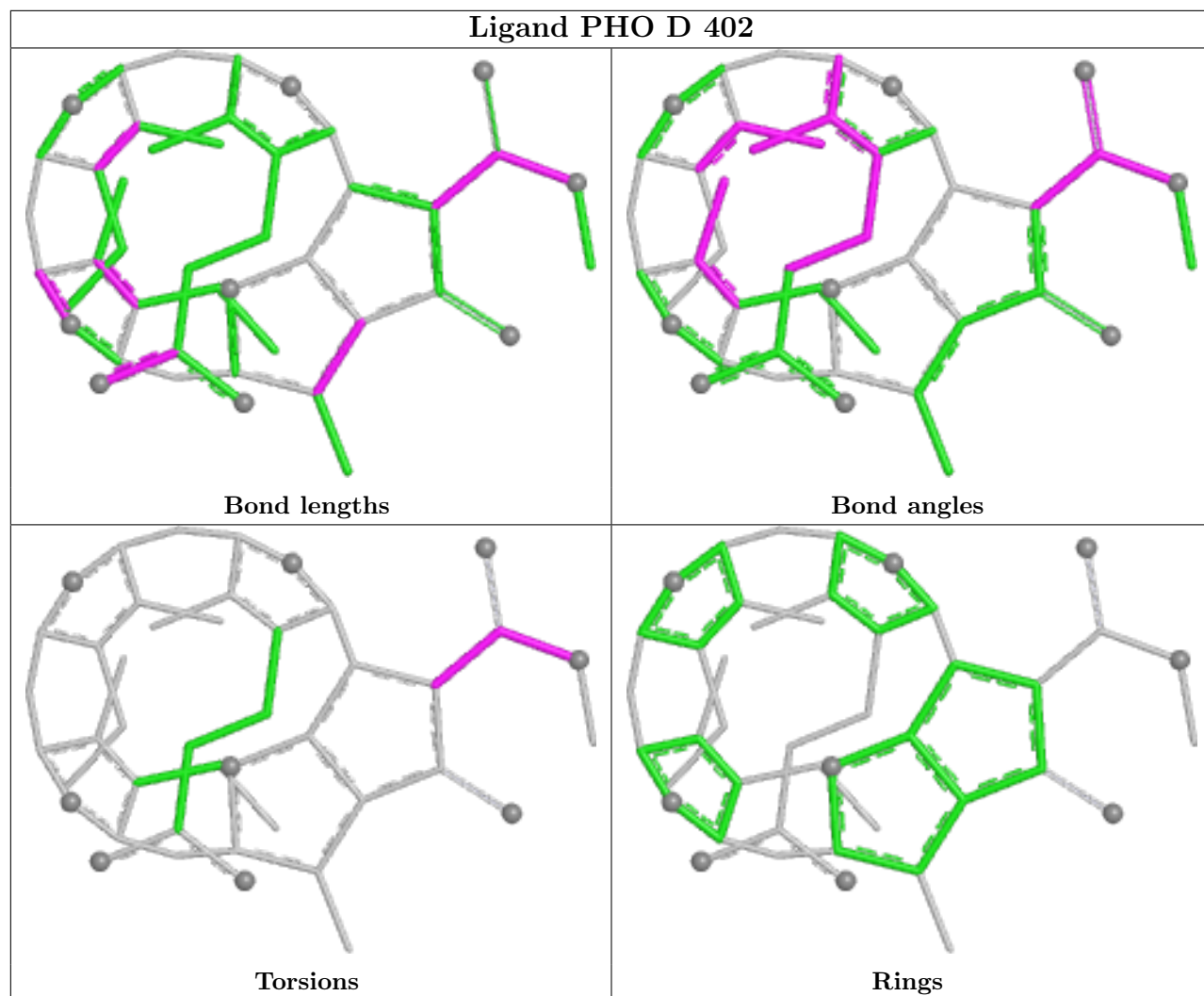


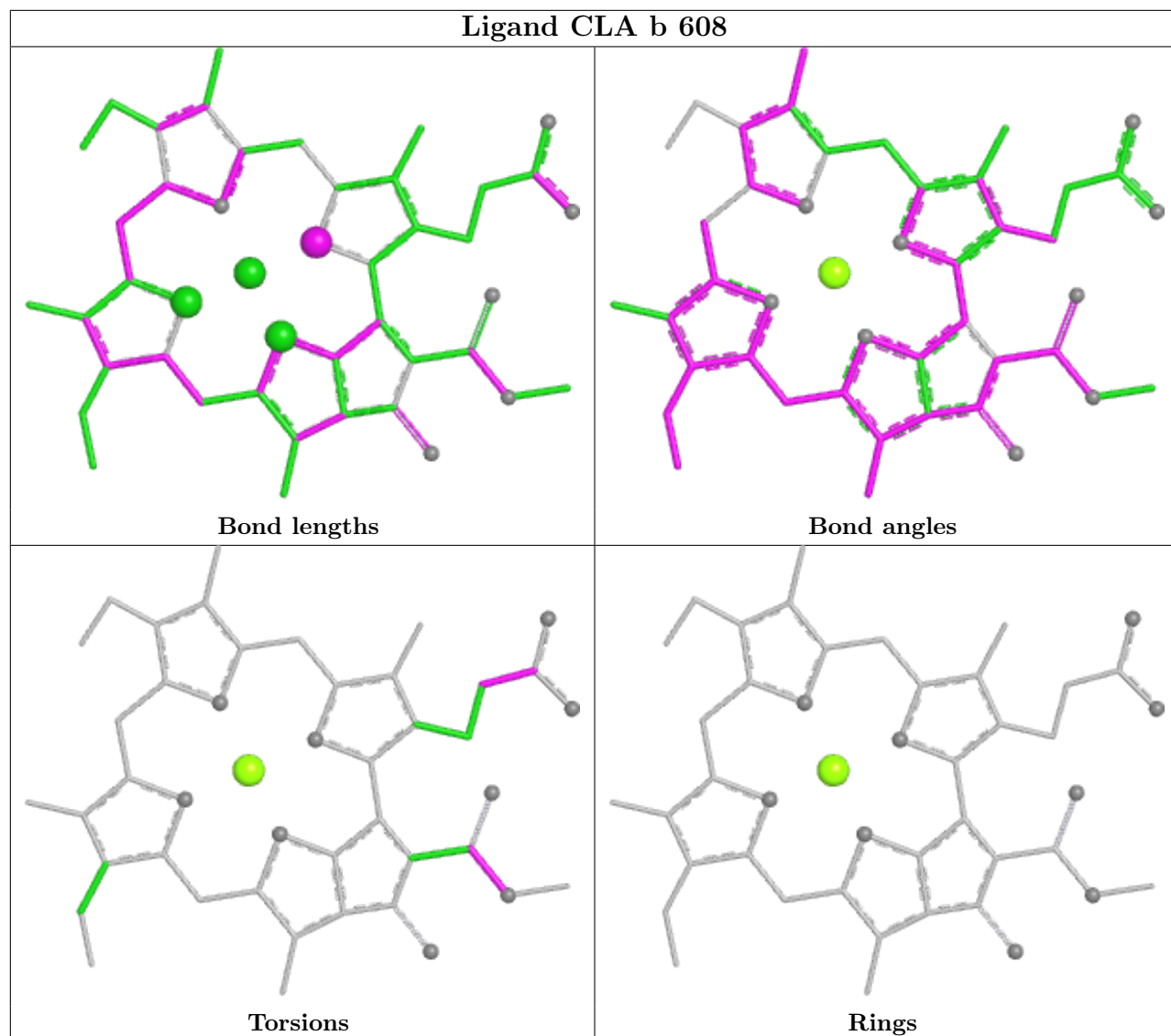


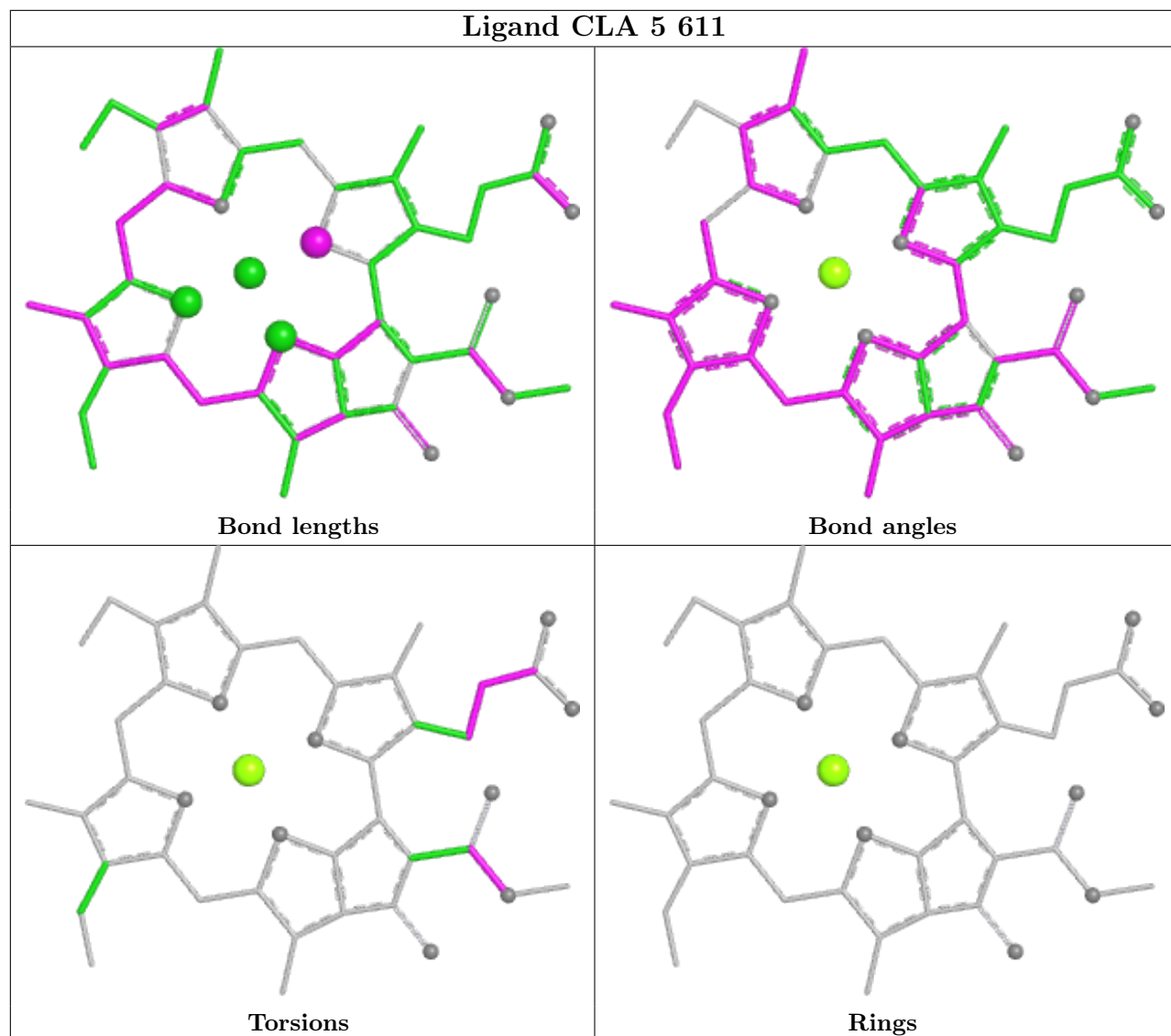




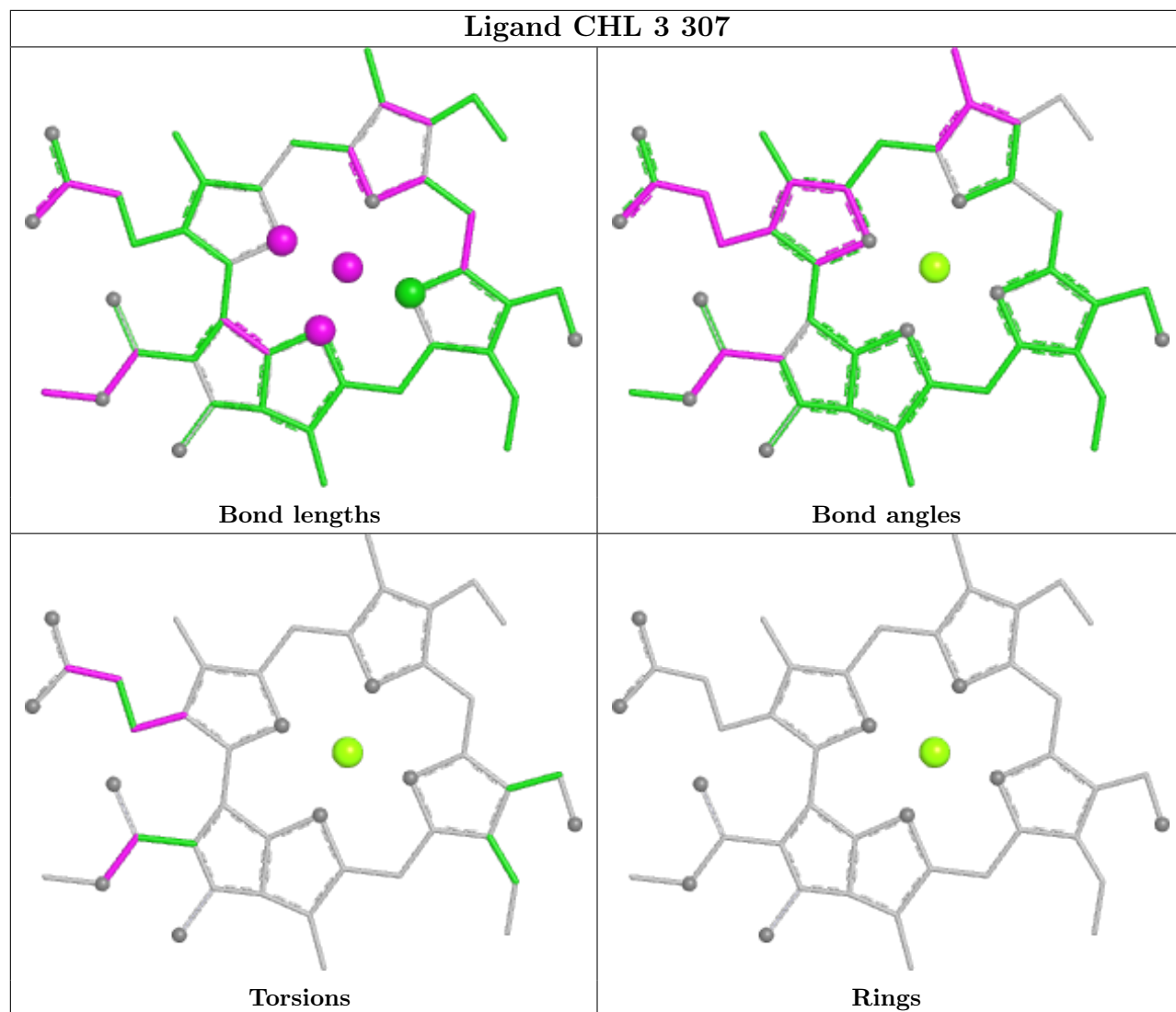


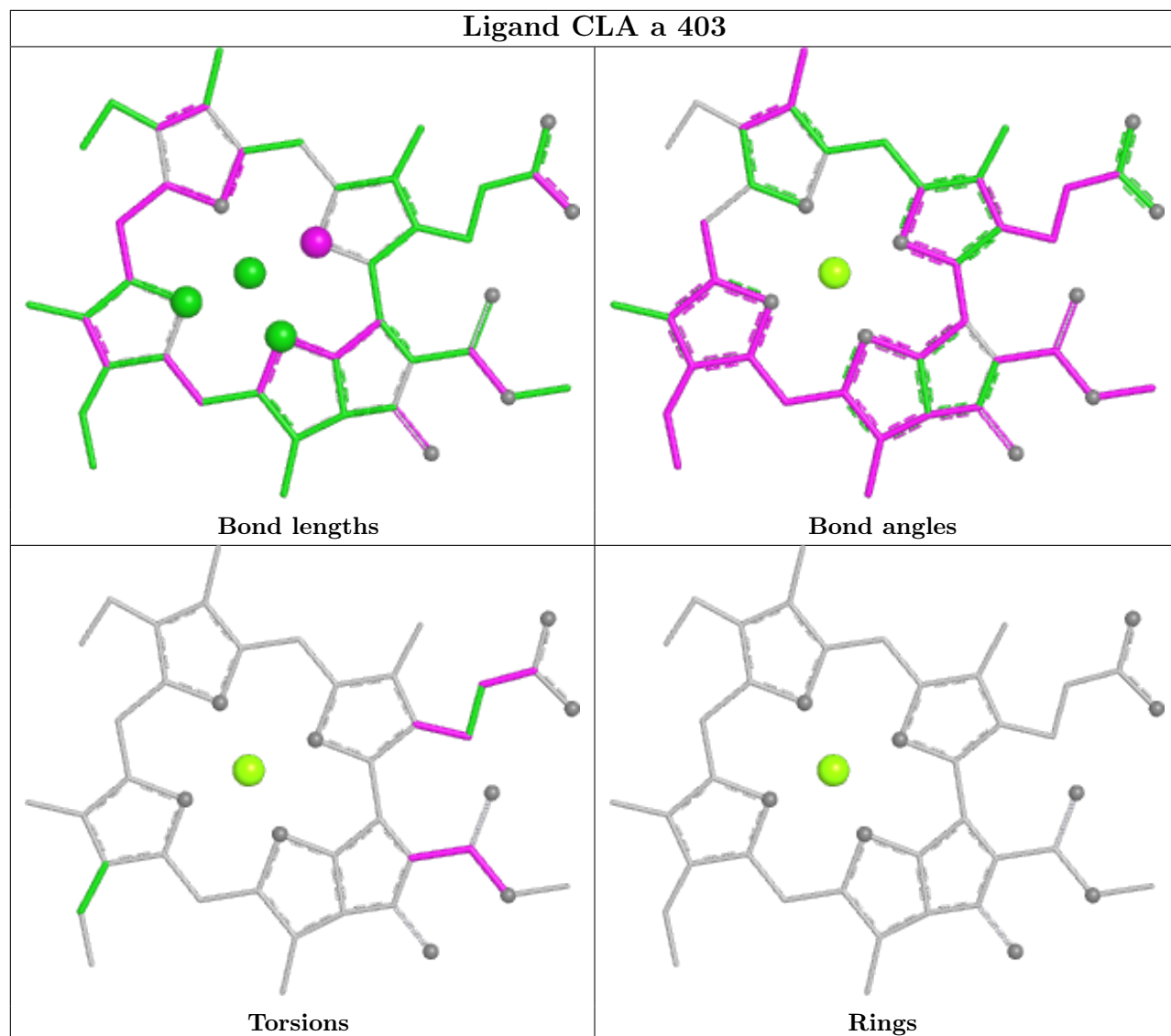


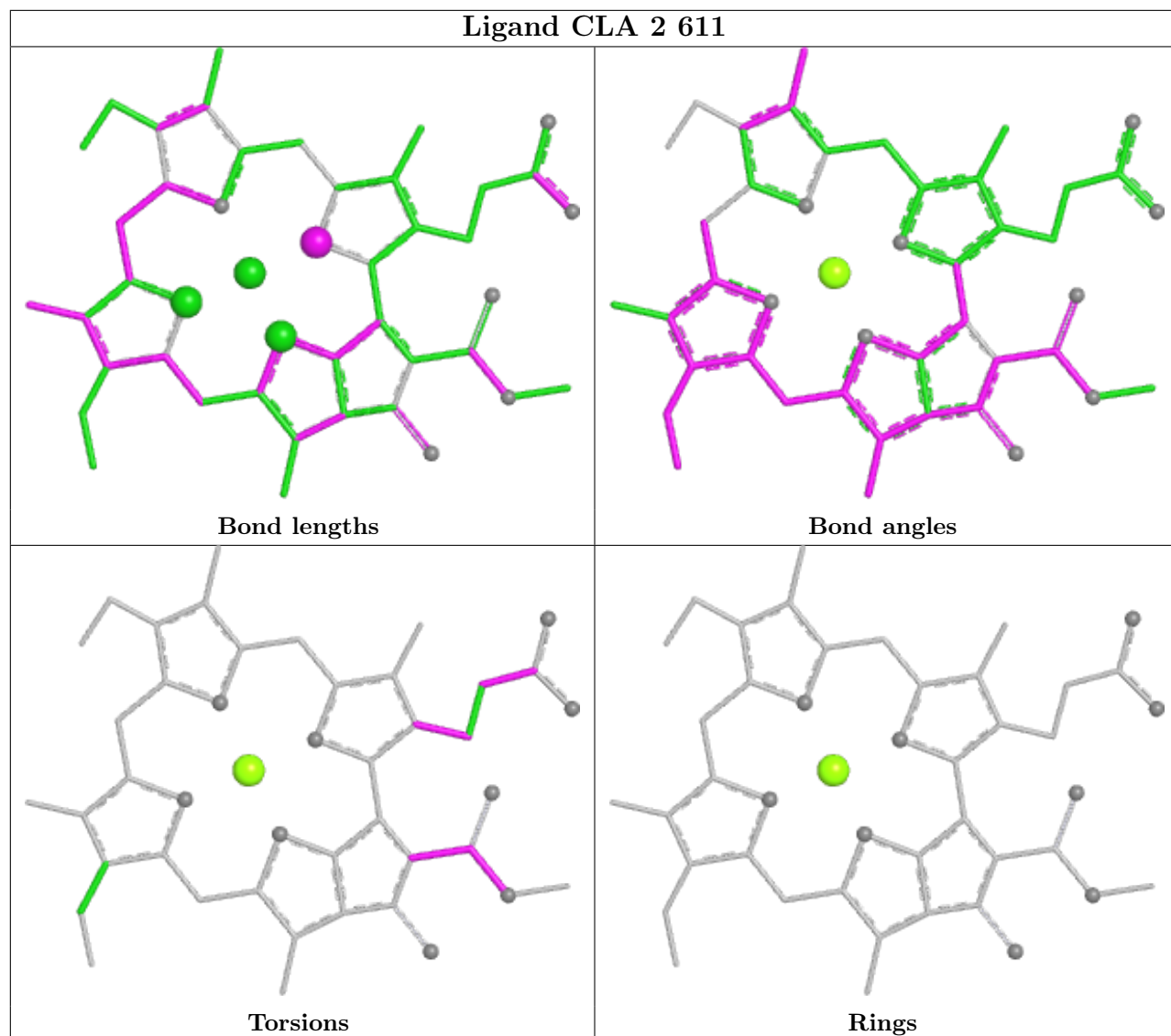


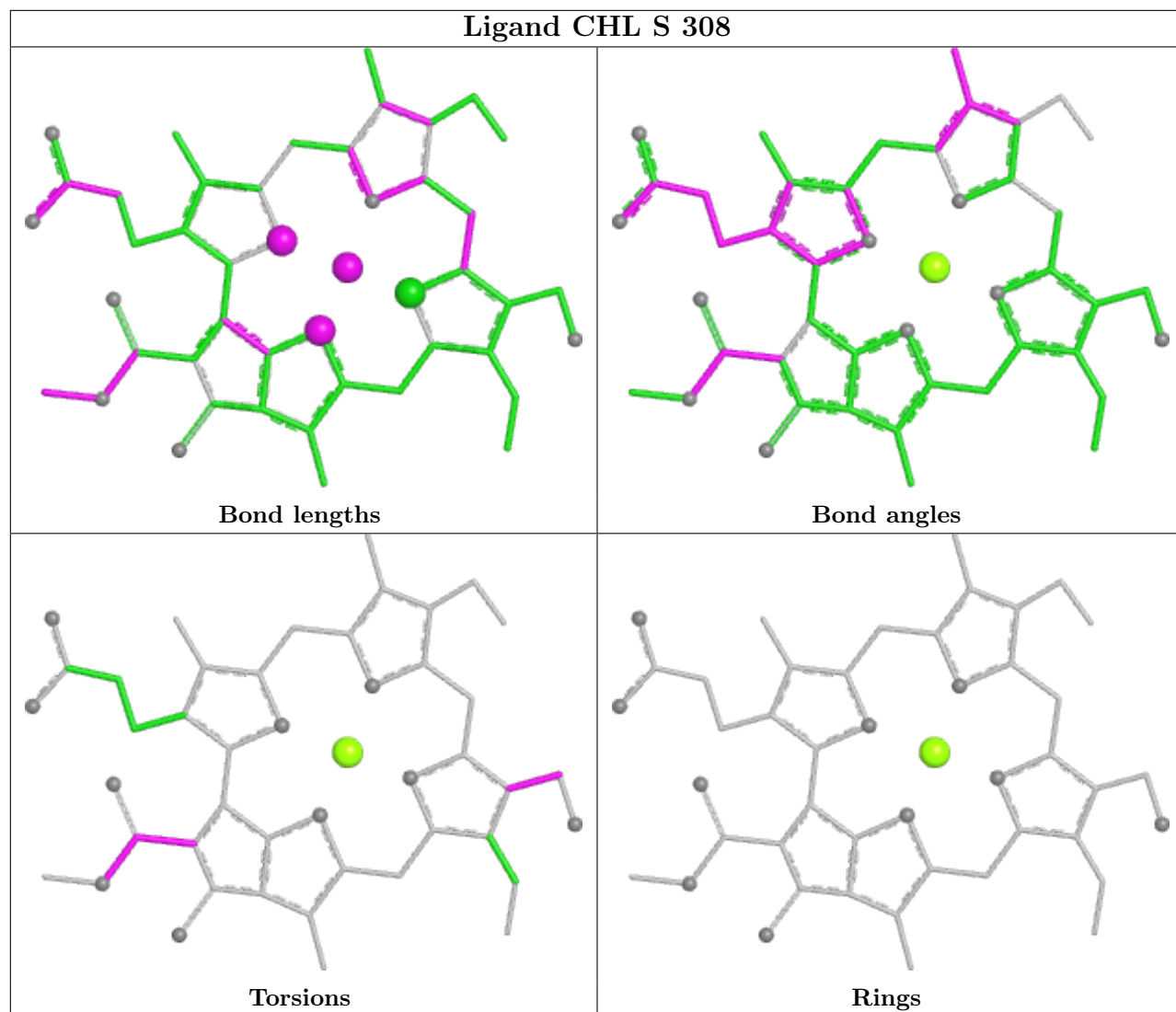


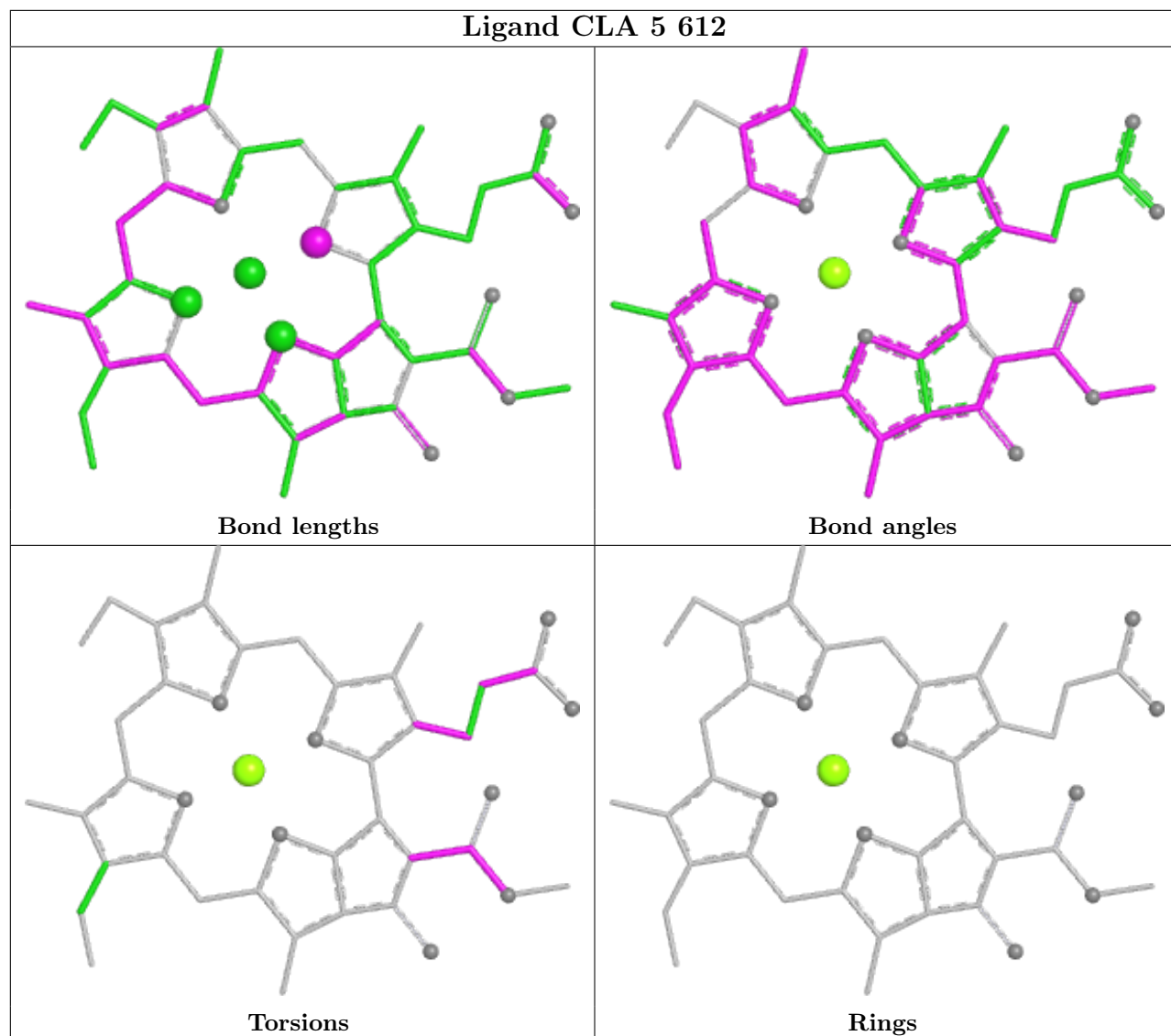
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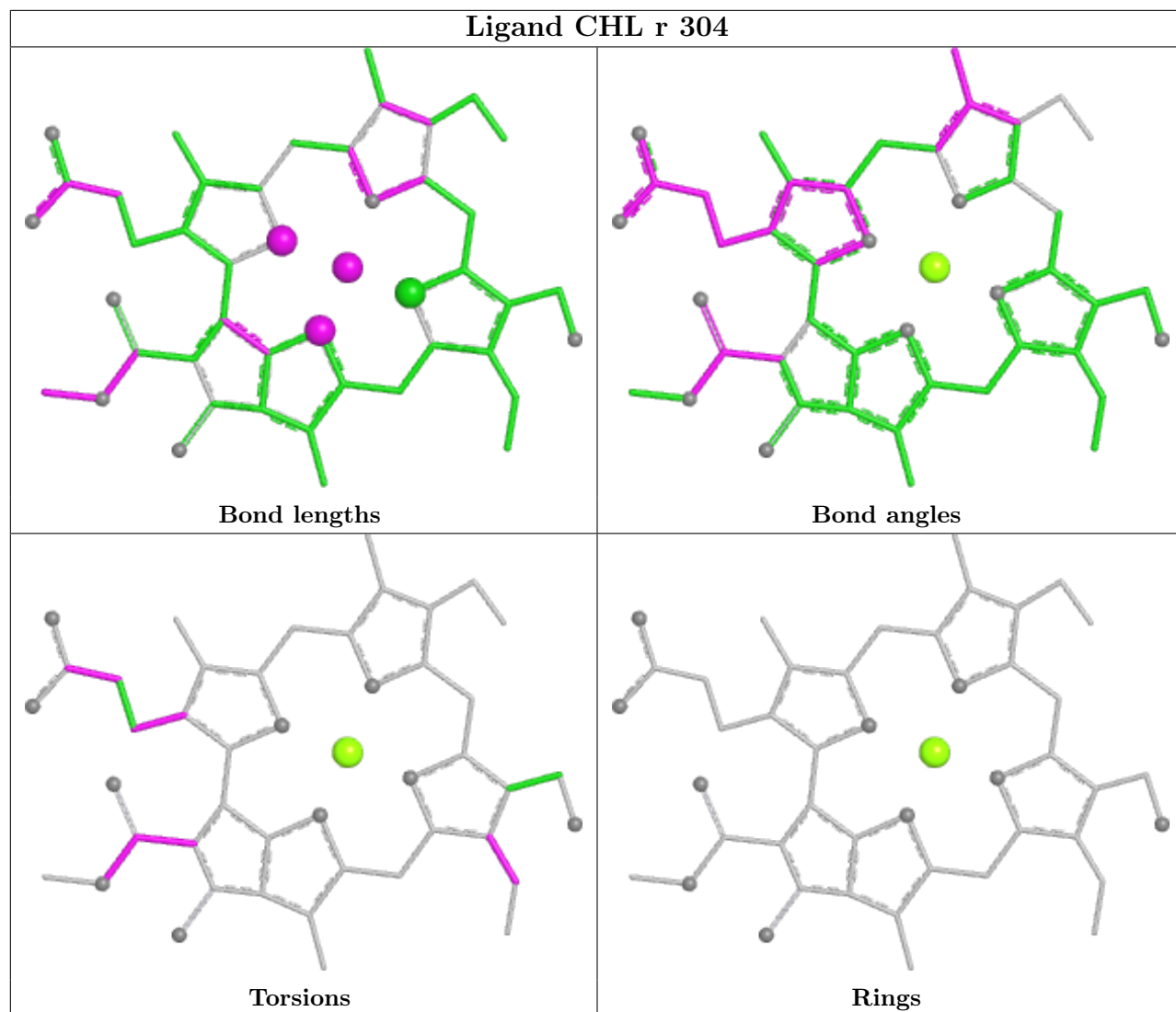


