



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 09:41 AM UTC

PDB ID : 9K7V / pdb_00009k7v
EMDB ID : EMD-62153
Title : Structural insights into photosystem II supercomplex of a a siphonous green algae *Bryopsis corticulans* from intertidal zone
Authors : Liu, X.Y.; Wang, W.D.
Deposited on : 2024-10-24
Resolution : 3.07 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

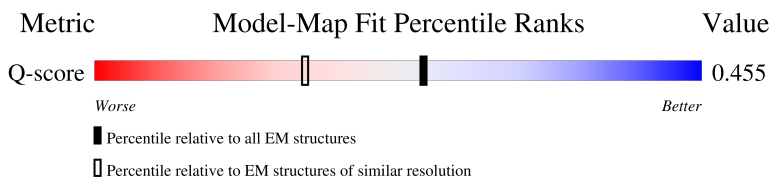
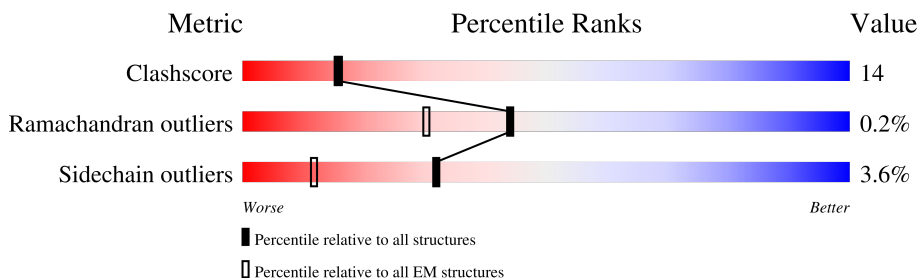
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 3.07 Å.

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







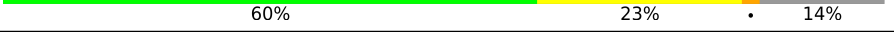


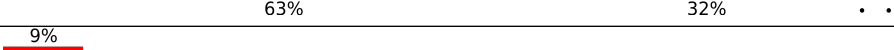
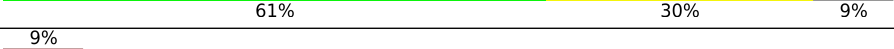

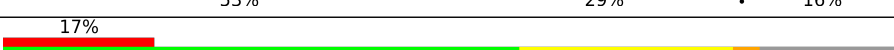
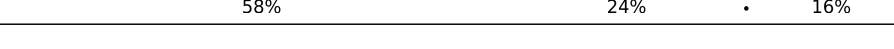



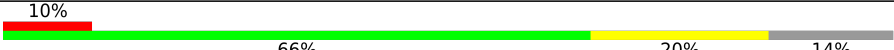



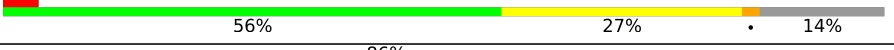





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	Z	62	
1	z	62	
2	E	82	
2	e	82	







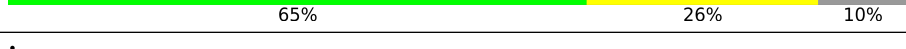

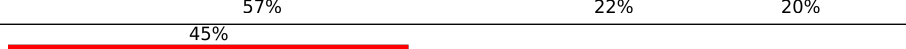
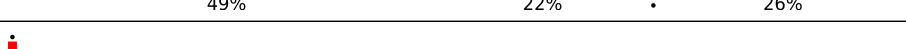




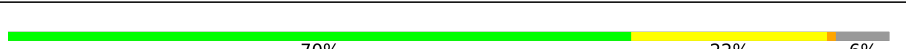





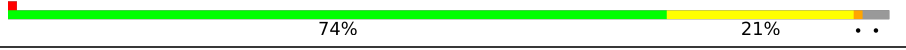
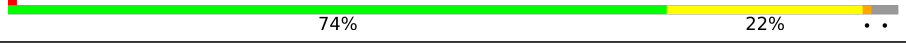



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Mol	Chain	Length	Quality of chain
3	H	75	
3	h	75	
4	I	36	
4	i	36	
5	K	43	
5	k	43	
6	L	38	
6	l	38	
7	M	33	
7	m	33	
8	R	267	
8	r	267	
9	F	42	
9	f	42	
10	1	212	
10	4	212	
11	2	256	
11	5	256	
12	3	254	
12	6	254	
12	7	254	
12	9	254	
12	p	254	
12	u	254	
13	S	308	

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Mol	Chain	Length	Quality of chain
13	s	308	
14	X	109	
14	x	109	
15	V	33	
15	v	33	
16	T	31	
16	t	31	
17	8	280	
17	G	280	
17	N	280	
17	Y	280	
17	g	280	
17	n	280	
17	q	280	
17	y	280	
18	B	508	
18	b	508	
19	A	327	
19	a	327	
20	C	461	
20	c	461	
21	D	352	
21	d	352	
22	W	118	
22	w	118	

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
24	CHL	1	304	X	-	-	-
24	CHL	1	305	X	-	-	-
24	CHL	1	308	X	-	-	-
24	CHL	1	309	X	-	-	-
24	CHL	1	310	X	-	-	-
24	CHL	1	311	X	-	-	-
24	CHL	1	312	X	-	-	-
24	CHL	1	317	X	-	-	-
24	CHL	2	305	X	-	-	-
24	CHL	2	306	X	-	-	-
24	CHL	2	309	X	-	-	-
24	CHL	2	310	X	-	-	-
24	CHL	2	311	X	-	-	-
24	CHL	2	312	X	-	-	-
24	CHL	2	313	X	-	-	-
24	CHL	2	318	X	-	-	-
24	CHL	3	304	X	-	-	-
24	CHL	3	305	X	-	-	-
24	CHL	3	308	X	-	-	-
24	CHL	3	309	X	-	-	-
24	CHL	3	310	X	-	-	-
24	CHL	3	311	X	-	-	-
24	CHL	3	312	X	-	-	-
24	CHL	3	317	X	-	-	-
24	CHL	4	304	X	-	-	-
24	CHL	4	305	X	-	-	-
24	CHL	4	308	X	-	-	-
24	CHL	4	309	X	-	-	-
24	CHL	4	310	X	-	-	-
24	CHL	4	311	X	-	-	-
24	CHL	4	312	X	-	-	-
24	CHL	4	317	X	-	-	-
24	CHL	5	305	X	-	-	-
24	CHL	5	306	X	-	-	-
24	CHL	5	309	X	-	-	-
24	CHL	5	310	X	-	-	-
24	CHL	5	311	X	-	-	-
24	CHL	5	312	X	-	-	-
24	CHL	5	313	X	-	-	-
24	CHL	5	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	6	304	X	-	-	-
24	CHL	6	305	X	-	-	-
24	CHL	6	308	X	-	-	-
24	CHL	6	309	X	-	-	-
24	CHL	6	310	X	-	-	-
24	CHL	6	311	X	-	-	-
24	CHL	6	312	X	-	-	-
24	CHL	6	317	X	-	-	-
24	CHL	7	305	X	-	-	-
24	CHL	7	306	X	-	-	-
24	CHL	7	309	X	-	-	-
24	CHL	7	310	X	-	-	-
24	CHL	7	311	X	-	-	-
24	CHL	7	312	X	-	-	-
24	CHL	7	313	X	-	-	-
24	CHL	7	318	X	-	-	-
24	CHL	8	303	X	-	-	-
24	CHL	8	304	X	-	-	-
24	CHL	8	307	X	-	-	-
24	CHL	8	308	X	-	-	-
24	CHL	8	309	X	-	-	-
24	CHL	8	310	X	-	-	-
24	CHL	8	315	X	-	-	-
24	CHL	9	304	X	-	-	-
24	CHL	9	305	X	-	-	-
24	CHL	9	308	X	-	-	-
24	CHL	9	309	X	-	-	-
24	CHL	9	310	X	-	-	-
24	CHL	9	311	X	-	-	-
24	CHL	9	312	X	-	-	-
24	CHL	9	317	X	-	-	-
24	CHL	G	305	X	-	-	-
24	CHL	G	306	X	-	-	-
24	CHL	G	309	X	-	-	-
24	CHL	G	310	X	-	-	-
24	CHL	G	311	X	-	-	-
24	CHL	G	312	X	-	-	-
24	CHL	G	313	X	-	-	-
24	CHL	G	318	X	-	-	-
24	CHL	N	304	X	-	-	-
24	CHL	N	305	X	-	-	-
24	CHL	N	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	N	309	X	-	-	-
24	CHL	N	310	X	-	-	-
24	CHL	N	311	X	-	-	-
24	CHL	N	312	X	-	-	-
24	CHL	N	317	X	-	-	-
24	CHL	R	601	X	-	-	-
24	CHL	R	602	X	-	-	-
24	CHL	R	605	X	-	-	-
24	CHL	R	606	X	-	-	-
24	CHL	R	607	X	-	-	-
24	CHL	R	608	X	-	-	-
24	CHL	S	601	X	-	-	-
24	CHL	S	602	X	-	-	-
24	CHL	S	605	X	-	-	-
24	CHL	S	606	X	-	-	-
24	CHL	S	607	X	-	-	-
24	CHL	S	608	X	-	-	-
24	CHL	S	613	X	-	-	-
24	CHL	Y	304	X	-	-	-
24	CHL	Y	305	X	-	-	-
24	CHL	Y	308	X	-	-	-
24	CHL	Y	309	X	-	-	-
24	CHL	Y	310	X	-	-	-
24	CHL	Y	311	X	-	-	-
24	CHL	Y	312	X	-	-	-
24	CHL	Y	317	X	-	-	-
24	CHL	Y	319	X	-	-	-
24	CHL	g	305	X	-	-	-
24	CHL	g	306	X	-	-	-
24	CHL	g	309	X	-	-	-
24	CHL	g	310	X	-	-	-
24	CHL	g	311	X	-	-	-
24	CHL	g	312	X	-	-	-
24	CHL	g	313	X	-	-	-
24	CHL	g	318	X	-	-	-
24	CHL	n	304	X	-	-	-
24	CHL	n	305	X	-	-	-
24	CHL	n	308	X	-	-	-
24	CHL	n	309	X	-	-	-
24	CHL	n	310	X	-	-	-
24	CHL	n	311	X	-	-	-
24	CHL	n	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	n	317	X	-	-	-
24	CHL	p	305	X	-	-	-
24	CHL	p	306	X	-	-	-
24	CHL	p	309	X	-	-	-
24	CHL	p	310	X	-	-	-
24	CHL	p	311	X	-	-	-
24	CHL	p	312	X	-	-	-
24	CHL	p	313	X	-	-	-
24	CHL	p	318	X	-	-	-
24	CHL	q	303	X	-	-	-
24	CHL	q	304	X	-	-	-
24	CHL	q	307	X	-	-	-
24	CHL	q	308	X	-	-	-
24	CHL	q	309	X	-	-	-
24	CHL	q	310	X	-	-	-
24	CHL	q	311	X	-	-	-
24	CHL	q	316	X	-	-	-
24	CHL	r	302	X	-	-	-
24	CHL	r	303	X	-	-	-
24	CHL	r	306	X	-	-	-
24	CHL	r	307	X	-	-	-
24	CHL	r	308	X	-	-	-
24	CHL	r	309	X	-	-	-
24	CHL	s	402	X	-	-	-
24	CHL	s	403	X	-	-	-
24	CHL	s	406	X	-	-	-
24	CHL	s	407	X	-	-	-
24	CHL	s	408	X	-	-	-
24	CHL	s	409	X	-	-	-
24	CHL	s	414	X	-	-	-
24	CHL	u	305	X	-	-	-
24	CHL	u	306	X	-	-	-
24	CHL	u	309	X	-	-	-
24	CHL	u	310	X	-	-	-
24	CHL	u	311	X	-	-	-
24	CHL	u	312	X	-	-	-
24	CHL	u	313	X	-	-	-
24	CHL	u	318	X	-	-	-
24	CHL	y	305	X	-	-	-
24	CHL	y	306	X	-	-	-
24	CHL	y	309	X	-	-	-
24	CHL	y	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	y	311	X	-	-	-
24	CHL	y	312	X	-	-	-
24	CHL	y	313	X	-	-	-
24	CHL	y	318	X	-	-	-
25	CLA	1	306	X	-	-	-
25	CLA	1	307	X	-	-	-
25	CLA	1	313	X	-	-	-
25	CLA	1	314	X	-	-	-
25	CLA	1	315	X	-	-	-
25	CLA	1	316	X	-	-	-
25	CLA	2	307	X	-	-	-
25	CLA	2	308	X	-	-	-
25	CLA	2	314	X	-	-	-
25	CLA	2	315	X	-	-	-
25	CLA	2	316	X	-	-	-
25	CLA	2	317	X	-	-	-
25	CLA	3	306	X	-	-	-
25	CLA	3	307	X	-	-	-
25	CLA	3	313	X	-	-	-
25	CLA	3	314	X	-	-	-
25	CLA	3	315	X	-	-	-
25	CLA	3	316	X	-	-	-
25	CLA	4	306	X	-	-	-
25	CLA	4	307	X	-	-	-
25	CLA	4	313	X	-	-	-
25	CLA	4	314	X	-	-	-
25	CLA	4	315	X	-	-	-
25	CLA	4	316	X	-	-	-
25	CLA	5	307	X	-	-	-
25	CLA	5	308	X	-	-	-
25	CLA	5	314	X	-	-	-
25	CLA	5	315	X	-	-	-
25	CLA	5	316	X	-	-	-
25	CLA	5	317	X	-	-	-
25	CLA	6	306	X	-	-	-
25	CLA	6	307	X	-	-	-
25	CLA	6	313	X	-	-	-
25	CLA	6	314	X	-	-	-
25	CLA	6	315	X	-	-	-
25	CLA	6	316	X	-	-	-
25	CLA	7	307	X	-	-	-
25	CLA	7	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	7	314	X	-	-	-
25	CLA	7	315	X	-	-	-
25	CLA	7	316	X	-	-	-
25	CLA	7	317	X	-	-	-
25	CLA	8	305	X	-	-	-
25	CLA	8	306	X	-	-	-
25	CLA	8	311	X	-	-	-
25	CLA	8	312	X	-	-	-
25	CLA	8	313	X	-	-	-
25	CLA	8	314	X	-	-	-
25	CLA	9	306	X	-	-	-
25	CLA	9	307	X	-	-	-
25	CLA	9	313	X	-	-	-
25	CLA	9	314	X	-	-	-
25	CLA	9	315	X	-	-	-
25	CLA	9	316	X	-	-	-
25	CLA	A	603	X	-	-	-
25	CLA	A	604	X	-	-	-
25	CLA	A	605	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	610	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	601	X	-	-	-
25	CLA	C	602	X	-	-	-
25	CLA	C	603	X	-	-	-
25	CLA	C	604	X	-	-	-
25	CLA	C	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	606	X	-	-	-
25	CLA	C	607	X	-	-	-
25	CLA	C	608	X	-	-	-
25	CLA	C	609	X	-	-	-
25	CLA	C	610	X	-	-	-
25	CLA	C	611	X	-	-	-
25	CLA	C	612	X	-	-	-
25	CLA	C	616	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	G	307	X	-	-	-
25	CLA	G	308	X	-	-	-
25	CLA	G	314	X	-	-	-
25	CLA	G	315	X	-	-	-
25	CLA	G	316	X	-	-	-
25	CLA	G	317	X	-	-	-
25	CLA	N	306	X	-	-	-
25	CLA	N	307	X	-	-	-
25	CLA	N	313	X	-	-	-
25	CLA	N	314	X	-	-	-
25	CLA	N	315	X	-	-	-
25	CLA	N	316	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	609	X	-	-	-
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	612	X	-	-	-
25	CLA	R	613	X	-	-	-
25	CLA	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	609	X	-	-	-
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	612	X	-	-	-
25	CLA	S	616	X	-	-	-
25	CLA	Y	306	X	-	-	-
25	CLA	Y	307	X	-	-	-
25	CLA	Y	313	X	-	-	-
25	CLA	Y	314	X	-	-	-
25	CLA	Y	315	X	-	-	-
25	CLA	Y	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	a	603	X	-	-	-
25	CLA	a	604	X	-	-	-
25	CLA	a	605	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	601	X	-	-	-
25	CLA	c	602	X	-	-	-
25	CLA	c	603	X	-	-	-
25	CLA	c	604	X	-	-	-
25	CLA	c	605	X	-	-	-
25	CLA	c	606	X	-	-	-
25	CLA	c	607	X	-	-	-
25	CLA	c	608	X	-	-	-
25	CLA	c	609	X	-	-	-
25	CLA	c	610	X	-	-	-
25	CLA	c	611	X	-	-	-
25	CLA	c	612	X	-	-	-
25	CLA	c	616	X	-	-	-
25	CLA	d	404	X	-	-	-
25	CLA	d	405	X	-	-	-
25	CLA	g	307	X	-	-	-
25	CLA	g	308	X	-	-	-
25	CLA	g	314	X	-	-	-
25	CLA	g	315	X	-	-	-
25	CLA	g	316	X	-	-	-
25	CLA	g	317	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	n	306	X	-	-	-
25	CLA	n	307	X	-	-	-
25	CLA	n	313	X	-	-	-
25	CLA	n	314	X	-	-	-
25	CLA	n	315	X	-	-	-
25	CLA	n	316	X	-	-	-
25	CLA	p	307	X	-	-	-
25	CLA	p	308	X	-	-	-
25	CLA	p	314	X	-	-	-
25	CLA	p	315	X	-	-	-
25	CLA	p	316	X	-	-	-
25	CLA	p	317	X	-	-	-
25	CLA	q	305	X	-	-	-
25	CLA	q	306	X	-	-	-
25	CLA	q	312	X	-	-	-
25	CLA	q	313	X	-	-	-
25	CLA	q	314	X	-	-	-
25	CLA	q	315	X	-	-	-
25	CLA	r	304	X	-	-	-
25	CLA	r	305	X	-	-	-
25	CLA	r	310	X	-	-	-
25	CLA	r	311	X	-	-	-
25	CLA	r	312	X	-	-	-
25	CLA	r	313	X	-	-	-
25	CLA	r	314	X	-	-	-
25	CLA	s	404	X	-	-	-
25	CLA	s	405	X	-	-	-
25	CLA	s	410	X	-	-	-
25	CLA	s	411	X	-	-	-
25	CLA	s	412	X	-	-	-
25	CLA	s	413	X	-	-	-
25	CLA	s	417	X	-	-	-
25	CLA	u	307	X	-	-	-
25	CLA	u	308	X	-	-	-
25	CLA	u	314	X	-	-	-
25	CLA	u	315	X	-	-	-
25	CLA	u	316	X	-	-	-
25	CLA	u	317	X	-	-	-
25	CLA	y	307	X	-	-	-
25	CLA	y	308	X	-	-	-
25	CLA	y	314	X	-	-	-
25	CLA	y	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	y	316	X	-	-	-
25	CLA	y	317	X	-	-	-
28	NEX	1	303	-	-	X	-
28	NEX	3	318	-	-	X	-
28	NEX	4	303	-	-	X	-
28	NEX	6	303	-	-	X	-
28	NEX	7	304	-	-	X	-
28	NEX	G	304	-	-	X	-
28	NEX	S	617	-	-	X	-
28	NEX	p	304	-	-	X	-
28	NEX	s	401	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 95298 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 reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	61	Total	C	N	O	S	0	0
			472	329	68	74	1		
1	z	61	Total	C	N	O	S	0	0
			472	329	68	74	1		

- Molecule 2 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	65	Total	C	N	O	0	0
			530	347	87	96		
2	e	65	Total	C	N	O	0	0
			530	347	87	96		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	68	Total	C	N	O	S	0	0
			513	337	74	98	4		
3	h	68	Total	C	N	O	S	0	0
			513	337	74	98	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	34	Total	C	N	O	S	0	0
			275	189	40	45	1		
4	i	34	Total	C	N	O	S	0	0
			275	189	40	45	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	26	ASP	ASN	conflict	UNP A0A2P0QH95

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Chain	Residue	Modelled	Actual	Comment	Reference
i	26	ASP	ASN	conflict	UNP A0A2P0QH95

- Molecule 5 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	37	Total	C	N	O	0	0
			299	208	43	48		
5	k	37	Total	C	N	O	0	0
			299	208	43	48		

- Molecule 6 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	37	Total	C	N	O	0	0
			304	204	48	52		
6	l	37	Total	C	N	O	0	0
			304	204	48	52		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	30	Total	C	N	O	0	0
			231	159	33	39		
7	m	30	Total	C	N	O	0	0
			231	159	33	39		

- Molecule 8 is a protein called PsbR.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	225	Total	C	N	O	S	0	0
			1711	1092	284	326	9		
8	r	225	Total	C	N	O	S	0	0
			1707	1089	283	326	9		

- Molecule 9 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	31	Total	C	N	O	S	0	0
			246	167	40	38	1		
9	f	31	Total	C	N	O	S	0	0
			251	170	42	38	1		

- Molecule 10 is a protein called Lhcb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	212	Total	C	N	O	S	0	0
			1609	1038	255	306	10		
10	4	212	Total	C	N	O	S	0	0
			1603	1035	252	306	10		

- Molecule 11 is a protein called Lhcb2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	221	Total	C	N	O	S	0	0
			1710	1108	278	316	8		
11	5	221	Total	C	N	O	S	0	0
			1711	1109	279	315	8		

- Molecule 12 is a protein called Lhcb3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	211	Total	C	N	O	S	0	0
			1606	1033	260	304	9		
12	9	219	Total	C	N	O	S	0	0
			1680	1081	271	319	9		
12	6	219	Total	C	N	O	S	0	0
			1670	1073	271	317	9		
12	u	219	Total	C	N	O	S	0	0
			1683	1084	271	319	9		
12	p	219	Total	C	N	O	S	0	0
			1680	1081	271	319	9		
12	7	219	Total	C	N	O	S	0	0
			1677	1080	271	317	9		

- Molecule 13 is a protein called LhcbS.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	249	Total	C	N	O	S	0	0
			1867	1203	309	349	6		
13	s	249	Total	C	N	O	S	0	0
			1867	1203	309	349	6		

- Molecule 14 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	34	Total	C	N	O	0	0
			226	146	36	44		
14	x	34	Total	C	N	O	0	0
			226	146	36	44		

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	25	Total	C	N	O	0	0
			179	118	30	31		
15	v	25	Total	C	N	O	0	0
			179	118	30	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	28	Total	C	N	O	S	0	0
			236	165	34	36	1		
16	t	28	Total	C	N	O	S	0	0
			236	165	34	36	1		

- Molecule 17 is a protein called LhcbG.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		
17	N	206	Total	C	N	O	S	0	0
			1551	1002	247	292	10		
17	Y	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		
17	8	206	Total	C	N	O	S	0	0
			1554	1005	247	292	10		
17	g	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		
17	n	206	Total	C	N	O	S	0	0
			1545	998	247	290	10		
17	y	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		
17	q	206	Total	C	N	O	S	0	0
			1554	1005	247	292	10		

- Molecule 18 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	478	Total	C	N	O	S	0	0
			3737	2447	625	652	13		
18	b	478	Total	C	N	O	S	0	0
			3737	2447	625	652	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	281	ALA	SER	conflict	UNP A0A0D6E1D0
B	353	GLU	GLN	conflict	UNP A0A0D6E1D0
B	355	HIS	TYR	conflict	UNP A0A0D6E1D0
b	281	ALA	SER	conflict	UNP A0A0D6E1D0
b	353	GLU	GLN	conflict	UNP A0A0D6E1D0
b	355	HIS	TYR	conflict	UNP A0A0D6E1D0

- Molecule 19 is a protein called PsbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	327	Total	C	N	O	S	0	0
			2558	1669	422	453	14		
19	a	327	Total	C	N	O	S	0	0
			2558	1669	422	453	14		

- Molecule 20 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	448	Total	C	N	O	S	0	0
			3472	2281	581	599	11		
20	c	448	Total	C	N	O	S	0	0
			3472	2281	581	599	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	VAL	MET	conflict	UNP D0EVT6
c	1	VAL	MET	conflict	UNP D0EVT6

- Molecule 21 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	340	Total	C	N	O	S	0	0
			2719	1803	447	458	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	340	Total	C	N	O	S	0	0
			2719	1803	447	458	11		

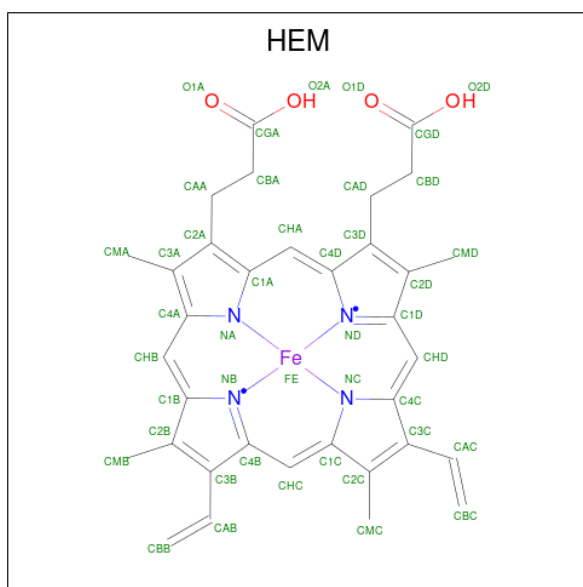
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	55	ILE	VAL	conflict	UNP A0A0B5GKA5
d	55	ILE	VAL	conflict	UNP A0A0B5GKA5

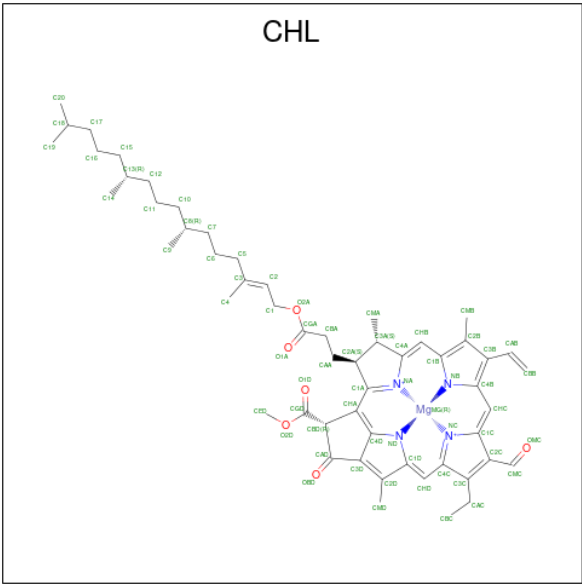
- Molecule 22 is a protein called PsbW.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	43	Total	C	N	O	0	0
			304	191	49	64		
22	w	43	Total	C	N	O	0	0
			304	191	49	64		

- Molecule 23 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	R	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	2	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	2	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	2	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	2	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	2	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	3	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	3	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	3	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	3	1	Total 51	C 40	Mg 1	N 4	O 6	0
24	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	3	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	3	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	3	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 58	C 47	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	S	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	G	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	G	1	Total 54	C 43	Mg 1	N 4	O 6	0
24	G	1	Total 51	C 40	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	9	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	9	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	9	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	9	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	9	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	N	1	Total 54	C 43	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	N	1	Total 60	C 49	Mg 1	N 4	O 6	0
24	N	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	N	1	Total 53	C 42	Mg 1	N 4	O 6	0
24	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	N	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	N	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	Y	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	Y	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	Y	1	Total 54	C 43	Mg 1	N 4	O 6	0
24	Y	1	Total 51	C 40	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	Y	1	Total 53	C 42	Mg 1	N 4	O 6	0
24	8	1	Total 54	C 43	Mg 1	N 4	O 6	0
24	8	1	Total 60	C 49	Mg 1	N 4	O 6	0
24	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	8	1	Total 50	C 39	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	8	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	4	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	4	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	4	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	5	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	5	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	5	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	5	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	5	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	5	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	5	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	6	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	6	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	6	1	Total 43	C 34	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	g	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	n	1	Total 54	C 43	Mg 1	N 4	O 6	0
24	n	1	Total 60	C 49	Mg 1	N 4	O 6	0
24	n	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	n	1	Total 53	C 42	Mg 1	N 4	O 6	0
24	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	n	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	n	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	y	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	y	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	y	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	y	1	Total 54	C 43	Mg 1	N 4	O 6	0
24	y	1	Total 51	C 40	Mg 1	N 4	O 6	0
24	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	y	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	p	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	p	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	p	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	p	1	Total 46	C 35	Mg 1	N 4	O 6	0

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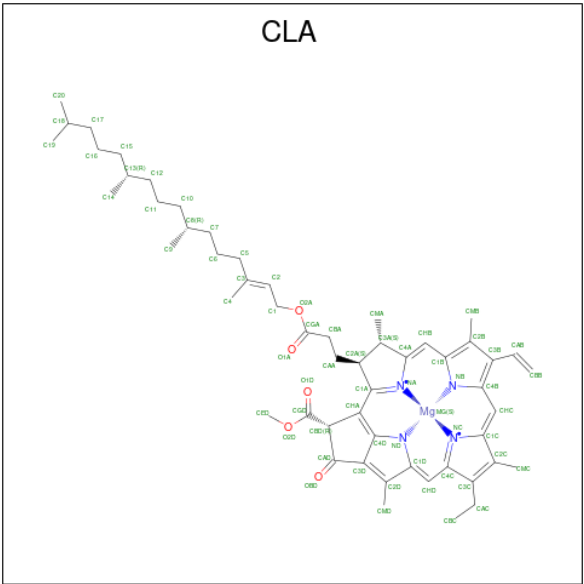
Mol	Chain	Residues	Atoms					AltConf
24	p	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	p	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	p	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	q	1	Total 54	C 43	Mg 1	N 4	O 6	0
24	q	1	Total 60	C 49	Mg 1	N 4	O 6	0
24	q	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	q	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	q	1	Total 53	C 42	Mg 1	N 4	O 6	0
24	q	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	q	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	q	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	s	1	Total 58	C 47	Mg 1	N 4	O 6	0
24	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	s	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	s	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	r	1	Total 47	C 36	Mg 1	N 4	O 6	0
24	r	1	Total 42	C 33	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	9	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	9	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	9	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	N	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	N	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	Y	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	Y	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	8	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	8	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	C	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	4	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	5	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	5	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	5	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	5	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	6	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	g	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	u	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	u	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	u	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	u	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	n	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	n	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	n	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	y	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	y	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	y	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	y	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	p	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	p	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	q	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	q	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	q	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	q	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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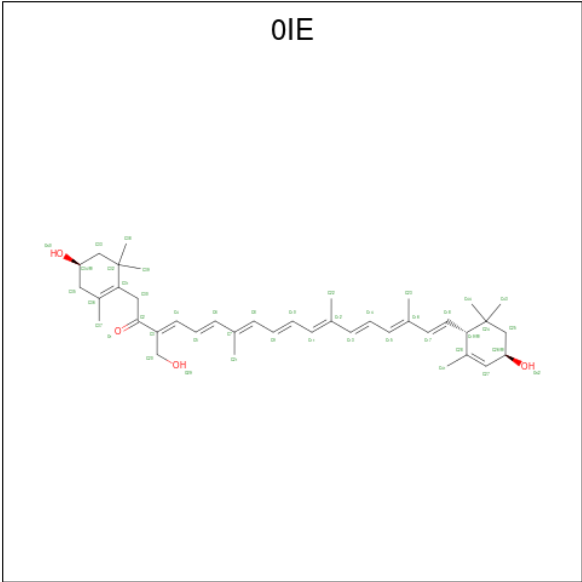
Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	a	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	c	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 26 is Siphonaxanthin (CCD ID: 0IE) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



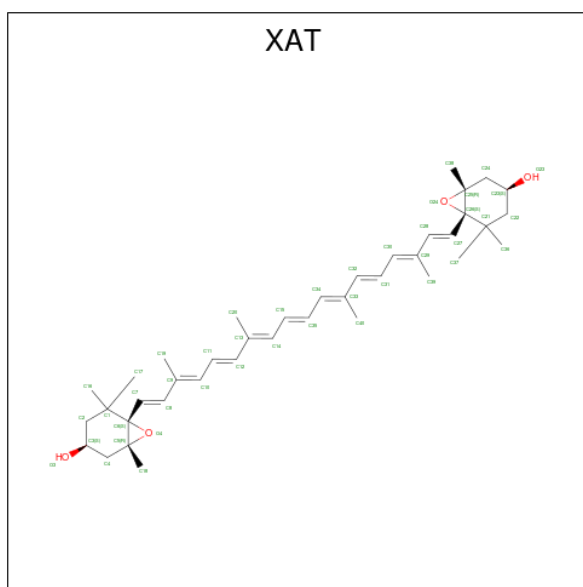
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26	R	1	Total	C	O	0
			44	40	4	
26	1	1	Total	C	O	0
			44	40	4	
26	2	1	Total	C	O	0
			44	40	4	
26	2	1	Total	C	O	0
			44	40	4	
26	3	1	Total	C	O	0
			43	39	4	
26	3	1	Total	C	O	0
			44	40	4	
26	G	1	Total	C	O	0
			44	40	4	
26	G	1	Total	C	O	0
			44	40	4	
26	9	1	Total	C	O	0
			44	40	4	
26	9	1	Total	C	O	0
			44	40	4	
26	N	1	Total	C	O	0
			44	40	4	
26	Y	1	Total	C	O	0
			44	40	4	
26	Y	1	Total	C	O	0
			44	40	4	
26	8	1	Total	C	O	0
			44	40	4	

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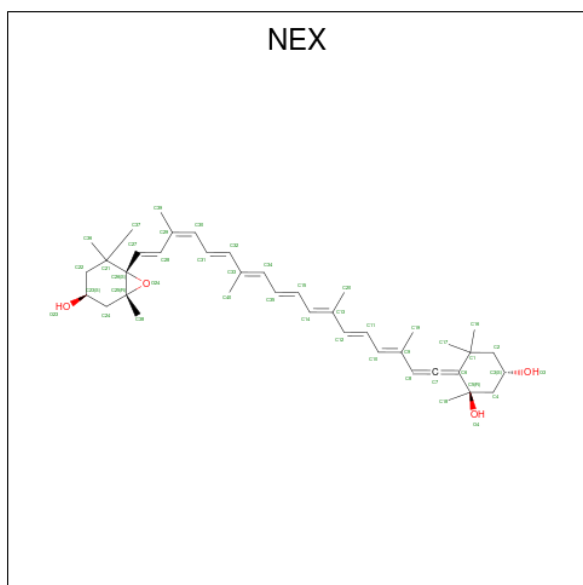
Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total	C	O	0
			44	40	4	
26	5	1	Total	C	O	0
			44	40	4	
26	5	1	Total	C	O	0
			44	40	4	
26	6	1	Total	C	O	0
			43	39	4	
26	g	1	Total	C	O	0
			44	40	4	
26	g	1	Total	C	O	0
			44	40	4	
26	u	1	Total	C	O	0
			44	40	4	
26	u	1	Total	C	O	0
			44	40	4	
26	n	1	Total	C	O	0
			44	40	4	
26	y	1	Total	C	O	0
			44	40	4	
26	y	1	Total	C	O	0
			44	40	4	
26	p	1	Total	C	O	0
			44	40	4	
26	p	1	Total	C	O	0
			44	40	4	
26	q	1	Total	C	O	0
			44	40	4	
26	r	1	Total	C	O	0
			44	40	4	
26	7	1	Total	C	O	0
			44	40	4	
26	7	1	Total	C	O	0
			44	40	4	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



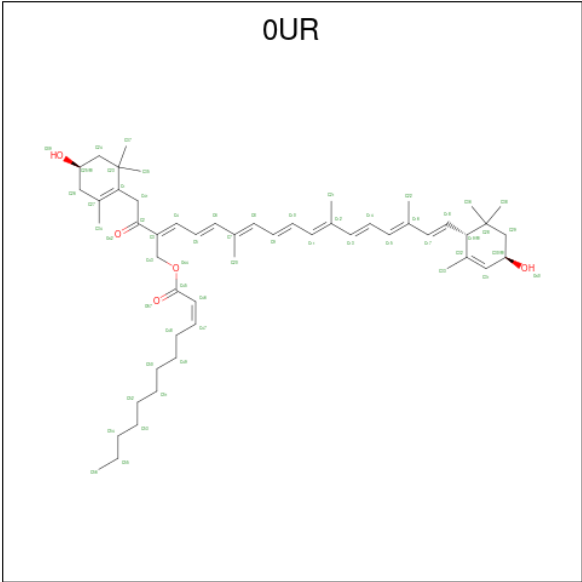
Mol	Chain	Residues	Atoms			AltConf
27	R	1	Total	C	O	0
			44	40	4	
27	r	1	Total	C	O	0
			44	40	4	

- Molecule 28 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	R	1	Total 44	C 40	O 4	0
28	1	1	Total 44	C 40	O 4	0
28	2	1	Total 44	C 40	O 4	0
28	3	1	Total 44	C 40	O 4	0
28	S	1	Total 44	C 40	O 4	0
28	G	1	Total 44	C 40	O 4	0
28	9	1	Total 44	C 40	O 4	0
28	N	1	Total 44	C 40	O 4	0
28	4	1	Total 44	C 40	O 4	0
28	5	1	Total 44	C 40	O 4	0
28	6	1	Total 44	C 40	O 4	0
28	g	1	Total 44	C 40	O 4	0
28	u	1	Total 44	C 40	O 4	0
28	n	1	Total 44	C 40	O 4	0
28	y	1	Total 44	C 40	O 4	0
28	p	1	Total 44	C 40	O 4	0
28	s	1	Total 44	C 40	O 4	0
28	r	1	Total 44	C 40	O 4	0
28	r	1	Total 44	C 40	O 4	0
28	7	1	Total 44	C 40	O 4	0

- Molecule 29 is Siphonein (CCD ID: 0UR) (formula: C₅₂H₇₆O₅) (labeled as "Ligand of Interest" by depositor).



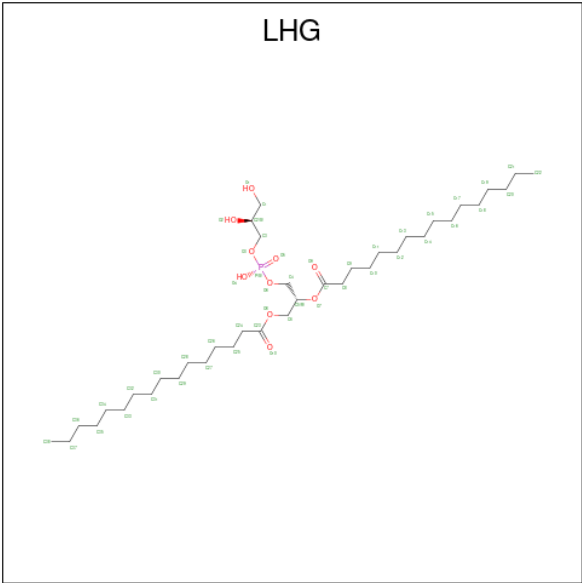
Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			52	47	5	
29	2	1	Total	C	O	0
			52	47	5	
29	3	1	Total	C	O	0
			52	47	5	
29	G	1	Total	C	O	0
			52	47	5	
29	9	1	Total	C	O	0
			52	47	5	
29	N	1	Total	C	O	0
			52	47	5	
29	Y	1	Total	C	O	0
			52	47	5	
29	8	1	Total	C	O	0
			52	47	5	
29	4	1	Total	C	O	0
			52	47	5	
29	5	1	Total	C	O	0
			52	47	5	
29	6	1	Total	C	O	0
			52	47	5	
29	g	1	Total	C	O	0
			52	47	5	
29	u	1	Total	C	O	0
			52	47	5	
29	n	1	Total	C	O	0
			52	47	5	

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Mol	Chain	Residues	Atoms			AltConf
29	y	1	Total	C	O	0
			52	47	5	
29	p	1	Total	C	O	0
			52	47	5	
29	q	1	Total	C	O	0
			52	47	5	
29	7	1	Total	C	O	0
			52	47	5	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	1	1	Total	C	O	P	0
			42	31	10	1	
30	2	1	Total	C	O	P	0
			40	29	10	1	
30	G	1	Total	C	O	P	0
			43	32	10	1	
30	9	1	Total	C	O	P	0
			43	32	10	1	
30	N	1	Total	C	O	P	0
			43	32	10	1	
30	Y	1	Total	C	O	P	0
			43	32	10	1	
30	A	1	Total	C	O	P	0
			45	34	10	1	

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Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			44	33	10	1	
30	C	1	Total	C	O	P	0
			32	21	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			39	28	10	1	
30	4	1	Total	C	O	P	0
			42	31	10	1	
30	5	1	Total	C	O	P	0
			43	32	10	1	
30	g	1	Total	C	O	P	0
			43	32	10	1	
30	n	1	Total	C	O	P	0
			43	32	10	1	
30	y	1	Total	C	O	P	0
			43	32	10	1	
30	p	1	Total	C	O	P	0
			43	32	10	1	
30	a	1	Total	C	O	P	0
			45	34	10	1	
30	a	1	Total	C	O	P	0
			44	33	10	1	
30	c	1	Total	C	O	P	0
			32	21	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			39	28	10	1	
30	7	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 31 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).

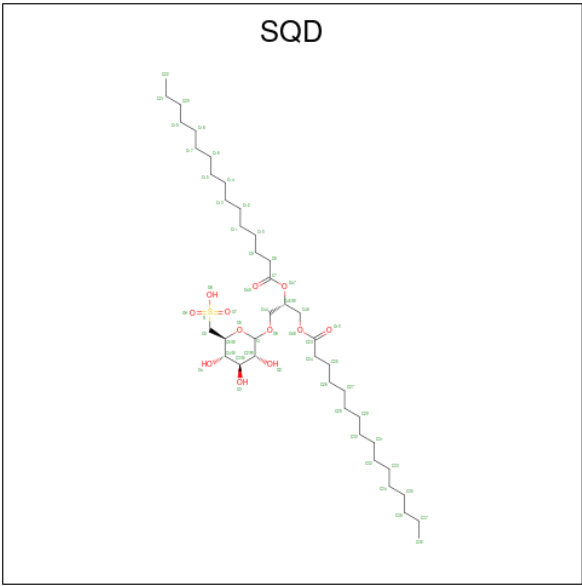


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Mol	Chain	Residues	Atoms	AltConf
31	b	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	s	1	Total C 40 40	0
31	s	1	Total C 40 40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



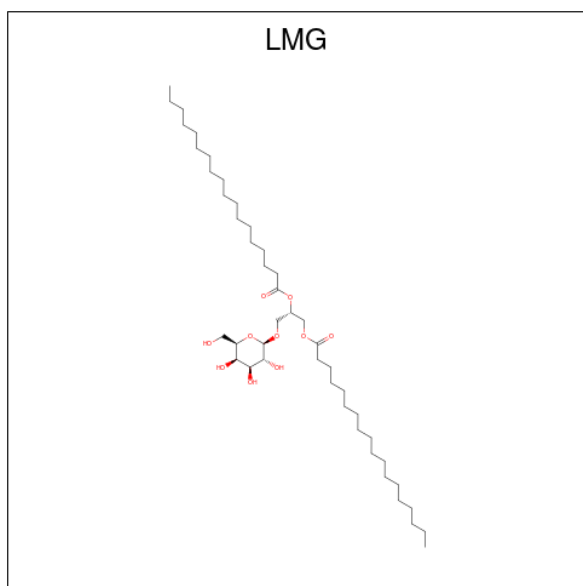
Mol	Chain	Residues	Atoms	AltConf
32	B	1	Total C O S 54 41 12 1	0
32	A	1	Total C O S 45 32 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
32	D	1	Total	C	O	S	0
			44	31	12	1	
32	b	1	Total	C	O	S	0
			54	41	12	1	
32	a	1	Total	C	O	S	0
			45	32	12	1	
32	d	1	Total	C	O	S	0
			44	31	12	1	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



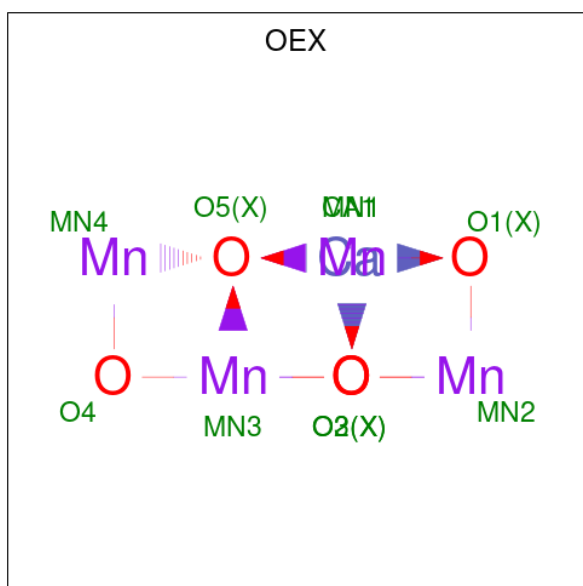
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O		0
			41	31	10		
33	C	1	Total	C	O		0
			42	32	10		
33	D	1	Total	C	O		0
			48	38	10		
33	D	1	Total	C	O		0
			46	36	10		
33	W	1	Total	C	O		0
			30	20	10		
33	i	1	Total	C	O		0
			48	38	10		
33	m	1	Total	C	O		0
			41	31	10		

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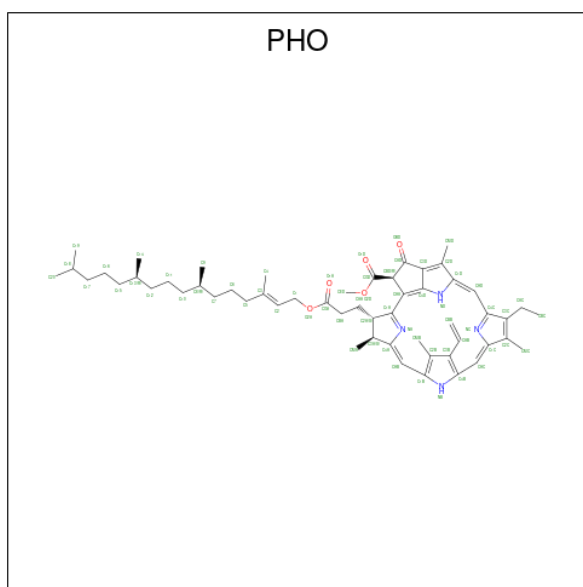
Mol	Chain	Residues	Atoms			AltConf
33	w	1	Total	C	O	0
			36	26	10	
33	d	1	Total	C	O	0
			48	38	10	
33	d	1	Total	C	O	0
			46	36	10	

- Molecule 34 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



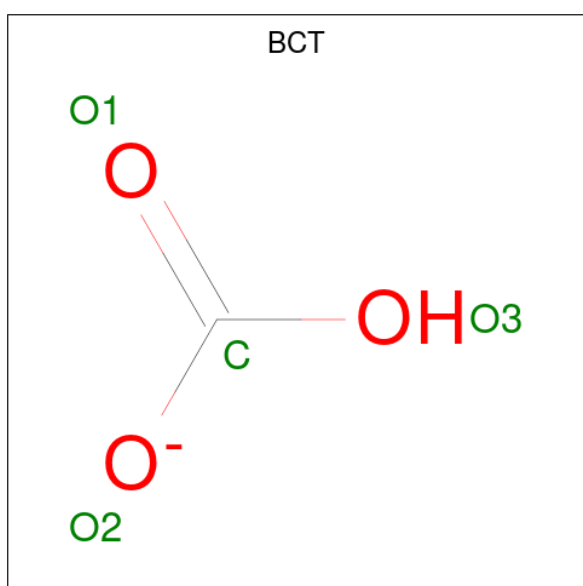
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
34	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 35 is PHEOPHYTIN A (CCD ID: PHO) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$) (labeled as "Ligand of Interest" by depositor).



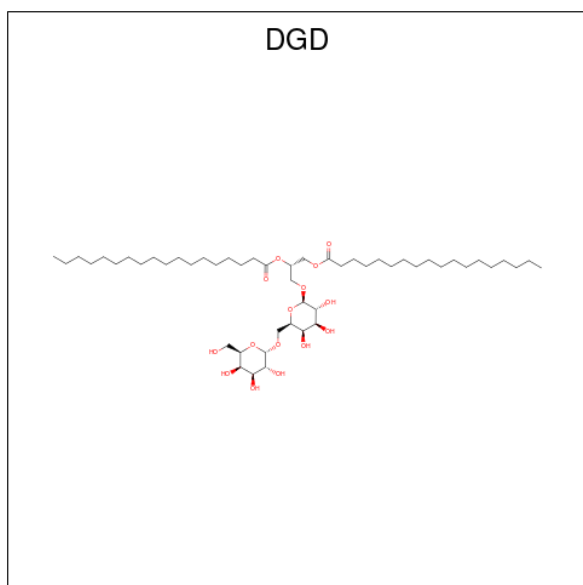
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			64	55	4	5	
35	D	1	Total	C	N	O	0
			64	55	4	5	
35	a	1	Total	C	N	O	0
			64	55	4	5	
35	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

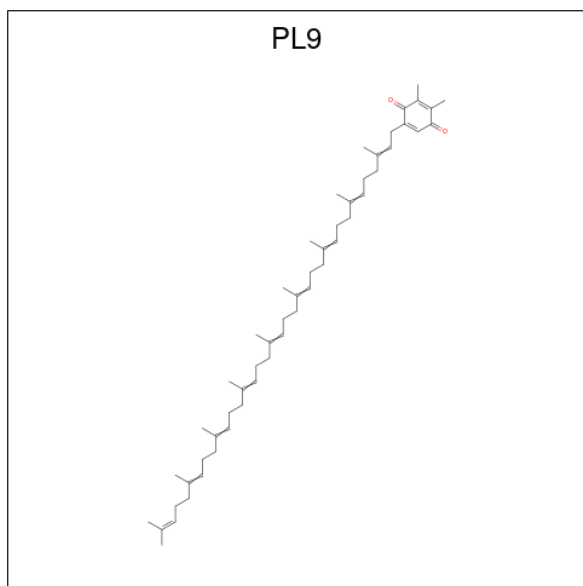


Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			50	35	15	
37	C	1	Total	C	O	0
			55	40	15	
37	c	1	Total	C	O	0
			50	35	15	
37	c	1	Total	C	O	0
			55	40	15	

- Molecule 38 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
38	D	1	Total	Fe	0
			1	1	
38	d	1	Total	Fe	0
			1	1	

- Molecule 39 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).




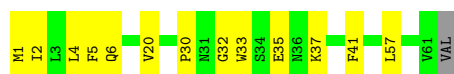
Mol	Chain	Residues	Atoms			AltConf
39	D	1	Total	C	O	0
			55	53	2	
39	d	1	Total	C	O	0
			55	53	2	

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 reaction center protein Z

Chain Z: 



- Molecule 1: Photosystem II reaction center protein Z

Chain z: 



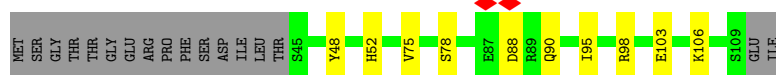
- Molecule 2: Cytochrome b559 subunit alpha

Chain E: 



- Molecule 2: Cytochrome b559 subunit alpha

Chain e: 

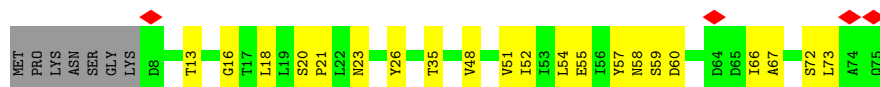


- Molecule 3: Photosystem II reaction center protein H

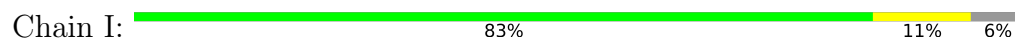
Chain H: 



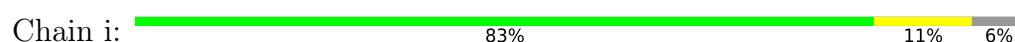
- Molecule 3: Photosystem II reaction center protein H



- Molecule 4: Photosystem II reaction center protein I



- Molecule 4: Photosystem II reaction center protein I



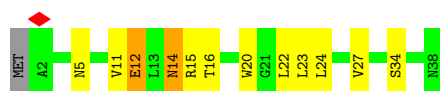
- Molecule 5: Photosystem II reaction center protein K



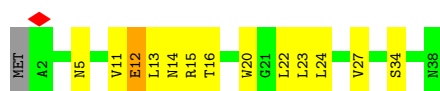
- Molecule 5: Photosystem II reaction center protein K



- Molecule 6: Photosystem II reaction center protein L



- Molecule 6: Photosystem II reaction center protein L



- Molecule 7: Photosystem II reaction center protein M

Chain M:

Chain m:

Chain R:

Chain r:

- Molecule 9: Cytochrome b559 subunit beta

Chain F:  55% 17% 26%

MET
ALA
SER
LYS
LYS
SER
SER
THR
TYR
PRO
I12
F13
T14
V15
R16
V25
P26
T35
R42

- Molecule 9: Cytochrome b559 subunit beta

Chain f:  55% 17% 26%


MET
ALA
SER
LYS
LYS
SER
SER
TYR
TYR
PRO
I12
F13
T14
V15
R16
V20
H21
V25
P26
R42

- Molecule 10: Lhcb1

Chain 1:  58% 68% 30%

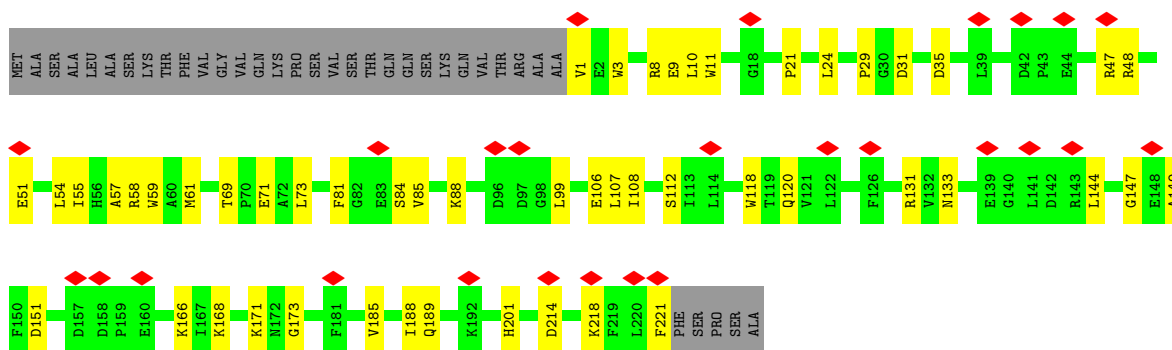
V1 E2 F3 Y4 G5 P6 D7 R8 A9 L10 W11 L12 G13 P14 Y15 S16 E17 G18 A19 V20 P21 S22 Y23 L24 T25 G26 E27 F28 D31 Y32 G33 W34 D35 S36 A37 G38 L39 D42 E51 L52 E53 L54 I55 H56 W58 W59 A60 M61 T64 V65 G66 C67 T69 P70
E71 A72 L73 E74 K75 Y76 G77 G78 V79 E80 F81 G82 E83 A84 V85 K88 A89 Q92 I93 F94 A95 E96 G97 G98 L99 D100 Y101 L102 G103 S106 V108 H109 A110 Q111 G125 L126 Y130 R131 C132 S133 G134 G135 P136 E139 A140 T141 F143 L144 Y145 E148 A149
F150 D151 P152 M153 G154 M155 A156 D157 D158 P159 E160 T161 F162 A163 E164 L165 K166 T167 K168 K171 N172 G173 R174 A175 L176 M177 F178 F181 G182 F183 F184 V185 Q186 S187 H188 Q189 T190 G191 K192 G193 P194 V195 E196 C197 W198 A199 E200 H201 I202 A203 D204 P205 V206 A207 N208 N209 G210 F211
V212

- Molecule 10: Lhcb1

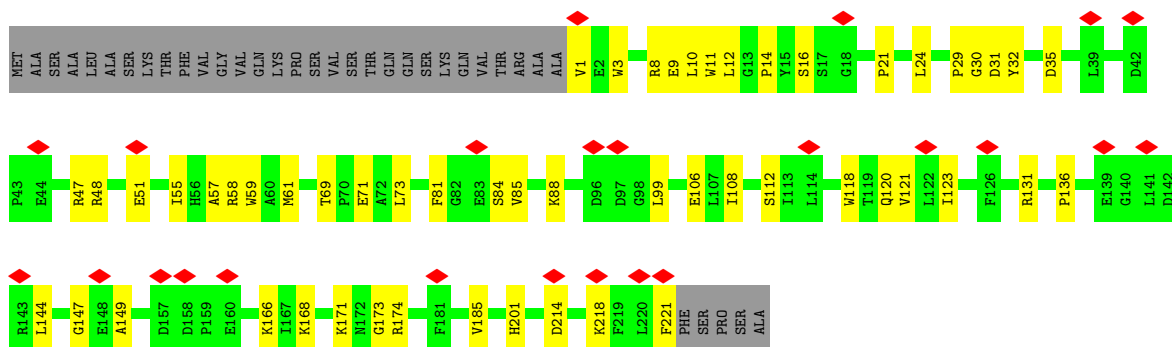
Chain 4:  58% 73% 25%

V1 E2 F3 Y4 G5 P6 D7 R8 A9 L10 W11 L12 G13 P14 Y15 S16 E17 G18 A19 V20 P21 S22 Y23 L24 T25 G26 E27 F28 D29 G30 D31 Y32 G33 W34 D35 S36 A37 G38 L39 S40 A41 D42 E51 L52 E53 L54 I55 H56 W58 W59 A60 M61 T64 V65 G66 C67 L68
T69 P70 E71 A72 L73 E74 K75 Y76 G77 G78 E80 F81 G82 E83 A84 V85 K88 A89 Q92 I93 F94 A95 E96 G97 G98 L99 D100 Y101 L102 G103 N104 P105 S106 L107 V108 H109 A110 Q111 G125 R131 C132 S133 G134 E139 A140 T141 F143 L144 Y145 E148 A149 F150
D151 P152 M153 G154 M155 A156 D157 D158 P159 E160 T161 F162 A163 E164 L165 K166 T167 K168 E169 I170 K171 G173 R174 L175 A176 M177 F178 F181 G182 F183 F184 V185 Q186 S187 H188 Q189 T190 G191 K192 G193 P194 V195 E196 C197 W198 A199 E200 H201 I202 A203 D204 P205 V206 A207 N208 N209 G210 F211
V212

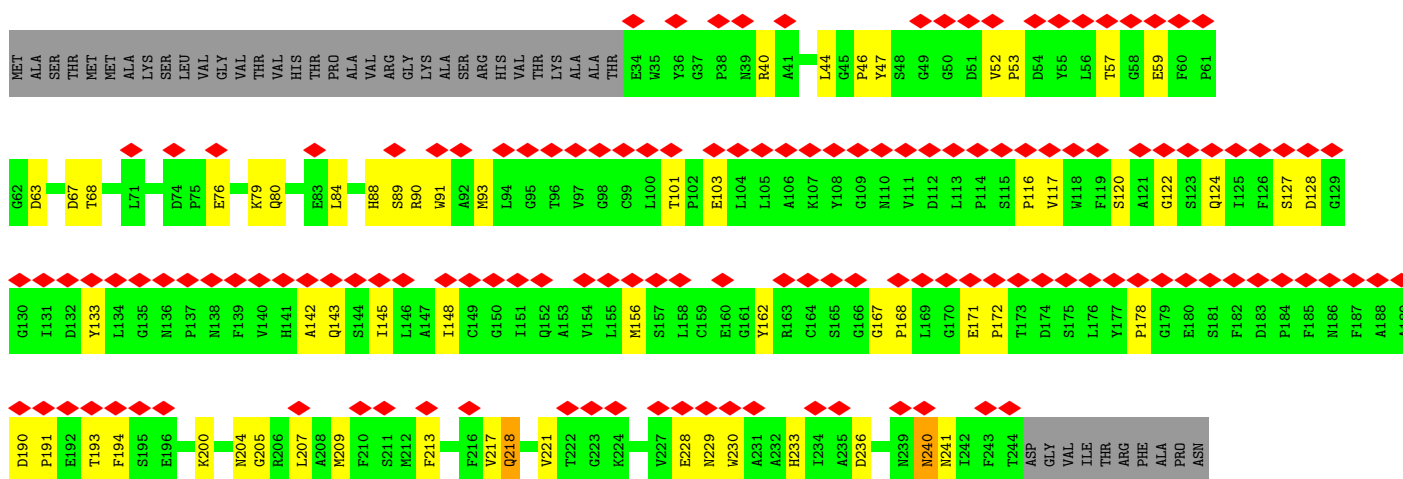
- Molecule 11: Lhcb2



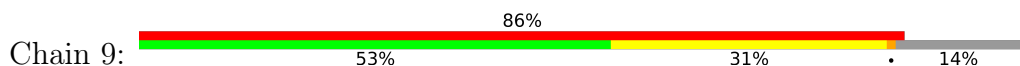
• Molecule 11: Lhcb2

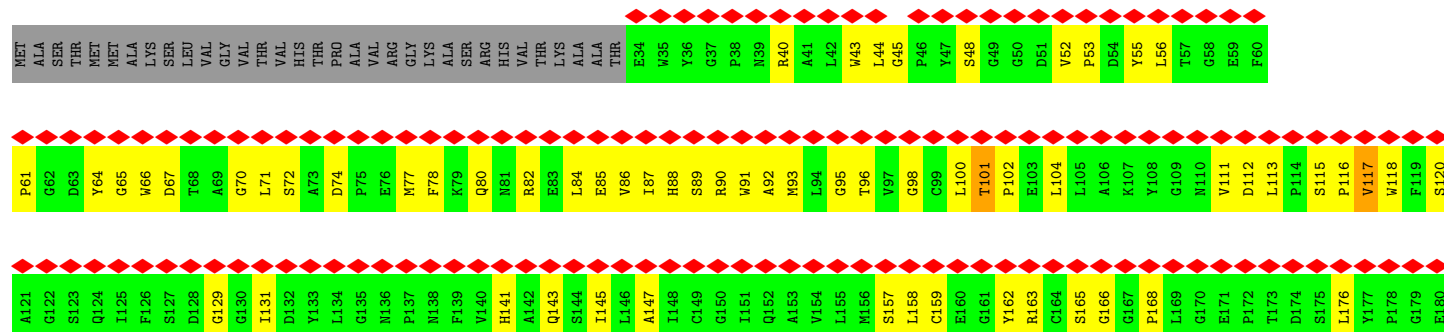


• Molecule 12: Lhcb3

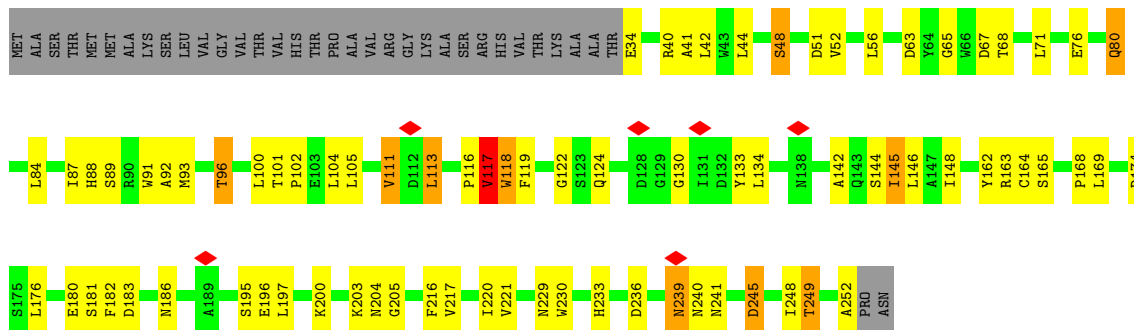


• Molecule 12: Lhcb3

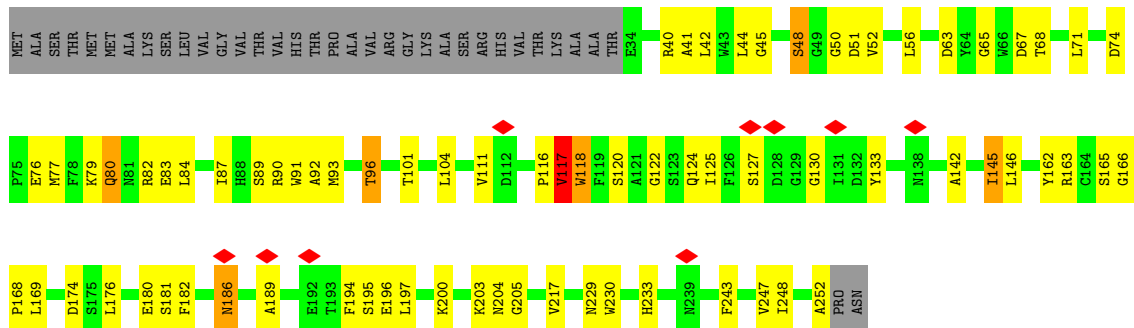




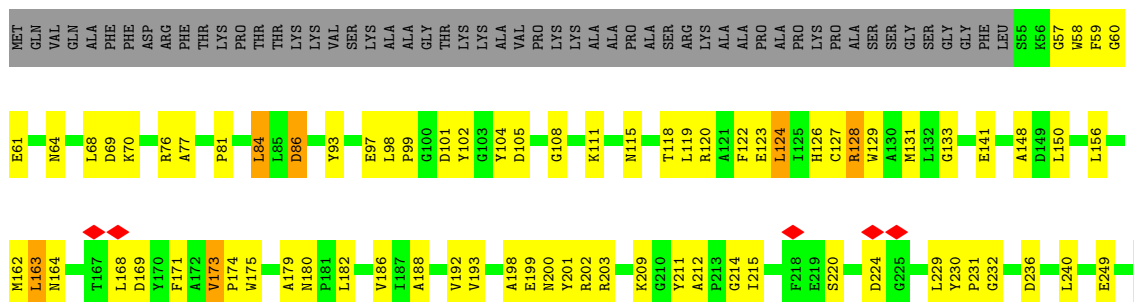
- Molecule 12: Lhcb3



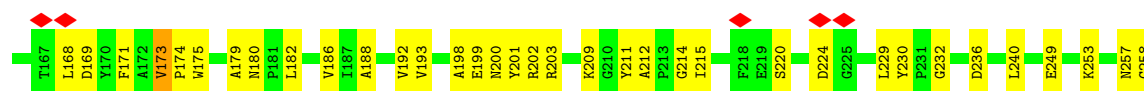
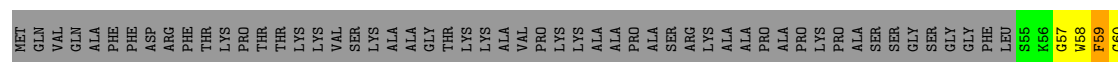
- Molecule 12: Lhcb3



- Molecule 13: LhcbS



- Molecule 13: LhcbS



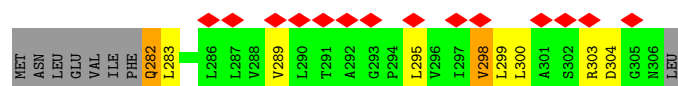
- Molecule 14: PsbX



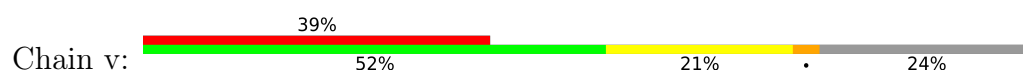
- Molecule 14: PsbX



- Molecule 15: Photosystem II reaction center protein Psb30



- Molecule 15: Photosystem II reaction center protein Psb30



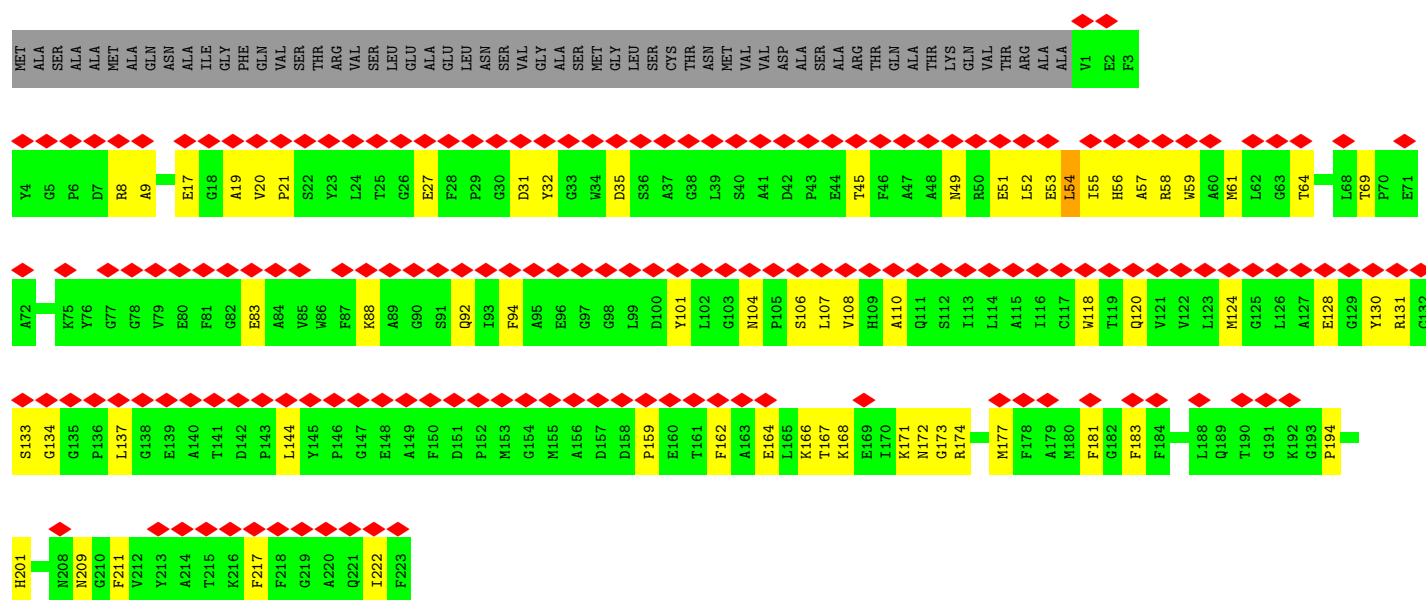
• Molecule 16: Photosystem II reaction center protein T



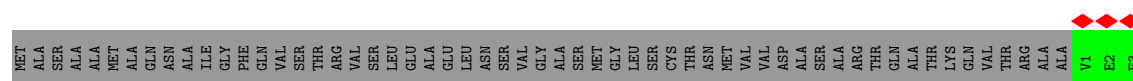
• Molecule 16: Photosystem II reaction center protein T

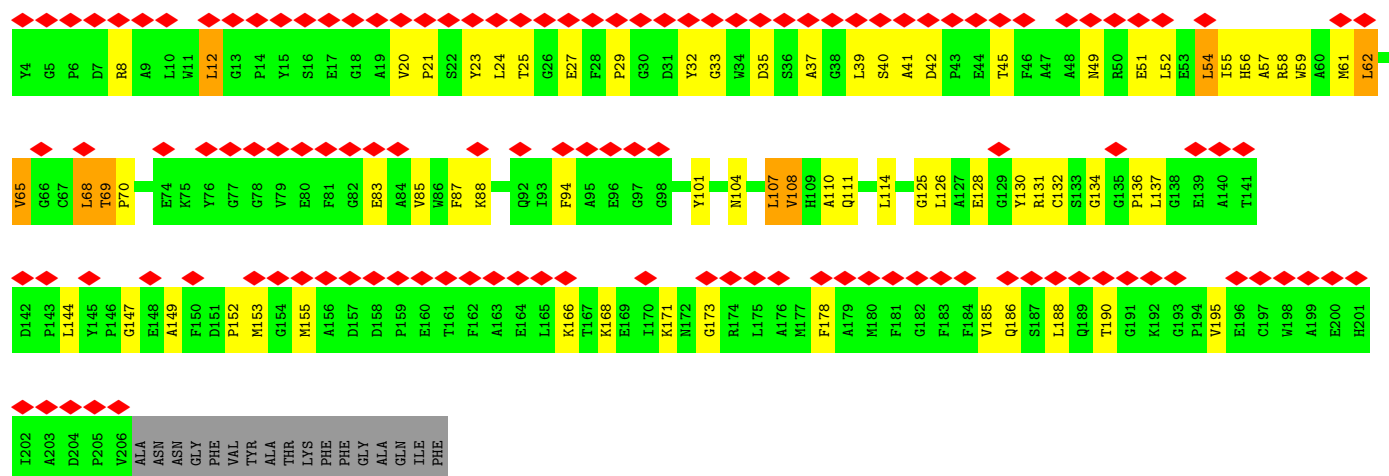


• Molecule 17: LhcbG

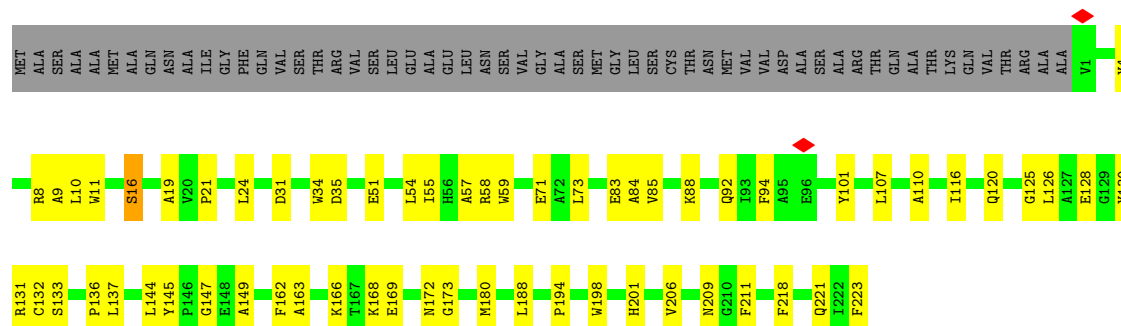


• Molecule 17: LhcbG

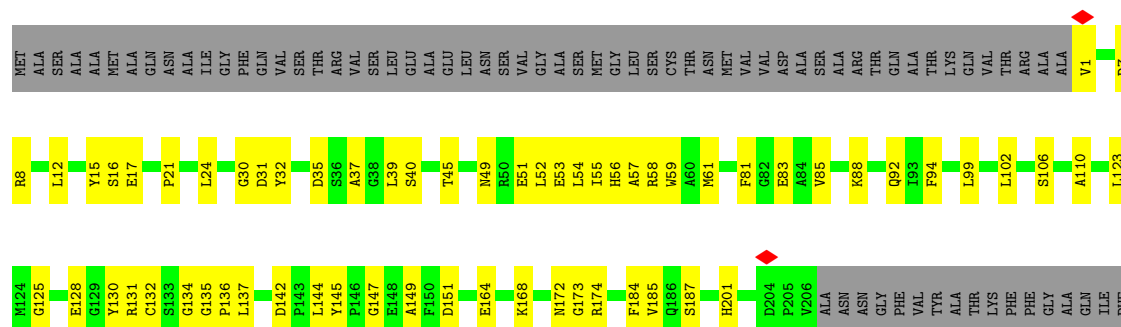




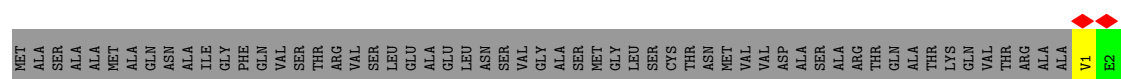
• Molecule 17: LhcbG

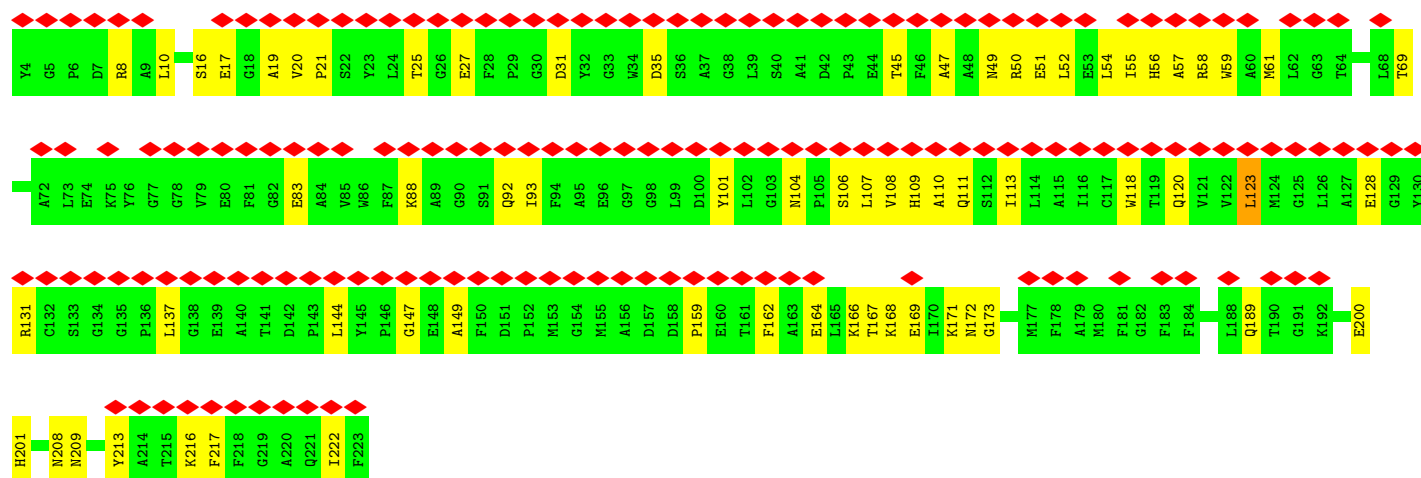


• Molecule 17: LhcbG

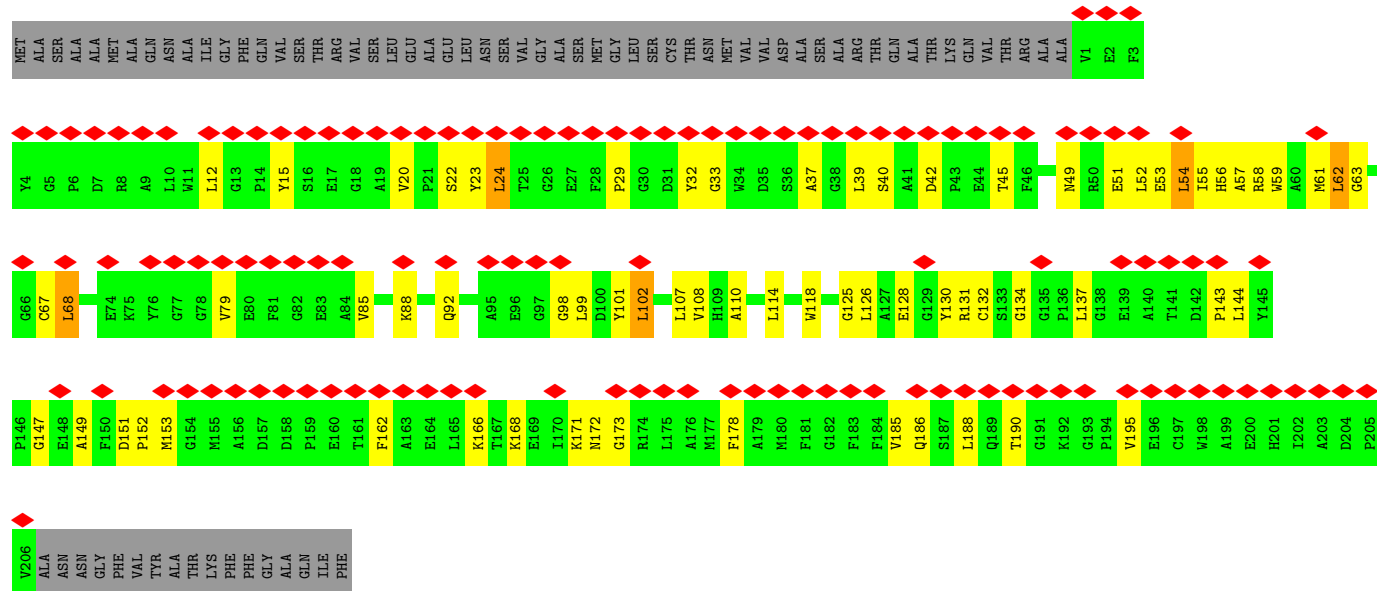


• Molecule 17: LhcbG

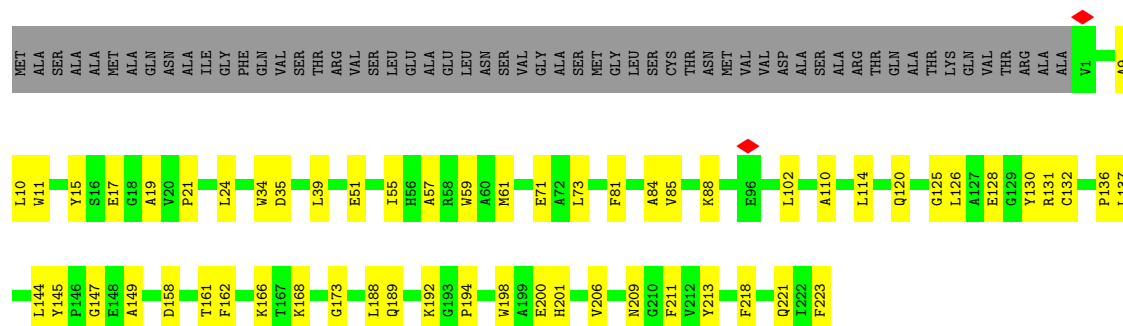




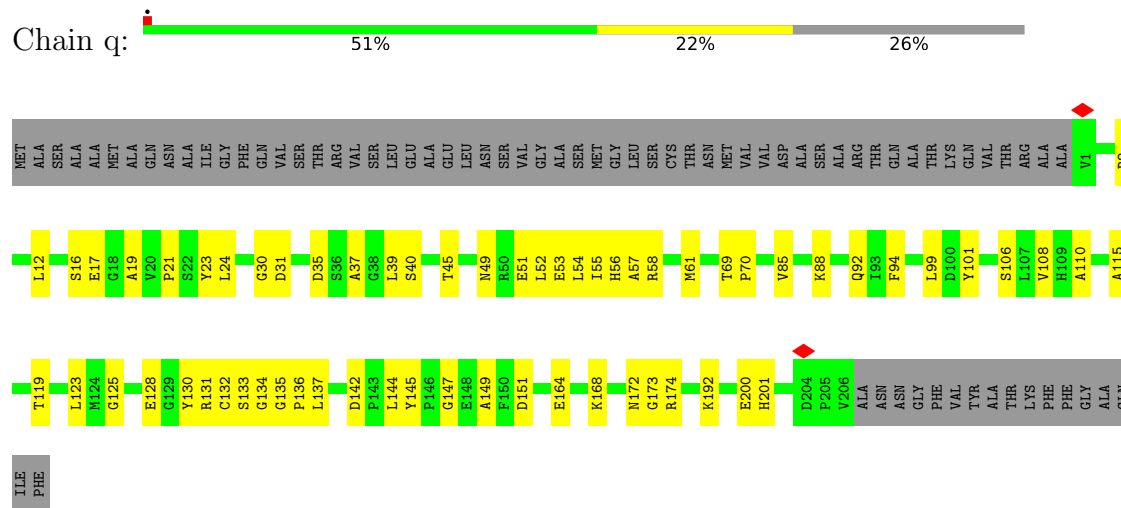
• Molecule 17: LhcbG



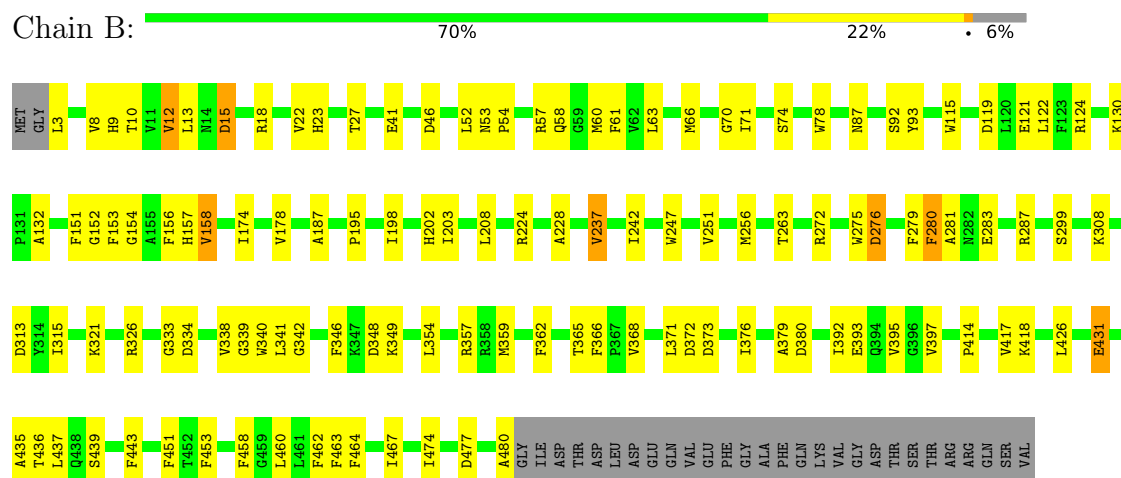
• Molecule 17: LhcbG



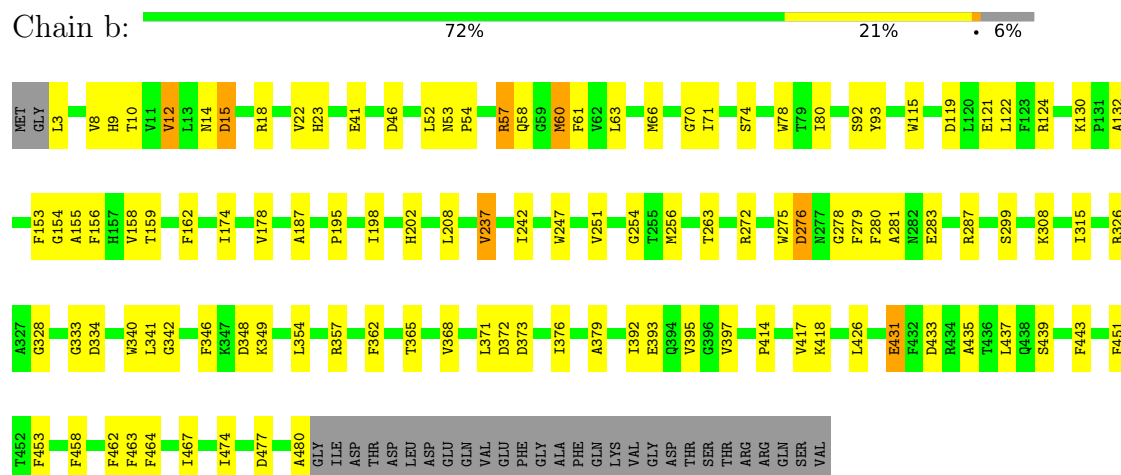
- Molecule 17: LhcbG



- Molecule 18: Photosystem II CP47 reaction center protein

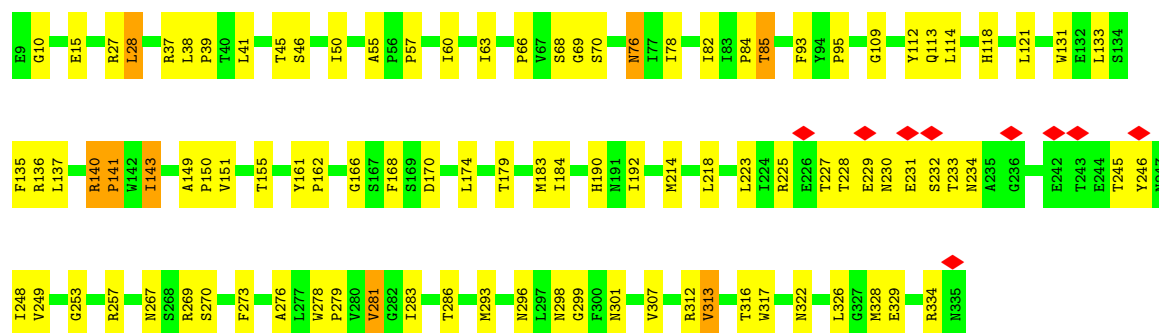


- Molecule 18: Photosystem II CP47 reaction center protein



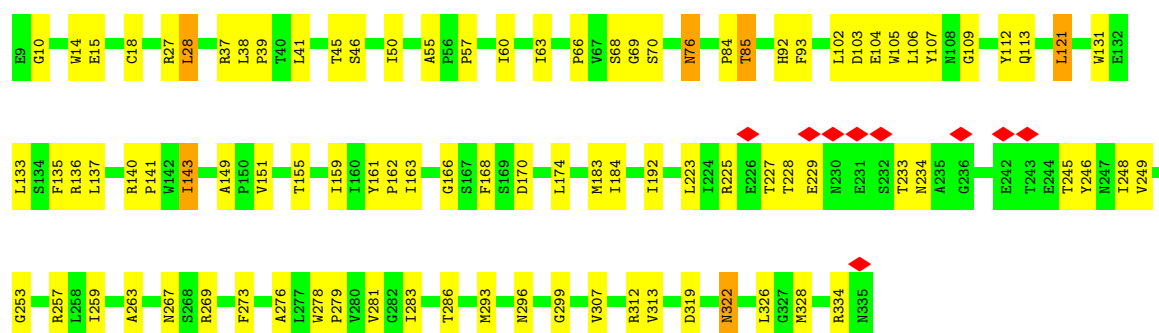
- Molecule 19: PsbA

Chain A: 




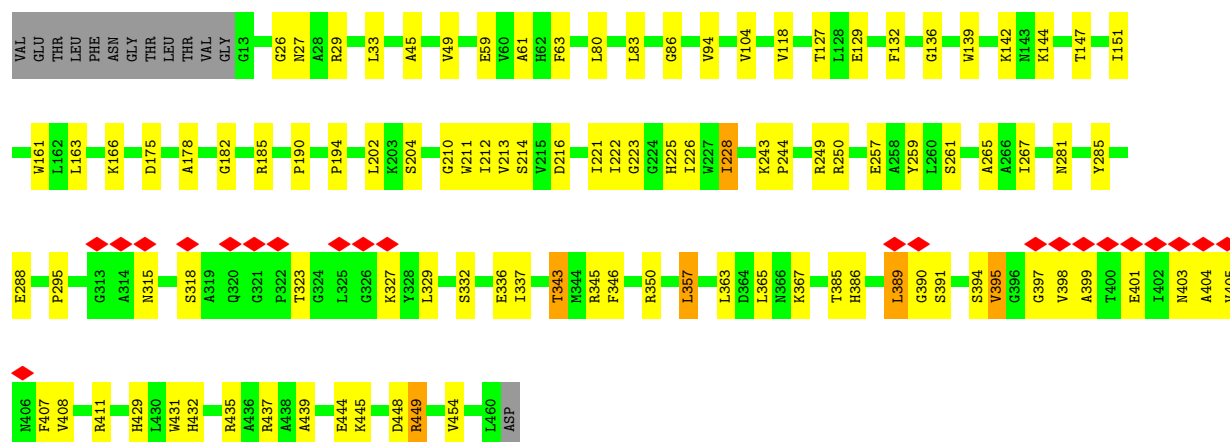
• Molecule 19: PsbA

Chain a: 




• Molecule 20: Photosystem II CP43 reaction center protein

Chain C: 



• Molecule 20: Photosystem II CP43 reaction center protein

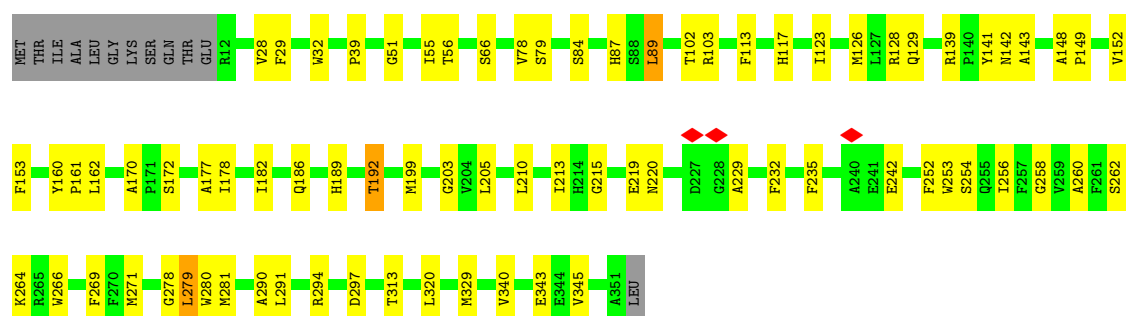
Chain c: 





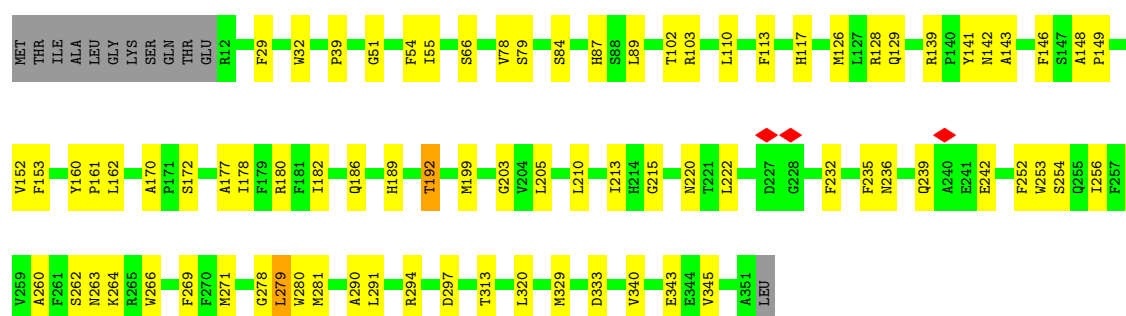
• Molecule 21: Photosystem II D2 protein

Chain D: 74% 21%



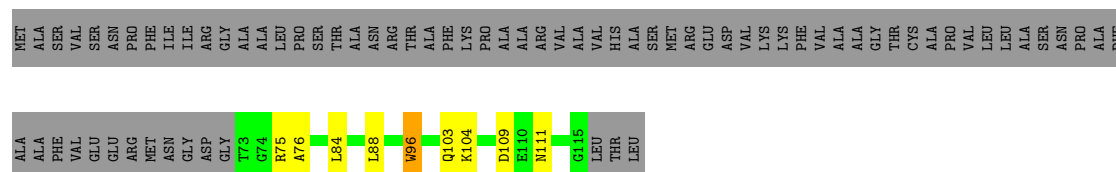
• Molecule 21: Photosystem II D2 protein

Chain d: 74% 22%



• Molecule 22: PsbW

Chain W: 29% 7% 64%



• Molecule 22: PsbW



MET	ALA	ALA	VAL	SER	ASN	PRO	PHE	ILE	ILE	ARG	GLY	ALA	ALA	LEU	PRO	SER	THR	ALA	ASN	ARG	THR	ALA	PHE	LYS	PRO	ALA	ALA	ARG	VAL	ALA	VAL	HIS	ALA	SER	MET	ARG	GLU	ASP	VAL	LYS	LYS	PHE	VAL	ALA	ALA	GLY	THR	CYS	ALA	PRO	VAL	LEU	ALA	SER	ASN	PRO	ALA	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	ALA	PHE	VAL	GLU	ARG	MET	ASN	GLY	ASP	GLY	T73	G74	R75	A76	L88	S93	W96	Q103	D109	E110	G115	LEU	THR	LEU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 10	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.922	Depositor
Minimum map value	-0.284	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.204	Depositor
Map size (Å)	624.0, 624.0, 624.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LMG, SQD, FE2, PL9, XAT, CHL, BCT, PHO, 8CT, LHG, OEX, 0UR, DGD, NEX, HEM, 0IE

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	Z	0.18	0/486	0.28	0/664
1	z	0.17	0/486	0.28	0/664
2	E	0.42	0/546	0.54	1/745 (0.1%)
2	e	0.23	0/546	0.35	0/745
3	H	0.22	0/523	0.29	0/713
3	h	0.23	0/523	0.32	0/713
4	I	0.33	0/283	0.28	0/383
4	i	0.34	0/283	0.38	0/383
5	K	0.26	0/310	0.52	0/426
5	k	0.25	0/310	0.35	0/426
6	L	0.27	0/312	0.30	0/424
6	l	0.27	0/312	0.29	0/424
7	M	0.16	0/234	0.31	0/320
7	m	0.15	0/234	0.30	0/320
8	R	0.18	0/1749	0.41	2/2373 (0.1%)
8	r	0.18	0/1745	0.42	2/2369 (0.1%)
9	F	0.21	0/252	0.41	0/341
9	f	0.21	0/258	0.38	0/349
10	1	0.11	0/1658	0.30	0/2257
10	4	0.11	0/1652	0.30	0/2250
11	2	0.15	0/1763	0.33	0/2394
11	5	0.14	0/1764	0.29	0/2395
12	3	0.14	0/1657	0.36	0/2261
12	6	0.14	0/1722	0.40	1/2349 (0.0%)
12	7	0.19	0/1730	0.43	0/2359
12	9	0.12	0/1733	0.37	0/2363
12	p	0.19	0/1733	0.45	0/2363
12	u	0.13	0/1736	0.38	0/2367
13	S	0.25	0/1920	0.43	1/2621 (0.0%)
13	s	0.28	0/1920	0.45	1/2621 (0.0%)
14	X	0.14	0/227	0.22	0/308

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	x	0.14	0/227	0.22	0/308
15	V	0.13	0/179	0.38	0/245
15	v	0.13	0/179	0.36	0/245
16	T	0.30	0/244	0.36	0/329
16	t	0.31	0/244	0.35	0/329
17	8	0.19	0/1602	0.29	0/2182
17	G	0.11	0/1743	0.27	0/2371
17	N	0.14	0/1599	0.30	0/2178
17	Y	0.24	0/1743	0.31	0/2371
17	g	0.11	0/1743	0.26	0/2371
17	n	0.13	0/1592	0.29	0/2168
17	q	0.19	0/1602	0.29	0/2182
17	y	0.23	0/1743	0.29	0/2371
18	B	0.33	0/3866	0.37	1/5266 (0.0%)
18	b	0.27	0/3866	0.34	0/5266
19	A	0.33	0/2637	0.36	0/3595
19	a	0.41	0/2637	0.39	0/3595
20	C	0.30	0/3591	0.38	0/4895
20	c	0.30	0/3591	0.39	0/4895
21	D	0.33	0/2813	0.37	0/3832
21	d	0.35	0/2813	0.37	0/3832
22	W	0.24	0/308	0.51	0/417
22	w	0.23	0/308	0.51	0/417
All	All	0.25	0/71477	0.36	9/97350 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	77	GLY	N-CA-C	7.09	123.47	114.25
8	r	68	ASP	CA-C-N	-6.62	113.97	120.52
8	r	68	ASP	C-N-CA	-6.62	113.97	120.52
8	R	68	ASP	CA-C-N	-6.58	114.00	120.52
8	R	68	ASP	C-N-CA	-6.58	114.00	120.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	472	0	496	9	0
1	z	472	0	496	6	0
2	E	530	0	517	20	0
2	e	530	0	517	9	0
3	H	513	0	517	18	0
3	h	513	0	517	17	0
4	I	275	0	282	4	0
4	i	275	0	282	4	0
5	K	299	0	311	7	0
5	k	299	0	311	4	0
6	L	304	0	313	16	0
6	l	304	0	313	14	0
7	M	231	0	261	9	0
7	m	231	0	261	11	0
8	R	1711	0	1670	83	0
8	r	1707	0	1659	70	0
9	F	246	0	256	4	0
9	f	251	0	261	4	0
10	1	1609	0	1517	52	0
10	4	1603	0	1506	50	0
11	2	1710	0	1616	46	0
11	5	1711	0	1620	48	0
12	3	1606	0	1501	44	0
12	6	1670	0	1564	50	0
12	7	1677	0	1573	66	0
12	9	1680	0	1575	71	0
12	p	1680	0	1575	65	0
12	u	1683	0	1584	74	0
13	S	1867	0	1797	79	0
13	s	1867	0	1797	75	0
14	X	226	0	242	4	0
14	x	226	0	242	2	0
15	V	179	0	205	7	0
15	v	179	0	205	5	0
16	T	236	0	239	5	0
16	t	236	0	239	5	0
17	8	1554	0	1467	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	G	1690	0	1593	57	0
17	N	1551	0	1458	64	0
17	Y	1690	0	1593	44	0
17	g	1690	0	1593	57	0
17	n	1545	0	1455	59	0
17	q	1554	0	1467	52	0
17	y	1690	0	1593	43	0
18	B	3737	0	3605	100	0
18	b	3737	0	3605	92	0
19	A	2558	0	2469	75	0
19	a	2558	0	2469	70	0
20	C	3472	0	3381	85	0
20	c	3472	0	3381	83	0
21	D	2719	0	2631	69	0
21	d	2719	0	2631	66	0
22	W	304	0	276	8	0
22	w	304	0	276	11	0
23	E	43	0	30	2	0
23	f	43	0	30	3	0
24	1	349	0	234	24	0
24	2	353	0	234	11	0
24	3	365	0	250	31	0
24	4	349	0	234	22	0
24	5	353	0	234	15	0
24	6	365	0	250	37	0
24	7	397	0	311	35	0
24	8	351	0	270	24	0
24	9	397	0	311	25	0
24	G	433	0	370	40	0
24	N	404	0	311	20	0
24	R	277	0	186	17	0
24	S	331	0	233	14	0
24	Y	486	0	411	26	0
24	g	433	0	370	28	0
24	n	404	0	311	21	0
24	p	397	0	311	37	0
24	q	404	0	311	23	0
24	r	277	0	186	19	0
24	s	331	0	233	14	0
24	u	397	0	311	21	0
24	y	433	0	370	26	0
25	1	268	0	204	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	2	305	0	258	10	0
25	3	256	0	186	6	0
25	4	268	0	204	23	0
25	5	305	0	258	11	0
25	6	256	0	186	7	0
25	7	321	0	280	27	0
25	8	310	0	267	12	0
25	9	324	0	284	16	0
25	A	280	0	271	12	0
25	B	980	0	1023	63	0
25	C	790	0	814	30	0
25	D	130	0	144	10	0
25	G	318	0	272	27	0
25	N	310	0	267	13	0
25	R	325	0	247	17	0
25	S	333	0	261	10	0
25	Y	321	0	278	8	0
25	a	280	0	271	13	0
25	b	980	0	1023	61	0
25	c	790	0	814	33	0
25	d	130	0	144	10	0
25	g	318	0	272	15	0
25	n	310	0	267	12	0
25	p	324	0	284	24	0
25	q	310	0	267	12	0
25	r	325	0	247	18	0
25	s	332	0	261	13	0
25	u	324	0	284	16	0
25	y	321	0	278	12	0
26	1	44	0	0	0	0
26	2	88	0	0	1	0
26	3	87	0	0	2	0
26	4	44	0	0	0	0
26	5	88	0	0	0	0
26	6	43	0	0	2	0
26	7	88	0	0	2	0
26	8	44	0	0	0	0
26	9	88	0	0	3	0
26	G	88	0	0	0	0
26	N	44	0	0	0	0
26	R	44	0	0	1	0
26	Y	88	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	g	88	0	0	0	0
26	n	44	0	0	0	0
26	p	88	0	0	2	0
26	q	44	0	0	0	0
26	r	44	0	0	1	0
26	u	88	0	0	1	0
26	y	88	0	0	2	0
27	R	44	0	56	16	0
27	r	44	0	56	8	0
28	1	44	0	56	22	0
28	2	44	0	56	9	0
28	3	44	0	56	22	0
28	4	44	0	56	21	0
28	5	44	0	56	10	0
28	6	44	0	56	21	0
28	7	44	0	56	32	0
28	9	44	0	56	6	0
28	G	44	0	56	32	0
28	N	44	0	56	7	0
28	R	44	0	56	6	0
28	S	44	0	56	24	0
28	g	44	0	56	15	0
28	n	44	0	56	7	0
28	p	44	0	56	27	0
28	r	88	0	112	15	0
28	s	44	0	56	21	0
28	u	44	0	56	9	0
28	y	44	0	56	4	0
29	1	52	0	0	0	0
29	2	52	0	0	1	0
29	3	52	0	0	0	0
29	4	52	0	0	1	0
29	5	52	0	0	0	0
29	6	52	0	0	1	0
29	7	52	0	0	0	0
29	8	52	0	0	1	0
29	9	52	0	0	1	0
29	G	52	0	0	1	0
29	N	52	0	0	0	0
29	Y	52	0	0	1	0
29	g	52	0	0	0	0
29	n	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	p	52	0	0	1	0
29	q	52	0	0	1	0
29	u	52	0	0	1	0
29	y	52	0	0	1	0
30	1	42	0	54	3	0
30	2	40	0	50	2	0
30	4	42	0	54	3	0
30	5	43	0	56	2	0
30	7	37	0	44	3	0
30	9	43	0	56	6	0
30	A	89	0	124	8	0
30	C	32	0	34	0	0
30	D	88	0	122	13	0
30	G	43	0	56	1	0
30	N	43	0	56	4	0
30	Y	43	0	56	0	0
30	a	89	0	124	7	0
30	c	32	0	34	0	0
30	d	88	0	122	11	0
30	g	43	0	56	2	0
30	n	43	0	56	4	0
30	p	43	0	56	3	0
30	y	43	0	56	2	0
31	A	40	0	0	0	0
31	B	40	0	0	0	0
31	C	120	0	0	1	0
31	D	40	0	0	0	0
31	S	80	0	0	0	0
31	T	40	0	0	0	0
31	V	40	0	0	1	0
31	X	40	0	0	0	0
31	a	40	0	0	0	0
31	b	40	0	0	0	0
31	c	120	0	0	1	0
31	d	40	0	0	0	0
31	s	80	0	0	0	0
31	t	40	0	0	0	0
31	v	40	0	0	1	0
31	x	40	0	0	0	0
32	A	45	0	54	2	0
32	B	54	0	78	4	0
32	D	44	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	a	45	0	54	4	0
32	b	54	0	78	5	0
32	d	44	0	52	1	0
33	B	41	0	52	5	0
33	C	42	0	54	6	0
33	D	94	0	128	8	0
33	W	30	0	30	2	0
33	d	94	0	128	8	0
33	i	48	0	66	3	0
33	m	41	0	52	6	0
33	w	36	0	42	6	0
34	A	10	0	0	0	0
34	a	10	0	0	0	0
35	A	64	0	74	4	0
35	D	64	0	74	6	0
35	a	64	0	74	4	0
35	d	64	0	74	6	0
36	A	4	0	1	0	0
36	a	4	0	1	0	0
37	C	105	0	126	7	0
37	c	105	0	126	8	0
38	D	1	0	0	0	0
38	d	1	0	0	0	0
39	D	55	0	80	2	0
39	d	55	0	80	2	0
All	All	95298	0	87326	2639	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 2639 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:58:TRP:HZ2	28:S:617:NEX:H183	1.14	1.10
12:u:158:LEU:HD23	28:u:304:NEX:H203	1.35	1.07
13:S:58:TRP:CZ2	28:S:617:NEX:H183	1.89	1.06
28:p:304:NEX:H31	24:p:310:CHL:HBA1	1.38	1.04
13:S:58:TRP:HE1	28:S:617:NEX:H192	1.19	1.03

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
1	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
2	E	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
2	e	63/82 (77%)	63 (100%)	0	0	100	100
3	H	66/75 (88%)	63 (96%)	3 (4%)	0	100	100
3	h	66/75 (88%)	63 (96%)	3 (4%)	0	100	100
4	I	32/36 (89%)	32 (100%)	0	0	100	100
4	i	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
5	K	35/43 (81%)	33 (94%)	2 (6%)	0	100	100
5	k	35/43 (81%)	34 (97%)	1 (3%)	0	100	100
6	L	35/38 (92%)	35 (100%)	0	0	100	100
6	l	35/38 (92%)	35 (100%)	0	0	100	100
7	M	28/33 (85%)	27 (96%)	1 (4%)	0	100	100
7	m	28/33 (85%)	27 (96%)	1 (4%)	0	100	100
8	R	223/267 (84%)	199 (89%)	23 (10%)	1 (0%)	30	58
8	r	223/267 (84%)	203 (91%)	20 (9%)	0	100	100
9	F	29/42 (69%)	27 (93%)	2 (7%)	0	100	100
9	f	29/42 (69%)	28 (97%)	1 (3%)	0	100	100
10	1	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
10	4	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
11	2	219/256 (86%)	205 (94%)	14 (6%)	0	100	100
11	5	219/256 (86%)	204 (93%)	15 (7%)	0	100	100
12	3	209/254 (82%)	189 (90%)	20 (10%)	0	100	100
12	6	217/254 (85%)	196 (90%)	21 (10%)	0	100	100
12	7	217/254 (85%)	188 (87%)	27 (12%)	2 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	9	217/254 (85%)	185 (85%)	31 (14%)	1 (0%)	24	54
12	p	217/254 (85%)	188 (87%)	26 (12%)	3 (1%)	9	31
12	u	217/254 (85%)	187 (86%)	30 (14%)	0	100	100
13	S	247/308 (80%)	211 (85%)	34 (14%)	2 (1%)	16	44
13	s	247/308 (80%)	209 (85%)	35 (14%)	3 (1%)	10	34
14	X	32/109 (29%)	32 (100%)	0	0	100	100
14	x	32/109 (29%)	32 (100%)	0	0	100	100
15	V	23/33 (70%)	18 (78%)	5 (22%)	0	100	100
15	v	23/33 (70%)	19 (83%)	4 (17%)	0	100	100
16	T	26/31 (84%)	24 (92%)	2 (8%)	0	100	100
16	t	26/31 (84%)	24 (92%)	2 (8%)	0	100	100
17	8	204/280 (73%)	195 (96%)	9 (4%)	0	100	100
17	G	221/280 (79%)	215 (97%)	6 (3%)	0	100	100
17	N	204/280 (73%)	196 (96%)	8 (4%)	0	100	100
17	Y	221/280 (79%)	212 (96%)	9 (4%)	0	100	100
17	g	221/280 (79%)	214 (97%)	7 (3%)	0	100	100
17	n	204/280 (73%)	192 (94%)	11 (5%)	1 (0%)	24	54
17	q	204/280 (73%)	196 (96%)	8 (4%)	0	100	100
17	y	221/280 (79%)	212 (96%)	9 (4%)	0	100	100
18	B	476/508 (94%)	455 (96%)	19 (4%)	2 (0%)	30	58
18	b	476/508 (94%)	457 (96%)	17 (4%)	2 (0%)	30	58
19	A	325/327 (99%)	307 (94%)	17 (5%)	1 (0%)	36	64
19	a	325/327 (99%)	304 (94%)	20 (6%)	1 (0%)	36	64
20	C	446/461 (97%)	409 (92%)	36 (8%)	1 (0%)	43	71
20	c	446/461 (97%)	407 (91%)	38 (8%)	1 (0%)	43	71
21	D	338/352 (96%)	313 (93%)	25 (7%)	0	100	100
21	d	338/352 (96%)	318 (94%)	20 (6%)	0	100	100
22	W	41/118 (35%)	30 (73%)	11 (27%)	0	100	100
22	w	41/118 (35%)	30 (73%)	11 (27%)	0	100	100
All	All	8900/10550 (84%)	8243 (93%)	636 (7%)	21 (0%)	44	71

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	B	279	PHE
18	B	299	SER
17	n	23	TYR
12	p	117	VAL
12	p	118	TRP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	51/52 (98%)	51 (100%)	0	100	100
1	z	51/52 (98%)	51 (100%)	0	100	100
2	E	58/73 (80%)	57 (98%)	1 (2%)	53	71
2	e	58/73 (80%)	57 (98%)	1 (2%)	53	71
3	H	56/62 (90%)	55 (98%)	1 (2%)	51	70
3	h	56/62 (90%)	55 (98%)	1 (2%)	51	70
4	I	31/32 (97%)	31 (100%)	0	100	100
4	i	31/32 (97%)	31 (100%)	0	100	100
5	K	33/39 (85%)	31 (94%)	2 (6%)	17	44
5	k	33/39 (85%)	32 (97%)	1 (3%)	36	62
6	L	34/35 (97%)	31 (91%)	3 (9%)	9	31
6	l	34/35 (97%)	32 (94%)	2 (6%)	18	45
7	M	27/30 (90%)	27 (100%)	0	100	100
7	m	27/30 (90%)	26 (96%)	1 (4%)	30	58
8	R	181/214 (85%)	173 (96%)	8 (4%)	25	54
8	r	180/214 (84%)	170 (94%)	10 (6%)	19	46
9	F	25/36 (69%)	22 (88%)	3 (12%)	5	19
9	f	26/36 (72%)	23 (88%)	3 (12%)	5	21
10	1	160/160 (100%)	153 (96%)	7 (4%)	25	54
10	4	159/160 (99%)	153 (96%)	6 (4%)	29	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	2	168/199 (84%)	168 (100%)	0	100	100
11	5	168/199 (84%)	168 (100%)	0	100	100
12	3	165/202 (82%)	158 (96%)	7 (4%)	26	55
12	6	172/202 (85%)	166 (96%)	6 (4%)	32	59
12	7	173/202 (86%)	164 (95%)	9 (5%)	21	49
12	9	174/202 (86%)	167 (96%)	7 (4%)	28	56
12	p	174/202 (86%)	161 (92%)	13 (8%)	12	37
12	u	175/202 (87%)	166 (95%)	9 (5%)	21	50
13	S	184/232 (79%)	172 (94%)	12 (6%)	15	42
13	s	184/232 (79%)	174 (95%)	10 (5%)	20	48
14	X	24/80 (30%)	23 (96%)	1 (4%)	26	55
14	x	24/80 (30%)	22 (92%)	2 (8%)	10	33
15	V	20/28 (71%)	18 (90%)	2 (10%)	7	26
15	v	20/28 (71%)	19 (95%)	1 (5%)	22	50
16	T	25/28 (89%)	23 (92%)	2 (8%)	11	35
16	t	25/28 (89%)	23 (92%)	2 (8%)	11	35
17	8	153/210 (73%)	152 (99%)	1 (1%)	76	80
17	G	165/210 (79%)	161 (98%)	4 (2%)	43	66
17	N	152/210 (72%)	143 (94%)	9 (6%)	18	45
17	Y	165/210 (79%)	162 (98%)	3 (2%)	51	70
17	g	165/210 (79%)	159 (96%)	6 (4%)	31	58
17	n	151/210 (72%)	144 (95%)	7 (5%)	24	53
17	q	153/210 (73%)	153 (100%)	0	100	100
17	y	165/210 (79%)	163 (99%)	2 (1%)	63	75
18	B	384/410 (94%)	371 (97%)	13 (3%)	32	60
18	b	384/410 (94%)	372 (97%)	12 (3%)	35	61
19	A	266/266 (100%)	251 (94%)	15 (6%)	19	46
19	a	266/266 (100%)	252 (95%)	14 (5%)	20	48
20	C	347/359 (97%)	338 (97%)	9 (3%)	40	65
20	c	347/359 (97%)	337 (97%)	10 (3%)	37	63
21	D	275/285 (96%)	266 (97%)	9 (3%)	33	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	d	275/285 (96%)	267 (97%)	8 (3%)	37	63
22	W	29/88 (33%)	27 (93%)	2 (7%)	14	40
22	w	29/88 (33%)	29 (100%)	0	100	100
All	All	7057/8308 (85%)	6800 (96%)	257 (4%)	32	58

5 of 257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	s	119	LEU
8	r	48	MET
19	A	281	VAL
19	A	232	SER
8	r	156	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
20	C	451	ASN
11	5	215	GLN
12	7	81	ASN
19	a	315	ASN
21	D	197	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 528 ligands modelled in this entry, 2 are monoatomic - leaving 526 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	CLA	9	315	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
25	CLA	q	312	-	59,63,73	1.24	9 (15%)	70,101,113	1.38	6 (8%)
37	DGD	c	618	-	51,51,67	0.94	2 (3%)	65,65,81	1.21	6 (9%)
39	PL9	d	406	-	55,55,55	1.65	11 (20%)	68,69,69	1.53	12 (17%)
25	CLA	N	307	-	54,58,73	1.30	8 (14%)	64,95,113	1.39	6 (9%)
26	OIE	p	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.50	10 (19%)
25	CLA	7	314	-	59,63,73	1.24	9 (15%)	70,101,113	1.34	6 (8%)
25	CLA	b	615	18	69,73,73	1.15	8 (11%)	82,113,113	1.26	5 (6%)
31	8CT	C	615	-	40,41,41	4.77	23 (57%)	51,56,56	2.80	19 (37%)
24	CHL	n	312	-	50,64,74	3.54	18 (36%)	46,102,114	2.81	19 (41%)
25	CLA	s	404	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	4 (6%)
26	OIE	3	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.61	10 (19%)
24	CHL	G	318	17	36,50,74	4.11	17 (47%)	29,85,114	3.09	15 (51%)
30	LHG	4	318	-	41,41,48	1.24	6 (14%)	44,47,54	0.99	3 (6%)
25	CLA	2	314	-	59,63,73	1.23	9 (15%)	70,101,113	1.33	5 (7%)
24	CHL	5	309	11	37,51,74	4.16	18 (48%)	30,86,114	3.22	16 (53%)
30	LHG	C	617	-	31,31,48	1.36	6 (19%)	34,37,54	1.15	3 (8%)
25	CLA	6	307	-	47,51,73	1.38	7 (14%)	55,86,113	1.44	4 (7%)
24	CHL	2	311	-	41,55,74	3.95	19 (46%)	35,91,114	2.99	14 (40%)
25	CLA	u	315	-	67,71,73	1.19	8 (11%)	79,110,113	1.31	6 (7%)
26	OIE	1	302	-	42,45,45	1.13	6 (14%)	51,63,63	1.53	12 (23%)
30	LHG	D	407	-	48,48,48	1.12	5 (10%)	51,54,54	0.97	2 (3%)
25	CLA	C	611	20	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
24	CHL	n	309	-	40,54,74	3.89	18 (45%)	34,90,114	3.47	16 (47%)
24	CHL	s	402	13	40,54,74	3.86	19 (47%)	34,90,114	3.17	16 (47%)
24	CHL	7	310	-	40,54,74	4.01	19 (47%)	34,90,114	3.06	14 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	NEX	g	304	-	40,46,46	1.12	3 (7%)	50,70,70	4.72	18 (36%)
25	CLA	C	605	20	60,64,73	1.23	9 (15%)	71,102,113	1.38	6 (8%)
25	CLA	c	609	20	69,73,73	1.17	9 (13%)	82,113,113	1.35	7 (8%)
24	CHL	N	312	-	50,64,74	3.55	18 (36%)	46,102,114	2.81	19 (41%)
32	SQD	D	409	-	42,44,54	1.06	3 (7%)	52,55,65	1.51	8 (15%)
24	CHL	8	308	-	40,54,74	3.85	19 (47%)	34,90,114	3.26	16 (47%)
25	CLA	B	615	18	69,73,73	1.15	8 (11%)	82,113,113	1.27	5 (6%)
24	CHL	Y	311	-	45,59,74	3.63	19 (42%)	40,96,114	2.97	17 (42%)
25	CLA	b	612	18	69,73,73	1.15	9 (13%)	82,113,113	1.33	9 (10%)
24	CHL	g	312	-	45,59,74	3.82	18 (40%)	40,96,114	2.93	18 (45%)
25	CLA	3	306	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	6 (11%)
25	CLA	6	314	-	45,49,73	1.40	7 (15%)	54,84,113	1.47	5 (9%)
26	OIE	9	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.53	11 (21%)
24	CHL	N	308	17	37,51,74	4.11	18 (48%)	30,86,114	3.16	13 (43%)
23	HEM	f	201	9,2	50,50,50	1.39	7 (14%)	67,82,82	1.00	0
25	CLA	A	603	19	69,73,73	1.17	9 (13%)	82,113,113	1.37	9 (10%)
24	CHL	y	311	-	48,62,74	3.54	19 (39%)	43,99,114	3.12	20 (46%)
26	OIE	q	302	-	42,45,45	1.14	5 (11%)	51,63,63	1.48	11 (21%)
25	CLA	y	316	17	49,53,73	1.36	9 (18%)	58,89,113	1.51	4 (6%)
26	OIE	8	302	-	42,45,45	1.14	5 (11%)	51,63,63	1.48	11 (21%)
27	XAT	r	316	-	41,47,47	0.92	1 (2%)	54,74,74	2.63	20 (37%)
24	CHL	N	309	-	40,54,74	3.89	19 (47%)	34,90,114	3.40	16 (47%)
24	CHL	y	313	-	60,74,74	3.17	19 (31%)	58,114,114	2.53	19 (32%)
24	CHL	9	308	12	37,51,74	4.28	18 (48%)	30,86,114	3.30	14 (46%)
24	CHL	5	318	11	36,50,74	4.21	17 (47%)	29,85,114	3.21	17 (58%)
30	LHG	1	318	-	41,41,48	1.24	6 (14%)	44,47,54	0.98	3 (6%)
25	CLA	C	616	20	50,54,73	1.33	7 (14%)	59,90,113	1.47	5 (8%)
25	CLA	7	308	-	54,58,73	1.30	9 (16%)	64,95,113	1.37	5 (7%)
25	CLA	c	601	20	69,73,73	1.15	9 (13%)	82,113,113	1.38	9 (10%)
25	CLA	a	603	19	69,73,73	1.16	10 (14%)	82,113,113	1.37	8 (9%)
24	CHL	9	317	-	36,50,74	4.35	17 (47%)	29,85,114	3.31	15 (51%)
24	CHL	4	304	-	36,50,74	4.30	18 (50%)	29,85,114	3.24	14 (48%)
33	LMG	m	101	-	41,41,55	0.99	2 (4%)	49,49,63	1.24	4 (8%)
25	CLA	p	315	30	67,71,73	1.17	9 (13%)	79,110,113	1.38	6 (7%)
24	CHL	y	306	-	58,72,74	3.15	19 (32%)	55,111,114	2.69	20 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	8	304	17	54,68,74	3.33	19 (35%)	50,106,114	2.83	19 (38%)
24	CHL	R	605	-	36,50,74	4.07	17 (47%)	29,85,114	3.34	16 (55%)
24	CHL	9	305	-	58,72,74	3.31	18 (31%)	55,111,114	2.57	19 (34%)
25	CLA	2	315	-	67,71,73	1.17	9 (13%)	79,110,113	1.29	4 (5%)
31	8CT	c	614	-	40,41,41	4.71	23 (57%)	51,56,56	2.81	21 (41%)
24	CHL	s	408	-	40,54,74	3.89	19 (47%)	34,90,114	3.20	16 (47%)
25	CLA	p	308	-	54,58,73	1.30	9 (16%)	64,95,113	1.36	5 (7%)
24	CHL	q	304	17	54,68,74	3.33	19 (35%)	50,106,114	2.84	19 (38%)
24	CHL	3	317	12	36,50,74	4.23	17 (47%)	29,85,114	3.21	14 (48%)
24	CHL	S	606	-	40,54,74	3.97	19 (47%)	34,90,114	3.03	14 (41%)
24	CHL	3	308	-	37,51,74	4.21	18 (48%)	30,86,114	3.25	15 (50%)
25	CLA	a	605	-	53,57,73	1.28	8 (15%)	61,93,113	1.41	5 (8%)
28	NEX	4	303	25	40,46,46	1.12	3 (7%)	50,70,70	4.73	18 (36%)
24	CHL	q	308	-	40,54,74	3.86	19 (47%)	34,90,114	3.30	16 (47%)
25	CLA	3	313	-	45,49,73	1.41	8 (17%)	54,84,113	1.49	6 (11%)
25	CLA	b	603	18	69,73,73	1.16	8 (11%)	82,113,113	1.29	8 (9%)
25	CLA	b	604	18	66,70,73	1.19	7 (10%)	78,109,113	1.39	7 (8%)
24	CHL	r	306	-	36,50,74	4.15	18 (50%)	29,85,114	3.02	14 (48%)
25	CLA	R	603	-	51,55,73	1.32	8 (15%)	60,91,113	1.43	4 (6%)
24	CHL	4	305	-	40,54,74	3.97	18 (45%)	34,90,114	3.14	14 (41%)
26	OIE	y	303	-	42,45,45	1.15	5 (11%)	51,63,63	1.43	9 (17%)
25	CLA	1	315	10	49,53,73	1.40	9 (18%)	58,89,113	1.44	4 (6%)
33	LMG	B	619	-	41,41,55	0.98	2 (4%)	49,49,63	1.31	4 (8%)
24	CHL	Y	319	-	47,61,74	3.61	19 (40%)	41,98,114	3.01	18 (43%)
25	CLA	5	316	-	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
29	OUR	8	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.82	14 (23%)
24	CHL	g	309	-	37,51,74	4.27	18 (48%)	30,86,114	3.32	15 (50%)
25	CLA	y	307	17	57,61,73	1.27	9 (15%)	67,98,113	1.39	6 (8%)
30	LHG	y	319	25	42,42,48	1.20	5 (11%)	45,48,54	1.09	3 (6%)
26	OIE	5	302	-	42,45,45	1.13	6 (14%)	51,63,63	1.49	10 (19%)
25	CLA	g	315	-	64,68,73	1.21	9 (14%)	76,107,113	1.28	5 (6%)
24	CHL	2	312	-	40,54,74	3.92	19 (47%)	34,90,114	3.13	15 (44%)
37	DGD	c	619	-	56,56,67	0.96	3 (5%)	70,70,81	1.24	5 (7%)
25	CLA	a	604	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
24	CHL	4	311	-	38,52,74	4.04	18 (47%)	31,87,114	3.25	14 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	4	314	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	5 (9%)
24	CHL	7	313	-	37,51,74	4.01	18 (48%)	30,86,114	3.21	14 (46%)
25	CLA	d	405	21	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
25	CLA	B	611	18	69,73,73	1.16	8 (11%)	82,113,113	1.38	6 (7%)
24	CHL	n	305	-	54,68,74	3.39	19 (35%)	50,106,114	2.73	18 (36%)
25	CLA	7	317	12	56,60,73	1.29	9 (16%)	65,97,113	1.40	5 (7%)
25	CLA	p	307	12	60,64,73	1.24	9 (15%)	71,102,113	1.38	6 (8%)
26	OIE	9	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.67	13 (25%)
25	CLA	1	316	10	46,50,73	1.41	9 (19%)	53,85,113	1.44	4 (7%)
25	CLA	s	410	-	59,63,73	1.23	9 (15%)	70,101,113	1.33	6 (8%)
32	SQD	b	618	-	52,54,54	0.96	3 (5%)	62,65,65	1.50	11 (17%)
24	CHL	8	307	17	37,51,74	4.03	18 (48%)	30,86,114	3.19	14 (46%)
25	CLA	8	313	17	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
28	NEX	r	301	-	40,46,46	1.23	3 (7%)	50,70,70	2.65	16 (32%)
30	LHG	n	318	-	42,42,48	1.22	6 (14%)	45,48,54	0.98	2 (4%)
26	OIE	7	302	-	42,45,45	1.14	6 (14%)	51,63,63	1.57	13 (25%)
25	CLA	C	609	20	69,73,73	1.16	9 (13%)	82,113,113	1.35	7 (8%)
28	NEX	5	304	-	40,46,46	1.11	3 (7%)	50,70,70	4.73	18 (36%)
25	CLA	g	317	17	59,63,73	1.25	9 (15%)	69,100,113	1.35	6 (8%)
25	CLA	B	614	18	60,64,73	1.23	9 (15%)	71,102,113	1.32	5 (7%)
25	CLA	C	601	20	69,73,73	1.15	8 (11%)	82,113,113	1.35	7 (8%)
26	OIE	3	302	-	41,44,45	1.13	6 (14%)	48,60,63	1.56	11 (22%)
37	DGD	C	619	-	51,51,67	0.94	2 (3%)	65,65,81	1.23	5 (7%)
24	CHL	q	303	17	48,62,74	3.65	19 (39%)	43,99,114	2.86	16 (37%)
24	CHL	6	312	-	37,51,74	4.20	18 (48%)	30,86,114	3.16	12 (40%)
25	CLA	q	305	17	58,62,73	1.26	9 (15%)	68,99,113	1.37	6 (8%)
29	OUR	4	301	-	50,53,58	1.01	1 (2%)	59,72,77	1.95	16 (27%)
24	CHL	q	307	17	37,51,74	4.05	18 (48%)	30,86,114	3.17	14 (46%)
25	CLA	b	606	18	69,73,73	1.14	10 (14%)	82,113,113	1.35	8 (9%)
25	CLA	p	314	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	6 (8%)
24	CHL	Y	304	17	60,74,74	3.10	19 (31%)	58,114,114	2.80	17 (29%)
29	OUR	p	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.65	12 (20%)
24	CHL	S	602	13	52,66,74	3.37	19 (36%)	48,104,114	2.94	19 (39%)
24	CHL	y	305	17	60,74,74	3.10	19 (31%)	58,114,114	2.78	15 (25%)
28	NEX	R	616	-	40,46,46	1.12	3 (7%)	50,70,70	4.72	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	606	20	57,61,73	1.26	9 (15%)	67,98,113	1.39	6 (8%)
25	CLA	Y	316	17	59,63,73	1.24	9 (15%)	69,100,113	1.38	5 (7%)
25	CLA	S	610	-	49,53,73	1.36	9 (18%)	58,89,113	1.40	4 (6%)
24	CHL	5	305	11	38,52,74	4.02	18 (47%)	31,87,114	3.12	15 (48%)
25	CLA	b	605	18	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
26	OIE	u	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.48	12 (23%)
29	OUR	1	301	-	50,53,58	1.01	2 (4%)	59,72,77	1.95	15 (25%)
24	CHL	9	310	-	40,54,74	4.08	18 (45%)	34,90,114	3.05	14 (41%)
29	OUR	g	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.82	17 (28%)
24	CHL	9	312	-	37,51,74	4.18	18 (48%)	30,86,114	3.27	14 (46%)
31	8CT	A	608	-	40,41,41	4.77	23 (57%)	51,56,56	2.80	18 (35%)
26	OIE	n	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.54	12 (23%)
24	CHL	9	304	12	60,74,74	3.30	18 (30%)	58,114,114	2.43	17 (29%)
25	CLA	G	307	-	57,61,73	1.29	8 (14%)	67,98,113	1.33	5 (7%)
25	CLA	B	613	18	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
25	CLA	4	316	-	46,50,73	1.41	8 (17%)	53,85,113	1.43	4 (7%)
25	CLA	c	610	-	69,73,73	1.15	10 (14%)	82,113,113	1.29	7 (8%)
30	LHG	9	318	25	42,42,48	1.22	6 (14%)	45,48,54	0.99	2 (4%)
25	CLA	S	604	-	47,51,73	1.36	7 (14%)	55,86,113	1.43	4 (7%)
25	CLA	1	314	-	45,49,73	1.41	8 (17%)	54,84,113	1.49	5 (9%)
25	CLA	d	404	21	69,73,73	1.15	10 (14%)	82,113,113	1.32	8 (9%)
28	NEX	u	304	-	40,46,46	1.11	3 (7%)	50,70,70	4.73	18 (36%)
25	CLA	D	405	21	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
29	OUR	7	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.64	12 (20%)
24	CHL	5	312	-	40,54,74	3.91	19 (47%)	34,90,114	3.14	15 (44%)
34	OEX	a	602	19	0,15,15	-	-	-	-	-
25	CLA	c	604	-	69,73,73	1.14	9 (13%)	82,113,113	1.32	6 (7%)
25	CLA	G	315	-	64,68,73	1.21	9 (14%)	76,107,113	1.28	5 (6%)
24	CHL	g	318	17	36,50,74	4.11	17 (47%)	29,85,114	3.08	14 (48%)
24	CHL	u	312	-	41,55,74	3.98	18 (43%)	35,91,114	3.03	14 (40%)
35	PHO	a	606	-	58,69,69	2.04	11 (18%)	55,99,99	1.43	6 (10%)
28	NEX	2	304	-	40,46,46	1.11	3 (7%)	50,70,70	4.72	18 (36%)
25	CLA	b	616	18	51,55,73	1.33	7 (13%)	60,91,113	1.46	5 (8%)
25	CLA	S	609	-	59,63,73	1.23	9 (15%)	70,101,113	1.32	6 (8%)
25	CLA	c	611	20	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	607	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	4 (4%)
25	CLA	s	412	13	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
24	CHL	1	317	-	36,50,74	4.34	17 (47%)	29,85,114	3.20	15 (51%)
30	LHG	A	612	-	43,43,48	1.20	5 (11%)	46,49,54	1.03	3 (6%)
25	CLA	n	315	17	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
31	8CT	V	401	-	40,41,41	4.80	23 (57%)	51,56,56	2.64	19 (37%)
26	0IE	7	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.47	10 (19%)
25	CLA	Y	314	30	67,71,73	1.16	7 (10%)	79,110,113	1.25	5 (6%)
24	CHL	G	310	-	41,55,74	4.00	18 (43%)	35,91,114	3.01	16 (45%)
23	HEM	E	201	2	50,50,50	1.36	8 (16%)	67,82,82	1.01	1 (1%)
24	CHL	3	311	-	38,52,74	4.06	17 (44%)	31,87,114	3.24	13 (41%)
24	CHL	8	310	-	50,64,74	3.45	19 (38%)	46,102,114	2.79	19 (41%)
25	CLA	r	304	-	51,55,73	1.32	8 (15%)	60,91,113	1.44	4 (6%)
30	LHG	7	319	25	36,36,48	1.30	6 (16%)	39,42,54	1.09	2 (5%)
25	CLA	5	308	-	54,58,73	1.30	9 (16%)	64,95,113	1.42	6 (9%)
30	LHG	D	408	-	38,38,48	1.26	6 (15%)	41,44,54	1.07	2 (4%)
26	0IE	2	302	-	42,45,45	1.13	6 (14%)	51,63,63	1.48	10 (19%)
25	CLA	9	316	12	59,63,73	1.27	9 (15%)	69,100,113	1.32	5 (7%)
24	CHL	q	310	-	44,58,74	3.66	19 (43%)	37,94,114	3.20	14 (37%)
24	CHL	8	309	-	44,58,74	3.65	19 (43%)	37,94,114	3.24	14 (37%)
25	CLA	5	307	11	47,51,73	1.38	9 (19%)	55,86,113	1.44	4 (7%)
26	0IE	g	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.47	10 (19%)
24	CHL	g	313	-	60,74,74	3.36	19 (31%)	58,114,114	2.47	16 (27%)
33	LMG	D	401	-	48,48,55	0.92	2 (4%)	56,56,63	1.18	5 (8%)
25	CLA	n	314	-	67,71,73	1.19	8 (11%)	79,110,113	1.28	6 (7%)
29	0UR	q	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.83	15 (25%)
29	0UR	G	301	-	50,53,58	0.96	1 (2%)	59,72,77	1.85	17 (28%)
24	CHL	n	311	-	44,58,74	3.75	18 (40%)	37,94,114	3.04	16 (43%)
24	CHL	4	308	10	37,51,74	4.22	17 (45%)	30,86,114	3.33	16 (53%)
25	CLA	b	610	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
24	CHL	y	310	-	41,55,74	3.79	19 (46%)	35,91,114	3.32	16 (45%)
31	8CT	c	615	-	40,41,41	4.77	23 (57%)	51,56,56	2.79	19 (37%)
25	CLA	Y	315	17	49,53,73	1.36	8 (16%)	58,89,113	1.51	4 (6%)
25	CLA	8	311	-	59,63,73	1.24	9 (15%)	70,101,113	1.37	6 (8%)
25	CLA	R	612	-	49,53,73	1.38	7 (14%)	58,89,113	1.45	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	p	312	-	41,55,74	3.78	19 (46%)	35,91,114	3.38	16 (45%)
25	CLA	n	306	17	58,62,73	1.27	9 (15%)	68,99,113	1.36	6 (8%)
25	CLA	9	307	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	5 (7%)
26	OIE	N	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.55	12 (23%)
30	LHG	Y	318	25	42,42,48	1.20	5 (11%)	45,48,54	1.11	3 (6%)
24	CHL	q	316	-	36,50,74	4.29	18 (50%)	29,85,114	3.17	13 (44%)
28	NEX	r	317	-	40,46,46	1.12	3 (7%)	50,70,70	4.73	18 (36%)
24	CHL	8	303	17	48,62,74	3.66	19 (39%)	43,99,114	2.88	17 (39%)
25	CLA	5	314	-	59,63,73	1.24	9 (15%)	70,101,113	1.34	5 (7%)
25	CLA	y	314	17	59,63,73	1.24	9 (15%)	70,101,113	1.36	7 (10%)
25	CLA	p	316	-	49,53,73	1.37	9 (18%)	58,89,113	1.44	4 (6%)
25	CLA	3	307	-	47,51,73	1.37	8 (17%)	55,86,113	1.44	4 (7%)
29	OUR	5	301	-	50,53,58	1.01	3 (6%)	59,72,77	1.80	14 (23%)
24	CHL	1	312	10	40,54,74	3.98	19 (47%)	34,90,114	3.10	17 (50%)
33	LMG	C	618	-	42,42,55	1.00	2 (4%)	50,50,63	1.24	4 (8%)
24	CHL	4	317	-	36,50,74	4.33	17 (47%)	29,85,114	3.21	15 (51%)
24	CHL	s	406	-	40,54,74	3.91	19 (47%)	34,90,114	3.09	16 (47%)
24	CHL	p	309	12	37,51,74	4.26	18 (48%)	30,86,114	3.34	15 (50%)
25	CLA	9	314	30	67,71,73	1.19	8 (11%)	79,110,113	1.31	6 (7%)
36	BCT	A	611	38	3,3,3	1.12	0	2,3,3	4.21	2 (100%)
24	CHL	1	304	-	36,50,74	4.29	18 (50%)	29,85,114	3.25	14 (48%)
24	CHL	S	601	13	40,54,74	3.84	19 (47%)	34,90,114	3.19	16 (47%)
24	CHL	7	311	-	40,54,74	3.97	19 (47%)	34,90,114	3.11	14 (41%)
29	OUR	3	301	-	50,53,58	0.95	1 (2%)	59,72,77	1.74	12 (20%)
24	CHL	9	311	-	41,55,74	3.98	18 (43%)	35,91,114	3.06	14 (40%)
24	CHL	1	305	10	40,54,74	3.97	18 (45%)	34,90,114	3.15	15 (44%)
24	CHL	g	305	17	60,74,74	3.26	18 (30%)	58,114,114	2.42	16 (27%)
24	CHL	s	409	-	41,55,74	3.90	19 (46%)	35,91,114	3.16	17 (48%)
25	CLA	r	314	-	51,55,73	1.36	7 (13%)	60,91,113	1.35	5 (8%)
25	CLA	n	307	-	54,58,73	1.30	9 (16%)	64,95,113	1.40	6 (9%)
25	CLA	3	314	-	45,49,73	1.40	7 (15%)	54,84,113	1.44	6 (11%)
31	8CT	C	614	-	40,41,41	4.71	23 (57%)	51,56,56	2.79	21 (41%)
25	CLA	n	316	-	47,51,73	1.38	9 (19%)	55,86,113	1.39	4 (7%)
25	CLA	c	605	20	60,64,73	1.23	9 (15%)	71,102,113	1.37	6 (8%)
24	CHL	s	414	-	36,50,74	4.01	18 (50%)	29,85,114	3.16	15 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	g	308	-	54,58,73	1.30	8 (14%)	64,95,113	1.38	6 (9%)
24	CHL	7	306	-	58,72,74	3.17	19 (32%)	55,111,114	2.80	18 (32%)
29	OUR	u	301	-	50,53,58	0.95	1 (2%)	59,72,77	1.86	15 (25%)
31	8CT	d	410	-	40,41,41	4.83	23 (57%)	51,56,56	2.56	19 (37%)
25	CLA	S	612	-	59,63,73	1.25	9 (15%)	69,100,113	1.35	5 (7%)
25	CLA	B	605	18	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
26	OIE	4	302	-	42,45,45	1.13	6 (14%)	51,63,63	1.54	12 (23%)
26	OIE	G	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.48	10 (19%)
24	CHL	G	313	-	60,74,74	3.35	19 (31%)	58,114,114	2.48	15 (25%)
24	CHL	Y	312	-	60,74,74	3.17	19 (31%)	58,114,114	2.56	19 (32%)
25	CLA	b	607	18	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
25	CLA	s	411	-	47,52,73	1.42	10 (21%)	55,87,113	1.42	4 (7%)
29	OUR	9	301	-	50,53,58	0.94	1 (2%)	59,72,77	1.82	13 (22%)
24	CHL	G	305	17	60,74,74	3.26	18 (30%)	58,114,114	2.43	17 (29%)
25	CLA	b	613	18	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
25	CLA	q	313	-	67,71,73	1.17	9 (13%)	79,110,113	1.27	6 (7%)
25	CLA	q	306	28	54,58,73	1.29	9 (16%)	64,95,113	1.38	7 (10%)
24	CHL	p	311	-	40,54,74	3.97	19 (47%)	34,90,114	3.03	14 (41%)
26	OIE	G	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.53	10 (19%)
25	CLA	s	405	-	47,51,73	1.36	8 (17%)	55,86,113	1.43	4 (7%)
25	CLA	n	313	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	6 (8%)
24	CHL	S	605	-	40,54,74	3.91	19 (47%)	34,90,114	3.11	16 (47%)
28	NEX	p	304	-	40,46,46	1.12	3 (7%)	50,70,70	4.73	19 (38%)
25	CLA	2	308	-	54,58,73	1.30	9 (16%)	64,95,113	1.43	6 (9%)
25	CLA	A	610	-	45,49,73	1.42	7 (15%)	54,84,113	1.50	6 (11%)
28	NEX	N	303	-	40,46,46	1.23	3 (7%)	50,70,70	2.66	16 (32%)
24	CHL	2	313	-	36,50,74	4.15	18 (50%)	29,85,114	3.04	13 (44%)
24	CHL	Y	309	-	41,55,74	3.78	19 (46%)	35,91,114	3.38	16 (45%)
25	CLA	2	317	-	53,57,73	1.30	9 (16%)	61,93,113	1.41	5 (8%)
28	NEX	3	318	-	40,46,46	1.23	3 (7%)	50,70,70	2.65	16 (32%)
25	CLA	S	603	-	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
25	CLA	B	612	18	69,73,73	1.14	9 (13%)	82,113,113	1.34	8 (9%)
30	LHG	d	407	-	48,48,48	1.12	5 (10%)	51,54,54	0.98	2 (3%)
25	CLA	a	607	19	64,68,73	1.19	8 (12%)	76,107,113	1.41	8 (10%)
25	CLA	S	611	13	49,53,73	1.36	9 (18%)	58,89,113	1.45	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	4	310	-	37,51,74	4.08	17 (45%)	30,86,114	3.20	13 (43%)
25	CLA	1	307	-	45,49,73	1.40	8 (17%)	54,84,113	1.46	6 (11%)
24	CHL	q	309	-	47,61,74	3.60	19 (40%)	41,98,114	2.98	19 (46%)
25	CLA	5	317	11	53,57,73	1.30	9 (16%)	61,93,113	1.43	5 (8%)
25	CLA	6	313	-	45,49,73	1.41	7 (15%)	54,84,113	1.50	6 (11%)
24	CHL	G	309	-	37,51,74	4.27	18 (48%)	30,86,114	3.31	15 (50%)
24	CHL	6	308	-	37,51,74	4.22	18 (48%)	30,86,114	3.25	15 (50%)
29	OUR	2	301	-	50,53,58	1.02	3 (6%)	59,72,77	1.80	14 (23%)
25	CLA	C	608	20	65,69,73	1.19	10 (15%)	77,108,113	1.36	7 (9%)
24	CHL	n	308	17	37,51,74	4.16	17 (45%)	30,86,114	3.14	15 (50%)
24	CHL	R	608	-	40,54,74	3.93	19 (47%)	34,90,114	3.23	14 (41%)
30	LHG	a	601	-	44,44,48	1.17	5 (11%)	47,50,54	0.99	2 (4%)
30	LHG	g	319	-	42,42,48	1.21	6 (14%)	45,48,54	1.00	2 (4%)
25	CLA	y	315	30	67,71,73	1.16	7 (10%)	79,110,113	1.25	5 (6%)
26	OIE	5	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.45	10 (19%)
24	CHL	5	313	-	36,50,74	4.15	18 (50%)	29,85,114	3.05	14 (48%)
25	CLA	A	607	19	64,68,73	1.18	8 (12%)	76,107,113	1.40	8 (10%)
24	CHL	u	313	-	37,51,74	4.20	17 (45%)	30,86,114	3.23	14 (46%)
25	CLA	9	313	-	59,63,73	1.26	7 (11%)	70,101,113	1.35	6 (8%)
35	PHO	A	606	-	58,69,69	2.05	11 (18%)	55,99,99	1.43	6 (10%)
28	NEX	G	304	-	40,46,46	1.12	3 (7%)	50,70,70	4.73	18 (36%)
24	CHL	6	305	-	42,56,74	3.84	19 (45%)	36,92,114	3.11	17 (47%)
25	CLA	G	308	-	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
25	CLA	B	604	18	66,70,73	1.19	7 (10%)	78,109,113	1.41	7 (8%)
25	CLA	b	602	18	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
26	OIE	6	302	-	41,44,45	1.14	6 (14%)	48,60,63	1.58	11 (22%)
24	CHL	u	306	-	58,72,74	3.32	18 (31%)	55,111,114	2.53	19 (34%)
35	PHO	d	403	-	58,69,69	2.04	9 (15%)	55,99,99	1.49	7 (12%)
24	CHL	y	312	-	45,59,74	3.64	19 (42%)	40,96,114	2.98	17 (42%)
28	NEX	n	303	-	40,46,46	1.22	3 (7%)	50,70,70	2.65	16 (32%)
25	CLA	4	307	28	45,49,73	1.41	9 (20%)	54,84,113	1.47	6 (11%)
24	CHL	r	308	-	42,56,74	3.79	19 (45%)	36,92,114	3.20	15 (41%)
25	CLA	A	604	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
25	CLA	C	610	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)
31	8CT	S	615	-	40,41,41	4.85	24 (60%)	51,56,56	6.92	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	NEX	s	401	25	40,46,46	1.23	3 (7%)	50,70,70	2.65	16 (32%)
25	CLA	g	314	-	59,63,73	1.26	9 (15%)	70,101,113	1.34	6 (8%)
31	8CT	v	401	-	40,41,41	4.81	23 (57%)	51,56,56	2.63	19 (37%)
25	CLA	9	306	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	5 (7%)
24	CHL	G	306	17	58,72,74	3.29	19 (32%)	55,111,114	2.65	19 (34%)
24	CHL	r	307	-	42,56,74	3.84	18 (42%)	36,92,114	3.09	15 (41%)
24	CHL	6	310	-	40,54,74	4.08	18 (45%)	34,90,114	3.05	12 (35%)
30	LHG	d	408	-	38,38,48	0.99	3 (7%)	41,44,54	1.26	4 (9%)
26	OIE	R	614	-	42,45,45	1.14	6 (14%)	51,63,63	1.48	11 (21%)
25	CLA	R	604	-	45,49,73	1.40	9 (20%)	54,84,113	1.52	6 (11%)
24	CHL	6	317	12	36,50,74	4.22	18 (50%)	29,85,114	3.20	13 (44%)
24	CHL	r	309	-	40,54,74	3.93	19 (47%)	34,90,114	3.23	14 (41%)
25	CLA	c	607	-	69,73,73	1.15	8 (11%)	82,113,113	1.32	4 (4%)
26	OIE	u	303	-	42,45,45	1.11	6 (14%)	51,63,63	1.58	10 (19%)
30	LHG	a	612	-	43,43,48	1.20	5 (11%)	46,49,54	1.03	3 (6%)
24	CHL	l	311	-	38,52,74	4.02	18 (47%)	31,87,114	3.29	14 (45%)
24	CHL	g	310	-	41,55,74	4.01	18 (43%)	35,91,114	3.04	16 (45%)
24	CHL	n	317	-	36,50,74	4.33	18 (50%)	29,85,114	3.26	16 (55%)
24	CHL	5	310	-	36,50,74	4.07	18 (50%)	29,85,114	3.03	14 (48%)
24	CHL	l	310	-	37,51,74	4.09	17 (45%)	30,86,114	3.19	13 (43%)
24	CHL	r	302	8	40,54,74	4.07	18 (45%)	34,90,114	3.08	14 (41%)
25	CLA	r	312	8	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
32	SQD	a	609	-	43,45,54	1.05	3 (6%)	53,56,65	1.59	10 (18%)
25	CLA	C	612	20	58,62,73	1.24	9 (15%)	68,99,113	1.42	5 (7%)
32	SQD	d	409	-	42,44,54	1.06	3 (7%)	52,55,65	1.50	8 (15%)
25	CLA	7	307	12	60,64,73	1.24	9 (15%)	71,102,113	1.38	6 (8%)
25	CLA	D	404	21	69,73,73	1.15	10 (14%)	82,113,113	1.31	8 (9%)
25	CLA	c	612	20	58,62,73	1.25	9 (15%)	68,99,113	1.41	6 (8%)
25	CLA	b	601	-	49,53,73	1.36	9 (18%)	58,89,113	1.44	4 (6%)
35	PHO	D	403	-	58,69,69	2.04	10 (17%)	55,99,99	1.49	7 (12%)
25	CLA	4	313	-	59,63,73	1.27	9 (15%)	70,101,113	1.34	6 (8%)
25	CLA	G	317	-	59,63,73	1.25	8 (13%)	69,100,113	1.35	5 (7%)
24	CHL	7	305	12	60,74,74	3.13	19 (31%)	58,114,114	2.82	17 (29%)
25	CLA	B	606	18	69,73,73	1.14	9 (13%)	82,113,113	1.35	8 (9%)
25	CLA	B	603	18	69,73,73	1.16	8 (11%)	82,113,113	1.29	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	2	310	-	36,50,74	4.08	18 (50%)	29,85,114	3.03	14 (48%)
24	CHL	p	313	-	37,51,74	4.02	18 (48%)	30,86,114	3.20	14 (46%)
24	CHL	G	311	-	48,62,74	3.68	18 (37%)	43,99,114	2.84	16 (37%)
25	CLA	q	314	17	49,53,73	1.38	9 (18%)	58,89,113	1.46	4 (6%)
24	CHL	g	311	-	48,62,74	3.70	18 (37%)	43,99,114	2.77	16 (37%)
25	CLA	8	305	17	58,62,73	1.26	9 (15%)	68,99,113	1.36	6 (8%)
33	LMG	W	201	-	30,30,55	1.14	2 (6%)	38,38,63	1.39	6 (15%)
24	CHL	3	309	-	45,59,74	3.84	18 (40%)	40,96,114	2.91	17 (42%)
27	XAT	R	615	-	41,47,47	0.91	1 (2%)	54,74,74	2.65	21 (38%)
25	CLA	R	610	-	49,53,73	1.36	8 (16%)	58,89,113	1.43	6 (10%)
24	CHL	q	311	-	50,64,74	3.44	19 (38%)	46,102,114	2.80	19 (41%)
24	CHL	l	308	10	37,51,74	4.21	18 (48%)	30,86,114	3.32	15 (50%)
25	CLA	B	616	18	51,55,73	1.33	7 (13%)	60,91,113	1.46	4 (6%)
24	CHL	3	310	-	40,54,74	4.07	18 (45%)	34,90,114	3.06	12 (35%)
26	OIE	p	302	-	42,45,45	1.14	6 (14%)	51,63,63	1.57	13 (25%)
24	CHL	Y	308	17	37,51,74	4.04	18 (48%)	30,86,114	3.17	13 (43%)
31	8CT	B	617	-	40,41,41	4.78	23 (57%)	51,56,56	2.97	18 (35%)
24	CHL	y	318	17	36,50,74	3.96	18 (50%)	29,85,114	3.10	17 (58%)
24	CHL	u	310	-	40,54,74	4.09	18 (45%)	34,90,114	3.07	14 (41%)
25	CLA	B	608	-	59,63,73	1.25	9 (15%)	70,101,113	1.34	6 (8%)
24	CHL	p	305	12	60,74,74	3.14	19 (31%)	58,114,114	2.79	17 (29%)
24	CHL	s	403	13	52,66,74	3.37	19 (36%)	48,104,114	2.93	19 (39%)
26	OIE	r	315	-	42,45,45	1.14	6 (14%)	51,63,63	1.49	11 (21%)
25	CLA	g	316	17	49,53,73	1.38	9 (18%)	58,89,113	1.46	4 (6%)
30	LHG	c	617	-	31,31,48	1.36	6 (19%)	34,37,54	1.15	3 (8%)
39	PL9	D	406	-	55,55,55	1.64	12 (21%)	68,69,69	1.53	13 (19%)
24	CHL	n	304	17	48,62,74	3.72	19 (39%)	43,99,114	2.79	16 (37%)
24	CHL	u	305	12	60,74,74	3.35	18 (30%)	58,114,114	2.47	18 (31%)
24	CHL	Y	305	-	58,72,74	3.16	19 (32%)	55,111,114	2.69	20 (36%)
24	CHL	g	306	-	58,72,74	3.27	19 (32%)	55,111,114	2.71	19 (34%)
24	CHL	y	309	17	37,51,74	4.04	18 (48%)	30,86,114	3.18	13 (43%)
26	OIE	2	303	-	42,45,45	1.12	6 (14%)	51,63,63	1.45	10 (19%)
24	CHL	N	305	-	54,68,74	3.39	19 (35%)	50,106,114	2.71	18 (36%)
30	LHG	5	319	-	42,42,48	1.21	6 (14%)	45,48,54	1.05	3 (6%)
24	CHL	n	310	-	47,61,74	3.73	18 (38%)	41,98,114	2.90	16 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	603	20	69,73,73	1.15	9 (13%)	82,113,113	1.32	8 (9%)
25	CLA	8	306	-	54,58,73	1.29	9 (16%)	64,95,113	1.38	7 (10%)
28	NEX	6	303	-	40,46,46	1.23	3 (7%)	50,70,70	2.66	16 (32%)
25	CLA	4	315	10	49,53,73	1.39	9 (18%)	58,89,113	1.44	4 (6%)
30	LHG	2	319	-	39,39,48	1.25	6 (15%)	42,45,54	1.07	3 (7%)
31	8CT	T	101	-	40,41,41	4.78	23 (57%)	51,56,56	3.07	17 (33%)
24	CHL	2	305	11	38,52,74	4.03	18 (47%)	31,87,114	3.12	14 (45%)
25	CLA	u	308	-	54,58,73	1.32	8 (14%)	64,95,113	1.39	6 (9%)
31	8CT	t	101	-	40,41,41	4.78	23 (57%)	51,56,56	3.08	17 (33%)
29	OUR	n	301	-	50,53,58	0.95	1 (2%)	59,72,77	1.84	13 (22%)
25	CLA	N	313	-	59,63,73	1.25	8 (13%)	70,101,113	1.36	6 (8%)
33	LMG	D	411	-	46,46,55	0.96	2 (4%)	54,54,63	1.14	4 (7%)
24	CHL	S	607	-	40,54,74	3.90	19 (47%)	34,90,114	3.09	17 (50%)
25	CLA	N	306	17	58,62,73	1.27	9 (15%)	68,99,113	1.36	6 (8%)
25	CLA	u	317	12	59,63,73	1.28	8 (13%)	69,100,113	1.34	5 (7%)
37	DGD	C	620	-	56,56,67	0.95	2 (3%)	70,70,81	1.22	5 (7%)
24	CHL	Y	317	17	36,50,74	3.97	18 (50%)	29,85,114	3.10	17 (58%)
25	CLA	r	311	-	49,53,73	1.36	9 (18%)	58,89,113	1.44	6 (10%)
25	CLA	G	316	17	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)
24	CHL	6	311	-	38,52,74	4.04	17 (44%)	31,87,114	3.24	13 (41%)
25	CLA	1	313	-	59,63,73	1.26	8 (13%)	70,101,113	1.35	6 (8%)
25	CLA	1	306	-	47,52,73	1.37	7 (14%)	55,87,113	1.43	5 (9%)
25	CLA	u	307	-	60,64,73	1.26	8 (13%)	71,102,113	1.33	5 (7%)
28	NEX	S	617	-	40,46,46	1.11	3 (7%)	50,70,70	4.73	18 (36%)
25	CLA	C	604	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
31	8CT	s	416	-	40,41,41	4.87	24 (60%)	51,56,56	6.92	21 (41%)
24	CHL	6	304	12	42,56,74	3.93	19 (45%)	36,92,114	2.95	15 (41%)
24	CHL	3	312	-	37,51,74	4.20	17 (45%)	30,86,114	3.15	12 (40%)
25	CLA	b	614	18	60,64,73	1.23	10 (16%)	71,102,113	1.33	5 (7%)
29	OUR	6	301	-	50,53,58	0.95	1 (2%)	59,72,77	1.82	15 (25%)
30	LHG	N	318	-	42,42,48	1.22	6 (14%)	45,48,54	0.98	2 (4%)
25	CLA	Y	306	17	57,61,73	1.27	9 (15%)	67,98,113	1.39	6 (8%)
25	CLA	r	310	8	59,63,73	1.24	9 (15%)	70,101,113	1.34	6 (8%)
26	OIE	Y	302	-	42,45,45	1.15	6 (14%)	51,63,63	1.51	11 (21%)
33	LMG	d	401	-	48,48,55	0.92	2 (4%)	56,56,63	1.20	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	7	315	30	67,71,73	1.17	9 (13%)	79,110,113	1.36	6 (7%)
24	CHL	2	318	11	36,50,74	4.21	17 (47%)	29,85,114	3.20	17 (58%)
25	CLA	C	602	20	69,73,73	1.16	8 (11%)	82,113,113	1.31	6 (7%)
24	CHL	2	309	11	37,51,74	4.15	18 (48%)	30,86,114	3.20	16 (53%)
28	NEX	y	304	-	40,46,46	1.12	3 (7%)	50,70,70	4.72	18 (36%)
25	CLA	c	616	20	50,54,73	1.32	8 (16%)	59,90,113	1.47	6 (10%)
25	CLA	R	609	8	59,63,73	1.24	9 (15%)	70,101,113	1.35	6 (8%)
24	CHL	8	315	-	36,50,74	4.29	18 (50%)	29,85,114	3.20	14 (48%)
25	CLA	3	315	12	49,53,73	1.39	9 (18%)	58,89,113	1.44	4 (6%)
25	CLA	N	315	17	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
30	LHG	G	319	-	42,42,48	1.21	6 (14%)	45,48,54	1.00	2 (4%)
24	CHL	N	304	17	48,62,74	3.72	19 (39%)	43,99,114	2.78	16 (37%)
25	CLA	Y	313	17	59,63,73	1.24	9 (15%)	70,101,113	1.36	7 (10%)
24	CHL	1	309	-	37,51,74	4.19	18 (48%)	30,86,114	3.25	14 (46%)
25	CLA	Y	307	-	54,58,73	1.29	9 (16%)	64,95,113	1.43	8 (12%)
24	CHL	5	311	-	41,55,74	3.96	19 (46%)	35,91,114	2.98	14 (40%)
25	CLA	c	606	20	57,61,73	1.27	9 (15%)	67,98,113	1.39	6 (8%)
25	CLA	8	312	-	67,71,73	1.18	9 (13%)	79,110,113	1.28	6 (7%)
34	OEX	A	602	19	0,15,15	-	-	-		
25	CLA	R	611	8	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
25	CLA	a	610	-	45,49,73	1.42	7 (15%)	54,84,113	1.49	6 (11%)
25	CLA	N	316	-	47,51,73	1.39	8 (17%)	55,86,113	1.39	4 (7%)
24	CHL	N	317	-	36,50,74	4.33	18 (50%)	29,85,114	3.25	15 (51%)
31	8CT	C	613	-	40,41,41	4.74	23 (57%)	51,56,56	2.80	20 (39%)
25	CLA	G	314	-	59,63,73	1.25	9 (15%)	70,101,113	1.33	6 (8%)
24	CHL	R	607	-	42,56,74	3.79	19 (45%)	36,92,114	3.21	15 (41%)
24	CHL	R	602	-	41,55,74	3.81	18 (43%)	35,91,114	3.31	16 (45%)
24	CHL	s	407	-	40,54,74	3.97	19 (47%)	34,90,114	3.02	14 (41%)
24	CHL	p	310	-	40,54,74	4.02	19 (47%)	34,90,114	3.06	14 (41%)
25	CLA	6	316	-	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
30	LHG	A	601	-	44,44,48	1.18	5 (11%)	47,50,54	0.99	2 (4%)
25	CLA	b	609	18	69,73,73	1.15	8 (11%)	82,113,113	1.31	7 (8%)
25	CLA	B	602	18	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
25	CLA	p	317	12	59,63,73	1.25	9 (15%)	69,100,113	1.38	6 (8%)
24	CHL	2	306	-	41,55,74	3.82	19 (46%)	35,91,114	3.23	17 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	NEX	1	303	-	40,46,46	1.12	3 (7%)	50,70,70	4.72	18 (36%)
31	8CT	b	617	-	40,41,41	4.80	23 (57%)	51,56,56	2.92	18 (35%)
24	CHL	R	601	8	40,54,74	4.09	19 (47%)	34,90,114	3.07	14 (41%)
24	CHL	S	613	-	36,50,74	4.03	18 (50%)	29,85,114	3.15	15 (51%)
30	LHG	p	319	25	42,42,48	1.22	6 (14%)	45,48,54	1.03	2 (4%)
25	CLA	B	607	18	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
29	OUR	Y	301	-	50,53,58	1.01	2 (4%)	59,72,77	1.71	13 (22%)
31	8CT	a	608	-	40,41,41	4.77	23 (57%)	51,56,56	2.80	18 (35%)
24	CHL	4	309	-	37,51,74	4.18	18 (48%)	30,86,114	3.26	15 (50%)
33	LMG	i	101	-	48,48,55	0.93	2 (4%)	56,56,63	1.21	4 (7%)
24	CHL	u	311	-	40,54,74	4.06	18 (45%)	34,90,114	3.05	14 (41%)
25	CLA	B	610	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
25	CLA	c	608	20	65,69,73	1.18	8 (12%)	77,108,113	1.35	7 (9%)
25	CLA	u	314	-	59,63,73	1.26	6 (10%)	70,101,113	1.34	7 (10%)
31	8CT	D	410	-	40,41,41	4.84	23 (57%)	51,56,56	2.54	20 (39%)
32	SQD	B	618	-	52,54,54	0.96	3 (5%)	62,65,65	1.50	11 (17%)
25	CLA	g	307	-	57,61,73	1.29	8 (14%)	67,98,113	1.32	5 (7%)
25	CLA	q	315	17	47,51,73	1.37	9 (19%)	55,86,113	1.42	4 (7%)
25	CLA	b	611	18	69,73,73	1.16	8 (11%)	82,113,113	1.38	6 (7%)
24	CHL	7	312	-	41,55,74	3.76	19 (46%)	35,91,114	3.41	16 (45%)
24	CHL	Y	310	-	48,62,74	3.52	19 (39%)	43,99,114	3.19	20 (46%)
26	OIE	y	302	-	42,45,45	1.16	6 (14%)	51,63,63	1.49	11 (21%)
25	CLA	6	306	-	45,49,73	1.40	8 (17%)	54,84,113	1.48	6 (11%)
25	CLA	R	613	-	51,55,73	1.36	7 (13%)	60,91,113	1.35	5 (8%)
24	CHL	3	304	12	42,56,74	3.90	19 (45%)	36,92,114	2.92	15 (41%)
24	CHL	7	318	12	36,50,74	4.16	18 (50%)	29,85,114	3.03	13 (44%)
25	CLA	N	314	-	67,71,73	1.18	8 (11%)	79,110,113	1.27	6 (7%)
26	OIE	g	302	-	42,45,45	1.12	6 (14%)	51,63,63	1.53	11 (21%)
24	CHL	u	318	-	36,50,74	4.35	17 (47%)	29,85,114	3.30	15 (51%)
25	CLA	r	313	-	49,53,73	1.38	7 (14%)	58,89,113	1.48	5 (8%)
29	OUR	N	301	-	50,53,58	0.95	1 (2%)	59,72,77	1.85	13 (22%)
25	CLA	7	316	12	49,53,73	1.36	9 (18%)	58,89,113	1.43	4 (6%)
25	CLA	u	316	-	49,53,73	1.39	9 (18%)	58,89,113	1.42	4 (6%)
25	CLA	c	602	20	69,73,73	1.17	8 (11%)	82,113,113	1.31	6 (7%)
24	CHL	5	306	-	41,55,74	3.83	19 (46%)	35,91,114	3.22	17 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	s	413	-	59,63,73	1.24	9 (15%)	69,100,113	1.36	5 (7%)
24	CHL	N	311	-	44,58,74	3.76	19 (43%)	37,94,114	3.01	16 (43%)
24	CHL	r	303	-	41,55,74	3.81	18 (43%)	35,91,114	3.33	16 (45%)
25	CLA	3	316	-	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)
24	CHL	p	318	12	36,50,74	4.16	18 (50%)	29,85,114	3.03	12 (41%)
25	CLA	4	306	-	47,52,73	1.38	8 (17%)	55,87,113	1.44	5 (9%)
25	CLA	B	609	18	69,73,73	1.15	8 (11%)	82,113,113	1.31	7 (8%)
31	8CT	S	614	-	40,41,41	4.85	23 (57%)	51,56,56	3.04	20 (39%)
24	CHL	7	309	12	37,51,74	4.26	18 (48%)	30,86,114	3.36	14 (46%)
25	CLA	2	316	-	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
31	8CT	c	613	-	40,41,41	4.75	23 (57%)	51,56,56	2.78	22 (43%)
36	BCT	a	611	38	3,3,3	1.12	0	2,3,3	4.19	2 (100%)
24	CHL	p	306	-	58,72,74	3.18	19 (32%)	55,111,114	2.79	18 (32%)
25	CLA	y	308	-	54,58,73	1.29	9 (16%)	64,95,113	1.42	8 (12%)
24	CHL	3	305	-	42,56,74	3.85	18 (42%)	36,92,114	3.08	17 (47%)
25	CLA	B	601	-	49,53,73	1.36	9 (18%)	58,89,113	1.44	4 (6%)
25	CLA	r	305	-	45,49,73	1.41	9 (20%)	54,84,113	1.53	7 (12%)
25	CLA	S	616	-	49,53,73	1.36	9 (18%)	58,89,113	1.41	4 (6%)
25	CLA	A	605	-	53,57,73	1.29	8 (15%)	61,93,113	1.42	5 (8%)
25	CLA	y	317	17	59,63,73	1.23	9 (15%)	69,100,113	1.38	5 (7%)
33	LMG	w	201	-	36,36,55	1.06	2 (5%)	44,44,63	1.36	5 (11%)
25	CLA	C	603	20	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
24	CHL	6	309	-	45,59,74	3.83	18 (40%)	40,96,114	2.92	18 (45%)
24	CHL	u	309	12	37,51,74	4.28	18 (48%)	30,86,114	3.26	14 (46%)
26	OIE	Y	303	-	42,45,45	1.14	5 (11%)	51,63,63	1.43	9 (17%)
24	CHL	N	310	-	47,61,74	3.72	19 (40%)	41,98,114	2.89	16 (39%)
25	CLA	8	314	-	47,51,73	1.38	9 (19%)	55,86,113	1.43	5 (9%)
31	8CT	x	601	-	40,41,41	4.77	23 (57%)	51,56,56	2.72	18 (35%)
25	CLA	6	315	12	49,53,73	1.39	9 (18%)	58,89,113	1.45	4 (6%)
28	NEX	7	304	-	40,46,46	1.11	3 (7%)	50,70,70	4.72	18 (36%)
24	CHL	R	606	-	42,56,74	3.84	18 (42%)	36,92,114	3.14	15 (41%)
24	CHL	S	608	-	41,55,74	3.90	19 (46%)	35,91,114	3.19	17 (48%)
32	SQD	A	609	-	43,45,54	1.06	3 (6%)	53,56,65	1.49	10 (18%)
25	CLA	5	315	-	67,71,73	1.18	9 (13%)	79,110,113	1.29	5 (6%)
31	8CT	s	415	-	40,41,41	4.86	23 (57%)	51,56,56	3.04	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	G	312	-	45,59,74	3.82	19 (42%)	40,96,114	2.89	18 (45%)
28	NEX	9	319	-	40,46,46	1.11	3 (7%)	50,70,70	4.72	18 (36%)
24	CHL	4	312	-	40,54,74	3.99	19 (47%)	34,90,114	3.09	16 (47%)
25	CLA	2	307	11	47,51,73	1.37	8 (17%)	55,86,113	1.42	4 (7%)
25	CLA	s	417	-	49,53,73	1.37	8 (16%)	58,89,113	1.41	4 (6%)
33	LMG	d	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.13	4 (7%)
24	CHL	9	309	-	40,54,74	4.08	18 (45%)	34,90,114	3.05	15 (44%)
31	8CT	X	601	-	40,41,41	4.78	23 (57%)	51,56,56	2.71	18 (35%)
29	OUR	y	301	-	50,53,58	1.00	1 (2%)	59,72,77	1.71	13 (22%)
25	CLA	b	608	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	6 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	9	315	-	1/1/11/20	6/15/91/115	-
25	CLA	q	312	-	1/1/13/20	2/27/103/115	-
37	DGD	c	618	-	-	27/39/79/95	0/2/2/2
39	PL9	d	406	-	-	10/53/73/73	0/1/1/1
25	CLA	N	307	-	1/1/12/20	5/21/97/115	-
26	OIE	p	303	-	-	2/33/72/72	0/2/2/2
25	CLA	7	314	-	1/1/13/20	6/27/103/115	-
25	CLA	b	615	18	1/1/15/20	5/39/115/115	-
31	8CT	C	615	-	-	13/29/63/63	0/2/2/2
24	CHL	n	312	-	3/3/18/26	14/27/125/137	-
25	CLA	s	404	-	1/1/11/20	6/15/91/115	-
26	OIE	3	303	-	-	1/33/72/72	0/2/2/2
24	CHL	G	318	17	3/3/15/26	6/10/108/137	-
30	LHG	4	318	-	-	21/46/46/53	-
25	CLA	2	314	-	1/1/13/20	4/27/103/115	-
24	CHL	5	309	11	3/3/15/26	3/12/110/137	-
30	LHG	C	617	-	-	17/36/36/53	-
25	CLA	6	307	-	1/1/10/20	6/13/89/115	-
24	CHL	2	311	-	3/3/16/26	8/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	u	315	-	1/1/14/20	11/37/113/115	-
26	OIE	1	302	-	-	2/33/72/72	0/2/2/2
30	LHG	D	407	-	-	29/53/53/53	-
25	CLA	C	611	20	1/1/15/20	10/39/115/115	-
24	CHL	n	309	-	3/3/16/26	6/15/113/137	-
24	CHL	s	402	13	3/3/16/26	13/15/113/137	-
24	CHL	7	310	-	3/3/16/26	7/15/113/137	-
28	NEX	g	304	-	-	5/27/83/83	0/3/3/3
25	CLA	C	605	20	1/1/13/20	7/29/105/115	-
25	CLA	c	609	20	1/1/15/20	5/39/115/115	-
24	CHL	N	312	-	3/3/18/26	14/27/125/137	-
32	SQD	D	409	-	-	13/39/59/69	0/1/1/1
24	CHL	8	308	-	3/3/16/26	5/15/113/137	-
25	CLA	B	615	18	1/1/15/20	4/39/115/115	-
24	CHL	Y	311	-	3/3/17/26	5/21/119/137	-
25	CLA	b	612	18	1/1/15/20	12/39/115/115	-
24	CHL	g	312	-	3/3/17/26	4/21/119/137	-
25	CLA	3	306	-	1/1/10/20	6/10/86/115	-
25	CLA	6	314	-	1/1/10/20	2/10/86/115	-
26	OIE	9	302	-	-	4/33/72/72	0/2/2/2
24	CHL	N	308	17	3/3/15/26	2/12/110/137	-
23	HEM	f	201	9,2	-	1/14/54/54	-
25	CLA	A	603	19	1/1/15/20	12/39/115/115	-
24	CHL	y	311	-	3/3/17/26	12/25/123/137	-
26	OIE	q	302	-	-	2/33/72/72	0/2/2/2
25	CLA	y	316	17	1/1/11/20	6/15/91/115	-
26	OIE	8	302	-	-	2/33/72/72	0/2/2/2
27	XAT	r	316	-	-	0/31/93/93	0/4/4/4
24	CHL	N	309	-	3/3/16/26	7/15/113/137	-
24	CHL	y	313	-	3/3/20/26	19/39/137/137	-
24	CHL	9	308	12	3/3/15/26	2/12/110/137	-
24	CHL	5	318	11	3/3/15/26	4/10/108/137	-
30	LHG	1	318	-	-	22/46/46/53	-
25	CLA	C	616	20	1/1/11/20	2/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	7	308	-	1/1/12/20	5/21/97/115	-
25	CLA	c	601	20	1/1/15/20	14/39/115/115	-
25	CLA	a	603	19	1/1/15/20	12/39/115/115	-
24	CHL	9	317	-	3/3/15/26	4/10/108/137	-
24	CHL	4	304	-	3/3/15/26	3/10/108/137	-
33	LMG	m	101	-	-	19/36/56/70	0/1/1/1
25	CLA	p	315	30	1/1/14/20	14/37/113/115	-
24	CHL	y	306	-	3/3/19/26	22/37/135/137	-
24	CHL	8	304	17	3/3/18/26	15/32/130/137	-
24	CHL	R	605	-	3/3/15/26	2/10/108/137	-
24	CHL	9	305	-	3/3/19/26	14/37/135/137	-
25	CLA	2	315	-	1/1/14/20	10/37/113/115	-
31	8CT	c	614	-	-	15/29/63/63	0/2/2/2
24	CHL	s	408	-	3/3/16/26	7/15/113/137	-
25	CLA	p	308	-	1/1/12/20	5/21/97/115	-
24	CHL	q	304	17	3/3/18/26	17/32/130/137	-
24	CHL	3	317	12	3/3/15/26	2/10/108/137	-
24	CHL	S	606	-	3/3/16/26	8/15/113/137	-
24	CHL	3	308	-	3/3/15/26	4/12/110/137	-
25	CLA	a	605	-	1/1/11/20	6/20/96/115	-
28	NEX	4	303	25	-	5/27/83/83	0/3/3/3
24	CHL	q	308	-	3/3/16/26	5/15/113/137	-
25	CLA	3	313	-	1/1/10/20	2/10/86/115	-
25	CLA	b	603	18	1/1/15/20	11/39/115/115	-
25	CLA	b	604	18	1/1/14/20	14/36/112/115	-
24	CHL	r	306	-	3/3/15/26	4/10/108/137	-
25	CLA	R	603	-	1/1/11/20	5/18/94/115	-
24	CHL	4	305	-	3/3/16/26	8/15/113/137	-
26	OIE	y	303	-	-	0/33/72/72	0/2/2/2
25	CLA	1	315	10	1/1/11/20	8/15/91/115	-
33	LMG	B	619	-	-	20/36/56/70	0/1/1/1
24	CHL	Y	319	-	3/3/17/26	7/24/122/137	-
25	CLA	5	316	-	1/1/11/20	4/15/91/115	-
29	OUR	8	301	-	-	9/42/81/86	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	g	309	-	3/3/15/26	2/12/110/137	-
25	CLA	y	307	17	1/1/12/20	4/25/101/115	-
30	LHG	y	319	25	-	23/47/47/53	-
26	OIE	5	302	-	-	2/33/72/72	0/2/2/2
25	CLA	g	315	-	1/1/14/20	7/33/109/115	-
24	CHL	2	312	-	3/3/16/26	8/15/113/137	-
37	DGD	c	619	-	-	17/44/84/95	0/2/2/2
25	CLA	a	604	-	1/1/15/20	8/39/115/115	-
24	CHL	4	311	-	3/3/15/26	3/13/111/137	-
25	CLA	4	314	-	1/1/10/20	4/10/86/115	-
24	CHL	7	313	-	3/3/15/26	6/12/110/137	-
25	CLA	d	405	21	1/1/15/20	13/39/115/115	-
25	CLA	B	611	18	1/1/15/20	4/39/115/115	-
24	CHL	n	305	-	3/3/18/26	16/32/130/137	-
25	CLA	7	317	12	1/1/12/20	5/24/100/115	-
25	CLA	p	307	12	1/1/13/20	7/29/105/115	-
26	OIE	9	303	-	-	5/33/72/72	0/2/2/2
25	CLA	l	316	10	1/1/10/20	0/12/88/115	-
25	CLA	s	410	-	1/1/13/20	5/27/103/115	-
32	SQD	b	618	-	-	14/49/69/69	0/1/1/1
24	CHL	8	307	17	3/3/15/26	2/12/110/137	-
25	CLA	8	313	17	1/1/11/20	4/15/91/115	-
28	NEX	r	301	-	-	4/27/83/83	0/3/3/3
30	LHG	n	318	-	-	18/47/47/53	-
26	OIE	7	302	-	-	4/33/72/72	0/2/2/2
25	CLA	C	609	20	1/1/15/20	5/39/115/115	-
28	NEX	5	304	-	-	5/27/83/83	0/3/3/3
25	CLA	g	317	17	1/1/12/20	6/27/103/115	-
25	CLA	B	614	18	1/1/13/20	13/29/105/115	-
25	CLA	C	601	20	1/1/15/20	14/39/115/115	-
26	OIE	3	302	-	-	4/33/69/72	0/2/2/2
37	DGD	C	619	-	-	27/39/79/95	0/2/2/2
24	CHL	q	303	17	3/3/17/26	10/25/123/137	-
24	CHL	6	312	-	3/3/15/26	5/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	q	305	17	1/1/12/20	9/26/102/115	-
29	OUR	4	301	-	-	13/42/81/86	0/2/2/2
24	CHL	q	307	17	3/3/15/26	1/12/110/137	-
25	CLA	b	606	18	1/1/15/20	16/39/115/115	-
25	CLA	p	314	-	1/1/13/20	4/27/103/115	-
24	CHL	Y	304	17	3/3/20/26	15/39/137/137	-
29	OUR	p	301	-	-	8/42/81/86	0/2/2/2
24	CHL	S	602	13	3/3/18/26	14/30/128/137	-
24	CHL	y	305	17	3/3/20/26	14/39/137/137	-
28	NEX	R	616	-	-	5/27/83/83	0/3/3/3
25	CLA	C	606	20	1/1/12/20	7/25/101/115	-
25	CLA	Y	316	17	1/1/12/20	6/27/103/115	-
25	CLA	S	610	-	1/1/11/20	2/15/91/115	-
24	CHL	5	305	11	3/3/15/26	9/13/111/137	-
25	CLA	b	605	18	1/1/15/20	13/39/115/115	-
26	OIE	u	302	-	-	4/33/72/72	0/2/2/2
29	OUR	1	301	-	-	13/42/81/86	0/2/2/2
24	CHL	9	310	-	3/3/16/26	4/15/113/137	-
29	OUR	g	301	-	-	10/42/81/86	0/2/2/2
24	CHL	9	312	-	3/3/15/26	3/12/110/137	-
31	8CT	A	608	-	-	8/29/63/63	0/2/2/2
26	OIE	n	302	-	-	2/33/72/72	0/2/2/2
24	CHL	9	304	12	3/3/20/26	15/39/137/137	-
25	CLA	G	307	-	1/1/12/20	5/25/101/115	-
25	CLA	B	613	18	1/1/15/20	9/39/115/115	-
25	CLA	4	316	-	1/1/10/20	0/12/88/115	-
25	CLA	c	610	-	1/1/15/20	8/39/115/115	-
30	LHG	9	318	25	-	24/47/47/53	-
25	CLA	S	604	-	1/1/10/20	3/13/89/115	-
25	CLA	1	314	-	1/1/10/20	4/10/86/115	-
25	CLA	d	404	21	1/1/15/20	9/39/115/115	-
28	NEX	u	304	-	-	5/27/83/83	0/3/3/3
25	CLA	D	405	21	1/1/15/20	13/39/115/115	-
29	OUR	7	301	-	-	8/42/81/86	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	5	312	-	3/3/16/26	8/15/113/137	-
25	CLA	c	604	-	1/1/15/20	16/39/115/115	-
25	CLA	G	315	-	1/1/14/20	7/33/109/115	-
24	CHL	g	318	17	3/3/15/26	6/10/108/137	-
24	CHL	u	312	-	3/3/16/26	6/17/115/137	-
35	PHO	a	606	-	-	6/37/103/103	0/5/6/6
28	NEX	2	304	-	-	5/27/83/83	0/3/3/3
25	CLA	b	616	18	1/1/11/20	6/18/94/115	-
25	CLA	S	609	-	1/1/13/20	4/27/103/115	-
25	CLA	c	611	20	1/1/15/20	10/39/115/115	-
25	CLA	C	607	-	1/1/15/20	11/39/115/115	-
25	CLA	s	412	13	1/1/11/20	6/15/91/115	-
24	CHL	l	317	-	3/3/15/26	6/10/108/137	-
30	LHG	A	612	-	-	14/48/48/53	-
25	CLA	n	315	17	1/1/11/20	8/15/91/115	-
31	8CT	V	401	-	-	10/29/63/63	0/2/2/2
26	0IE	7	303	-	-	2/33/72/72	0/2/2/2
25	CLA	Y	314	30	1/1/14/20	11/37/113/115	-
24	CHL	G	310	-	3/3/16/26	7/17/115/137	-
23	HEM	E	201	2	-	0/14/54/54	-
24	CHL	3	311	-	3/3/15/26	7/13/111/137	-
24	CHL	8	310	-	3/3/18/26	13/27/125/137	-
25	CLA	r	304	-	1/1/11/20	4/18/94/115	-
30	LHG	7	319	25	-	24/41/41/53	-
25	CLA	5	308	-	1/1/12/20	4/21/97/115	-
30	LHG	D	408	-	-	21/43/43/53	-
26	0IE	2	302	-	-	2/33/72/72	0/2/2/2
25	CLA	9	316	12	1/1/12/20	9/27/103/115	-
24	CHL	q	310	-	3/3/16/26	5/20/118/137	-
24	CHL	8	309	-	3/3/16/26	5/20/118/137	-
25	CLA	5	307	11	1/1/10/20	8/13/89/115	-
26	0IE	g	303	-	-	0/33/72/72	0/2/2/2
24	CHL	g	313	-	3/3/20/26	20/39/137/137	-
33	LMG	D	401	-	-	10/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	n	314	-	1/1/14/20	2/37/113/115	-
29	OUR	q	301	-	-	9/42/81/86	0/2/2/2
29	OUR	G	301	-	-	10/42/81/86	0/2/2/2
24	CHL	n	311	-	3/3/16/26	7/20/118/137	-
24	CHL	4	308	10	3/3/15/26	4/12/110/137	-
25	CLA	b	610	-	1/1/15/20	4/39/115/115	-
24	CHL	y	310	-	3/3/16/26	6/17/115/137	-
31	8CT	c	615	-	-	12/29/63/63	0/2/2/2
25	CLA	Y	315	17	1/1/11/20	6/15/91/115	-
25	CLA	8	311	-	1/1/13/20	2/27/103/115	-
25	CLA	R	612	-	1/1/11/20	6/15/91/115	-
24	CHL	p	312	-	3/3/16/26	7/17/115/137	-
25	CLA	n	306	17	1/1/12/20	8/26/102/115	-
25	CLA	9	307	-	1/1/12/20	7/21/97/115	-
26	OIE	N	302	-	-	2/33/72/72	0/2/2/2
30	LHG	Y	318	25	-	21/47/47/53	-
24	CHL	q	316	-	3/3/15/26	1/10/108/137	-
28	NEX	r	317	-	-	5/27/83/83	0/3/3/3
24	CHL	8	303	17	3/3/17/26	10/25/123/137	-
25	CLA	5	314	-	1/1/13/20	4/27/103/115	-
25	CLA	y	314	17	1/1/13/20	5/27/103/115	-
25	CLA	p	316	-	1/1/11/20	4/15/91/115	-
25	CLA	3	307	-	1/1/10/20	4/13/89/115	-
29	OUR	5	301	-	-	14/42/81/86	0/2/2/2
24	CHL	1	312	10	3/3/16/26	8/15/113/137	-
33	LMG	C	618	-	-	17/37/57/70	0/1/1/1
24	CHL	4	317	-	3/3/15/26	6/10/108/137	-
24	CHL	s	406	-	3/3/16/26	5/15/113/137	-
24	CHL	p	309	12	3/3/15/26	3/12/110/137	-
25	CLA	9	314	30	1/1/14/20	11/37/113/115	-
24	CHL	1	304	-	3/3/15/26	3/10/108/137	-
24	CHL	S	601	13	3/3/16/26	12/15/113/137	-
24	CHL	7	311	-	3/3/16/26	2/15/113/137	-
29	OUR	3	301	-	-	9/42/81/86	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	9	311	-	3/3/16/26	6/17/115/137	-
24	CHL	1	305	10	3/3/16/26	8/15/113/137	-
24	CHL	g	305	17	3/3/20/26	16/39/137/137	-
24	CHL	s	409	-	3/3/16/26	7/17/115/137	-
25	CLA	r	314	-	1/1/11/20	7/18/94/115	-
25	CLA	n	307	-	1/1/12/20	5/21/97/115	-
25	CLA	3	314	-	1/1/10/20	2/10/86/115	-
31	8CT	C	614	-	-	15/29/63/63	0/2/2/2
25	CLA	n	316	-	1/1/10/20	2/13/89/115	-
25	CLA	c	605	20	1/1/13/20	7/29/105/115	-
24	CHL	s	414	-	3/3/15/26	2/10/108/137	-
25	CLA	g	308	-	1/1/12/20	6/21/97/115	-
24	CHL	7	306	-	3/3/19/26	24/37/135/137	-
29	0UR	u	301	-	-	9/42/81/86	0/2/2/2
31	8CT	d	410	-	-	9/29/63/63	0/2/2/2
25	CLA	S	612	-	1/1/12/20	9/27/103/115	-
25	CLA	B	605	18	1/1/15/20	13/39/115/115	-
26	0IE	4	302	-	-	2/33/72/72	0/2/2/2
26	0IE	G	303	-	-	0/33/72/72	0/2/2/2
24	CHL	G	313	-	3/3/20/26	20/39/137/137	-
24	CHL	Y	312	-	3/3/20/26	17/39/137/137	-
25	CLA	b	607	18	1/1/15/20	12/39/115/115	-
25	CLA	s	411	-	1/1/10/20	4/14/90/115	-
29	0UR	9	301	-	-	9/42/81/86	0/2/2/2
24	CHL	G	305	17	3/3/20/26	18/39/137/137	-
25	CLA	b	613	18	1/1/15/20	9/39/115/115	-
25	CLA	q	313	-	1/1/14/20	8/37/113/115	-
25	CLA	q	306	28	1/1/12/20	6/21/97/115	-
24	CHL	p	311	-	3/3/16/26	3/15/113/137	-
26	0IE	G	302	-	-	2/33/72/72	0/2/2/2
25	CLA	s	405	-	1/1/10/20	2/13/89/115	-
25	CLA	n	313	-	1/1/13/20	5/27/103/115	-
24	CHL	S	605	-	3/3/16/26	5/15/113/137	-
28	NEX	p	304	-	-	5/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	2	308	-	1/1/12/20	4/21/97/115	-
25	CLA	A	610	-	1/1/10/20	2/10/86/115	-
28	NEX	N	303	-	-	4/27/83/83	0/3/3/3
24	CHL	2	313	-	3/3/15/26	3/10/108/137	-
24	CHL	Y	309	-	3/3/16/26	5/17/115/137	-
25	CLA	2	317	-	1/1/11/20	7/20/96/115	-
28	NEX	3	318	-	-	4/27/83/83	0/3/3/3
25	CLA	S	603	-	1/1/11/20	6/15/91/115	-
25	CLA	B	612	18	1/1/15/20	12/39/115/115	-
30	LHG	d	407	-	-	27/53/53/53	-
25	CLA	a	607	19	1/1/14/20	6/33/109/115	-
25	CLA	S	611	13	1/1/11/20	6/15/91/115	-
24	CHL	4	310	-	3/3/15/26	4/12/110/137	-
25	CLA	1	307	-	1/1/10/20	4/10/86/115	-
24	CHL	q	309	-	3/3/17/26	10/24/122/137	-
25	CLA	5	317	11	1/1/11/20	7/20/96/115	-
25	CLA	6	313	-	1/1/10/20	2/10/86/115	-
24	CHL	G	309	-	3/3/15/26	2/12/110/137	-
24	CHL	6	308	-	3/3/15/26	4/12/110/137	-
29	OUR	2	301	-	-	14/42/81/86	0/2/2/2
25	CLA	C	608	20	1/1/14/20	11/35/111/115	-
24	CHL	n	308	17	3/3/15/26	2/12/110/137	-
24	CHL	R	608	-	3/3/16/26	6/15/113/137	-
30	LHG	a	601	-	-	24/49/49/53	-
30	LHG	g	319	-	-	23/47/47/53	-
25	CLA	y	315	30	1/1/14/20	11/37/113/115	-
26	OIE	5	303	-	-	0/33/72/72	0/2/2/2
24	CHL	5	313	-	3/3/15/26	2/10/108/137	-
25	CLA	A	607	19	1/1/14/20	5/33/109/115	-
24	CHL	u	313	-	3/3/15/26	4/12/110/137	-
25	CLA	9	313	-	1/1/13/20	3/27/103/115	-
35	PHO	A	606	-	-	7/37/103/103	0/5/6/6
28	NEX	G	304	-	-	5/27/83/83	0/3/3/3
24	CHL	6	305	-	3/3/16/26	7/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	G	308	-	1/1/12/20	8/21/97/115	-
25	CLA	B	604	18	1/1/14/20	14/36/112/115	-
25	CLA	b	602	18	1/1/15/20	11/39/115/115	-
26	OIE	6	302	-	-	4/33/69/72	0/2/2/2
24	CHL	u	306	-	3/3/19/26	15/37/135/137	-
35	PHO	d	403	-	-	9/37/103/103	0/5/6/6
24	CHL	y	312	-	3/3/17/26	5/21/119/137	-
28	NEX	n	303	-	-	4/27/83/83	0/3/3/3
25	CLA	4	307	28	1/1/10/20	4/10/86/115	-
24	CHL	r	308	-	3/3/16/26	9/18/116/137	-
25	CLA	A	604	-	1/1/15/20	7/39/115/115	-
25	CLA	C	610	-	1/1/15/20	9/39/115/115	-
31	8CT	S	615	-	-	12/29/63/63	0/2/2/2
28	NEX	s	401	25	-	4/27/83/83	0/3/3/3
25	CLA	g	314	-	1/1/13/20	3/27/103/115	-
31	8CT	v	401	-	-	10/29/63/63	0/2/2/2
25	CLA	9	306	-	1/1/13/20	7/29/105/115	-
24	CHL	G	306	17	3/3/19/26	26/37/135/137	-
24	CHL	r	307	-	3/3/16/26	10/18/116/137	-
24	CHL	6	310	-	3/3/16/26	7/15/113/137	-
30	LHG	d	408	-	-	25/43/43/53	-
26	OIE	R	614	-	-	1/33/72/72	0/2/2/2
25	CLA	R	604	-	1/1/10/20	4/10/86/115	-
24	CHL	6	317	12	3/3/15/26	0/10/108/137	-
24	CHL	r	309	-	3/3/16/26	6/15/113/137	-
25	CLA	c	607	-	1/1/15/20	11/39/115/115	-
26	OIE	u	303	-	-	2/33/72/72	0/2/2/2
30	LHG	a	612	-	-	14/48/48/53	-
24	CHL	1	311	-	3/3/15/26	3/13/111/137	-
24	CHL	g	310	-	3/3/16/26	7/17/115/137	-
24	CHL	n	317	-	3/3/15/26	6/10/108/137	-
24	CHL	5	310	-	3/3/15/26	2/10/108/137	-
24	CHL	1	310	-	3/3/15/26	4/12/110/137	-
24	CHL	r	302	8	3/3/16/26	7/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	r	312	8	1/1/11/20	8/15/91/115	-
32	SQD	a	609	-	-	19/40/60/69	0/1/1/1
25	CLA	C	612	20	1/1/12/20	8/26/102/115	-
32	SQD	d	409	-	-	13/39/59/69	0/1/1/1
25	CLA	7	307	12	1/1/13/20	7/29/105/115	-
25	CLA	D	404	21	1/1/15/20	7/39/115/115	-
25	CLA	c	612	20	1/1/12/20	9/26/102/115	-
25	CLA	b	601	-	1/1/11/20	9/15/91/115	-
35	PHO	D	403	-	-	9/37/103/103	0/5/6/6
25	CLA	4	313	-	1/1/13/20	5/27/103/115	-
25	CLA	G	317	-	1/1/12/20	6/27/103/115	-
24	CHL	7	305	12	3/3/20/26	17/39/137/137	-
25	CLA	B	606	18	1/1/15/20	16/39/115/115	-
25	CLA	B	603	18	1/1/15/20	12/39/115/115	-
24	CHL	2	310	-	3/3/15/26	2/10/108/137	-
24	CHL	p	313	-	3/3/15/26	6/12/110/137	-
24	CHL	G	311	-	3/3/17/26	12/25/123/137	-
25	CLA	q	314	17	1/1/11/20	4/15/91/115	-
24	CHL	g	311	-	3/3/17/26	10/25/123/137	-
25	CLA	8	305	17	1/1/12/20	9/26/102/115	-
33	LMG	W	201	-	-	11/25/45/70	0/1/1/1
24	CHL	3	309	-	3/3/17/26	9/21/119/137	-
27	XAT	R	615	-	-	0/31/93/93	0/4/4/4
25	CLA	R	610	-	1/1/11/20	2/15/91/115	-
24	CHL	q	311	-	3/3/18/26	13/27/125/137	-
24	CHL	1	308	10	3/3/15/26	4/12/110/137	-
25	CLA	B	616	18	1/1/11/20	6/18/94/115	-
24	CHL	3	310	-	3/3/16/26	7/15/113/137	-
26	OIE	p	302	-	-	4/33/72/72	0/2/2/2
24	CHL	Y	308	17	3/3/15/26	4/12/110/137	-
31	8CT	B	617	-	-	13/29/63/63	0/2/2/2
24	CHL	y	318	17	3/3/15/26	4/10/108/137	-
24	CHL	u	310	-	3/3/16/26	9/15/113/137	-
25	CLA	B	608	-	1/1/13/20	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	p	305	12	3/3/20/26	17/39/137/137	-
24	CHL	s	403	13	3/3/18/26	14/30/128/137	-
26	0IE	r	315	-	-	1/33/72/72	0/2/2/2
25	CLA	g	316	17	1/1/11/20	5/15/91/115	-
30	LHG	c	617	-	-	17/36/36/53	-
39	PL9	D	406	-	-	10/53/73/73	0/1/1/1
24	CHL	n	304	17	3/3/17/26	8/25/123/137	-
24	CHL	u	305	12	3/3/20/26	15/39/137/137	-
24	CHL	Y	305	-	3/3/19/26	22/37/135/137	-
24	CHL	g	306	-	3/3/19/26	25/37/135/137	-
24	CHL	y	309	17	3/3/15/26	4/12/110/137	-
26	0IE	2	303	-	-	0/33/72/72	0/2/2/2
24	CHL	N	305	-	3/3/18/26	13/32/130/137	-
30	LHG	5	319	-	-	21/47/47/53	-
24	CHL	n	310	-	3/3/17/26	11/24/122/137	-
25	CLA	c	603	20	1/1/15/20	12/39/115/115	-
25	CLA	8	306	-	1/1/12/20	7/21/97/115	-
28	NEX	6	303	-	-	4/27/83/83	0/3/3/3
25	CLA	4	315	10	1/1/11/20	8/15/91/115	-
30	LHG	2	319	-	-	20/44/44/53	-
31	8CT	T	101	-	-	12/29/63/63	0/2/2/2
24	CHL	2	305	11	3/3/15/26	9/13/111/137	-
25	CLA	u	308	-	1/1/12/20	5/21/97/115	-
31	8CT	t	101	-	-	12/29/63/63	0/2/2/2
29	0UR	n	301	-	-	9/42/81/86	0/2/2/2
25	CLA	N	313	-	1/1/13/20	5/27/103/115	-
33	LMG	D	411	-	-	26/41/61/70	0/1/1/1
24	CHL	S	607	-	3/3/16/26	6/15/113/137	-
25	CLA	N	306	17	1/1/12/20	7/26/102/115	-
25	CLA	u	317	12	1/1/12/20	6/27/103/115	-
37	DGD	C	620	-	-	25/44/84/95	0/2/2/2
24	CHL	Y	317	17	3/3/15/26	4/10/108/137	-
25	CLA	r	311	-	1/1/11/20	4/15/91/115	-
25	CLA	G	316	17	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	6	311	-	3/3/15/26	5/13/111/137	-
25	CLA	1	313	-	1/1/13/20	4/27/103/115	-
25	CLA	1	306	-	1/1/10/20	5/14/90/115	-
25	CLA	u	307	-	1/1/13/20	6/29/105/115	-
28	NEX	S	617	-	-	5/27/83/83	0/3/3/3
25	CLA	C	604	-	1/1/15/20	16/39/115/115	-
31	8CT	s	416	-	-	12/29/63/63	0/2/2/2
24	CHL	6	304	12	3/3/16/26	10/18/116/137	-
24	CHL	3	312	-	3/3/15/26	7/12/110/137	-
25	CLA	b	614	18	1/1/13/20	12/29/105/115	-
29	0UR	6	301	-	-	9/42/81/86	0/2/2/2
30	LHG	N	318	-	-	17/47/47/53	-
25	CLA	Y	306	17	1/1/12/20	4/25/101/115	-
25	CLA	r	310	8	1/1/13/20	4/27/103/115	-
26	0IE	Y	302	-	-	2/33/72/72	0/2/2/2
33	LMG	d	401	-	-	12/43/63/70	0/1/1/1
25	CLA	7	315	30	1/1/14/20	14/37/113/115	-
24	CHL	2	318	11	3/3/15/26	4/10/108/137	-
25	CLA	C	602	20	1/1/15/20	17/39/115/115	-
24	CHL	2	309	11	3/3/15/26	3/12/110/137	-
28	NEX	y	304	-	-	5/27/83/83	0/3/3/3
25	CLA	c	616	20	1/1/11/20	2/17/93/115	-
25	CLA	R	609	8	1/1/13/20	4/27/103/115	-
24	CHL	8	315	-	3/3/15/26	0/10/108/137	-
25	CLA	3	315	12	1/1/11/20	8/15/91/115	-
25	CLA	N	315	17	1/1/11/20	8/15/91/115	-
30	LHG	G	319	-	-	23/47/47/53	-
24	CHL	N	304	17	3/3/17/26	8/25/123/137	-
25	CLA	Y	313	17	1/1/13/20	5/27/103/115	-
24	CHL	1	309	-	3/3/15/26	4/12/110/137	-
25	CLA	Y	307	-	1/1/12/20	7/21/97/115	-
24	CHL	5	311	-	3/3/16/26	8/17/115/137	-
25	CLA	c	606	20	1/1/12/20	7/25/101/115	-
25	CLA	8	312	-	1/1/14/20	10/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	R	611	8	1/1/11/20	8/15/91/115	-
25	CLA	a	610	-	1/1/10/20	2/10/86/115	-
25	CLA	N	316	-	1/1/10/20	1/13/89/115	-
24	CHL	N	317	-	3/3/15/26	5/10/108/137	-
31	8CT	C	613	-	-	8/29/63/63	0/2/2/2
25	CLA	G	314	-	1/1/13/20	3/27/103/115	-
24	CHL	R	607	-	3/3/16/26	9/18/116/137	-
24	CHL	R	602	-	3/3/16/26	6/17/115/137	-
24	CHL	s	407	-	3/3/16/26	7/15/113/137	-
24	CHL	p	310	-	3/3/16/26	7/15/113/137	-
25	CLA	6	316	-	1/1/11/20	8/15/91/115	-
30	LHG	A	601	-	-	24/49/49/53	-
25	CLA	b	609	18	1/1/15/20	19/39/115/115	-
25	CLA	B	602	18	1/1/15/20	11/39/115/115	-
25	CLA	p	317	12	1/1/12/20	7/27/103/115	-
24	CHL	2	306	-	3/3/16/26	10/17/115/137	-
28	NEX	1	303	-	-	5/27/83/83	0/3/3/3
31	8CT	b	617	-	-	13/29/63/63	0/2/2/2
24	CHL	R	601	8	3/3/16/26	7/15/113/137	-
24	CHL	S	613	-	3/3/15/26	2/10/108/137	-
30	LHG	p	319	25	-	26/47/47/53	-
25	CLA	B	607	18	1/1/15/20	13/39/115/115	-
29	OUR	Y	301	-	-	11/42/81/86	0/2/2/2
31	8CT	a	608	-	-	8/29/63/63	0/2/2/2
24	CHL	4	309	-	3/3/15/26	6/12/110/137	-
33	LMG	i	101	-	-	14/43/63/70	0/1/1/1
24	CHL	u	311	-	3/3/16/26	5/15/113/137	-
25	CLA	B	610	-	1/1/15/20	3/39/115/115	-
25	CLA	c	608	20	1/1/14/20	11/35/111/115	-
25	CLA	u	314	-	1/1/13/20	3/27/103/115	-
31	8CT	D	410	-	-	10/29/63/63	0/2/2/2
32	SQD	B	618	-	-	14/49/69/69	0/1/1/1
25	CLA	g	307	-	1/1/12/20	5/25/101/115	-
25	CLA	q	315	17	1/1/10/20	3/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	611	18	1/1/15/20	4/39/115/115	-
24	CHL	7	312	-	3/3/16/26	7/17/115/137	-
24	CHL	Y	310	-	3/3/17/26	11/25/123/137	-
26	OIE	y	302	-	-	2/33/72/72	0/2/2/2
25	CLA	6	306	-	1/1/10/20	6/10/86/115	-
25	CLA	R	613	-	1/1/11/20	7/18/94/115	-
24	CHL	3	304	12	3/3/16/26	11/18/116/137	-
24	CHL	7	318	12	3/3/15/26	4/10/108/137	-
25	CLA	N	314	-	1/1/14/20	2/37/113/115	-
26	OIE	g	302	-	-	2/33/72/72	0/2/2/2
24	CHL	u	318	-	3/3/15/26	4/10/108/137	-
25	CLA	r	313	-	1/1/11/20	6/15/91/115	-
29	OUR	N	301	-	-	10/42/81/86	0/2/2/2
25	CLA	7	316	12	1/1/11/20	4/15/91/115	-
25	CLA	u	316	-	1/1/11/20	6/15/91/115	-
25	CLA	c	602	20	1/1/15/20	16/39/115/115	-
24	CHL	5	306	-	3/3/16/26	10/17/115/137	-
25	CLA	s	413	-	1/1/12/20	9/27/103/115	-
24	CHL	N	311	-	3/3/16/26	7/20/118/137	-
24	CHL	r	303	-	3/3/16/26	6/17/115/137	-
25	CLA	3	316	-	1/1/11/20	6/15/91/115	-
24	CHL	p	318	12	3/3/15/26	4/10/108/137	-
25	CLA	4	306	-	1/1/10/20	5/14/90/115	-
25	CLA	B	609	18	1/1/15/20	16/39/115/115	-
31	8CT	S	614	-	-	7/29/63/63	0/2/2/2
24	CHL	7	309	12	3/3/15/26	3/12/110/137	-
25	CLA	2	316	-	1/1/11/20	4/15/91/115	-
31	8CT	c	613	-	-	8/29/63/63	0/2/2/2
24	CHL	p	306	-	3/3/19/26	24/37/135/137	-
25	CLA	y	308	-	1/1/12/20	7/21/97/115	-
24	CHL	3	305	-	3/3/16/26	8/18/116/137	-
25	CLA	B	601	-	1/1/11/20	9/15/91/115	-
25	CLA	r	305	-	1/1/10/20	2/10/86/115	-
25	CLA	S	616	-	1/1/11/20	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	605	-	1/1/11/20	5/20/96/115	-
25	CLA	y	317	17	1/1/12/20	6/27/103/115	-
33	LMG	w	201	-	-	17/31/51/70	0/1/1/1
25	CLA	C	603	20	1/1/15/20	13/39/115/115	-
24	CHL	6	309	-	3/3/17/26	7/21/119/137	-
24	CHL	u	309	12	3/3/15/26	2/12/110/137	-
26	0IE	Y	303	-	-	0/33/72/72	0/2/2/2
24	CHL	N	310	-	3/3/17/26	11/24/122/137	-
25	CLA	8	314	-	1/1/10/20	3/13/89/115	-
31	8CT	x	601	-	-	10/29/63/63	0/2/2/2
25	CLA	6	315	12	1/1/11/20	8/15/91/115	-
28	NEX	7	304	-	-	5/27/83/83	0/3/3/3
24	CHL	R	606	-	3/3/16/26	10/18/116/137	-
24	CHL	S	608	-	3/3/16/26	7/17/115/137	-
32	SQD	A	609	-	-	16/40/60/69	0/1/1/1
25	CLA	5	315	-	1/1/14/20	10/37/113/115	-
31	8CT	s	415	-	-	7/29/63/63	0/2/2/2
24	CHL	G	312	-	3/3/17/26	4/21/119/137	-
28	NEX	9	319	-	-	5/27/83/83	0/3/3/3
24	CHL	4	312	-	3/3/16/26	8/15/113/137	-
25	CLA	2	307	11	1/1/10/20	7/13/89/115	-
25	CLA	s	417	-	1/1/11/20	8/15/91/115	-
33	LMG	d	411	-	-	20/41/61/70	0/1/1/1
24	CHL	9	309	-	3/3/16/26	9/15/113/137	-
31	8CT	X	601	-	-	10/29/63/63	0/2/2/2
29	0UR	y	301	-	-	11/42/81/86	0/2/2/2
25	CLA	b	608	-	1/1/13/20	9/27/103/115	-

The worst 5 of 5928 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	410	8CT	C02-C03	15.16	1.59	1.34
31	d	410	8CT	C02-C03	15.02	1.59	1.34
31	S	614	8CT	C02-C03	14.75	1.59	1.34
31	s	415	8CT	C02-C03	14.74	1.59	1.34
31	A	608	8CT	C02-C03	14.72	1.59	1.34

The worst 5 of 5455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	416	8CT	C22-C21-C20	-27.08	78.94	122.82
31	S	615	8CT	C22-C21-C20	-27.07	78.96	122.82
31	S	615	8CT	C22-C21-C23	-26.12	78.18	118.09
31	s	416	8CT	C22-C21-C23	-26.11	78.20	118.09
31	S	615	8CT	C23-C21-C20	24.21	157.09	119.01

5 of 718 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	R	601	CHL	NA
24	R	601	CHL	NC
24	R	601	CHL	ND
24	R	602	CHL	NA
24	R	602	CHL	NC

5 of 4267 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	R	601	CHL	C1C-C2C-CMC-OMC
24	R	601	CHL	C3C-C2C-CMC-OMC
24	R	606	CHL	C1A-C2A-CAA-CBA
24	R	607	CHL	C1C-C2C-CMC-OMC
24	R	607	CHL	C3C-C2C-CMC-OMC

There are no ring outliers.

