



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:14 AM UTC

PDB ID : 5MDX / pdb_00005mdx
EMDB ID : EMD-3491
Title : Cryo-EM structure of the PSII supercomplex from Arabidopsis thaliana
Authors : van Bezouwen, L.S.; Caffarri, S.; Kale, R.S.; Kouril, R.; Thunnissen, A.M.W.H.; Oostergetel, G.T.; Boekema, E.J.
Deposited on : 2016-11-13
Resolution : 5.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

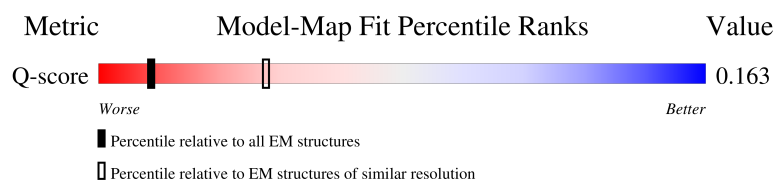
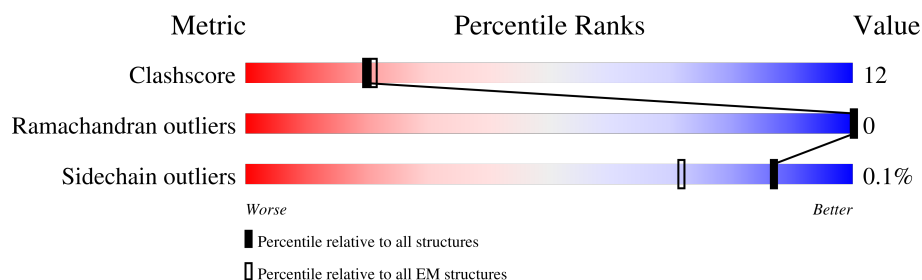
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 5.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	625 (4.80 - 5.80)

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

Mol	Chain	Length	Quality of chain
1	A	343	
1	a	343	
2	B	507	
2	b	507	

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Mol	Chain	Length	Quality of chain
3	C	459	
3	c	459	
4	D	352	
4	d	352	
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	H	72	
7	h	72	
8	I	36	
8	i	36	
9	K	37	
9	k	37	
10	L	38	
10	l	38	
11	M	34	
11	m	34	
12	O	247	
12	o	247	
13	T	33	
13	t	33	
14	W	54	
14	w	54	
15	X	116	

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Mol	Chain	Length	Quality of chain
15	x	116	
16	Z	62	
16	z	62	
17	R	250	
17	r	250	
18	S	232	
18	s	232	
19	1	224	
19	2	224	
19	3	224	
19	5	224	
19	6	224	
19	7	224	
19	G	224	
19	N	224	
19	Y	224	
19	g	224	
19	n	224	
19	y	224	
20	4	210	
20	8	210	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	604	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	2	602	X	-	-	-
22	CLA	2	603	X	-	-	-
22	CLA	2	604	X	-	-	-
22	CLA	2	609	X	-	-	-
22	CLA	2	610	X	-	-	-
22	CLA	2	611	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	2	613	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	-	-
22	CLA	3	313	X	-	-	-
22	CLA	3	314	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	613	X	-	-	-
22	CLA	5	614	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	6	613	X	-	-	-
22	CLA	7	303	X	-	-	-
22	CLA	7	304	X	-	-	-
22	CLA	7	305	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-
22	CLA	7	314	X	-	-	-
22	CLA	8	302	X	-	-	-
22	CLA	8	303	X	-	-	-
22	CLA	8	304	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	D	404	X	-	-	-
22	CLA	G	602	X	-	-	-
22	CLA	G	603	X	-	-	-
22	CLA	G	604	X	-	-	-
22	CLA	G	610	X	-	-	-
22	CLA	G	611	X	-	-	-
22	CLA	G	612	X	-	-	-
22	CLA	G	613	X	-	-	-
22	CLA	G	614	X	-	-	-
22	CLA	N	602	X	-	-	-
22	CLA	N	603	X	-	-	-
22	CLA	N	604	X	-	-	-
22	CLA	N	610	X	-	-	-
22	CLA	N	611	X	-	-	-
22	CLA	N	612	X	-	-	-
22	CLA	N	613	X	-	-	-
22	CLA	N	614	X	-	-	-
22	CLA	R	301	X	-	-	-
22	CLA	R	302	X	-	X	-
22	CLA	R	303	X	-	-	-
22	CLA	R	307	X	-	-	-
22	CLA	R	308	X	-	-	-
22	CLA	R	309	X	-	-	-
22	CLA	R	310	X	-	-	-
22	CLA	R	311	X	-	-	-
22	CLA	R	312	X	-	X	-
22	CLA	S	301	X	-	-	-
22	CLA	S	303	X	-	-	-
22	CLA	S	304	X	-	-	-
22	CLA	S	305	X	-	-	-
22	CLA	S	309	X	-	-	-
22	CLA	S	310	X	-	-	-
22	CLA	S	311	X	-	-	-
22	CLA	S	312	X	-	-	-
22	CLA	S	313	X	-	-	-
22	CLA	S	314	X	-	-	-
22	CLA	Y	602	X	-	-	-
22	CLA	Y	603	X	-	-	-
22	CLA	Y	604	X	-	-	-
22	CLA	Y	610	X	-	-	-
22	CLA	Y	611	X	-	-	-
22	CLA	Y	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	Y	613	X	-	-	-
22	CLA	Y	614	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	g	602	X	-	-	-
22	CLA	g	603	X	-	-	-
22	CLA	g	604	X	-	-	-
22	CLA	g	610	X	-	-	-
22	CLA	g	611	X	-	-	-
22	CLA	g	612	X	-	-	-
22	CLA	g	613	X	-	-	-
22	CLA	g	614	X	-	-	-
22	CLA	n	602	X	-	-	-
22	CLA	n	603	X	-	-	-
22	CLA	n	604	X	-	-	-
22	CLA	n	610	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	2	608	X	-	-	-
25	CHL	3	301	X	-	-	-
25	CHL	3	302	X	-	-	-
25	CHL	3	306	X	-	-	-
25	CHL	3	307	X	-	-	-
25	CHL	3	308	X	-	-	-
25	CHL	3	309	X	-	-	-
25	CHL	4	301	X	-	-	-
25	CHL	4	305	X	-	-	-
25	CHL	4	306	X	-	-	-
25	CHL	4	307	X	-	-	-
25	CHL	4	308	X	-	-	-
25	CHL	5	601	X	-	-	-
25	CHL	5	605	X	-	-	-
25	CHL	5	606	X	-	-	-
25	CHL	5	607	X	-	-	-
25	CHL	5	608	X	-	-	-
25	CHL	5	609	X	-	-	-
25	CHL	5	615	X	-	-	-
25	CHL	6	601	X	-	-	-
25	CHL	6	605	X	-	-	-
25	CHL	6	606	X	-	-	-
25	CHL	6	607	X	-	-	-
25	CHL	6	608	X	-	-	-
25	CHL	7	301	X	-	-	-
25	CHL	7	302	X	-	-	-
25	CHL	7	306	X	-	-	-
25	CHL	7	307	X	-	-	-
25	CHL	7	308	X	-	-	-
25	CHL	7	309	X	-	-	-
25	CHL	8	301	X	-	-	-
25	CHL	8	305	X	-	-	-
25	CHL	8	306	X	-	-	-
25	CHL	8	307	X	-	-	-
25	CHL	8	308	X	-	-	-
25	CHL	G	601	X	-	-	-
25	CHL	G	605	X	-	-	-
25	CHL	G	606	X	-	-	-
25	CHL	G	607	X	-	-	-
25	CHL	G	608	X	-	-	-
25	CHL	G	609	X	-	-	-
25	CHL	N	601	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	y	609	X	-	-	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 78324 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	308	Total	C	N	O	S	0	0
			2388	1558	392	426	12		
1	a	330	Total	C	N	O	S	0	0
			2584	1688	426	457	13		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

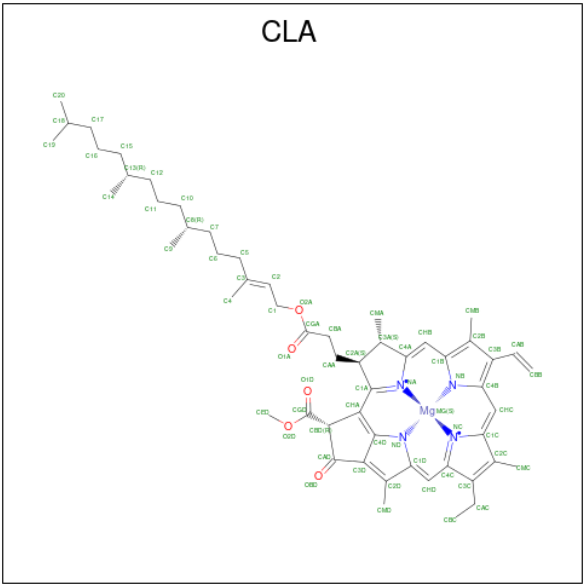
- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	y	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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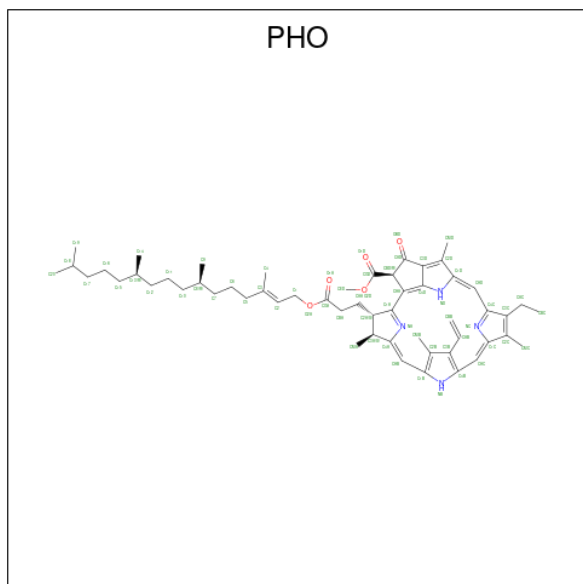
Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	8	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	8	1	45	35	1	4	5	0

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



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

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



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

- Molecule 25 is CHLOROPHYLL B (CCD ID: CHL) (formula: $\text{C}_{55}\text{H}_{70}\text{MgN}_4\text{O}_6$).



Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	R	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	G	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	N	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	Y	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
25	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	g	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	n	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	n	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	y	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	1	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	2	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	3	1	Total 42	C 33	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	5	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	6	1	Total 42	C 33	Mg 1	N 4	O 4	0
25	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
25	7	1	Total 46	C 35	Mg 1	N 4	O 6	0

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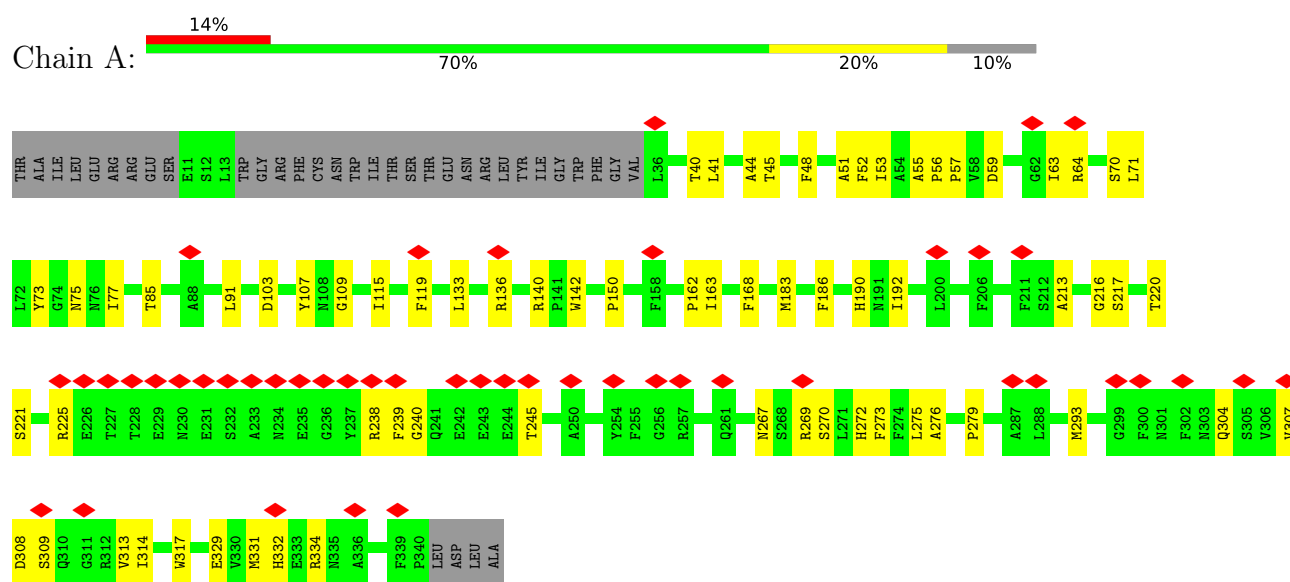
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Mol	Chain	Residues	Atoms					AltConf
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

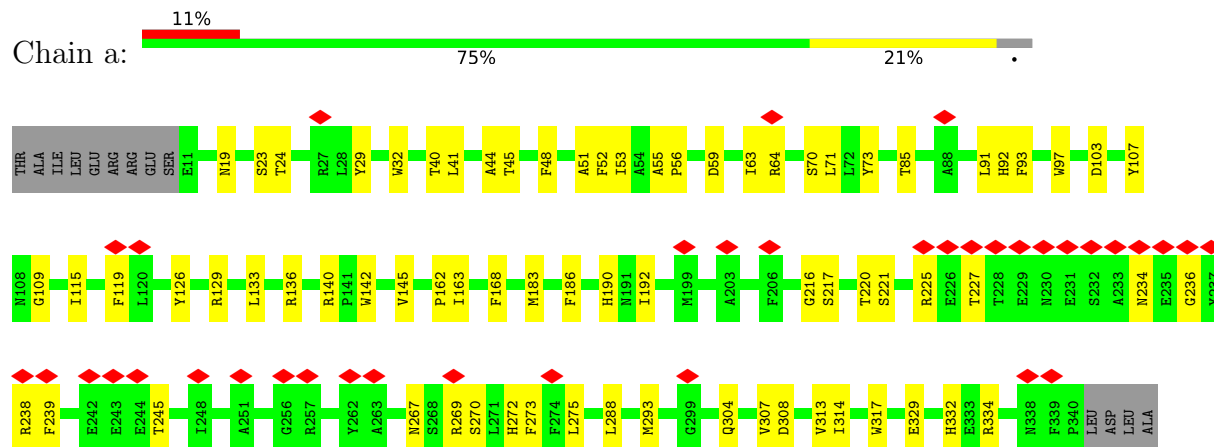
3 Residue-property plots

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

• Molecule 1: Photosystem II protein D1



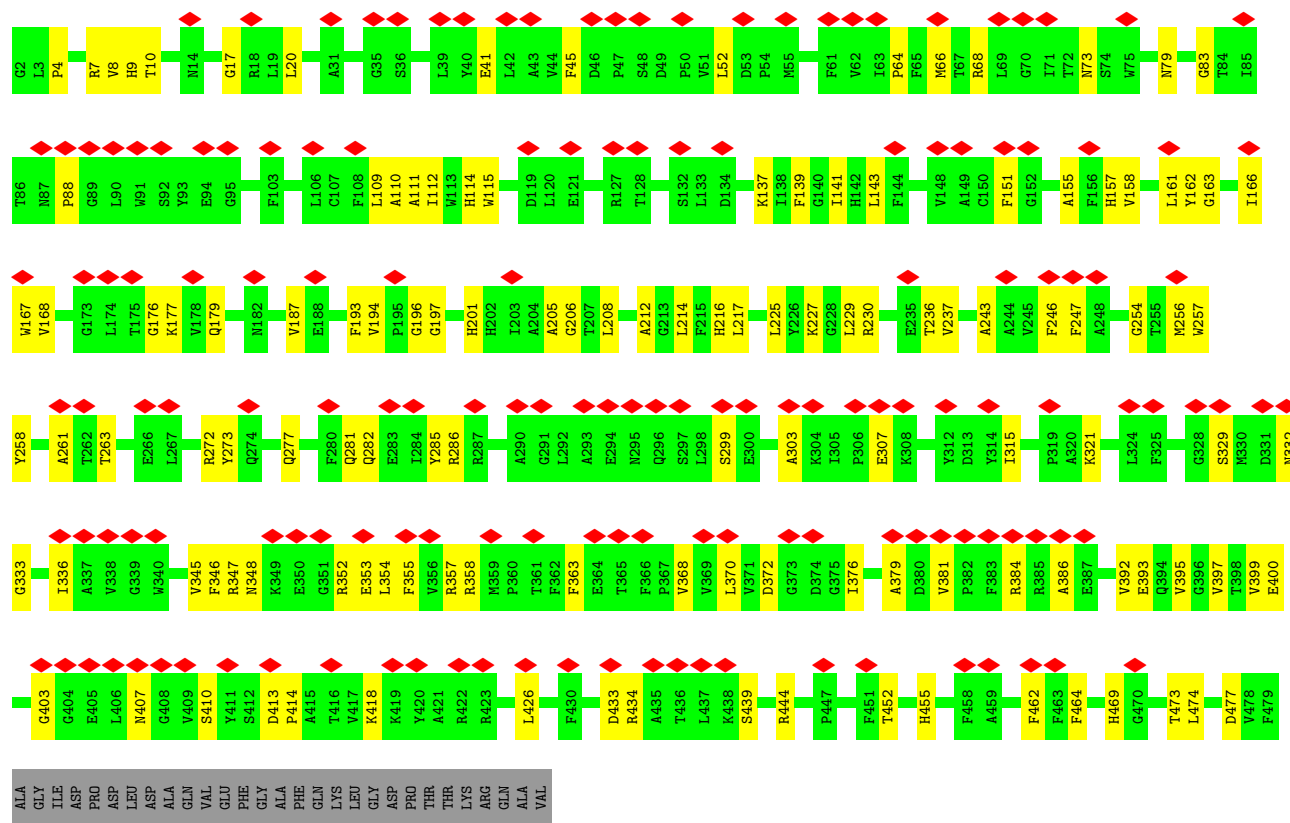
• Molecule 1: Photosystem II protein D1



• Molecule 2: Photosystem II CP47 reaction center protein

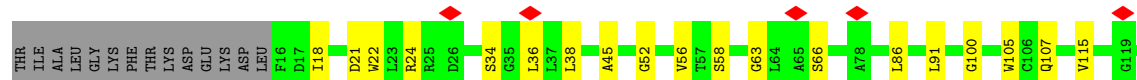


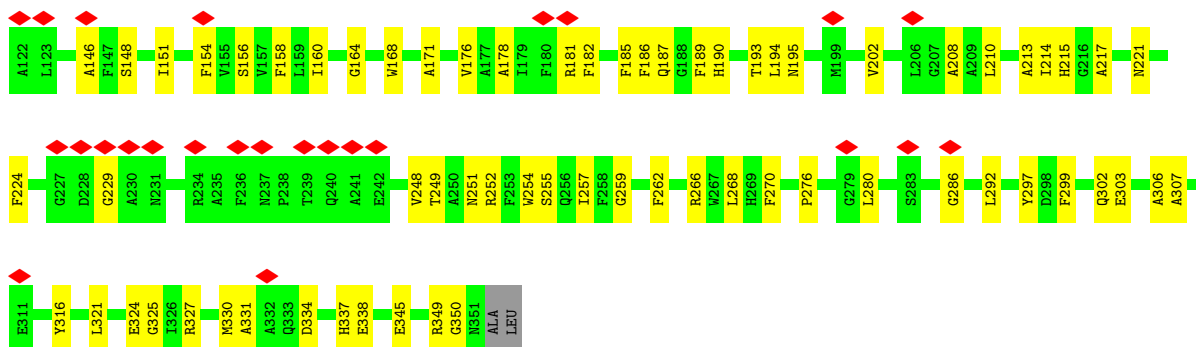
- Molecule 2: Photosystem II CP47 reaction center protein



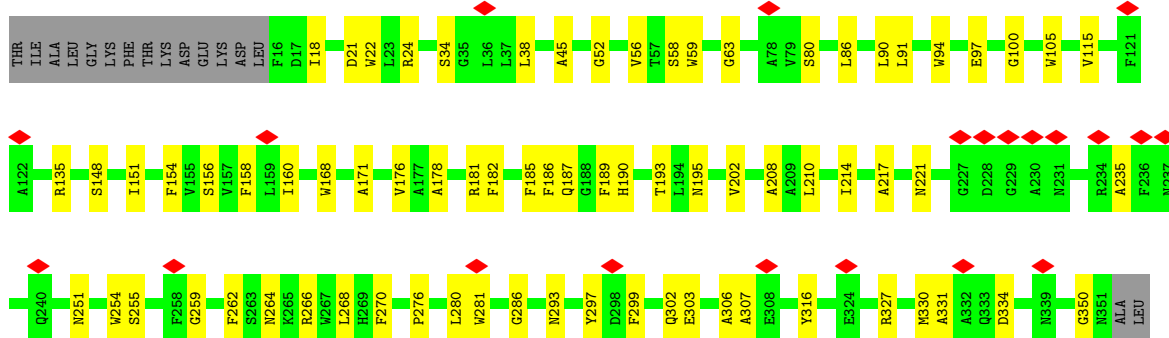
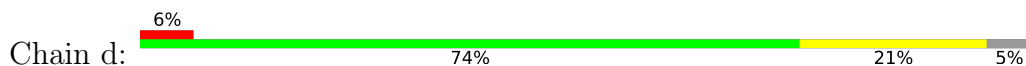
- Molecule 3: Photosystem II CP43 reaction center protein







• Molecule 4: Photosystem II D2 protein



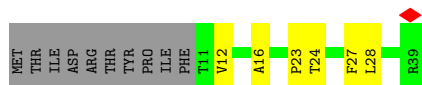
• Molecule 5: Cytochrome b559 subunit alpha



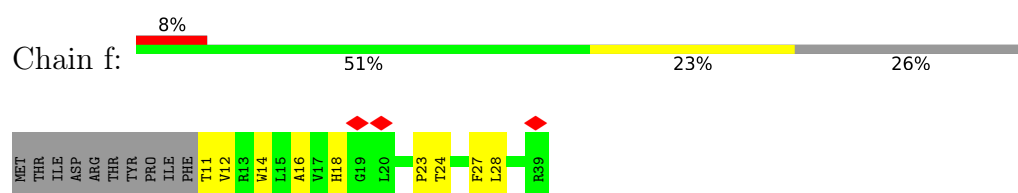
• Molecule 5: Cytochrome b559 subunit alpha



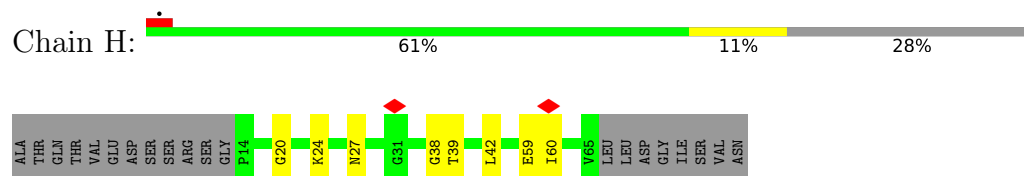
• Molecule 6: Cytochrome b559 subunit beta (PsbF)



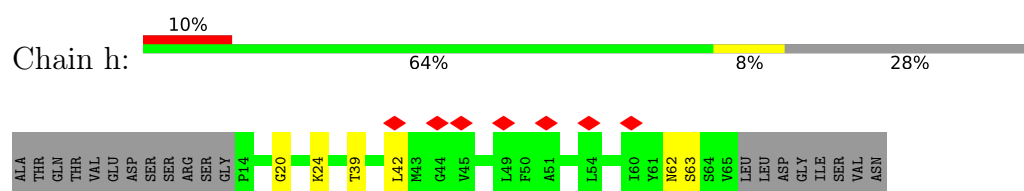
• Molecule 6: Cytochrome b559 subunit beta (PsbF)



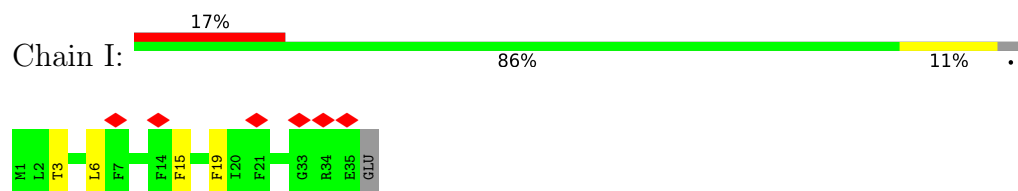
• Molecule 7: Photosystem II reaction center protein H



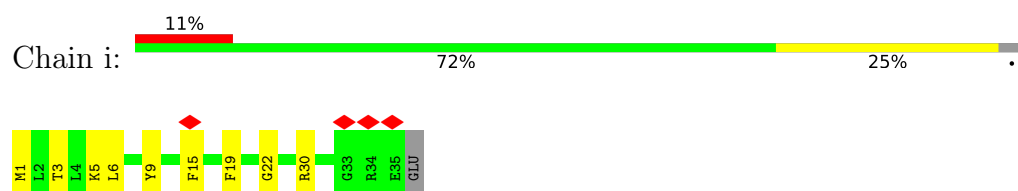
• Molecule 7: Photosystem II reaction center protein H



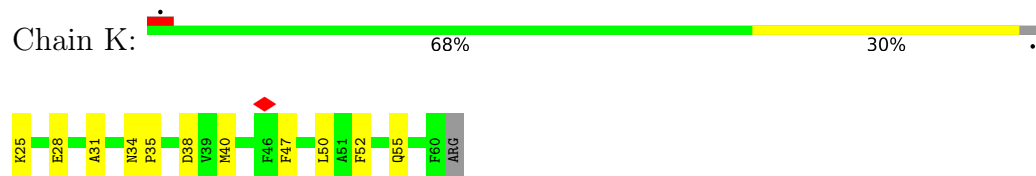
• Molecule 8: Photosystem II reaction center protein I



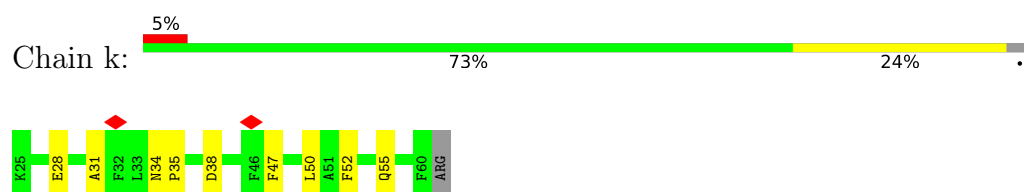
• Molecule 8: Photosystem II reaction center protein I



• Molecule 9: Photosystem II reaction center protein K



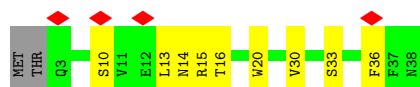
• Molecule 9: Photosystem II reaction center protein K



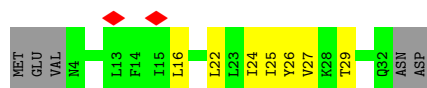
- Molecule 10: Photosystem II reaction center protein L



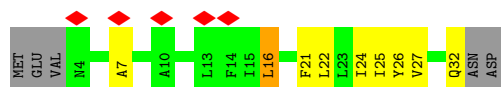
- Molecule 10: Photosystem II reaction center protein L



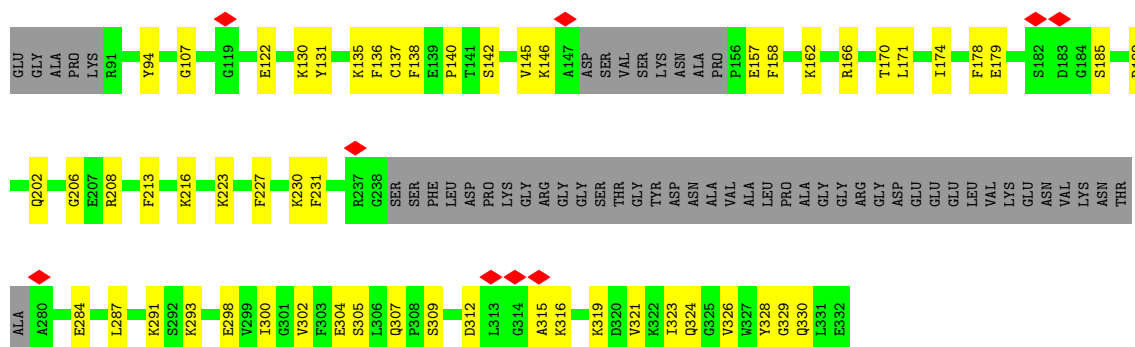
- Molecule 11: Photosystem II reaction center protein M



- Molecule 11: Photosystem II reaction center protein M

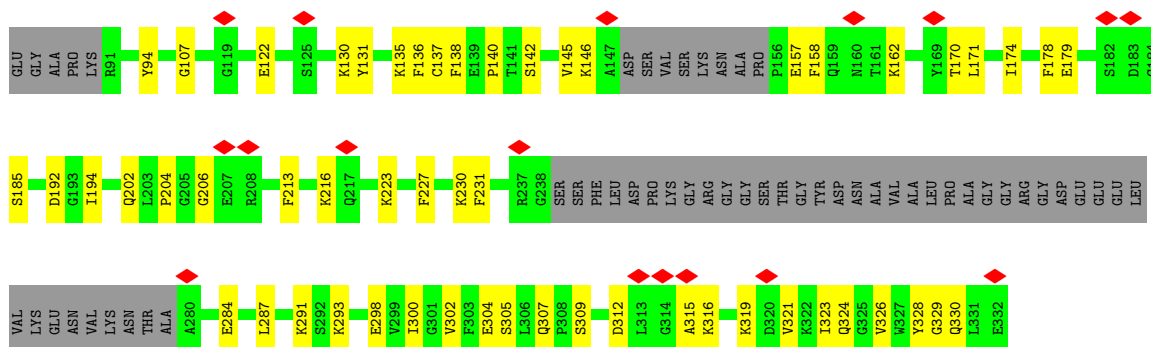


- Molecule 12: Oxygen-evolving enhancer protein 1-1, chloroplastic

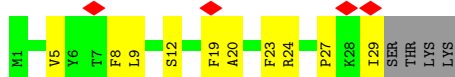


- Molecule 12: Oxygen-evolving enhancer protein 1-1, chloroplastic

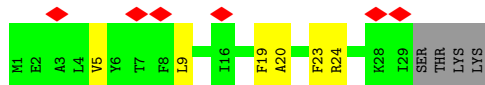




• Molecule 13: Photosystem II reaction center protein T



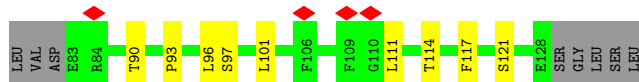
• Molecule 13: Photosystem II reaction center protein T



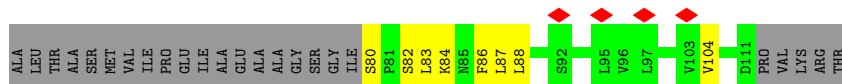
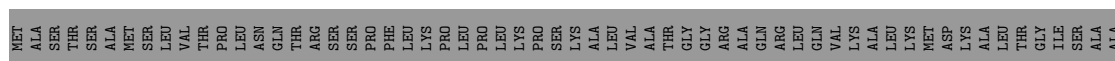
• Molecule 14: Photosystem II reaction center W protein, chloroplastic



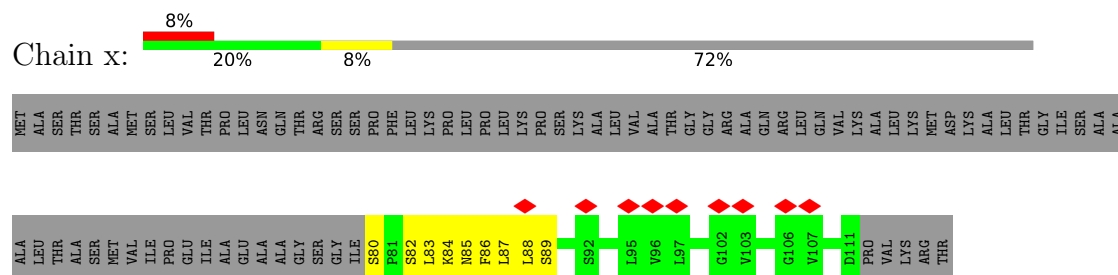
• Molecule 14: Photosystem II reaction center W protein, chloroplastic



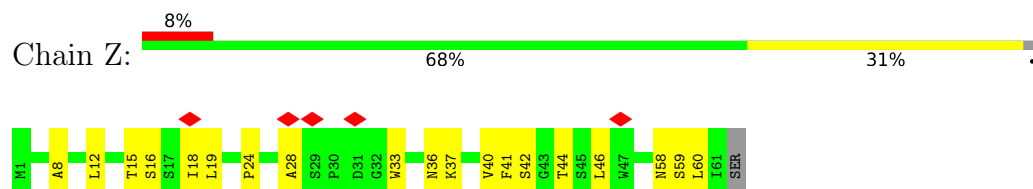
• Molecule 15: Photosystem II reaction center protein X



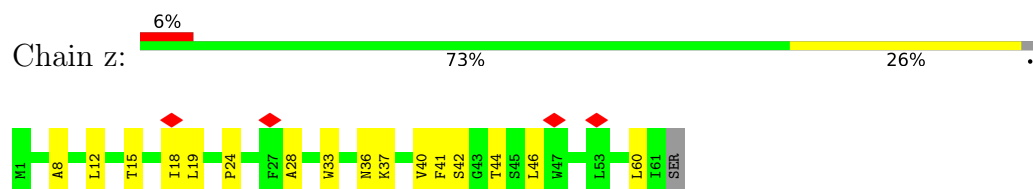
- Molecule 15: Photosystem II reaction center protein X



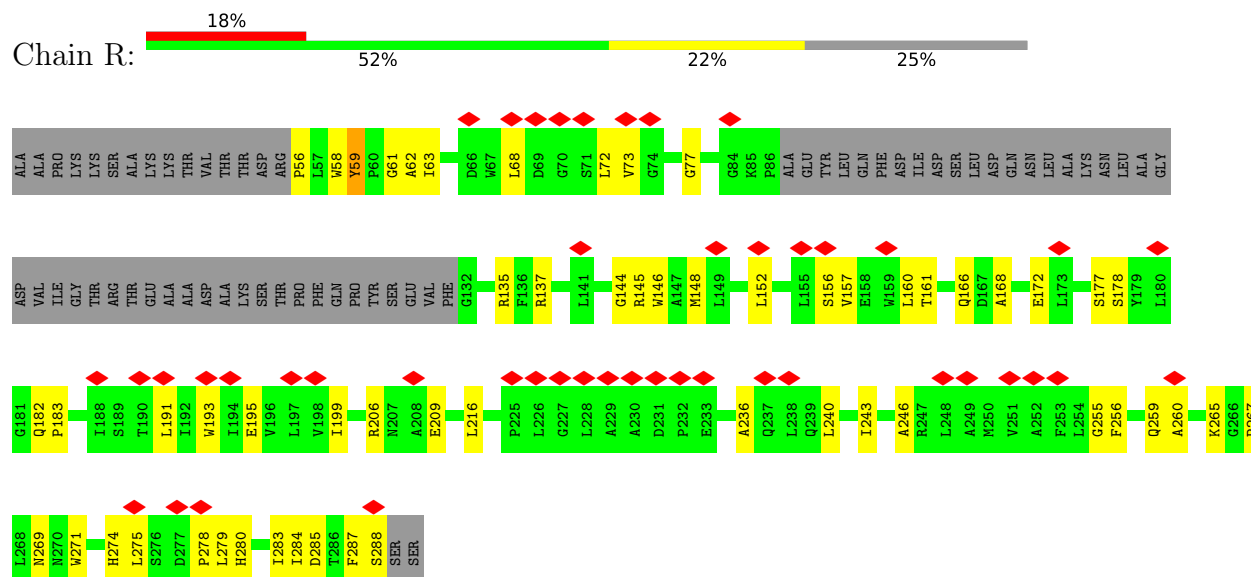
- Molecule 16: Photosystem II reaction center protein Z



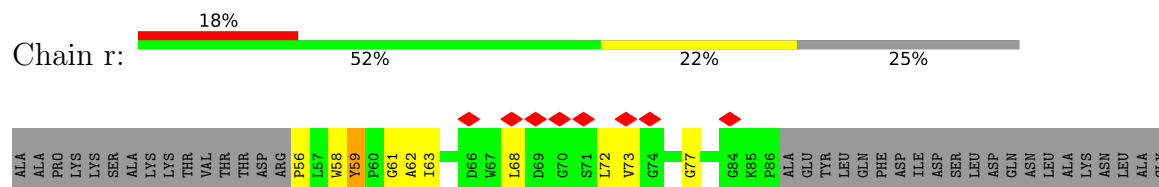
- Molecule 16: Photosystem II reaction center protein Z

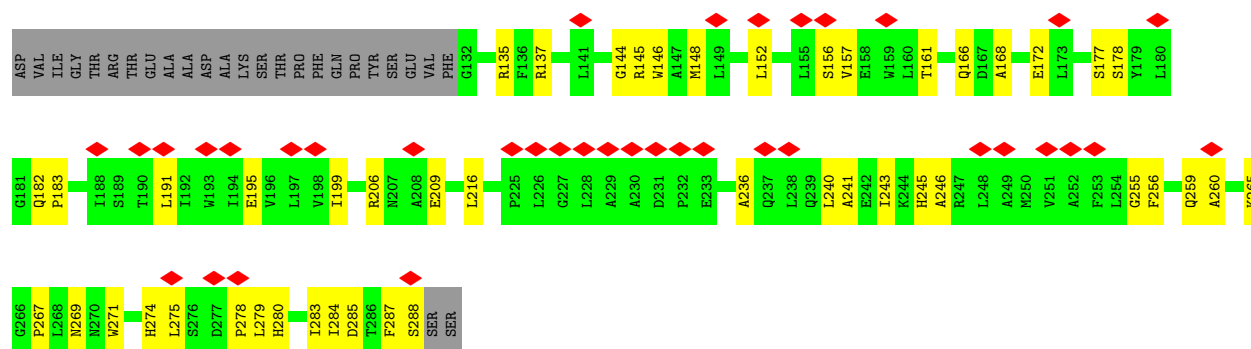


- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic



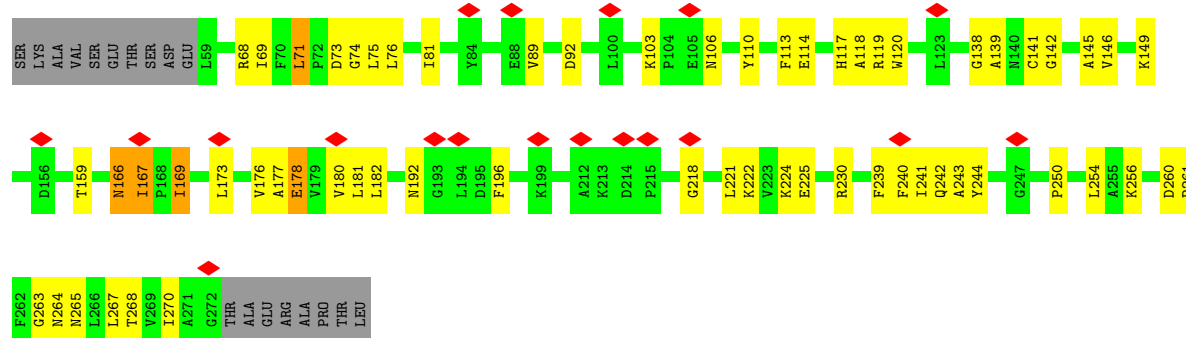
- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic





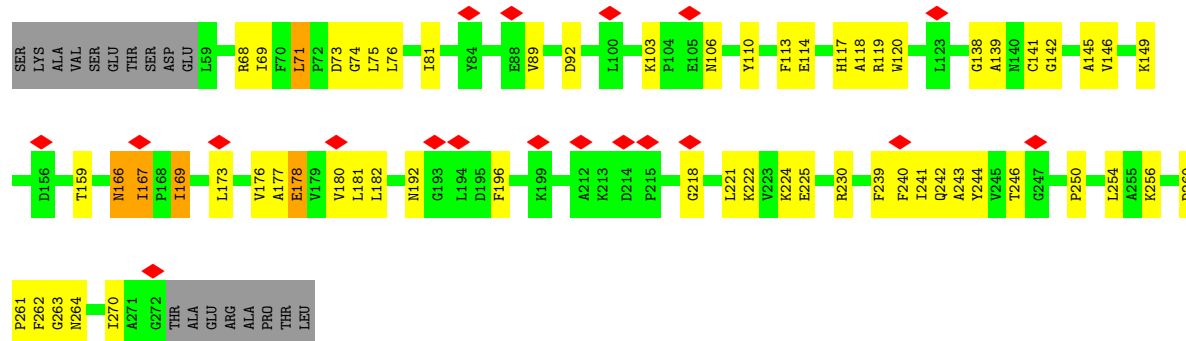
- Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic

Chain S: 8% 66% 25% 8%



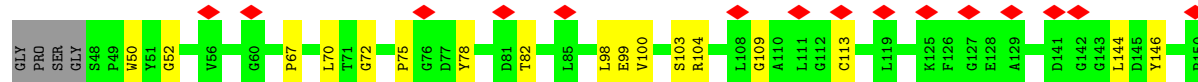
- Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic

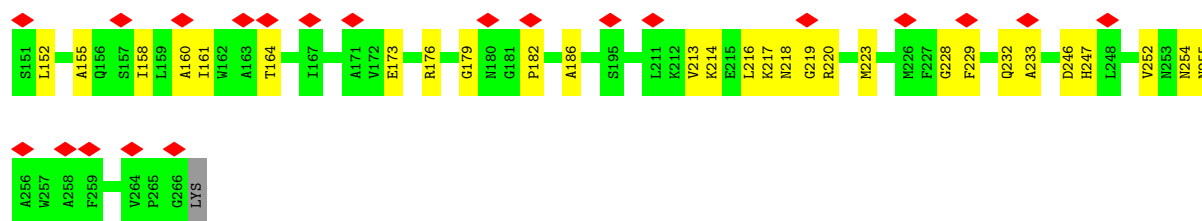
Chain s: 8% 66% 24% 8%



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

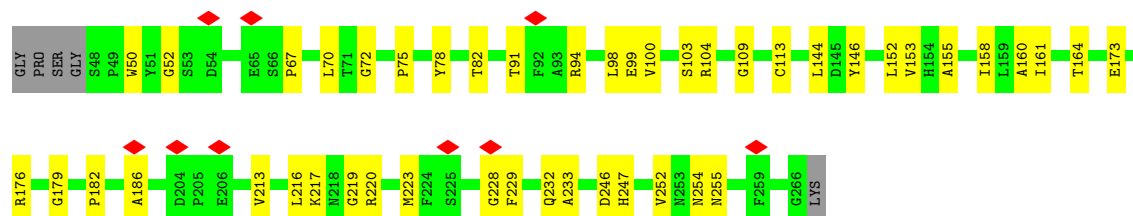
Chain G: 16% 78% 20%





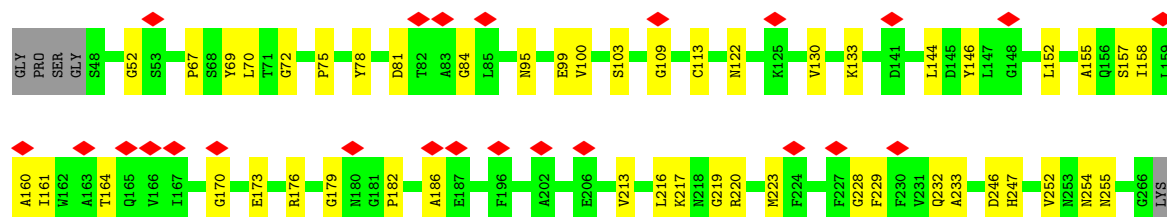
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain N: 77% 21% .



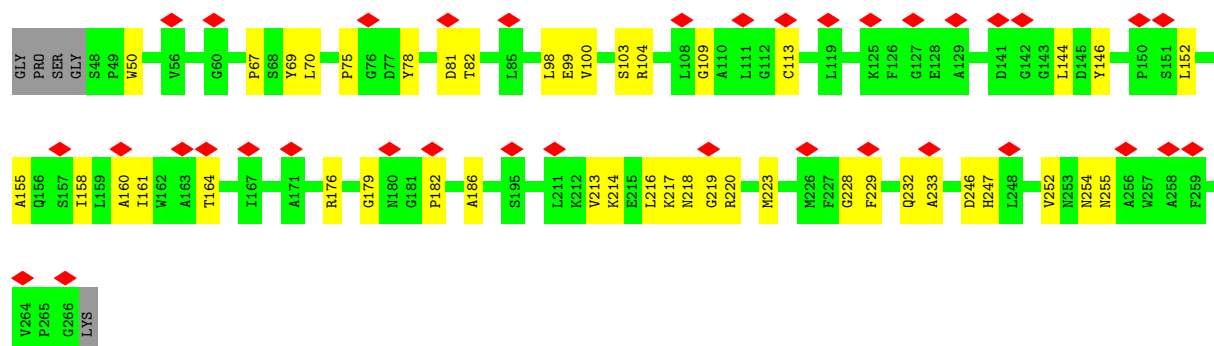
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain Y: 11% 76% 21% .



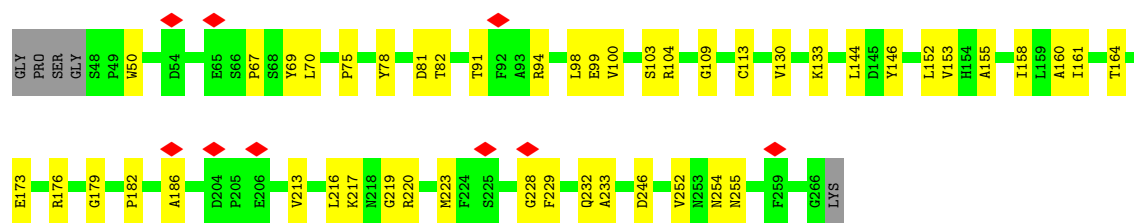
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain g: 16% 78% 20% .

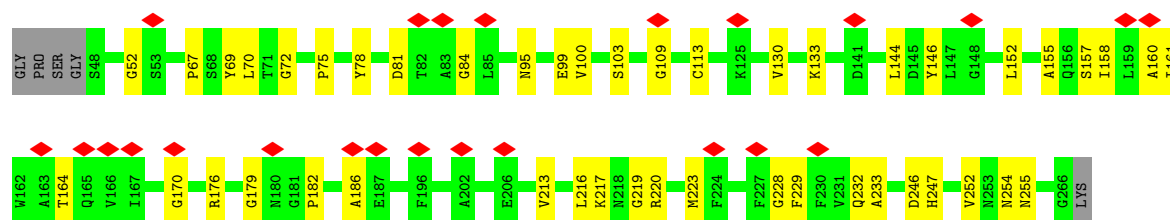
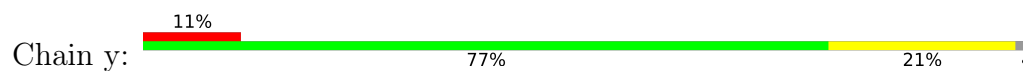


- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

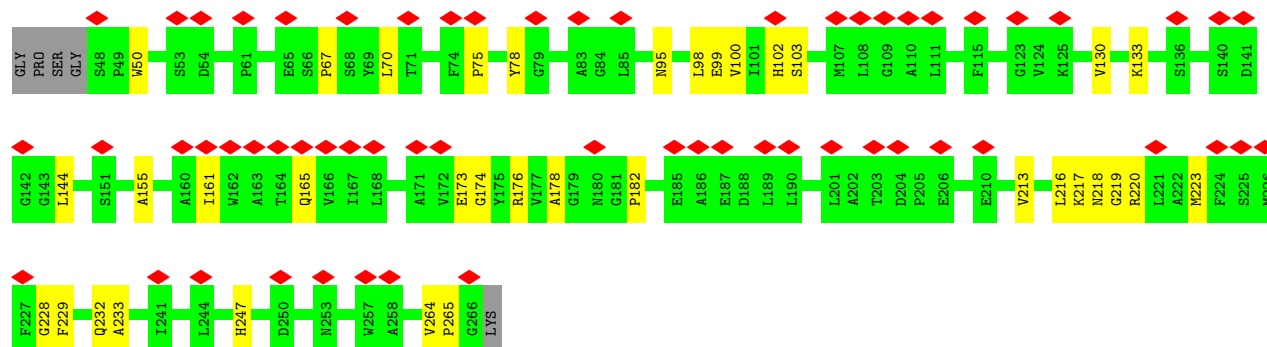
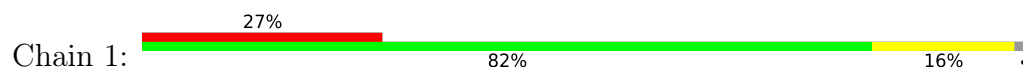
Chain n: 77% 21% .



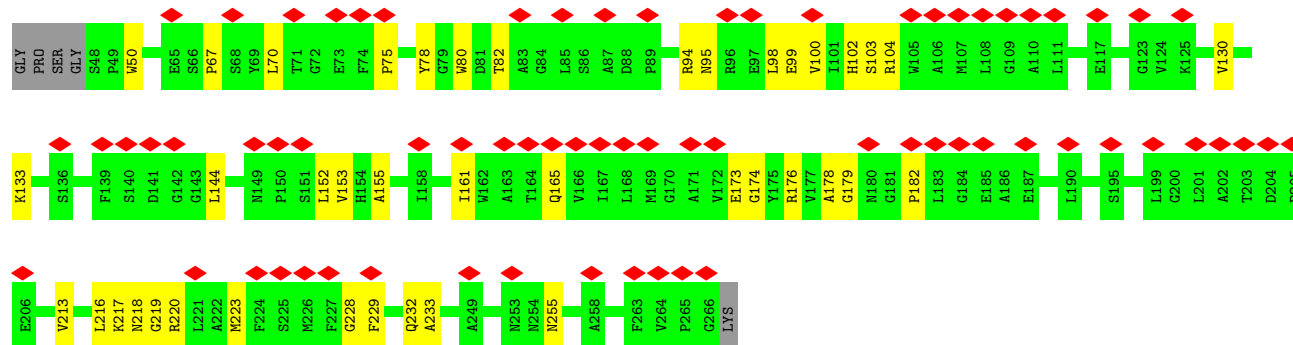
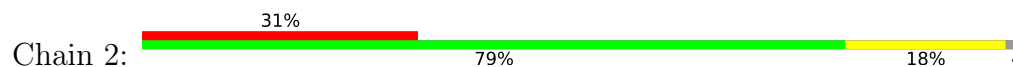
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



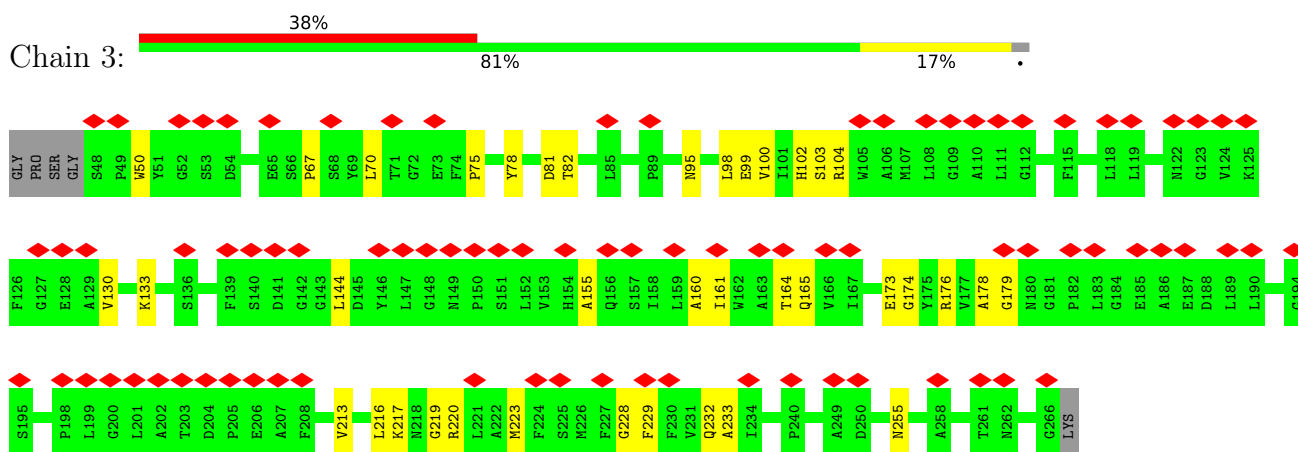
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



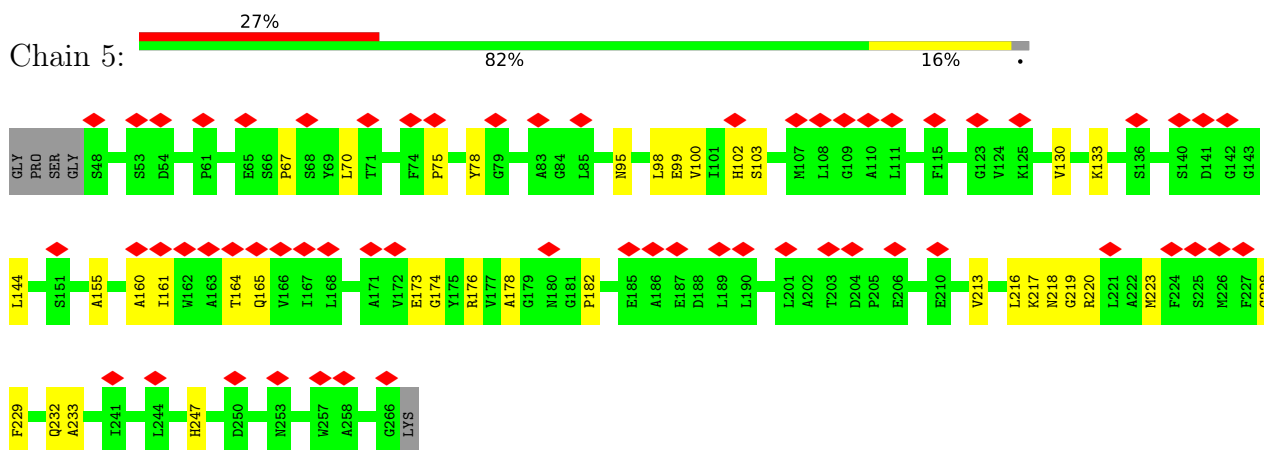
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



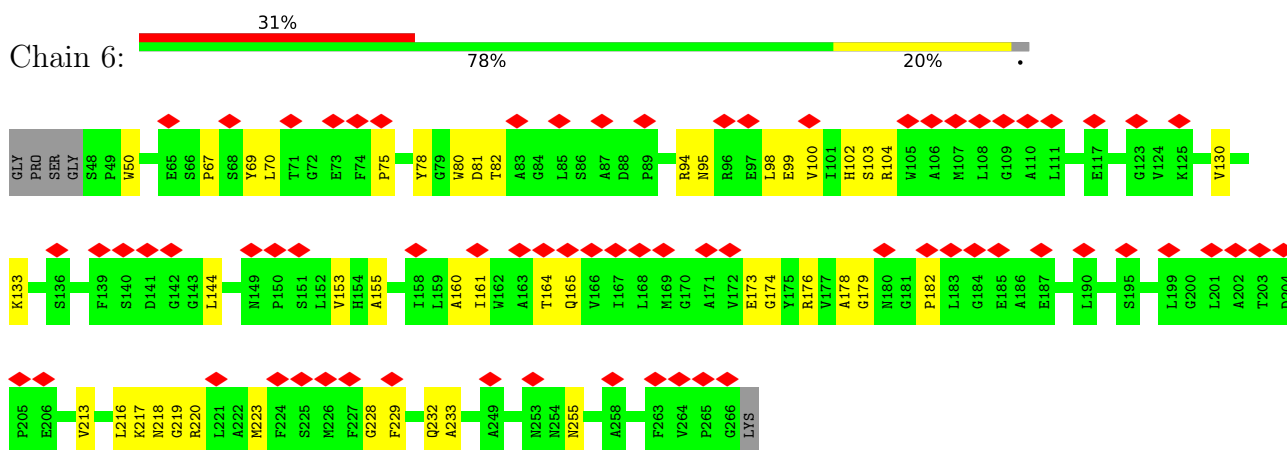
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



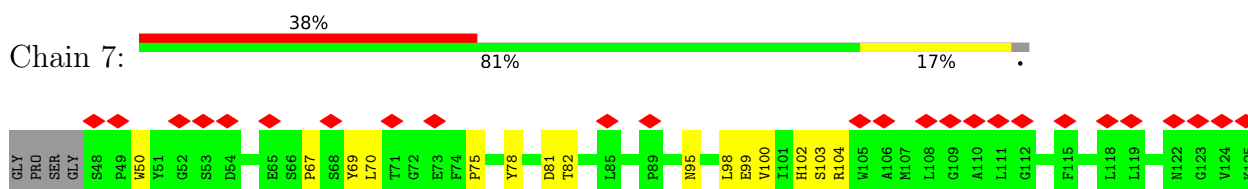
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

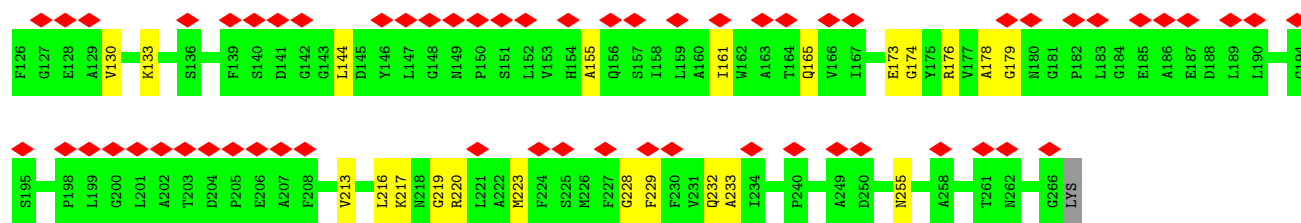


- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

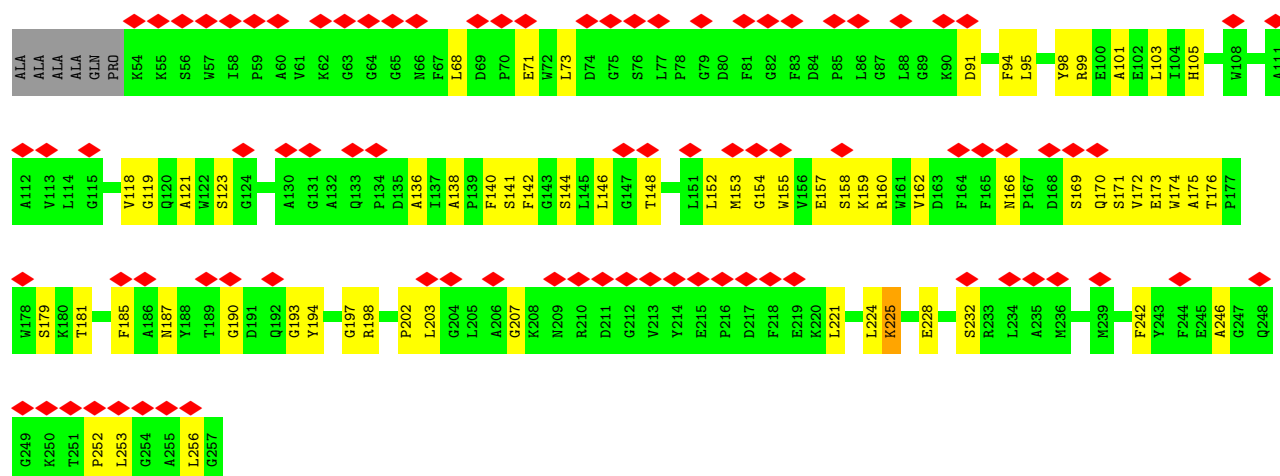
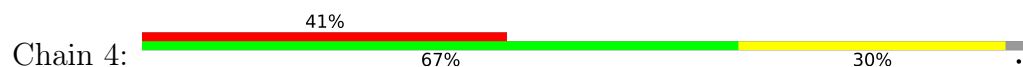


- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

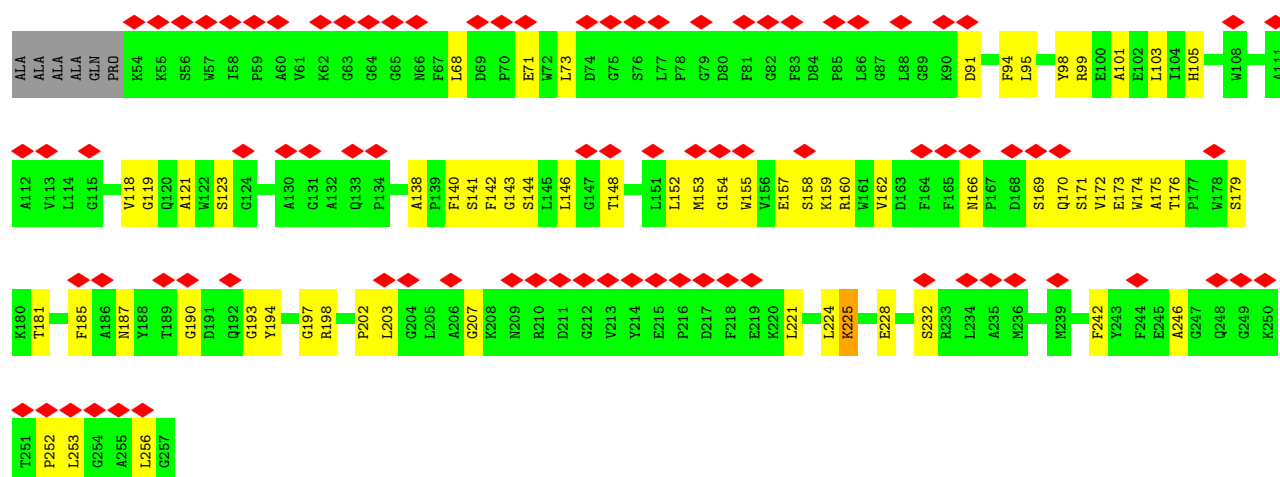
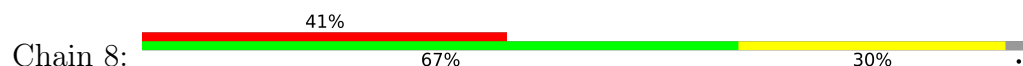




- Molecule 20: Chlorophyll a-b binding protein, chloroplastic



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



4 Experimental information

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/2458	0.70	0/3348
1	a	0.30	0/2665	0.70	0/3634
2	B	0.28	0/3881	0.70	0/5286
2	b	0.28	0/3881	0.70	0/5286
3	C	0.29	0/3487	0.72	2/4750 (0.0%)
3	c	0.29	0/3487	0.72	2/4750 (0.0%)
4	D	0.30	0/2768	0.74	1/3774 (0.0%)
4	d	0.30	0/2768	0.74	1/3774 (0.0%)
5	E	0.34	0/603	0.90	2/819 (0.2%)
5	e	0.34	0/603	0.90	2/819 (0.2%)
6	F	0.31	0/229	0.78	0/311
6	f	0.31	0/229	0.78	0/311
7	H	0.30	0/398	0.70	0/541
7	h	0.30	0/398	0.70	0/541
8	I	0.35	0/294	0.87	0/397
8	i	0.35	0/294	0.87	0/397
9	K	0.37	0/301	0.93	0/414
9	k	0.37	0/301	0.93	0/414
10	L	0.32	0/310	0.86	0/421
10	l	0.32	0/310	0.86	0/421
11	M	0.37	0/230	0.79	0/315
11	m	0.37	0/230	0.79	0/315
12	O	0.28	0/1518	0.72	2/2049 (0.1%)
12	o	0.28	0/1518	0.72	2/2049 (0.1%)
13	T	0.29	0/246	0.72	0/333
13	t	0.29	0/246	0.72	0/333
14	W	0.27	0/383	0.76	0/519
14	w	0.27	0/383	0.76	0/519
15	X	0.29	0/228	0.60	0/310
15	x	0.28	0/228	0.59	0/310
16	Z	0.27	0/468	0.67	0/641
16	z	0.28	0/468	0.68	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.26	0/1502	0.58	0/2047
17	r	0.26	0/1502	0.58	0/2047
18	S	0.32	0/1698	0.96	11/2305 (0.5%)
18	s	0.32	0/1698	0.96	11/2305 (0.5%)
19	1	0.23	0/1716	0.60	0/2336
19	2	0.23	0/1716	0.60	0/2336
19	3	0.23	0/1716	0.60	0/2336
19	5	0.23	0/1716	0.60	0/2336
19	6	0.23	0/1716	0.60	0/2336
19	7	0.23	0/1716	0.60	0/2336
19	G	0.27	0/1716	0.63	0/2336
19	N	0.27	0/1716	0.63	0/2336
19	Y	0.27	0/1716	0.63	0/2336
19	g	0.27	0/1716	0.63	0/2336
19	n	0.27	0/1716	0.63	0/2336
19	y	0.27	0/1716	0.63	0/2336
20	4	0.29	0/1652	1.10	5/2242 (0.2%)
20	8	0.29	0/1652	1.10	5/2242 (0.2%)
All	All	0.28	0/66107	0.73	46/89962 (0.1%)

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

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

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	207	GLY	CA-C-O	28.04	152.19	121.90
20	8	207	GLY	CA-C-O	28.04	152.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	207	GLY	O-C-N	-27.56	87.76	122.76
20	8	207	GLY	O-C-N	-27.56	87.76	122.76
20	4	207	GLY	CA-C-N	6.29	131.37	122.05

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2309	59	0
1	a	2584	0	2490	55	0
2	B	3752	0	3636	109	0
2	b	3752	0	3636	115	0
3	C	3373	0	3302	127	0
3	c	3373	0	3302	111	0
4	D	2675	0	2565	86	0
4	d	2675	0	2565	64	0
5	E	586	0	566	13	0
5	e	586	0	566	12	0
6	F	224	0	233	4	0
6	f	224	0	233	6	0
7	H	389	0	411	8	0
7	h	389	0	411	4	0
8	I	286	0	295	2	0
8	i	286	0	295	8	0
9	K	290	0	300	7	0
9	k	290	0	300	5	0
10	L	302	0	291	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	l	302	0	291	7	0
11	M	226	0	252	6	0
11	m	226	0	252	9	0
12	O	1487	0	1462	36	0
12	o	1487	0	1462	35	0
13	T	239	0	255	9	0
13	t	239	0	255	3	0
14	W	372	0	346	7	0
14	w	372	0	346	6	0
15	X	226	0	244	6	0
15	x	226	0	244	6	0
16	Z	458	0	490	32	0
16	z	458	0	489	23	0
17	R	1459	0	1428	132	0
17	r	1459	0	1428	127	0
18	S	1653	0	1639	79	0
18	s	1653	0	1639	73	0
19	1	1666	0	1593	29	0
19	2	1666	0	1593	33	0
19	3	1666	0	1593	29	0
19	5	1666	0	1593	28	0
19	6	1666	0	1593	37	0
19	7	1666	0	1593	30	0
19	G	1666	0	1593	33	0
19	N	1666	0	1593	33	0
19	Y	1666	0	1593	36	0
19	g	1666	0	1593	31	0
19	n	1666	0	1593	33	0
19	y	1666	0	1593	35	0
20	4	1597	0	1526	159	0
20	8	1597	0	1526	162	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	1	360	0	264	3	0
22	2	360	0	264	22	0
22	3	360	0	264	2	0
22	4	225	0	165	5	0
22	5	360	0	264	3	0
22	6	360	0	264	22	0
22	7	360	0	264	2	0
22	8	225	0	165	5	0
22	A	135	0	99	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	720	0	528	23	0
22	C	540	0	396	15	0
22	D	135	0	99	3	0
22	G	360	0	264	7	0
22	N	360	0	264	4	0
22	R	405	0	295	67	0
22	S	450	0	330	13	0
22	Y	360	0	264	8	0
22	a	135	0	99	3	0
22	b	720	0	528	19	0
22	c	540	0	396	13	0
22	d	135	0	99	4	0
22	g	360	0	264	6	0
22	n	360	0	264	4	0
22	r	405	0	295	46	0
22	s	450	0	330	23	0
22	y	360	0	264	5	0
23	A	44	0	35	2	0
23	D	44	0	35	1	0
23	a	44	0	35	2	0
23	d	44	0	35	2	0
24	E	43	0	30	3	0
24	e	43	0	30	3	0
25	1	318	0	213	9	0
25	2	226	0	151	13	0
25	3	272	0	182	6	0
25	4	230	0	155	14	0
25	5	318	0	213	7	0
25	6	226	0	151	13	0
25	7	272	0	182	7	0
25	8	230	0	155	15	0
25	G	272	0	182	11	0
25	N	272	0	182	9	0
25	R	138	0	93	6	0
25	S	184	0	124	4	0
25	Y	272	0	182	12	0
25	g	272	0	182	11	0
25	n	272	0	182	8	0
25	r	138	0	93	3	0
25	s	184	0	124	3	0
25	y	272	0	182	11	0
All	All	78324	0	72516	1876	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 12.

The worst 5 of 1876 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:PHE:CZ	18:S:261:PRO:HG2	1.17	1.70
16:Z:59:SER:CB	18:S:267:LEU:CD2	1.74	1.58
17:r:280:HIS:HA	20:4:141:SER:N	1.20	1.48
16:Z:59:SER:CB	18:S:267:LEU:HD23	1.02	1.47
22:b:214:LEU:HD22	22:R:302:CLA:CED	1.42	1.47

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	26/343 (8%)	25 (96%)	1 (4%)	0	100	100
2	b	136/507 (27%)	125 (92%)	11 (8%)	0	100	100
3	c	429/459 (94%)	402 (94%)	27 (6%)	0	100	100
4	d	313/352 (89%)	288 (92%)	25 (8%)	0	100	100
5	e	68/83 (82%)	59 (87%)	9 (13%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	0	100	100
7	h	50/72 (69%)	44 (88%)	6 (12%)	0	100	100
8	i	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
9	k	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
10	l	29/38 (76%)	23 (79%)	6 (21%)	0	100	100
11	m	7/34 (21%)	7 (100%)	0	0	100	100
12	o	111/247 (45%)	99 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	t	27/33 (82%)	27 (100%)	0	0	100	100
14	w	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
15	x	8/116 (7%)	8 (100%)	0	0	100	100
16	z	59/62 (95%)	59 (100%)	0	0	100	100
17	R	184/250 (74%)	172 (94%)	12 (6%)	0	100	100
17	r	12/250 (5%)	10 (83%)	2 (17%)	0	100	100
18	S	212/232 (91%)	171 (81%)	41 (19%)	0	100	100
18	s	141/232 (61%)	116 (82%)	25 (18%)	0	100	100
19	1	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	2	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	3	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	5	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	6	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	7	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	G	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	N	149/224 (66%)	138 (93%)	11 (7%)	0	100	100
19	Y	107/224 (48%)	102 (95%)	5 (5%)	0	100	100
19	g	201/224 (90%)	189 (94%)	12 (6%)	0	100	100
19	n	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	y	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
20	4	202/210 (96%)	184 (91%)	18 (9%)	0	100	100
20	8	202/210 (96%)	184 (91%)	18 (9%)	0	100	100
All	All	4764/6584 (72%)	4388 (92%)	376 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/278 (89%)	247 (100%)	0	100	100
1	a	267/278 (96%)	267 (100%)	0	100	100
2	B	379/401 (94%)	379 (100%)	0	100	100
2	b	379/401 (94%)	379 (100%)	0	100	100
3	C	340/359 (95%)	340 (100%)	0	100	100
3	c	340/359 (95%)	340 (100%)	0	100	100
4	D	269/282 (95%)	269 (100%)	0	100	100
4	d	269/282 (95%)	269 (100%)	0	100	100
5	E	63/73 (86%)	63 (100%)	0	100	100
5	e	63/73 (86%)	63 (100%)	0	100	100
6	F	24/34 (71%)	24 (100%)	0	100	100
6	f	24/34 (71%)	24 (100%)	0	100	100
7	H	43/60 (72%)	43 (100%)	0	100	100
7	h	43/60 (72%)	43 (100%)	0	100	100
8	I	32/33 (97%)	32 (100%)	0	100	100
8	i	32/33 (97%)	32 (100%)	0	100	100
9	K	31/32 (97%)	31 (100%)	0	100	100
9	k	31/32 (97%)	31 (100%)	0	100	100
10	L	34/36 (94%)	34 (100%)	0	100	100
10	l	34/36 (94%)	34 (100%)	0	100	100
11	M	25/30 (83%)	25 (100%)	0	100	100
11	m	25/30 (83%)	24 (96%)	1 (4%)	28	48
12	O	164/204 (80%)	164 (100%)	0	100	100
12	o	164/204 (80%)	164 (100%)	0	100	100
13	T	26/30 (87%)	26 (100%)	0	100	100
13	t	26/30 (87%)	26 (100%)	0	100	100
14	W	40/47 (85%)	40 (100%)	0	100	100
14	w	40/47 (85%)	40 (100%)	0	100	100
15	X	27/92 (29%)	27 (100%)	0	100	100
15	x	27/92 (29%)	27 (100%)	0	100	100
16	Z	53/54 (98%)	53 (100%)	0	100	100
16	z	53/54 (98%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	R	150/201 (75%)	149 (99%)	1 (1%)	76	80
17	r	150/201 (75%)	149 (99%)	1 (1%)	76	80
18	S	165/180 (92%)	163 (99%)	2 (1%)	63	74
18	s	165/180 (92%)	163 (99%)	2 (1%)	63	74
19	1	167/170 (98%)	167 (100%)	0	100	100
19	2	167/170 (98%)	167 (100%)	0	100	100
19	3	167/170 (98%)	167 (100%)	0	100	100
19	5	167/170 (98%)	167 (100%)	0	100	100
19	6	167/170 (98%)	167 (100%)	0	100	100
19	7	167/170 (98%)	167 (100%)	0	100	100
19	G	167/170 (98%)	167 (100%)	0	100	100
19	N	167/170 (98%)	167 (100%)	0	100	100
19	Y	167/170 (98%)	167 (100%)	0	100	100
19	g	167/170 (98%)	167 (100%)	0	100	100
19	n	167/170 (98%)	167 (100%)	0	100	100
19	y	167/170 (98%)	167 (100%)	0	100	100
20	4	156/158 (99%)	156 (100%)	0	100	100
20	8	156/158 (99%)	156 (100%)	0	100	100
All	All	6560/7208 (91%)	6553 (100%)	7 (0%)	87	88

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

Mol	Chain	Res	Type
18	S	169	ILE
17	r	199	ILE
18	s	169	ILE
18	s	81	ILE
18	S	81	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
18	s	257	HIS
20	4	133	GLN
19	g	156	GLN

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Mol	Chain	Res	Type
19	y	156	GLN
20	8	166	ASN

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	R	306	-	40,54,74	2.24	11 (27%)	34,90,114	2.96	18 (52%)
22	CLA	C	507	-	49,53,73	2.15	17 (34%)	58,89,113	2.83	32 (55%)
22	CLA	3	305	-	49,53,73	2.23	19 (38%)	58,89,113	2.79	27 (46%)
22	CLA	7	305	-	49,53,73	2.23	19 (38%)	58,89,113	2.79	27 (46%)
22	CLA	c	509	-	49,53,73	2.19	14 (28%)	58,89,113	2.73	27 (46%)
22	CLA	G	603	-	49,53,73	2.19	19 (38%)	58,89,113	2.83	32 (55%)
22	CLA	N	604	-	49,53,73	2.19	16 (32%)	58,89,113	2.82	30 (51%)
22	CLA	N	612	19	49,53,73	2.17	16 (32%)	58,89,113	2.80	30 (51%)
25	CHL	y	607	-	40,54,74	2.22	12 (30%)	34,90,114	3.04	20 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	1	607	-	40,54,74	2.22	11 (27%)	34,90,114	3.14	18 (52%)
22	CLA	S	313	18	49,53,73	2.19	16 (32%)	58,89,113	2.87	32 (55%)
22	CLA	N	611	-	49,53,73	2.18	17 (34%)	58,89,113	2.86	30 (51%)
25	CHL	8	301	-	40,54,74	2.26	12 (30%)	34,90,114	2.95	19 (55%)
22	CLA	b	603	-	49,53,73	2.24	18 (36%)	58,89,113	2.89	32 (55%)
25	CHL	7	301	-	40,54,74	2.23	12 (30%)	34,90,114	3.11	19 (55%)
22	CLA	1	602	19	49,53,73	2.21	19 (38%)	58,89,113	2.74	28 (48%)
23	PHO	a	404	-	38,49,69	2.77	13 (34%)	31,75,99	3.75	14 (45%)
22	CLA	b	602	-	49,53,73	2.16	15 (30%)	58,89,113	2.79	30 (51%)
25	CHL	n	607	-	40,54,74	2.18	12 (30%)	34,90,114	3.13	19 (55%)
22	CLA	c	510	-	49,53,73	2.23	18 (36%)	58,89,113	2.76	27 (46%)
22	CLA	N	610	19	49,53,73	2.19	15 (30%)	58,89,113	2.76	26 (44%)
22	CLA	4	309	20	49,53,73	2.22	18 (36%)	58,89,113	2.70	29 (50%)
22	CLA	D	404	-	49,53,73	2.20	18 (36%)	58,89,113	2.78	30 (51%)
25	CHL	N	608	-	40,54,74	2.24	11 (27%)	34,90,114	2.94	20 (58%)
25	CHL	7	308	-	40,54,74	2.25	11 (27%)	34,90,114	2.97	18 (52%)
22	CLA	d	403	-	49,53,73	2.21	16 (32%)	58,89,113	2.96	34 (58%)
22	CLA	R	303	-	49,53,73	2.18	15 (30%)	58,89,113	2.96	32 (55%)
22	CLA	6	603	-	49,53,73	2.21	19 (38%)	58,89,113	2.73	28 (48%)
22	CLA	G	610	19	49,53,73	2.19	15 (30%)	58,89,113	2.76	28 (48%)
25	CHL	G	606	-	40,54,74	2.24	10 (25%)	34,90,114	2.98	15 (44%)
22	CLA	7	310	19	49,53,73	2.24	17 (34%)	58,89,113	2.76	27 (46%)
22	CLA	B	609	-	49,53,73	2.21	18 (36%)	58,89,113	2.90	33 (56%)
22	CLA	6	602	19	49,53,73	2.22	20 (40%)	58,89,113	2.75	29 (50%)
22	CLA	5	612	19	49,53,73	2.23	19 (38%)	58,89,113	2.76	29 (50%)
25	CHL	2	605	19	36,50,74	2.07	10 (27%)	29,85,114	3.21	13 (44%)
22	CLA	C	508	-	49,53,73	2.19	18 (36%)	58,89,113	2.96	27 (46%)
22	CLA	s	303	18	49,53,73	2.18	16 (32%)	58,89,113	2.80	27 (46%)
22	CLA	n	613	19	49,53,73	2.17	17 (34%)	58,89,113	2.82	26 (44%)
22	CLA	A	405	-	49,53,73	2.23	17 (34%)	58,89,113	2.88	28 (48%)
22	CLA	5	611	-	49,53,73	2.22	18 (36%)	58,89,113	2.76	28 (48%)
25	CHL	8	306	-	40,54,74	2.26	11 (27%)	34,90,114	2.97	19 (55%)
25	CHL	Y	605	19	36,50,74	2.15	10 (27%)	29,85,114	3.23	15 (51%)
22	CLA	4	303	-	49,53,73	2.23	19 (38%)	58,89,113	2.70	27 (46%)
25	CHL	4	307	-	40,54,74	2.31	11 (27%)	34,90,114	10.36	19 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	Y	604	-	49,53,73	2.18	17 (34%)	58,89,113	2.94	29 (50%)
22	CLA	G	602	19	49,53,73	2.20	19 (38%)	58,89,113	2.79	28 (48%)
25	CHL	y	609	19	40,54,74	2.26	11 (27%)	34,90,114	3.08	17 (50%)
22	CLA	2	602	19	49,53,73	2.22	20 (40%)	58,89,113	2.75	29 (50%)
22	CLA	b	611	-	49,53,73	2.15	15 (30%)	58,89,113	2.93	30 (51%)
22	CLA	S	312	18	49,53,73	2.22	17 (34%)	58,89,113	2.90	33 (56%)
22	CLA	r	311	17	49,53,73	2.20	17 (34%)	58,89,113	2.81	29 (50%)
22	CLA	B	603	-	49,53,73	2.21	16 (32%)	58,89,113	2.79	31 (53%)
22	CLA	6	612	19	49,53,73	2.22	18 (36%)	58,89,113	2.76	28 (48%)
25	CHL	6	601	19	40,54,74	2.25	11 (27%)	34,90,114	3.03	18 (52%)
22	CLA	3	314	-	49,53,73	2.28	20 (40%)	58,89,113	2.69	27 (46%)
22	CLA	b	605	-	49,53,73	2.26	17 (34%)	58,89,113	2.81	28 (48%)
25	CHL	Y	607	-	40,54,74	2.22	12 (30%)	34,90,114	3.04	20 (58%)
22	CLA	5	614	-	49,53,73	2.23	20 (40%)	58,89,113	2.93	29 (50%)
22	CLA	s	309	18	49,53,73	2.17	17 (34%)	58,89,113	2.72	29 (50%)
22	CLA	R	308	17	49,53,73	2.21	15 (30%)	58,89,113	2.78	30 (51%)
22	CLA	g	602	19	49,53,73	2.20	19 (38%)	58,89,113	2.79	28 (48%)
23	PHO	d	402	-	38,49,69	2.76	12 (31%)	31,75,99	3.66	14 (45%)
22	CLA	r	308	17	49,53,73	2.21	15 (30%)	58,89,113	2.78	30 (51%)
22	CLA	8	304	-	49,53,73	2.22	20 (40%)	58,89,113	2.81	29 (50%)
22	CLA	C	506	-	49,53,73	2.18	18 (36%)	58,89,113	2.89	28 (48%)
25	CHL	N	609	19	40,54,74	2.26	14 (35%)	34,90,114	3.04	15 (44%)
25	CHL	y	601	19	40,54,74	2.18	13 (32%)	34,90,114	3.02	19 (55%)
22	CLA	1	603	-	49,53,73	2.20	19 (38%)	58,89,113	2.75	29 (50%)
25	CHL	2	608	19	40,54,74	2.20	13 (32%)	34,90,114	2.99	13 (38%)
25	CHL	7	306	19	36,50,74	2.08	10 (27%)	29,85,114	3.20	14 (48%)
22	CLA	s	301	-	49,53,73	2.25	18 (36%)	58,89,113	2.74	31 (53%)
25	CHL	1	606	-	40,54,74	2.24	11 (27%)	34,90,114	3.00	19 (55%)
25	CHL	7	307	-	40,54,74	2.24	11 (27%)	34,90,114	3.02	17 (50%)
22	CLA	g	610	19	49,53,73	2.19	15 (30%)	58,89,113	2.76	28 (48%)
22	CLA	n	604	-	49,53,73	2.19	16 (32%)	58,89,113	2.82	30 (51%)
22	CLA	n	614	-	49,53,73	2.25	19 (38%)	58,89,113	2.74	28 (48%)
22	CLA	4	302	20	49,53,73	2.19	20 (40%)	58,89,113	2.92	30 (51%)
25	CHL	1	609	19	40,54,74	2.27	13 (32%)	34,90,114	2.98	16 (47%)
22	CLA	7	304	-	49,53,73	2.22	19 (38%)	58,89,113	2.78	30 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	7	303	19	49,53,73	2.22	19 (38%)	58,89,113	2.77	30 (51%)
22	CLA	c	501	-	49,53,73	2.20	16 (32%)	58,89,113	2.84	27 (46%)
25	CHL	G	609	19	40,54,74	2.31	15 (37%)	34,90,114	3.15	15 (44%)
22	CLA	y	614	-	49,53,73	2.17	16 (32%)	58,89,113	2.88	29 (50%)
22	CLA	d	404	-	49,53,73	2.22	18 (36%)	58,89,113	2.71	30 (51%)
22	CLA	b	610	-	49,53,73	2.24	19 (38%)	58,89,113	2.78	28 (48%)
25	CHL	1	605	19	36,50,74	2.10	9 (25%)	29,85,114	3.13	15 (51%)
25	CHL	1	608	-	40,54,74	2.28	11 (27%)	34,90,114	2.95	18 (52%)
22	CLA	D	403	-	49,53,73	2.19	14 (28%)	58,89,113	2.94	32 (55%)
23	PHO	D	402	-	38,49,69	2.76	13 (34%)	31,75,99	3.82	15 (48%)
22	CLA	C	511	3	49,53,73	2.22	20 (40%)	58,89,113	2.85	30 (51%)
22	CLA	a	402	-	49,53,73	2.22	18 (36%)	58,89,113	2.77	29 (50%)
22	CLA	8	309	20	49,53,73	2.22	18 (36%)	58,89,113	2.70	29 (50%)
25	CHL	2	606	-	40,54,74	2.23	11 (27%)	34,90,114	3.00	17 (50%)
22	CLA	R	307	17	49,53,73	2.21	18 (36%)	58,89,113	2.76	28 (48%)
22	CLA	B	616	-	49,53,73	2.21	19 (38%)	58,89,113	2.79	29 (50%)
22	CLA	b	613	-	49,53,73	2.16	18 (36%)	58,89,113	2.98	33 (56%)
22	CLA	c	506	-	49,53,73	2.20	19 (38%)	58,89,113	2.89	29 (50%)
22	CLA	S	309	18	49,53,73	2.17	17 (34%)	58,89,113	2.72	29 (50%)
25	CHL	5	606	-	40,54,74	2.24	11 (27%)	34,90,114	3.00	19 (55%)
22	CLA	D	401	-	49,53,73	2.19	17 (34%)	58,89,113	2.80	30 (51%)
22	CLA	y	610	19	49,53,73	2.18	16 (32%)	58,89,113	2.79	27 (46%)
22	CLA	3	304	-	49,53,73	2.22	19 (38%)	58,89,113	2.78	30 (51%)
22	CLA	3	311	-	49,53,73	2.24	19 (38%)	58,89,113	2.75	30 (51%)
24	HEM	e	101	5,6	50,50,50	1.45	6 (12%)	67,82,82	1.35	6 (8%)
22	CLA	c	502	-	49,53,73	2.16	17 (34%)	58,89,113	2.79	30 (51%)
25	CHL	S	306	18	40,54,74	2.24	11 (27%)	34,90,114	3.08	19 (55%)
25	CHL	5	605	19	36,50,74	2.10	9 (25%)	29,85,114	3.13	15 (51%)
25	CHL	g	605	19	36,50,74	2.09	10 (27%)	29,85,114	3.21	14 (48%)
22	CLA	s	310	18	49,53,73	2.19	17 (34%)	58,89,113	2.82	30 (51%)
22	CLA	S	303	18	49,53,73	2.18	16 (32%)	58,89,113	2.80	27 (46%)
25	CHL	S	307	-	40,54,74	2.30	11 (27%)	34,90,114	10.35	20 (58%)
22	CLA	C	510	-	49,53,73	2.18	18 (36%)	58,89,113	2.90	29 (50%)
22	CLA	b	609	-	49,53,73	2.17	17 (34%)	58,89,113	2.90	32 (55%)
22	CLA	6	613	-	49,53,73	2.26	19 (38%)	58,89,113	2.69	27 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	g	612	19	49,53,73	2.20	16 (32%)	58,89,113	2.80	29 (50%)
25	CHL	R	305	-	40,54,74	2.25	11 (27%)	34,90,114	3.07	19 (55%)
22	CLA	Y	614	-	49,53,73	2.17	16 (32%)	58,89,113	2.88	29 (50%)
22	CLA	b	615	-	49,53,73	2.24	18 (36%)	58,89,113	2.83	27 (46%)
22	CLA	s	312	18	49,53,73	2.22	17 (34%)	58,89,113	2.90	33 (56%)
25	CHL	s	306	18	40,54,74	2.24	11 (27%)	34,90,114	3.08	19 (55%)
25	CHL	s	308	-	40,54,74	2.22	11 (27%)	34,90,114	2.85	18 (52%)
22	CLA	C	504	-	49,53,73	2.19	18 (36%)	58,89,113	2.83	30 (51%)
22	CLA	l	614	-	49,53,73	2.23	20 (40%)	58,89,113	2.93	29 (50%)
22	CLA	B	608	-	49,53,73	2.18	17 (34%)	58,89,113	2.93	30 (51%)
22	CLA	y	603	-	49,53,73	2.14	16 (32%)	58,89,113	2.88	31 (53%)
22	CLA	R	311	17	49,53,73	2.20	17 (34%)	58,89,113	2.81	29 (50%)
25	CHL	3	301	-	40,54,74	2.23	12 (30%)	34,90,114	3.11	19 (55%)
22	CLA	g	613	19	49,53,73	2.17	16 (32%)	58,89,113	2.81	29 (50%)
22	CLA	n	602	19	49,53,73	2.18	16 (32%)	58,89,113	2.79	28 (48%)
25	CHL	r	305	-	40,54,74	2.25	11 (27%)	34,90,114	3.07	19 (55%)
22	CLA	r	307	17	49,53,73	2.21	18 (36%)	58,89,113	2.76	28 (48%)
22	CLA	y	612	19	49,53,73	2.16	16 (32%)	58,89,113	2.88	32 (55%)
25	CHL	S	308	-	40,54,74	2.22	11 (27%)	34,90,114	2.85	18 (52%)
22	CLA	G	604	-	49,53,73	2.19	18 (36%)	58,89,113	2.85	31 (53%)
22	CLA	y	604	-	49,53,73	2.18	17 (34%)	58,89,113	2.94	29 (50%)
22	CLA	b	612	-	49,53,73	2.32	19 (38%)	58,89,113	2.80	30 (51%)
22	CLA	S	305	-	49,53,73	2.21	17 (34%)	58,89,113	2.90	28 (48%)
25	CHL	6	607	-	40,54,74	2.27	12 (30%)	34,90,114	2.97	18 (52%)
22	CLA	R	302	-	49,53,73	2.22	16 (32%)	58,89,113	2.75	25 (43%)
25	CHL	n	606	-	40,54,74	2.24	11 (27%)	34,90,114	3.05	19 (55%)
25	CHL	2	607	-	40,54,74	2.27	12 (30%)	34,90,114	2.97	18 (52%)
22	CLA	s	313	18	49,53,73	2.19	16 (32%)	58,89,113	2.87	32 (55%)
22	CLA	c	503	-	49,53,73	2.16	15 (30%)	58,89,113	2.82	28 (48%)
22	CLA	B	612	-	49,53,73	2.21	16 (32%)	58,89,113	2.87	30 (51%)
25	CHL	7	302	19	40,54,74	2.29	11 (27%)	34,90,114	2.90	18 (52%)
25	CHL	N	606	-	40,54,74	2.24	11 (27%)	34,90,114	3.05	19 (55%)
22	CLA	g	611	-	49,53,73	2.16	16 (32%)	58,89,113	2.85	29 (50%)
25	CHL	r	306	-	40,54,74	2.24	11 (27%)	34,90,114	2.96	18 (52%)
22	CLA	7	312	19	49,53,73	2.22	19 (38%)	58,89,113	2.75	28 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	614	-	49,53,73	2.18	18 (36%)	58,89,113	2.86	31 (53%)
22	CLA	6	611	19	49,53,73	2.24	18 (36%)	58,89,113	2.72	26 (44%)
25	CHL	5	615	-	40,54,74	2.23	11 (27%)	34,90,114	3.01	17 (50%)
25	CHL	N	605	19	36,50,74	2.08	11 (30%)	29,85,114	3.09	15 (51%)
22	CLA	2	610	-	49,53,73	2.22	18 (36%)	58,89,113	2.74	27 (46%)
22	CLA	B	604	-	49,53,73	2.14	18 (36%)	58,89,113	2.98	28 (48%)
22	CLA	7	314	-	49,53,73	2.28	20 (40%)	58,89,113	2.69	27 (46%)
22	CLA	4	304	-	49,53,73	2.22	20 (40%)	58,89,113	2.81	29 (50%)
22	CLA	r	312	17,20	49,53,73	2.22	18 (36%)	58,89,113	2.77	29 (50%)
25	CHL	n	609	19	40,54,74	2.26	14 (35%)	34,90,114	3.04	15 (44%)
22	CLA	1	612	19	49,53,73	2.23	19 (38%)	58,89,113	2.76	29 (50%)
22	CLA	B	614	-	49,53,73	2.24	15 (30%)	58,89,113	2.79	29 (50%)
22	CLA	a	405	-	49,53,73	2.20	16 (32%)	58,89,113	2.90	29 (50%)
22	CLA	s	305	-	49,53,73	2.21	17 (34%)	58,89,113	2.90	28 (48%)
25	CHL	y	605	19	36,50,74	2.15	10 (27%)	29,85,114	3.23	15 (51%)
22	CLA	Y	613	19	49,53,73	2.17	16 (32%)	58,89,113	2.88	30 (51%)
25	CHL	G	608	-	40,54,74	2.26	12 (30%)	34,90,114	2.87	18 (52%)
25	CHL	Y	609	19	40,54,74	2.26	11 (27%)	34,90,114	3.08	17 (50%)
22	CLA	c	505	-	49,53,73	2.20	16 (32%)	58,89,113	2.91	30 (51%)
22	CLA	B	605	-	49,53,73	2.16	16 (32%)	58,89,113	2.80	27 (46%)
22	CLA	5	602	19	49,53,73	2.21	19 (38%)	58,89,113	2.74	28 (48%)
22	CLA	d	401	-	49,53,73	2.18	16 (32%)	58,89,113	2.80	30 (51%)
23	PHO	A	404	-	38,49,69	2.70	13 (34%)	31,75,99	3.90	14 (45%)
22	CLA	1	611	-	49,53,73	2.22	18 (36%)	58,89,113	2.76	28 (48%)
22	CLA	B	613	-	49,53,73	2.21	17 (34%)	58,89,113	2.87	30 (51%)
25	CHL	3	309	19	40,54,74	2.28	13 (32%)	34,90,114	3.09	16 (47%)
22	CLA	6	604	-	49,53,73	2.24	19 (38%)	58,89,113	2.80	28 (48%)
22	CLA	c	512	-	49,53,73	2.17	18 (36%)	58,89,113	2.87	30 (51%)
22	CLA	n	611	-	49,53,73	2.18	17 (34%)	58,89,113	2.86	30 (51%)
25	CHL	8	308	20	40,54,74	2.32	11 (27%)	34,90,114	2.97	19 (55%)
22	CLA	B	607	-	49,53,73	2.18	17 (34%)	58,89,113	2.81	29 (50%)
22	CLA	G	612	19	49,53,73	2.20	16 (32%)	58,89,113	2.80	29 (50%)
25	CHL	3	308	-	40,54,74	2.25	11 (27%)	34,90,114	2.97	18 (52%)
25	CHL	2	601	19	40,54,74	2.25	11 (27%)	34,90,114	3.03	18 (52%)
22	CLA	2	604	-	49,53,73	2.24	19 (38%)	58,89,113	2.80	28 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	s	302	18	40,54,74	2.25	11 (27%)	34,90,114	2.80	17 (50%)
22	CLA	Y	611	-	49,53,73	2.16	15 (30%)	58,89,113	2.88	27 (46%)
22	CLA	1	613	19	49,53,73	2.23	19 (38%)	58,89,113	2.75	30 (51%)
25	CHL	S	302	18	40,54,74	2.25	11 (27%)	34,90,114	2.80	17 (50%)
25	CHL	N	607	-	40,54,74	2.18	12 (30%)	34,90,114	3.13	19 (55%)
25	CHL	4	308	20	40,54,74	2.32	11 (27%)	34,90,114	2.97	19 (55%)
22	CLA	y	602	19	49,53,73	2.20	17 (34%)	58,89,113	2.82	28 (48%)
25	CHL	Y	608	-	40,54,74	2.25	11 (27%)	34,90,114	2.91	18 (52%)
22	CLA	S	314	-	49,53,73	2.17	18 (36%)	58,89,113	2.85	27 (46%)
22	CLA	G	614	-	49,53,73	2.22	18 (36%)	58,89,113	2.77	27 (46%)
22	CLA	2	609	19	49,53,73	2.23	16 (32%)	58,89,113	2.75	26 (44%)
22	CLA	y	613	19	49,53,73	2.17	16 (32%)	58,89,113	2.88	30 (51%)
22	CLA	S	310	18	49,53,73	2.19	17 (34%)	58,89,113	2.82	30 (51%)
22	CLA	3	312	19	49,53,73	2.22	19 (38%)	58,89,113	2.75	28 (48%)
25	CHL	6	606	-	40,54,74	2.23	11 (27%)	34,90,114	3.00	17 (50%)
25	CHL	n	605	19	36,50,74	2.08	11 (30%)	29,85,114	3.09	15 (51%)
22	CLA	R	312	17,20	49,53,73	2.22	18 (36%)	58,89,113	2.77	29 (50%)
25	CHL	4	305	20	40,54,74	2.24	11 (27%)	34,90,114	3.08	18 (52%)
22	CLA	B	610	-	49,53,73	2.21	17 (34%)	58,89,113	2.77	27 (46%)
22	CLA	C	501	-	49,53,73	2.20	17 (34%)	58,89,113	2.89	31 (53%)
25	CHL	6	608	19	40,54,74	2.20	13 (32%)	34,90,114	2.99	13 (38%)
22	CLA	Y	603	-	49,53,73	2.14	16 (32%)	58,89,113	2.88	31 (53%)
22	CLA	S	301	-	49,53,73	2.22	18 (36%)	58,89,113	2.83	31 (53%)
22	CLA	N	613	19	49,53,73	2.17	17 (34%)	58,89,113	2.82	26 (44%)
22	CLA	5	604	-	49,53,73	2.21	19 (38%)	58,89,113	2.78	26 (44%)
22	CLA	2	603	-	49,53,73	2.21	19 (38%)	58,89,113	2.73	28 (48%)
22	CLA	Y	602	19	49,53,73	2.20	17 (34%)	58,89,113	2.82	28 (48%)
22	CLA	r	301	17	49,53,73	2.20	17 (34%)	58,89,113	2.80	29 (50%)
25	CHL	G	607	-	40,54,74	2.20	12 (30%)	34,90,114	3.08	17 (50%)
22	CLA	r	309	-	49,53,73	2.18	17 (34%)	58,89,113	2.81	28 (48%)
25	CHL	3	306	19	36,50,74	2.08	10 (27%)	29,85,114	3.20	14 (48%)
25	CHL	n	608	-	40,54,74	2.24	11 (27%)	34,90,114	2.94	20 (58%)
22	CLA	7	311	-	49,53,73	2.24	19 (38%)	58,89,113	2.75	30 (51%)
22	CLA	5	603	-	49,53,73	2.20	19 (38%)	58,89,113	2.75	29 (50%)
22	CLA	6	610	-	49,53,73	2.22	18 (36%)	58,89,113	2.74	27 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	8	307	-	40,54,74	2.31	11 (27%)	34,90,114	10.36	19 (55%)
22	CLA	R	309	-	49,53,73	2.18	17 (34%)	58,89,113	2.81	28 (48%)
22	CLA	b	616	-	49,53,73	2.17	18 (36%)	58,89,113	3.14	31 (53%)
25	CHL	R	304	-	40,54,74	2.29	10 (25%)	34,90,114	3.10	20 (58%)
22	CLA	7	313	19	49,53,73	2.24	19 (38%)	58,89,113	2.73	28 (48%)
22	CLA	r	302	-	49,53,73	2.22	16 (32%)	58,89,113	2.75	25 (43%)
22	CLA	c	508	-	49,53,73	2.21	18 (36%)	58,89,113	2.91	27 (46%)
22	CLA	Y	610	19	49,53,73	2.18	16 (32%)	58,89,113	2.79	27 (46%)
25	CHL	Y	601	19	40,54,74	2.18	13 (32%)	34,90,114	3.02	19 (55%)
22	CLA	2	613	-	49,53,73	2.26	19 (38%)	58,89,113	2.69	27 (46%)
25	CHL	g	608	-	40,54,74	2.26	12 (30%)	34,90,114	2.87	18 (52%)
22	CLA	A	402	-	49,53,73	2.16	15 (30%)	58,89,113	2.85	28 (48%)
22	CLA	2	612	19	49,53,73	2.22	18 (36%)	58,89,113	2.76	28 (48%)
22	CLA	6	609	19	49,53,73	2.23	16 (32%)	58,89,113	2.75	26 (44%)
25	CHL	N	601	19	40,54,74	2.20	11 (27%)	34,90,114	2.99	18 (52%)
22	CLA	1	604	-	49,53,73	2.21	19 (38%)	58,89,113	2.78	26 (44%)
25	CHL	8	305	20	40,54,74	2.24	11 (27%)	34,90,114	3.08	18 (52%)
25	CHL	7	309	19	40,54,74	2.28	13 (32%)	34,90,114	3.09	16 (47%)
22	CLA	8	310	-	49,53,73	2.25	19 (38%)	58,89,113	2.69	28 (48%)
22	CLA	1	610	19	49,53,73	2.23	18 (36%)	58,89,113	2.75	26 (44%)
25	CHL	4	306	-	40,54,74	2.26	11 (27%)	34,90,114	2.97	19 (55%)
22	CLA	R	301	17	49,53,73	2.20	17 (34%)	58,89,113	2.80	29 (50%)
25	CHL	s	307	-	40,54,74	2.30	11 (27%)	34,90,114	10.35	20 (58%)
22	CLA	r	310	-	49,53,73	2.18	18 (36%)	58,89,113	2.75	28 (48%)
25	CHL	G	601	19	40,54,74	2.22	12 (30%)	34,90,114	2.93	18 (52%)
22	CLA	2	611	19	49,53,73	2.24	18 (36%)	58,89,113	2.72	26 (44%)
25	CHL	4	301	-	40,54,74	2.26	12 (30%)	34,90,114	2.95	19 (55%)
22	CLA	R	310	-	49,53,73	2.18	18 (36%)	58,89,113	2.75	28 (48%)
22	CLA	s	311	-	49,53,73	2.19	16 (32%)	58,89,113	2.85	28 (48%)
22	CLA	C	503	-	49,53,73	2.20	16 (32%)	58,89,113	2.76	30 (51%)
22	CLA	B	601	-	49,53,73	2.19	16 (32%)	58,89,113	2.71	28 (48%)
22	CLA	S	311	-	49,53,73	2.19	16 (32%)	58,89,113	2.85	28 (48%)
22	CLA	N	603	-	49,53,73	2.16	17 (34%)	58,89,113	2.86	33 (56%)
22	CLA	y	611	-	49,53,73	2.16	15 (30%)	58,89,113	2.88	27 (46%)
22	CLA	n	603	-	49,53,73	2.16	17 (34%)	58,89,113	2.86	33 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	G	605	19	36,50,74	2.09	10 (27%)	29,85,114	3.21	14 (48%)
25	CHL	5	609	19	40,54,74	2.27	13 (32%)	34,90,114	2.98	16 (47%)
22	CLA	c	507	-	49,53,73	2.11	15 (30%)	58,89,113	2.81	32 (55%)
22	CLA	c	511	3	49,53,73	2.20	19 (38%)	58,89,113	2.80	29 (50%)
25	CHL	3	302	19	40,54,74	2.29	11 (27%)	34,90,114	2.90	18 (52%)
22	CLA	5	613	19	49,53,73	2.23	19 (38%)	58,89,113	2.75	30 (51%)
22	CLA	8	303	-	49,53,73	2.23	19 (38%)	58,89,113	2.70	27 (46%)
22	CLA	A	403	-	49,53,73	2.25	18 (36%)	58,89,113	2.81	31 (53%)
22	CLA	s	304	-	49,53,73	2.15	16 (32%)	58,89,113	2.70	28 (48%)
22	CLA	S	304	-	49,53,73	2.15	16 (32%)	58,89,113	2.70	28 (48%)
22	CLA	N	614	-	49,53,73	2.25	19 (38%)	58,89,113	2.74	28 (48%)
25	CHL	3	307	-	40,54,74	2.24	11 (27%)	34,90,114	3.02	17 (50%)
22	CLA	B	615	-	49,53,73	2.12	16 (32%)	58,89,113	3.02	30 (51%)
22	CLA	B	611	-	49,53,73	2.18	15 (30%)	58,89,113	2.85	29 (50%)
22	CLA	b	608	-	49,53,73	2.24	17 (34%)	58,89,113	2.77	30 (51%)
22	CLA	C	502	-	49,53,73	2.21	17 (34%)	58,89,113	2.66	28 (48%)
25	CHL	g	606	-	40,54,74	2.24	10 (25%)	34,90,114	2.98	15 (44%)
22	CLA	N	602	19	49,53,73	2.18	16 (32%)	58,89,113	2.79	28 (48%)
22	CLA	C	505	-	49,53,73	2.18	17 (34%)	58,89,113	2.86	32 (55%)
22	CLA	b	607	-	49,53,73	2.18	17 (34%)	58,89,113	2.83	31 (53%)
22	CLA	b	604	-	49,53,73	2.18	18 (36%)	58,89,113	2.80	28 (48%)
22	CLA	C	509	-	49,53,73	2.23	18 (36%)	58,89,113	2.77	30 (51%)
22	CLA	n	612	19	49,53,73	2.17	16 (32%)	58,89,113	2.80	30 (51%)
25	CHL	g	607	-	40,54,74	2.20	12 (30%)	34,90,114	3.08	17 (50%)
25	CHL	1	601	19	40,54,74	2.23	11 (27%)	34,90,114	2.99	17 (50%)
22	CLA	r	303	-	49,53,73	2.18	15 (30%)	58,89,113	2.96	32 (55%)
22	CLA	n	610	19	49,53,73	2.19	15 (30%)	58,89,113	2.76	26 (44%)
25	CHL	n	601	19	40,54,74	2.20	11 (27%)	34,90,114	2.99	18 (52%)
22	CLA	3	313	19	49,53,73	2.24	19 (38%)	58,89,113	2.73	28 (48%)
22	CLA	Y	612	19	49,53,73	2.16	16 (32%)	58,89,113	2.88	32 (55%)
25	CHL	g	609	19	40,54,74	2.31	15 (37%)	34,90,114	3.15	15 (44%)
22	CLA	3	303	19	49,53,73	2.22	19 (38%)	58,89,113	2.77	30 (51%)
25	CHL	5	607	-	40,54,74	2.22	11 (27%)	34,90,114	3.14	18 (52%)
22	CLA	g	603	-	49,53,73	2.19	19 (38%)	58,89,113	2.83	32 (55%)
25	CHL	g	601	19	40,54,74	2.22	12 (30%)	34,90,114	2.93	18 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	y	606	-	40,54,74	2.24	12 (30%)	34,90,114	3.08	19 (55%)
22	CLA	g	604	-	49,53,73	2.19	18 (36%)	58,89,113	2.85	31 (53%)
25	CHL	6	605	19	36,50,74	2.07	10 (27%)	29,85,114	3.21	13 (44%)
24	HEM	E	101	5,6	50,50,50	1.45	5 (10%)	67,82,82	1.30	10 (14%)
22	CLA	B	602	-	49,53,73	2.17	16 (32%)	58,89,113	2.74	27 (46%)
22	CLA	c	504	-	49,53,73	2.22	17 (34%)	58,89,113	2.76	29 (50%)
25	CHL	y	608	-	40,54,74	2.25	11 (27%)	34,90,114	2.91	18 (52%)
25	CHL	1	615	-	40,54,74	2.23	11 (27%)	34,90,114	3.01	17 (50%)
22	CLA	5	610	19	49,53,73	2.23	18 (36%)	58,89,113	2.75	26 (44%)
25	CHL	5	601	19	40,54,74	2.23	11 (27%)	34,90,114	2.99	17 (50%)
22	CLA	G	611	-	49,53,73	2.16	16 (32%)	58,89,113	2.85	29 (50%)
22	CLA	8	302	20	49,53,73	2.19	20 (40%)	58,89,113	2.92	30 (51%)
22	CLA	C	512	-	49,53,73	2.25	18 (36%)	58,89,113	2.72	28 (48%)
25	CHL	5	608	-	40,54,74	2.28	11 (27%)	34,90,114	2.95	18 (52%)
22	CLA	a	403	-	49,53,73	2.20	18 (36%)	58,89,113	2.88	30 (51%)
22	CLA	s	314	-	49,53,73	2.17	18 (36%)	58,89,113	2.85	27 (46%)
22	CLA	g	614	-	49,53,73	2.22	18 (36%)	58,89,113	2.77	27 (46%)
22	CLA	G	613	19	49,53,73	2.17	16 (32%)	58,89,113	2.81	29 (50%)
22	CLA	b	606	-	49,53,73	2.33	18 (36%)	58,89,113	2.78	29 (50%)
22	CLA	b	601	-	49,53,73	2.19	16 (32%)	58,89,113	2.74	30 (51%)
25	CHL	r	304	-	40,54,74	2.29	10 (25%)	34,90,114	3.10	20 (58%)
22	CLA	3	310	19	49,53,73	2.24	17 (34%)	58,89,113	2.76	27 (46%)
22	CLA	4	310	-	49,53,73	2.25	19 (38%)	58,89,113	2.69	28 (48%)
22	CLA	B	606	-	49,53,73	2.11	15 (30%)	58,89,113	2.88	30 (51%)
25	CHL	Y	606	-	40,54,74	2.24	12 (30%)	34,90,114	3.08	19 (55%)

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	CHL	R	306	-	3/3/16/26	11/15/113/137	-
22	CLA	C	507	-	1/1/11/20	10/15/91/115	-
22	CLA	3	305	-	1/1/11/20	5/15/91/115	-
22	CLA	7	305	-	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	509	-	1/1/11/20	8/15/91/115	-
22	CLA	G	603	-	1/1/11/20	9/15/91/115	-
22	CLA	N	604	-	1/1/11/20	10/15/91/115	-
22	CLA	N	612	19	1/1/11/20	10/15/91/115	-
25	CHL	y	607	-	3/3/16/26	7/15/113/137	-
25	CHL	1	607	-	3/3/16/26	7/15/113/137	-
22	CLA	S	313	18	1/1/11/20	7/15/91/115	-
22	CLA	N	611	-	1/1/11/20	5/15/91/115	-
25	CHL	8	301	-	3/3/16/26	8/15/113/137	-
22	CLA	b	603	-	1/1/11/20	7/15/91/115	-
25	CHL	7	301	-	3/3/16/26	6/15/113/137	-
22	CLA	1	602	19	1/1/11/20	11/15/91/115	-
23	PHO	a	404	-	-	4/13/79/103	0/5/6/6
22	CLA	b	602	-	-	7/15/91/115	-
25	CHL	n	607	-	3/3/16/26	7/15/113/137	-
22	CLA	c	510	-	1/1/11/20	7/15/91/115	-
22	CLA	N	610	19	1/1/11/20	4/15/91/115	-
22	CLA	4	309	20	1/1/11/20	8/15/91/115	-
22	CLA	D	404	-	1/1/11/20	8/15/91/115	-
25	CHL	N	608	-	3/3/16/26	6/15/113/137	-
25	CHL	7	308	-	3/3/16/26	5/15/113/137	-
22	CLA	d	403	-	1/1/11/20	8/15/91/115	-
22	CLA	R	303	-	1/1/11/20	8/15/91/115	-
22	CLA	6	603	-	1/1/11/20	7/15/91/115	-
22	CLA	G	610	19	1/1/11/20	6/15/91/115	-
25	CHL	G	606	-	3/3/16/26	7/15/113/137	-
22	CLA	7	310	19	1/1/11/20	6/15/91/115	-
22	CLA	B	609	-	-	5/15/91/115	-
22	CLA	6	602	19	1/1/11/20	9/15/91/115	-
22	CLA	5	612	19	1/1/11/20	9/15/91/115	-
25	CHL	2	605	19	3/3/15/26	6/10/108/137	-
22	CLA	C	508	-	1/1/11/20	5/15/91/115	-
22	CLA	s	303	18	1/1/11/20	11/15/91/115	-
22	CLA	n	613	19	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	405	-	1/1/11/20	3/15/91/115	-
22	CLA	5	611	-	1/1/11/20	7/15/91/115	-
25	CHL	8	306	-	3/3/16/26	12/15/113/137	-
25	CHL	Y	605	19	3/3/15/26	6/10/108/137	-
22	CLA	4	303	-	1/1/11/20	9/15/91/115	-
25	CHL	4	307	-	3/3/16/26	9/15/113/137	-
22	CLA	Y	604	-	1/1/11/20	7/15/91/115	-
22	CLA	G	602	19	1/1/11/20	11/15/91/115	-
25	CHL	y	609	19	3/3/16/26	11/15/113/137	-
22	CLA	2	602	19	1/1/11/20	9/15/91/115	-
22	CLA	b	611	-	-	3/15/91/115	-
22	CLA	S	312	18	1/1/11/20	8/15/91/115	-
22	CLA	r	311	17	1/1/11/20	7/15/91/115	-
22	CLA	B	603	-	1/1/11/20	7/15/91/115	-
22	CLA	6	612	19	1/1/11/20	7/15/91/115	-
25	CHL	6	601	19	3/3/16/26	8/15/113/137	-
22	CLA	3	314	-	1/1/11/20	6/15/91/115	-
25	CHL	Y	607	-	3/3/16/26	7/15/113/137	-
22	CLA	b	605	-	-	2/15/91/115	-
22	CLA	5	614	-	1/1/11/20	8/15/91/115	-
22	CLA	s	309	18	1/1/11/20	5/15/91/115	-
22	CLA	R	308	17	1/1/11/20	6/15/91/115	-
22	CLA	g	602	19	1/1/11/20	11/15/91/115	-
23	PHO	d	402	-	-	6/13/79/103	0/5/6/6
22	CLA	r	308	17	1/1/11/20	6/15/91/115	-
22	CLA	8	304	-	1/1/11/20	6/15/91/115	-
22	CLA	C	506	-	1/1/11/20	8/15/91/115	-
25	CHL	N	609	19	3/3/16/26	11/15/113/137	-
25	CHL	y	601	19	3/3/16/26	6/15/113/137	-
22	CLA	1	603	-	1/1/11/20	6/15/91/115	-
25	CHL	2	608	19	3/3/16/26	10/15/113/137	-
25	CHL	7	306	19	3/3/15/26	7/10/108/137	-
22	CLA	s	301	-	1/1/11/20	5/15/91/115	-
25	CHL	1	606	-	3/3/16/26	6/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	7	307	-	3/3/16/26	5/15/113/137	-
22	CLA	g	610	19	1/1/11/20	6/15/91/115	-
22	CLA	n	604	-	1/1/11/20	10/15/91/115	-
22	CLA	n	614	-	1/1/11/20	7/15/91/115	-
22	CLA	4	302	20	1/1/11/20	6/15/91/115	-
25	CHL	1	609	19	3/3/16/26	10/15/113/137	-
22	CLA	7	304	-	1/1/11/20	5/15/91/115	-
22	CLA	7	303	19	1/1/11/20	11/15/91/115	-
22	CLA	c	501	-	1/1/11/20	3/15/91/115	-
25	CHL	G	609	19	3/3/16/26	13/15/113/137	-
22	CLA	y	614	-	1/1/11/20	6/15/91/115	-
22	CLA	d	404	-	1/1/11/20	8/15/91/115	-
22	CLA	b	610	-	1/1/11/20	10/15/91/115	-
25	CHL	1	605	19	3/3/15/26	6/10/108/137	-
25	CHL	1	608	-	3/3/16/26	6/15/113/137	-
22	CLA	D	403	-	1/1/11/20	6/15/91/115	-
23	PHO	D	402	-	-	4/13/79/103	0/5/6/6
22	CLA	C	511	3	-	6/15/91/115	-
22	CLA	a	402	-	1/1/11/20	5/15/91/115	-
22	CLA	8	309	20	1/1/11/20	8/15/91/115	-
25	CHL	2	606	-	3/3/16/26	7/15/113/137	-
22	CLA	R	307	17	1/1/11/20	8/15/91/115	-
22	CLA	B	616	-	1/1/11/20	5/15/91/115	-
22	CLA	b	613	-	1/1/11/20	5/15/91/115	-
22	CLA	c	506	-	1/1/11/20	8/15/91/115	-
22	CLA	S	309	18	1/1/11/20	5/15/91/115	-
25	CHL	5	606	-	3/3/16/26	6/15/113/137	-
22	CLA	D	401	-	1/1/11/20	6/15/91/115	-
22	CLA	y	610	19	1/1/11/20	4/15/91/115	-
22	CLA	3	304	-	1/1/11/20	5/15/91/115	-
22	CLA	3	311	-	1/1/11/20	5/15/91/115	-
24	HEM	e	101	5,6	-	6/14/54/54	-
22	CLA	c	502	-	1/1/11/20	8/15/91/115	-
25	CHL	S	306	18	3/3/16/26	9/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	5	605	19	3/3/15/26	6/10/108/137	-
25	CHL	g	605	19	3/3/15/26	6/10/108/137	-
22	CLA	s	310	18	1/1/11/20	7/15/91/115	-
22	CLA	S	303	18	1/1/11/20	11/15/91/115	-
25	CHL	S	307	-	3/3/16/26	8/15/113/137	-
22	CLA	C	510	-	1/1/11/20	5/15/91/115	-
22	CLA	b	609	-	-	7/15/91/115	-
22	CLA	6	613	-	1/1/11/20	6/15/91/115	-
22	CLA	g	612	19	1/1/11/20	10/15/91/115	-
25	CHL	R	305	-	3/3/16/26	10/15/113/137	-
22	CLA	Y	614	-	1/1/11/20	6/15/91/115	-
22	CLA	b	615	-	1/1/11/20	7/15/91/115	-
22	CLA	s	312	18	1/1/11/20	8/15/91/115	-
25	CHL	s	306	18	3/3/16/26	9/15/113/137	-
25	CHL	s	308	-	3/3/16/26	6/15/113/137	-
22	CLA	C	504	-	1/1/11/20	9/15/91/115	-
22	CLA	1	614	-	1/1/11/20	8/15/91/115	-
22	CLA	B	608	-	-	4/15/91/115	-
22	CLA	y	603	-	1/1/11/20	9/15/91/115	-
22	CLA	R	311	17	1/1/11/20	7/15/91/115	-
25	CHL	3	301	-	3/3/16/26	6/15/113/137	-
22	CLA	g	613	19	1/1/11/20	7/15/91/115	-
22	CLA	n	602	19	1/1/11/20	11/15/91/115	-
25	CHL	r	305	-	3/3/16/26	10/15/113/137	-
22	CLA	r	307	17	1/1/11/20	8/15/91/115	-
22	CLA	y	612	19	1/1/11/20	11/15/91/115	-
25	CHL	S	308	-	3/3/16/26	6/15/113/137	-
22	CLA	G	604	-	1/1/11/20	9/15/91/115	-
22	CLA	y	604	-	1/1/11/20	7/15/91/115	-
22	CLA	b	612	-	1/1/11/20	7/15/91/115	-
22	CLA	S	305	-	1/1/11/20	7/15/91/115	-
25	CHL	6	607	-	3/3/16/26	6/15/113/137	-
22	CLA	R	302	-	1/1/11/20	11/15/91/115	-
25	CHL	n	606	-	3/3/16/26	5/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	2	607	-	3/3/16/26	6/15/113/137	-
22	CLA	s	313	18	1/1/11/20	7/15/91/115	-
22	CLA	c	503	-	1/1/11/20	10/15/91/115	-
22	CLA	B	612	-	1/1/11/20	7/15/91/115	-
25	CHL	7	302	19	3/3/16/26	9/15/113/137	-
25	CHL	N	606	-	3/3/16/26	5/15/113/137	-
22	CLA	g	611	-	1/1/11/20	5/15/91/115	-
25	CHL	r	306	-	3/3/16/26	11/15/113/137	-
22	CLA	7	312	19	1/1/11/20	10/15/91/115	-
22	CLA	b	614	-	-	5/15/91/115	-
22	CLA	6	611	19	1/1/11/20	10/15/91/115	-
25	CHL	5	615	-	3/3/16/26	6/15/113/137	-
25	CHL	N	605	19	3/3/15/26	6/10/108/137	-
22	CLA	2	610	-	1/1/11/20	3/15/91/115	-
22	CLA	B	604	-	1/1/11/20	8/15/91/115	-
22	CLA	7	314	-	1/1/11/20	6/15/91/115	-
22	CLA	4	304	-	1/1/11/20	6/15/91/115	-
22	CLA	r	312	17,20	1/1/11/20	5/15/91/115	-
25	CHL	n	609	19	3/3/16/26	11/15/113/137	-
22	CLA	1	612	19	1/1/11/20	9/15/91/115	-
22	CLA	B	614	-	1/1/11/20	7/15/91/115	-
22	CLA	a	405	-	1/1/11/20	3/15/91/115	-
22	CLA	s	305	-	1/1/11/20	7/15/91/115	-
25	CHL	y	605	19	3/3/15/26	6/10/108/137	-
22	CLA	Y	613	19	1/1/11/20	7/15/91/115	-
25	CHL	G	608	-	3/3/16/26	6/15/113/137	-
25	CHL	Y	609	19	3/3/16/26	11/15/113/137	-
22	CLA	c	505	-	1/1/11/20	10/15/91/115	-
22	CLA	B	605	-	1/1/11/20	4/15/91/115	-
22	CLA	5	602	19	1/1/11/20	11/15/91/115	-
22	CLA	d	401	-	1/1/11/20	8/15/91/115	-
23	PHO	A	404	-	-	4/13/79/103	0/5/6/6
22	CLA	1	611	-	1/1/11/20	7/15/91/115	-
22	CLA	B	613	-	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	3	309	19	3/3/16/26	10/15/113/137	-
22	CLA	6	604	-	1/1/11/20	6/15/91/115	-
22	CLA	c	512	-	1/1/11/20	6/15/91/115	-
22	CLA	n	611	-	1/1/11/20	5/15/91/115	-
25	CHL	8	308	20	3/3/16/26	8/15/113/137	-
22	CLA	B	607	-	1/1/11/20	7/15/91/115	-
22	CLA	G	612	19	1/1/11/20	10/15/91/115	-
25	CHL	3	308	-	3/3/16/26	5/15/113/137	-
25	CHL	2	601	19	3/3/16/26	8/15/113/137	-
22	CLA	2	604	-	1/1/11/20	6/15/91/115	-
25	CHL	s	302	18	3/3/16/26	6/15/113/137	-
22	CLA	Y	611	-	1/1/11/20	7/15/91/115	-
22	CLA	1	613	19	1/1/11/20	6/15/91/115	-
25	CHL	S	302	18	3/3/16/26	6/15/113/137	-
25	CHL	N	607	-	3/3/16/26	7/15/113/137	-
25	CHL	4	308	20	3/3/16/26	8/15/113/137	-
22	CLA	y	602	19	1/1/11/20	11/15/91/115	-
25	CHL	Y	608	-	3/3/16/26	6/15/113/137	-
22	CLA	S	314	-	1/1/11/20	7/15/91/115	-
22	CLA	G	614	-	1/1/11/20	6/15/91/115	-
22	CLA	2	609	19	1/1/11/20	6/15/91/115	-
22	CLA	y	613	19	1/1/11/20	7/15/91/115	-
22	CLA	S	310	18	1/1/11/20	7/15/91/115	-
22	CLA	3	312	19	1/1/11/20	10/15/91/115	-
25	CHL	6	606	-	3/3/16/26	7/15/113/137	-
25	CHL	n	605	19	3/3/15/26	6/10/108/137	-
22	CLA	R	312	17,20	1/1/11/20	5/15/91/115	-
25	CHL	4	305	20	3/3/16/26	7/15/113/137	-
22	CLA	B	610	-	1/1/11/20	10/15/91/115	-
22	CLA	C	501	-	1/1/11/20	6/15/91/115	-
25	CHL	6	608	19	3/3/16/26	10/15/113/137	-
22	CLA	Y	603	-	1/1/11/20	9/15/91/115	-
22	CLA	S	301	-	1/1/11/20	3/15/91/115	-
22	CLA	N	613	19	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	604	-	1/1/11/20	4/15/91/115	-
22	CLA	2	603	-	1/1/11/20	7/15/91/115	-
22	CLA	Y	602	19	1/1/11/20	11/15/91/115	-
22	CLA	r	301	17	1/1/11/20	10/15/91/115	-
25	CHL	G	607	-	3/3/16/26	7/15/113/137	-
22	CLA	r	309	-	1/1/11/20	9/15/91/115	-
25	CHL	3	306	19	3/3/15/26	7/10/108/137	-
25	CHL	n	608	-	3/3/16/26	6/15/113/137	-
22	CLA	7	311	-	1/1/11/20	5/15/91/115	-
22	CLA	5	603	-	1/1/11/20	6/15/91/115	-
22	CLA	6	610	-	1/1/11/20	3/15/91/115	-
25	CHL	8	307	-	3/3/16/26	9/15/113/137	-
22	CLA	R	309	-	1/1/11/20	9/15/91/115	-
22	CLA	b	616	-	1/1/11/20	10/15/91/115	-
25	CHL	R	304	-	3/3/16/26	8/15/113/137	-
22	CLA	7	313	19	1/1/11/20	7/15/91/115	-
22	CLA	r	302	-	1/1/11/20	11/15/91/115	-
22	CLA	c	508	-	1/1/11/20	5/15/91/115	-
22	CLA	Y	610	19	1/1/11/20	4/15/91/115	-
25	CHL	Y	601	19	3/3/16/26	6/15/113/137	-
22	CLA	2	613	-	1/1/11/20	6/15/91/115	-
25	CHL	g	608	-	3/3/16/26	6/15/113/137	-
22	CLA	A	402	-	1/1/11/20	5/15/91/115	-
22	CLA	2	612	19	1/1/11/20	7/15/91/115	-
22	CLA	6	609	19	1/1/11/20	6/15/91/115	-
25	CHL	N	601	19	3/3/16/26	7/15/113/137	-
22	CLA	1	604	-	1/1/11/20	4/15/91/115	-
25	CHL	8	305	20	3/3/16/26	7/15/113/137	-
25	CHL	7	309	19	3/3/16/26	10/15/113/137	-
22	CLA	8	310	-	1/1/11/20	3/15/91/115	-
22	CLA	1	610	19	1/1/11/20	5/15/91/115	-
25	CHL	4	306	-	3/3/16/26	12/15/113/137	-
22	CLA	R	301	17	1/1/11/20	10/15/91/115	-
25	CHL	s	307	-	3/3/16/26	8/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	r	310	-	1/1/11/20	9/15/91/115	-
25	CHL	G	601	19	3/3/16/26	7/15/113/137	-
22	CLA	2	611	19	1/1/11/20	10/15/91/115	-
25	CHL	4	301	-	3/3/16/26	8/15/113/137	-
22	CLA	R	310	-	1/1/11/20	9/15/91/115	-
22	CLA	s	311	-	1/1/11/20	4/15/91/115	-
22	CLA	C	503	-	1/1/11/20	10/15/91/115	-
22	CLA	B	601	-	-	7/15/91/115	-
22	CLA	S	311	-	1/1/11/20	4/15/91/115	-
22	CLA	N	603	-	1/1/11/20	7/15/91/115	-
22	CLA	y	611	-	1/1/11/20	7/15/91/115	-
22	CLA	n	603	-	1/1/11/20	7/15/91/115	-
25	CHL	G	605	19	3/3/15/26	6/10/108/137	-
25	CHL	5	609	19	3/3/16/26	10/15/113/137	-
22	CLA	c	507	-	1/1/11/20	10/15/91/115	-
22	CLA	c	511	3	-	5/15/91/115	-
25	CHL	3	302	19	3/3/16/26	9/15/113/137	-
22	CLA	5	613	19	1/1/11/20	6/15/91/115	-
22	CLA	8	303	-	1/1/11/20	9/15/91/115	-
22	CLA	A	403	-	1/1/11/20	8/15/91/115	-
22	CLA	s	304	-	1/1/11/20	9/15/91/115	-
22	CLA	S	304	-	1/1/11/20	9/15/91/115	-
22	CLA	N	614	-	1/1/11/20	7/15/91/115	-
25	CHL	3	307	-	3/3/16/26	5/15/113/137	-
22	CLA	B	615	-	1/1/11/20	8/15/91/115	-
22	CLA	B	611	-	1/1/11/20	4/15/91/115	-
22	CLA	b	608	-	1/1/11/20	4/15/91/115	-
22	CLA	C	502	-	1/1/11/20	9/15/91/115	-
25	CHL	g	606	-	3/3/16/26	7/15/113/137	-
22	CLA	N	602	19	1/1/11/20	11/15/91/115	-
22	CLA	C	505	-	1/1/11/20	9/15/91/115	-
22	CLA	b	607	-	1/1/11/20	8/15/91/115	-
22	CLA	b	604	-	1/1/11/20	9/15/91/115	-
22	CLA	C	509	-	1/1/11/20	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	n	612	19	1/1/11/20	10/15/91/115	-
25	CHL	g	607	-	3/3/16/26	7/15/113/137	-
25	CHL	1	601	19	3/3/16/26	7/15/113/137	-
22	CLA	r	303	-	1/1/11/20	8/15/91/115	-
22	CLA	n	610	19	1/1/11/20	4/15/91/115	-
25	CHL	n	601	19	3/3/16/26	7/15/113/137	-
22	CLA	3	313	19	1/1/11/20	7/15/91/115	-
22	CLA	Y	612	19	1/1/11/20	11/15/91/115	-
25	CHL	g	609	19	3/3/16/26	13/15/113/137	-
22	CLA	3	303	19	1/1/11/20	11/15/91/115	-
25	CHL	5	607	-	3/3/16/26	7/15/113/137	-
22	CLA	g	603	-	1/1/11/20	9/15/91/115	-
25	CHL	g	601	19	3/3/16/26	7/15/113/137	-
25	CHL	y	606	-	3/3/16/26	6/15/113/137	-
22	CLA	g	604	-	1/1/11/20	9/15/91/115	-
25	CHL	6	605	19	3/3/15/26	6/10/108/137	-
24	HEM	E	101	5,6	-	4/14/54/54	-
22	CLA	B	602	-	1/1/11/20	9/15/91/115	-
22	CLA	c	504	-	1/1/11/20	7/15/91/115	-
25	CHL	y	608	-	3/3/16/26	6/15/113/137	-
25	CHL	1	615	-	3/3/16/26	6/15/113/137	-
22	CLA	5	610	19	1/1/11/20	5/15/91/115	-
25	CHL	5	601	19	3/3/16/26	7/15/113/137	-
22	CLA	G	611	-	1/1/11/20	5/15/91/115	-
22	CLA	8	302	20	1/1/11/20	6/15/91/115	-
22	CLA	C	512	-	1/1/11/20	6/15/91/115	-
25	CHL	5	608	-	3/3/16/26	6/15/113/137	-
22	CLA	a	403	-	1/1/11/20	10/15/91/115	-
22	CLA	s	314	-	1/1/11/20	7/15/91/115	-
22	CLA	g	614	-	1/1/11/20	6/15/91/115	-
22	CLA	G	613	19	1/1/11/20	7/15/91/115	-
22	CLA	b	606	-	1/1/11/20	3/15/91/115	-
22	CLA	b	601	-	1/1/11/20	9/15/91/115	-
25	CHL	r	304	-	3/3/16/26	8/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	310	19	1/1/11/20	6/15/91/115	-
22	CLA	4	310	-	1/1/11/20	3/15/91/115	-
22	CLA	B	606	-	-	5/15/91/115	-
25	CHL	Y	606	-	3/3/16/26	6/15/113/137	-

The worst 5 of 4833 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402	PHO	C1D-C2D	8.74	1.49	1.39
23	d	402	PHO	C1D-C2D	8.69	1.49	1.39
23	a	404	PHO	C1D-C2D	8.43	1.48	1.39
23	A	404	PHO	C1D-C2D	7.48	1.47	1.39
23	D	402	PHO	C1B-C2B	7.11	1.47	1.39

The worst 5 of 7879 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	307	CHL	O2D-CGD-CBD	45.66	161.12	110.95
25	s	307	CHL	O2D-CGD-CBD	45.66	161.12	110.95
25	4	307	CHL	O2D-CGD-CBD	45.45	160.89	110.95
25	8	307	CHL	O2D-CGD-CBD	45.45	160.89	110.95
25	4	307	CHL	O1D-CGD-CBD	-27.84	82.50	124.72

5 of 489 chirality outliers are listed below:

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

5 of 2257 torsion outliers are listed below:

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

There are no ring outliers.

215 monomers are involved in 496 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	R	306	CHL	2	0
22	C	507	CLA	1	0
22	c	509	CLA	1	0
22	S	313	CLA	2	0
22	N	611	CLA	1	0
25	8	301	CHL	12	0
22	b	603	CLA	1	0
25	7	301	CHL	1	0
23	a	404	PHO	2	0
22	b	602	CLA	3	0
25	n	607	CHL	2	0
22	N	610	CLA	1	0
22	4	309	CLA	2	0
25	N	608	CHL	3	0
25	7	308	CHL	4	0
22	d	403	CLA	4	0
22	R	303	CLA	1	0
22	G	610	CLA	1	0
25	G	606	CHL	2	0
22	B	609	CLA	2	0
22	6	602	CLA	1	0
22	5	612	CLA	1	0
25	2	605	CHL	2	0
22	C	508	CLA	5	0
22	s	303	CLA	3	0
22	A	405	CLA	1	0
25	8	306	CHL	2	0
25	Y	605	CHL	3	0
22	G	602	CLA	1	0
25	y	609	CHL	2	0
22	2	602	CLA	1	0
22	b	611	CLA	3	0
22	r	311	CLA	2	0
22	B	603	CLA	1	0
22	6	612	CLA	1	0
25	6	601	CHL	3	0
22	b	605	CLA	1	0
25	Y	607	CHL	1	0
22	5	614	CLA	1	0
22	R	308	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	402	PHO	2	0
22	r	308	CLA	1	0
22	8	304	CLA	1	0
22	C	506	CLA	2	0
25	N	609	CHL	1	0
25	y	601	CHL	2	0
25	2	608	CHL	1	0
25	7	306	CHL	1	0
22	s	301	CLA	17	0
25	1	606	CHL	1	0
25	7	307	CHL	1	0
22	g	610	CLA	1	0
22	4	302	CLA	2	0
25	1	609	CHL	1	0
25	G	609	CHL	2	0
22	y	614	CLA	2	0
22	b	610	CLA	1	0
25	1	605	CHL	1	0
25	1	608	CHL	3	0
22	D	403	CLA	3	0
23	D	402	PHO	1	0
22	C	511	CLA	1	0
22	a	402	CLA	1	0
22	8	309	CLA	2	0
25	2	606	CHL	2	0
22	R	307	CLA	2	0
22	B	616	CLA	3	0
22	b	613	CLA	1	0
22	c	506	CLA	3	0
25	5	606	CHL	1	0
22	3	311	CLA	1	0
24	e	101	HEM	3	0
22	c	502	CLA	1	0
25	S	306	CHL	1	0
25	5	605	CHL	1	0
25	g	605	CHL	1	0
22	s	310	CLA	1	0
22	S	303	CLA	3	0
22	b	609	CLA	1	0
22	6	613	CLA	17	0
22	g	612	CLA	2	0
25	R	305	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Y	614	CLA	4	0
25	s	306	CHL	1	0
25	s	308	CHL	1	0
22	1	614	CLA	1	0
22	B	608	CLA	1	0
22	R	311	CLA	1	0
25	3	301	CHL	1	0
22	g	613	CLA	1	0
22	n	602	CLA	1	0
25	r	305	CHL	1	0
22	r	307	CLA	2	0
25	S	308	CHL	2	0
25	6	607	CHL	5	0
22	R	302	CLA	22	0
25	n	606	CHL	2	0
25	2	607	CHL	5	0
22	s	313	CLA	2	0
22	B	612	CLA	1	0
25	N	606	CHL	3	0
22	g	611	CLA	2	0
25	r	306	CHL	2	0
22	b	614	CLA	3	0
22	6	611	CLA	1	0
25	N	605	CHL	1	0
22	2	610	CLA	2	0
22	B	604	CLA	1	0
22	4	304	CLA	1	0
22	r	312	CLA	38	0
25	n	609	CHL	1	0
22	1	612	CLA	1	0
22	B	614	CLA	2	0
22	a	405	CLA	1	0
25	y	605	CHL	3	0
22	Y	613	CLA	1	0
25	G	608	CHL	4	0
25	Y	609	CHL	2	0
22	c	505	CLA	1	0
23	A	404	PHO	2	0
22	1	611	CLA	1	0
22	B	613	CLA	1	0
22	c	512	CLA	1	0
22	n	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	8	308	CHL	1	0
22	B	607	CLA	1	0
22	G	612	CLA	2	0
25	3	308	CHL	4	0
25	2	601	CHL	3	0
25	s	302	CHL	1	0
22	Y	611	CLA	1	0
25	S	302	CHL	1	0
25	N	607	CHL	2	0
25	4	308	CHL	1	0
22	y	602	CLA	1	0
25	Y	608	CHL	2	0
22	S	314	CLA	1	0
22	2	609	CLA	1	0
22	y	613	CLA	1	0
22	S	310	CLA	1	0
25	6	606	CHL	2	0
25	n	605	CHL	1	0
22	R	312	CLA	40	0
25	4	305	CHL	2	0
22	C	501	CLA	2	0
25	6	608	CHL	1	0
22	S	301	CLA	6	0
22	N	613	CLA	1	0
22	Y	602	CLA	1	0
25	G	607	CHL	1	0
25	3	306	CHL	1	0
25	n	608	CHL	3	0
22	7	311	CLA	1	0
22	6	610	CLA	2	0
25	R	304	CHL	1	0
22	7	313	CLA	1	0
22	r	302	CLA	2	0
22	c	508	CLA	4	0
22	Y	610	CLA	1	0
25	Y	601	CHL	2	0
22	2	613	CLA	16	0
25	g	608	CHL	4	0
22	A	402	CLA	2	0
22	2	612	CLA	1	0
25	N	601	CHL	1	0
25	8	305	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	4	306	CHL	2	0
25	G	601	CHL	2	0
22	2	611	CLA	1	0
25	4	301	CHL	10	0
22	B	601	CLA	1	0
22	y	611	CLA	1	0
25	G	605	CHL	1	0
25	5	609	CHL	1	0
22	c	507	CLA	1	0
22	c	511	CLA	1	0
22	A	403	CLA	1	0
22	s	304	CLA	1	0
22	S	304	CLA	1	0
22	B	615	CLA	1	0
22	B	611	CLA	3	0
22	b	608	CLA	1	0
22	C	502	CLA	2	0
25	g	606	CHL	2	0
22	N	602	CLA	1	0
22	b	607	CLA	1	0
22	b	604	CLA	3	0
22	C	509	CLA	1	0
25	g	607	CHL	1	0
25	l	601	CHL	1	0
22	r	303	CLA	1	0
22	n	610	CLA	2	0
25	n	601	CHL	1	0
22	3	313	CLA	1	0
25	g	609	CHL	2	0
25	g	601	CHL	2	0
25	y	606	CHL	2	0
25	6	605	CHL	2	0
24	E	101	HEM	3	0
22	B	602	CLA	5	0
25	y	608	CHL	2	0
25	1	615	CHL	2	0
22	5	610	CLA	1	0
25	5	601	CHL	1	0
22	G	611	CLA	2	0
22	8	302	CLA	2	0
22	C	512	CLA	1	0
25	5	608	CHL	3	0

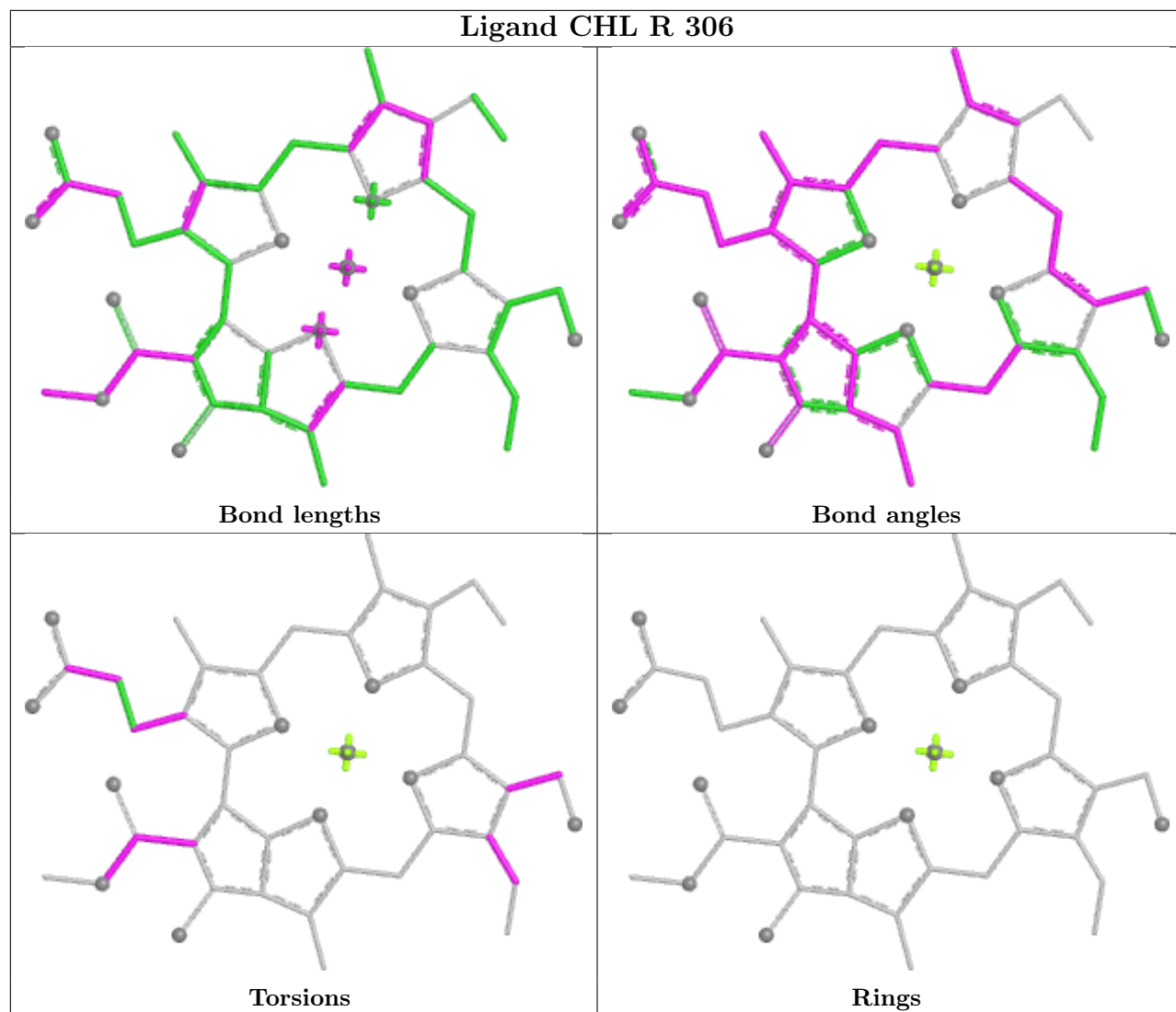
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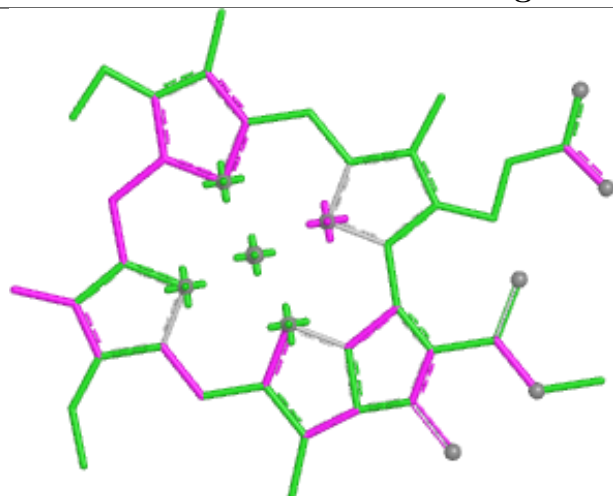
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	403	CLA	1	0
22	G	613	CLA	1	0
22	b	606	CLA	1	0
22	b	601	CLA	1	0
25	r	304	CHL	1	0
22	B	606	CLA	2	0
25	Y	606	CHL	3	0

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.