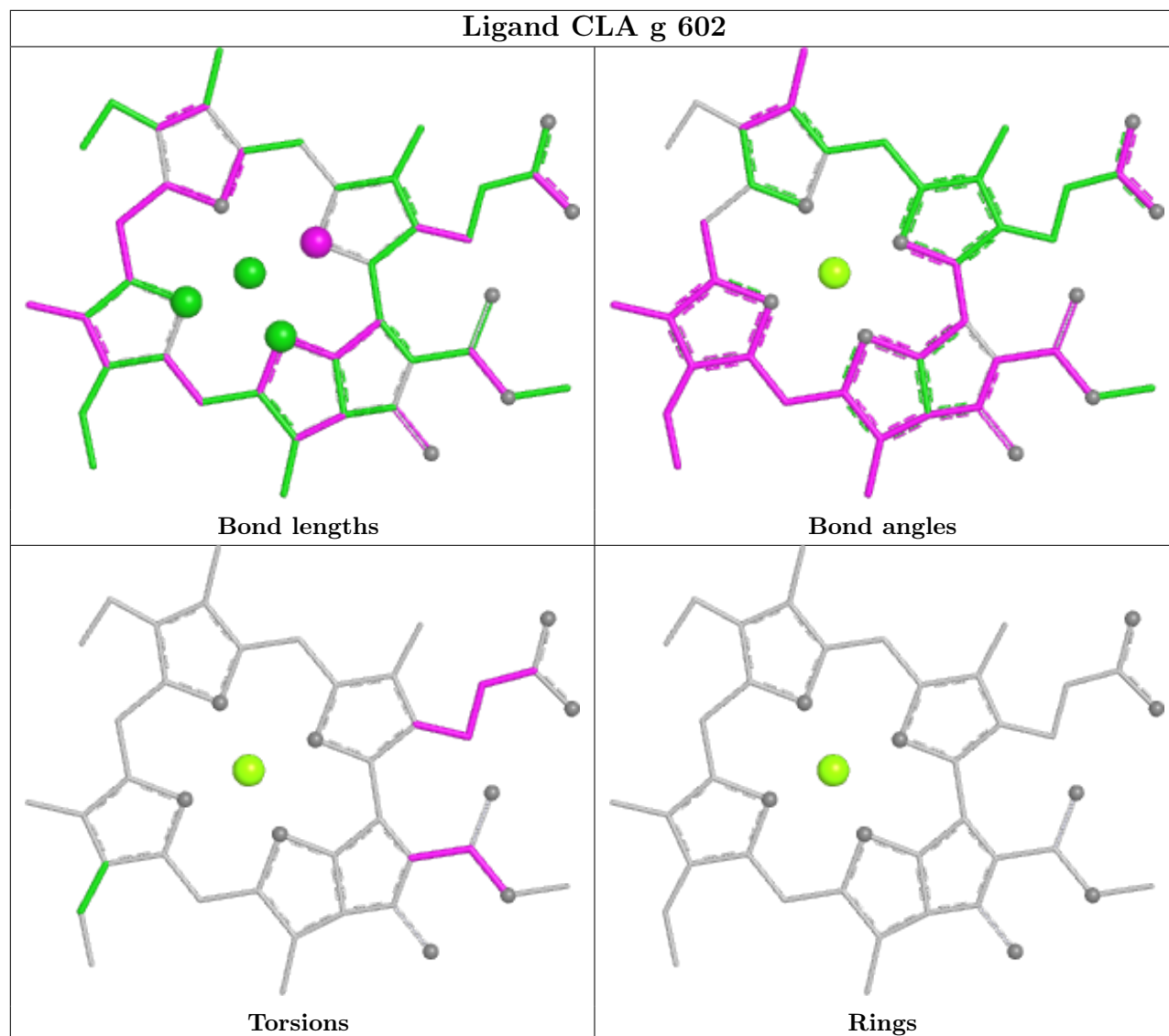


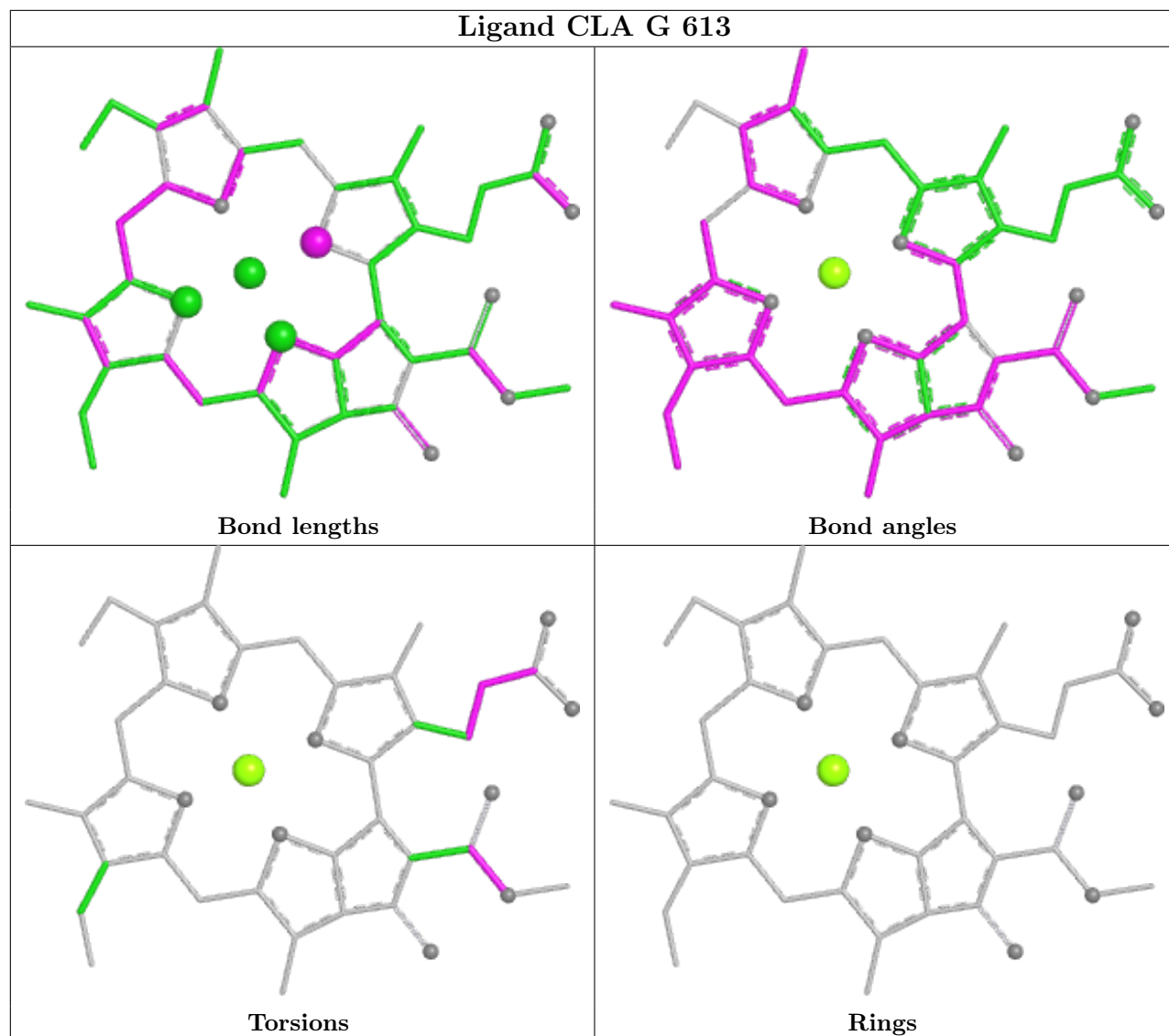


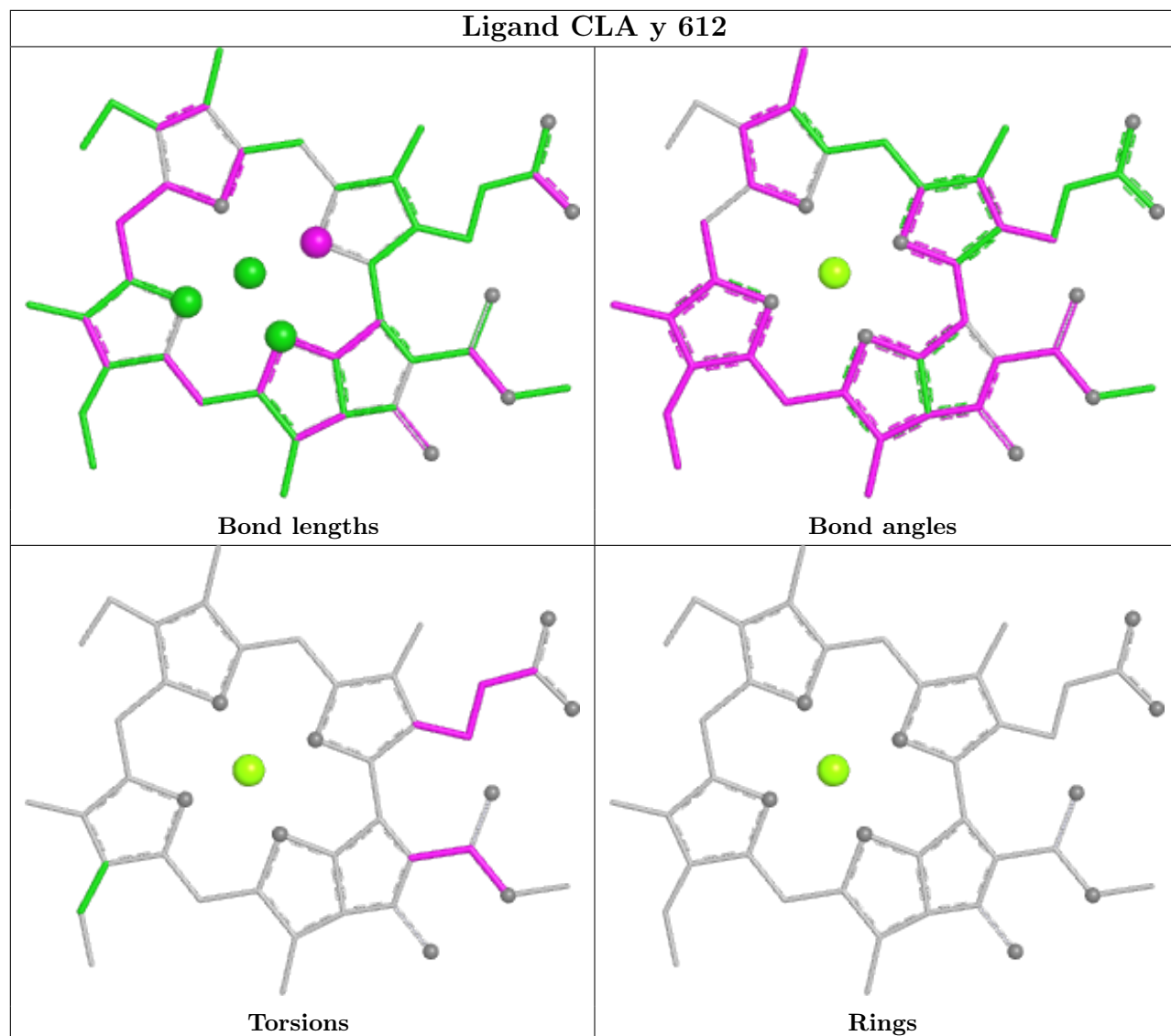


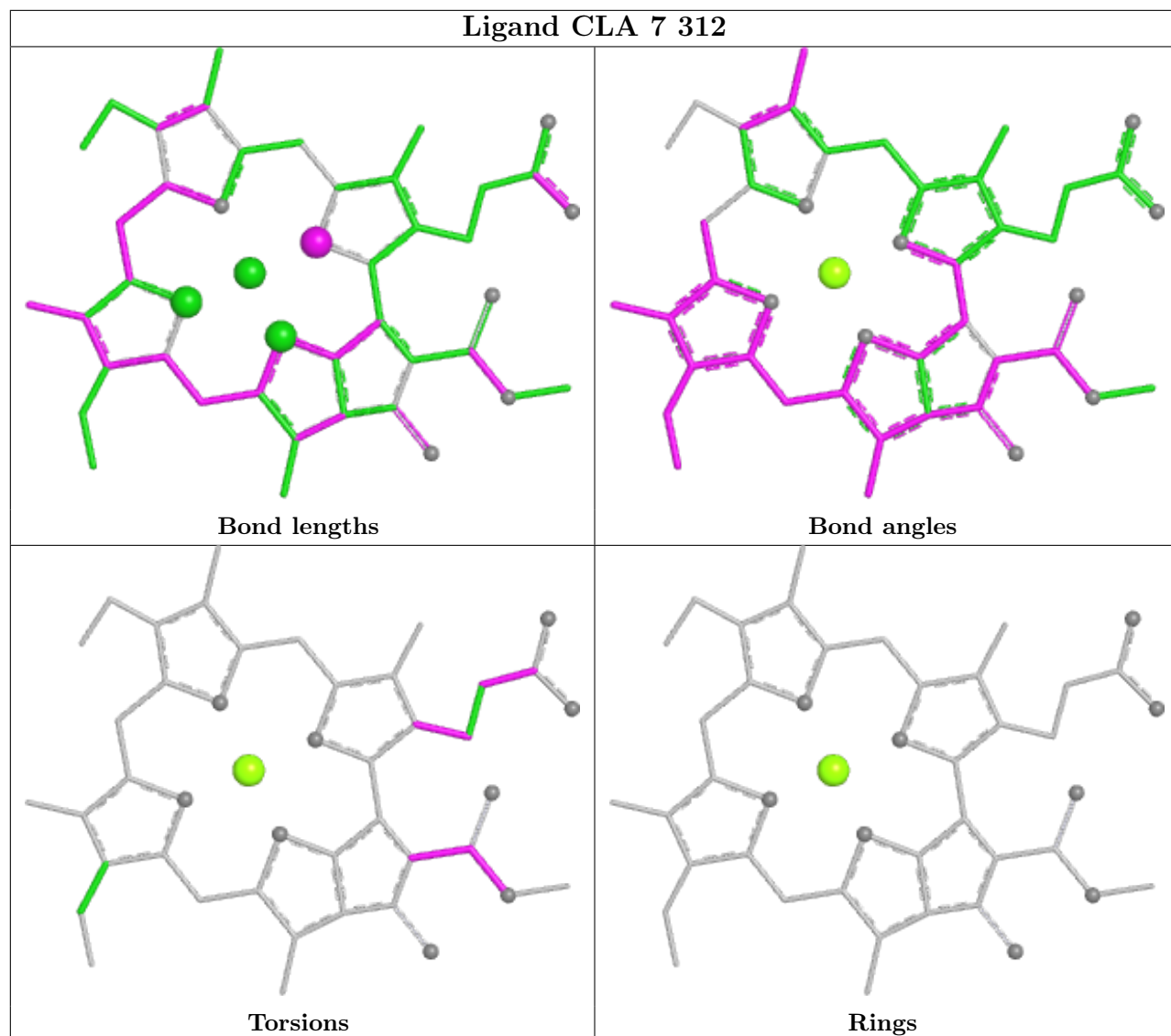


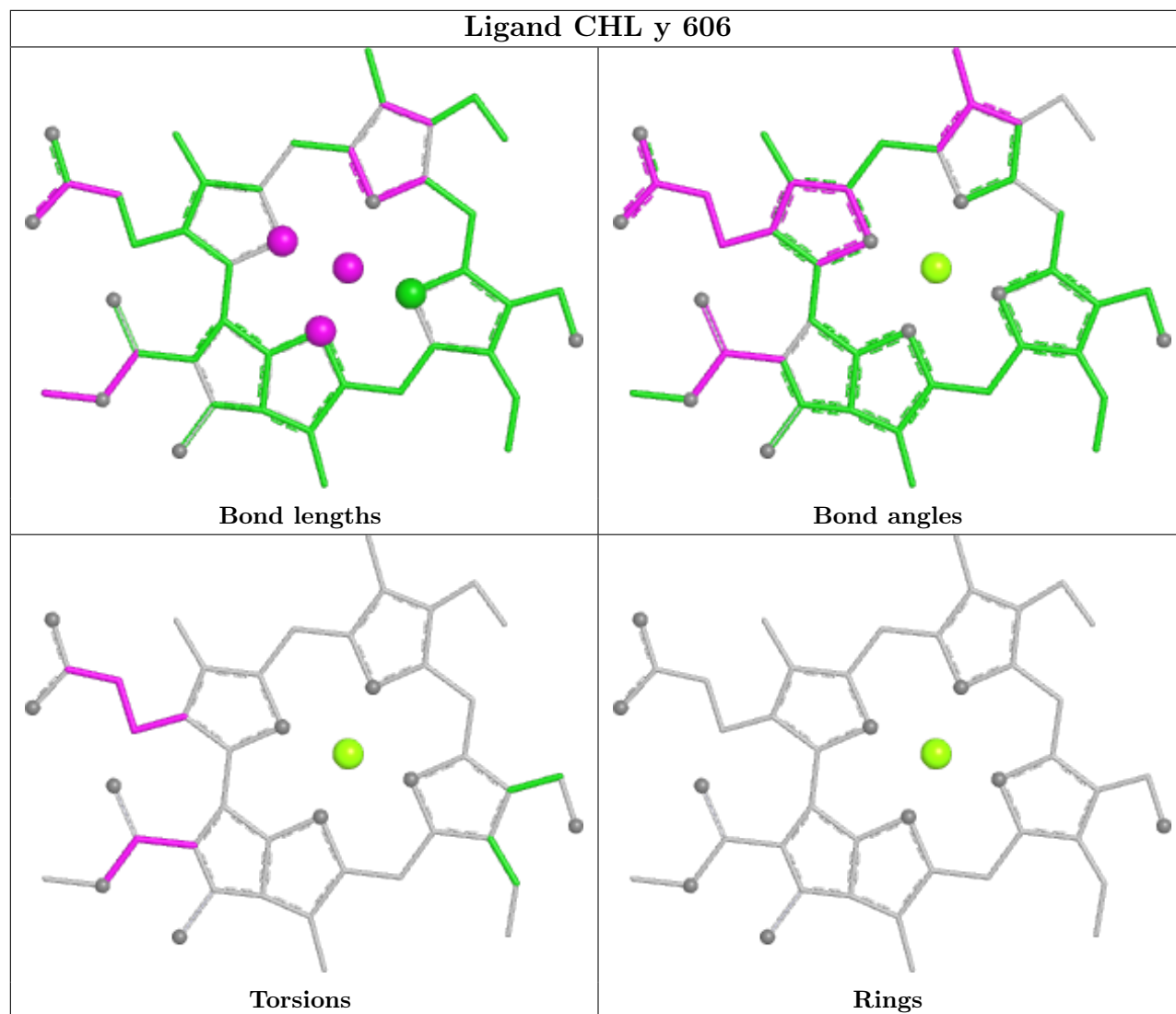


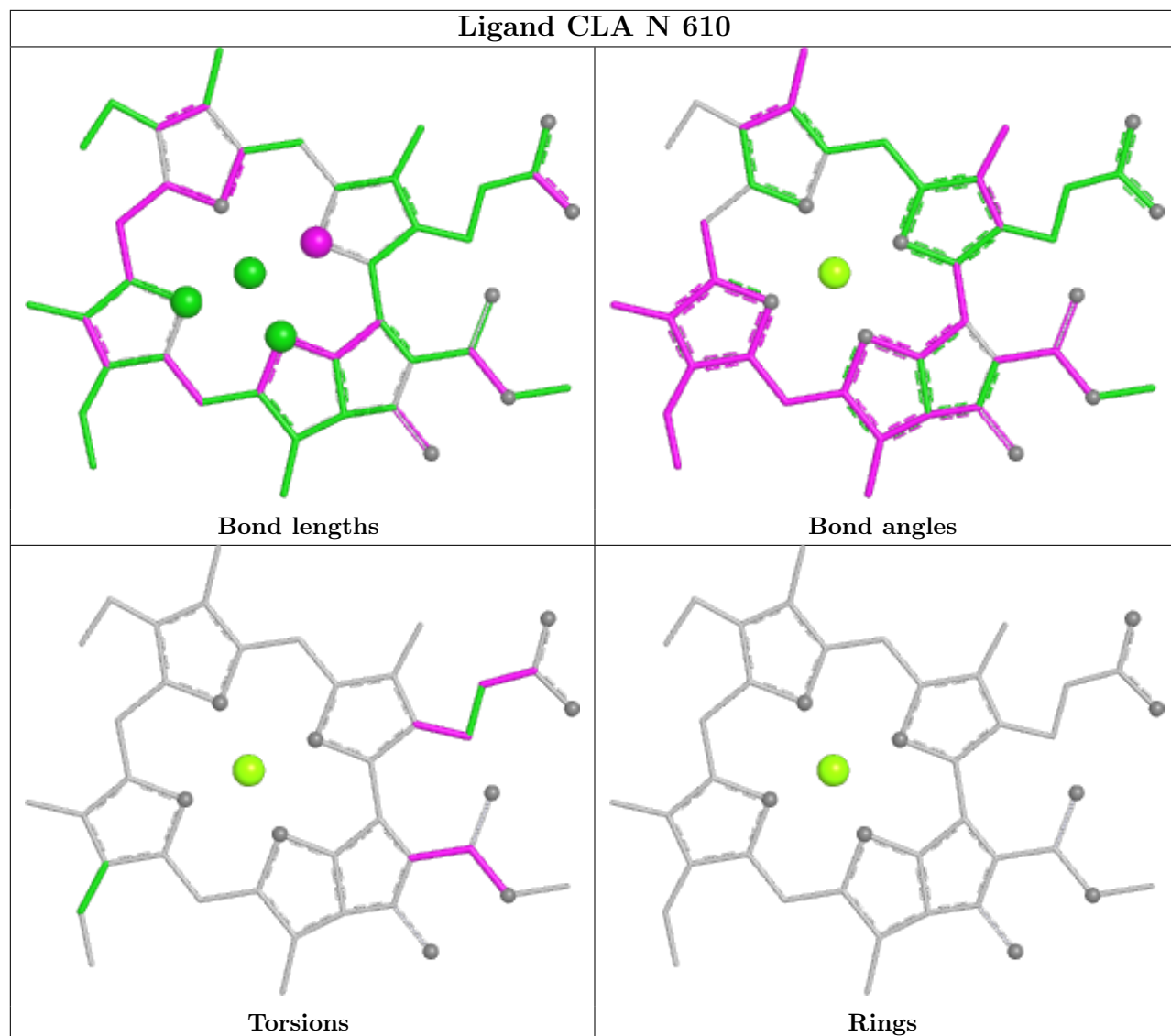


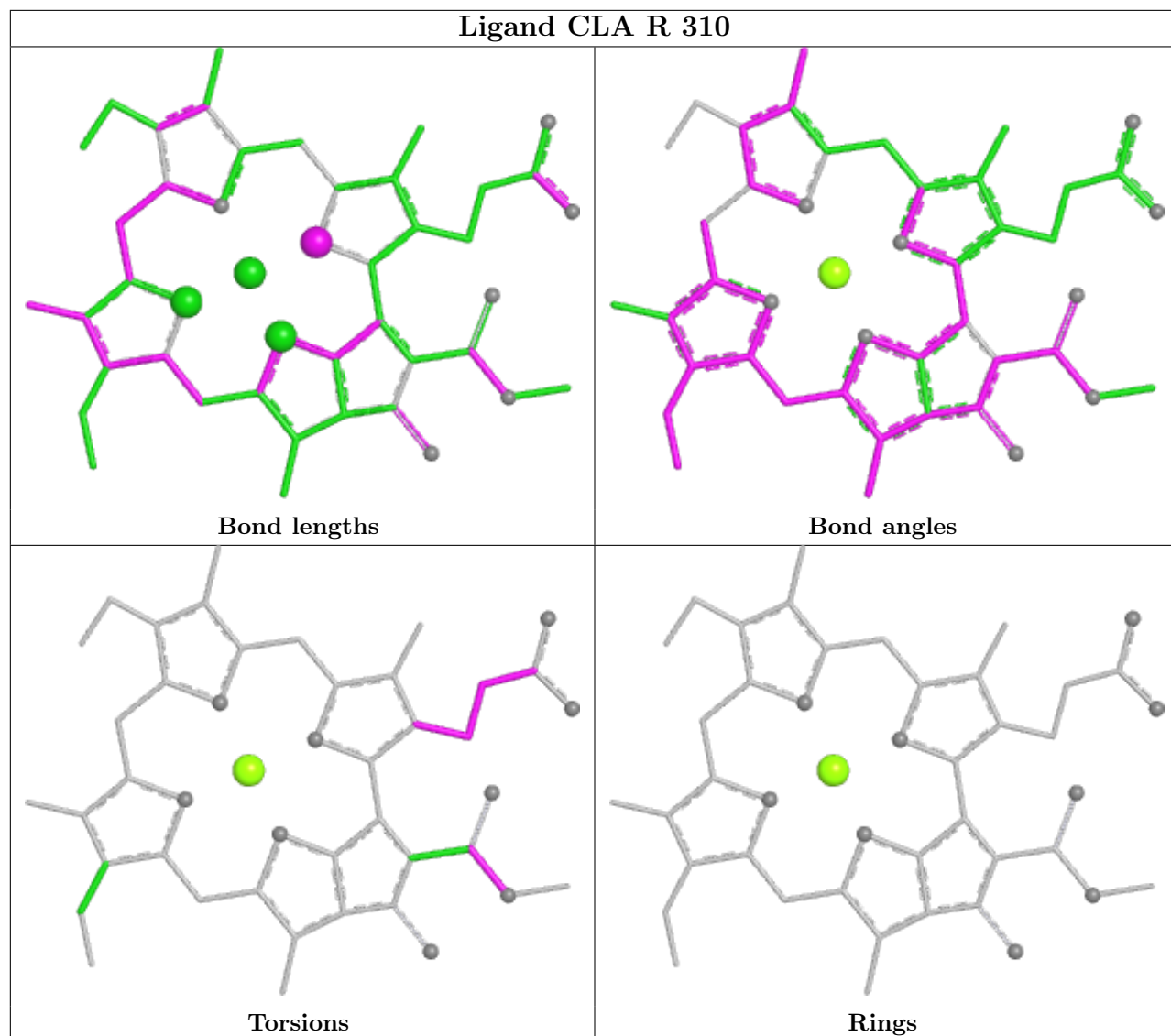


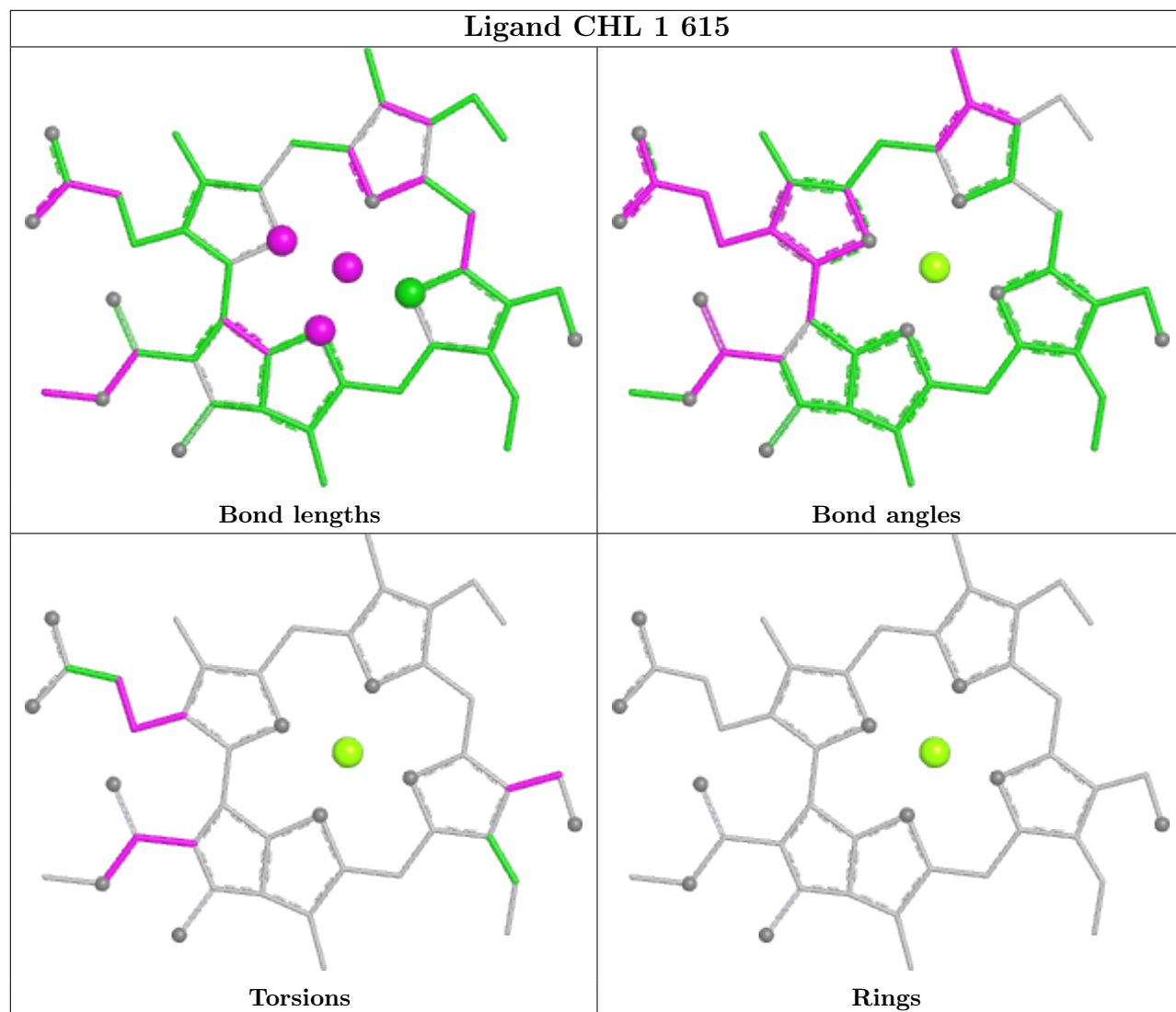


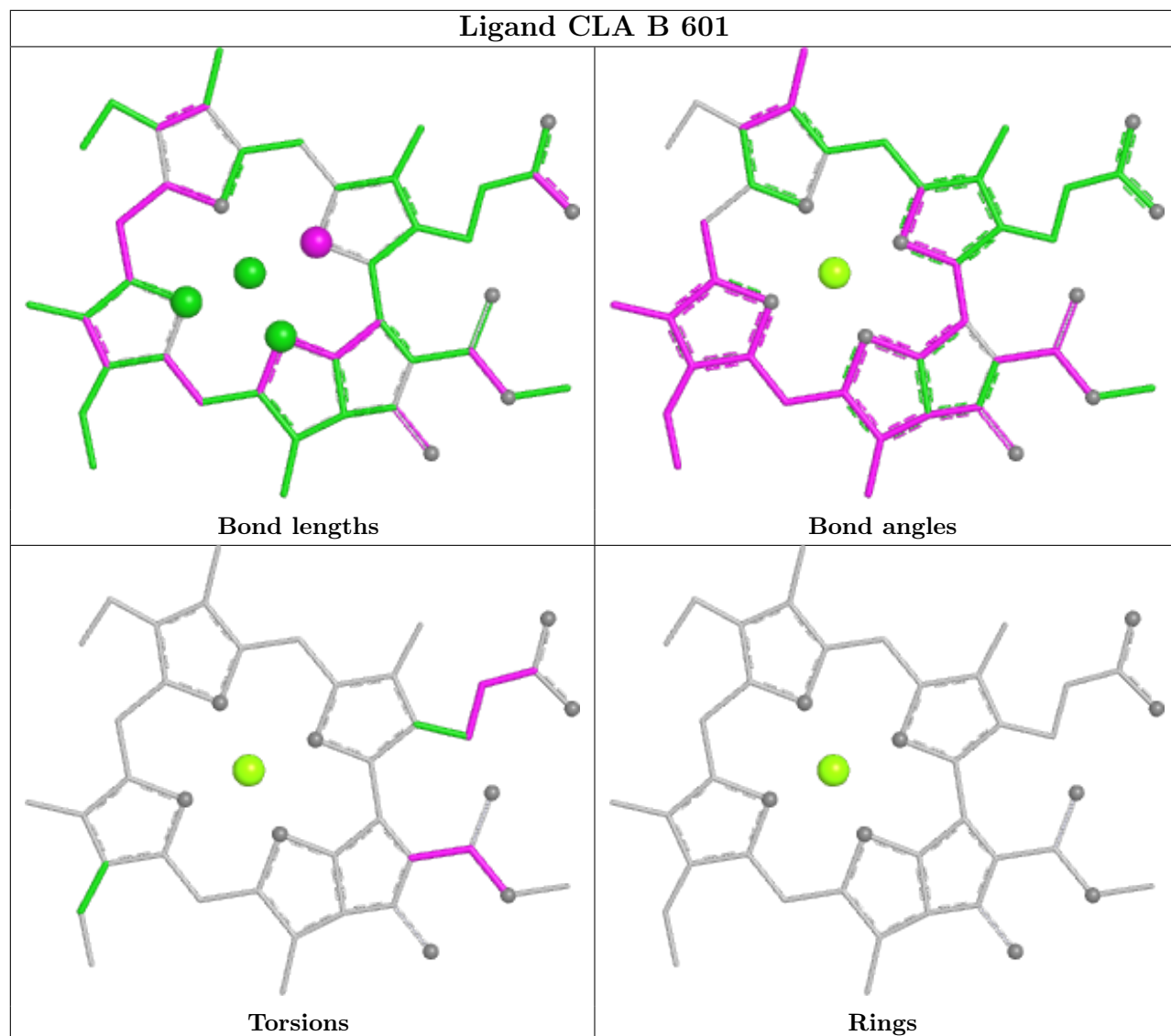


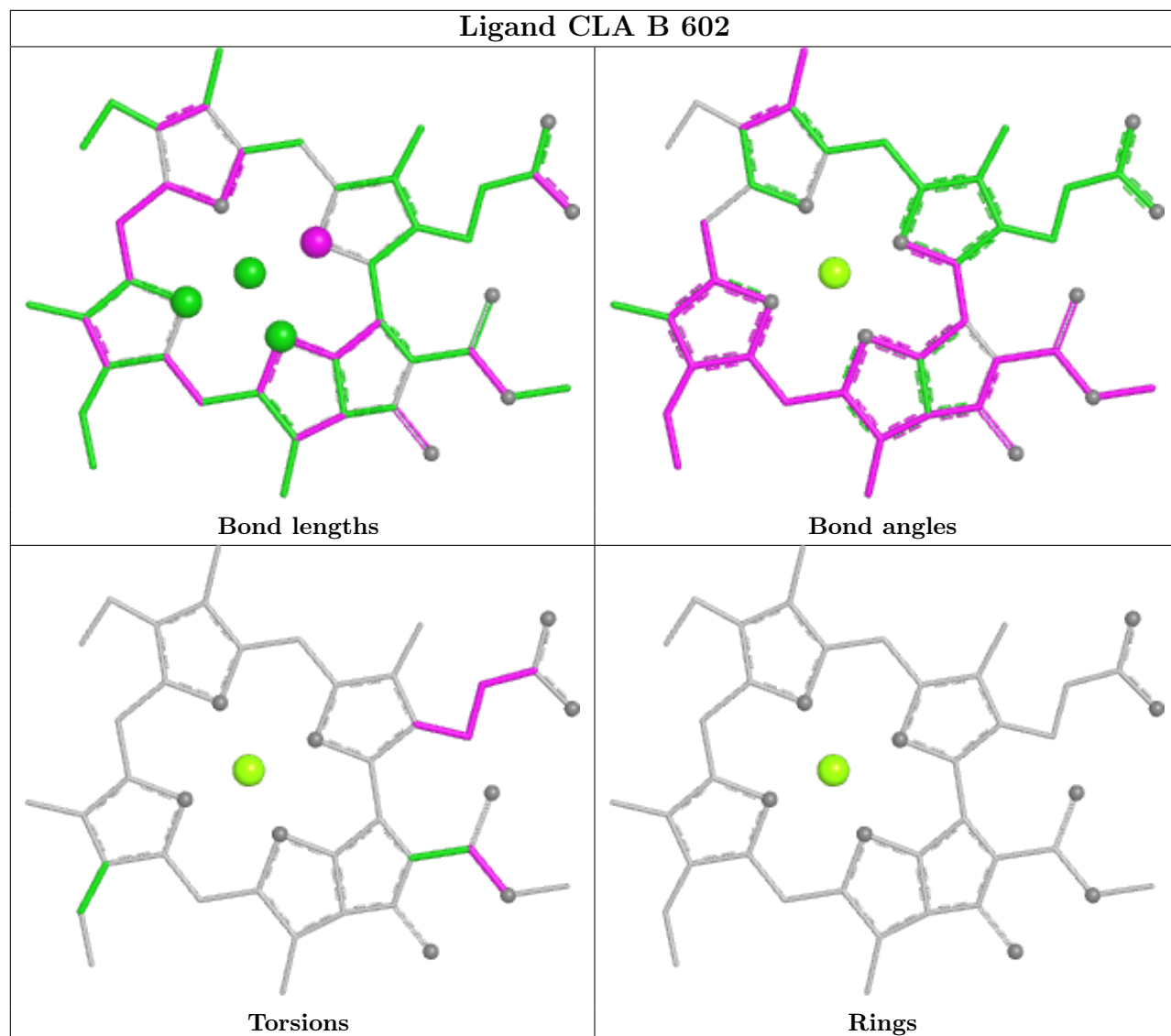


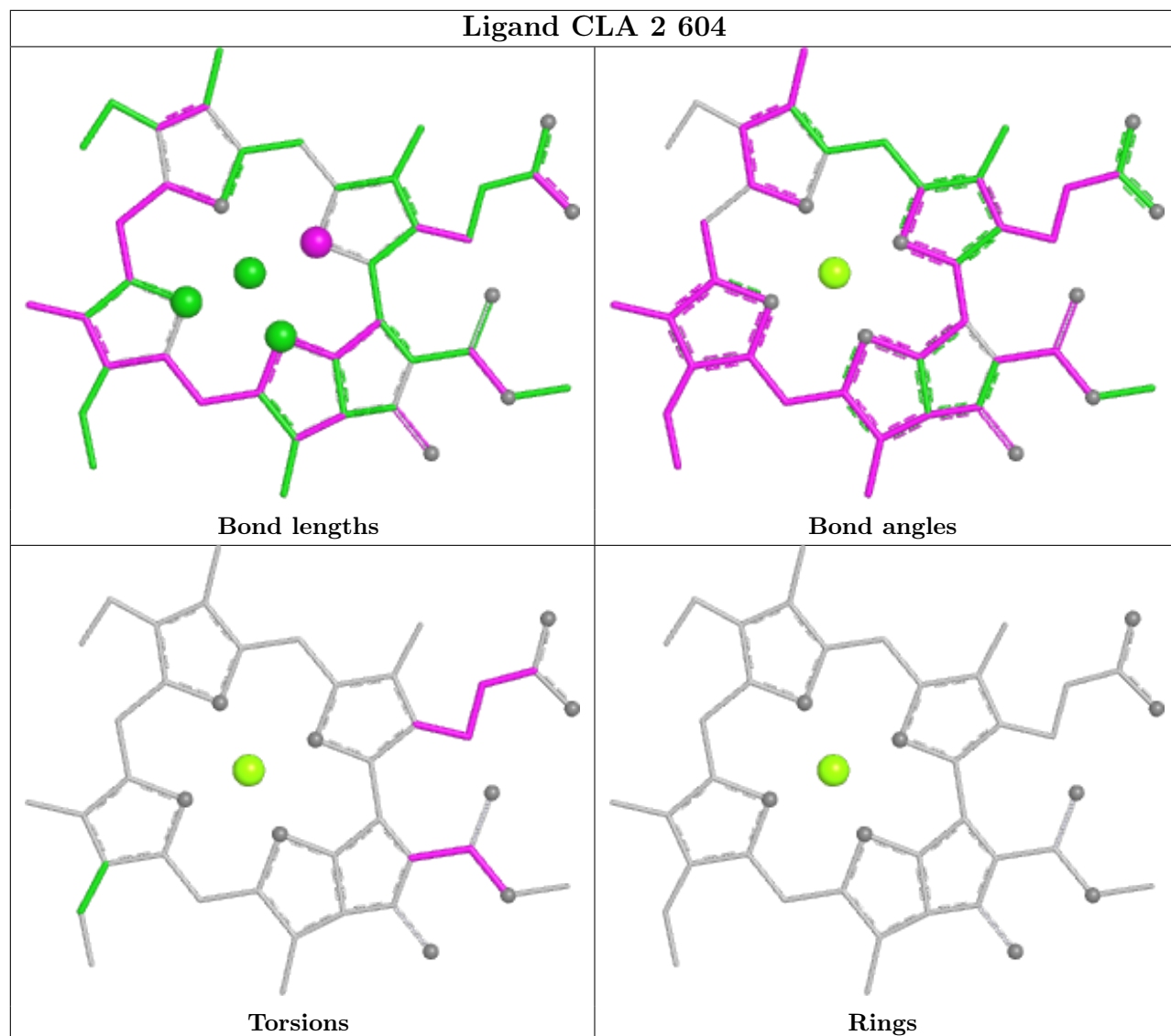


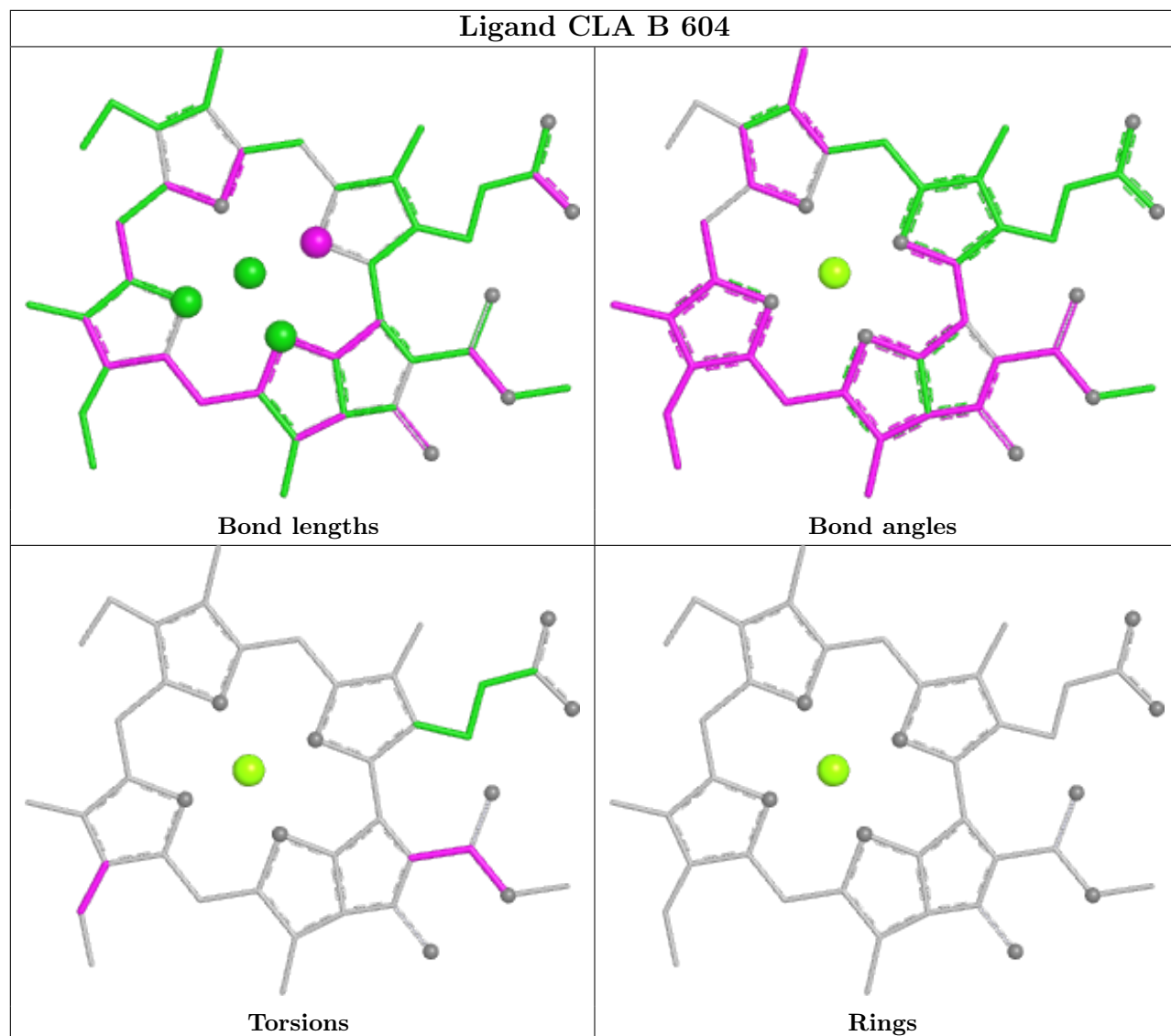


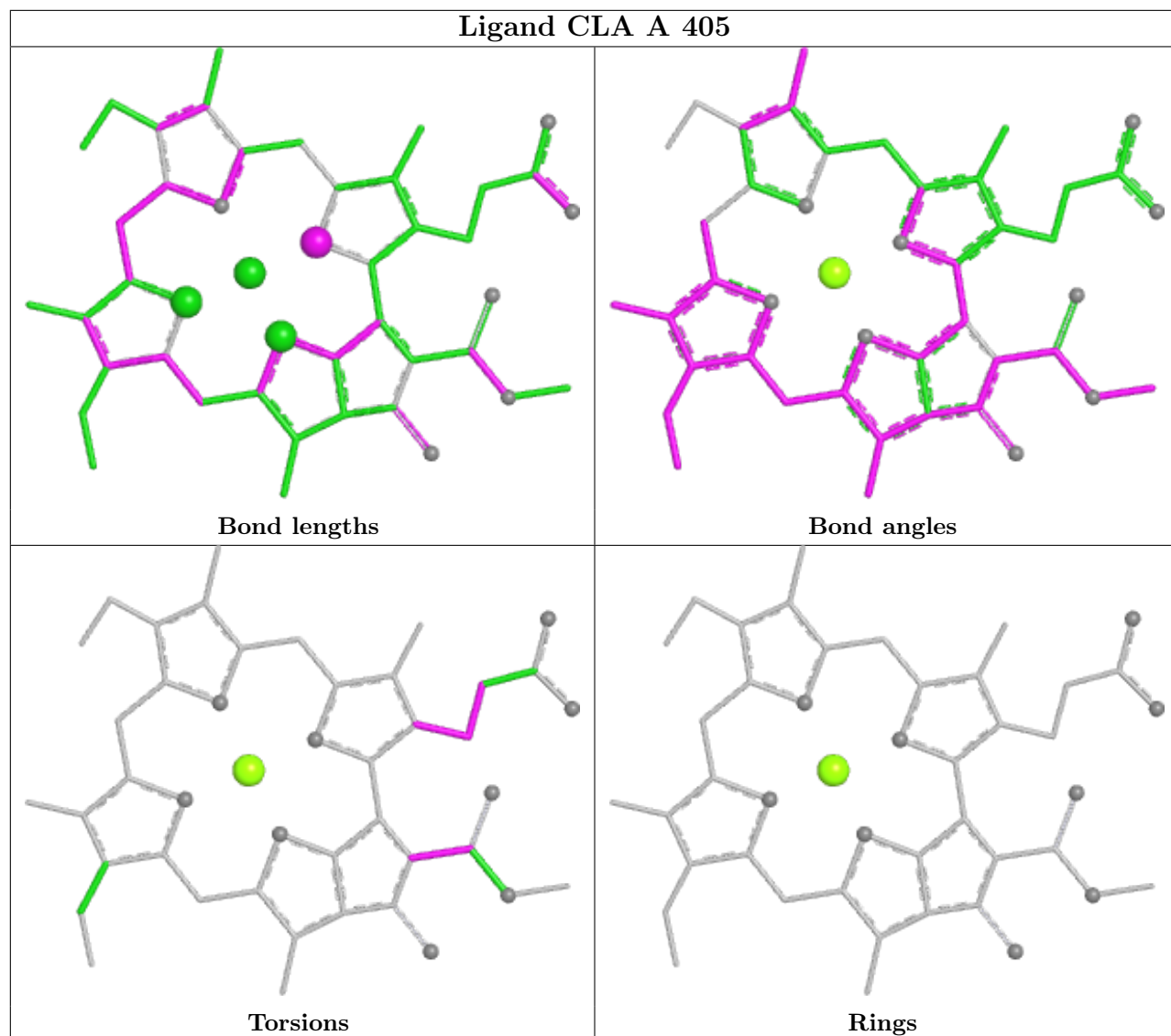


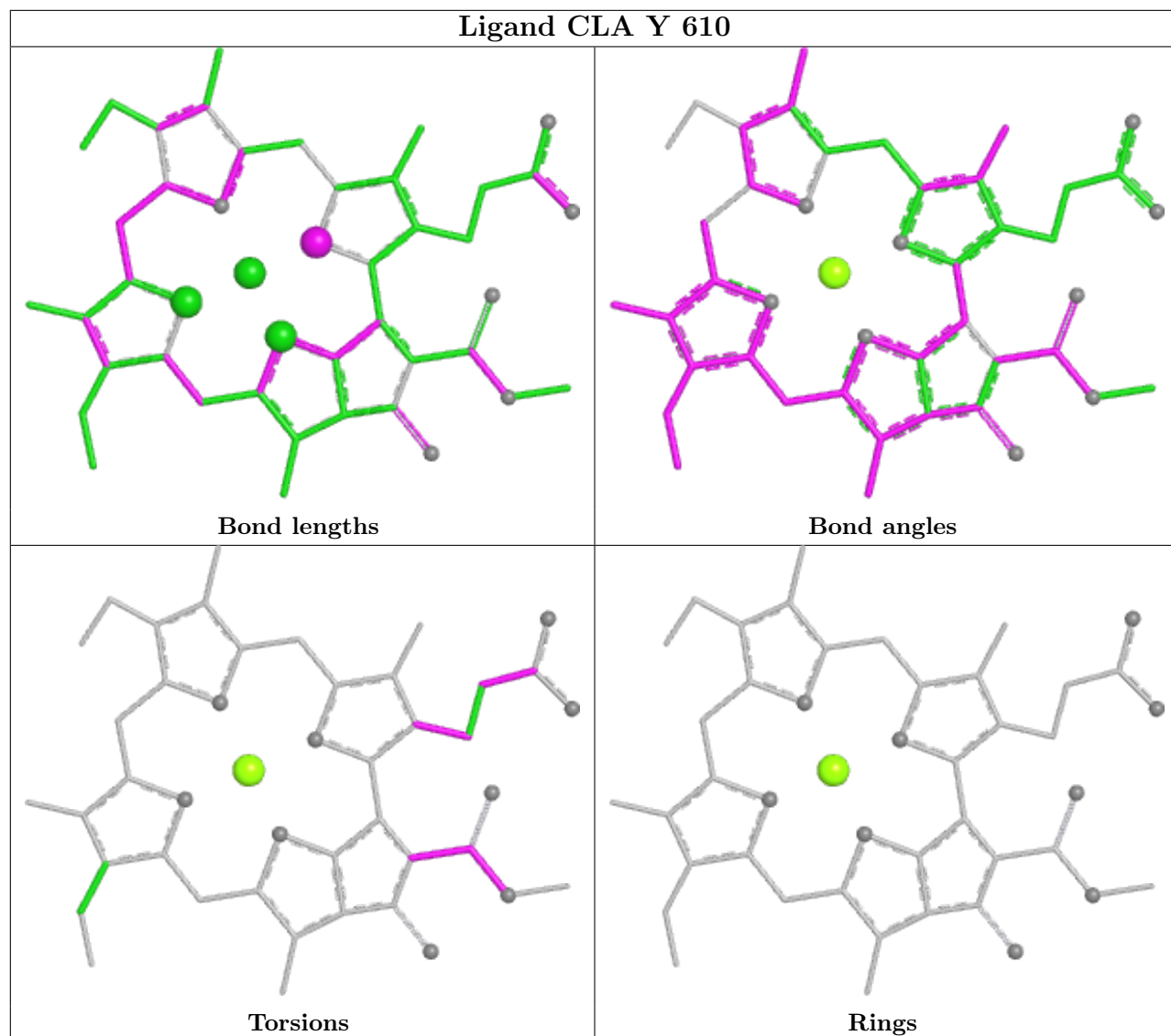


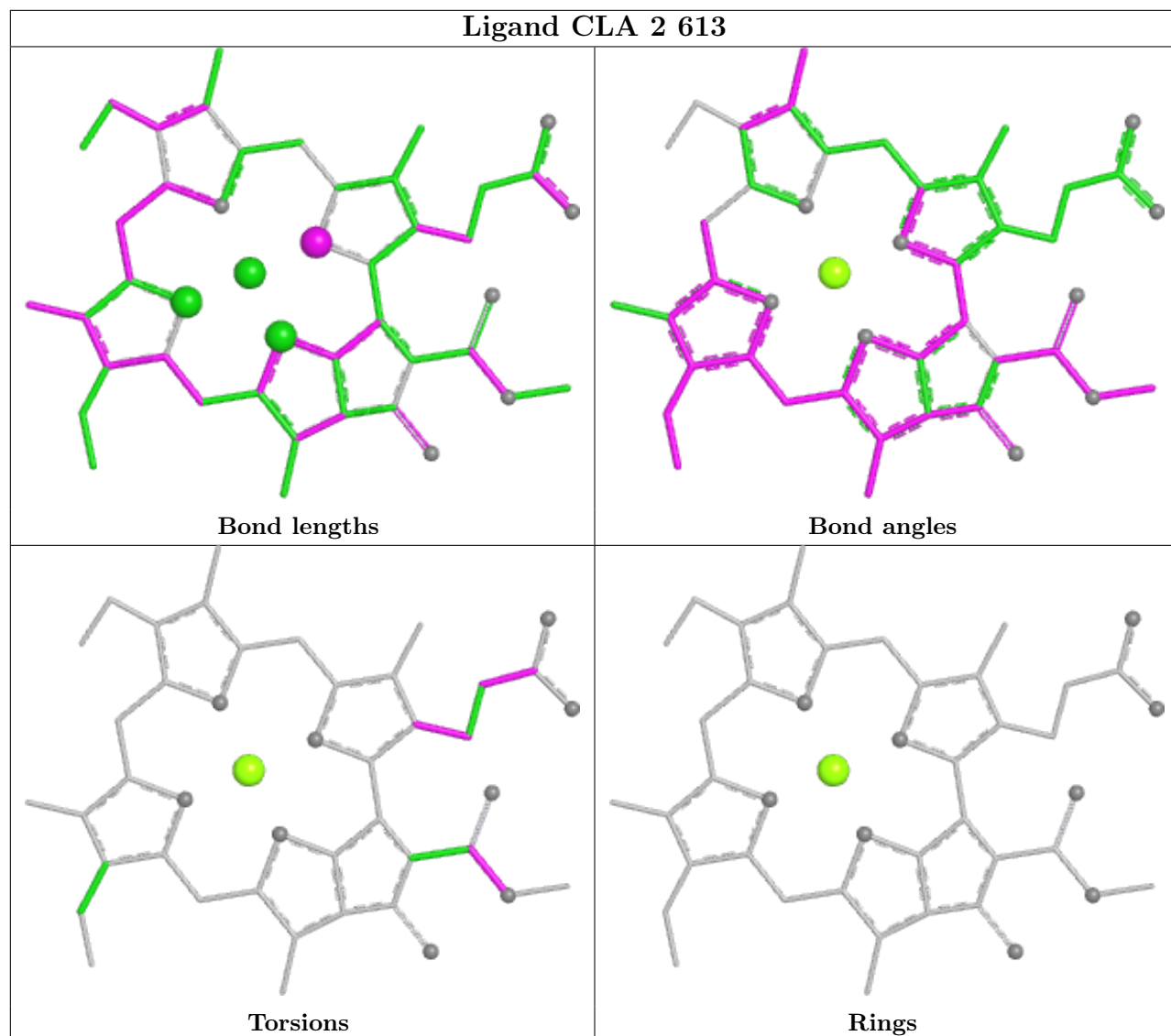


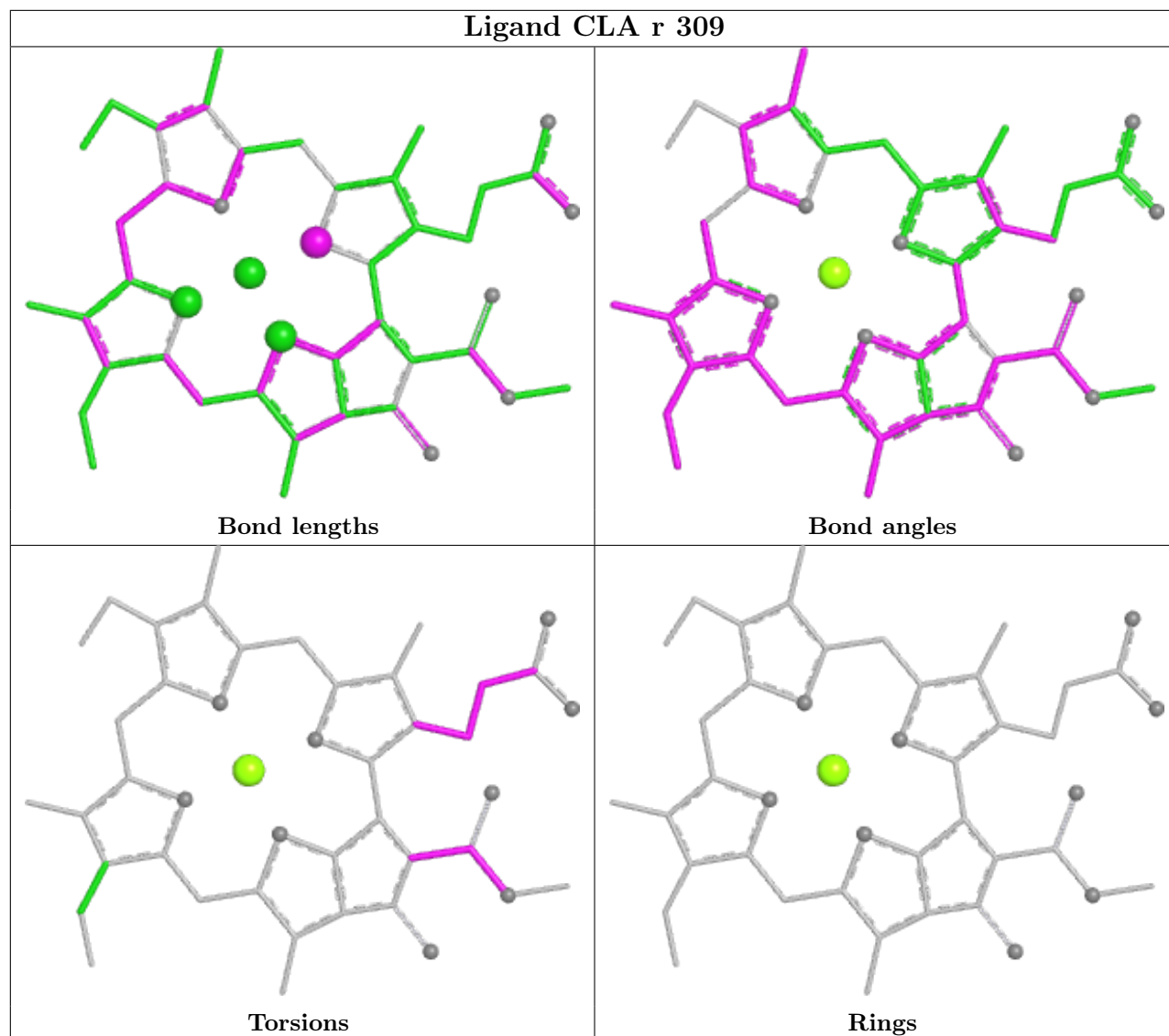


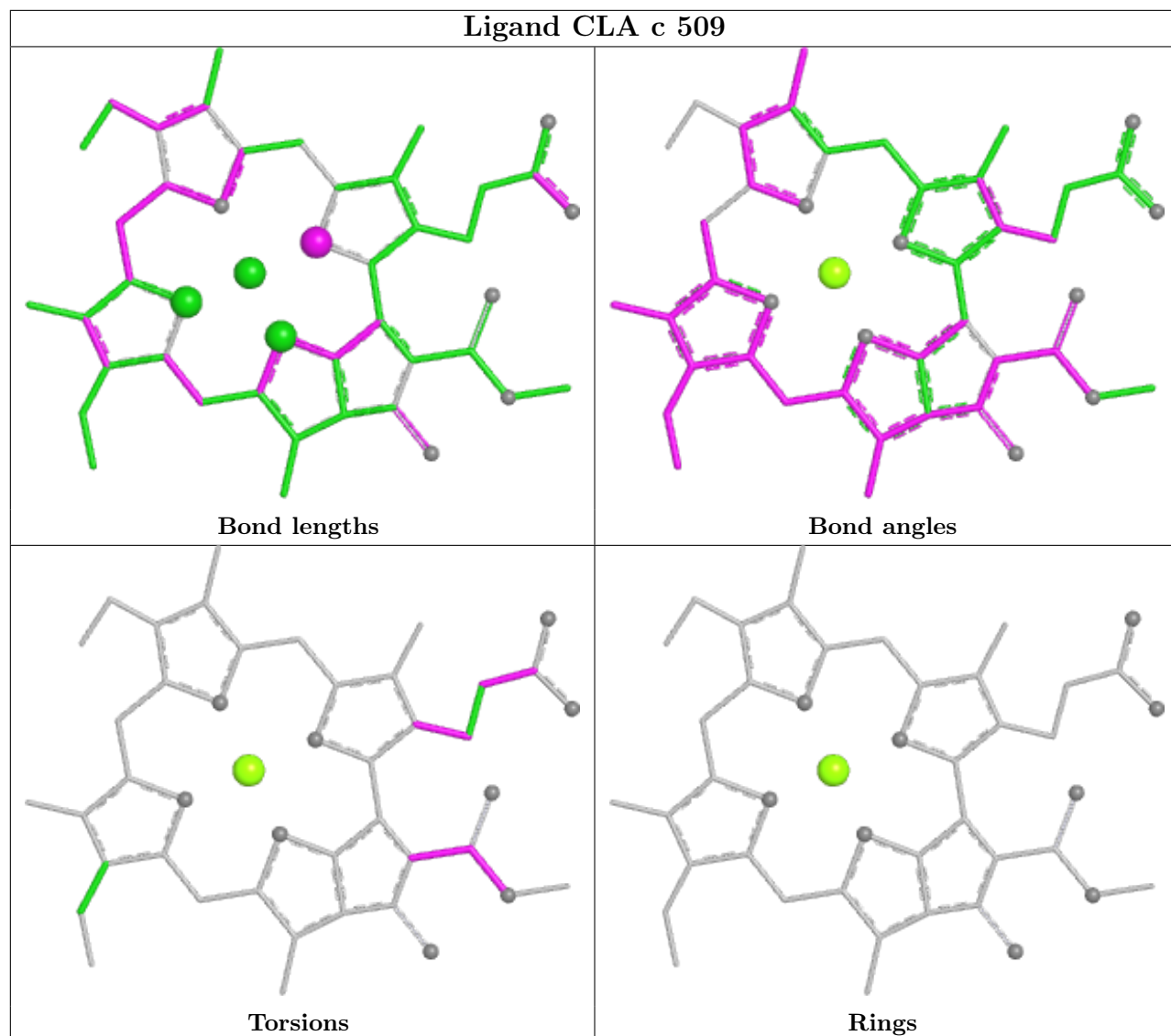


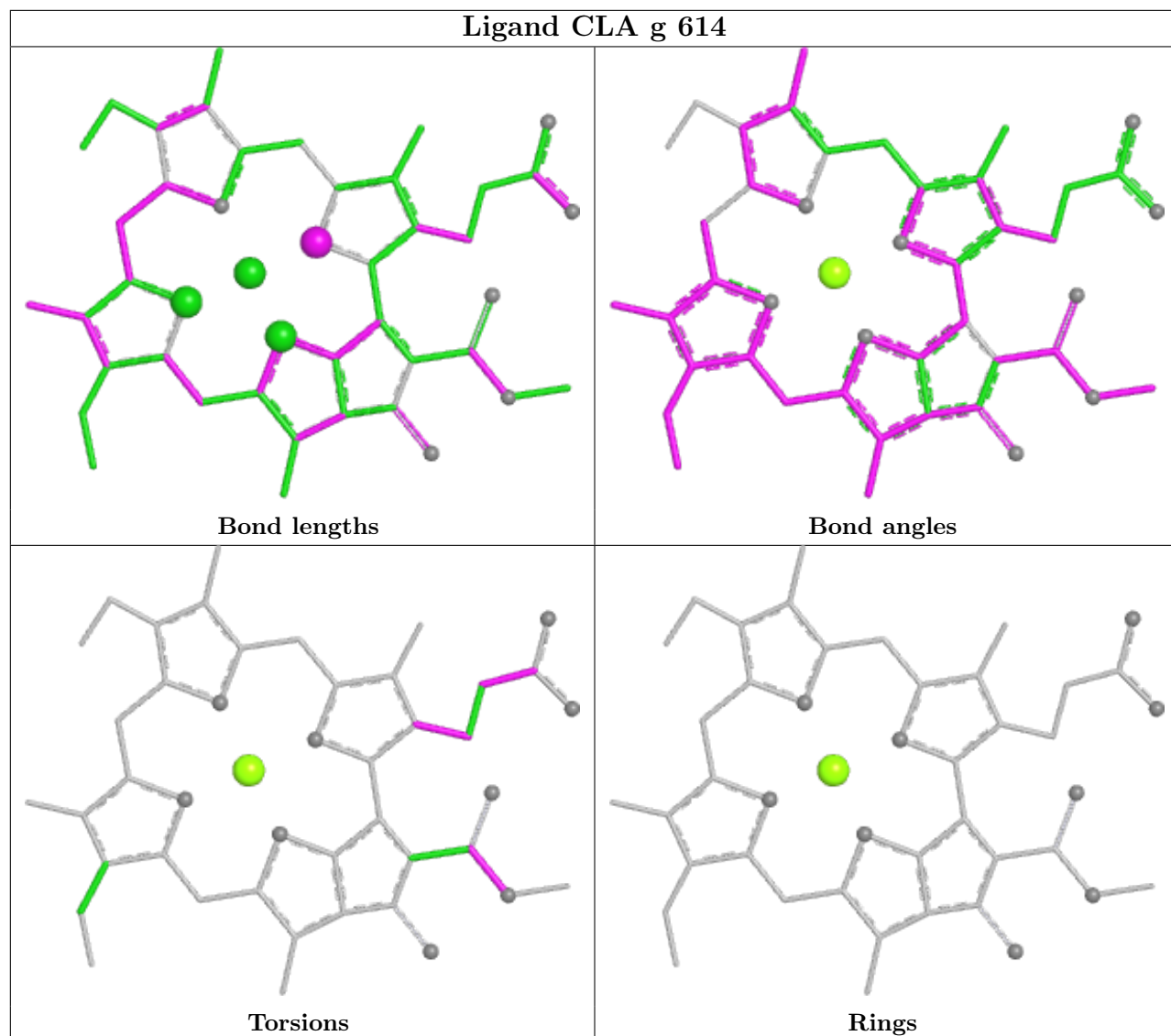


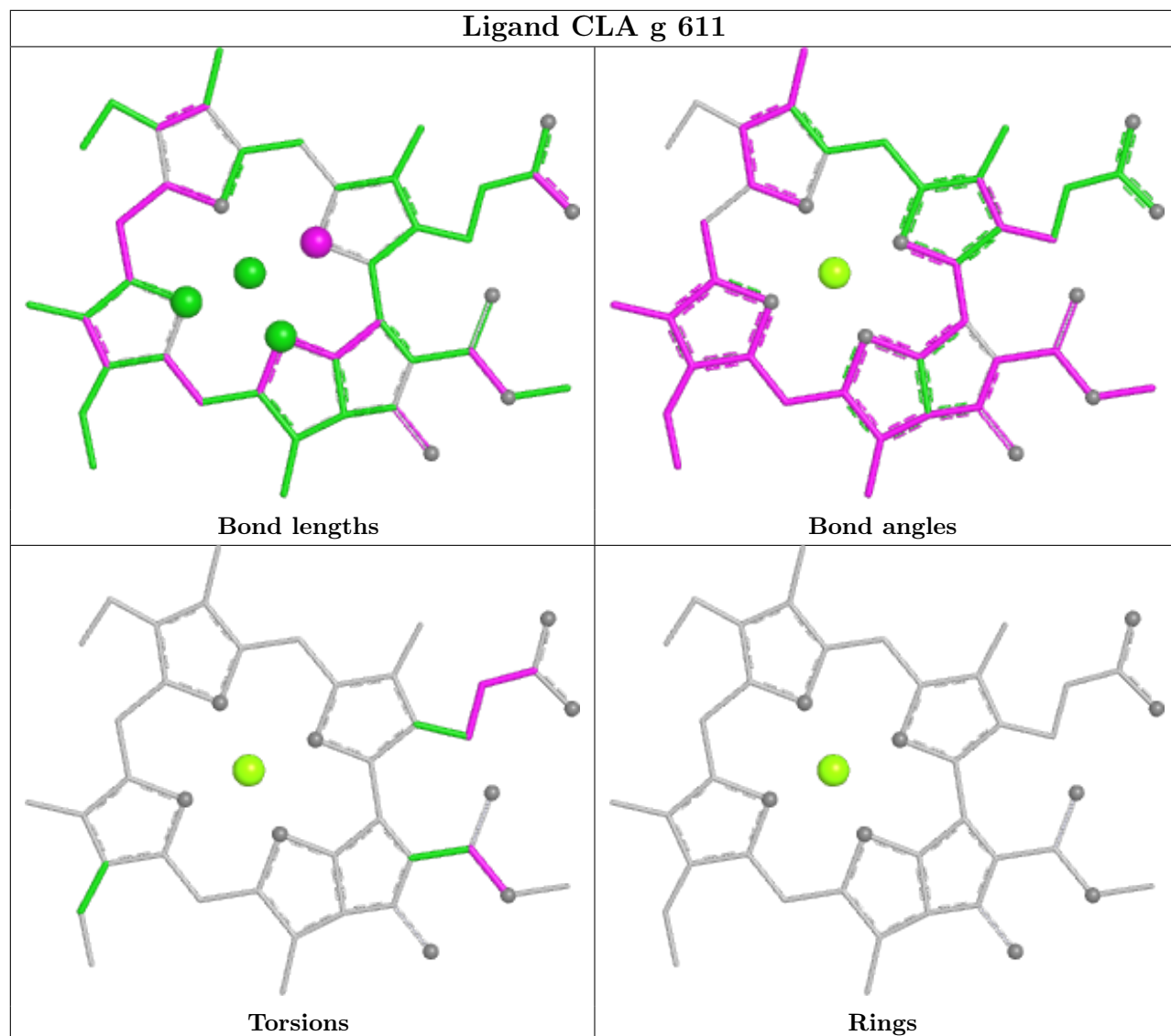


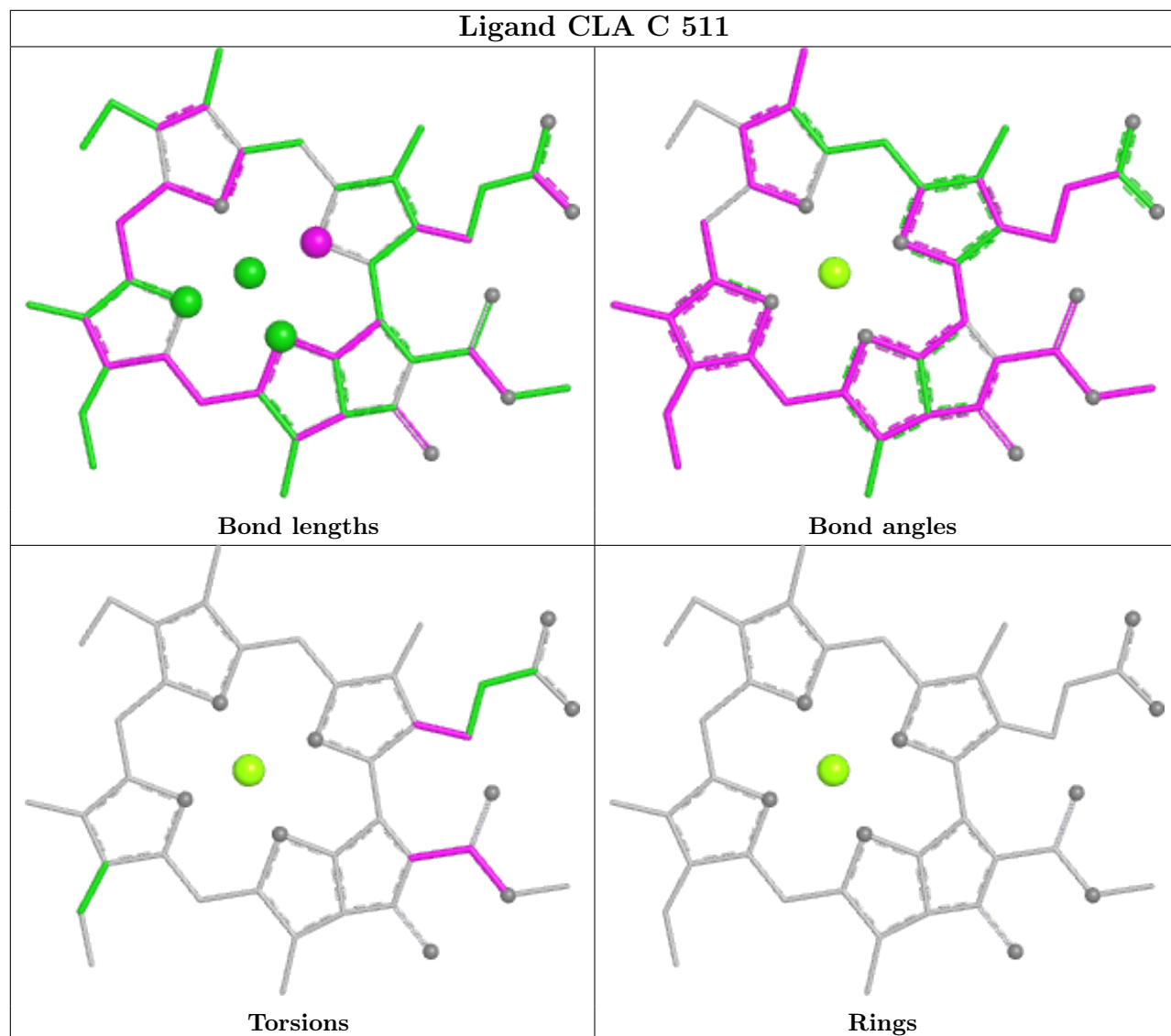


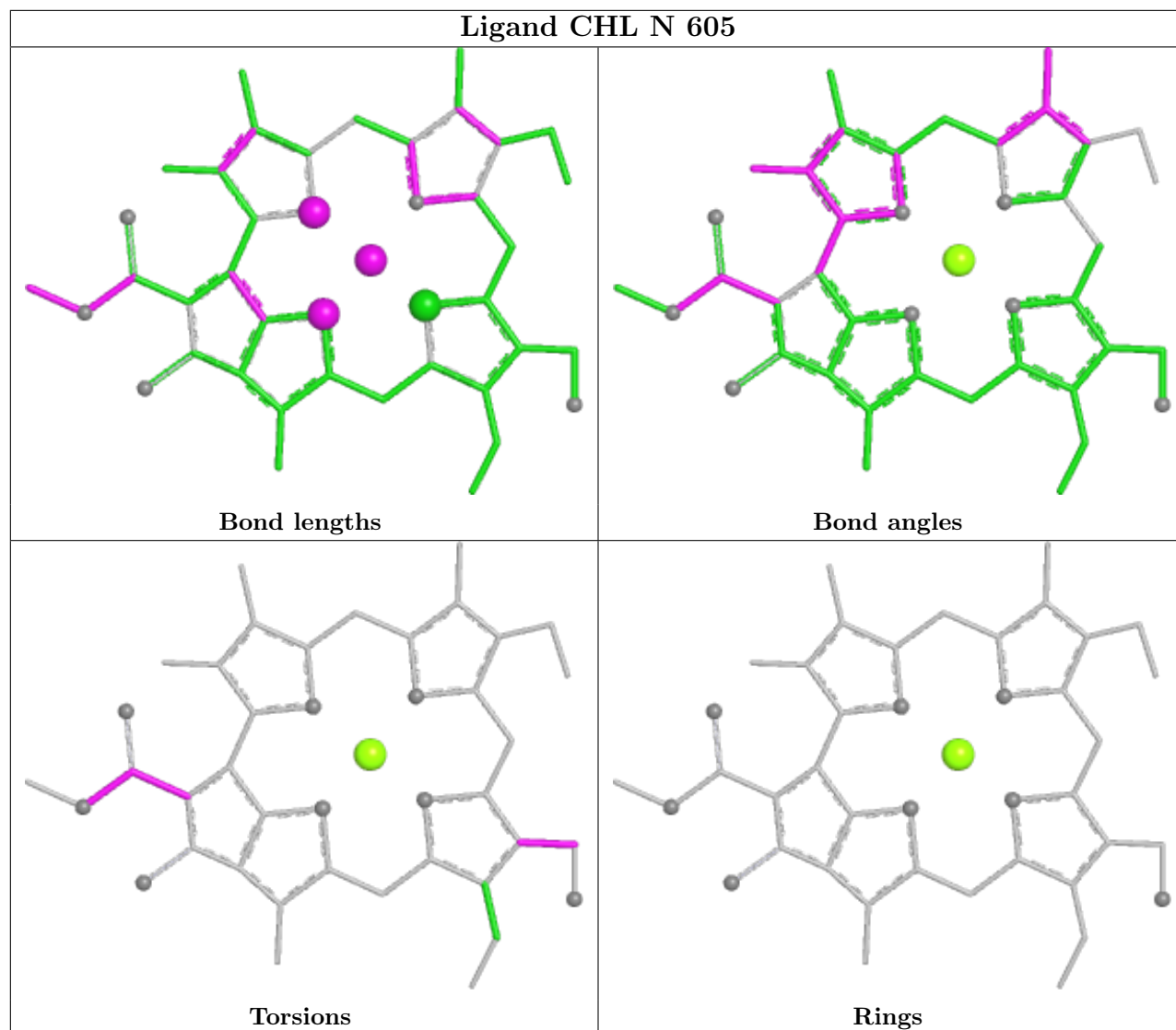


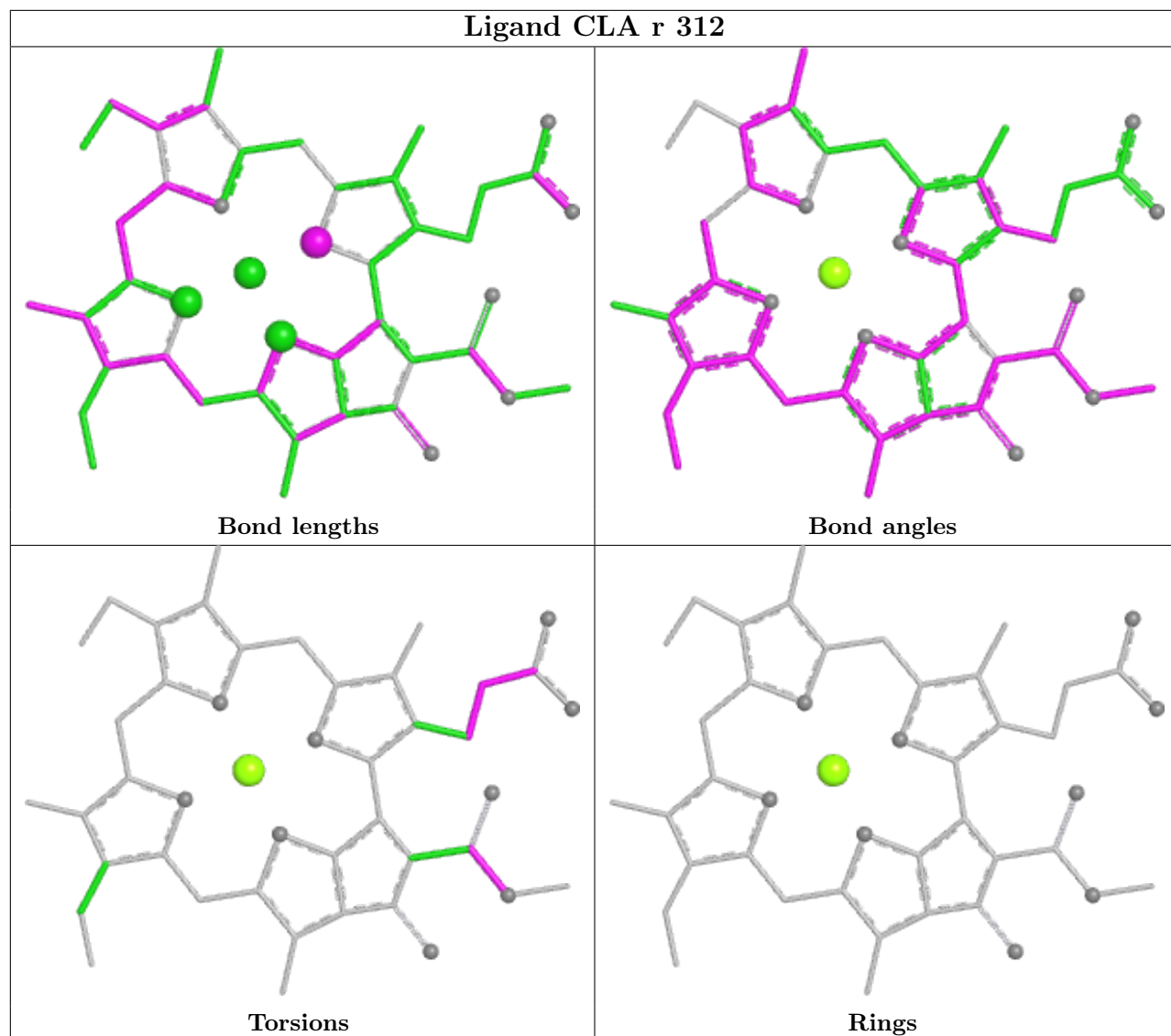


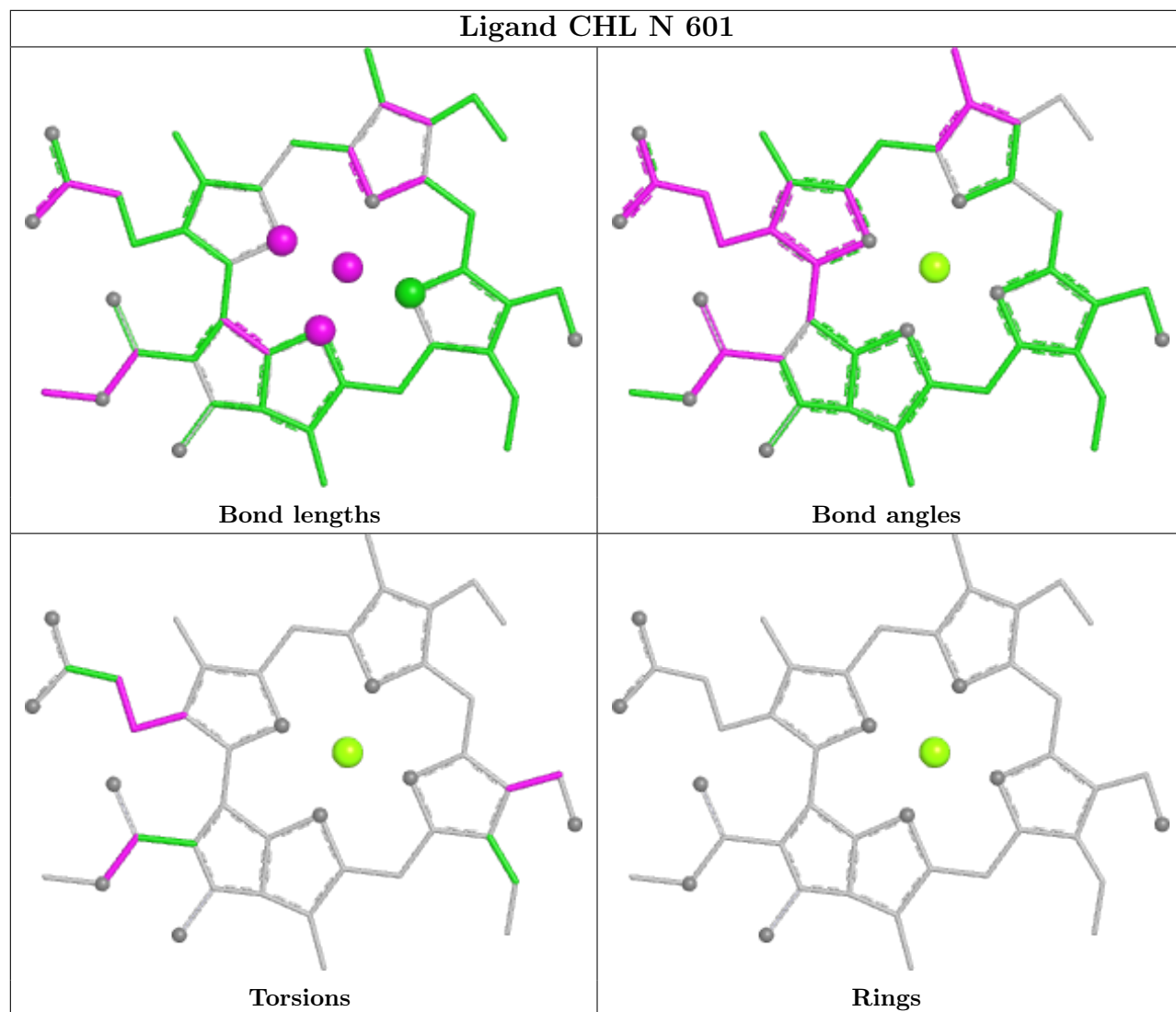


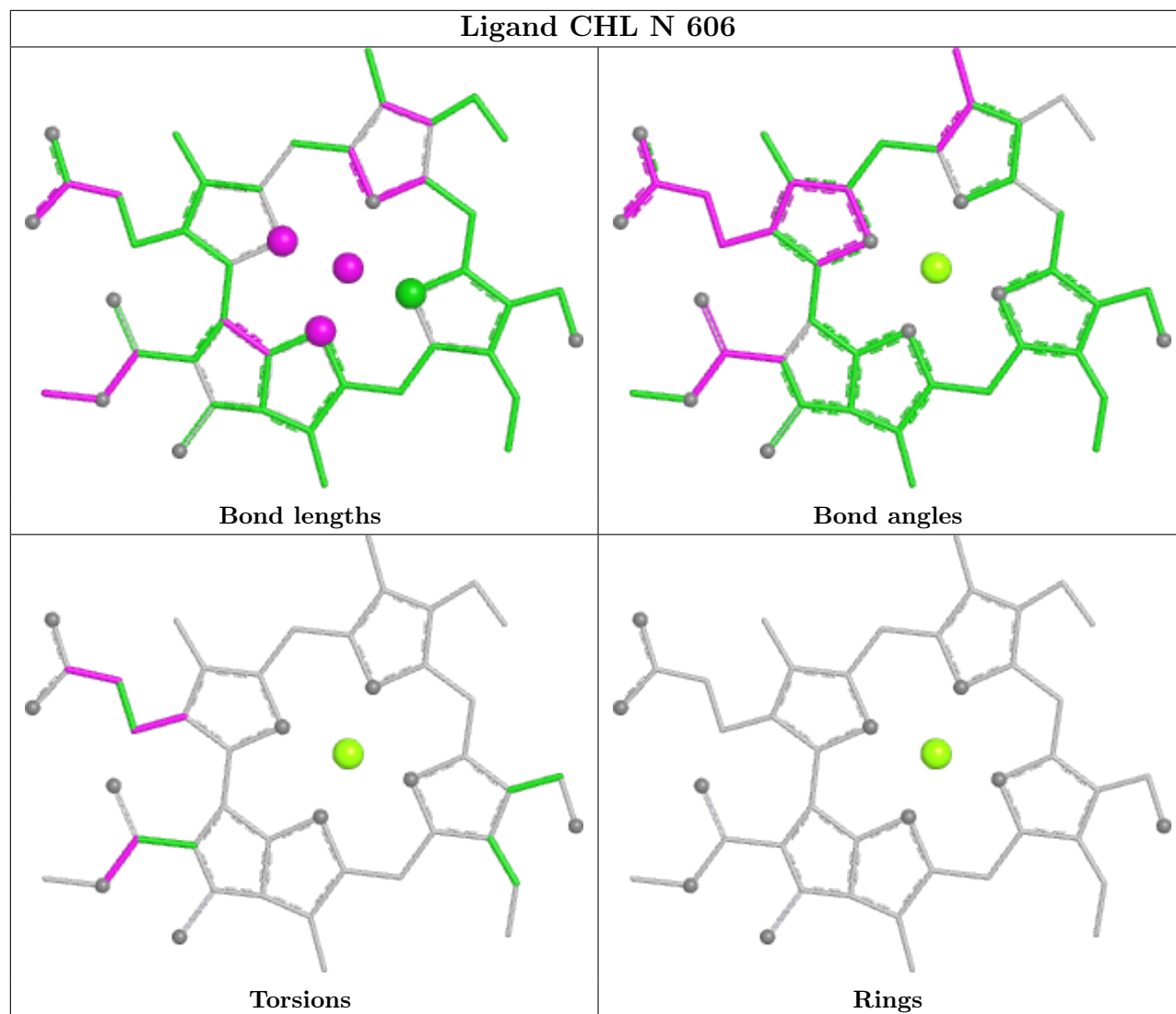


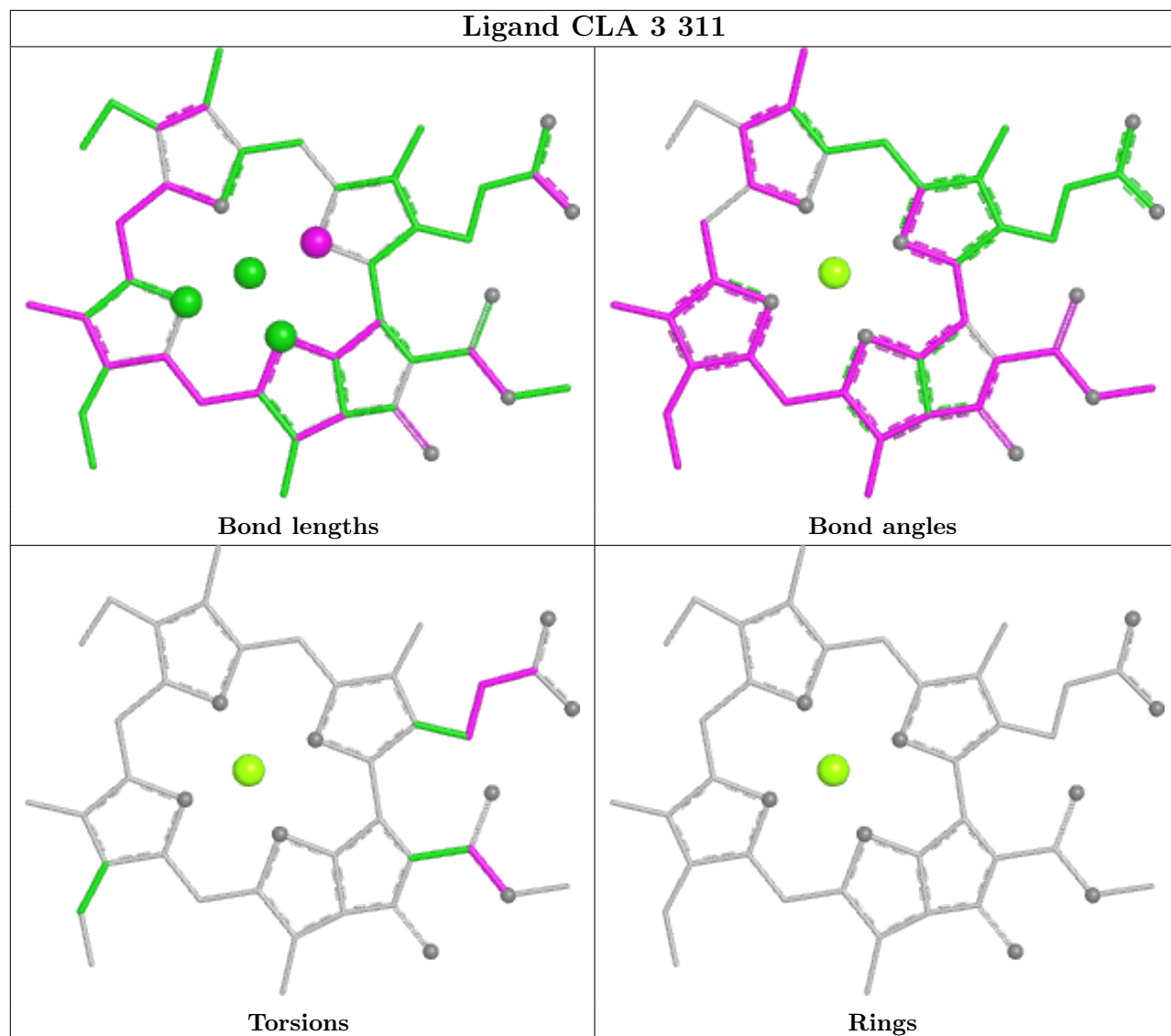


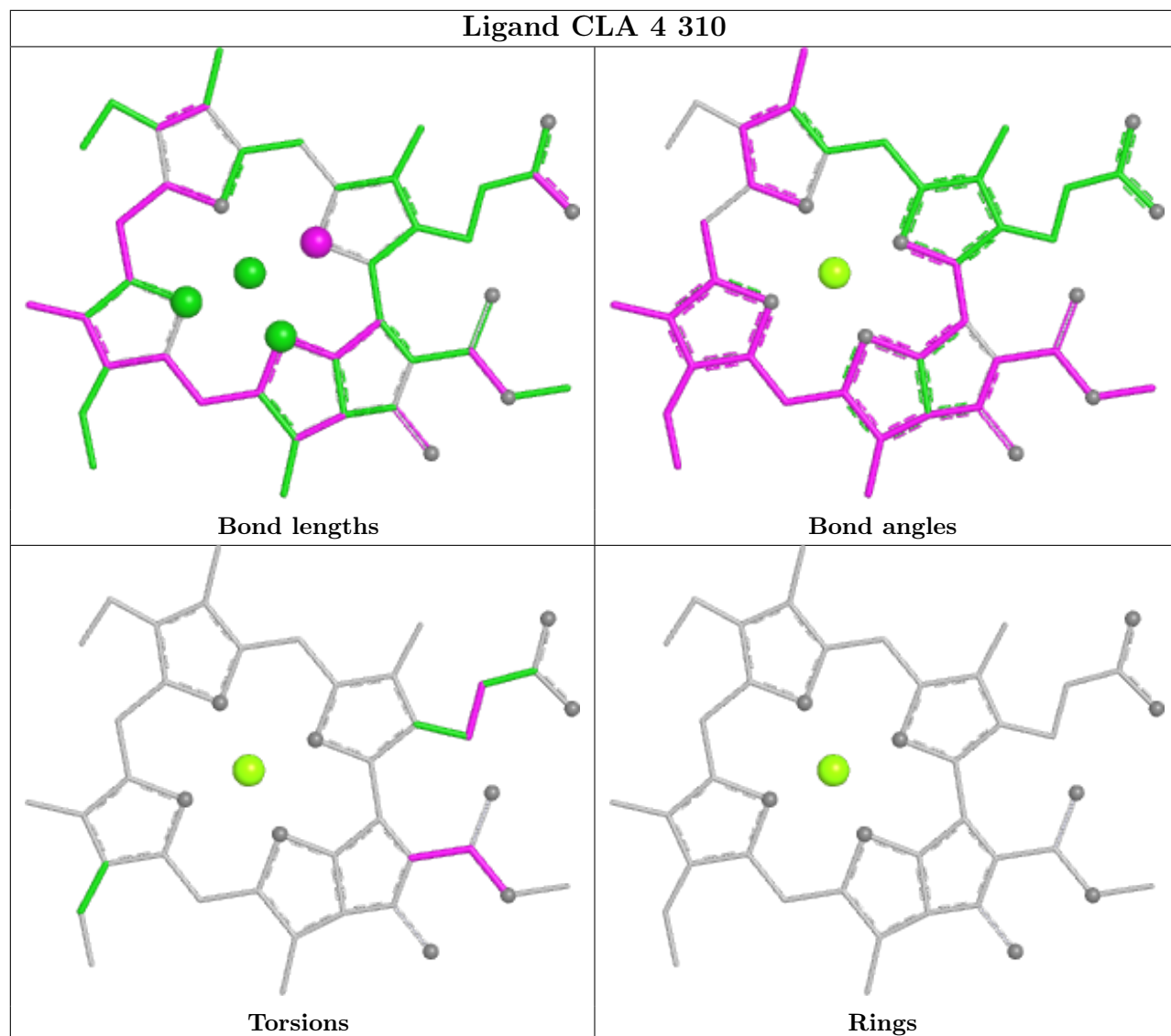


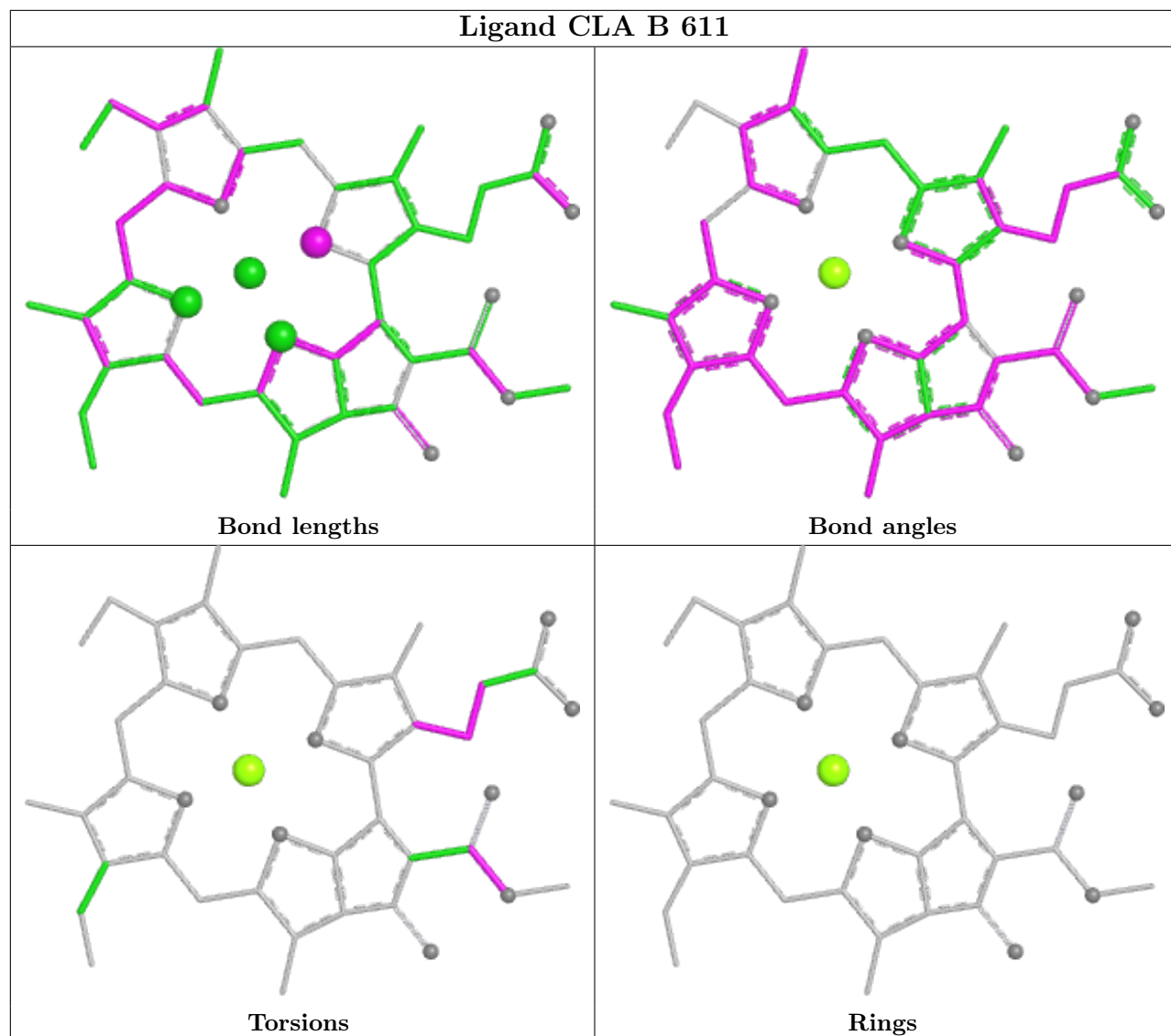


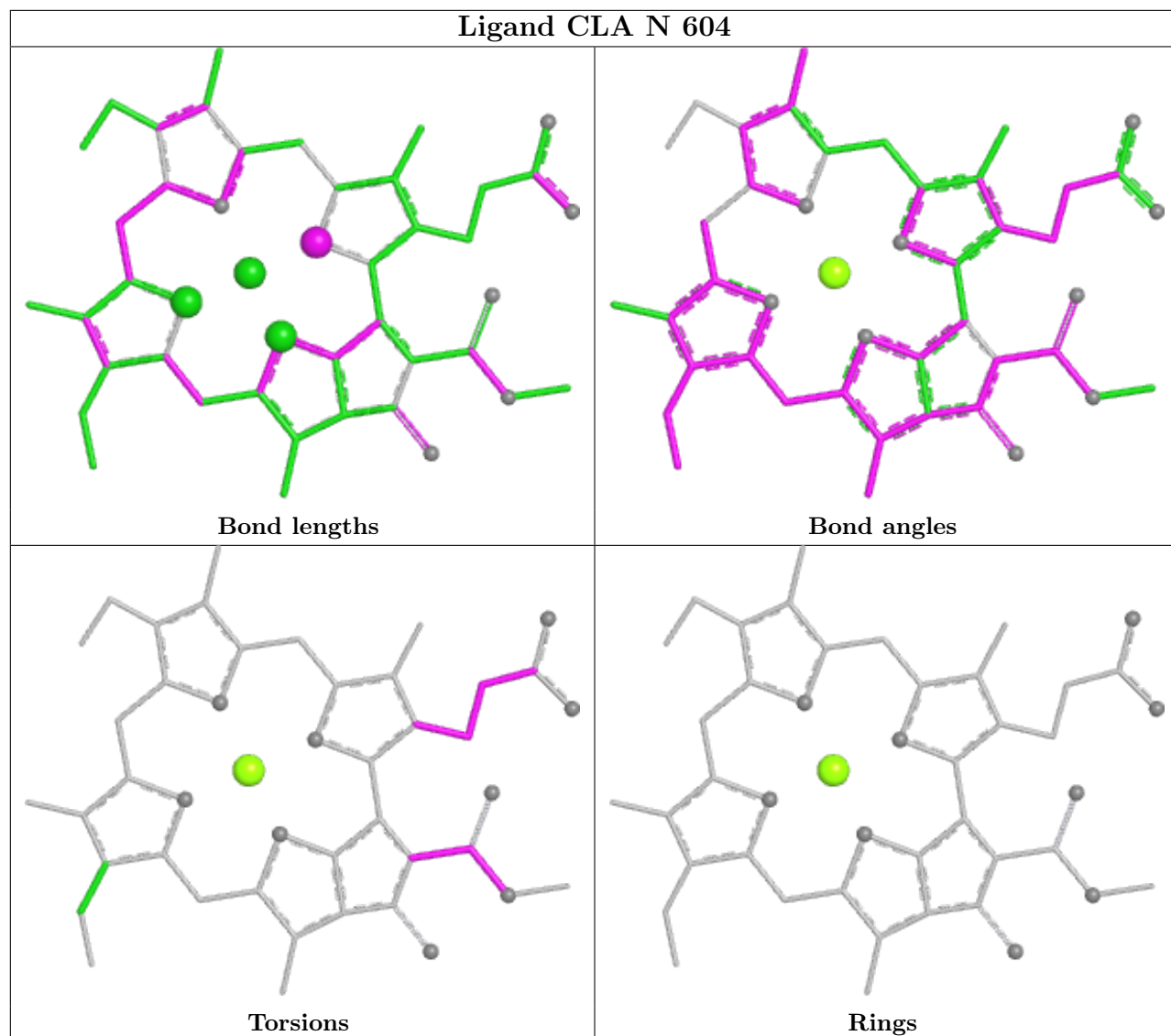


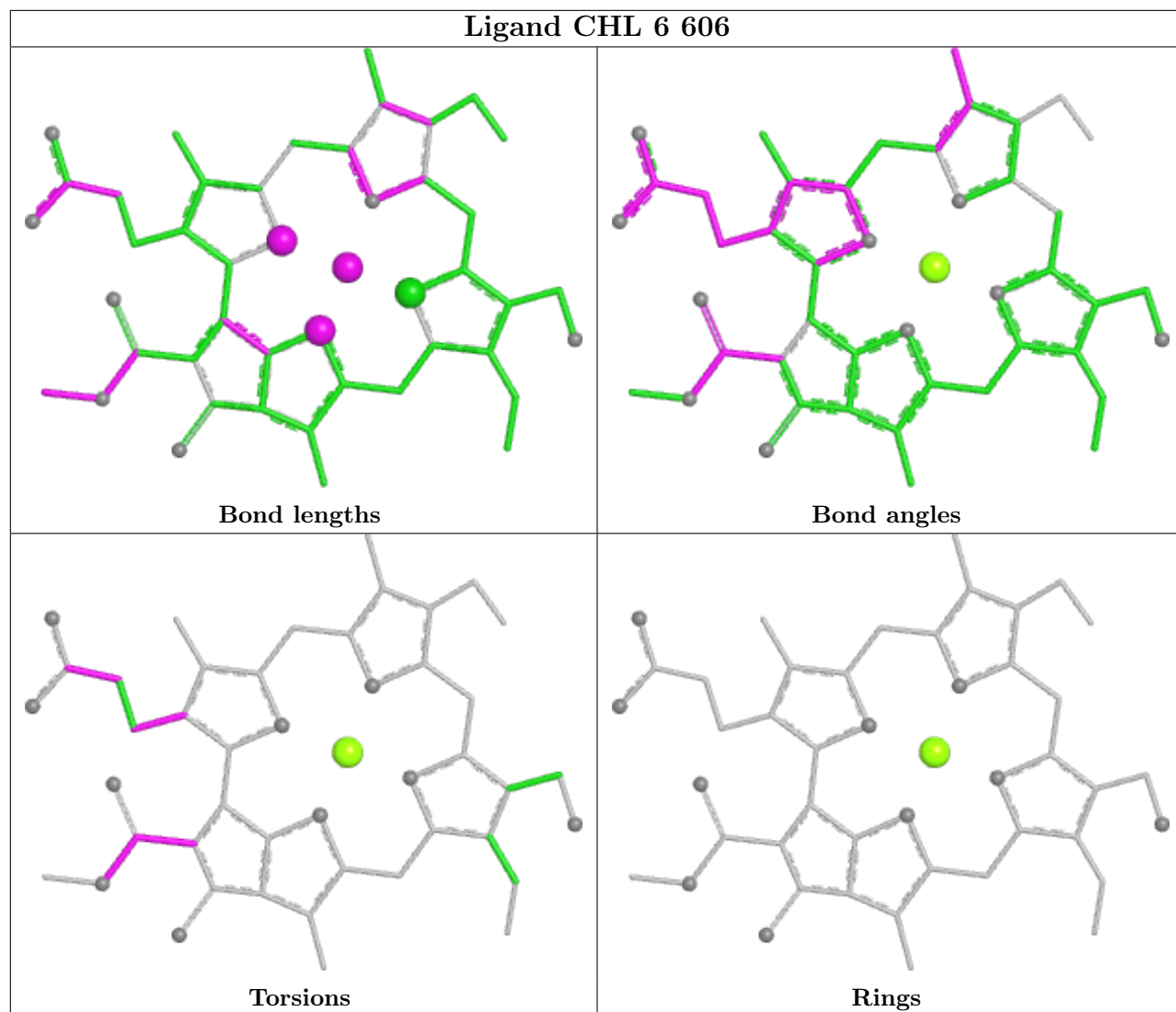


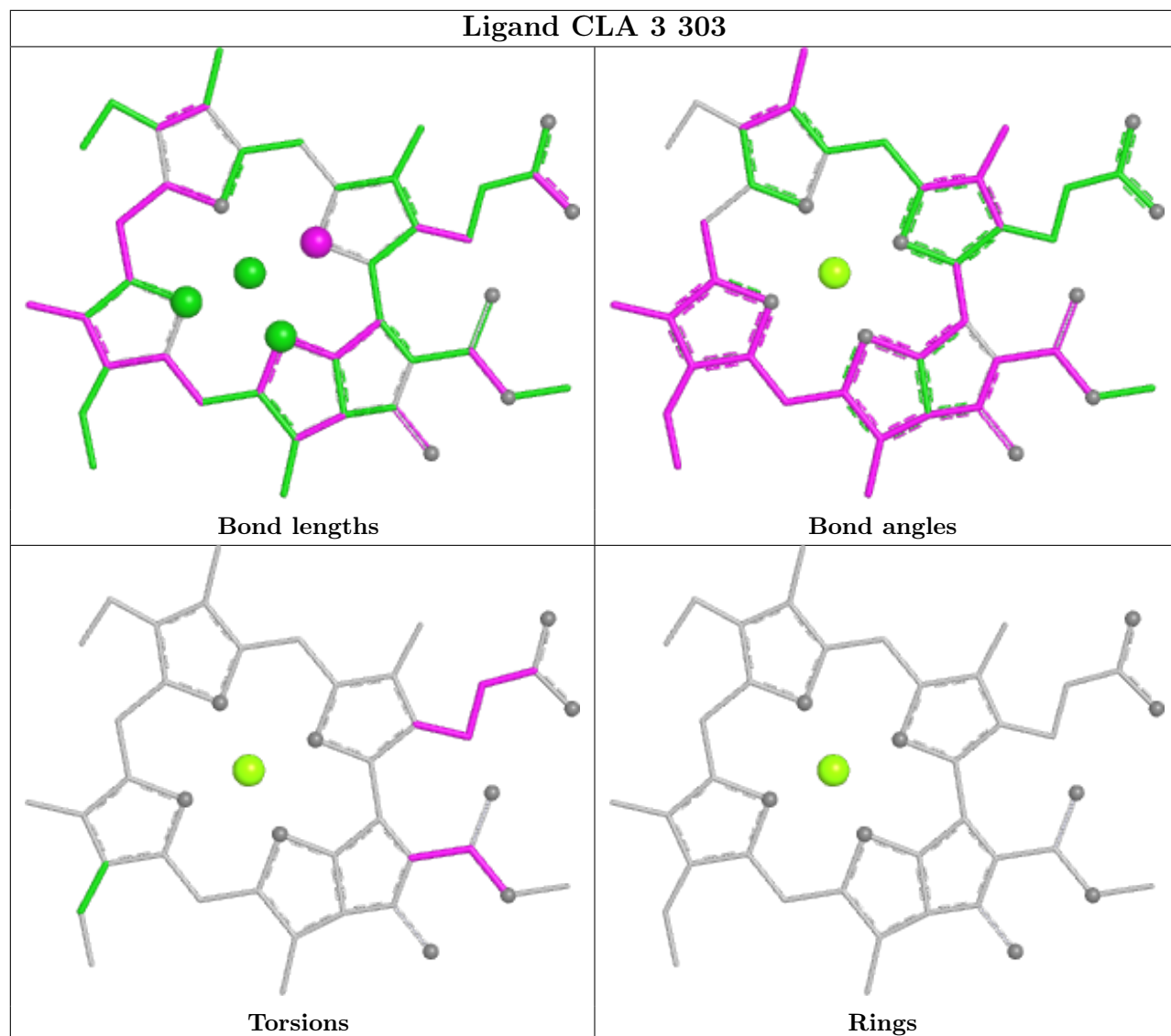