435 monomers are involved in 1342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	9	315	CLA	4	0
25	q	312	CLA	2	0
37	c	618	DGD	4	0
39	d	406	PL9	2	0
25	N	307	CLA	4	0
25	7	314	CLA	2	0
25	b	615	CLA	7	0
24	n	312	CHL	2	0
24	G	318	CHL	1	0
30	4	318	LHG	3	0
25	2	314	CLA	1	0
24	5	309	CHL	1	0
25	6	307	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	u	315	CLA	4	0
30	D	407	LHG	7	0
25	C	611	CLA	5	0
24	n	309	CHL	1	0
24	s	402	CHL	3	0
24	7	310	CHL	14	0
28	g	304	NEX	15	0
25	C	605	CLA	1	0
25	c	609	CLA	3	0
24	N	312	CHL	4	0
32	D	409	SQD	1	0
24	8	308	CHL	3	0
25	B	615	CLA	8	0
24	Y	311	CHL	4	0
25	b	612	CLA	8	0
24	g	312	CHL	3	0
25	3	306	CLA	1	0
26	9	302	OIE	2	0
24	N	308	CHL	3	0
23	f	201	HEM	3	0
25	A	603	CLA	5	0
24	y	311	CHL	1	0
25	y	316	CLA	3	0
27	r	316	XAT	8	0
24	N	309	CHL	1	0
24	y	313	CHL	6	0
24	9	308	CHL	1	0
30	1	318	LHG	3	0
25	C	616	CLA	2	0
25	7	308	CLA	15	0
25	c	601	CLA	3	0
25	a	603	CLA	5	0
24	9	317	CHL	1	0
24	4	304	CHL	2	0
33	m	101	LMG	6	0
25	p	315	CLA	2	0
24	y	306	CHL	2	0
24	8	304	CHL	6	0
24	R	605	CHL	3	0
24	9	305	CHL	6	0
25	2	315	CLA	1	0
24	s	408	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	p	308	CLA	12	0
24	q	304	CHL	4	0
24	3	317	CHL	2	0
24	S	606	CHL	2	0
24	3	308	CHL	2	0
25	a	605	CLA	1	0
28	4	303	NEX	21	0
24	q	308	CHL	3	0
25	b	603	CLA	4	0
25	b	604	CLA	10	0
24	r	306	CHL	3	0
25	R	603	CLA	1	0
24	4	305	CHL	1	0
26	y	303	0IE	1	0
25	1	315	CLA	2	0
33	B	619	LMG	5	0
25	5	316	CLA	2	0
29	8	301	0UR	1	0
24	g	309	CHL	2	0
25	y	307	CLA	2	0
30	y	319	LHG	2	0
25	g	315	CLA	3	0
24	2	312	CHL	2	0
37	c	619	DGD	4	0
25	a	604	CLA	6	0
24	4	311	CHL	5	0
25	4	314	CLA	1	0
24	7	313	CHL	3	0
25	d	405	CLA	6	0
25	B	611	CLA	5	0
24	n	305	CHL	5	0
25	7	317	CLA	4	0
25	p	307	CLA	2	0
26	9	303	0IE	1	0
25	1	316	CLA	2	0
25	s	410	CLA	4	0
32	b	618	SQD	5	0
24	8	307	CHL	1	0
25	8	313	CLA	1	0
28	r	301	NEX	6	0
30	n	318	LHG	4	0
26	7	302	0IE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	609	CLA	2	0
28	5	304	NEX	10	0
25	g	317	CLA	1	0
25	B	614	CLA	3	0
25	C	601	CLA	4	0
26	3	302	0IE	2	0
37	C	619	DGD	5	0
24	q	303	CHL	3	0
25	q	305	CLA	2	0
29	4	301	0UR	1	0
24	q	307	CHL	1	0
25	b	606	CLA	9	0
25	p	314	CLA	2	0
24	Y	304	CHL	5	0
29	p	301	0UR	1	0
24	S	602	CHL	5	0
24	y	305	CHL	8	0
28	R	616	NEX	6	0
25	Y	316	CLA	2	0
24	5	305	CHL	6	0
25	b	605	CLA	4	0
26	u	302	0IE	1	0
24	9	310	CHL	2	0
24	9	312	CHL	3	0
24	9	304	CHL	6	0
25	G	307	CLA	2	0
25	B	613	CLA	5	0
25	4	316	CLA	2	0
25	c	610	CLA	4	0
30	9	318	LHG	6	0
25	1	314	CLA	1	0
25	d	404	CLA	4	0
28	u	304	NEX	9	0
25	D	405	CLA	5	0
24	5	312	CHL	3	0
25	c	604	CLA	3	0
25	G	315	CLA	3	0
24	g	318	CHL	2	0
24	u	312	CHL	4	0
35	a	606	PHO	4	0
28	2	304	NEX	9	0
25	b	616	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	S	609	CLA	4	0
25	c	611	CLA	3	0
25	C	607	CLA	2	0
25	s	412	CLA	3	0
24	l	317	CHL	2	0
30	A	612	LHG	2	0
25	n	315	CLA	2	0
31	V	401	8CT	1	0
25	Y	314	CLA	1	0
24	G	310	CHL	3	0
23	E	201	HEM	2	0
24	3	311	CHL	6	0
24	8	310	CHL	6	0
25	r	304	CLA	1	0
30	7	319	LHG	3	0
25	5	308	CLA	5	0
30	D	408	LHG	6	0
25	9	316	CLA	4	0
24	q	310	CHL	6	0
24	8	309	CHL	5	0
24	g	313	CHL	6	0
33	D	401	LMG	3	0
29	q	301	0UR	1	0
29	G	301	0UR	1	0
24	n	311	CHL	4	0
24	4	308	CHL	1	0
25	b	610	CLA	3	0
24	y	310	CHL	1	0
25	Y	315	CLA	1	0
25	8	311	CLA	2	0
25	R	612	CLA	7	0
24	p	312	CHL	5	0
25	n	306	CLA	2	0
25	9	307	CLA	4	0
28	r	317	NEX	9	0
24	8	303	CHL	3	0
25	5	314	CLA	2	0
25	y	314	CLA	2	0
25	p	316	CLA	2	0
25	3	307	CLA	2	0
24	l	312	CHL	4	0
33	C	618	LMG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	4	317	CHL	2	0
24	s	406	CHL	2	0
24	p	309	CHL	3	0
25	9	314	CLA	3	0
24	1	304	CHL	3	0
24	S	601	CHL	1	0
24	7	311	CHL	2	0
24	9	311	CHL	4	0
24	1	305	CHL	2	0
24	g	305	CHL	4	0
24	s	409	CHL	2	0
25	r	314	CLA	1	0
25	n	307	CLA	4	0
25	n	316	CLA	4	0
25	c	605	CLA	2	0
24	s	414	CHL	2	0
25	g	308	CLA	6	0
24	7	306	CHL	4	0
29	u	301	0UR	1	0
25	S	612	CLA	1	0
25	B	605	CLA	6	0
24	G	313	CHL	10	0
24	Y	312	CHL	7	0
25	b	607	CLA	3	0
25	s	411	CLA	3	0
29	9	301	0UR	1	0
24	G	305	CHL	4	0
25	b	613	CLA	5	0
25	q	313	CLA	1	0
25	q	306	CLA	5	0
24	p	311	CHL	2	0
24	S	605	CHL	2	0
28	p	304	NEX	27	0
25	2	308	CLA	5	0
28	N	303	NEX	7	0
24	2	313	CHL	3	0
24	Y	309	CHL	2	0
25	2	317	CLA	2	0
28	3	318	NEX	22	0
25	B	612	CLA	8	0
30	d	407	LHG	7	0
25	a	607	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	S	611	CLA	1	0
24	4	310	CHL	3	0
25	1	307	CLA	9	0
25	5	317	CLA	2	0
24	G	309	CHL	2	0
24	6	308	CHL	1	0
29	2	301	0UR	1	0
24	n	308	CHL	3	0
24	R	608	CHL	2	0
30	a	601	LHG	5	0
30	g	319	LHG	2	0
25	y	315	CLA	3	0
24	5	313	CHL	4	0
25	A	607	CLA	2	0
24	u	313	CHL	1	0
25	9	313	CLA	2	0
35	A	606	PHO	4	0
28	G	304	NEX	32	0
24	6	305	CHL	1	0
25	G	308	CLA	16	0
25	B	604	CLA	12	0
25	b	602	CLA	8	0
26	6	302	0IE	2	0
24	u	306	CHL	4	0
35	d	403	PHO	6	0
24	y	312	CHL	4	0
28	n	303	NEX	7	0
25	4	307	CLA	16	0
24	r	308	CHL	3	0
25	A	604	CLA	5	0
25	C	610	CLA	4	0
28	s	401	NEX	21	0
25	g	314	CLA	2	0
31	v	401	8CT	1	0
25	9	306	CLA	1	0
24	G	306	CHL	6	0
24	r	307	CHL	4	0
24	6	310	CHL	2	0
30	d	408	LHG	4	0
26	R	614	0IE	1	0
25	R	604	CLA	7	0
24	6	317	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	r	309	CHL	2	0
25	c	607	CLA	3	0
30	a	612	LHG	2	0
24	1	311	CHL	7	0
24	g	310	CHL	6	0
24	1	310	CHL	3	0
24	r	302	CHL	3	0
32	a	609	SQD	4	0
25	C	612	CLA	2	0
32	d	409	SQD	1	0
25	7	307	CLA	2	0
25	D	404	CLA	5	0
25	c	612	CLA	4	0
25	b	601	CLA	1	0
35	D	403	PHO	6	0
25	4	313	CLA	2	0
25	G	317	CLA	2	0
24	7	305	CHL	6	0
25	B	606	CLA	8	0
25	B	603	CLA	3	0
24	p	313	CHL	3	0
24	G	311	CHL	4	0
25	q	314	CLA	1	0
24	g	311	CHL	3	0
25	8	305	CLA	2	0
33	W	201	LMG	2	0
24	3	309	CHL	19	0
27	R	615	XAT	16	0
25	R	610	CLA	1	0
24	q	311	CHL	6	0
25	B	616	CLA	3	0
24	3	310	CHL	1	0
26	p	302	OIE	2	0
24	Y	308	CHL	3	0
24	y	318	CHL	2	0
24	u	310	CHL	4	0
25	B	608	CLA	6	0
24	p	305	CHL	7	0
24	s	403	CHL	3	0
26	r	315	OIE	1	0
25	g	316	CLA	2	0
39	D	406	PL9	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	n	304	CHL	4	0
24	u	305	CHL	5	0
24	Y	305	CHL	2	0
24	g	306	CHL	3	0
24	y	309	CHL	2	0
26	2	303	0IE	1	0
24	N	305	CHL	2	0
30	5	319	LHG	2	0
24	n	310	CHL	2	0
25	c	603	CLA	3	0
25	8	306	CLA	4	0
28	6	303	NEX	21	0
25	4	315	CLA	2	0
30	2	319	LHG	2	0
24	2	305	CHL	5	0
25	u	308	CLA	1	0
29	n	301	0UR	1	0
25	N	313	CLA	1	0
33	D	411	LMG	5	0
24	S	607	CHL	2	0
25	N	306	CLA	1	0
25	u	317	CLA	5	0
37	C	620	DGD	2	0
24	Y	317	CHL	2	0
25	r	311	CLA	1	0
25	G	316	CLA	3	0
24	6	311	CHL	9	0
25	1	313	CLA	2	0
25	u	307	CLA	2	0
28	S	617	NEX	24	0
25	C	604	CLA	4	0
24	6	304	CHL	3	0
25	b	614	CLA	3	0
29	6	301	0UR	1	0
30	N	318	LHG	4	0
25	Y	306	CLA	2	0
25	r	310	CLA	1	0
26	Y	302	0IE	1	0
33	d	401	LMG	3	0
25	7	315	CLA	2	0
25	C	602	CLA	2	0
24	2	309	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	y	304	NEX	4	0
25	c	616	CLA	2	0
25	R	609	CLA	1	0
25	3	315	CLA	1	0
25	N	315	CLA	3	0
30	G	319	LHG	1	0
24	N	304	CHL	5	0
25	Y	313	CLA	2	0
24	1	309	CHL	5	0
24	5	311	CHL	1	0
25	8	312	CLA	1	0
25	N	316	CLA	4	0
31	C	613	8CT	1	0
25	G	314	CLA	2	0
24	R	607	CHL	3	0
24	R	602	CHL	4	0
24	s	407	CHL	2	0
24	p	310	CHL	12	0
25	6	316	CLA	3	0
30	A	601	LHG	6	0
25	b	609	CLA	4	0
25	B	602	CLA	7	0
25	p	317	CLA	5	0
28	1	303	NEX	22	0
24	R	601	CHL	3	0
24	S	613	CHL	2	0
30	p	319	LHG	3	0
25	B	607	CLA	4	0
29	Y	301	0UR	1	0
24	4	309	CHL	7	0
33	i	101	LMG	3	0
24	u	311	CHL	1	0
25	B	610	CLA	2	0
25	c	608	CLA	3	0
25	u	314	CLA	2	0
32	B	618	SQD	4	0
25	g	307	CLA	2	0
25	q	315	CLA	1	0
25	b	611	CLA	3	0
24	7	312	CHL	6	0
24	Y	310	CHL	1	0
26	y	302	0IE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	6	306	CLA	1	0
24	3	304	CHL	1	0
24	7	318	CHL	2	0
24	u	318	CHL	1	0
25	r	313	CLA	5	0
25	7	316	CLA	3	0
25	u	316	CLA	4	0
25	c	602	CLA	2	0
25	s	413	CLA	1	0
24	N	311	CHL	4	0
24	r	303	CHL	5	0
25	3	316	CLA	2	0
24	p	318	CHL	3	0
25	B	609	CLA	3	0
25	2	316	CLA	1	0
31	c	613	8CT	1	0
24	p	306	CHL	4	0
25	y	308	CLA	1	0
24	3	305	CHL	1	0
25	B	601	CLA	1	0
25	r	305	CLA	9	0
25	S	616	CLA	4	0
25	A	605	CLA	1	0
25	y	317	CLA	2	0
33	w	201	LMG	6	0
25	C	603	CLA	5	0
24	6	309	CHL	20	0
24	u	309	CHL	2	0
24	N	310	CHL	2	0
25	8	314	CLA	2	0
25	6	315	CLA	1	0
28	7	304	NEX	32	0
24	R	606	CHL	2	0
24	S	608	CHL	1	0
32	A	609	SQD	2	0
25	5	315	CLA	1	0
24	G	312	CHL	12	0
28	9	319	NEX	6	0
24	4	312	CHL	3	0
25	s	417	CLA	4	0
33	d	411	LMG	5	0
24	9	309	CHL	3	0

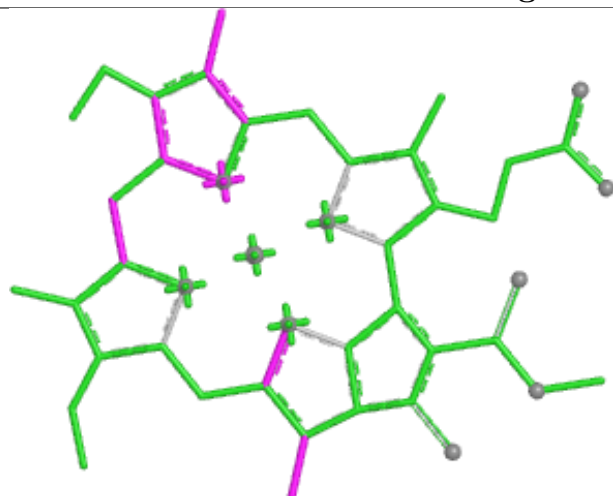
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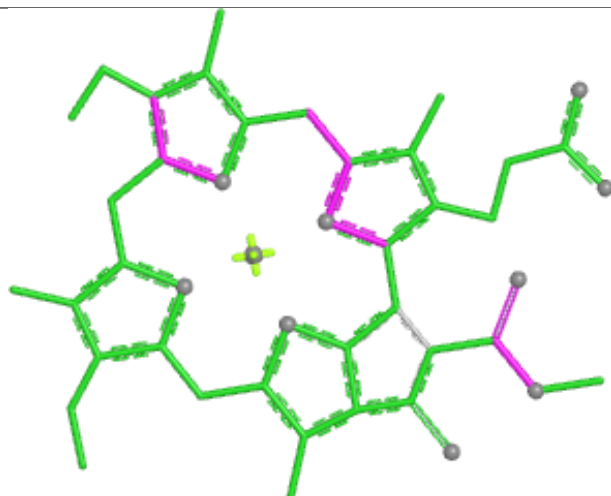
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	y	301	0UR	1	0
25	b	608	CLA	5	0

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

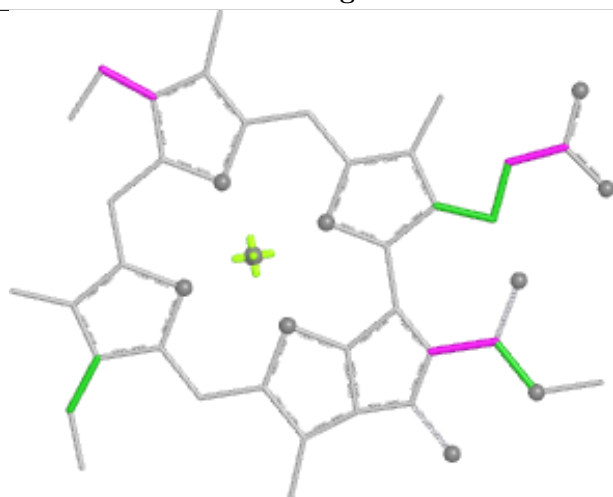
Ligand CLA 9 315



Bond lengths



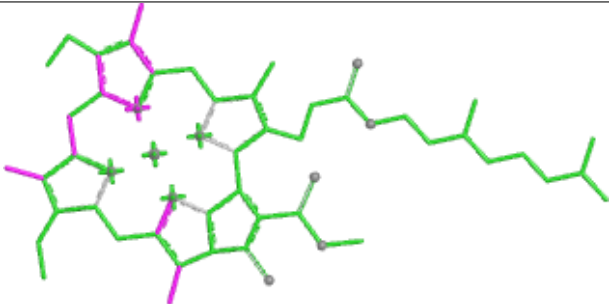
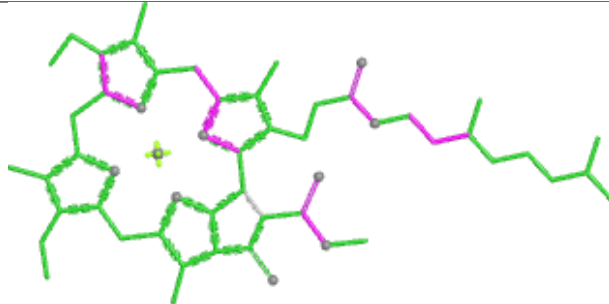
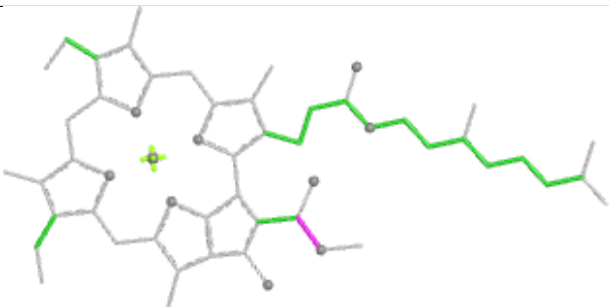
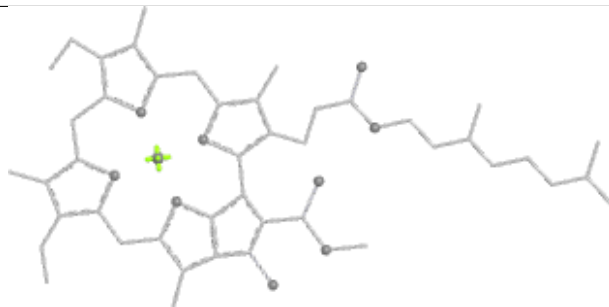
Bond angles

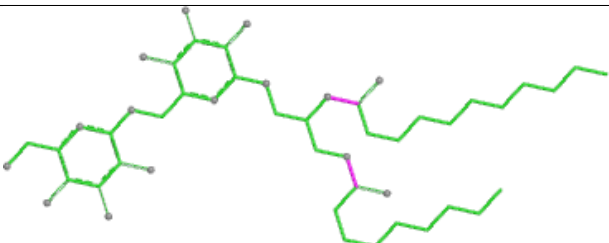
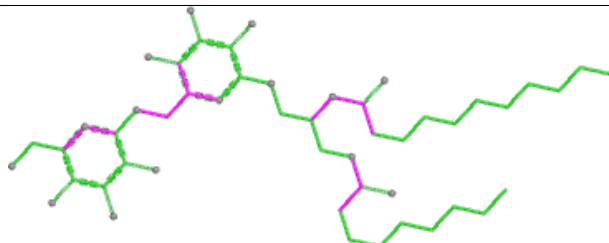
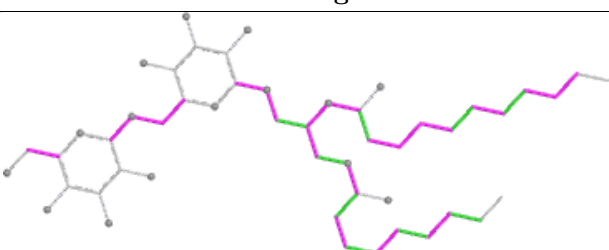
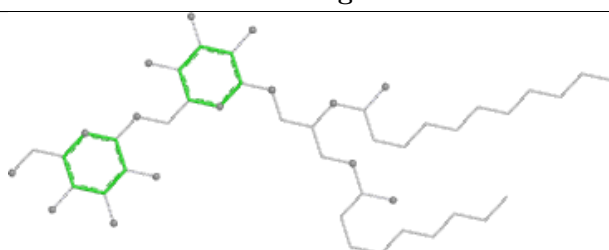


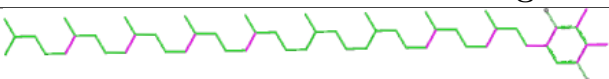
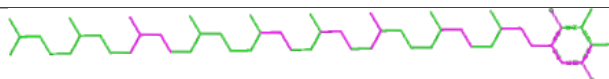
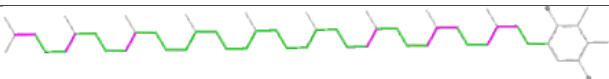
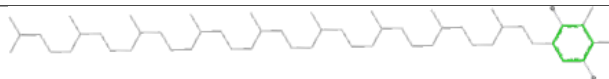
Torsions

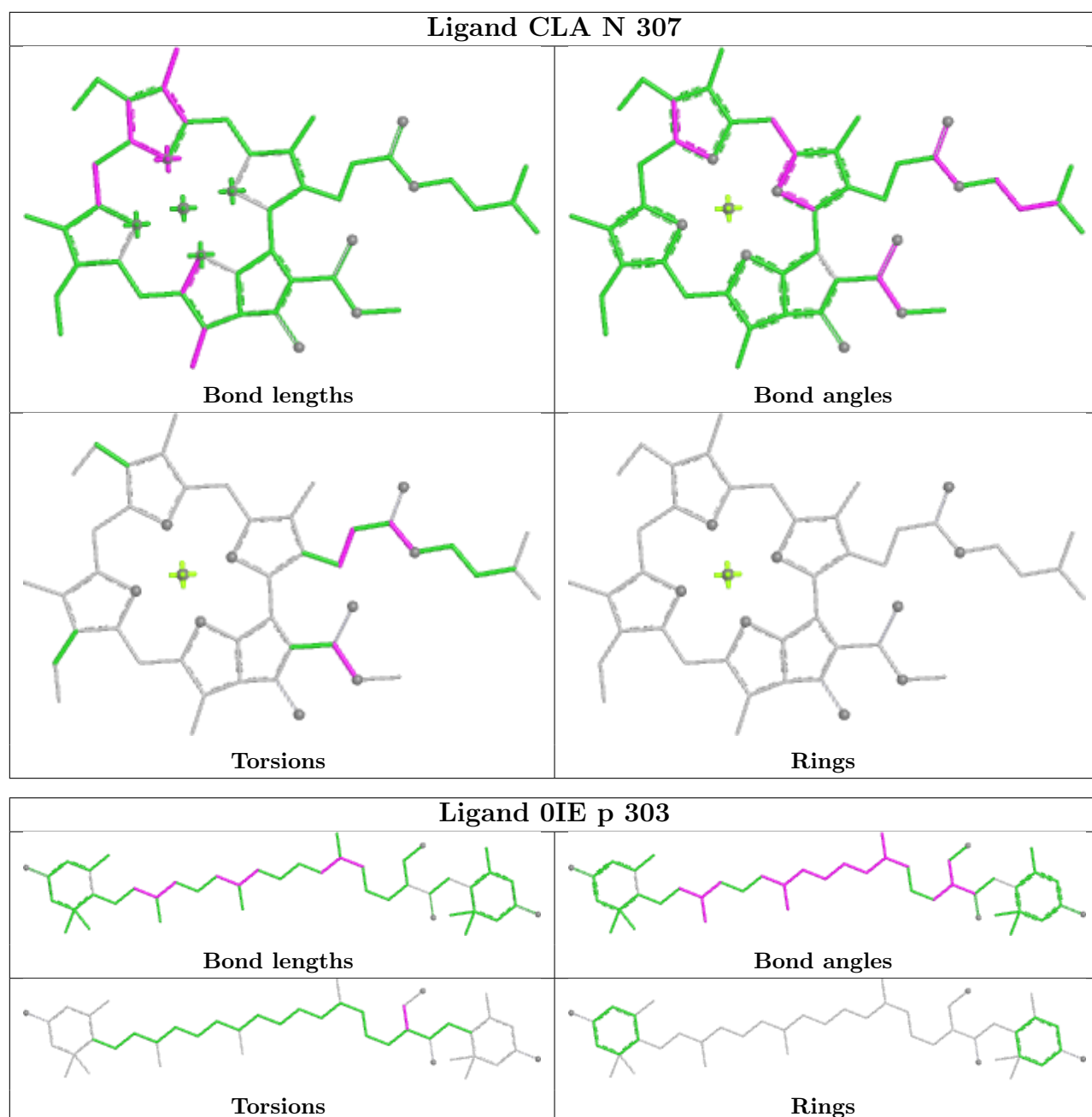


Rings

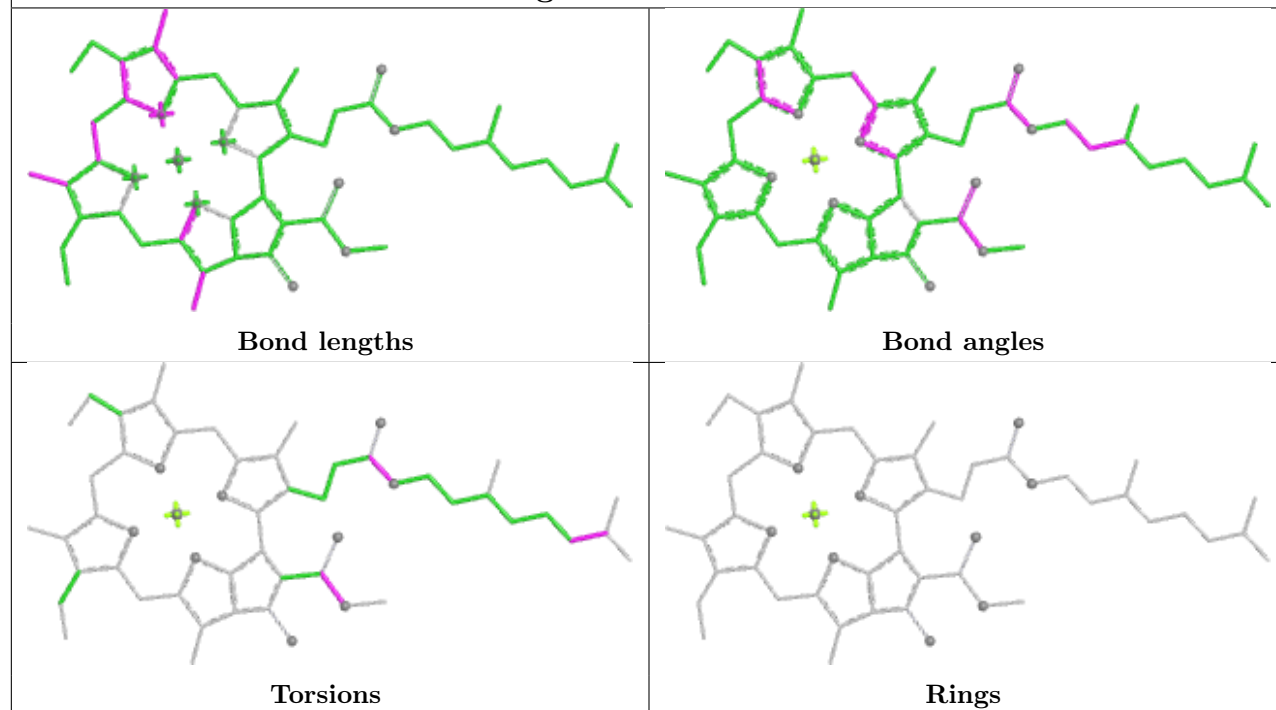
Ligand CLA q 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD c 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

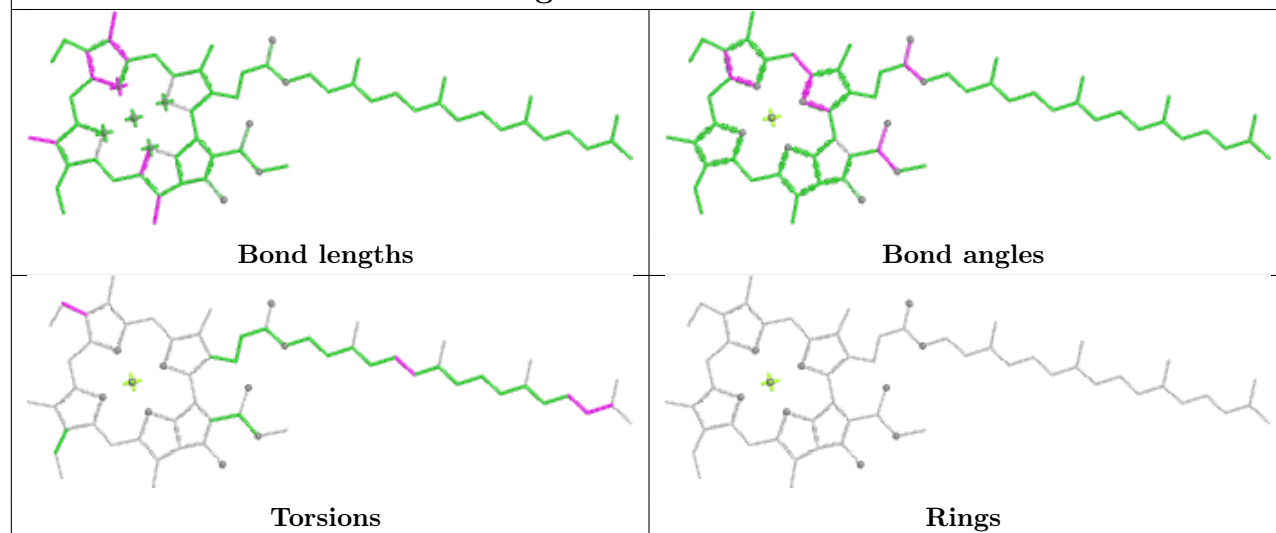
Ligand PL9 d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings



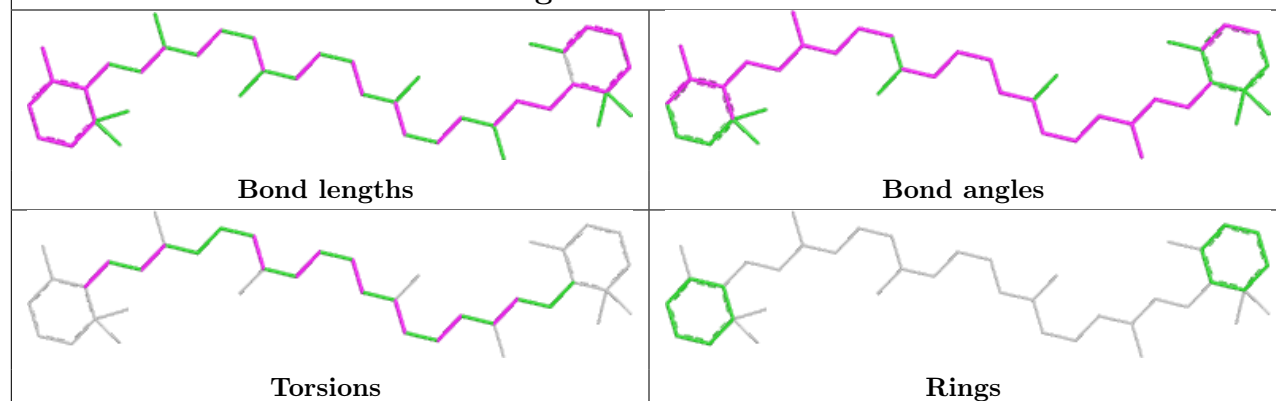
Ligand CLA 7 314

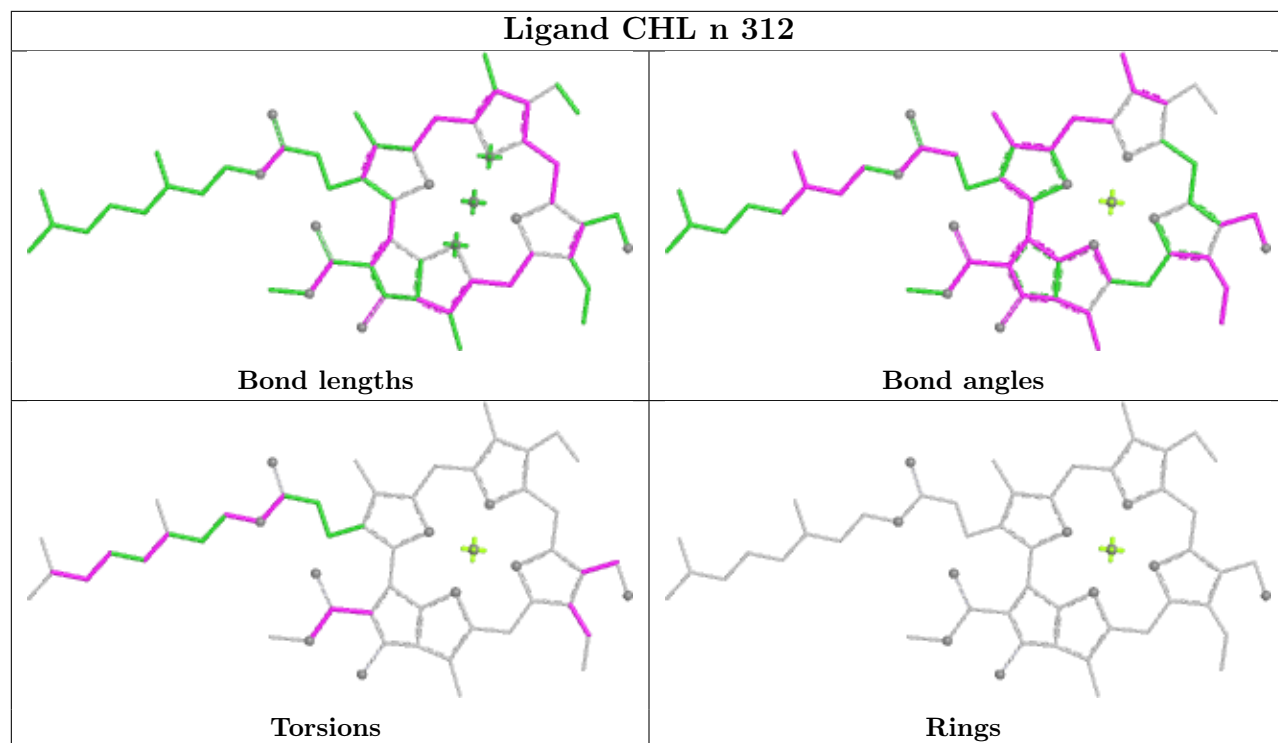


Ligand CLA b 615

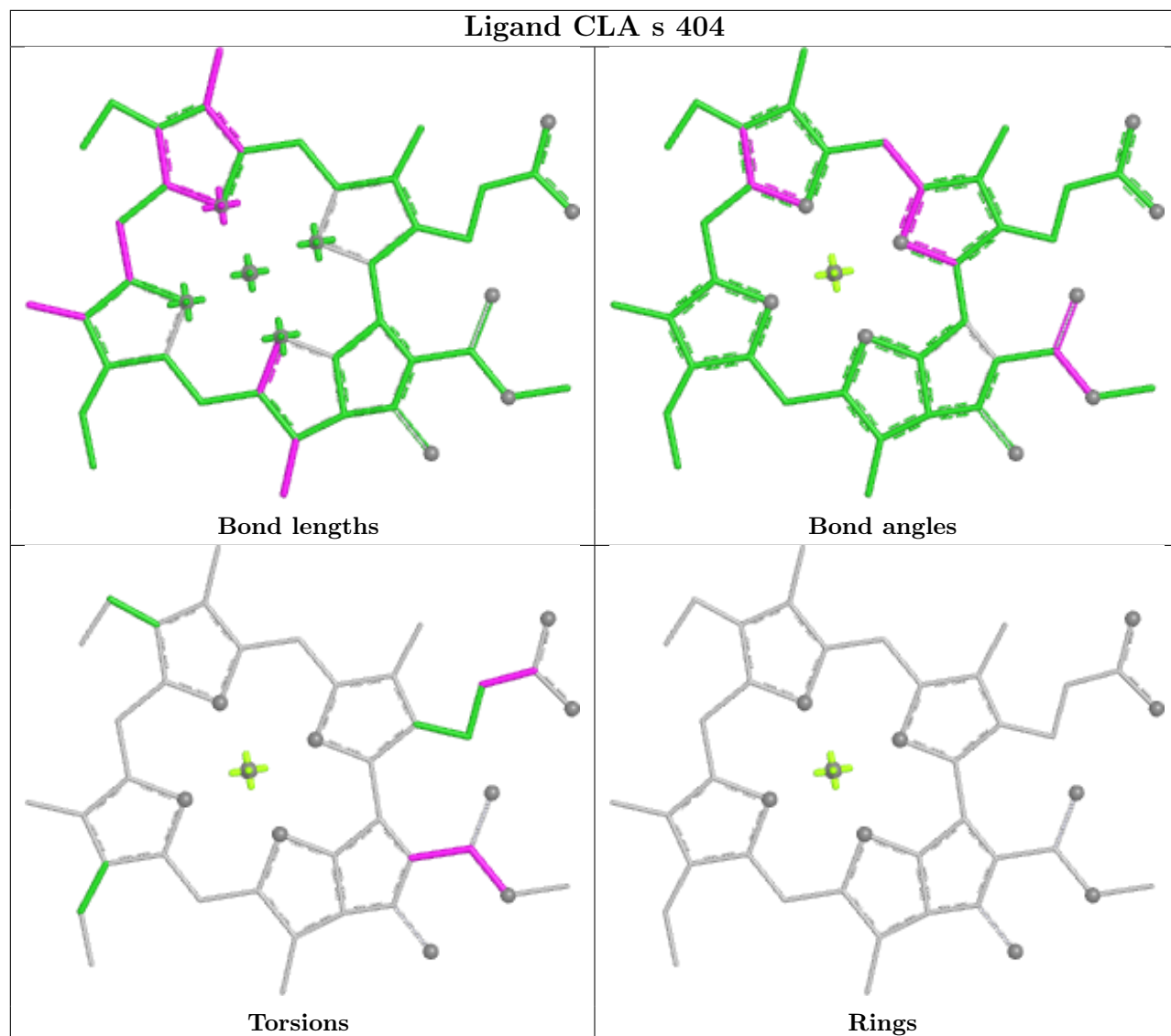


Ligand 8CT C 615

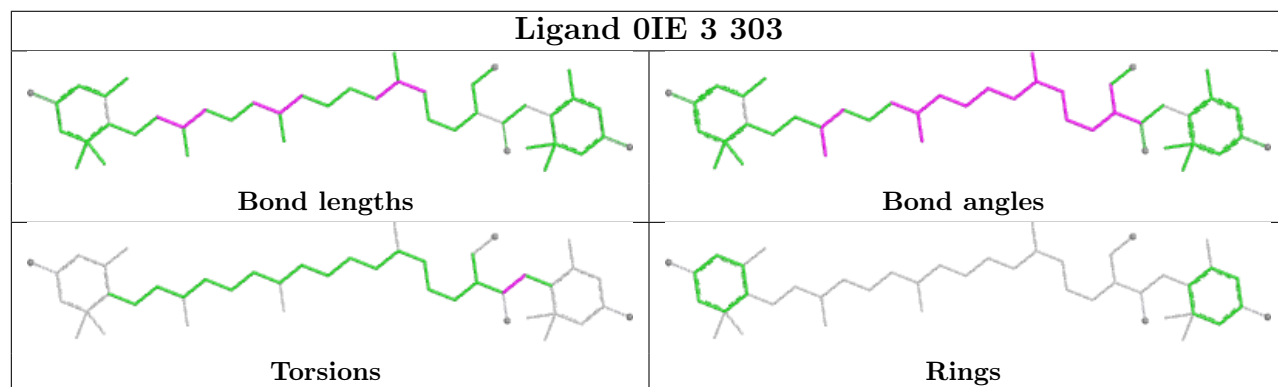


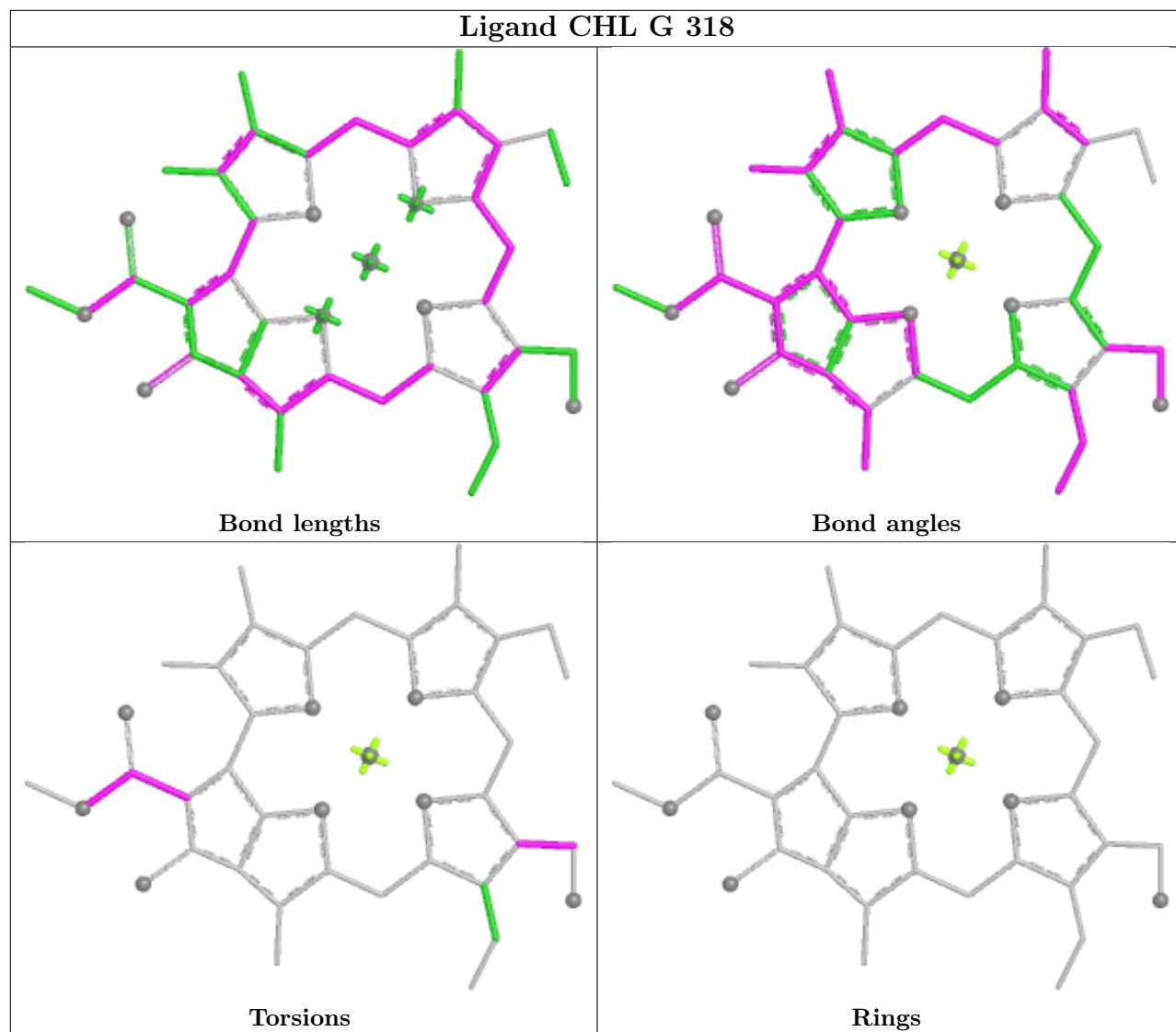


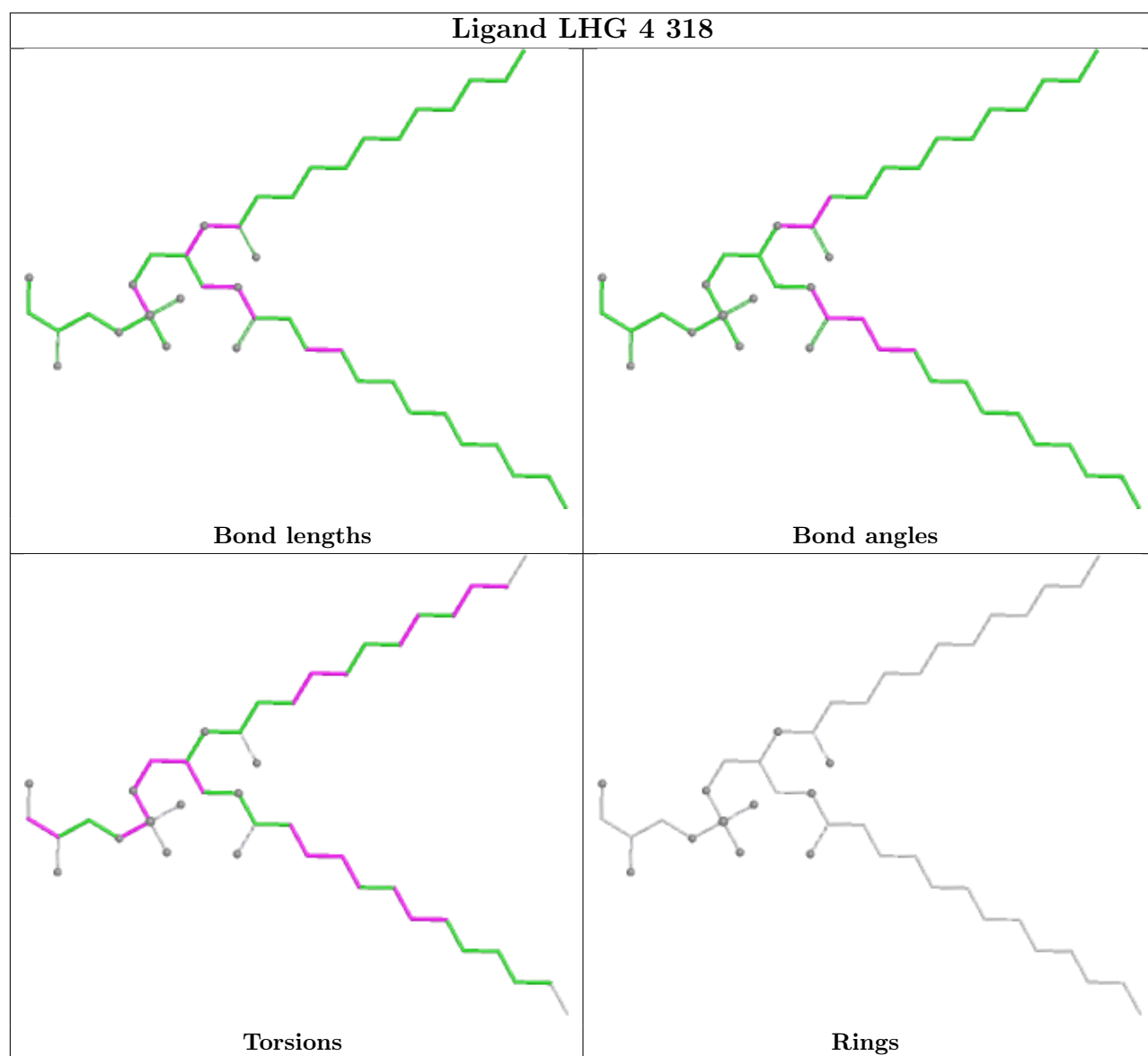
Ligand CLA s 404

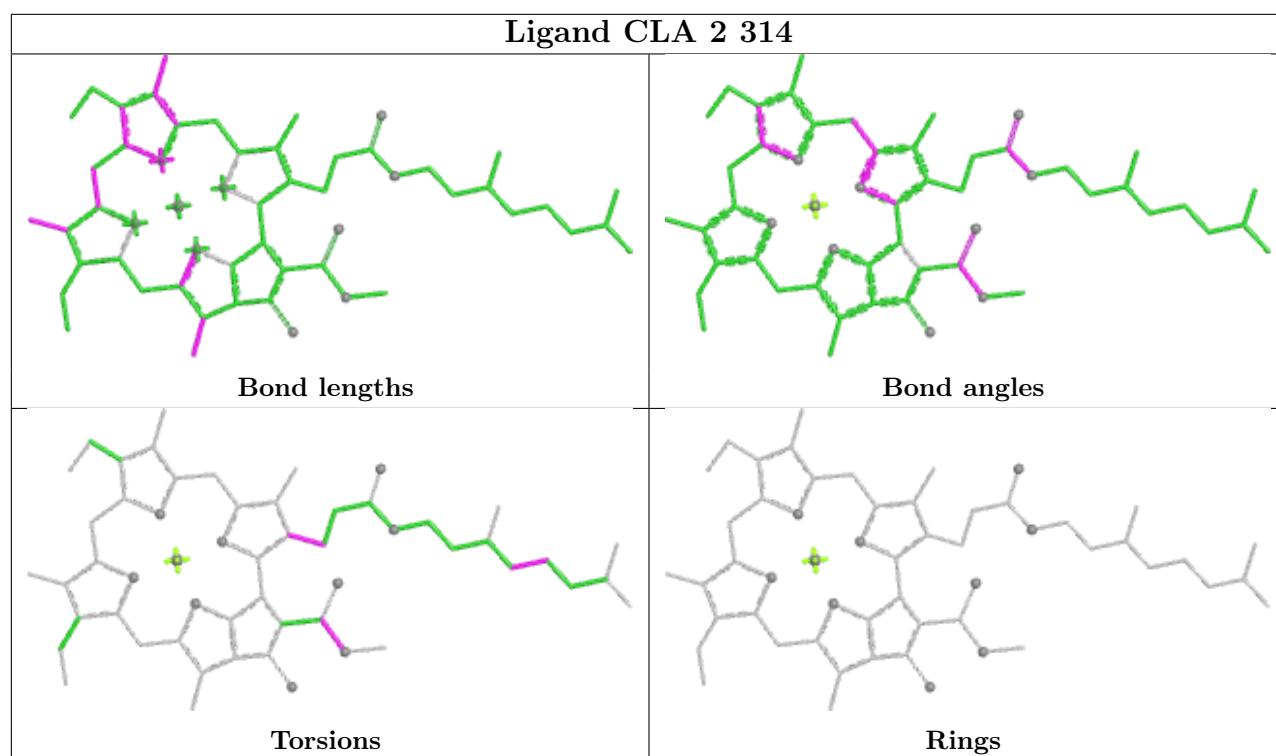


Ligand OIE 3 303

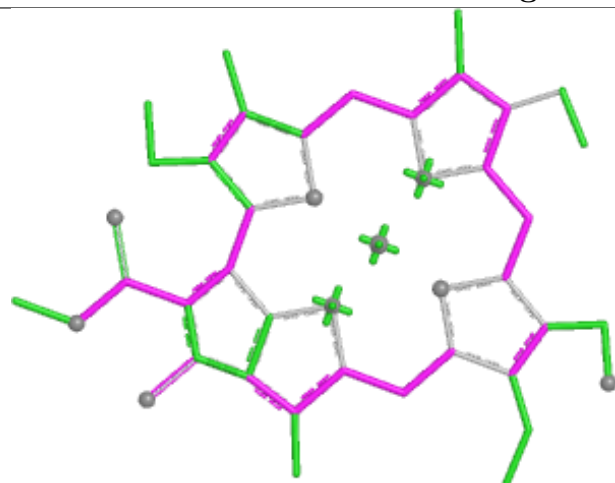




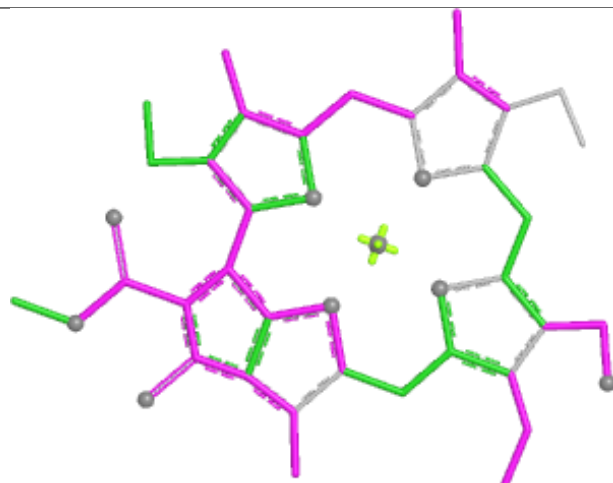




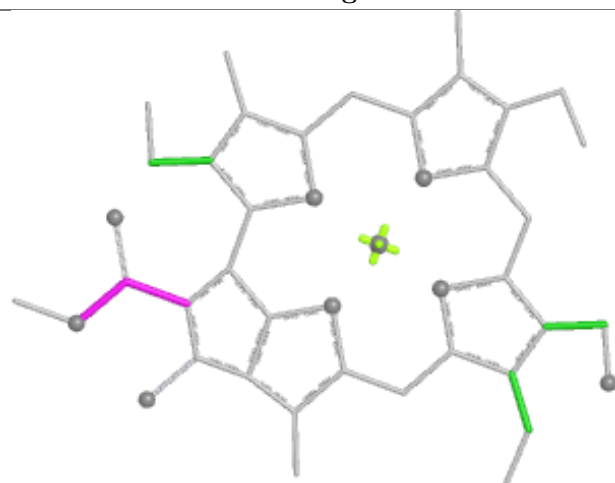
Ligand CHL 5 309



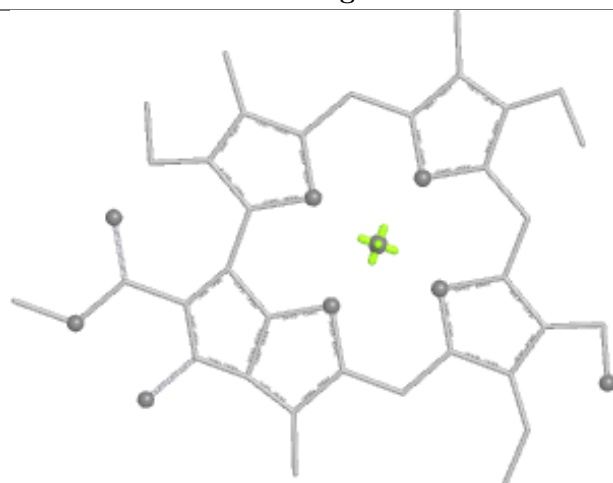
Bond lengths



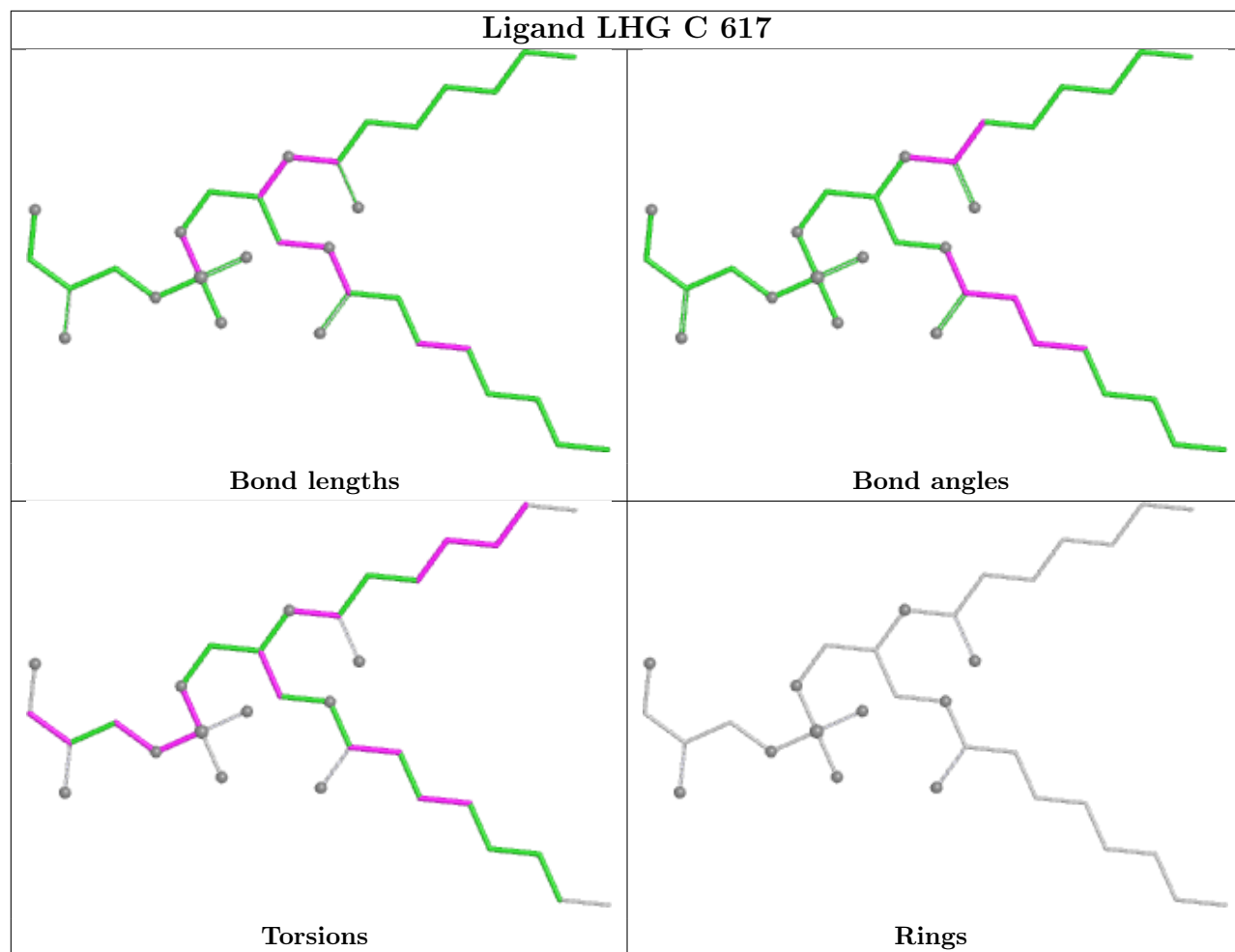
Bond angles



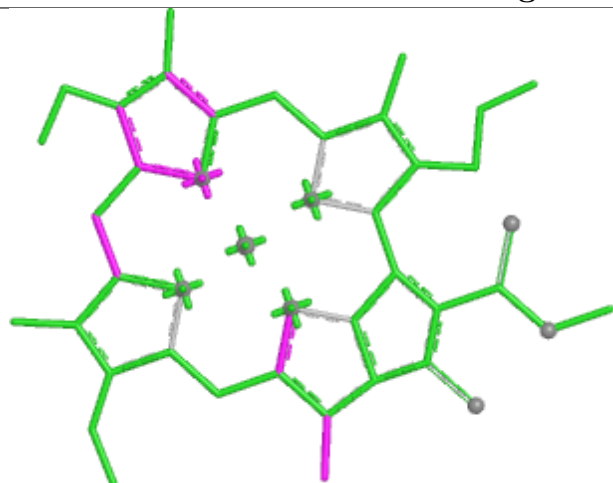
Torsions



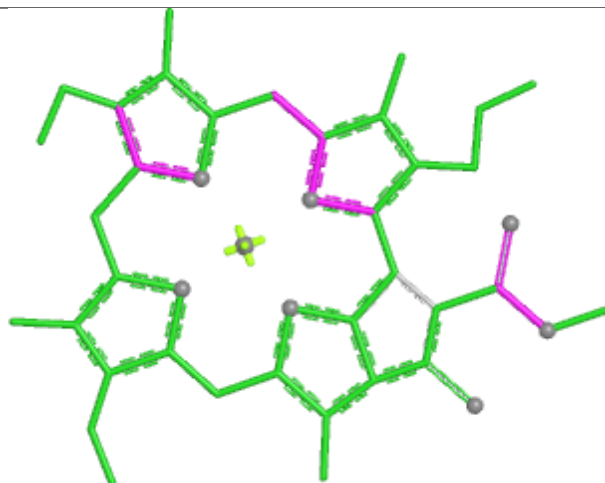
Rings



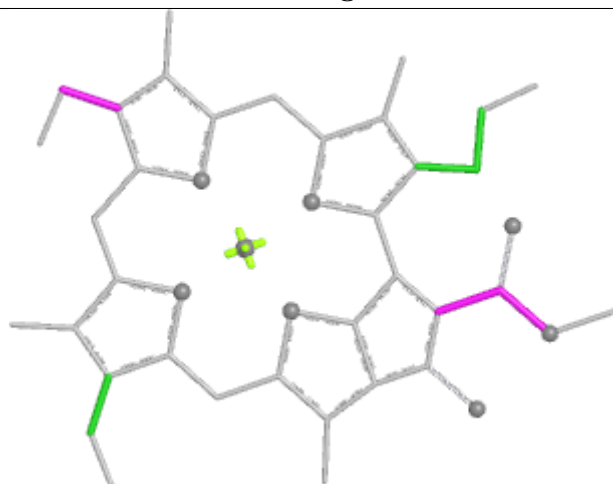
Ligand CLA 6 307



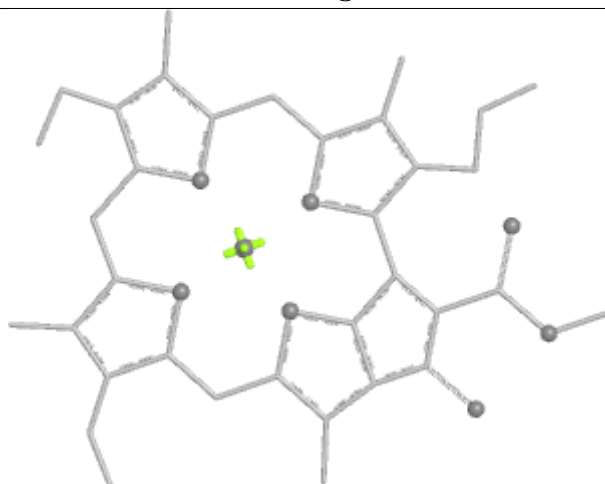
Bond lengths



Bond angles

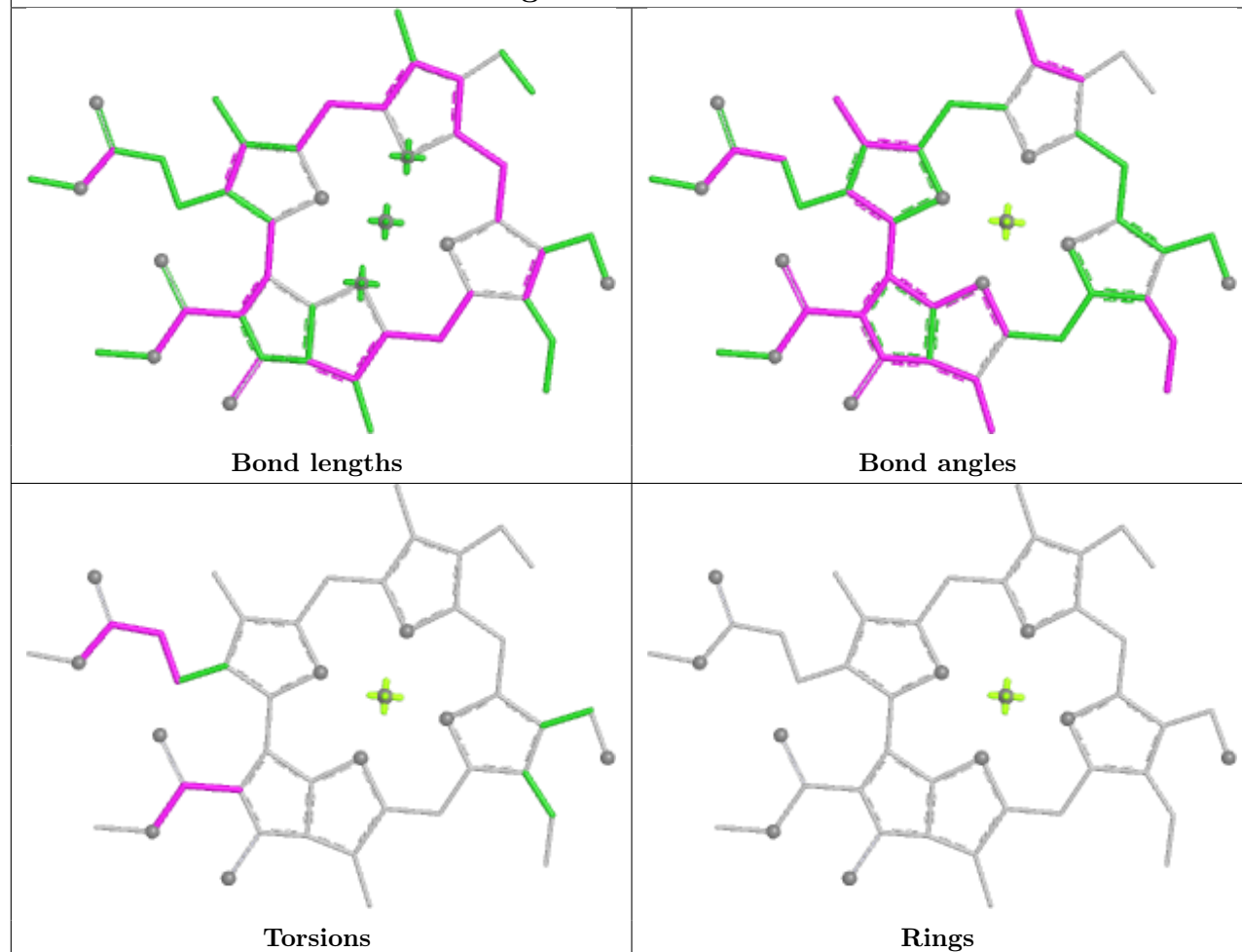


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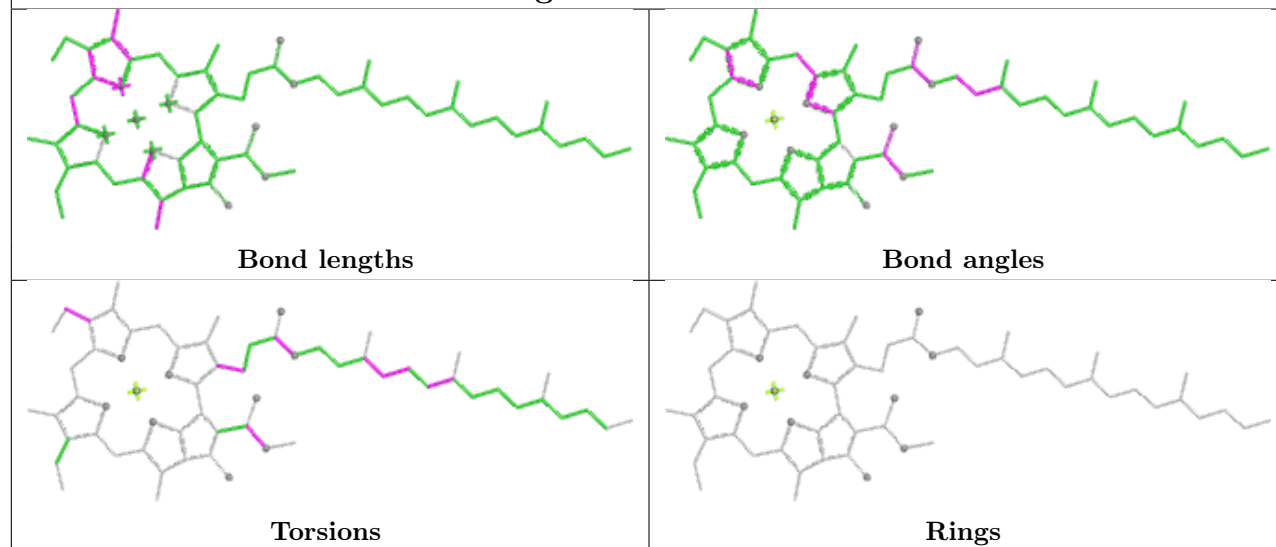


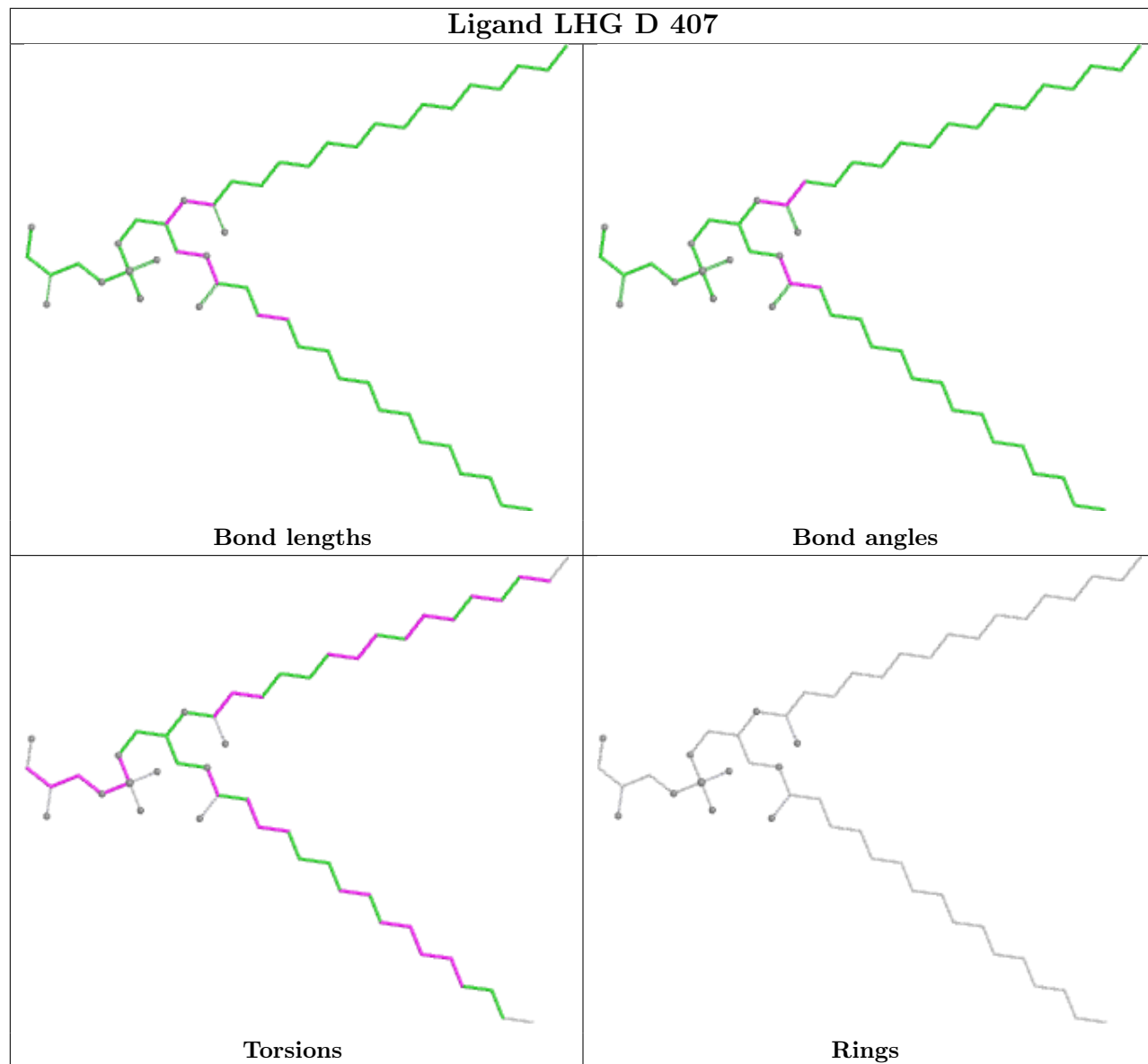
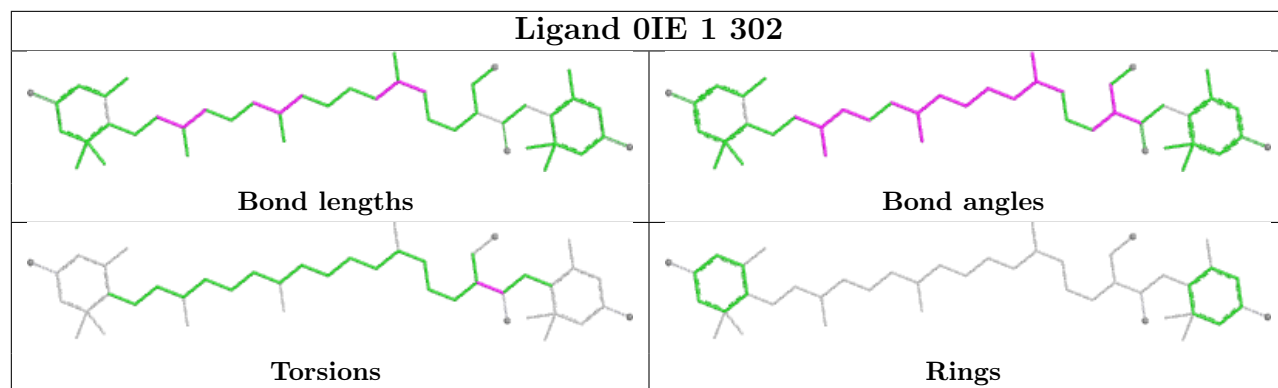
Rings

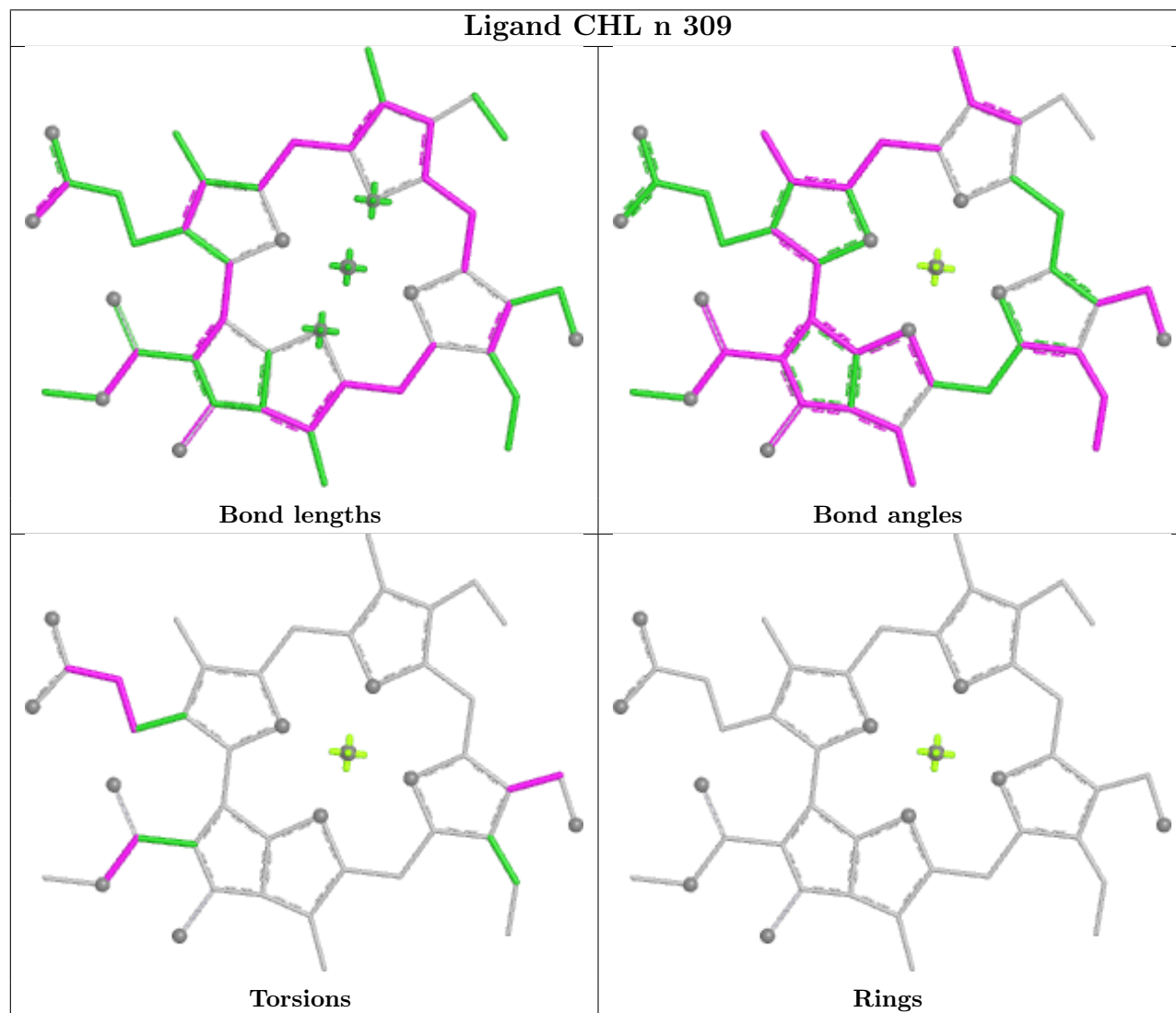
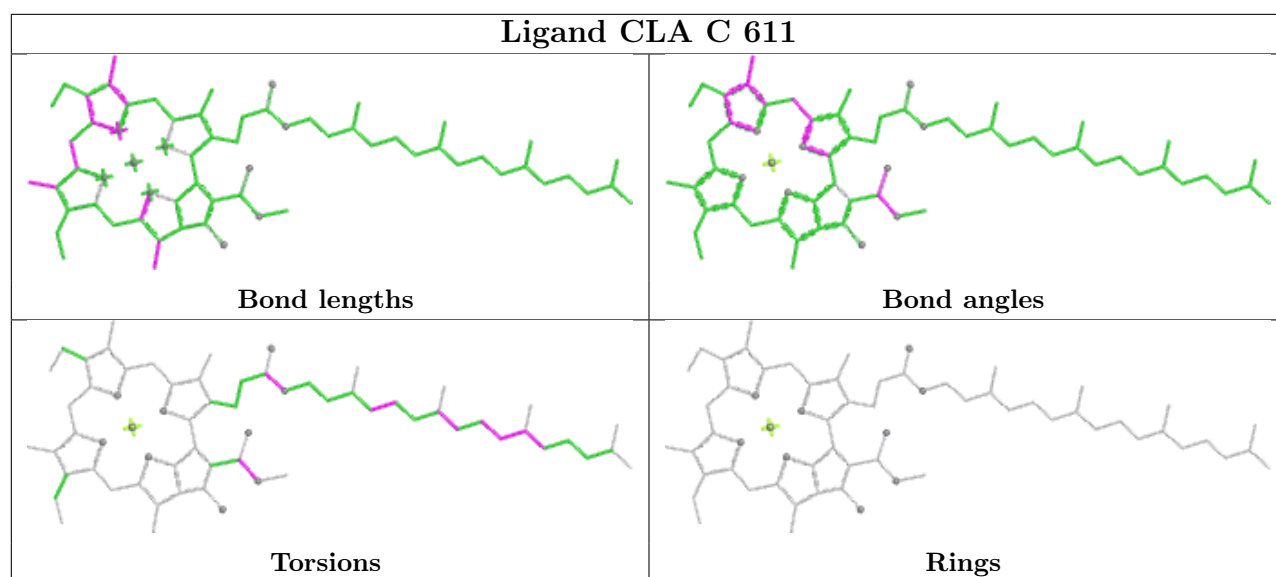
Ligand CHL 2 311



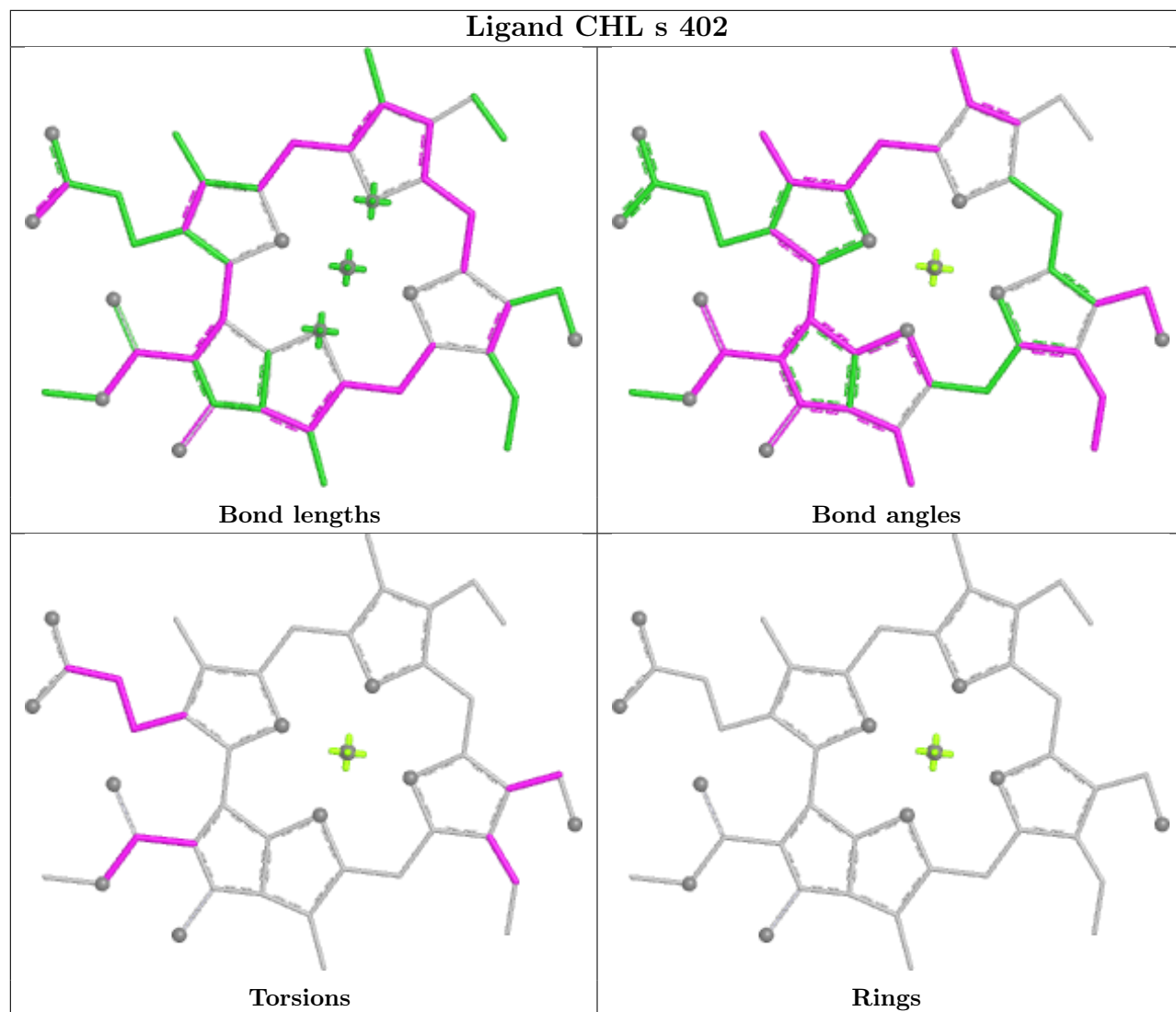
Ligand CLA u 315



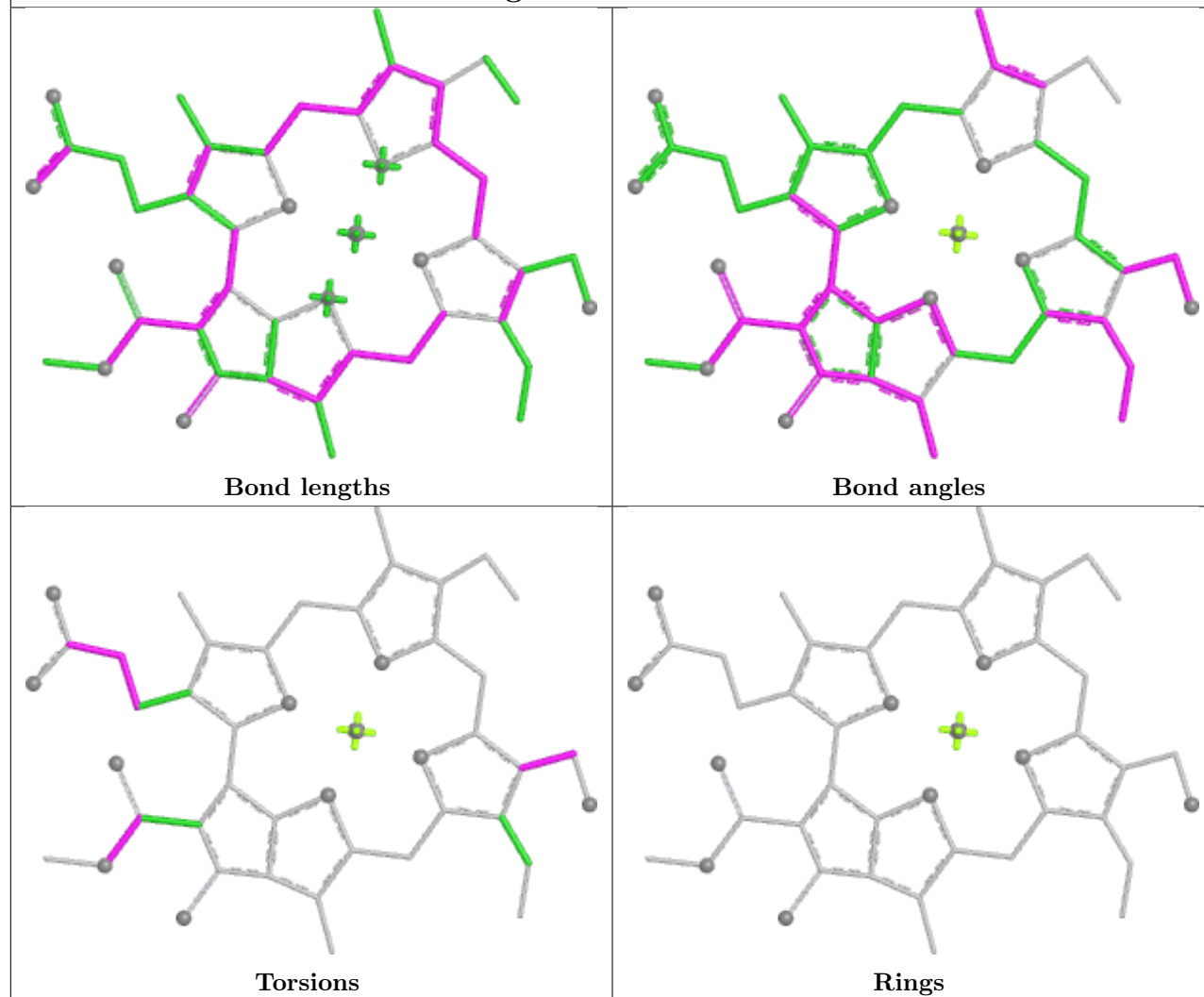




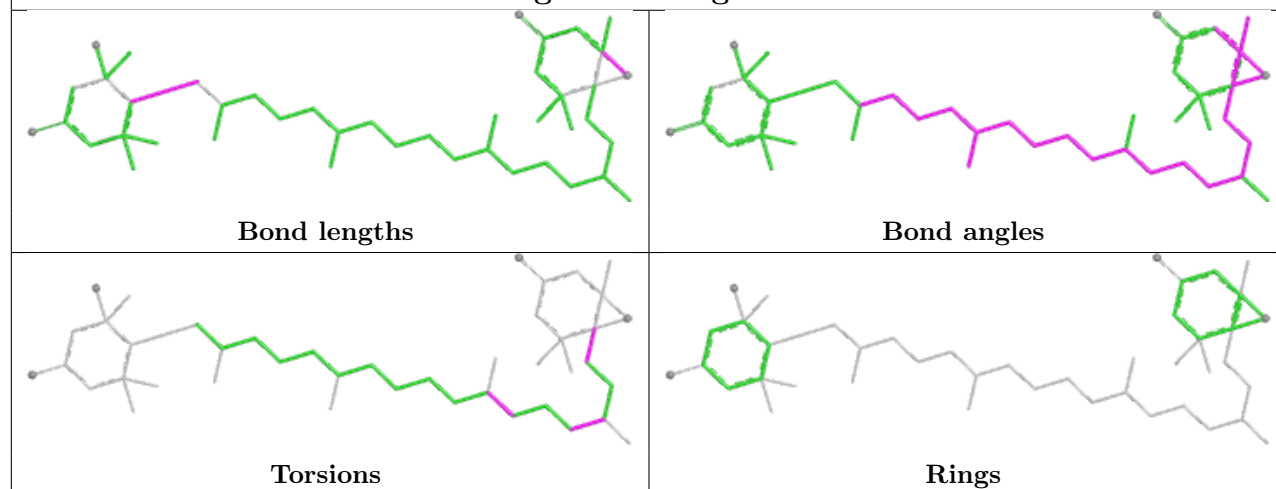
Ligand CHL s 402

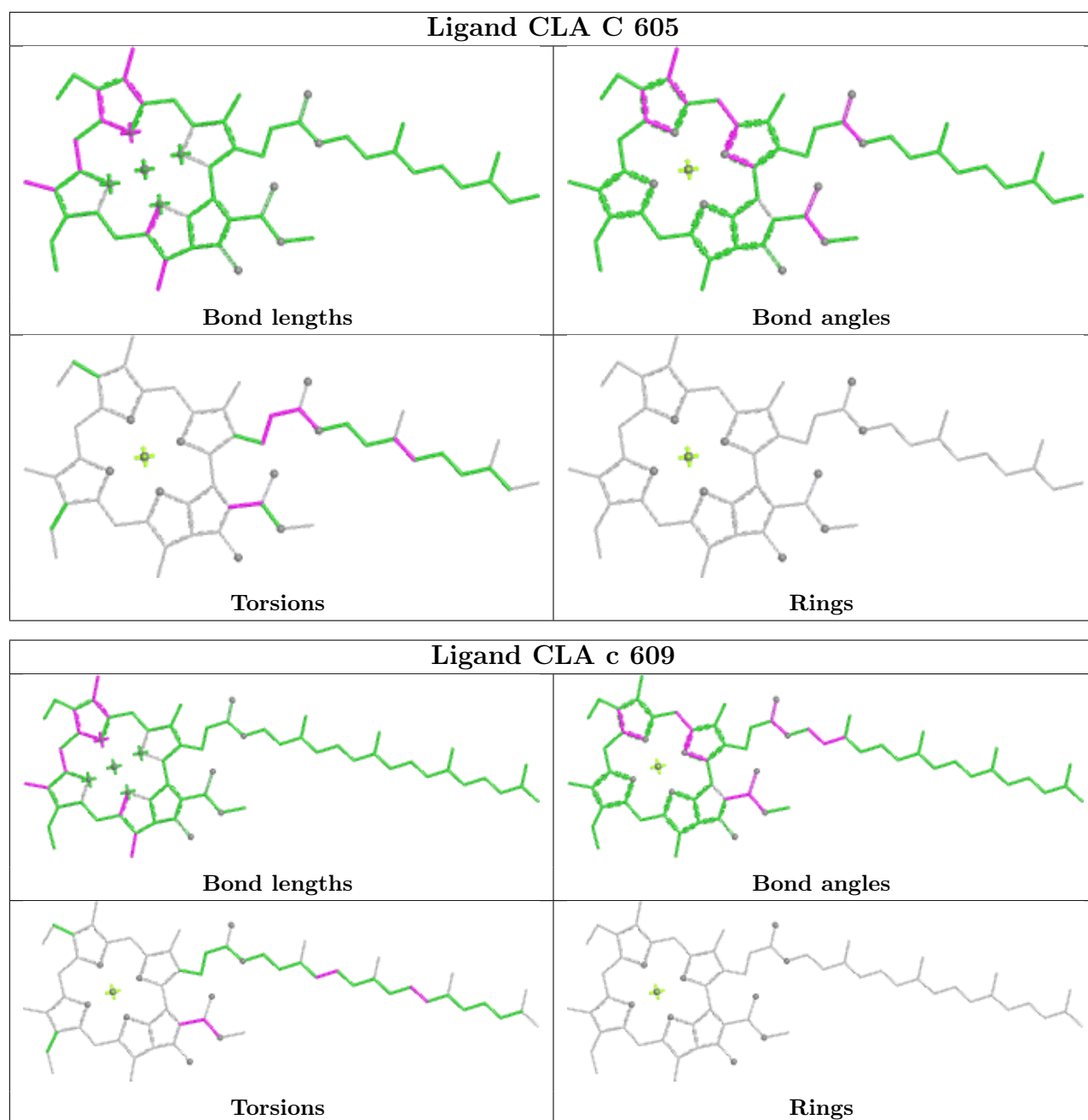


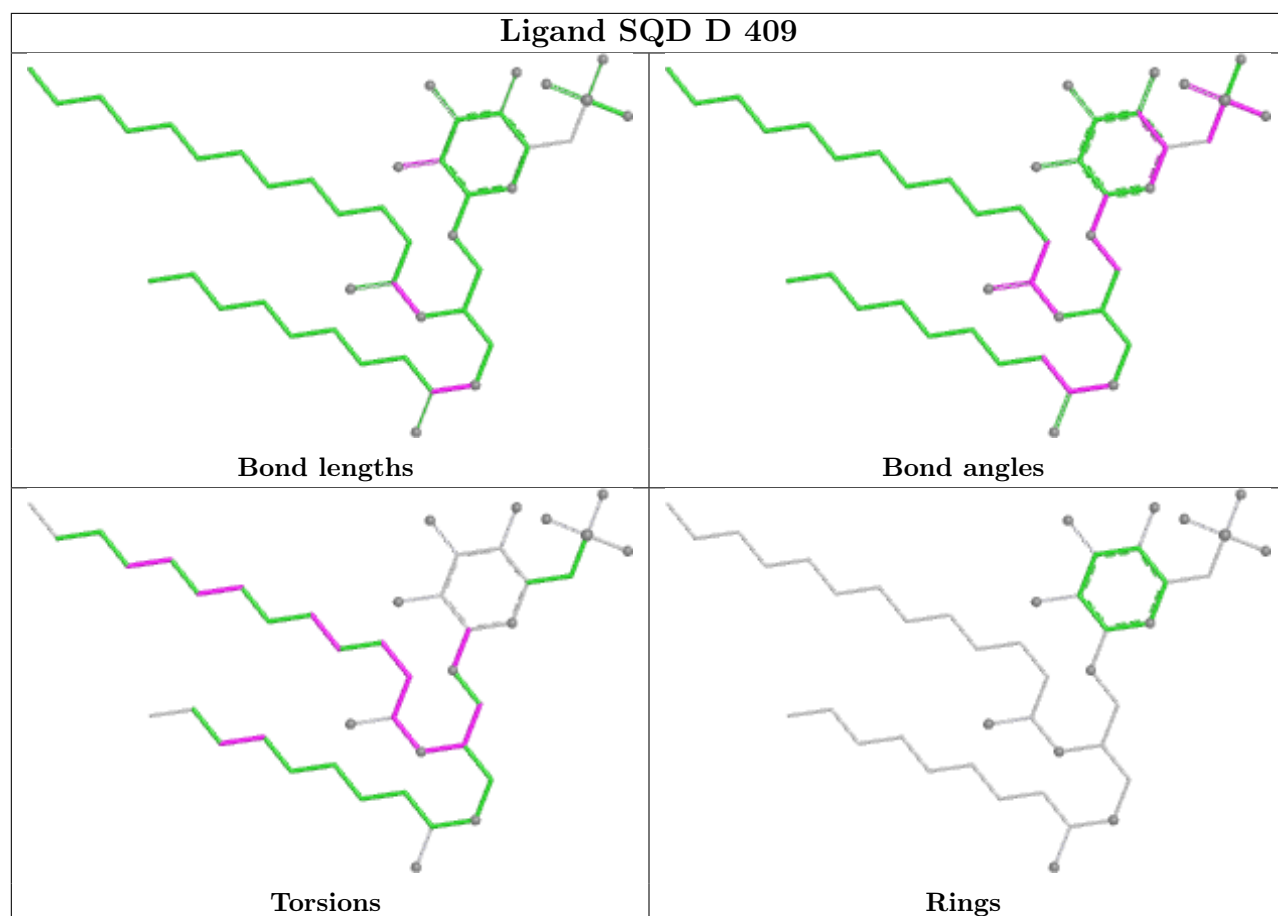
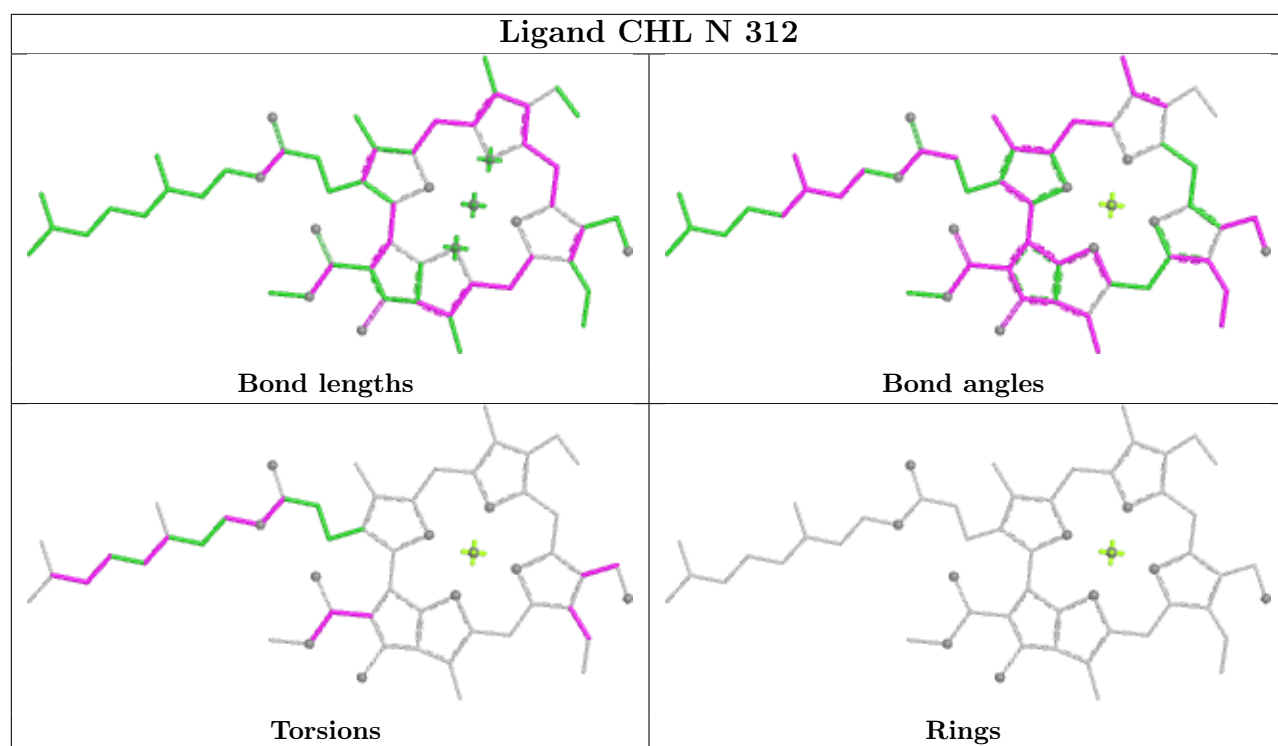
Ligand CHL 7 310



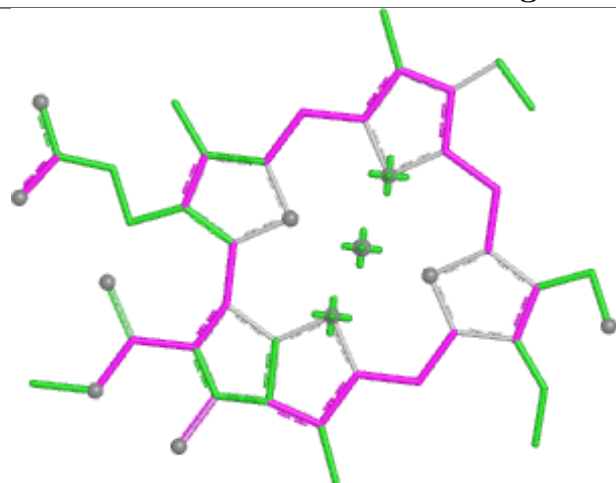
Ligand NEX g 304



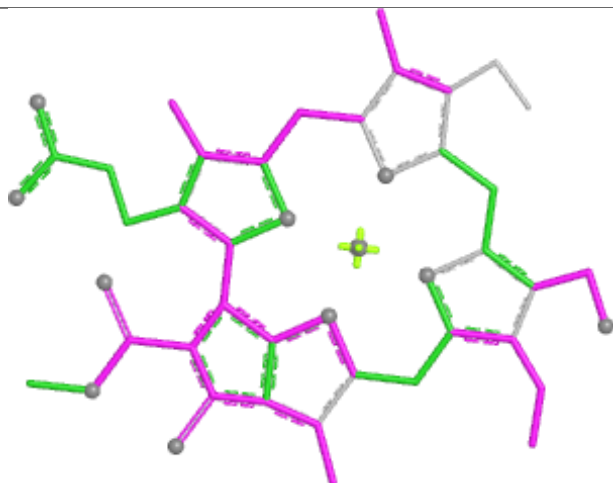




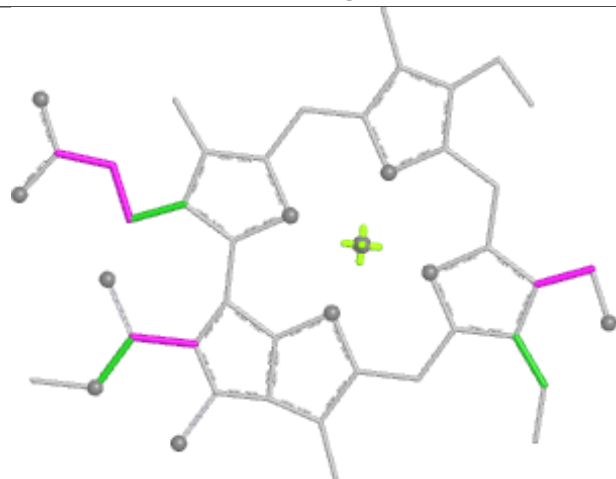
Ligand CHL 8 308



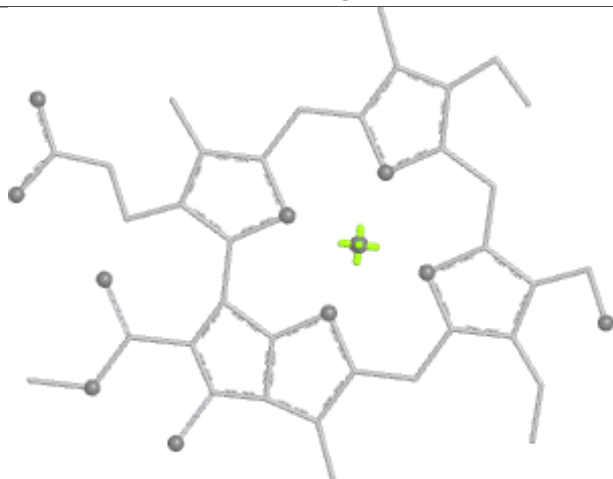
Bond lengths



Bond angles

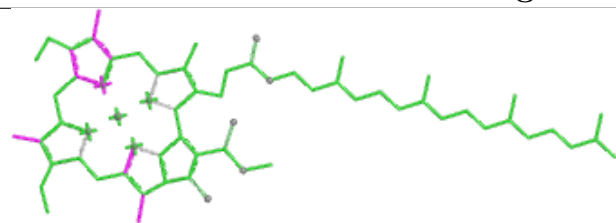


Torsions

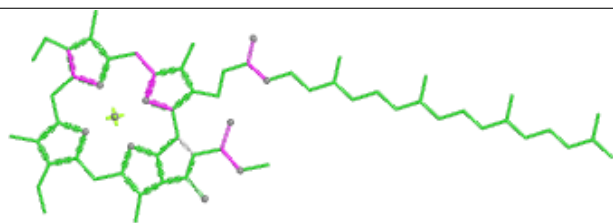


Rings

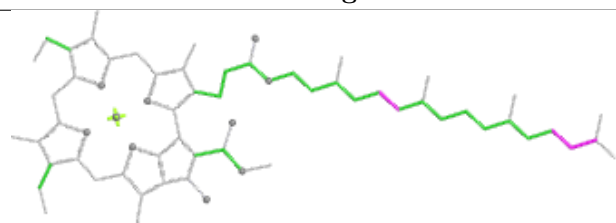
Ligand CLA B 615



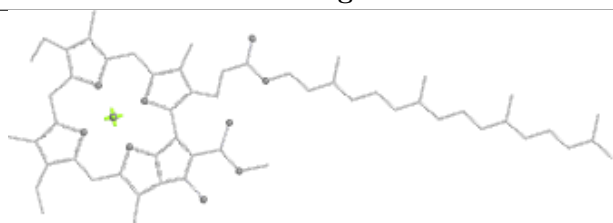
Bond lengths



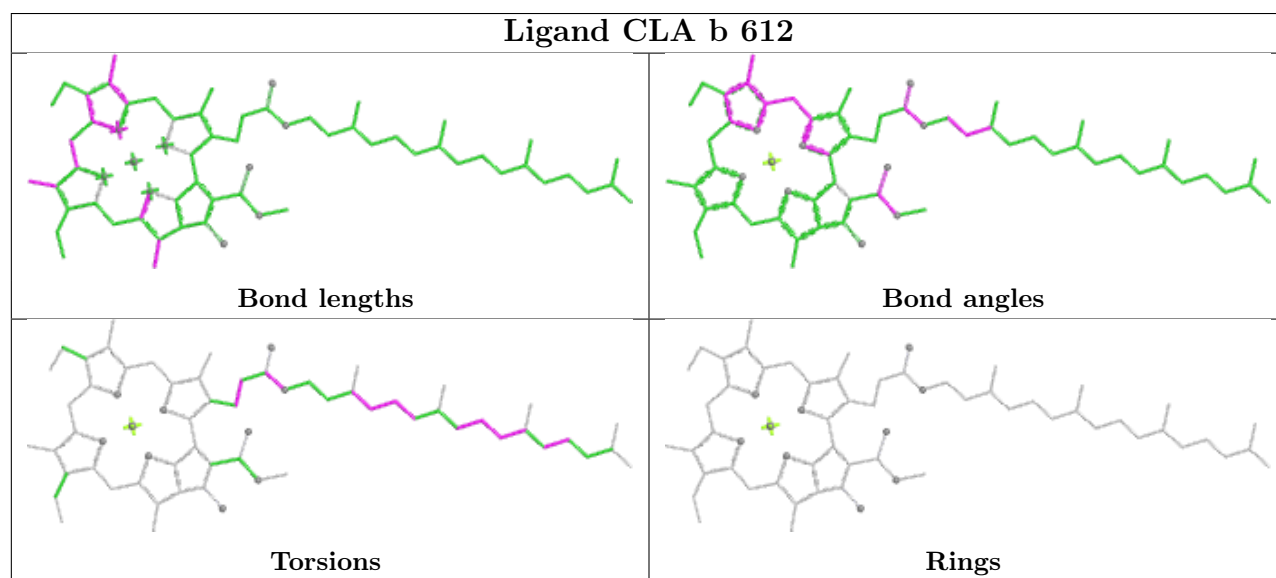
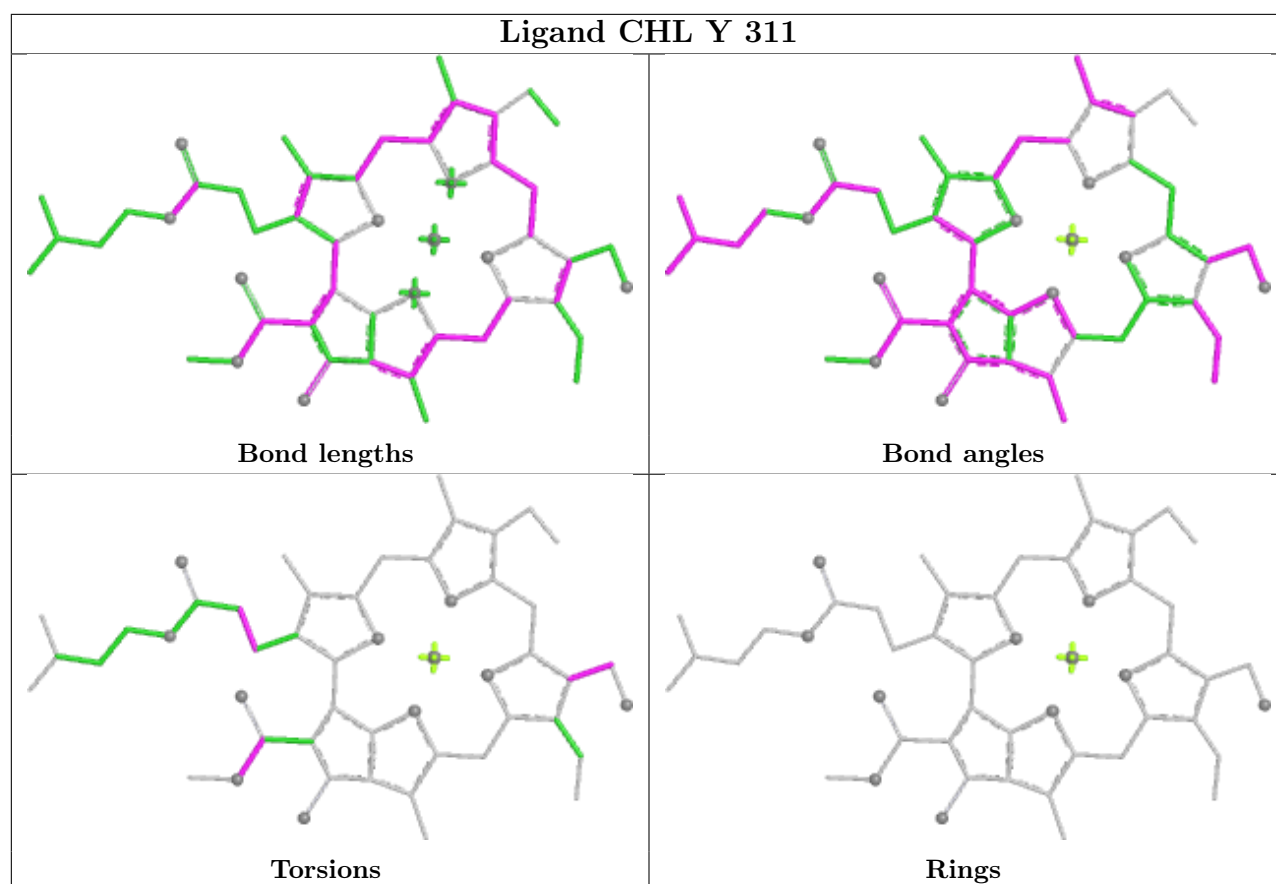
Bond angles

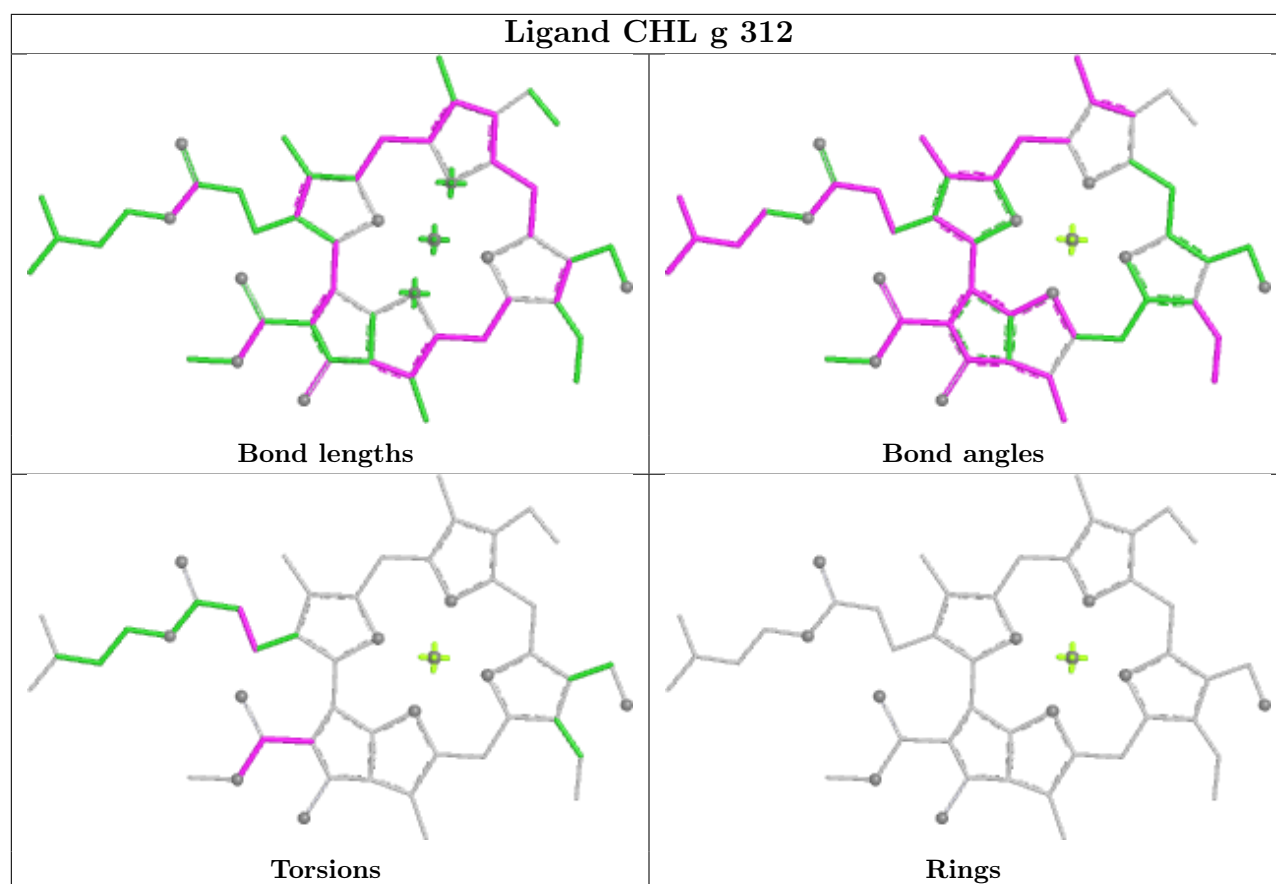


Torsions

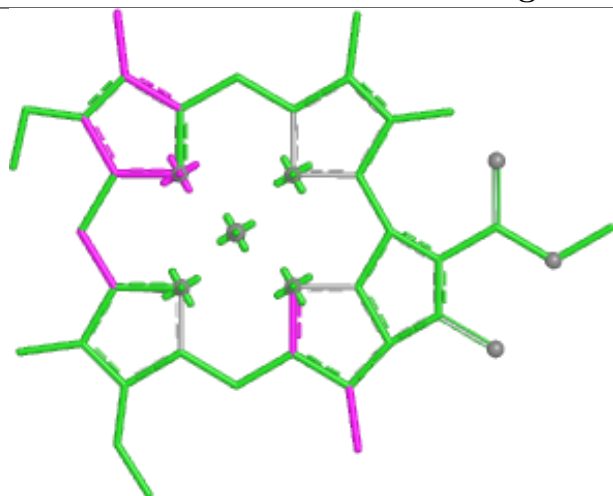


Rings

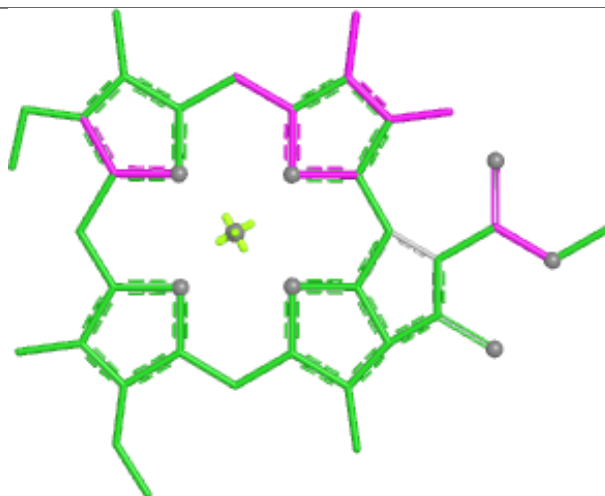




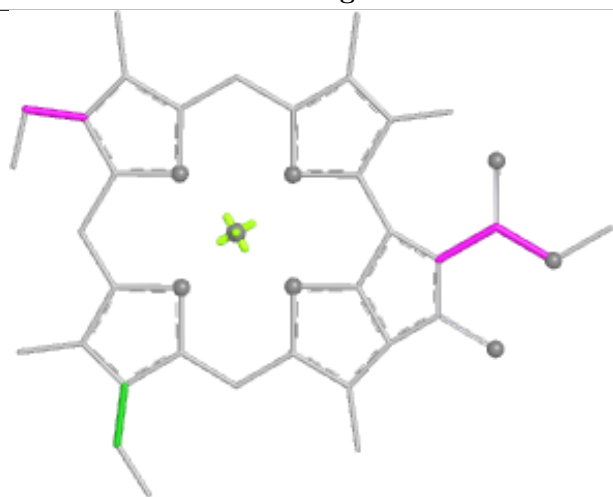
Ligand CLA 3 306



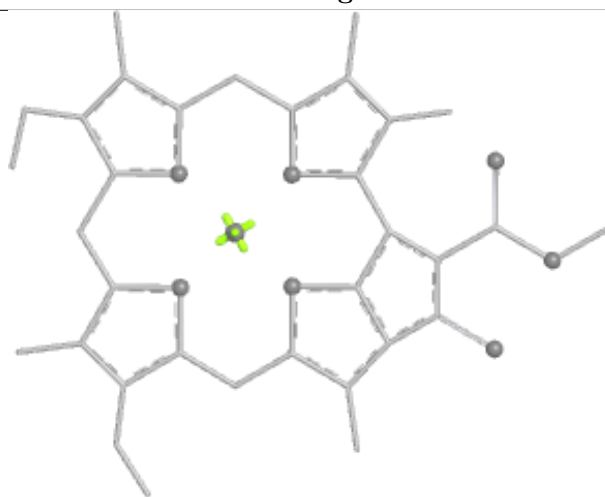
Bond lengths



Bond angles

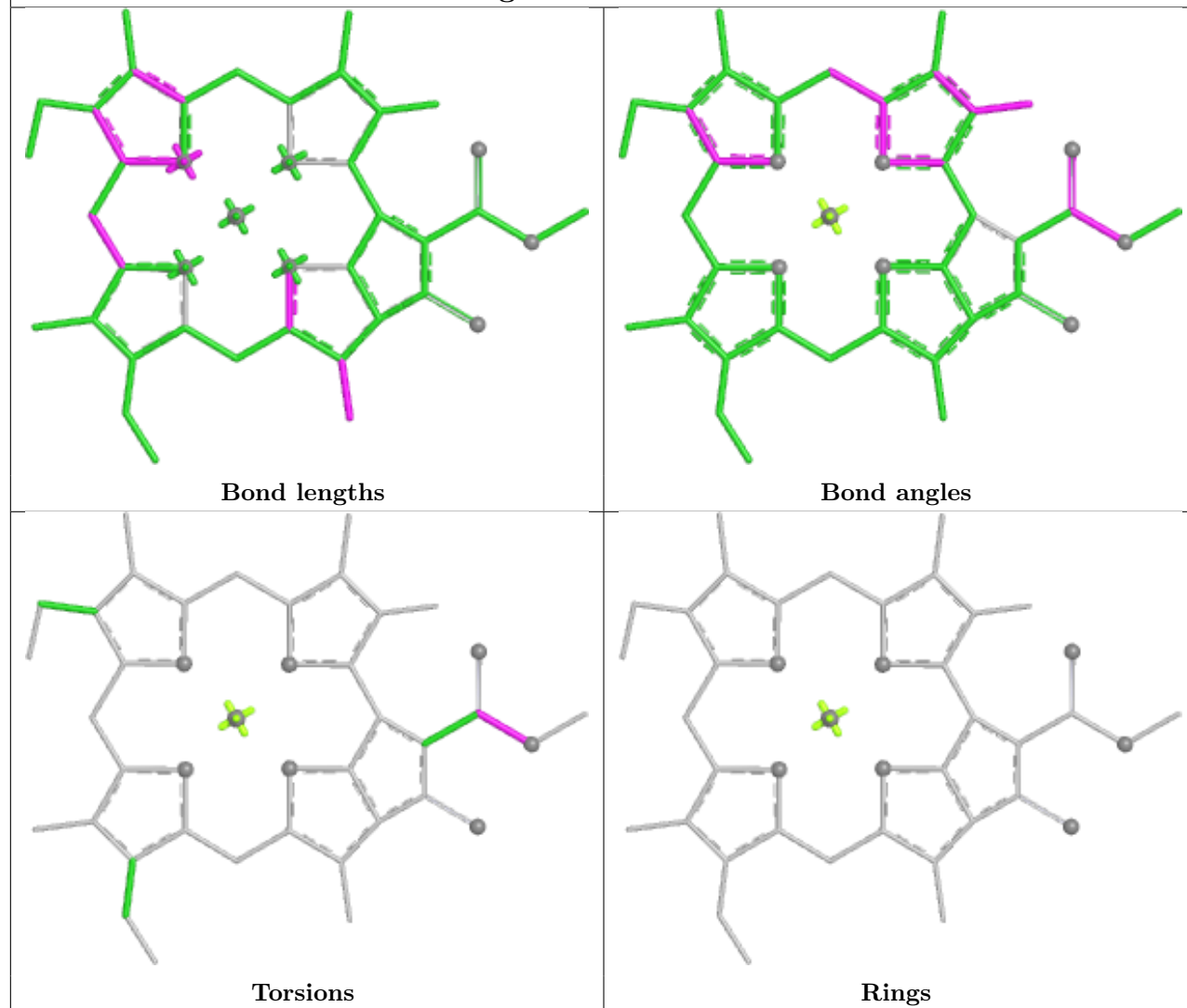


Torsions

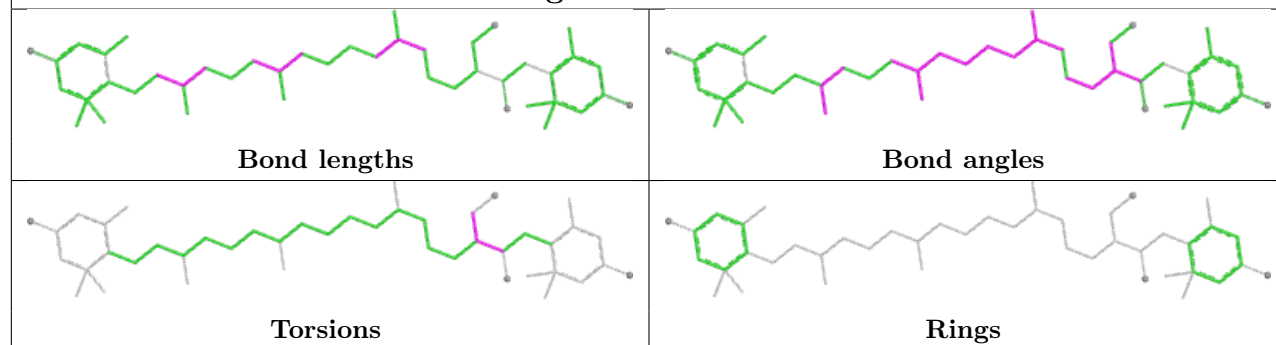


Rings

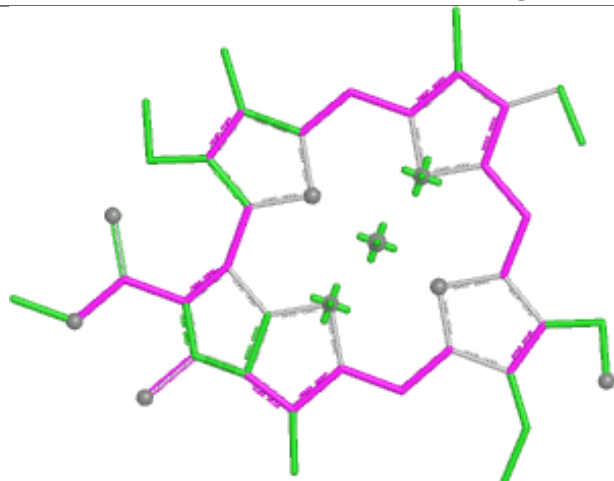
Ligand CLA 6 314



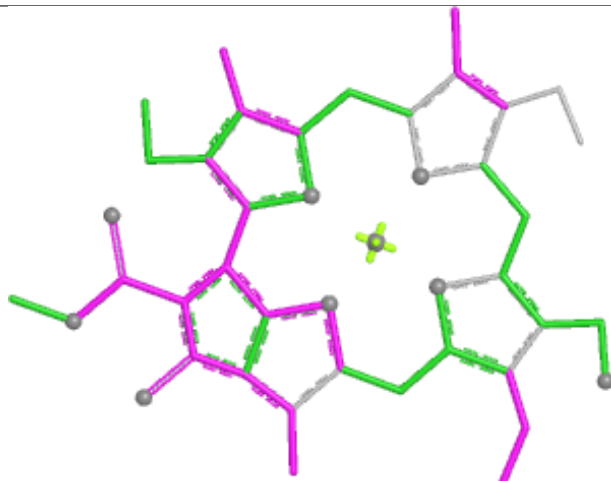
Ligand OIE 9 302



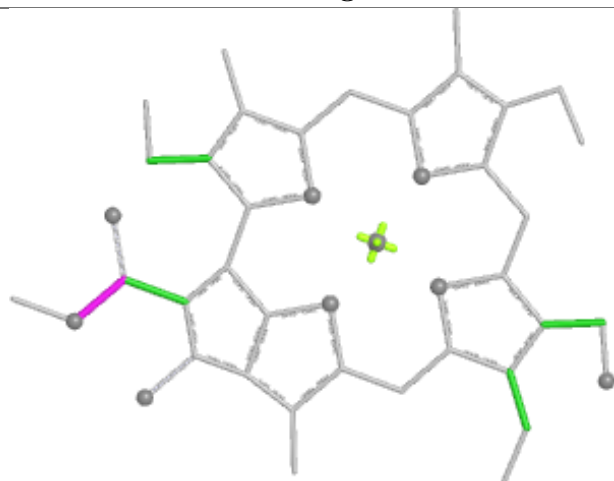
Ligand CHL N 308



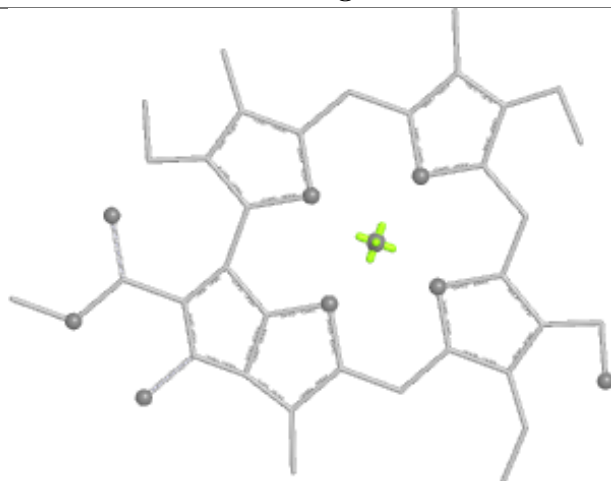
Bond lengths



Bond angles

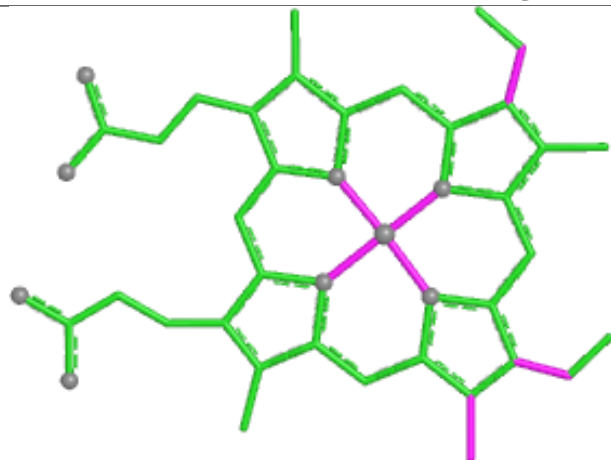


Torsions

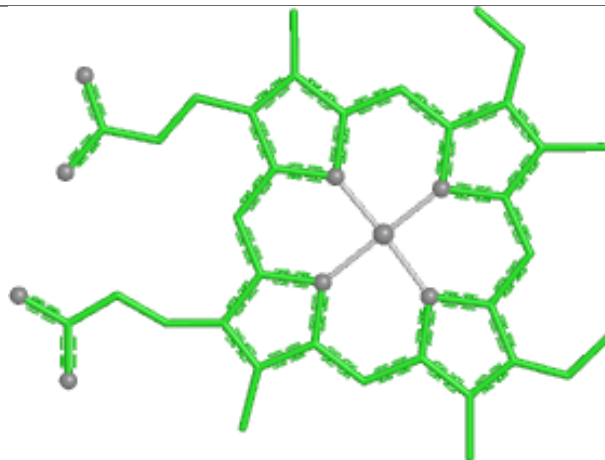


Rings

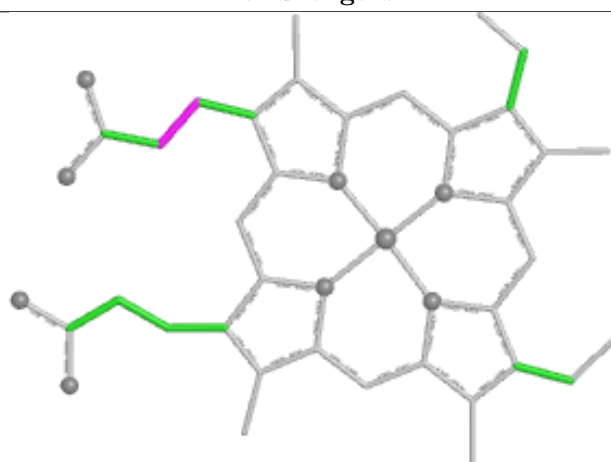
Ligand HEM f 201



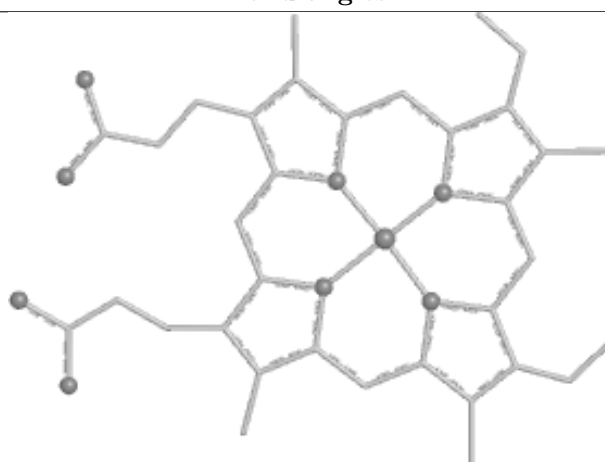
Bond lengths



Bond angles

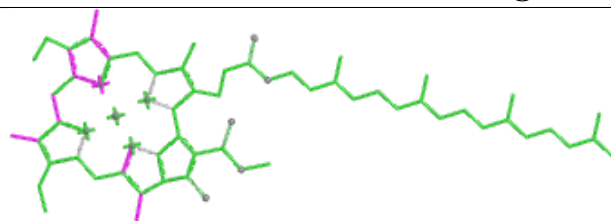


Torsions

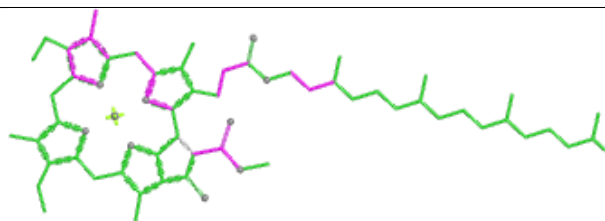


Rings

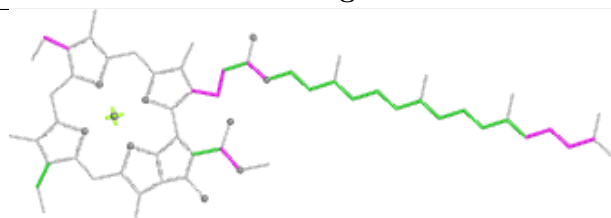
Ligand CLA A 603



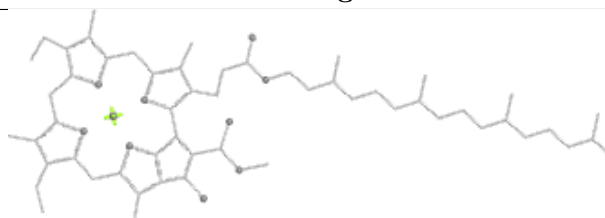
Bond lengths



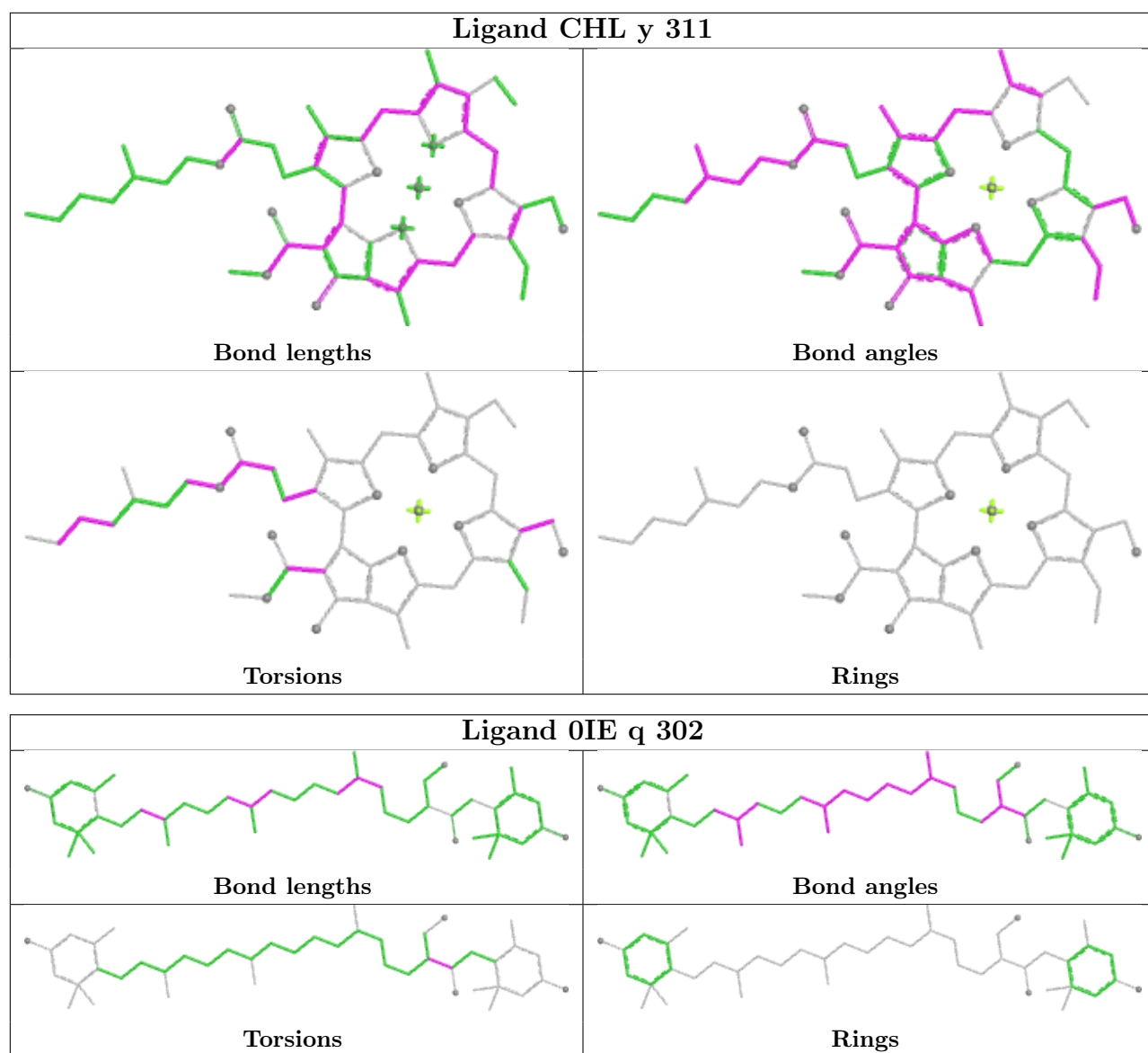
Bond angles



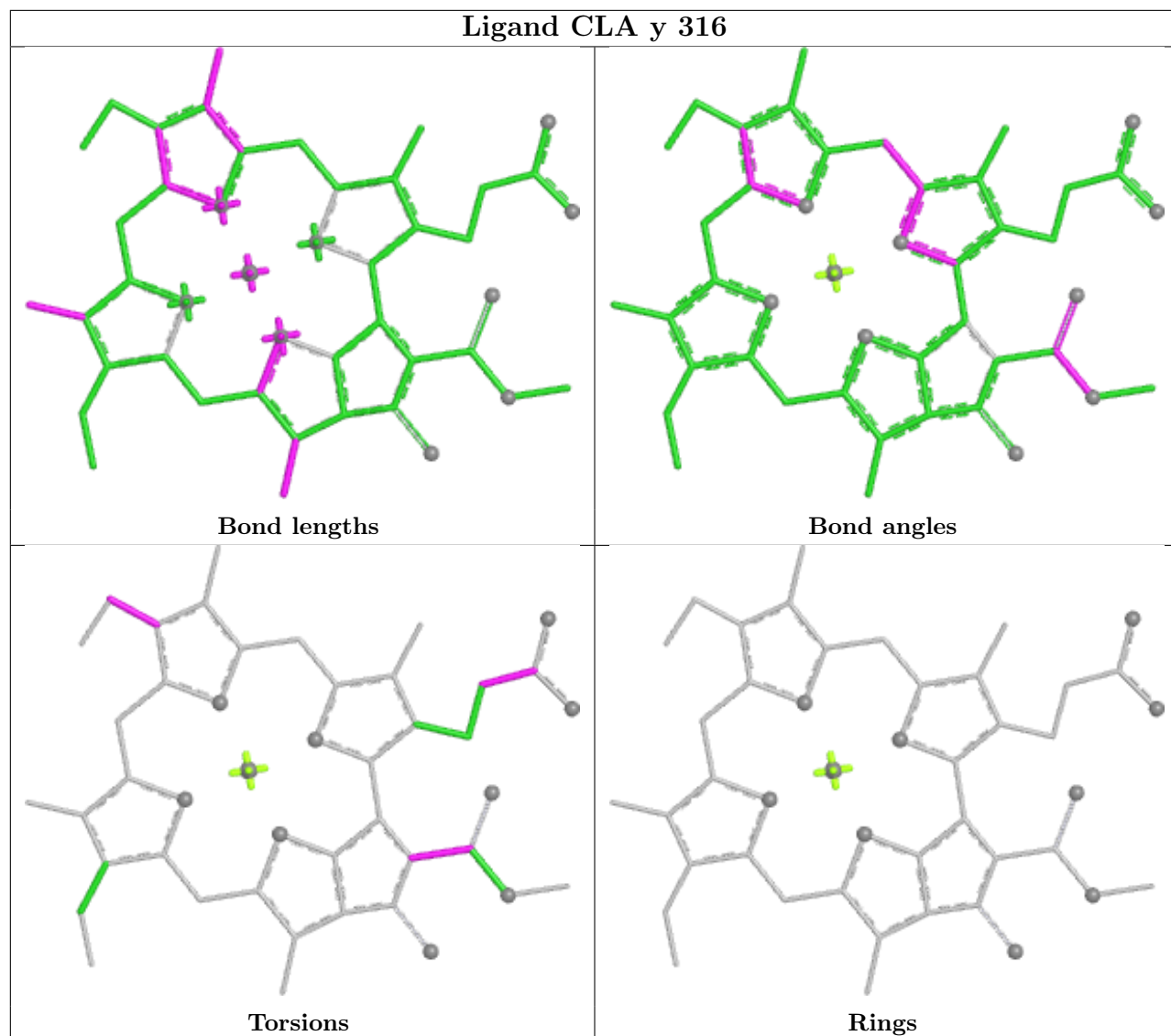
Torsions



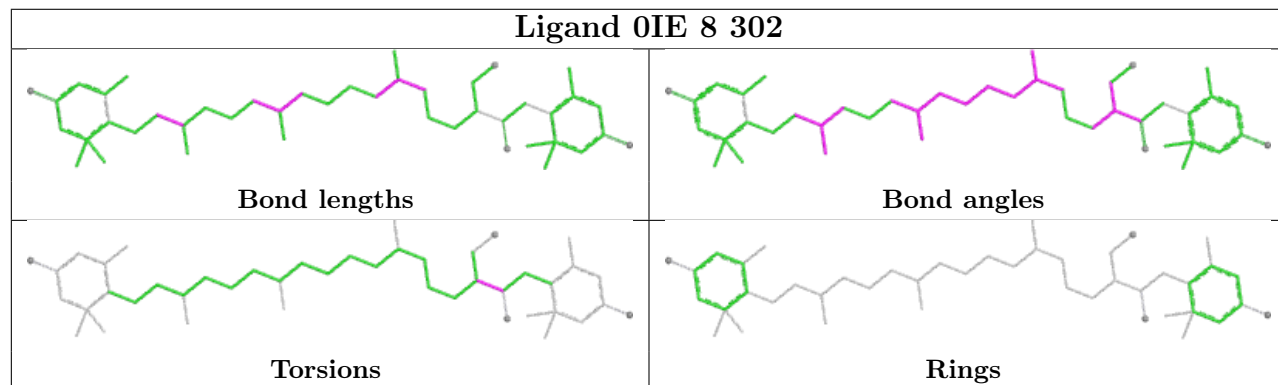
Rings

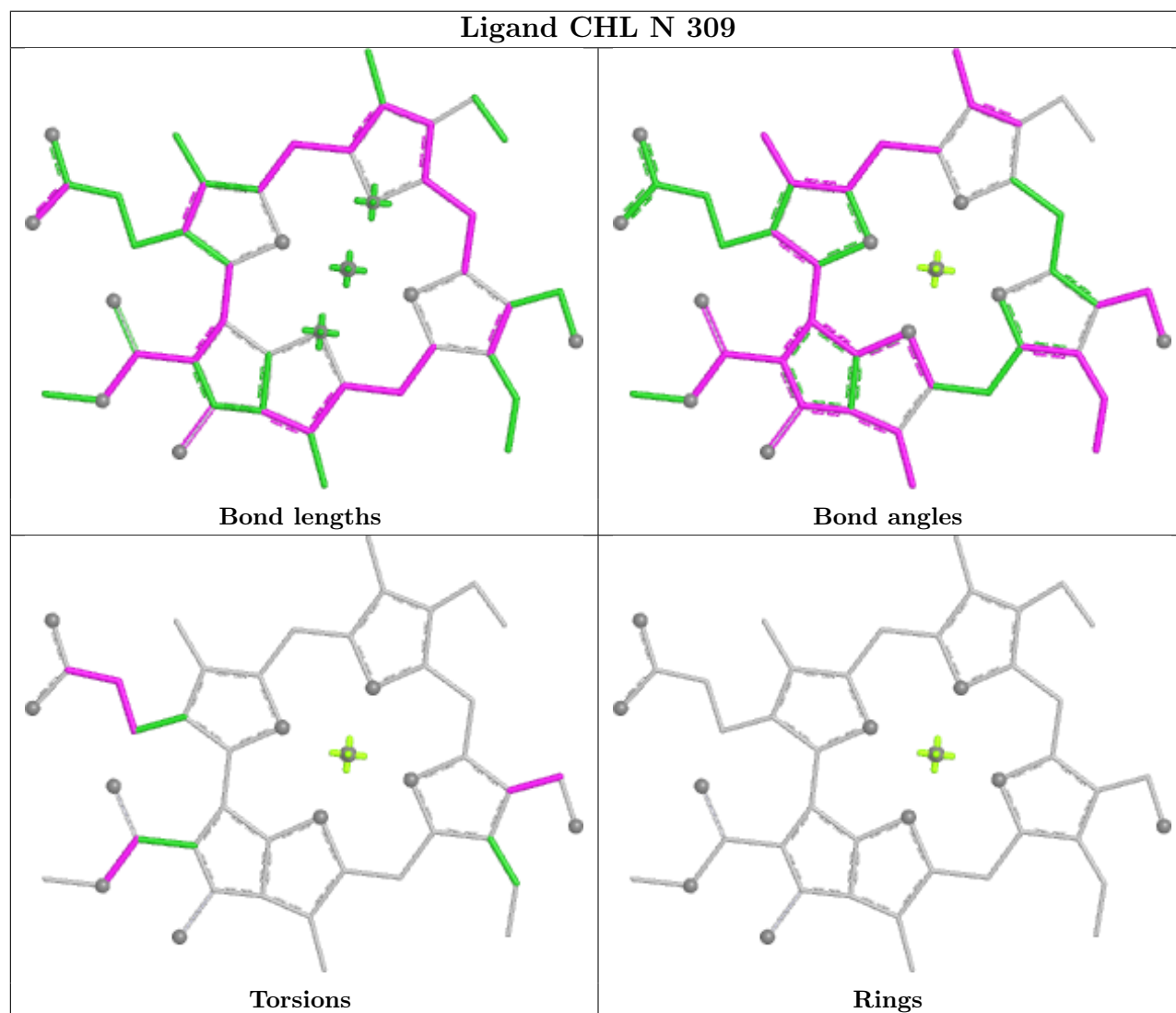
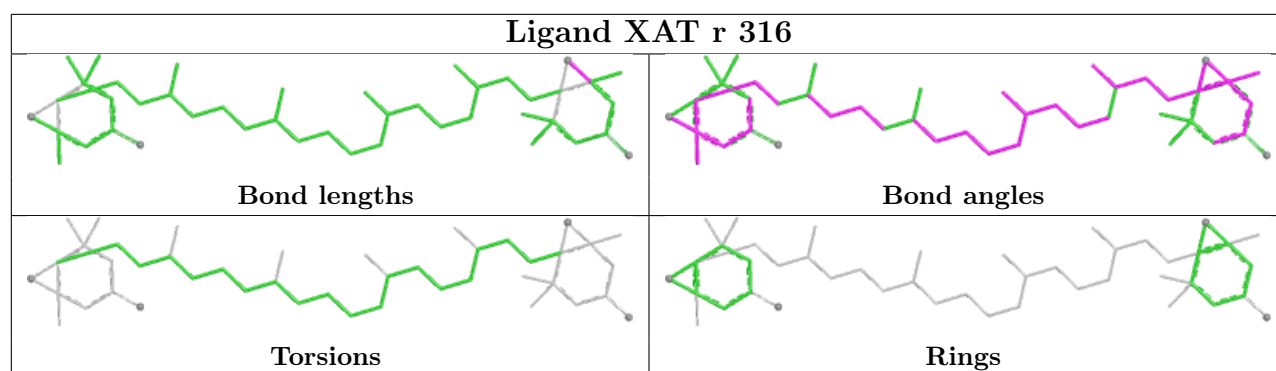


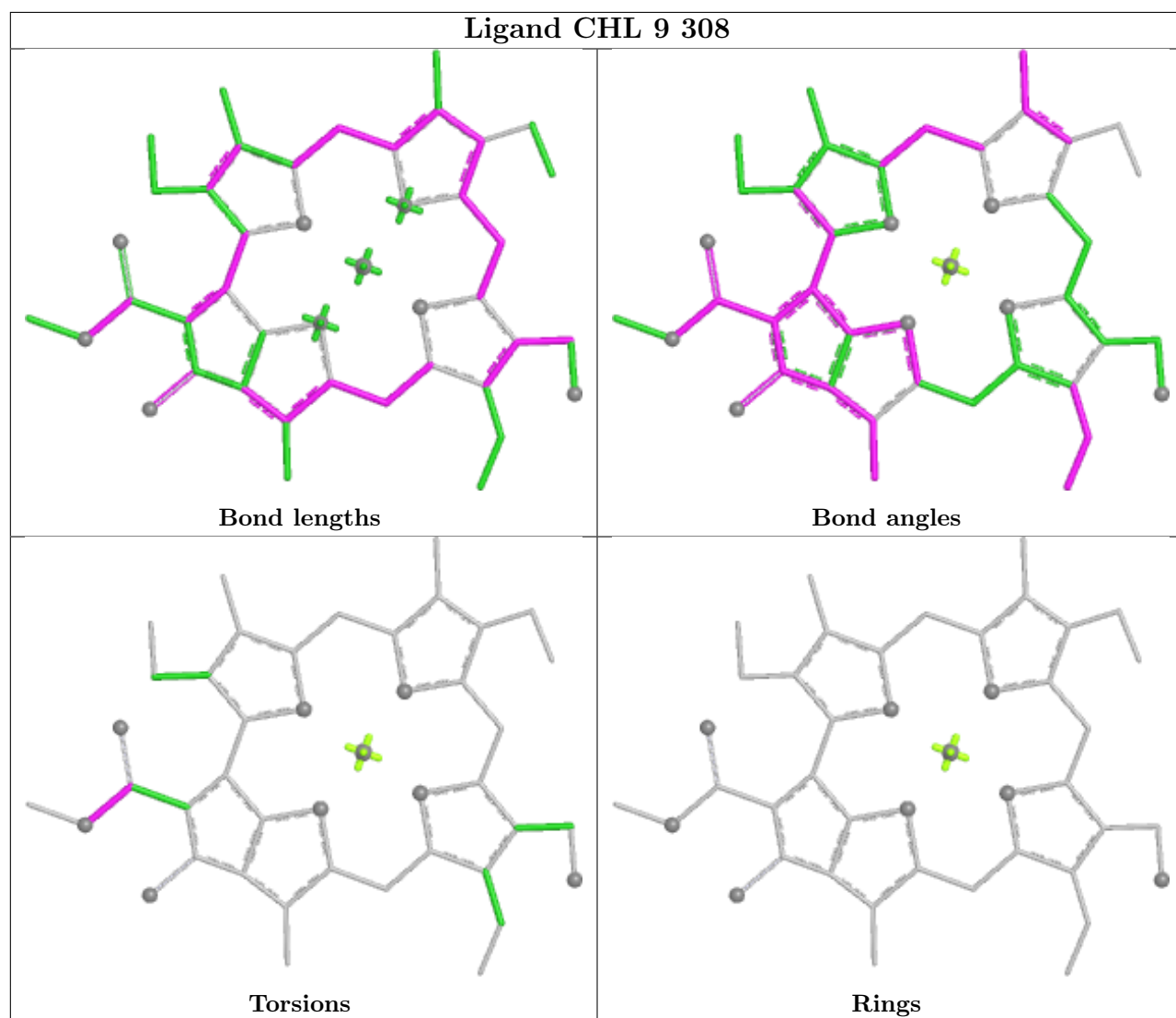
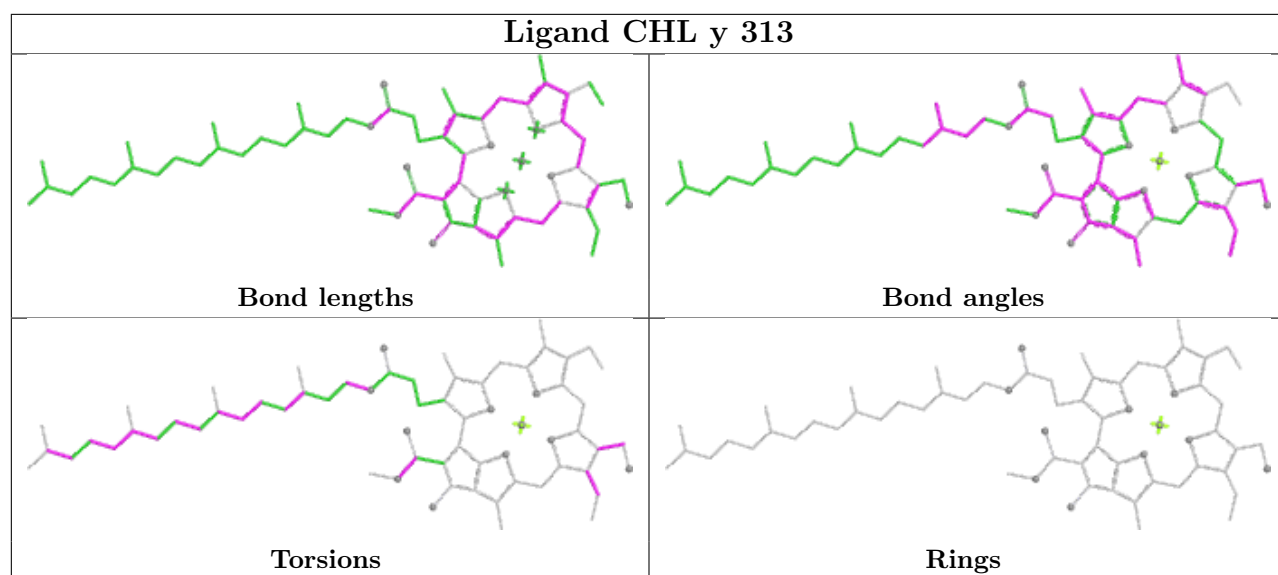
Ligand CLA y 316



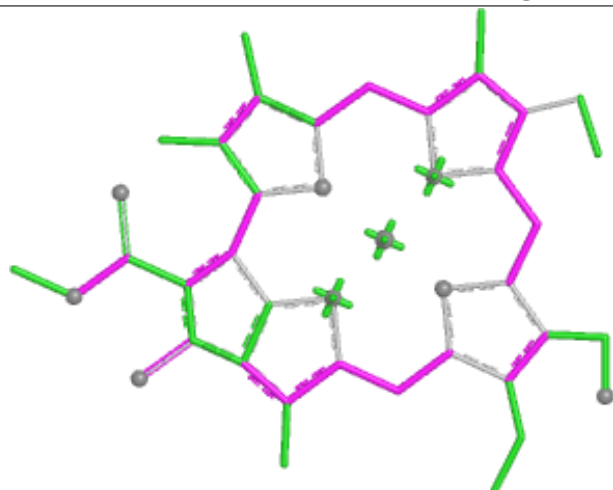
Ligand OIE 8 302



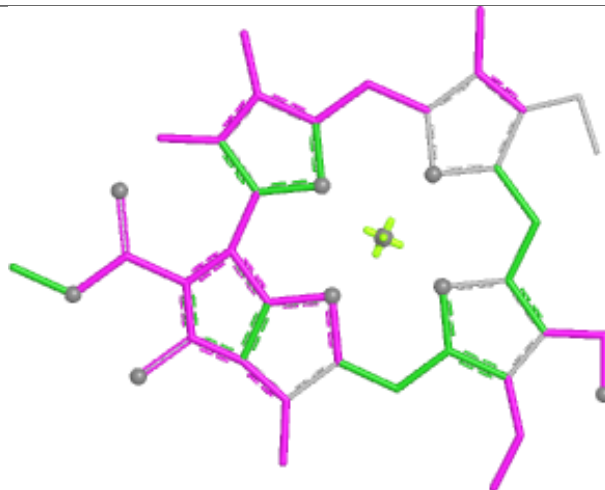




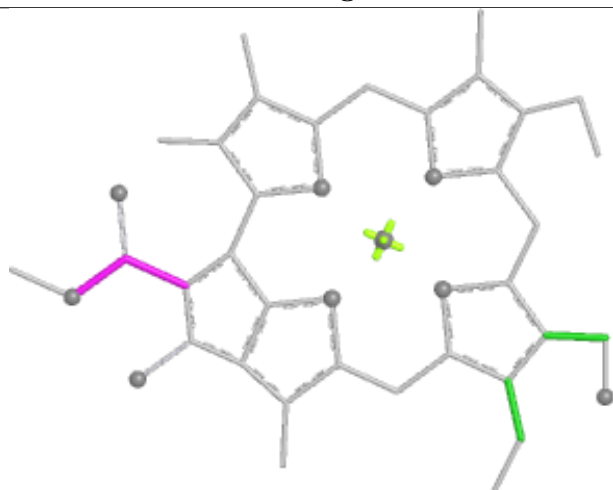
Ligand CHL 5 318



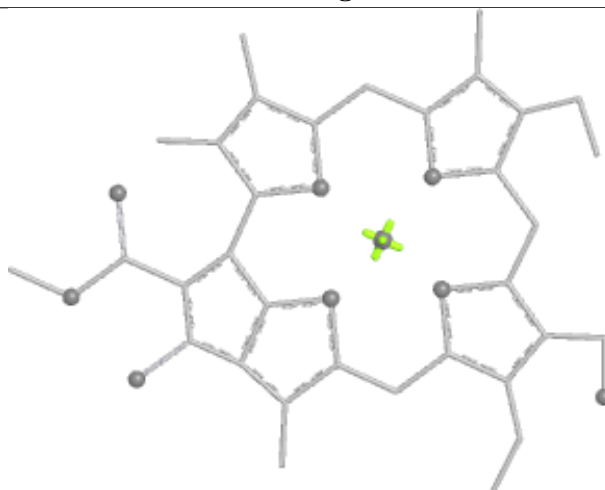
Bond lengths



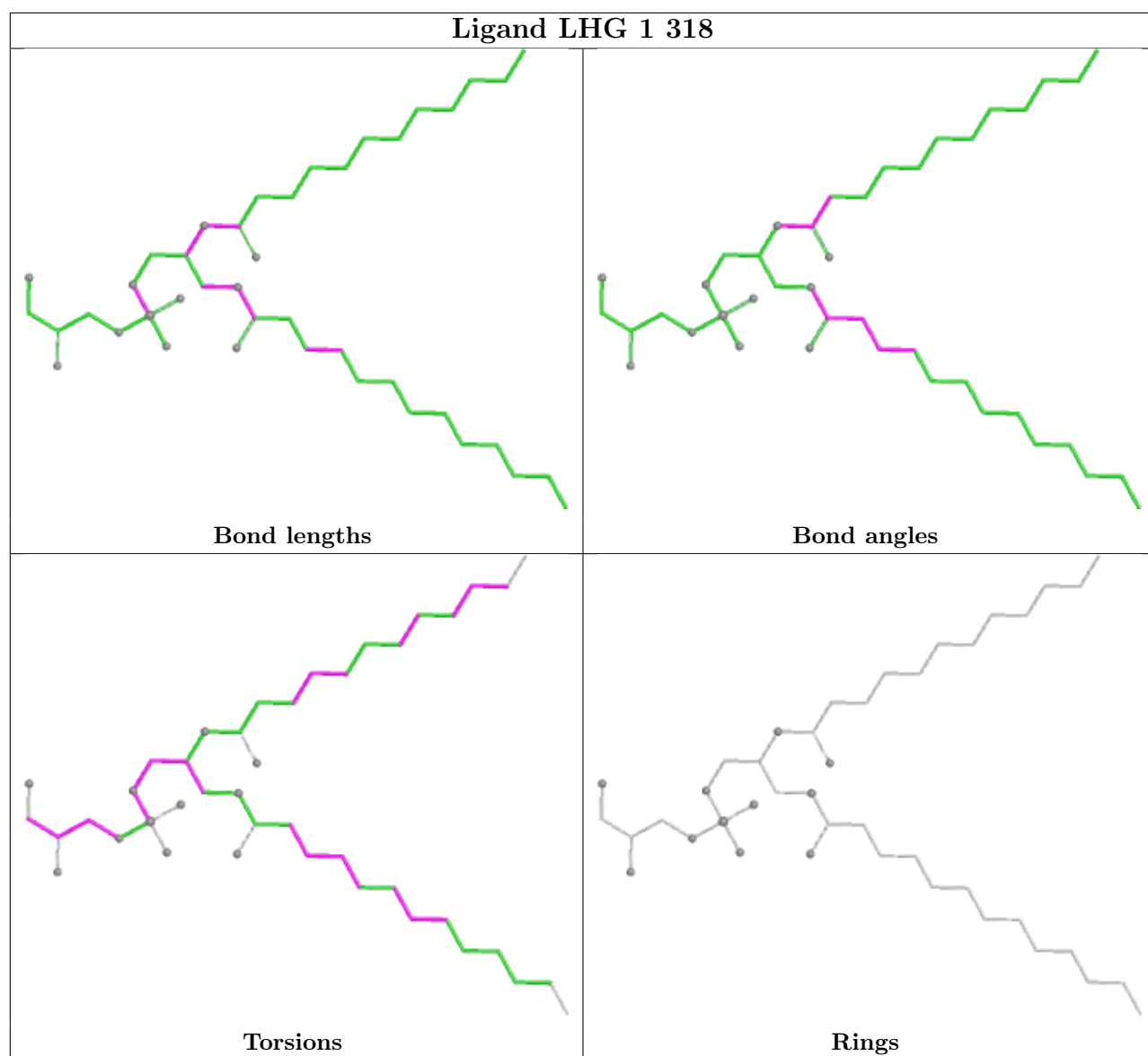
Bond angles



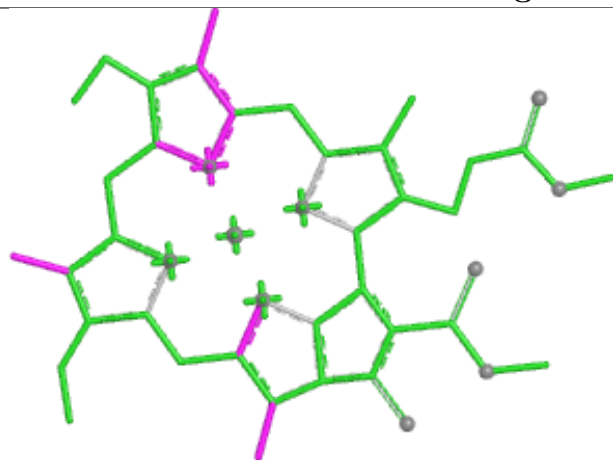
Torsions



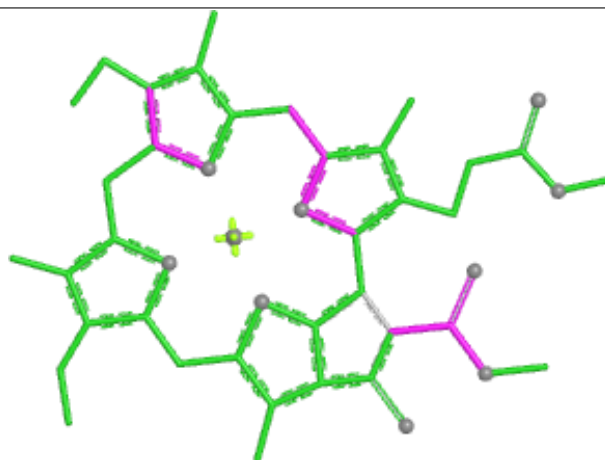
Rings



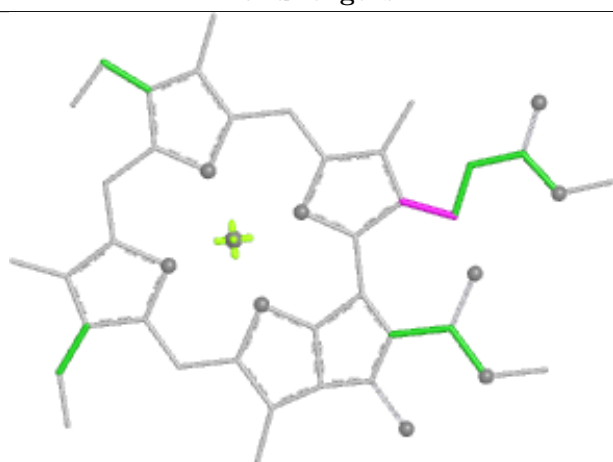
Ligand CLA C 616



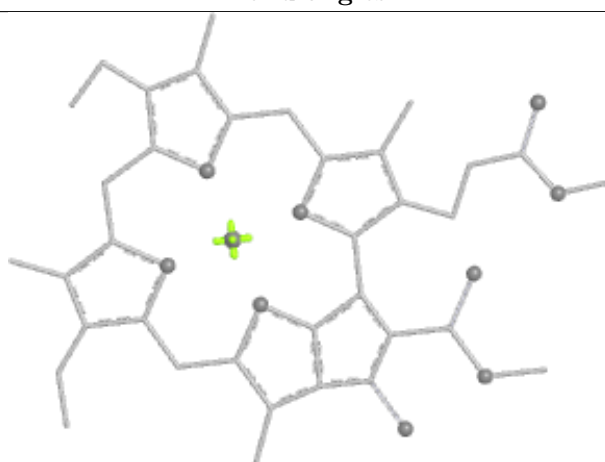
Bond lengths



Bond angles

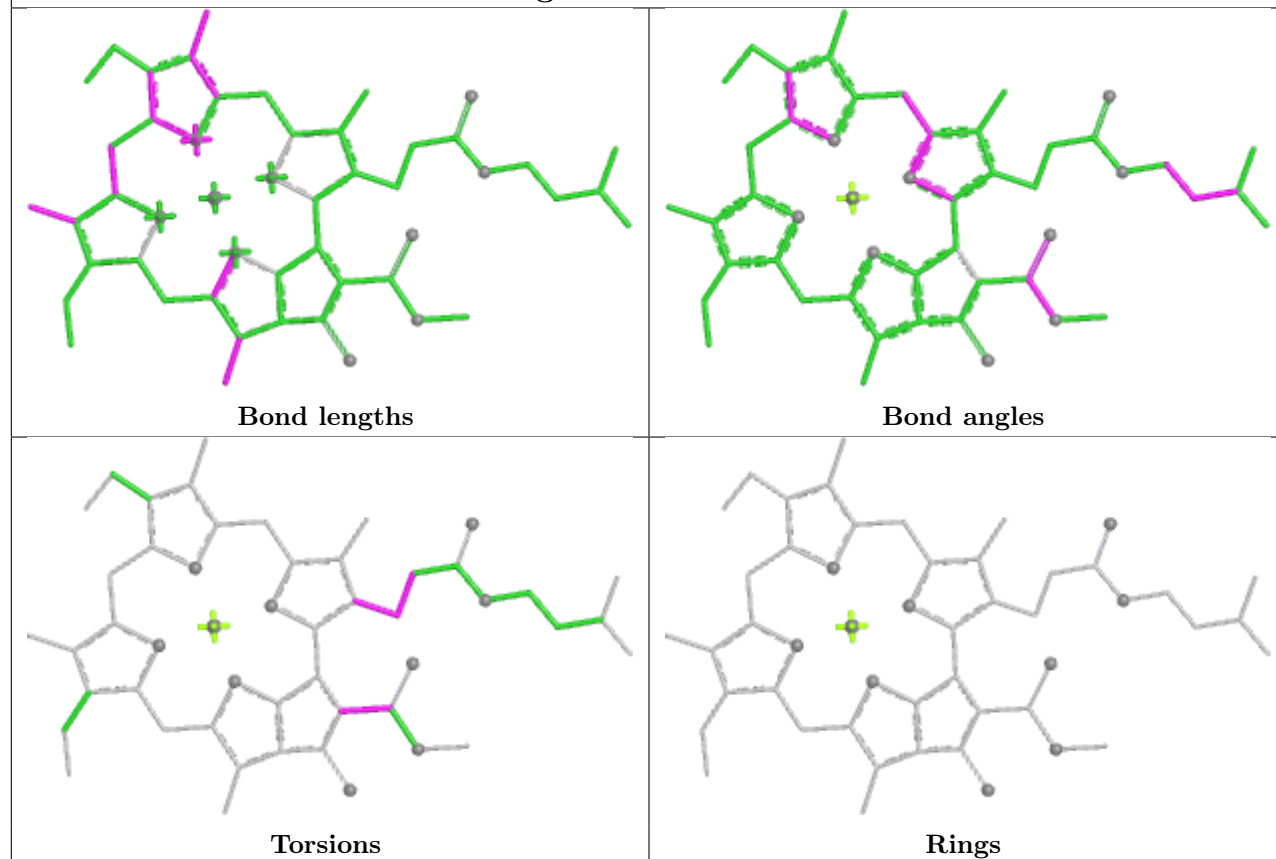


Torsions

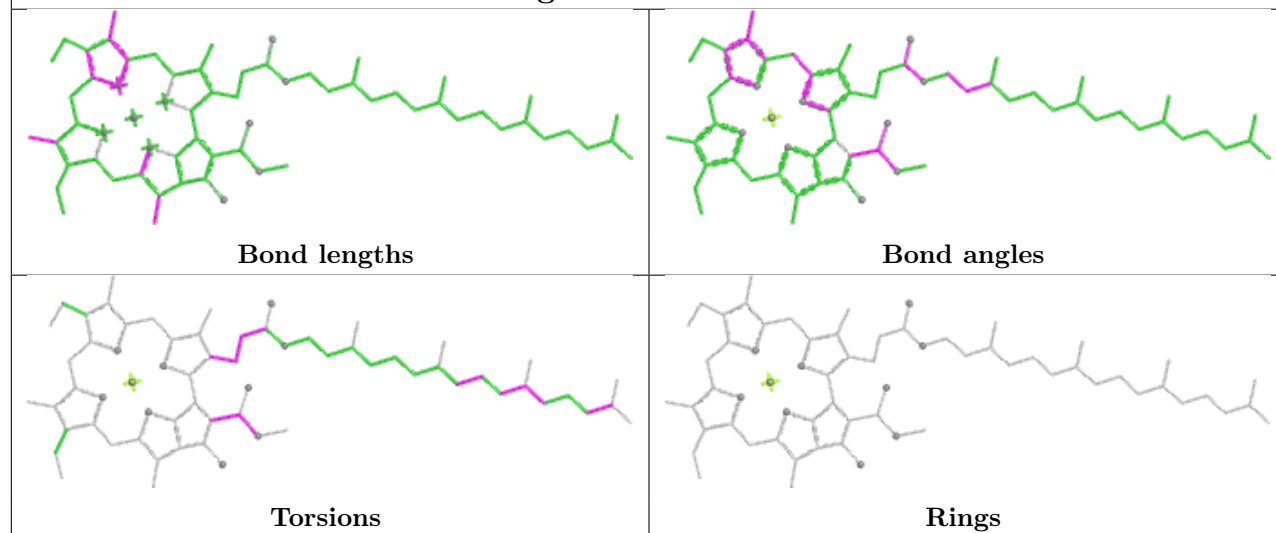


Rings

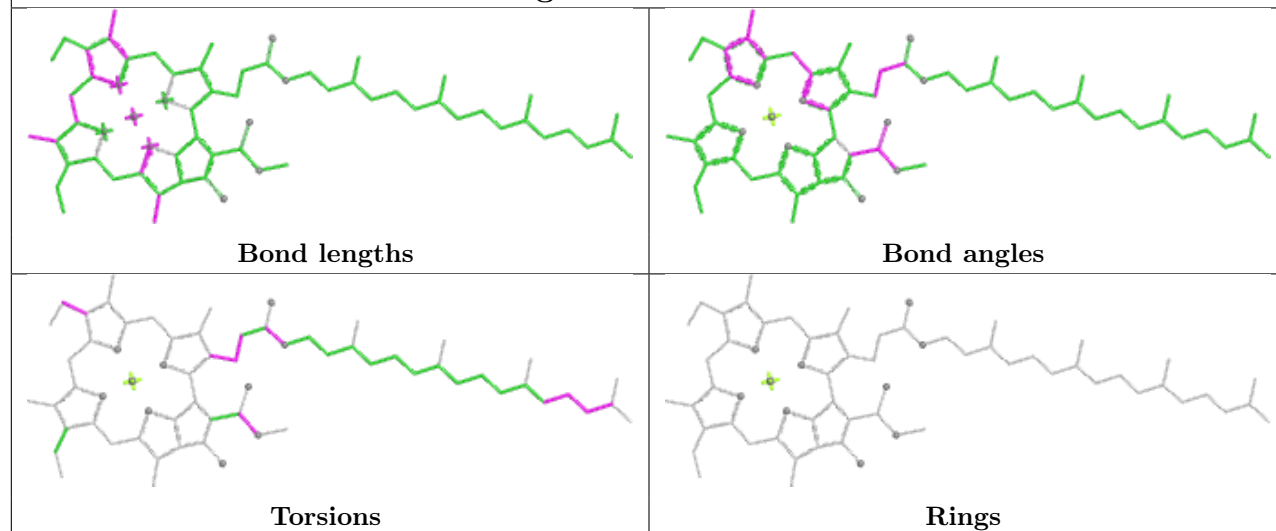
Ligand CLA 7 308



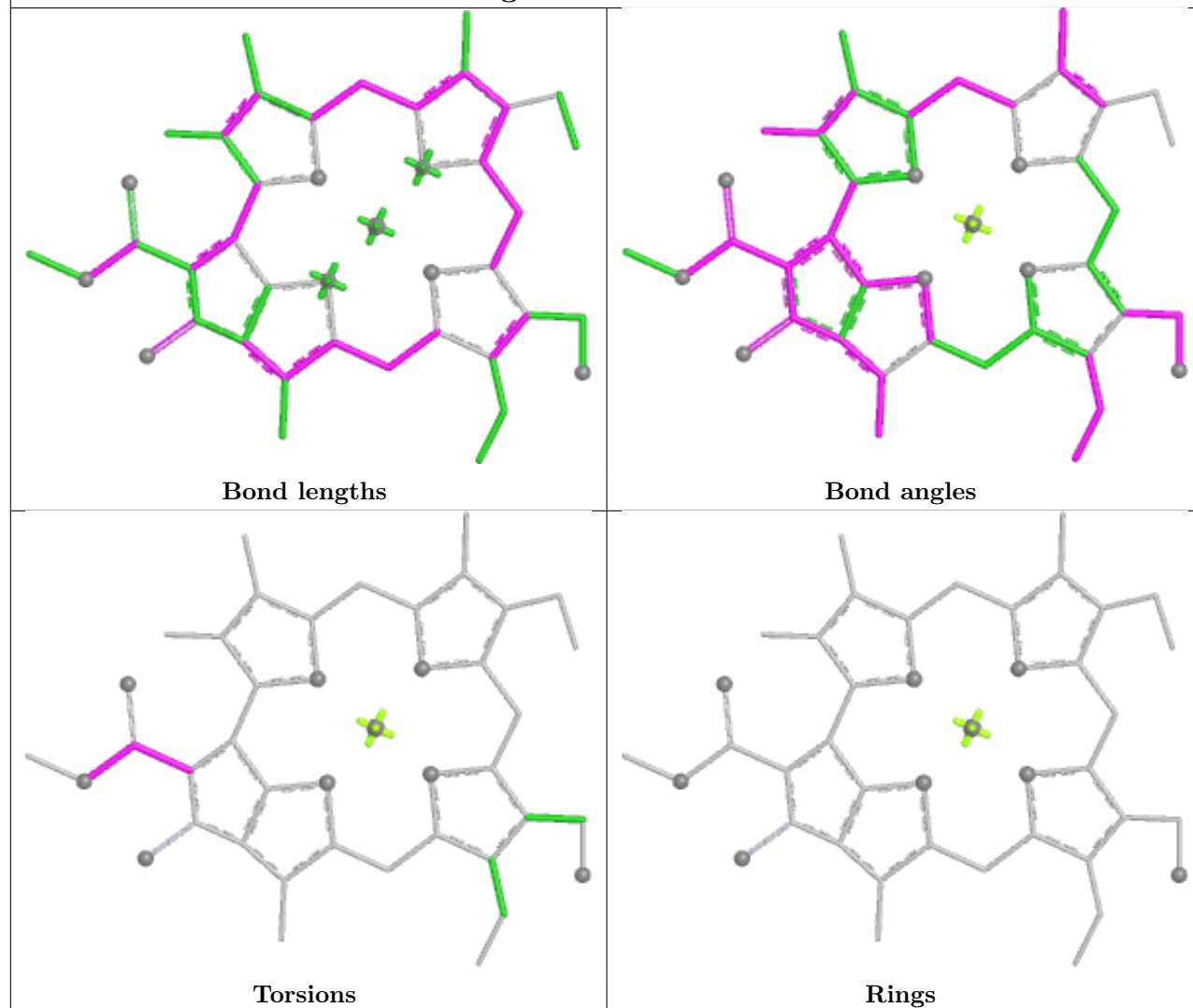
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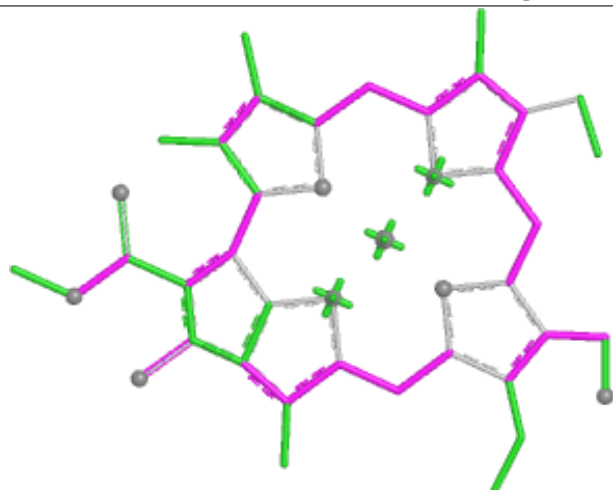
Ligand CLA a 603



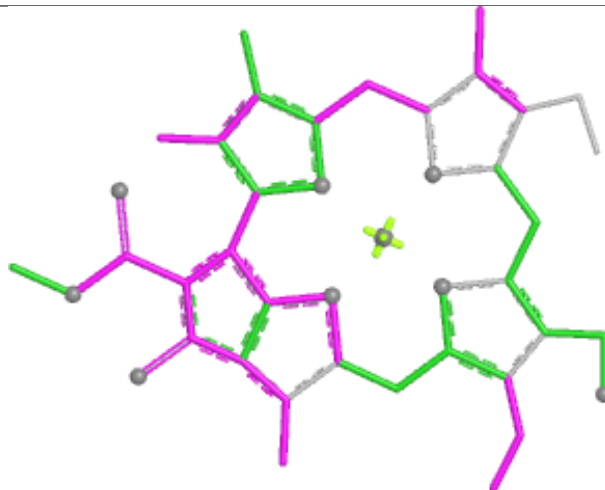
Ligand CHL 9 317



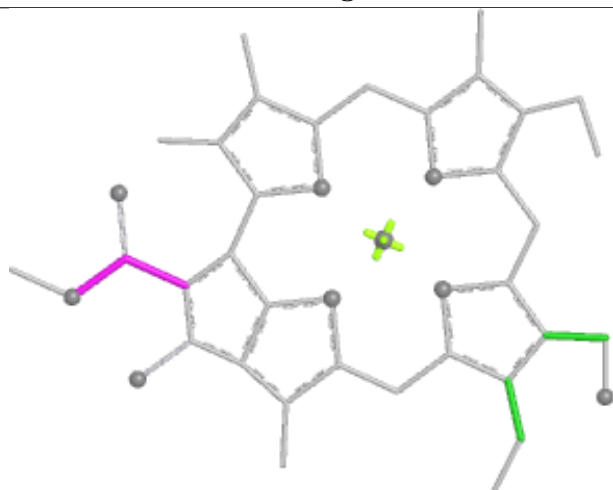
Ligand CHL 4 304



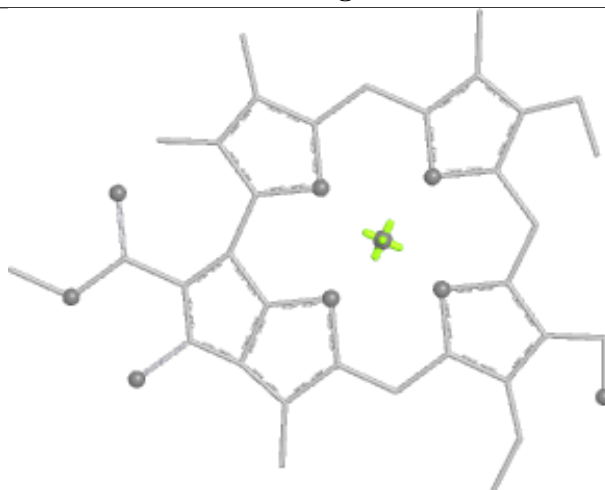
Bond lengths



Bond angles

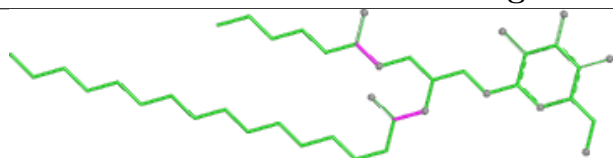


Torsions

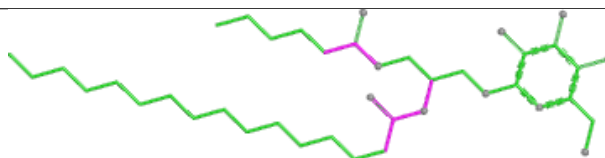


Rings

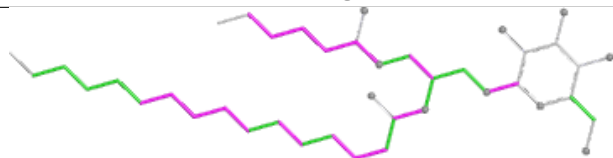
Ligand LMG m 101



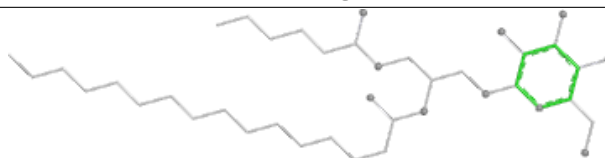
Bond lengths



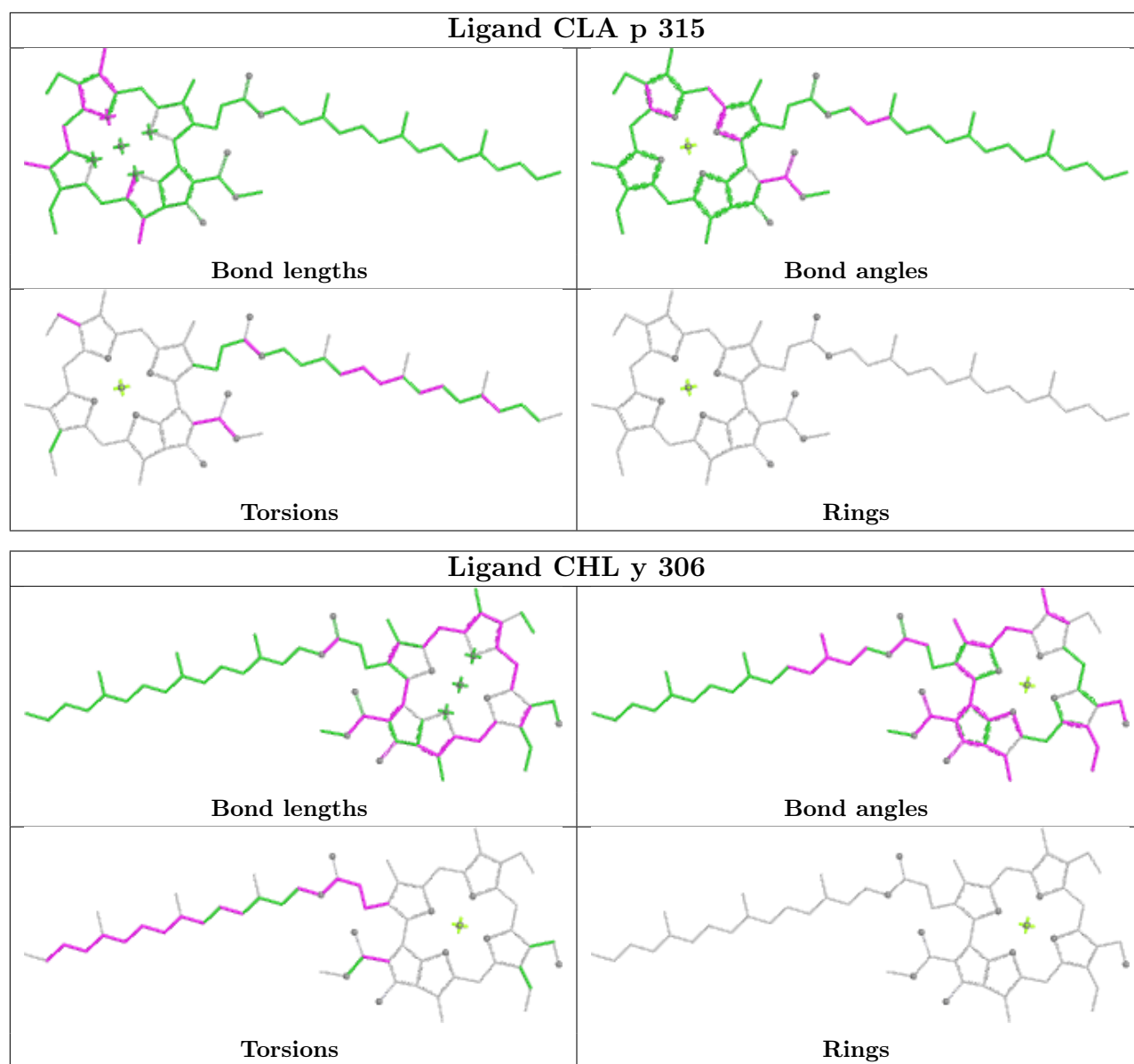
Bond angles



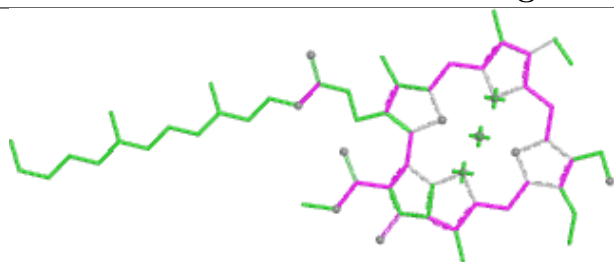
Torsions



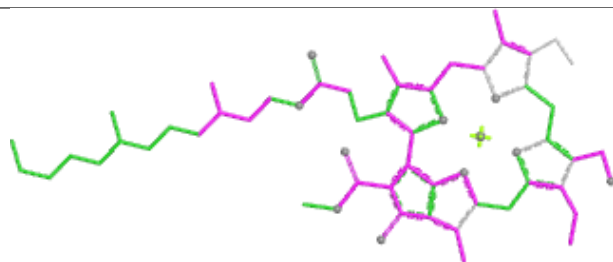
Rings



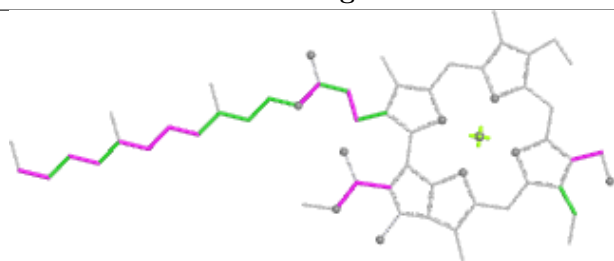
Ligand CHL 8 304



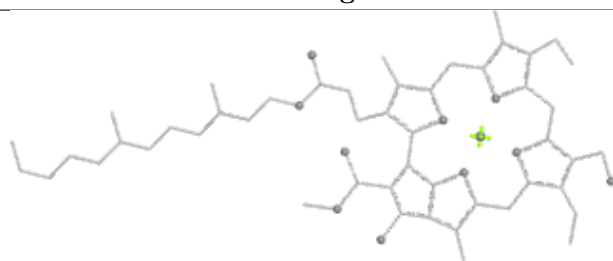
Bond lengths



Bond angles

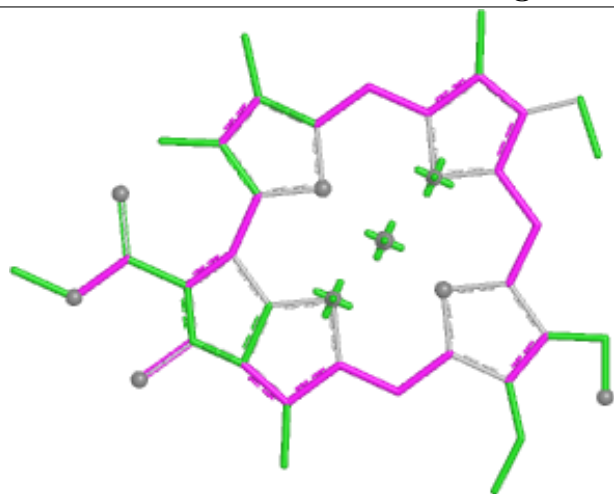


Torsions



Rings

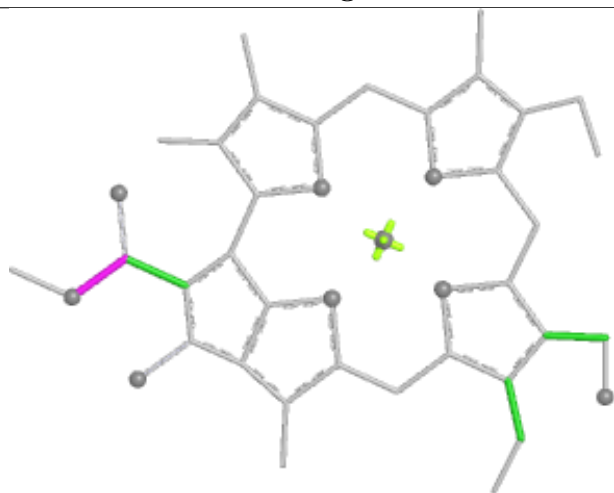
Ligand CHL R 605



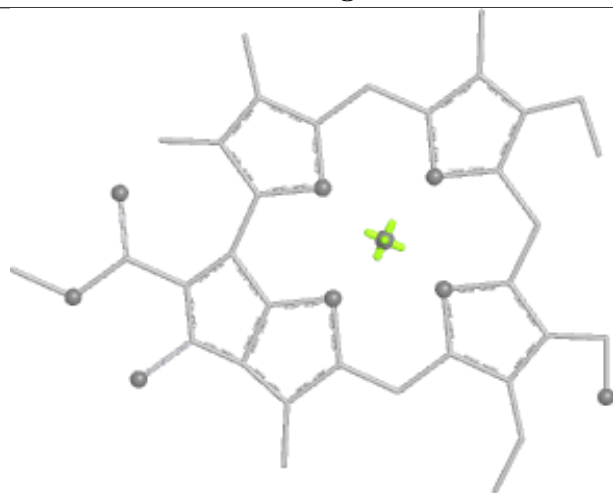
Bond lengths



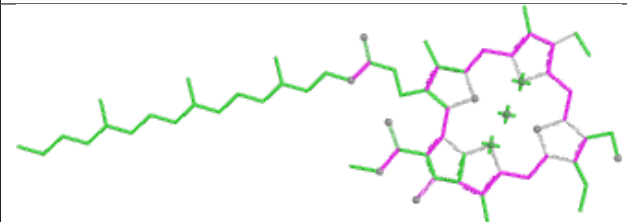
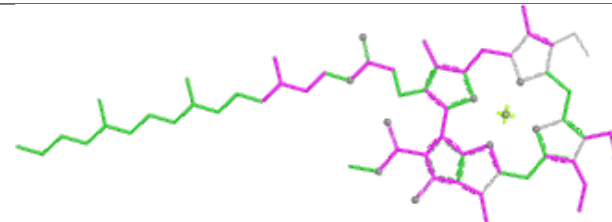
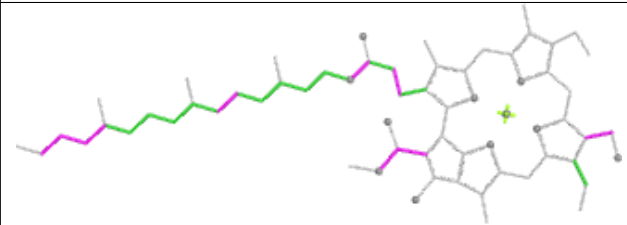
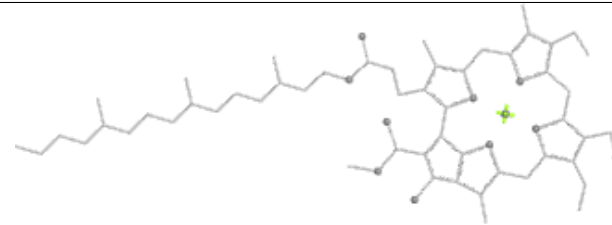
Bond angles

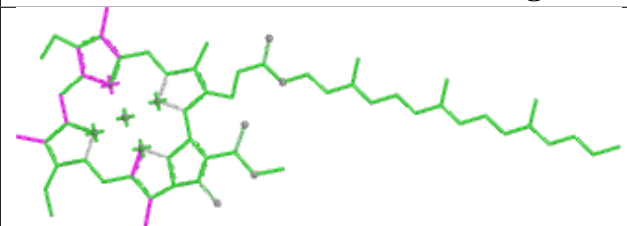
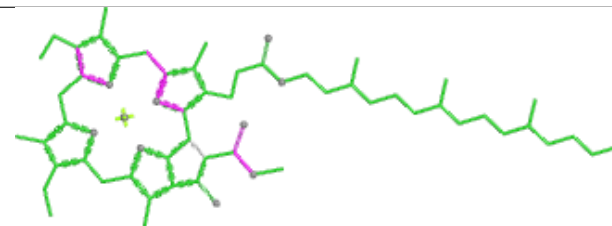
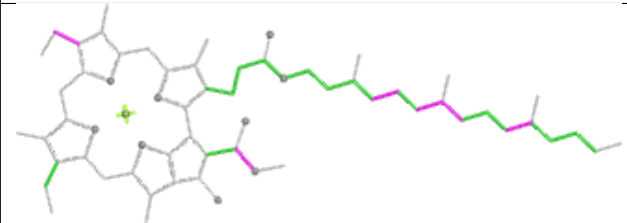
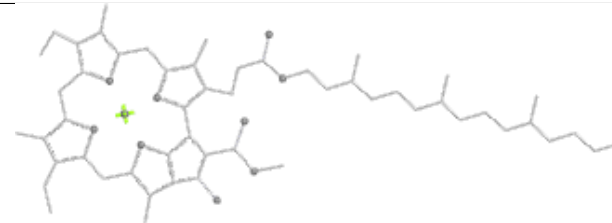


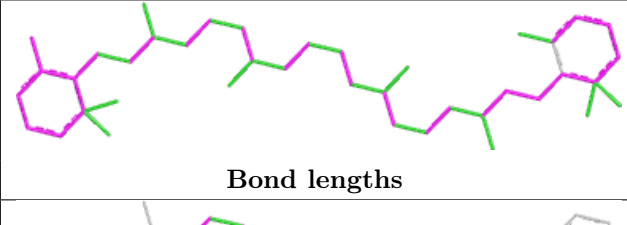
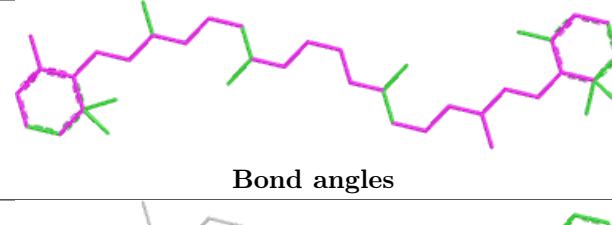


Torsions



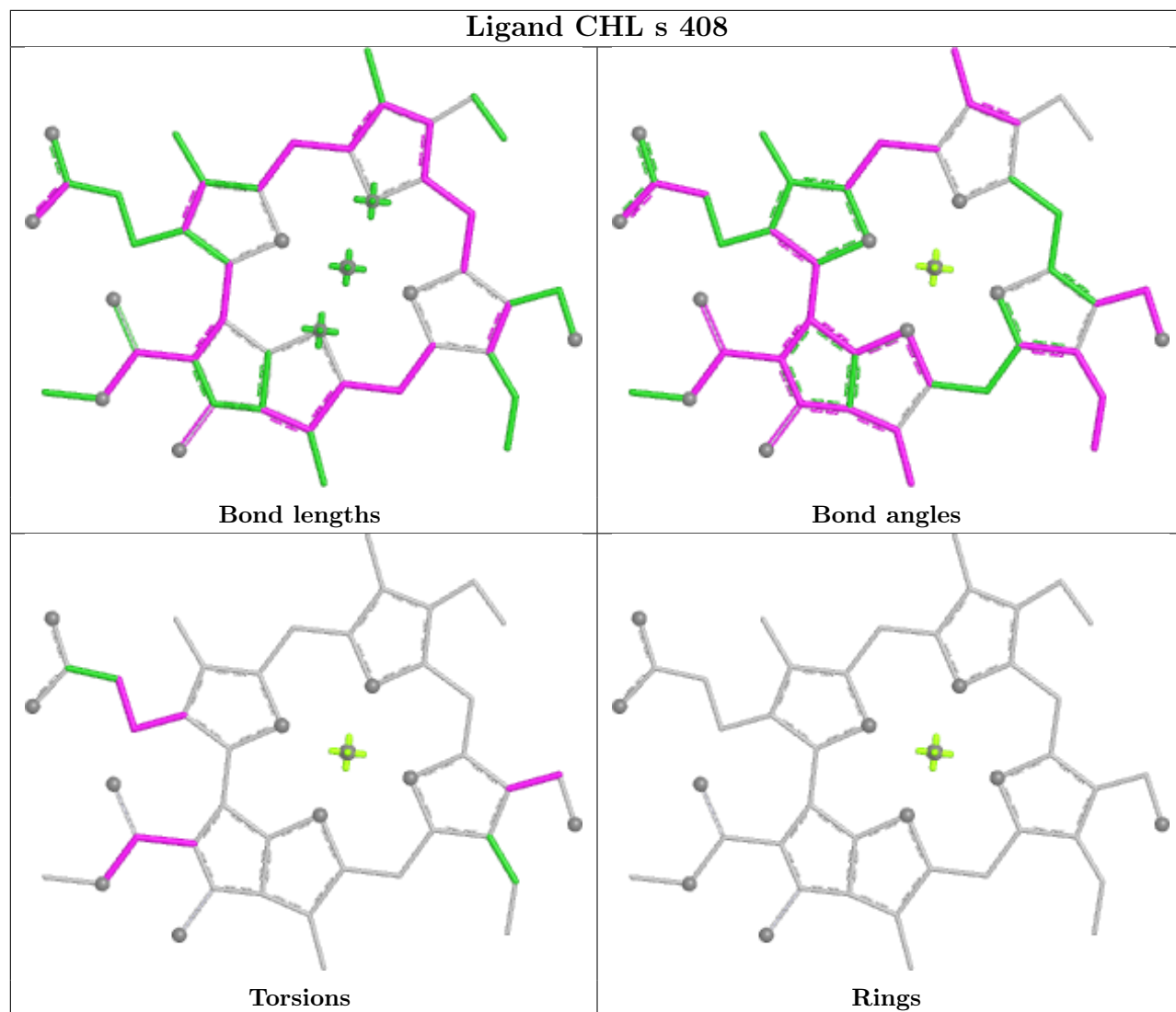
Rings

Ligand CHL 9 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

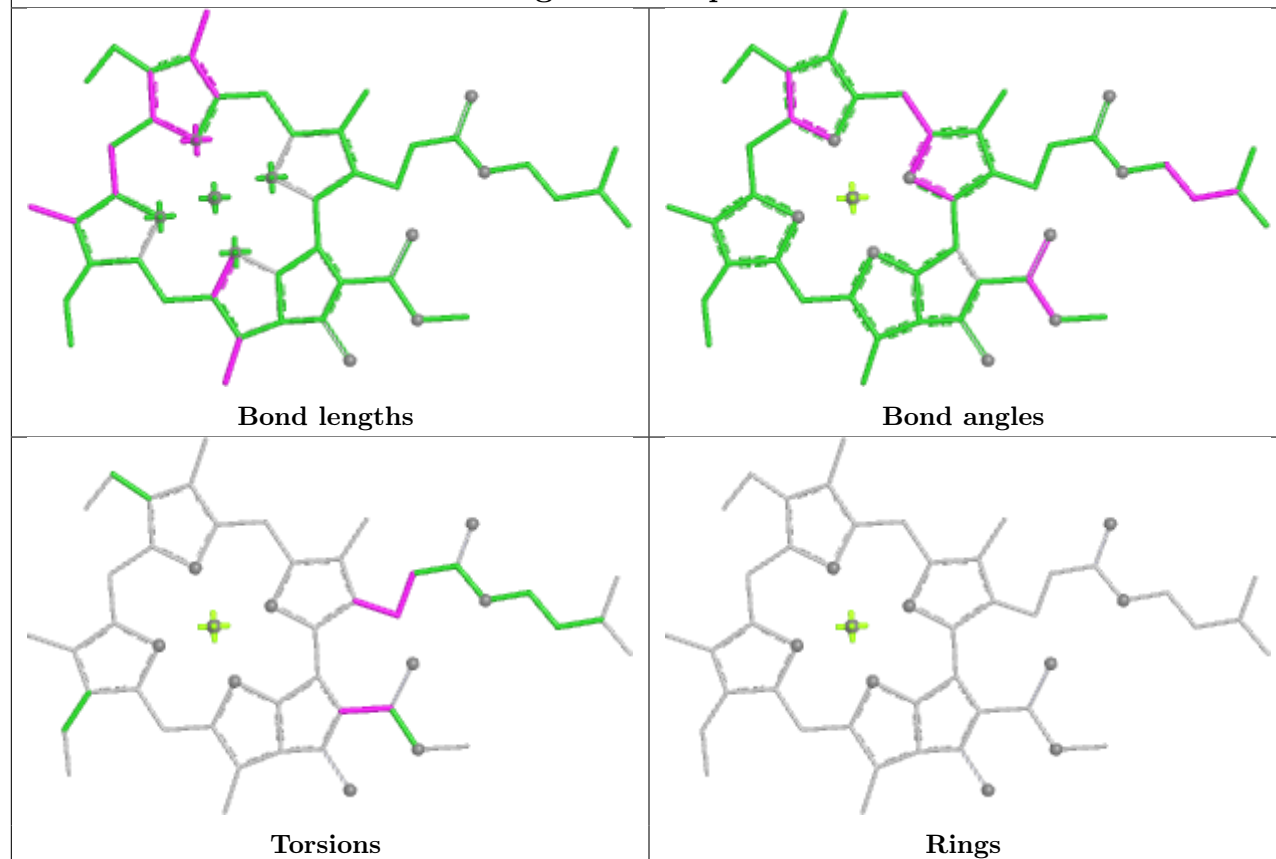
Ligand CLA 2 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT c 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