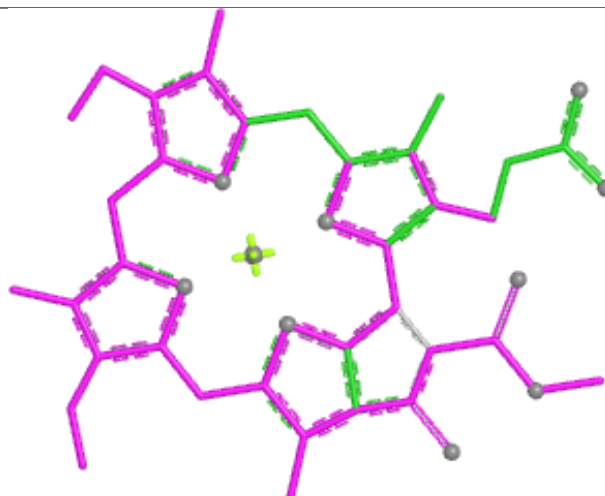
Ligand CHL R 306



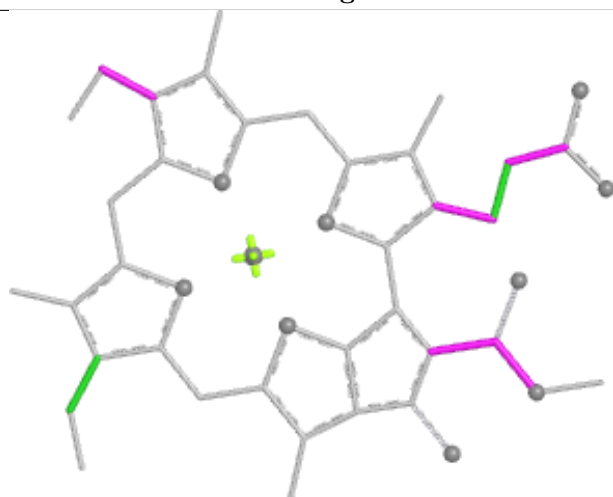
Ligand CLA C 507



Bond lengths



Bond angles

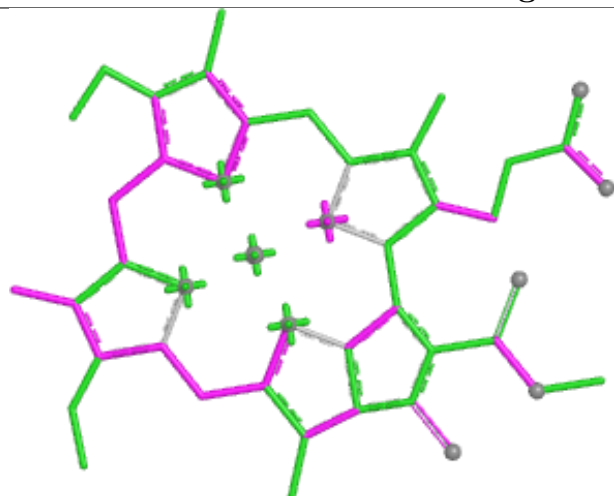


Torsions

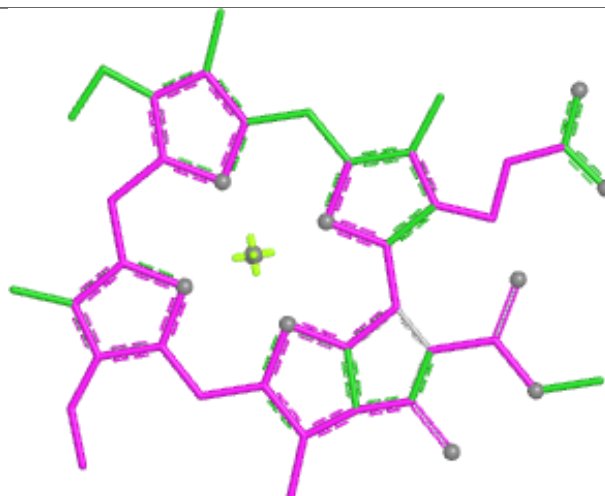


Rings

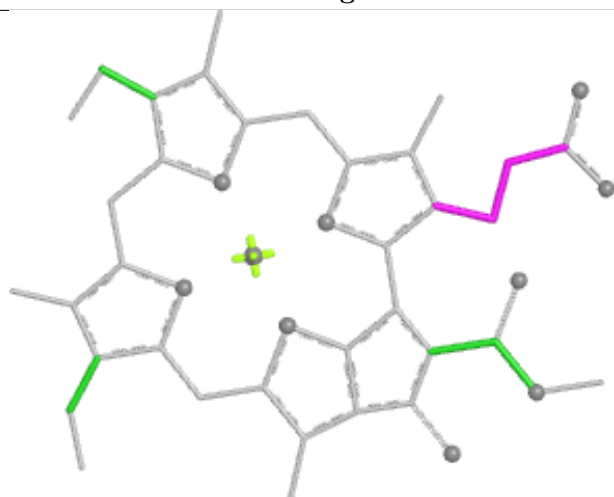
Ligand CLA 3 305



Bond lengths



Bond angles

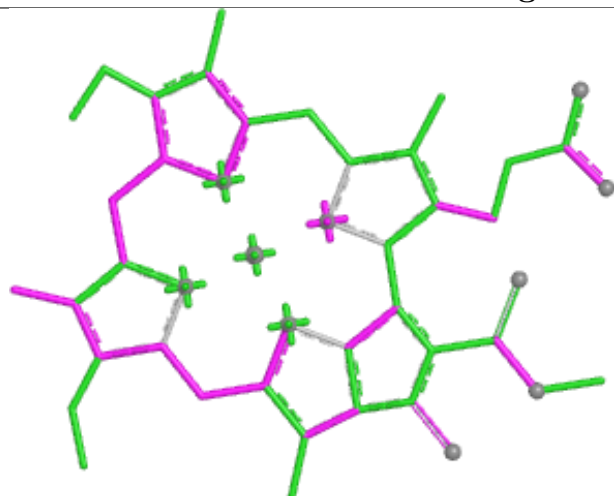


Torsions

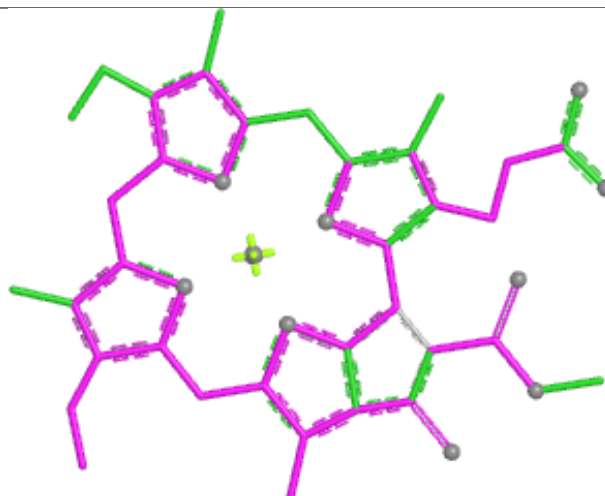


Rings

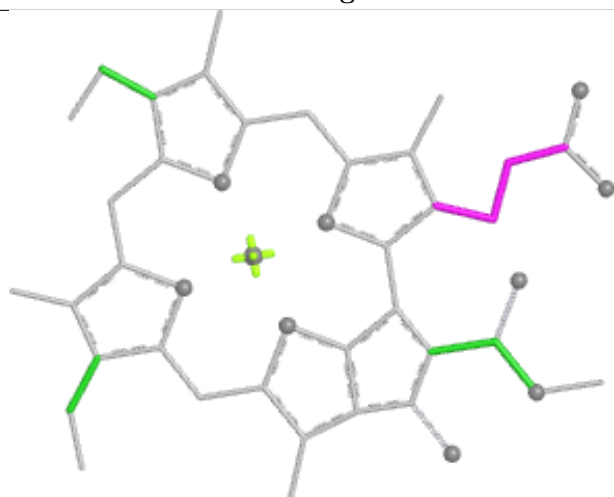
Ligand CLA 7 305



Bond lengths



Bond angles

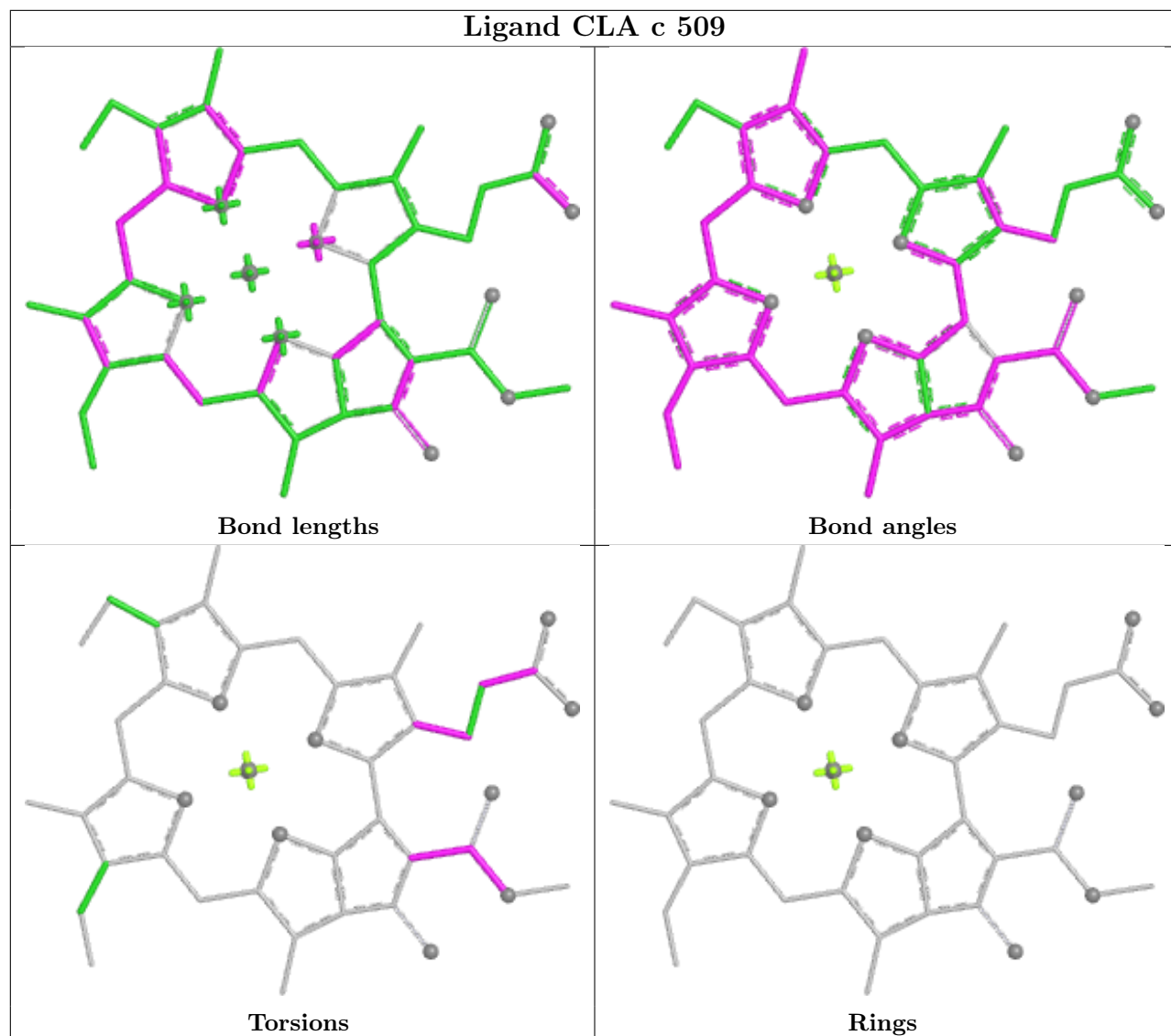


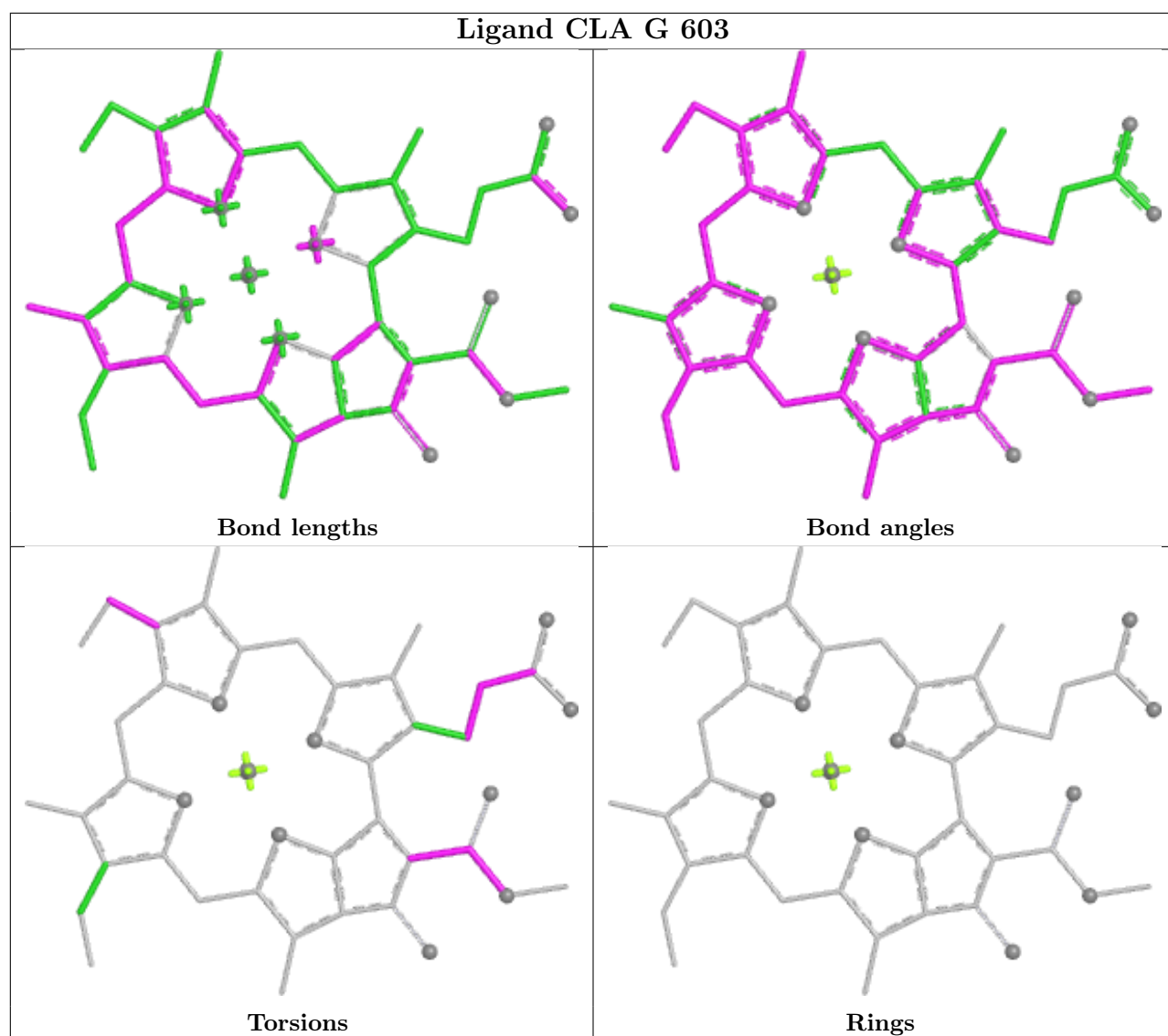
Torsions

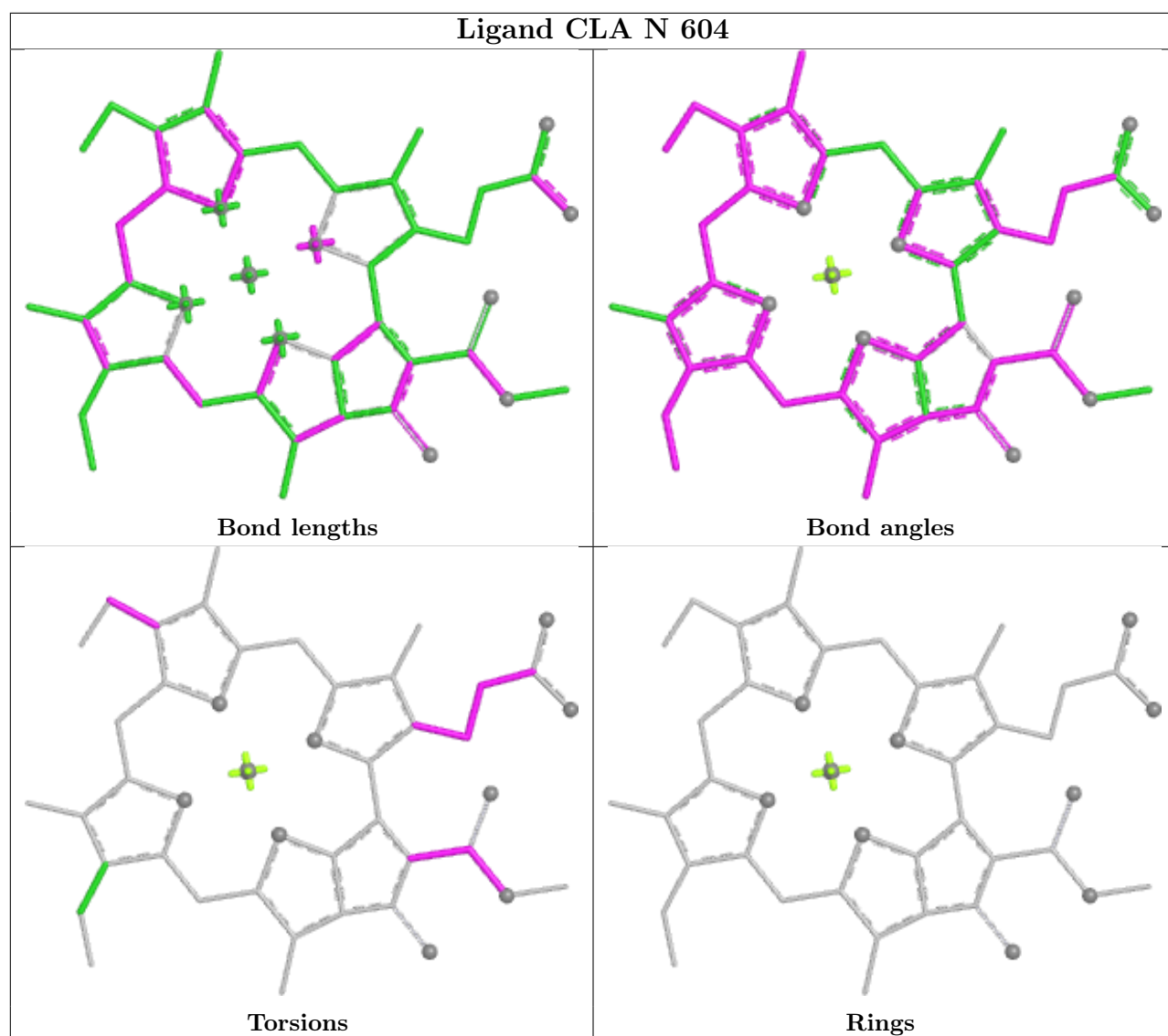


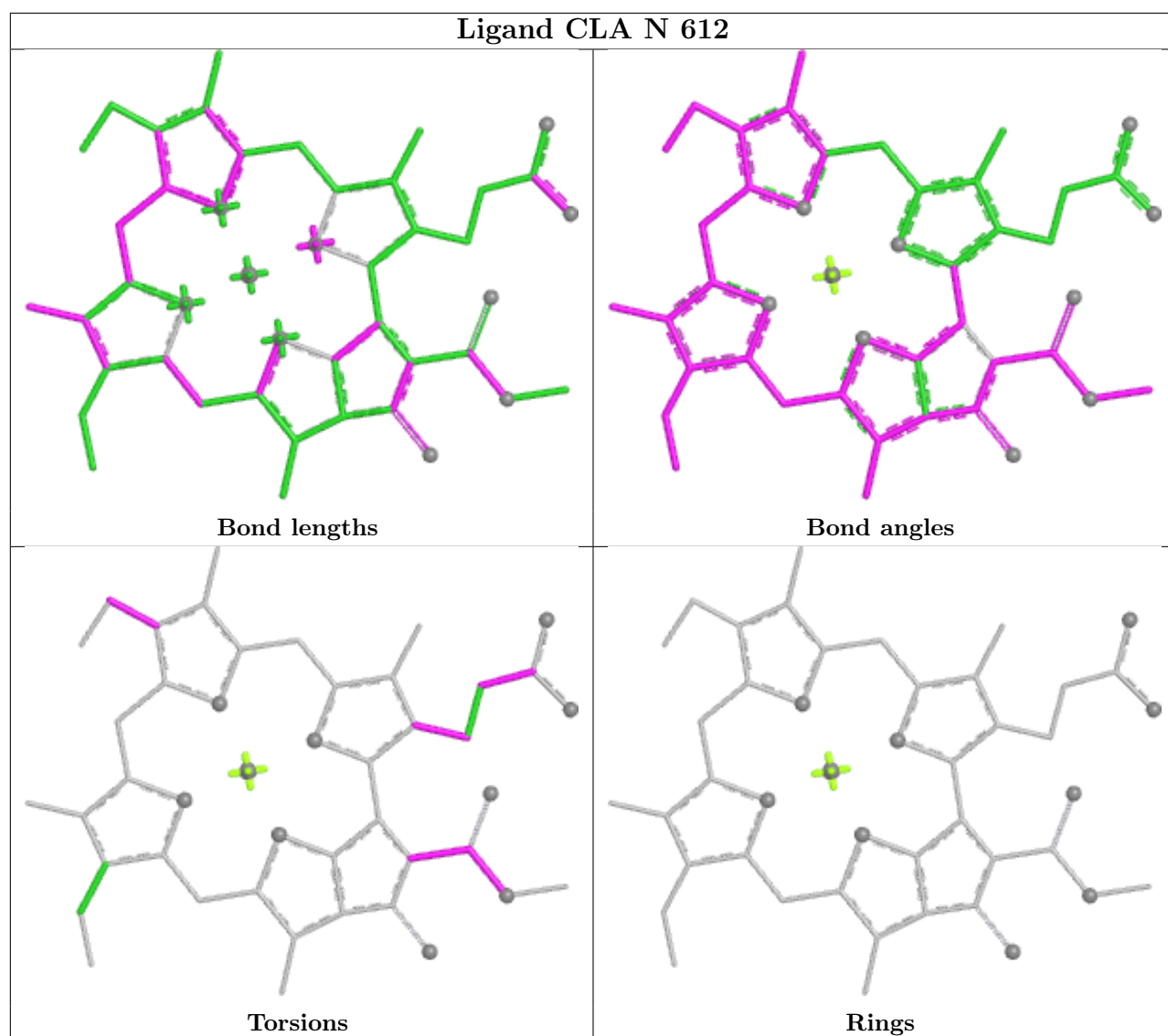
Rings

Ligand CLA c 509

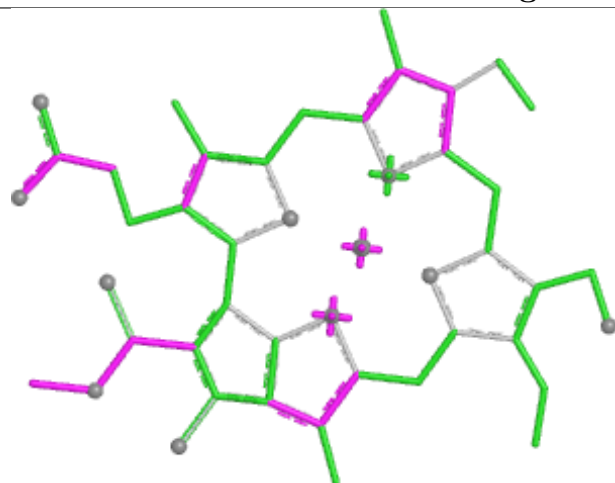




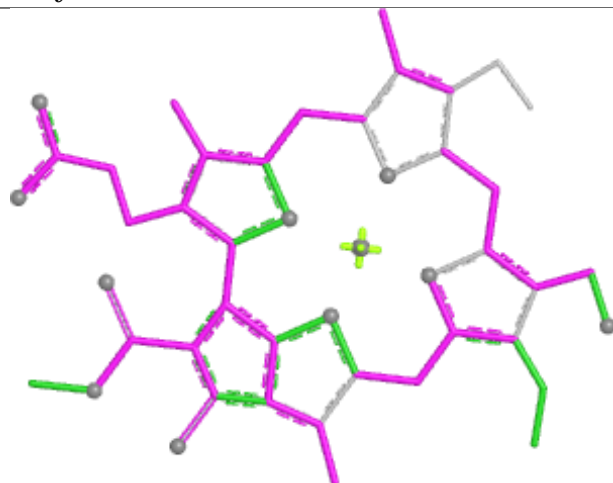




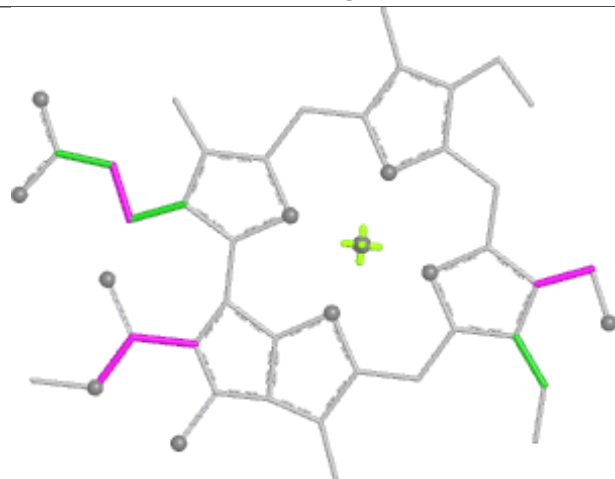
Ligand CHL y 607



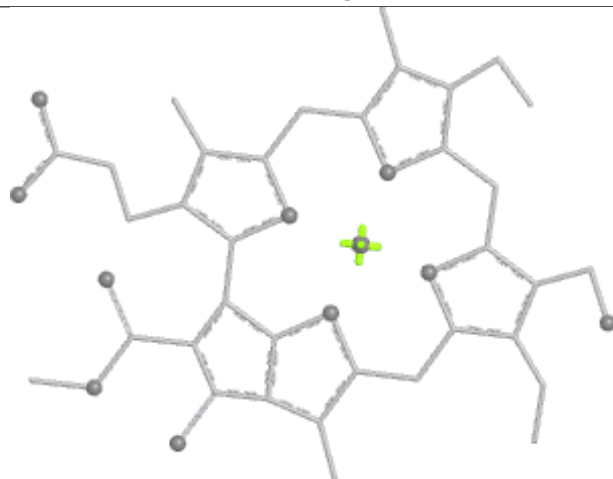
Bond lengths



Bond angles

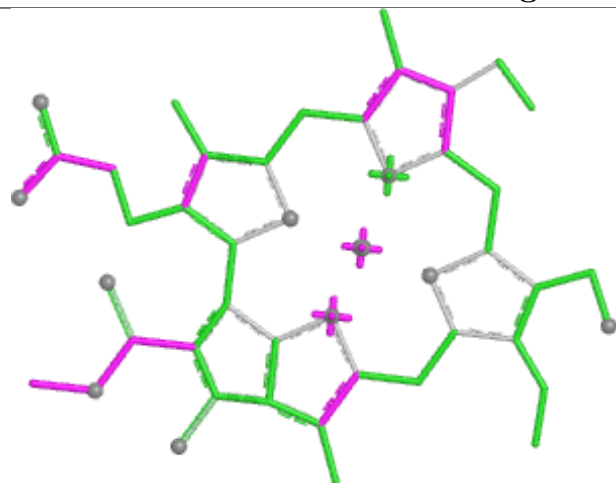


Torsions

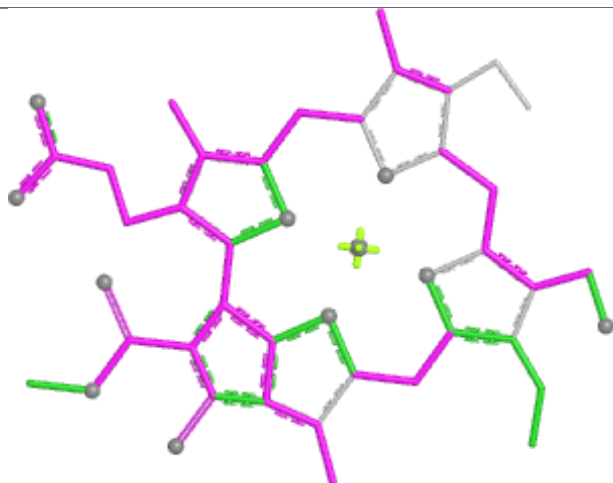


Rings

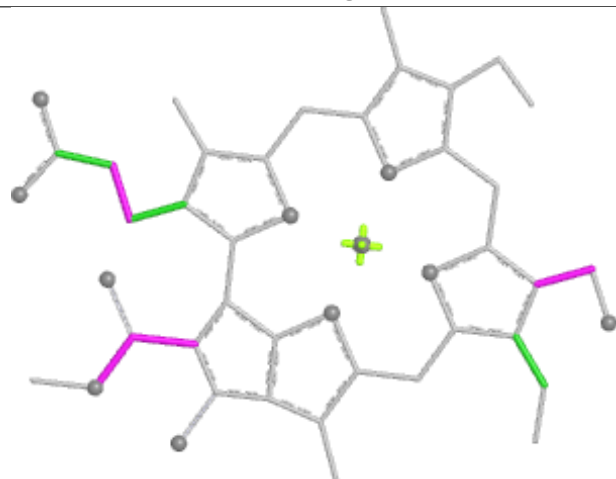
Ligand CHL 1 607



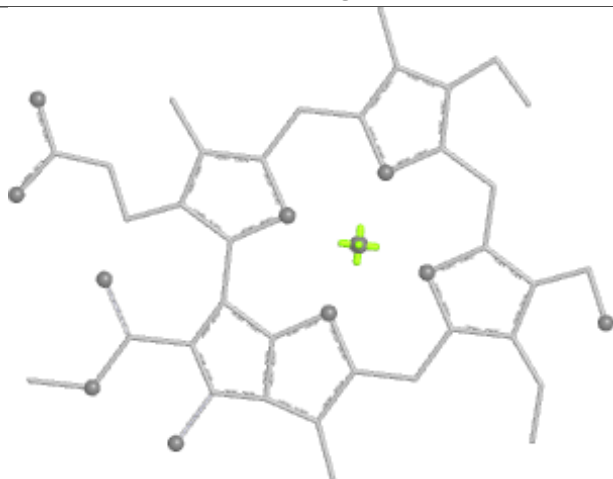
Bond lengths



Bond angles

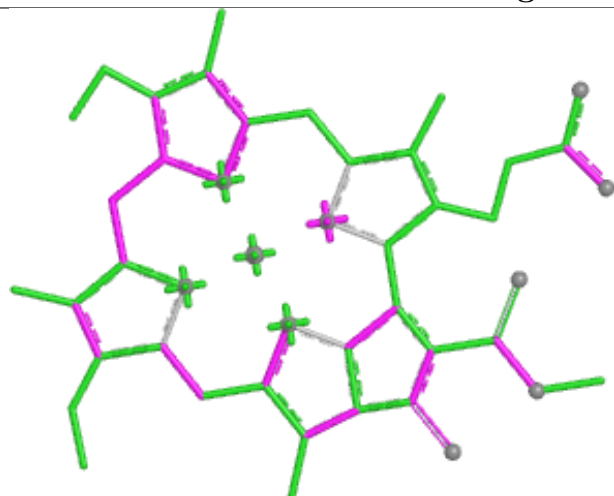


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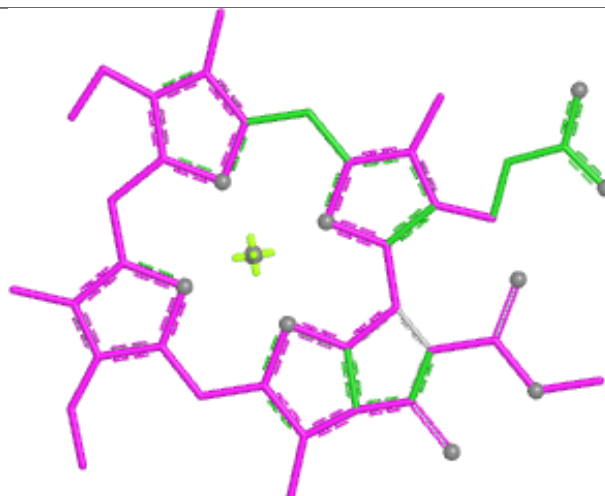


Rings

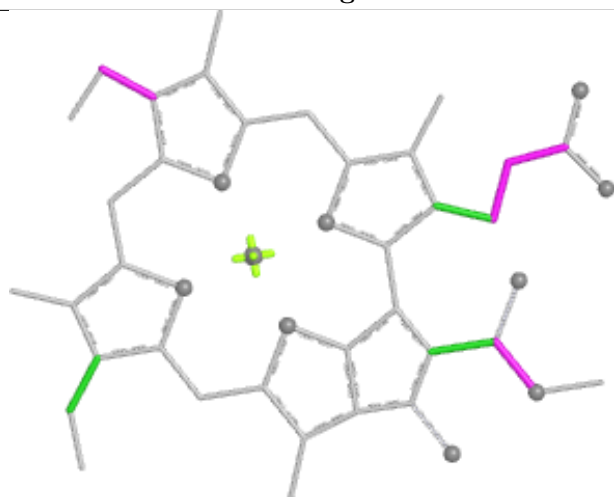
Ligand CLA S 313



Bond lengths



Bond angles

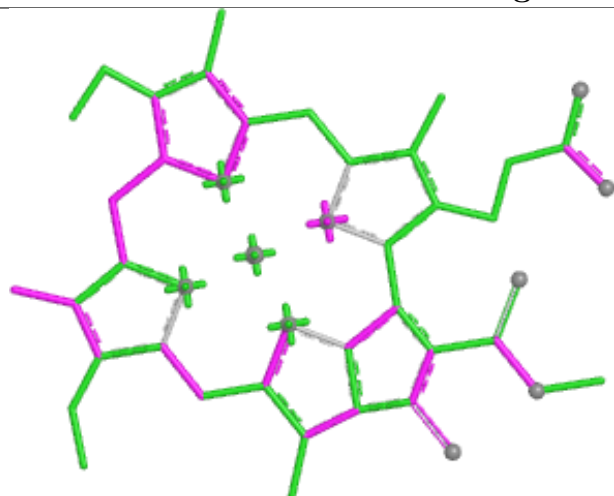


Torsions

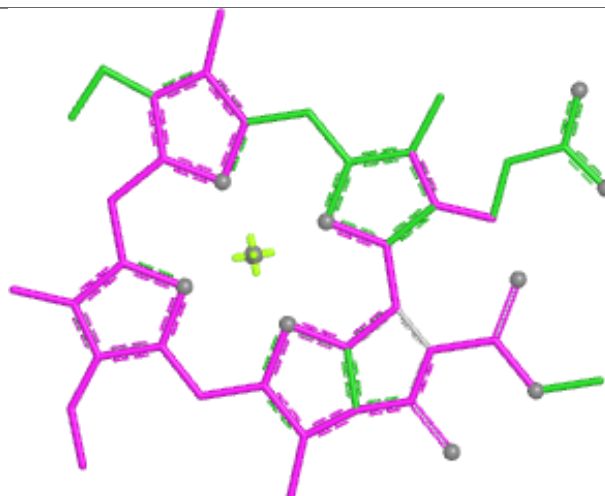


Rings

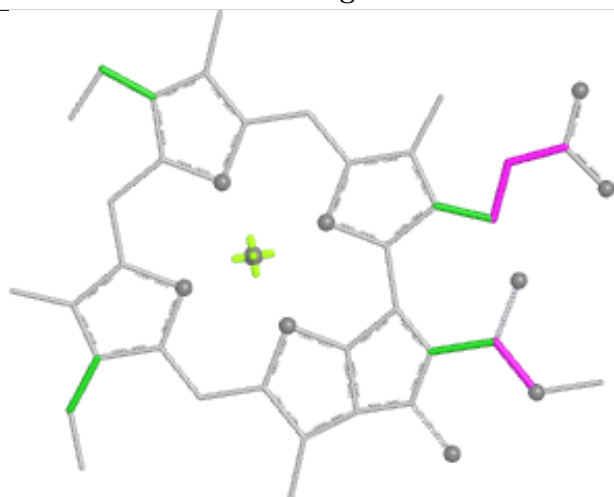
Ligand CLA N 611



Bond lengths



Bond angles

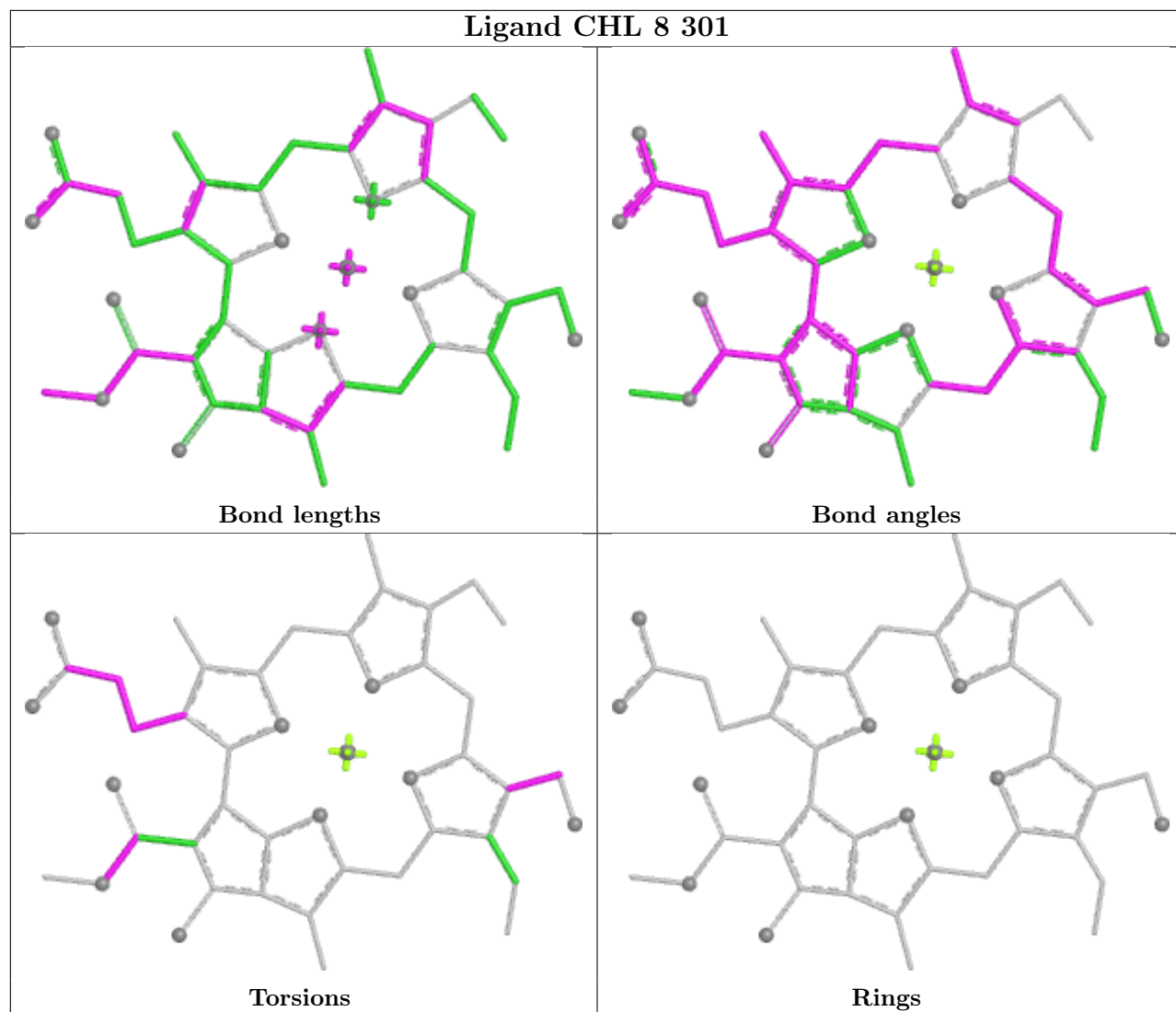


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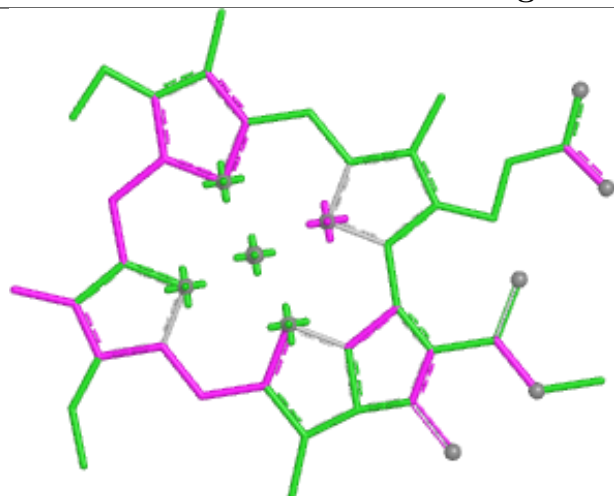


Rings

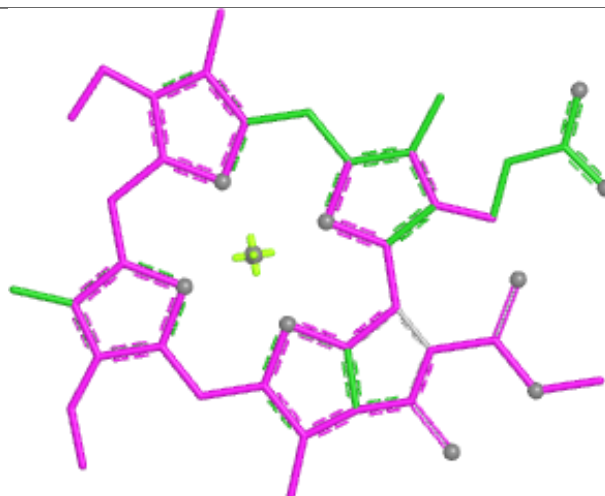
Ligand CHL 8 301



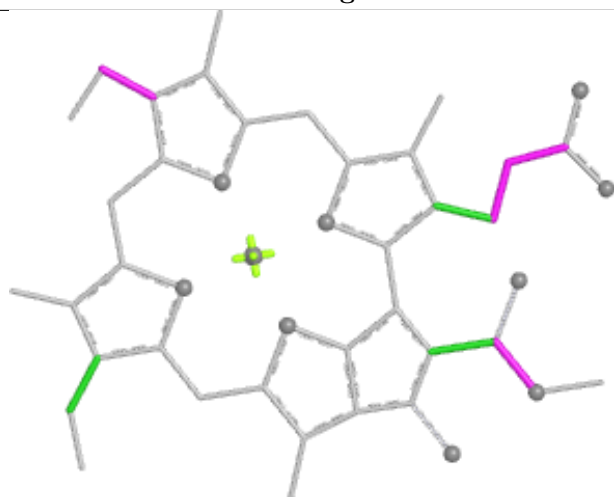
Ligand CLA b 603



Bond lengths



Bond angles

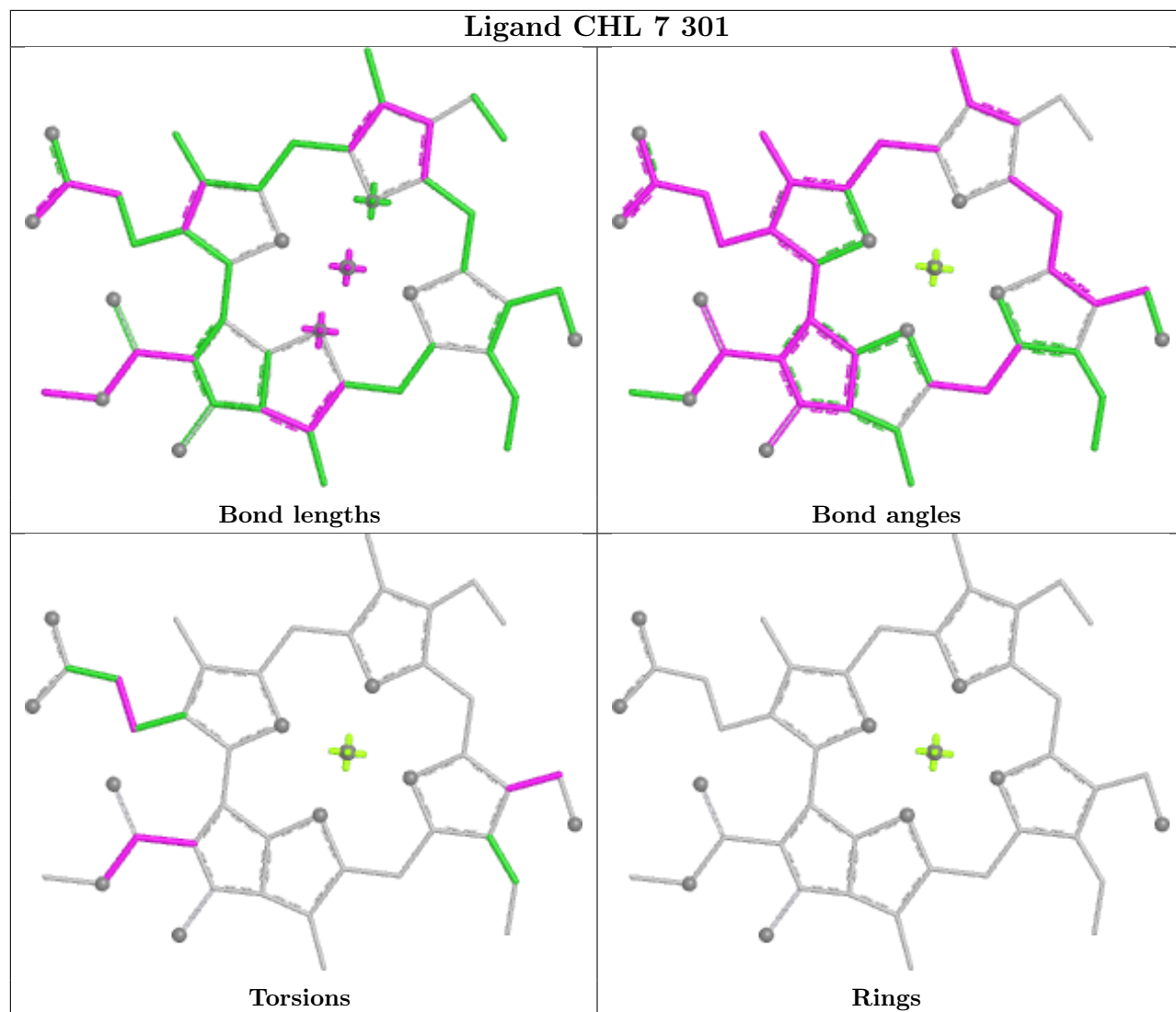


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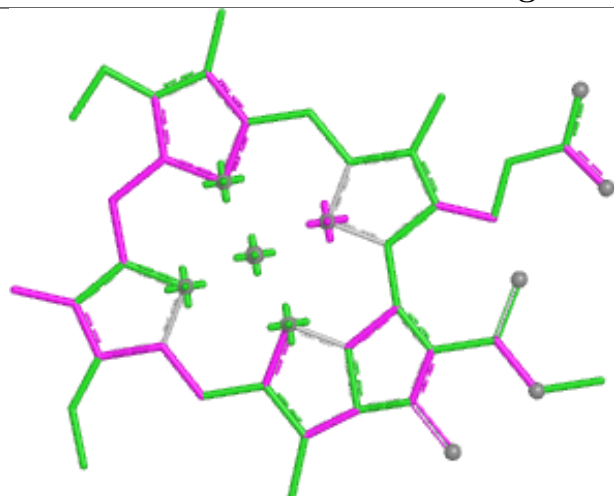


Rings

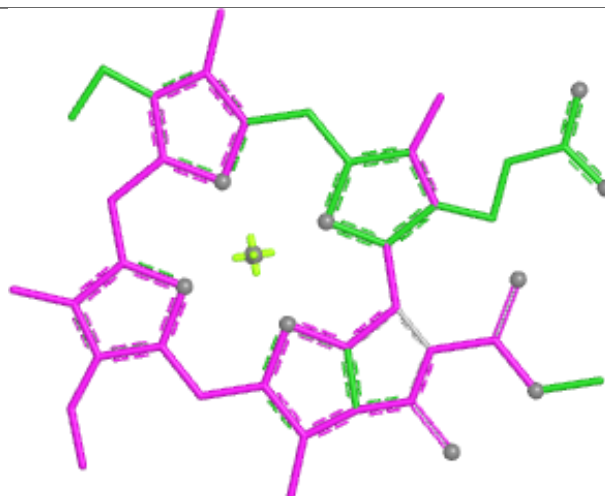
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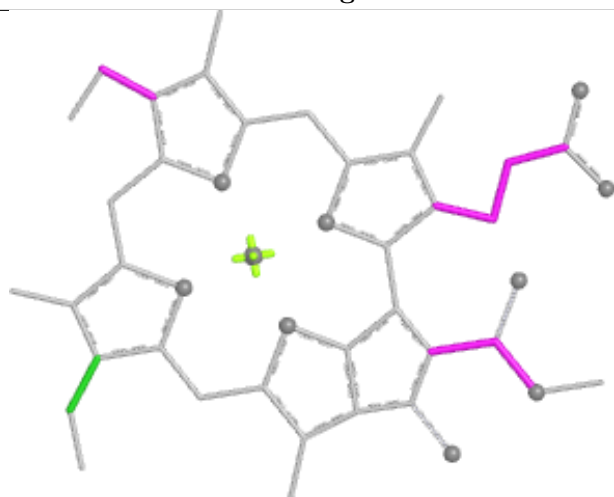
Ligand CLA 1 602



Bond lengths



Bond angles

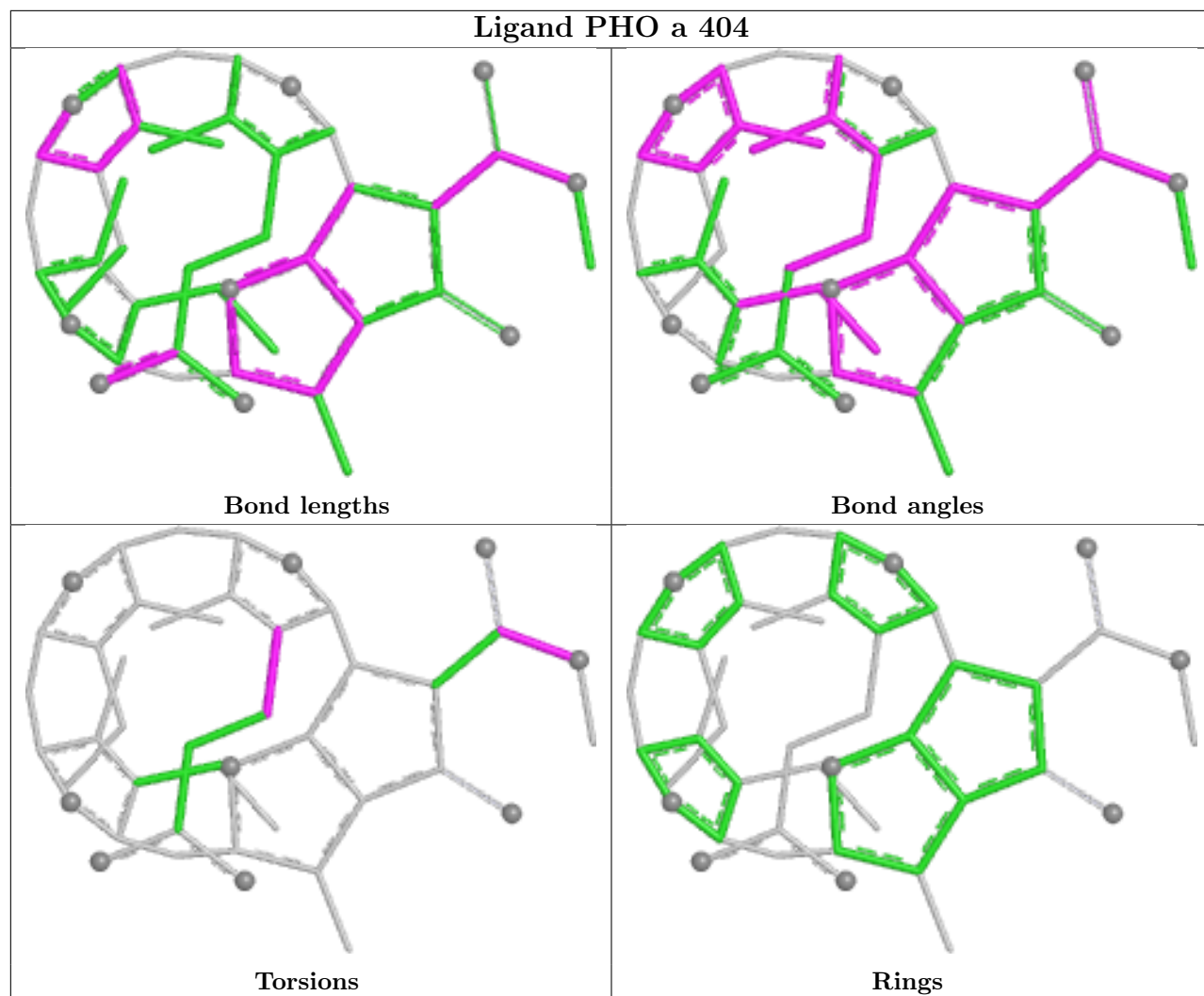


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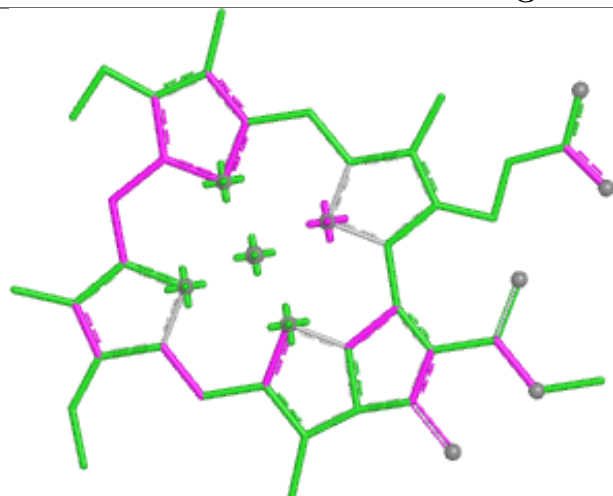


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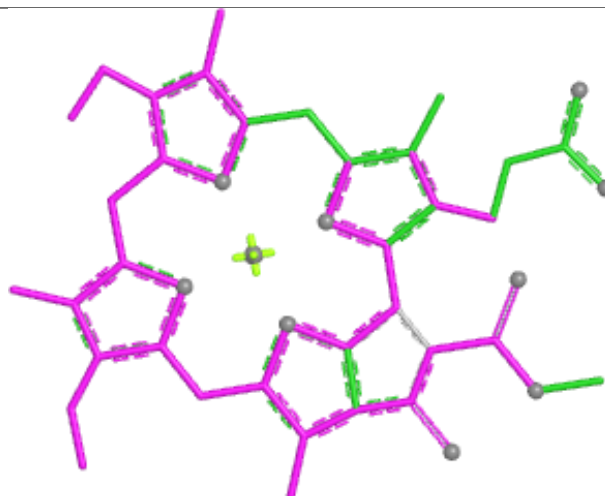
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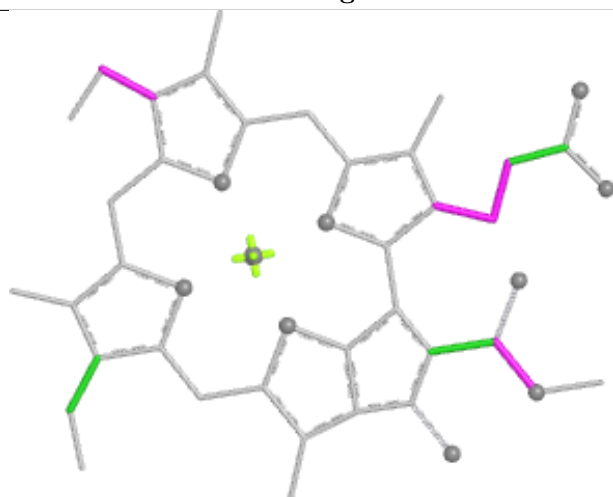
Ligand CLA b 602



Bond lengths



Bond angles

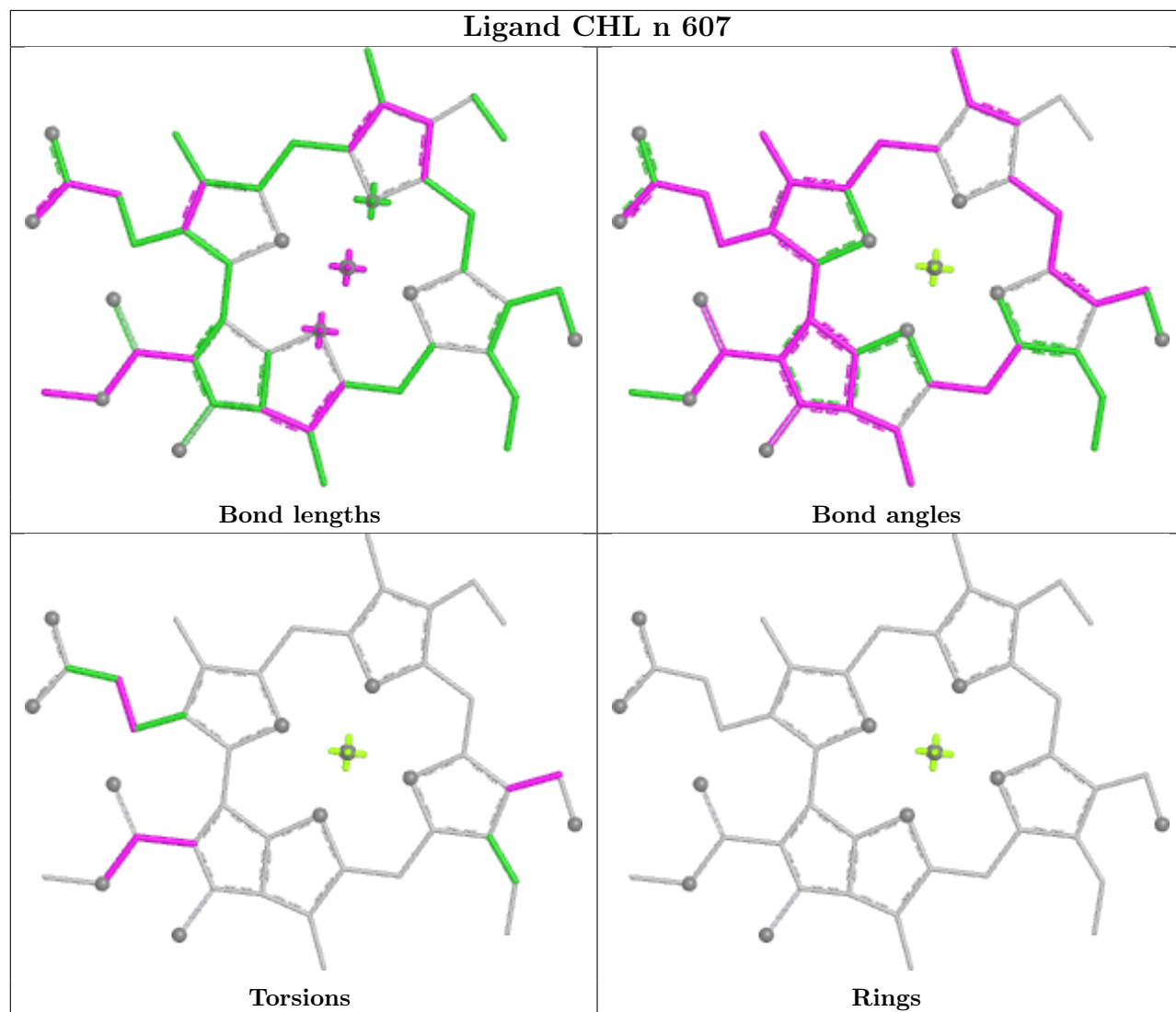


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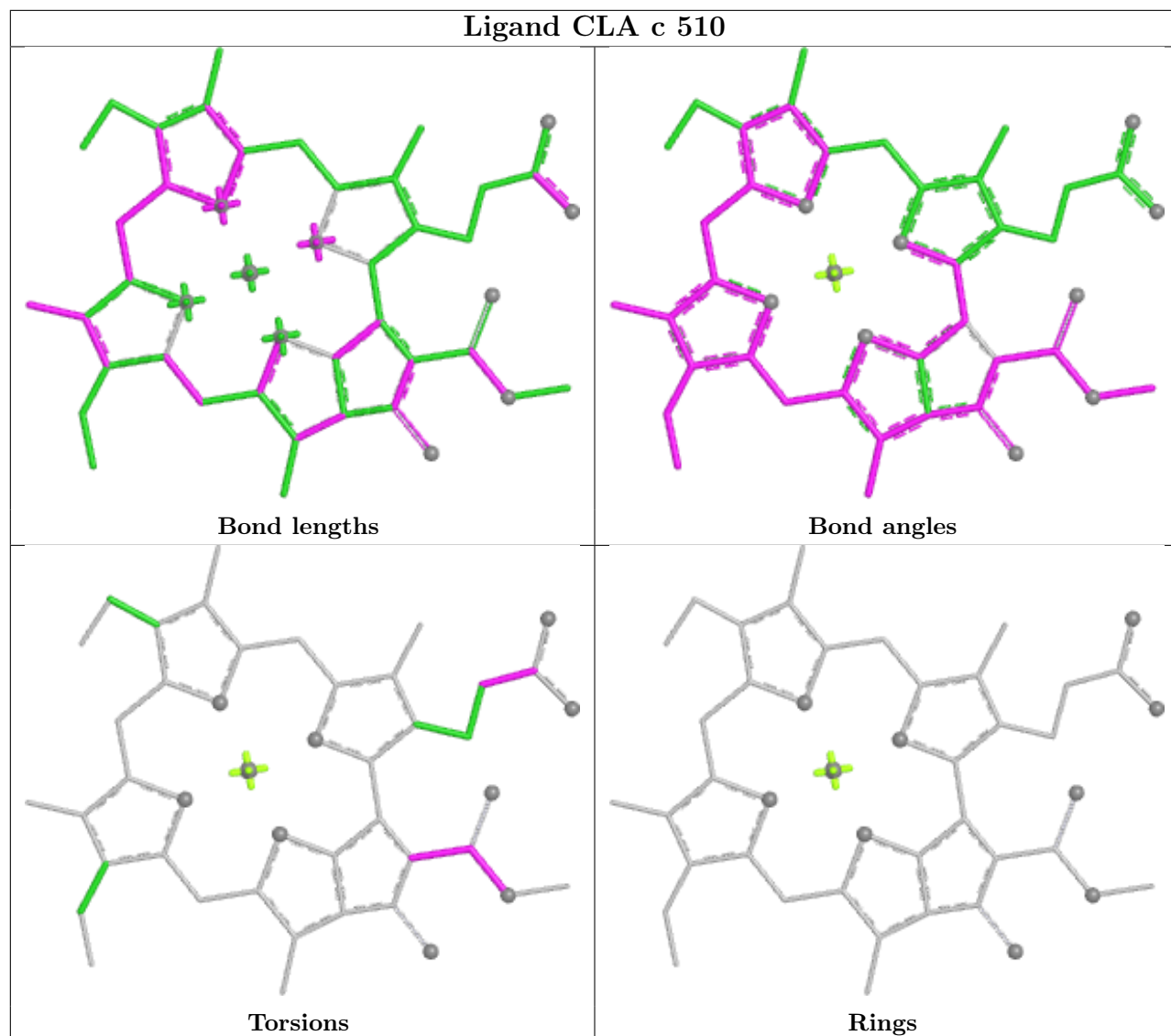


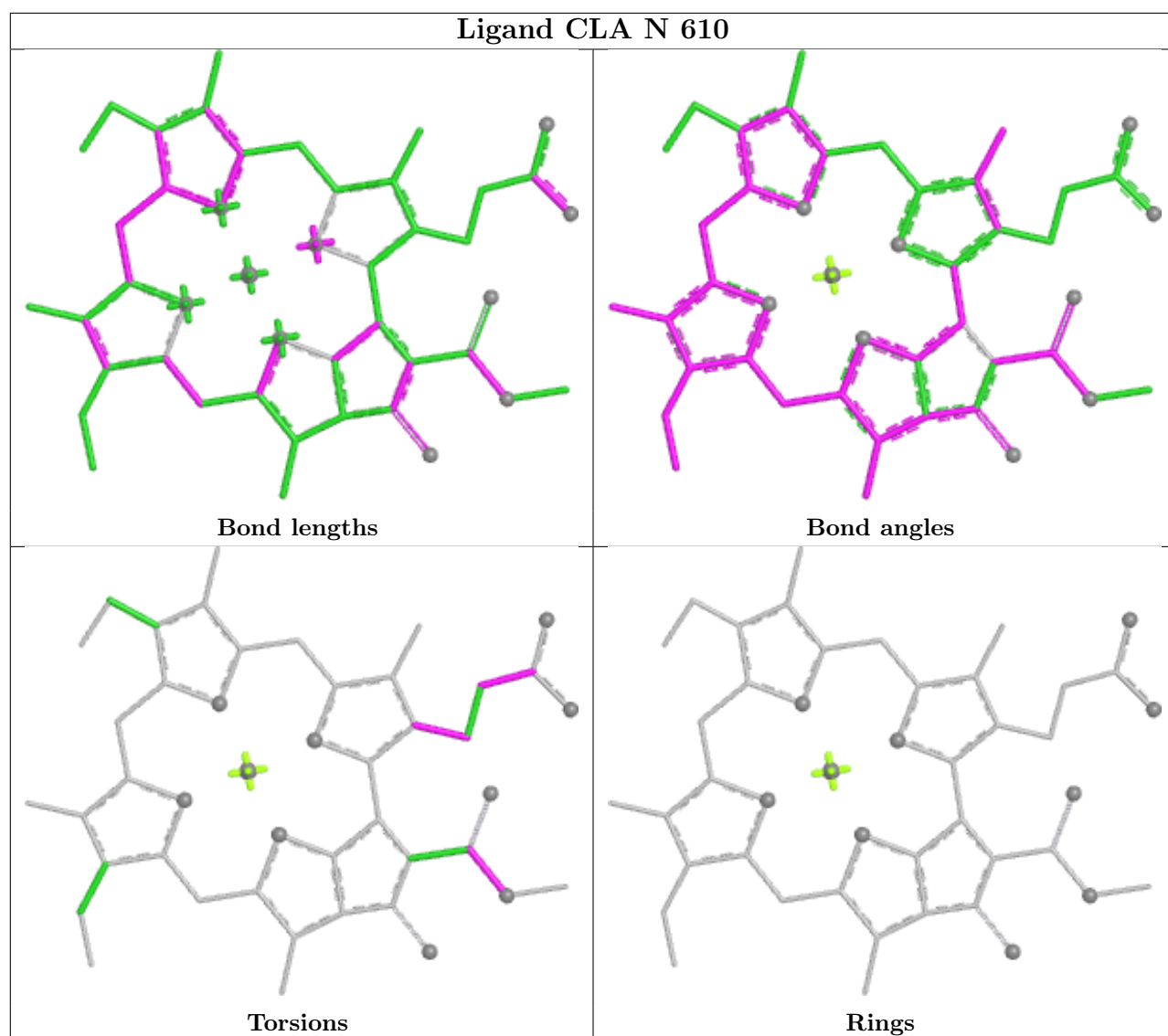
Rings

Ligand CHL n 607

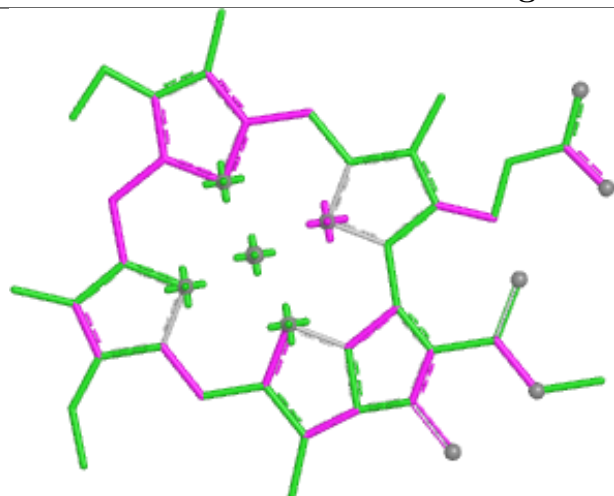


Ligand CLA c 510

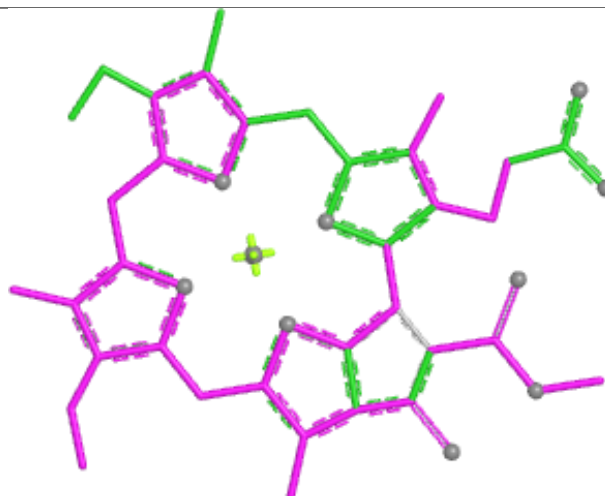




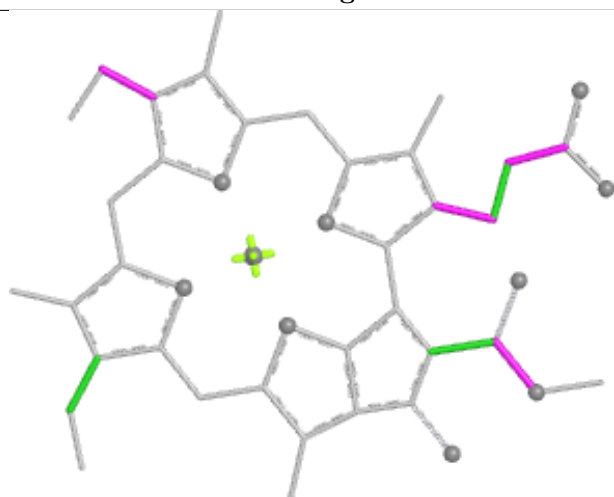
Ligand CLA 4 309



Bond lengths



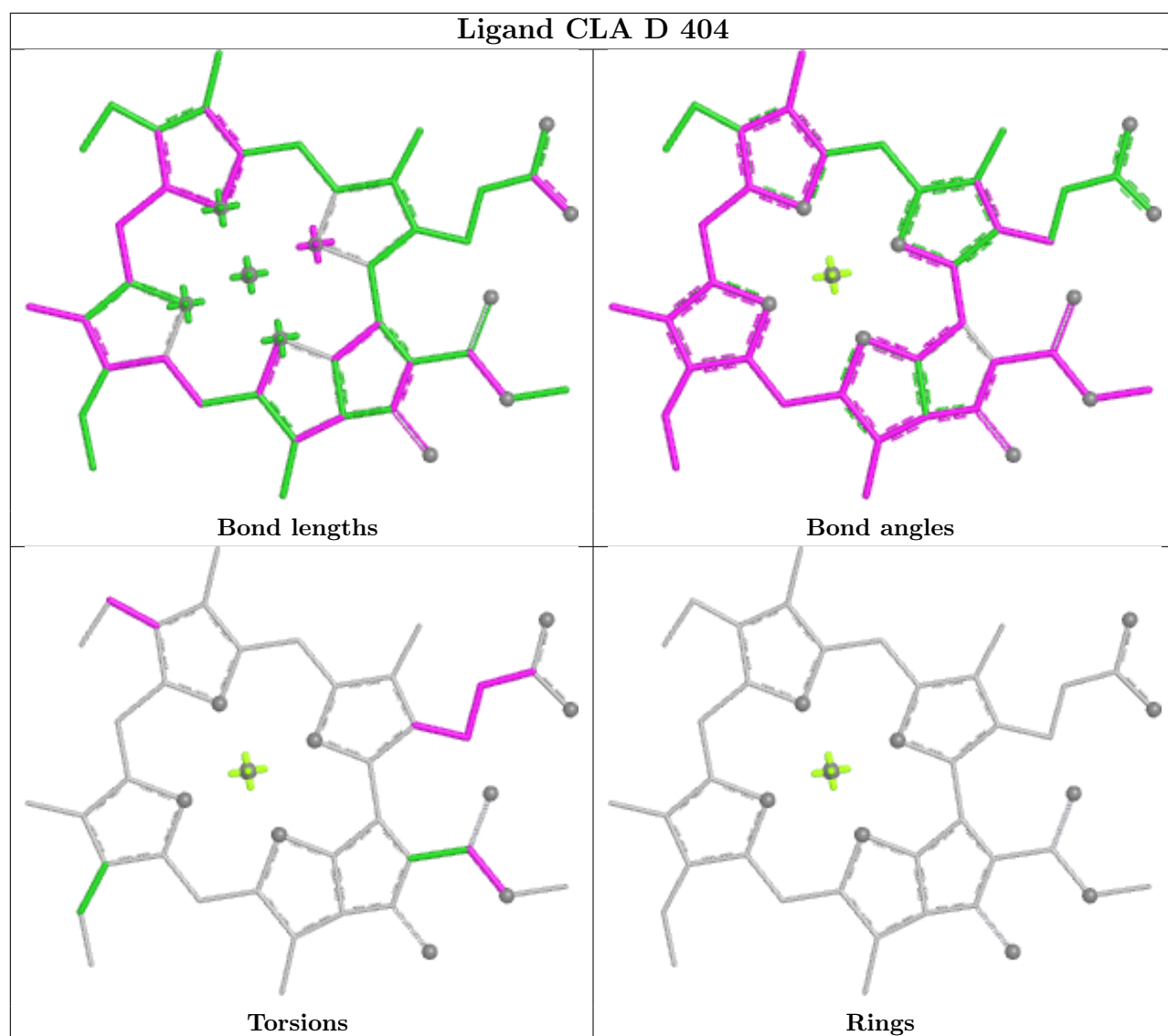
Bond angles



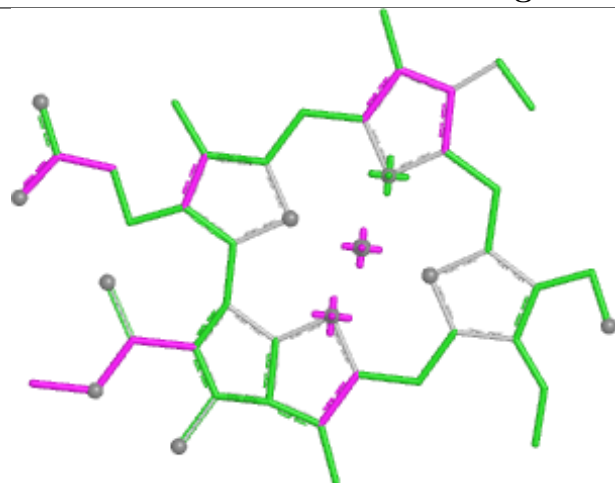
Torsions



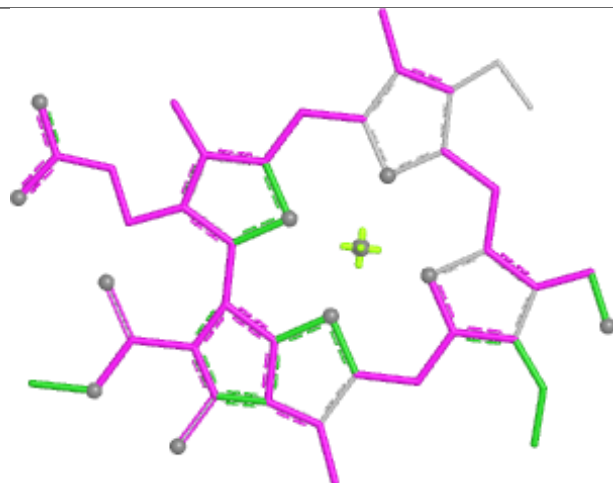
Rings



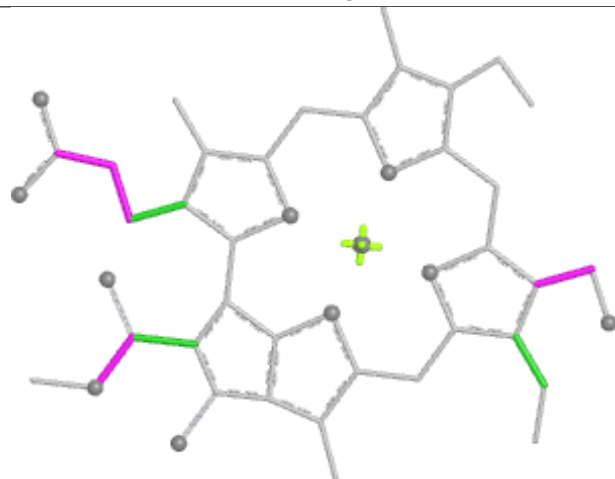
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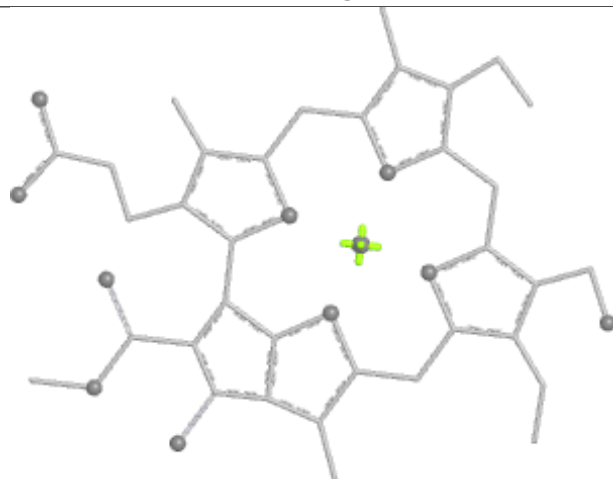
Bond lengths



Bond angles

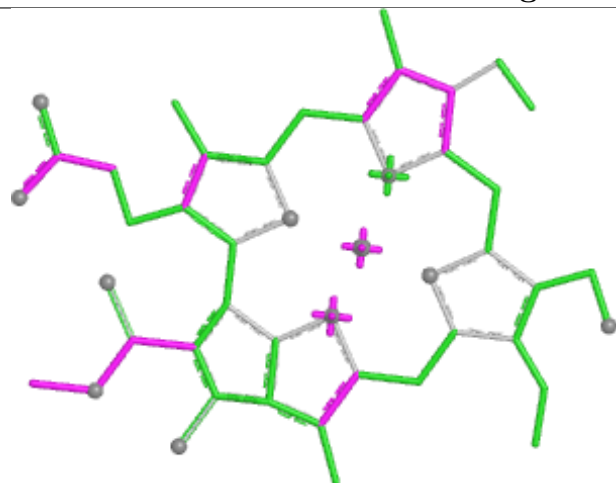


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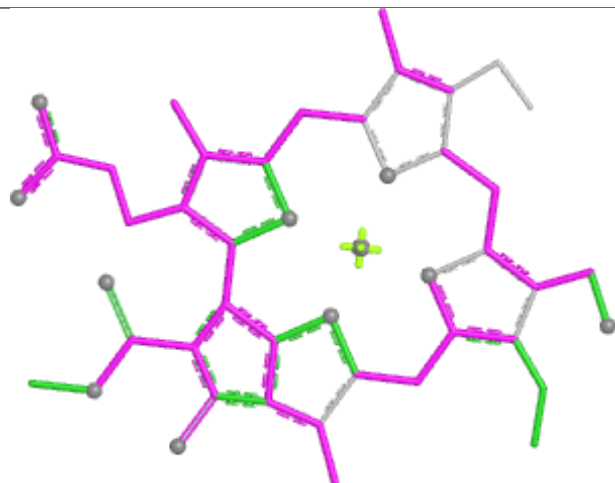


Rings

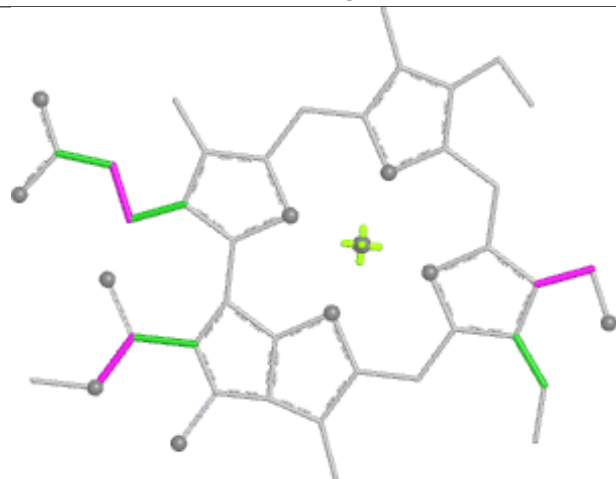
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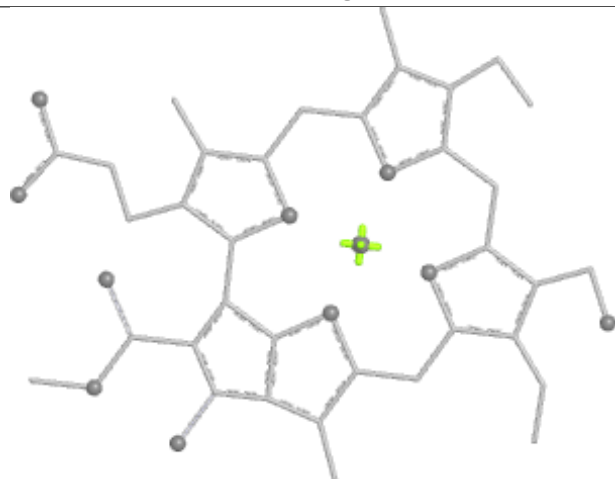
Bond lengths



Bond angles

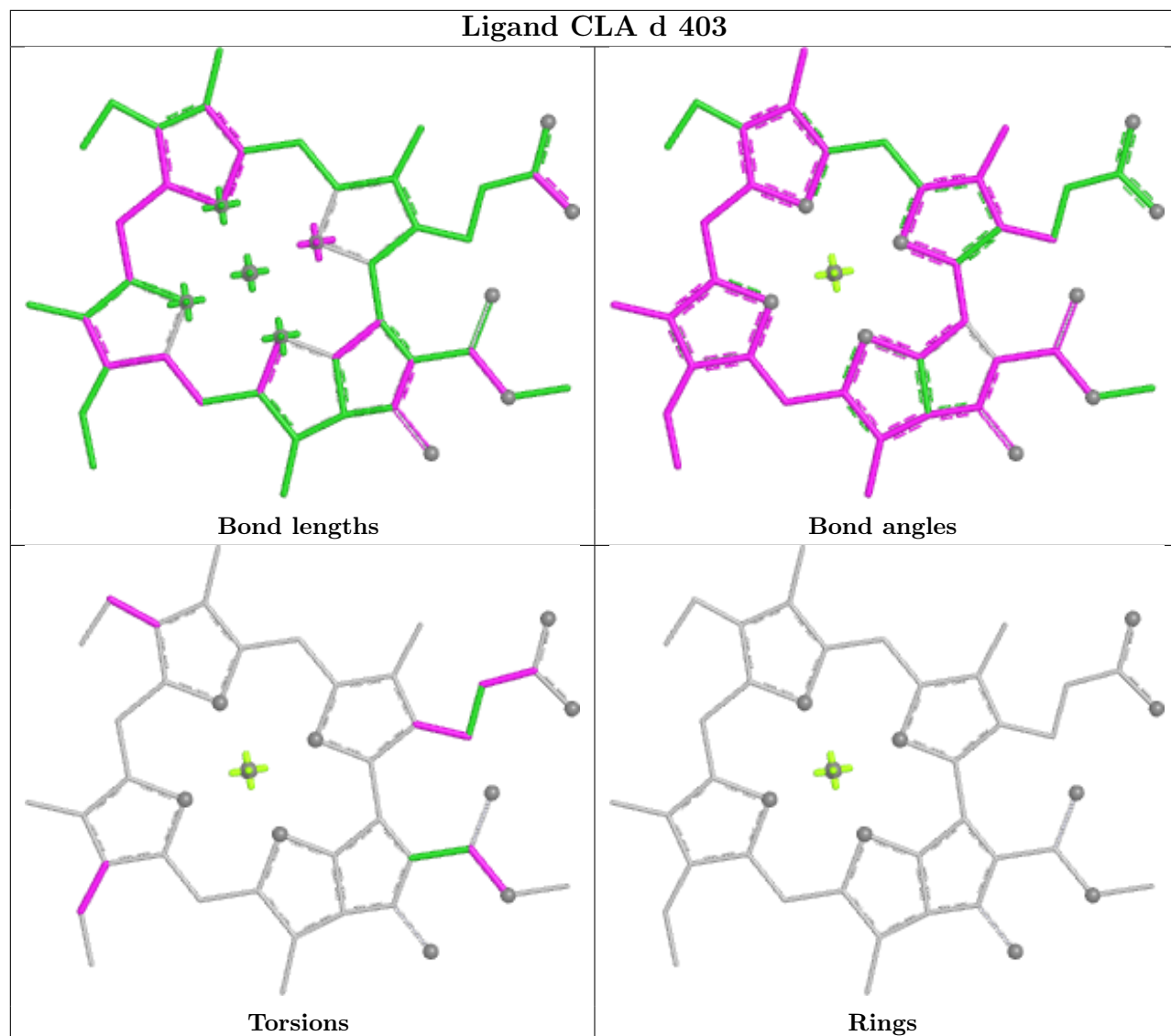


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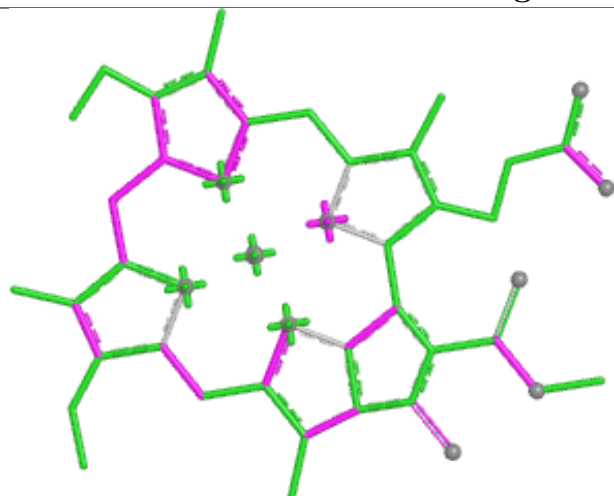


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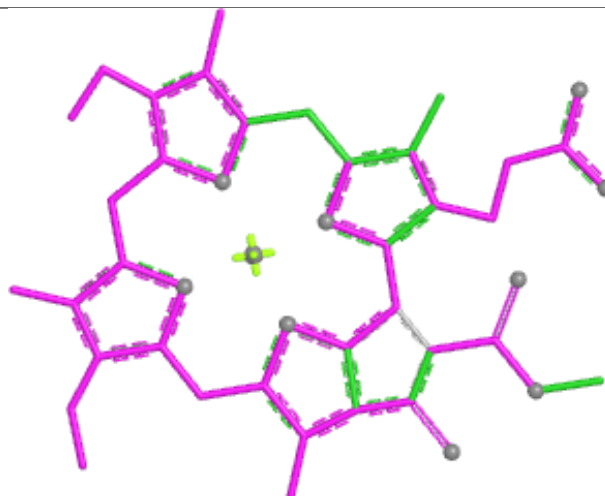
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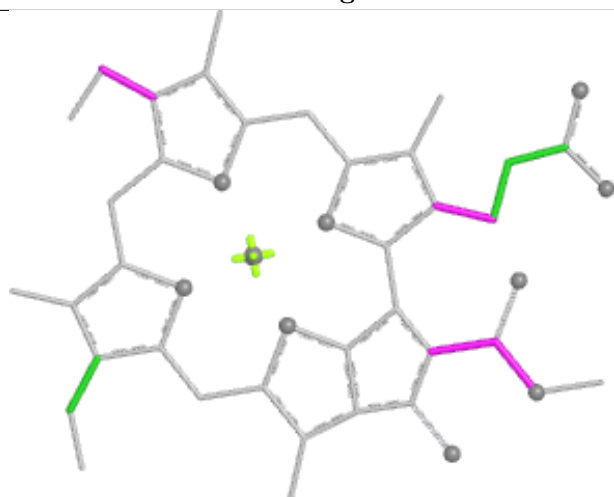
Ligand CLA R 303



Bond lengths



Bond angles

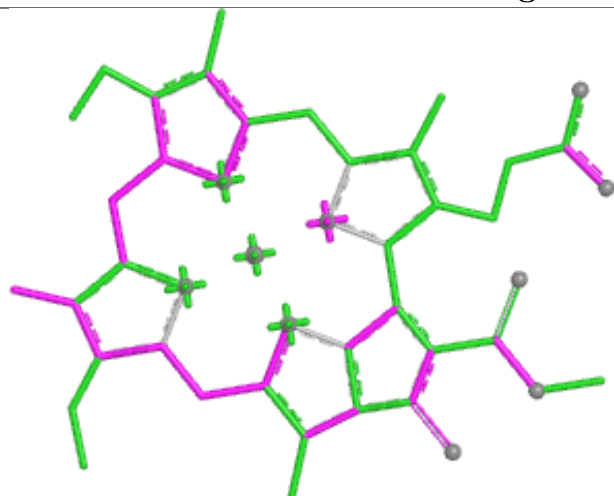


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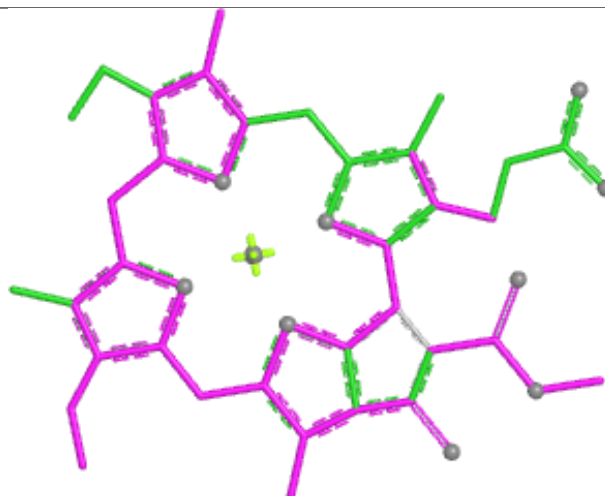


Rings

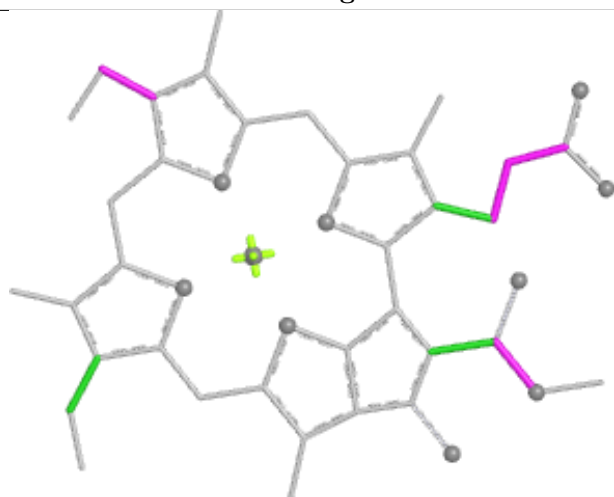
Ligand CLA 6 603



Bond lengths



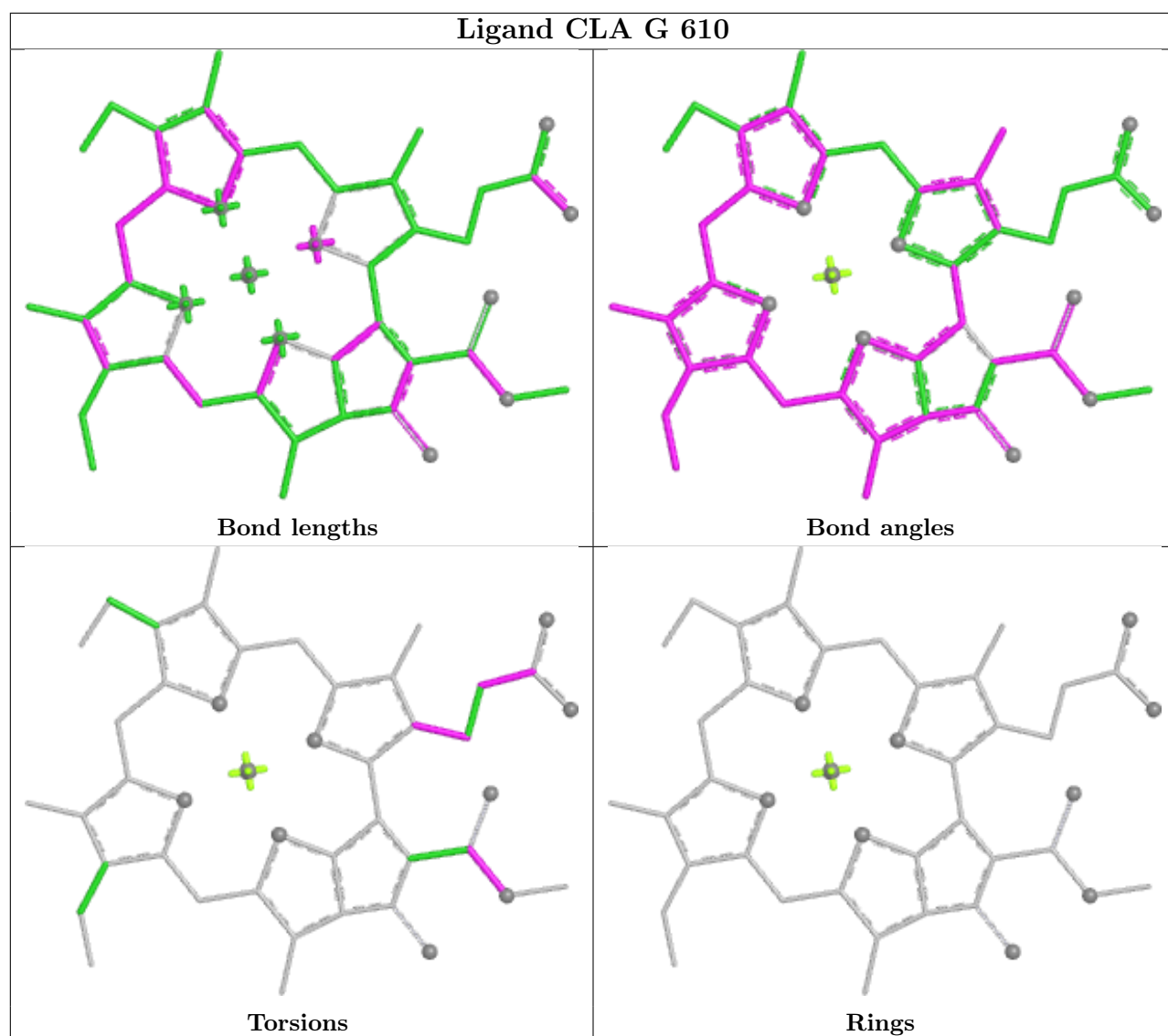
Bond angles

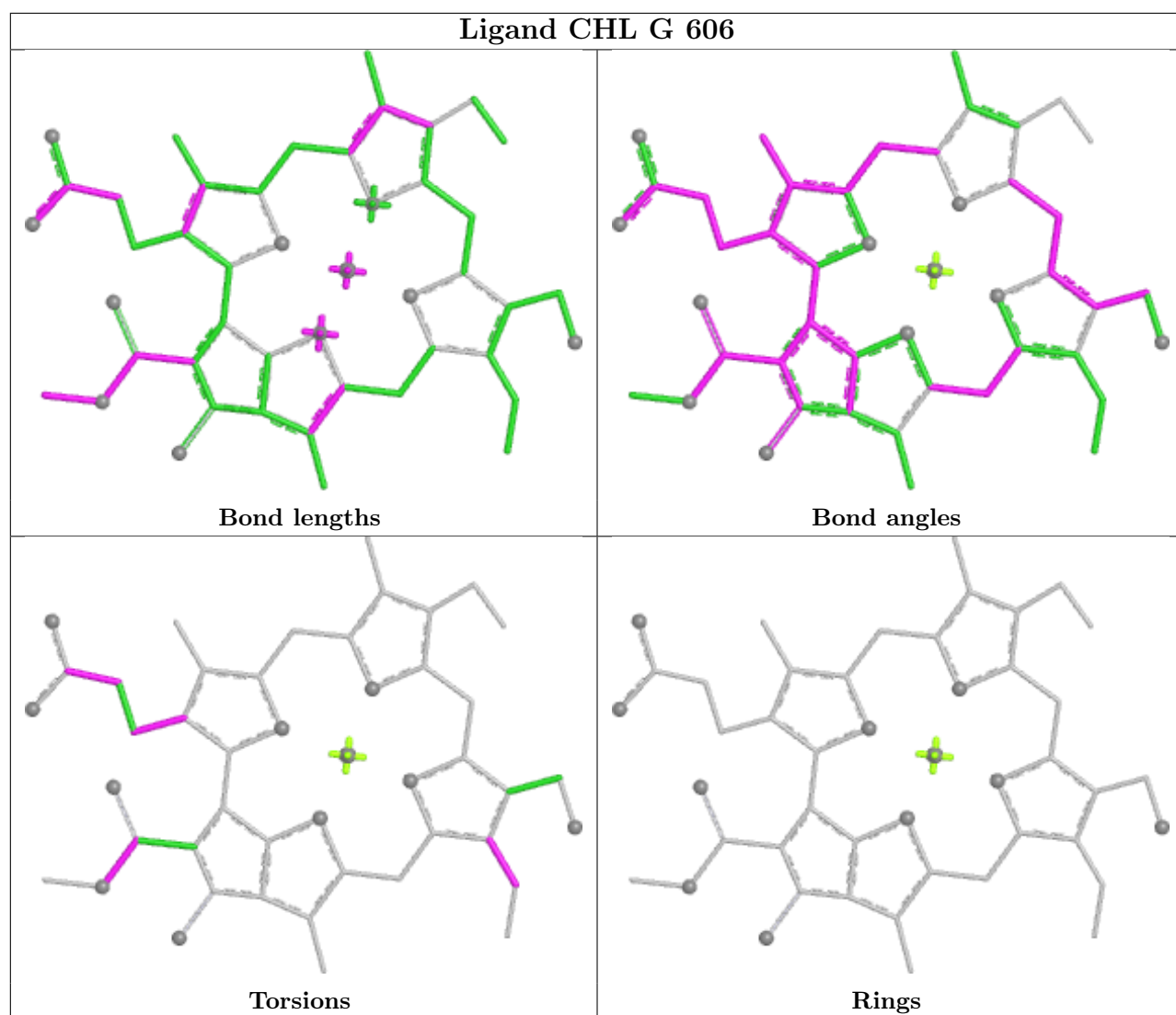


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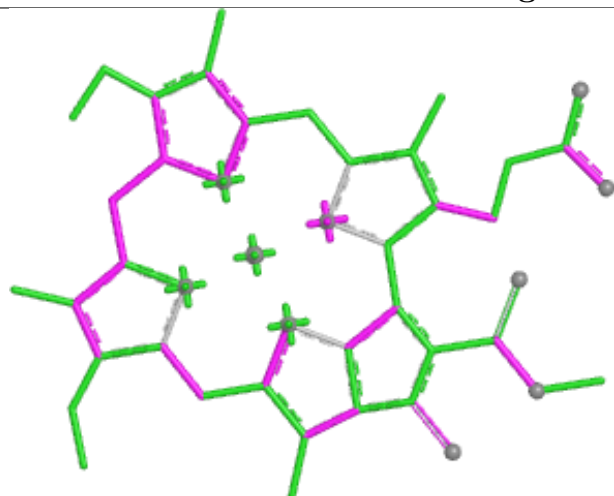


Rings

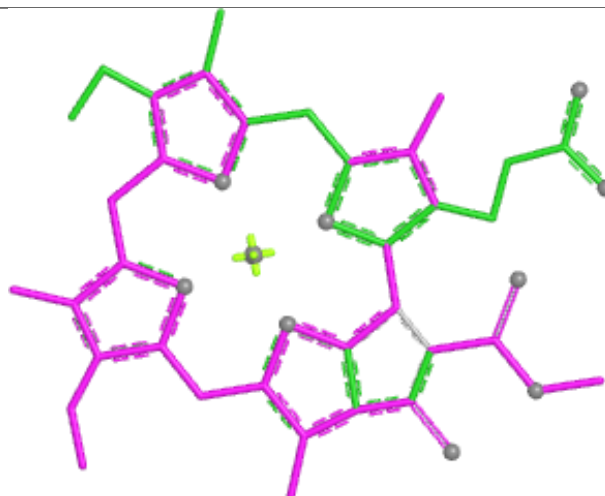




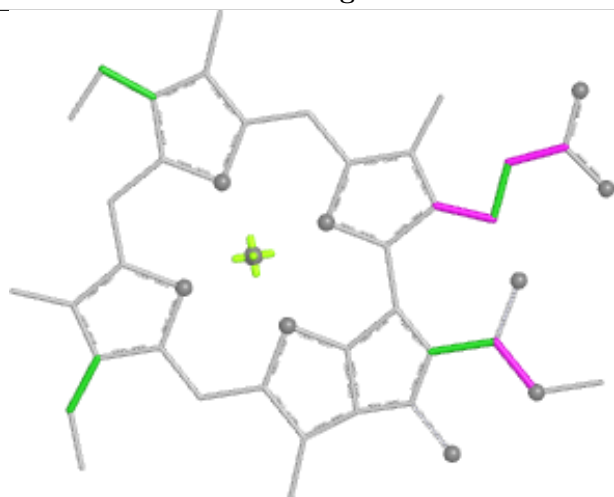
Ligand CLA 7 310



Bond lengths



Bond angles

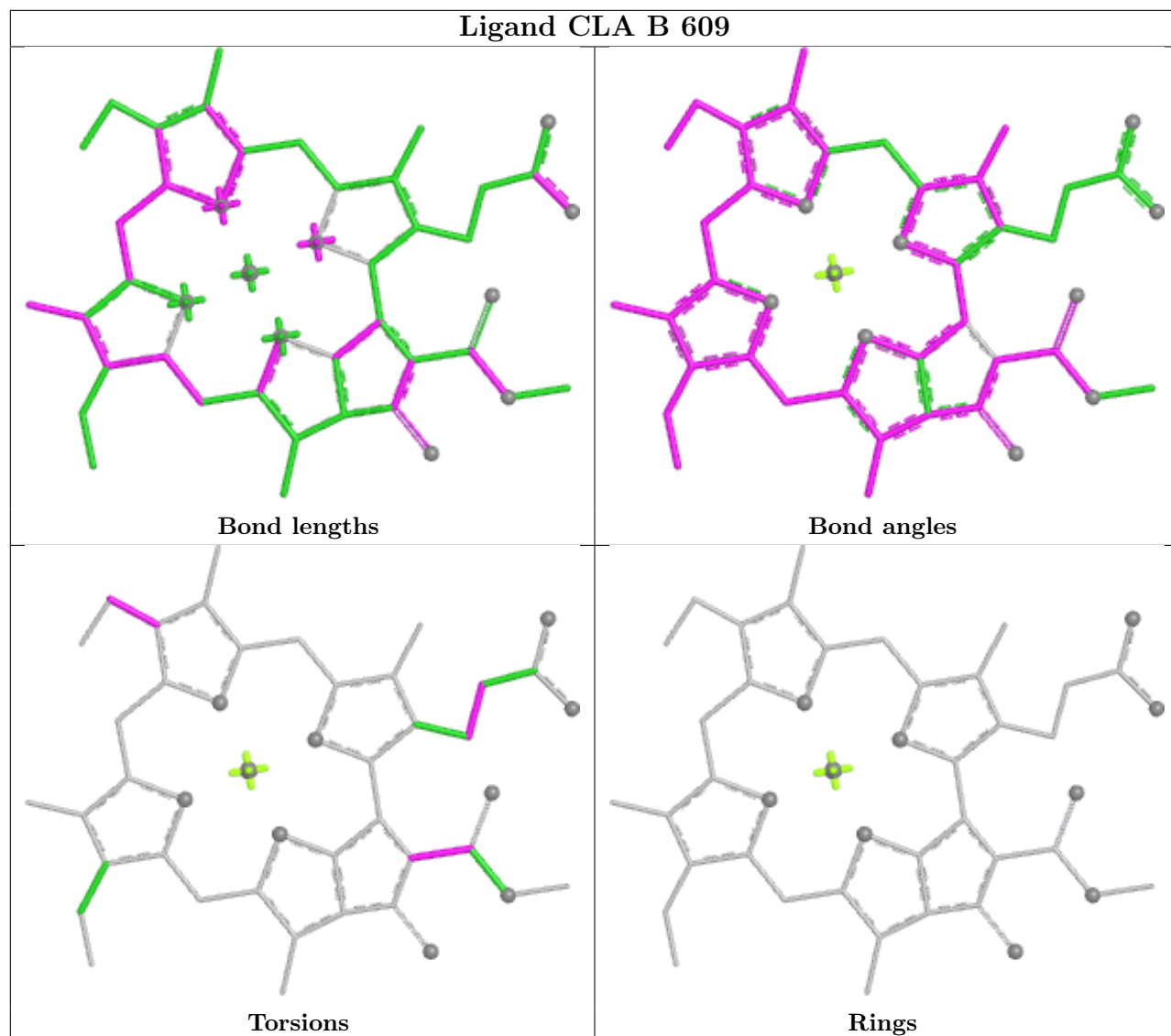


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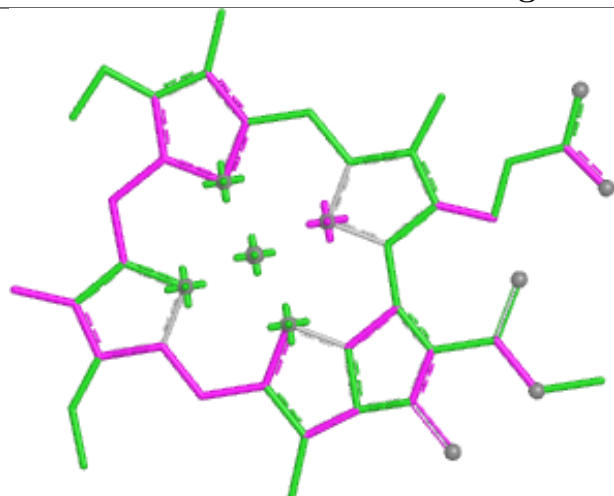


Rings

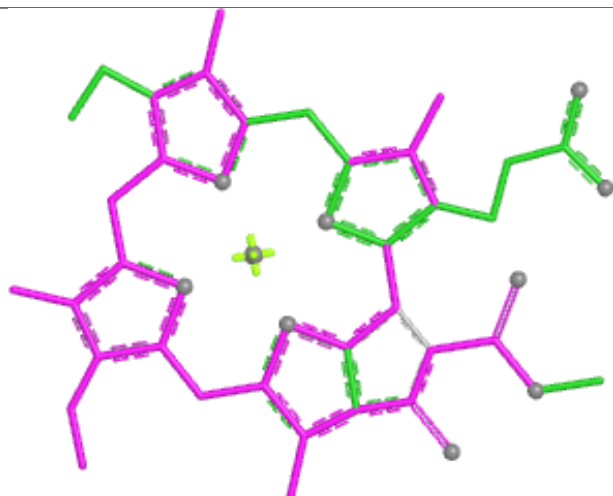
Ligand CLA B 609



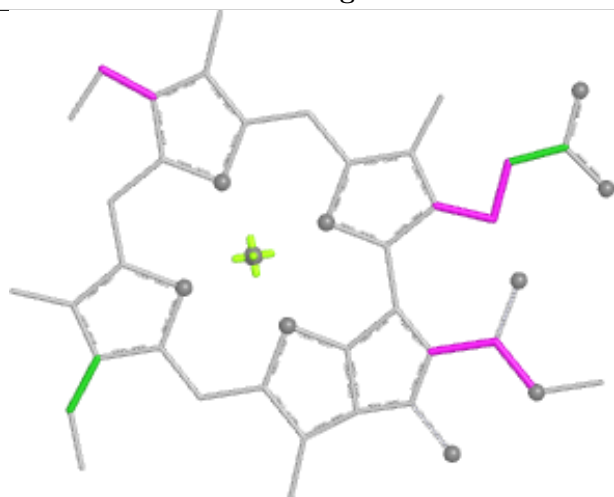
Ligand CLA 6 602



Bond lengths



Bond angles

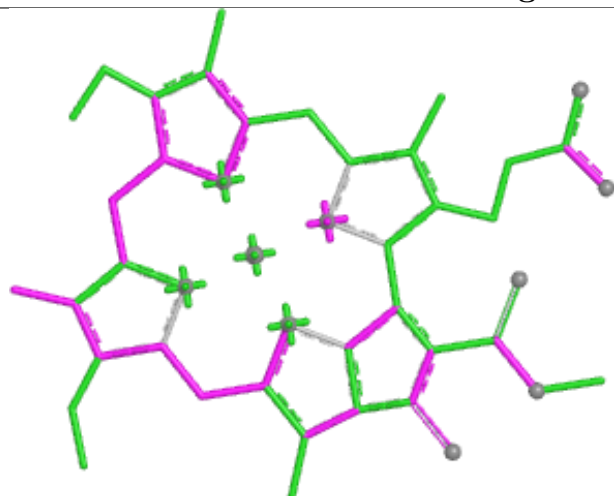


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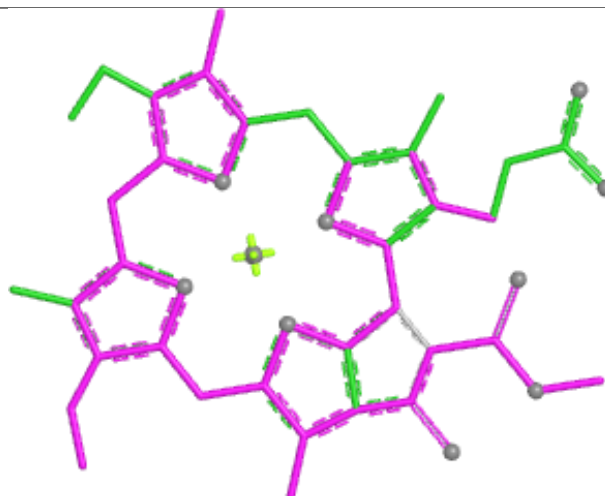


Rings

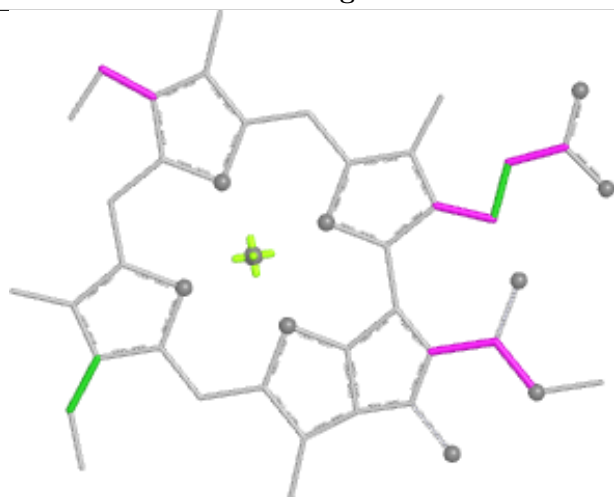
Ligand CLA 5 612



Bond lengths



Bond angles

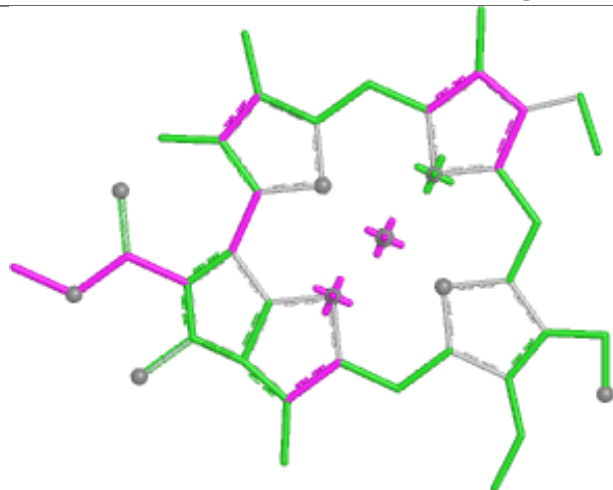


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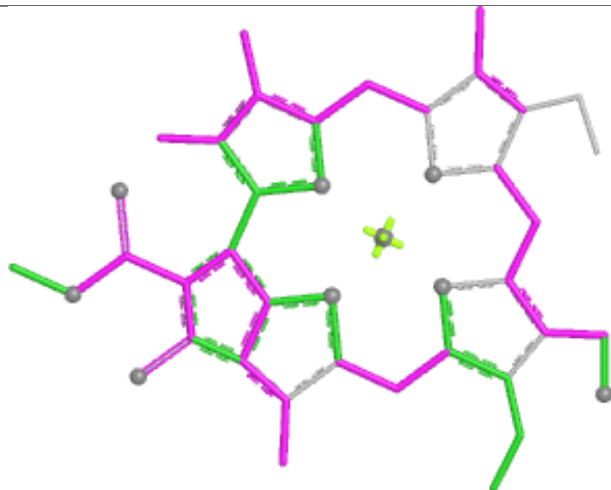


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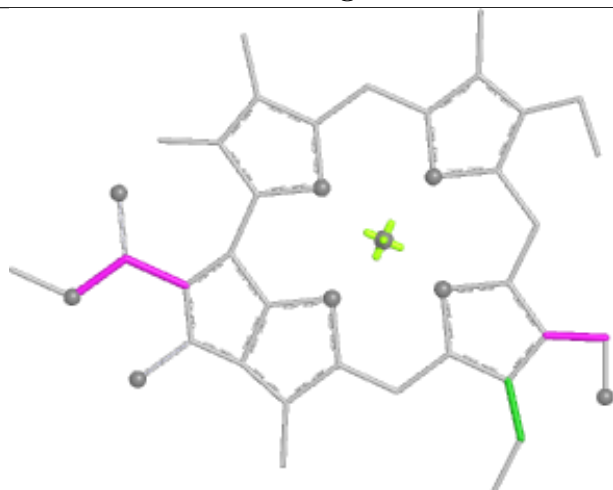
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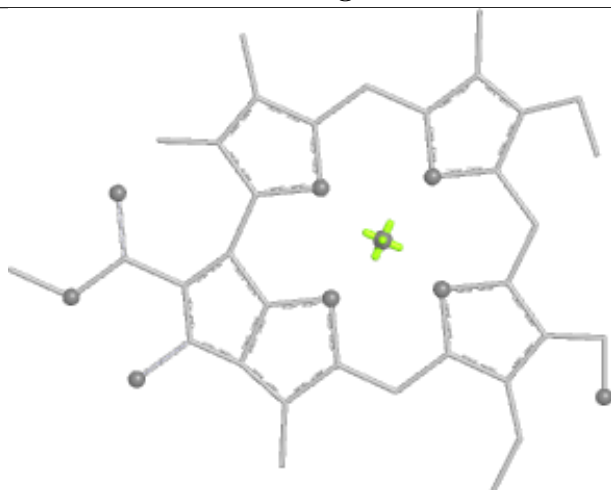
Bond lengths



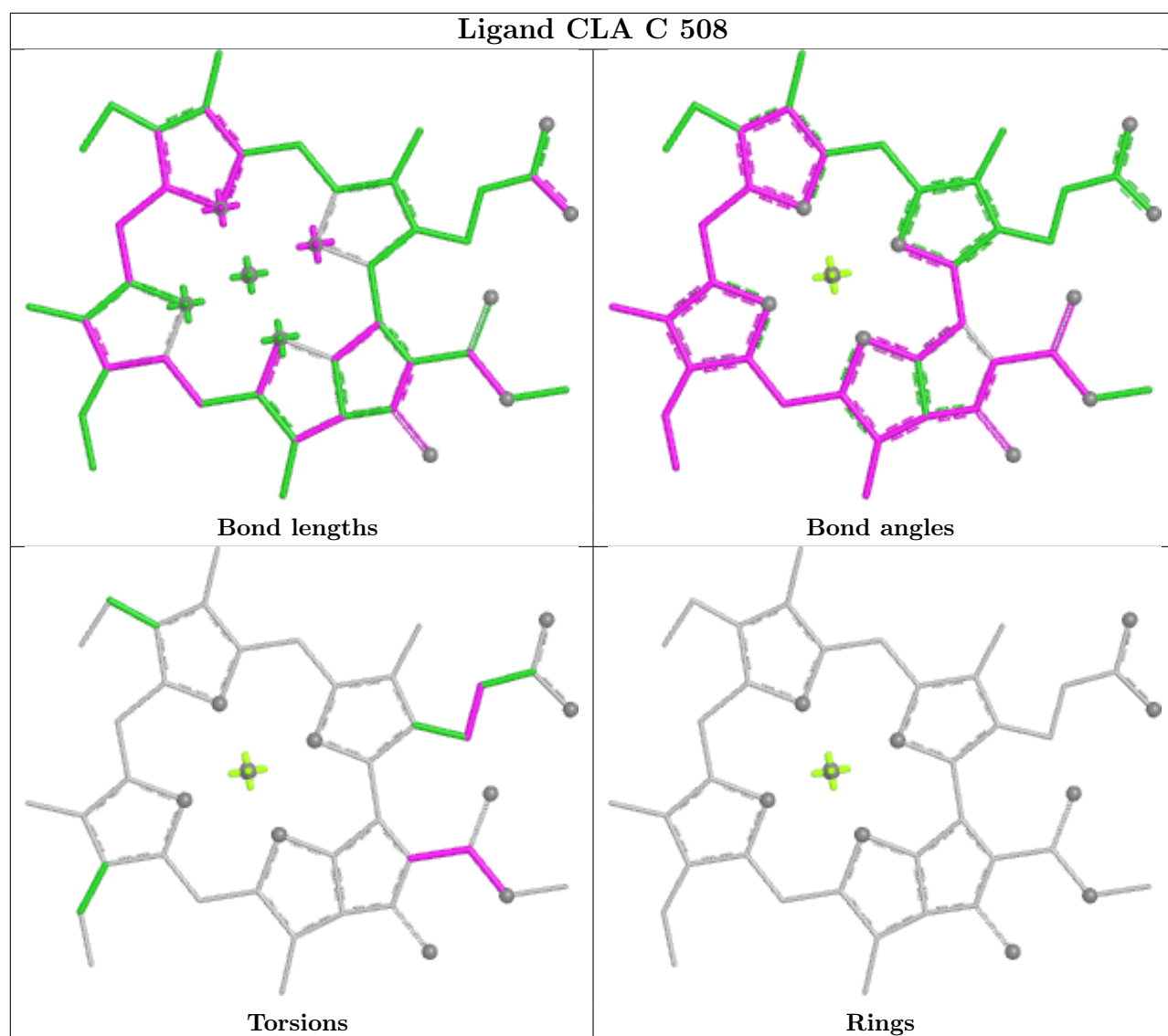
Bond angles



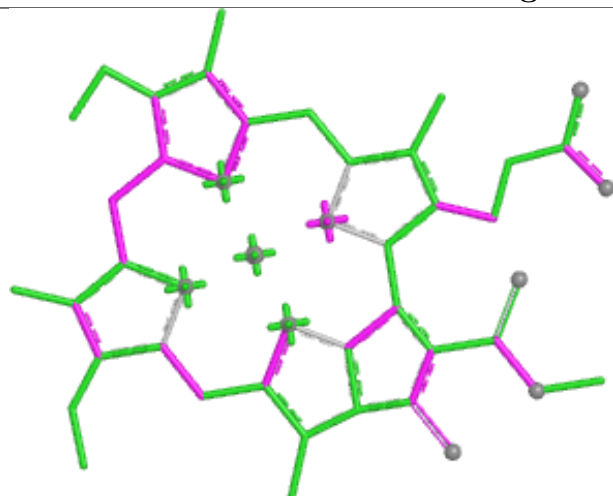
Torsions



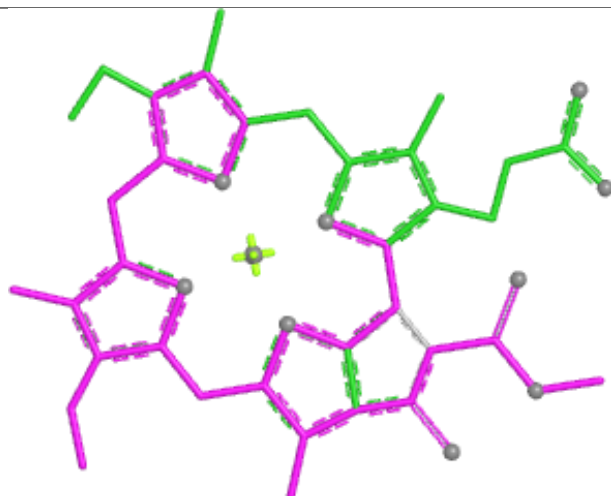
Rings



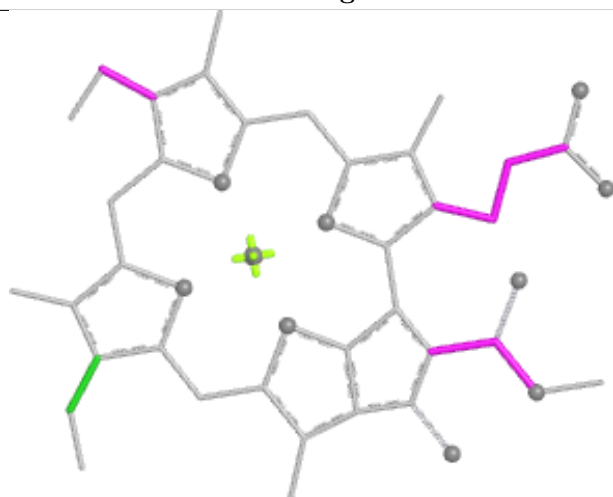
Ligand CLA s 303



Bond lengths



Bond angles

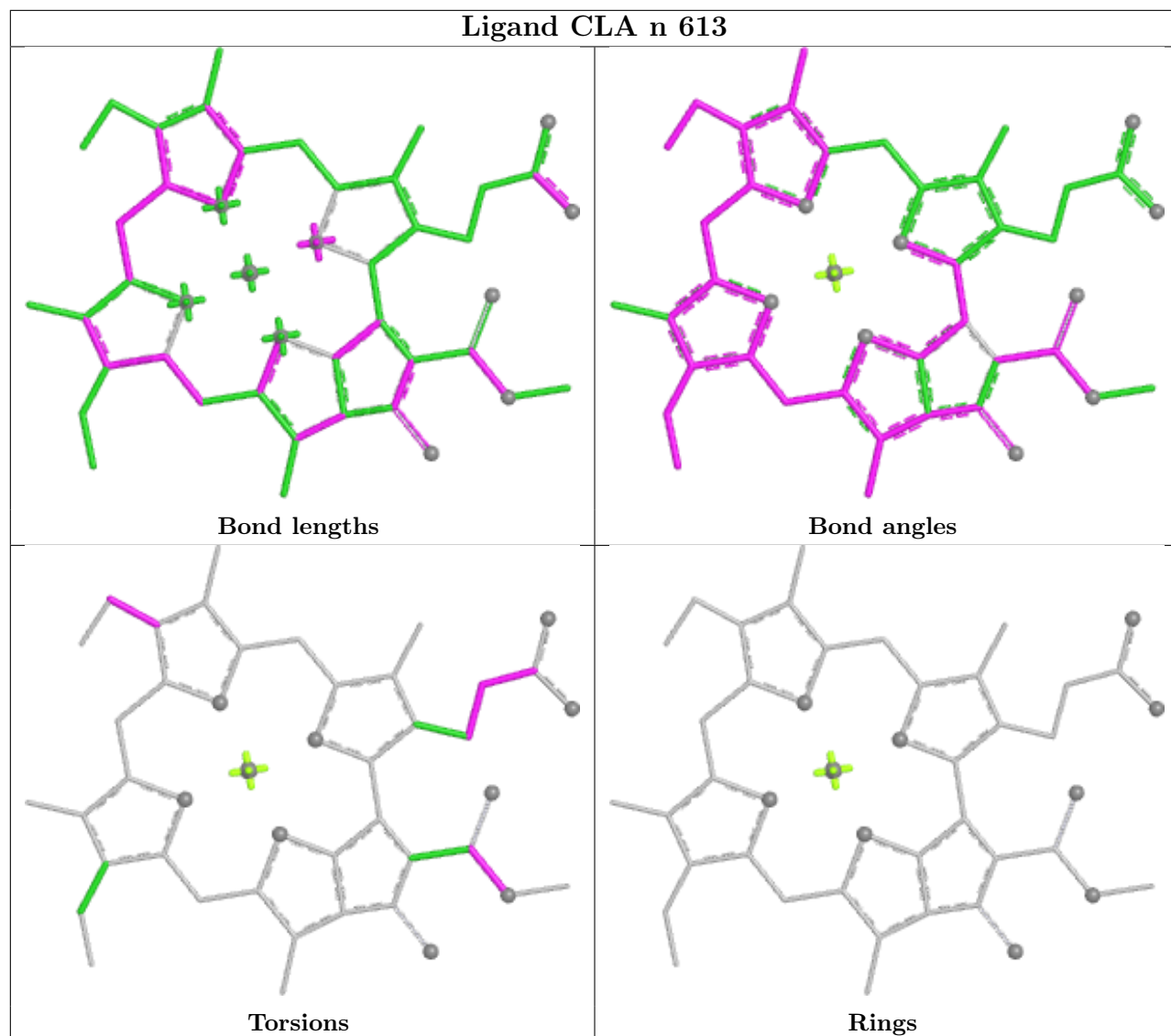


Torsions

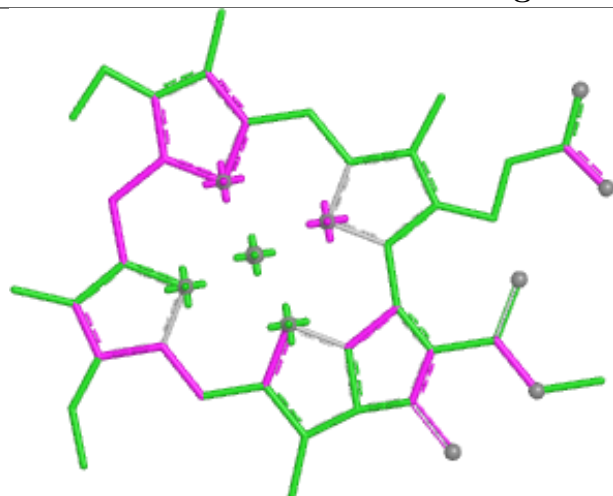


Rings

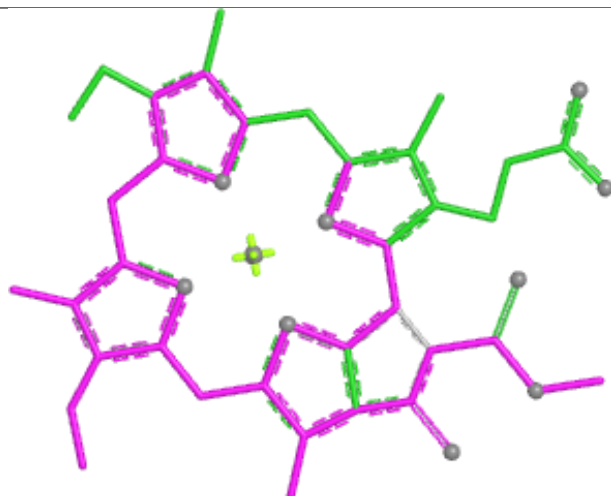
Ligand CLA n 613



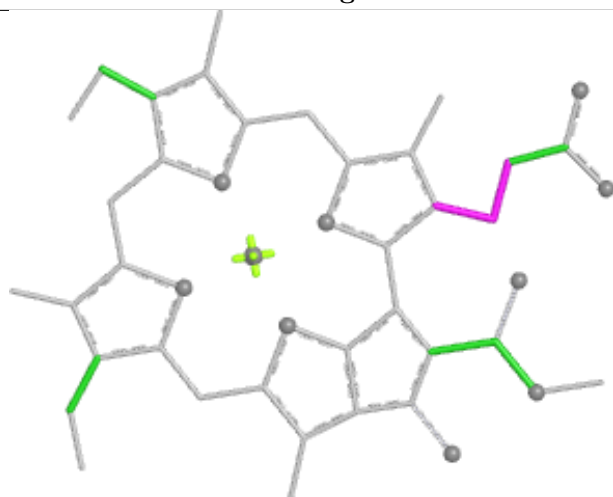
Ligand CLA A 405



Bond lengths



Bond angles

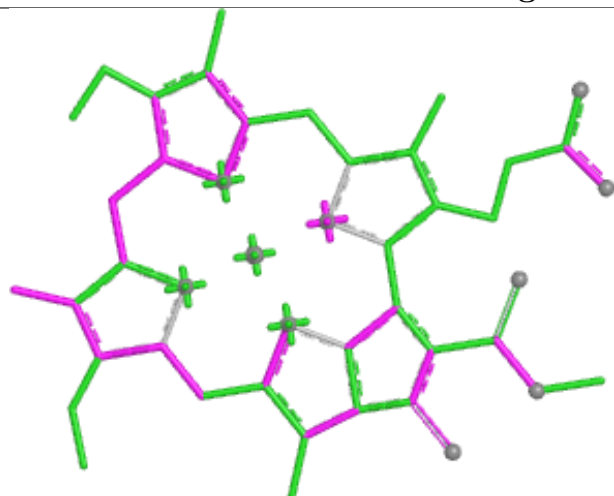


Torsions

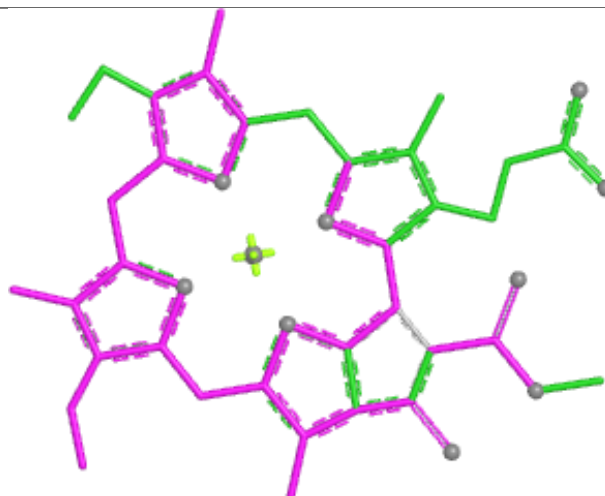


Rings

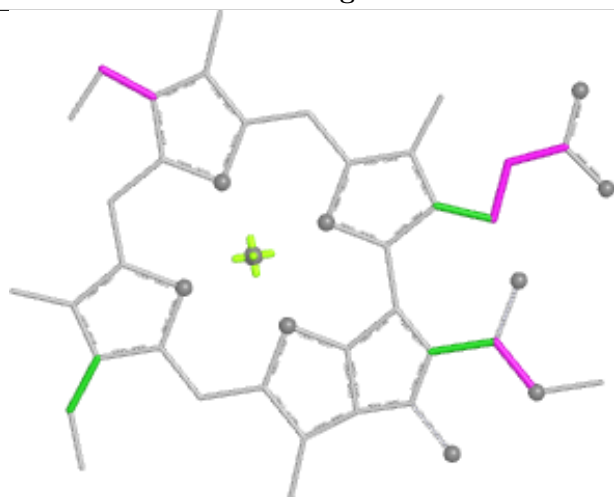
Ligand CLA 5 611



Bond lengths



Bond angles

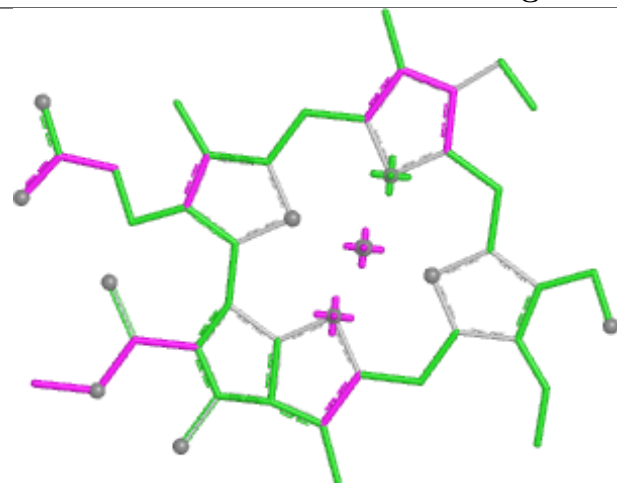


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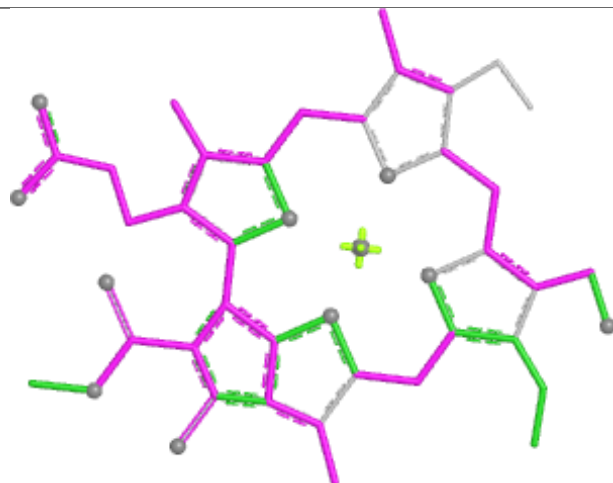


Rings

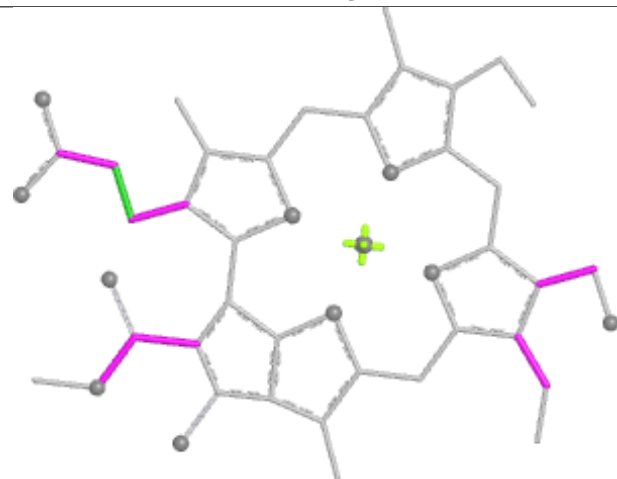
Ligand CHL 8 306



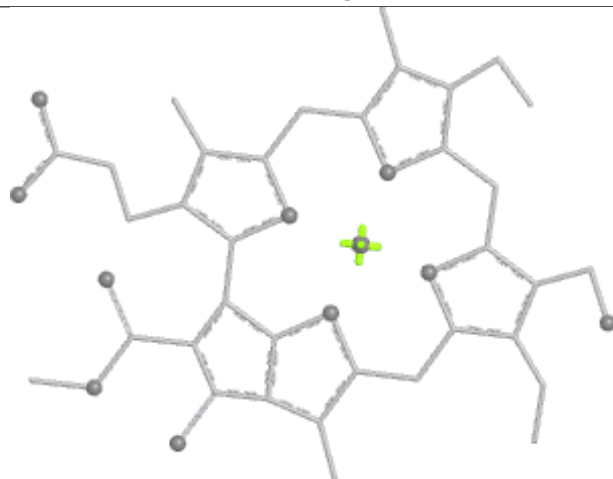
Bond lengths



Bond angles

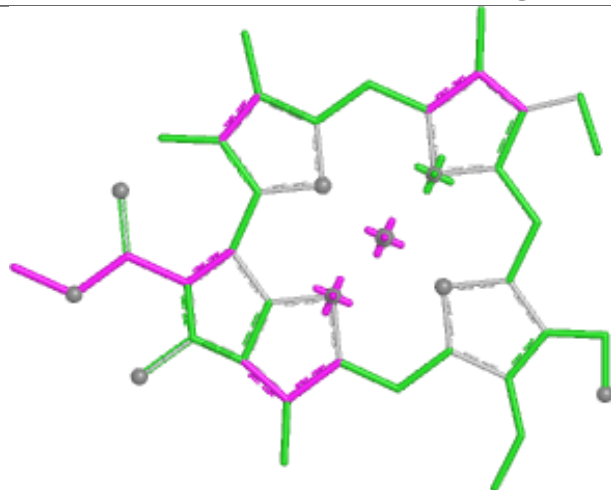


Torsions

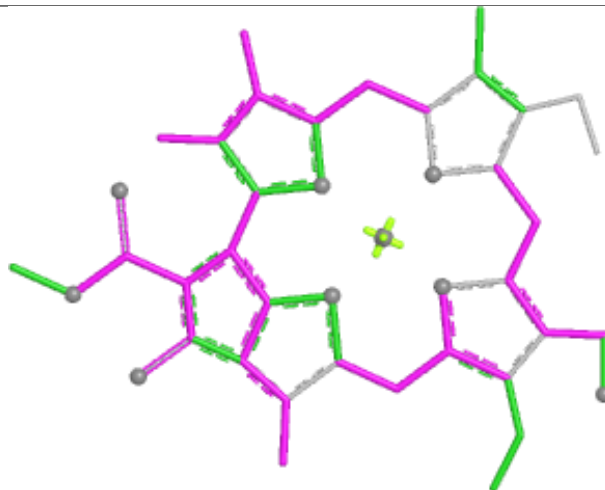


Rings

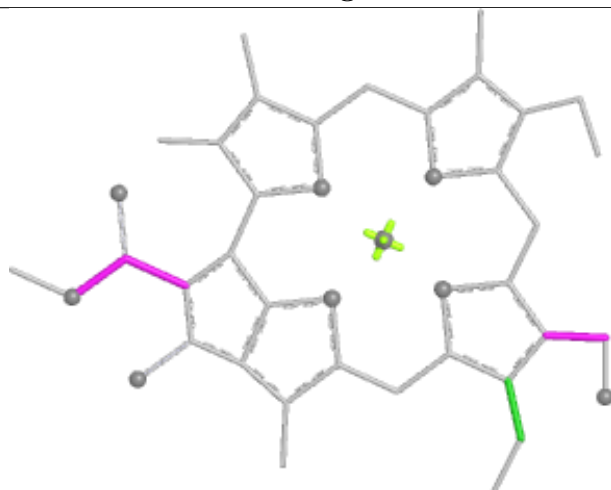
Ligand CHL Y 605



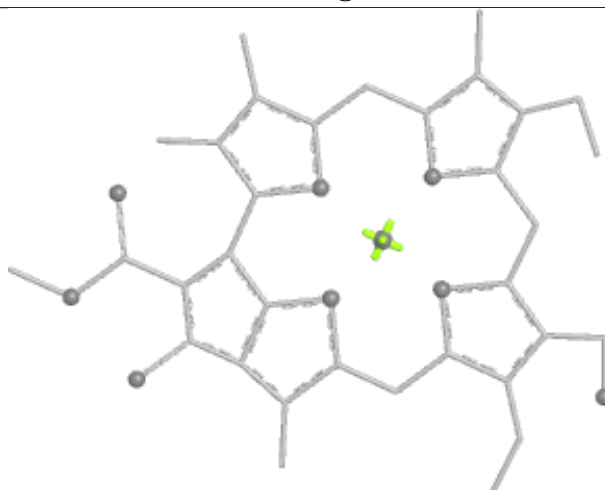
Bond lengths



Bond angles

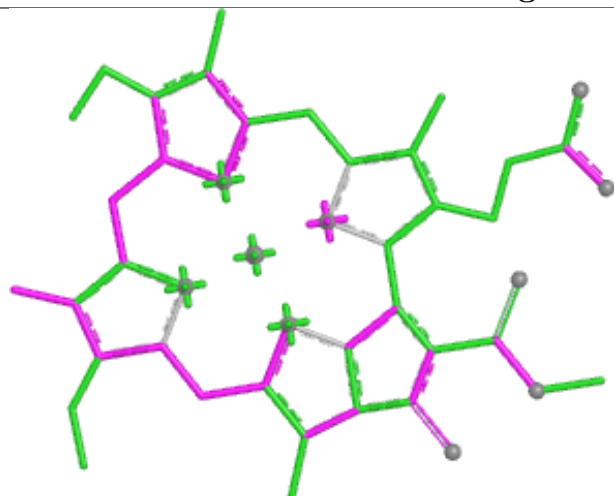


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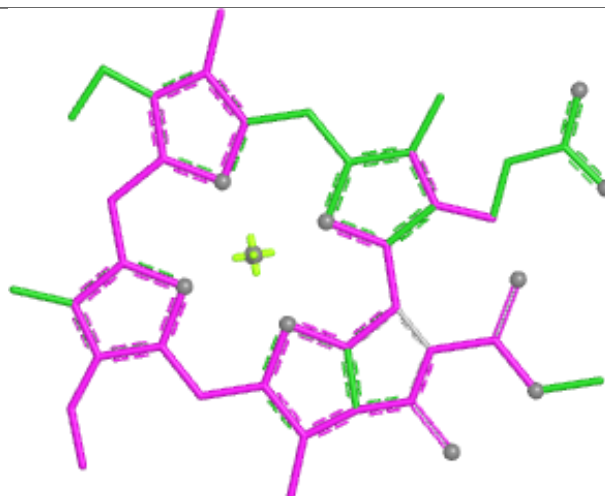


Rings

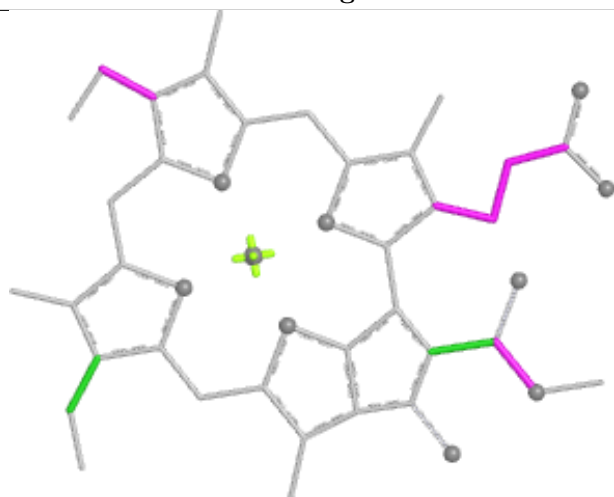
Ligand CLA 4 303



Bond lengths



Bond angles

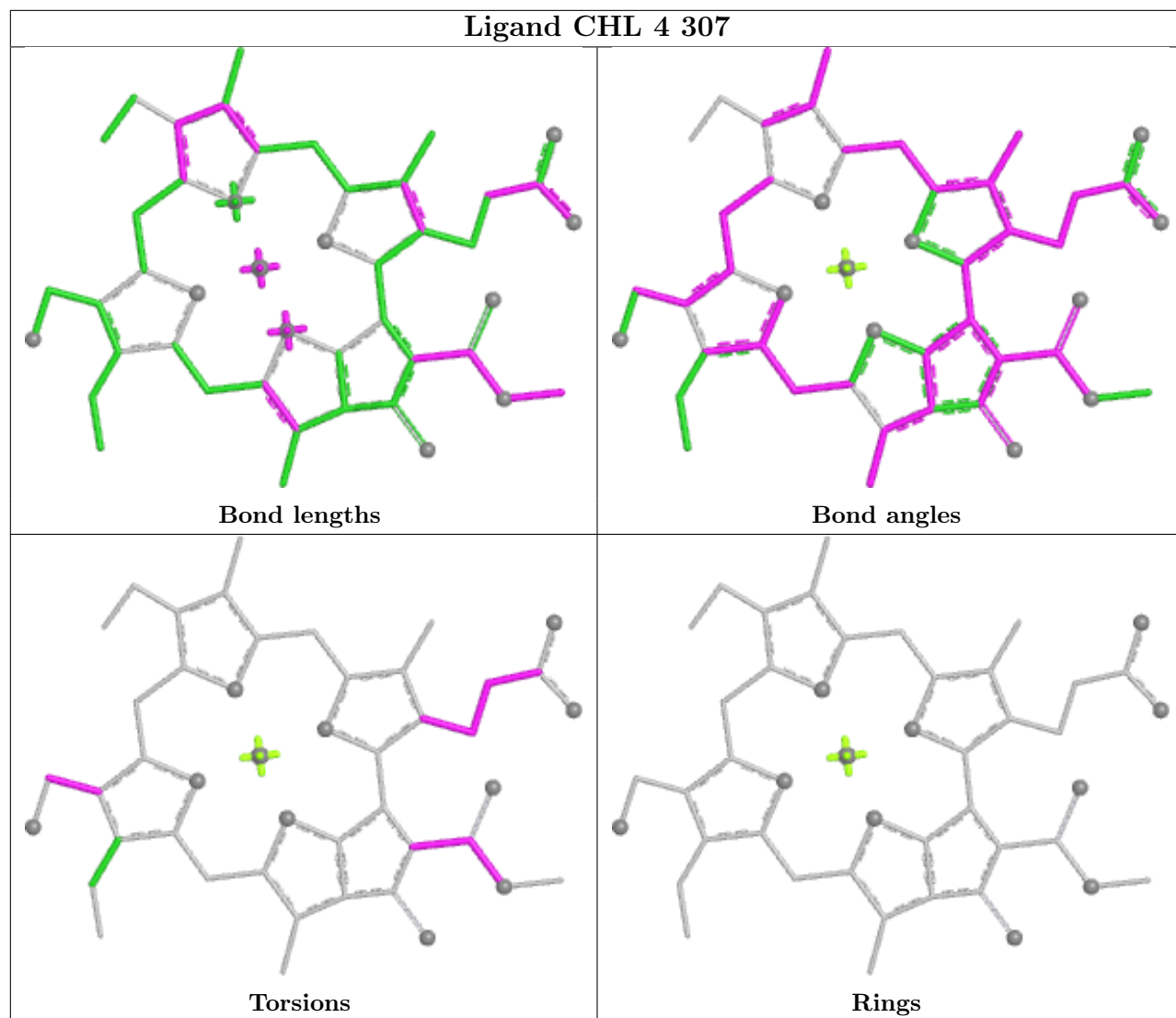


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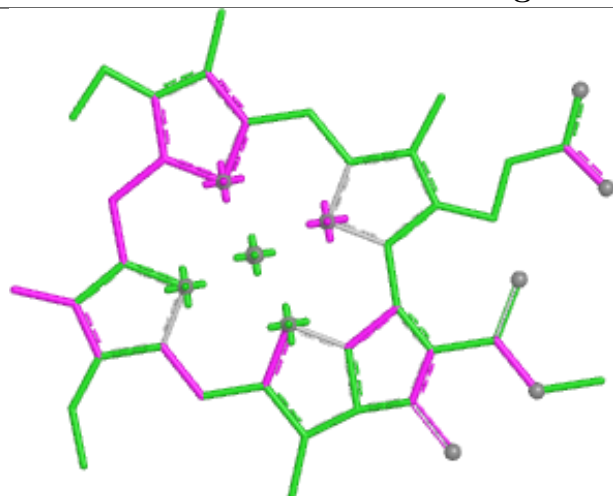


Rings

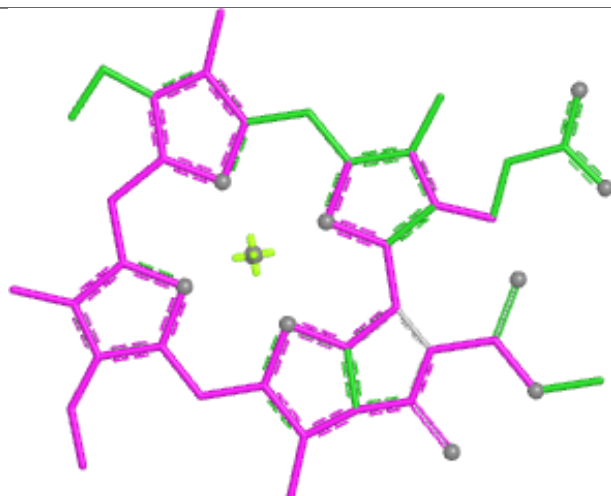
Ligand CHL 4 307



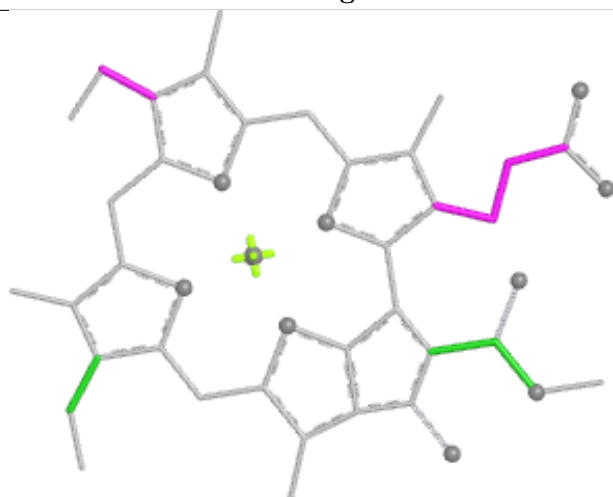
Ligand CLA Y 604



Bond lengths



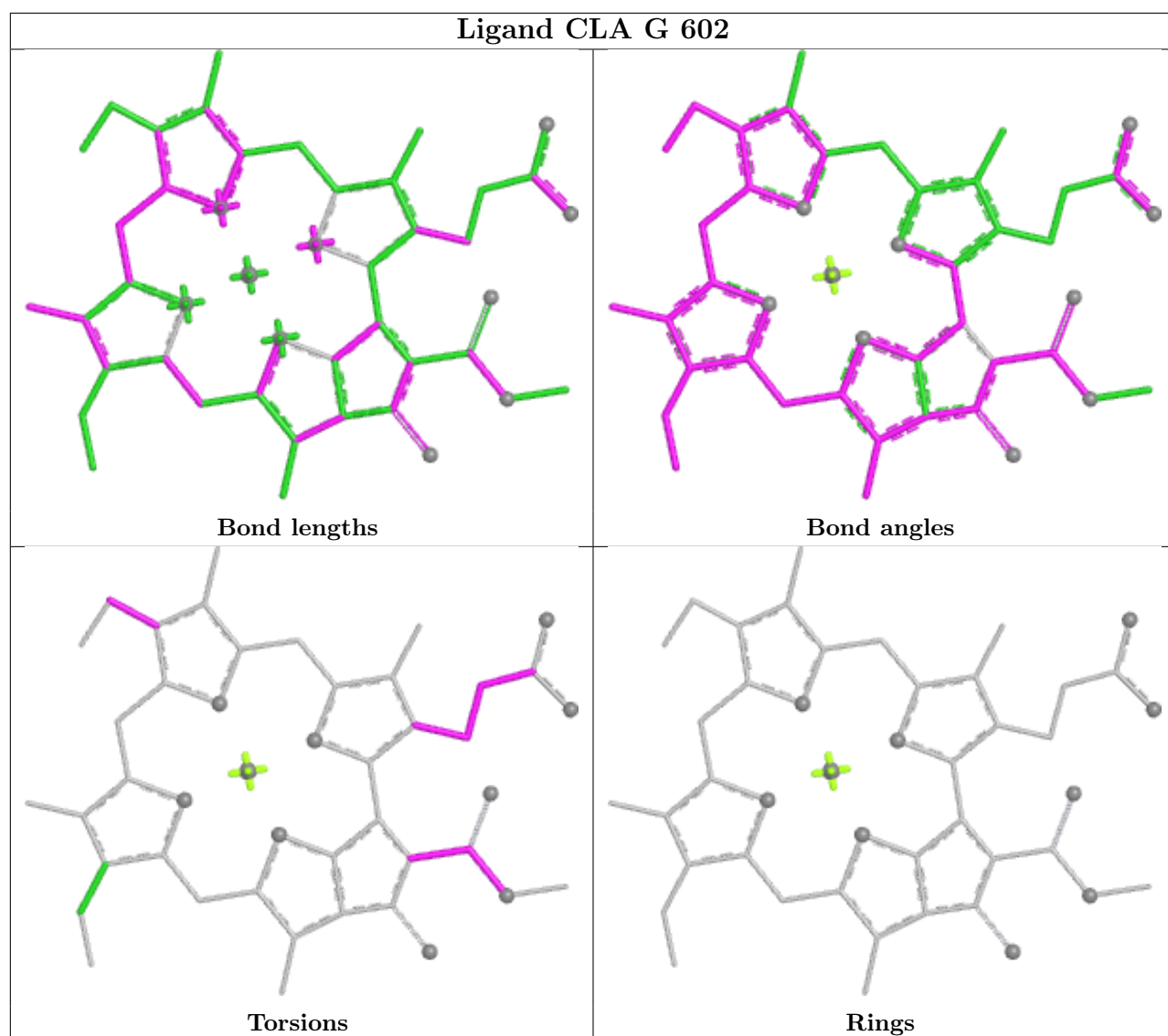
Bond angles



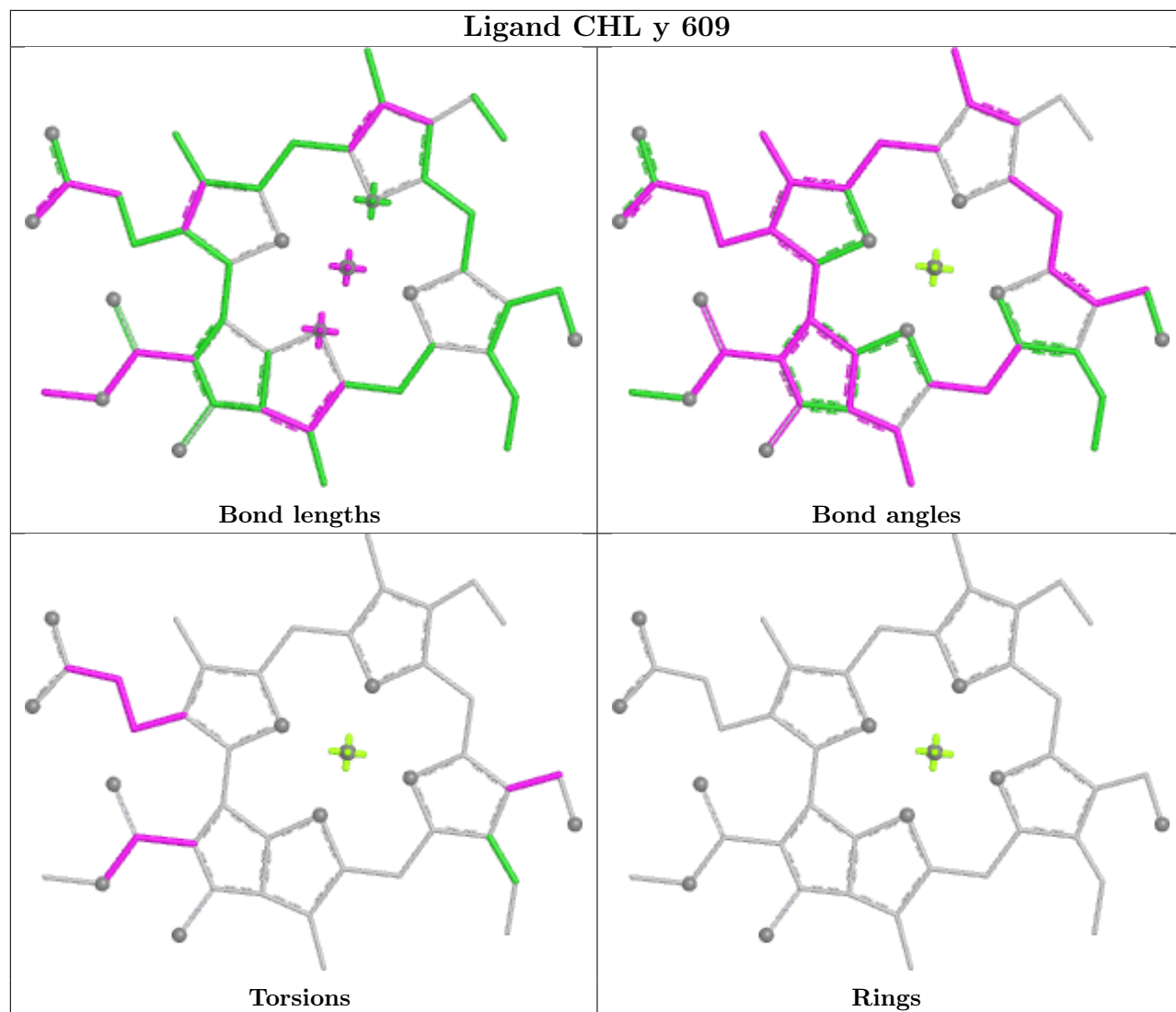
Torsions



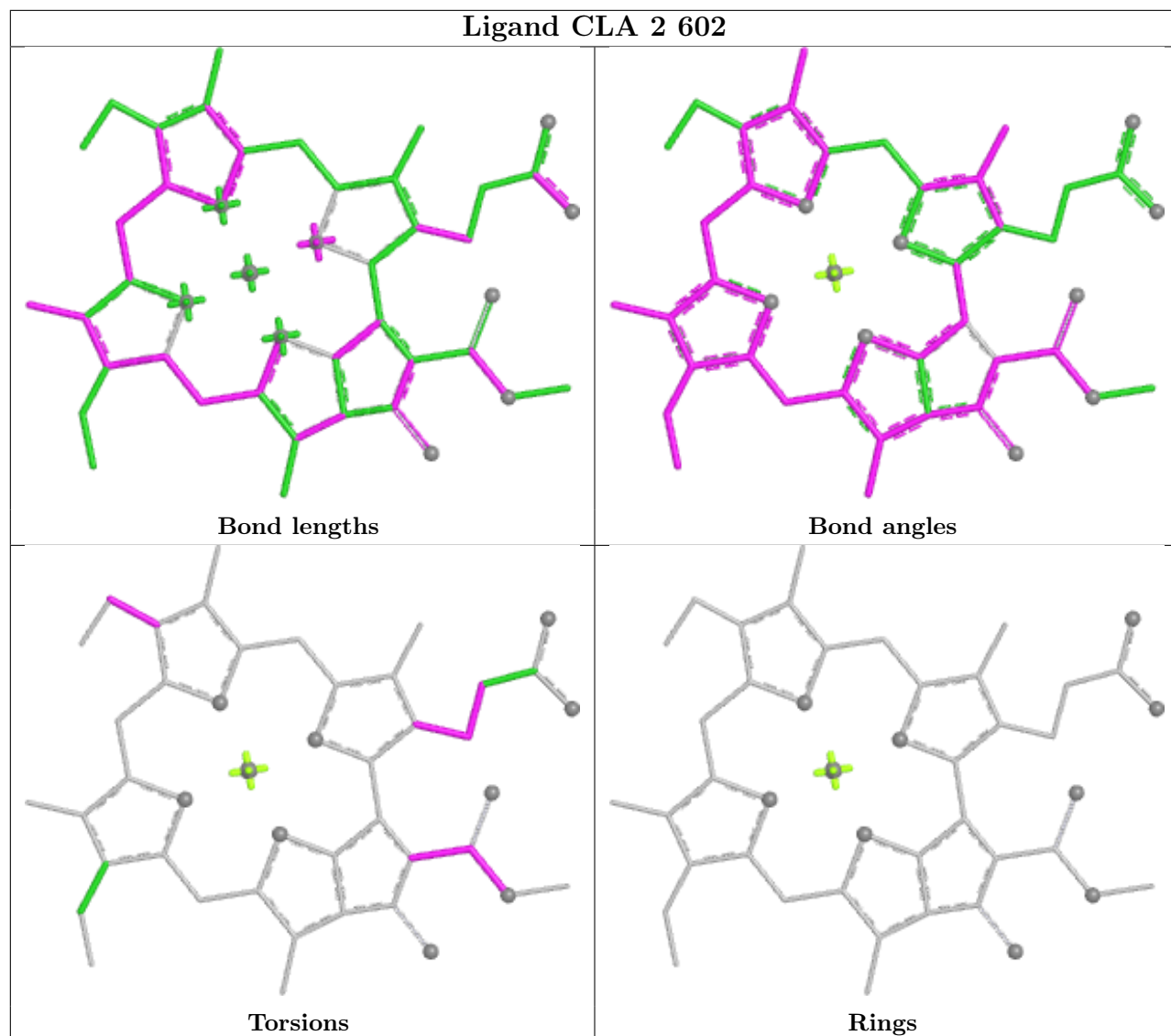
Rings



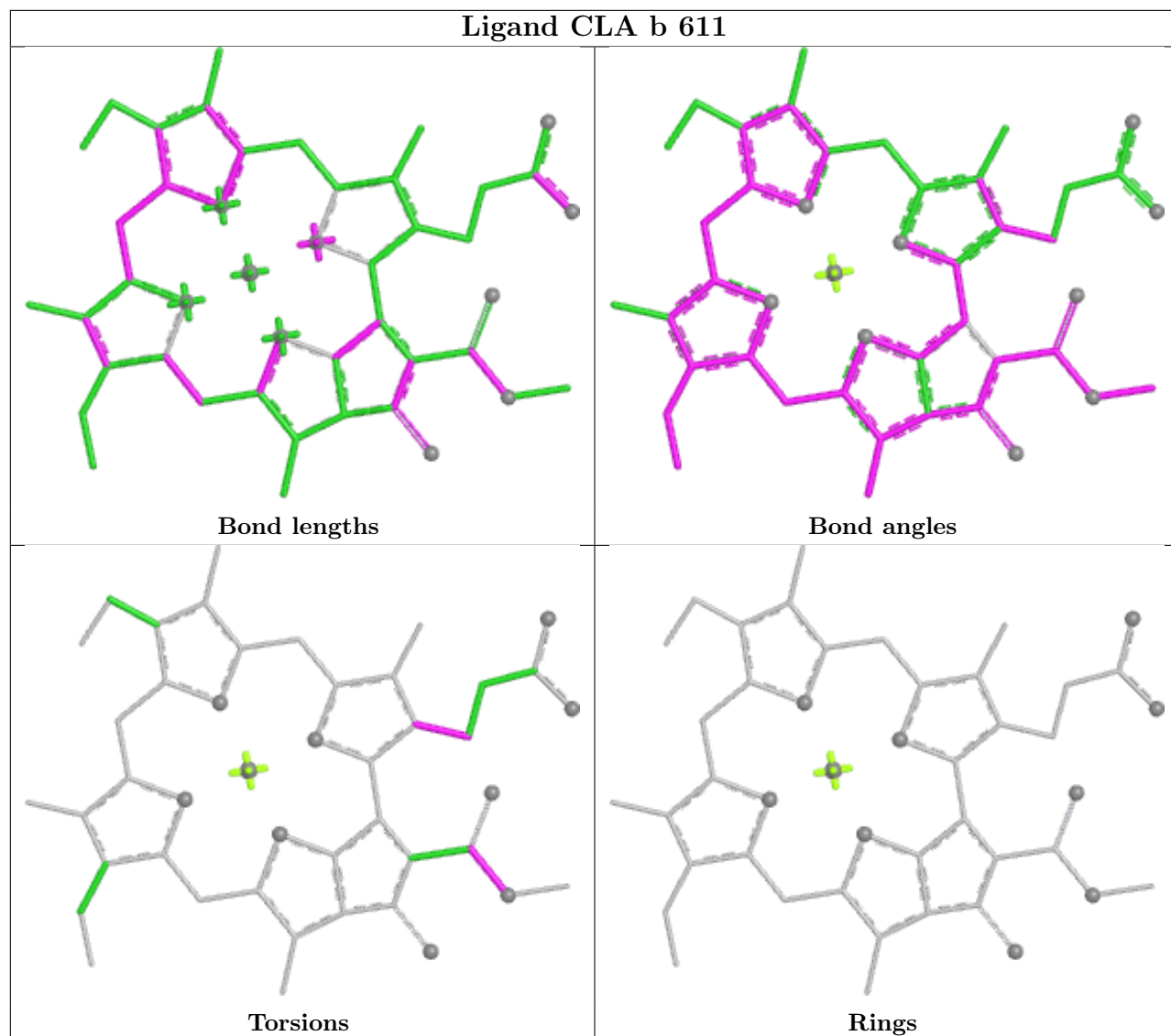
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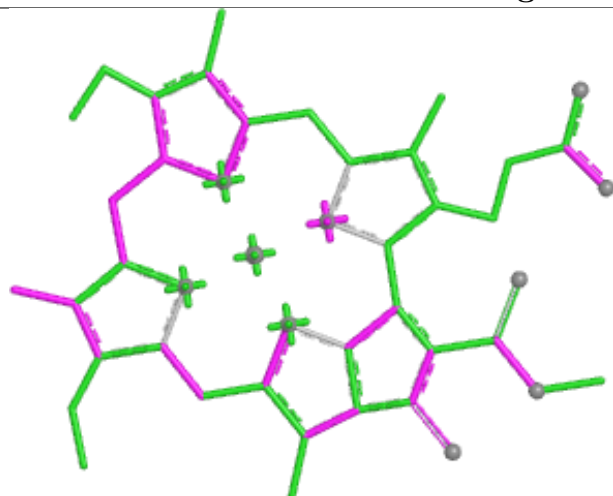
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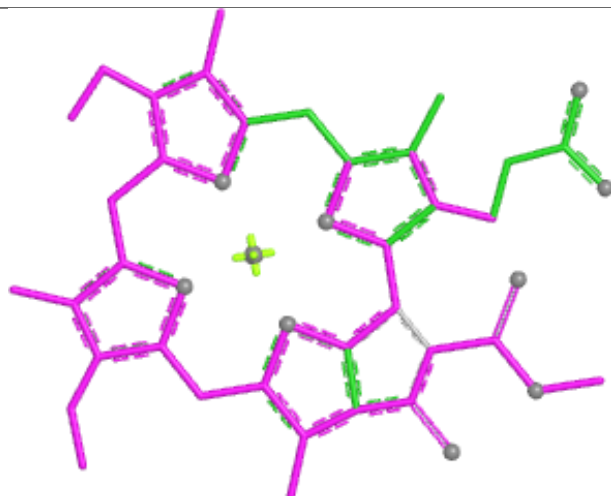
Ligand CLA b 611