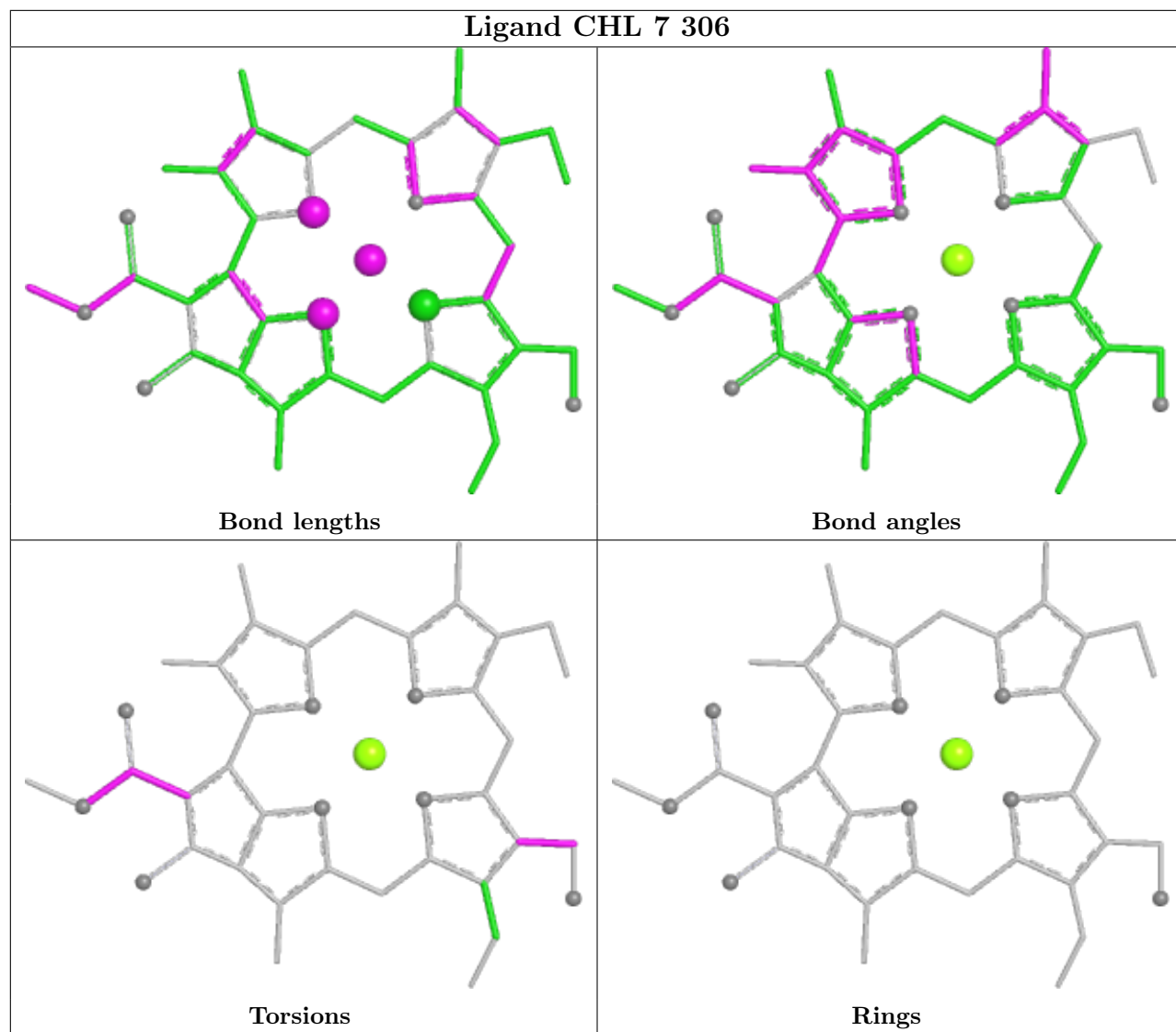


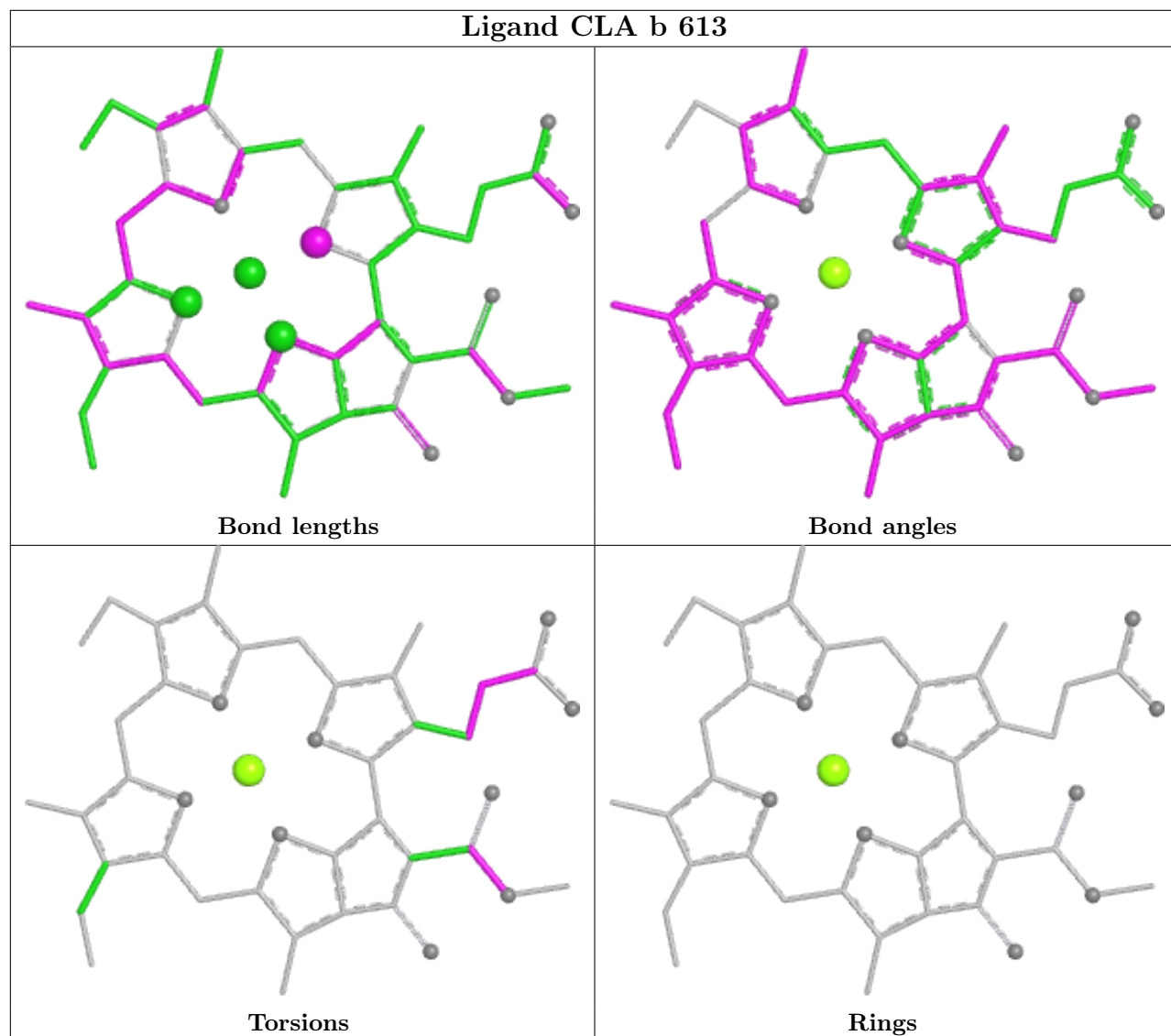


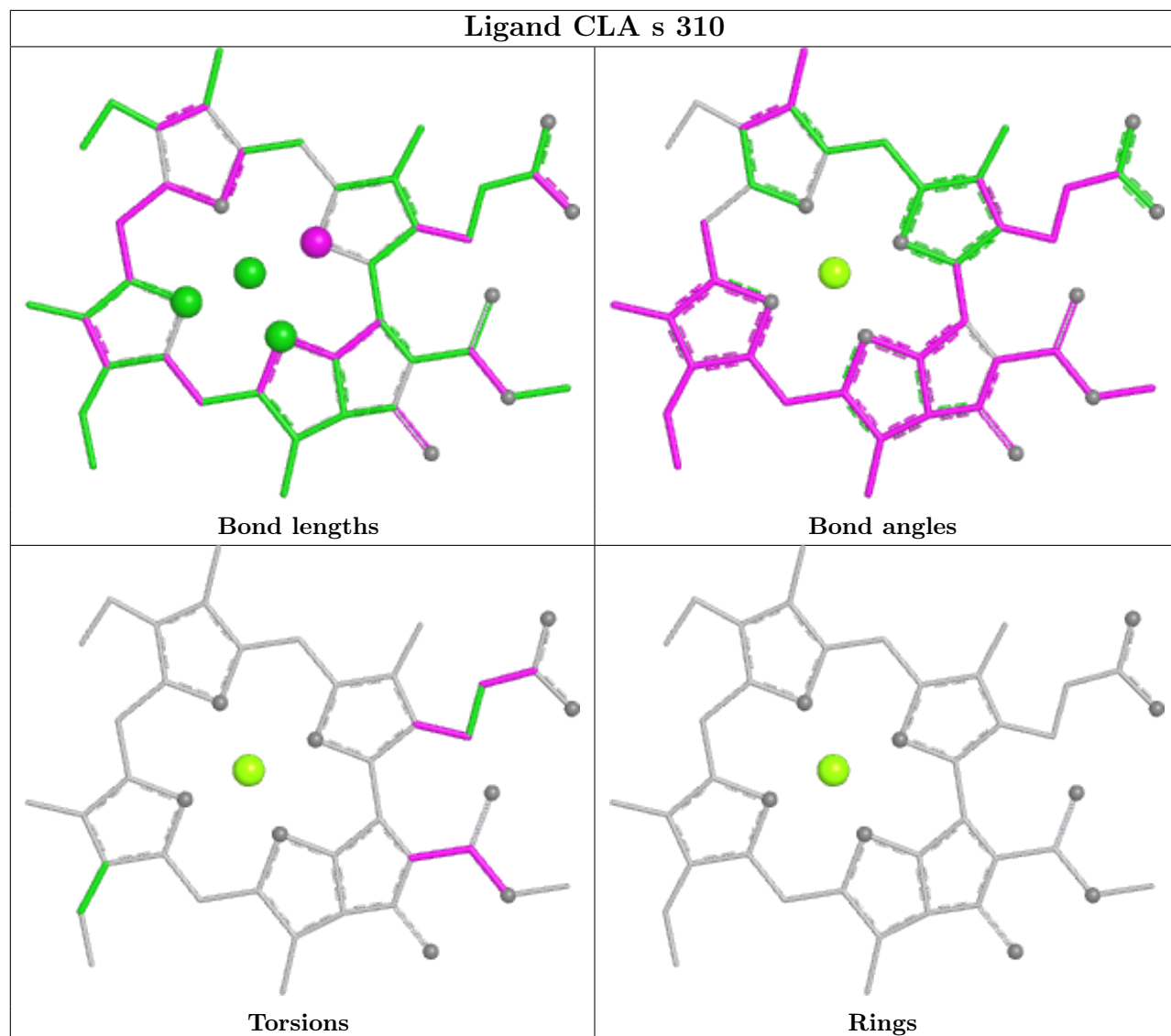


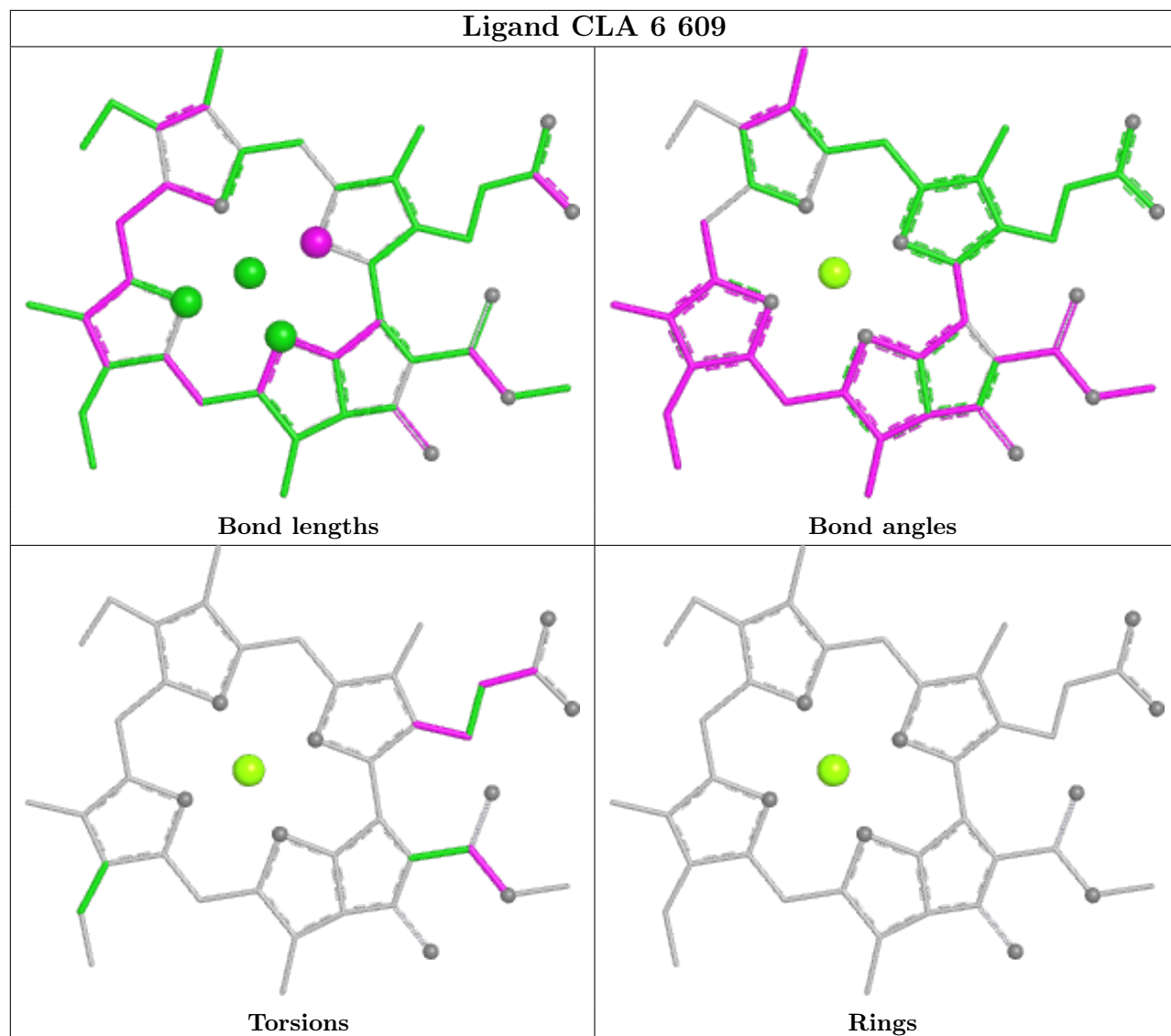


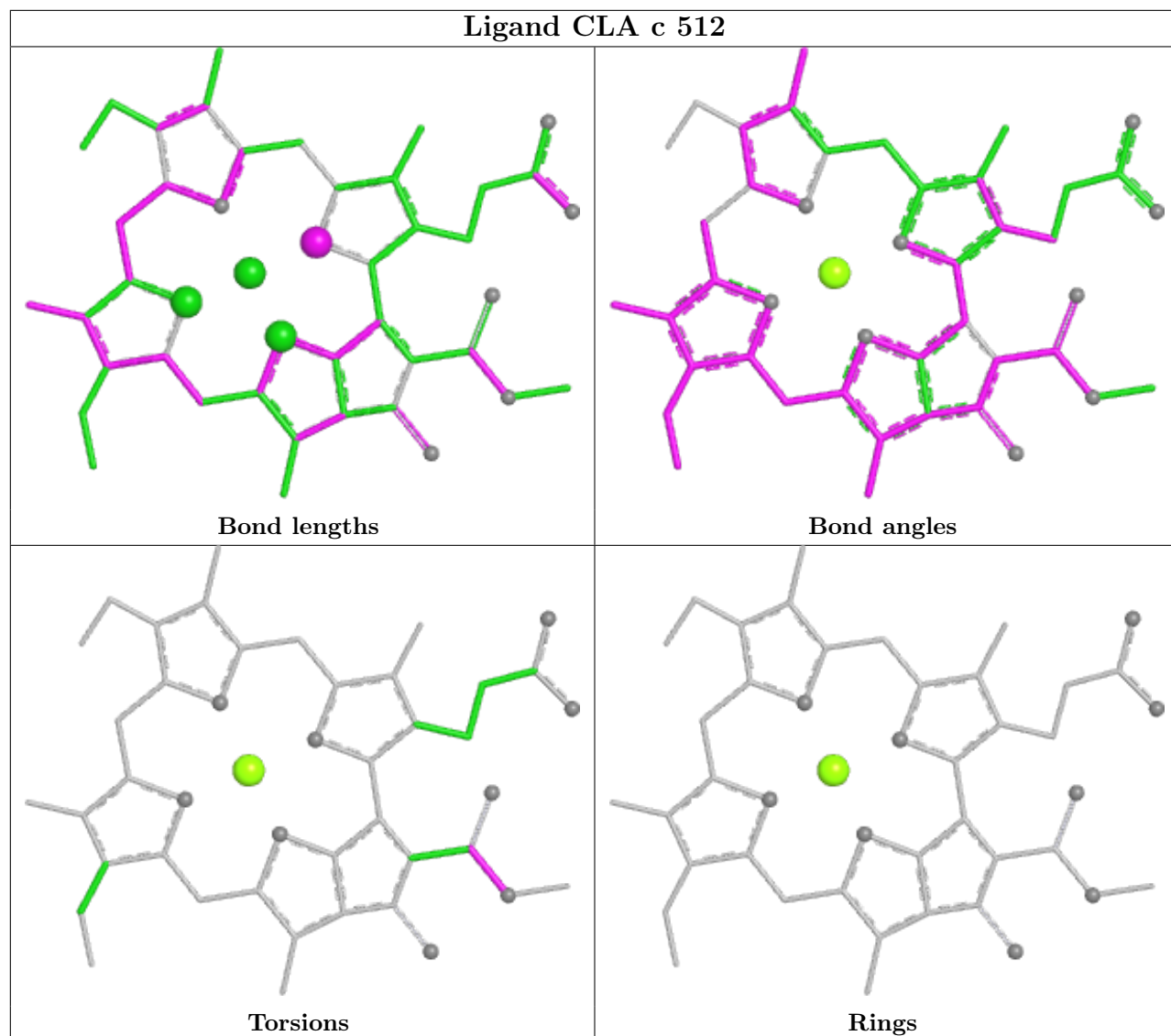


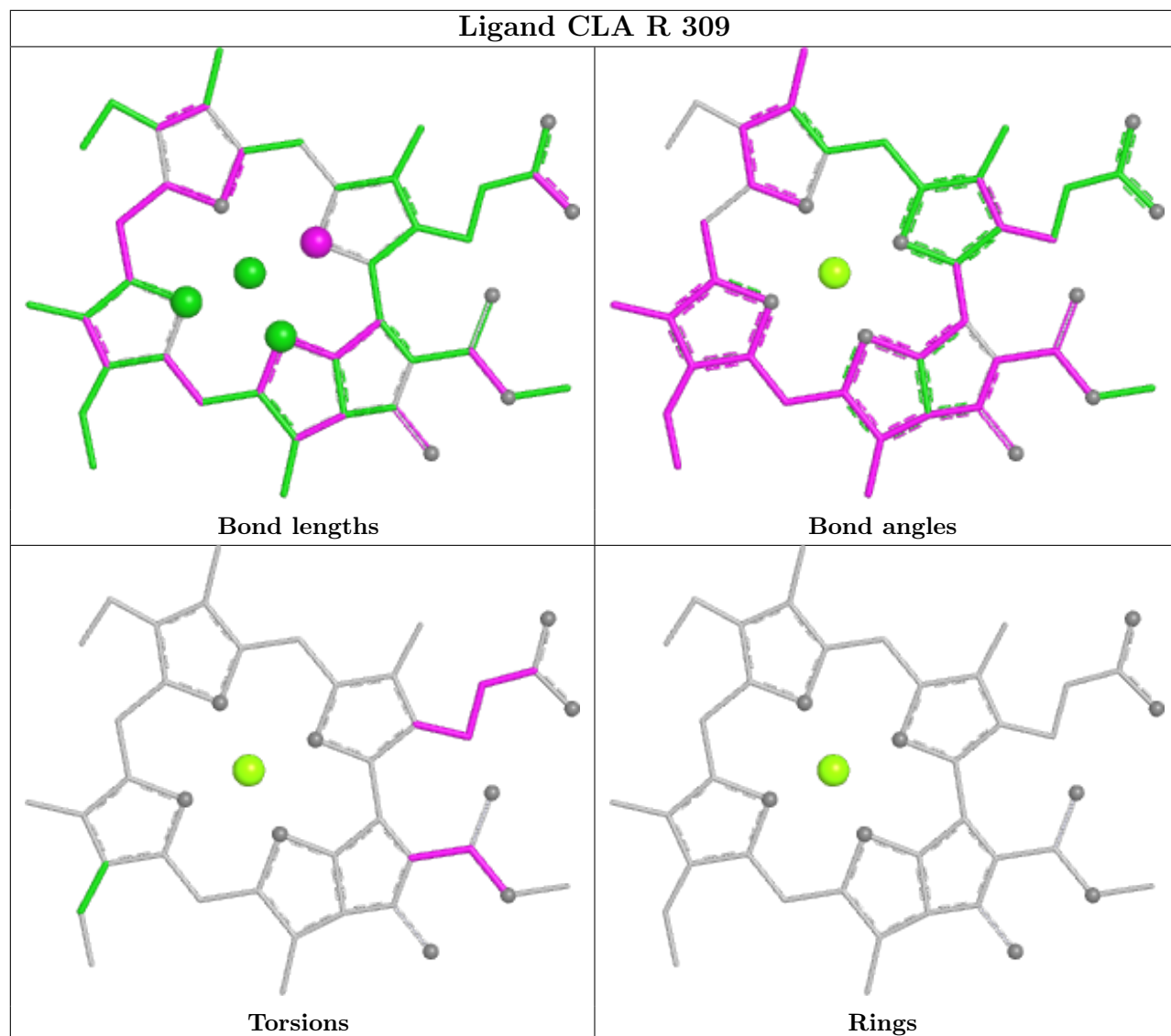


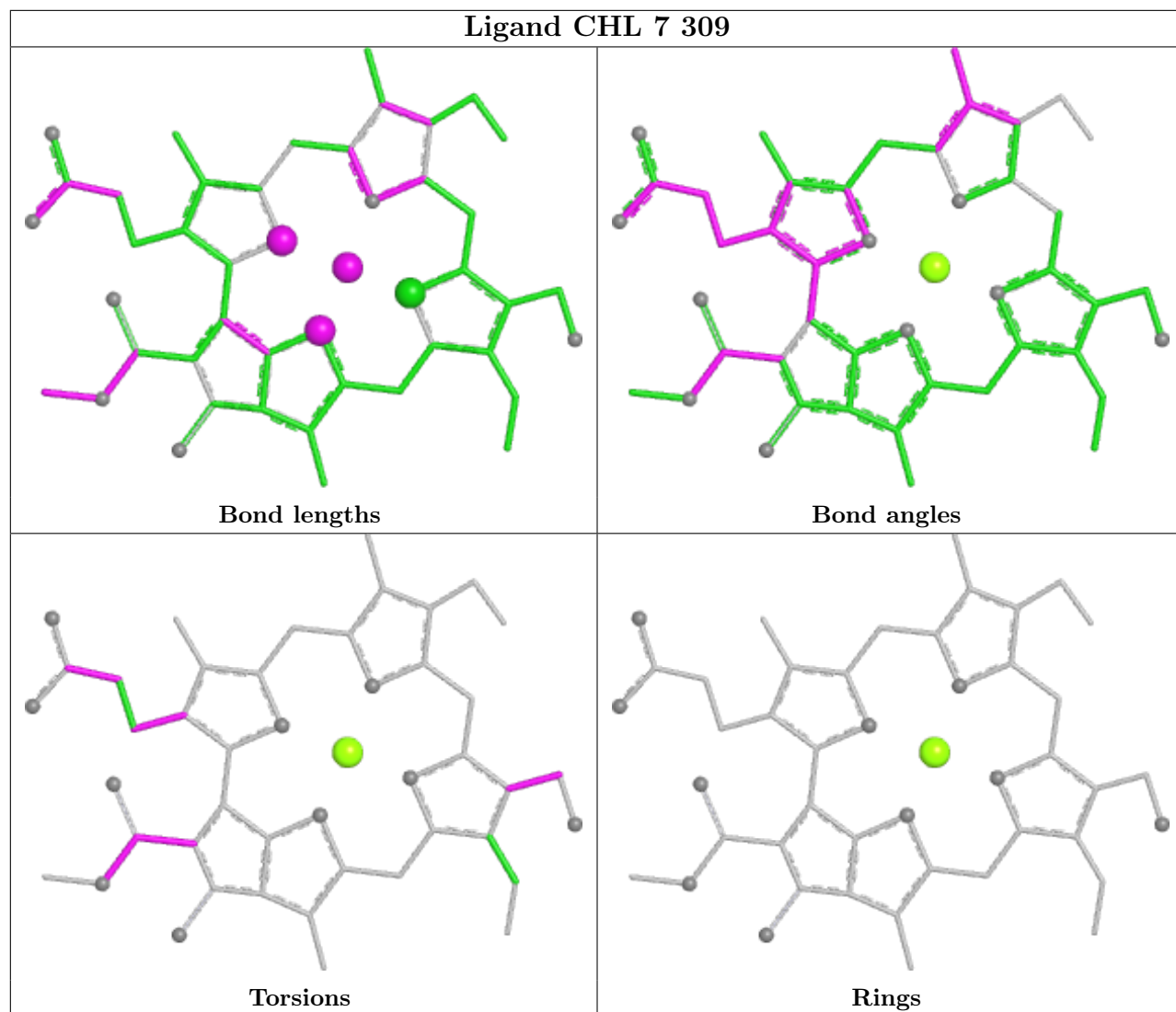


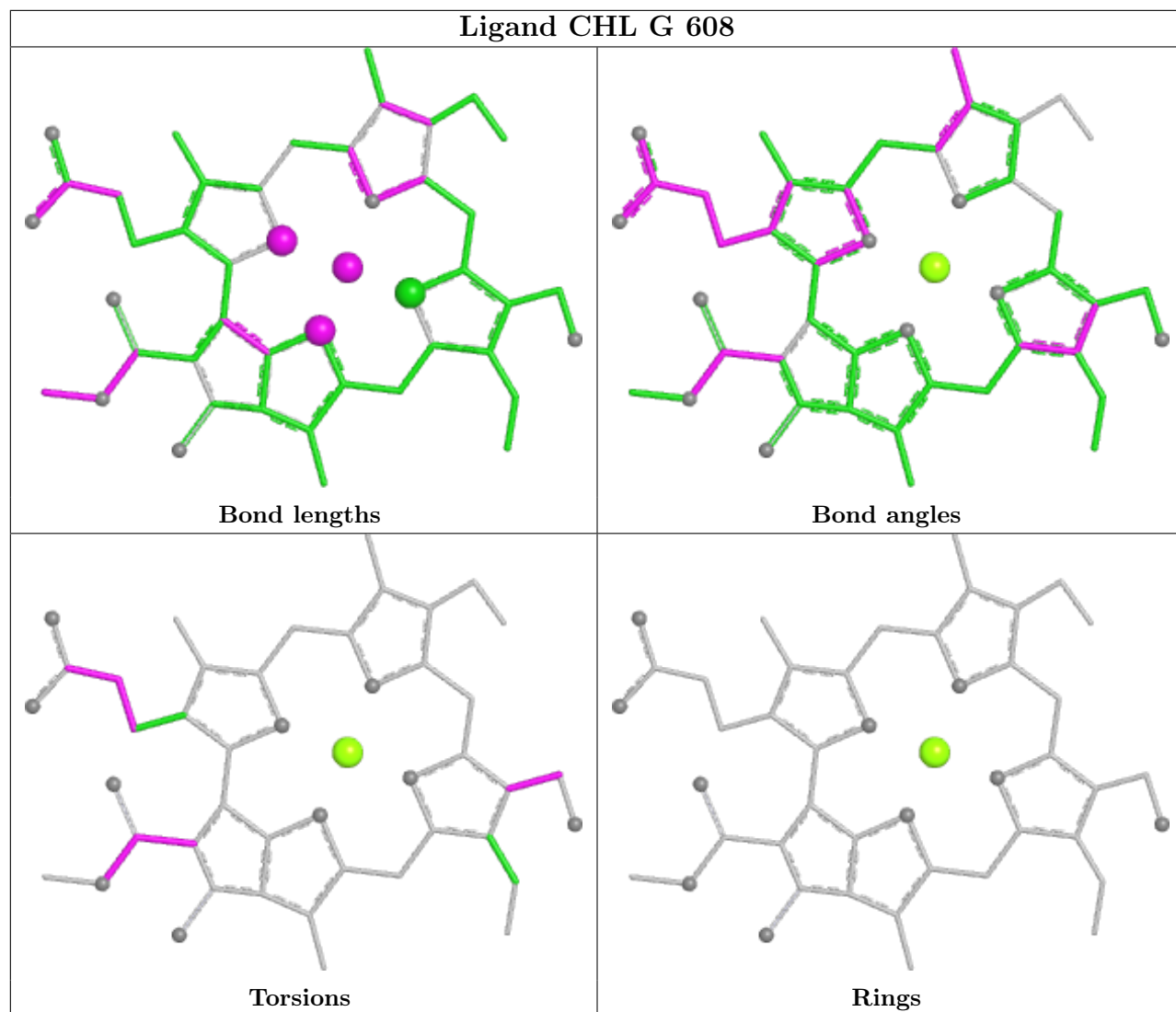


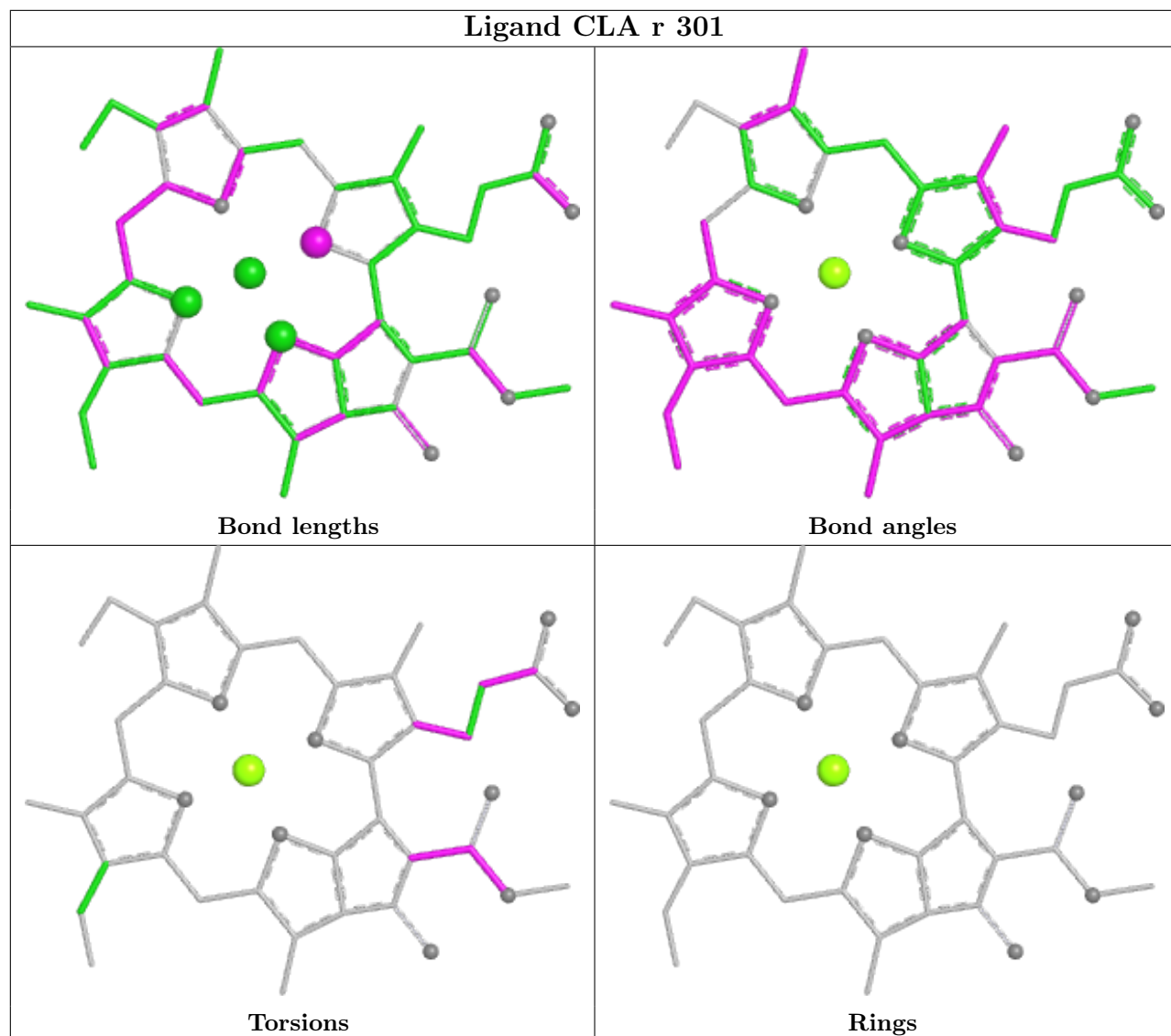


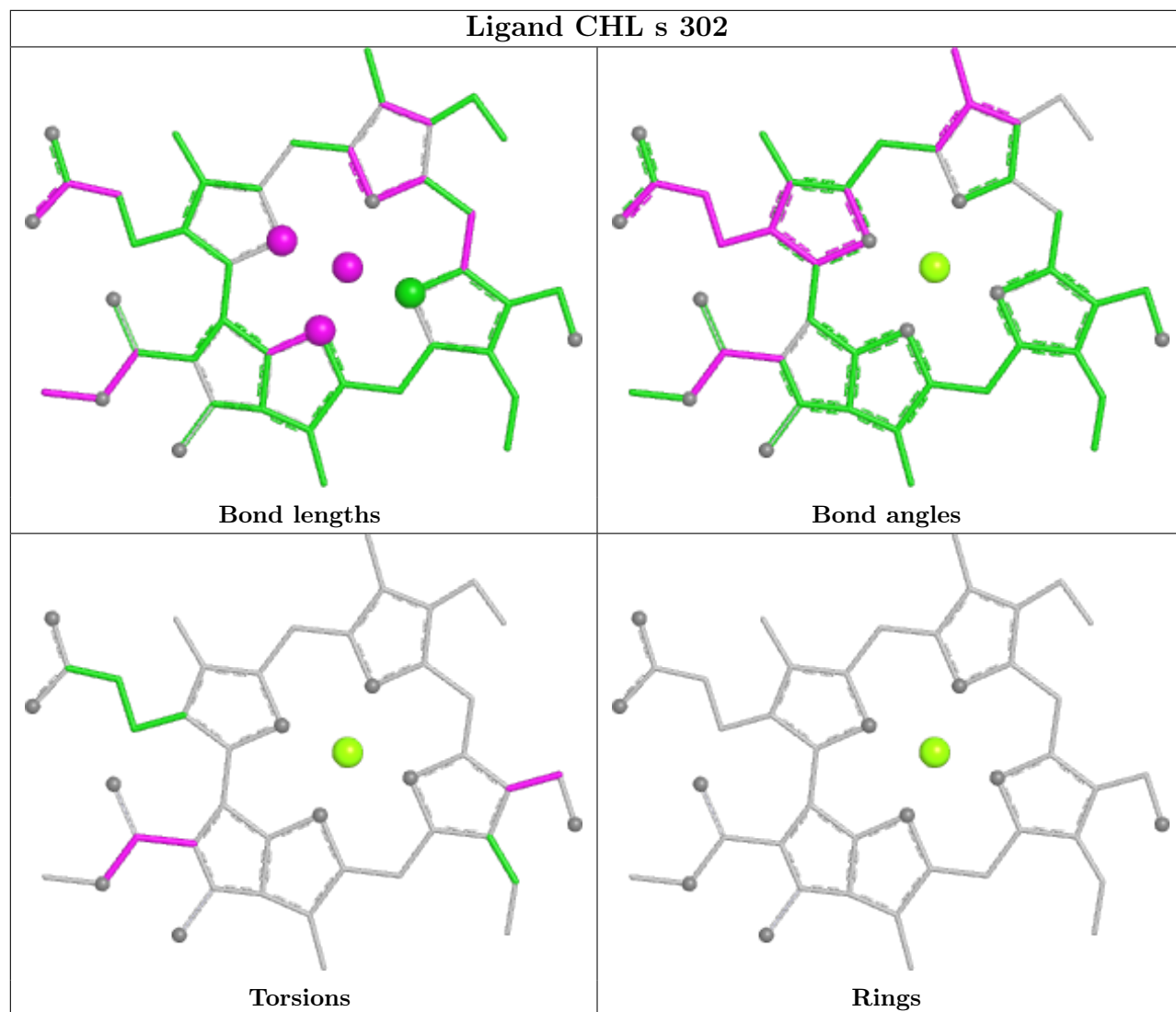


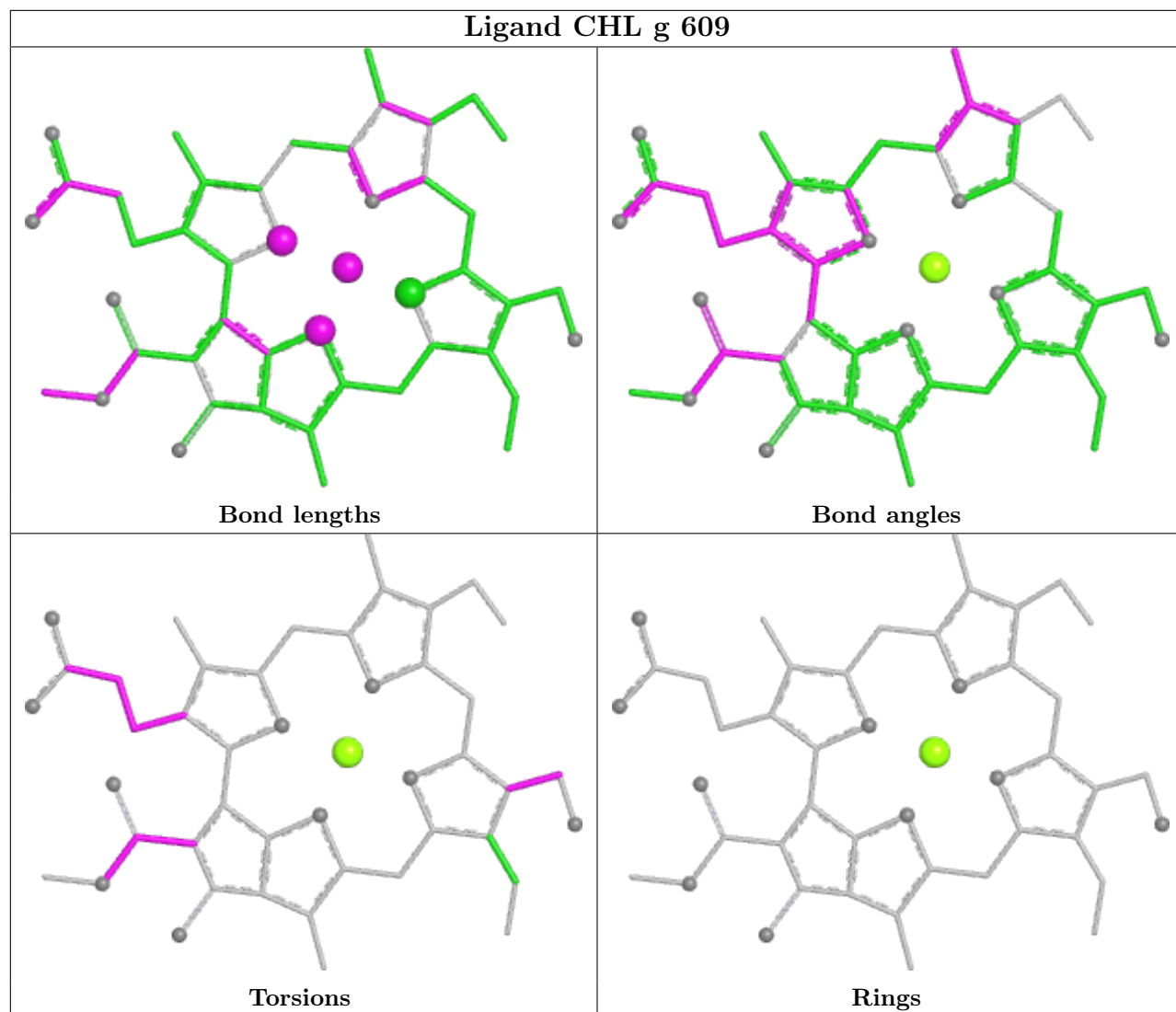


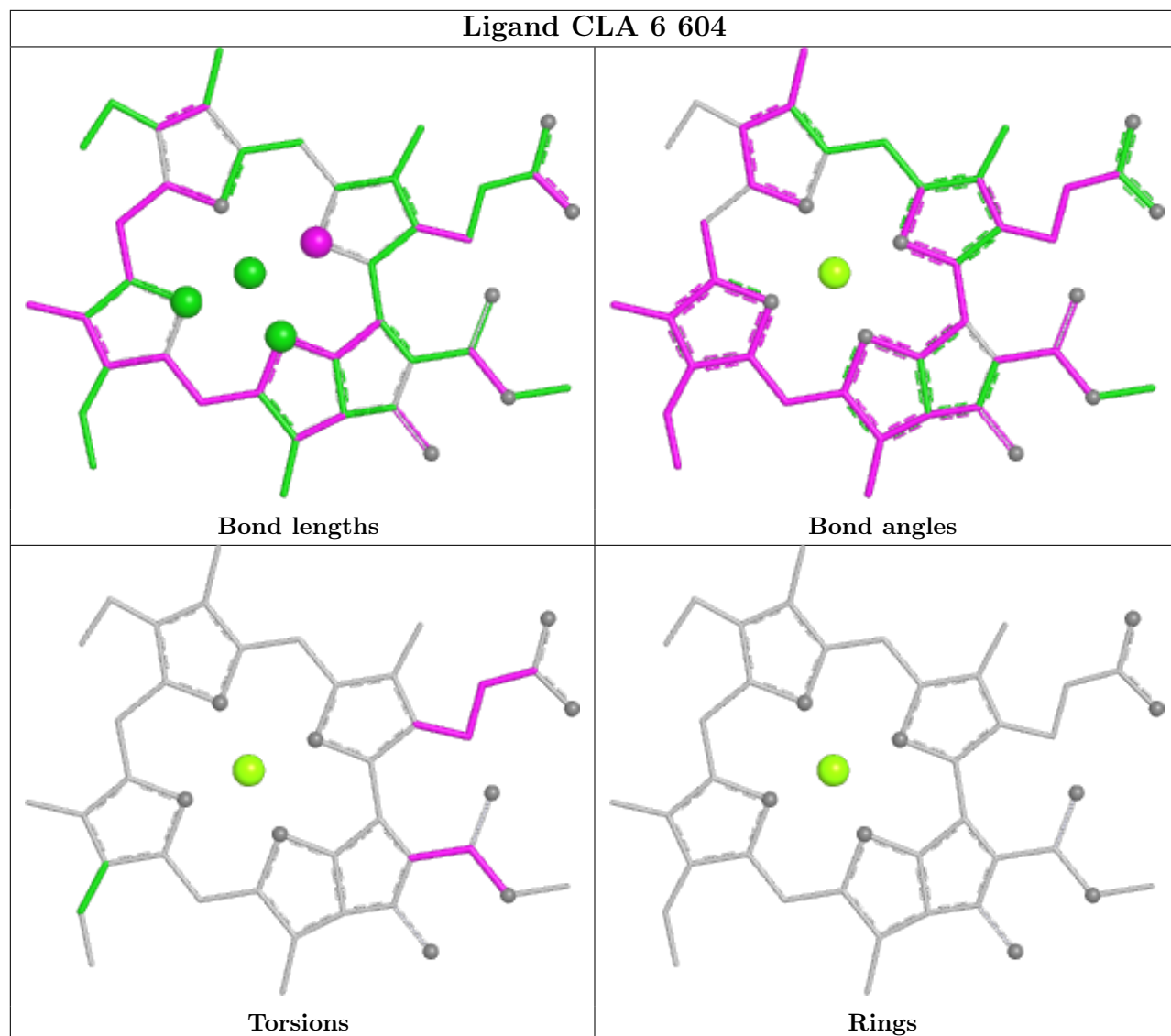


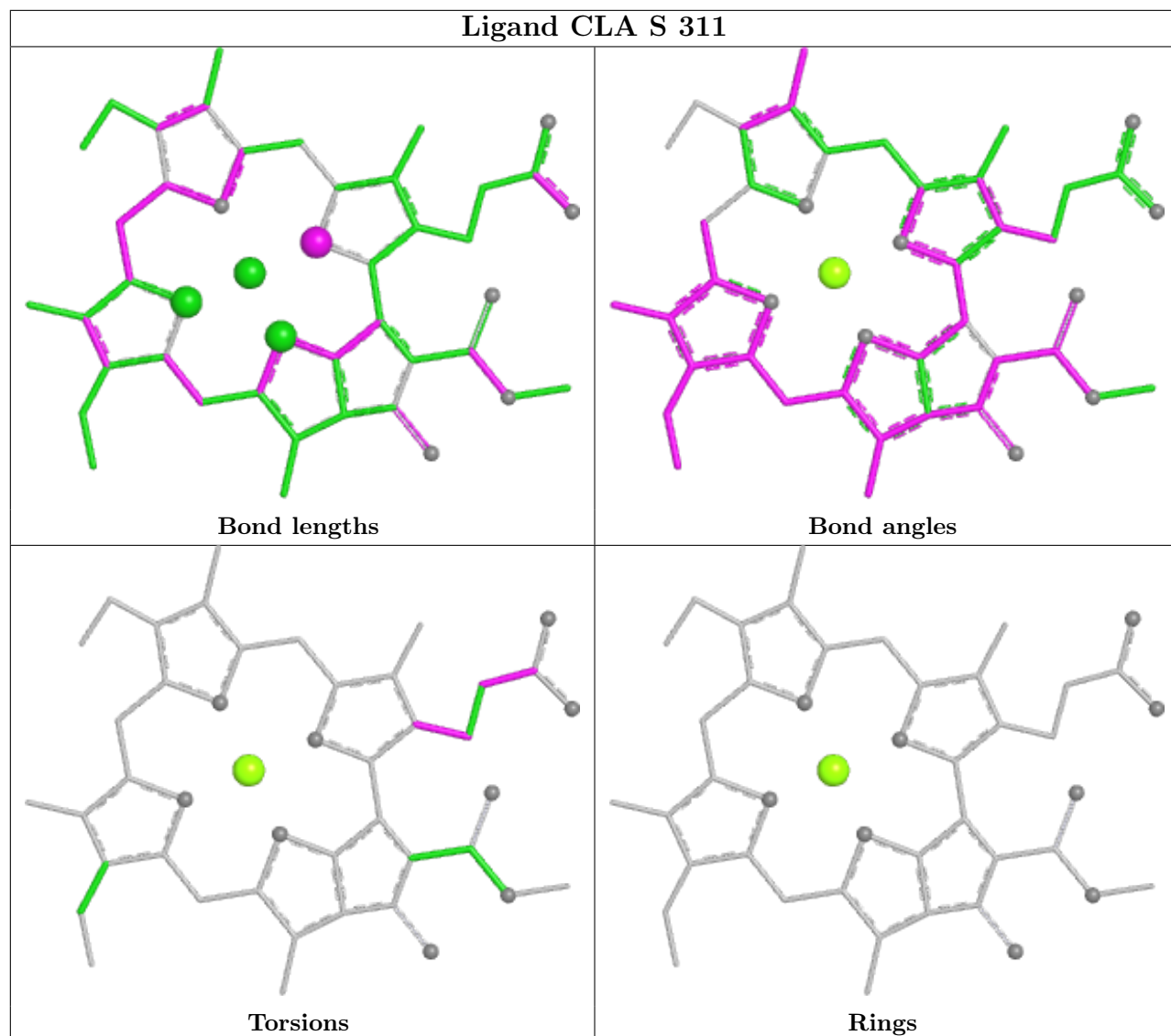


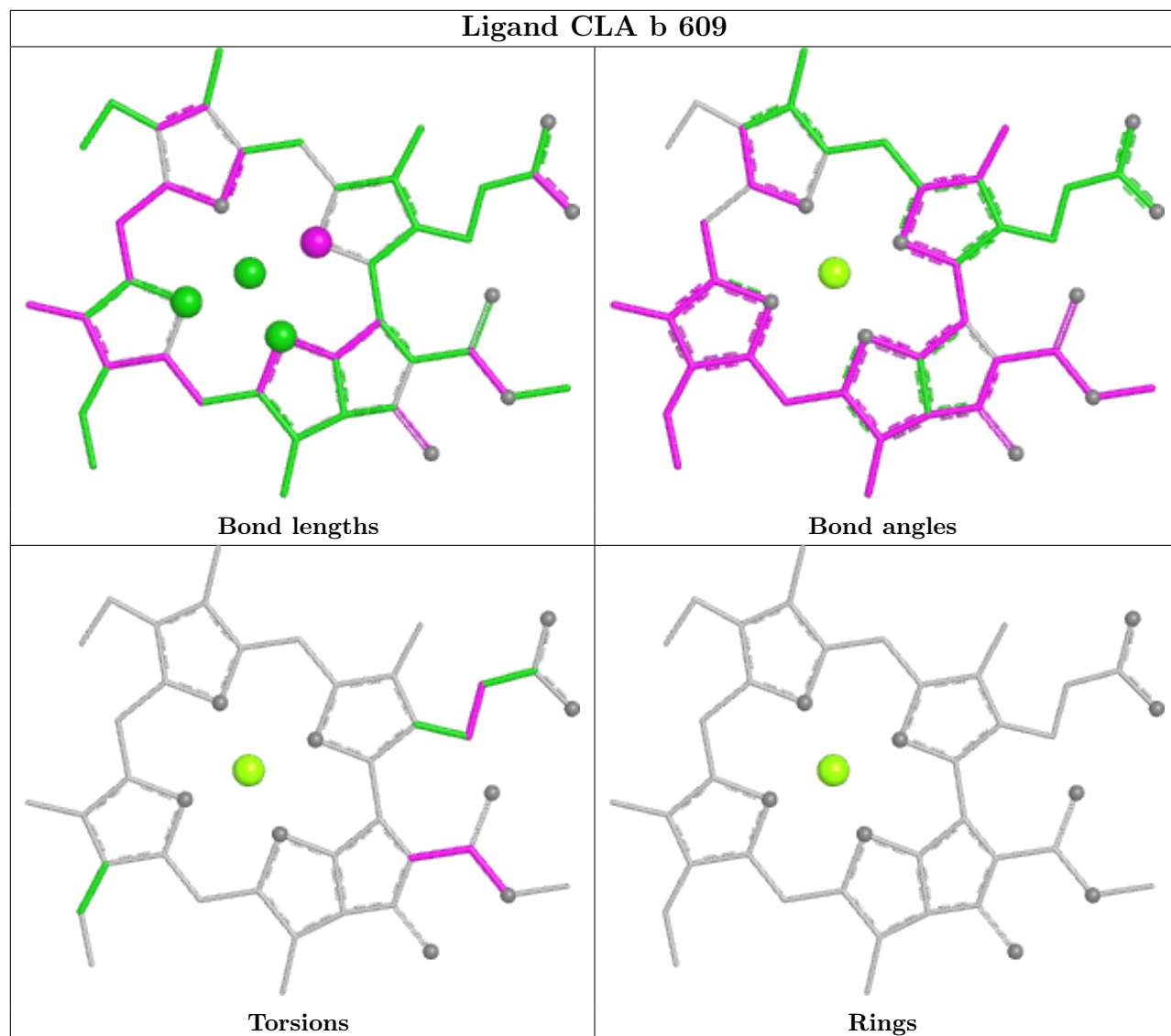


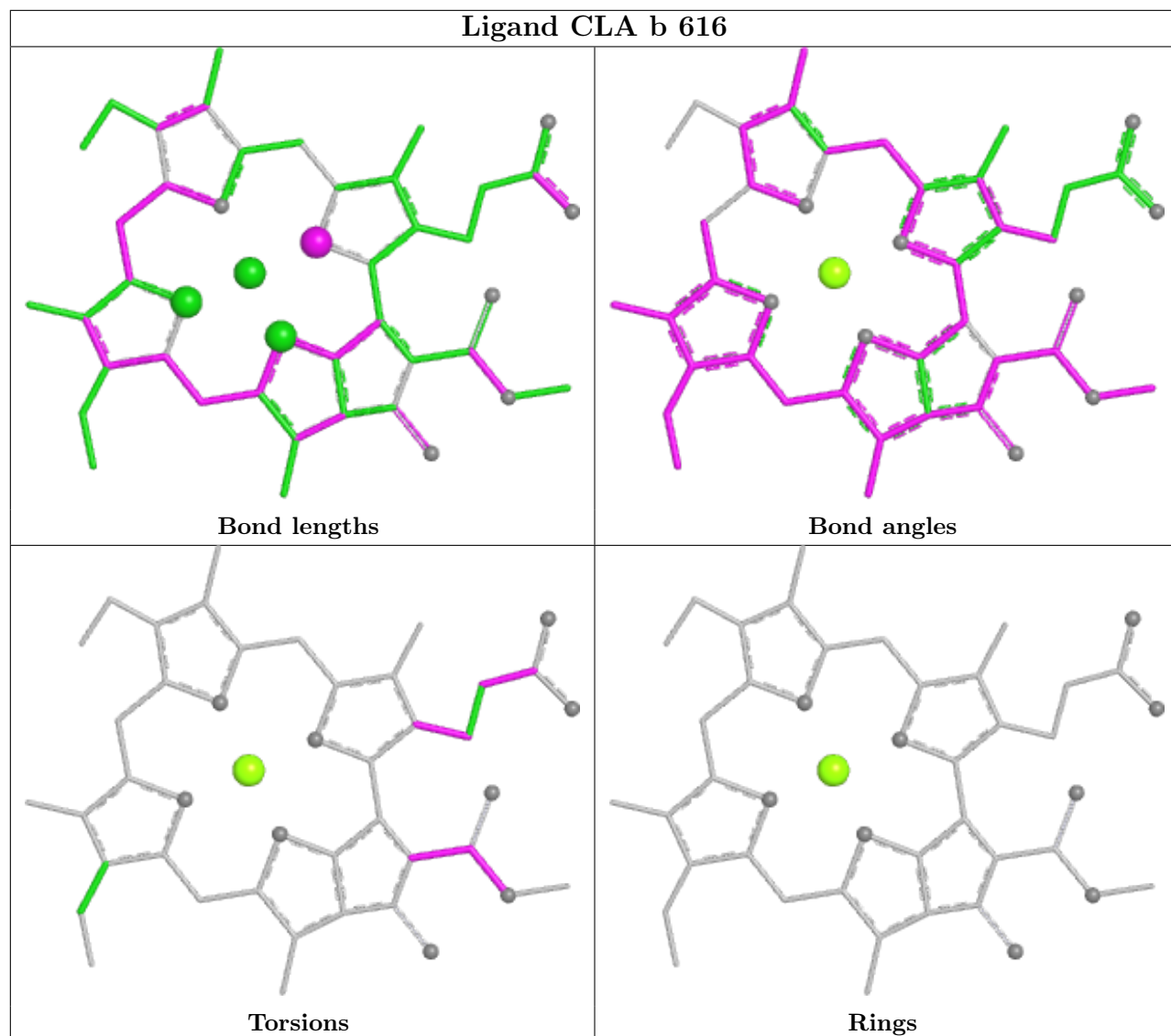


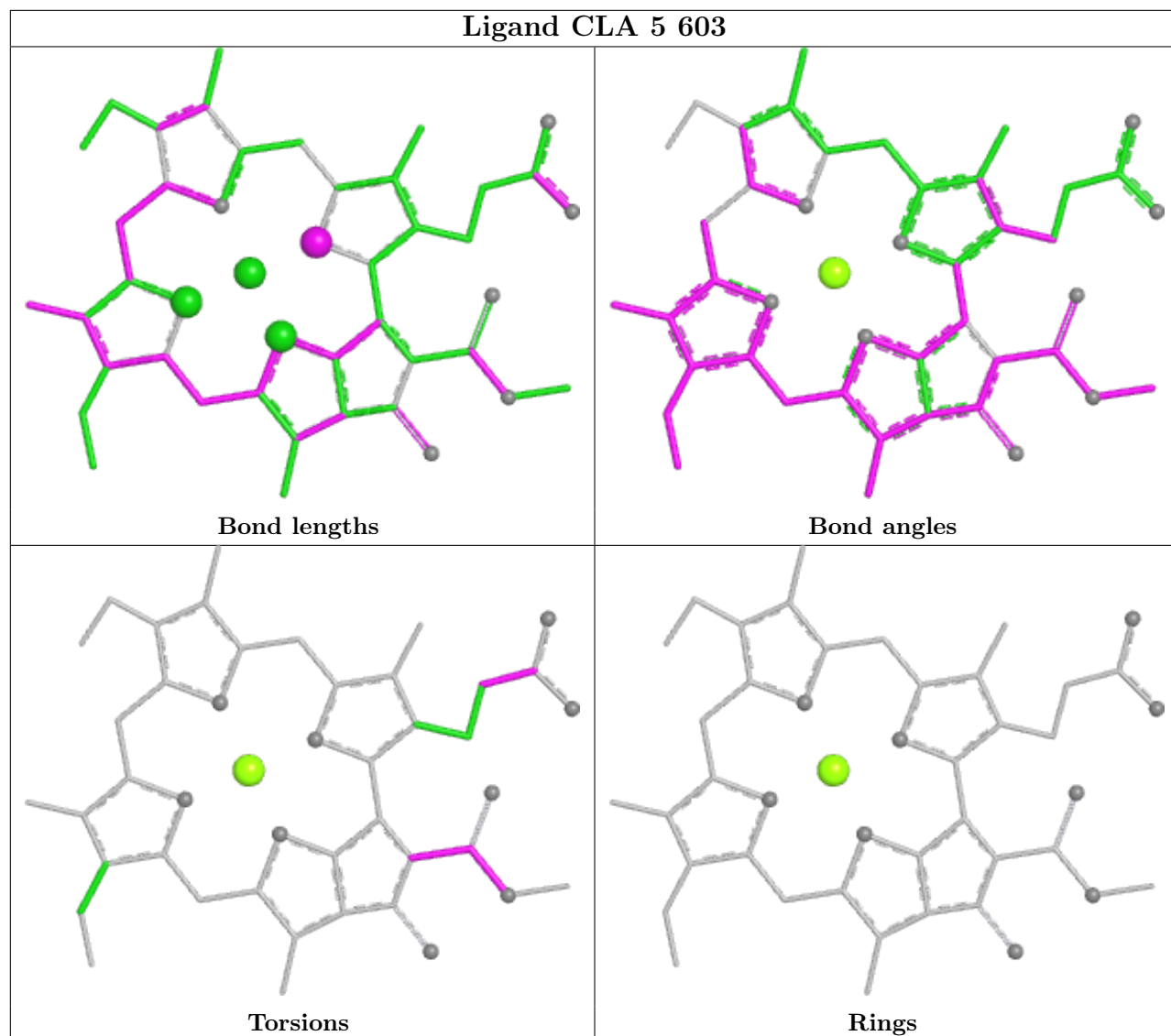


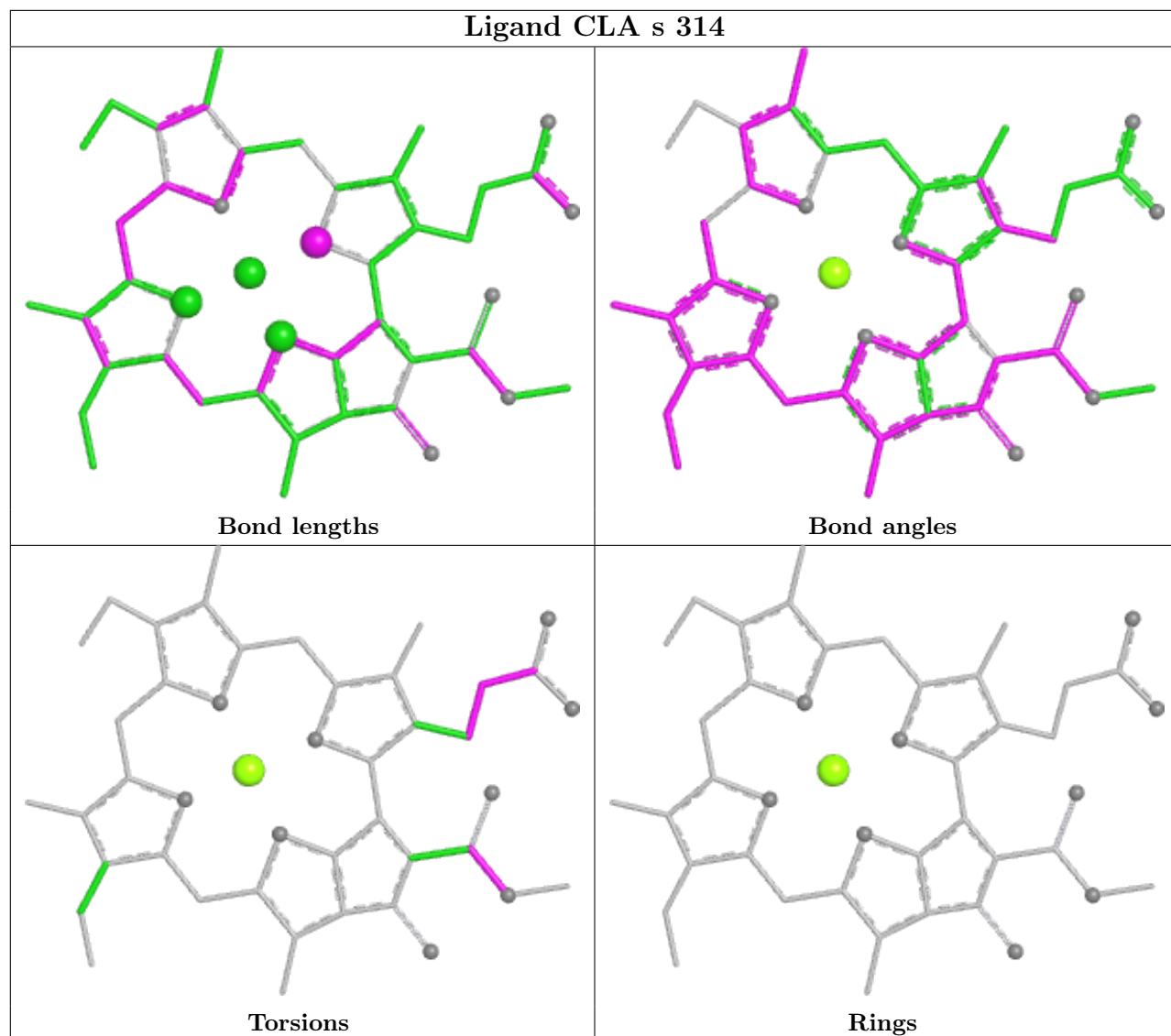


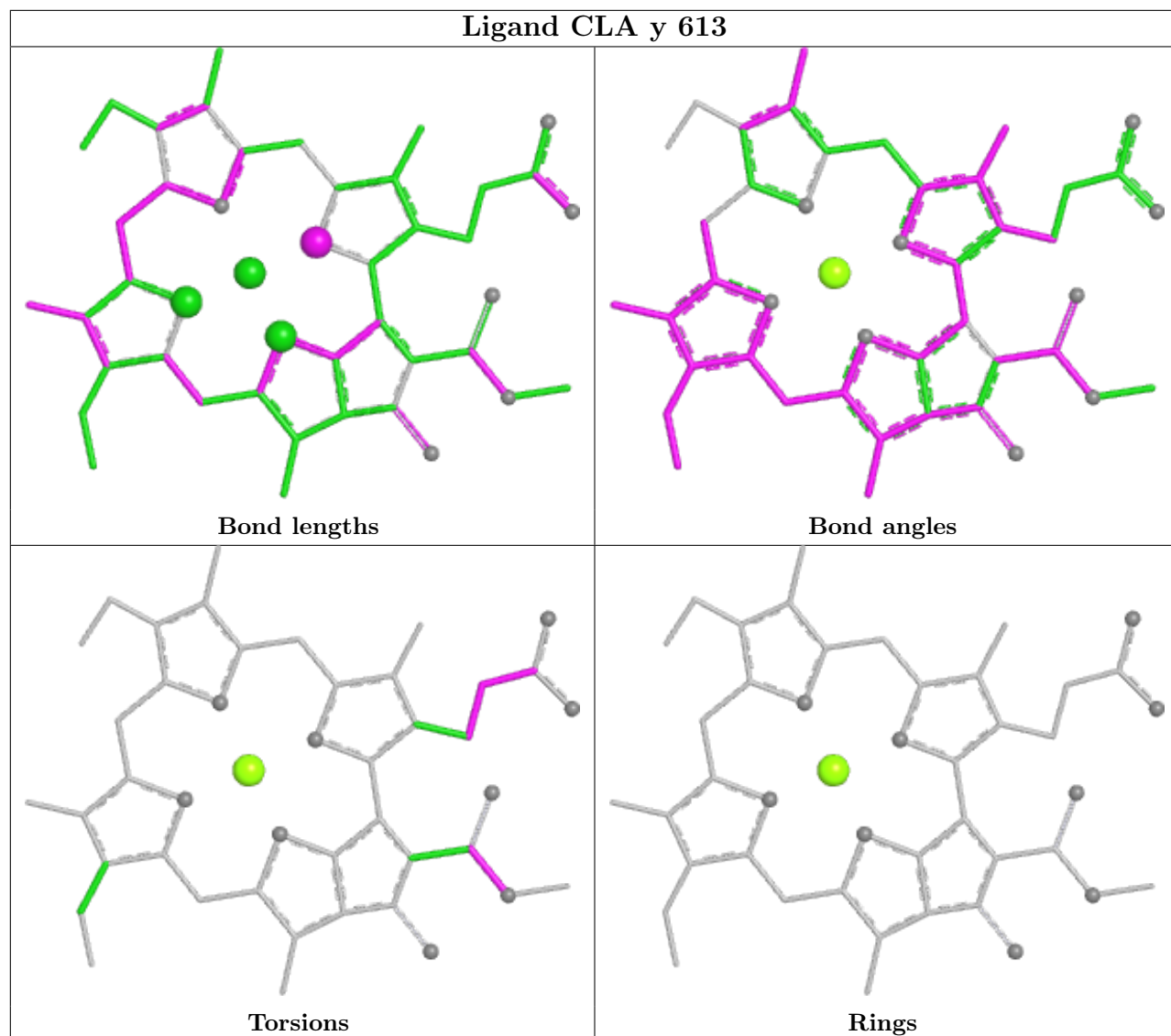


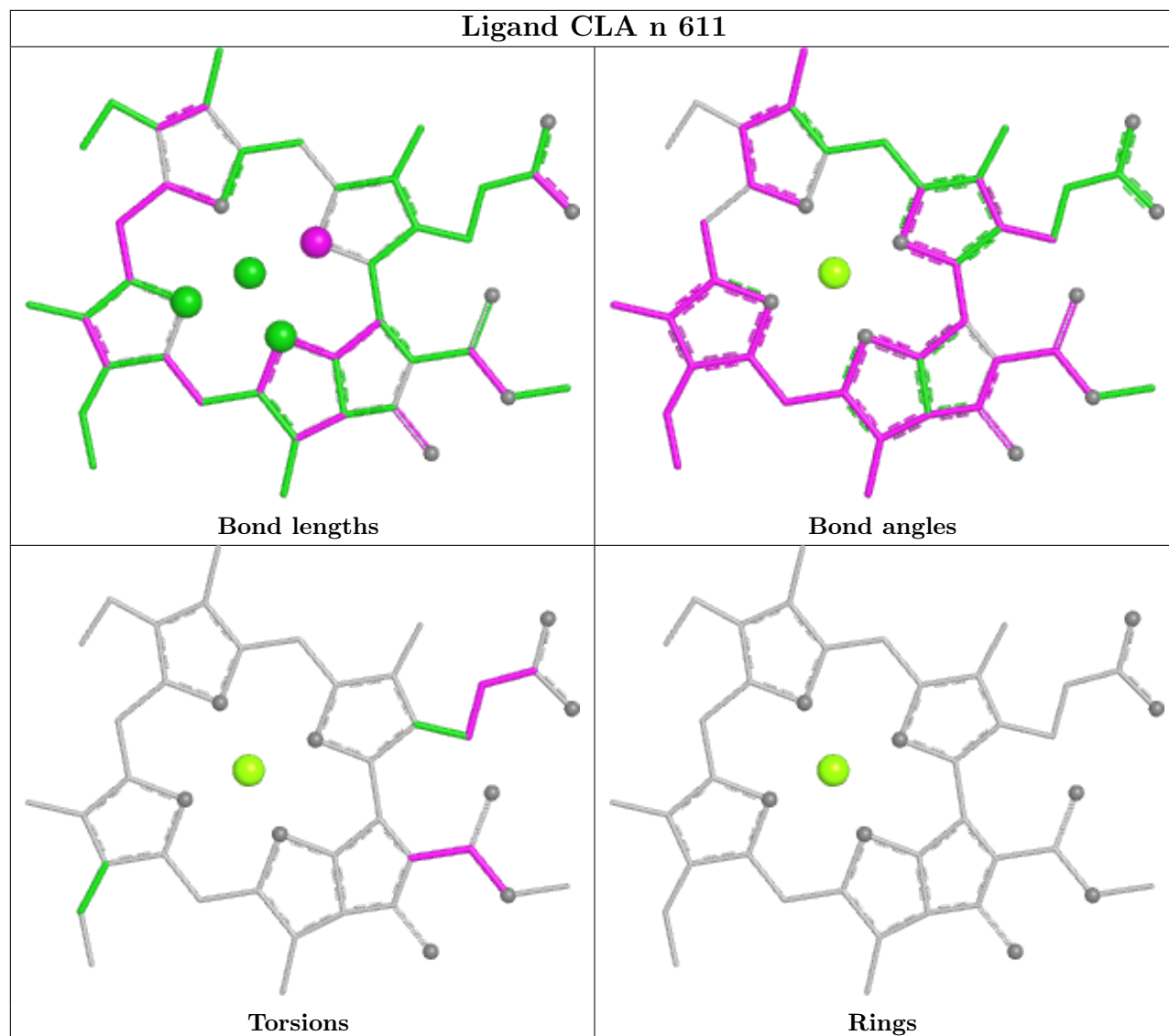


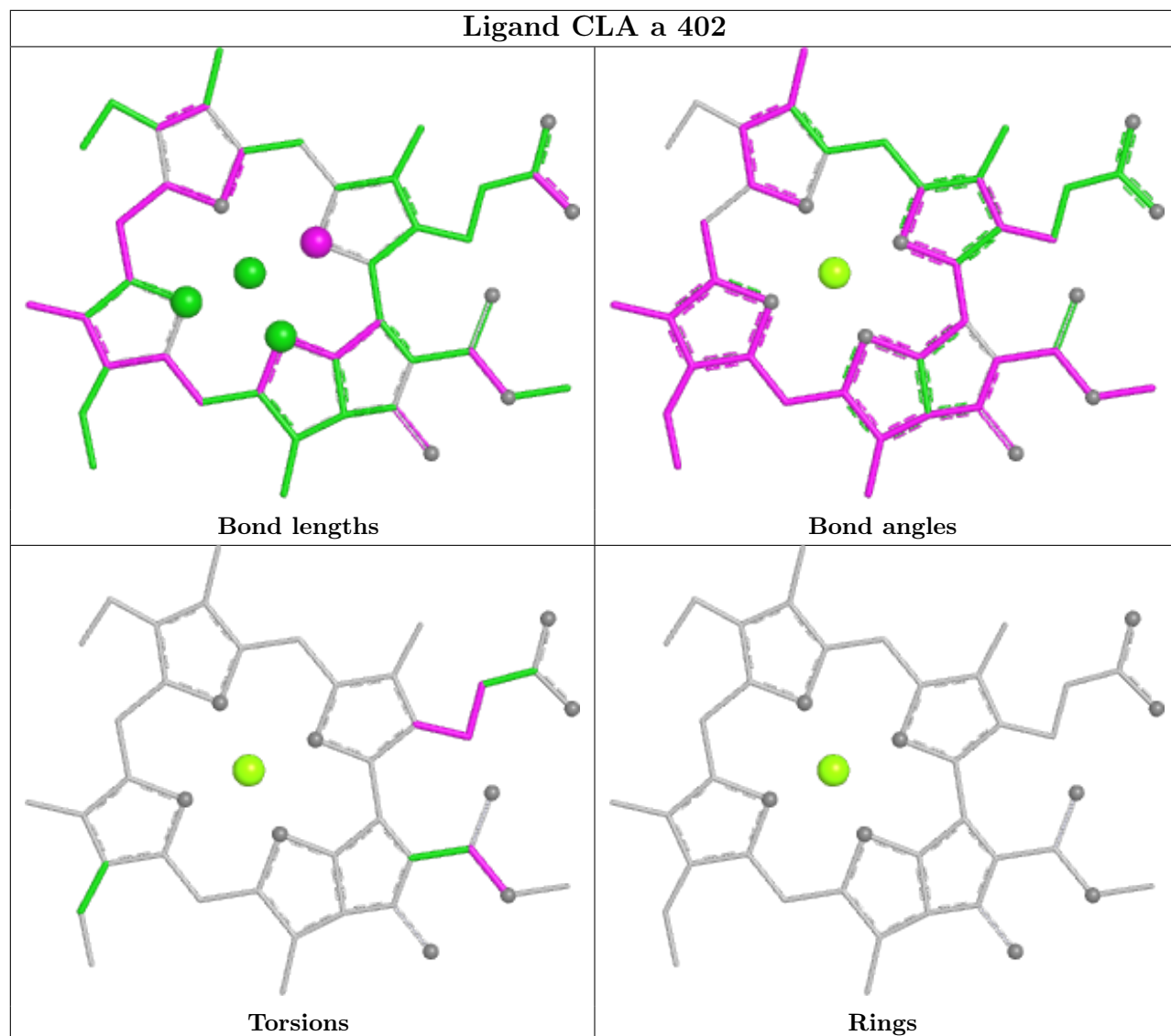


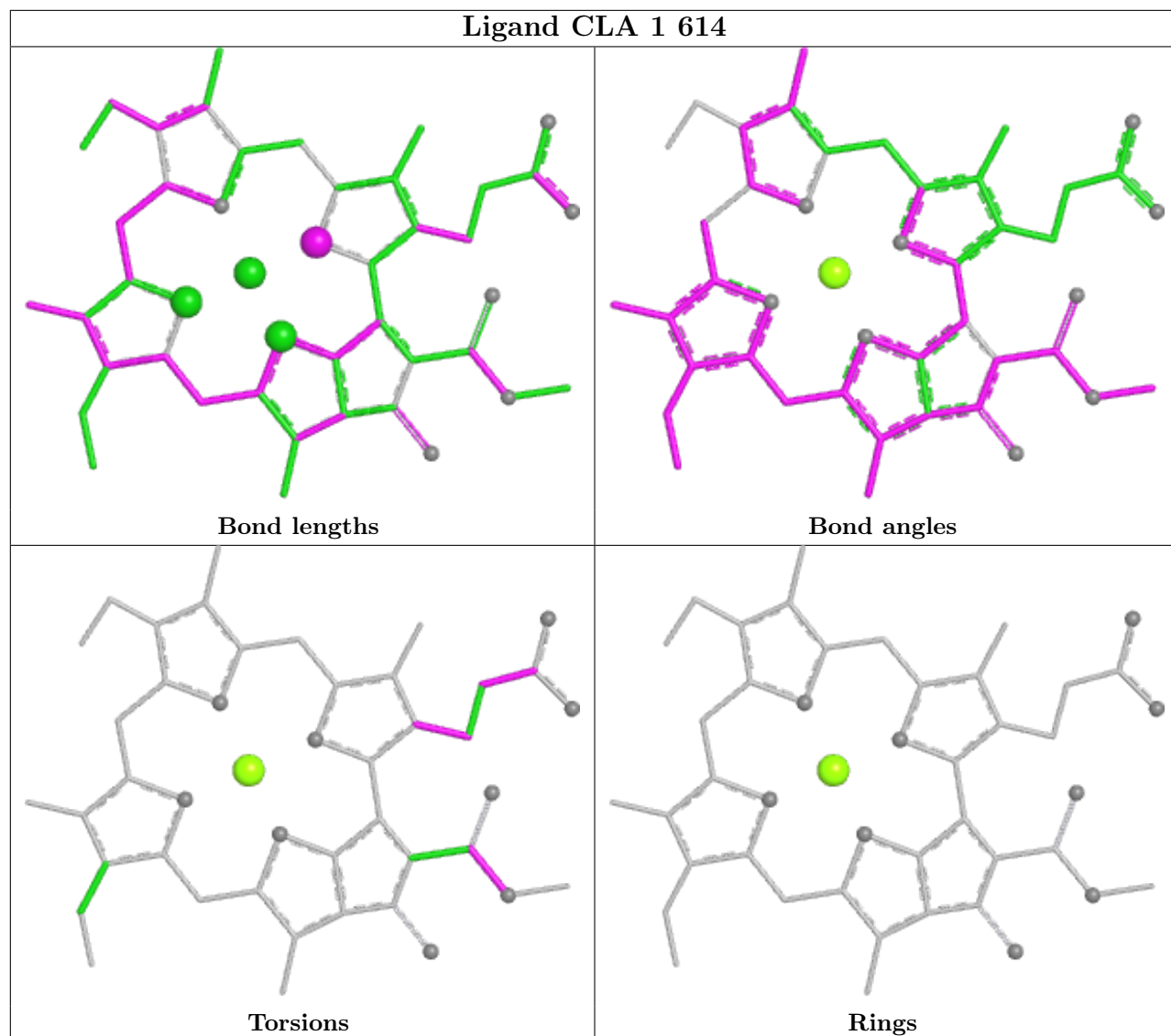


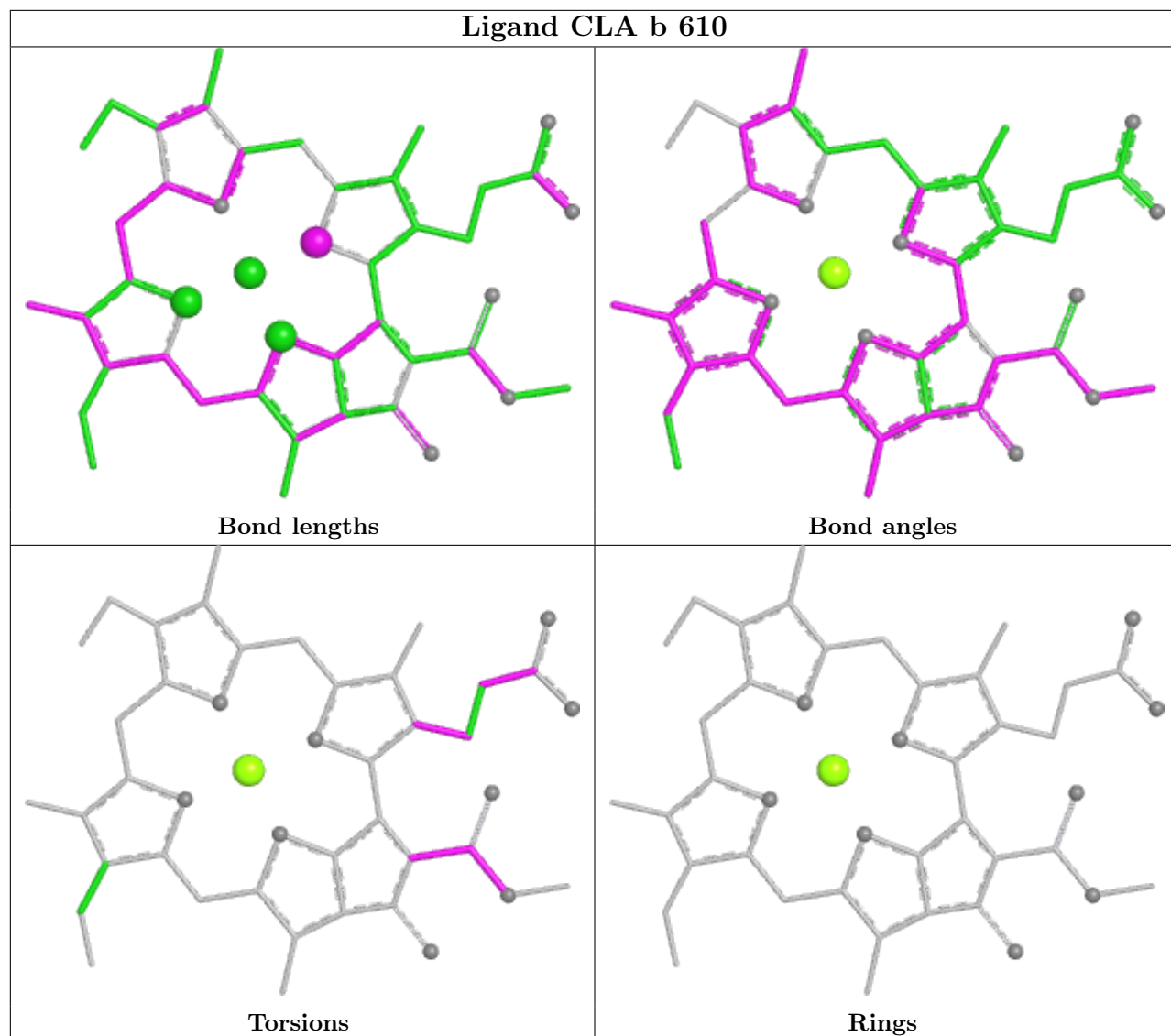


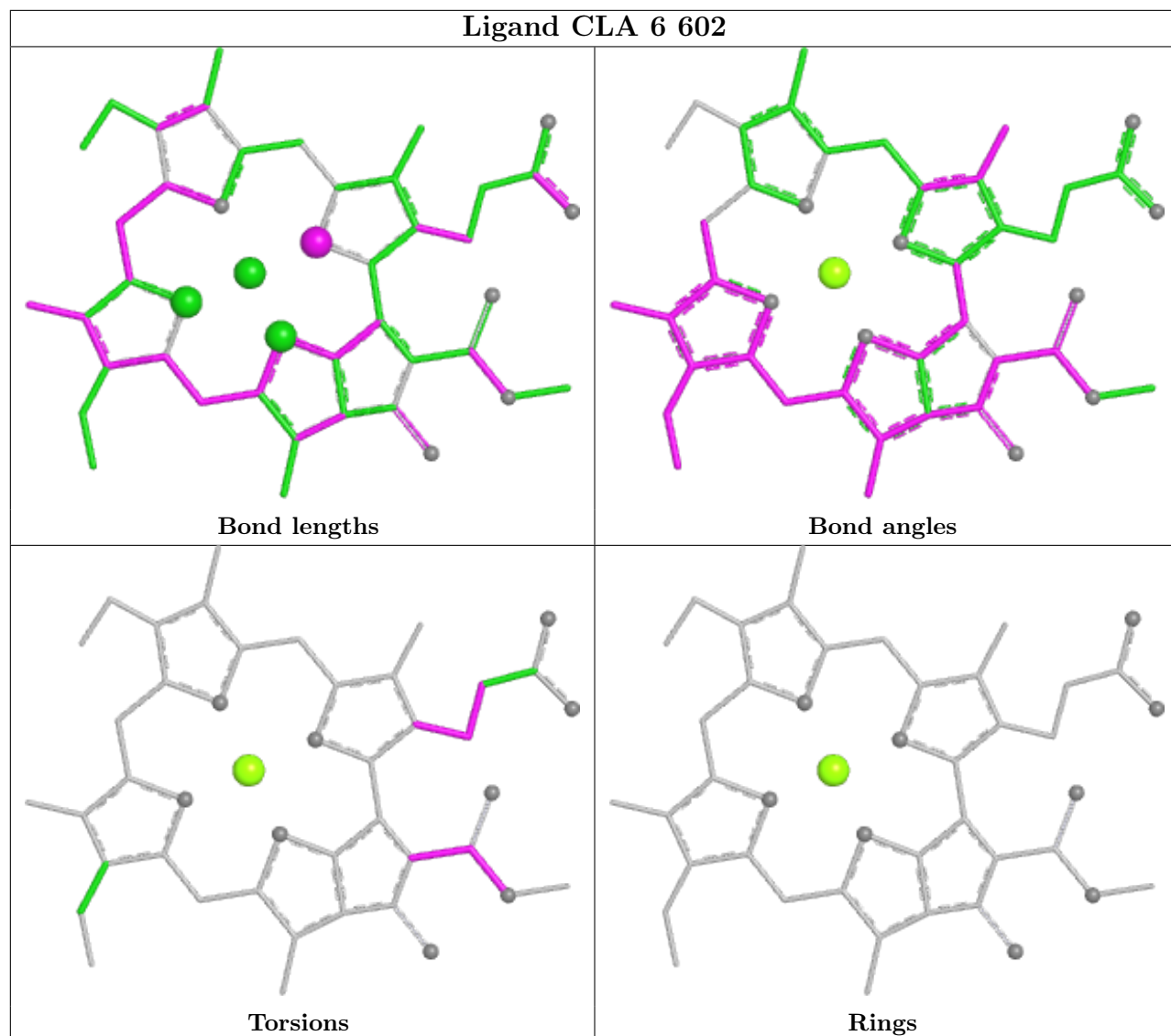


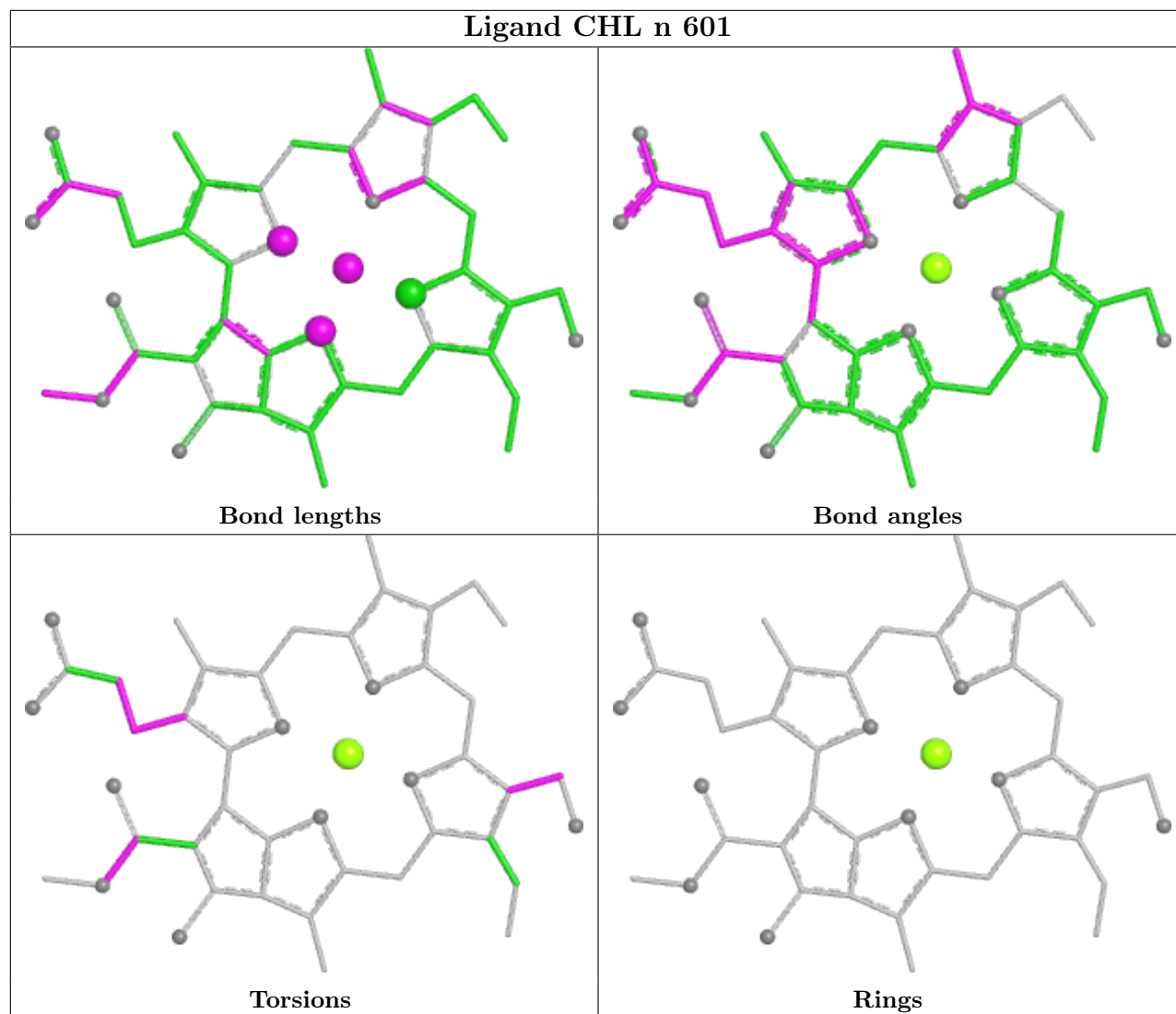


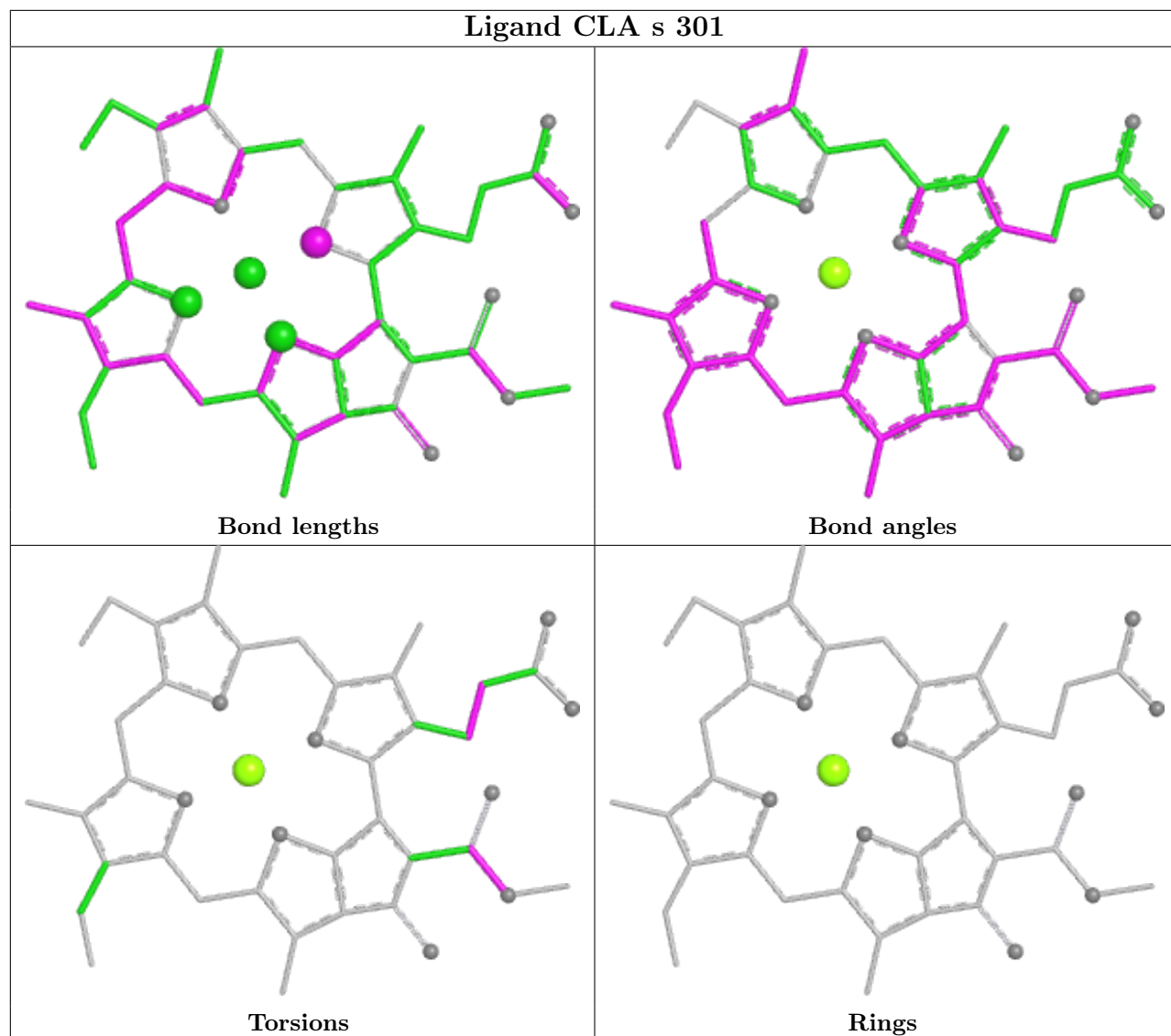


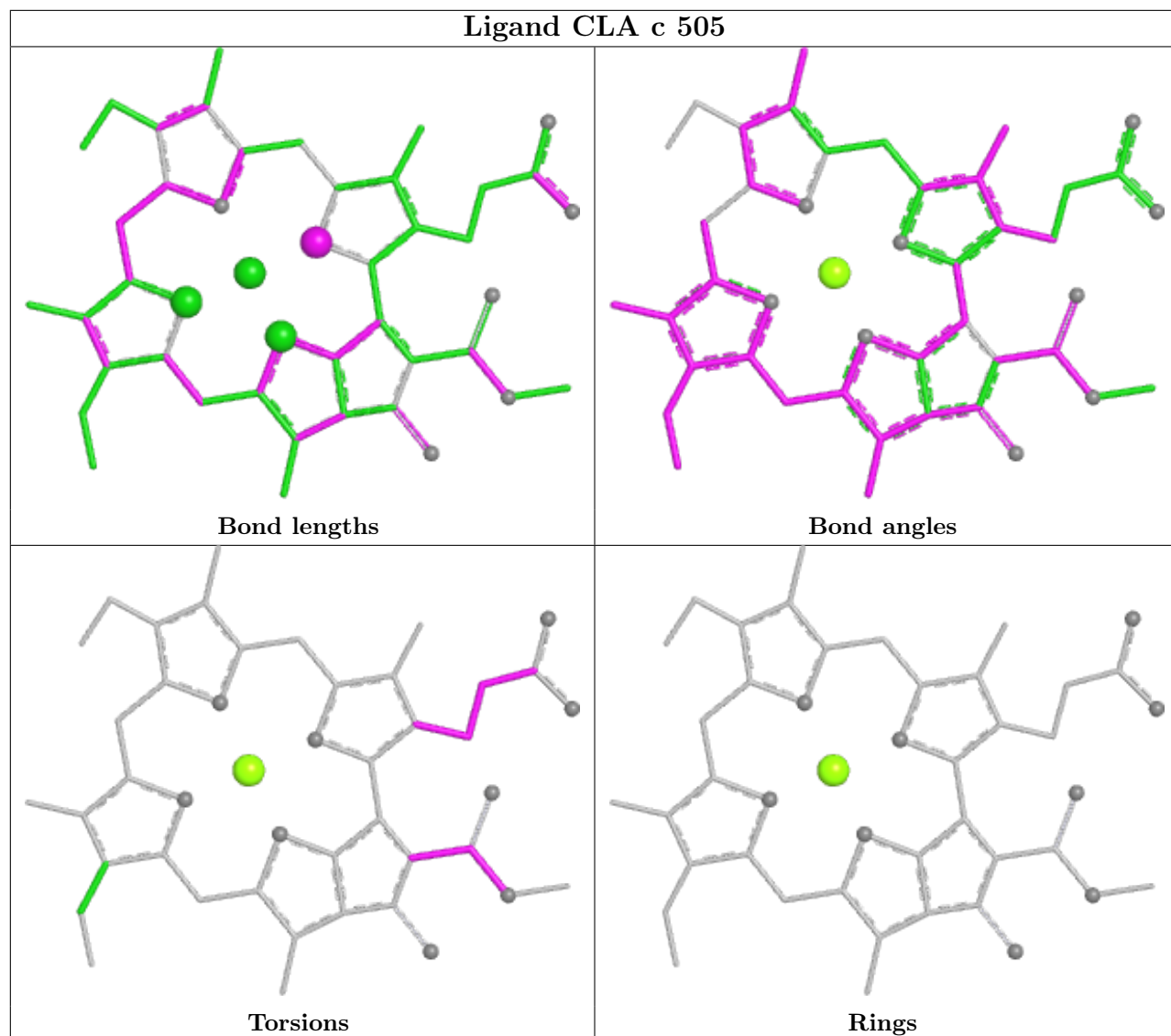


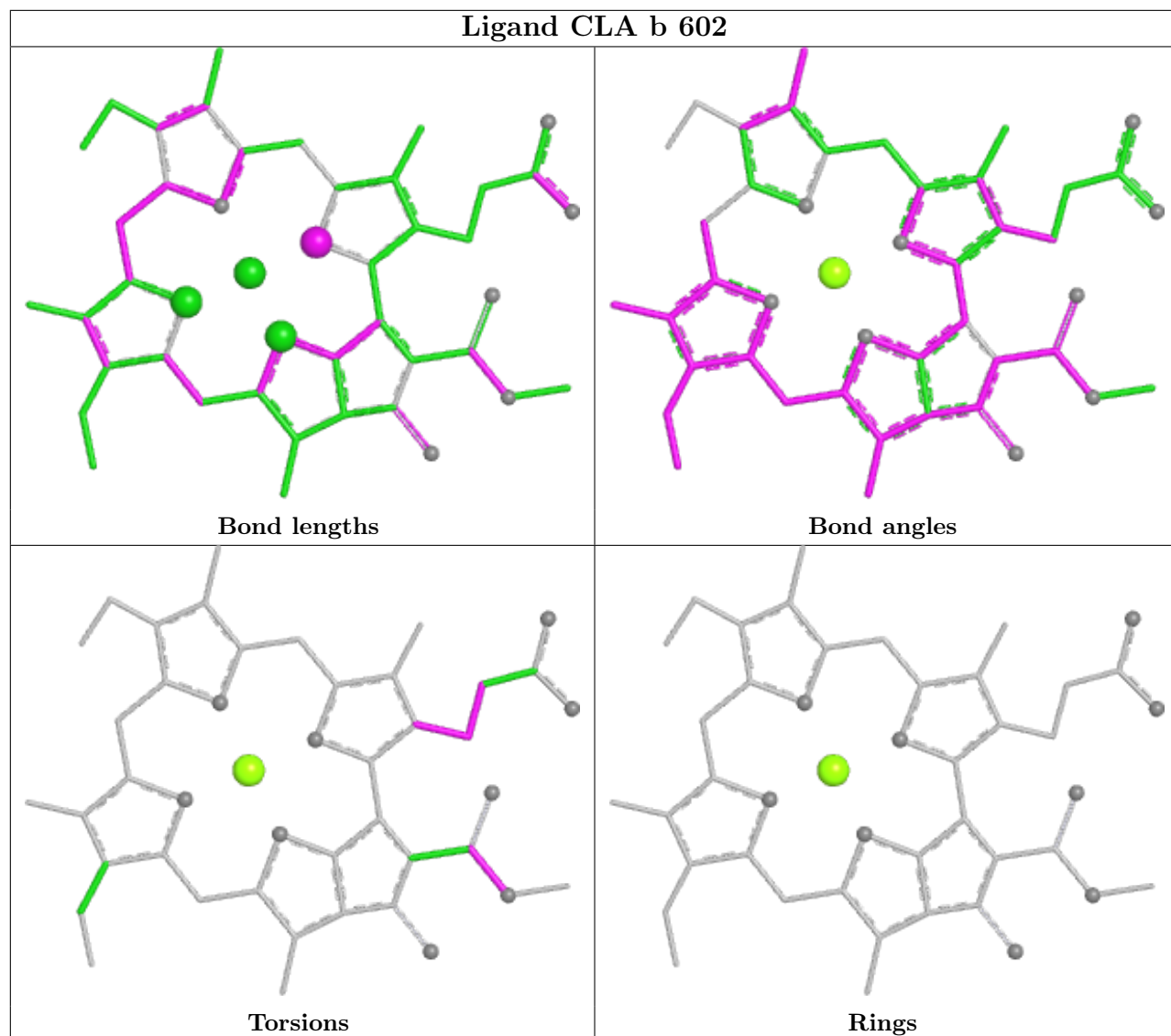


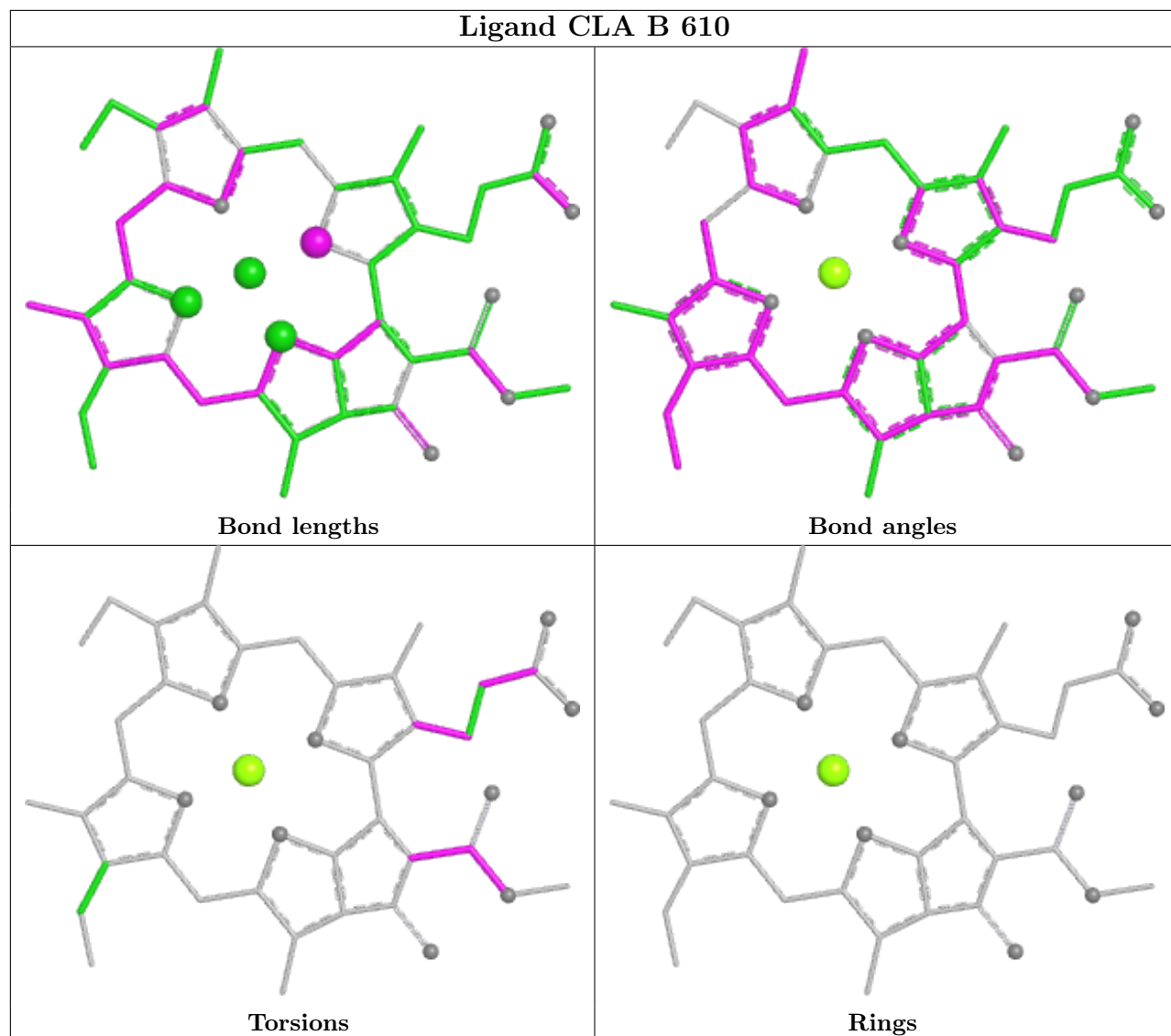


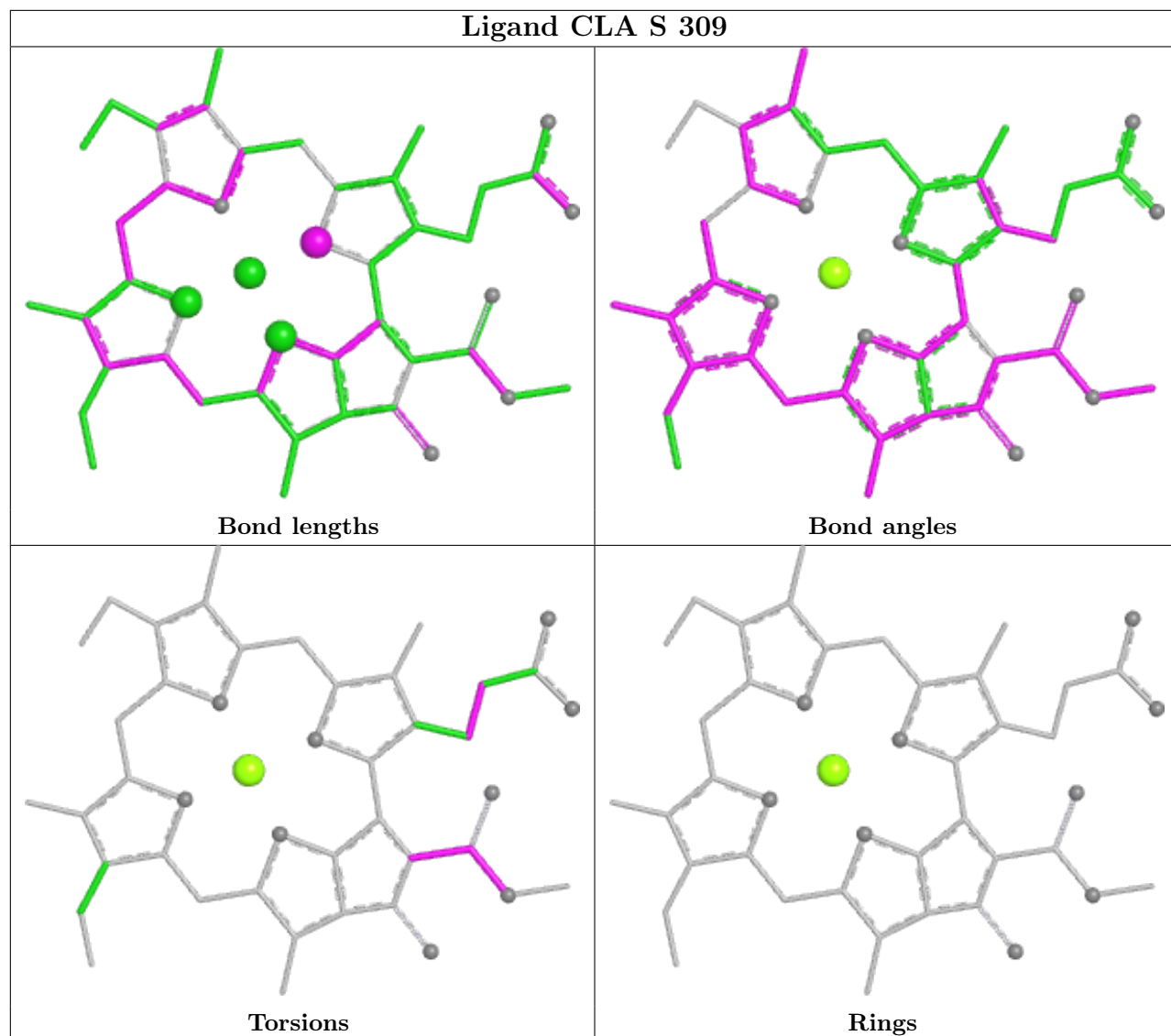


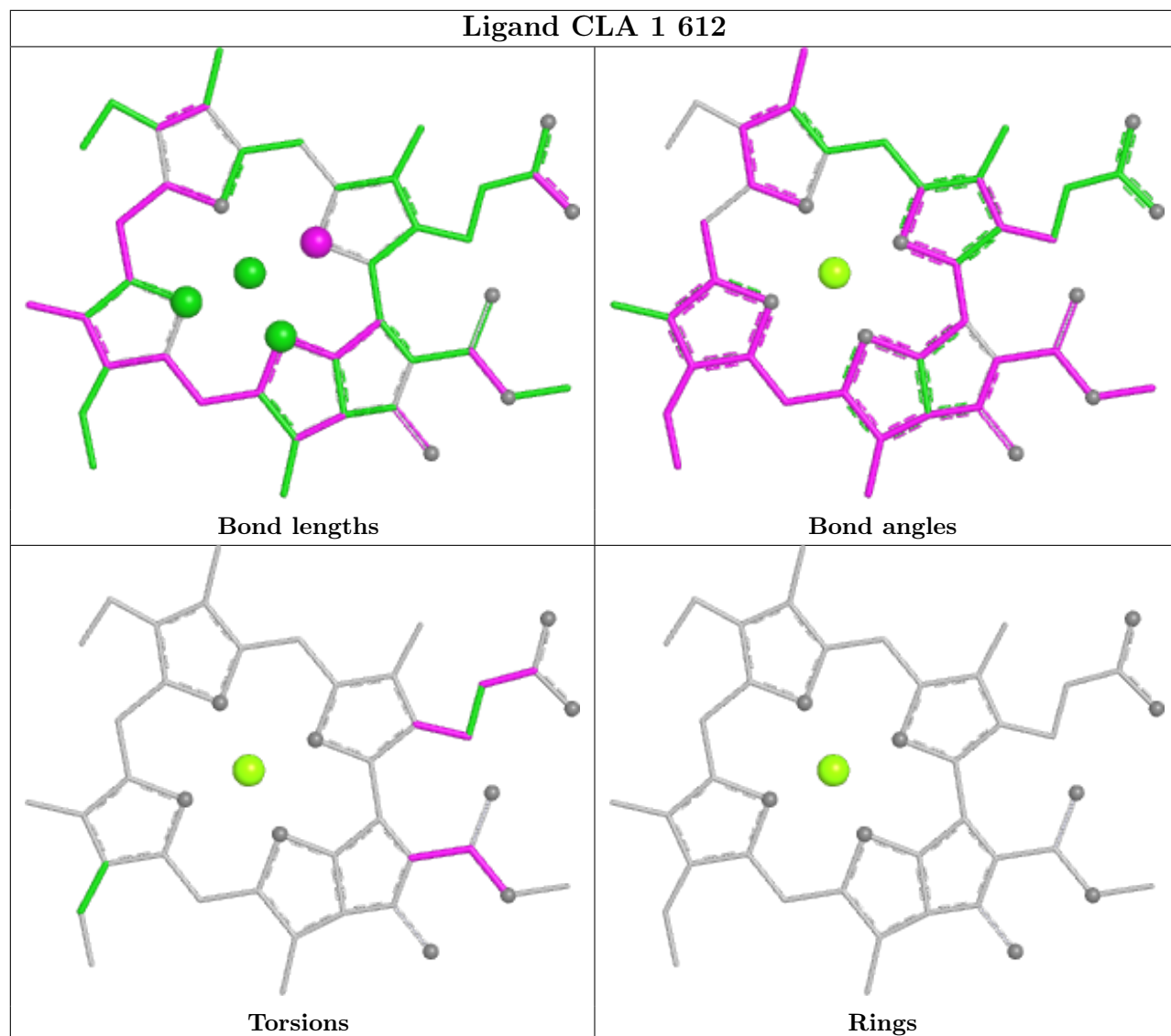