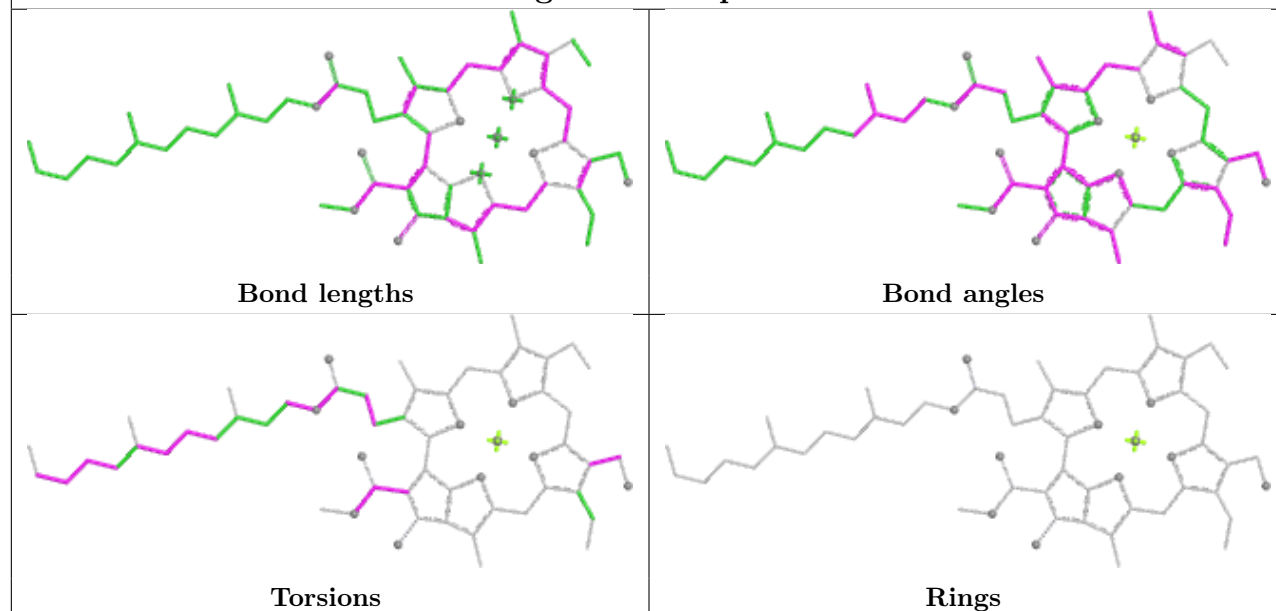
Ligand CHL s 408



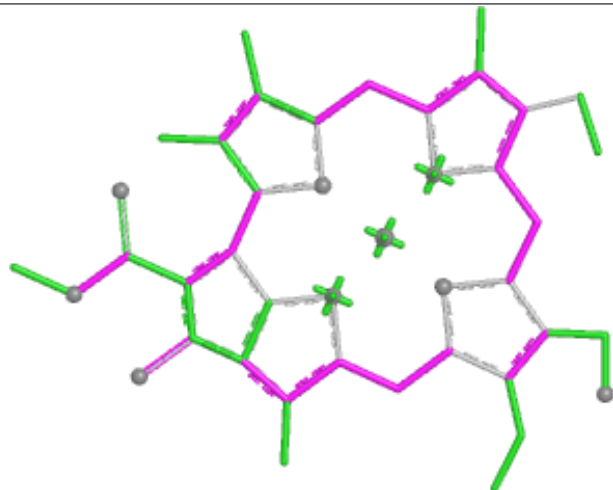
Ligand CLA p 308



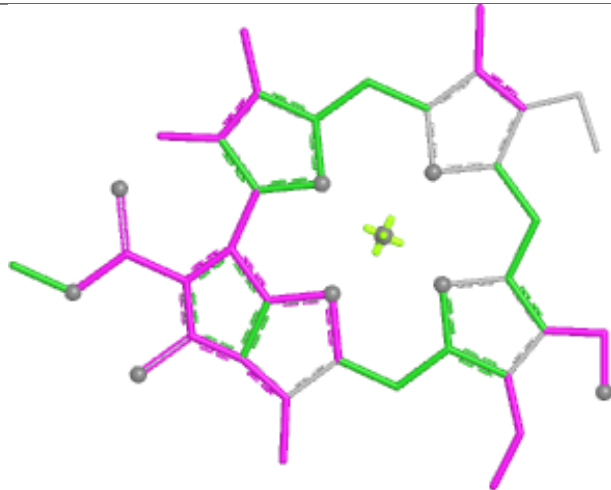
Ligand CHL q 304



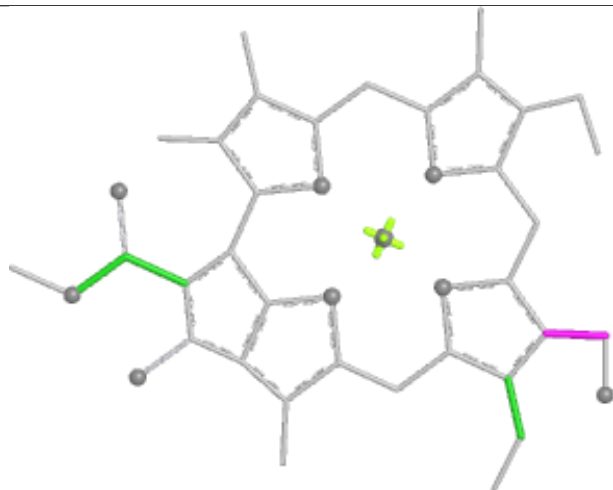
Ligand CHL 3 317



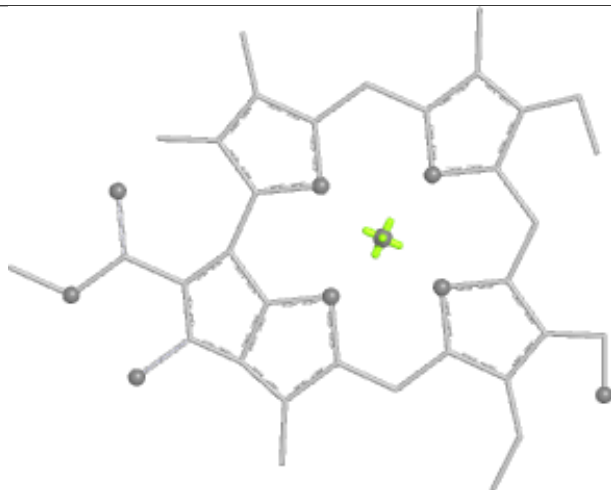
Bond lengths



Bond angles

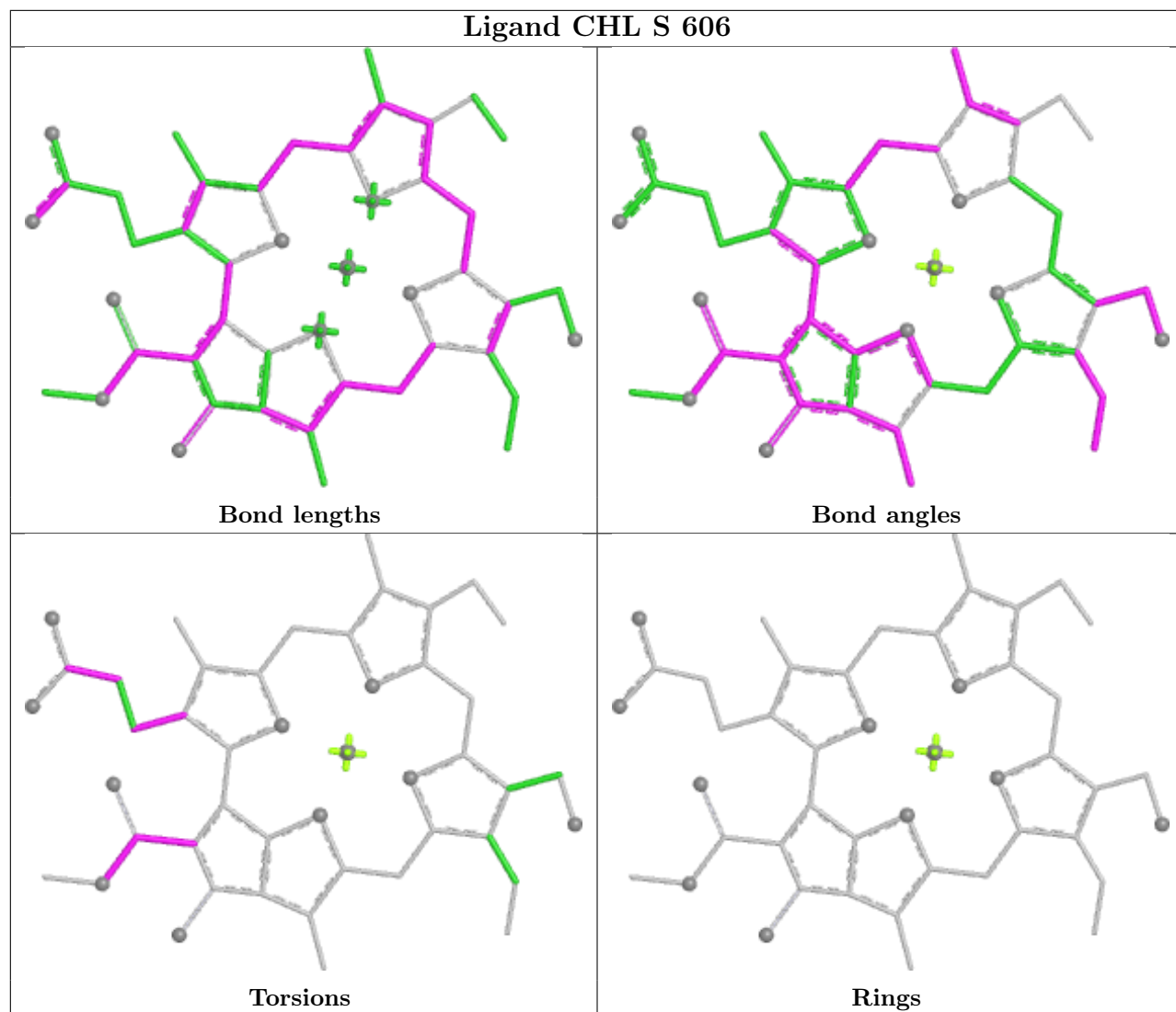


Torsions

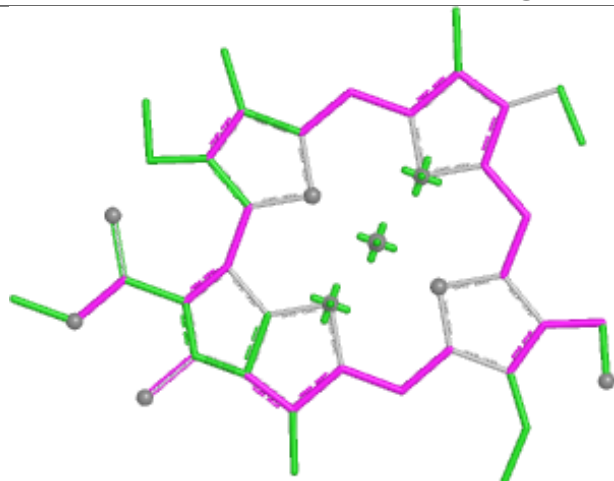


Rings

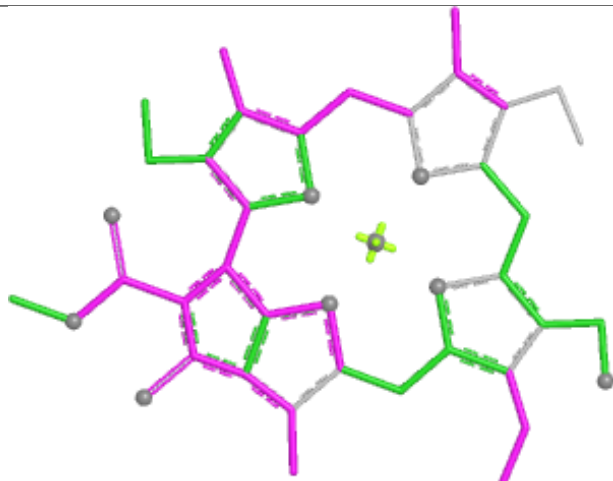
Ligand CHL S 606



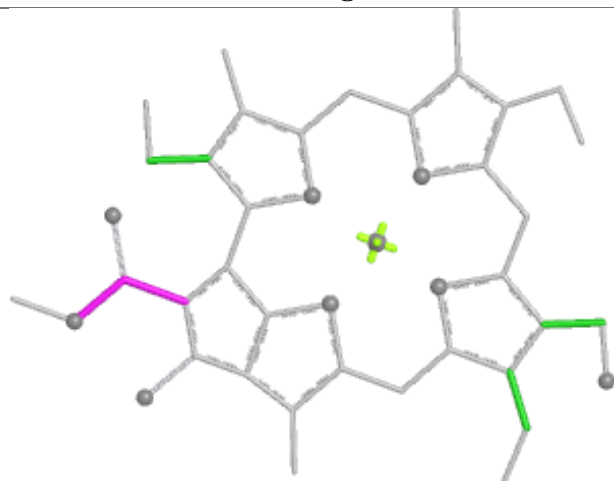
Ligand CHL 3 308



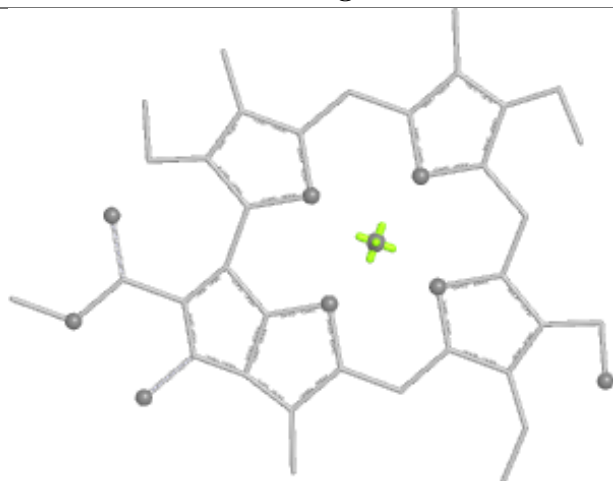
Bond lengths



Bond angles

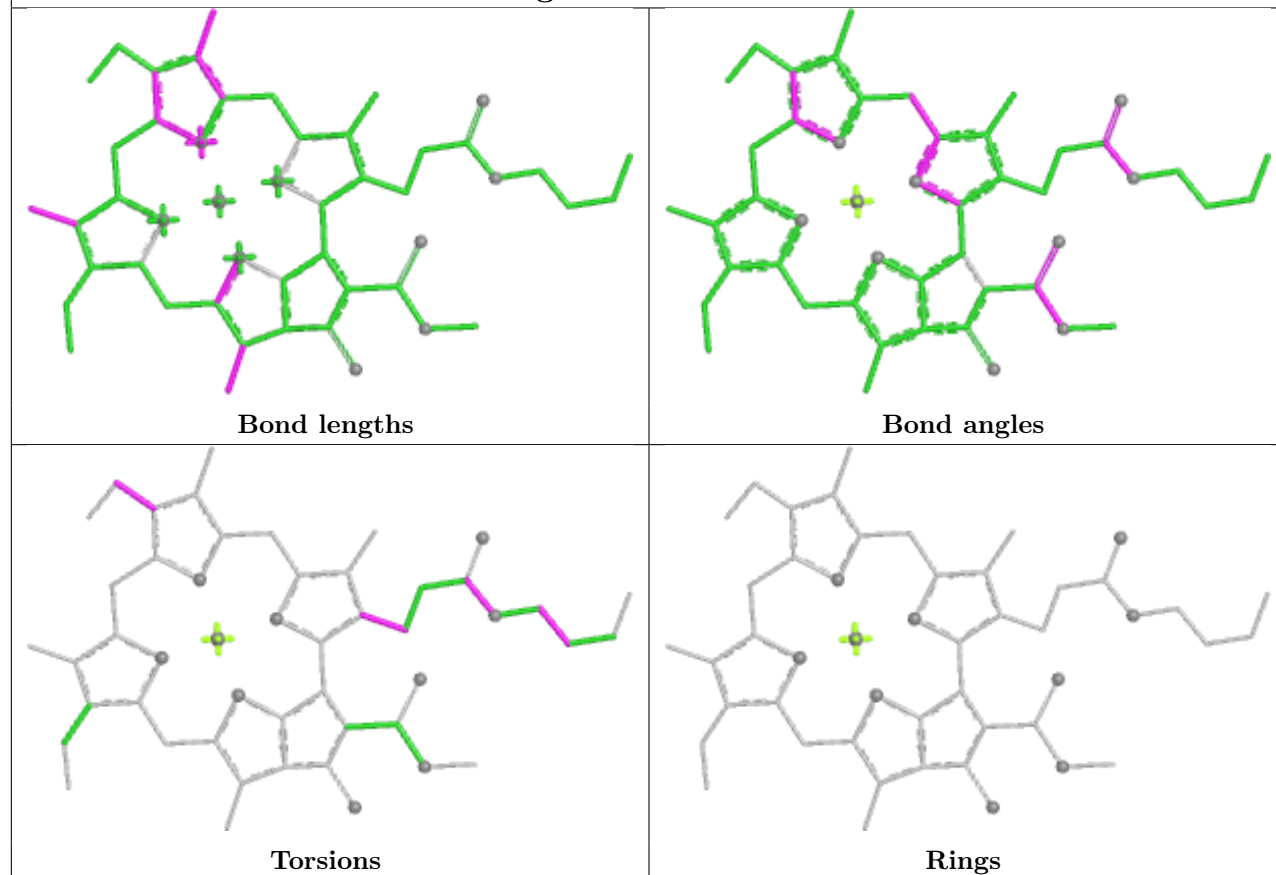


Torsions

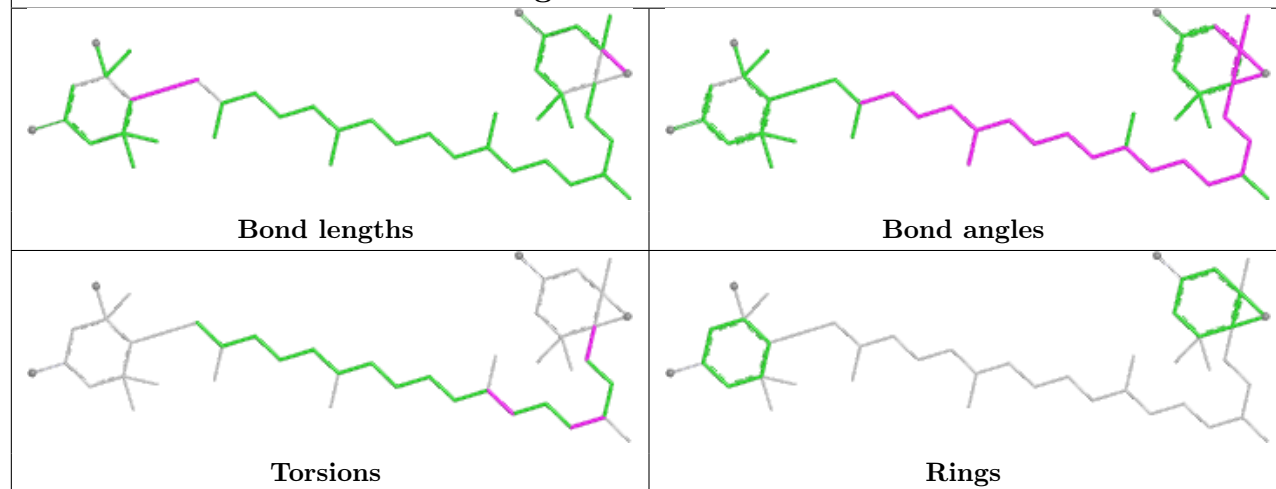


Rings

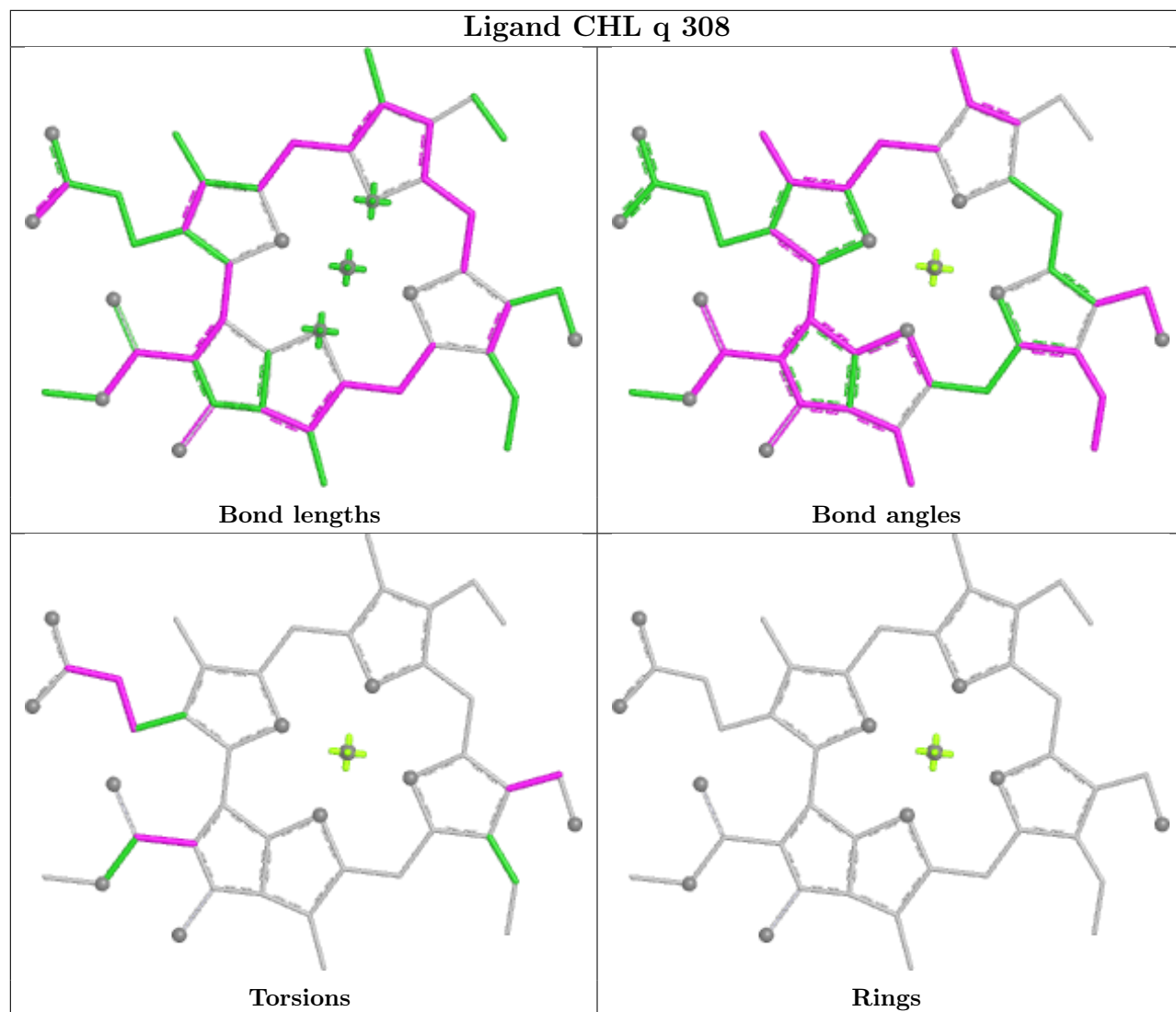
Ligand CLA a 605



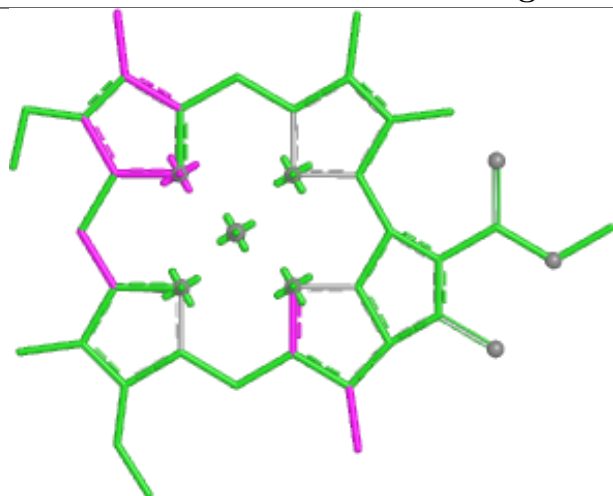
Ligand NEX 4 303



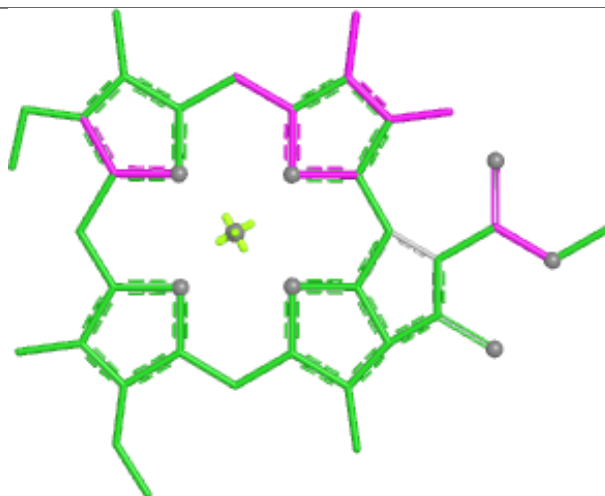
Ligand CHL q 308



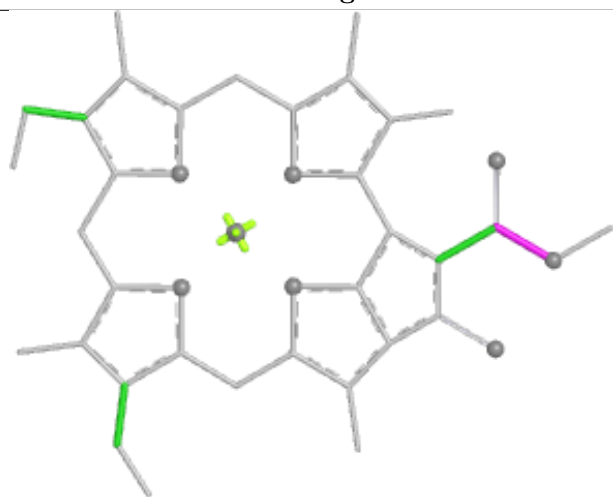
Ligand CLA 3 313



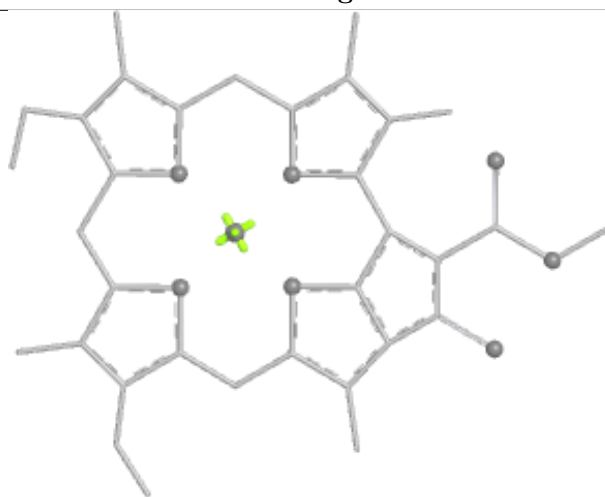
Bond lengths



Bond angles

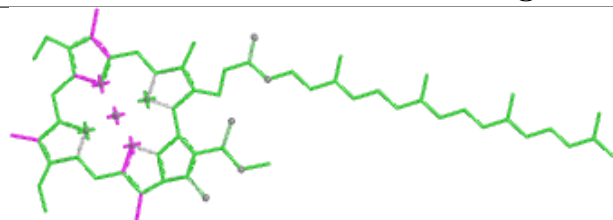


Torsions

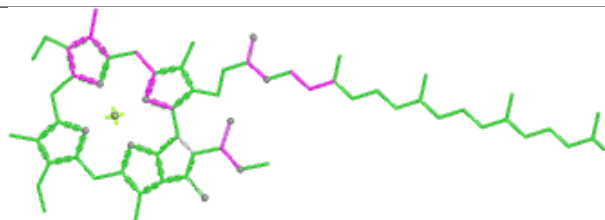


Rings

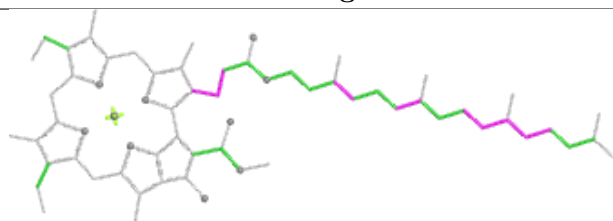
Ligand CLA b 603



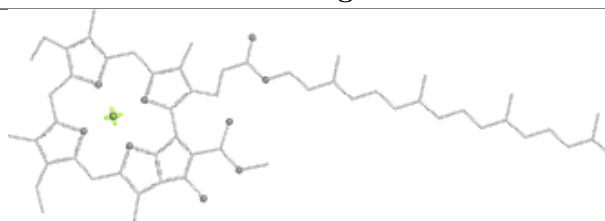
Bond lengths



Bond angles

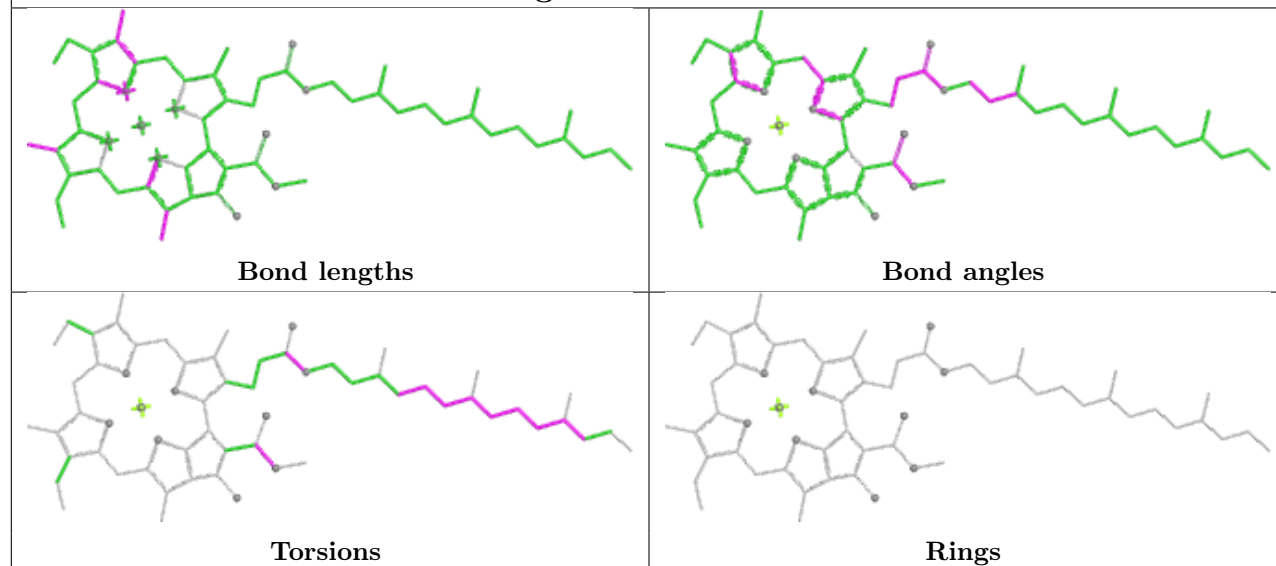


Torsions

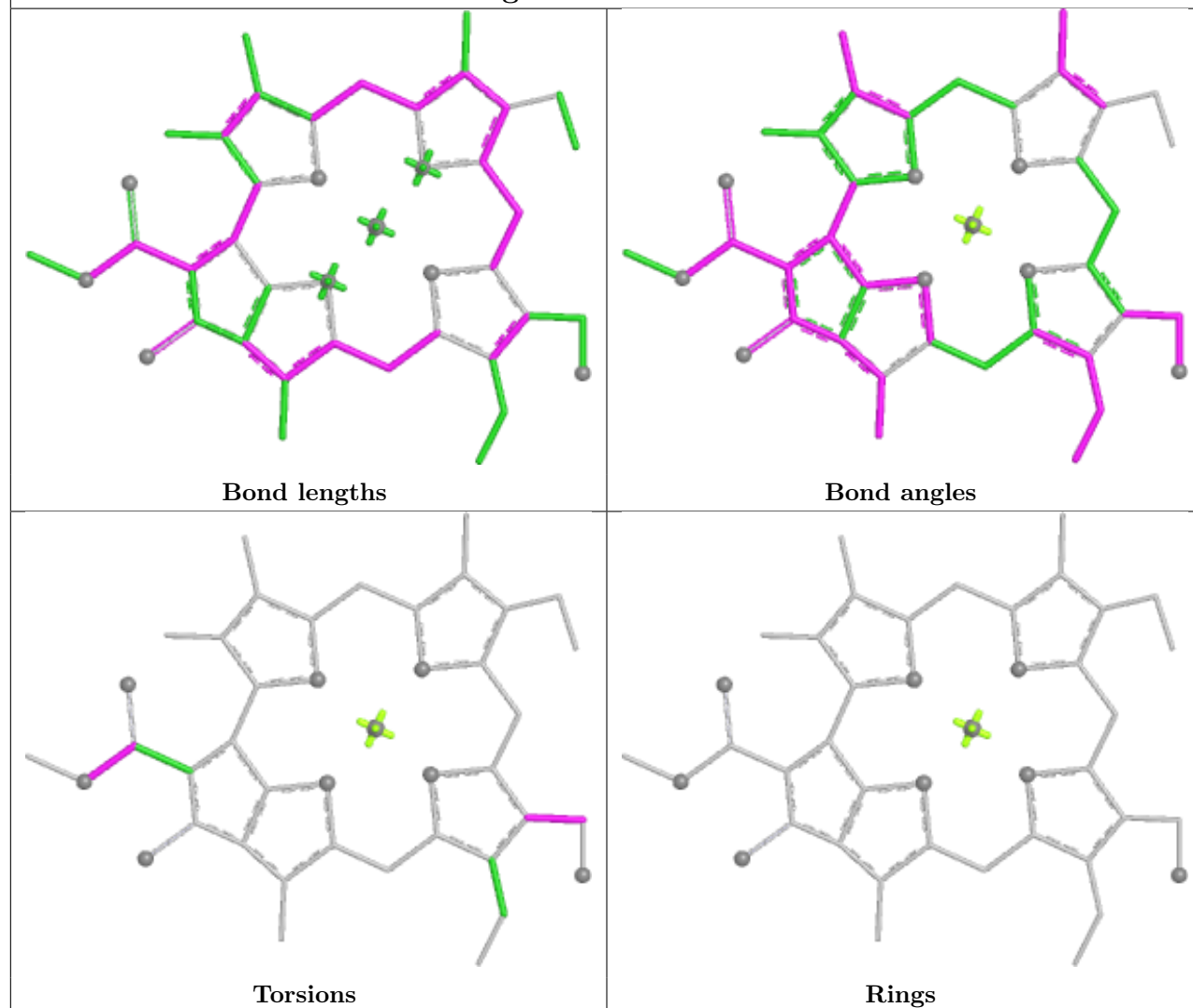


Rings

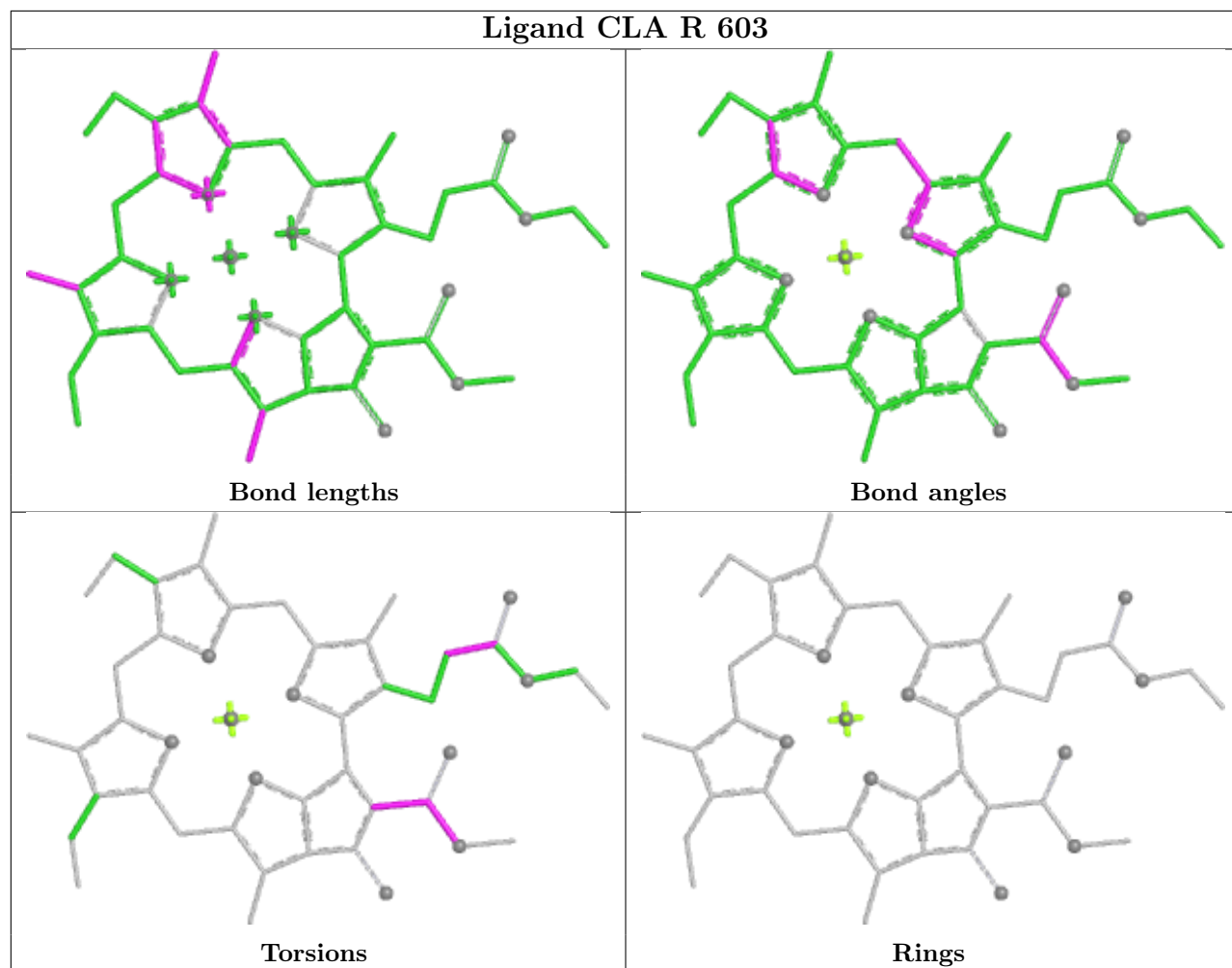
Ligand CLA b 604



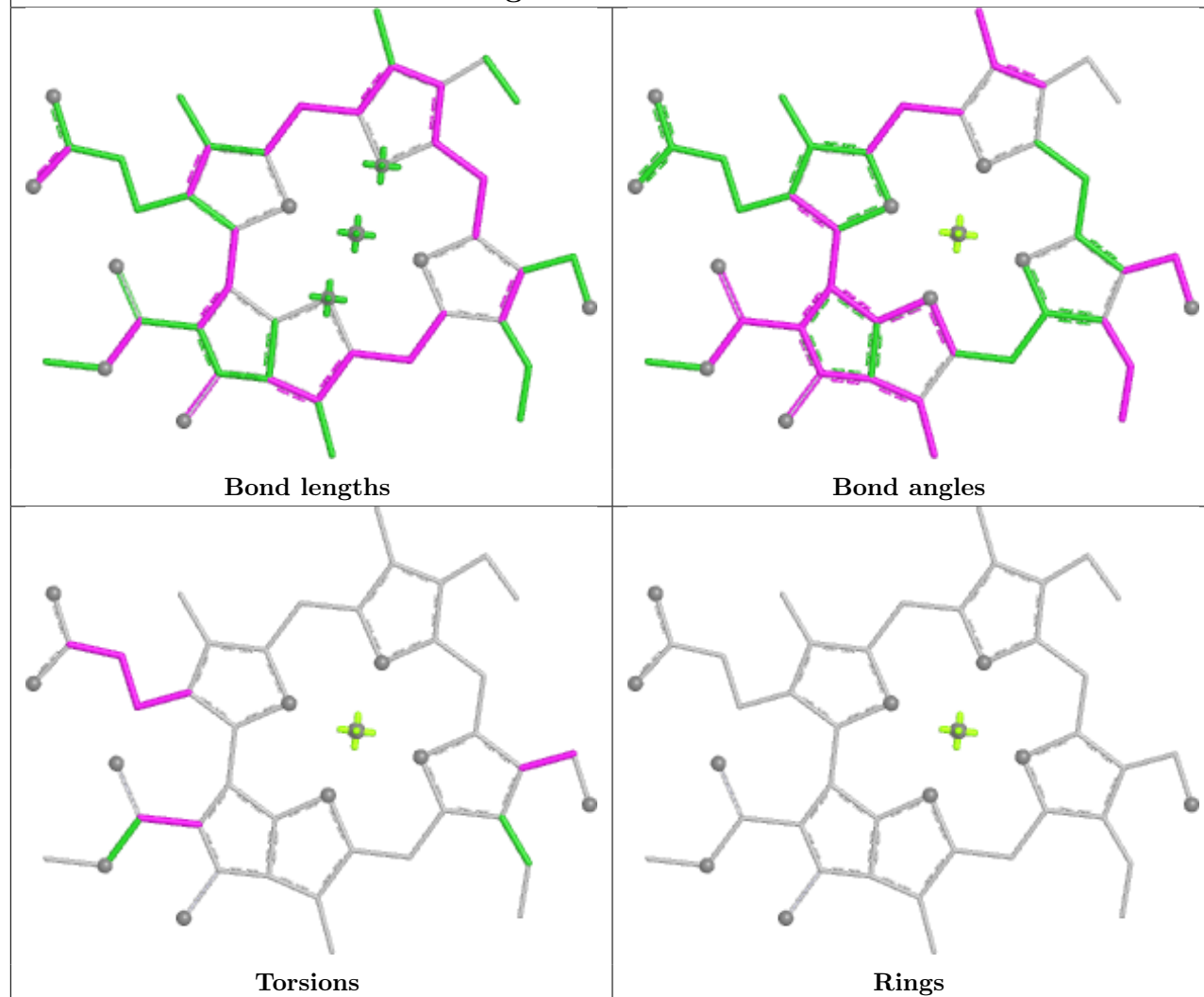
Ligand CHL r 306



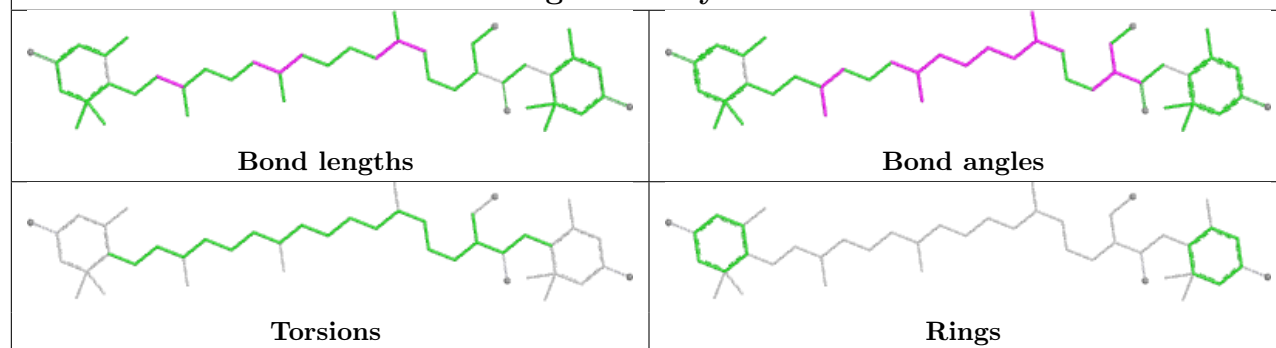
Ligand CLA R 603



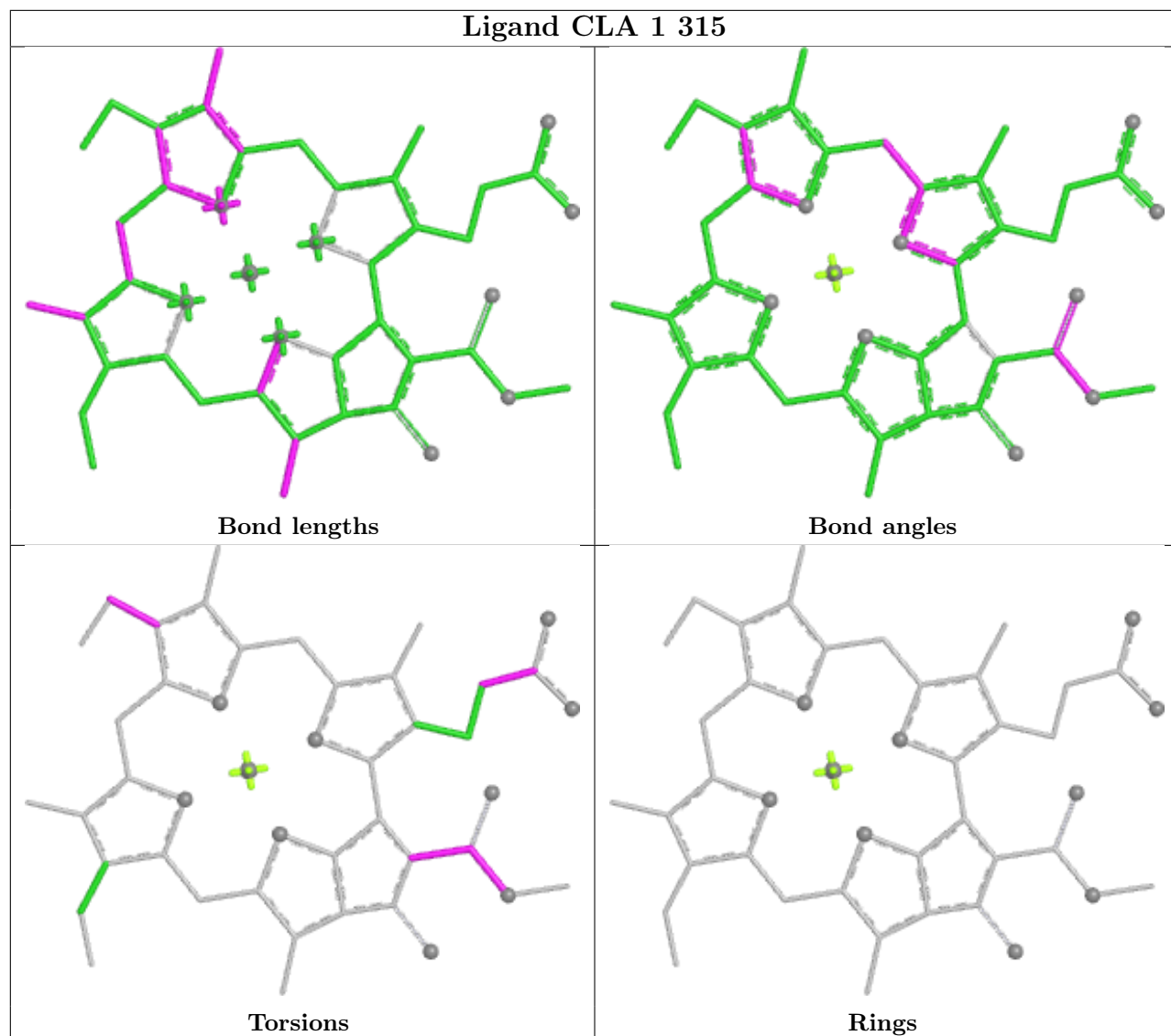
Ligand CHL 4 305



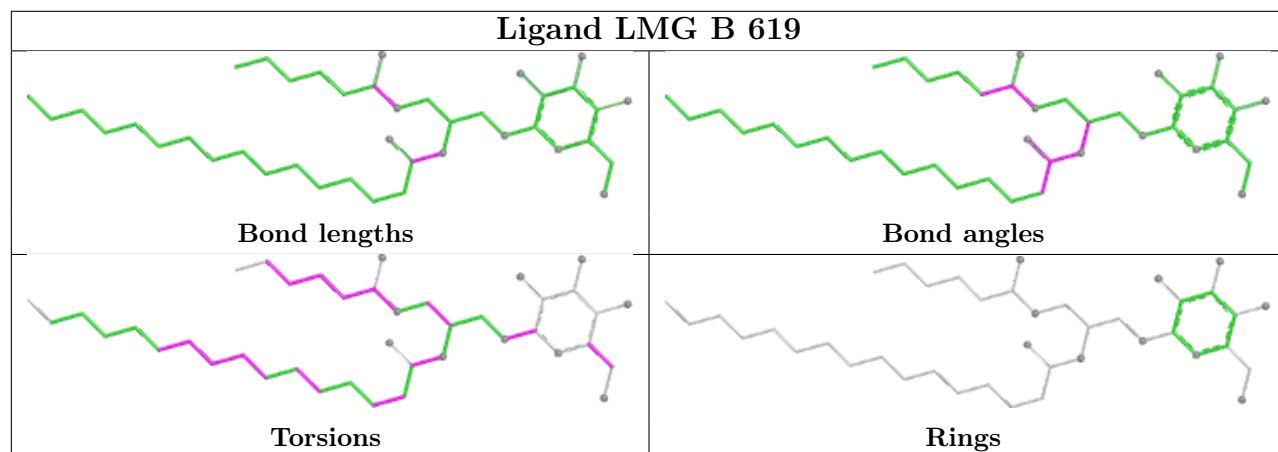
Ligand OIE y 303

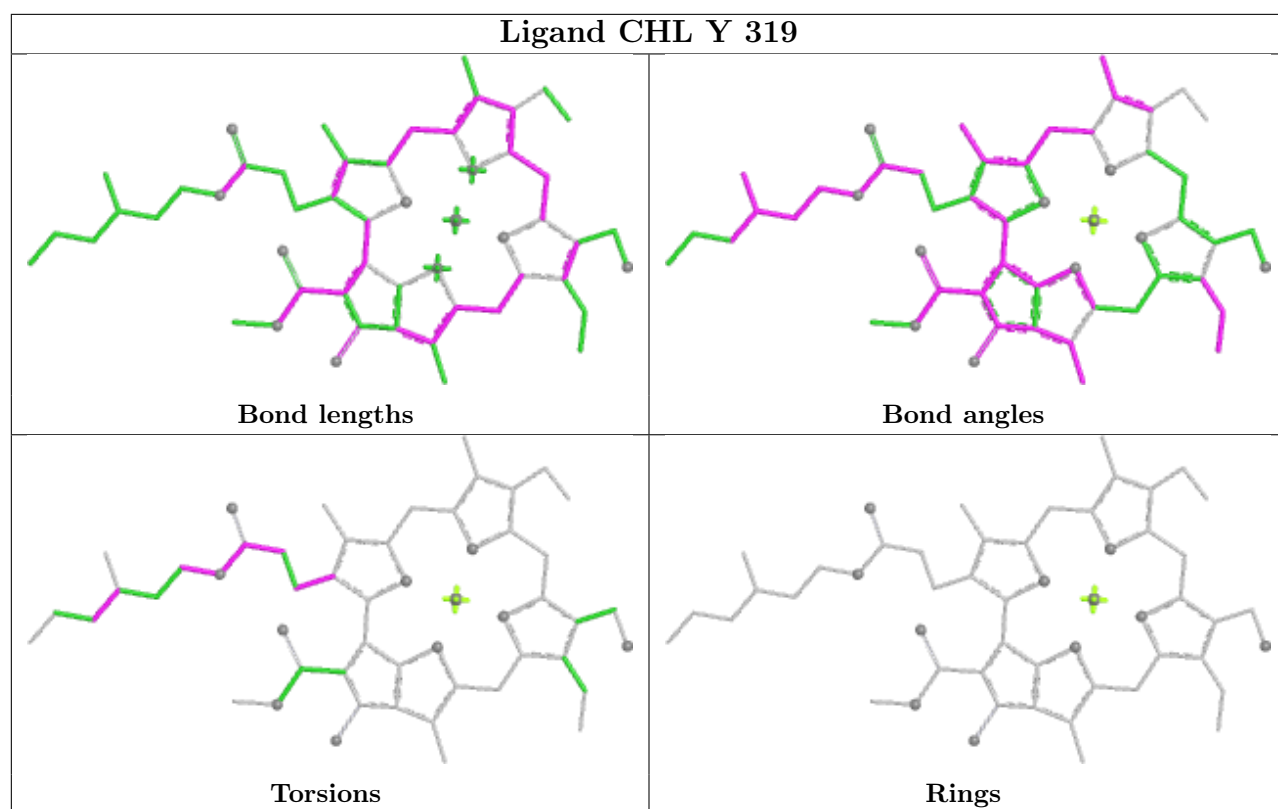


Ligand CLA 1 315

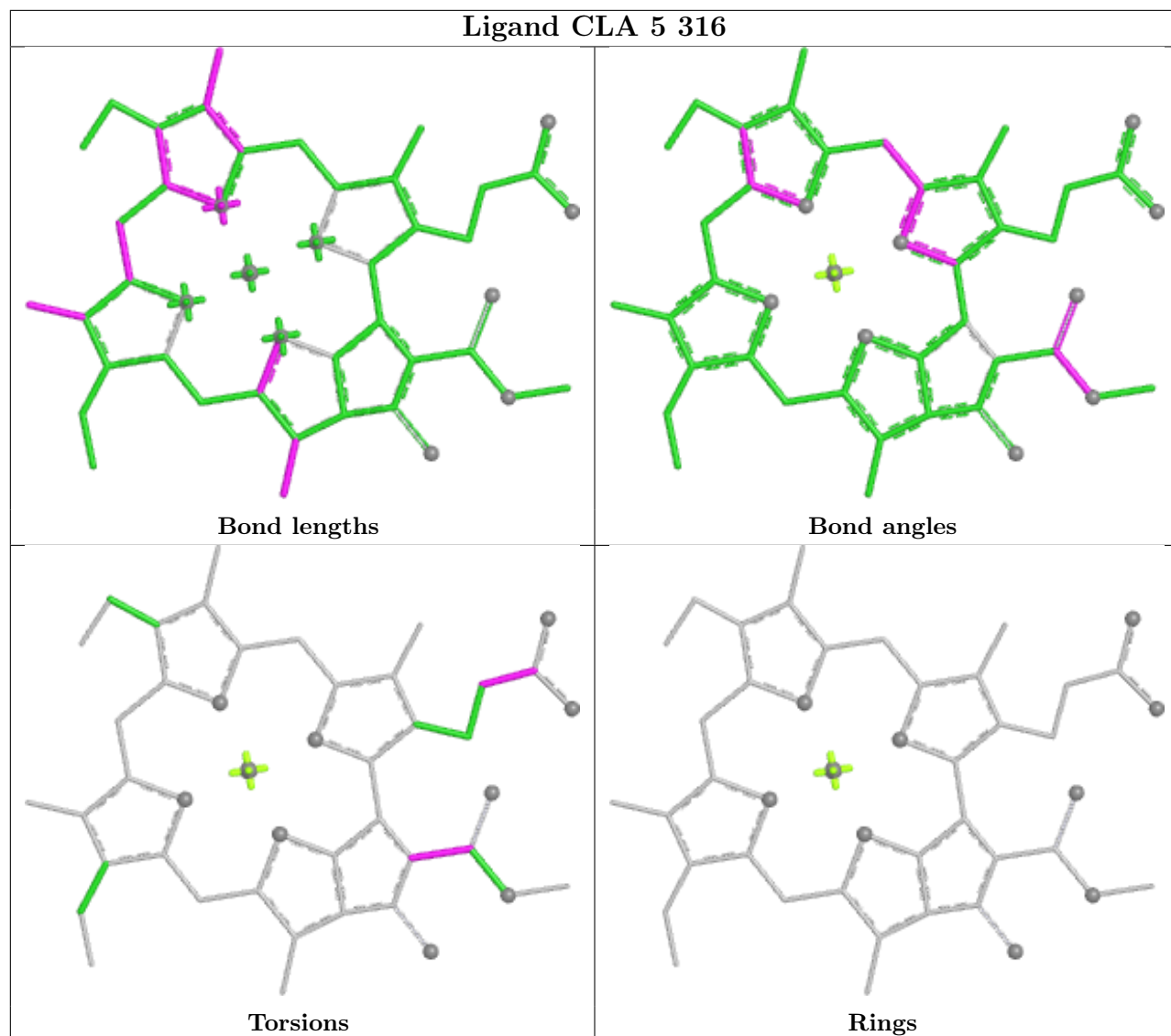


Ligand LMG B 619

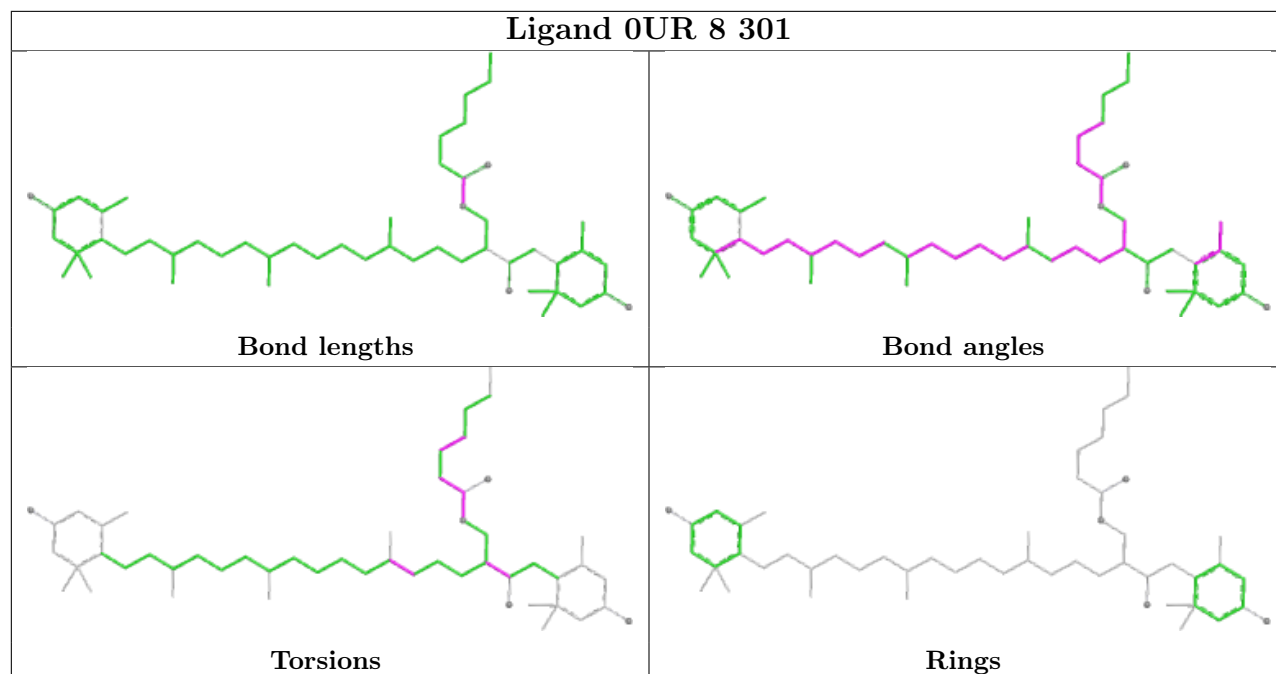




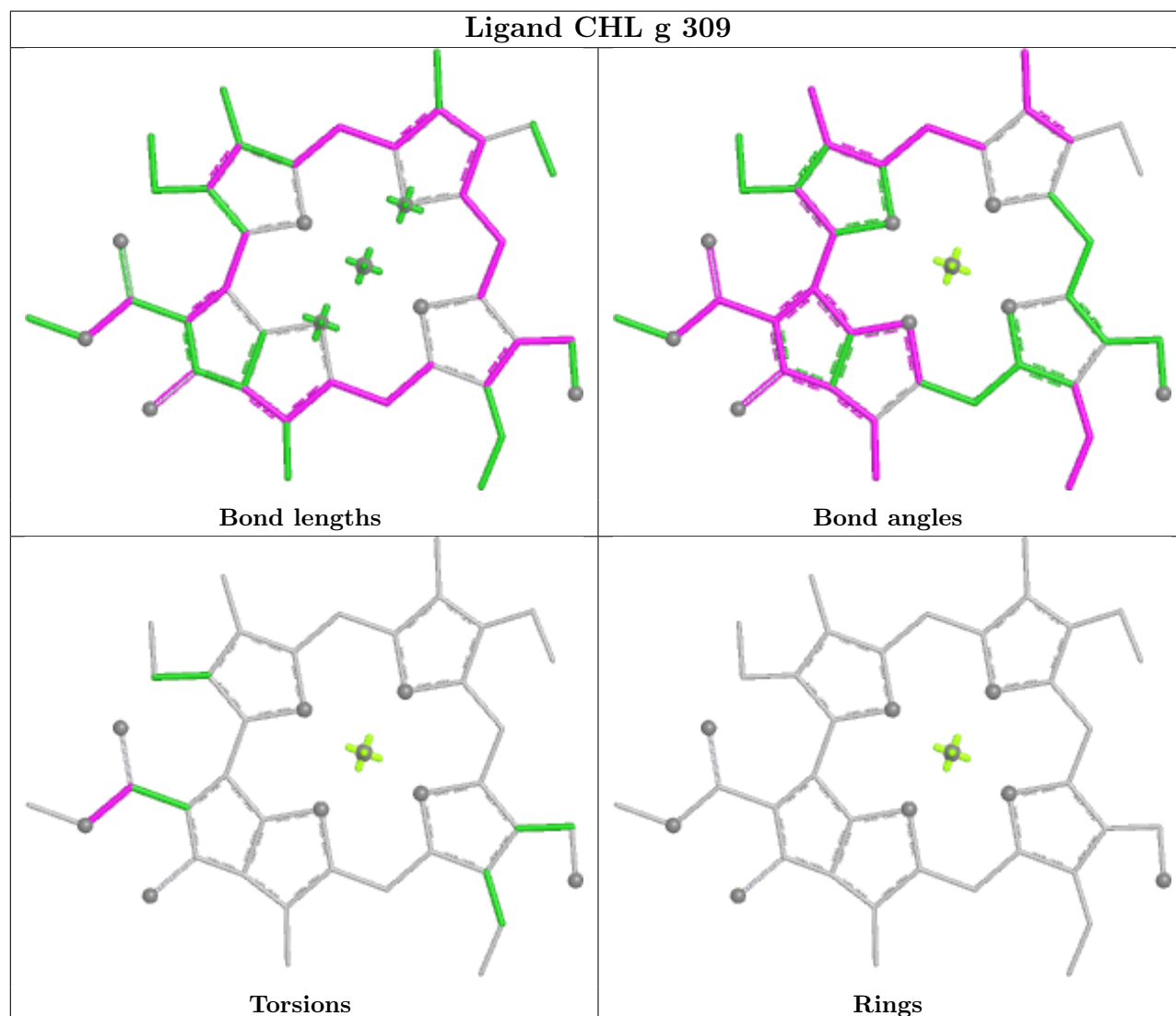
Ligand CLA 5 316



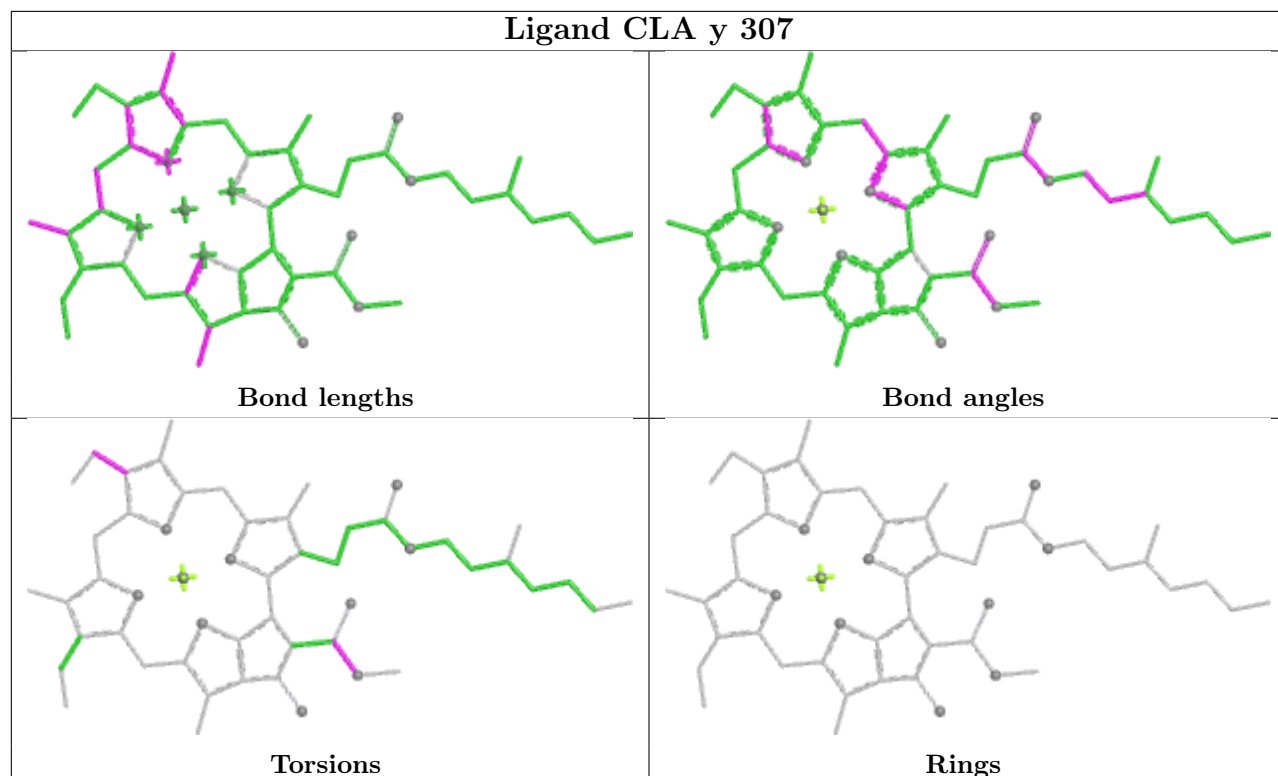
Ligand OUR 8 301



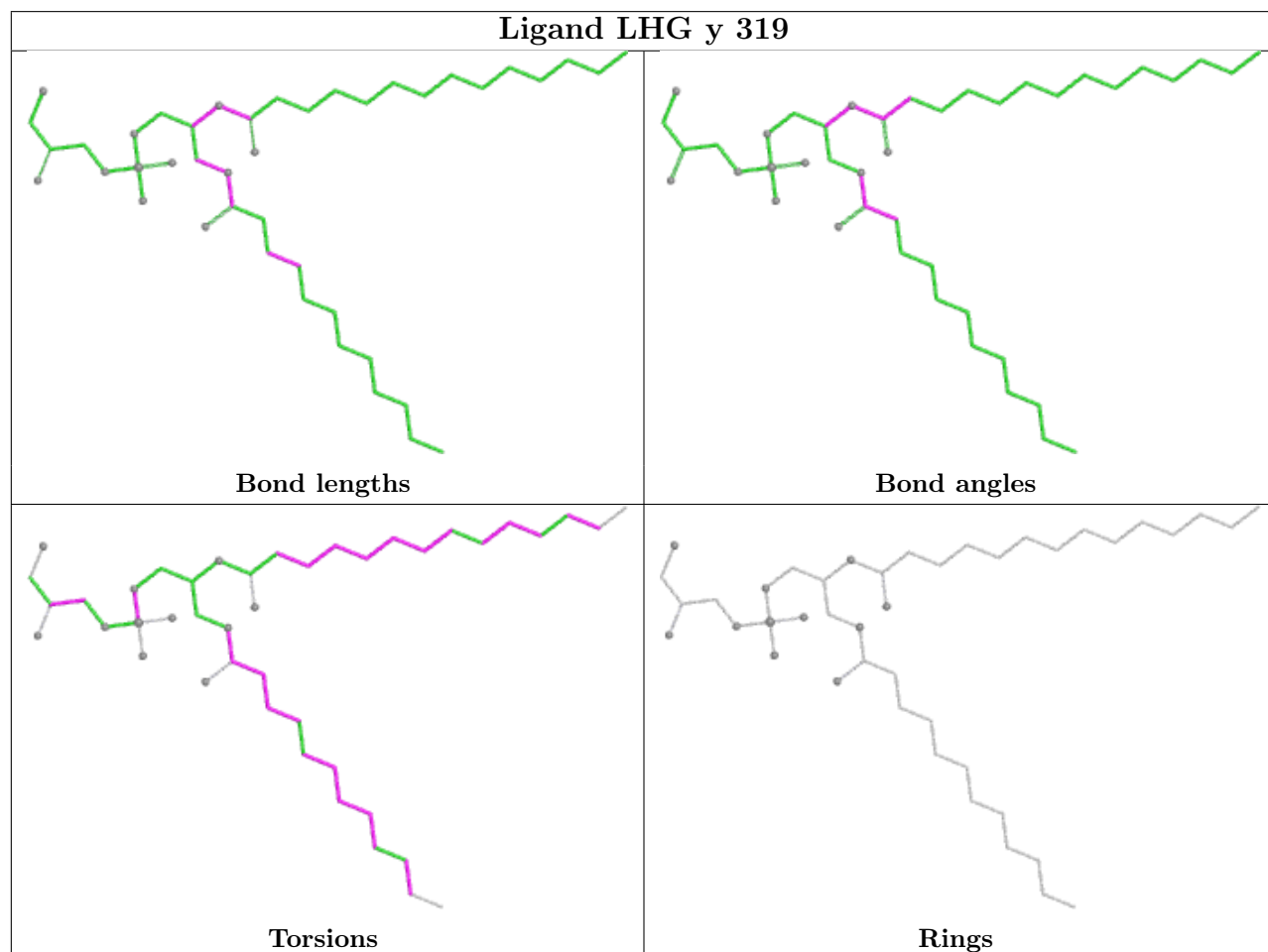
Ligand CHL g 309

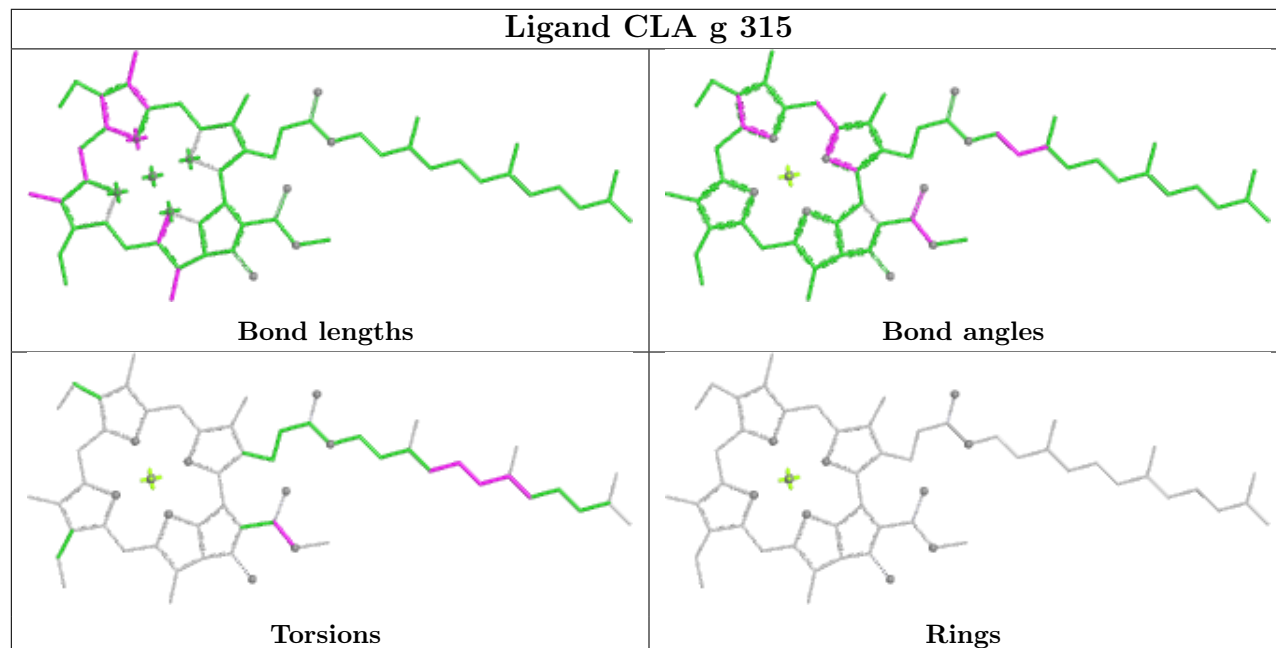
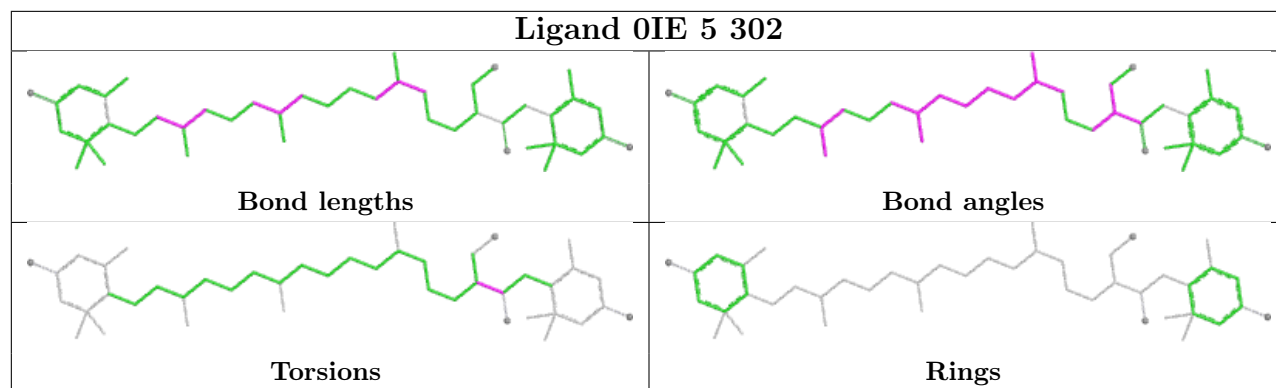


Ligand CLA y 307

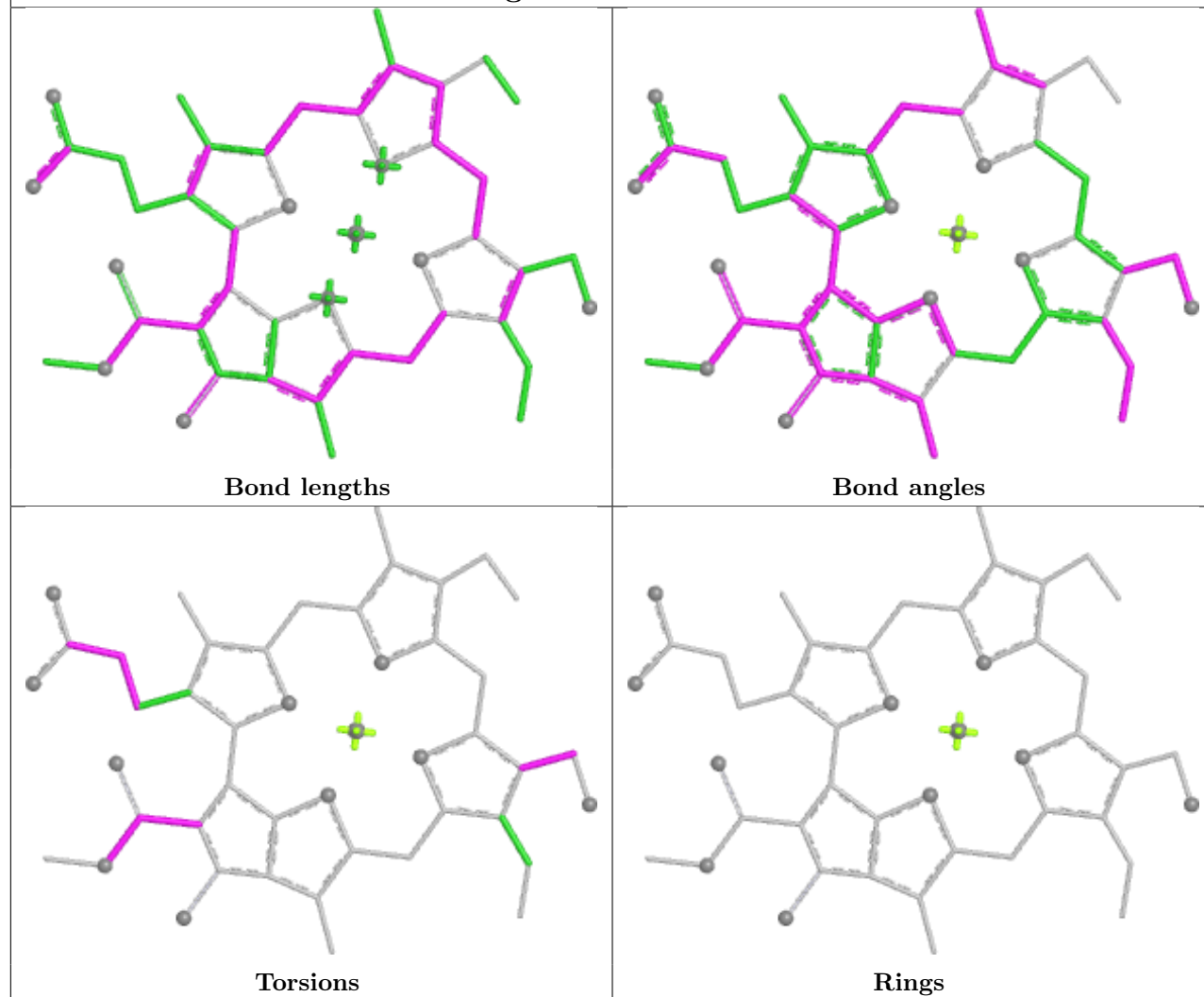


Ligand LHG y 319

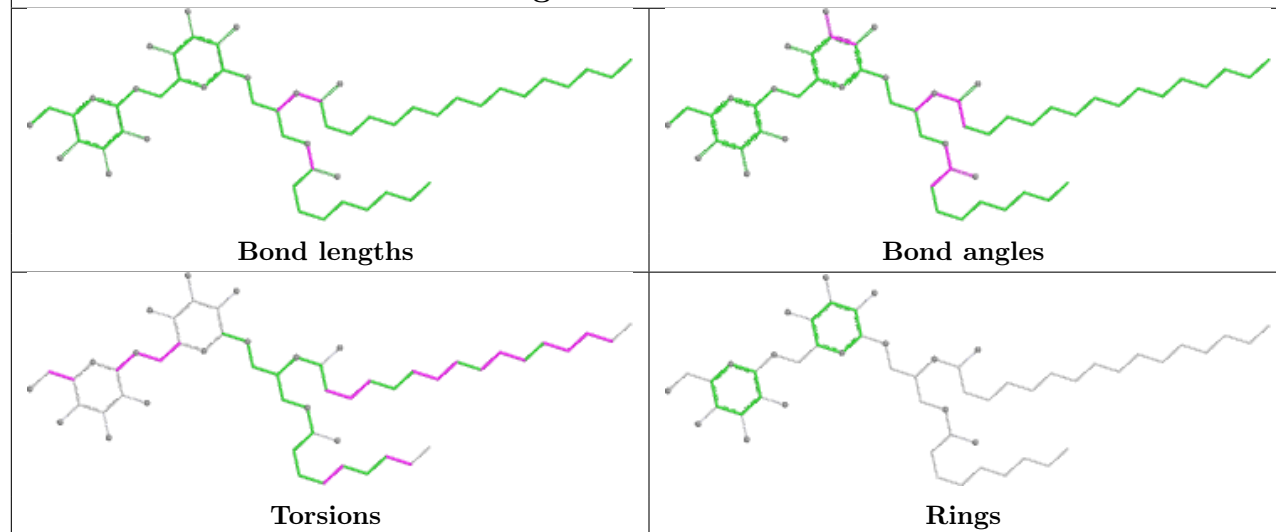




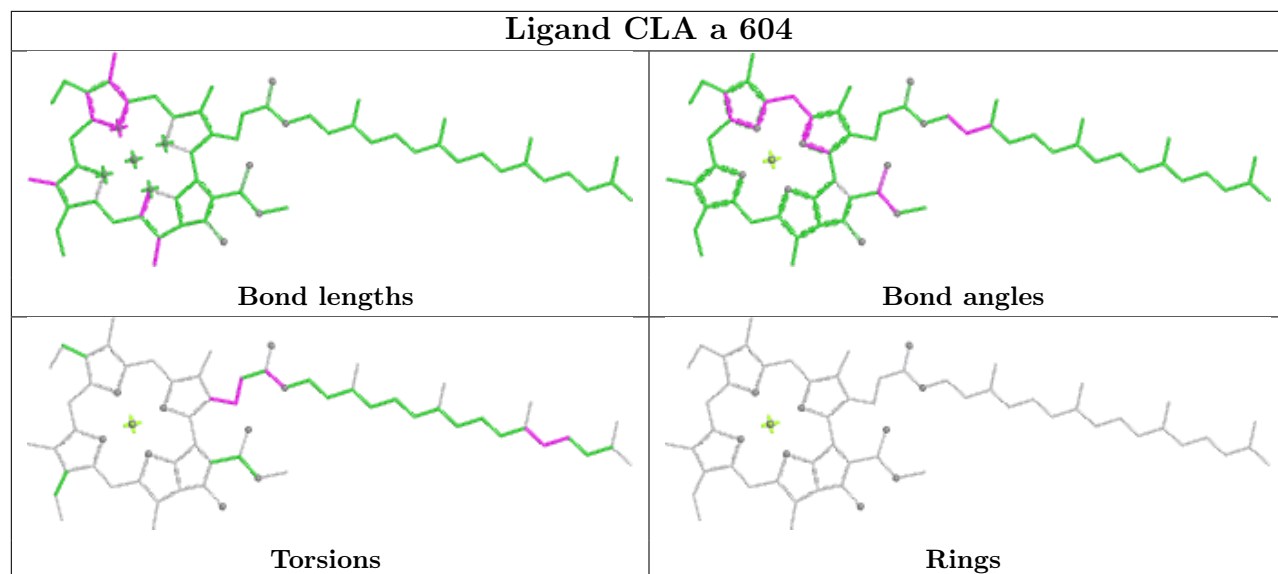
Ligand CHL 2 312



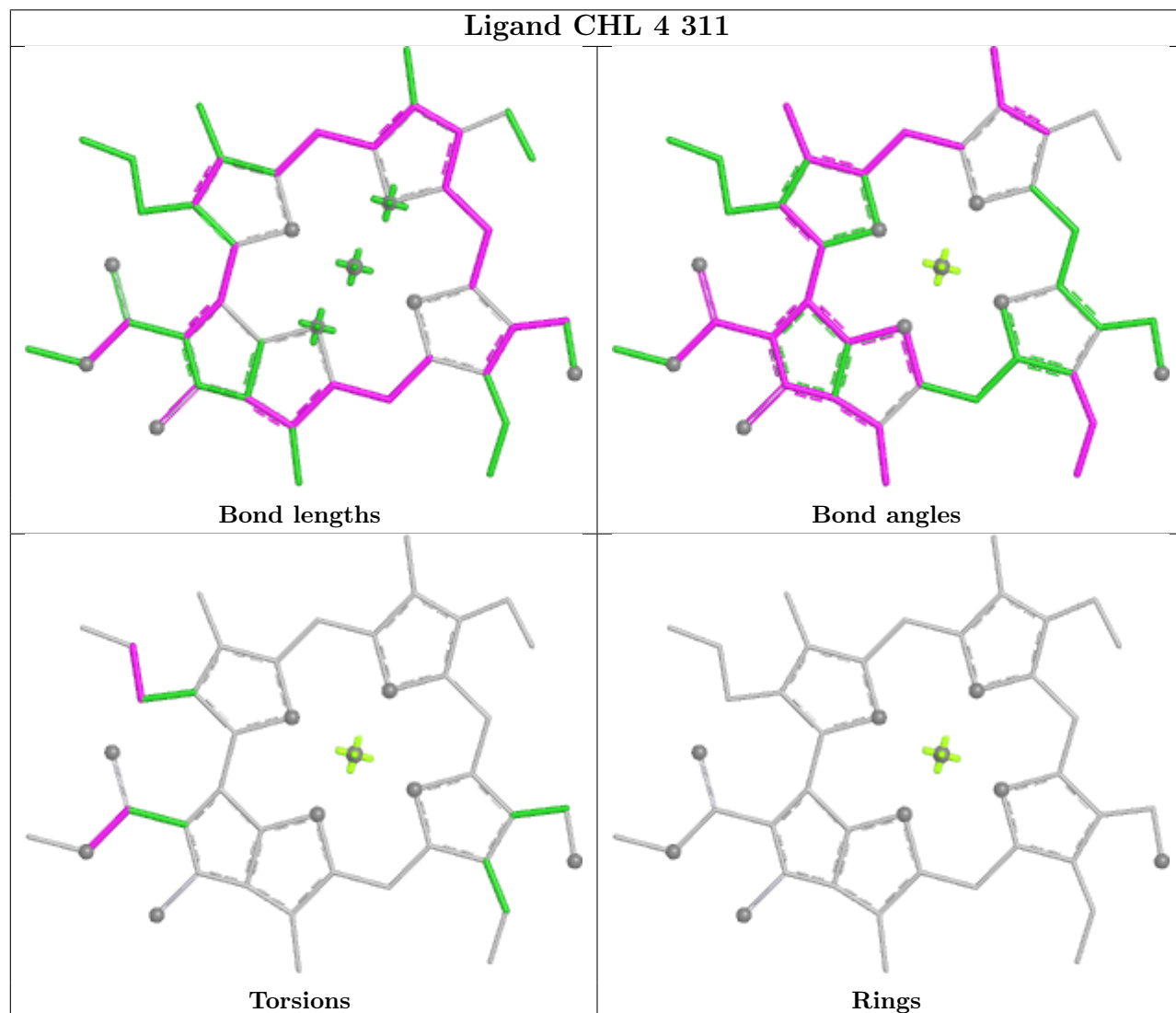
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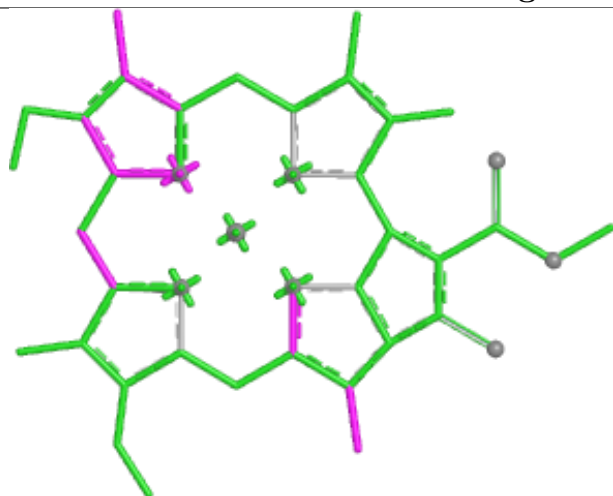
Ligand CLA a 604



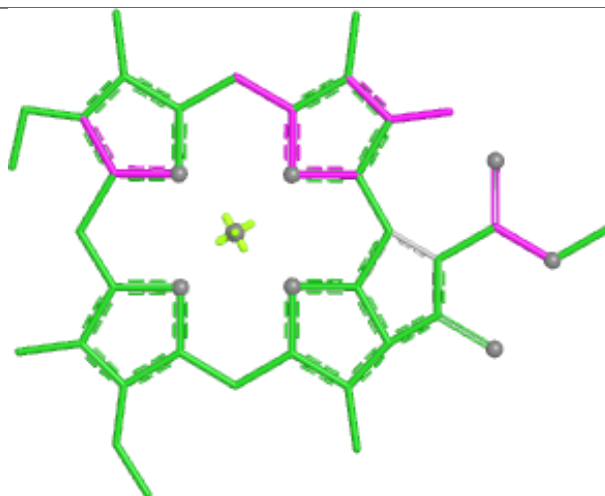
Ligand CHL 4 311



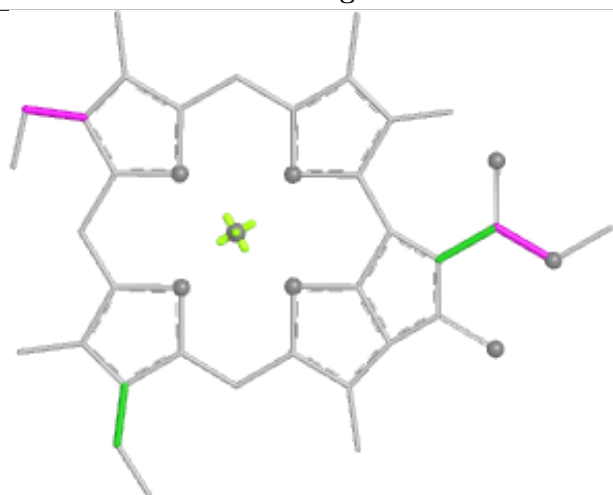
Ligand CLA 4 314



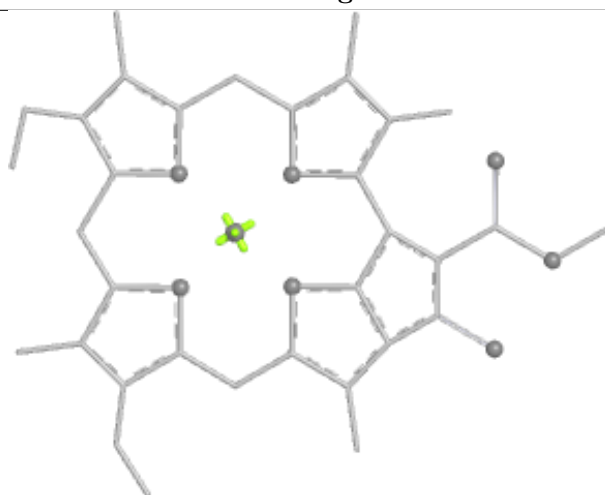
Bond lengths



Bond angles

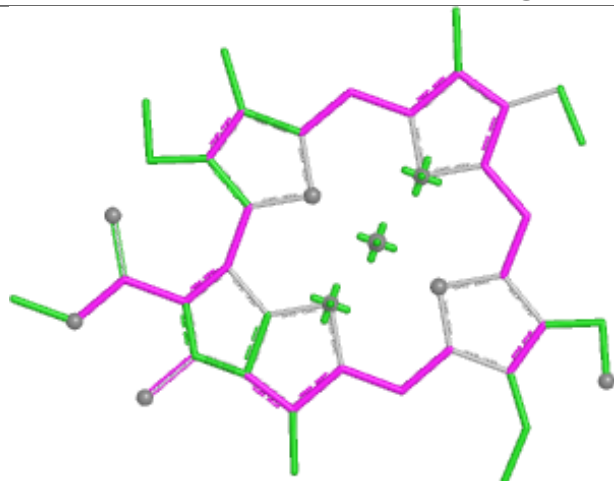


Torsions

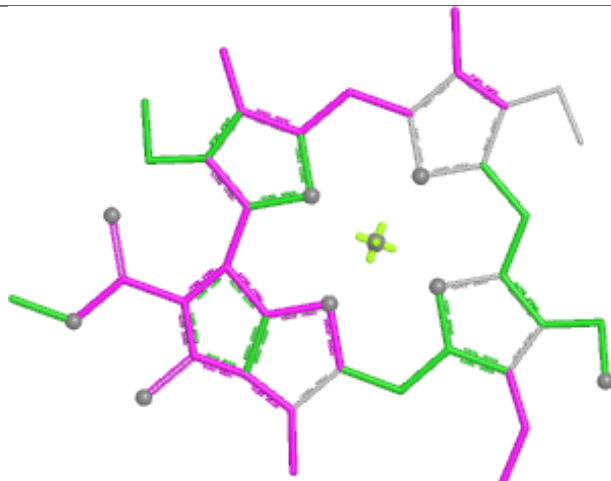


Rings

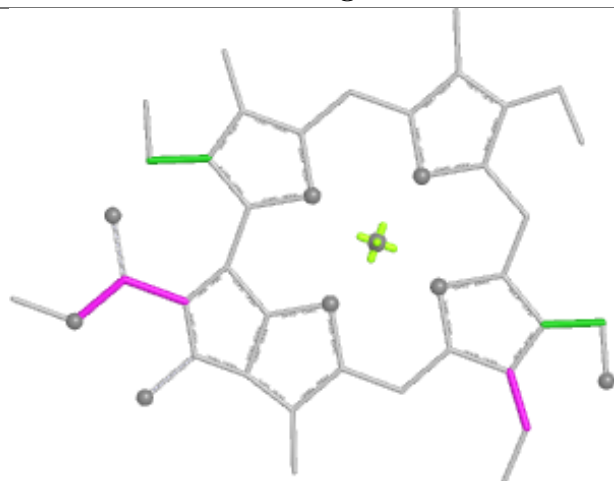
Ligand CHL 7 313



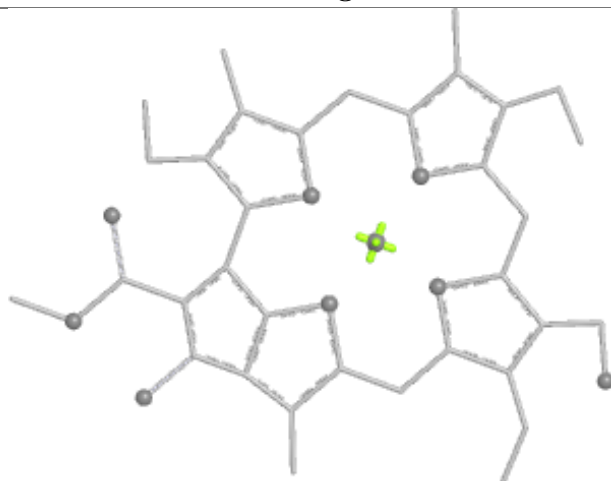
Bond lengths



Bond angles

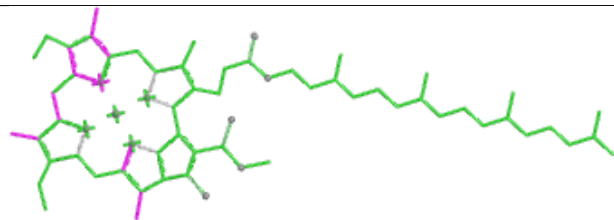


Torsions

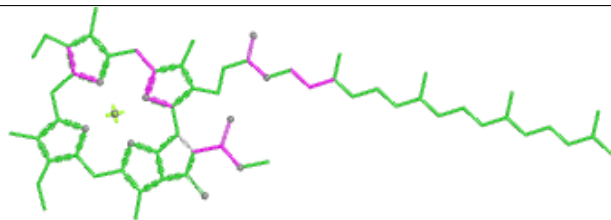


Rings

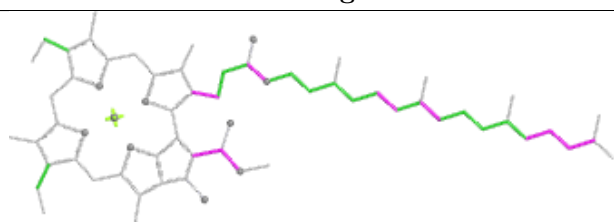
Ligand CLA d 405



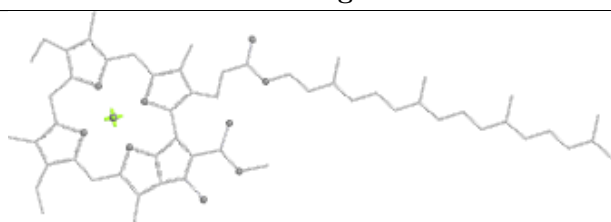
Bond lengths



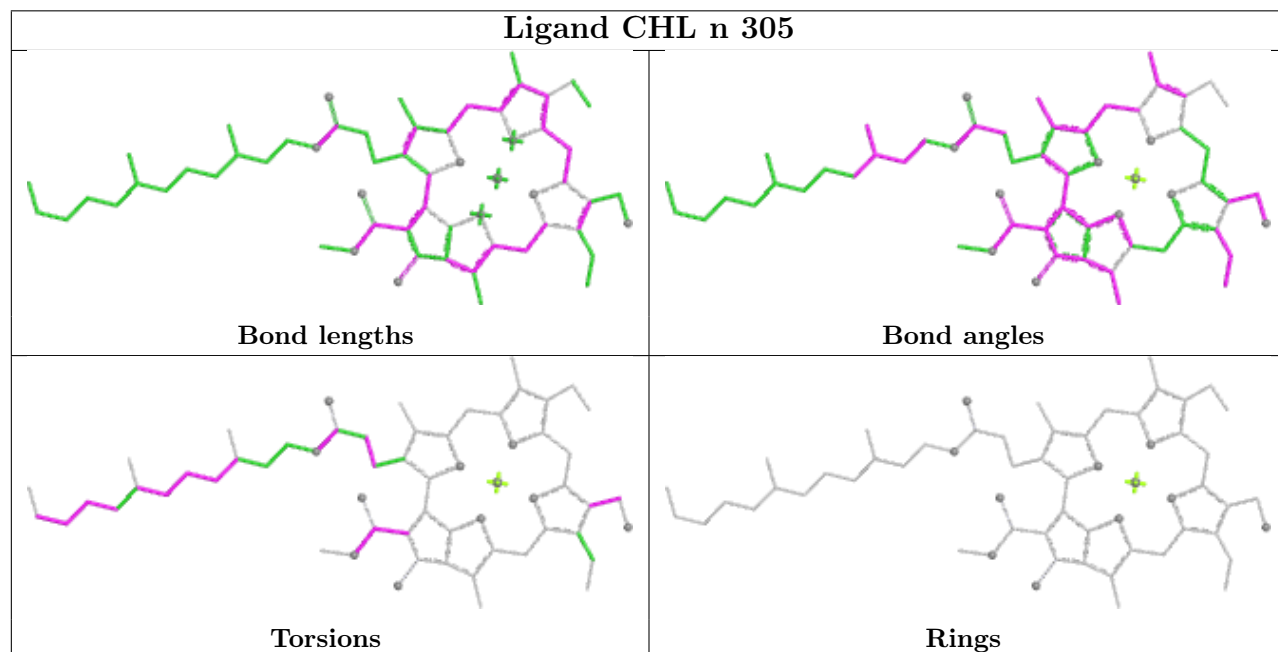
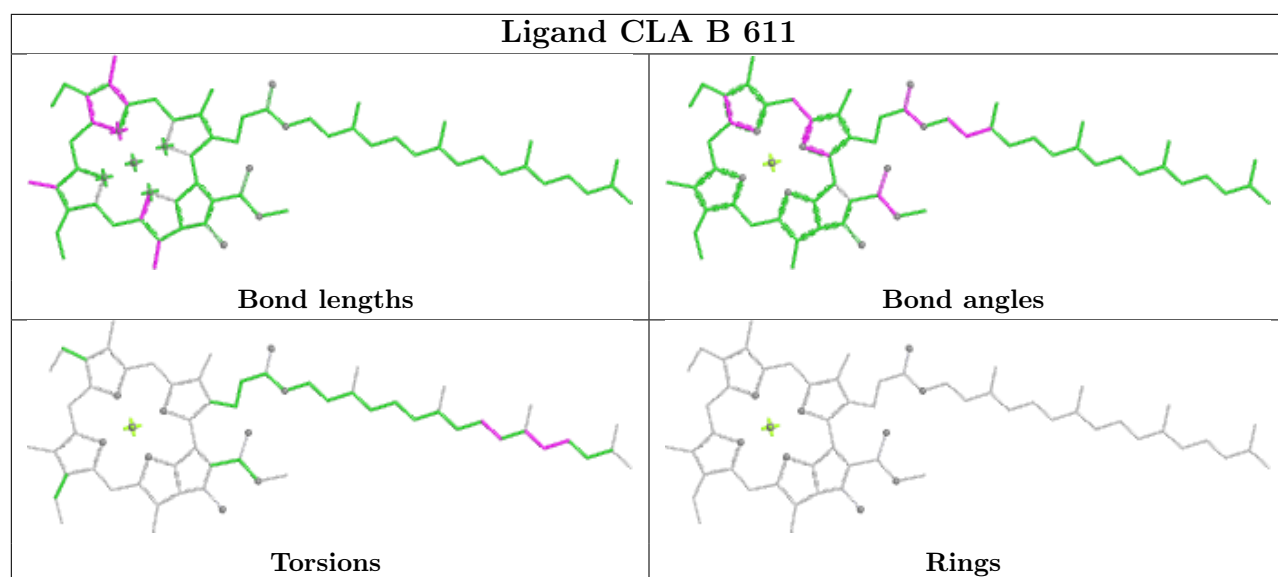
Bond angles



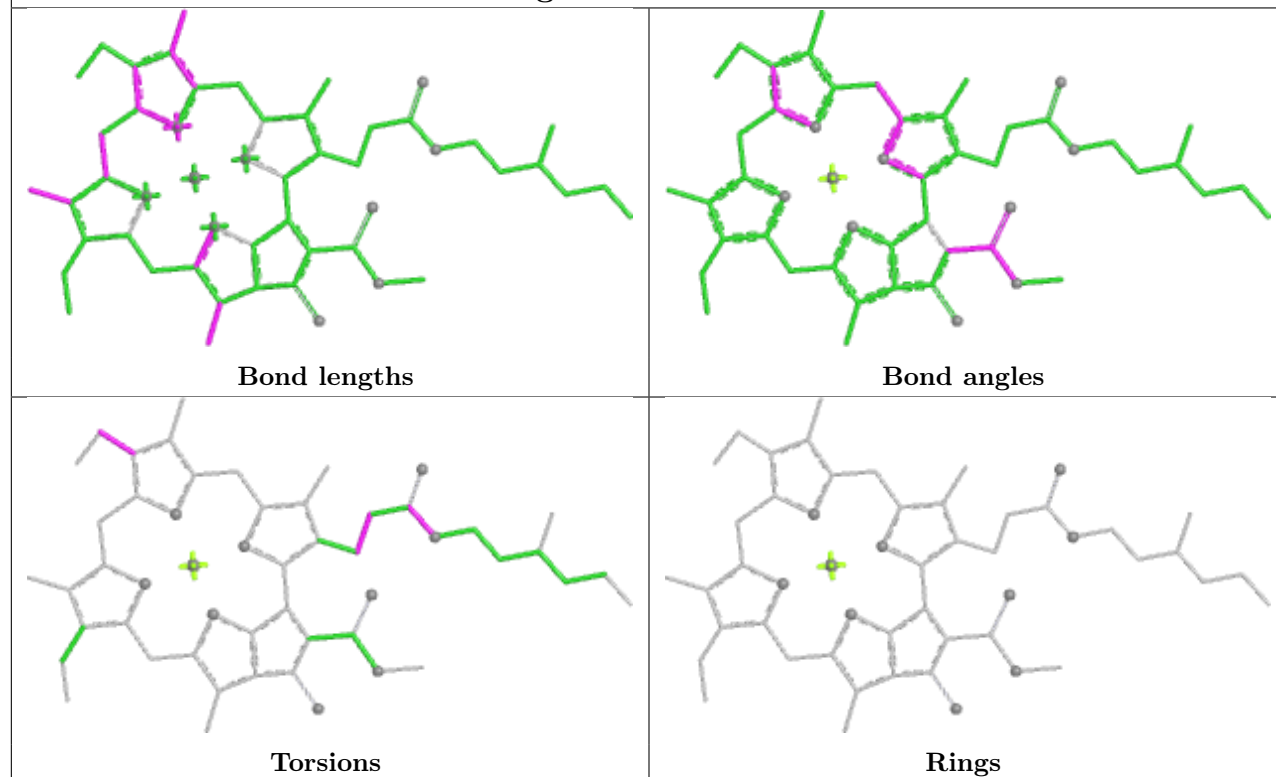
Torsions



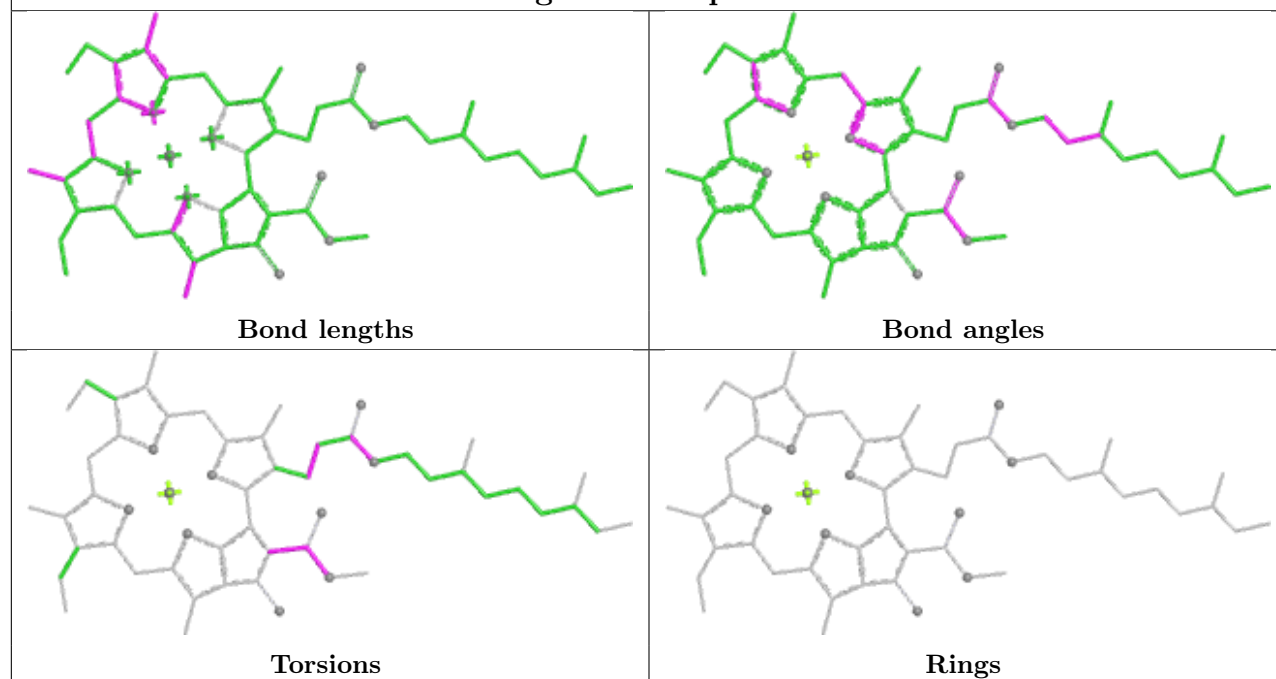
Rings



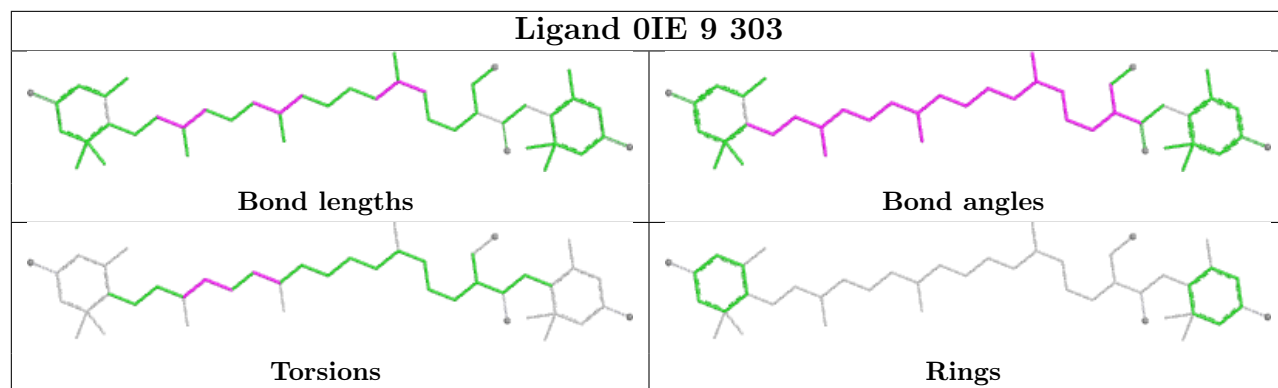
Ligand CLA 7 317



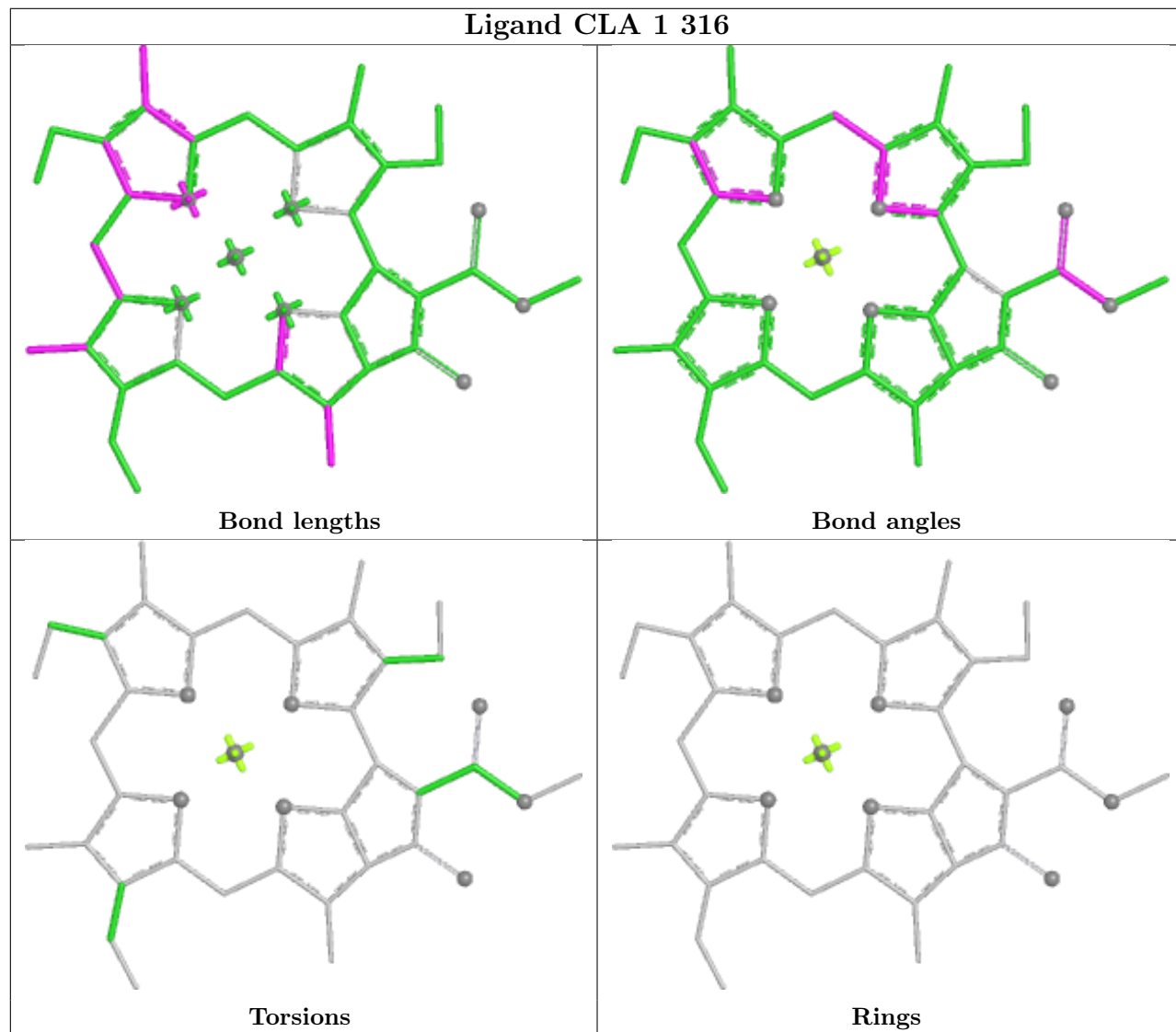
Ligand CLA p 307

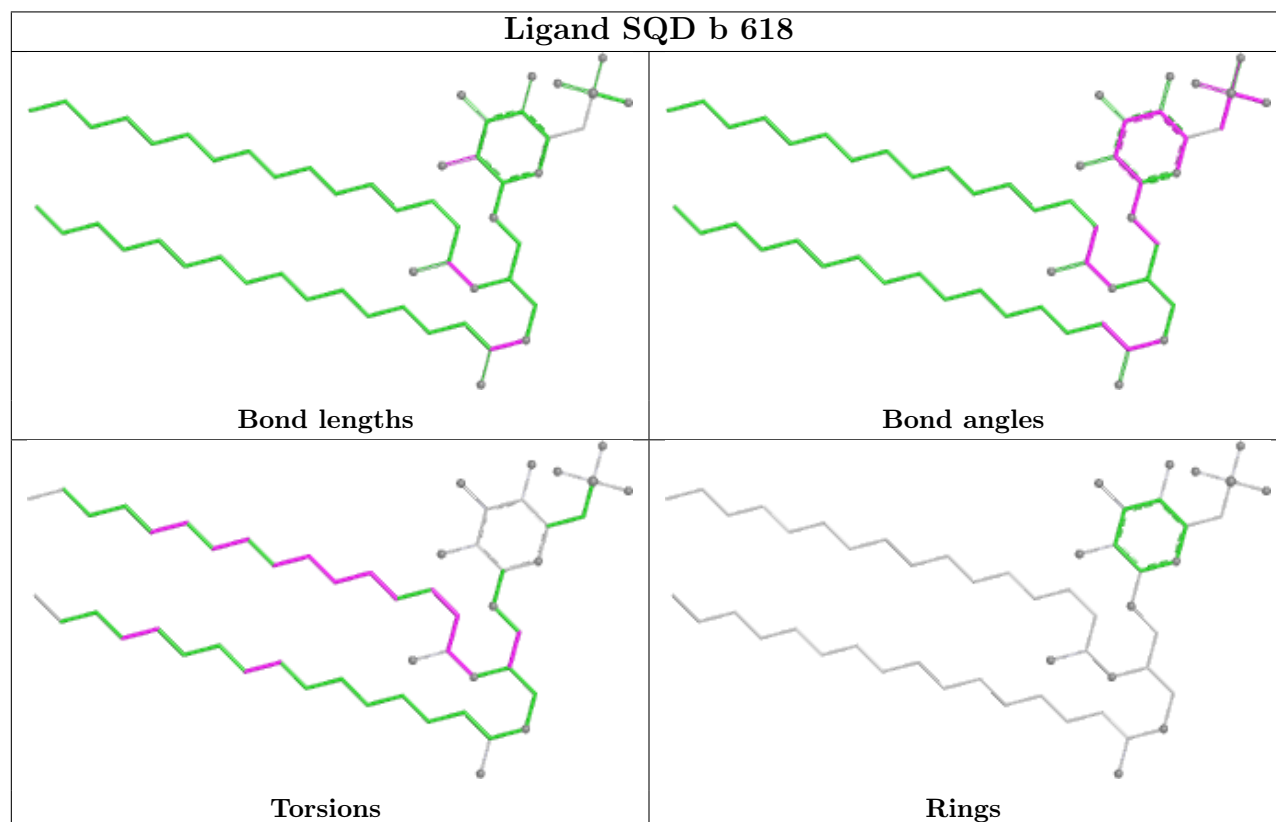
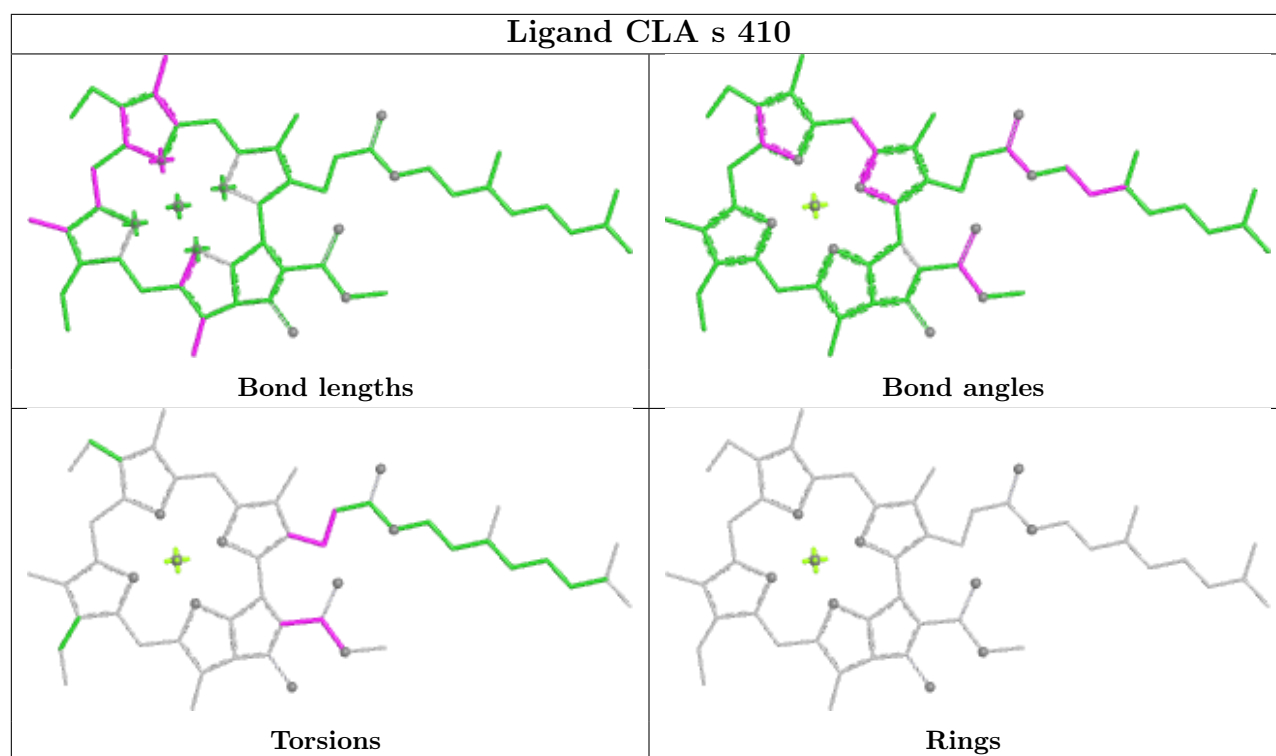


Ligand OIE 9 303

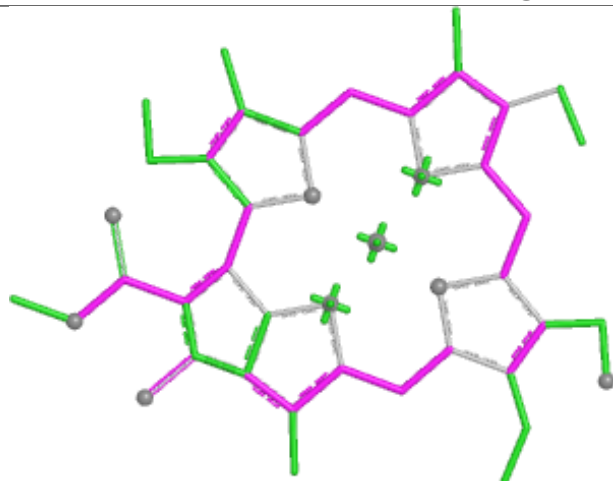


Ligand CLA 1 316

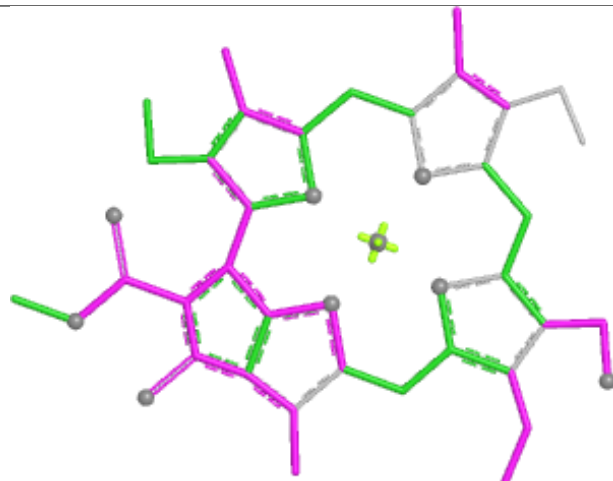




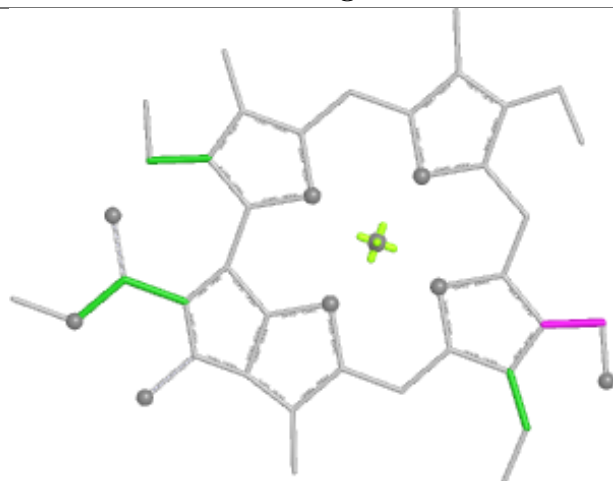
Ligand CHL 8 307



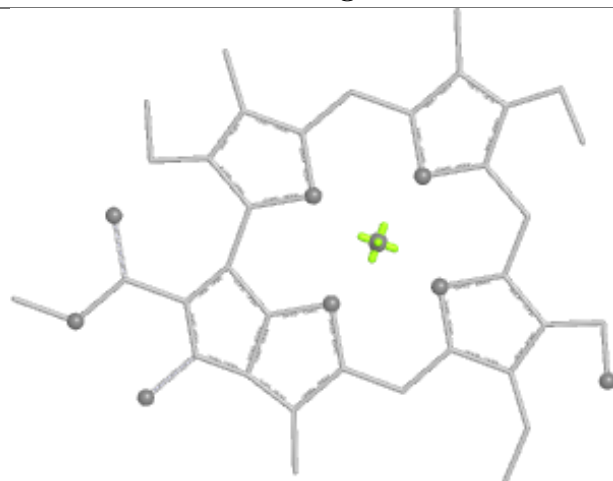
Bond lengths



Bond angles

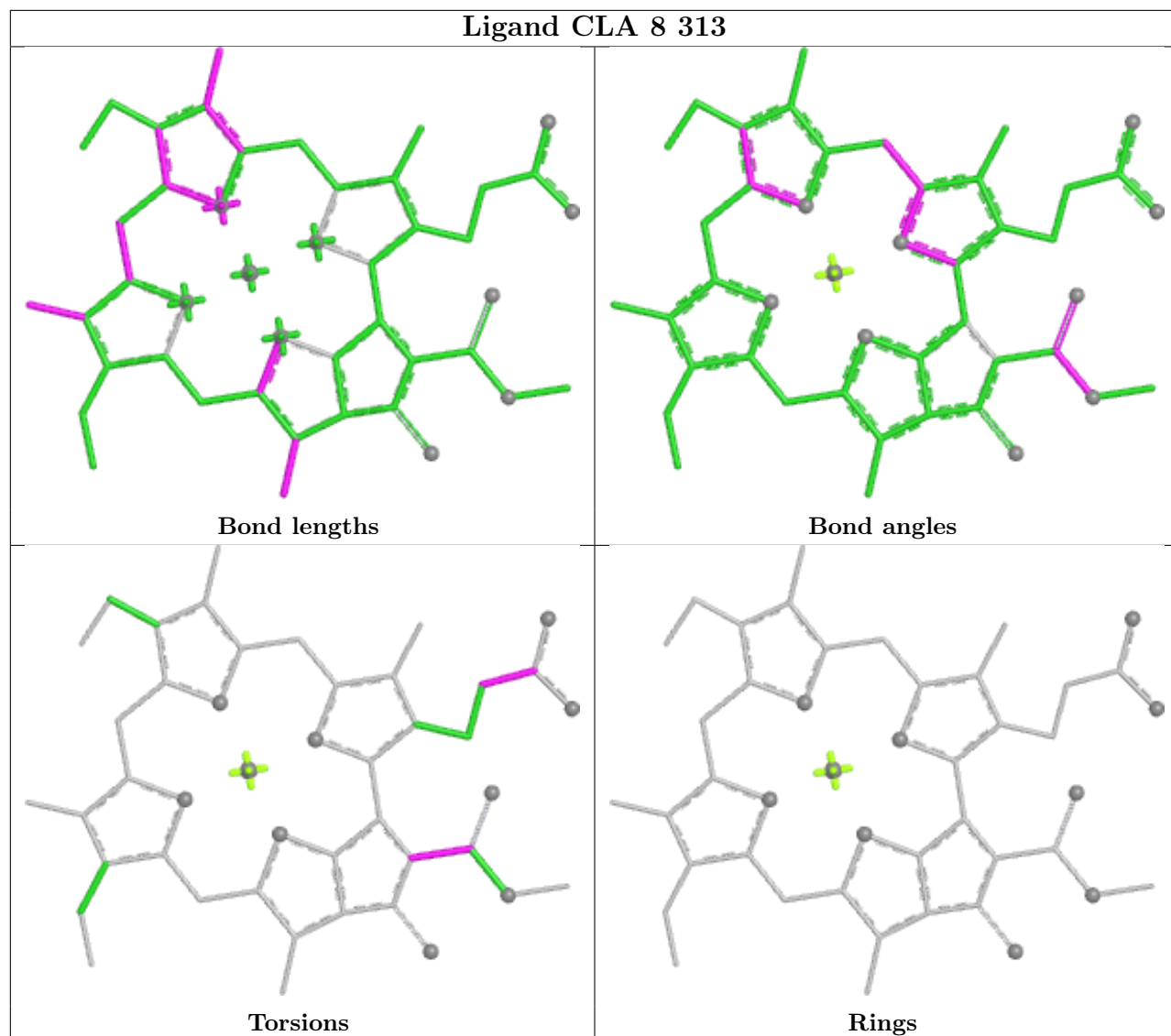


Torsions

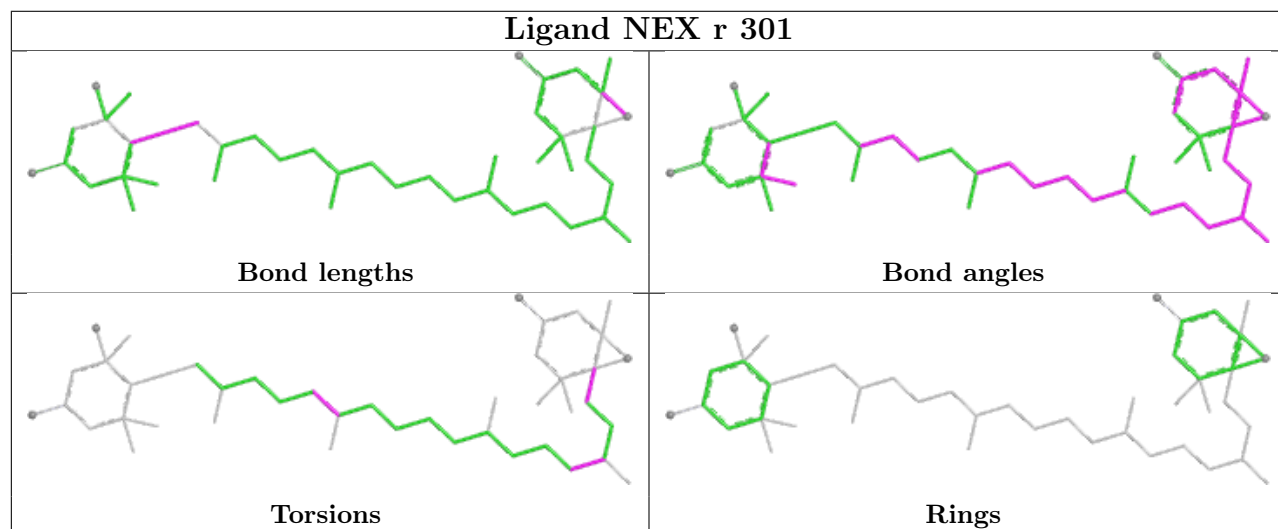


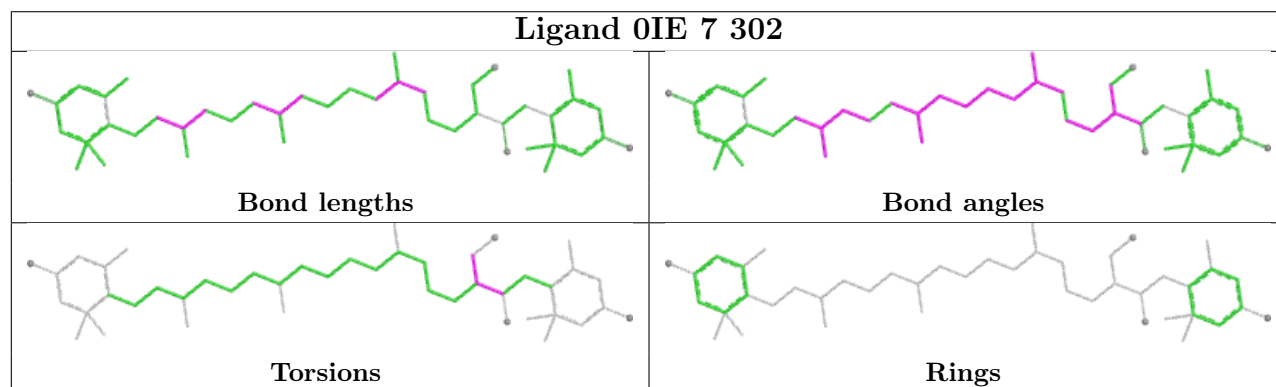
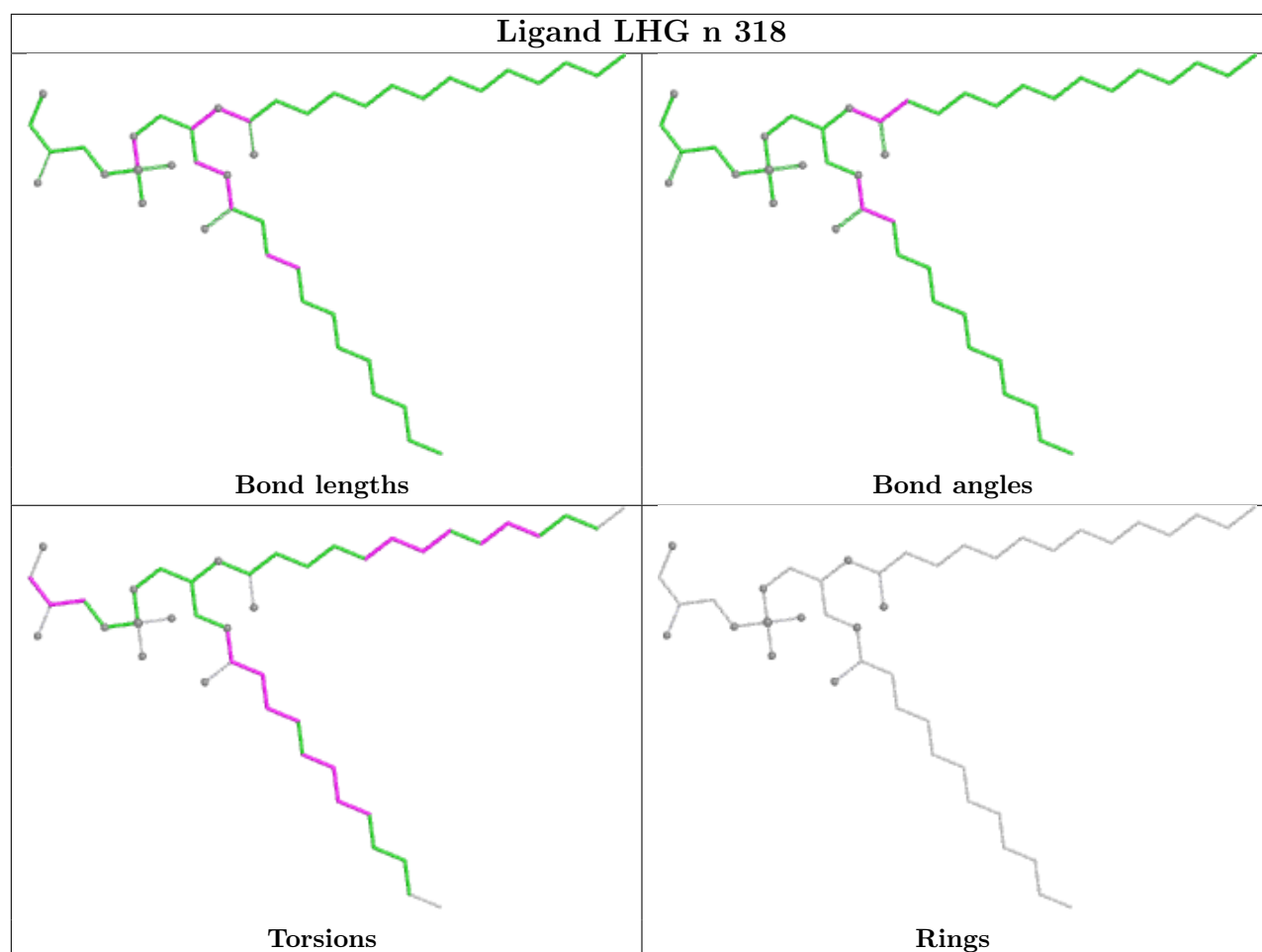
Rings

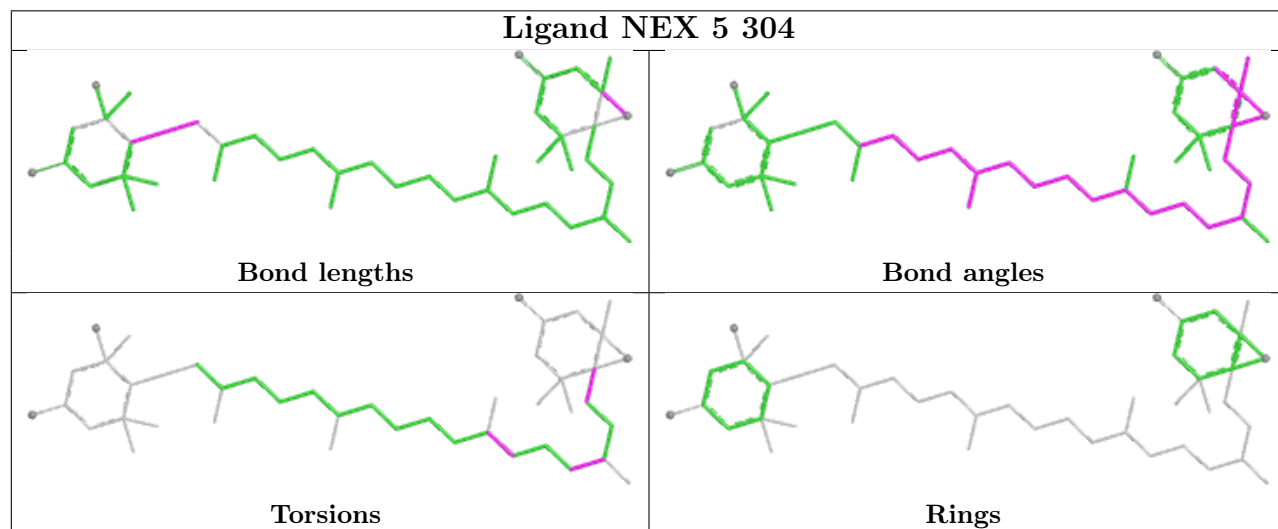
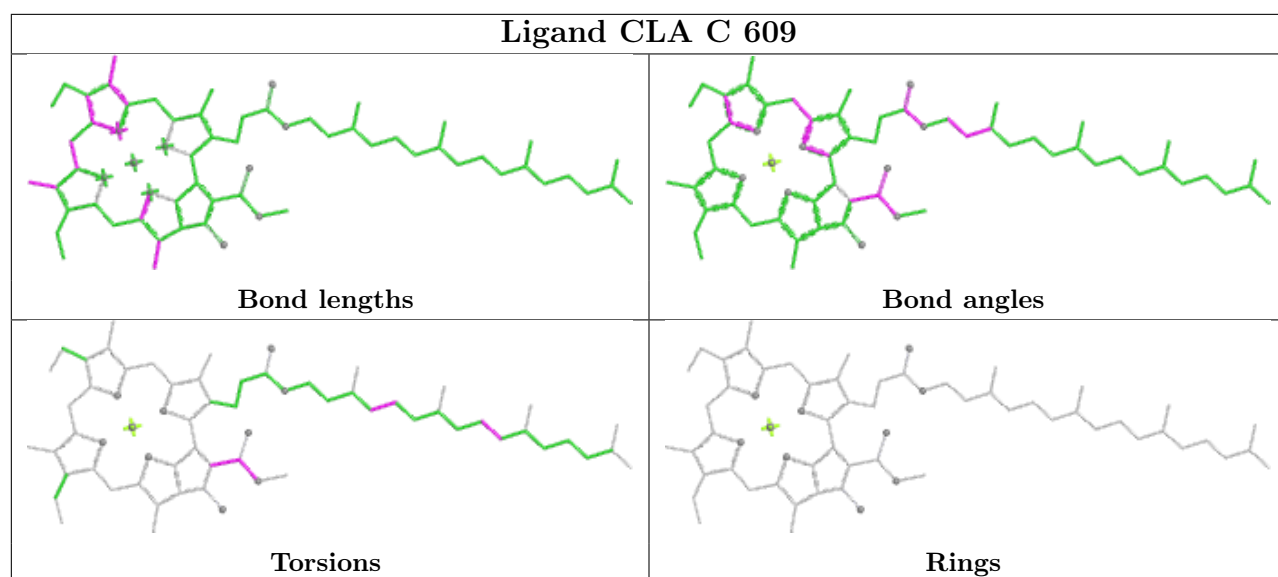
Ligand CLA 8 313



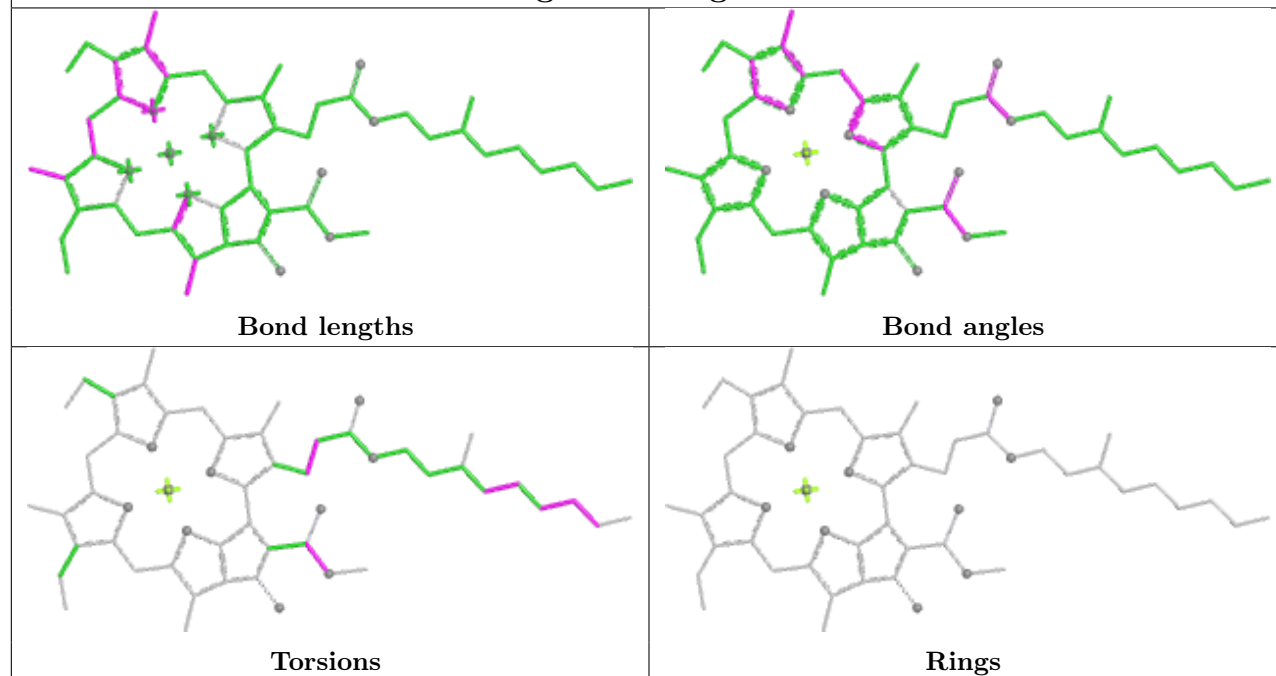
Ligand NEX r 301



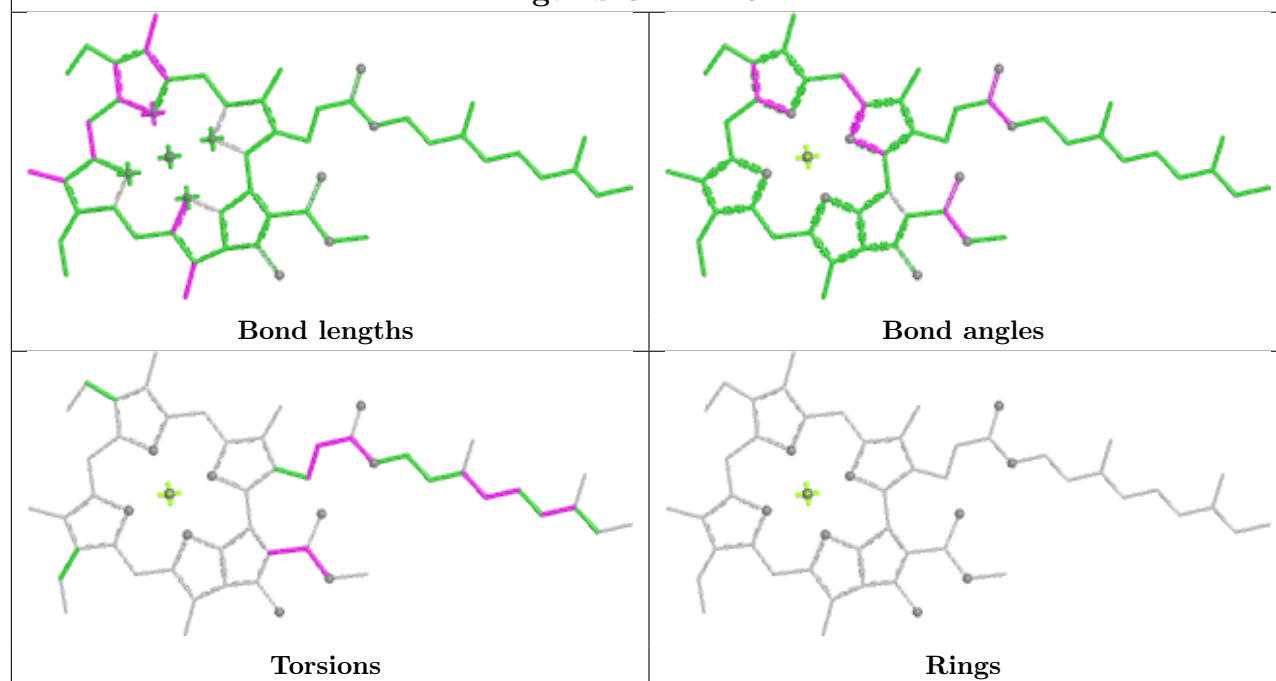


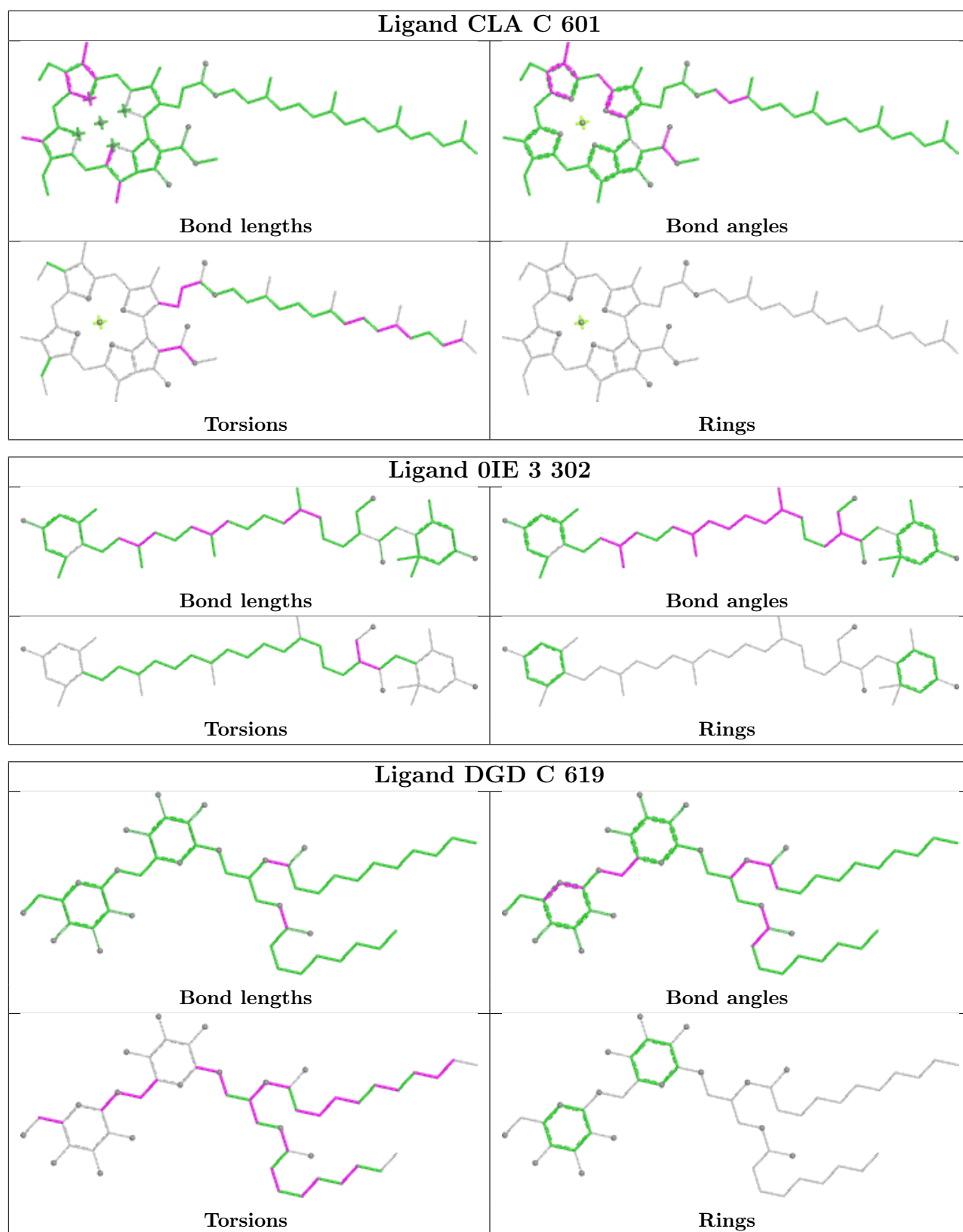


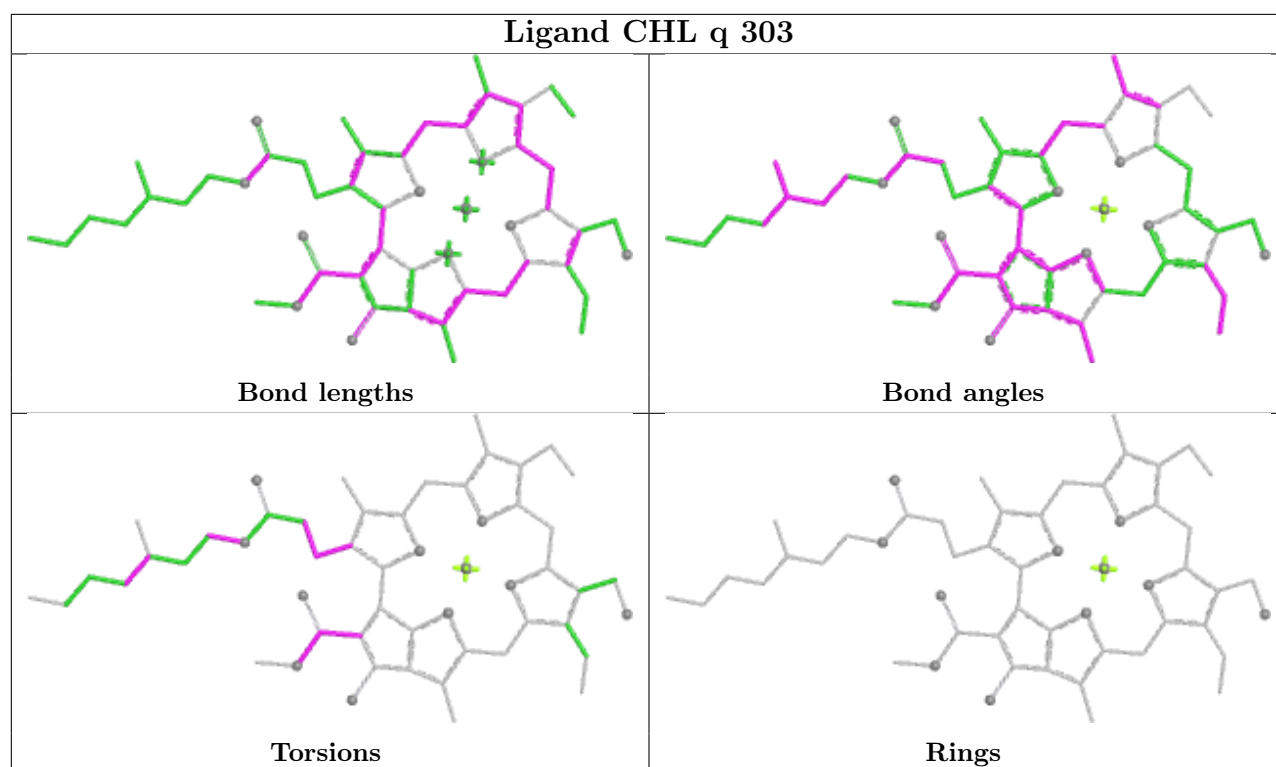
Ligand CLA g 317



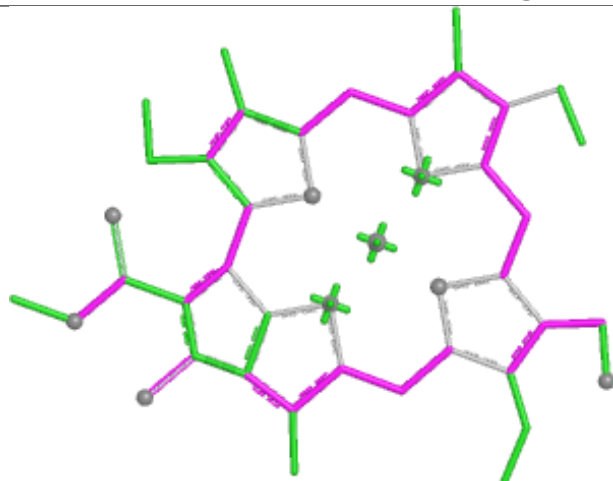
Ligand CLA B 614



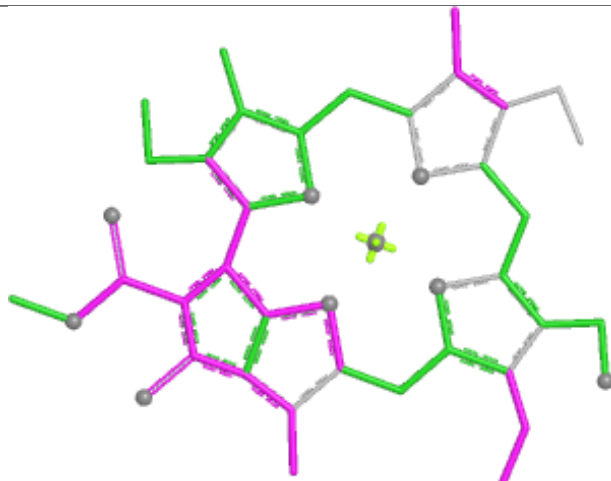




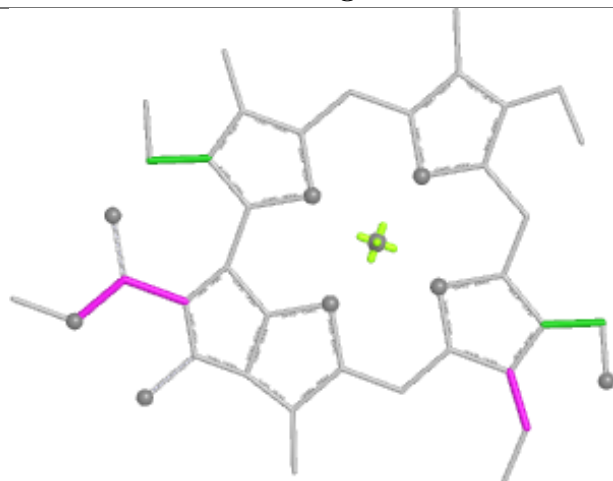
Ligand CHL 6 312



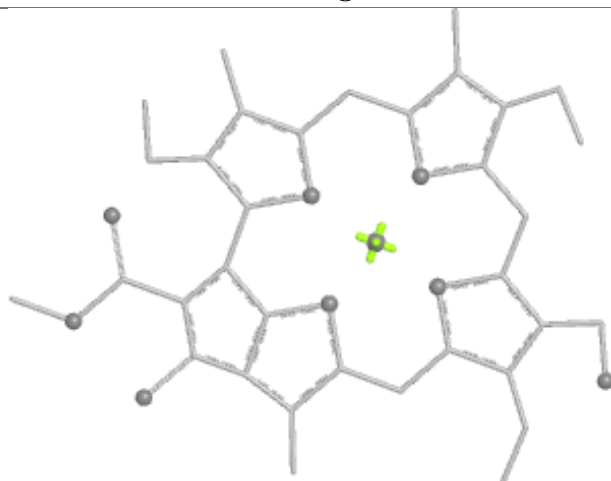
Bond lengths



Bond angles

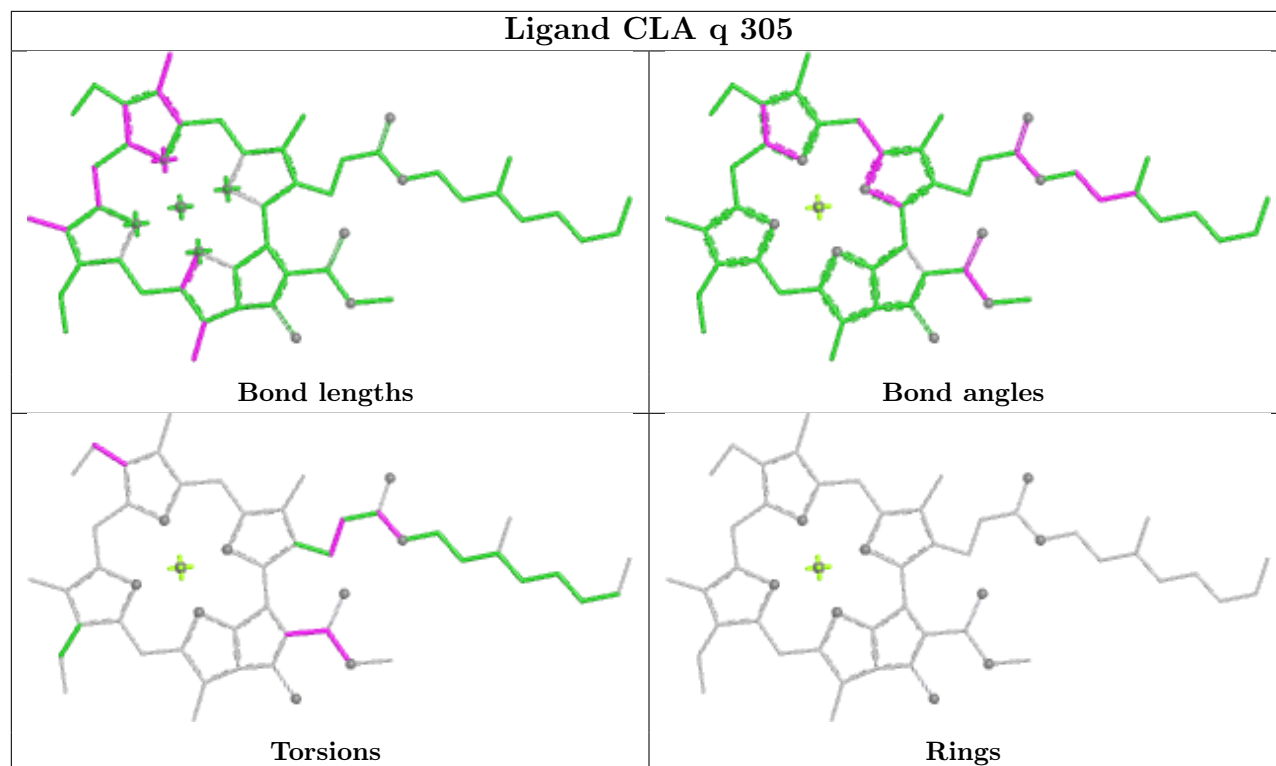


Torsions

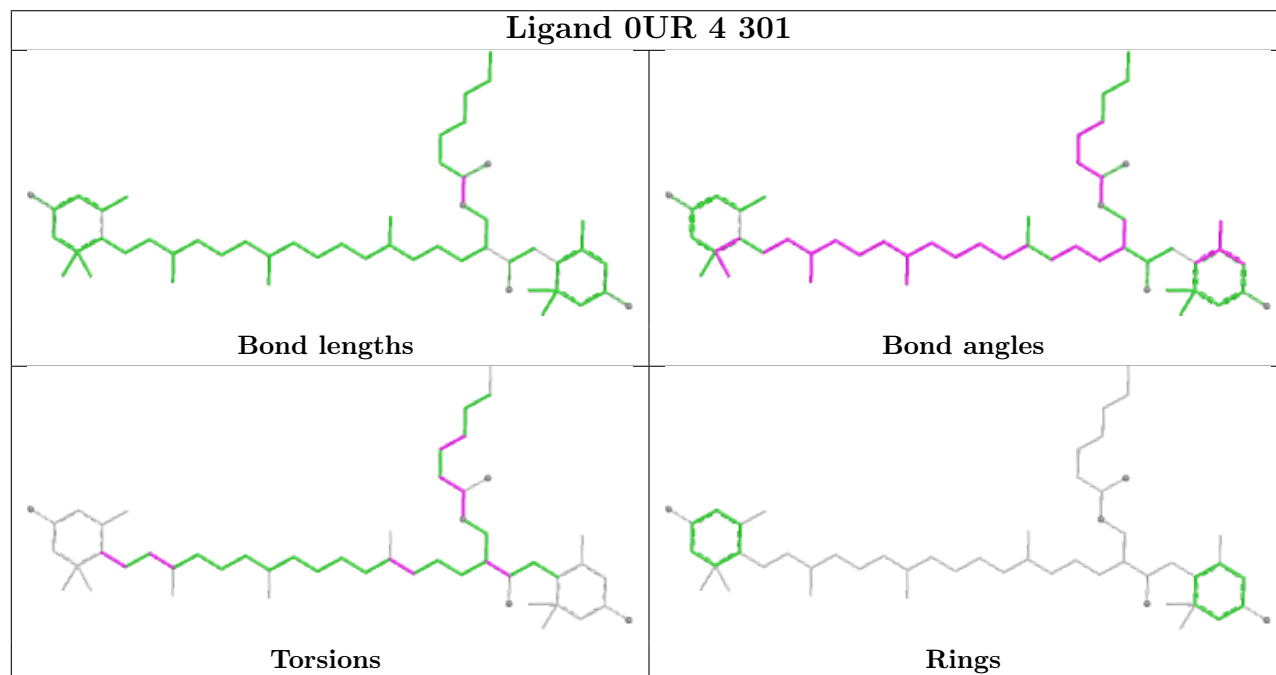


Rings

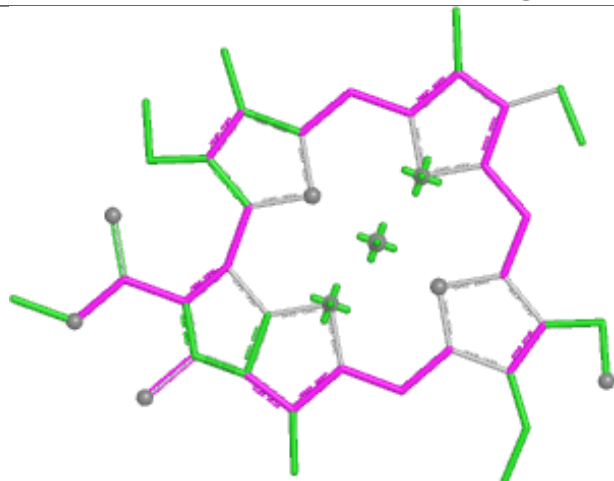
Ligand CLA q 305



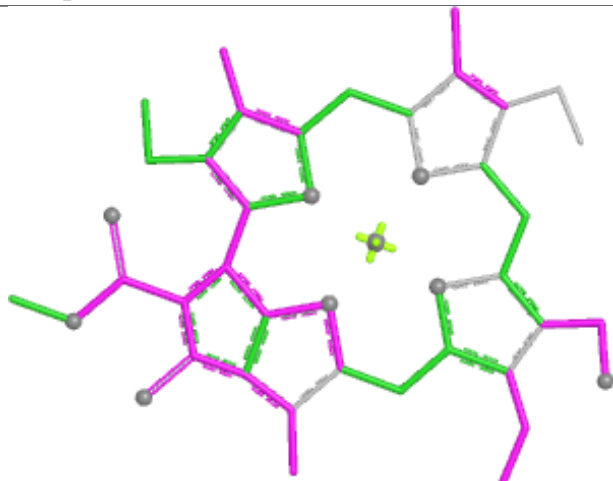
Ligand OUR 4 301



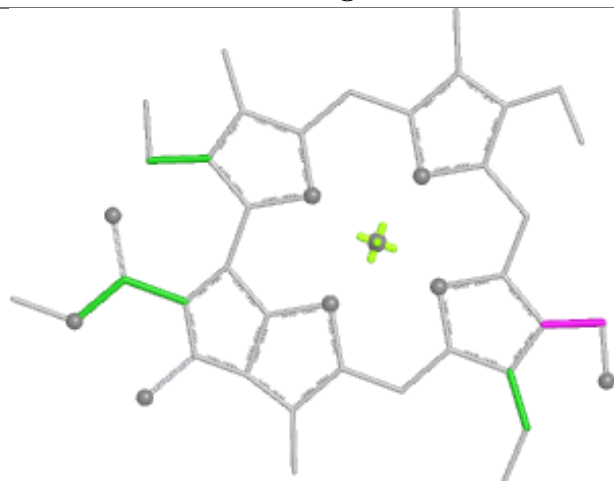
Ligand CHL q 307



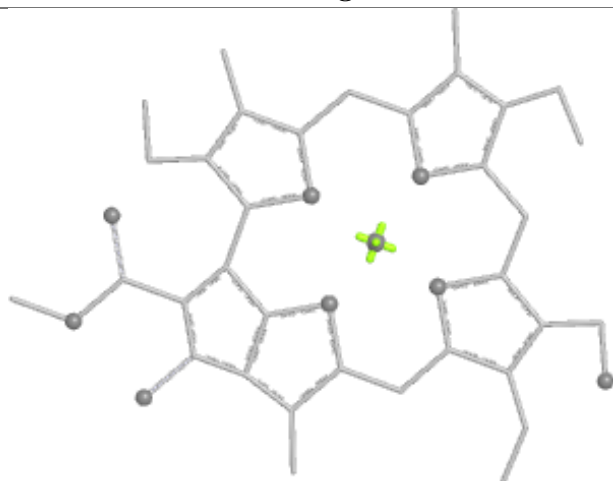
Bond lengths



Bond angles

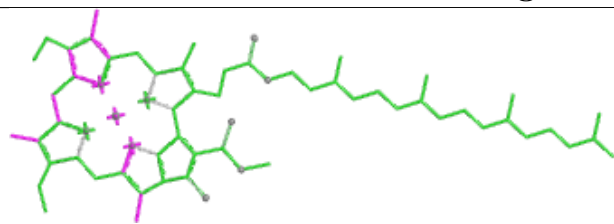


Torsions

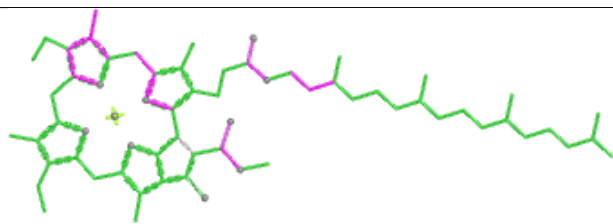


Rings

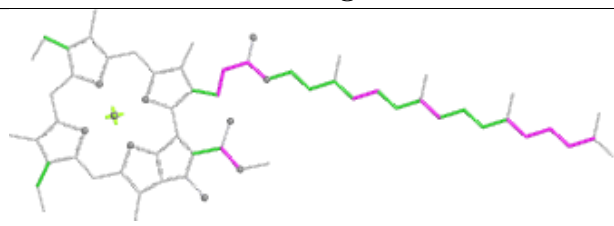
Ligand CLA b 606



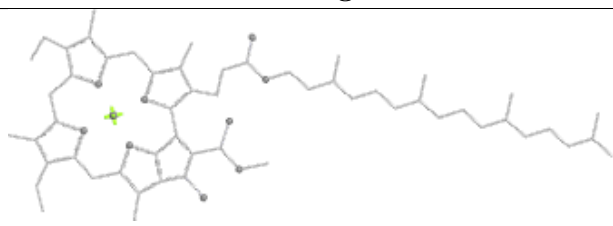
Bond lengths



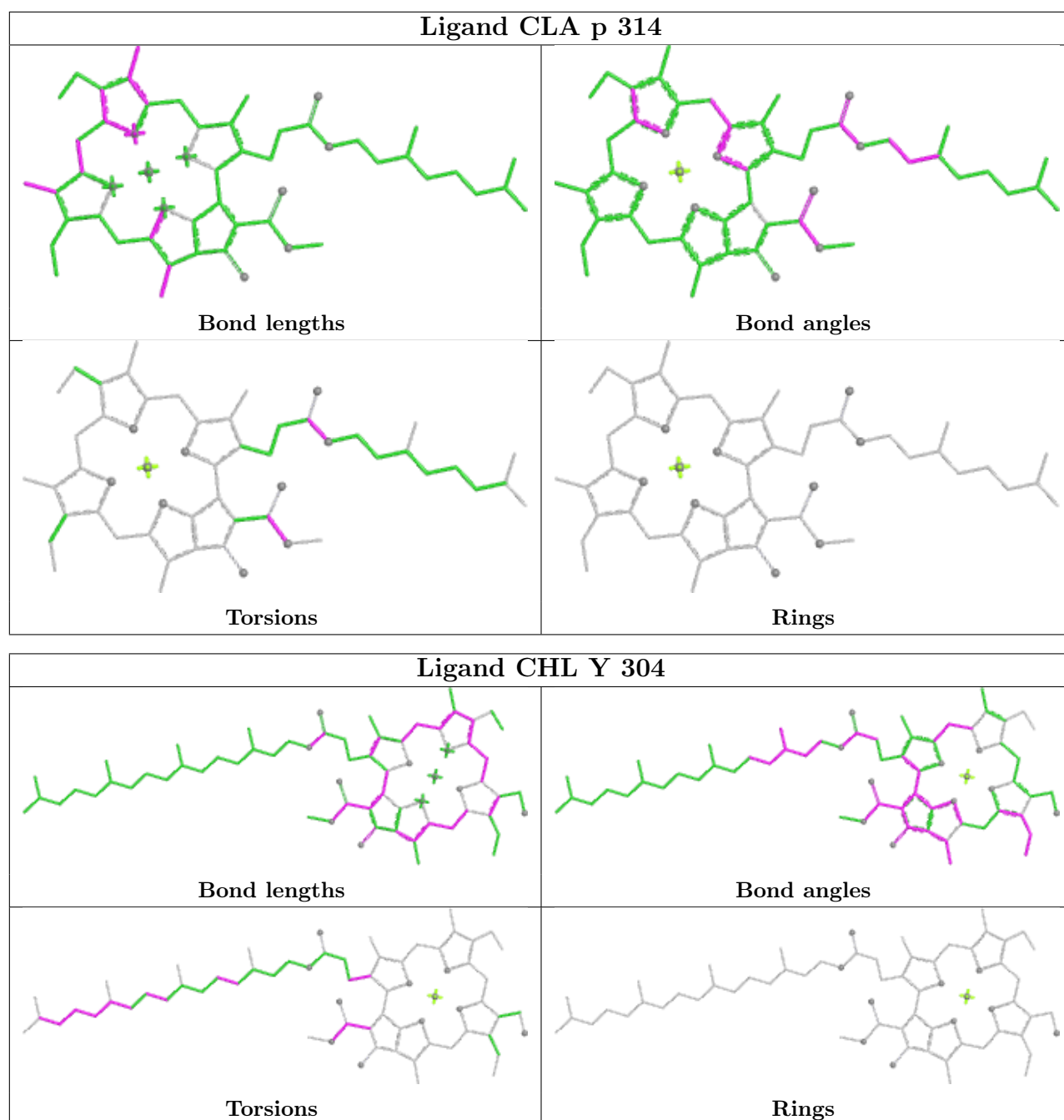
Bond angles

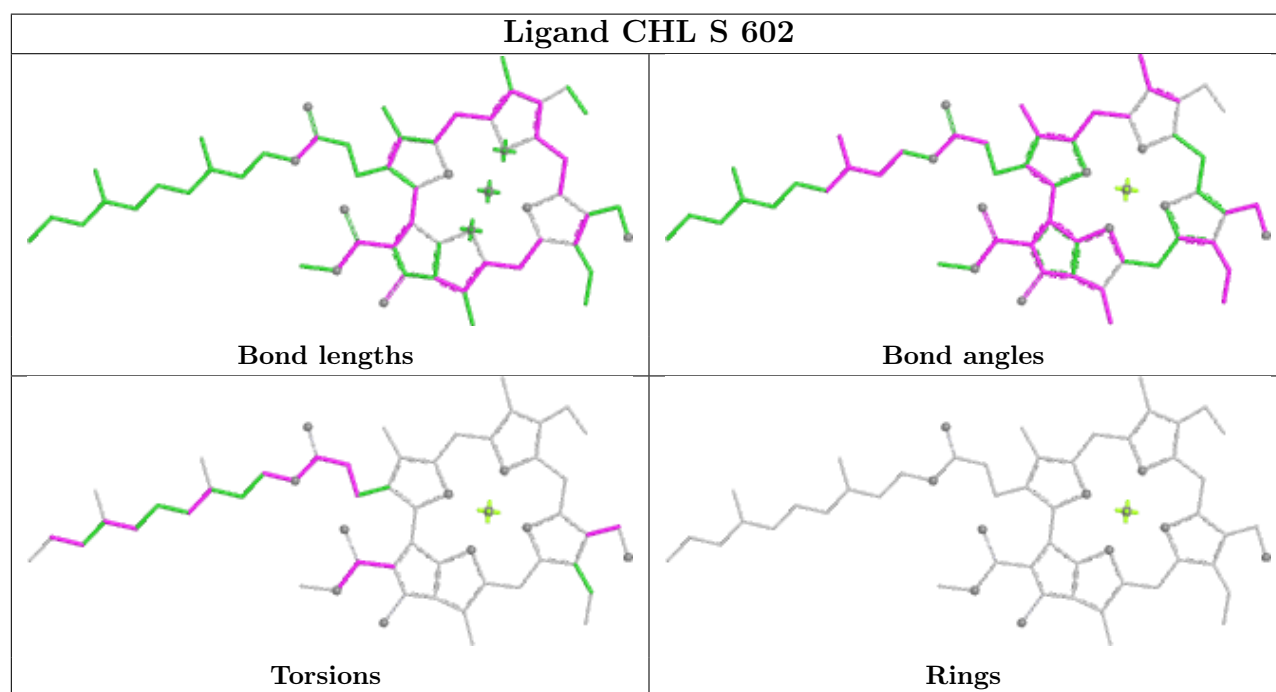
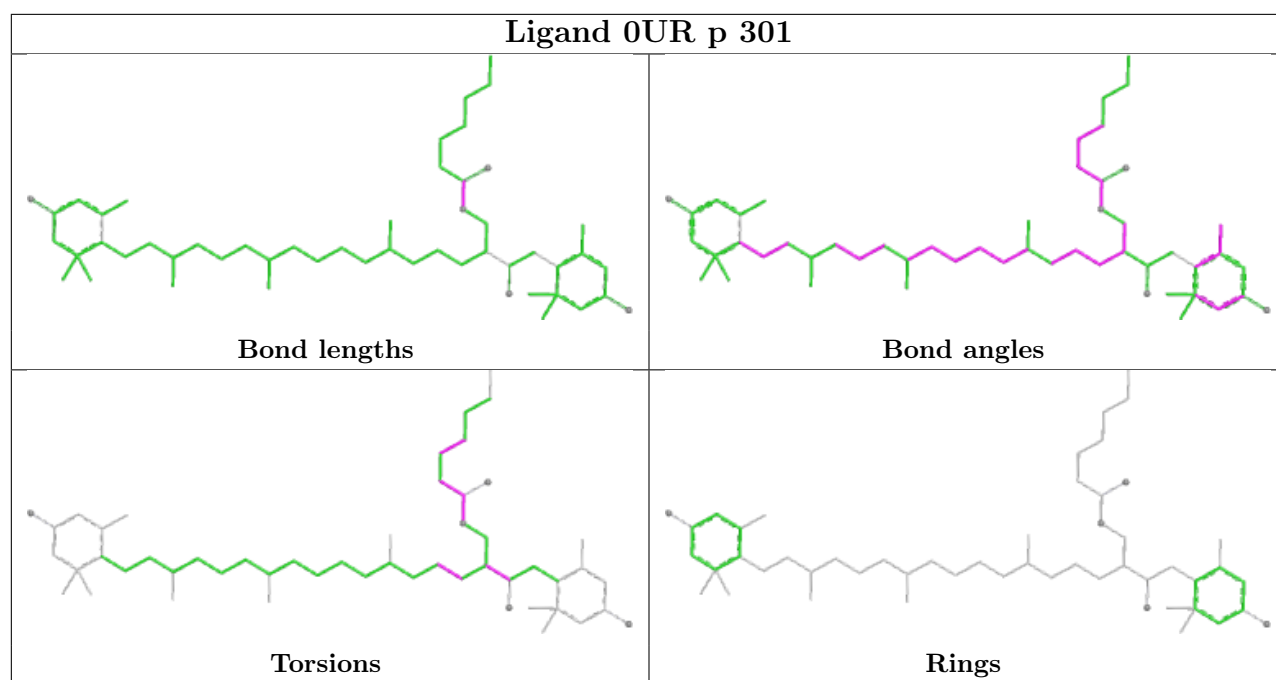


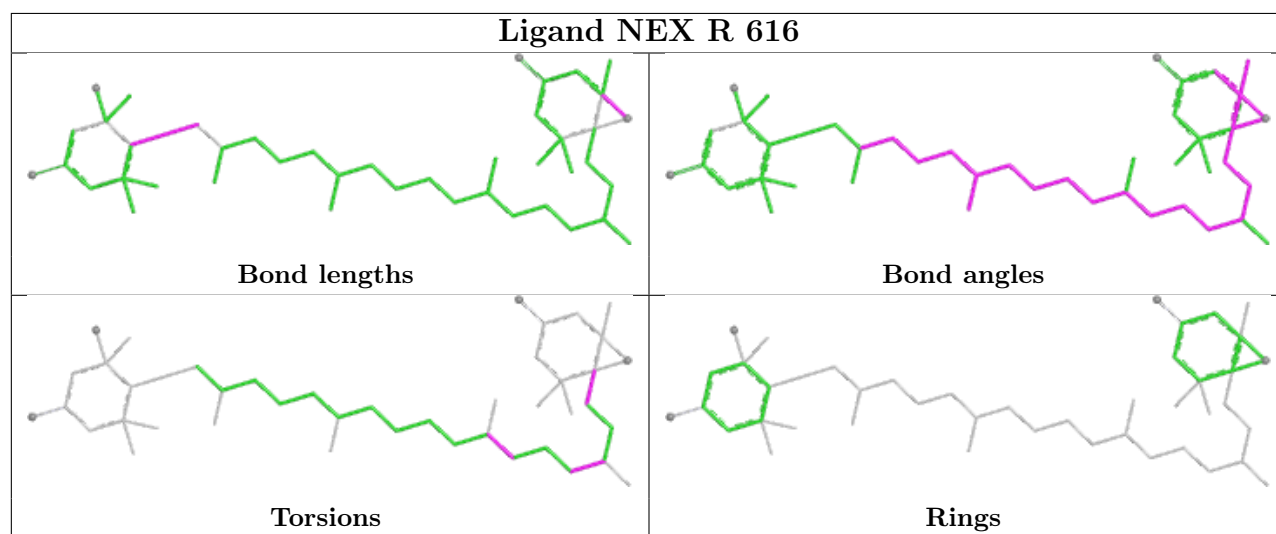
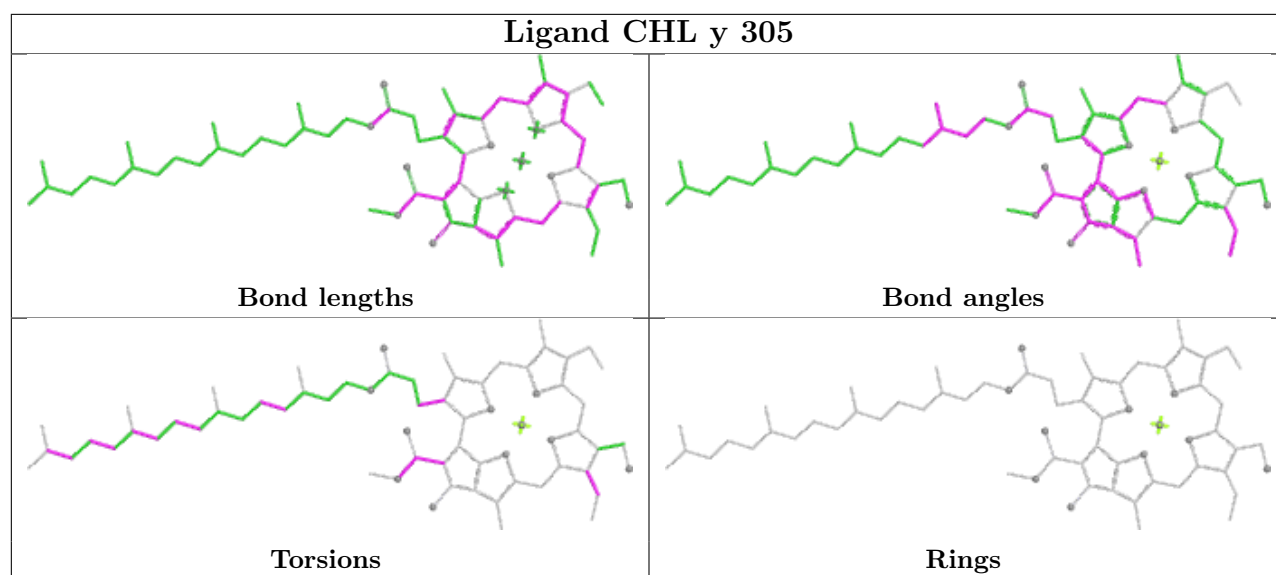
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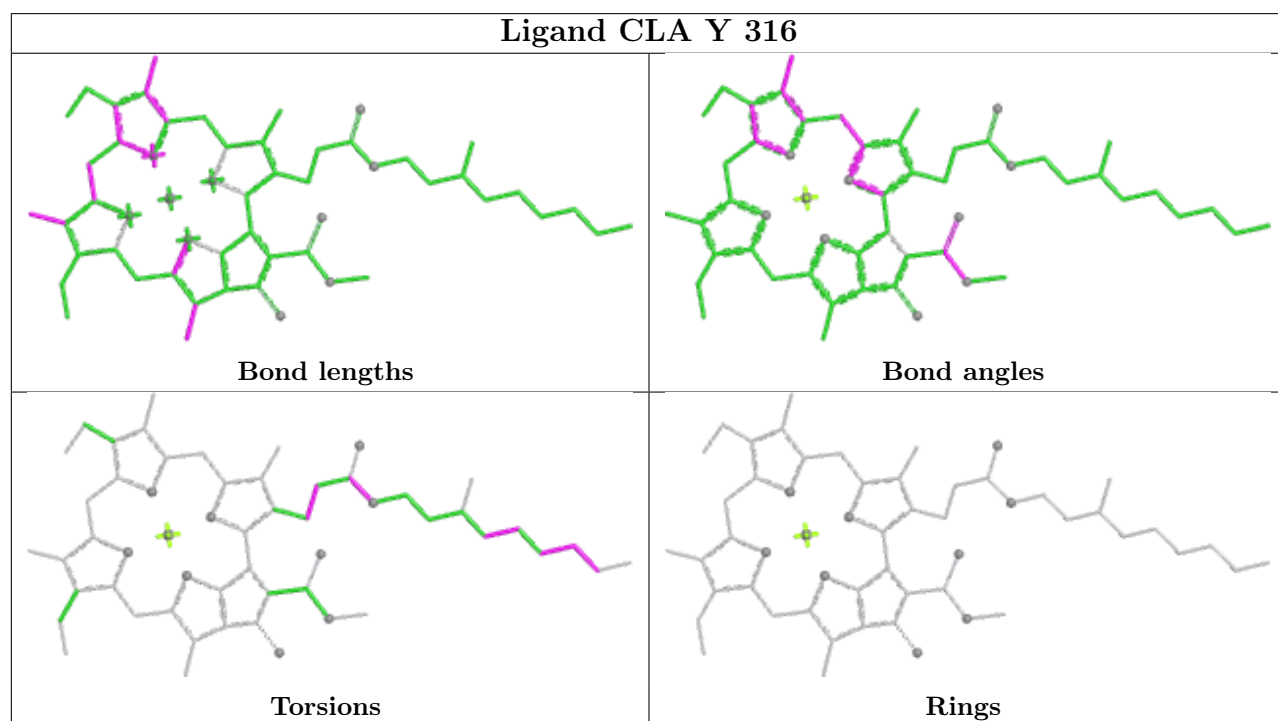
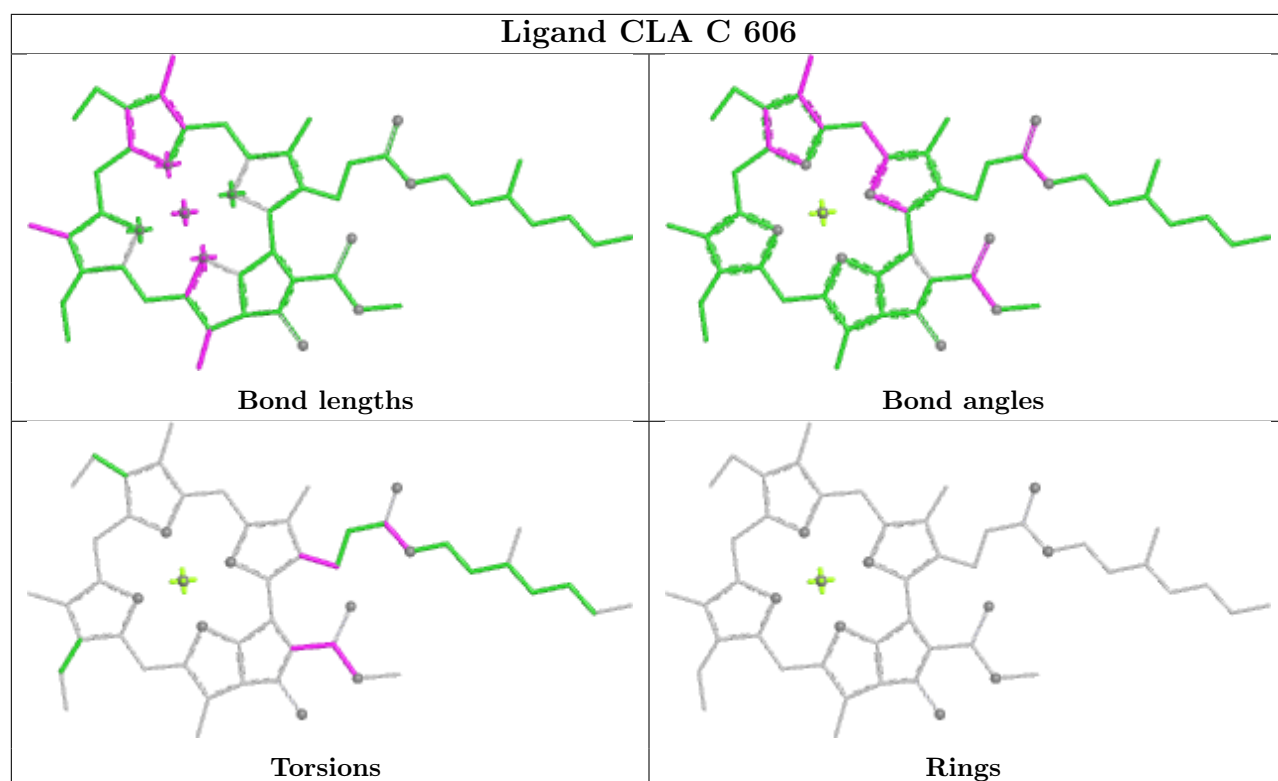


Rings

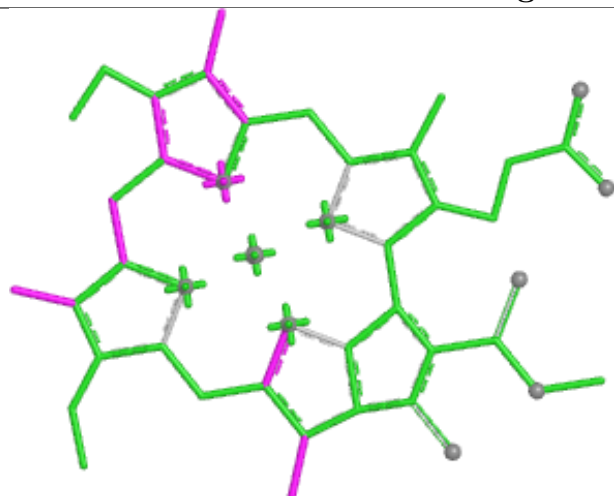




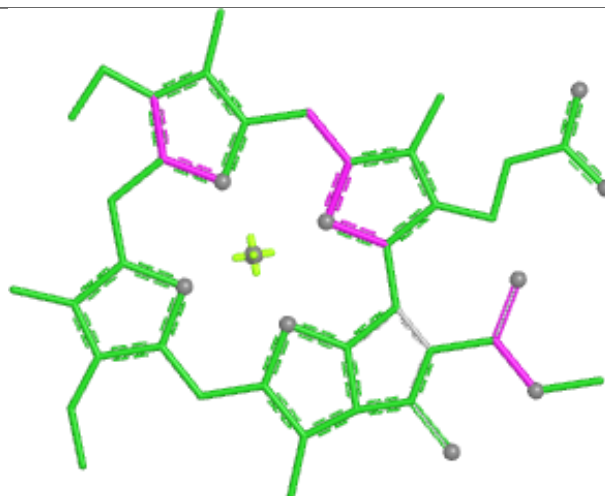




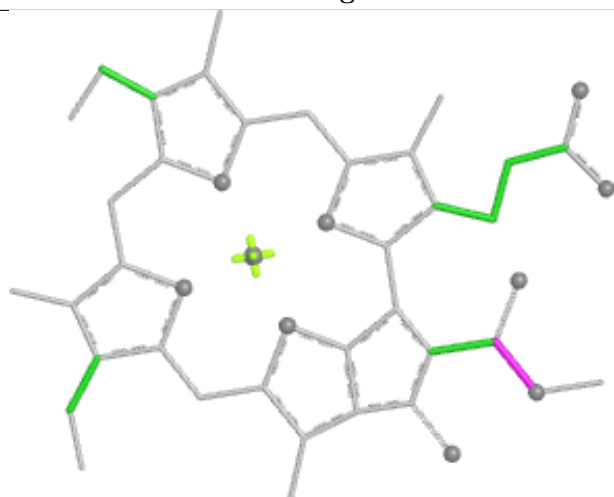
Ligand CLA S 610



Bond lengths



Bond angles

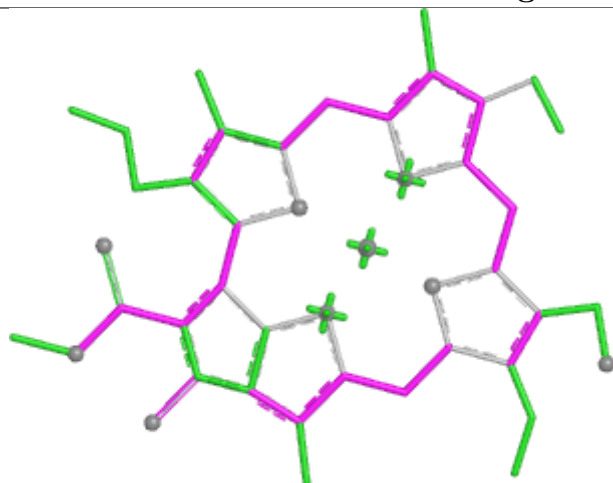


Torsions

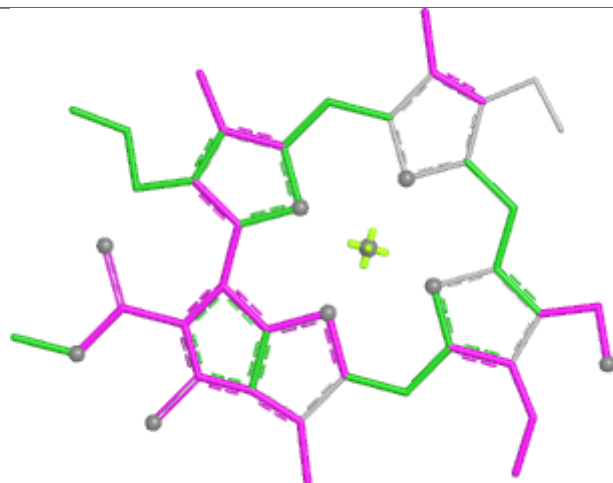


Rings

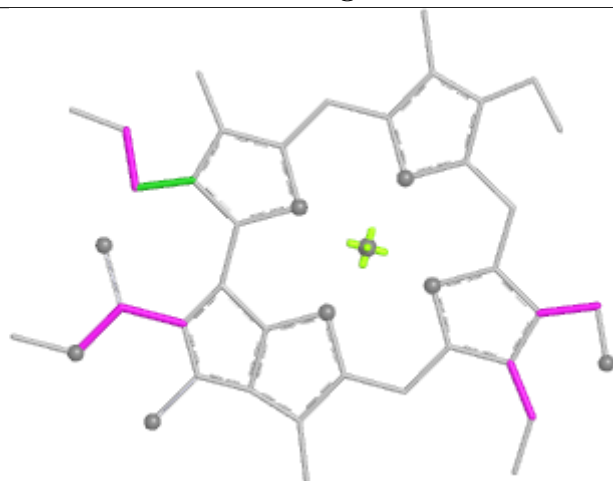
Ligand CHL 5 305



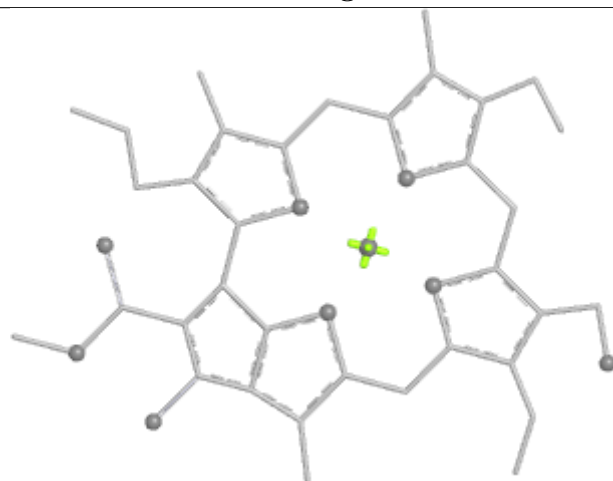
Bond lengths



Bond angles

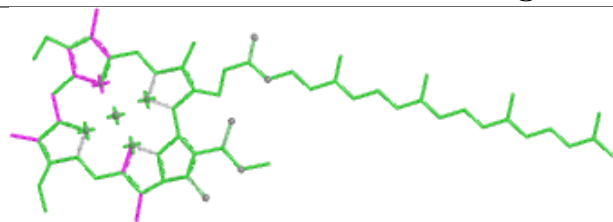


Torsions

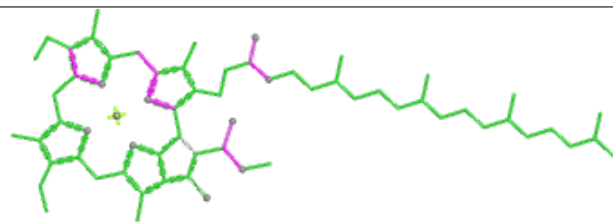


Rings

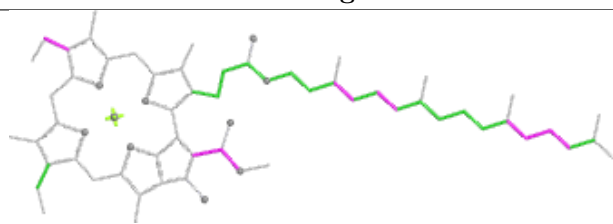
Ligand CLA b 605



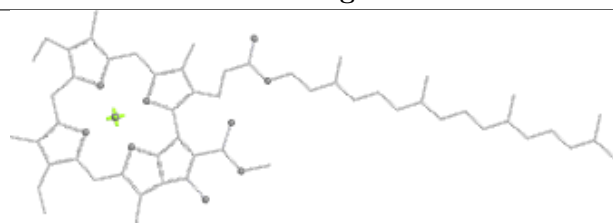
Bond lengths



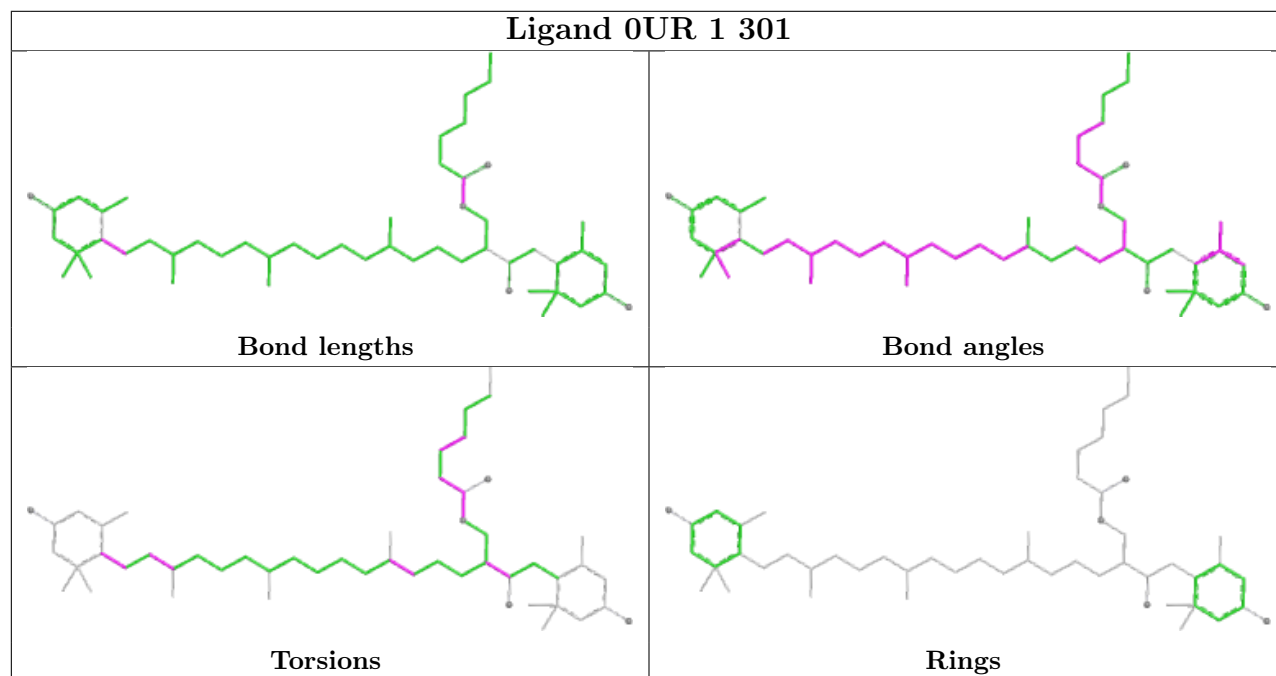
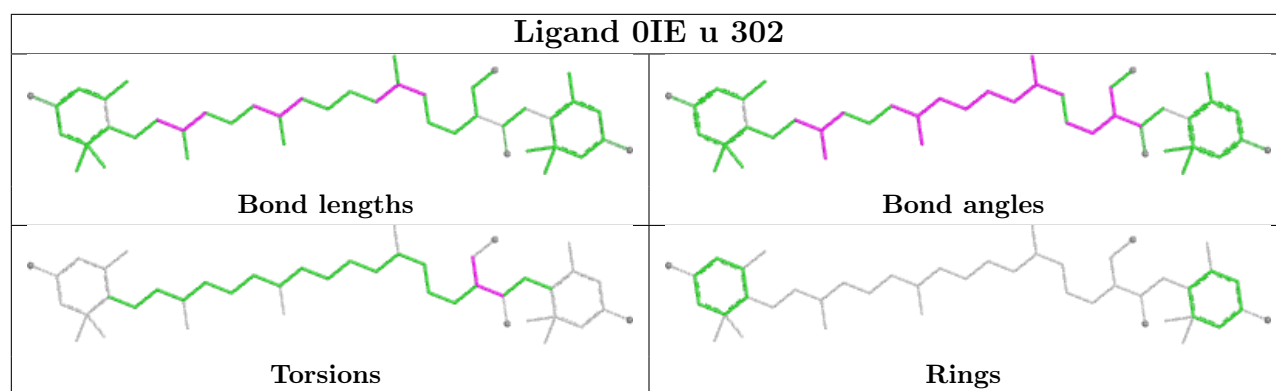
Bond angles



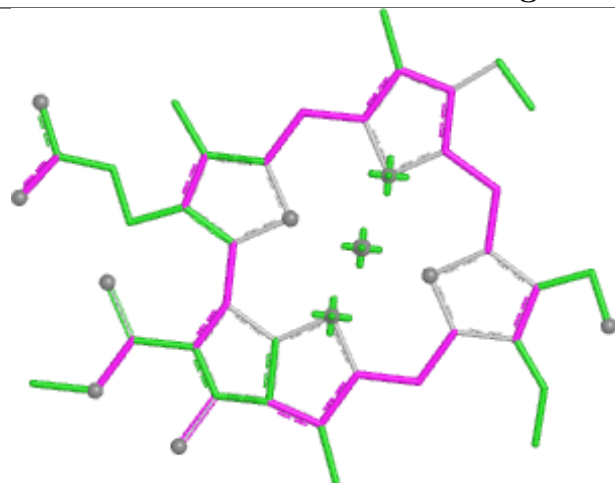
Torsions



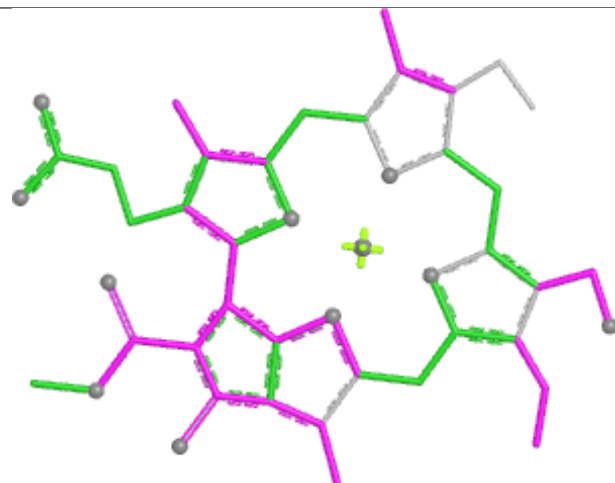
Rings



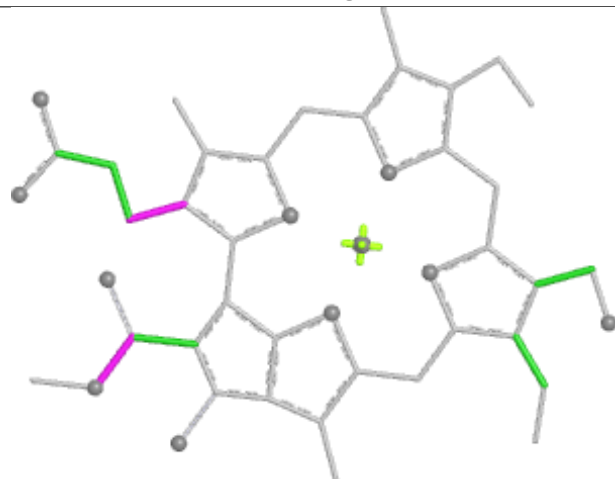
Ligand CHL 9 310



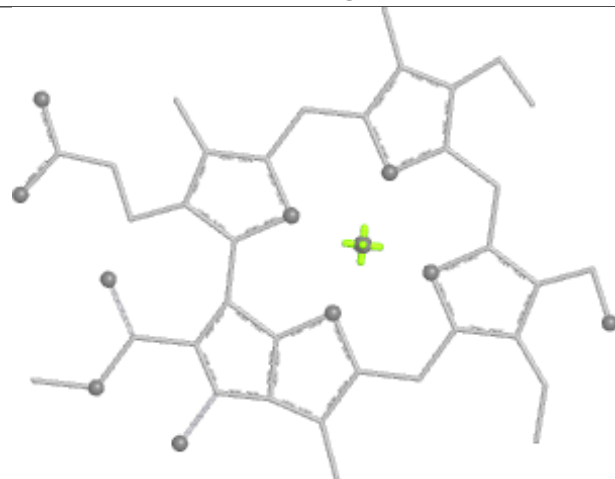
Bond lengths



Bond angles

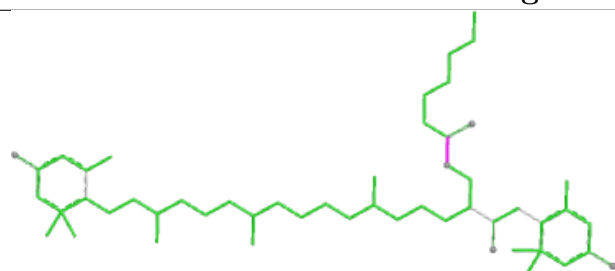


Torsions

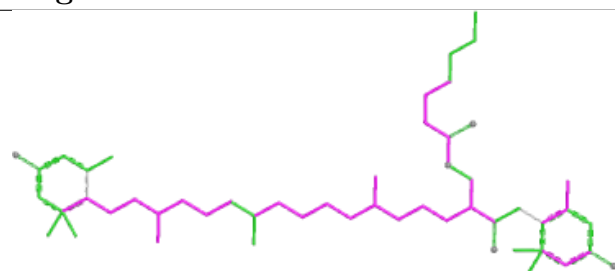


Rings

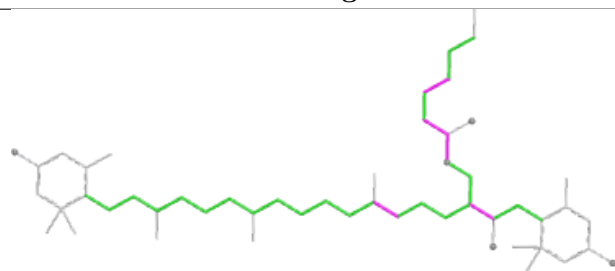
Ligand OUR g 301



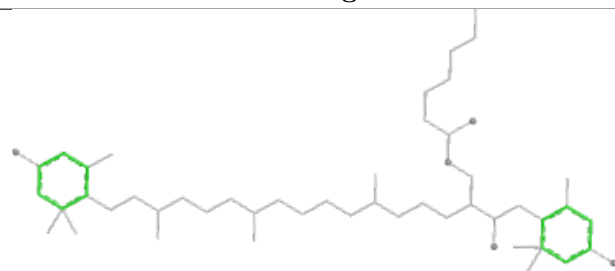
Bond lengths



Bond angles

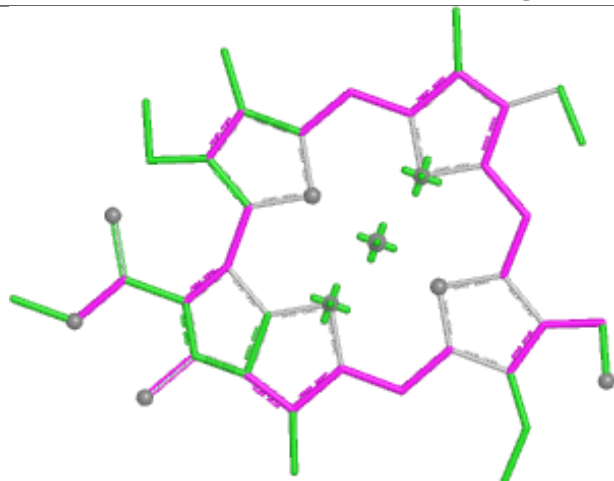


Torsions

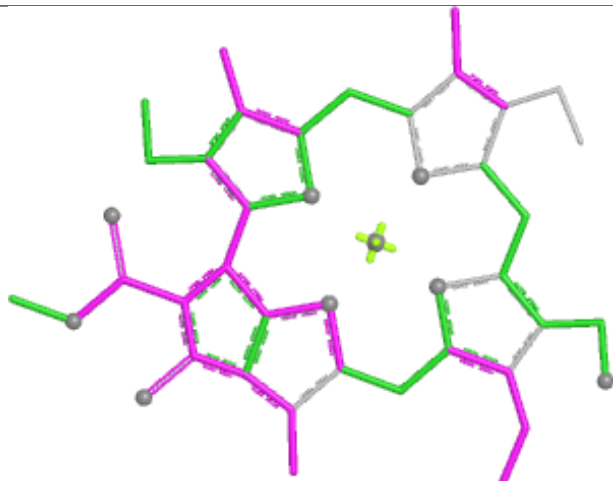


Rings

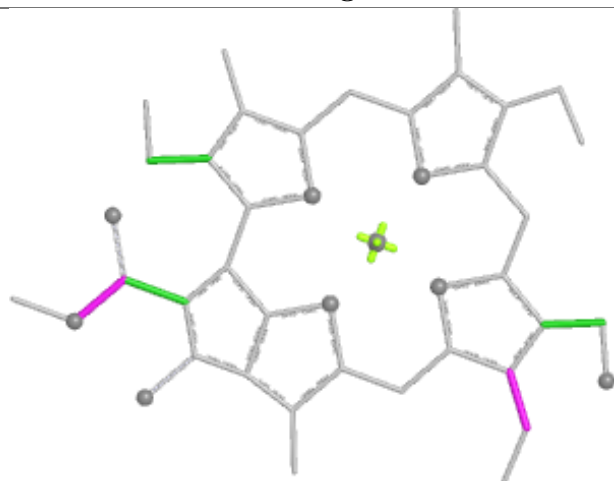
Ligand CHL 9 312



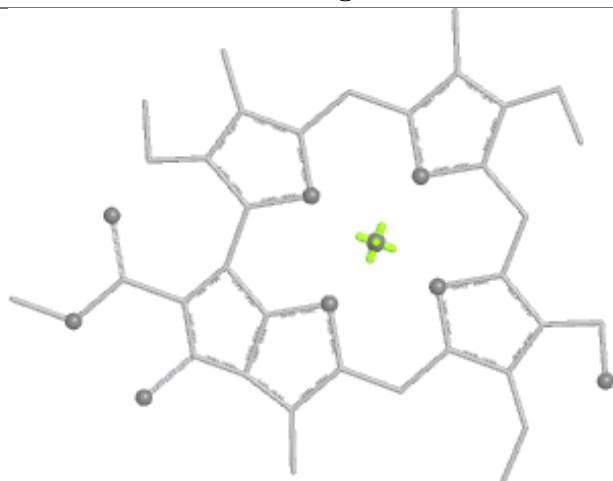
Bond lengths



Bond angles

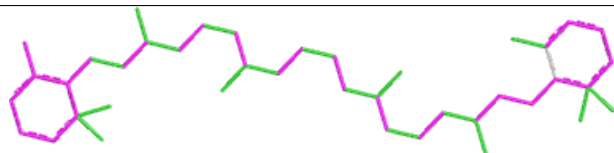


Torsions

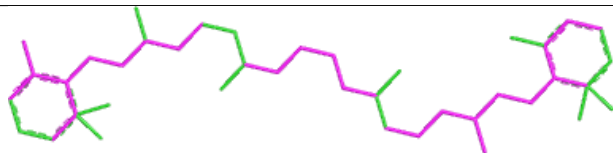


Rings

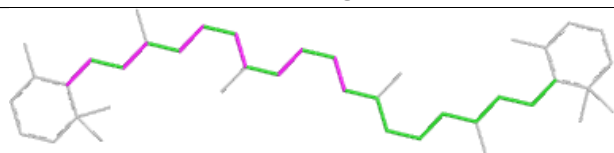
Ligand 8CT A 608



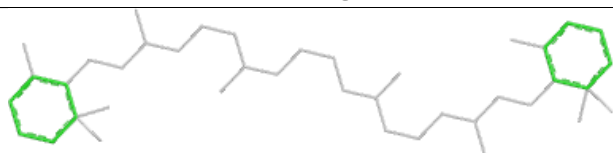
Bond lengths



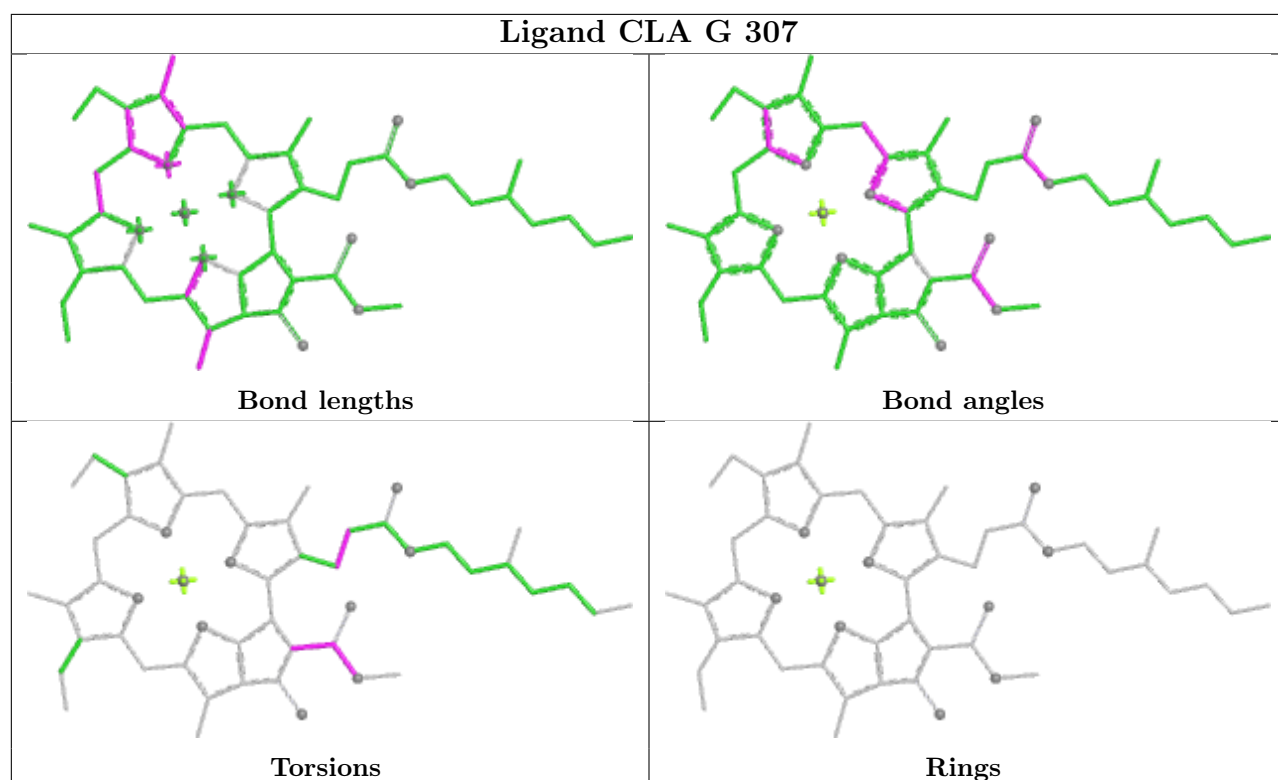
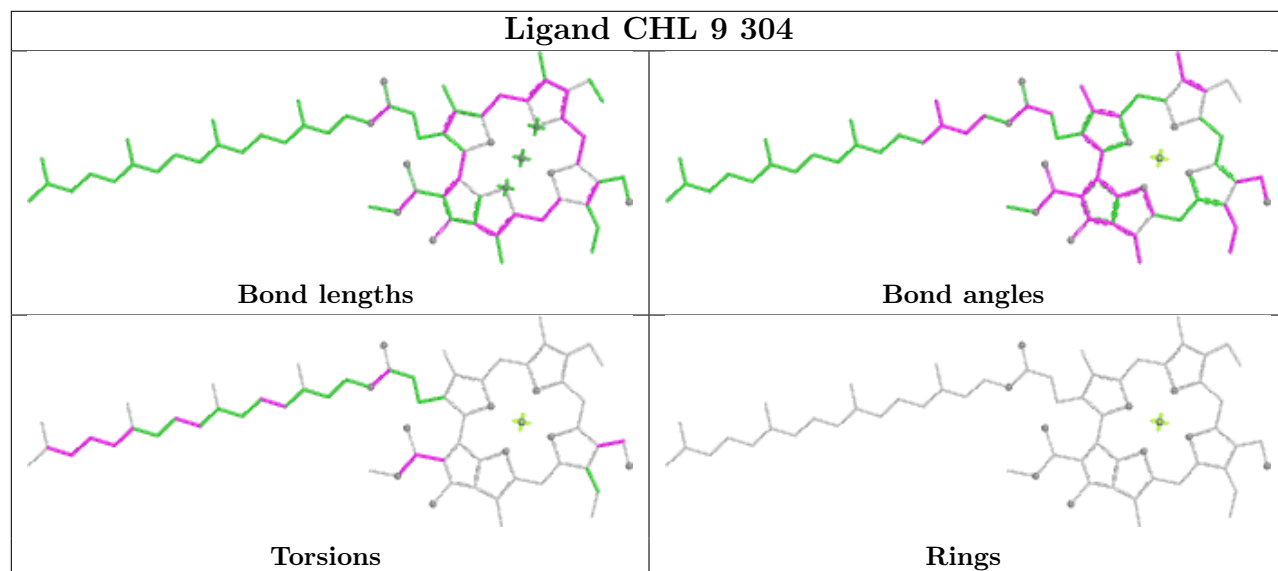
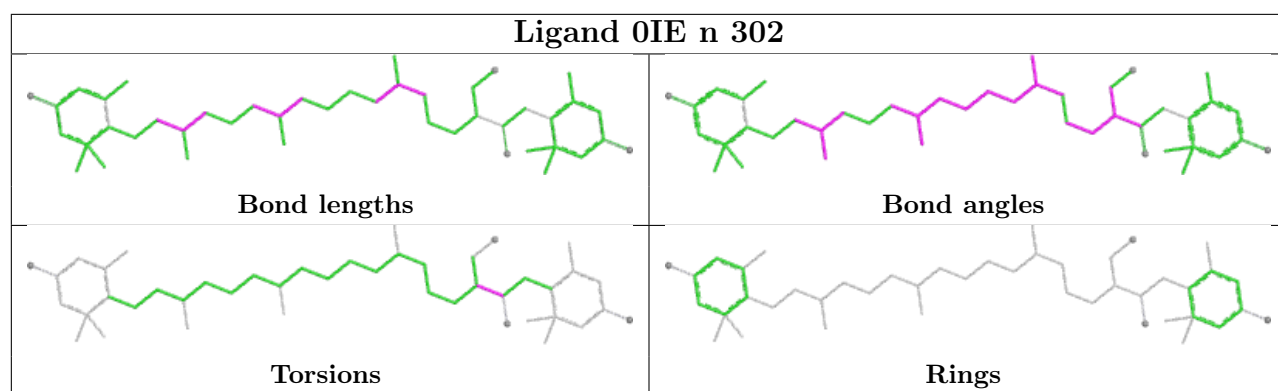
Bond angles



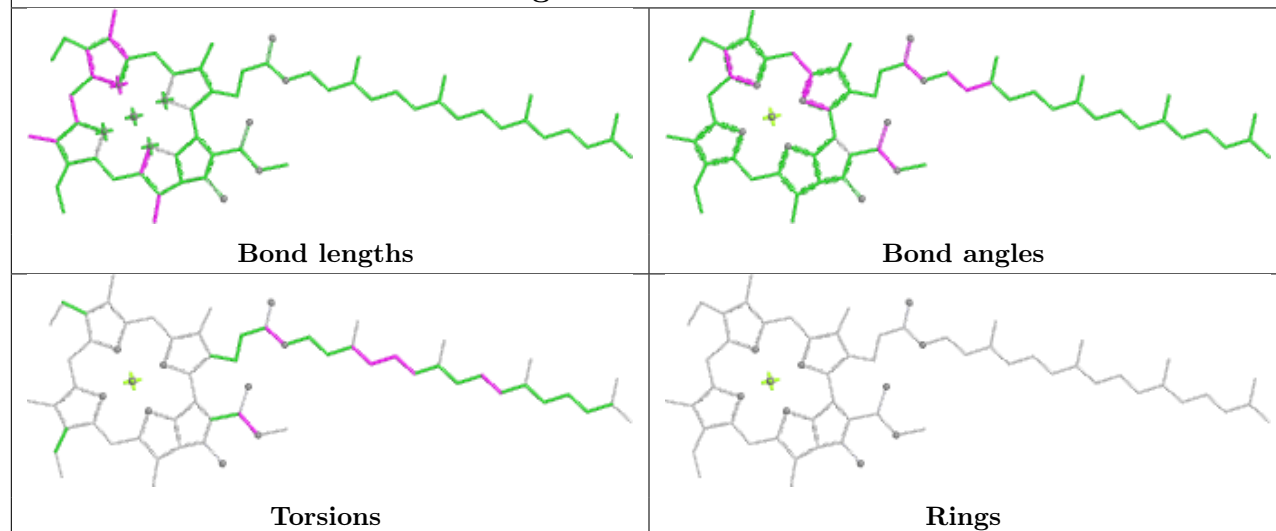
Torsions



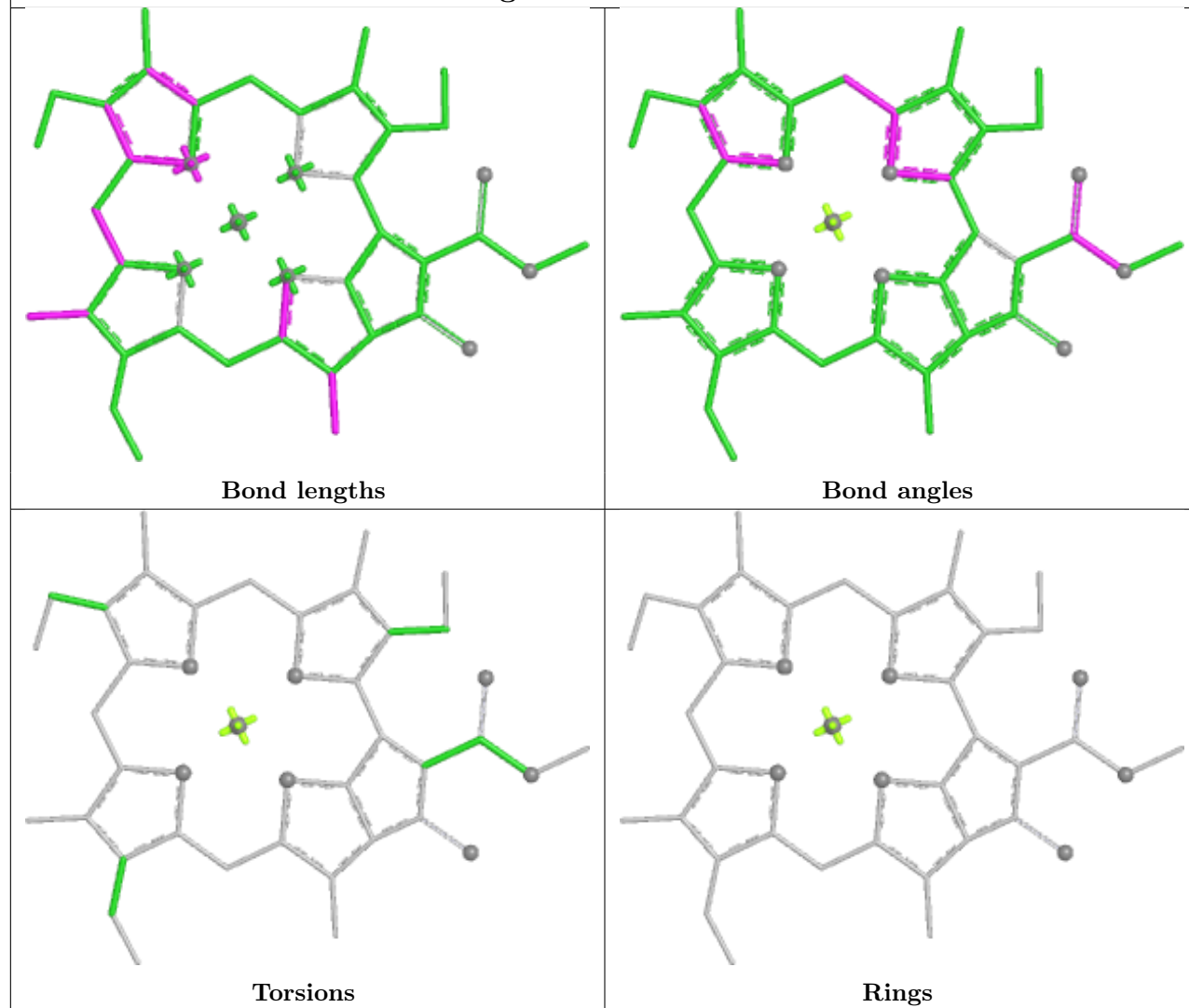
Rings

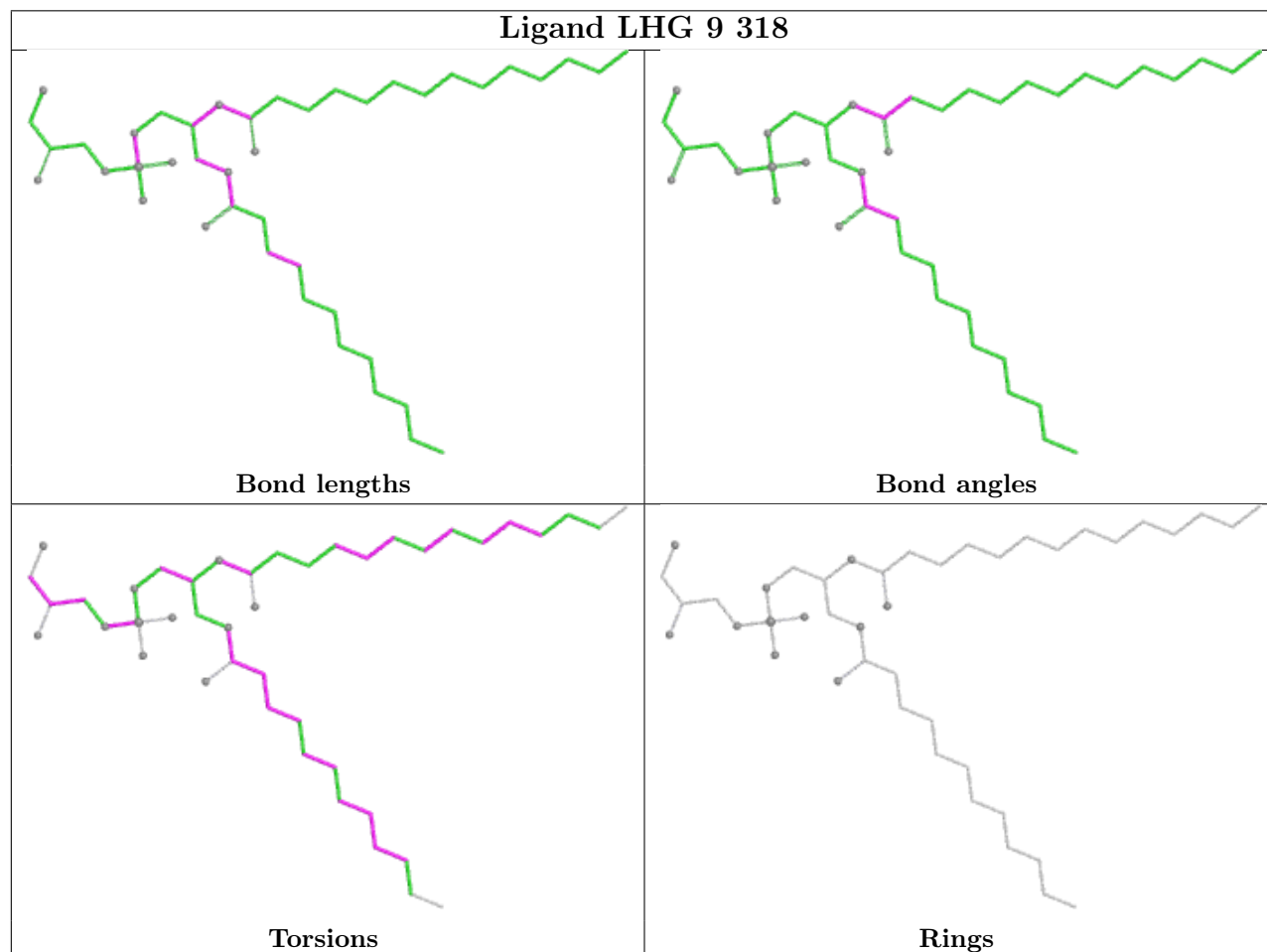
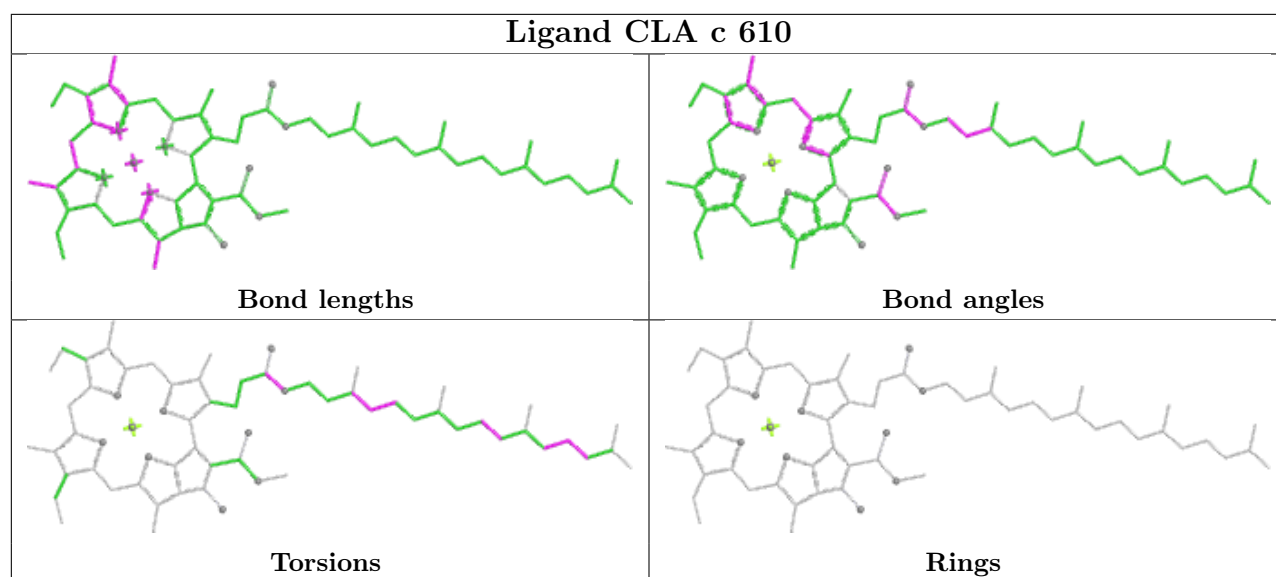


Ligand CLA B 613

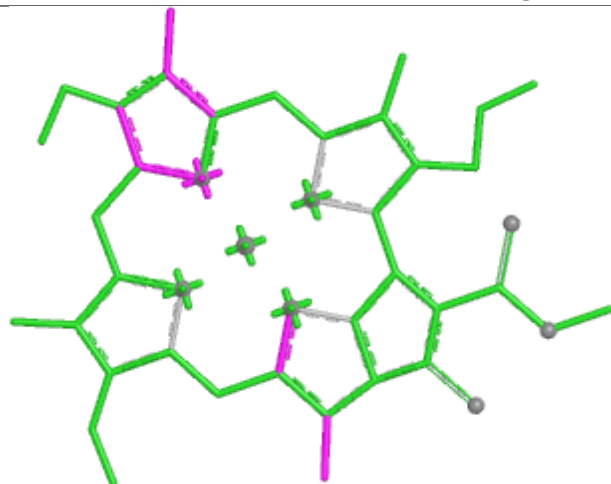


Ligand CLA 4 316

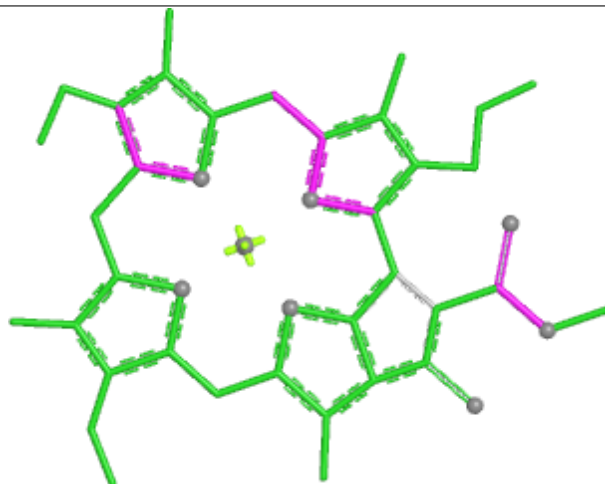




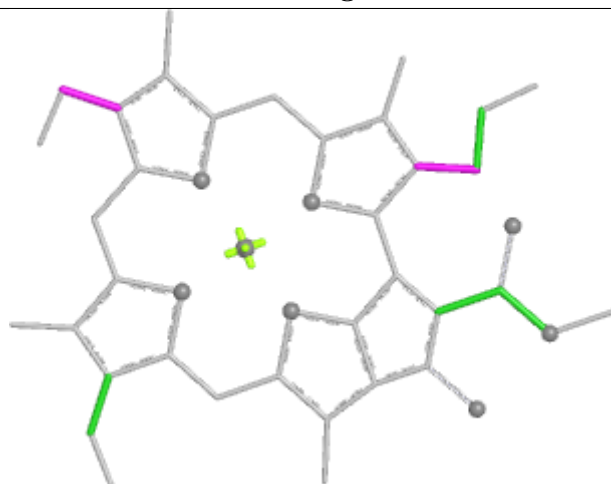
Ligand CLA S 604



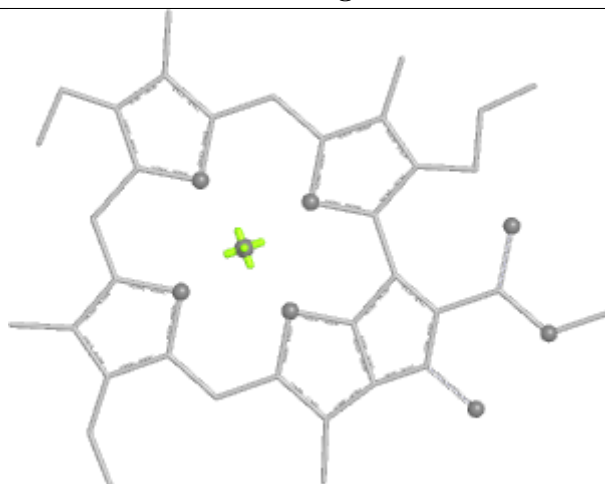
Bond lengths



Bond angles

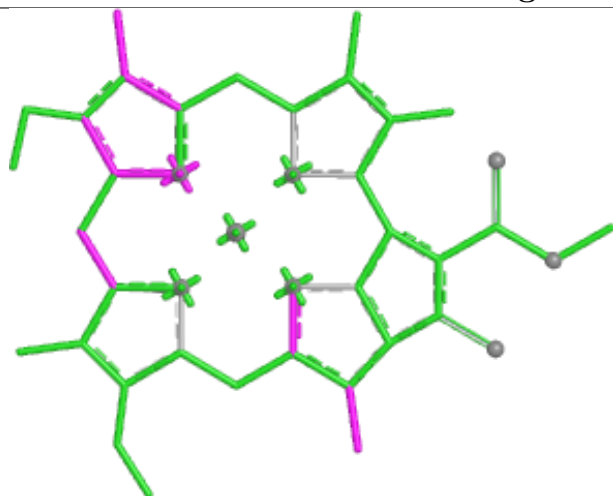


Torsions

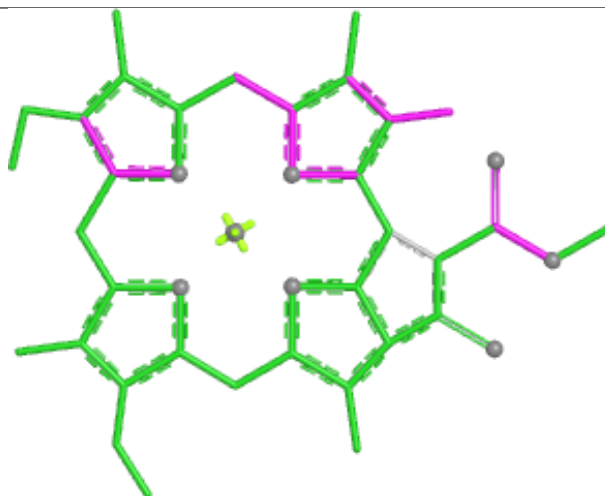


Rings

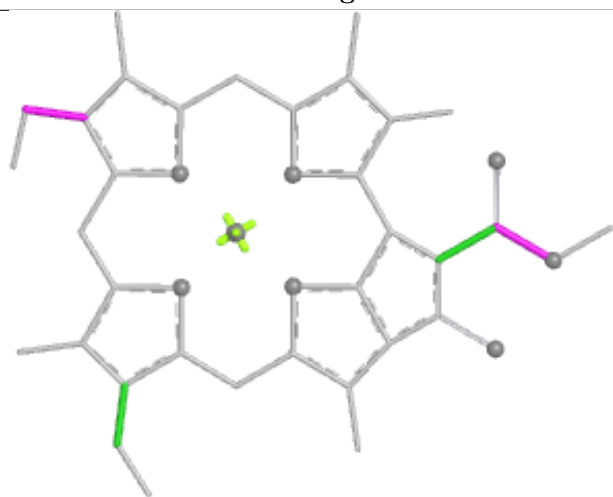
Ligand CLA 1 314



Bond lengths



Bond angles

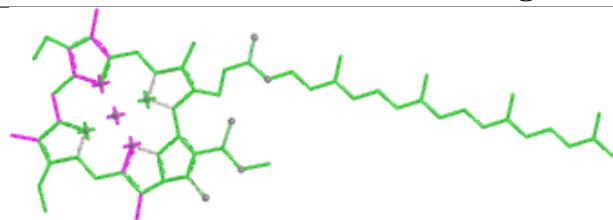


Torsions

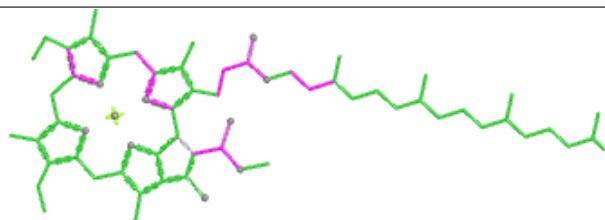


Rings

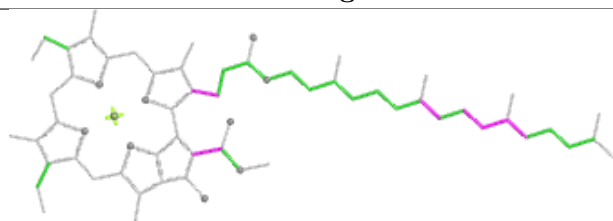
Ligand CLA d 404



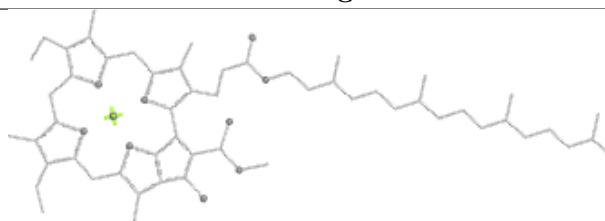
Bond lengths



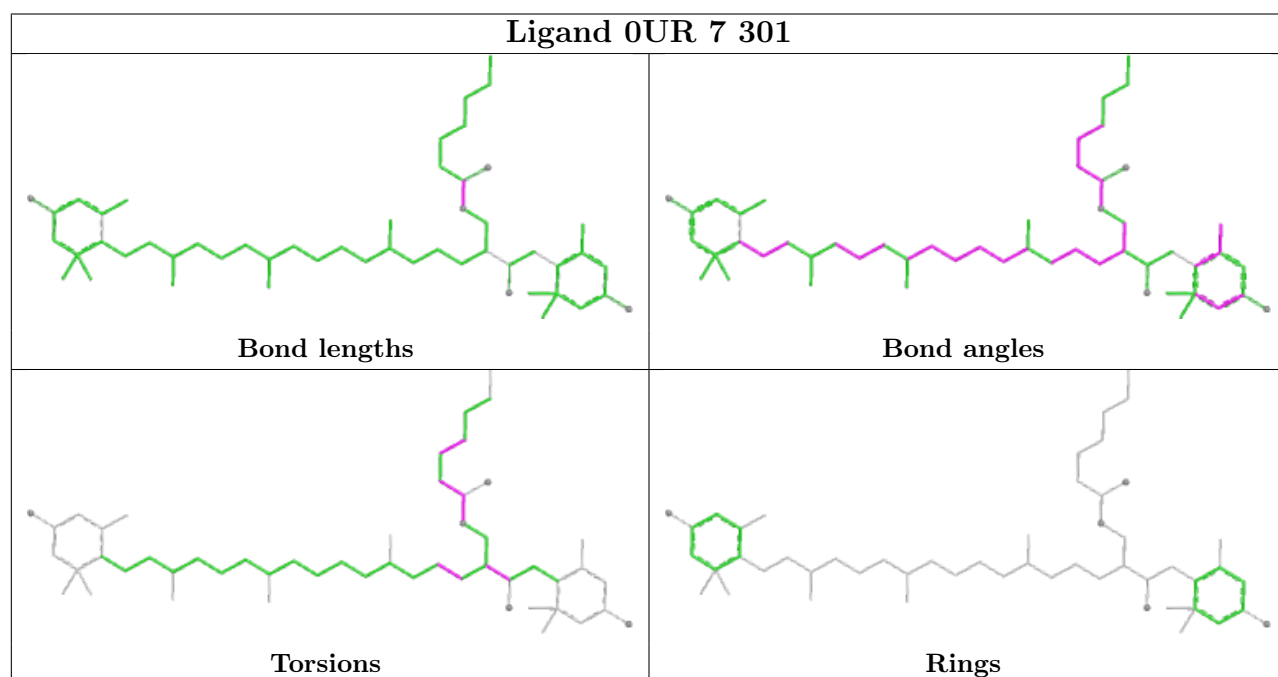
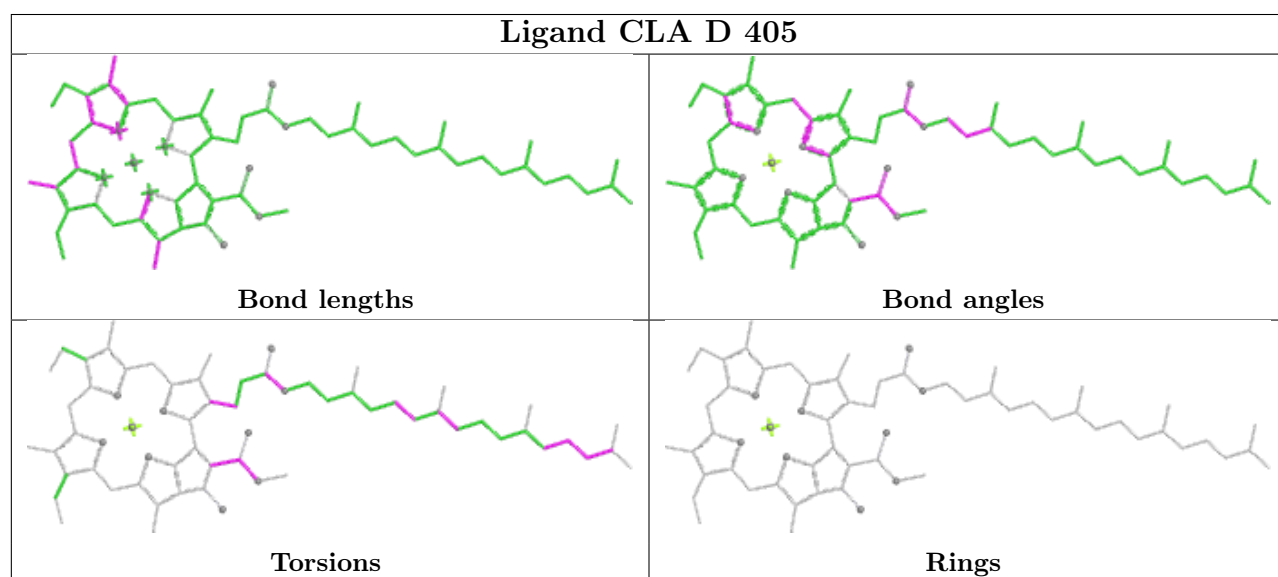
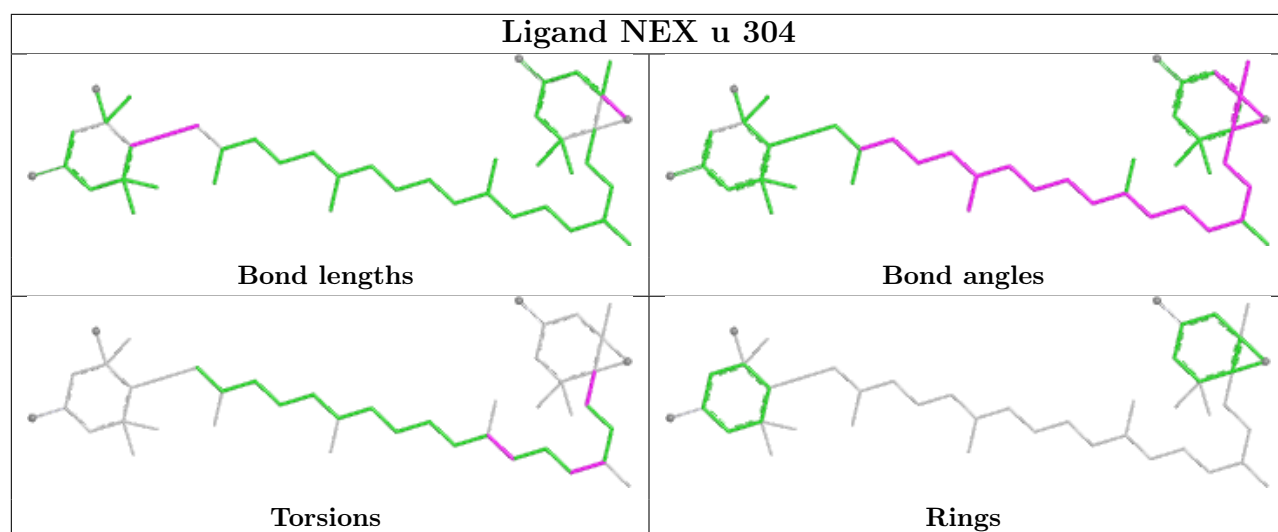
Bond angles