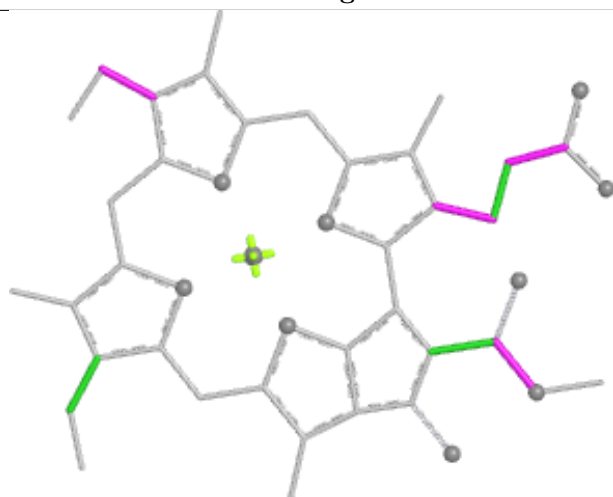
Ligand CLA S 312



Bond lengths



Bond angles

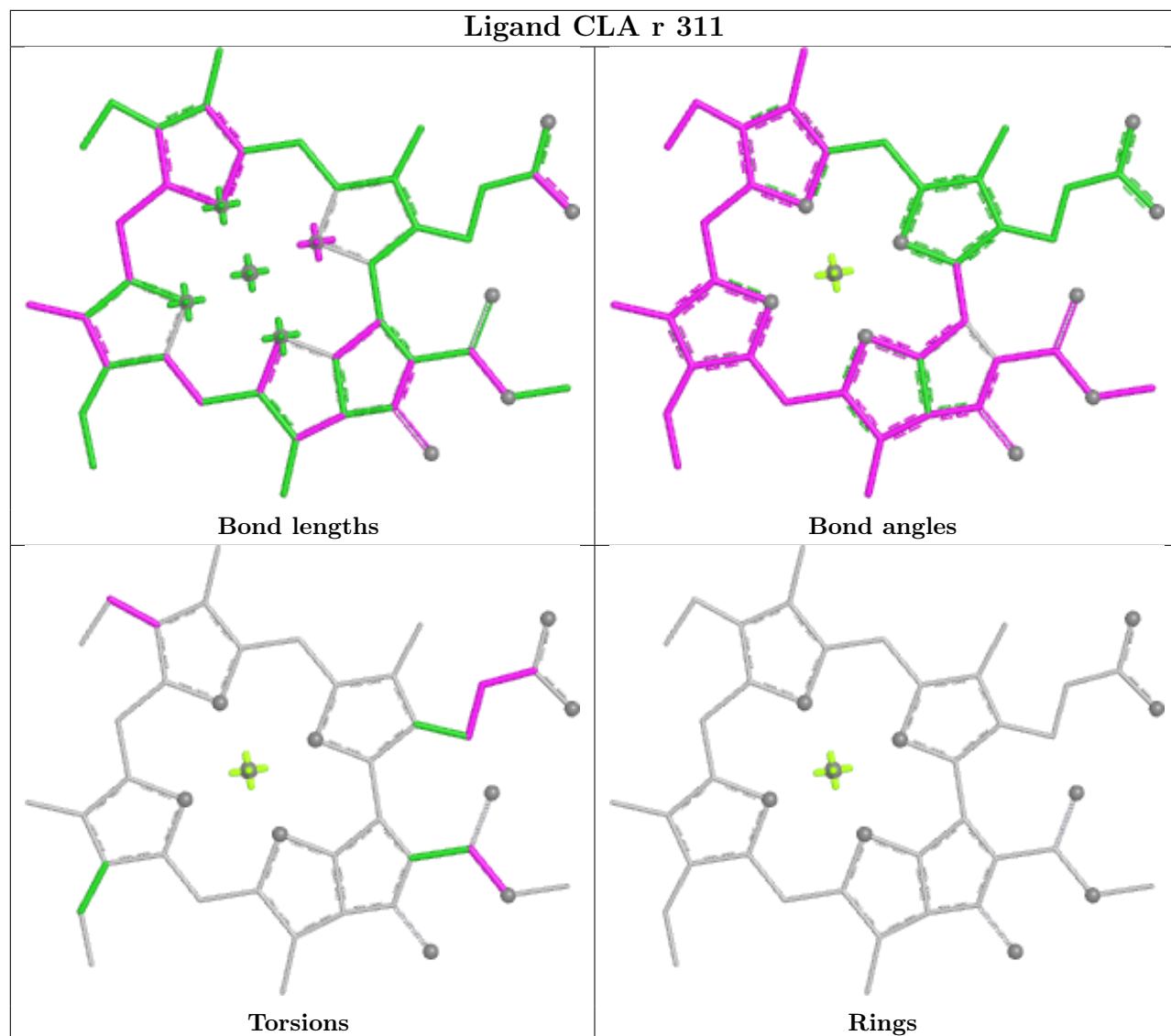


Torsions

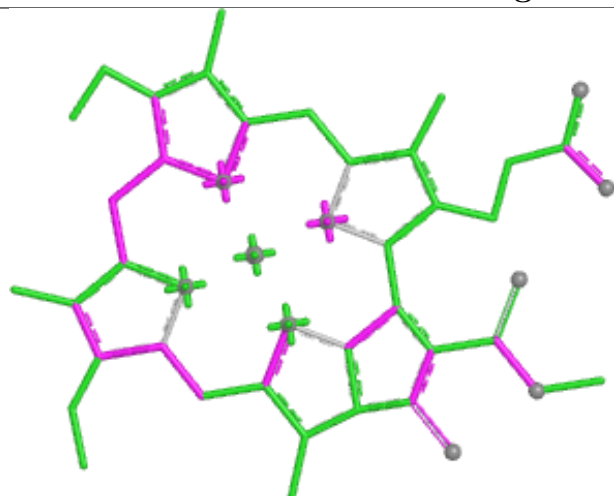


Rings

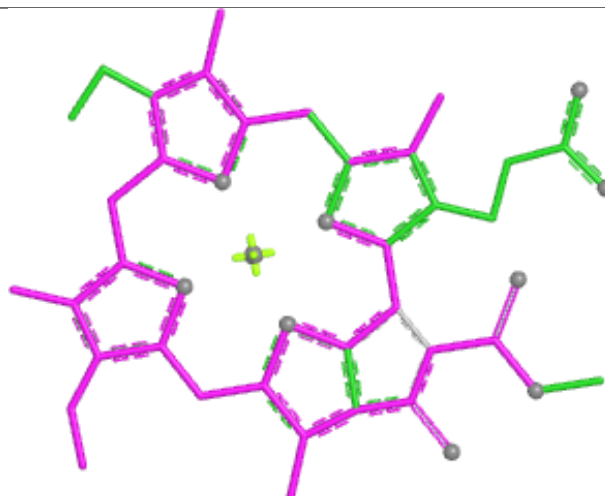
Ligand CLA r 311



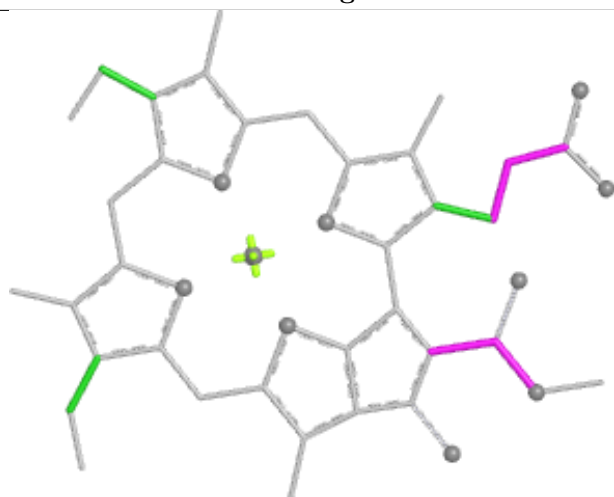
Ligand CLA B 603



Bond lengths



Bond angles

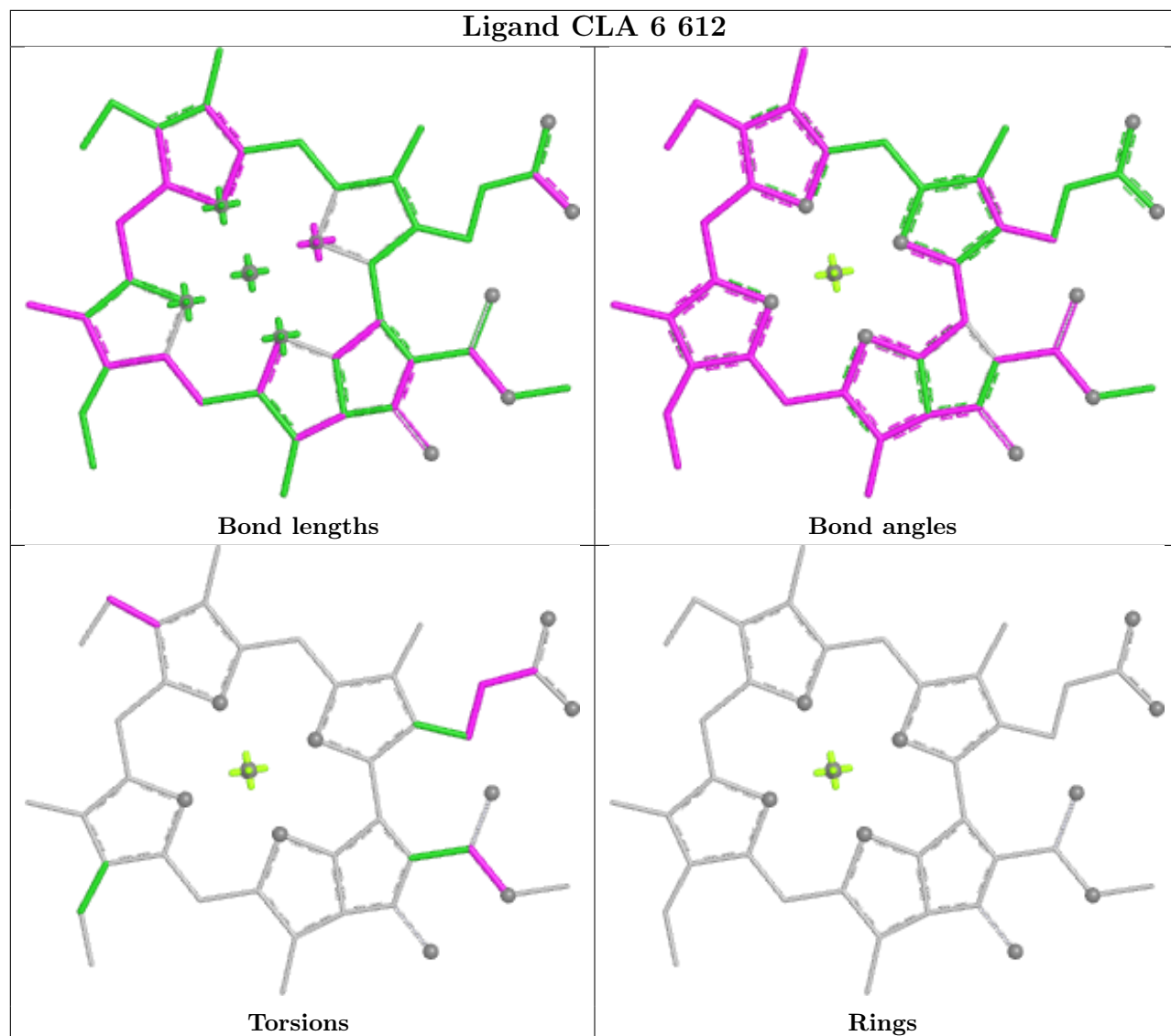


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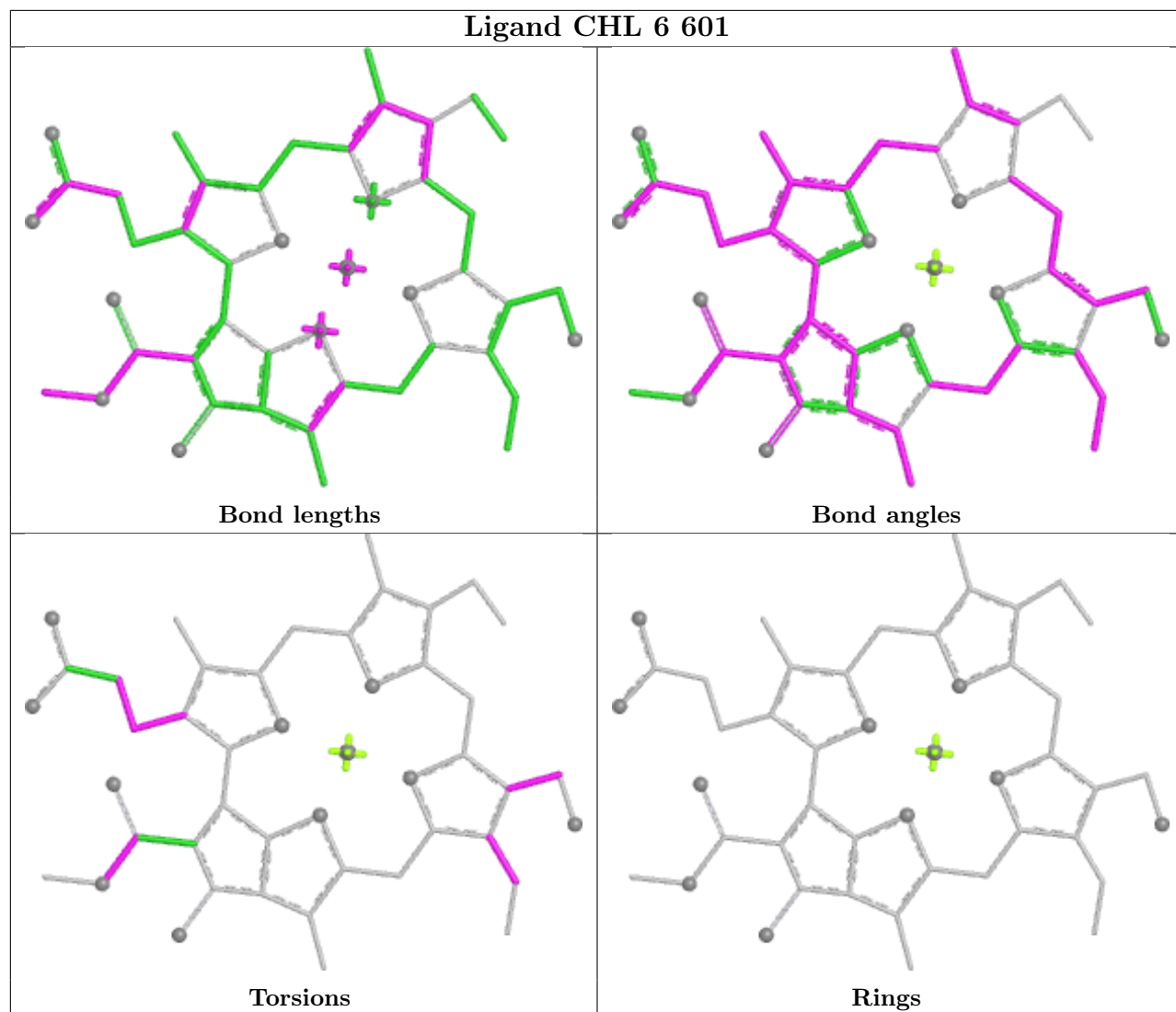


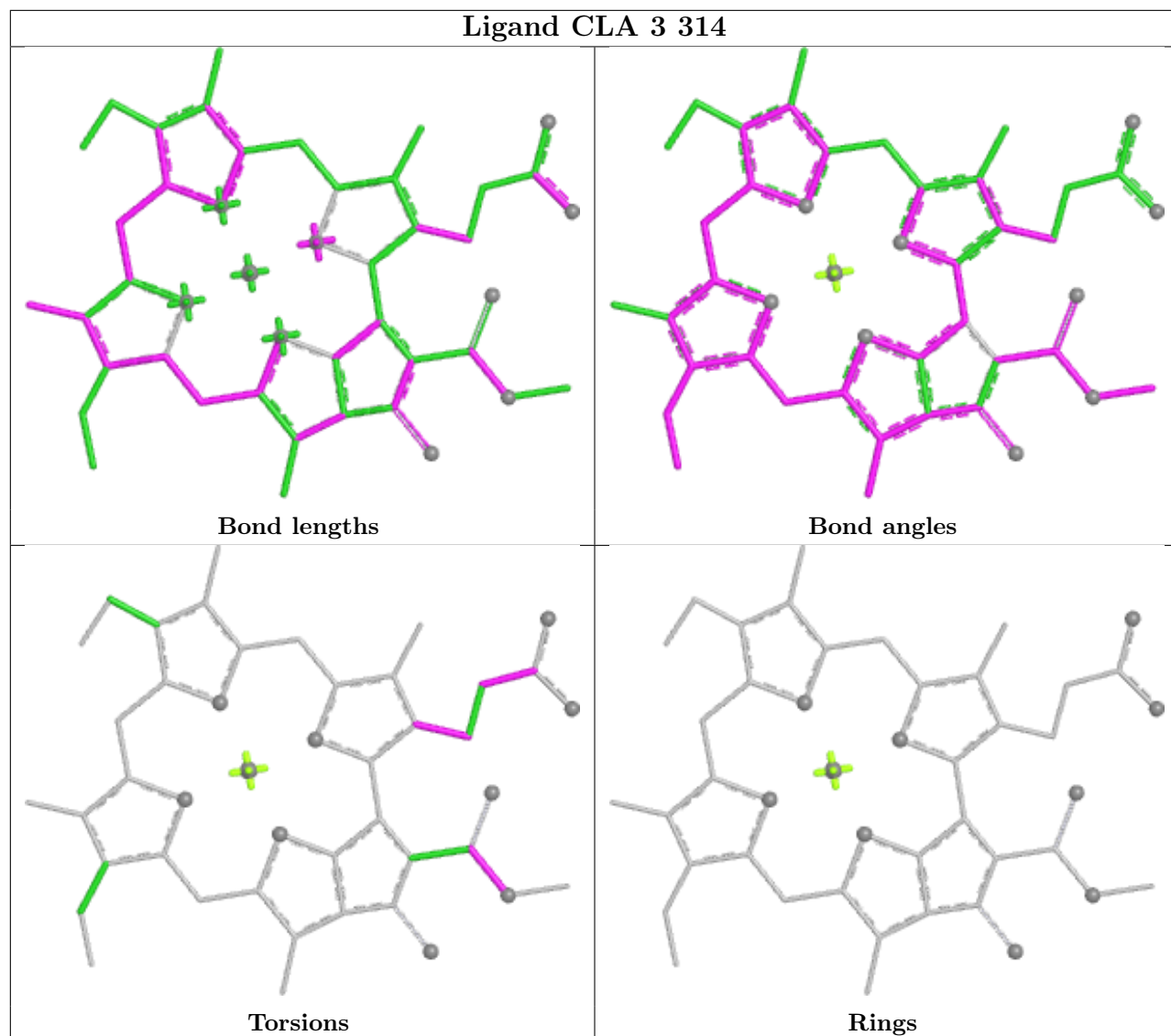
Rings

Ligand CLA 6 612

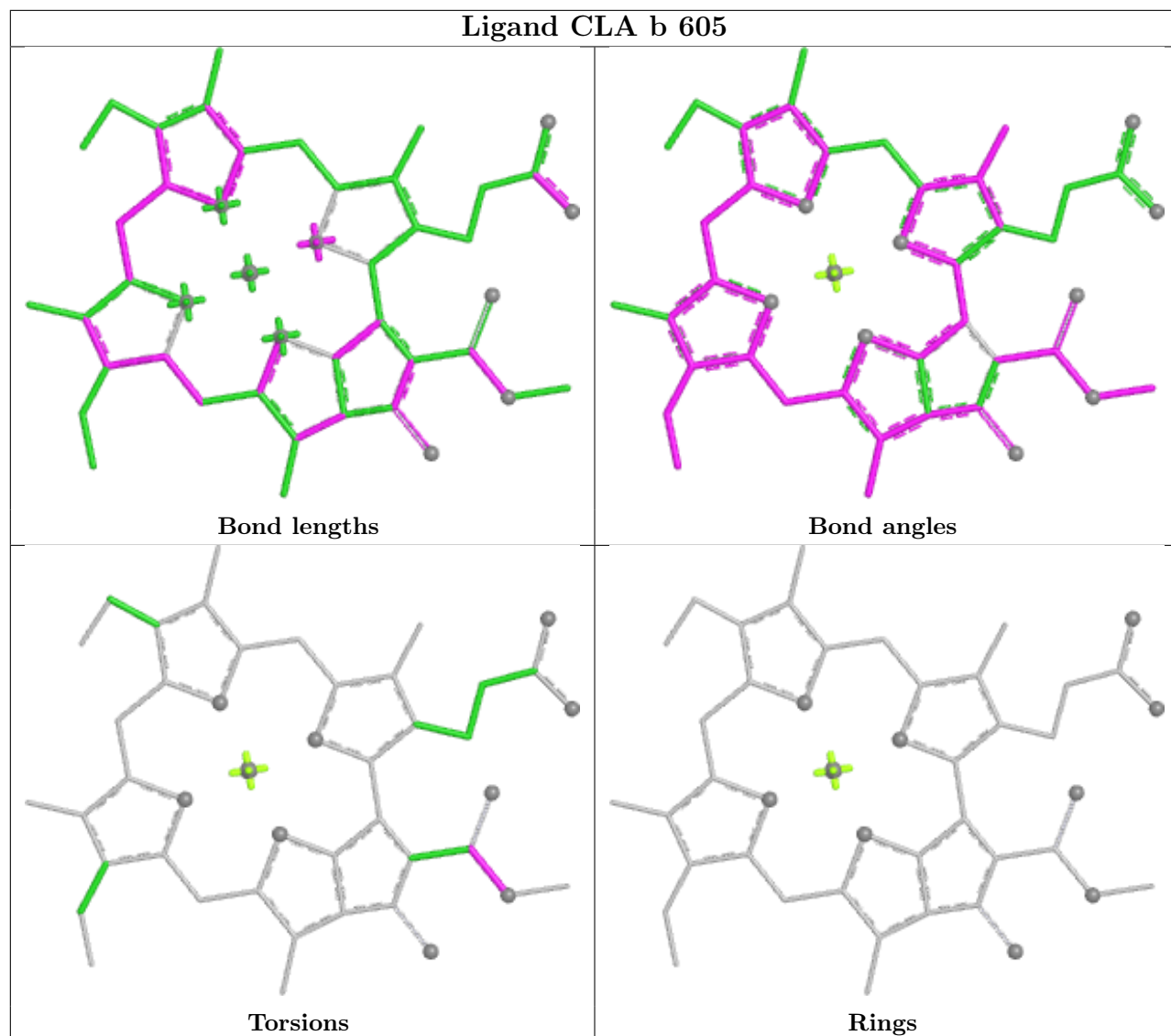


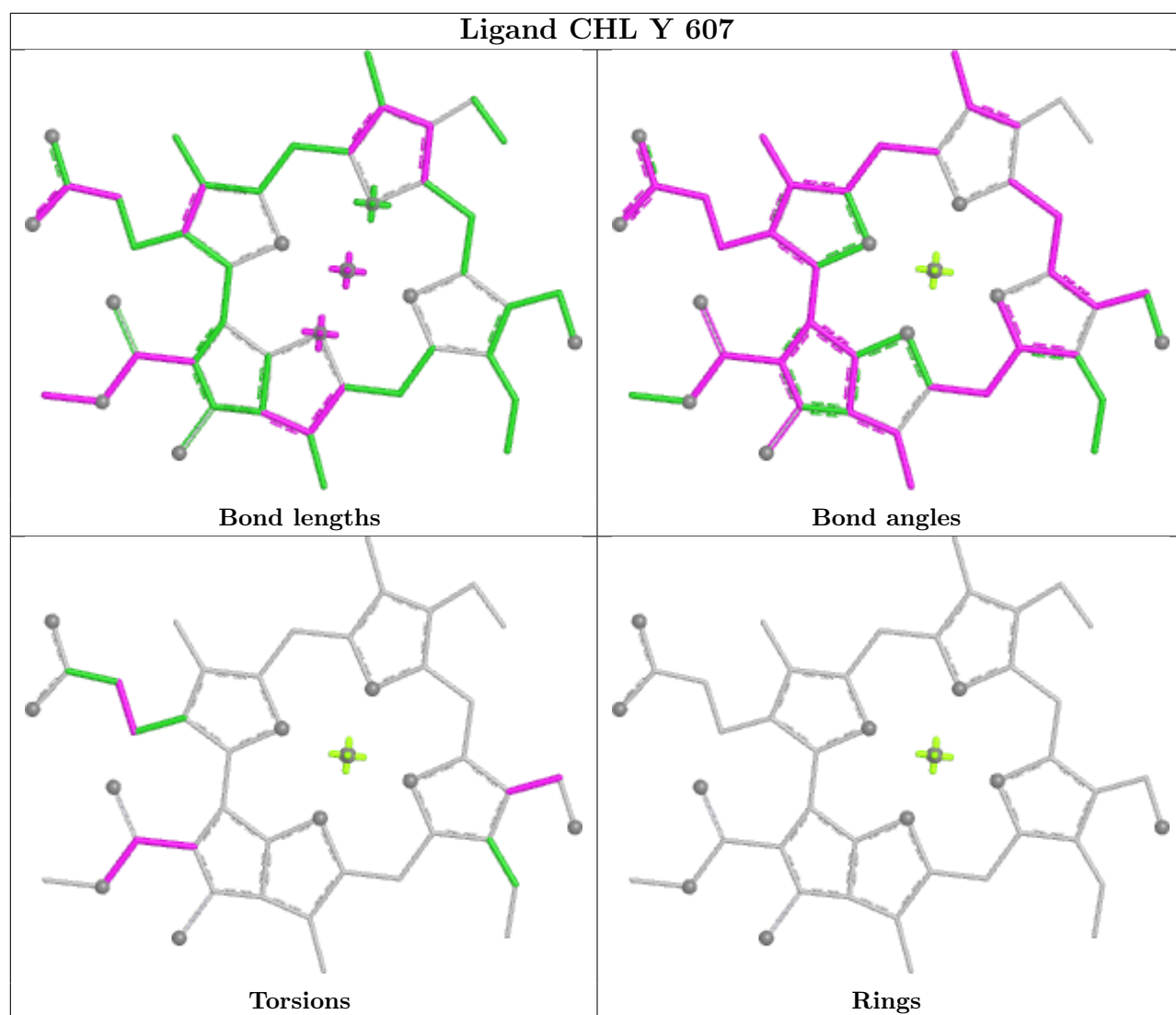
Ligand CHL 6 601



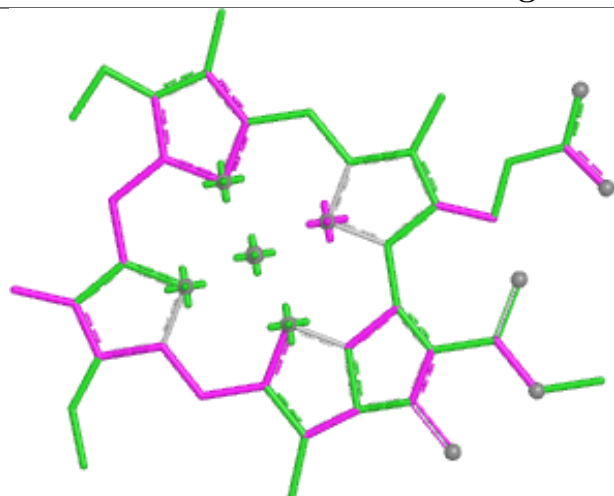


Ligand CLA b 605

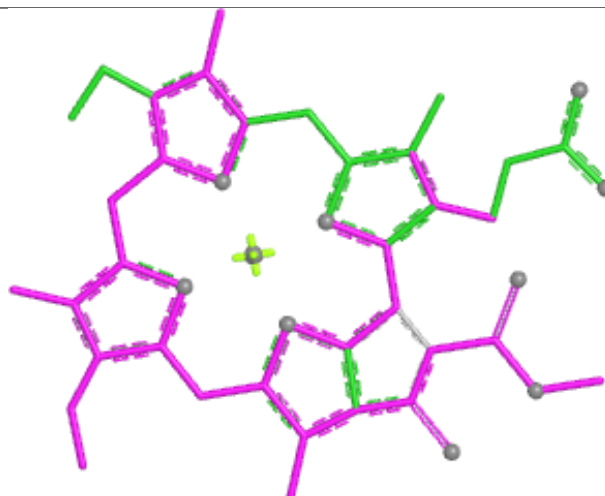




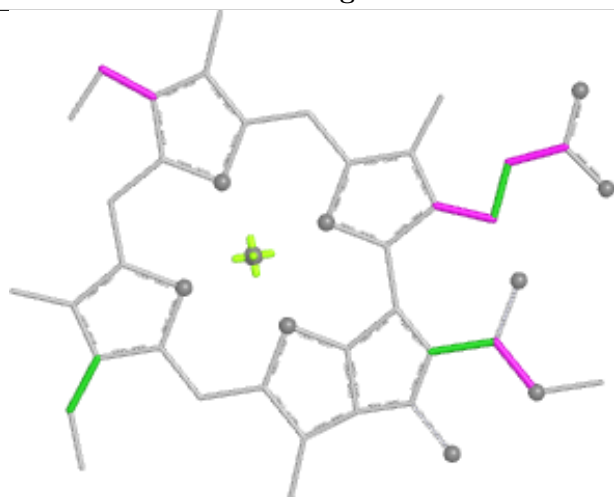
Ligand CLA 5 614



Bond lengths



Bond angles

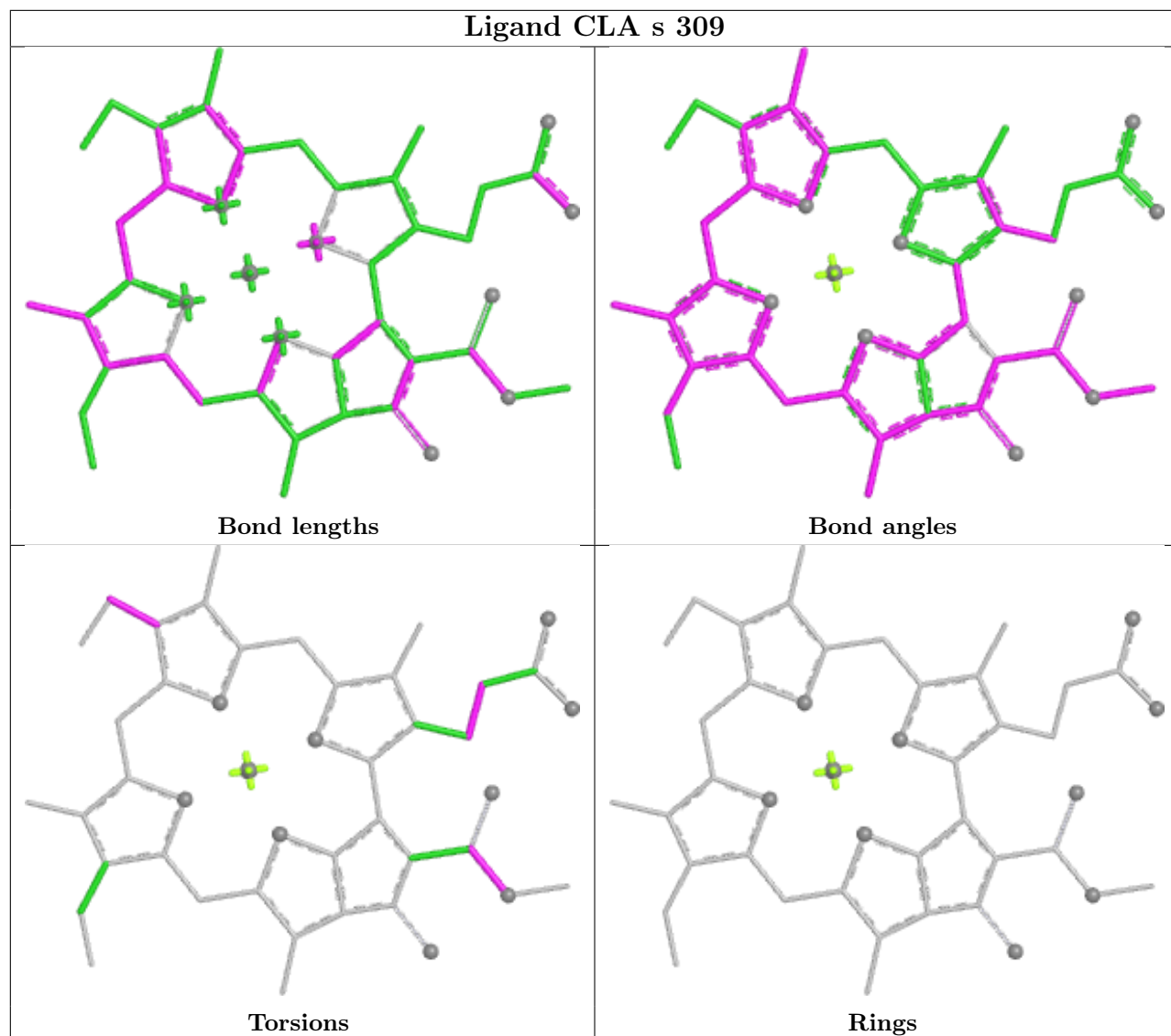


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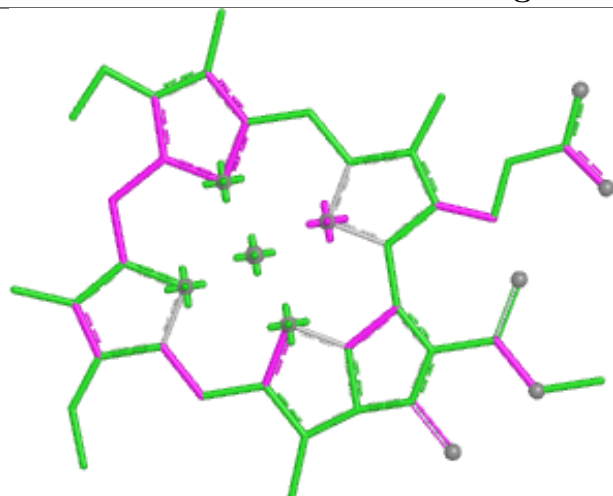


Rings

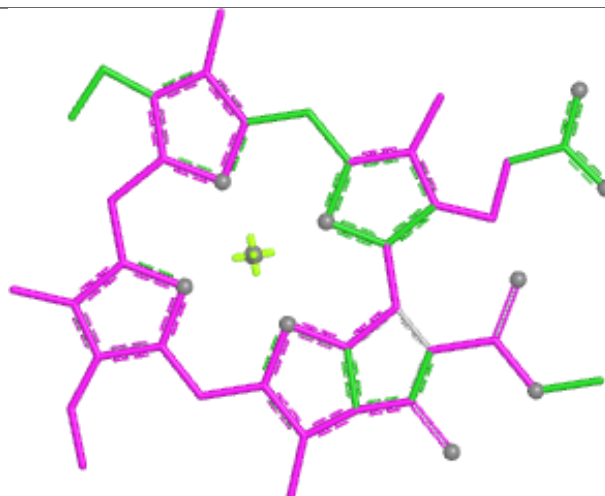
Ligand CLA s 309



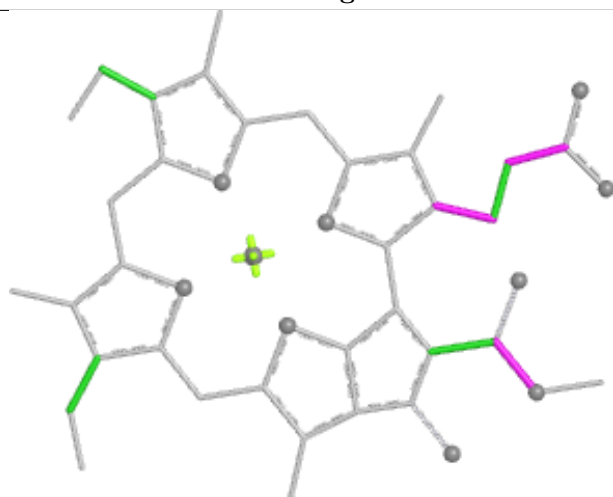
Ligand CLA R 308



Bond lengths



Bond angles

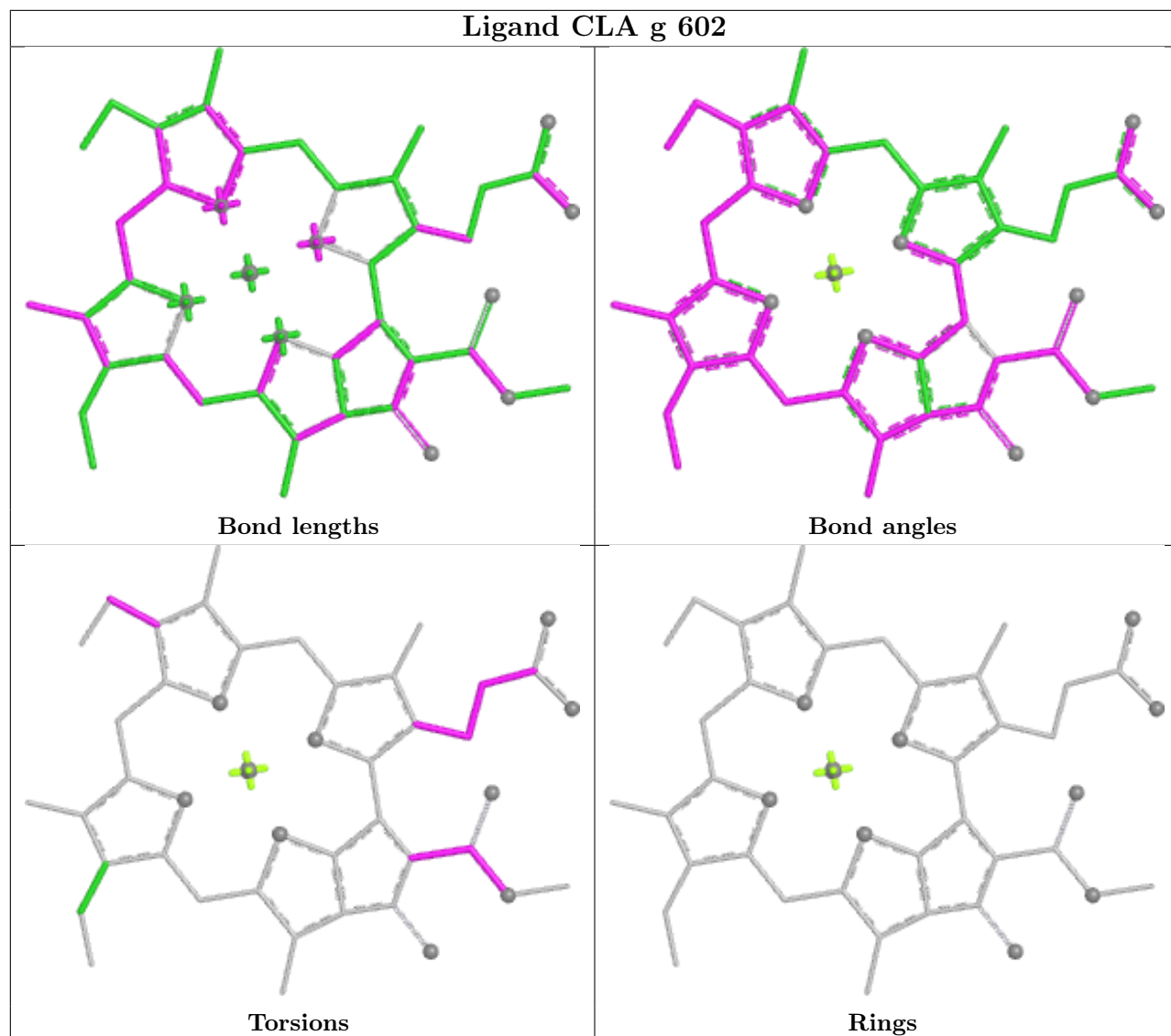


Torsions

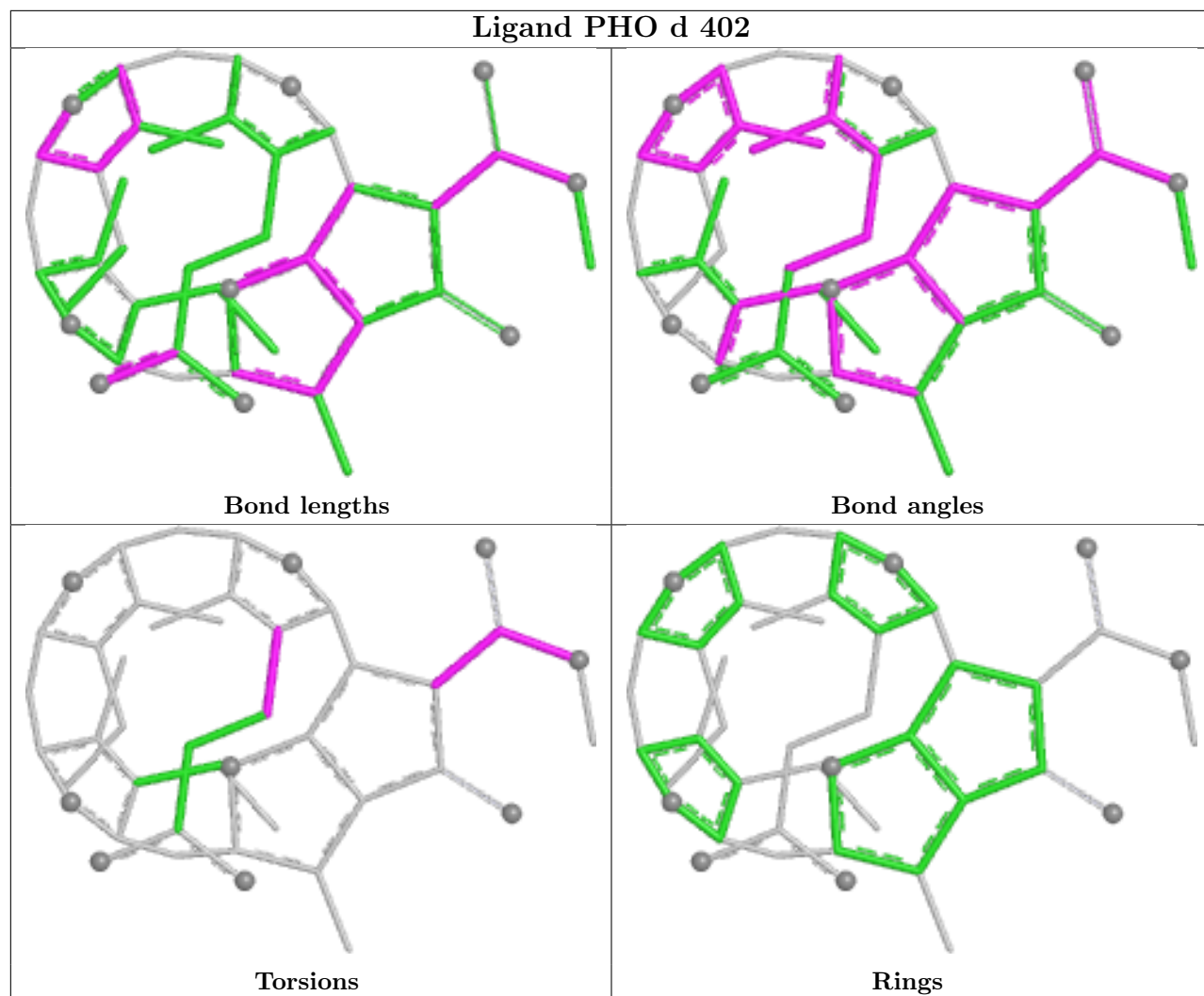


Rings

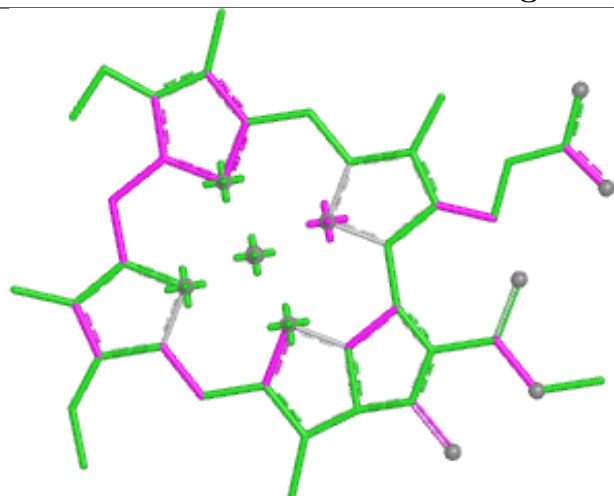
Ligand CLA g 602



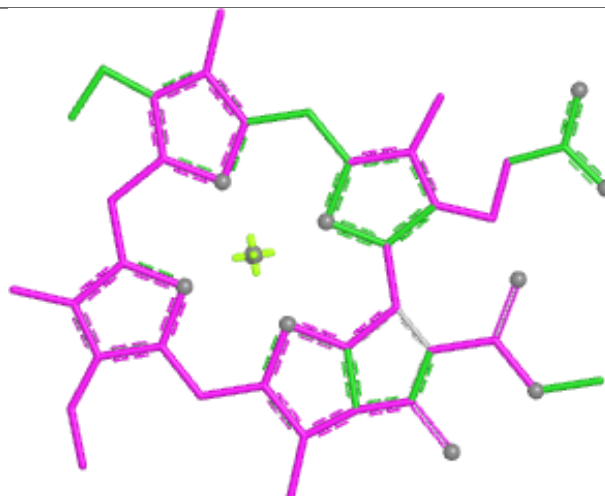
Ligand PHO d 402



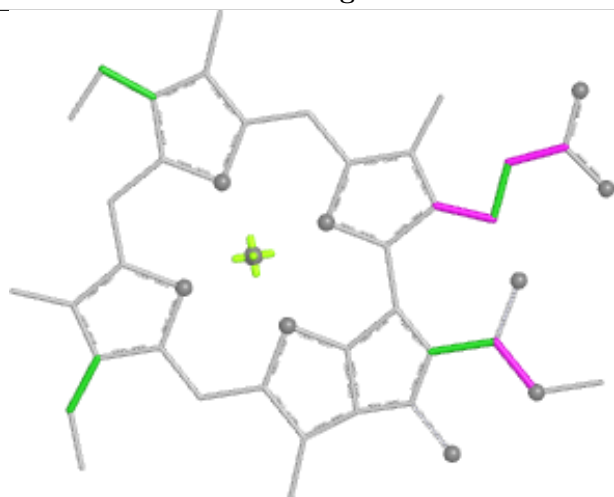
Ligand CLA r 308



Bond lengths



Bond angles

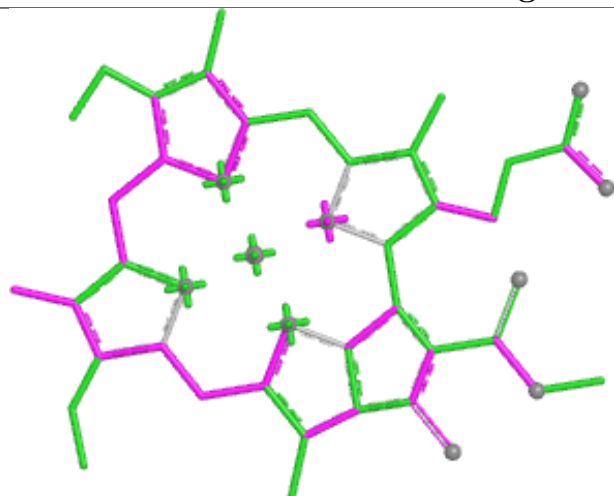


Torsions

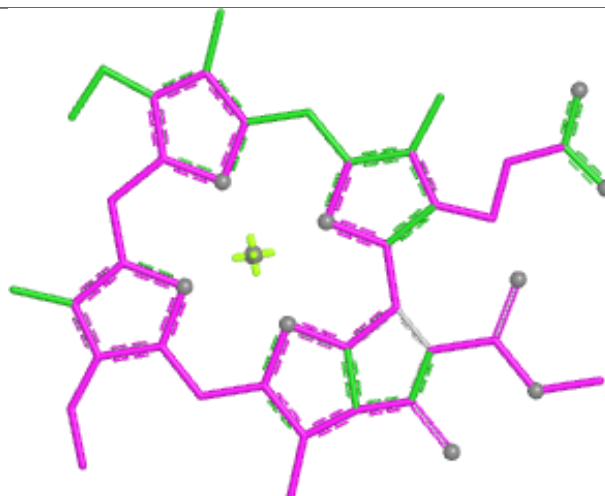


Rings

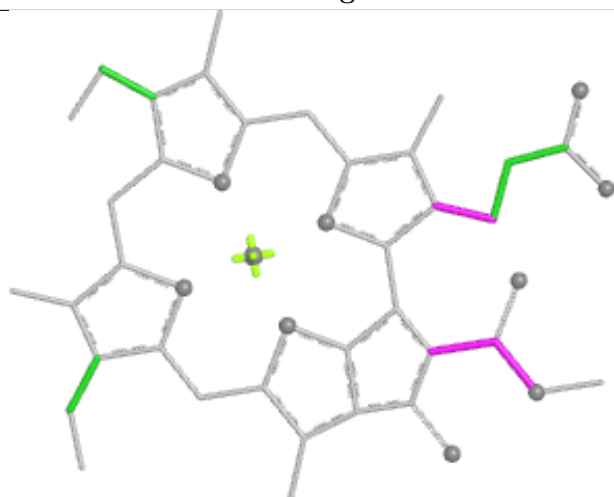
Ligand CLA 8 304



Bond lengths



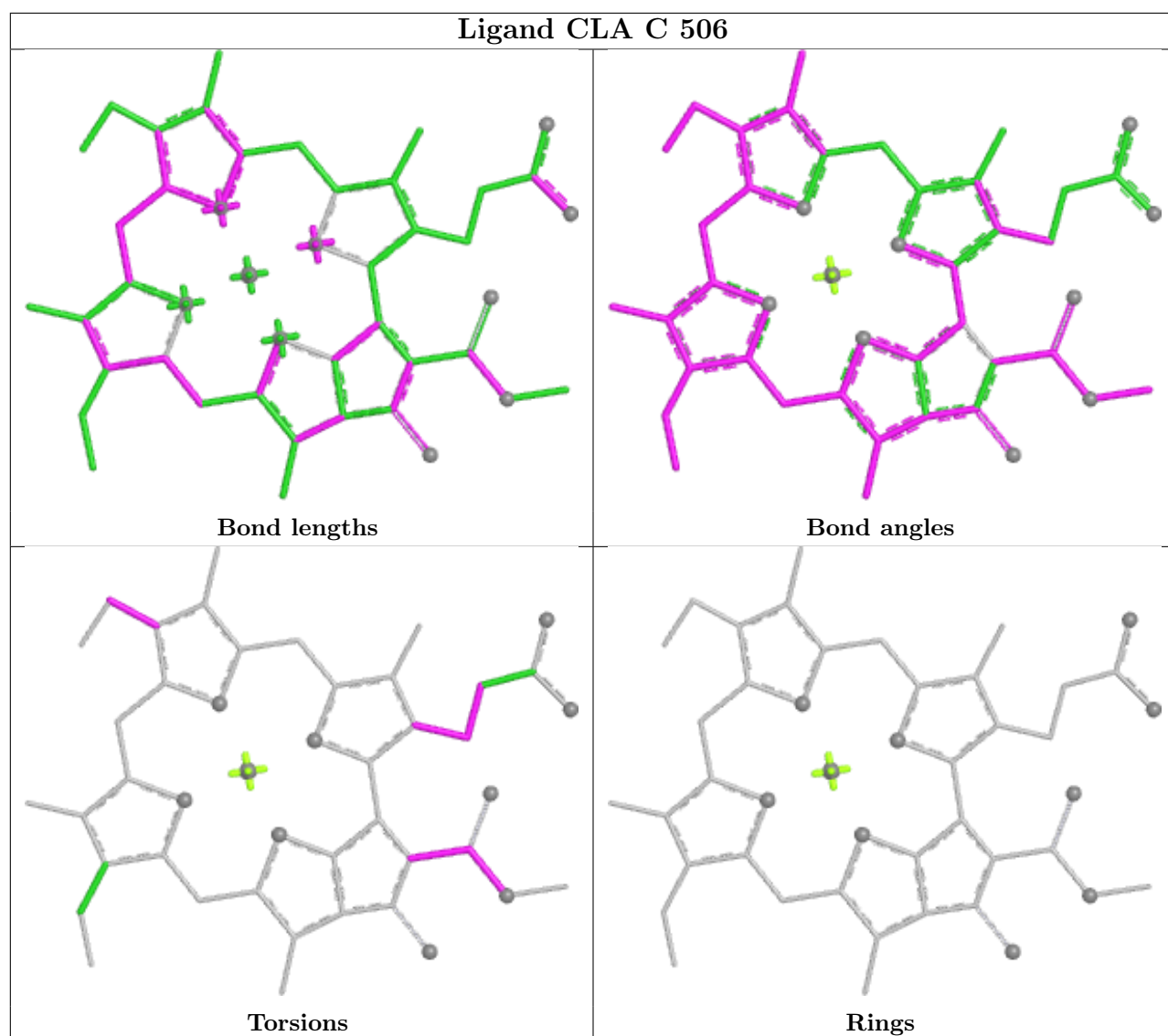
Bond angles

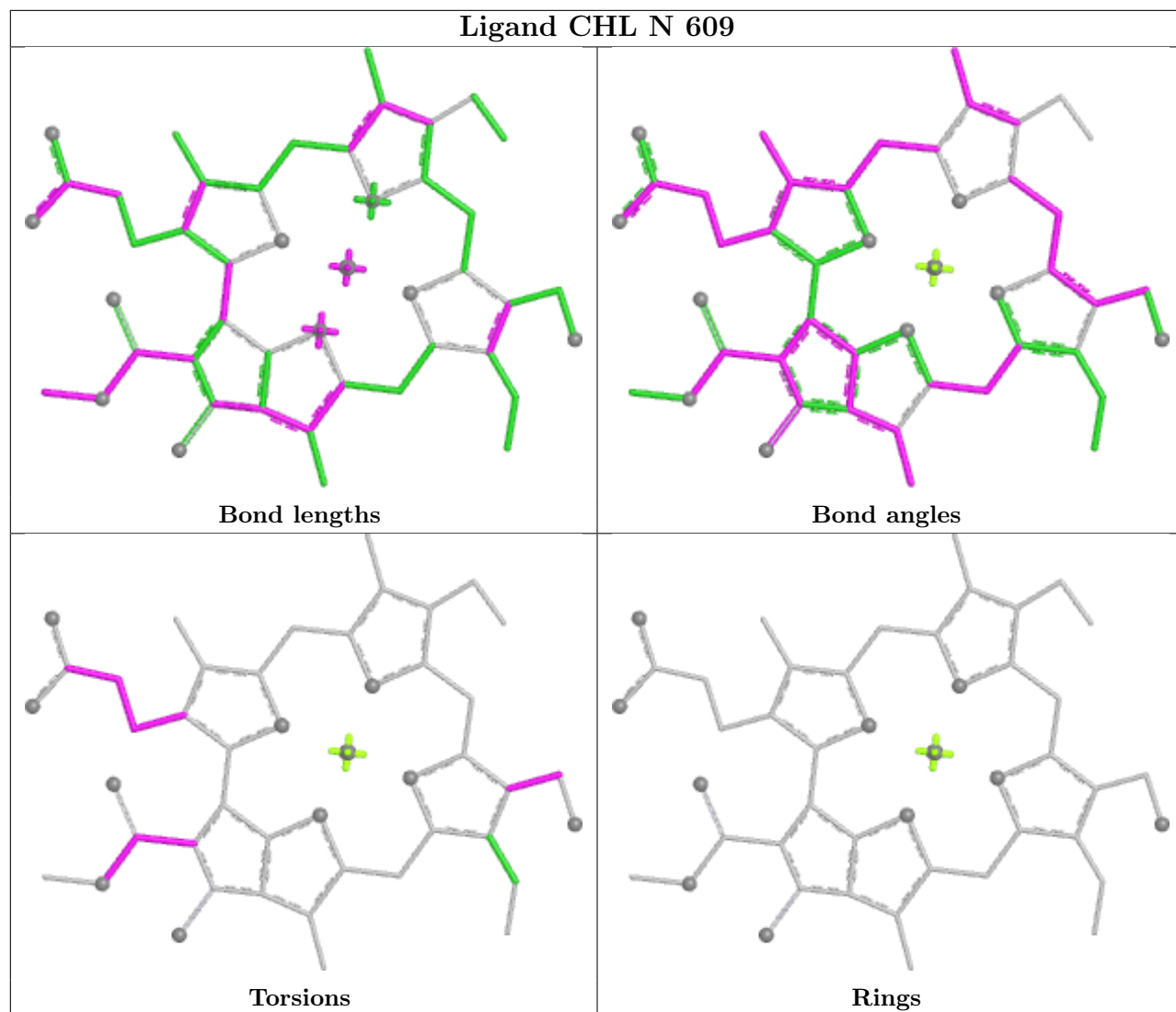


Torsions

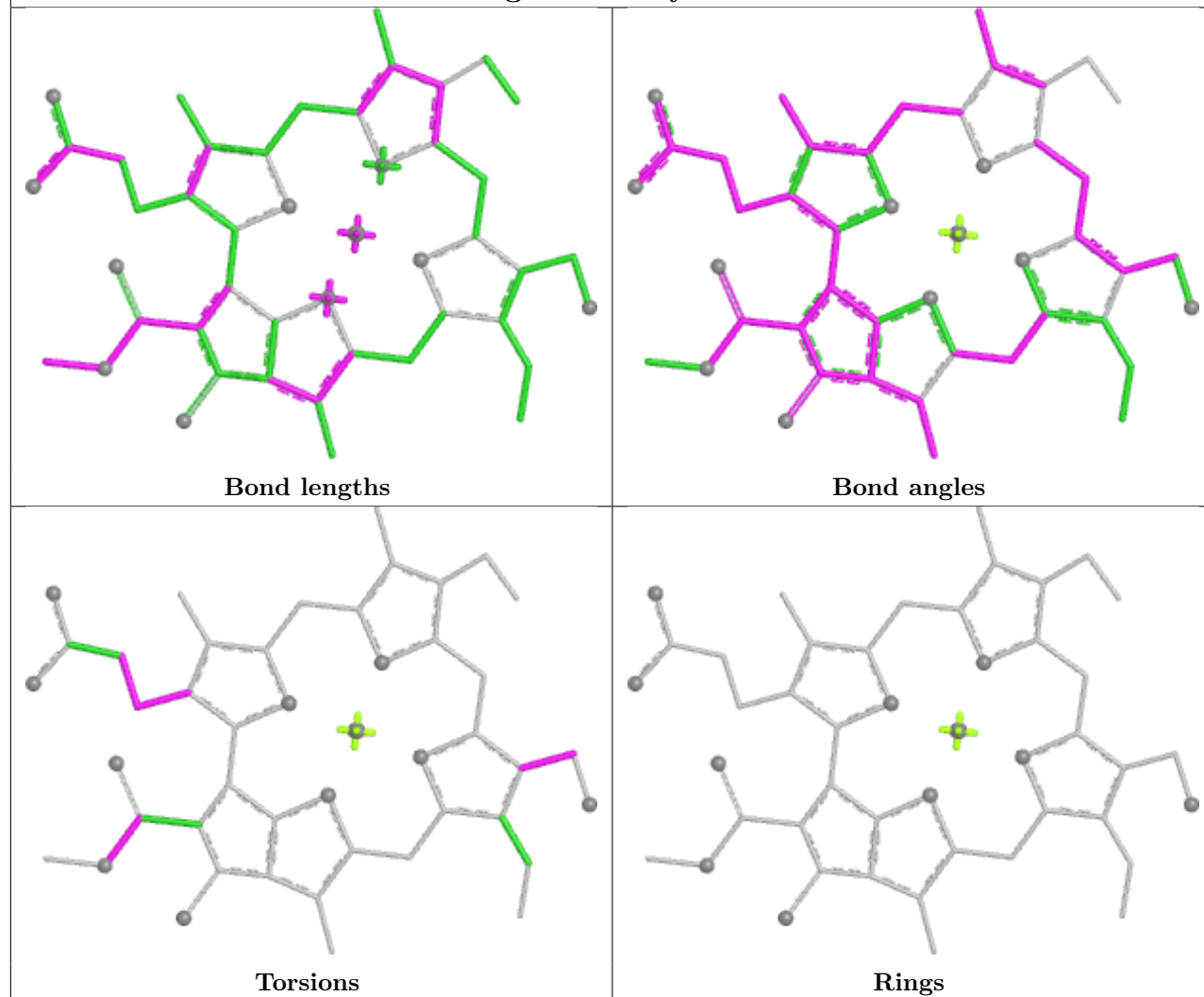


Rings

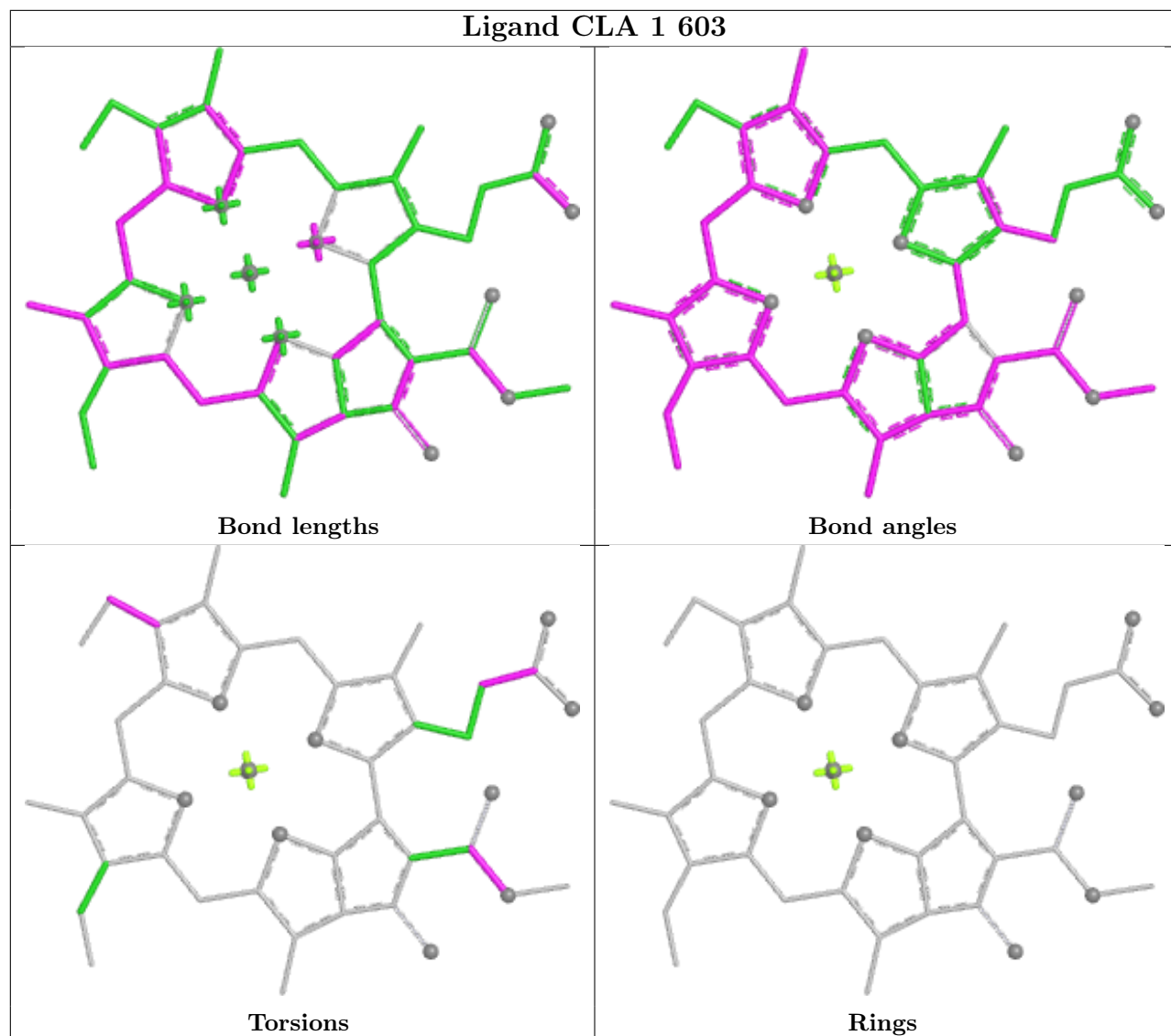




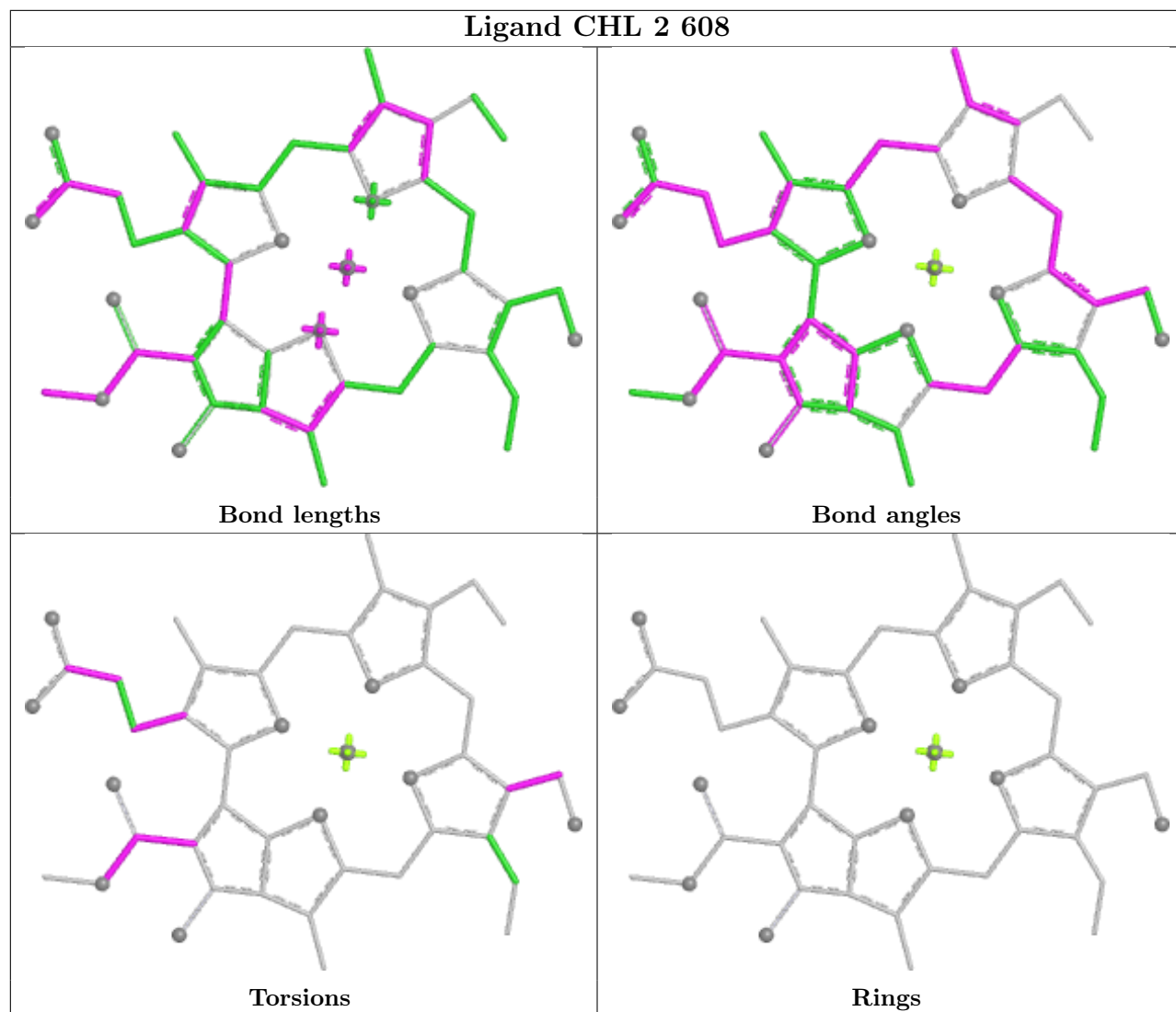
Ligand CHL y 601



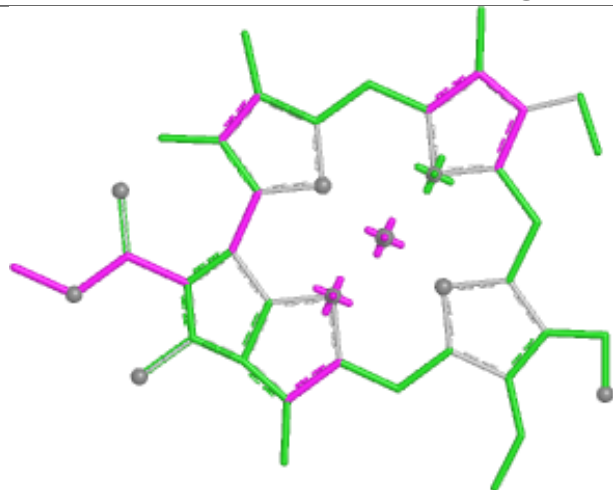
Ligand CLA 1 603



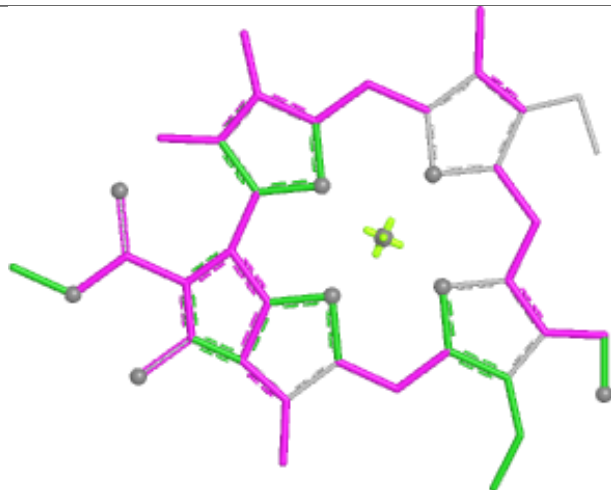
Ligand CHL 2 608



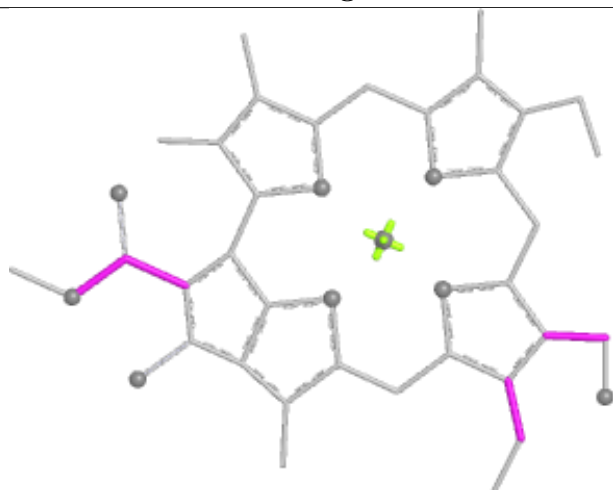
Ligand CHL 7 306



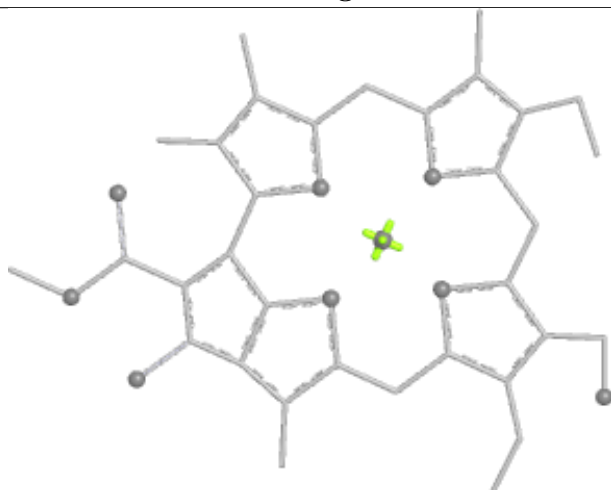
Bond lengths



Bond angles

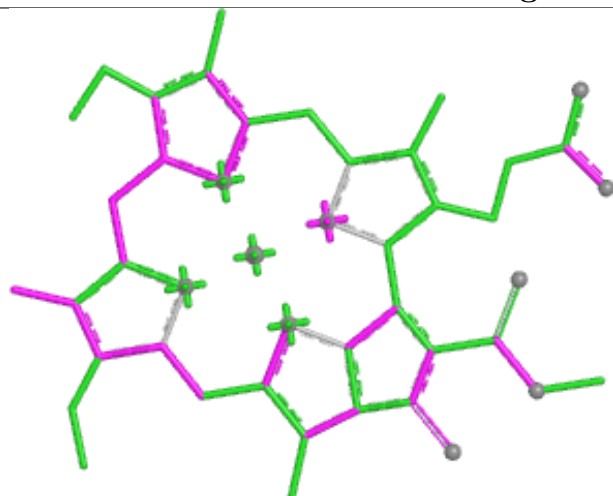


Torsions

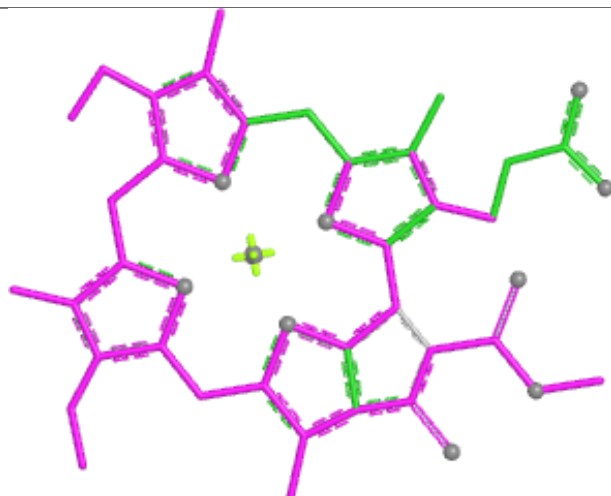


Rings

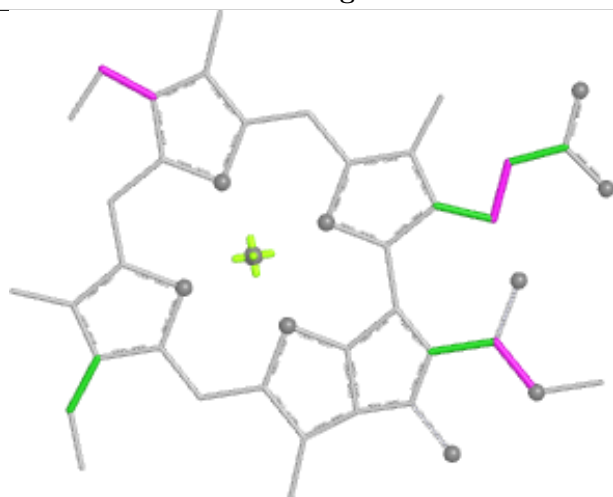
Ligand CLA s 301



Bond lengths



Bond angles

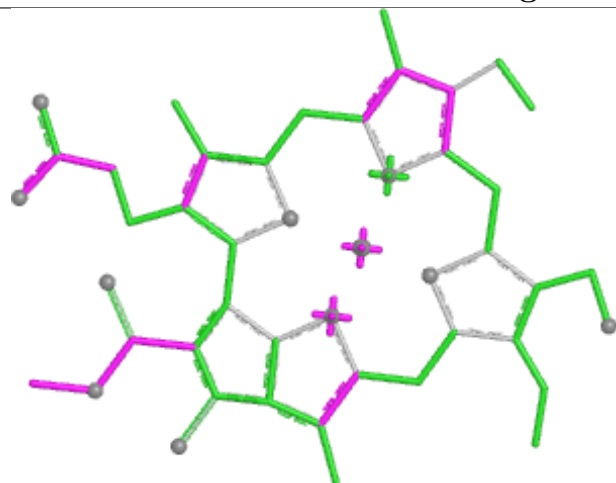


Torsions

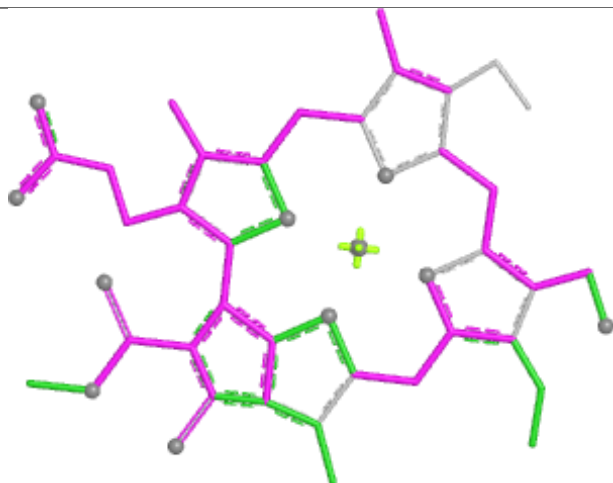


Rings

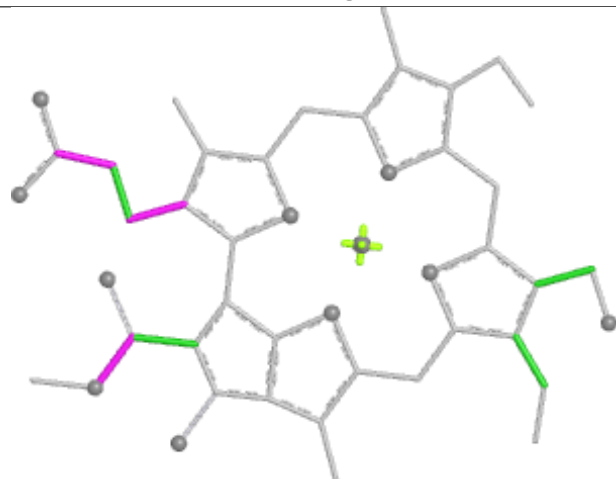
Ligand CHL 1 606



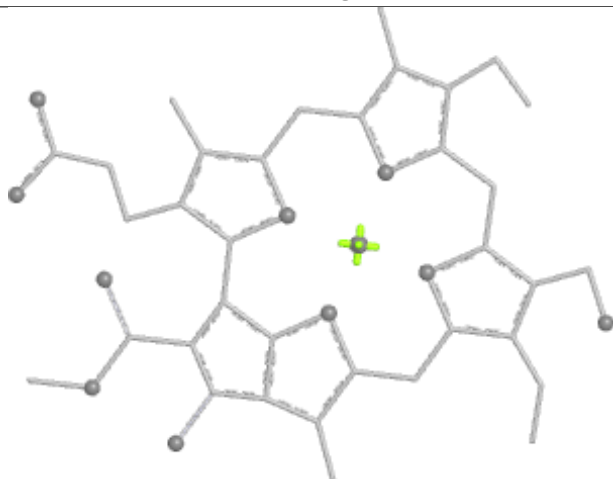
Bond lengths



Bond angles

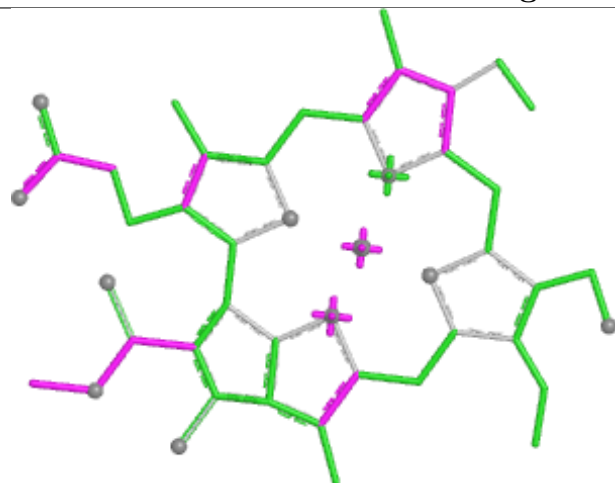


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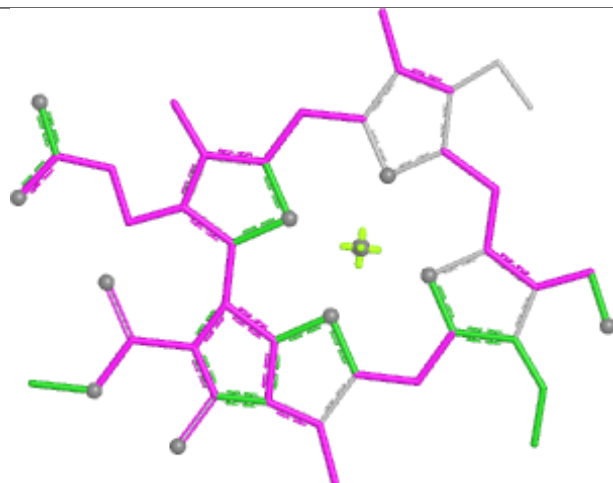


Rings

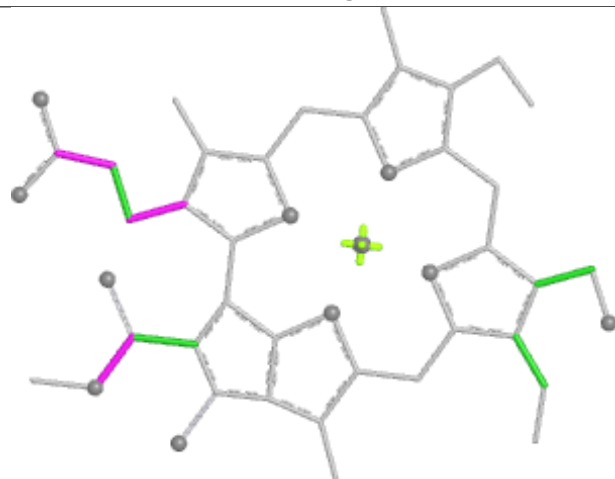
Ligand CHL 7 307



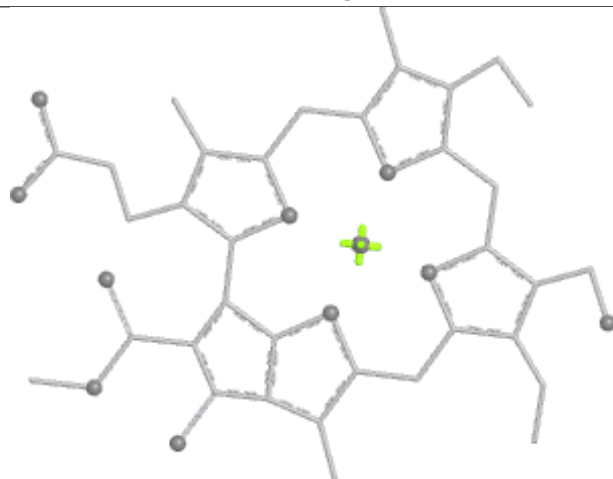
Bond lengths



Bond angles

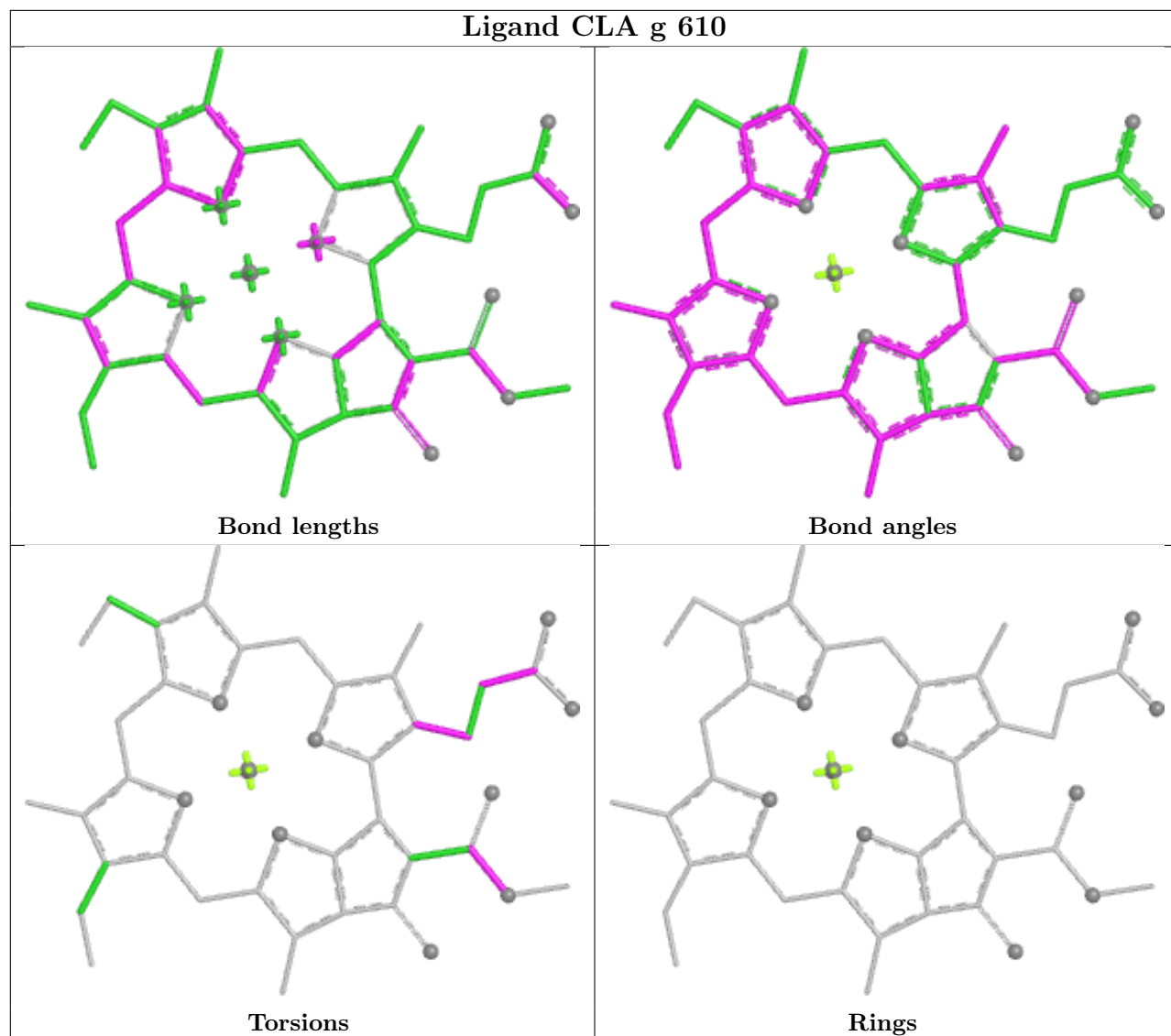


Torsions

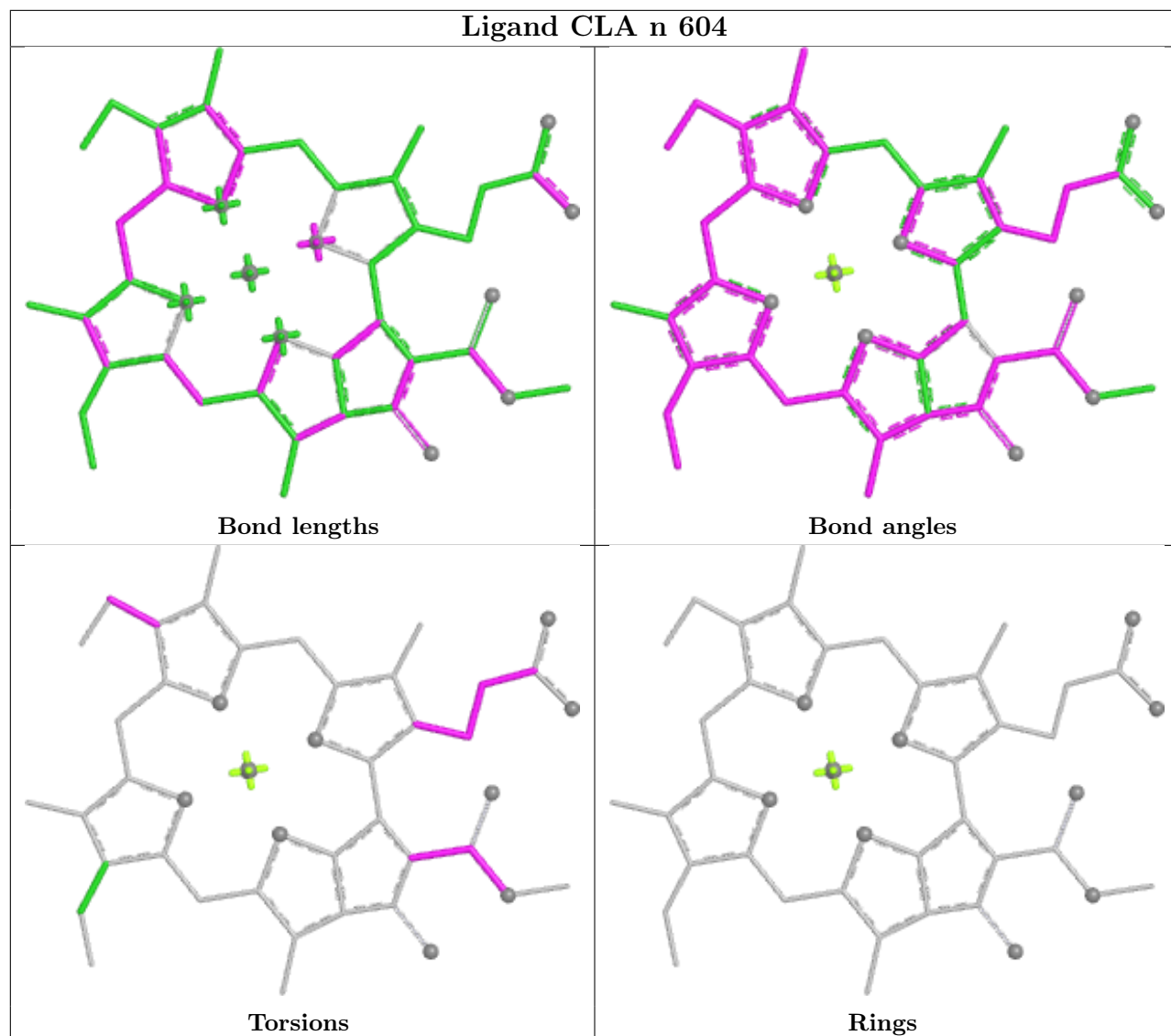


Rings

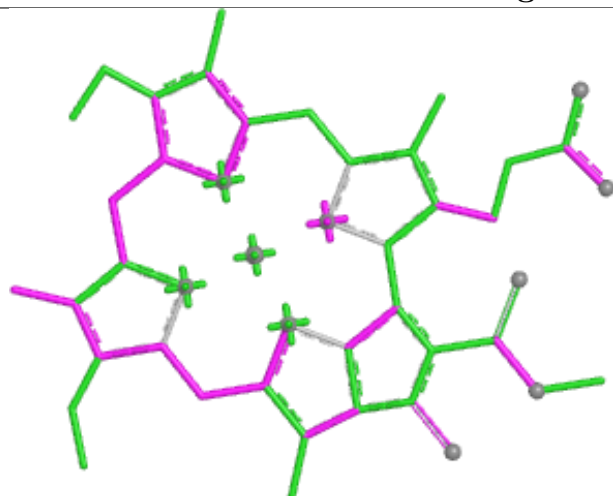
Ligand CLA g 610



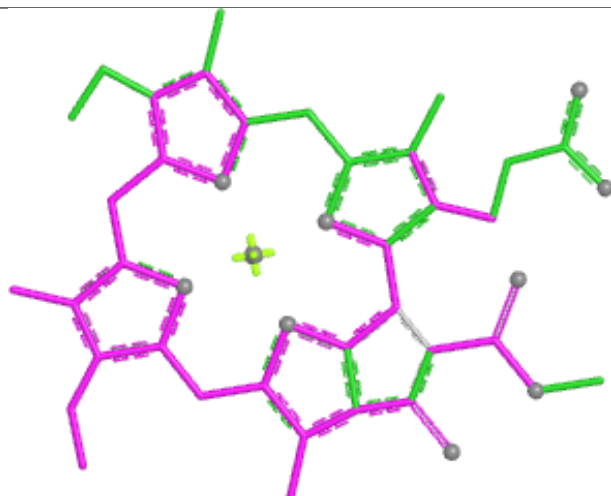
Ligand CLA n 604



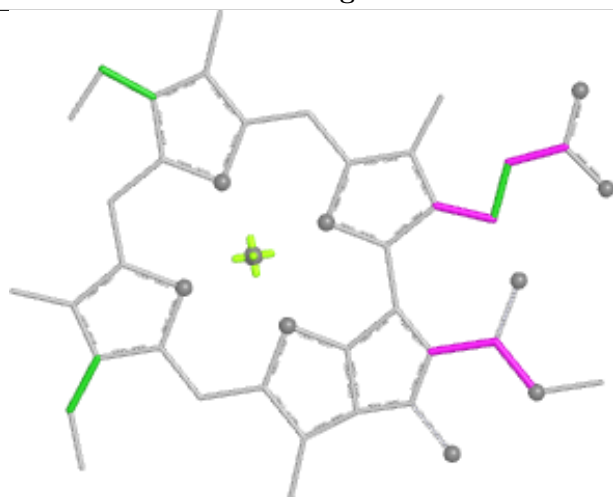
Ligand CLA n 614



Bond lengths



Bond angles

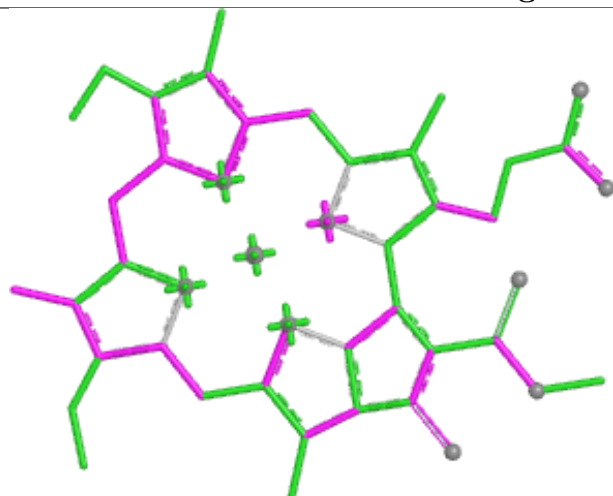


Torsions

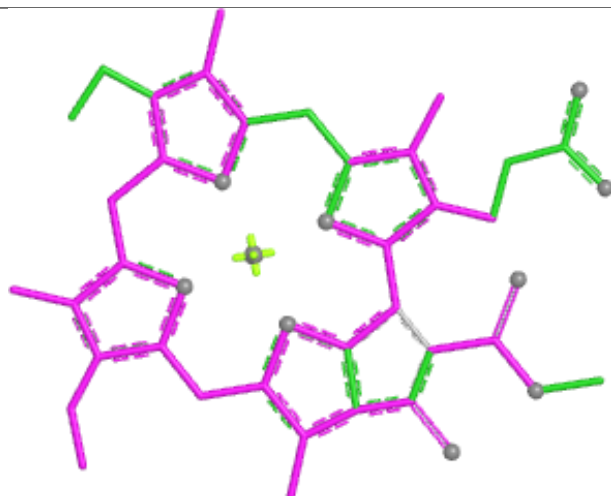


Rings

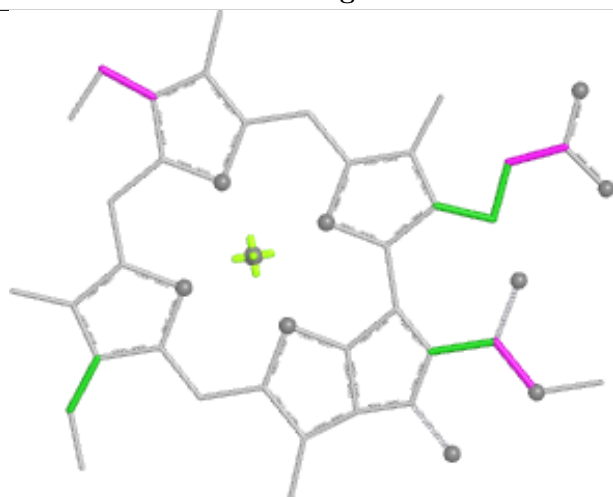
Ligand CLA 4 302



Bond lengths



Bond angles

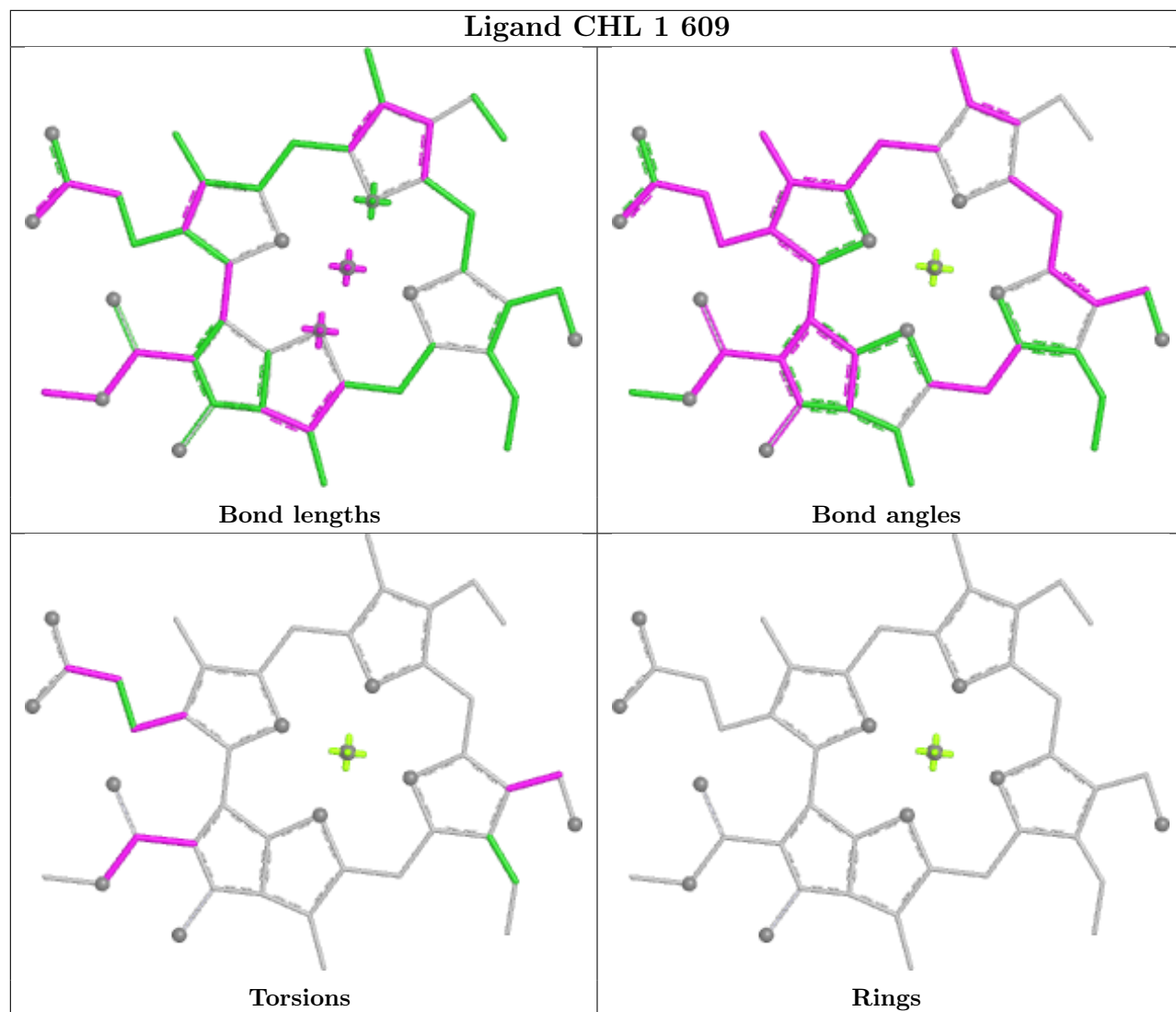


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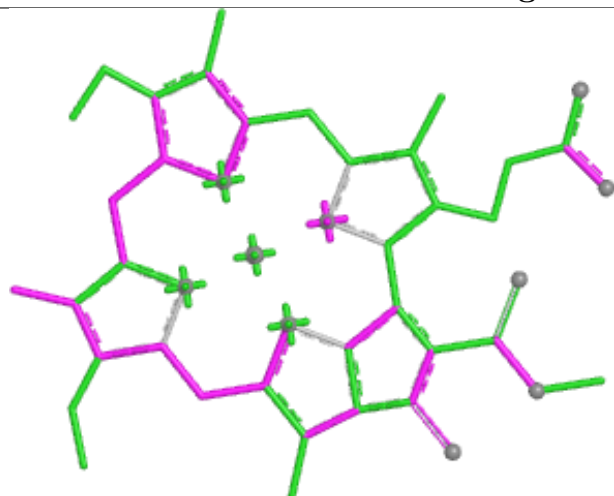


Rings

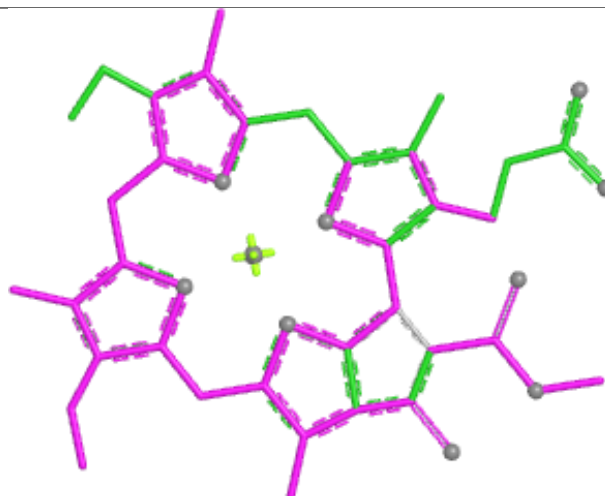
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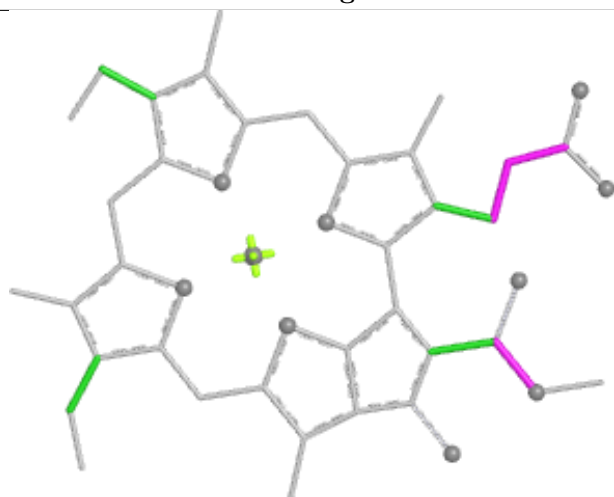
Ligand CLA 7 304