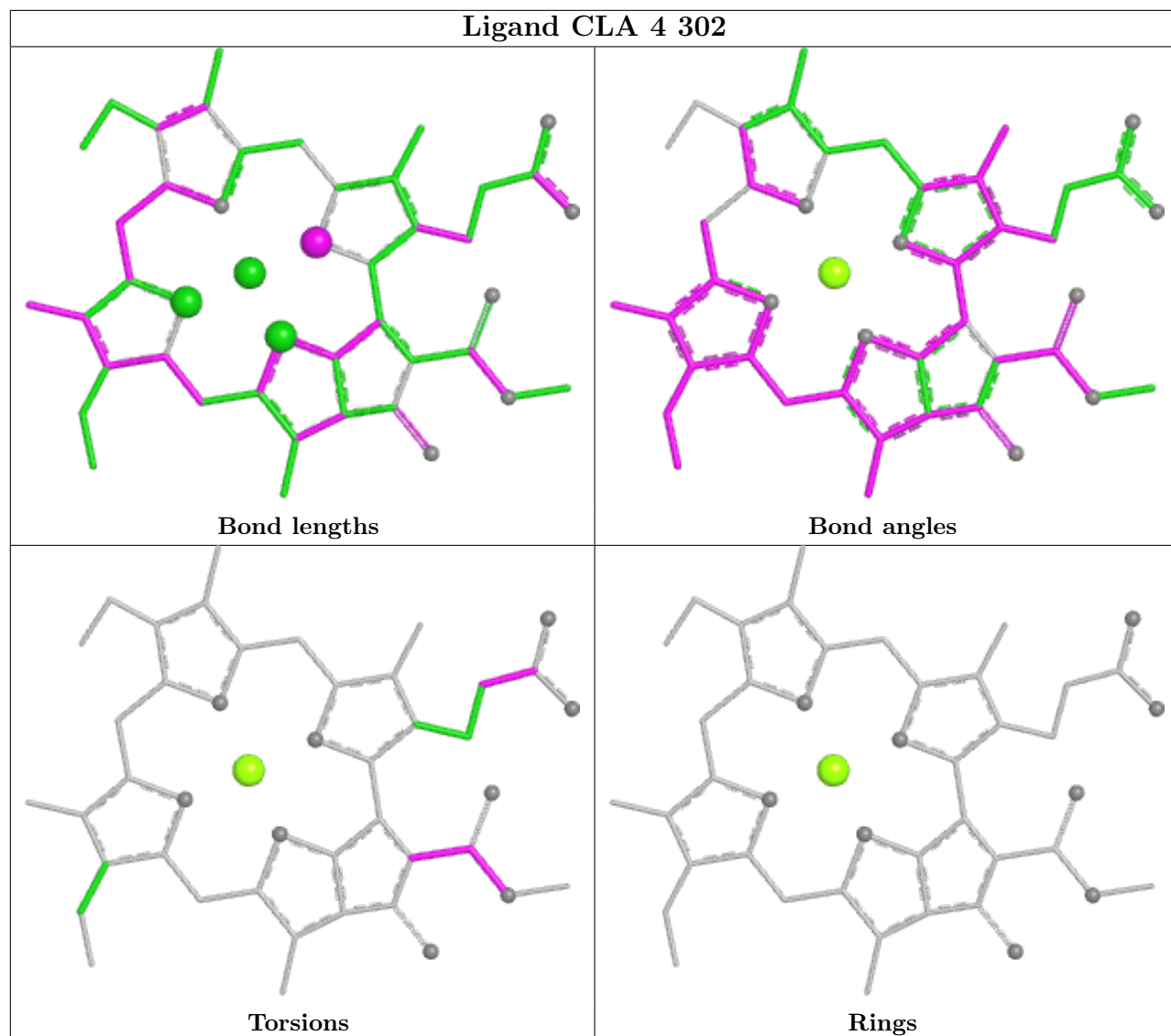


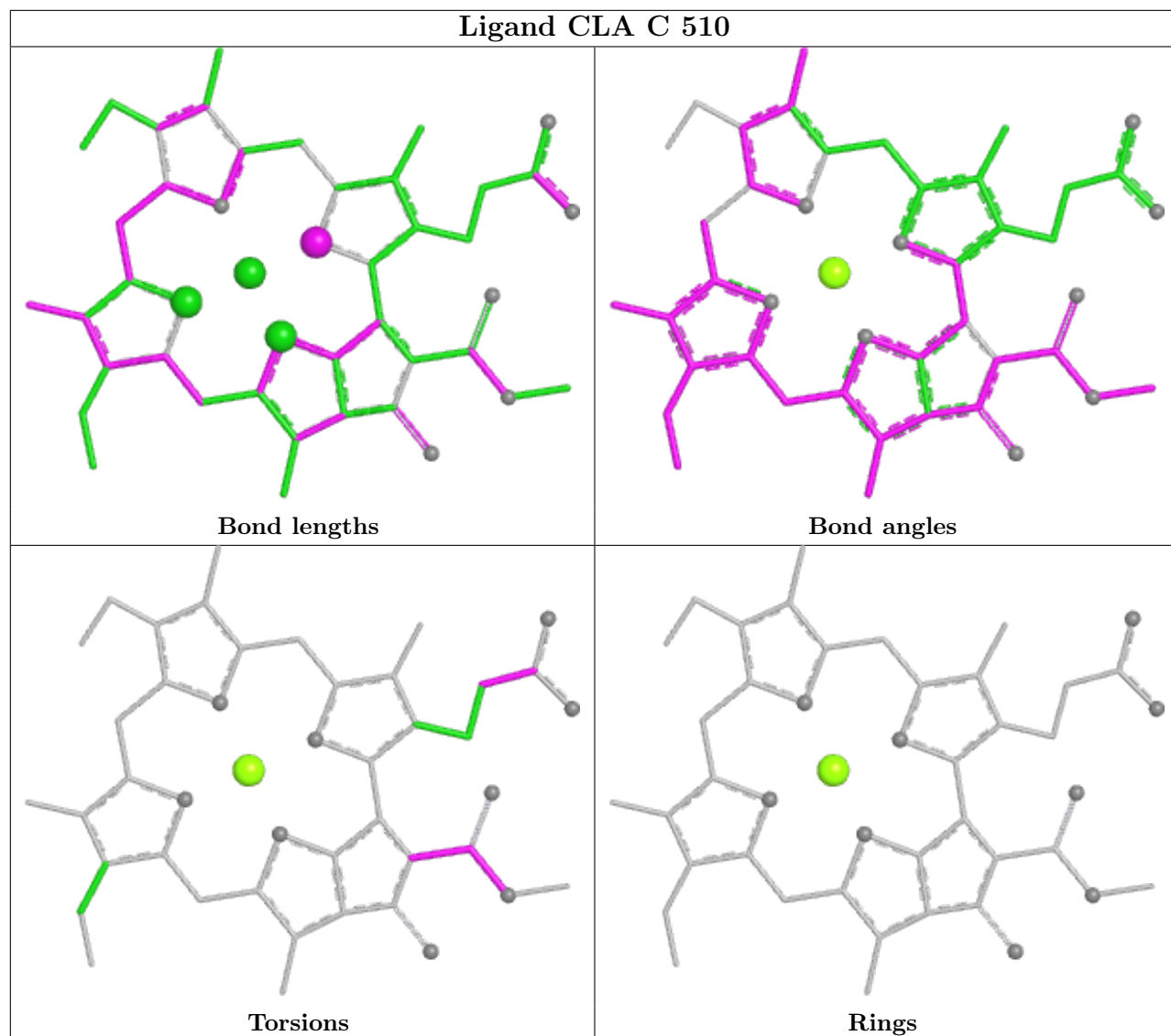


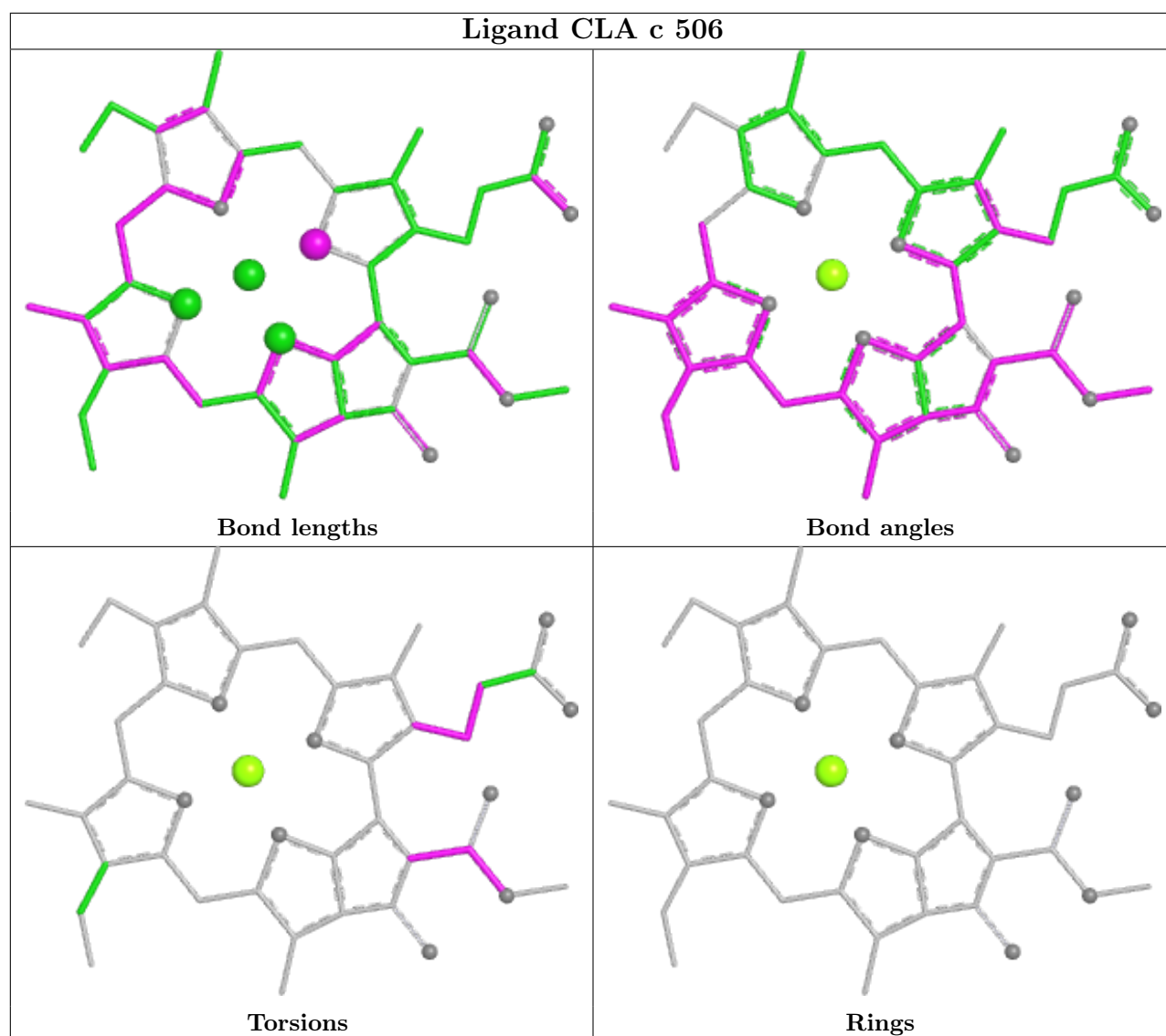


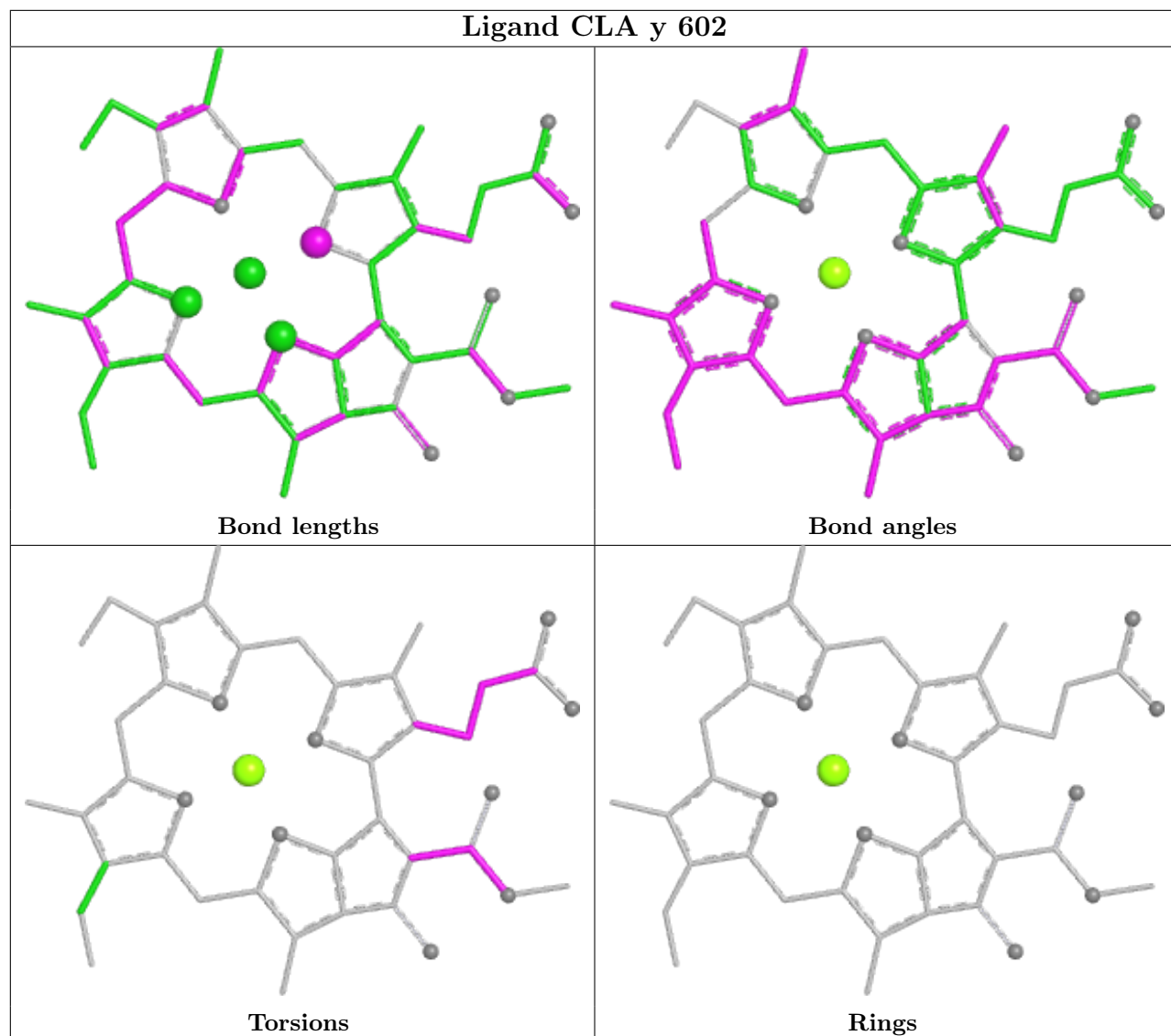


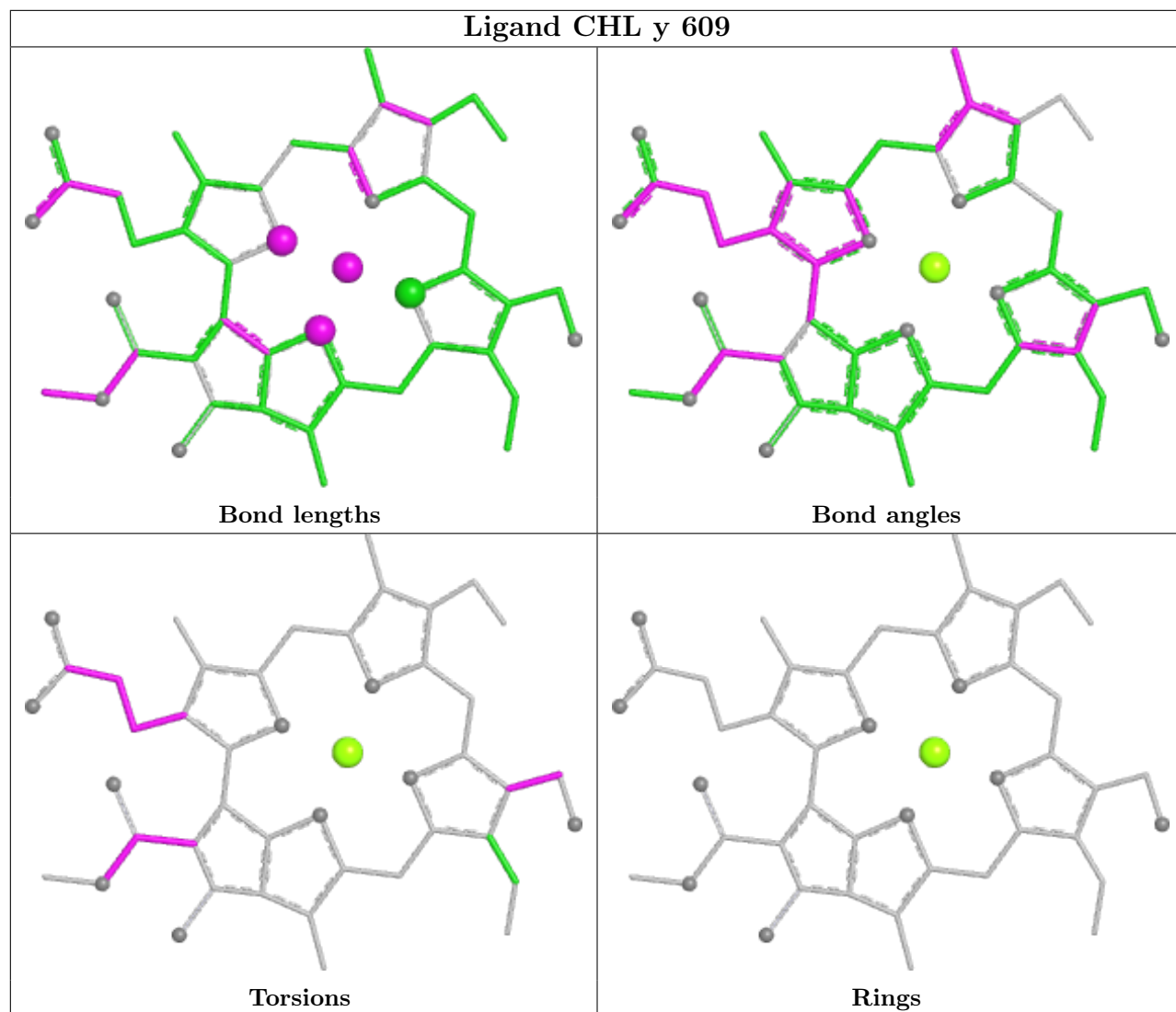


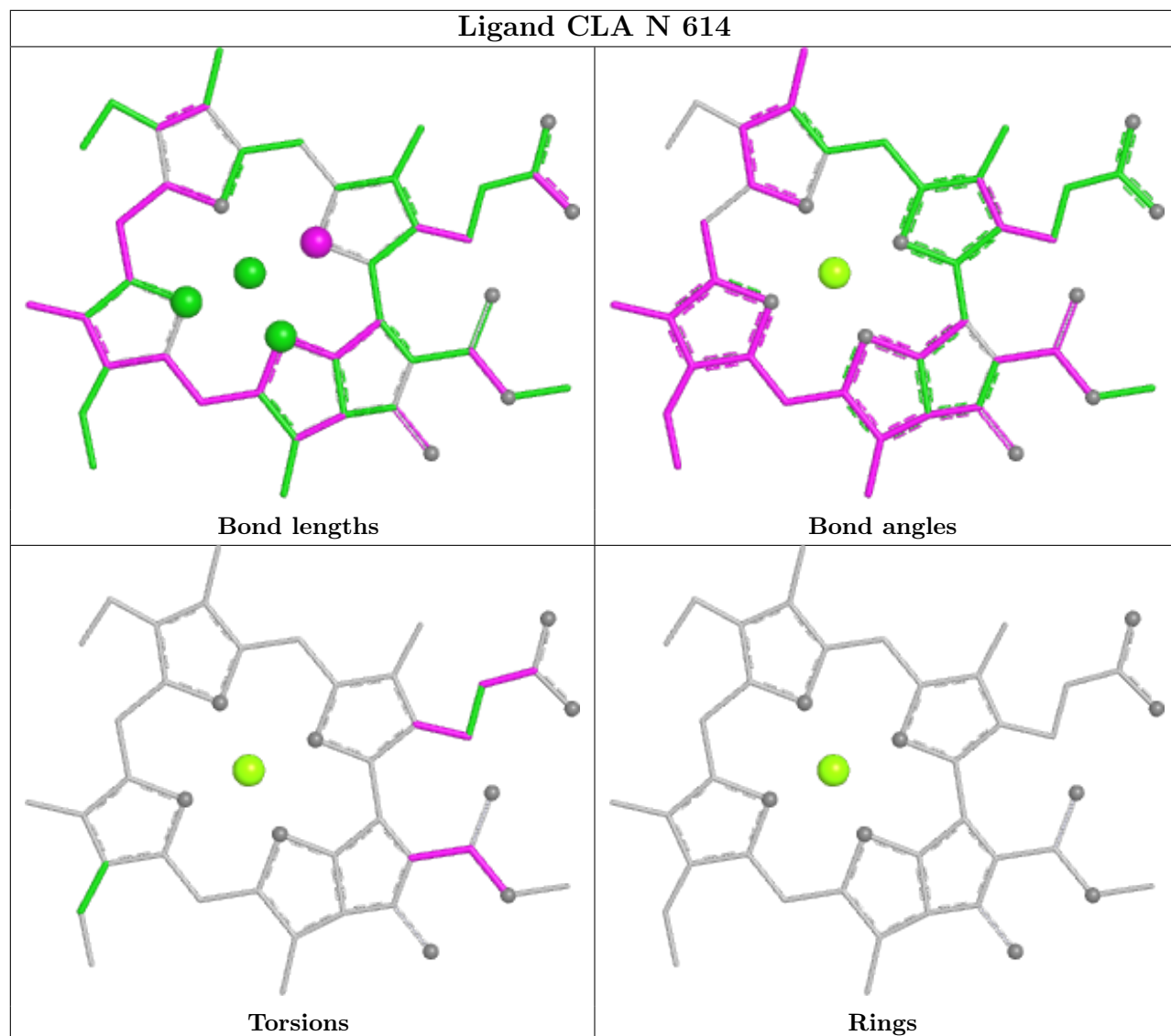


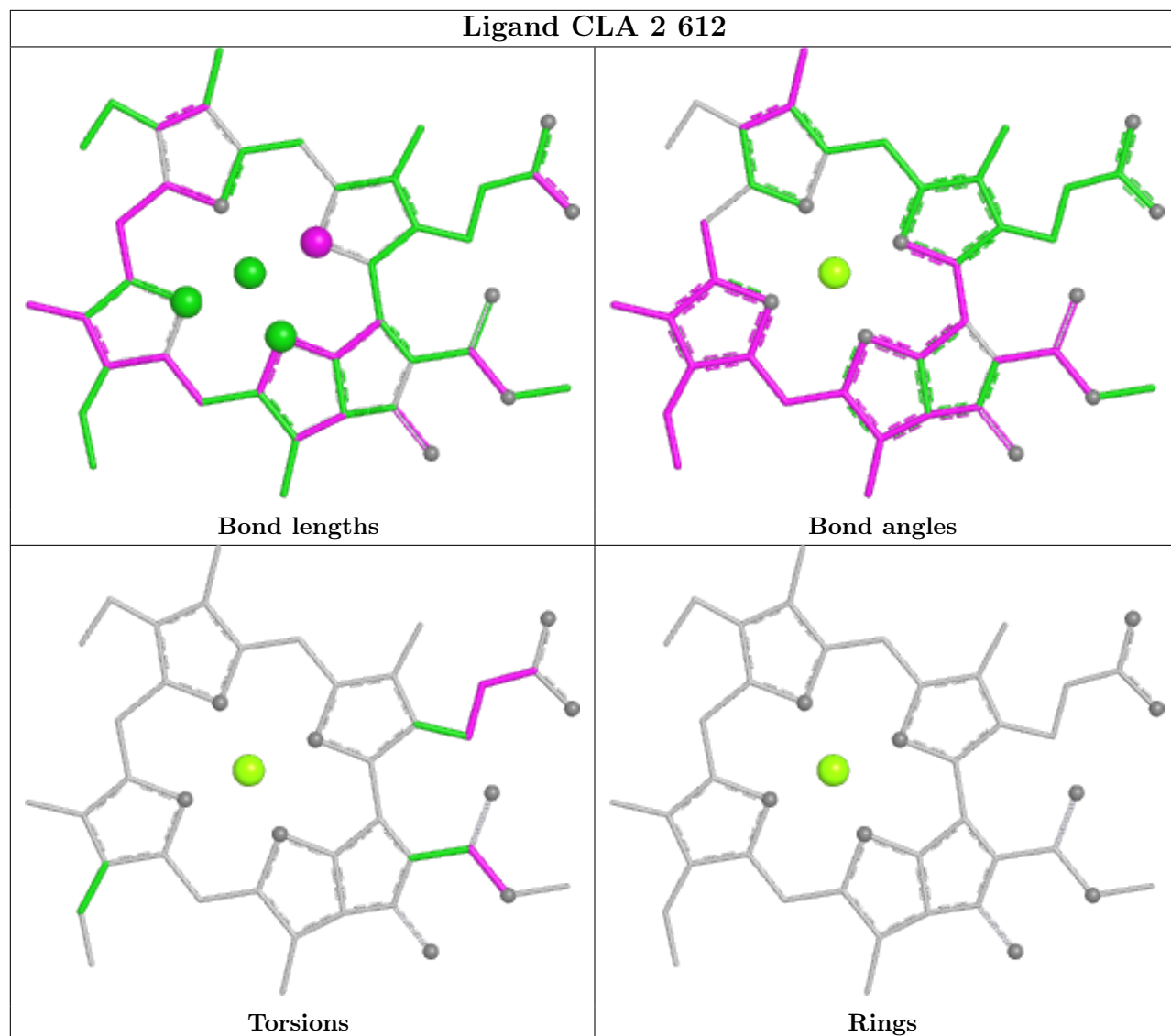


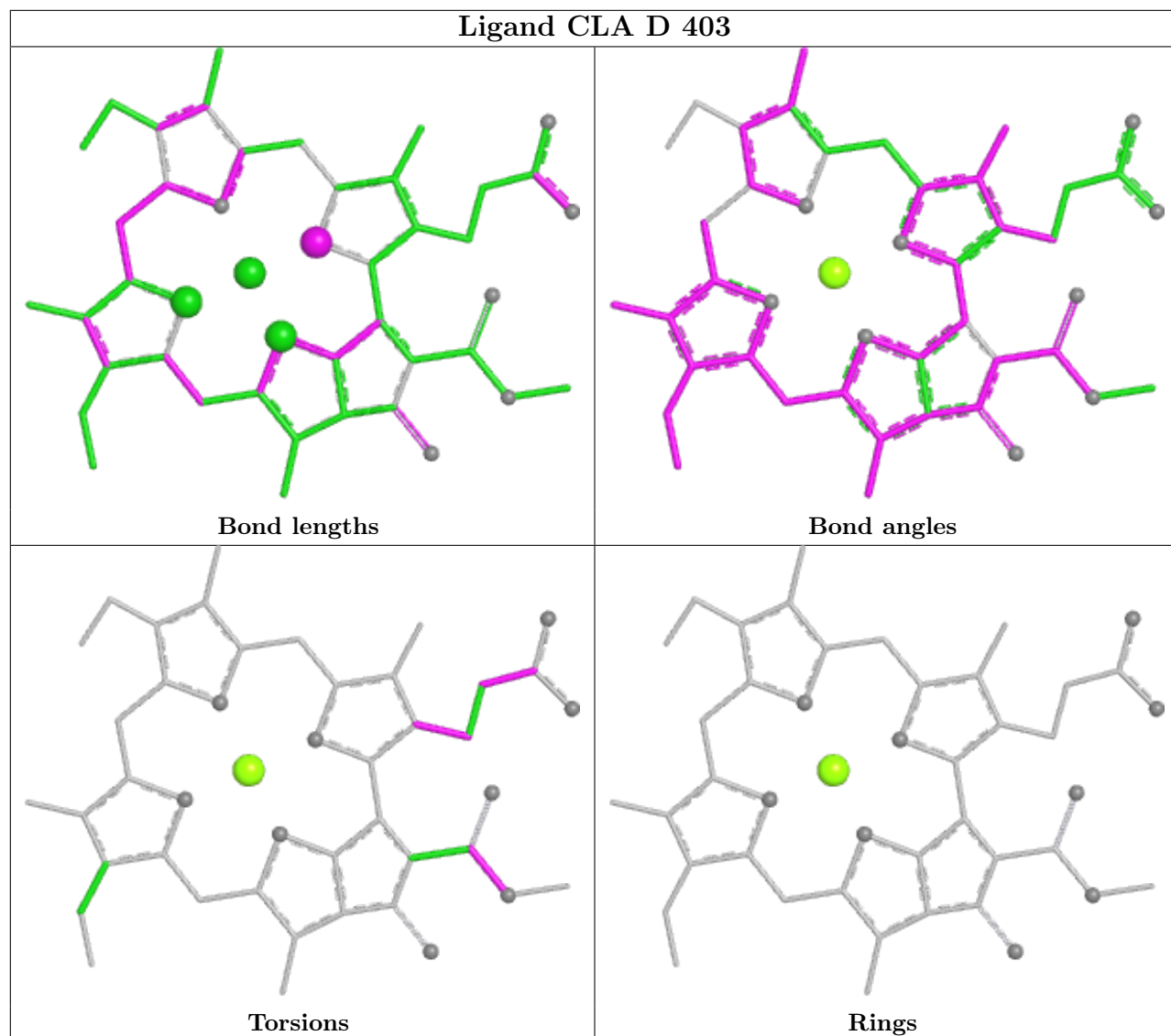


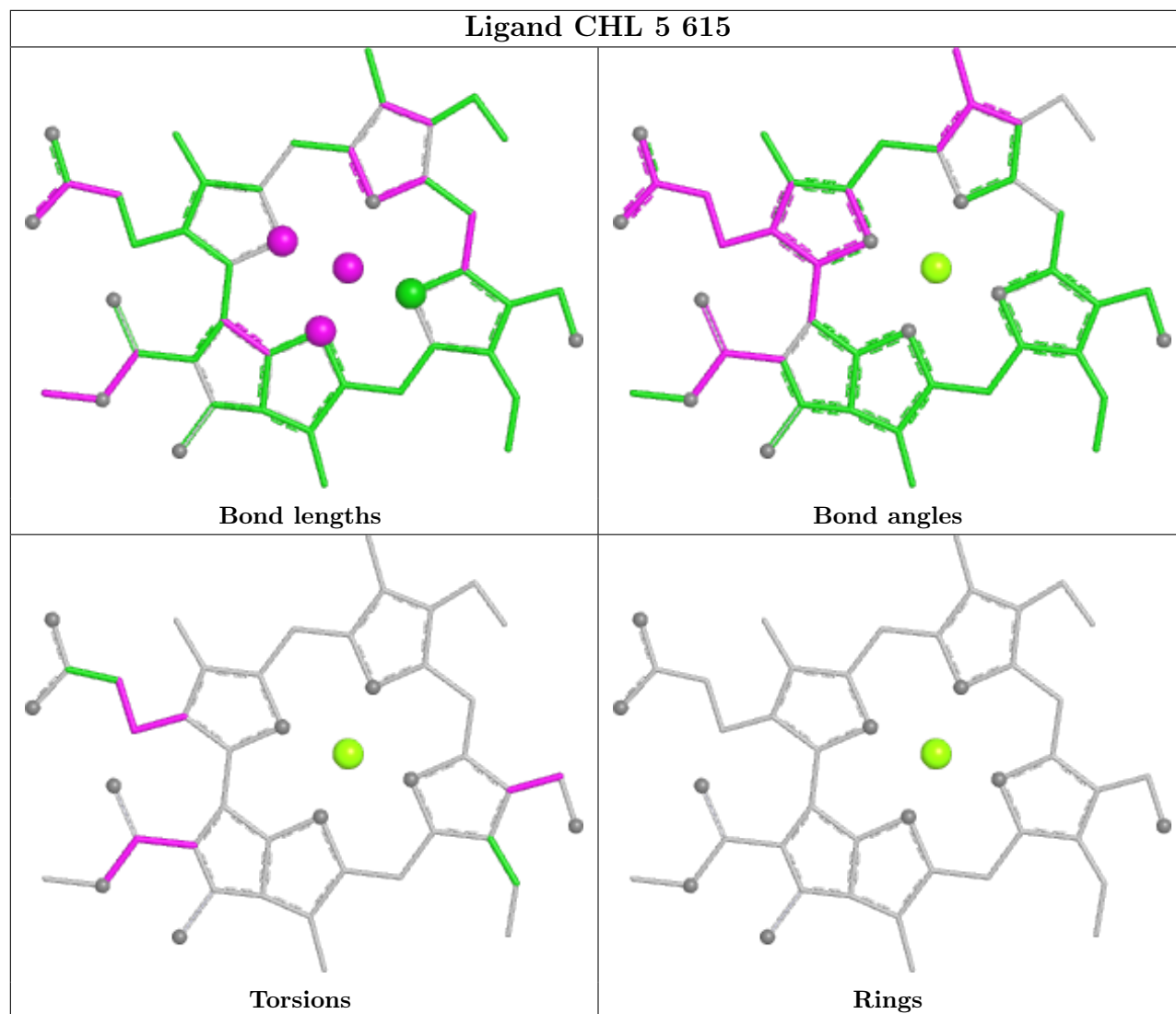


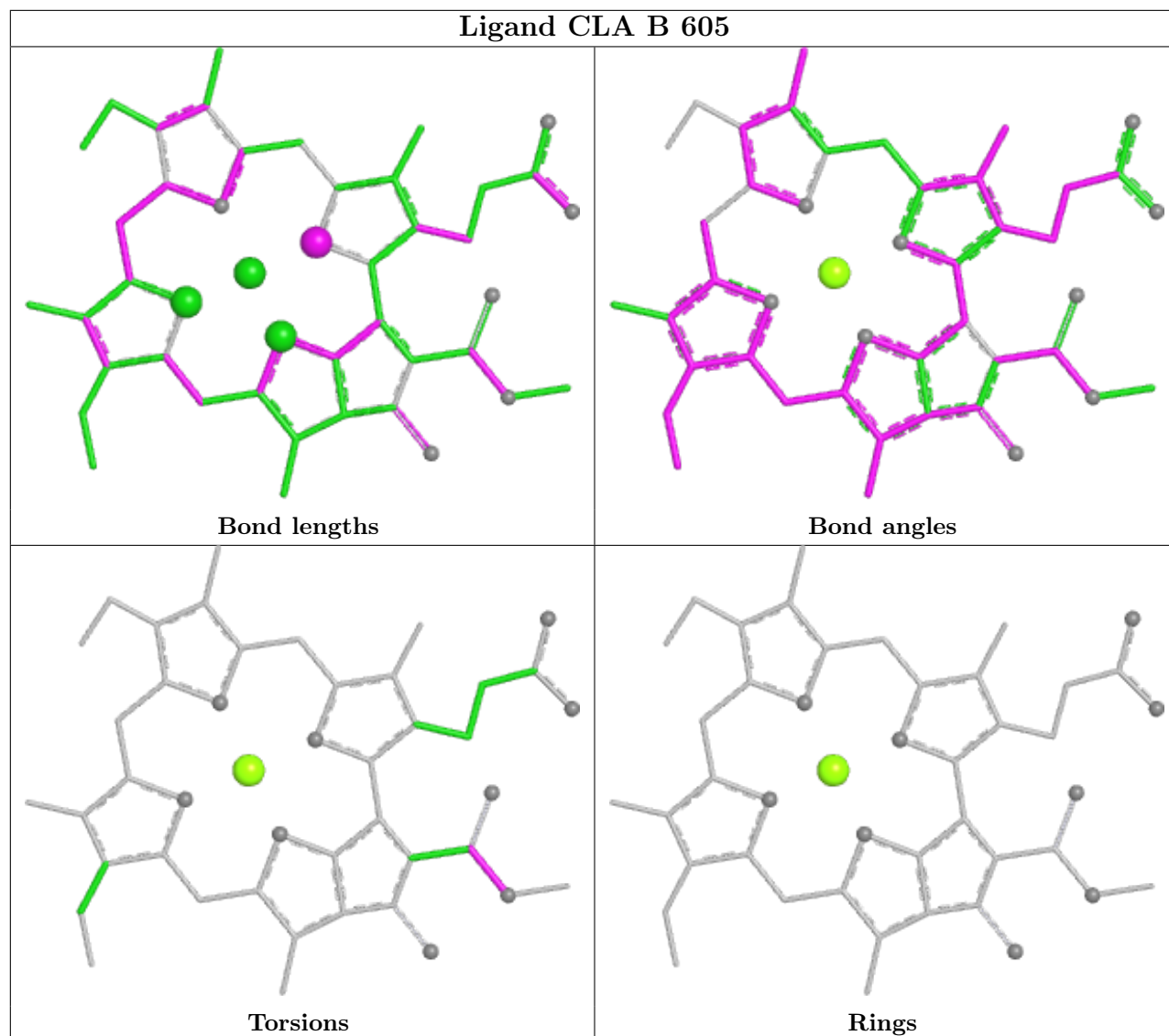


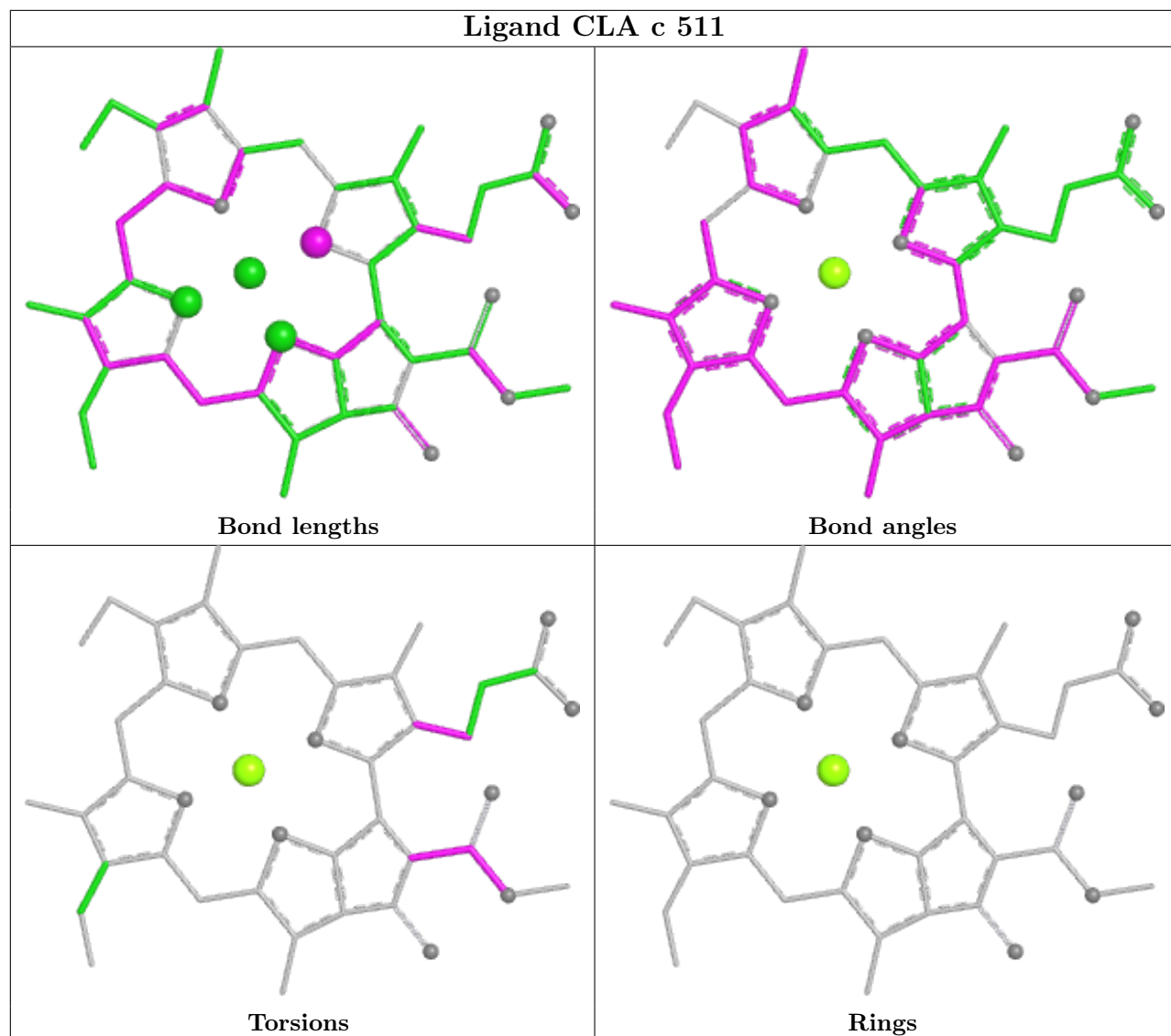


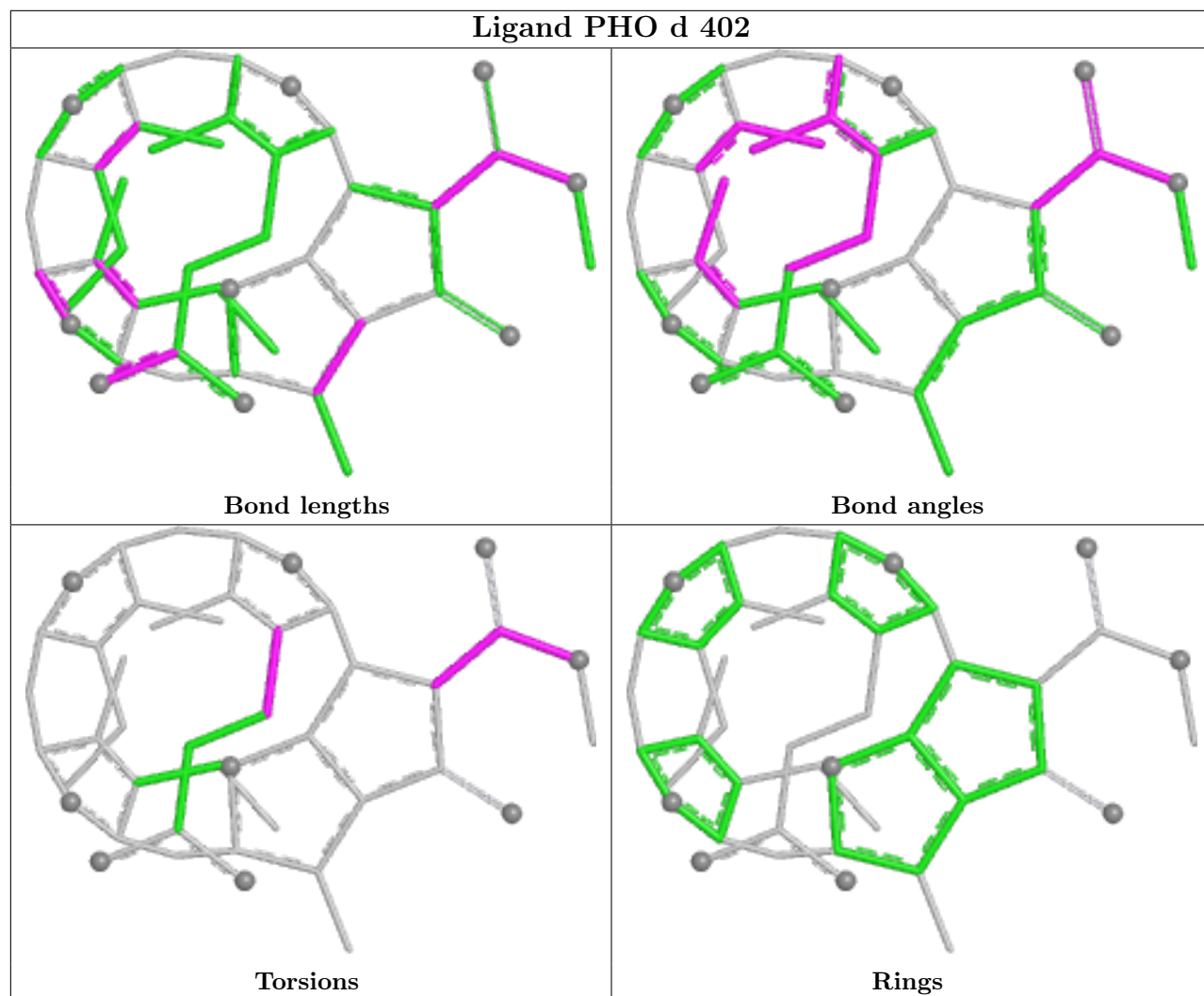


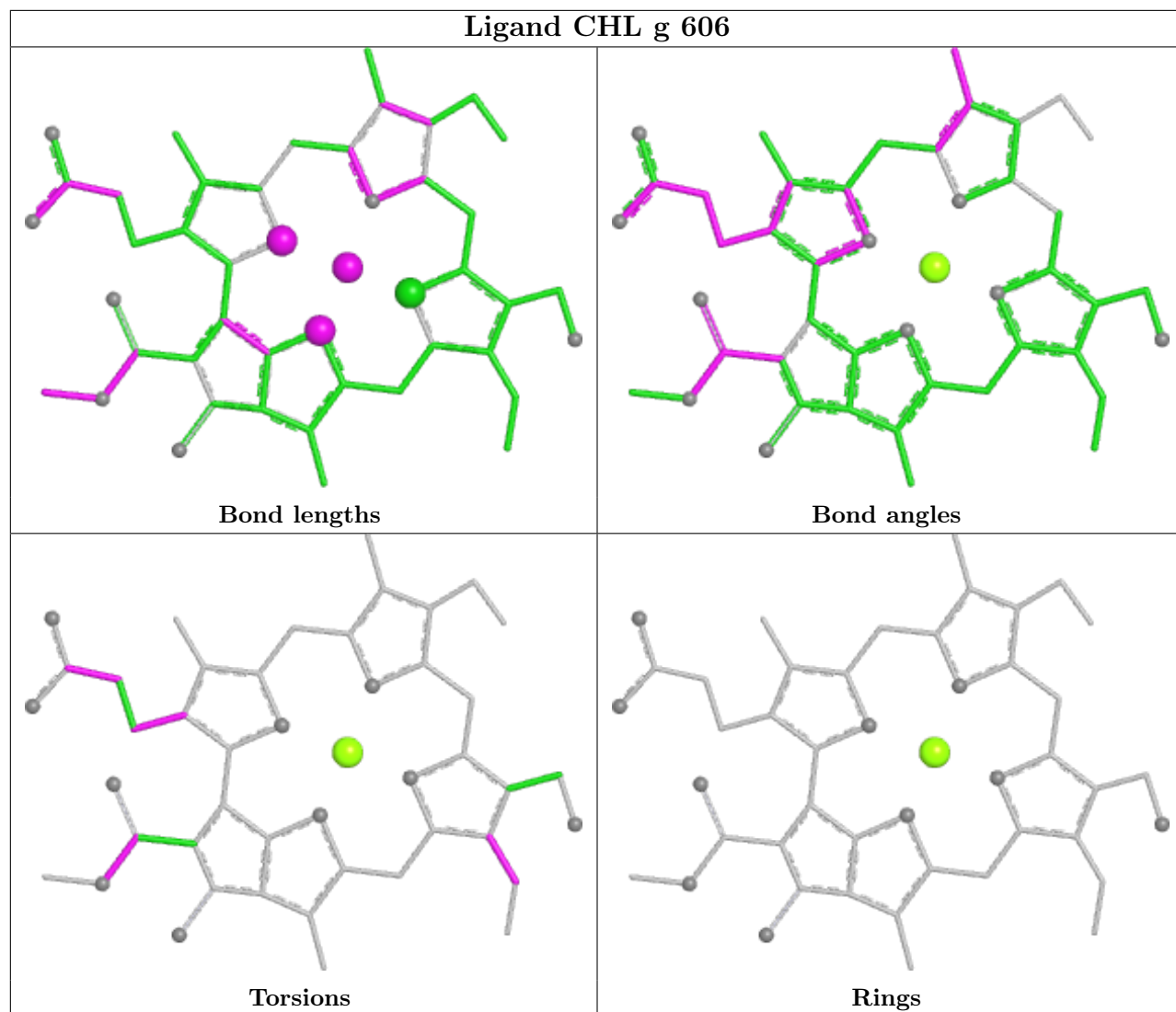


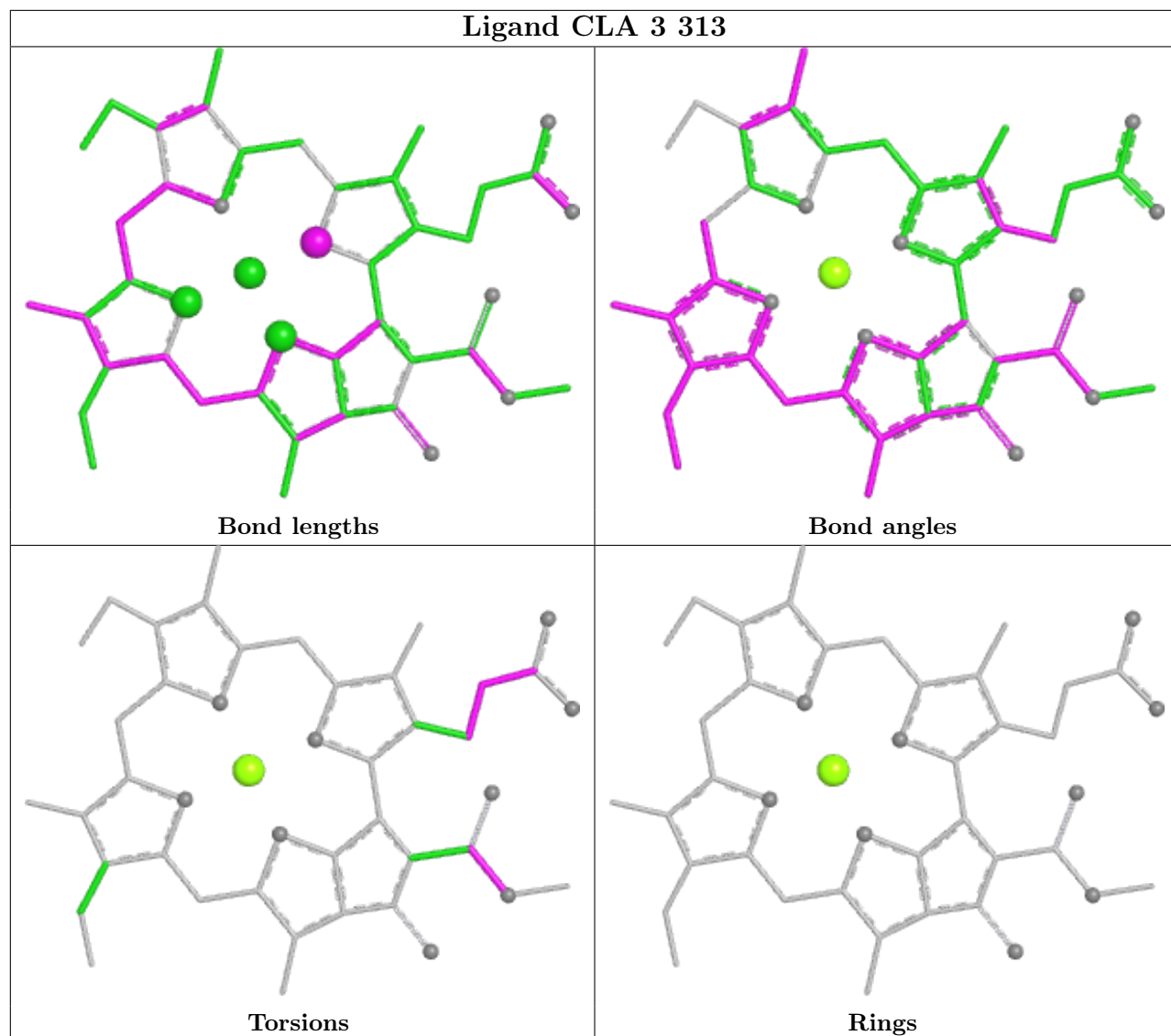


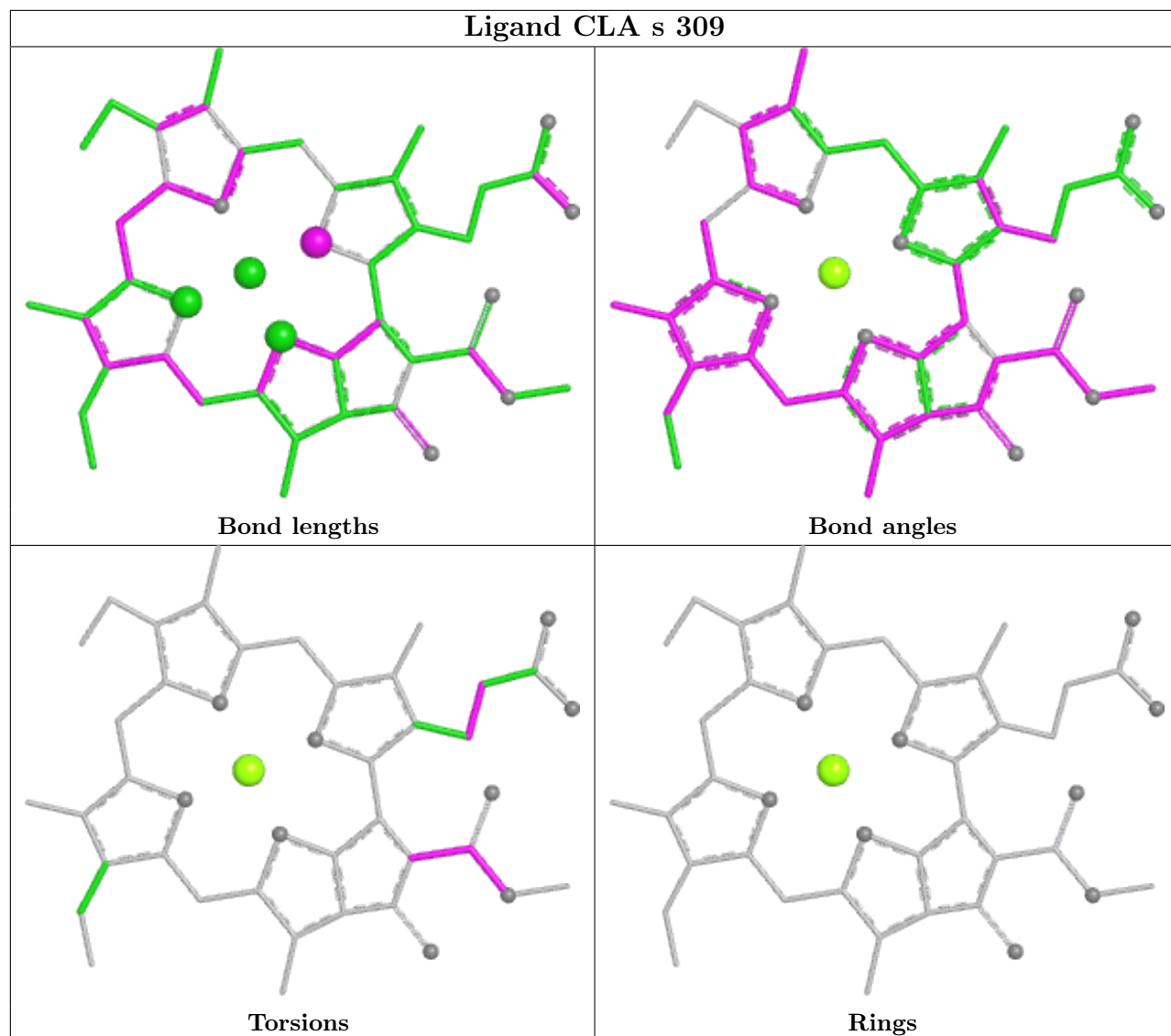


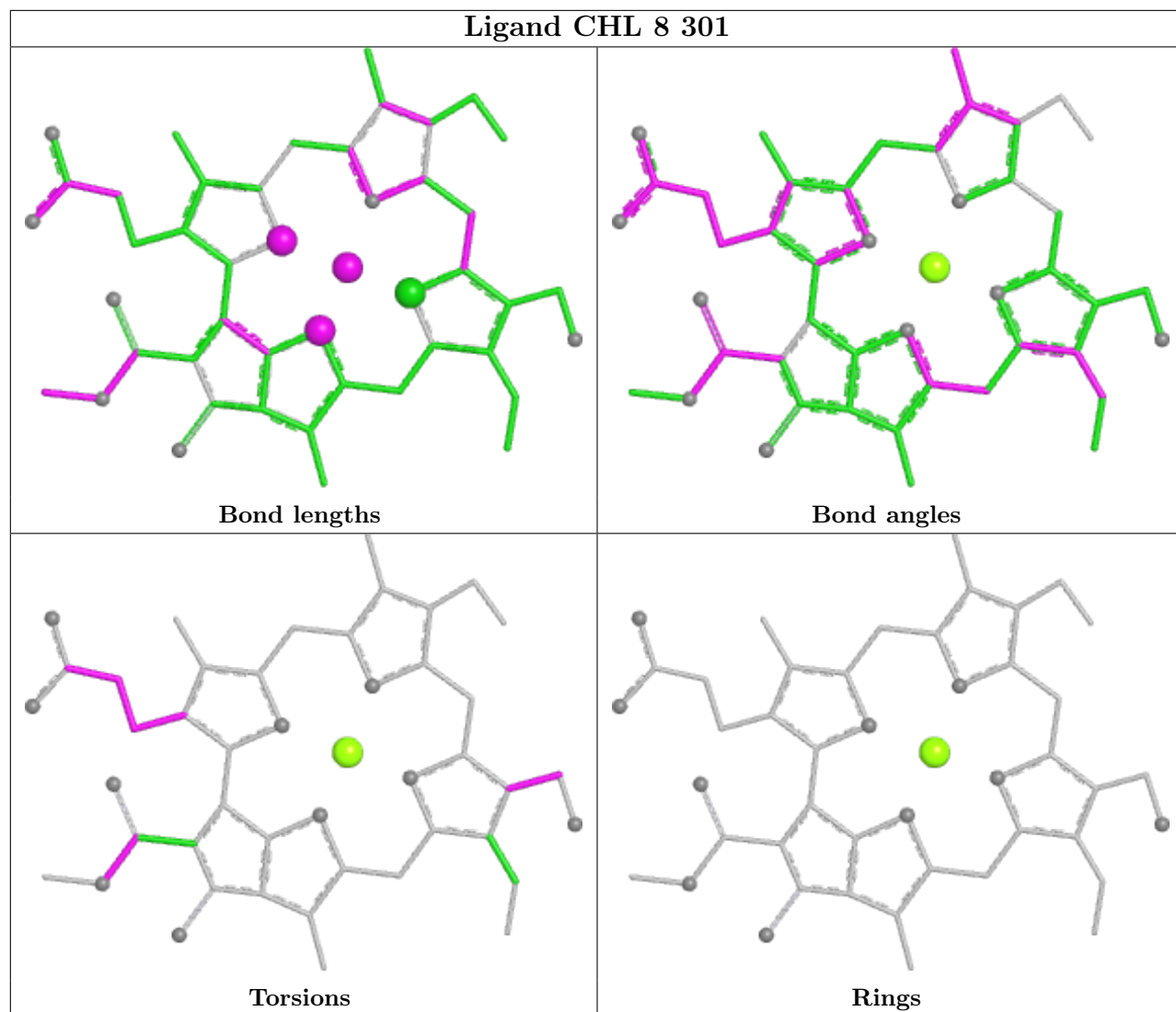


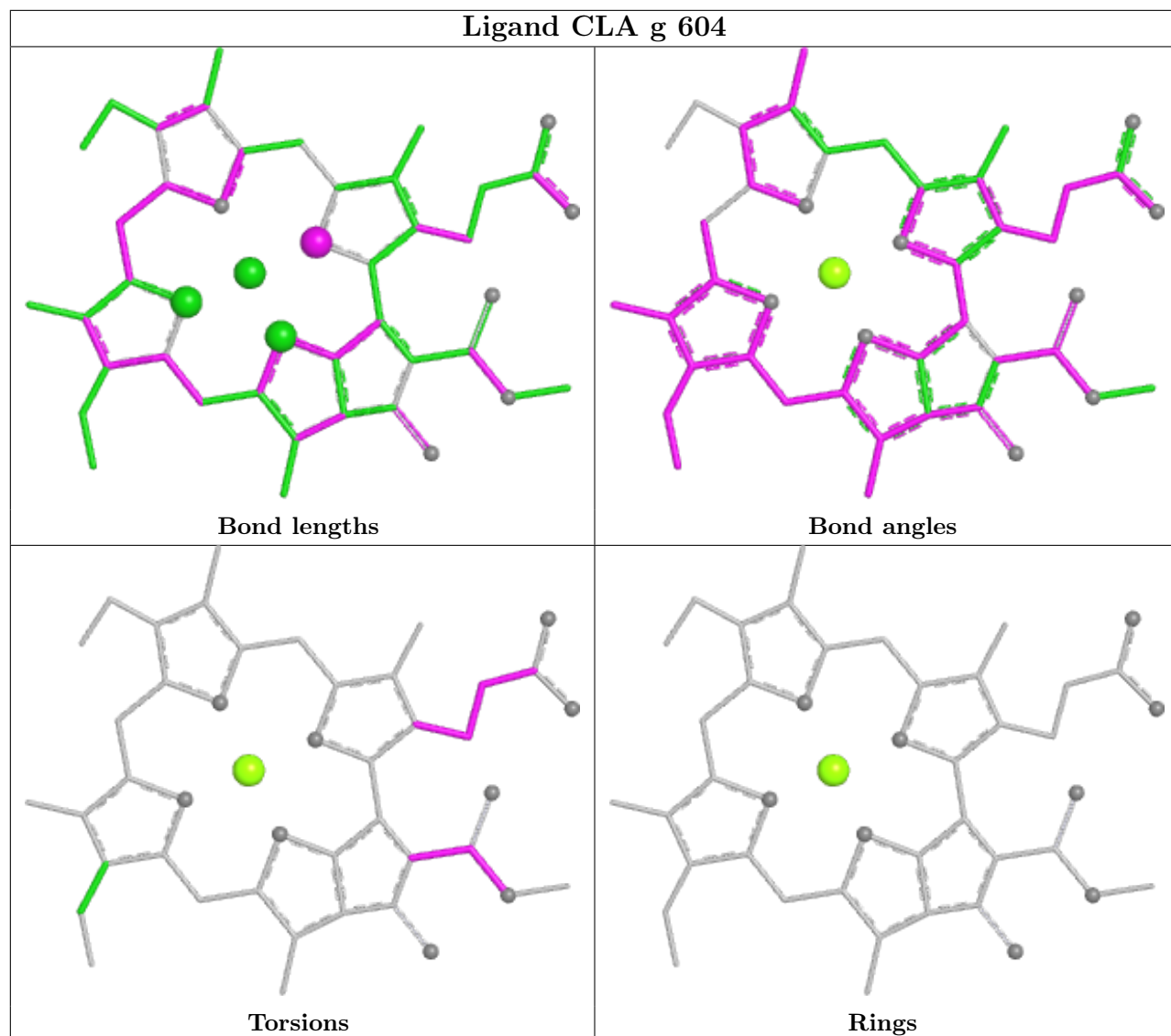


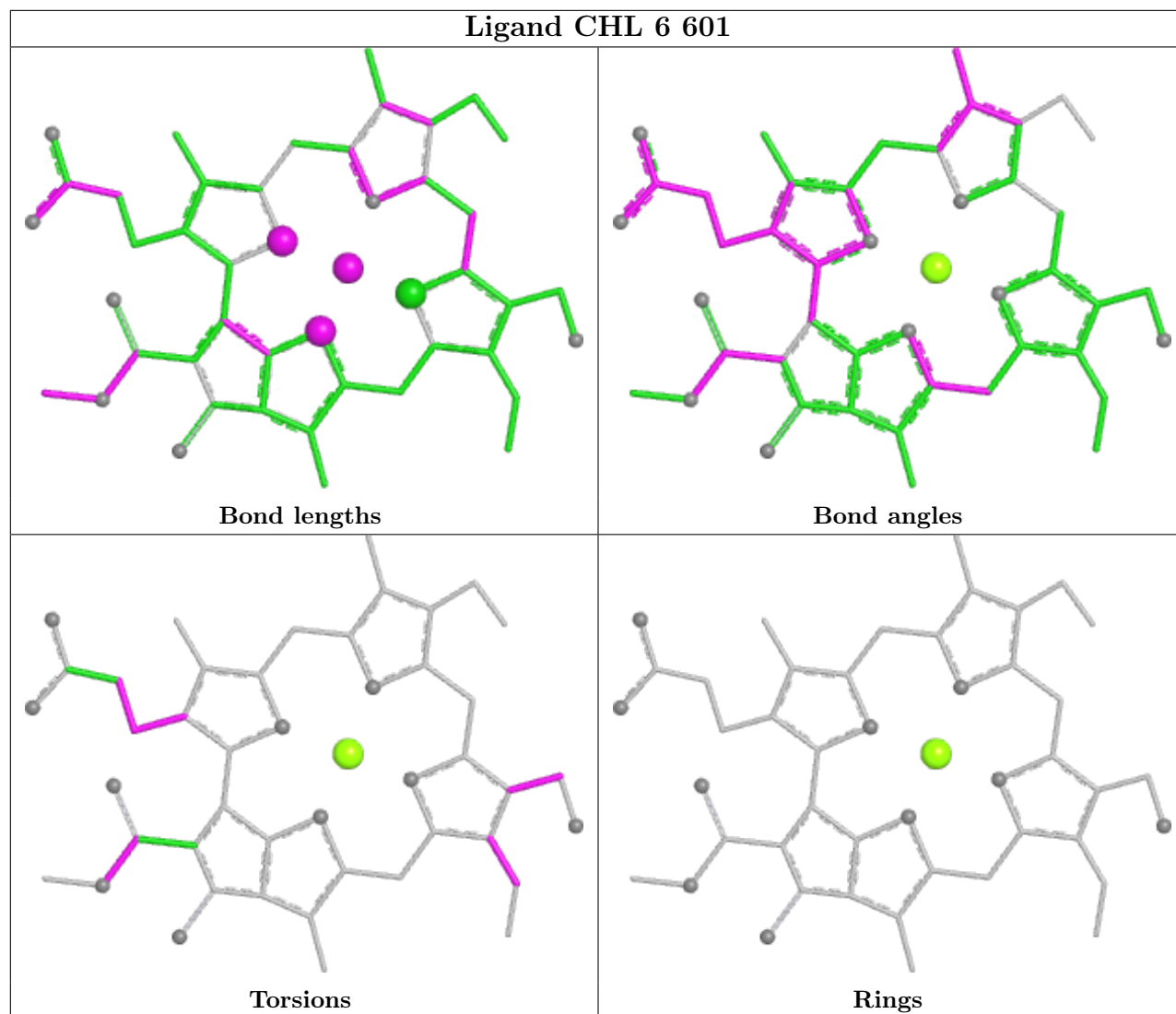


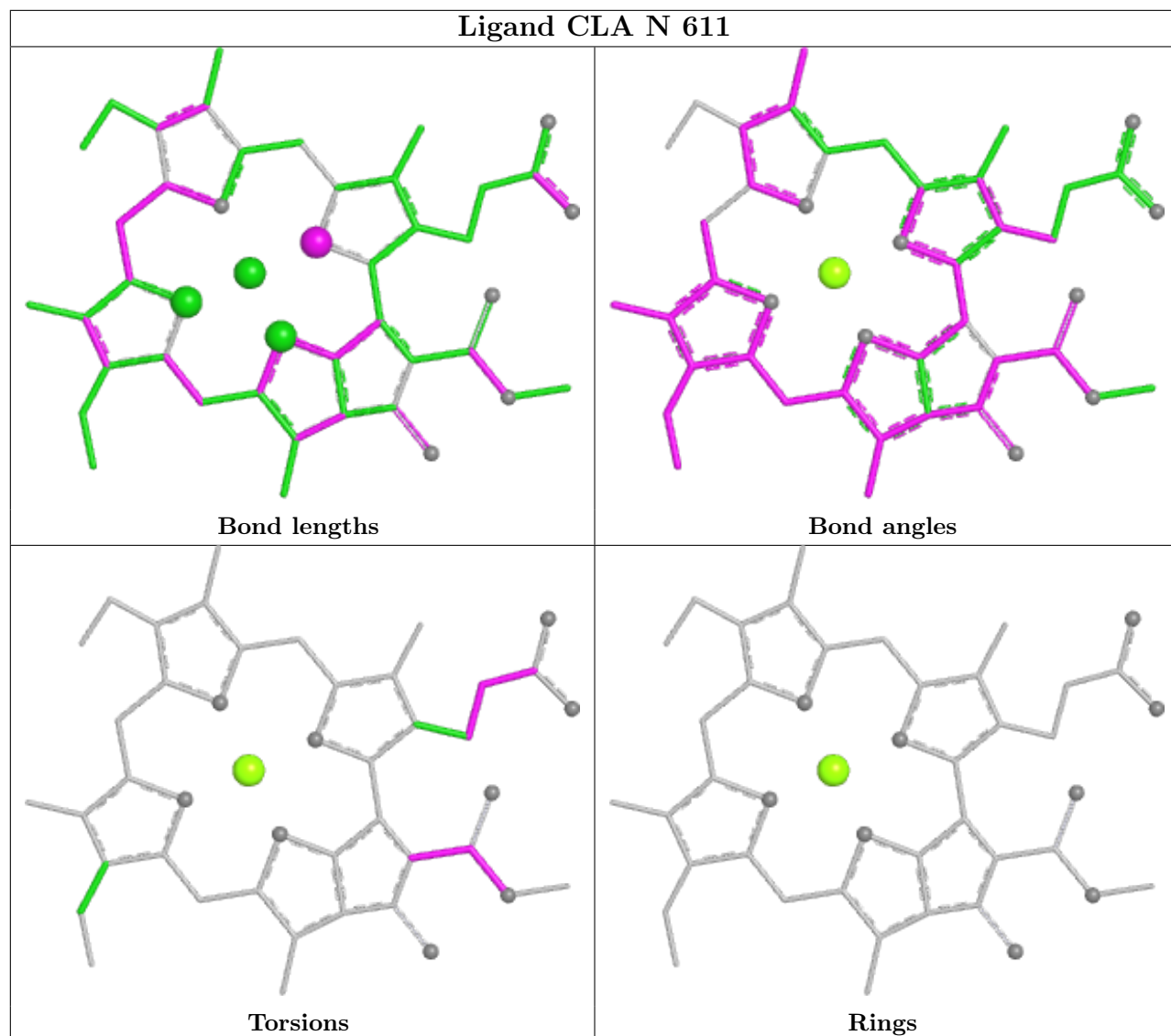


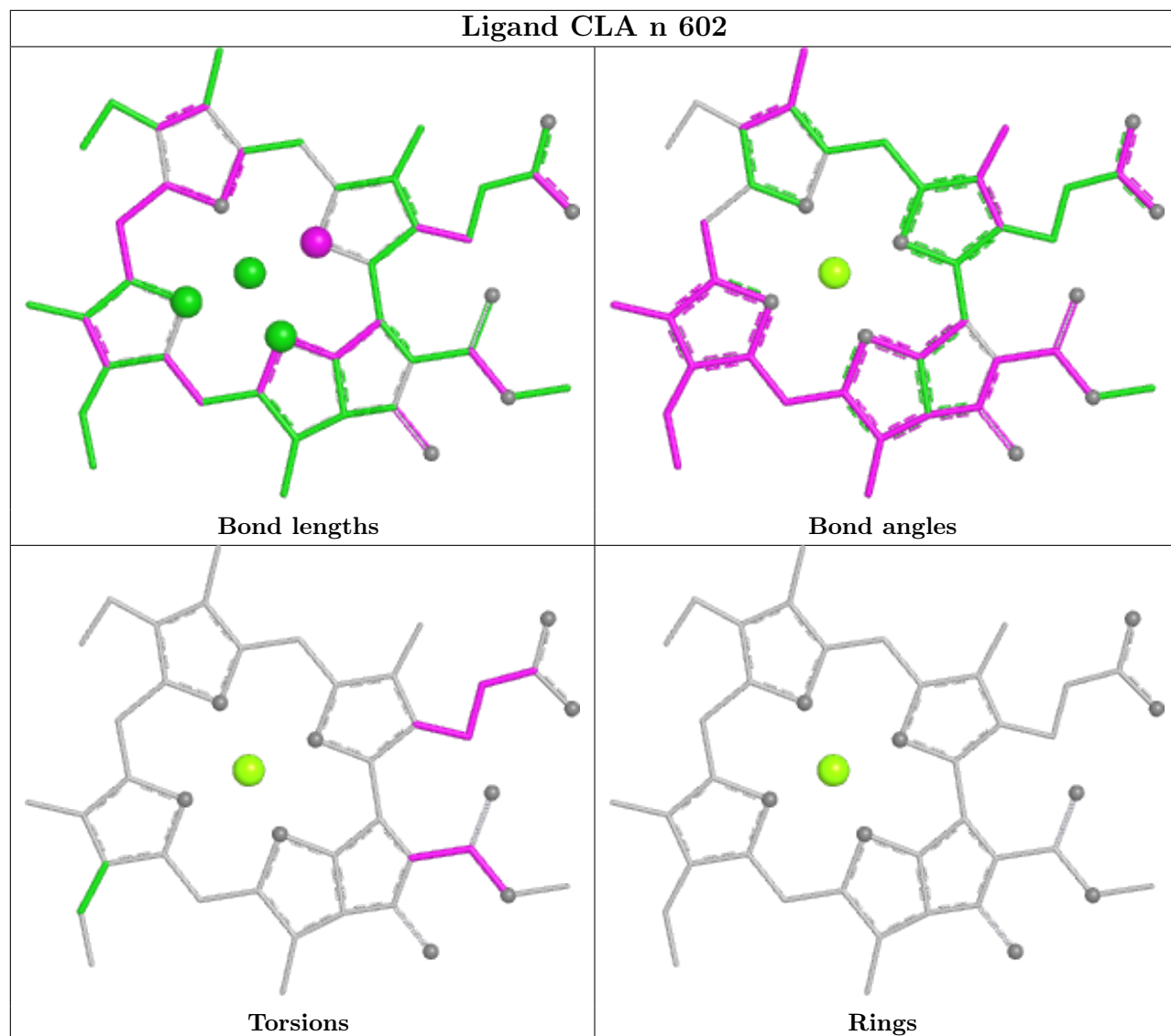


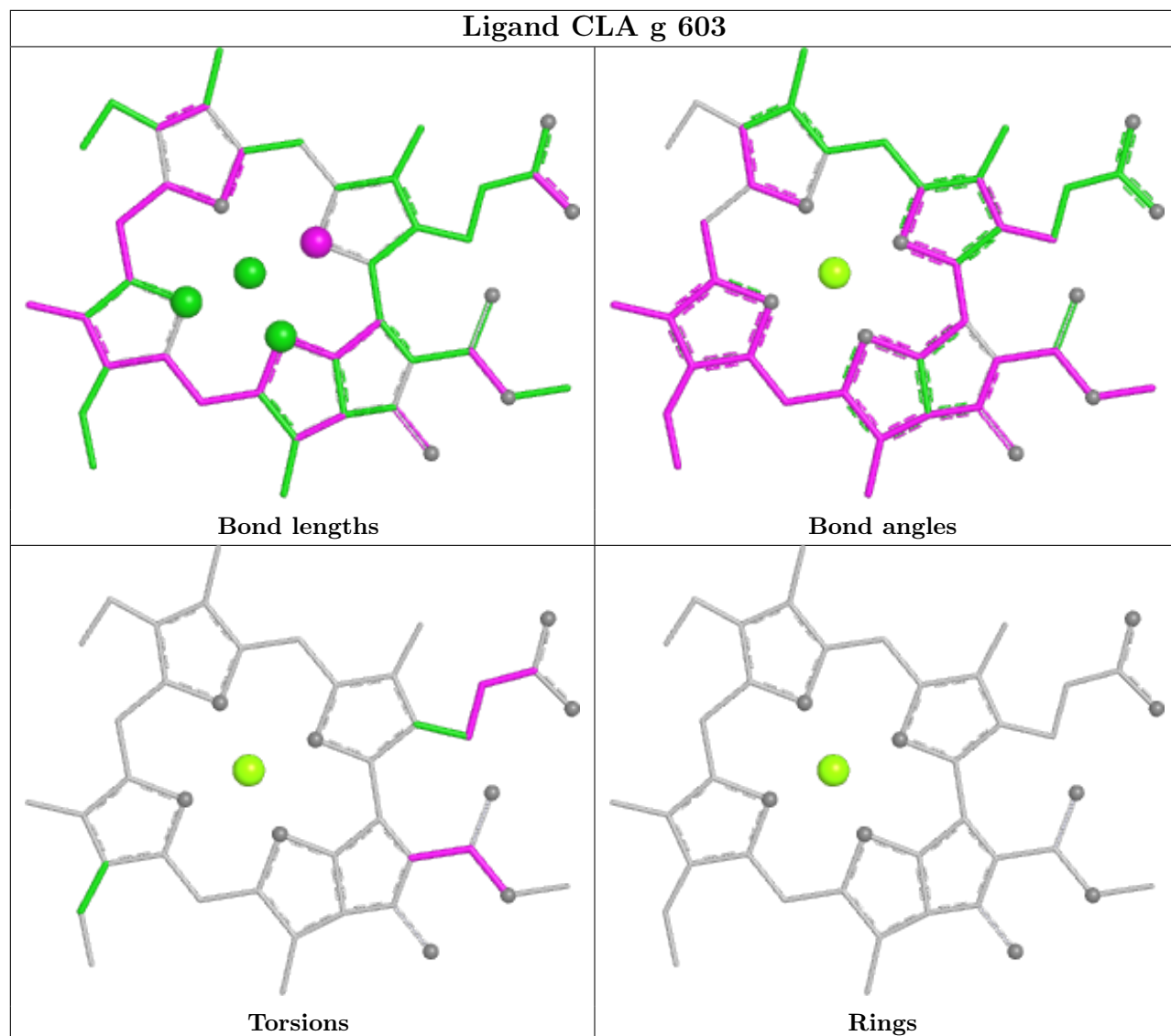


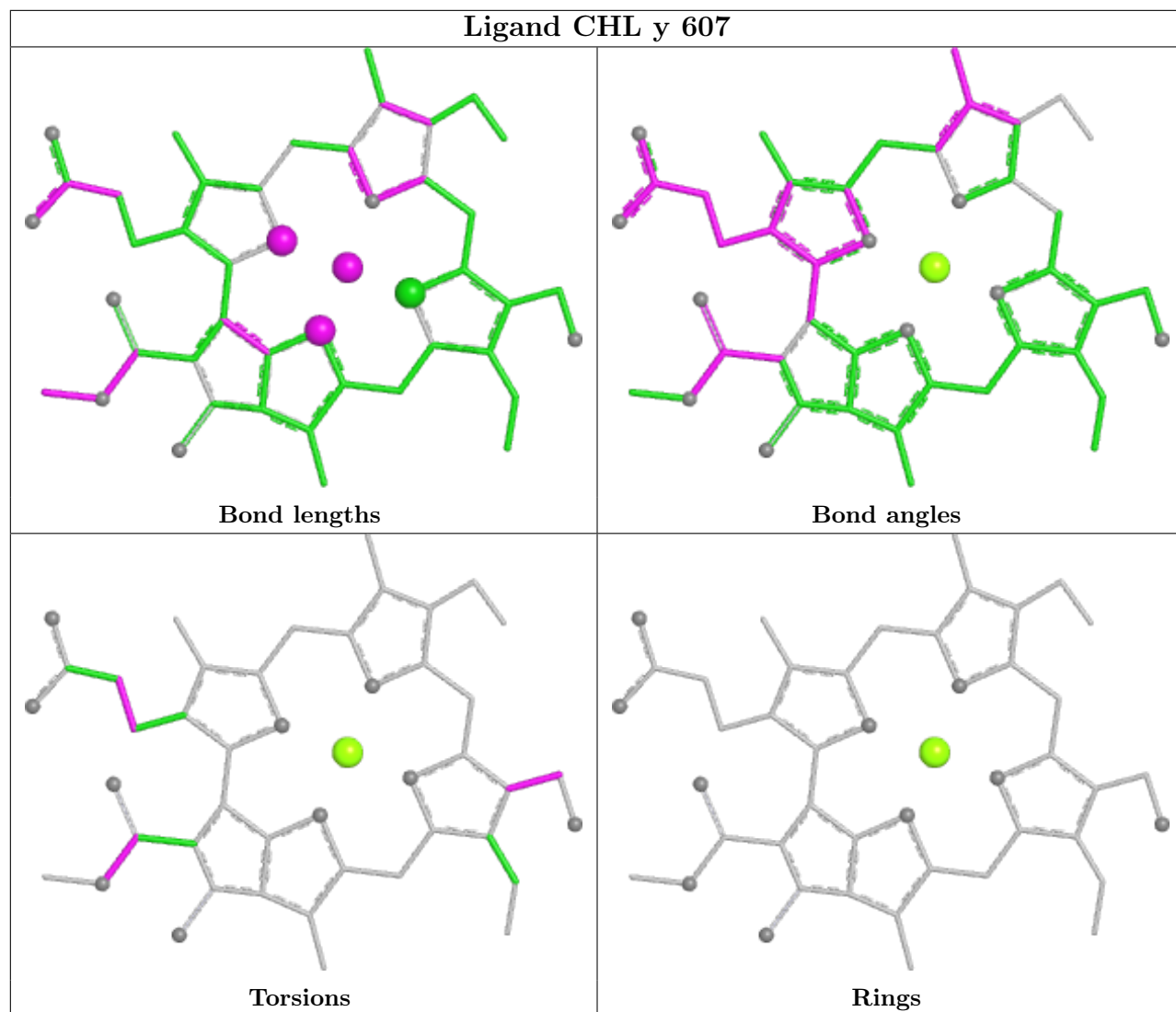


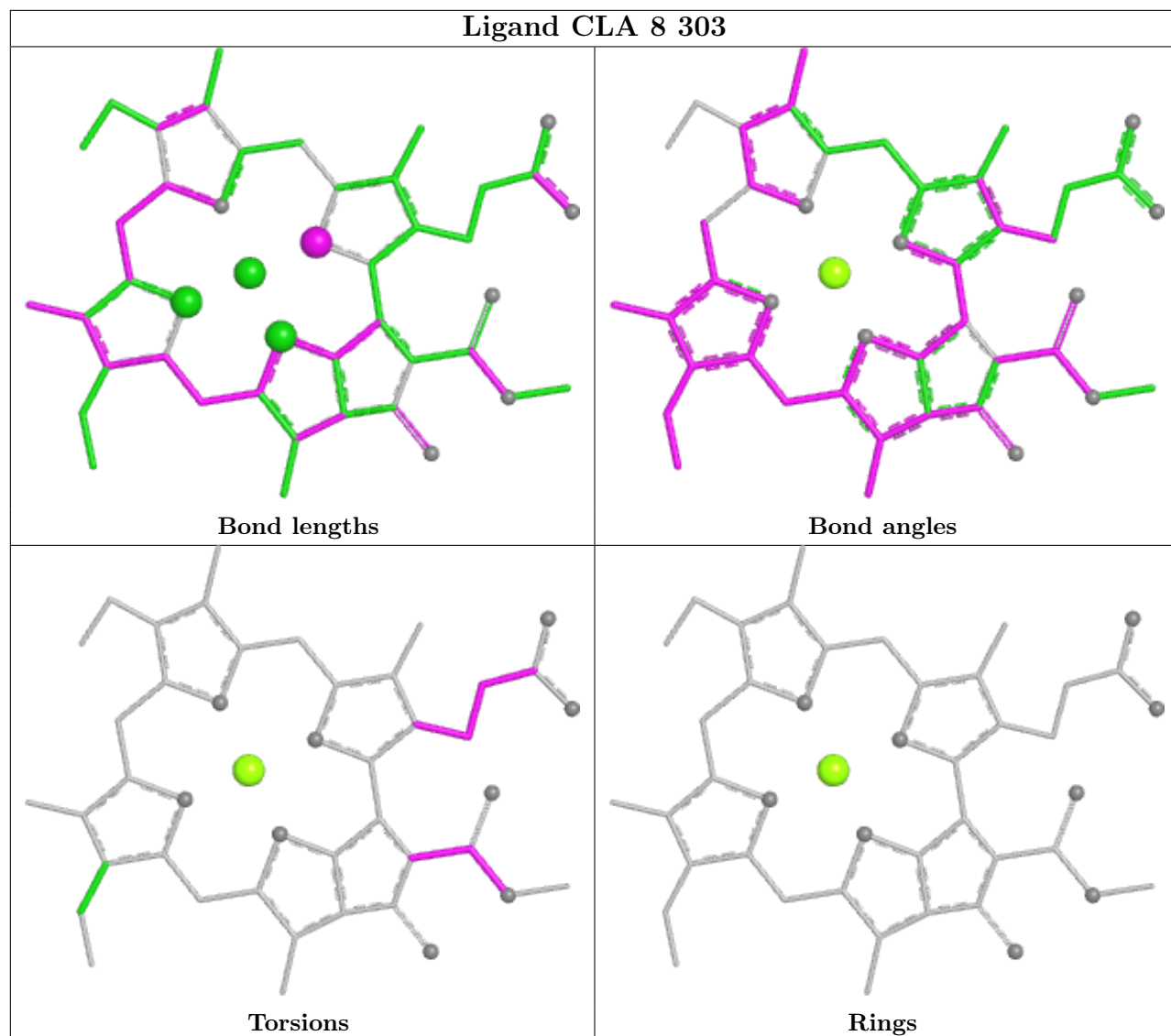


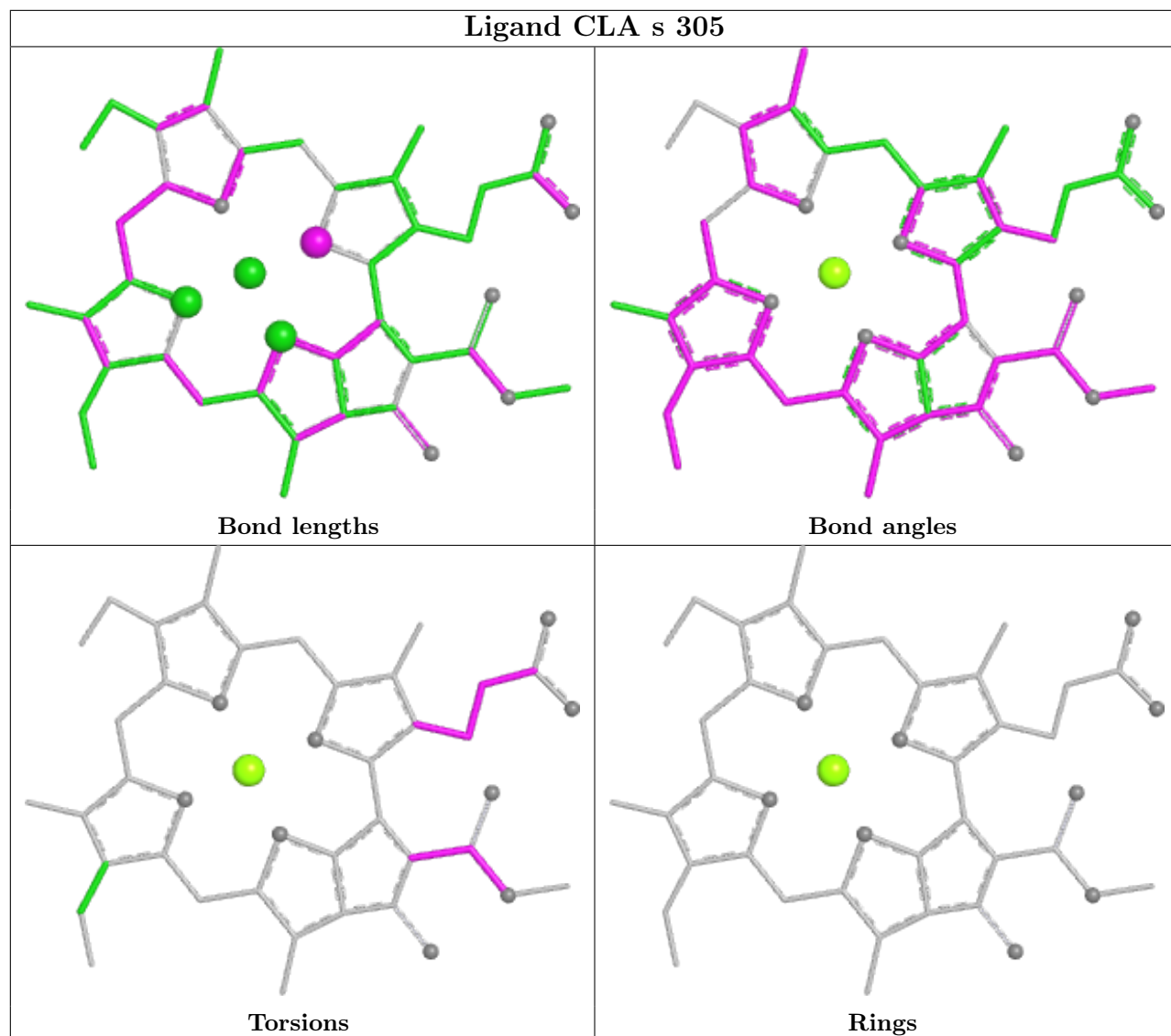


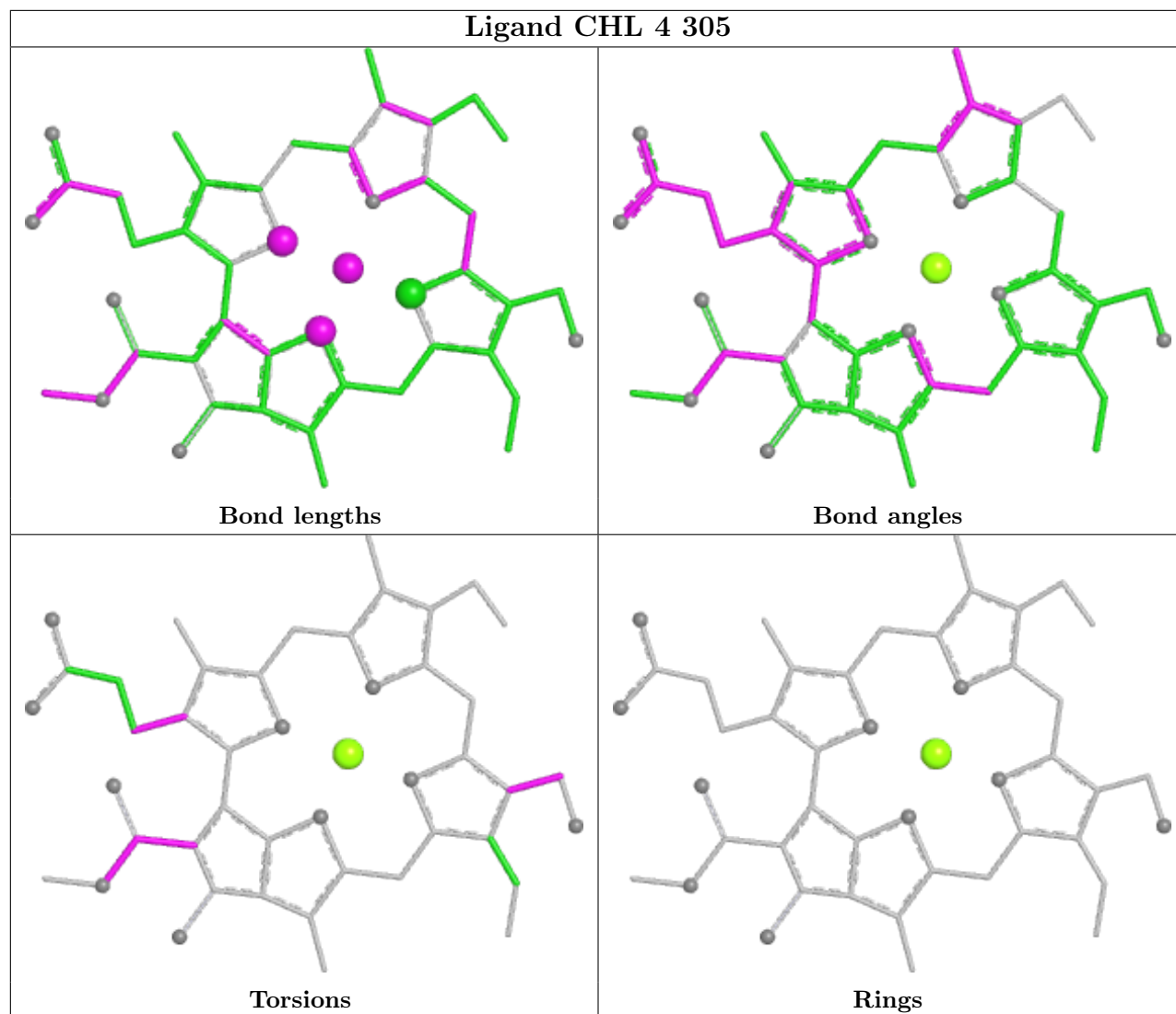


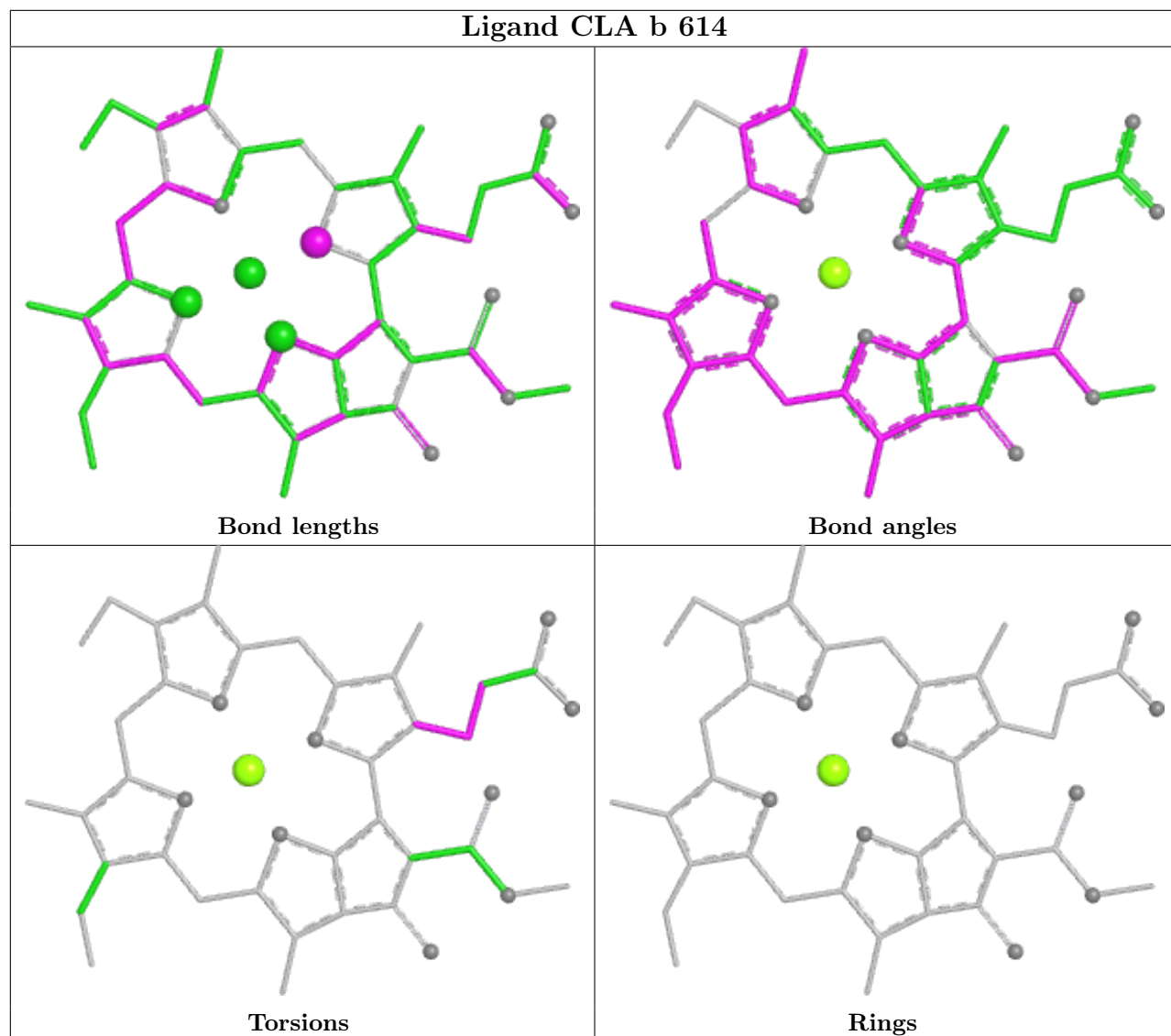


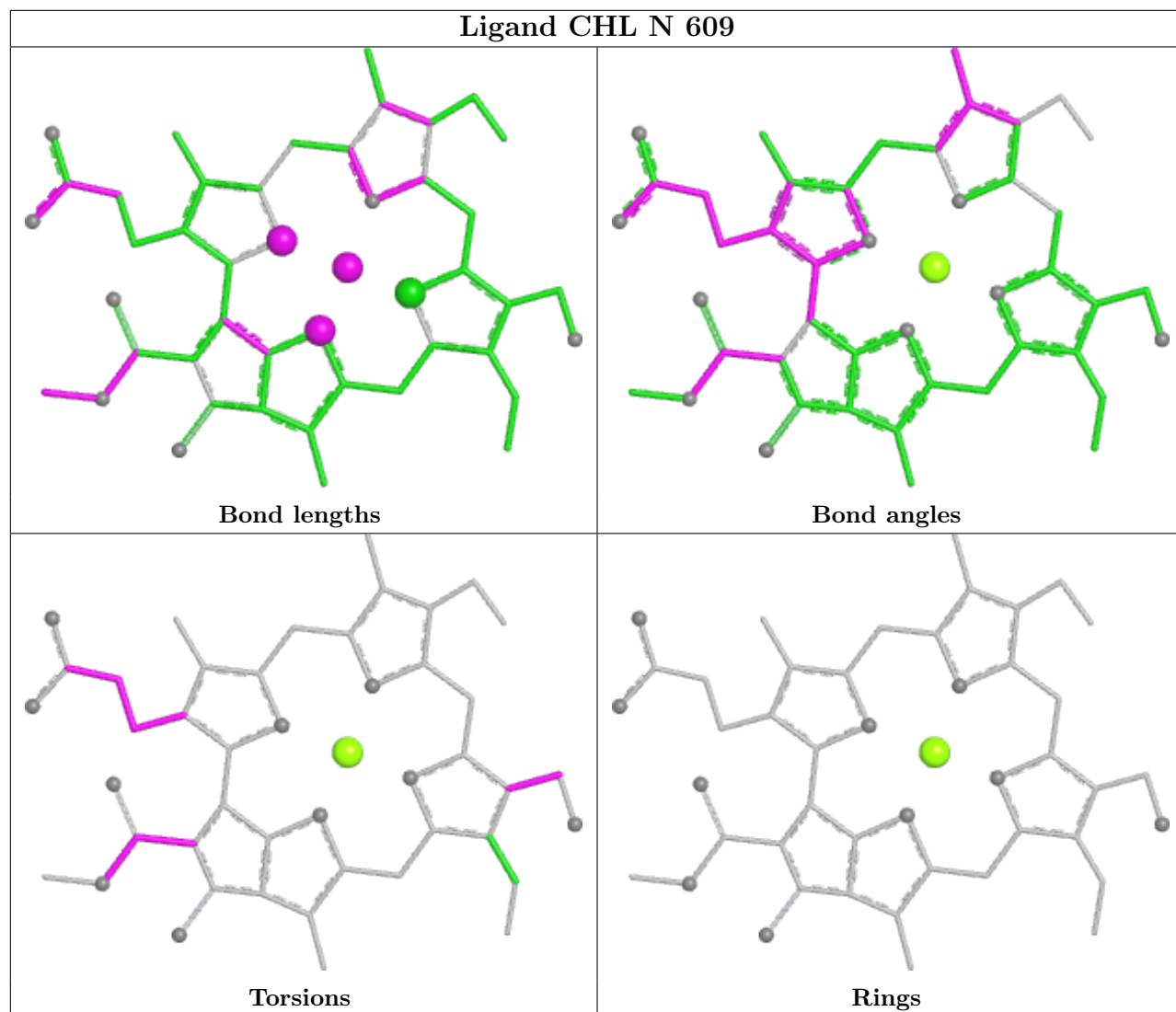


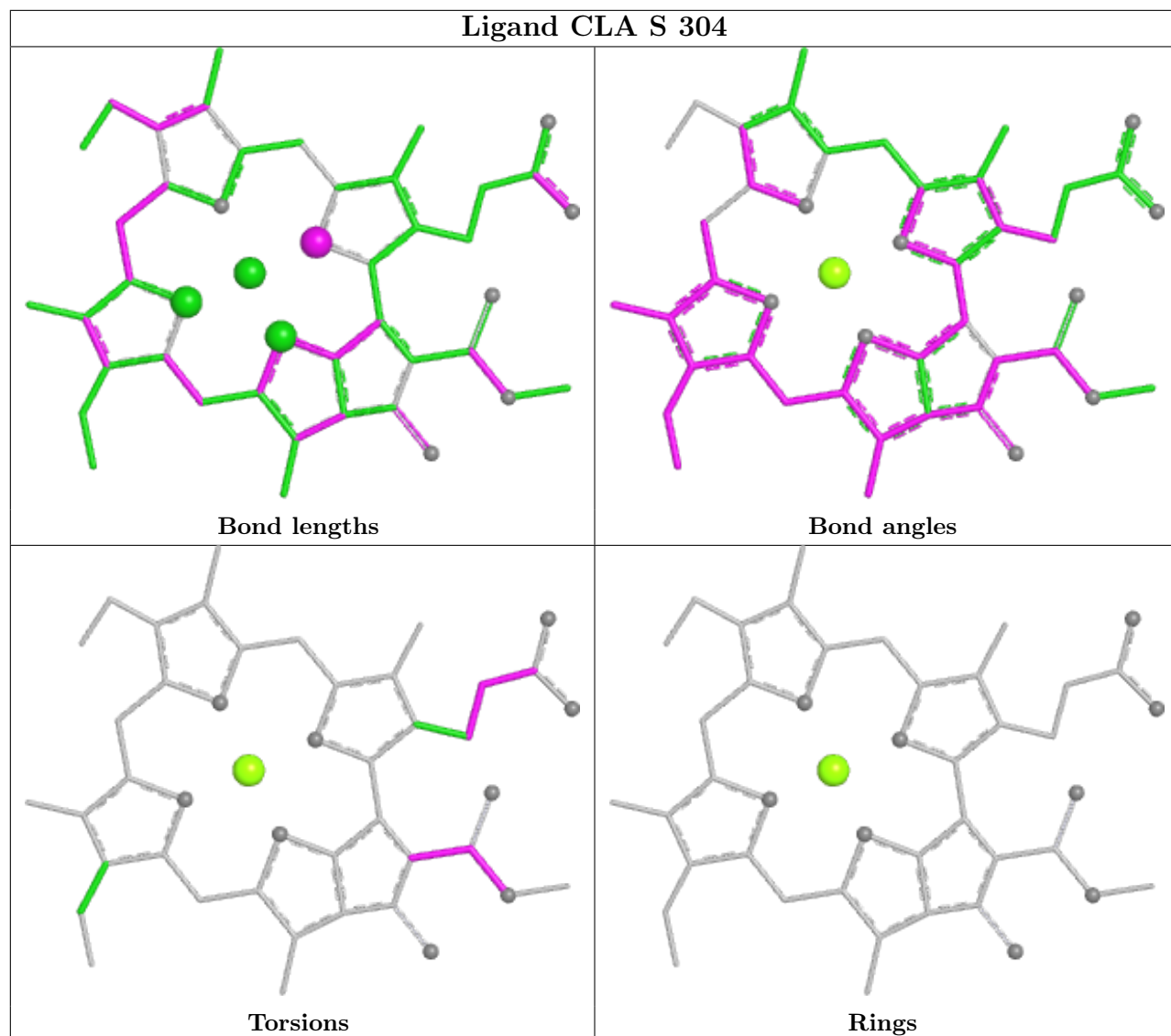


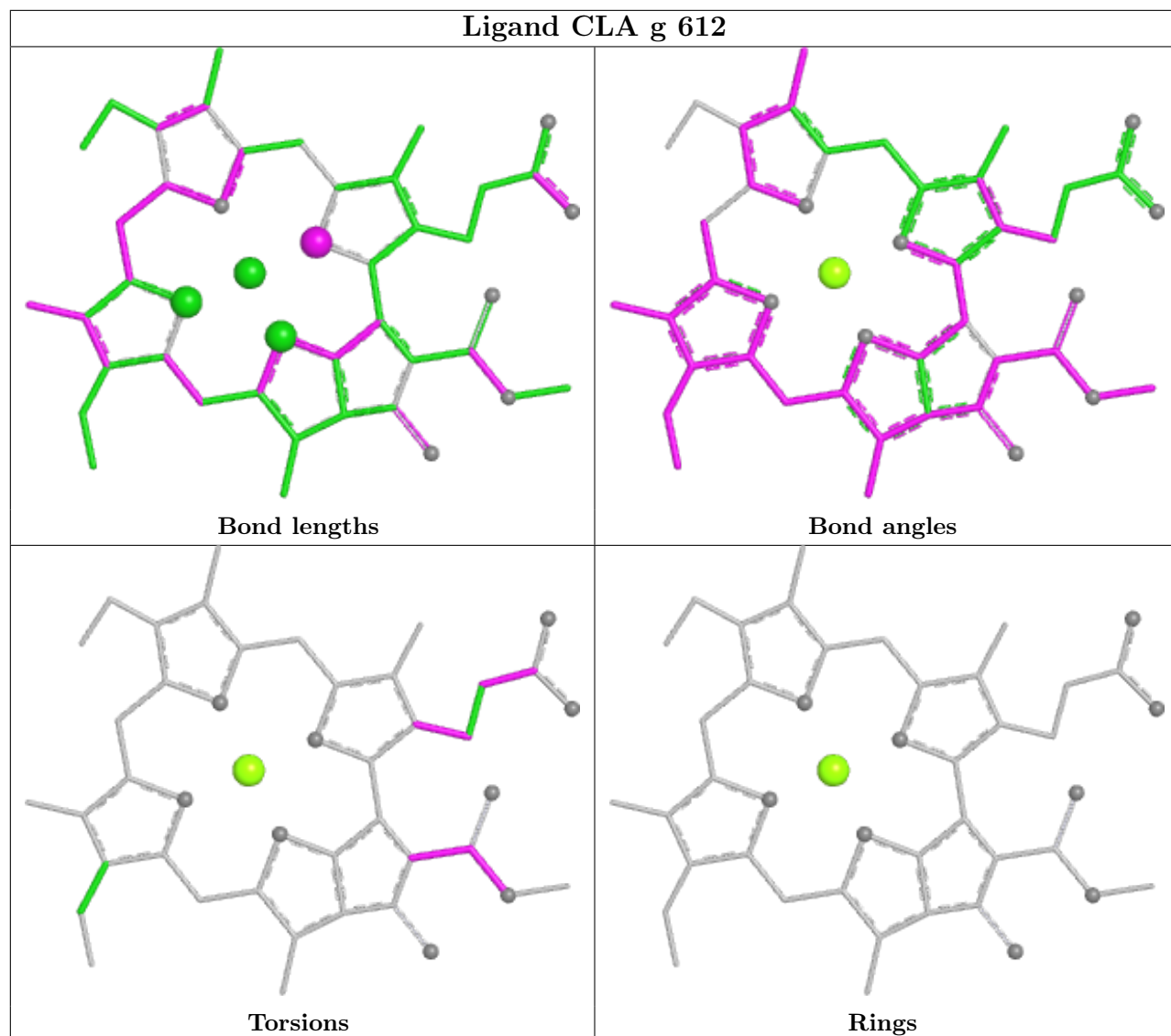


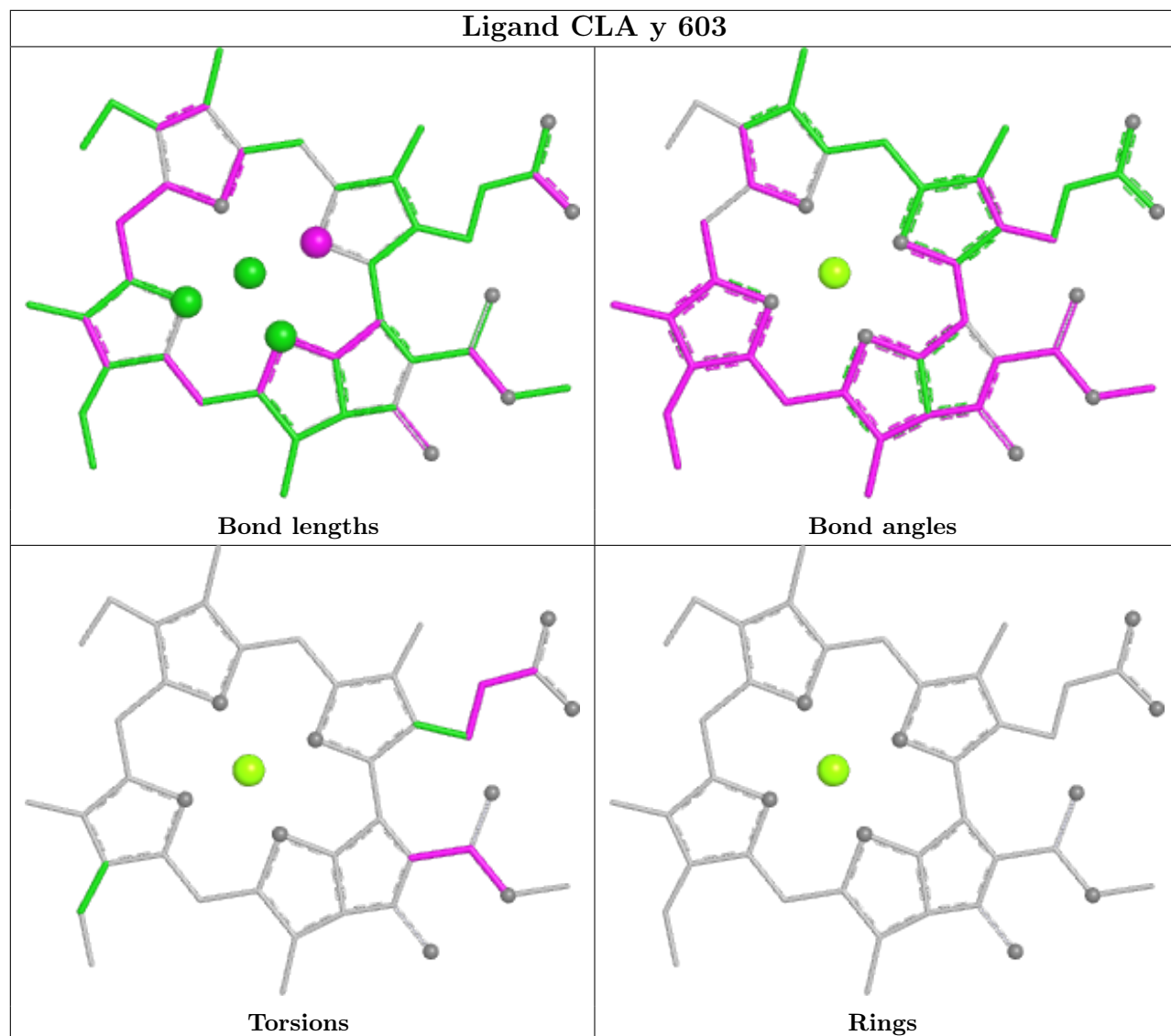