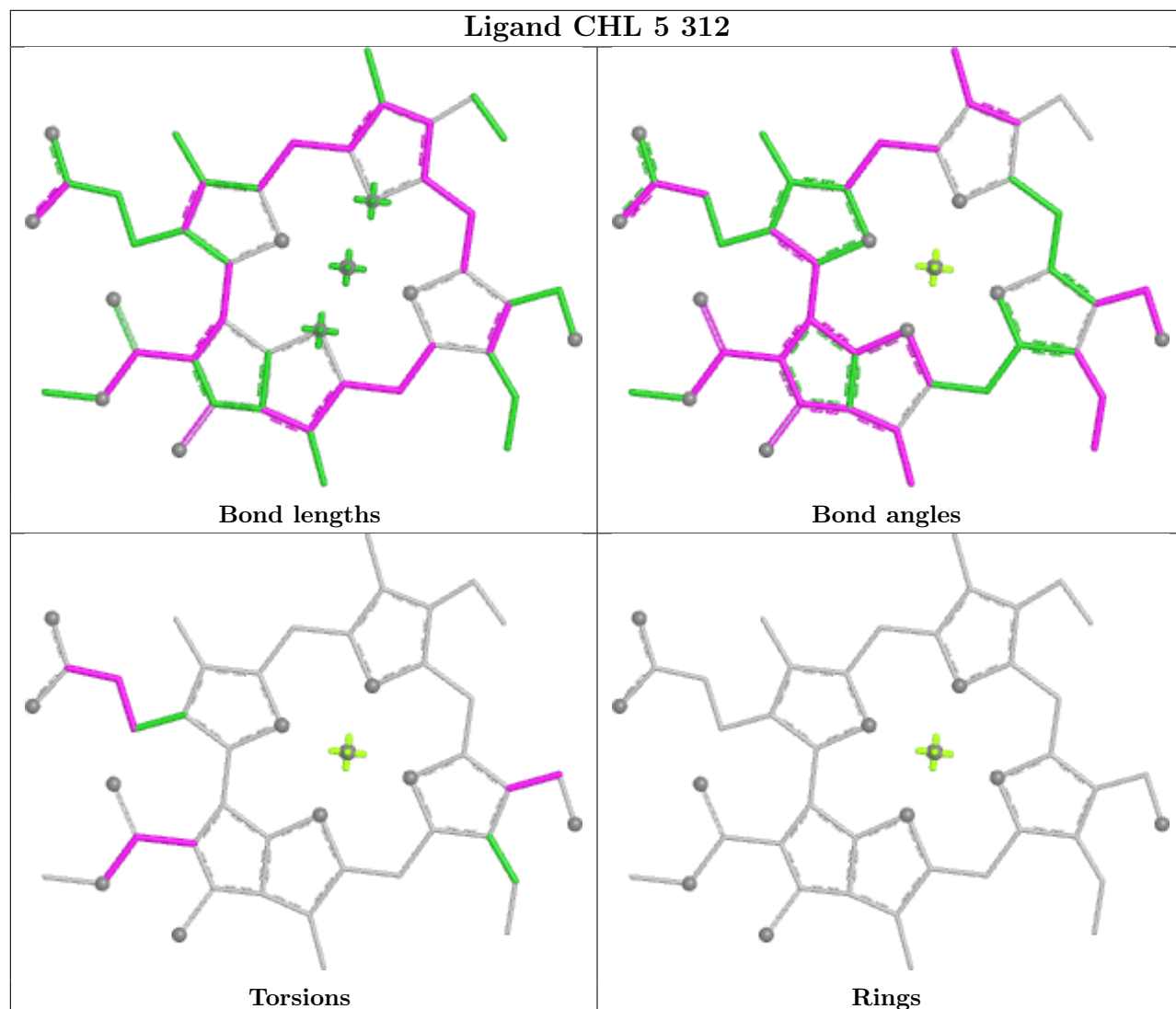
Torsions

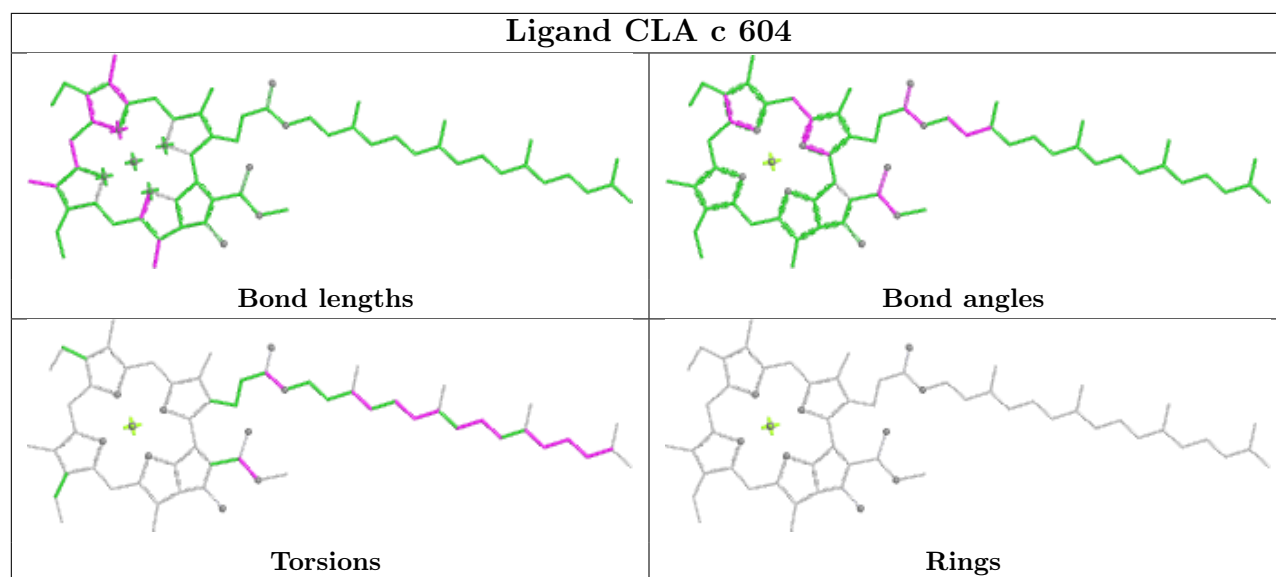
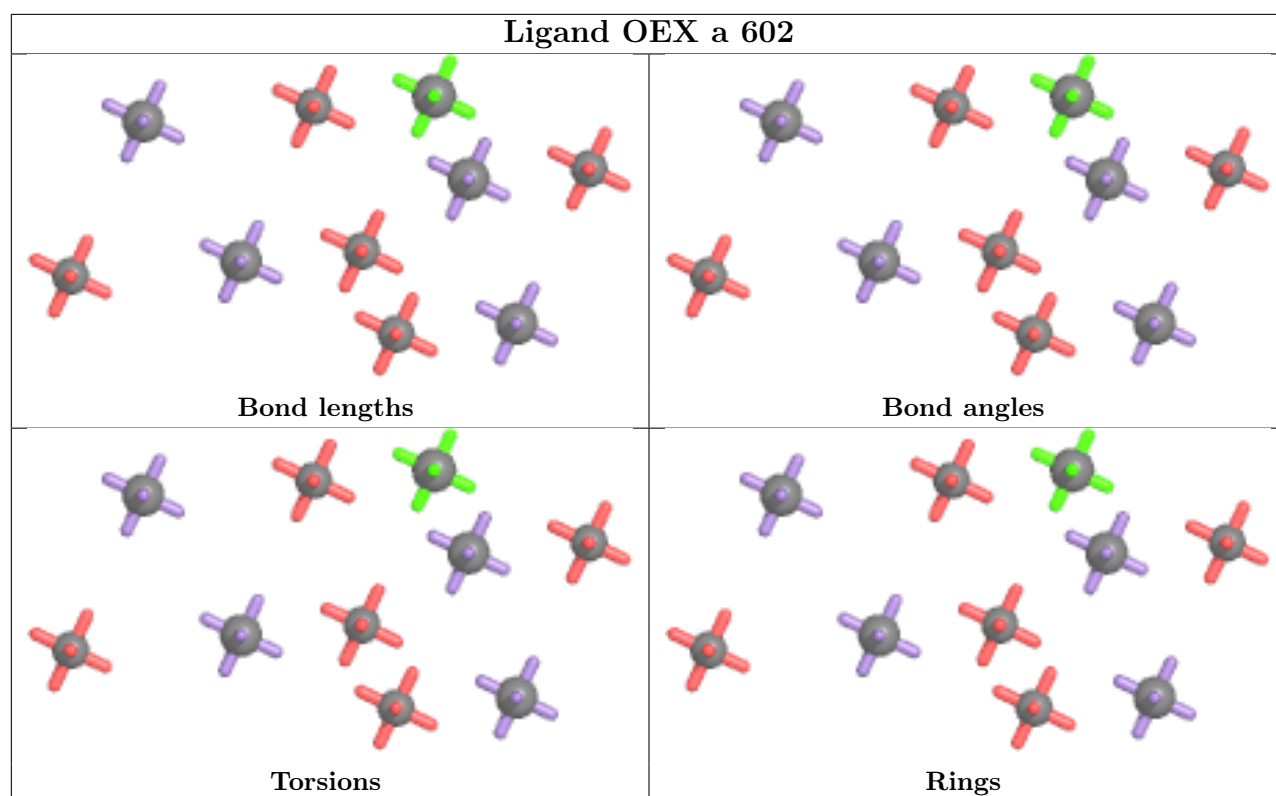


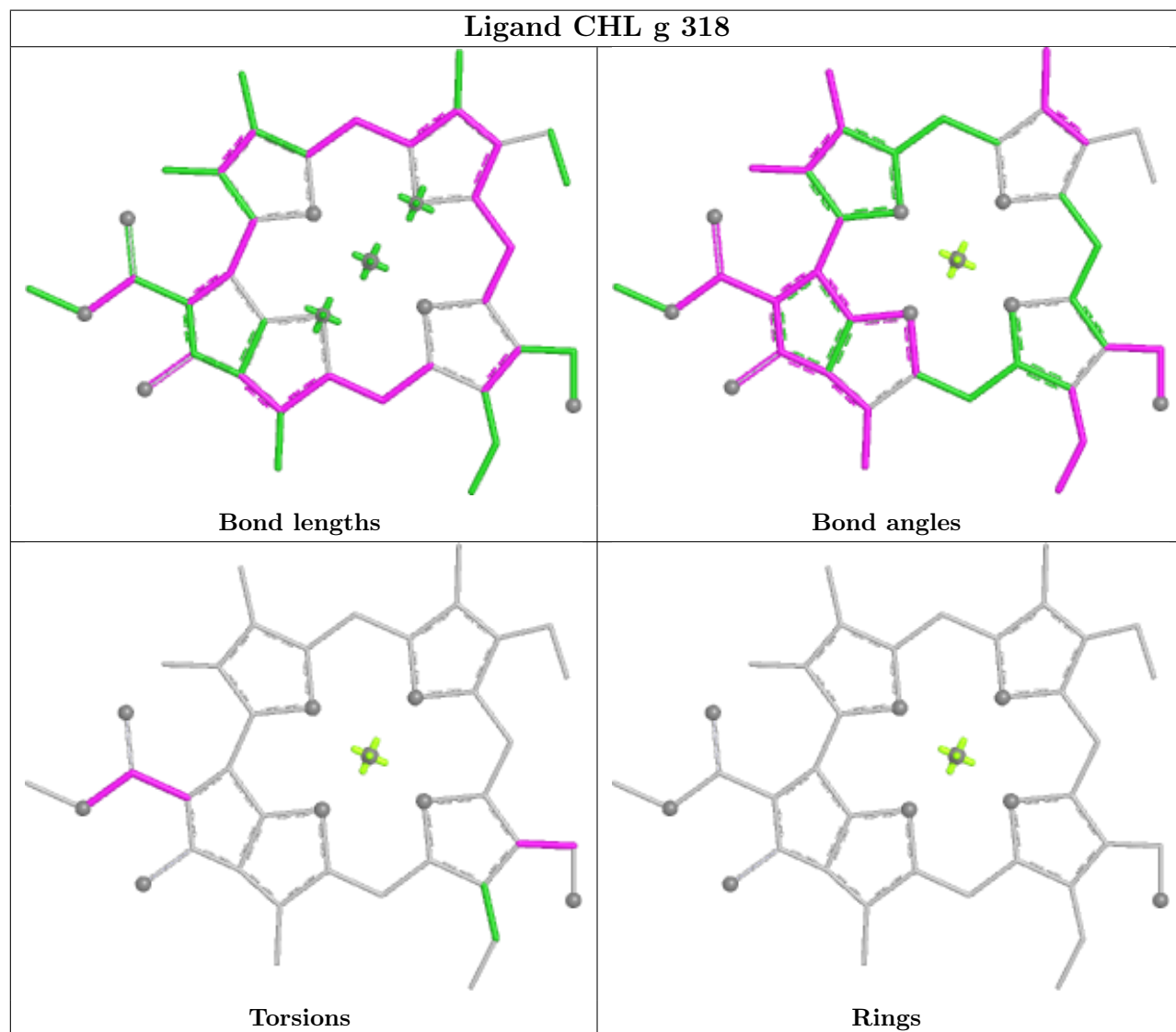
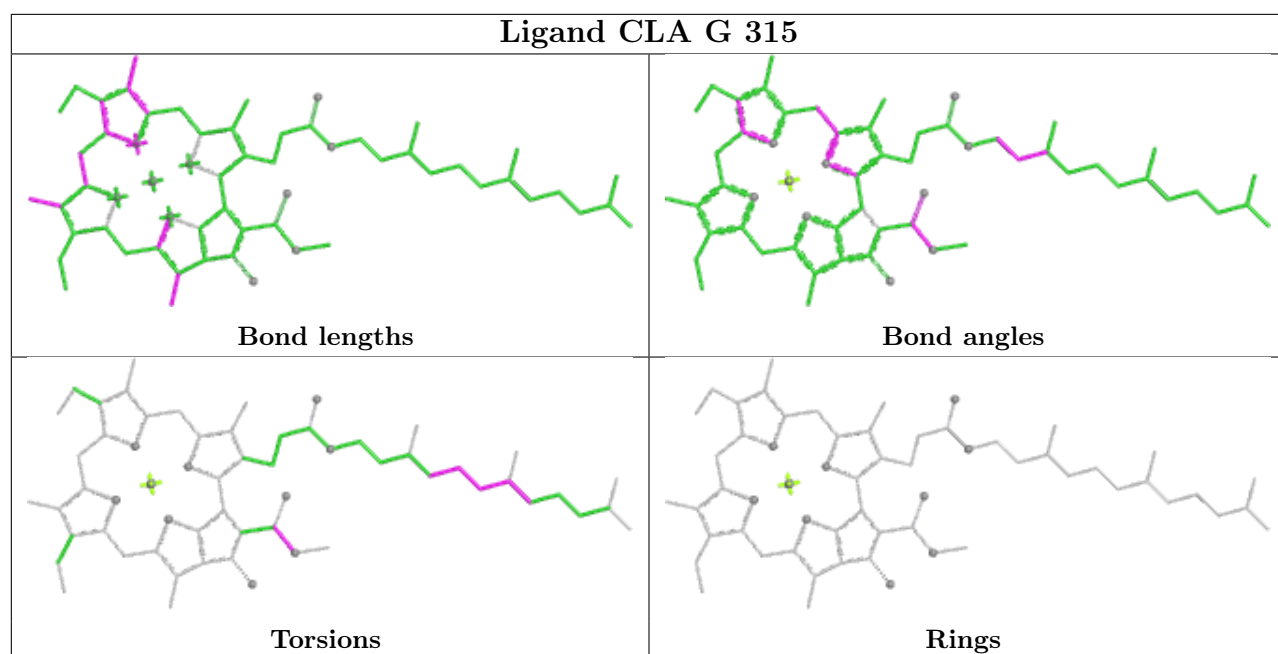
Rings



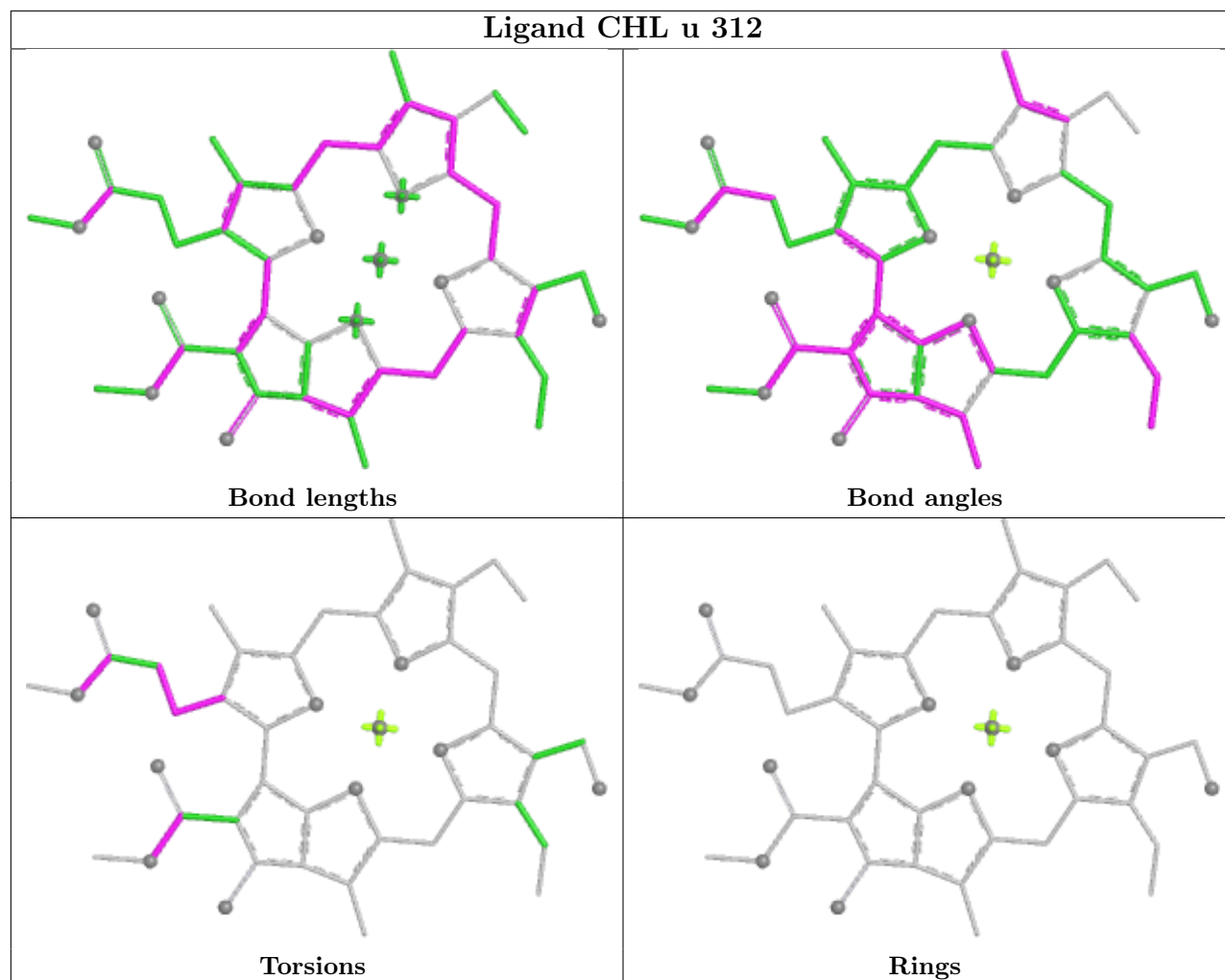
Ligand CHL 5 312



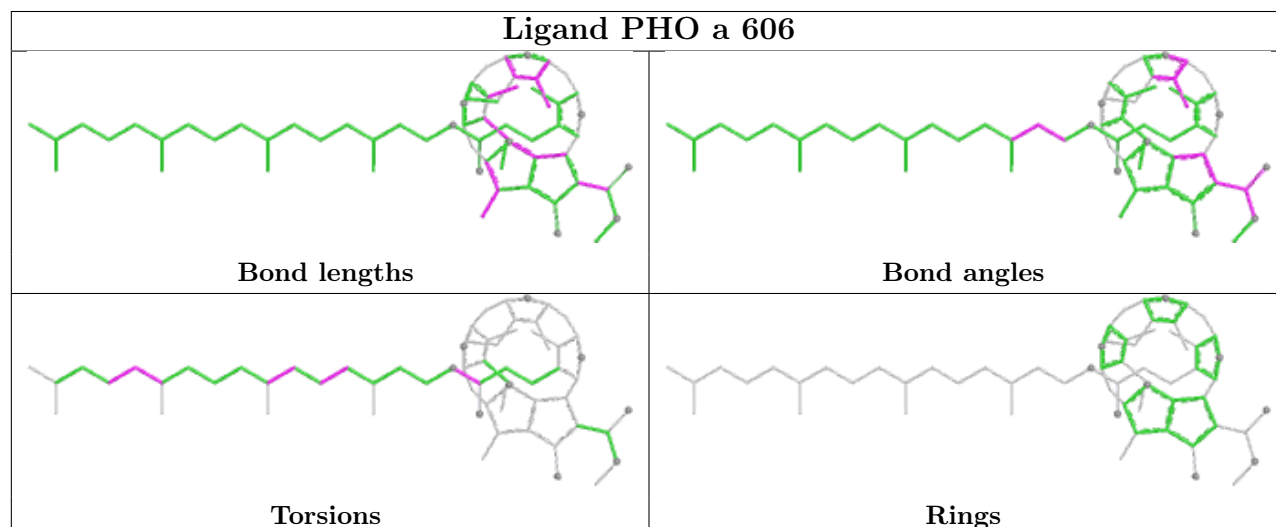


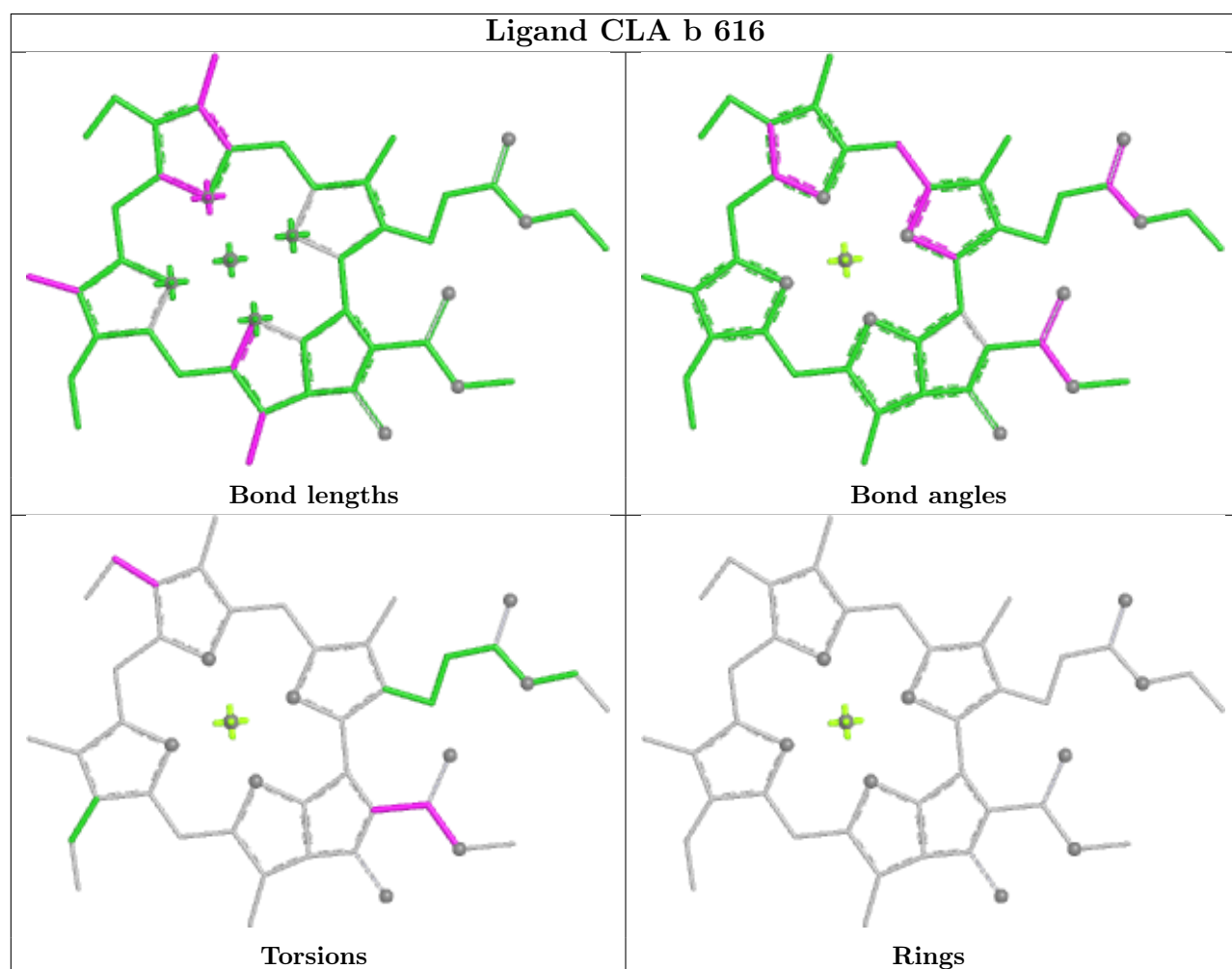
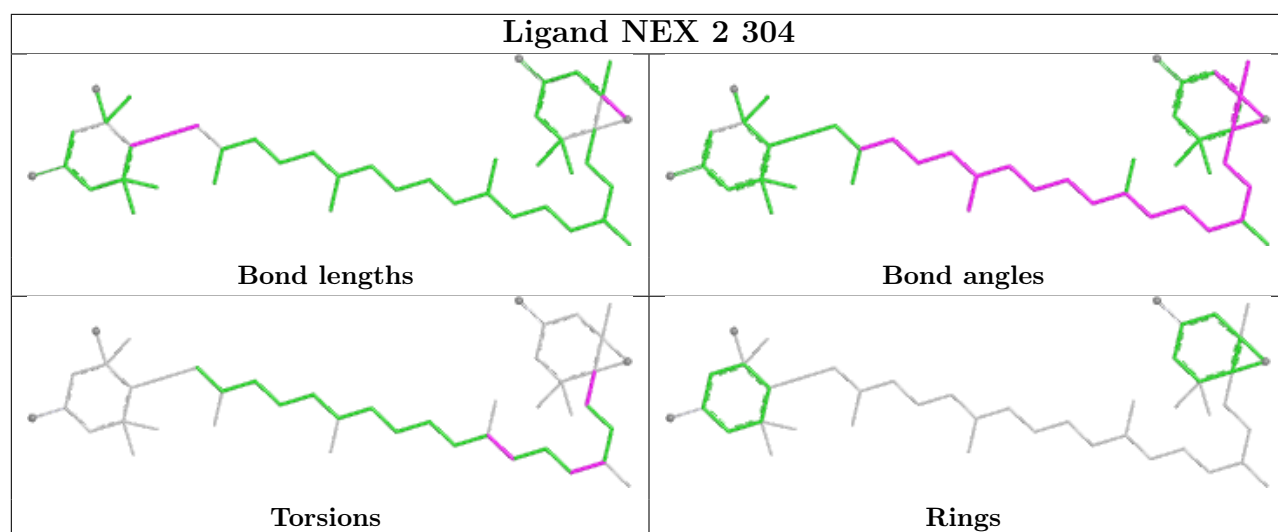


Ligand CHL u 312

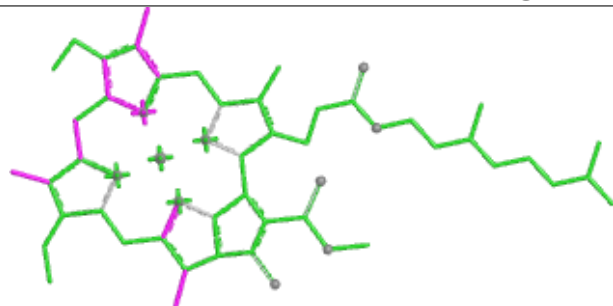


Ligand PHO a 606

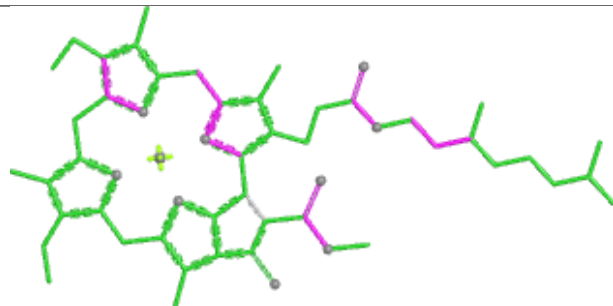




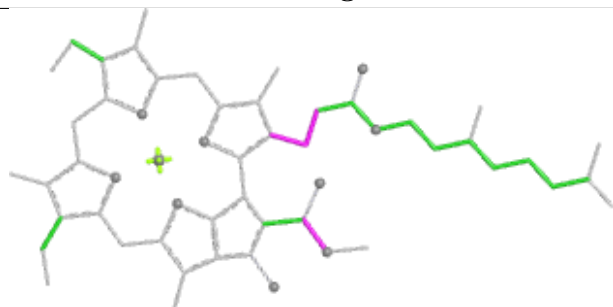
Ligand CLA S 609



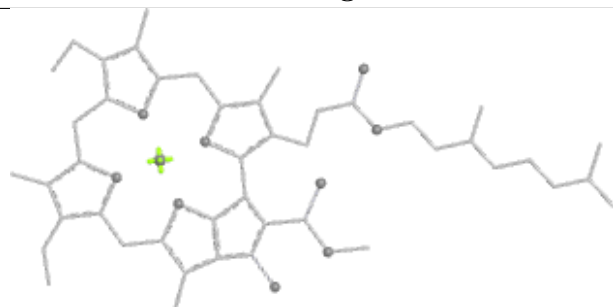
Bond lengths



Bond angles

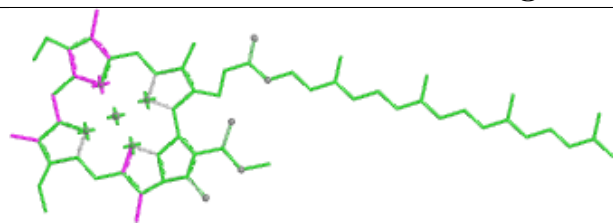


Torsions

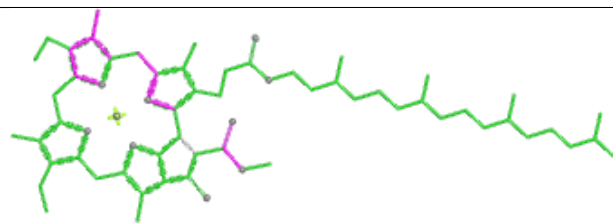


Rings

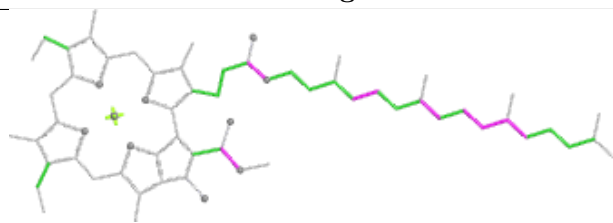
Ligand CLA c 611



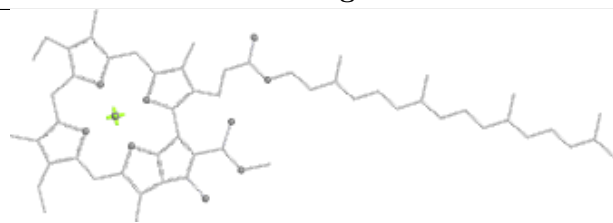
Bond lengths



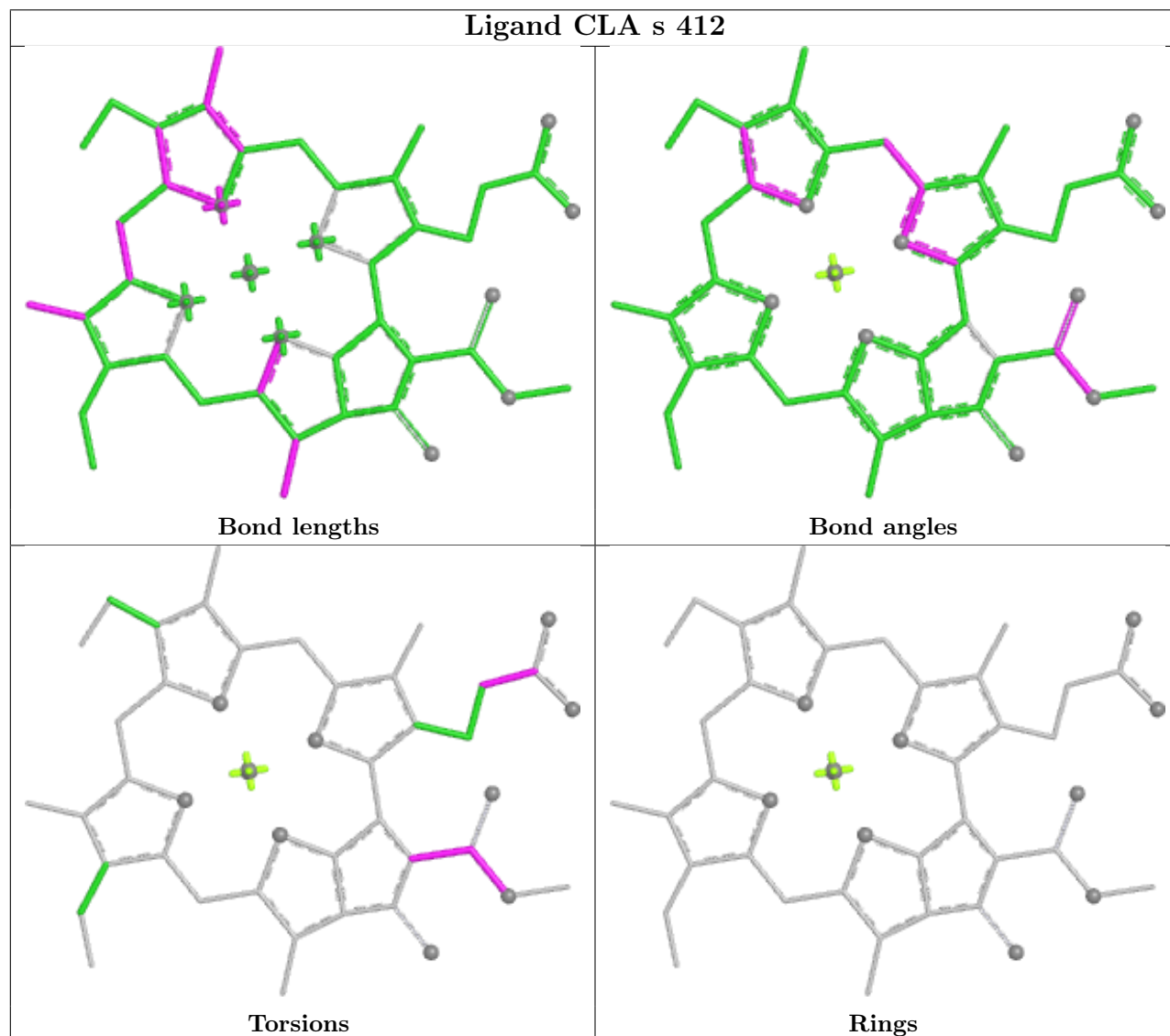
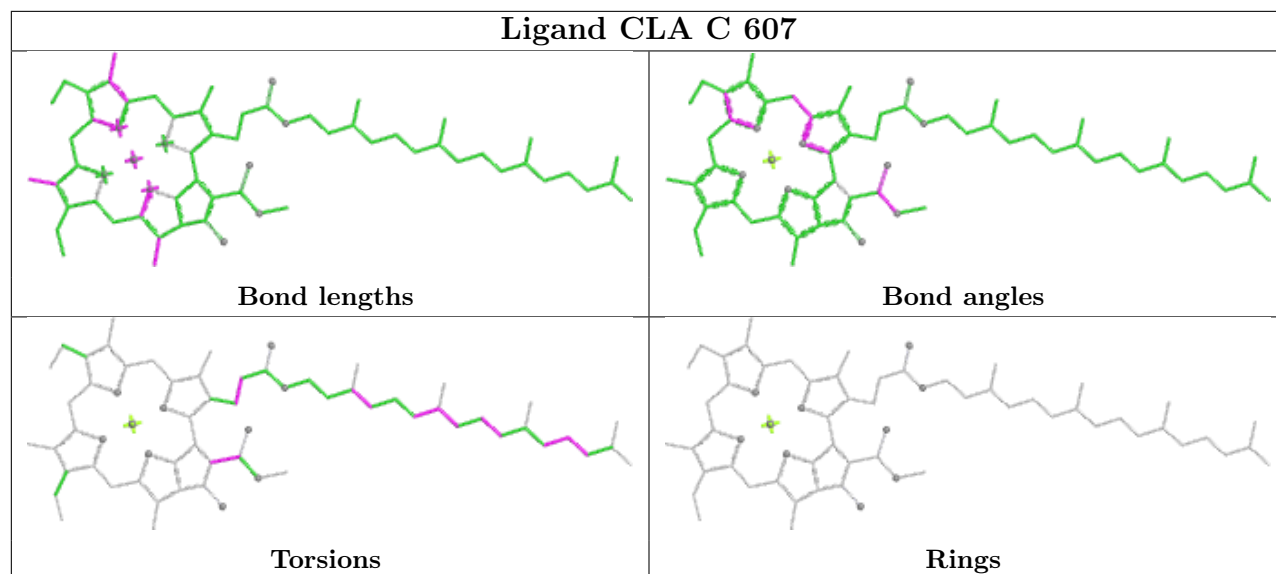
Bond angles



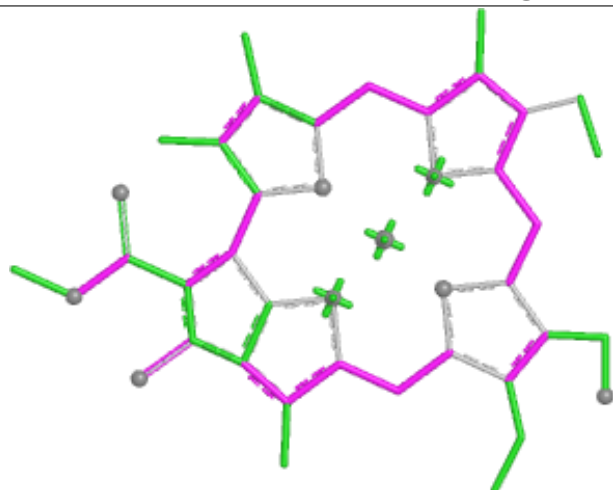
Torsions



Rings



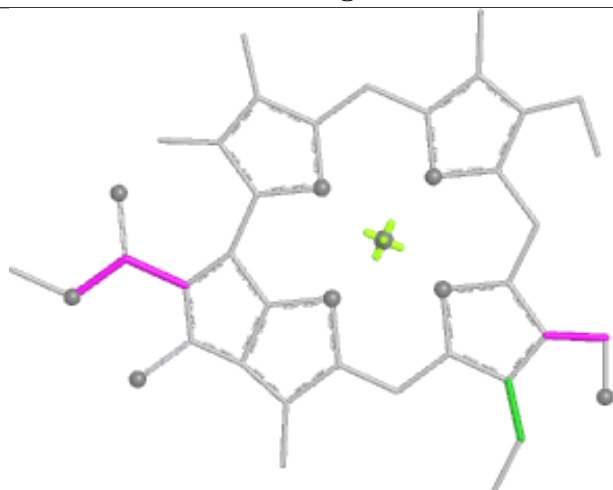
Ligand CHL 1 317



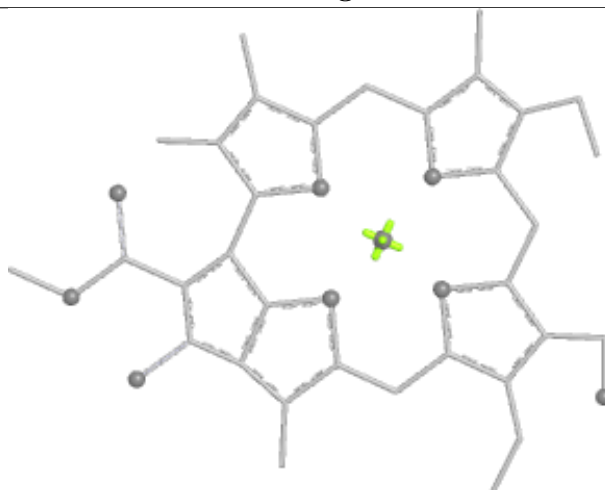
Bond lengths



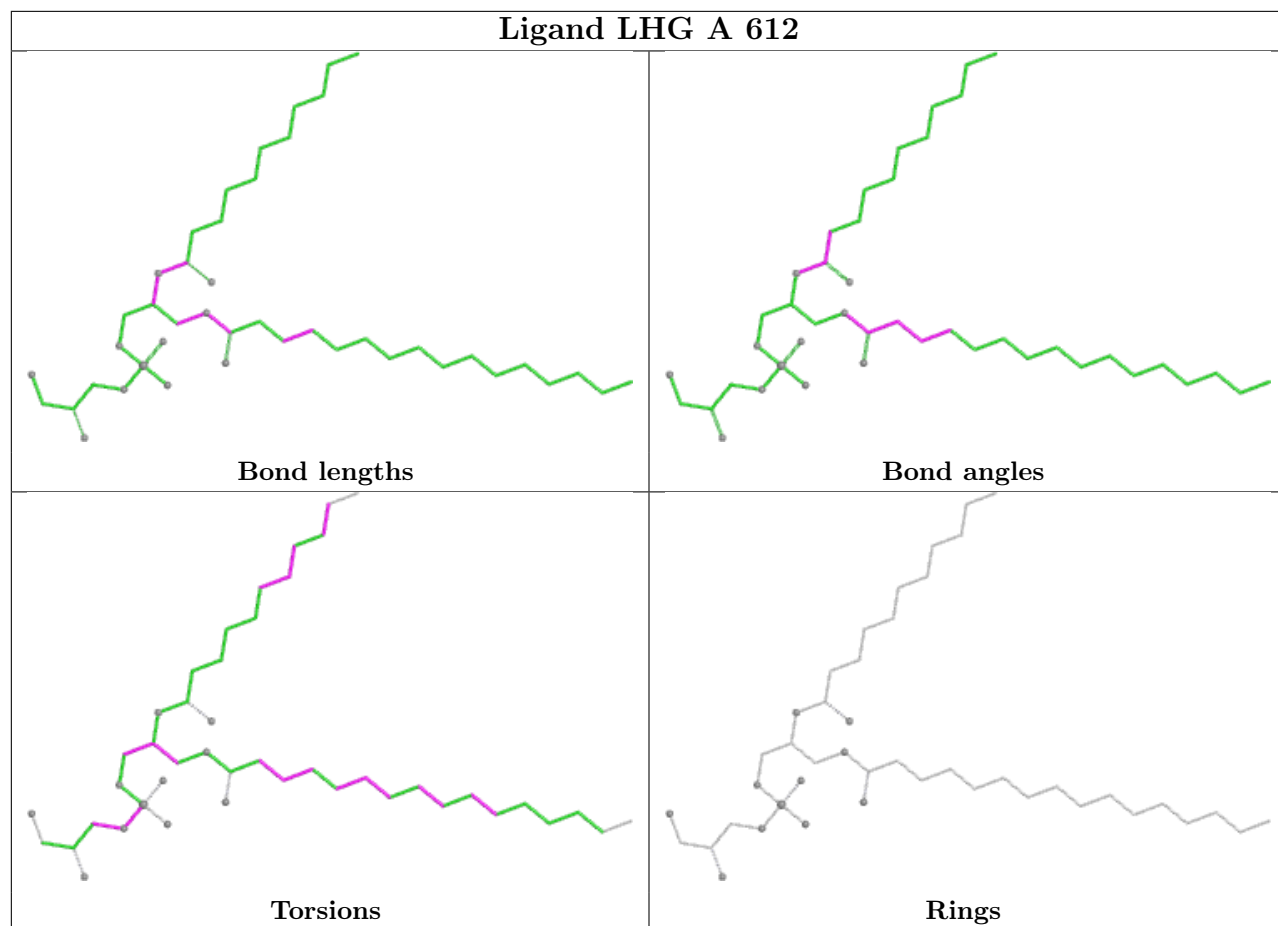
Bond angles



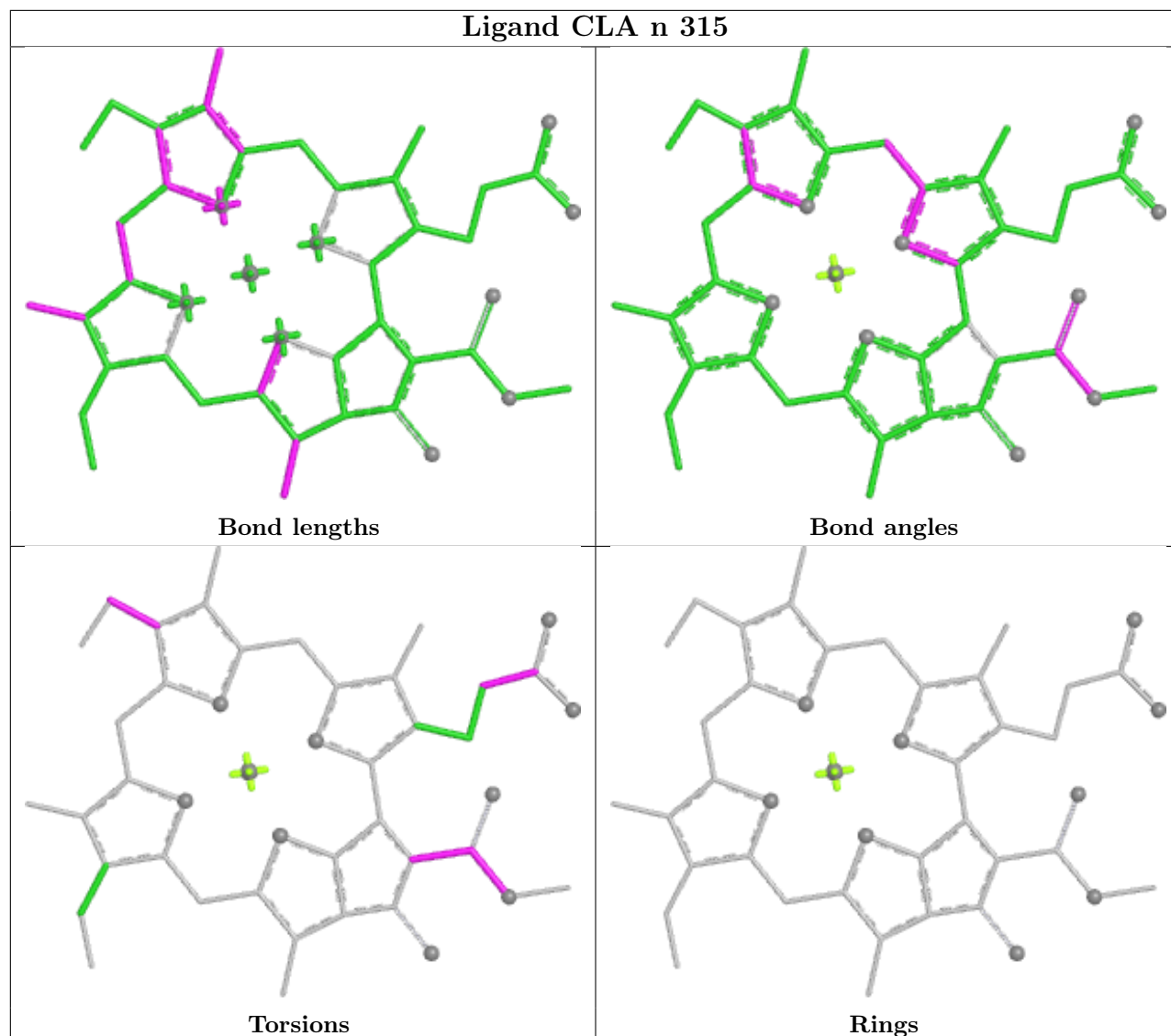
Torsions



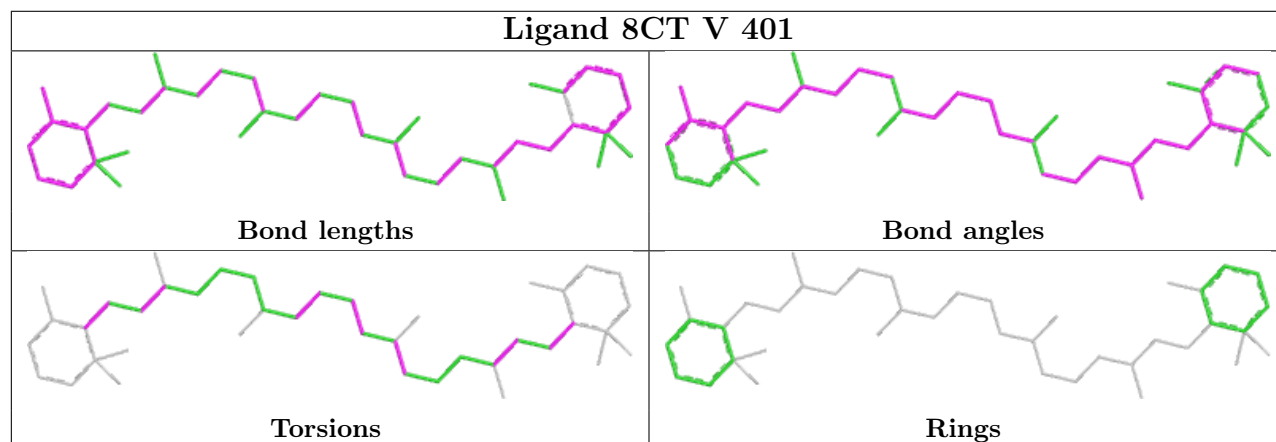
Rings




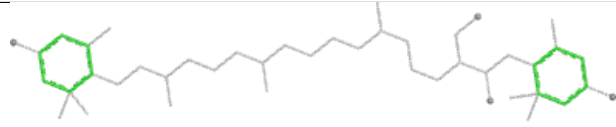


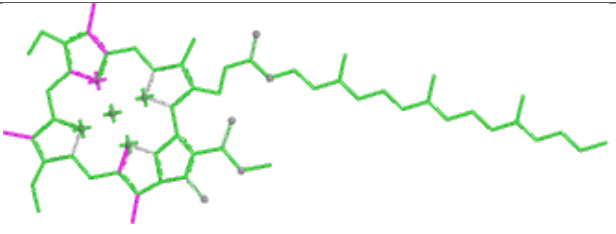
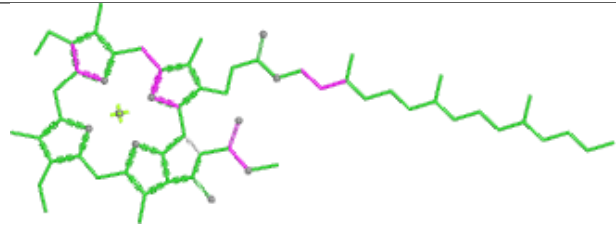
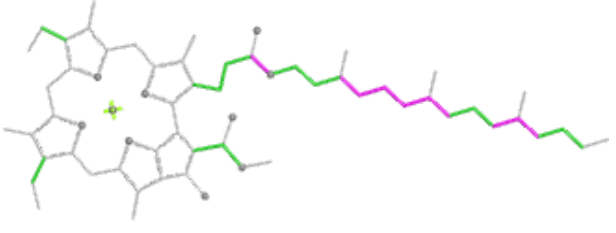
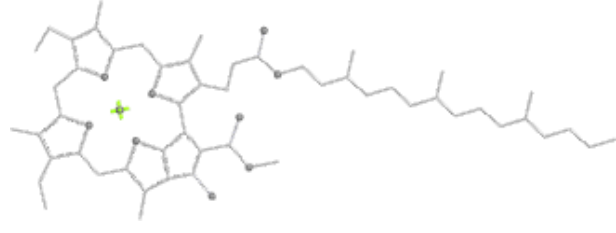
Ligand CLA n 315

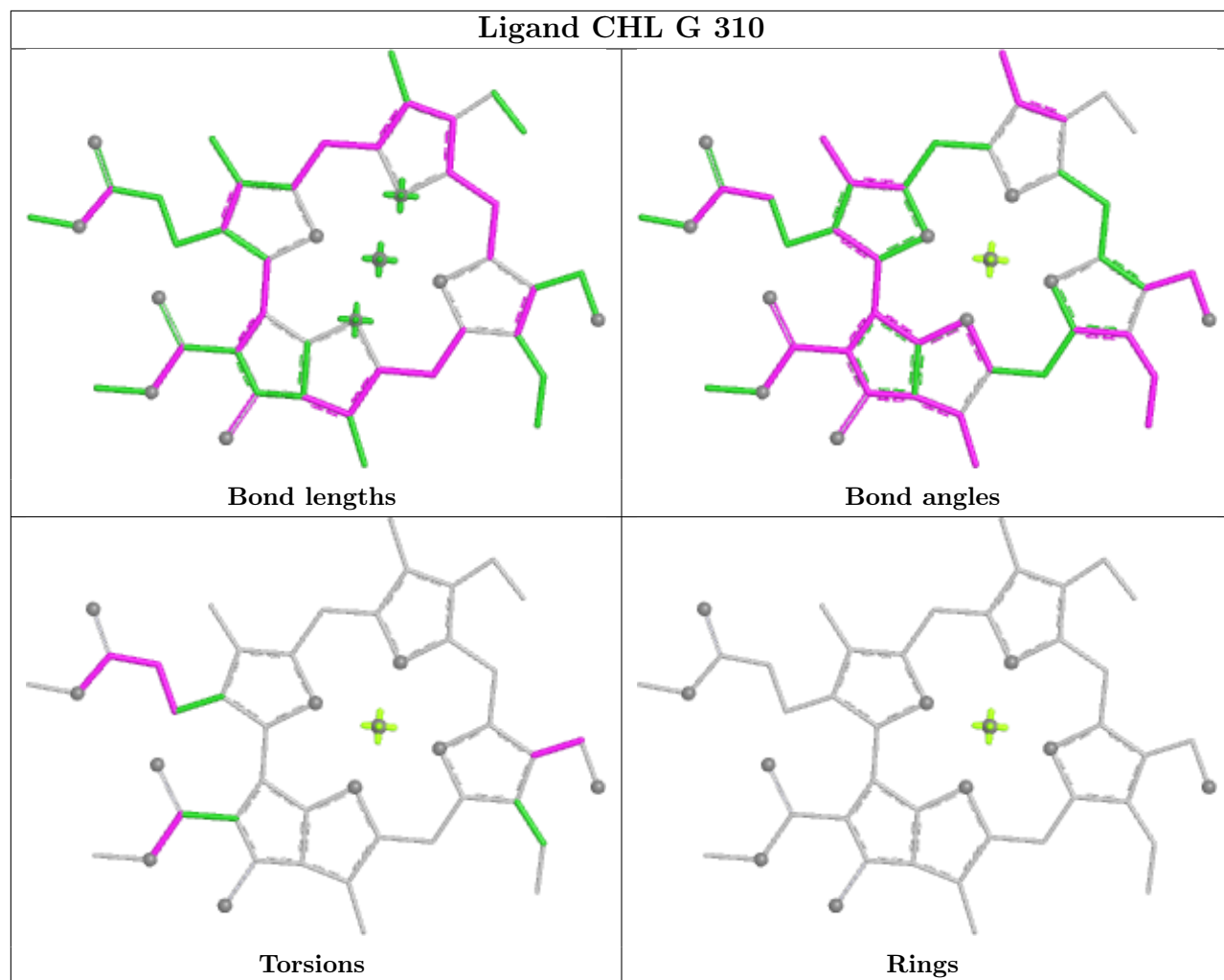


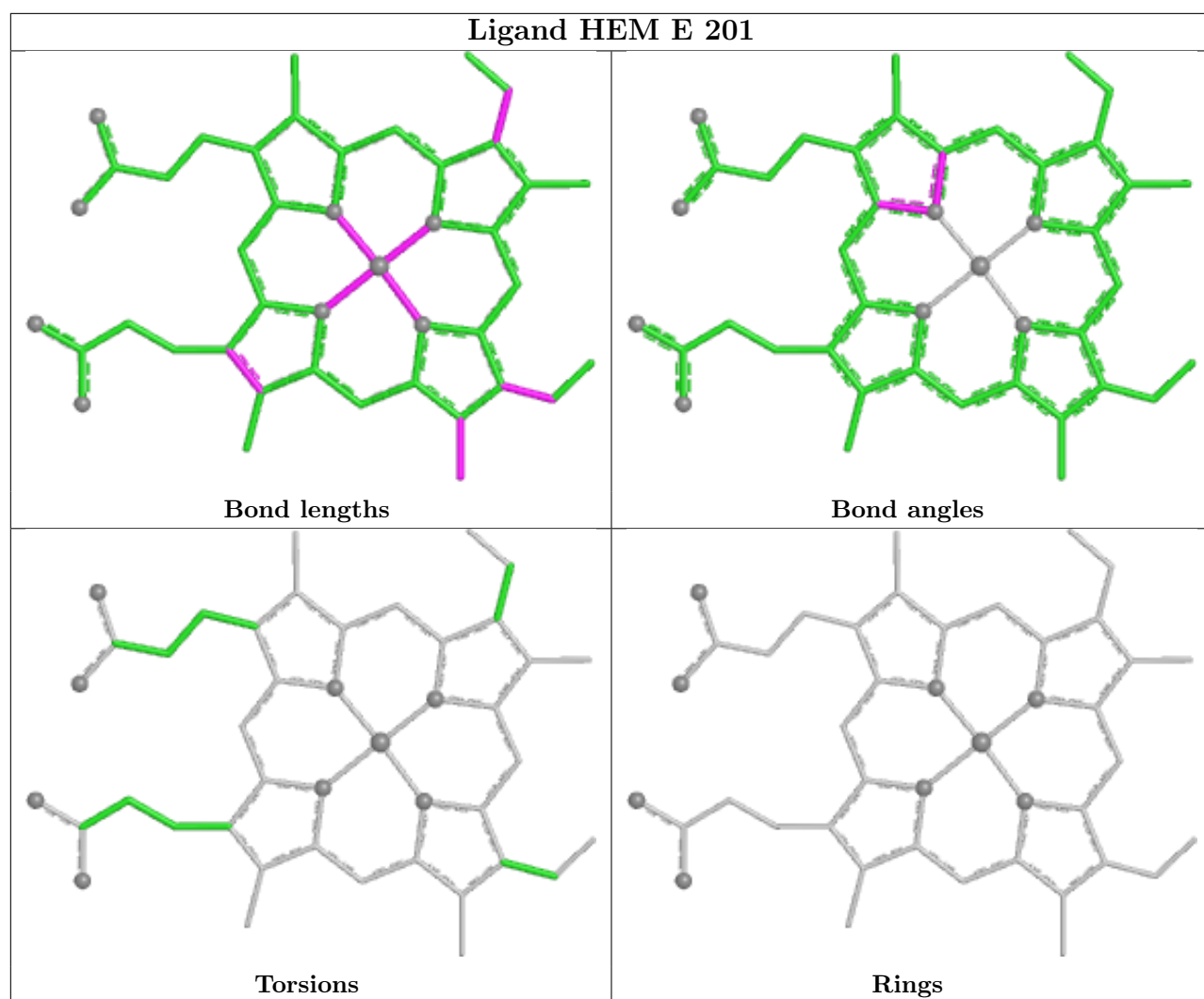
Ligand 8CT V 401



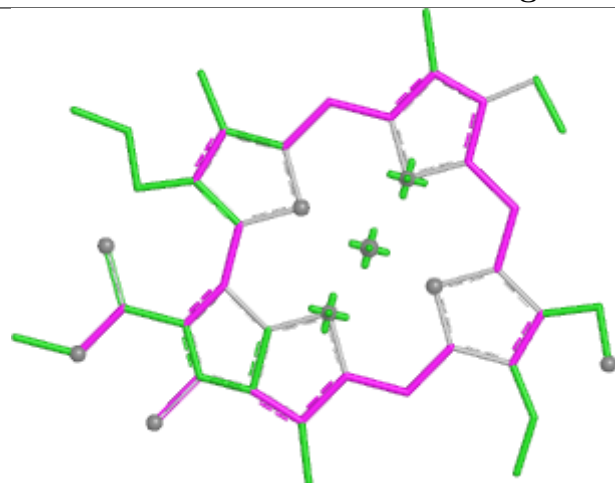
Ligand OIE 7 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

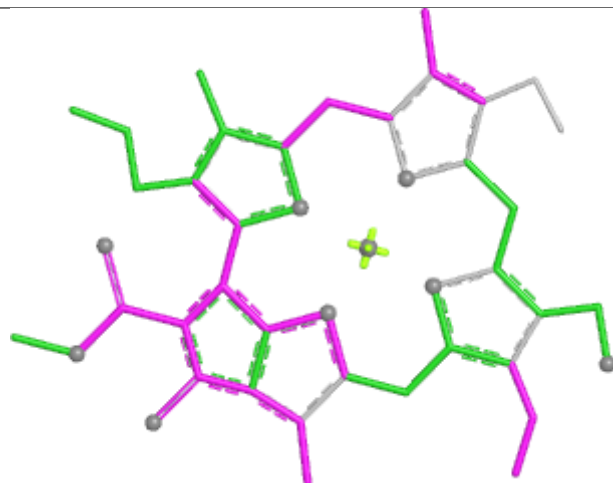




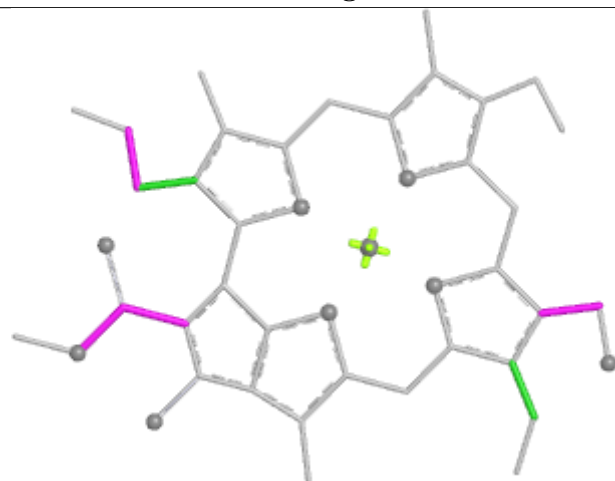
Ligand CHL 3 311



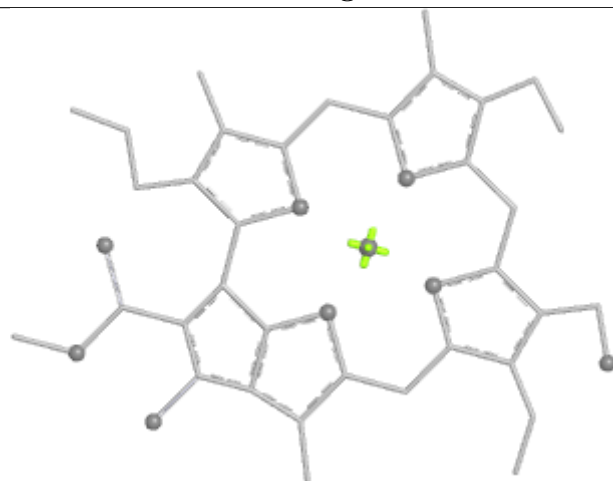
Bond lengths



Bond angles

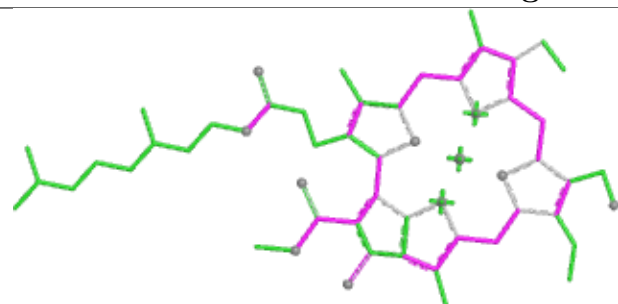


Torsions

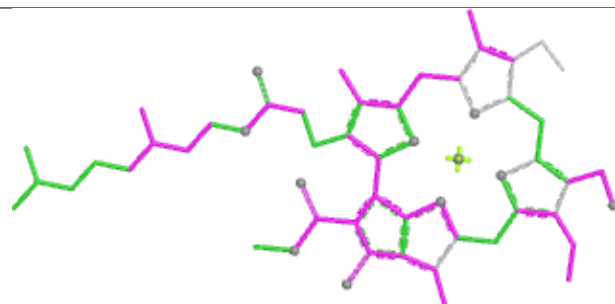


Rings

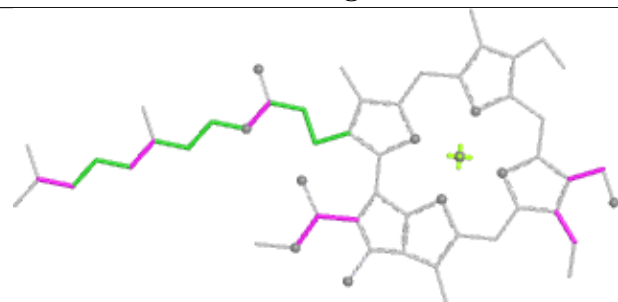
Ligand CHL 8 310



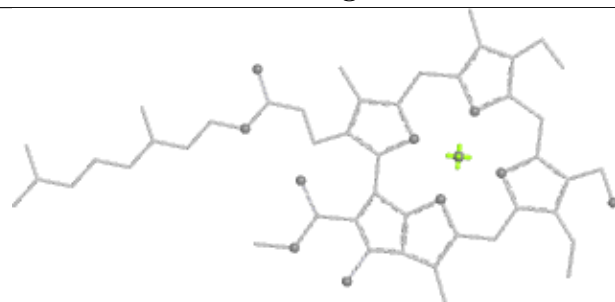
Bond lengths



Bond angles

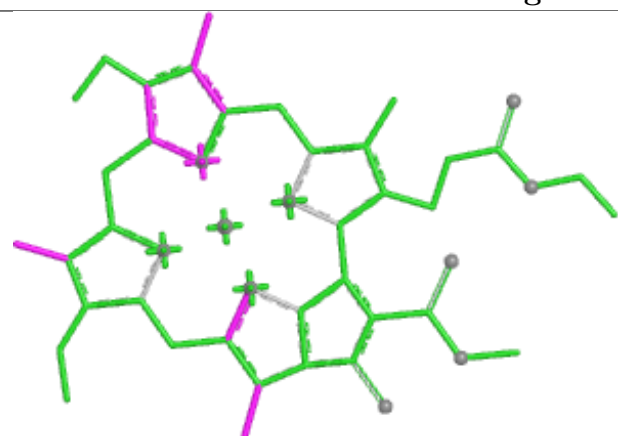


Torsions

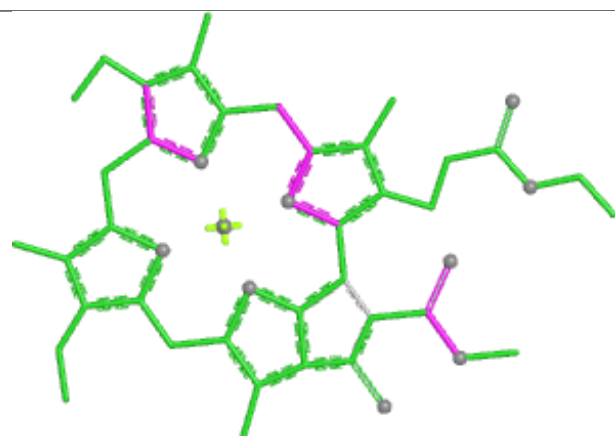


Rings

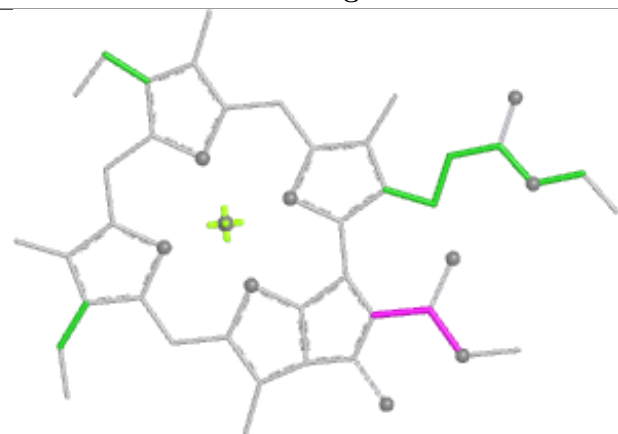
Ligand CLA r 304



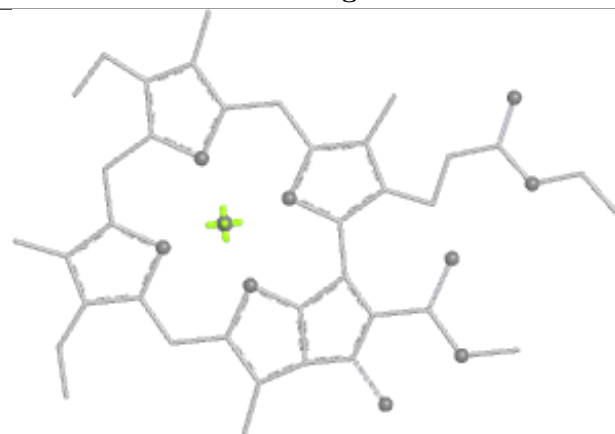
Bond lengths



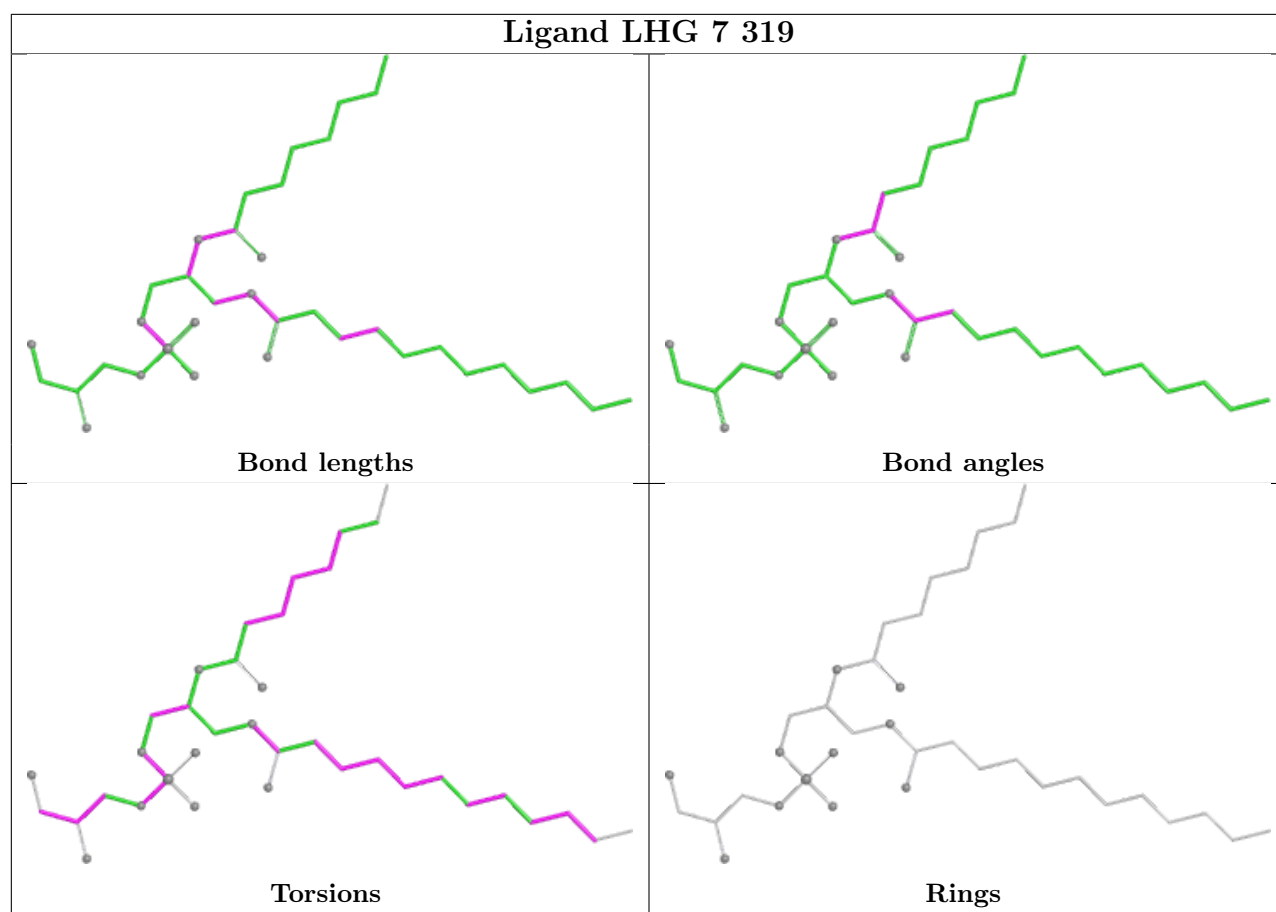
Bond angles



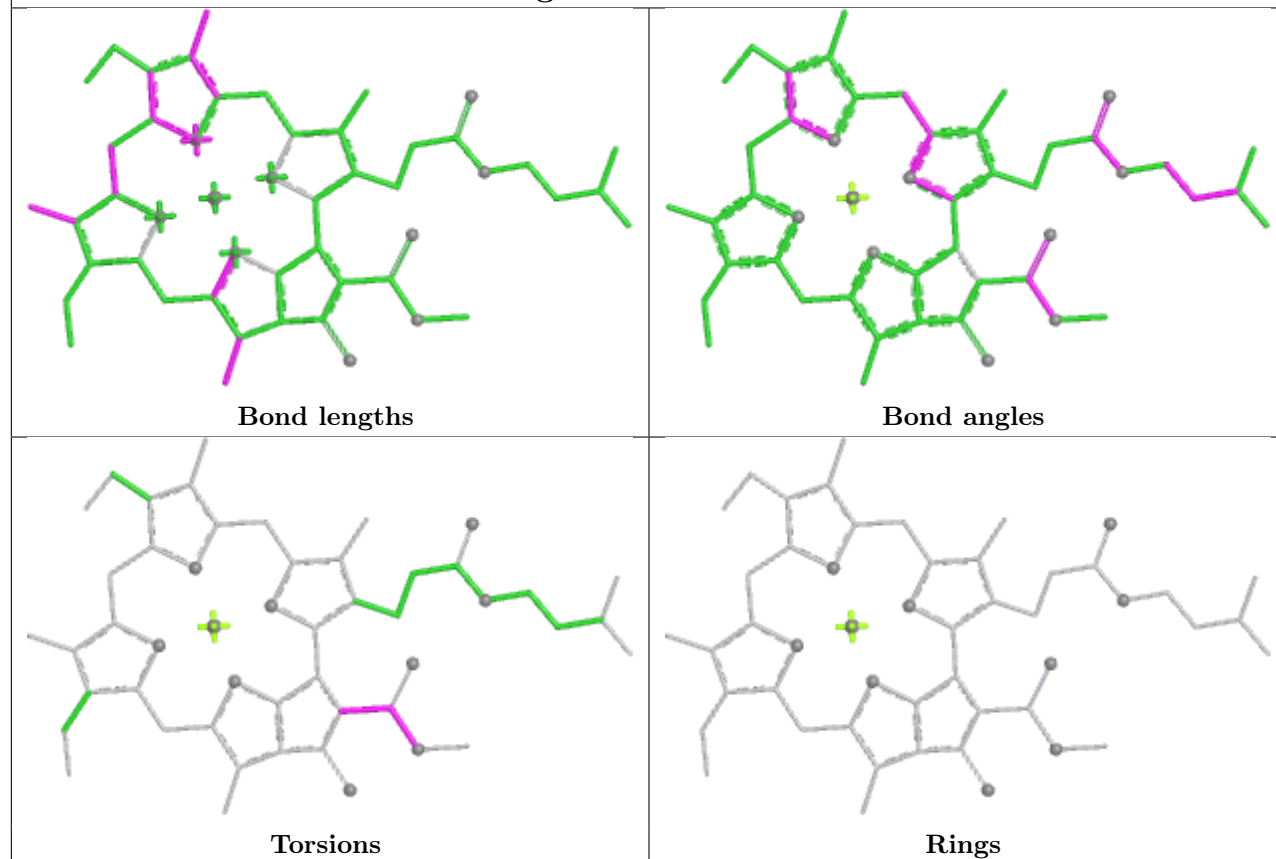
Torsions



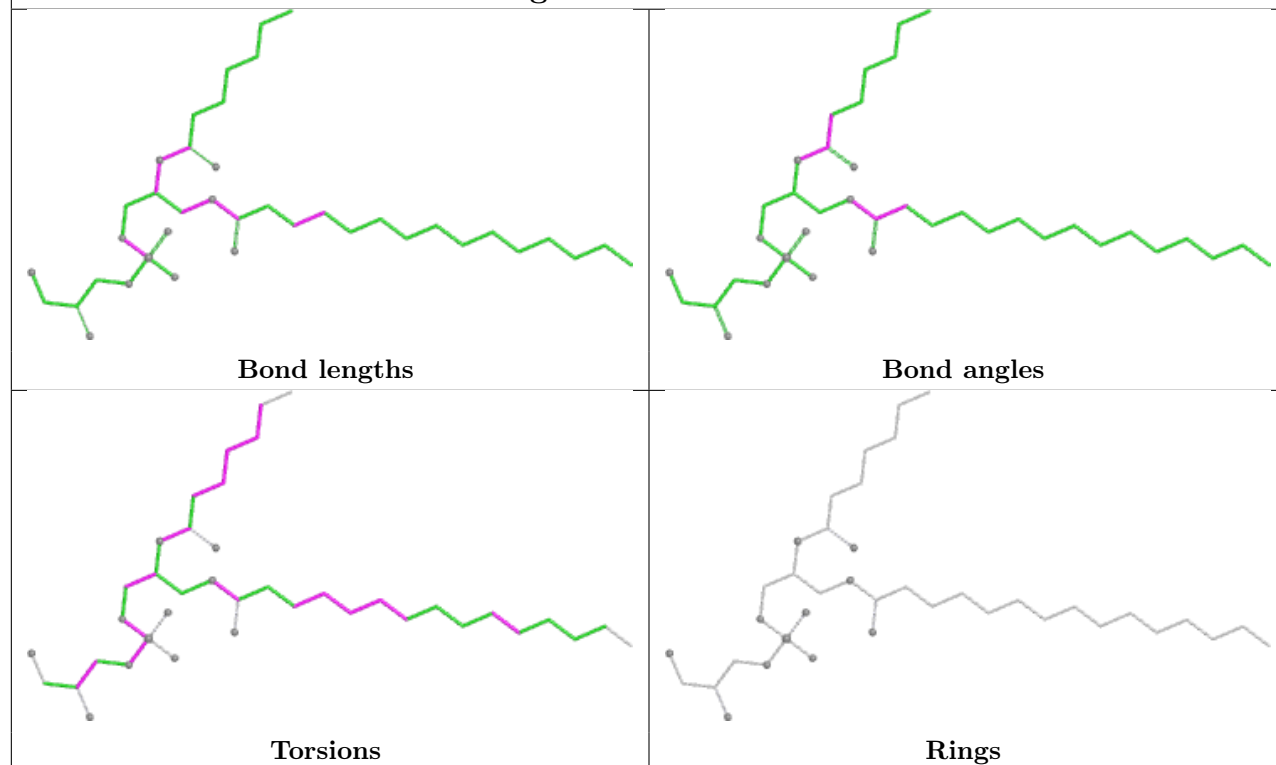
Rings

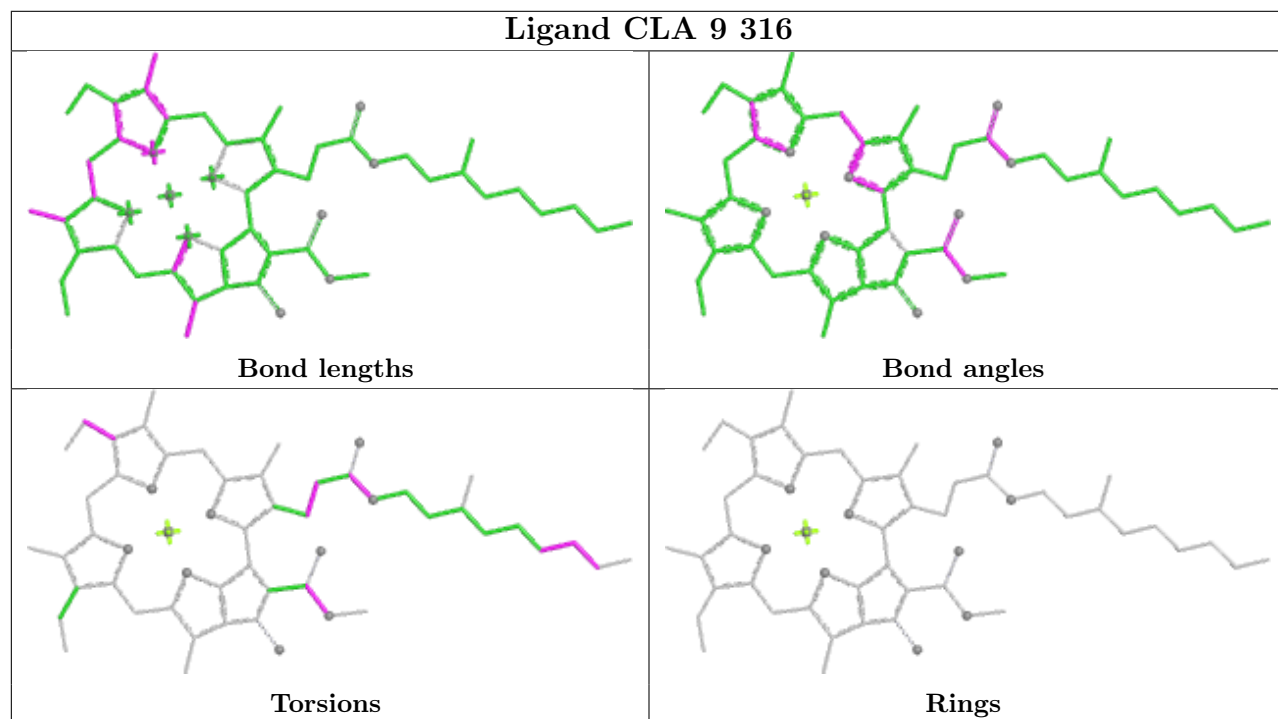
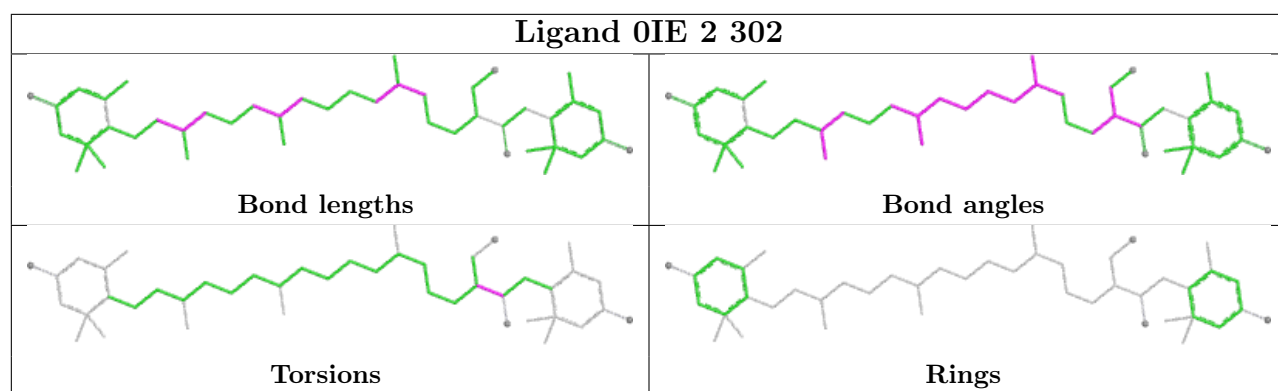


Ligand CLA 5 308

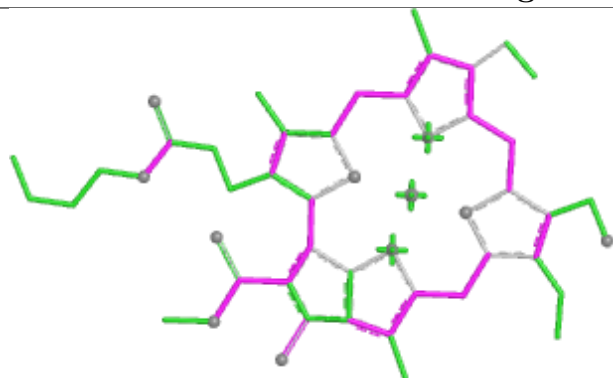


Ligand LHG D 408

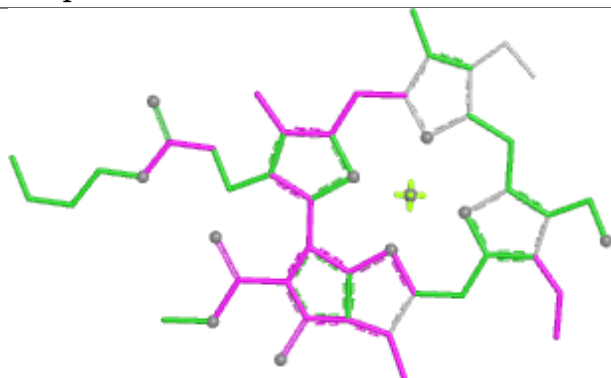




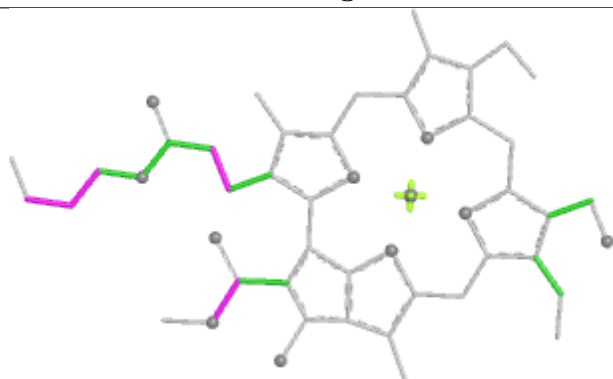
Ligand CHL q 310



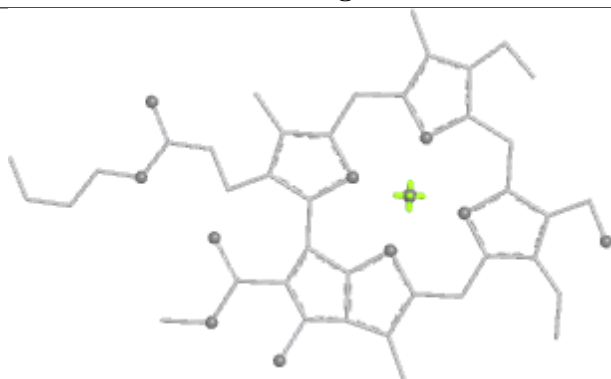
Bond lengths



Bond angles

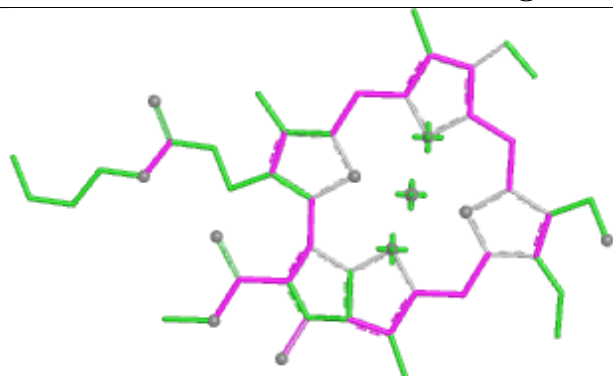


Torsions

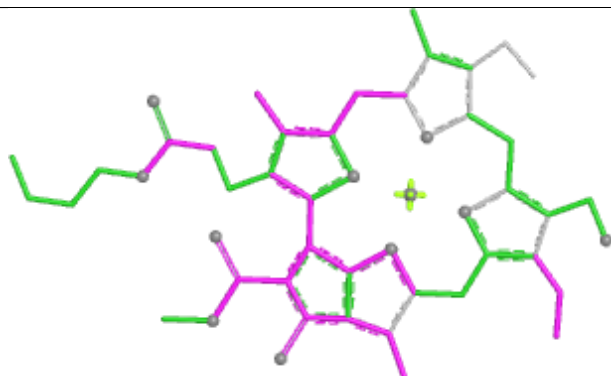


Rings

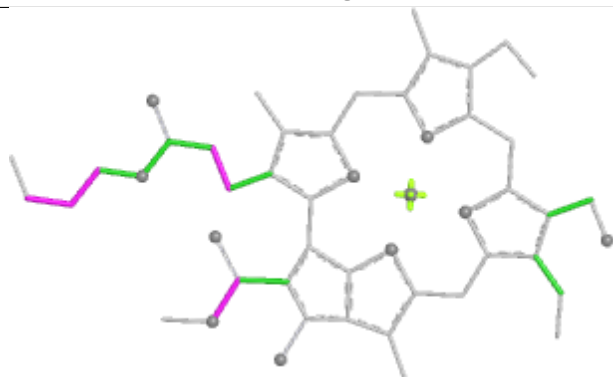
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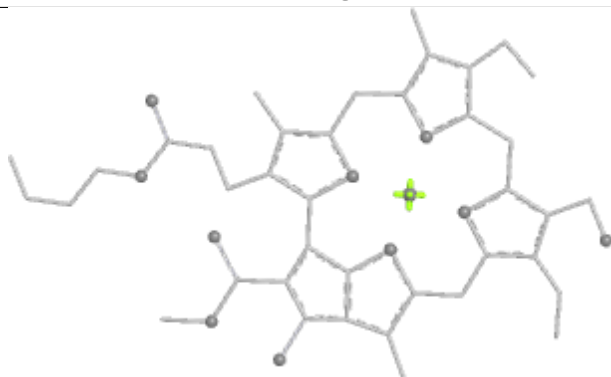
Bond lengths



Bond angles

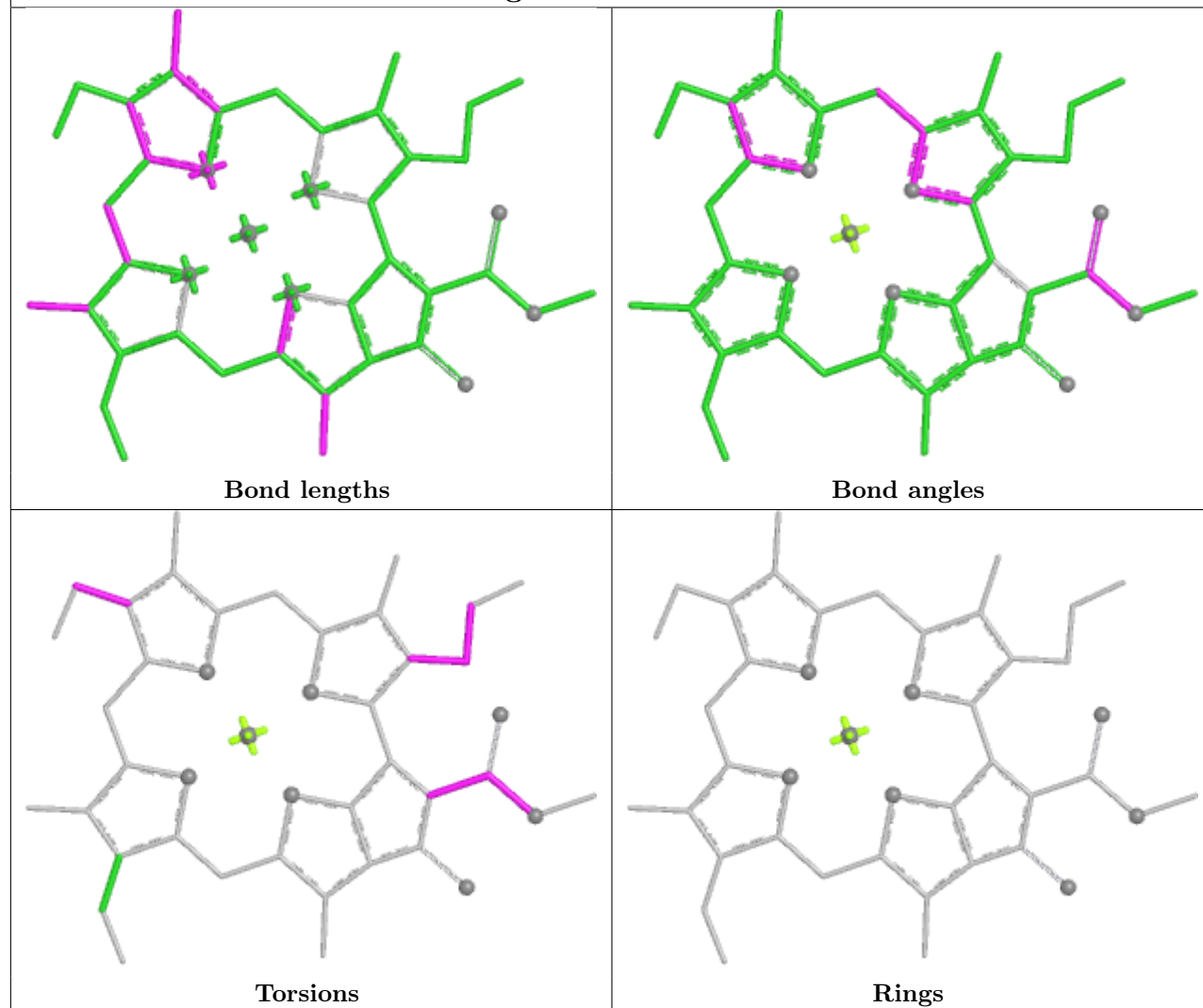


Torsions

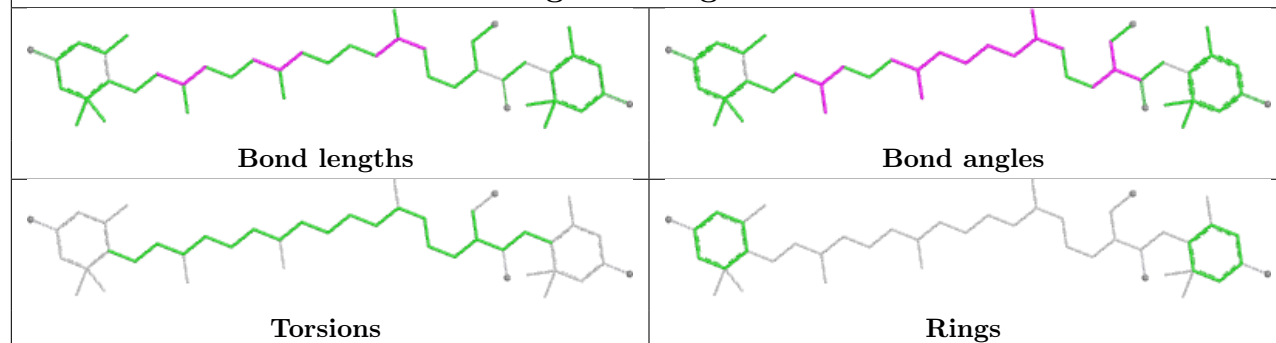


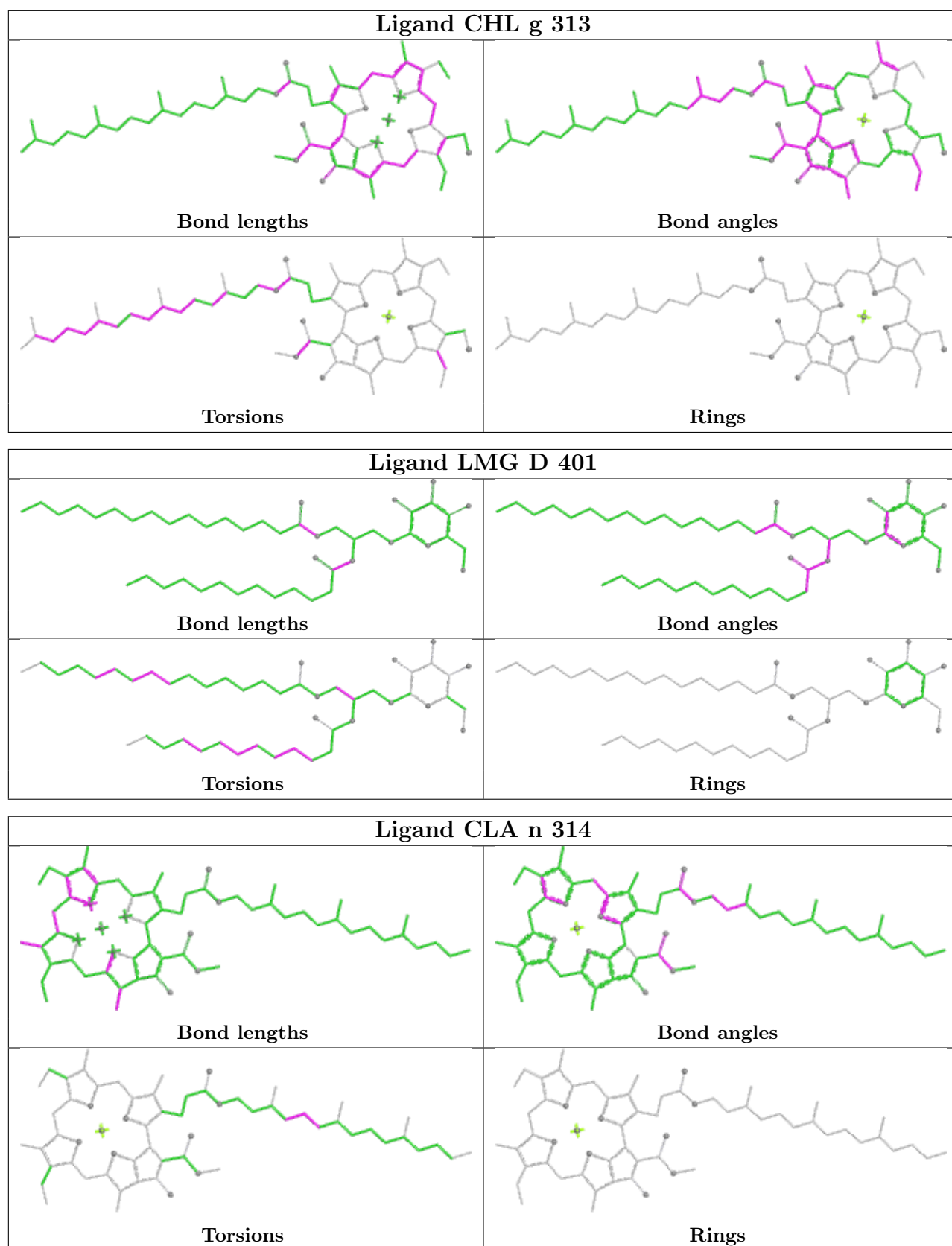
Rings

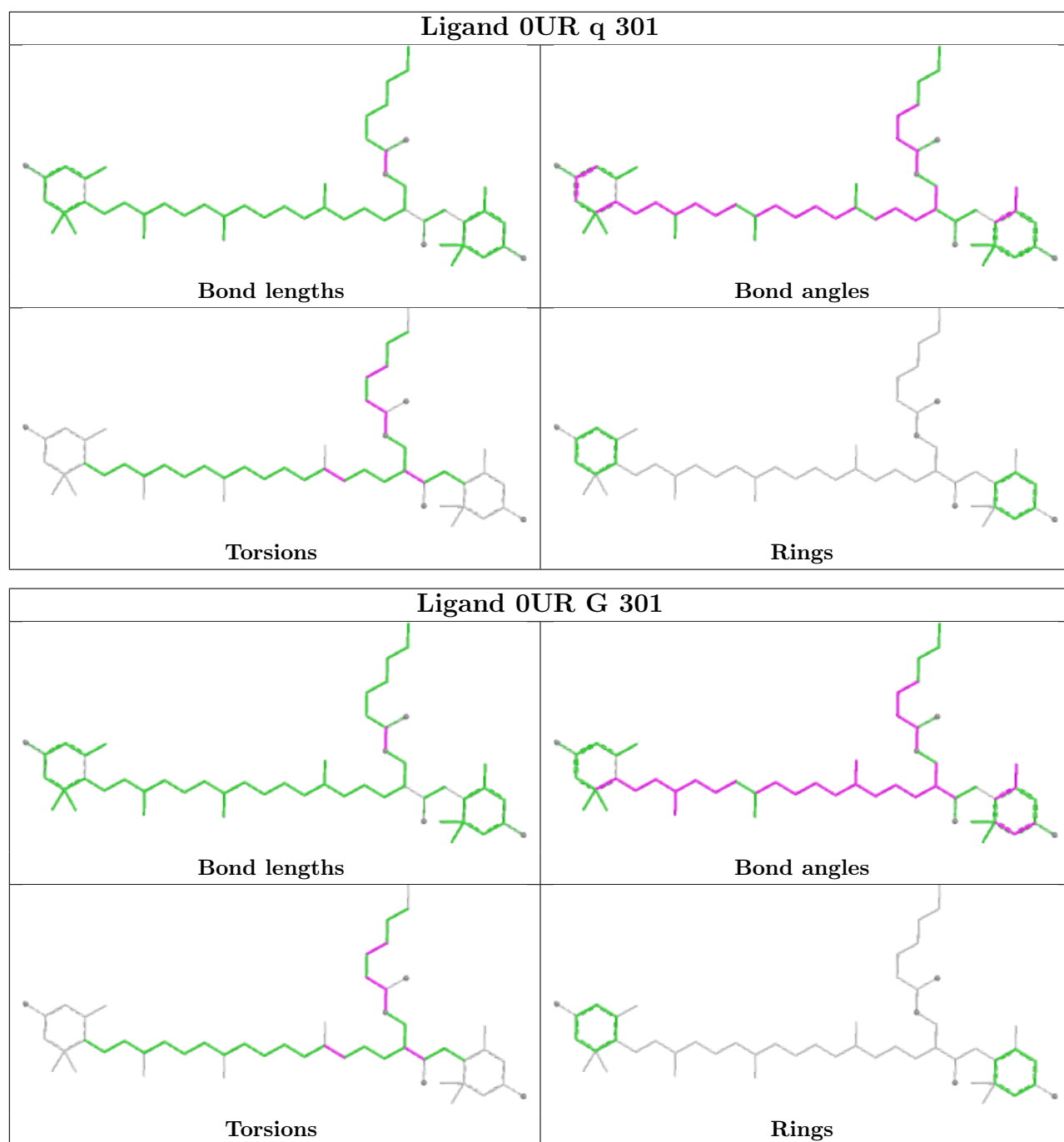
Ligand CLA 5 307

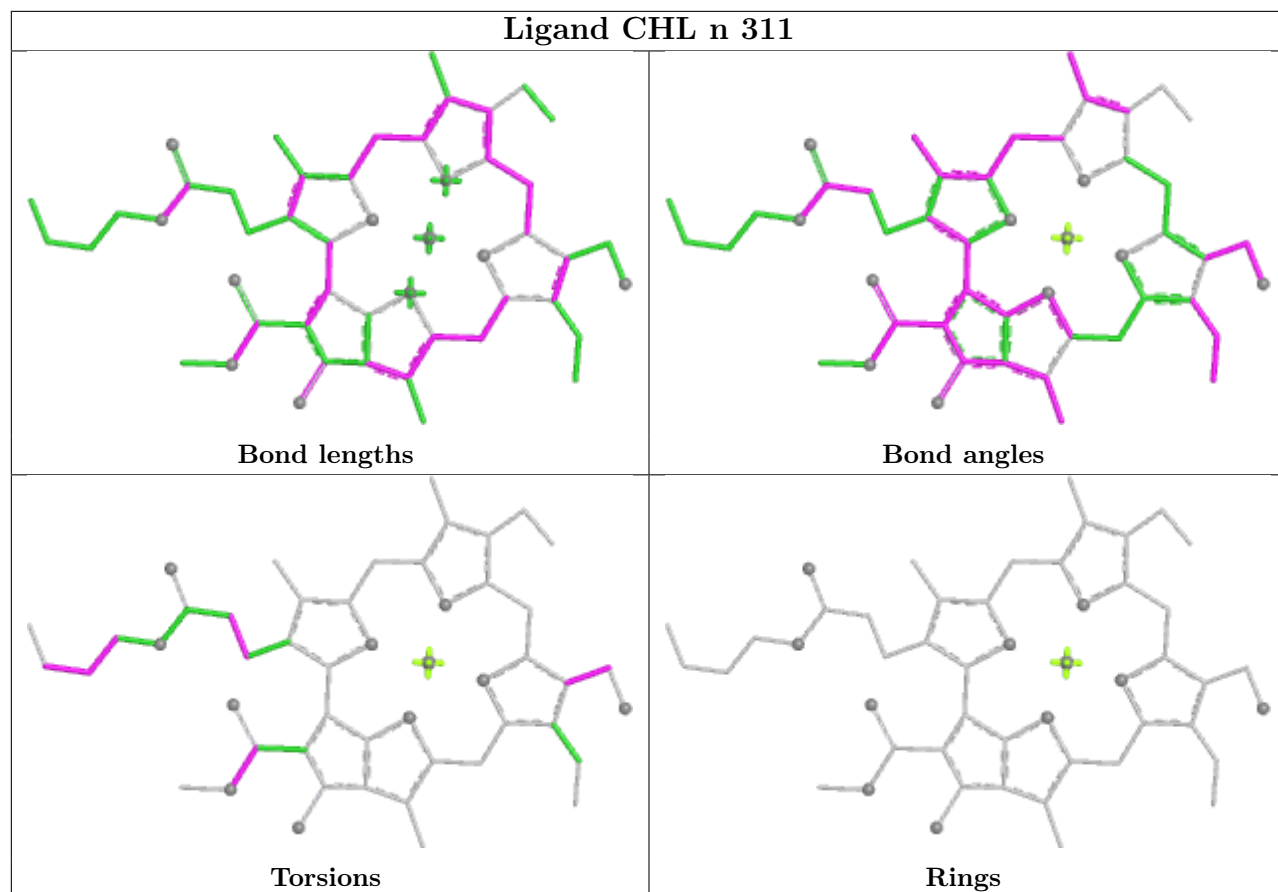


Ligand OIE g 303

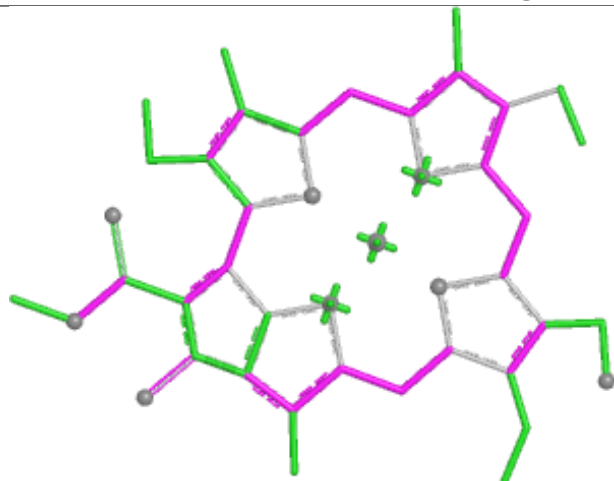




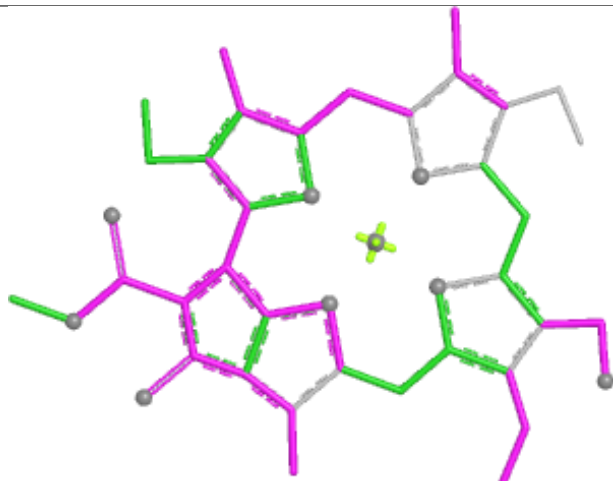




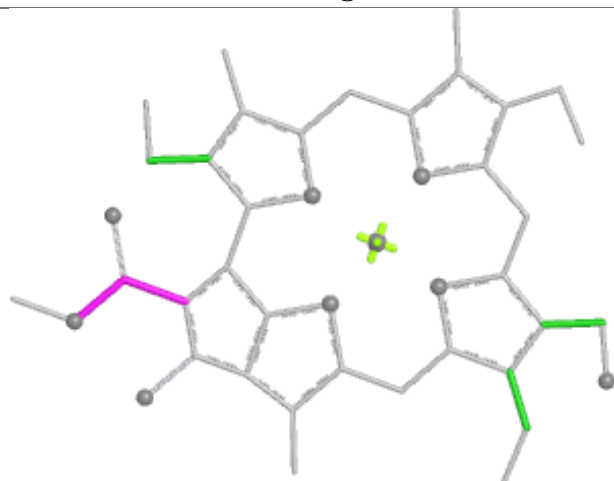
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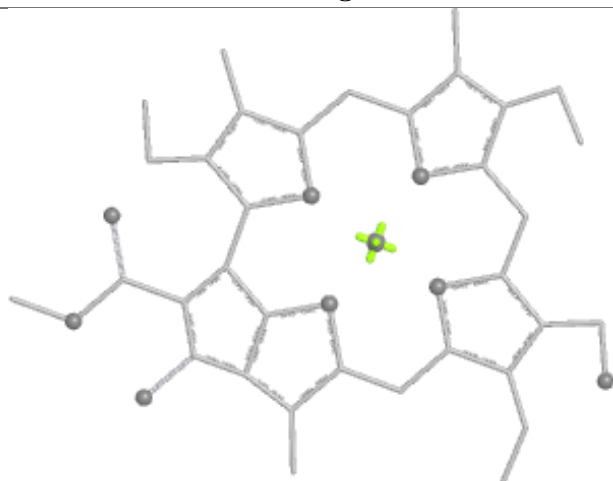
Bond lengths



Bond angles

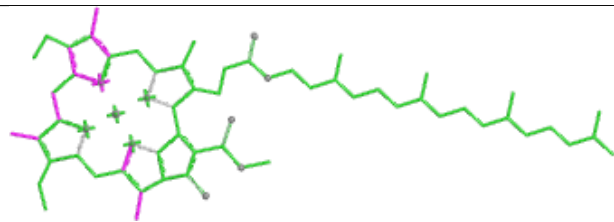


Torsions

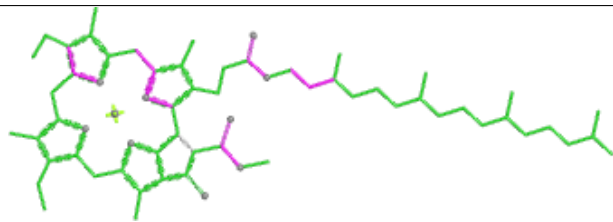


Rings

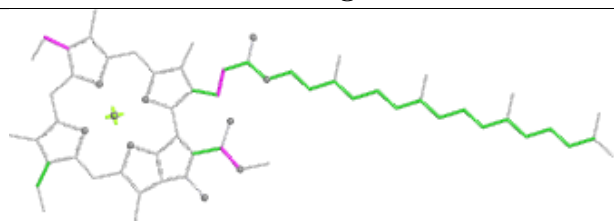
Ligand CLA b 610



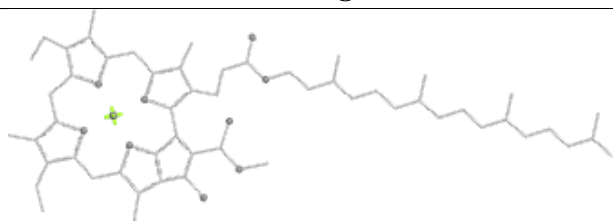
Bond lengths



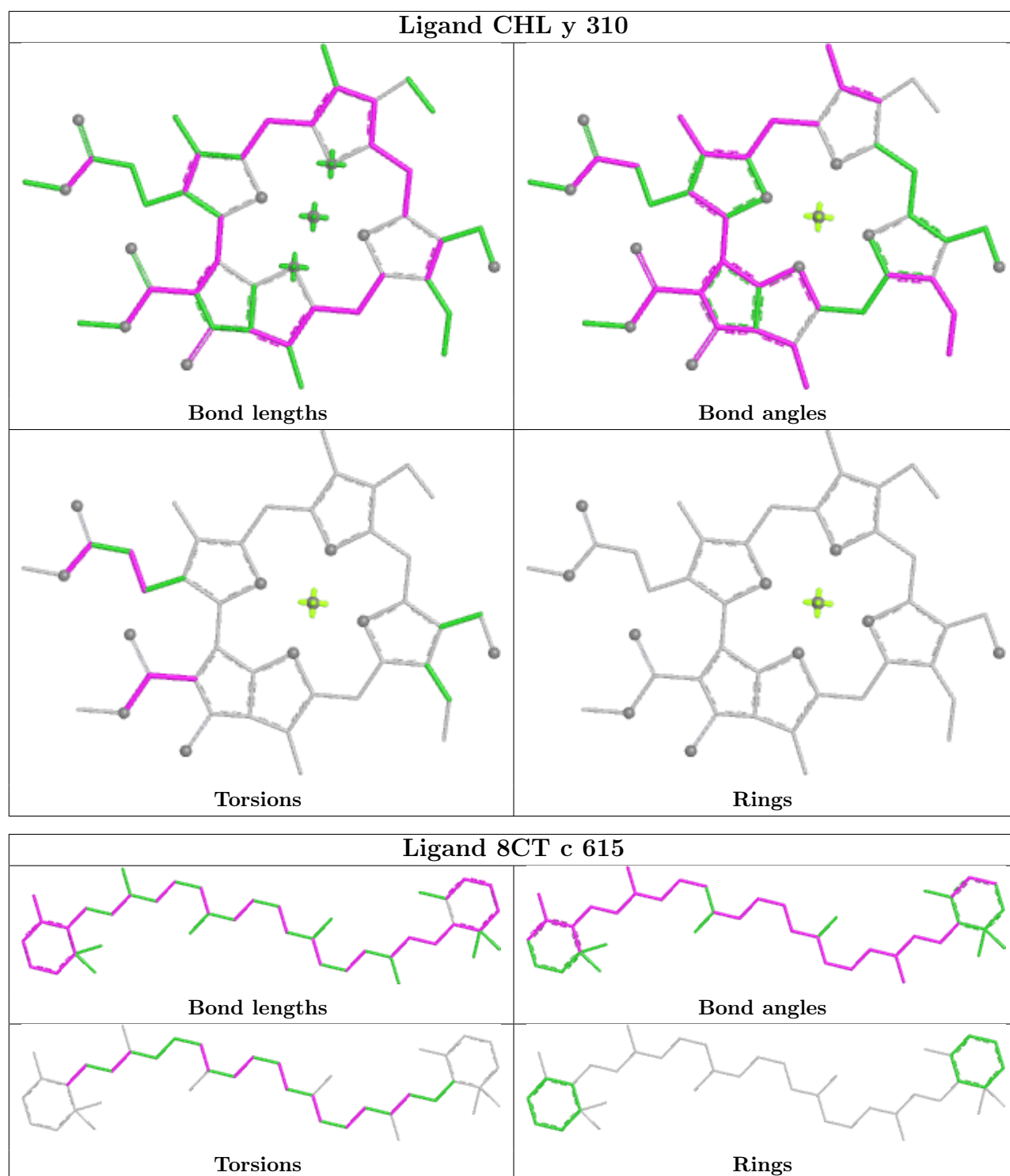
Bond angles



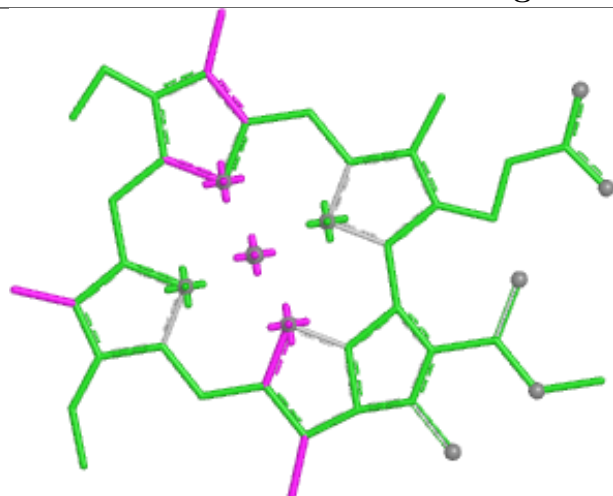
Torsions



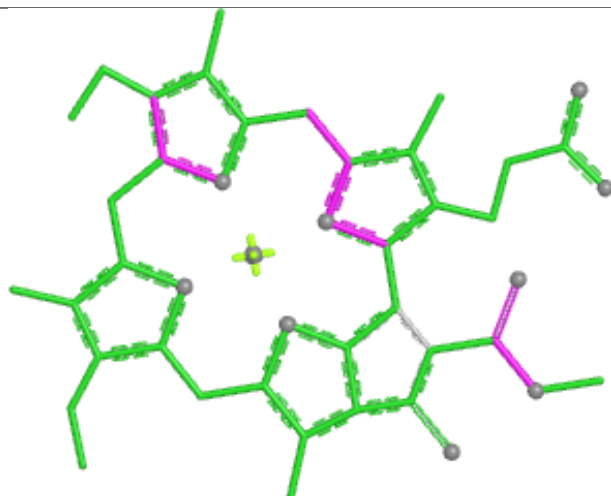
Rings



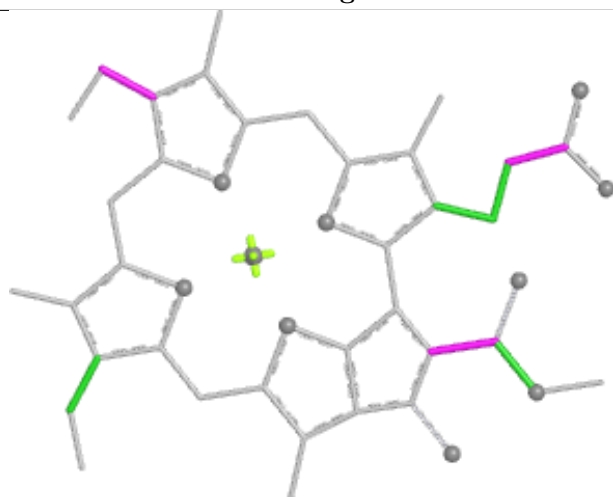
Ligand CLA Y 315



Bond lengths



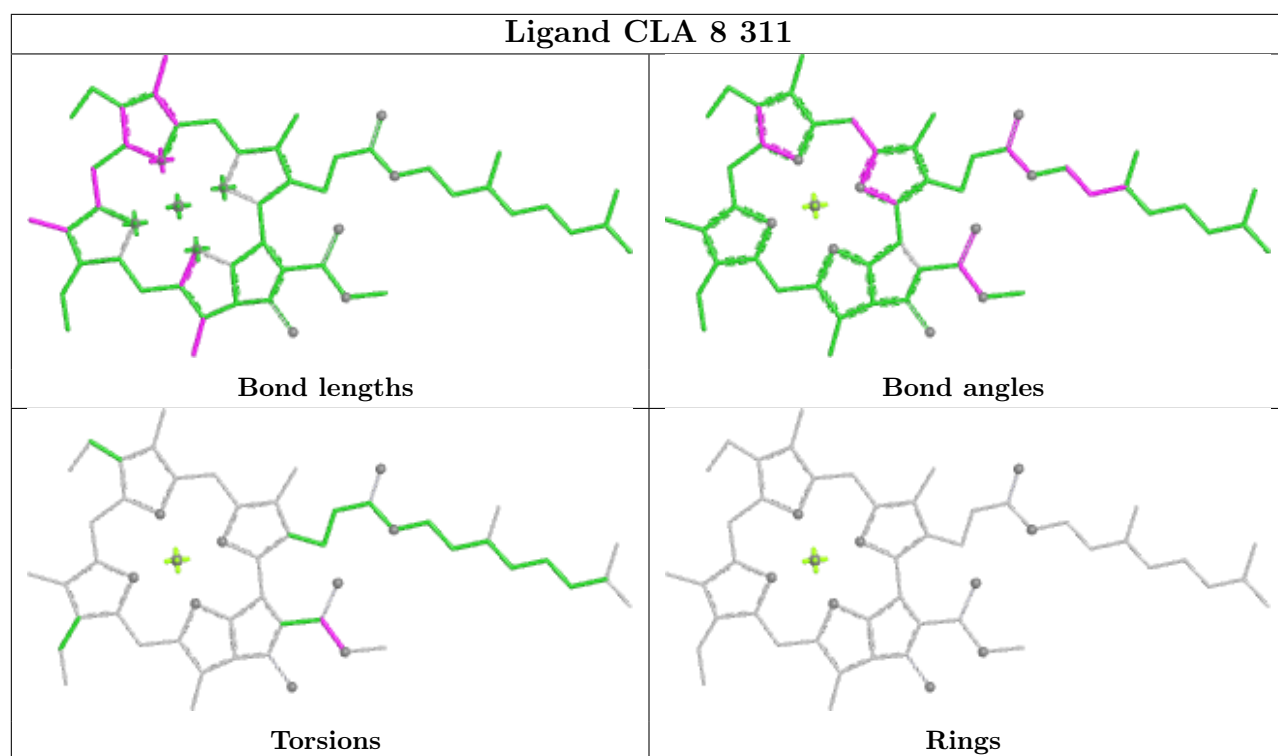
Bond angles



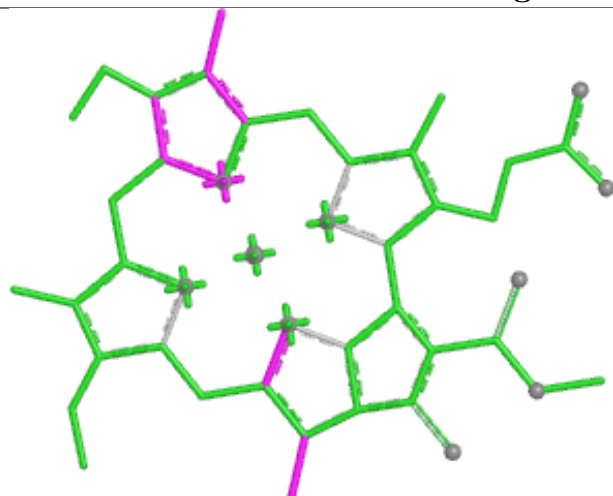
Torsions



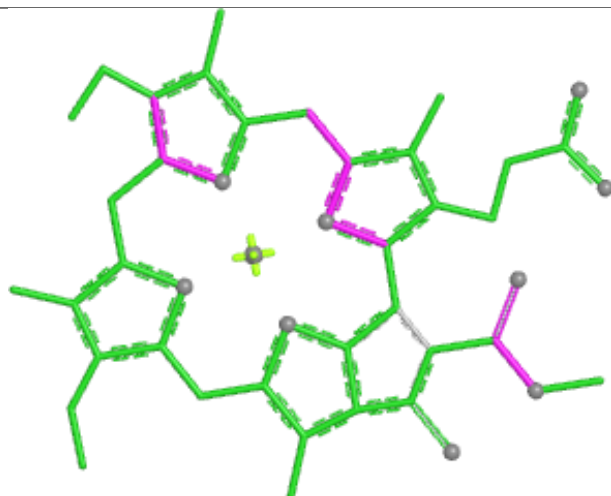
Rings



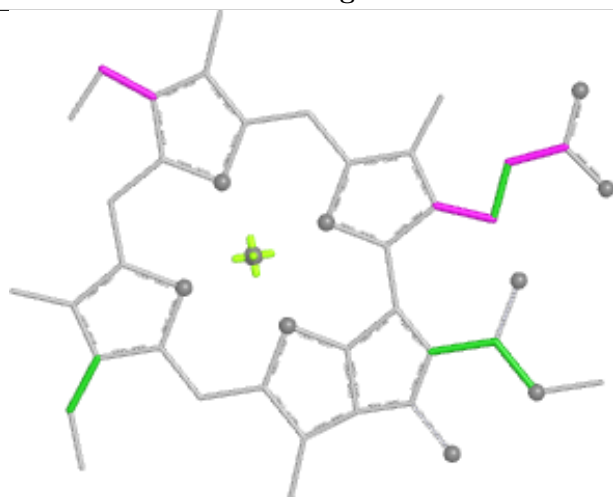
Ligand CLA R 612



Bond lengths



Bond angles

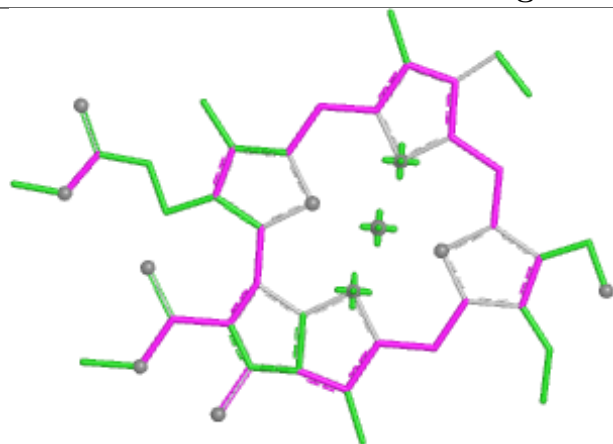


Torsions

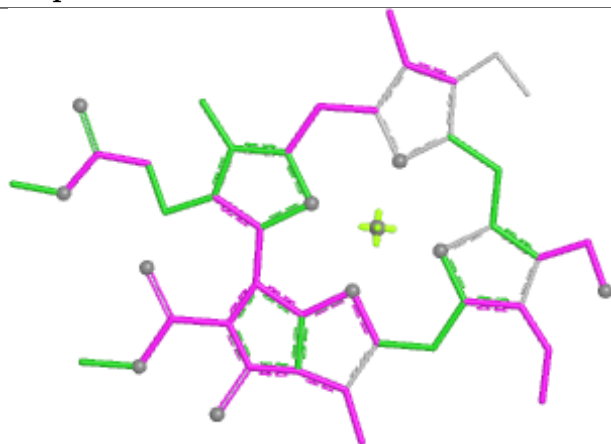


Rings

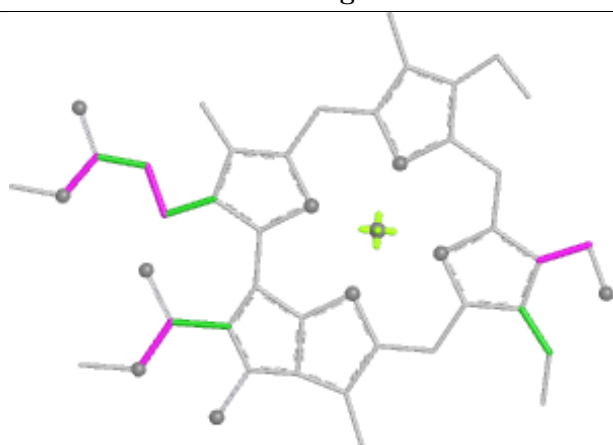
Ligand CHL p 312



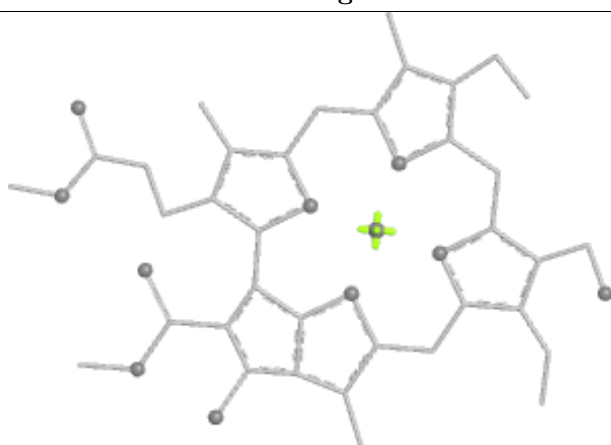
Bond lengths



Bond angles

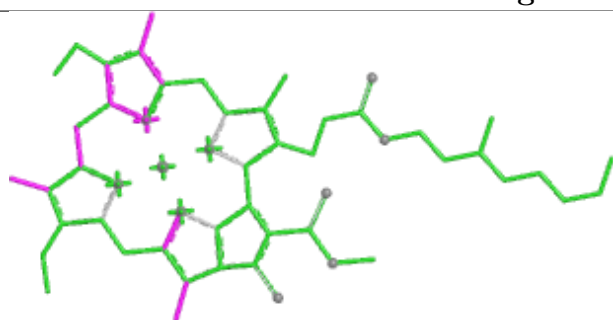


Torsions

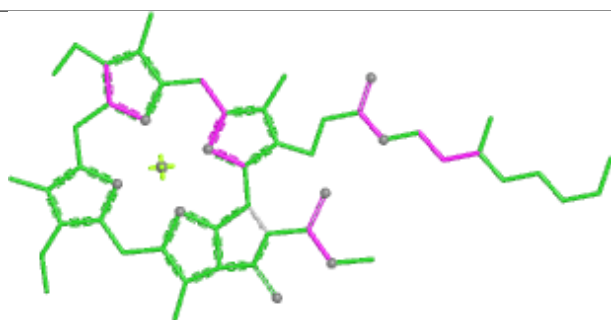


Rings

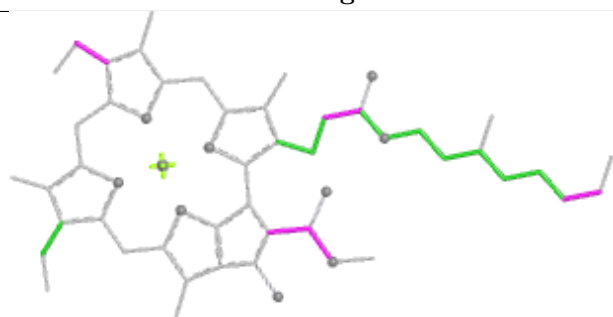
Ligand CLA n 306



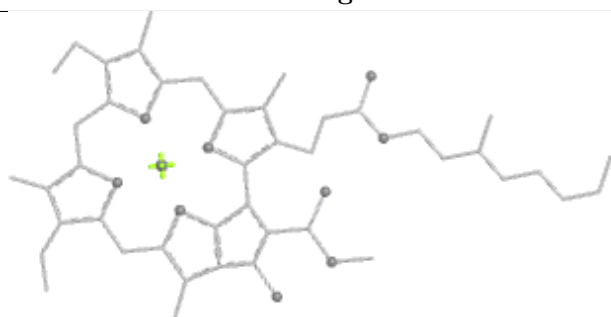
Bond lengths



Bond angles

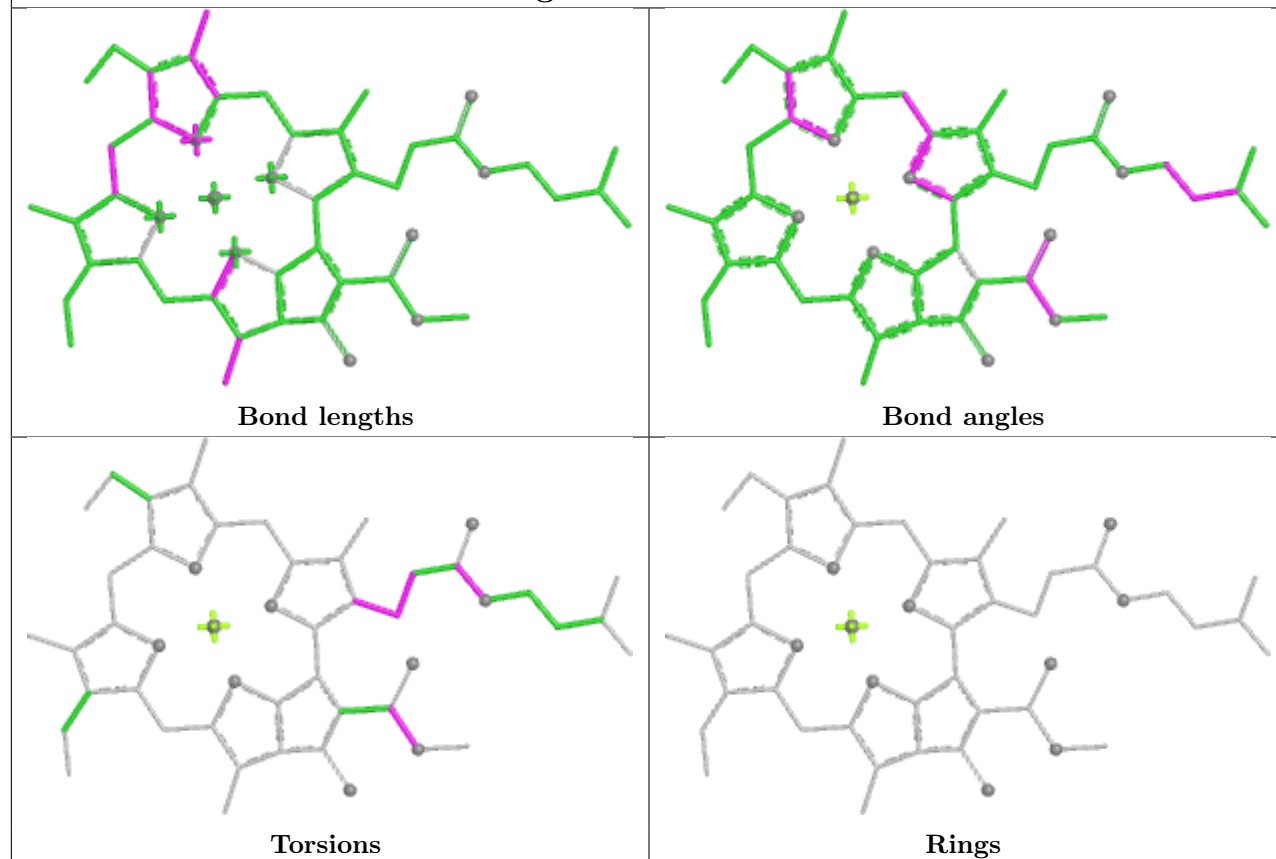


Torsions

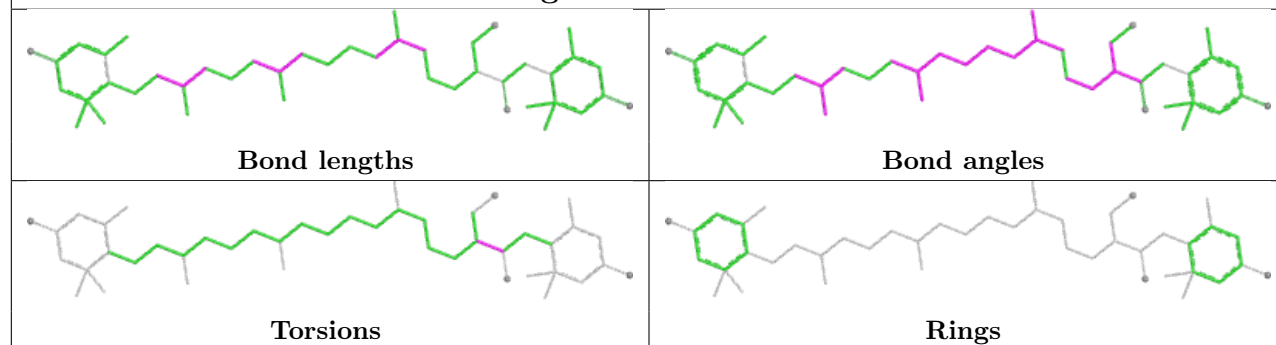


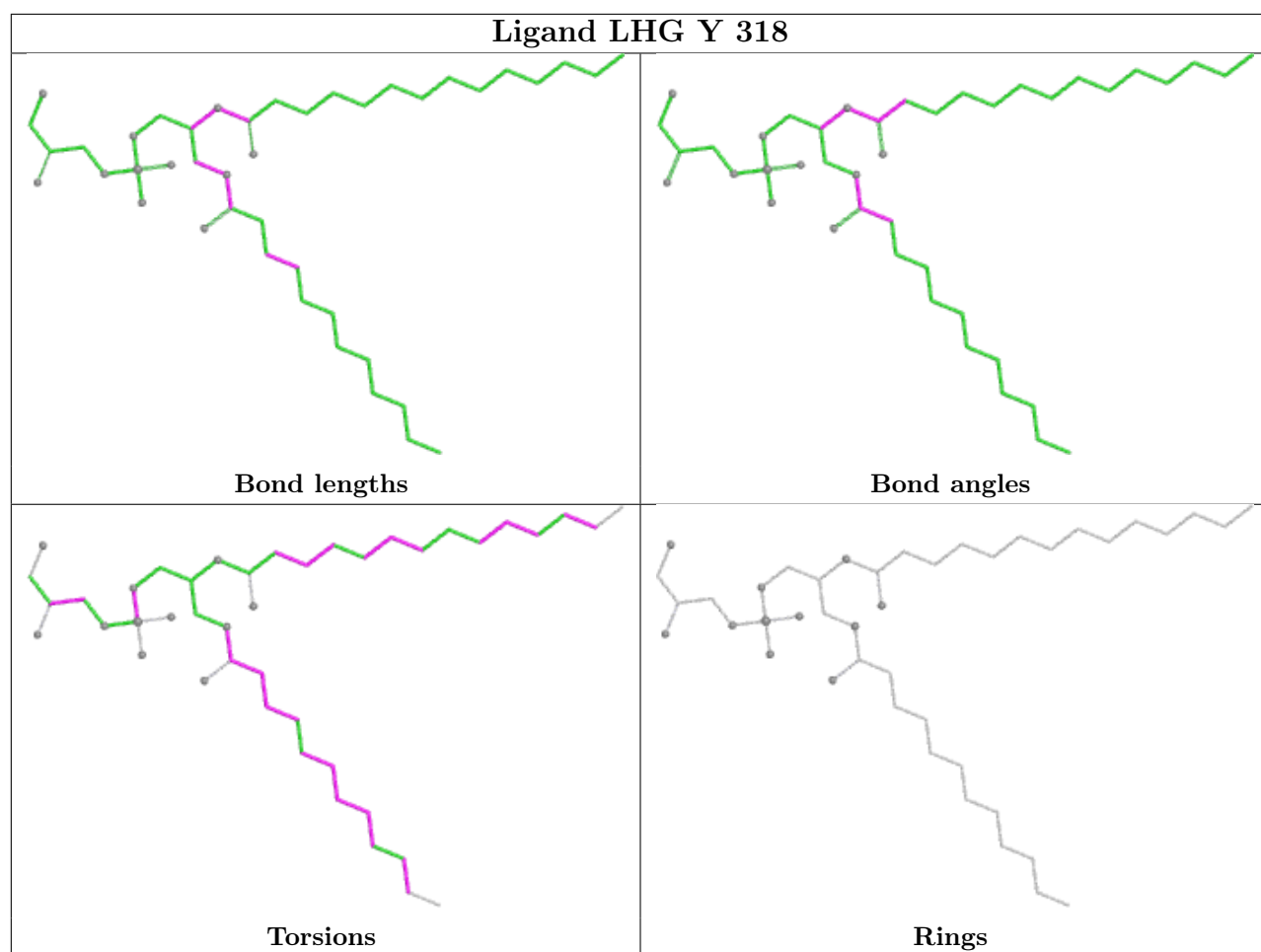
Rings

Ligand CLA 9 307

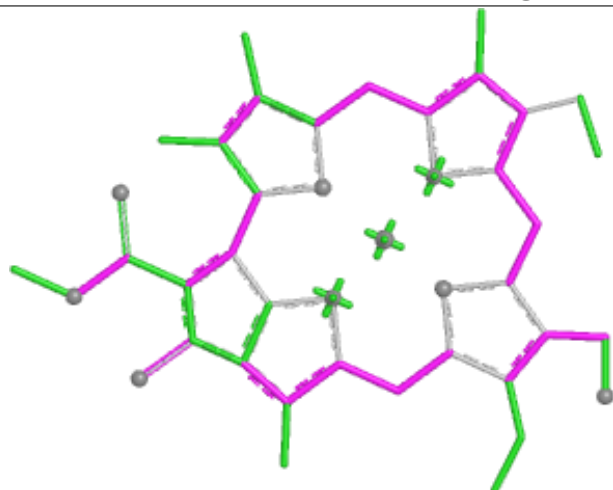


Ligand OIE N 302

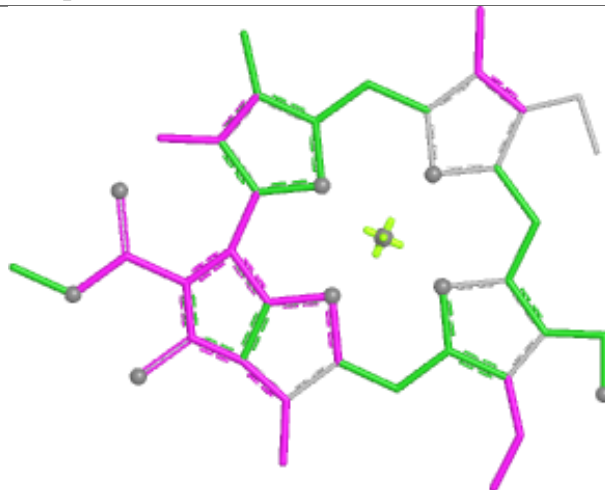




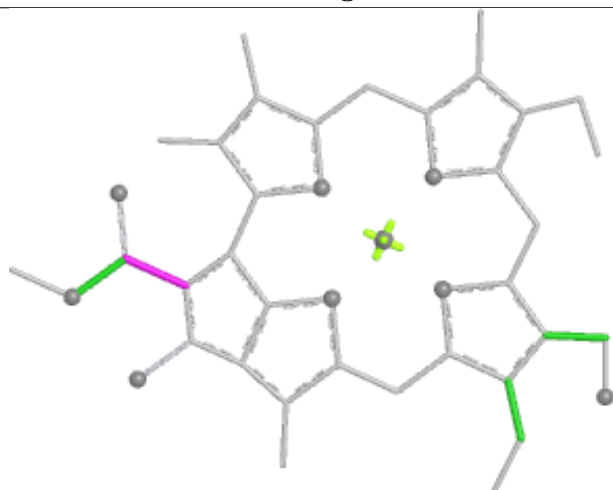
Ligand CHL q 316



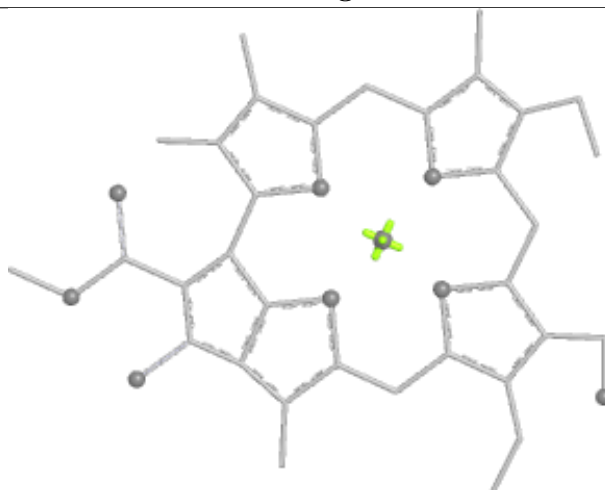
Bond lengths



Bond angles

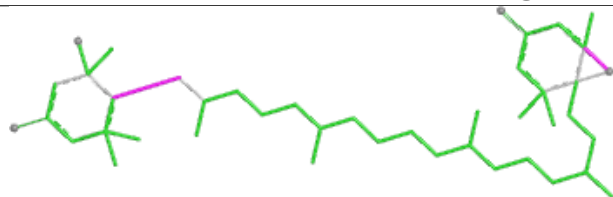


Torsions

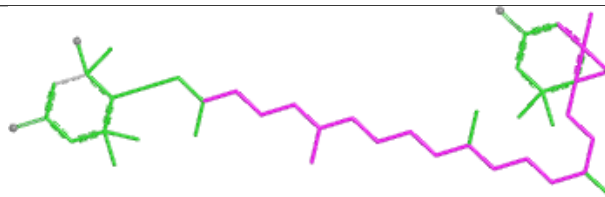


Rings

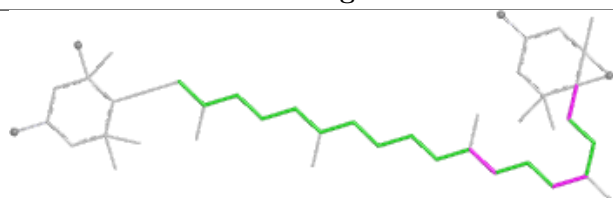
Ligand NEX r 317



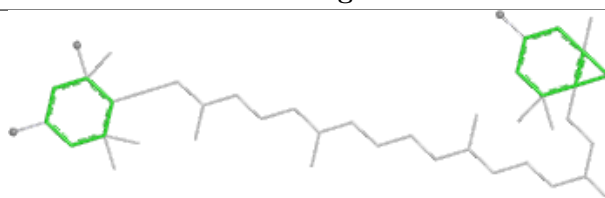
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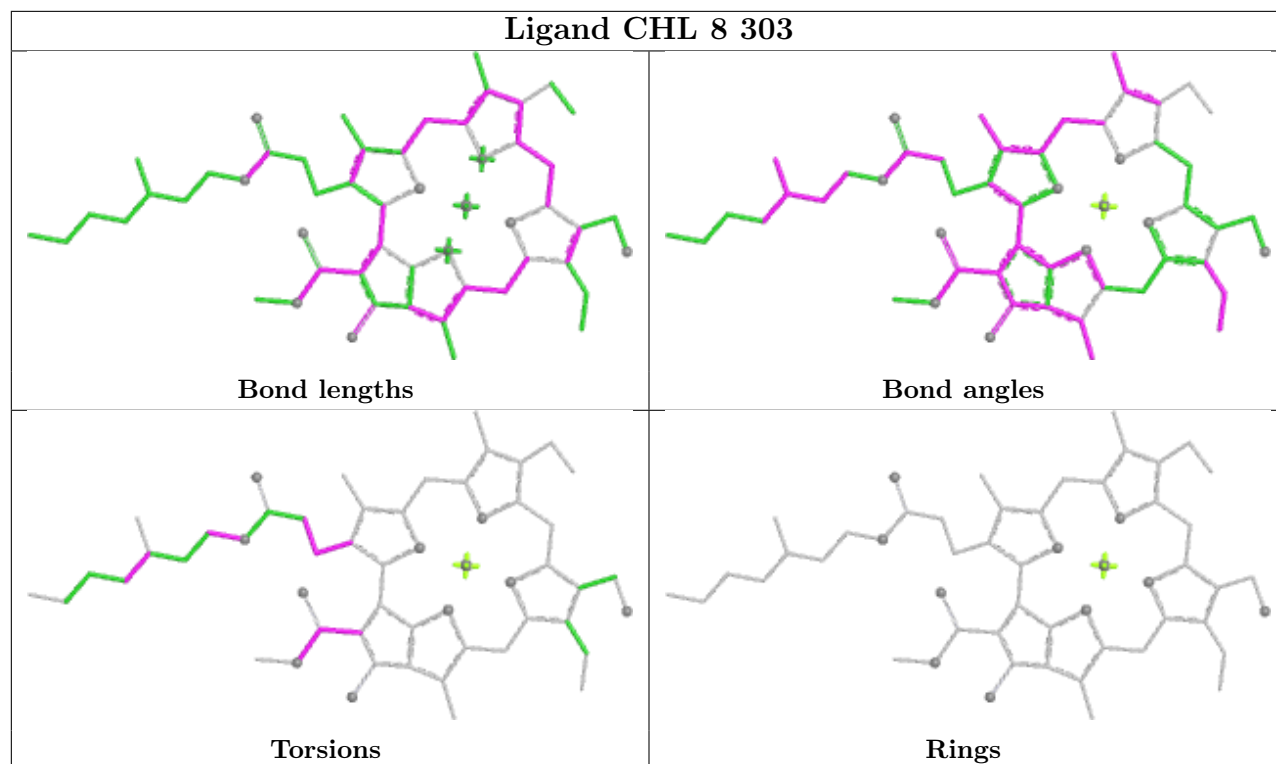
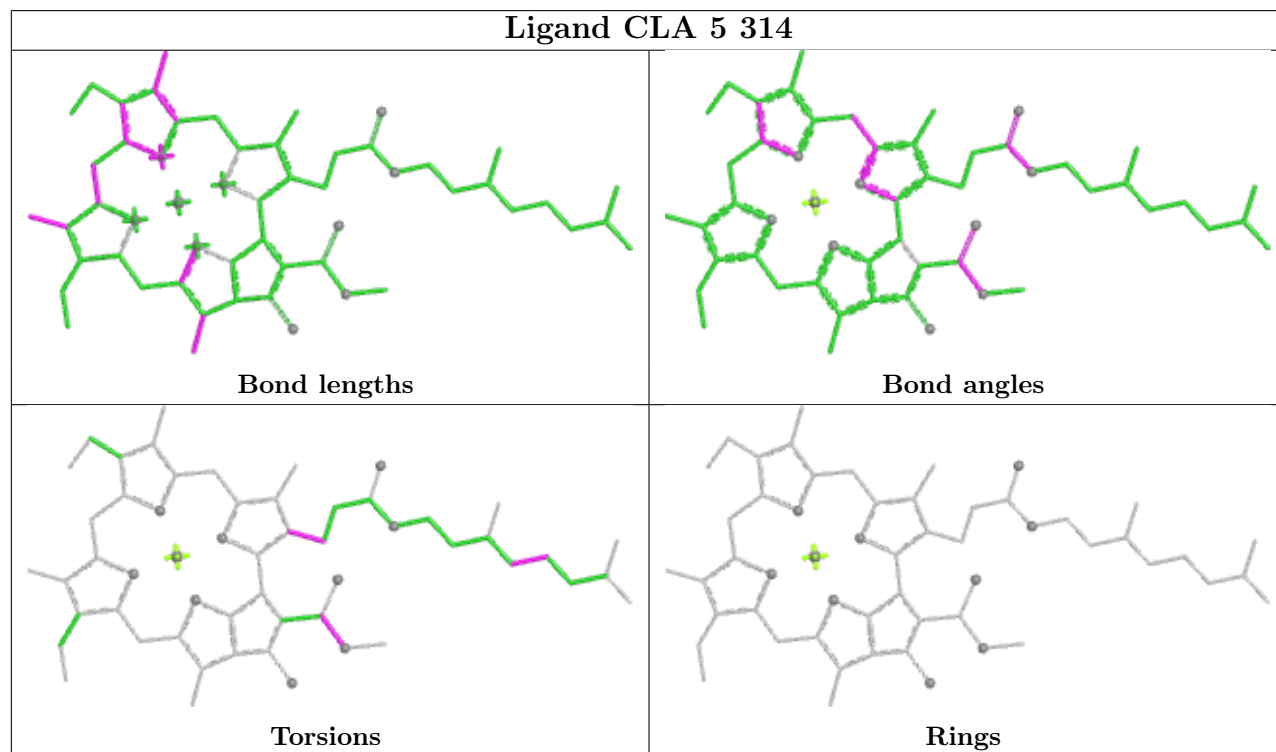
Bond angles

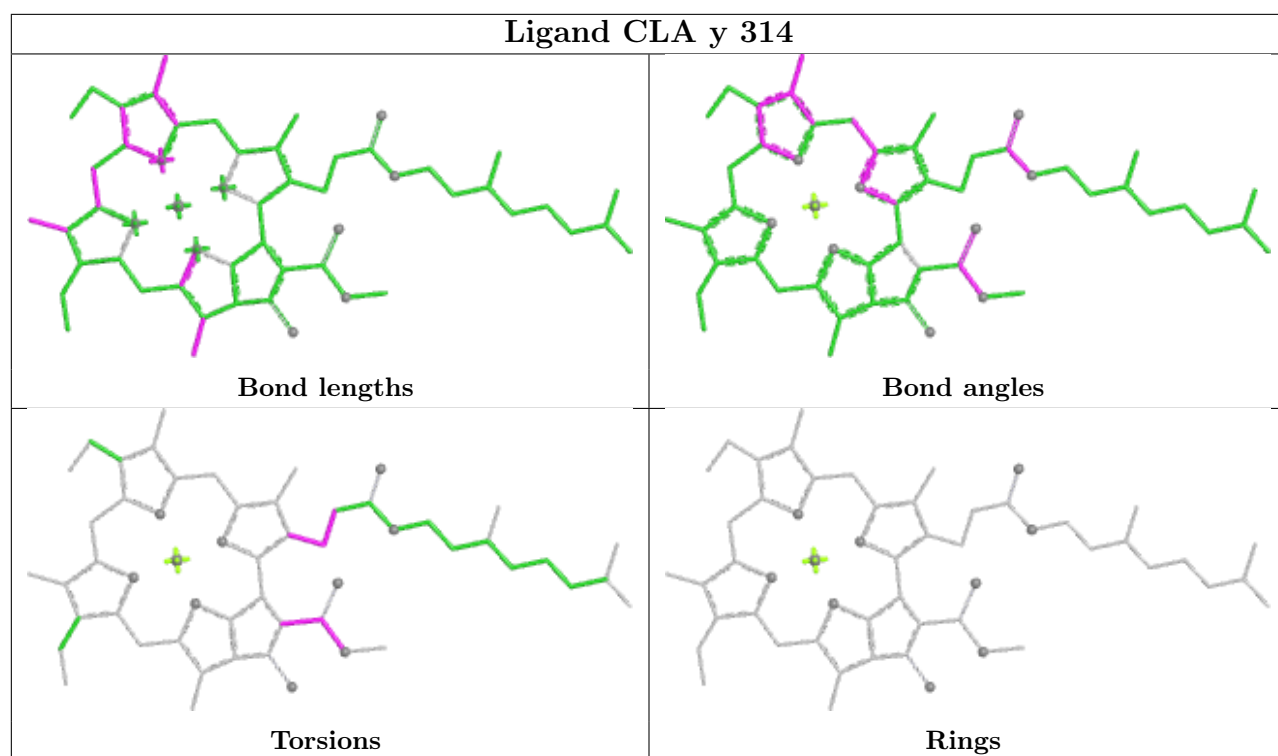


Torsions

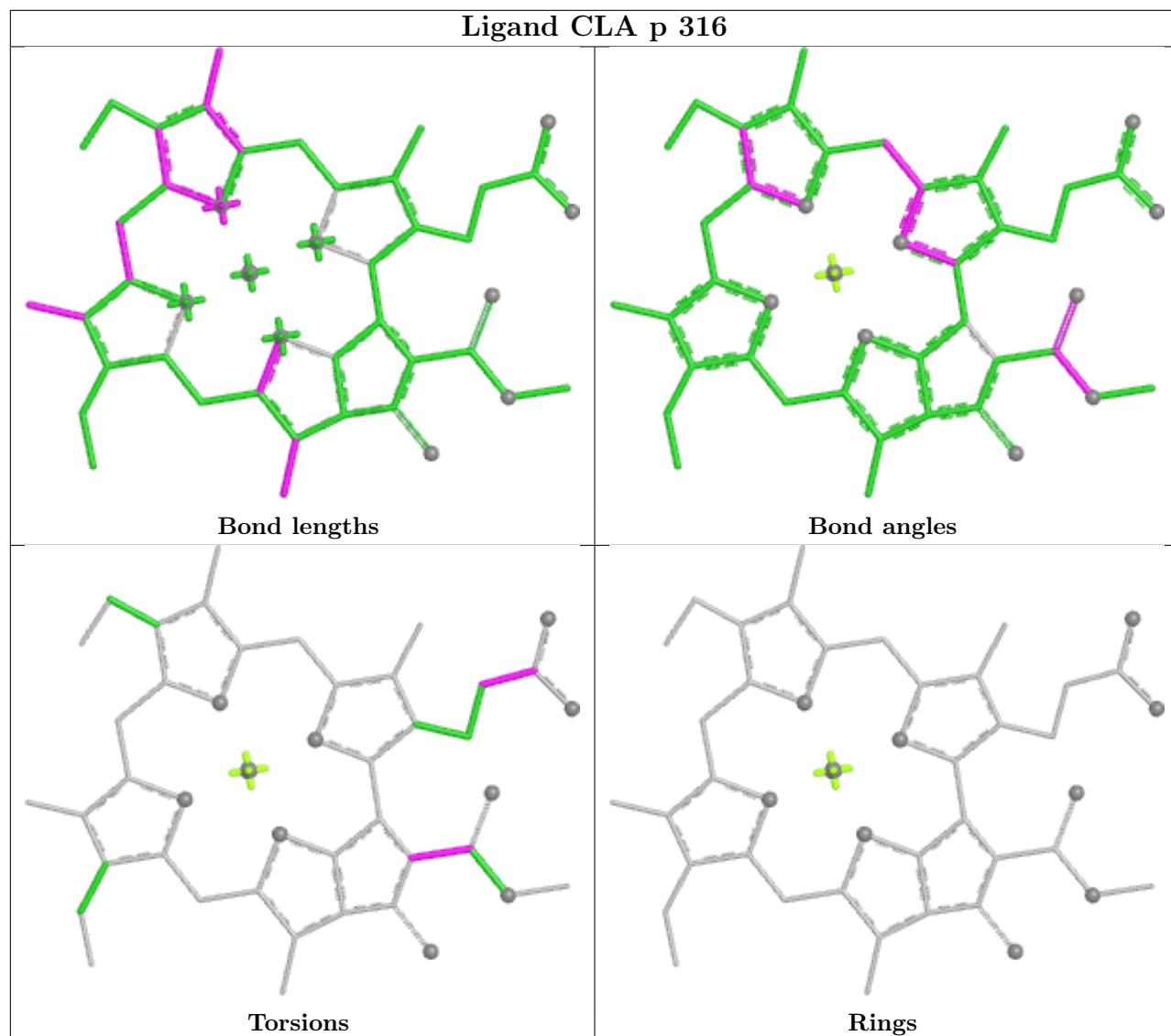


Rings

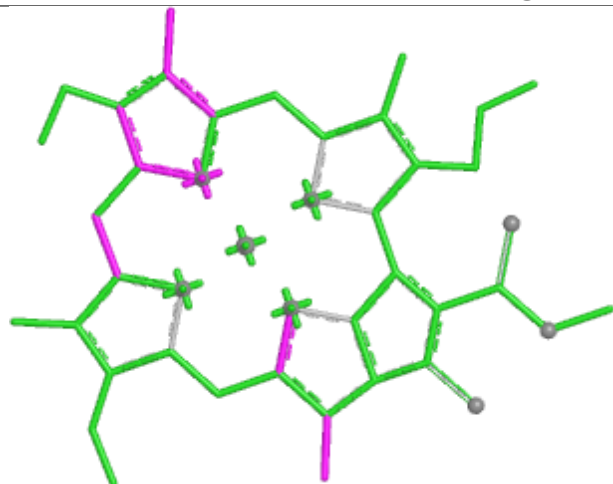
Ligand CHL 8 303**Ligand CLA 5 314**



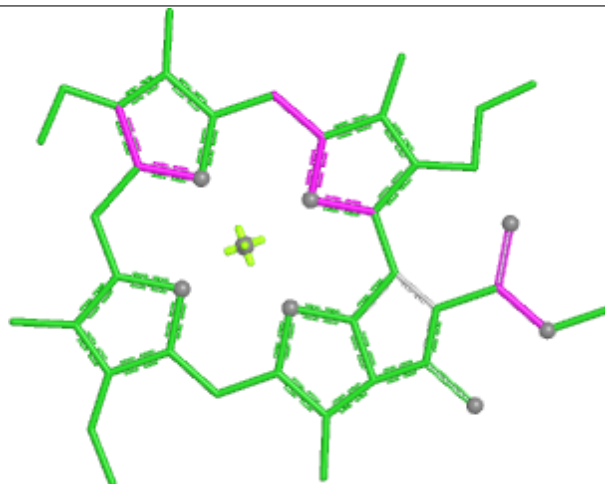
Ligand CLA p 316



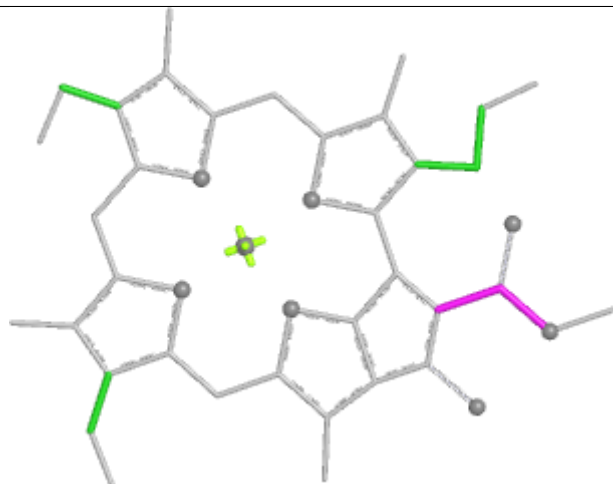
Ligand CLA 3 307



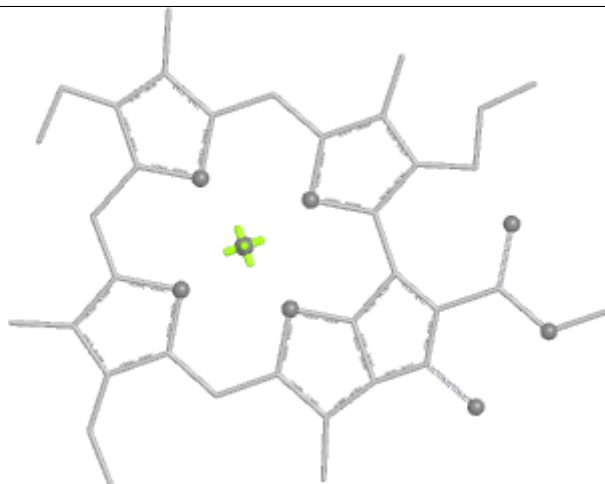
Bond lengths



Bond angles

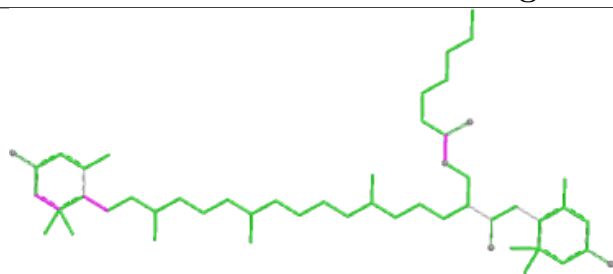


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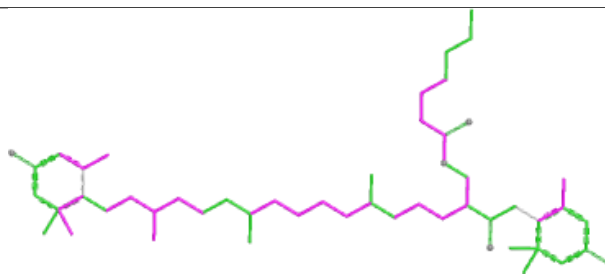


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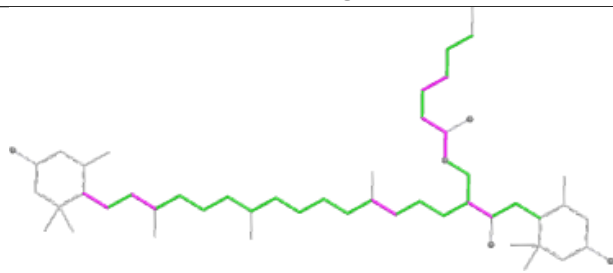
Ligand OUR 5 301



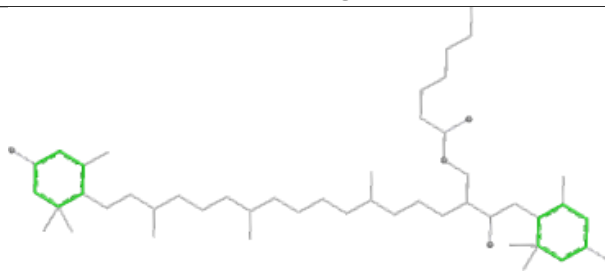
Bond lengths



Bond angles

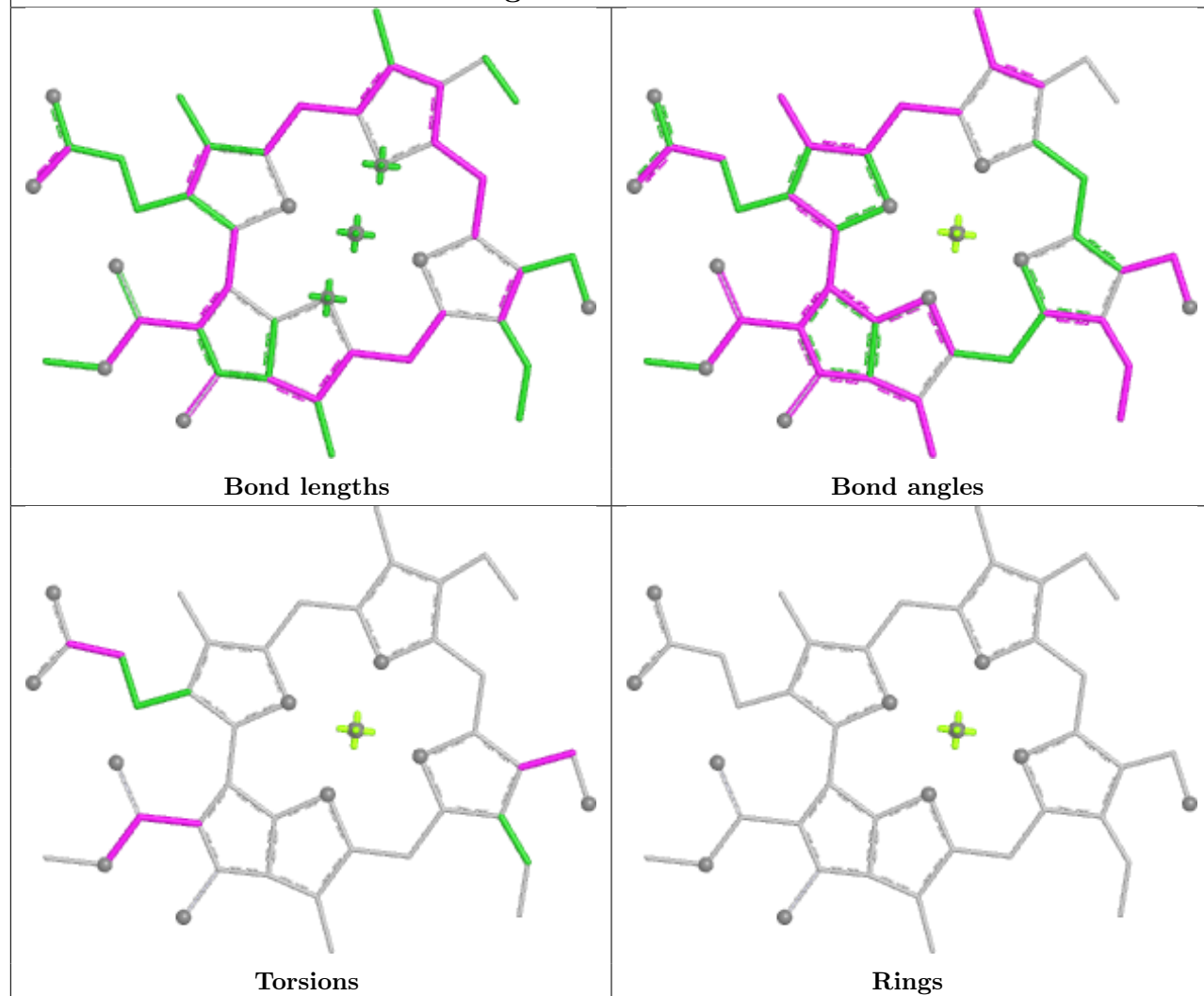


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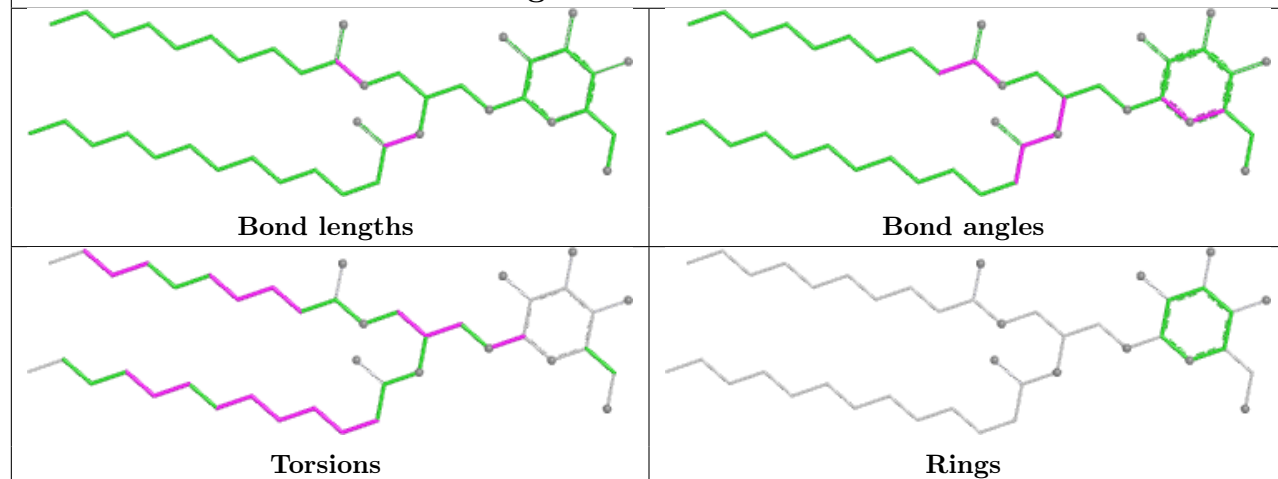


Rings

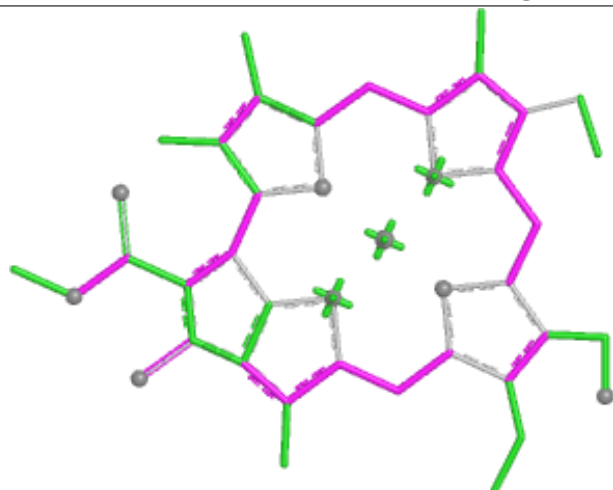
Ligand CHL 1 312



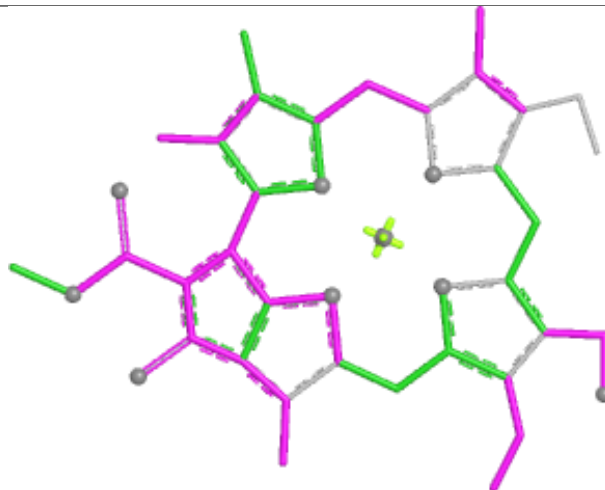
Ligand LMG C 618



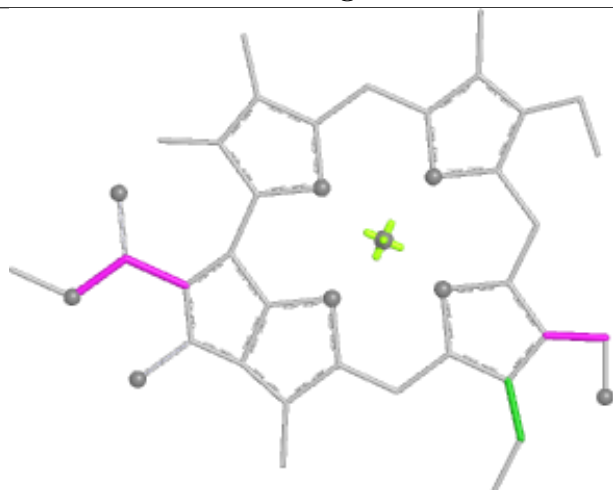
Ligand CHL 4 317



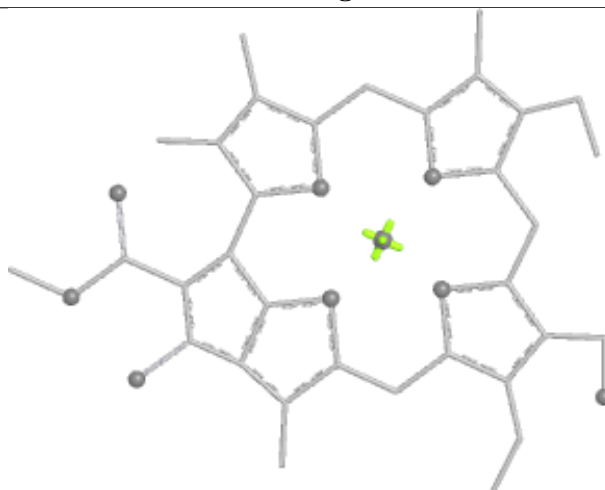
Bond lengths



Bond angles

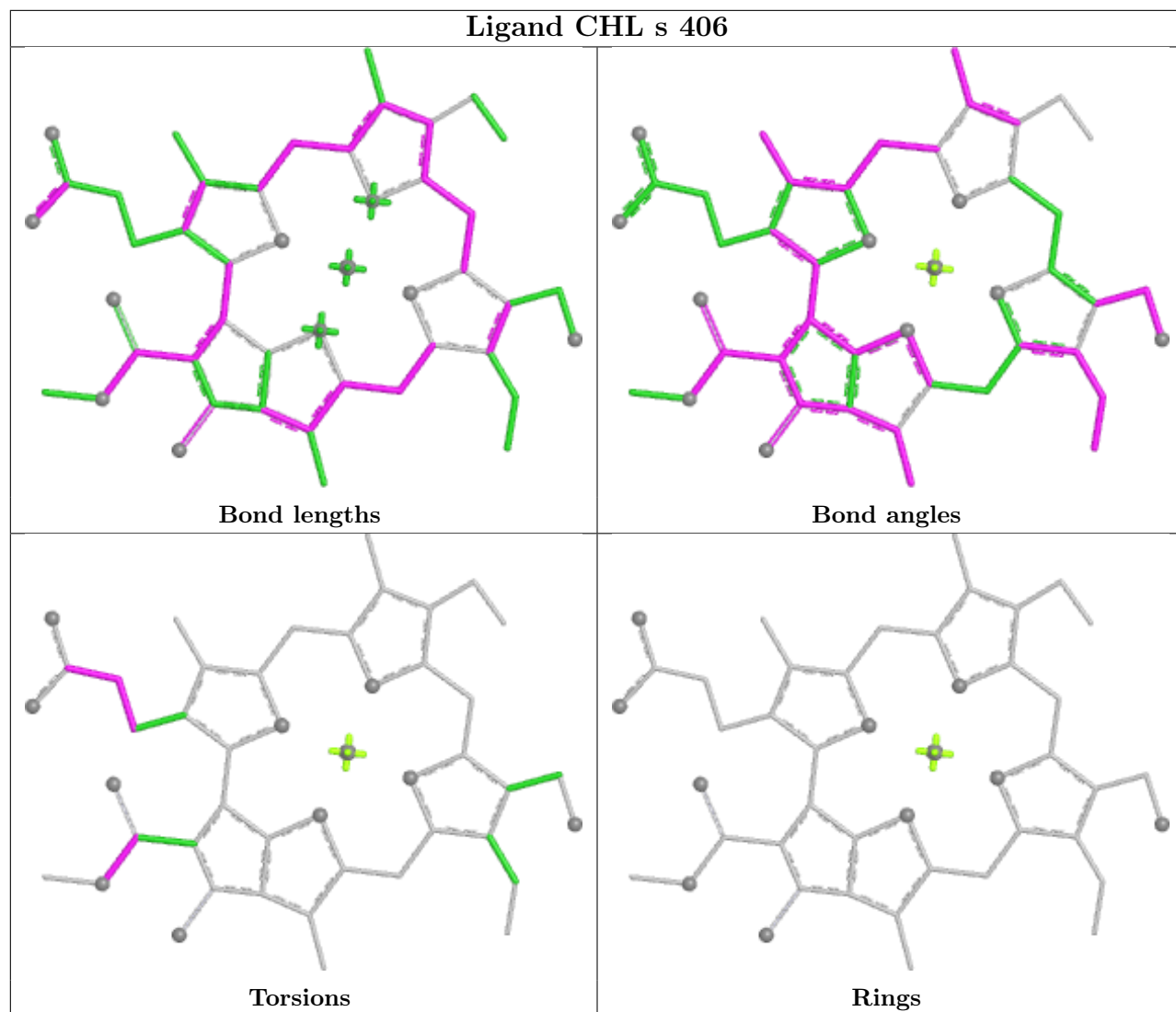


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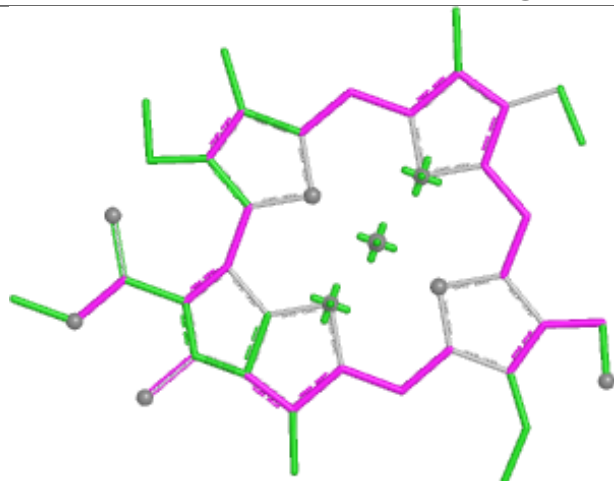


Rings

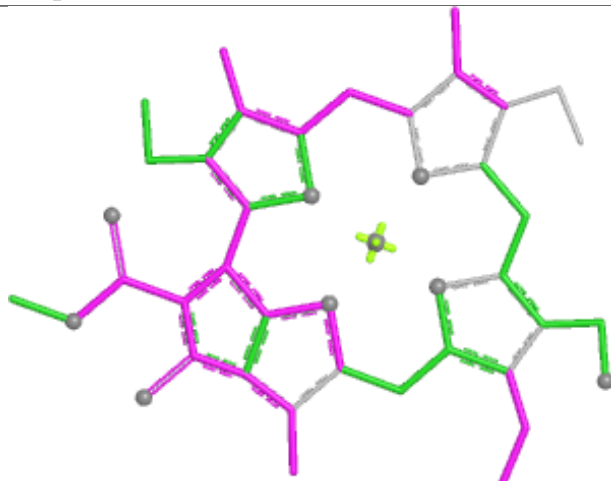
Ligand CHL s 406



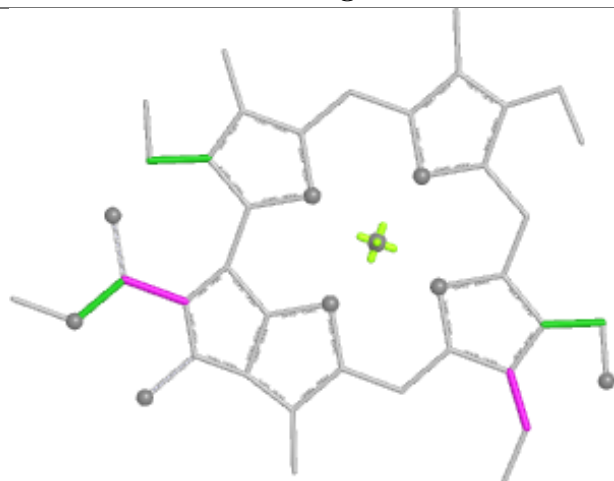
Ligand CHL p 309



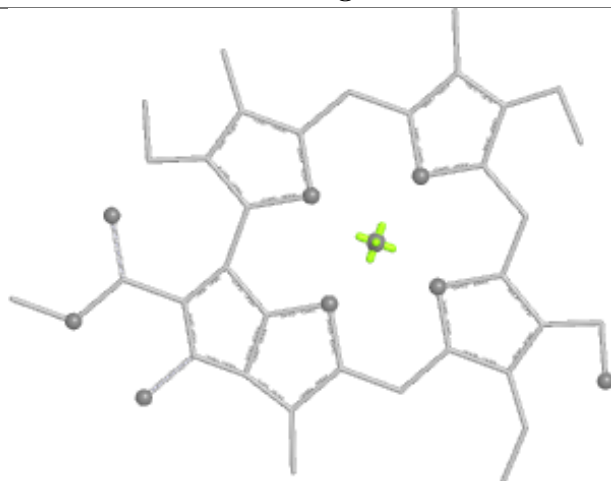
Bond lengths



Bond angles

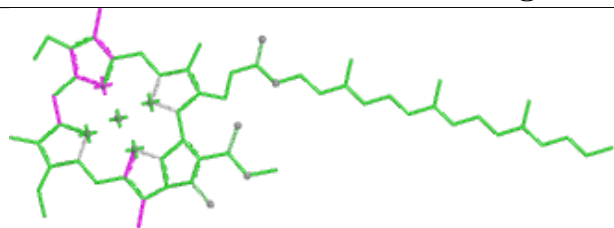


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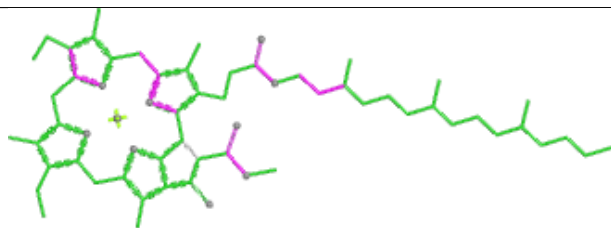


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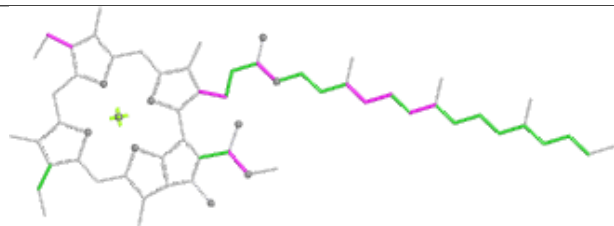
Ligand CLA 9 314



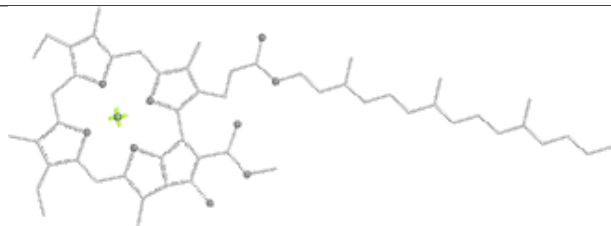
Bond lengths



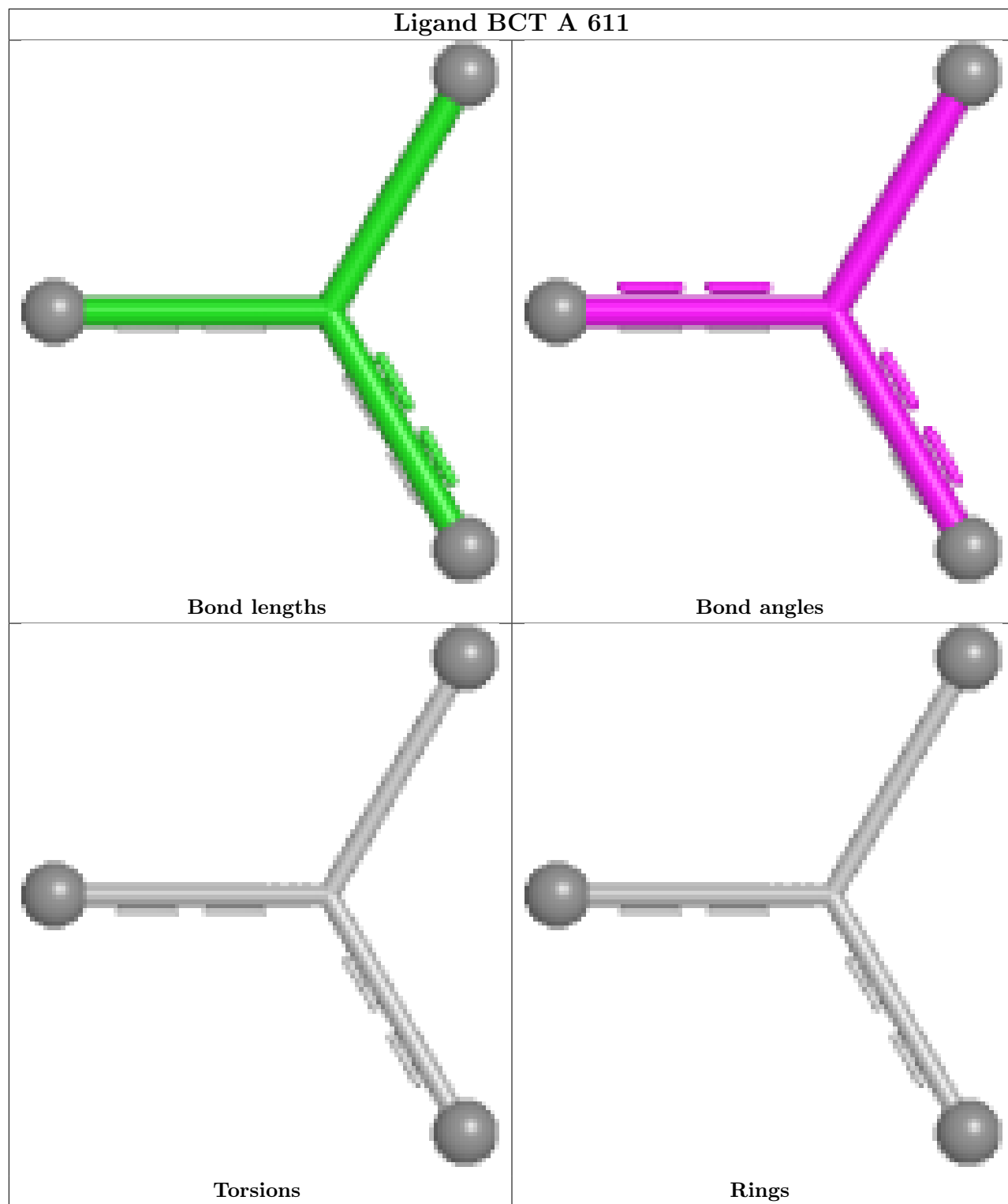
Bond angles



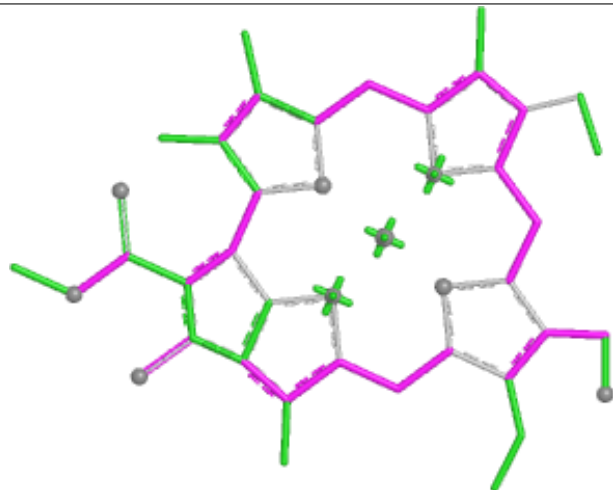
Torsions



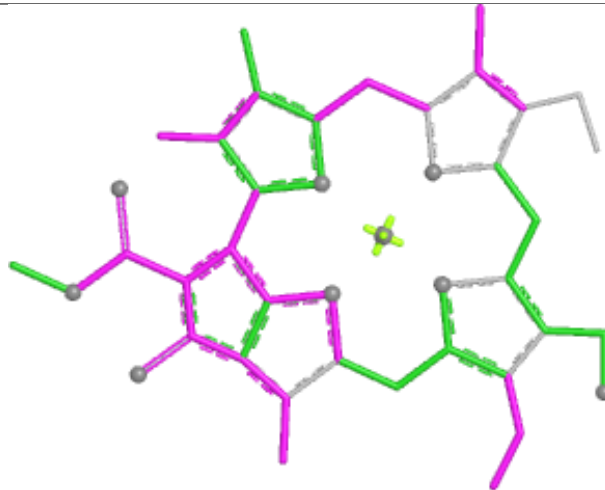
Rings



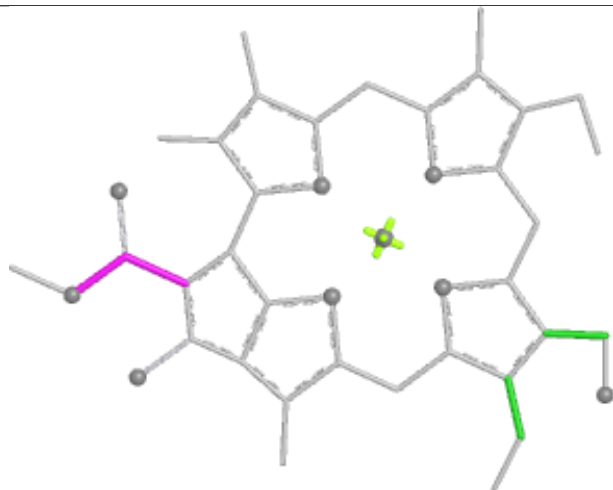
Ligand CHL 1 304



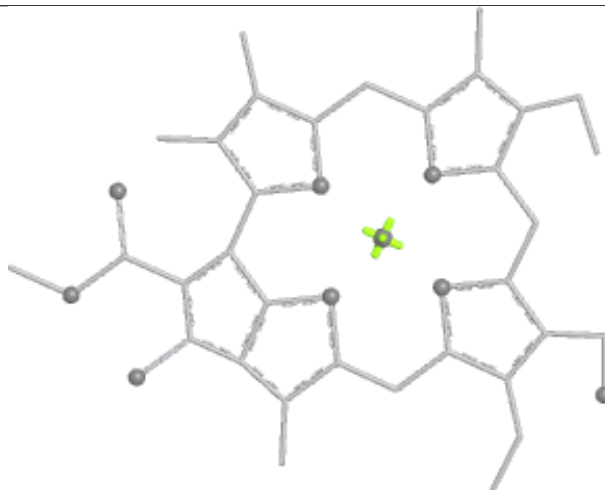
Bond lengths



Bond angles

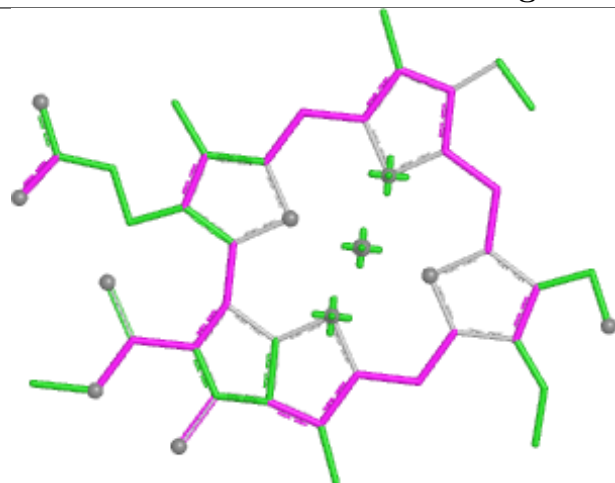


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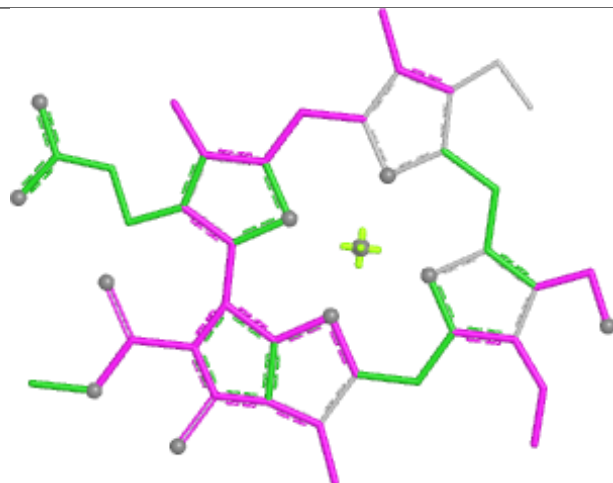


Rings

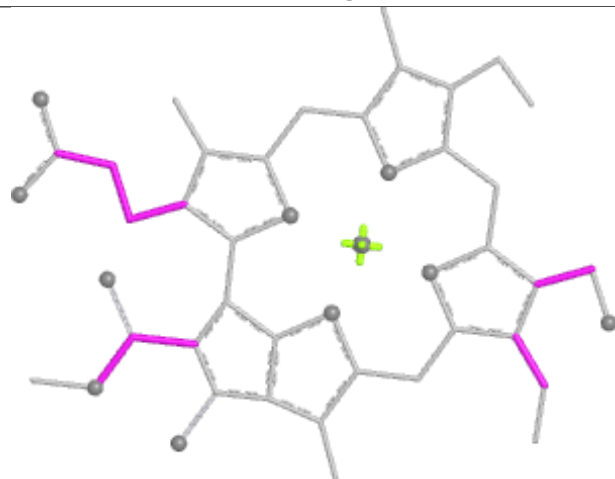
Ligand CHL S 601



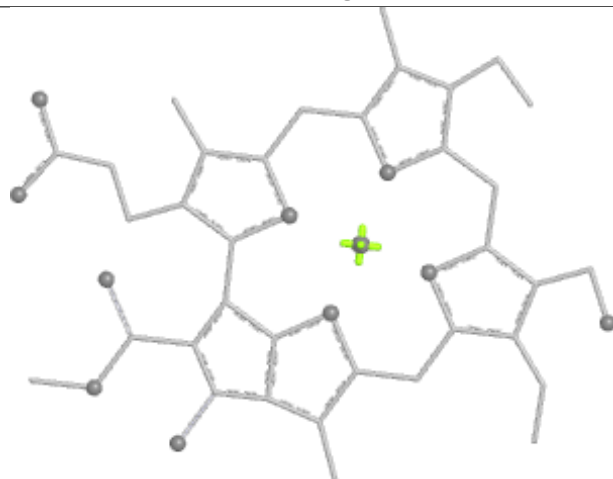
Bond lengths



Bond angles

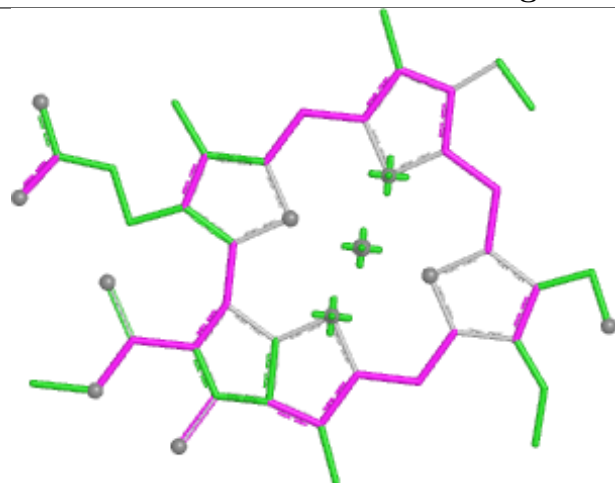


Torsions

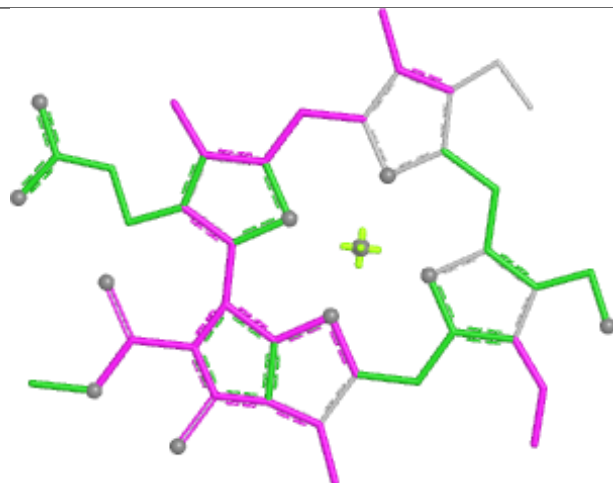


Rings

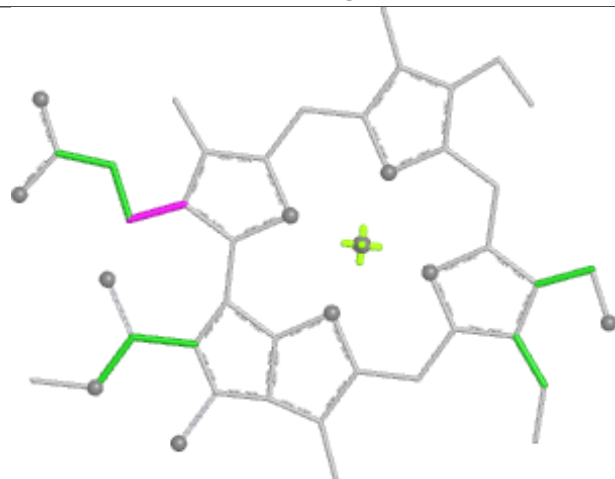
Ligand CHL 7 311



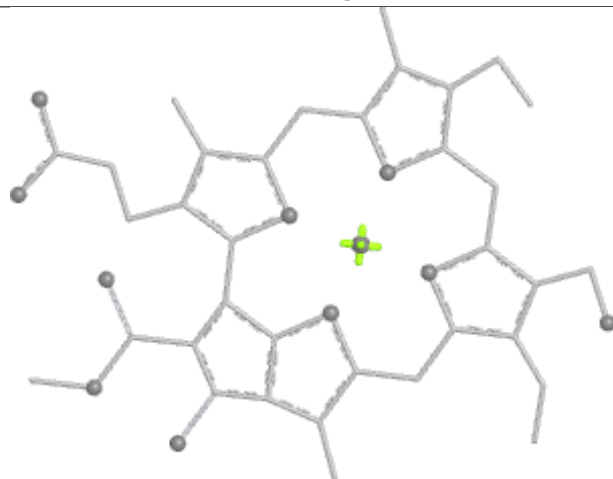
Bond lengths



Bond angles

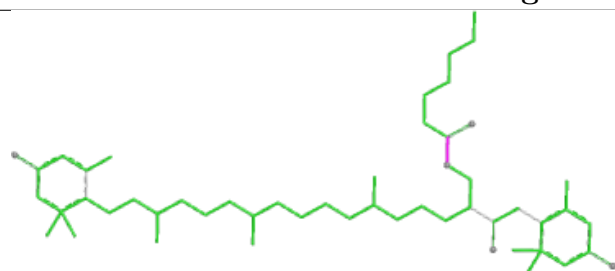


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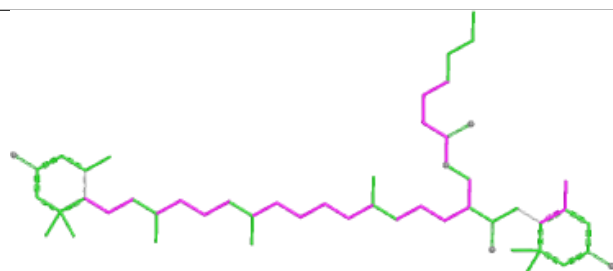


Rings

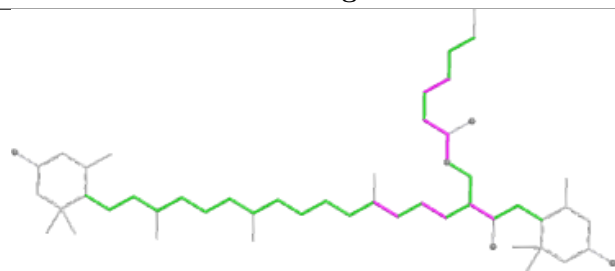
Ligand OUR 3 301



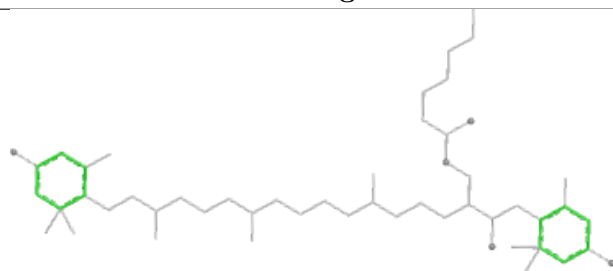
Bond lengths



Bond angles

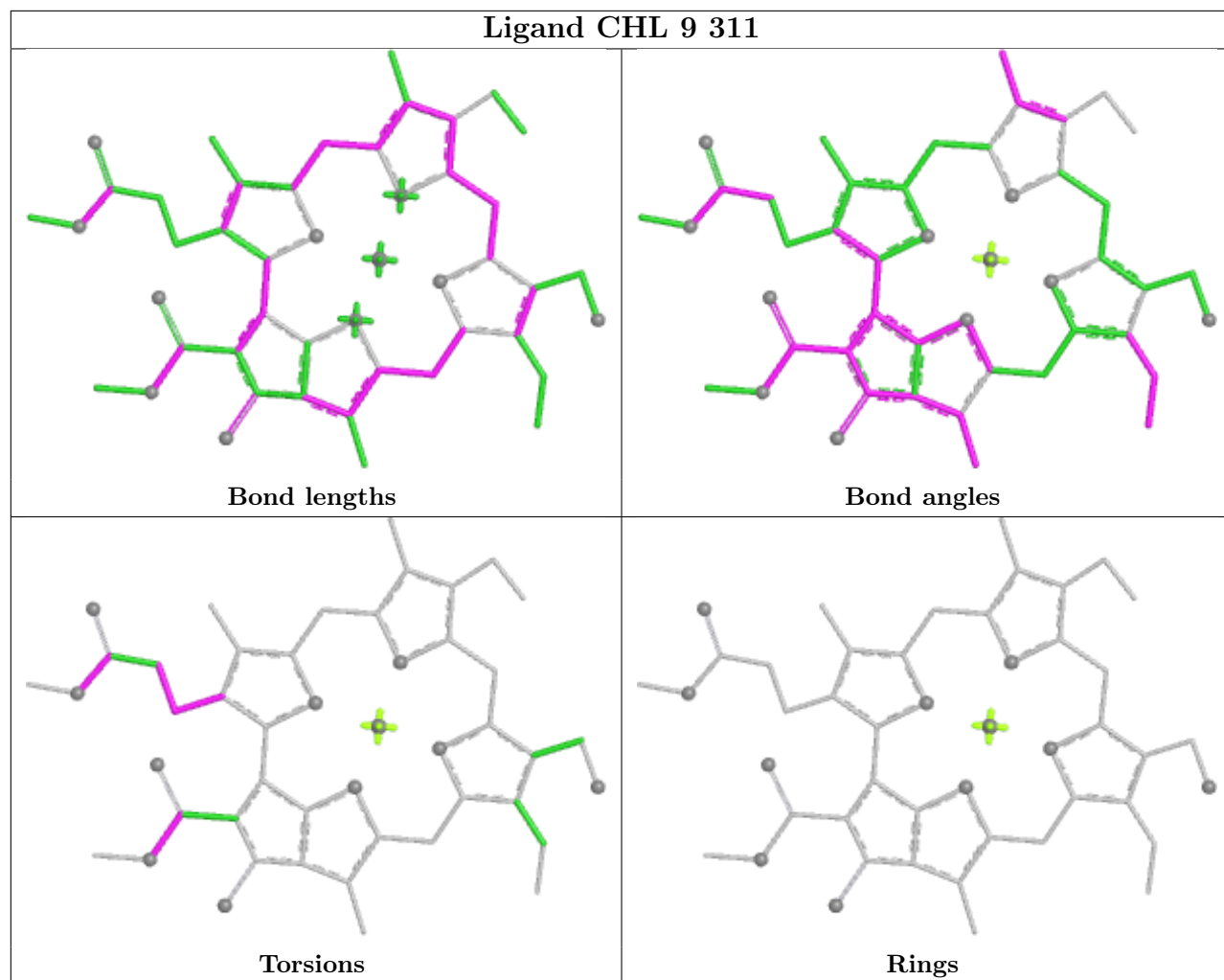


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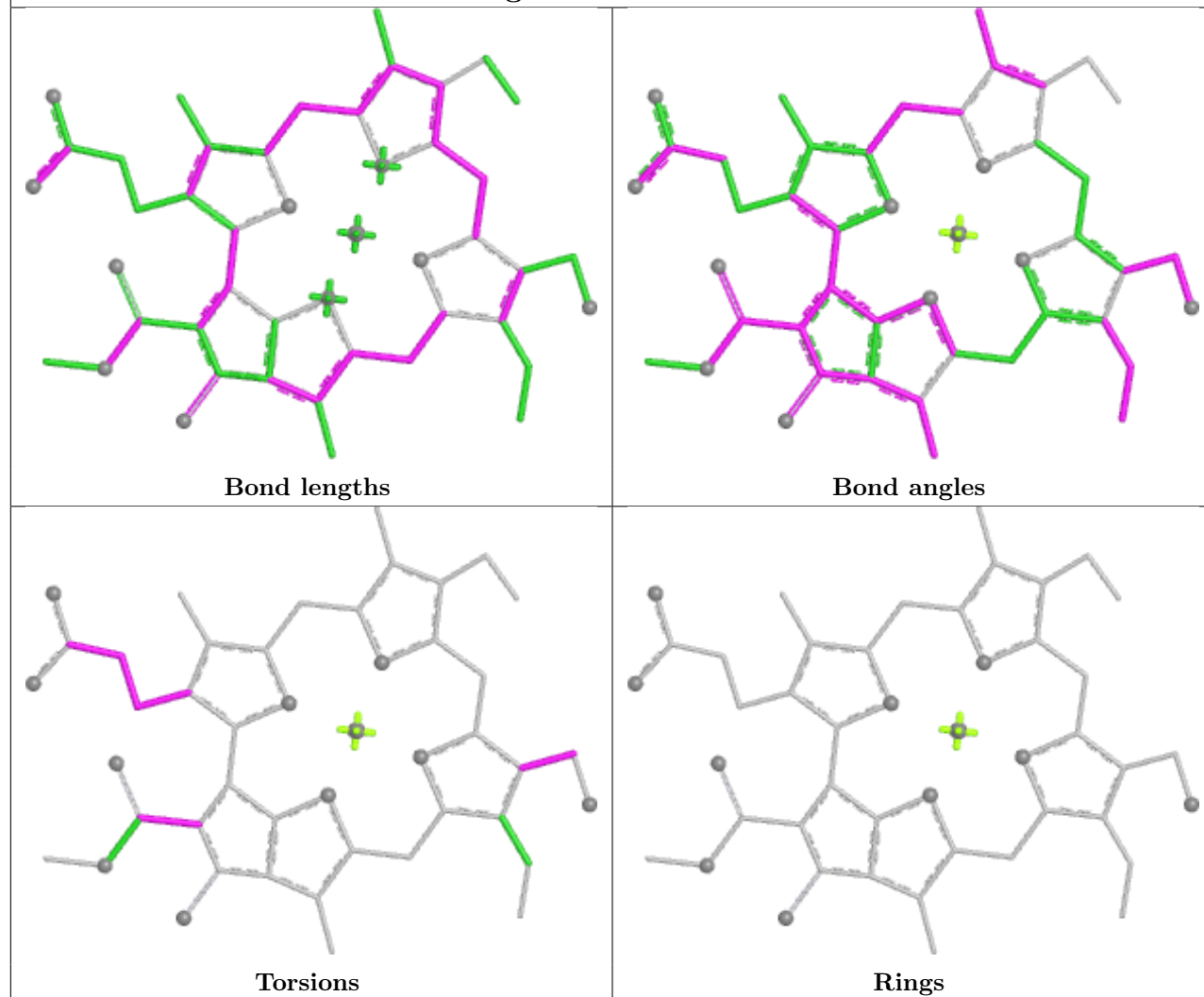


Rings

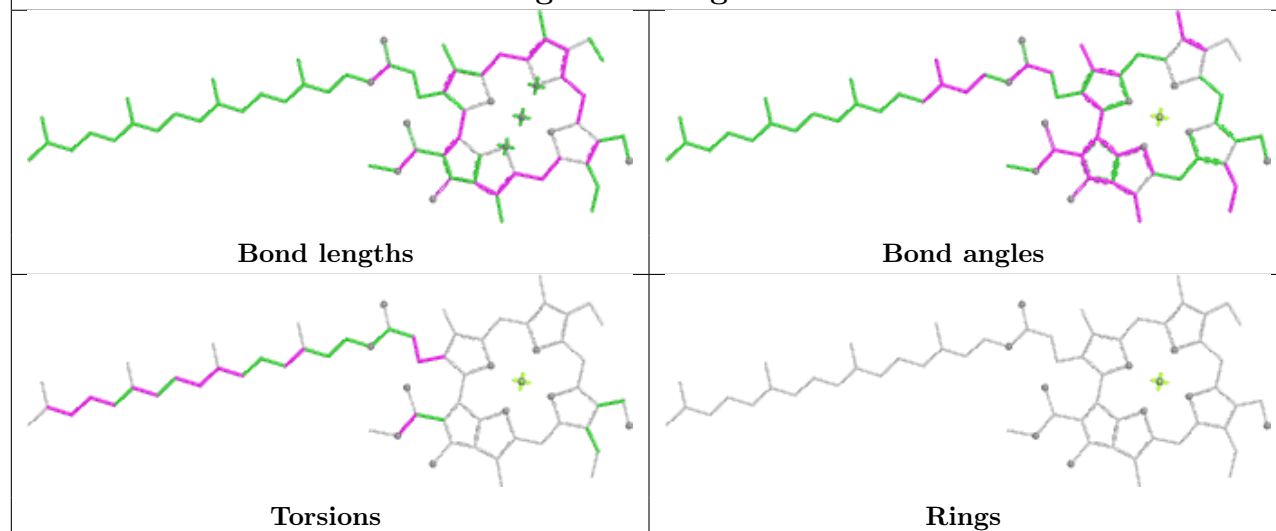
Ligand CHL 9 311



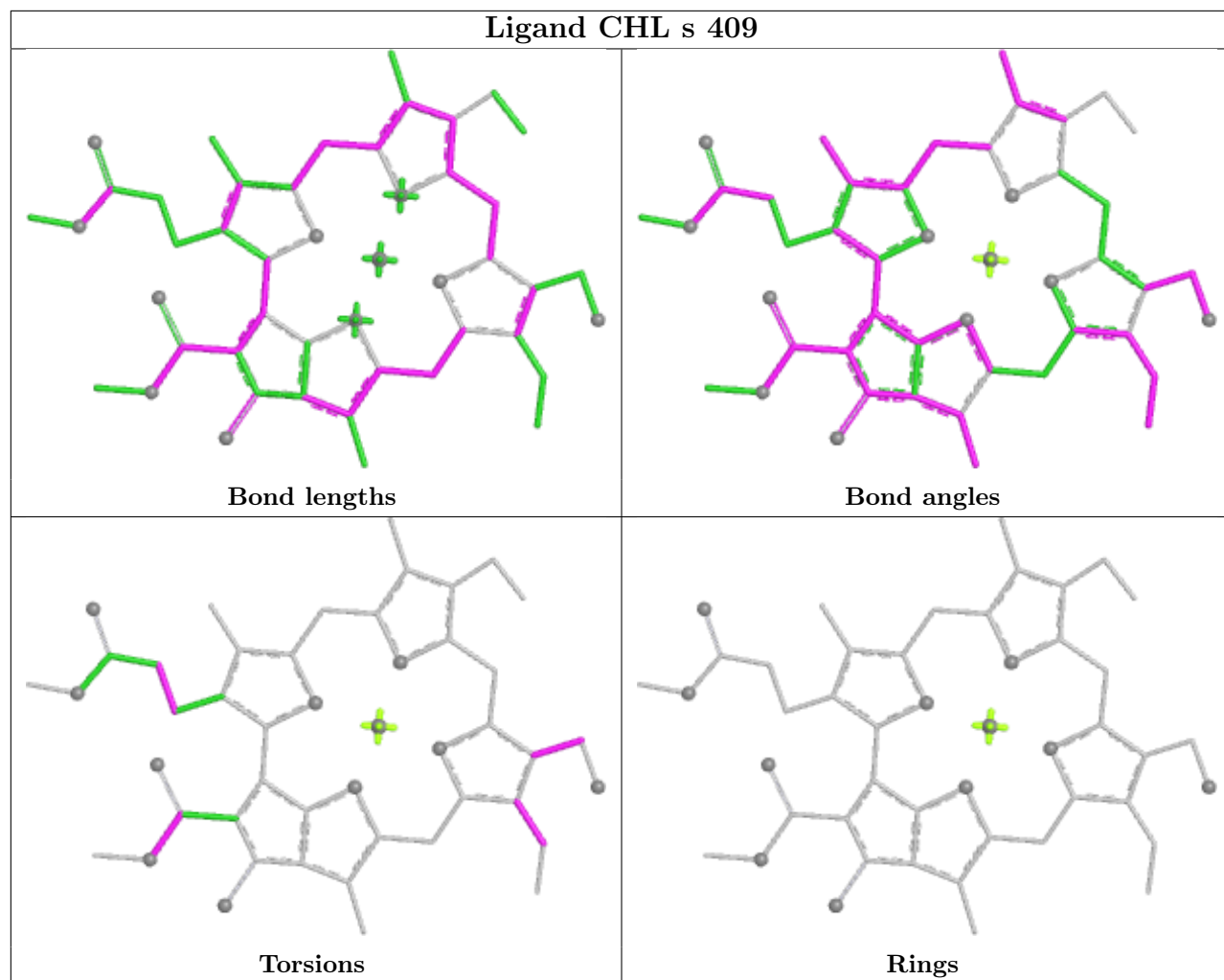
Ligand CHL 1 305



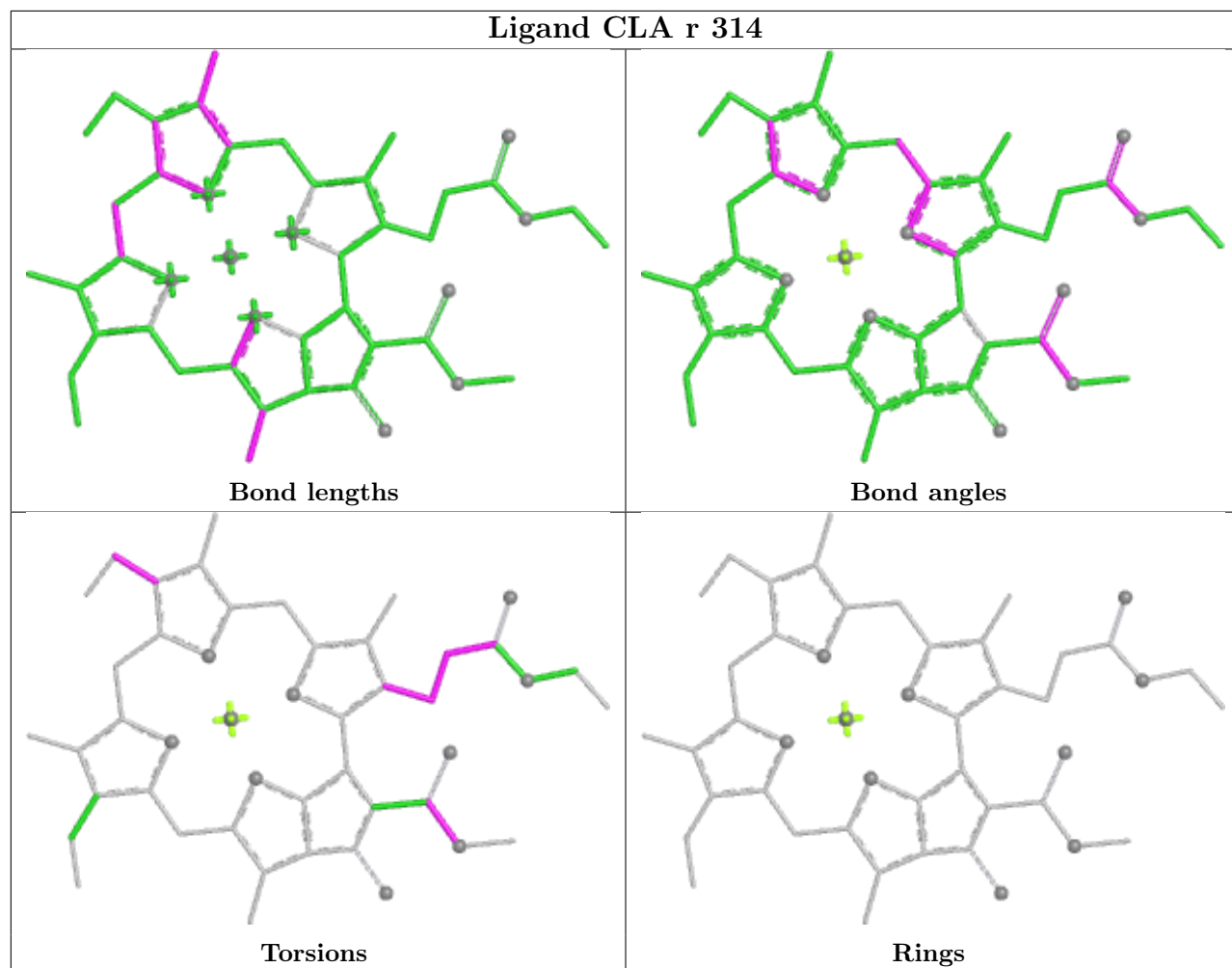
Ligand CHL g 305

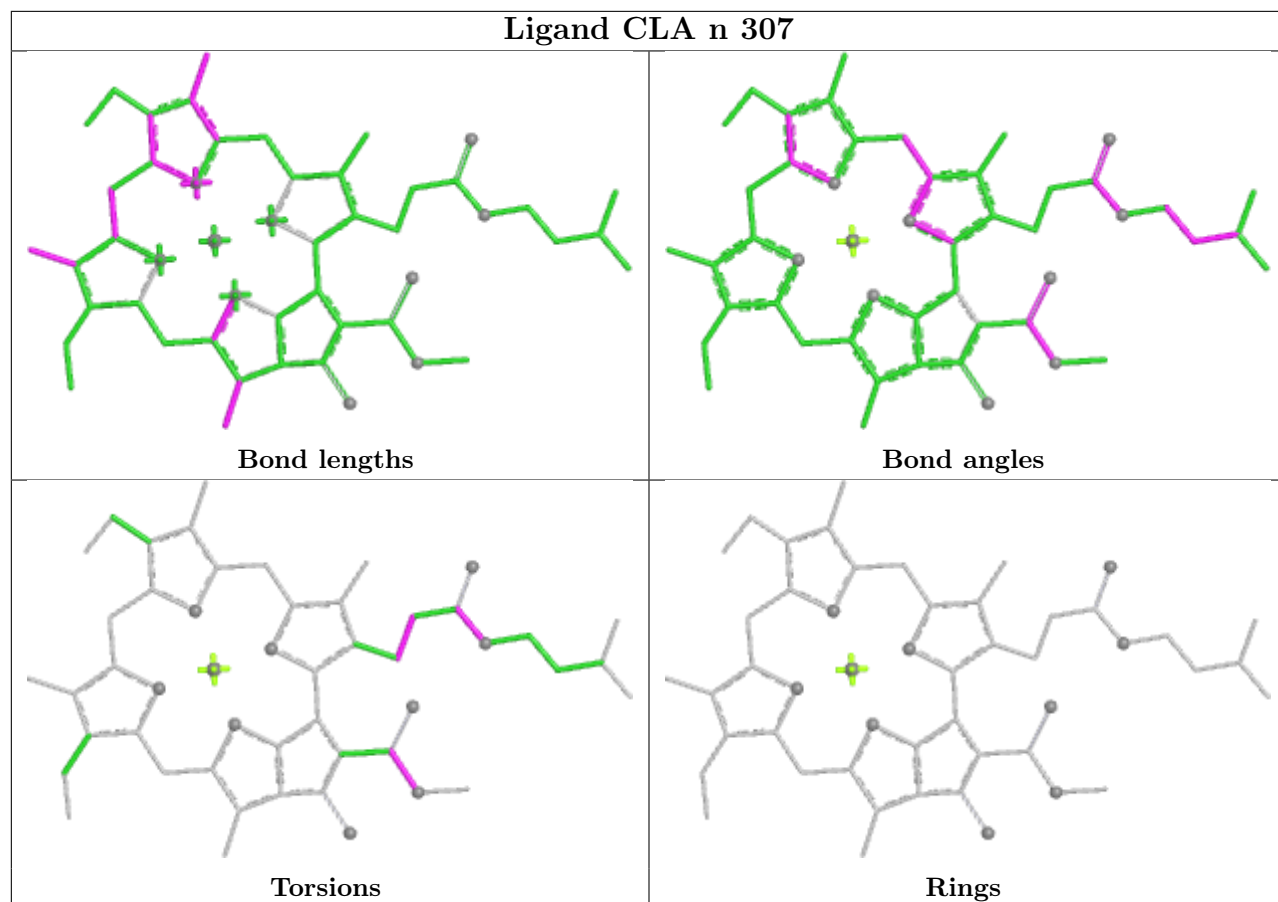


Ligand CHL s 409

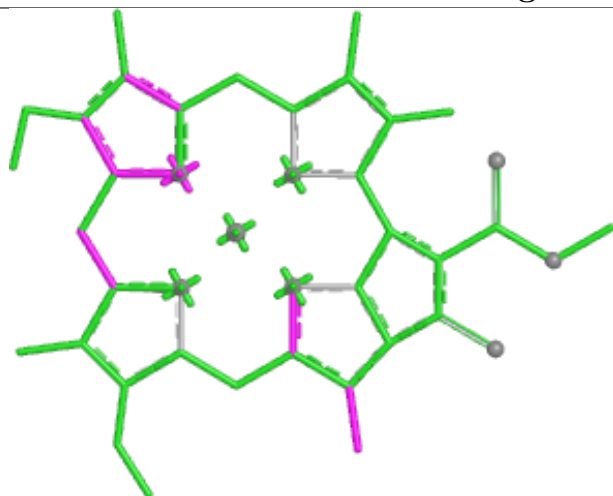


Ligand CLA r 314

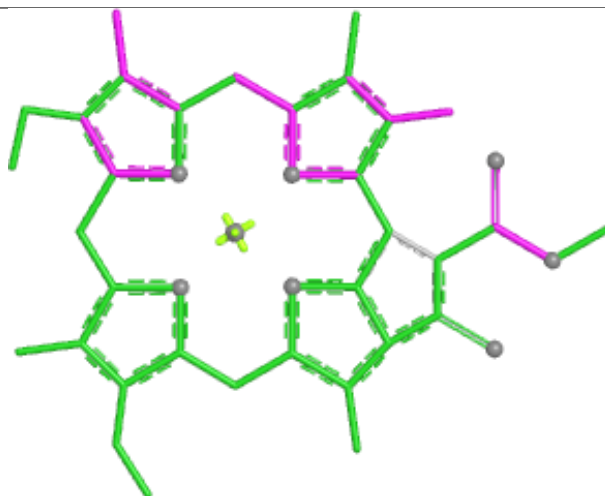




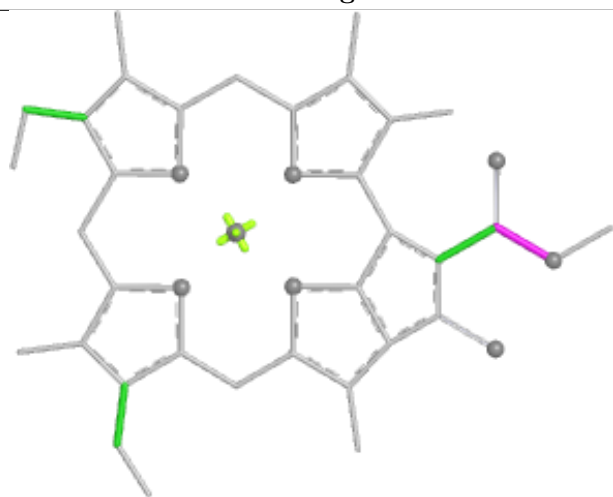
Ligand CLA 3 314



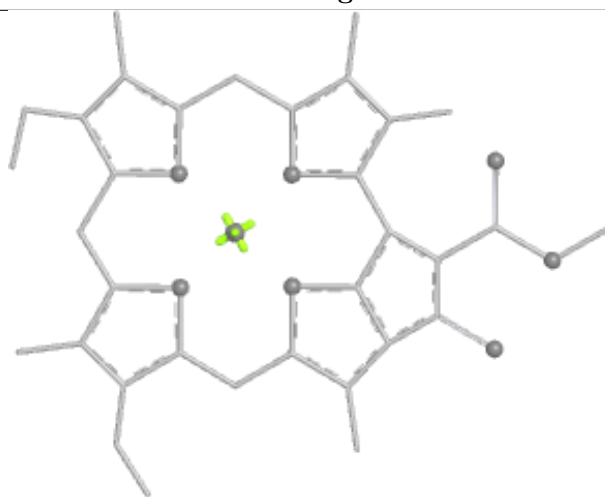
Bond lengths



Bond angles

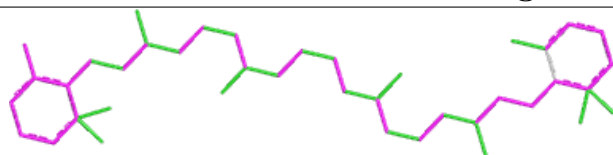


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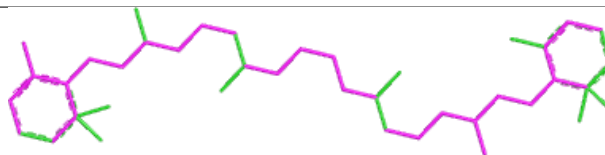