Bond lengths



Bond angles

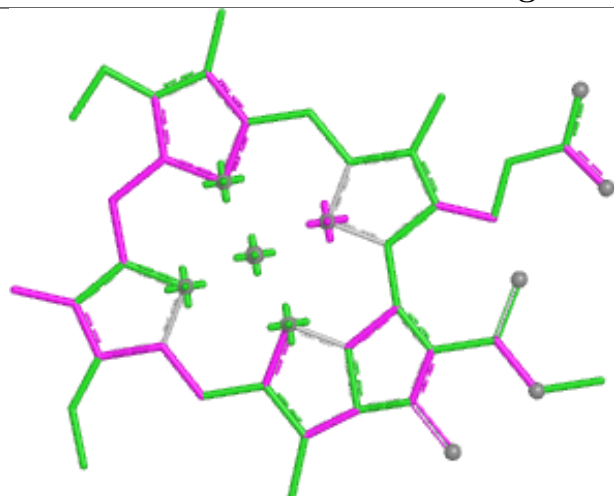


Torsions

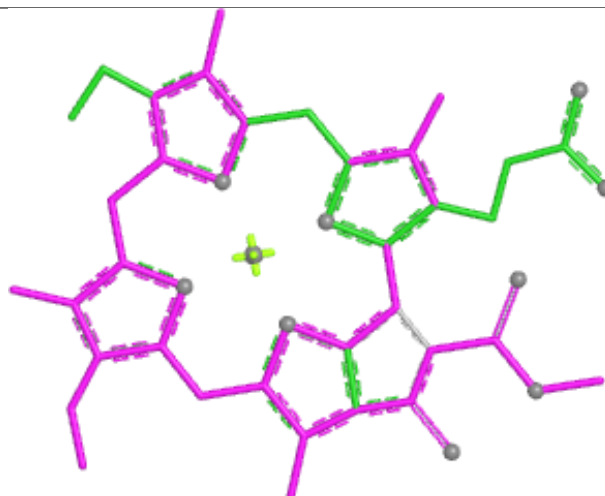


Rings

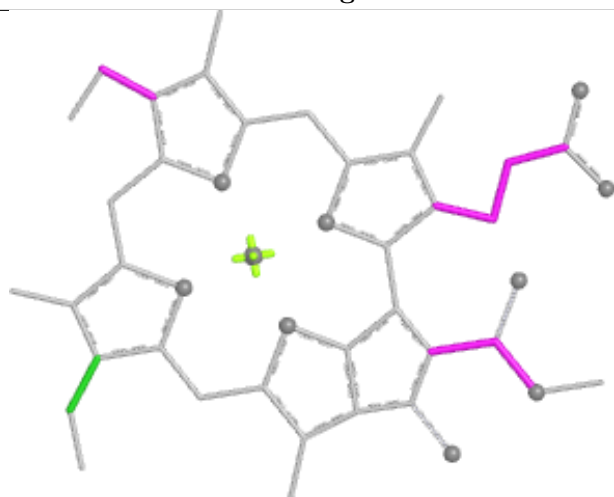
Ligand CLA 7 303



Bond lengths



Bond angles

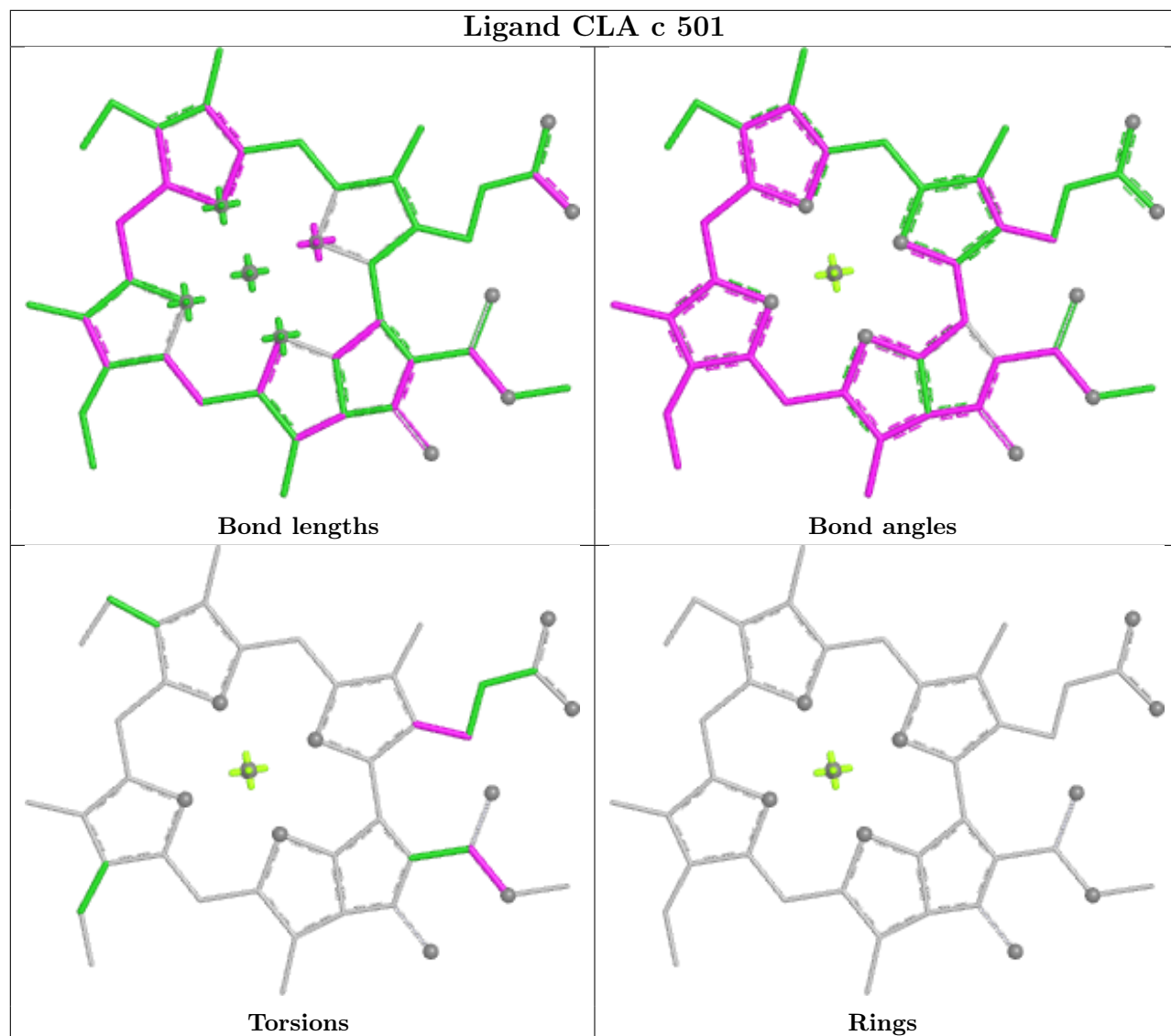


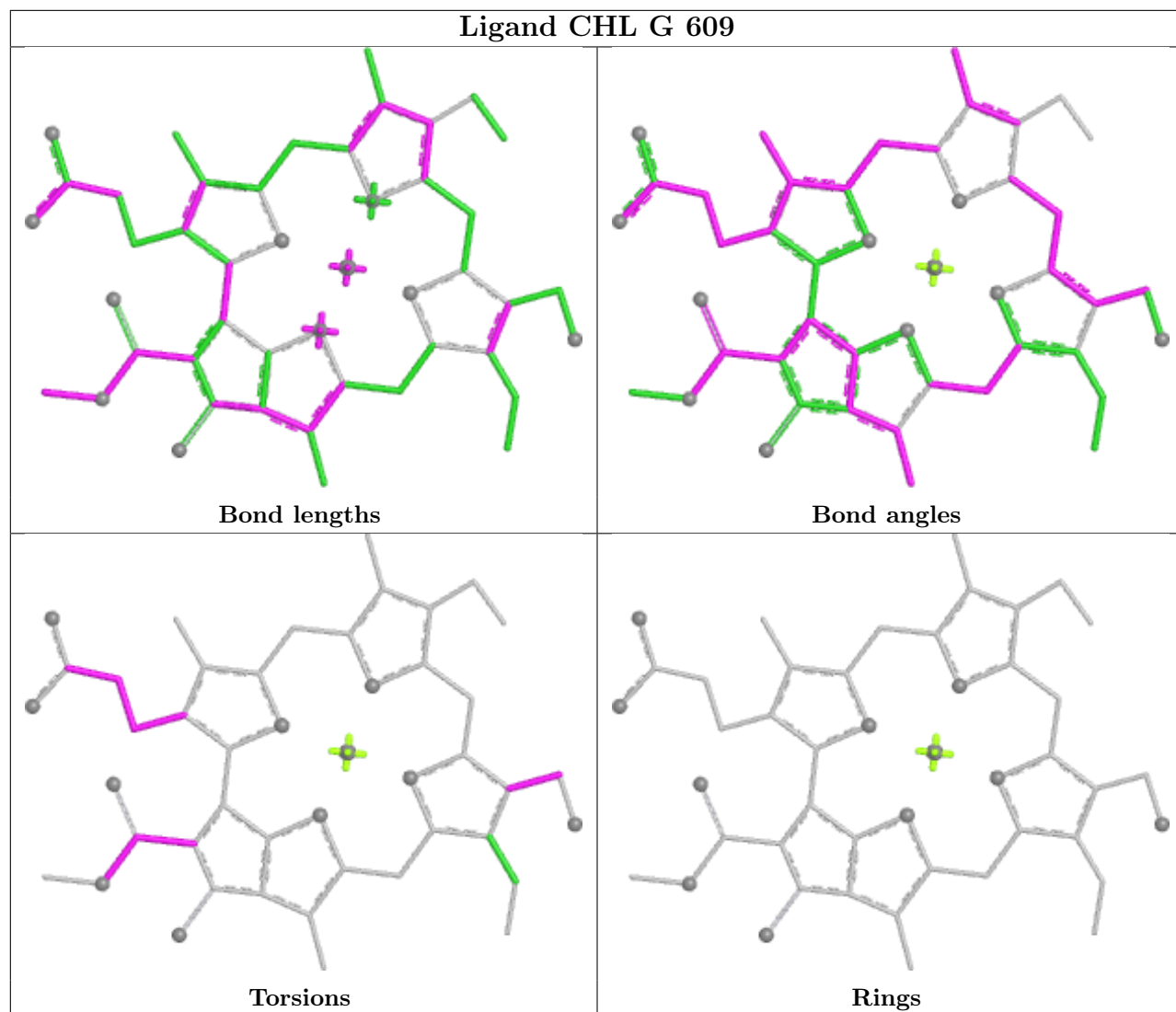
Torsions



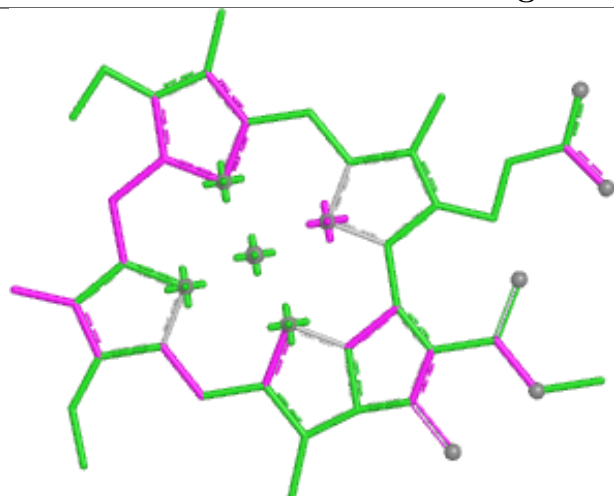
Rings

Ligand CLA c 501

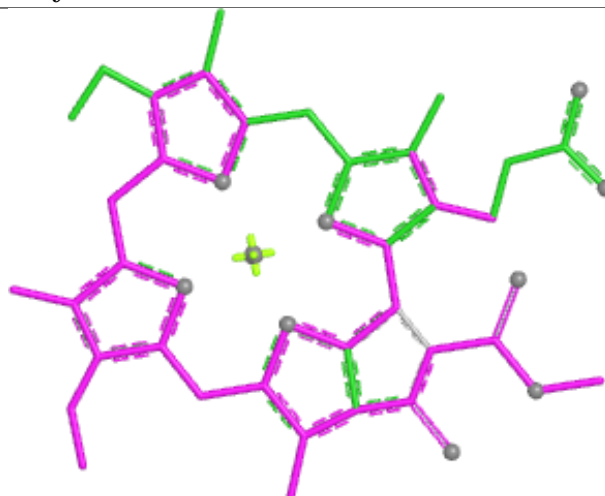




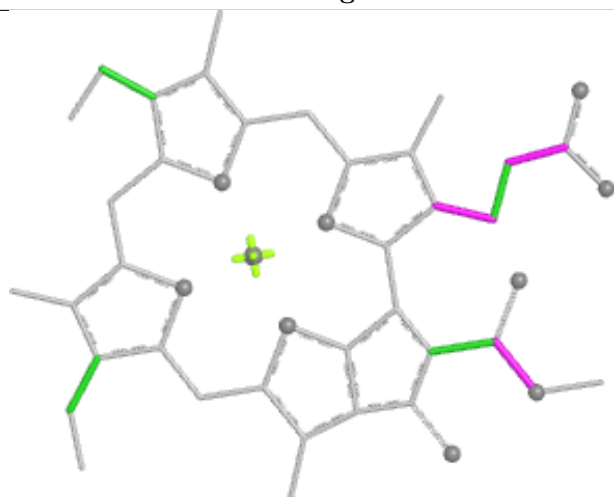
Ligand CLA y 614



Bond lengths



Bond angles

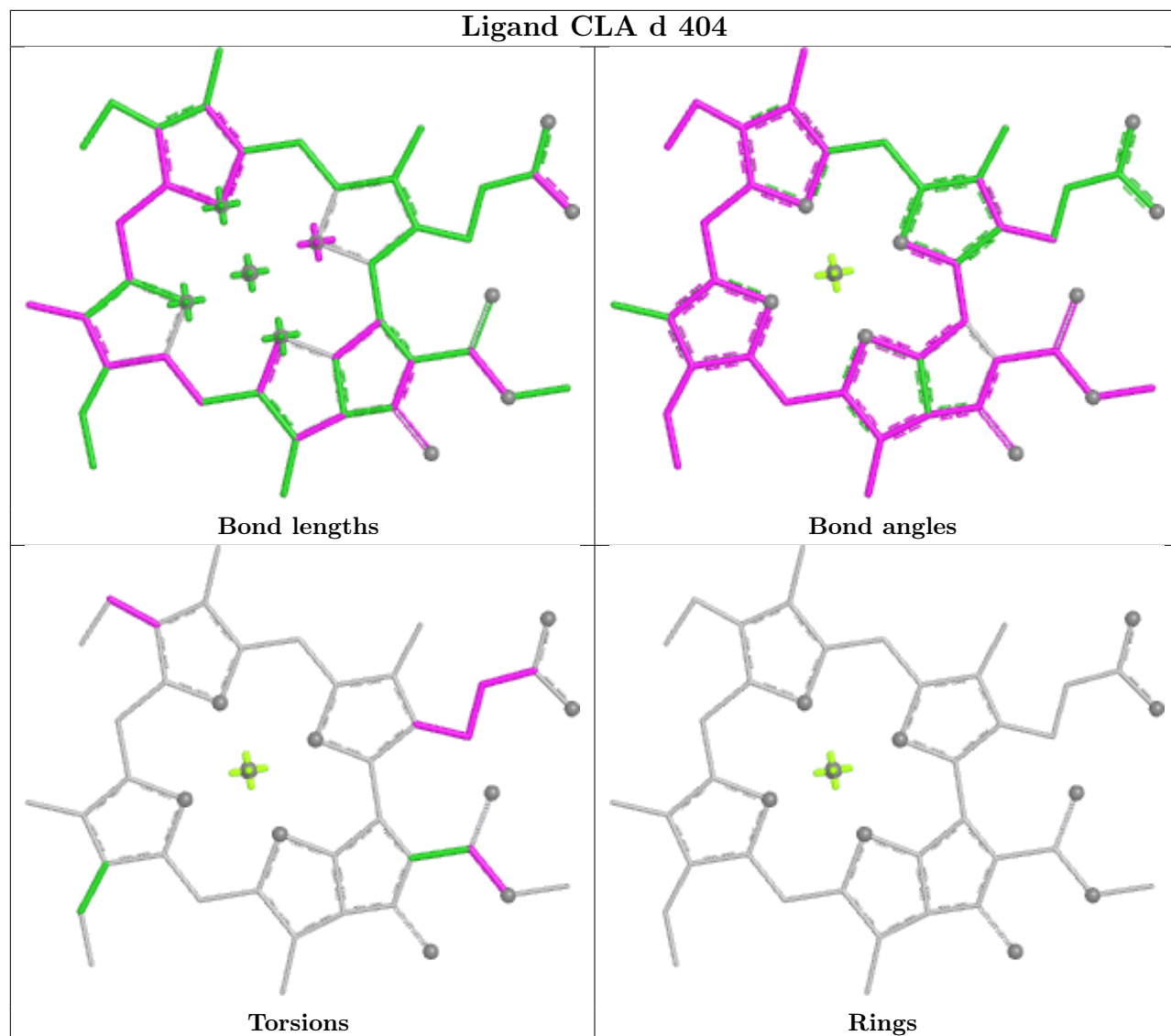


Torsions

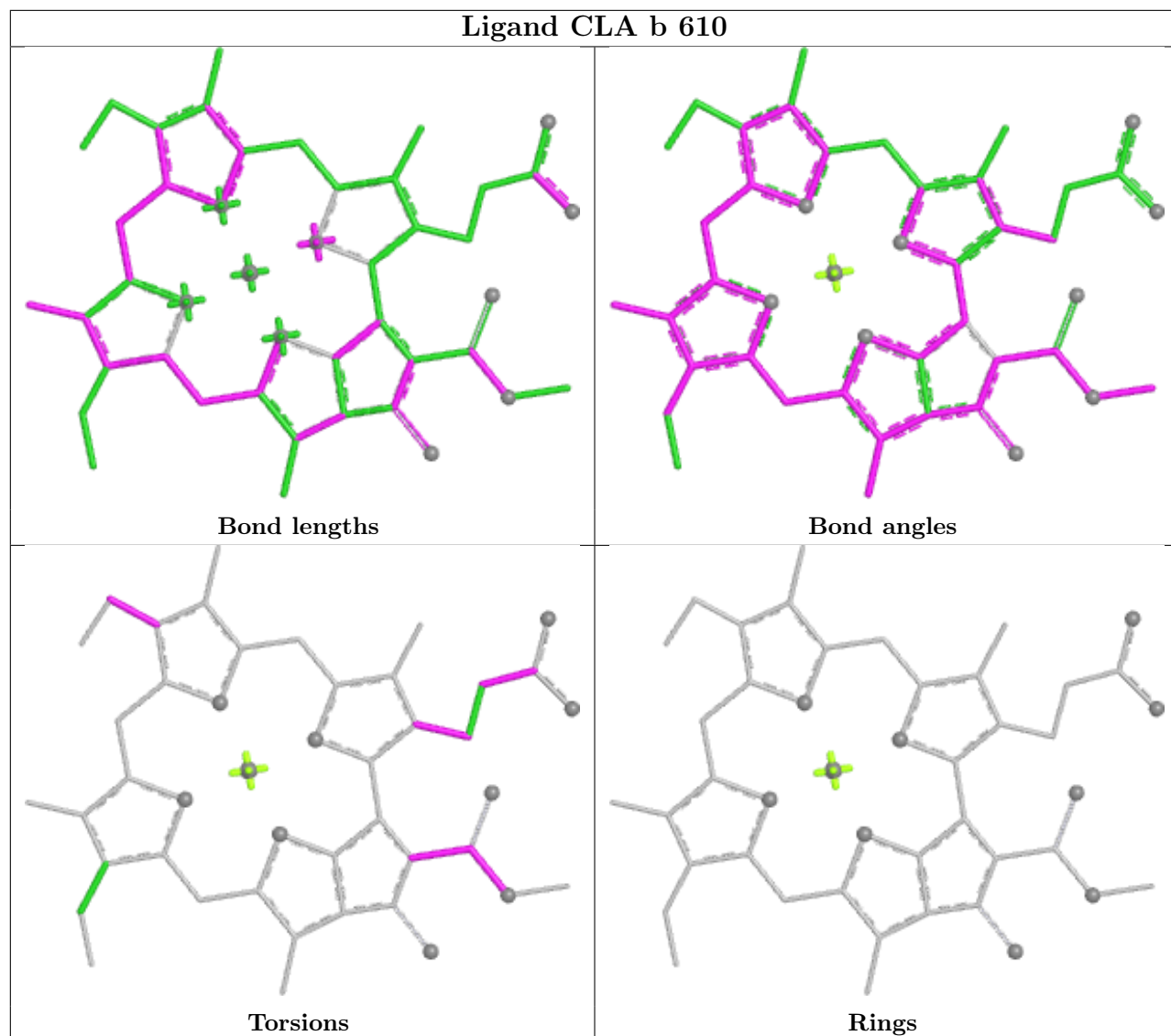


Rings

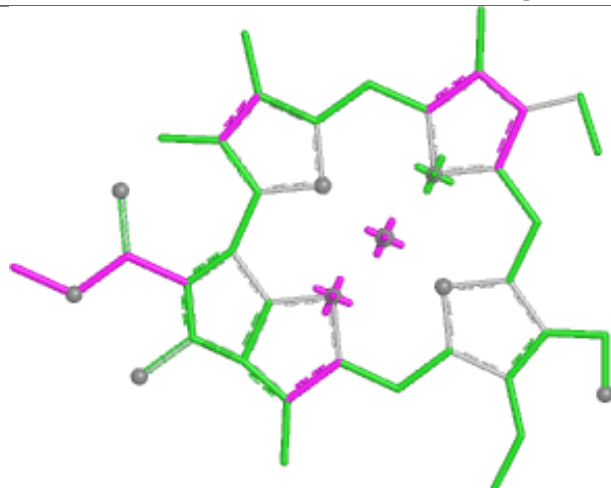
Ligand CLA d 404



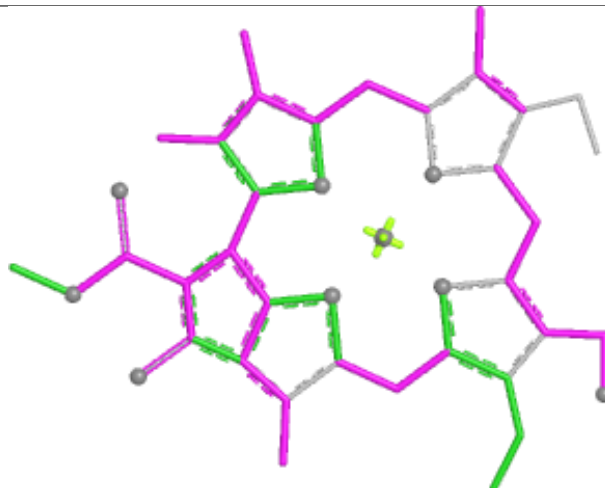
Ligand CLA b 610



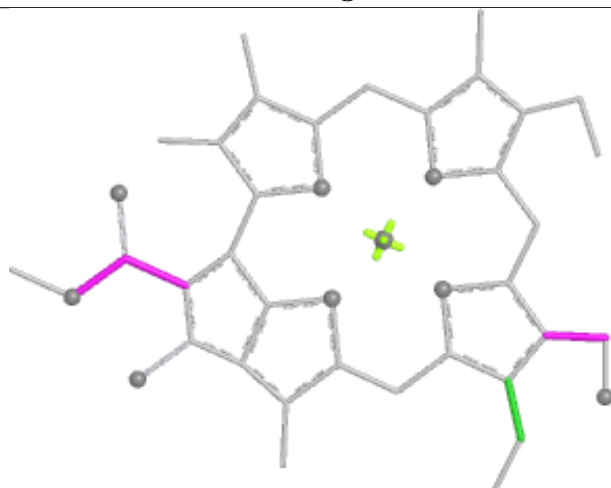
Ligand CHL 1 605



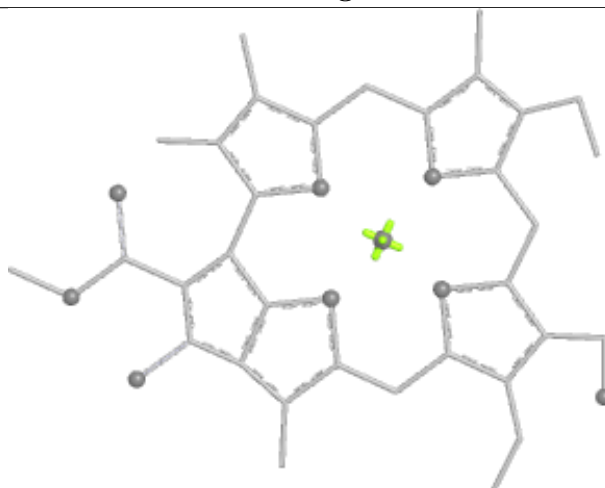
Bond lengths



Bond angles

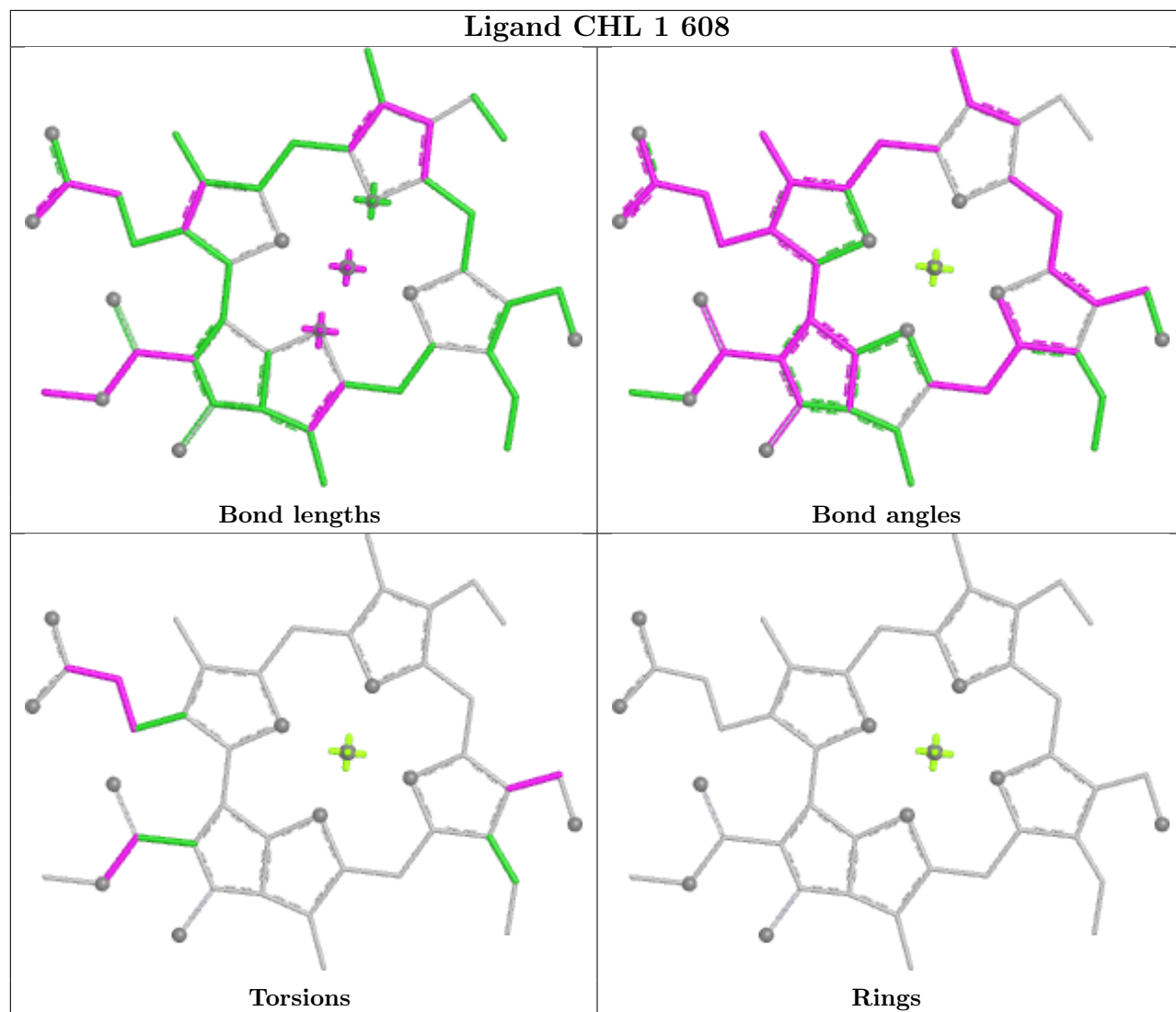


Torsions

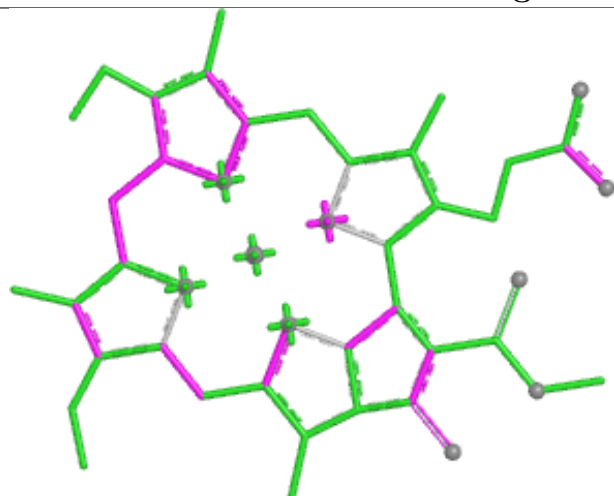


Rings

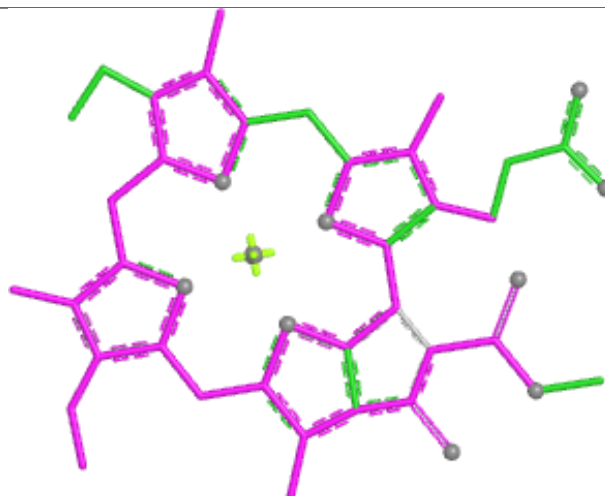
Ligand CHL 1 608



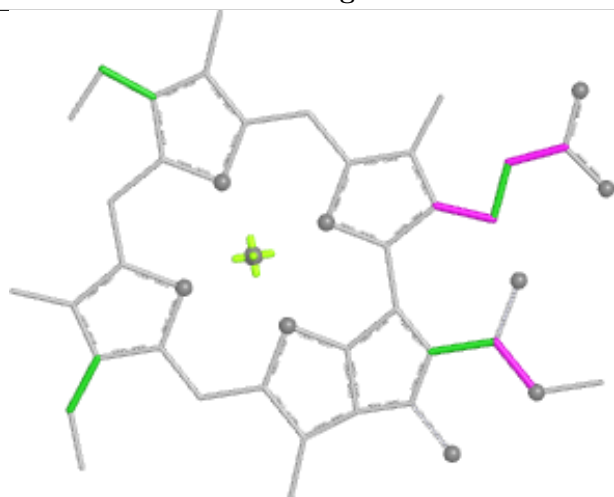
Ligand CLA D 403



Bond lengths



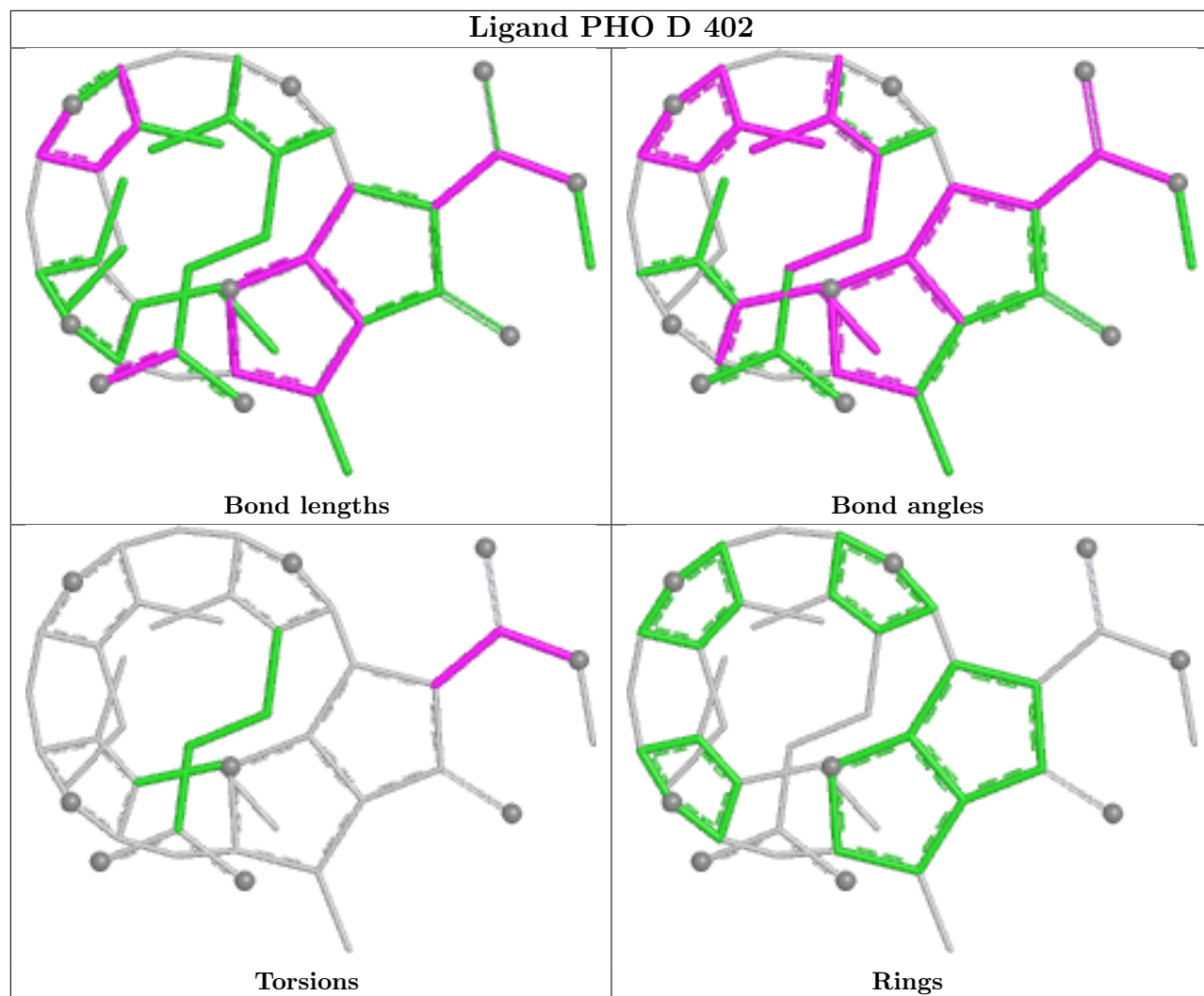
Bond angles



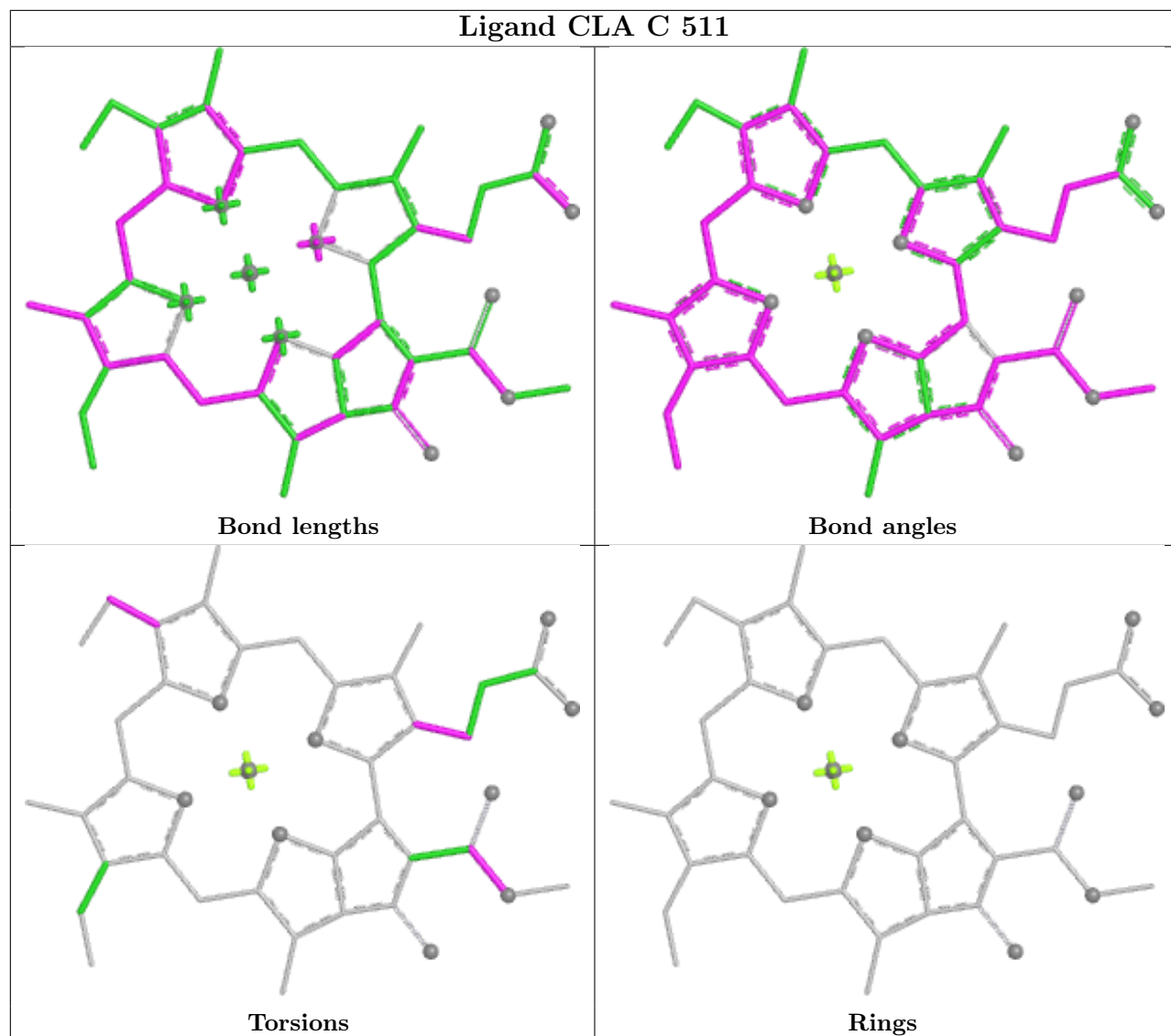
Torsions



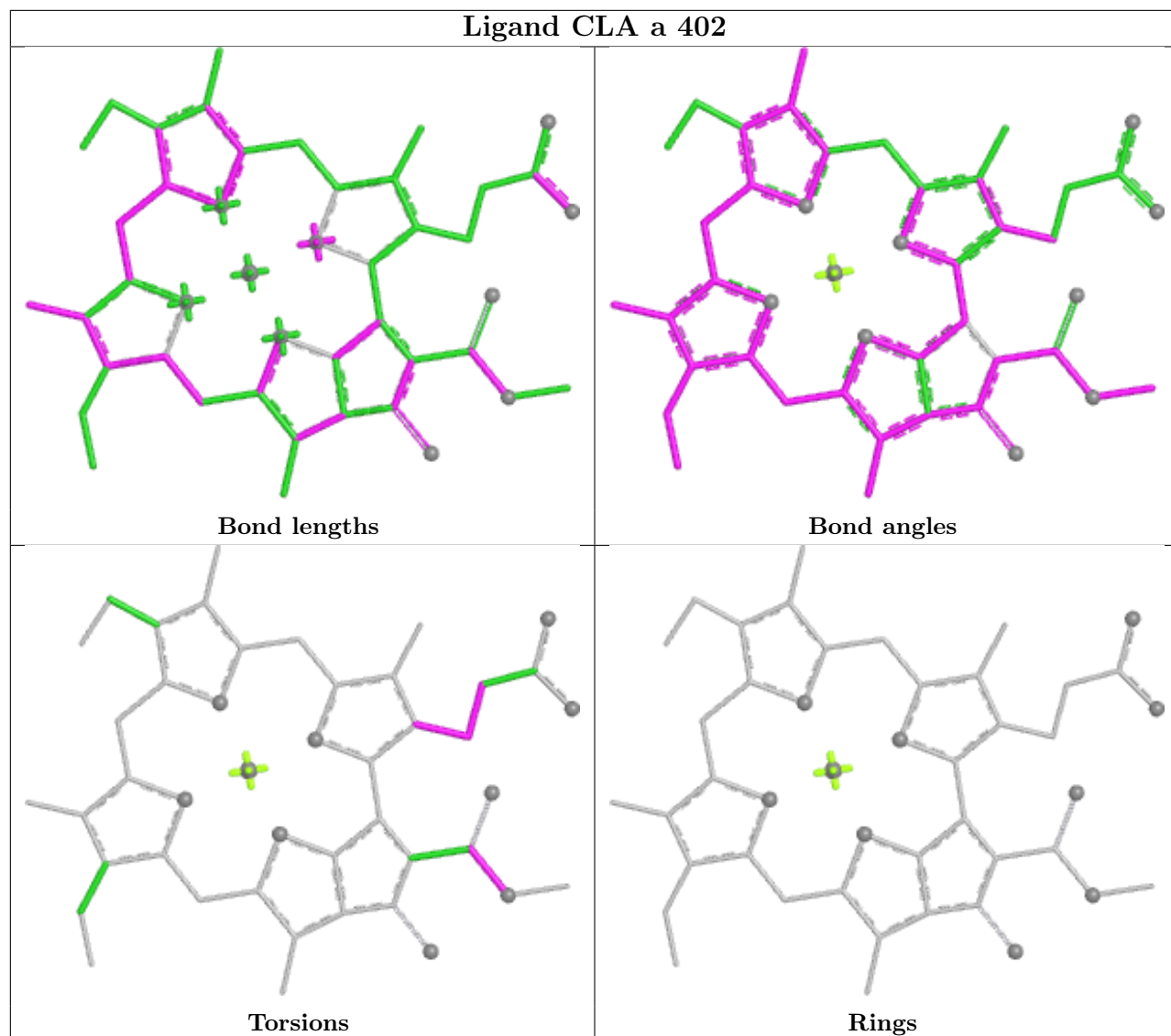
Rings



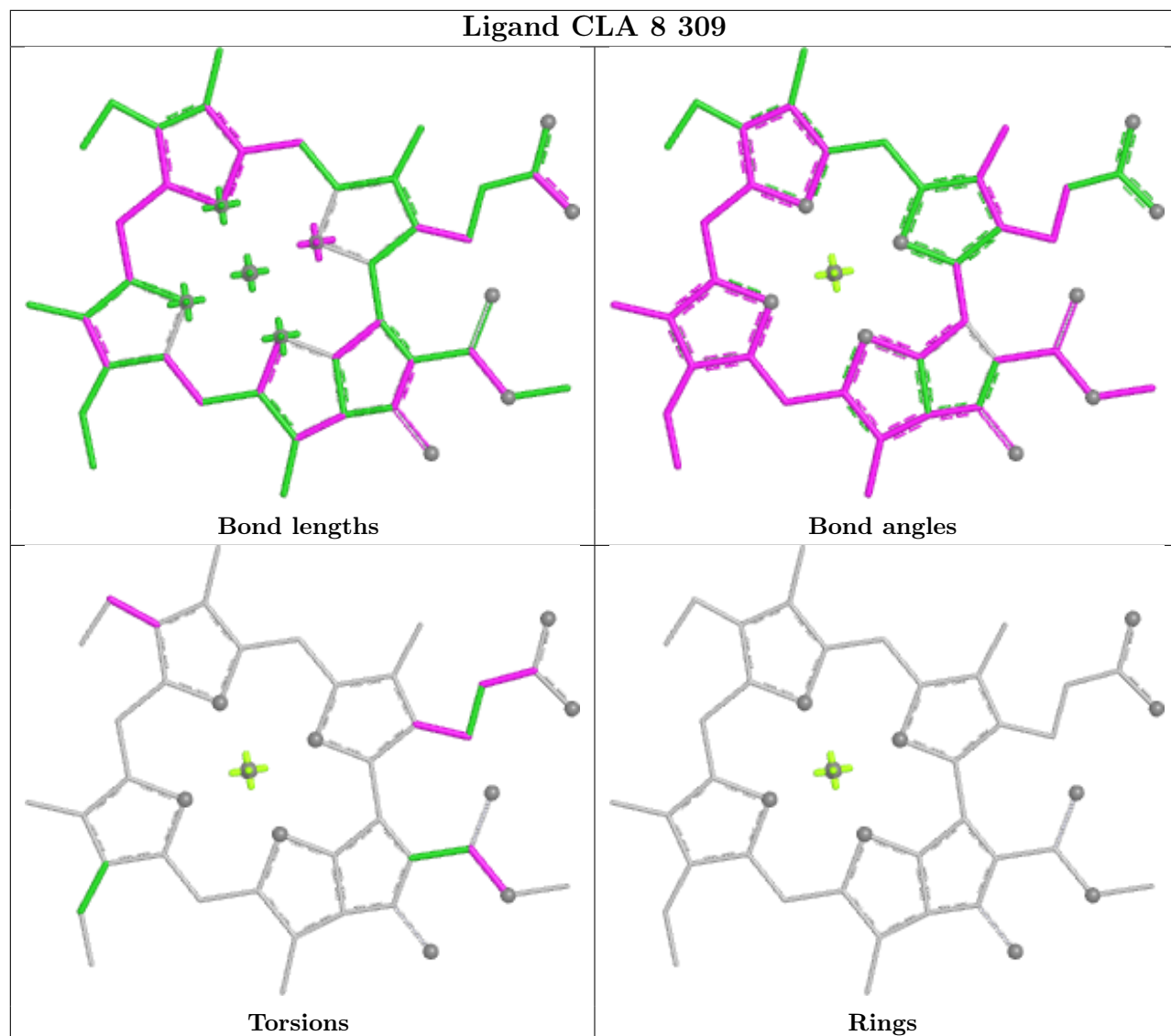
Ligand CLA C 511



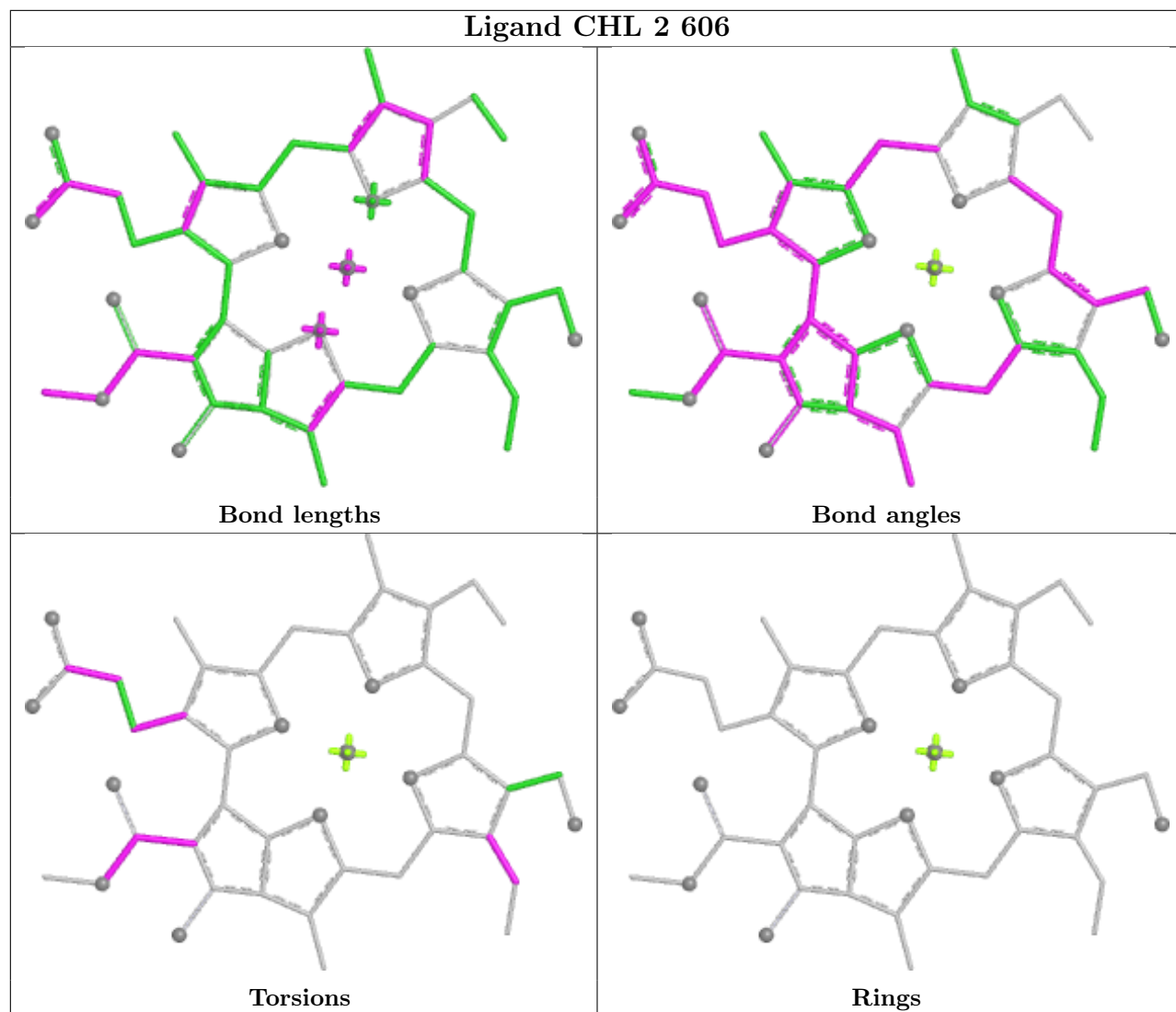
Ligand CLA a 402



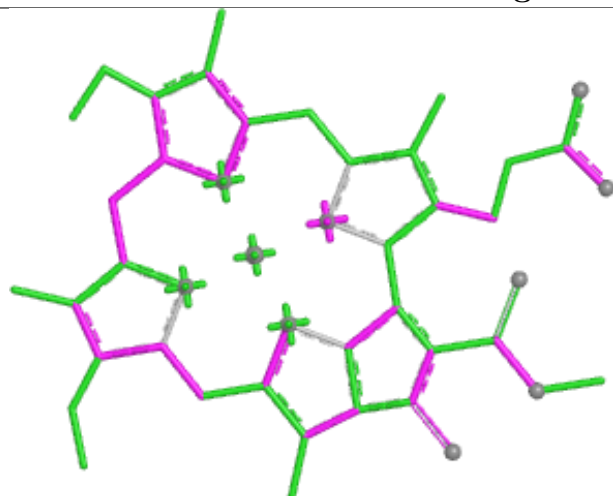
Ligand CLA 8 309



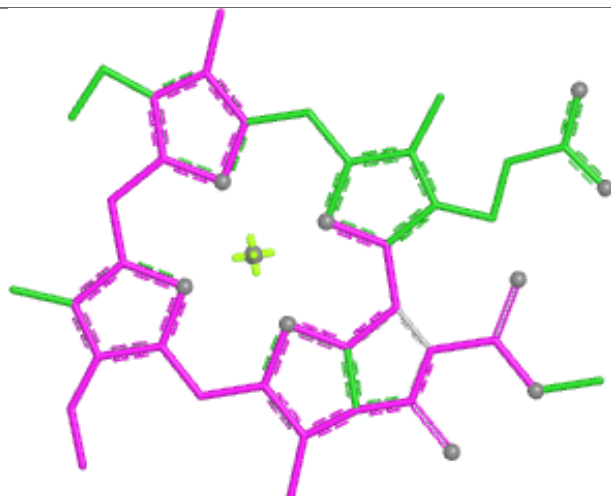
Ligand CHL 2 606



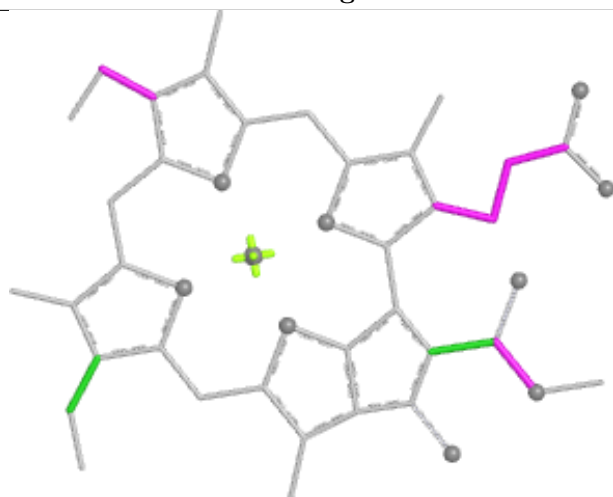
Ligand CLA R 307



Bond lengths



Bond angles

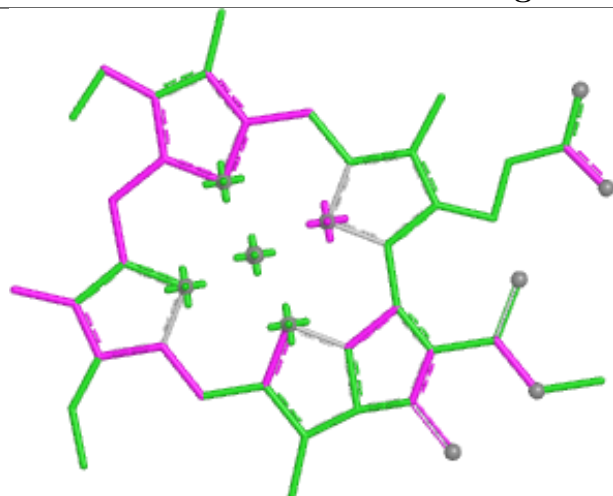


Torsions

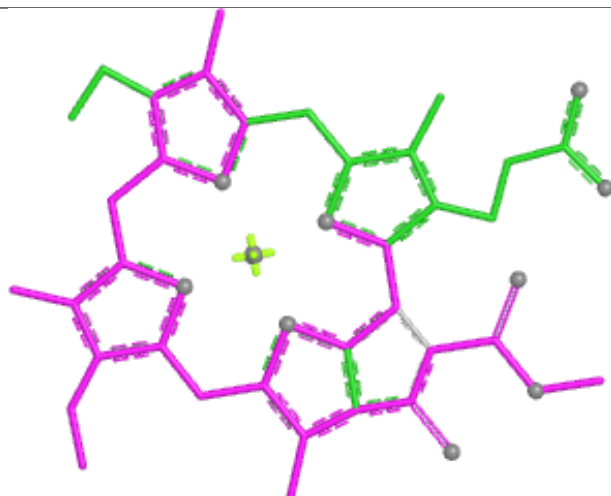


Rings

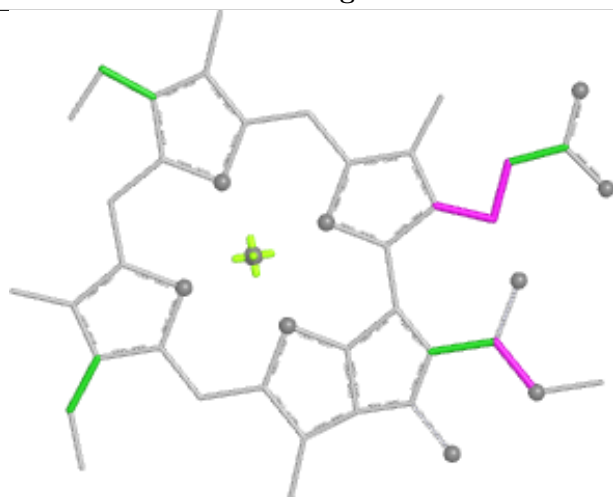
Ligand CLA B 616



Bond lengths



Bond angles

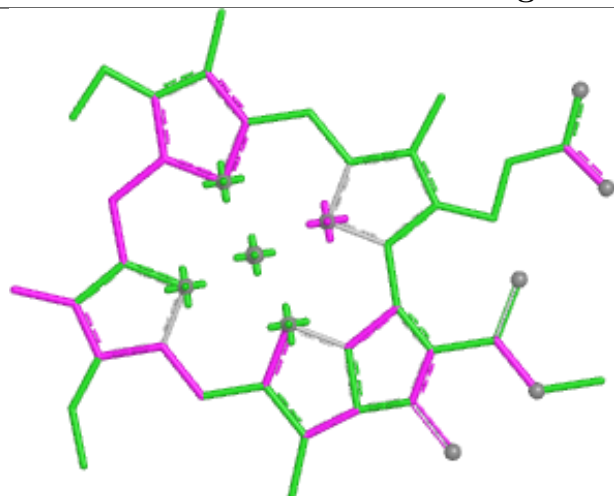


Torsions

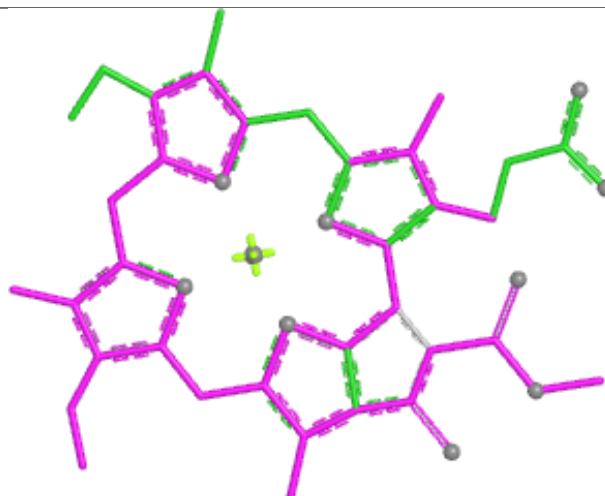


Rings

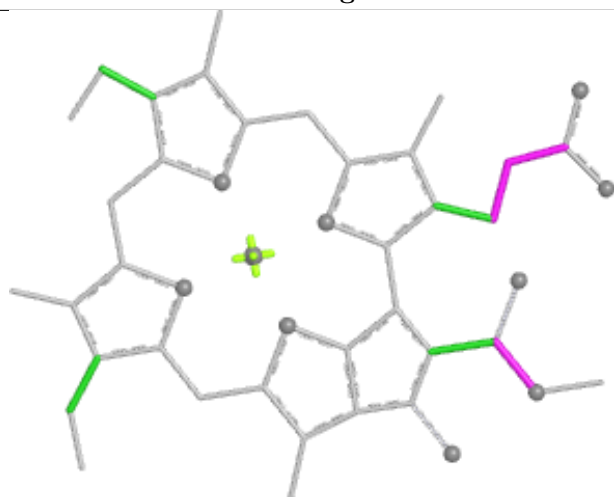
Ligand CLA b 613



Bond lengths



Bond angles

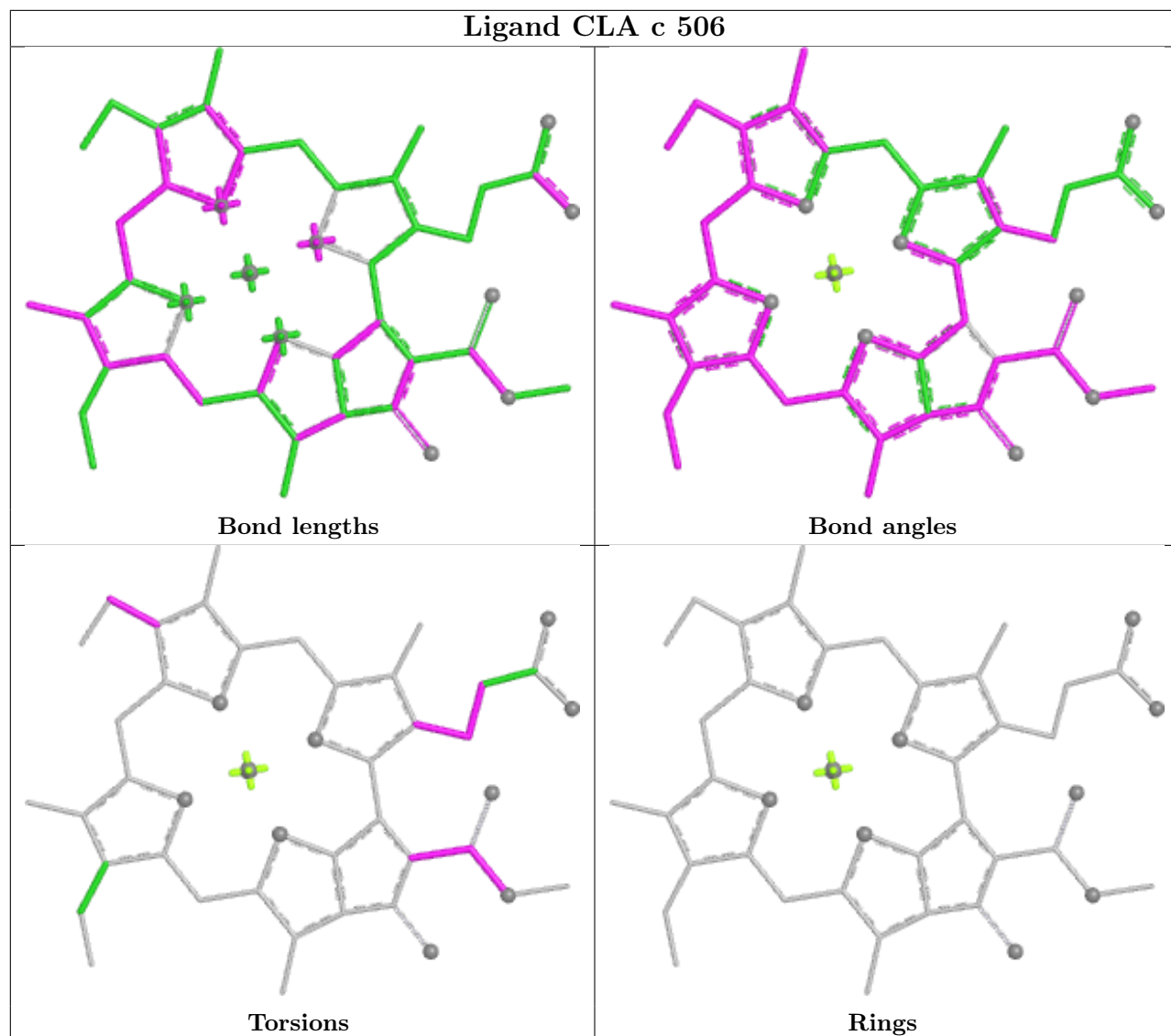


Torsions

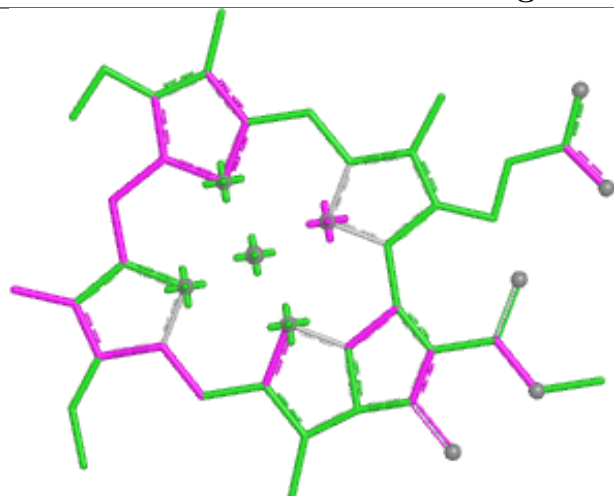


Rings

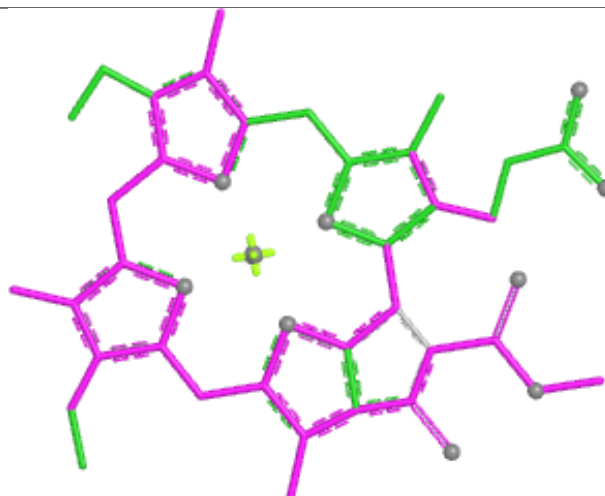
Ligand CLA c 506



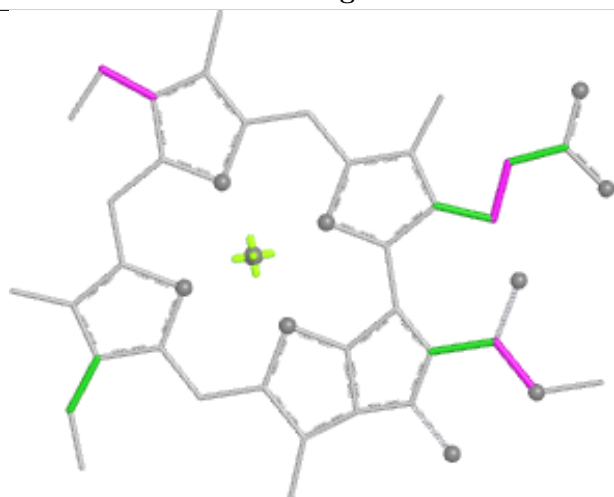
Ligand CLA S 309



Bond lengths



Bond angles

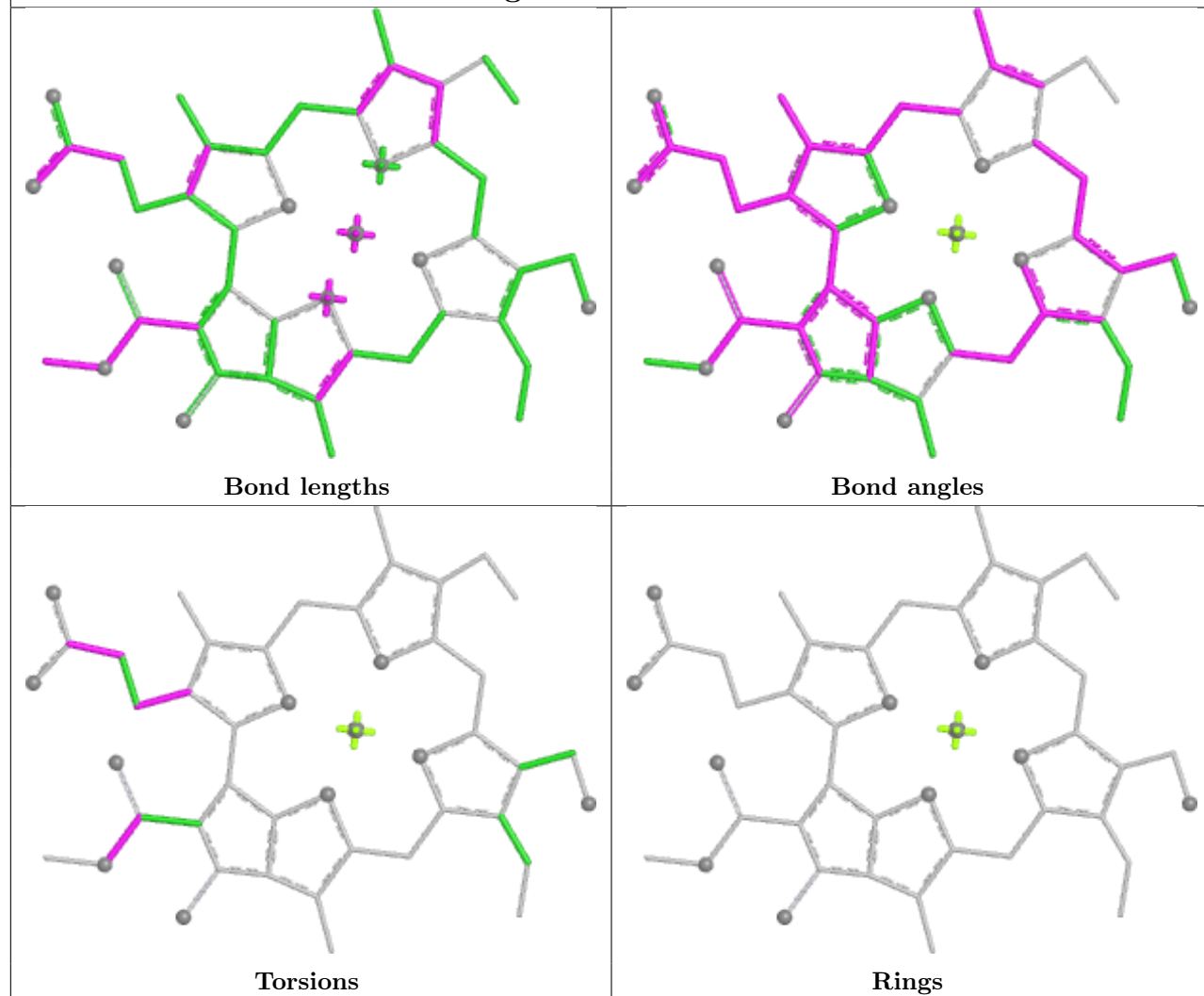


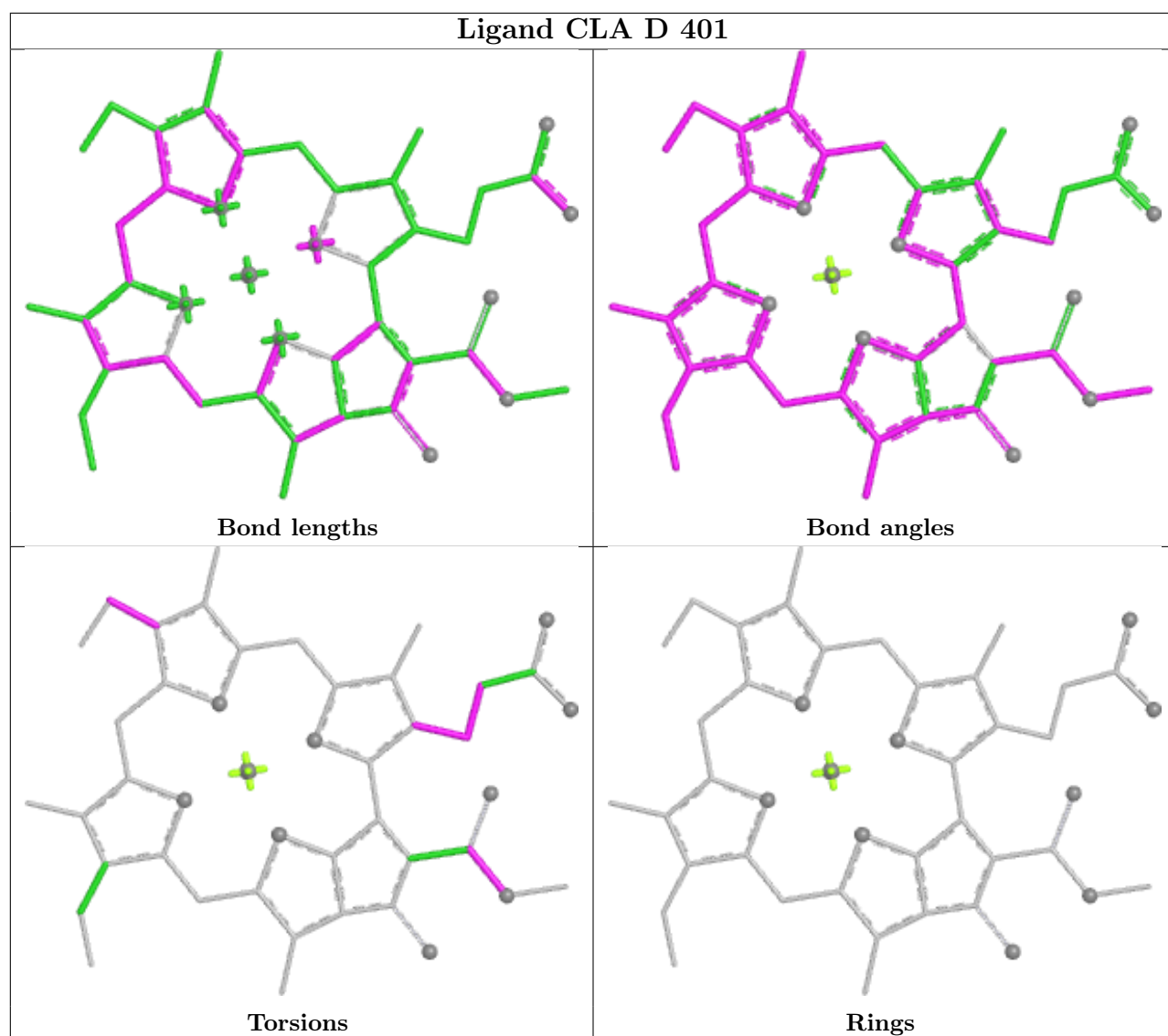
Torsions



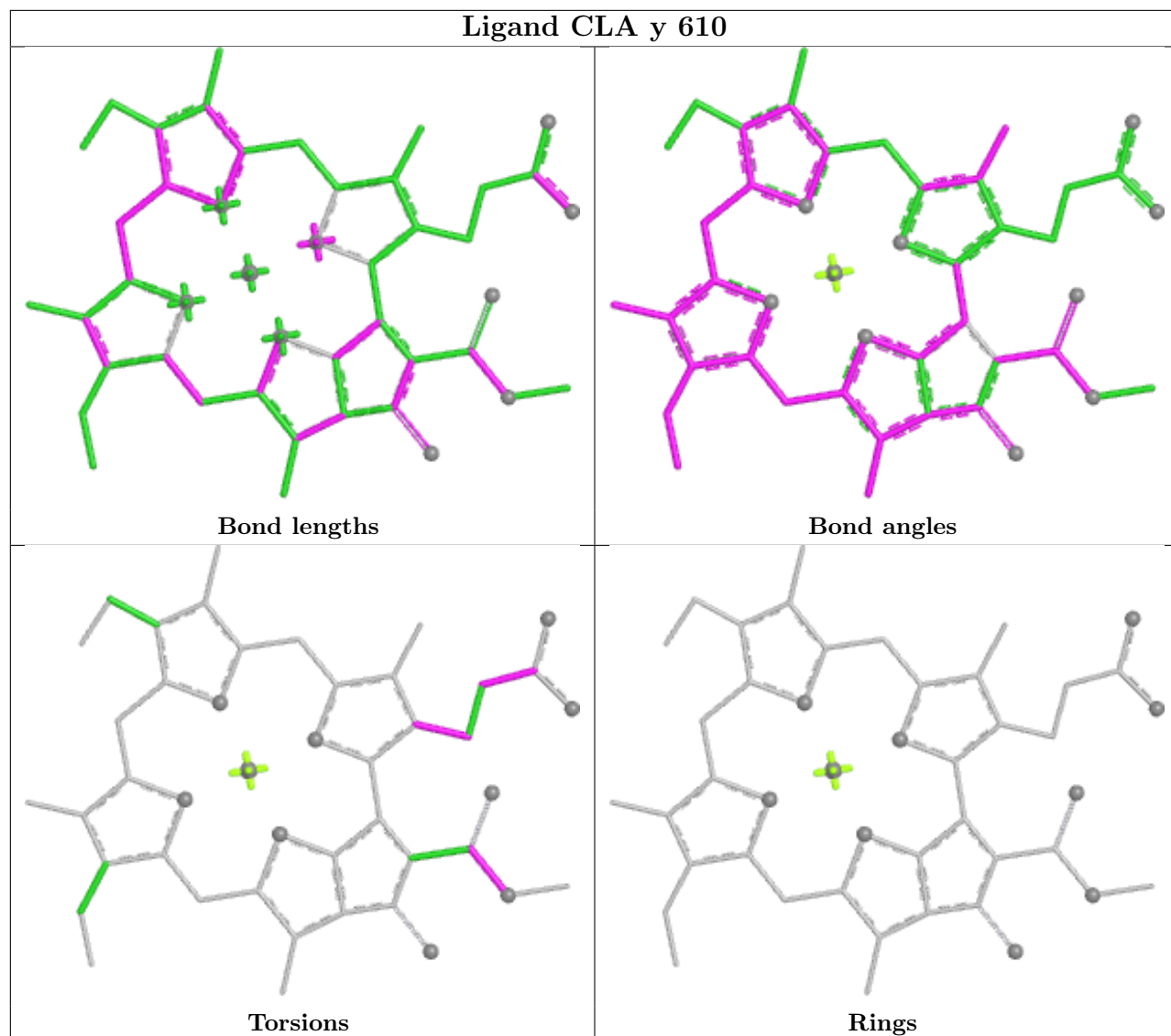
Rings

Ligand CHL 5 606

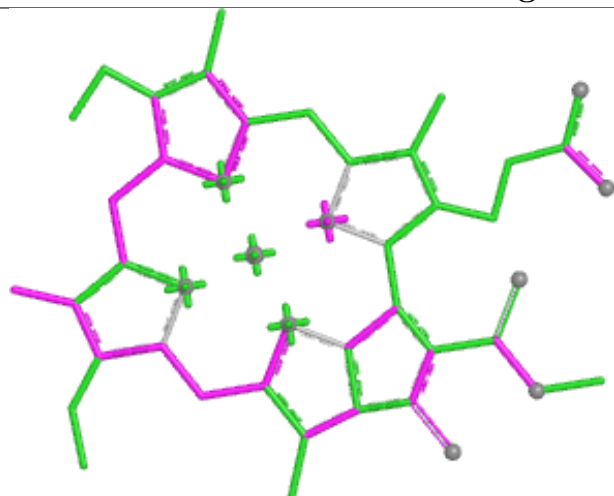




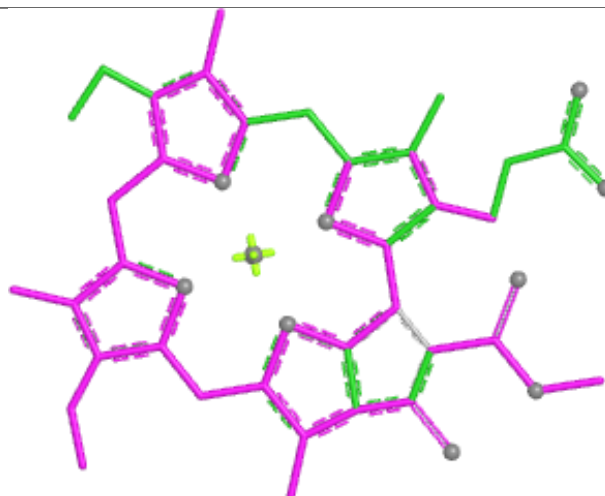
Ligand CLA y 610



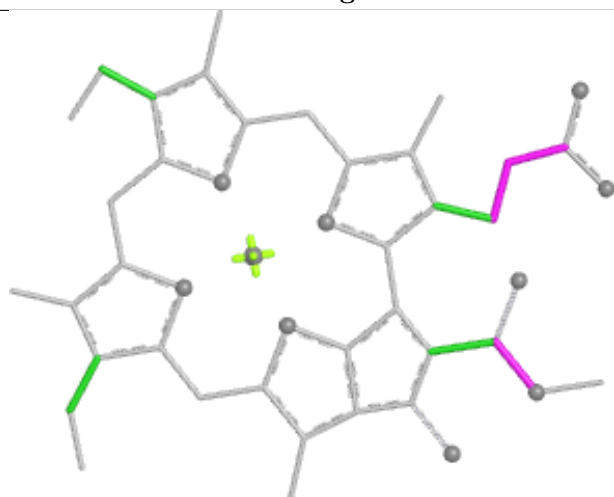
Ligand CLA 3 304



Bond lengths



Bond angles

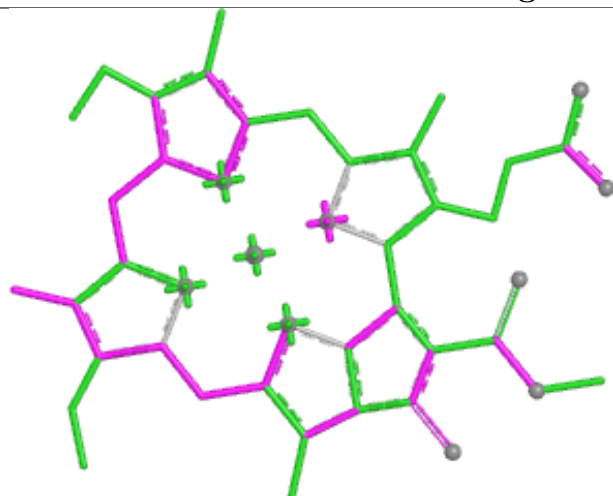


Torsions

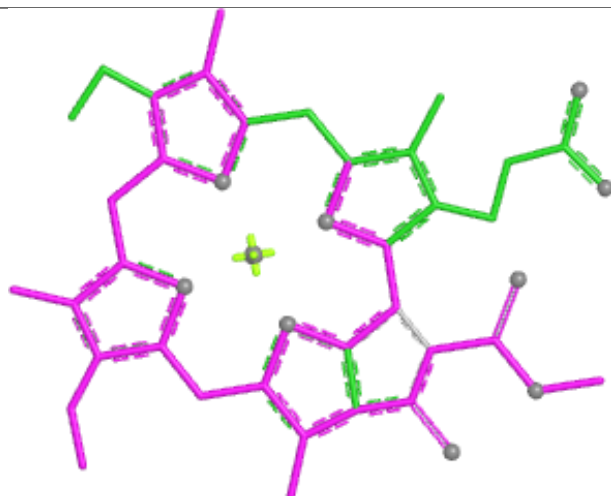


Rings

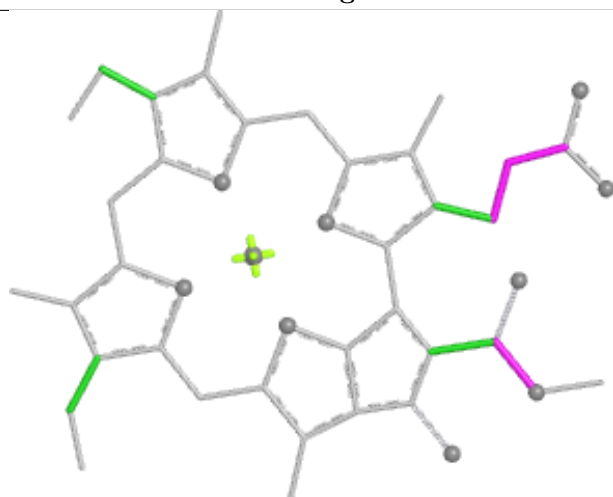
Ligand CLA 3 311



Bond lengths



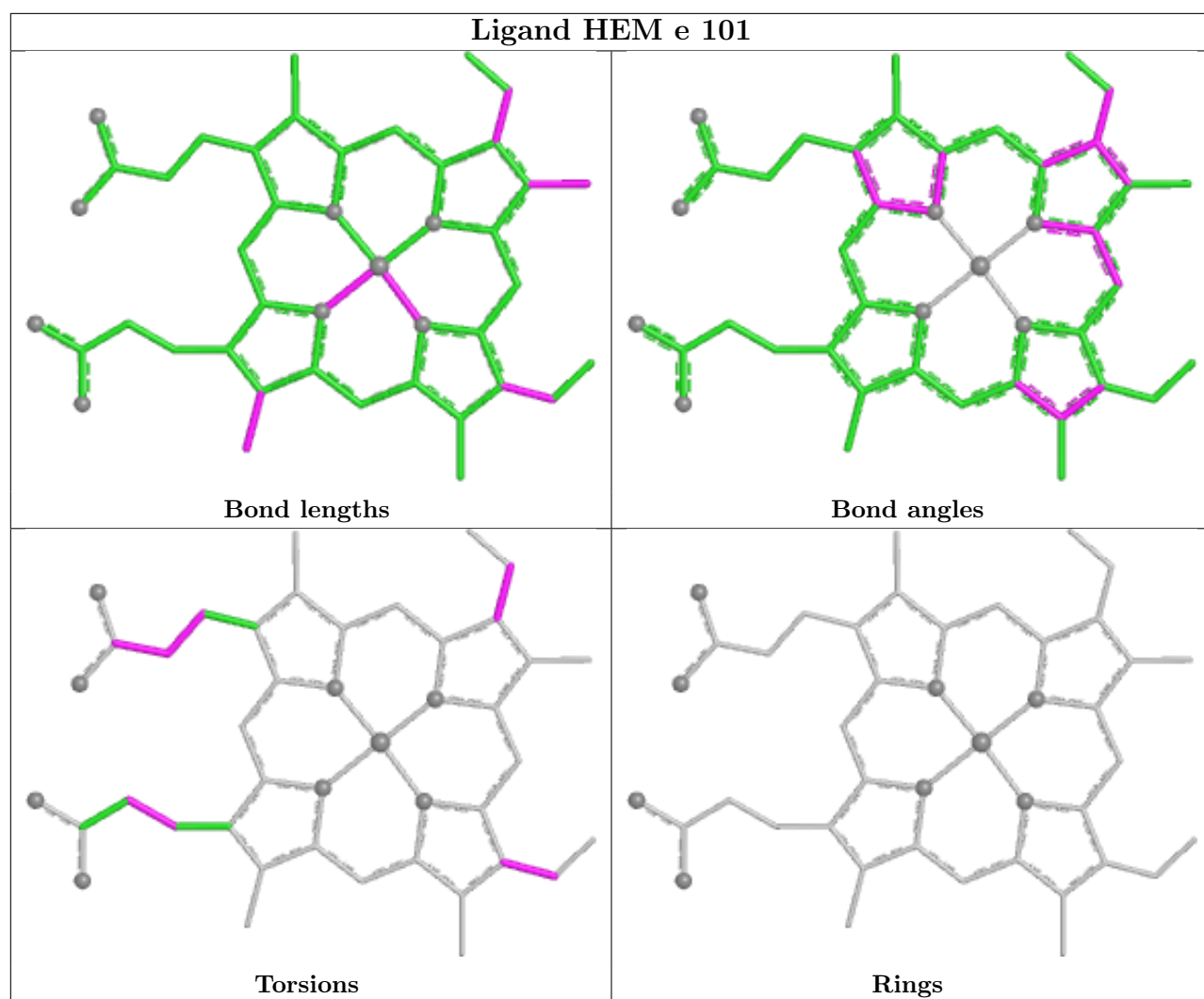
Bond angles



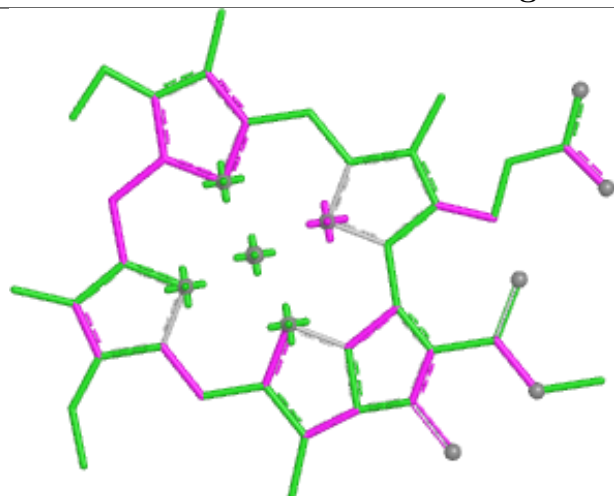
Torsions



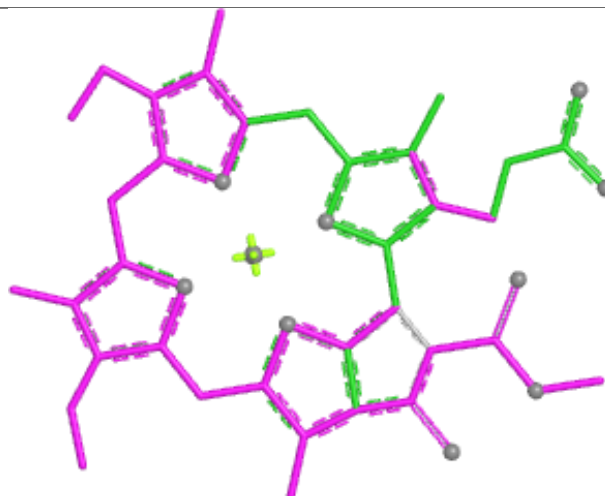
Rings



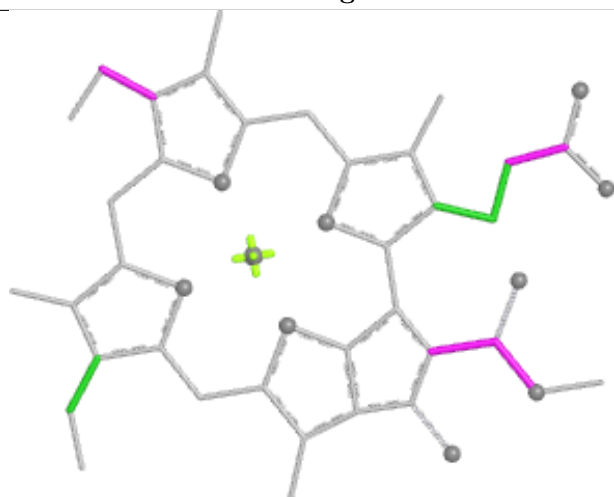
Ligand CLA c 502



Bond lengths



Bond angles

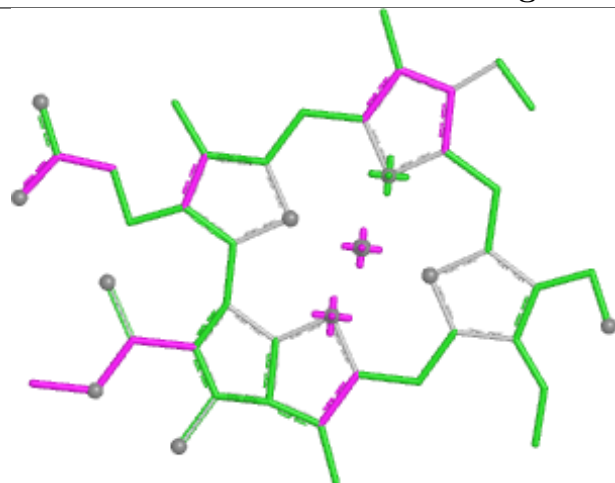


Torsions

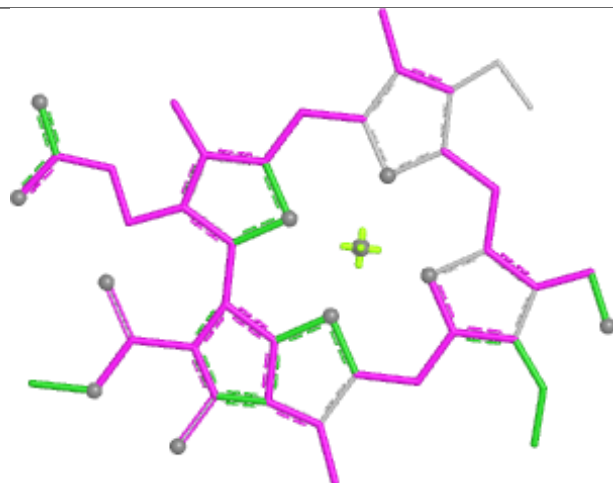


Rings

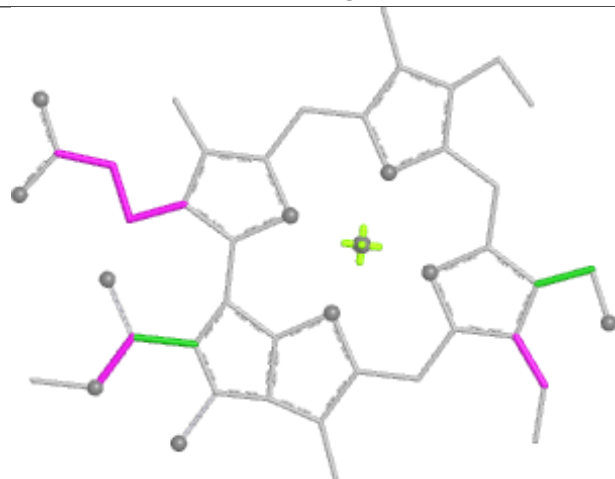
Ligand CHL S 306



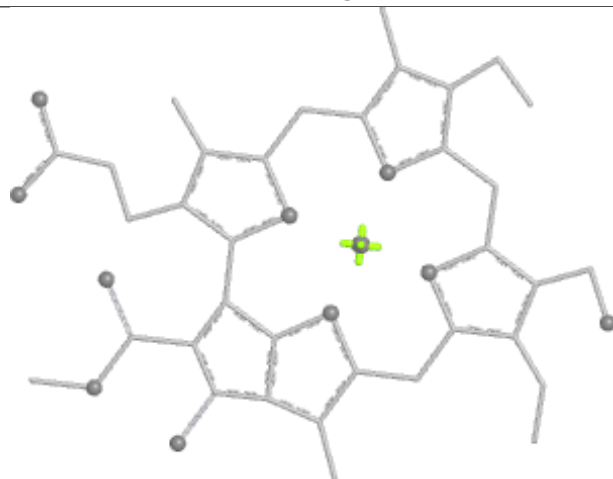
Bond lengths



Bond angles

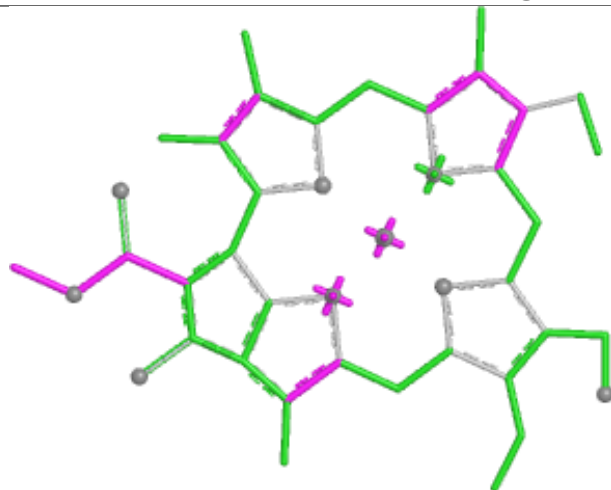


Torsions

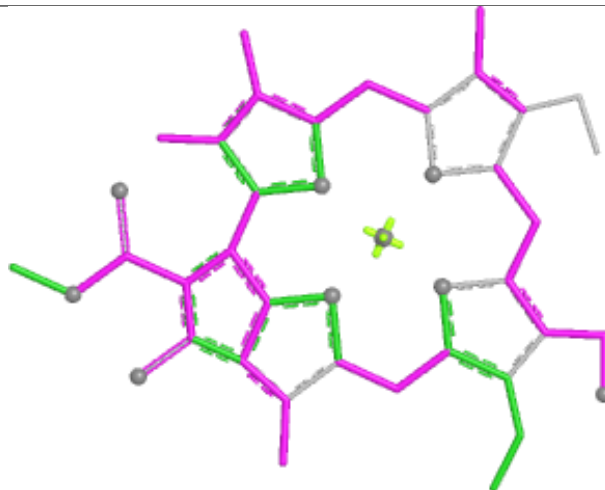


Rings

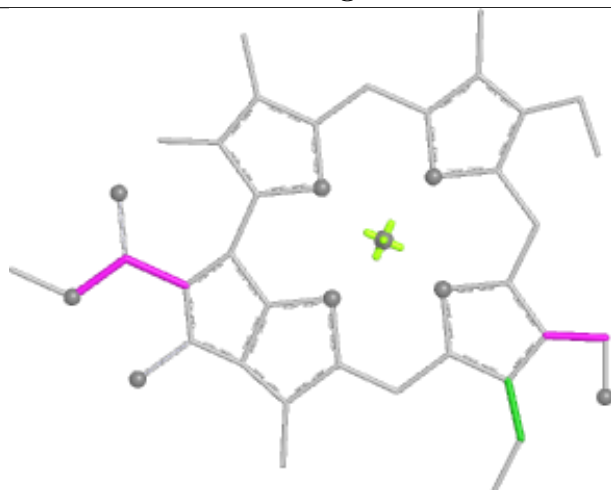
Ligand CHL 5 605



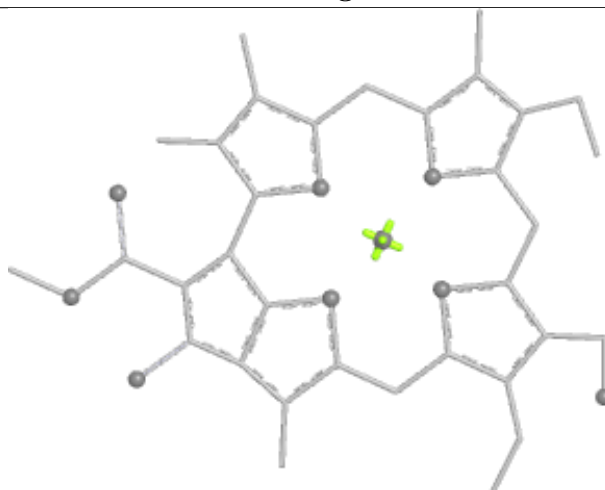
Bond lengths



Bond angles

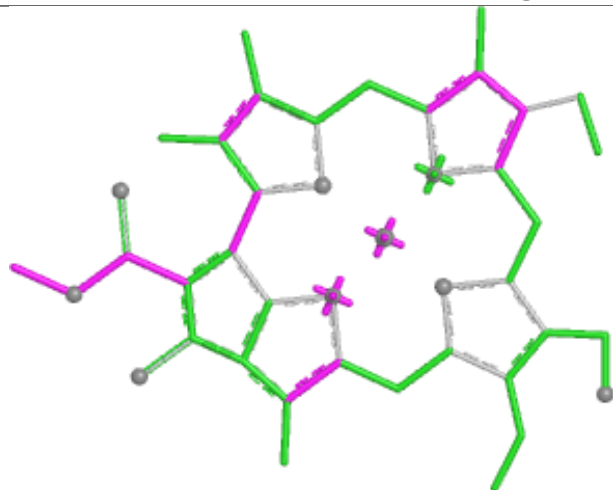


Torsions

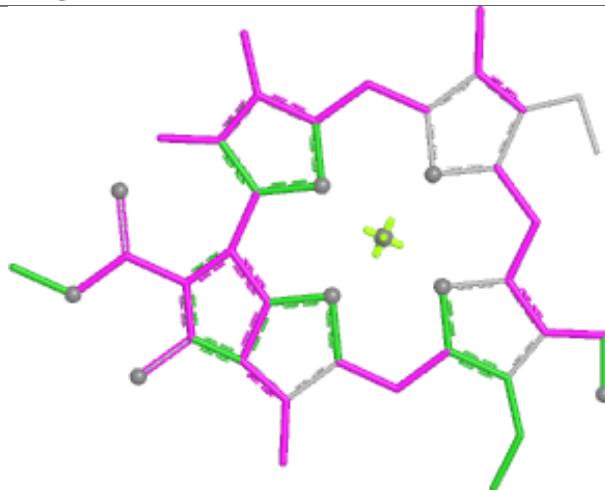


Rings

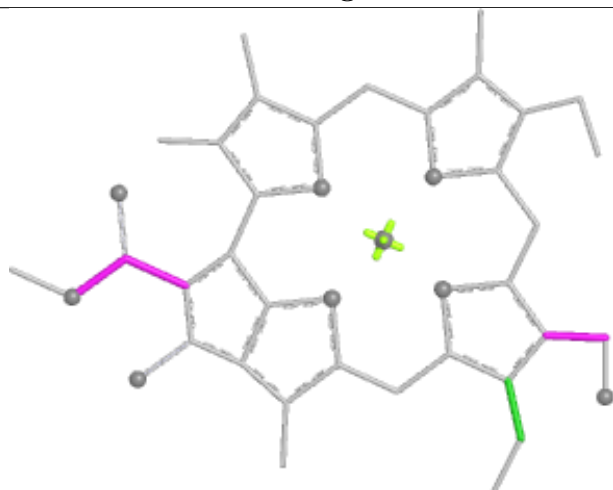
Ligand CHL g 605



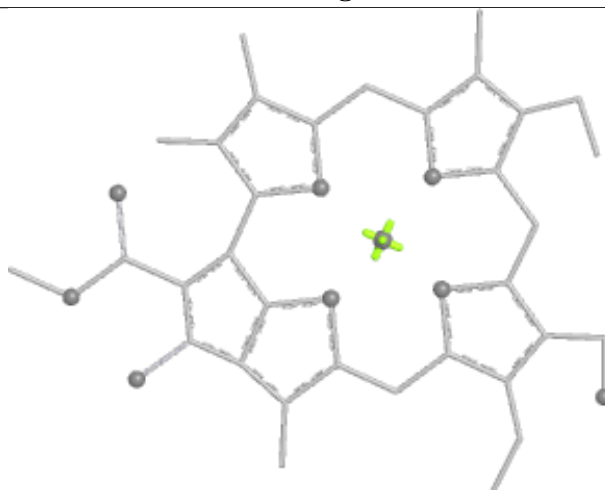
Bond lengths



Bond angles

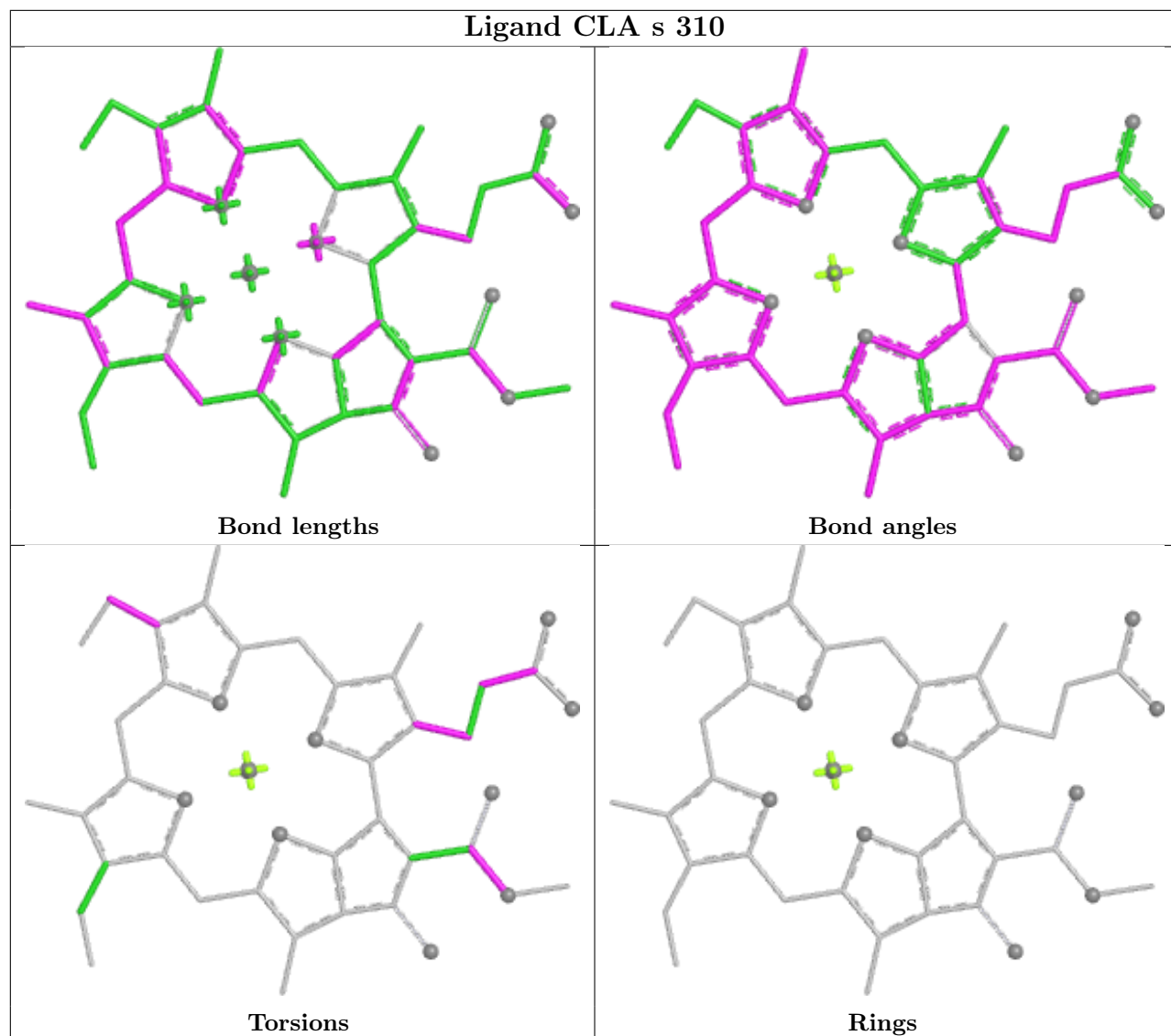


Torsions

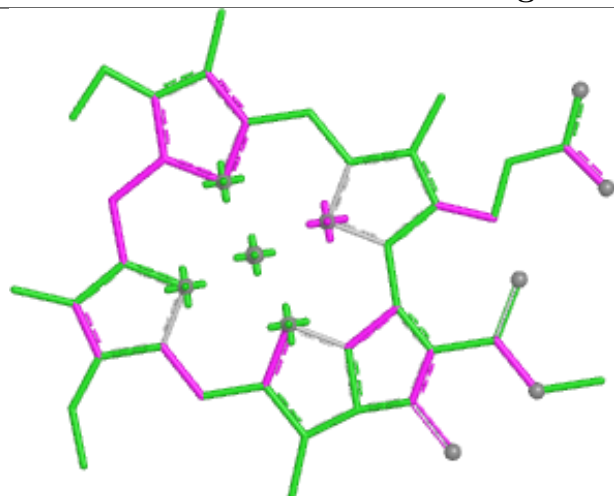


Rings

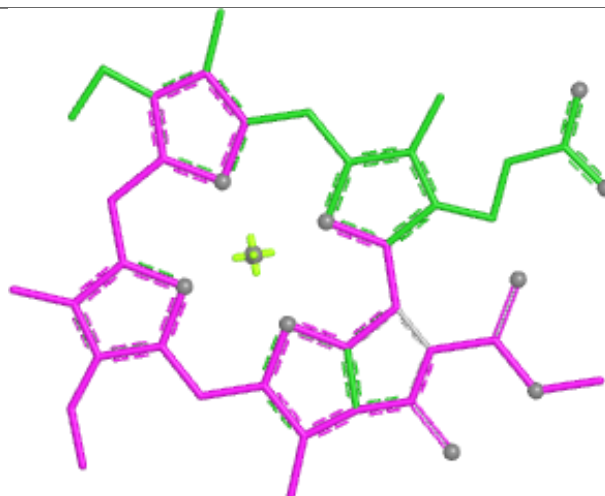
Ligand CLA s 310



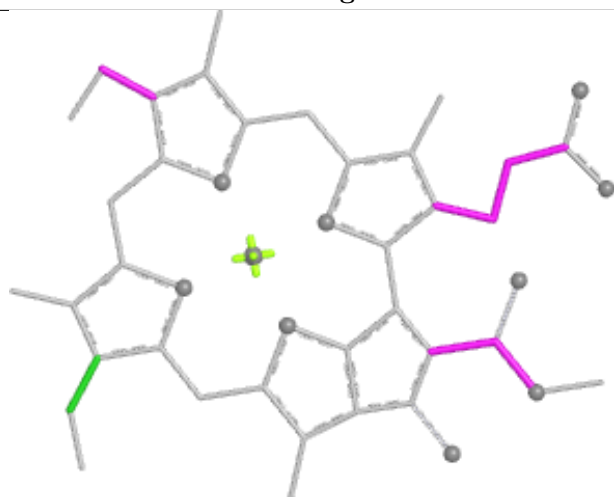
Ligand CLA S 303



Bond lengths



Bond angles

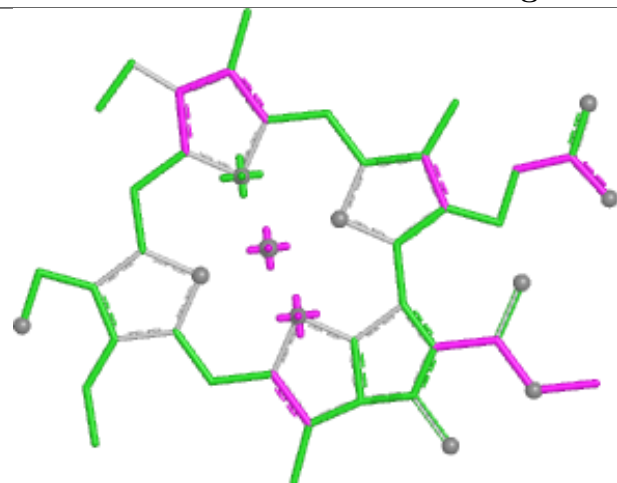


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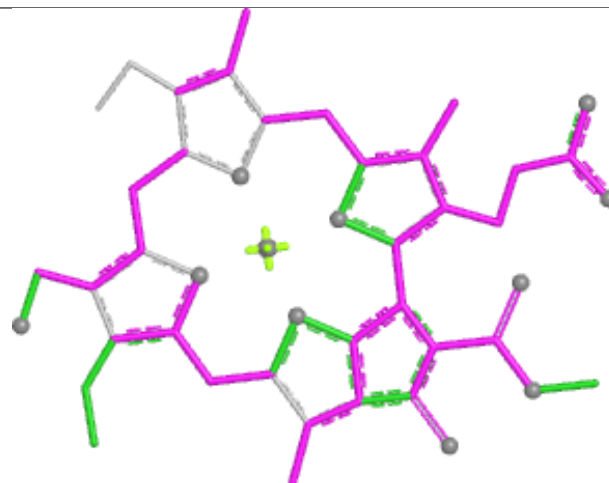


Rings

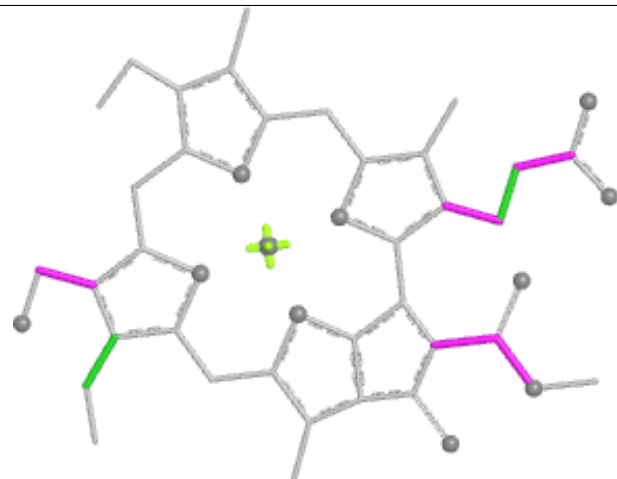
Ligand CHL S 307



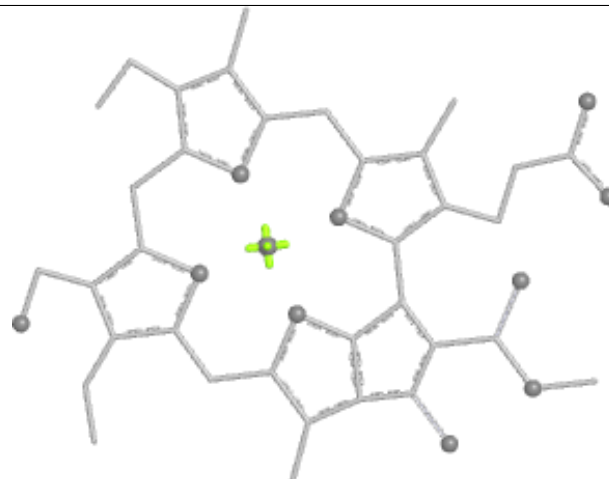
Bond lengths



Bond angles

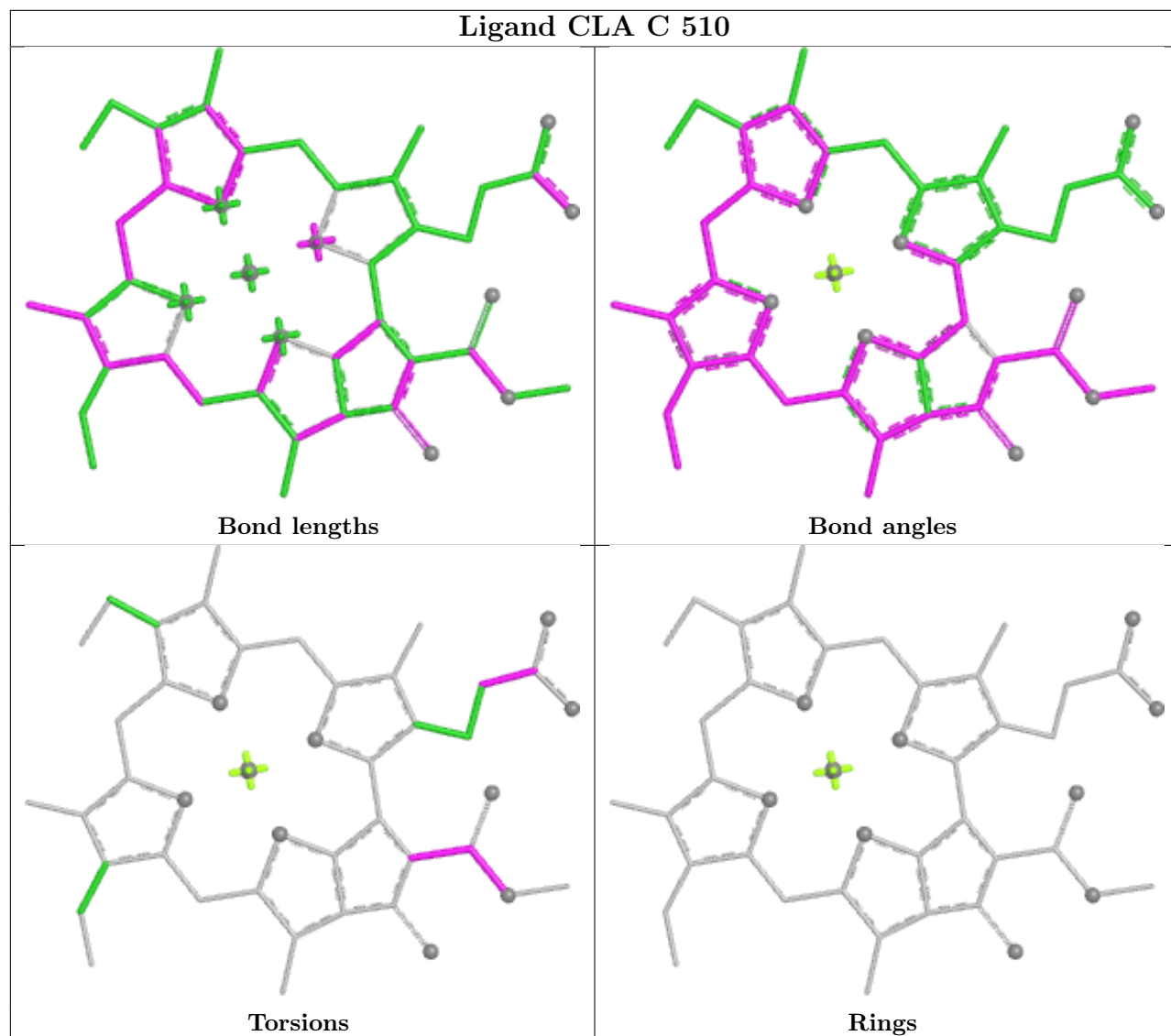


Torsions

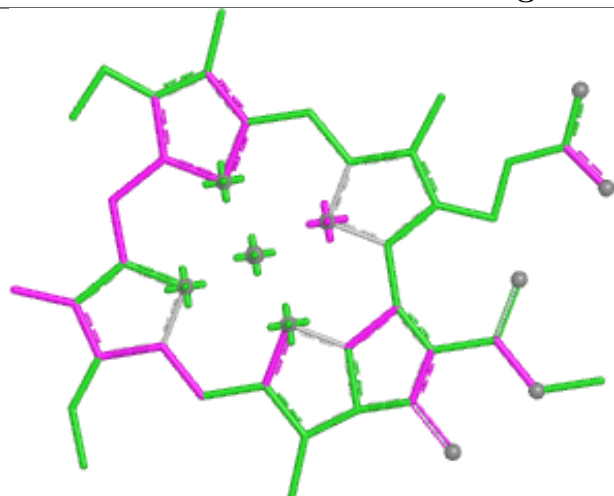


Rings

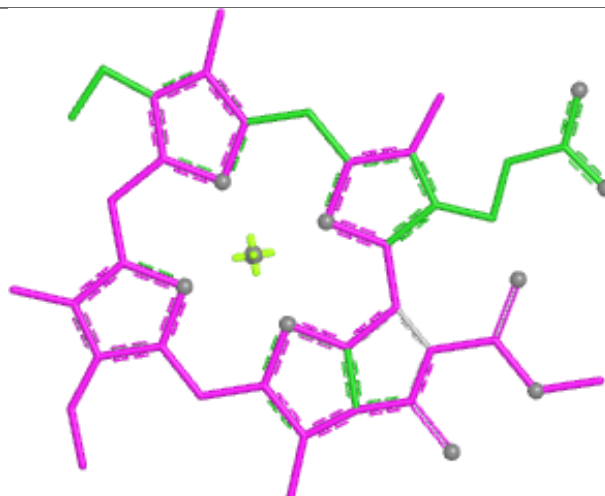
Ligand CLA C 510



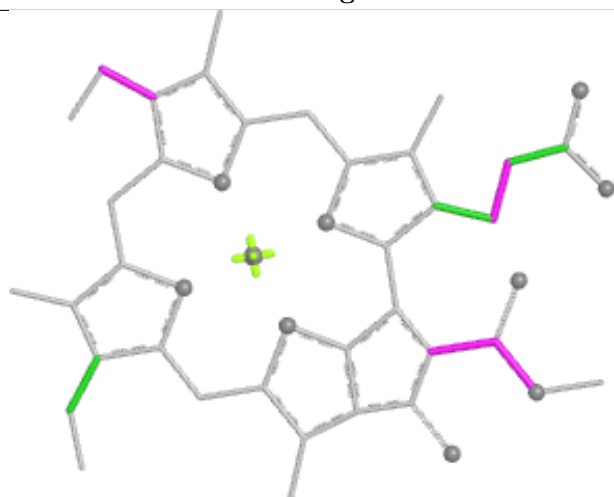
Ligand CLA b 609



Bond lengths



Bond angles

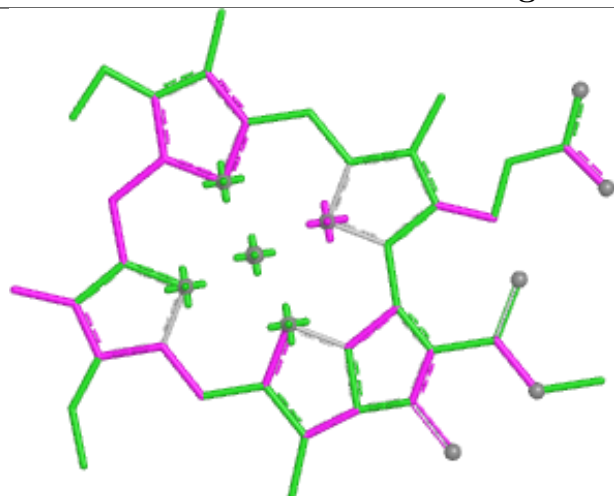


Torsions

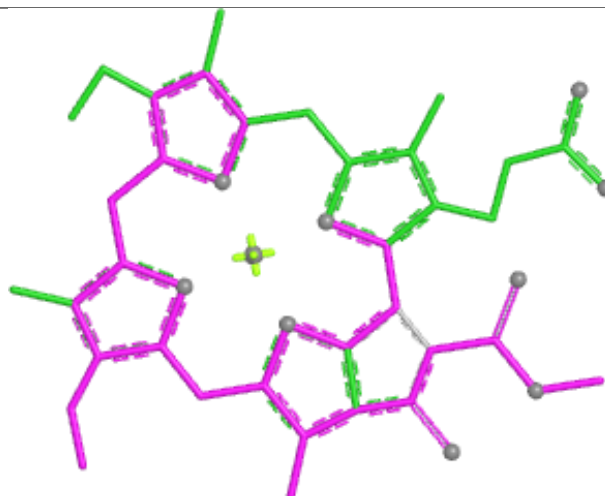


Rings

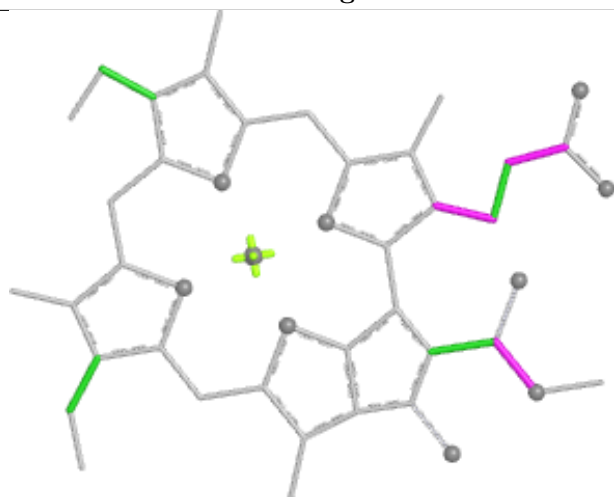
Ligand CLA 6 613



Bond lengths



Bond angles

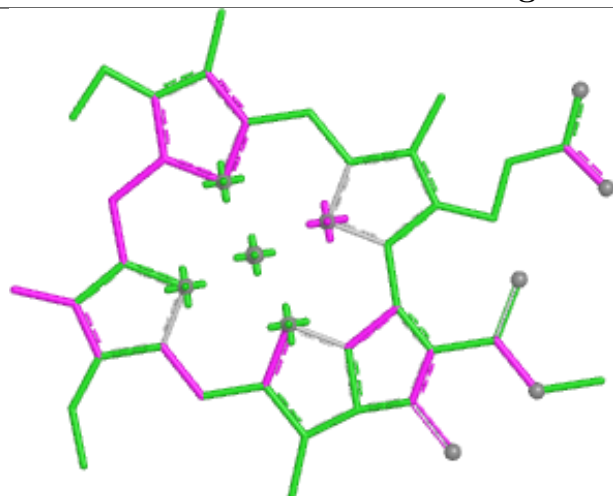


Torsions

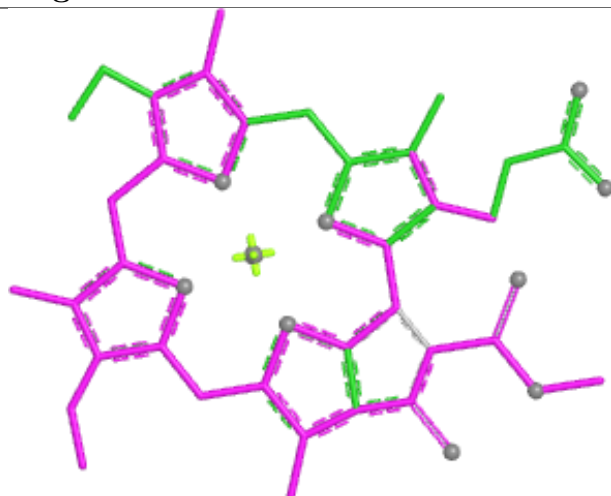


Rings

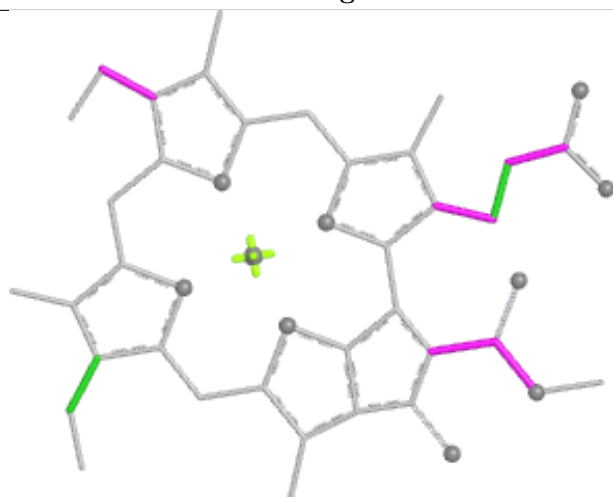
Ligand CLA g 612



Bond lengths



Bond angles

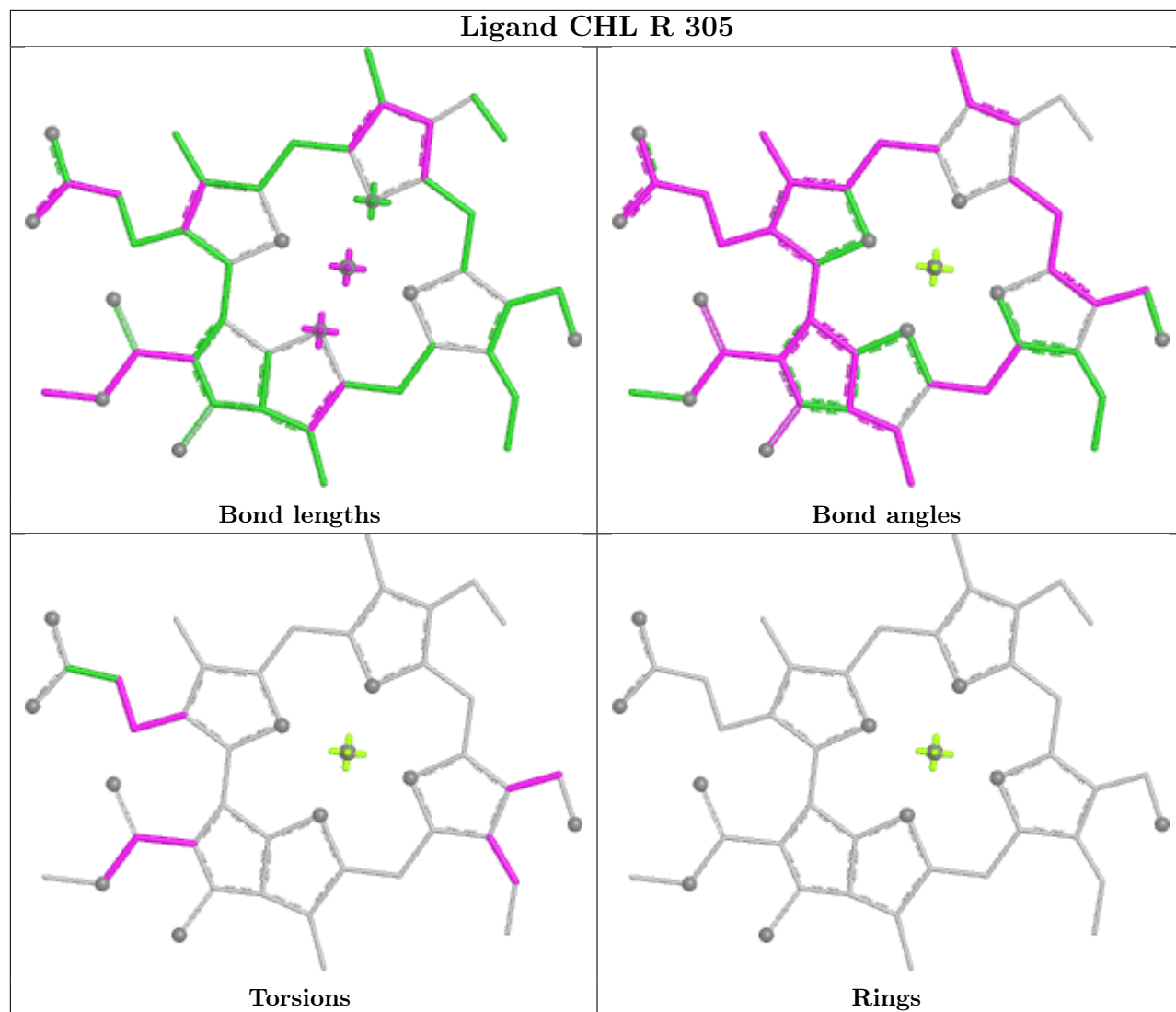


Torsions

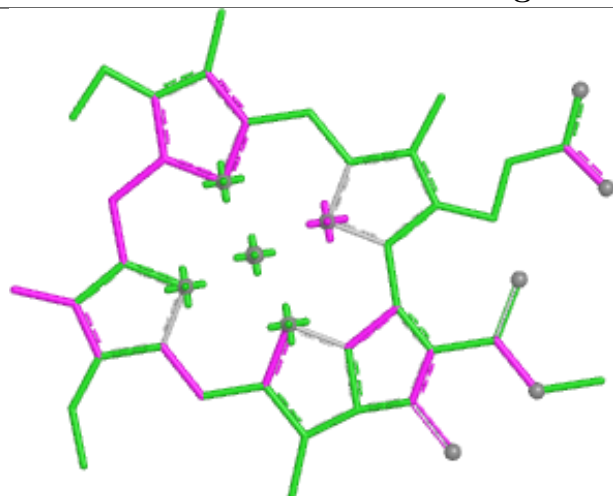


Rings

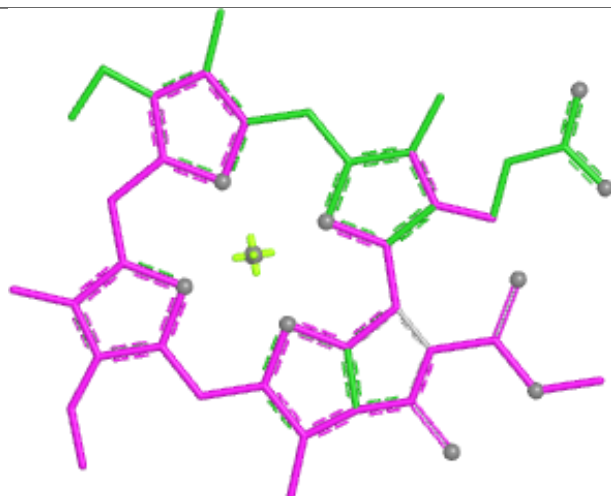
Ligand CHL R 305



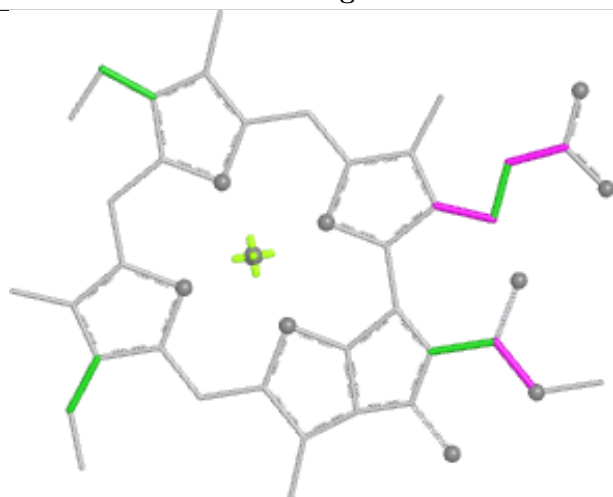
Ligand CLA Y 614



Bond lengths



Bond angles

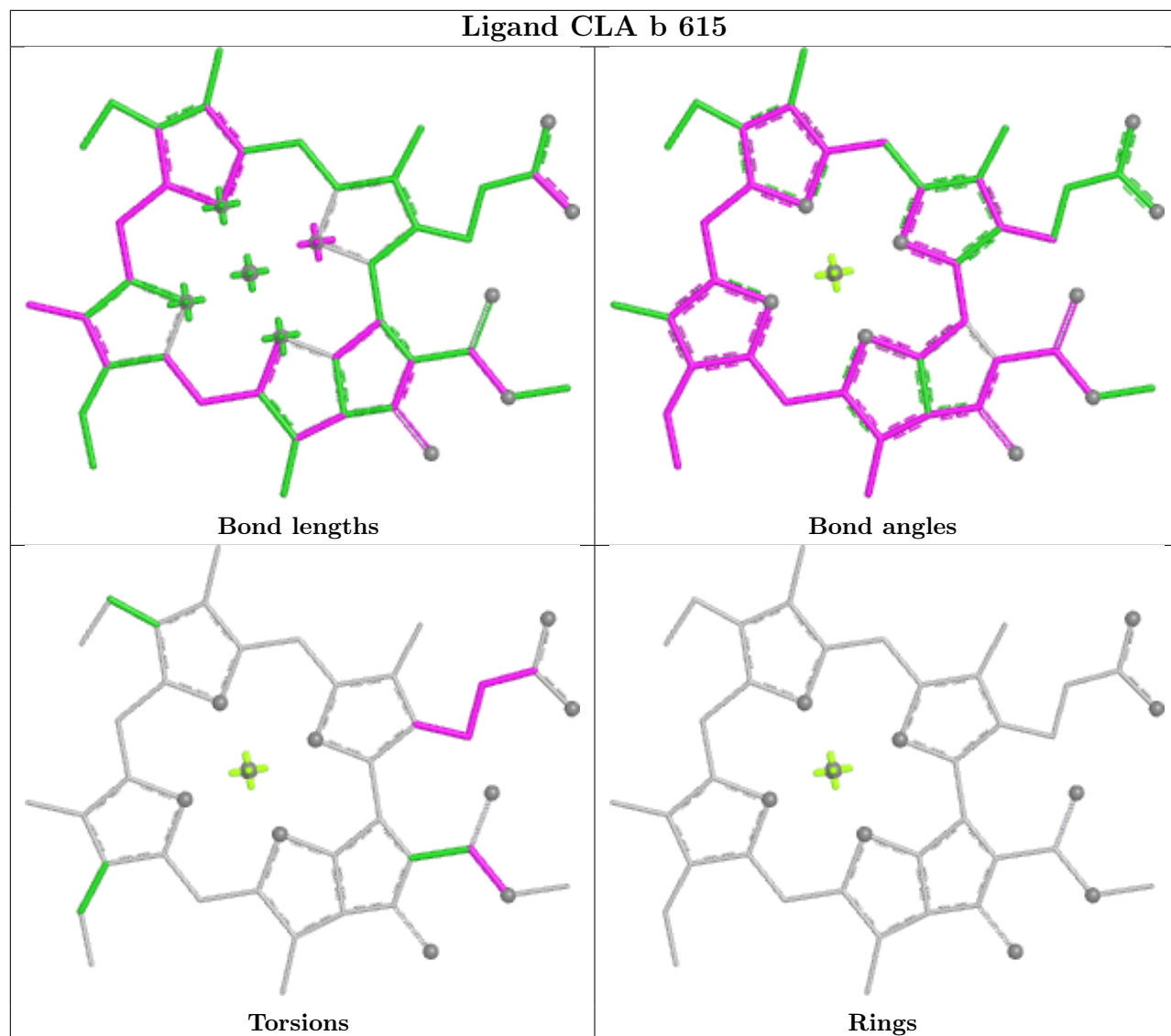


Torsions

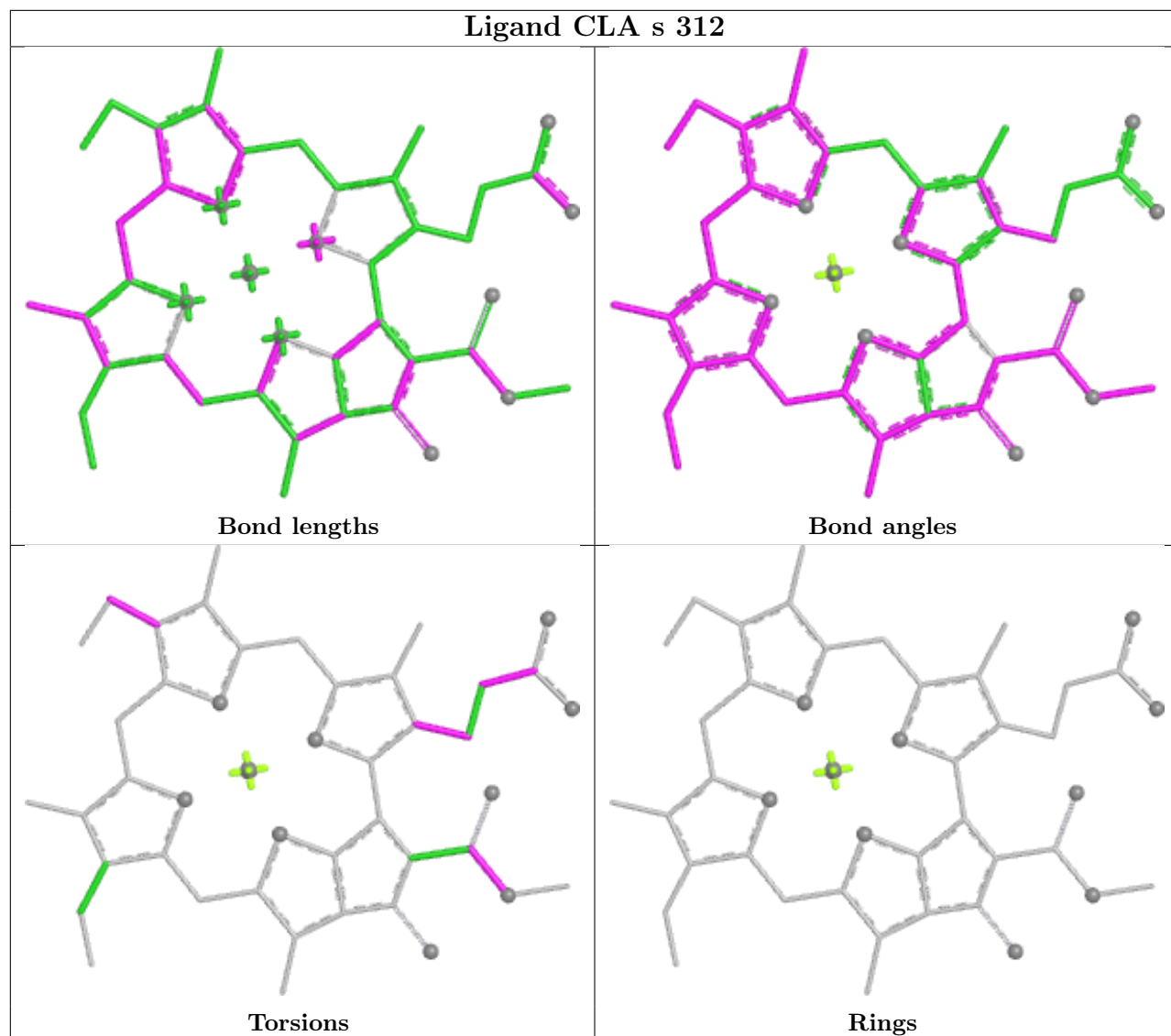


Rings

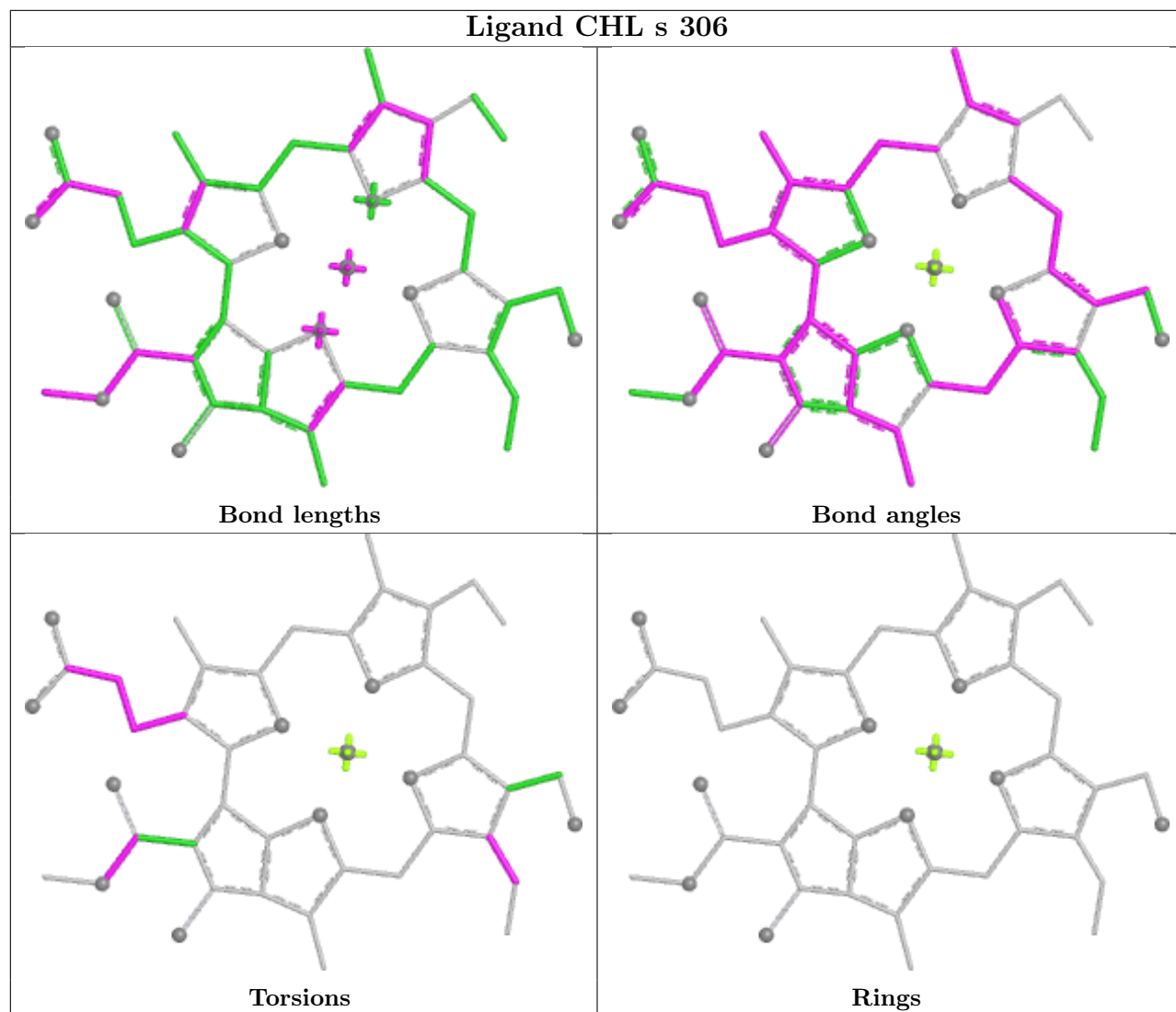
Ligand CLA b 615



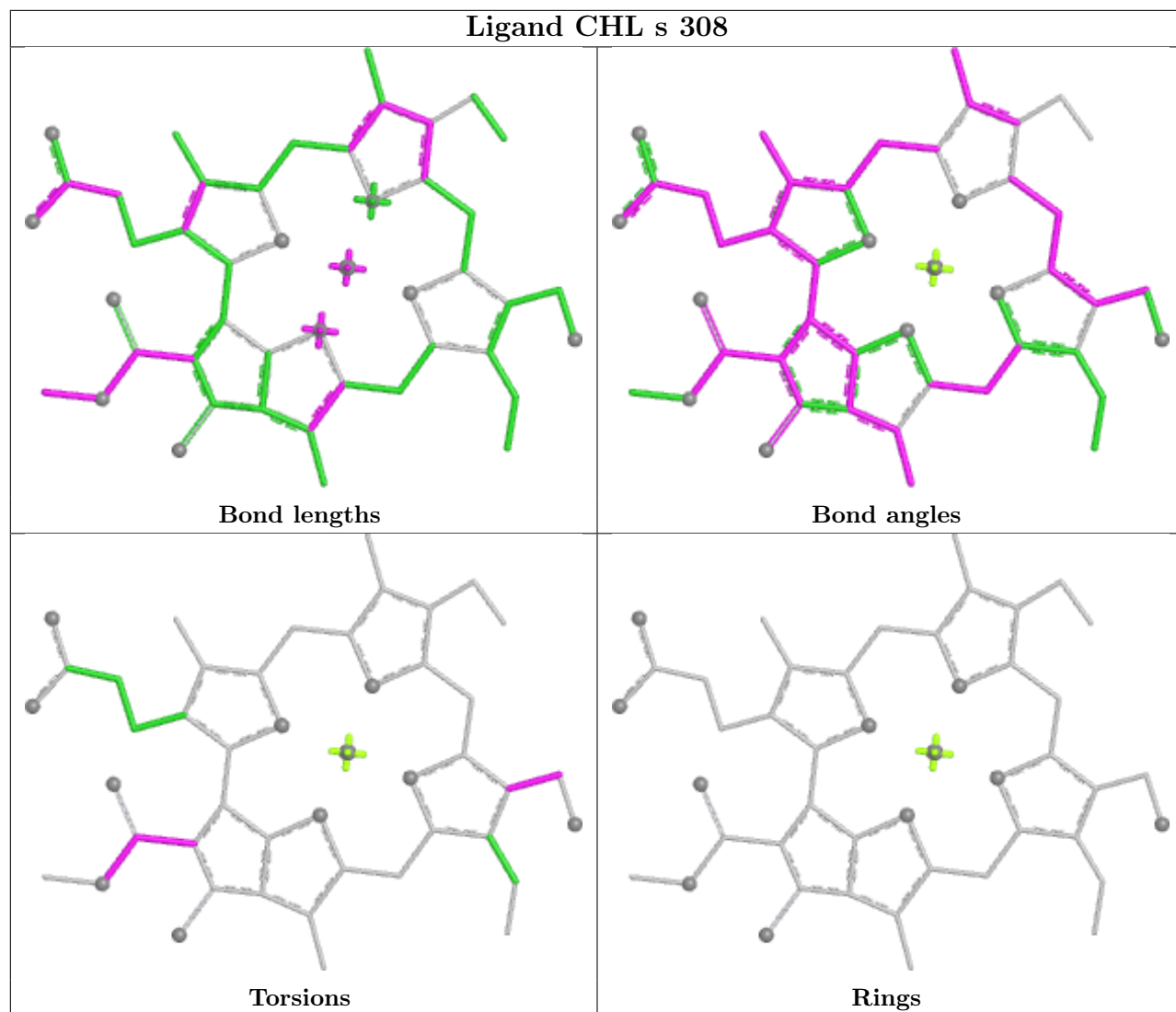
Ligand CLA s 312



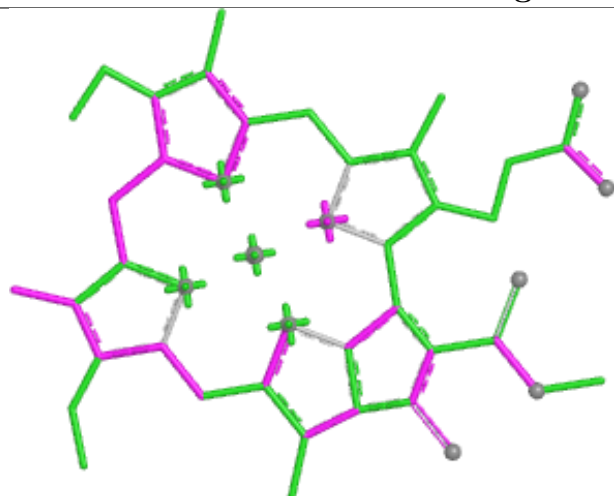
Ligand CHL s 306



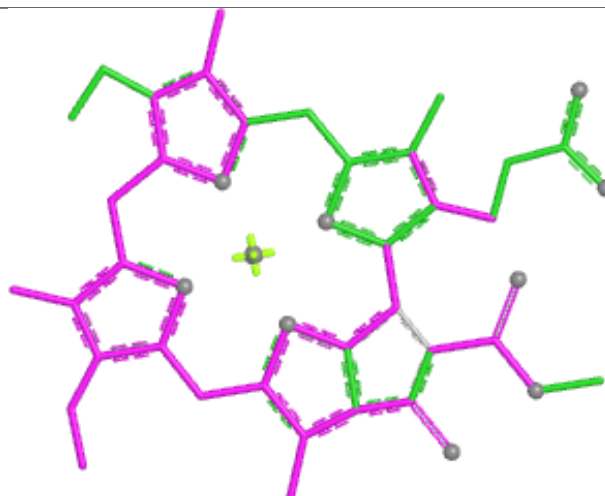
Ligand CHL s 308



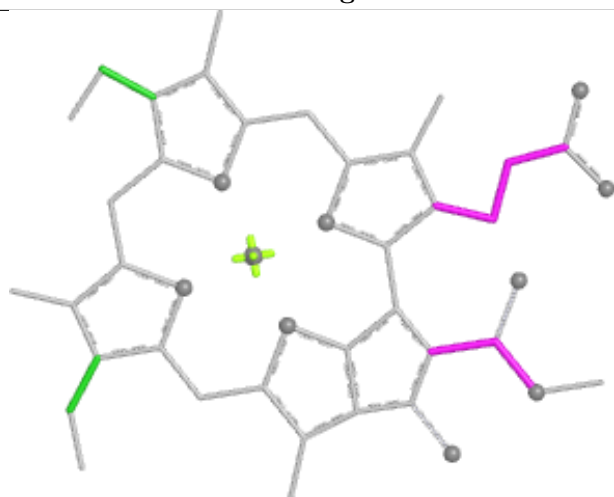
Ligand CLA C 504



Bond lengths



Bond angles

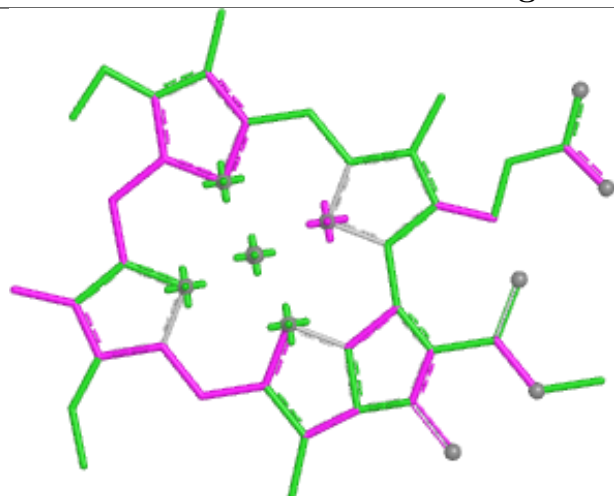


Torsions

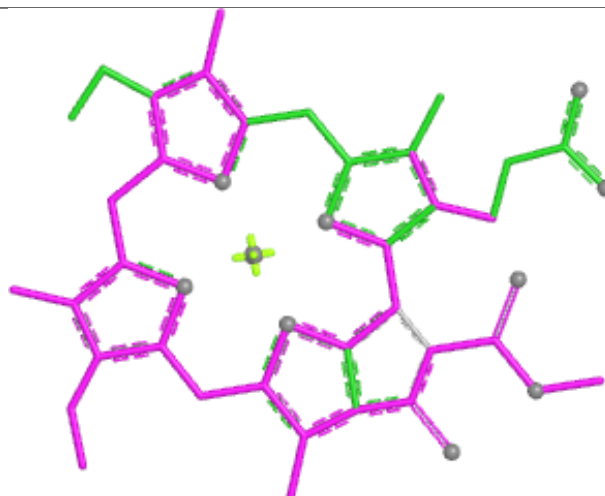


Rings

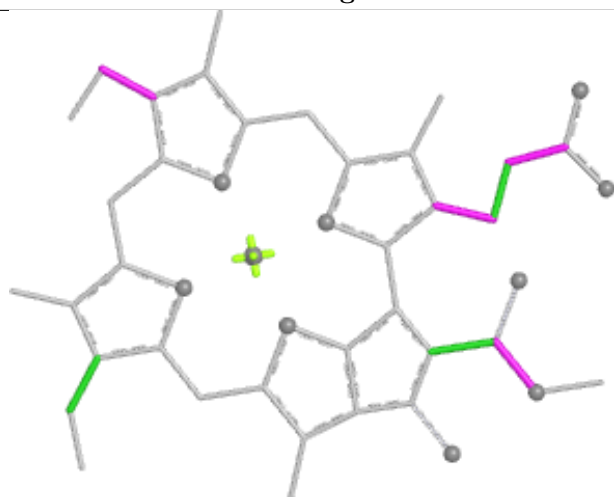
Ligand CLA 1 614



Bond lengths



Bond angles

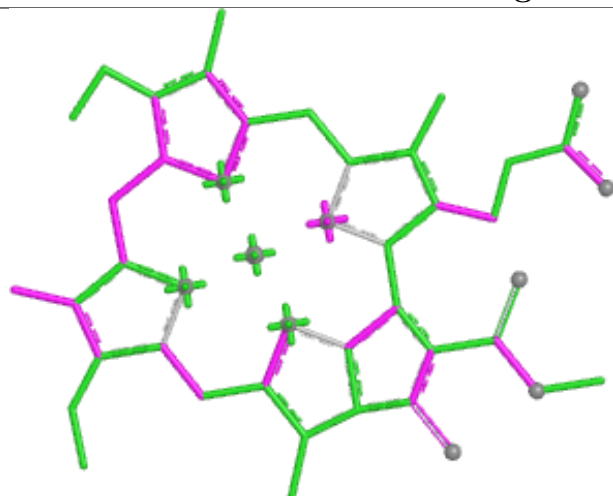


Torsions

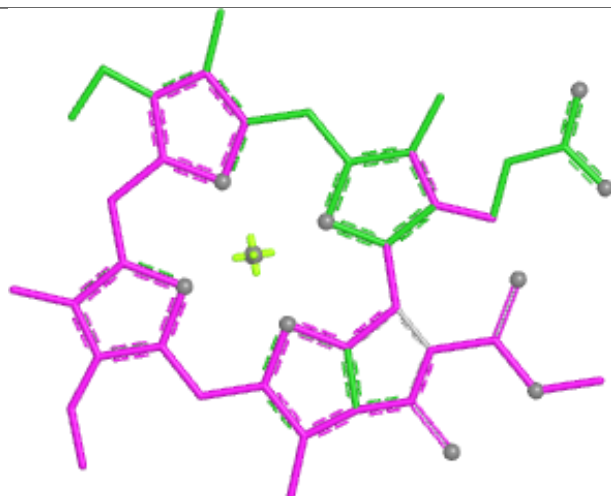


Rings

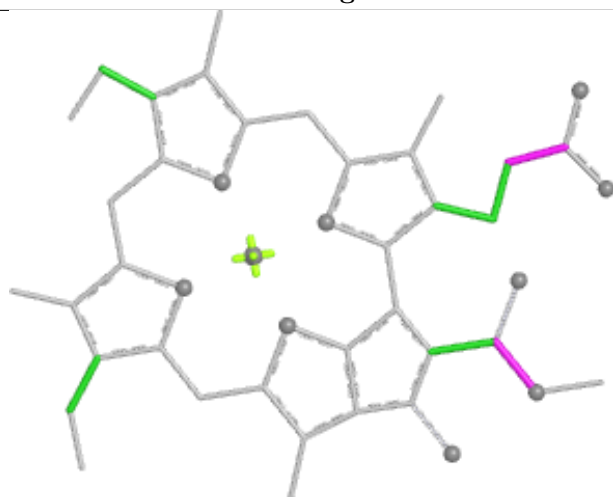
Ligand CLA B 608



Bond lengths



Bond angles

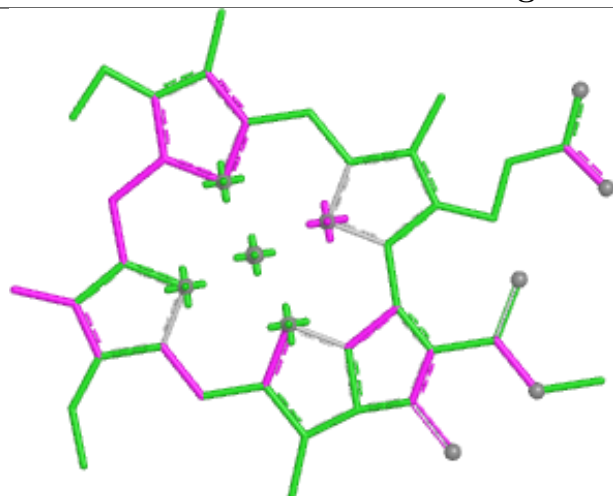


Torsions

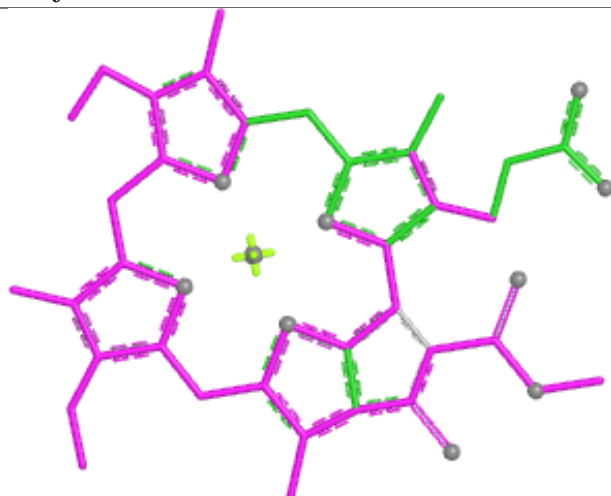


Rings

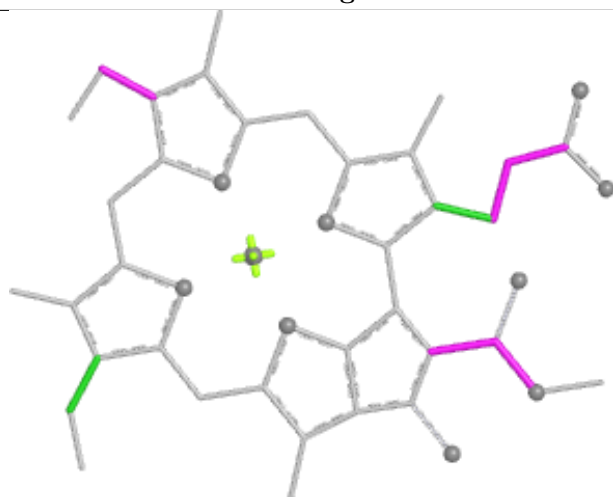
Ligand CLA y 603



Bond lengths



Bond angles

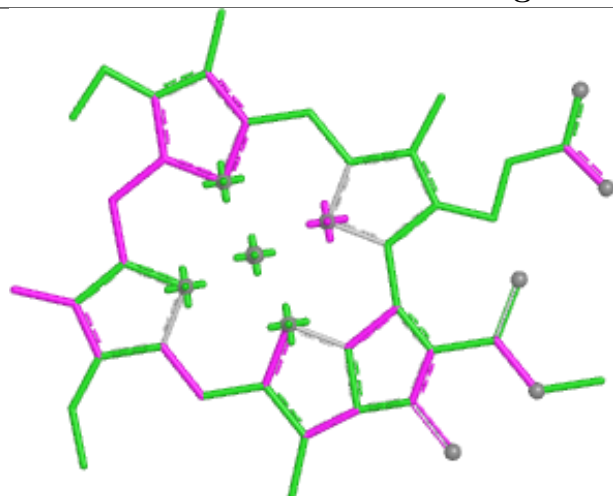


Torsions

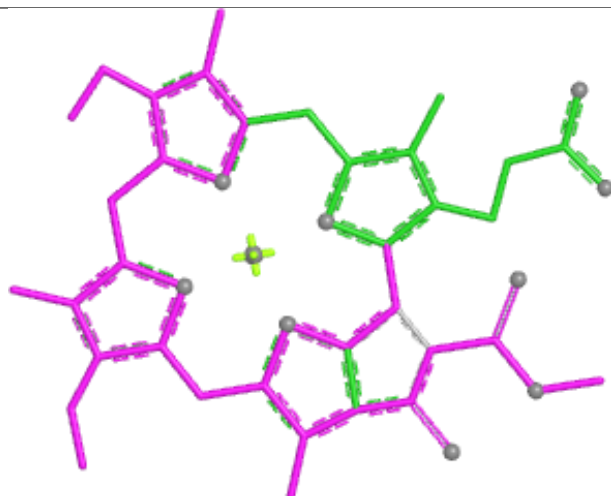


Rings

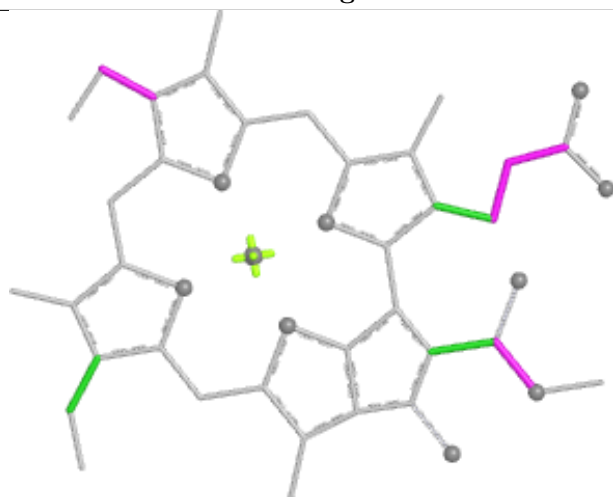
Ligand CLA R 311



Bond lengths



Bond angles

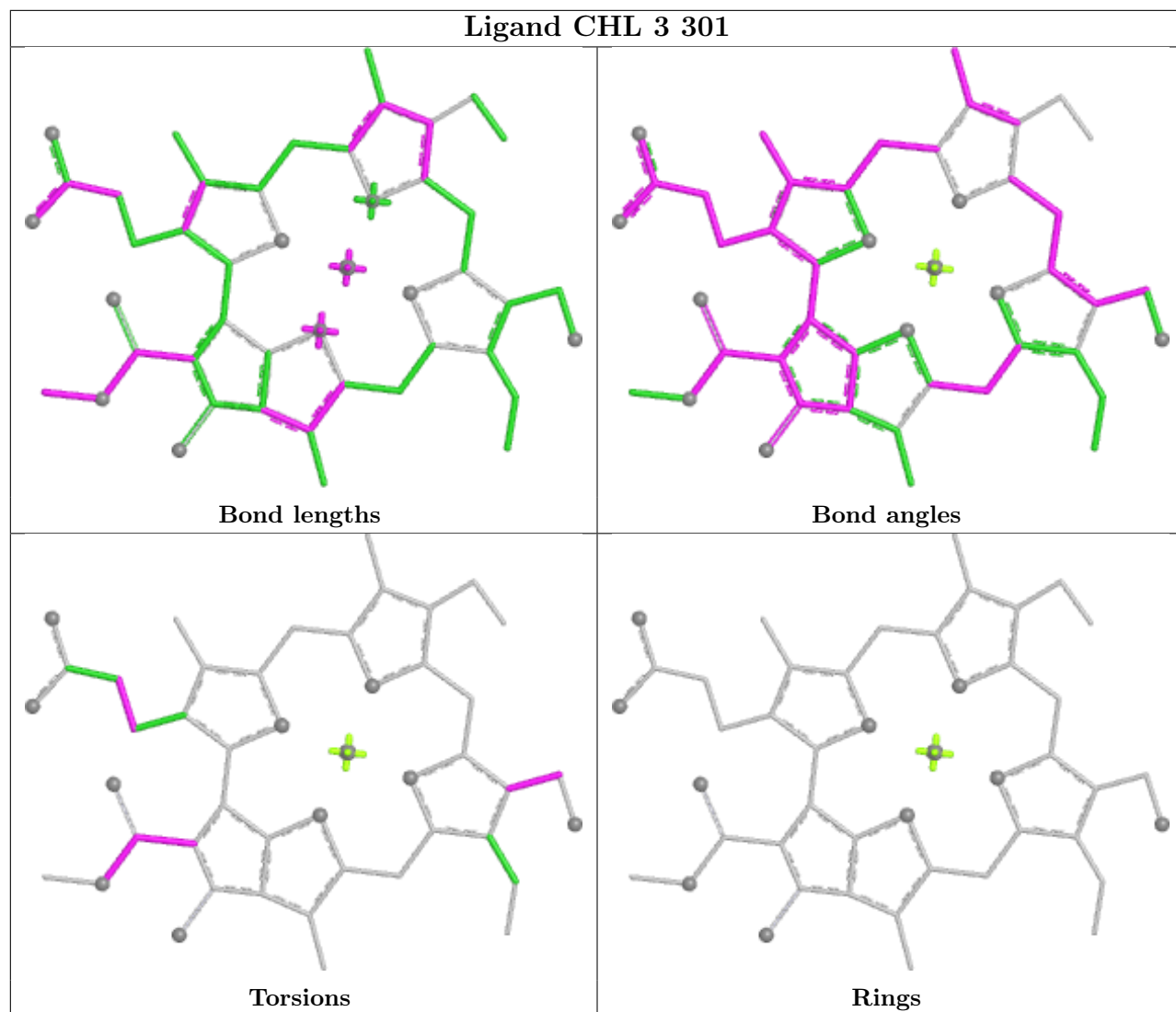


Torsions

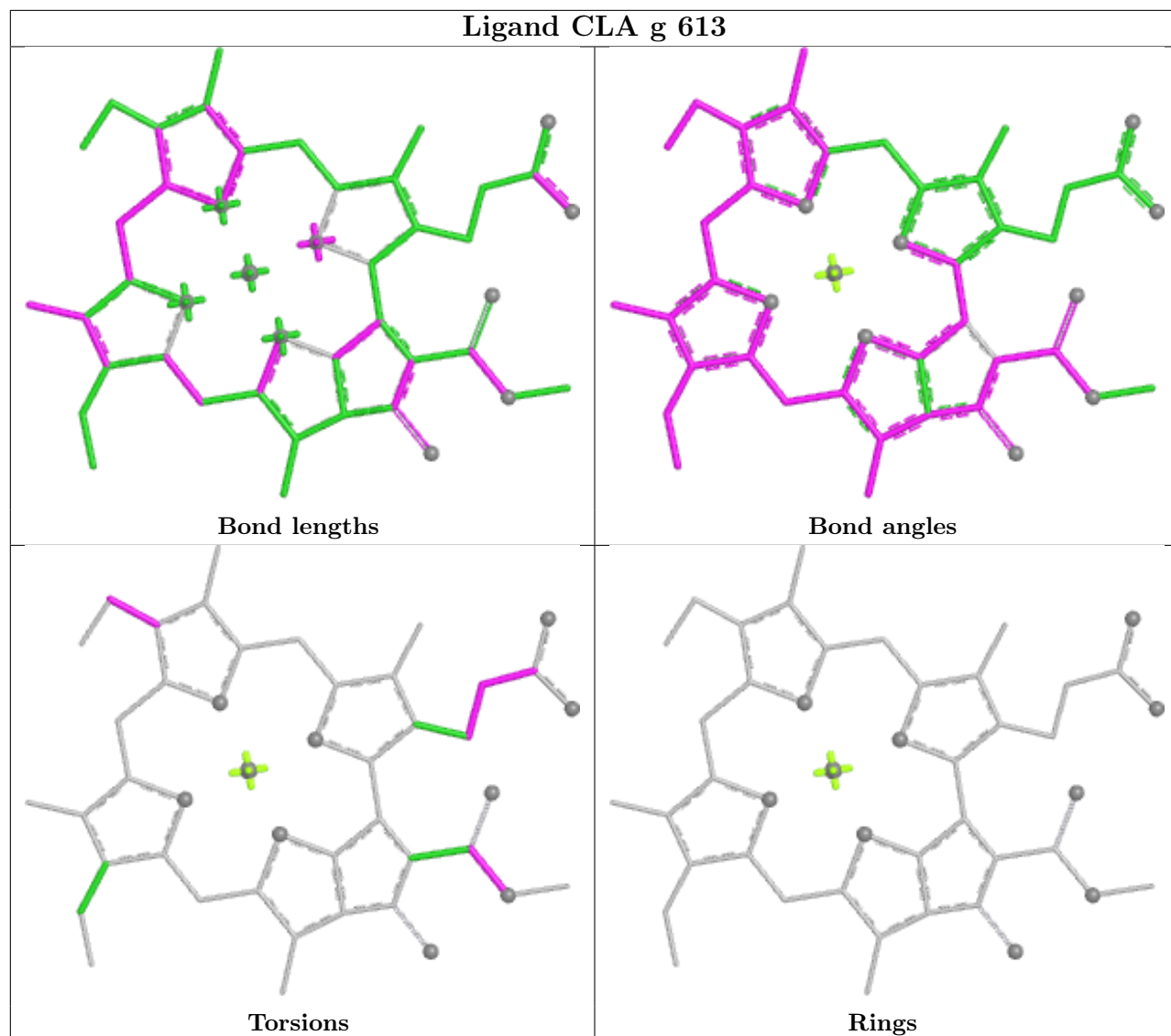


Rings

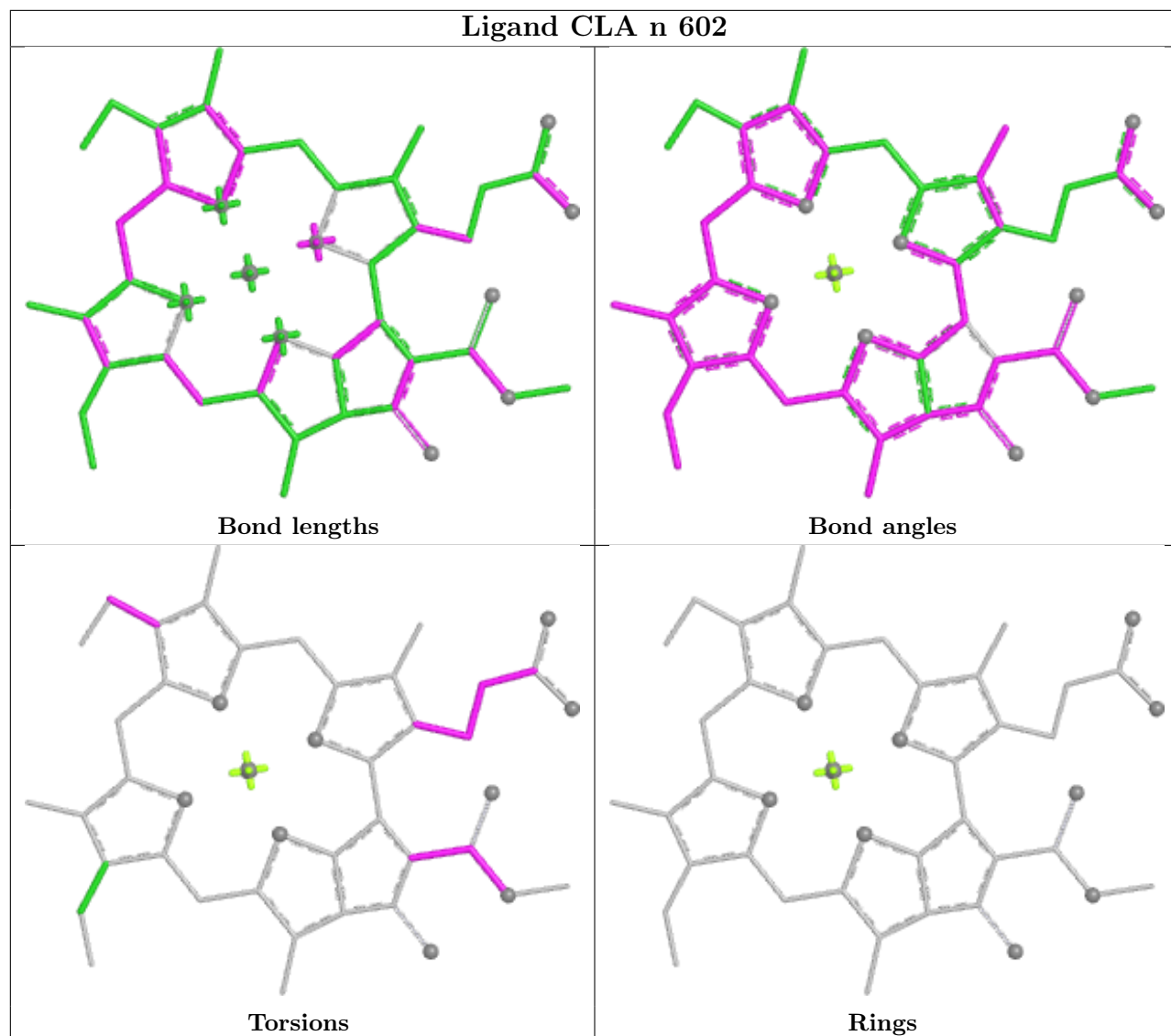
Ligand CHL 3 301



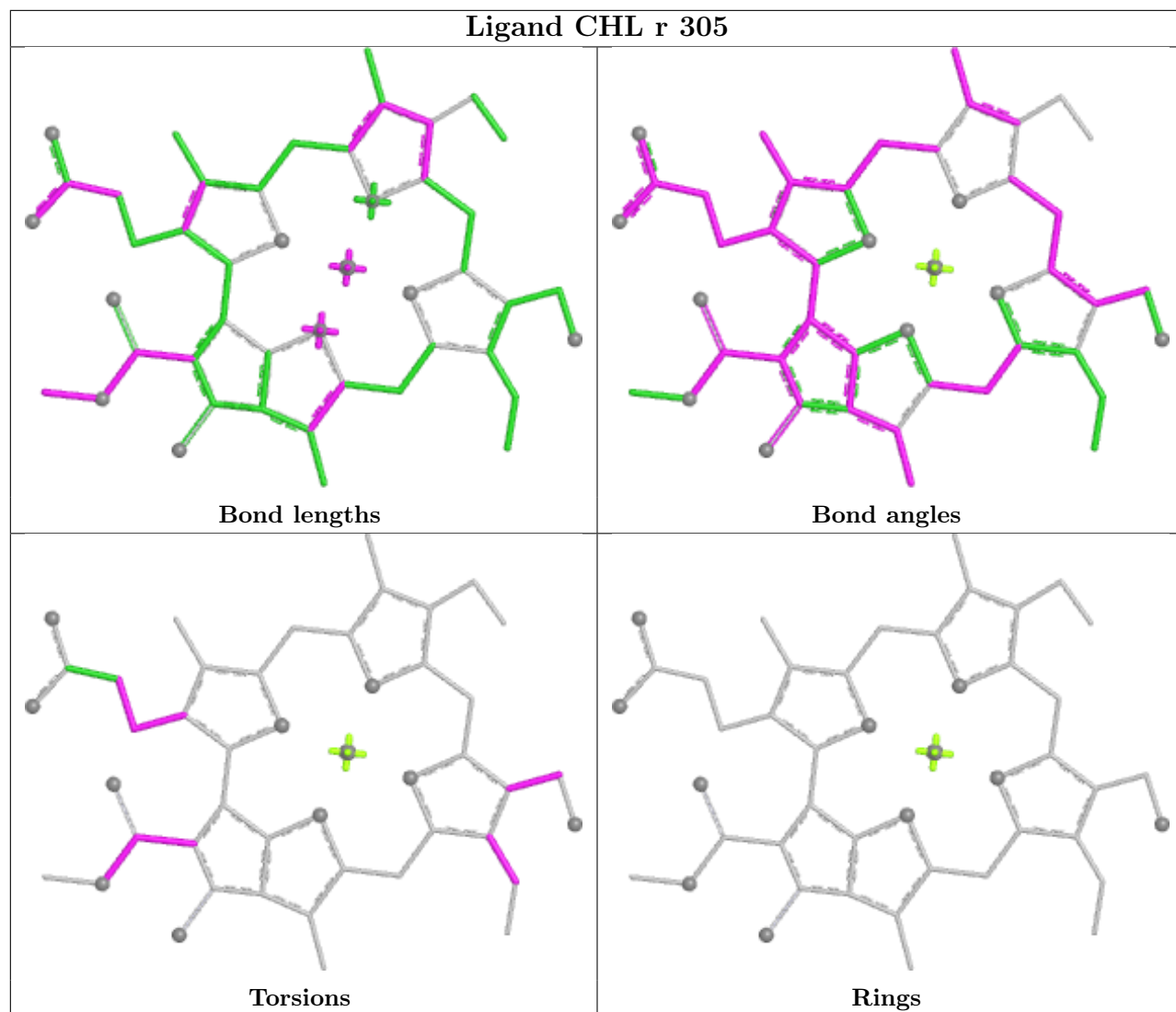
Ligand CLA g 613



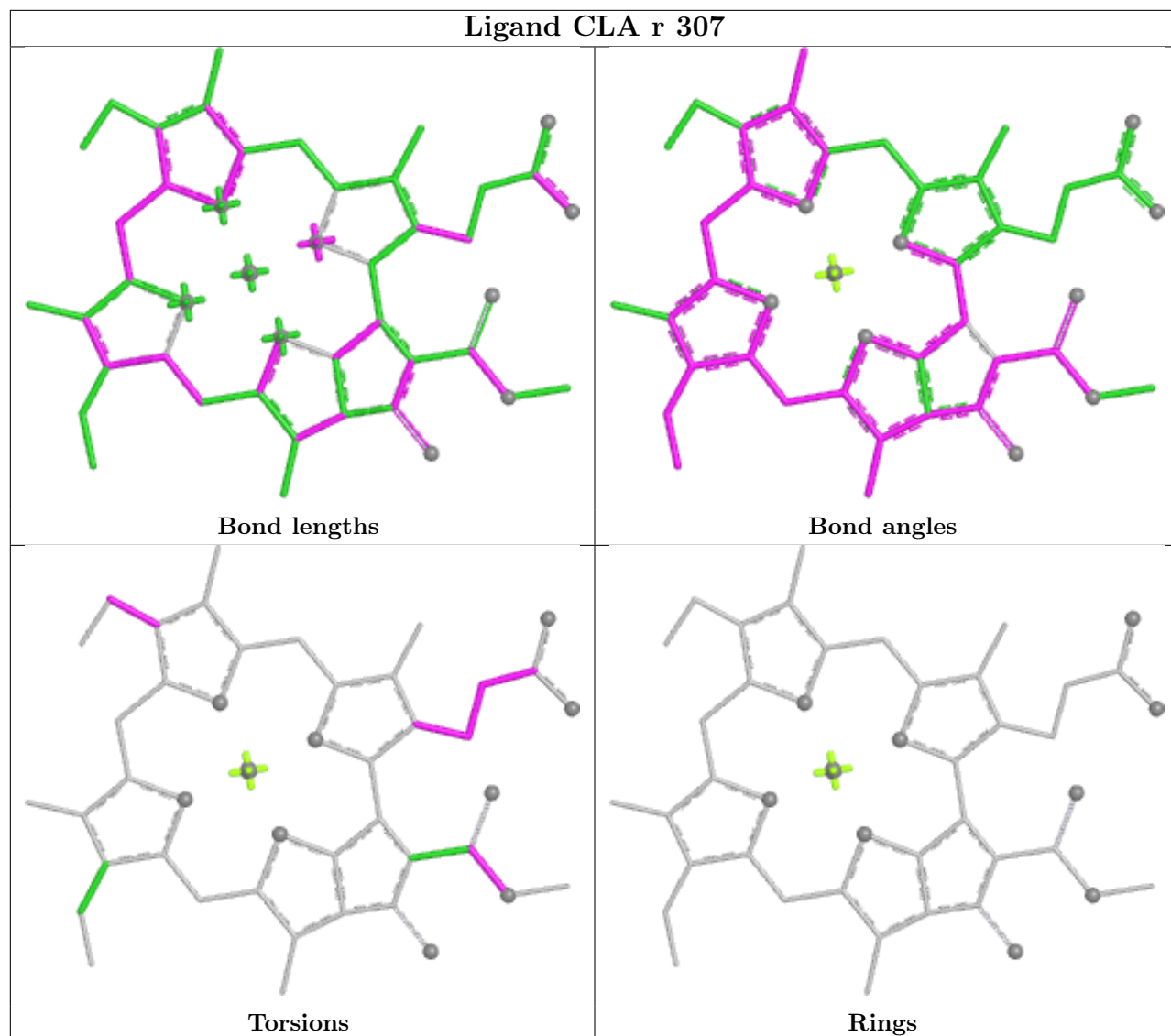
Ligand CLA n 602



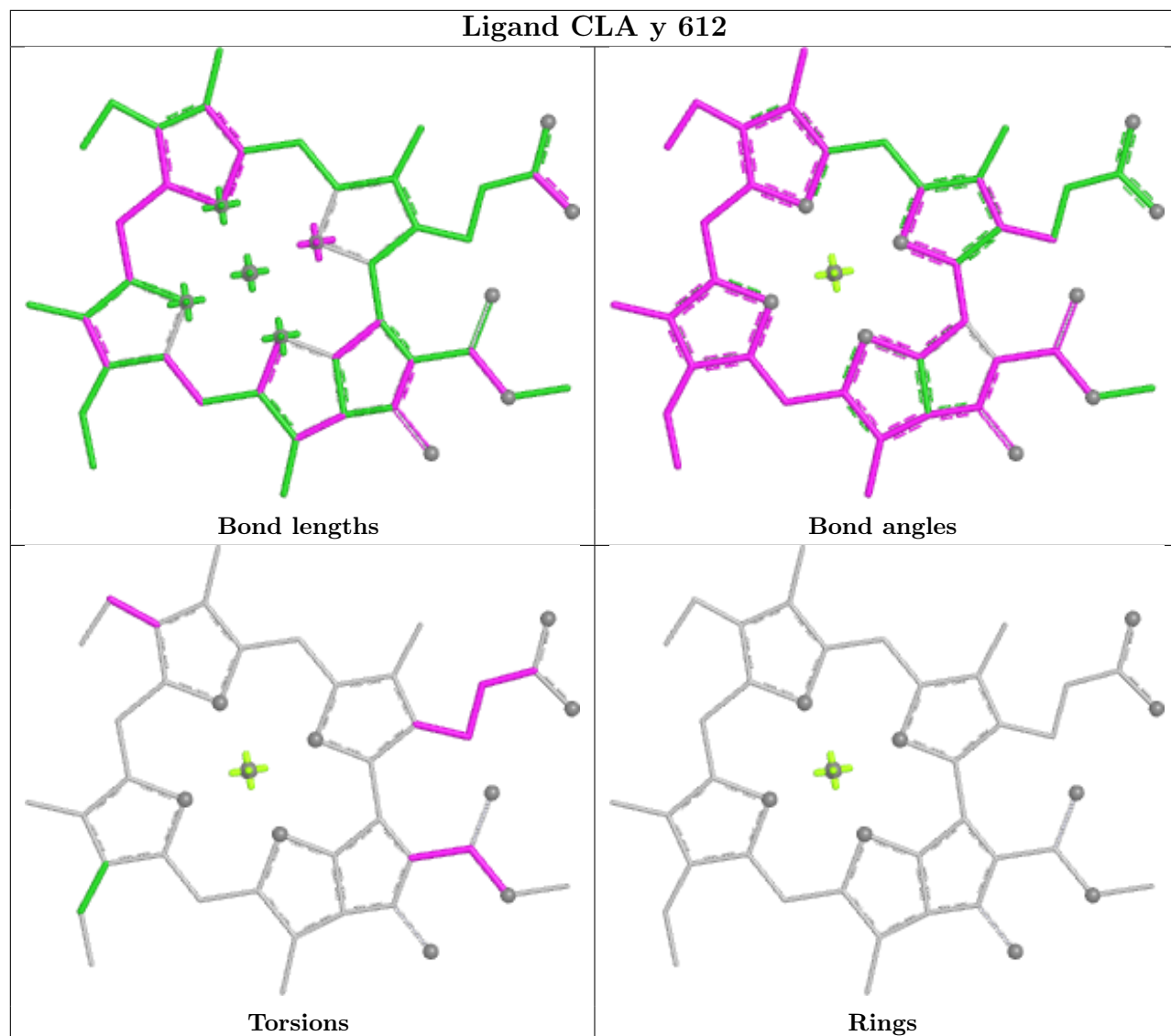
Ligand CHL r 305



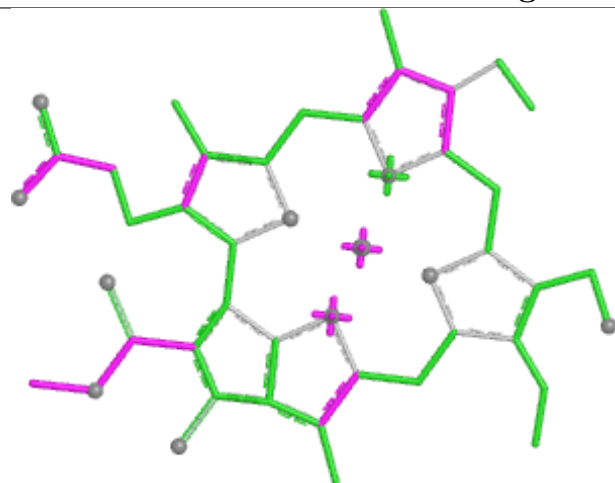
Ligand CLA r 307



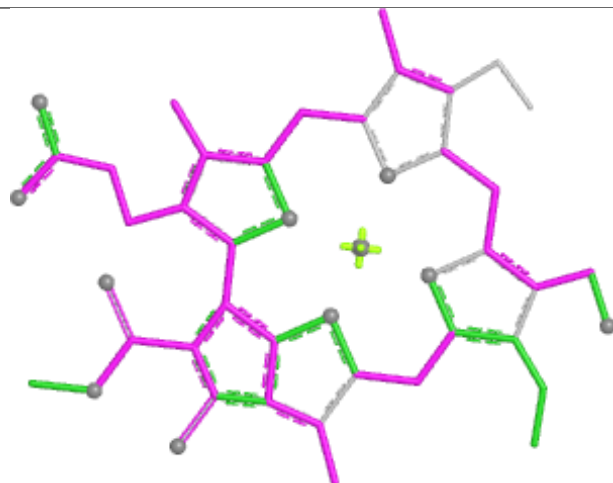
Ligand CLA y 612



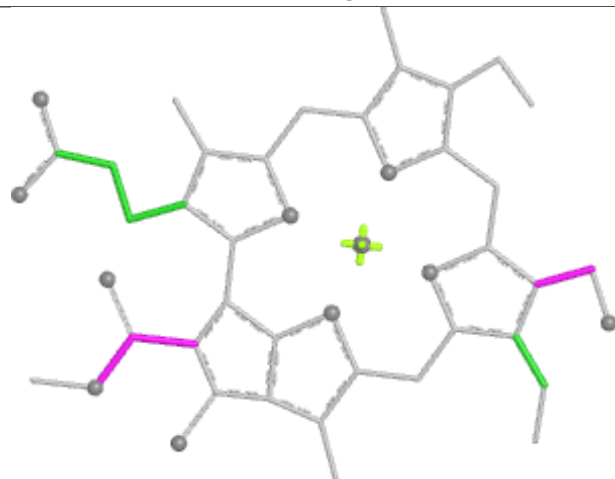
Ligand CHL S 308



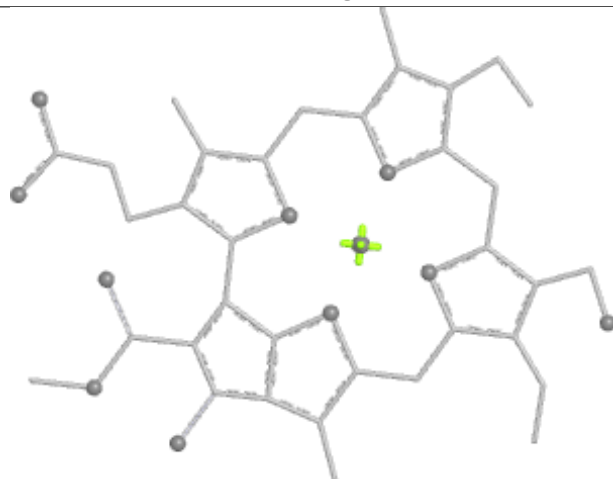
Bond lengths



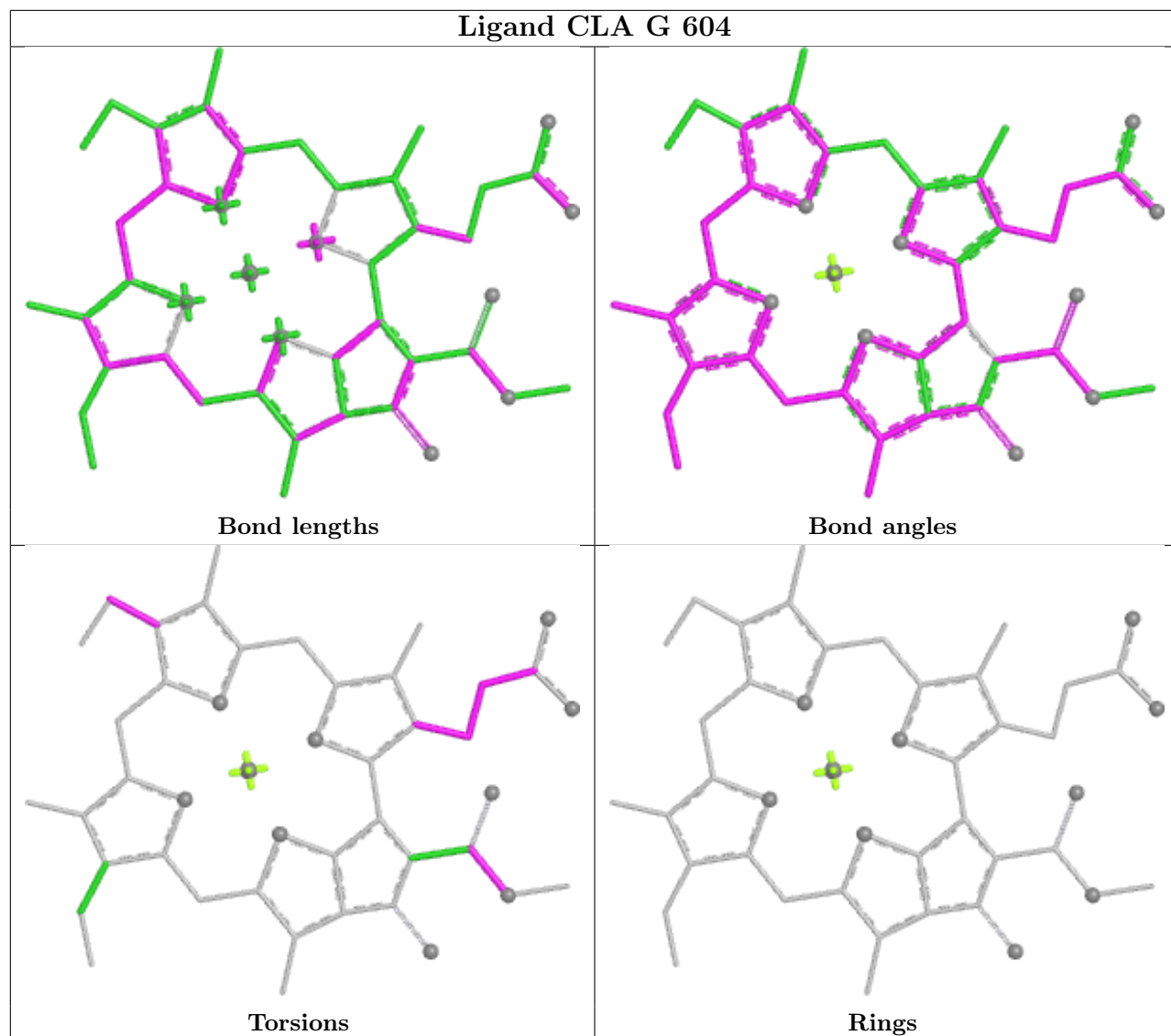
Bond angles



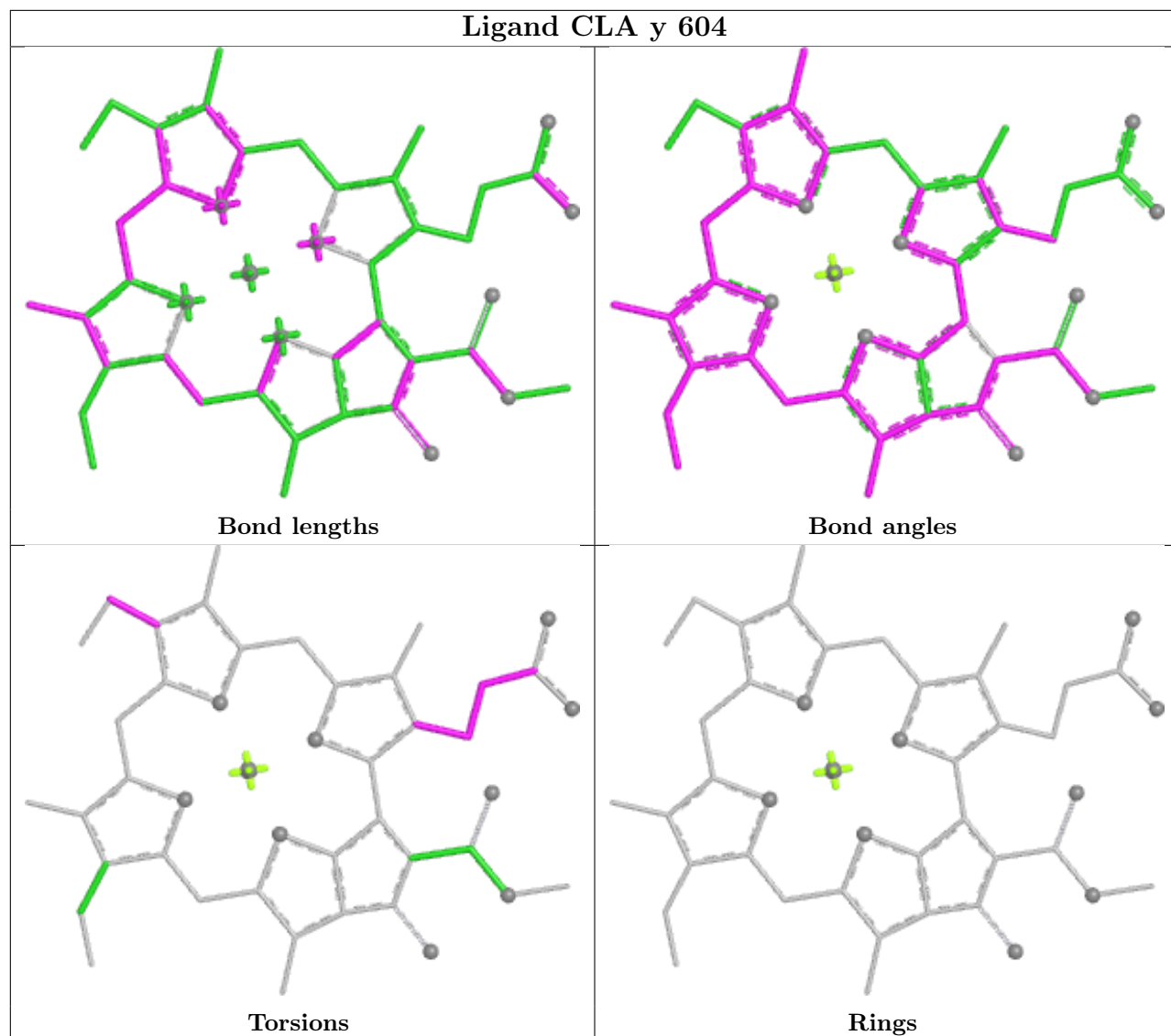
Torsions



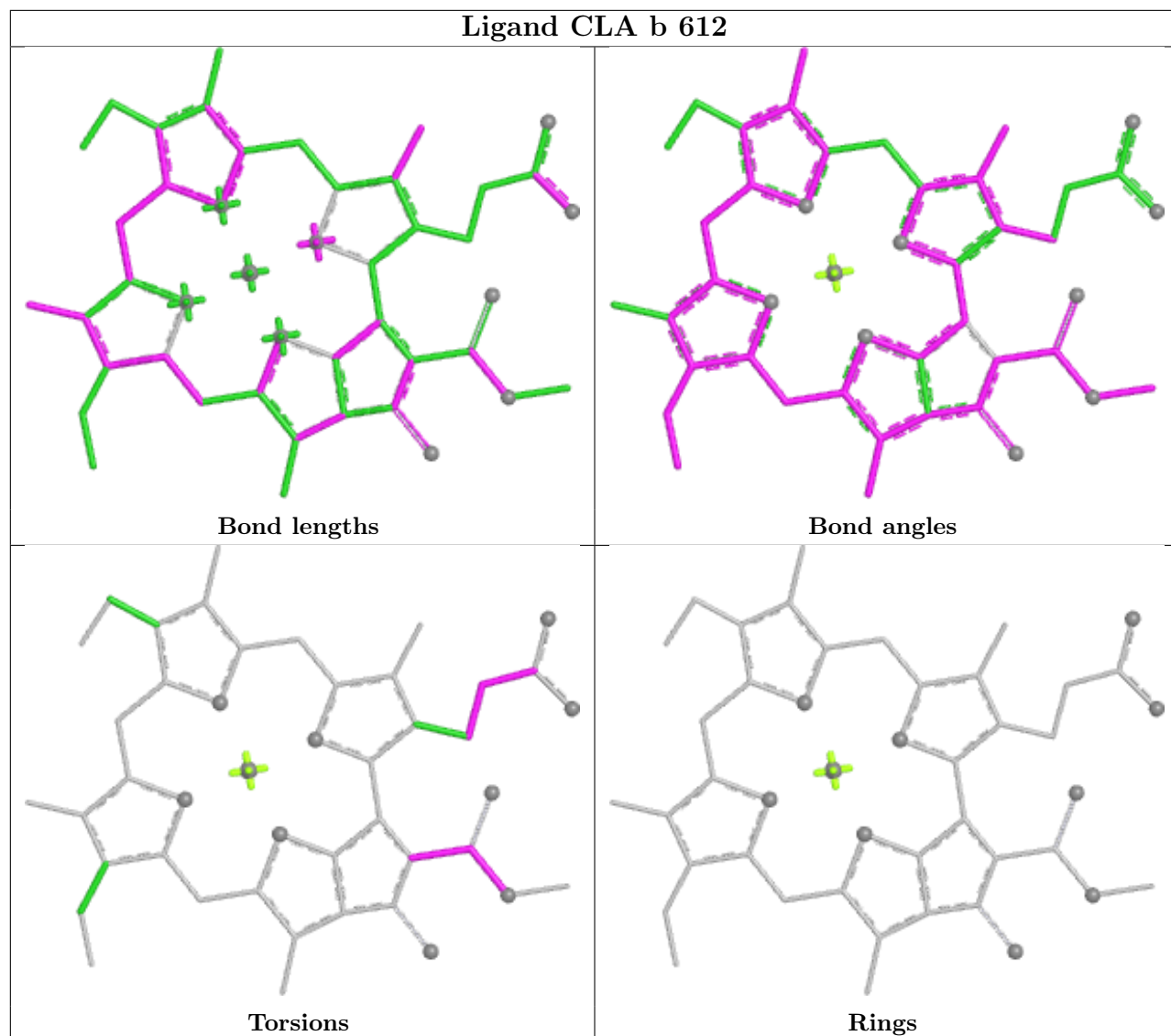
Rings



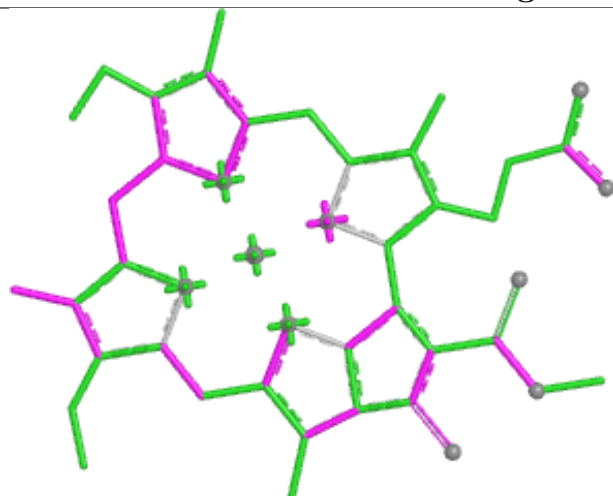
Ligand CLA y 604



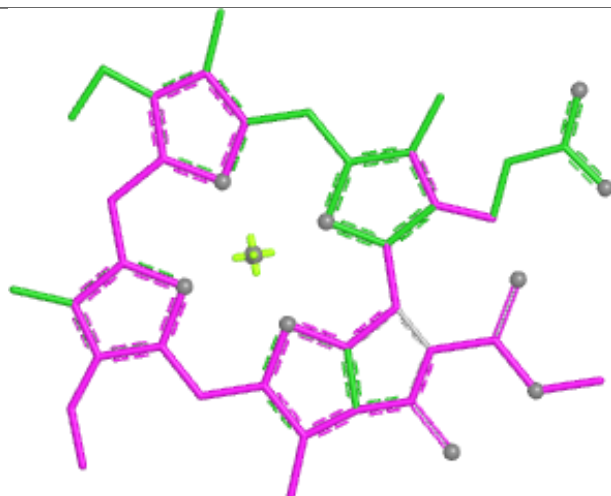
Ligand CLA b 612



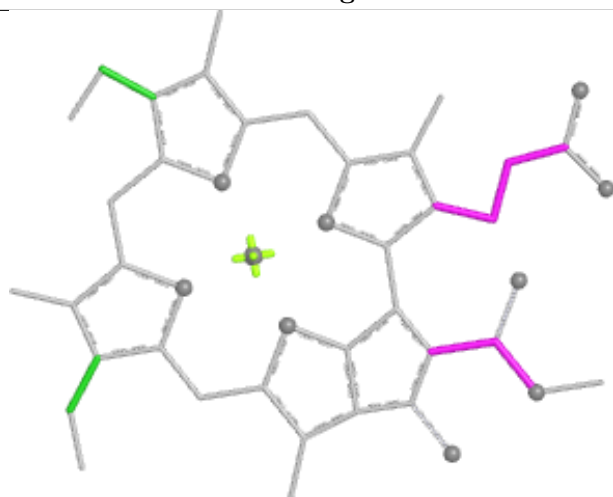
Ligand CLA S 305



Bond lengths



Bond angles

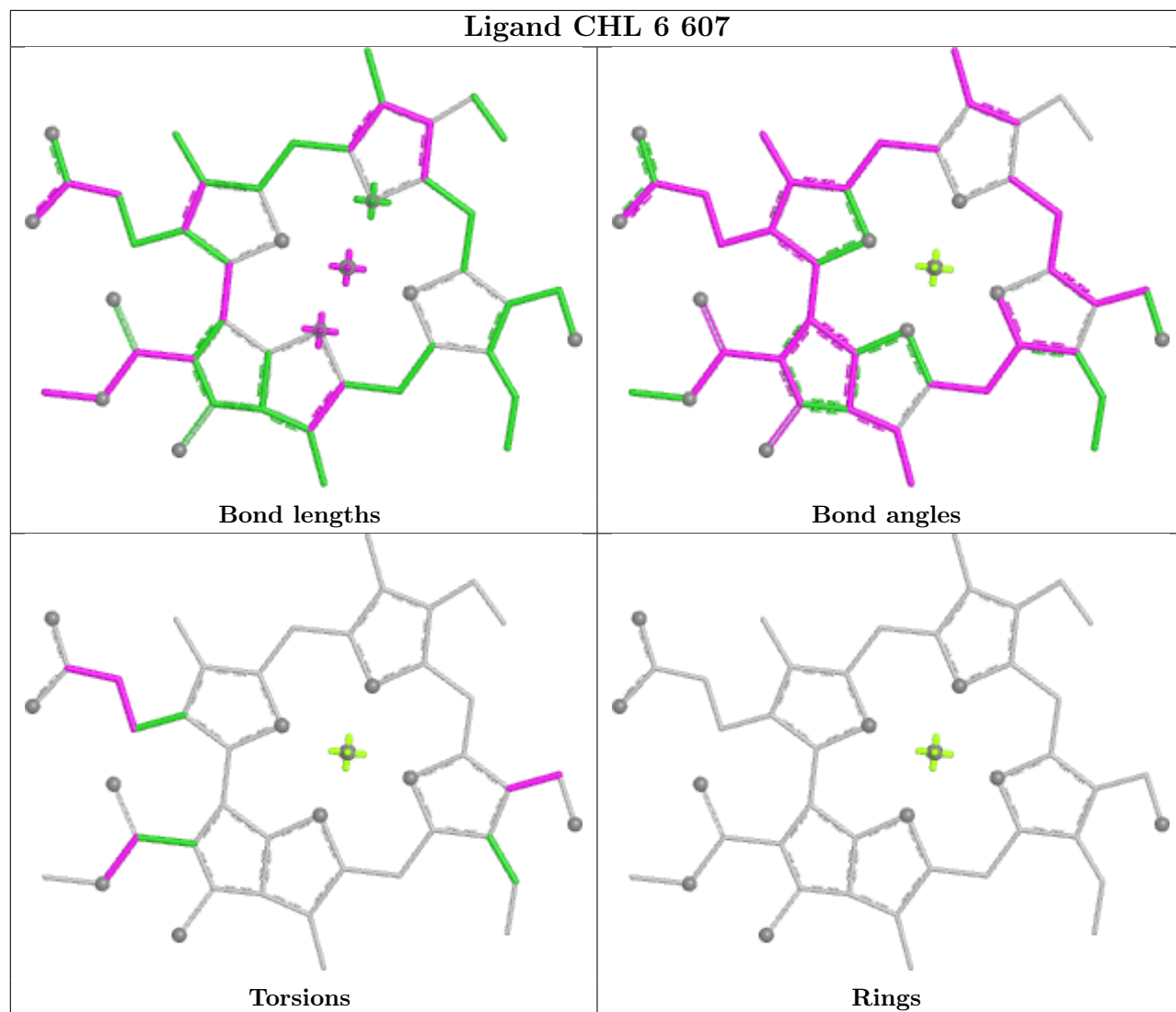


Torsions

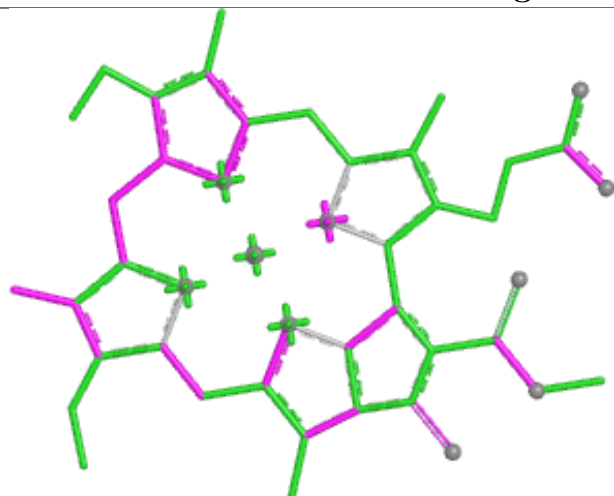


Rings

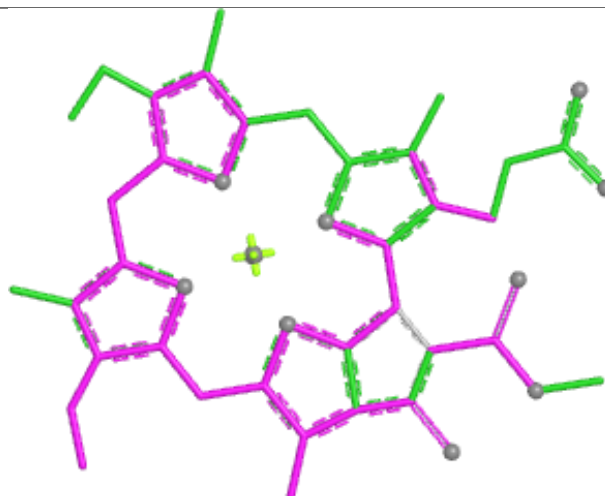
Ligand CHL 6 607



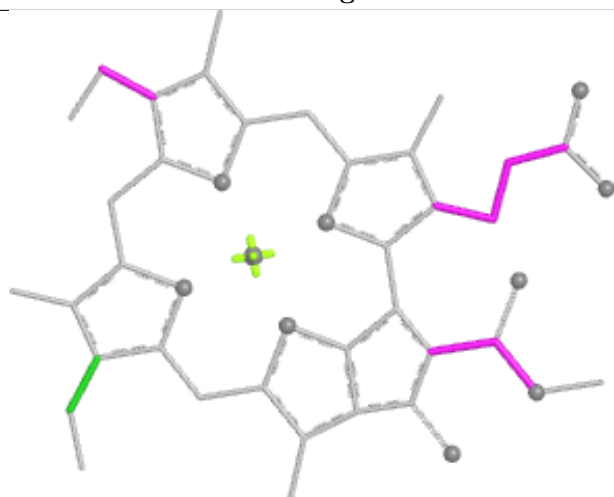
Ligand CLA R 302



Bond lengths



Bond angles

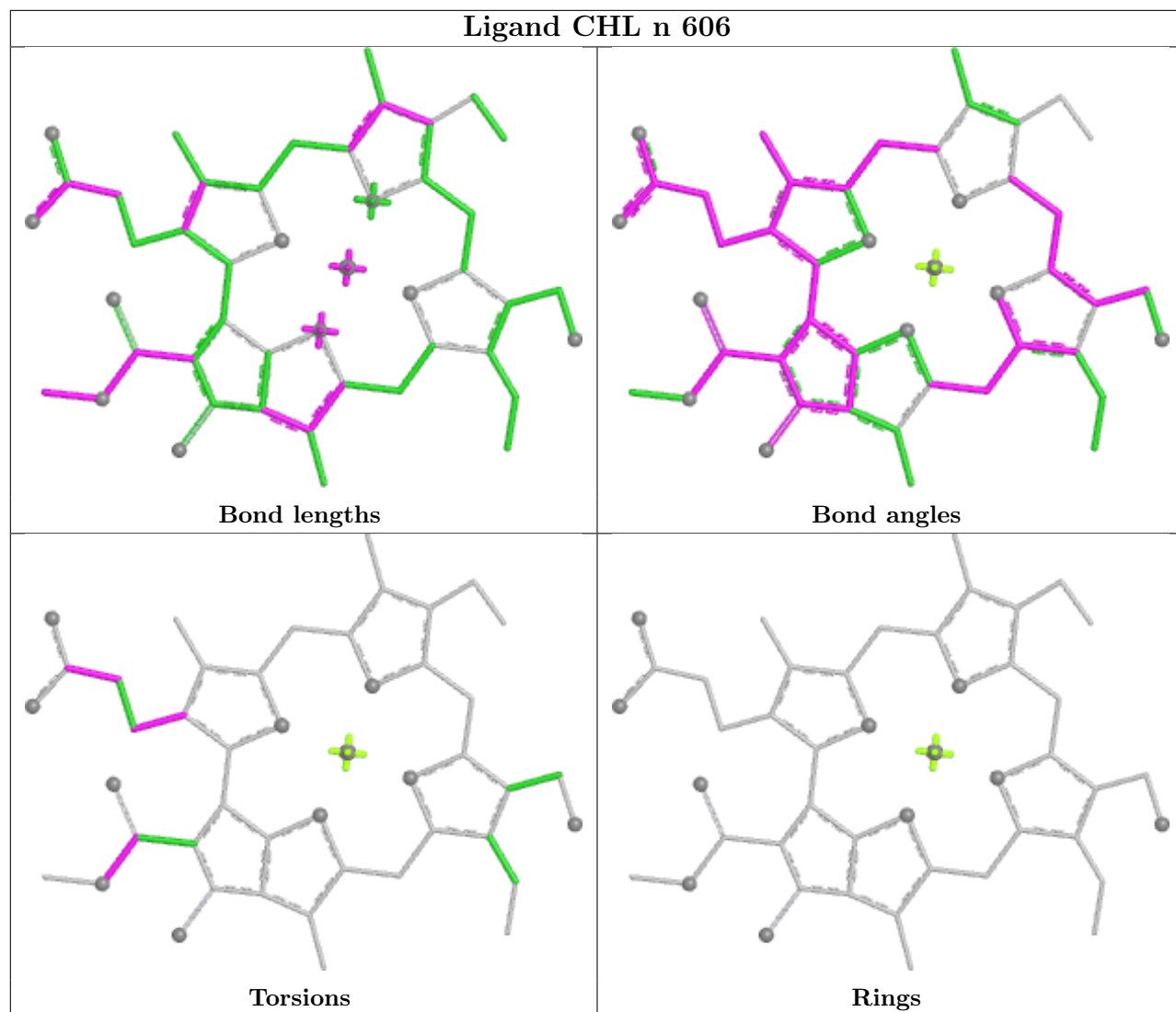


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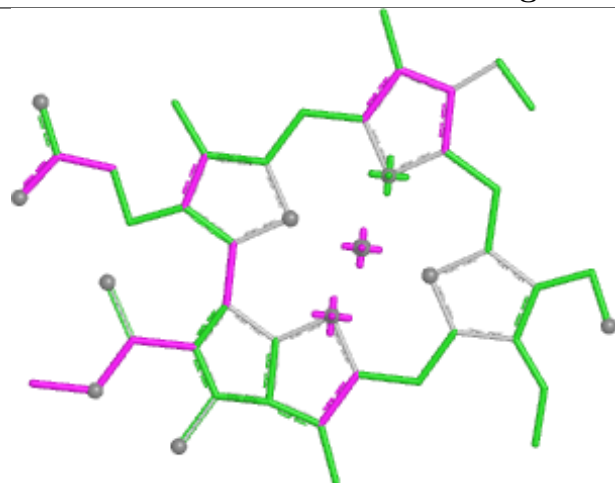