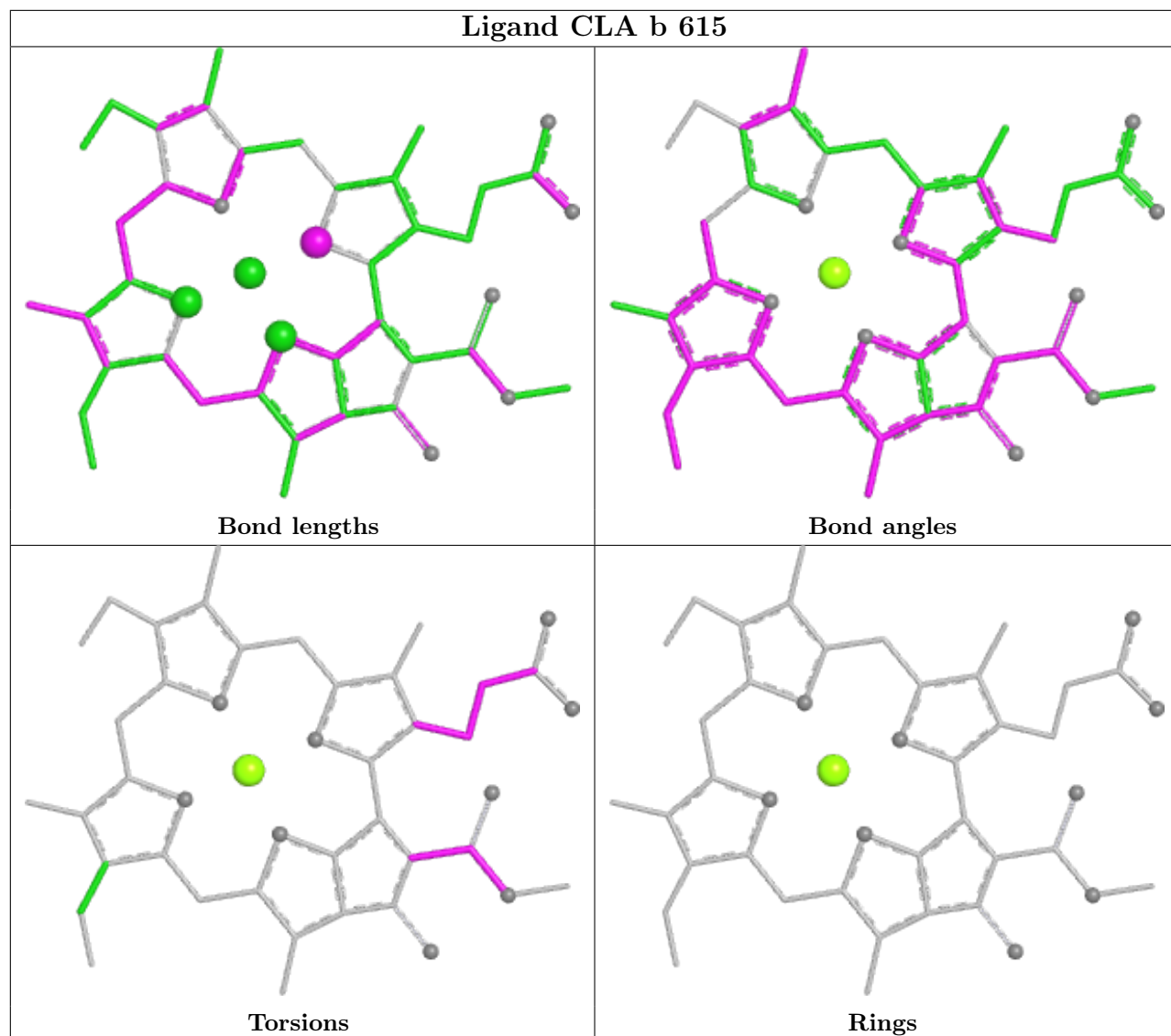


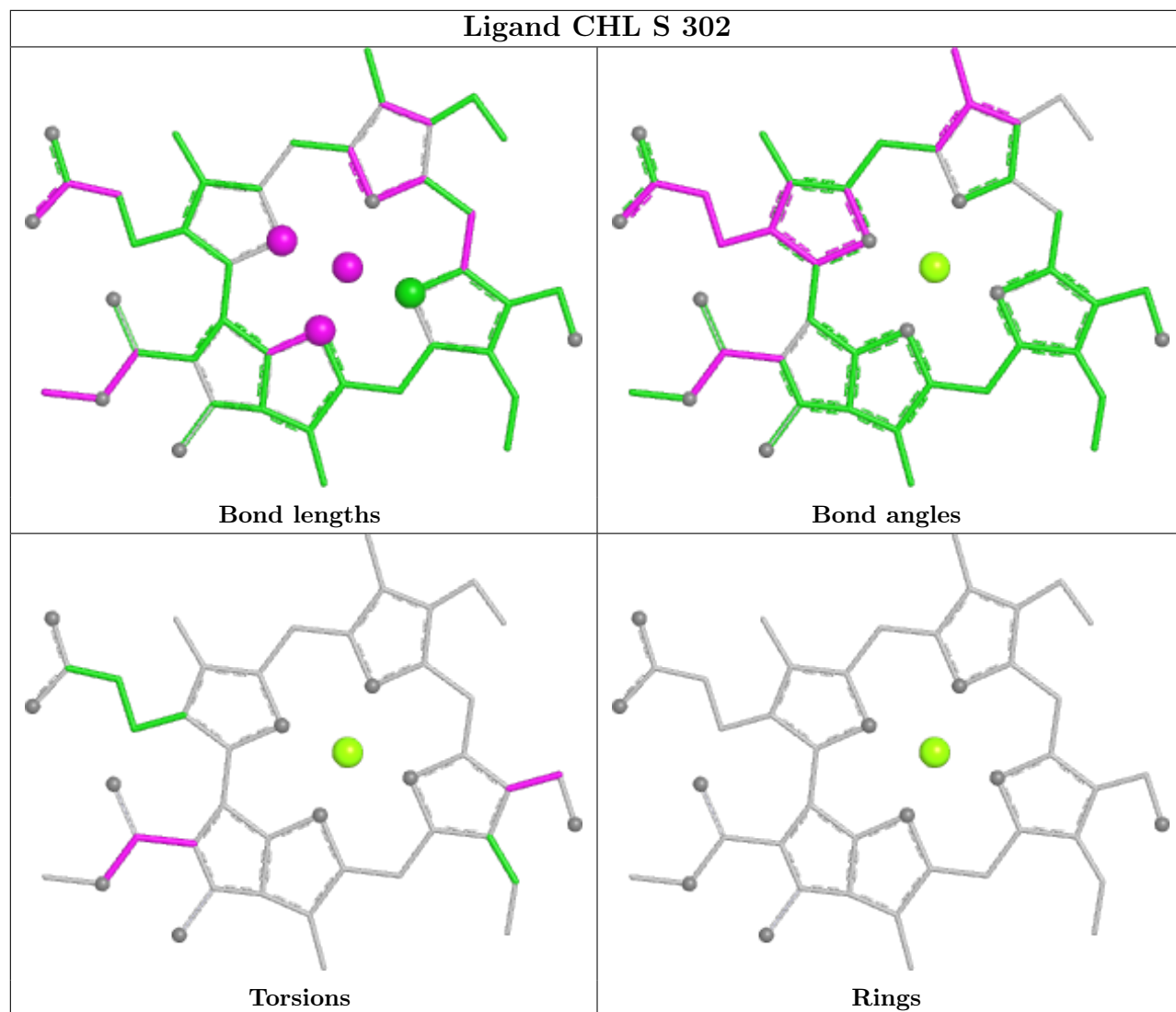


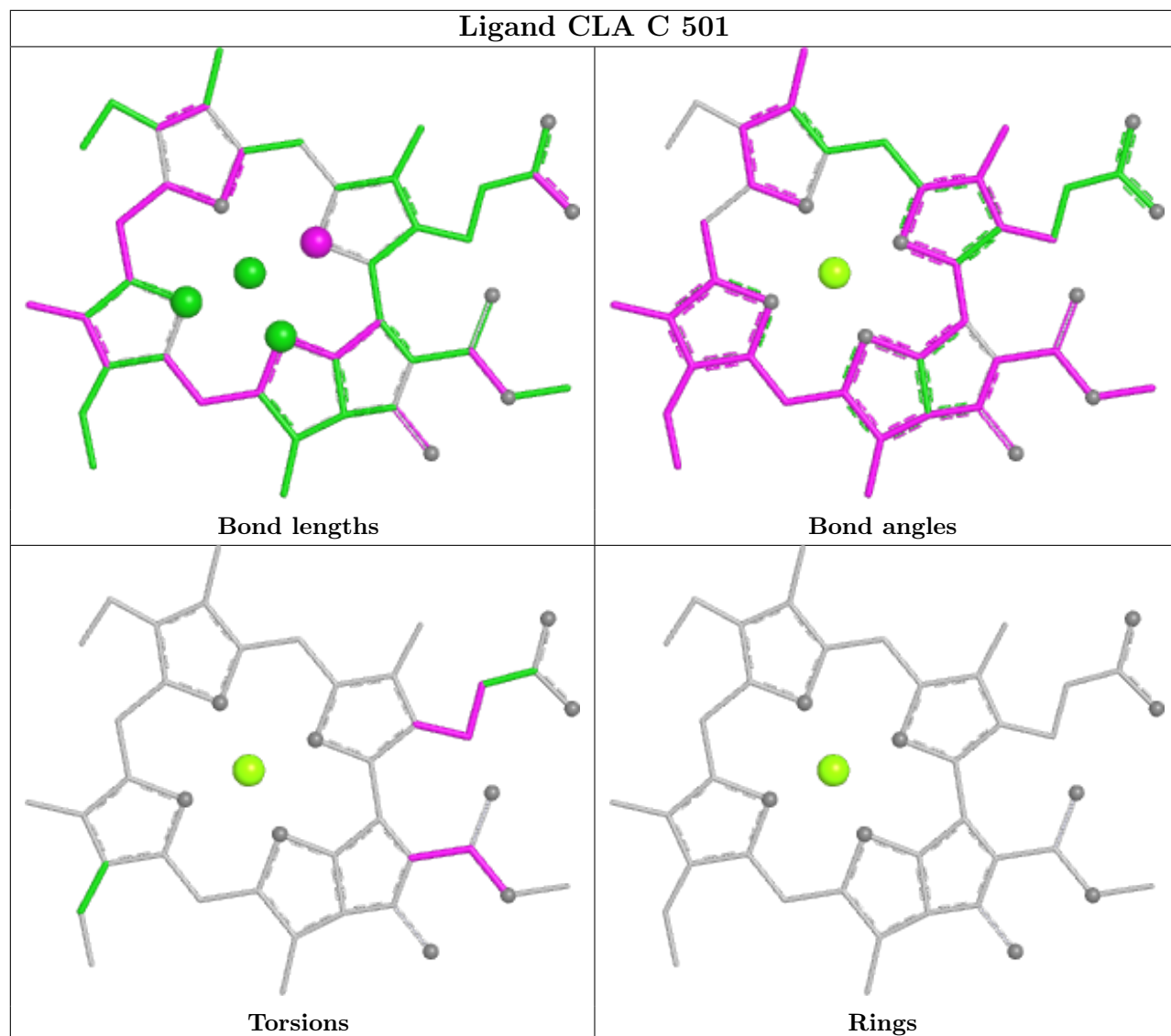


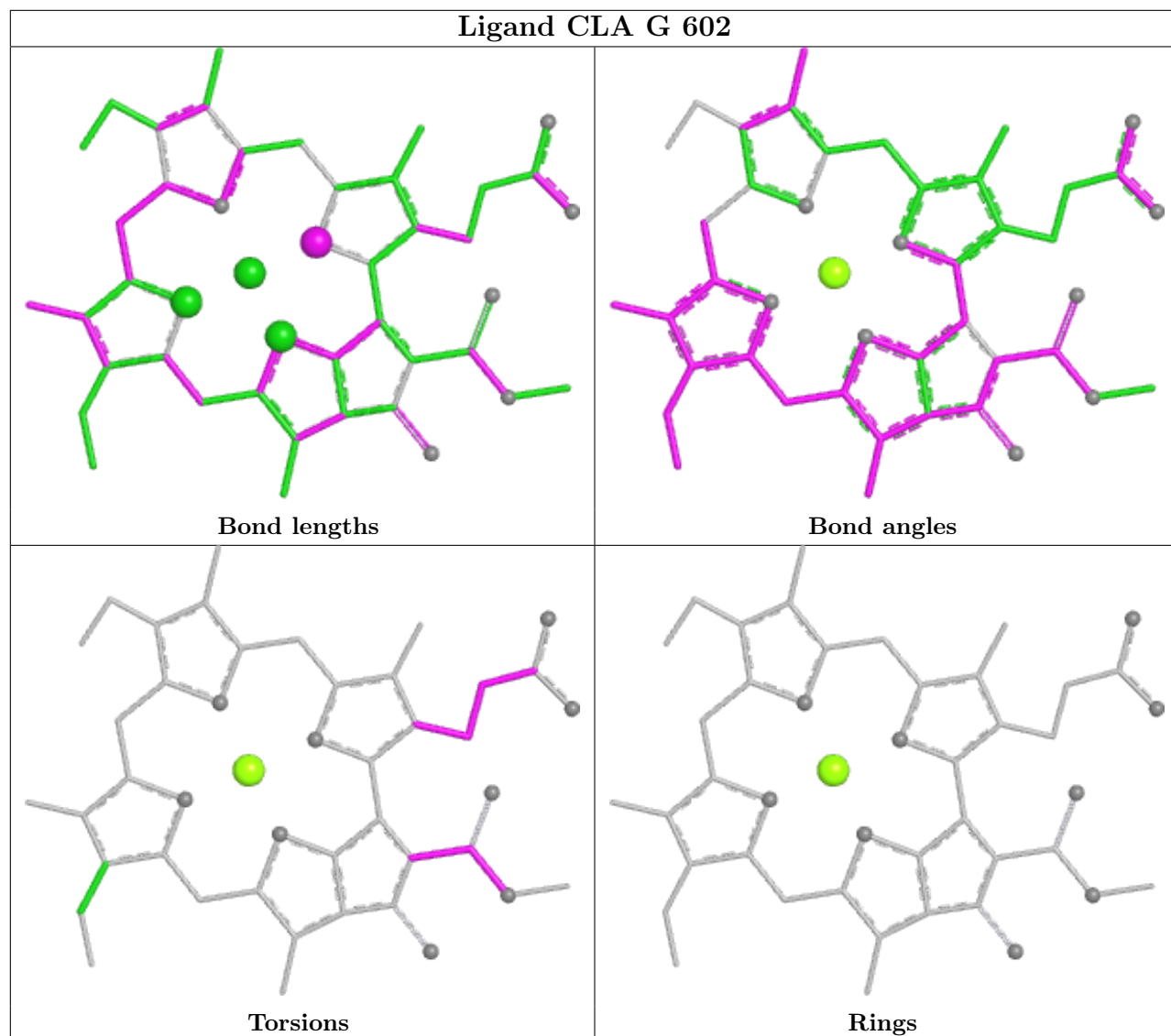


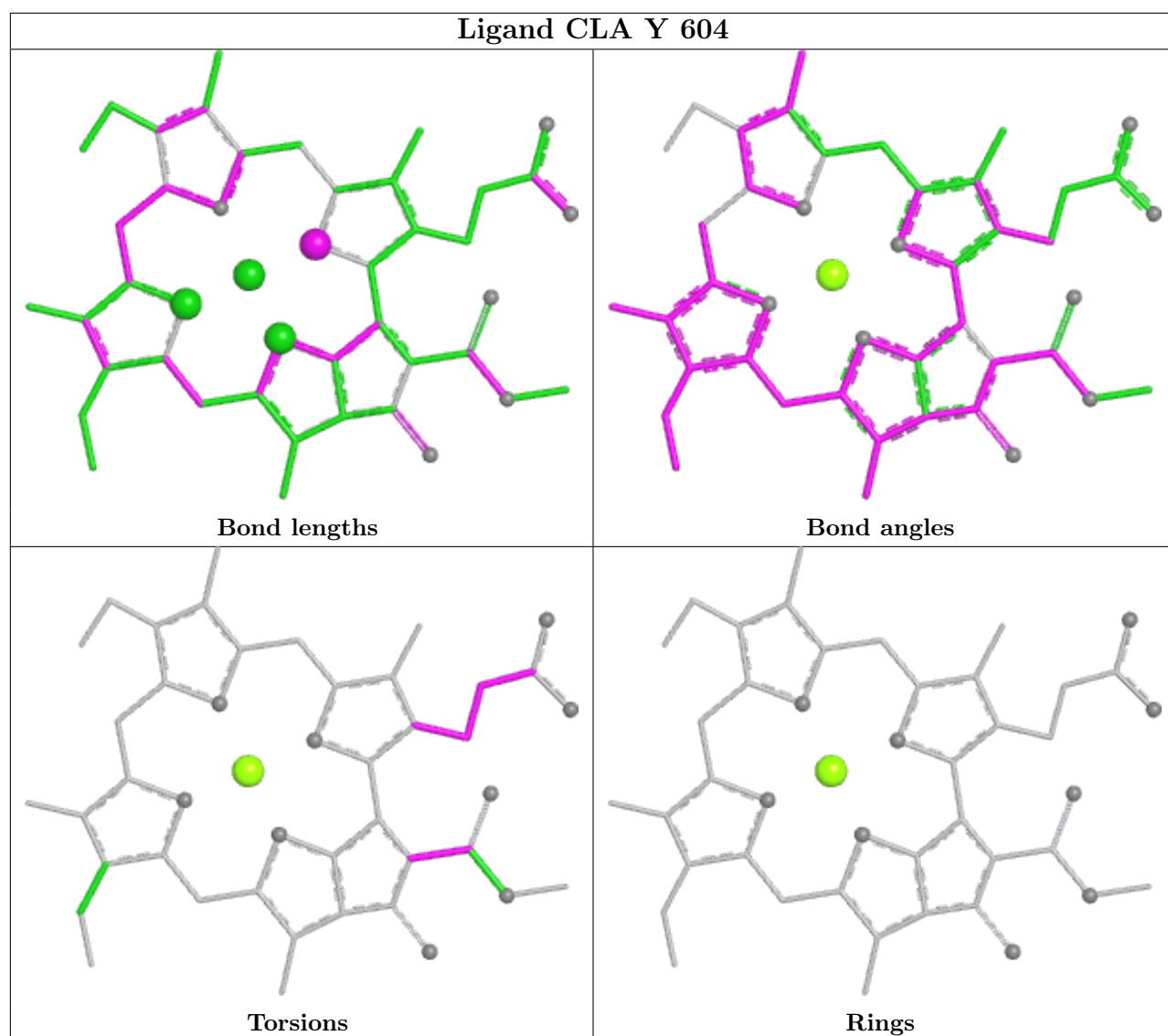


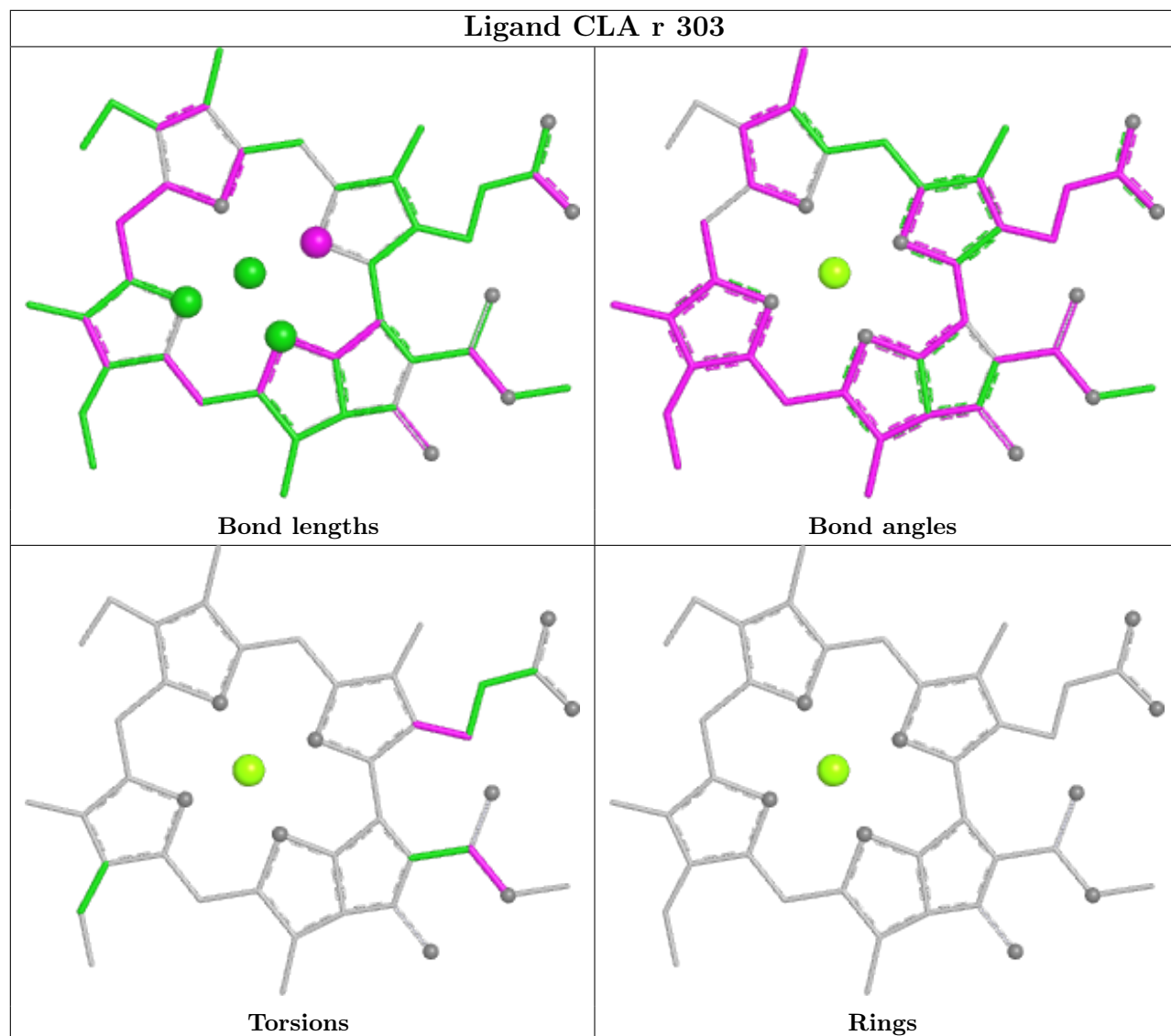


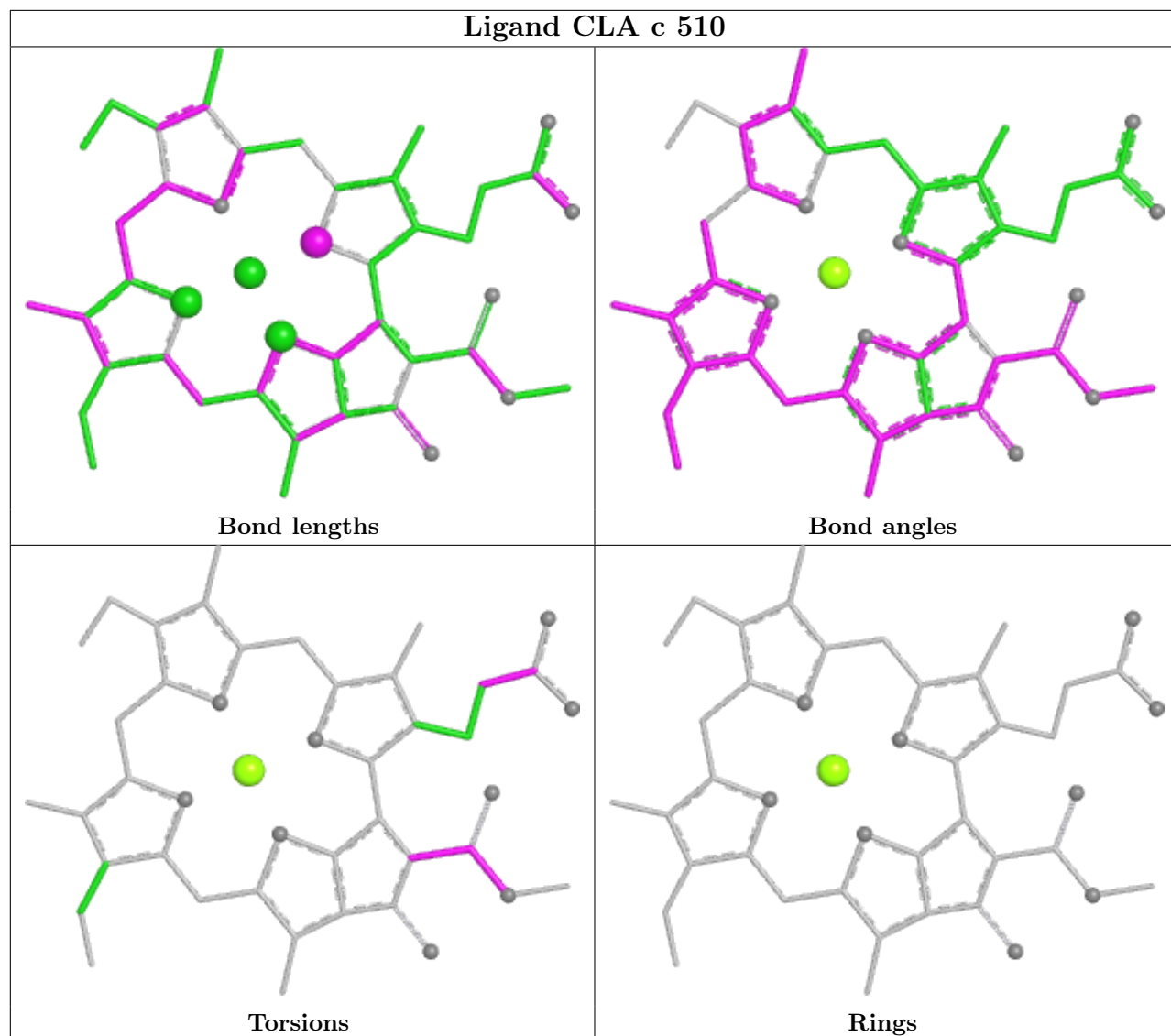


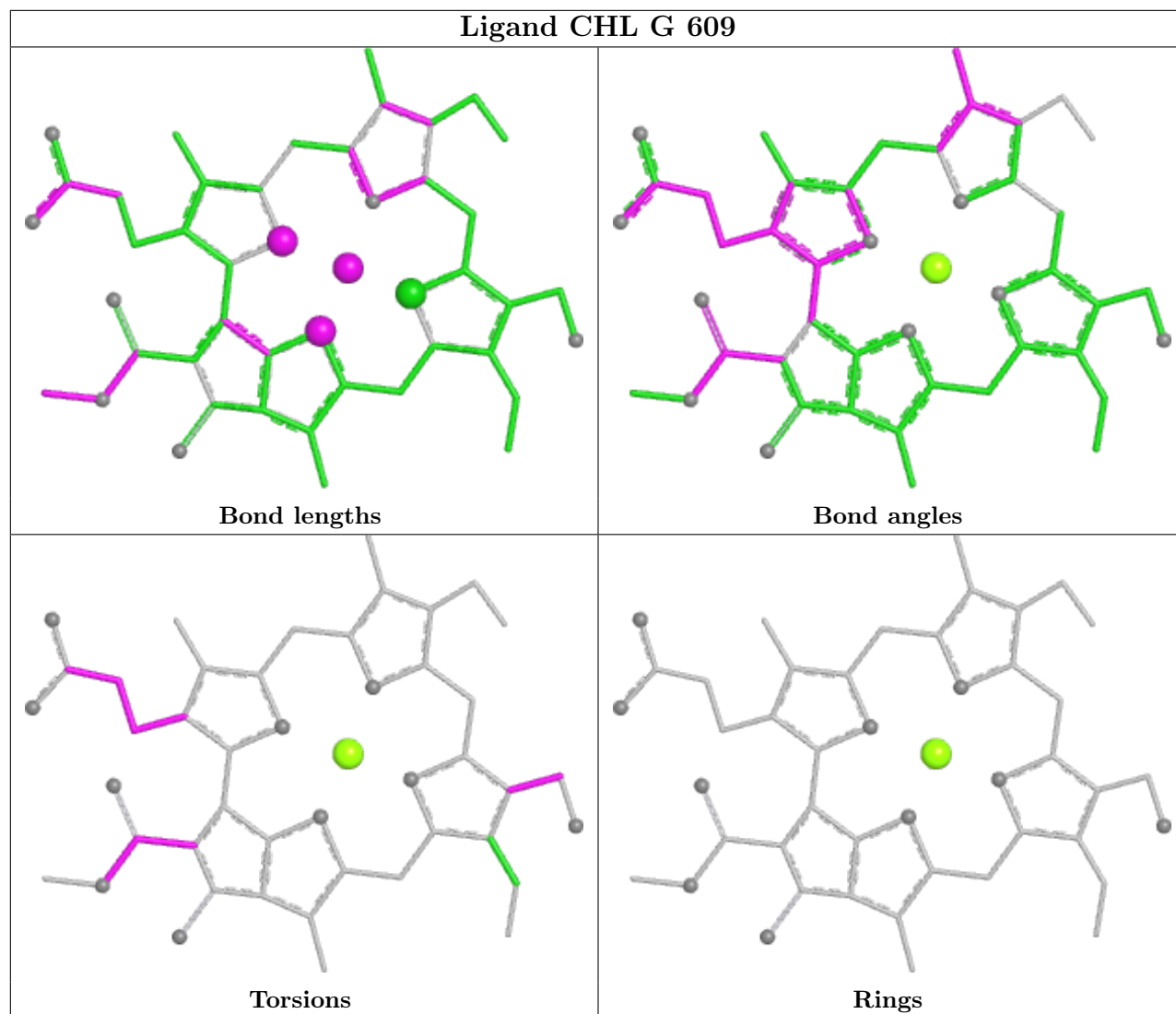


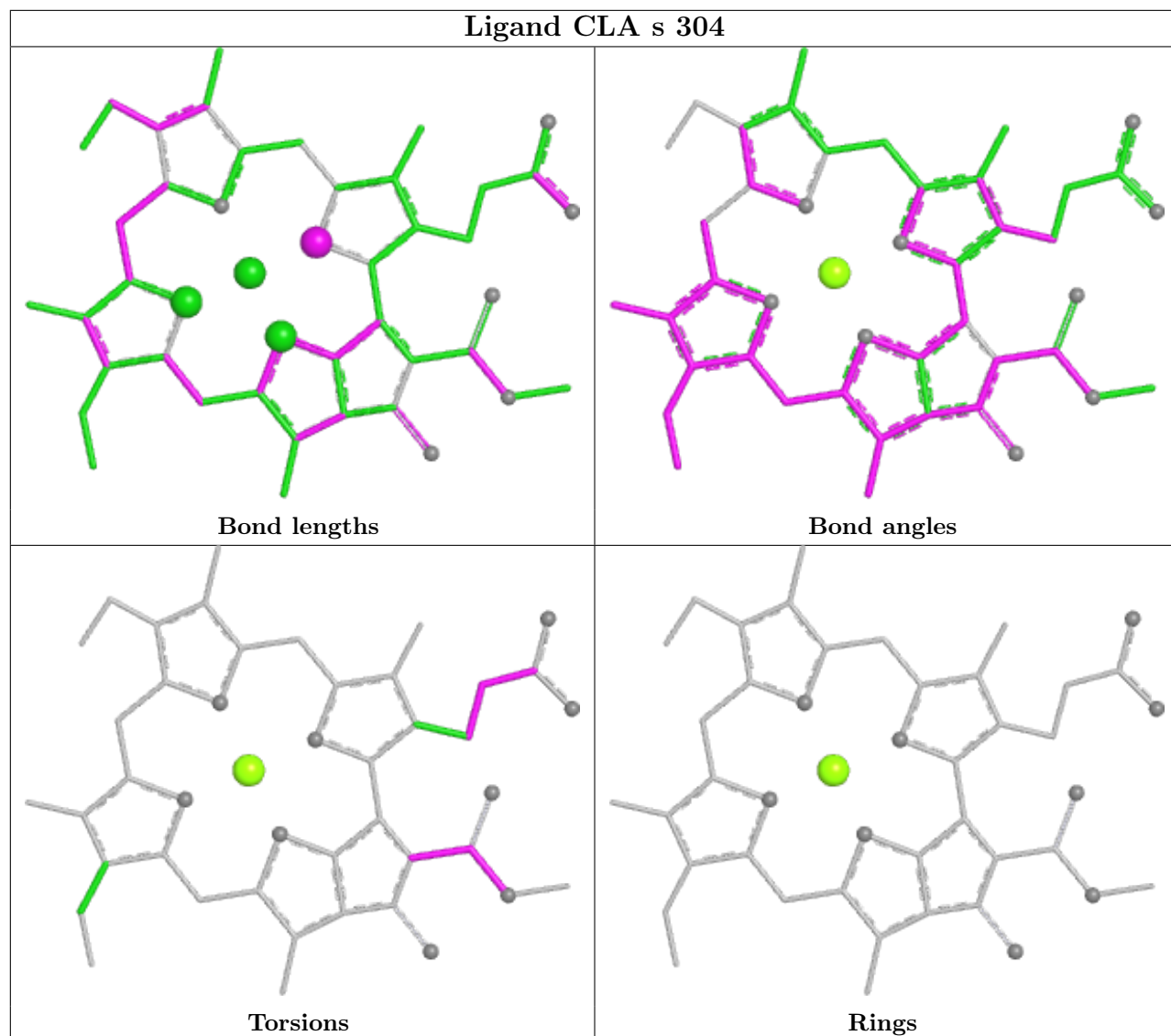


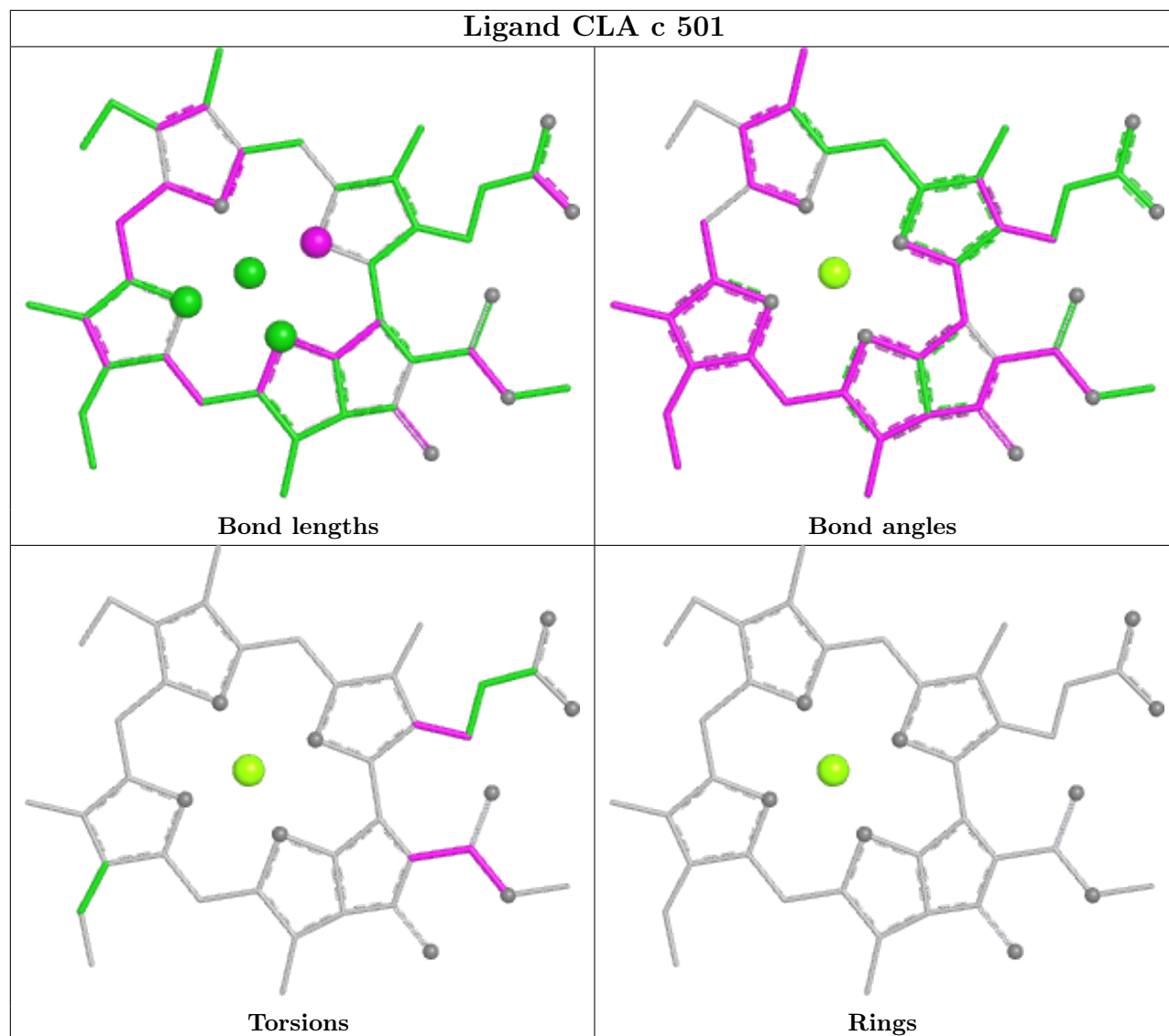


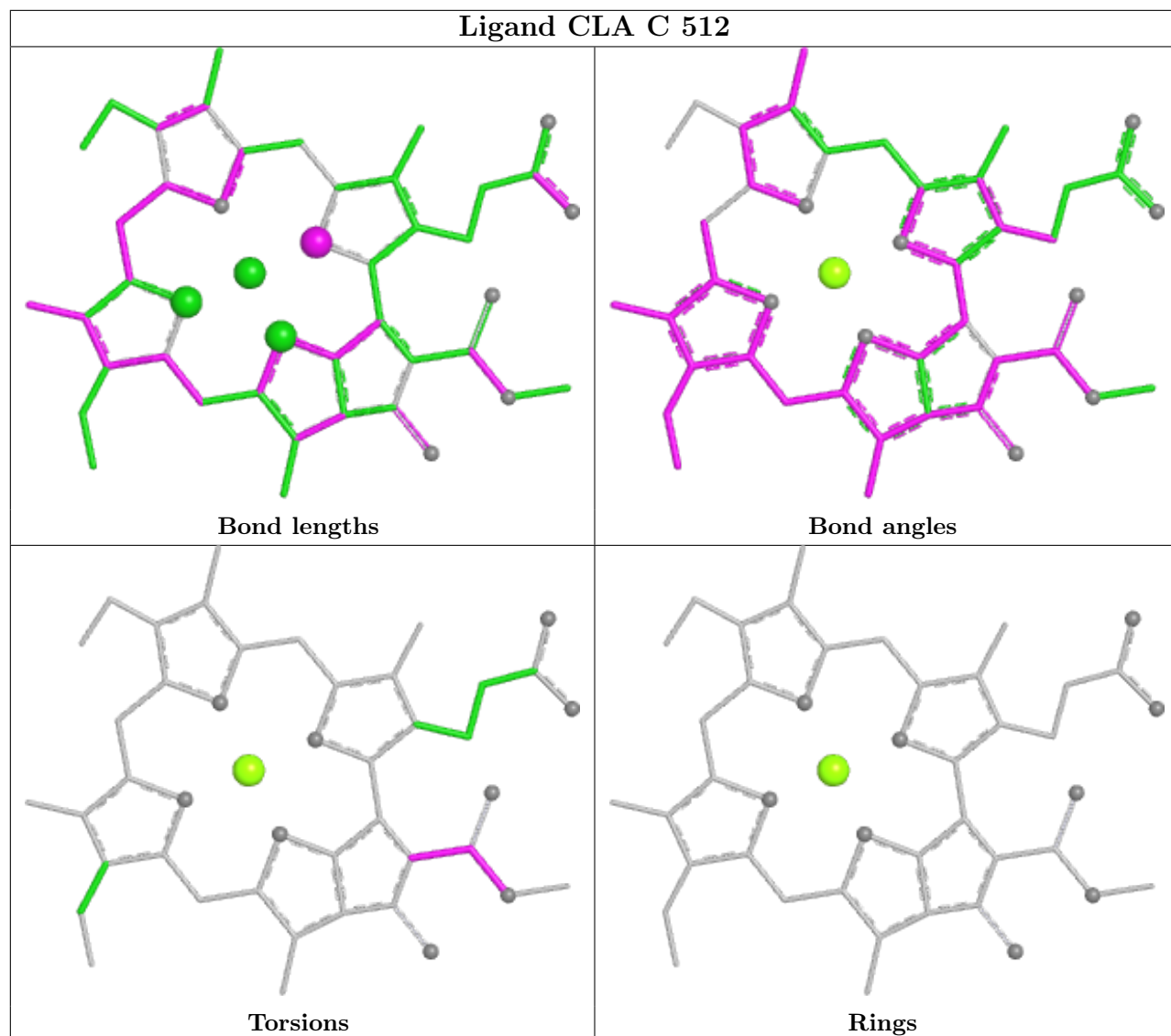


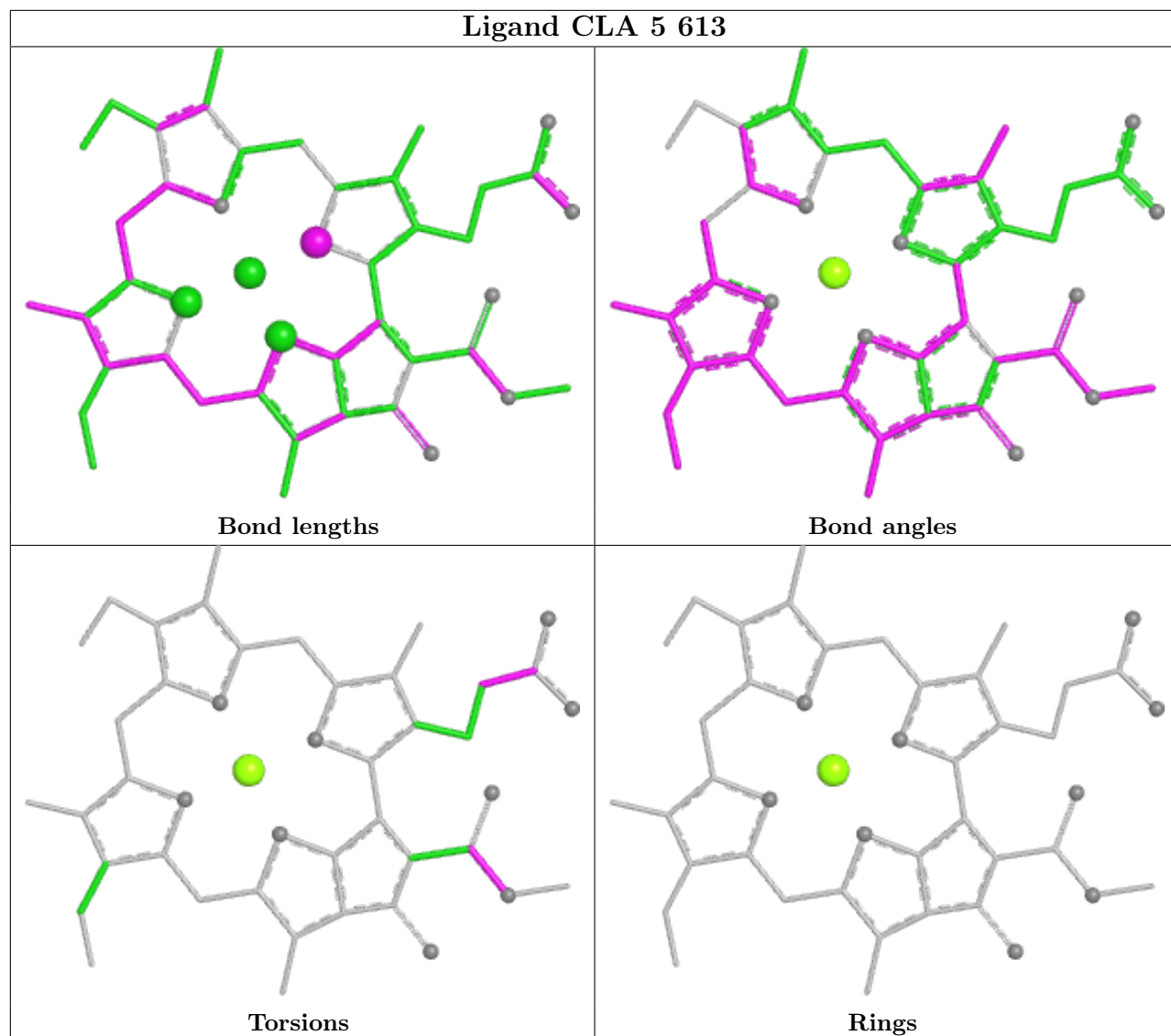


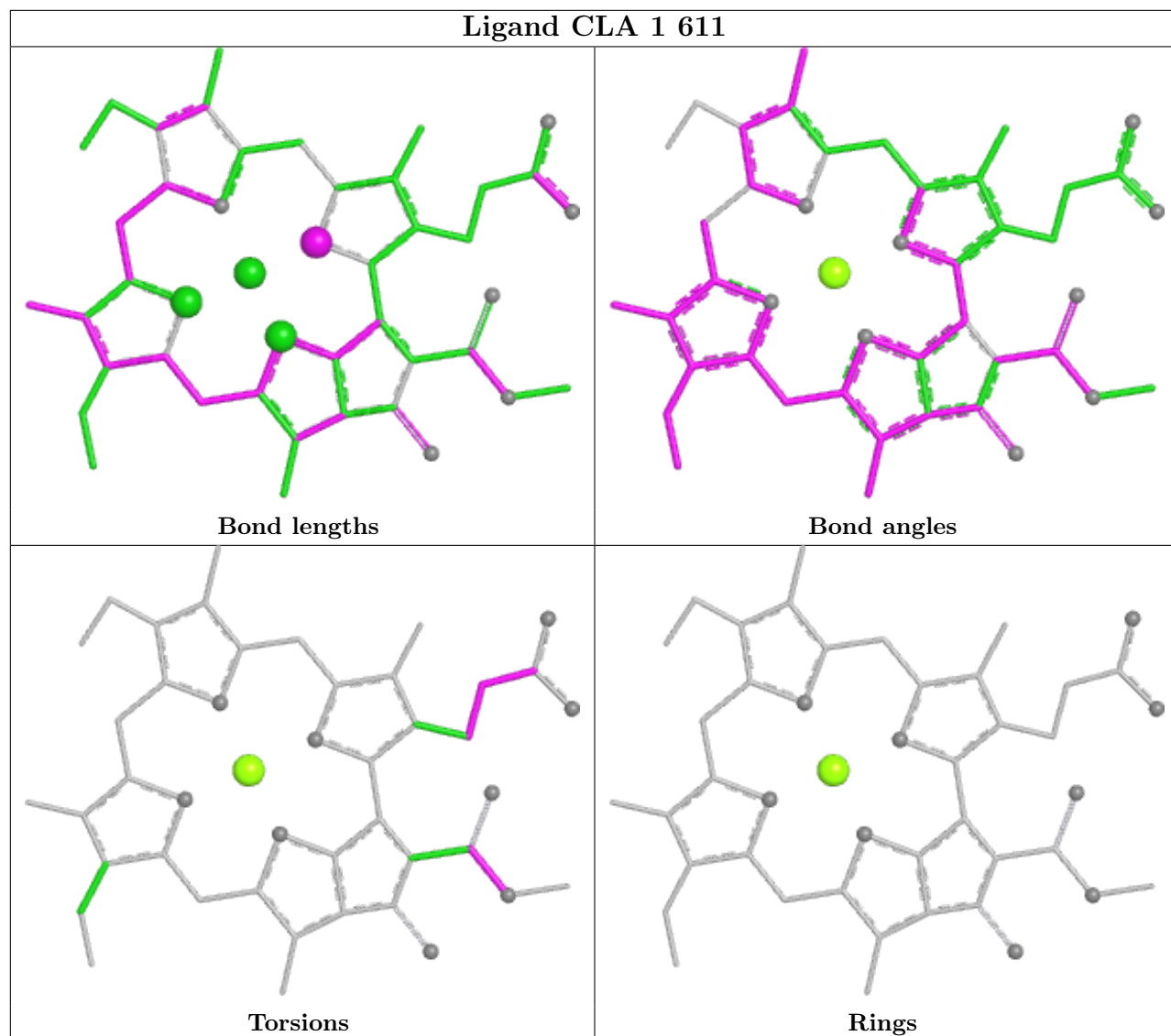


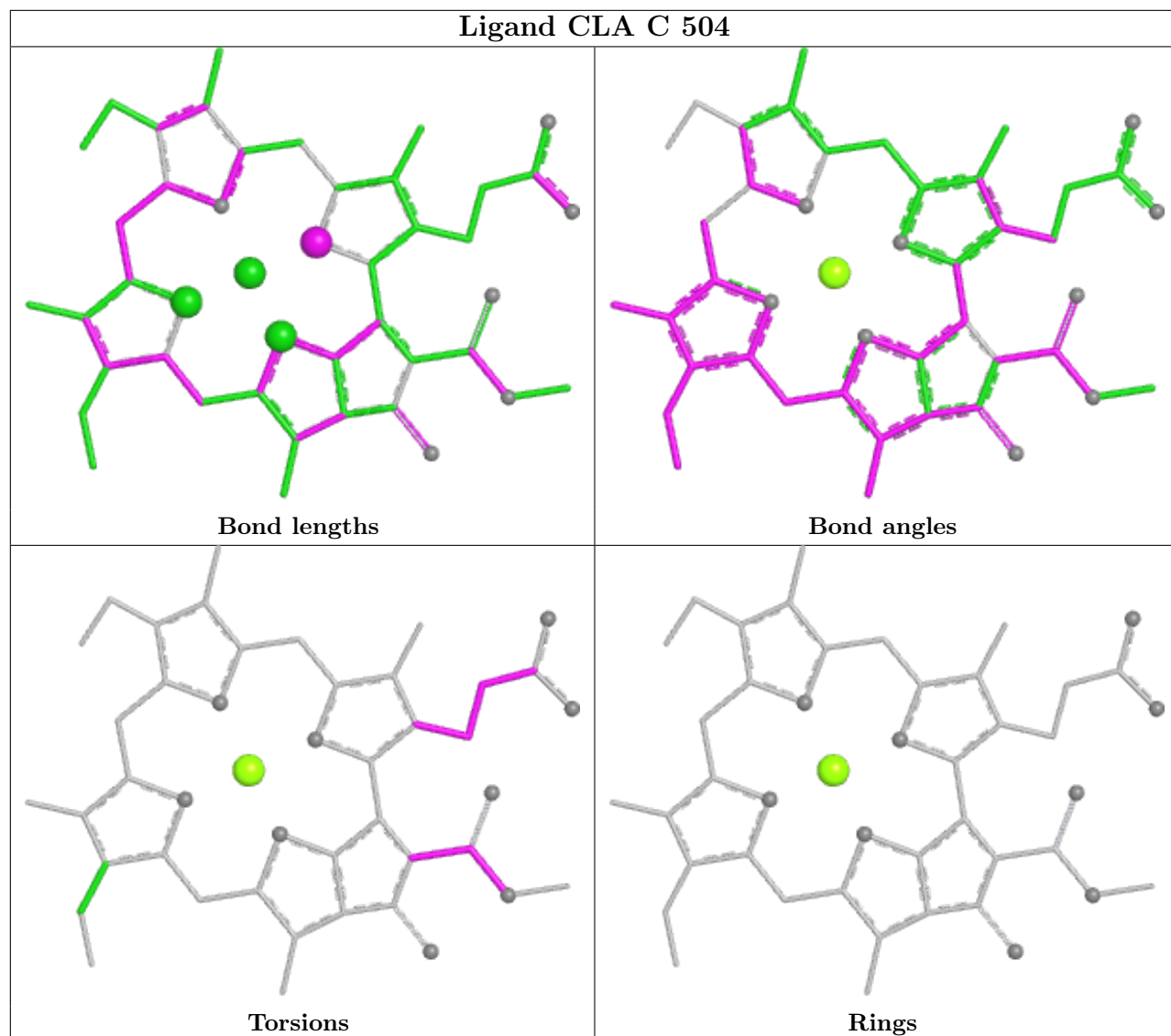


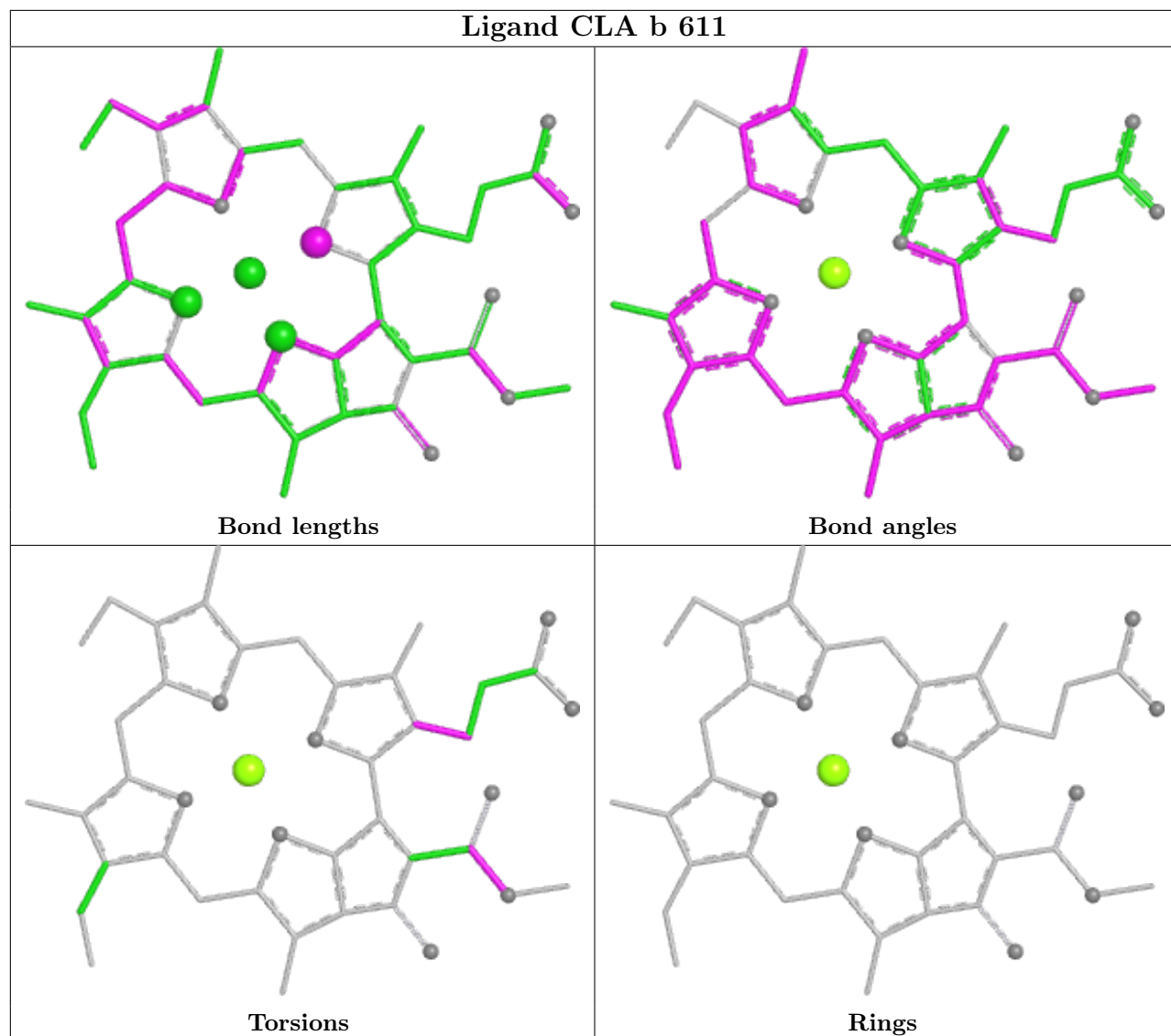


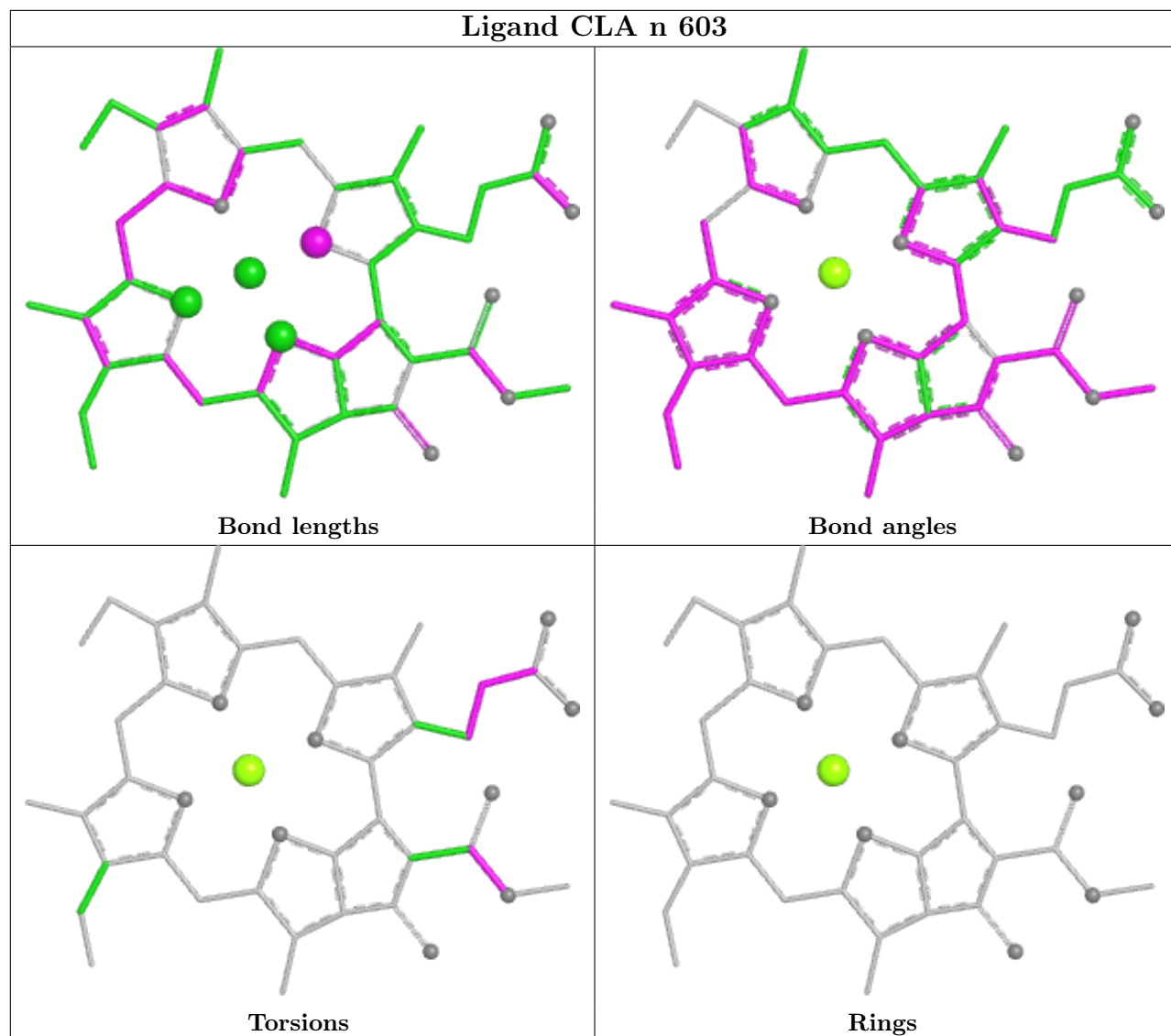


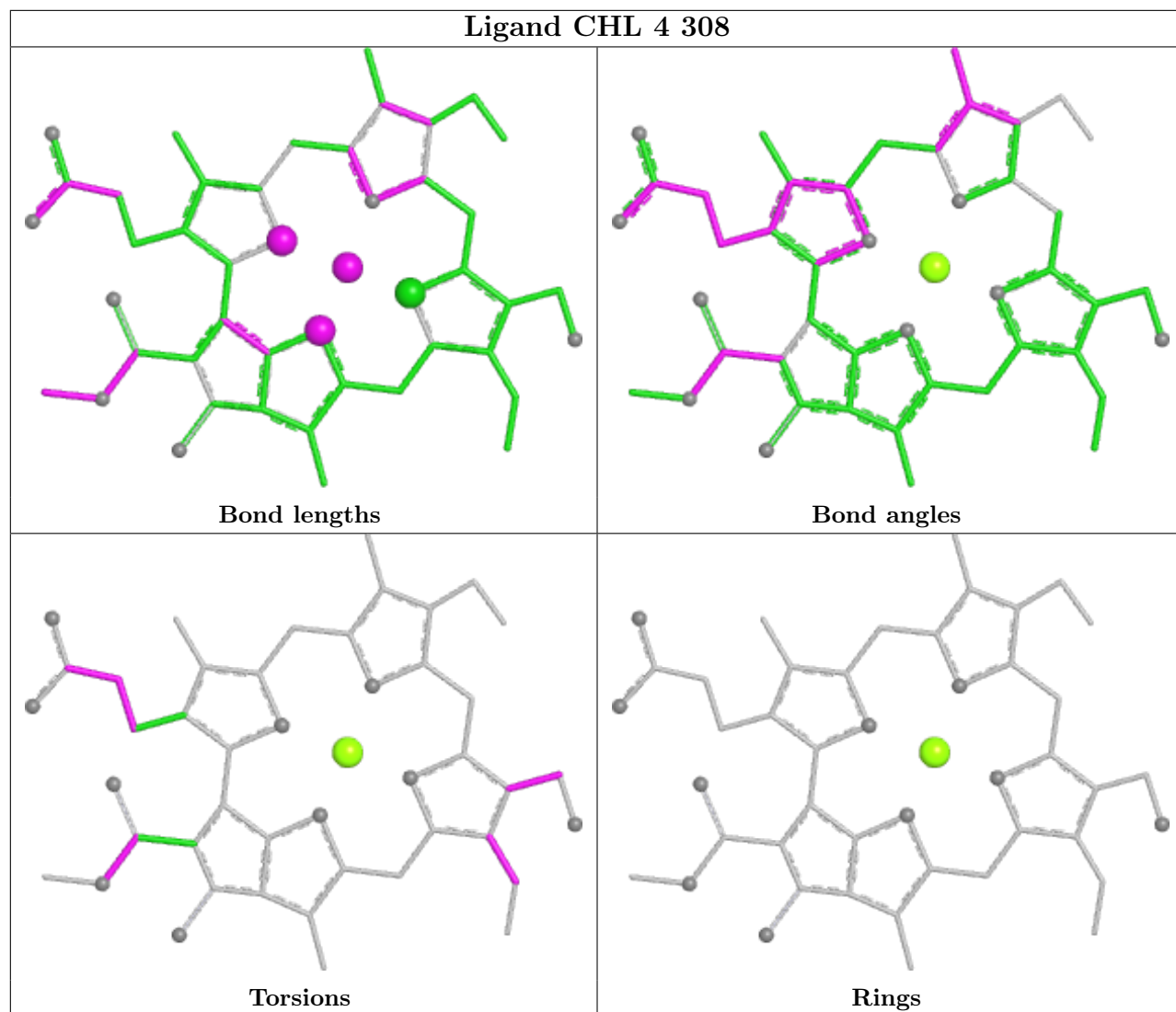


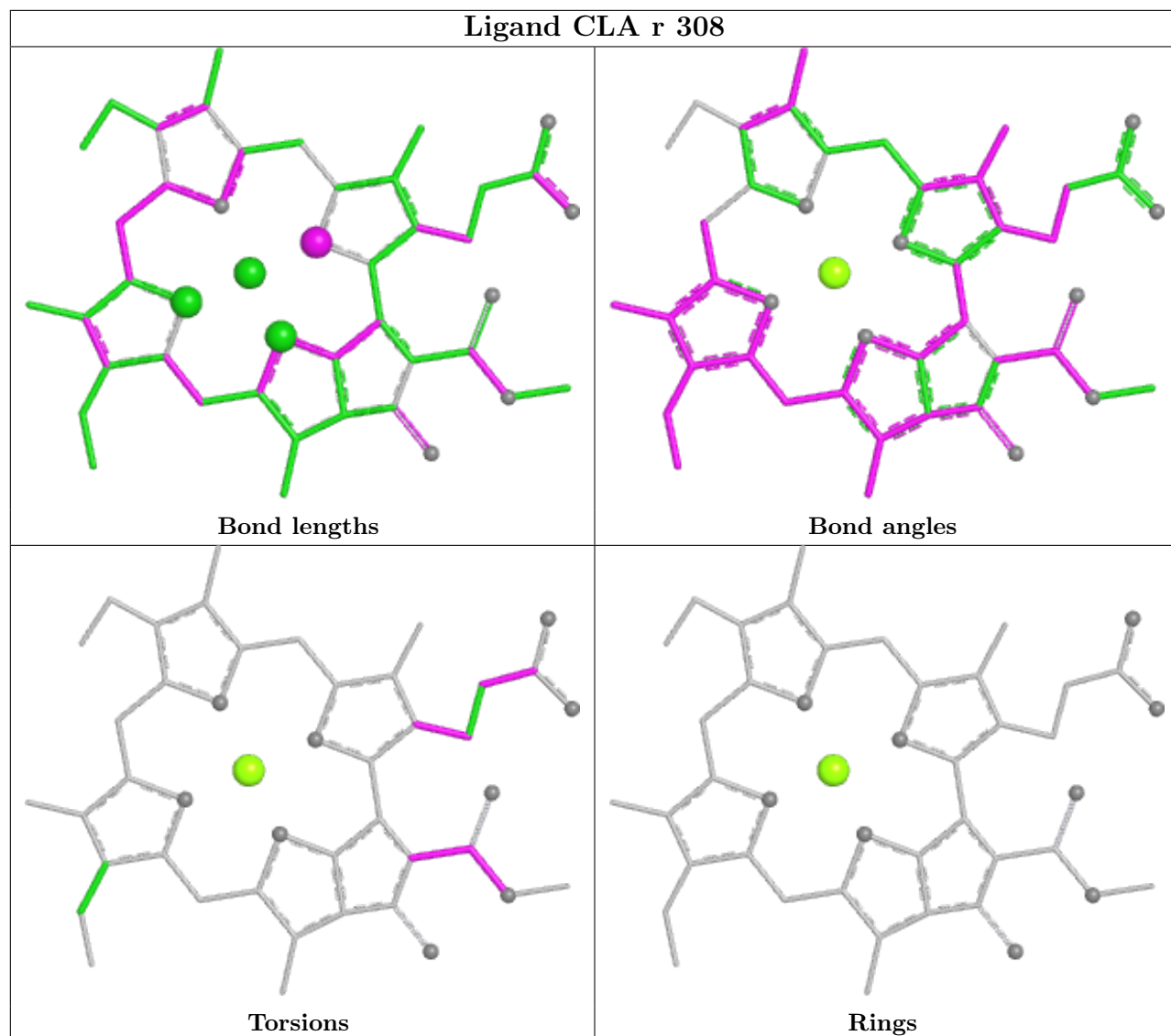


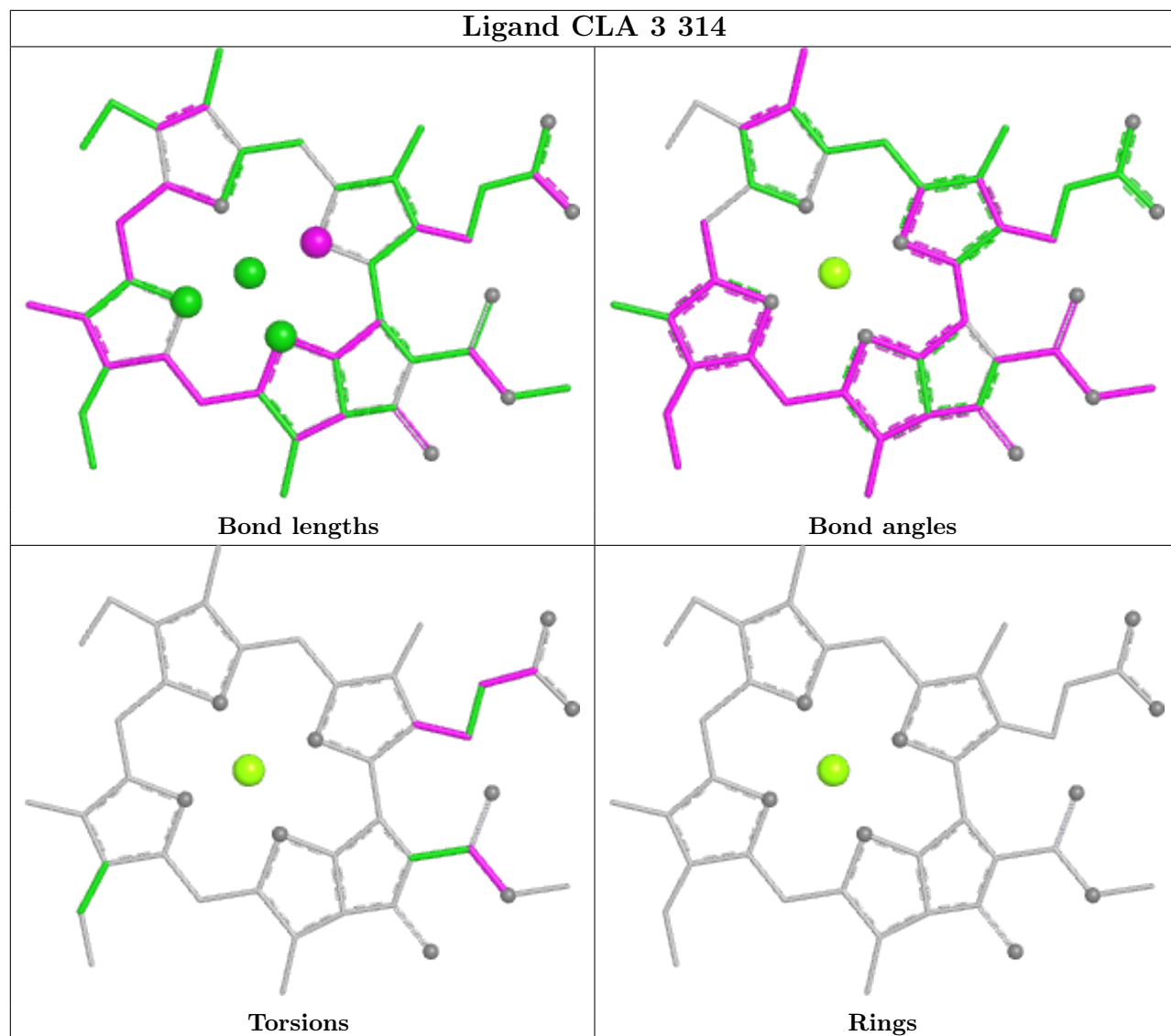


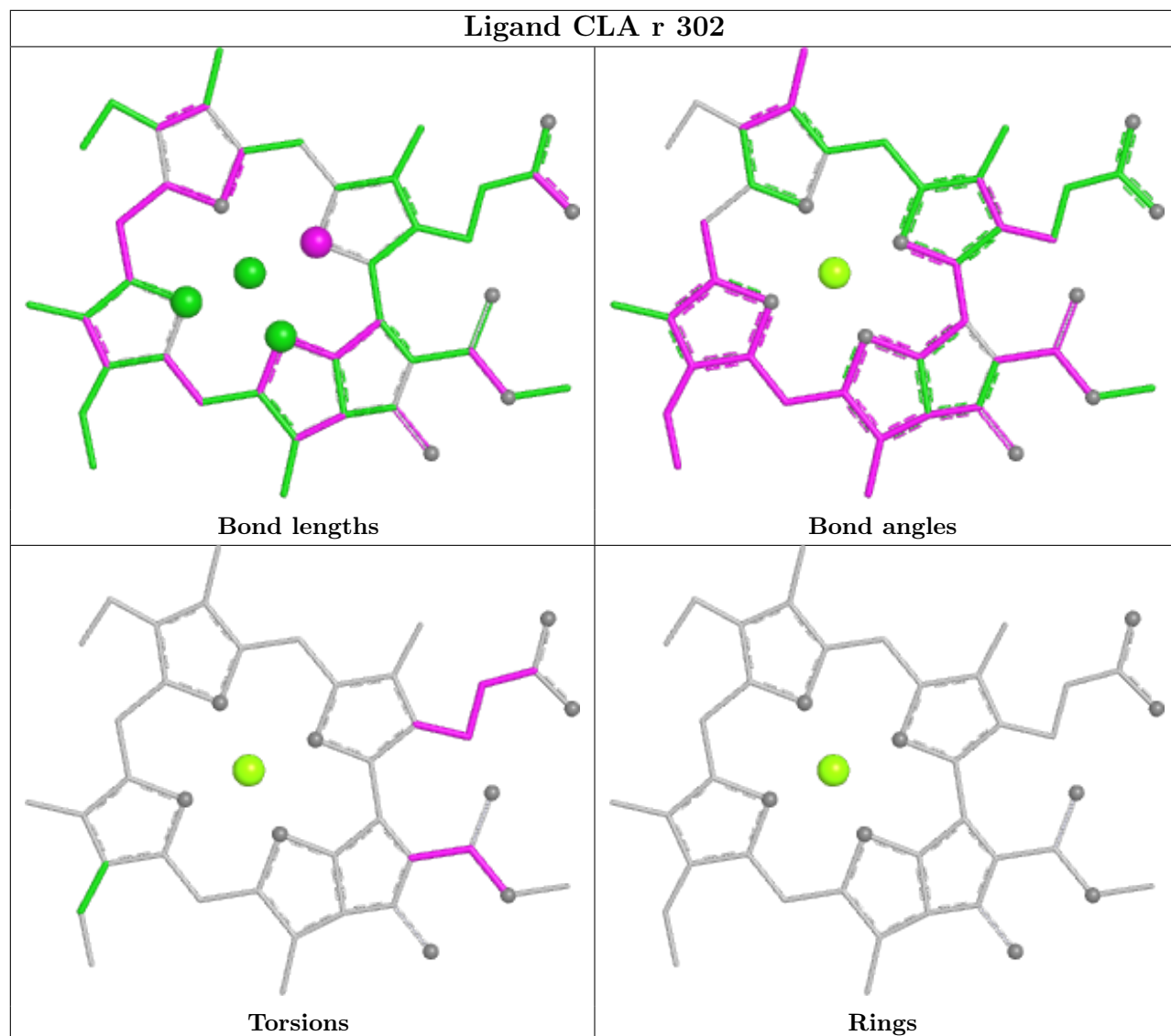


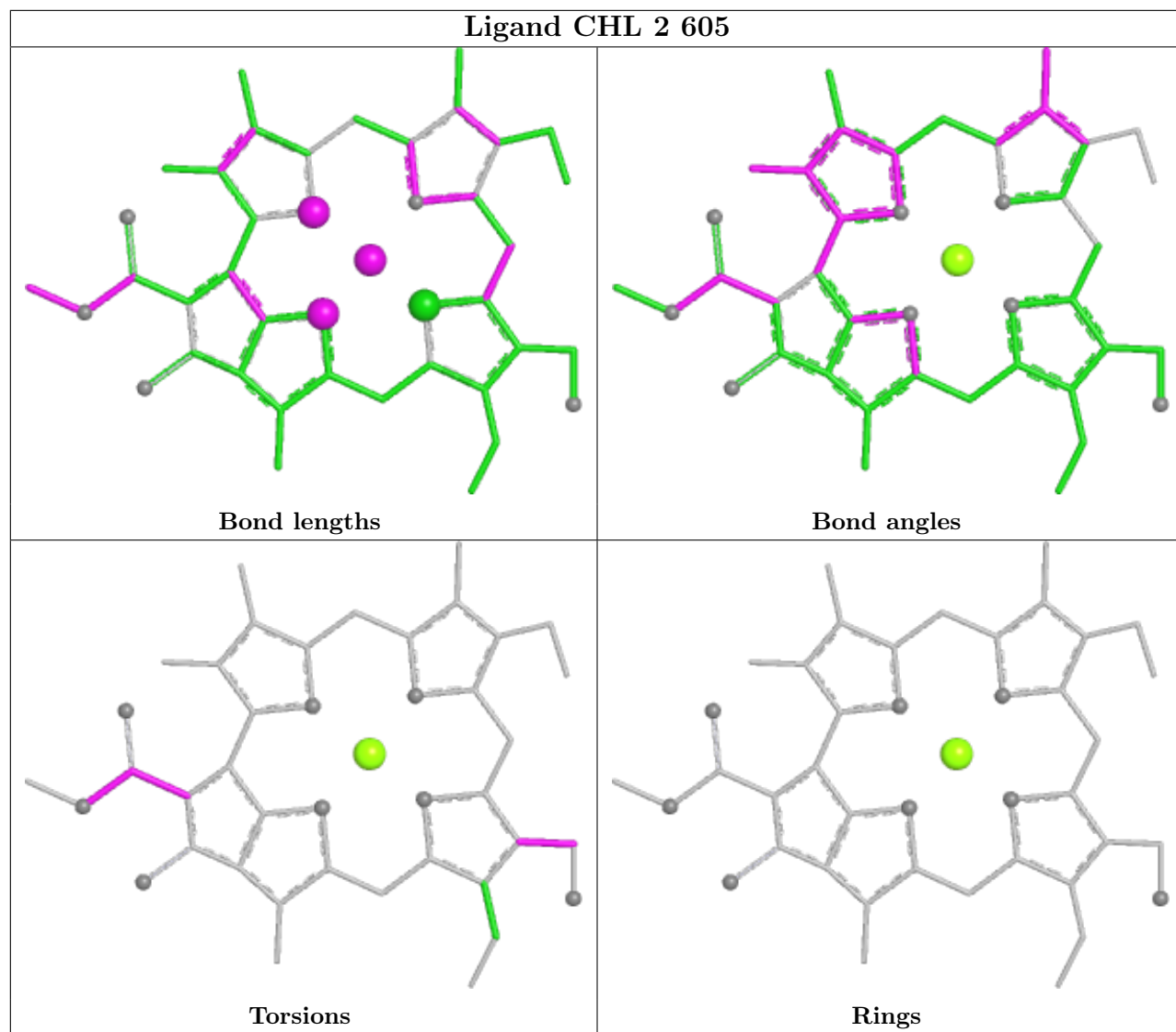


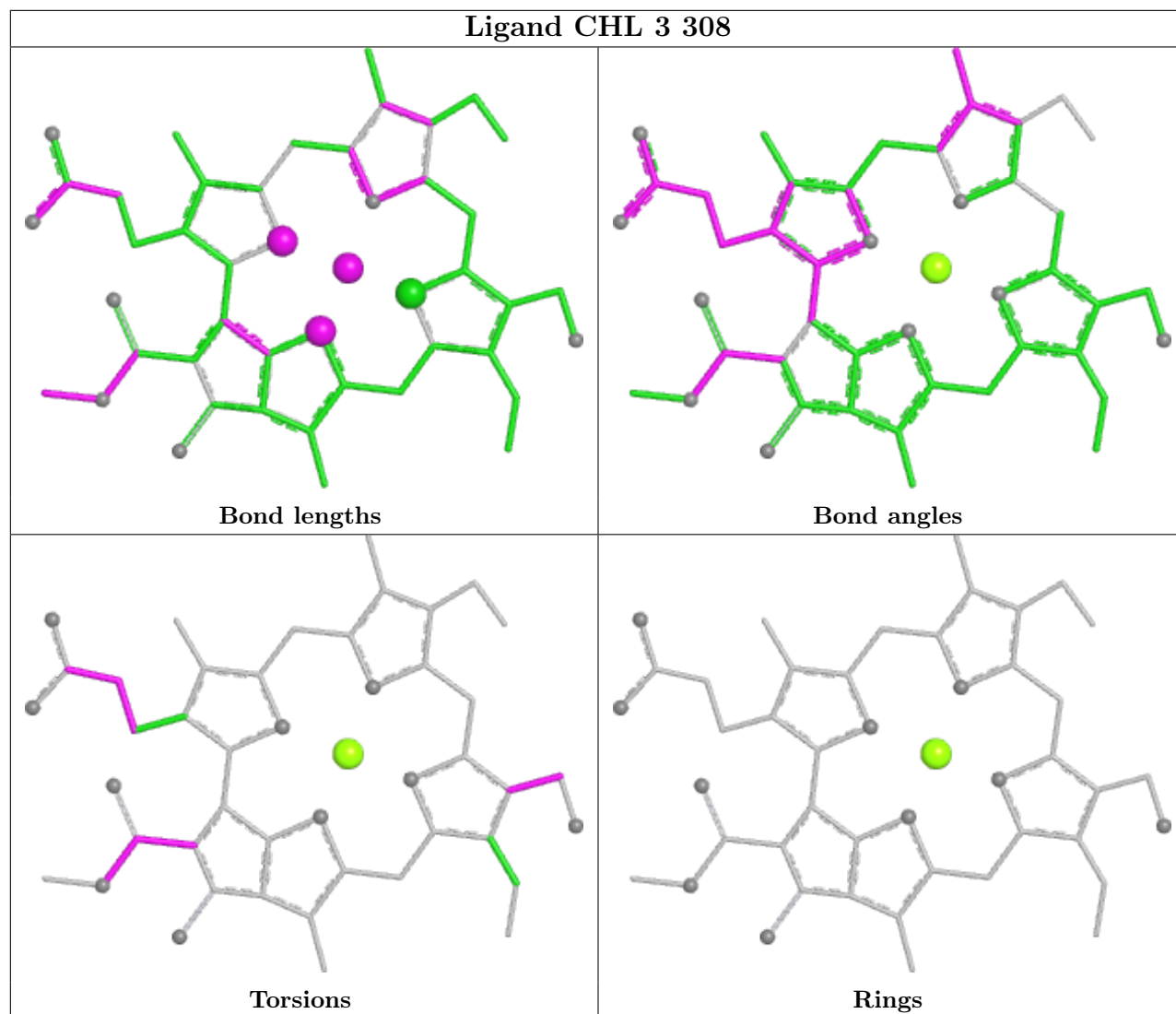


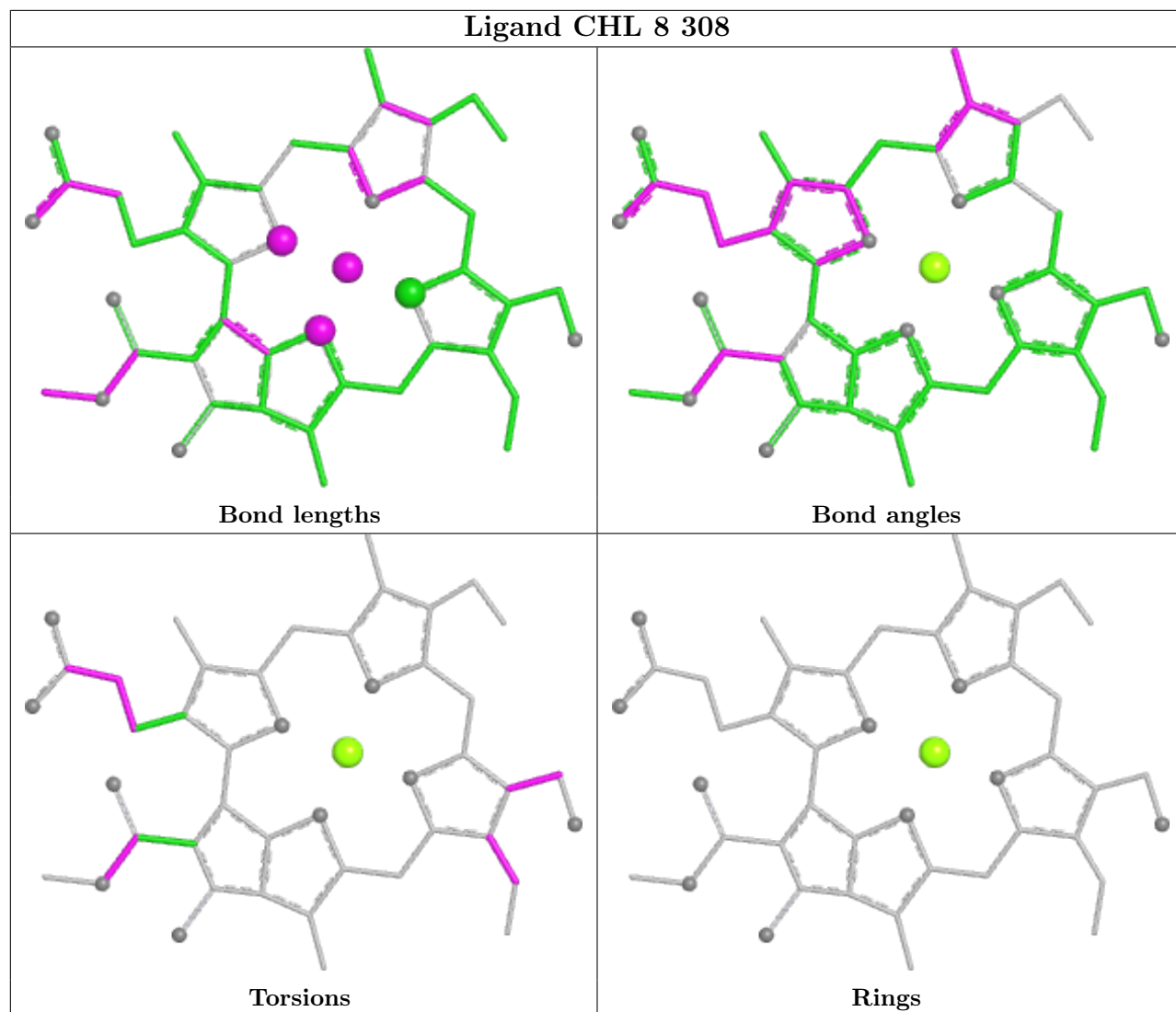


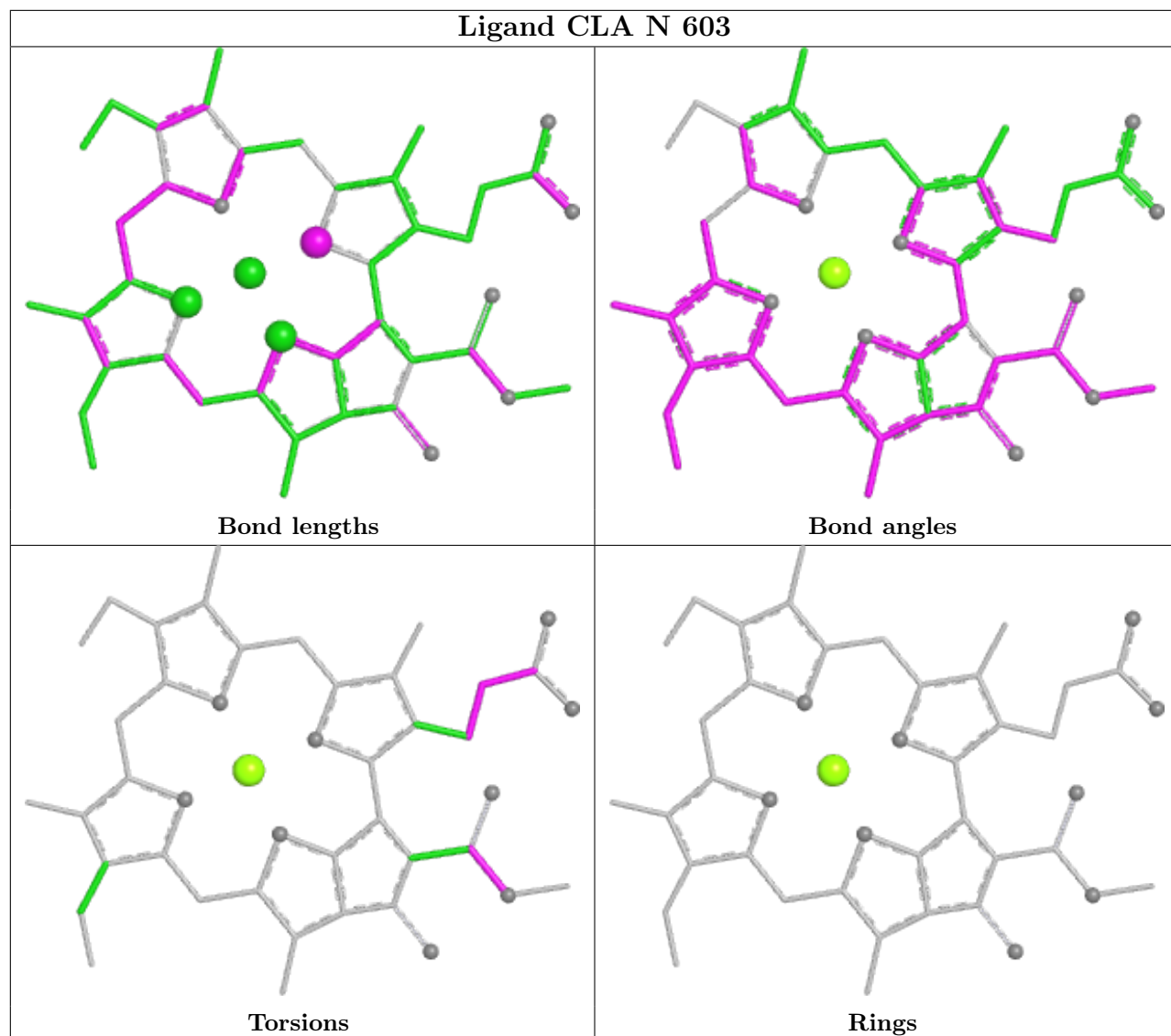


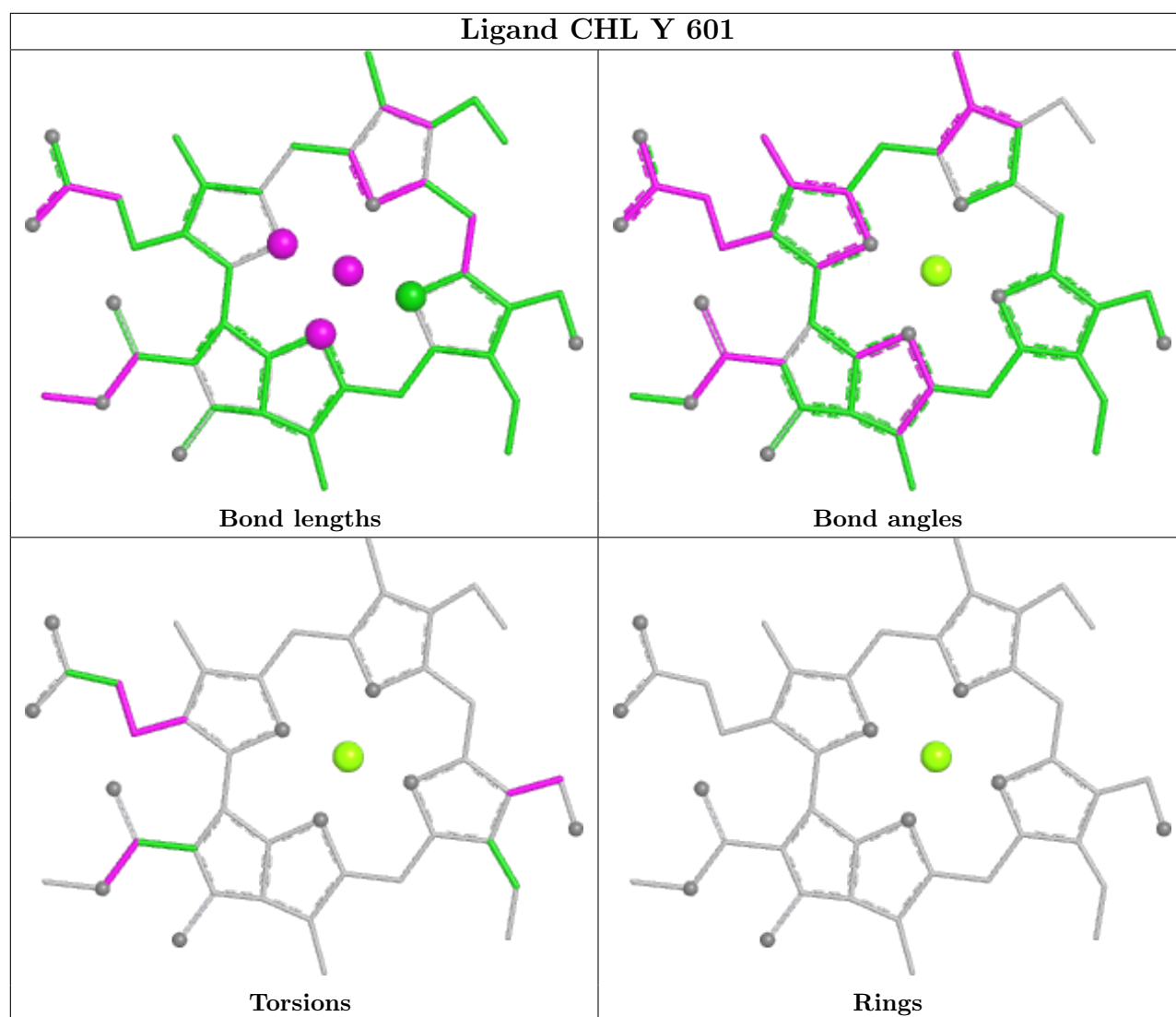












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

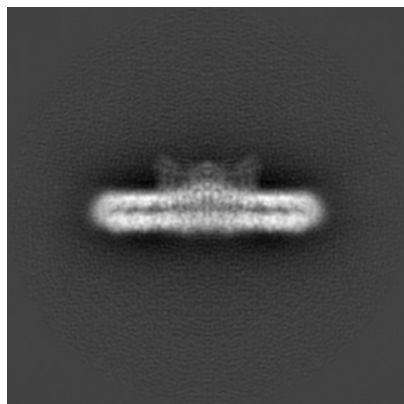
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3491. These allow visual inspection of the internal detail of the map and identification of artifacts.