Rings

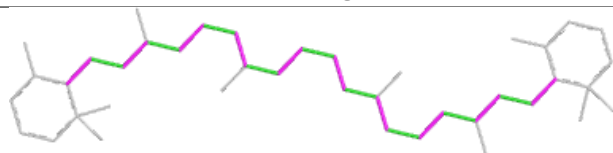
Ligand 8CT C 614



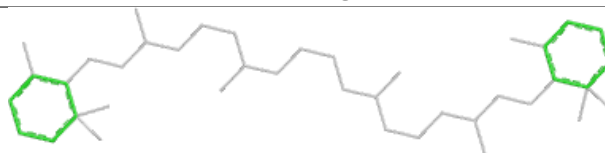
Bond lengths



Bond angles

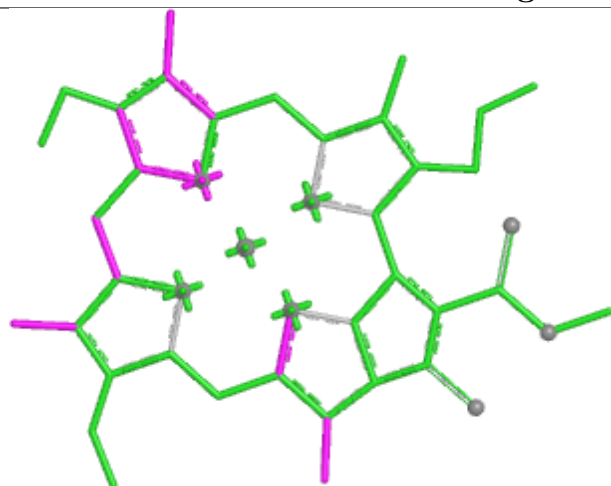


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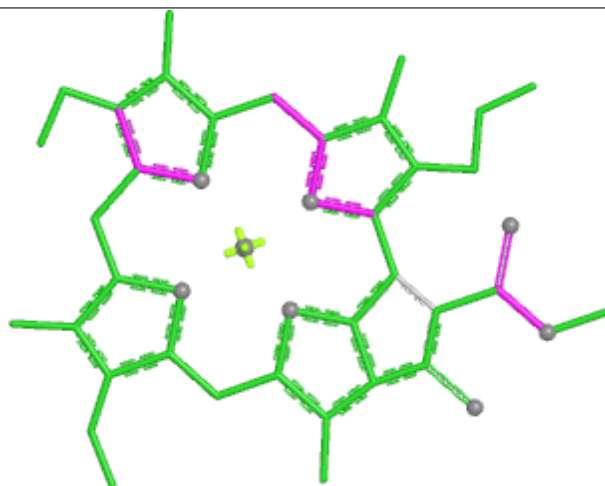


Rings

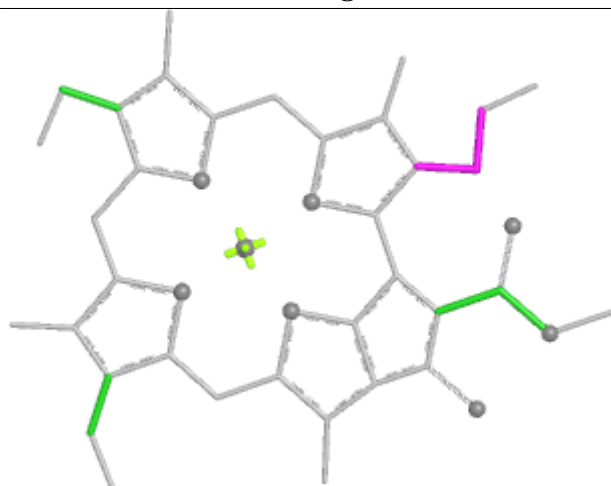
Ligand CLA n 316



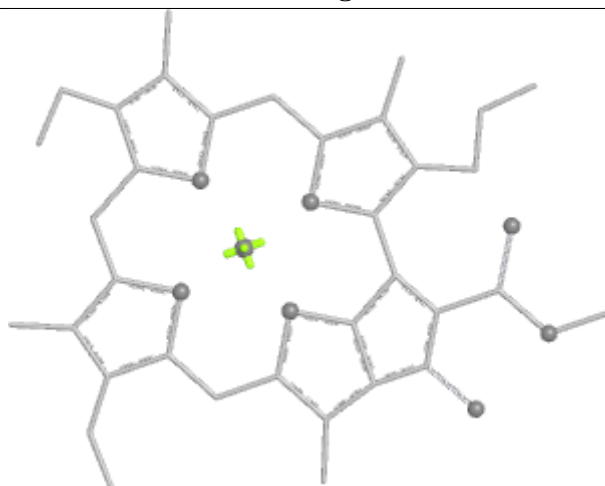
Bond lengths



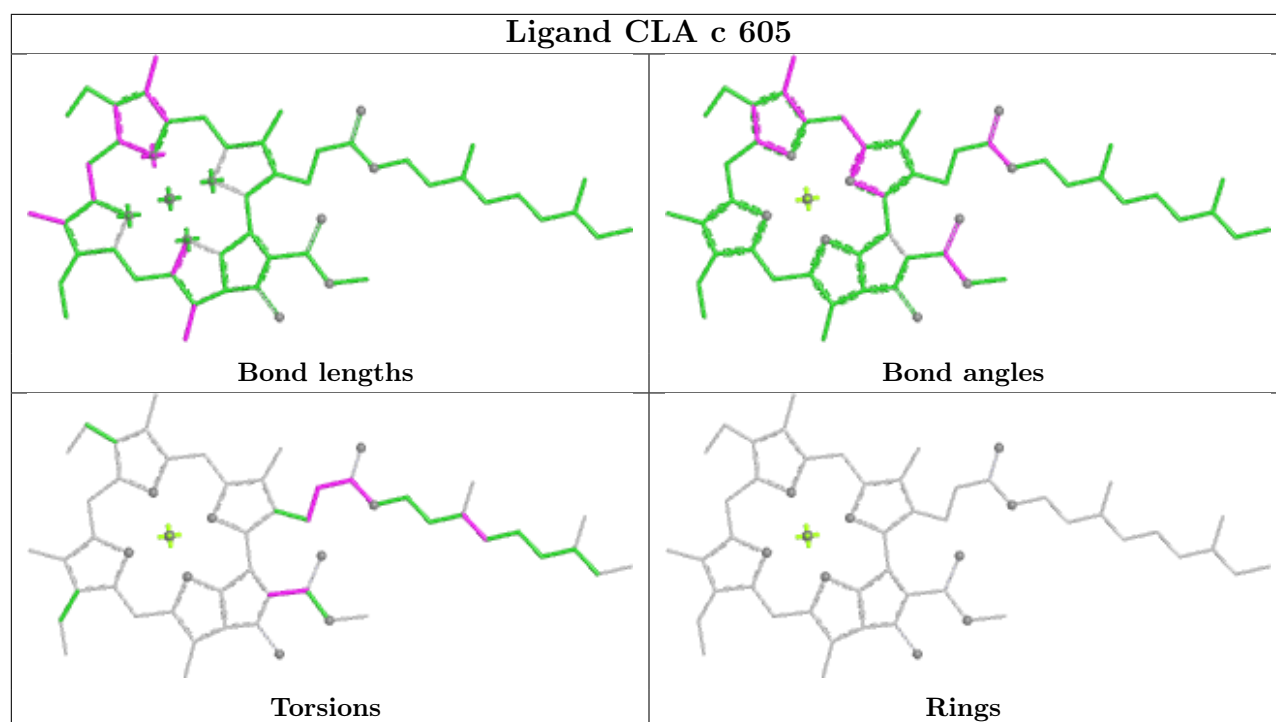
Bond angles



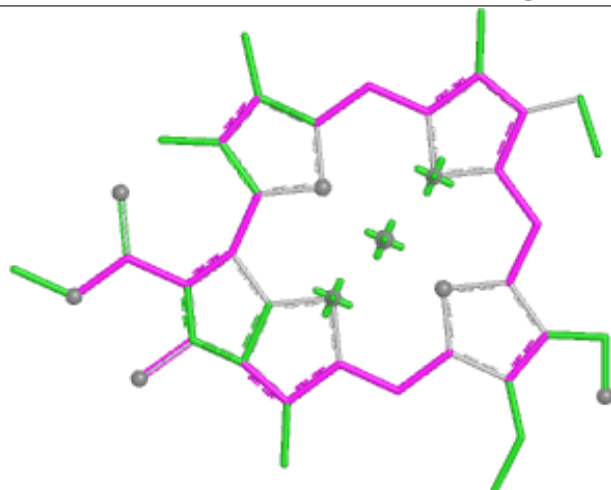
Torsions



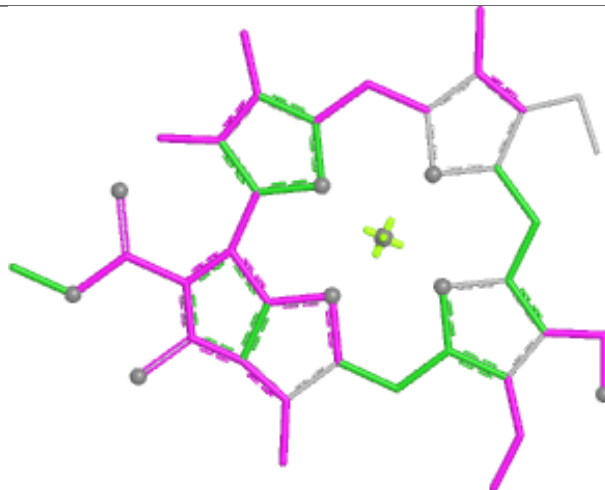
Rings



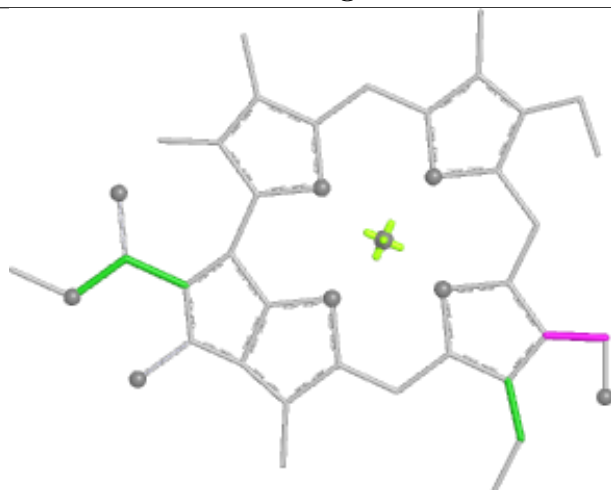
Ligand CHL s 414



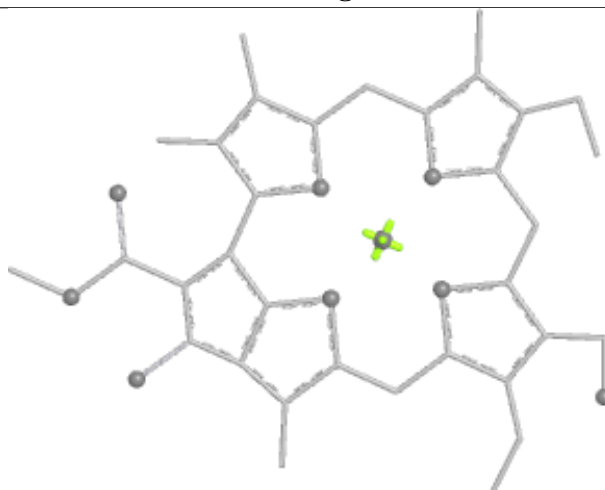
Bond lengths



Bond angles

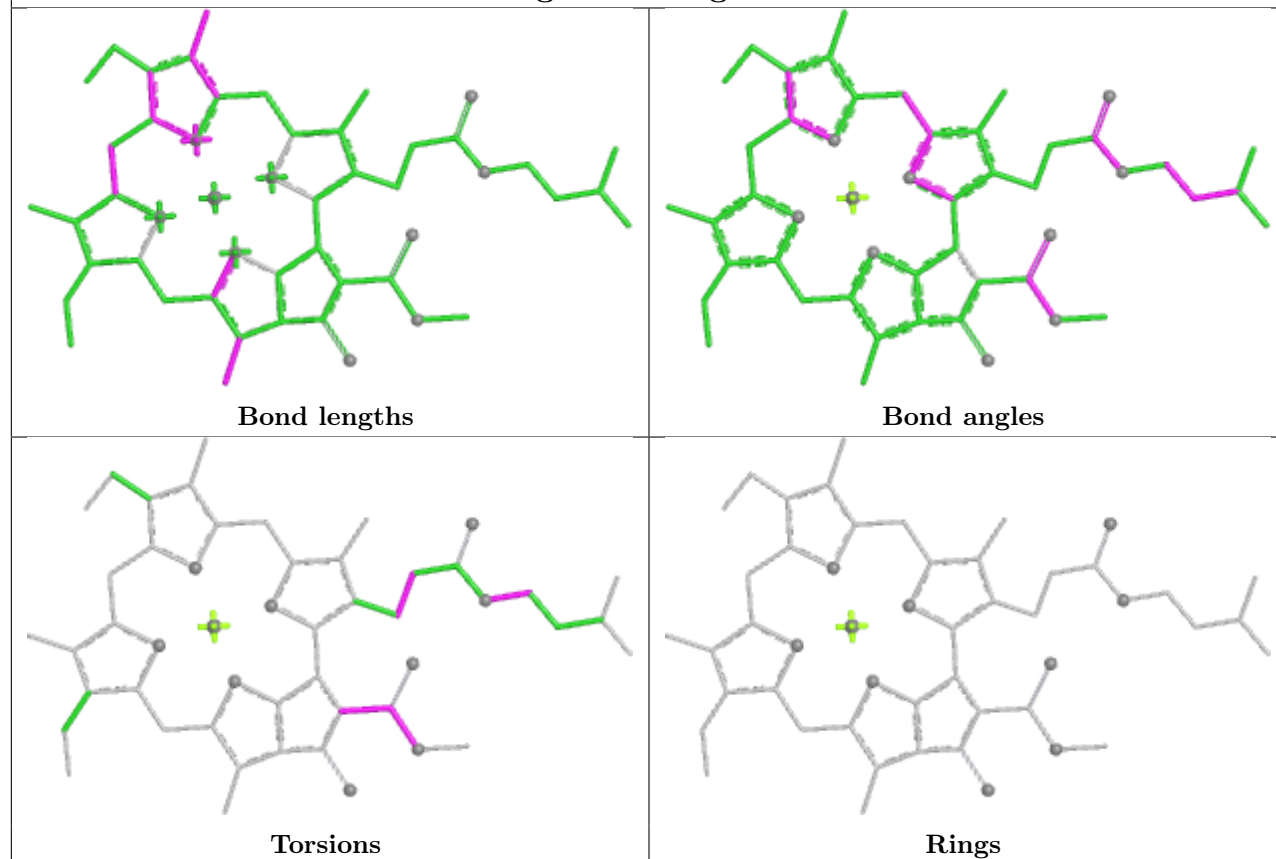


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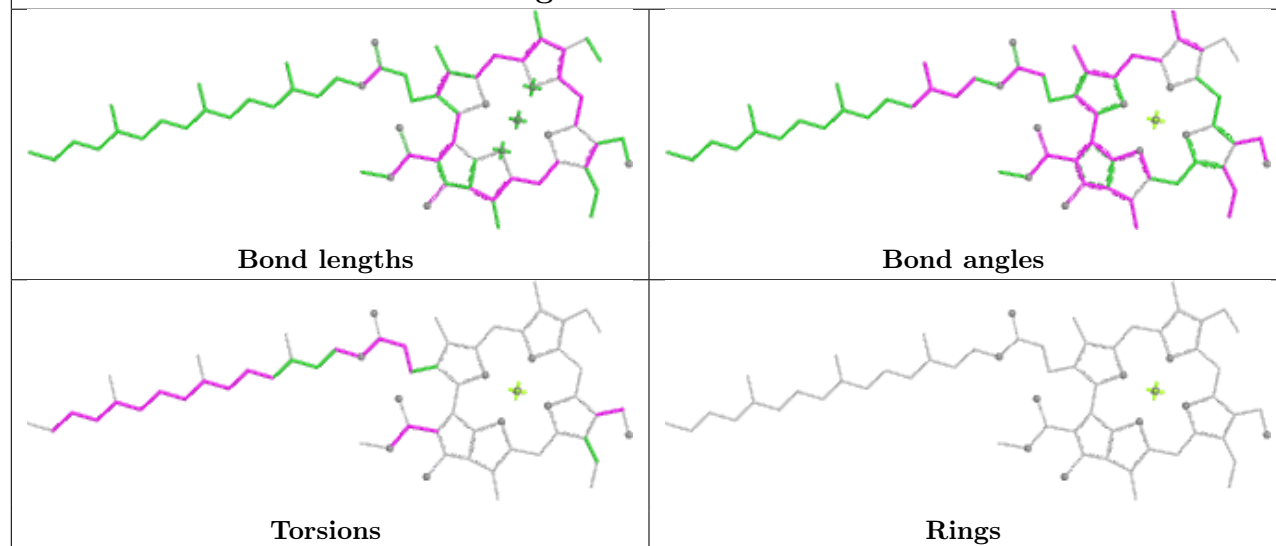


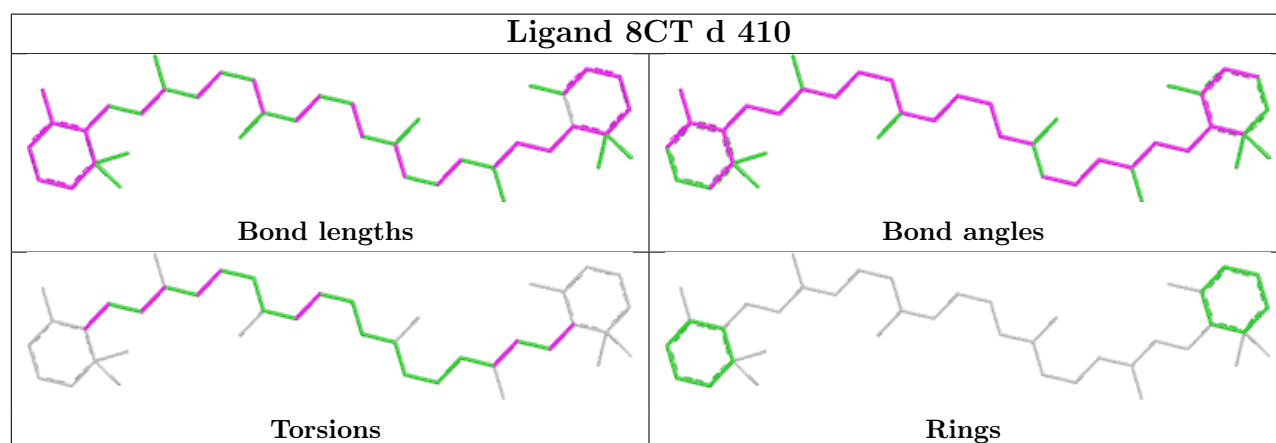
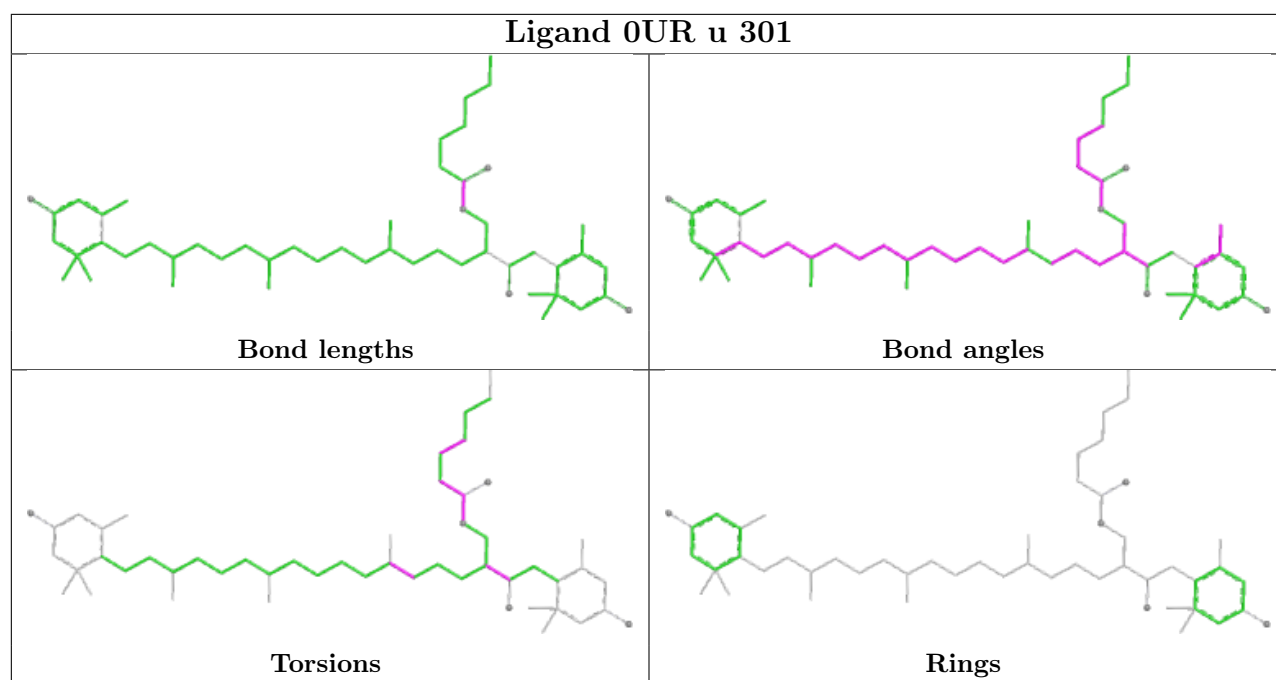
Rings

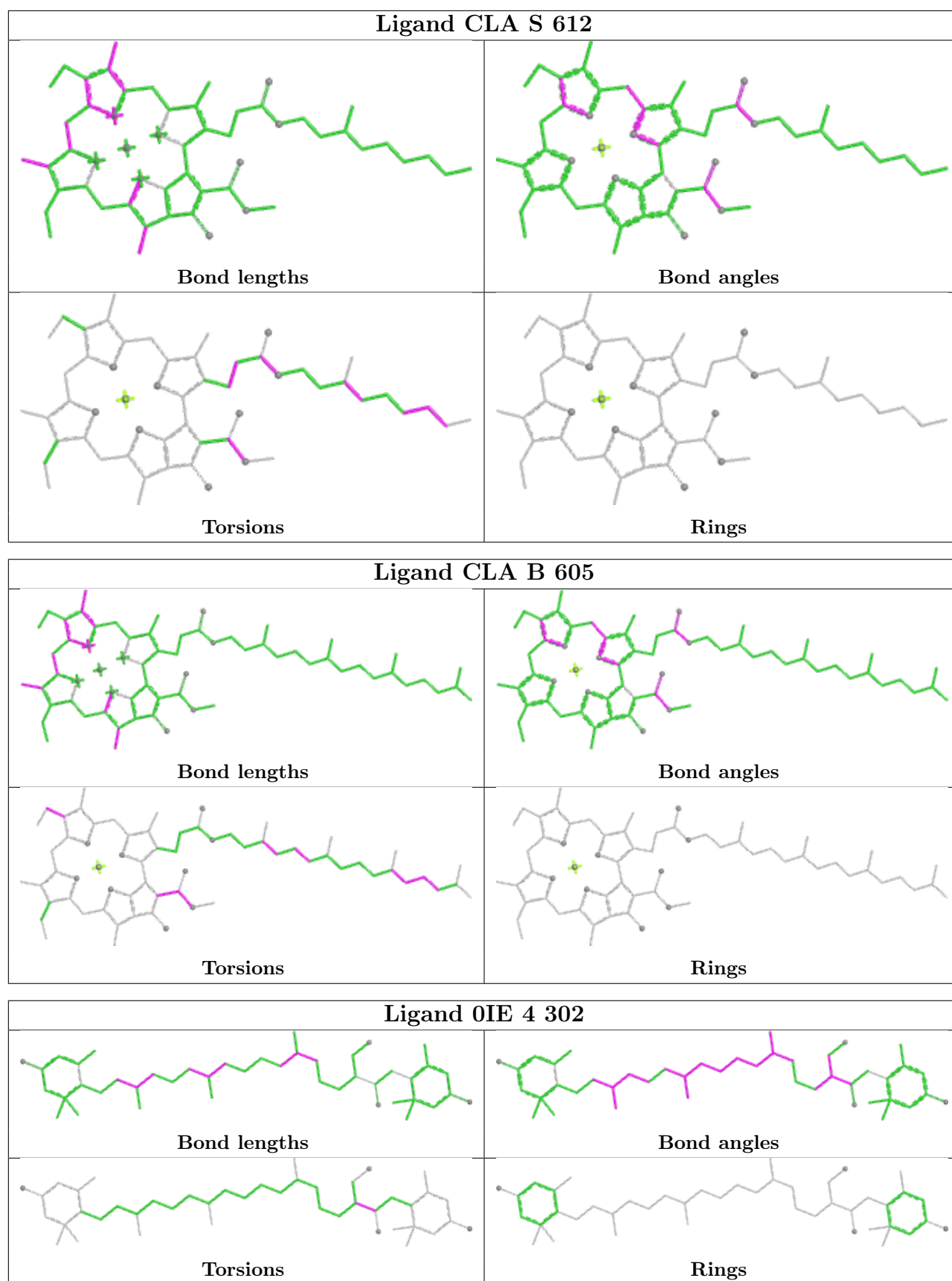
Ligand CLA g 308

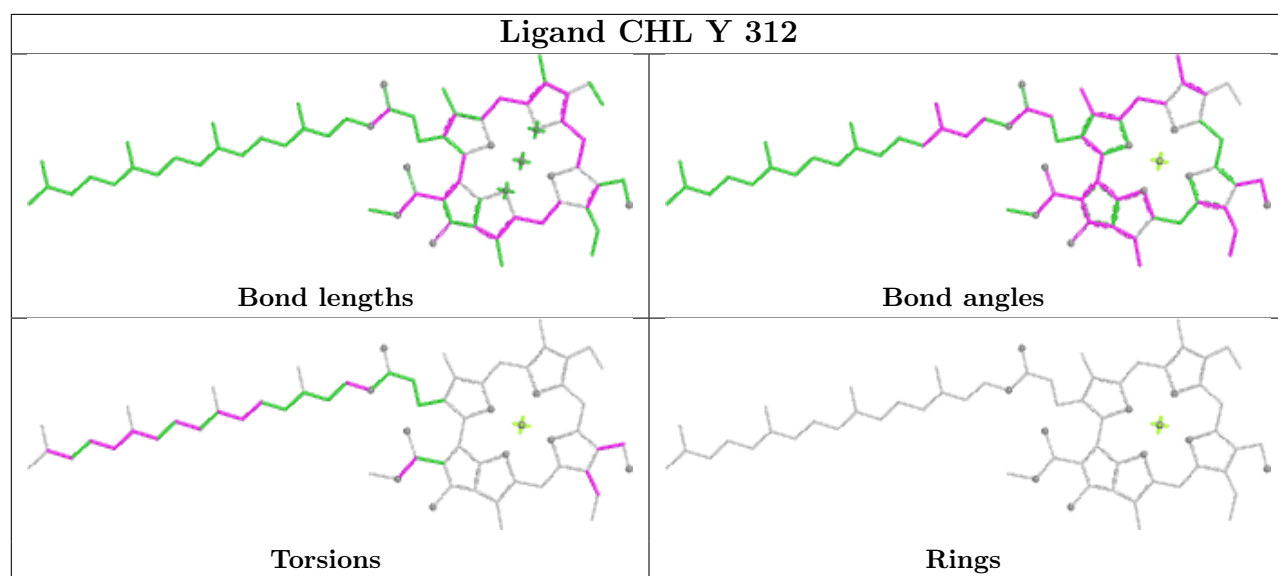
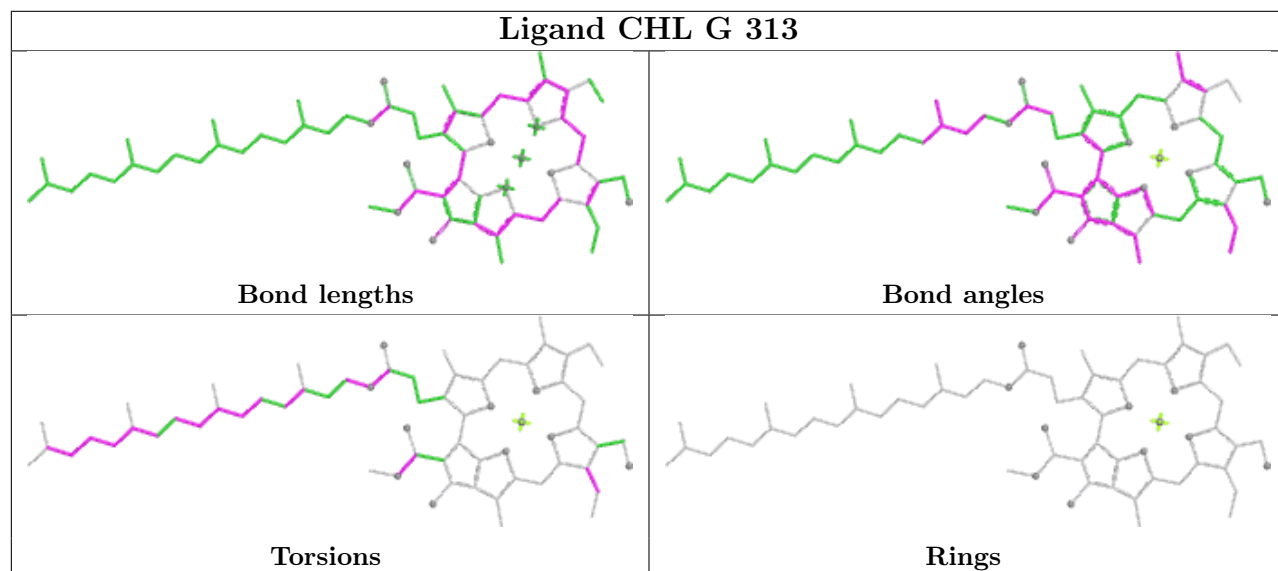
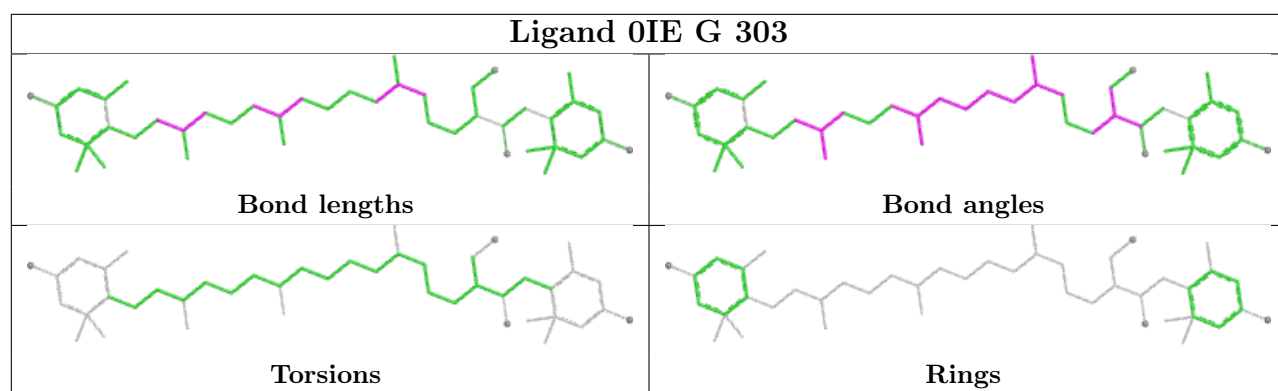


Ligand CHL 7 306

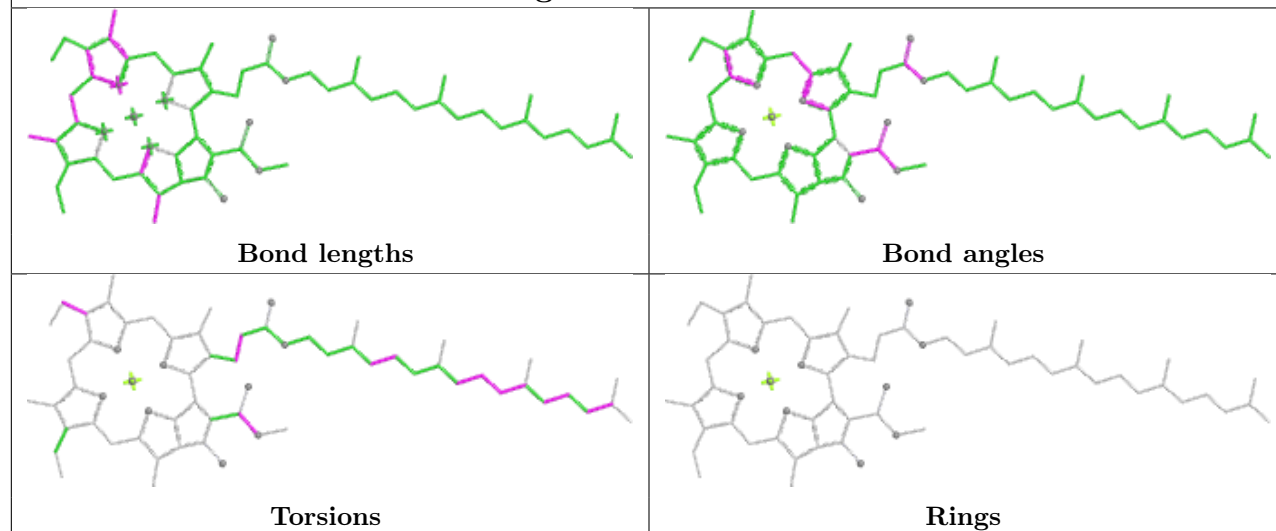




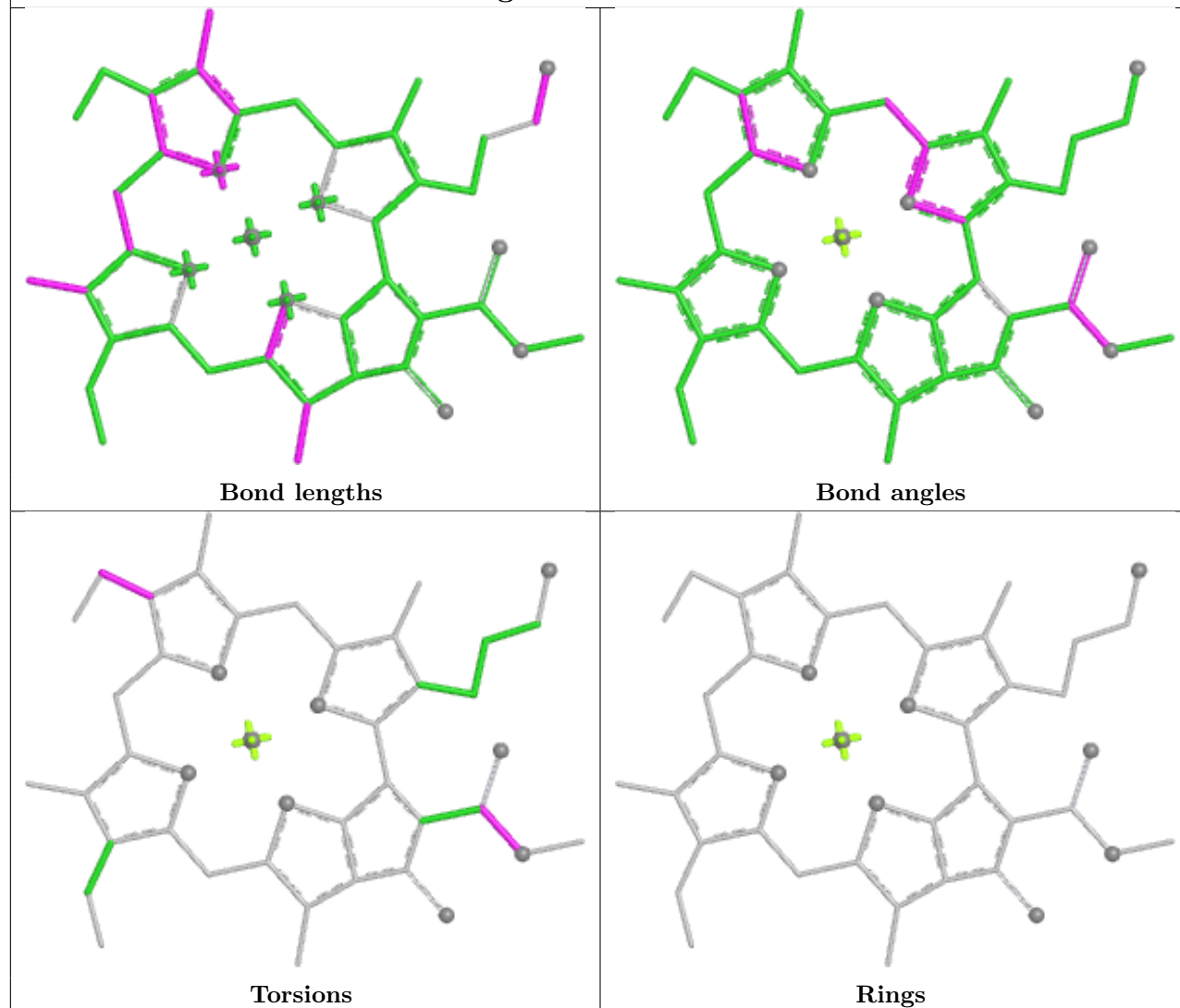


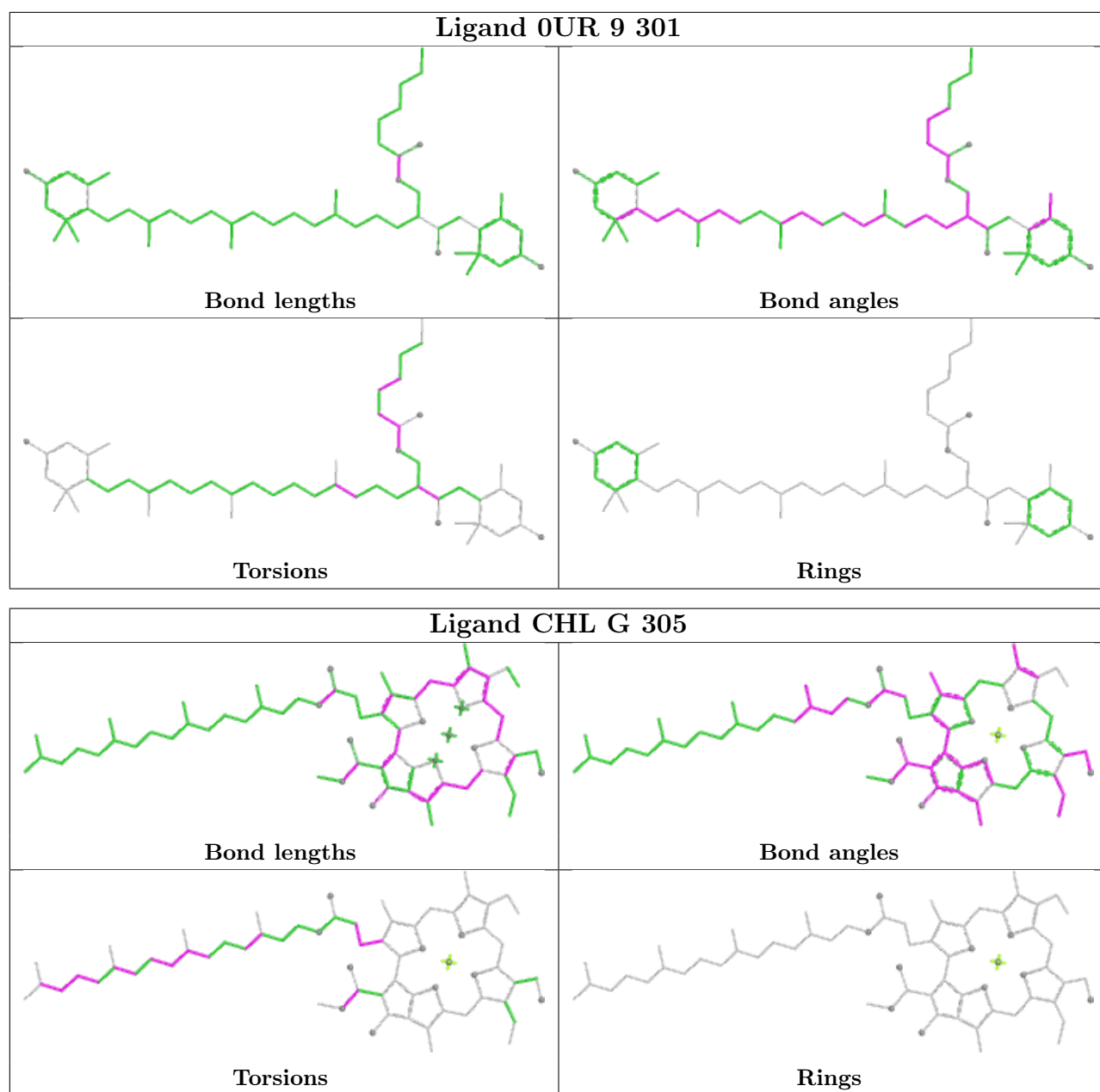


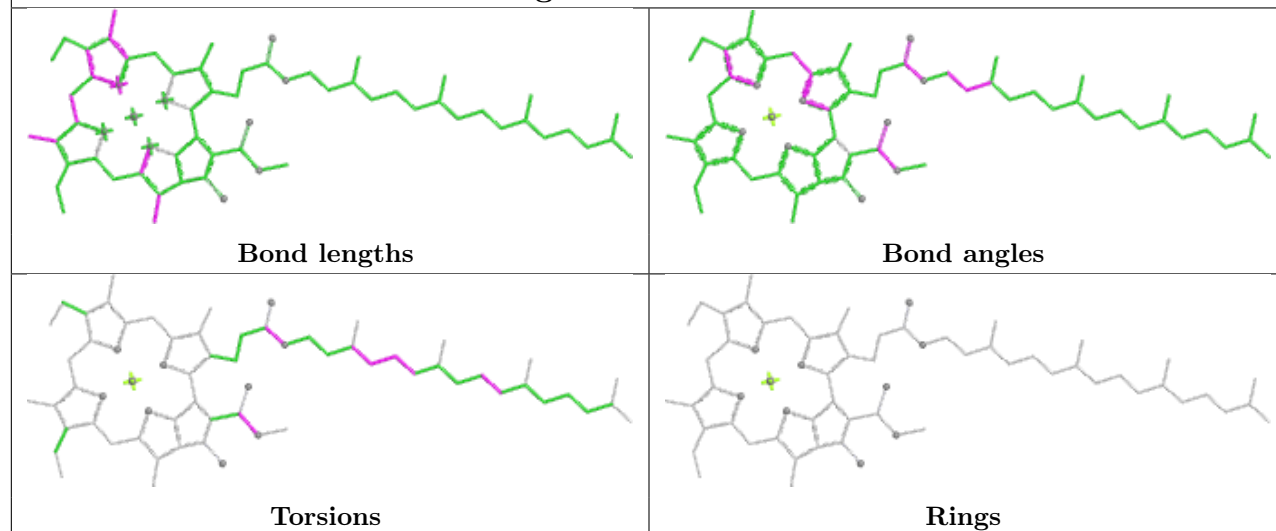
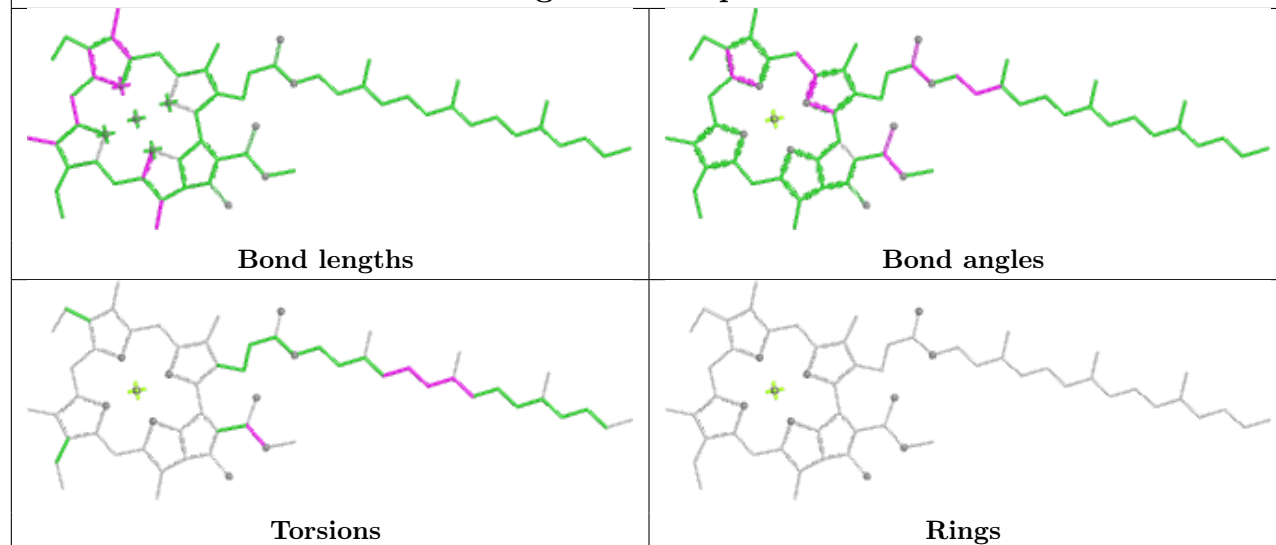
Ligand CLA b 607



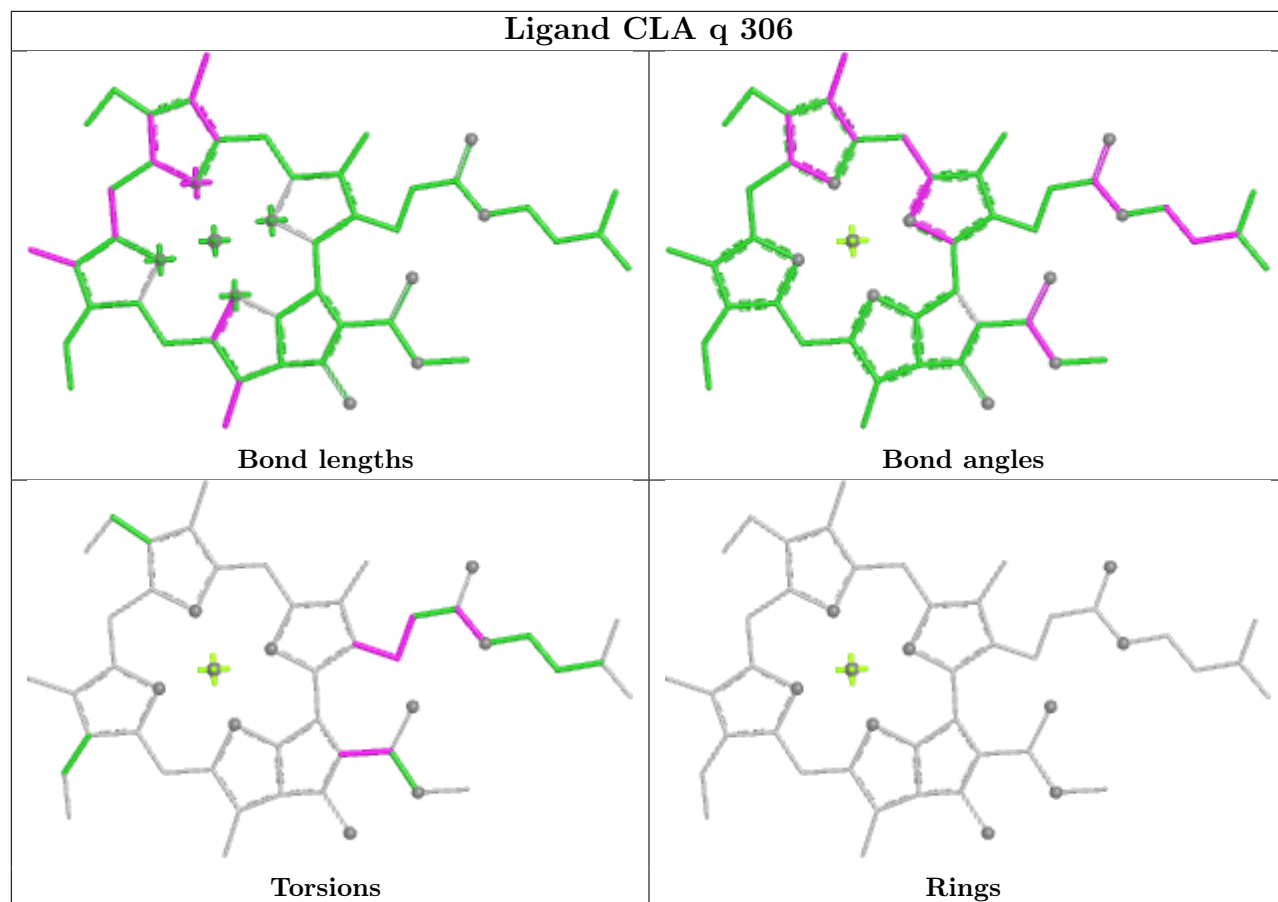
Ligand CLA s 411



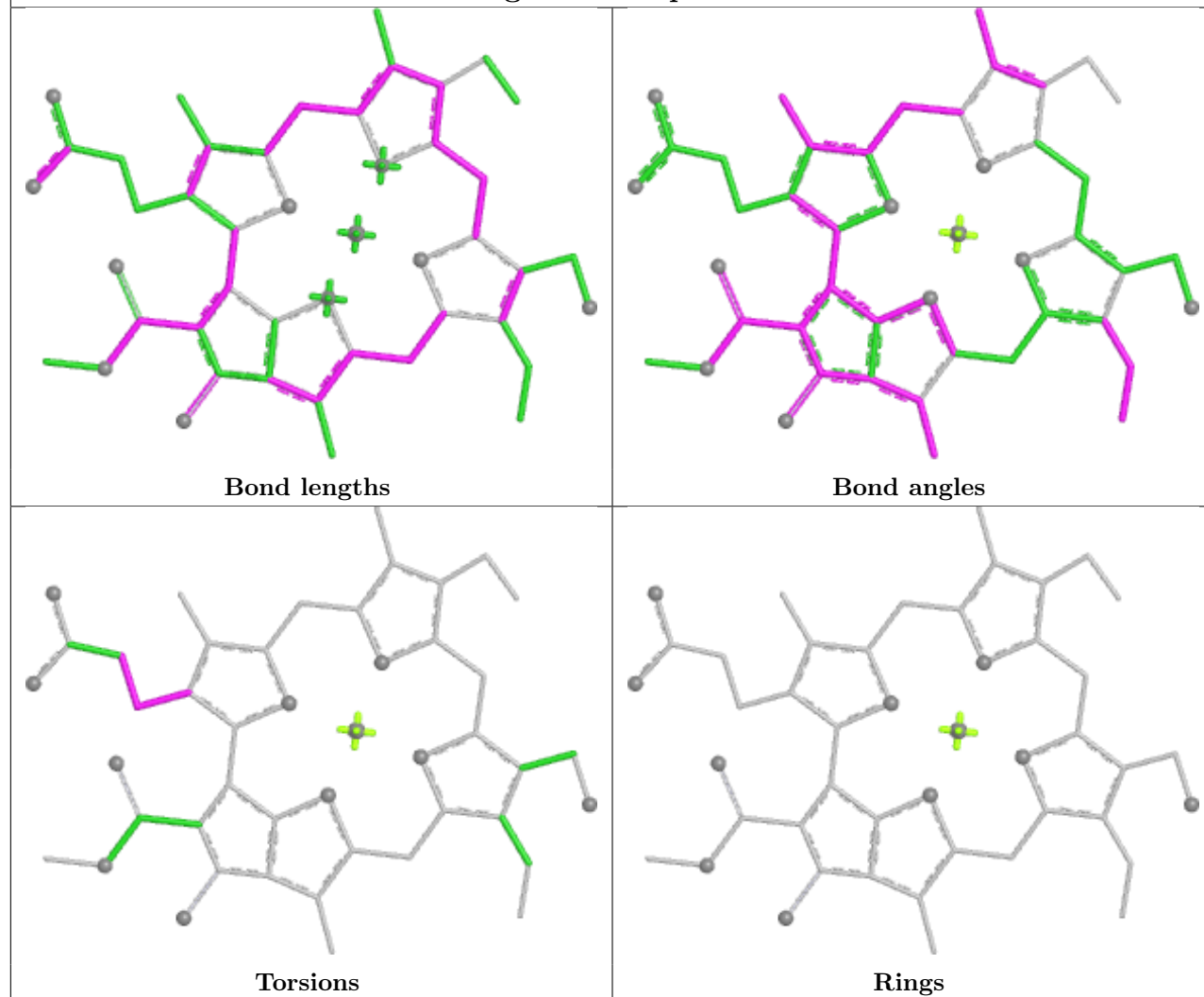


Ligand CLA b 613**Ligand CLA q 313**

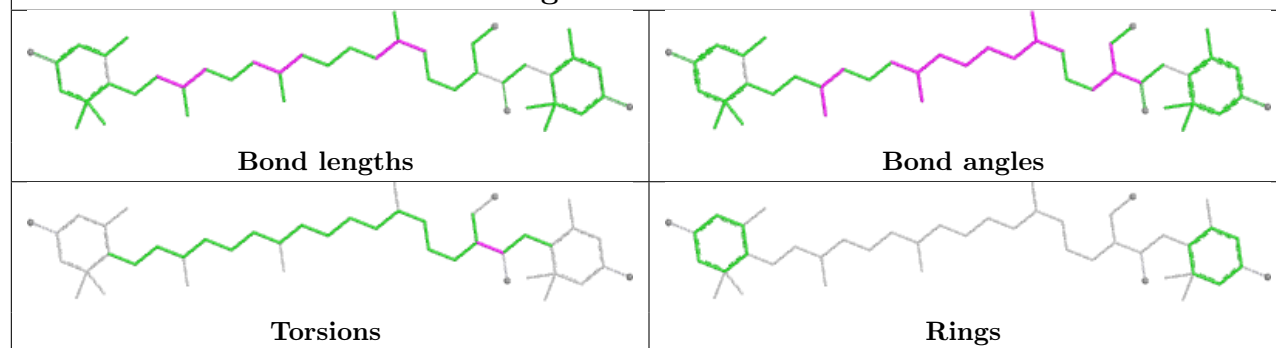
Ligand CLA q 306



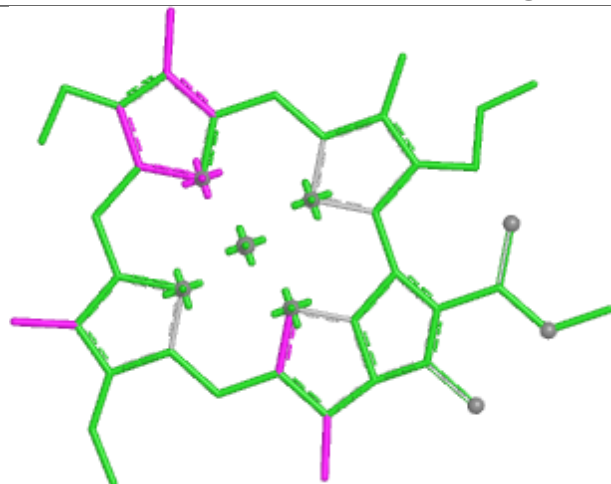
Ligand CHL p 311



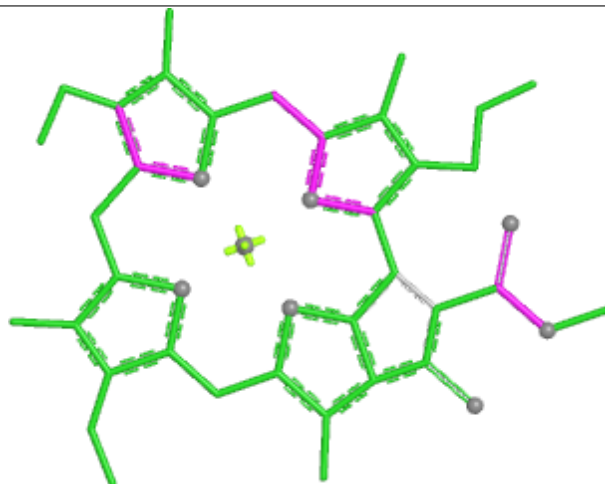
Ligand OIE G 302



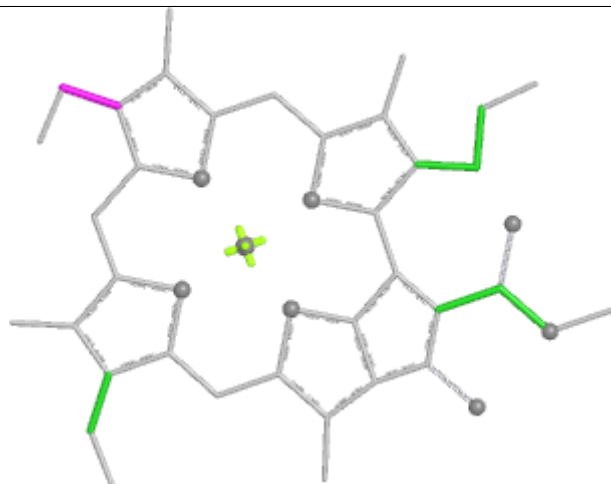
Ligand CLA s 405



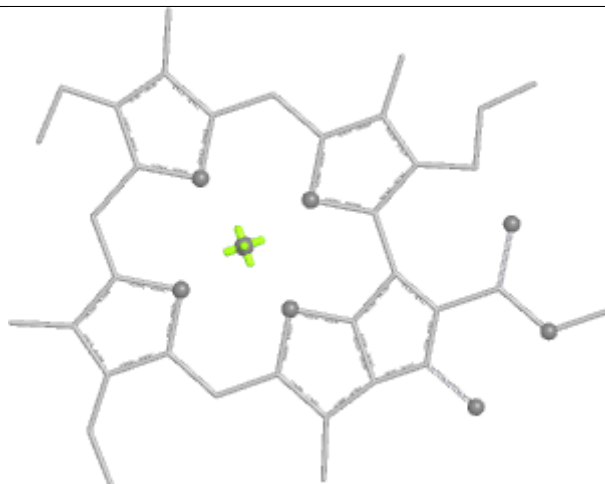
Bond lengths



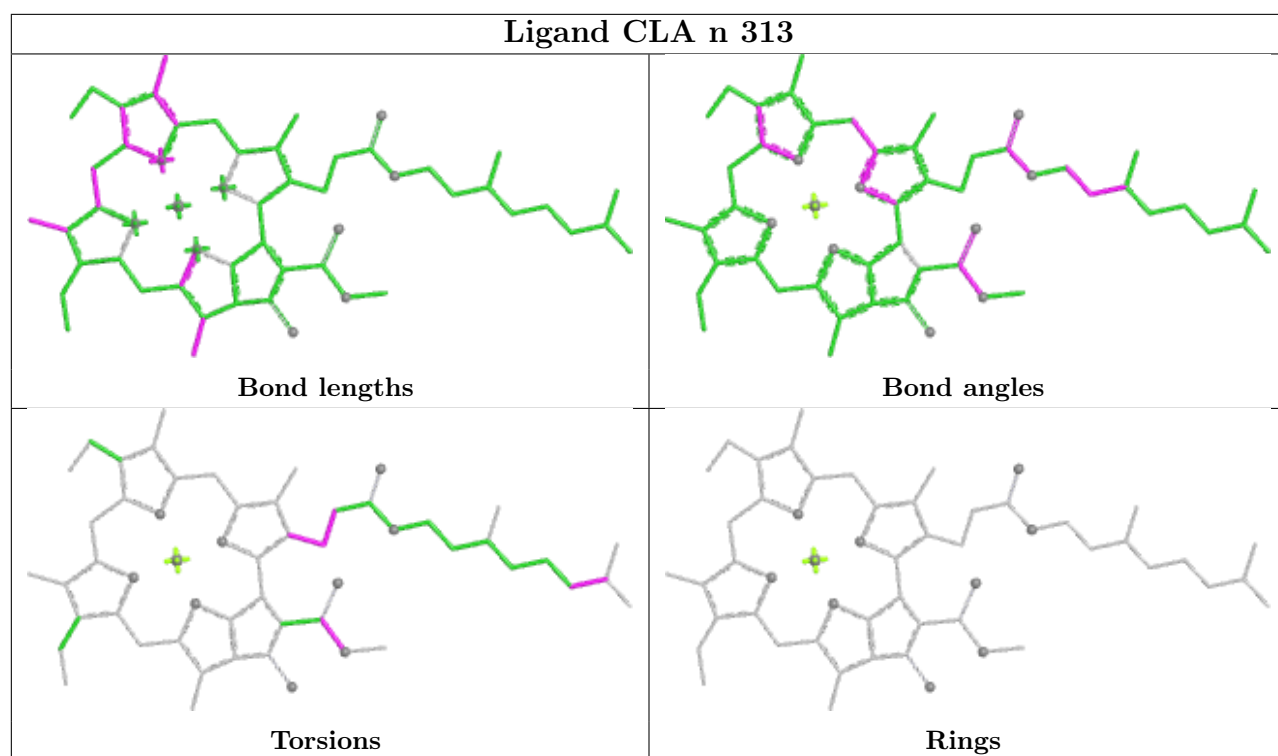
Bond angles



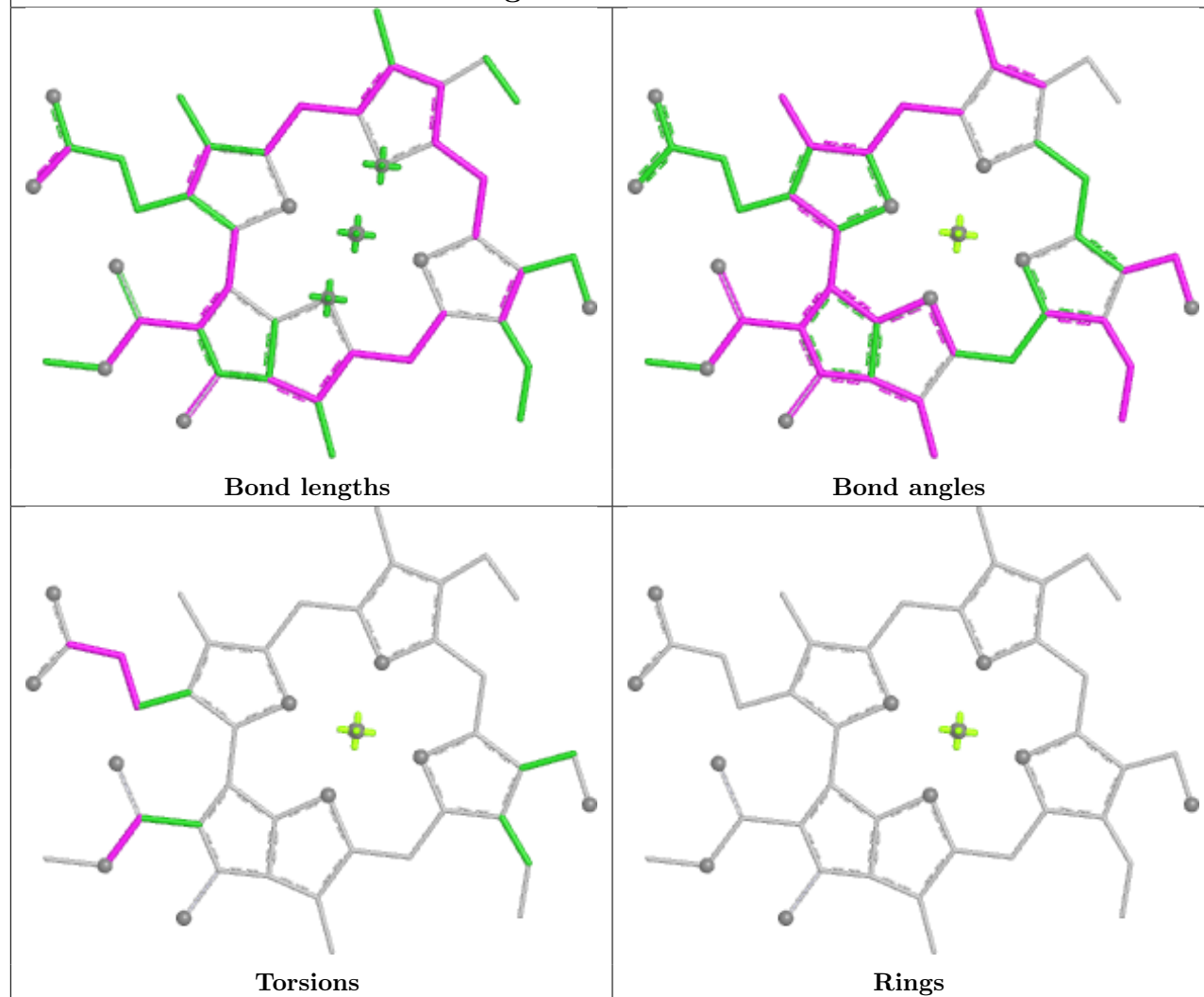
Torsions



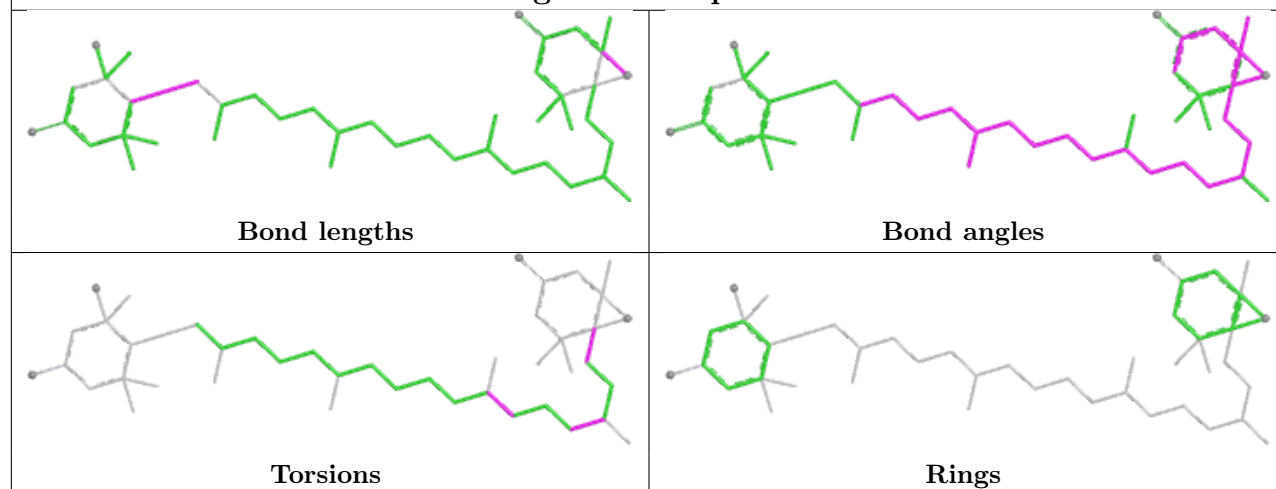
Rings



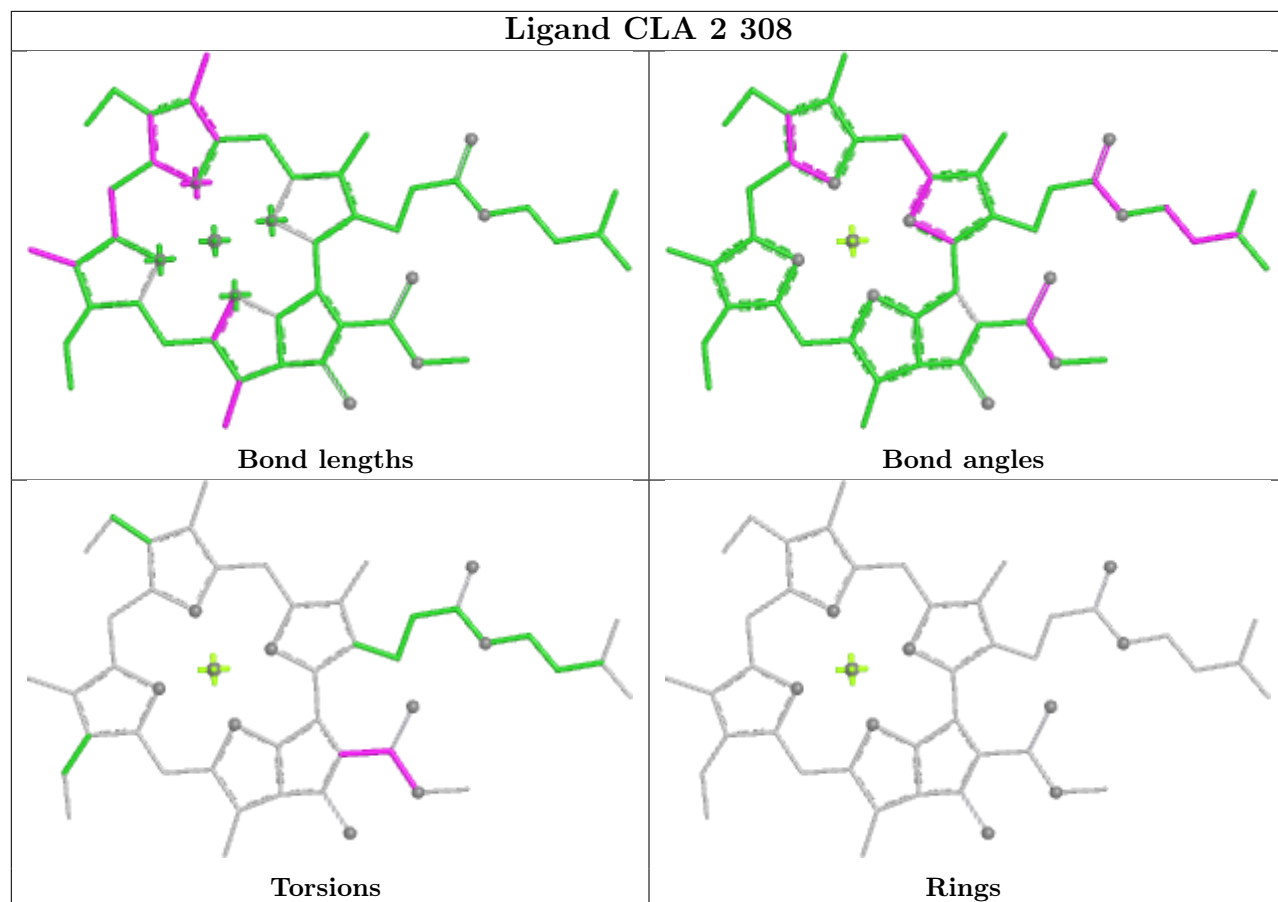
Ligand CHL S 605



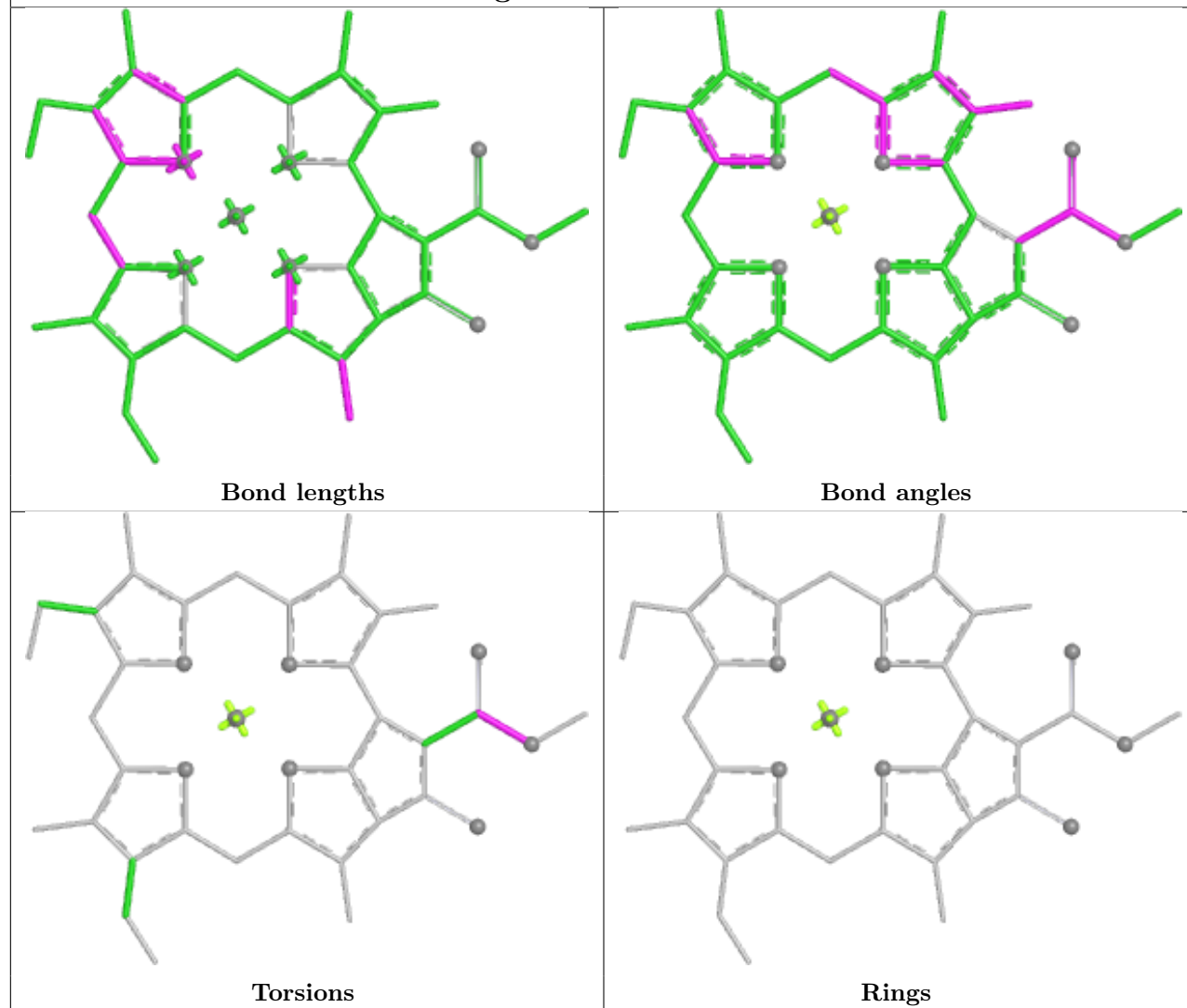
Ligand NEX p 304



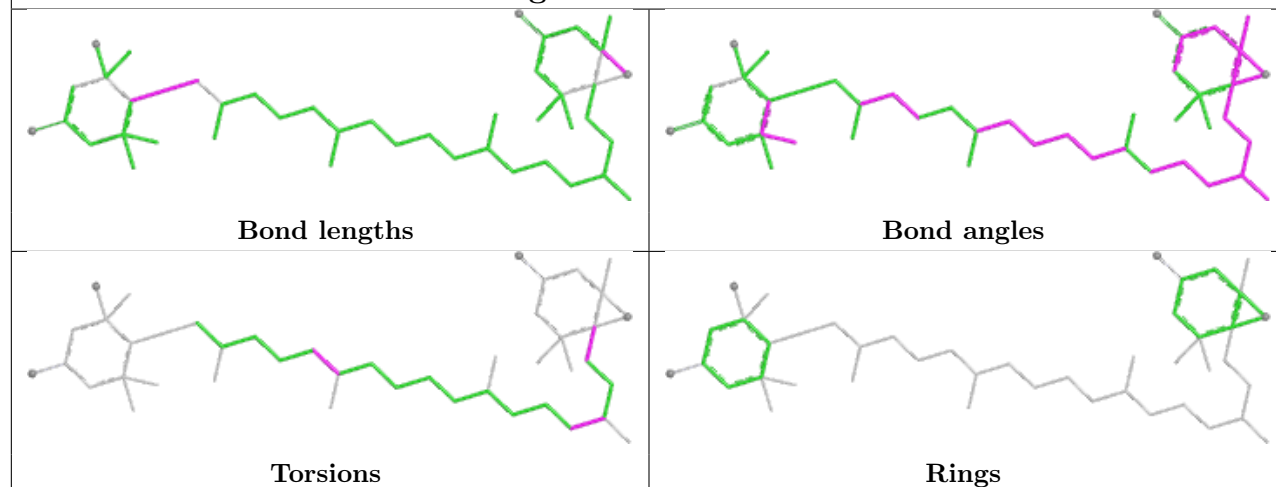
Ligand CLA 2 308



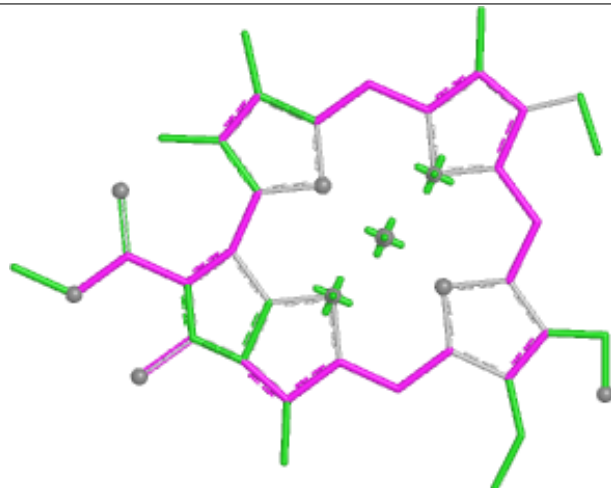
Ligand CLA A 610



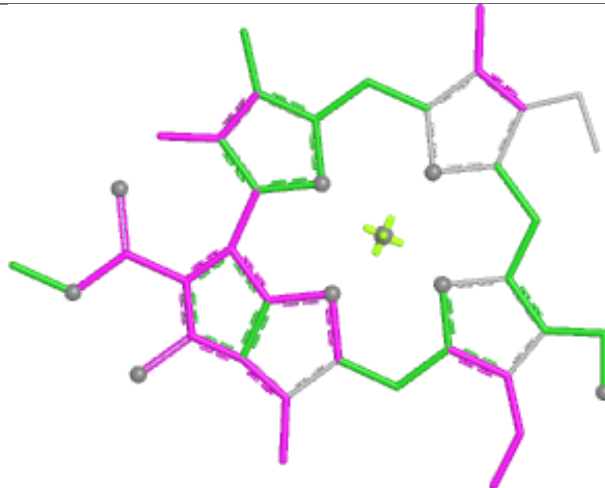
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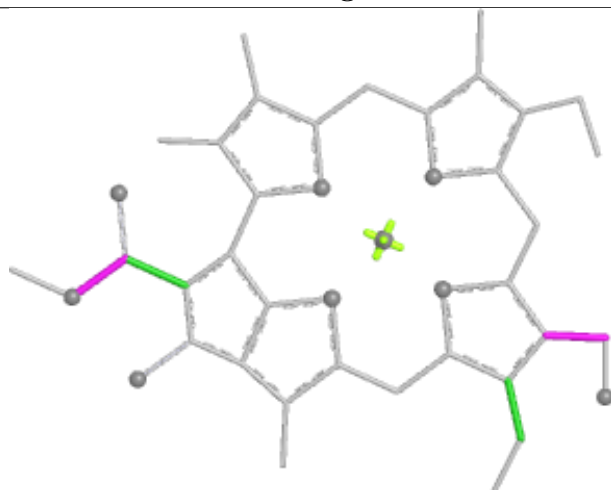
Ligand CHL 2 313



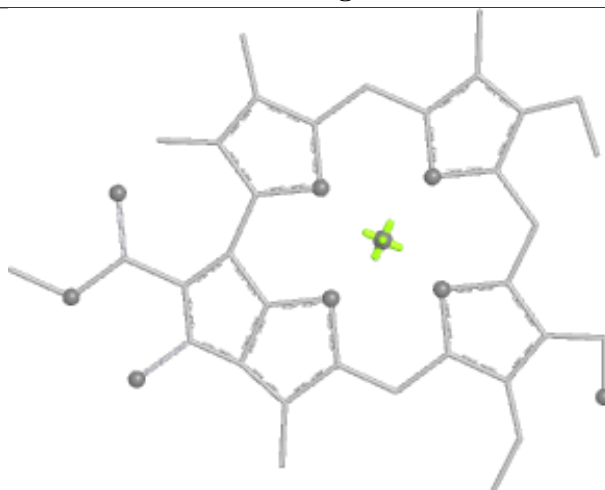
Bond lengths



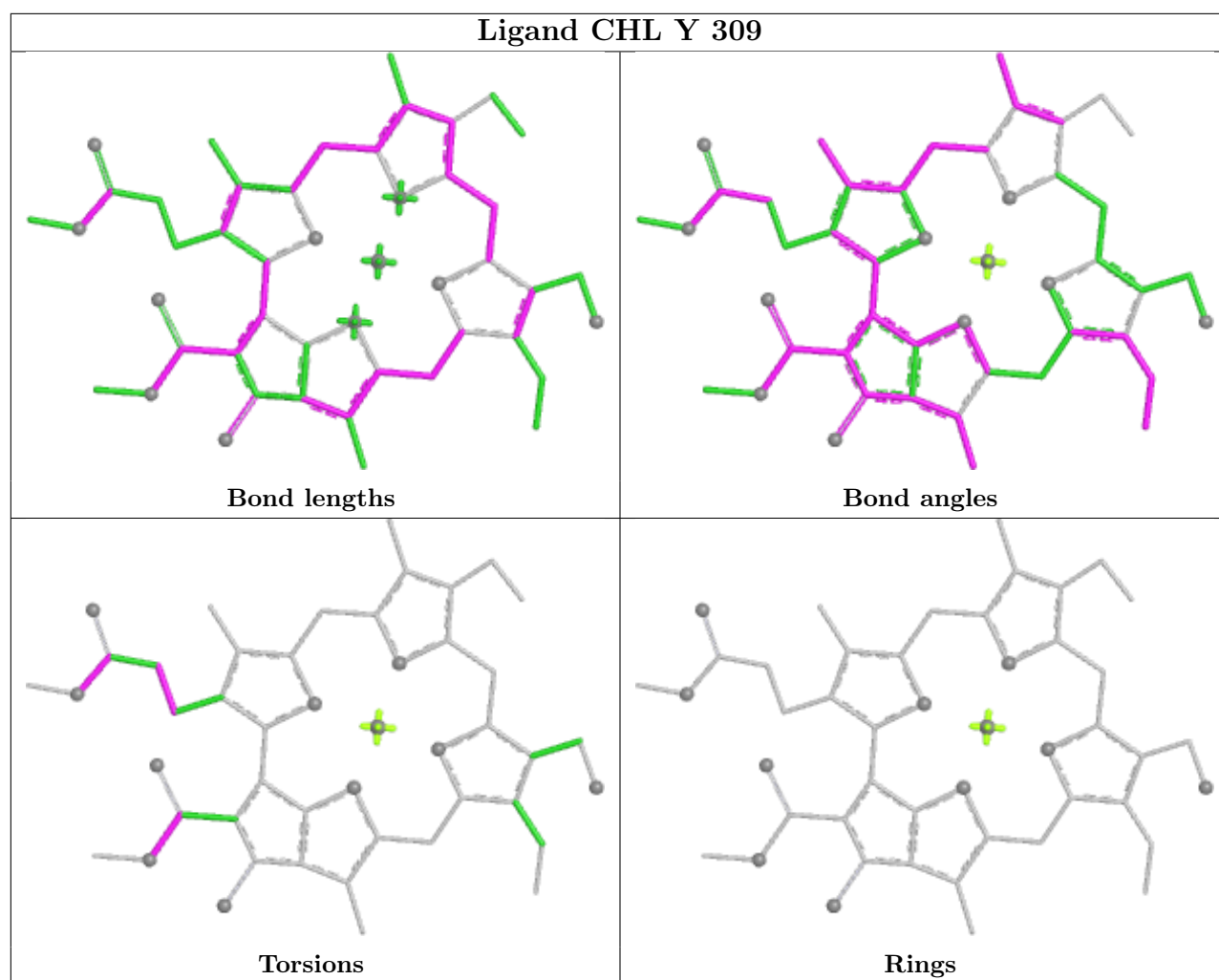
Bond angles



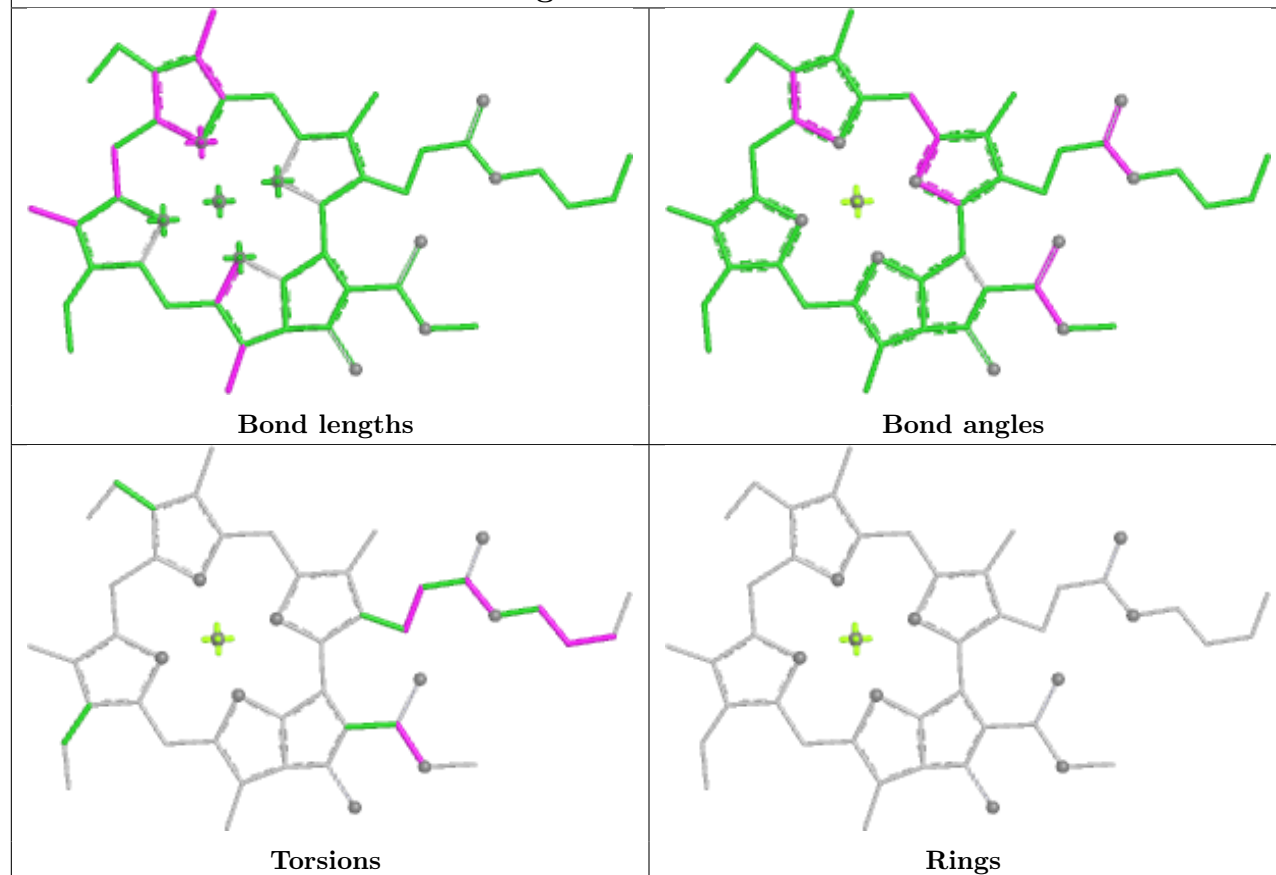
Torsions



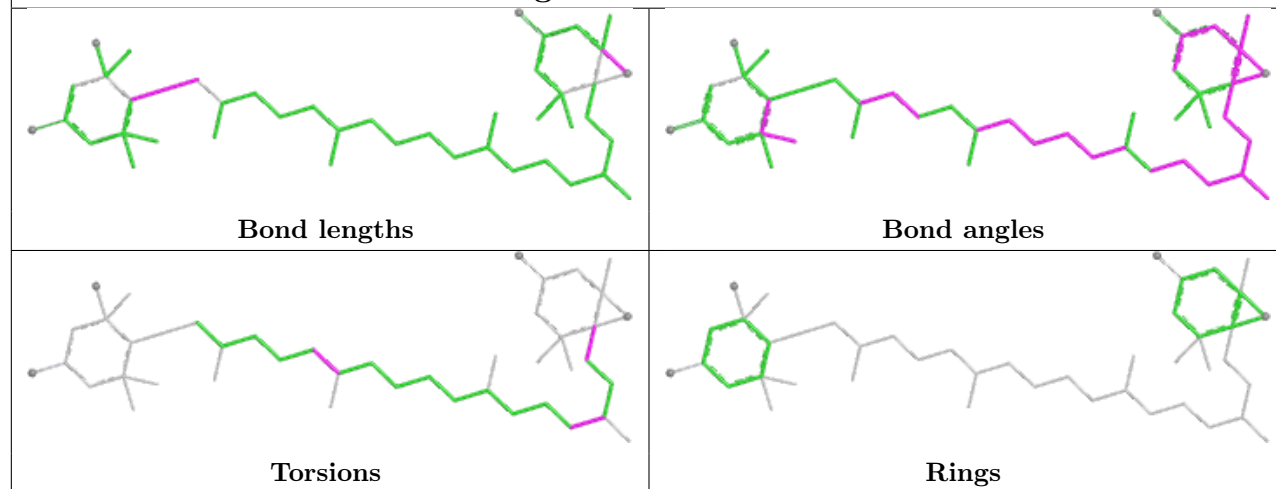
Rings



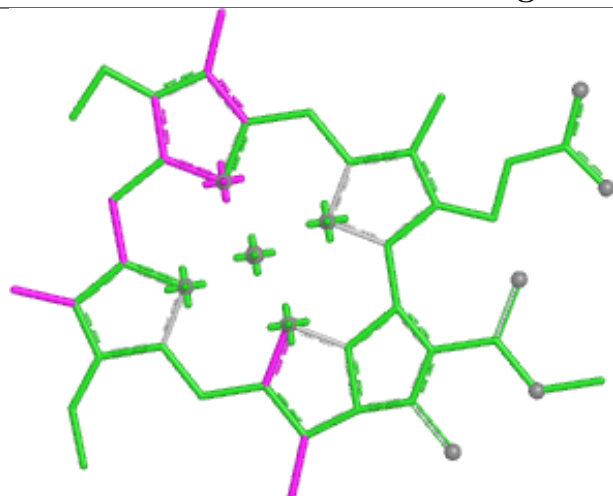
Ligand CLA 2 317



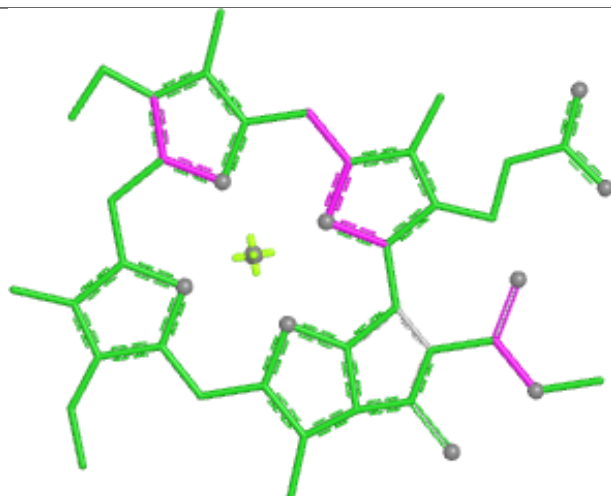
Ligand NEX 3 318



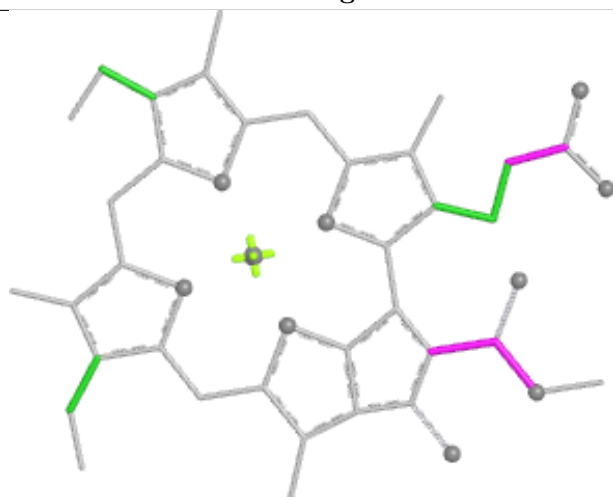
Ligand CLA S 603



Bond lengths



Bond angles

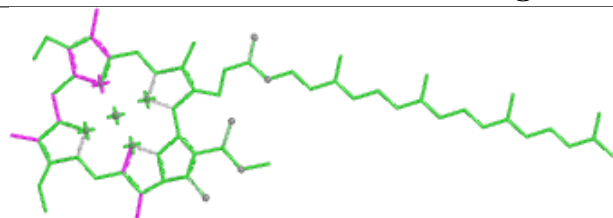


Torsions

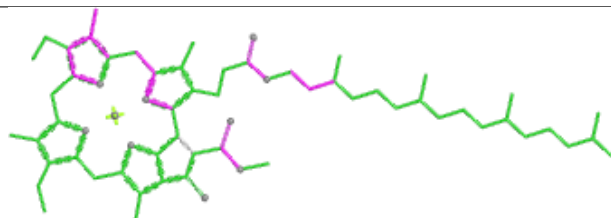


Rings

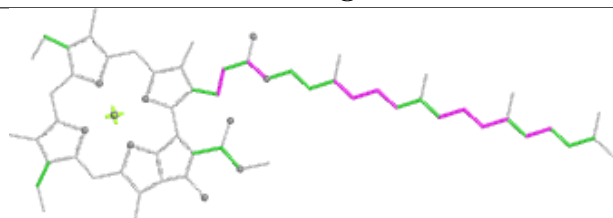
Ligand CLA B 612



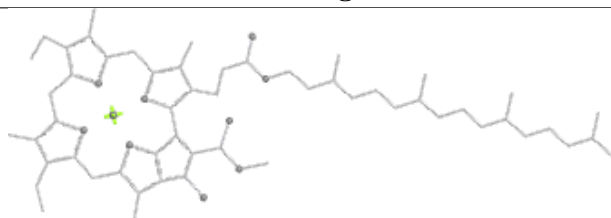
Bond lengths



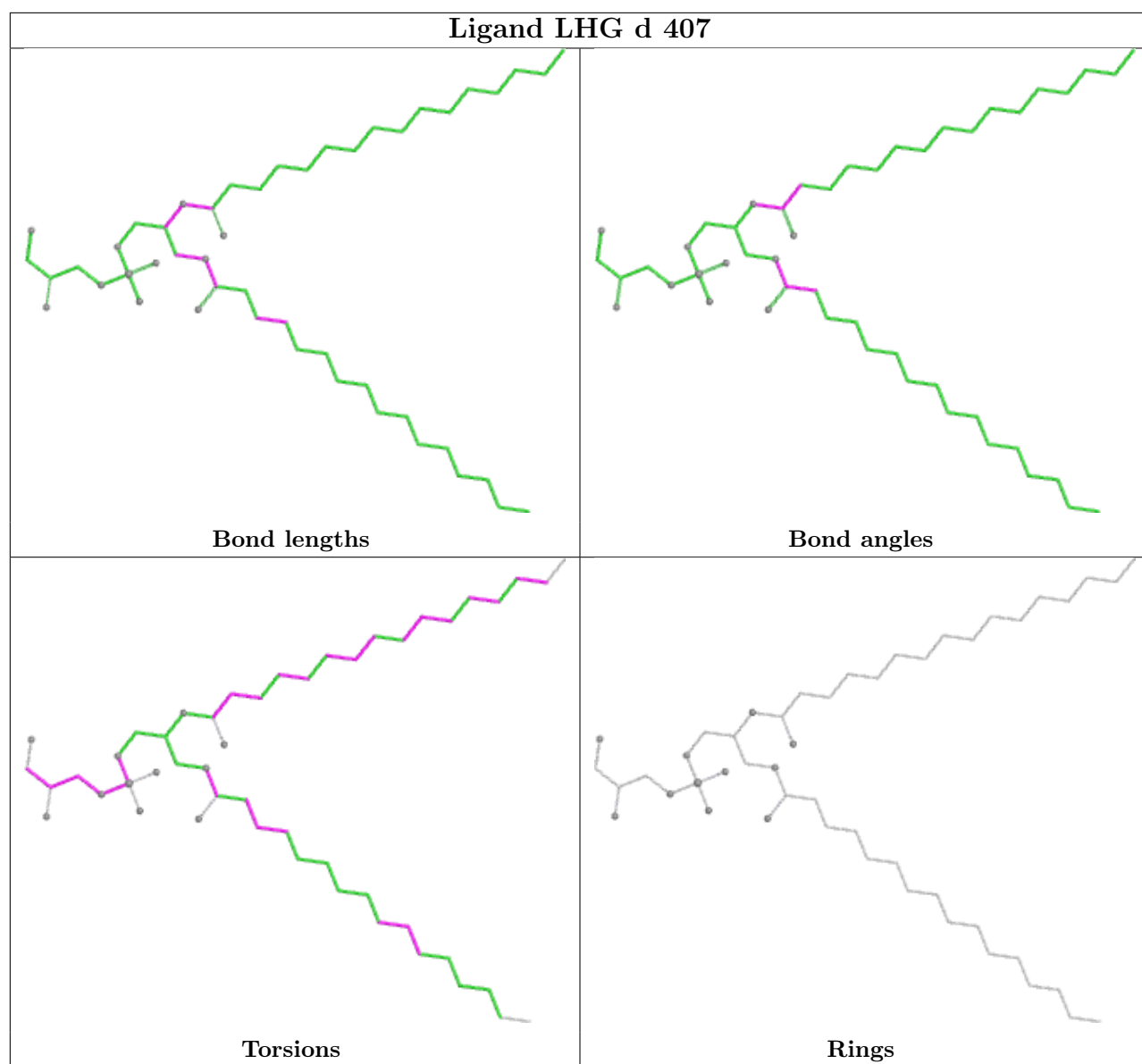
Bond angles



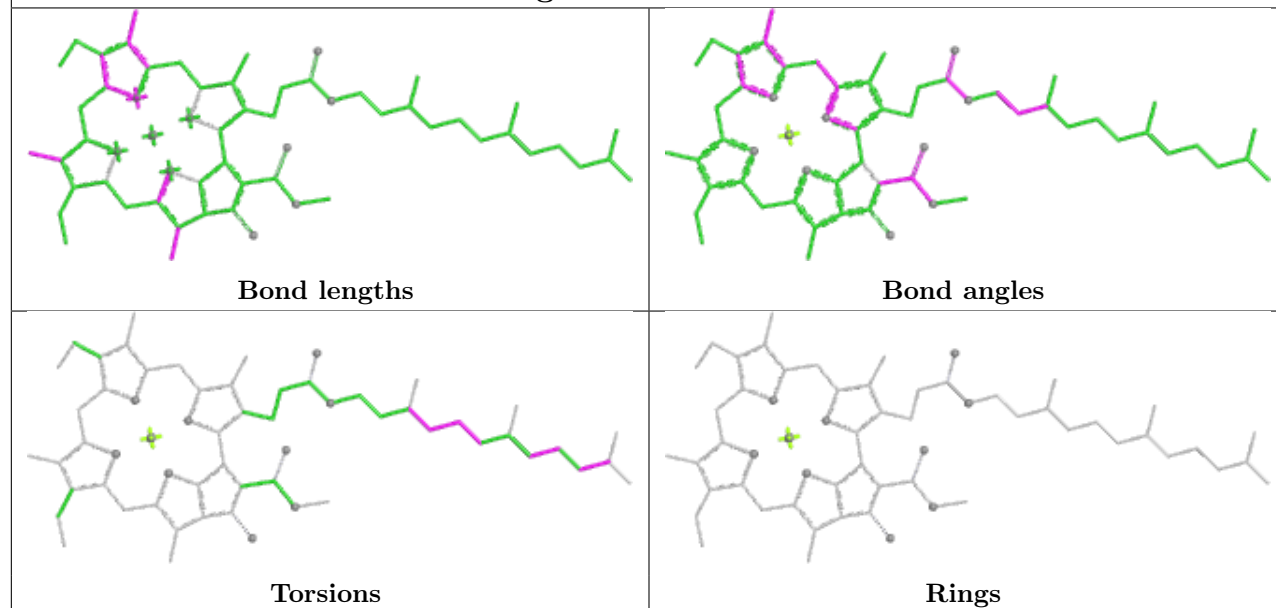
Torsions



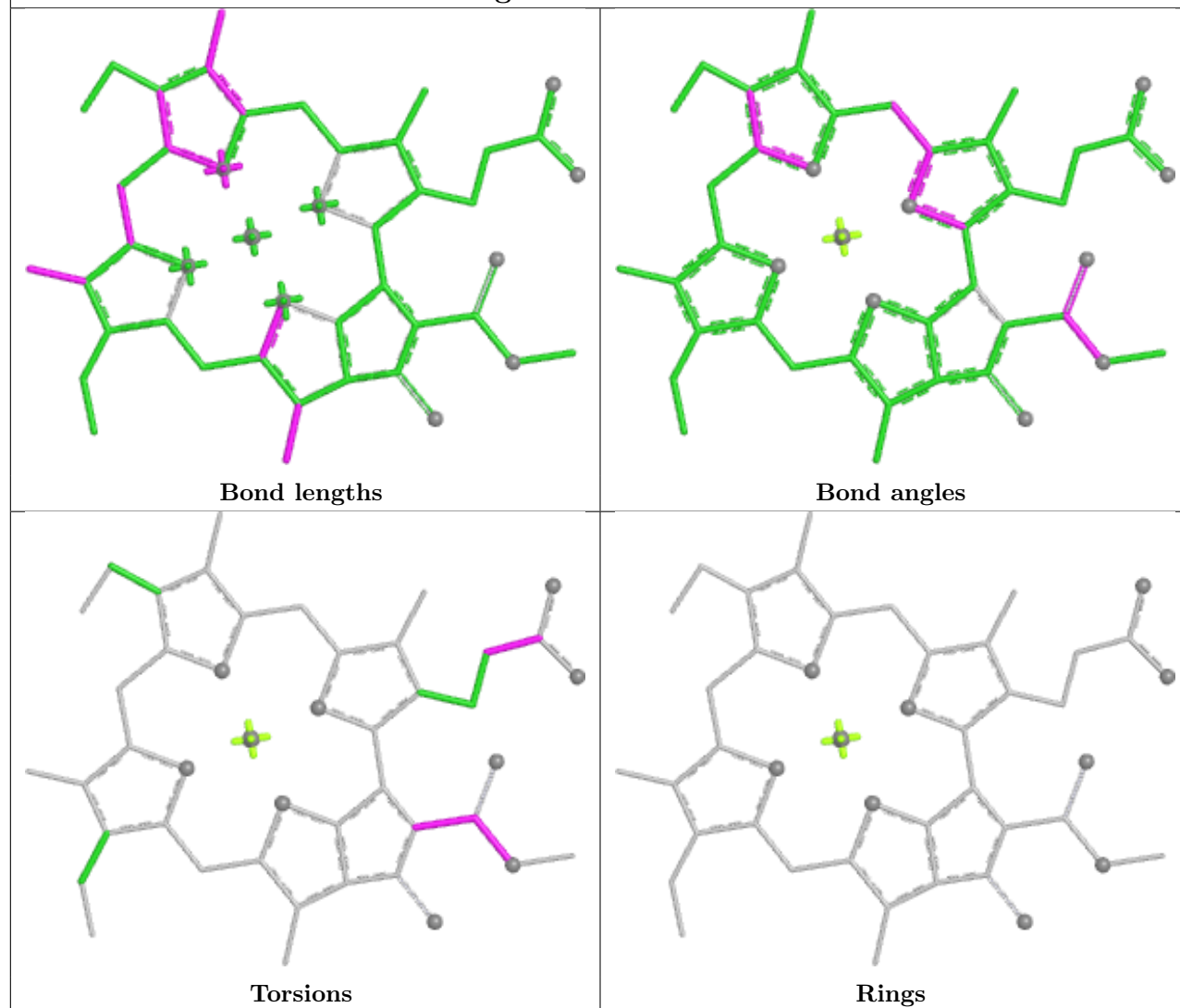
Rings



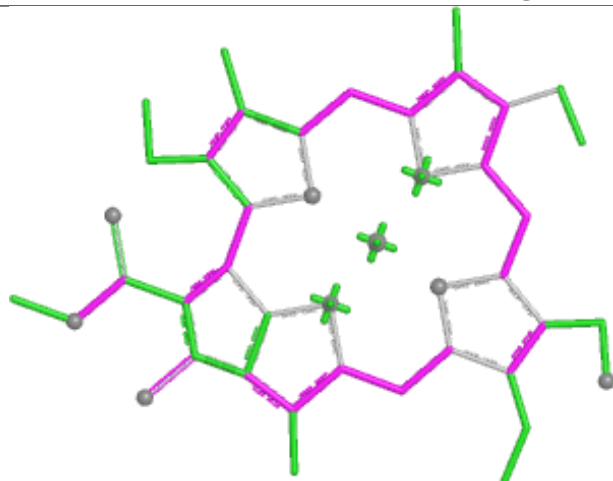
Ligand CLA a 607



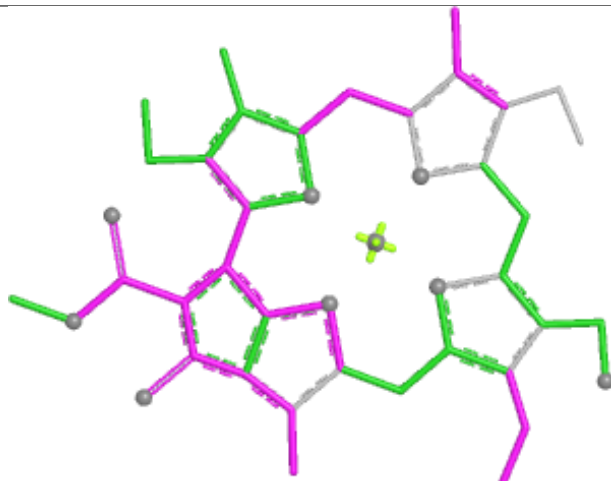
Ligand CLA S 611



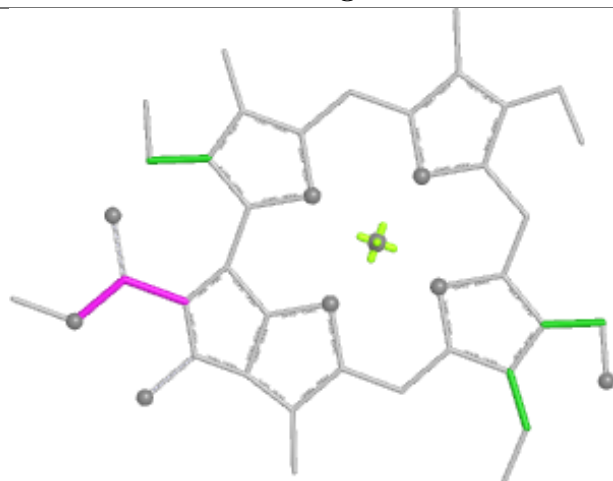
Ligand CHL 4 310



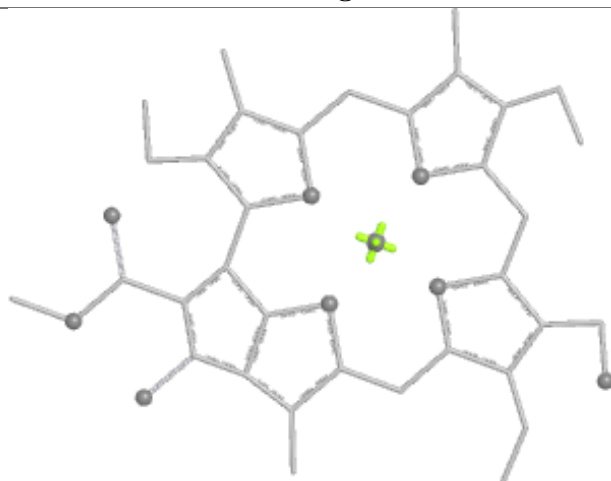
Bond lengths



Bond angles

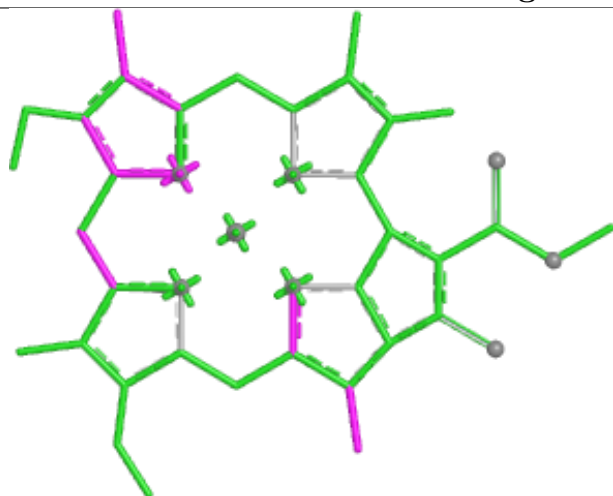


Torsions

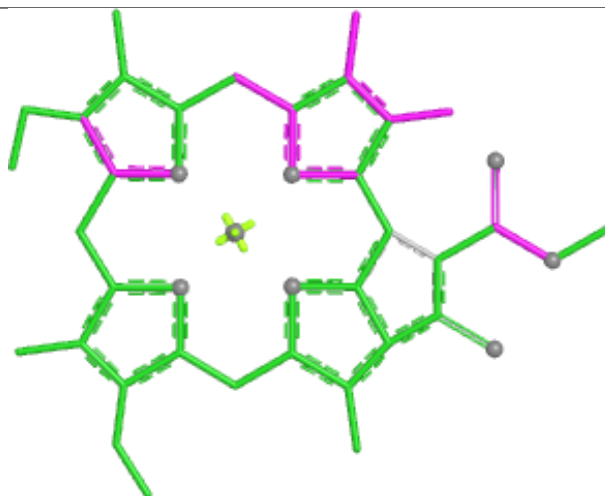


Rings

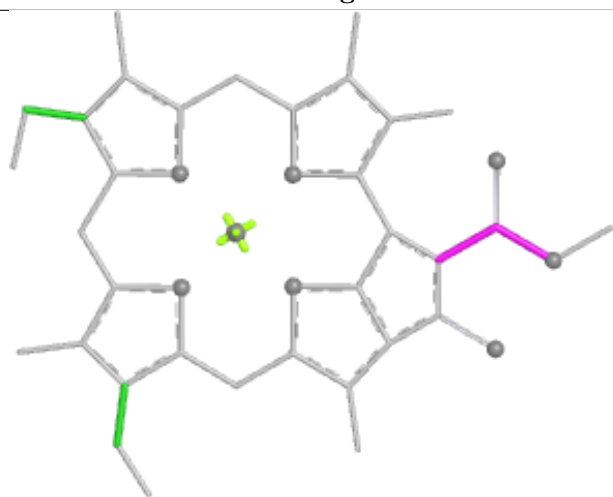
Ligand CLA 1 307



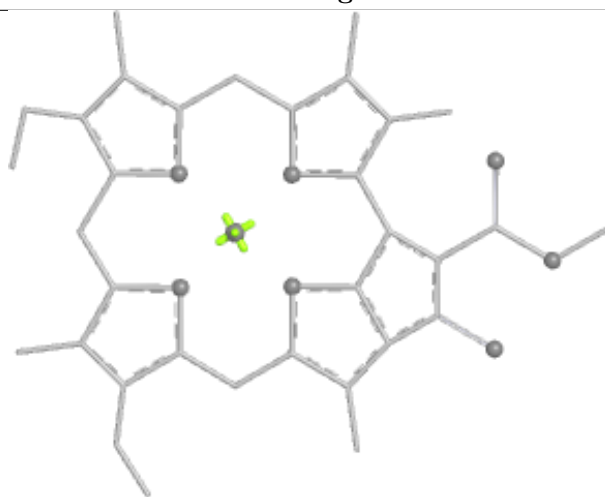
Bond lengths



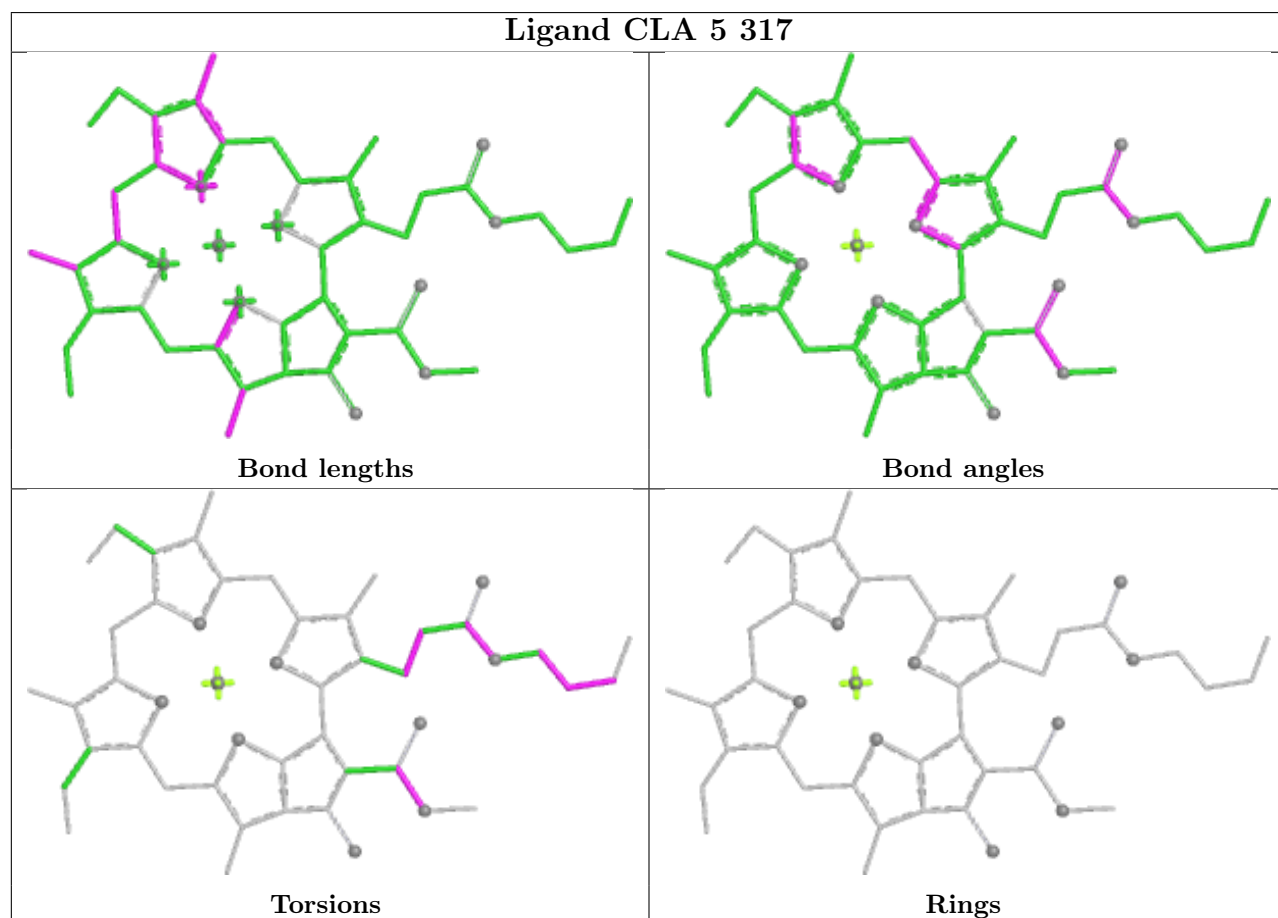
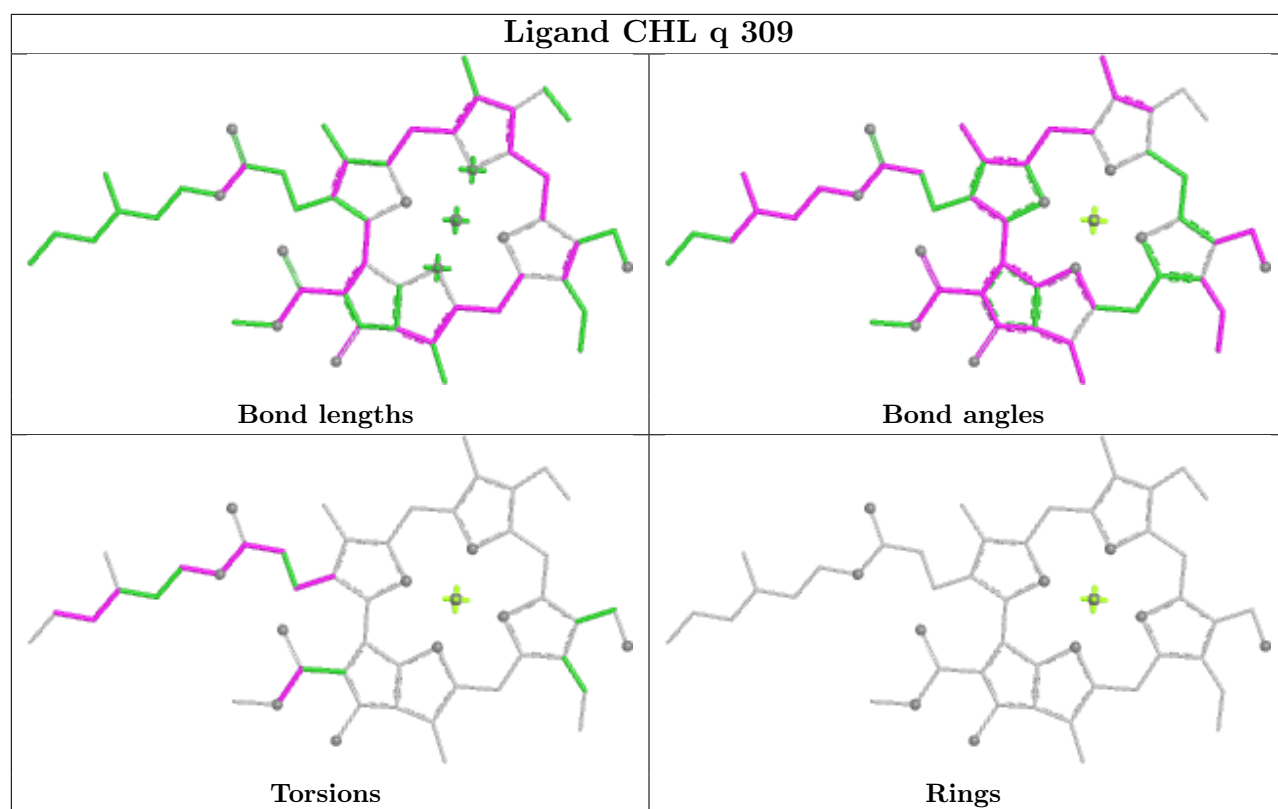
Bond angles



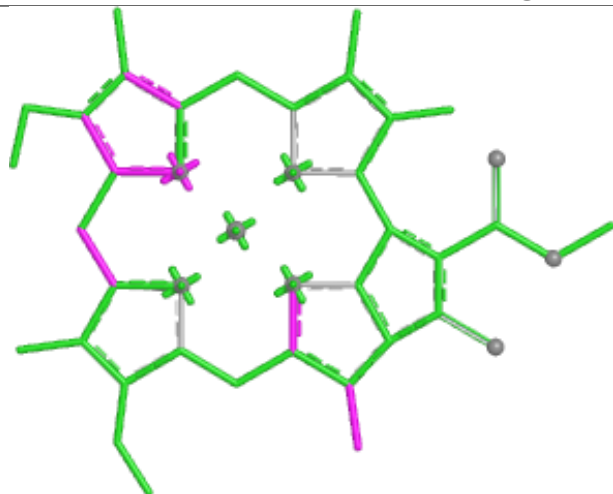
Torsions



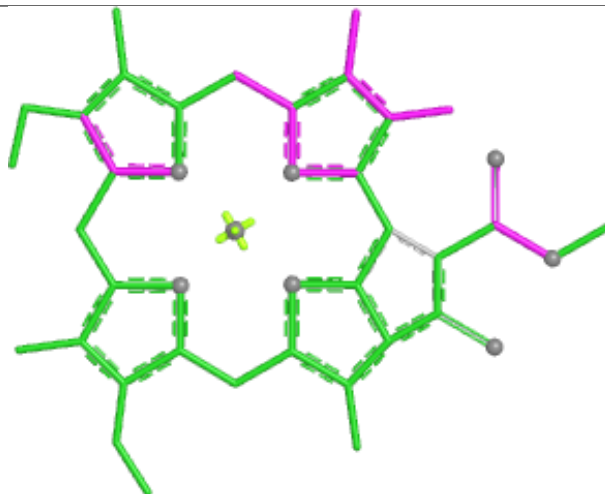
Rings



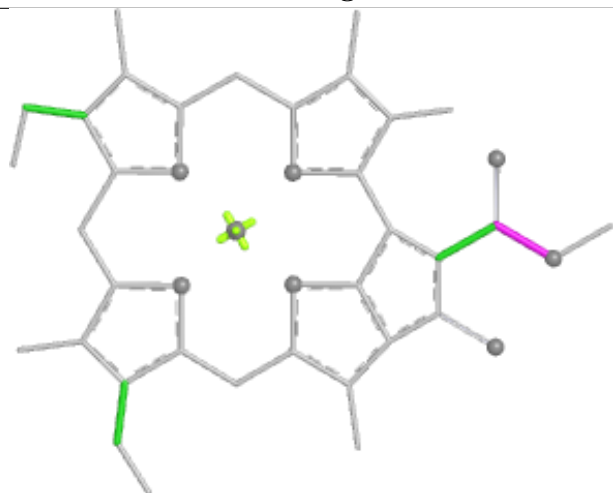
Ligand CLA 6 313



Bond lengths



Bond angles

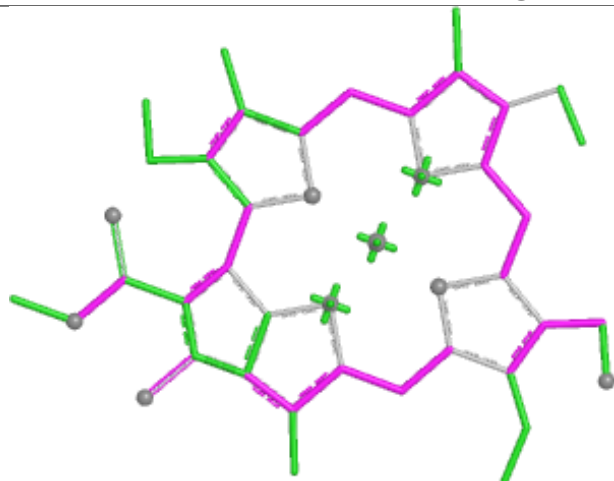


Torsions

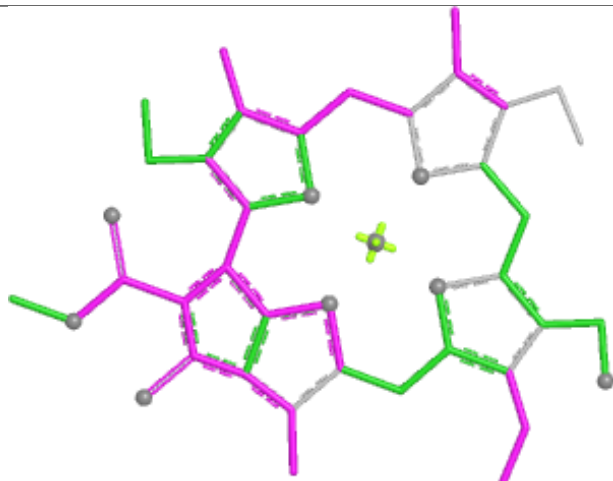


Rings

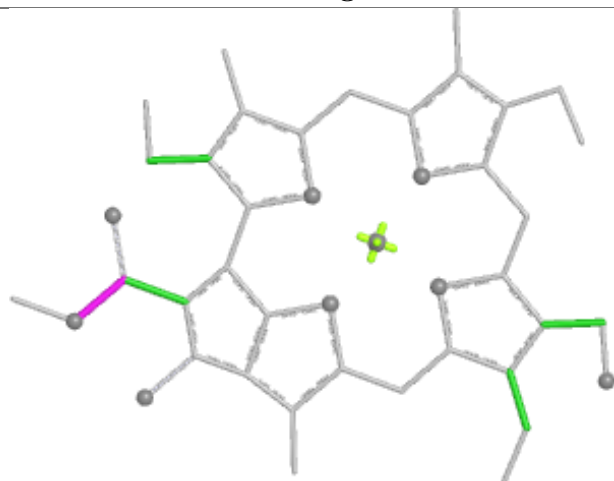
Ligand CHL G 309



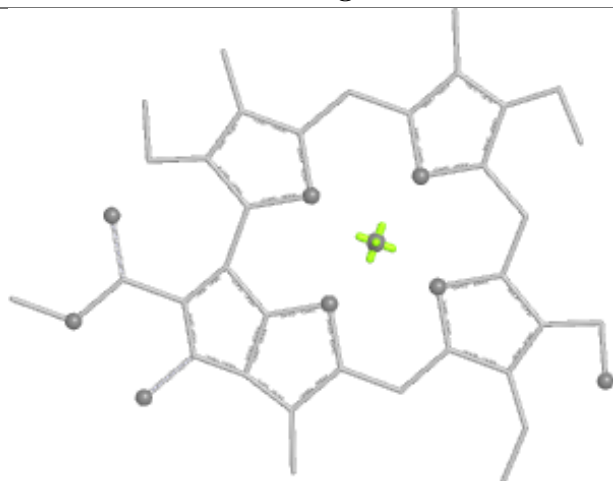
Bond lengths



Bond angles

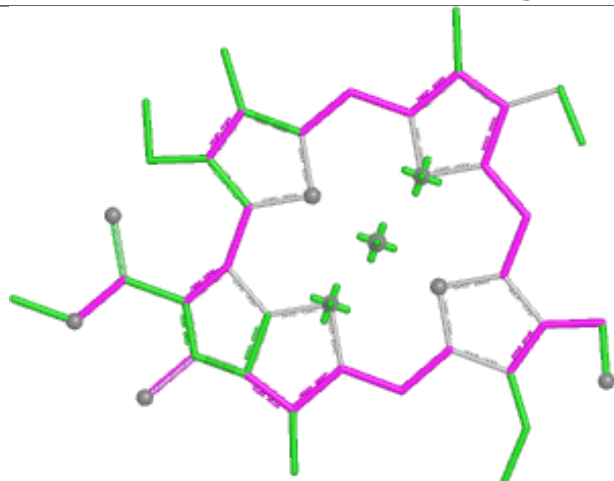


Torsions

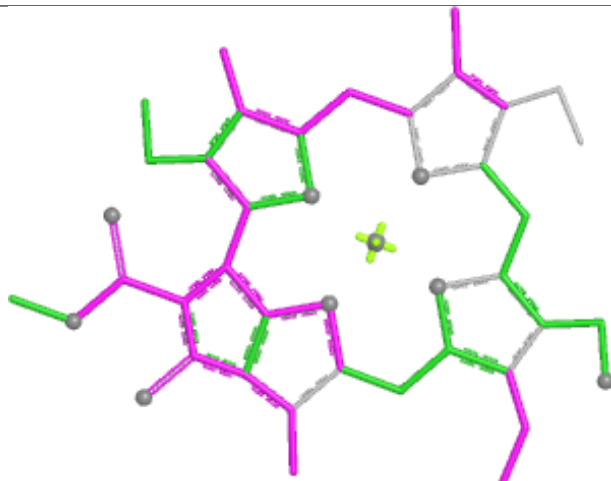


Rings

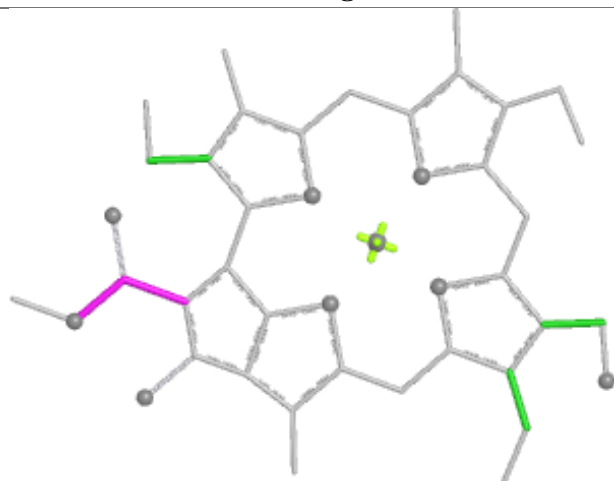
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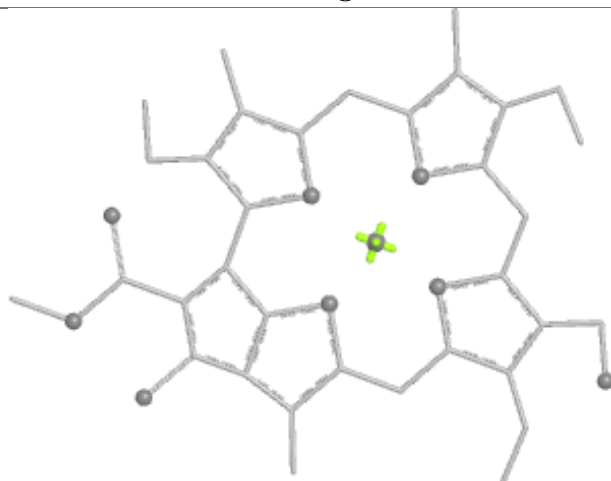
Bond lengths



Bond angles

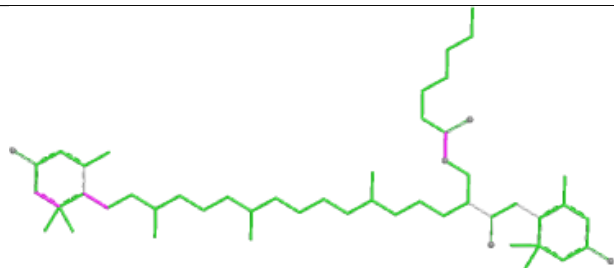


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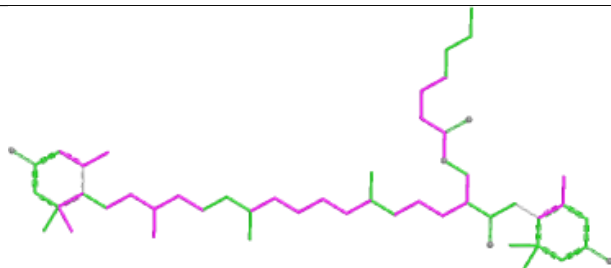


Rings

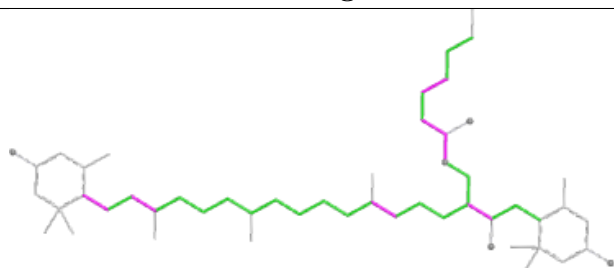
Ligand OUR 2 301



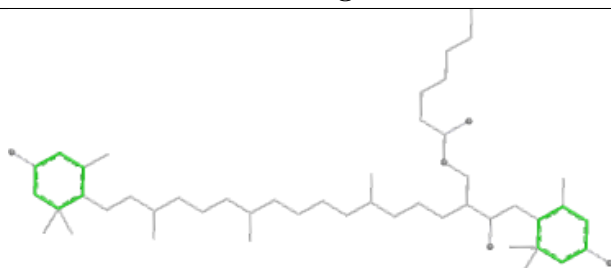
Bond lengths



Bond angles

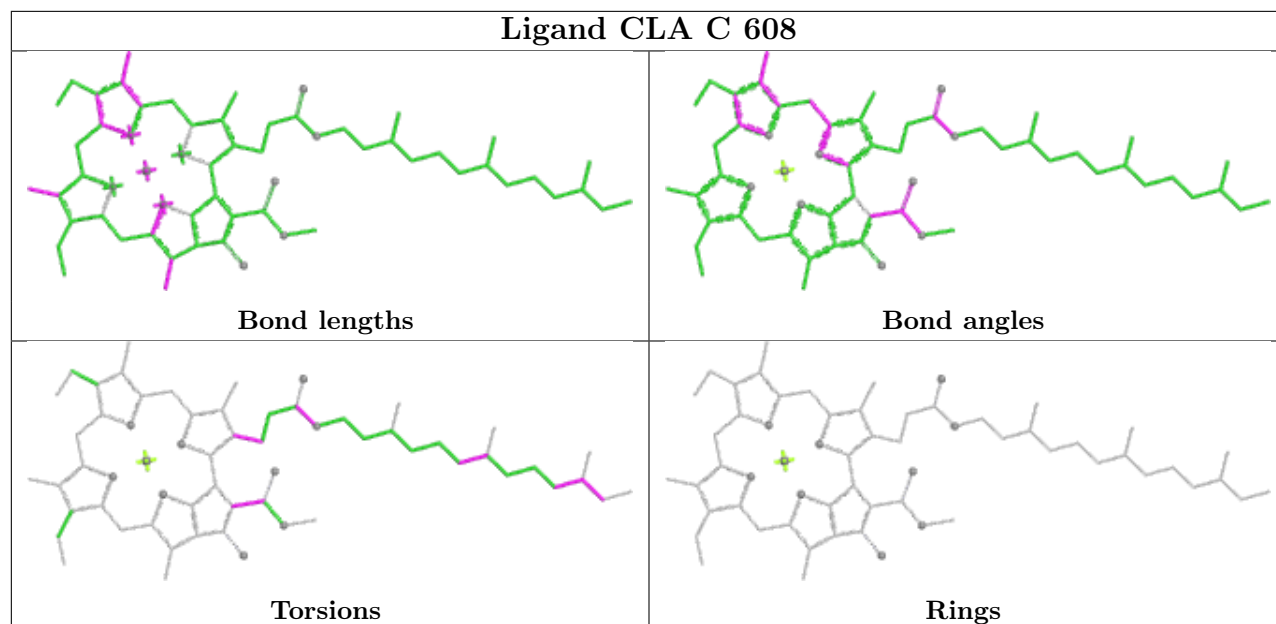


Torsions

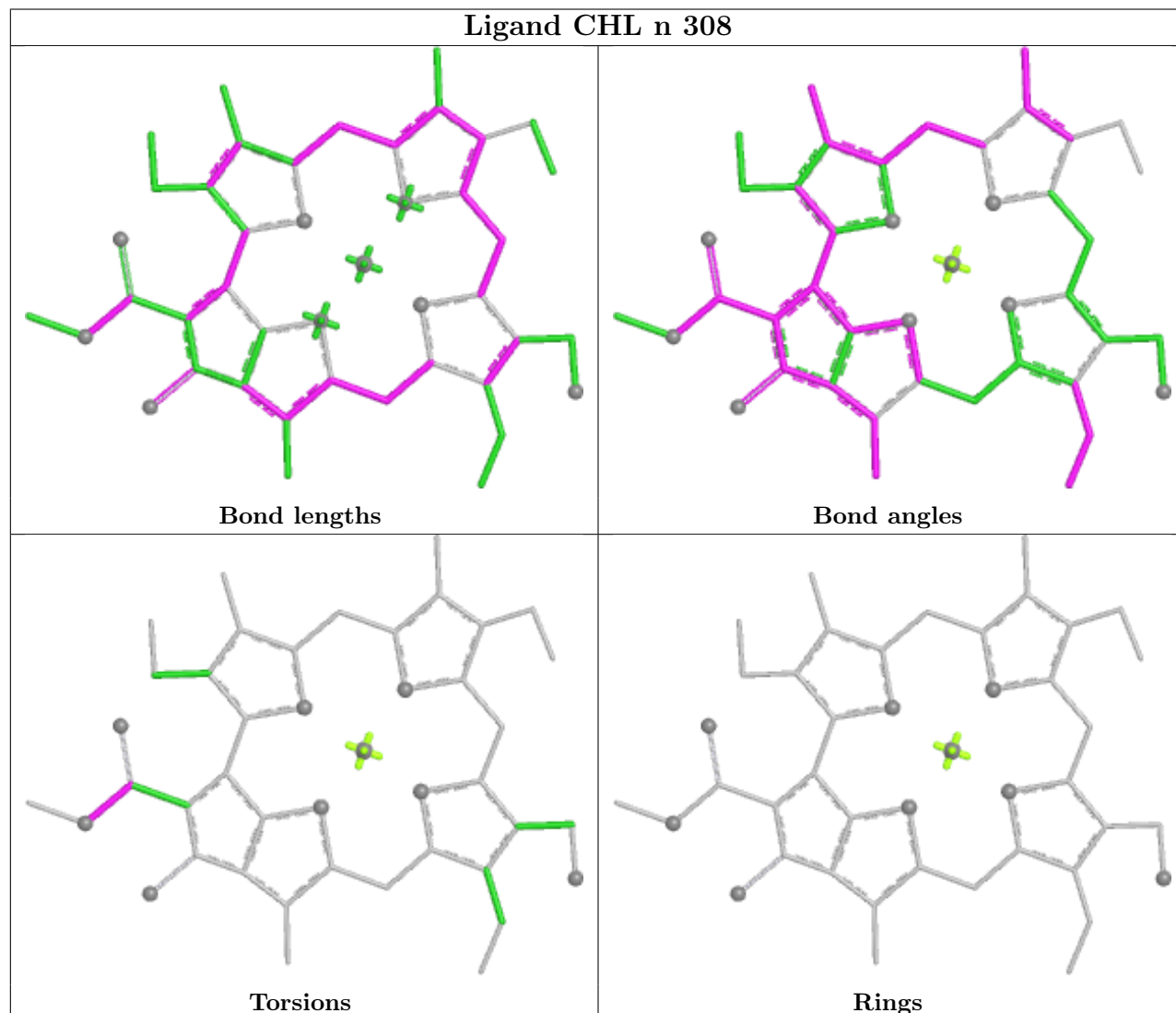


Rings

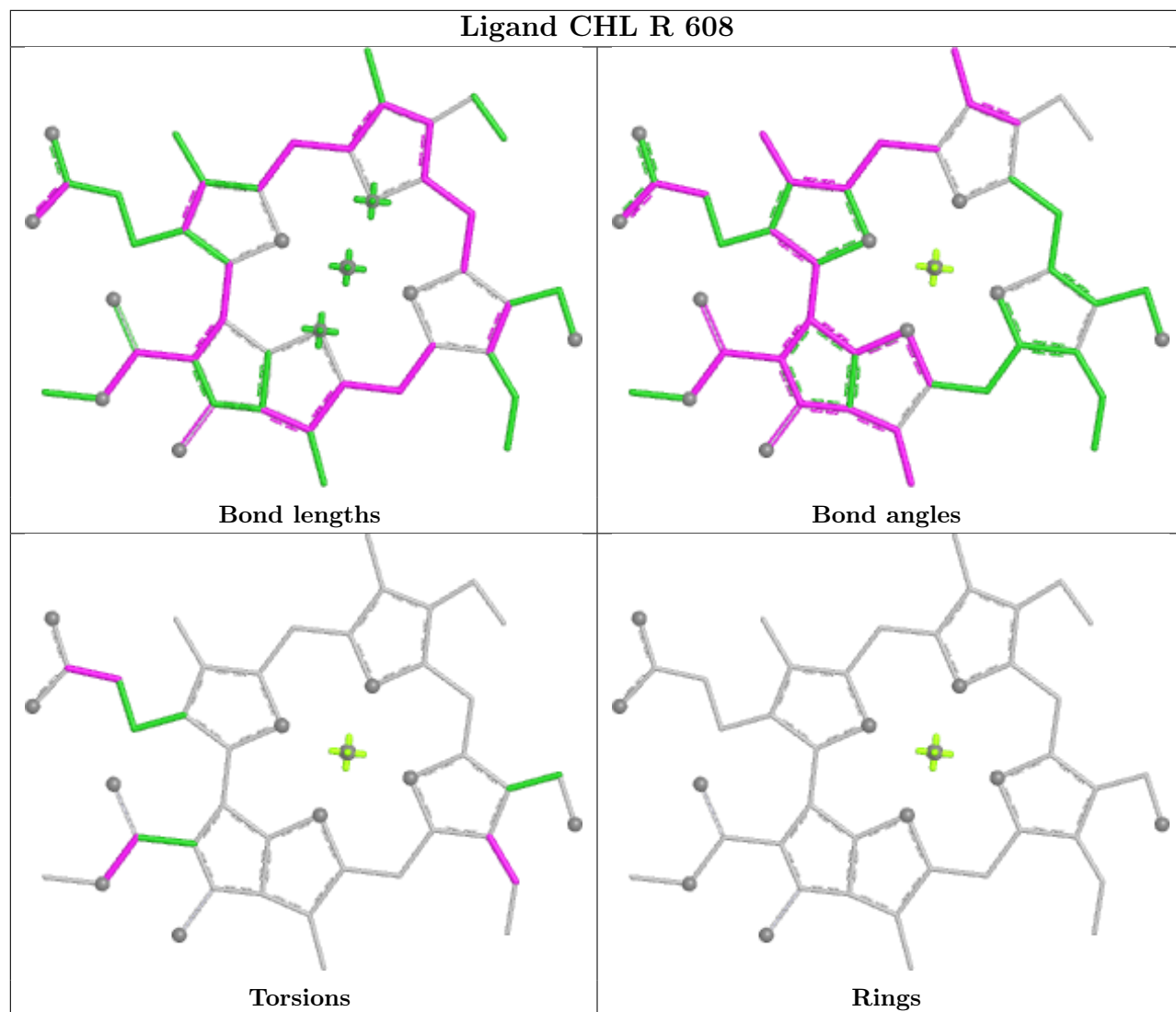
Ligand CLA C 608

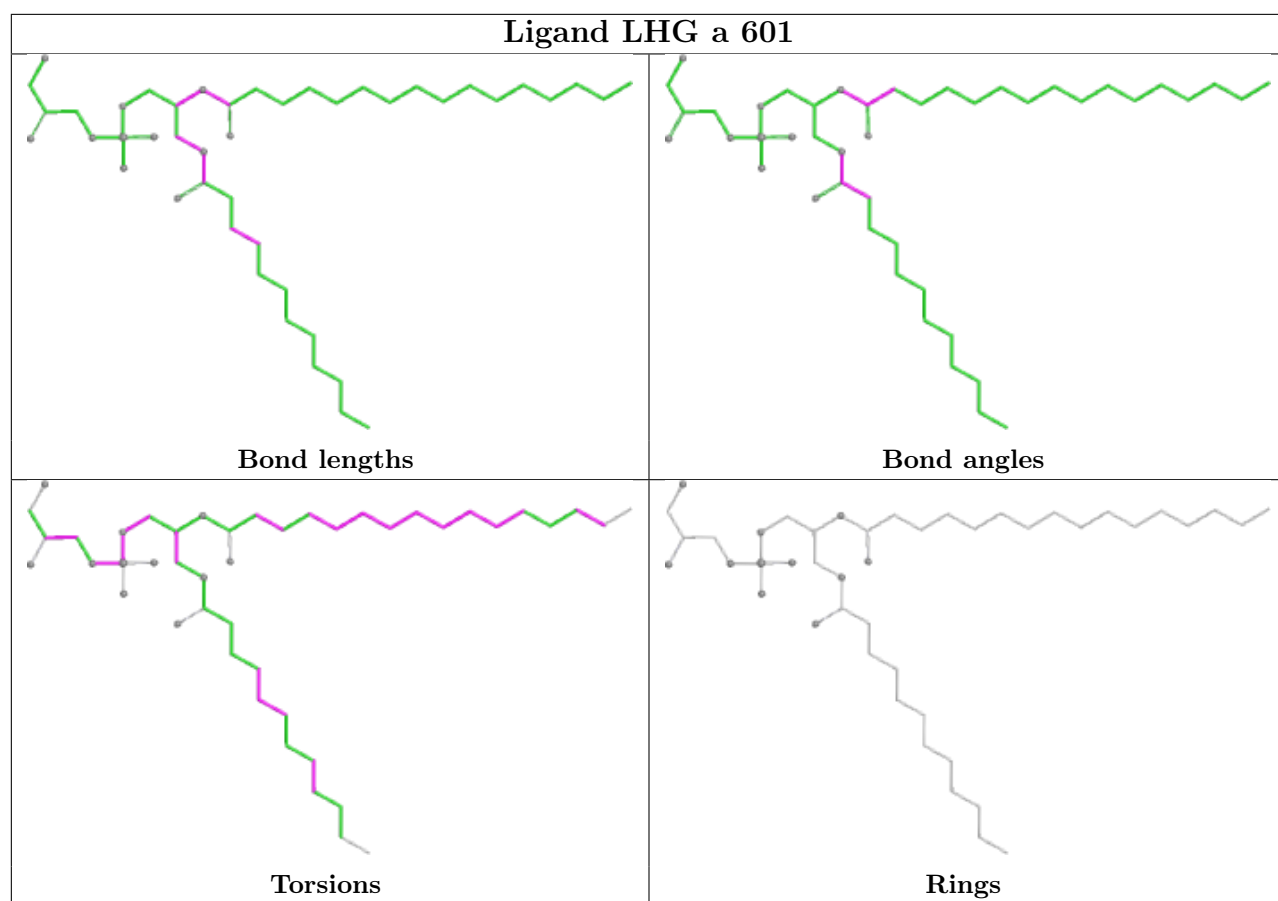


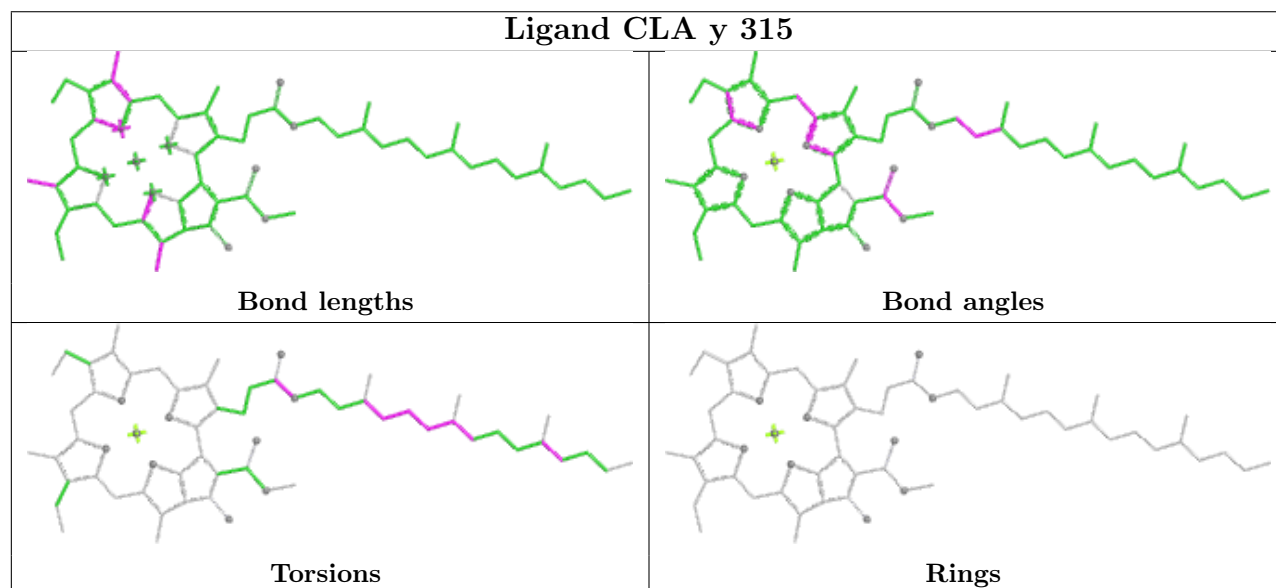
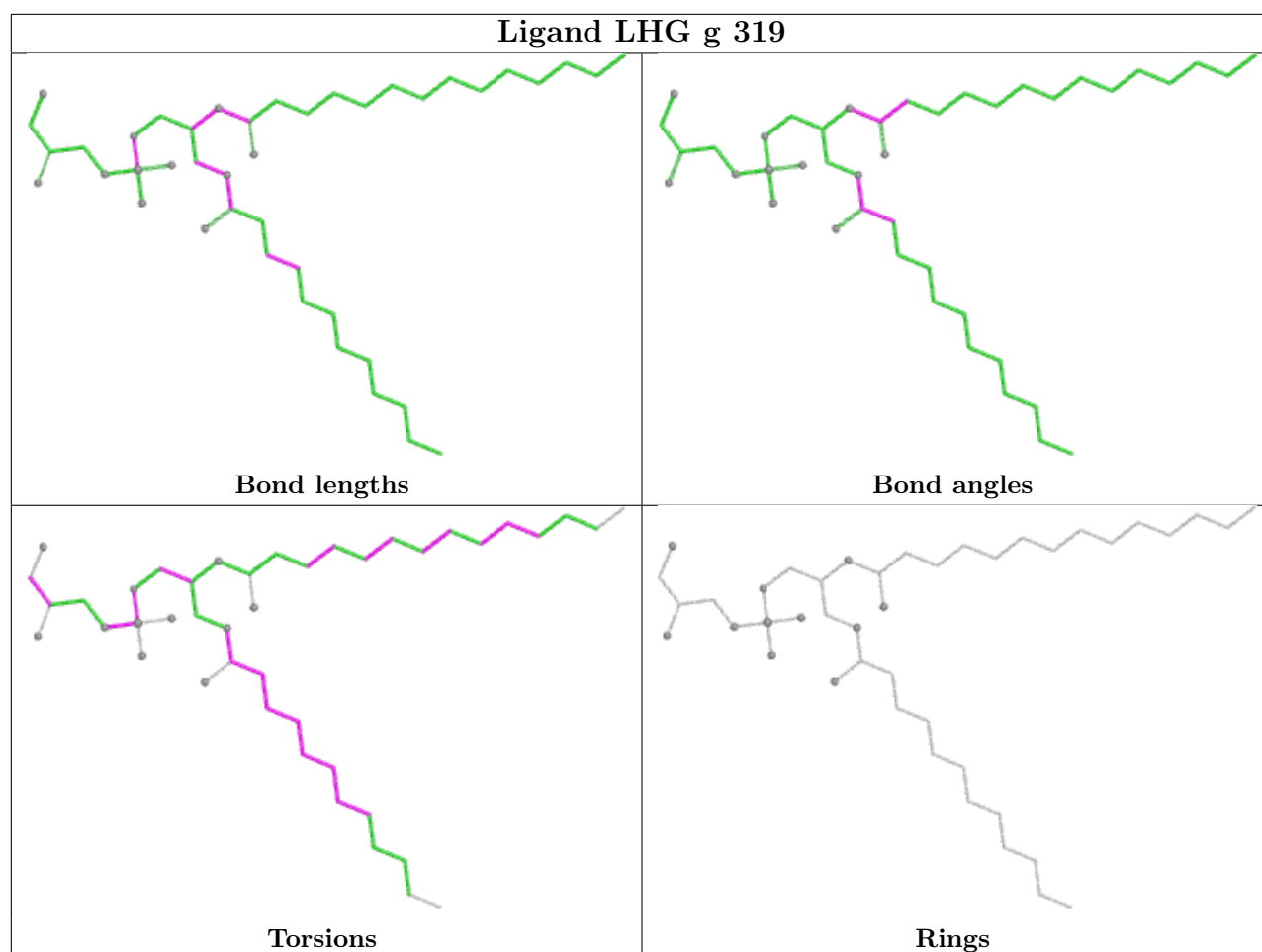
Ligand CHL n 308

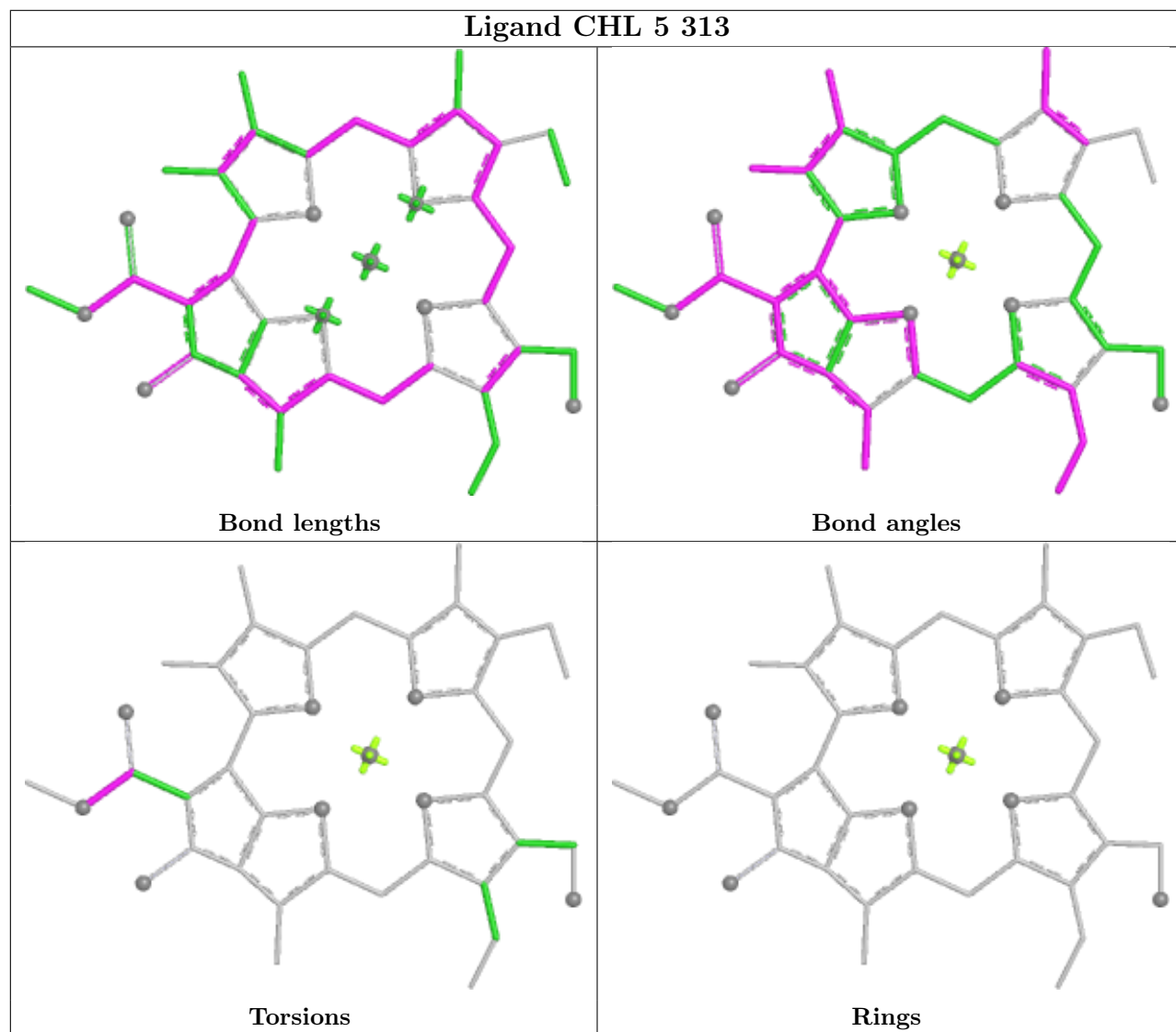
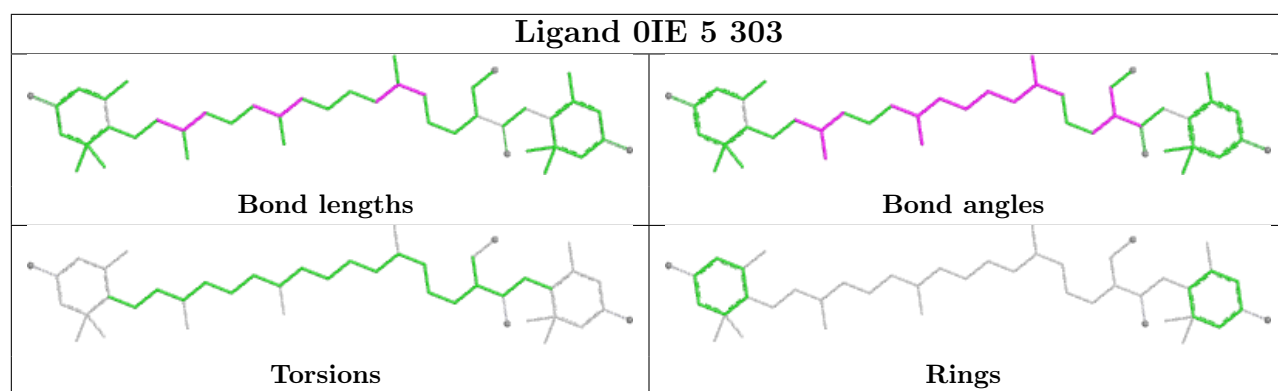


Ligand CHL R 608

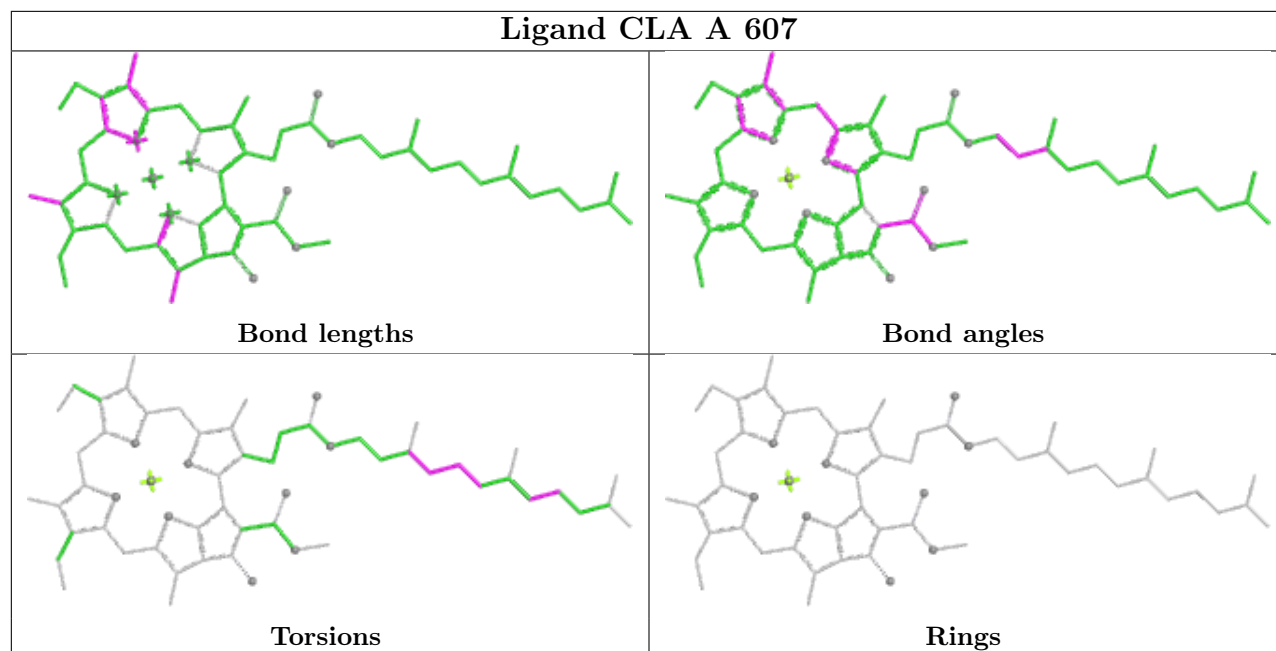




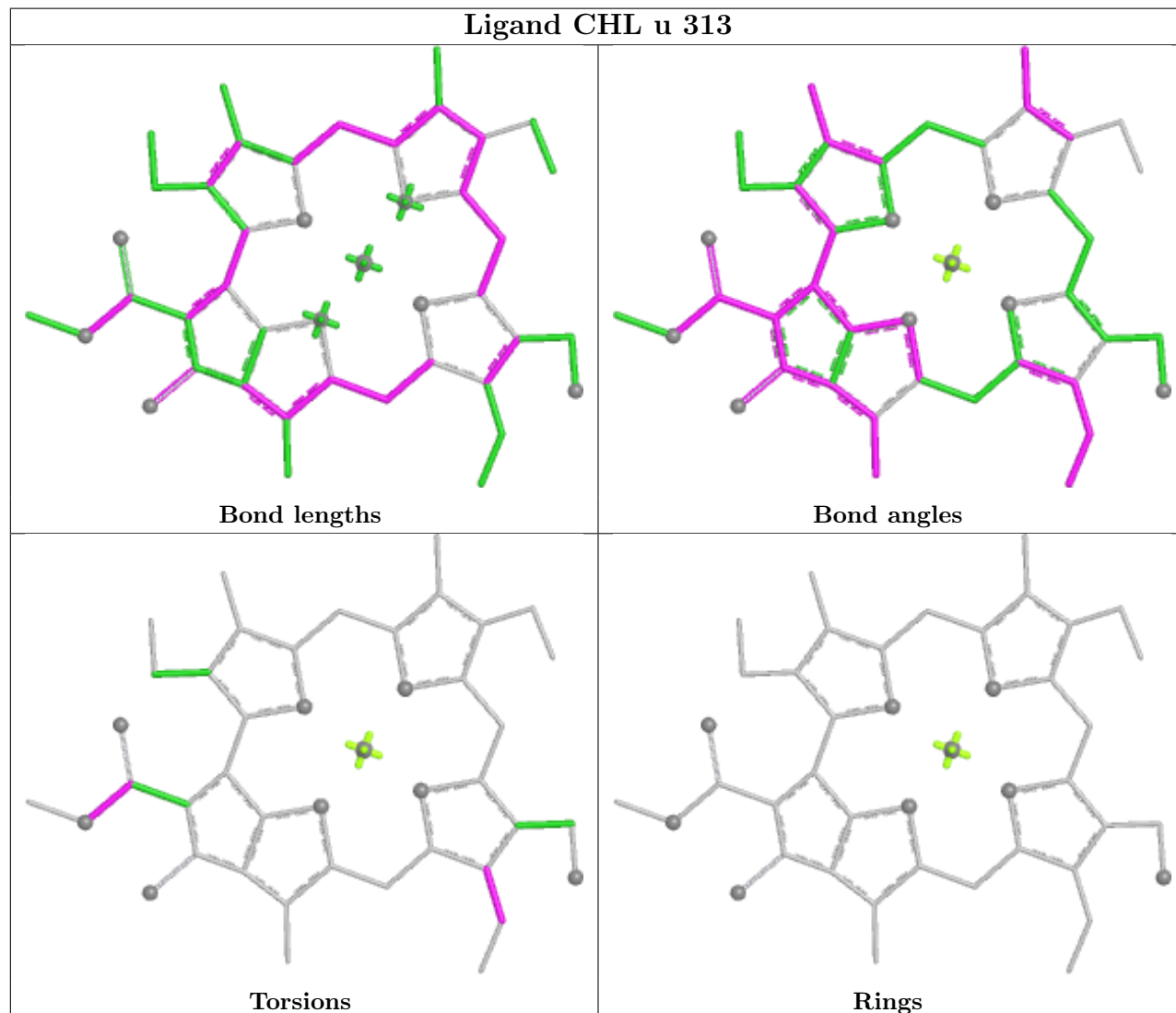


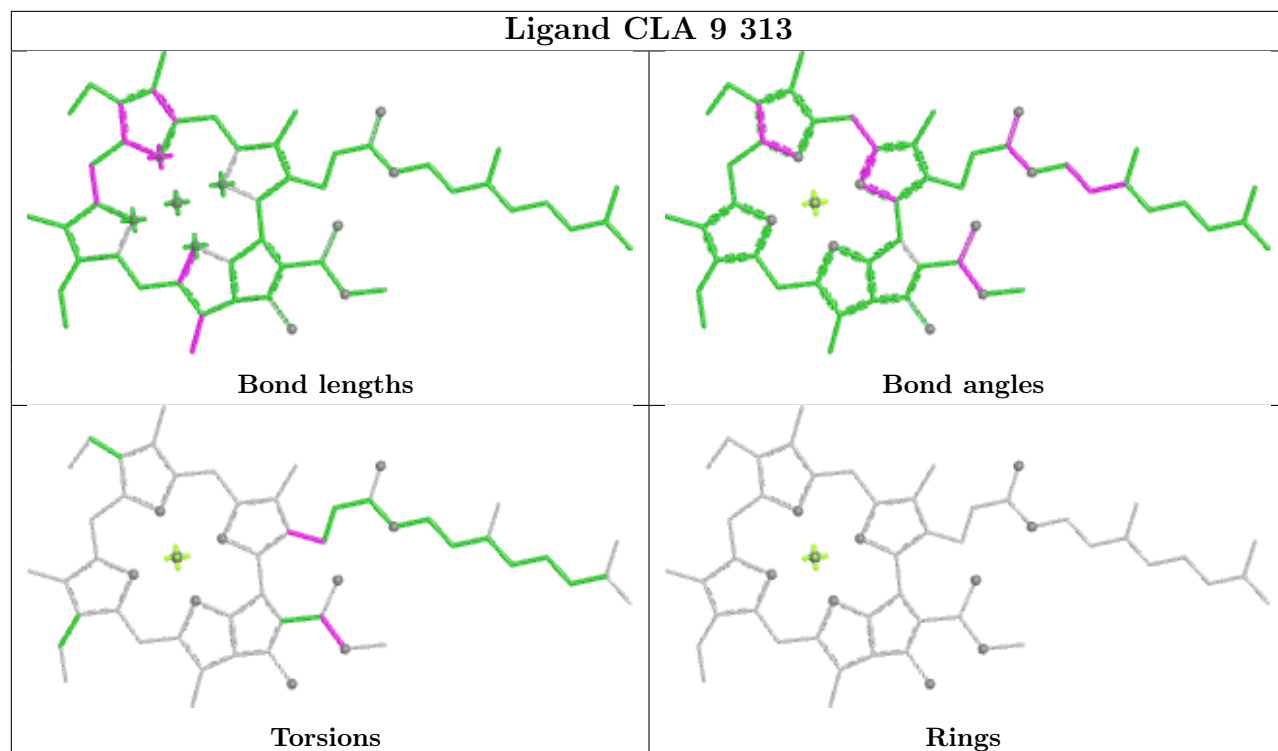
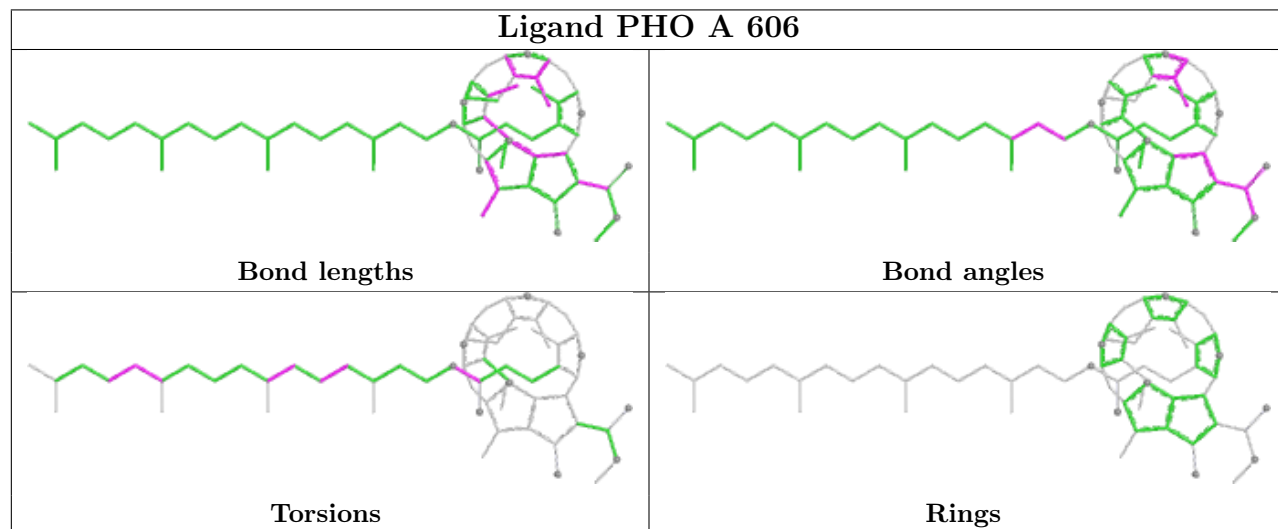


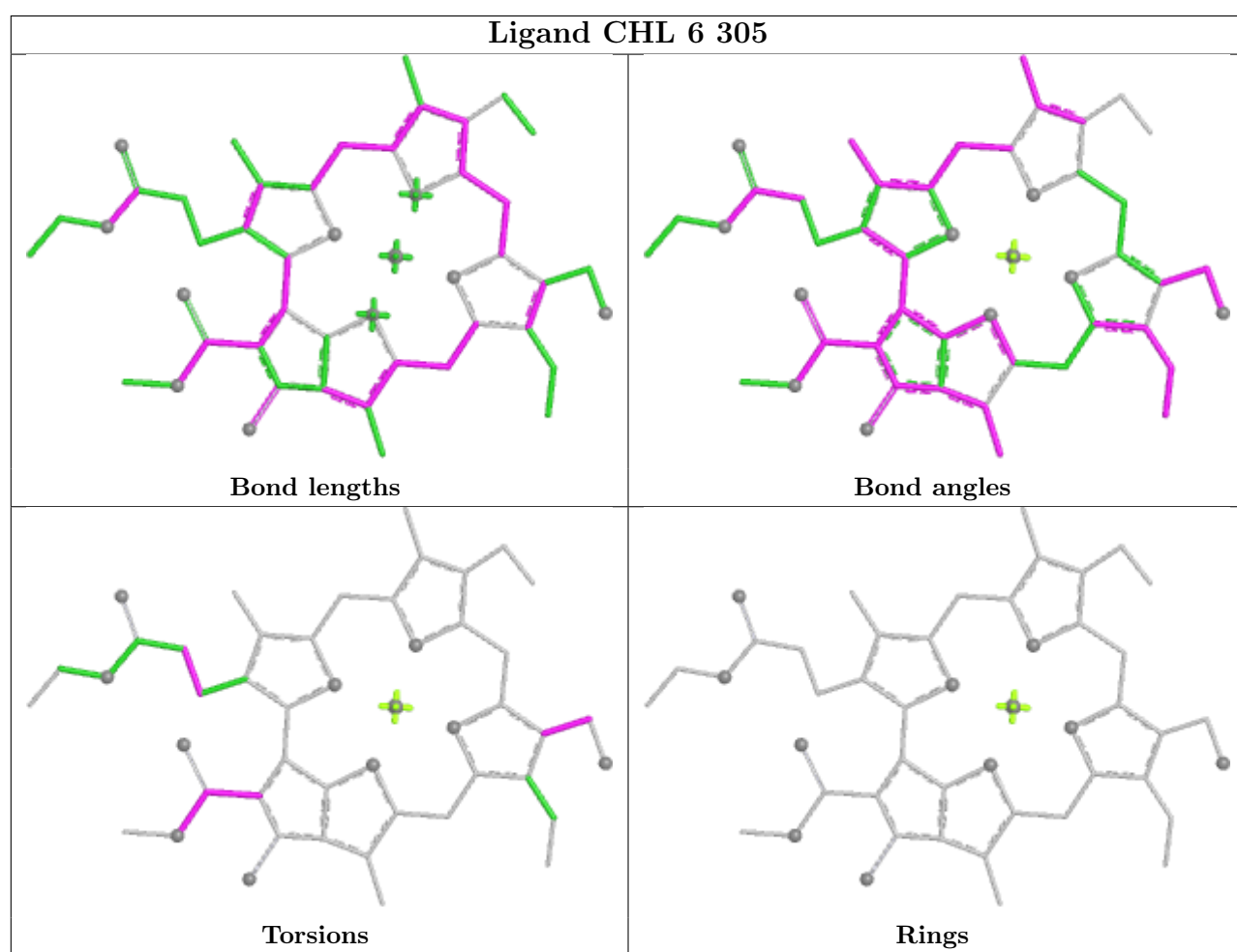
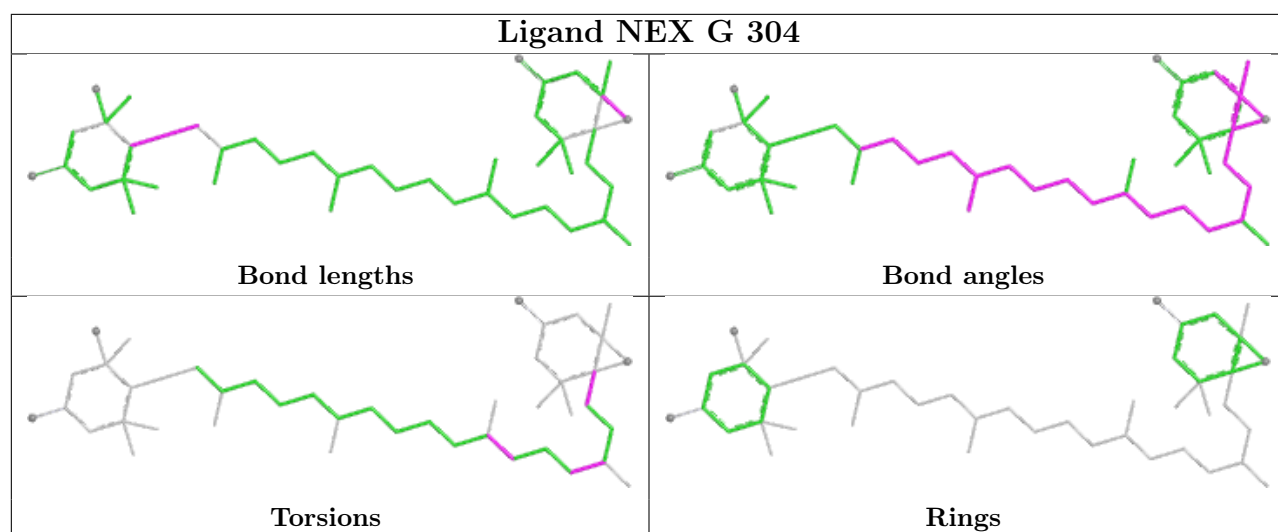
Ligand CLA A 607



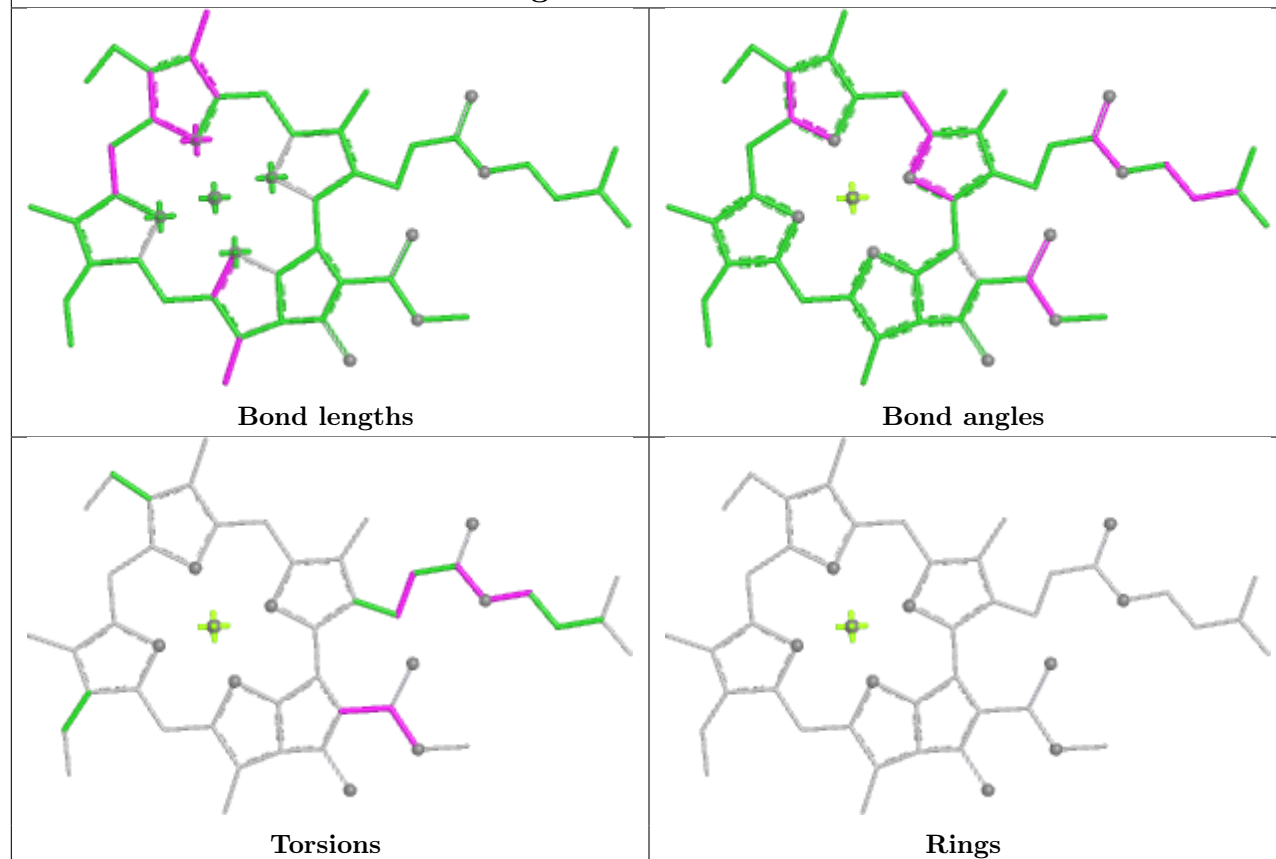
Ligand CHL u 313



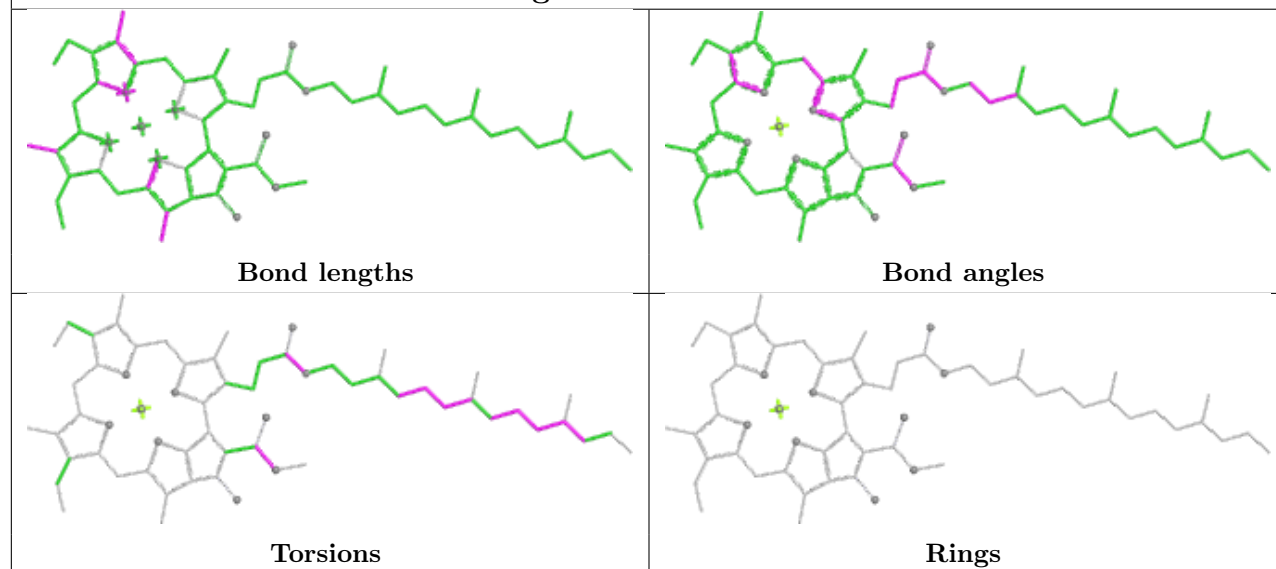
Ligand CLA 9 313**Ligand PHO A 606**

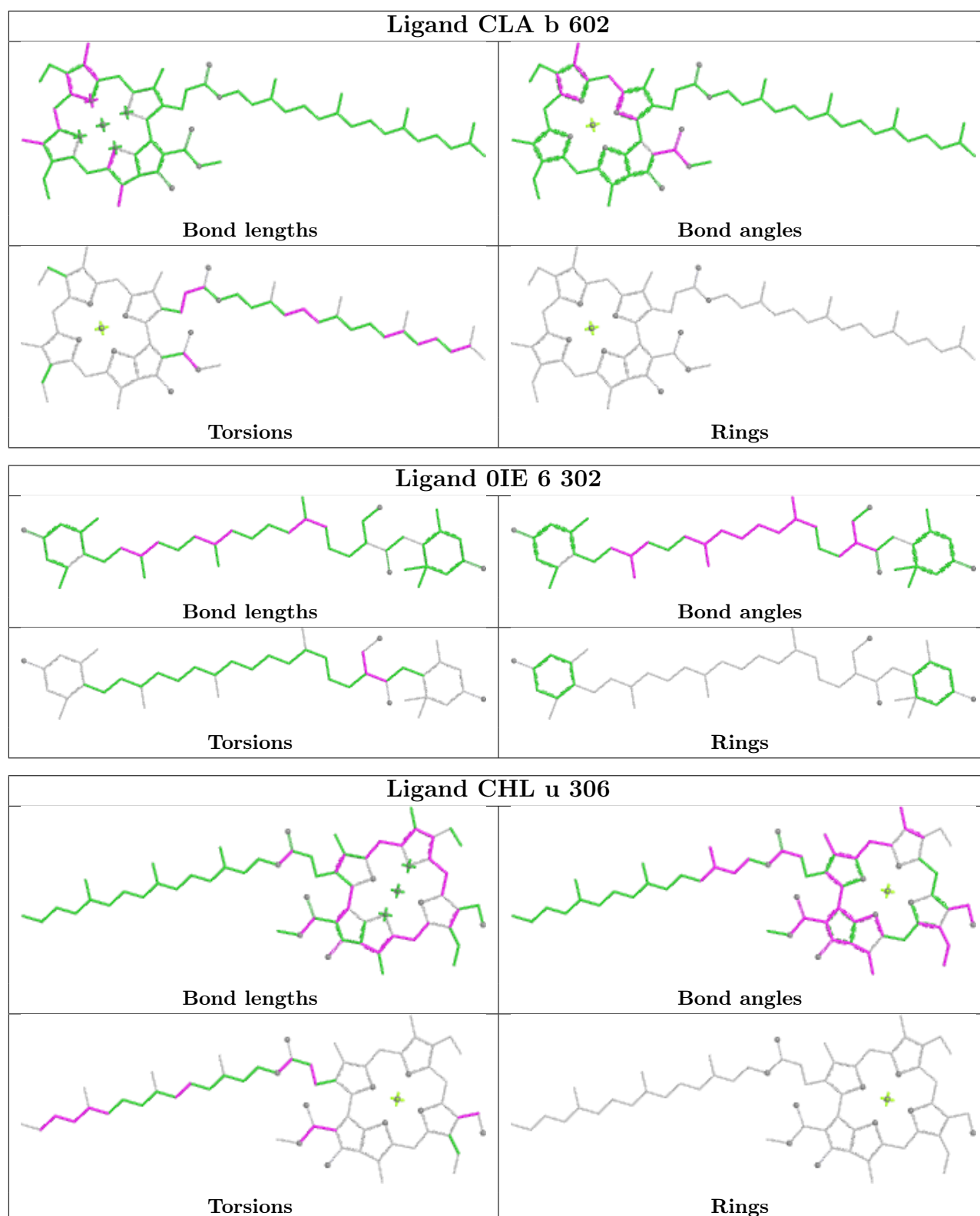


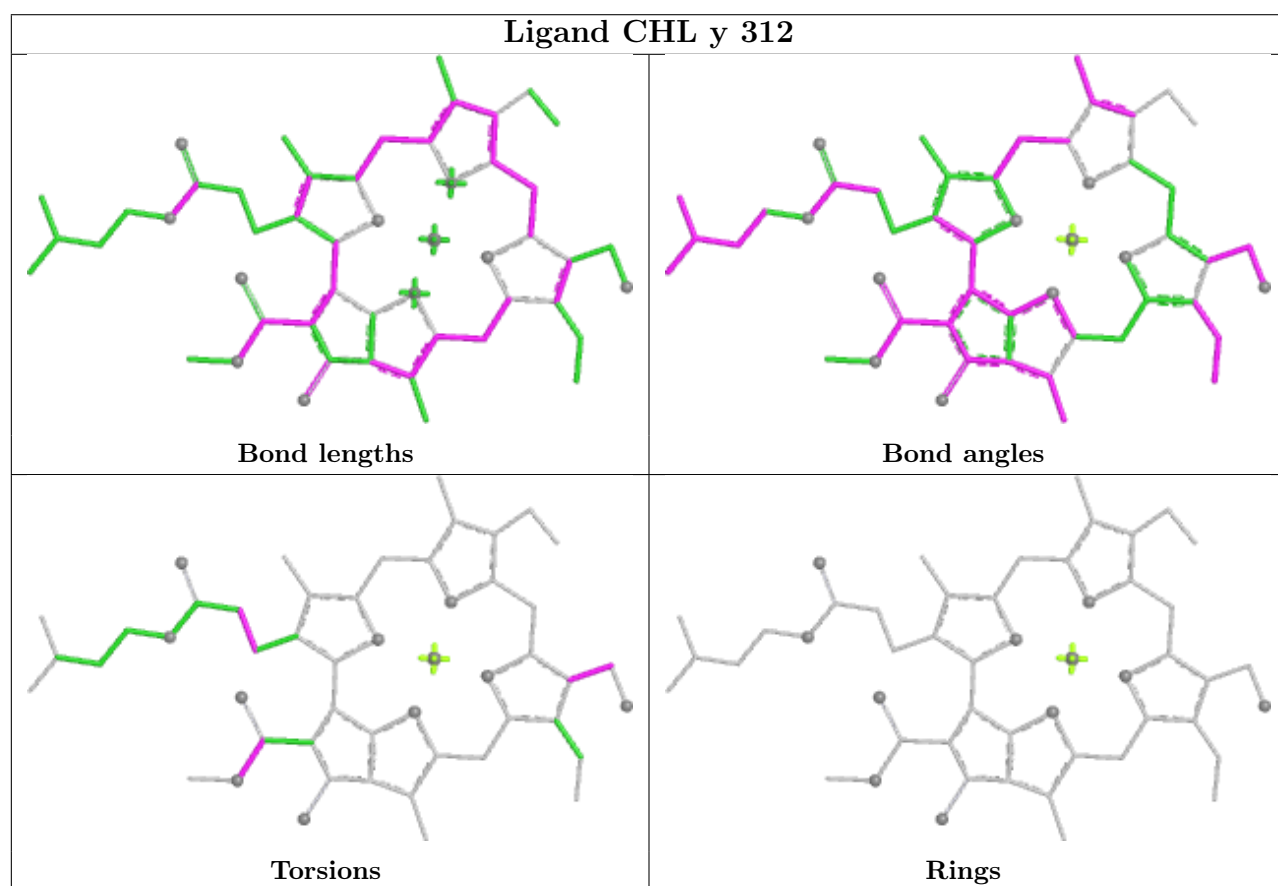
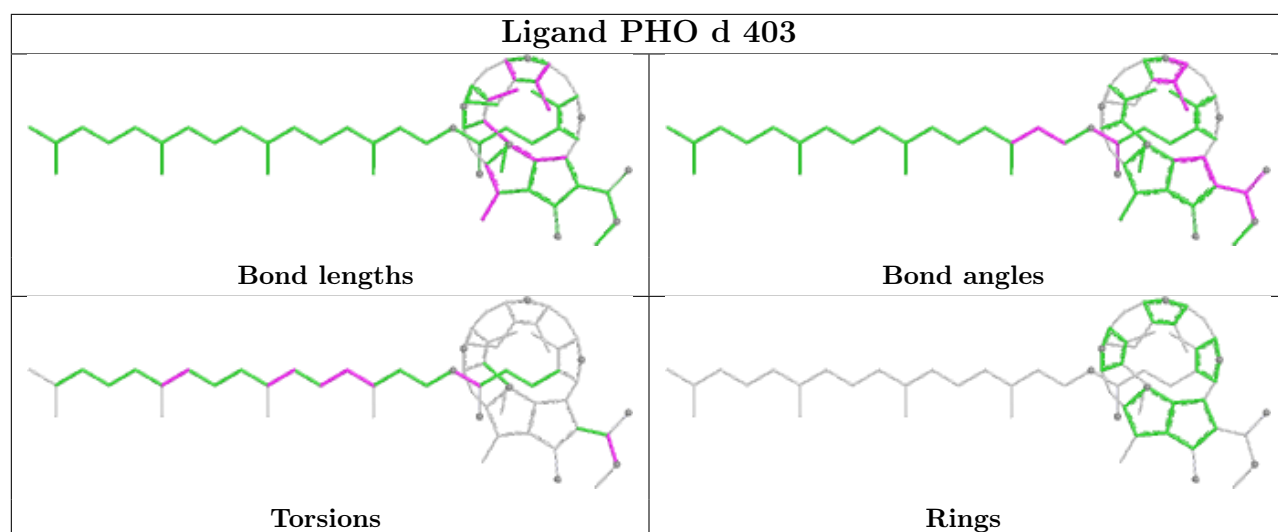
Ligand CLA G 308

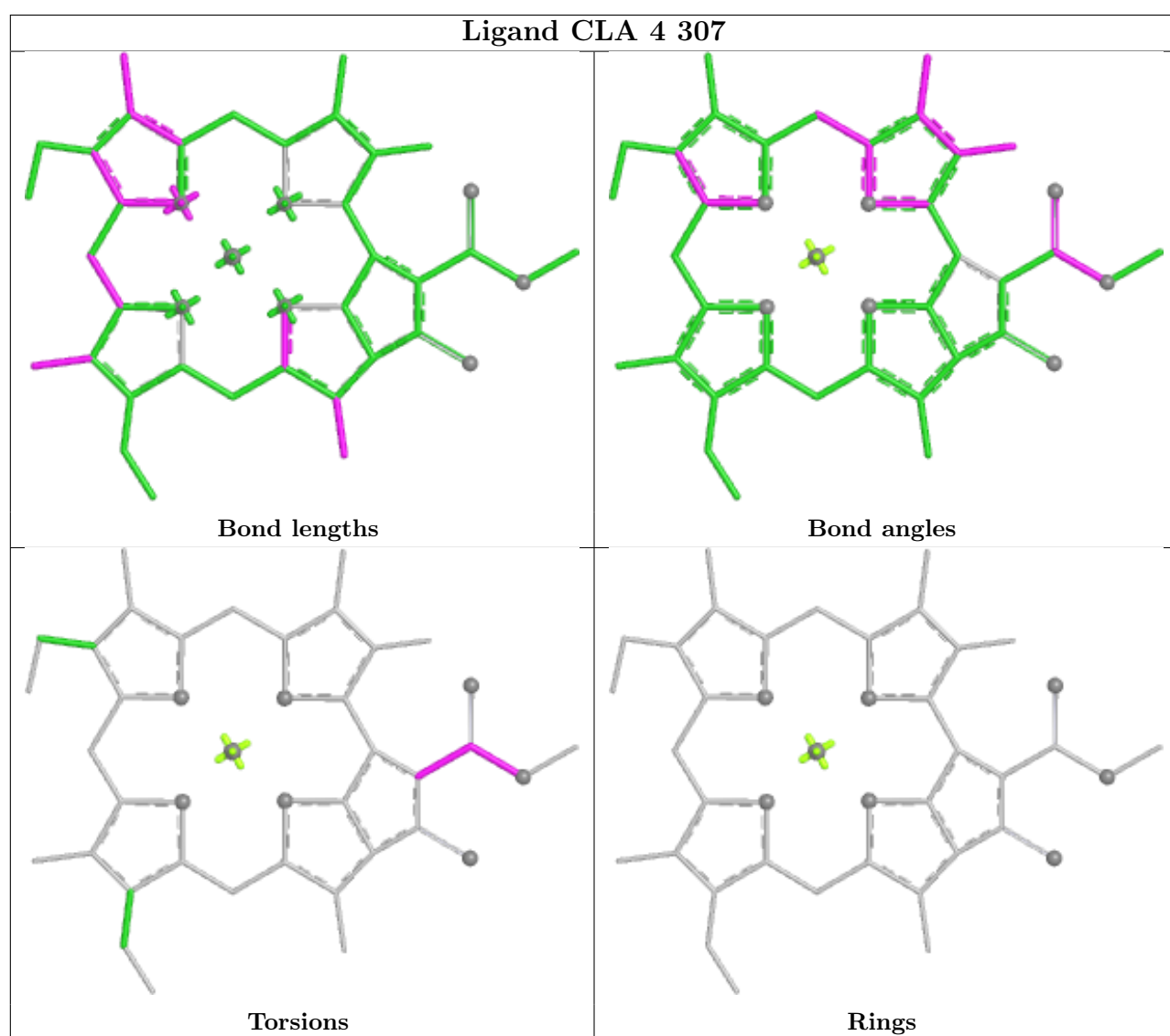
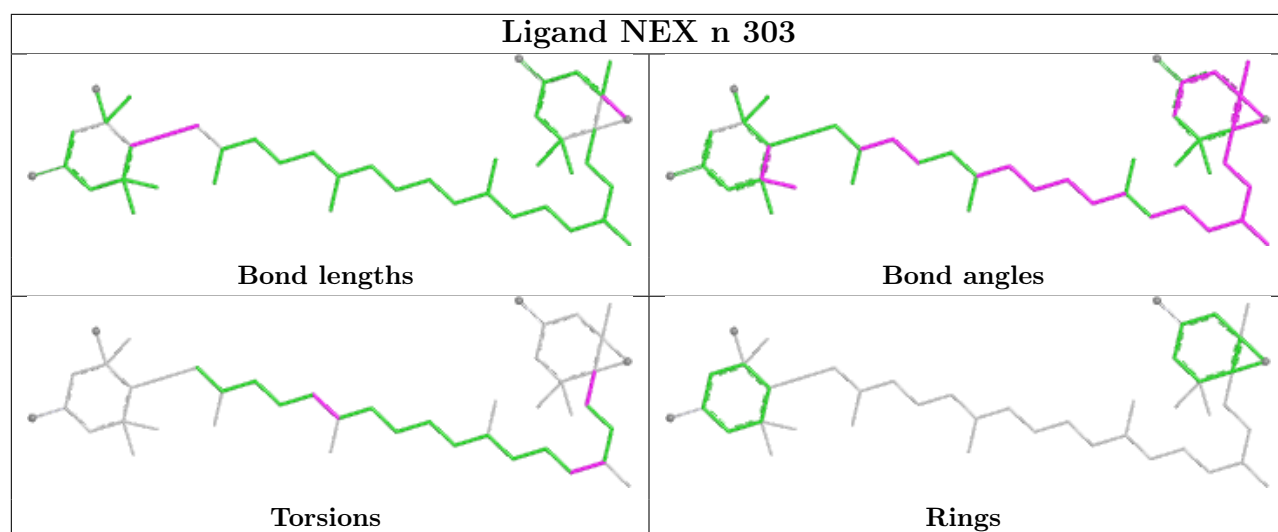


Ligand CLA B 604

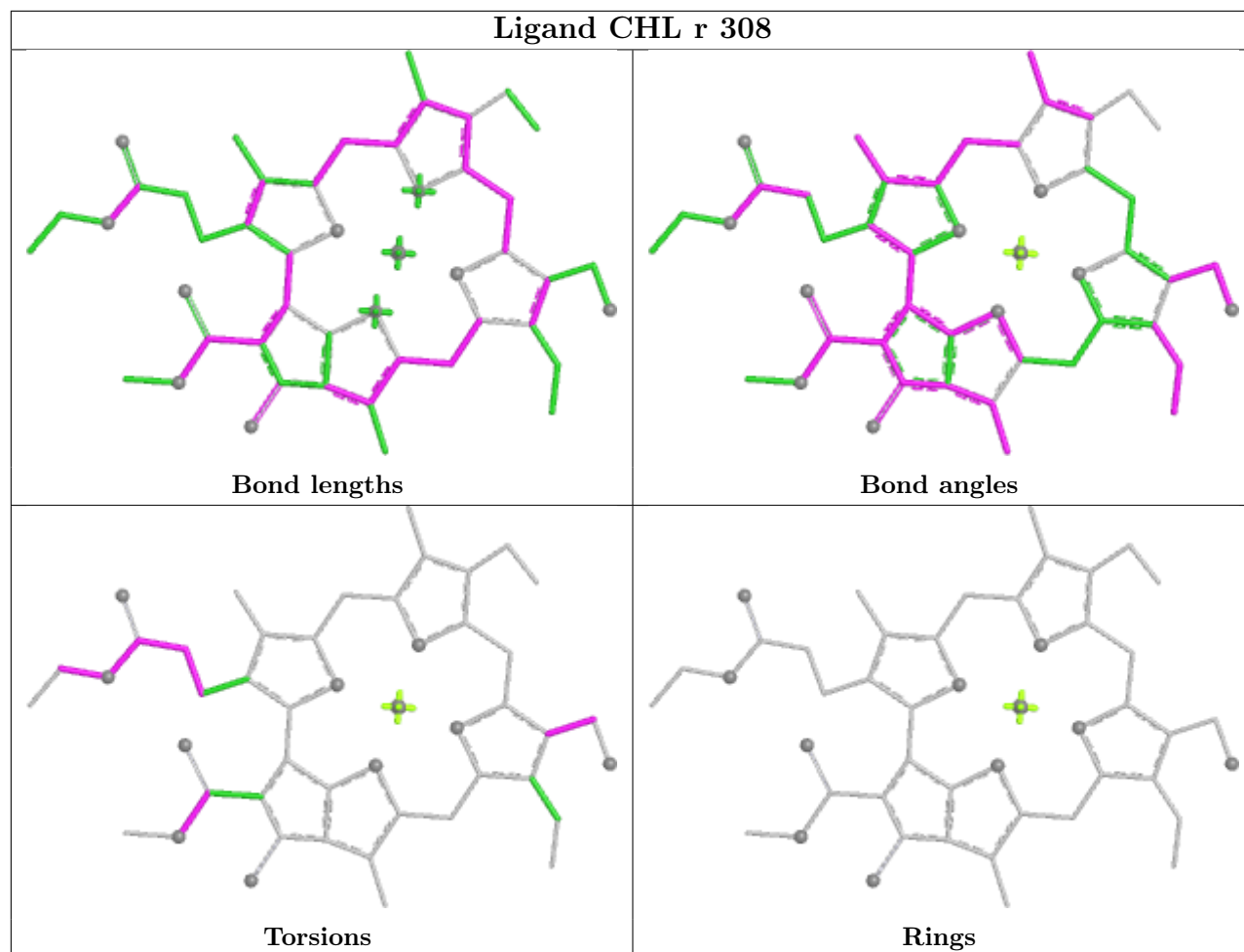




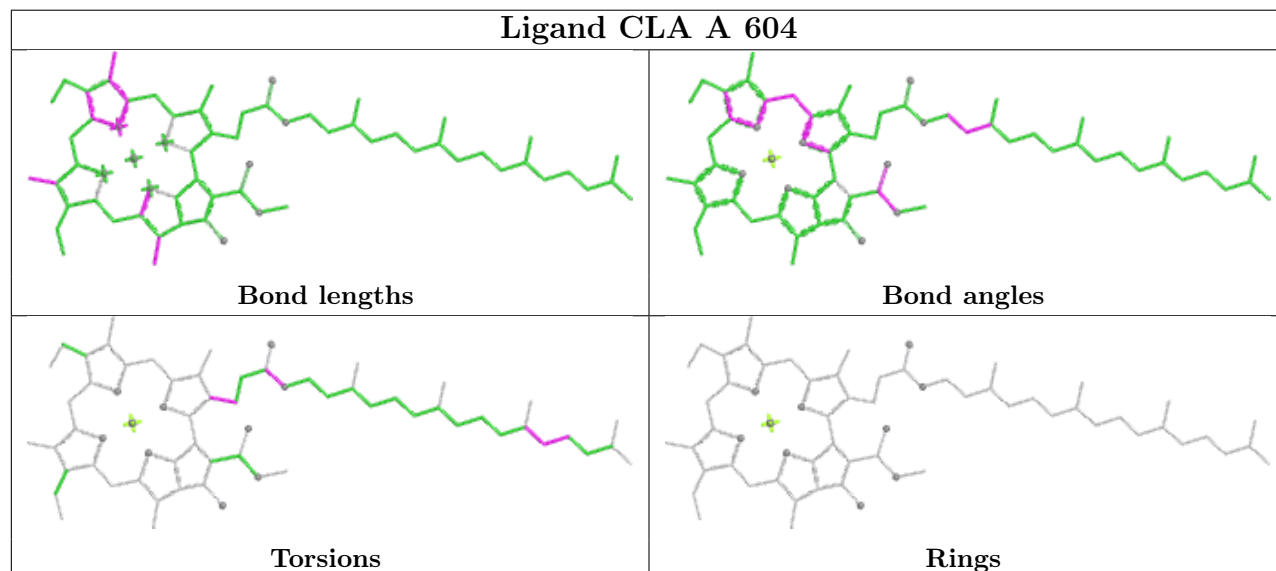


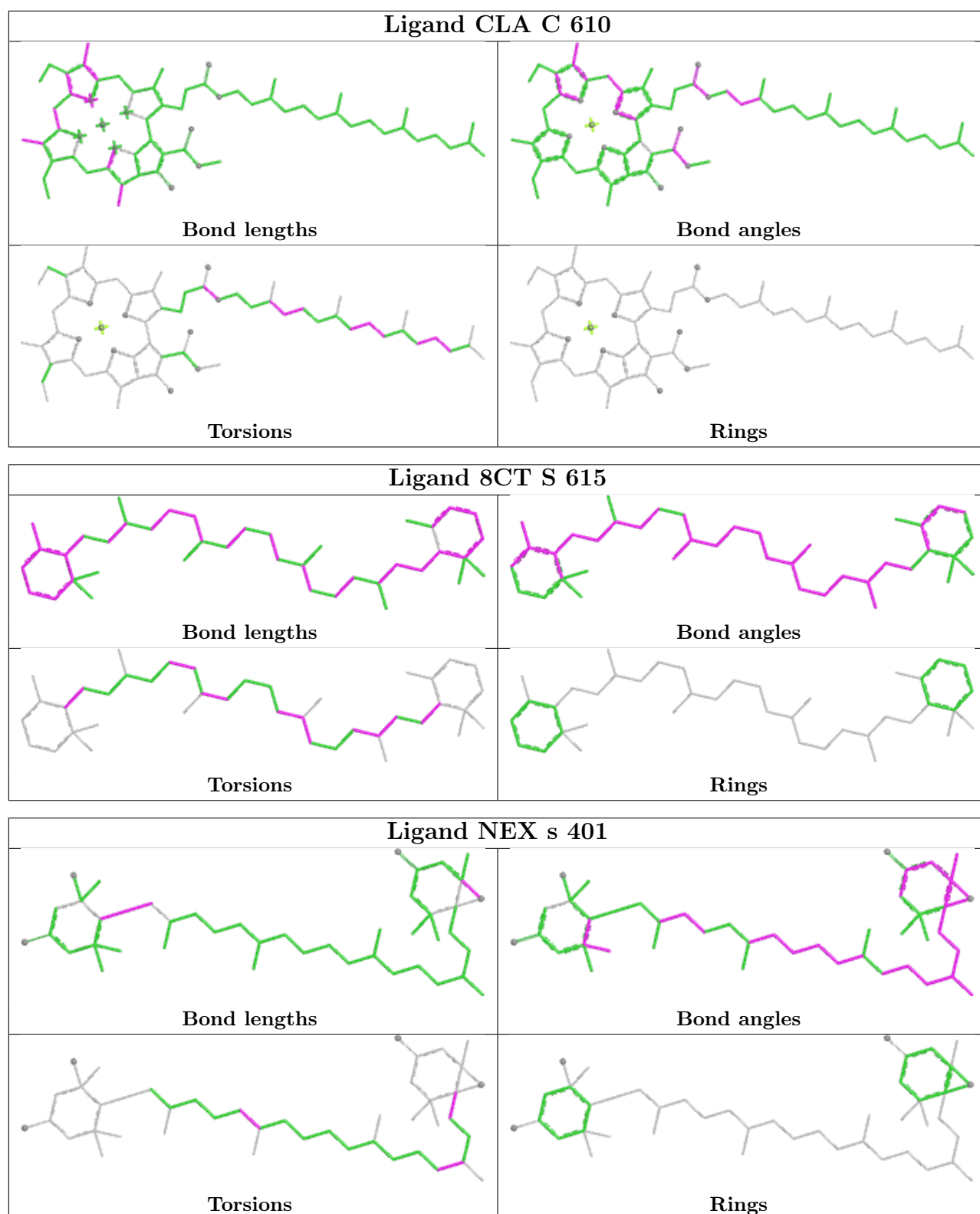


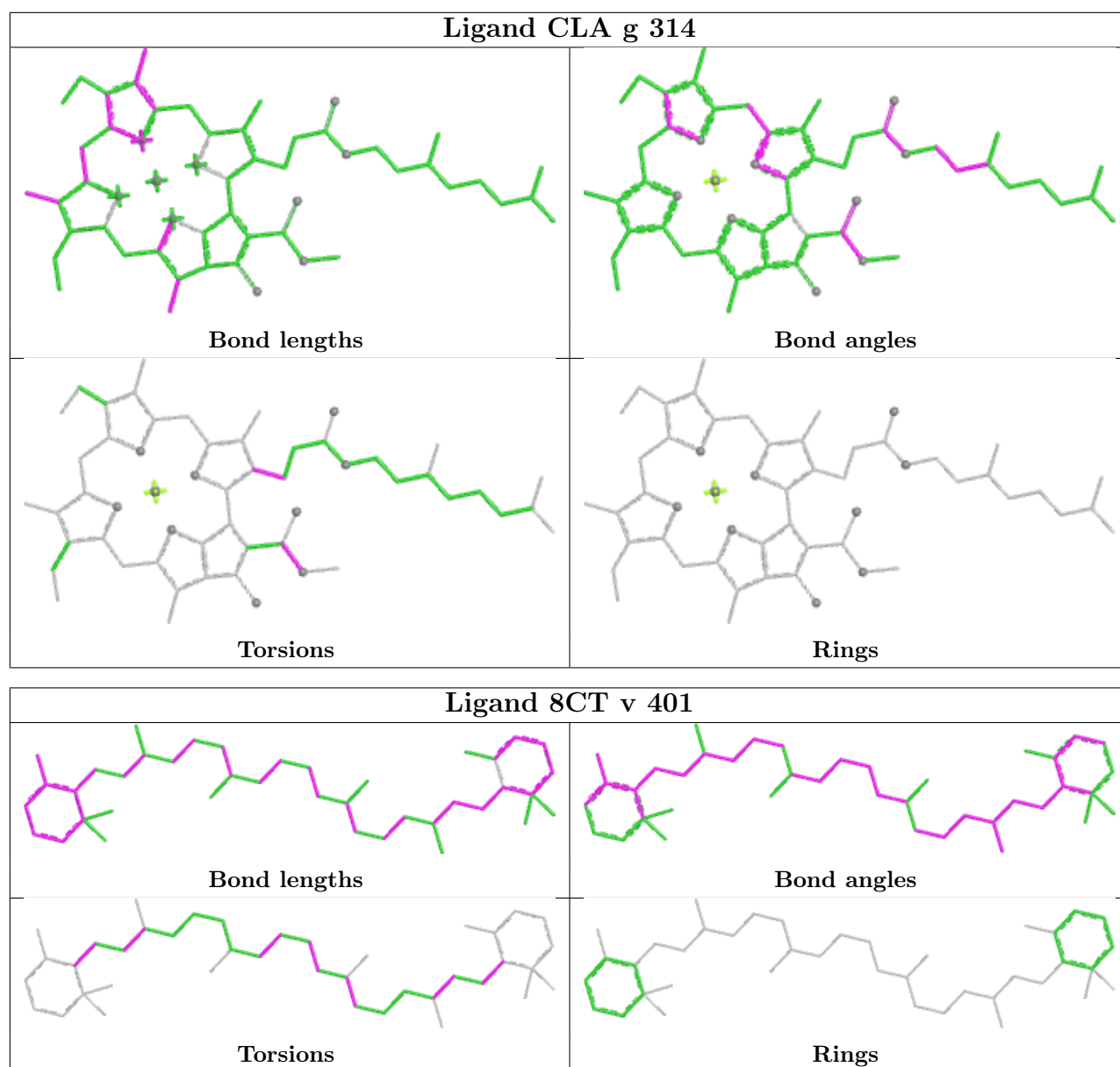
Ligand CHL r 308

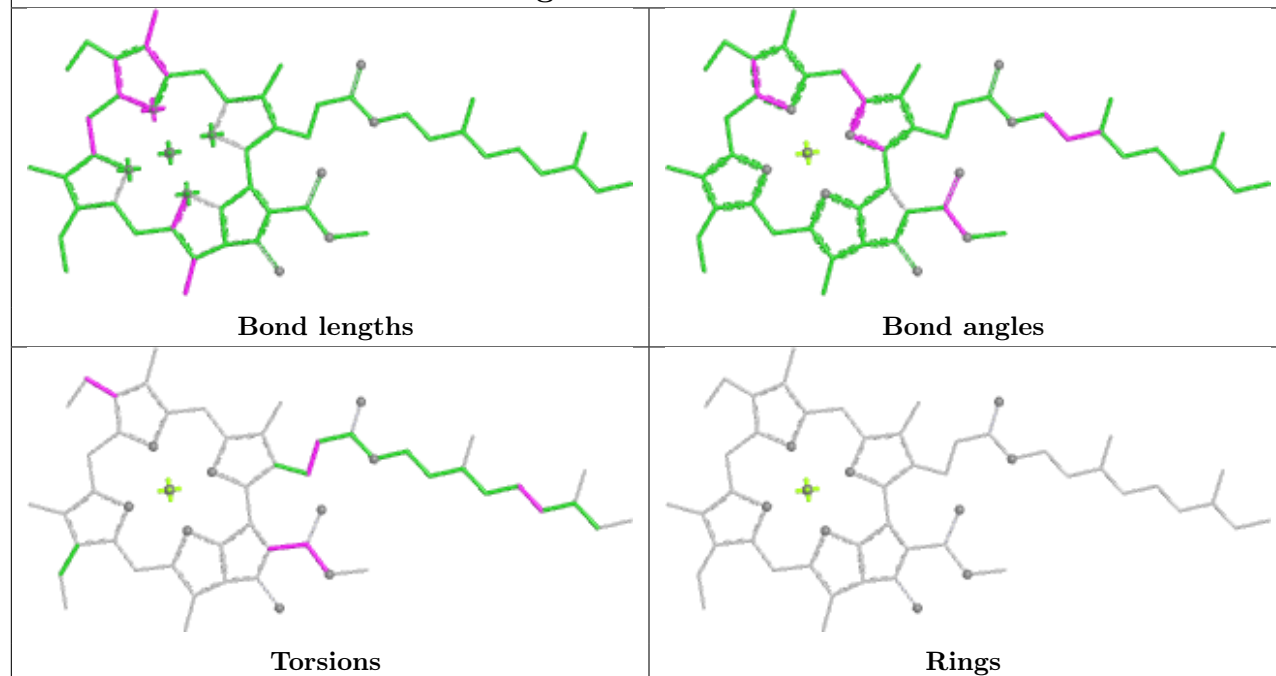
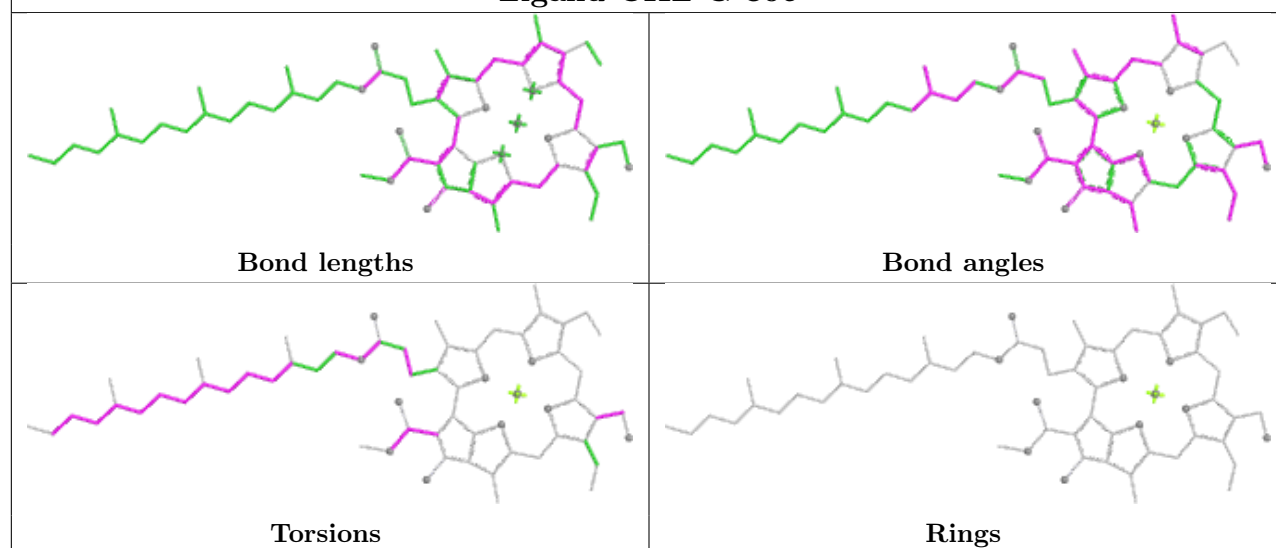