Rings

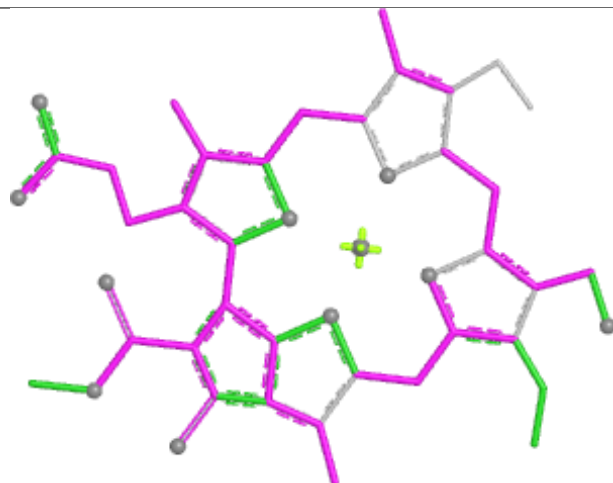
Ligand CHL n 606



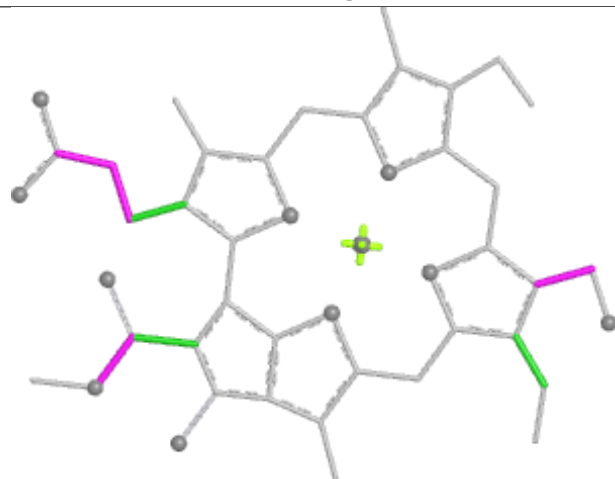
Ligand CHL 2 607



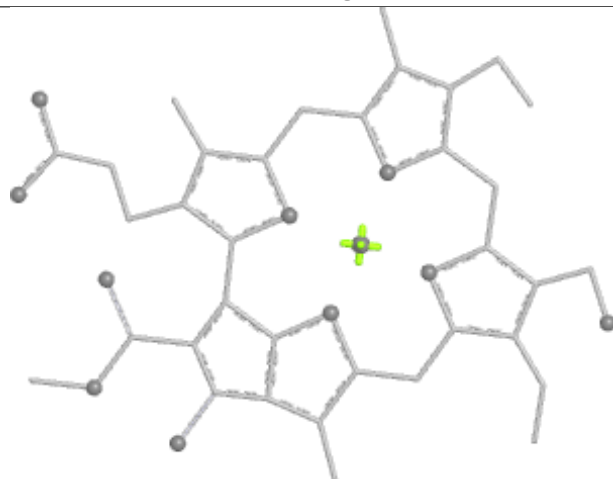
Bond lengths



Bond angles

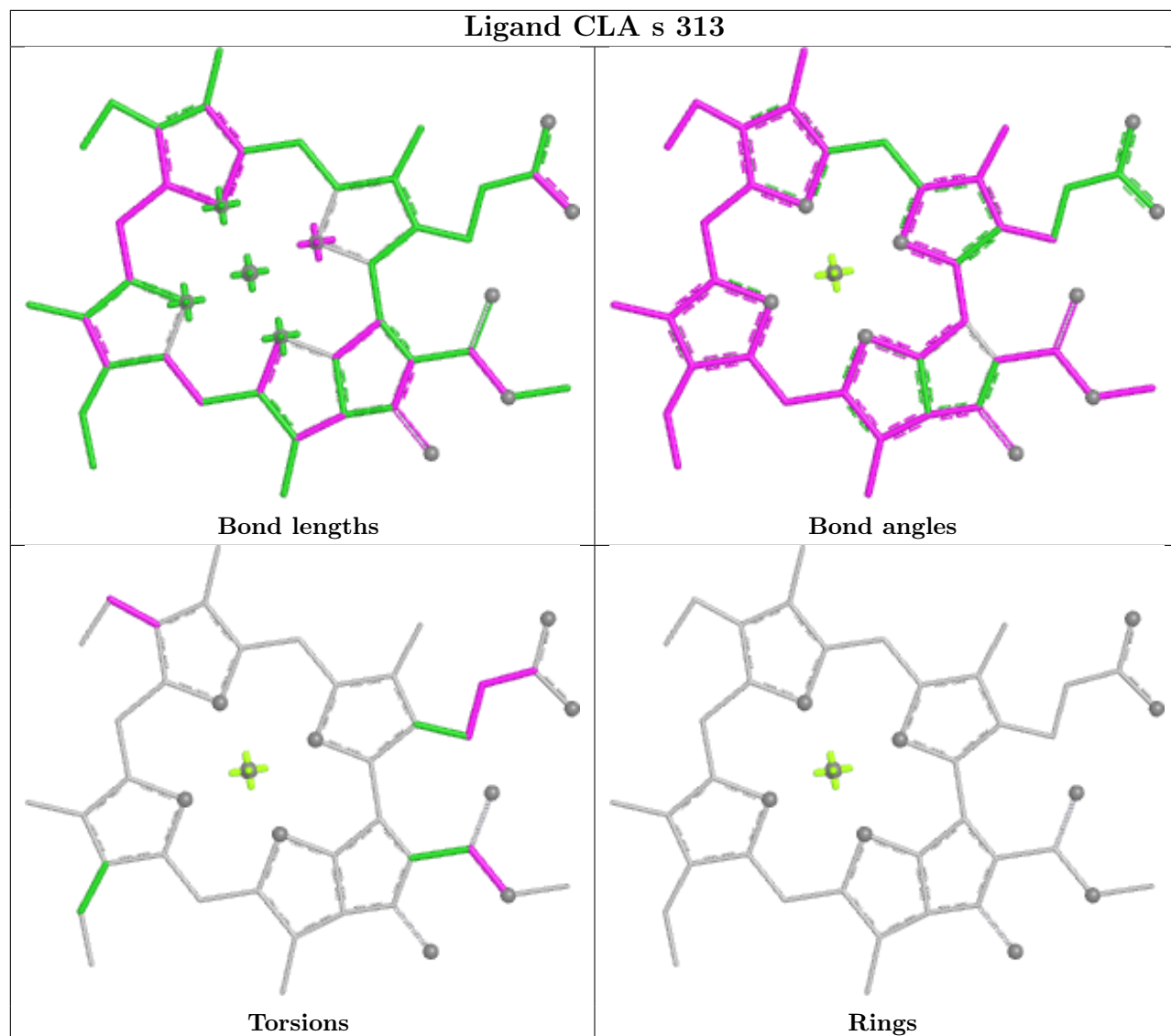


Torsions

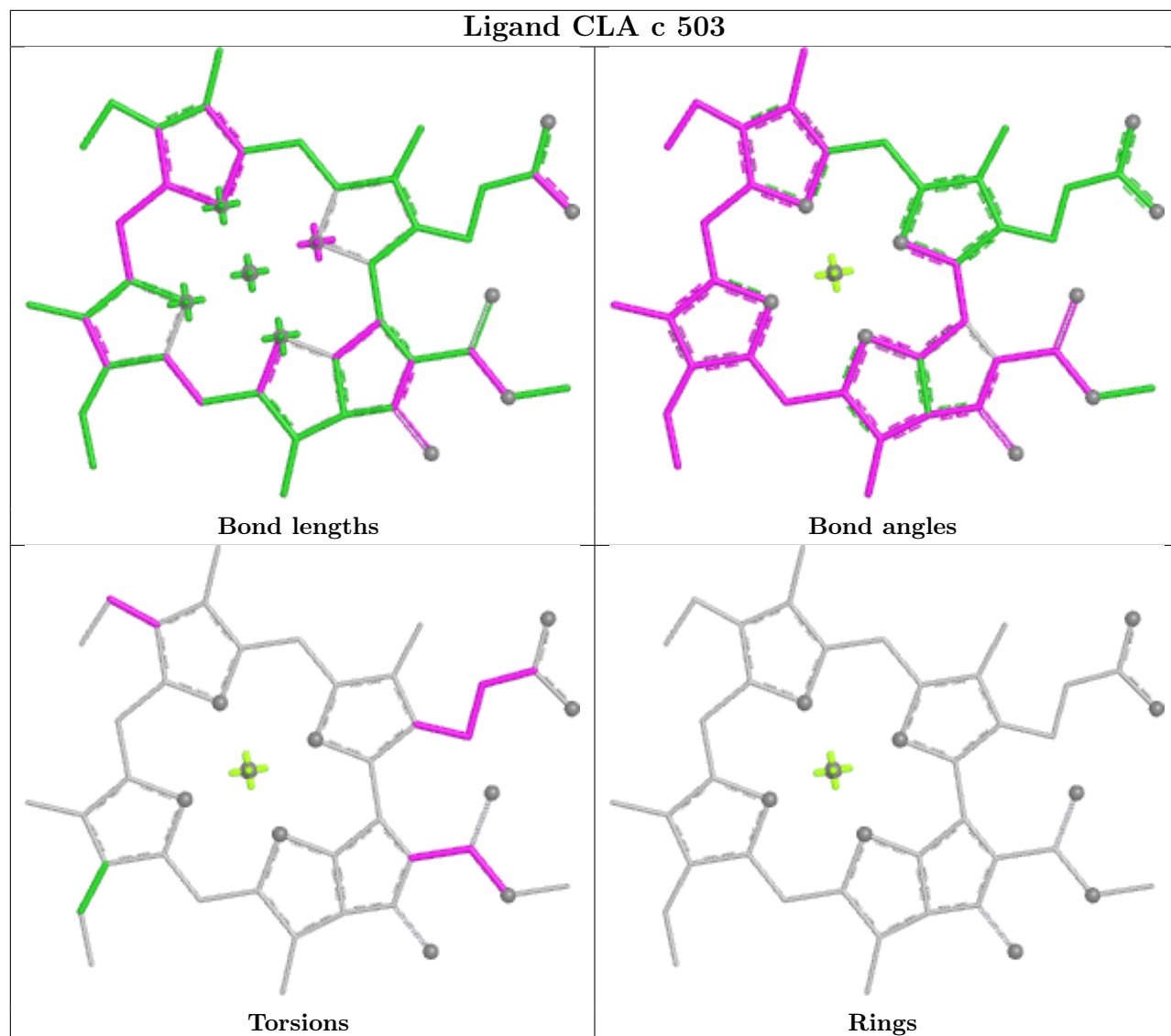


Rings

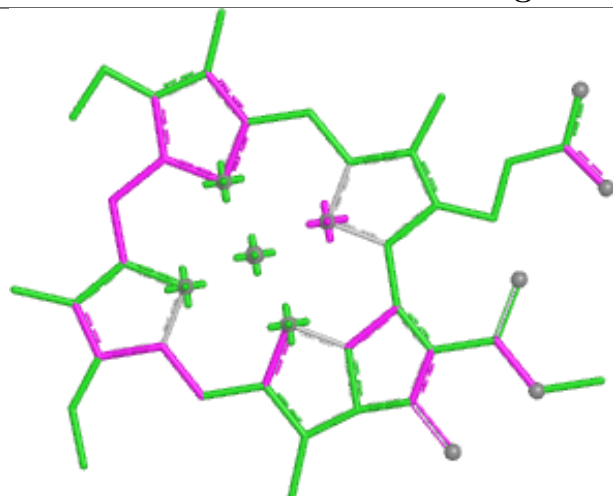
Ligand CLA s 313



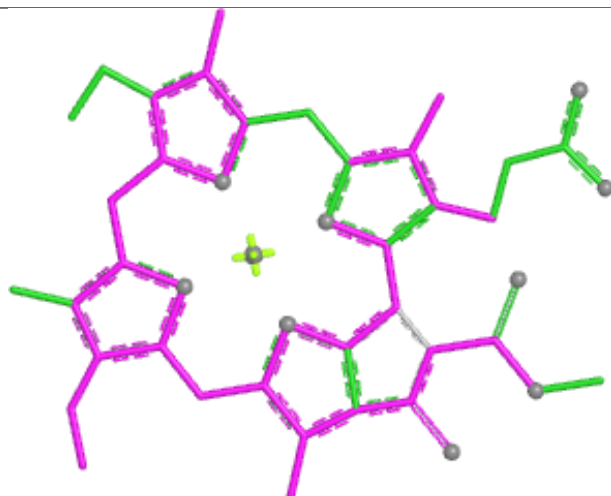
Ligand CLA c 503



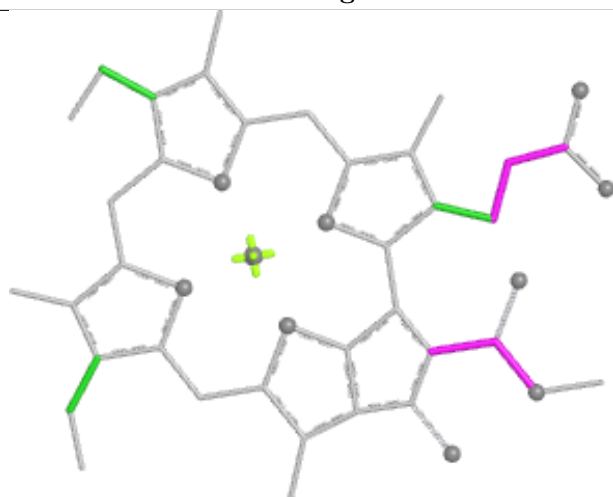
Ligand CLA B 612



Bond lengths



Bond angles

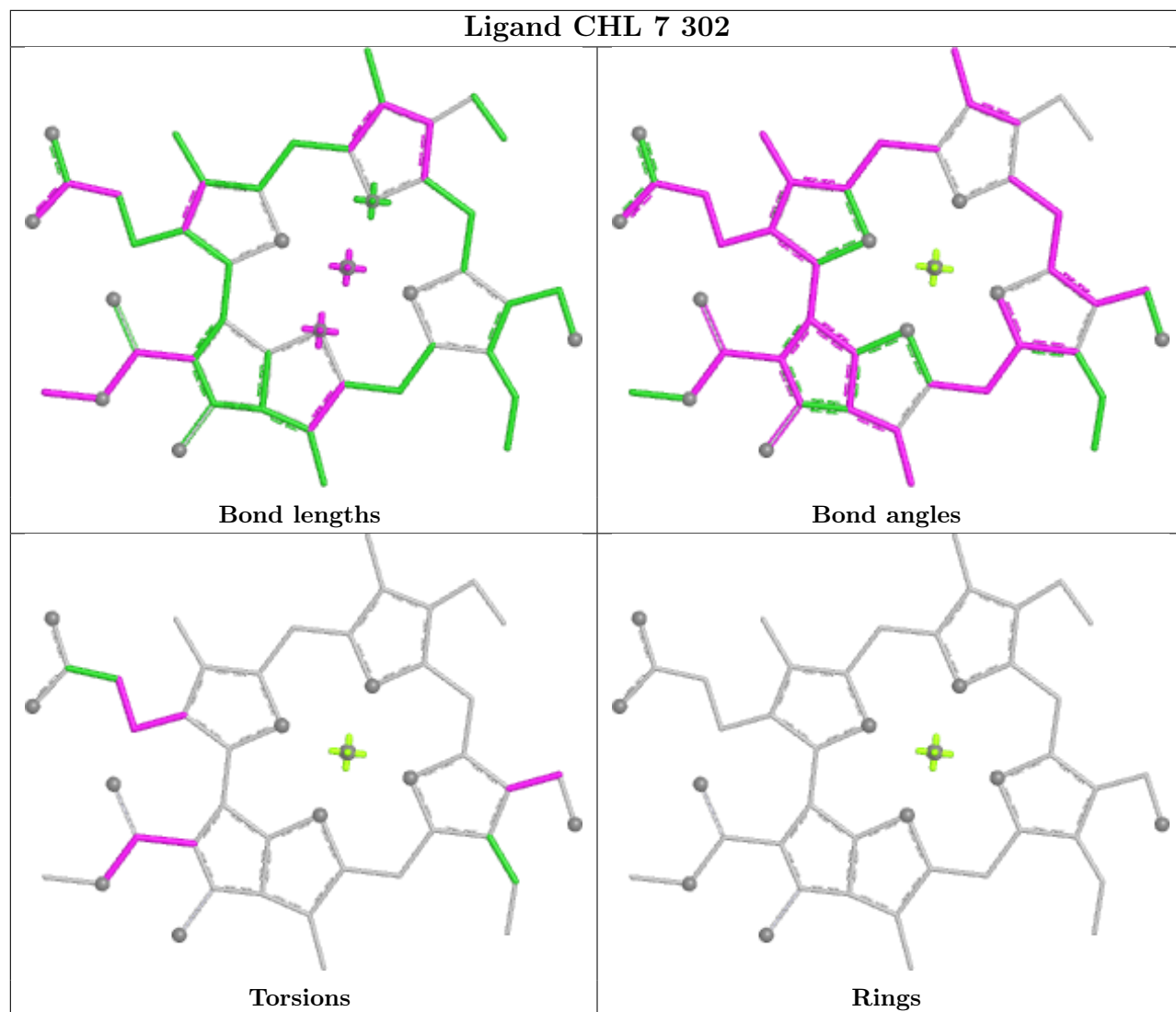


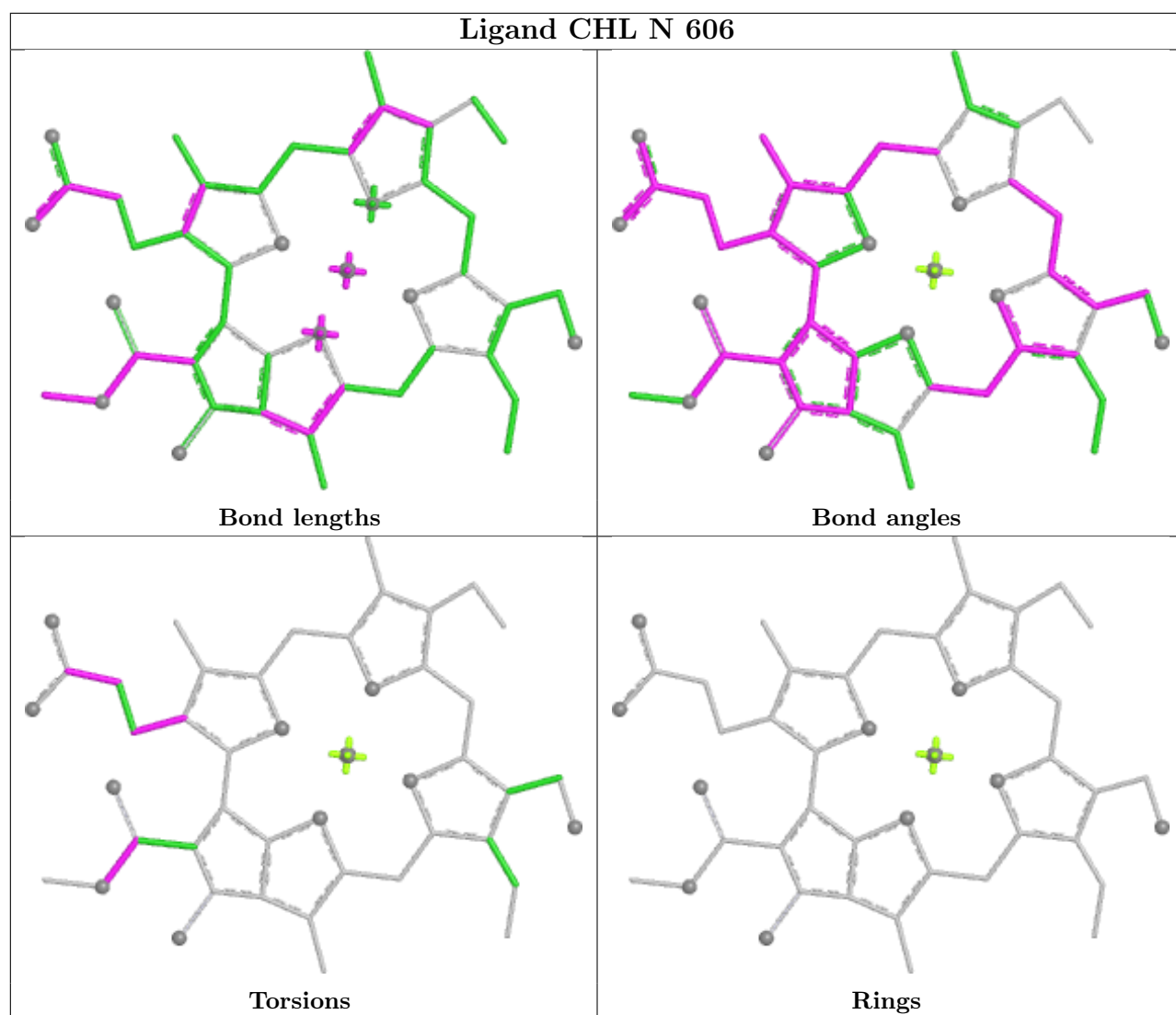
Torsions



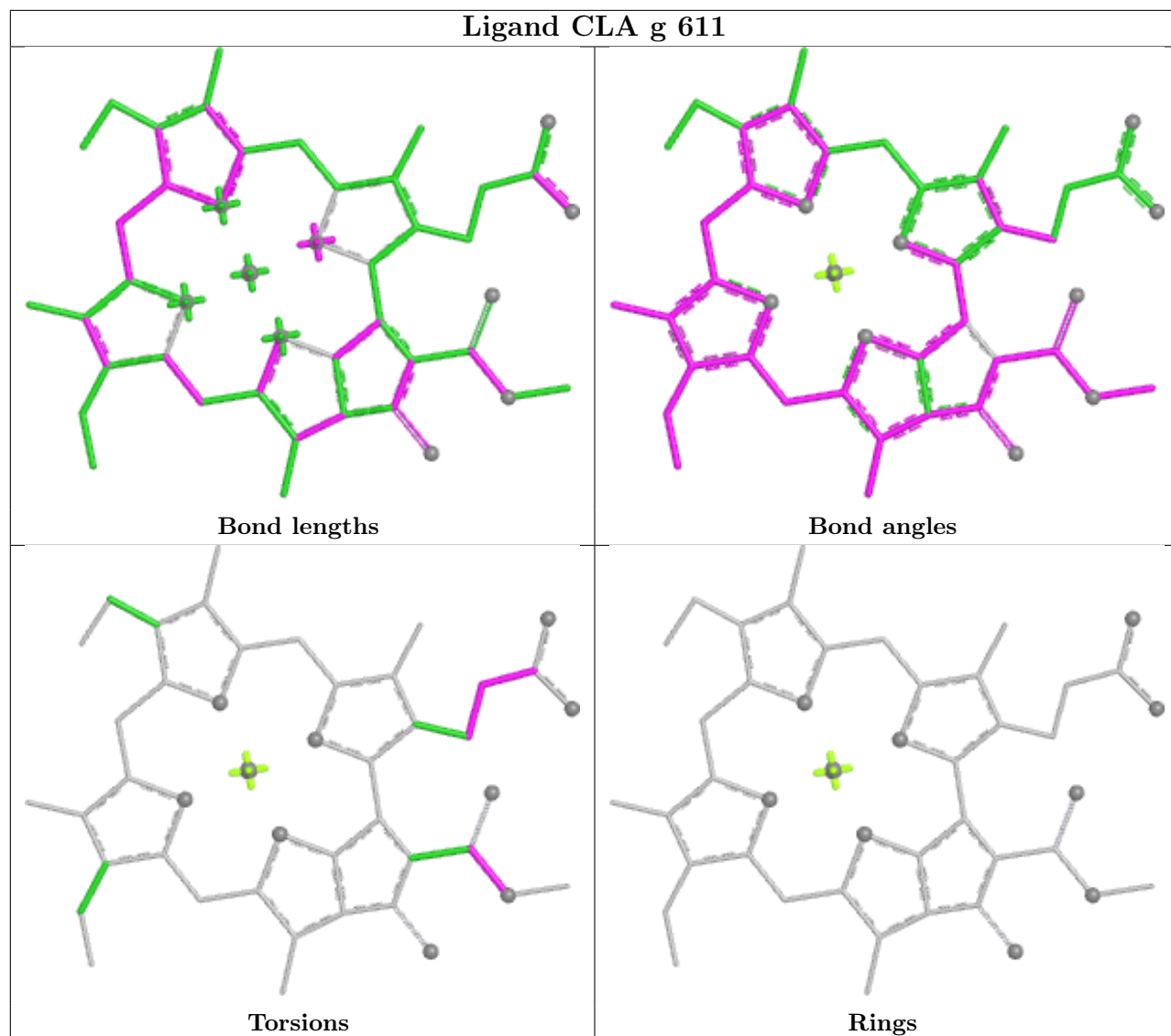
Rings

Ligand CHL 7 302

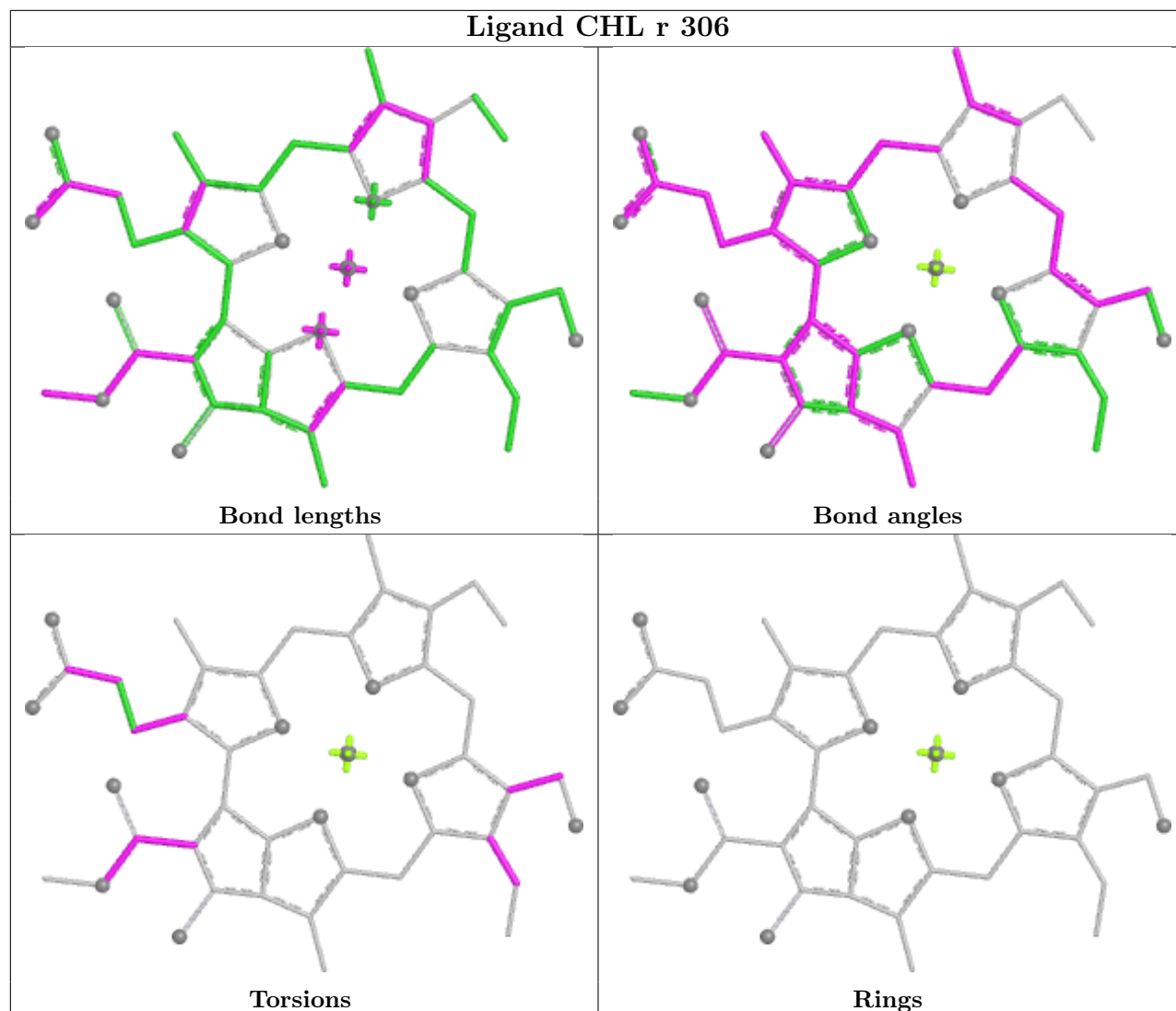




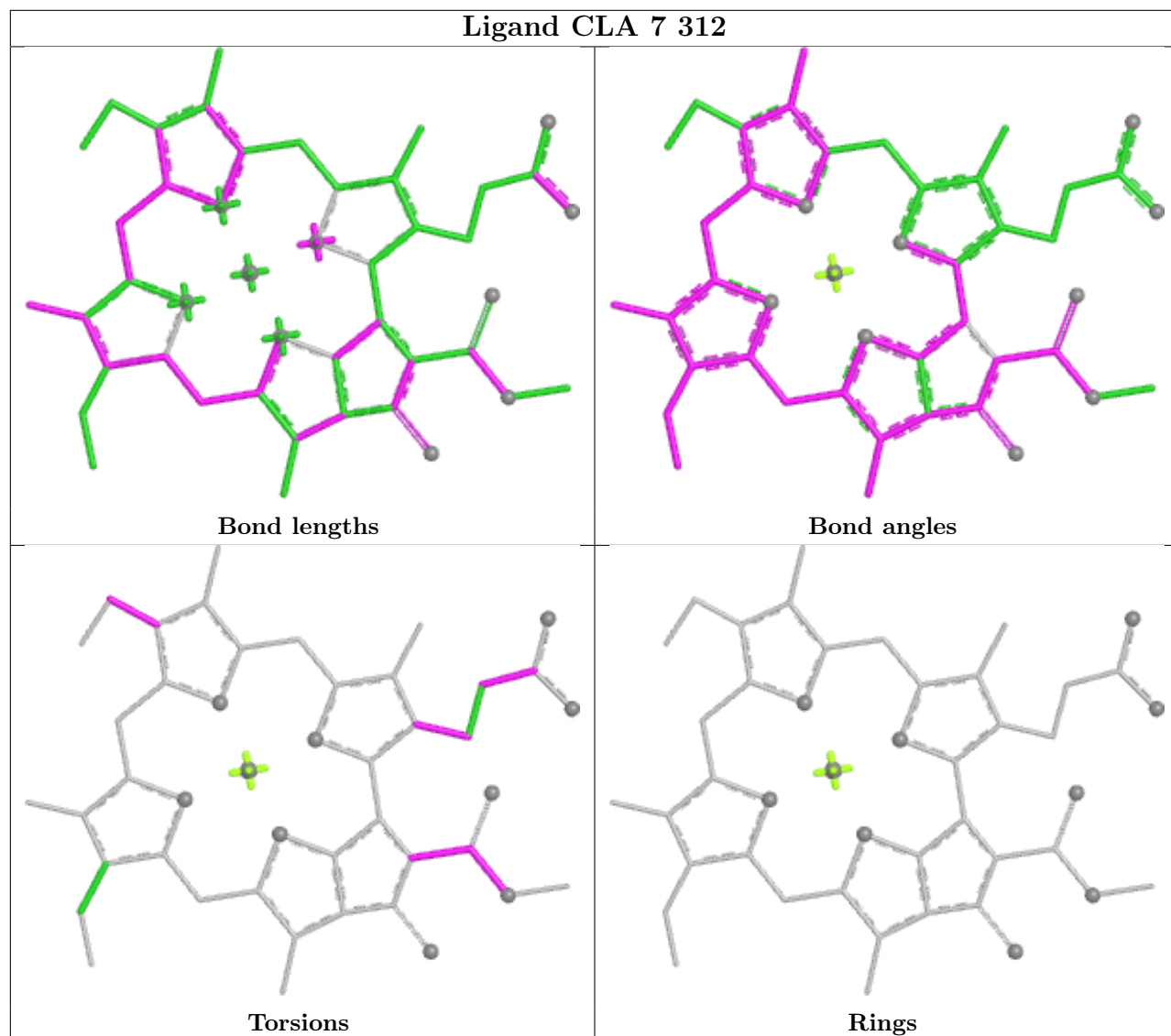
Ligand CLA g 611



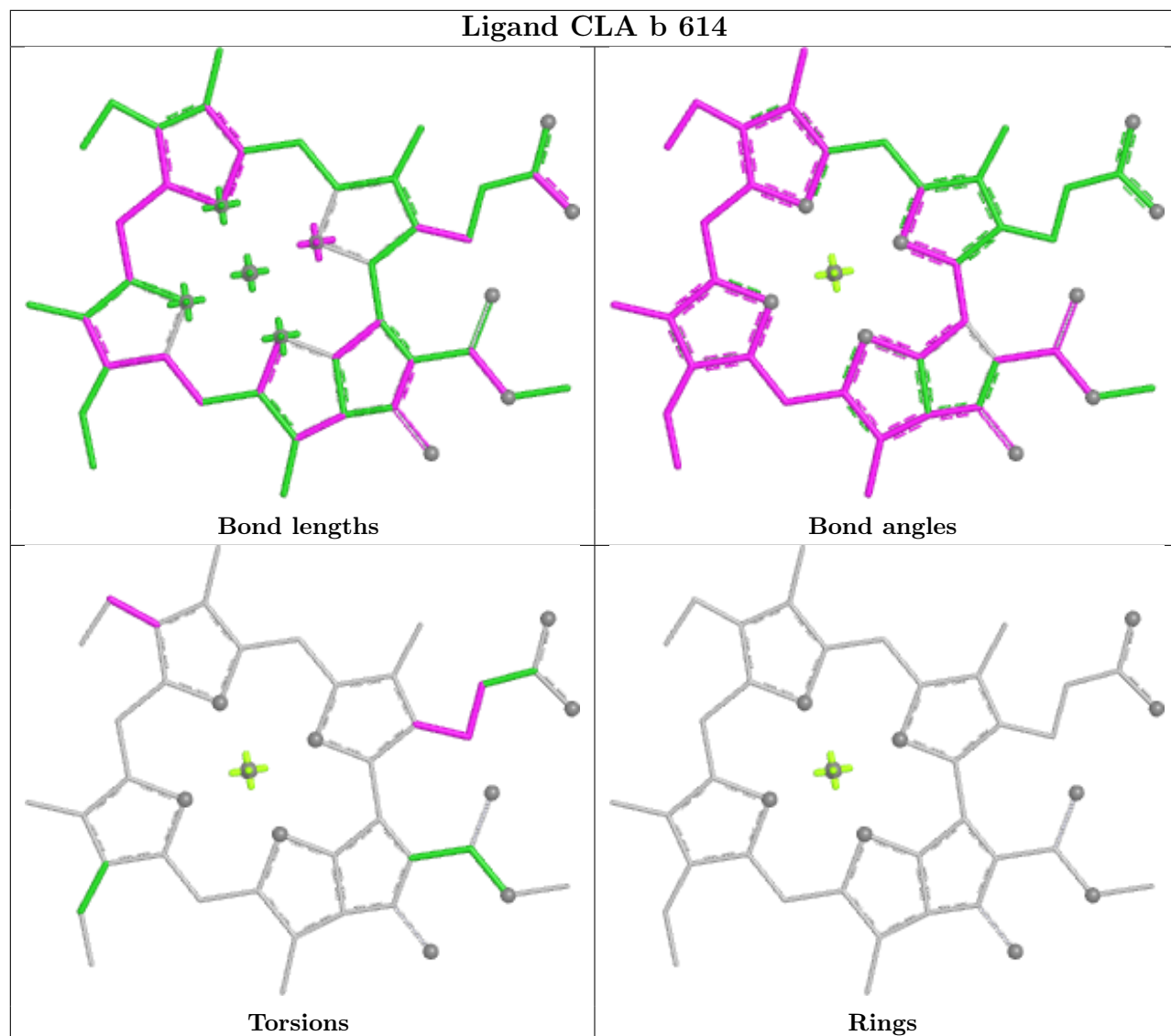
Ligand CHL r 306



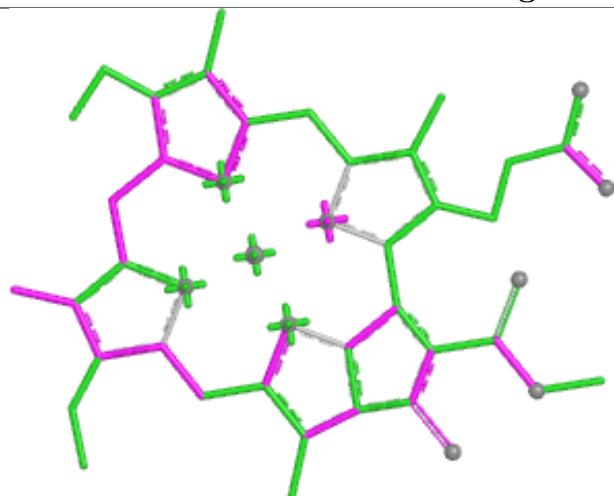
Ligand CLA 7 312



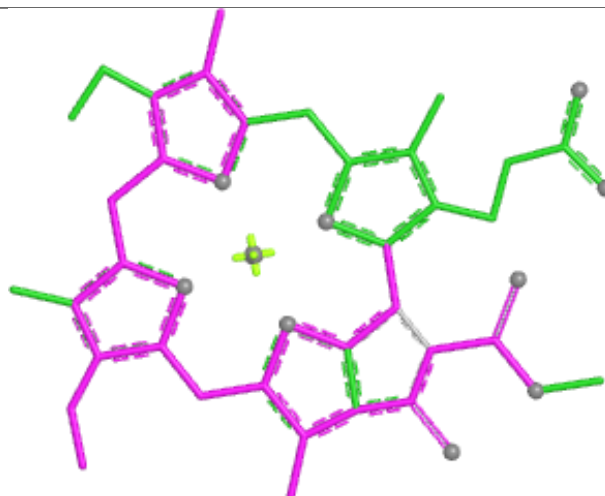
Ligand CLA b 614



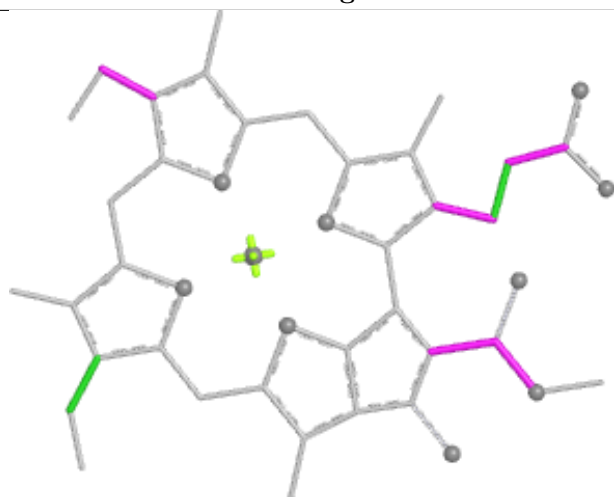
Ligand CLA 6 611



Bond lengths



Bond angles

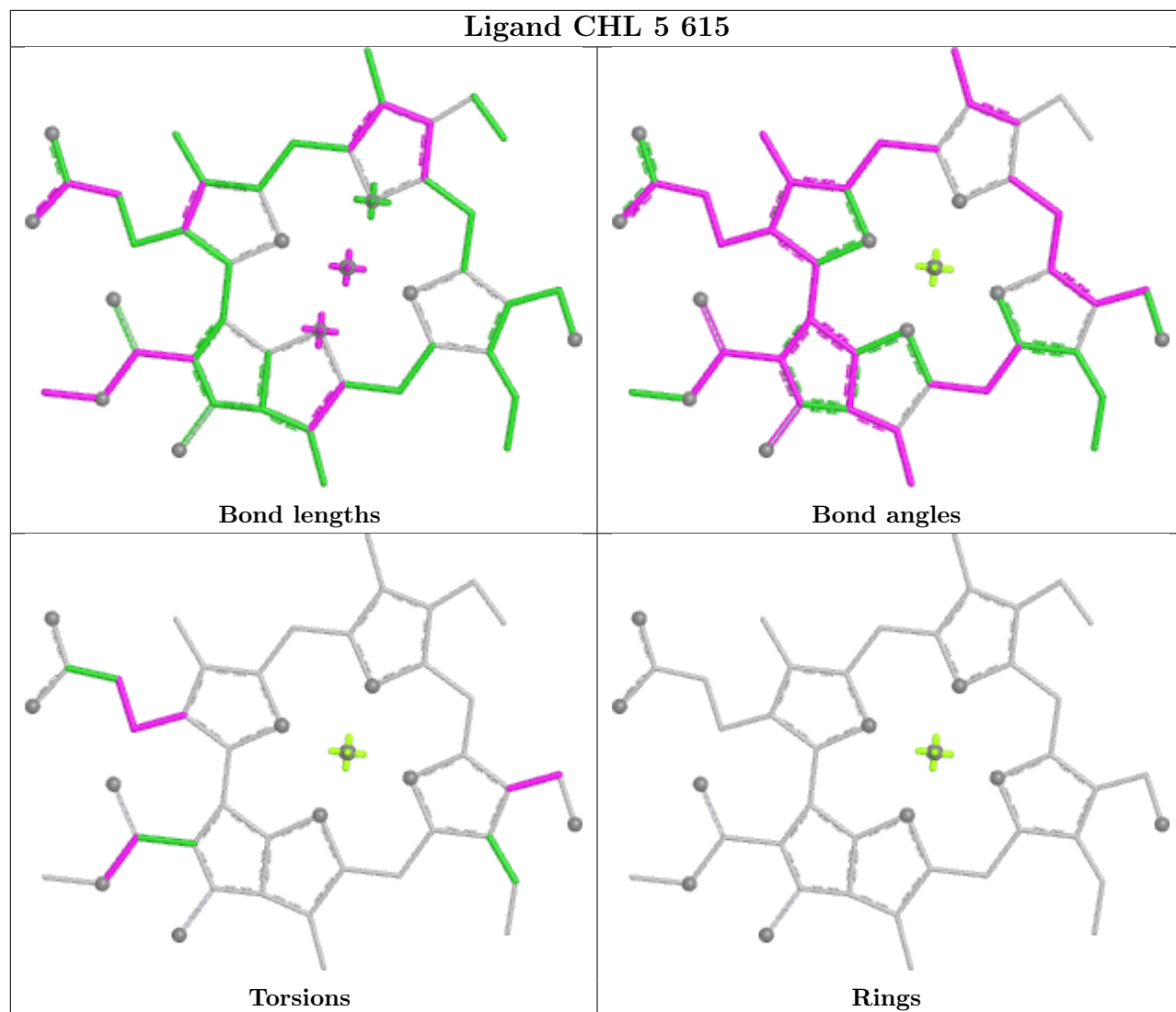


Torsions

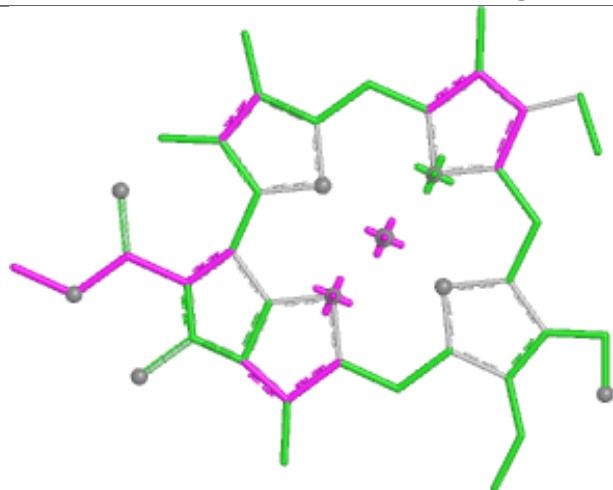


Rings

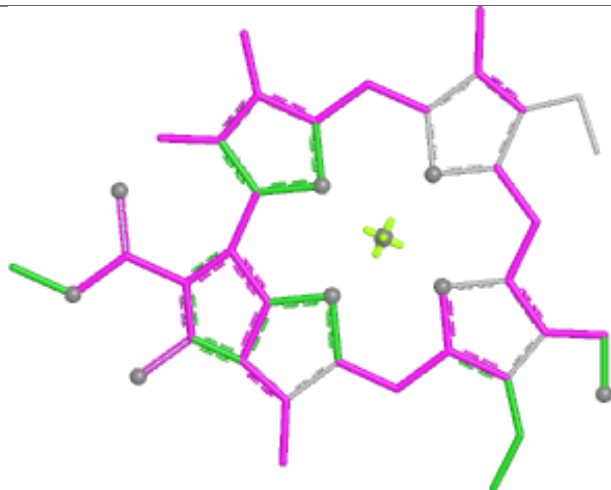
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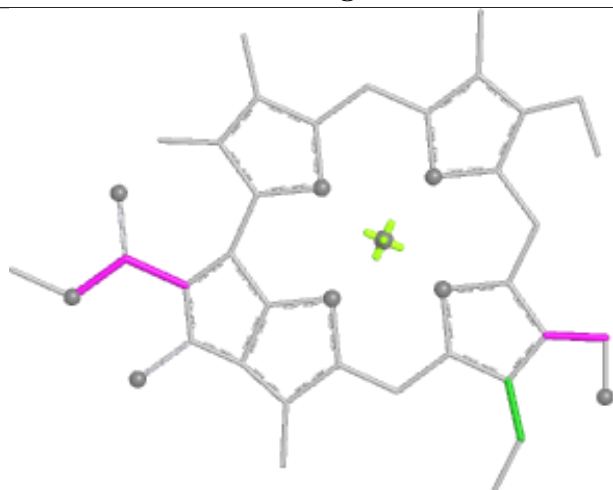
Ligand CHL N 605



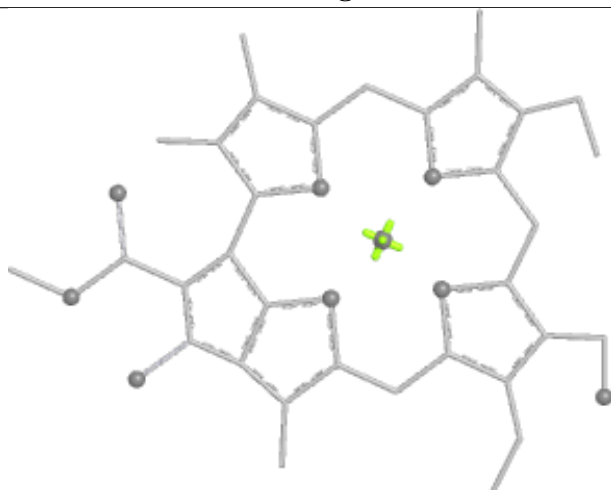
Bond lengths



Bond angles

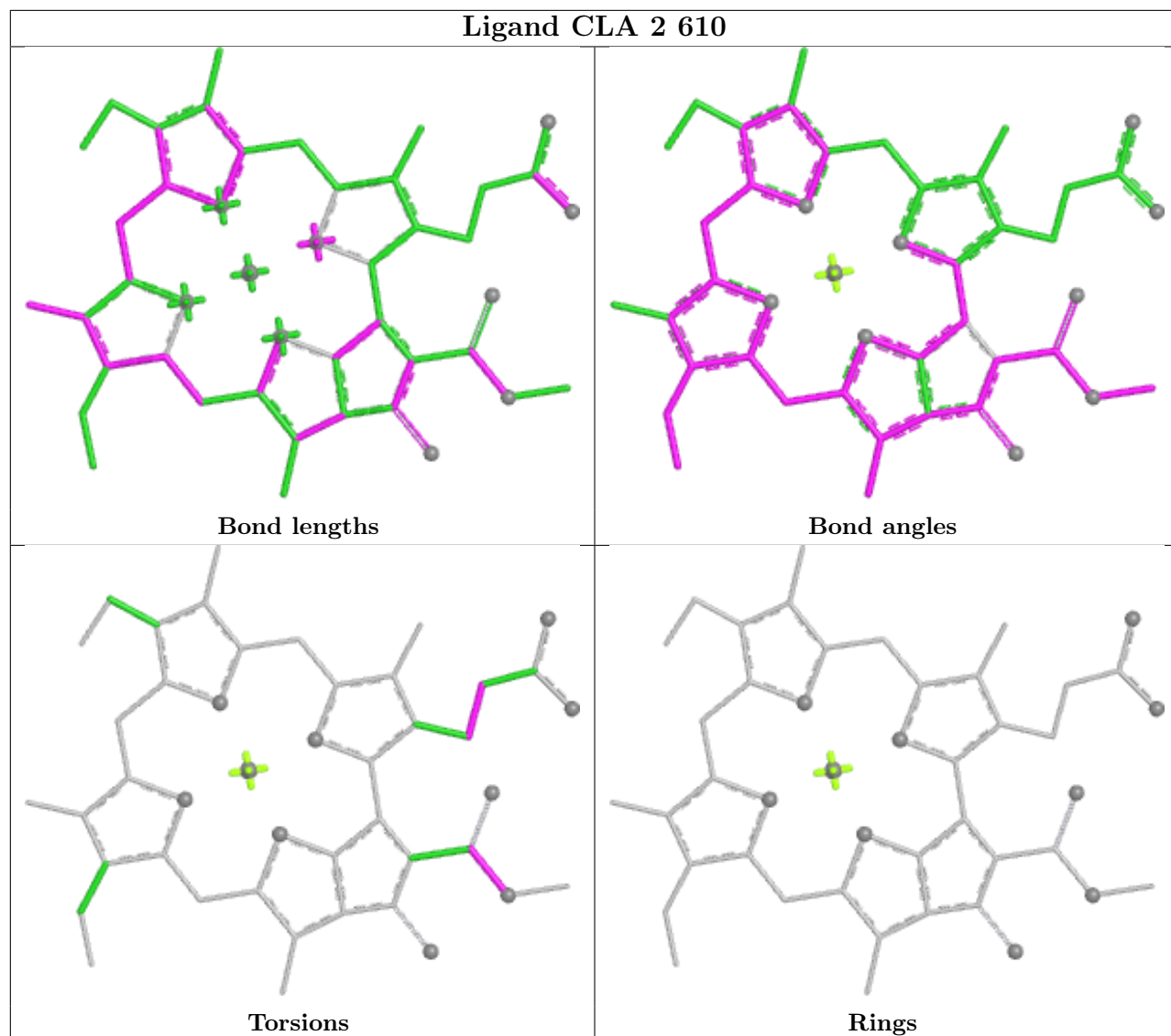


Torsions

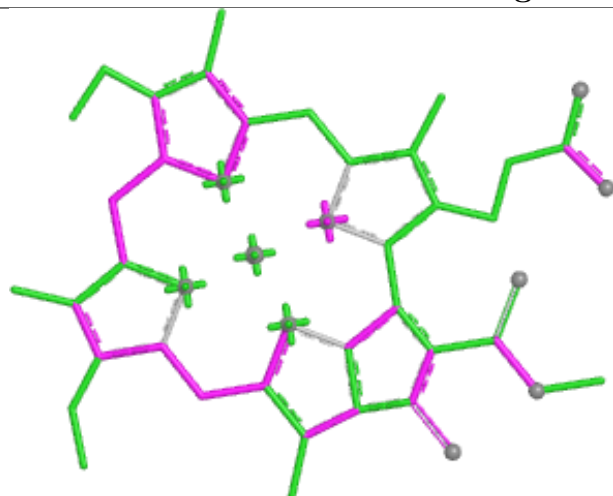


Rings

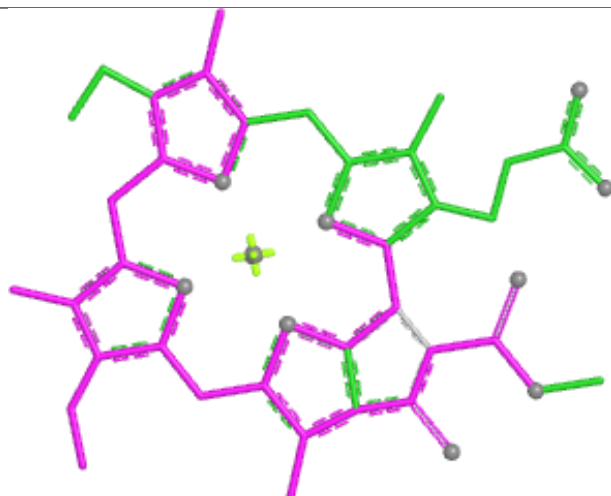
Ligand CLA 2 610



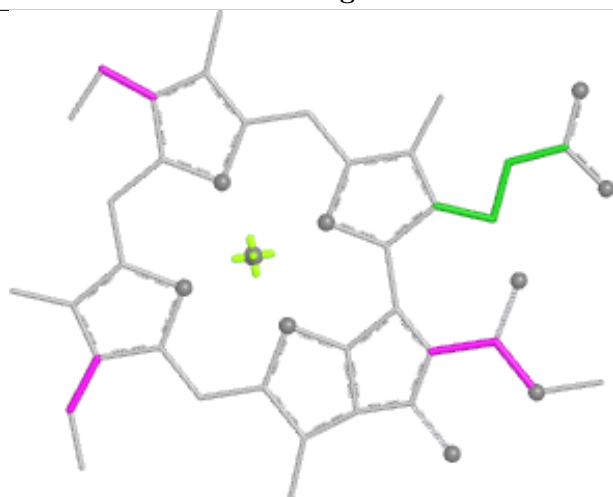
Ligand CLA B 604



Bond lengths



Bond angles

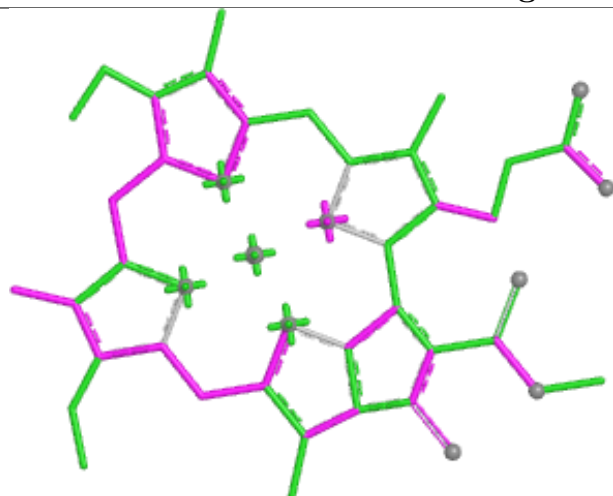


Torsions

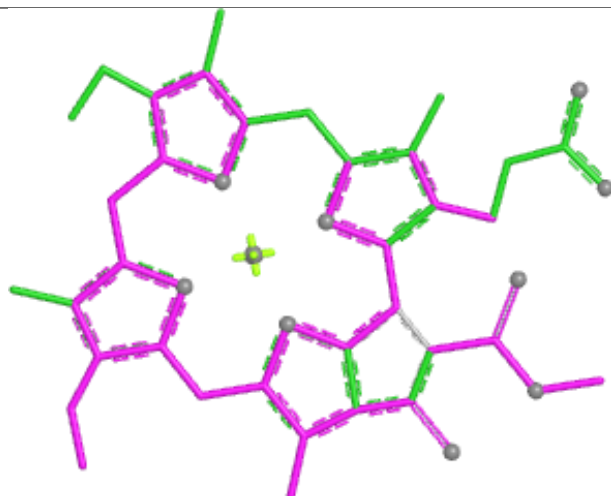


Rings

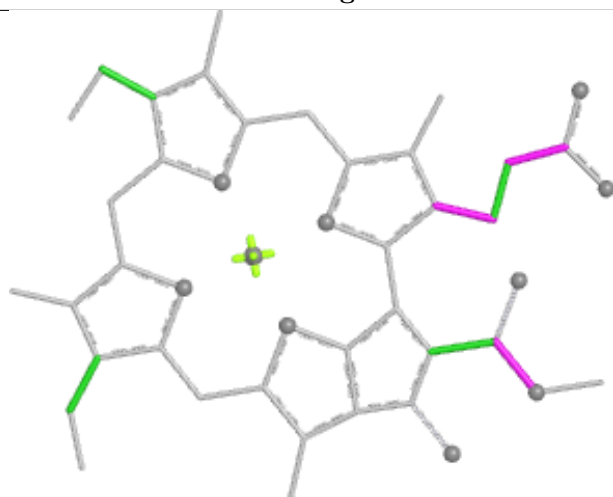
Ligand CLA 7 314



Bond lengths



Bond angles

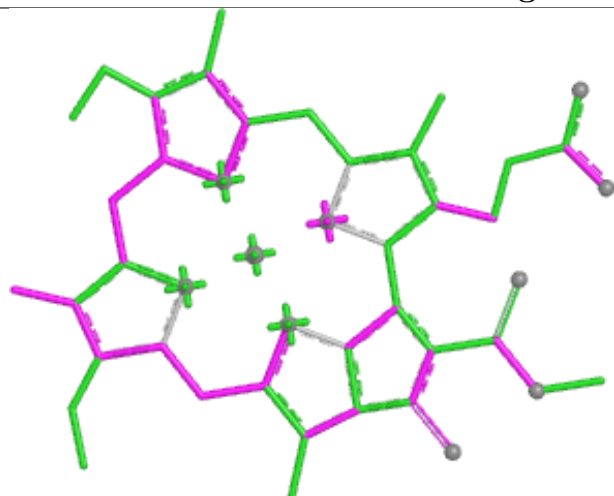


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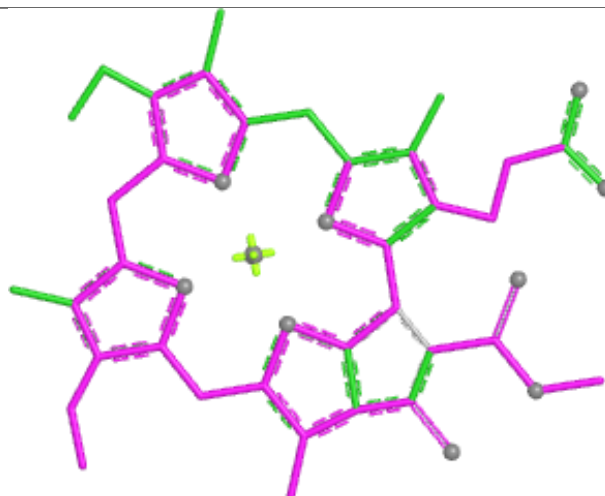


Rings

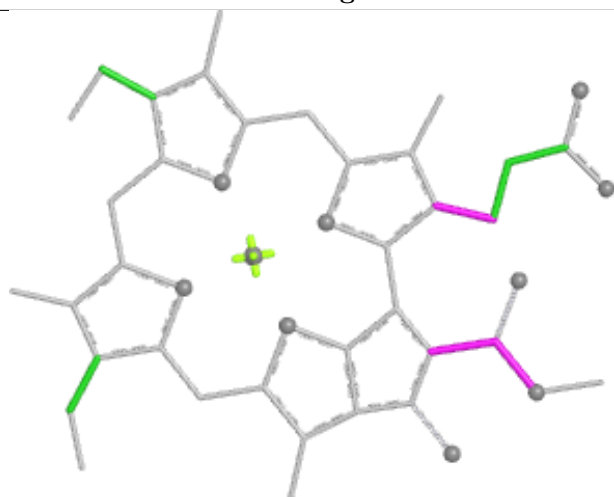
Ligand CLA 4 304



Bond lengths



Bond angles

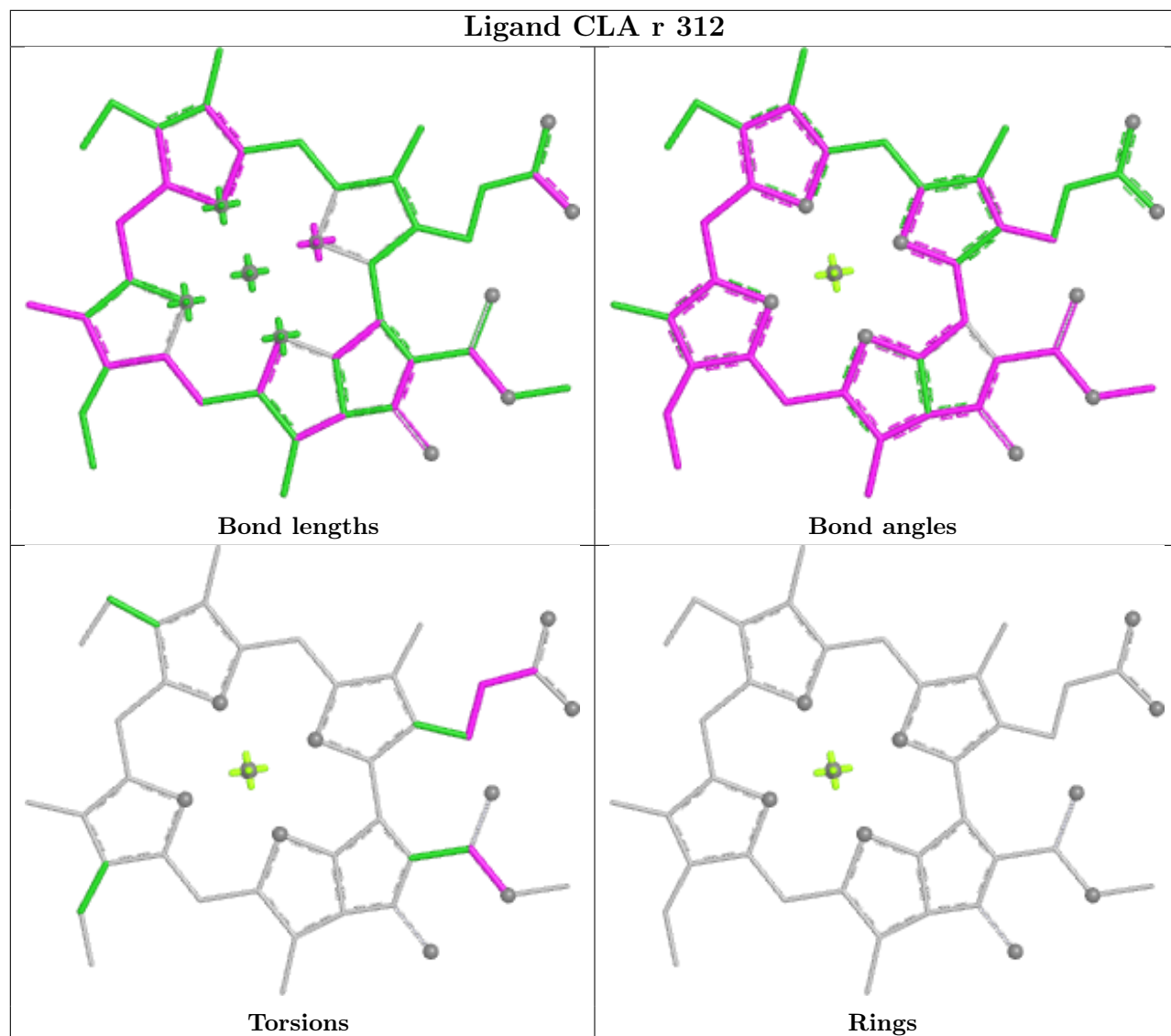


Torsions

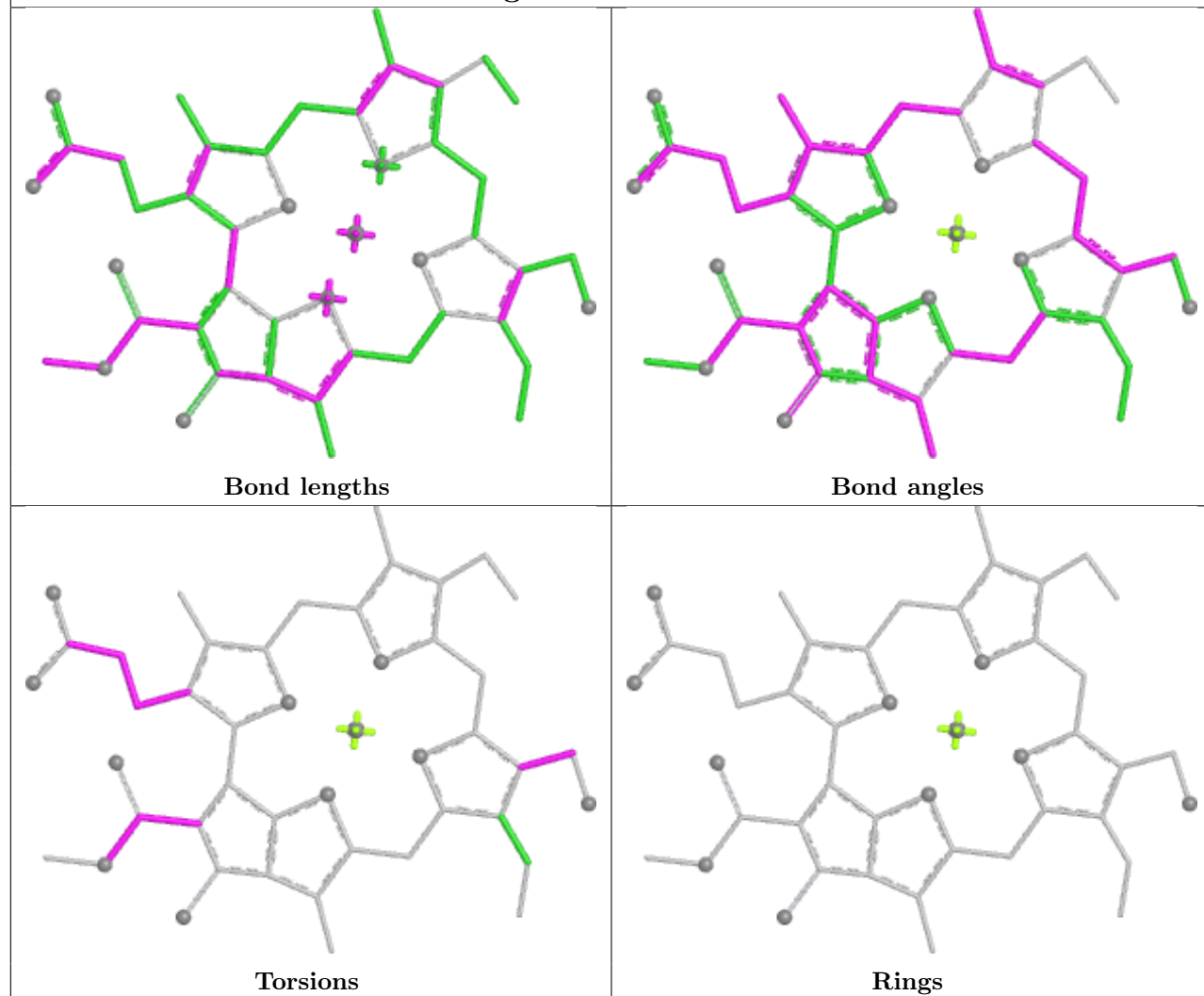


Rings

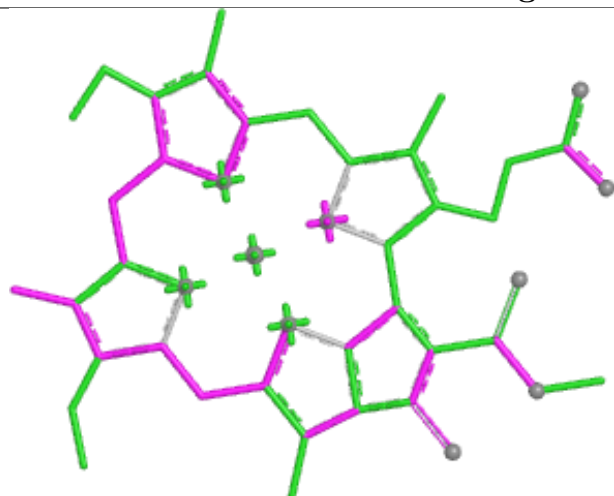
Ligand CLA r 312



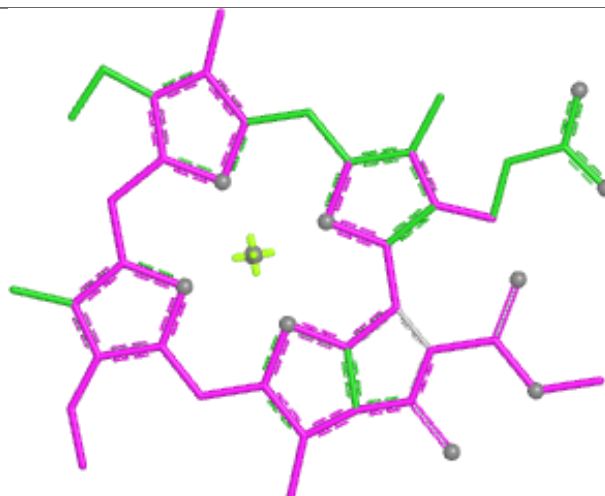
Ligand CHL n 609



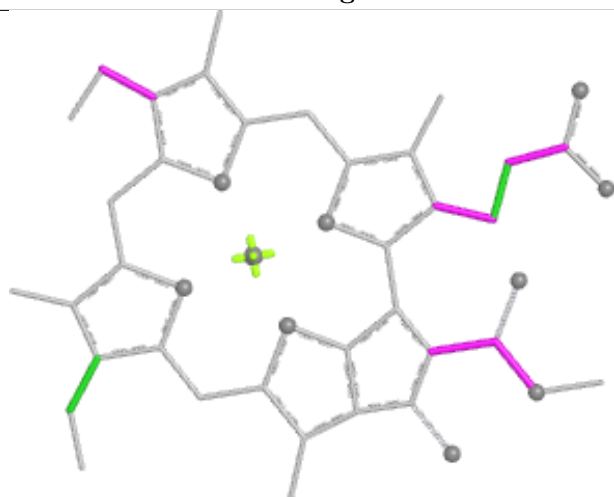
Ligand CLA 1 612



Bond lengths



Bond angles

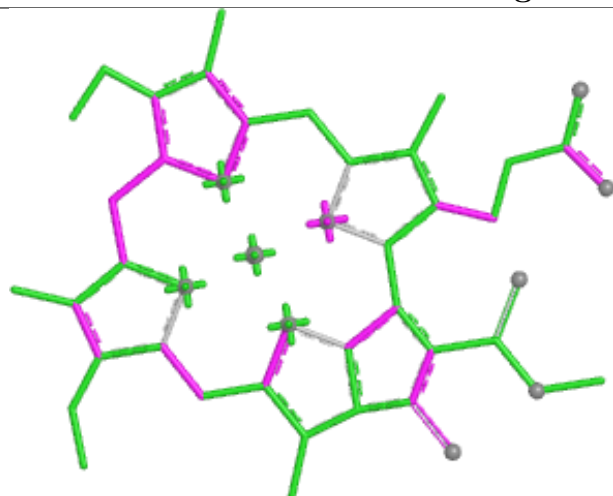


Torsions

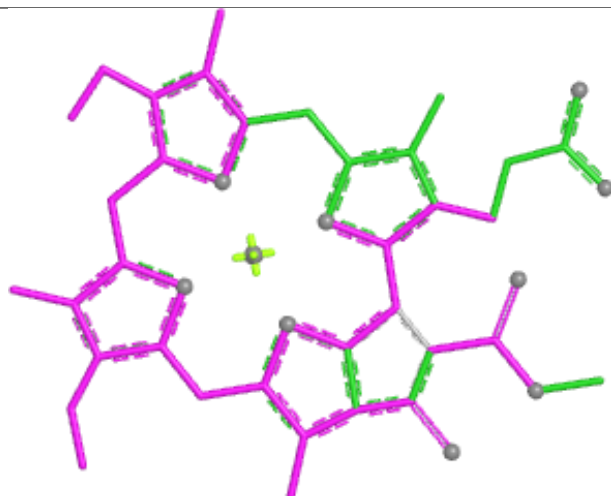


Rings

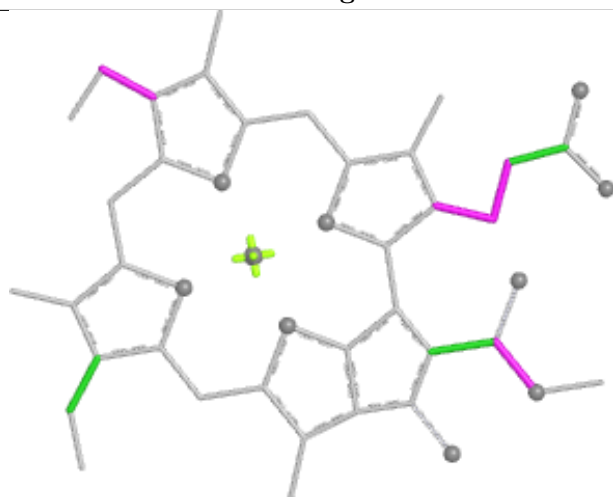
Ligand CLA B 614



Bond lengths



Bond angles

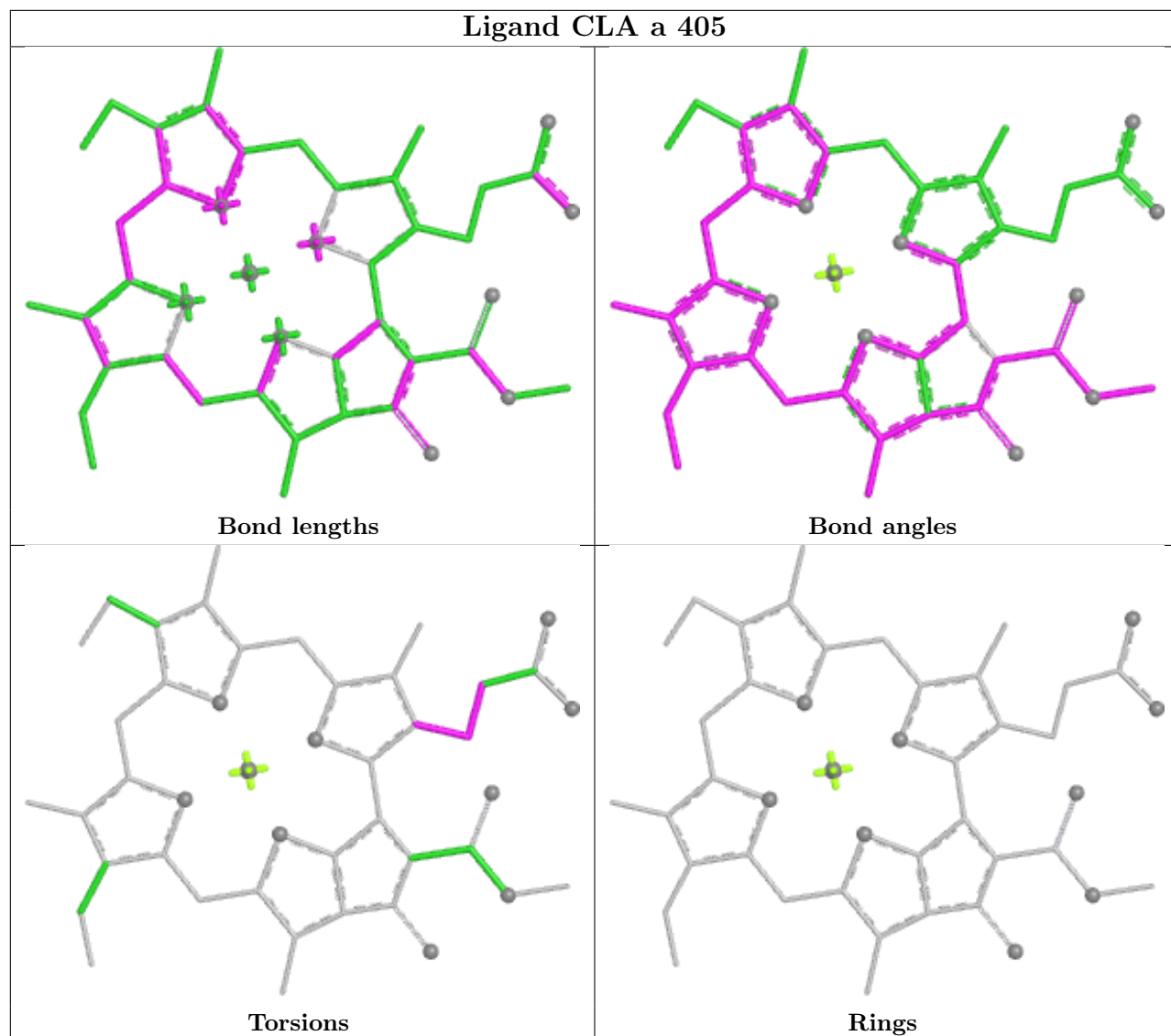


Torsions

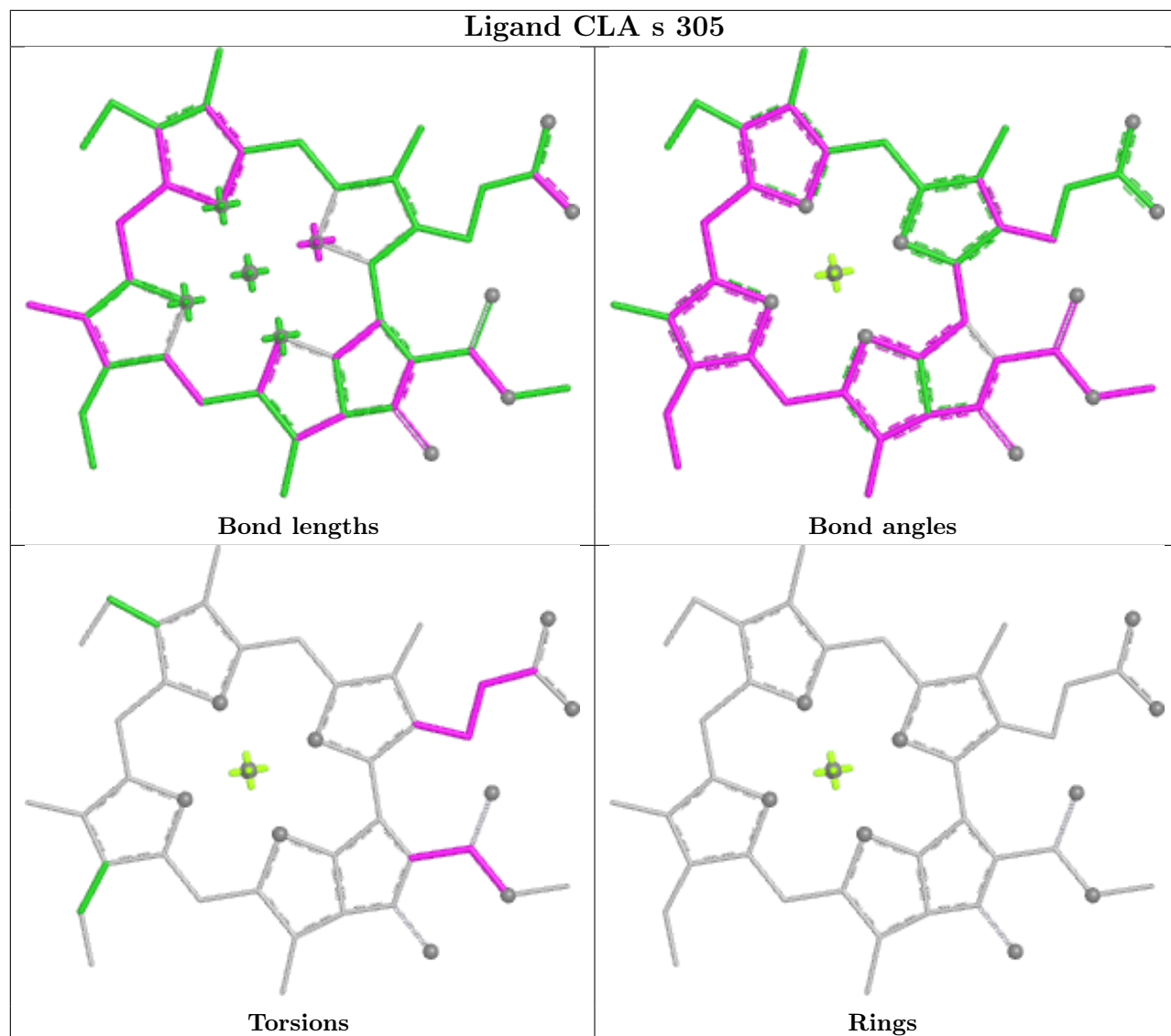


Rings

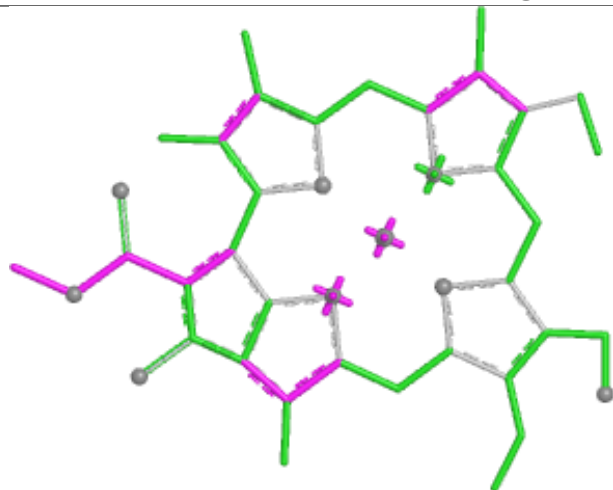
Ligand CLA a 405



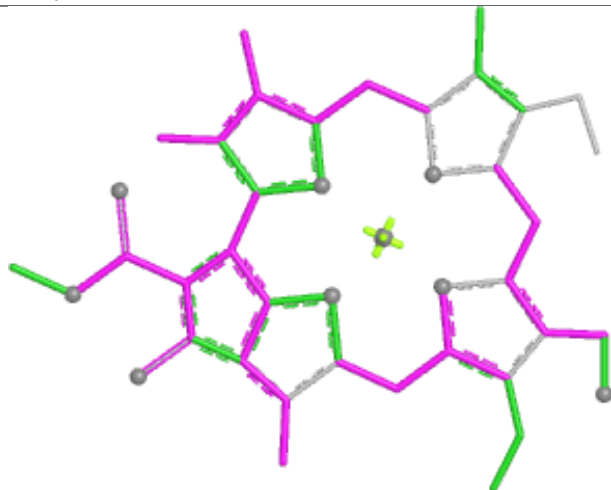
Ligand CLA s 305



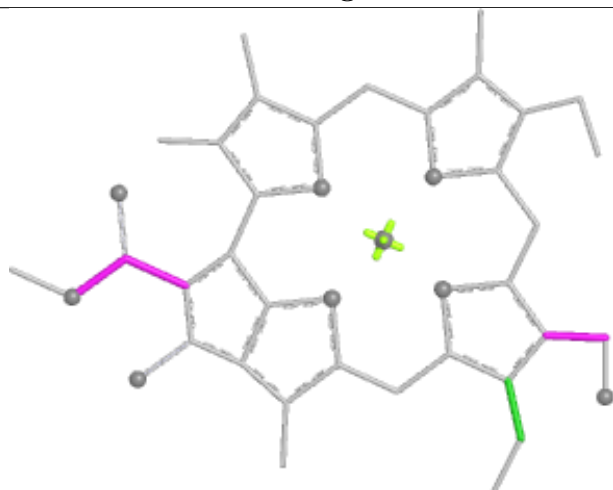
Ligand CHL y 605



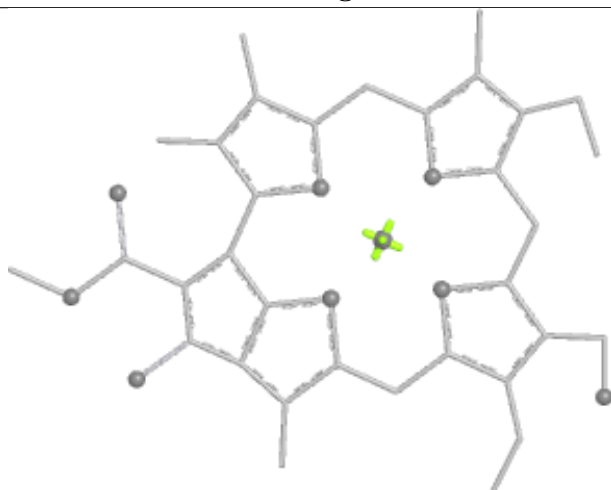
Bond lengths



Bond angles

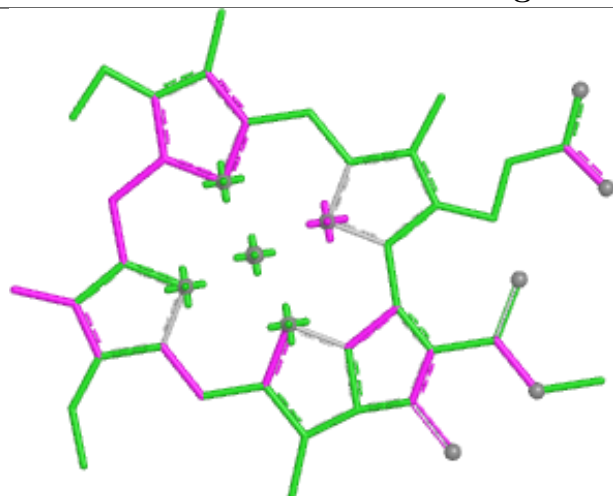


Torsions

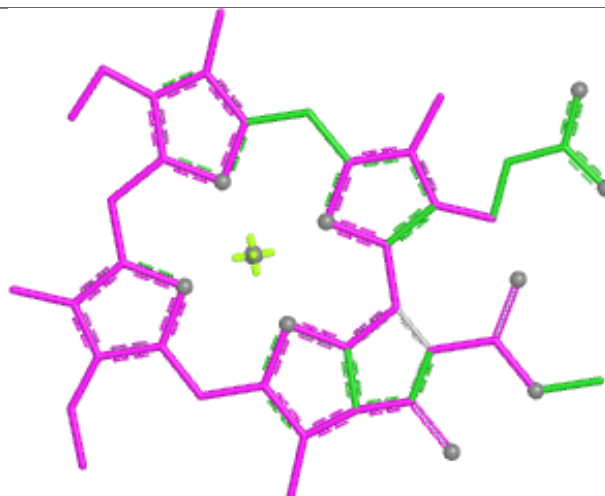


Rings

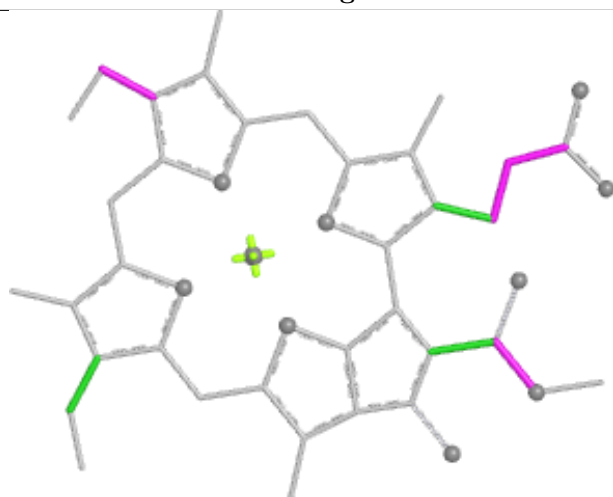
Ligand CLA Y 613



Bond lengths



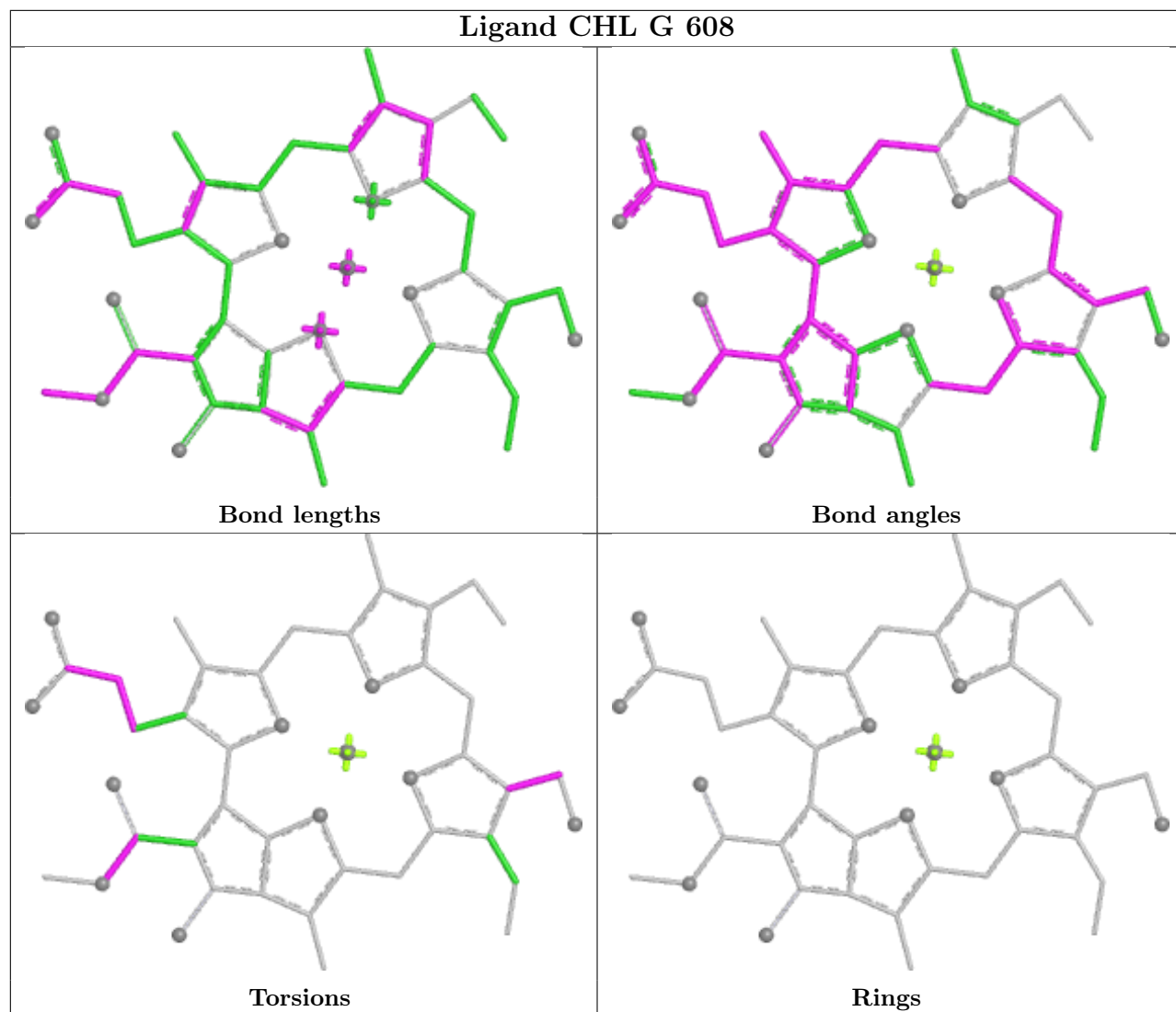
Bond angles



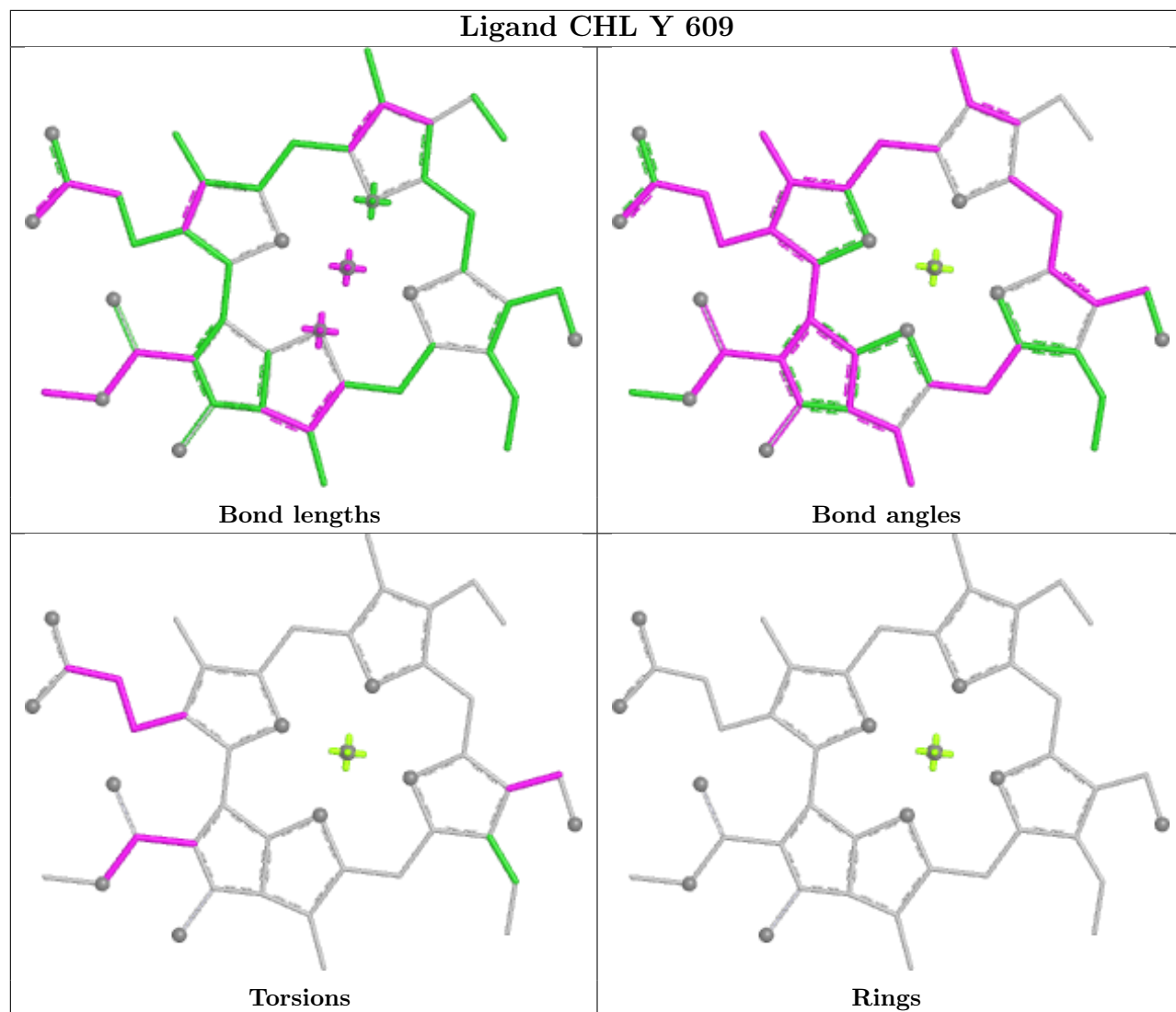
Torsions



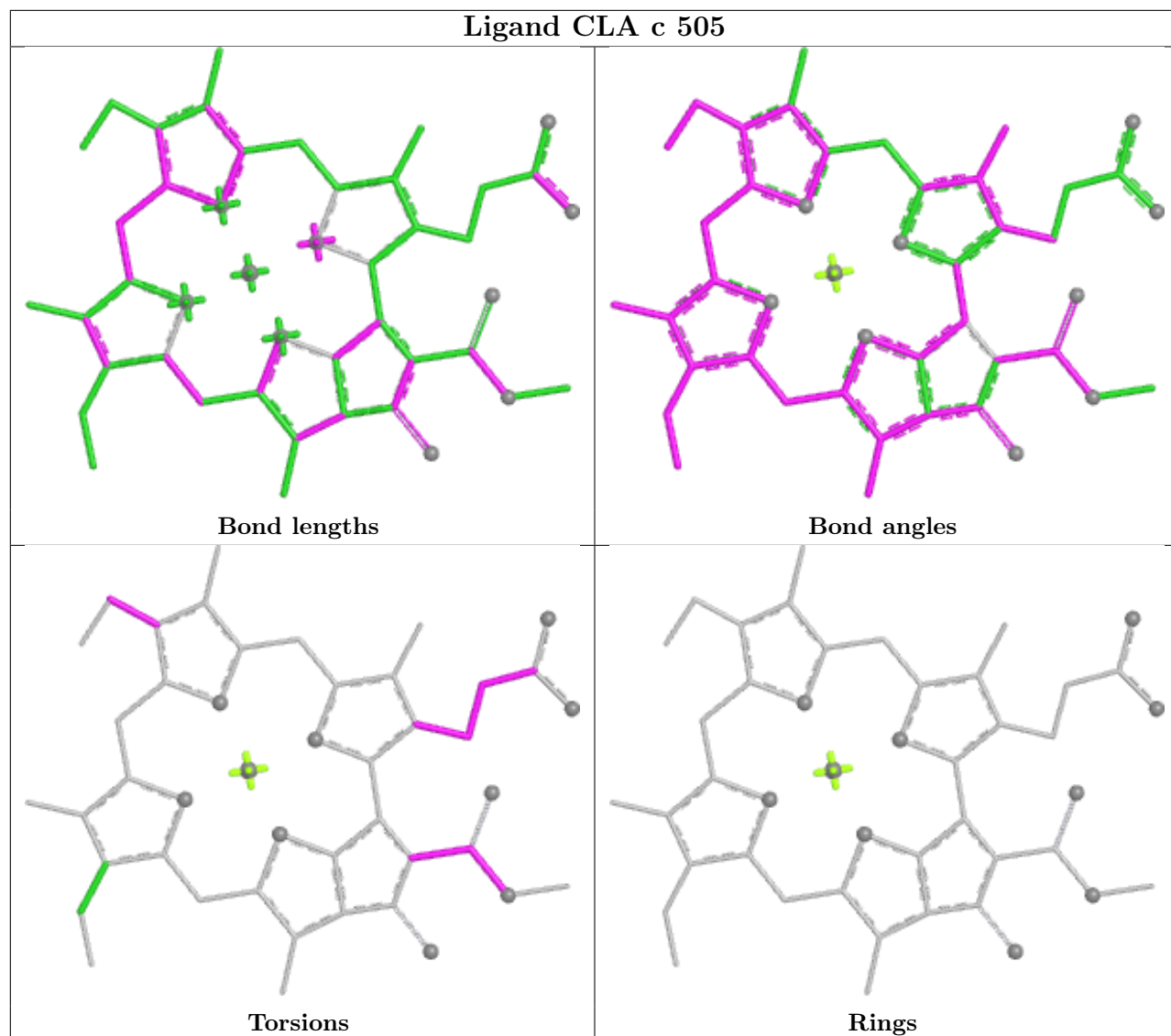
Rings



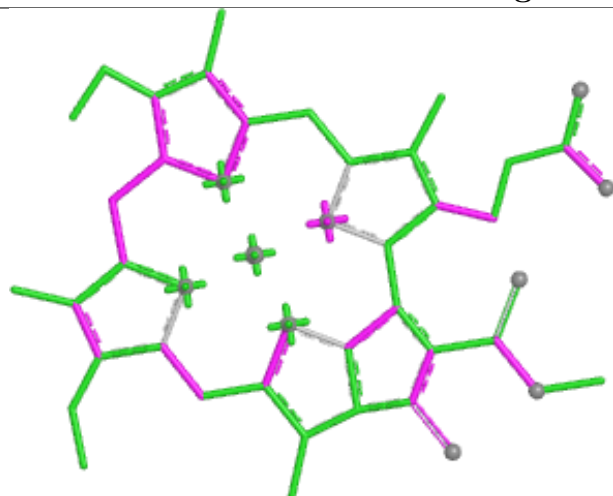
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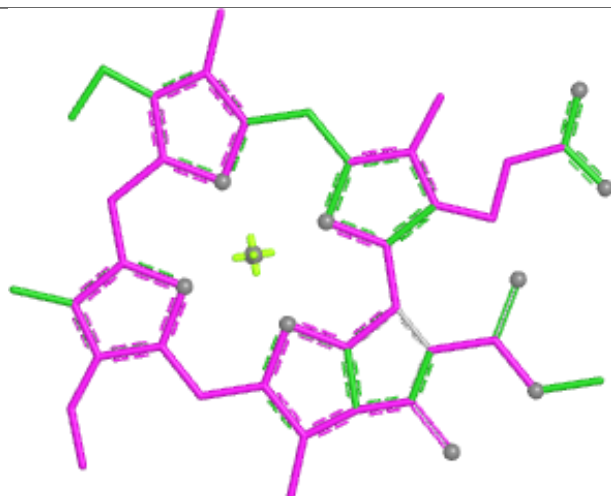
Ligand CLA c 505