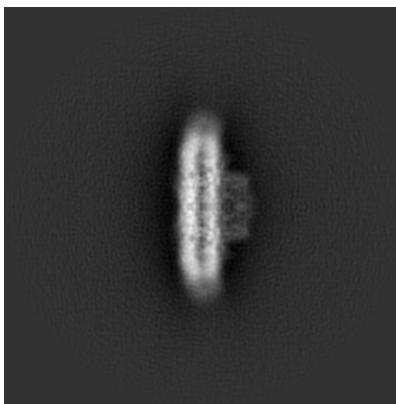
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

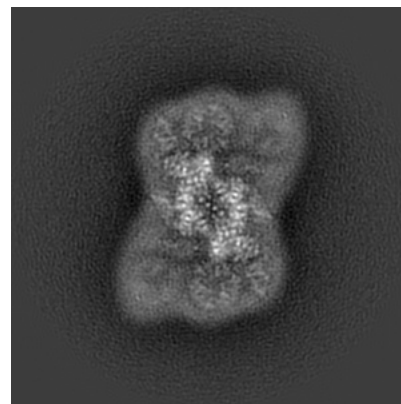
6.1.1 Primary map



X

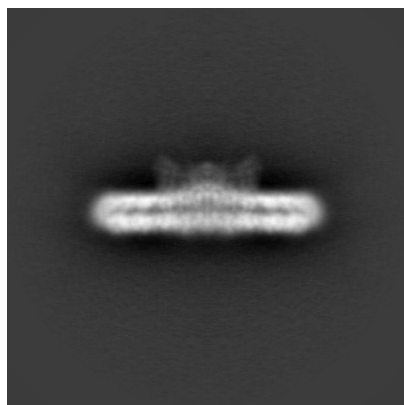


Y

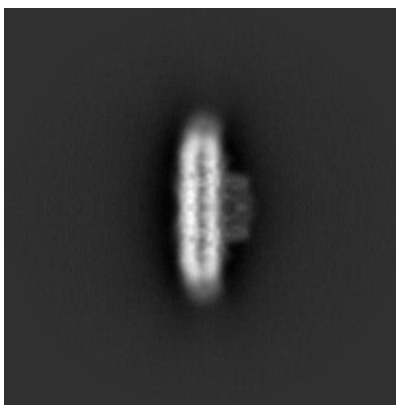


Z

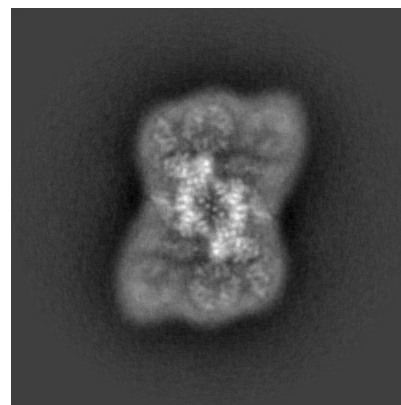
6.1.2 Raw map



X



Y

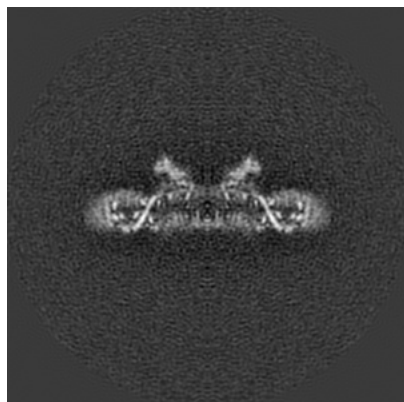


Z

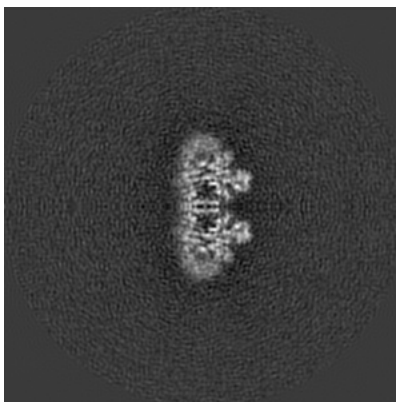
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

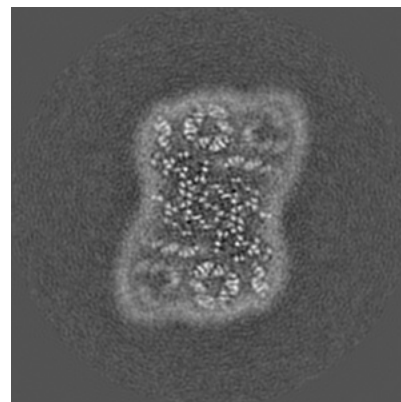
6.2.1 Primary map



X Index: 234

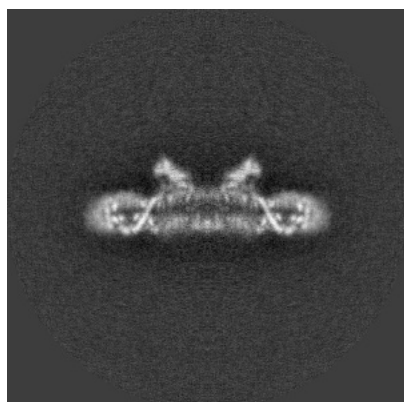


Y Index: 234

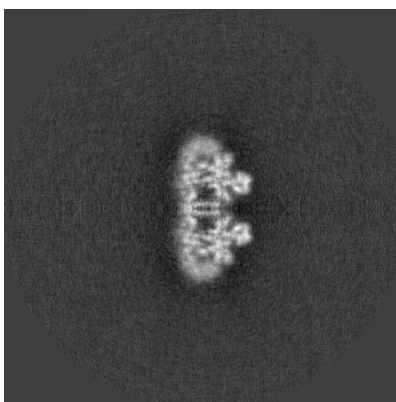


Z Index: 234

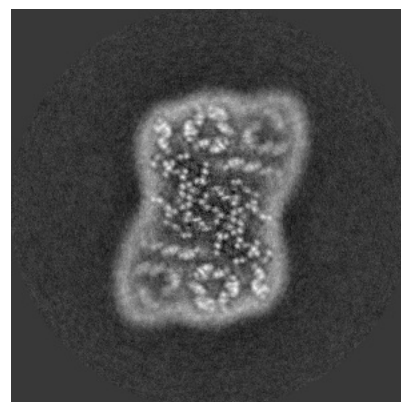
6.2.2 Raw map



X Index: 234



Y Index: 234

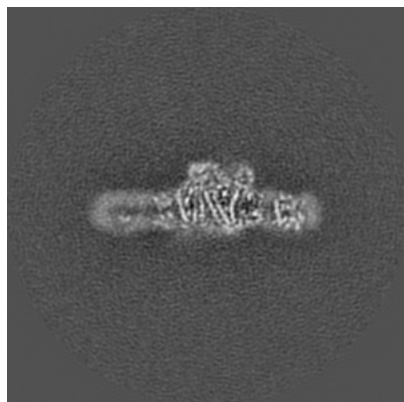


Z Index: 234

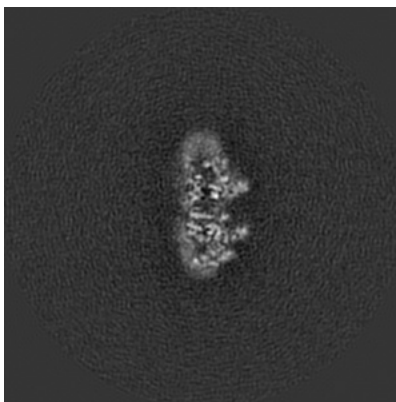
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

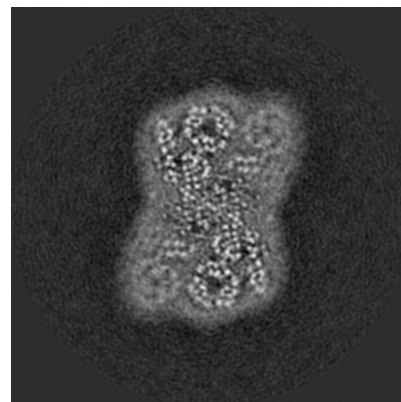
6.3.1 Primary map



X Index: 208

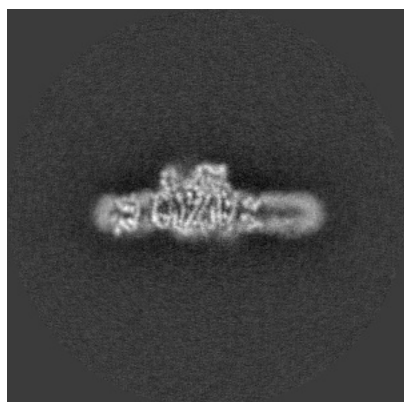


Y Index: 243

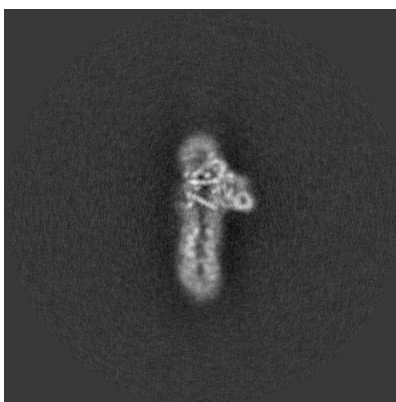


Z Index: 218

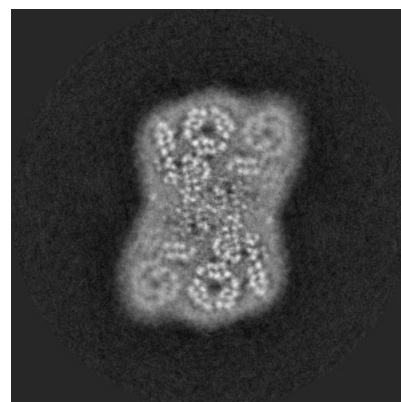
6.3.2 Raw map



X Index: 262



Y Index: 190



Z Index: 218

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