Ligand CLA A 604

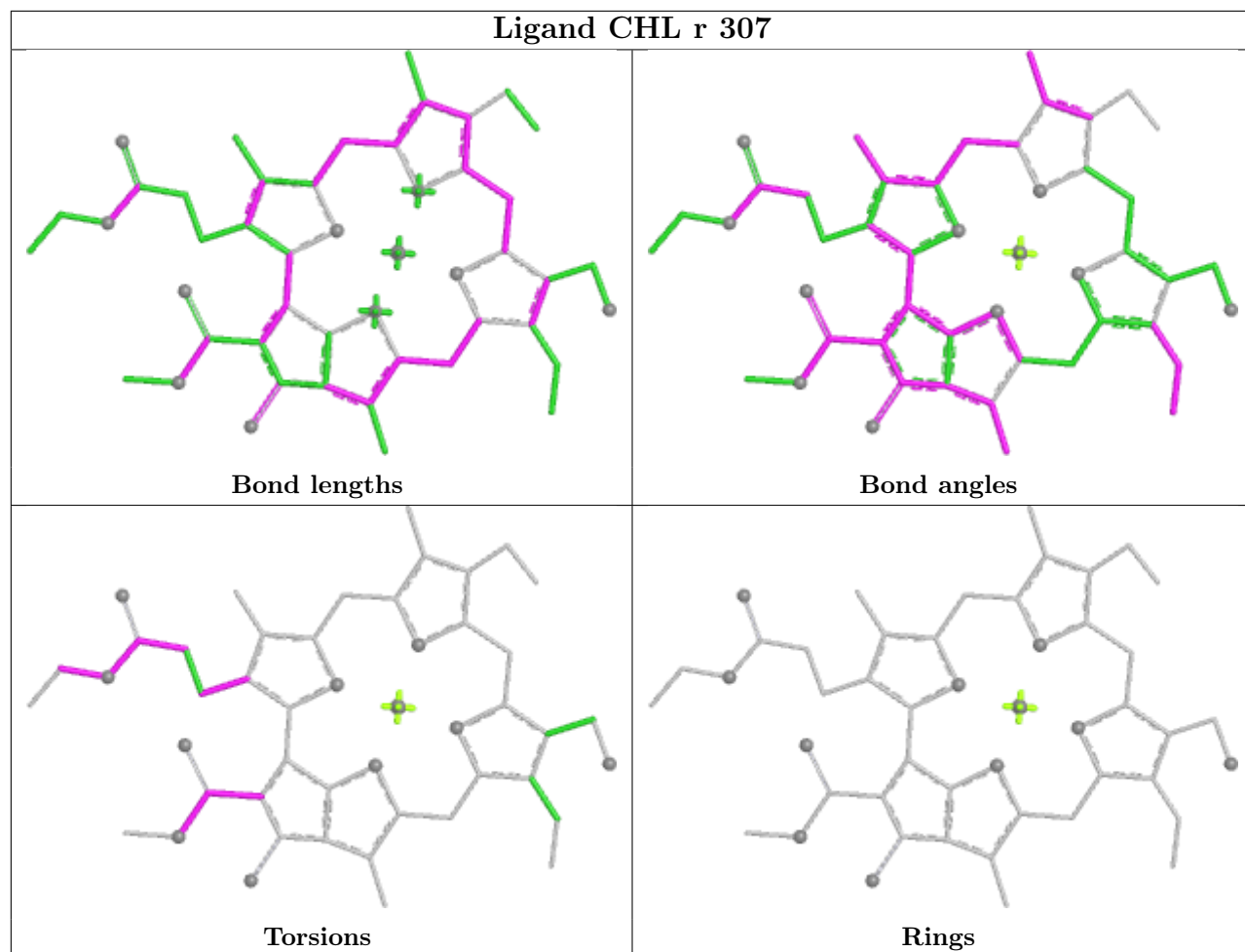




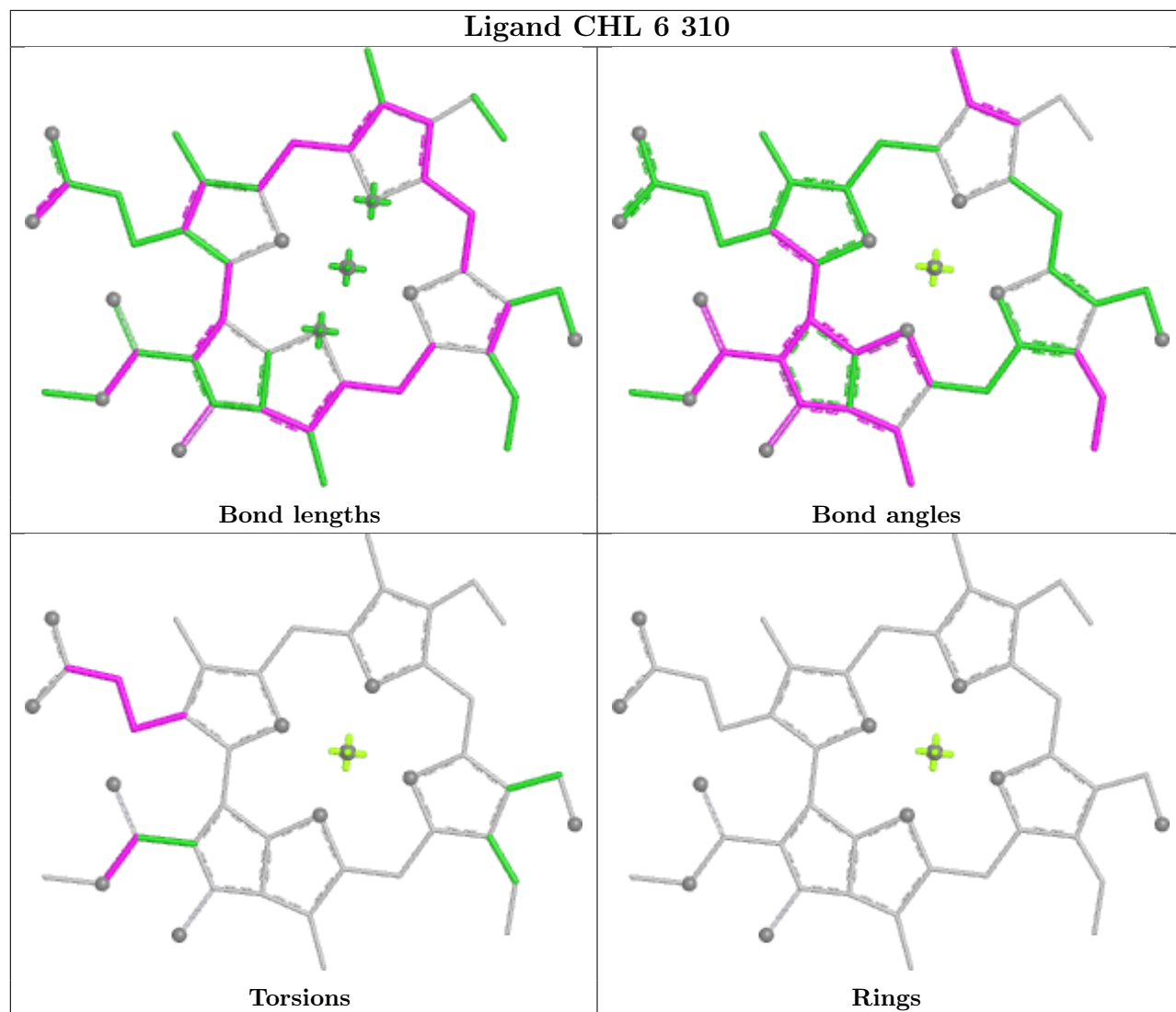


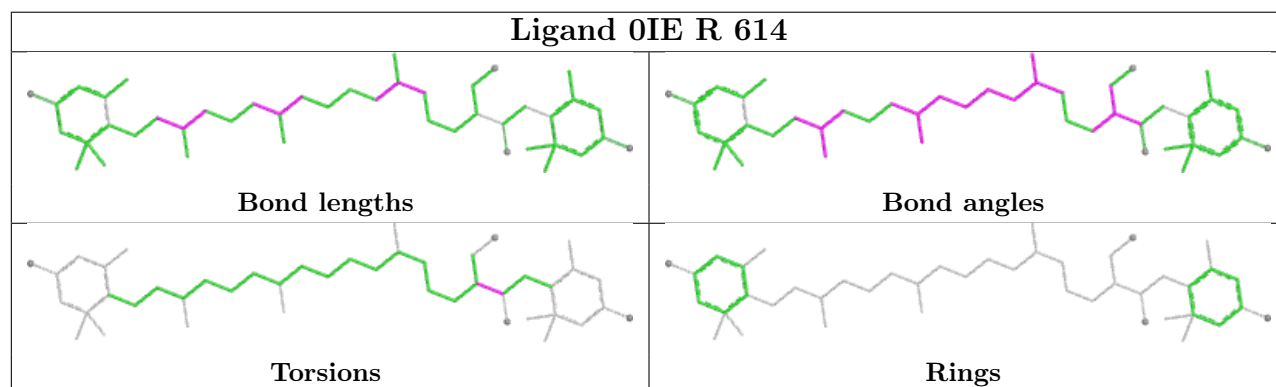
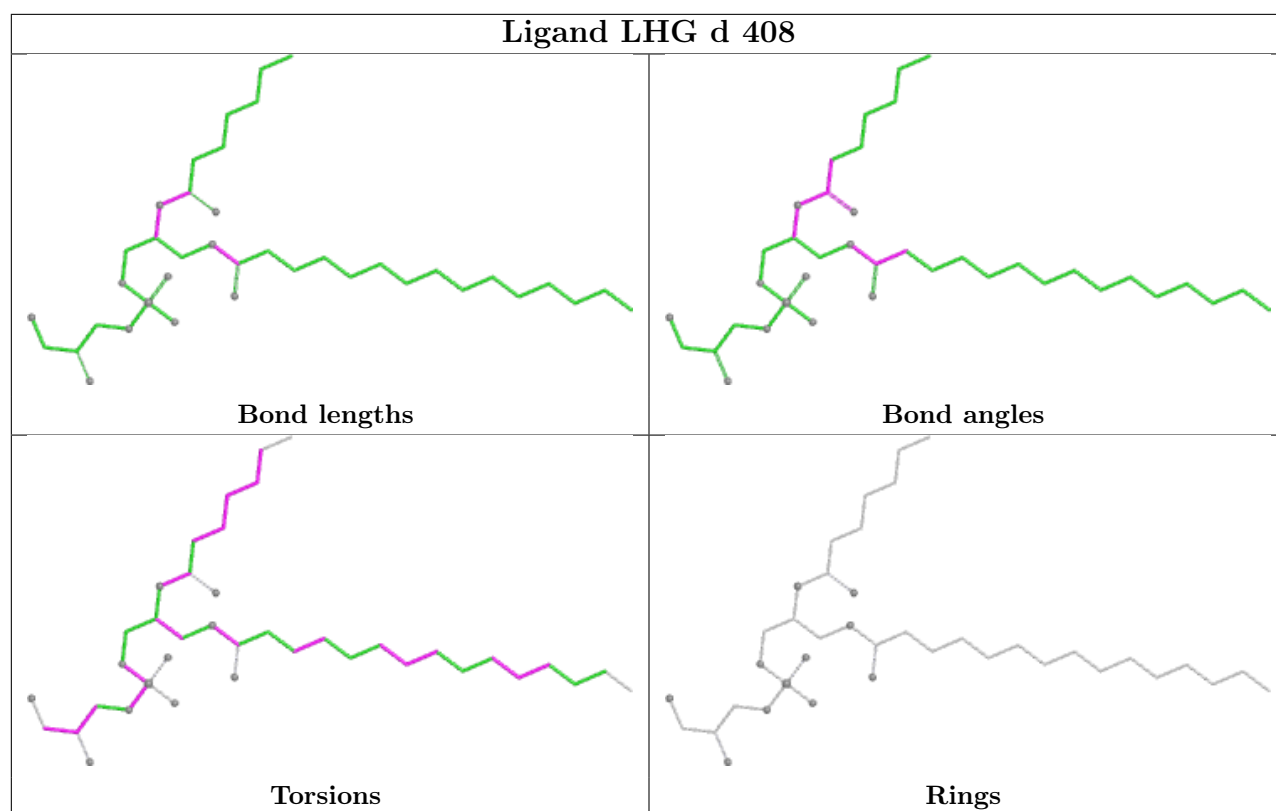
Ligand CLA 9 306**Ligand CHL G 306**

Ligand CHL r 307

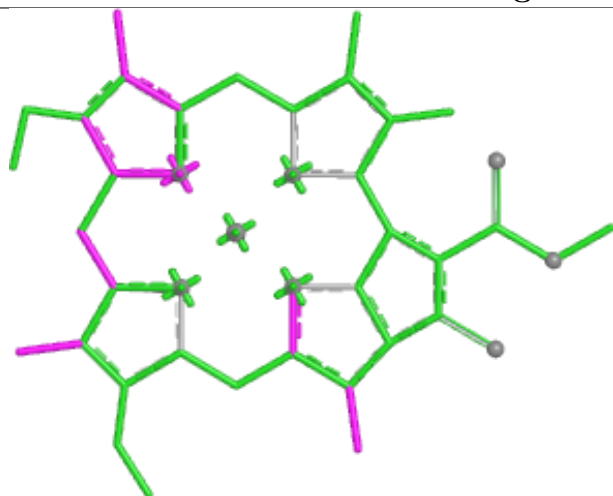


Ligand CHL 6 310

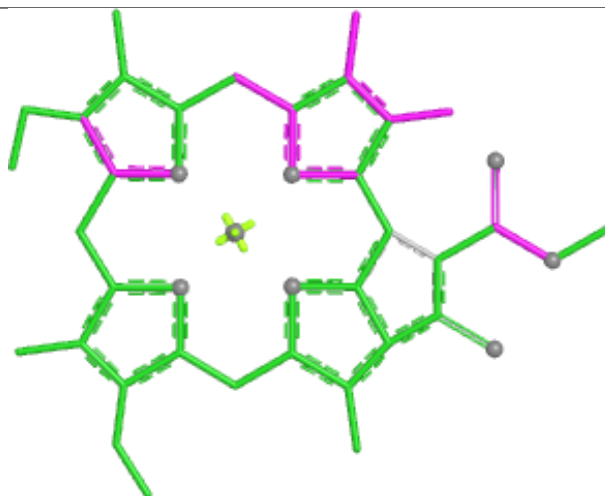




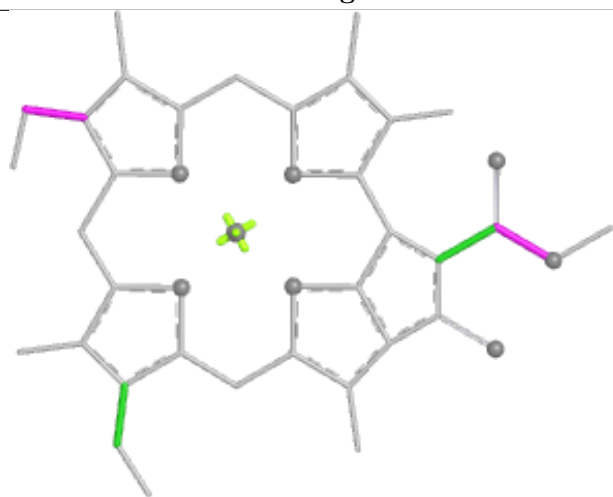
Ligand CLA R 604



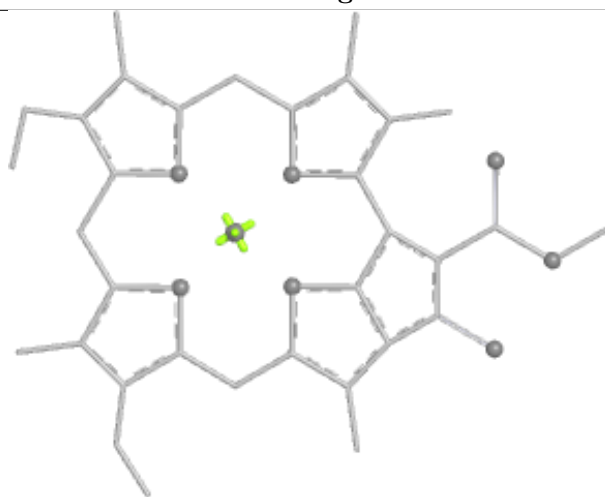
Bond lengths



Bond angles

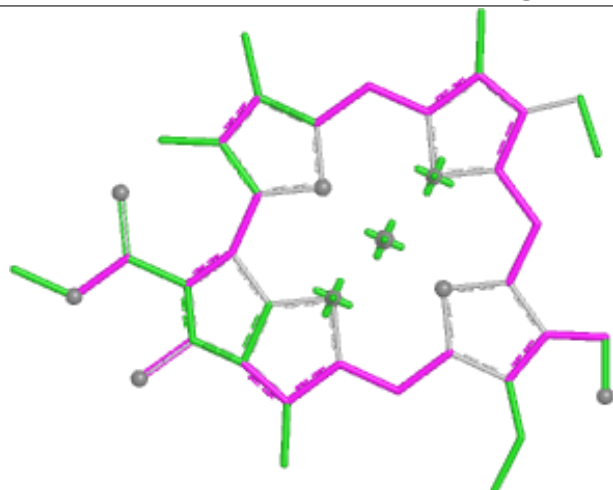


Torsions

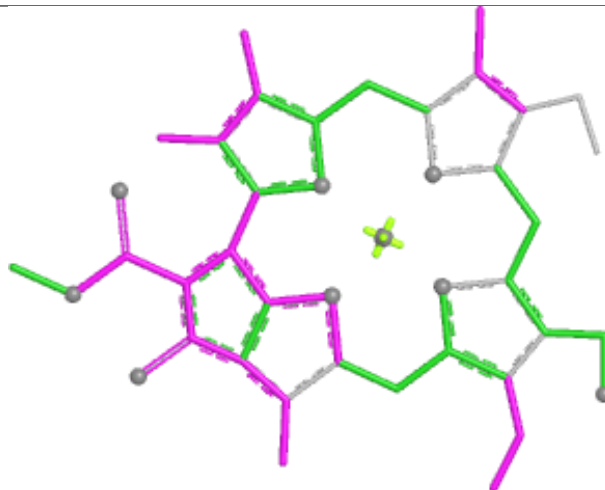


Rings

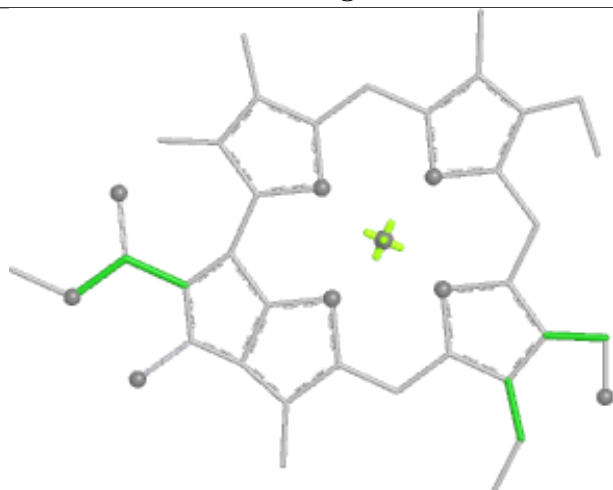
Ligand CHL 6 317



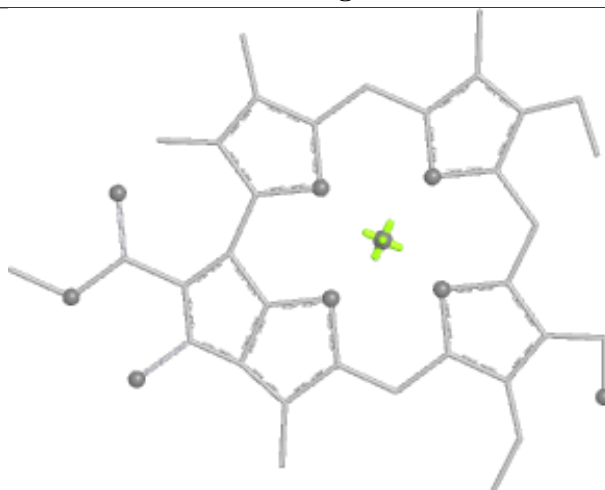
Bond lengths



Bond angles

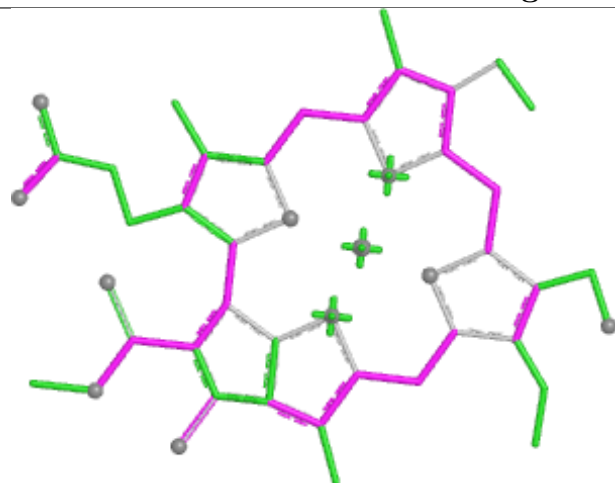


Torsions

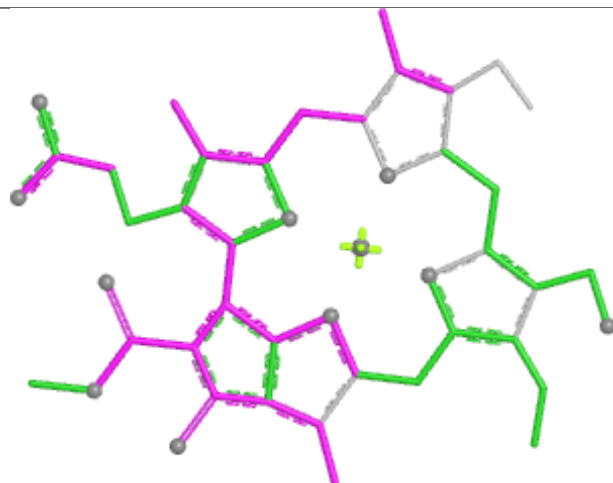


Rings

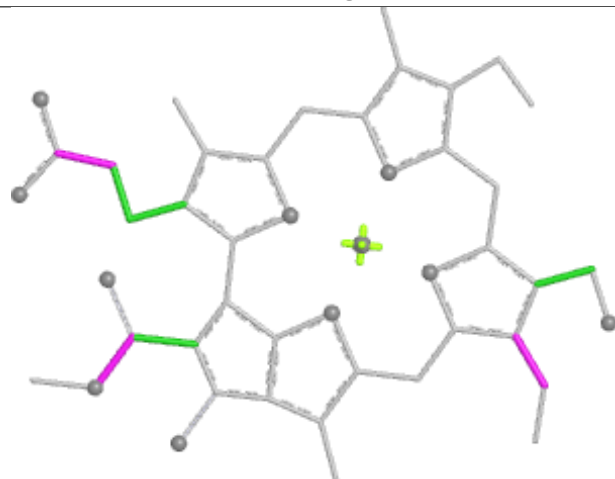
Ligand CHL r 309



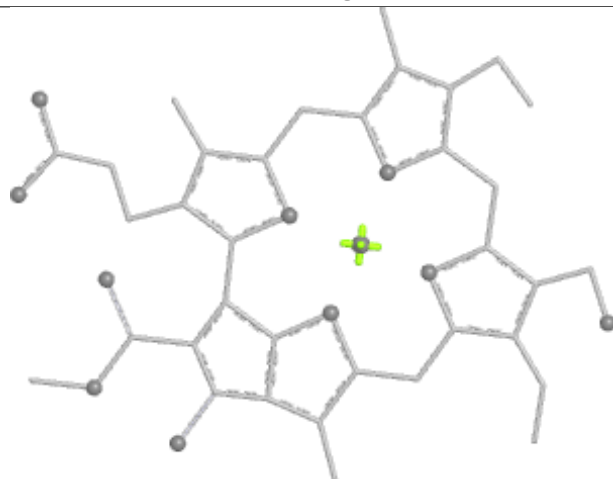
Bond lengths



Bond angles

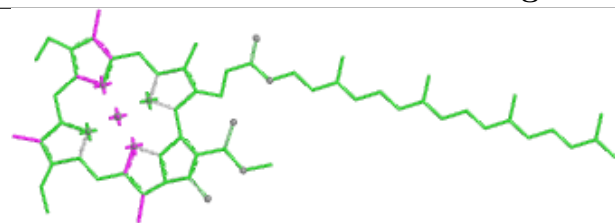


Torsions

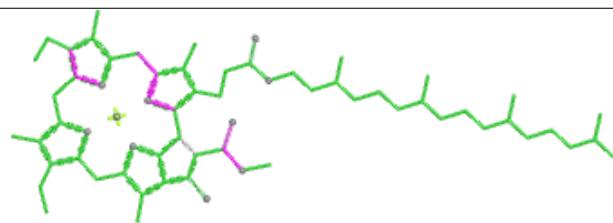


Rings

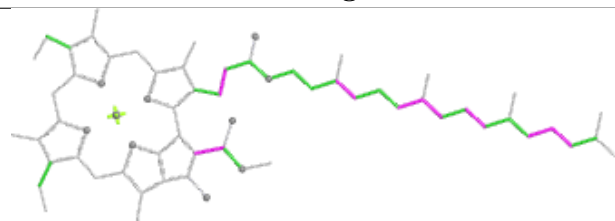
Ligand CLA c 607



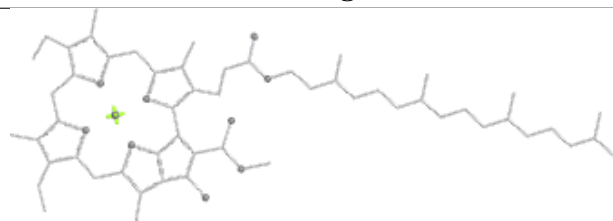
Bond lengths



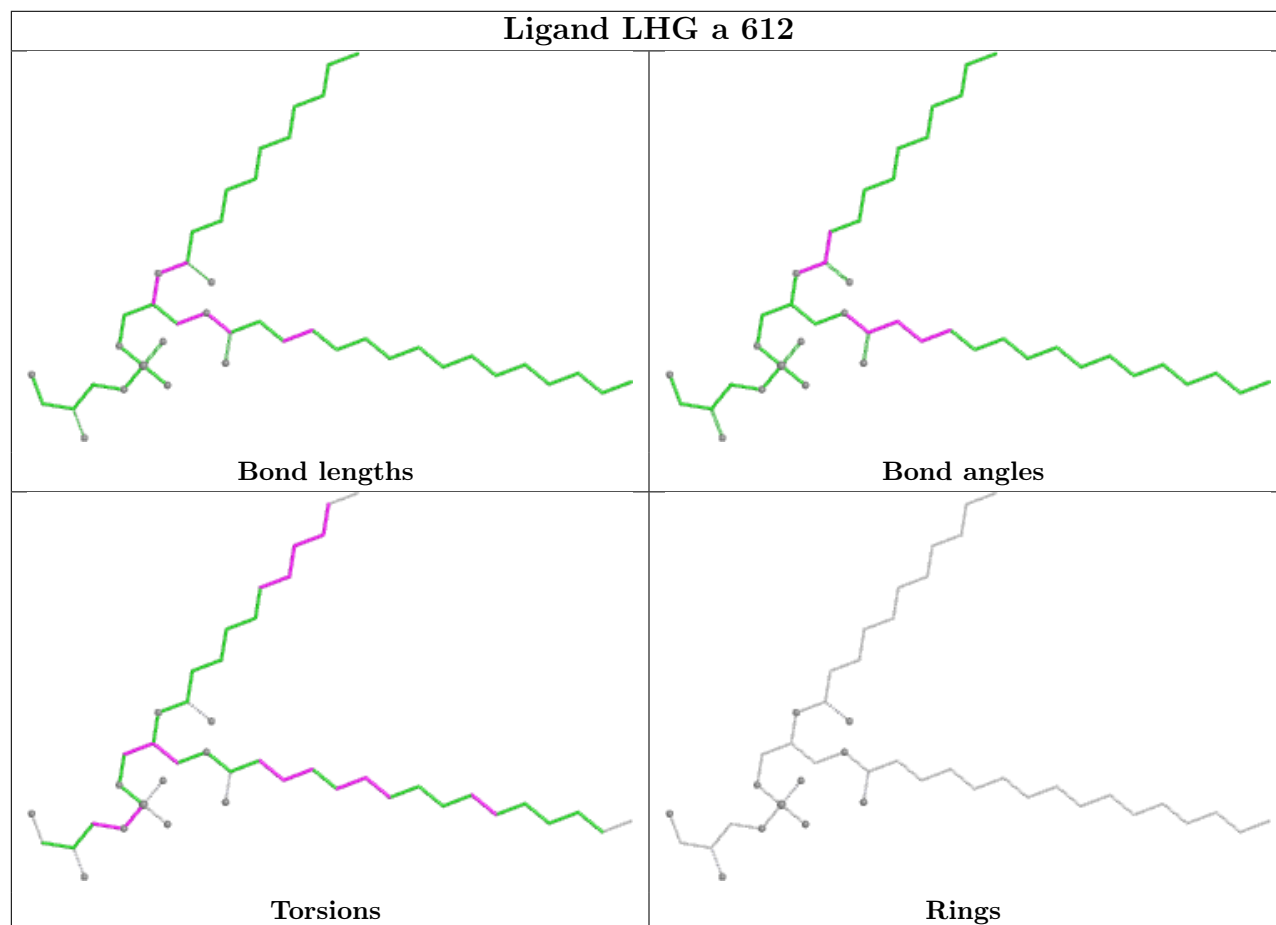
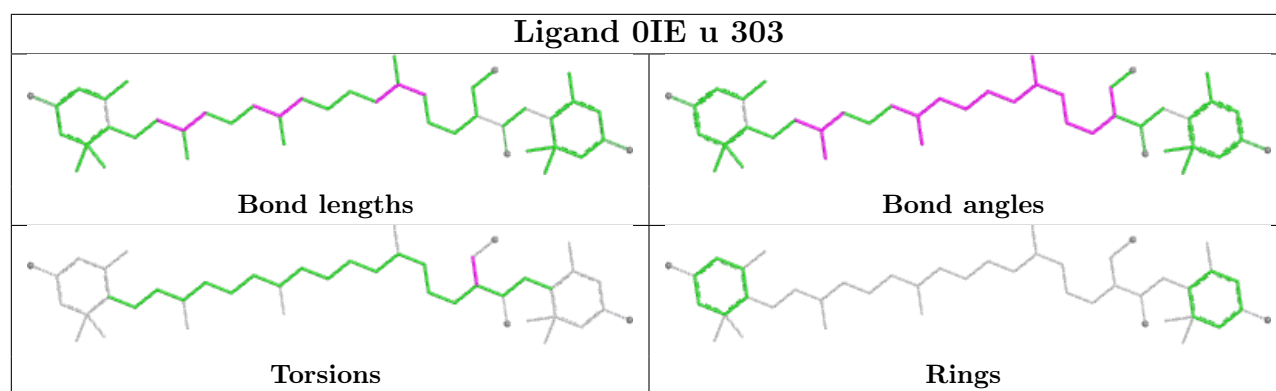
Bond angles



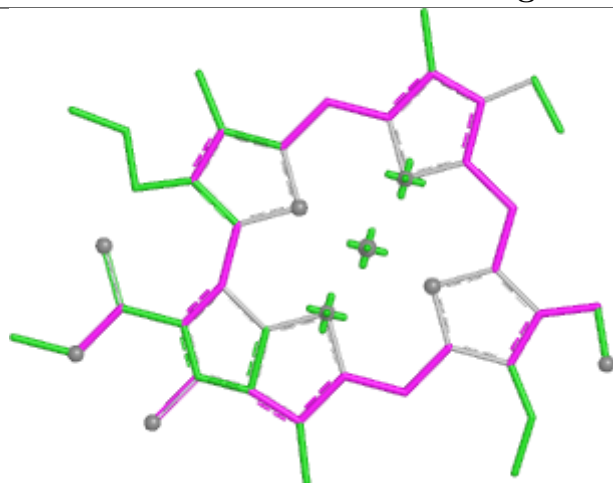
Torsions



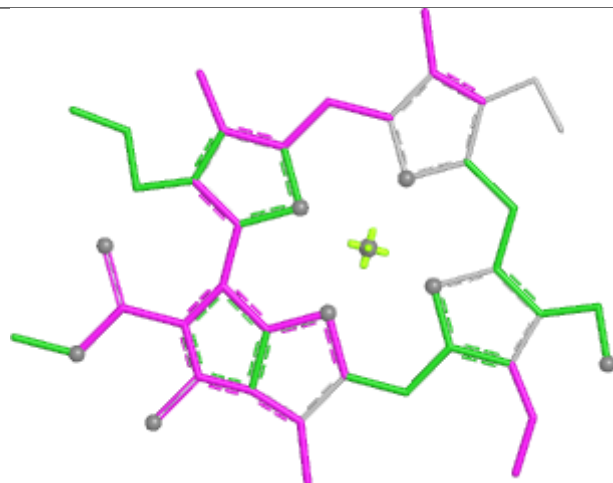
Rings



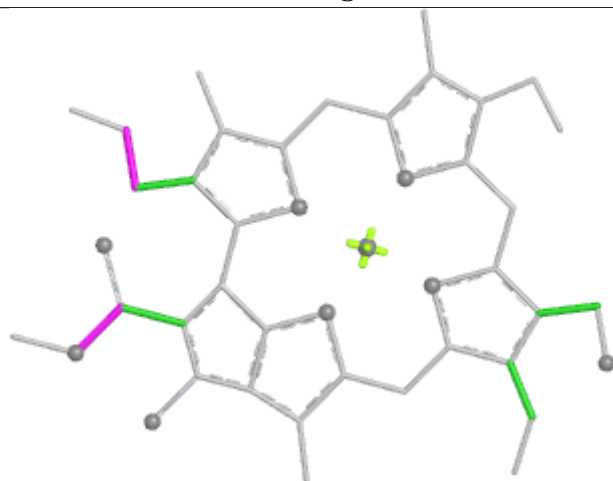
Ligand CHL 1 311



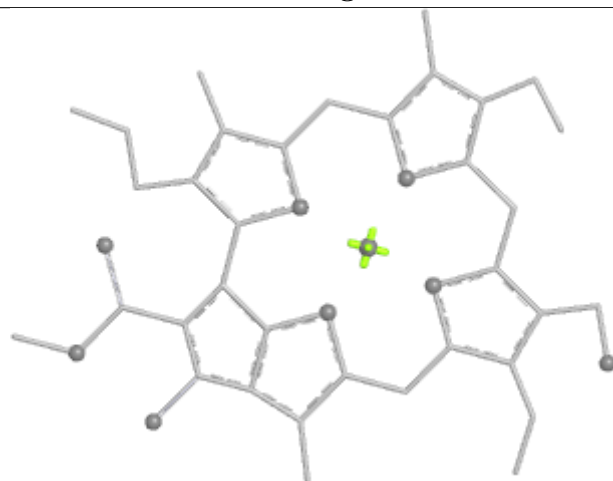
Bond lengths



Bond angles

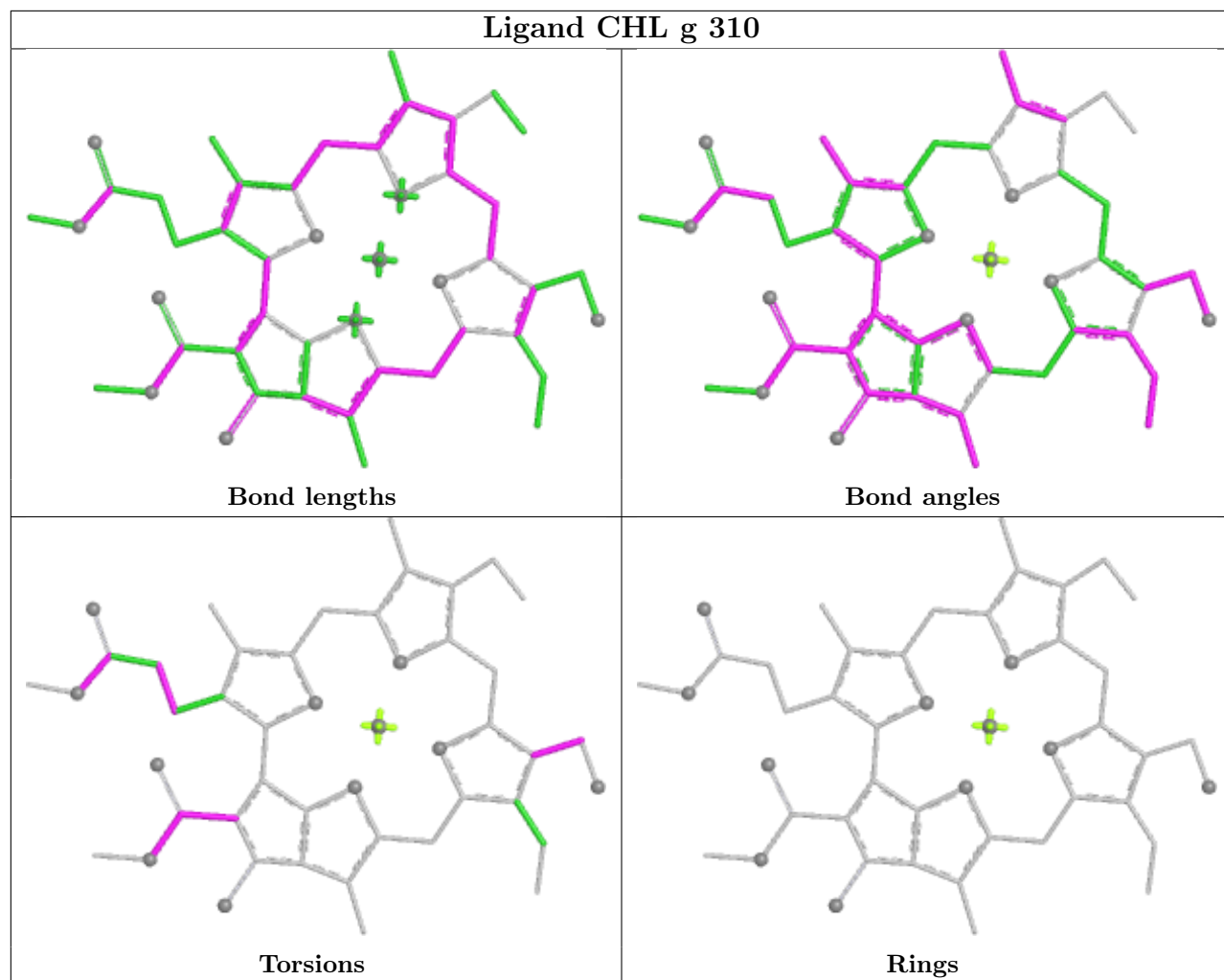


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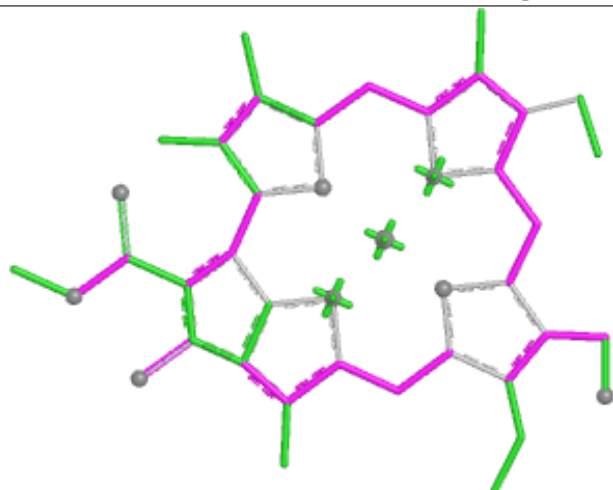


Rings

Ligand CHL g 310



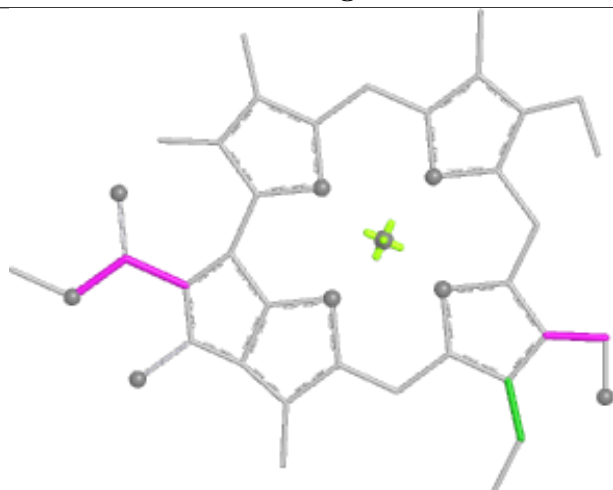
Ligand CHL n 317



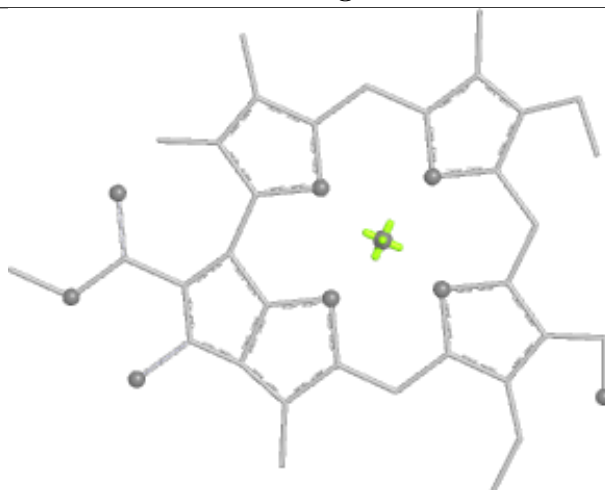
Bond lengths



Bond angles

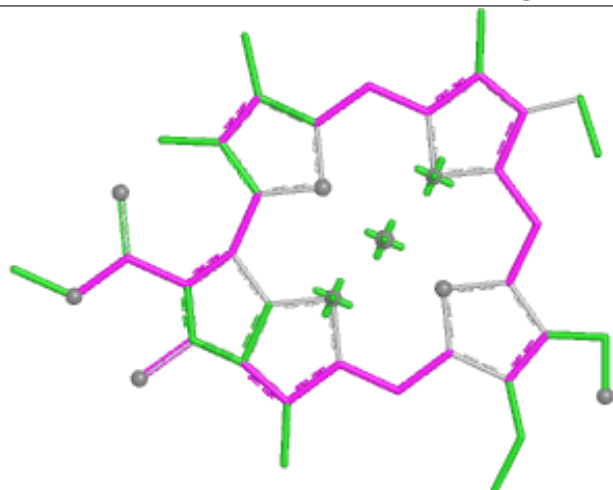


Torsions

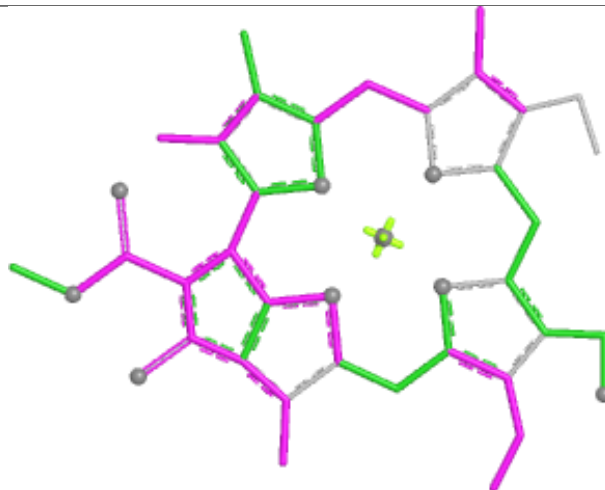


Rings

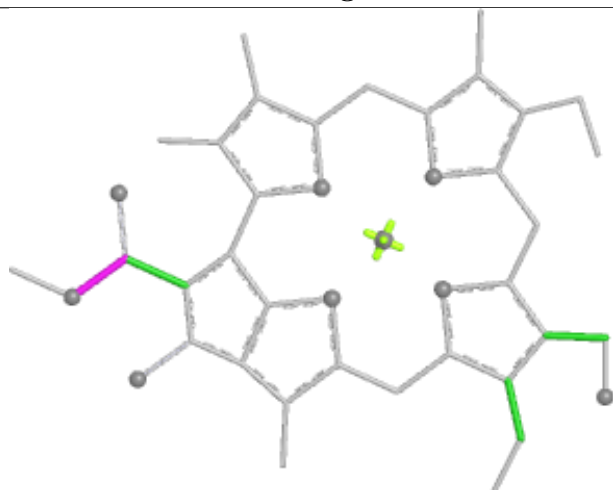
Ligand CHL 5 310



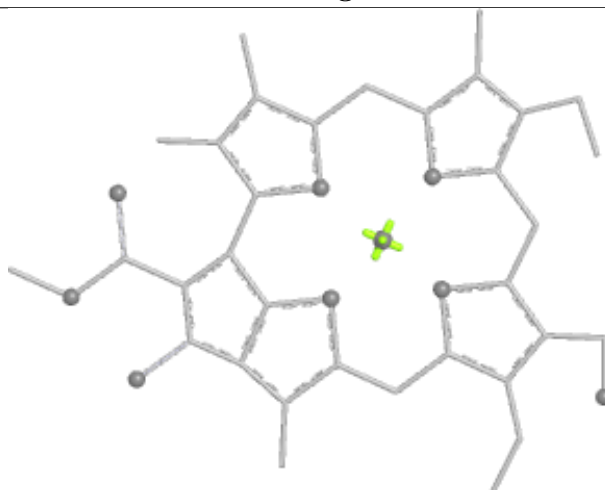
Bond lengths



Bond angles

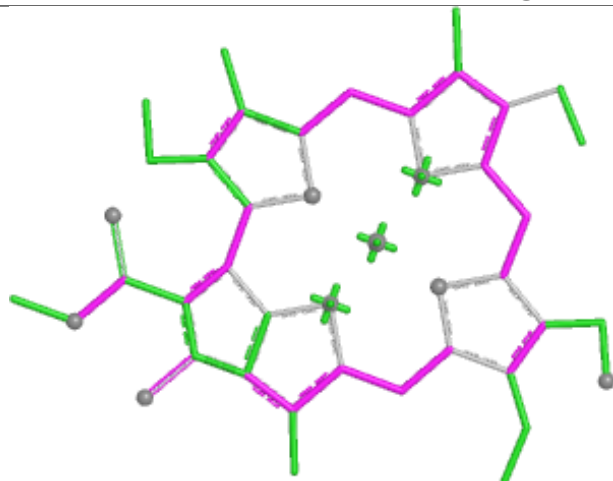


Torsions

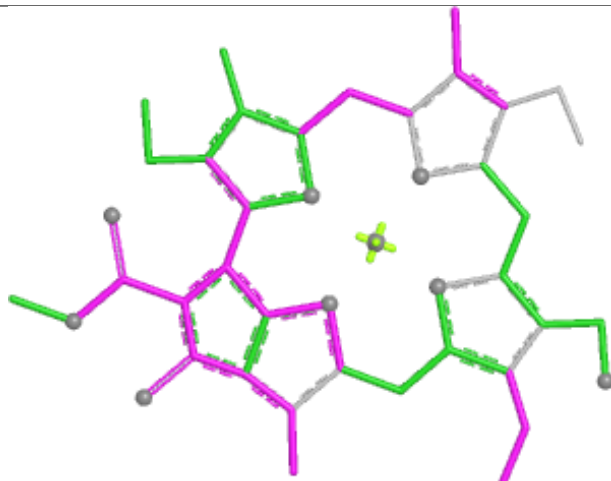


Rings

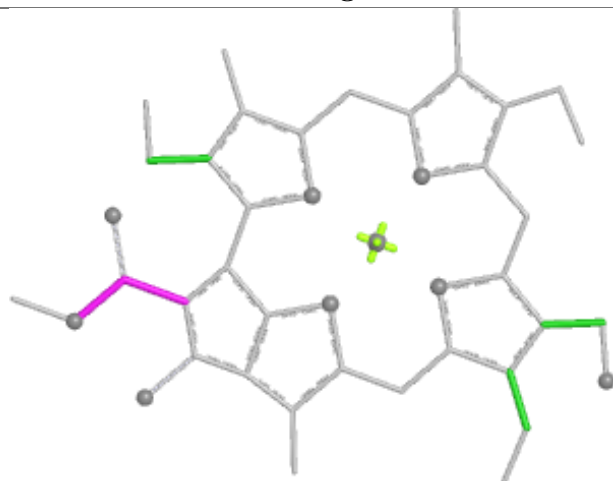
Ligand CHL 1 310



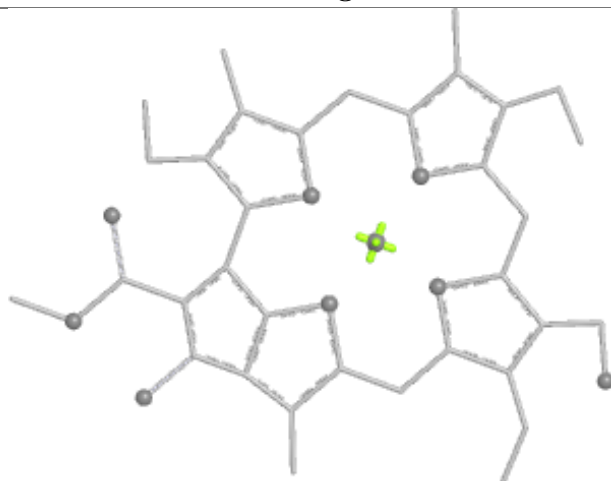
Bond lengths



Bond angles

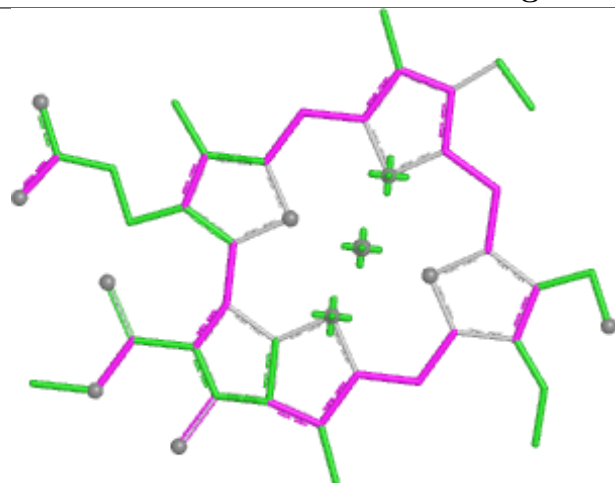


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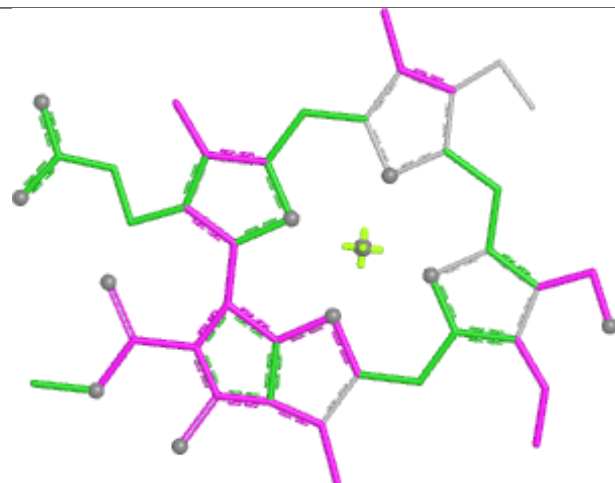


Rings

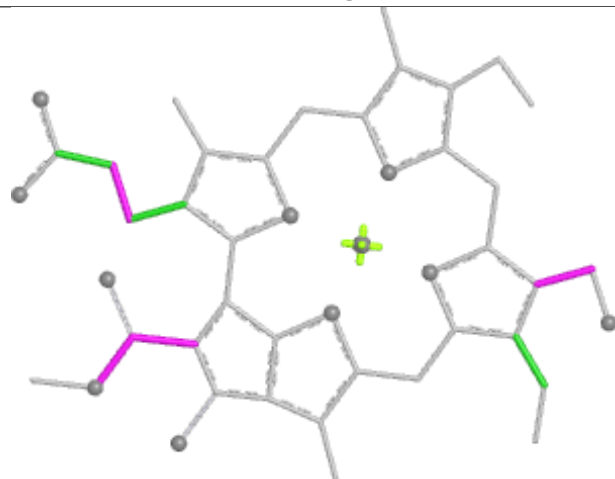
Ligand CHL r 302



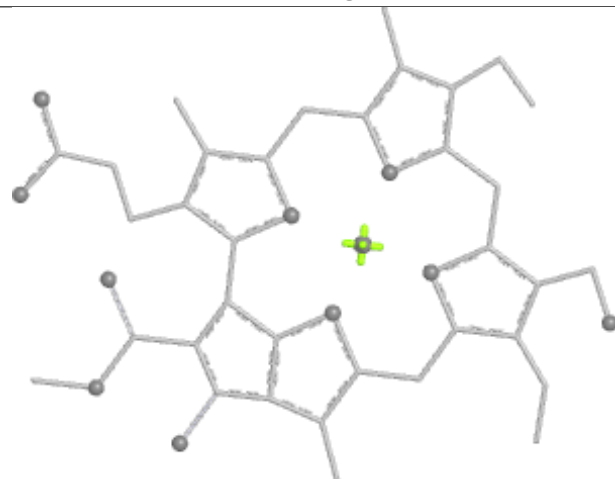
Bond lengths



Bond angles

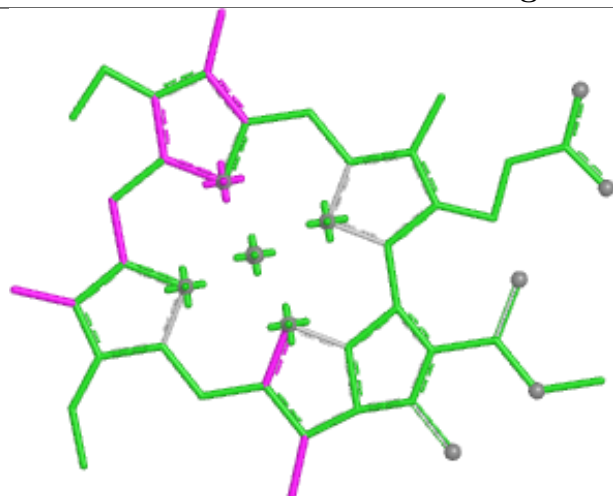


Torsions

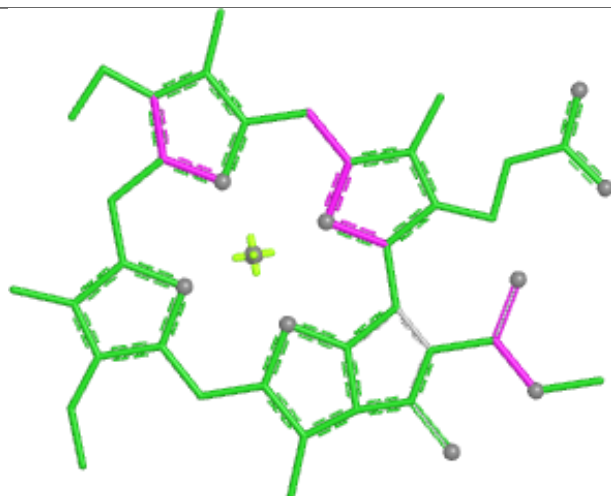


Rings

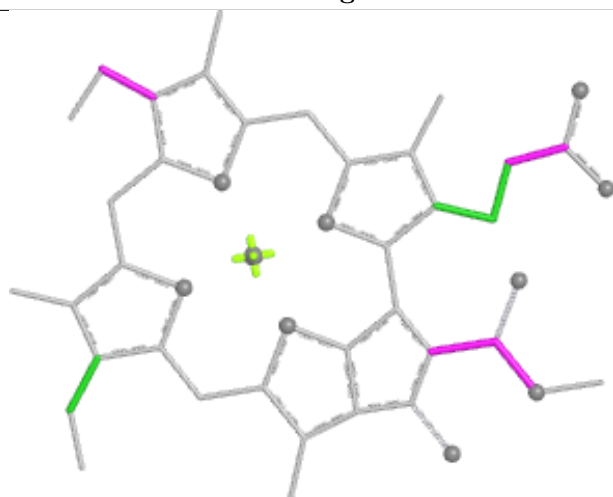
Ligand CLA r 312



Bond lengths



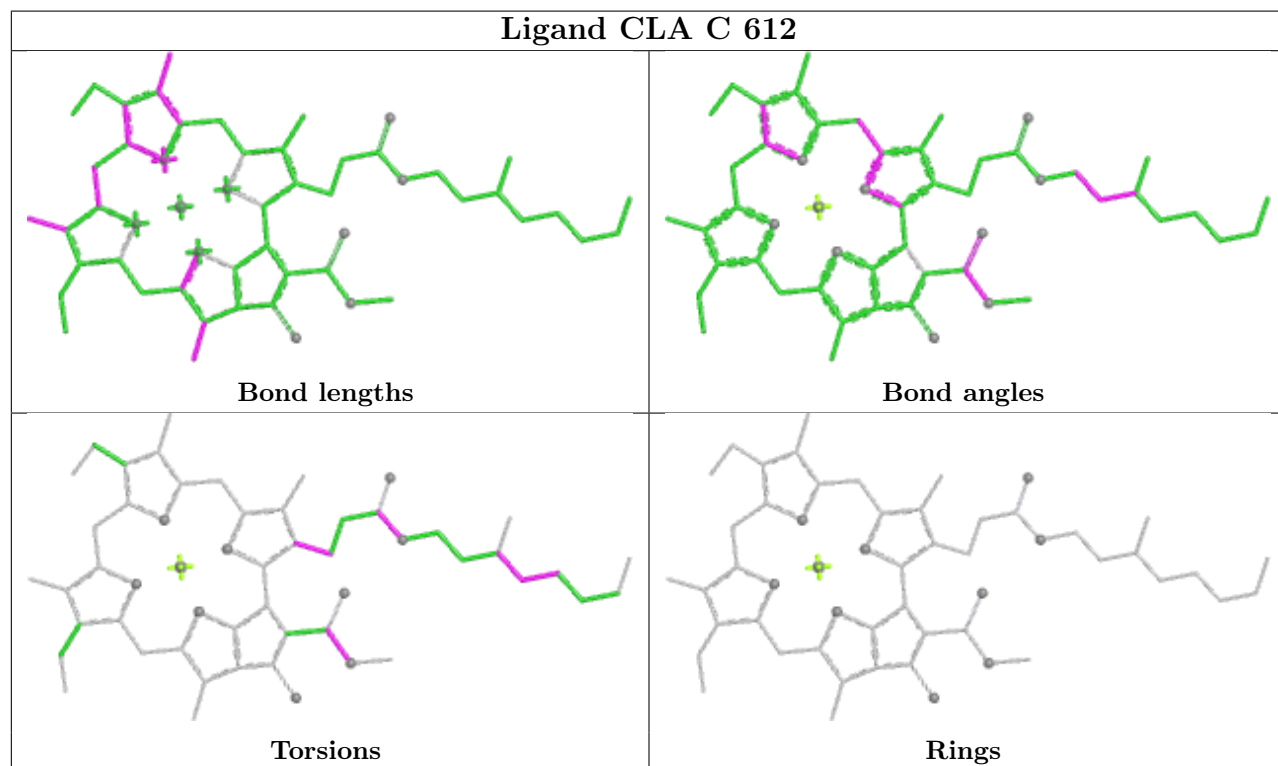
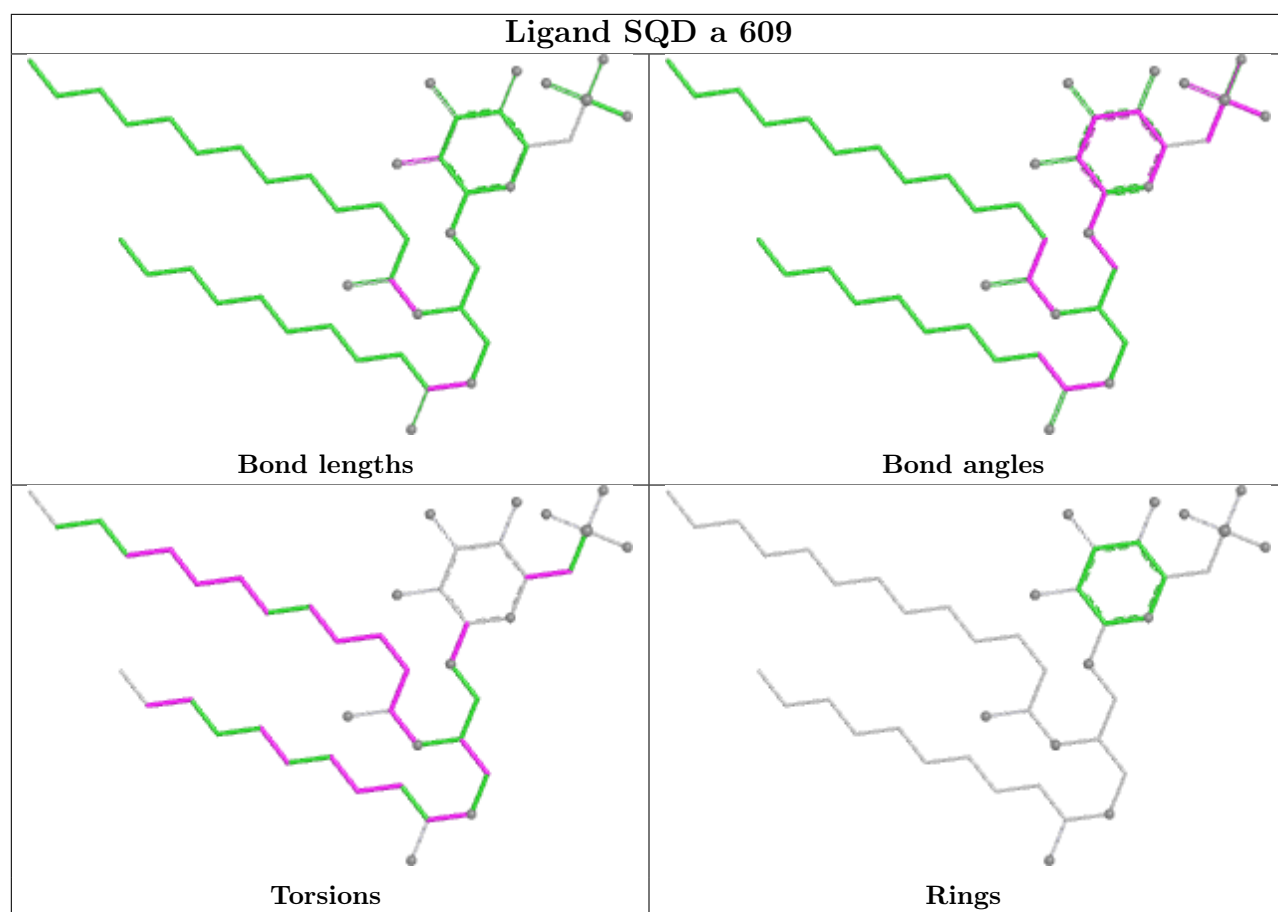
Bond angles



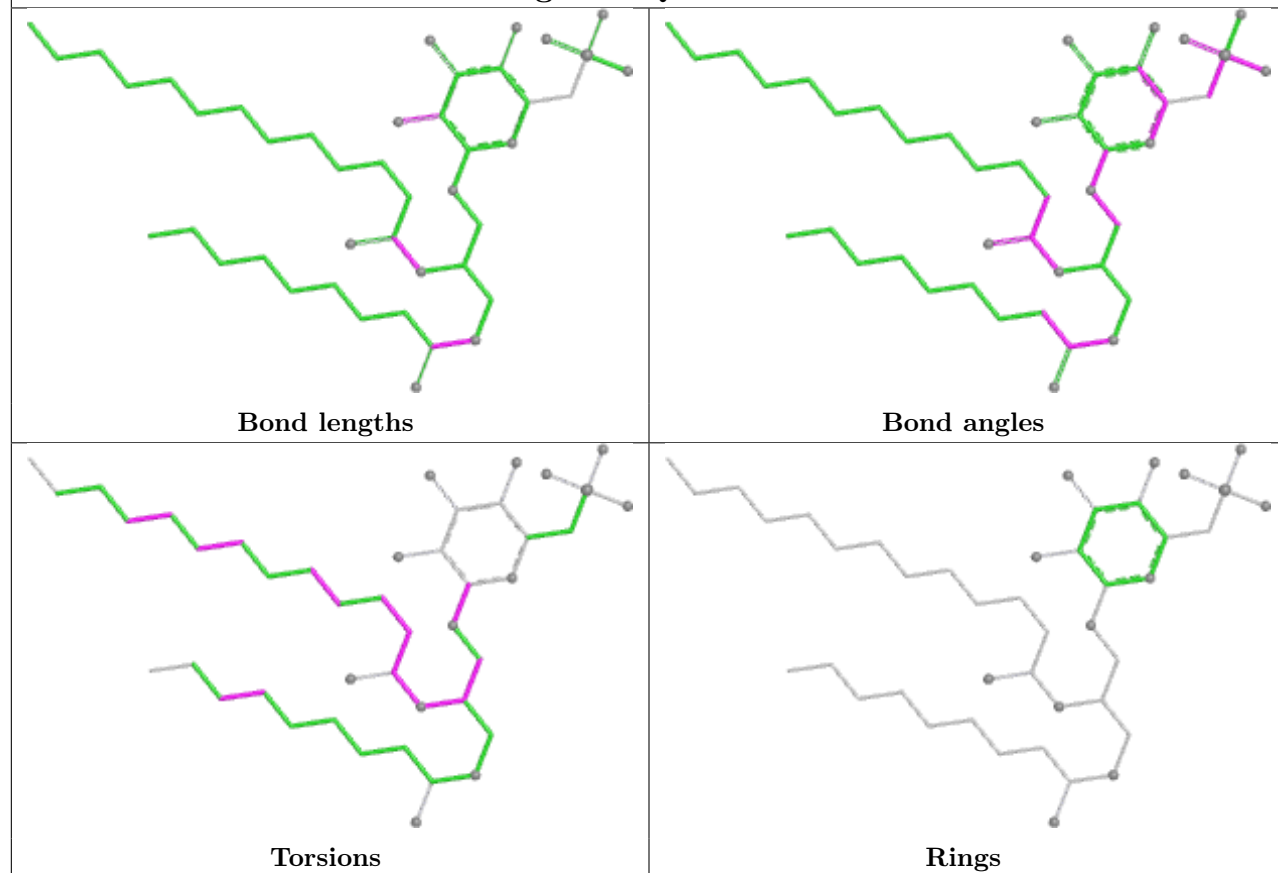
Torsions



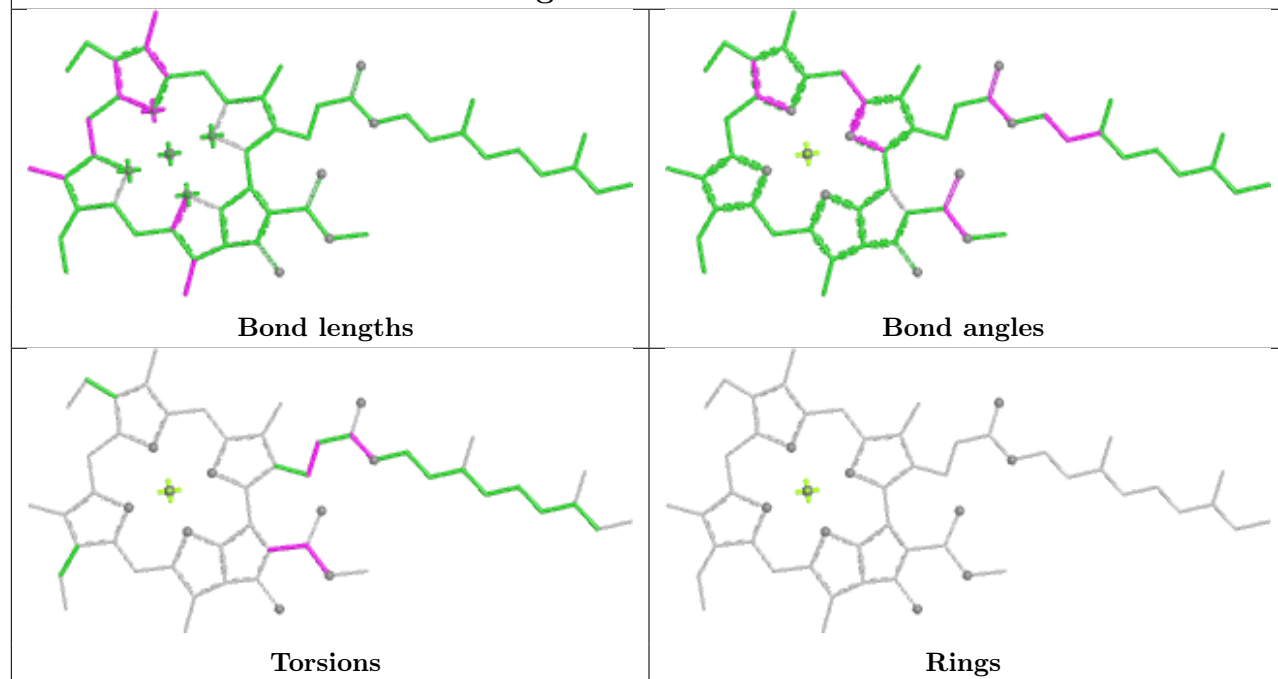
Rings

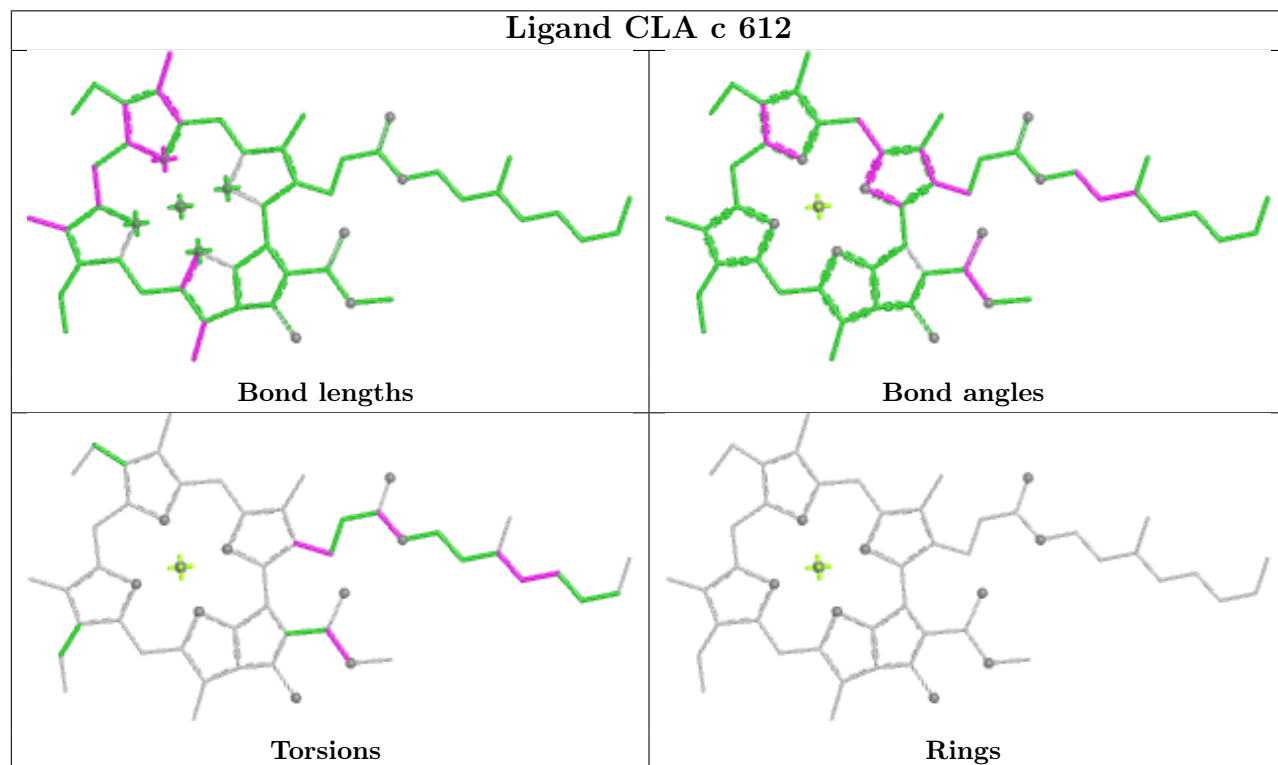
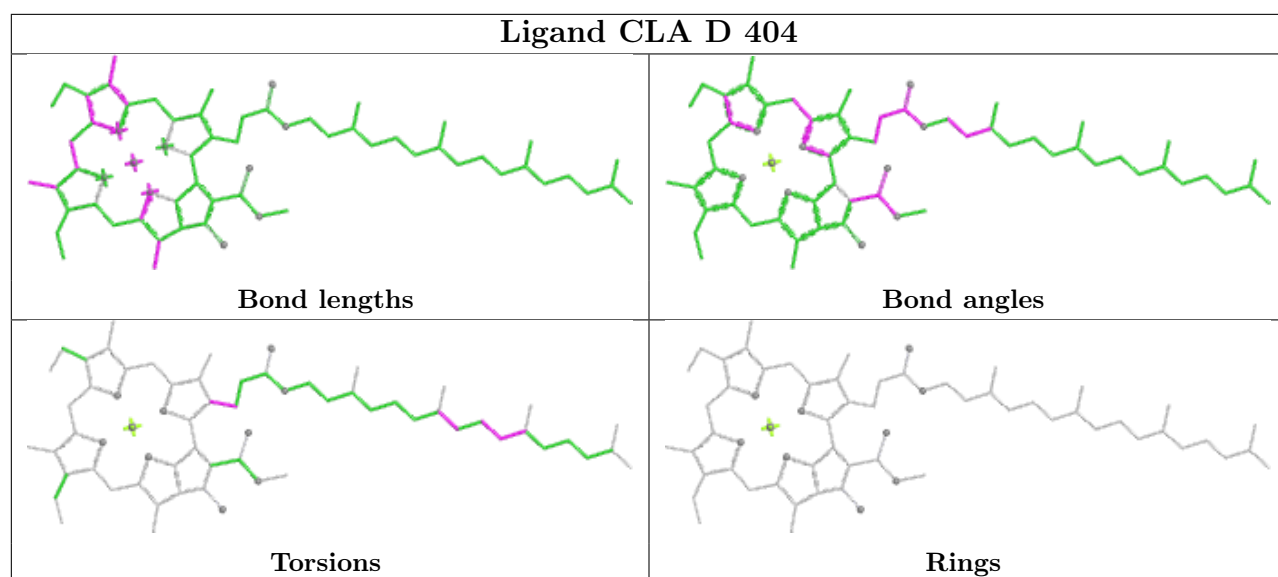


Ligand SQD d 409

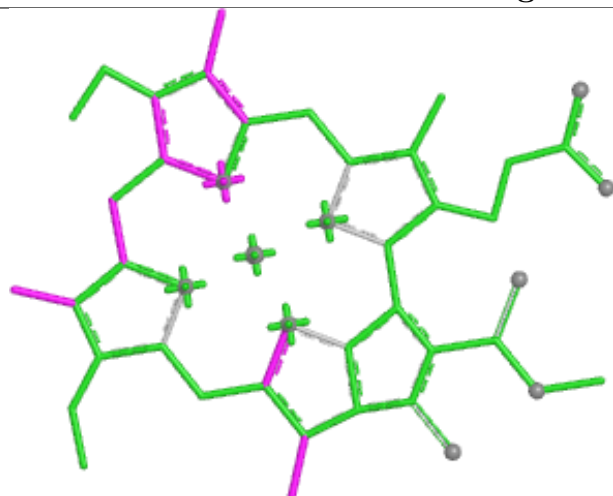


Ligand CLA 7 307

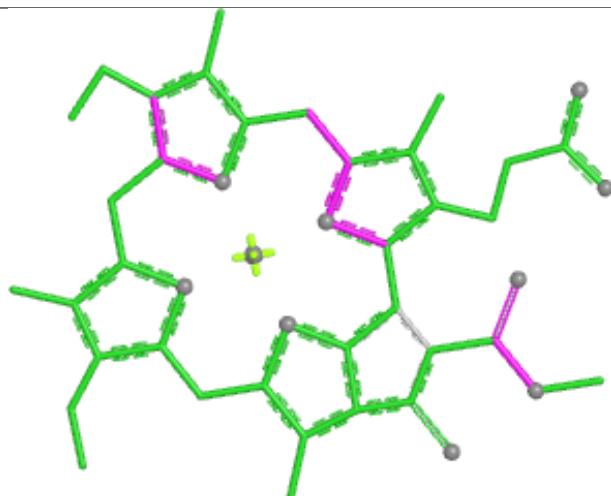




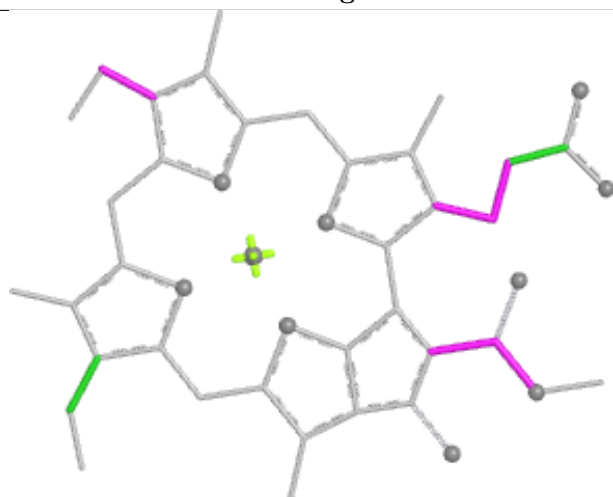
Ligand CLA b 601



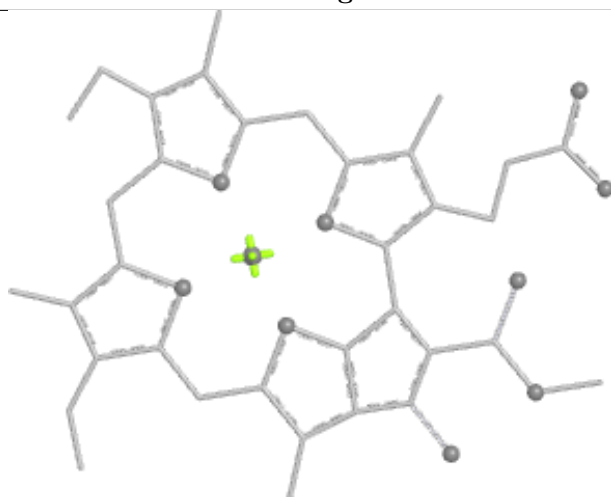
Bond lengths



Bond angles

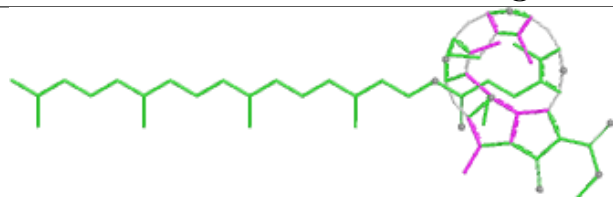


Torsions

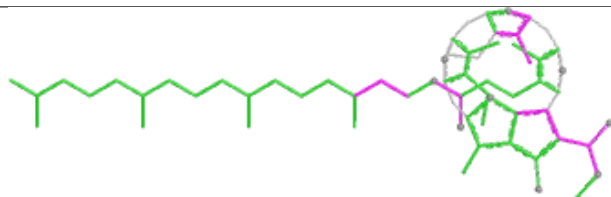


Rings

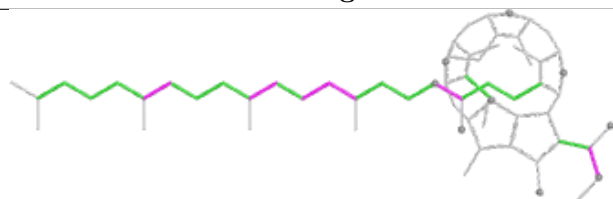
Ligand PHO D 403



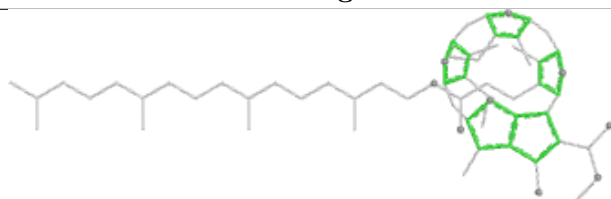
Bond lengths



Bond angles

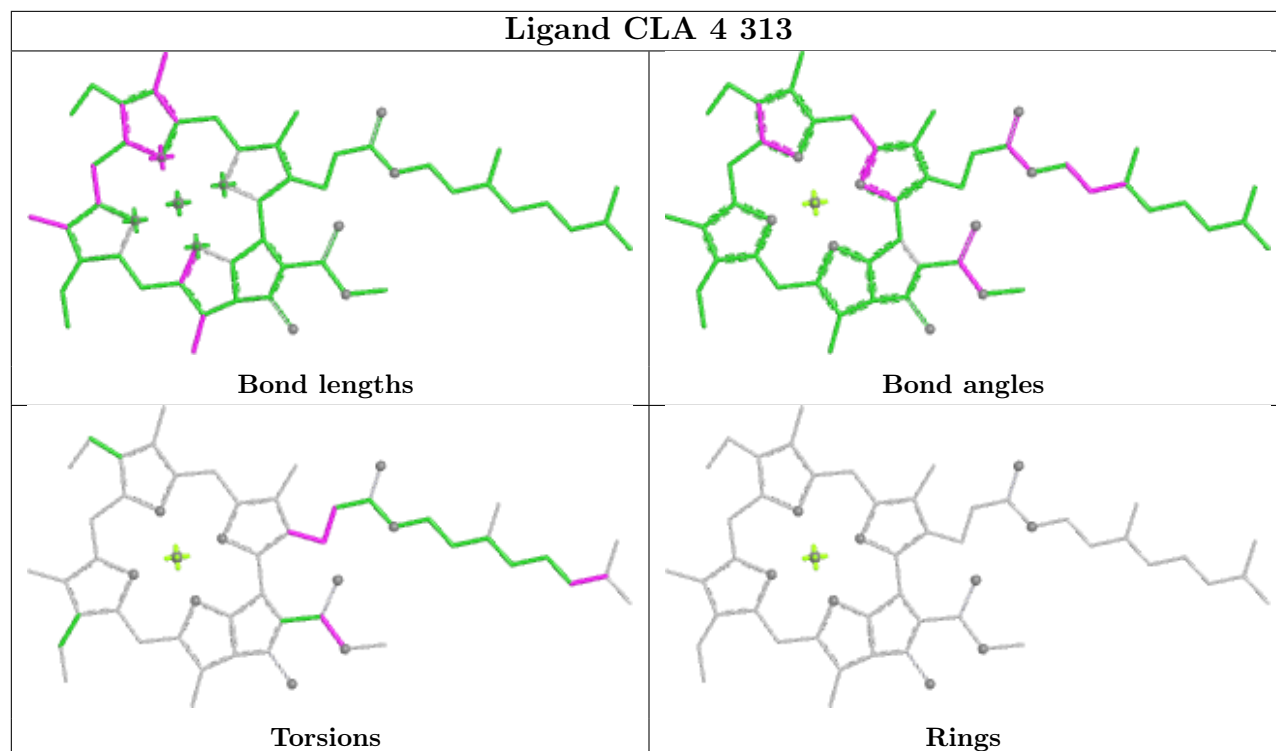


Torsions

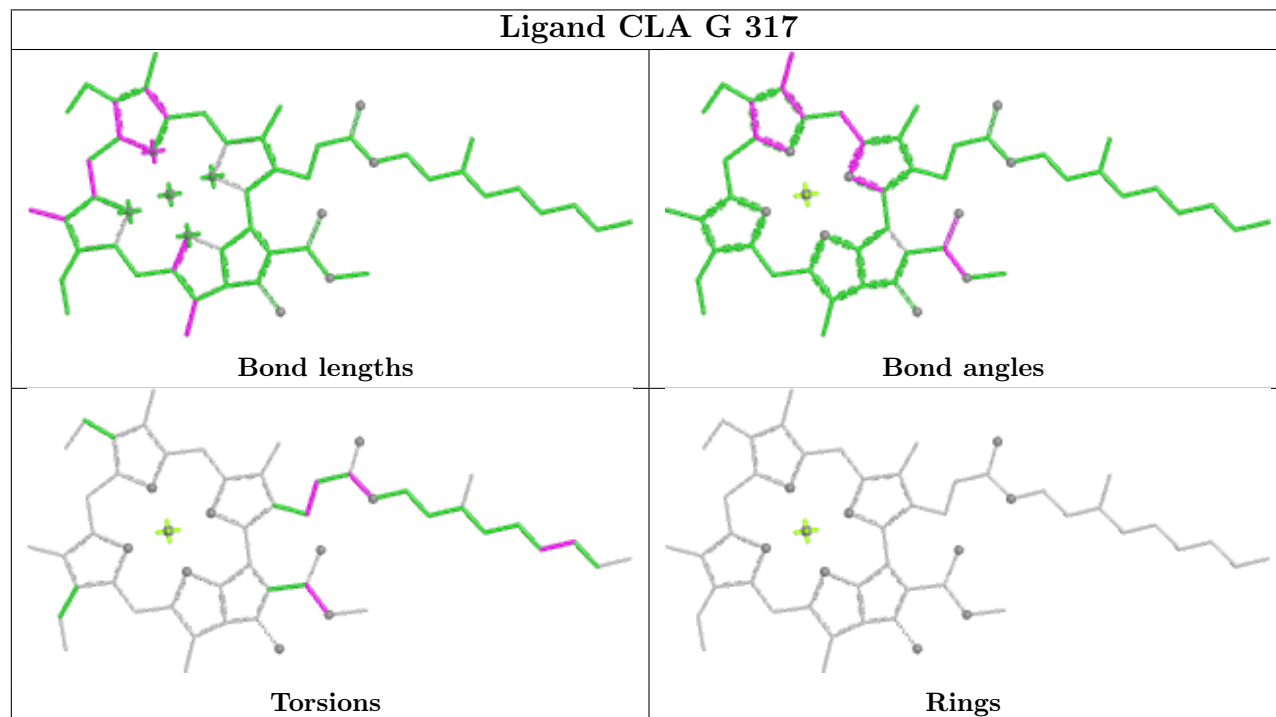


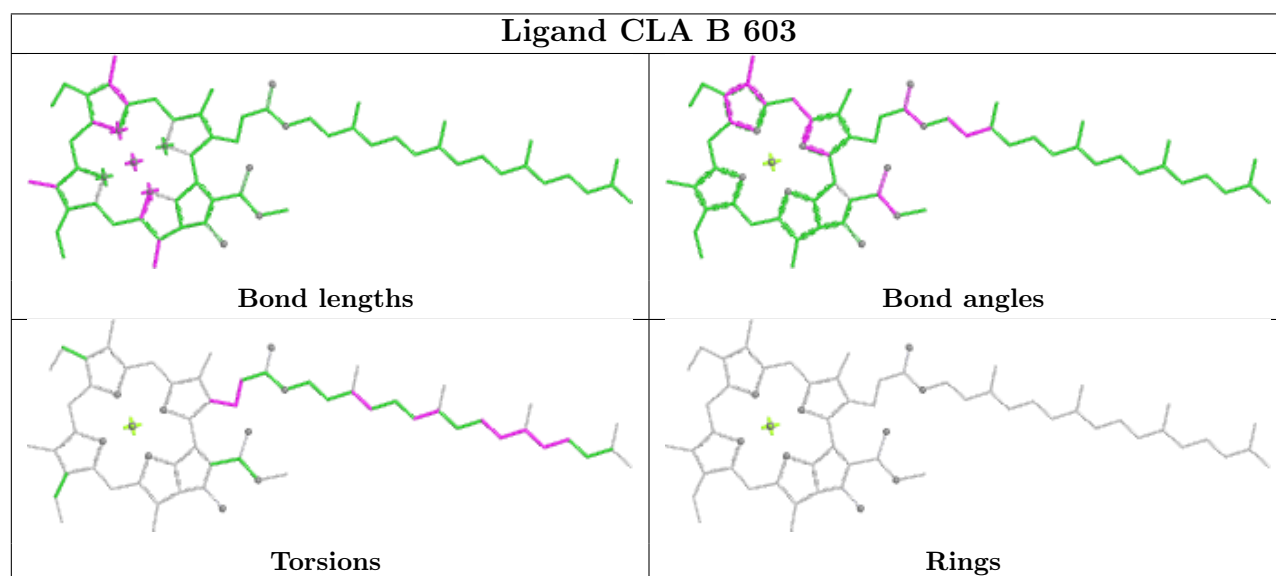
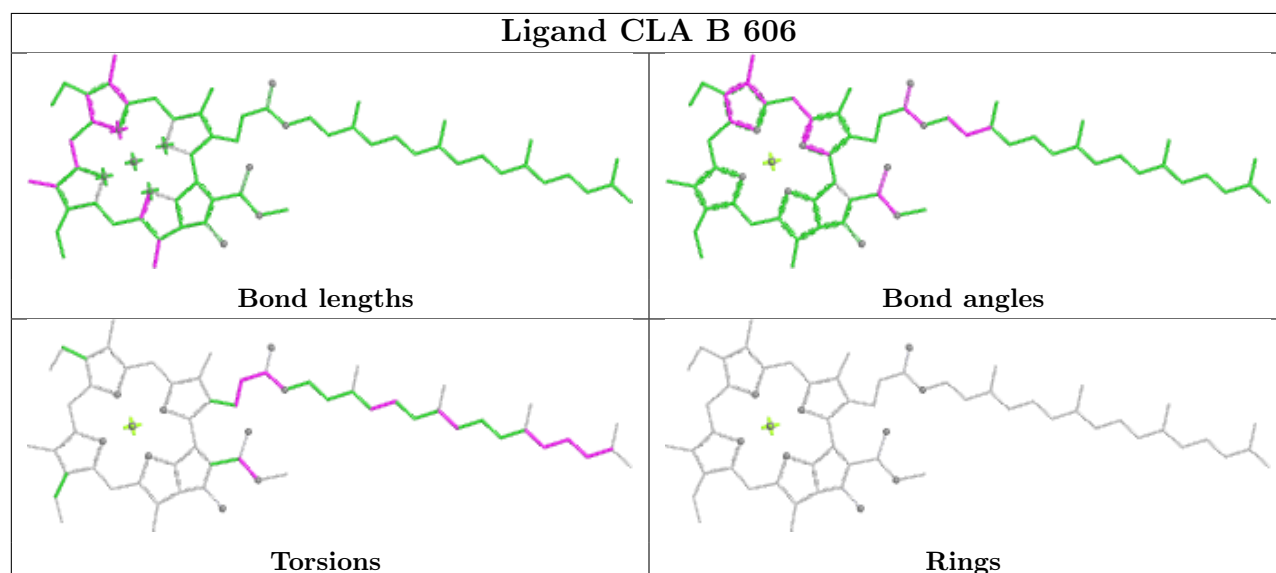
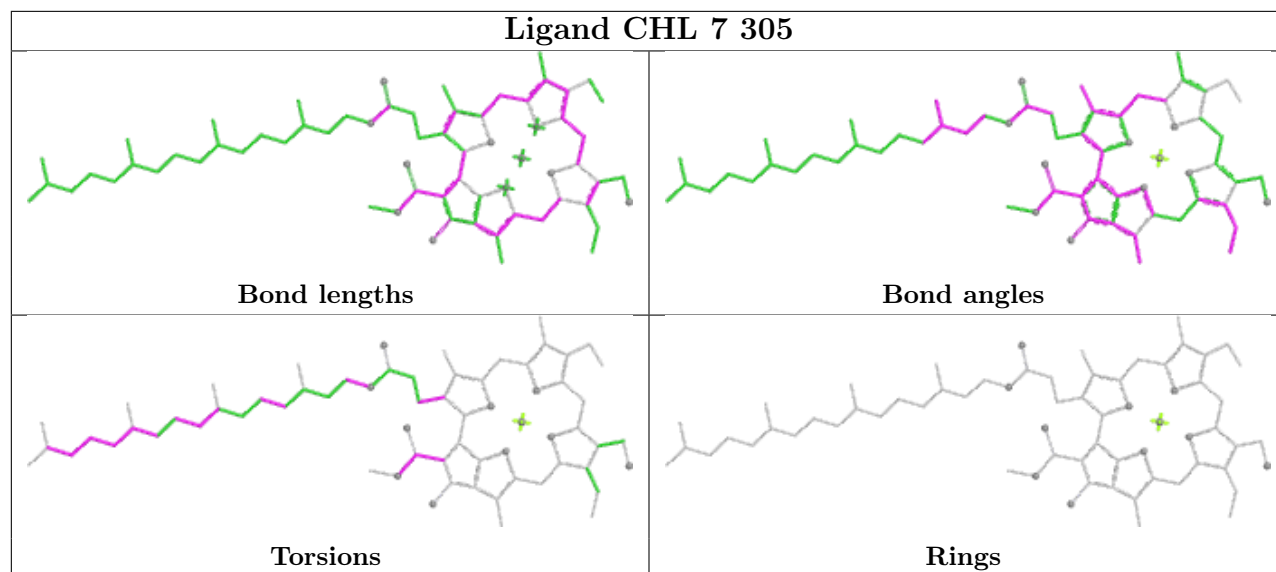
Rings

Ligand CLA 4 313

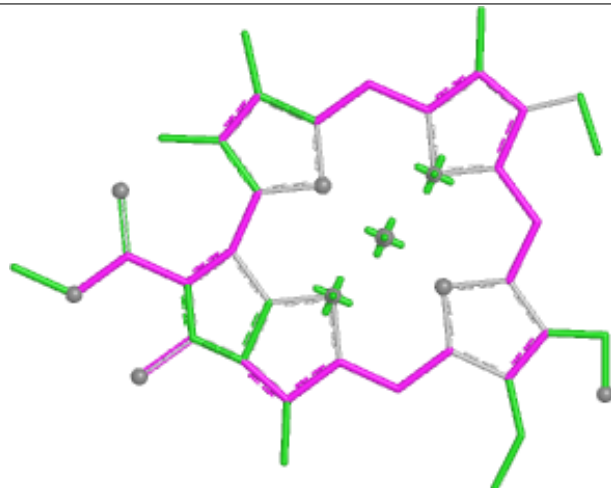


Ligand CLA G 317

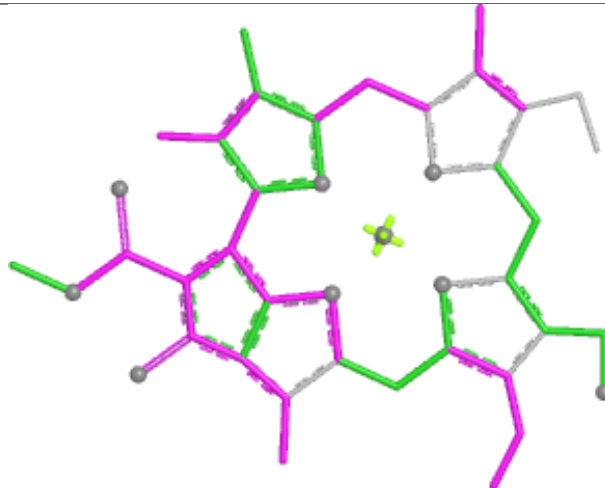




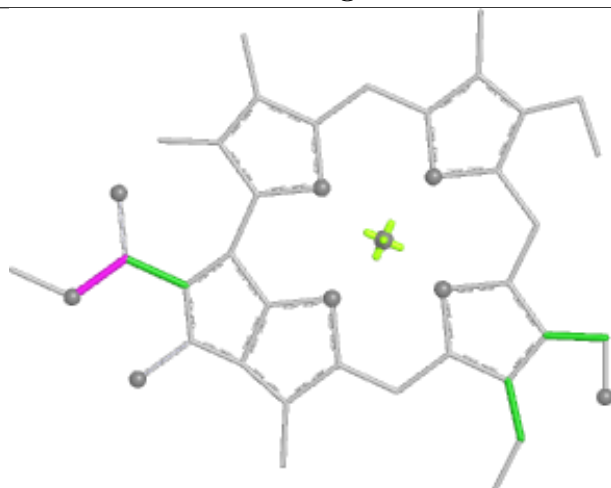
Ligand CHL 2 310



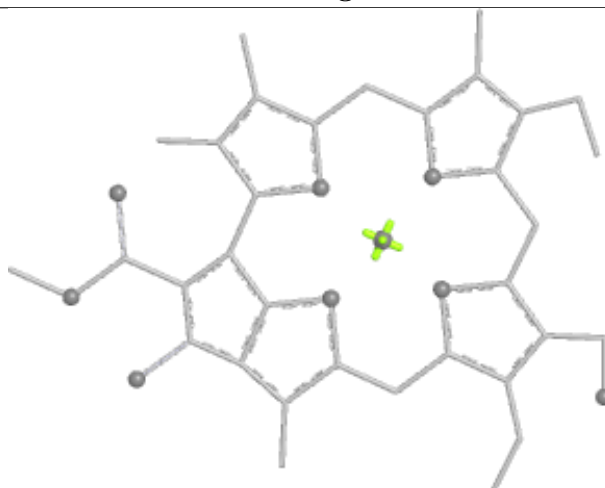
Bond lengths



Bond angles

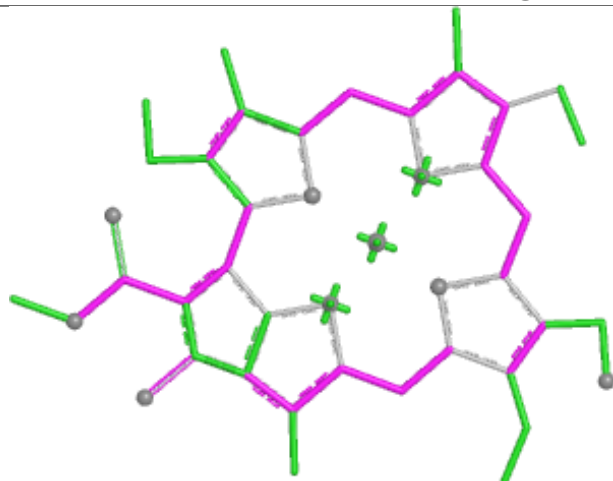


Torsions

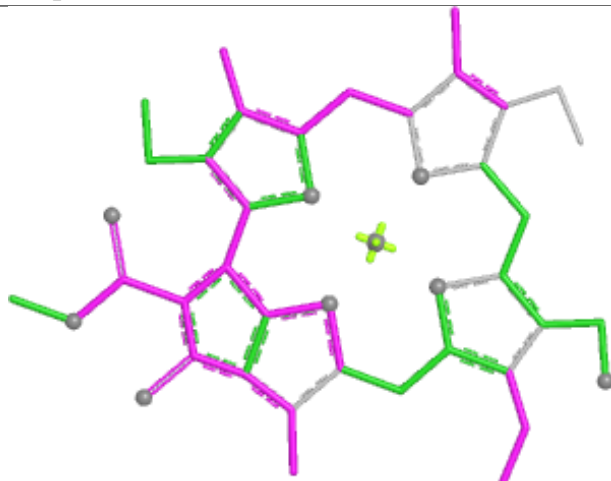


Rings

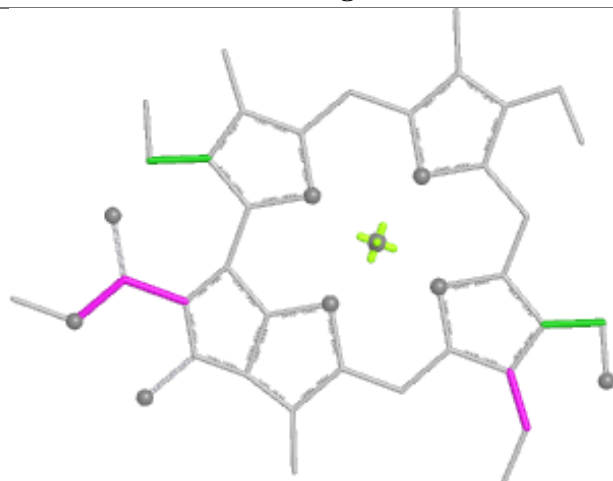
Ligand CHL p 313



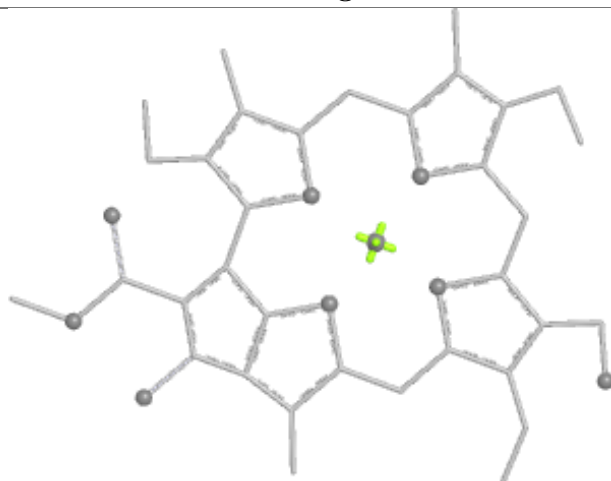
Bond lengths



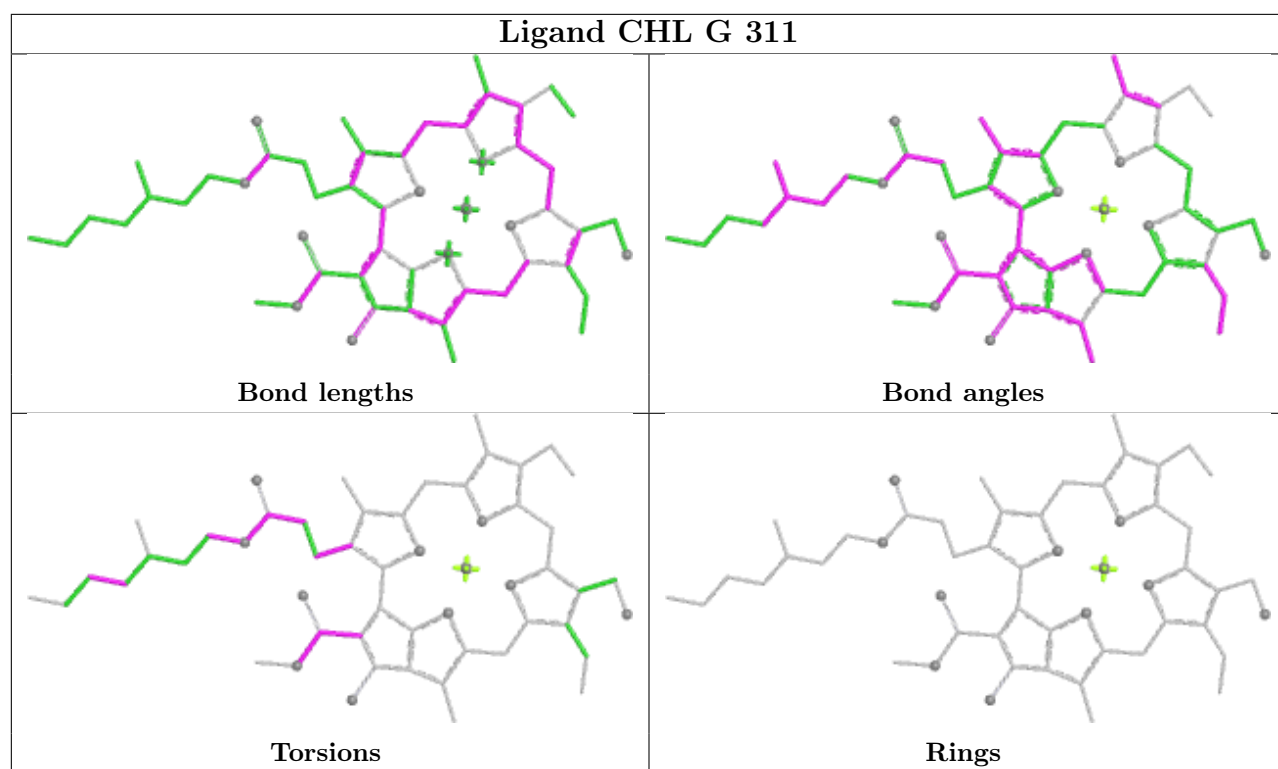
Bond angles



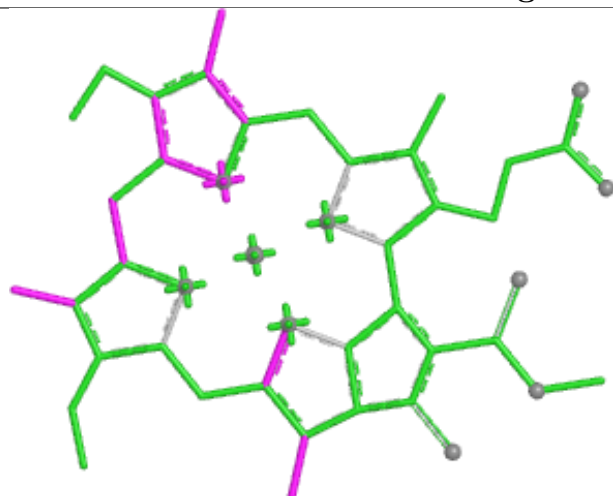
Torsions



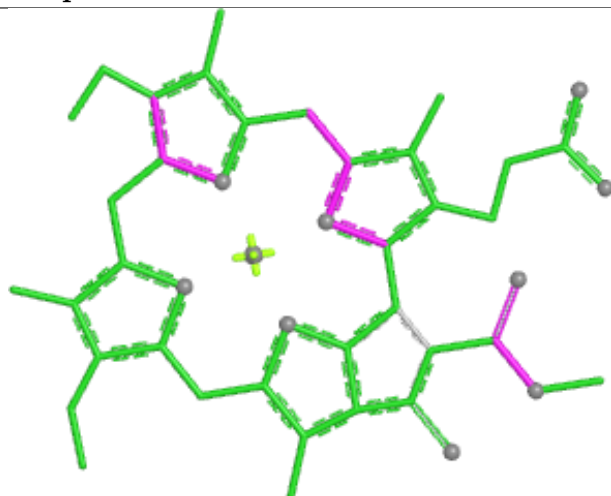
Rings



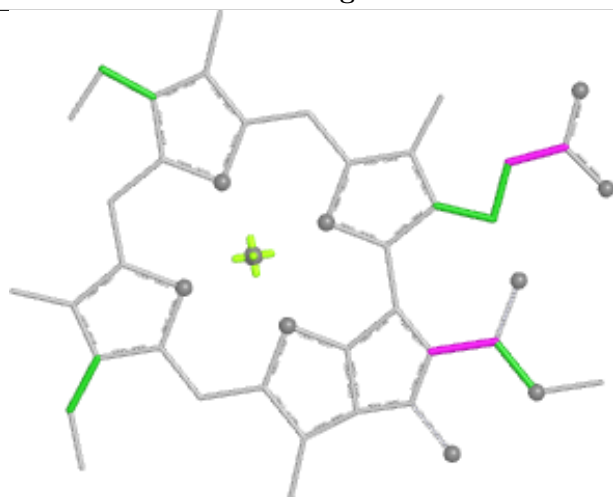
Ligand CLA q 314



Bond lengths



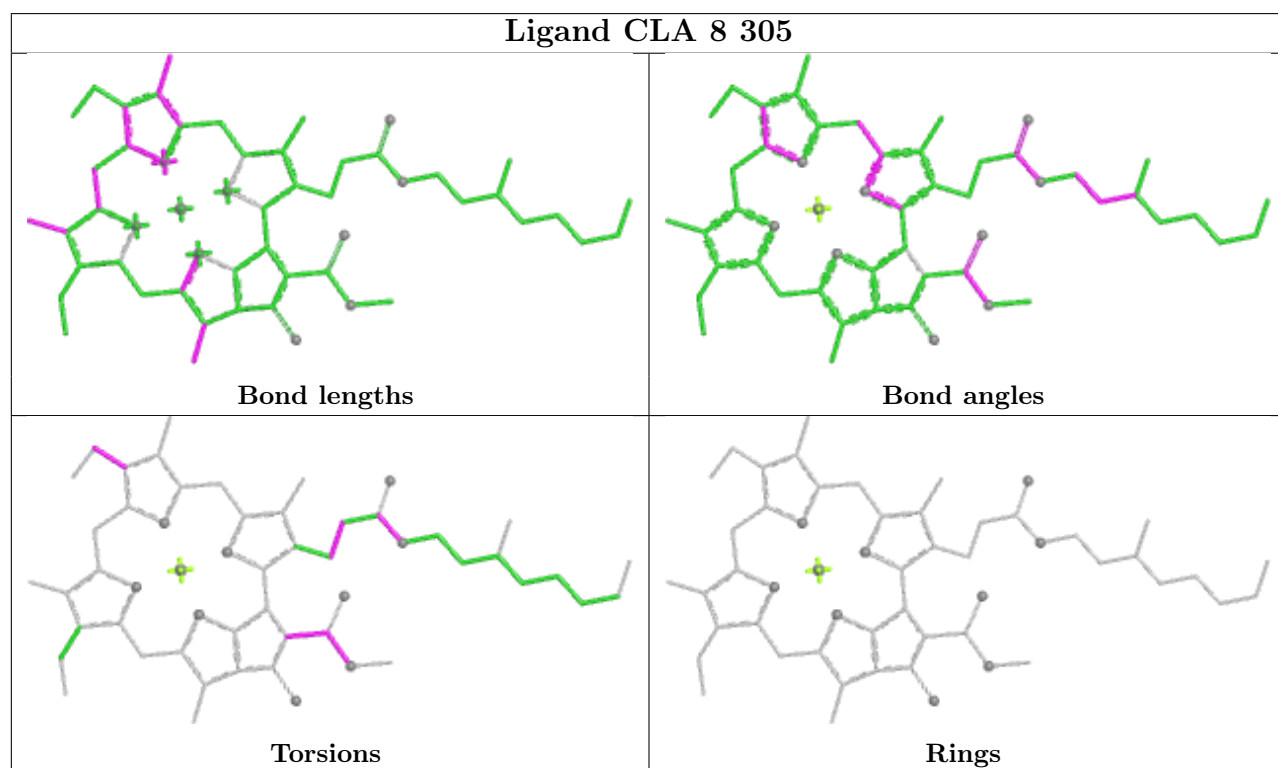
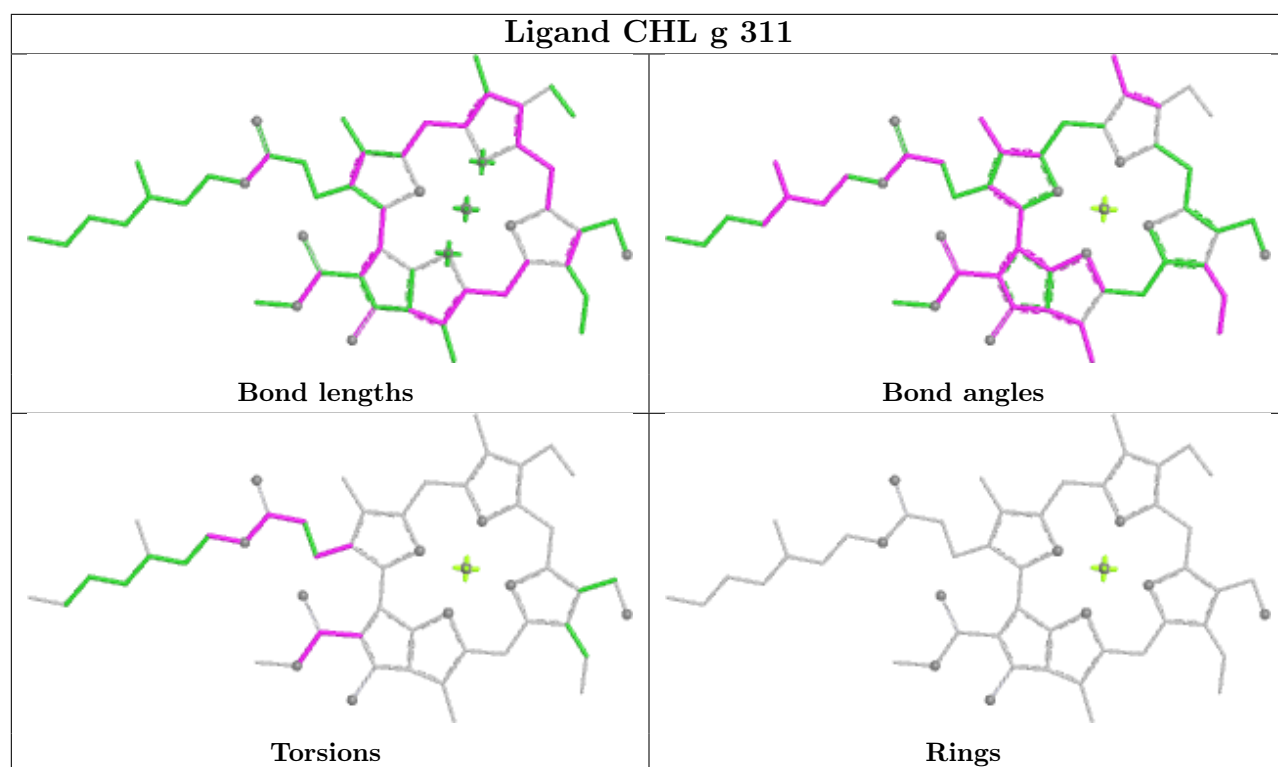
Bond angles

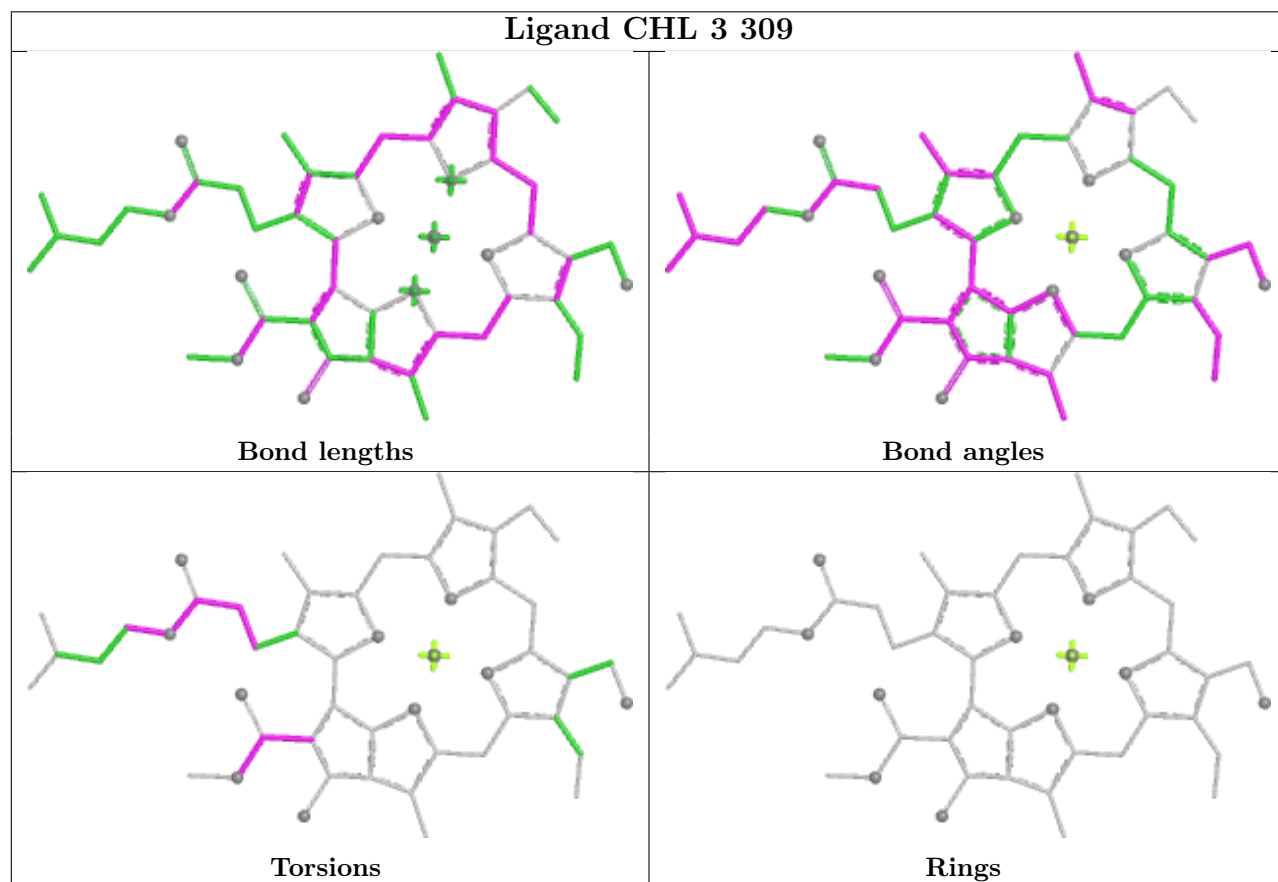
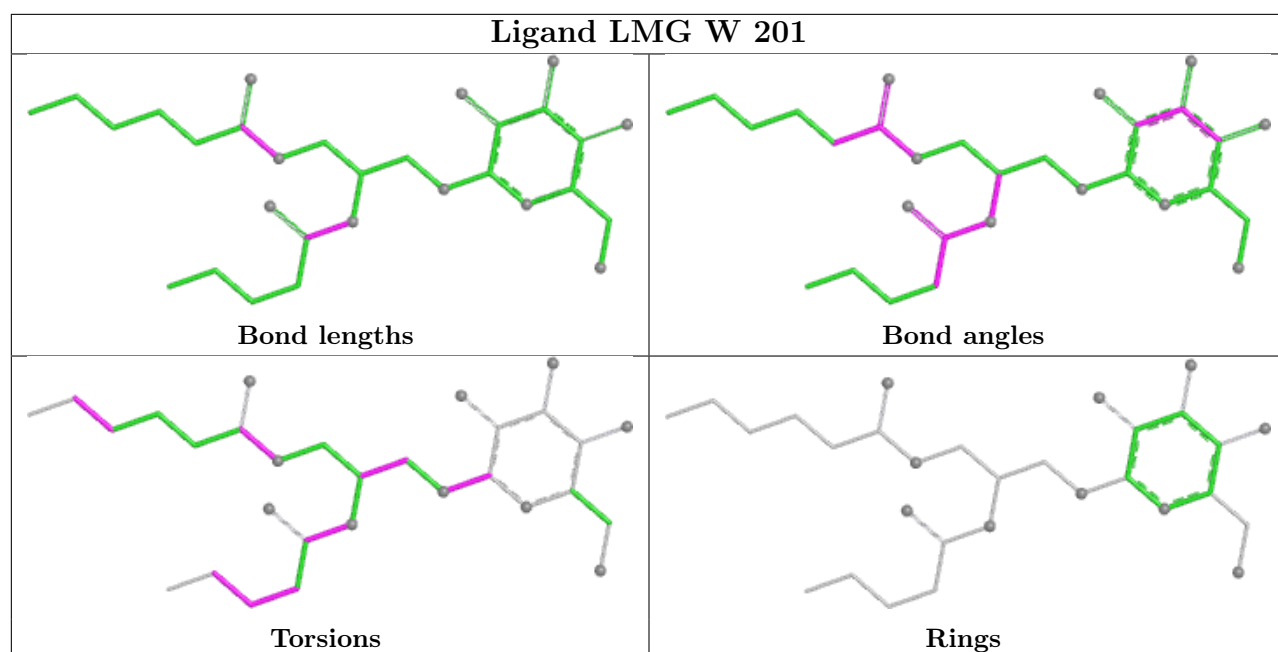


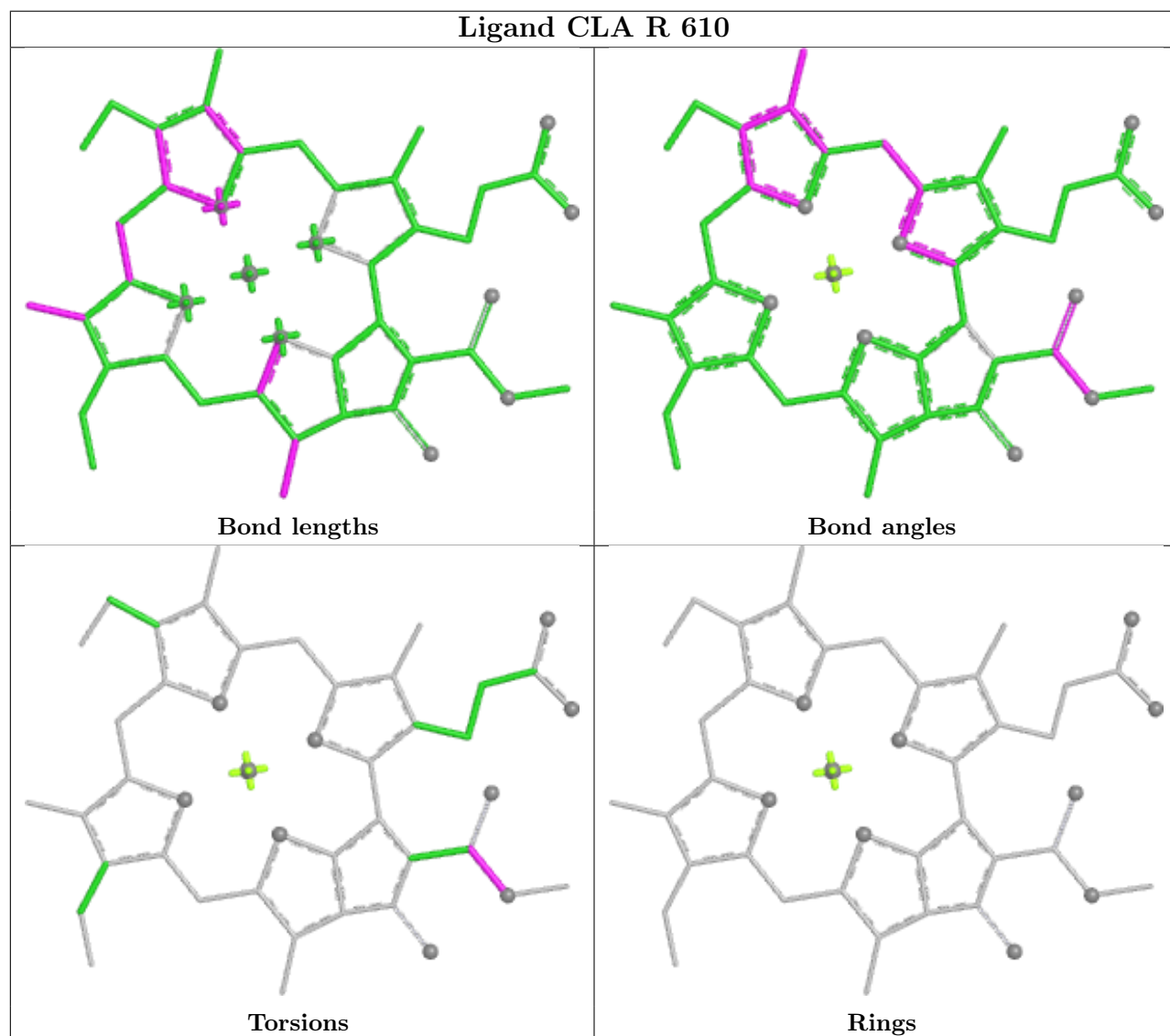
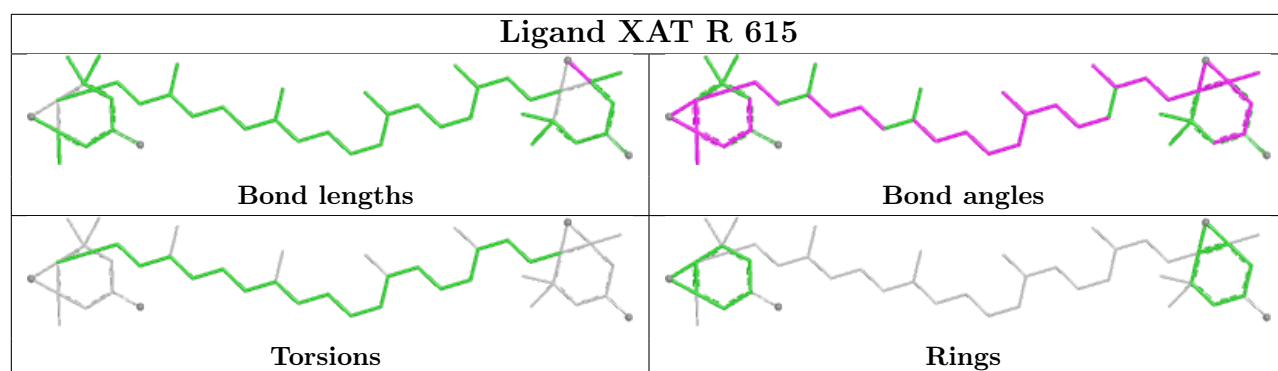
Torsions

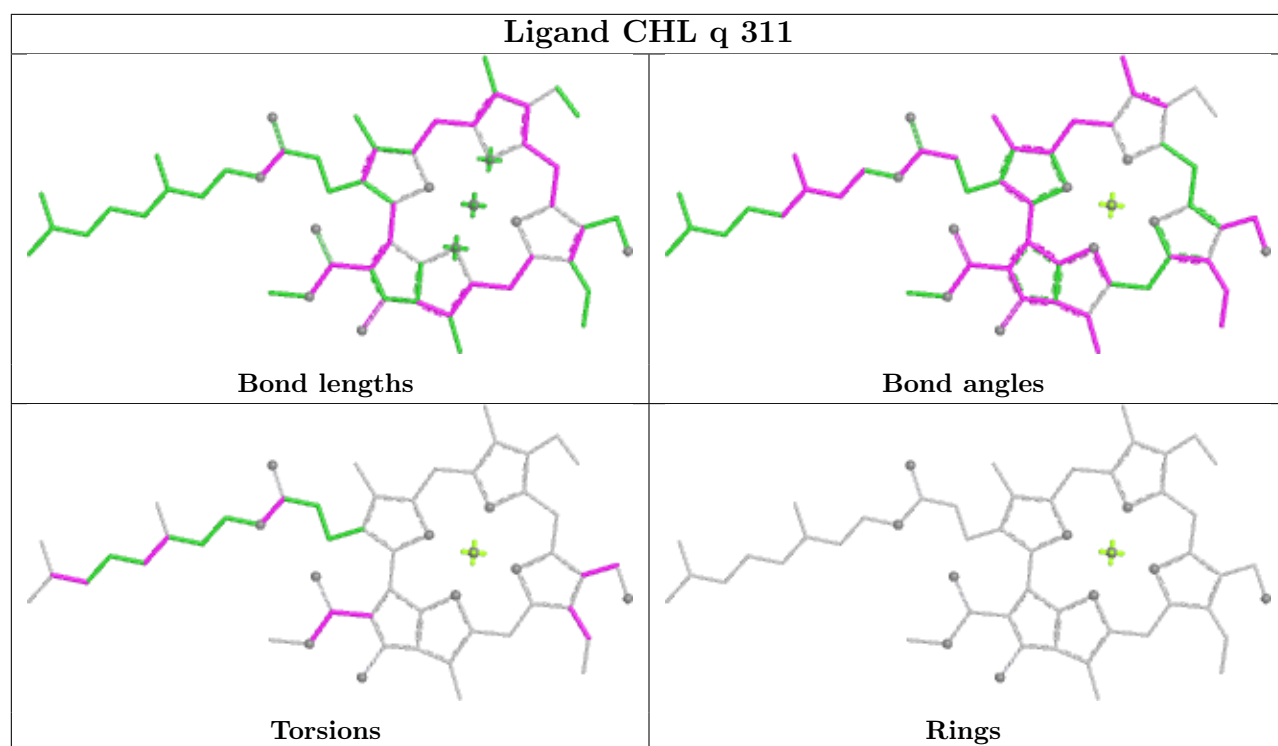


Rings

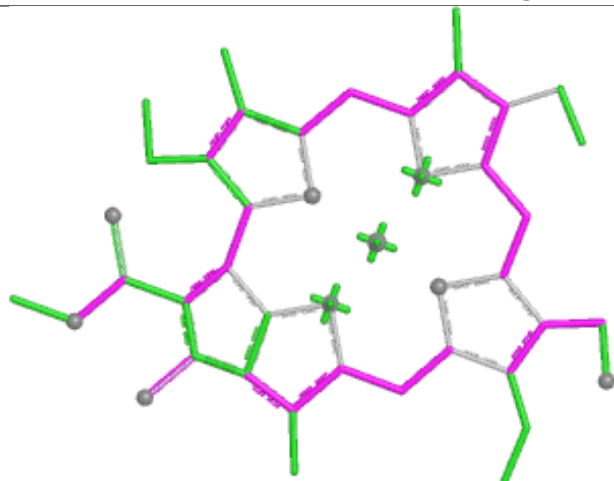




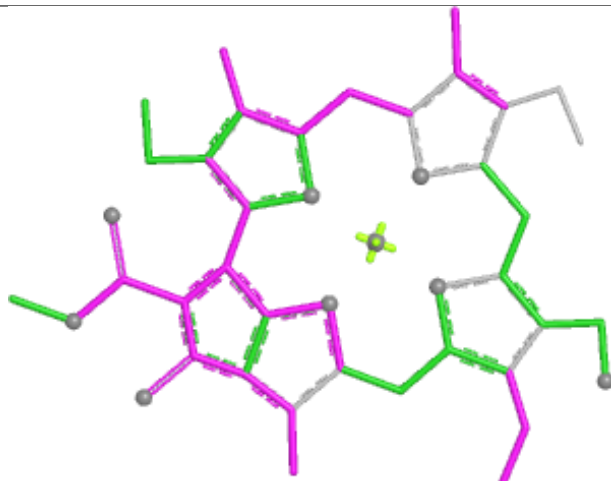




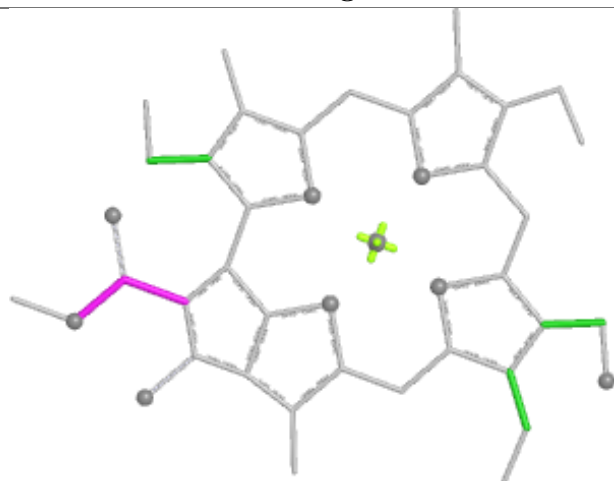
Ligand CHL 1 308



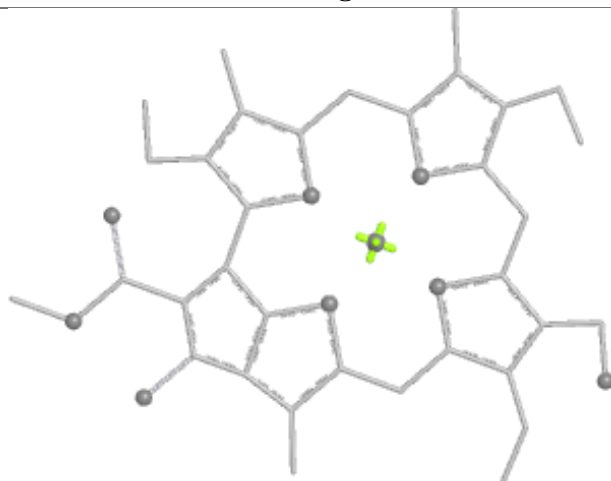
Bond lengths



Bond angles

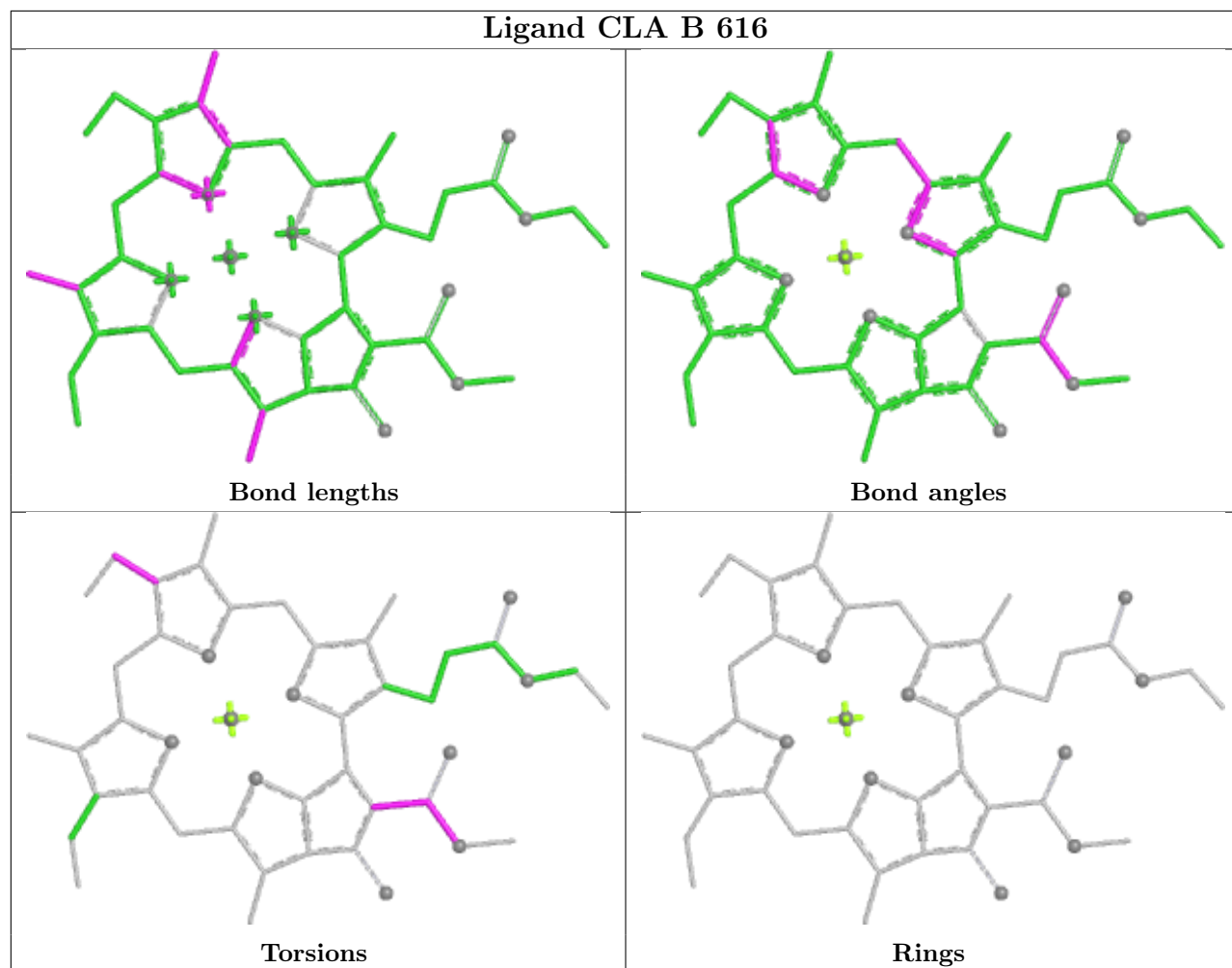


Torsions

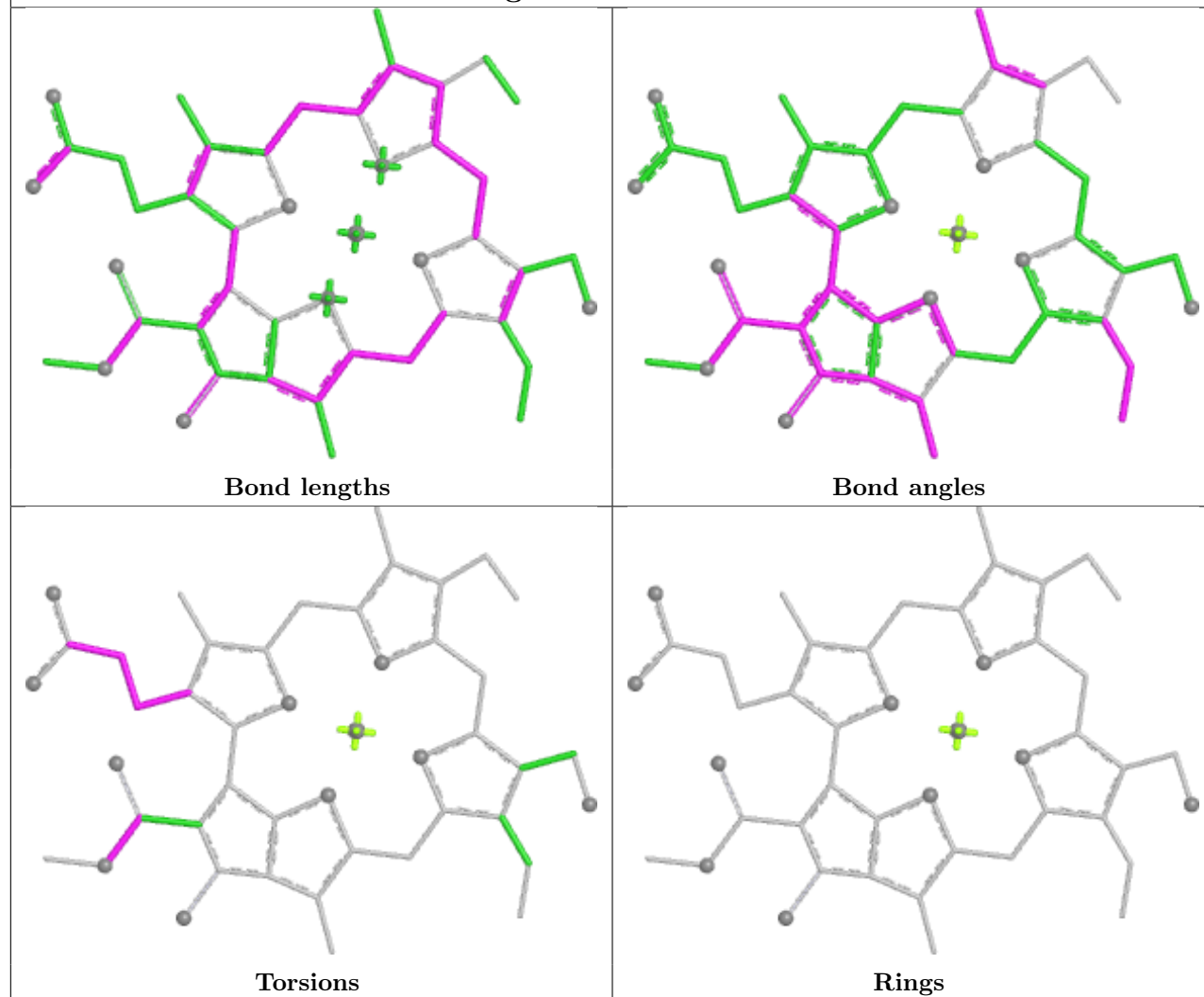


Rings

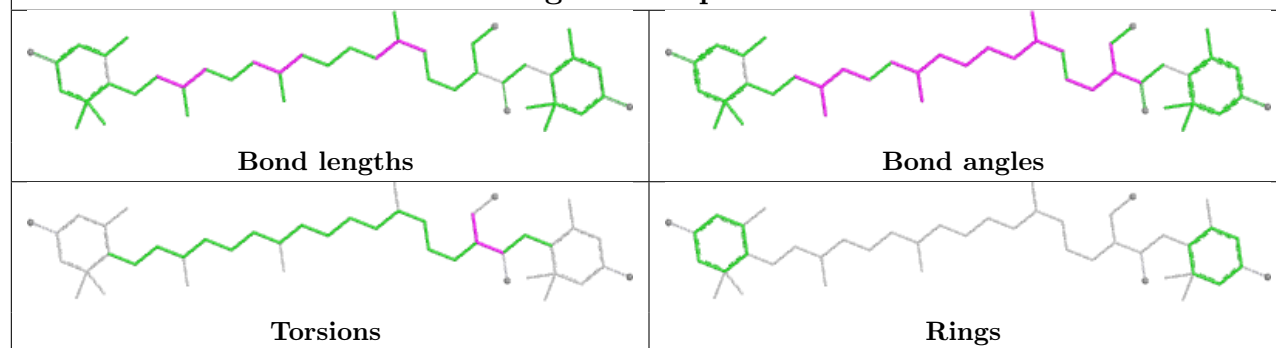
Ligand CLA B 616



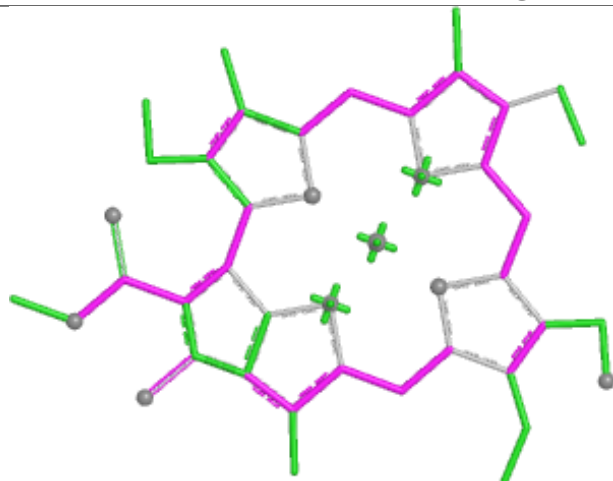
Ligand CHL 3 310



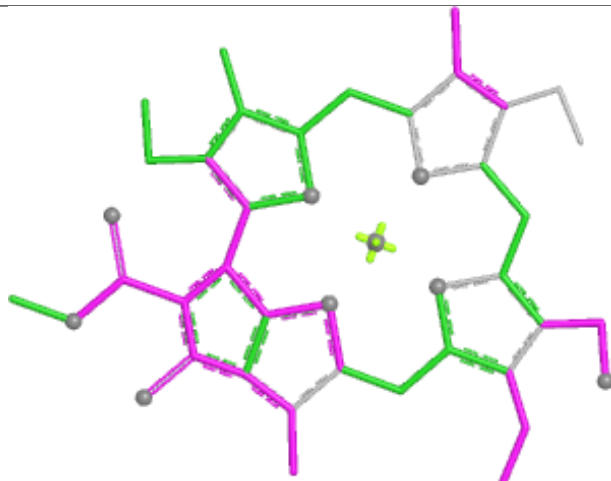
Ligand OIE p 302



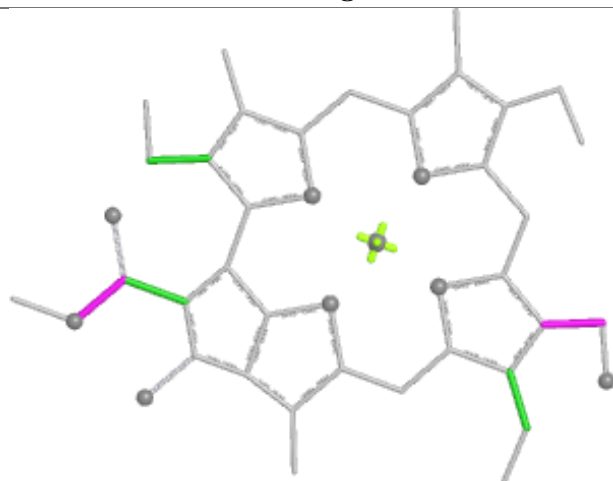
Ligand CHL Y 308



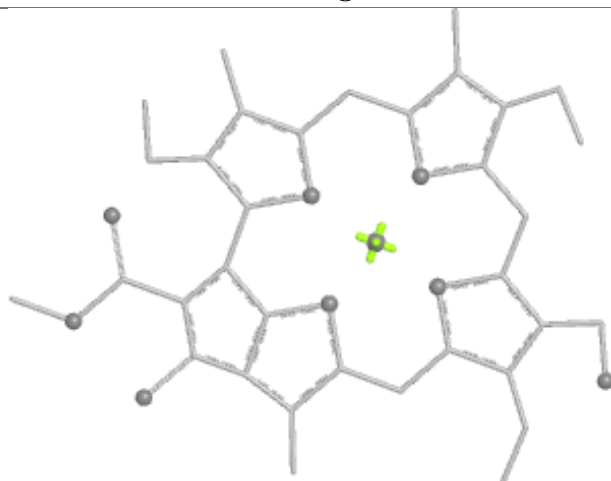
Bond lengths



Bond angles

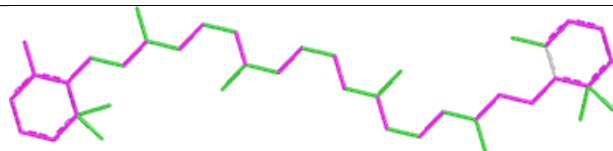


Torsions

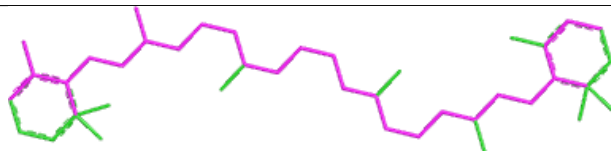


Rings

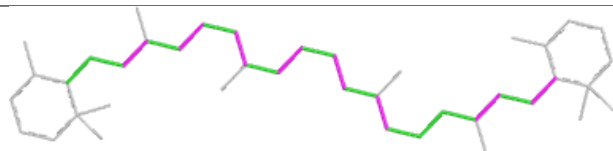
Ligand 8CT B 617



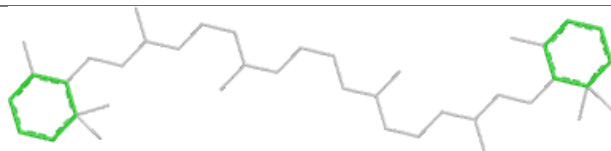
Bond lengths



Bond angles

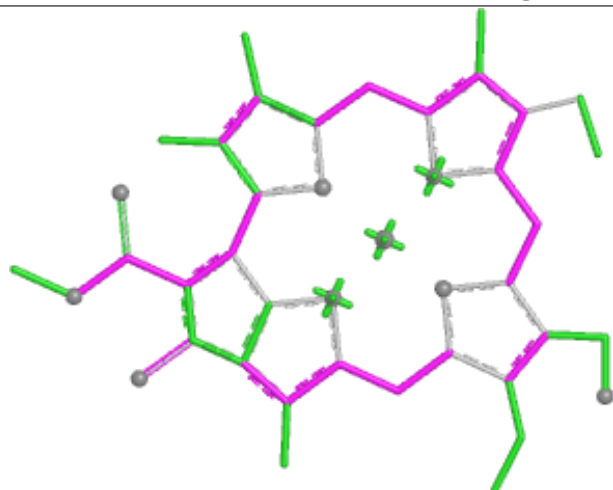


Torsions



Rings

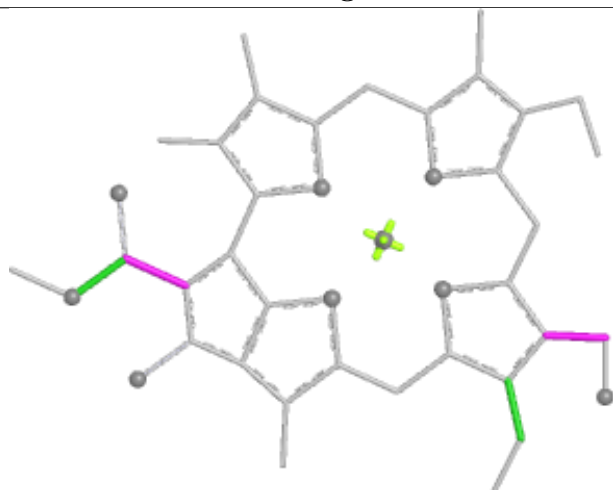
Ligand CHL y 318



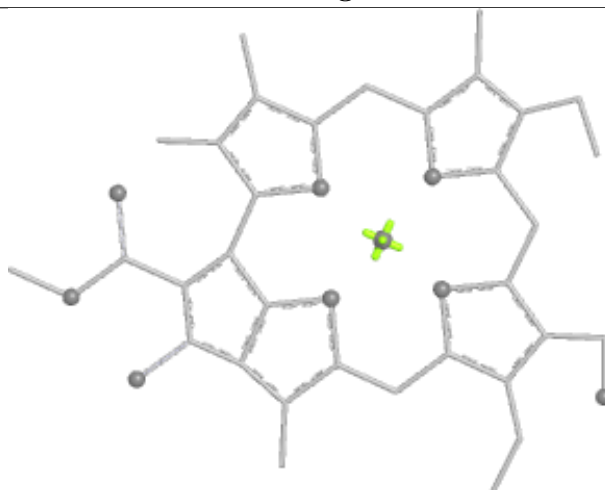
Bond lengths



Bond angles

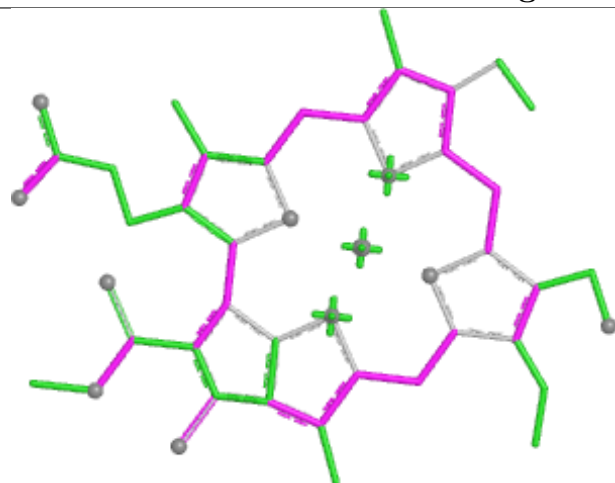


Torsions

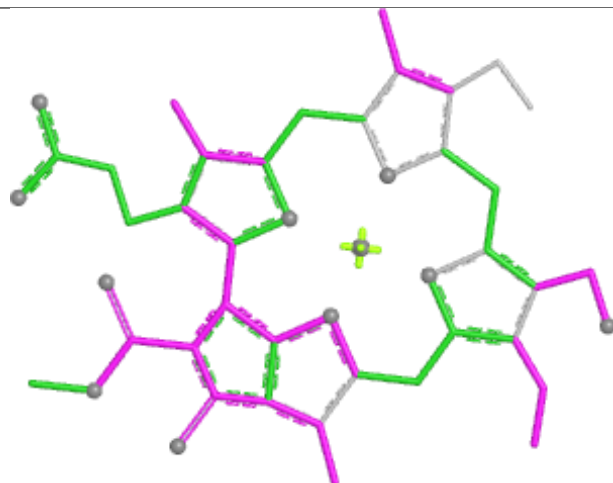


Rings

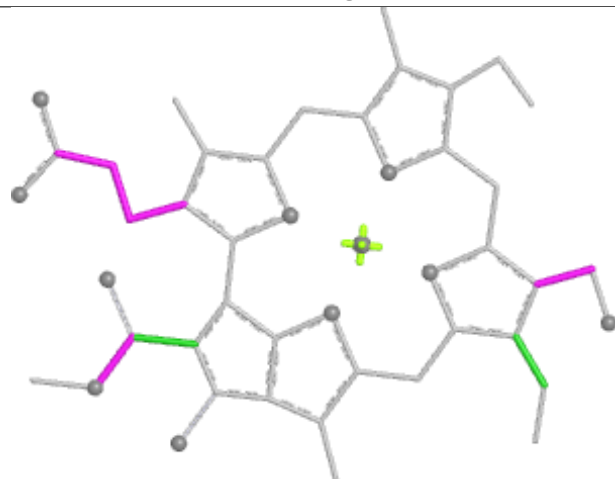
Ligand CHL u 310



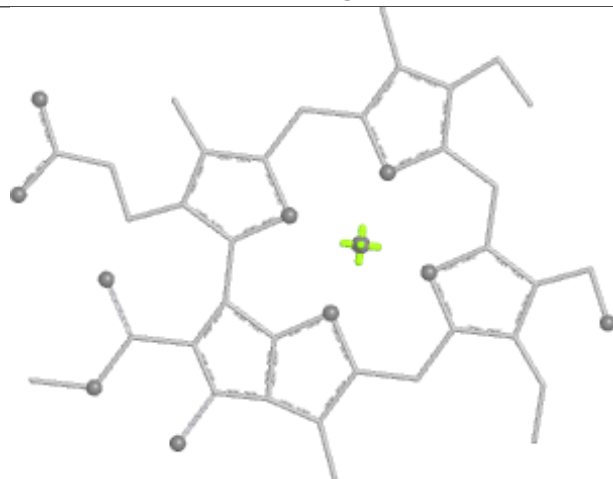
Bond lengths



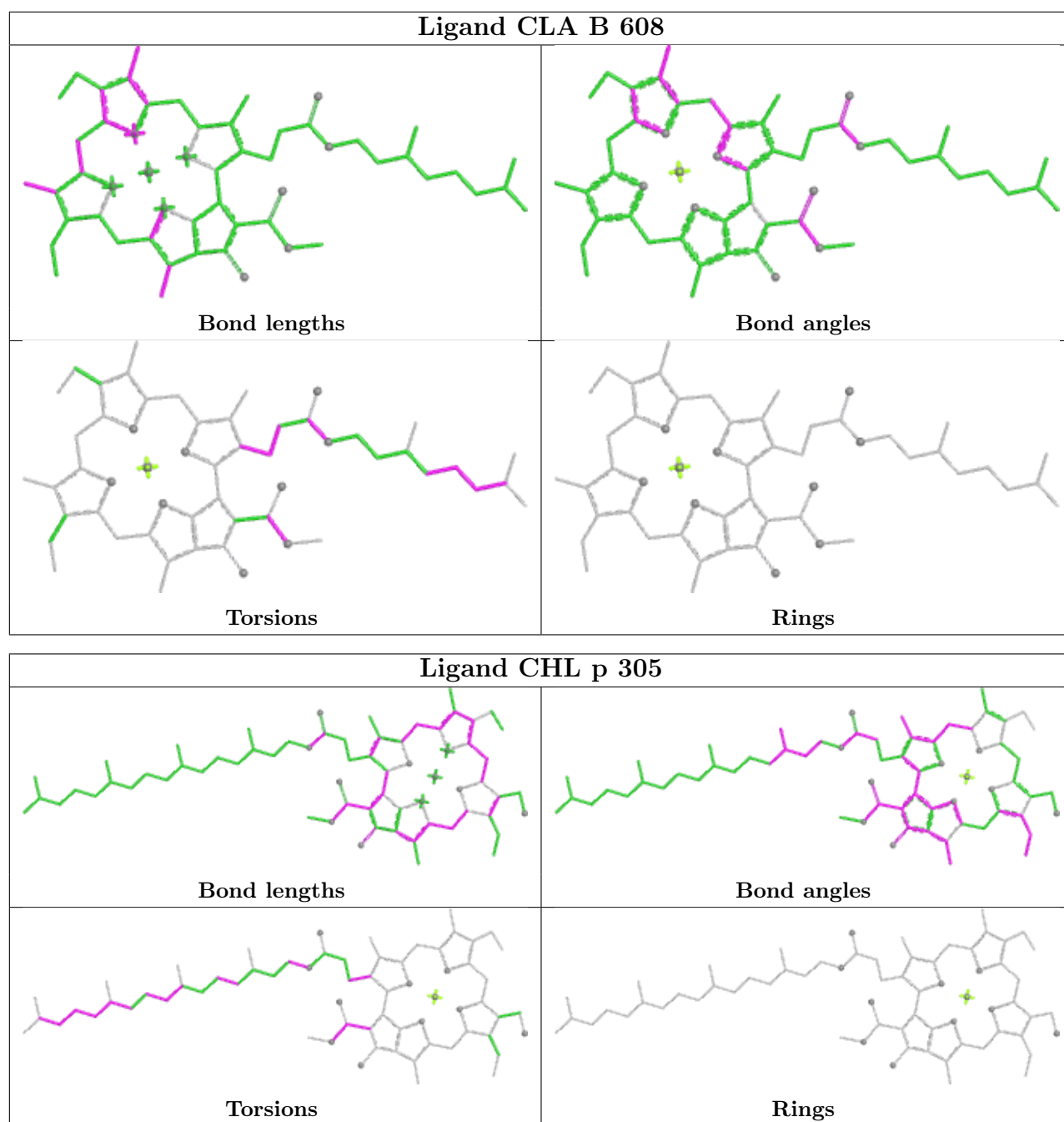
Bond angles

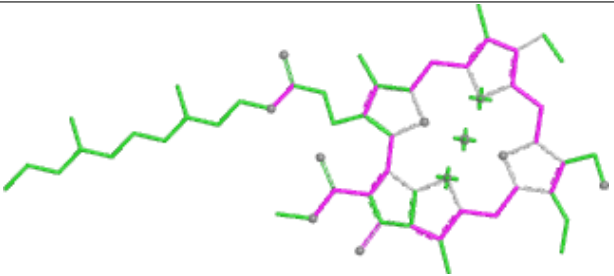
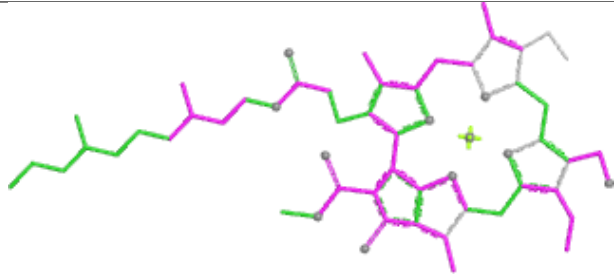
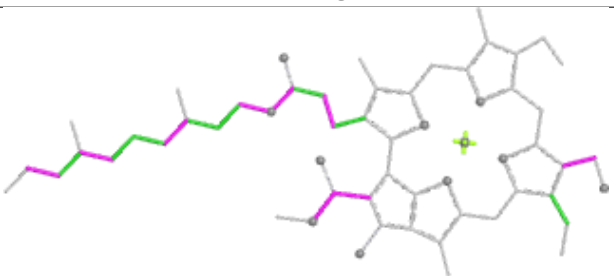
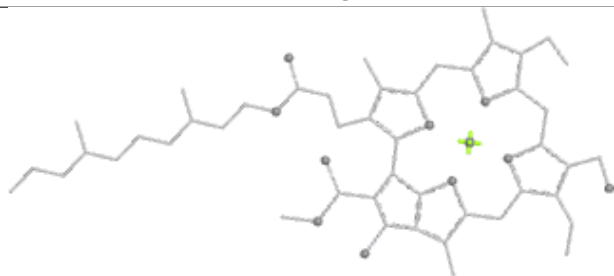




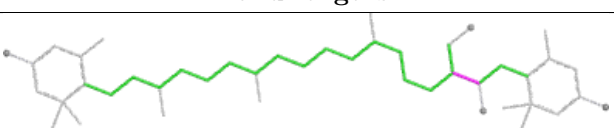
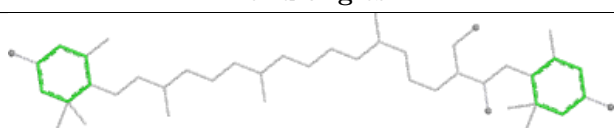
Torsions



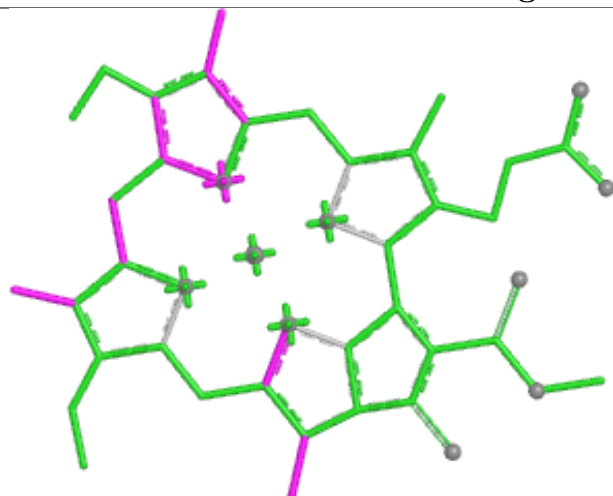
Rings



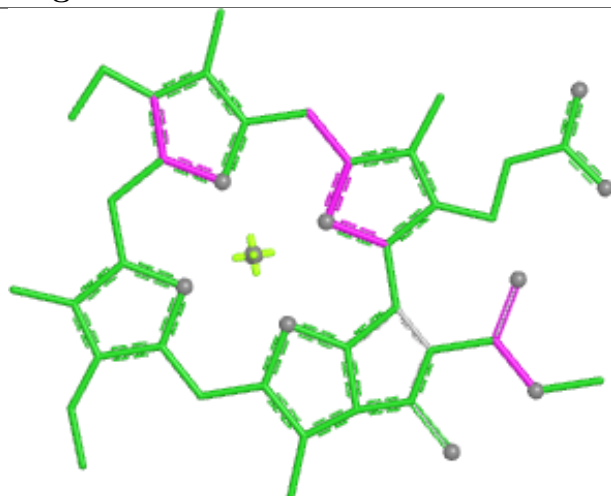
Ligand CHL s 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 0IE r 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

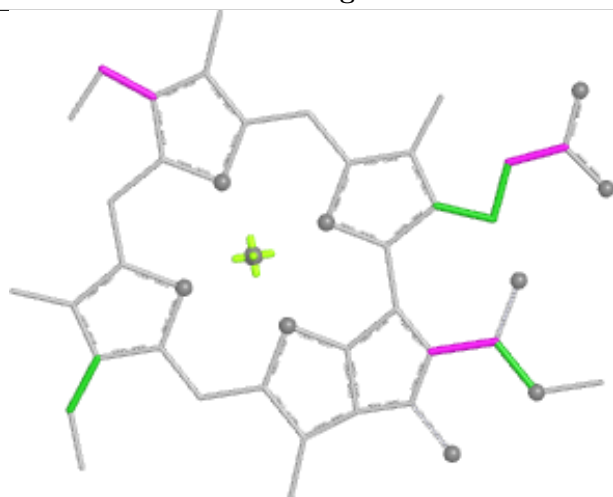
Ligand CLA g 316



Bond lengths



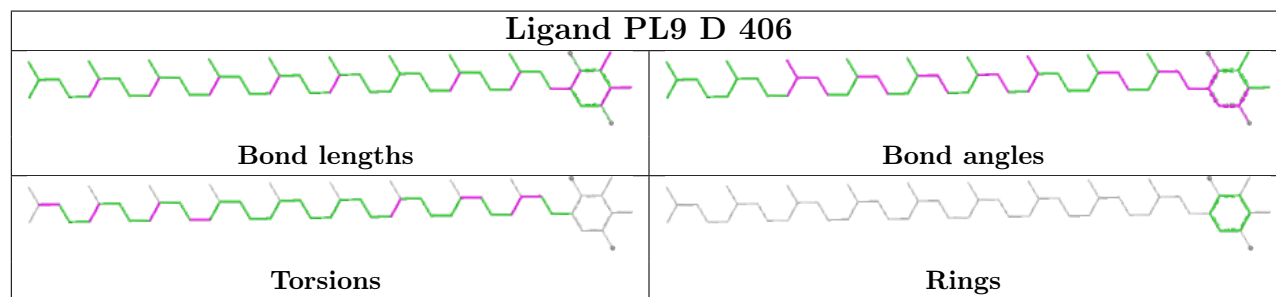
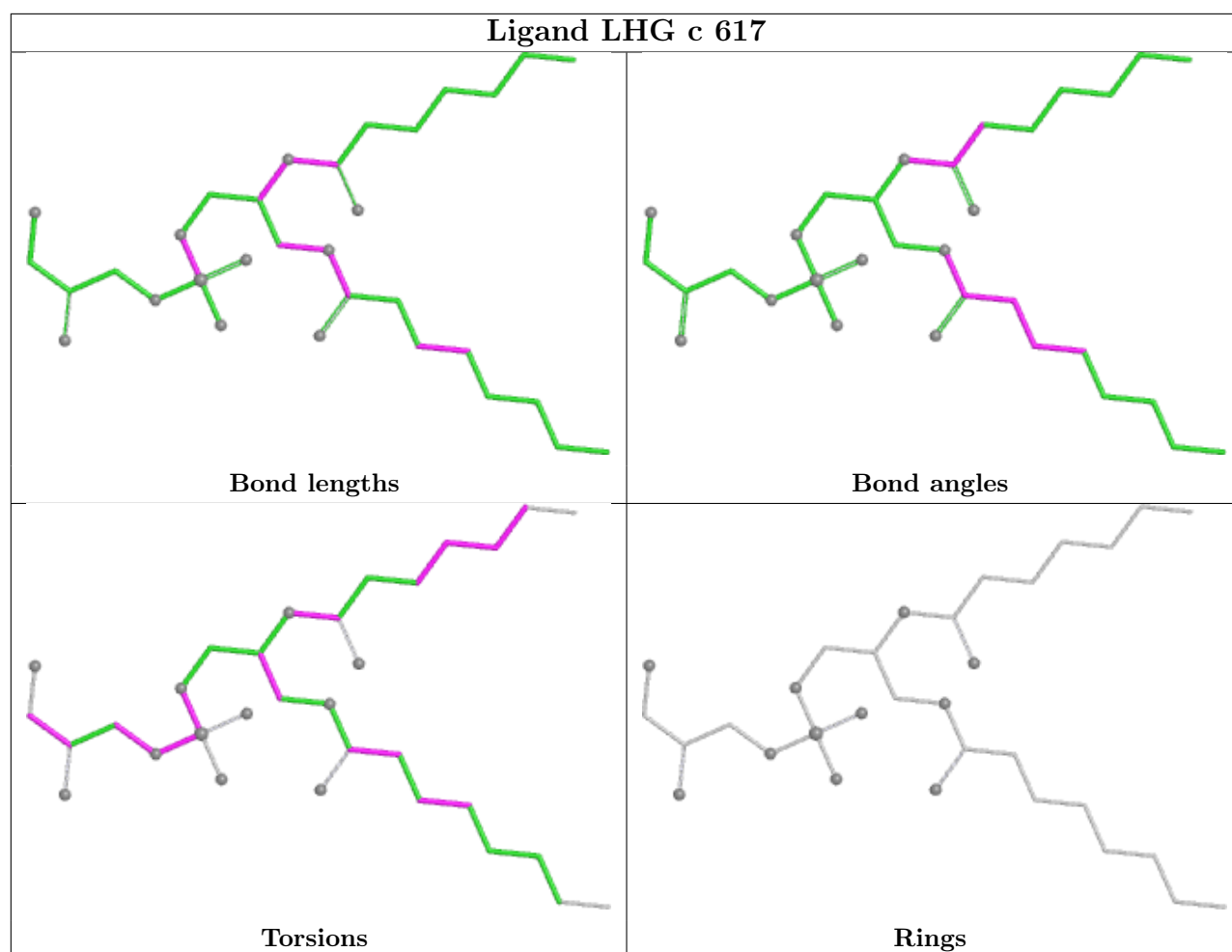
Bond angles

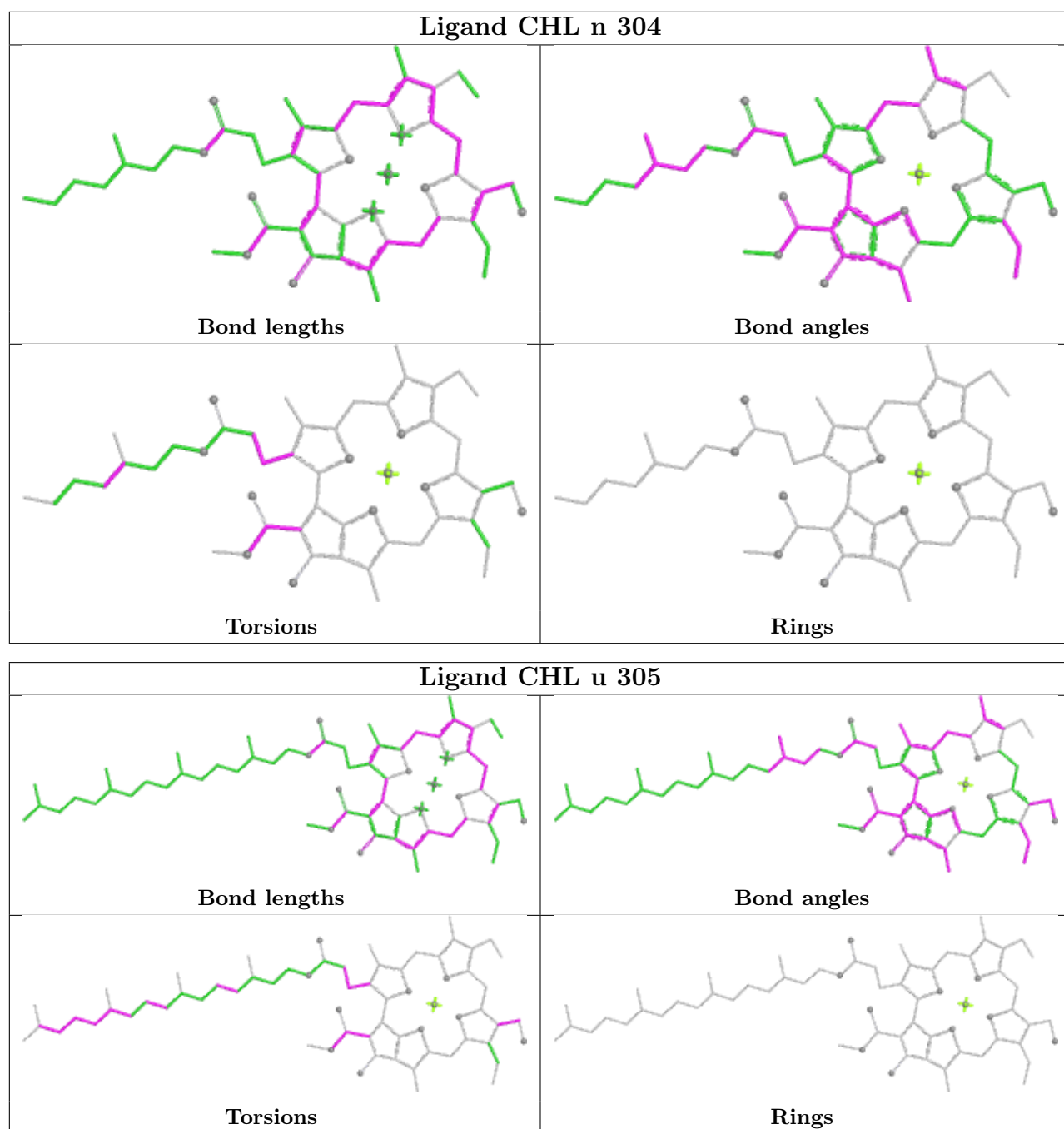


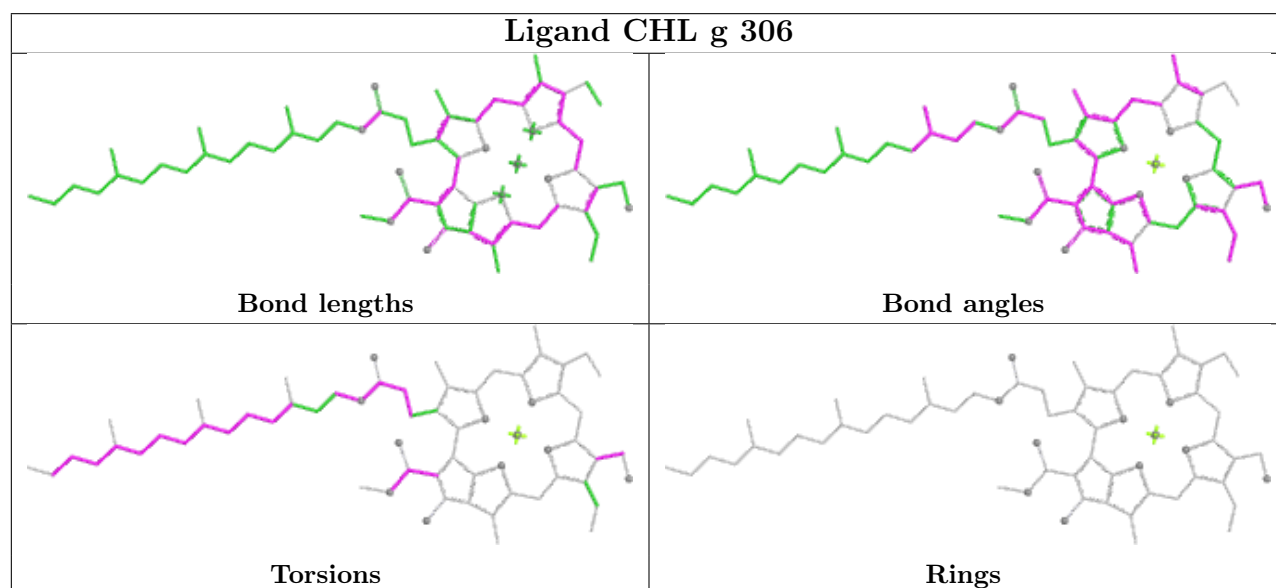
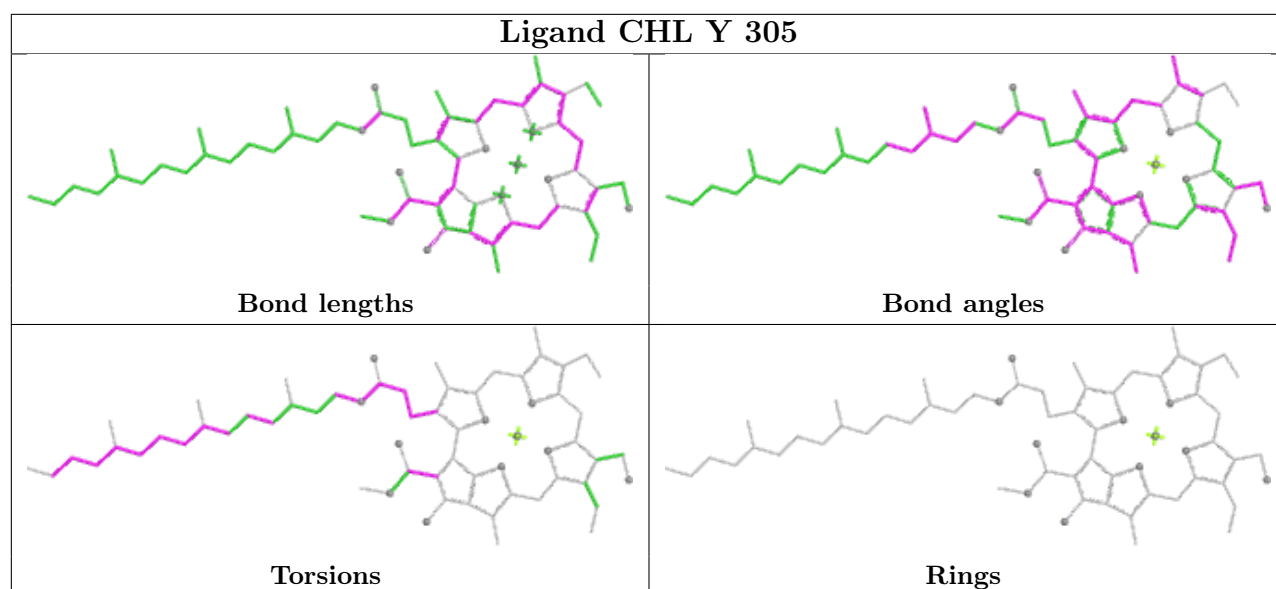
Torsions



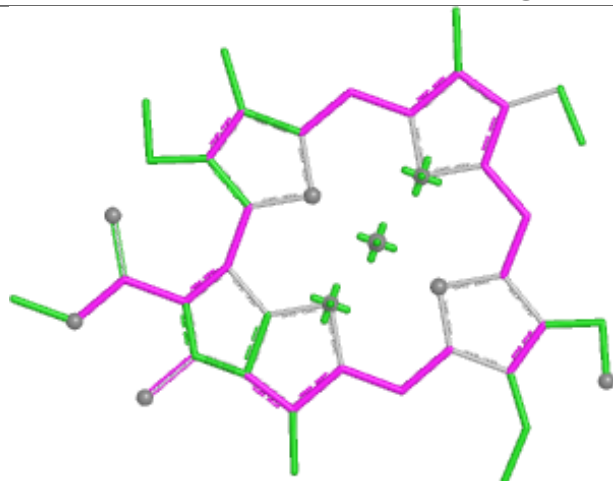
Rings



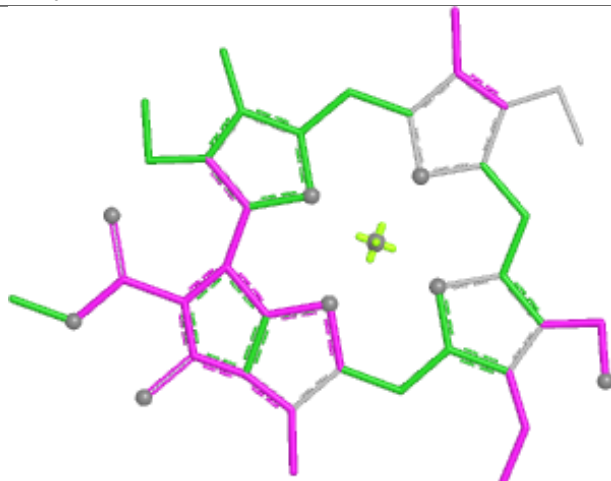




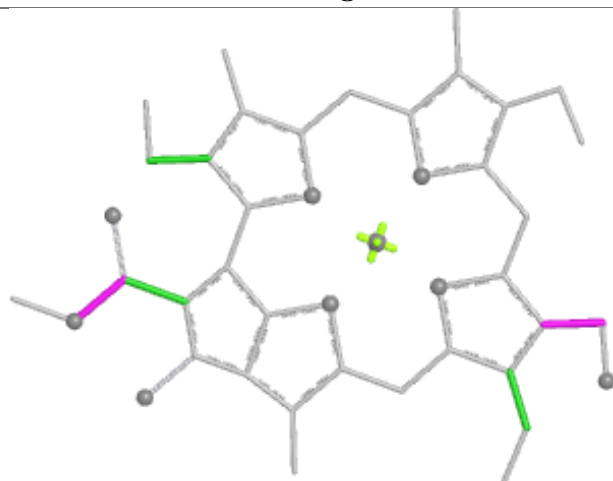
Ligand CHL y 309



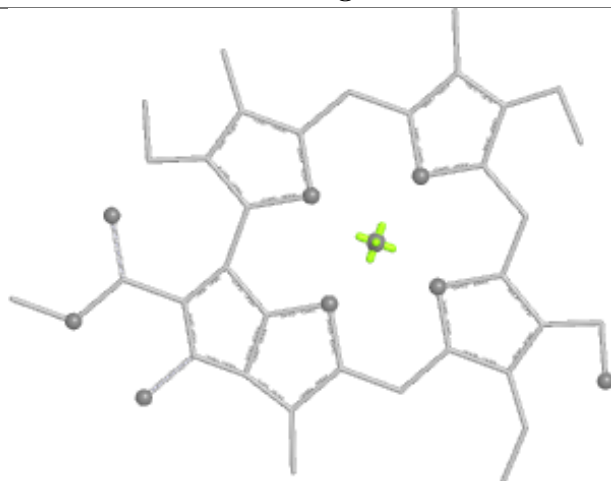
Bond lengths



Bond angles

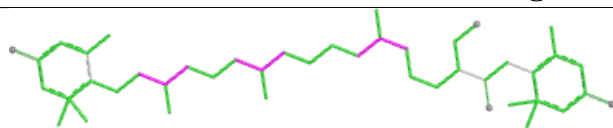


Torsions

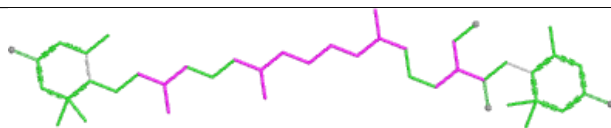


Rings

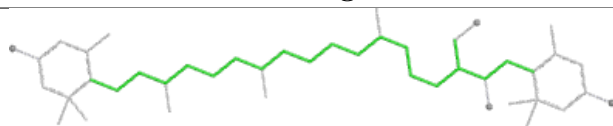
Ligand OIE 2 303



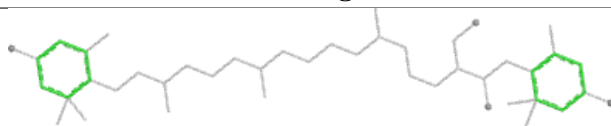
Bond lengths



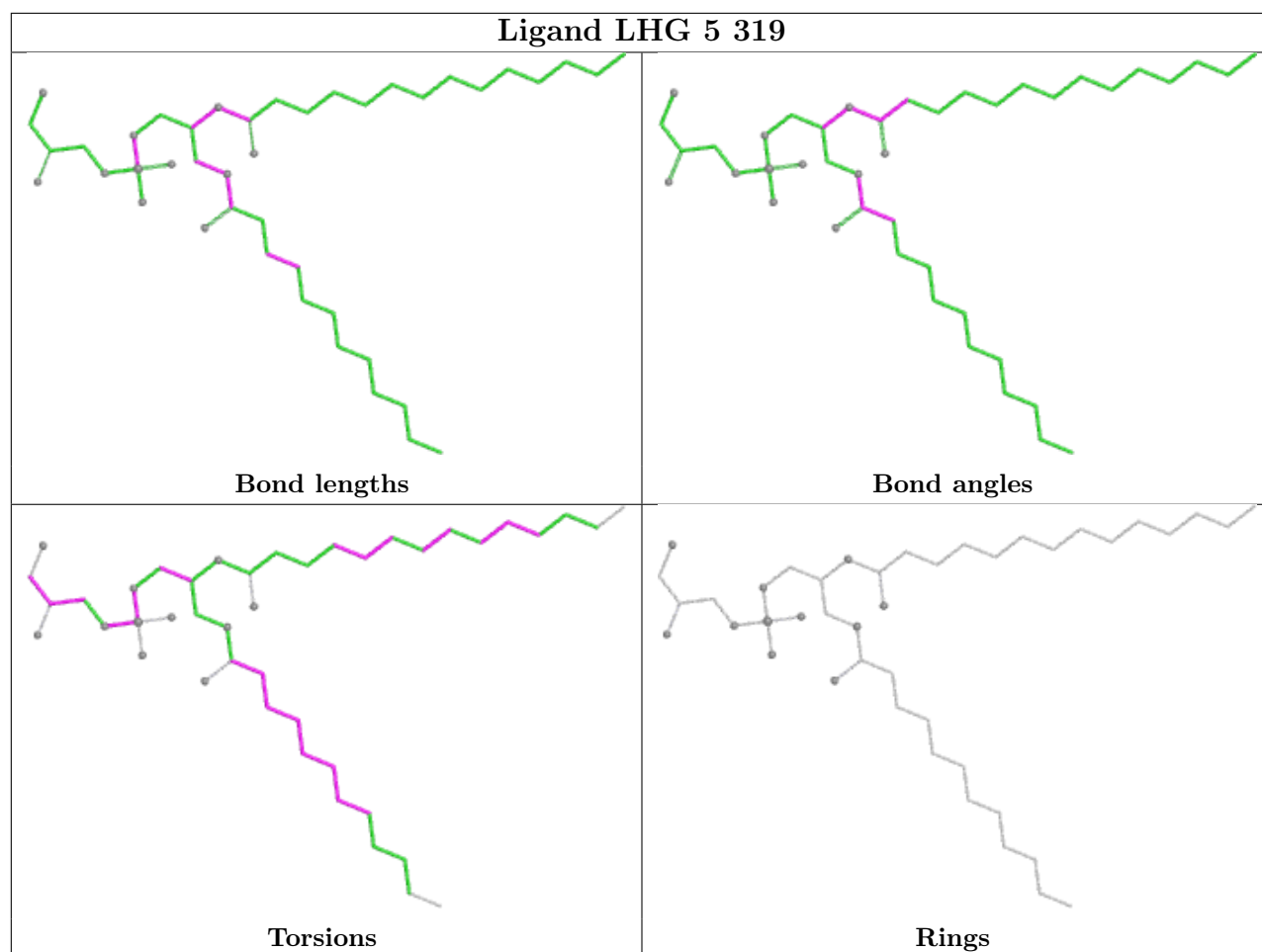
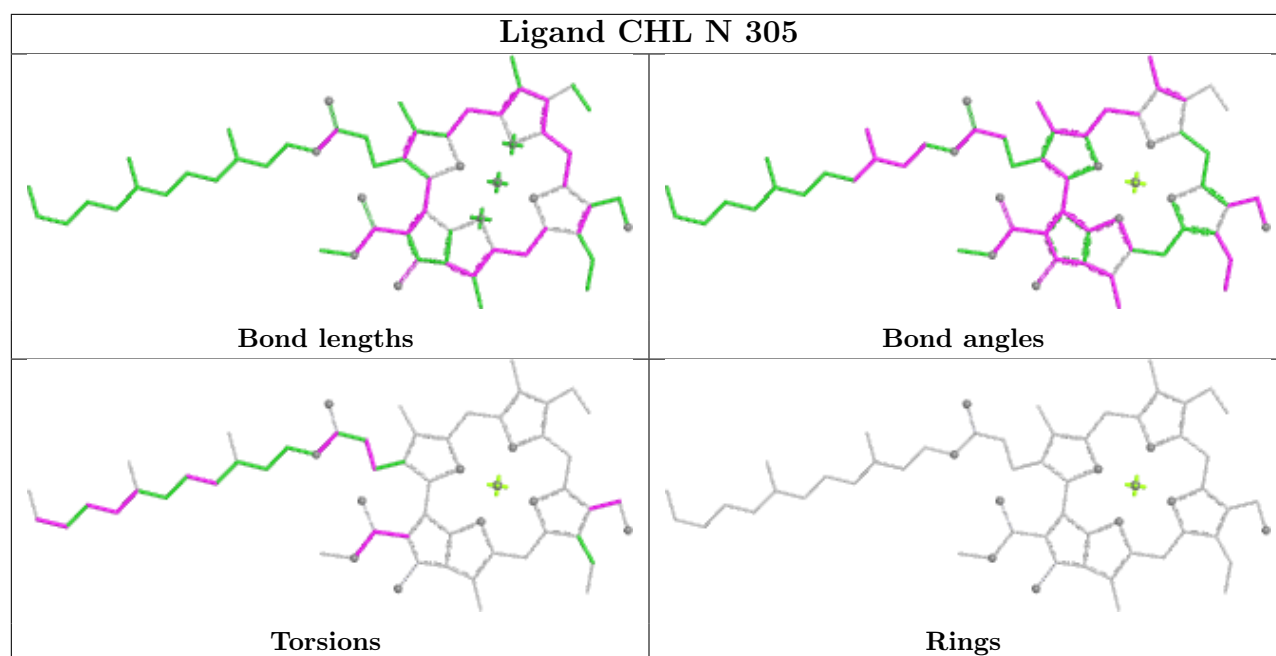
Bond angles

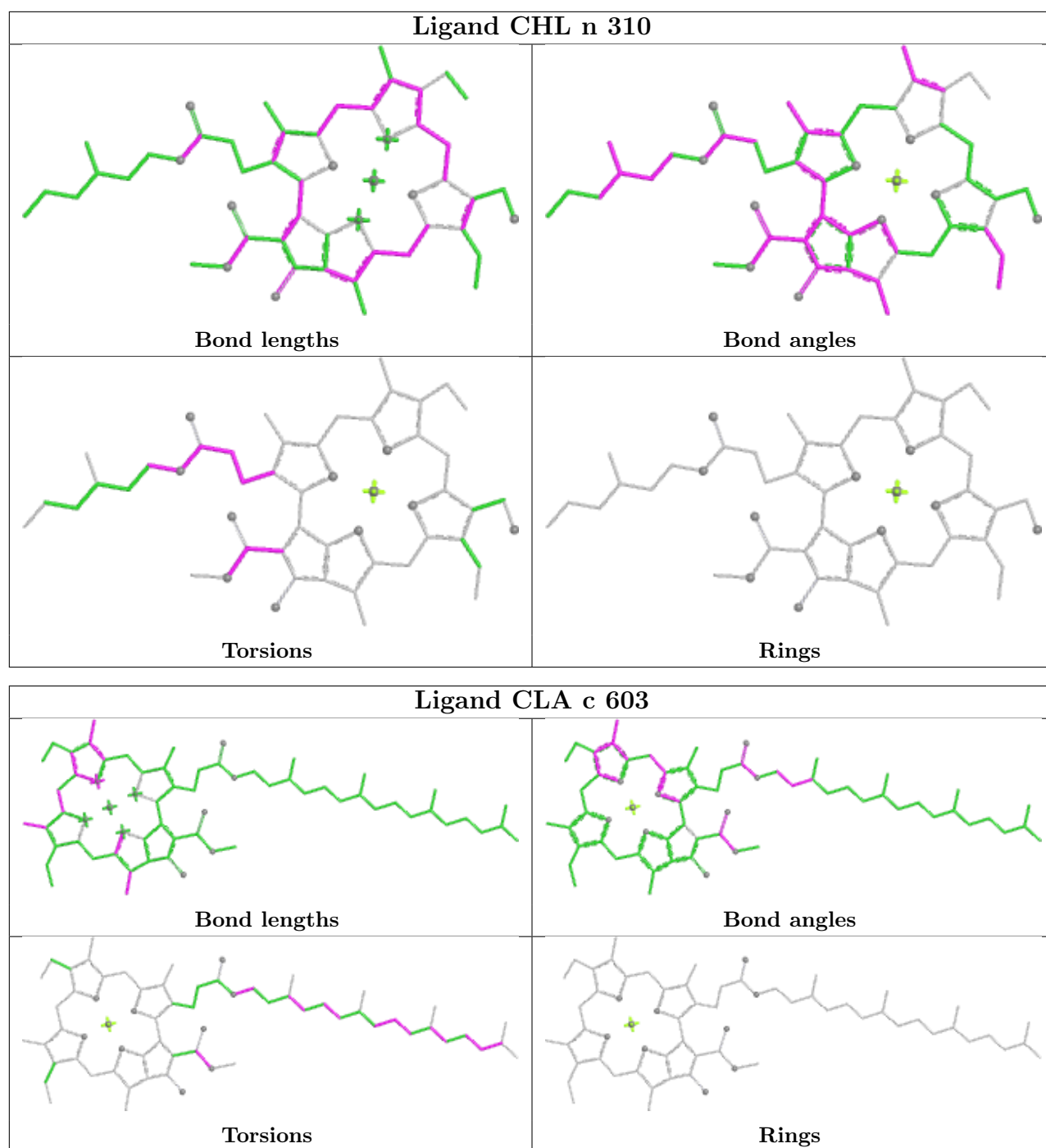


Torsions

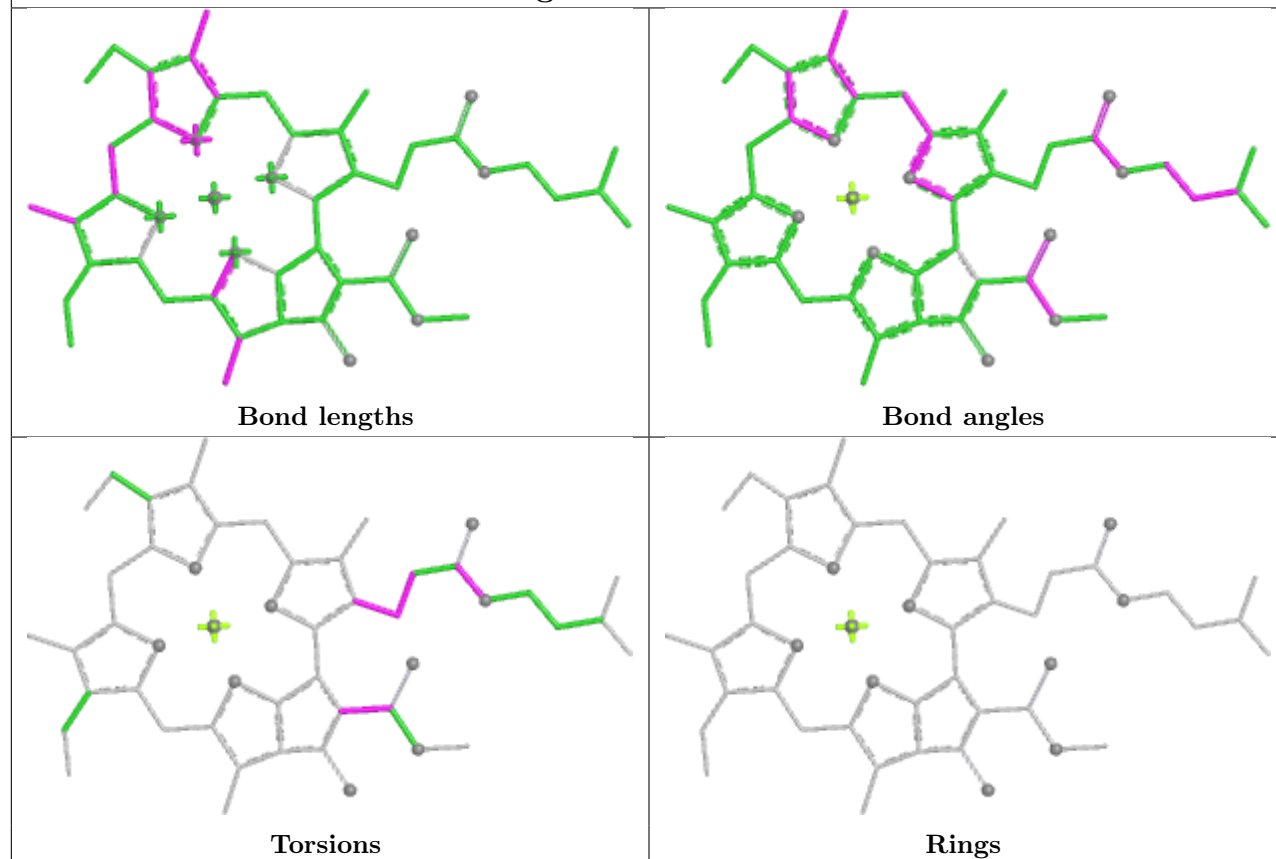


Rings

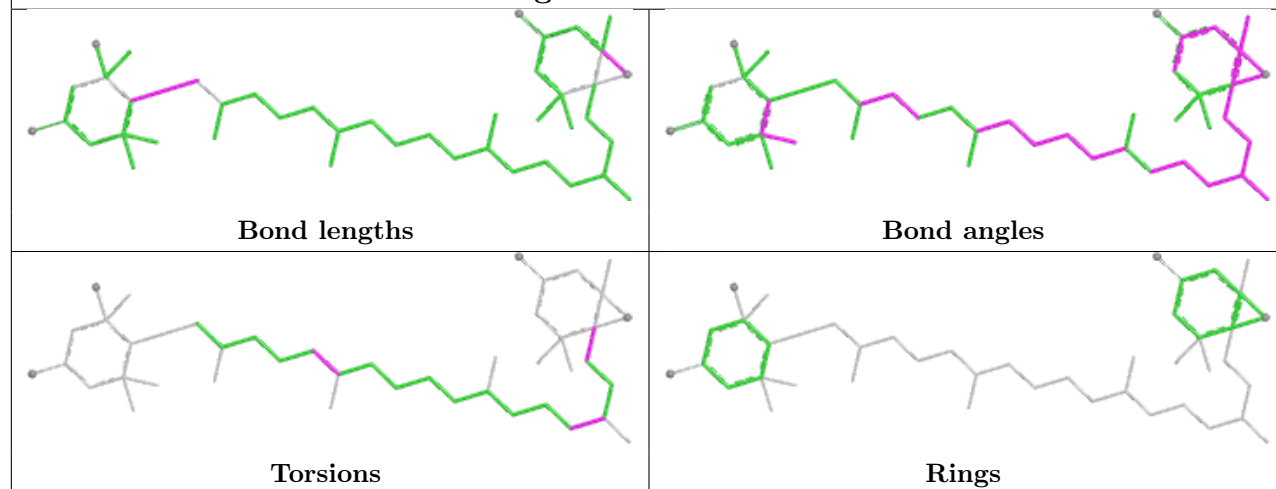




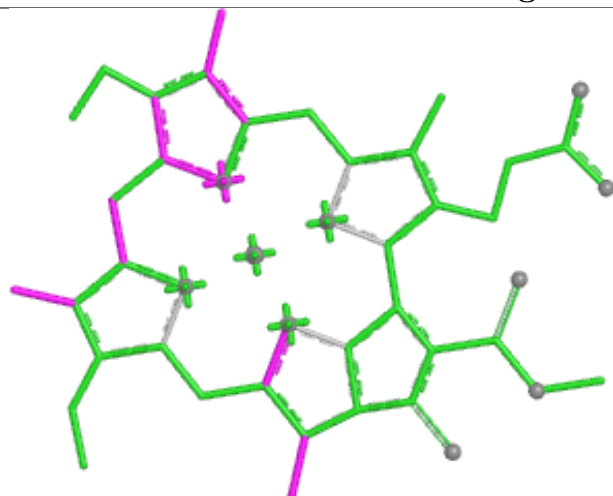
Ligand CLA 8 306



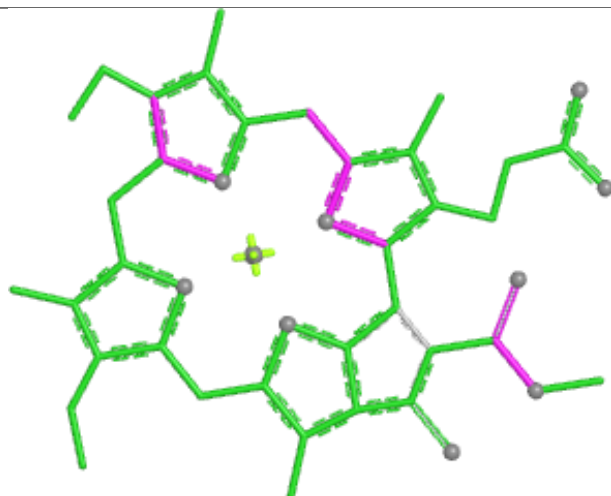
Ligand NEX 6 303



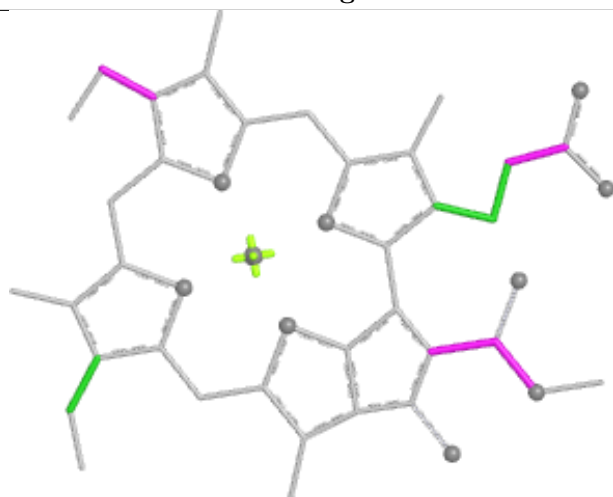
Ligand CLA 4 315



Bond lengths



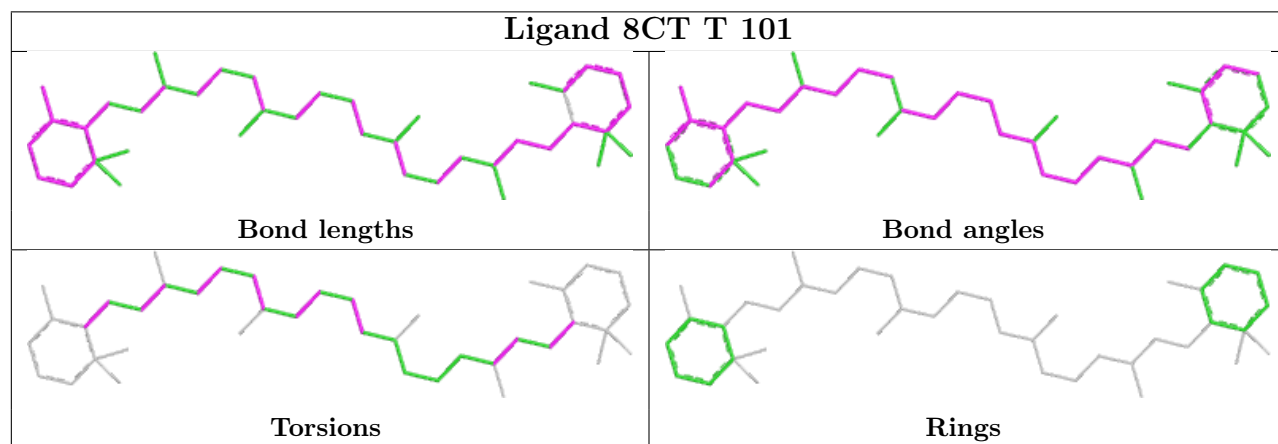
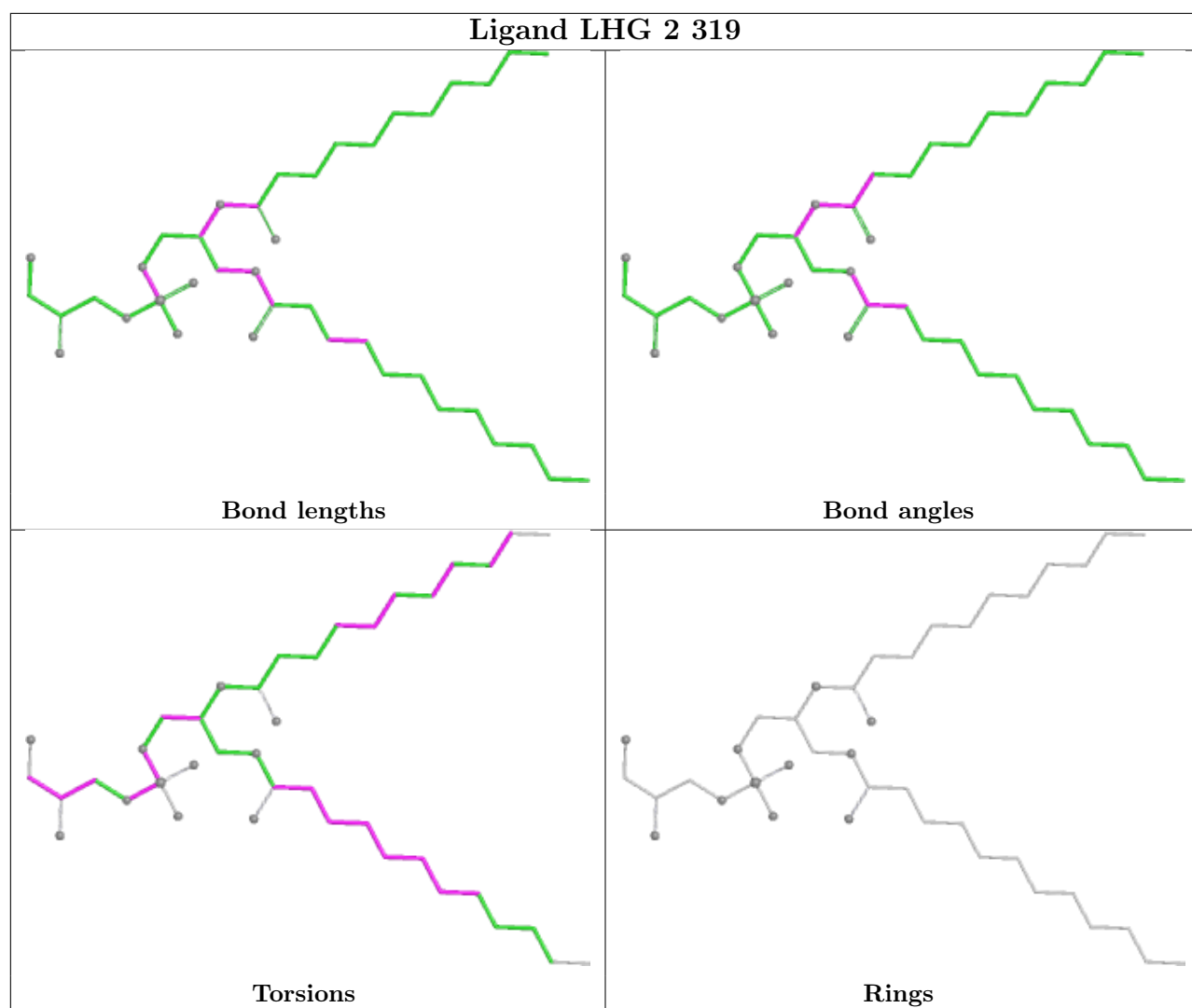
Bond angles



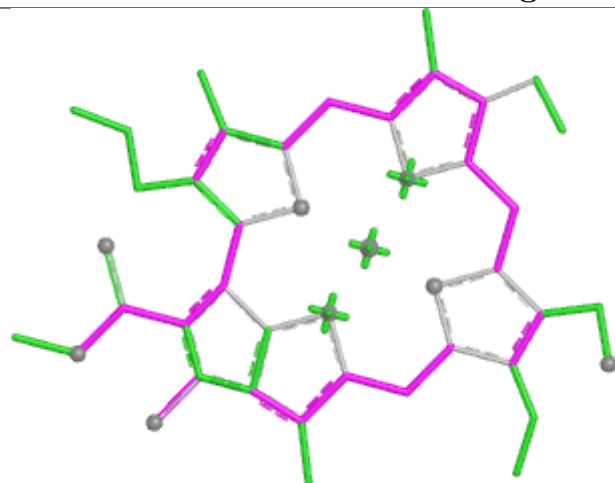
Torsions



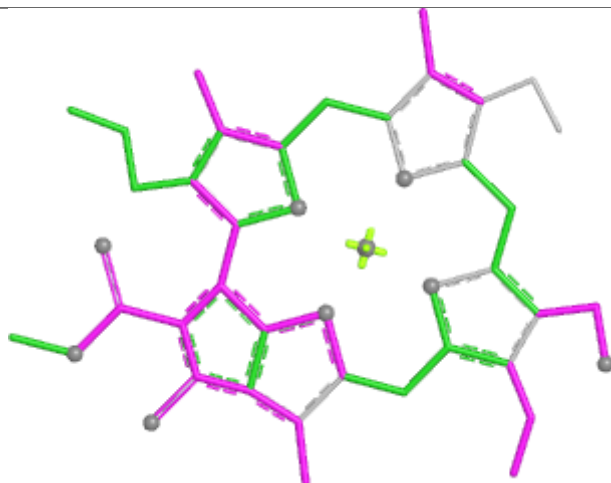
Rings



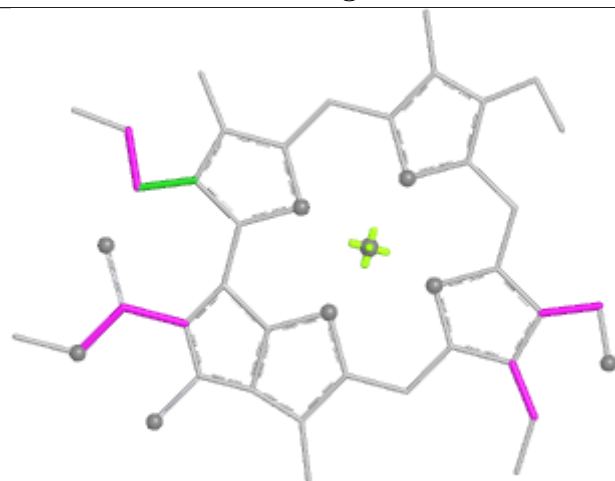
Ligand CHL 2 305



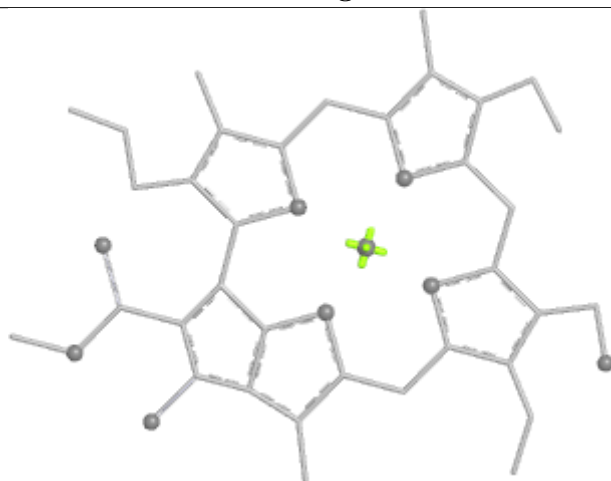
Bond lengths



Bond angles

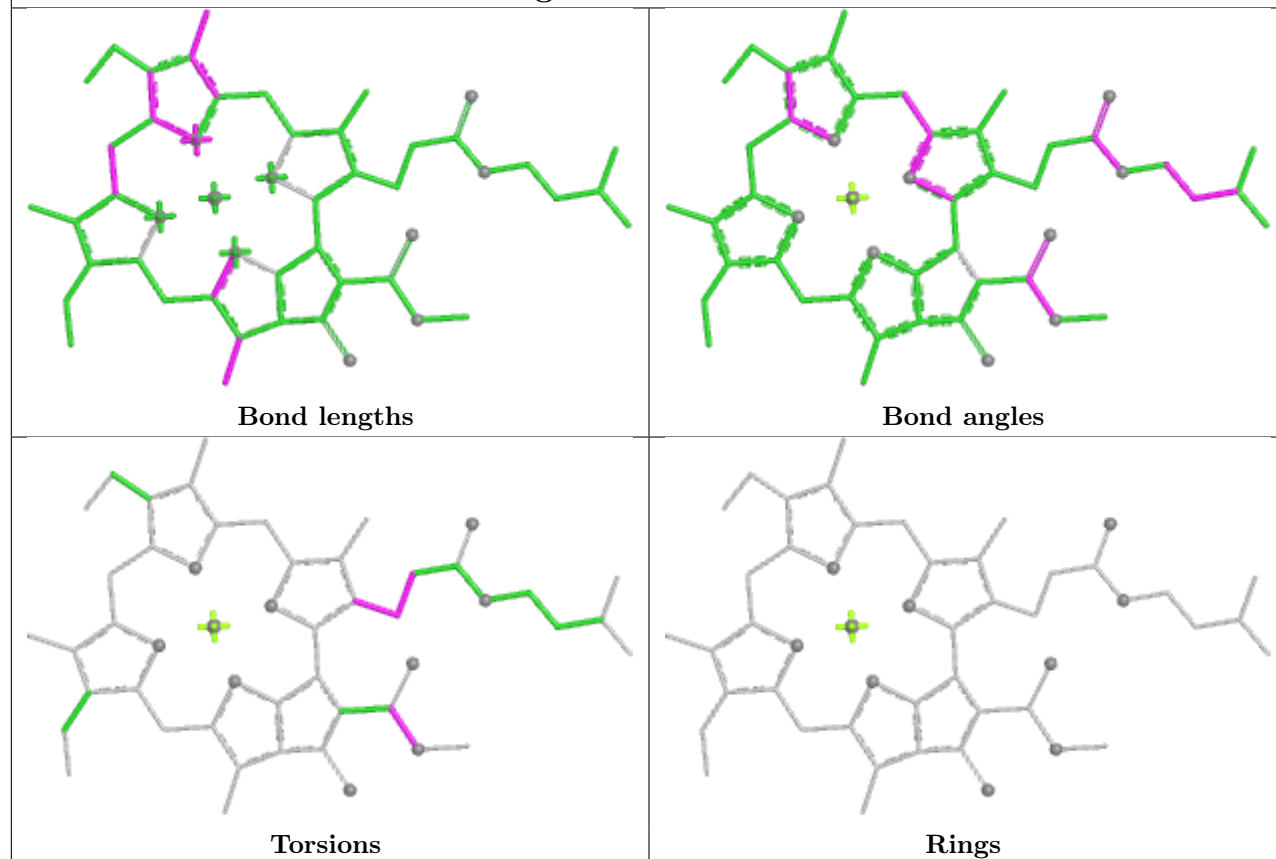


Torsions

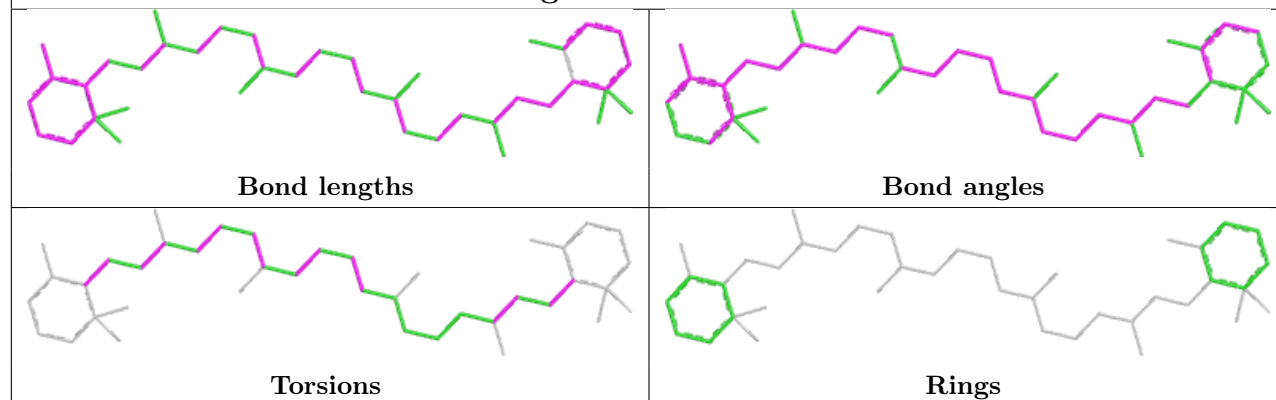


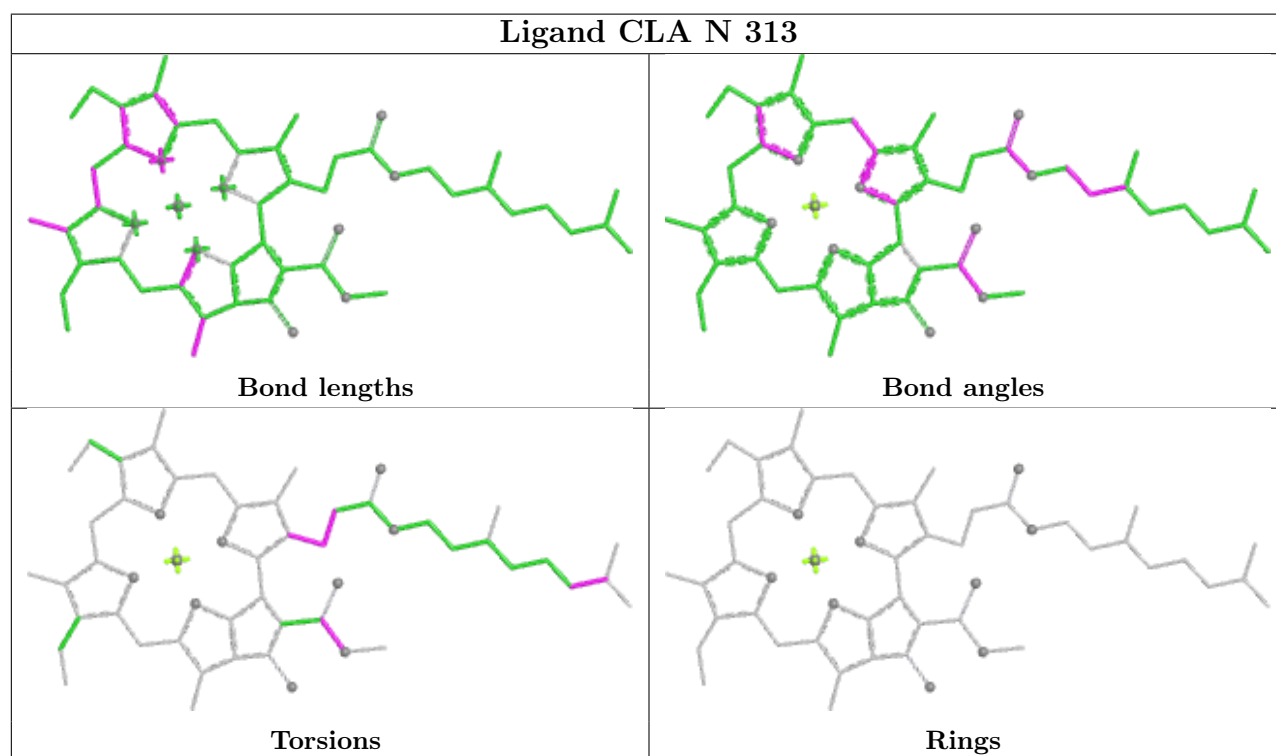
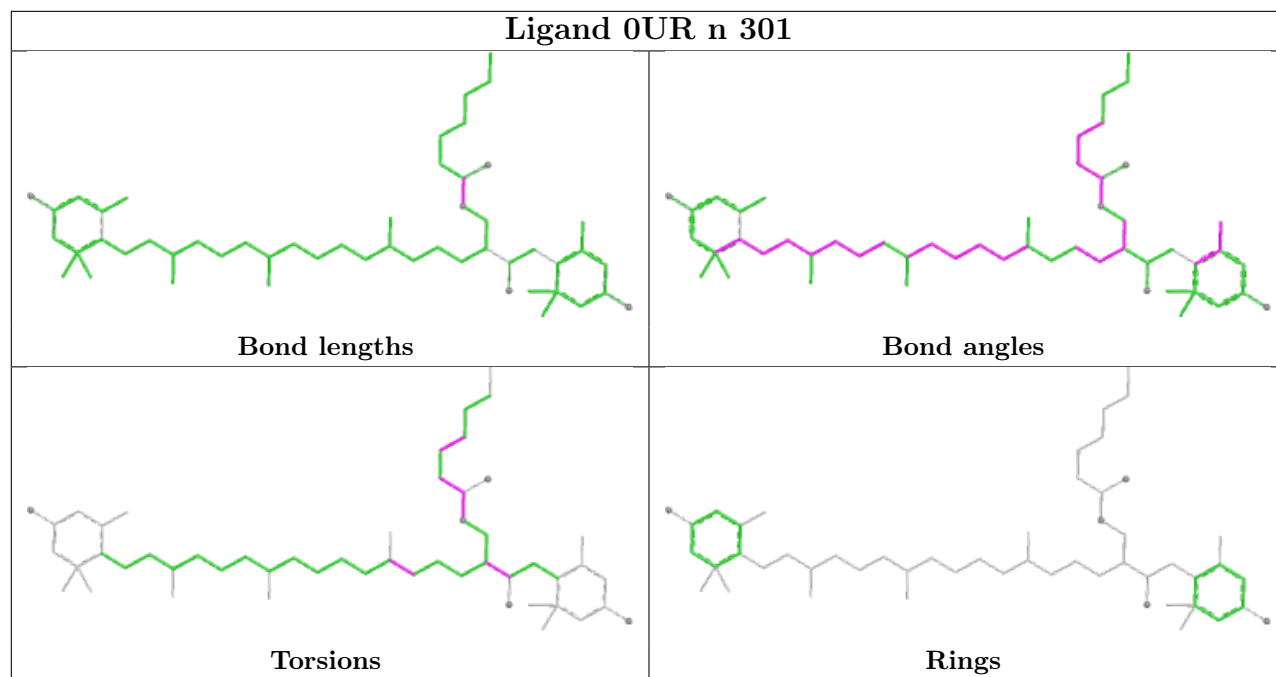
Rings

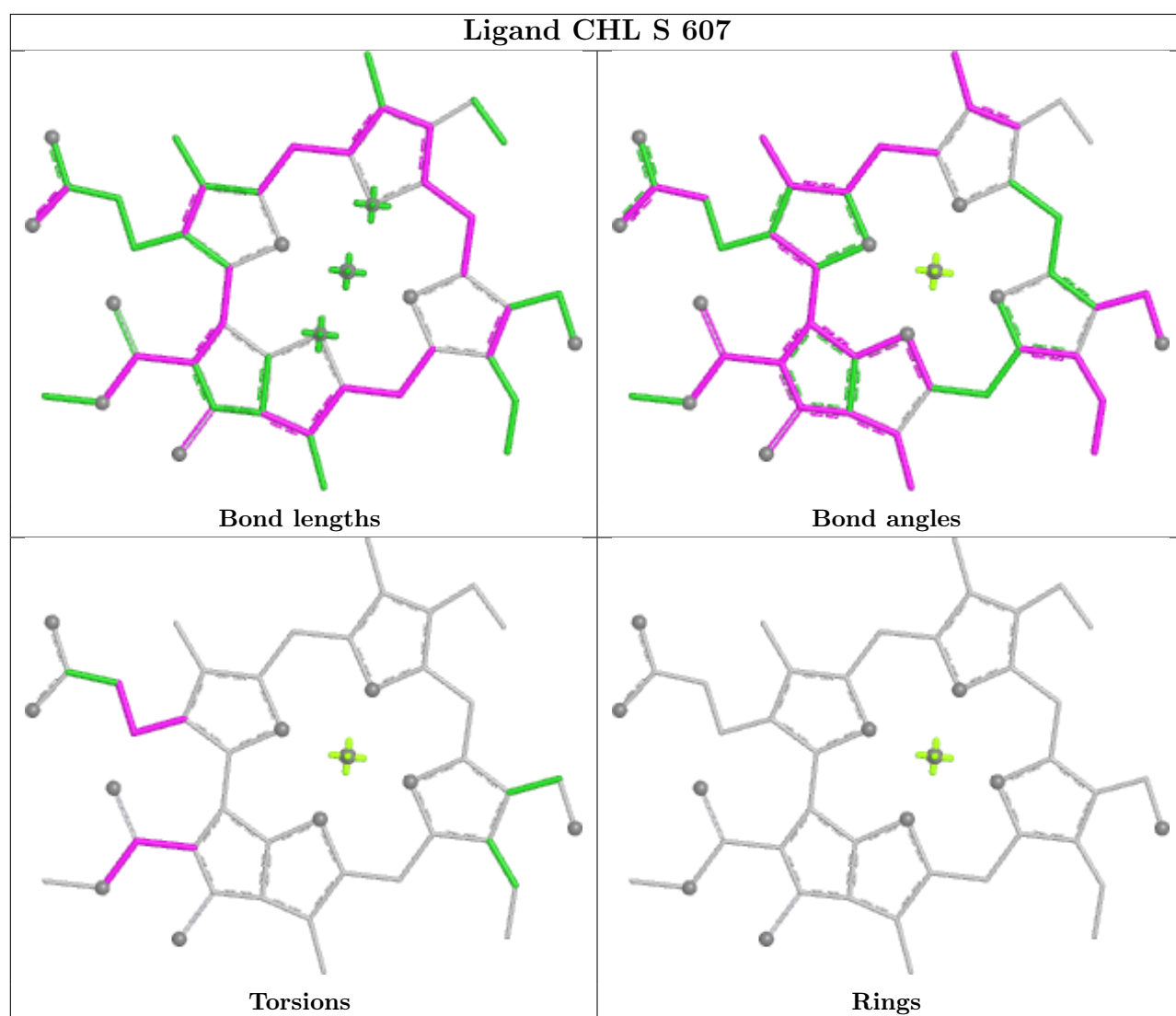
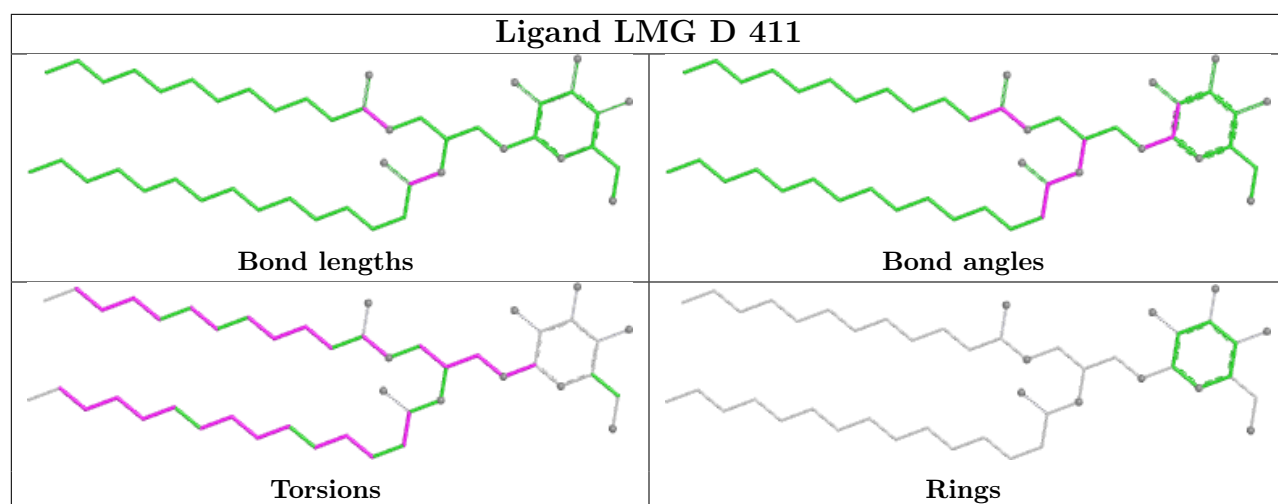
Ligand CLA u 308