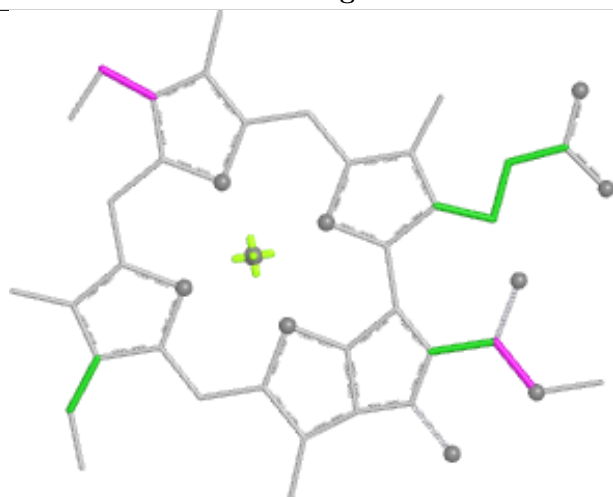
Ligand CLA B 605



Bond lengths



Bond angles

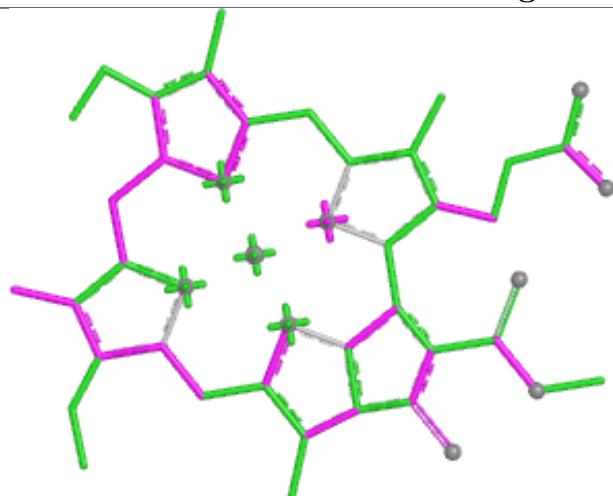


Torsions

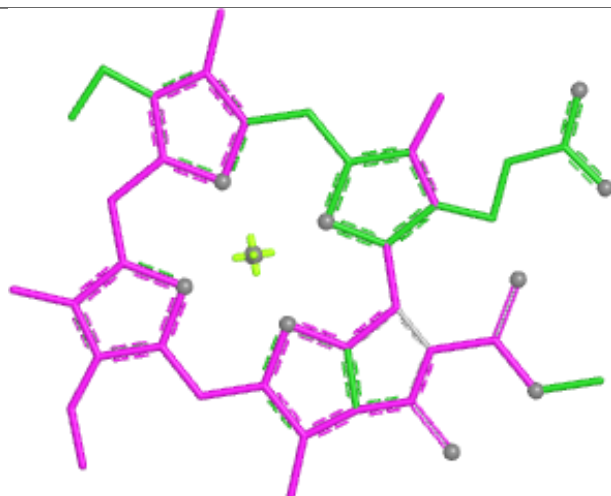


Rings

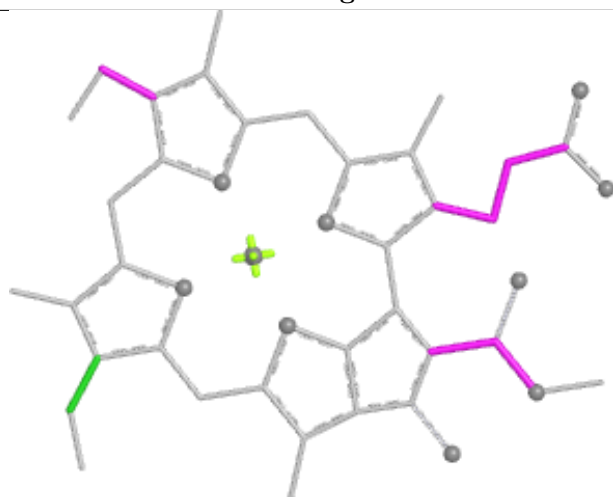
Ligand CLA 5 602



Bond lengths



Bond angles

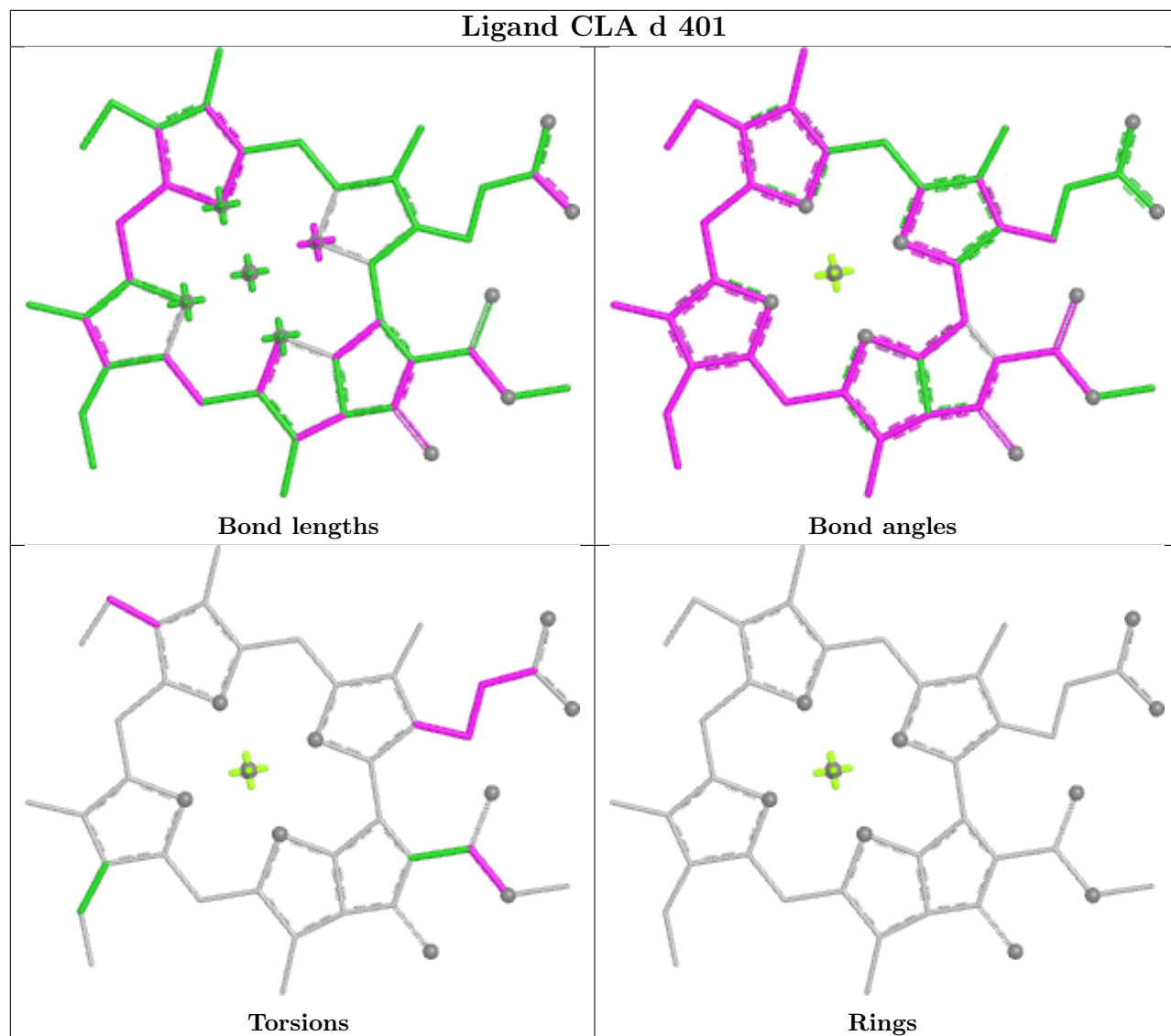


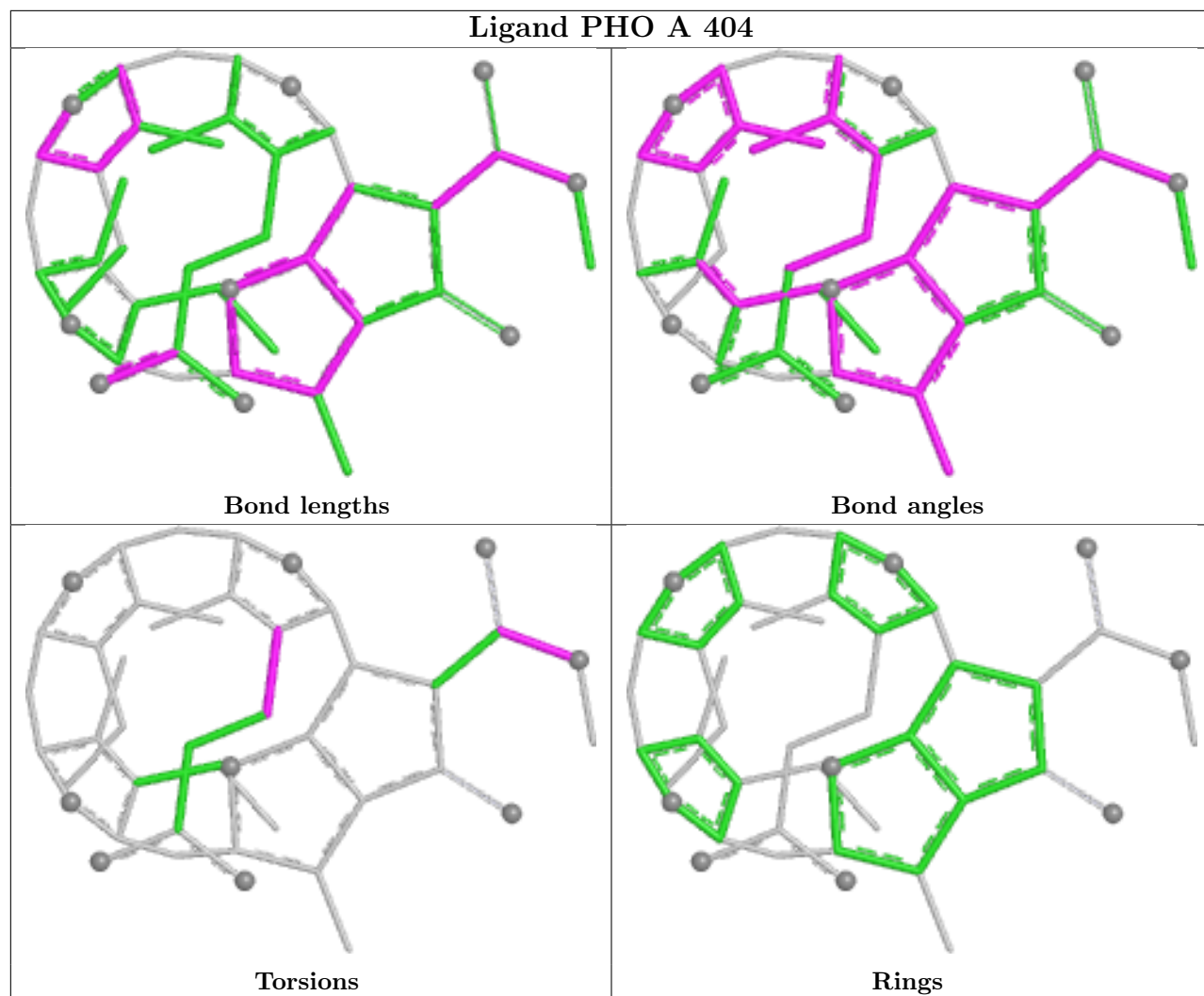
Torsions



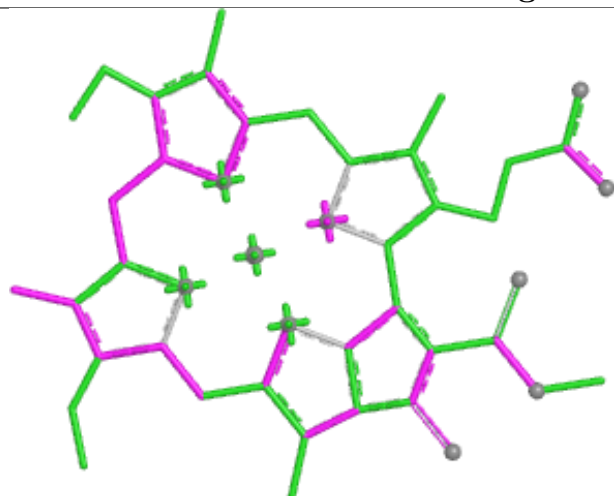
Rings

Ligand CLA d 401

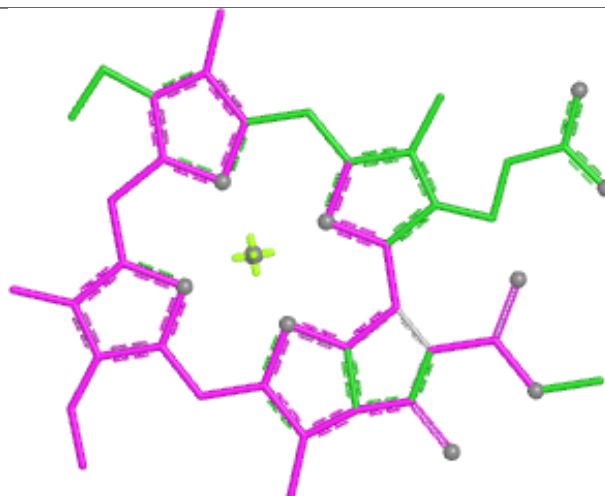




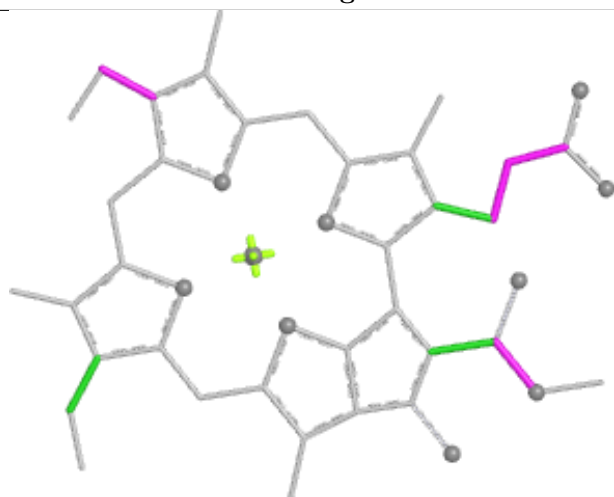
Ligand CLA 1 611



Bond lengths



Bond angles

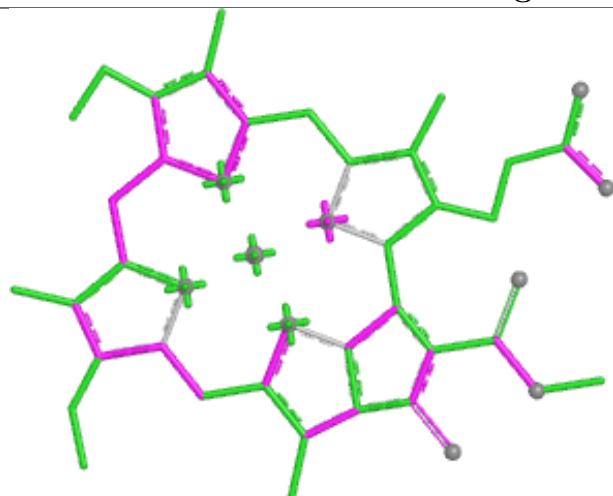


Torsions

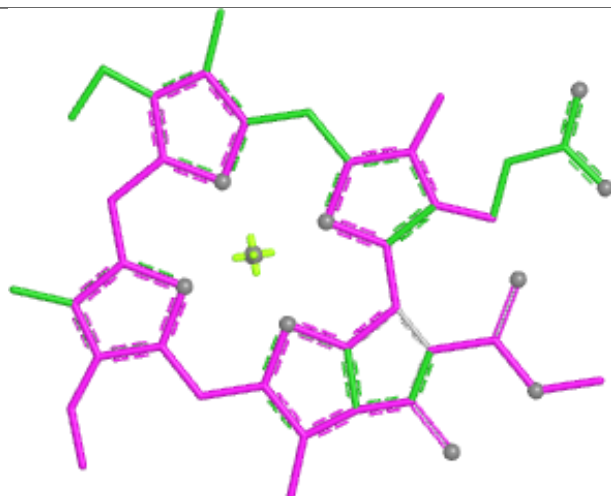


Rings

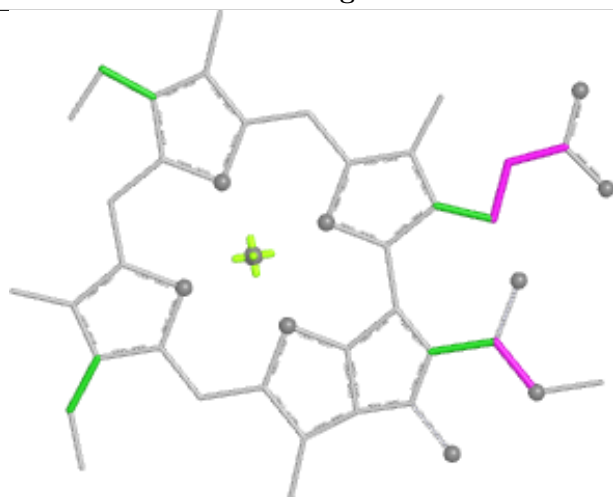
Ligand CLA B 613



Bond lengths



Bond angles

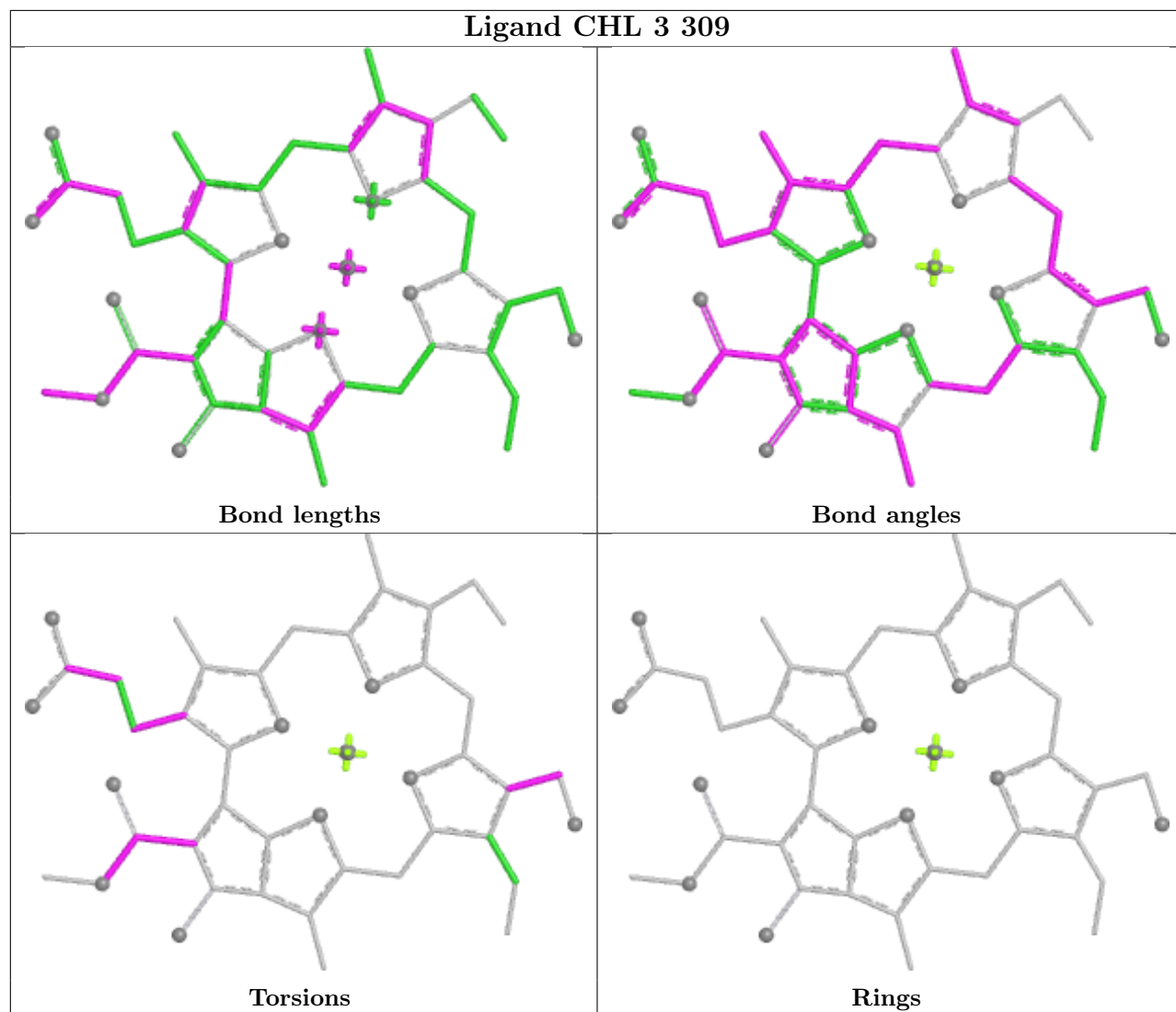


Torsions

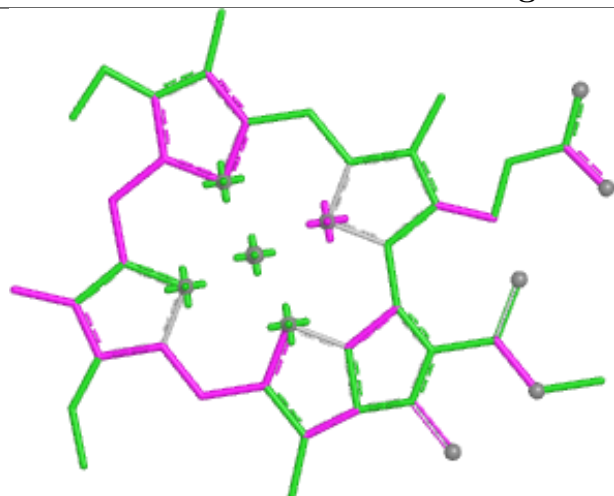


Rings

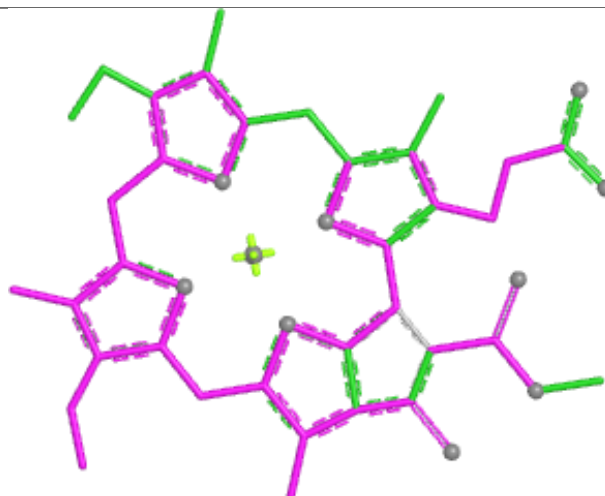
Ligand CHL 3 309



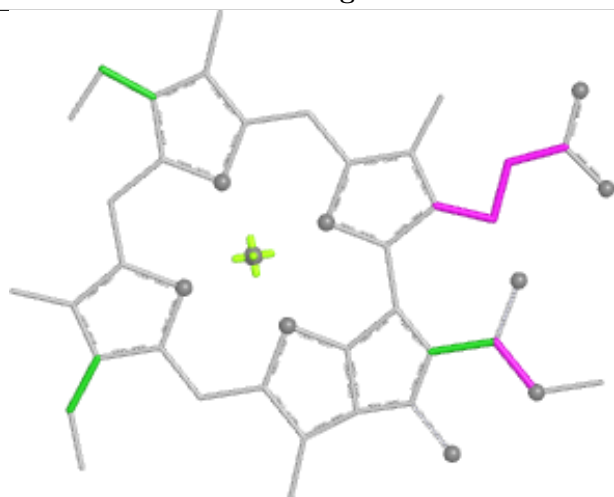
Ligand CLA 6 604



Bond lengths



Bond angles

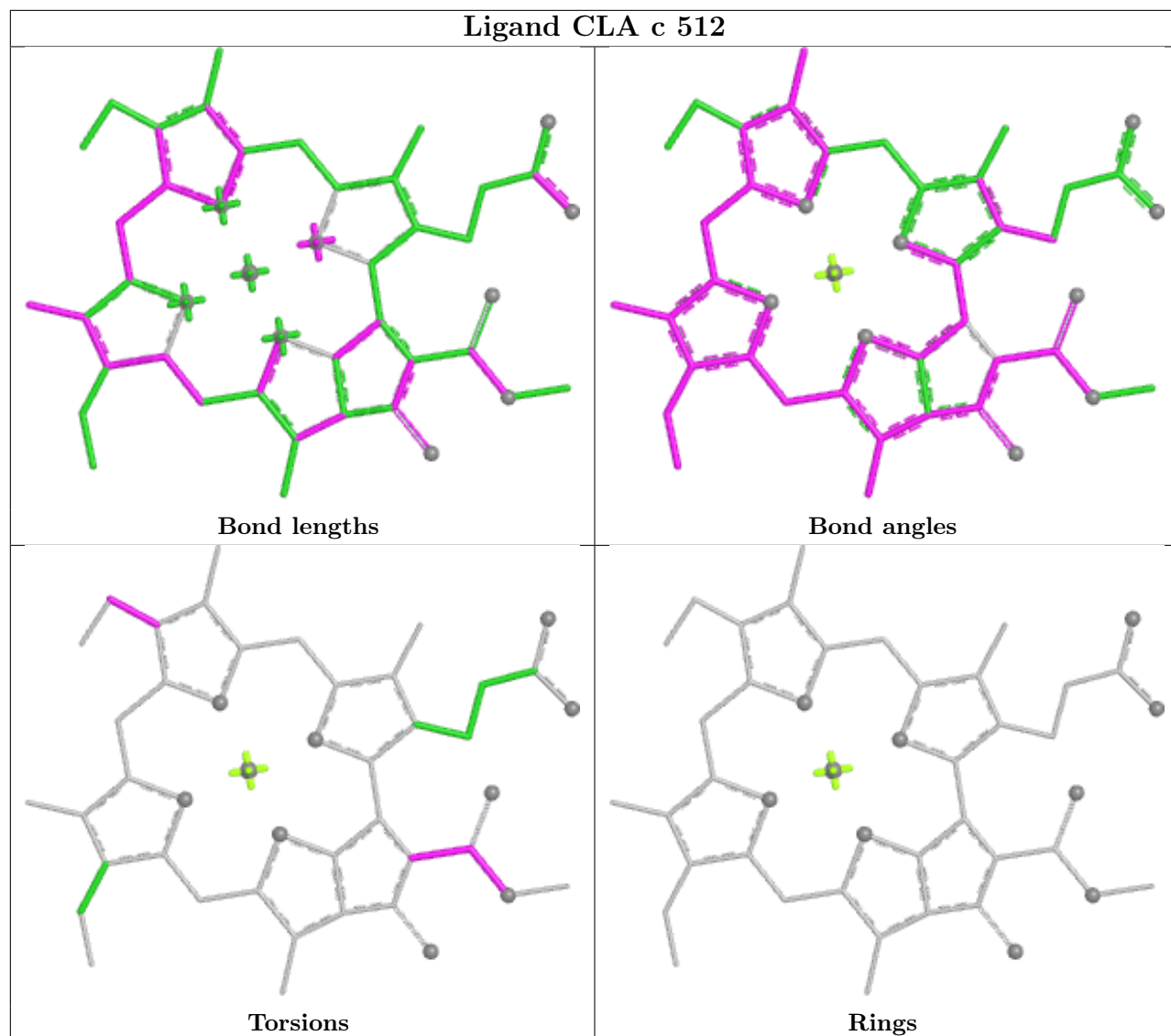


Torsions

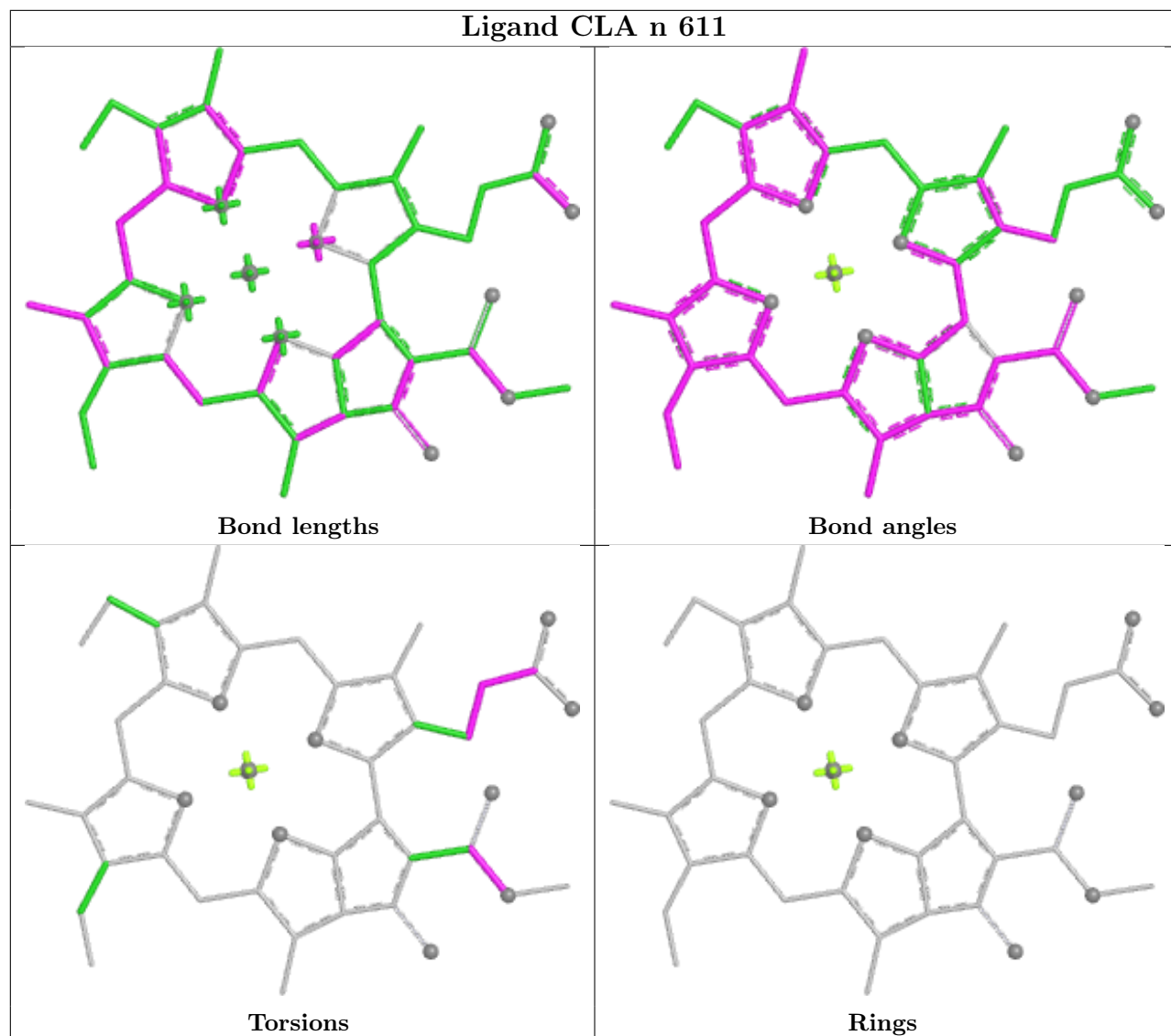


Rings

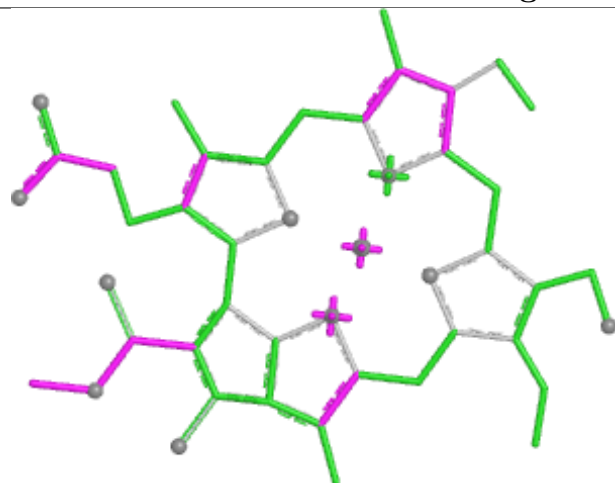
Ligand CLA c 512



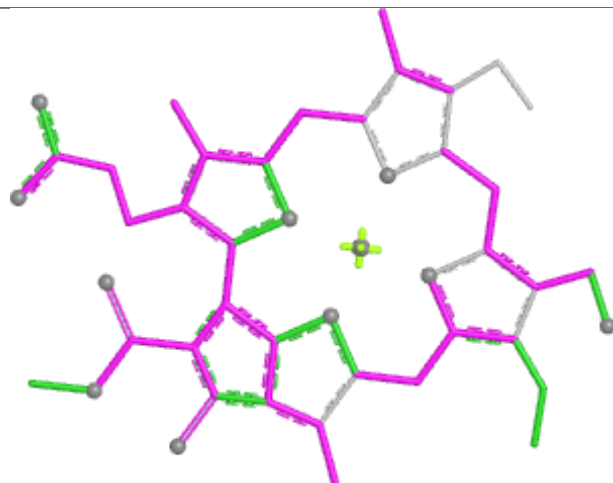
Ligand CLA n 611



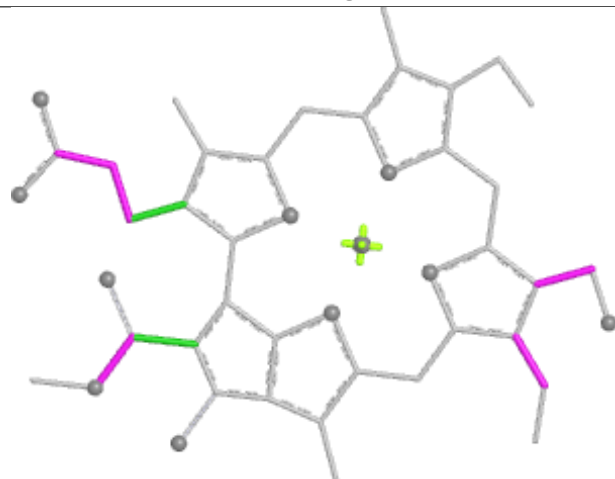
Ligand CHL 8 308



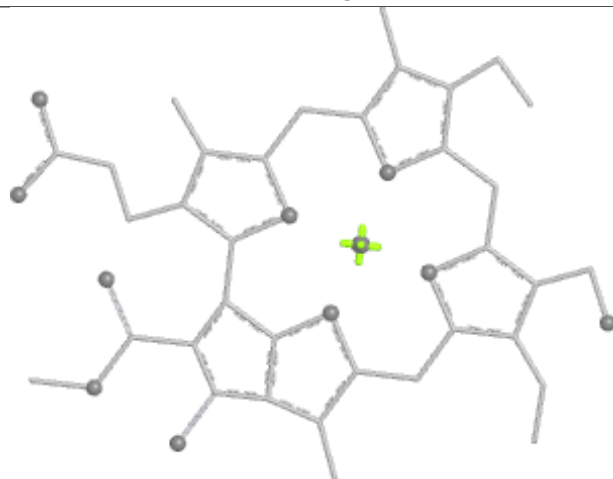
Bond lengths



Bond angles

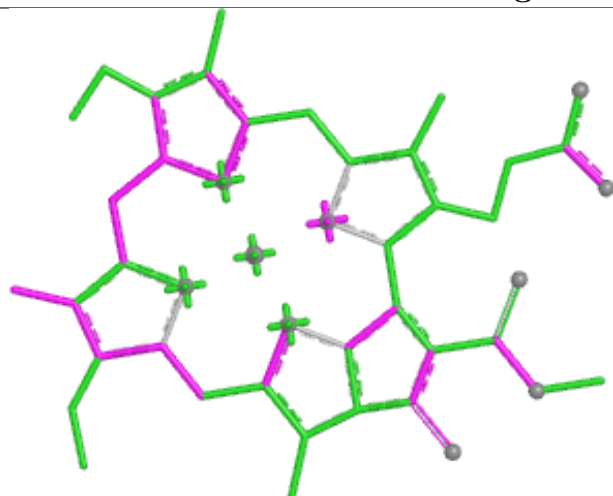


Torsions

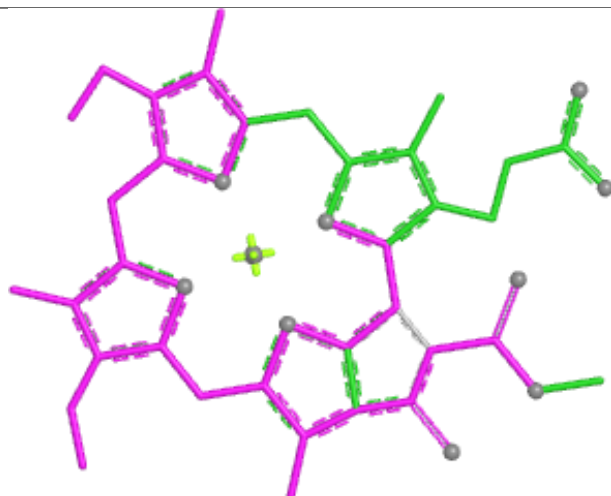


Rings

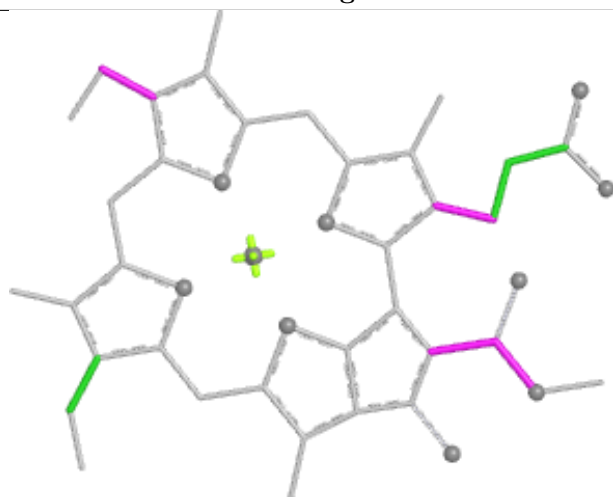
Ligand CLA B 607



Bond lengths



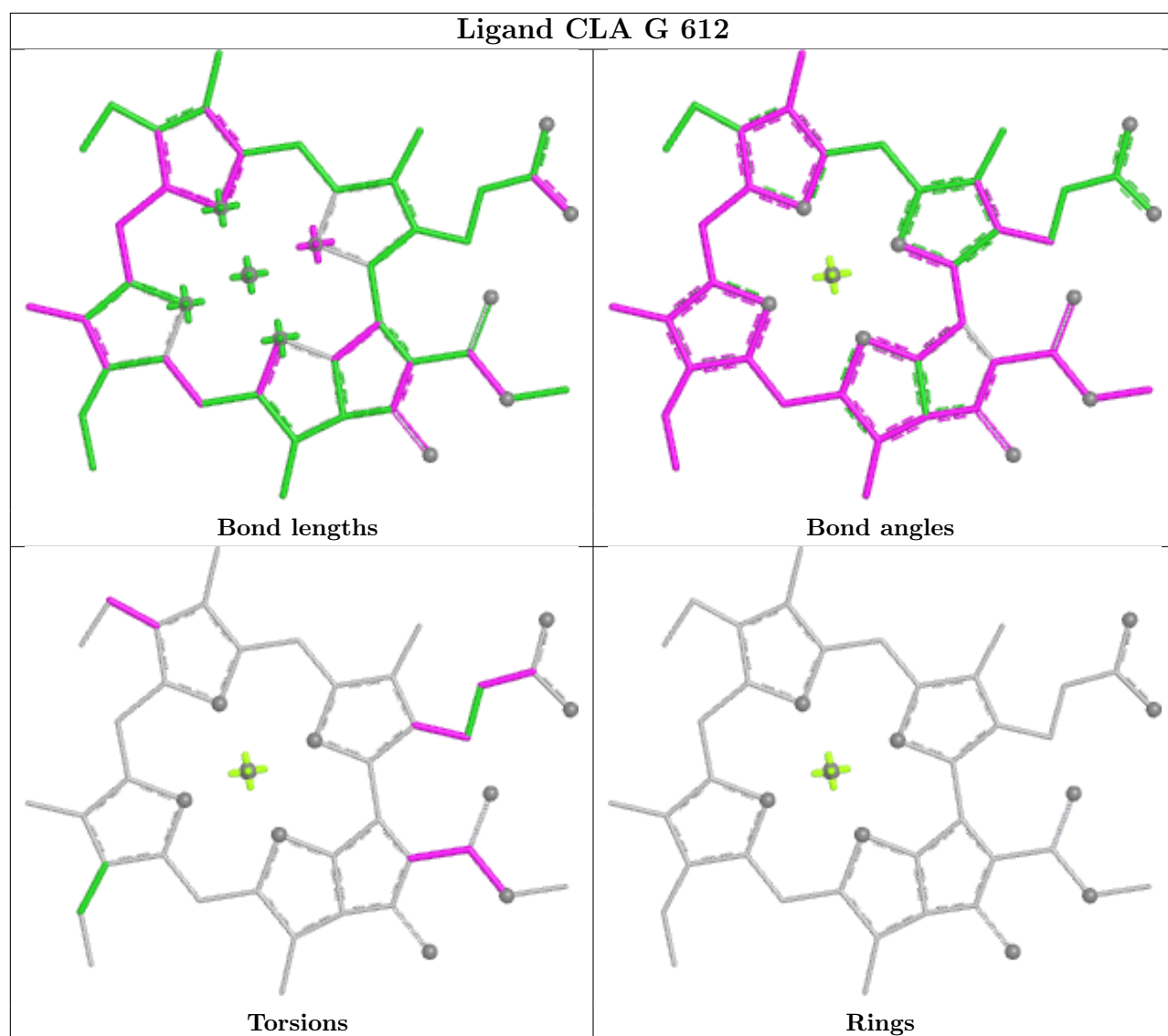
Bond angles



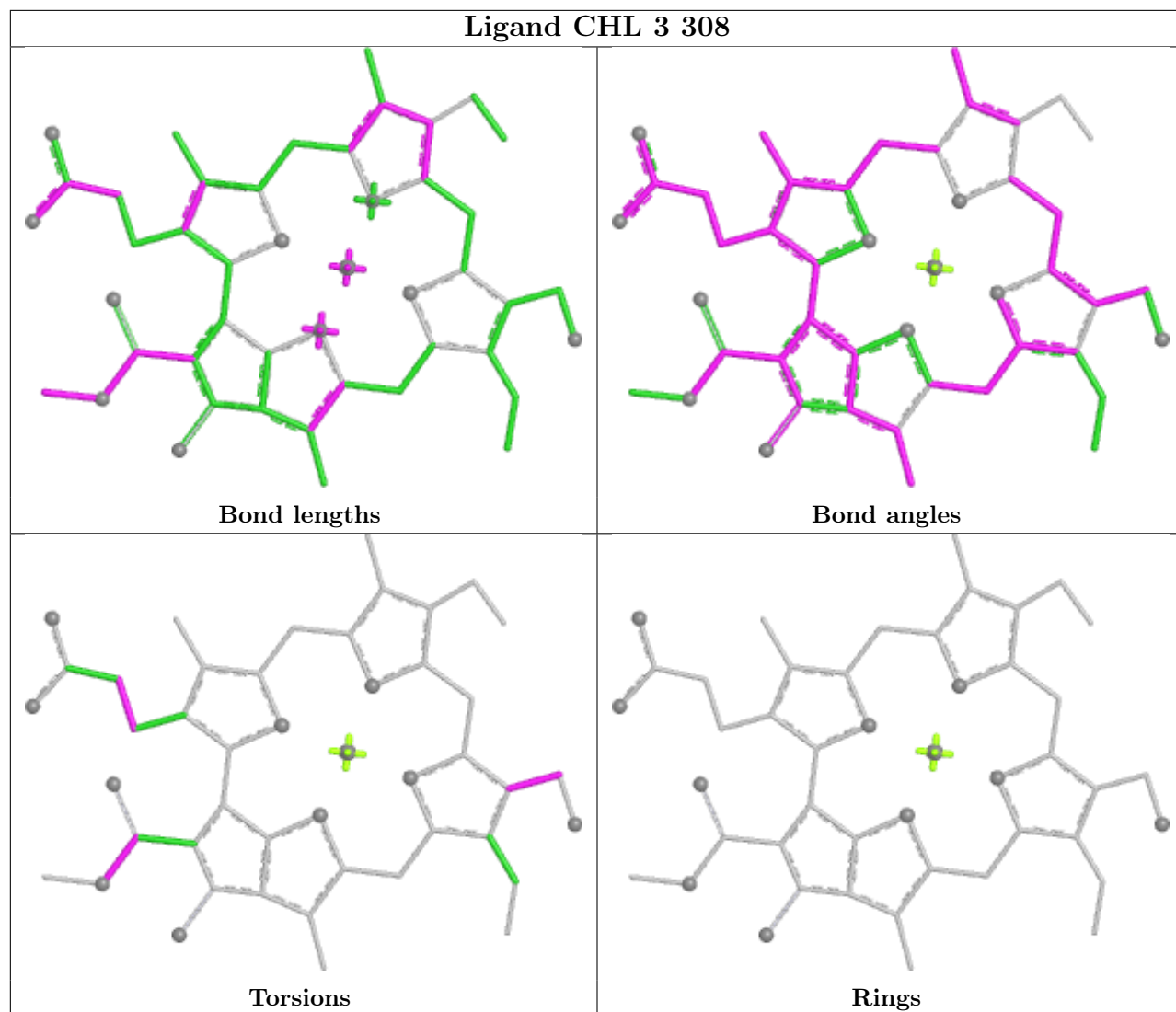
Torsions



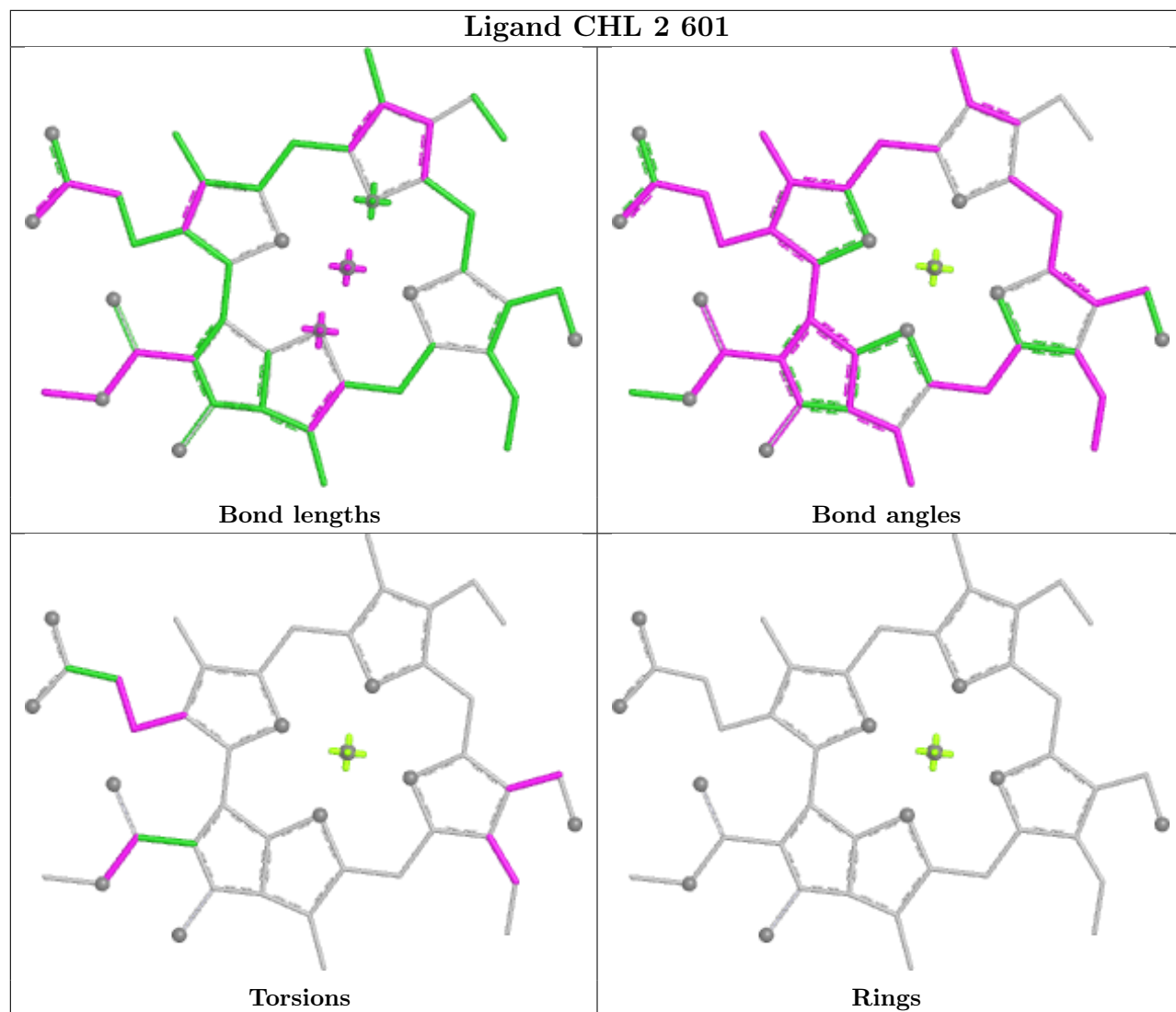
Rings



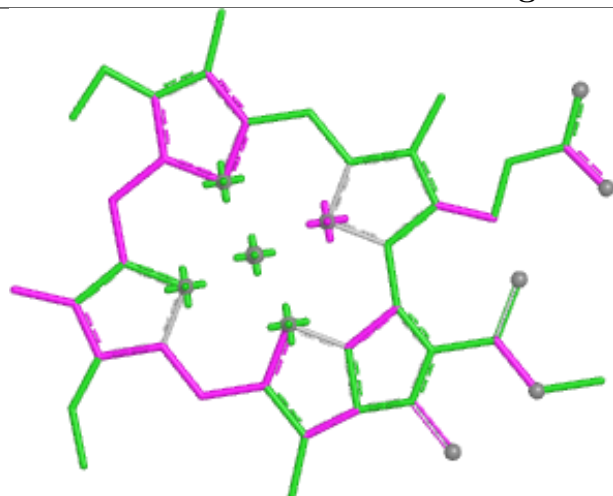
Ligand CHL 3 308



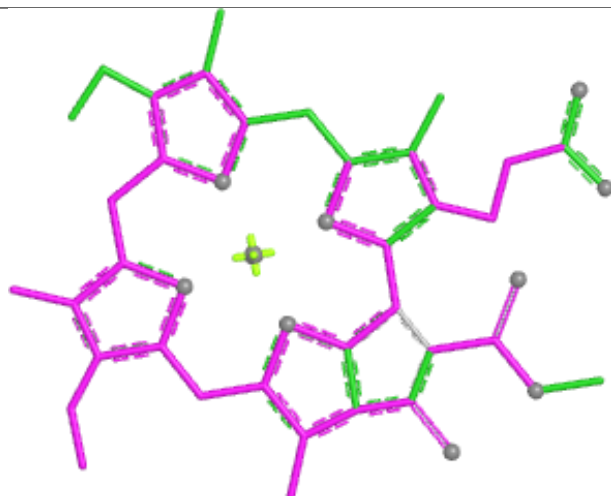
Ligand CHL 2 601



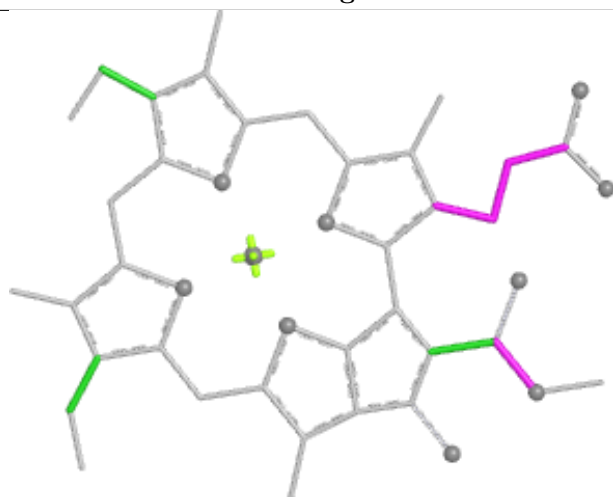
Ligand CLA 2 604



Bond lengths



Bond angles

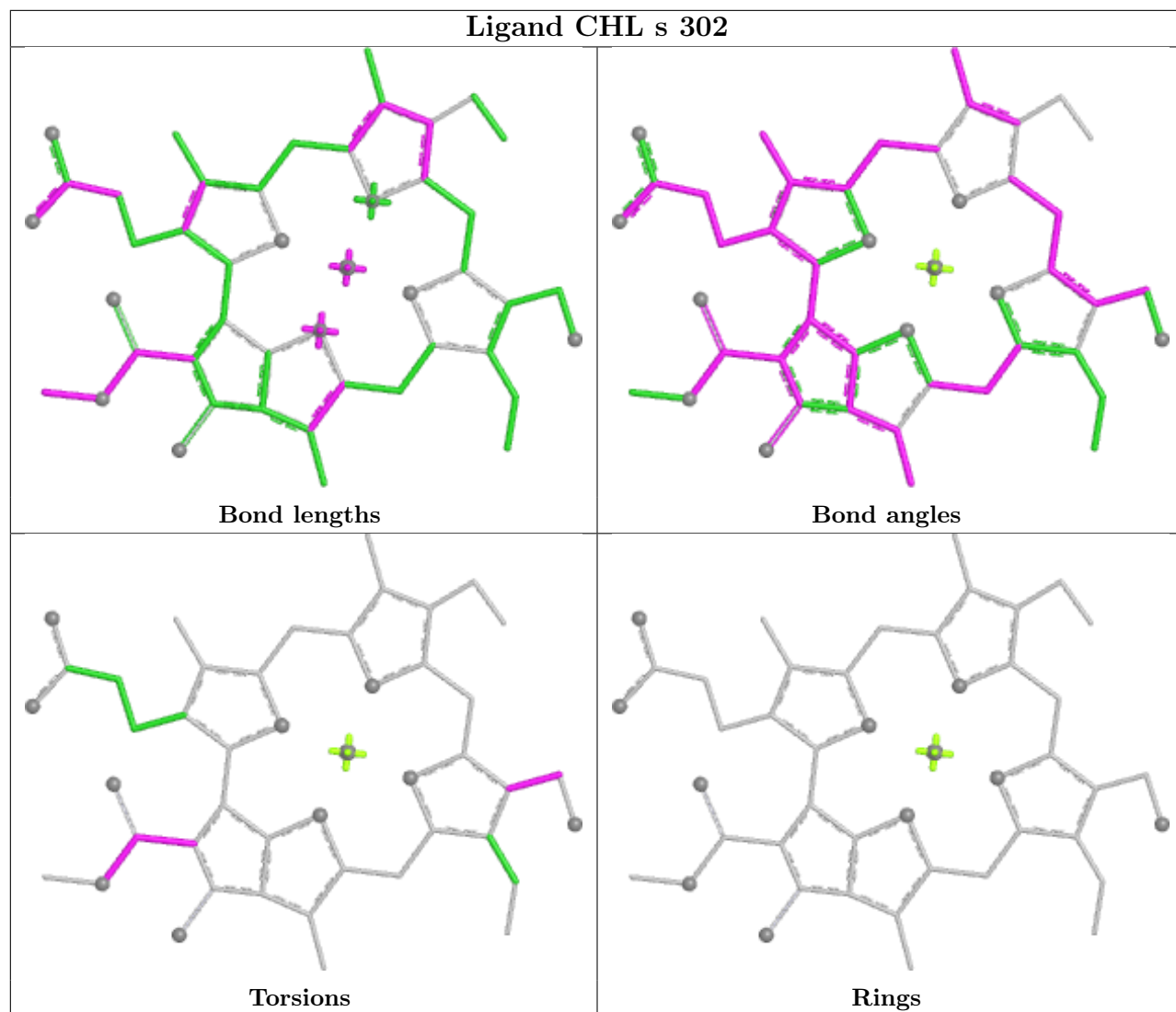


Torsions

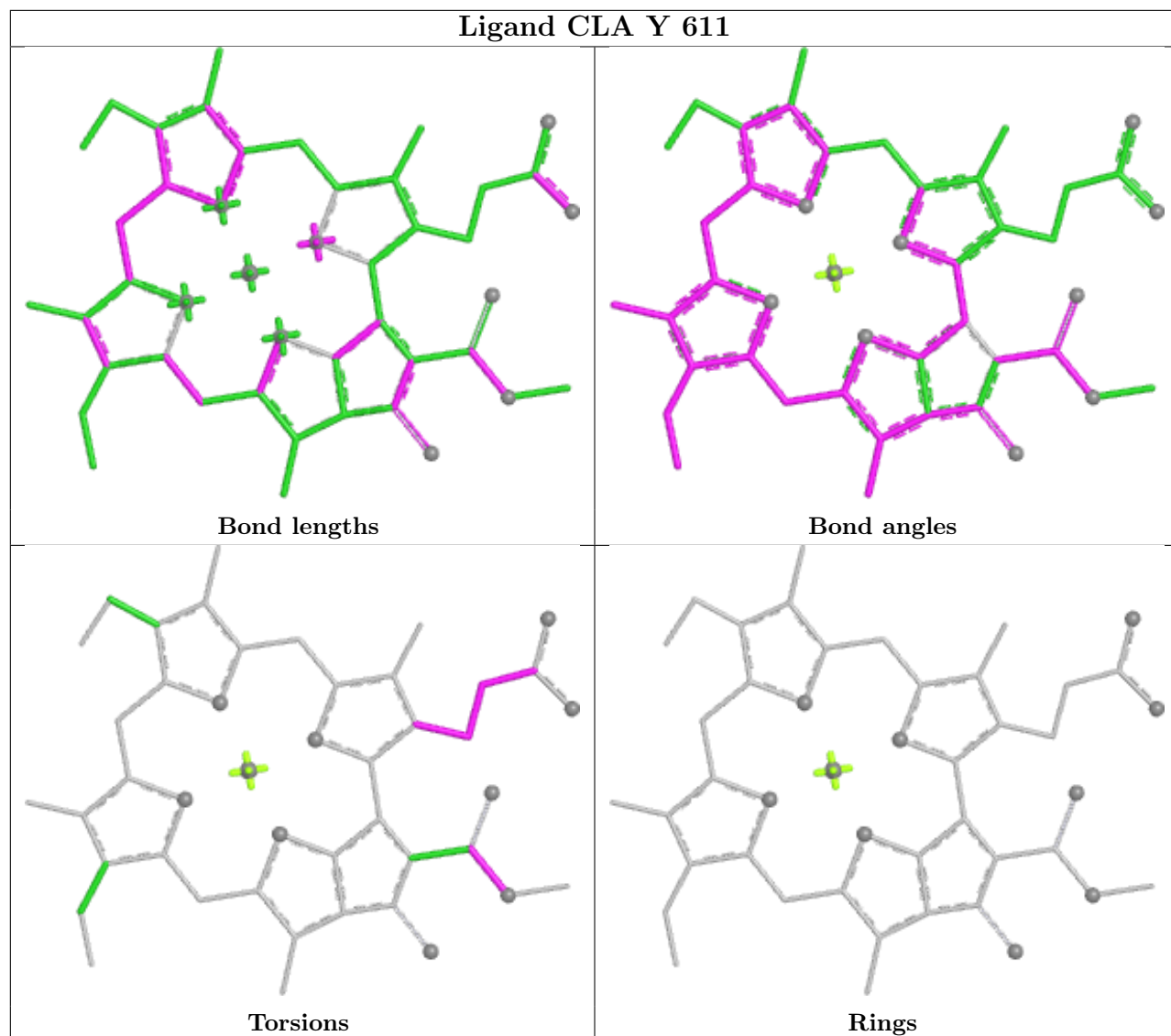


Rings

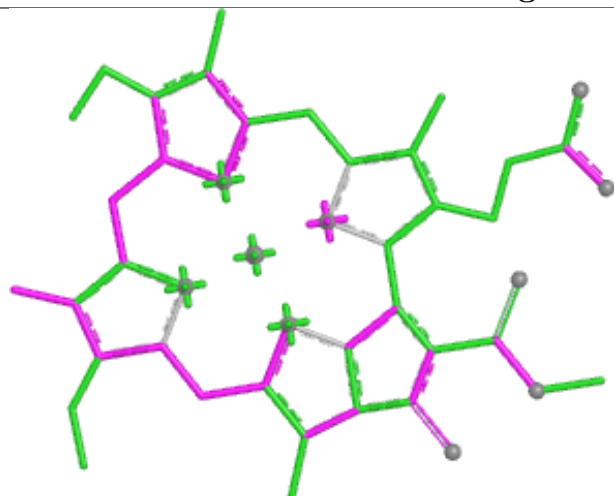
Ligand CHL s 302



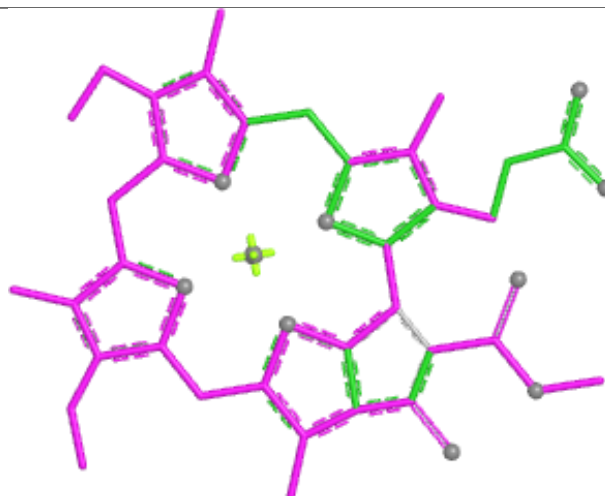
Ligand CLA Y 611



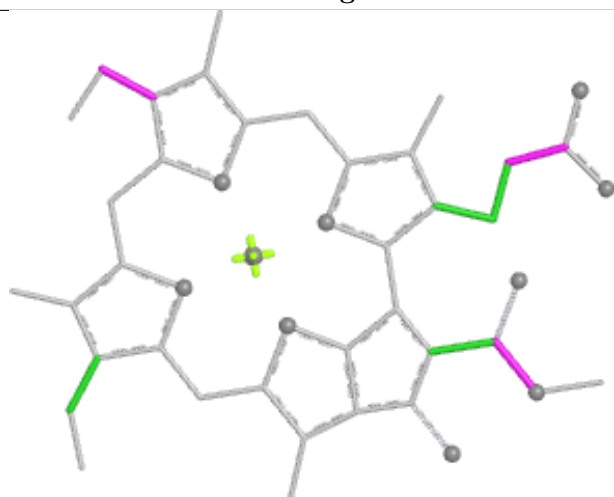
Ligand CLA 1 613



Bond lengths



Bond angles

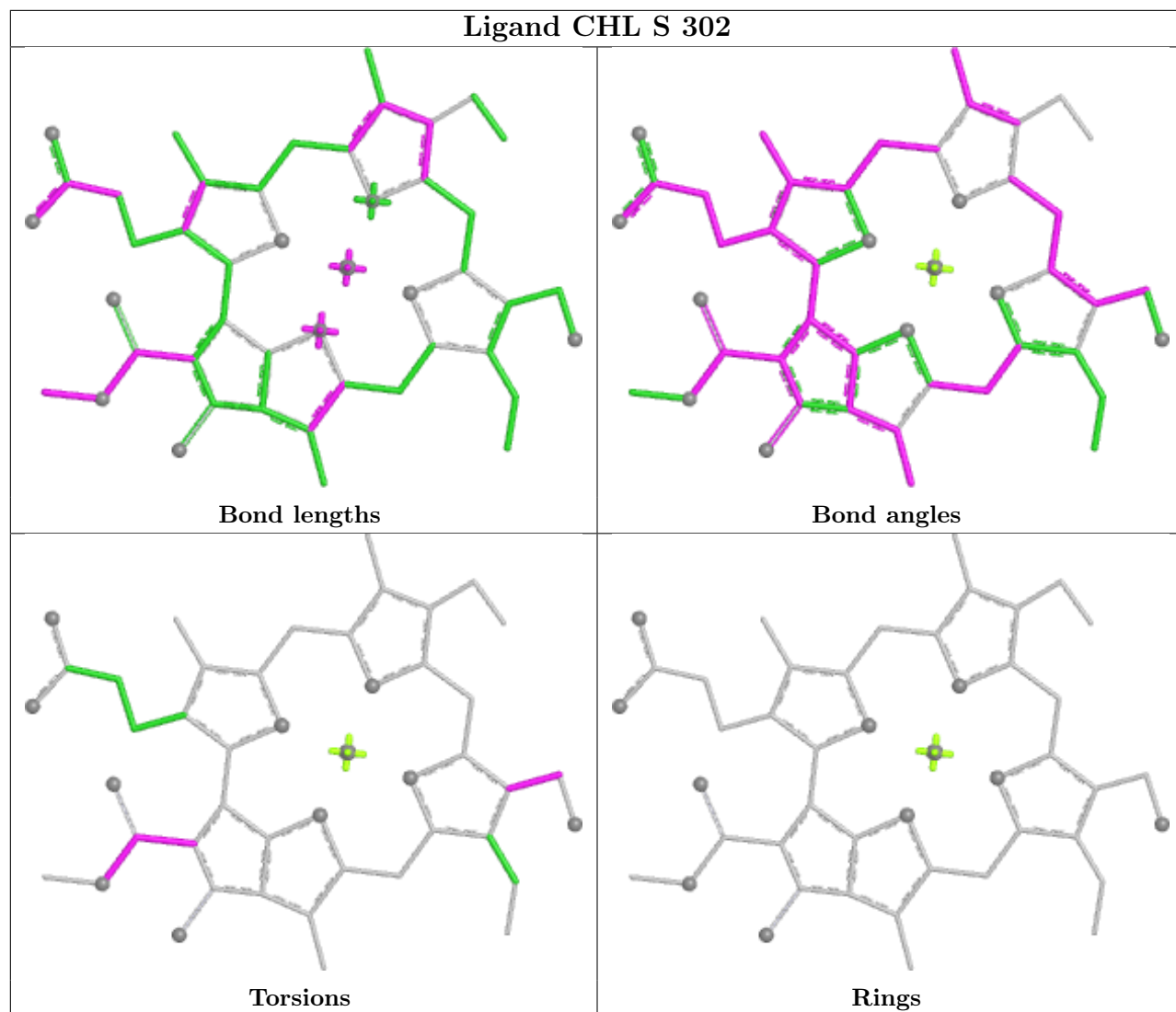


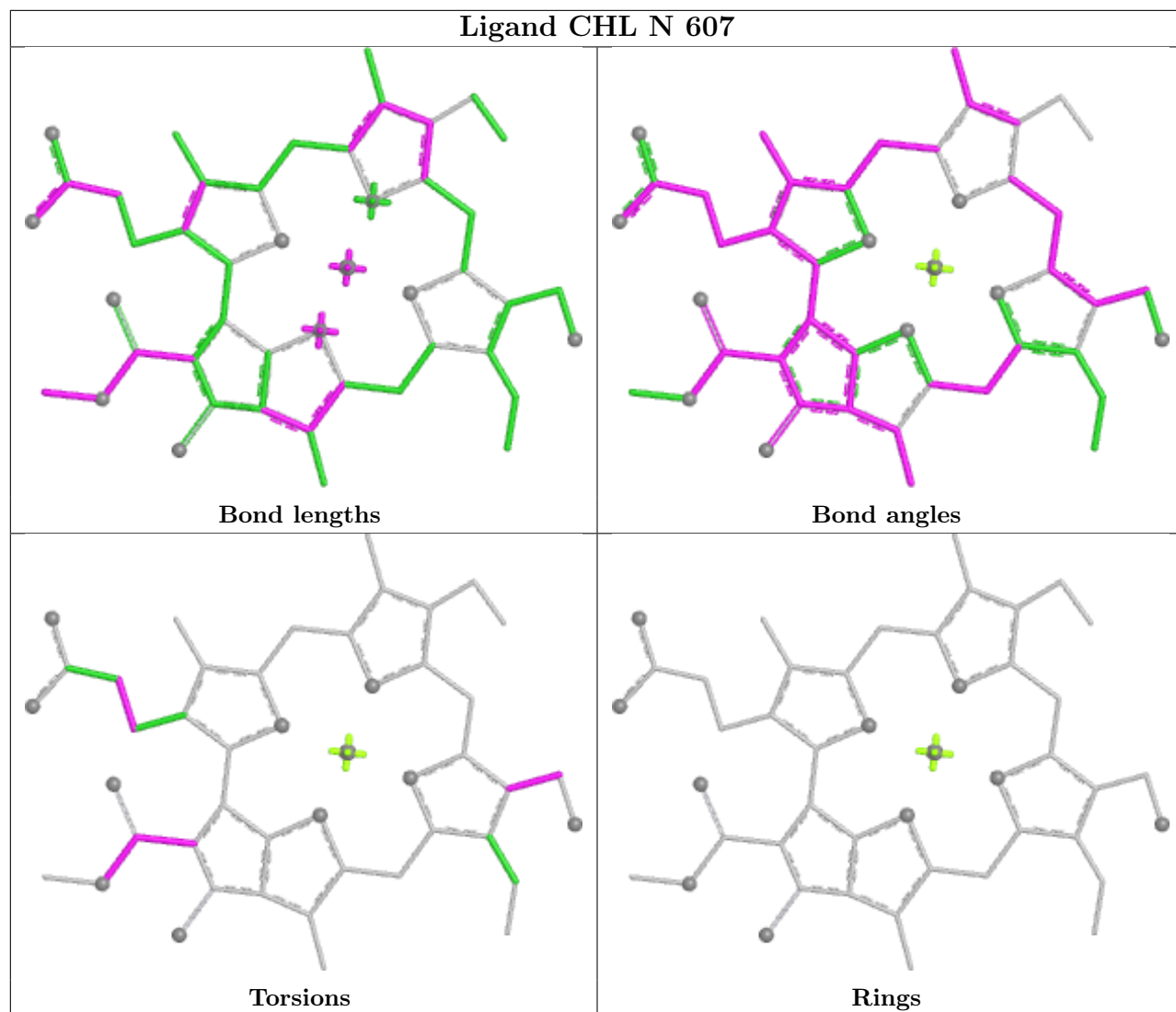
Torsions



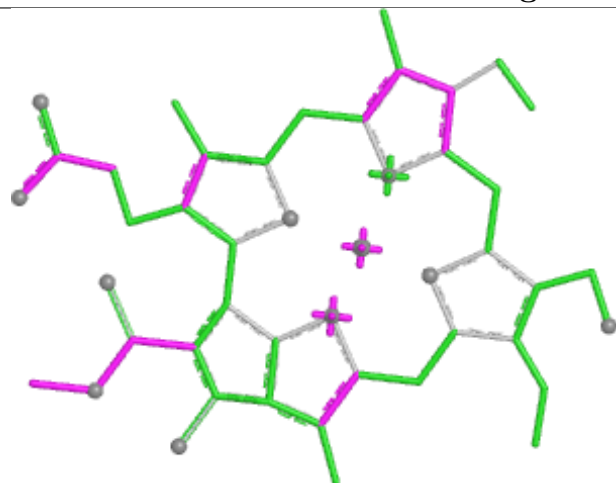
Rings

Ligand CHL S 302

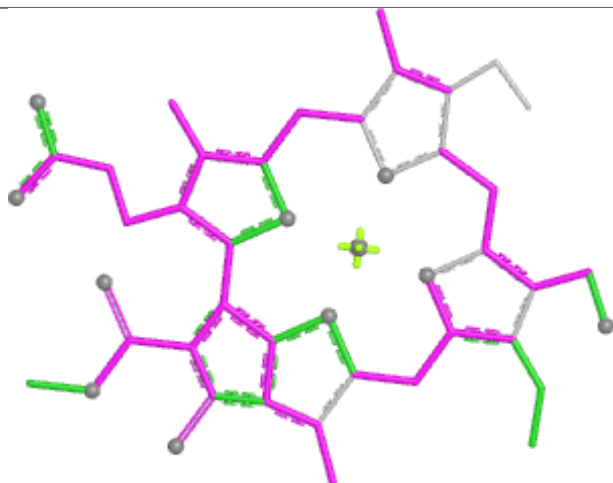




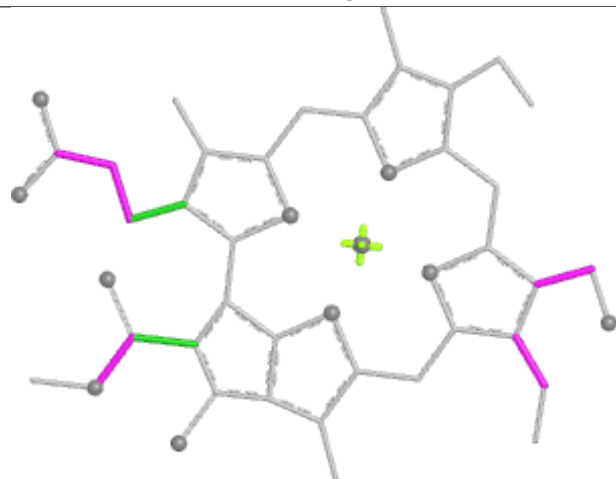
Ligand CHL 4 308



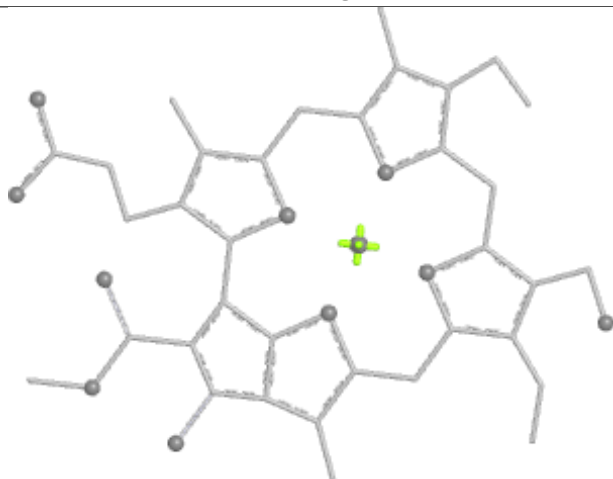
Bond lengths



Bond angles

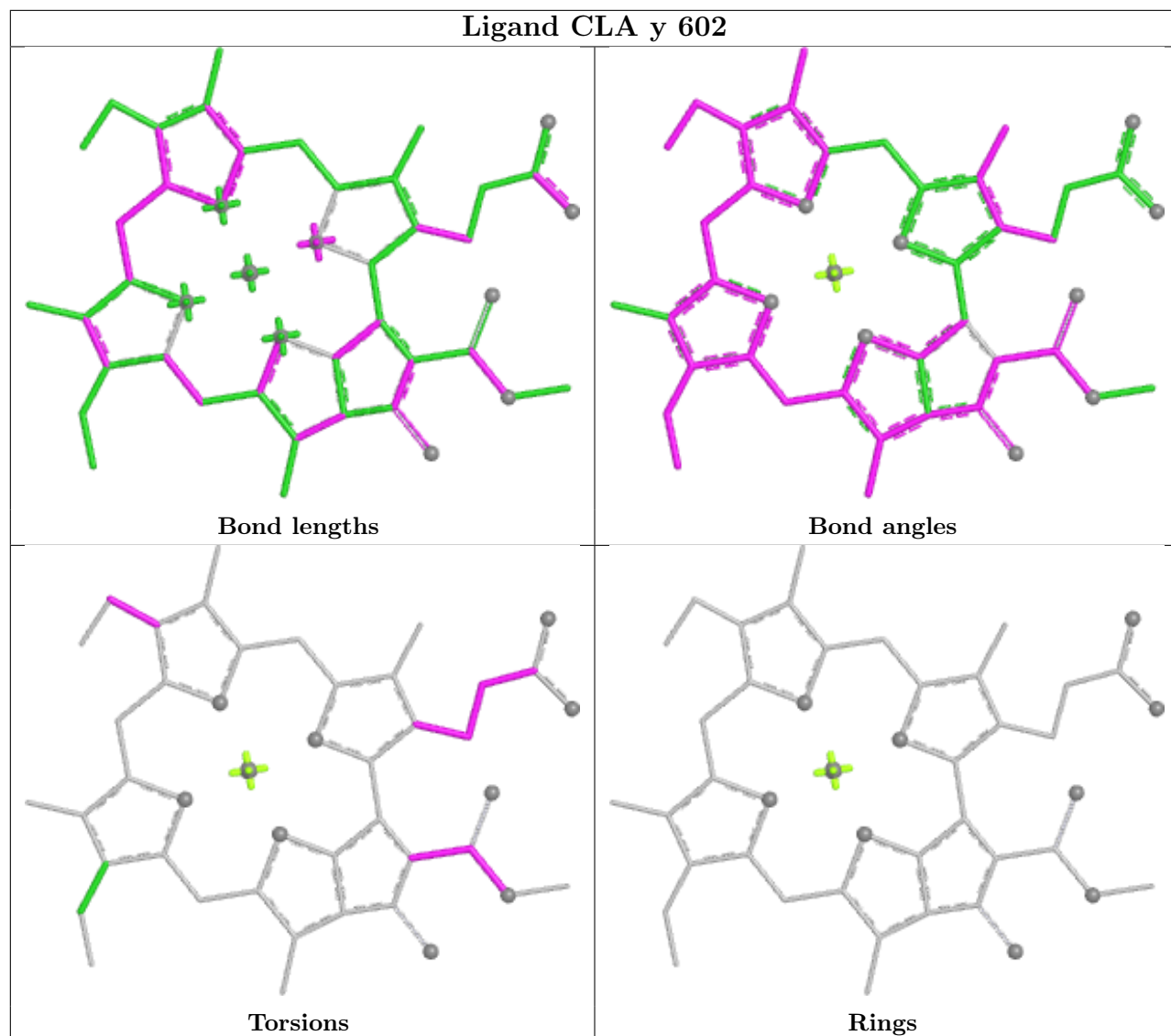


Torsions

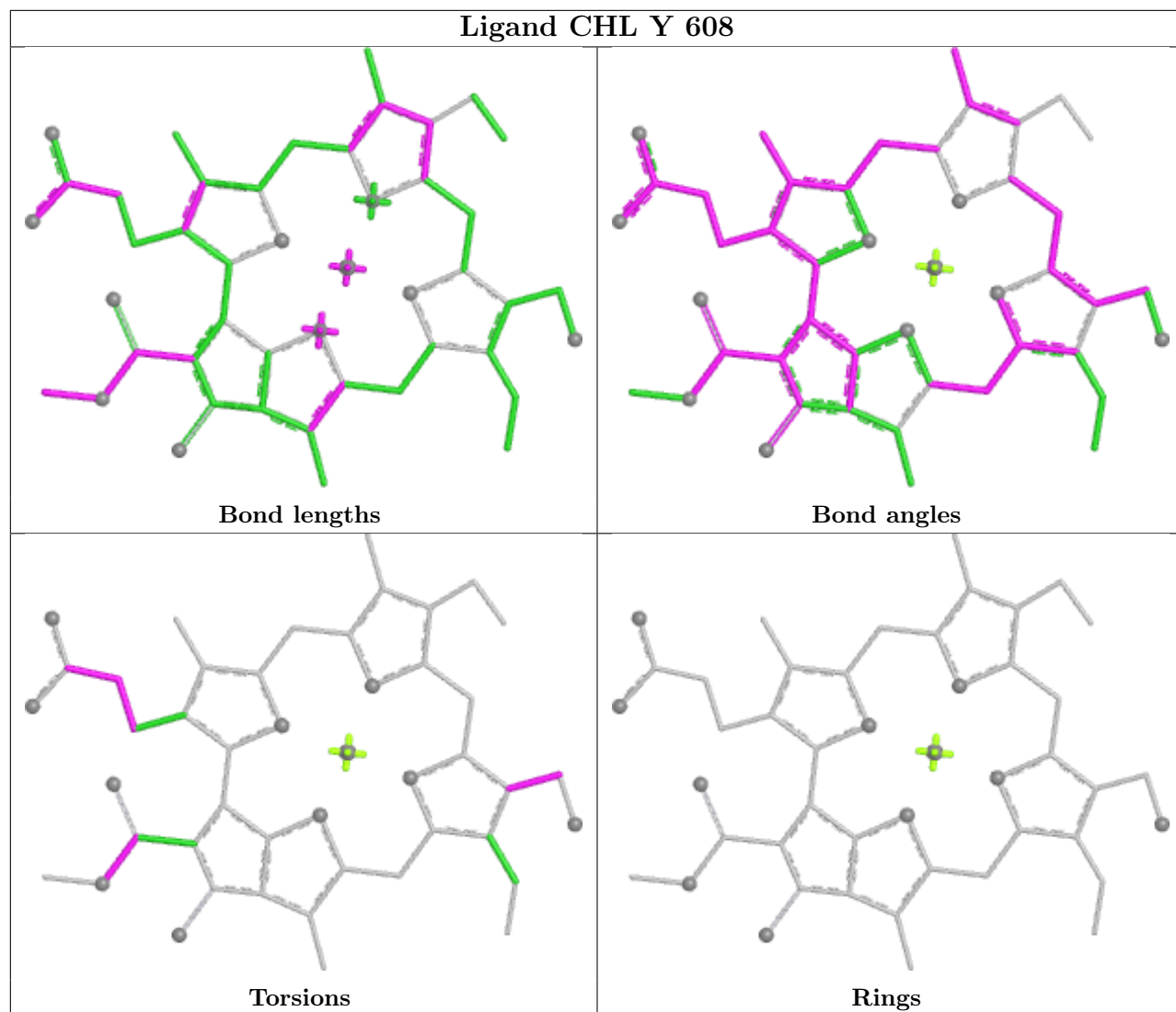


Rings

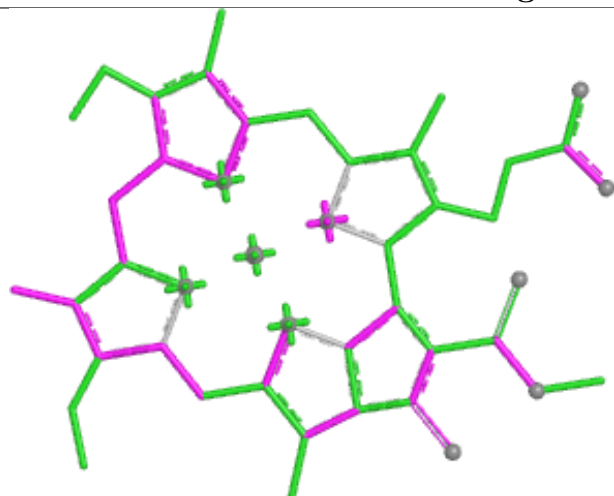
Ligand CLA y 602



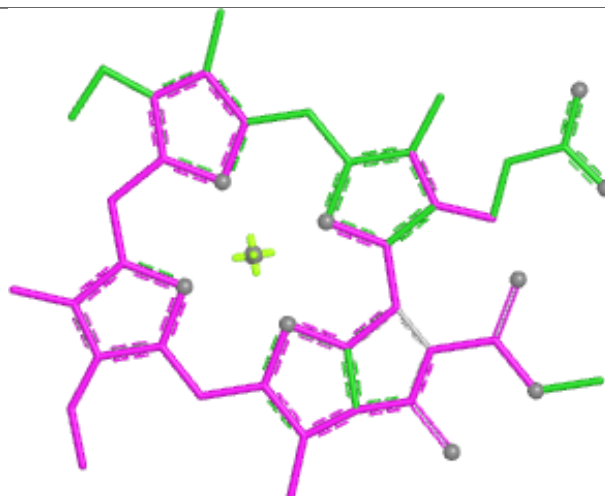
Ligand CHL Y 608



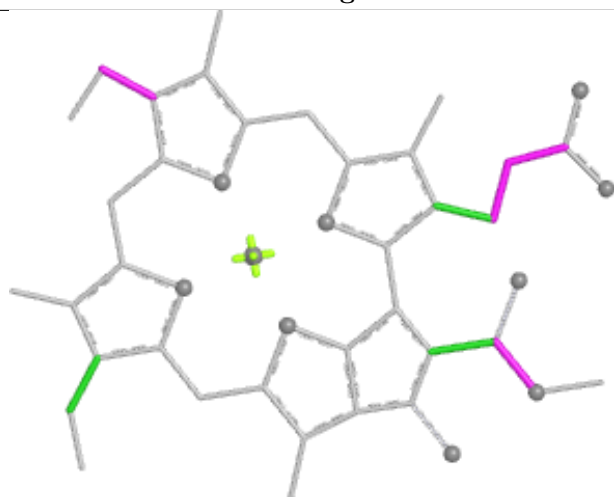
Ligand CLA S 314



Bond lengths



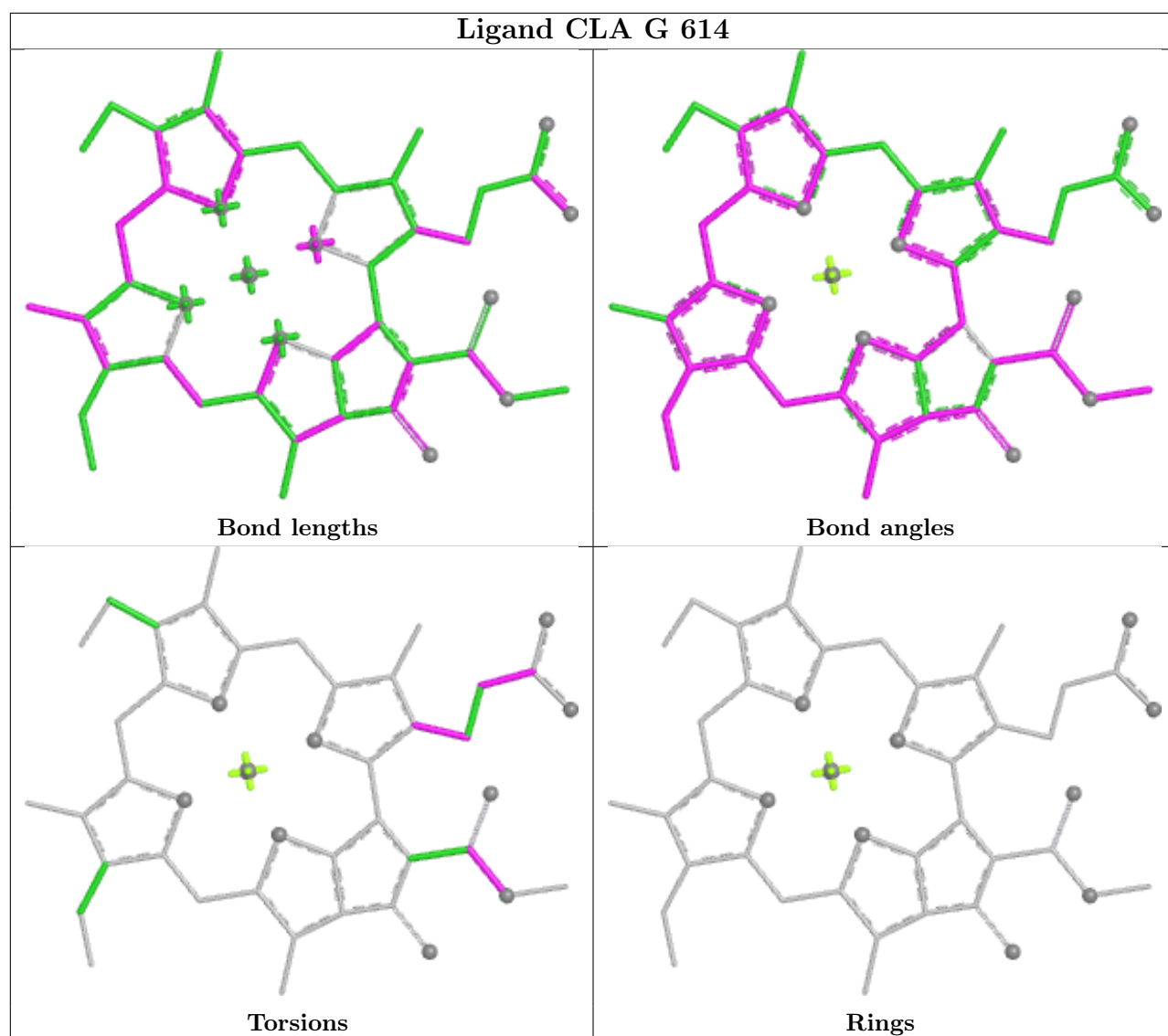
Bond angles



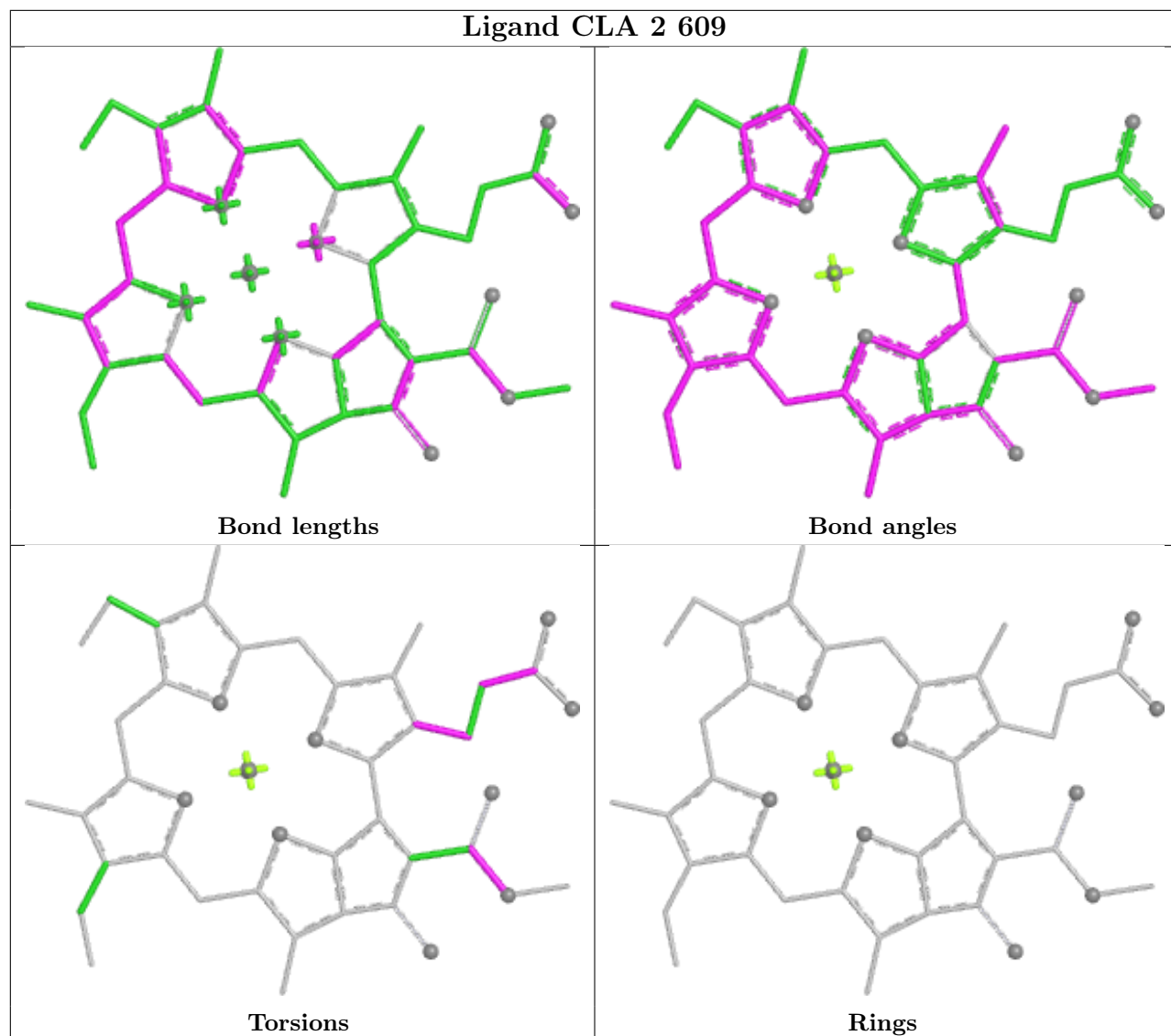
Torsions



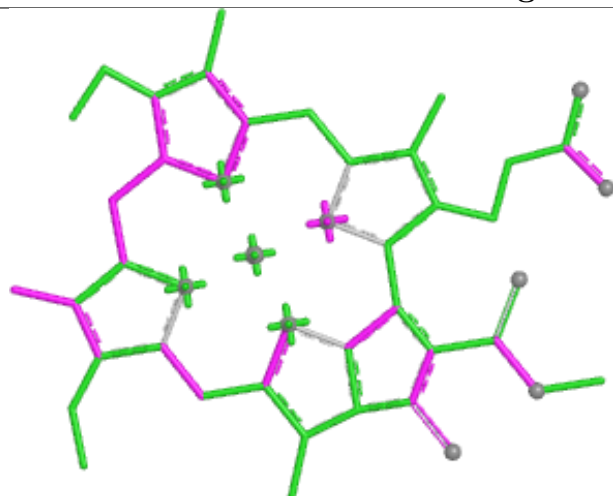
Rings



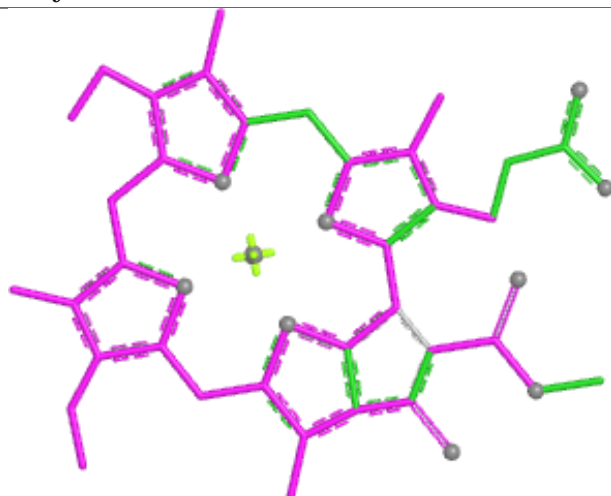
Ligand CLA 2 609



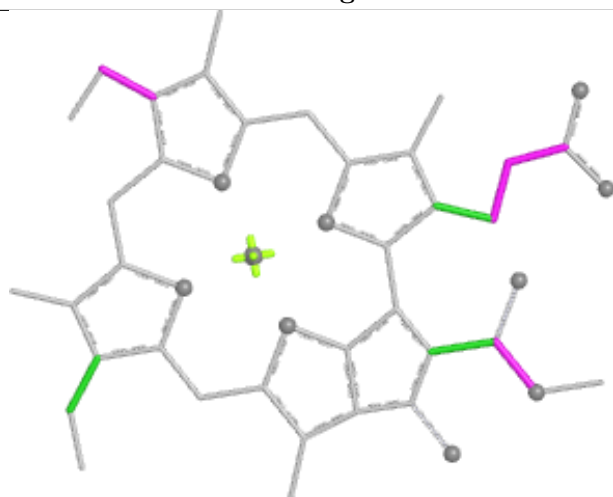
Ligand CLA y 613



Bond lengths



Bond angles

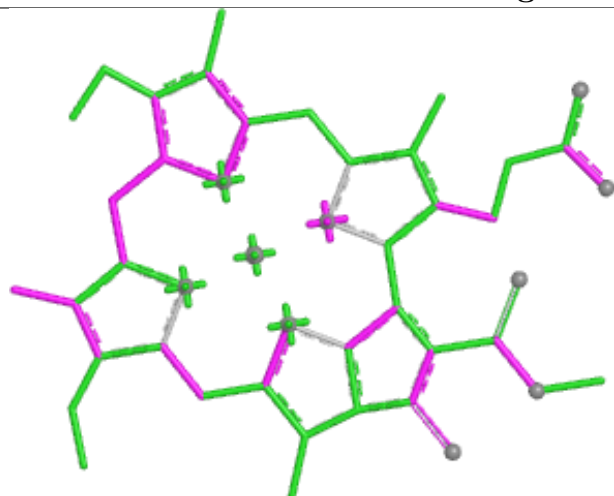


Torsions

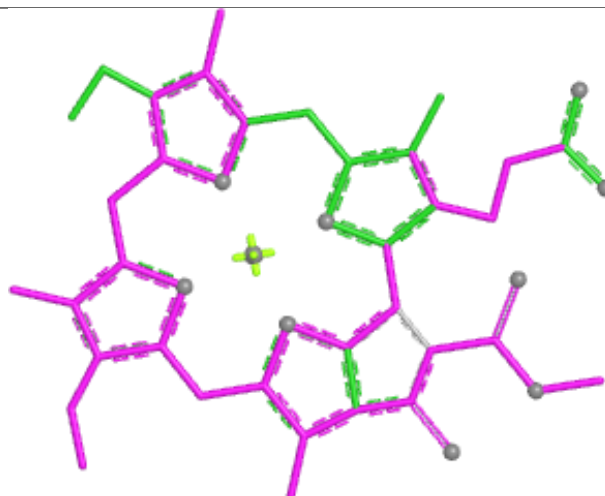


Rings

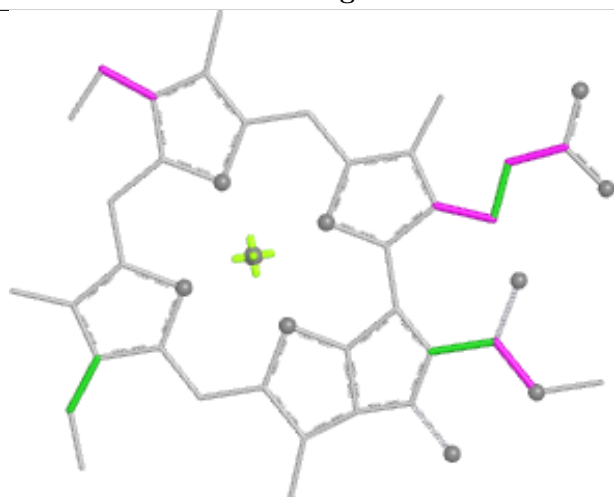
Ligand CLA S 310



Bond lengths



Bond angles

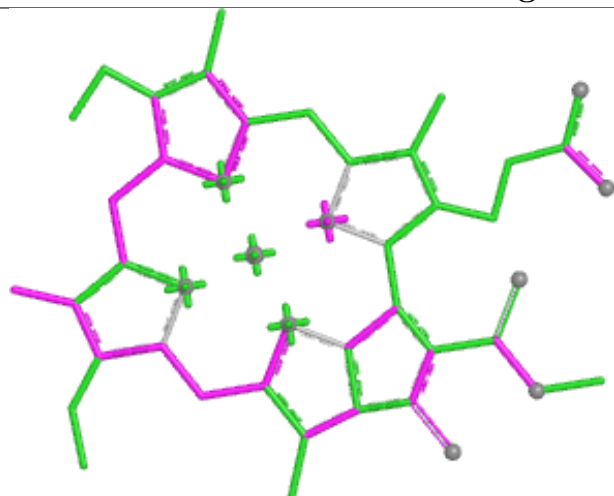


Torsions

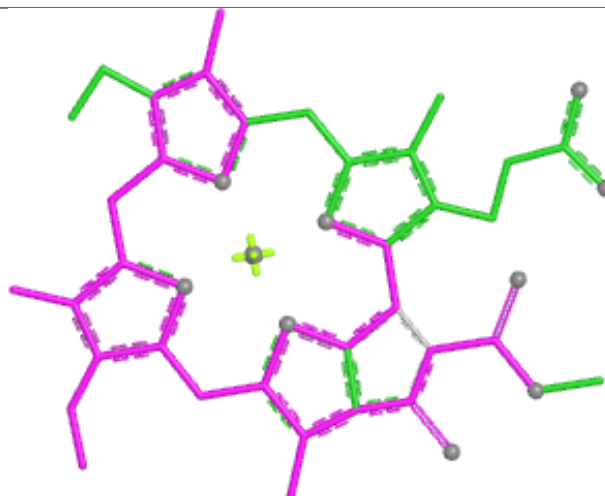


Rings

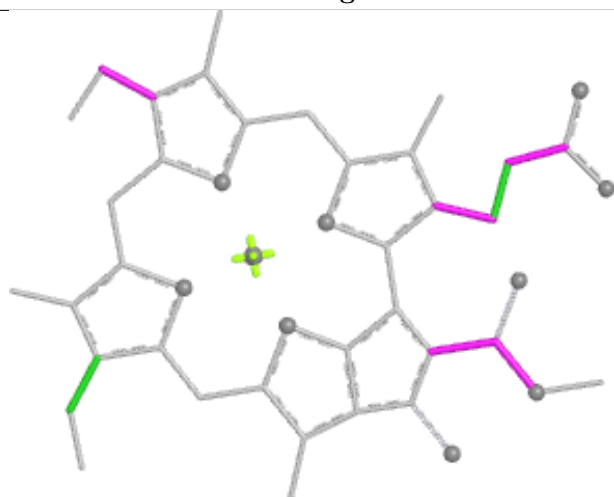
Ligand CLA 3 312



Bond lengths



Bond angles

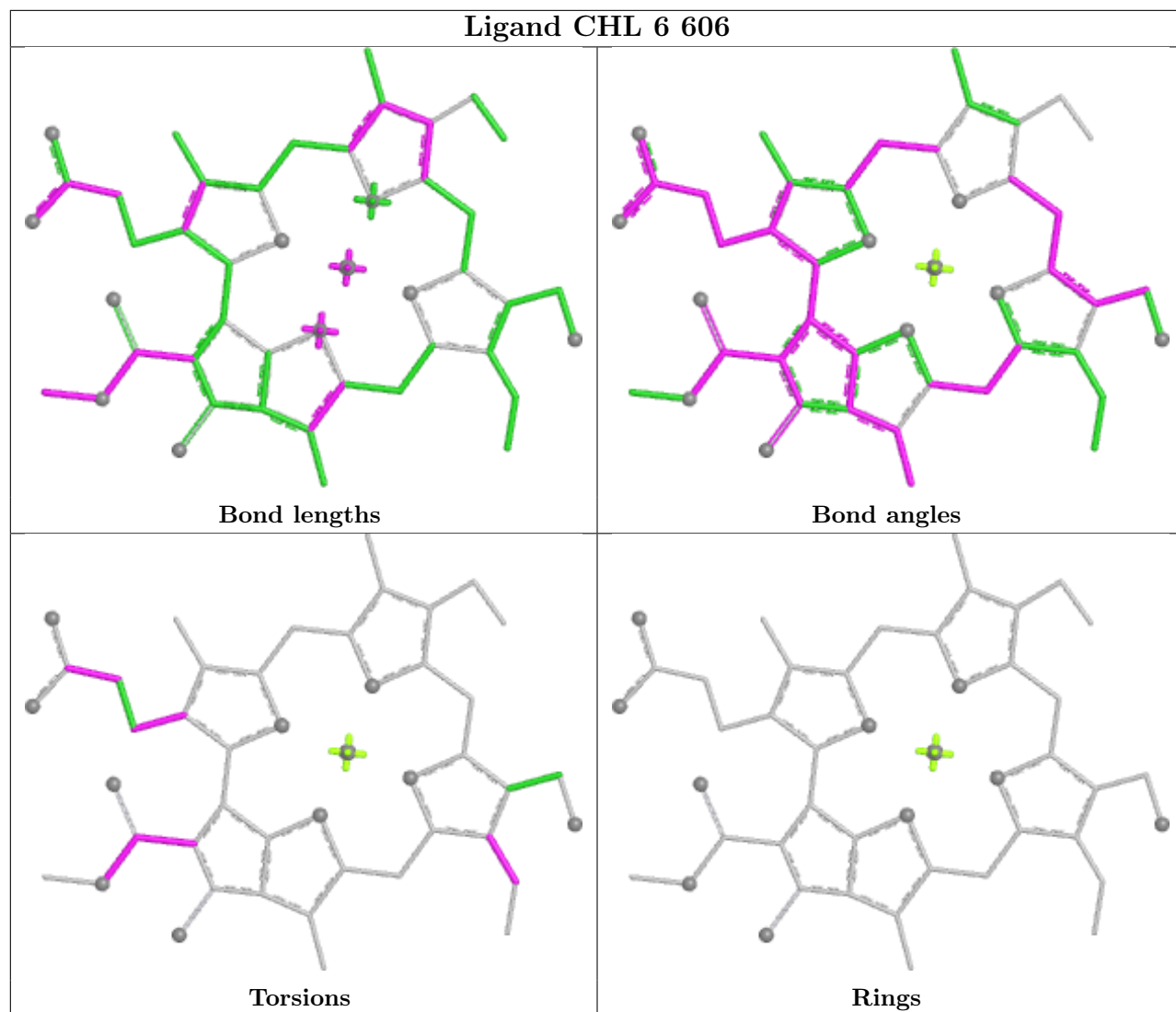


Torsions

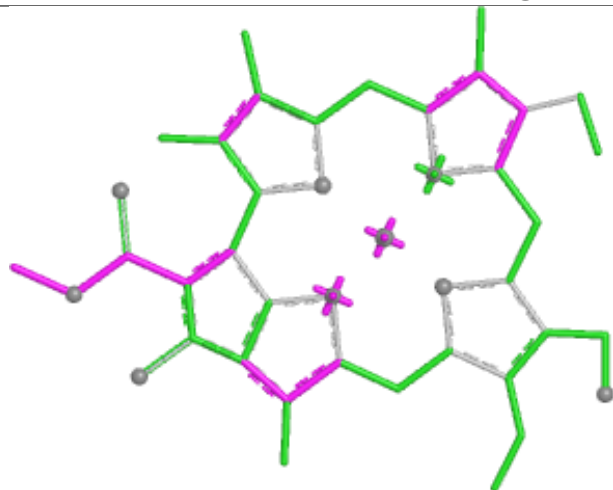


Rings

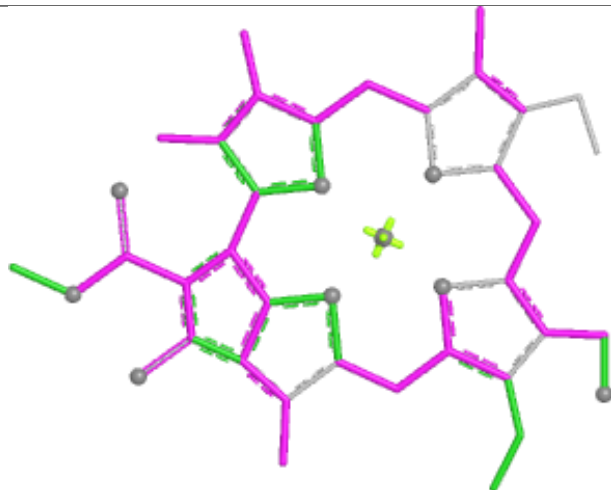
Ligand CHL 6 606



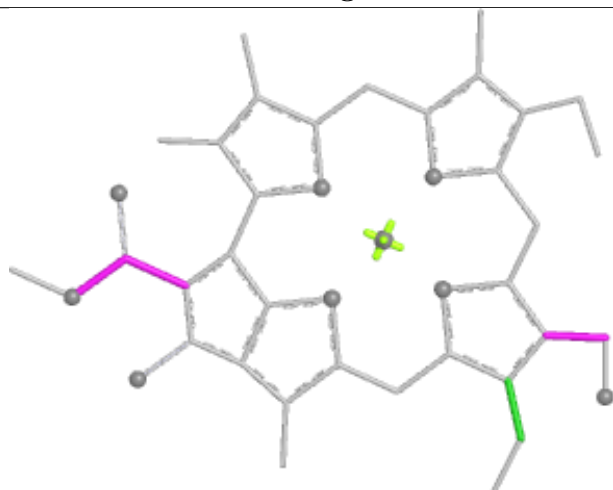
Ligand CHL n 605



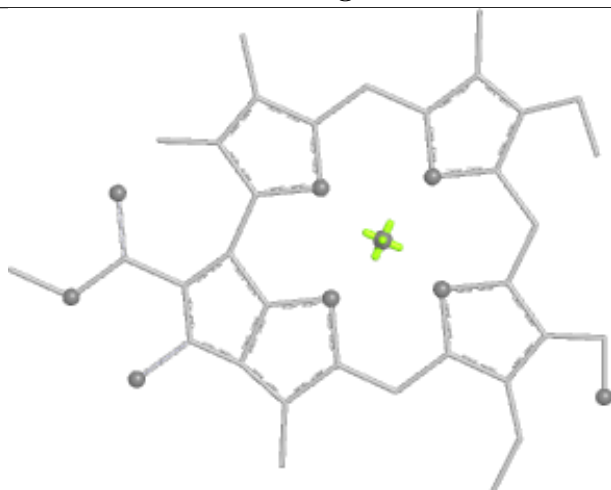
Bond lengths



Bond angles

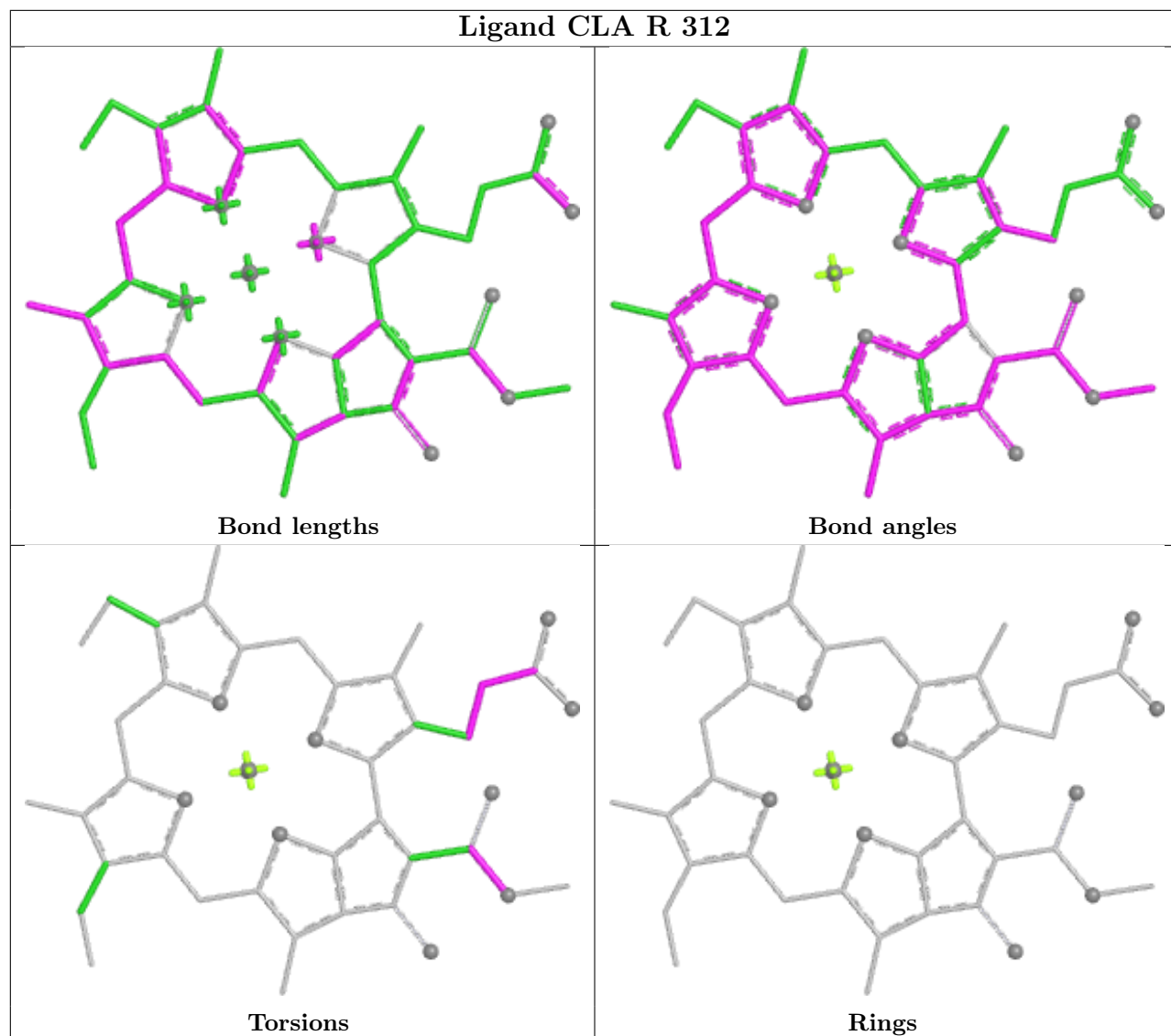


Torsions

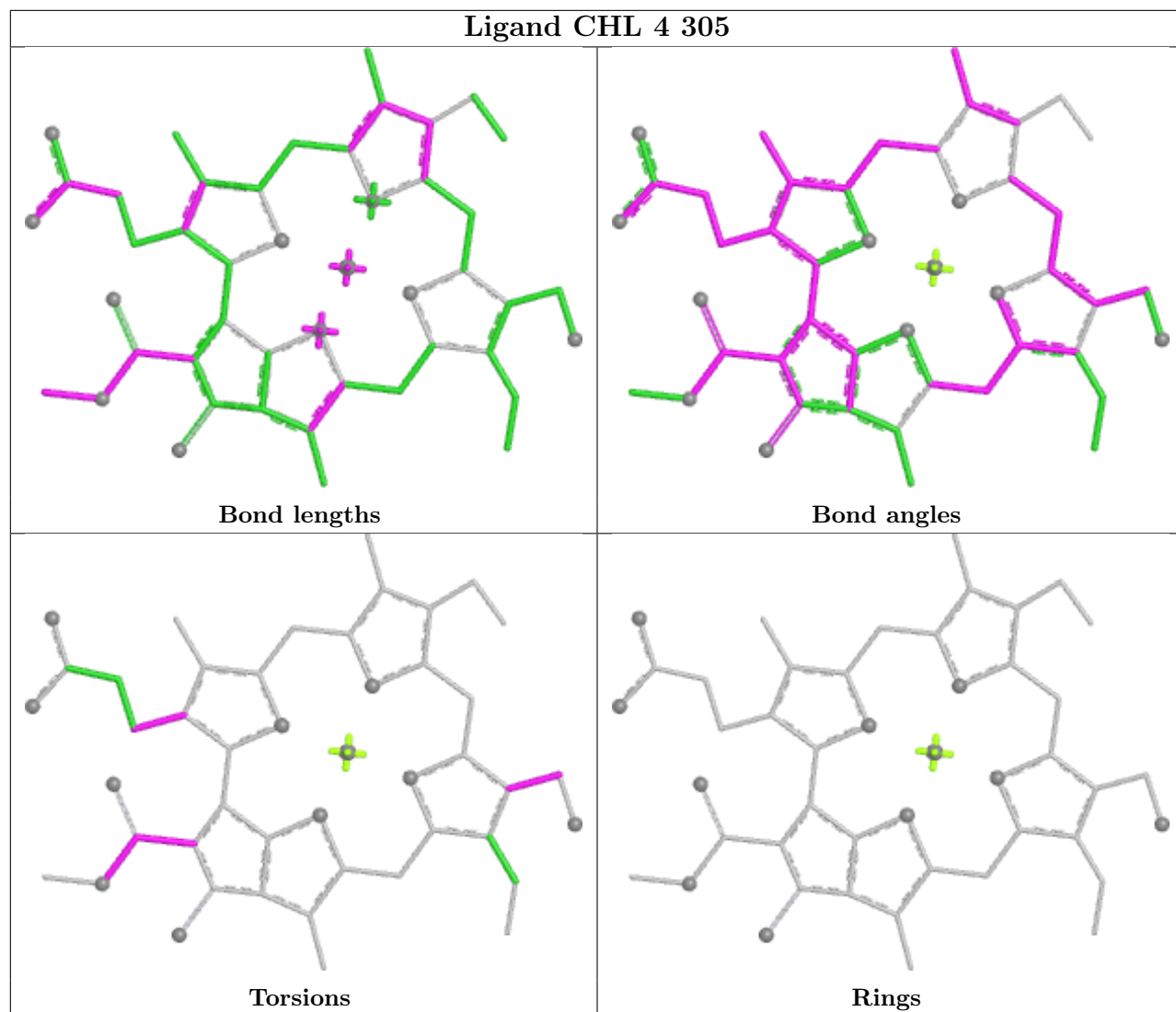


Rings

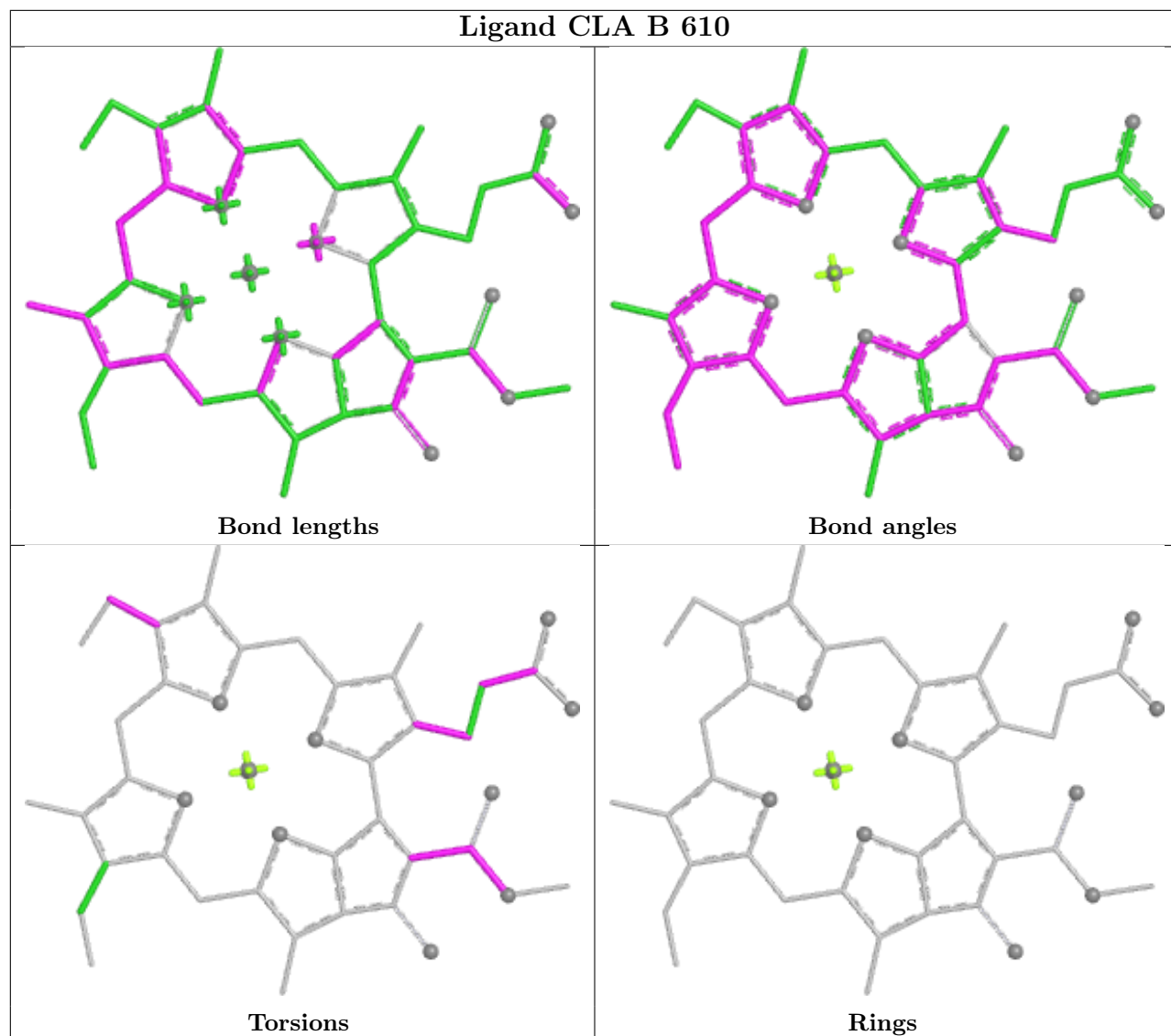
Ligand CLA R 312



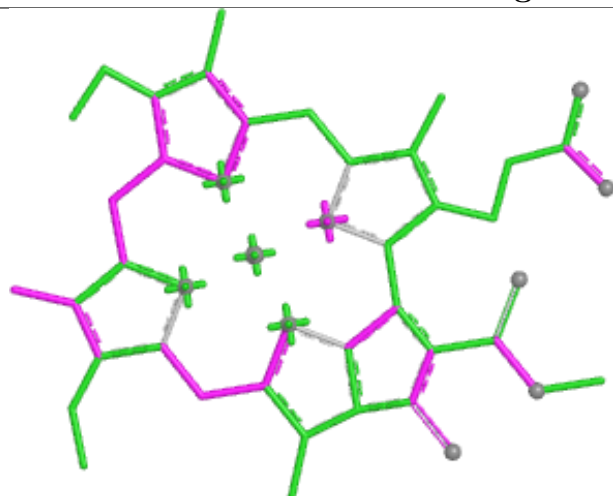
Ligand CHL 4 305



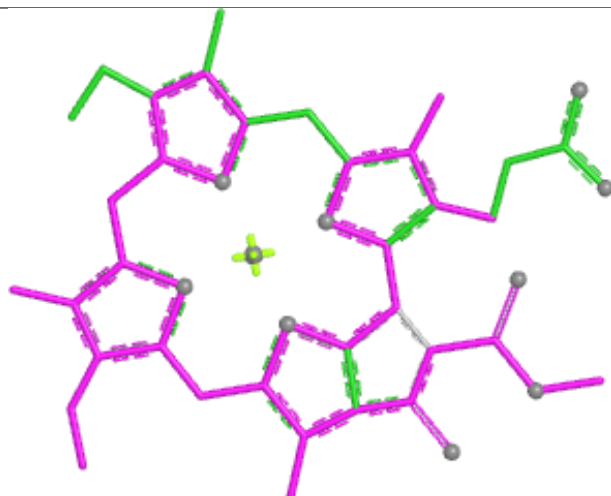
Ligand CLA B 610



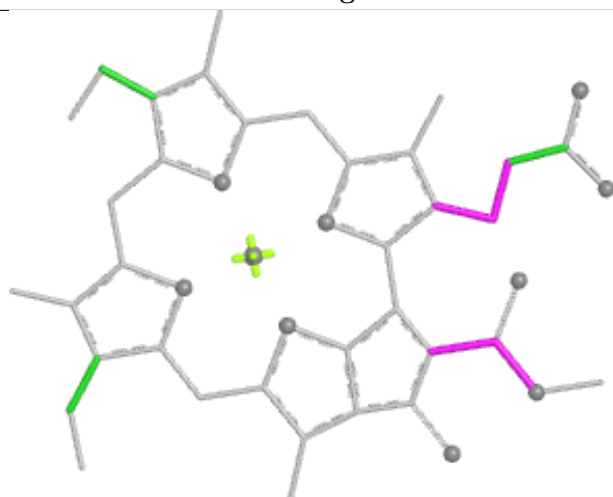
Ligand CLA C 501



Bond lengths



Bond angles

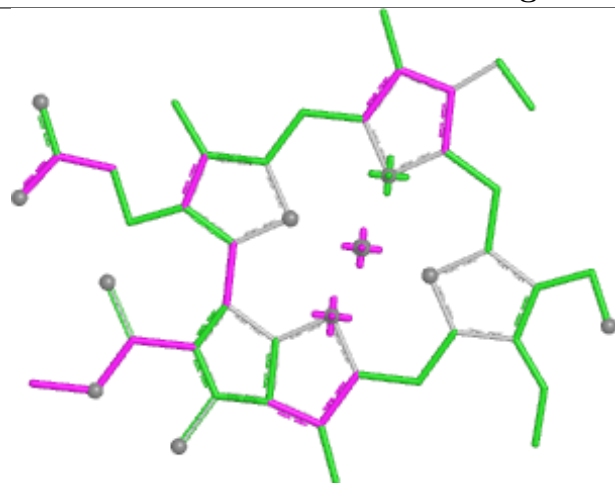


Torsions

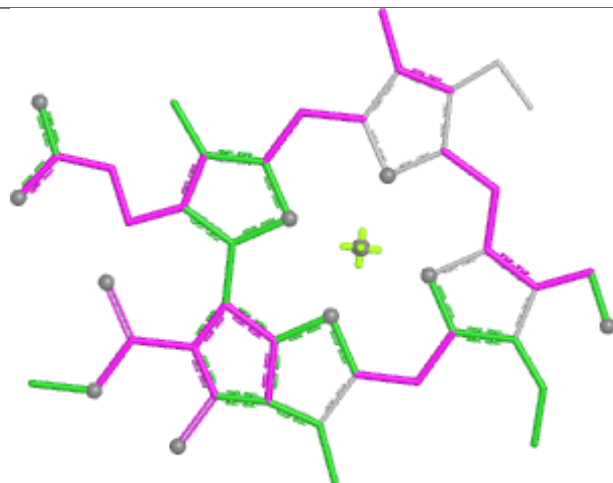


Rings

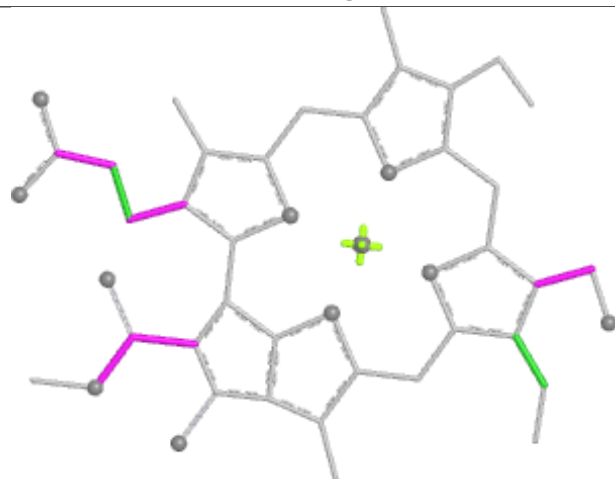
Ligand CHL 6 608



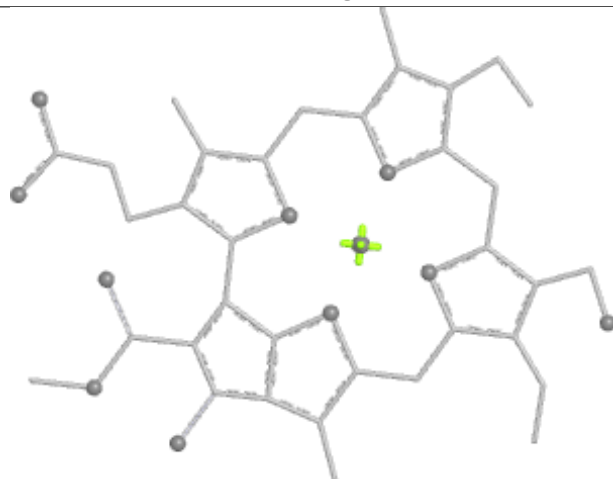
Bond lengths



Bond angles

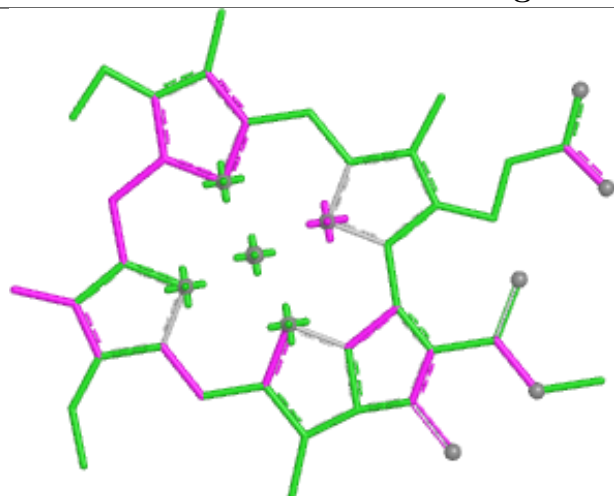


Torsions

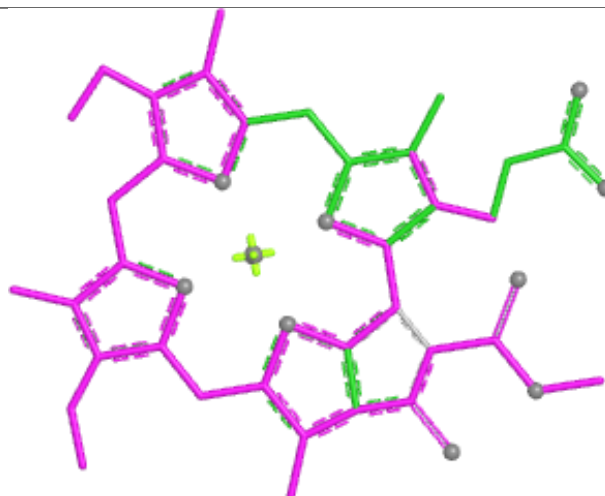


Rings

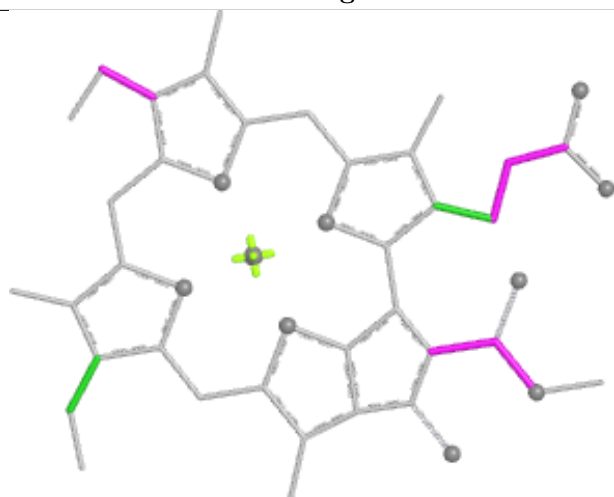
Ligand CLA Y 603



Bond lengths



Bond angles

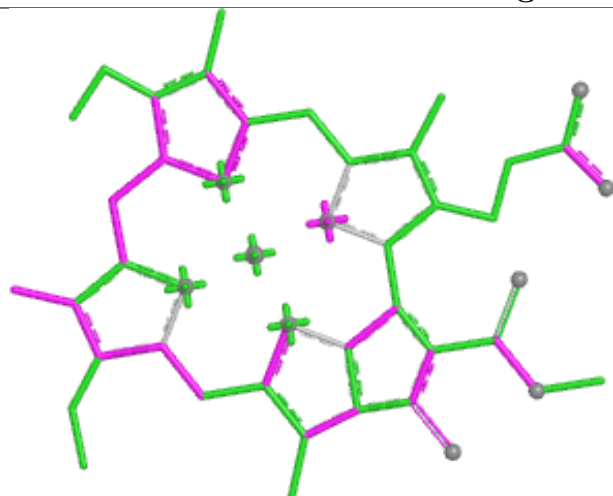


Torsions

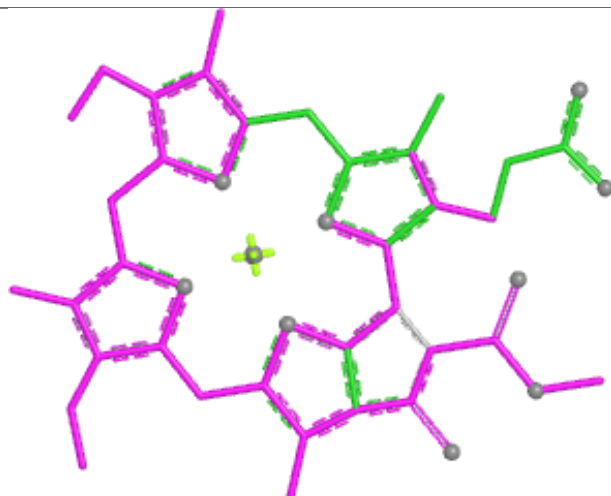


Rings

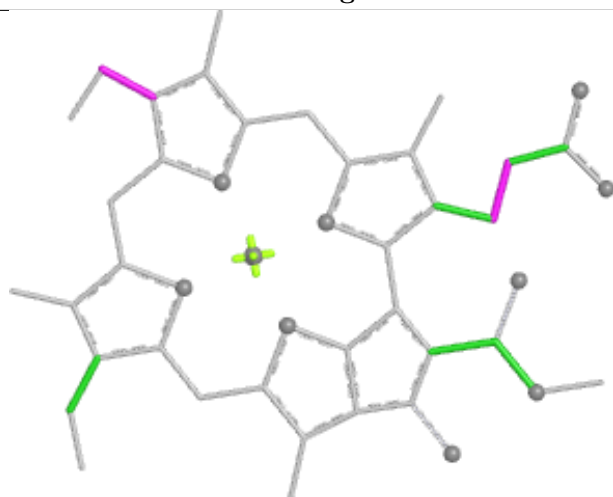
Ligand CLA S 301



Bond lengths



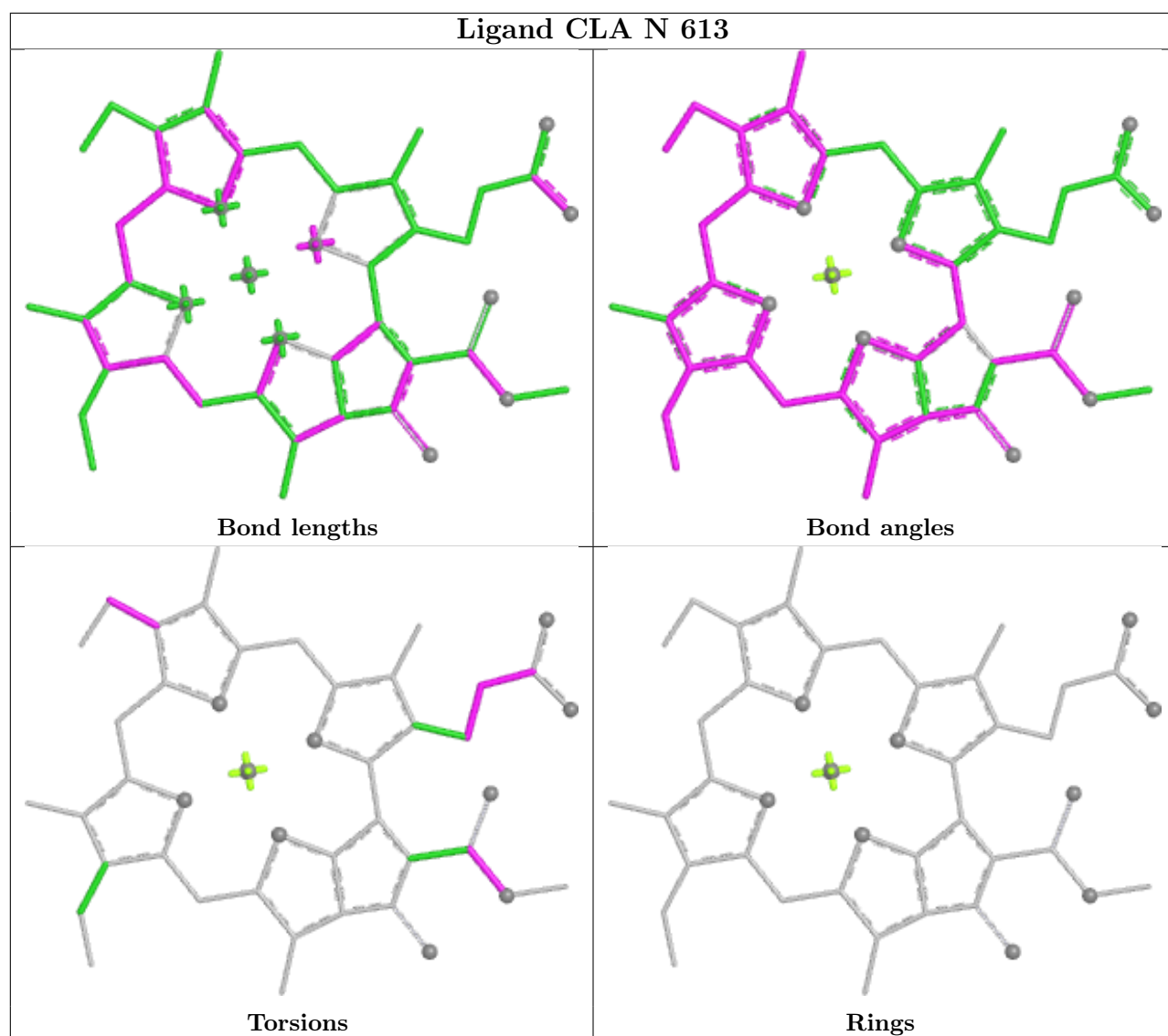
Bond angles



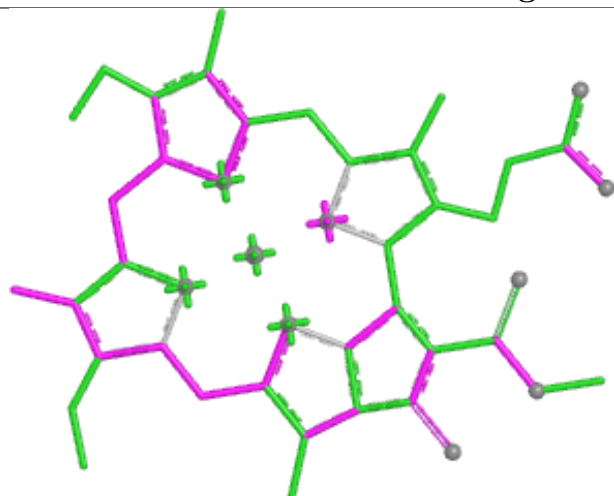
Torsions



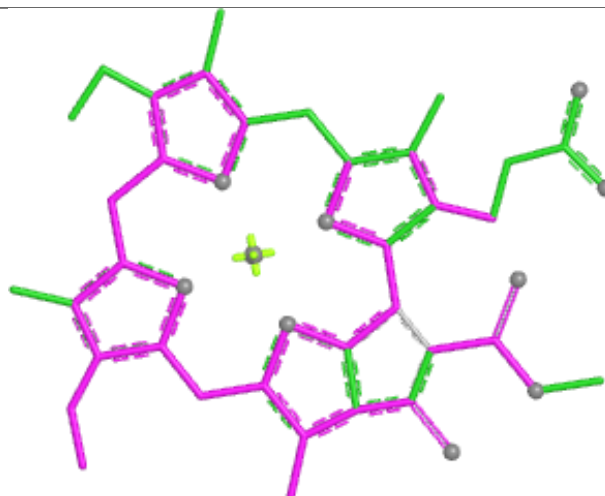
Rings



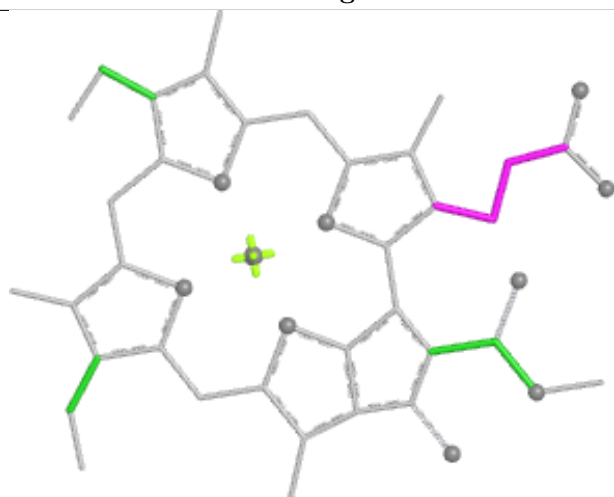
Ligand CLA 5 604



Bond lengths



Bond angles

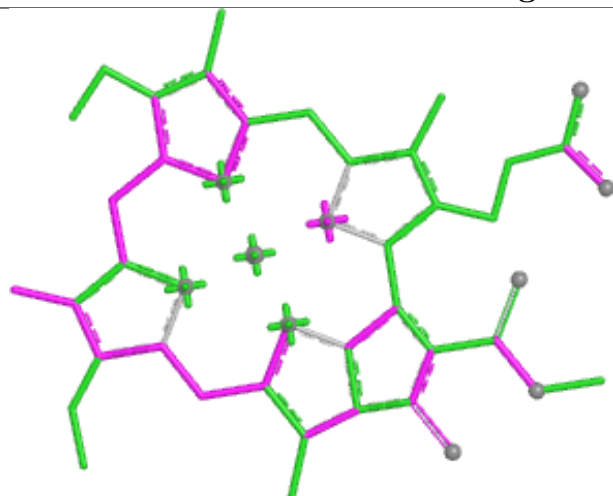


Torsions

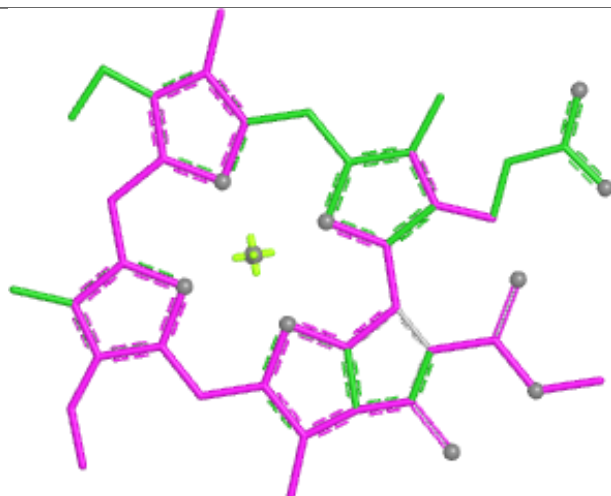


Rings

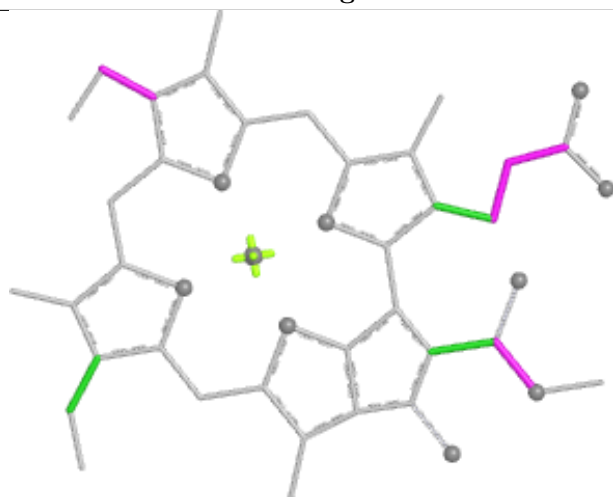
Ligand CLA 2 603



Bond lengths



Bond angles

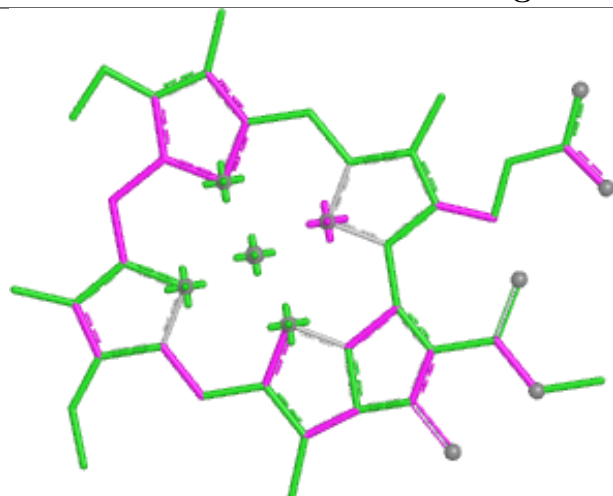


Torsions

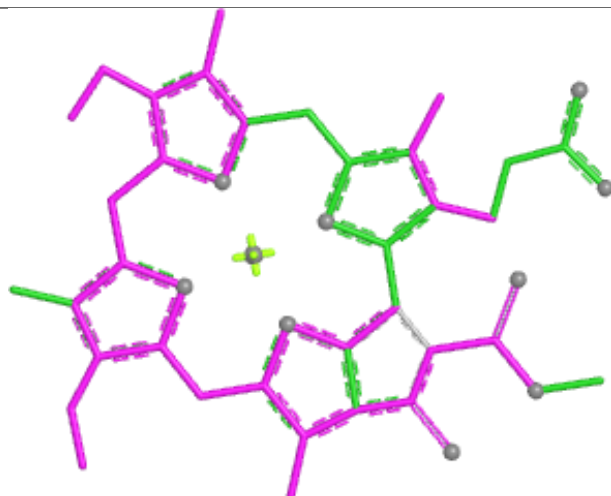


Rings

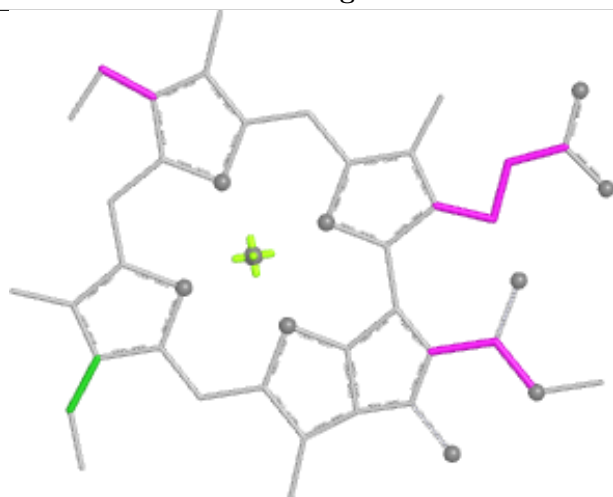
Ligand CLA Y 602



Bond lengths



Bond angles

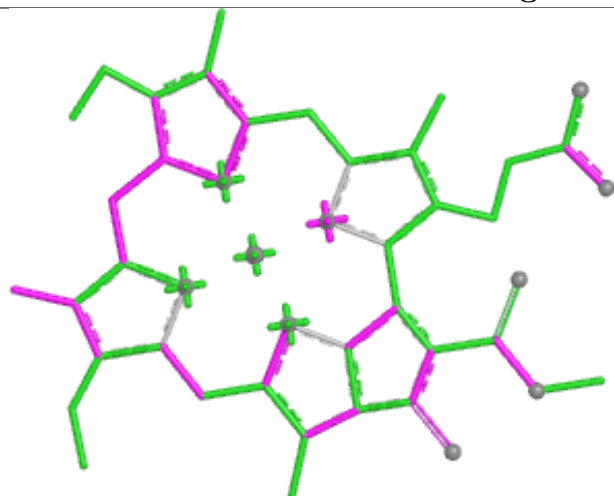


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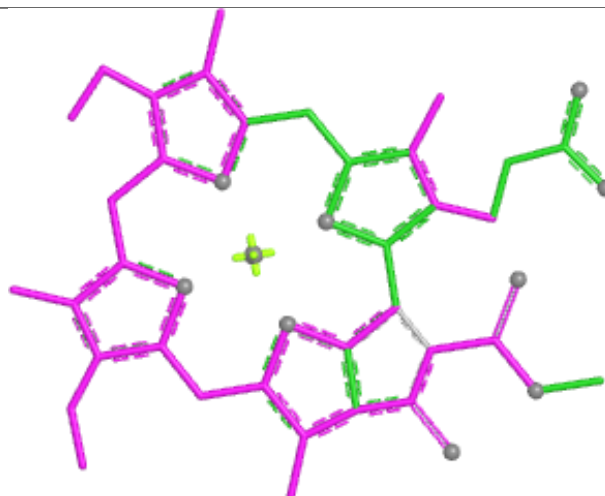


Rings

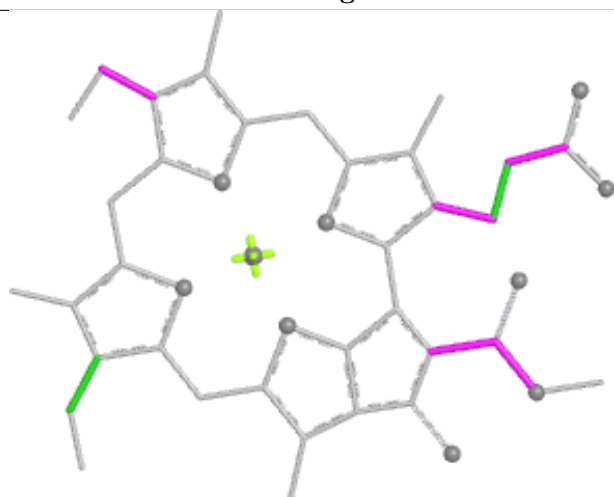
Ligand CLA r 301



Bond lengths



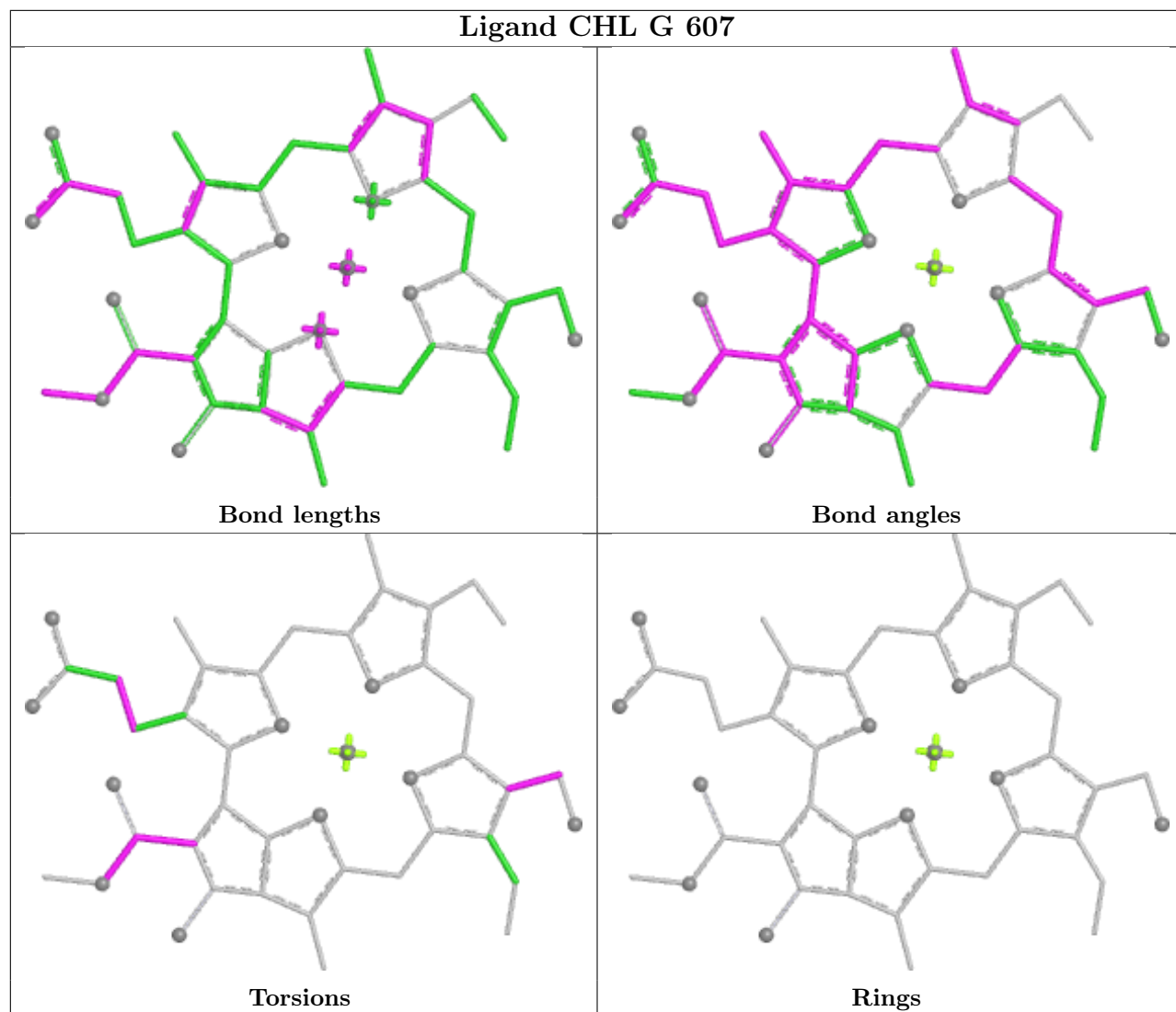
Bond angles



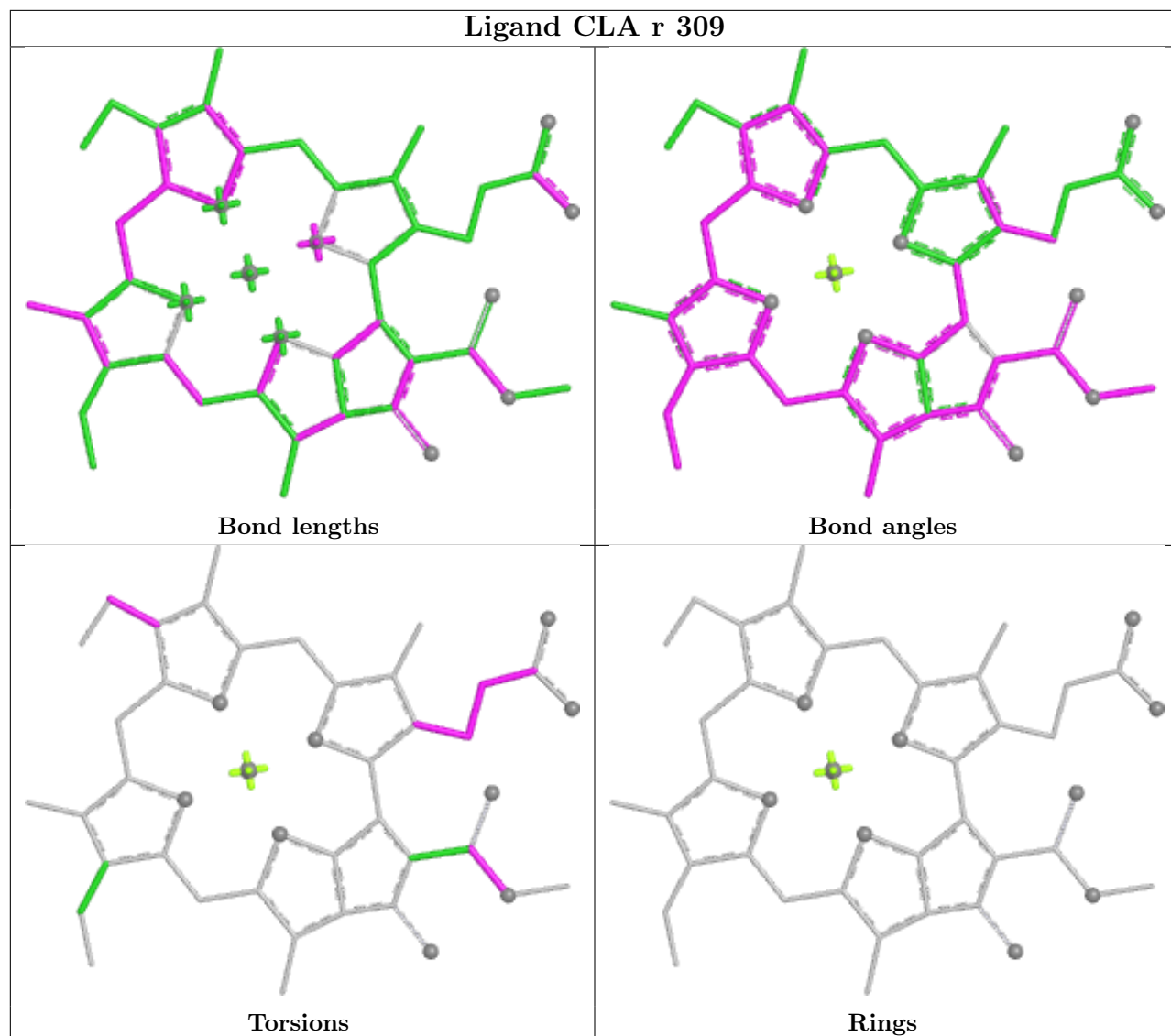
Torsions



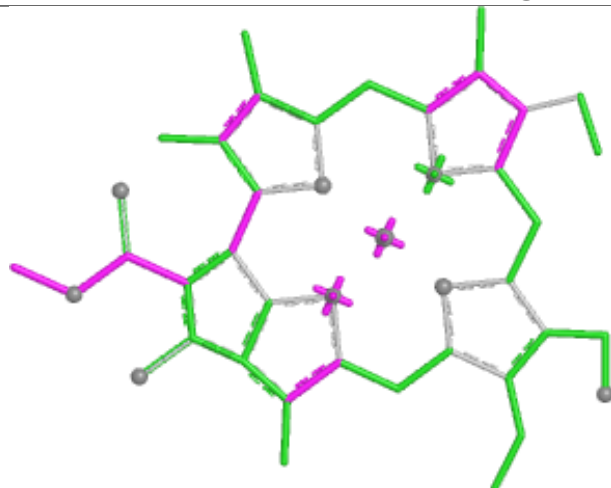
Rings



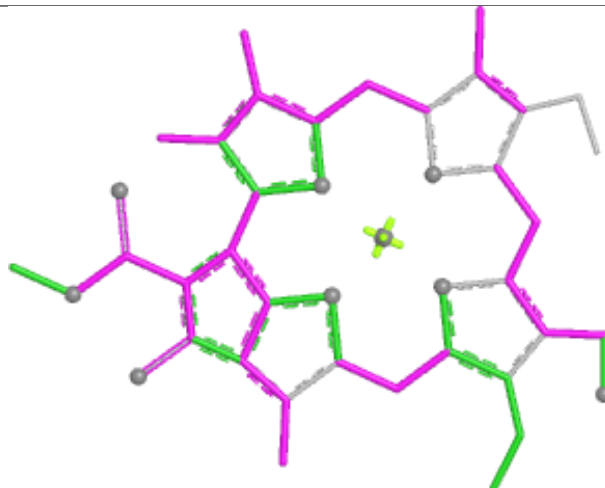
Ligand CLA r 309



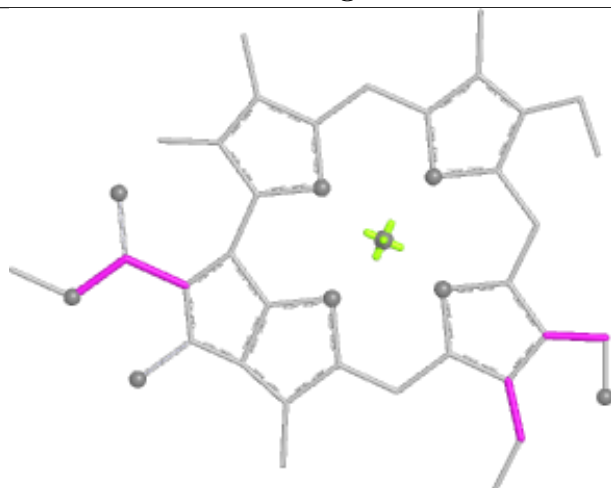
Ligand CHL 3 306



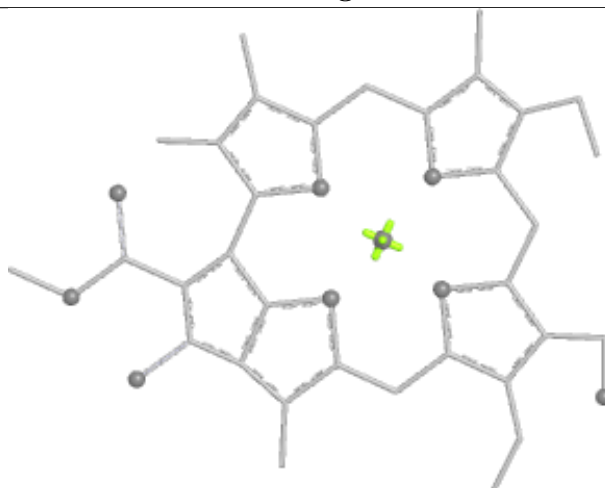
Bond lengths



Bond angles

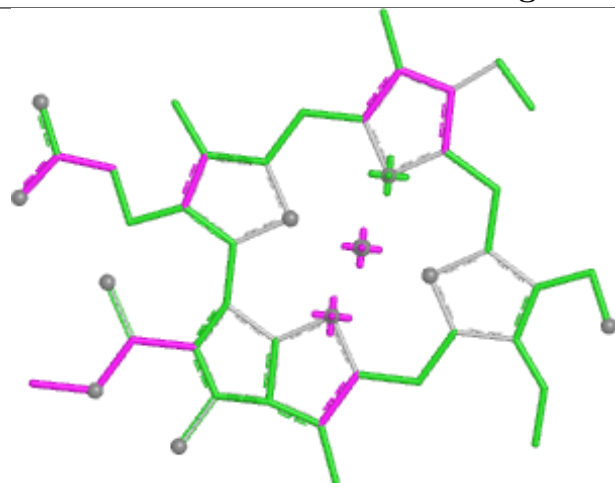


Torsions

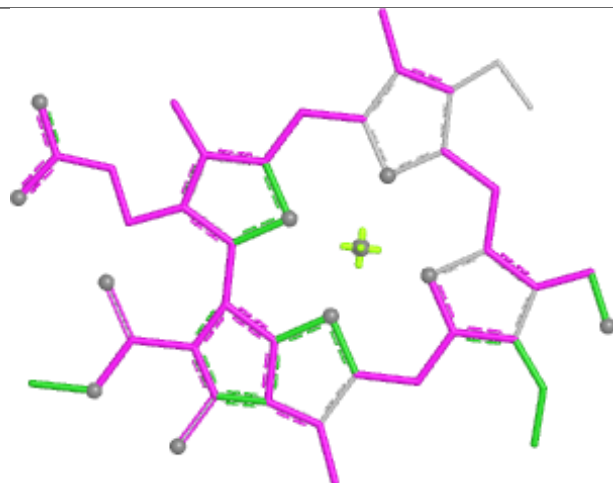


Rings

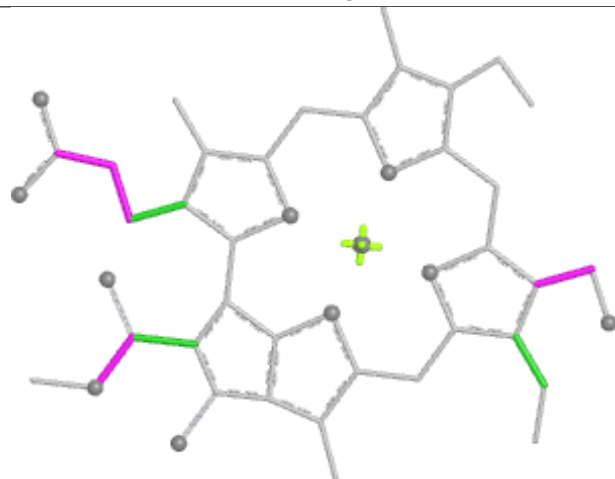
Ligand CHL n 608



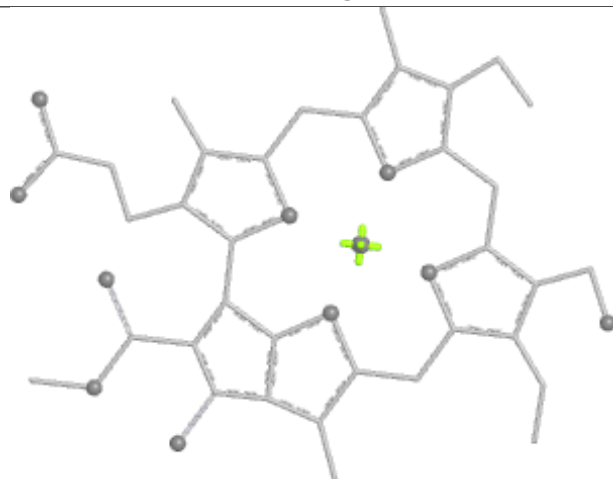
Bond lengths



Bond angles

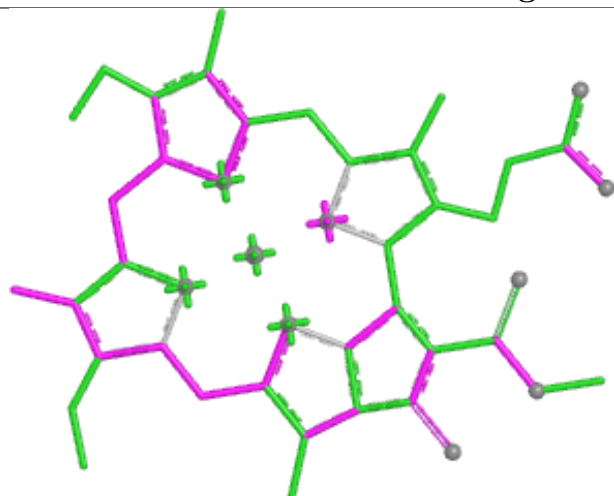


Torsions

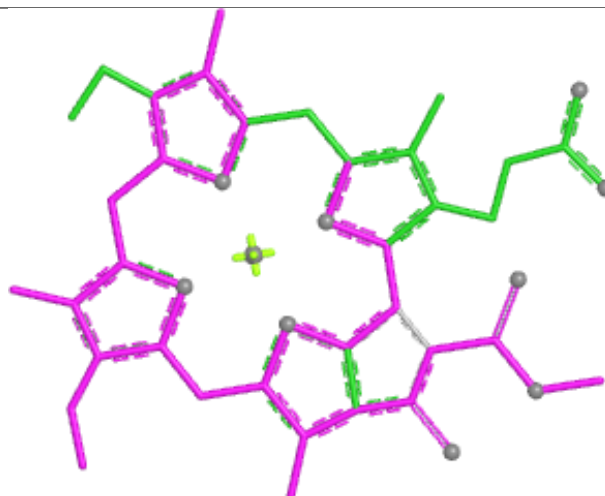


Rings

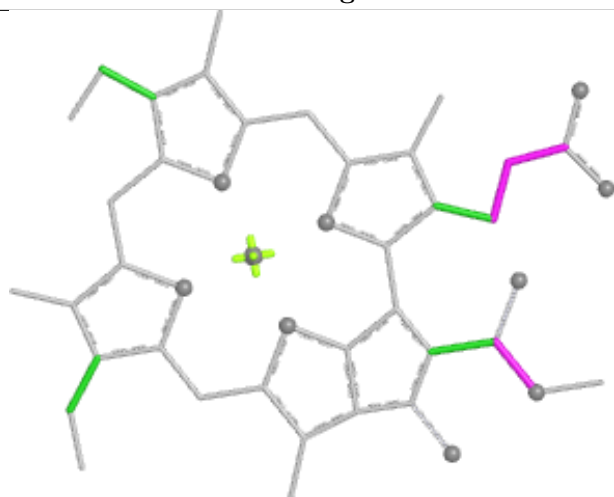
Ligand CLA 7 311



Bond lengths



Bond angles

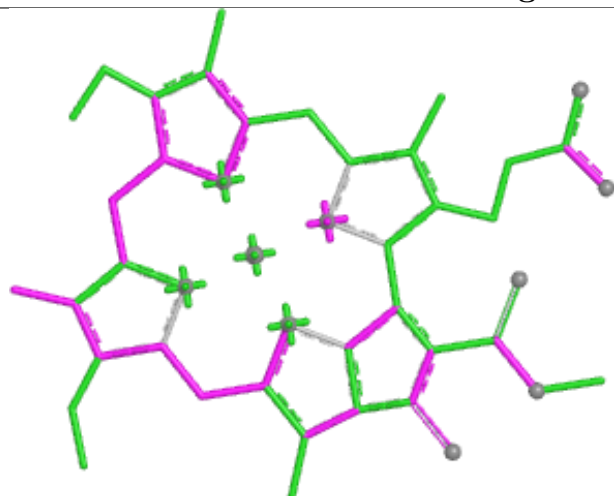


Torsions

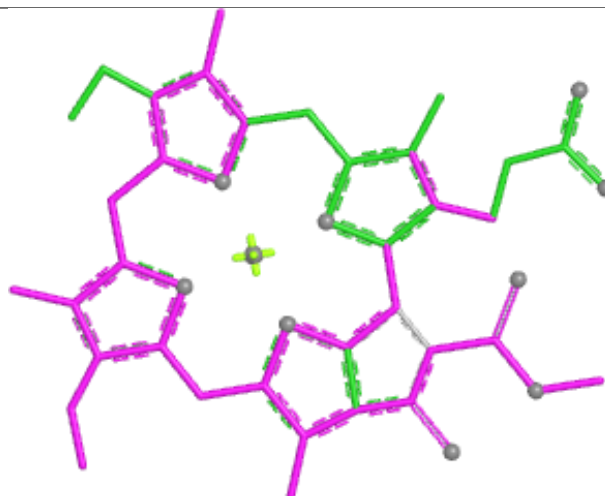


Rings

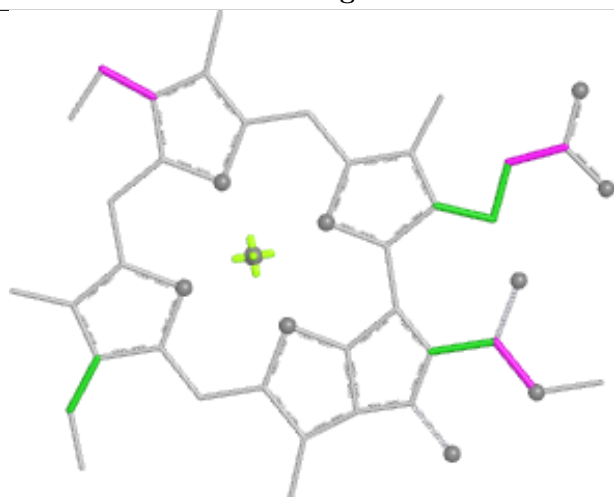
Ligand CLA 5 603



Bond lengths



Bond angles

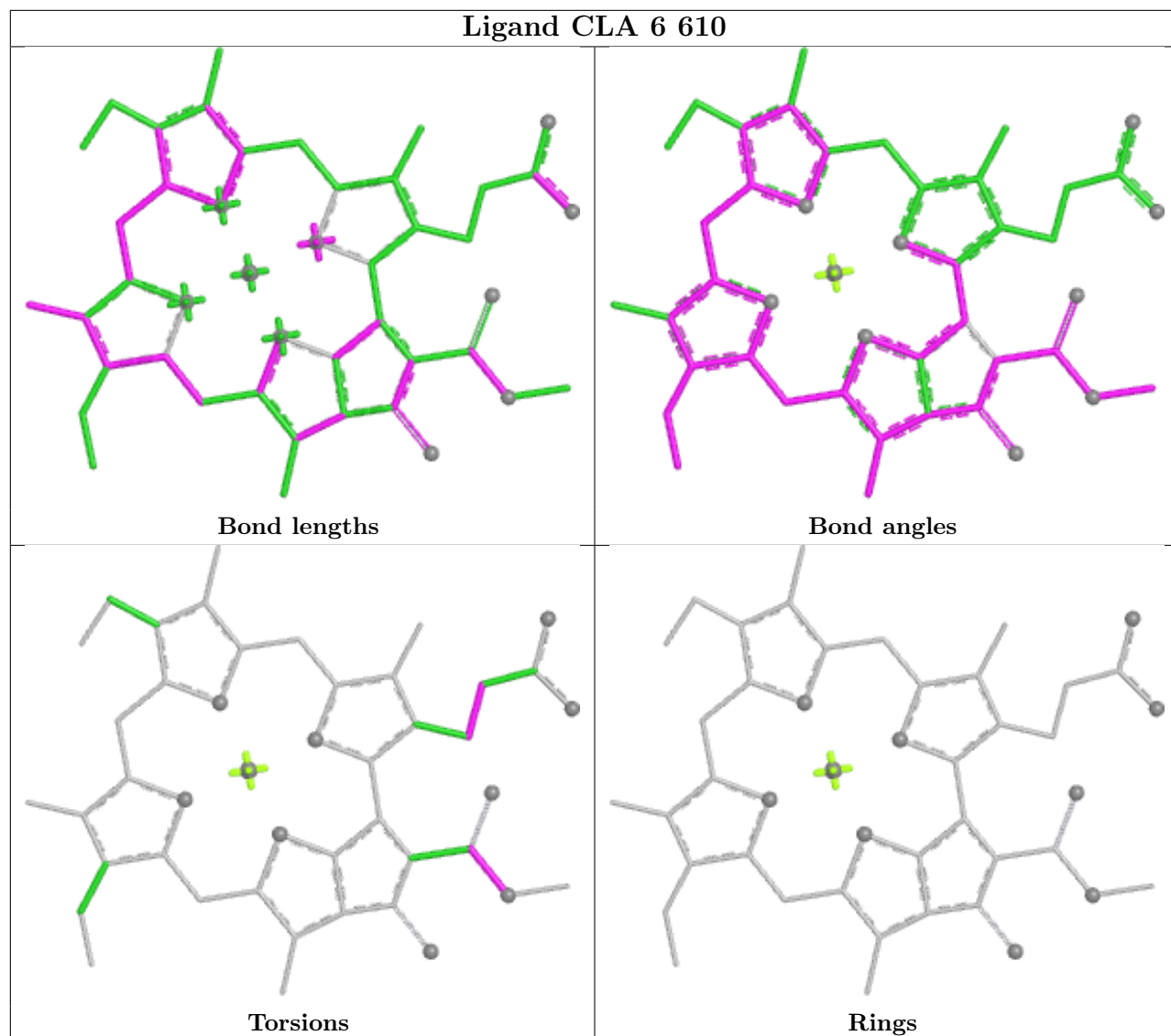


Torsions

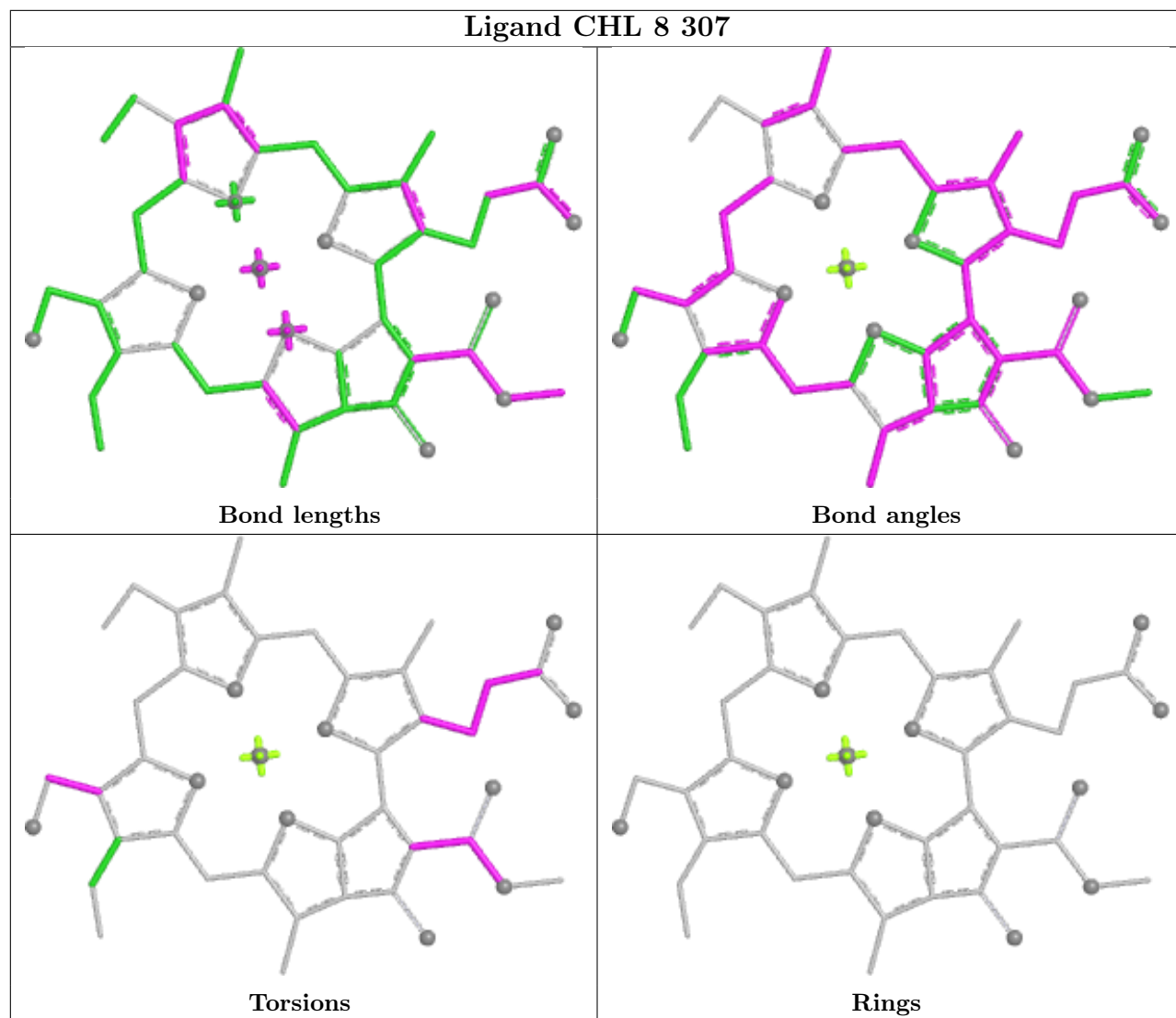


Rings

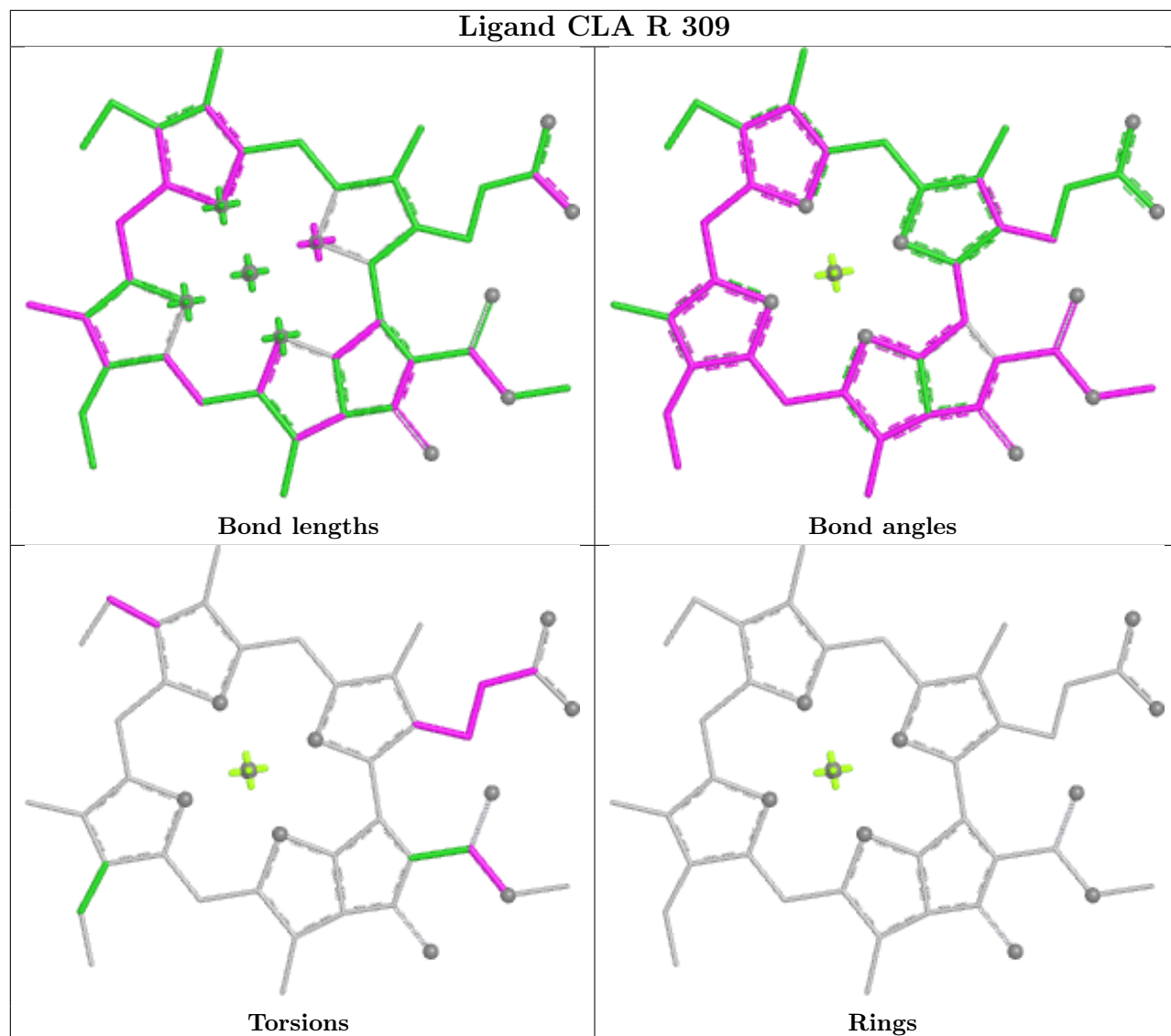
Ligand CLA 6 610



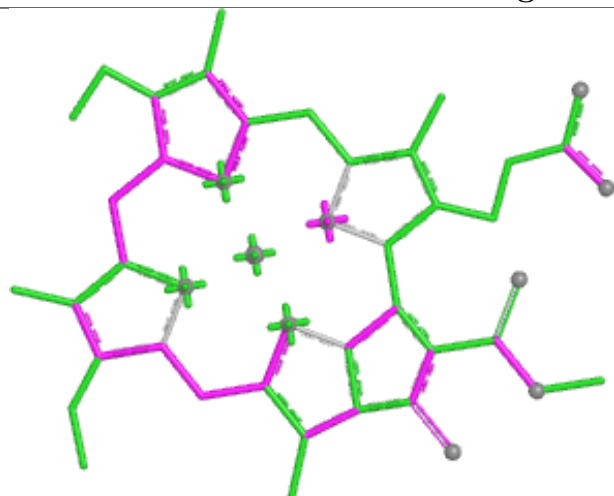
Ligand CHL 8 307



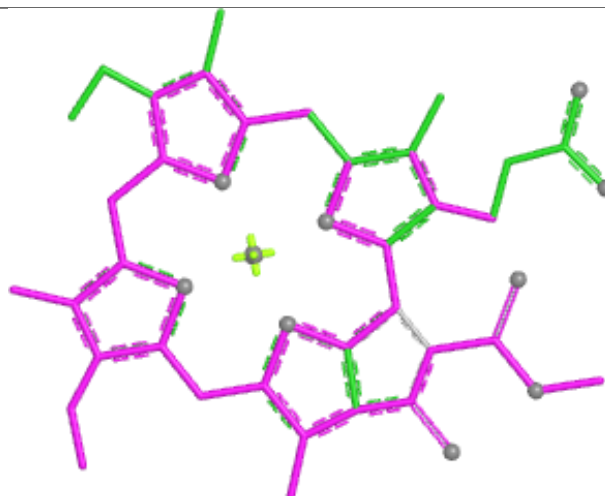
Ligand CLA R 309



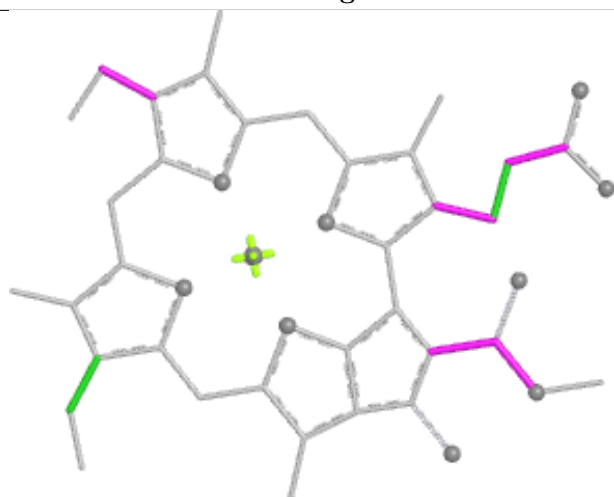
Ligand CLA b 616



Bond lengths



Bond angles

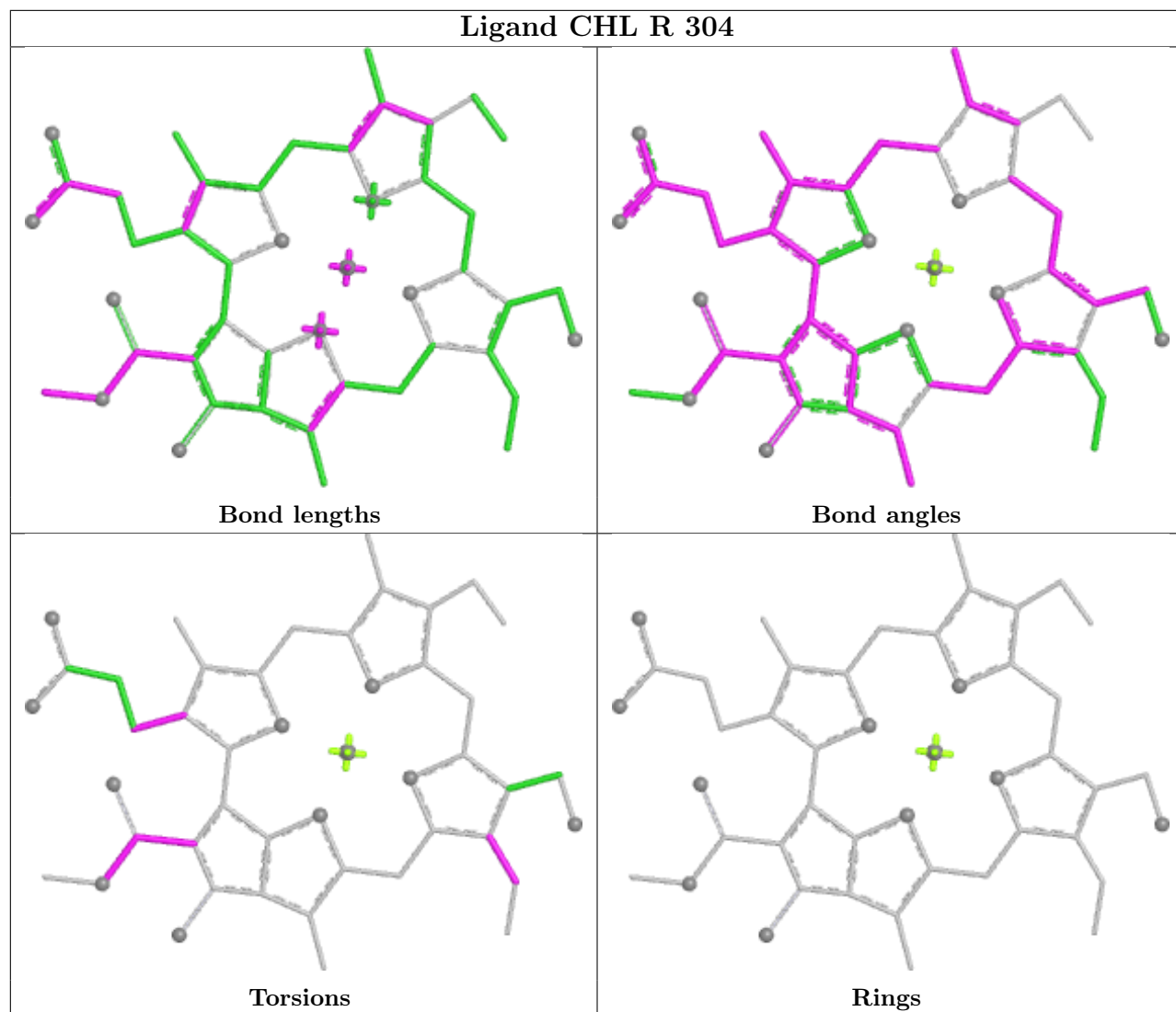


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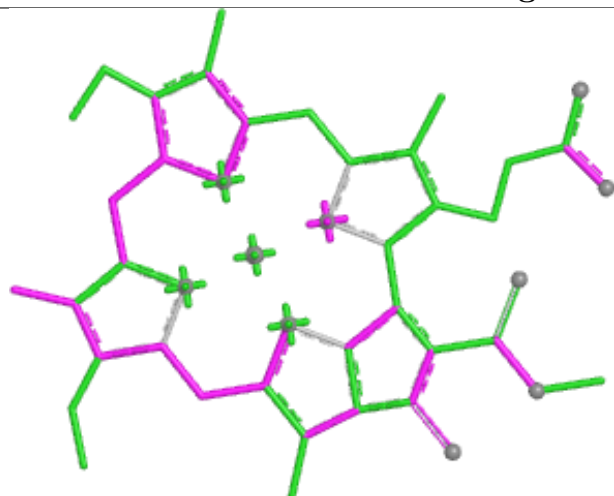