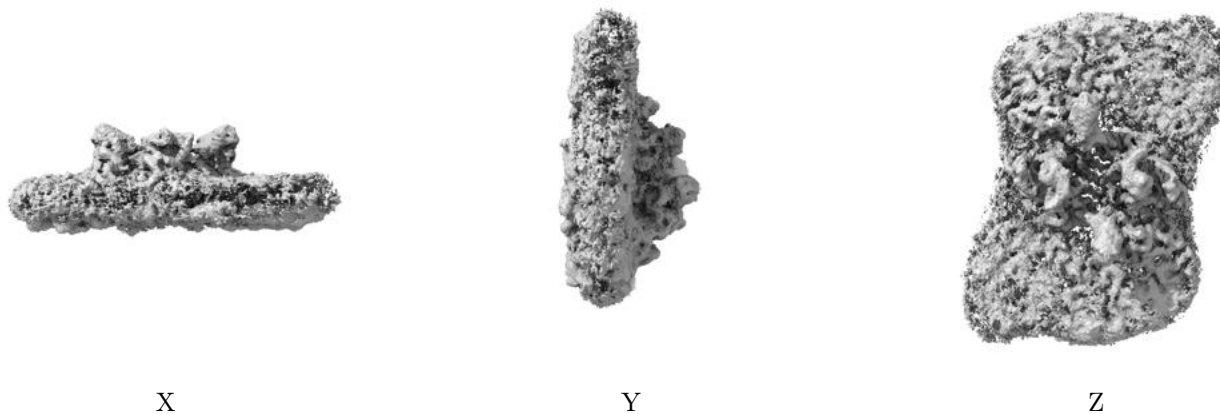
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

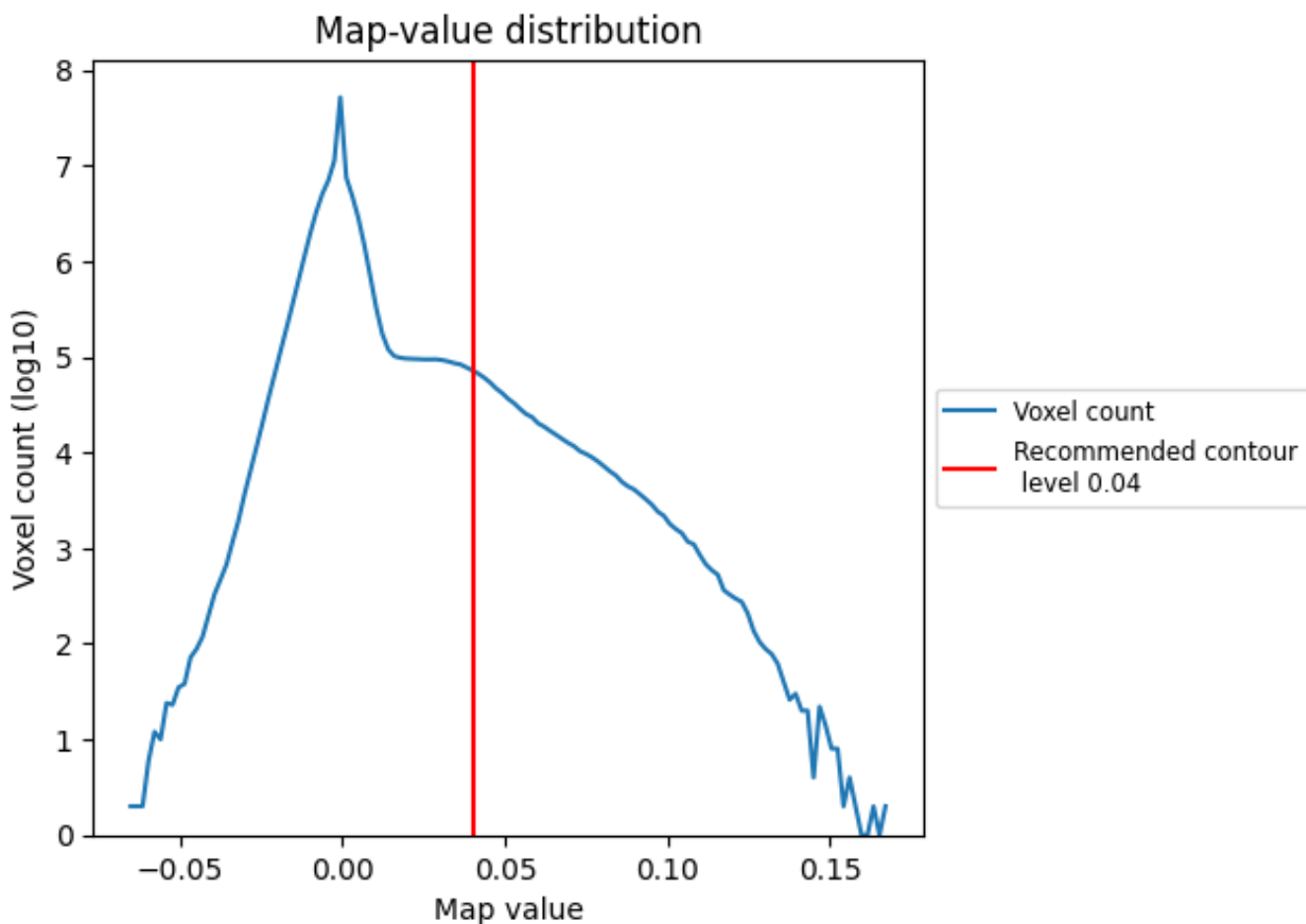
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

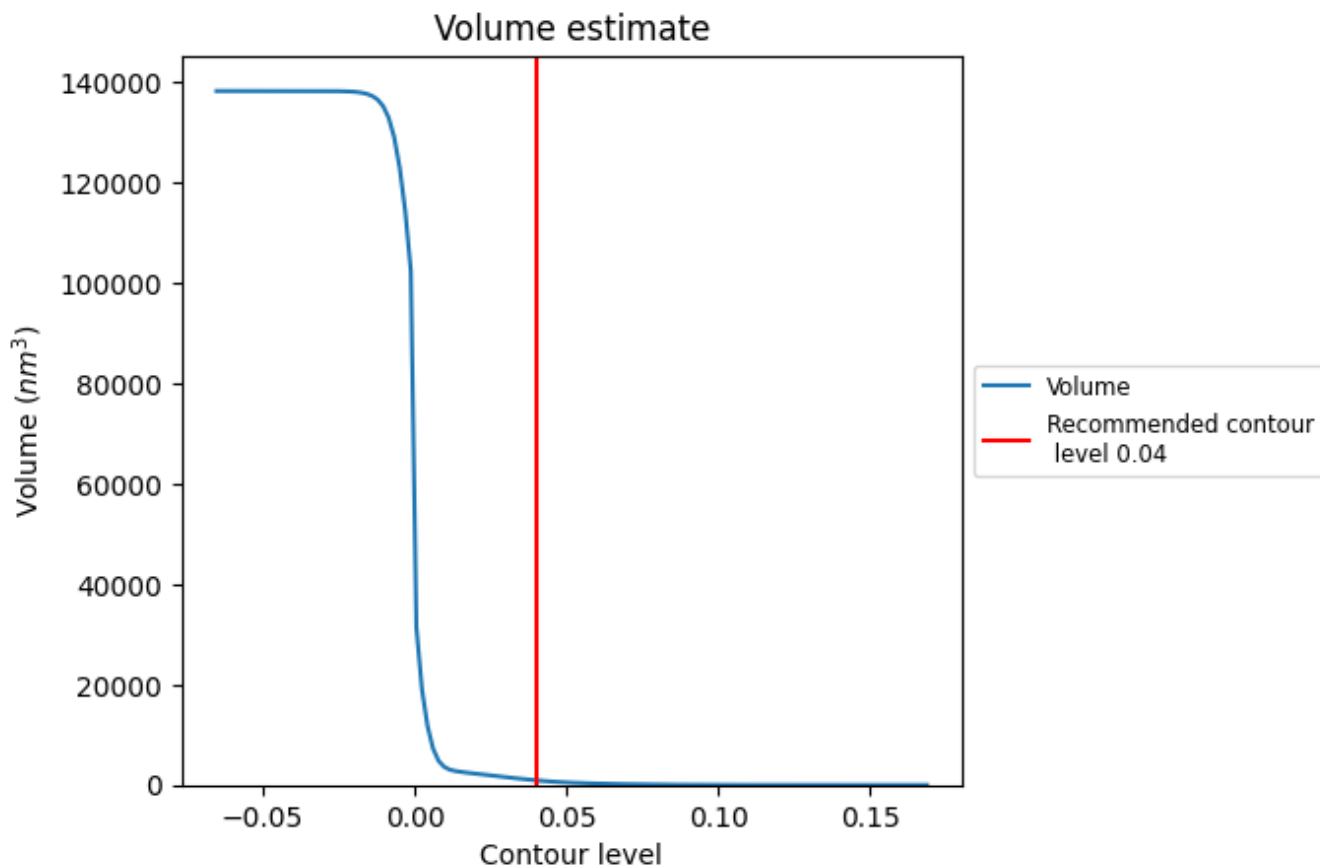
This section contains the results of statistical analysis of the map.

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.

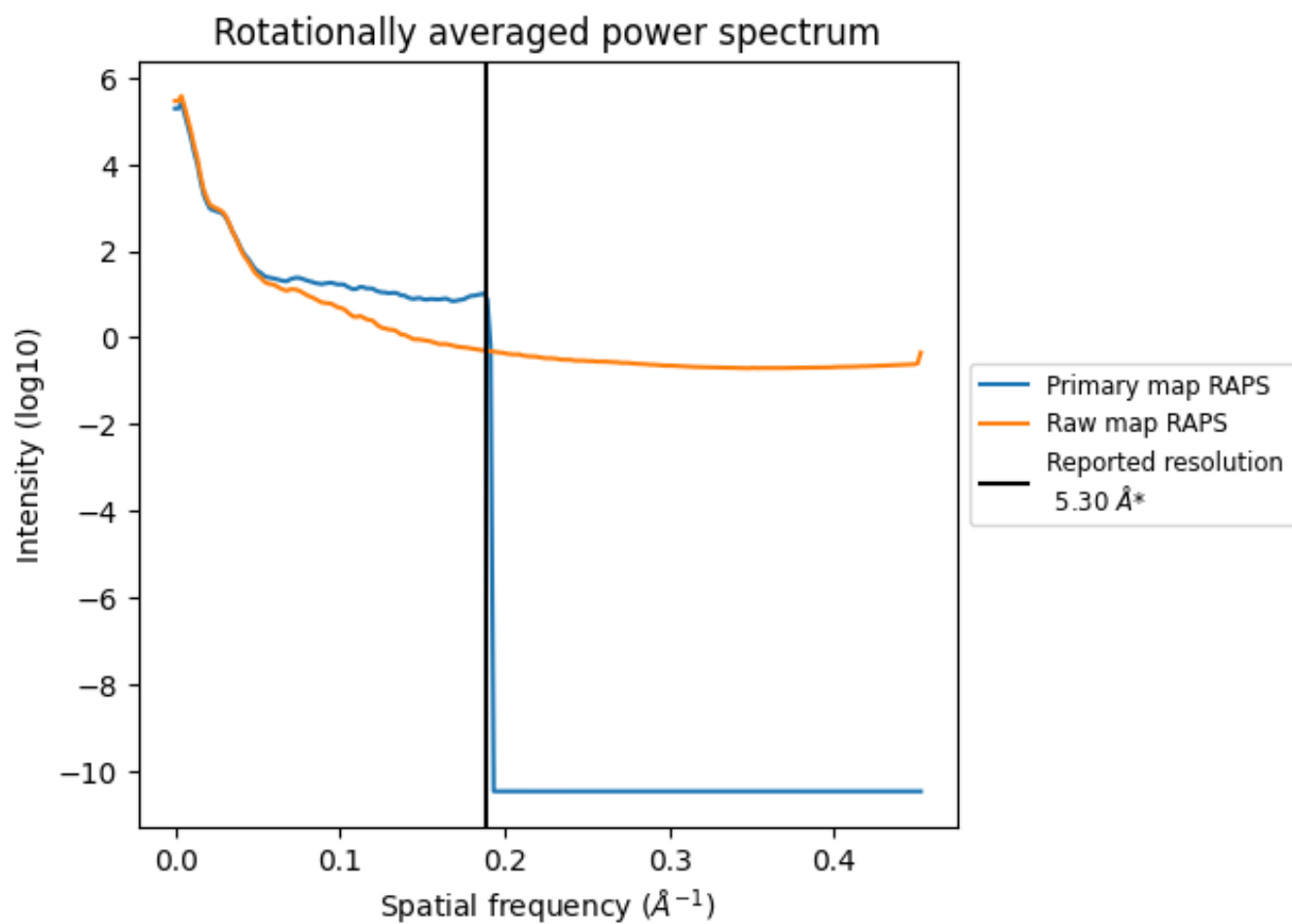
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 930 nm^3 ; this corresponds to an approximate mass of 840 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

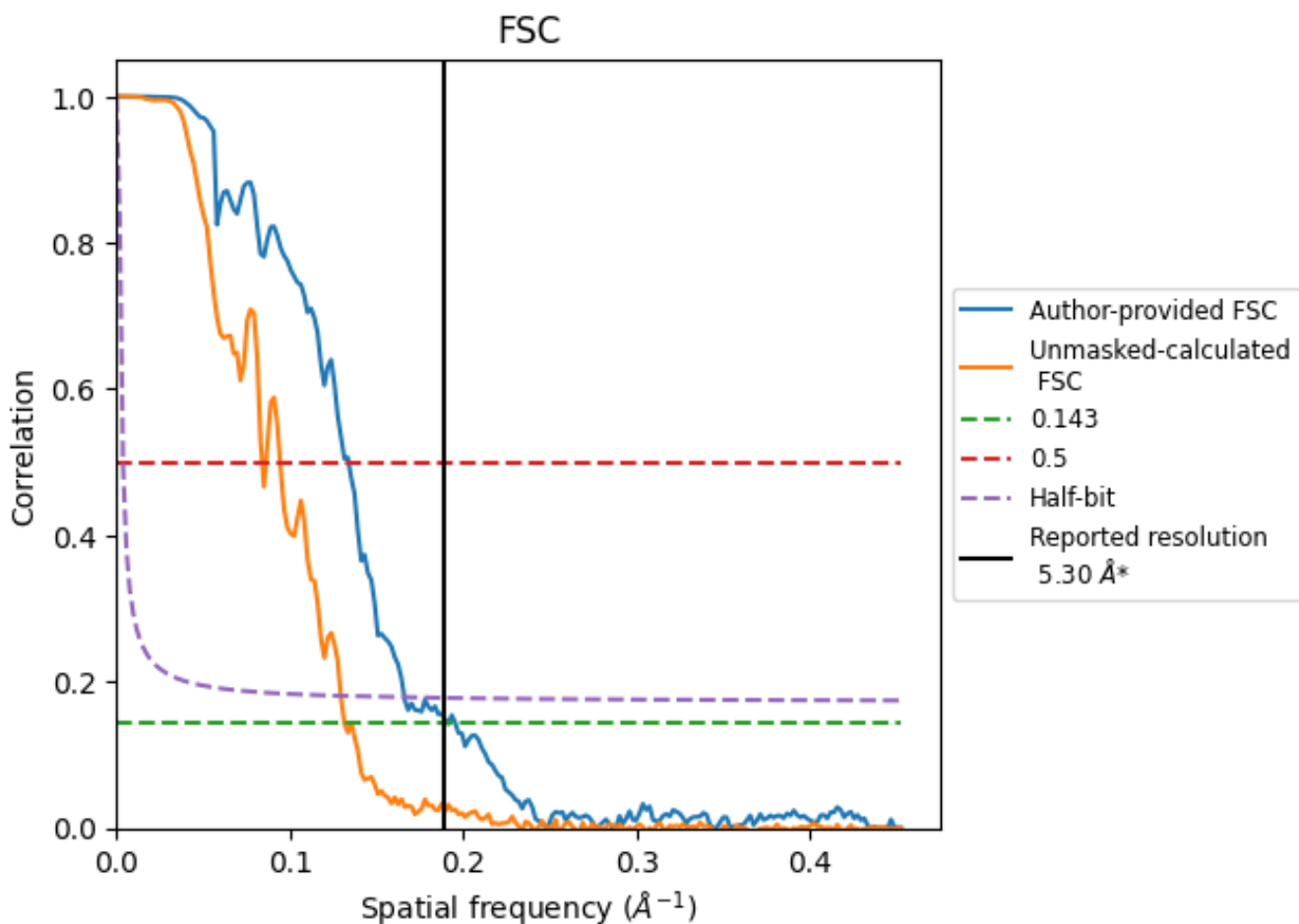


*Reported resolution corresponds to spatial frequency of 0.189 Å⁻¹

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 0.189 Å⁻¹

8.2 Resolution estimates

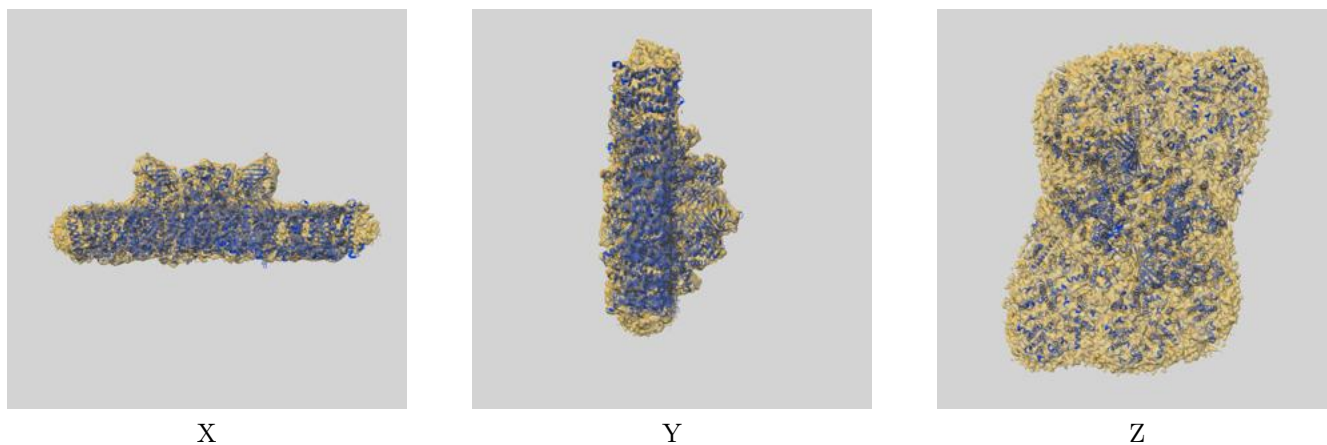
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.23	7.47	6.02
Unmasked-calculated*	7.60	11.90	7.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.60 differs from the reported value 5.3 by more than 10 %

9 Map-model fit [i](#)

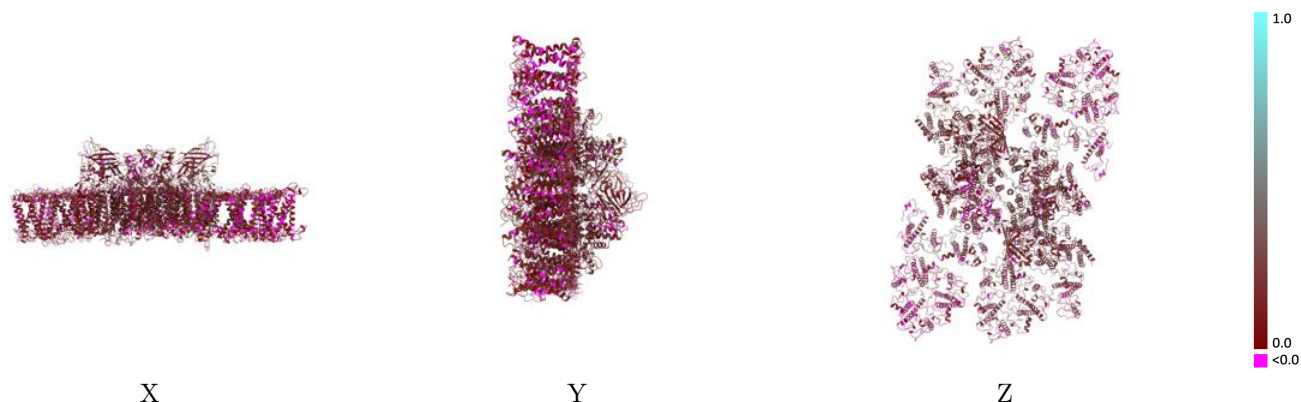
This section contains information regarding the fit between EMDB map EMD-3491 and PDB model 5MDX. Per-residue inclusion information can be found in section [3](#) on page [34](#).