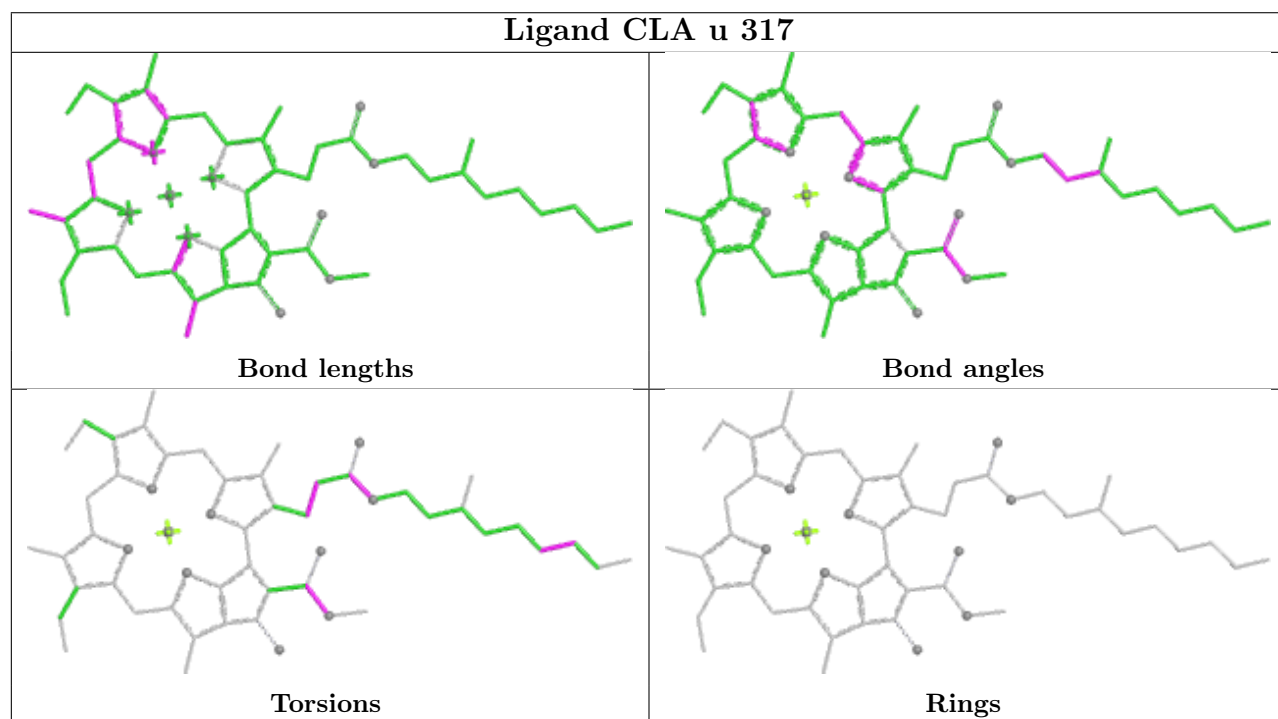
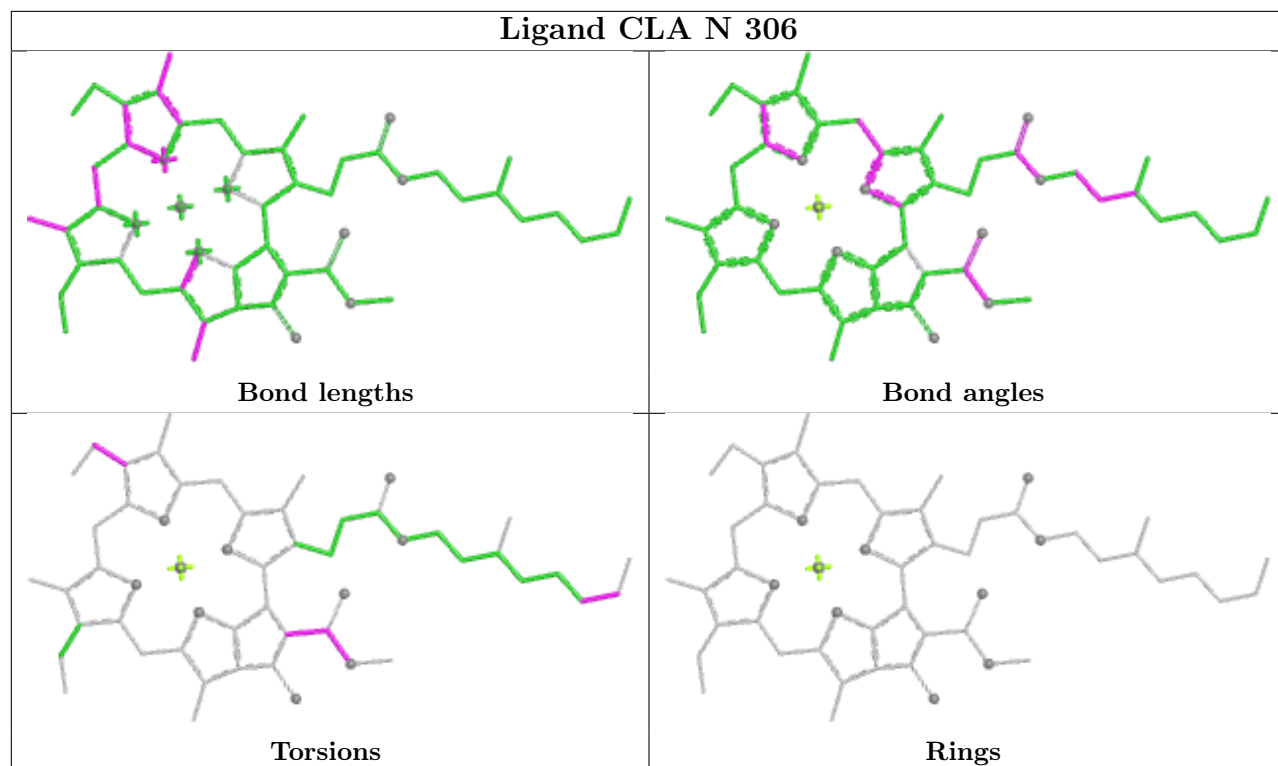


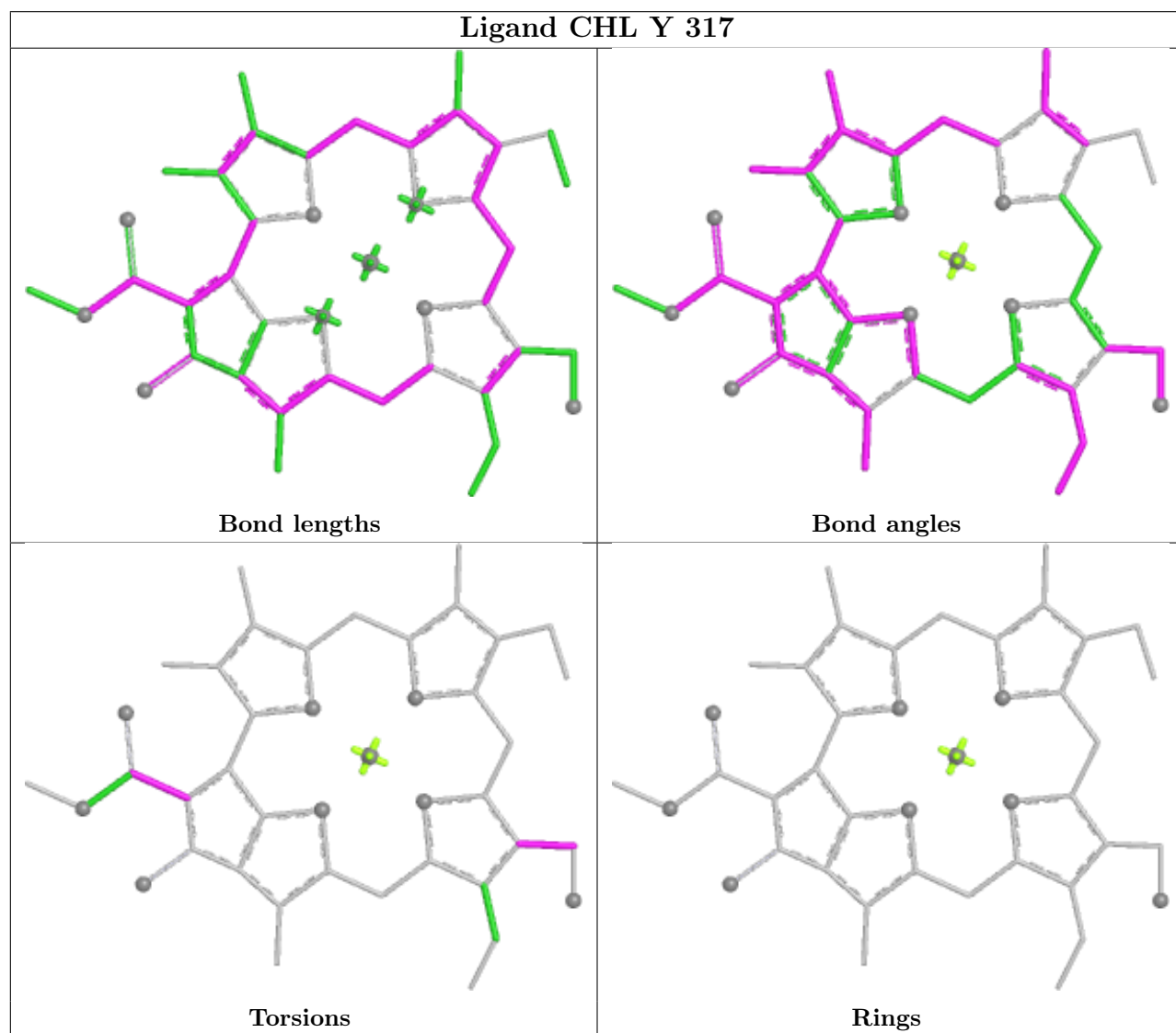
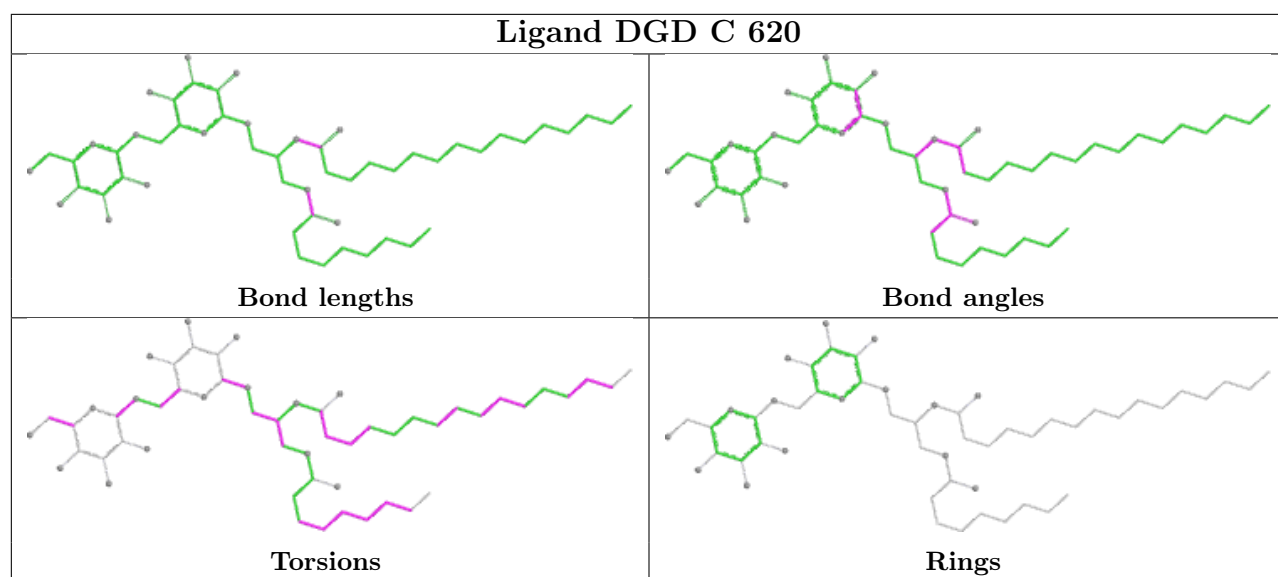
Ligand 8CT t 101



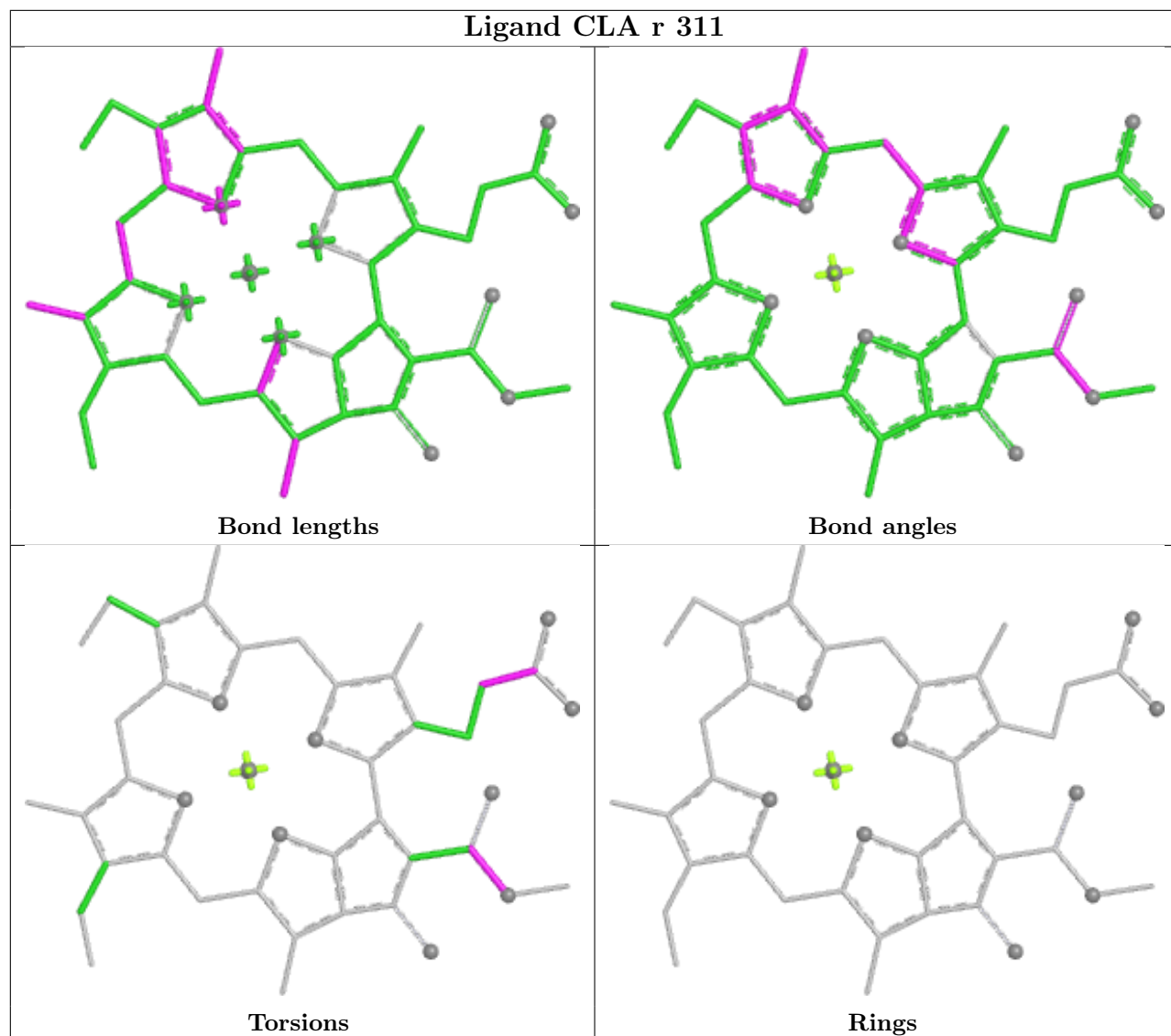




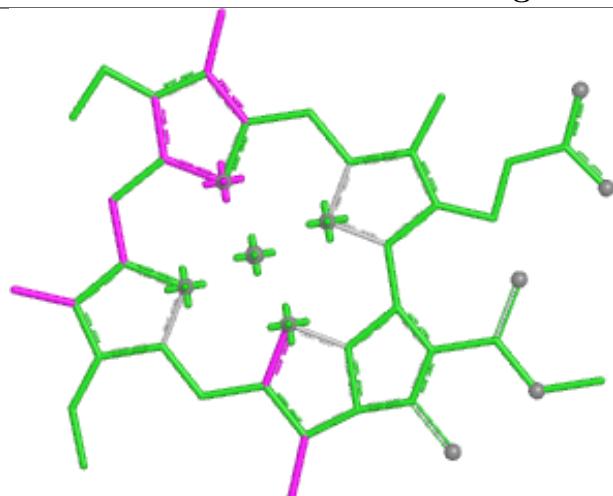




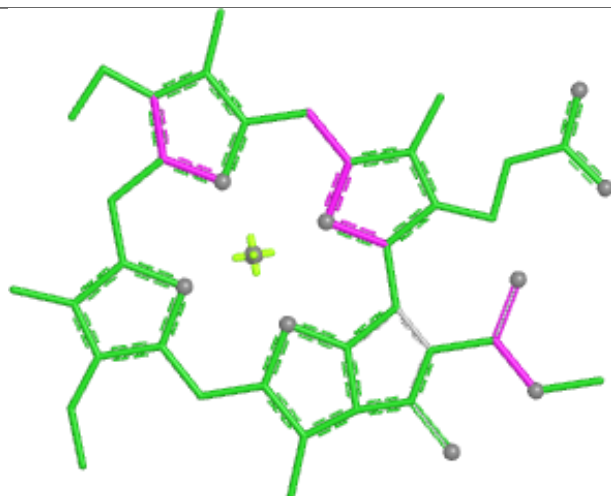
Ligand CLA r 311



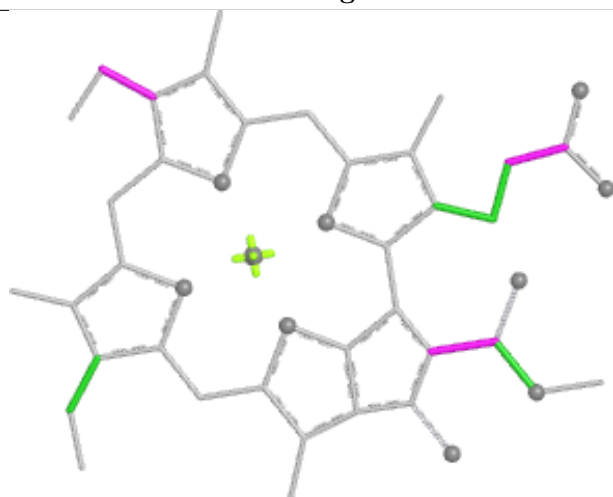
Ligand CLA G 316



Bond lengths



Bond angles

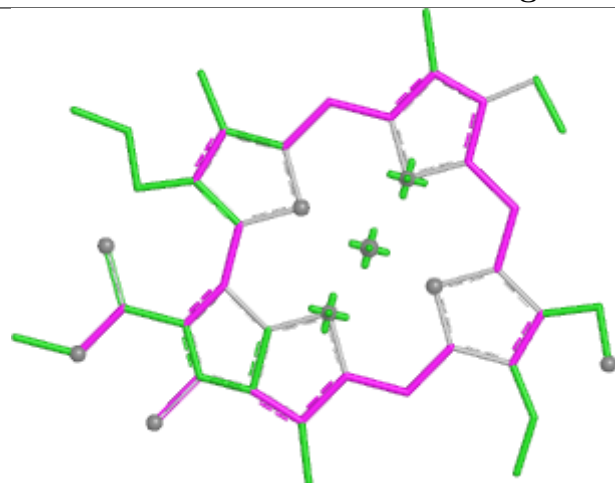


Torsions

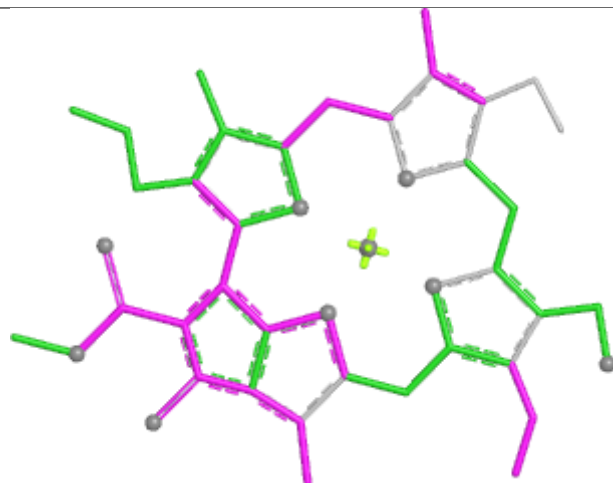


Rings

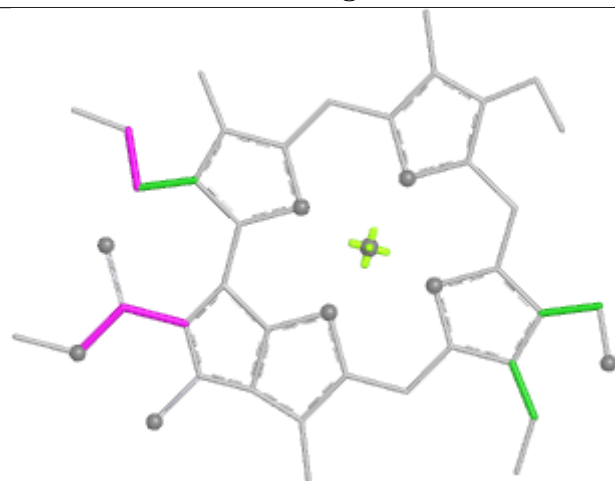
Ligand CHL 6 311



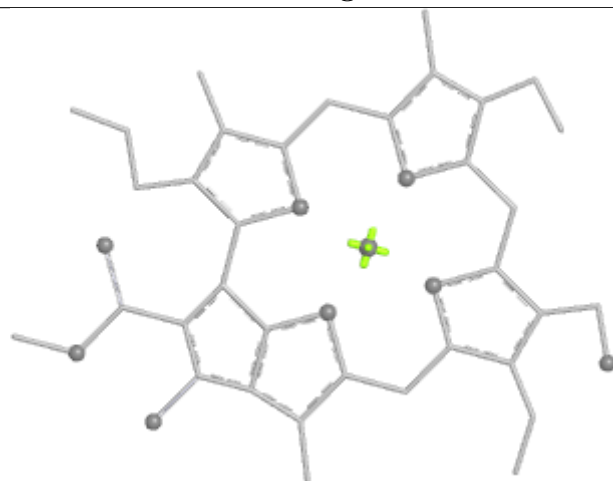
Bond lengths



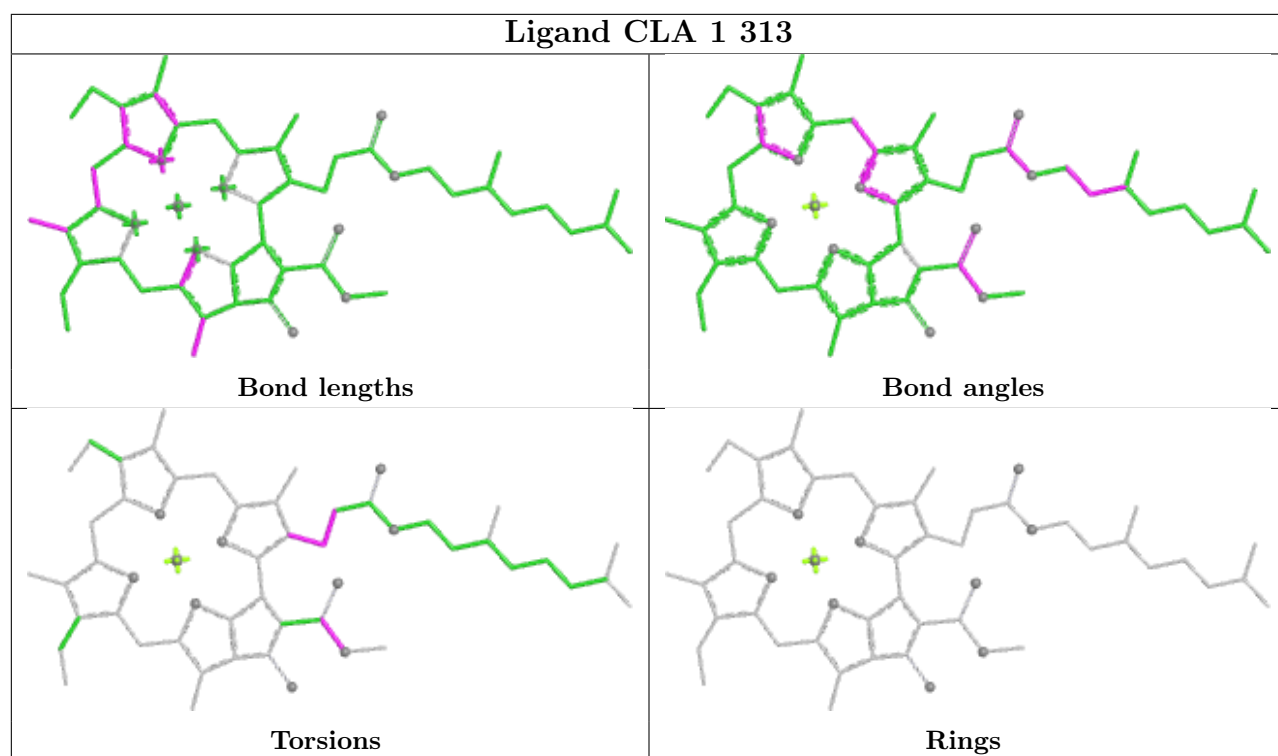
Bond angles



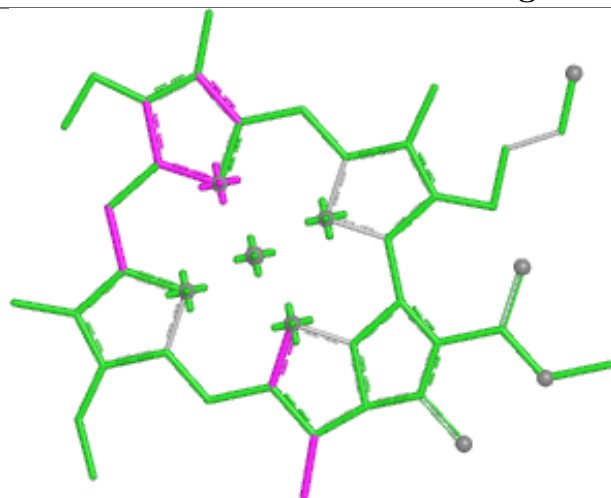
Torsions



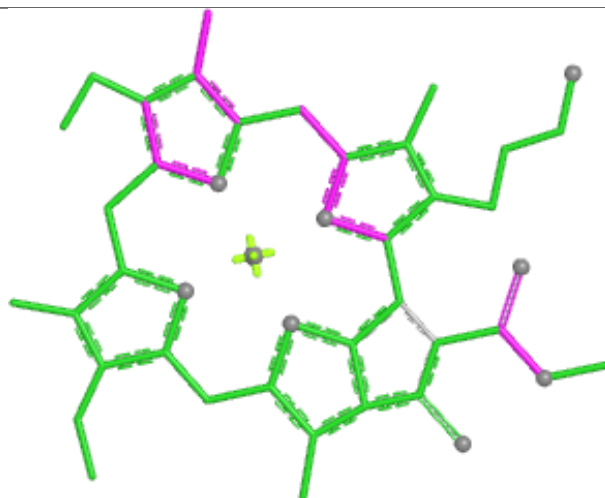
Rings



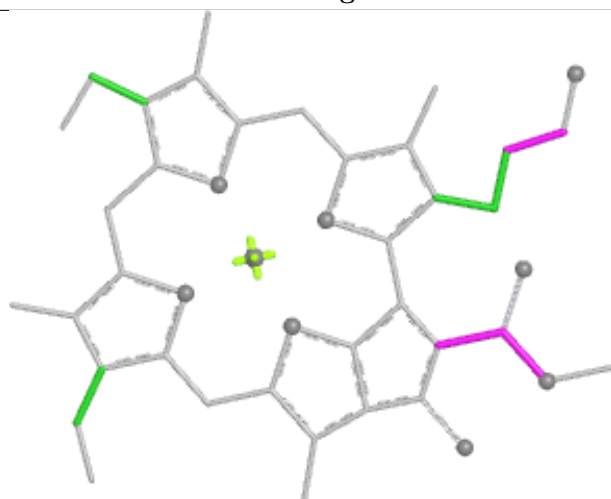
Ligand CLA 1 306



Bond lengths



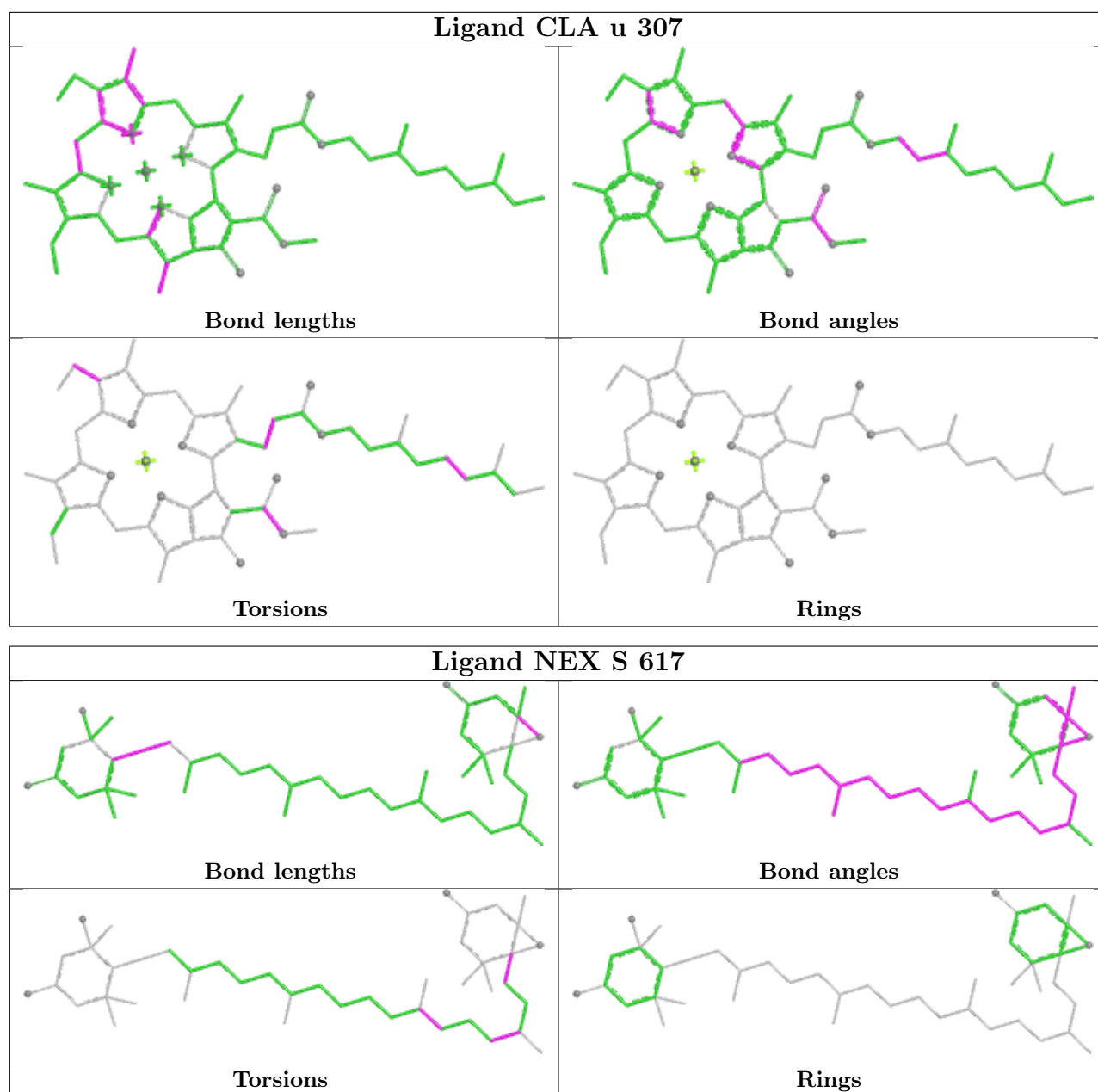
Bond angles

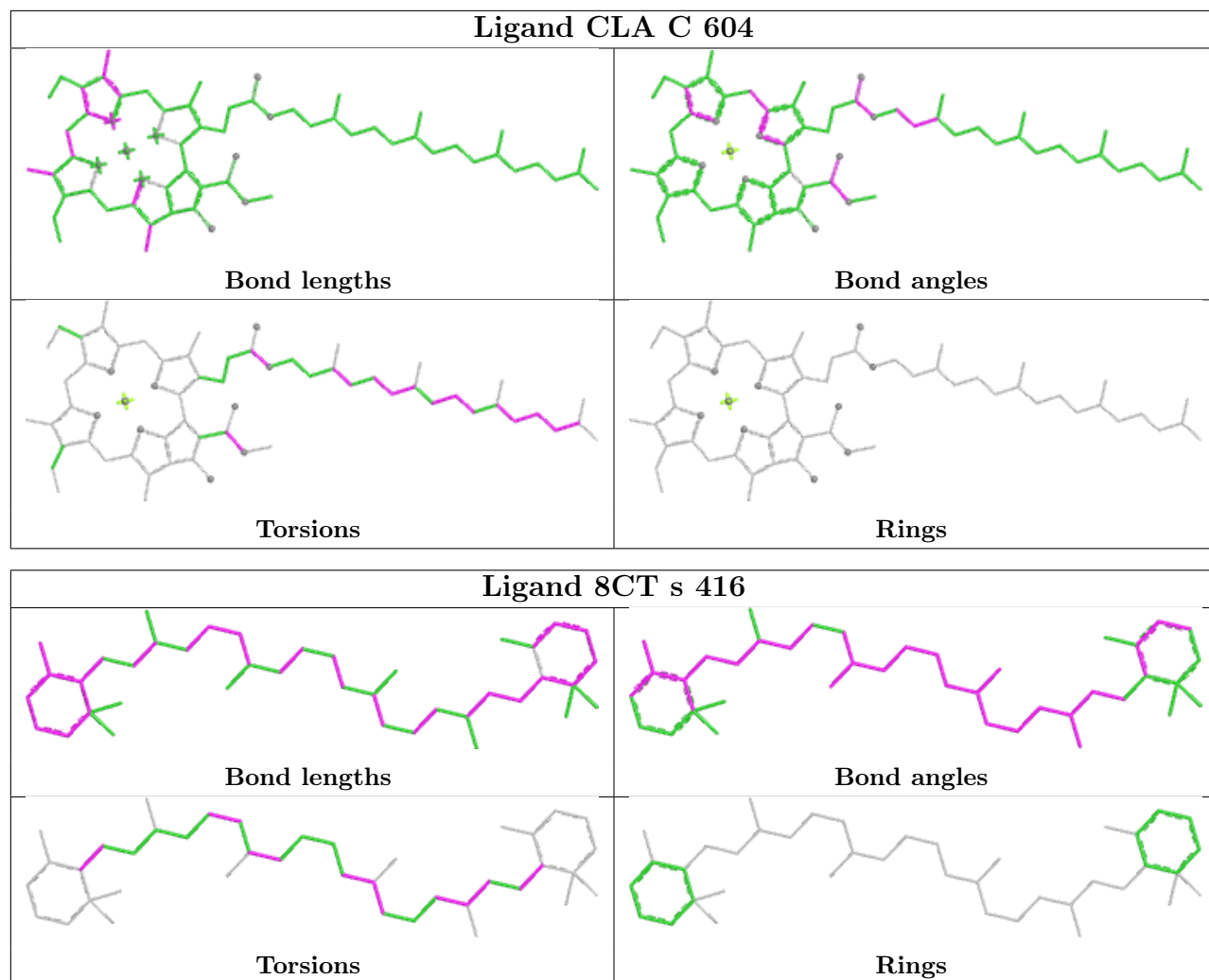


Torsions

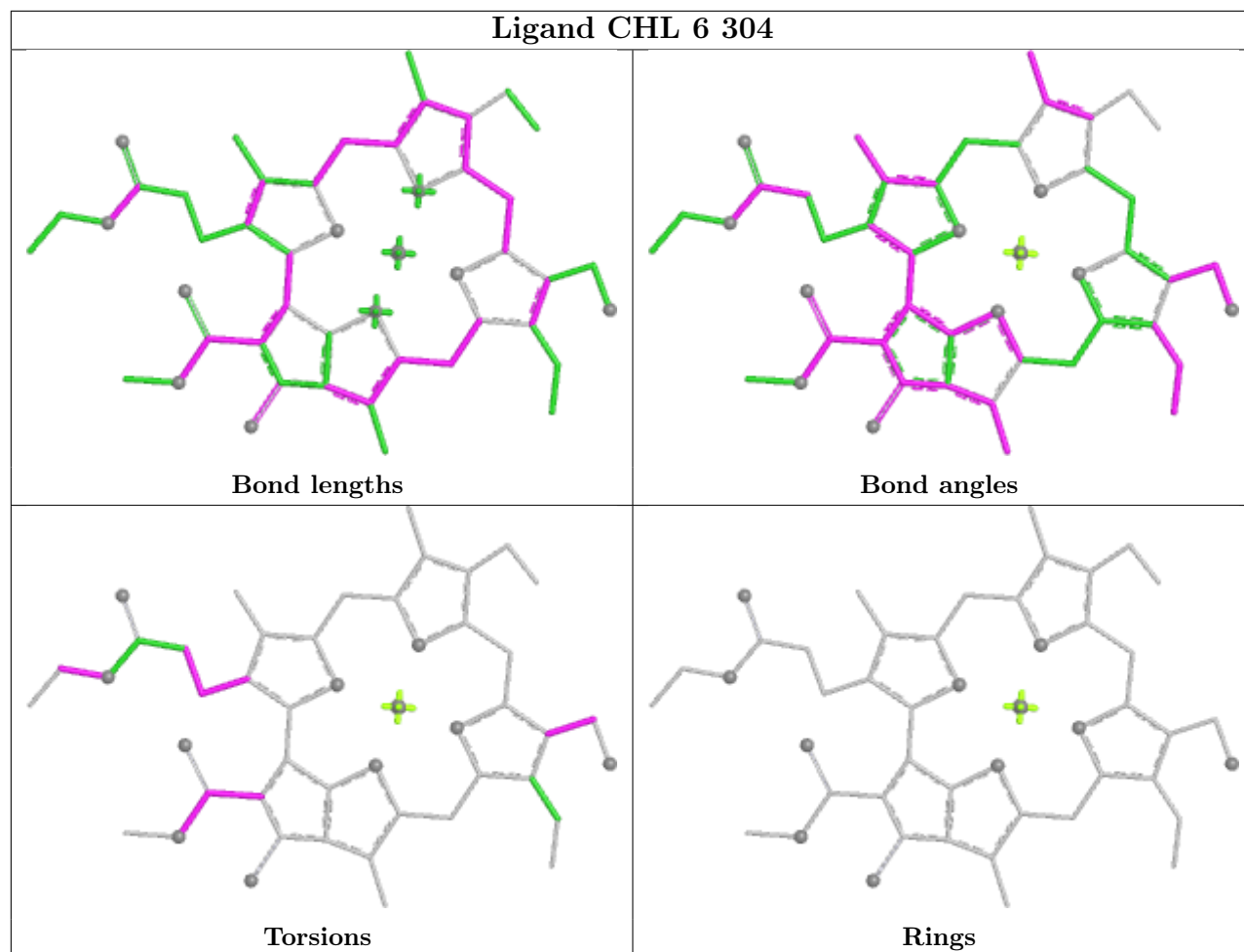


Rings

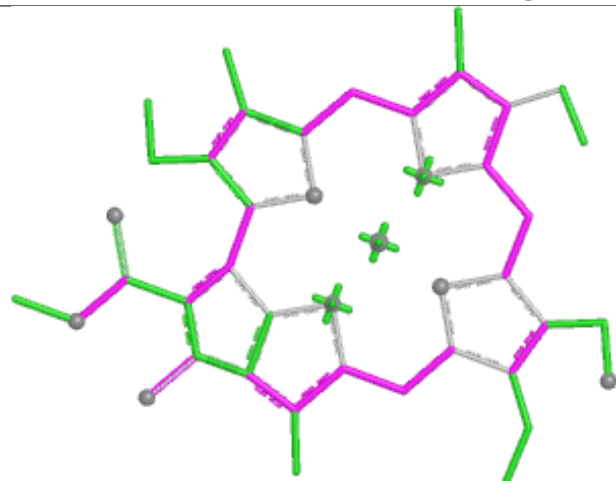




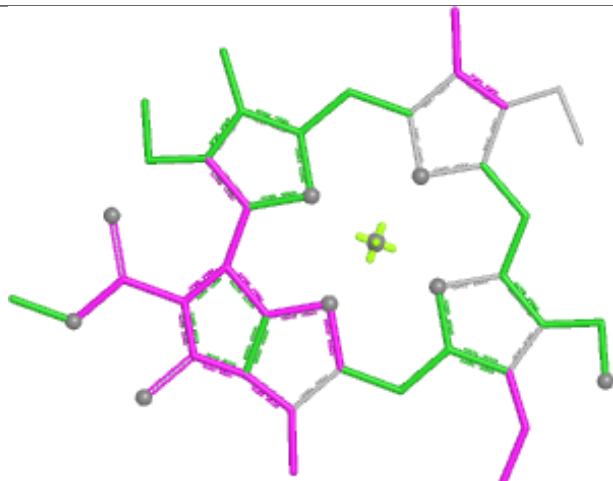
Ligand CHL 6 304



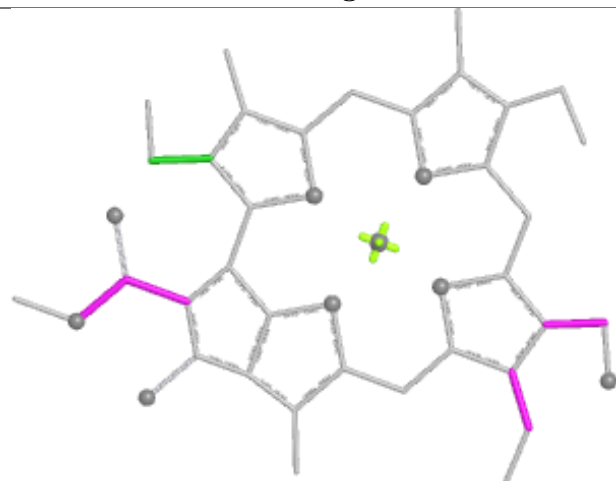
Ligand CHL 3 312



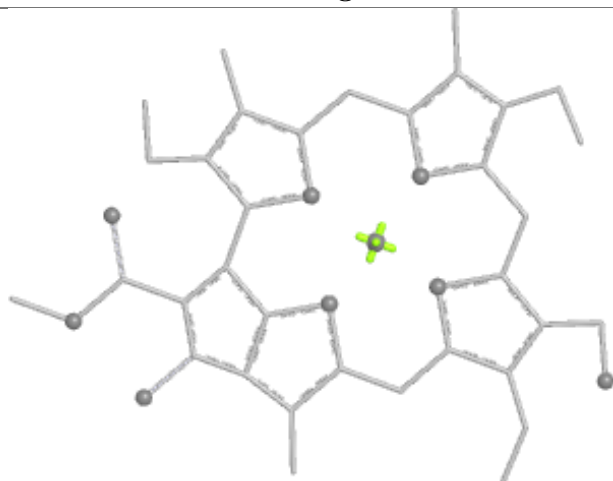
Bond lengths



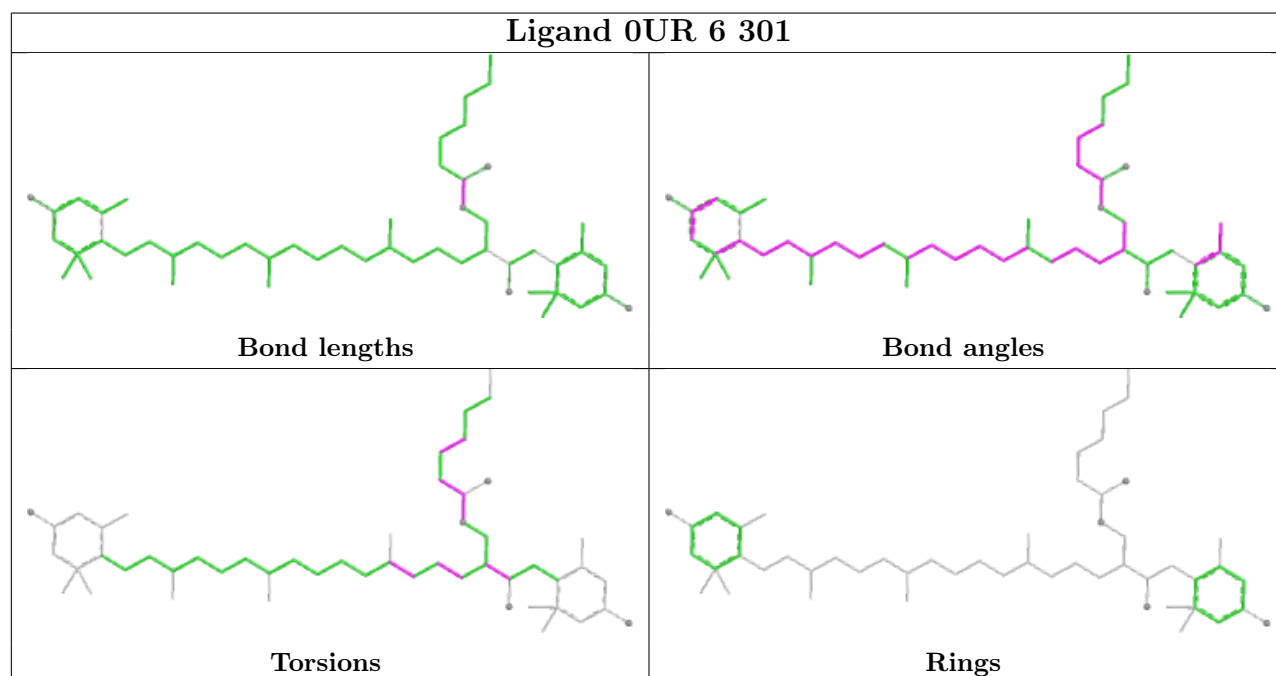
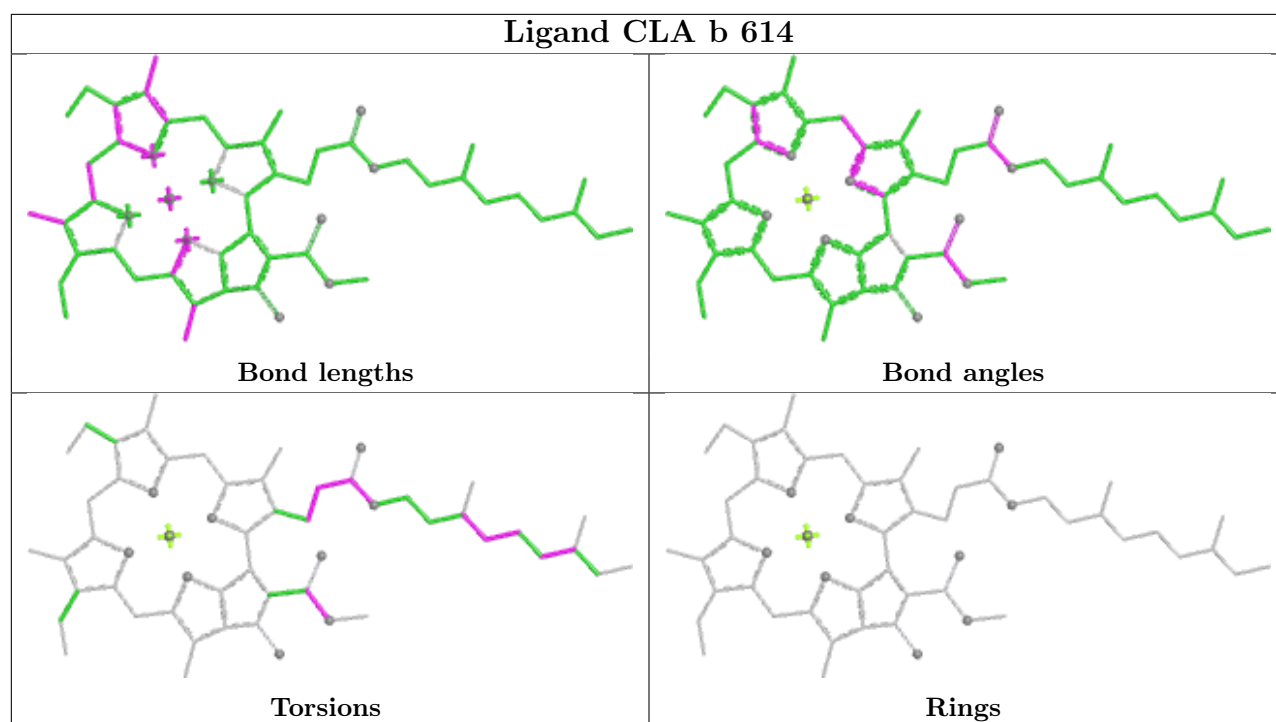
Bond angles

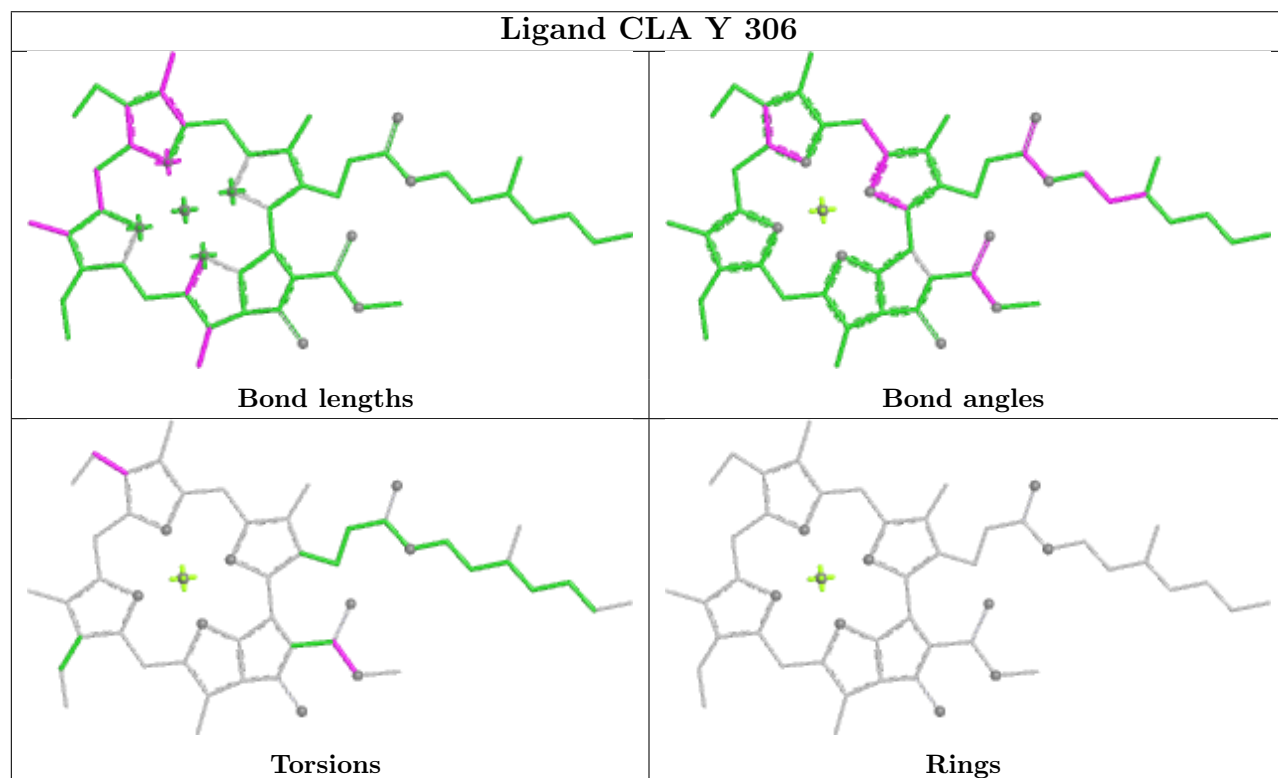
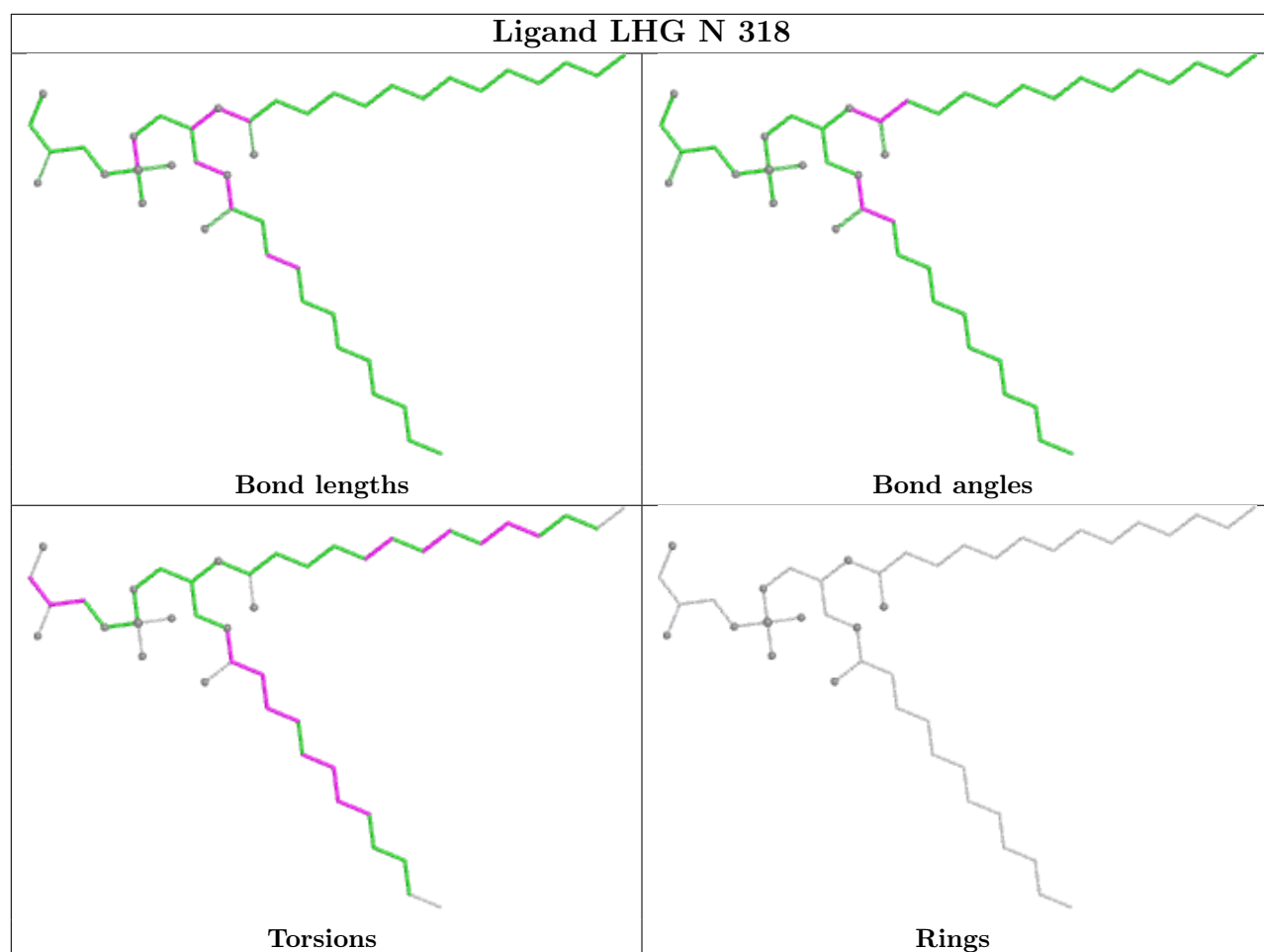


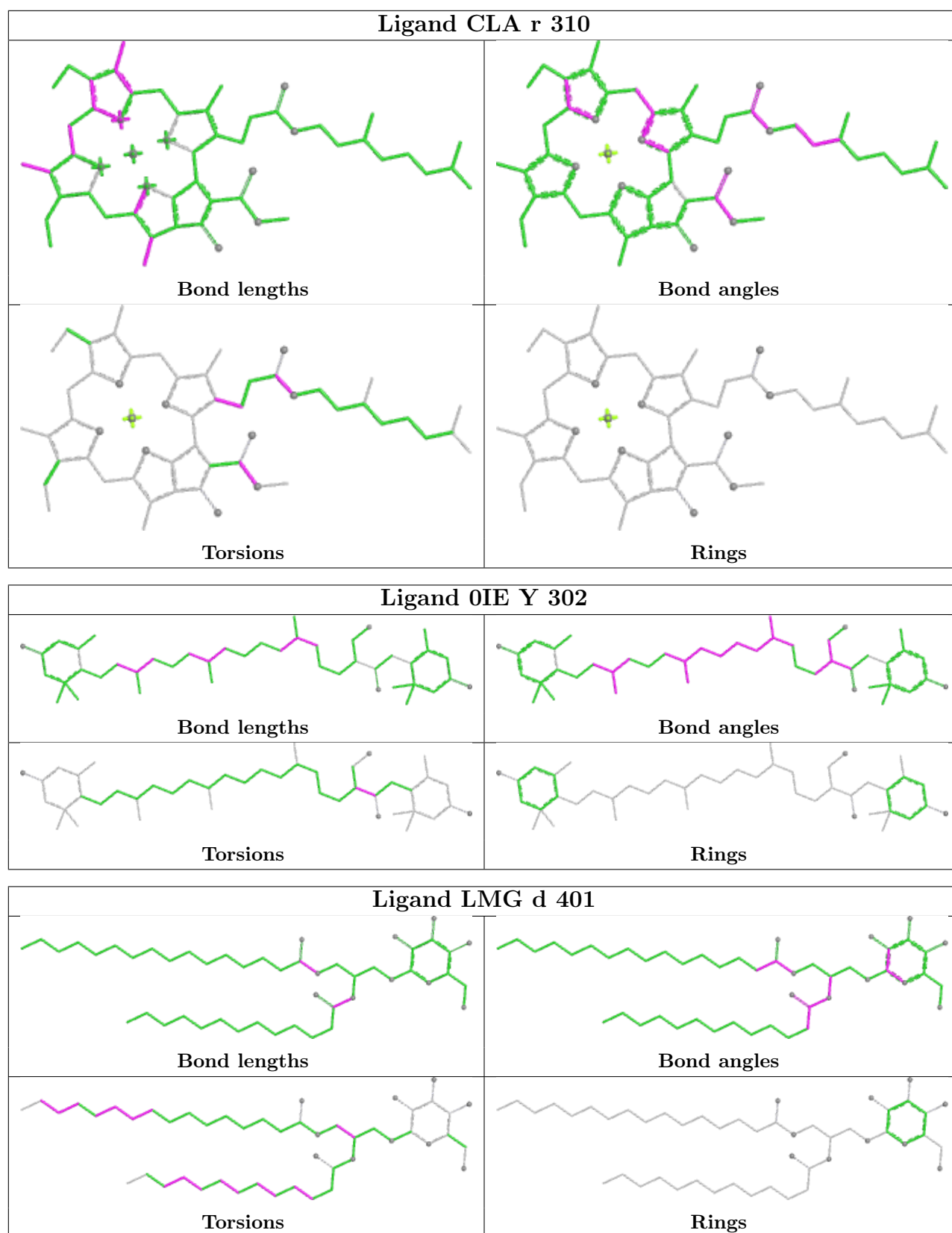
Torsions



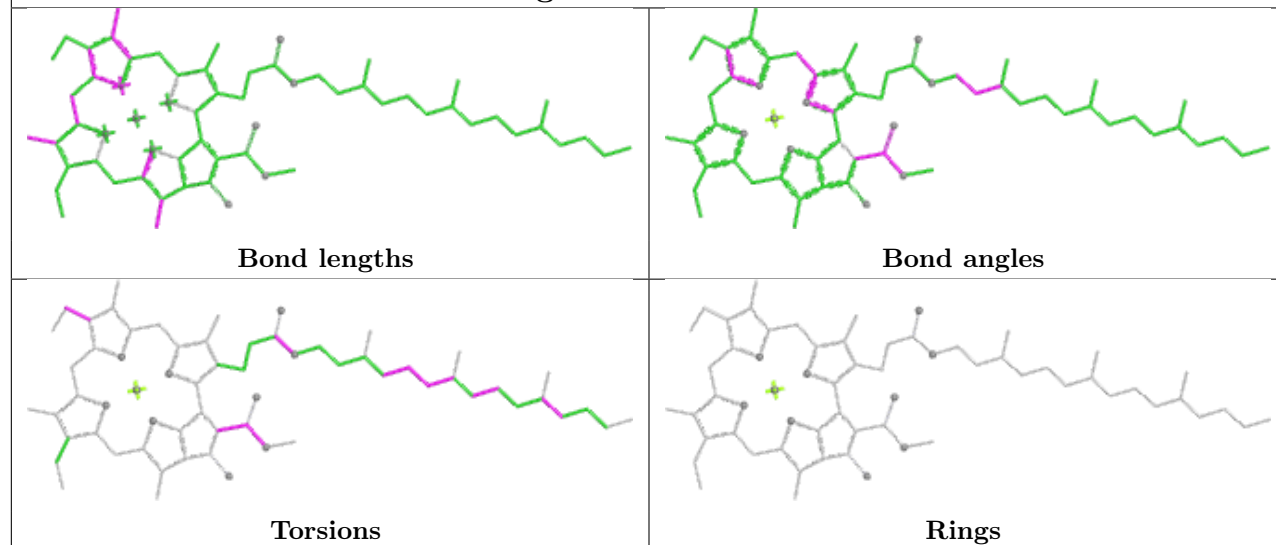
Rings



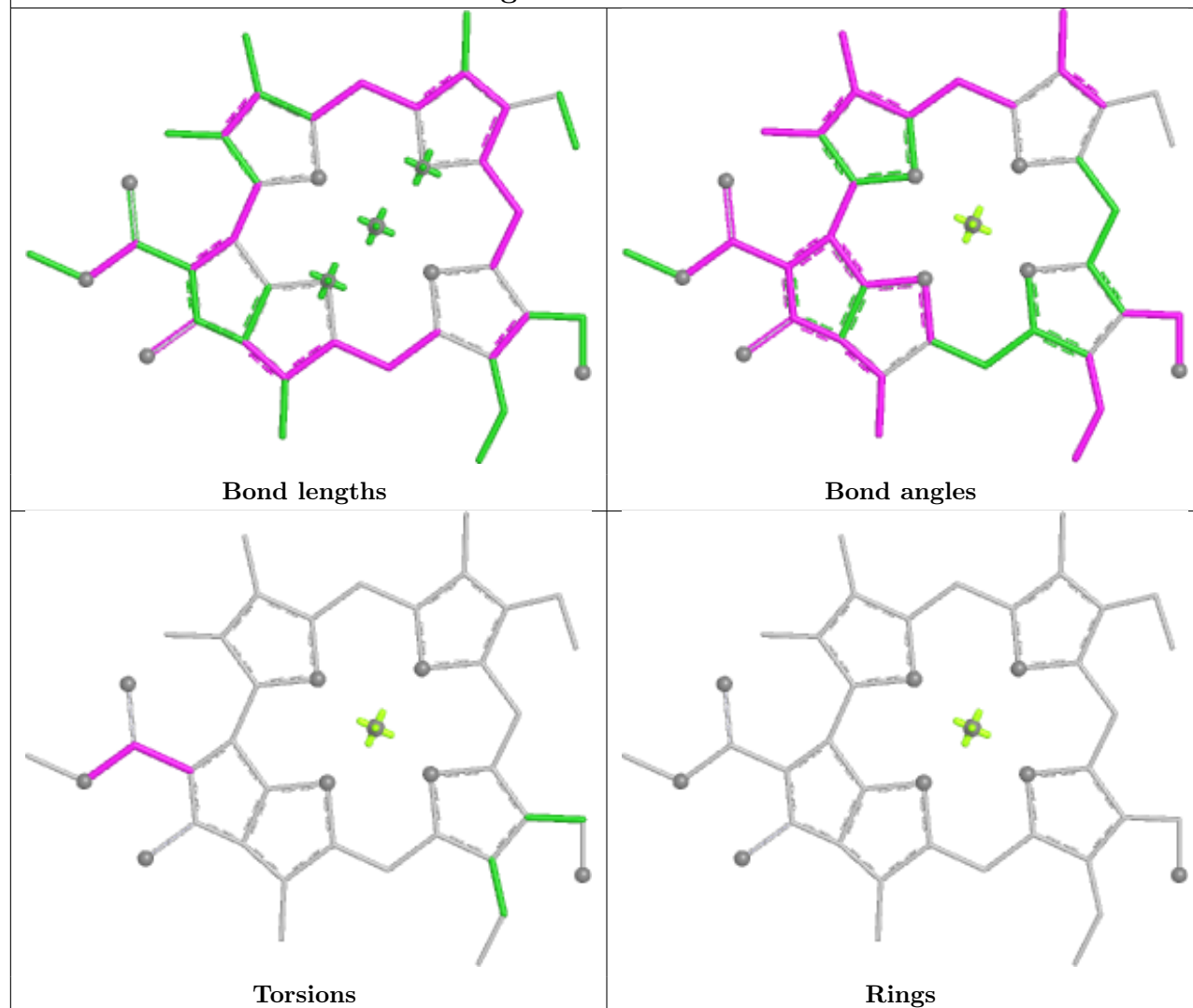




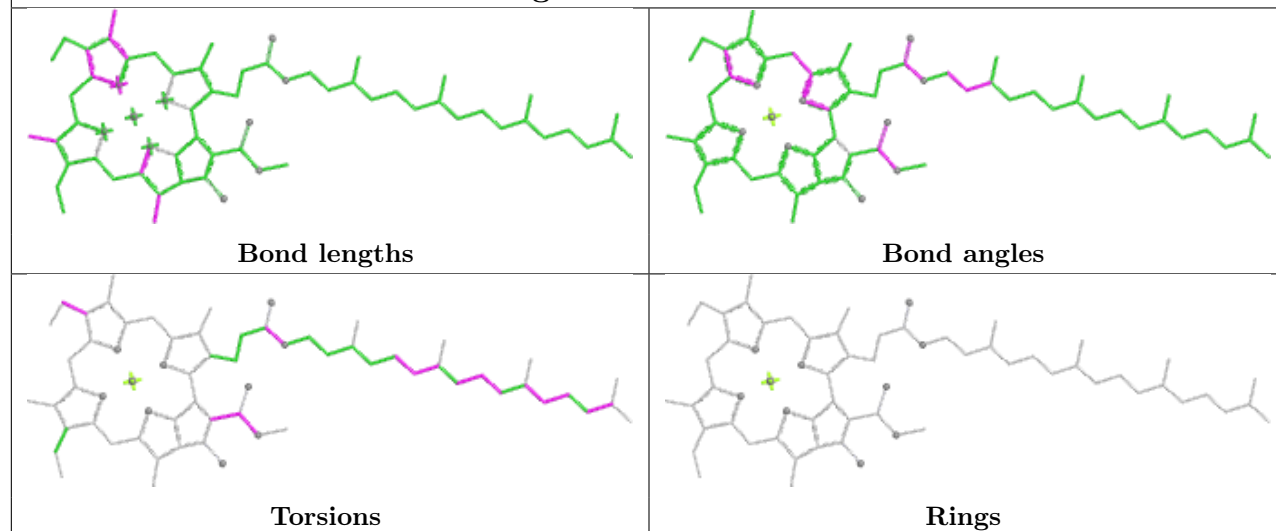
Ligand CLA 7 315



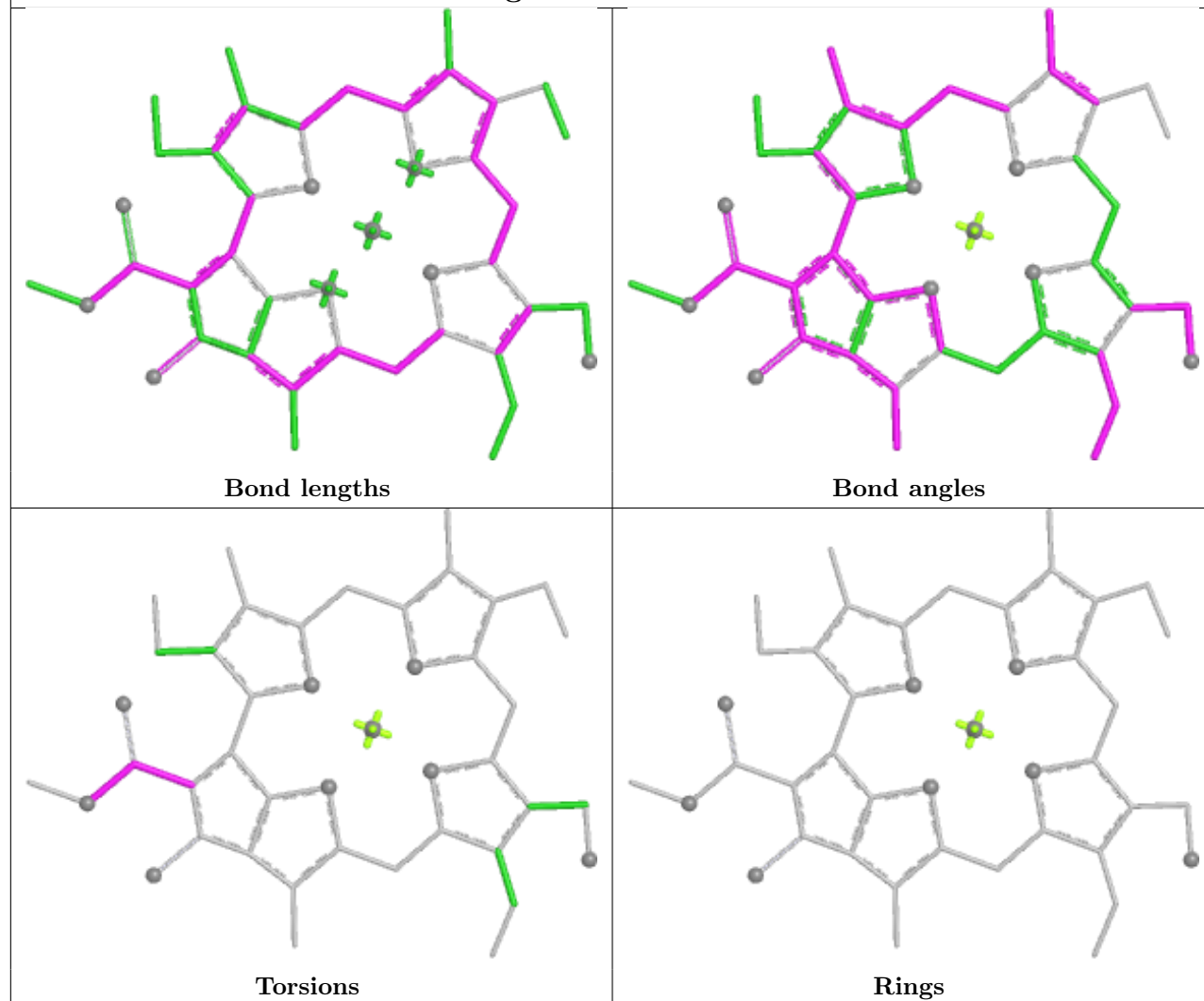
Ligand CHL 2 318

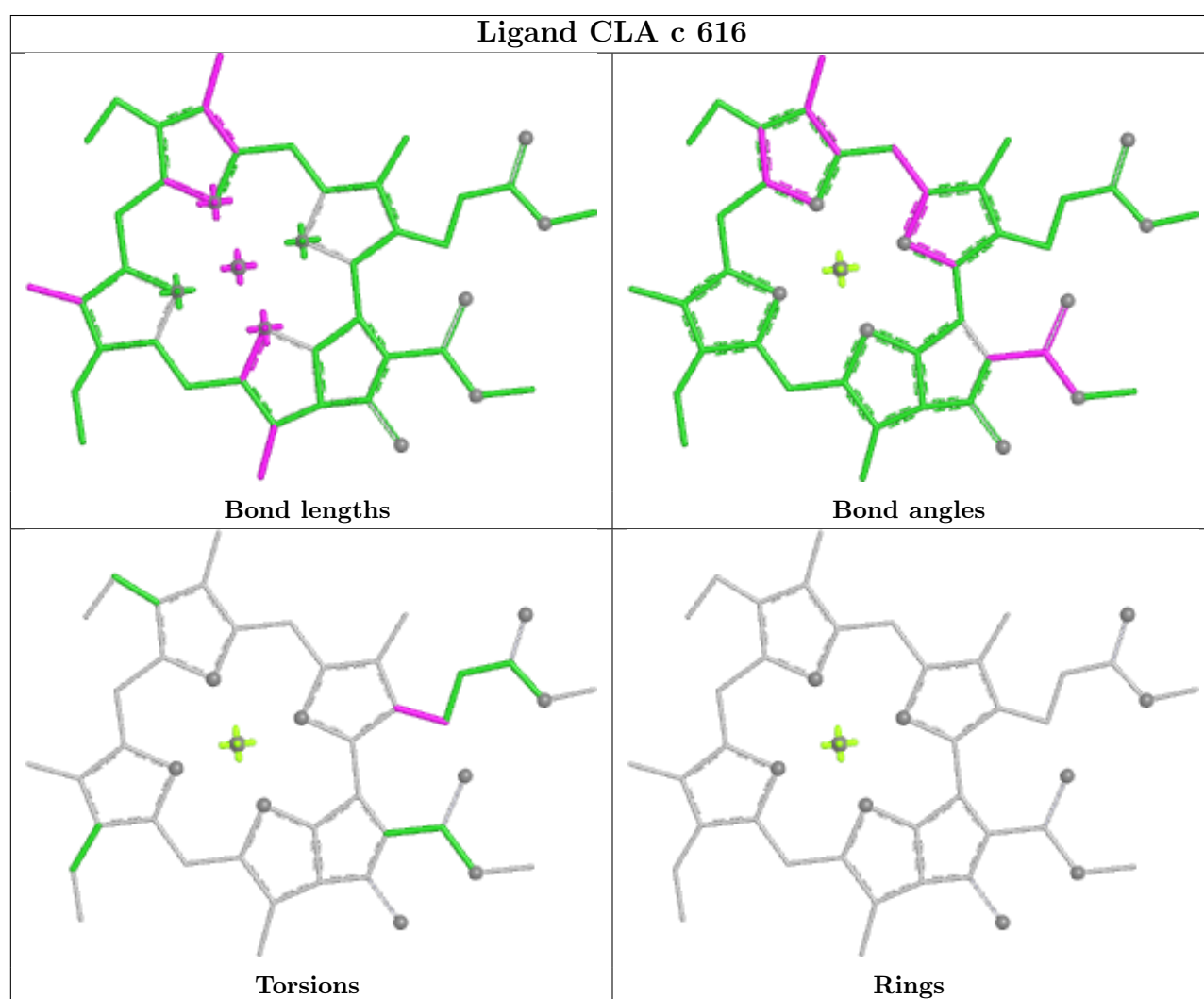
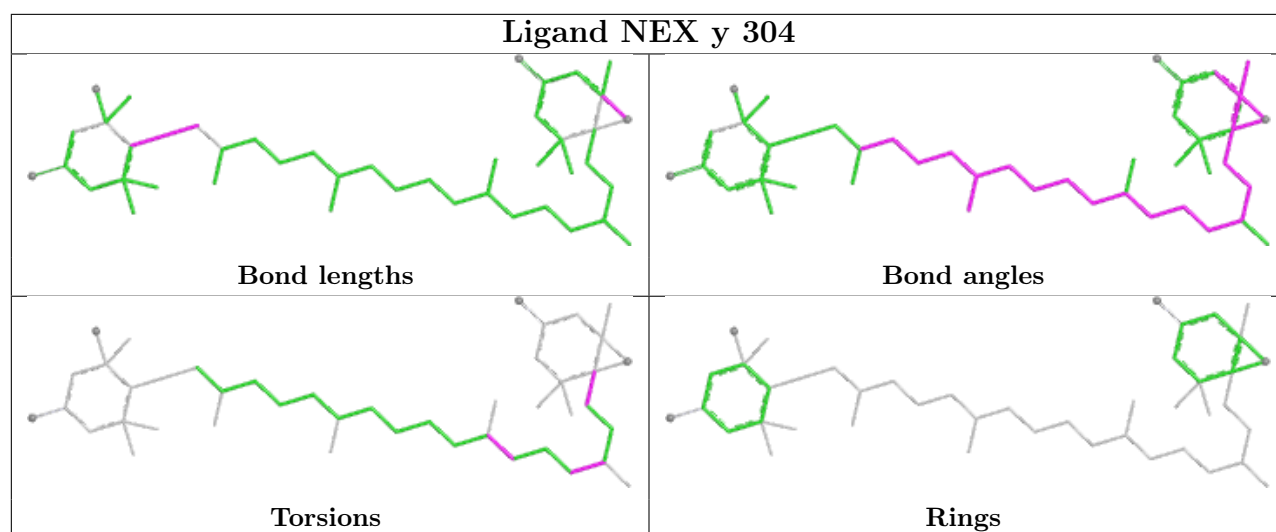


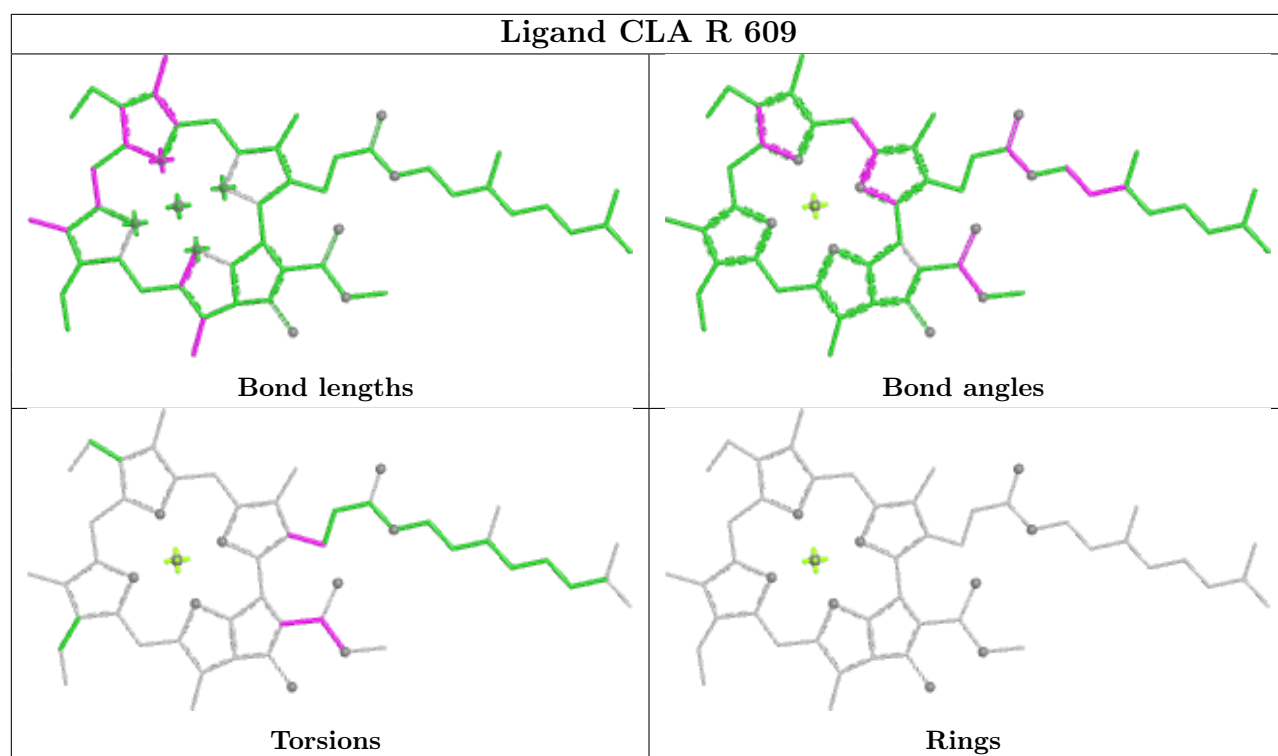
Ligand CLA C 602



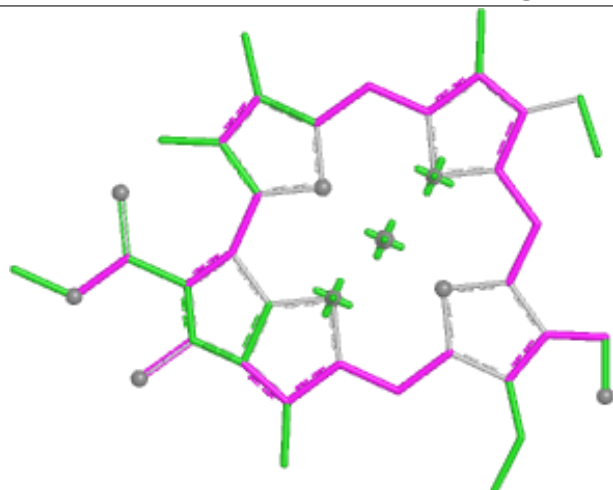
Ligand CHL 2 309



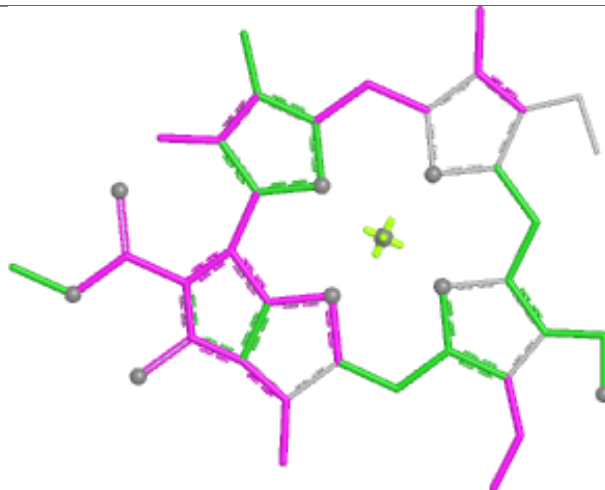




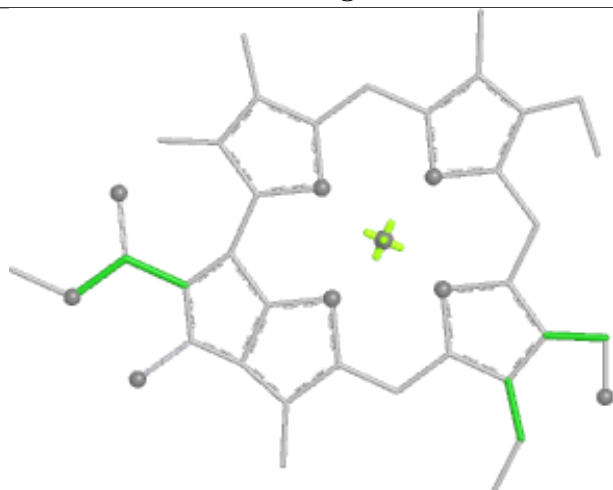
Ligand CHL 8 315



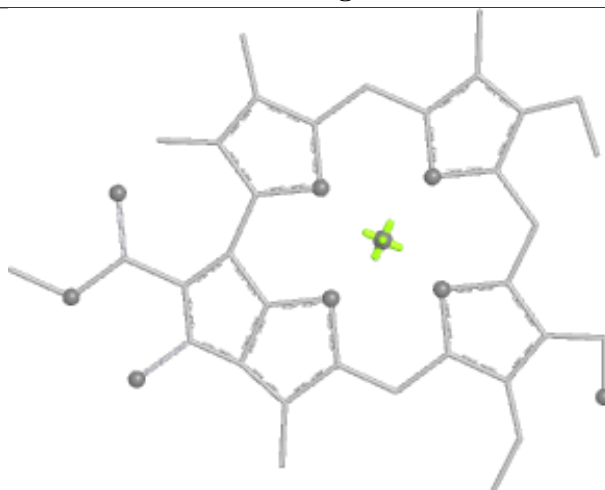
Bond lengths



Bond angles

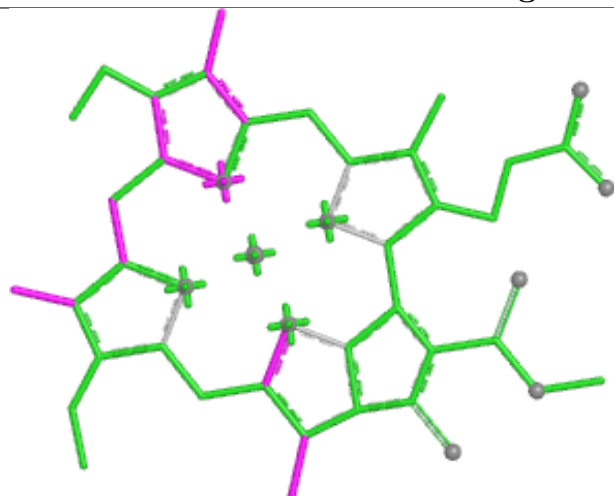


Torsions

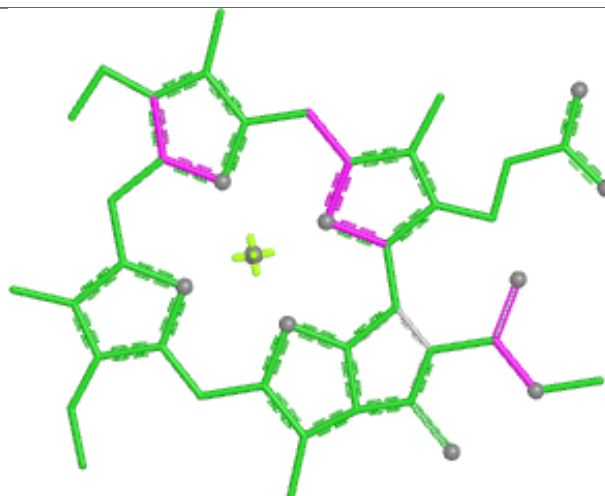


Rings

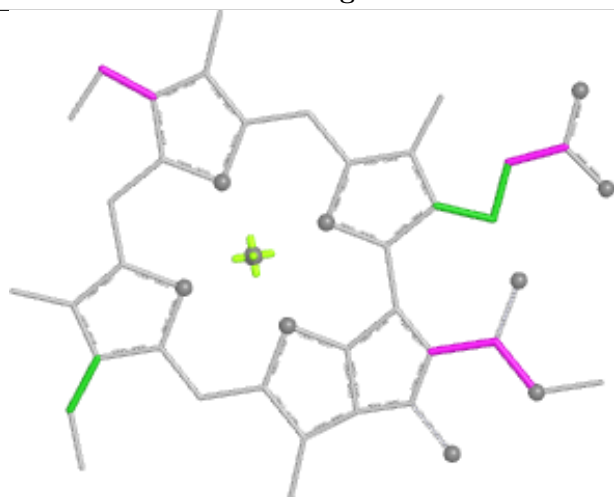
Ligand CLA 3 315



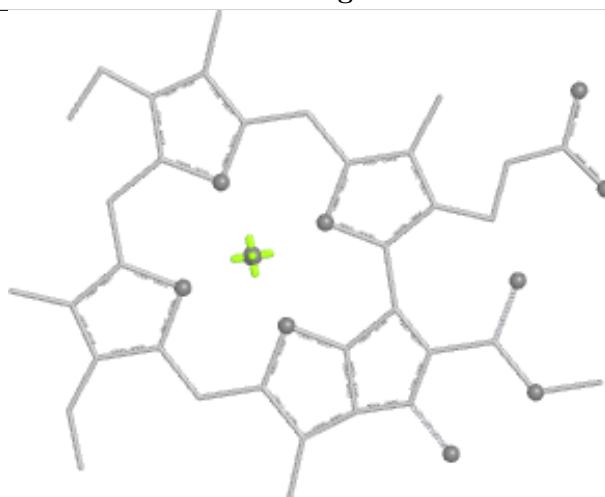
Bond lengths



Bond angles

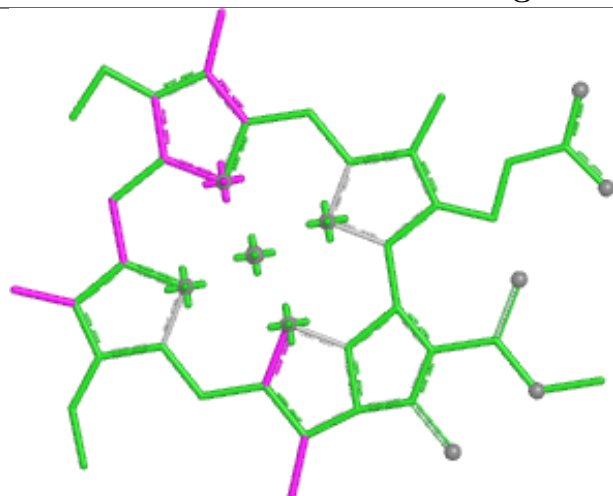


Torsions

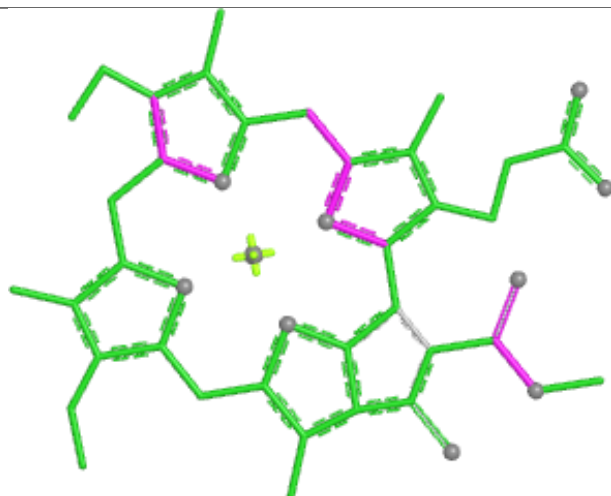


Rings

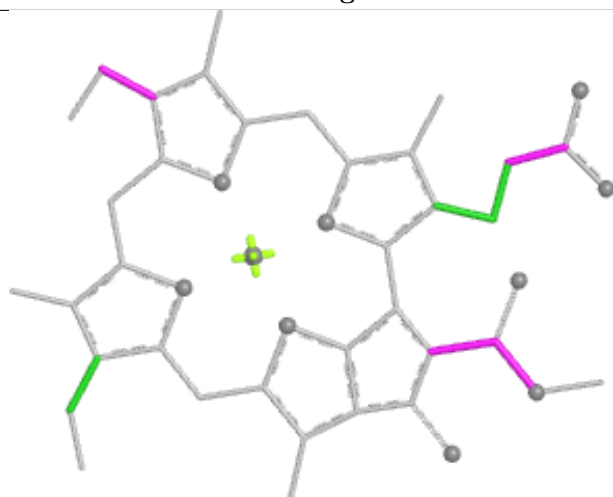
Ligand CLA N 315



Bond lengths



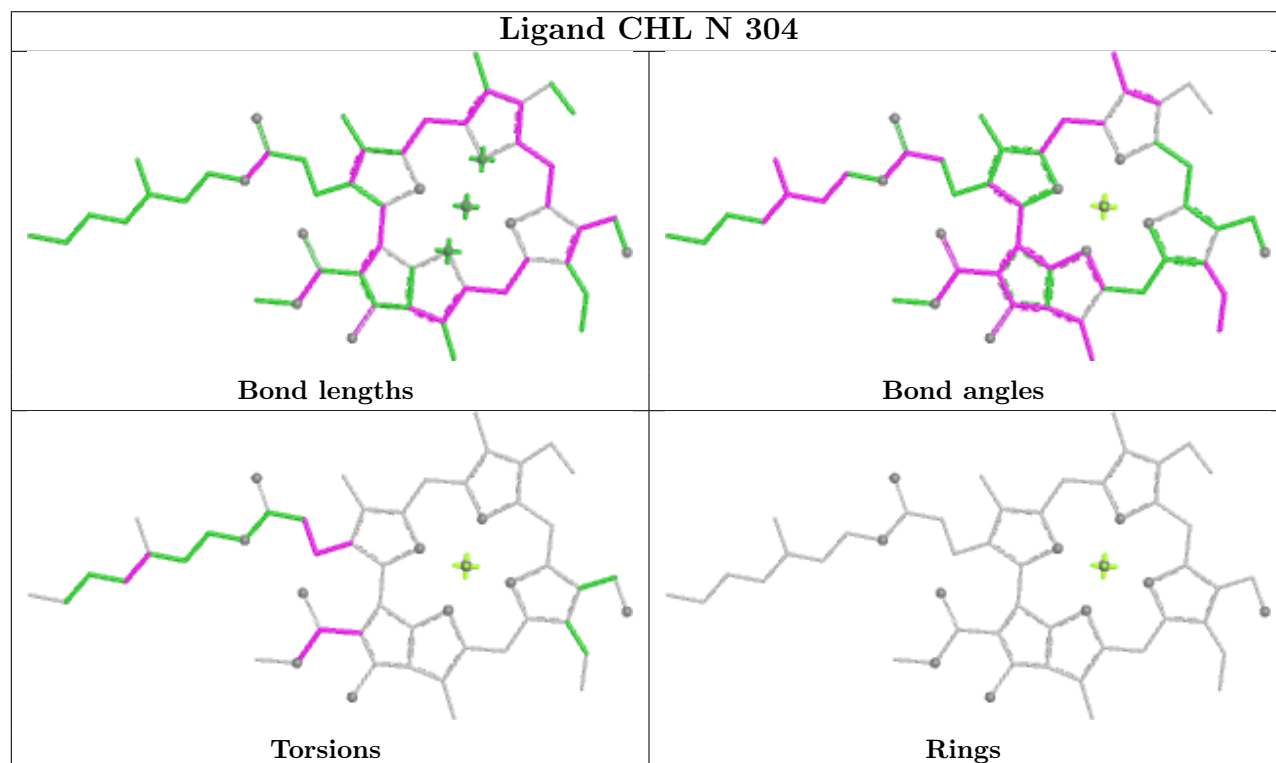
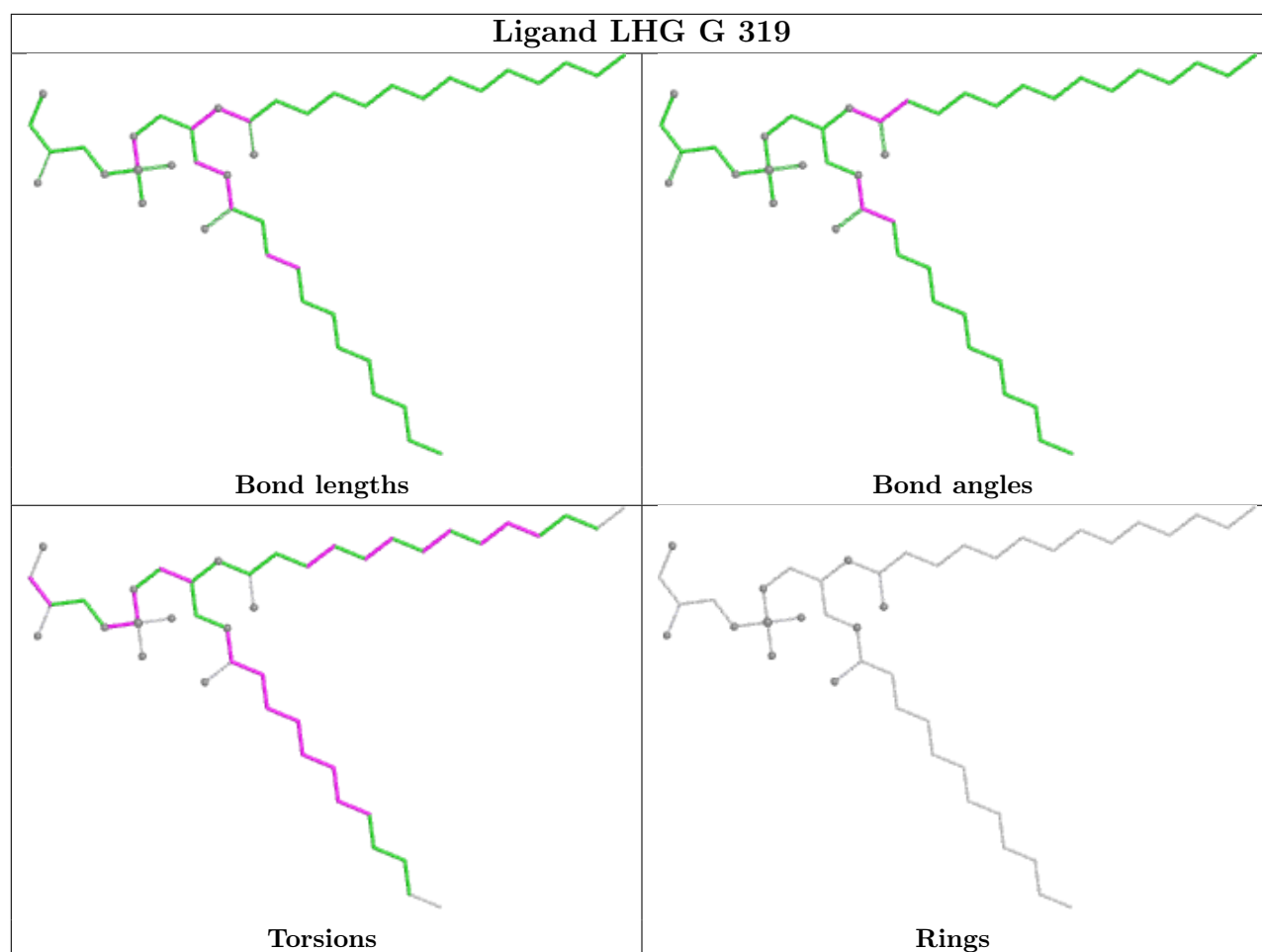
Bond angles

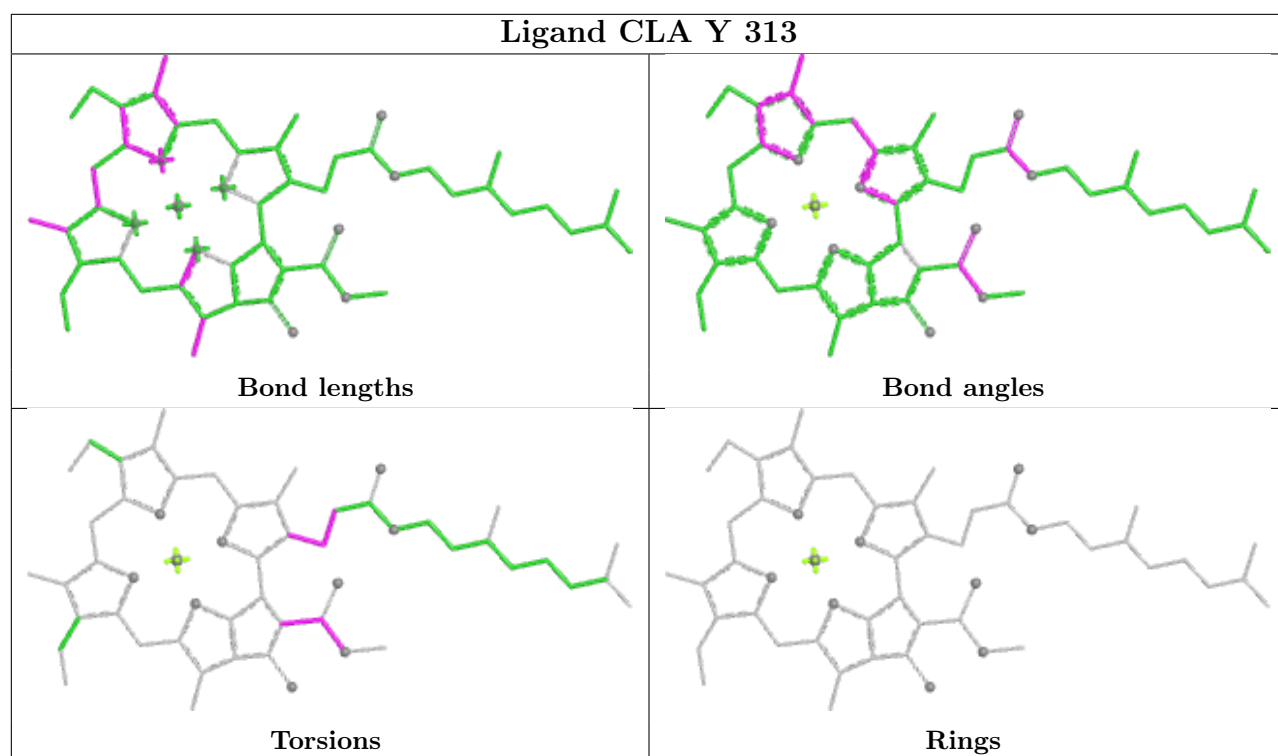


Torsions

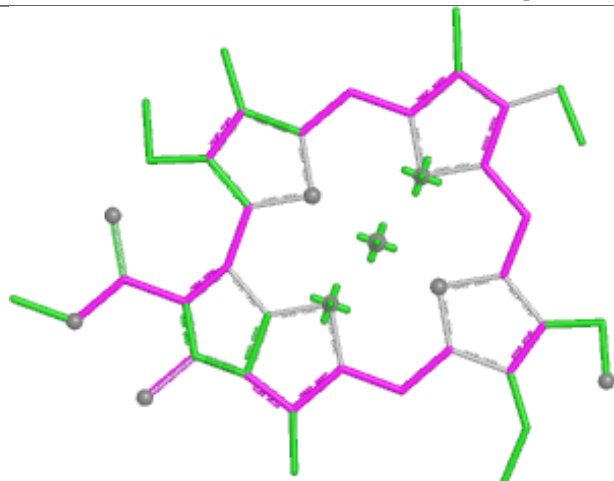


Rings

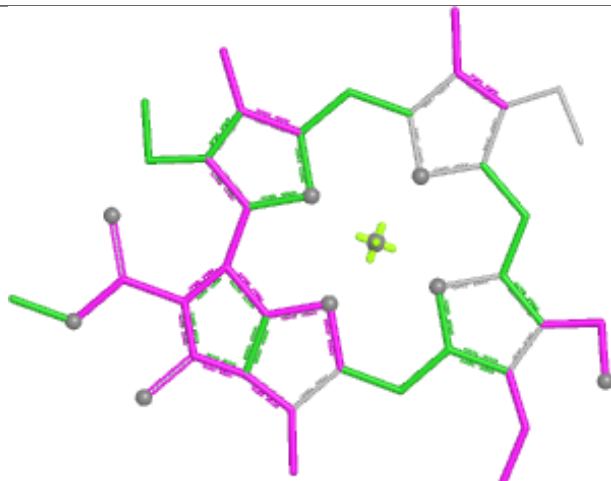




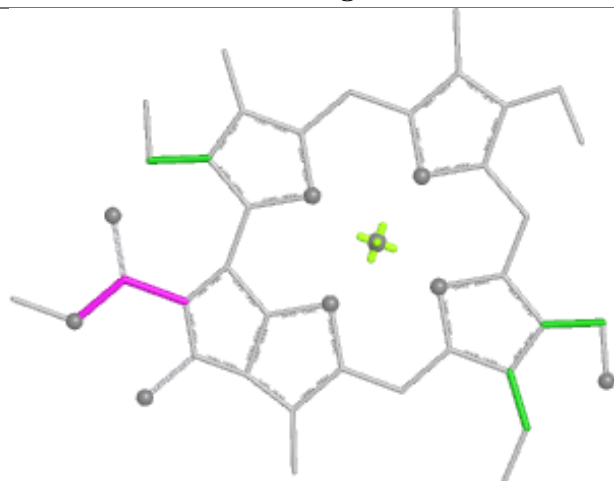
Ligand CHL 1 309



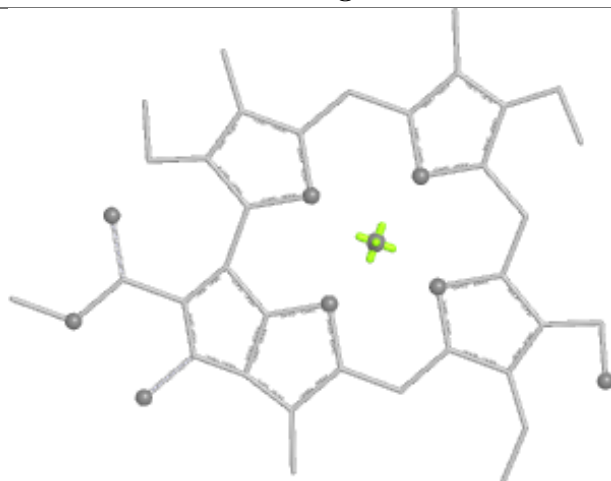
Bond lengths



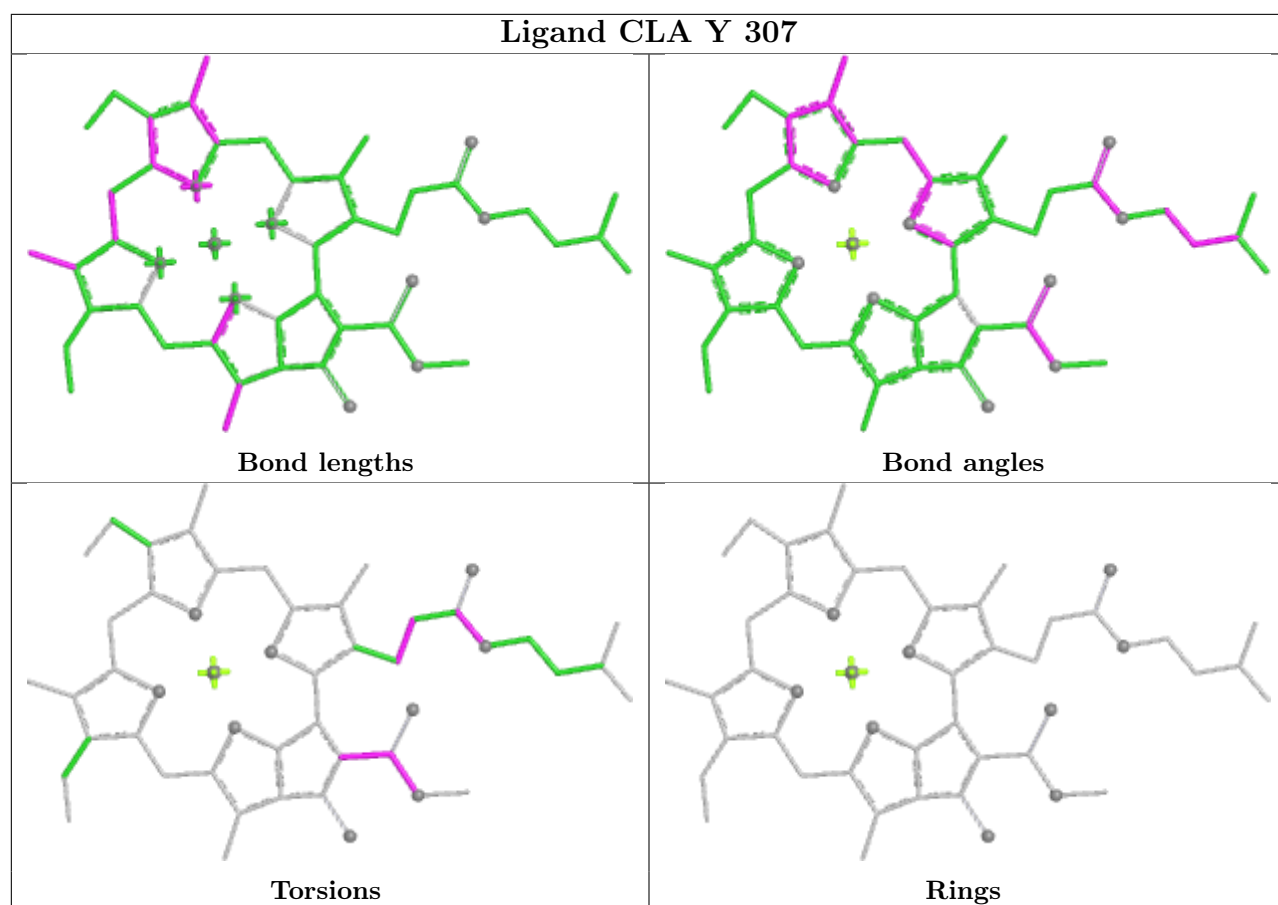
Bond angles



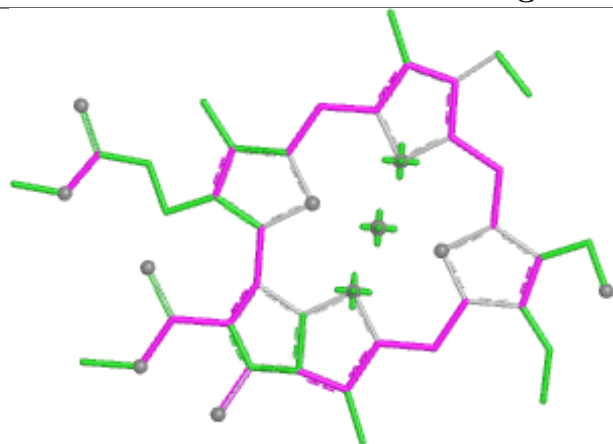
Torsions



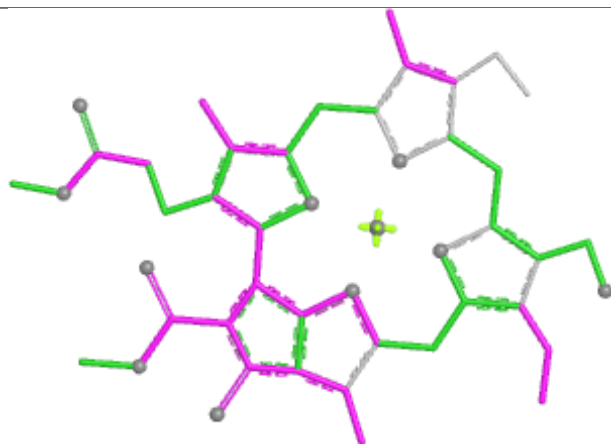
Rings



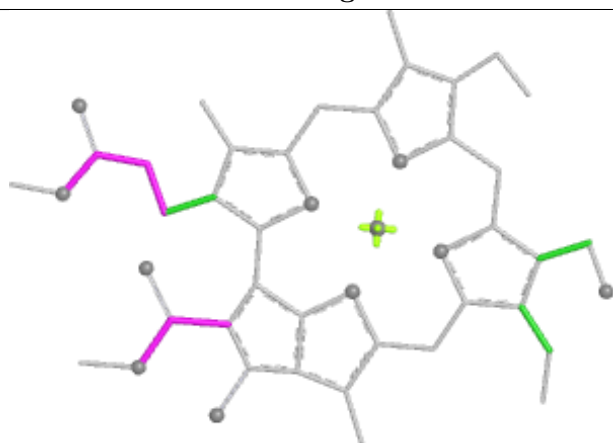
Ligand CHL 5 311



Bond lengths



Bond angles

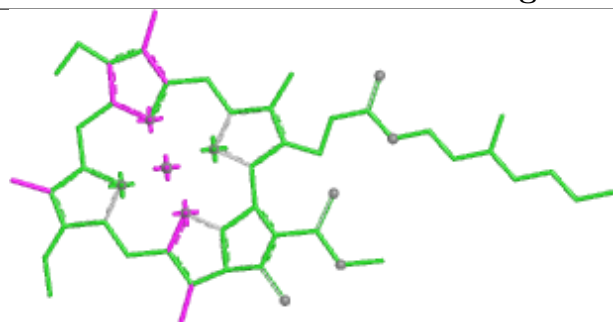


Torsions

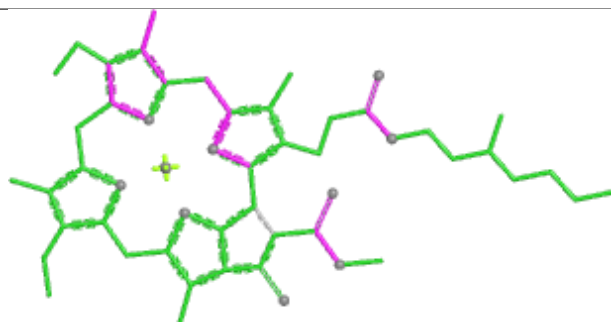


Rings

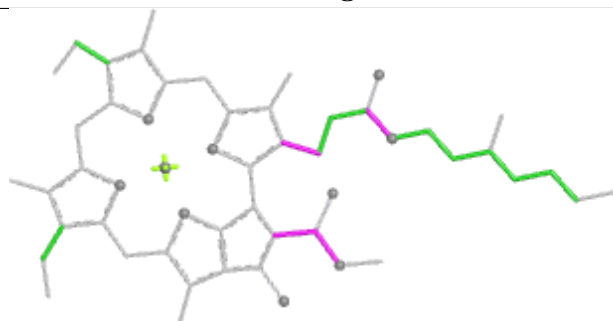
Ligand CLA c 606



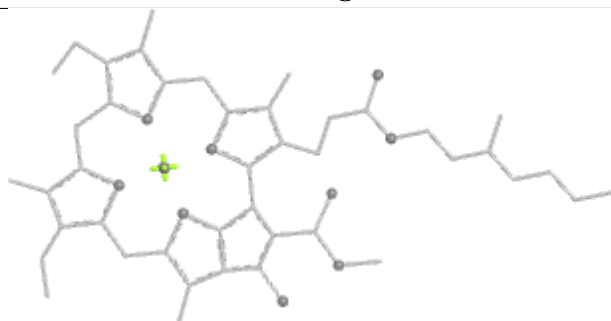
Bond lengths



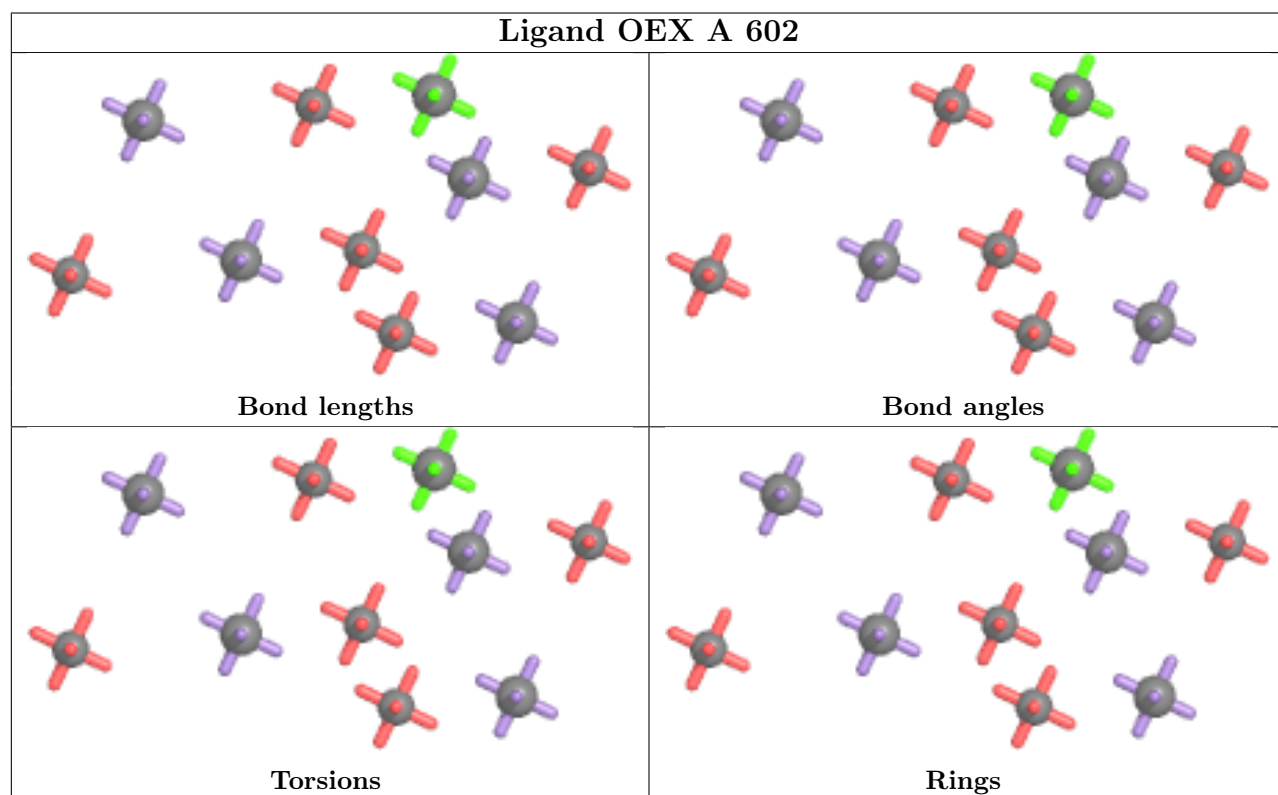
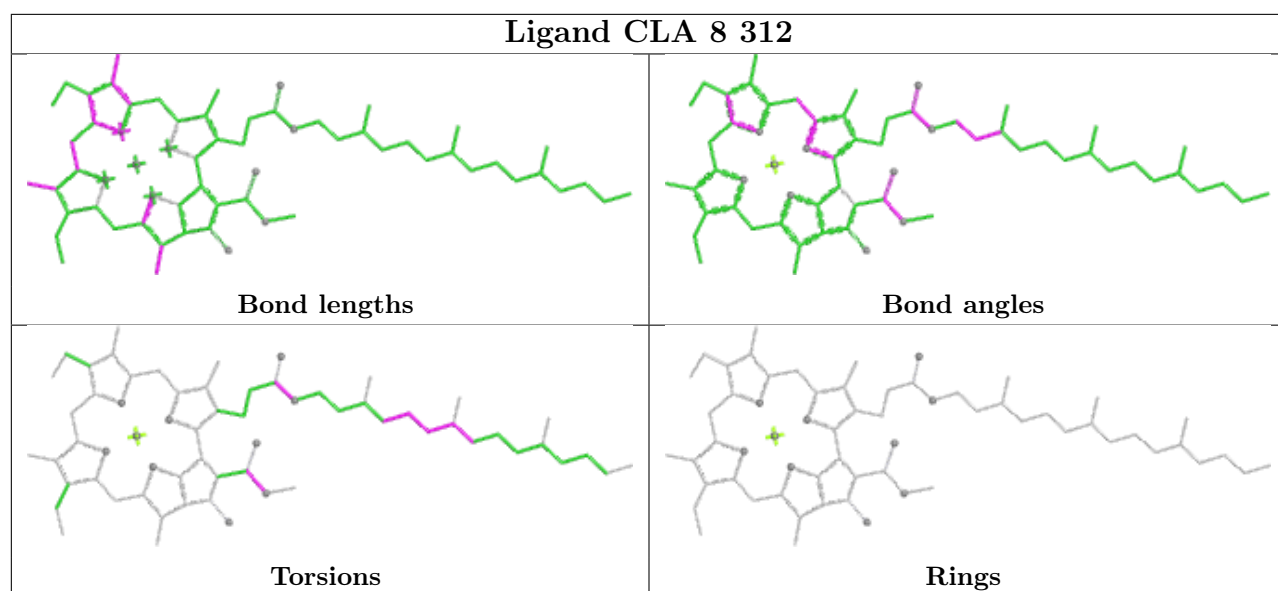
Bond angles



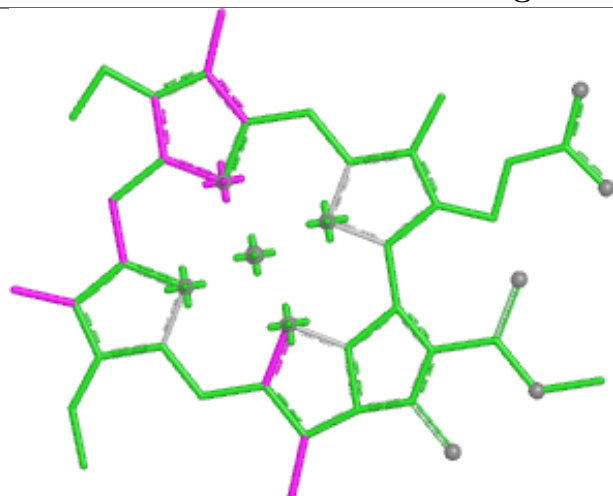
Torsions



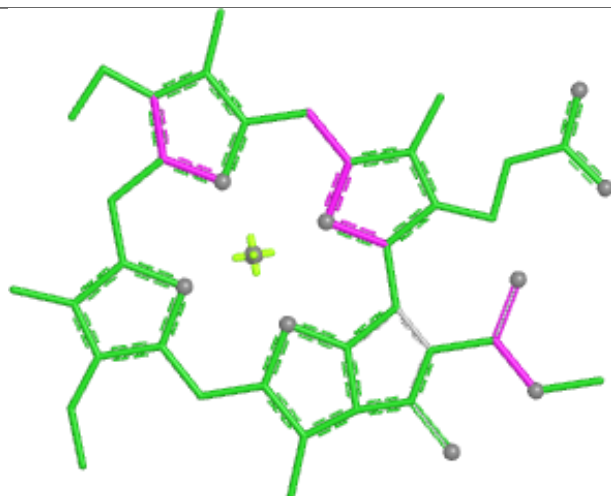
Rings



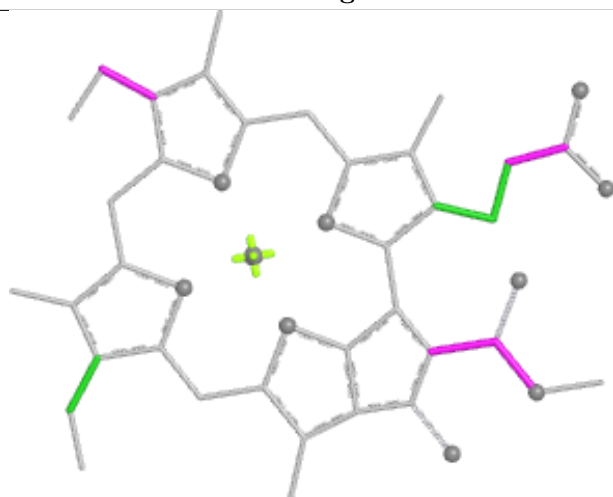
Ligand CLA R 611



Bond lengths



Bond angles

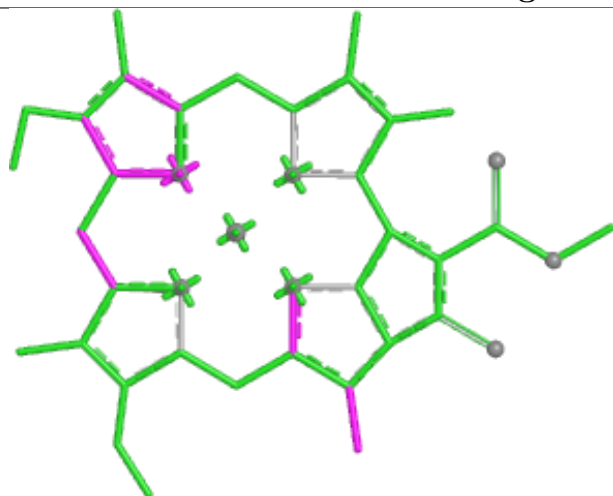


Torsions

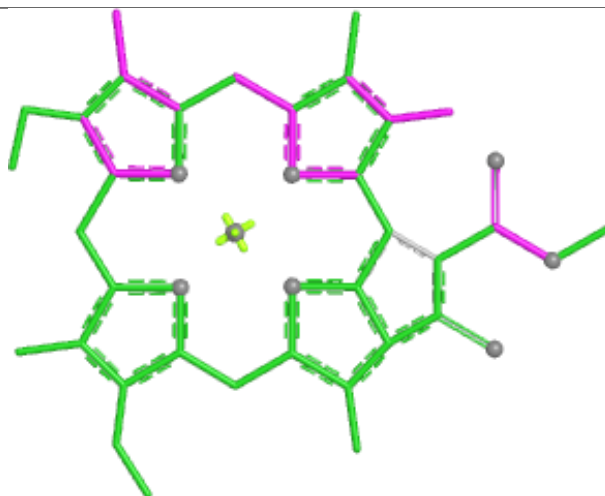


Rings

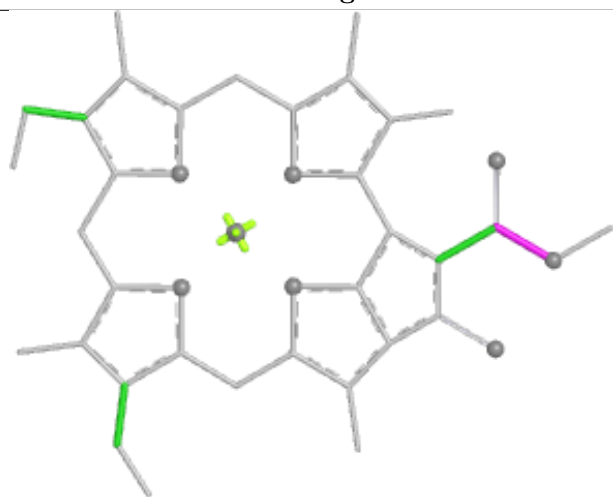
Ligand CLA a 610



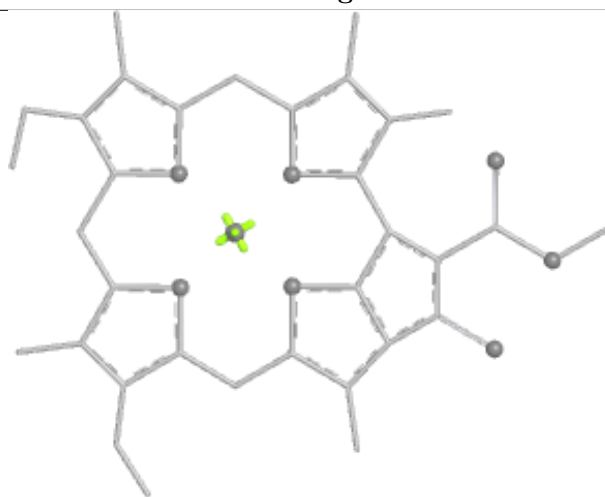
Bond lengths



Bond angles

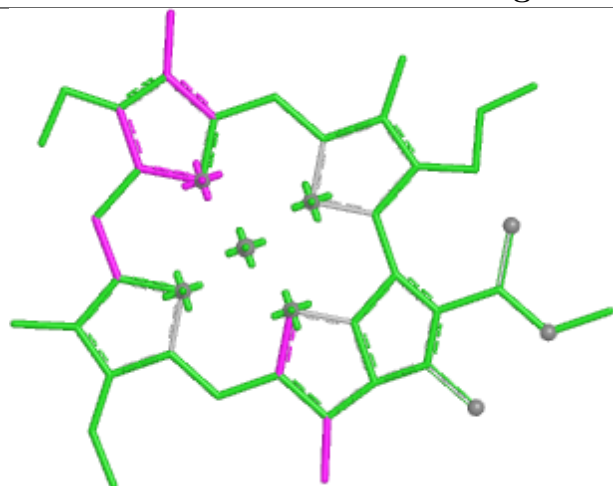


Torsions

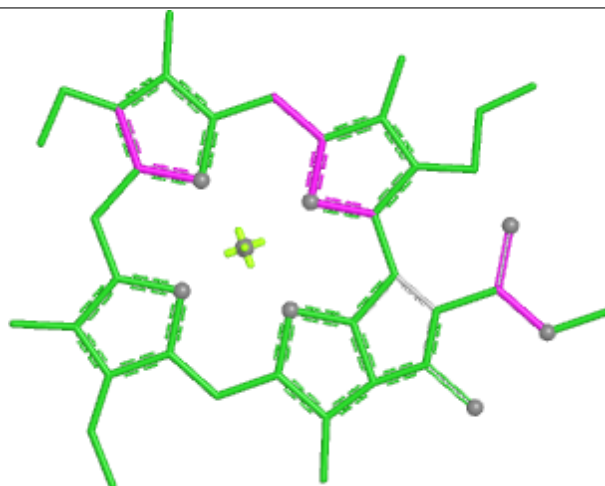


Rings

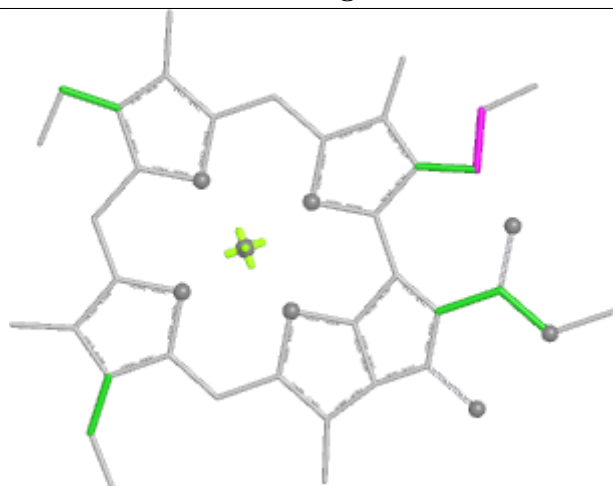
Ligand CLA N 316



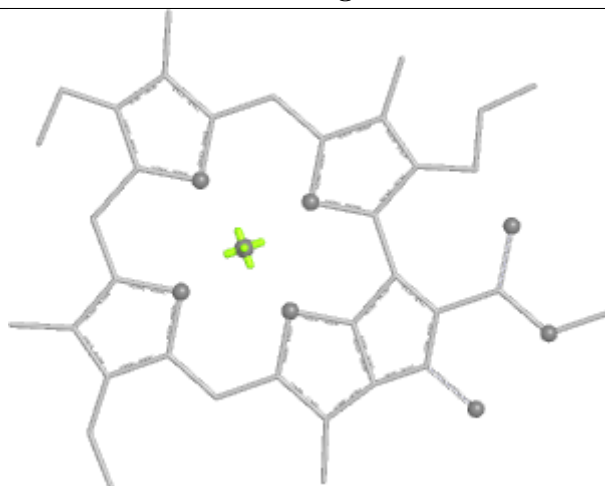
Bond lengths



Bond angles

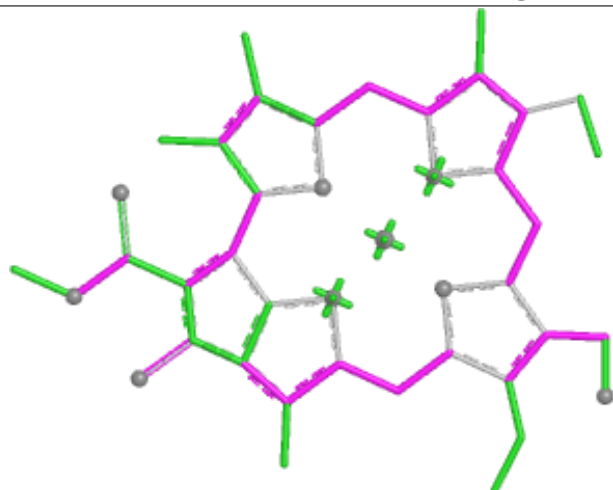


Torsions



Rings

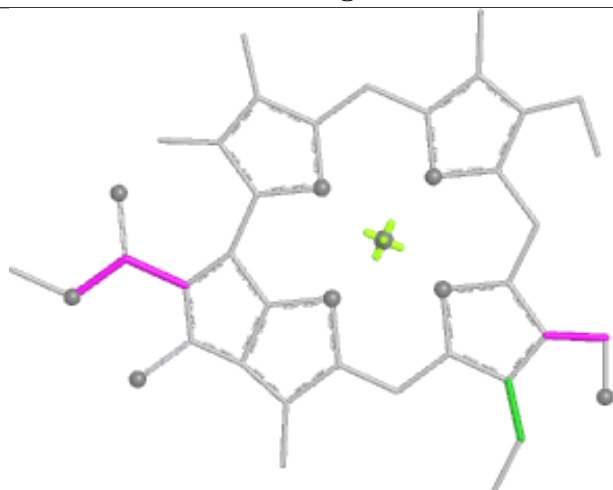
Ligand CHL N 317



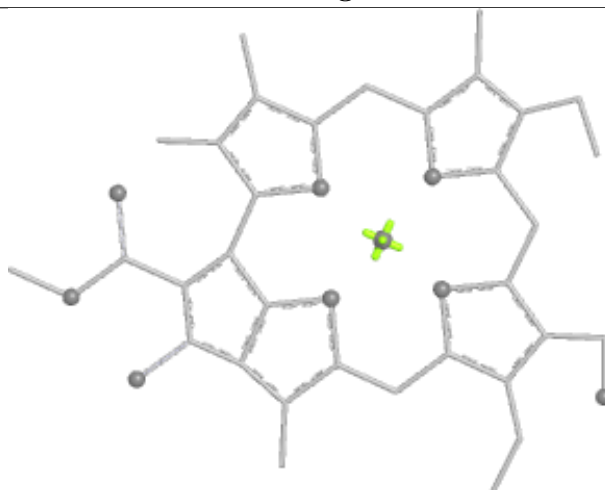
Bond lengths



Bond angles

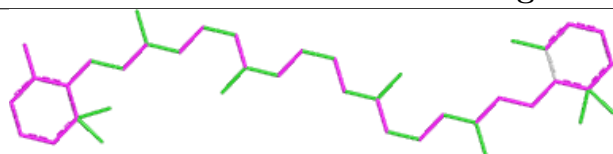


Torsions

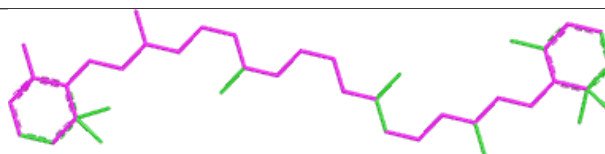


Rings

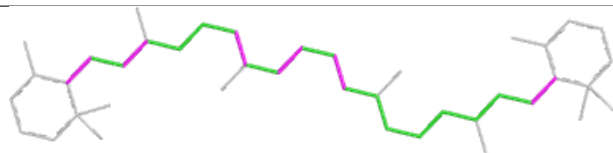
Ligand 8CT C 613



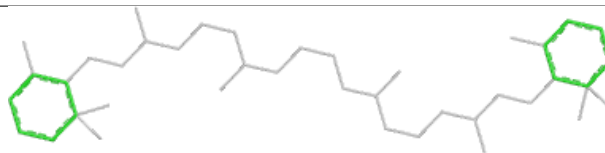
Bond lengths



Bond angles

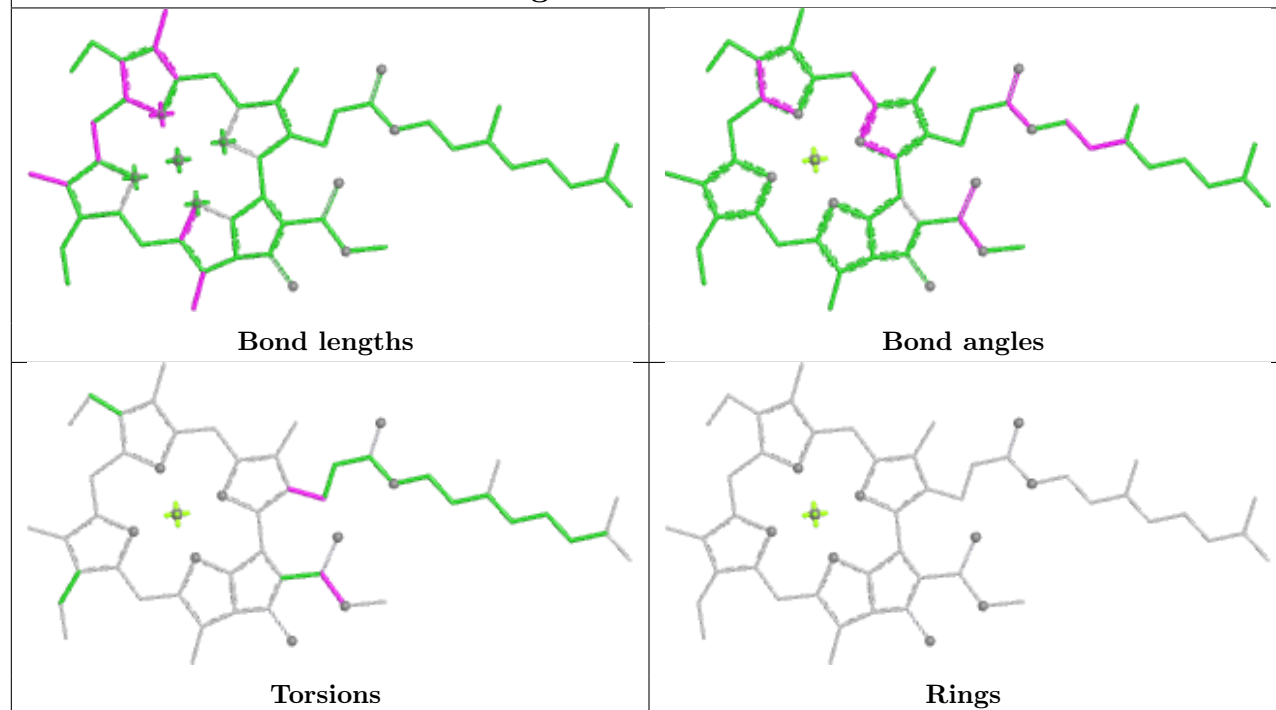


Torsions

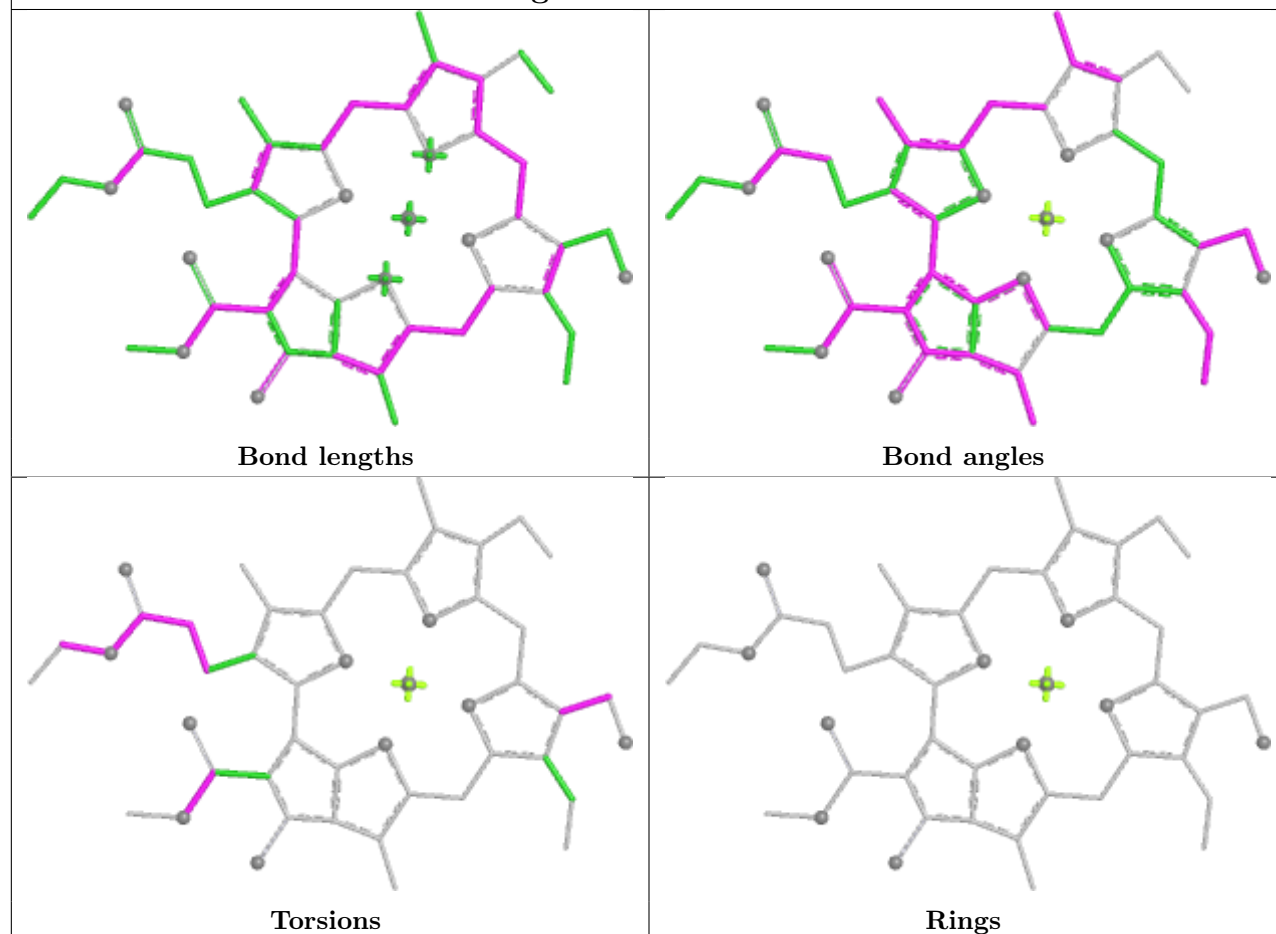


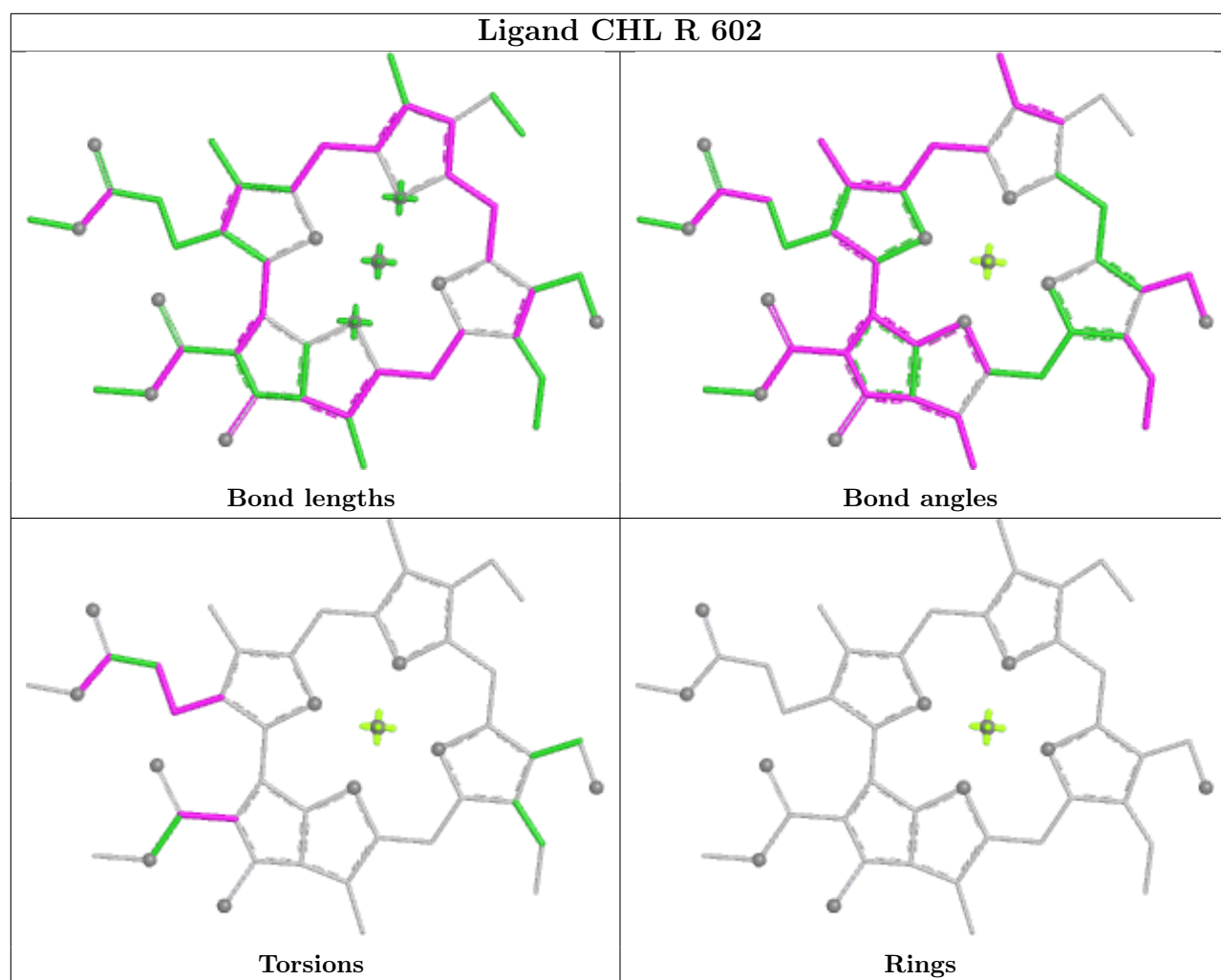
Rings

Ligand CLA G 314

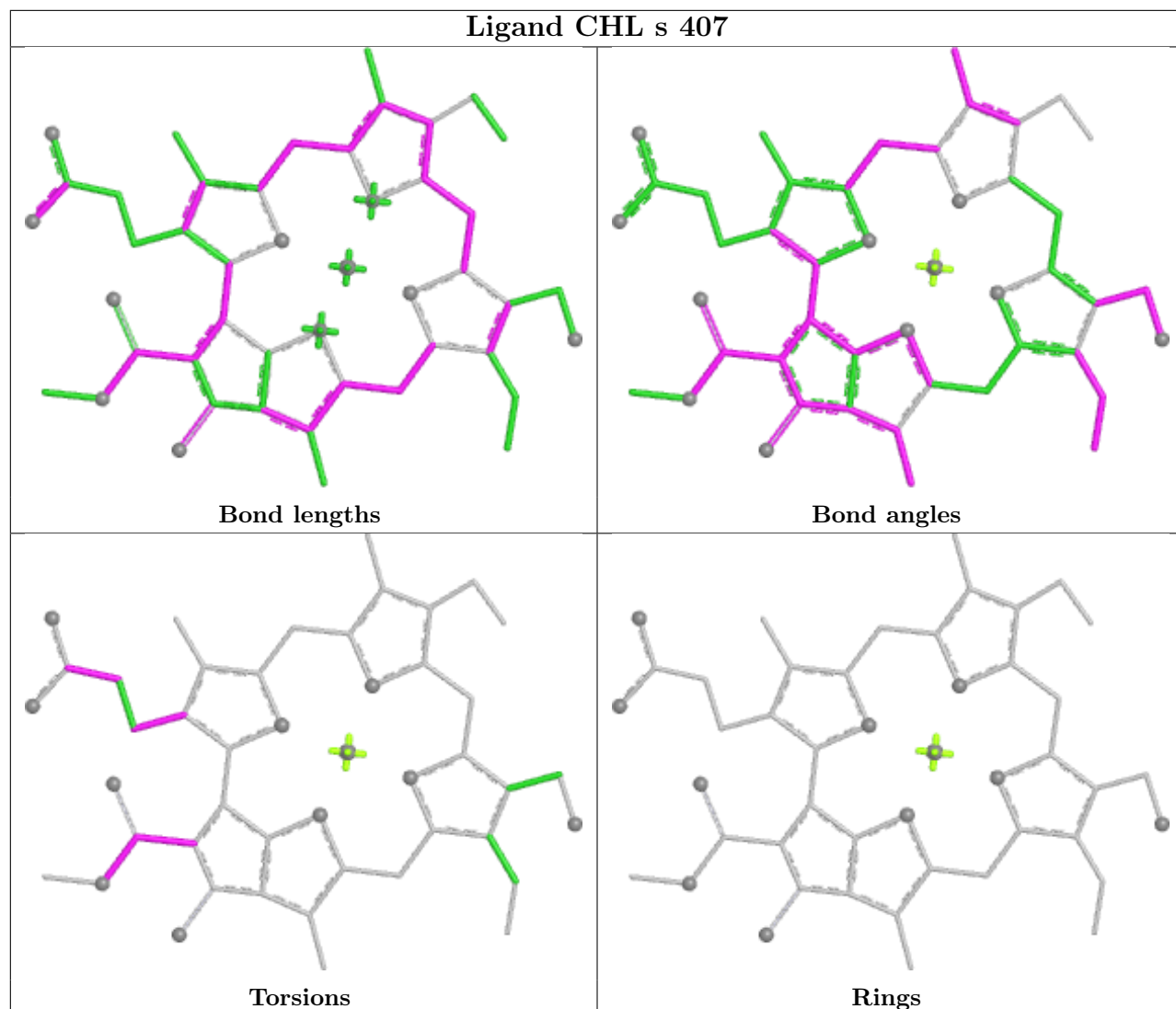


Ligand CHL R 607

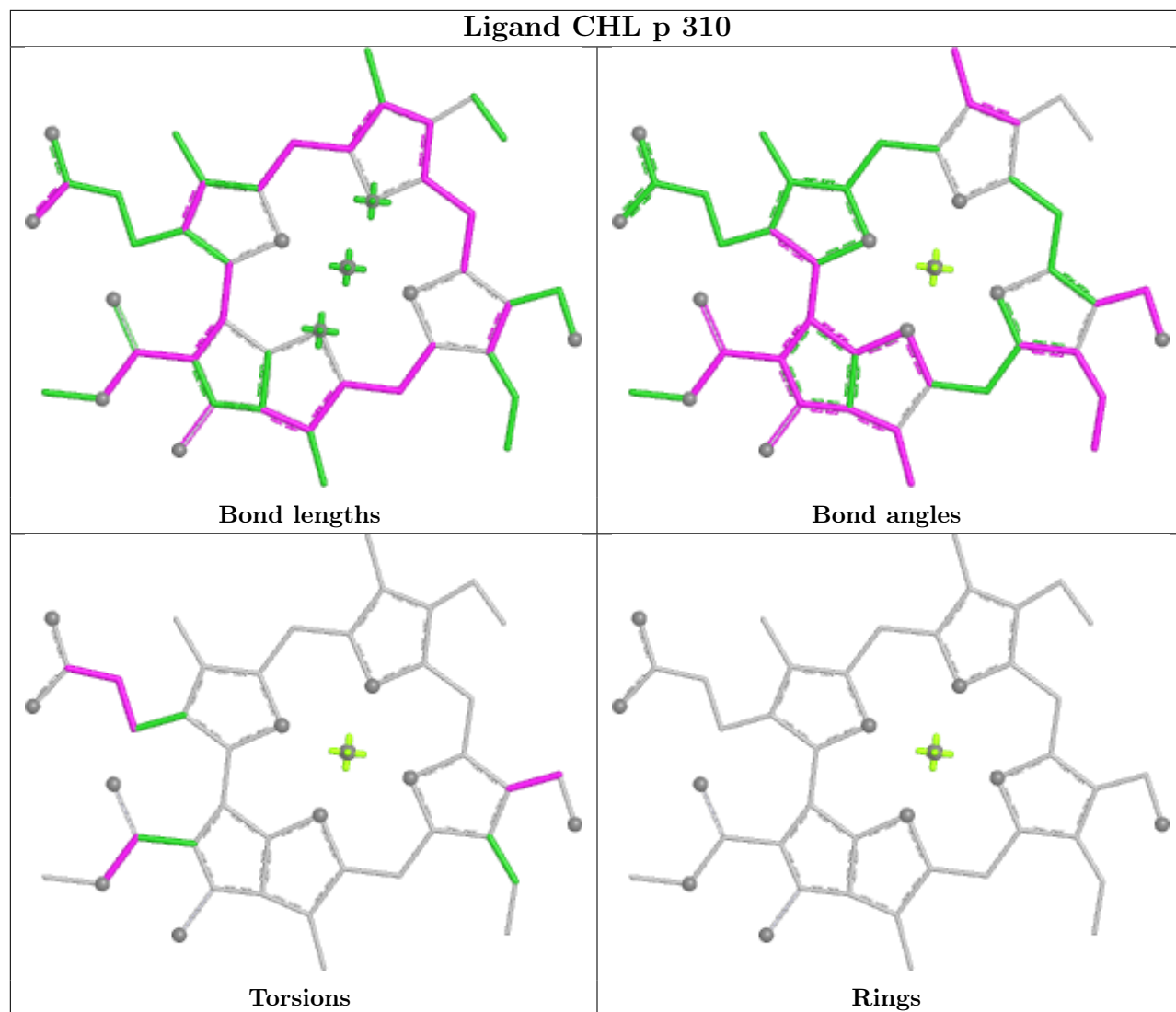




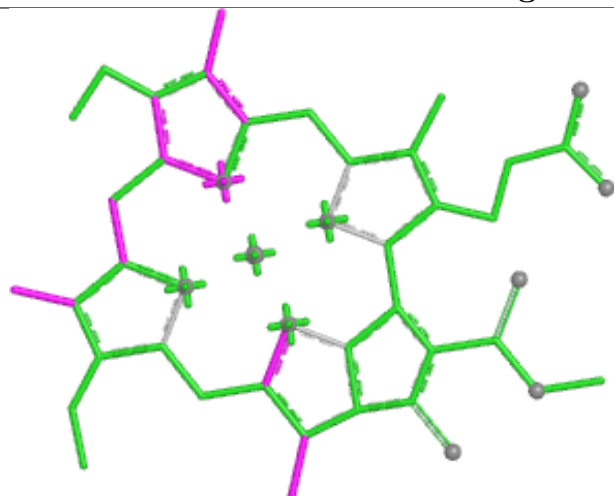
Ligand CHL s 407



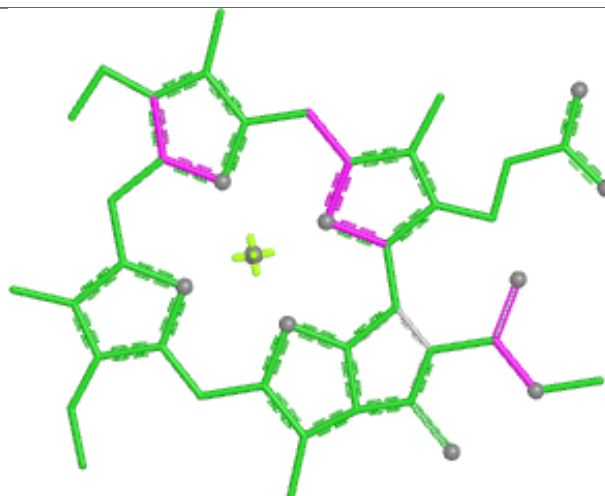
Ligand CHL p 310



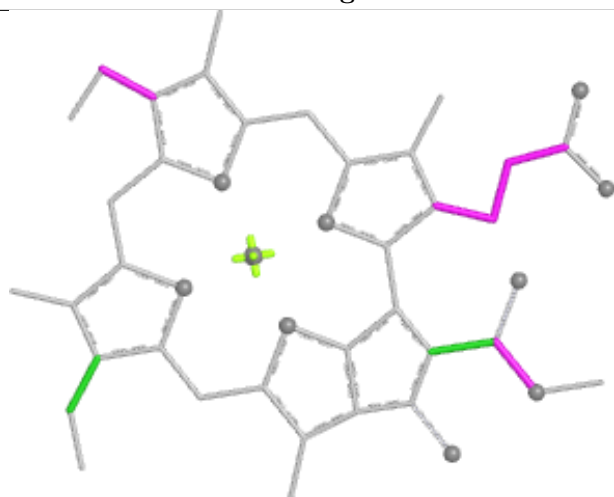
Ligand CLA 6 316



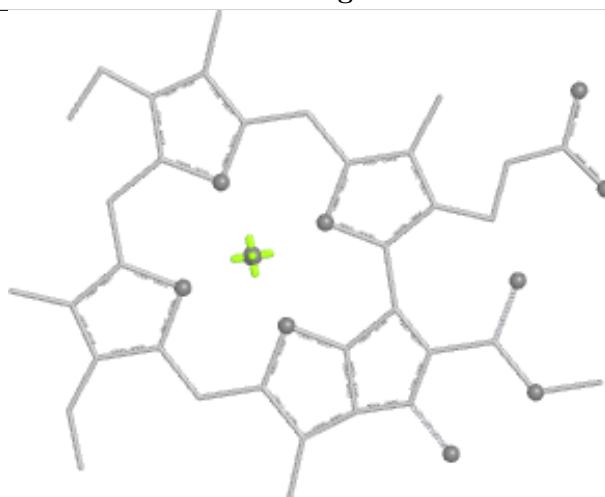
Bond lengths



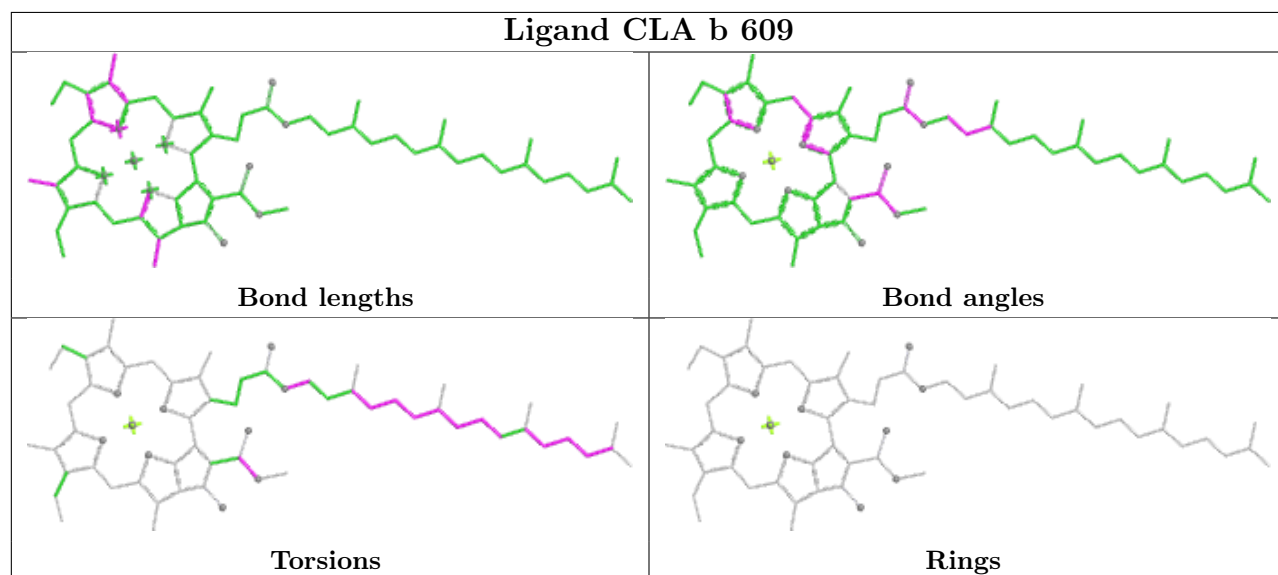
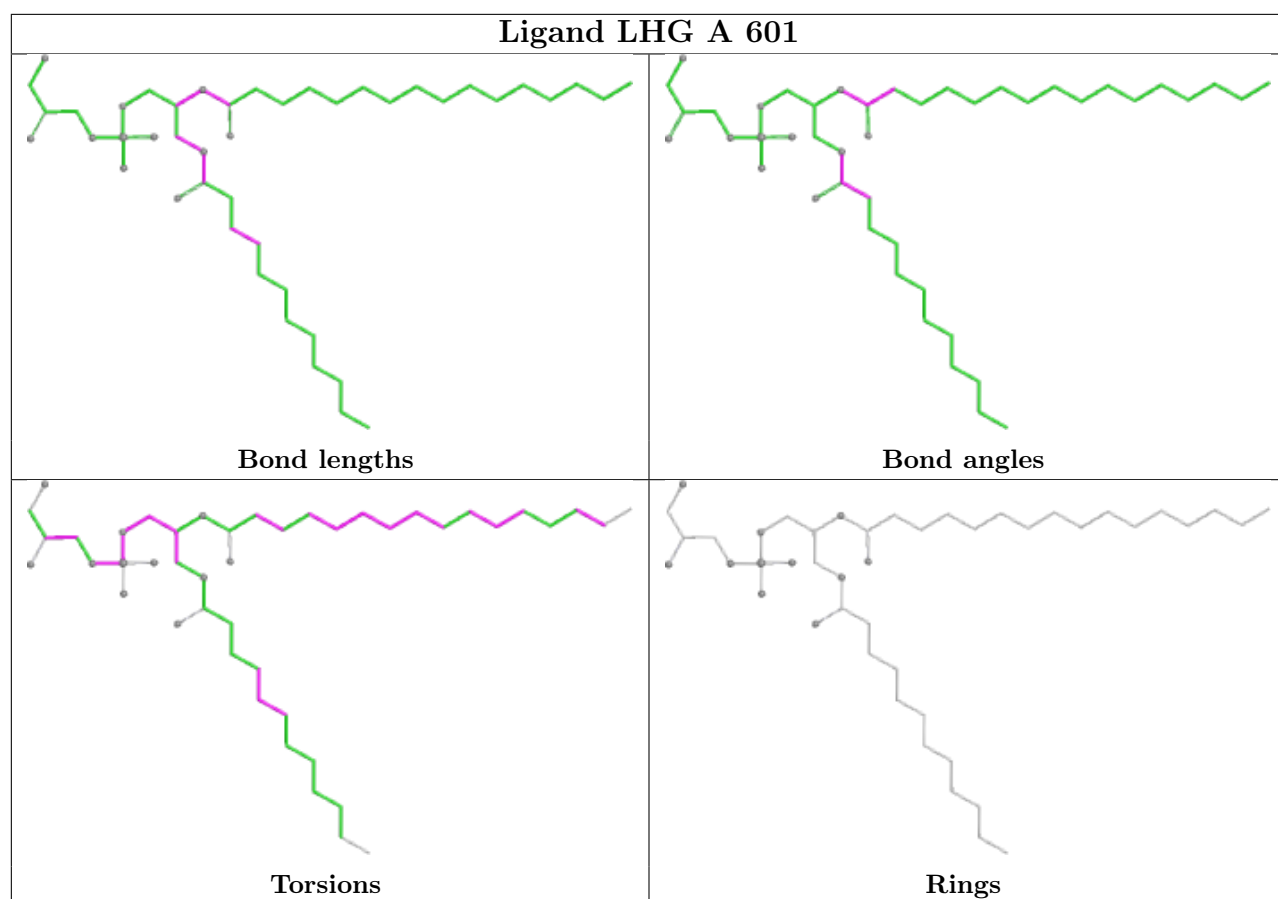
Bond angles

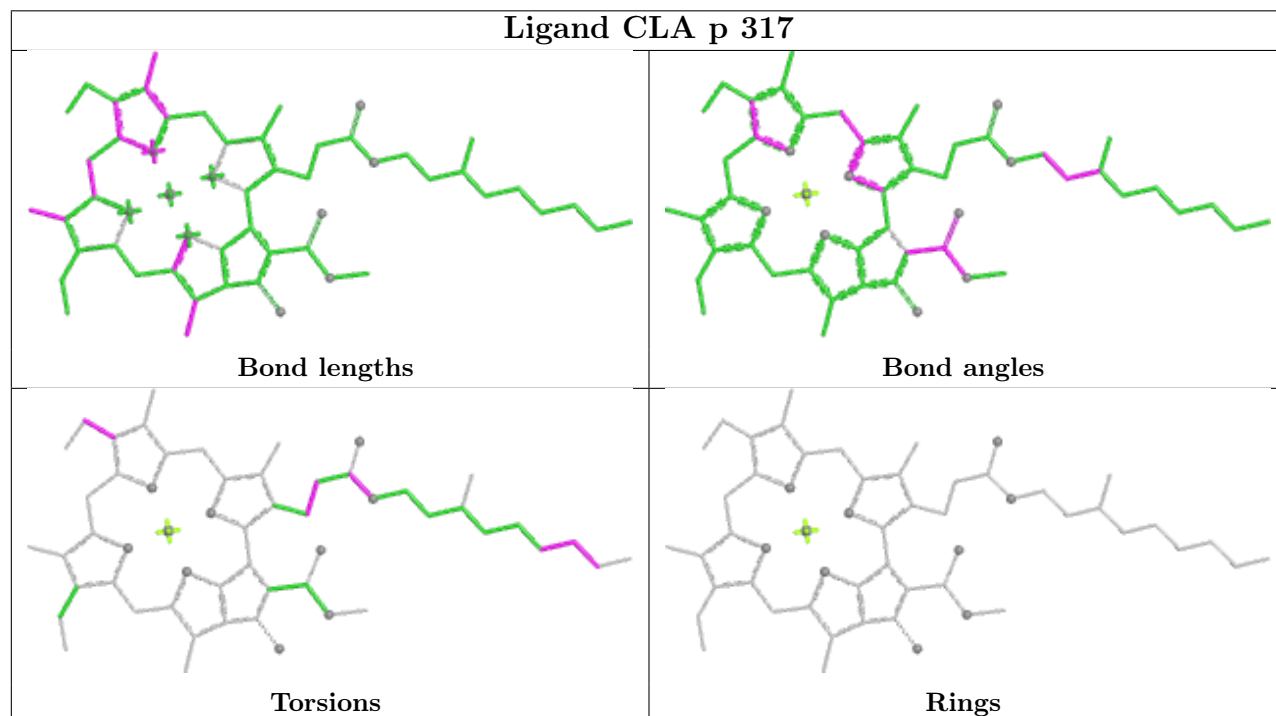
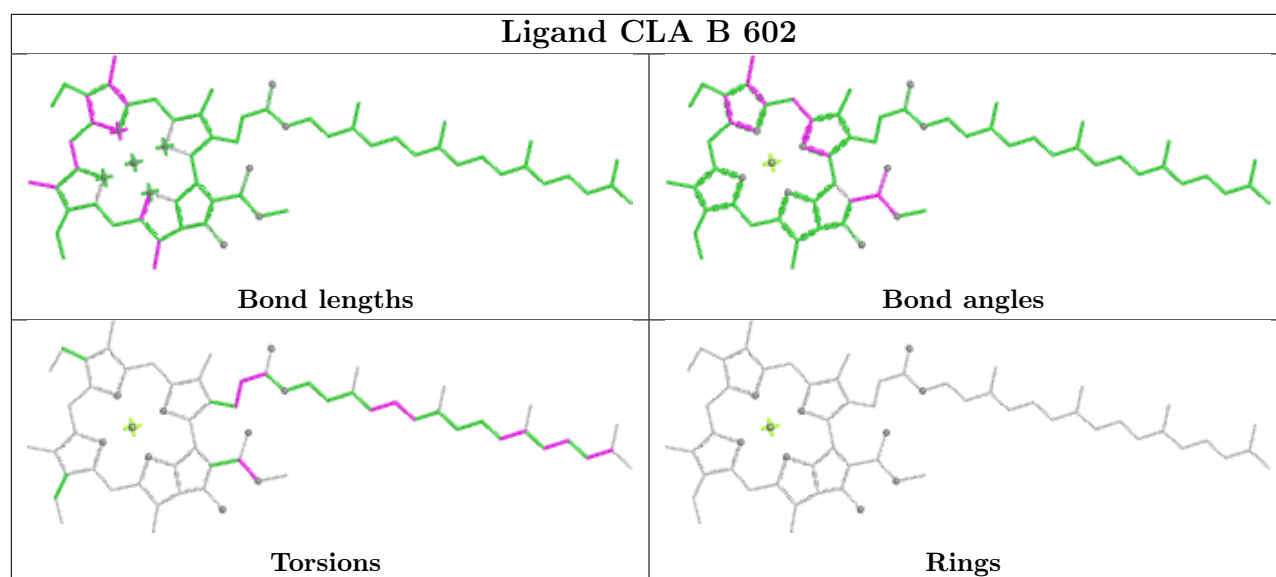


Torsions

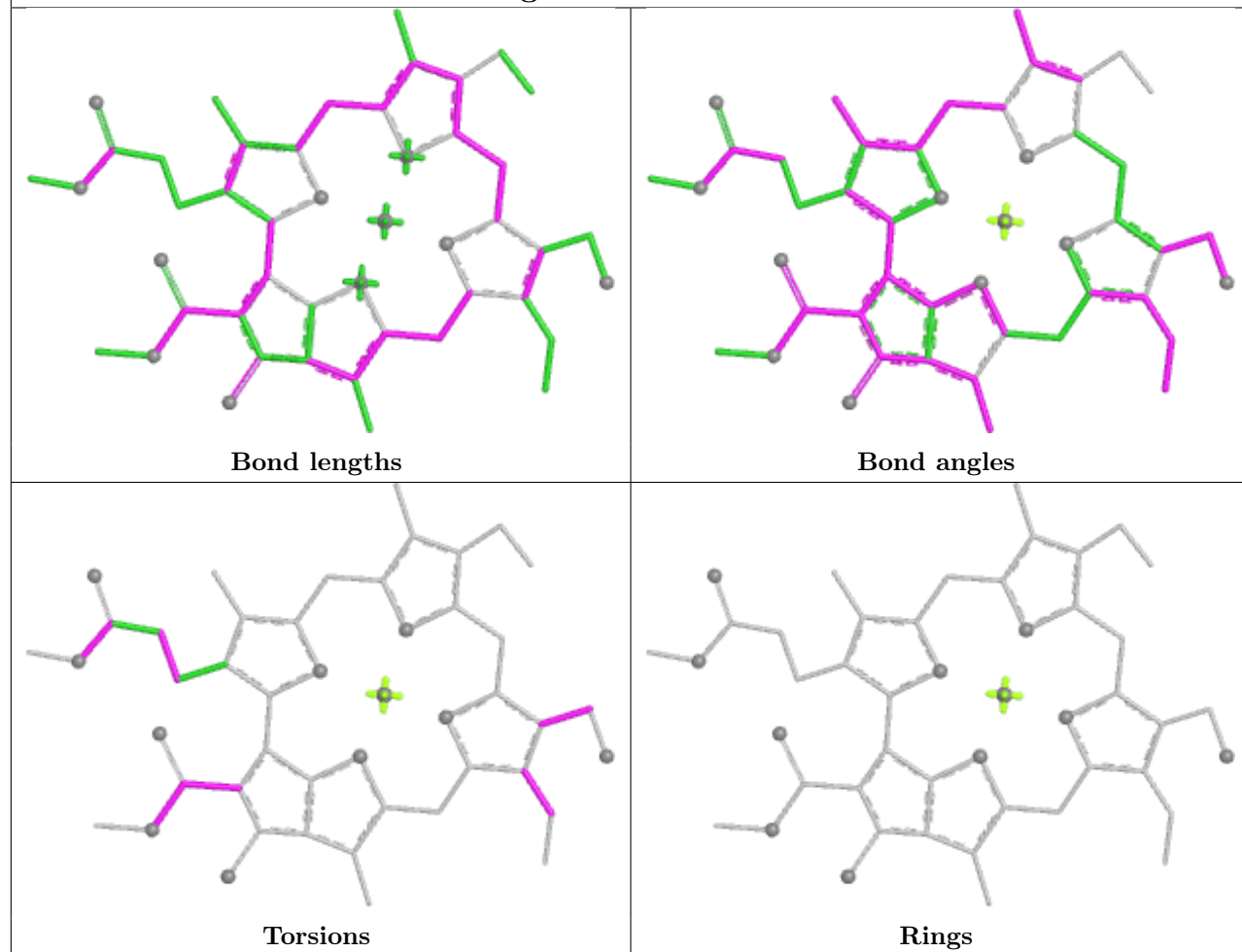


Rings

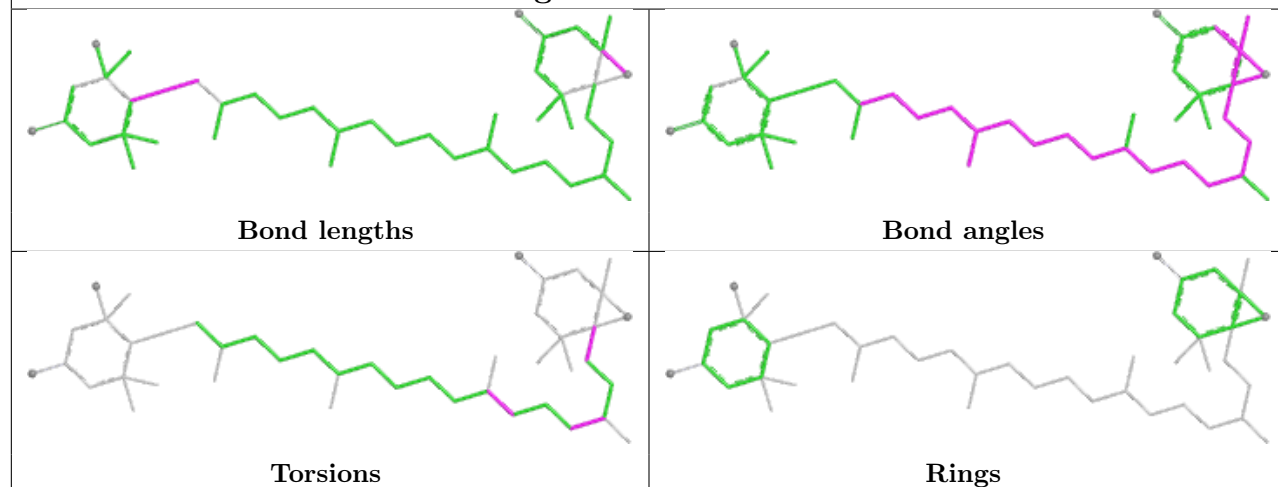


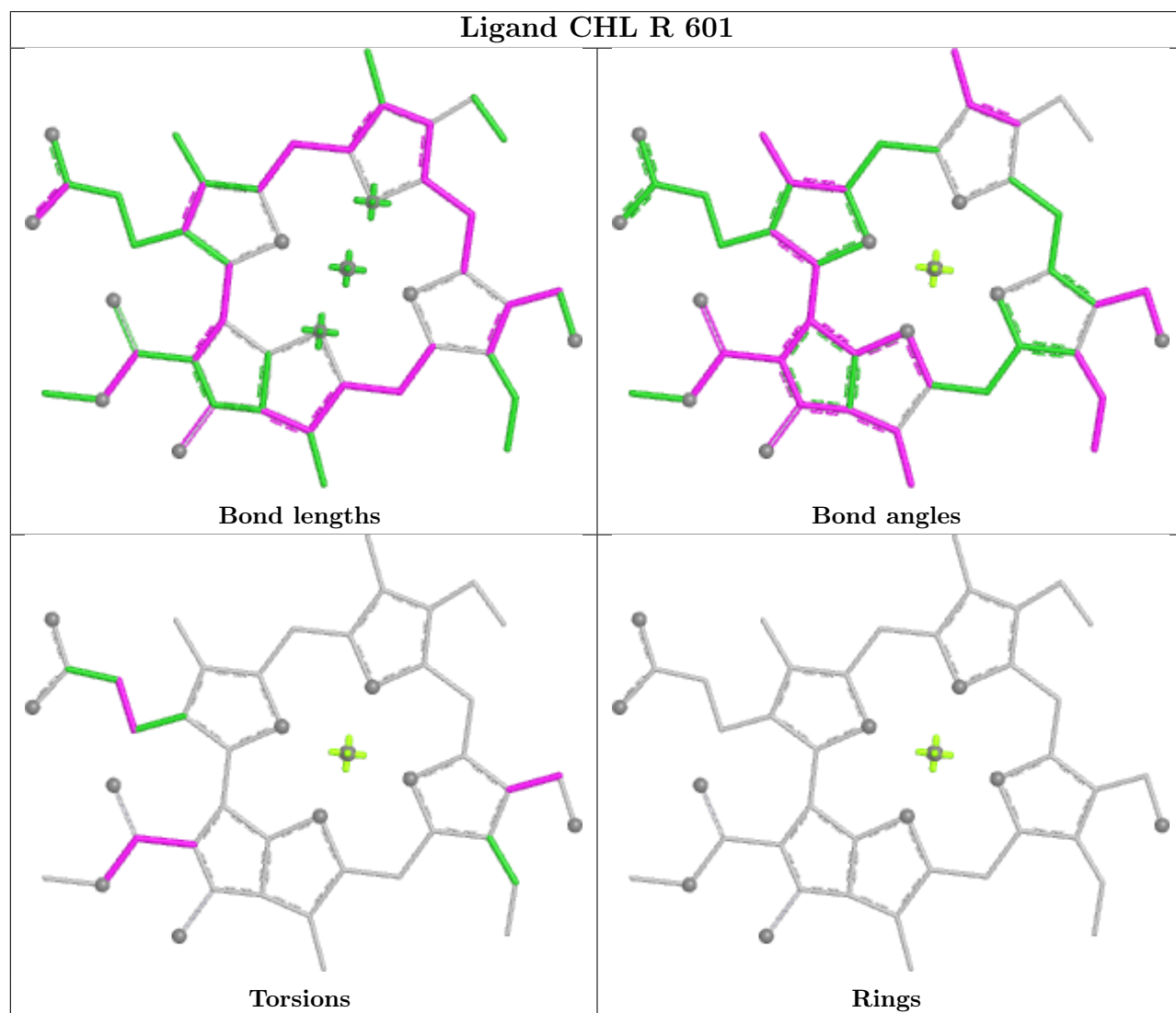
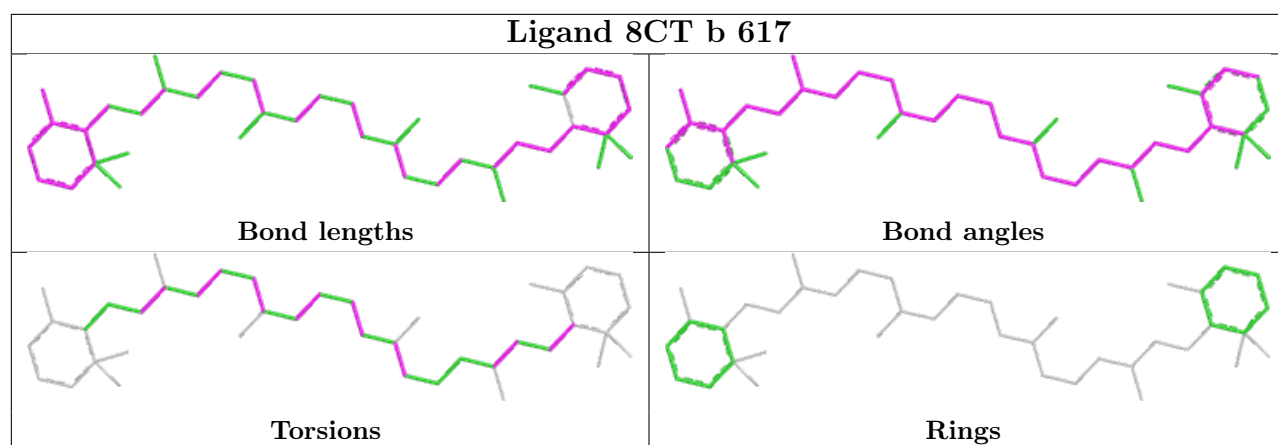


Ligand CHL 2 306

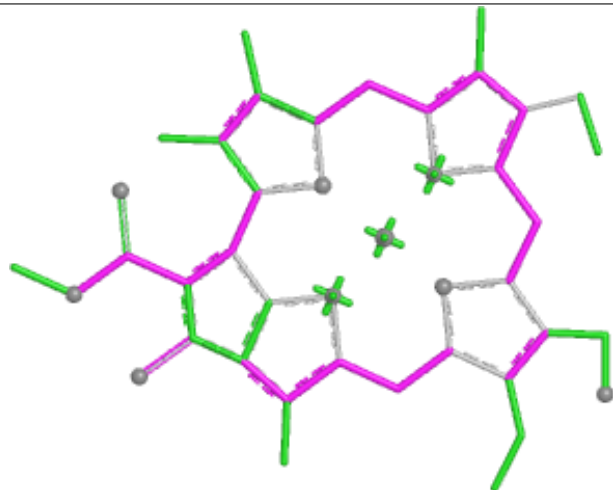


Ligand NEX 1 303





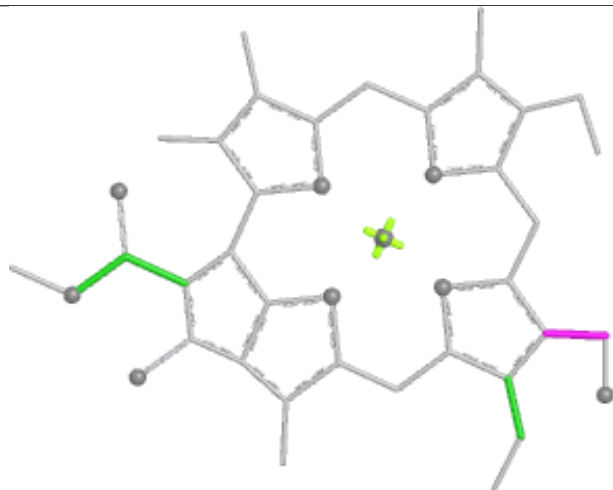
Ligand CHL S 613



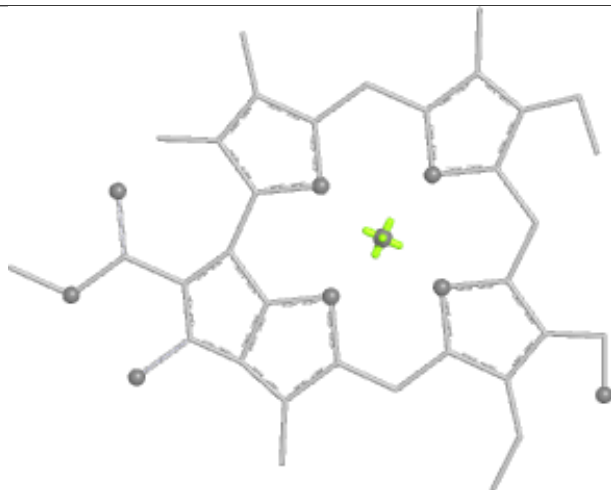
Bond lengths



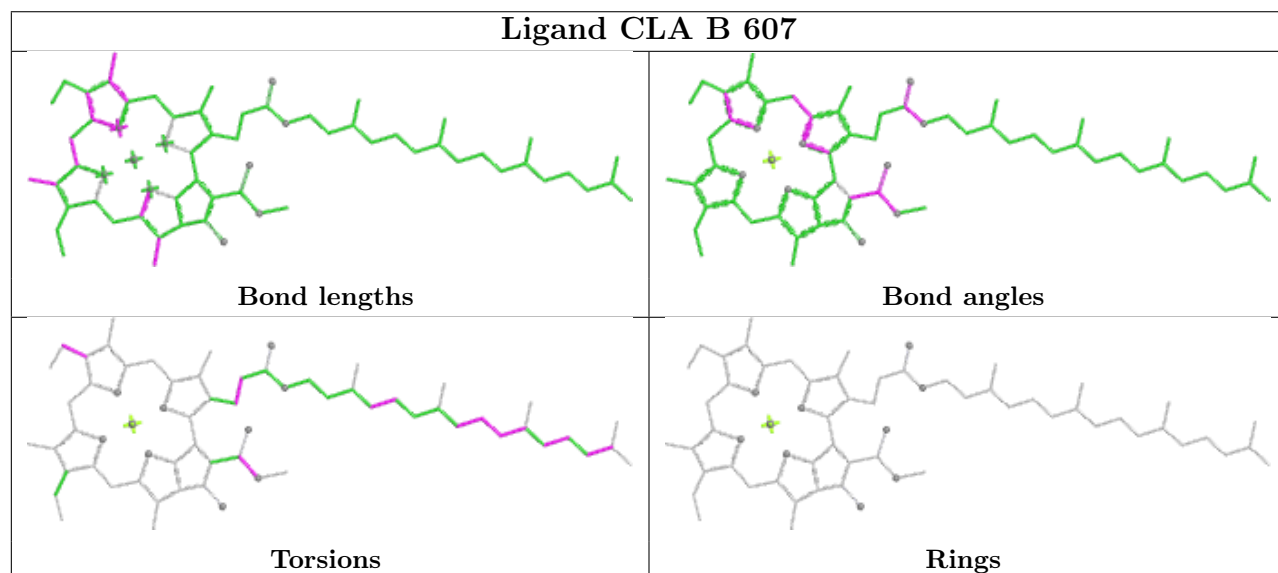
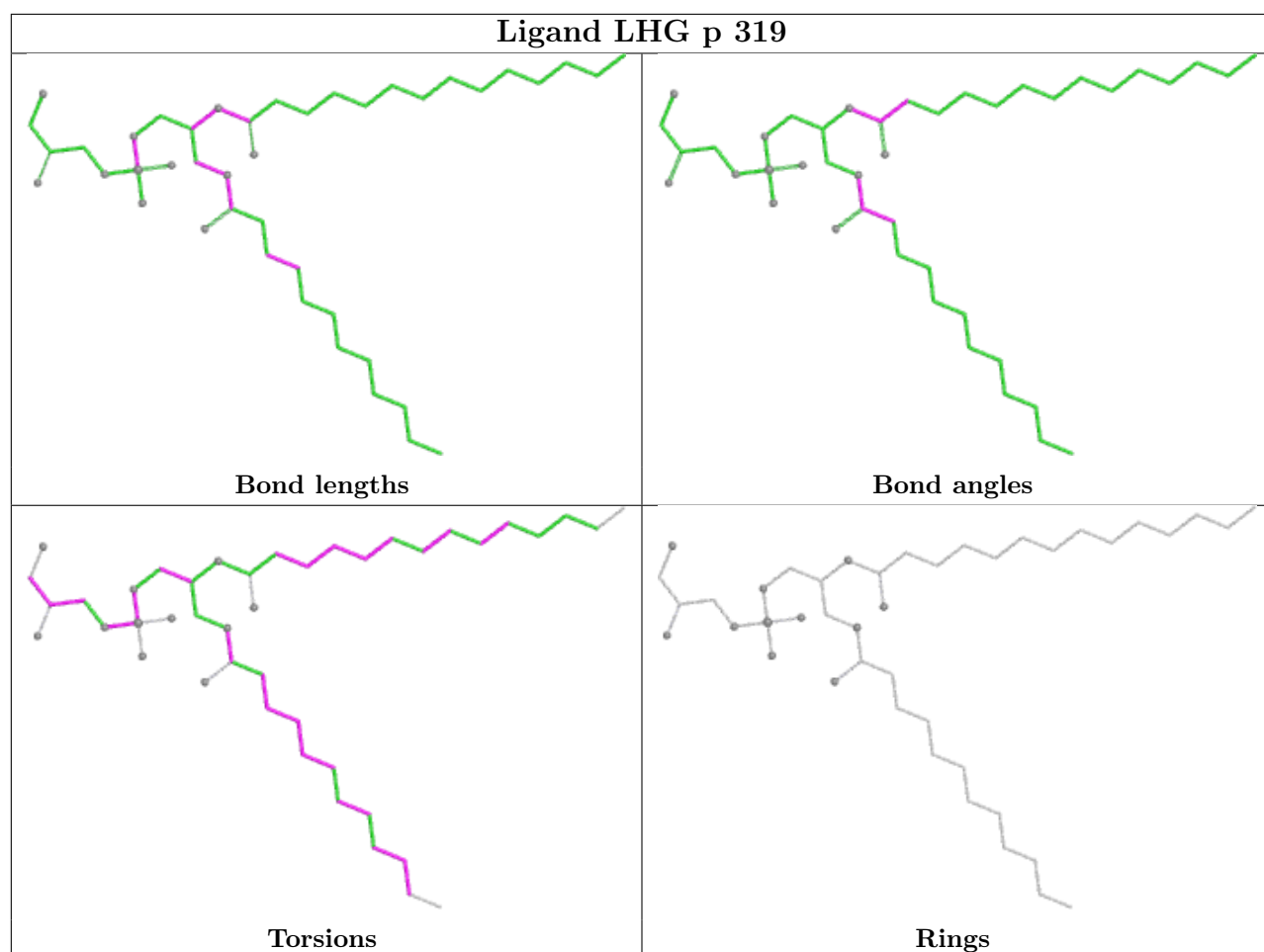
Bond angles

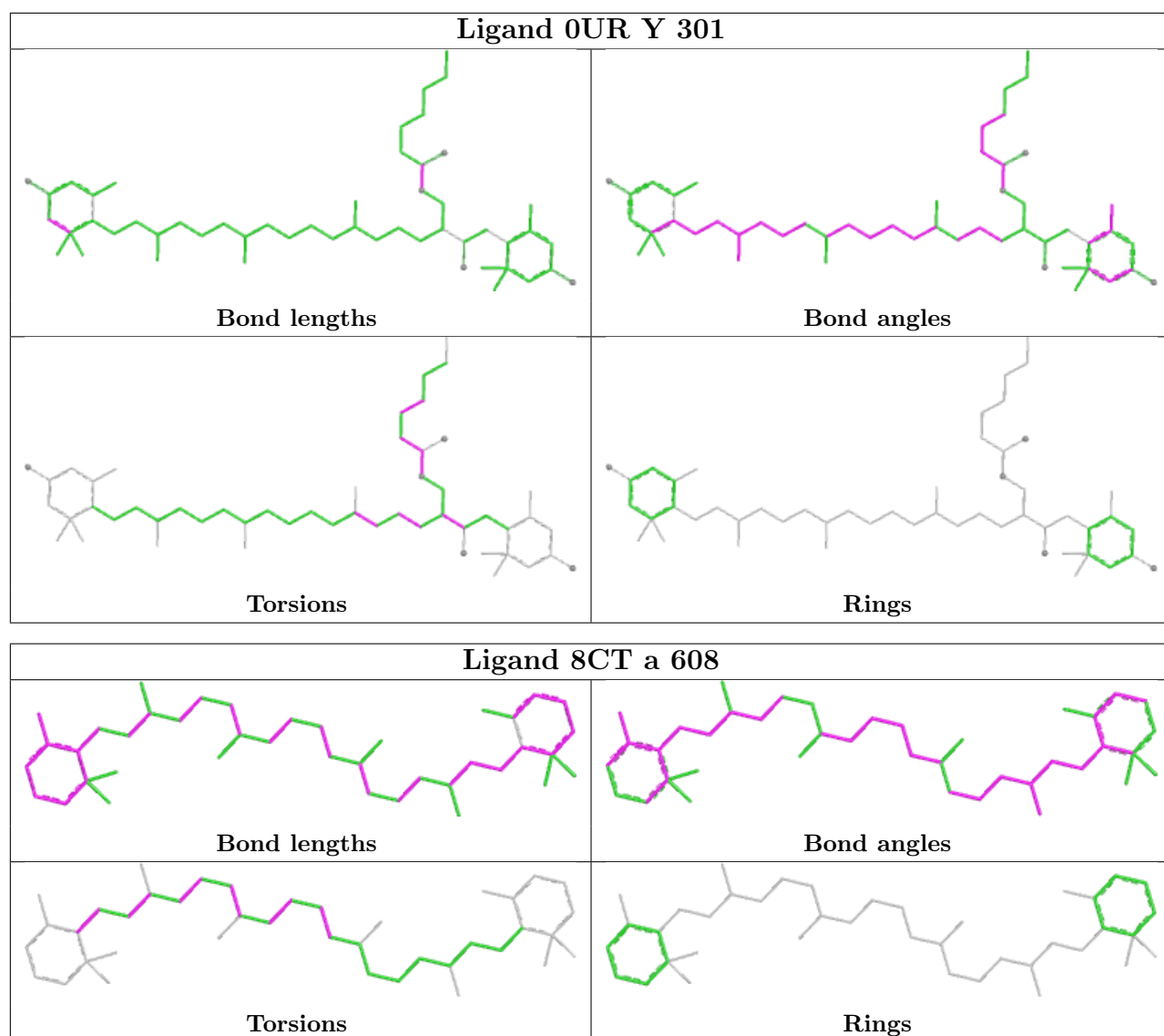


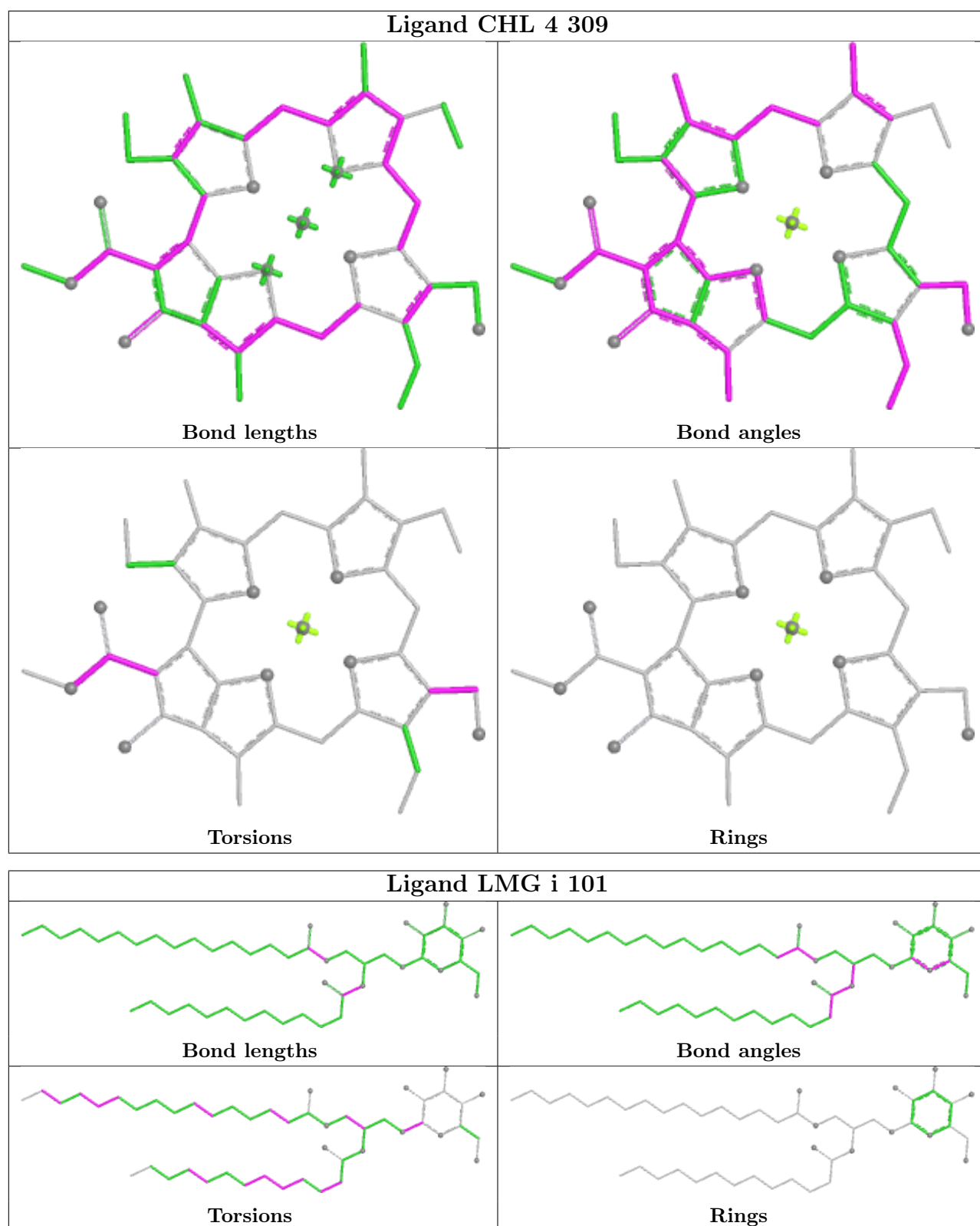
Torsions

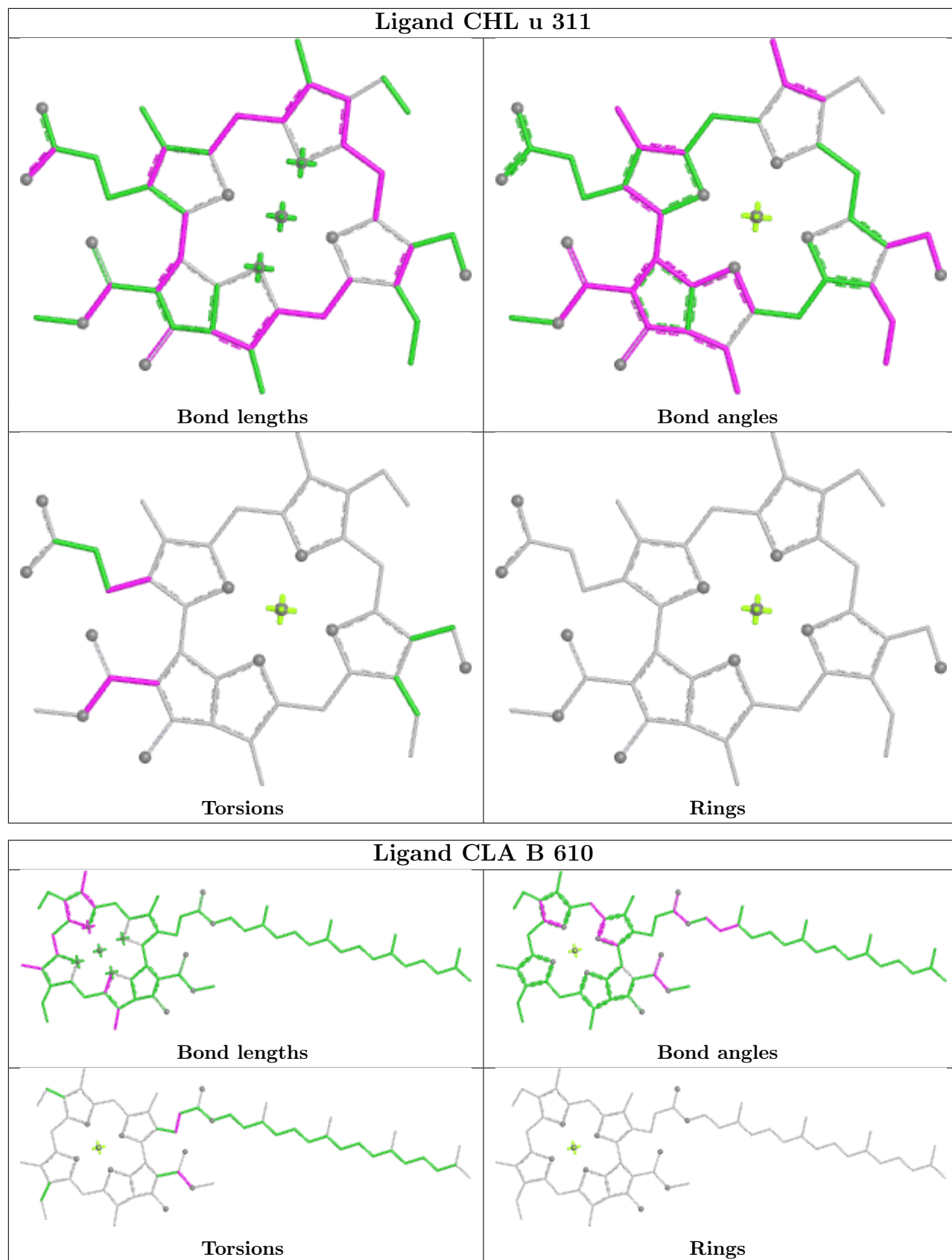


Rings

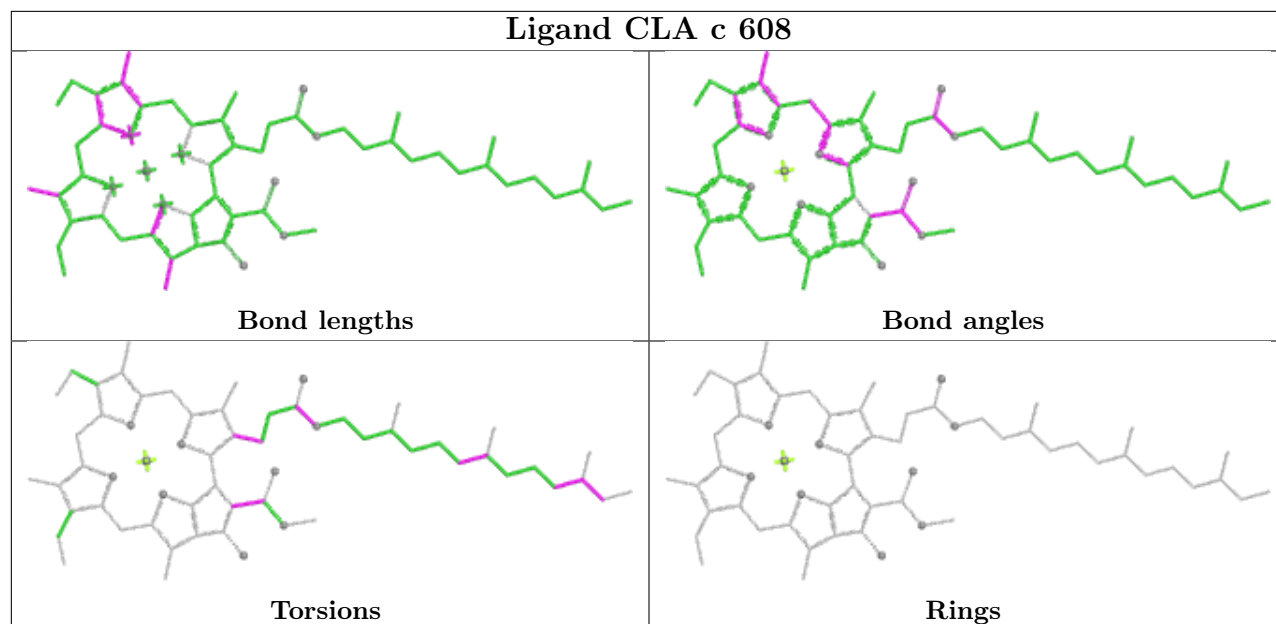




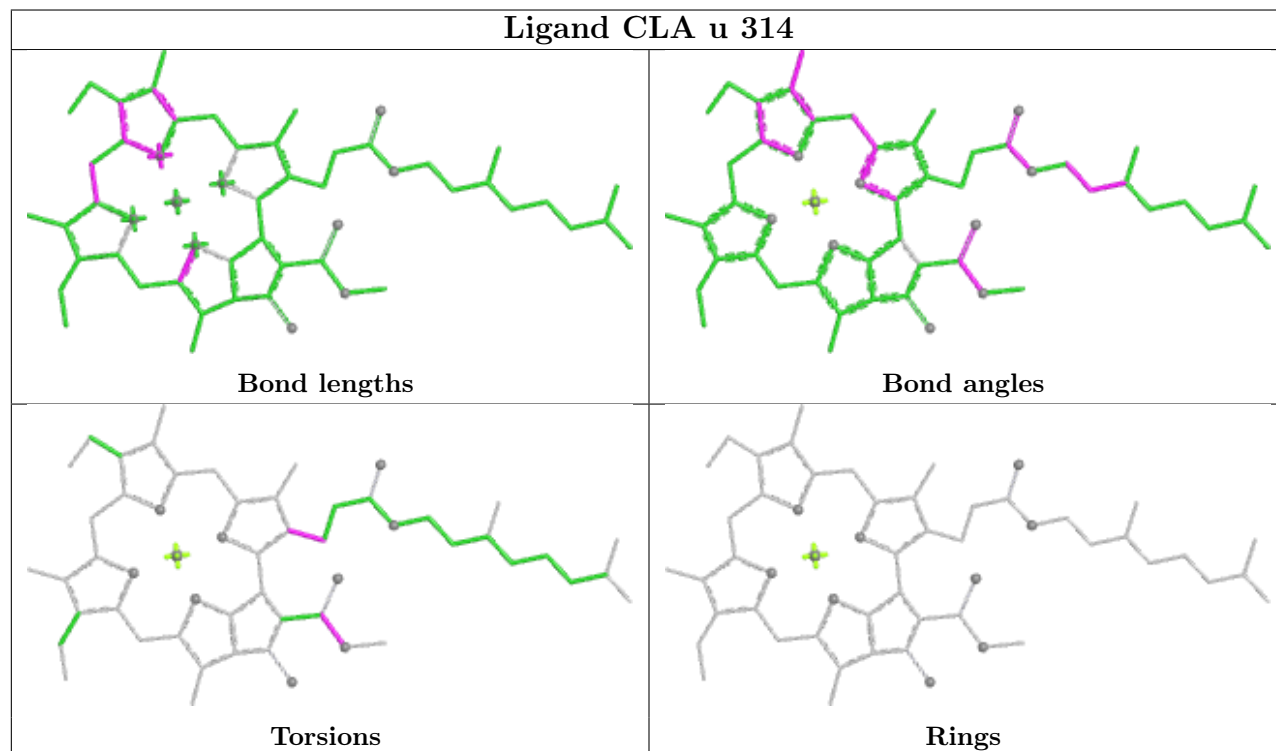


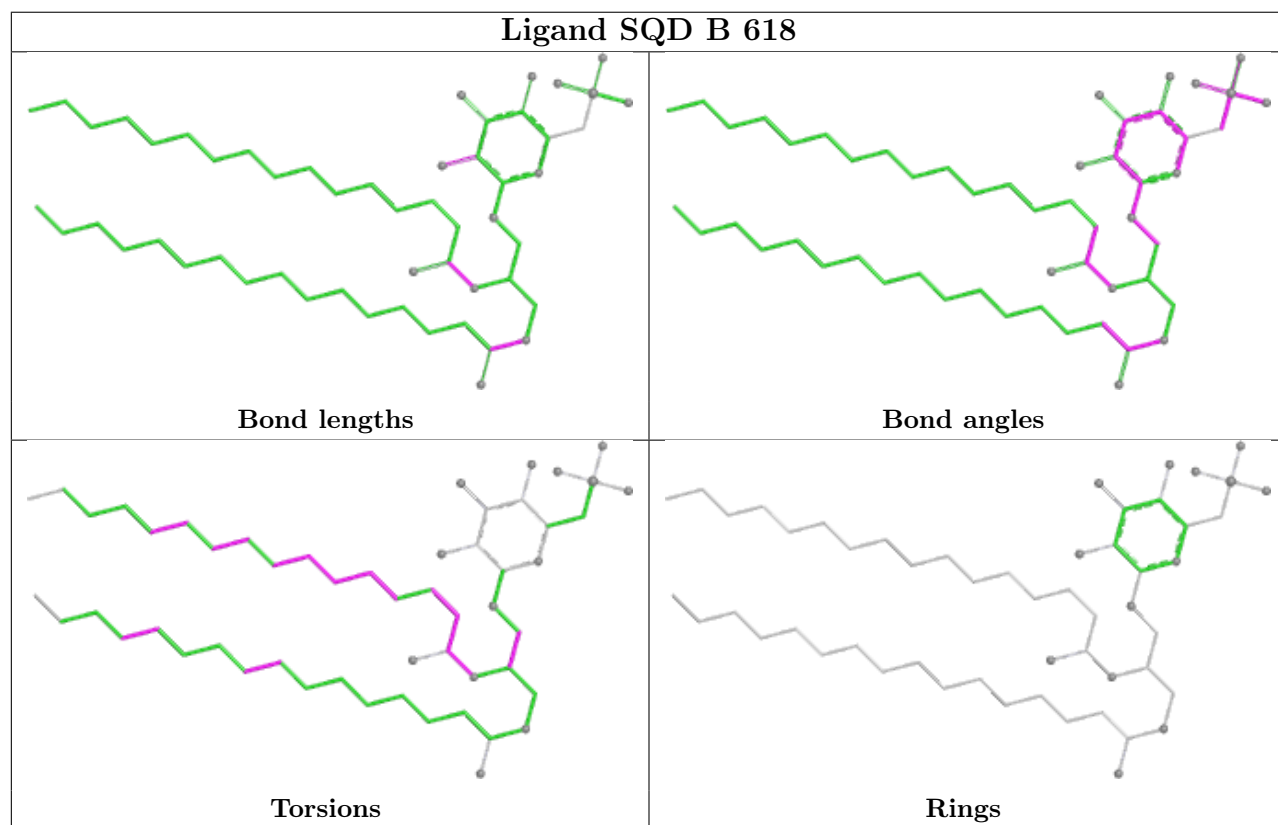
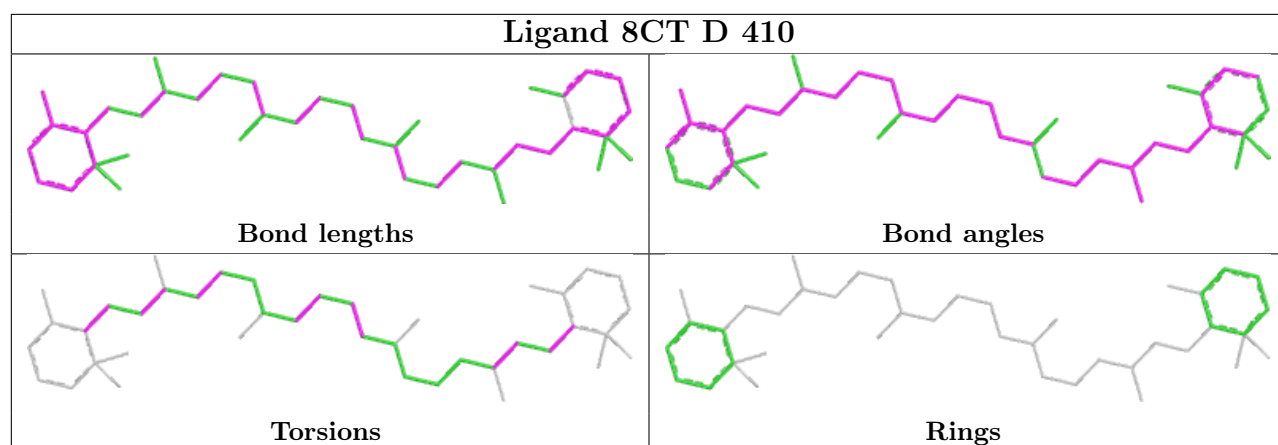