Rings

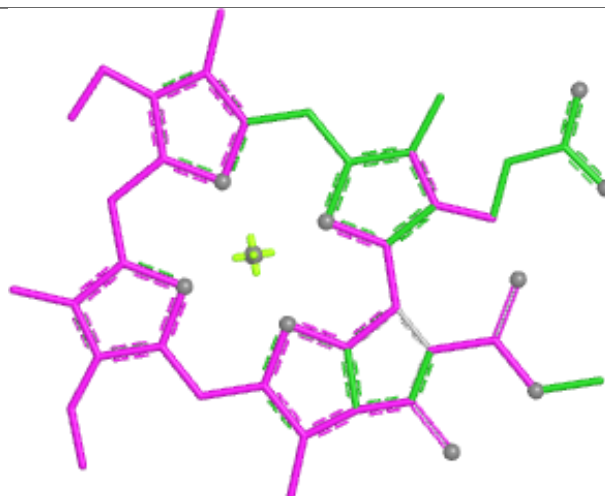
Ligand CHL R 304



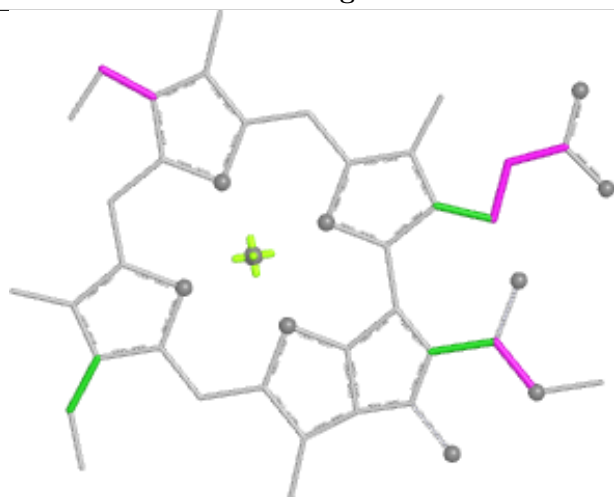
Ligand CLA 7 313



Bond lengths



Bond angles

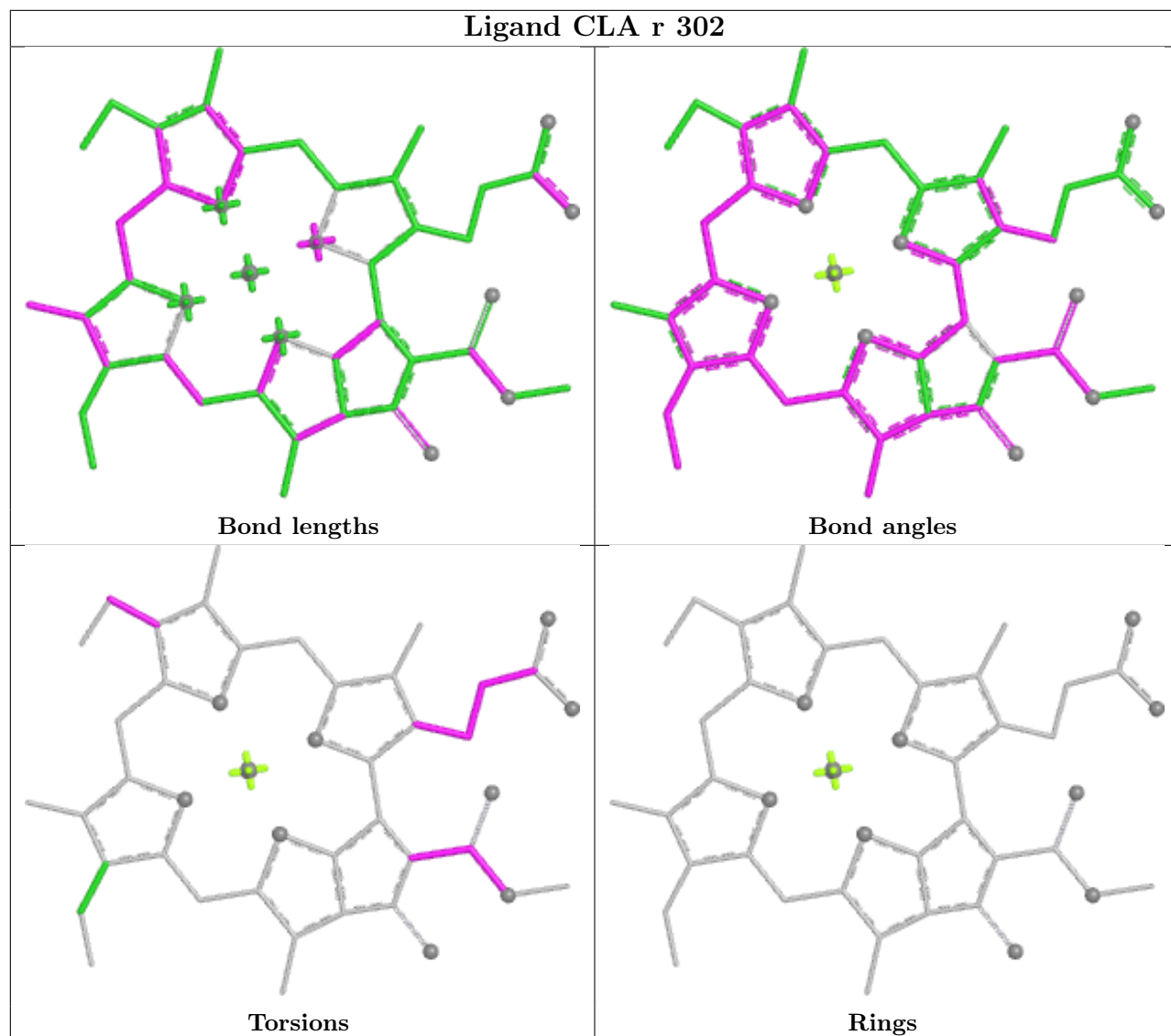


Torsions

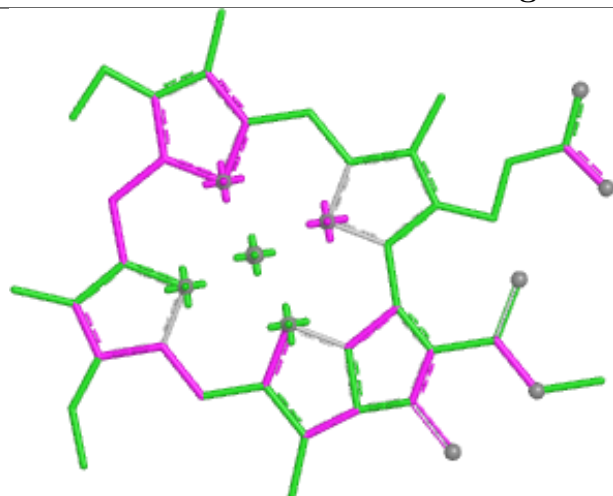


Rings

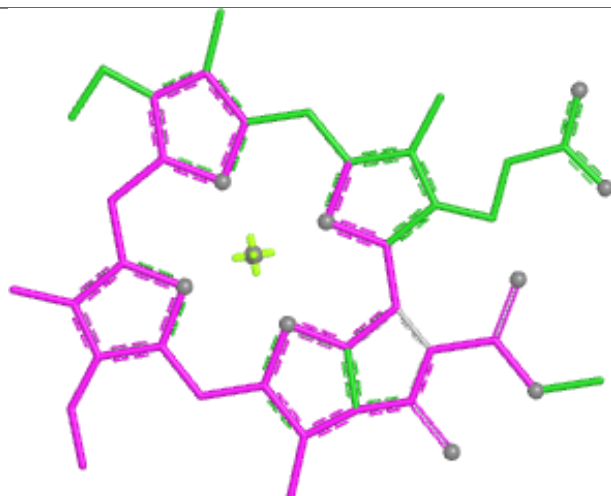
Ligand CLA r 302



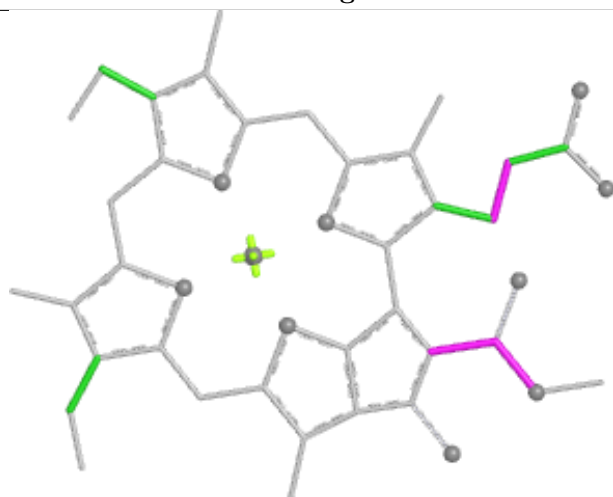
Ligand CLA c 508



Bond lengths



Bond angles

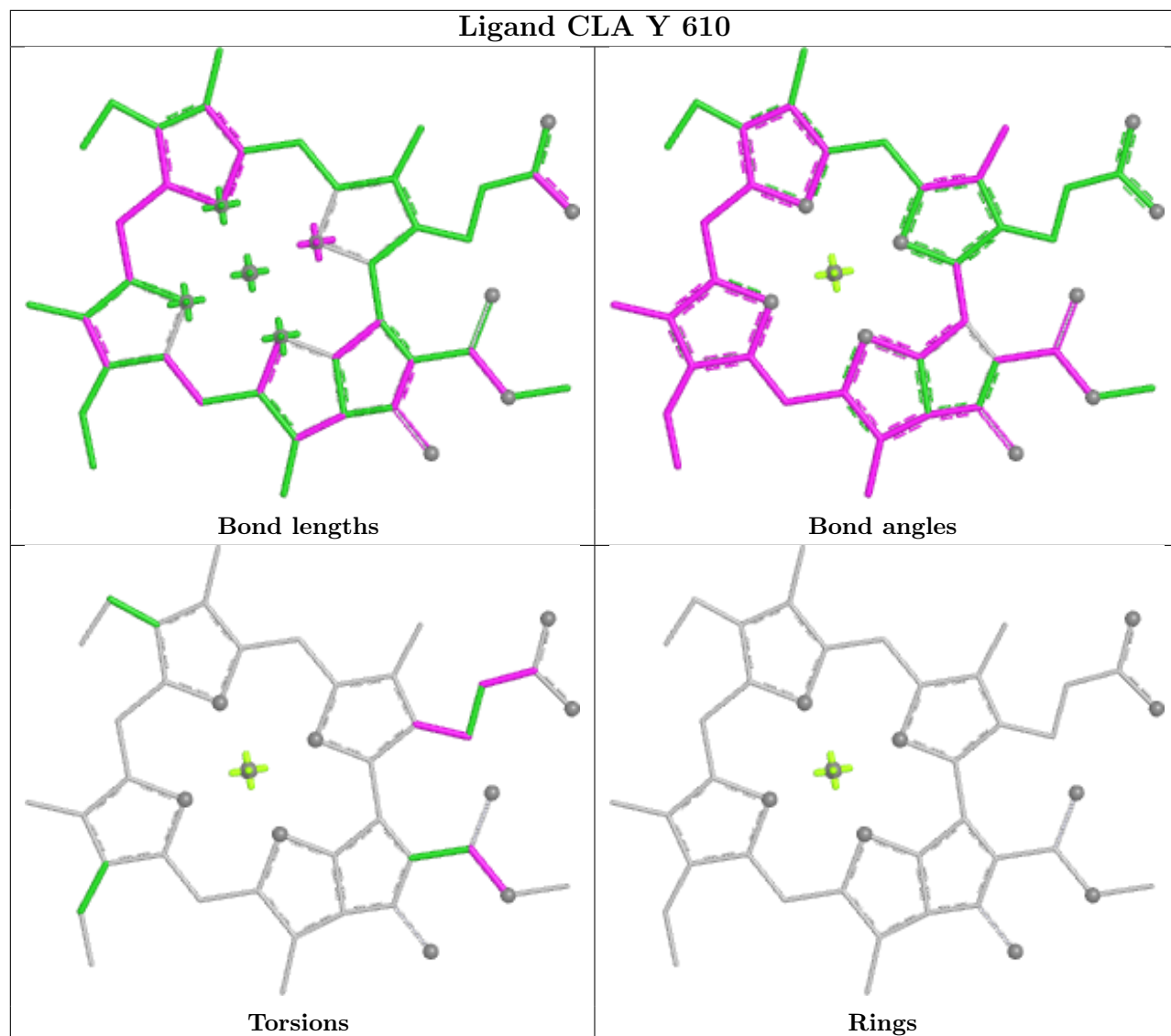


Torsions

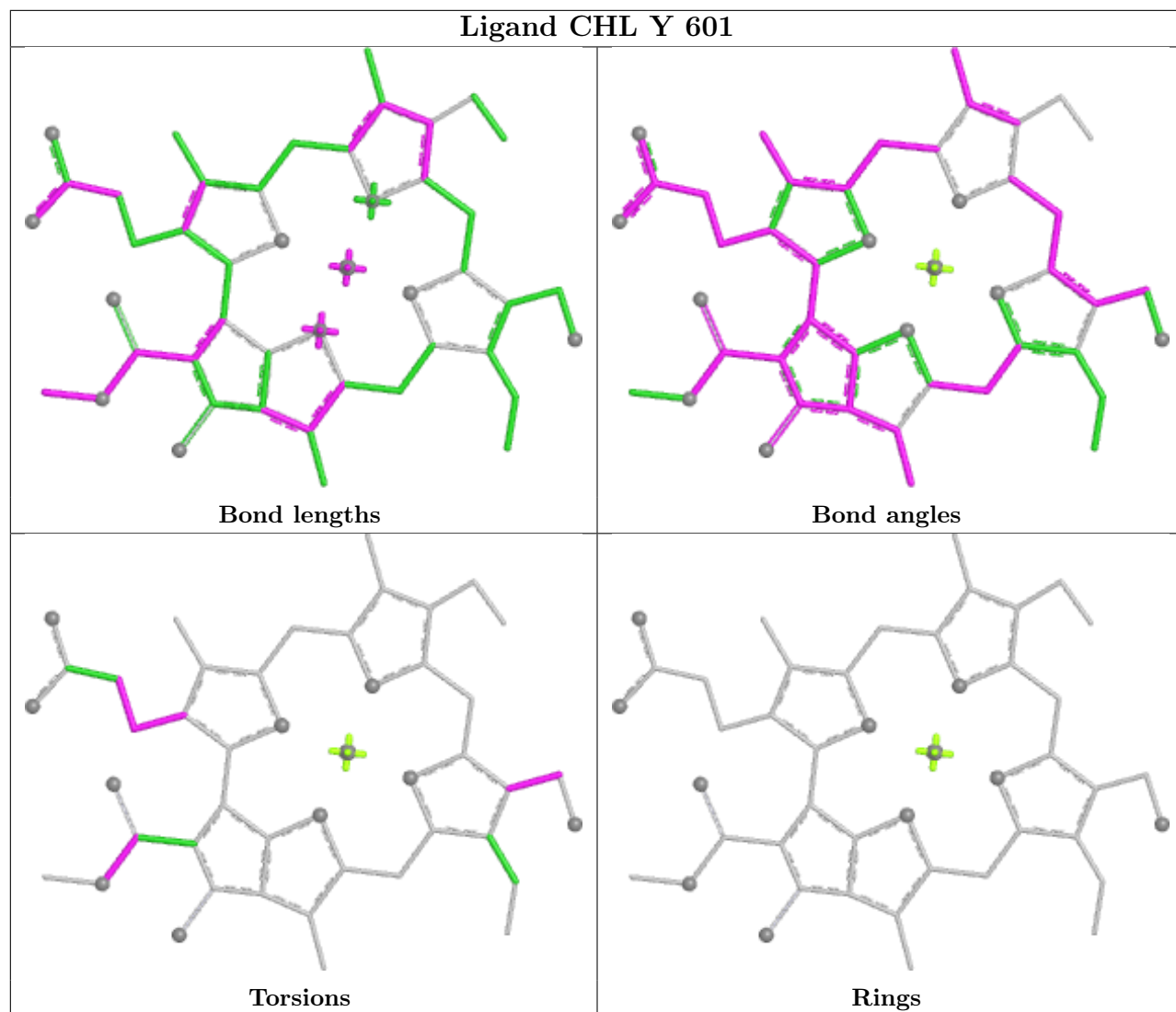


Rings

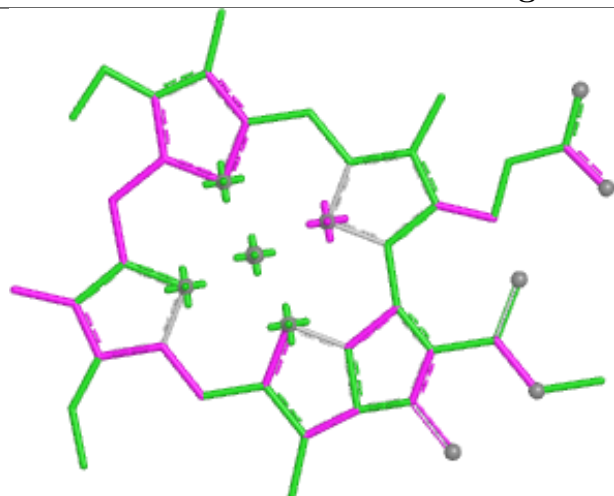
Ligand CLA Y 610



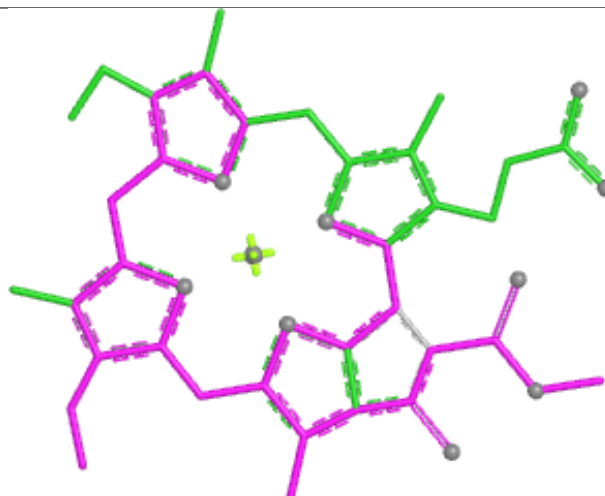
Ligand CHL Y 601



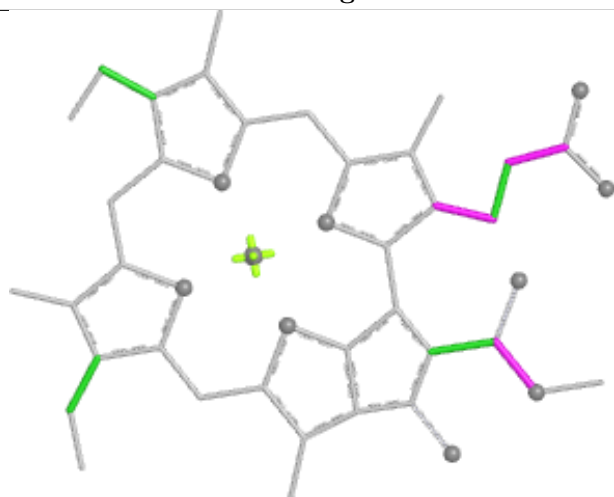
Ligand CLA 2 613



Bond lengths



Bond angles

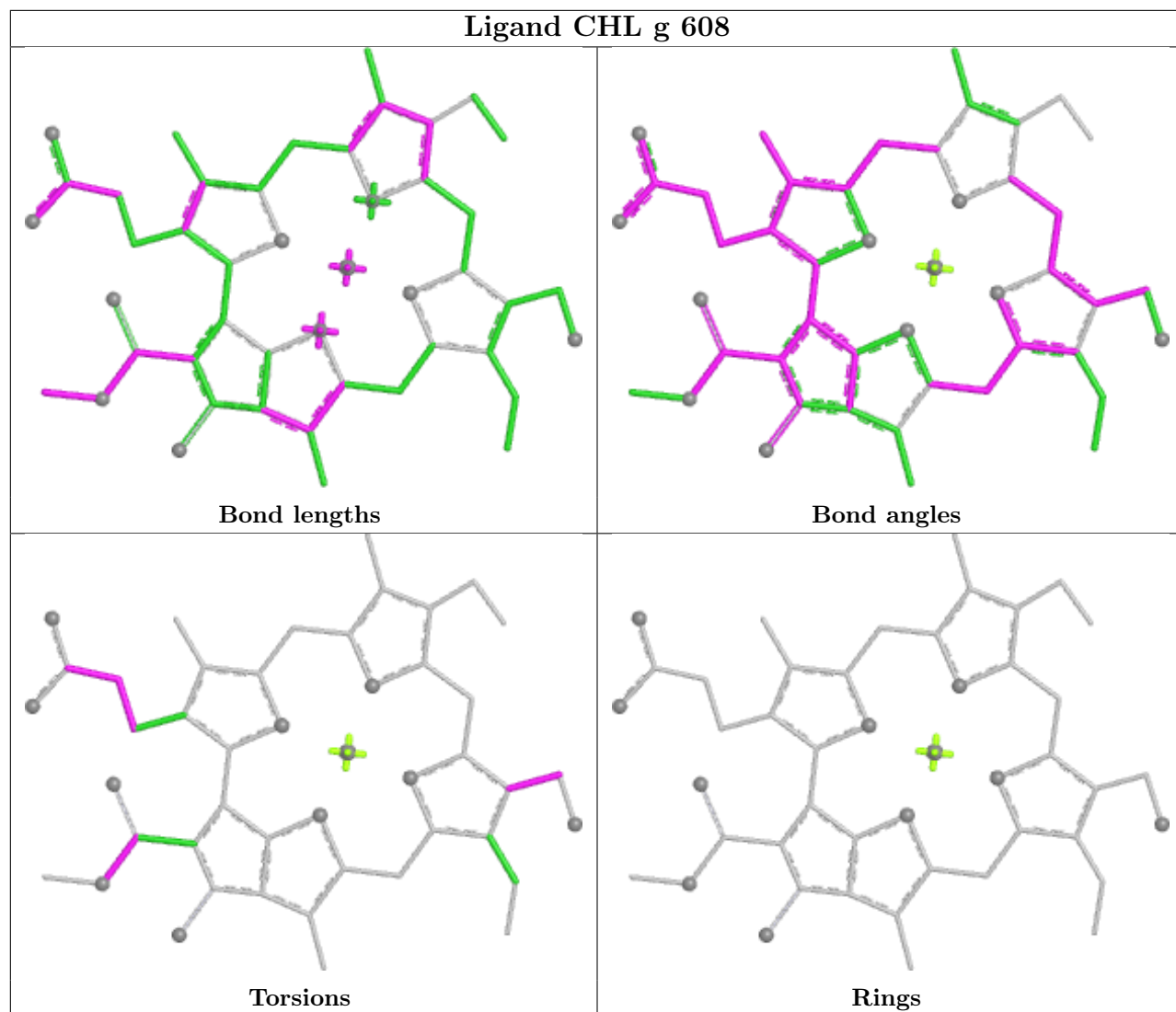


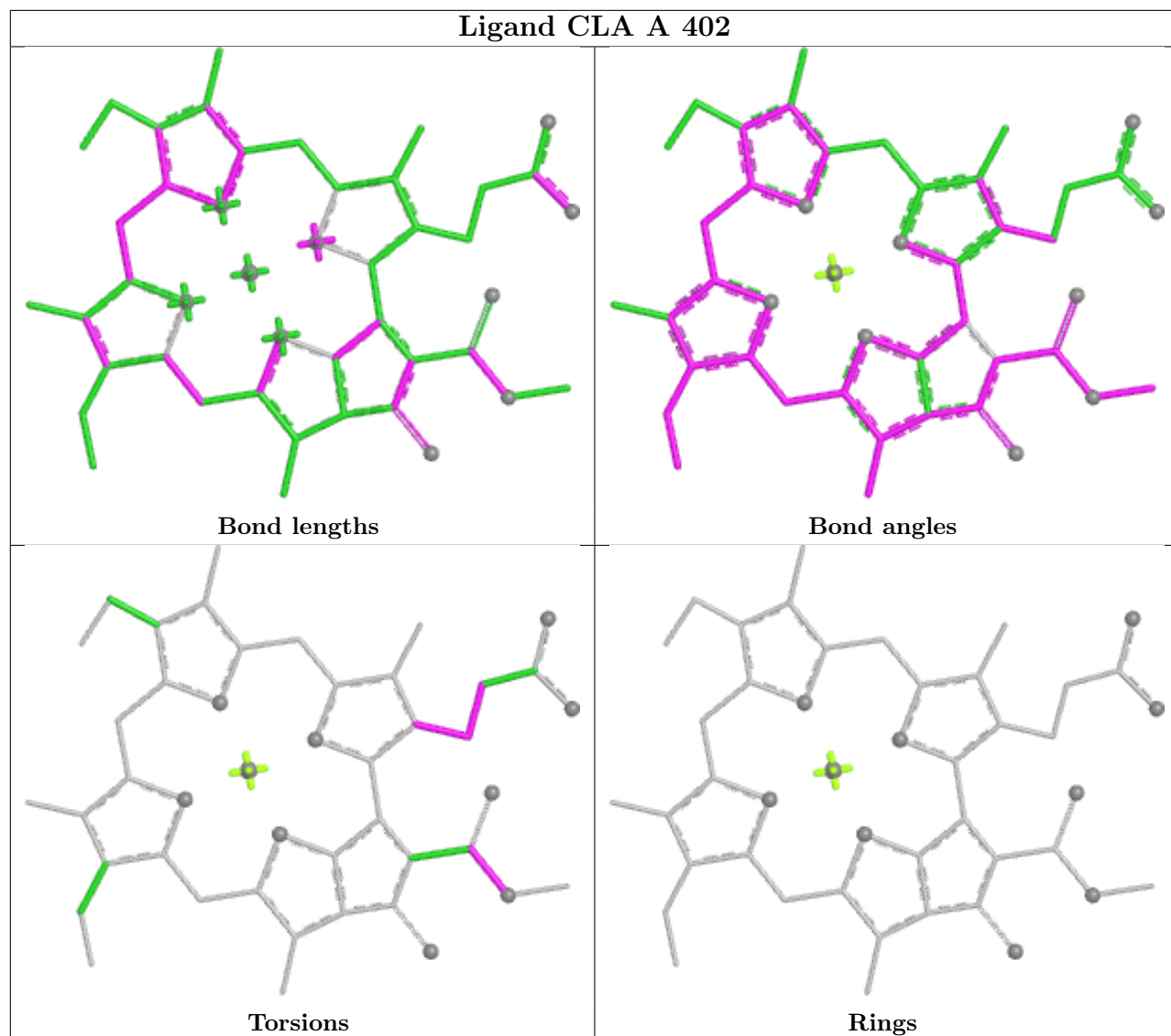
Torsions



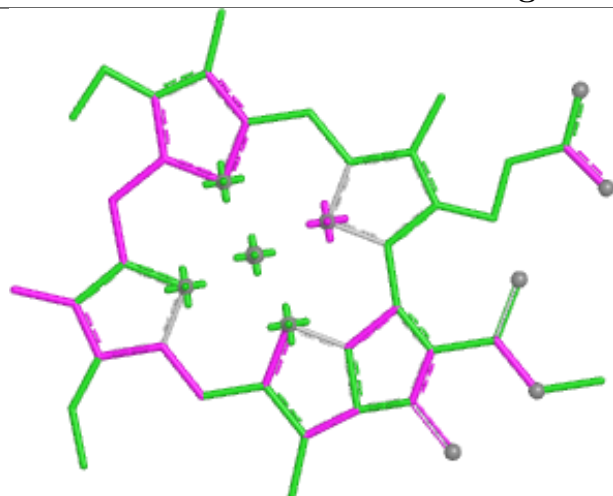
Rings

Ligand CHL g 608

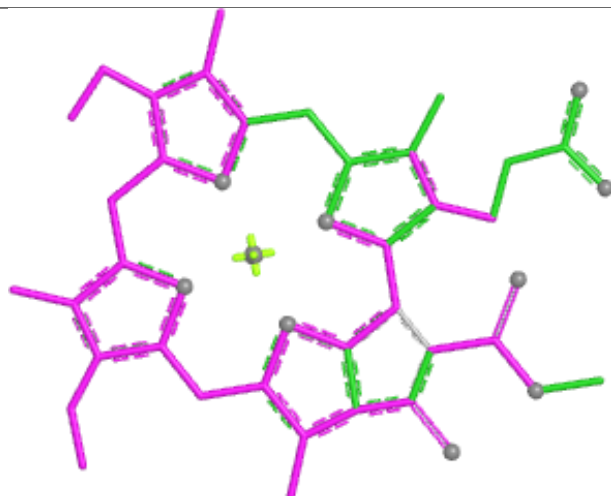




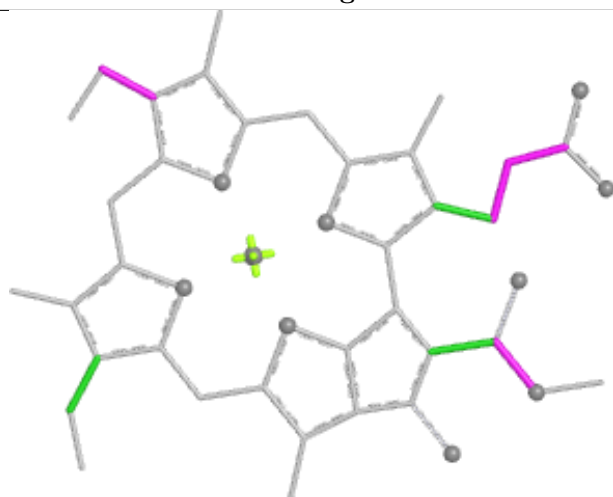
Ligand CLA 2 612



Bond lengths



Bond angles

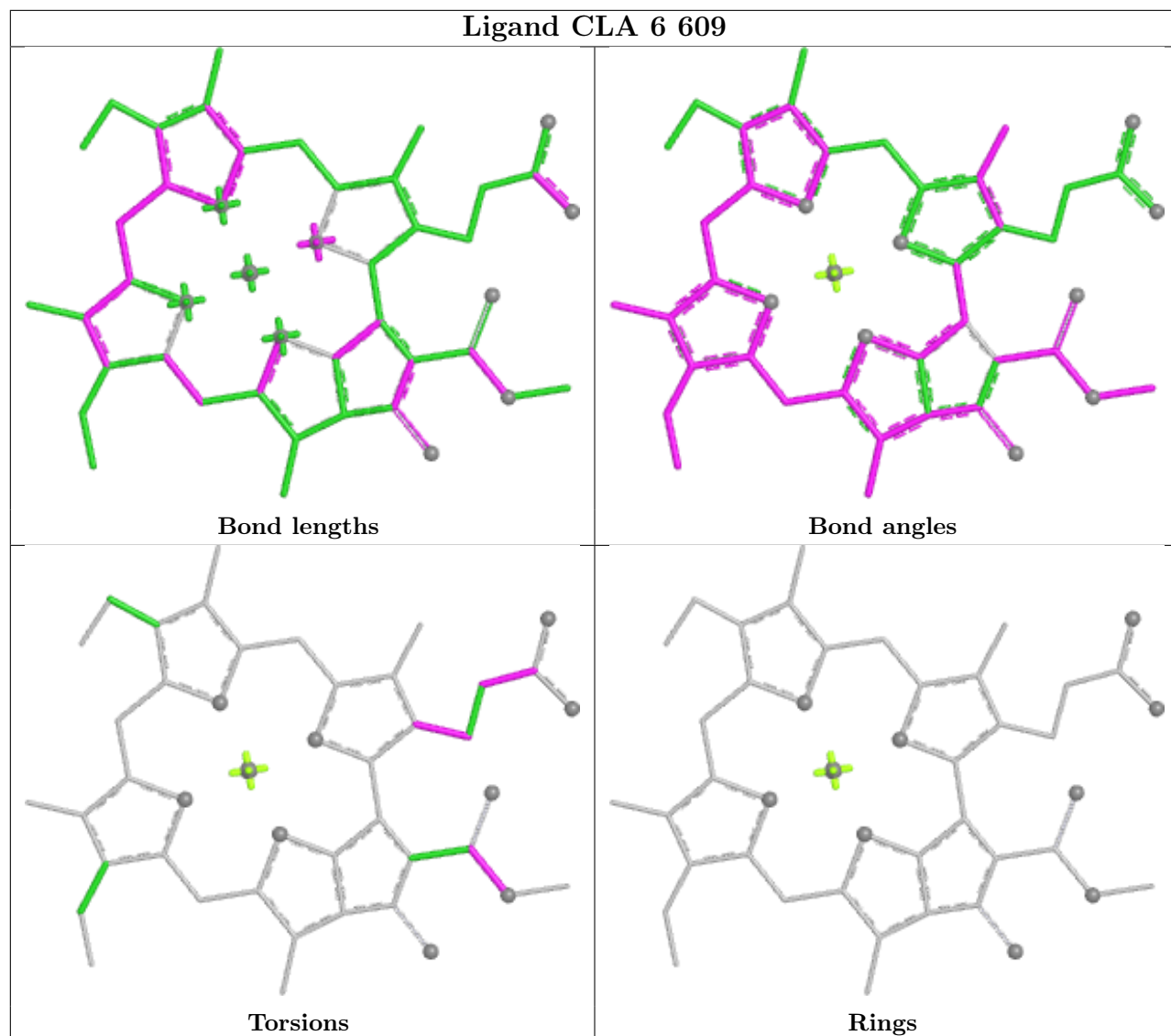


Torsions

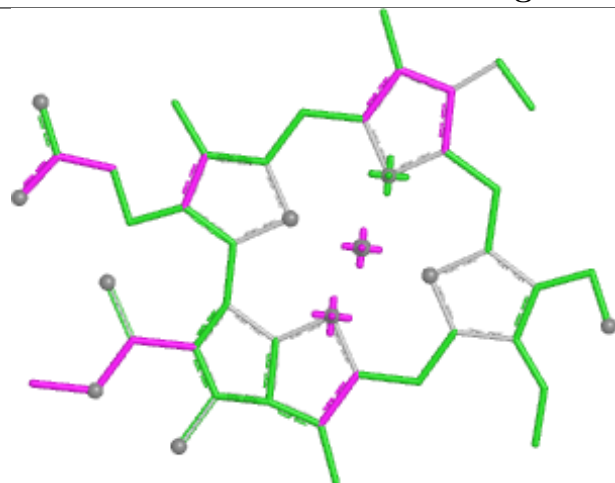


Rings

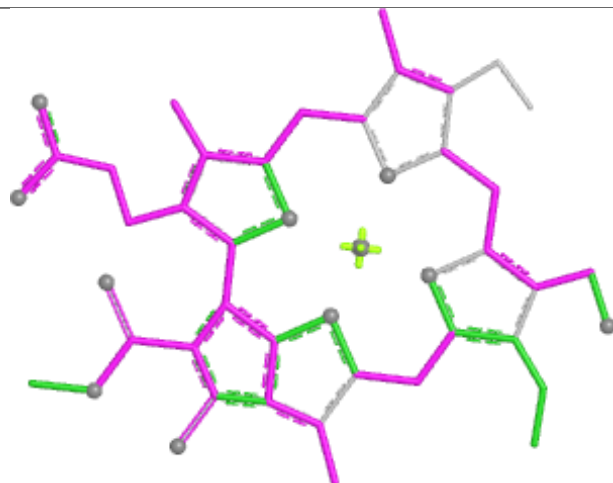
Ligand CLA 6 609



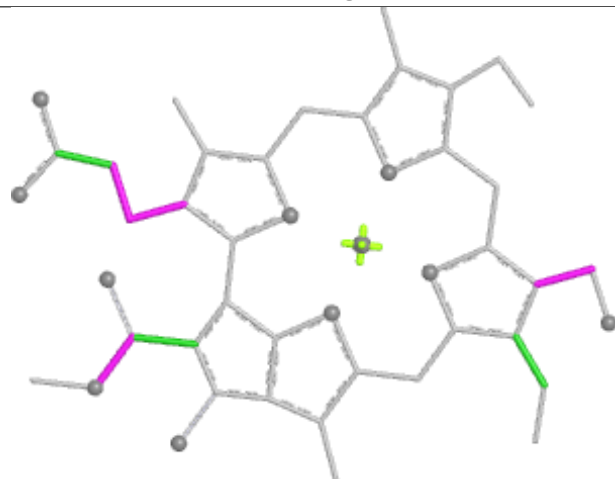
Ligand CHL N 601



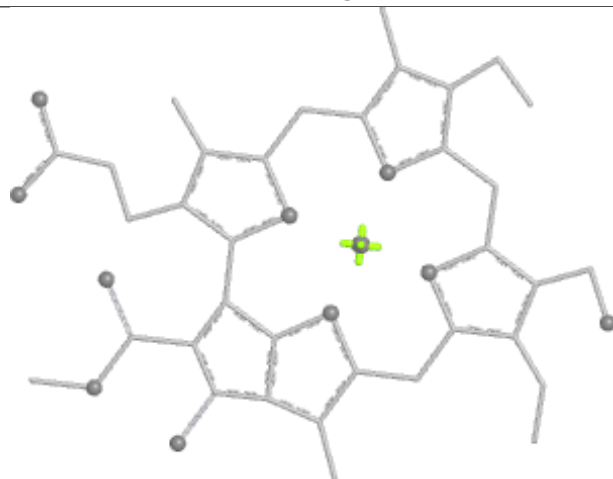
Bond lengths



Bond angles

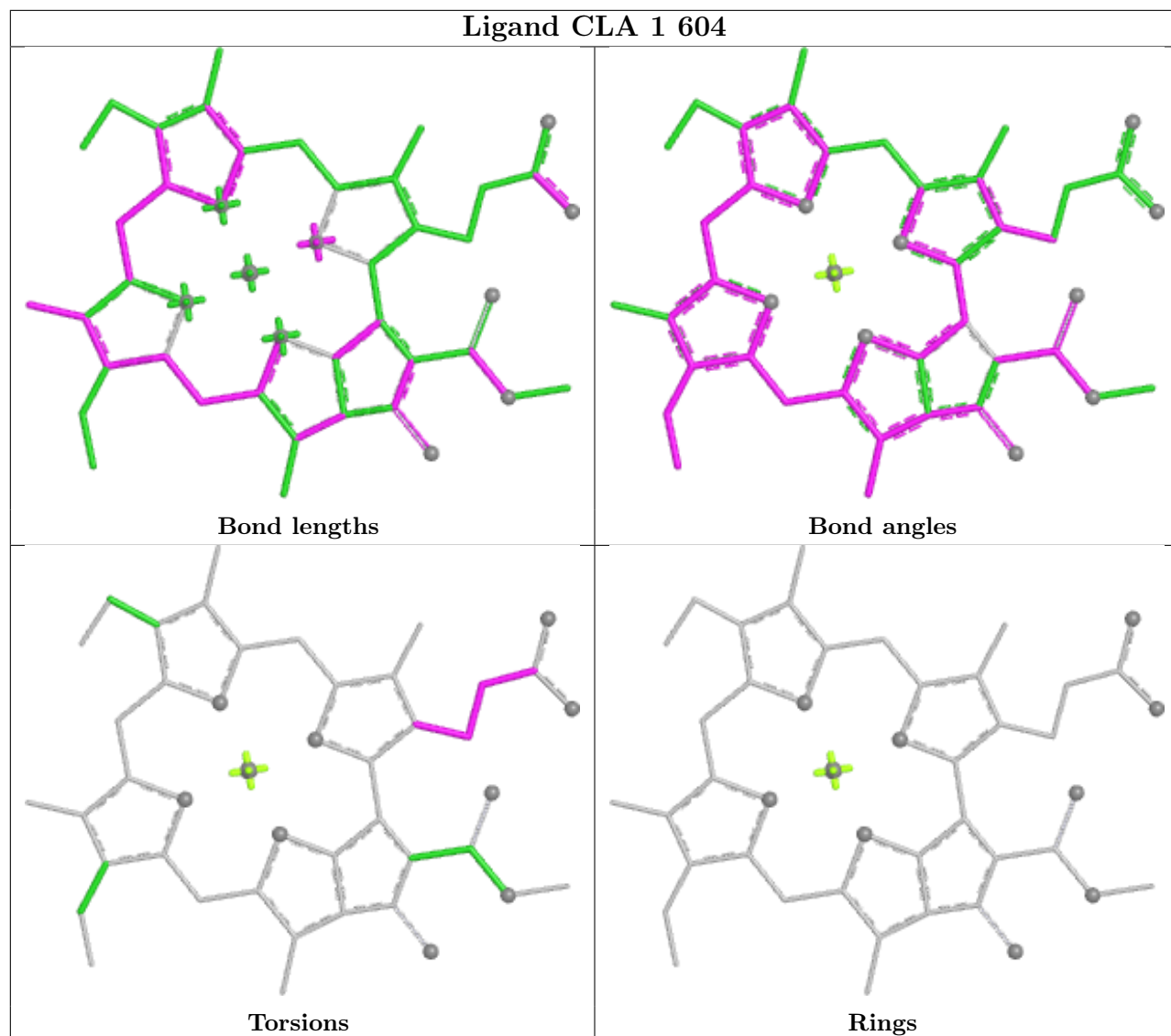


Torsions

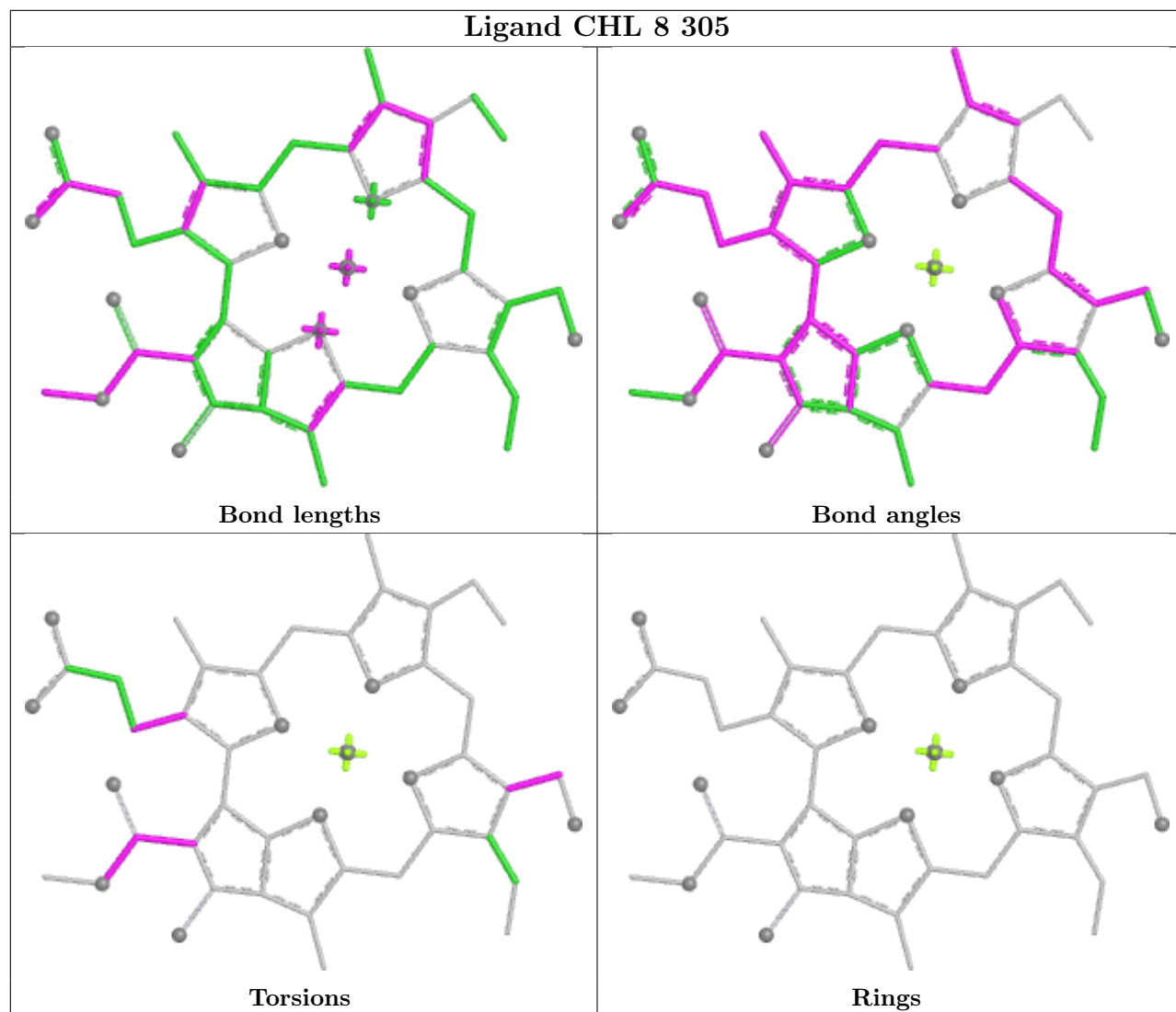


Rings

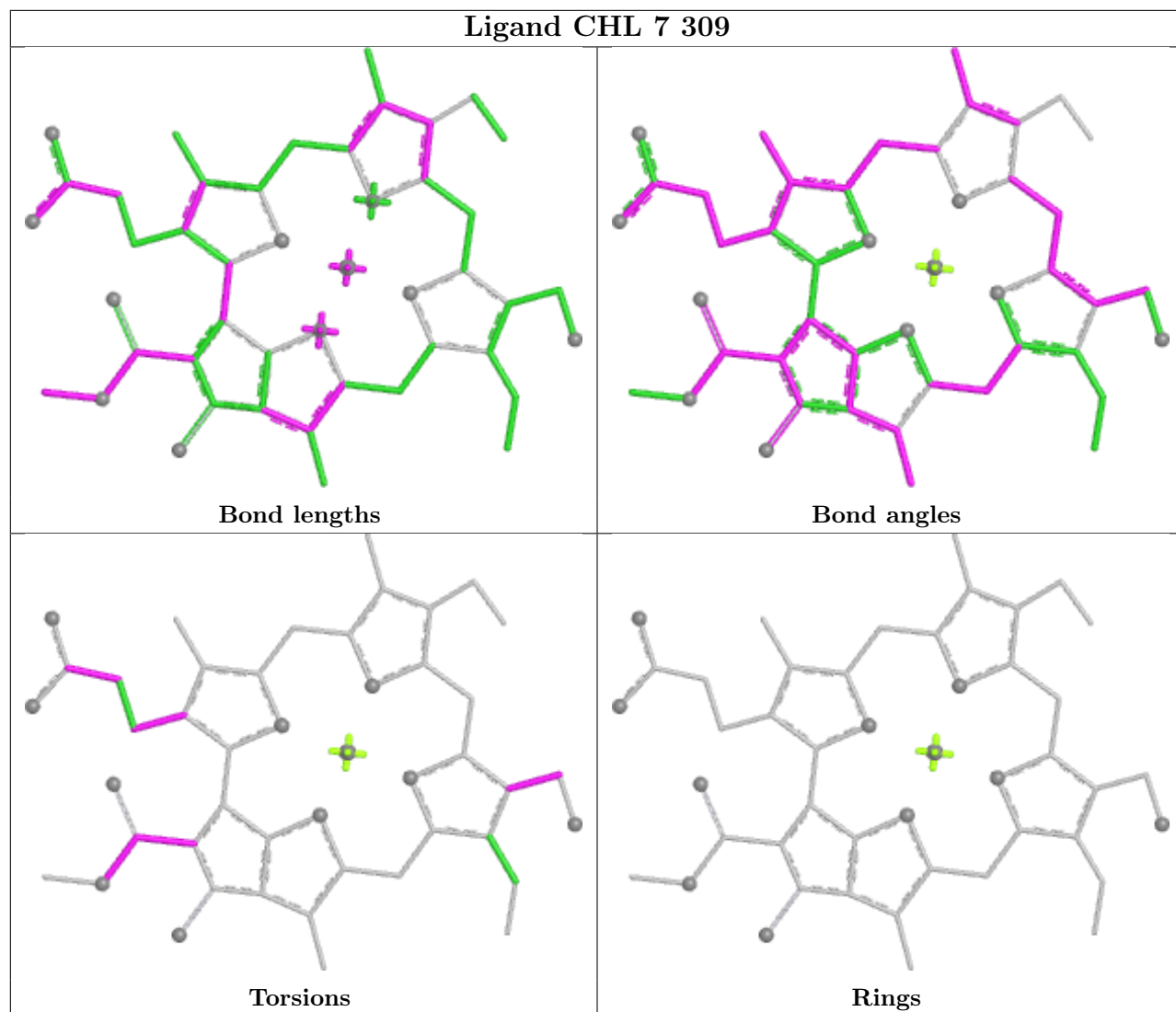
Ligand CLA 1 604



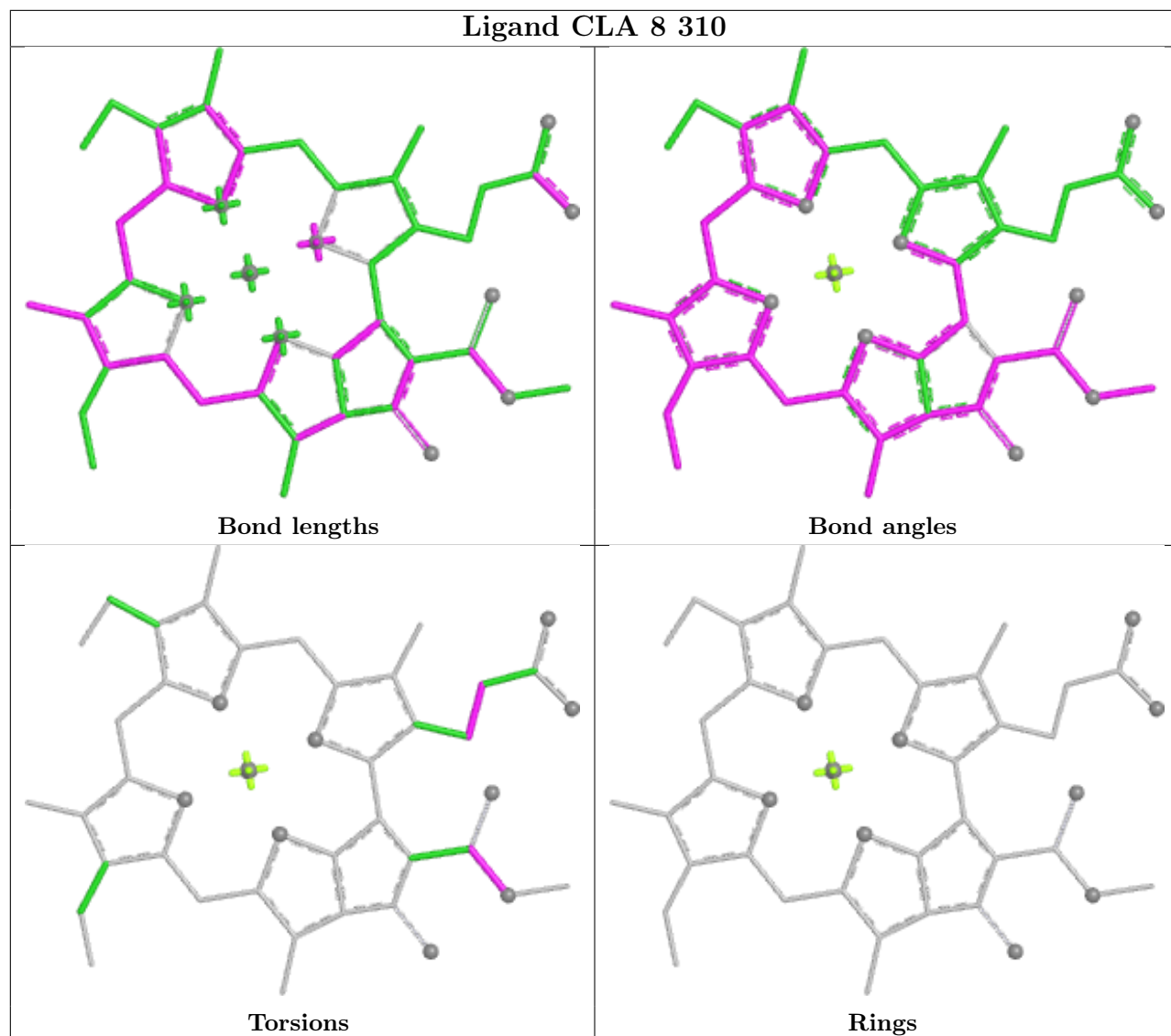
Ligand CHL 8 305



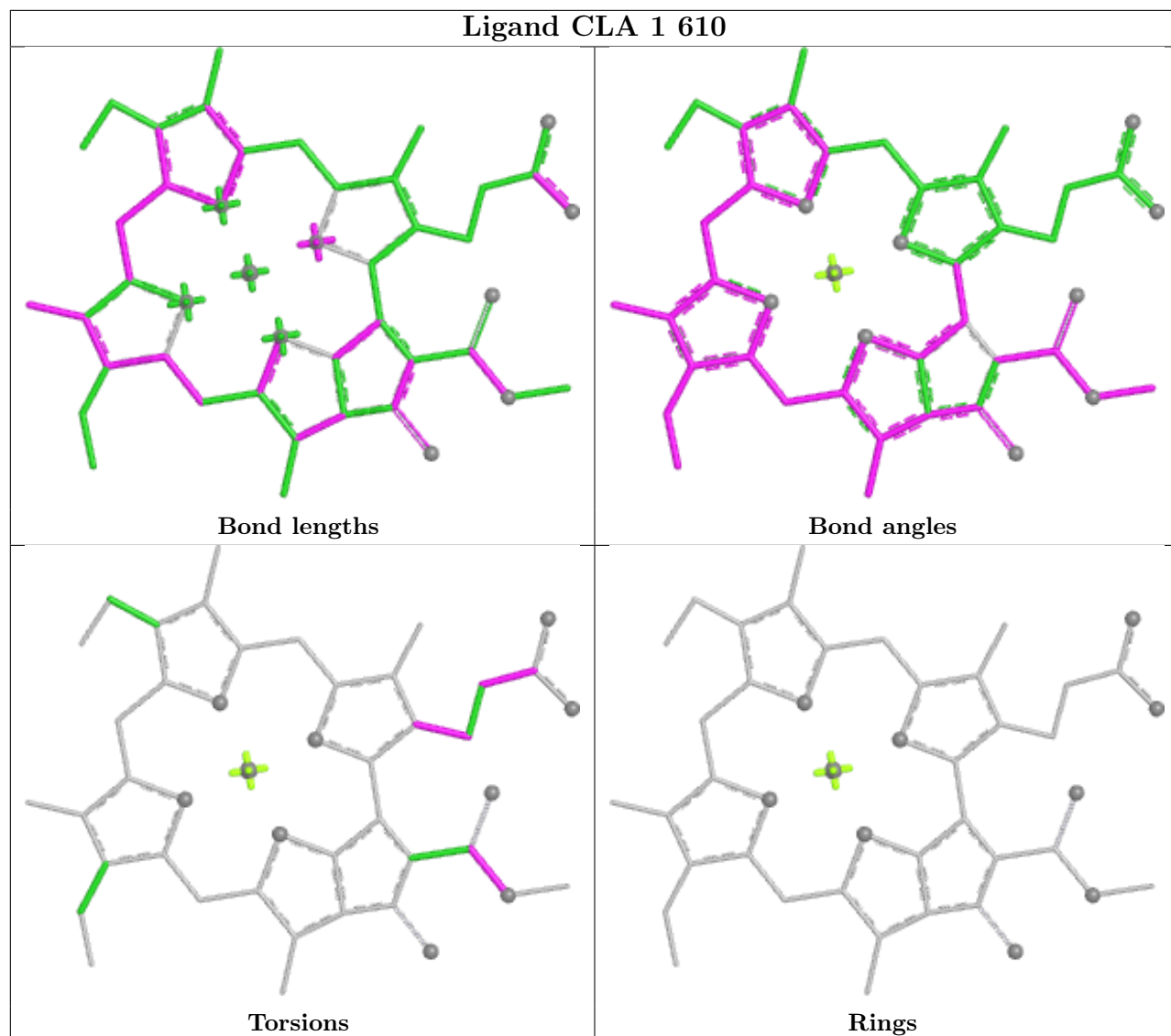
Ligand CHL 7 309



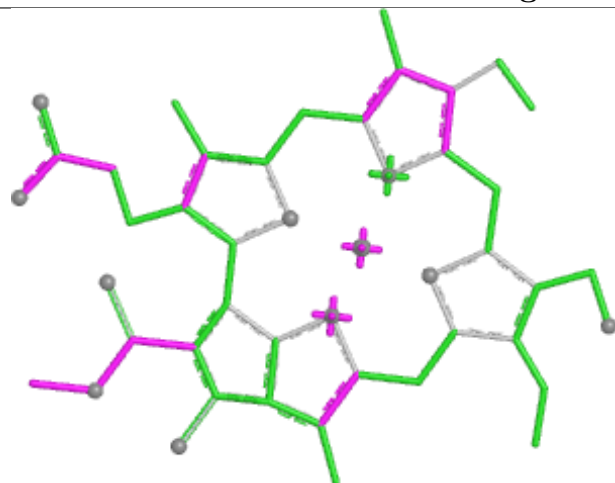
Ligand CLA 8 310



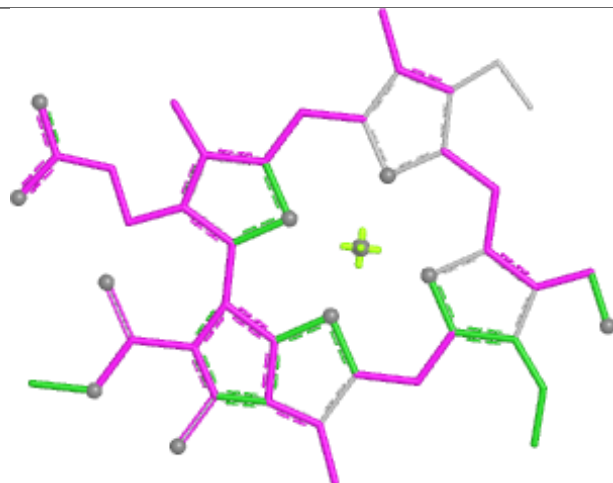
Ligand CLA 1 610



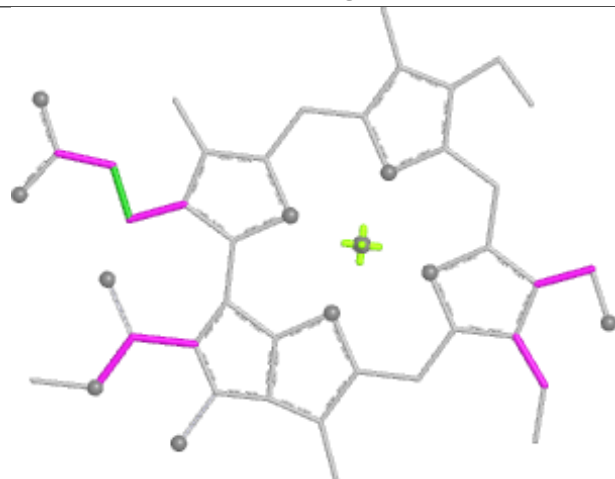
Ligand CHL 4 306



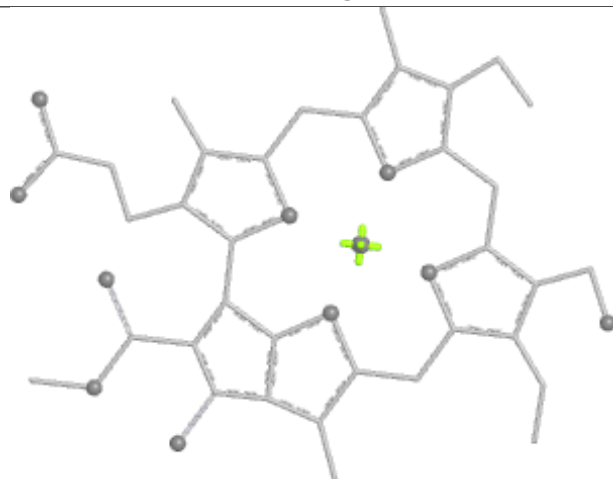
Bond lengths



Bond angles

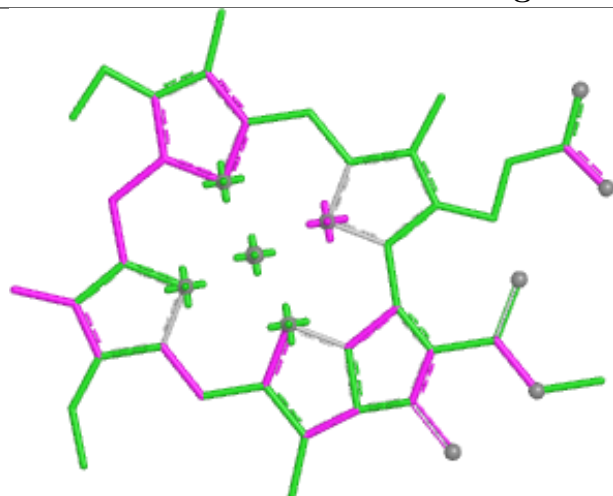


Torsions

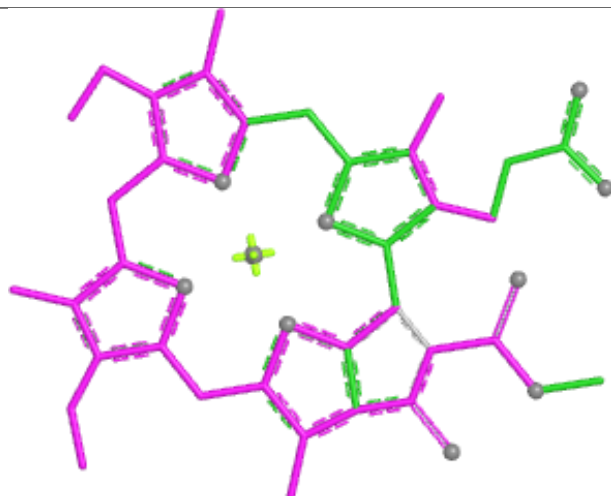


Rings

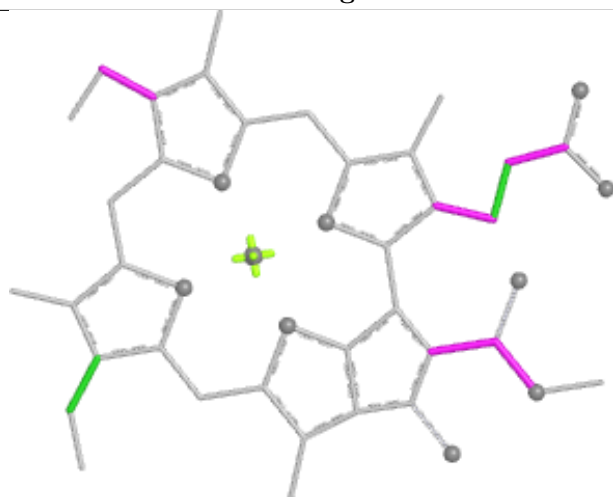
Ligand CLA R 301



Bond lengths



Bond angles

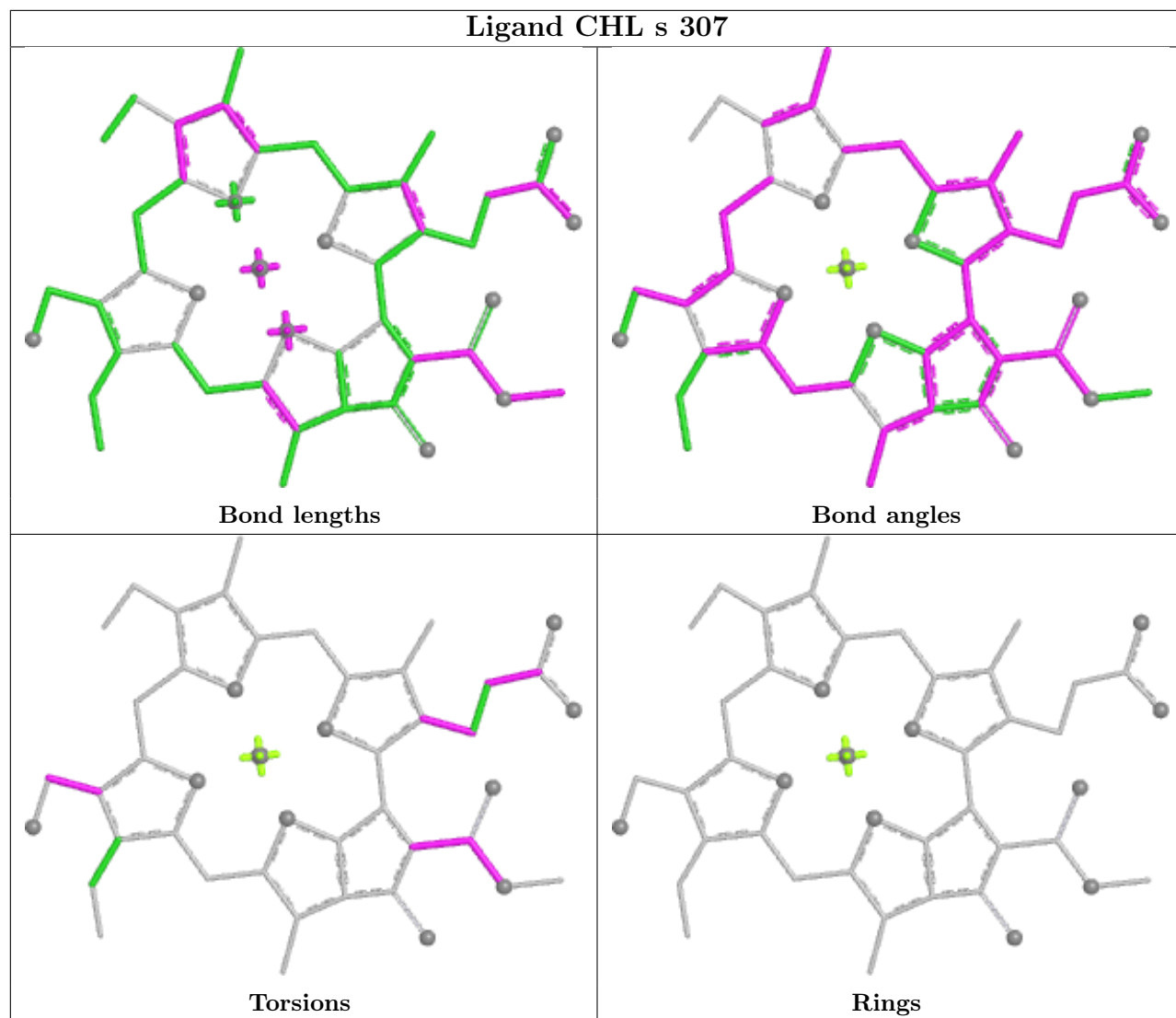


Torsions

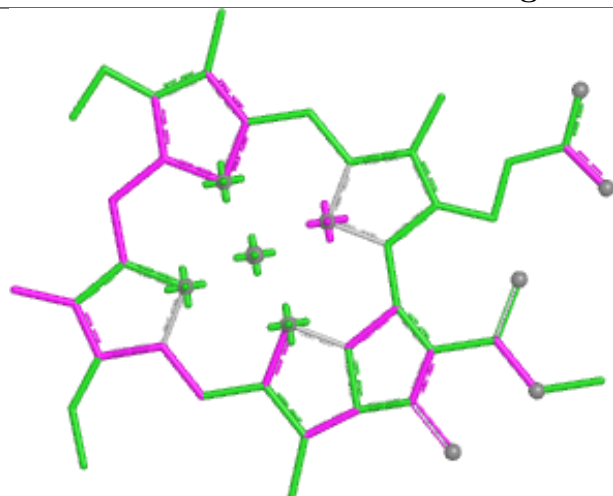


Rings

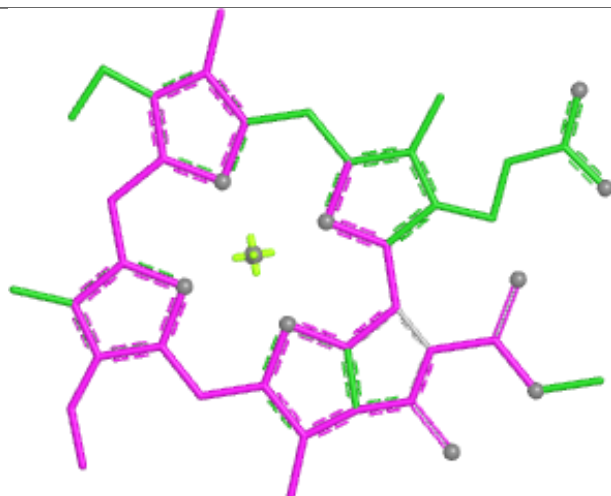
Ligand CHL s 307



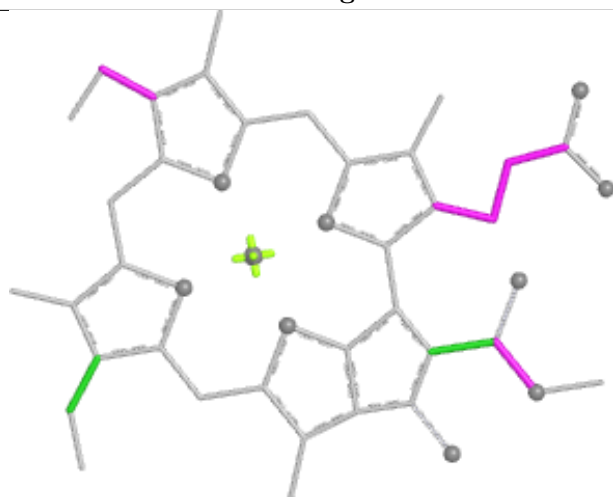
Ligand CLA r 310



Bond lengths



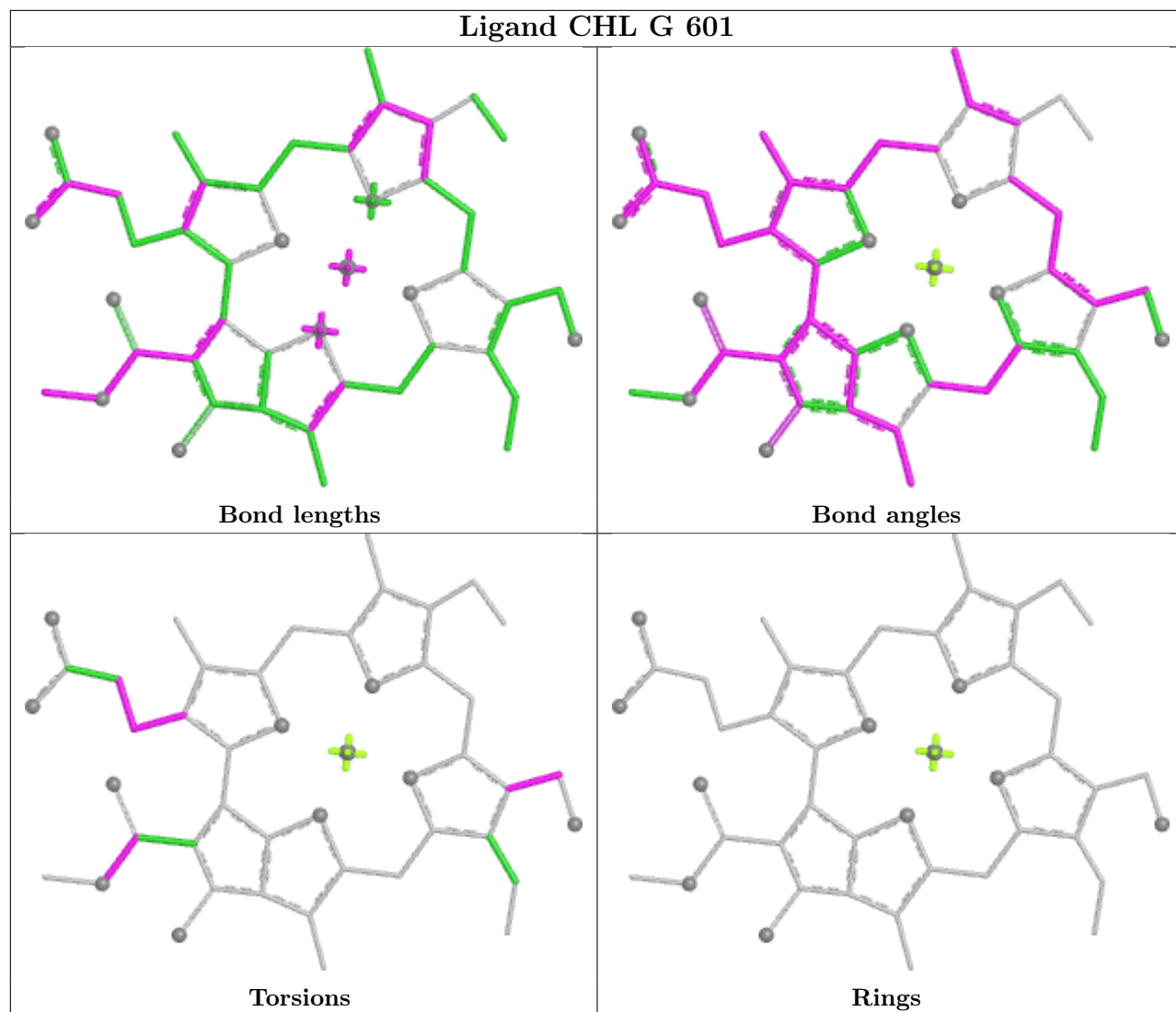
Bond angles



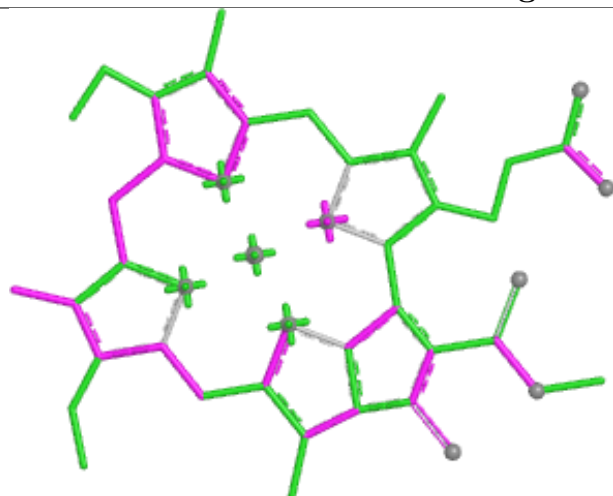
Torsions



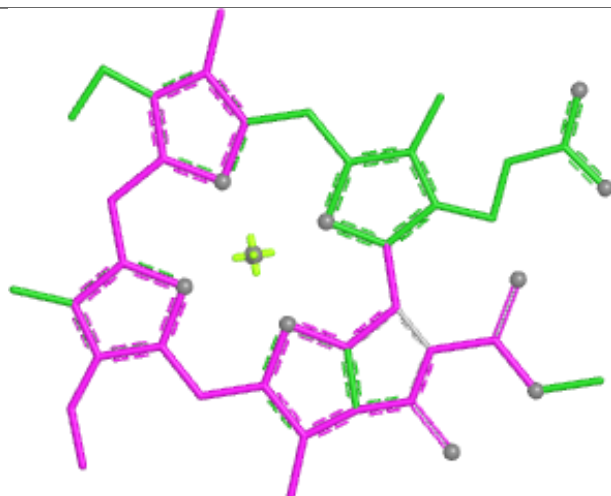
Rings



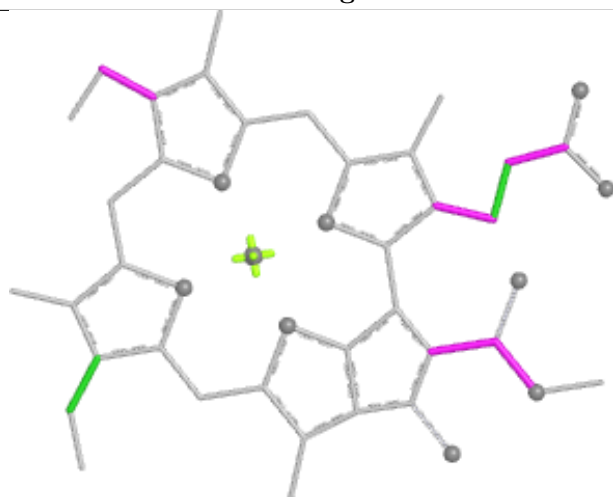
Ligand CLA 2 611



Bond lengths



Bond angles

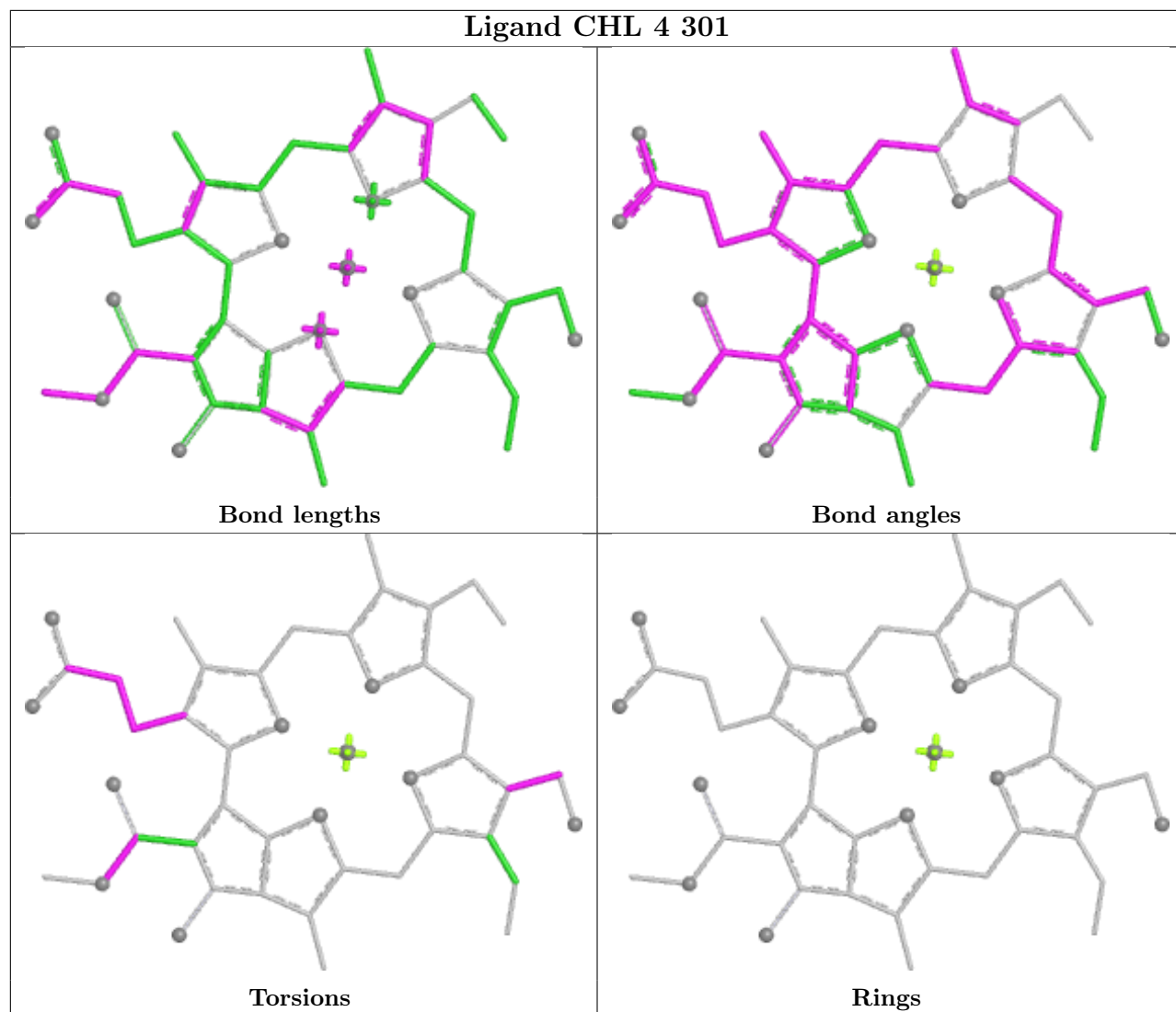


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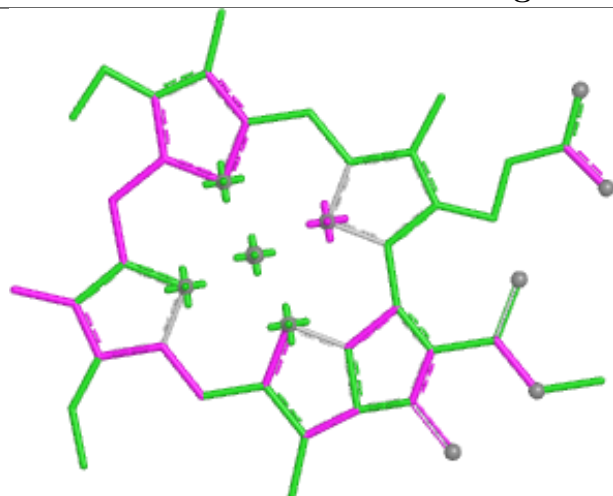


Rings

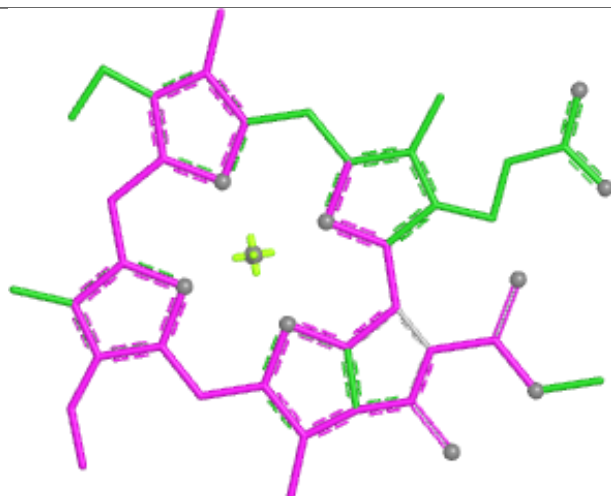
Ligand CHL 4 301



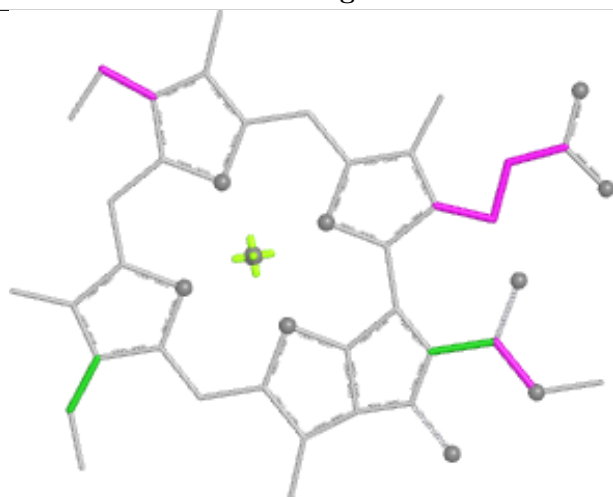
Ligand CLA R 310



Bond lengths



Bond angles

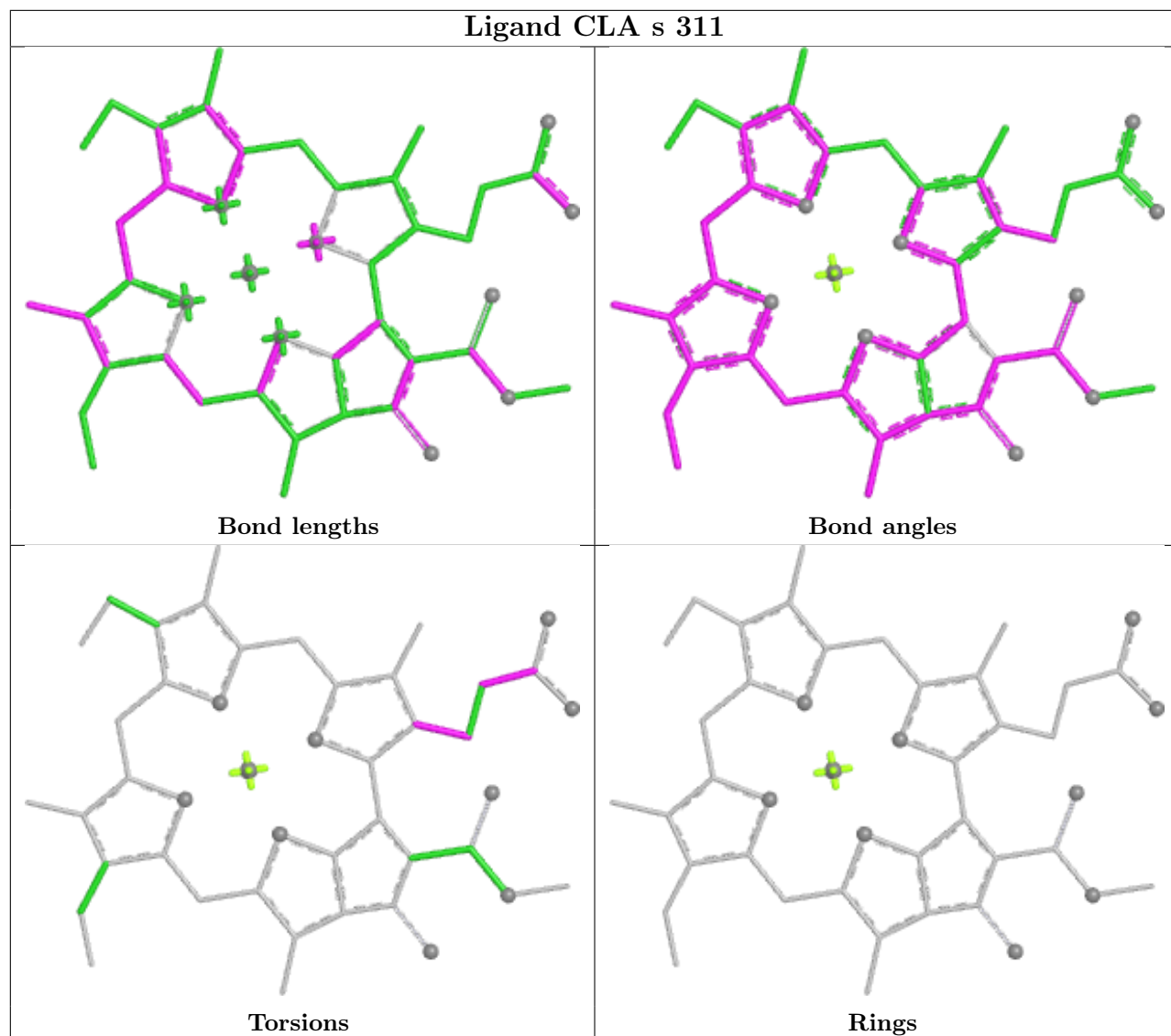


Torsions

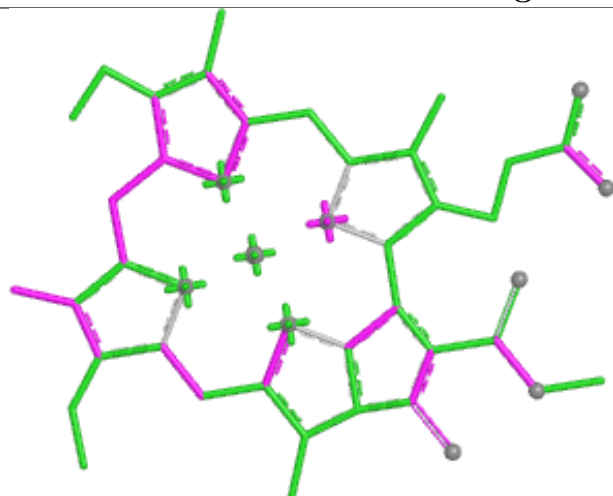


Rings

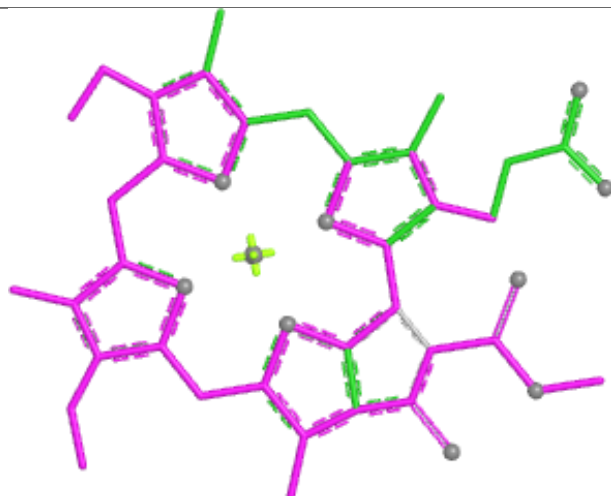
Ligand CLA s 311



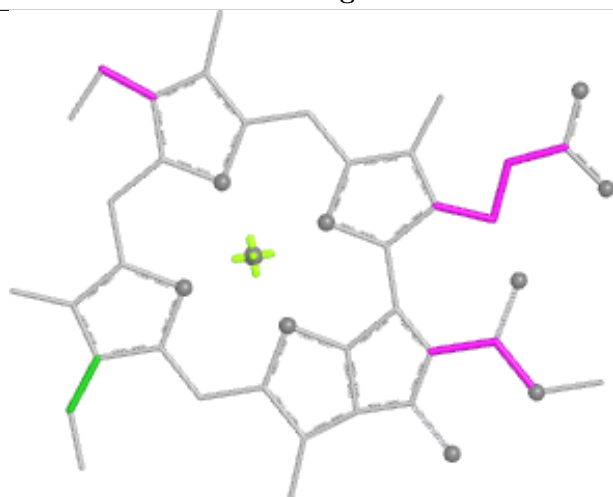
Ligand CLA C 503



Bond lengths



Bond angles

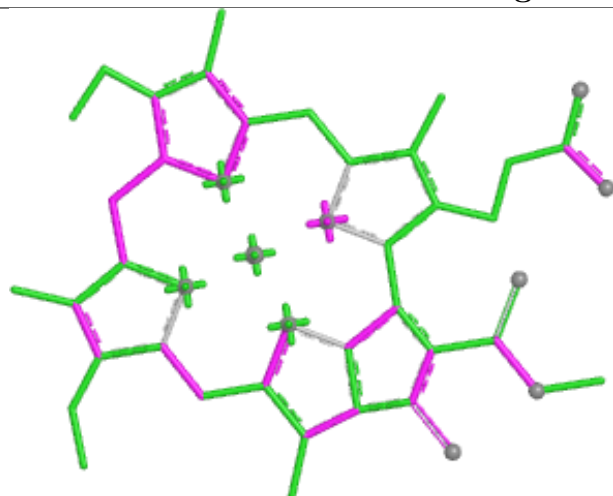


Torsions

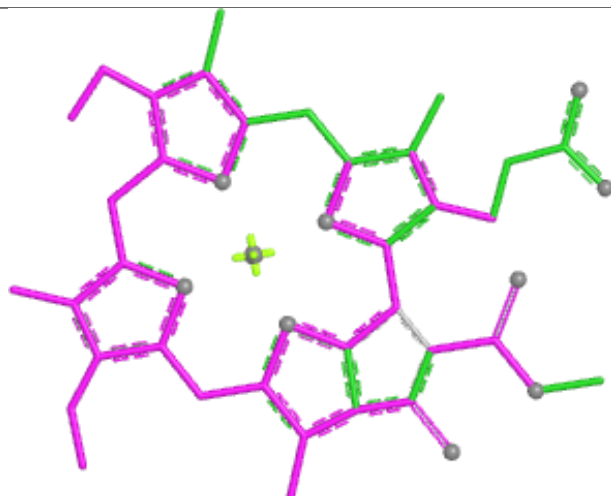


Rings

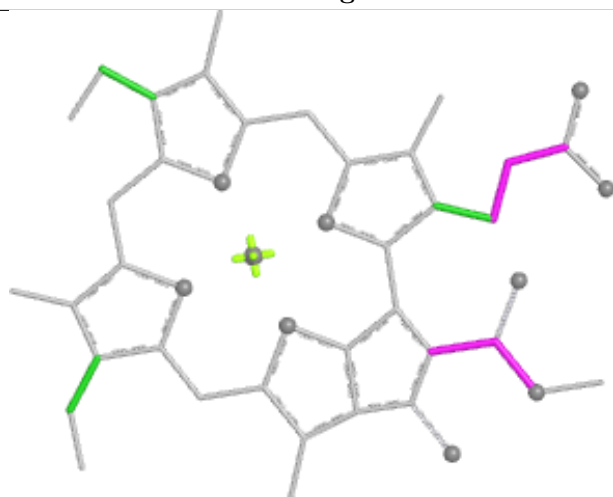
Ligand CLA B 601



Bond lengths



Bond angles

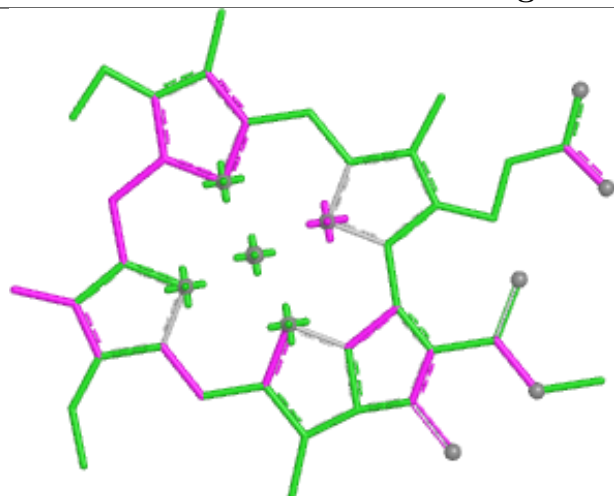


Torsions

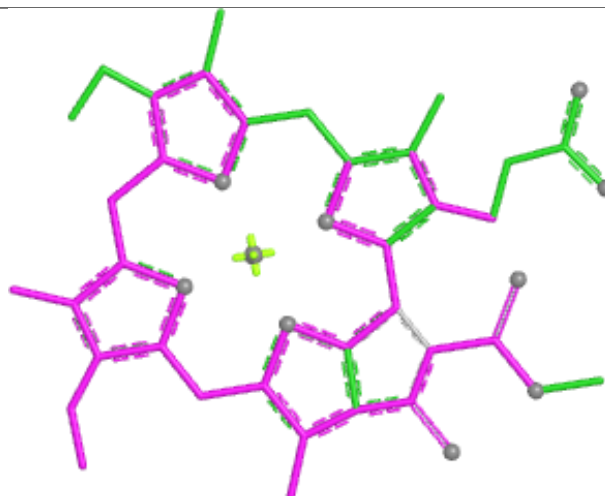


Rings

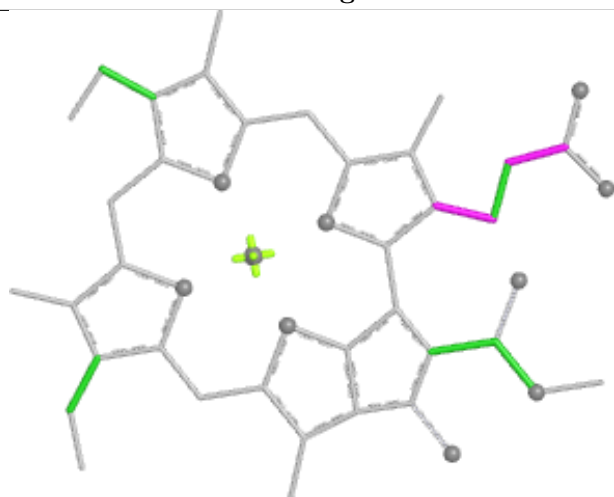
Ligand CLA S 311



Bond lengths



Bond angles

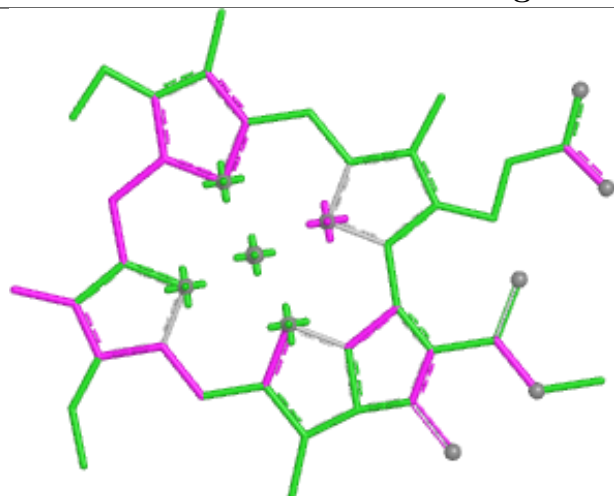


Torsions

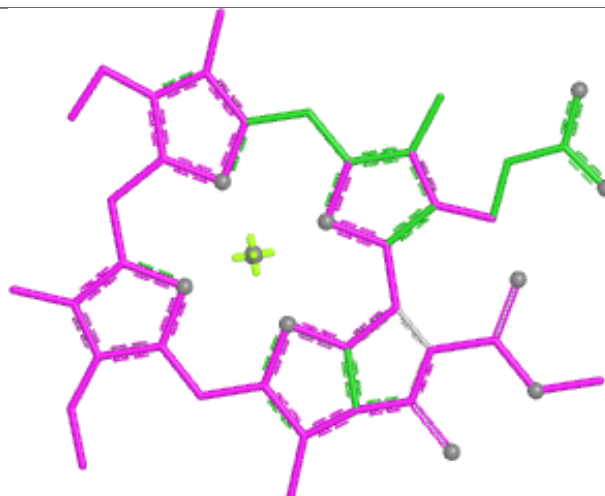


Rings

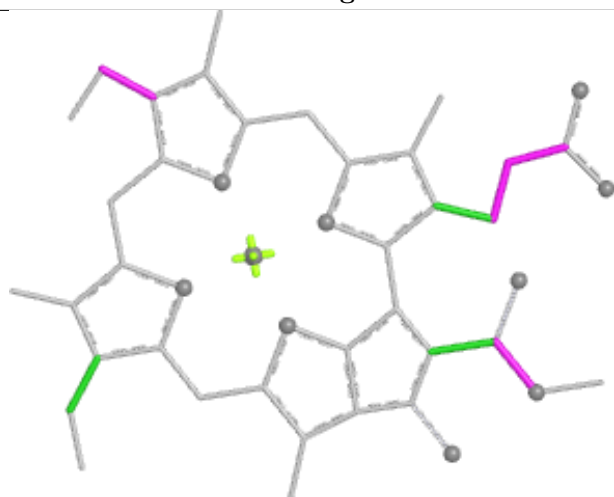
Ligand CLA N 603



Bond lengths



Bond angles

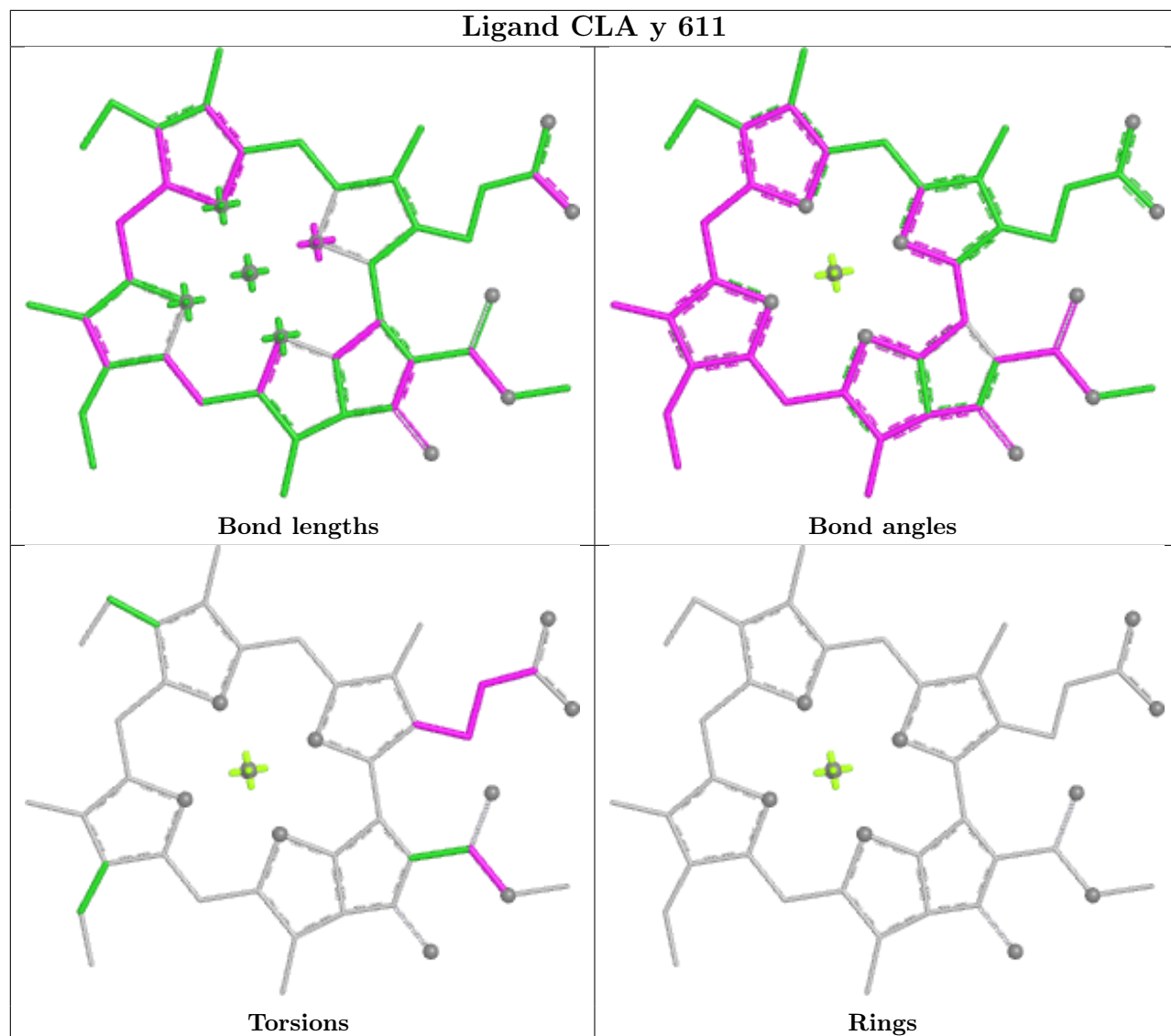


Torsions

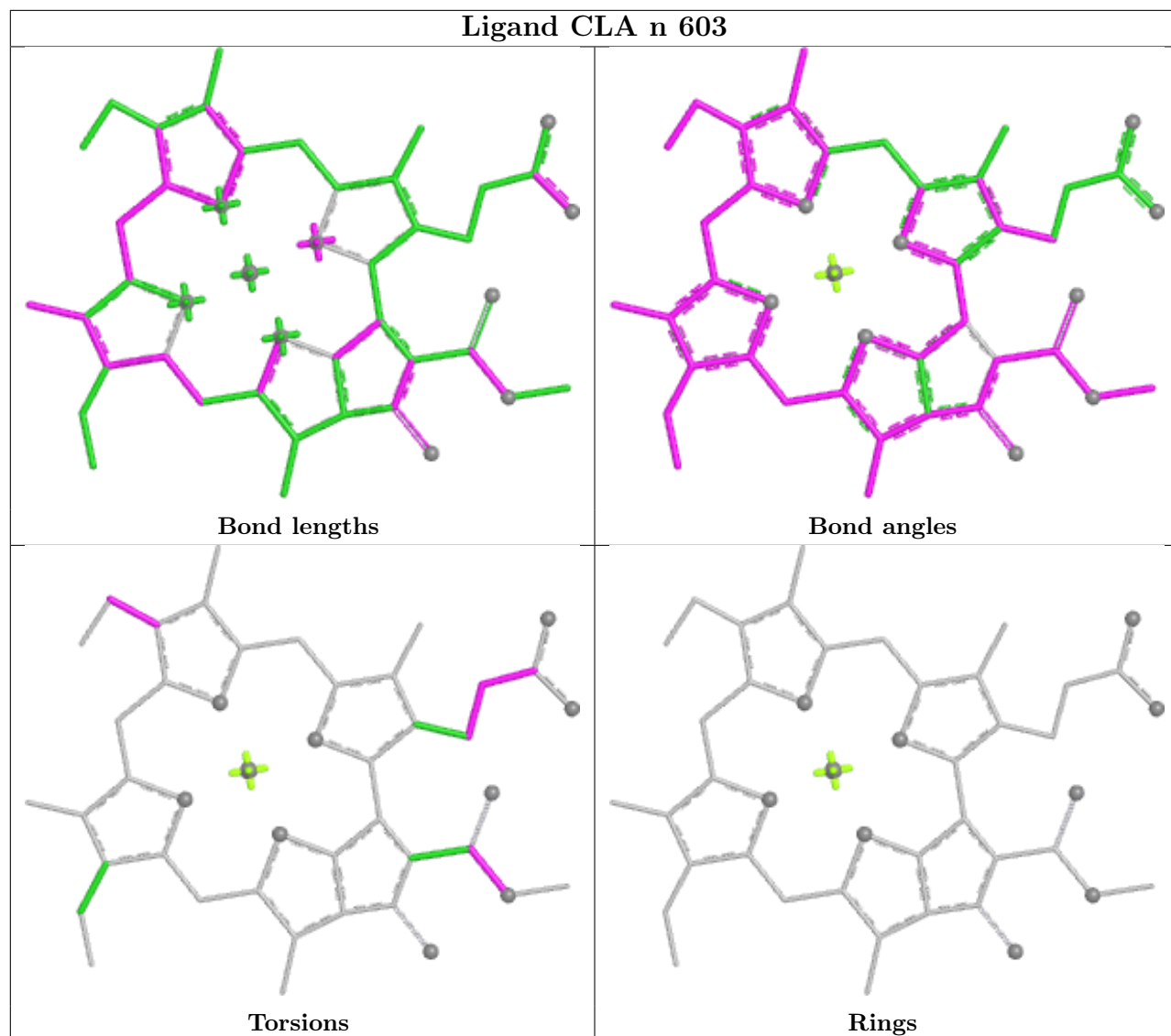


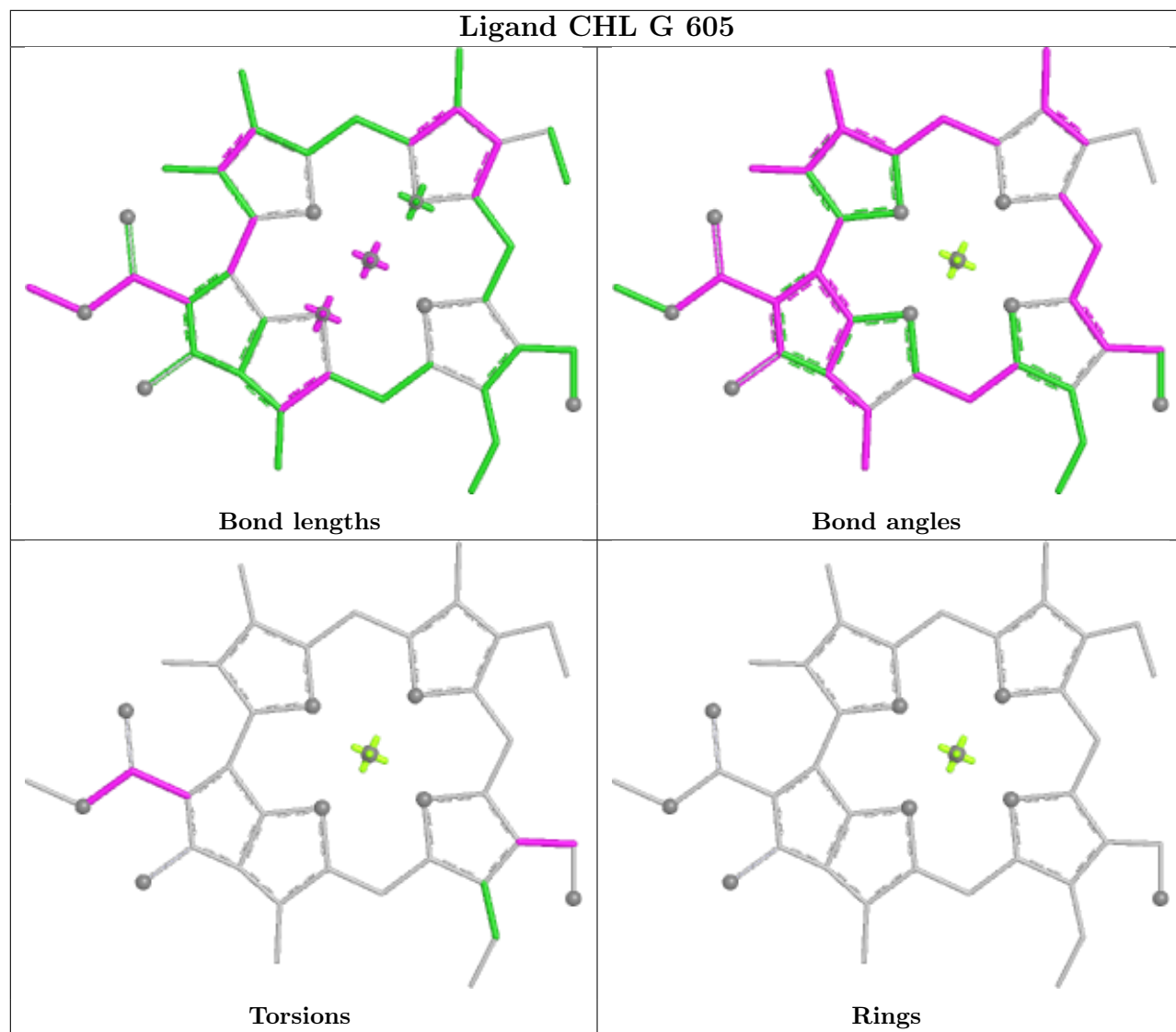
Rings

Ligand CLA y 611

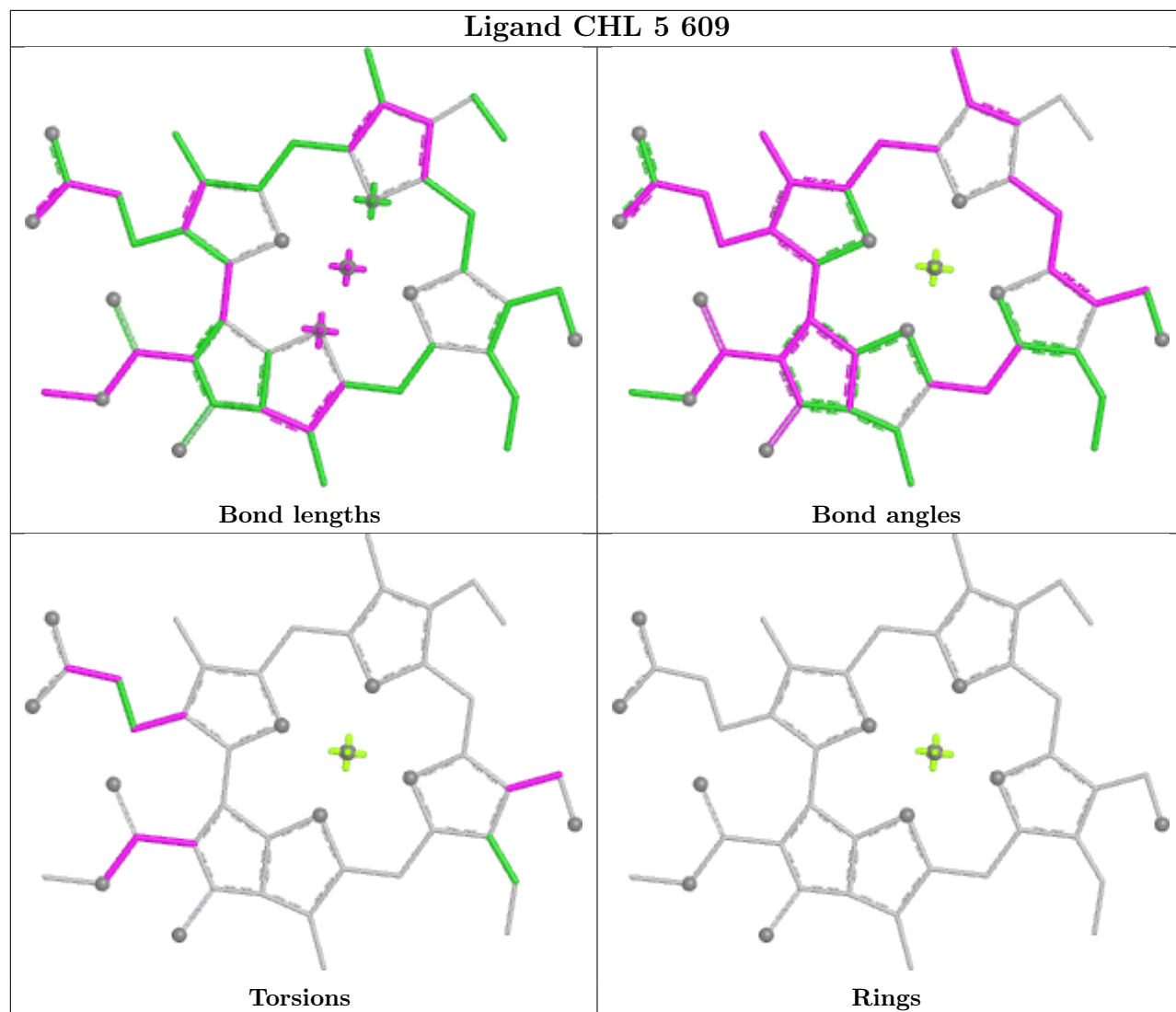


Ligand CLA n 603

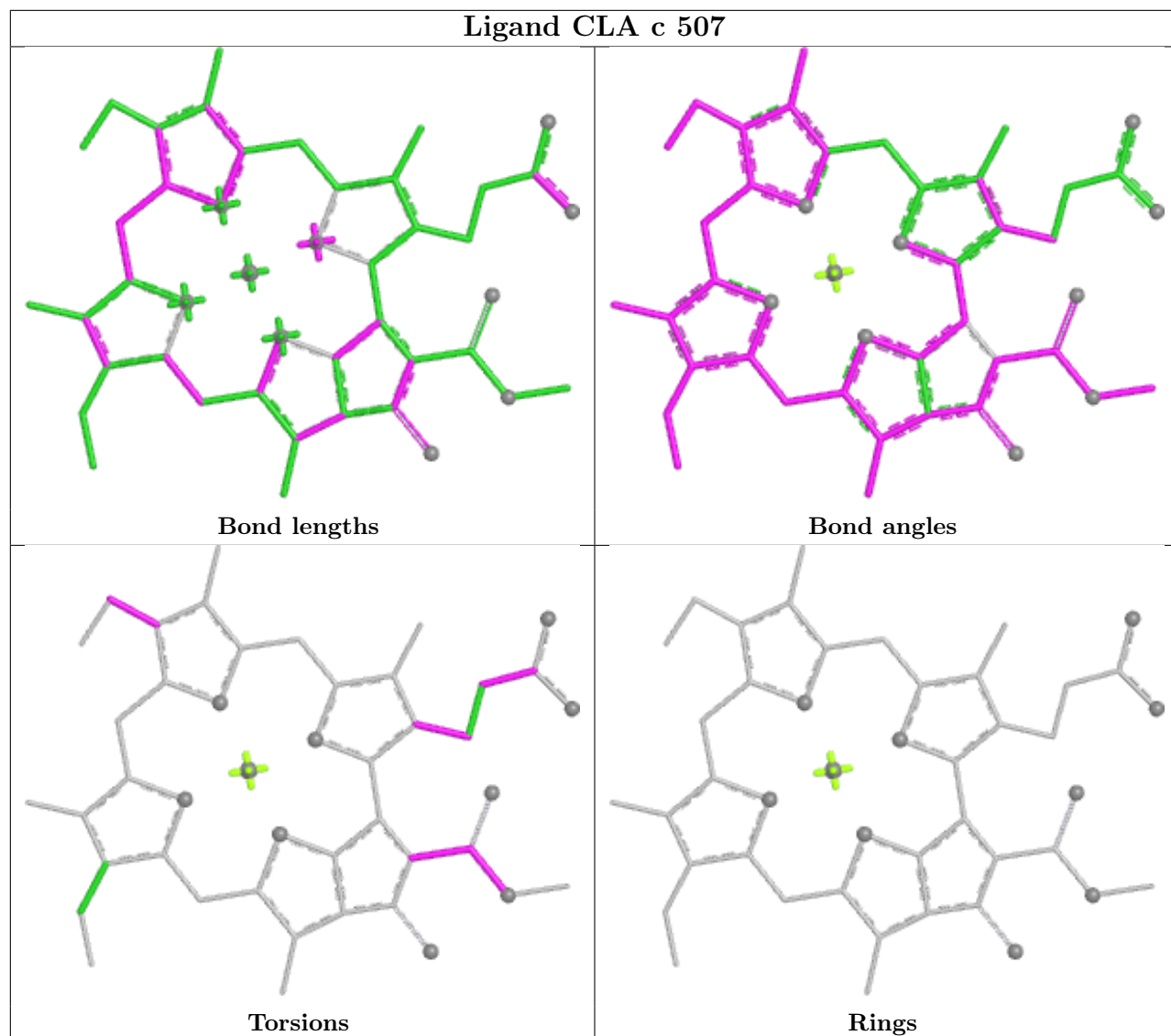




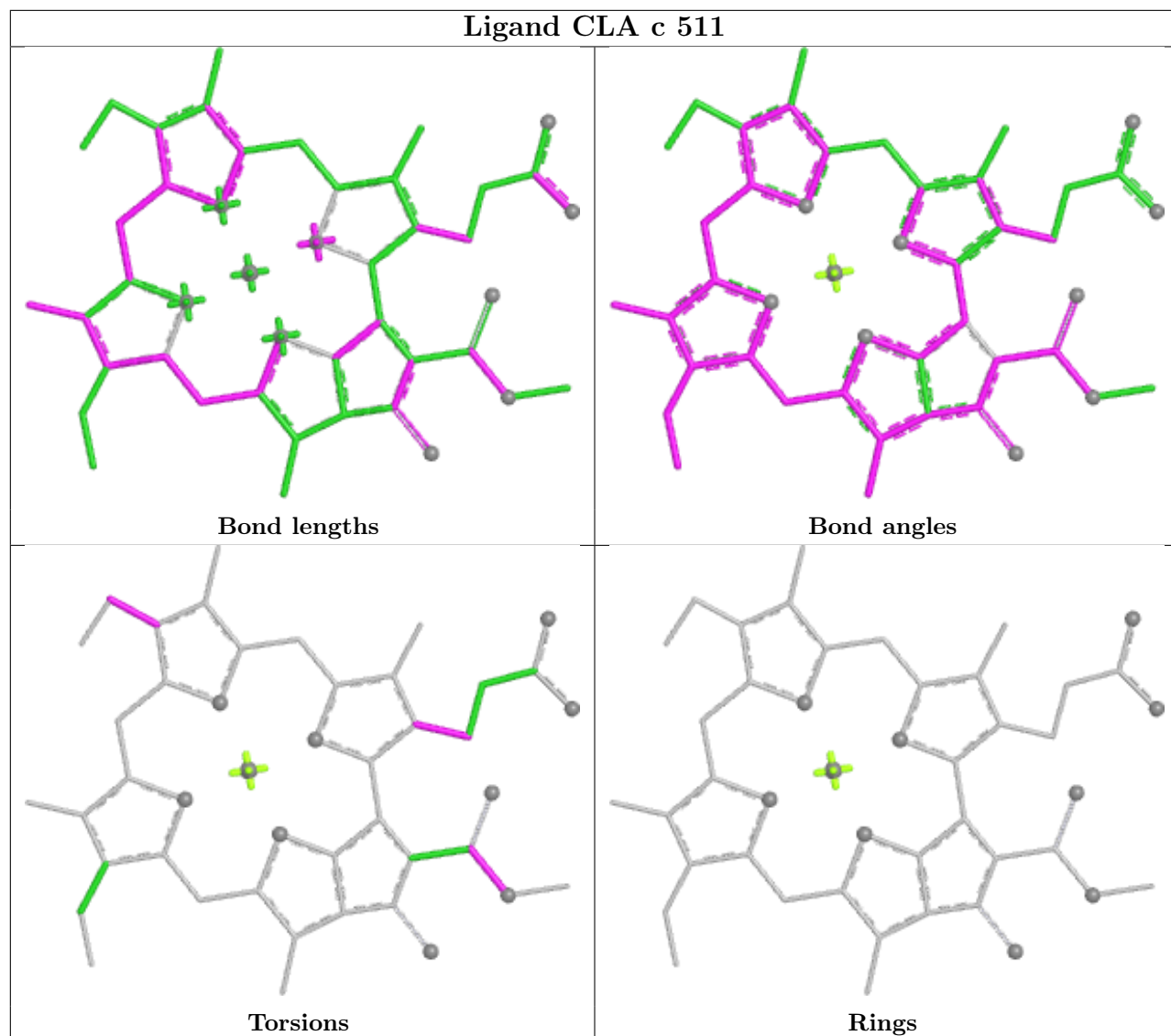
Ligand CHL 5 609



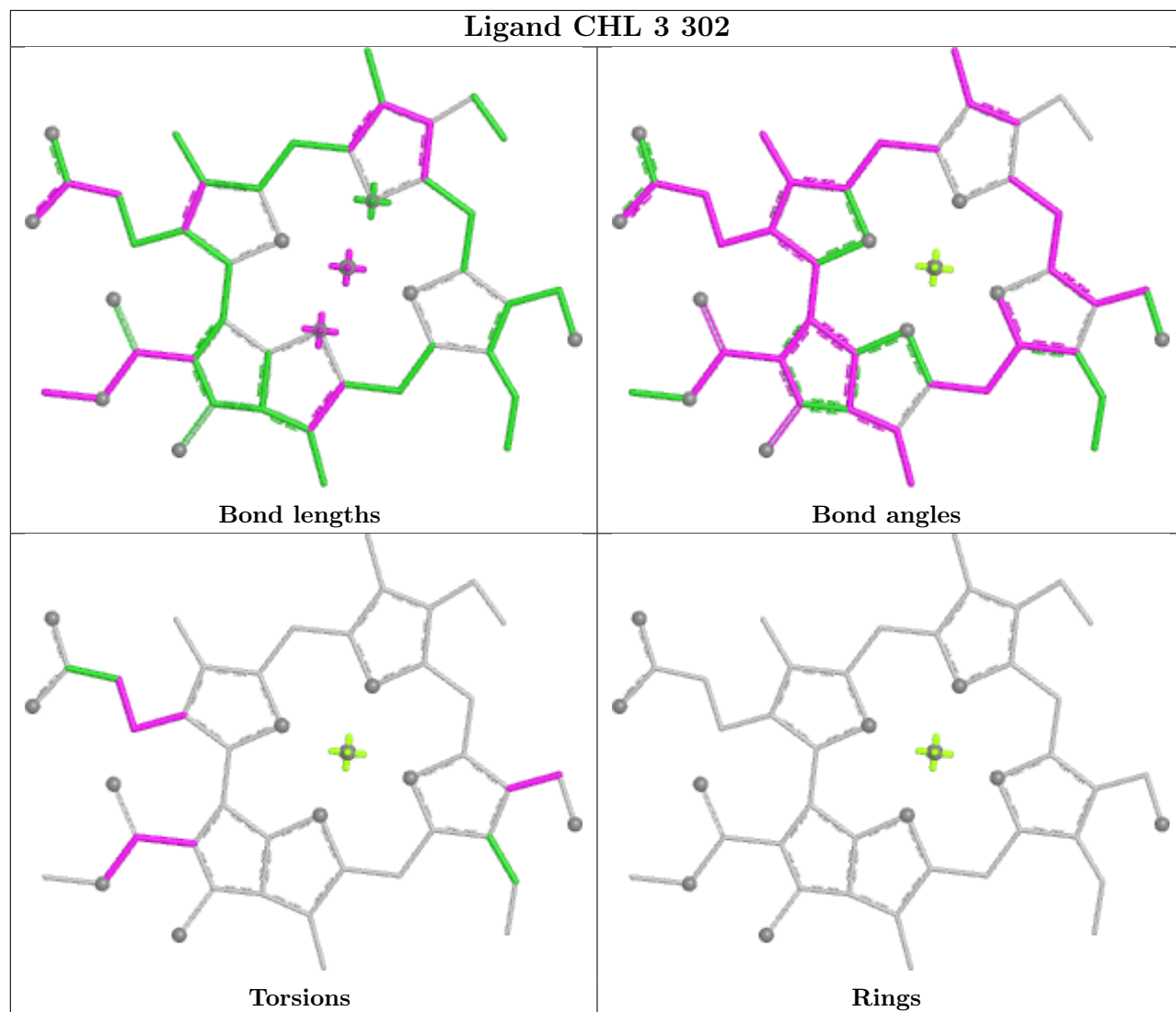
Ligand CLA c 507



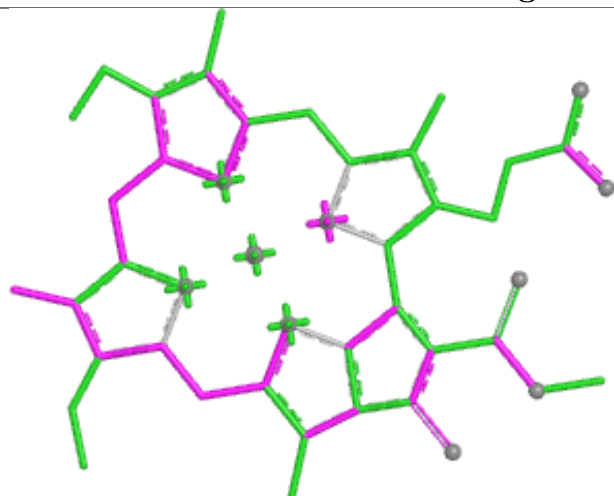
Ligand CLA c 511



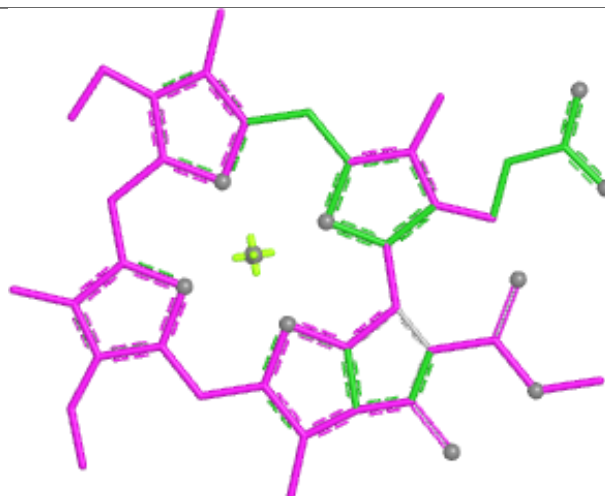
Ligand CHL 3 302



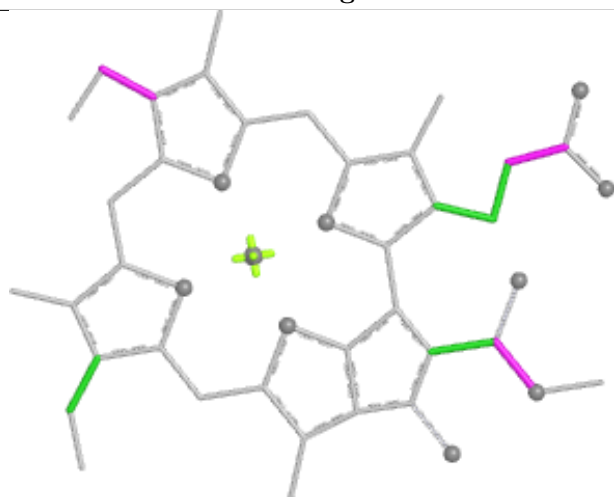
Ligand CLA 5 613



Bond lengths



Bond angles

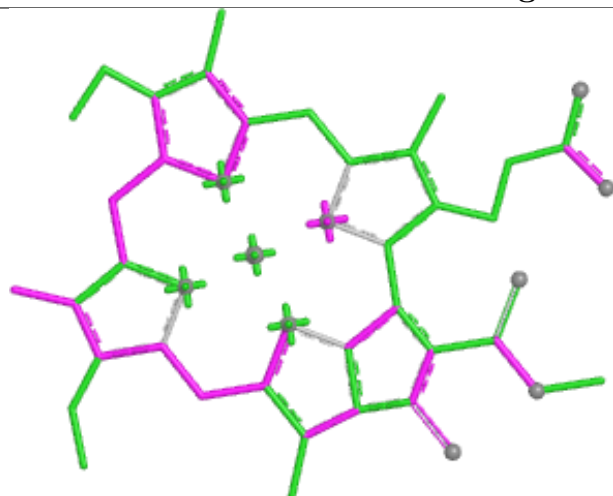


Torsions

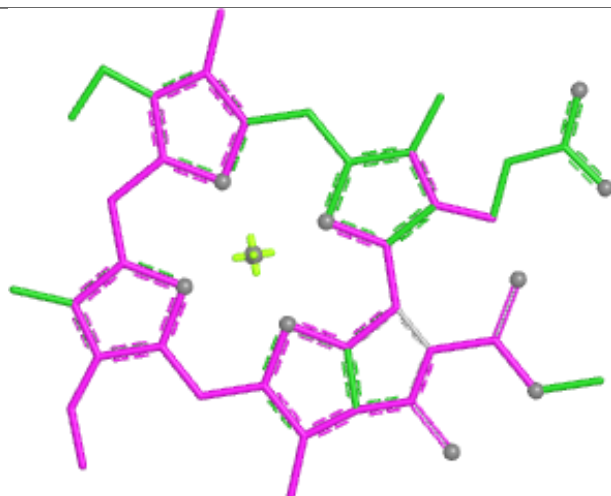


Rings

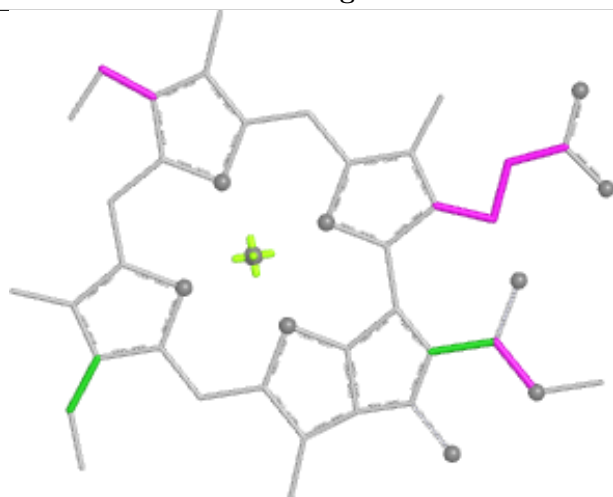
Ligand CLA 8 303



Bond lengths



Bond angles

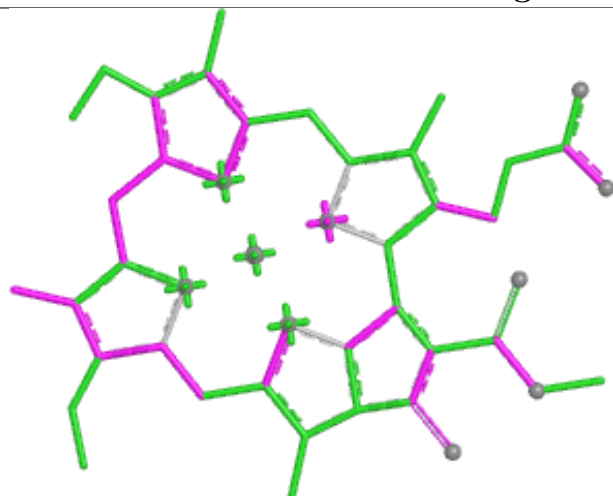


Torsions

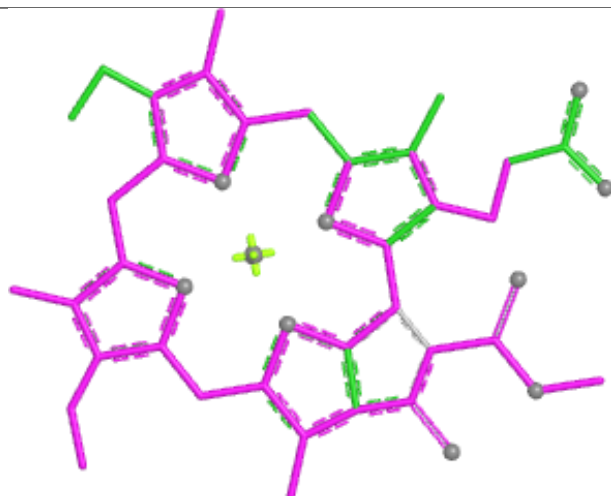


Rings

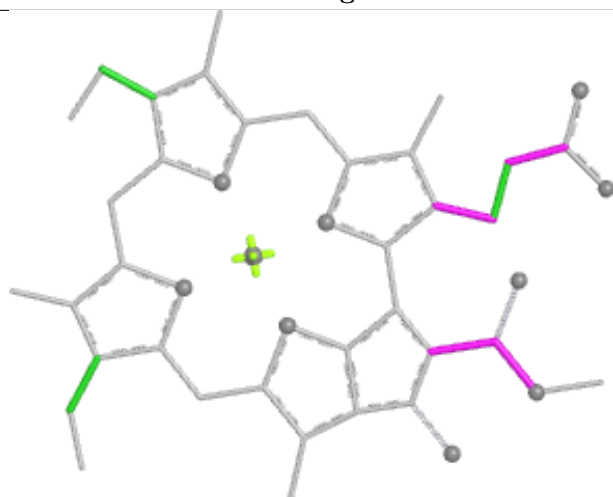
Ligand CLA A 403



Bond lengths



Bond angles

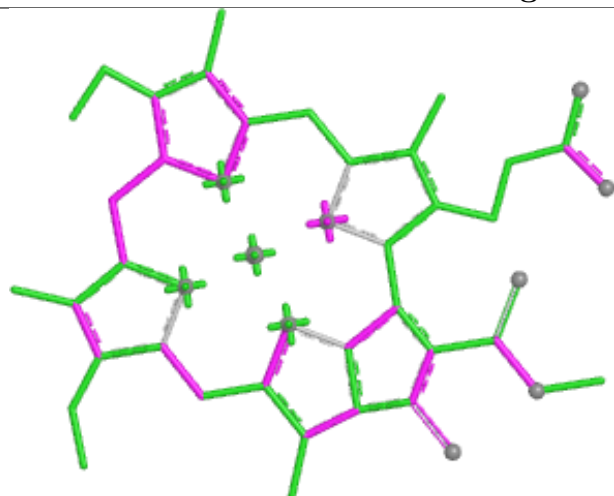


Torsions

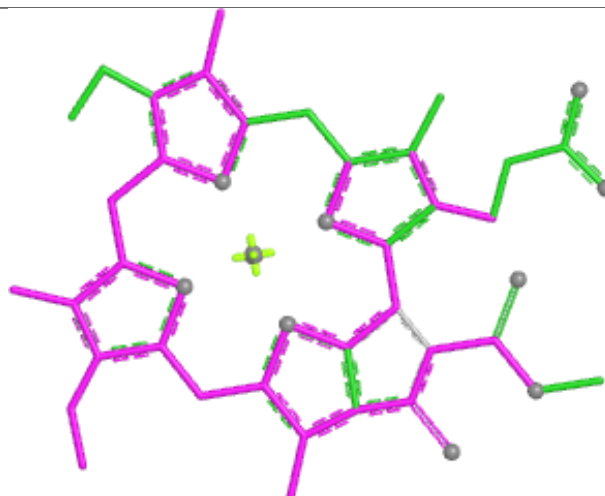


Rings

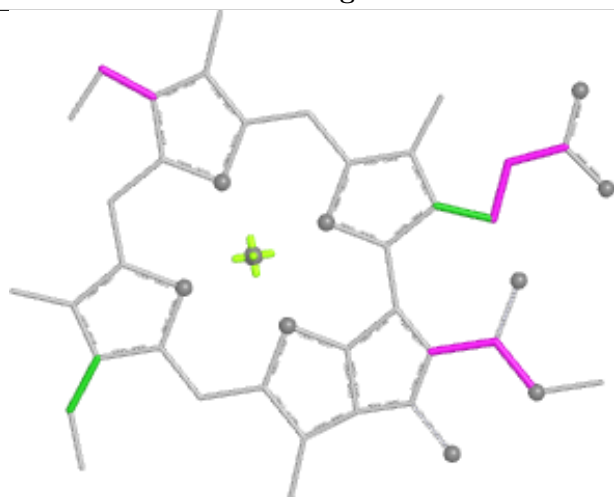
Ligand CLA s 304



Bond lengths



Bond angles

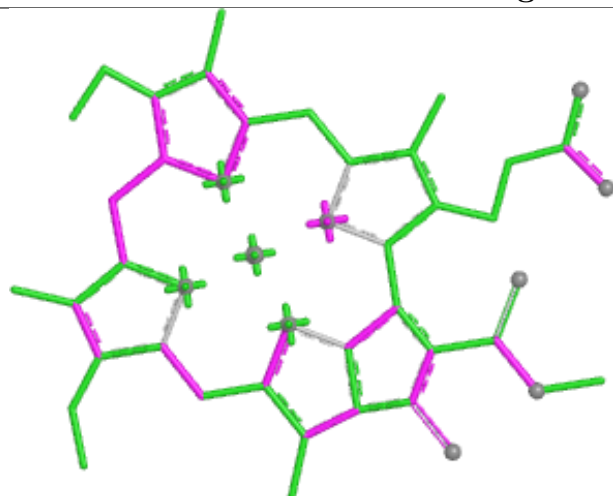


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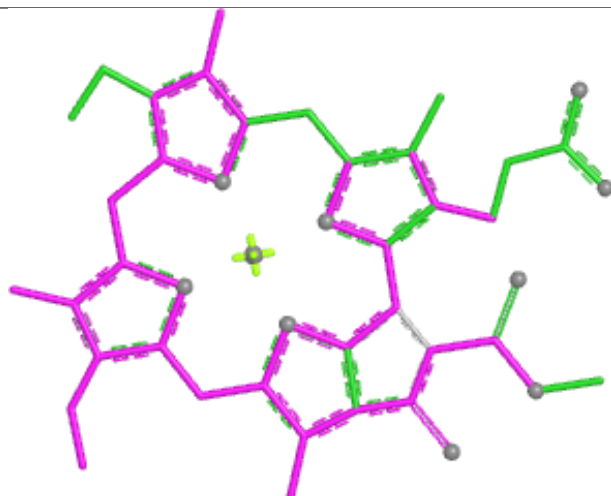


Rings

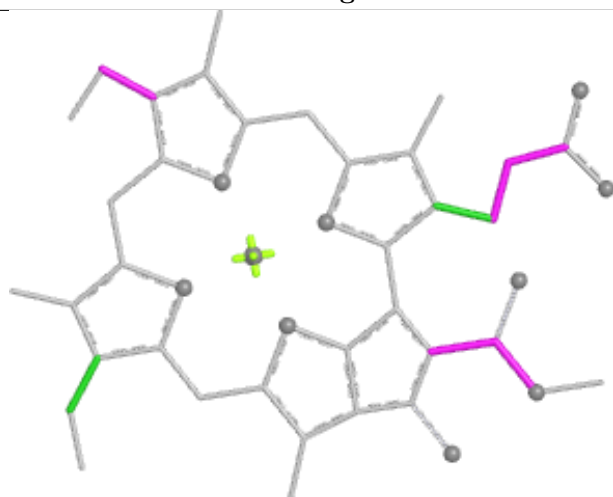
Ligand CLA S 304



Bond lengths



Bond angles

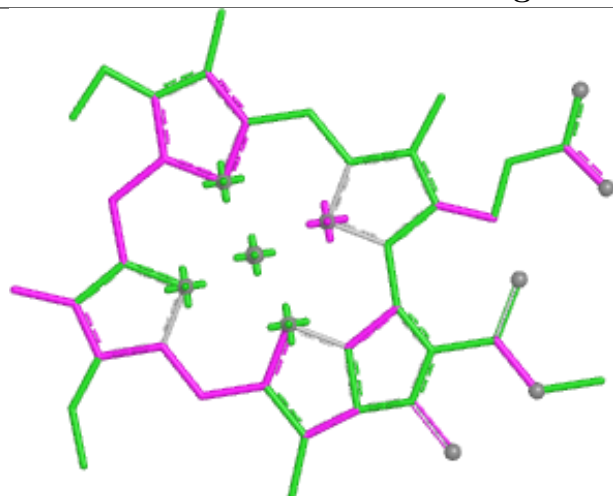


Torsions

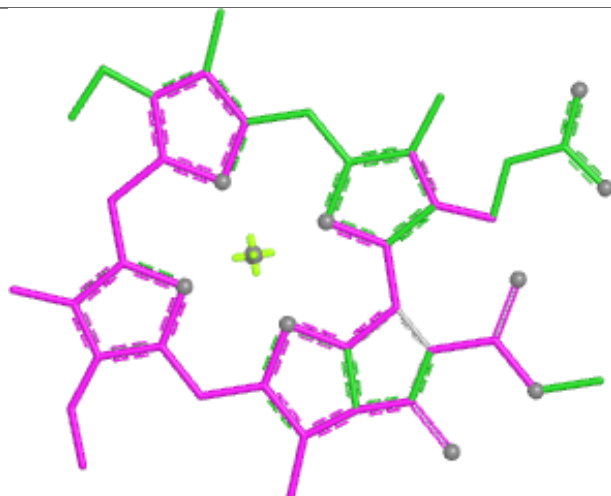


Rings

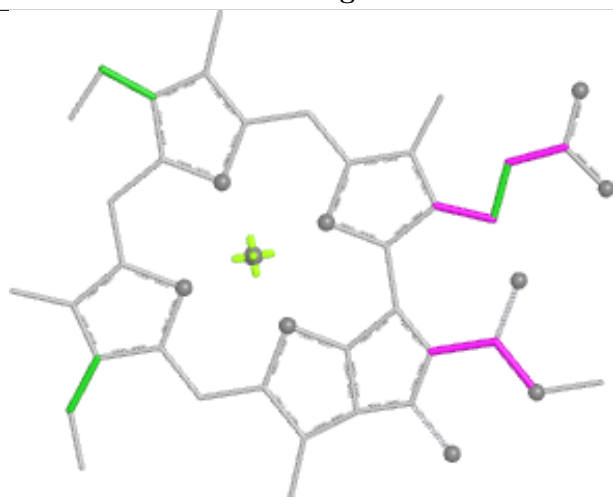
Ligand CLA N 614



Bond lengths



Bond angles

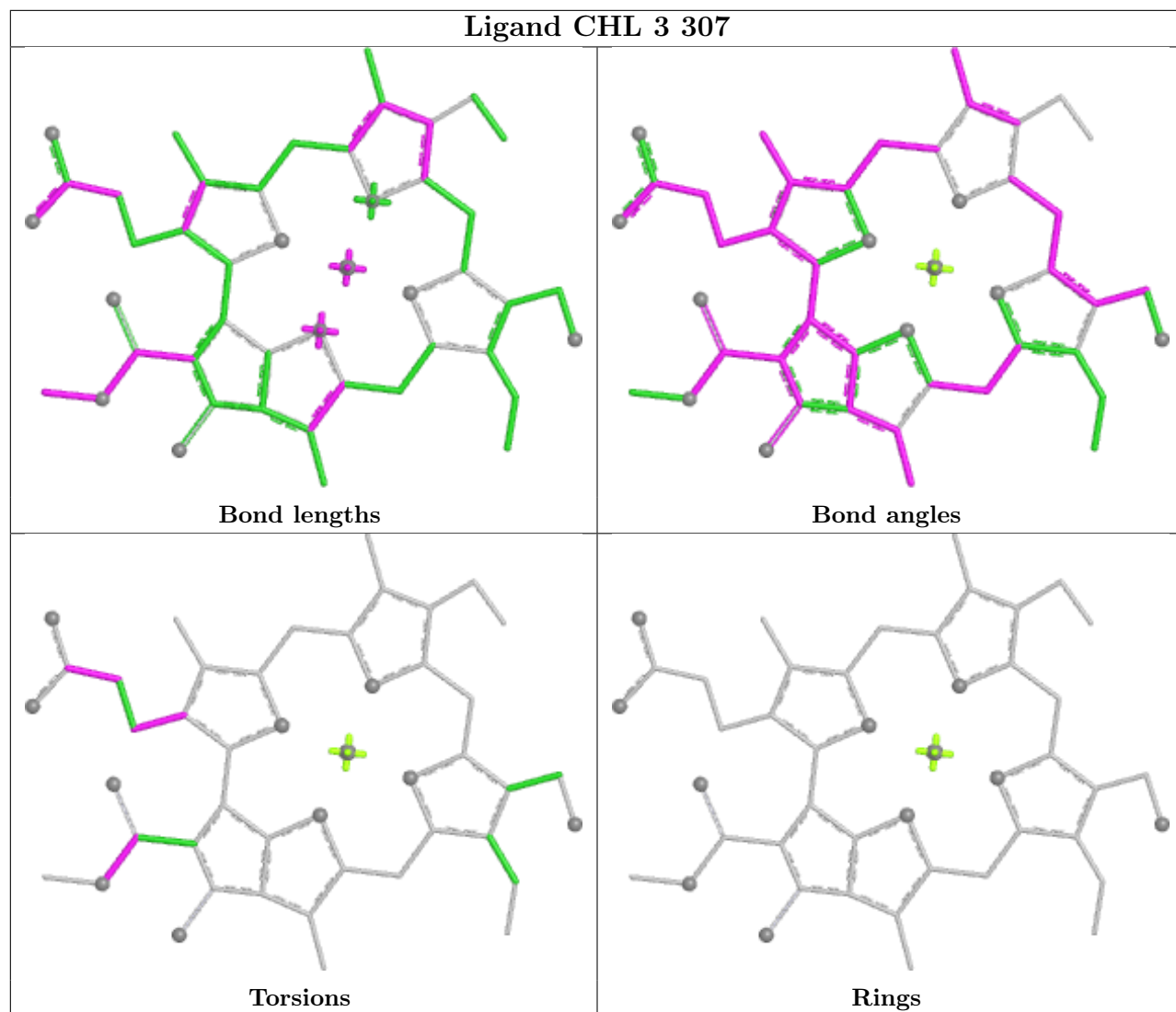


Torsions

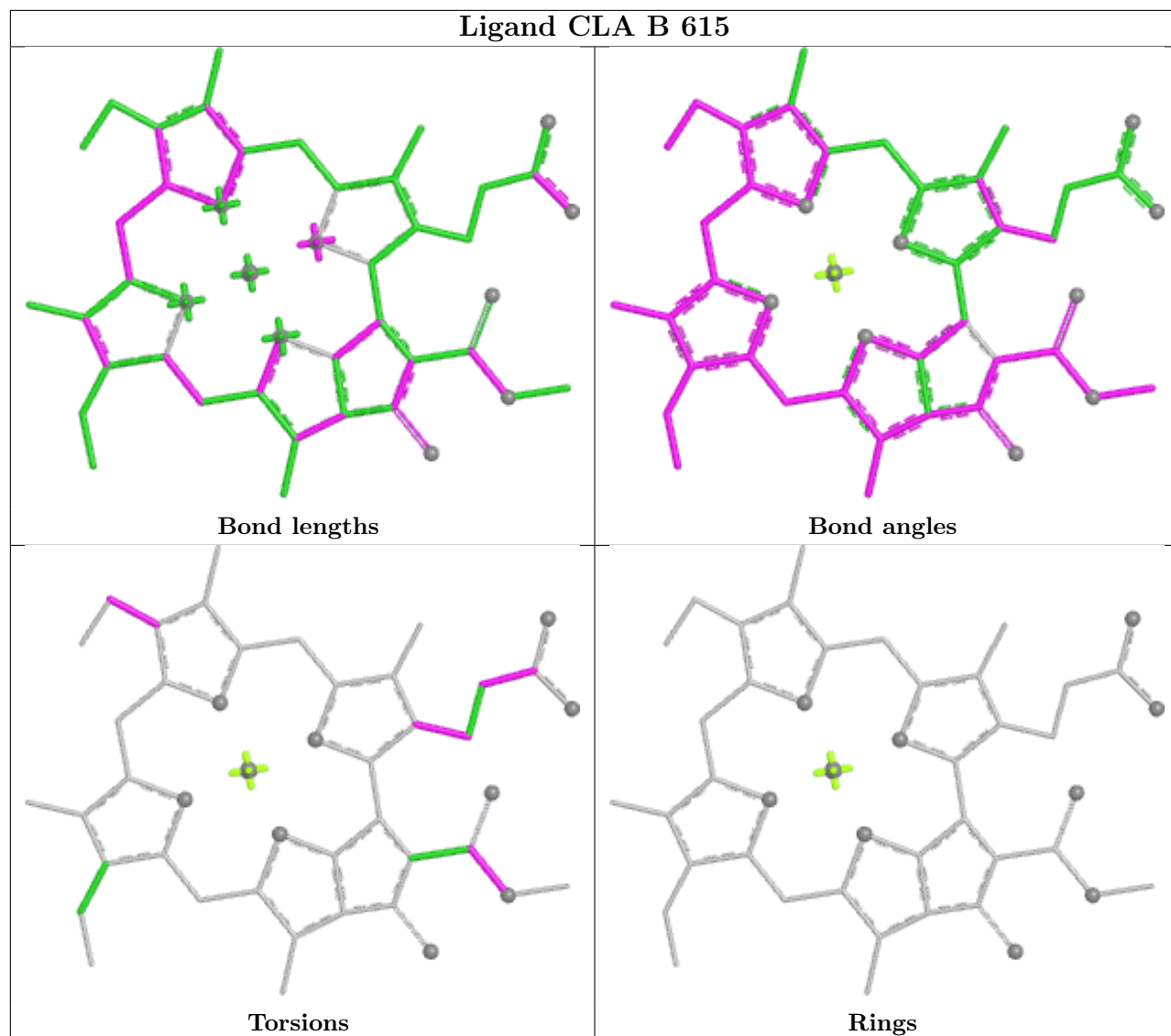


Rings

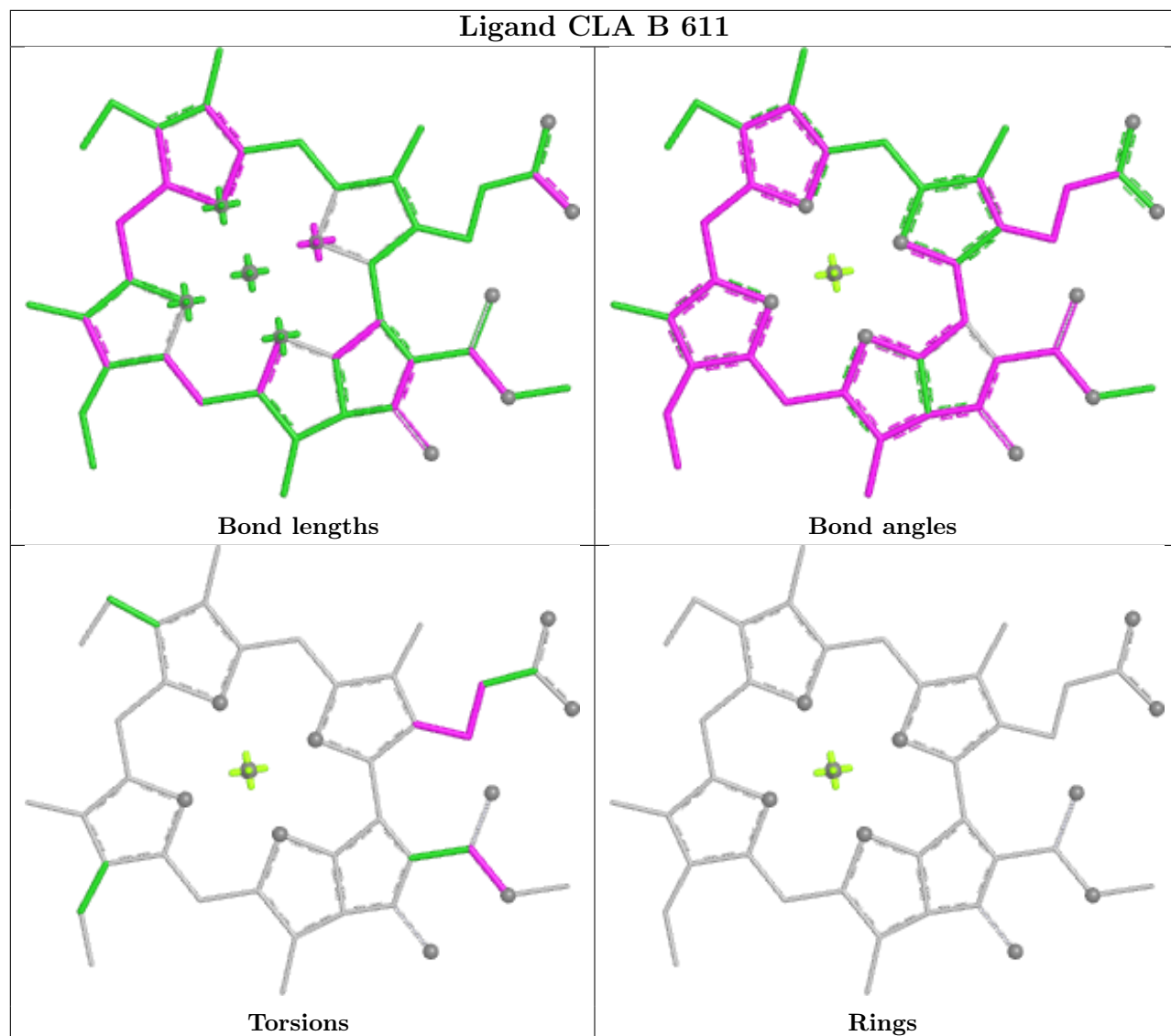
Ligand CHL 3 307



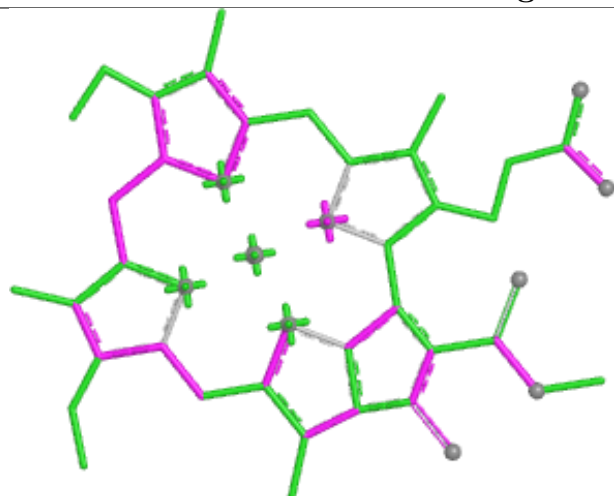
Ligand CLA B 615



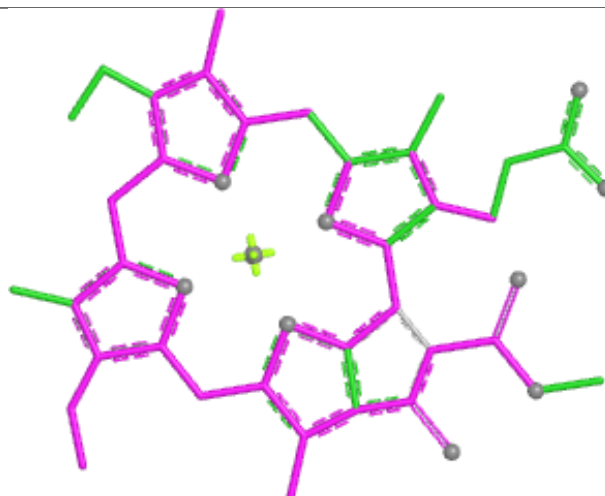
Ligand CLA B 611



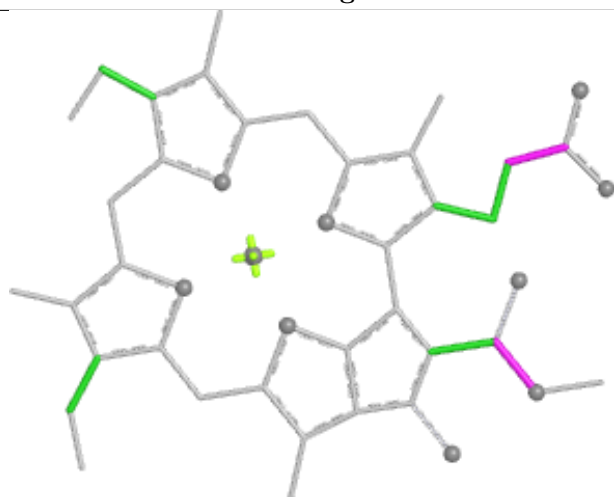
Ligand CLA b 608



Bond lengths



Bond angles

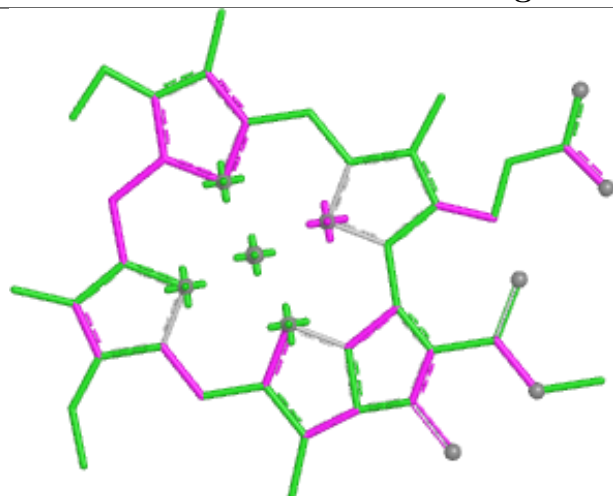


Torsions

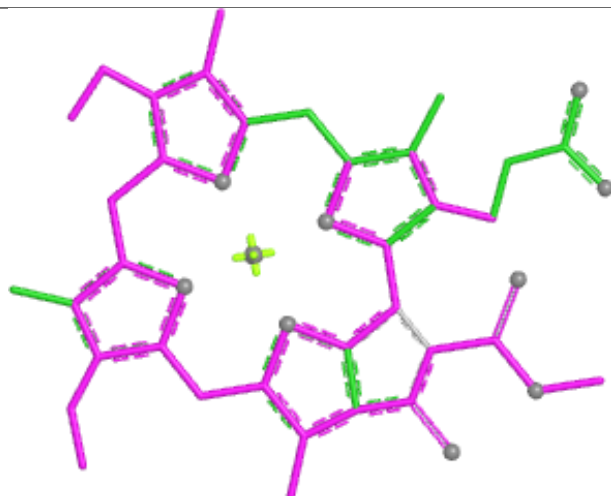


Rings

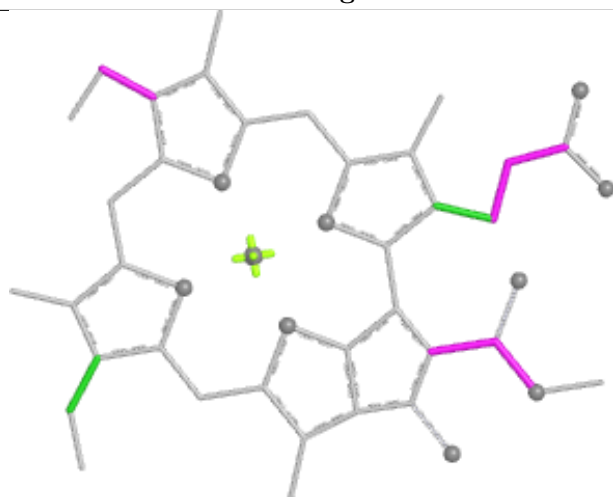
Ligand CLA C 502



Bond lengths



Bond angles

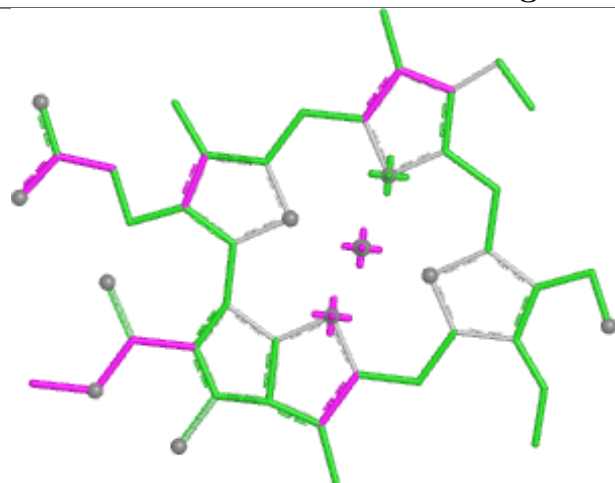


Torsions

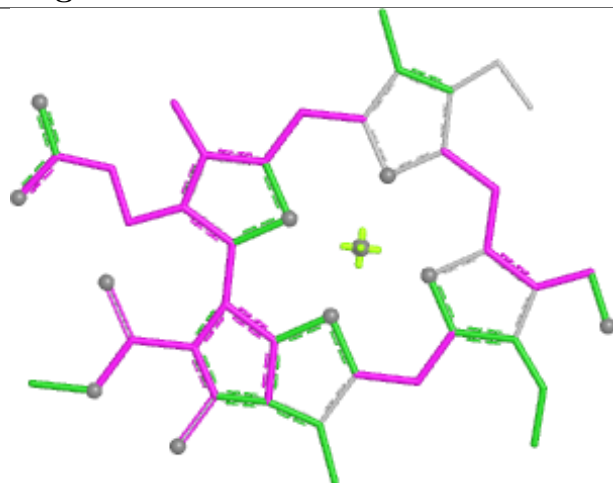


Rings

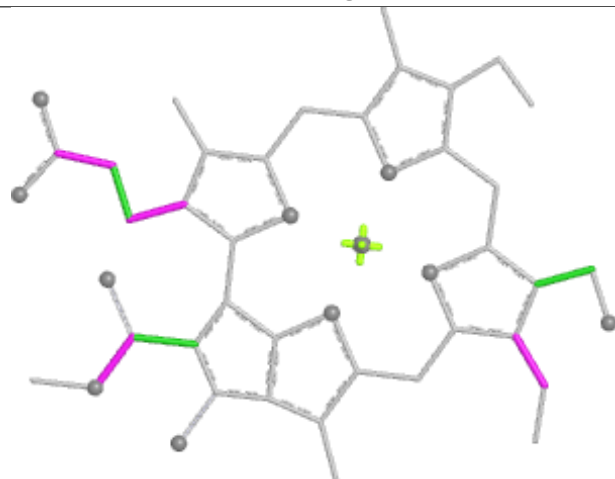
Ligand CHL g 606



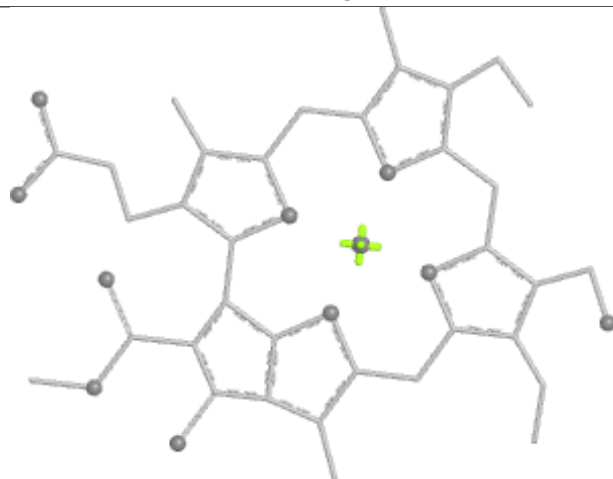
Bond lengths



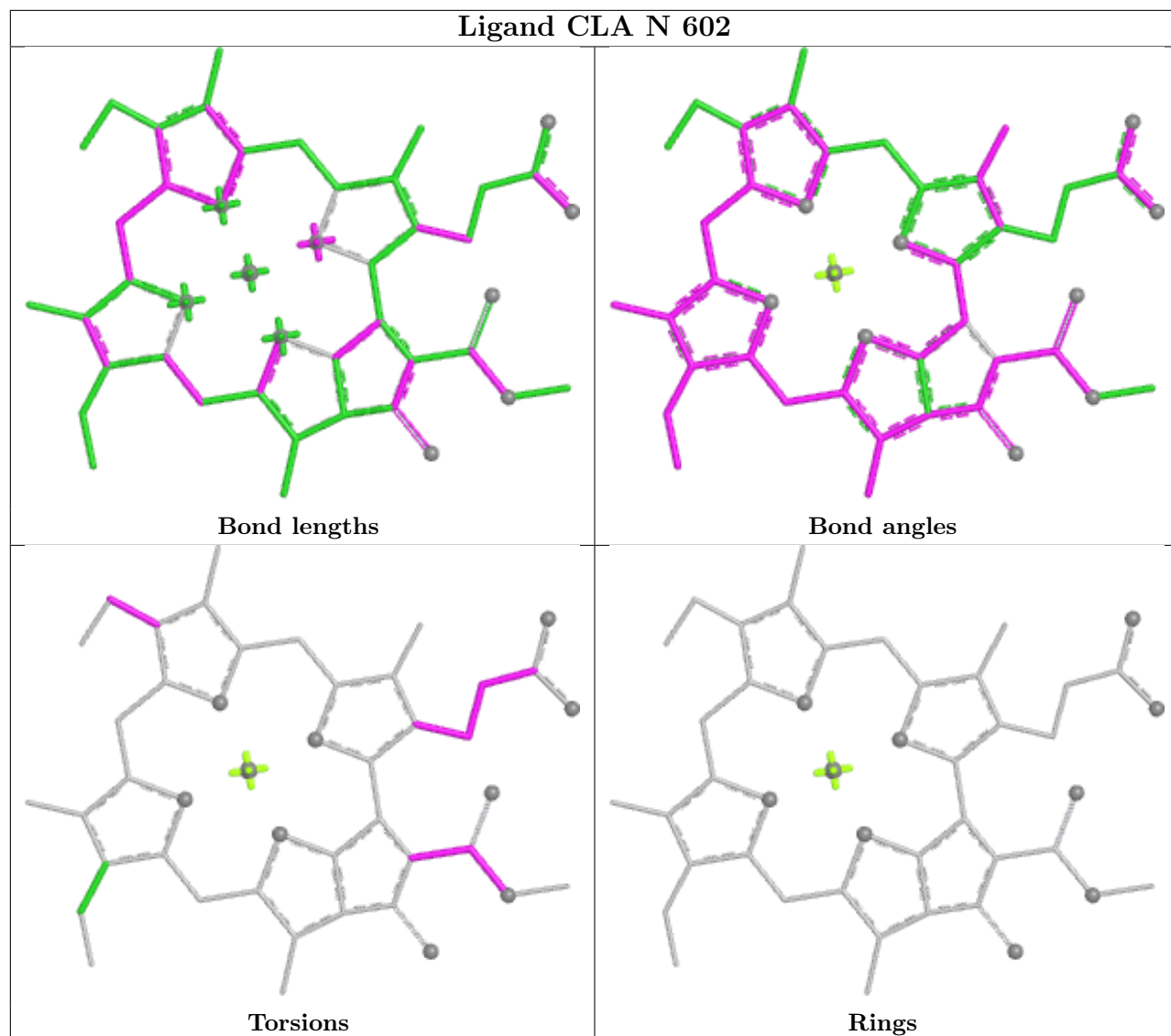
Bond angles

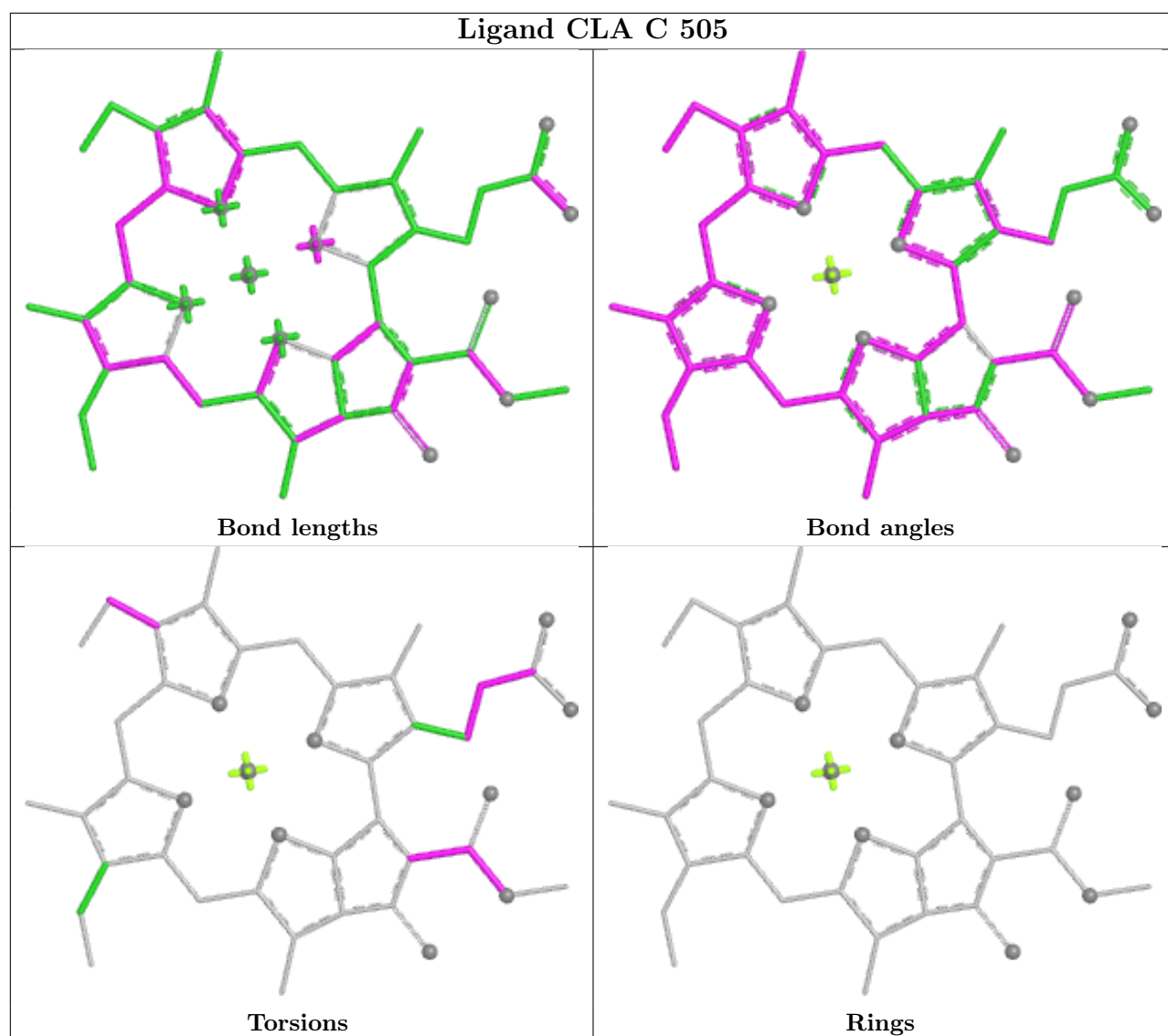


Torsions

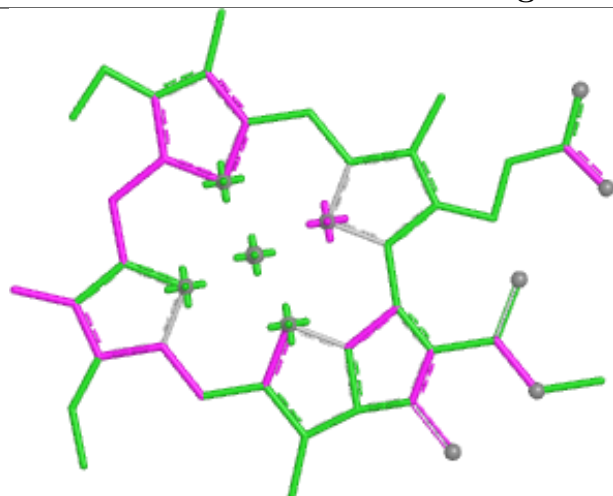


Rings

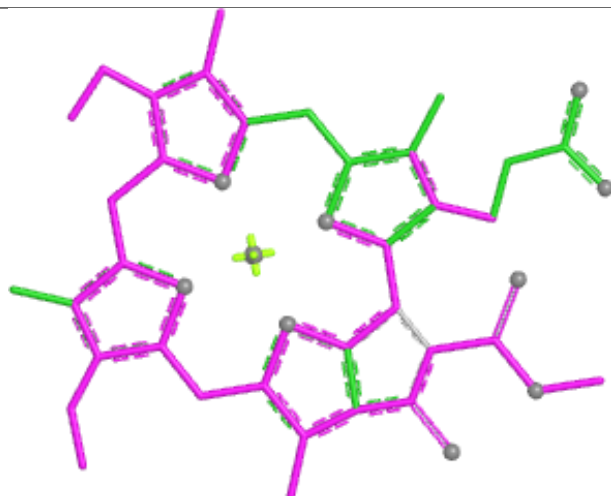




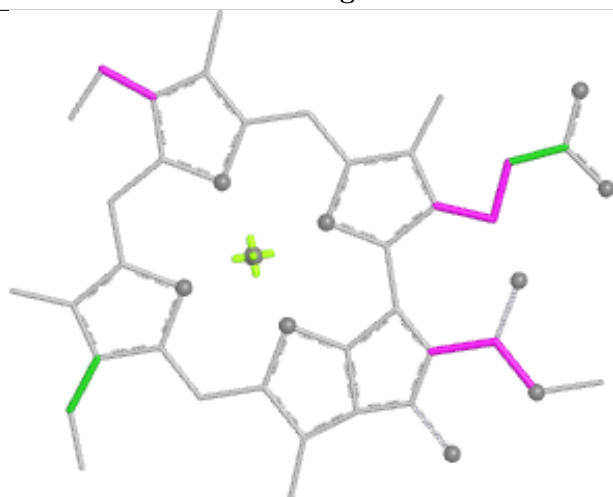
Ligand CLA b 607



Bond lengths



Bond angles

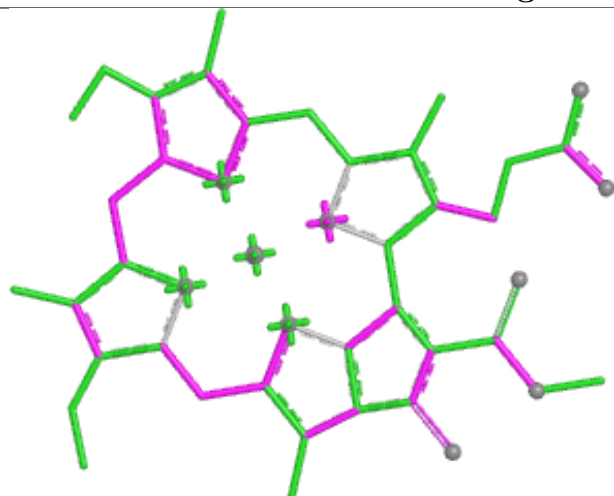


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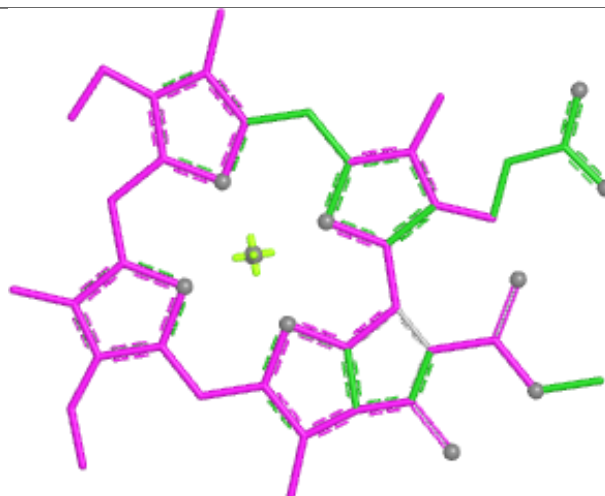