9.1 Map-model overlay [i](#)



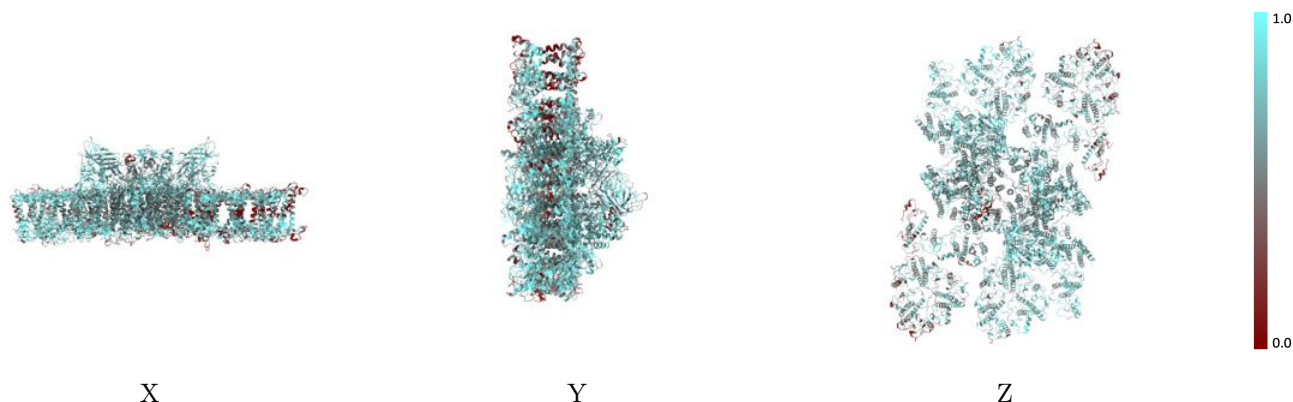
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



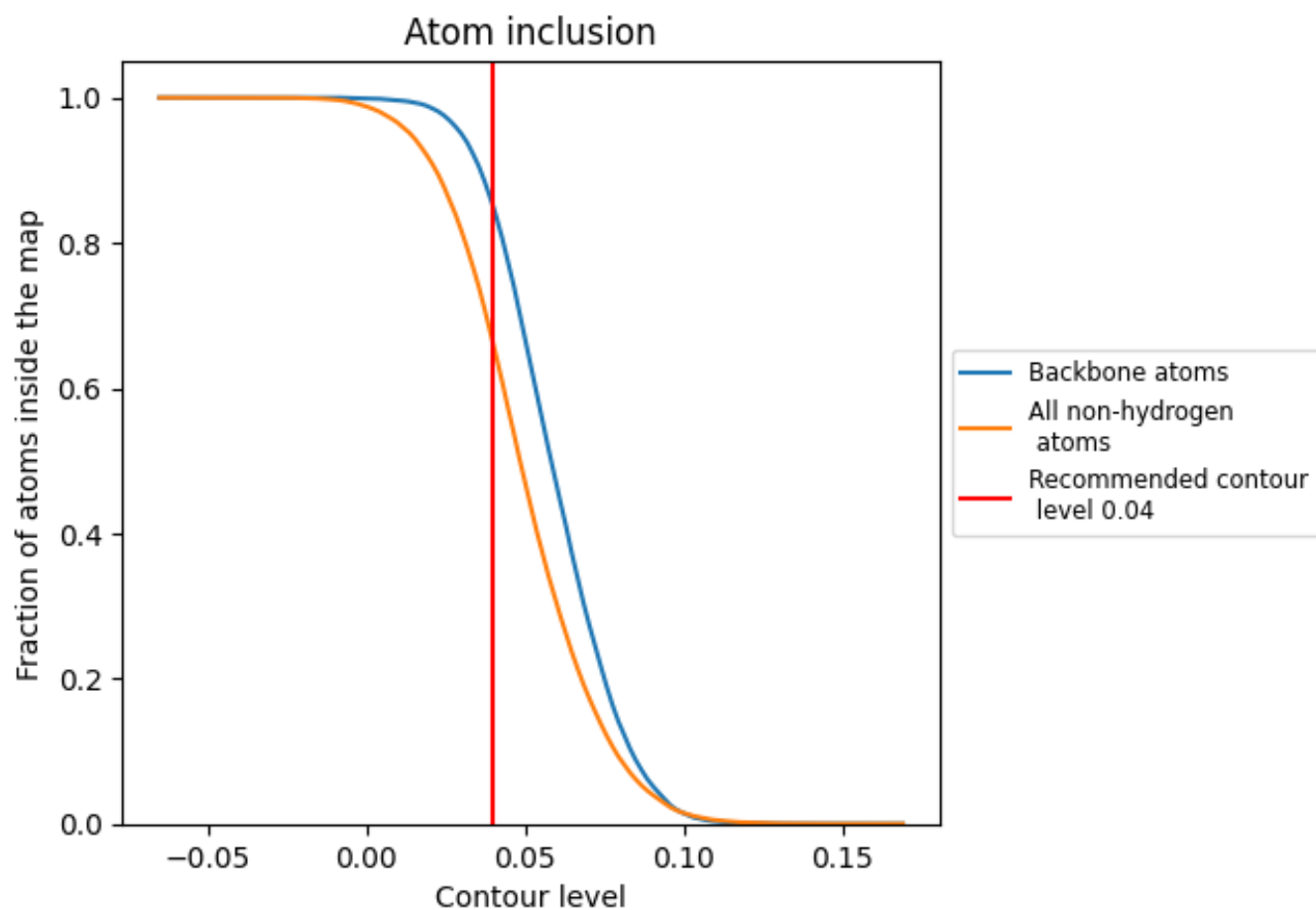
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 66% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6598	 0.1630
1	 0.6194	 0.1070
2	 0.5794	 0.1060
3	 0.5535	 0.0770
4	 0.5144	 0.1140
5	 0.6194	 0.1080
6	 0.5794	 0.1060
7	 0.5535	 0.0780
8	 0.5144	 0.1150
A	 0.6302	 0.2030
B	 0.6971	 0.1970
C	 0.7379	 0.2150
D	 0.6566	 0.2030
E	 0.6984	 0.1580
F	 0.7397	 0.1420
G	 0.7097	 0.1470
H	 0.7057	 0.2160
I	 0.5872	 0.1800
K	 0.6736	 0.2180
L	 0.6330	 0.1940
M	 0.5867	 0.1950
N	 0.7540	 0.1700
O	 0.7247	 0.2070
R	 0.6523	 0.1620
S	 0.7371	 0.1660
T	 0.5424	 0.1940
W	 0.6512	 0.2050
X	 0.6062	 0.1600
Y	 0.7029	 0.1760
Z	 0.6689	 0.1580
a	 0.6504	 0.2110
b	 0.5831	 0.1220
c	 0.7455	 0.2260
d	 0.6656	 0.2030
e	 0.7246	 0.1830



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Chain	Atom inclusion	Q-score
f	 0.6849	 0.1790
g	 0.7097	 0.1450
h	 0.6615	 0.1880
i	 0.5801	 0.1780
k	 0.6910	 0.2100
l	 0.6229	 0.1810
m	 0.5556	 0.1770
n	 0.7540	 0.1690
o	 0.7002	 0.1850
r	 0.6523	 0.1610
s	 0.7366	 0.1640
t	 0.5424	 0.2050
w	 0.6267	 0.2140
x	 0.5752	 0.1480
y	 0.7029	 0.1760
z	 0.6732	 0.1730