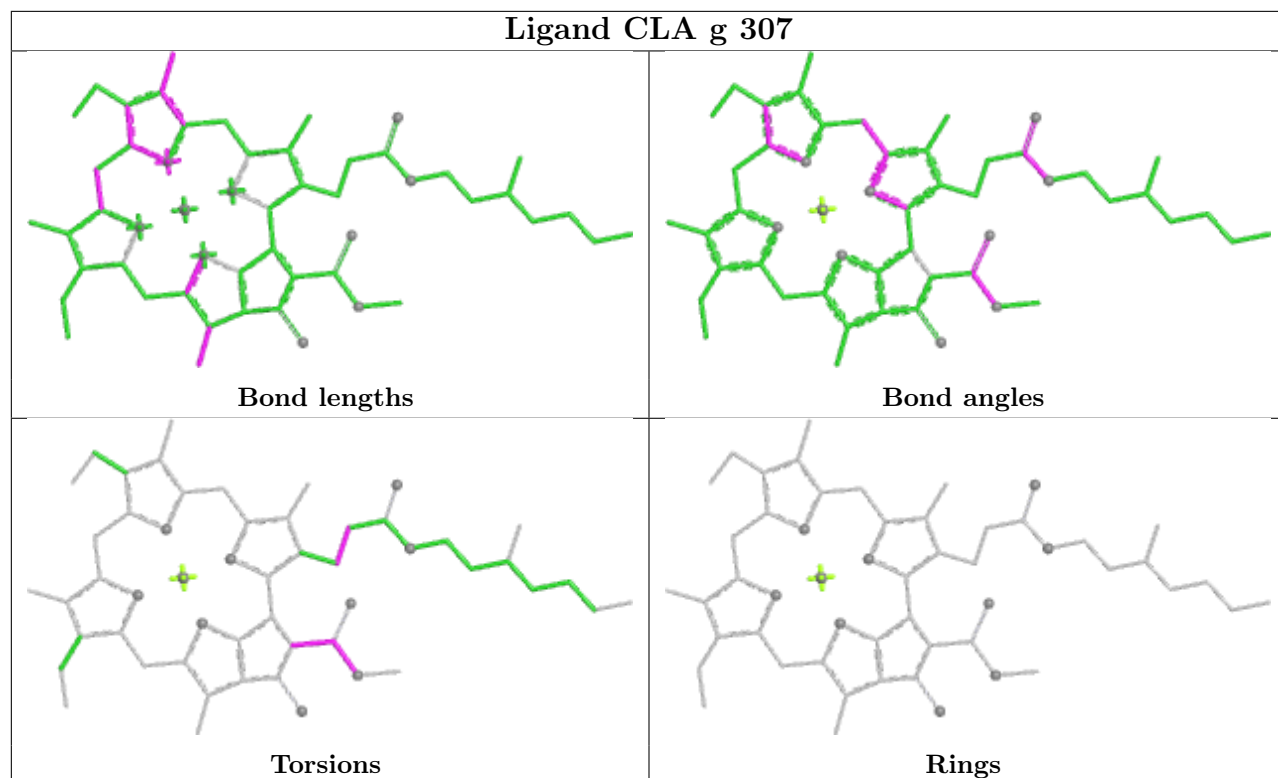
Ligand CLA c 608



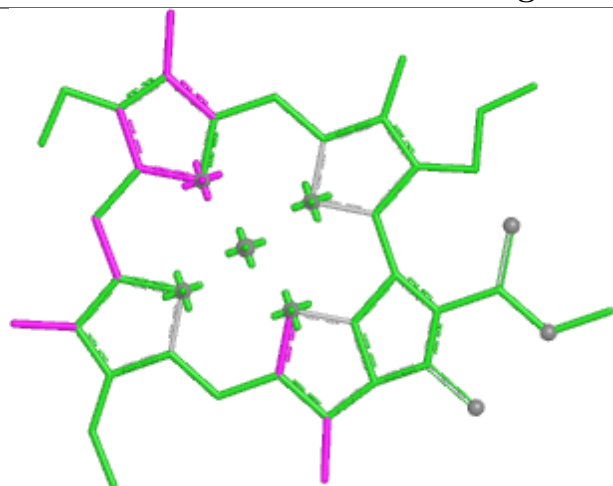
Ligand CLA u 314



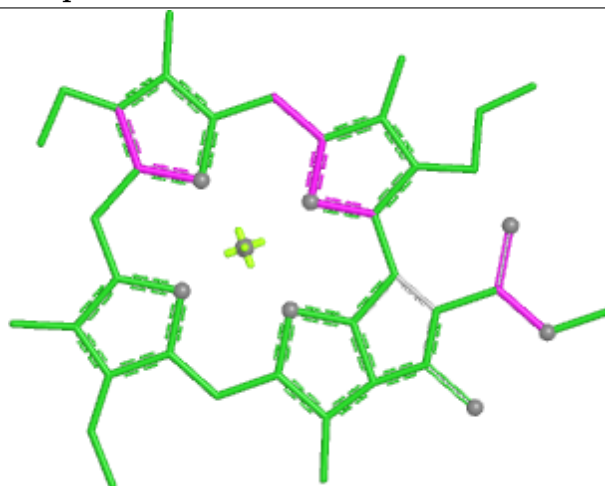




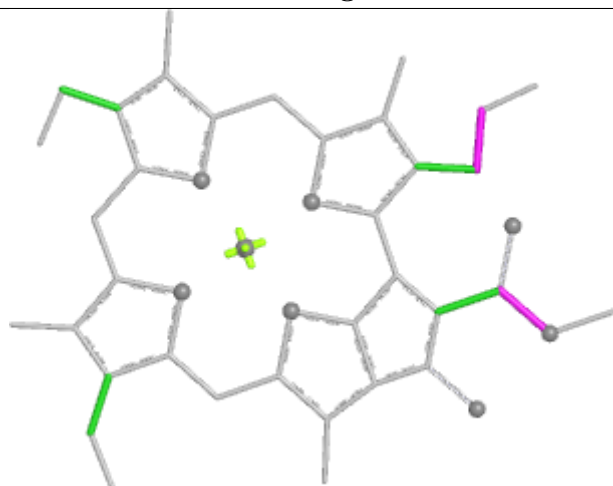
Ligand CLA q 315



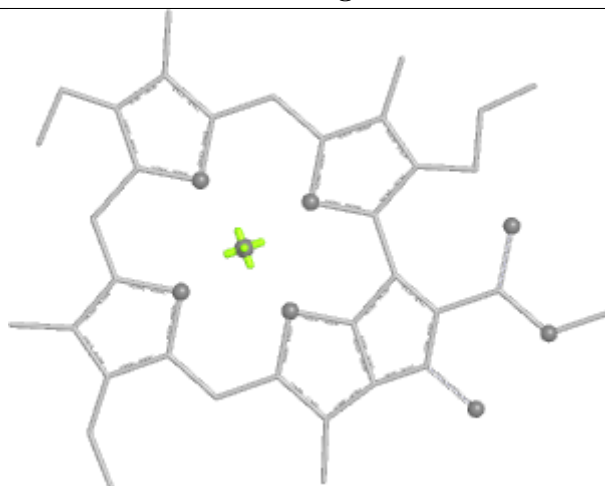
Bond lengths



Bond angles

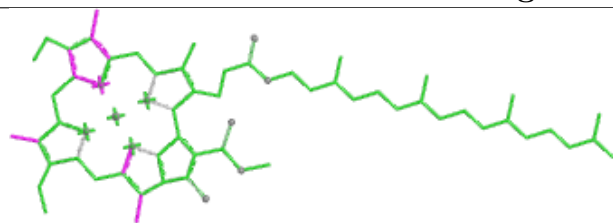


Torsions

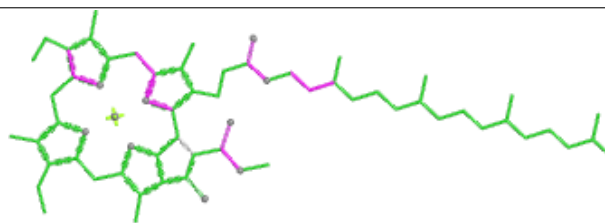


Rings

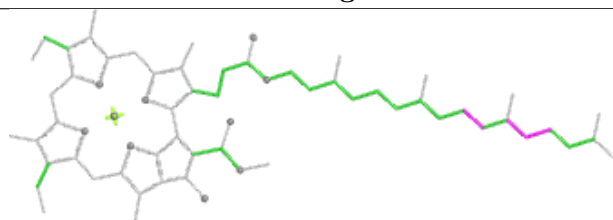
Ligand CLA b 611



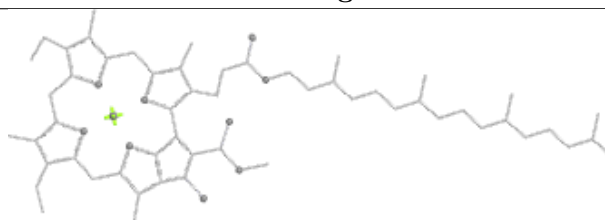
Bond lengths



Bond angles

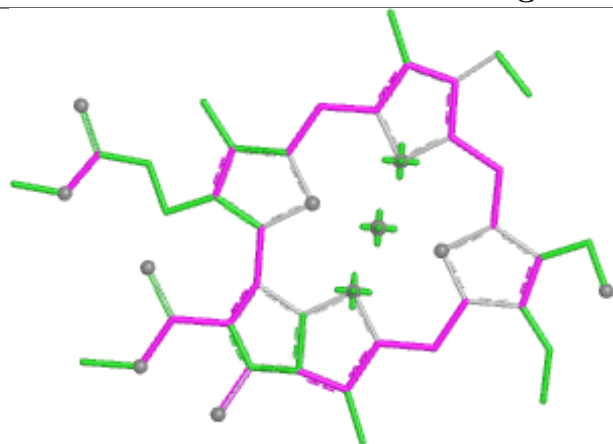


Torsions

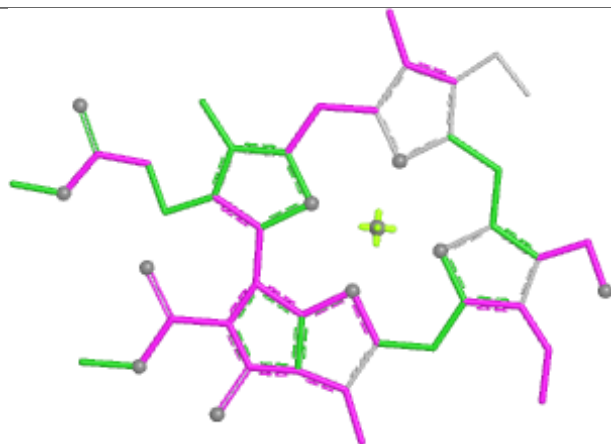


Rings

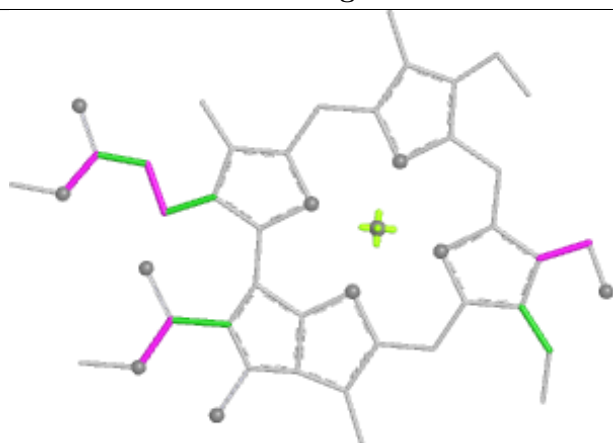
Ligand CHL 7 312



Bond lengths



Bond angles

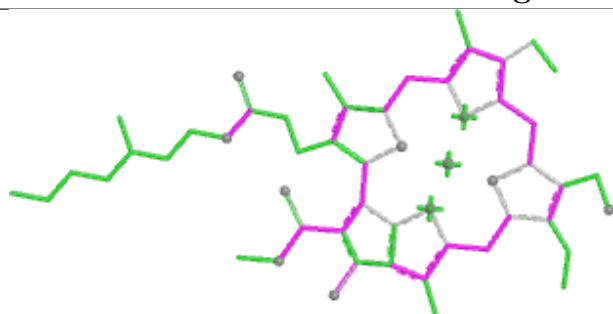


Torsions

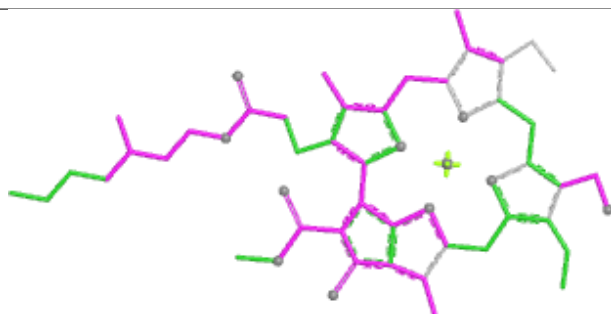


Rings

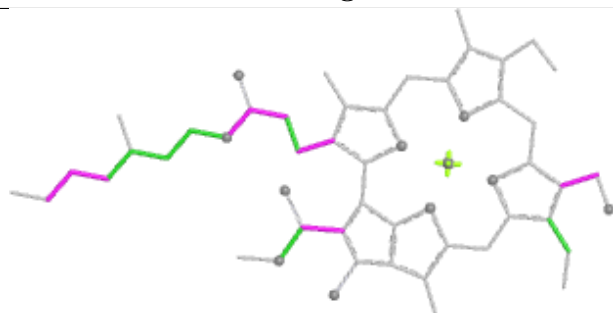
Ligand CHL Y 310



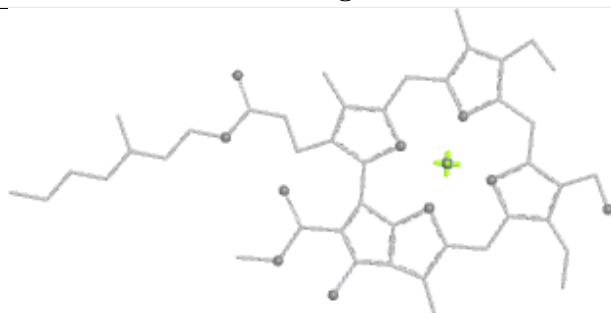
Bond lengths



Bond angles

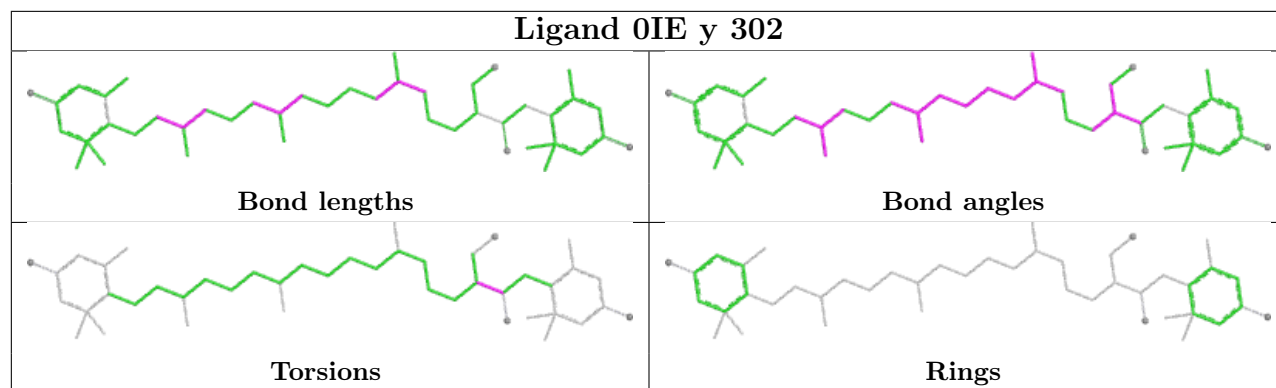


Torsions

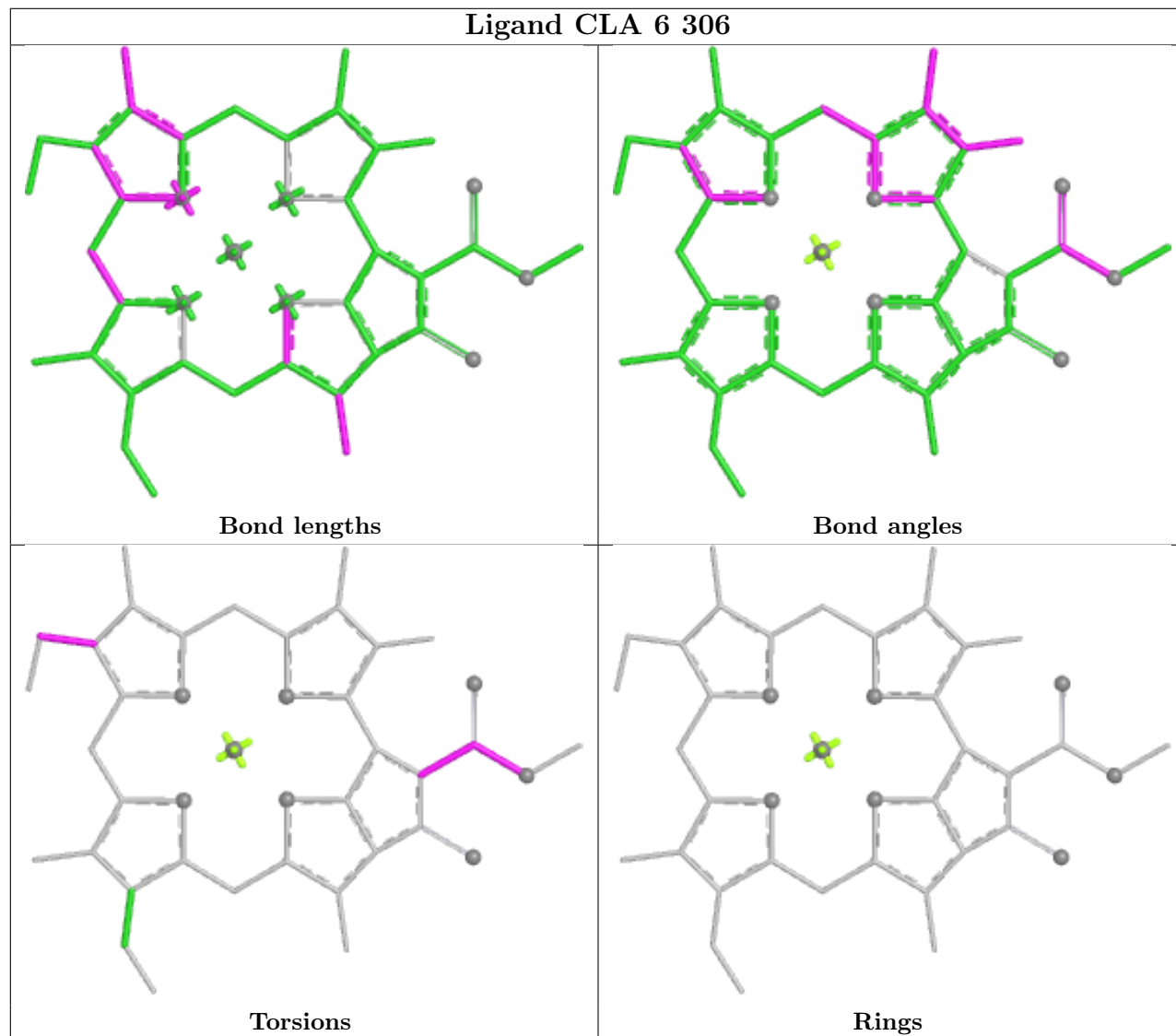


Rings

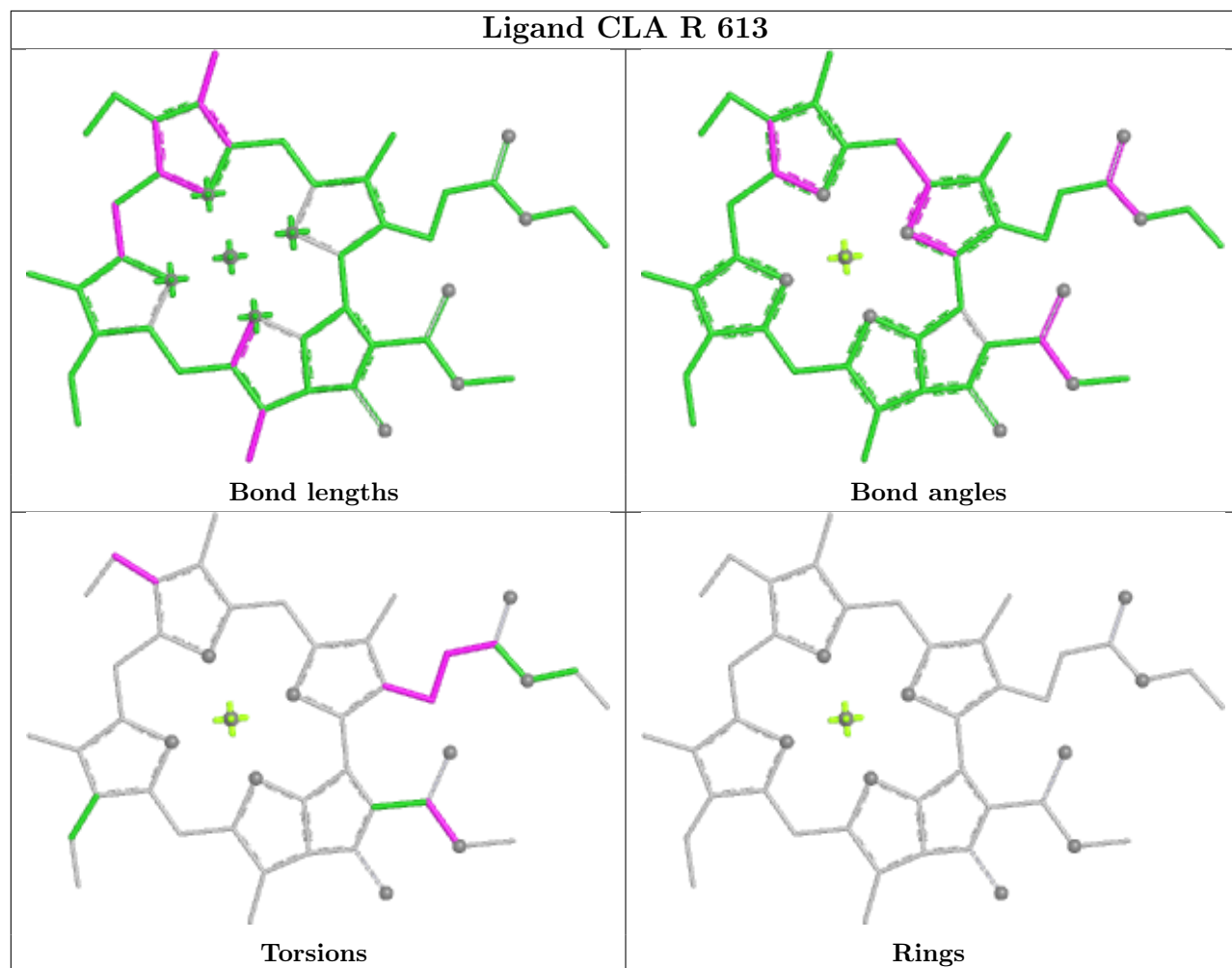
Ligand 0IE y 302



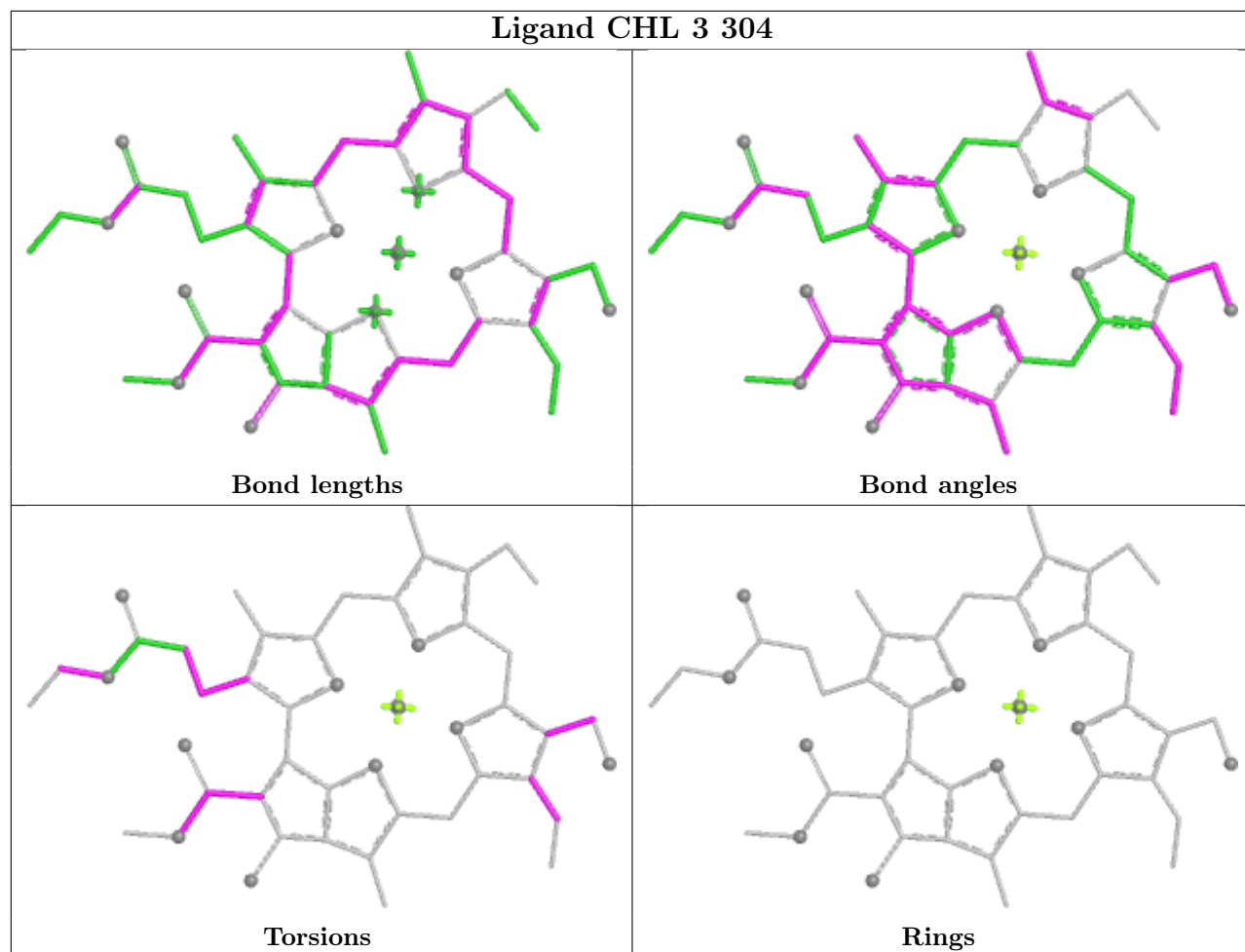
Ligand CLA 6 306



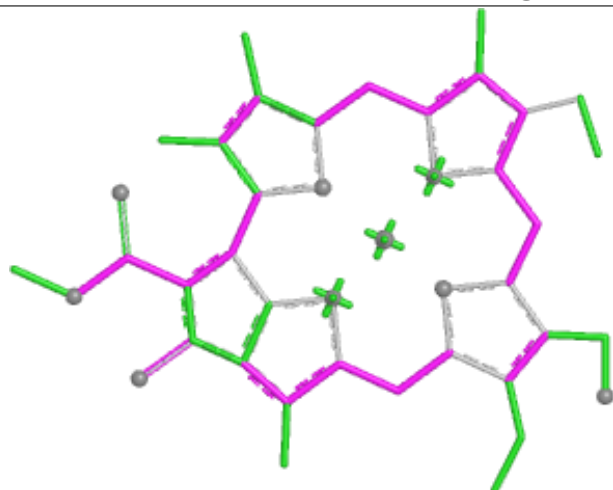
Ligand CLA R 613



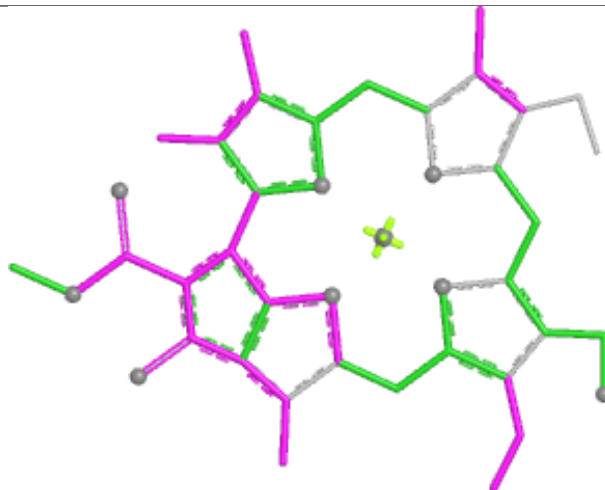
Ligand CHL 3 304



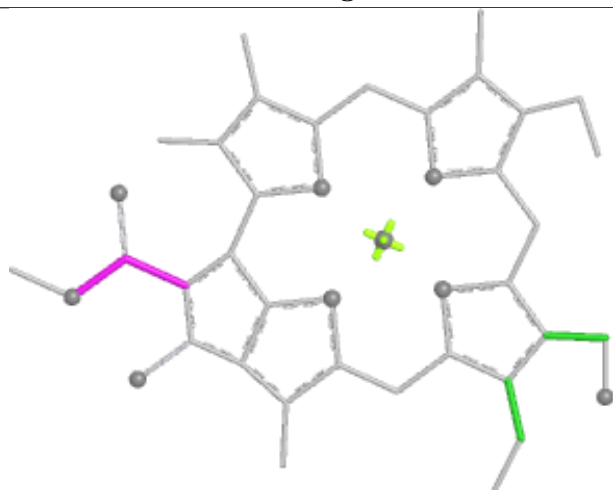
Ligand CHL 7 318



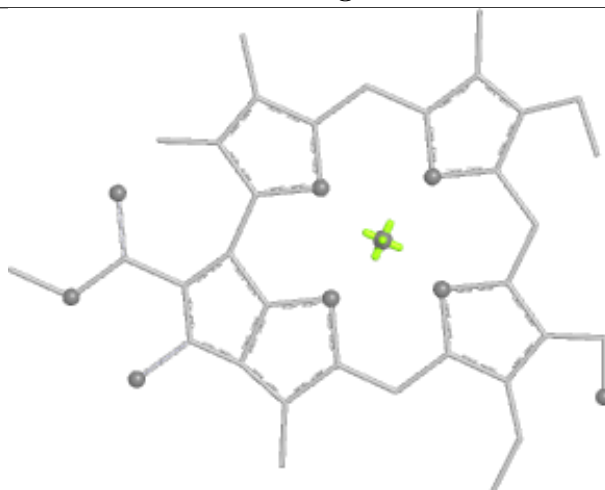
Bond lengths



Bond angles

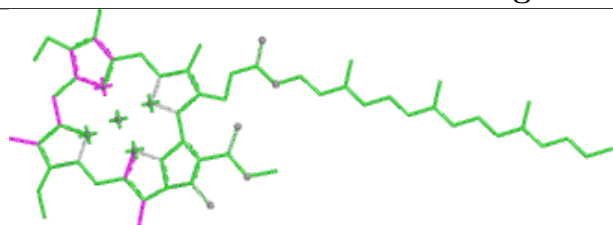


Torsions

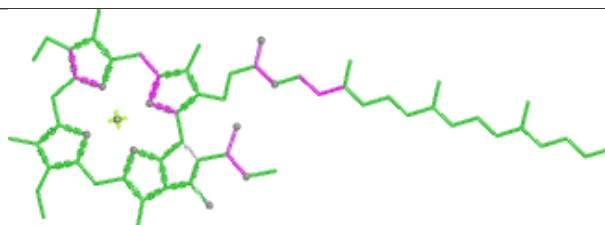


Rings

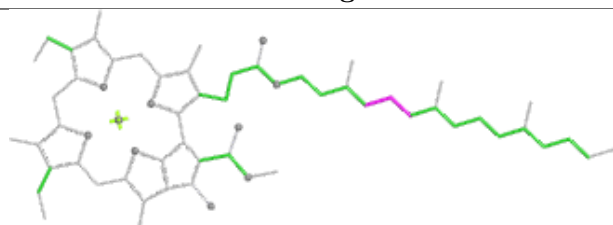
Ligand CLA N 314



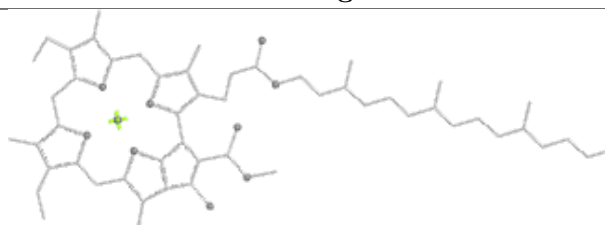
Bond lengths



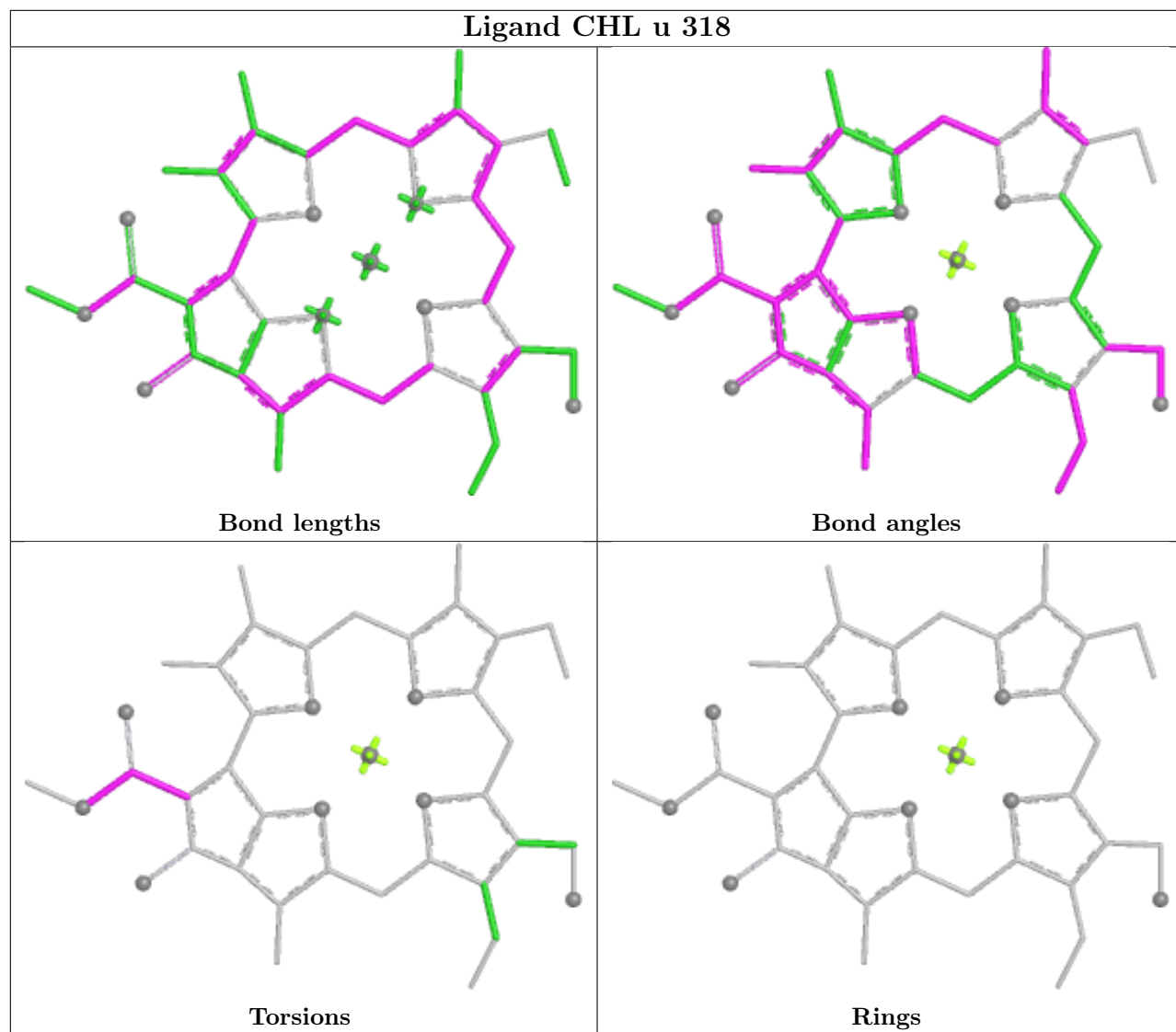
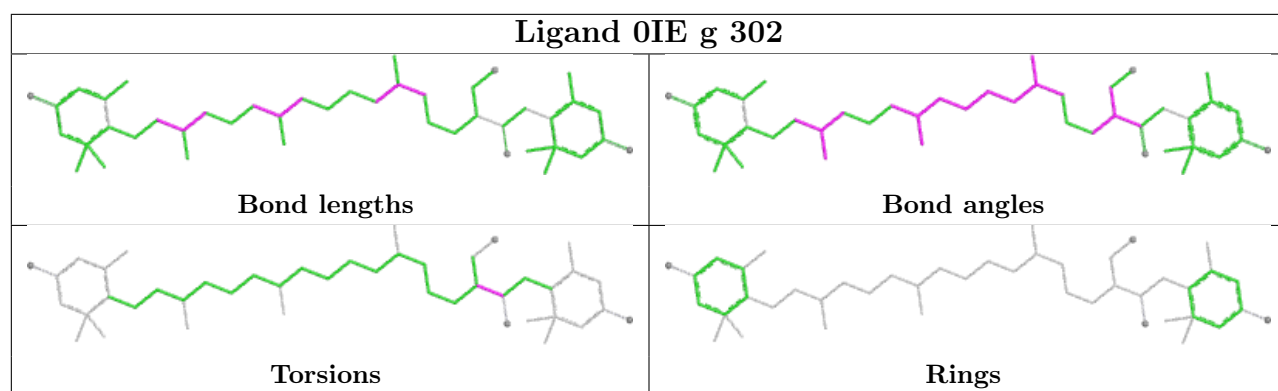
Bond angles



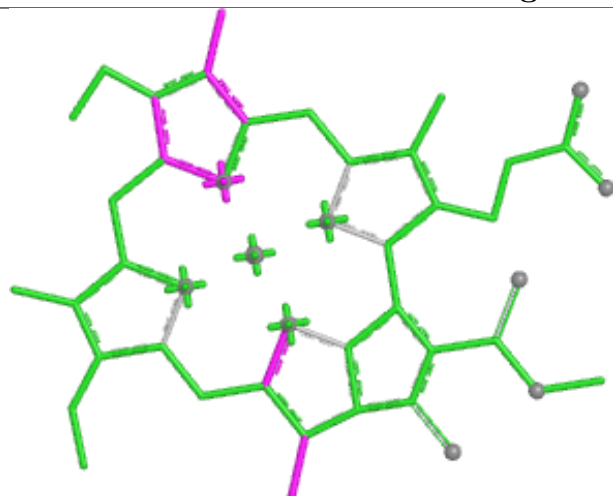
Torsions



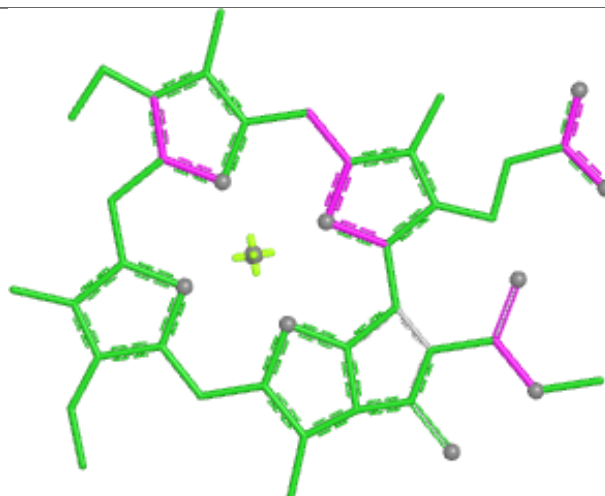
Rings



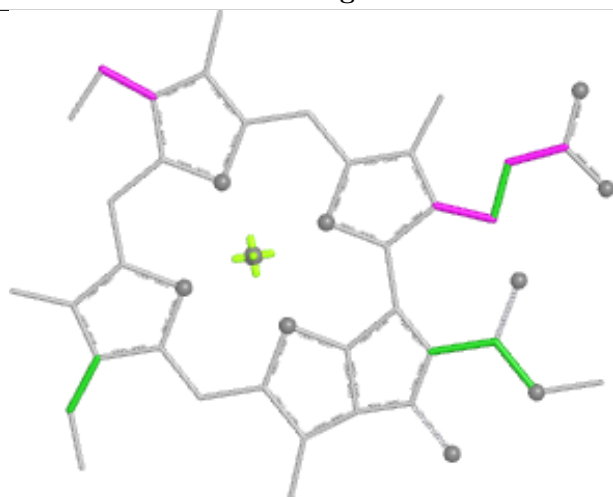
Ligand CLA r 313



Bond lengths



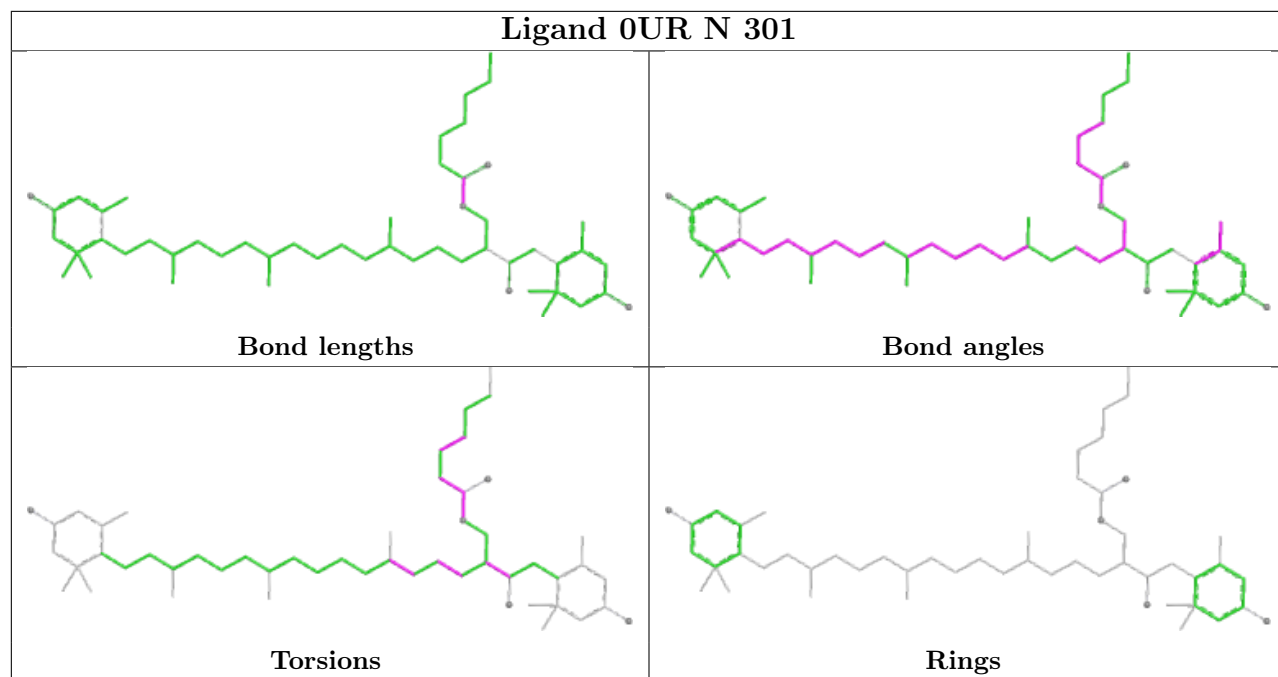
Bond angles



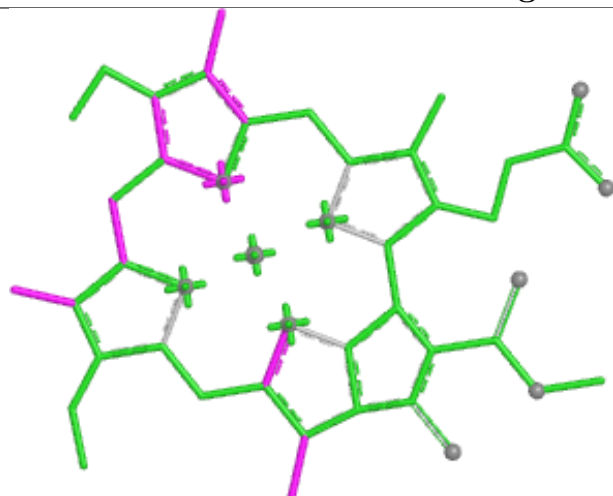
Torsions



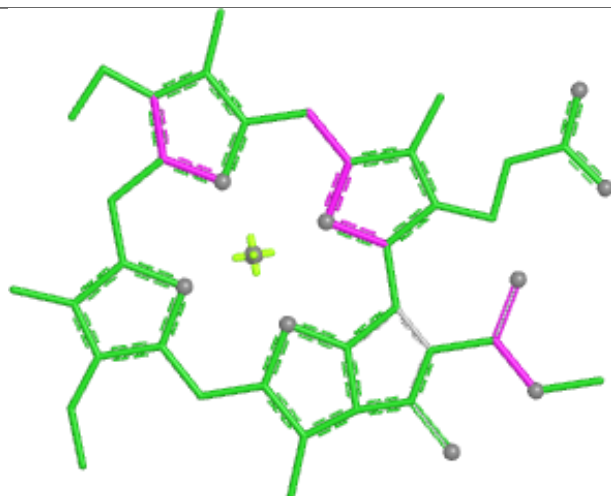
Rings



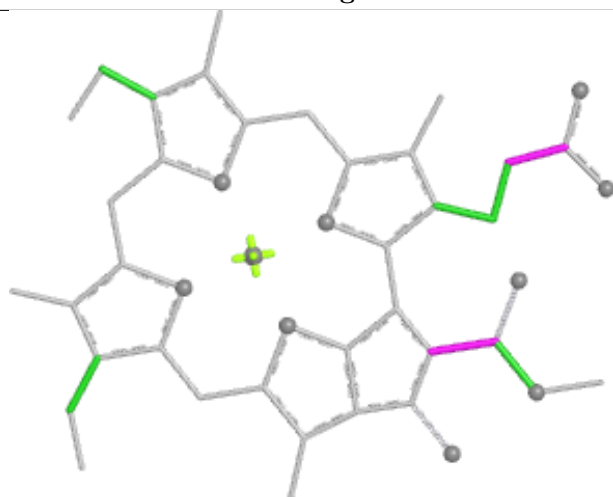
Ligand CLA 7 316



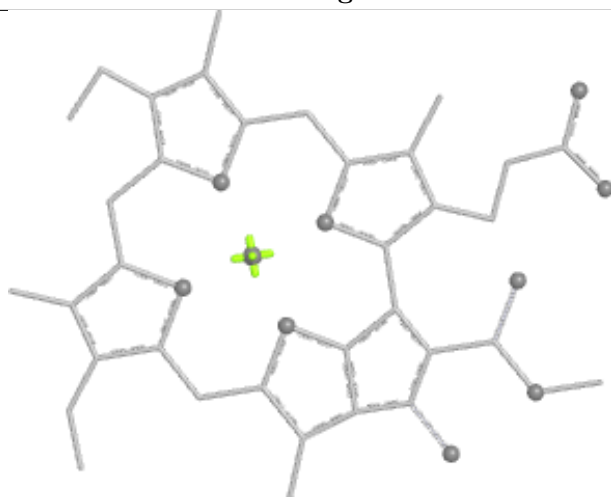
Bond lengths



Bond angles

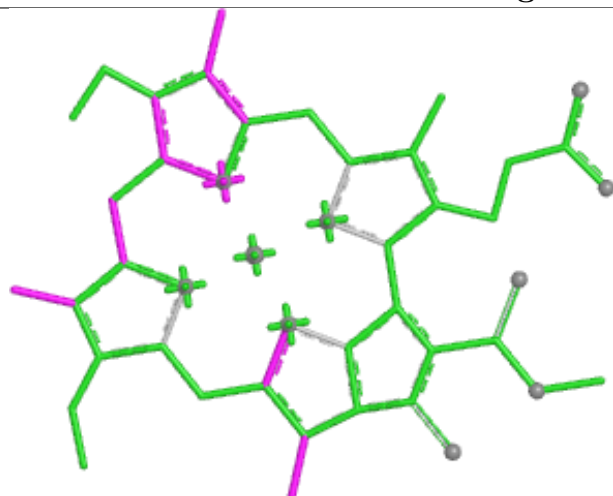


Torsions

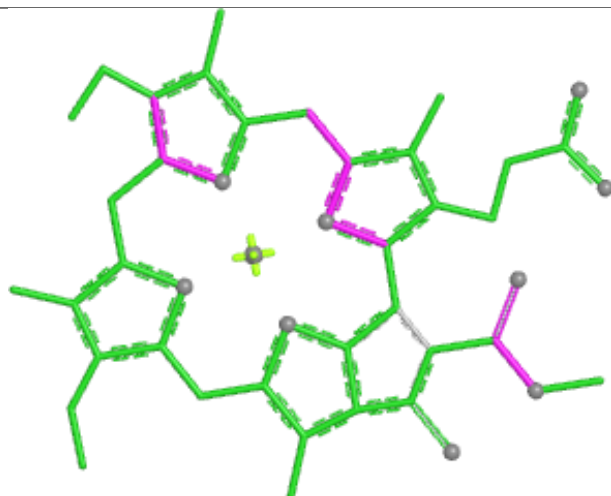


Rings

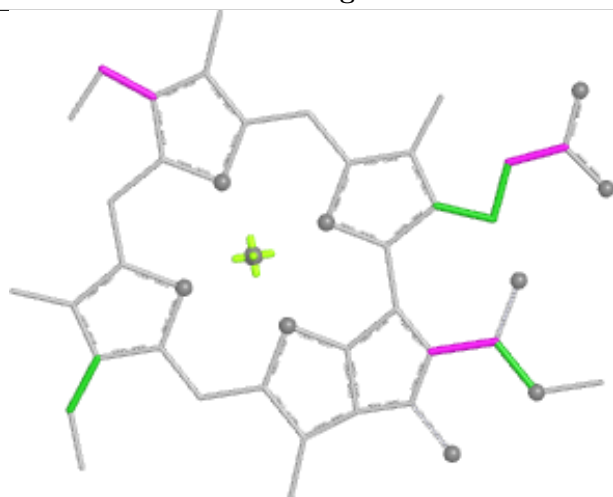
Ligand CLA u 316



Bond lengths



Bond angles

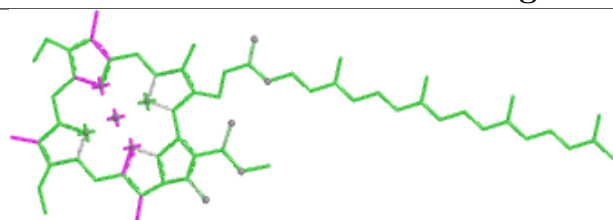


Torsions

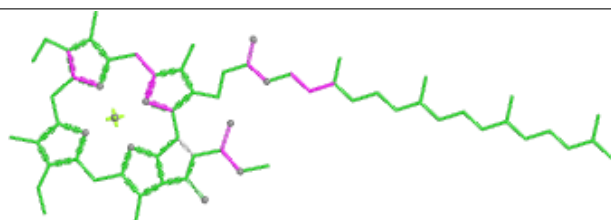


Rings

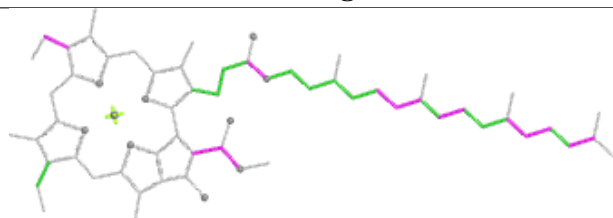
Ligand CLA c 602



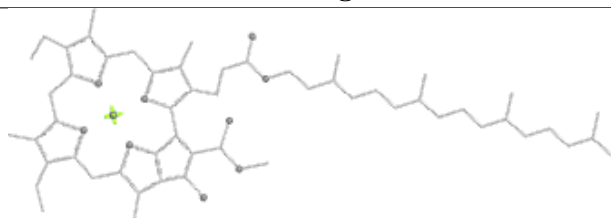
Bond lengths



Bond angles

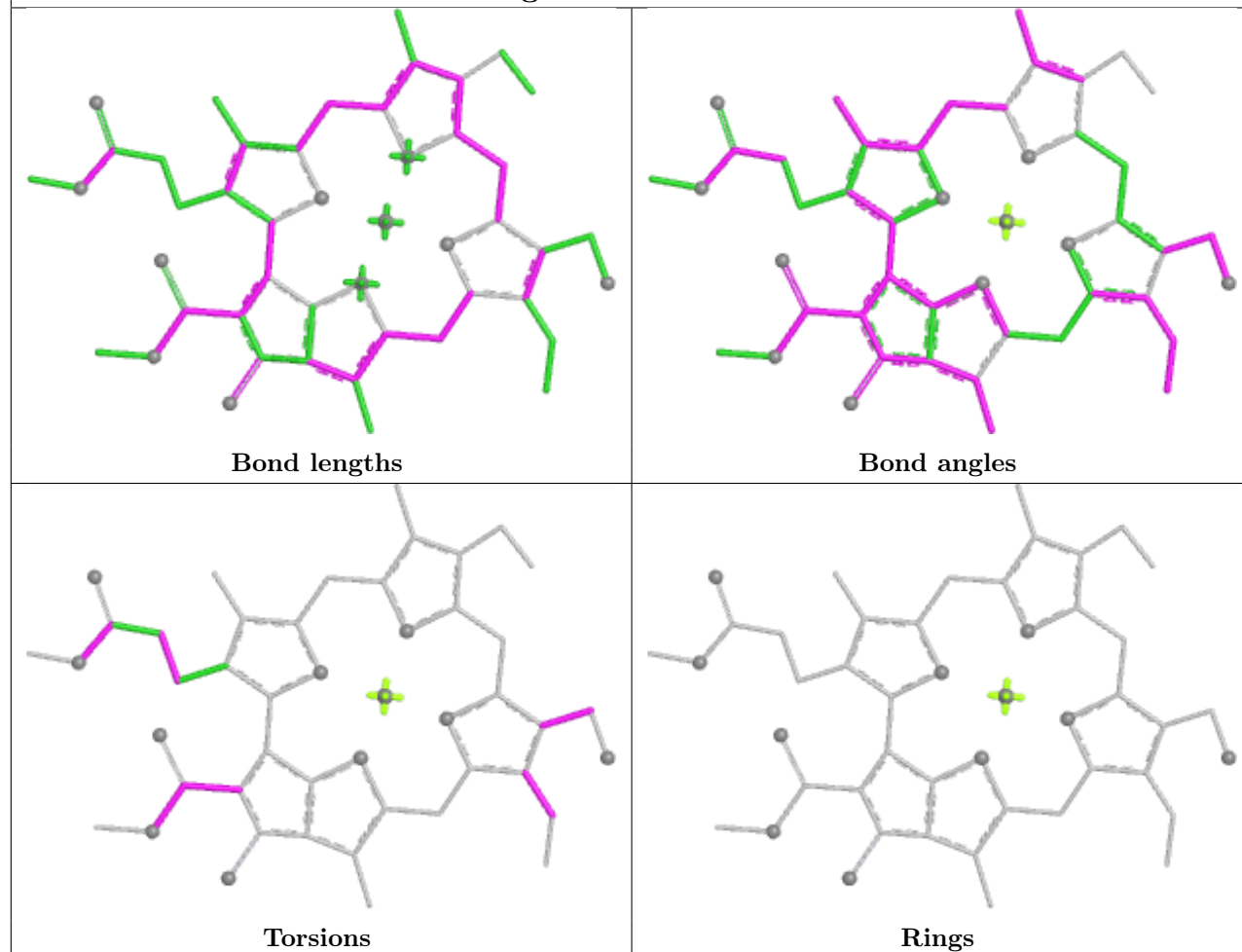


Torsions

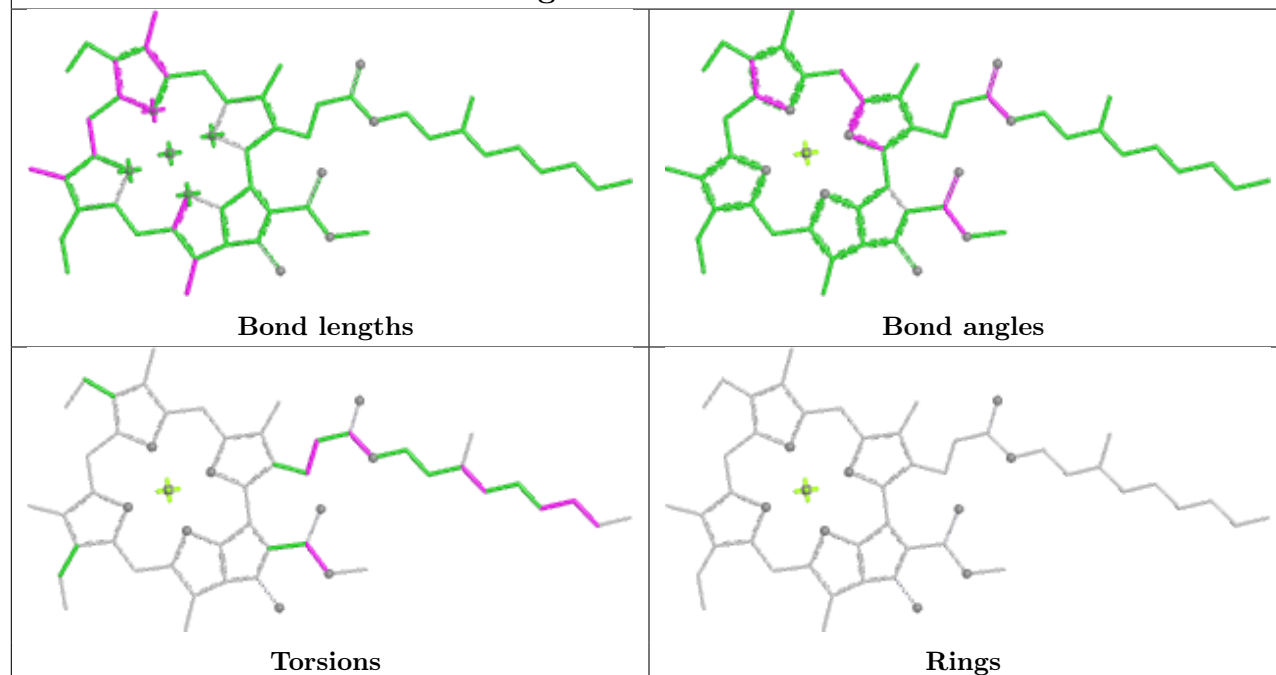


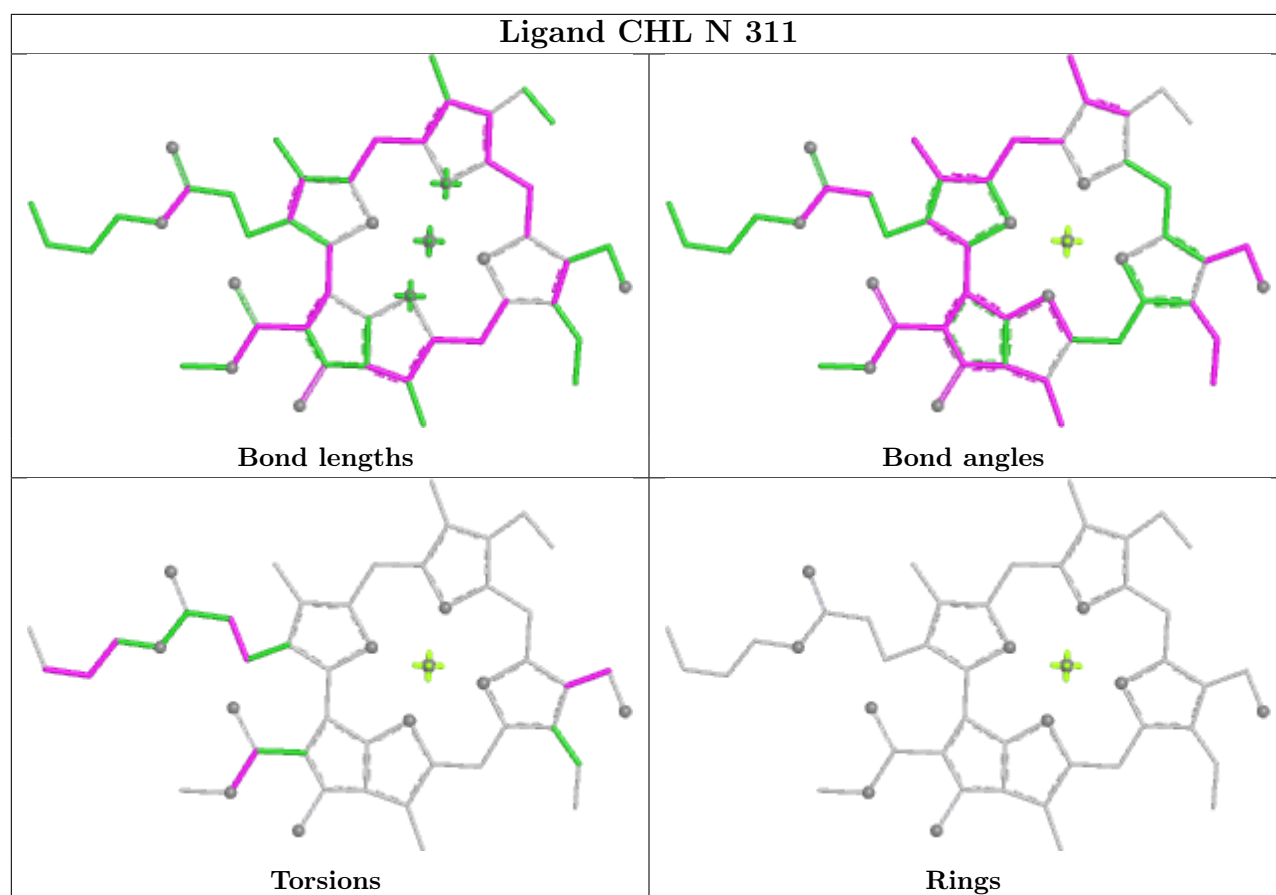
Rings

Ligand CHL 5 306

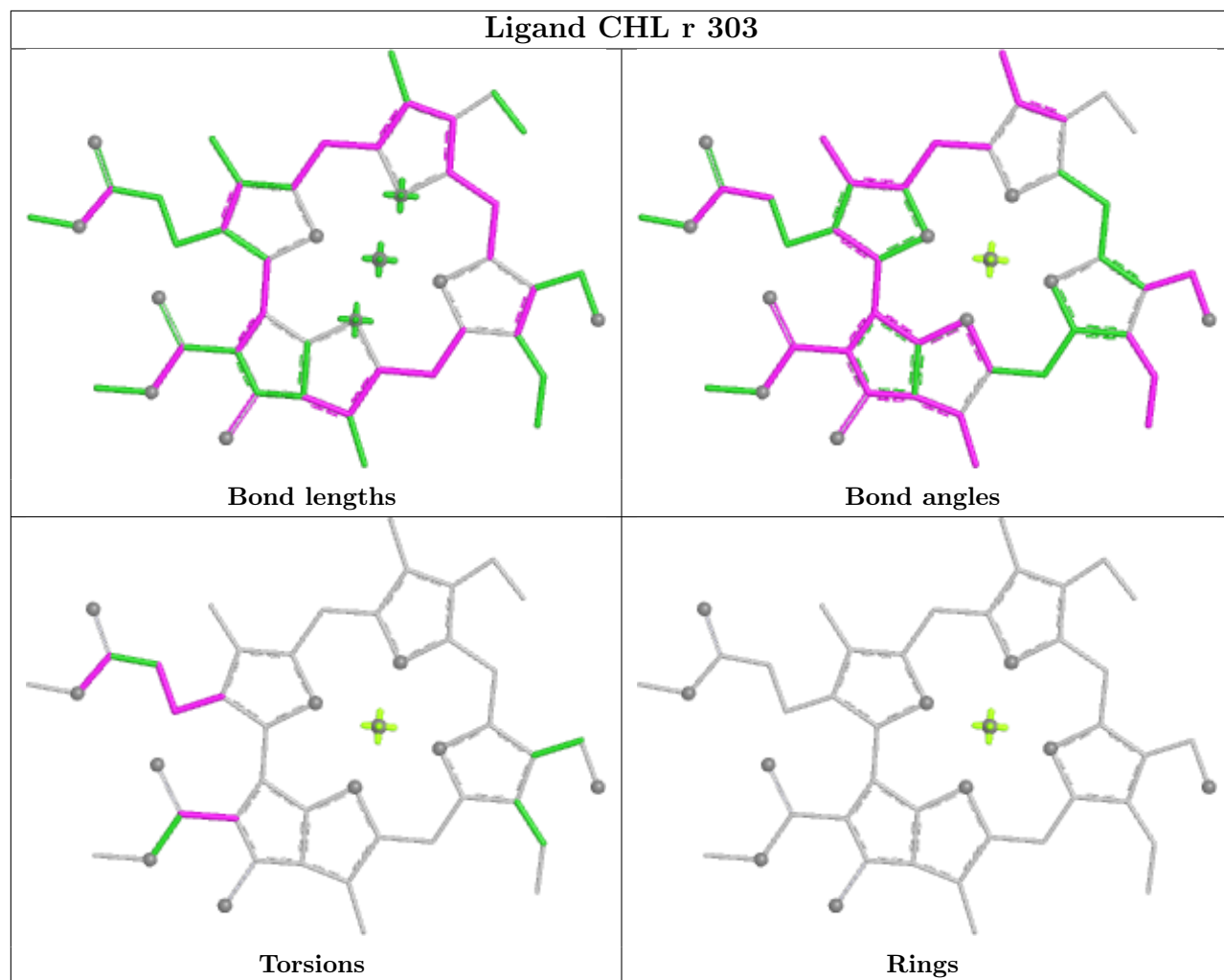


Ligand CLA s 413

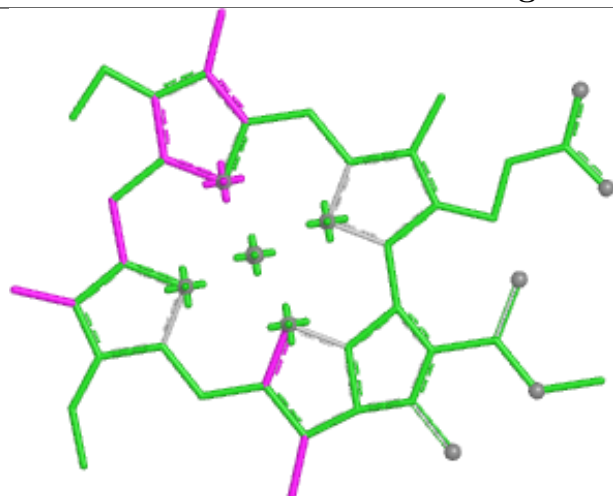




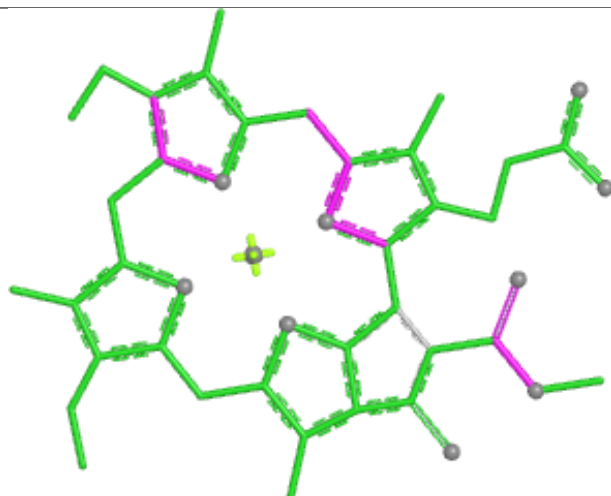
Ligand CHL r 303



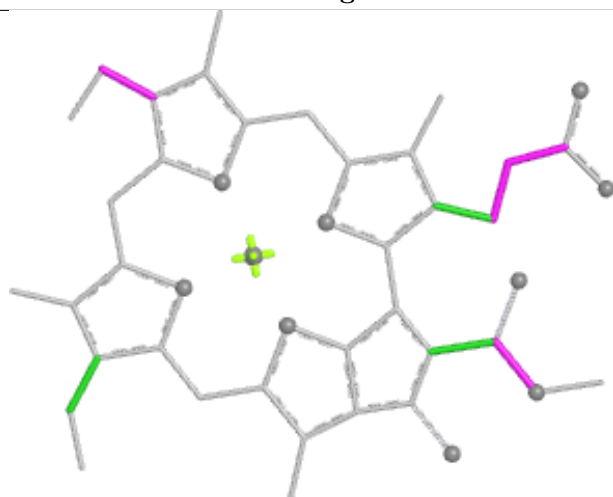
Ligand CLA 3 316



Bond lengths



Bond angles

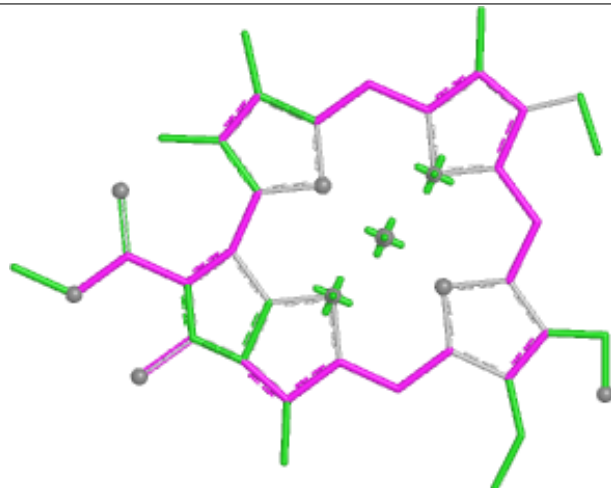


Torsions

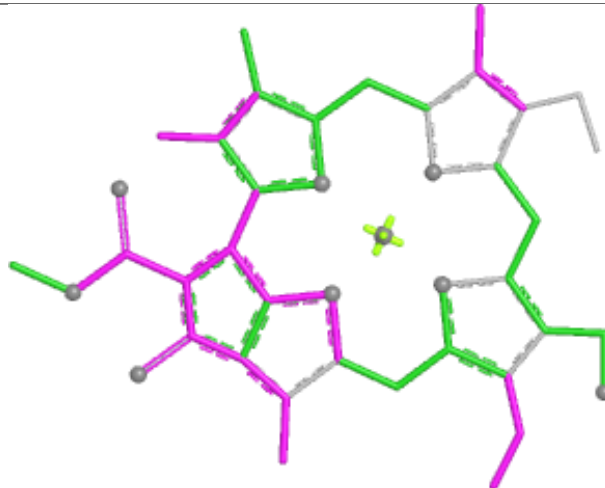


Rings

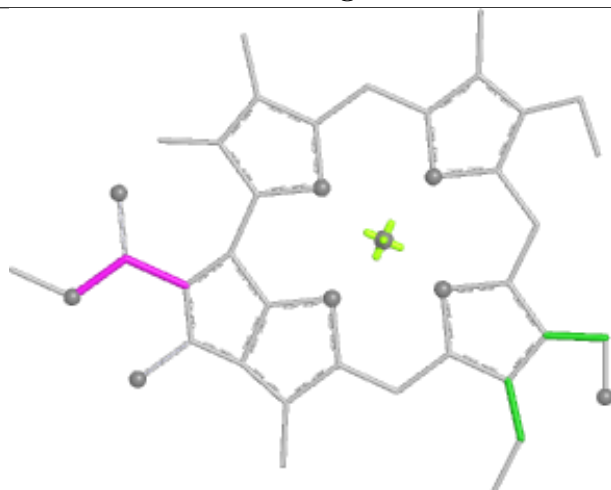
Ligand CHL p 318



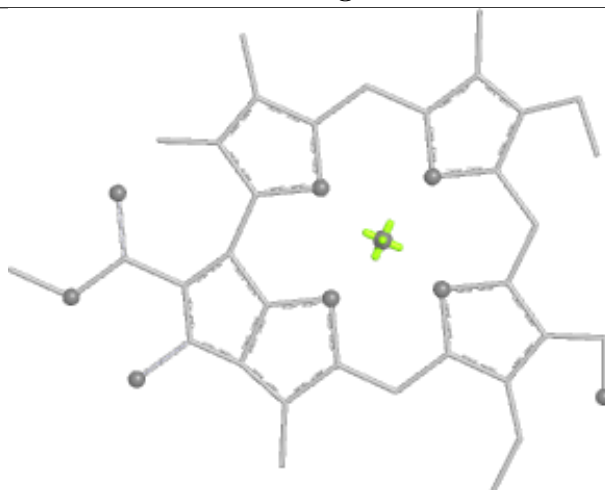
Bond lengths



Bond angles

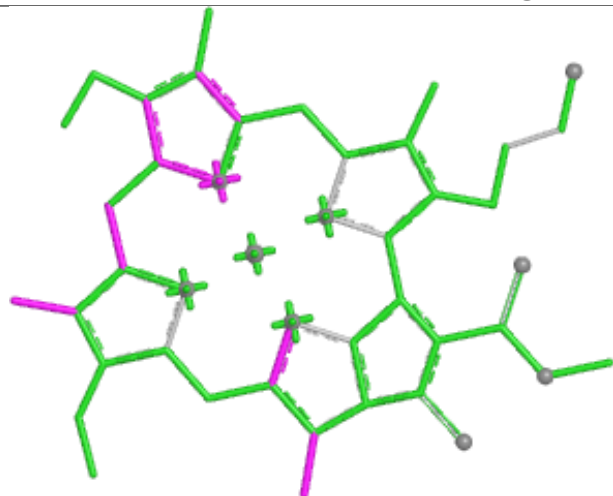


Torsions

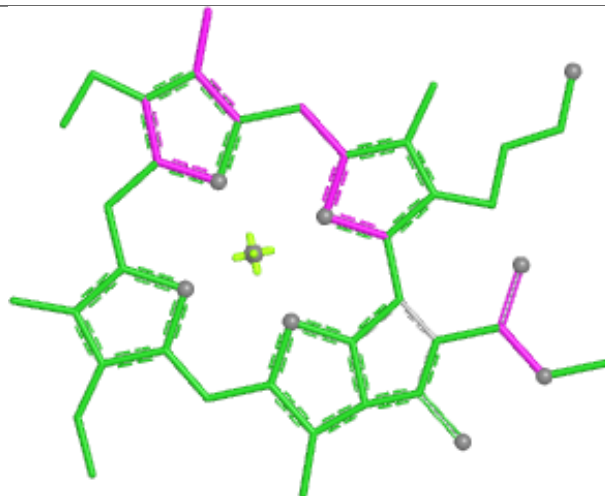


Rings

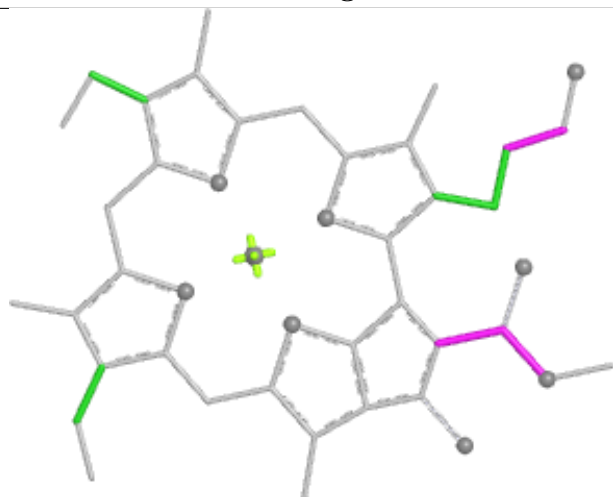
Ligand CLA 4 306



Bond lengths



Bond angles

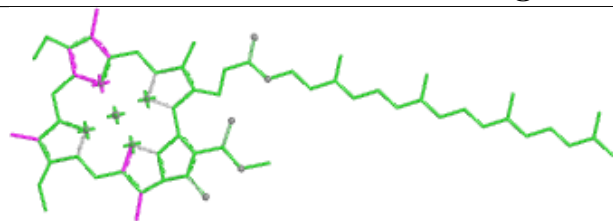


Torsions

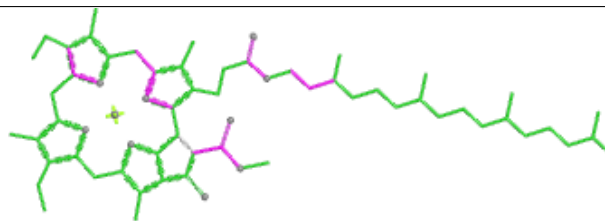


Rings

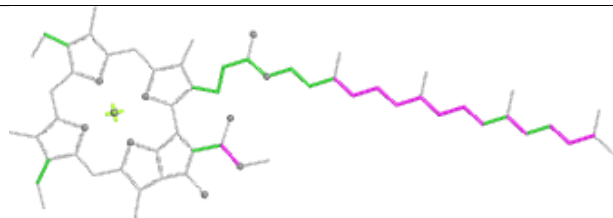
Ligand CLA B 609



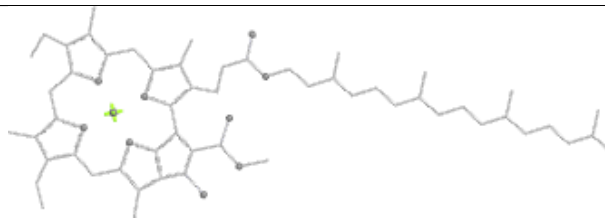
Bond lengths



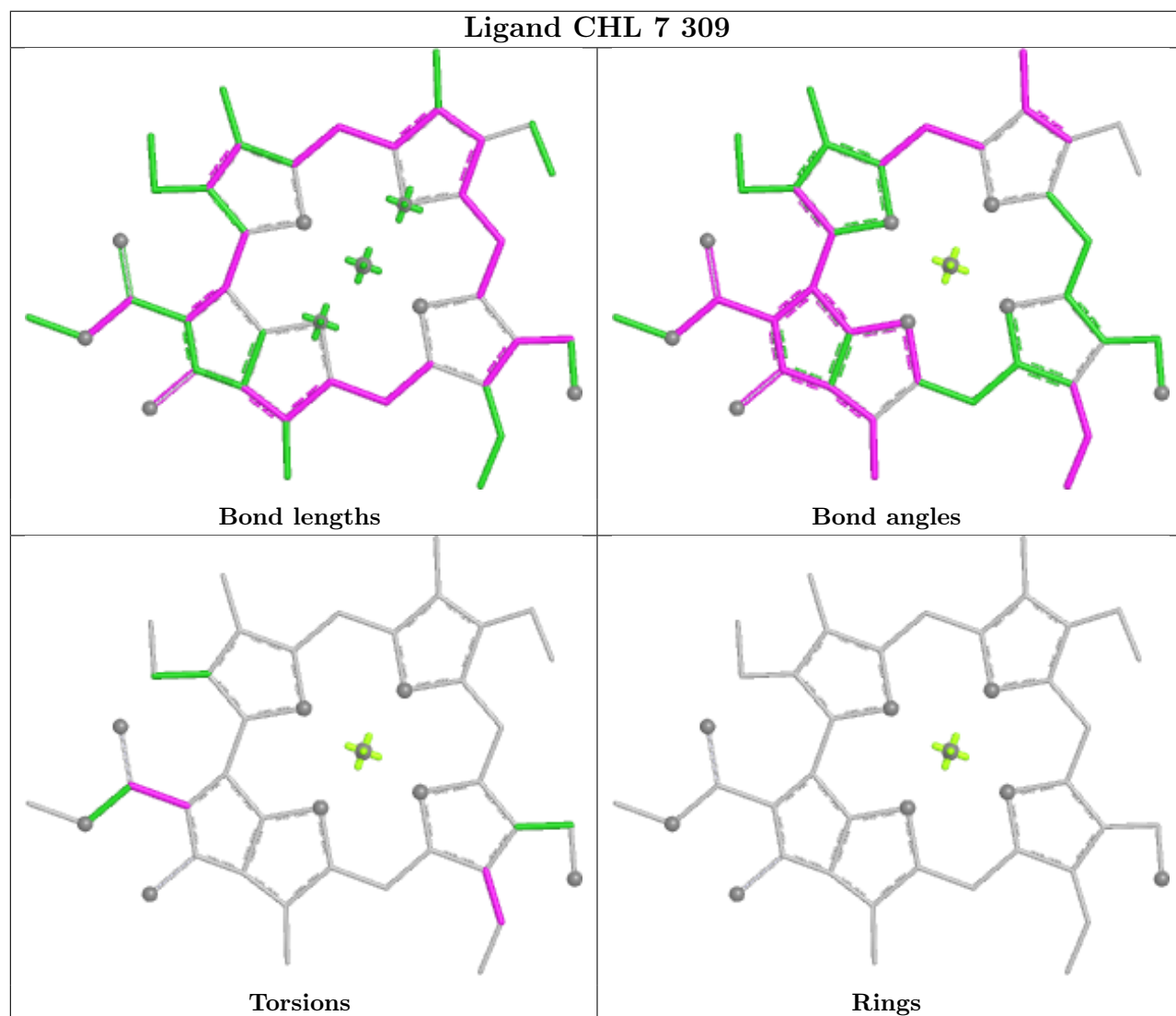
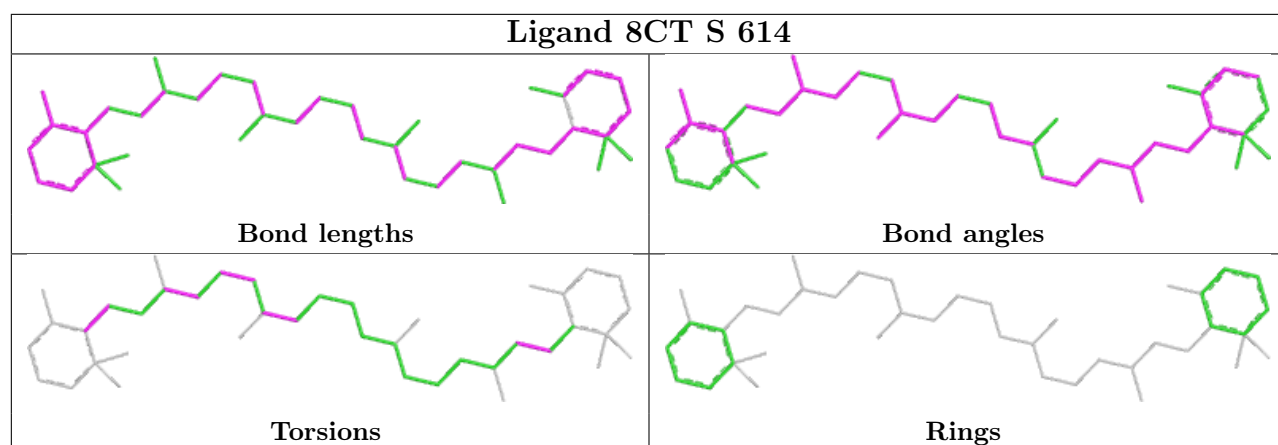
Bond angles



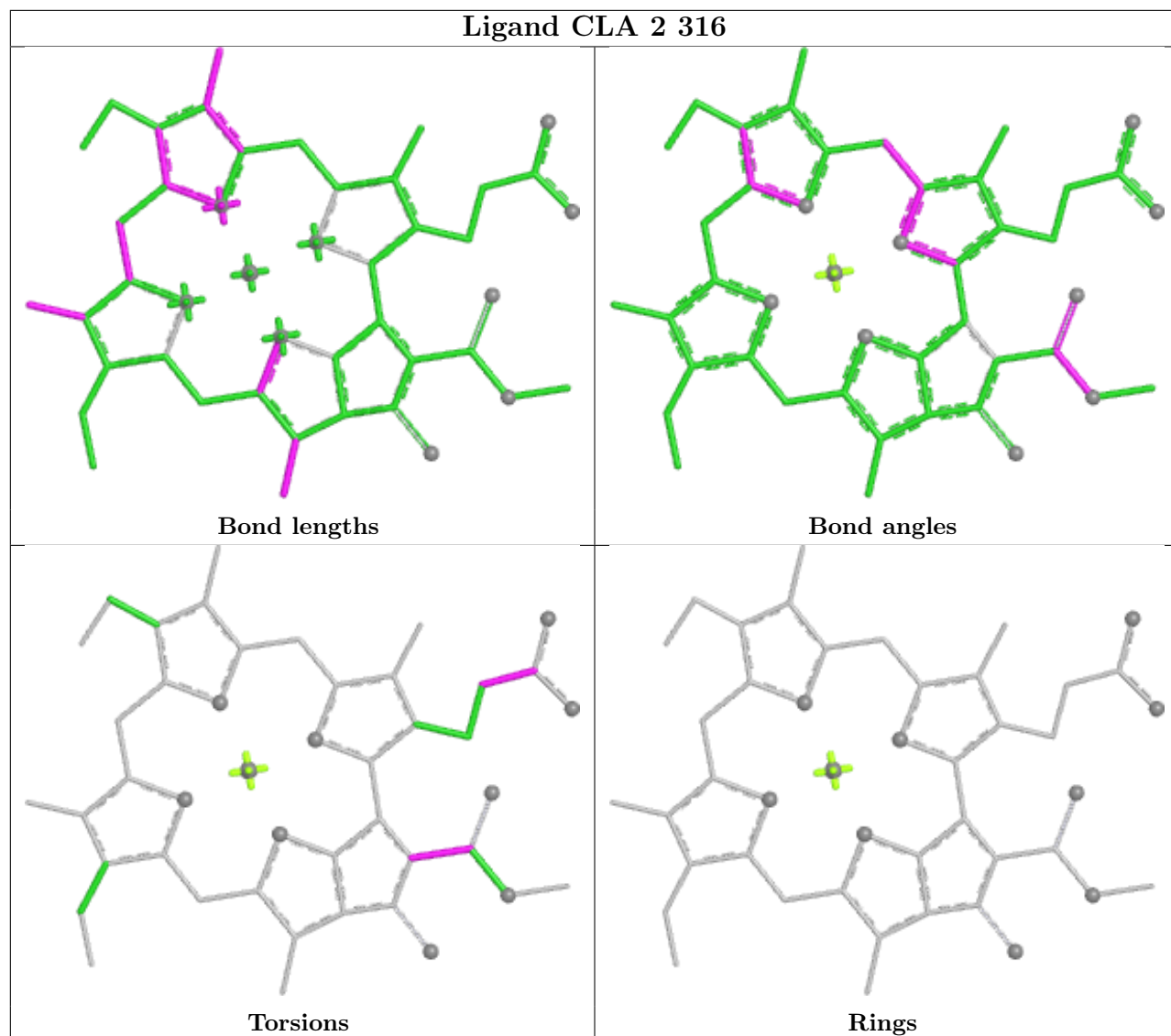
Torsions



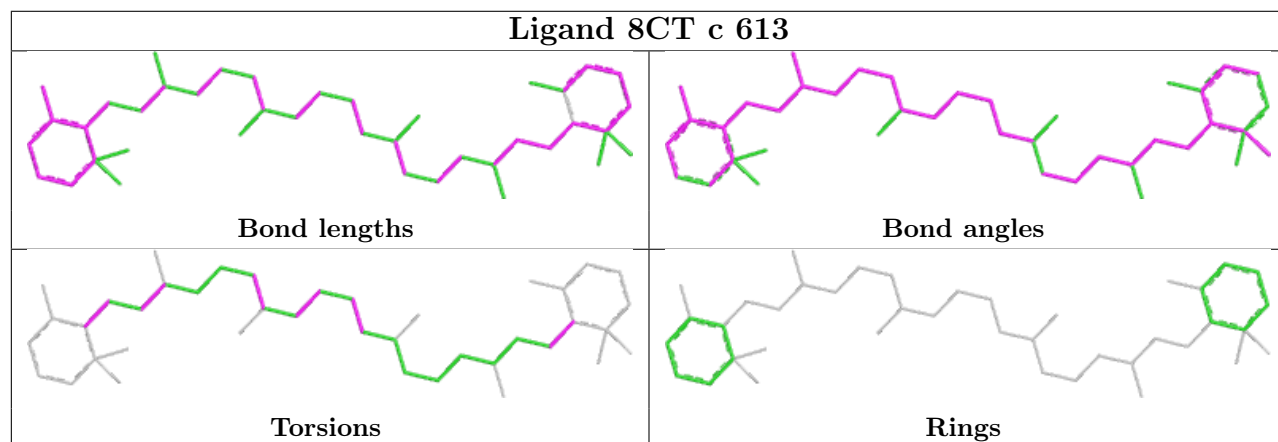
Rings

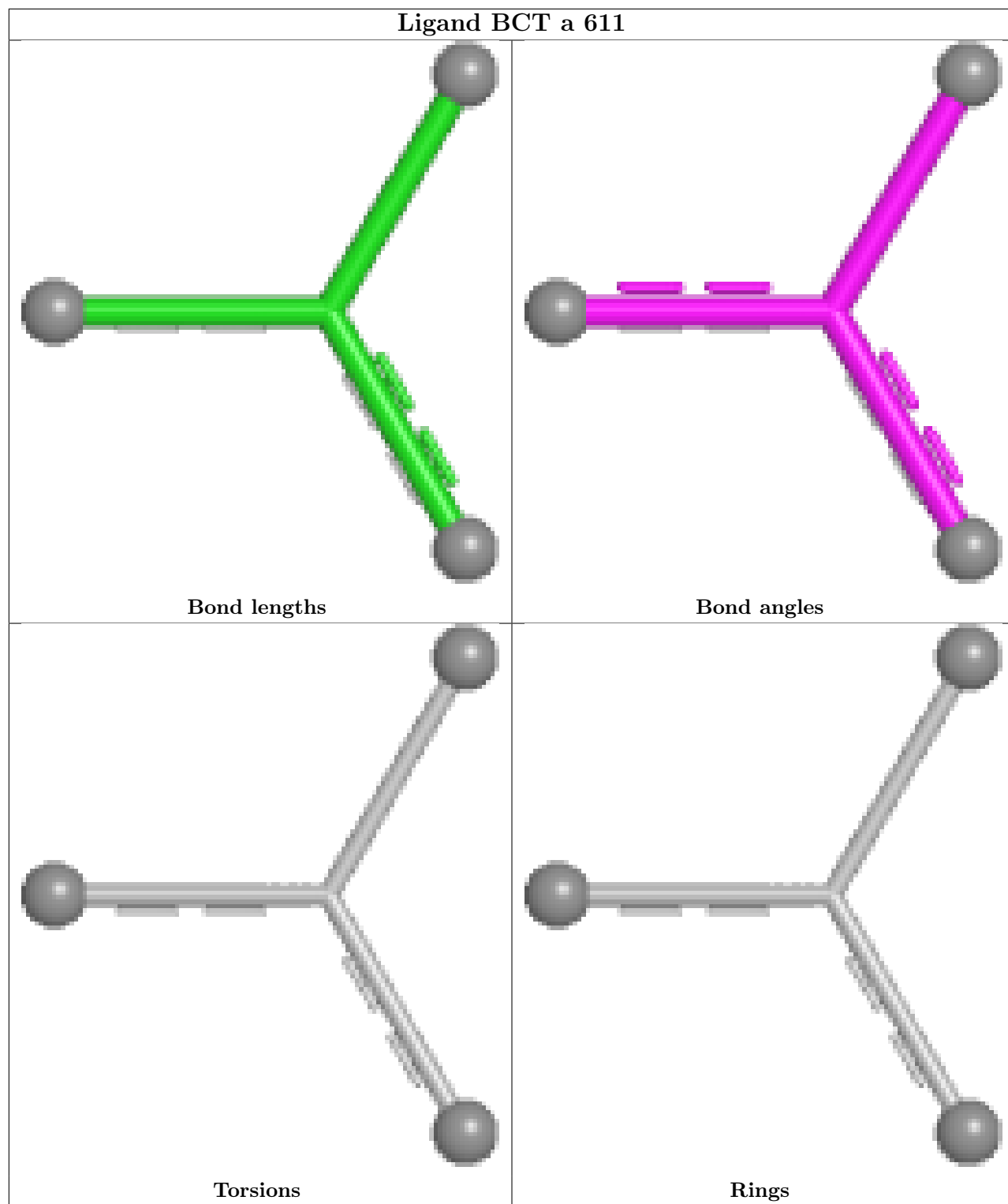


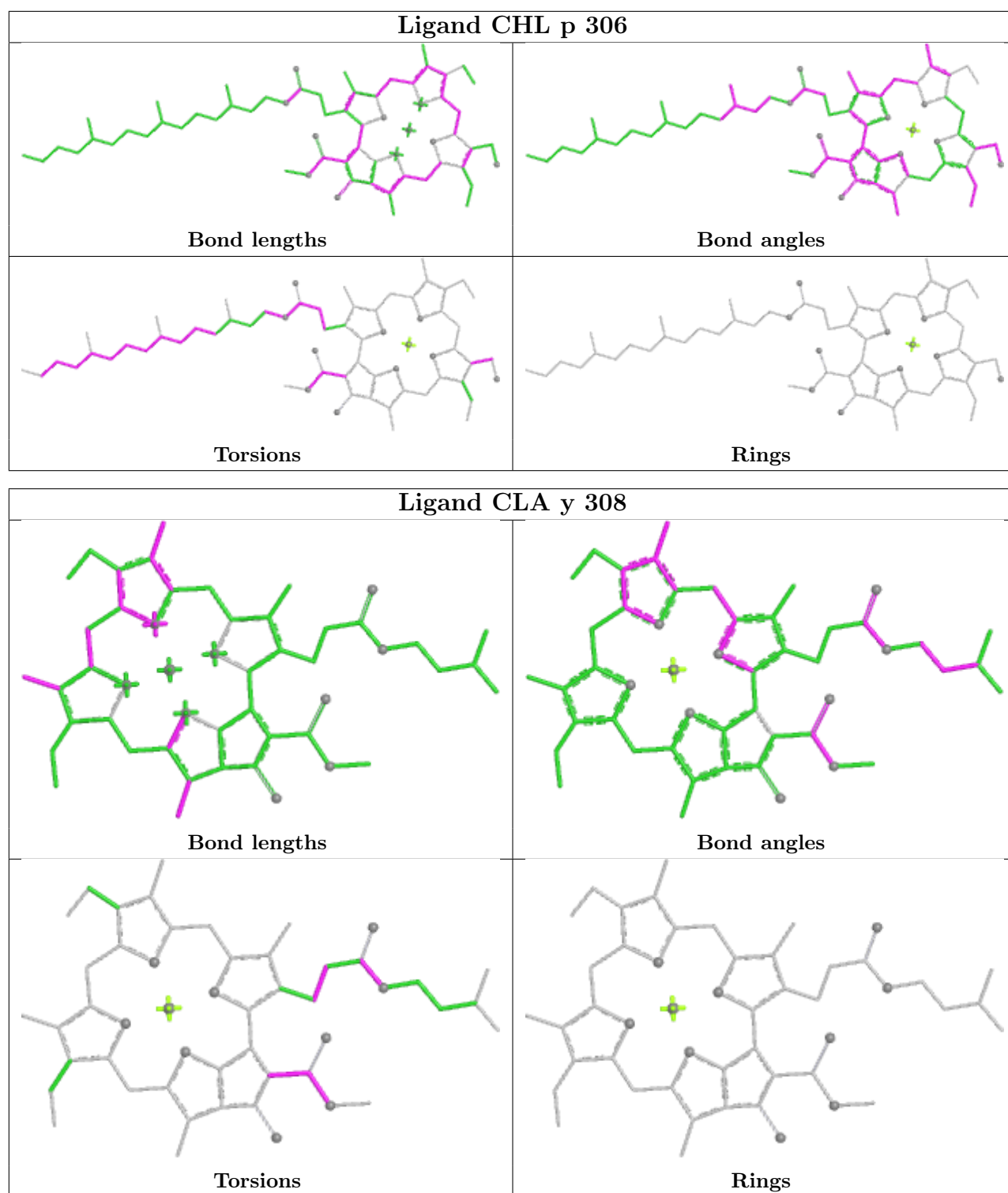
Ligand CLA 2 316



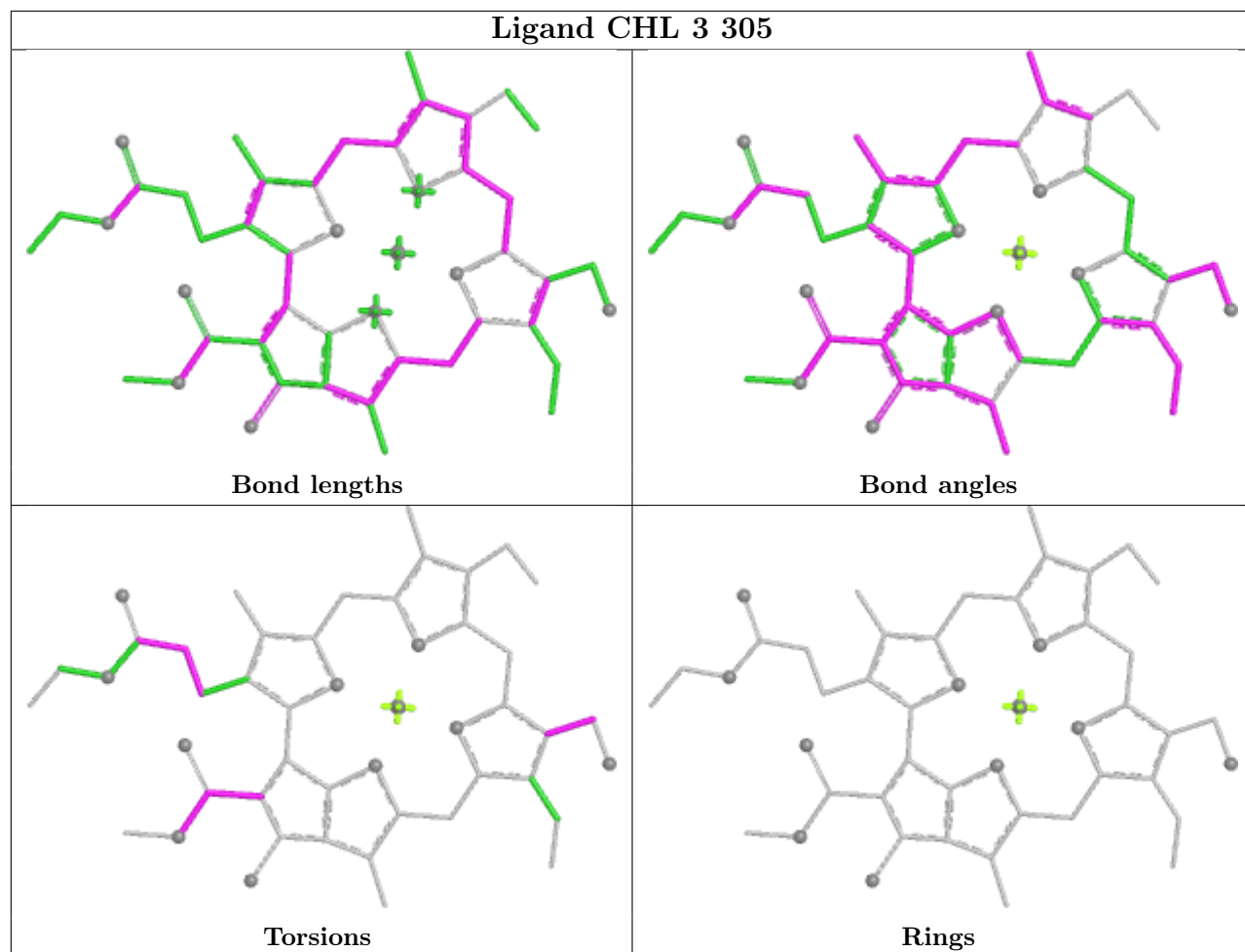
Ligand 8CT c 613



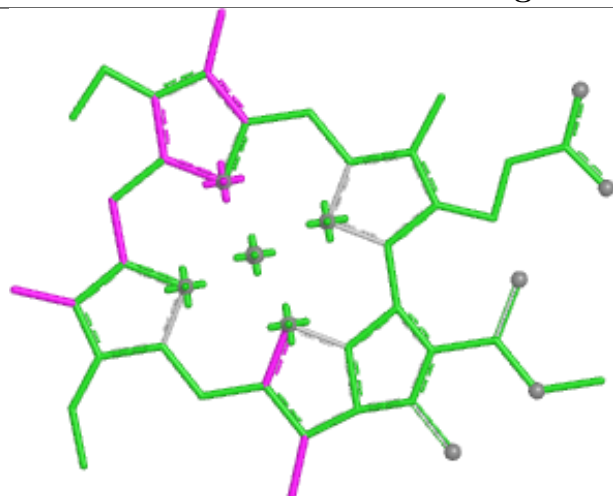




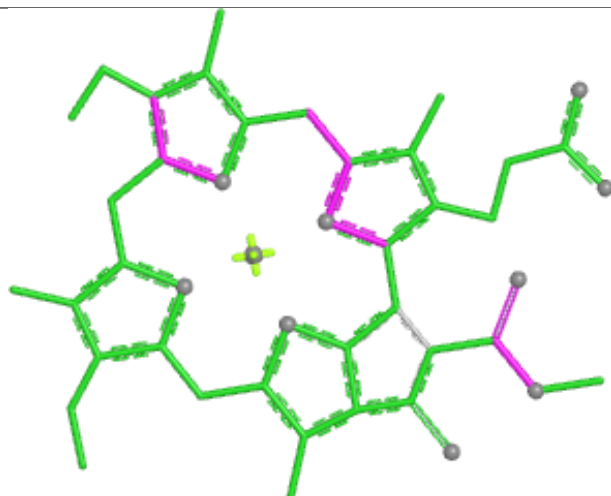
Ligand CHL 3 305



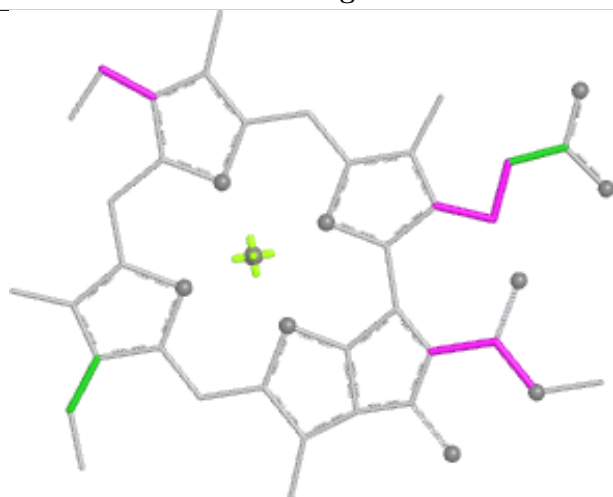
Ligand CLA B 601



Bond lengths



Bond angles

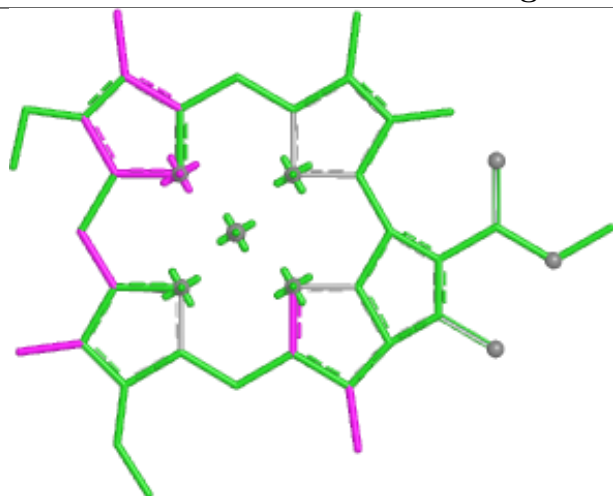


Torsions

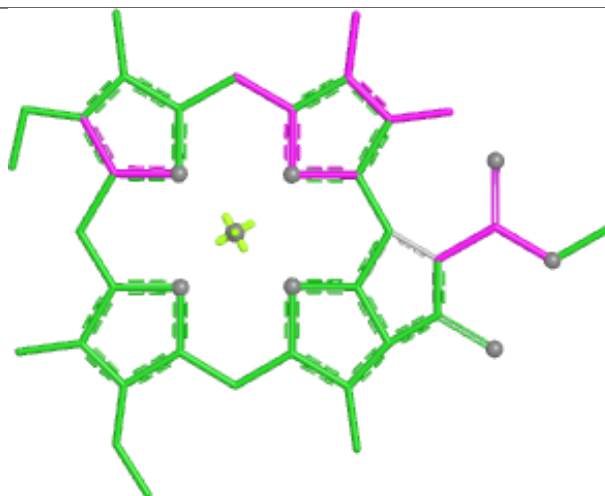


Rings

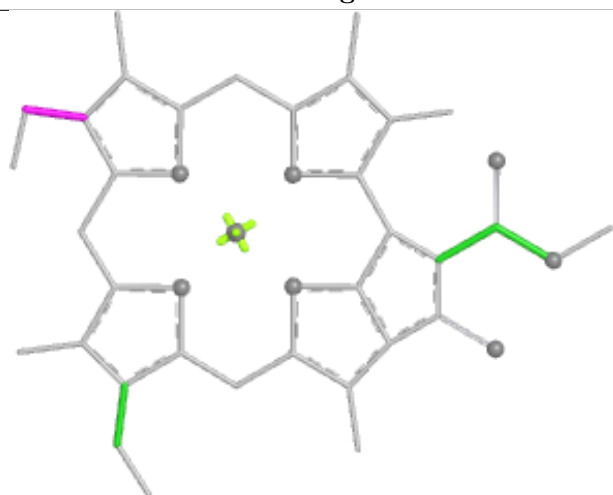
Ligand CLA r 305



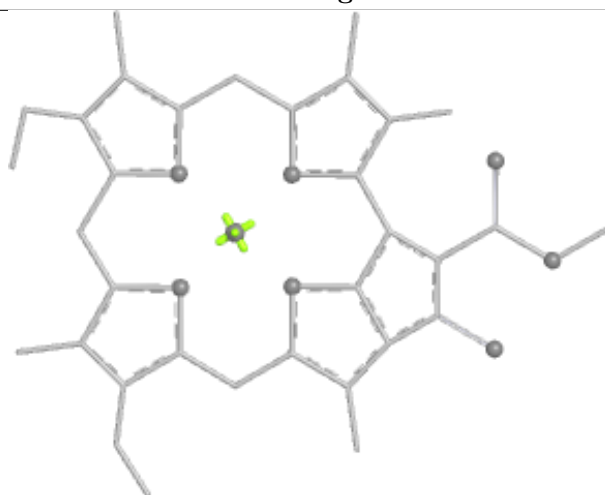
Bond lengths



Bond angles

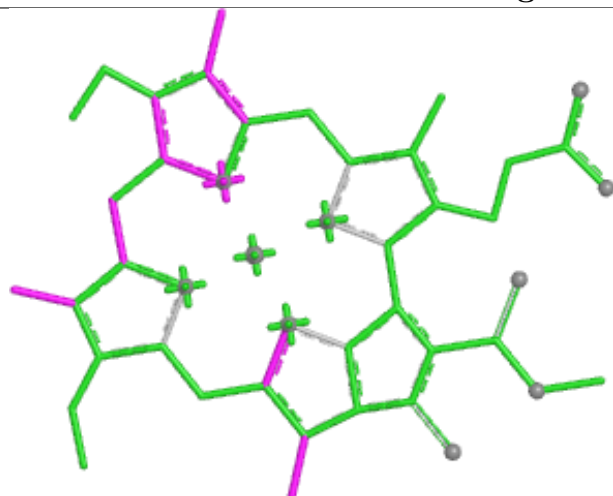


Torsions

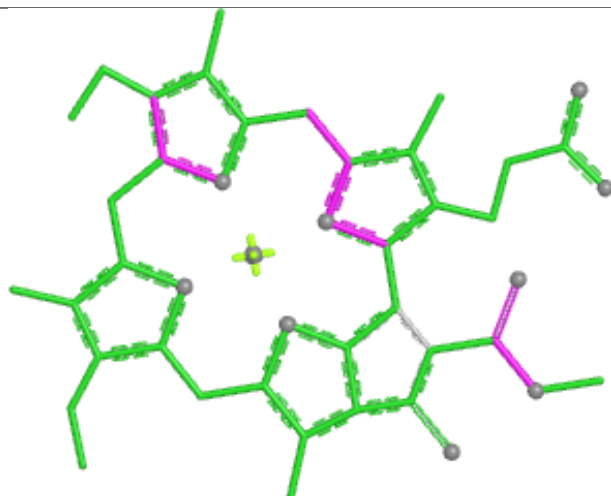


Rings

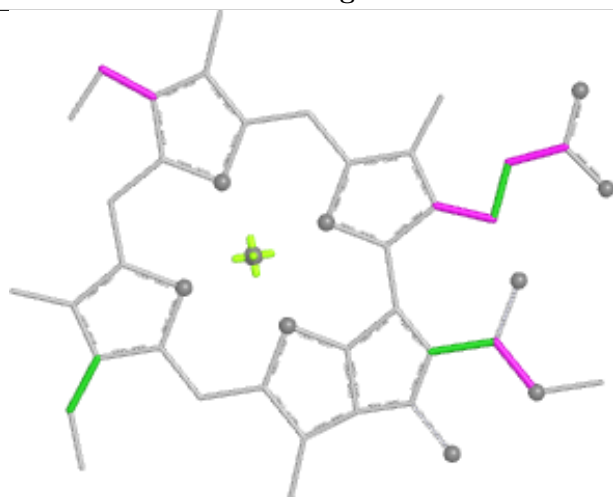
Ligand CLA S 616



Bond lengths



Bond angles

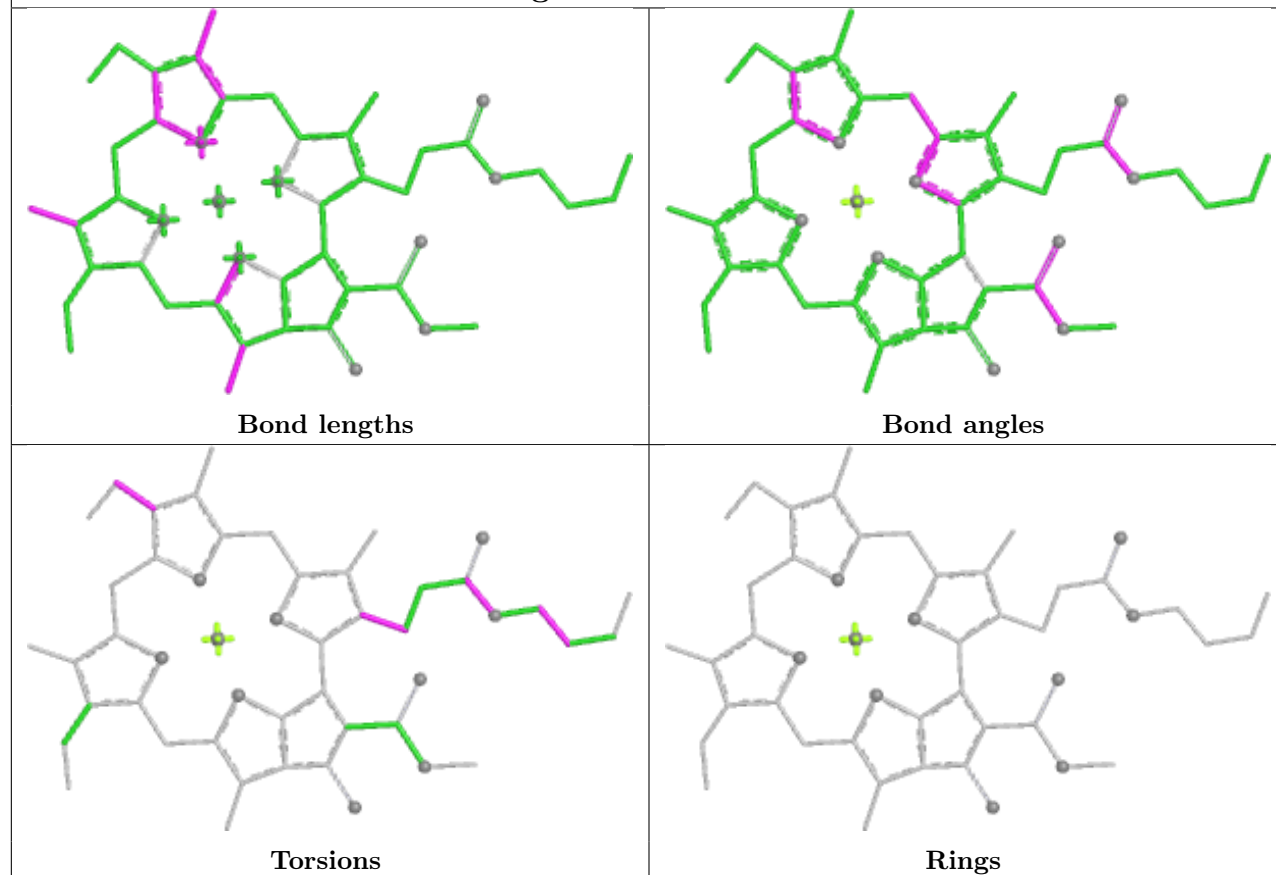


Torsions

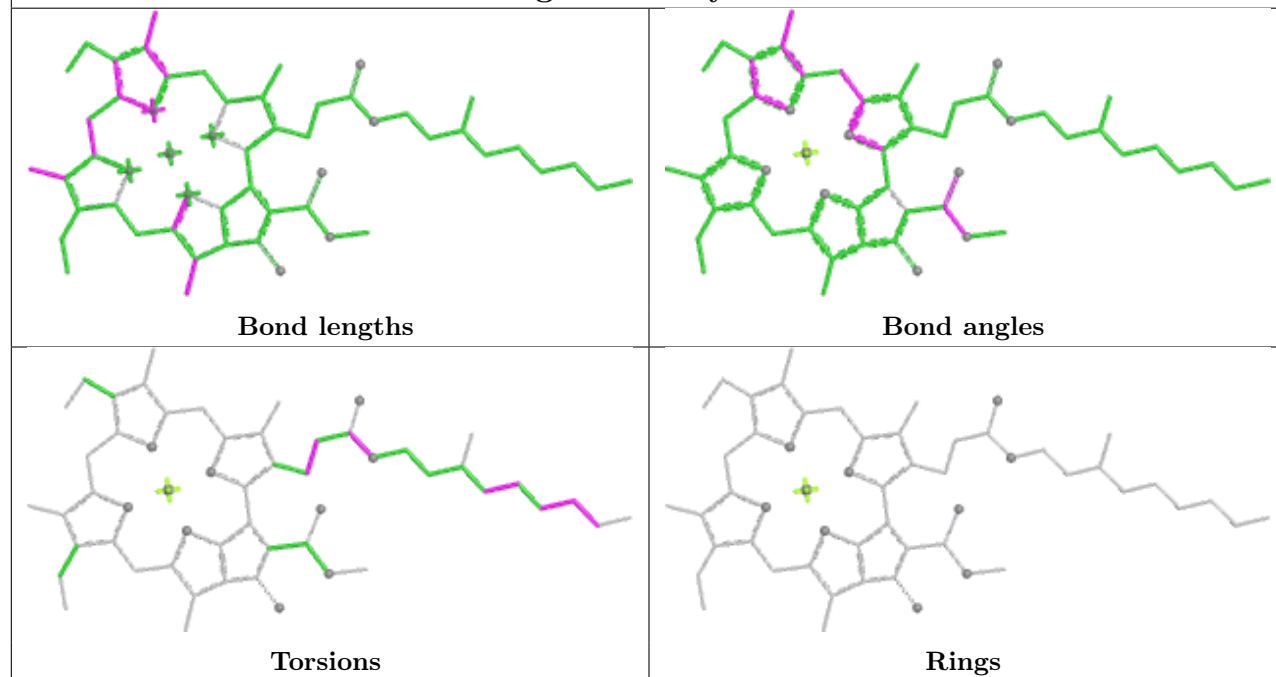


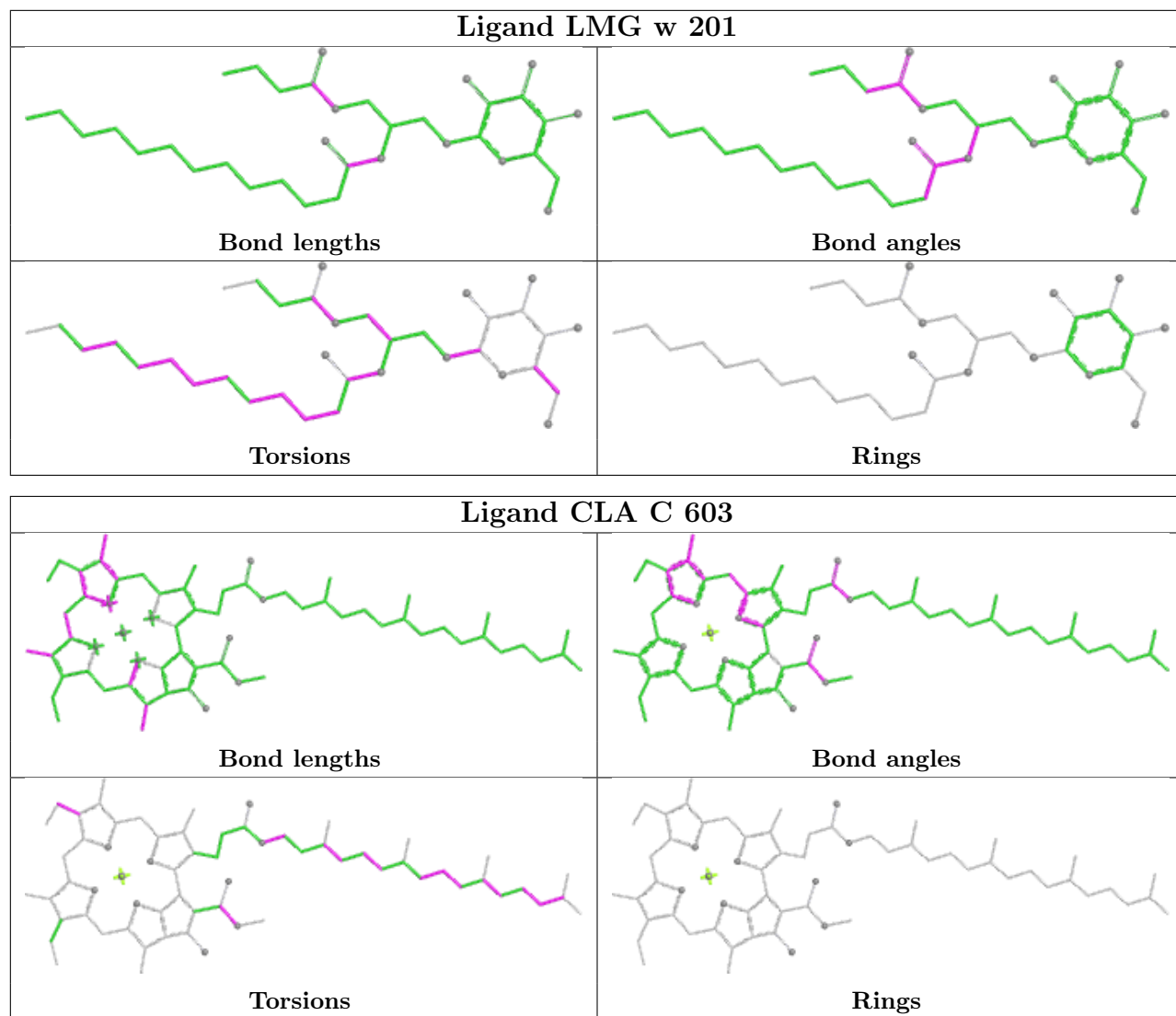
Rings

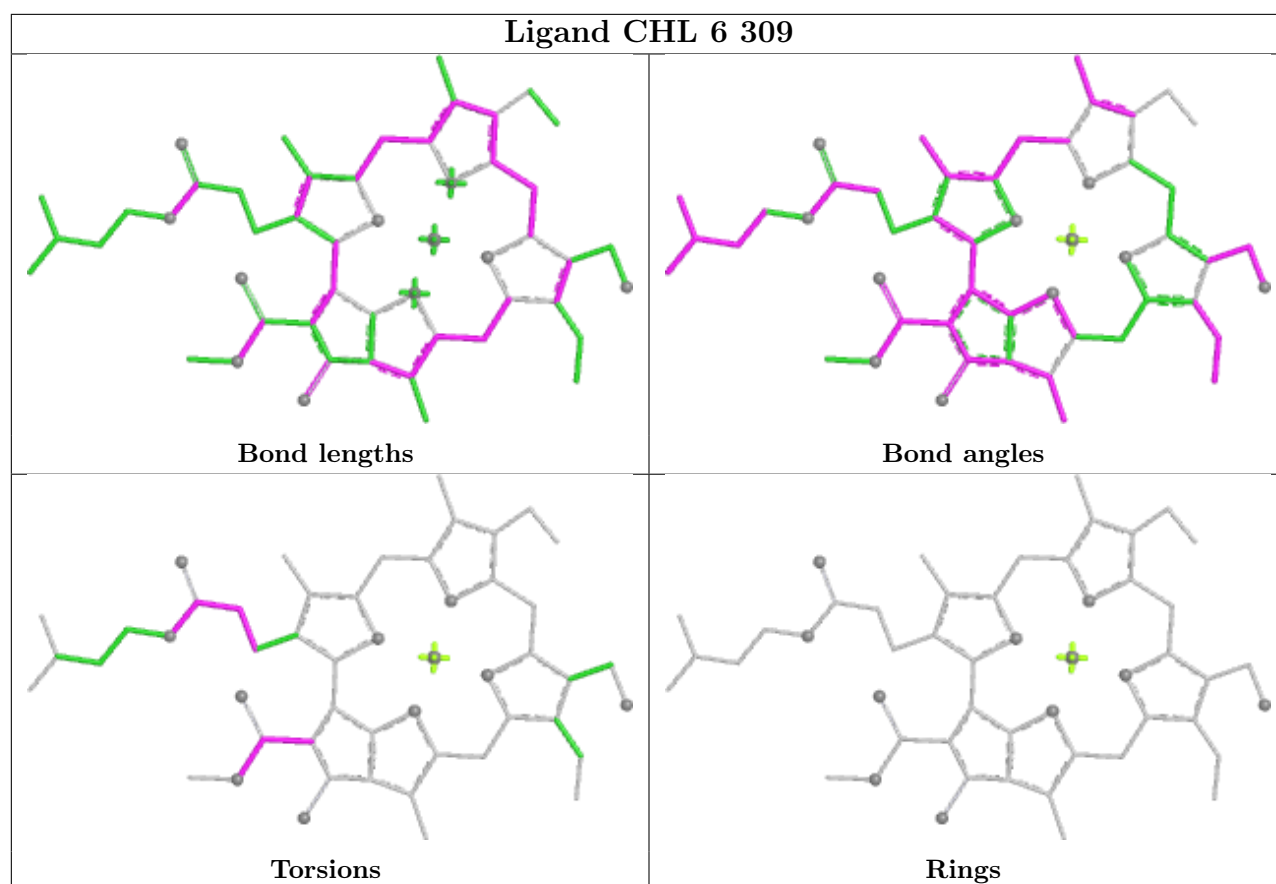
Ligand CLA A 605



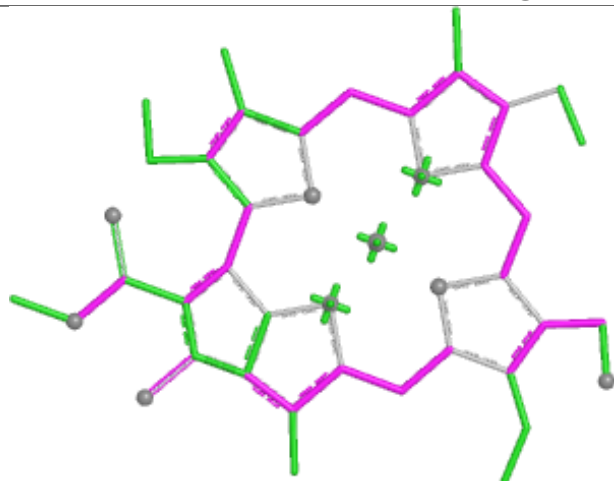
Ligand CLA y 317



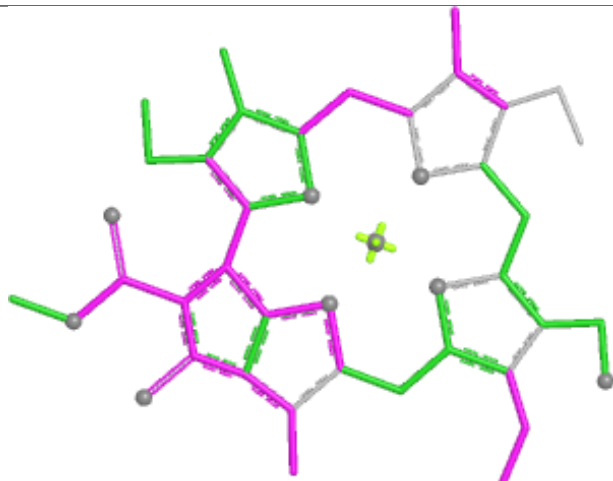




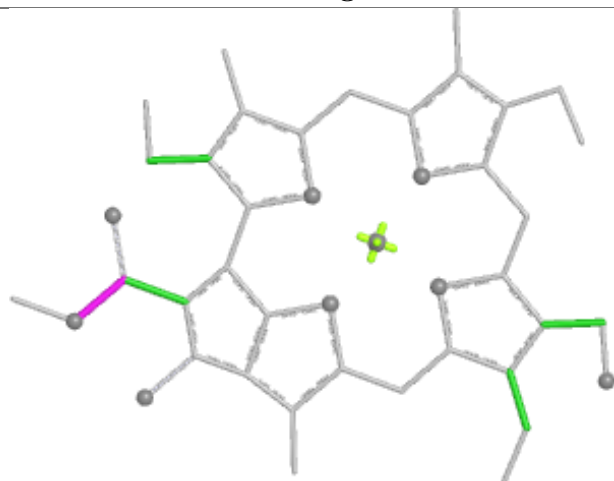
Ligand CHL u 309



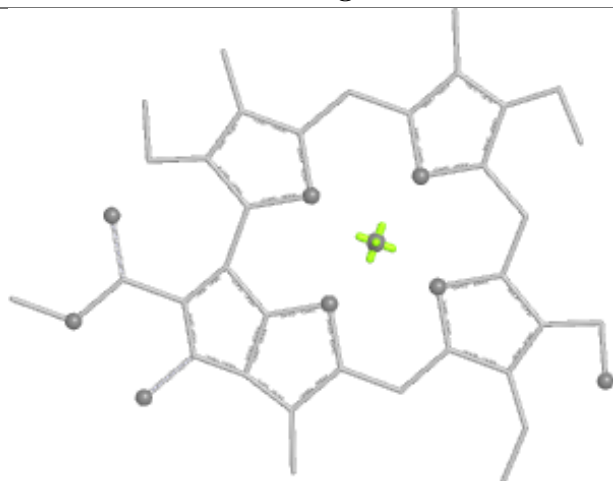
Bond lengths



Bond angles

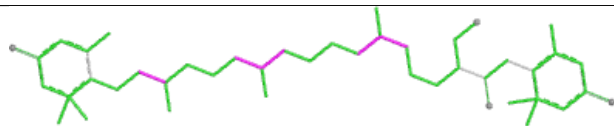


Torsions

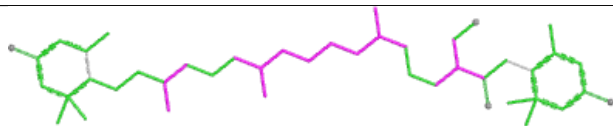


Rings

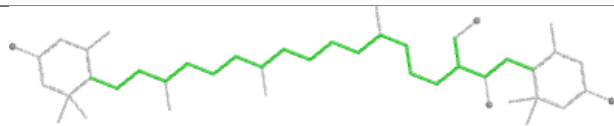
Ligand 0IE Y 303



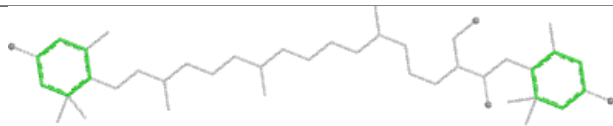
Bond lengths



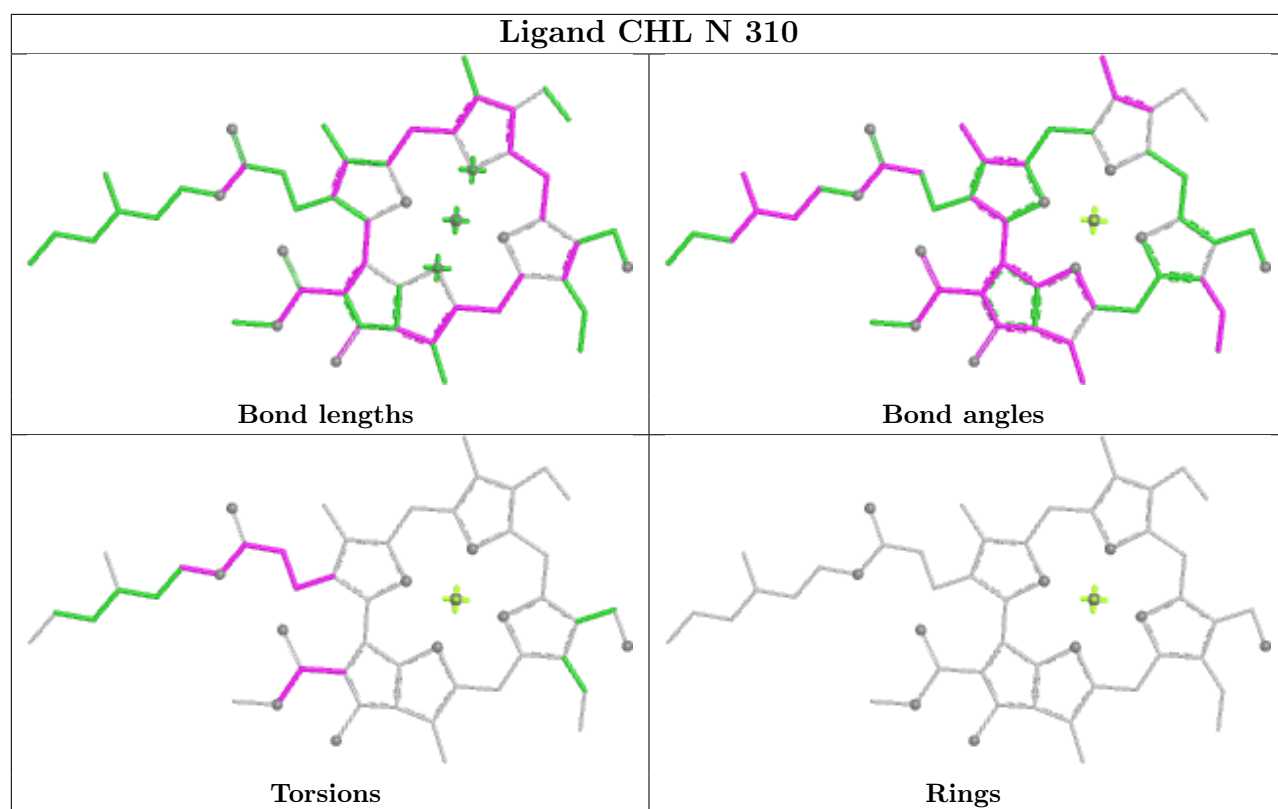
Bond angles



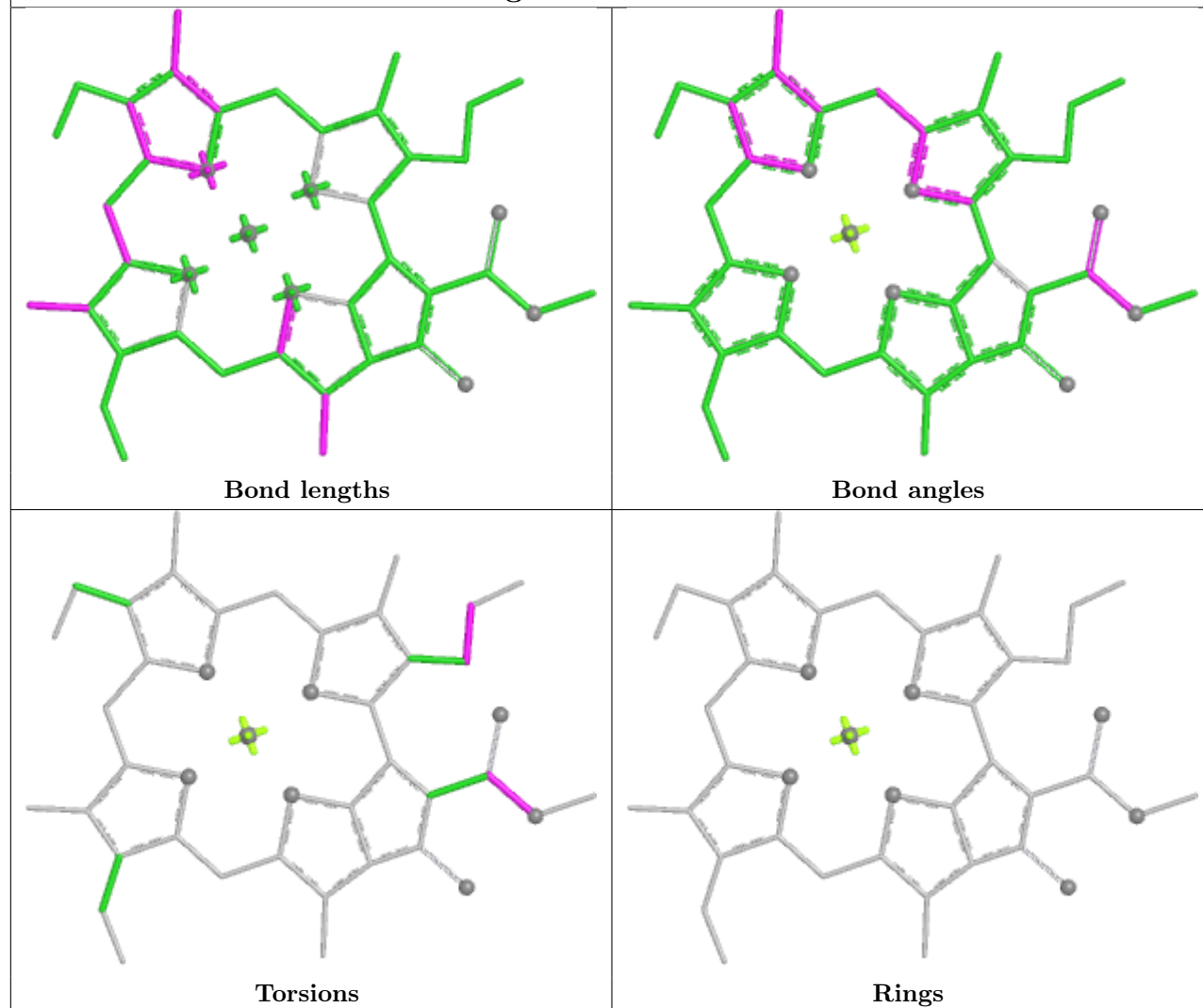
Torsions



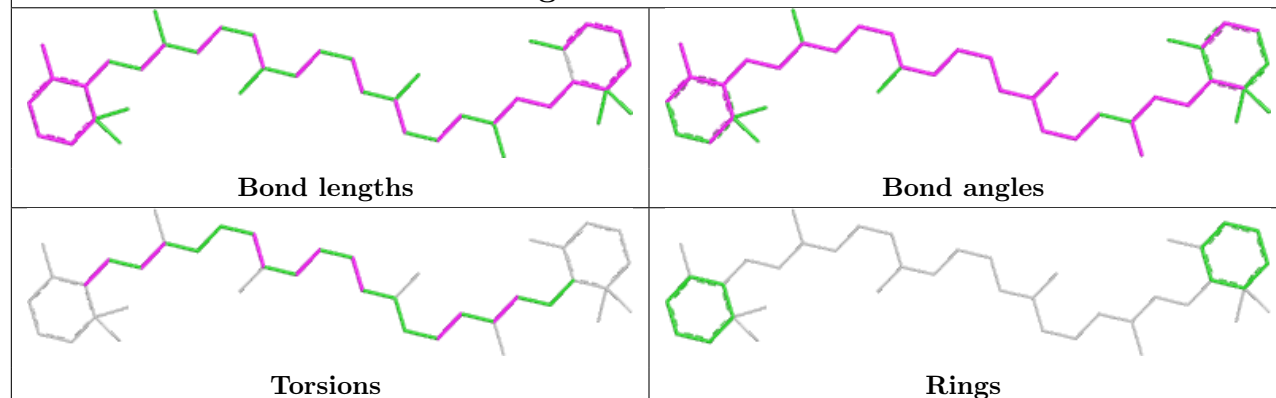
Rings



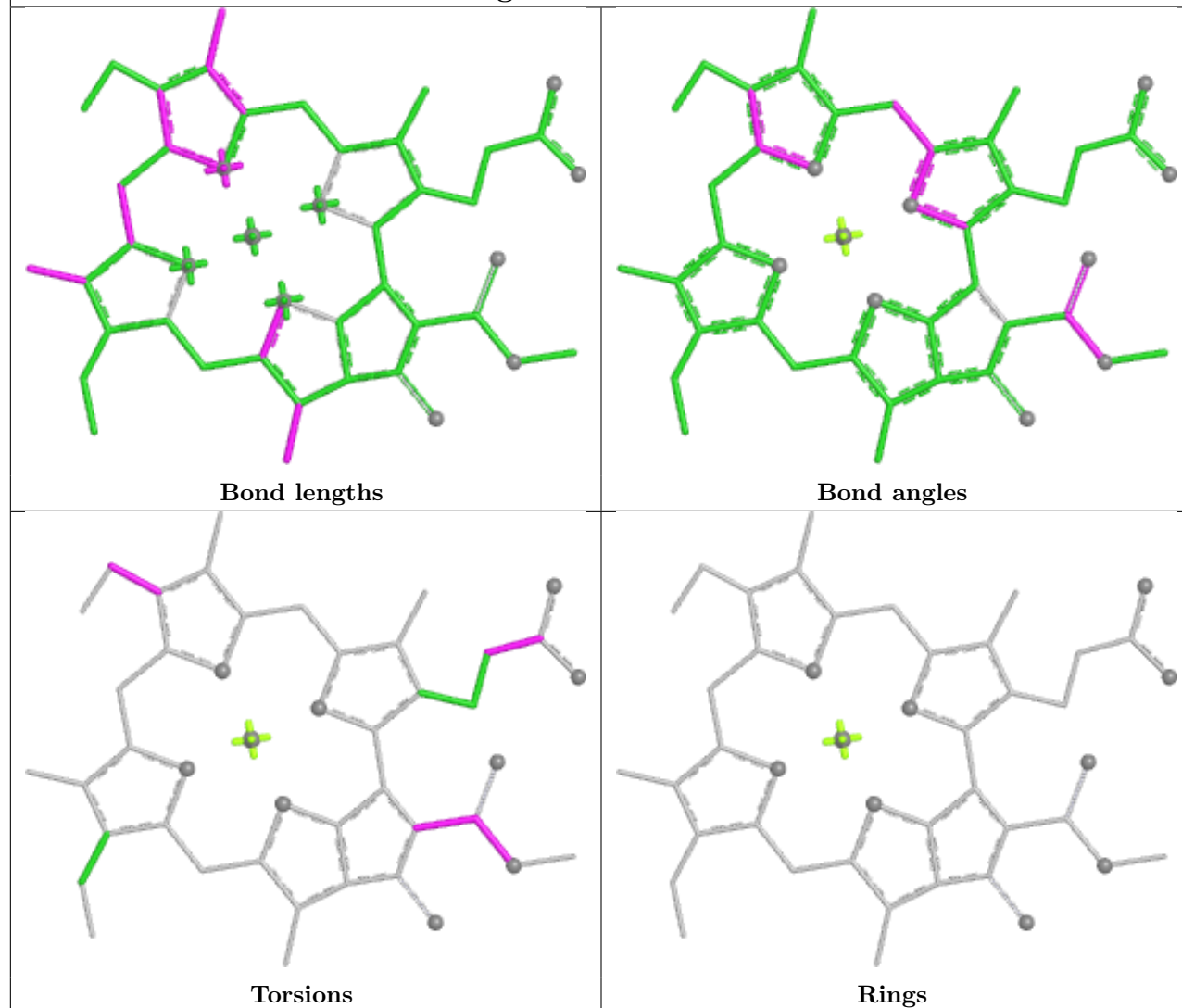
Ligand CLA 8 314



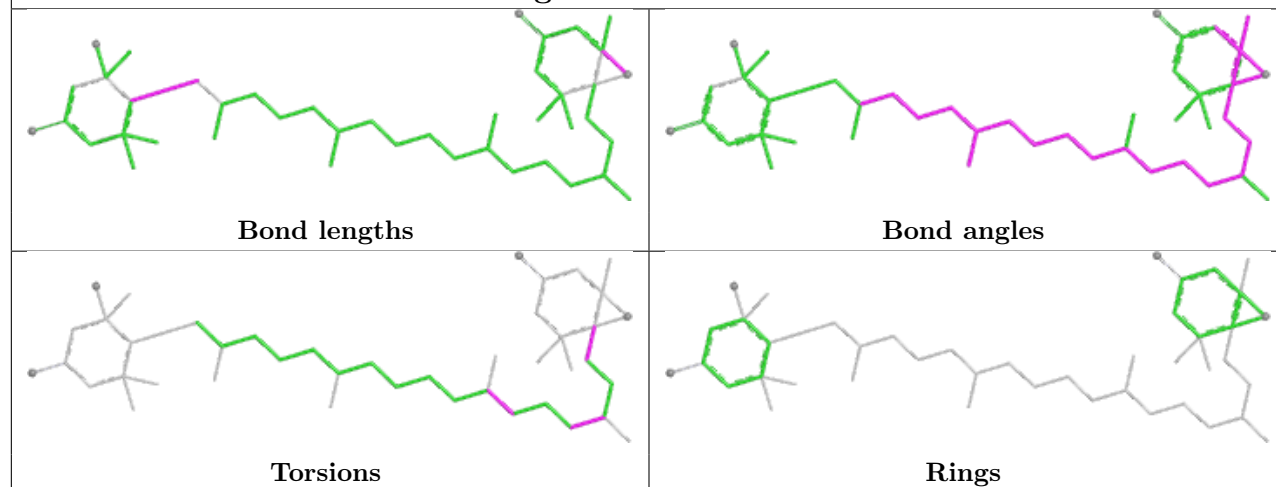
Ligand 8CT x 601

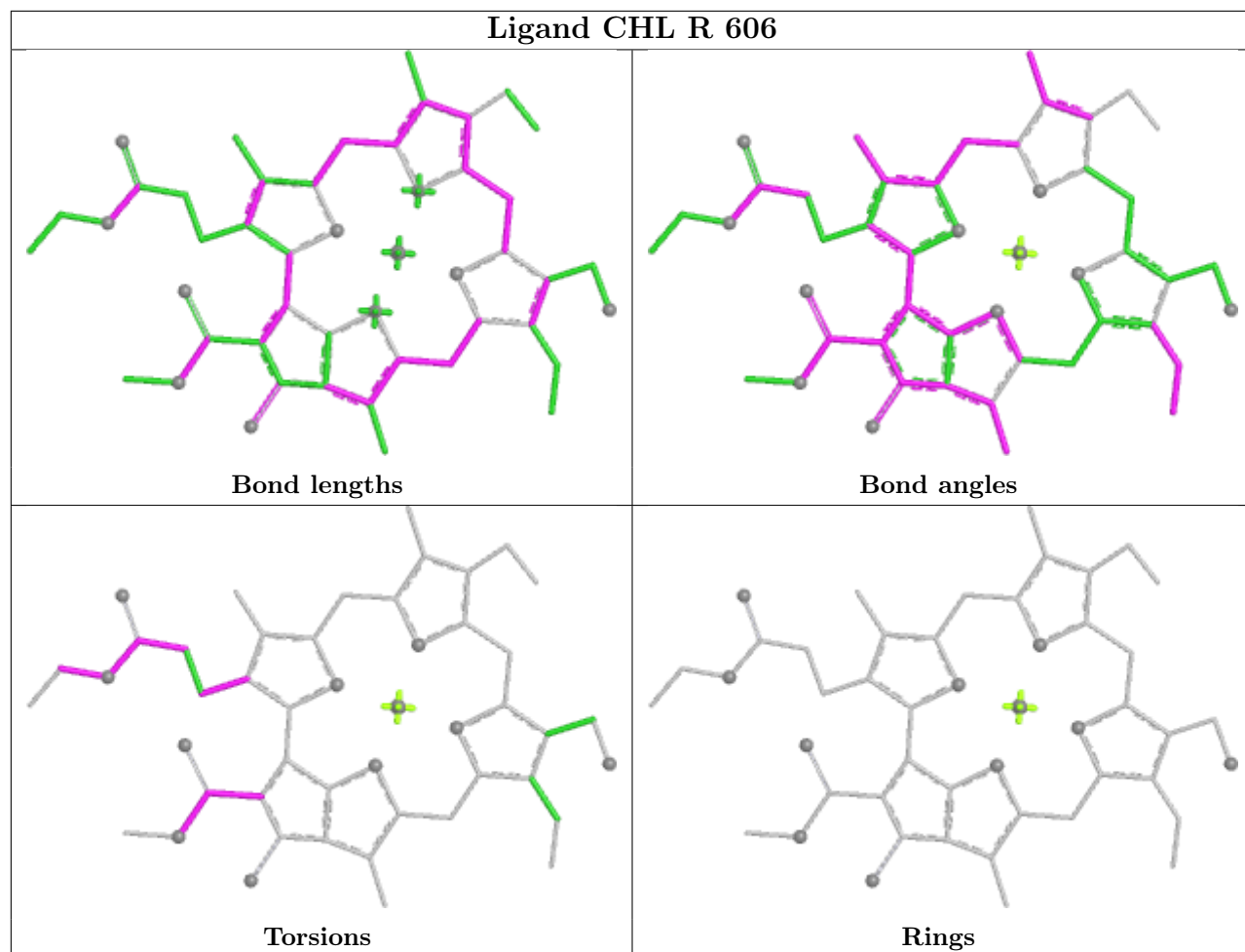


Ligand CLA 6 315

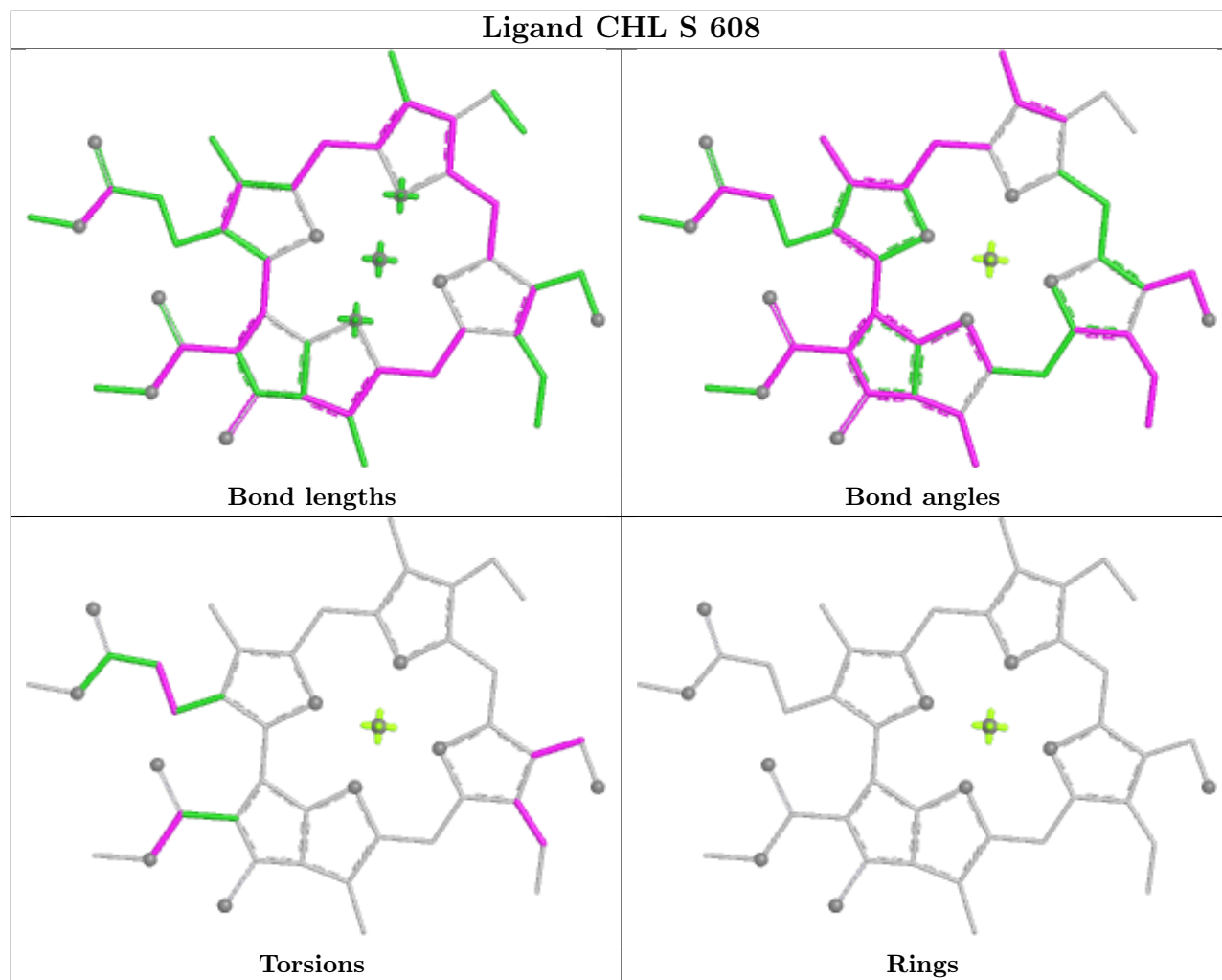


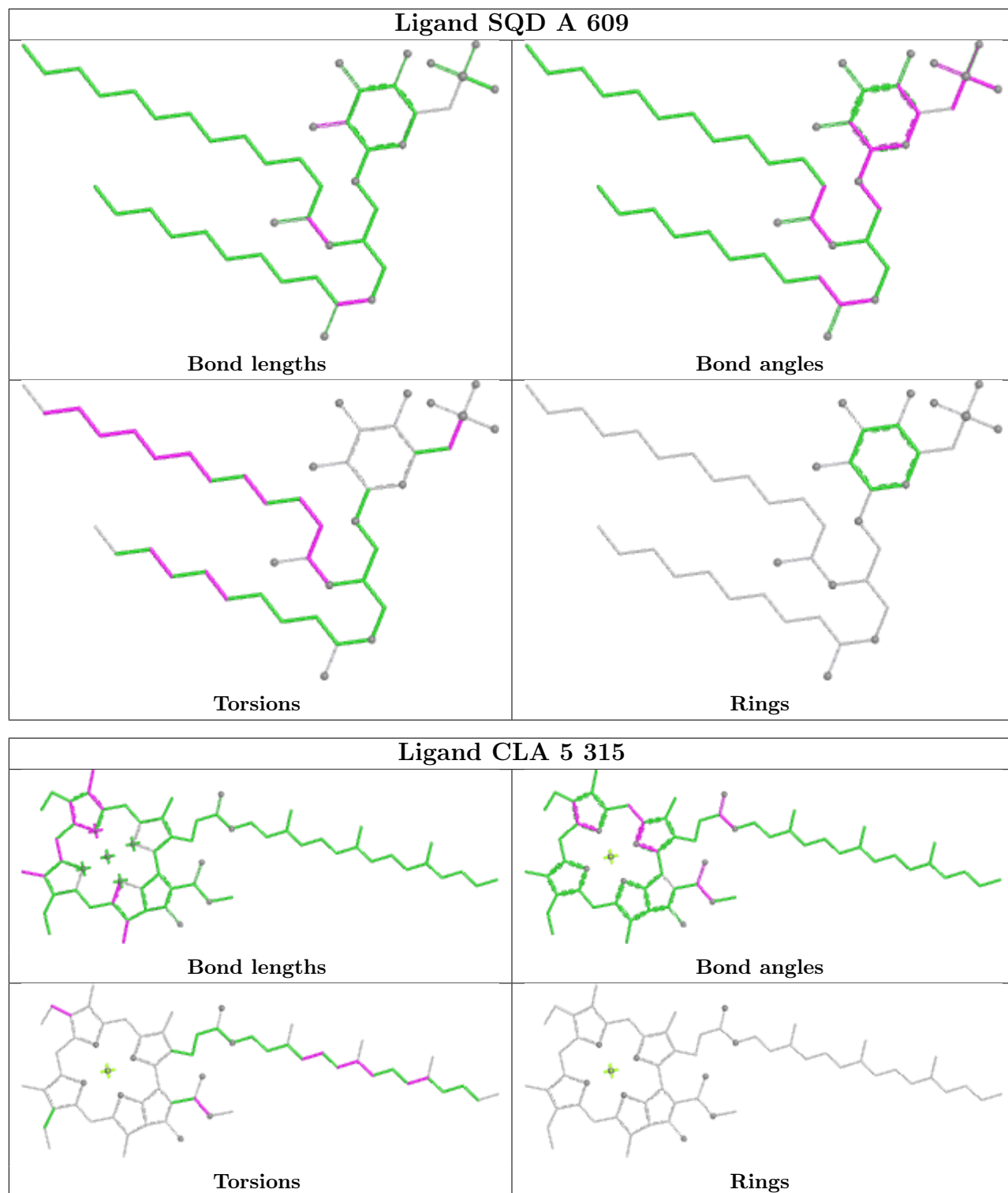
Ligand NEX 7 304

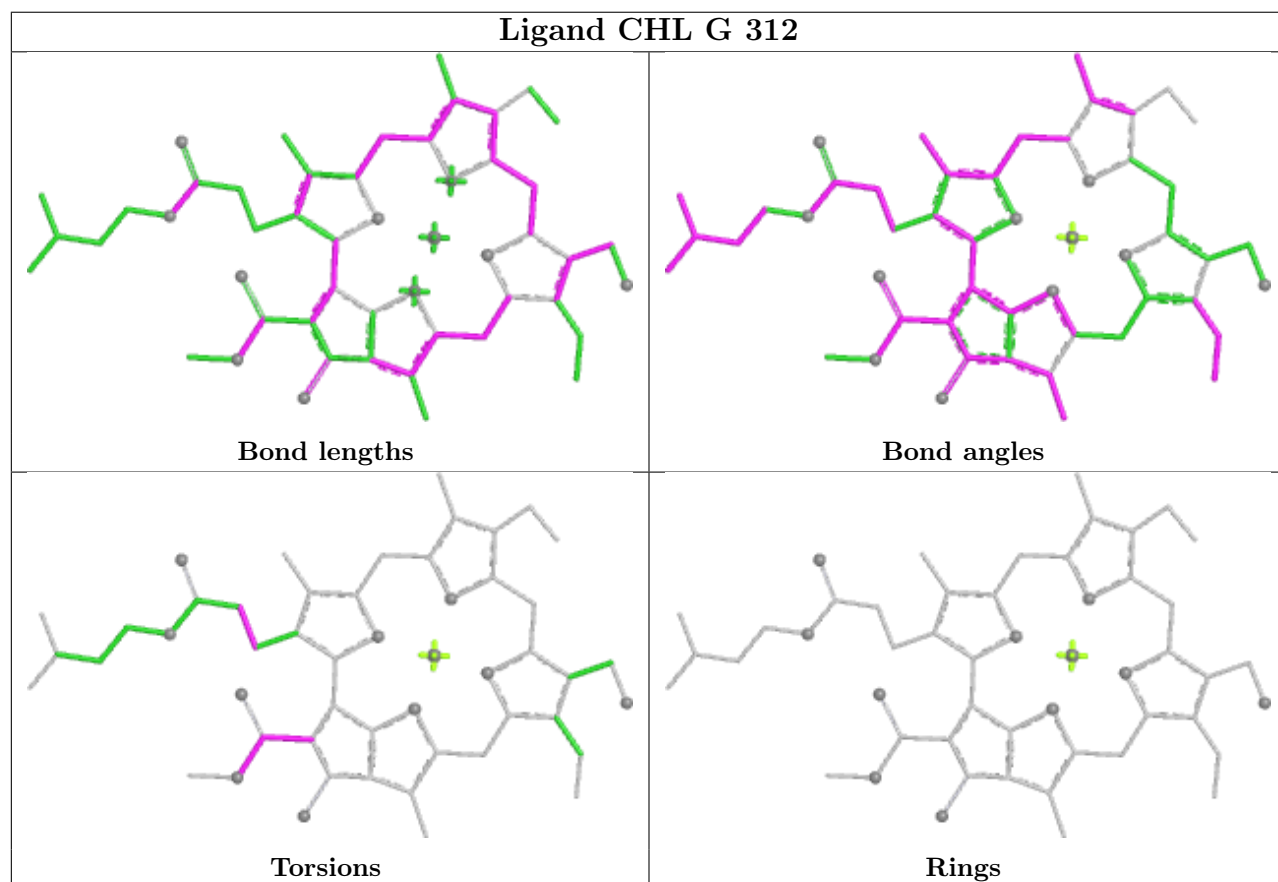
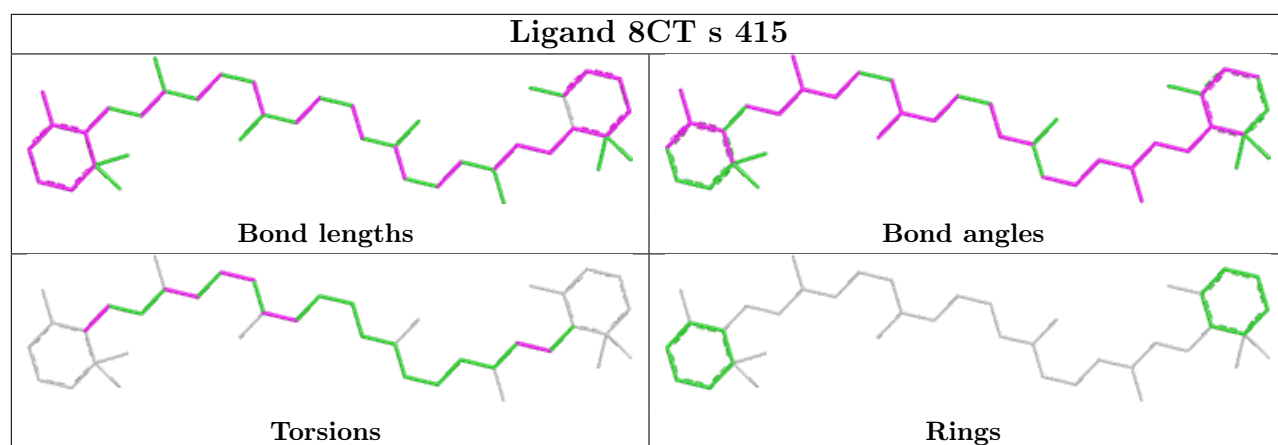


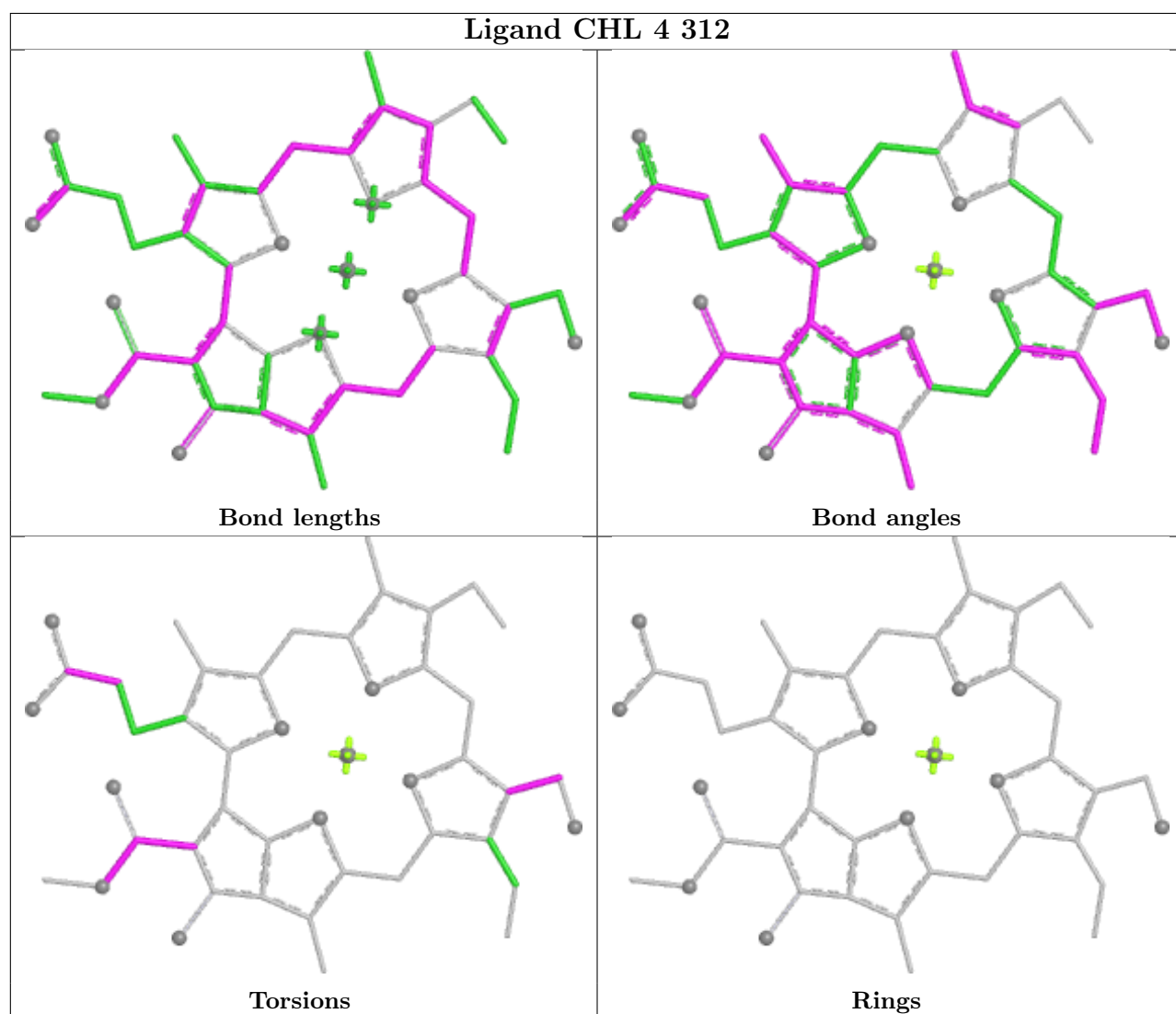
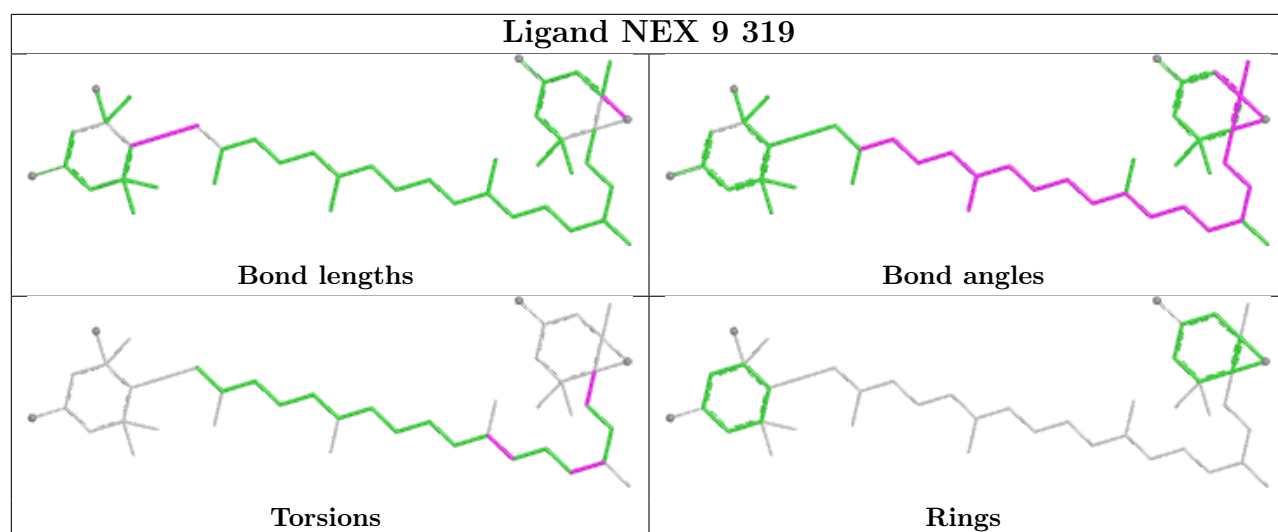


Ligand CHL S 608

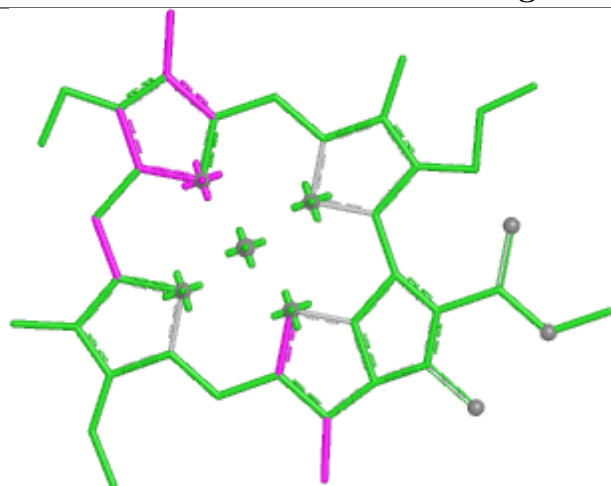




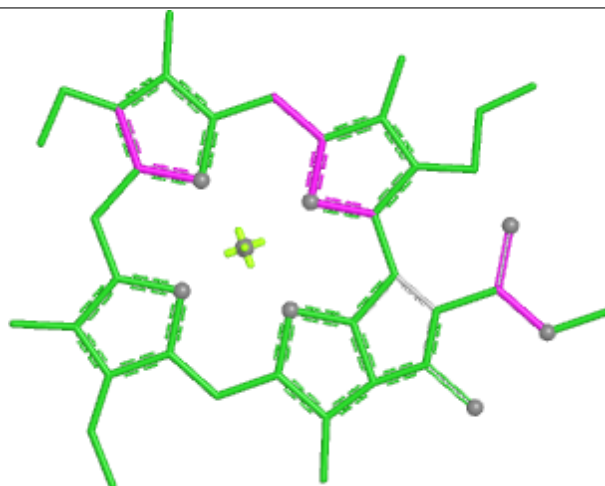




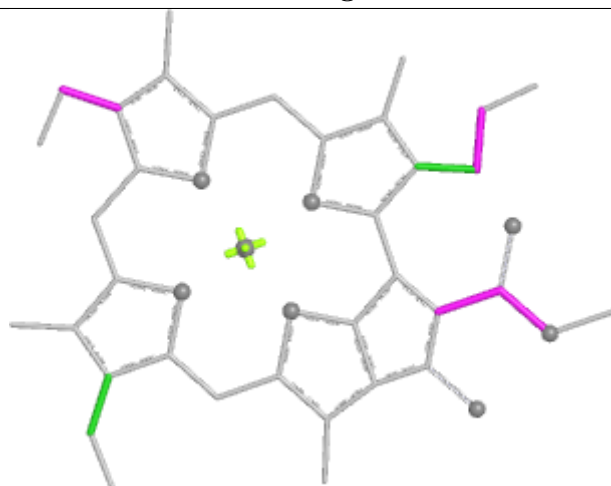
Ligand CLA 2 307



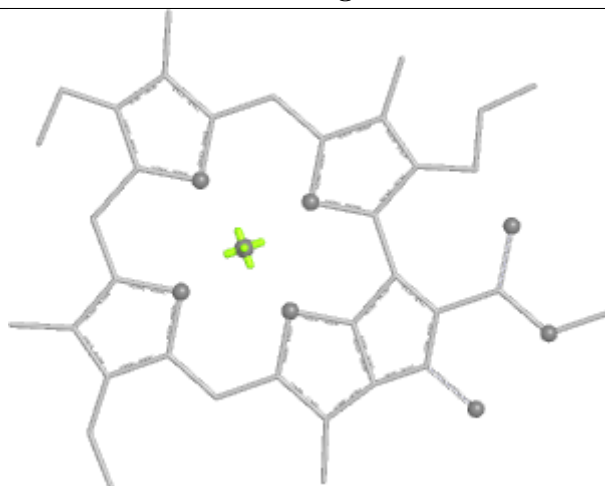
Bond lengths



Bond angles

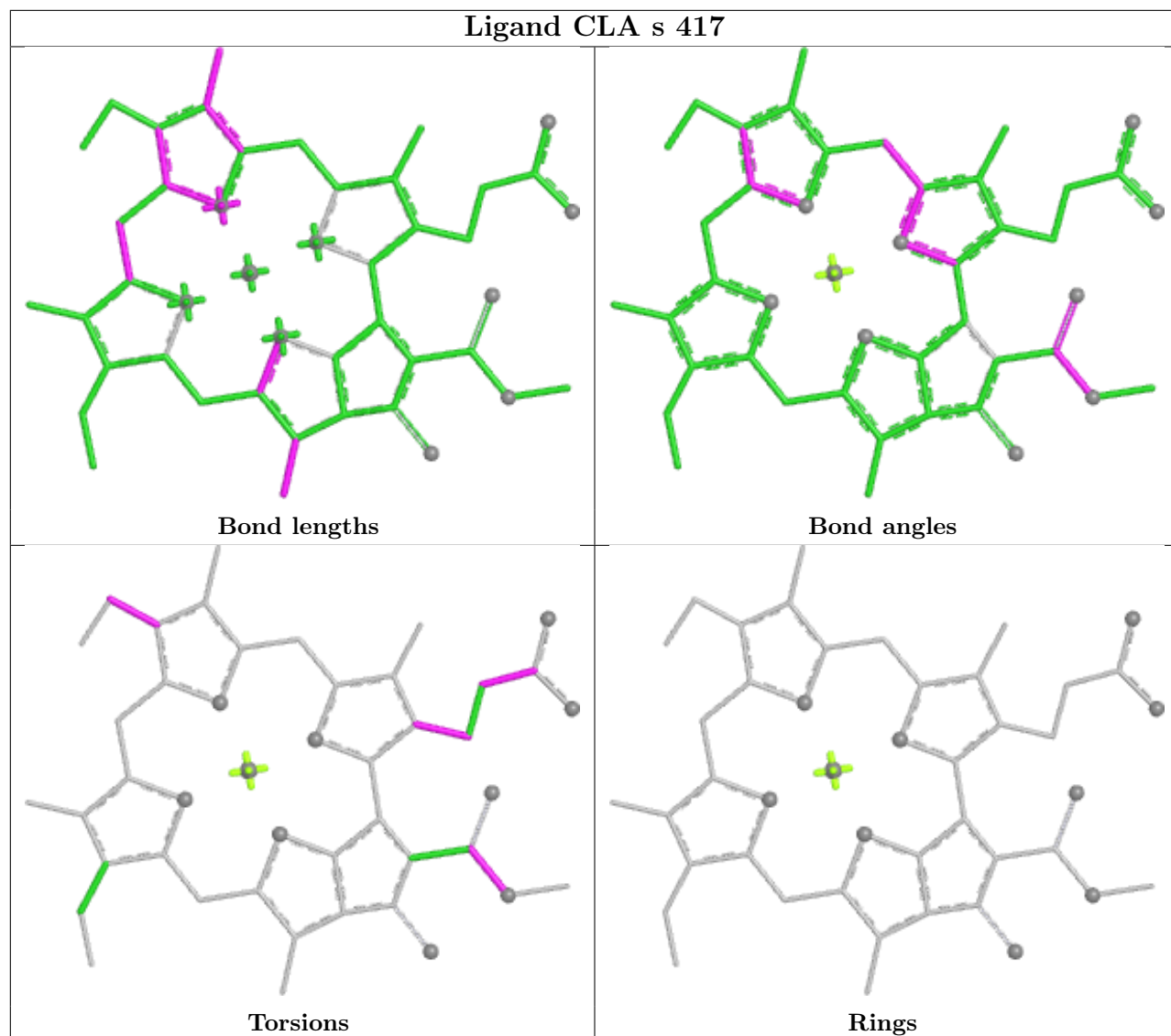


Torsions

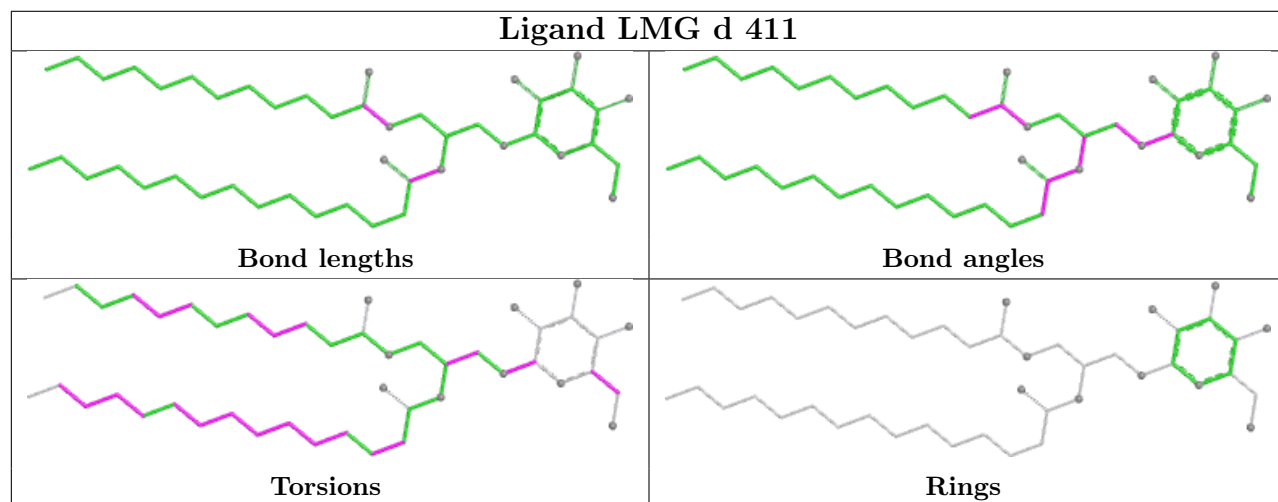


Rings

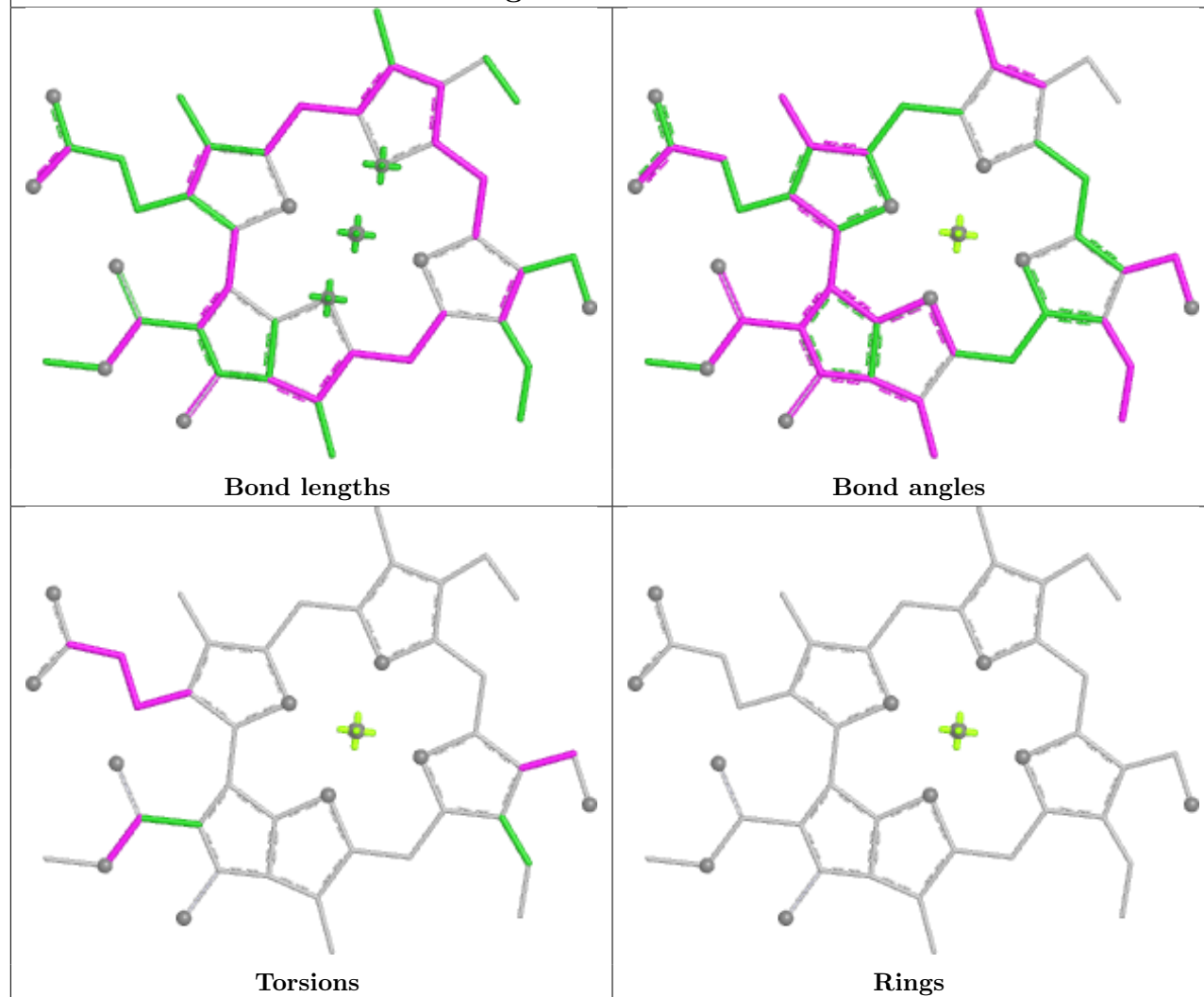
Ligand CLA s 417



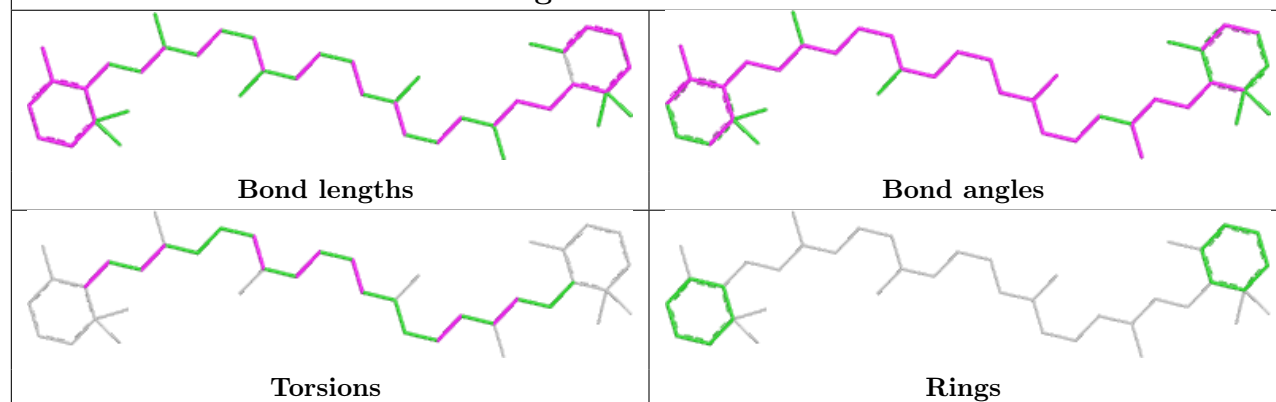
Ligand LMG d 411

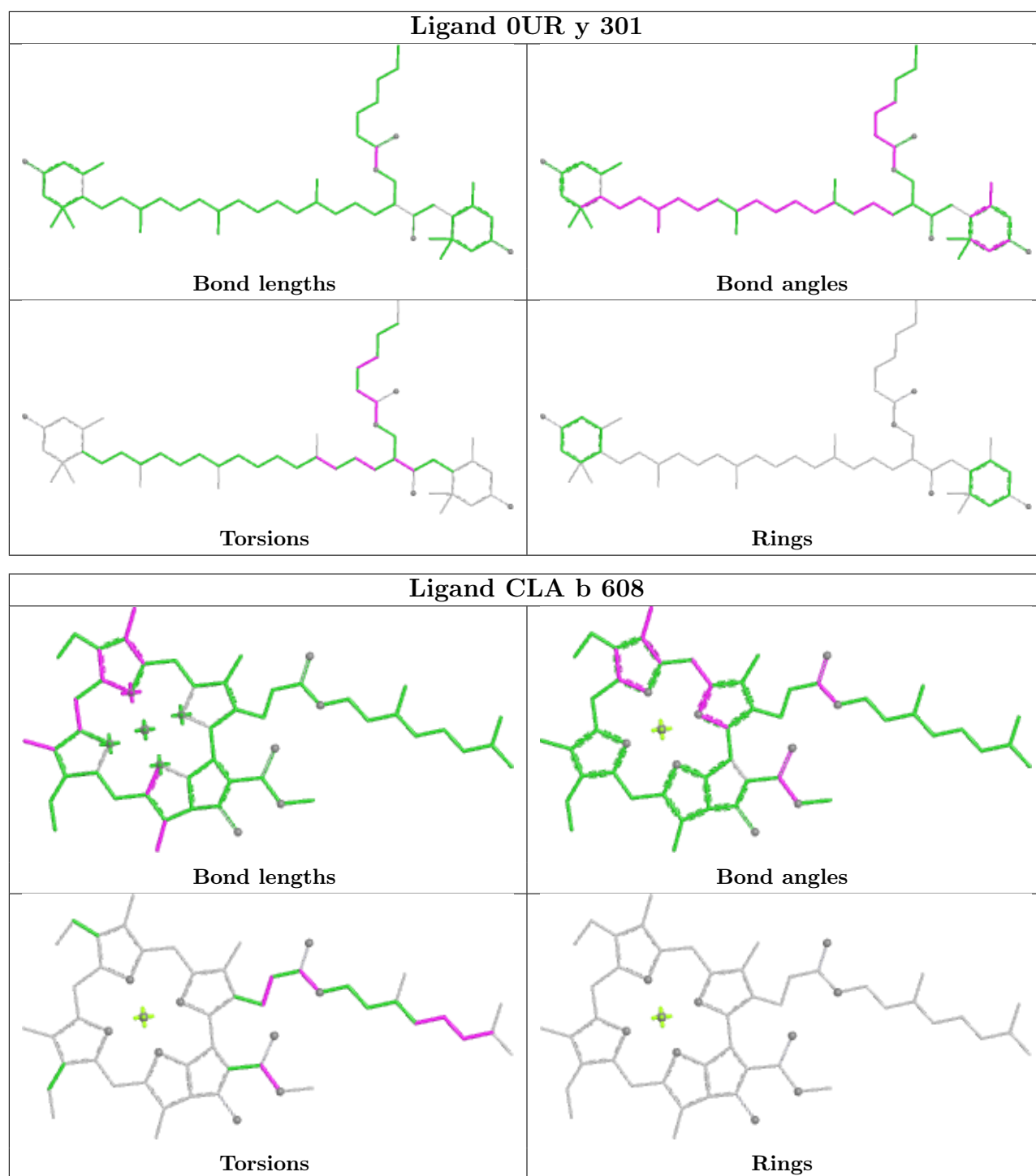


Ligand CHL 9 309



Ligand 8CT X 601





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.

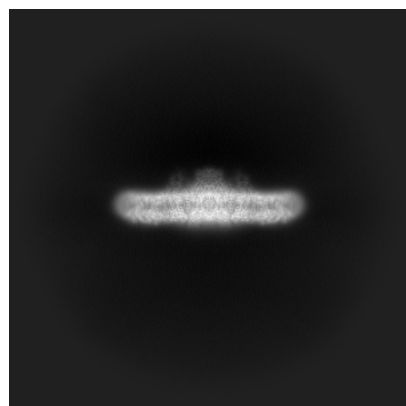
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62153. These allow visual inspection of the internal detail of the map and identification of artifacts.

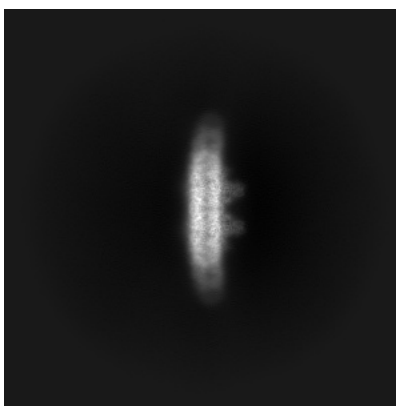
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

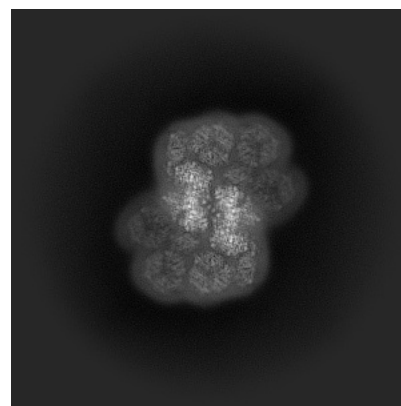
6.1.1 Primary map



X

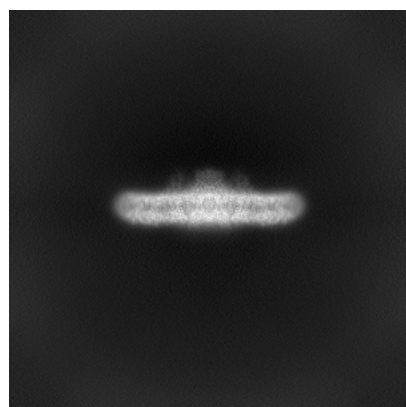


Y

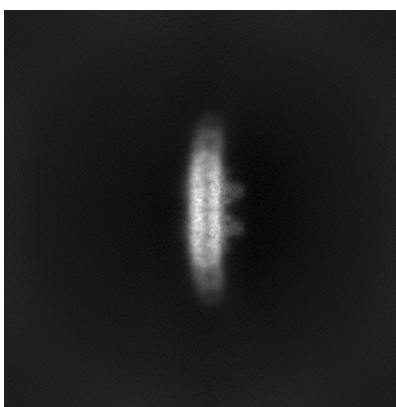


Z

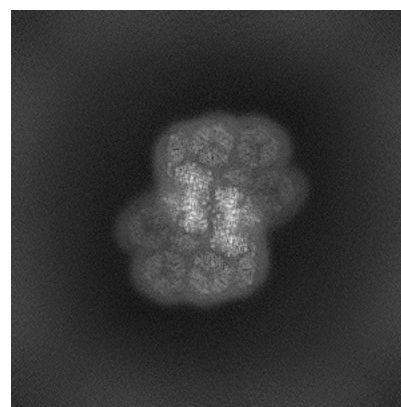
6.1.2 Raw map



X



Y

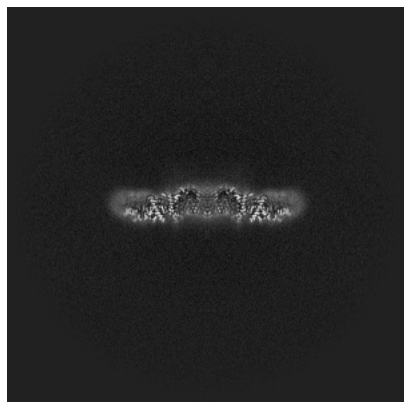


Z

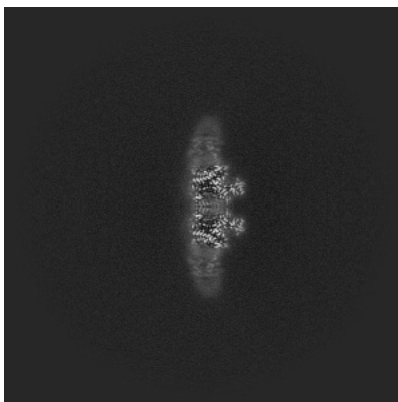
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

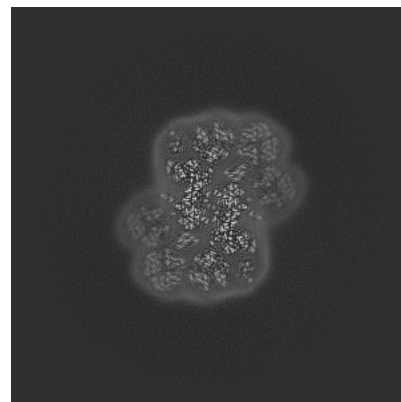
6.2.1 Primary map



X Index: 300

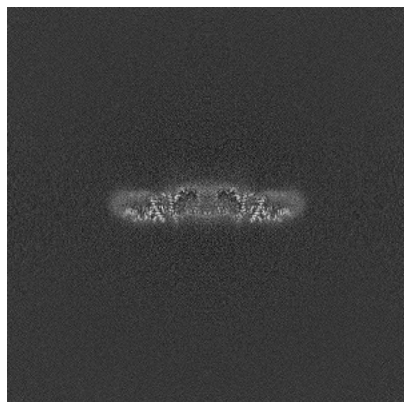


Y Index: 300

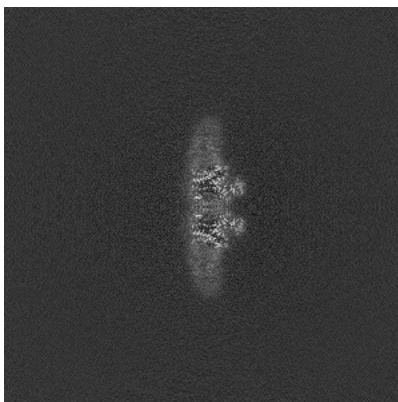


Z Index: 300

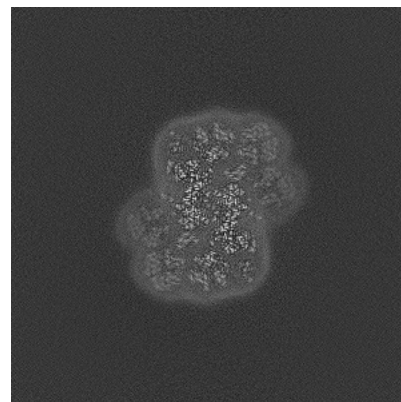
6.2.2 Raw map



X Index: 300



Y Index: 300

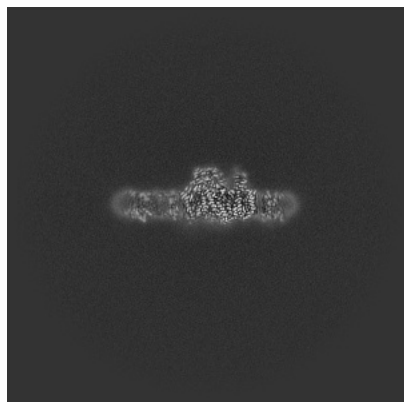


Z Index: 300

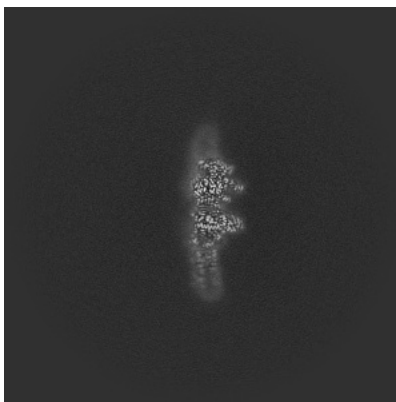
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

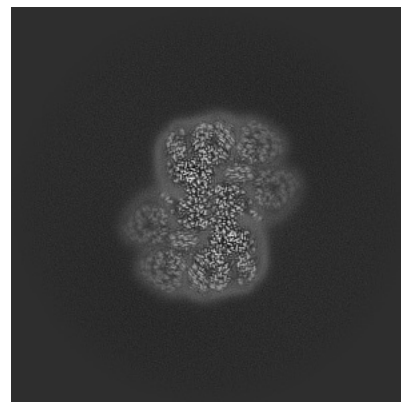
6.3.1 Primary map



X Index: 273

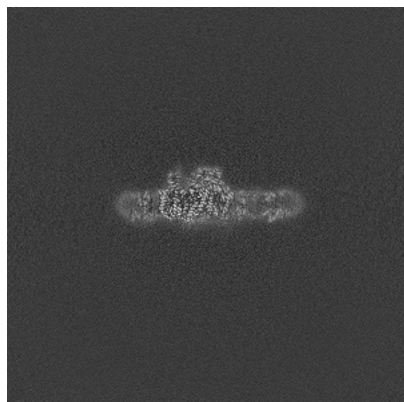


Y Index: 288

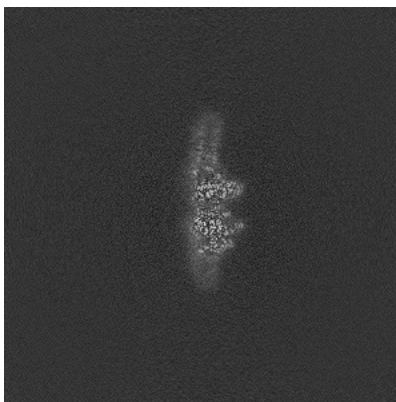


Z Index: 293

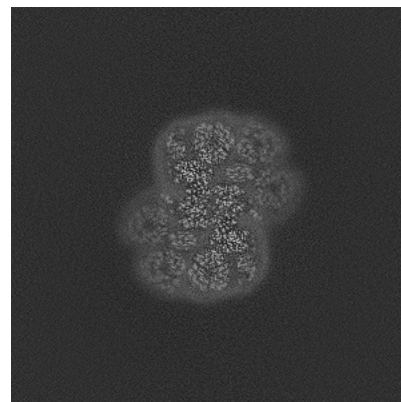
6.3.2 Raw map



X Index: 327



Y Index: 312

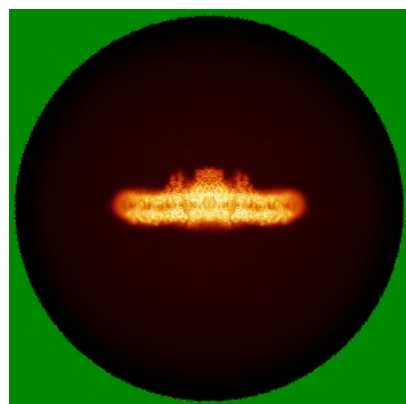


Z Index: 294

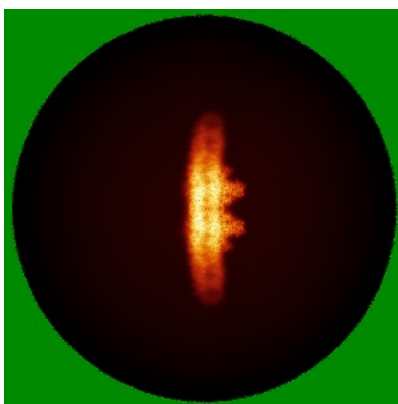
The images above show the largest variance slices of the map in three orthogonal directions.

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

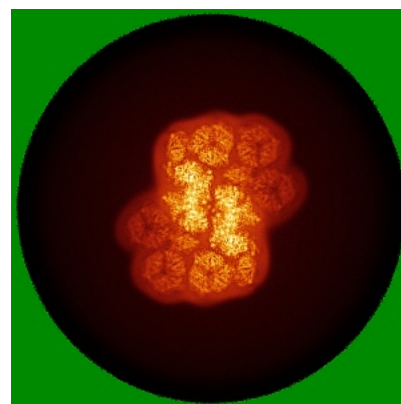
6.4.1 Primary map



X

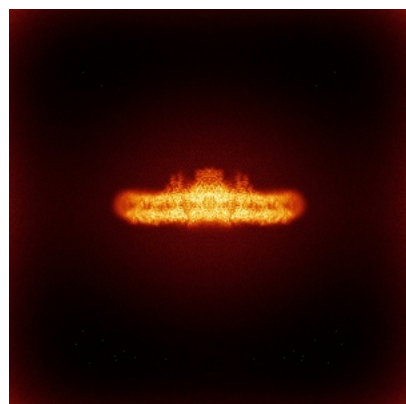


Y

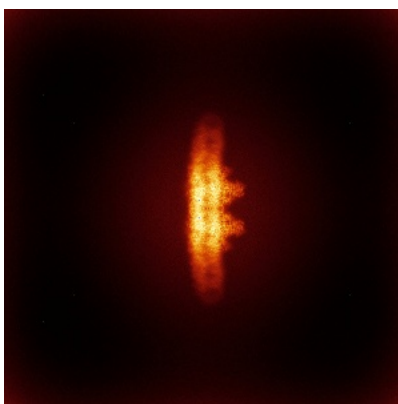


Z

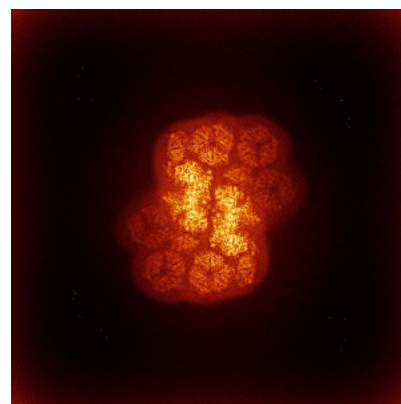
6.4.2 Raw map



X



Y

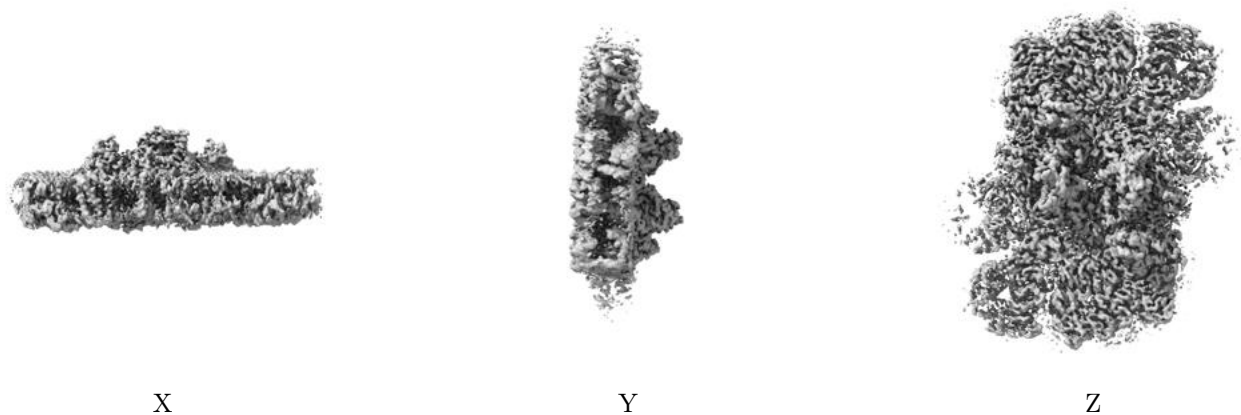


Z

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

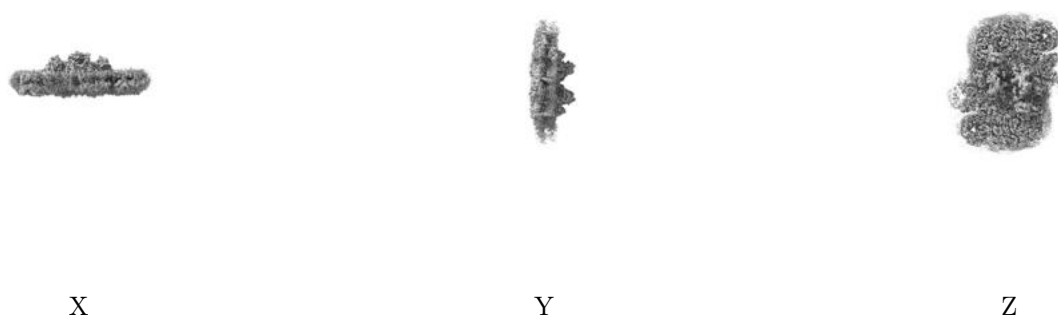
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.204. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

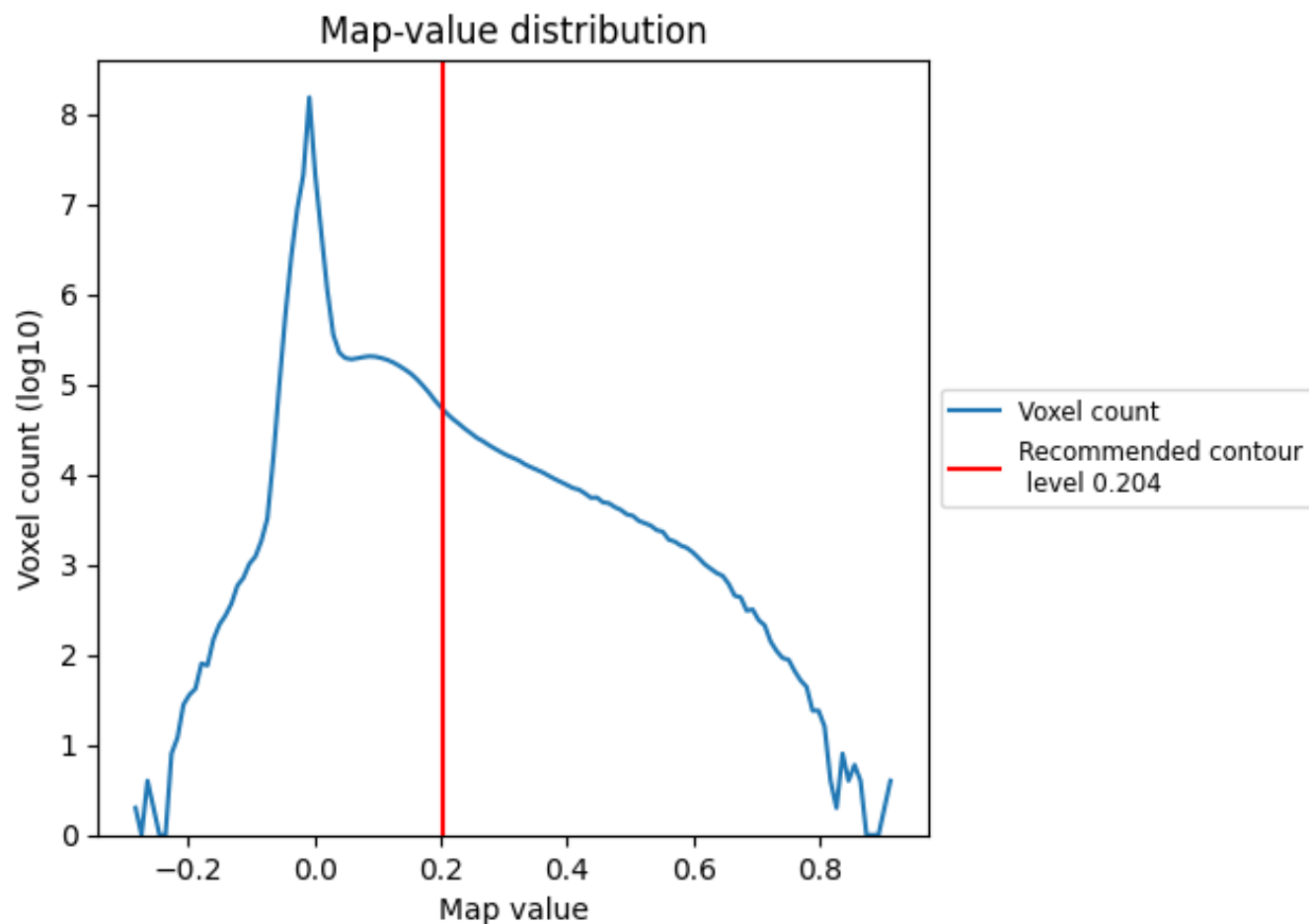
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

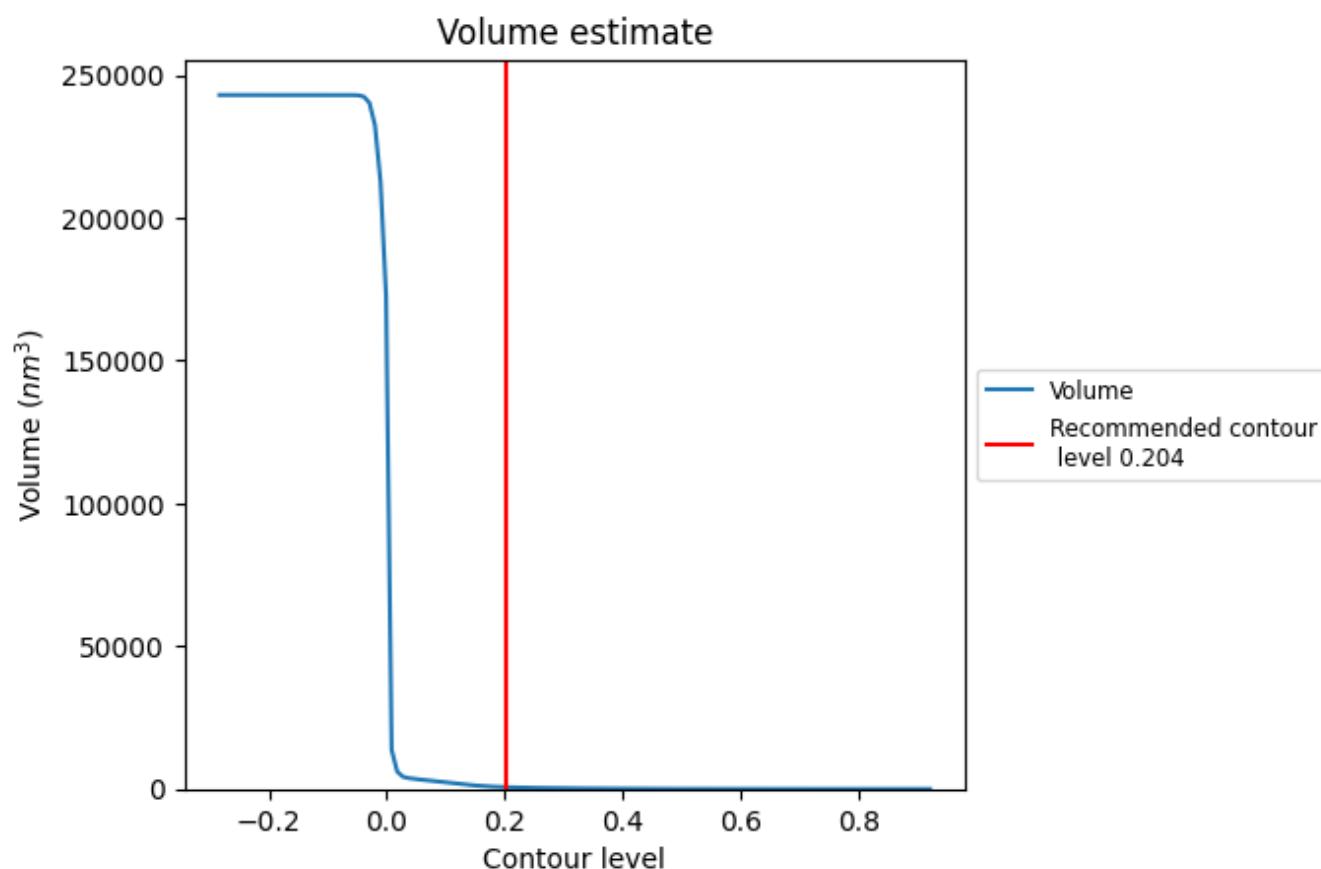
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

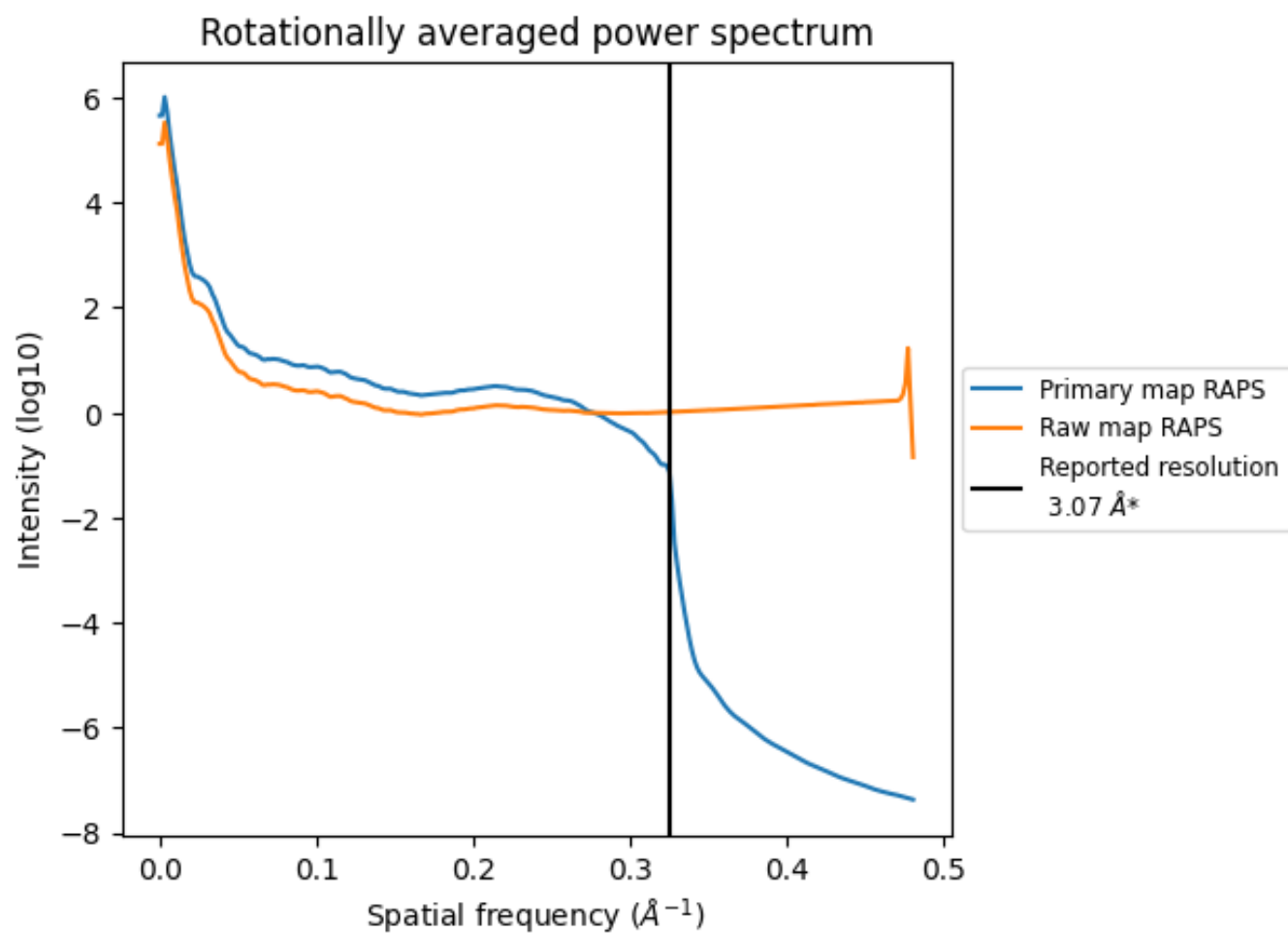
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 606 nm³; this corresponds to an approximate mass of 548 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

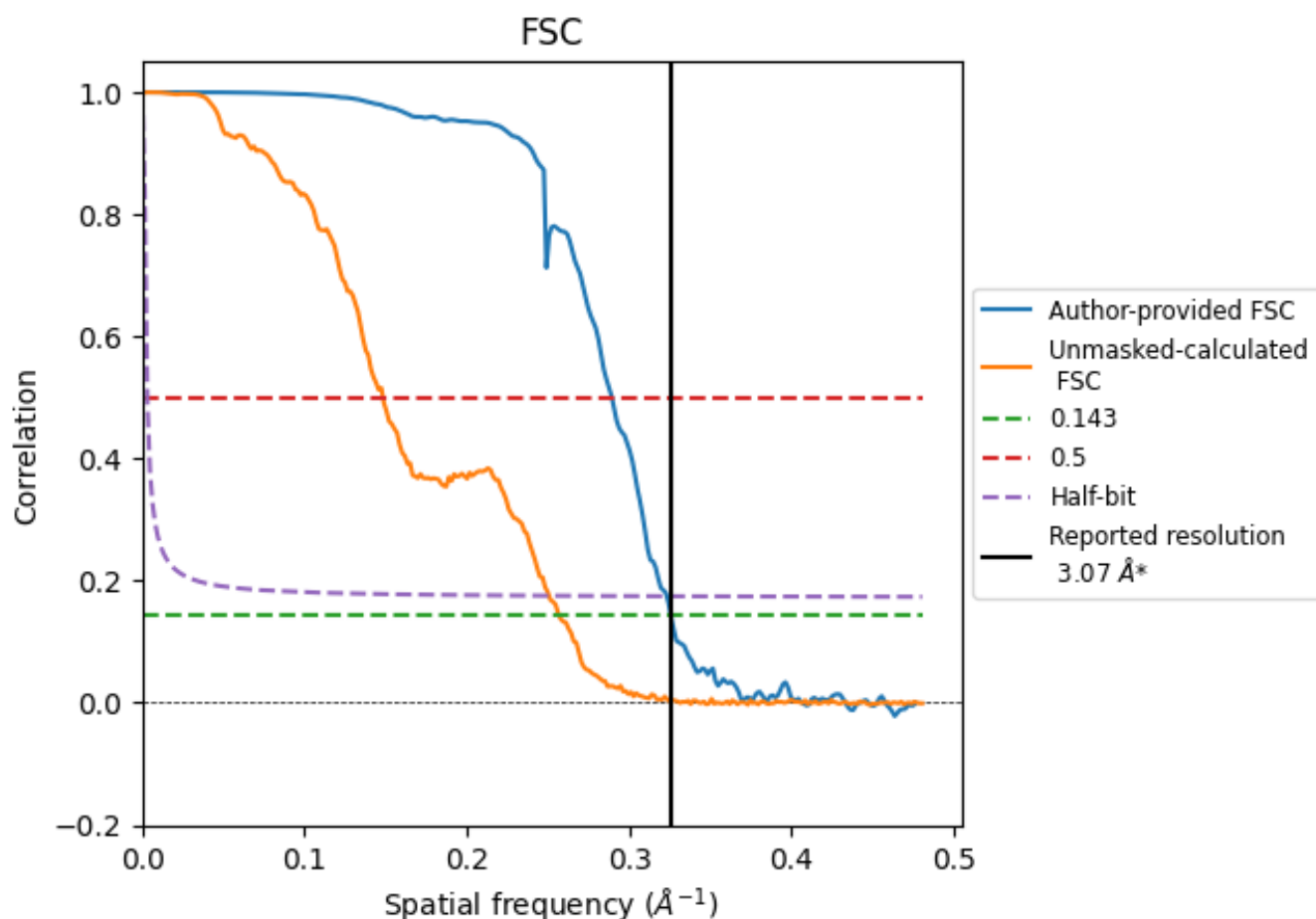


*Reported resolution corresponds to spatial frequency of 0.326 \AA^{-1}

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 0.326 \AA^{-1}

8.2 Resolution estimates [i](#)

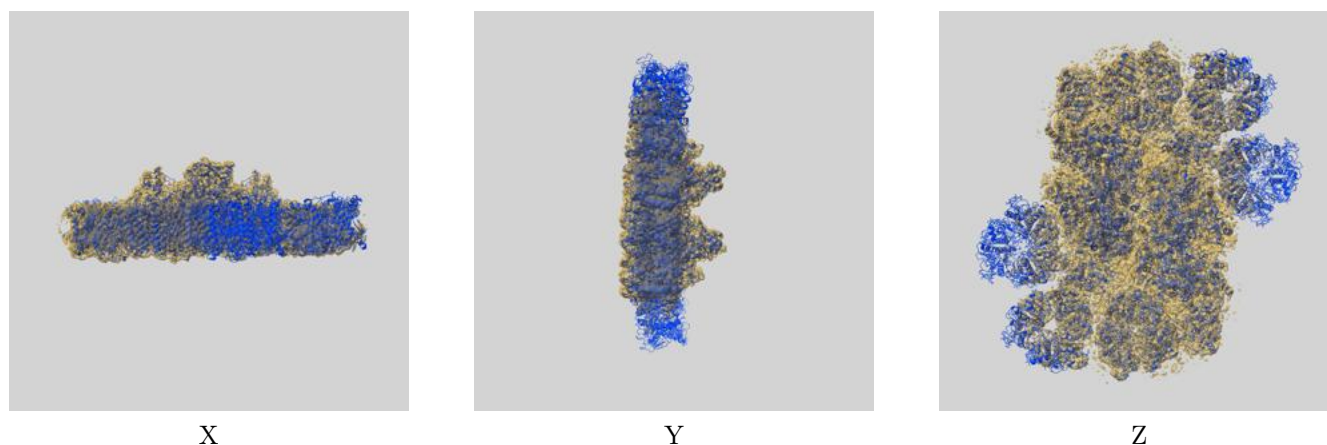
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.07	3.45	3.09
Unmasked-calculated*	3.89	6.74	3.99

*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 3.89 differs from the reported value 3.07 by more than 10 %

9 Map-model fit [i](#)

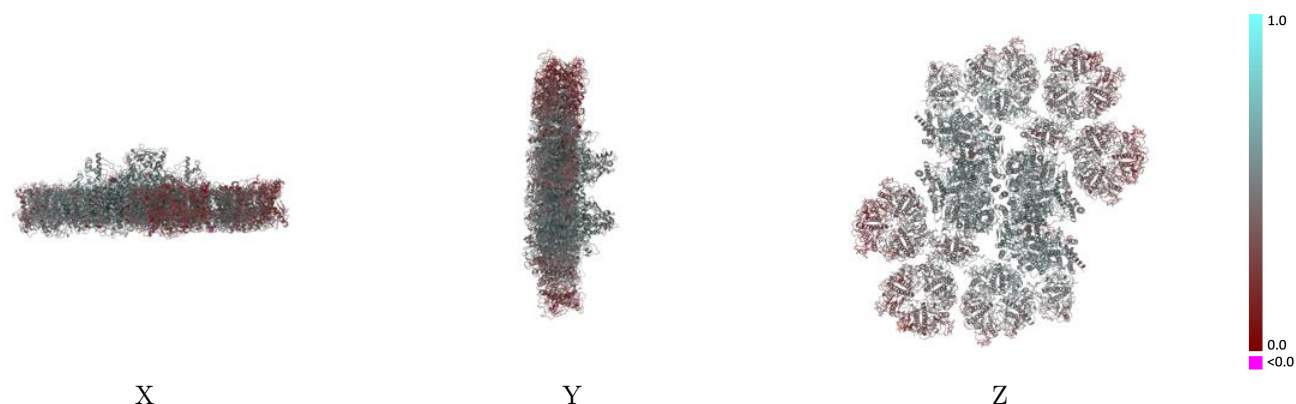
This section contains information regarding the fit between EMDB map EMD-62153 and PDB model 9K7V. Per-residue inclusion information can be found in [section 3](#) on [page 54](#).

9.1 Map-model overlay [i](#)



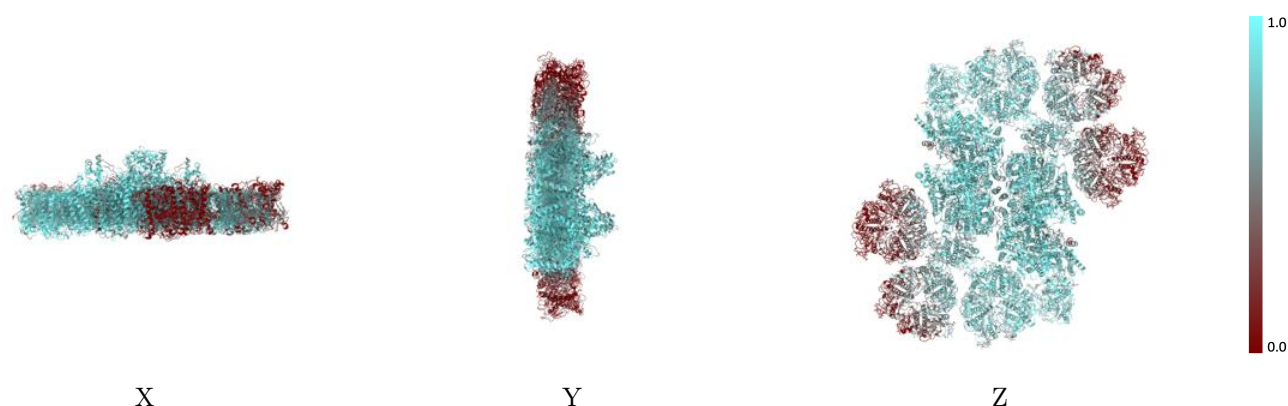
The images above show the 3D surface view of the map at the recommended contour level 0.204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



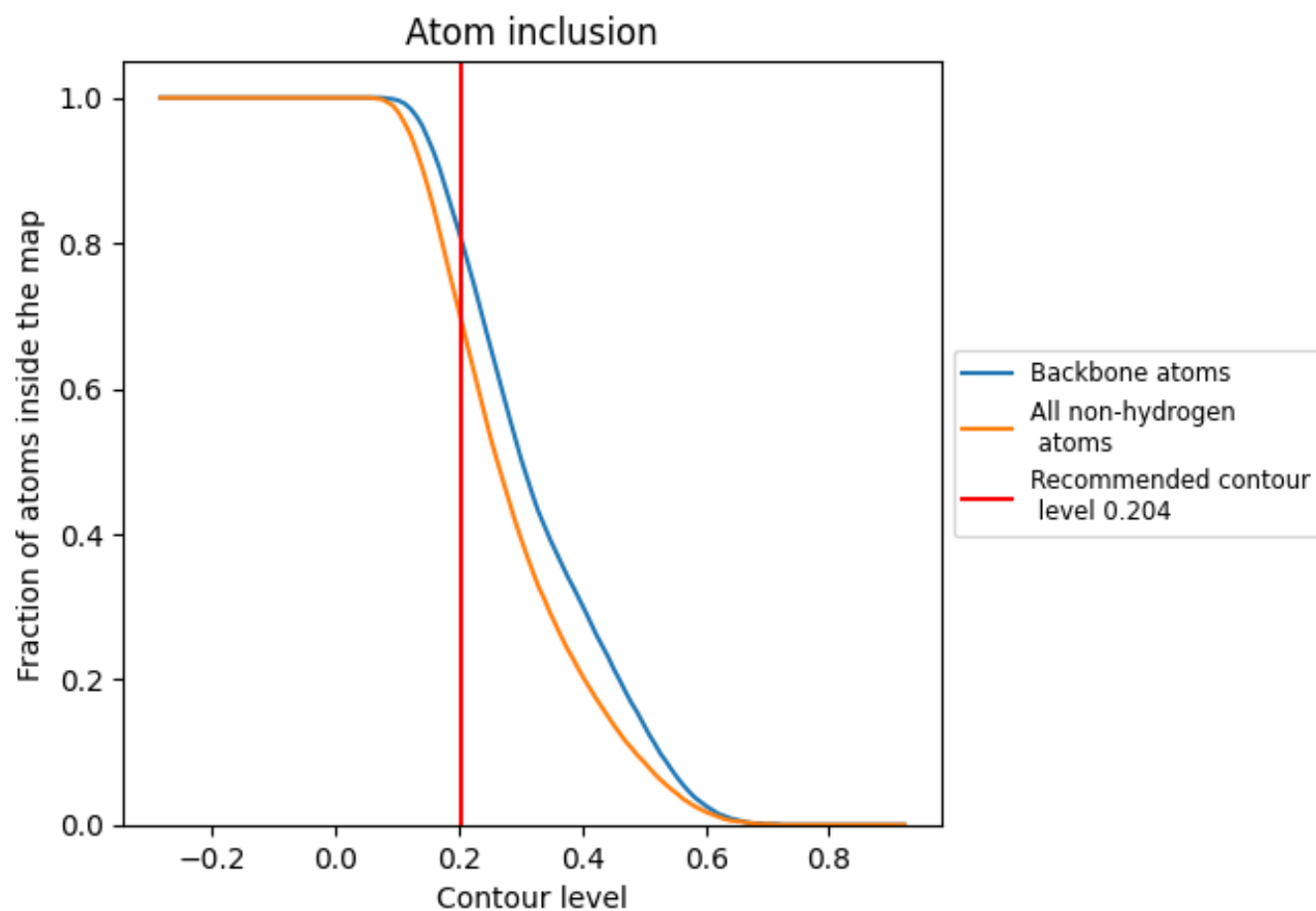
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.204).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% 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 (0.204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6920	 0.4550
1	 0.3620	 0.3400
2	 0.6680	 0.4570
3	 0.3050	 0.3320
4	 0.3660	 0.3380
5	 0.6660	 0.4580
6	 0.3020	 0.3250
7	 0.7880	 0.4340
8	 0.8580	 0.4730
9	 0.0130	 0.2470
A	 0.9160	 0.5370
B	 0.9140	 0.5310
C	 0.9100	 0.5370
D	 0.9260	 0.5490
E	 0.8090	 0.4670
F	 0.8670	 0.4710
G	 0.2460	 0.3830
H	 0.8510	 0.5070
I	 0.9600	 0.5430
K	 0.9220	 0.5170
L	 0.9060	 0.5290
M	 0.7130	 0.4500
N	 0.3140	 0.3920
R	 0.7010	 0.4140
S	 0.8320	 0.4570
T	 0.8600	 0.5220
V	 0.4290	 0.3920
W	 0.9000	 0.5010
X	 0.8040	 0.4860
Y	 0.9010	 0.5210
Z	 0.8080	 0.4380
a	 0.9160	 0.5370
b	 0.9140	 0.5320
c	 0.9080	 0.5350
d	 0.9240	 0.5490



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Chain	Atom inclusion	Q-score
e	 0.8140	 0.4640
f	 0.8530	 0.4640
g	 0.2490	 0.3850
h	 0.8430	 0.5070
i	 0.9500	 0.5570
k	 0.9290	 0.5150
l	 0.9100	 0.5340
m	 0.7310	 0.4650
n	 0.3180	 0.3910
p	 0.7870	 0.4340
q	 0.8550	 0.4720
r	 0.7020	 0.4130
s	 0.8340	 0.4560
t	 0.8640	 0.5190
u	 0.0150	 0.2460
v	 0.4470	 0.3850
w	 0.8840	 0.4930
x	 0.7970	 0.4900
y	 0.8990	 0.5210
z	 0.8080	 0.4370