Rings

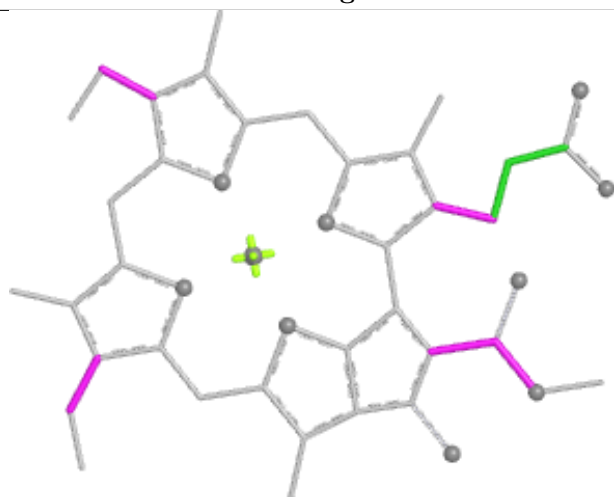
Ligand CLA b 604



Bond lengths



Bond angles

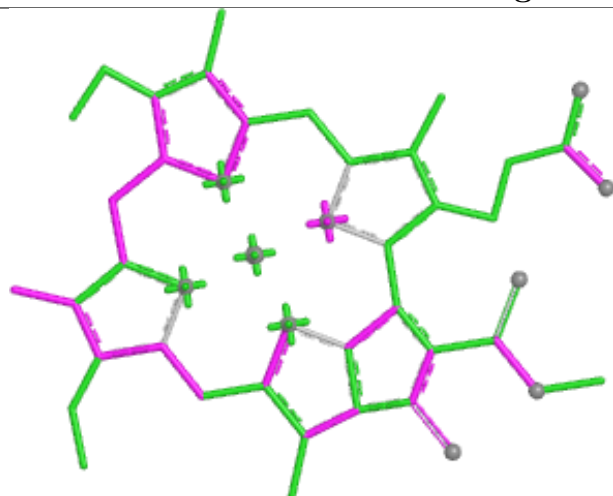


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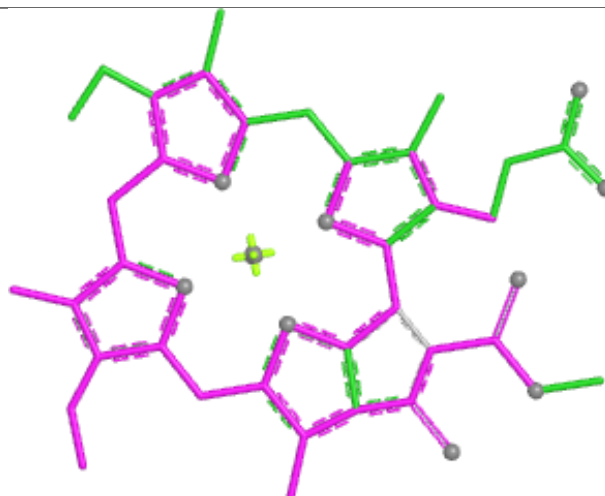


Rings

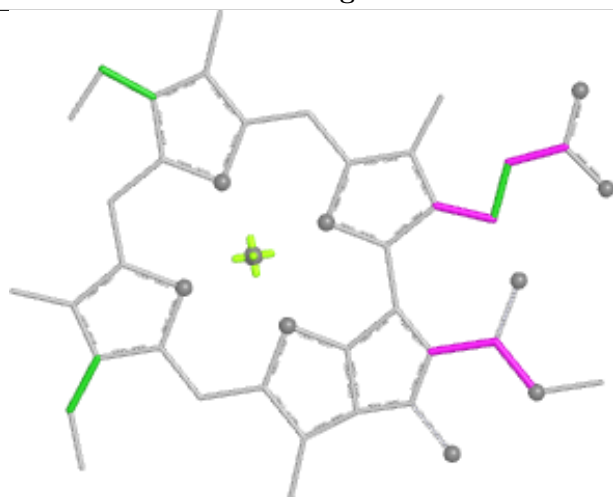
Ligand CLA C 509



Bond lengths



Bond angles

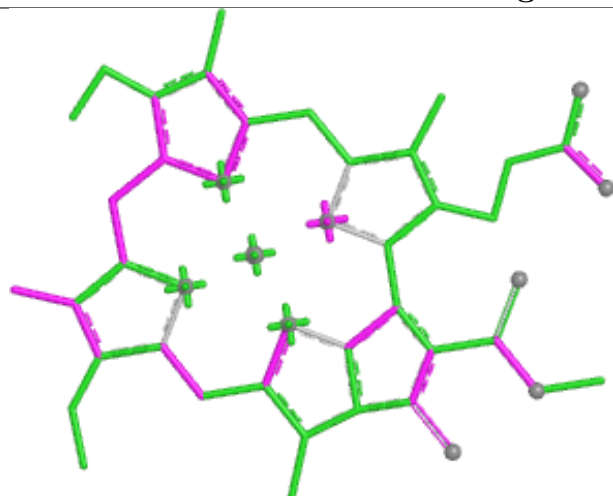


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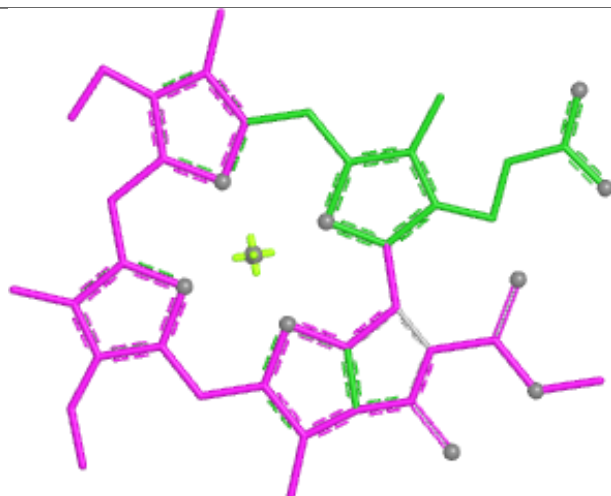


Rings

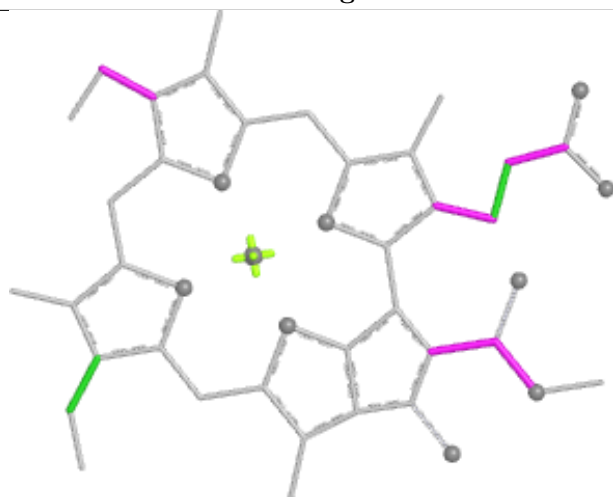
Ligand CLA n 612



Bond lengths



Bond angles

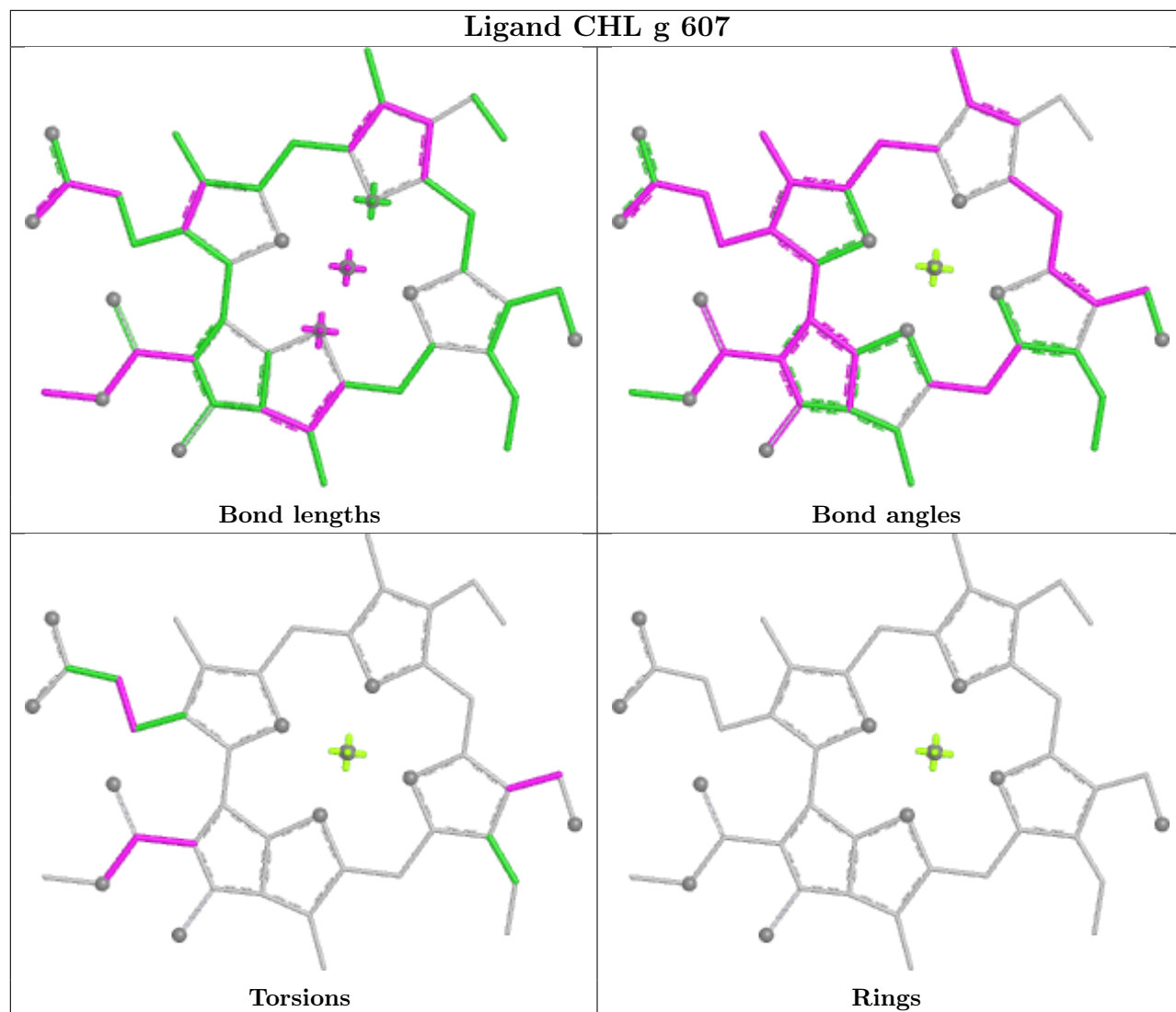


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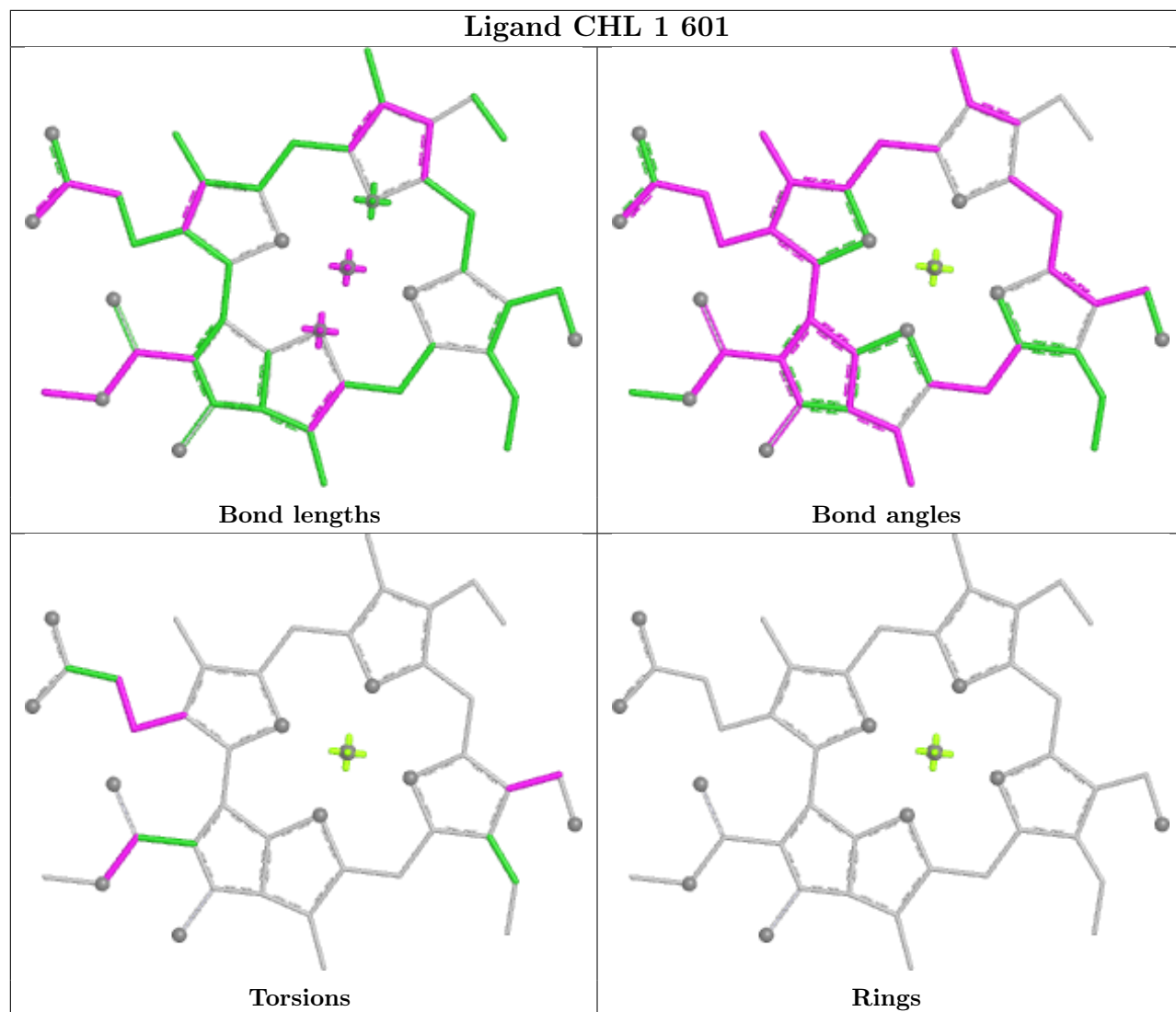


Rings

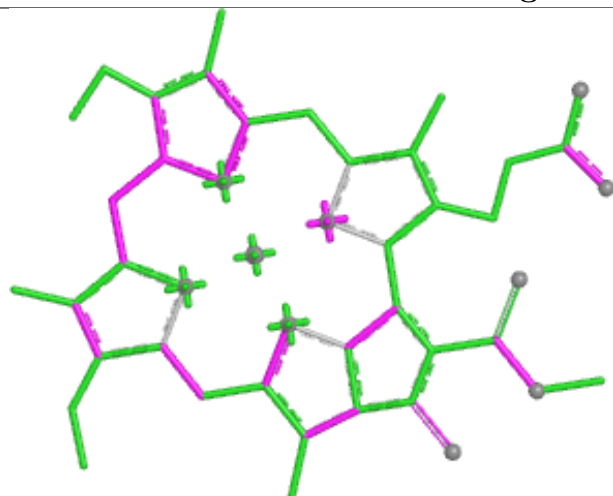
Ligand CHL g 607



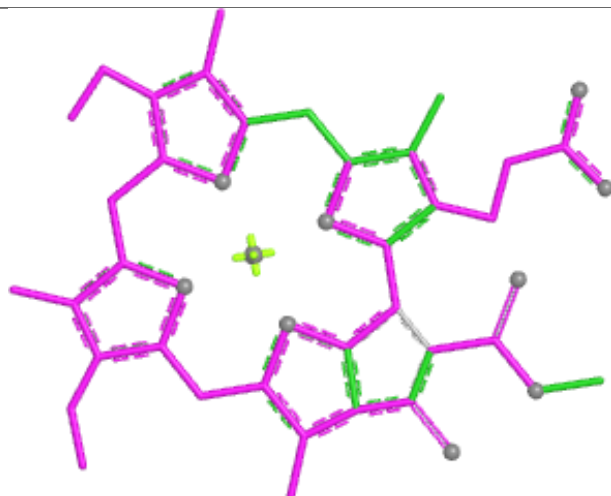
Ligand CHL 1 601



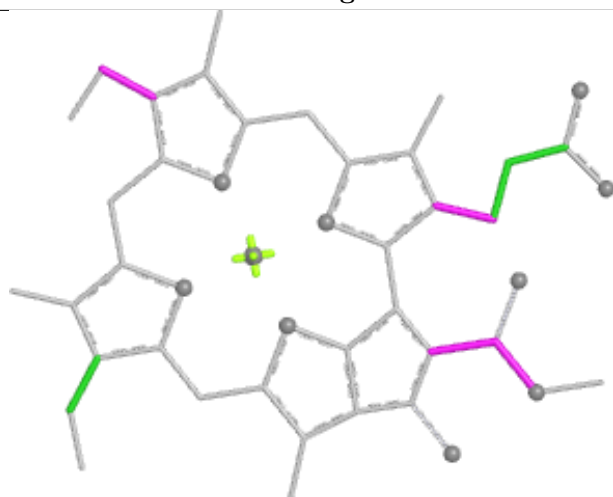
Ligand CLA r 303



Bond lengths



Bond angles

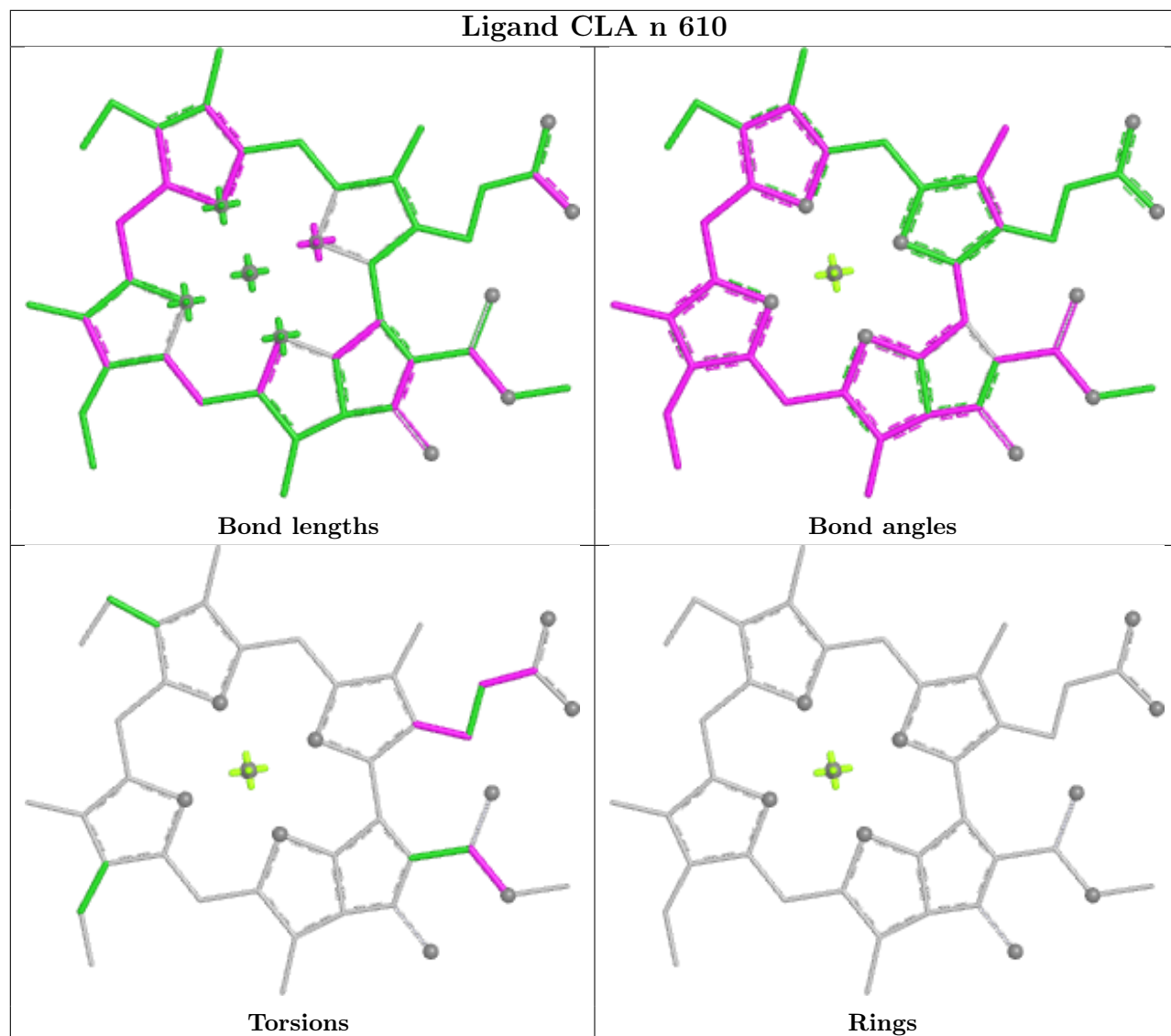


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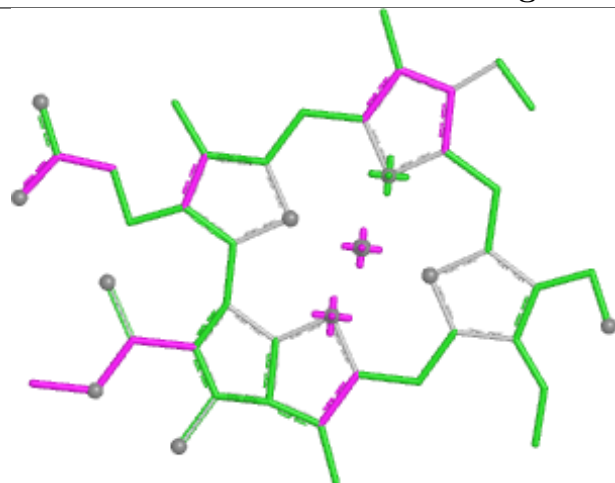


Rings

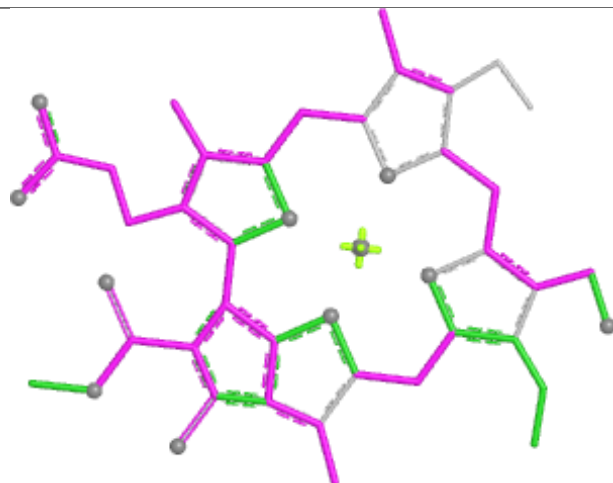
Ligand CLA n 610



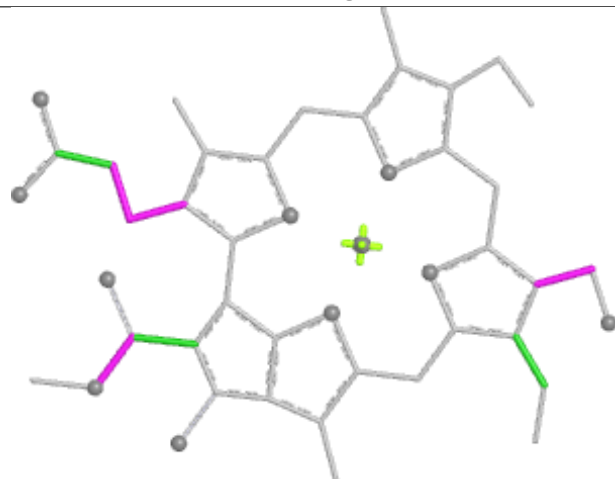
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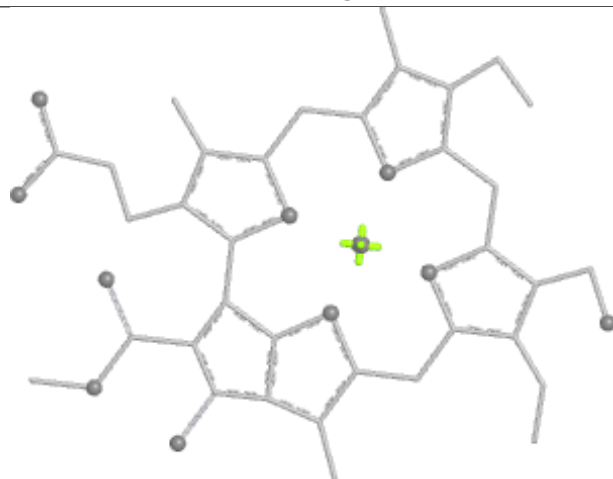
Bond lengths



Bond angles

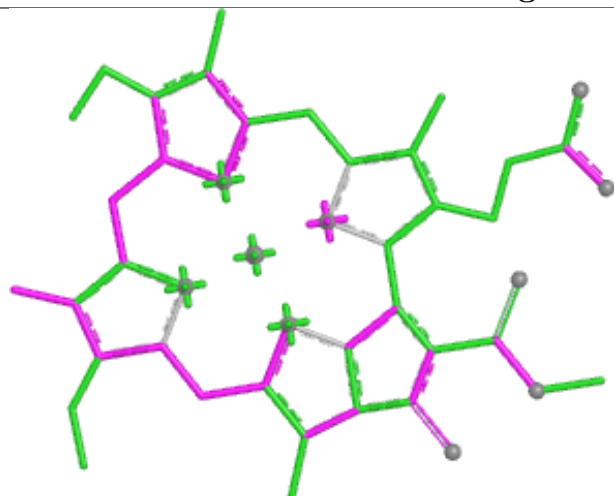


Torsions

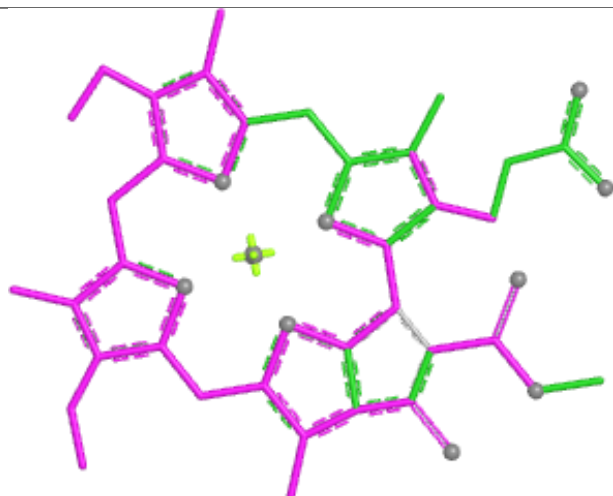


Rings

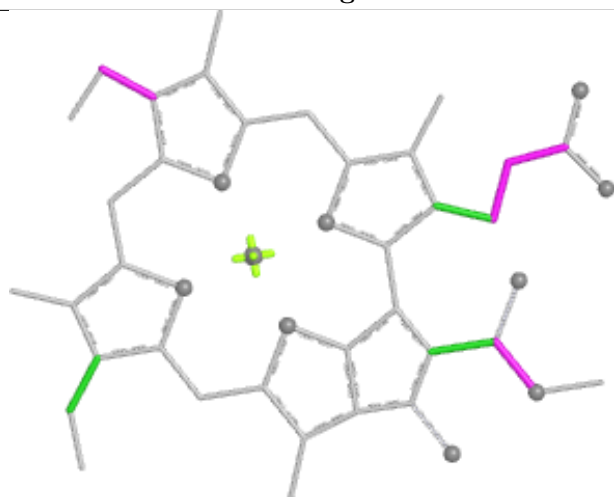
Ligand CLA 3 313



Bond lengths



Bond angles

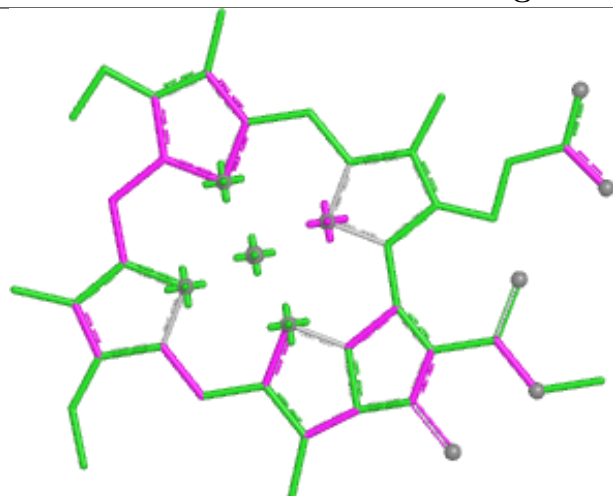


Torsions

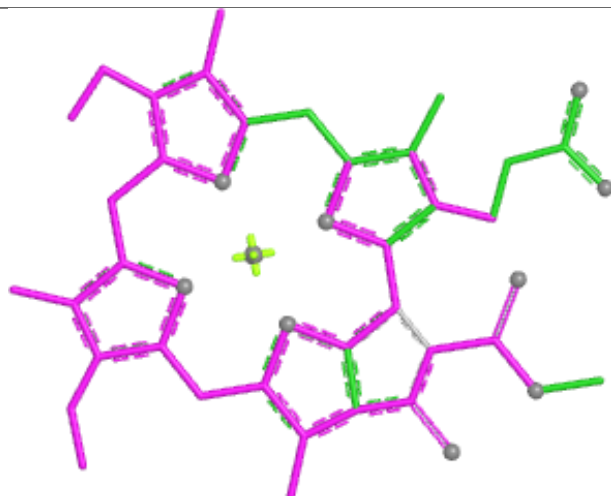


Rings

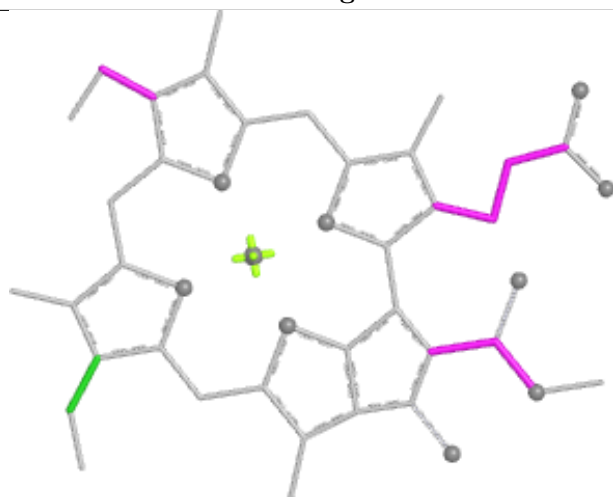
Ligand CLA Y 612



Bond lengths



Bond angles

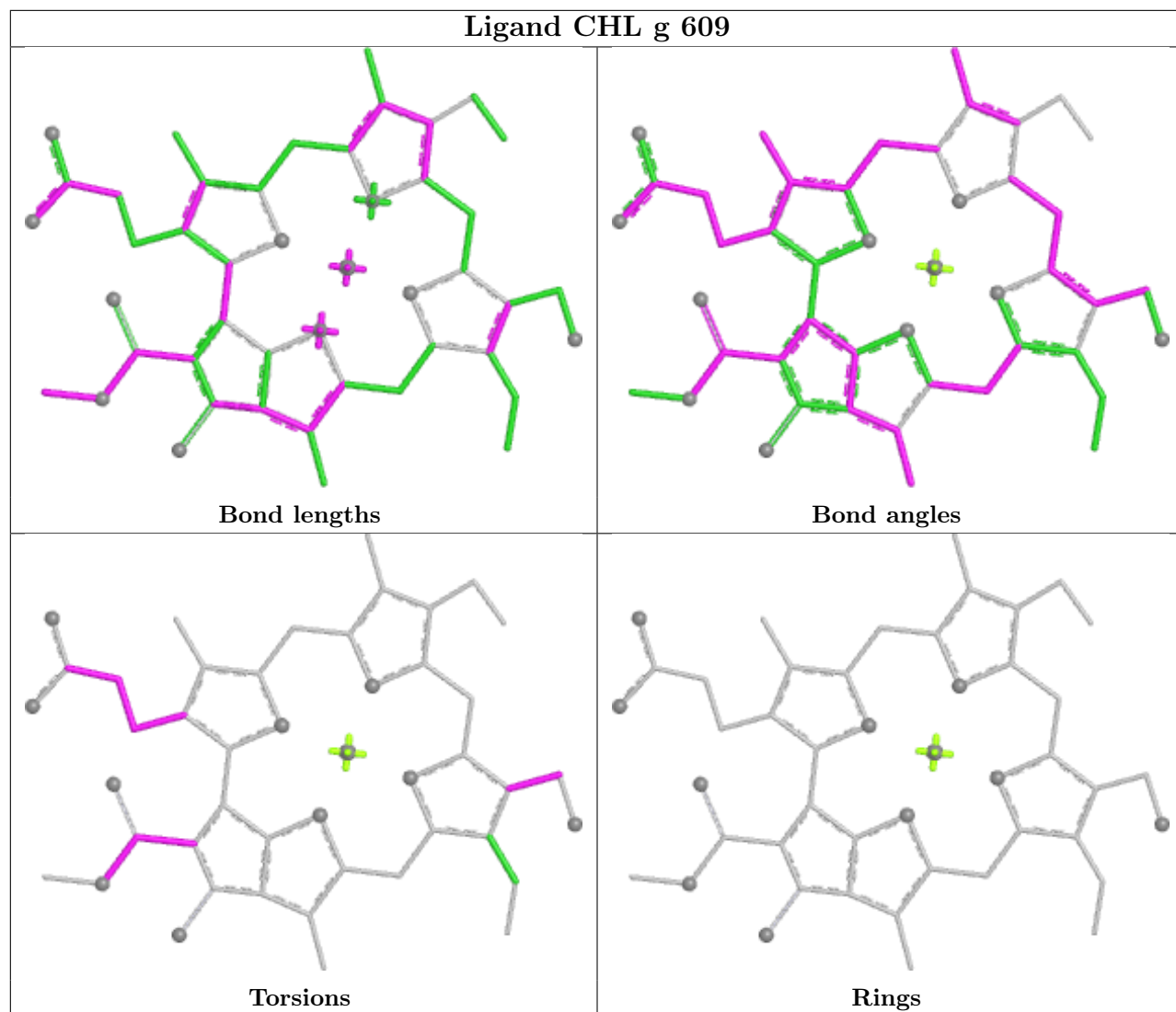


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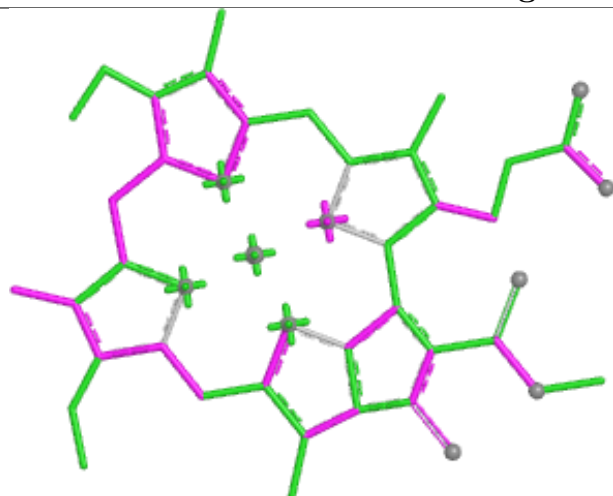


Rings

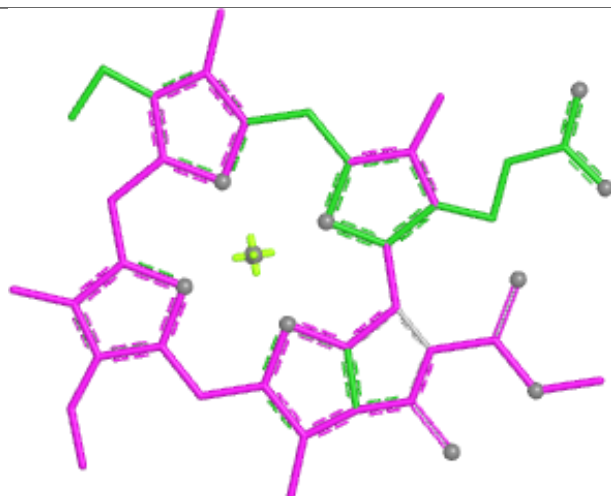
Ligand CHL g 609



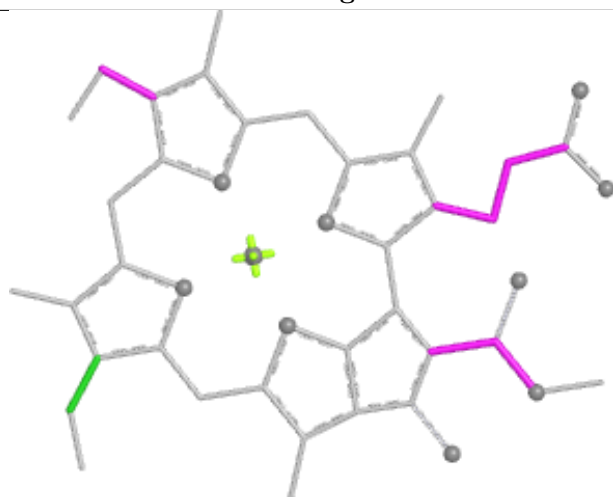
Ligand CLA 3 303



Bond lengths



Bond angles

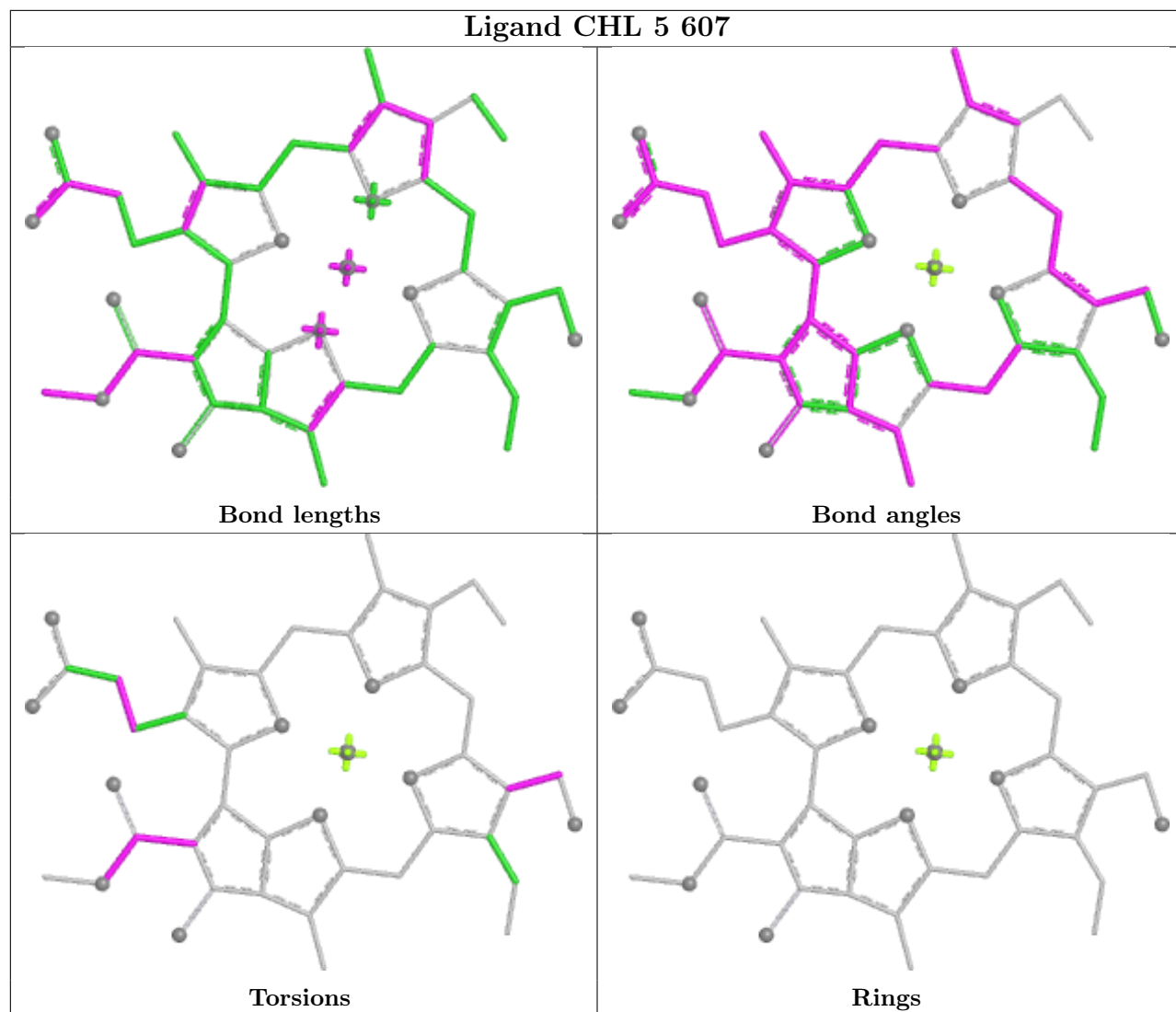


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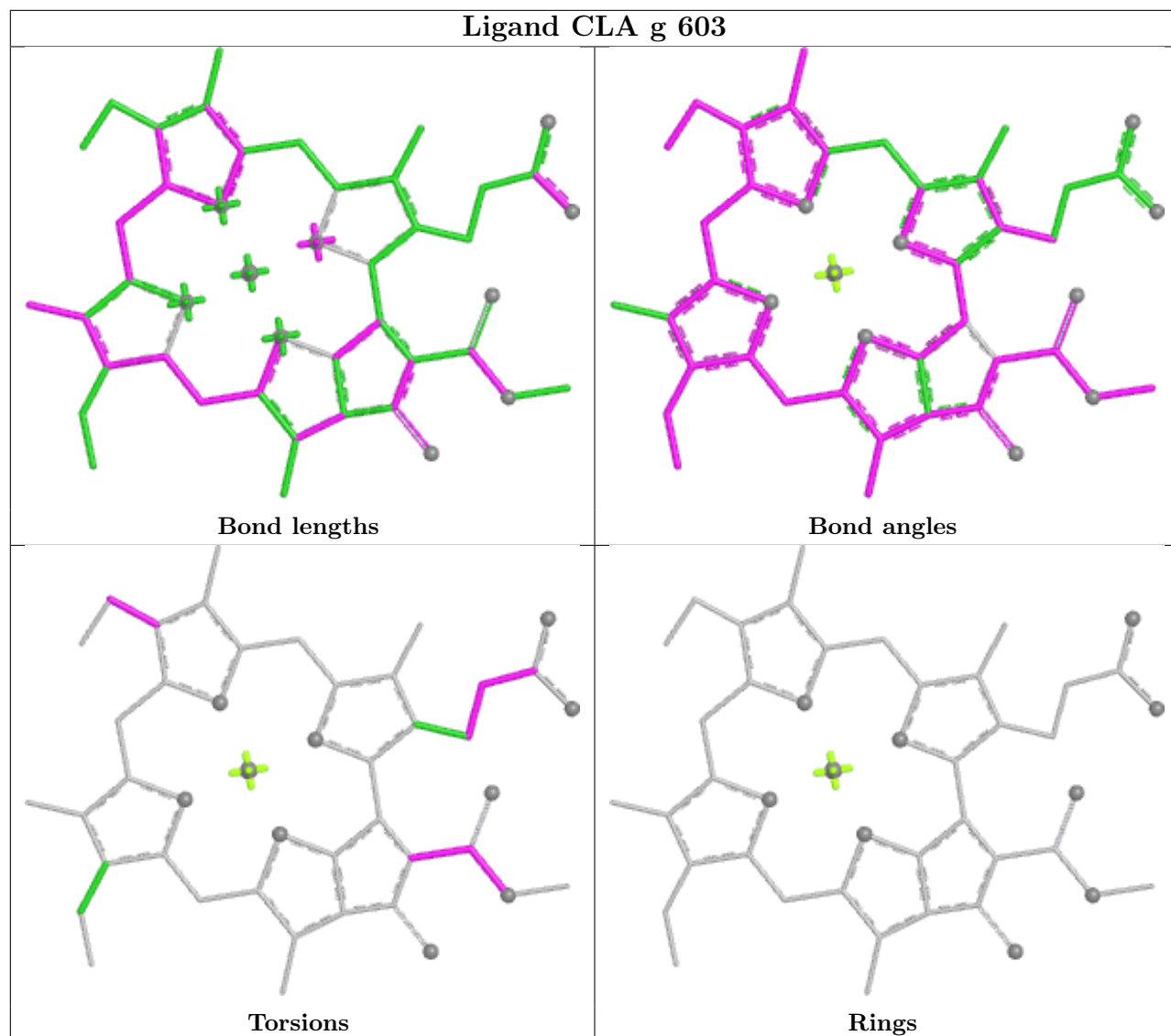


Rings

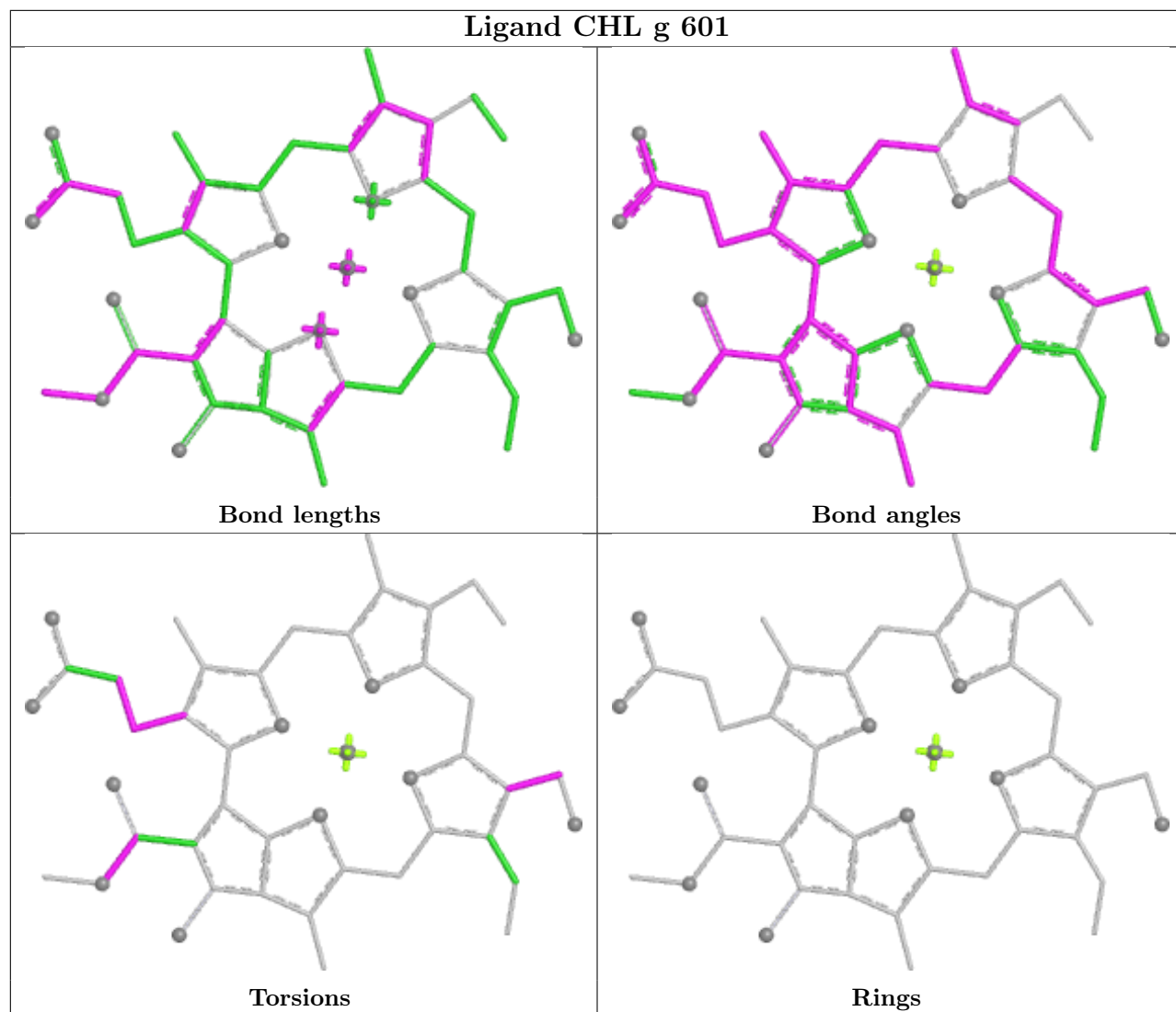
Ligand CHL 5 607



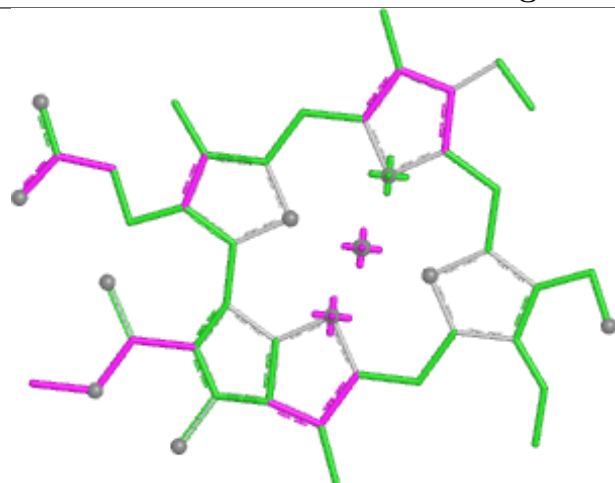
Ligand CLA g 603



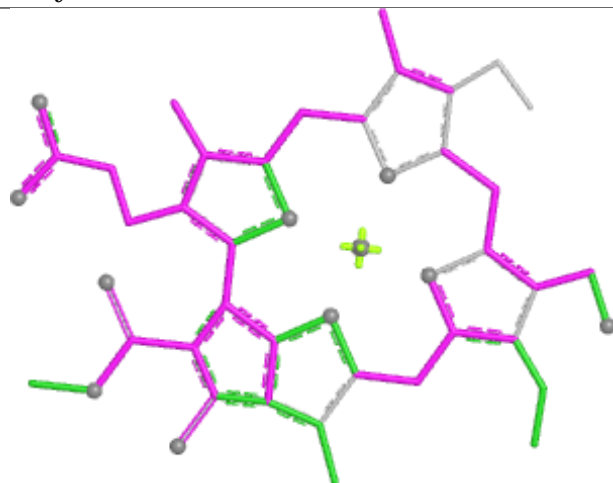
Ligand CHL g 601



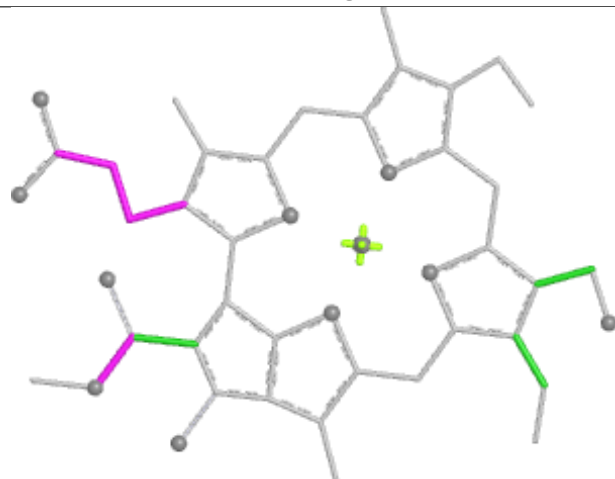
Ligand CHL y 606



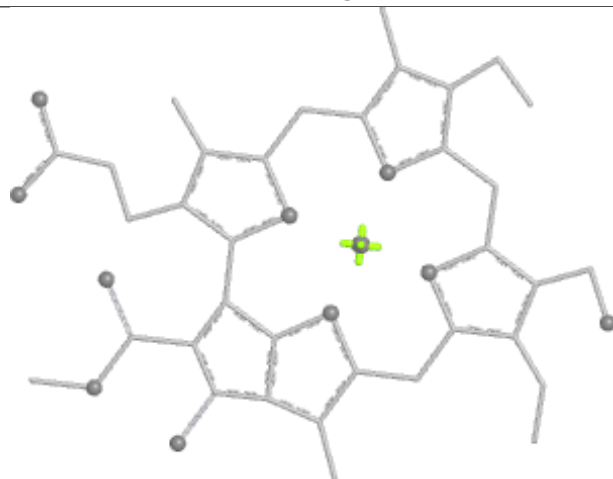
Bond lengths



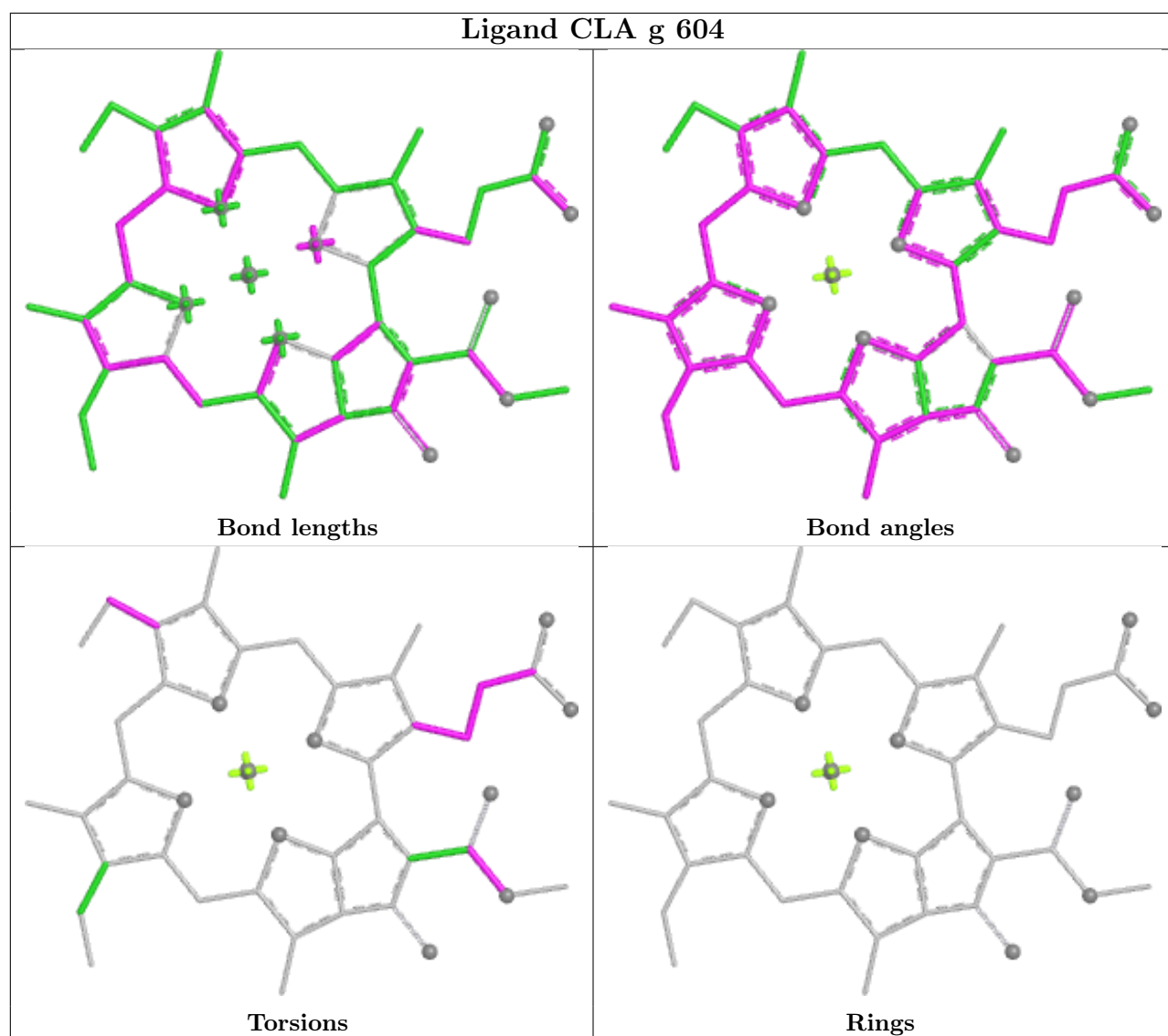
Bond angles



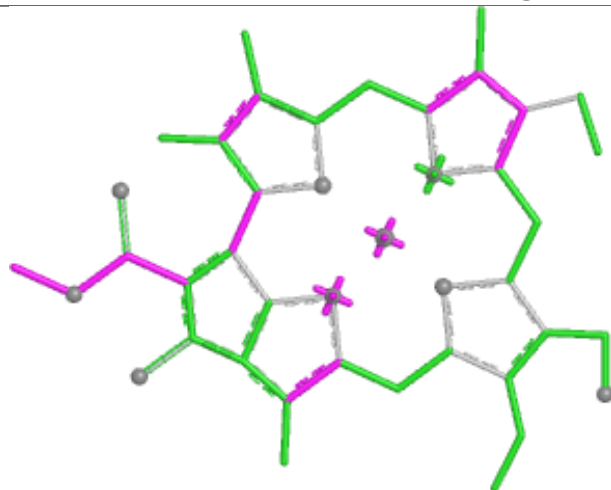
Torsions



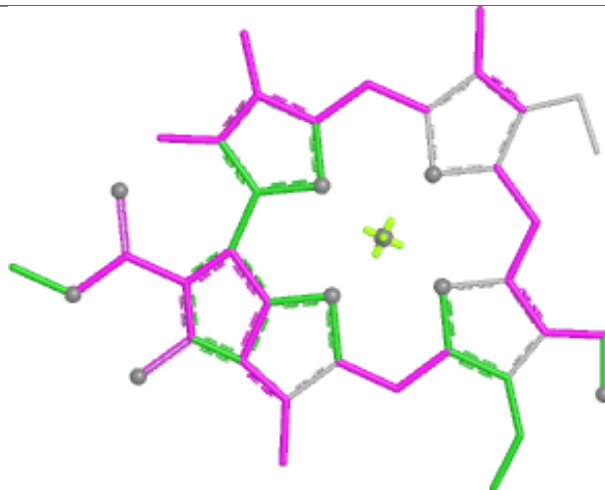
Rings



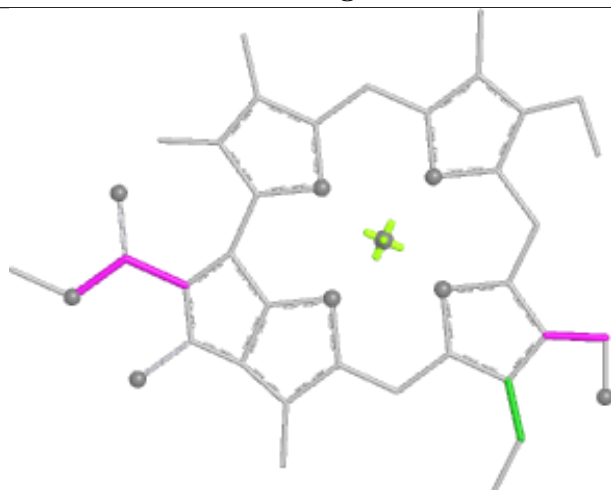
Ligand CHL 6 605



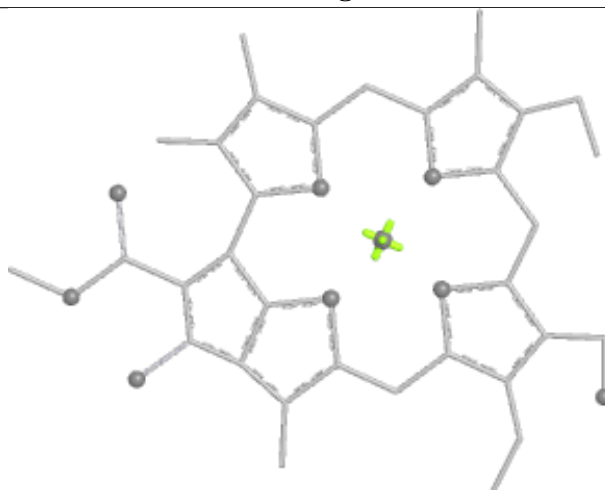
Bond lengths



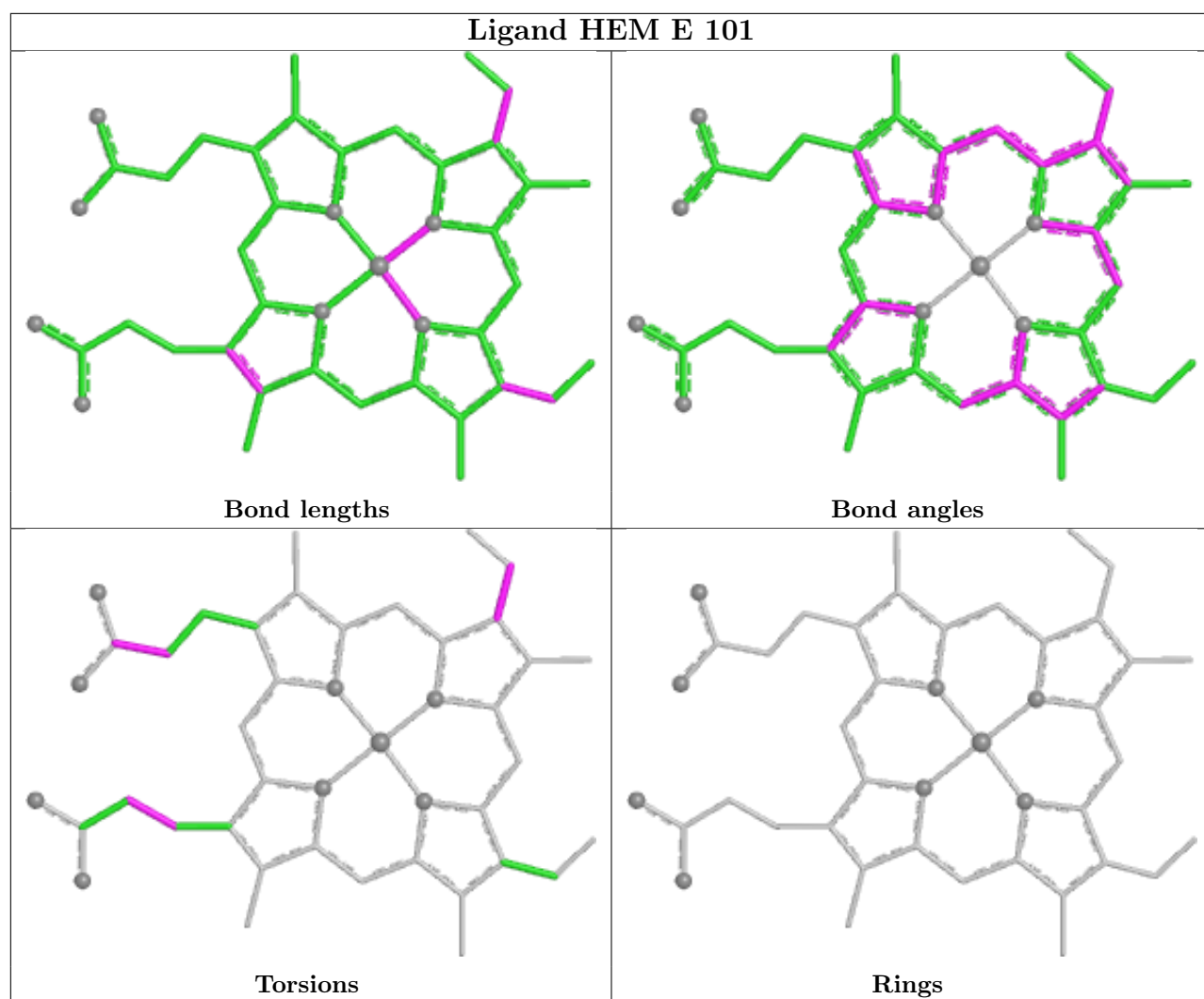
Bond angles



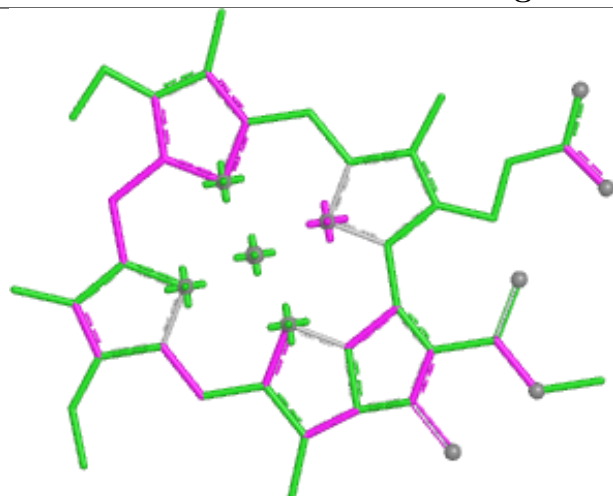
Torsions



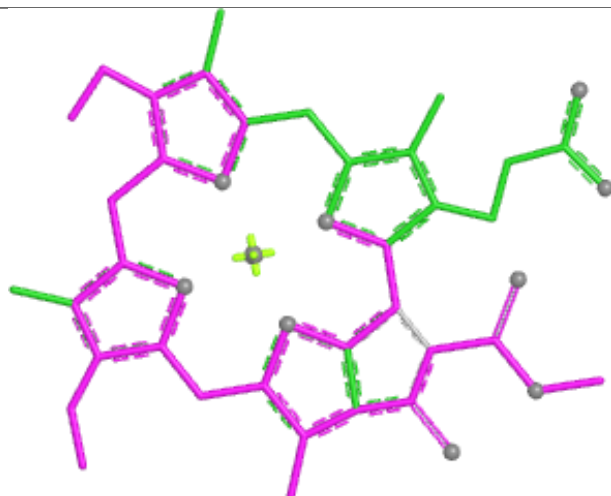
Rings



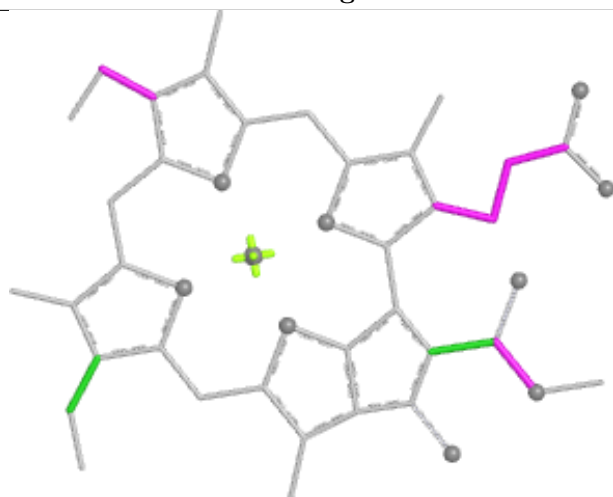
Ligand CLA B 602



Bond lengths



Bond angles

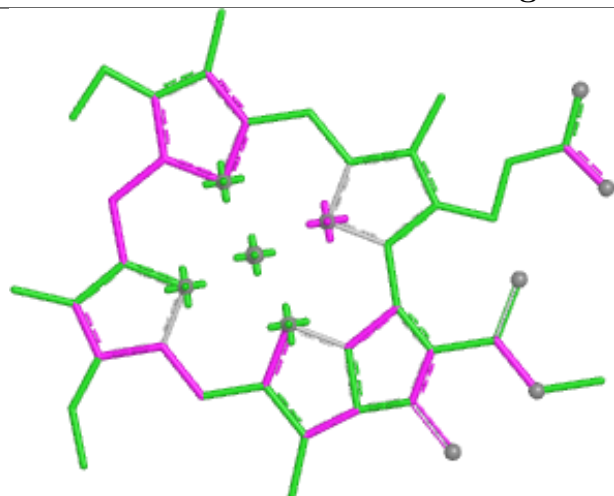


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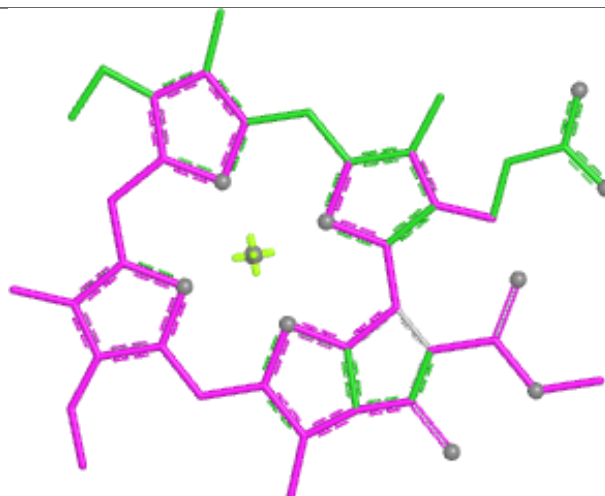


Rings

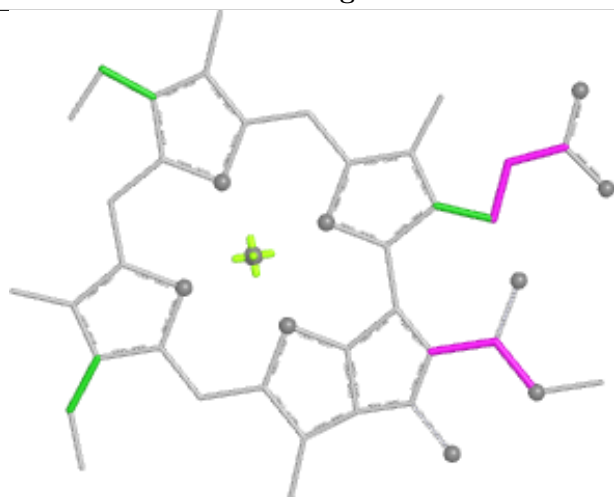
Ligand CLA c 504



Bond lengths



Bond angles

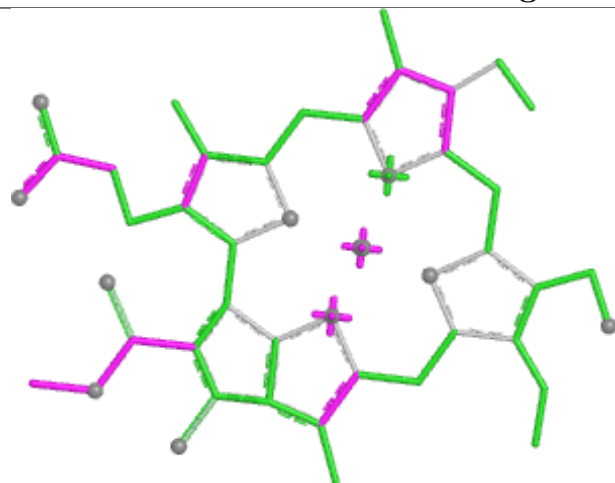


Torsions

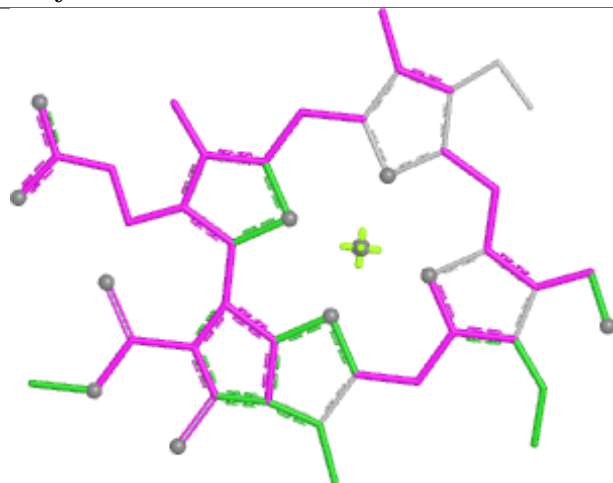


Rings

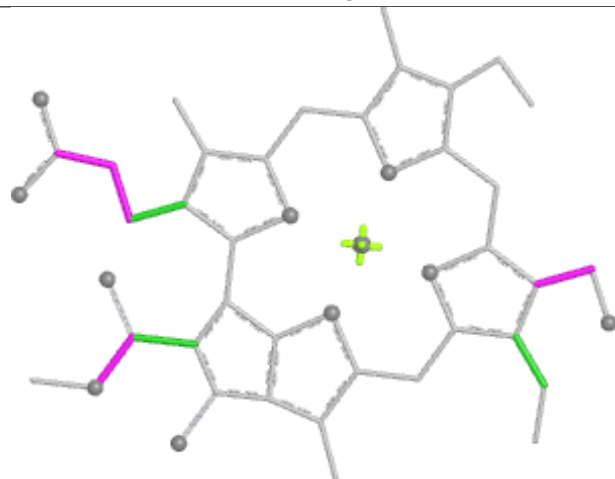
Ligand CHL y 608



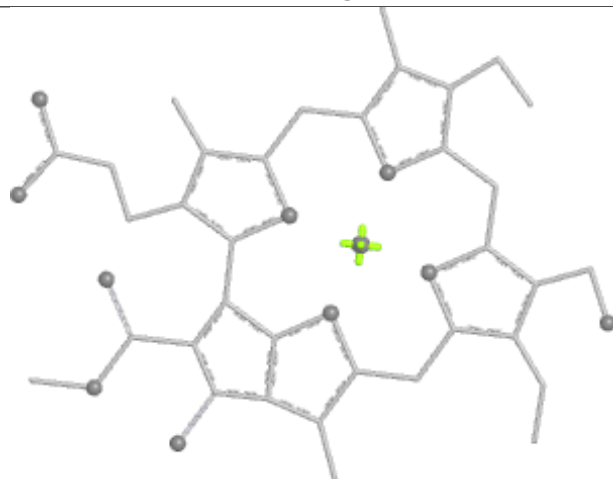
Bond lengths



Bond angles

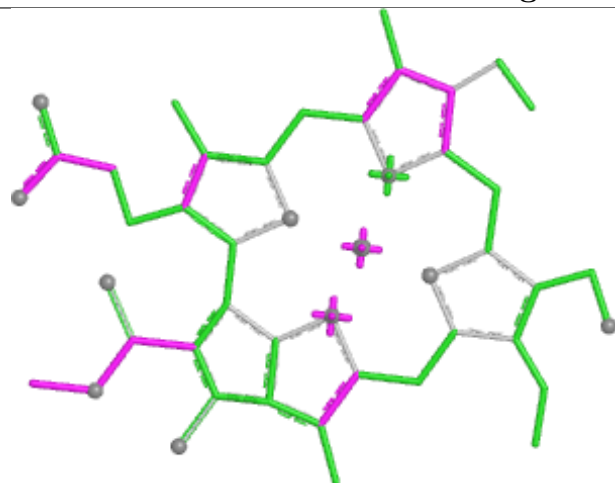


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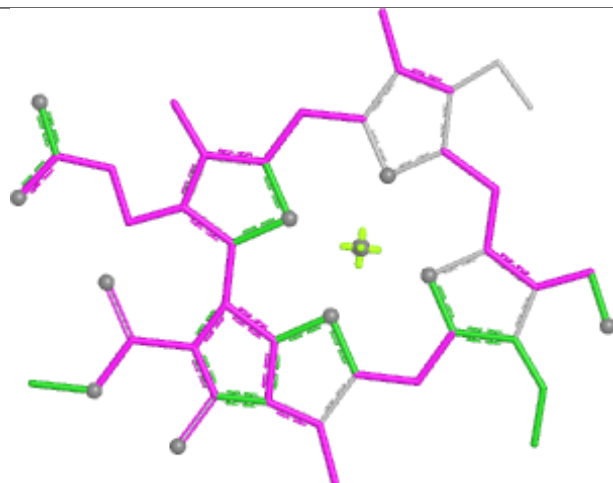


Rings

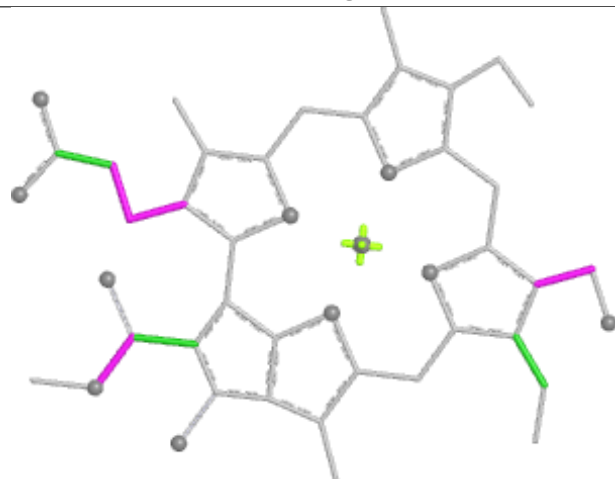
Ligand CHL 1 615



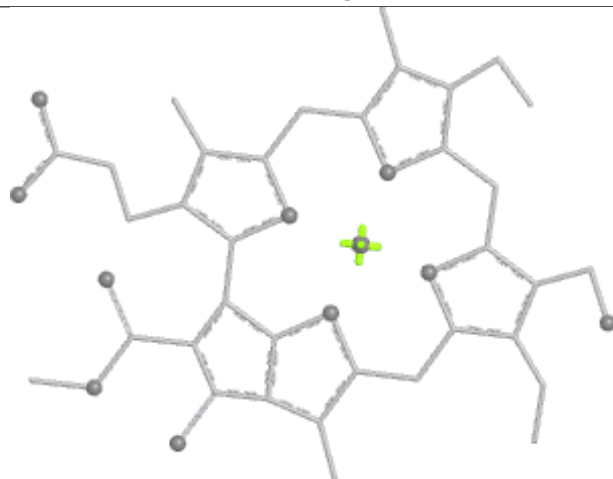
Bond lengths



Bond angles

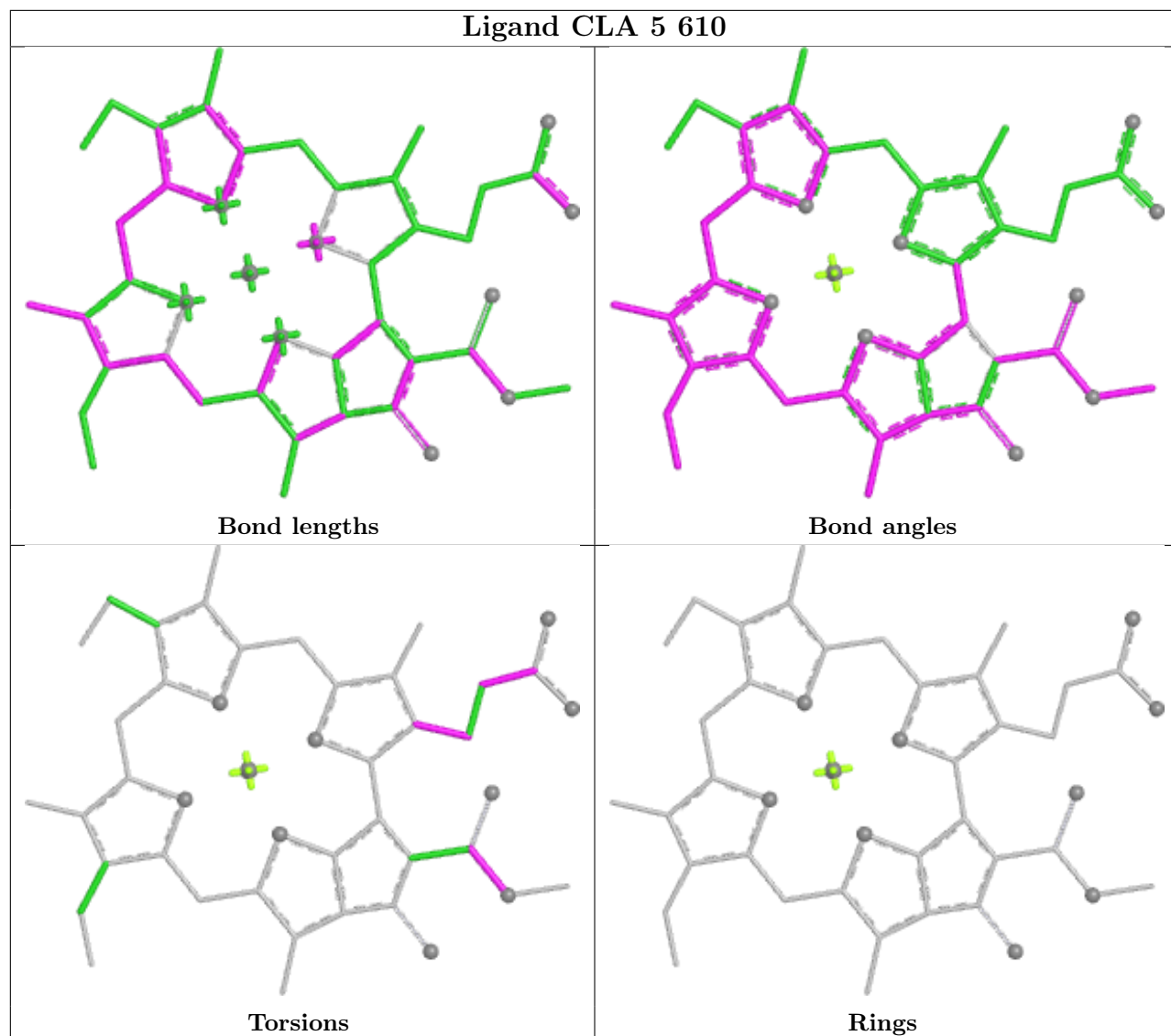


Torsions

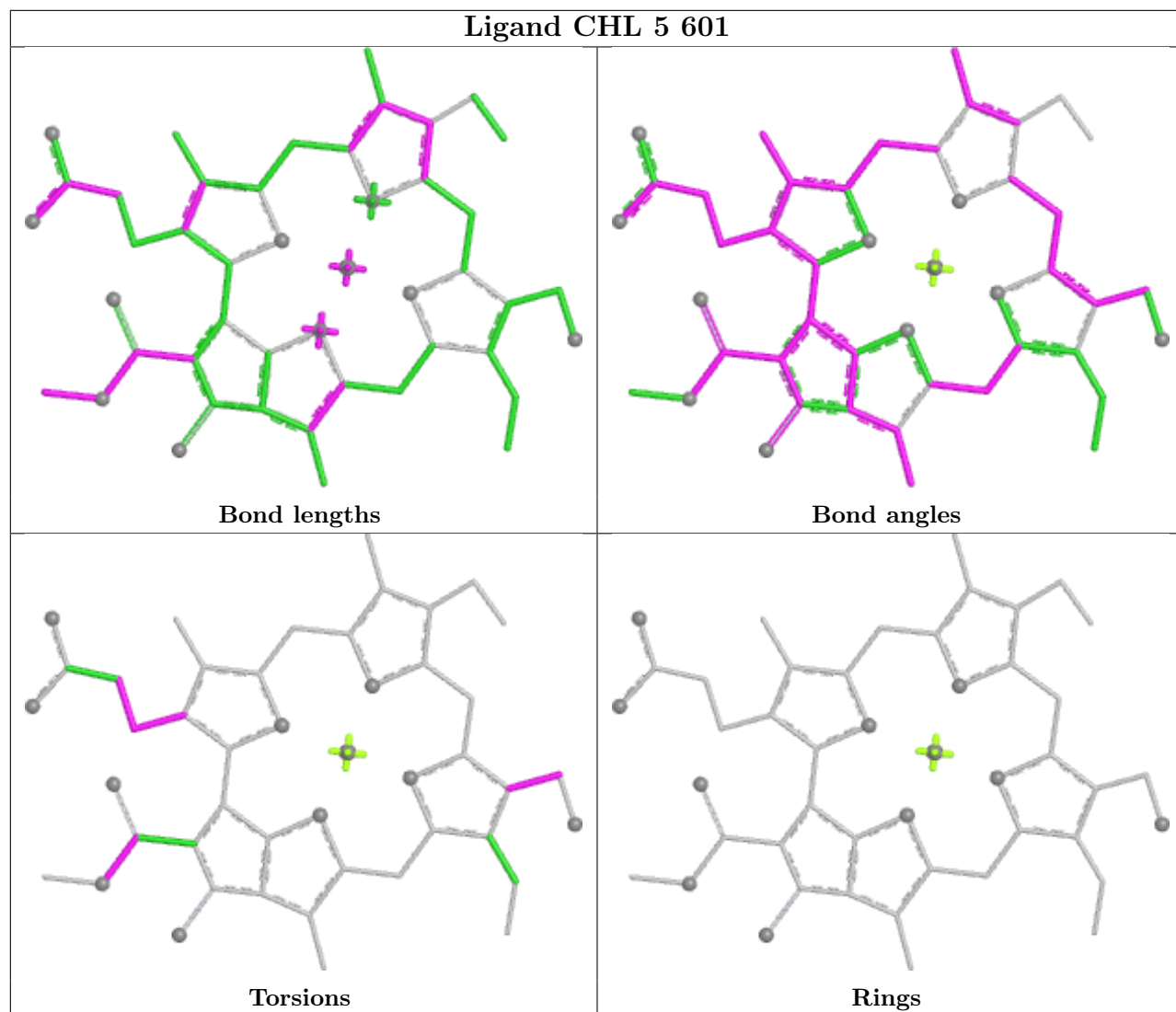


Rings

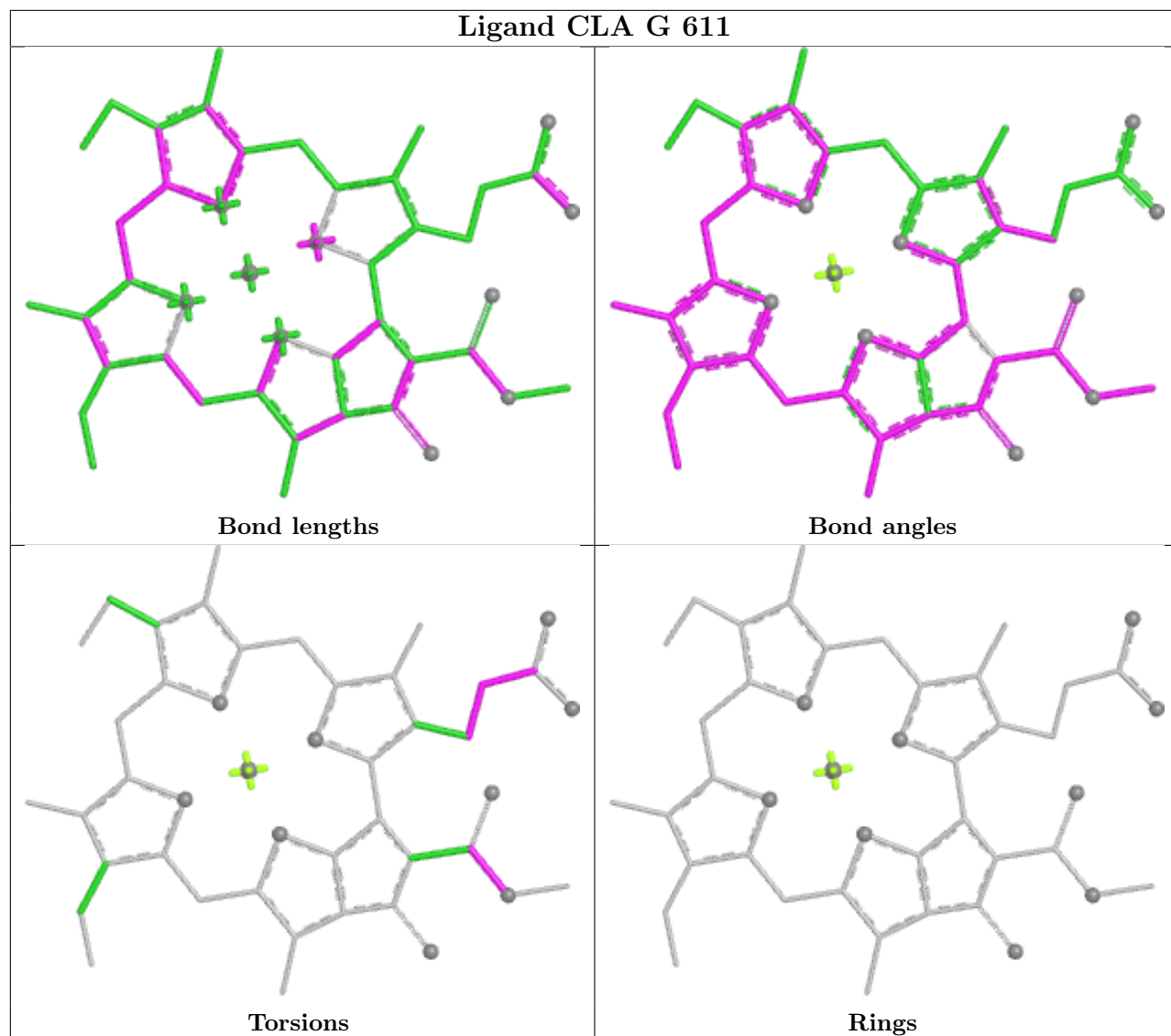
Ligand CLA 5 610



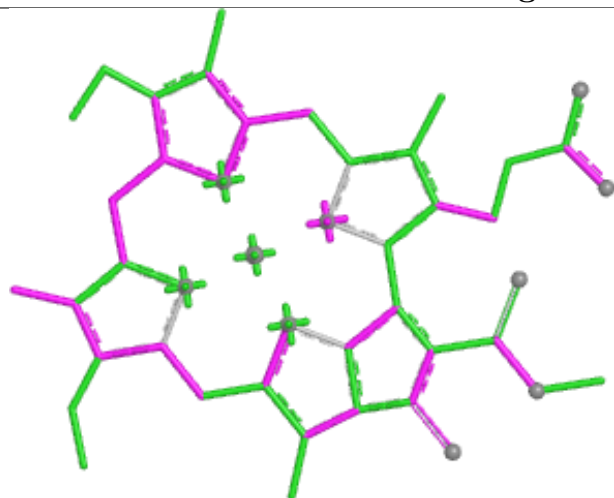
Ligand CHL 5 601



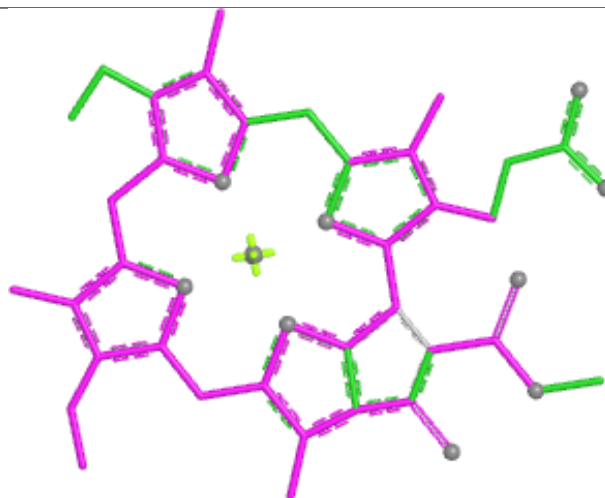
Ligand CLA G 611



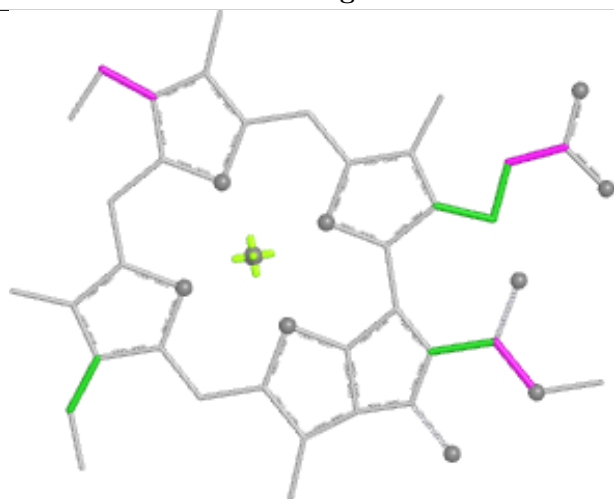
Ligand CLA 8 302



Bond lengths



Bond angles

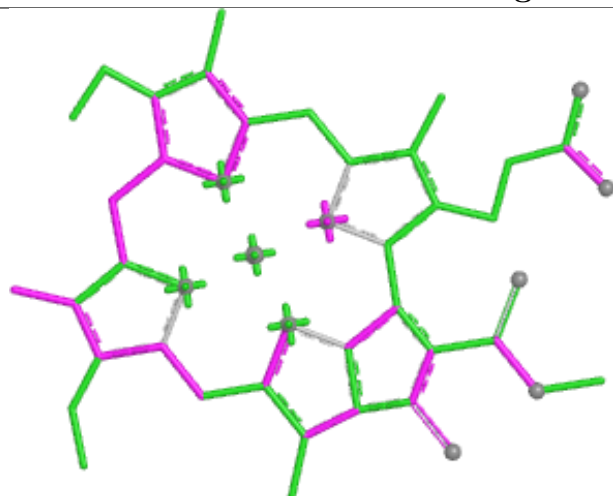


Torsions

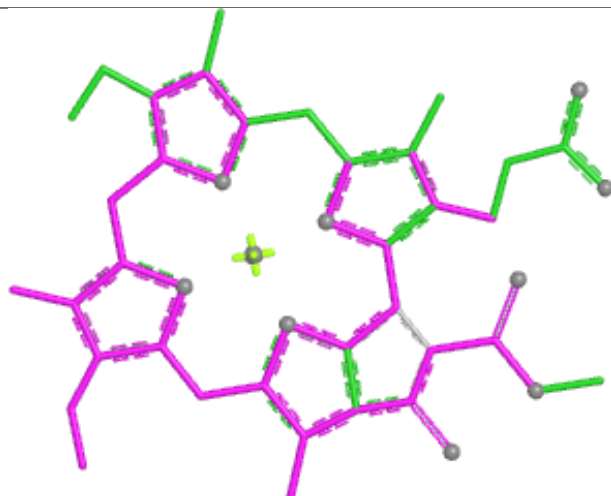


Rings

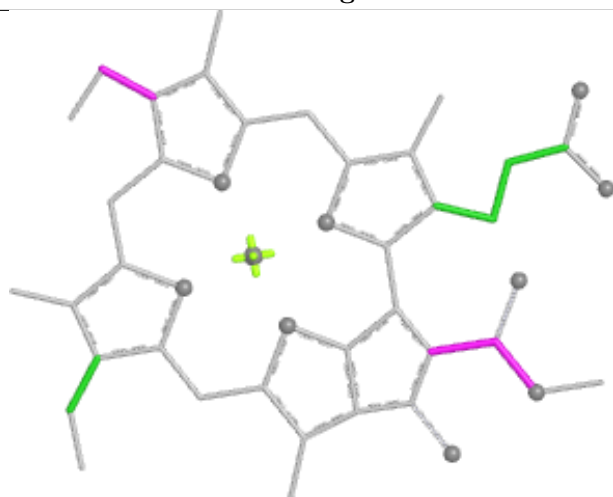
Ligand CLA C 512



Bond lengths



Bond angles

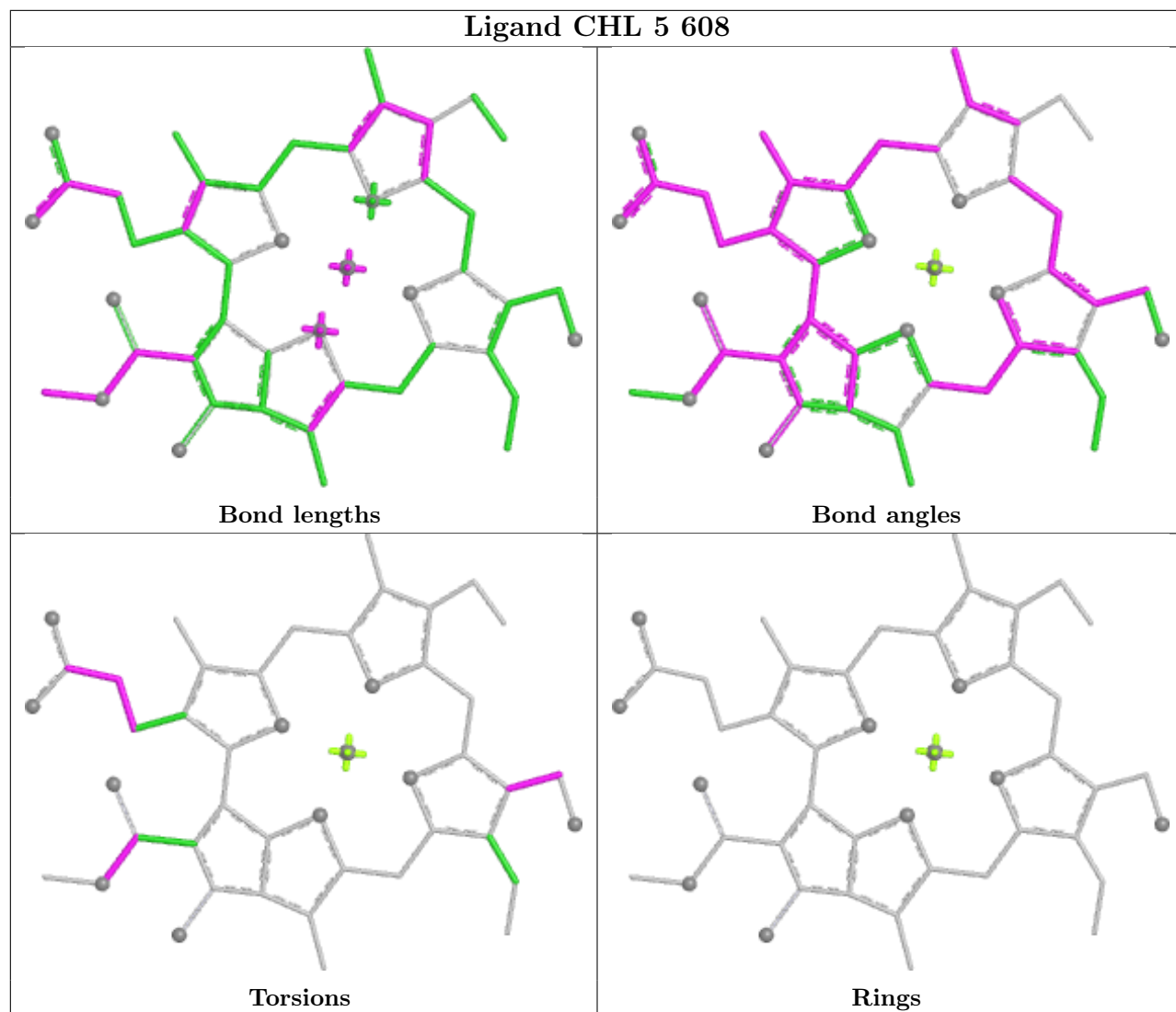


Torsions

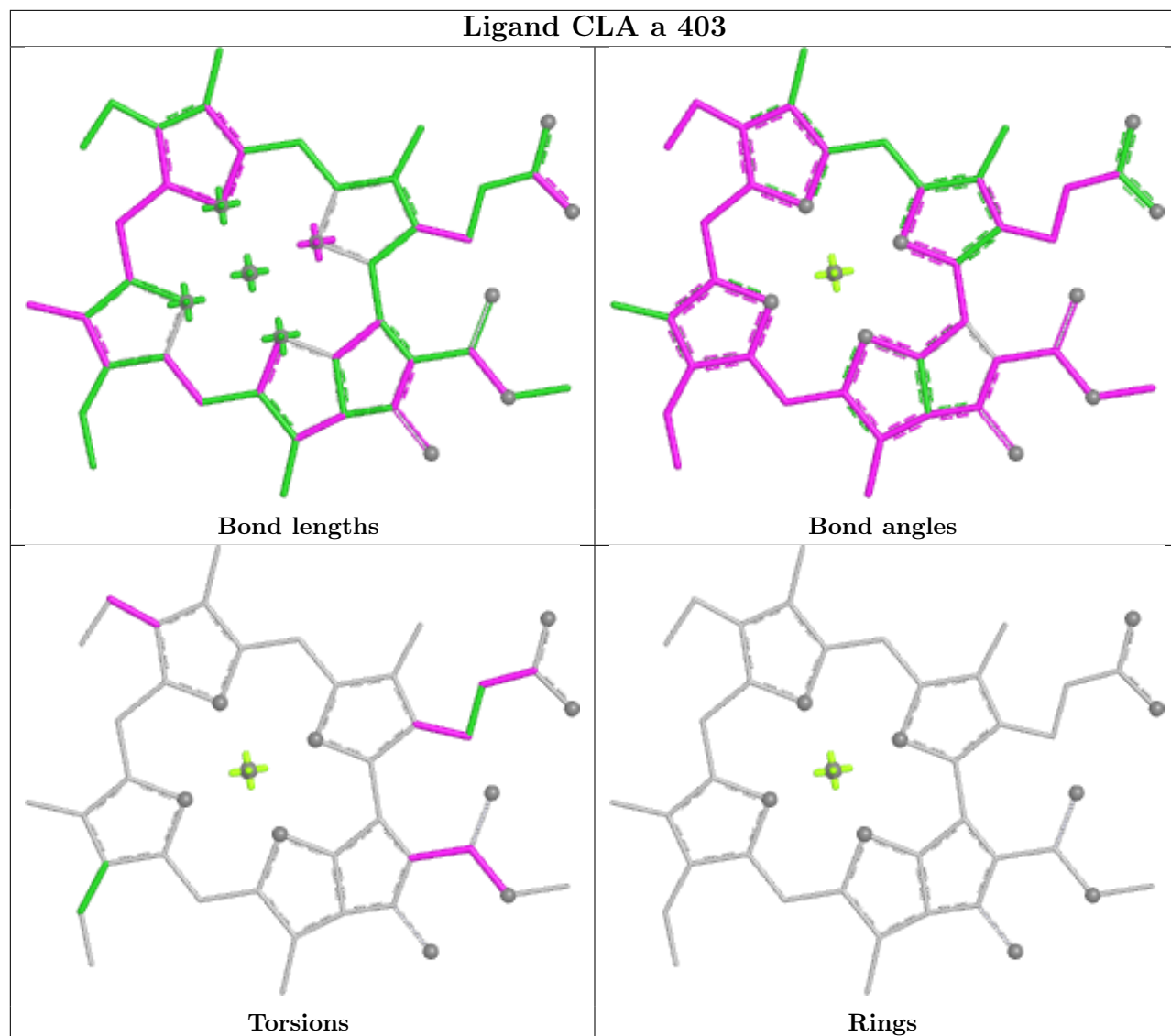


Rings

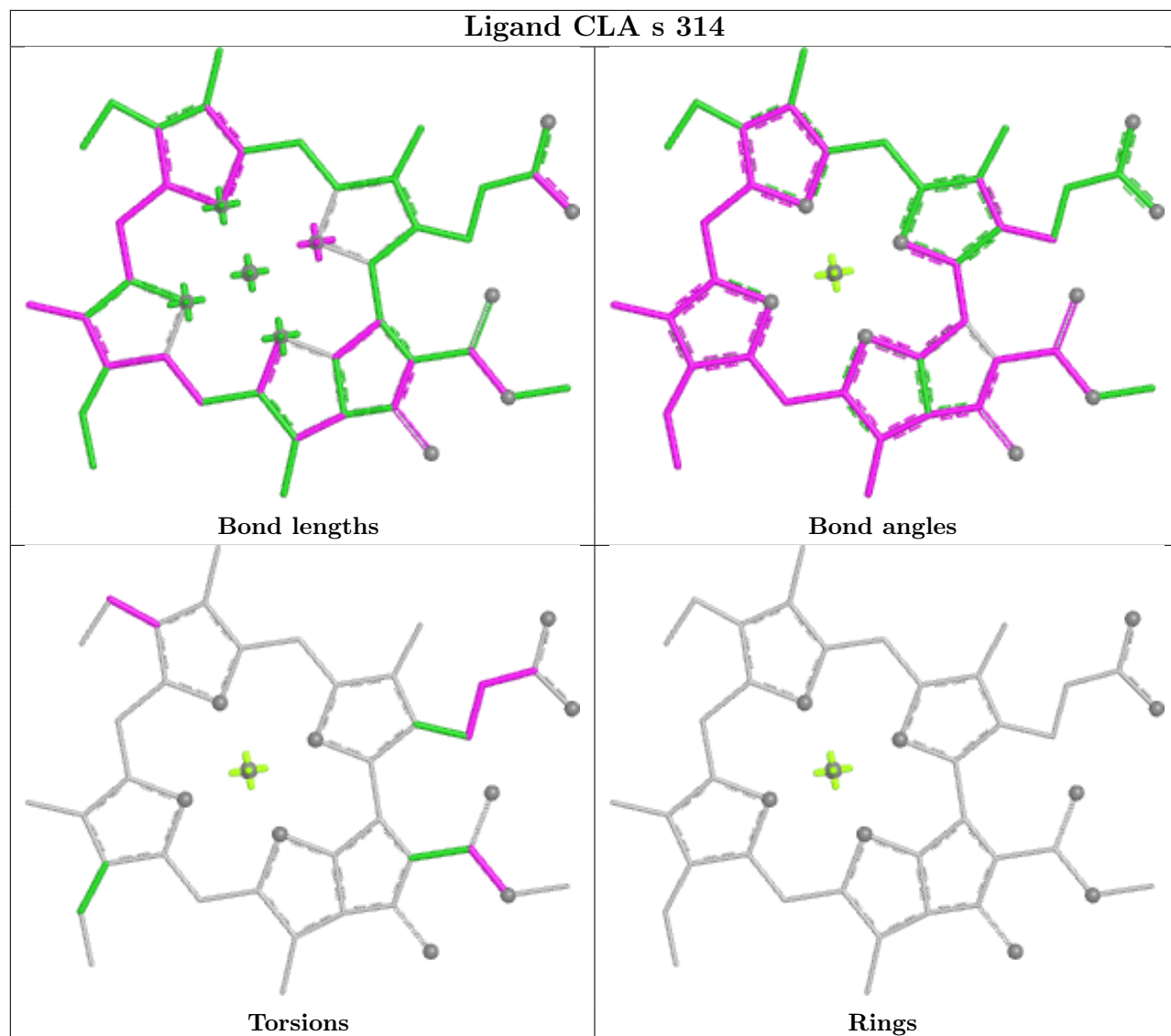
Ligand CHL 5 608



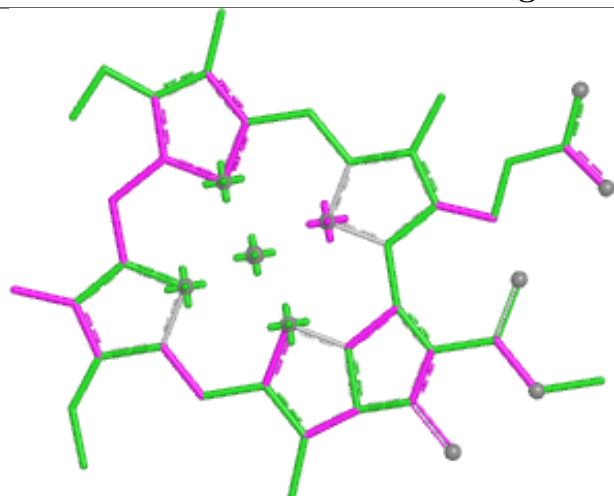
Ligand CLA a 403



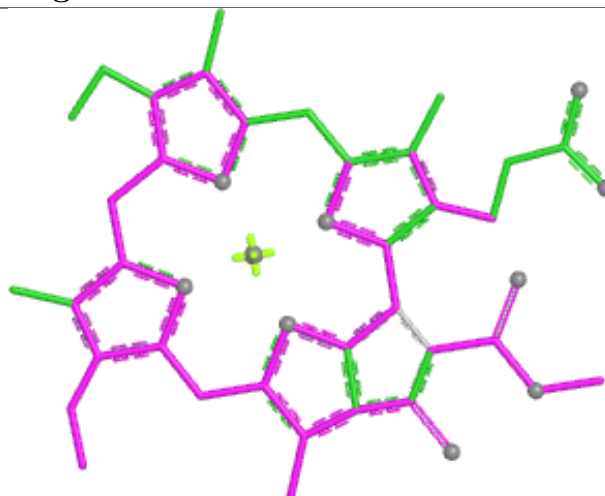
Ligand CLA s 314



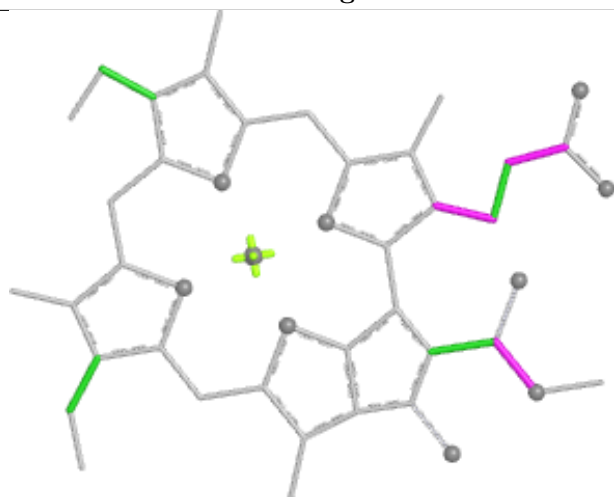
Ligand CLA g 614



Bond lengths



Bond angles

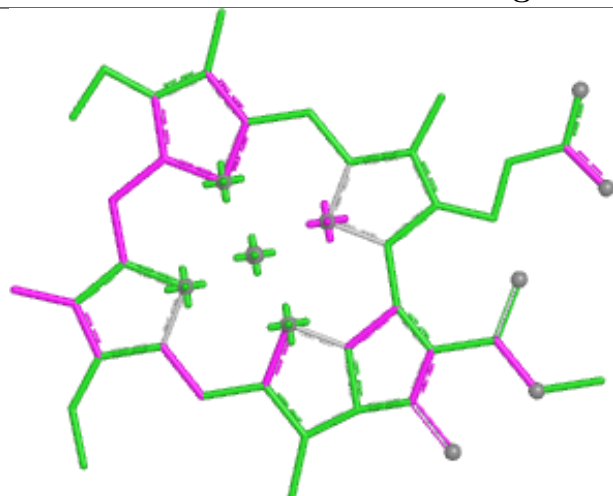


Torsions

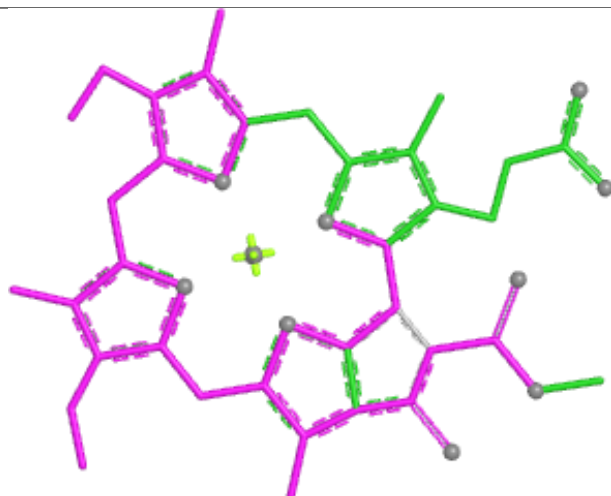


Rings

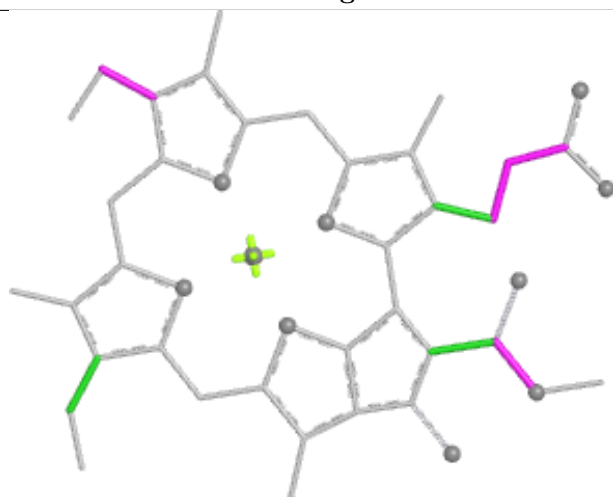
Ligand CLA G 613



Bond lengths



Bond angles

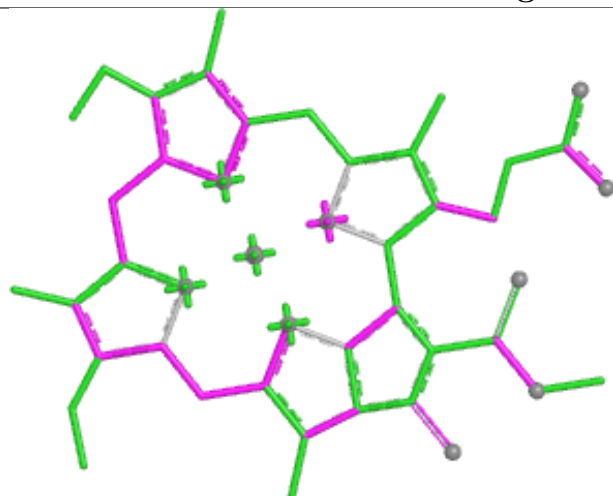


Torsions

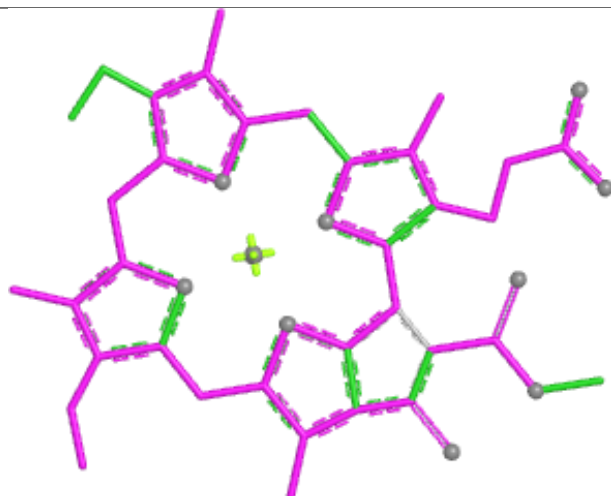


Rings

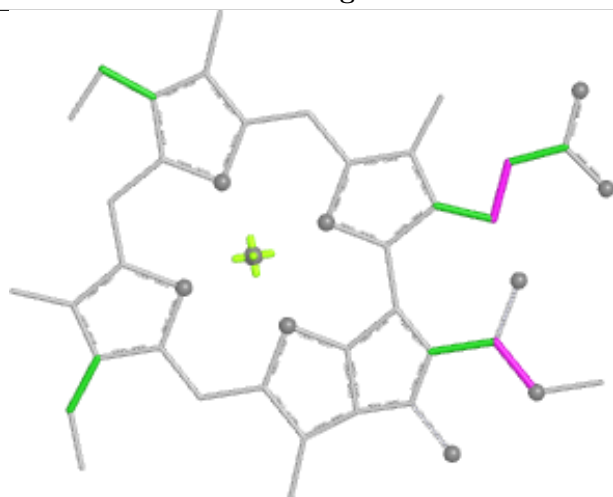
Ligand CLA b 606



Bond lengths



Bond angles

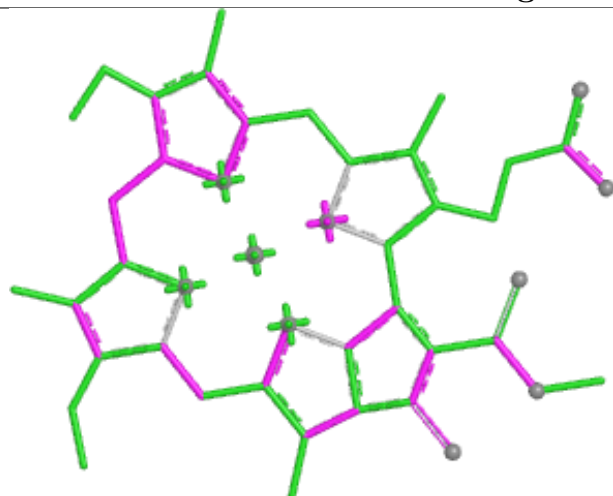


Torsions

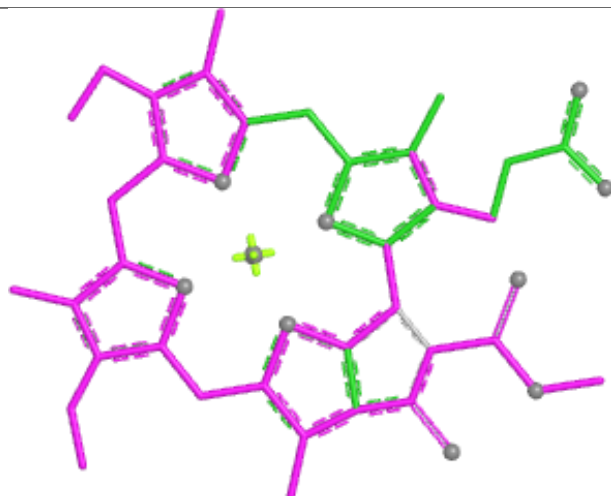


Rings

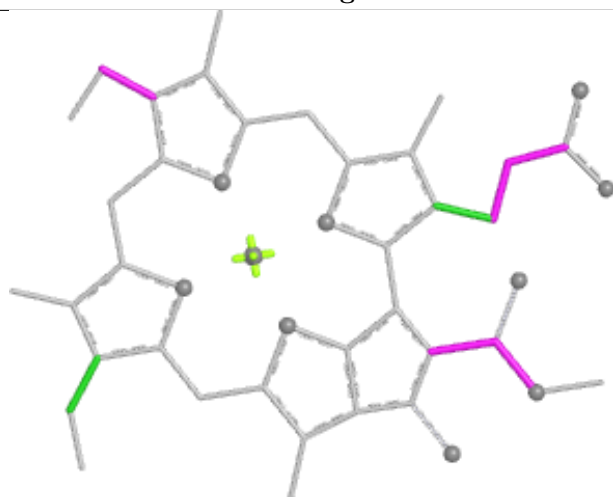
Ligand CLA b 601



Bond lengths



Bond angles

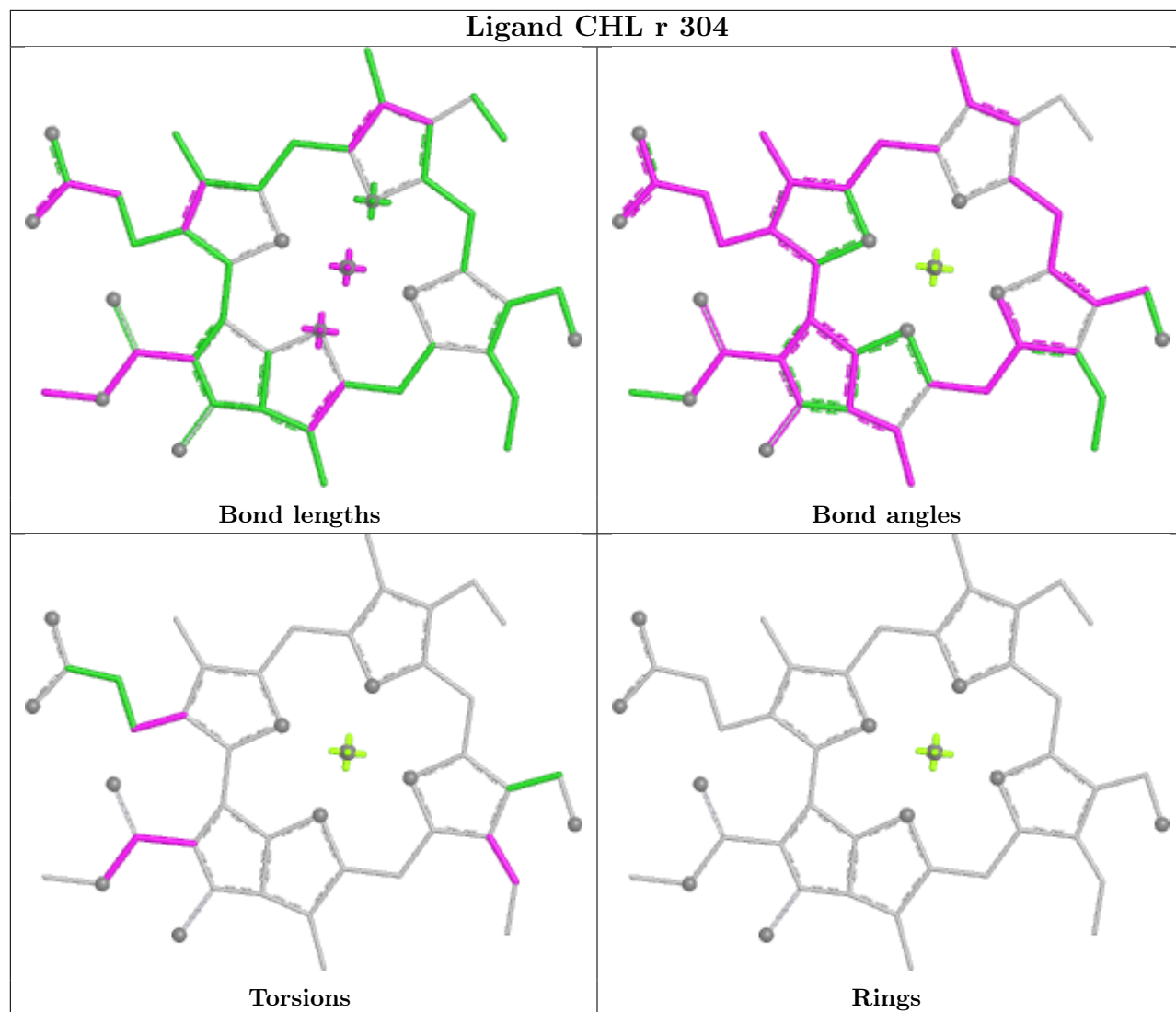


Torsions

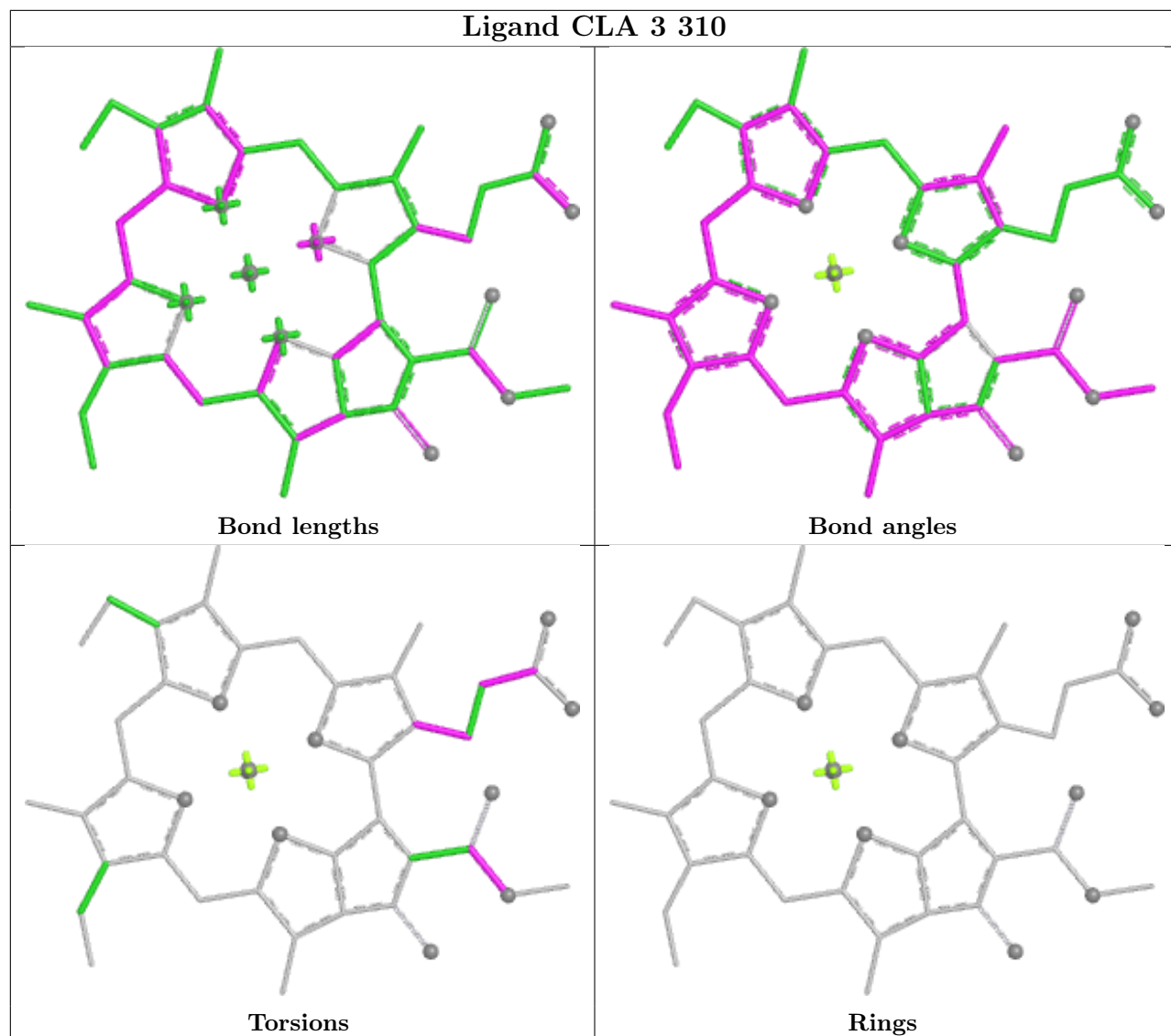


Rings

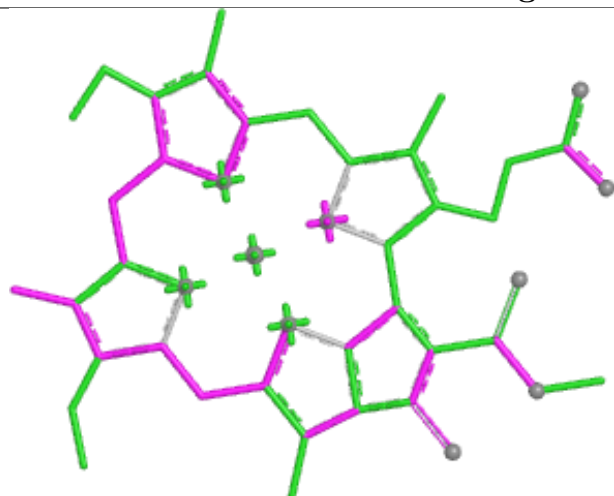
Ligand CHL r 304



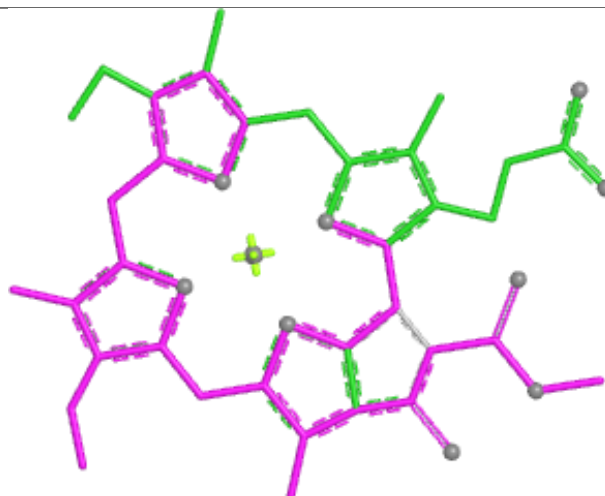
Ligand CLA 3 310



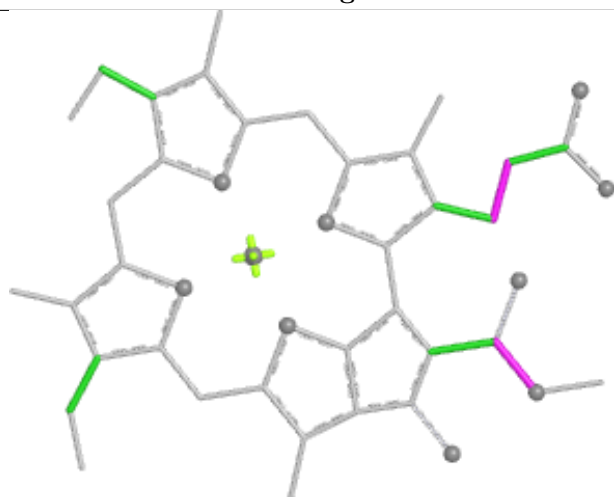
Ligand CLA 4 310



Bond lengths



Bond angles

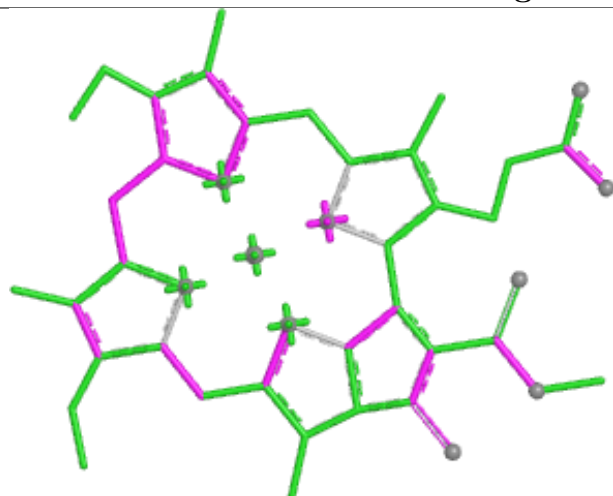


Torsions

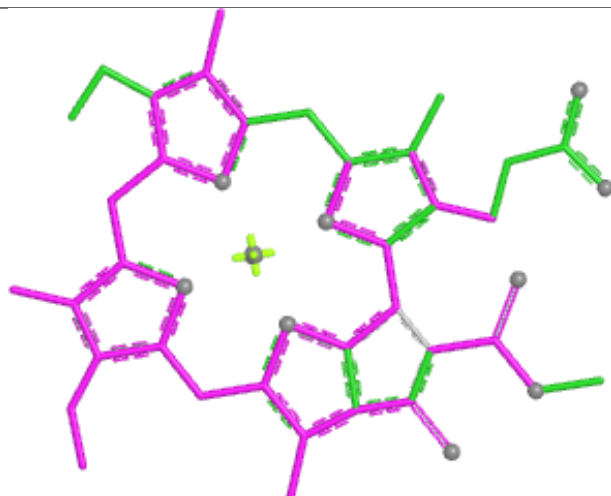


Rings

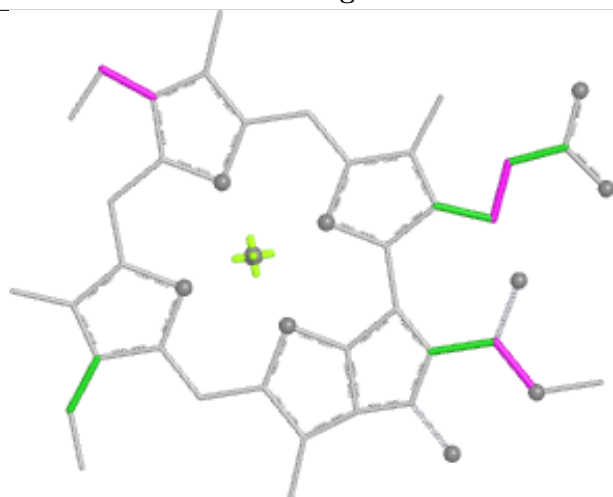
Ligand CLA B 606



Bond lengths



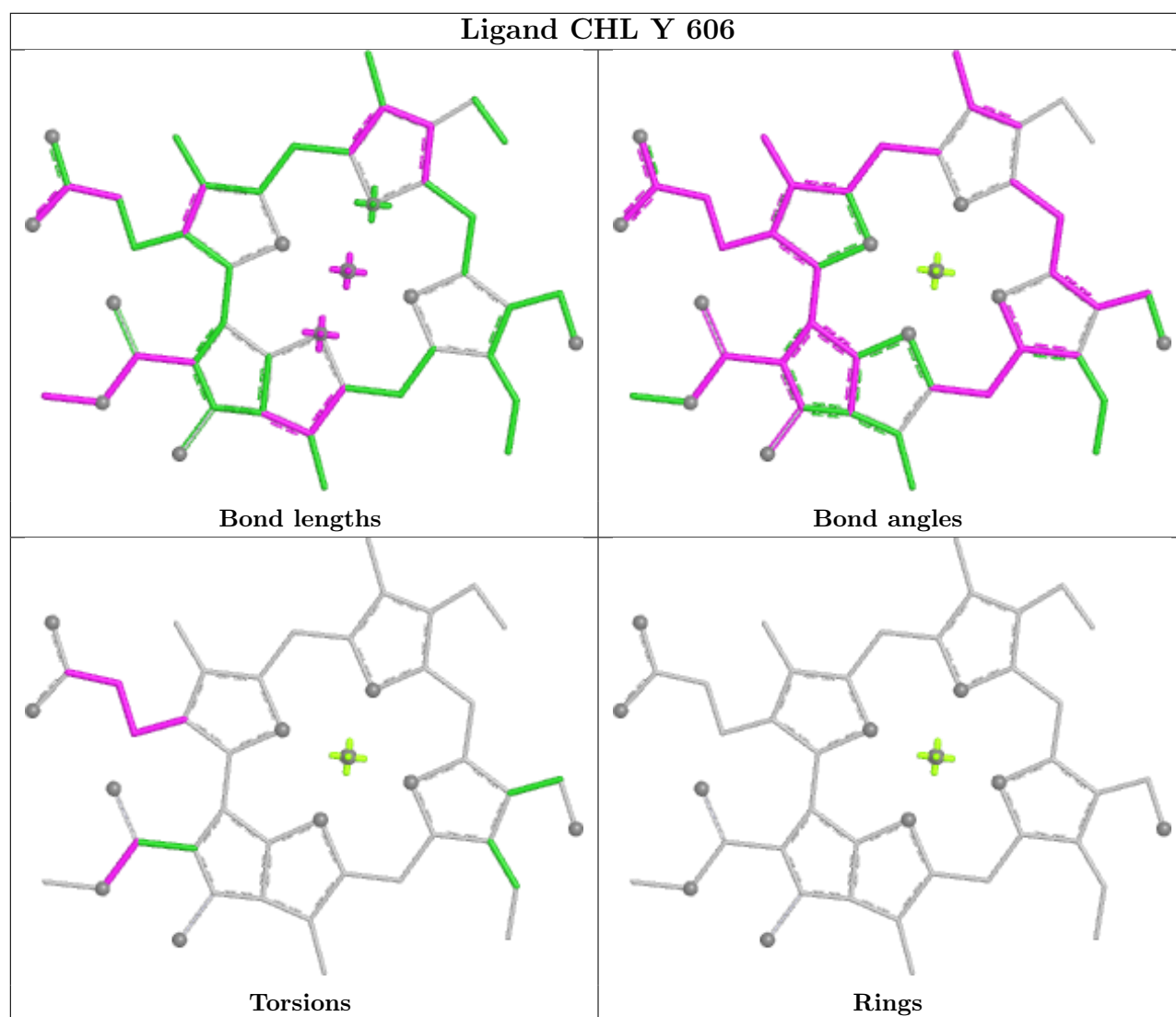
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

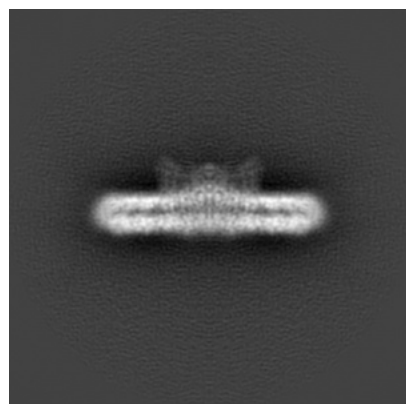
6 Map visualisation [i](#)

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

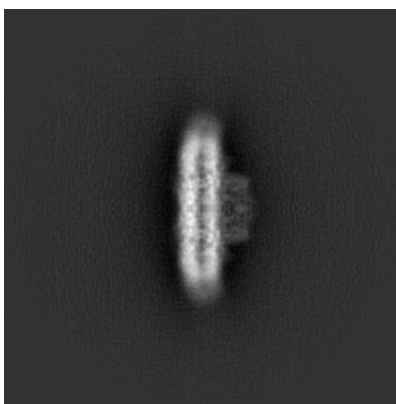
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

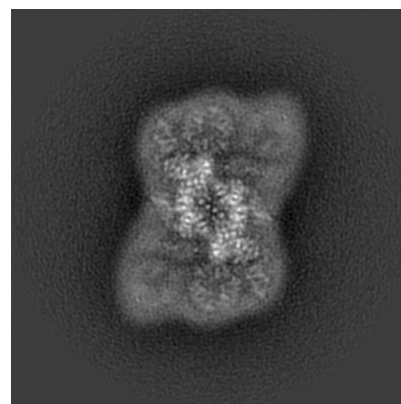
6.1.1 Primary map



X

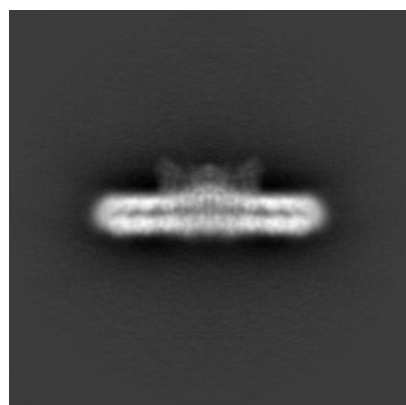


Y

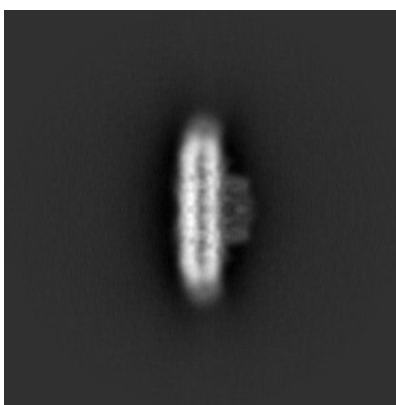


Z

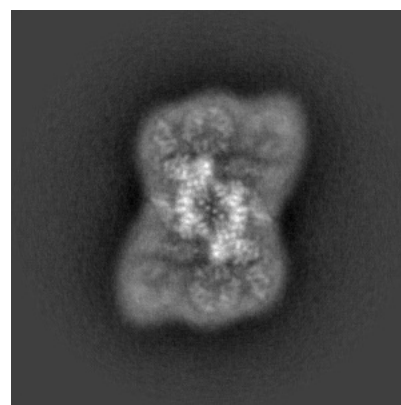
6.1.2 Raw map



X



Y

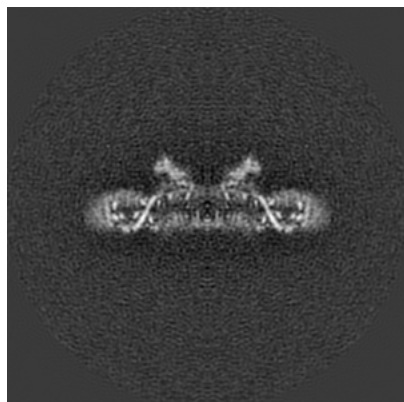


Z

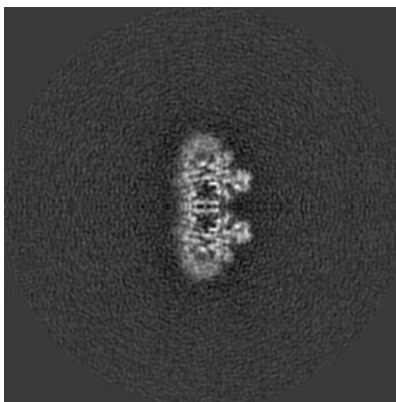
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

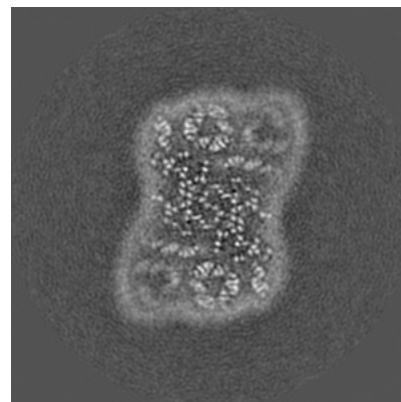
6.2.1 Primary map



X Index: 234

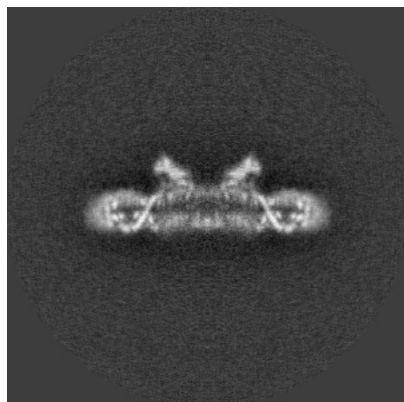


Y Index: 234

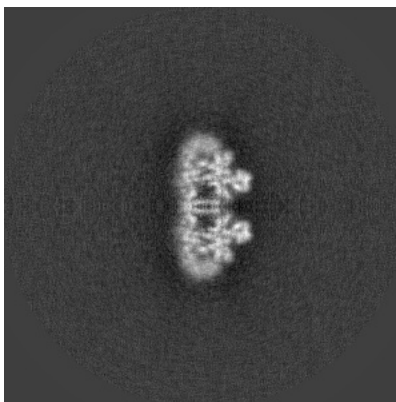


Z Index: 234

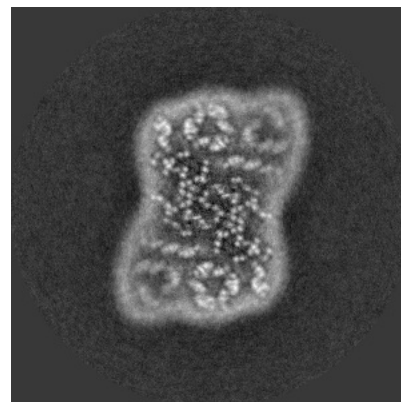
6.2.2 Raw map



X Index: 234



Y Index: 234

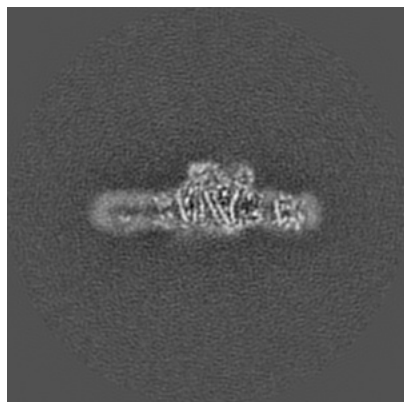


Z Index: 234

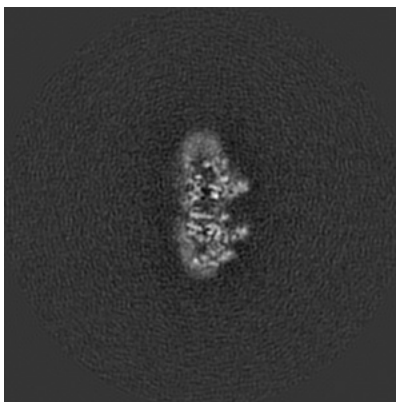
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

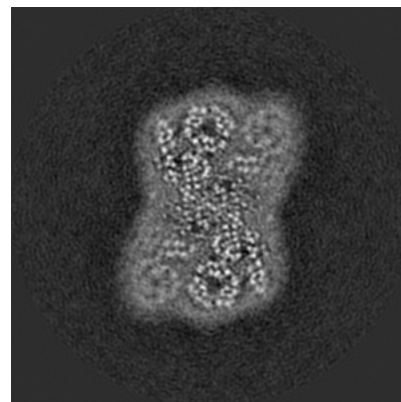
6.3.1 Primary map



X Index: 208

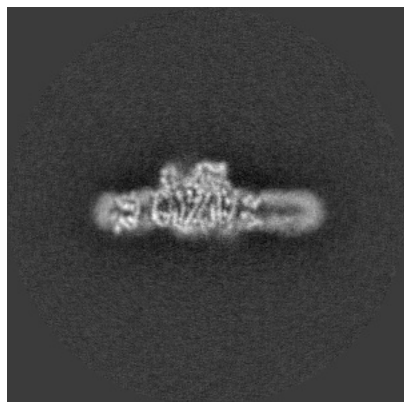


Y Index: 243

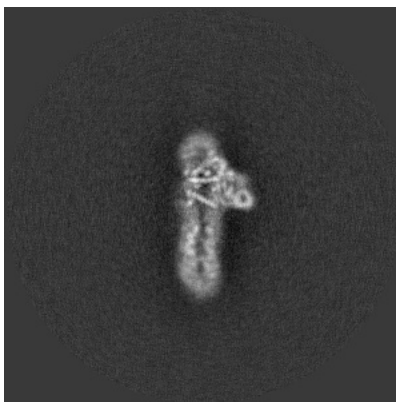


Z Index: 218

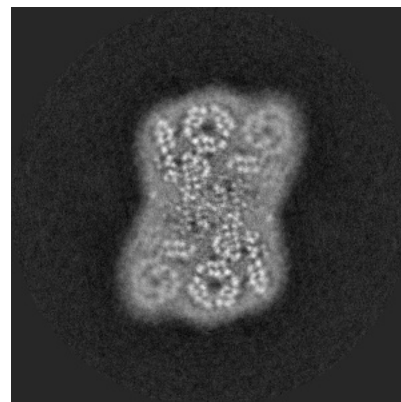
6.3.2 Raw map



X Index: 262



Y Index: 190

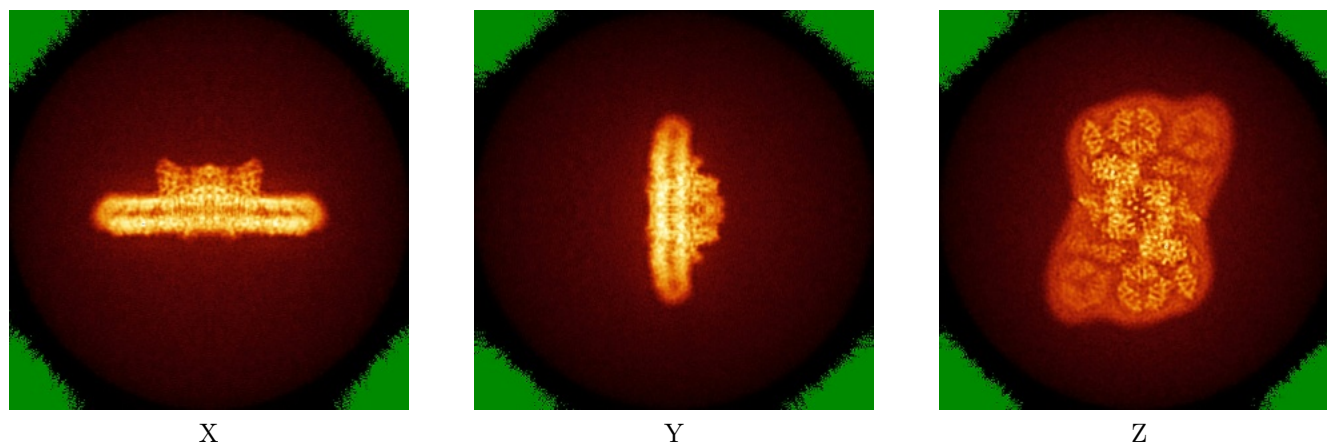


Z Index: 218

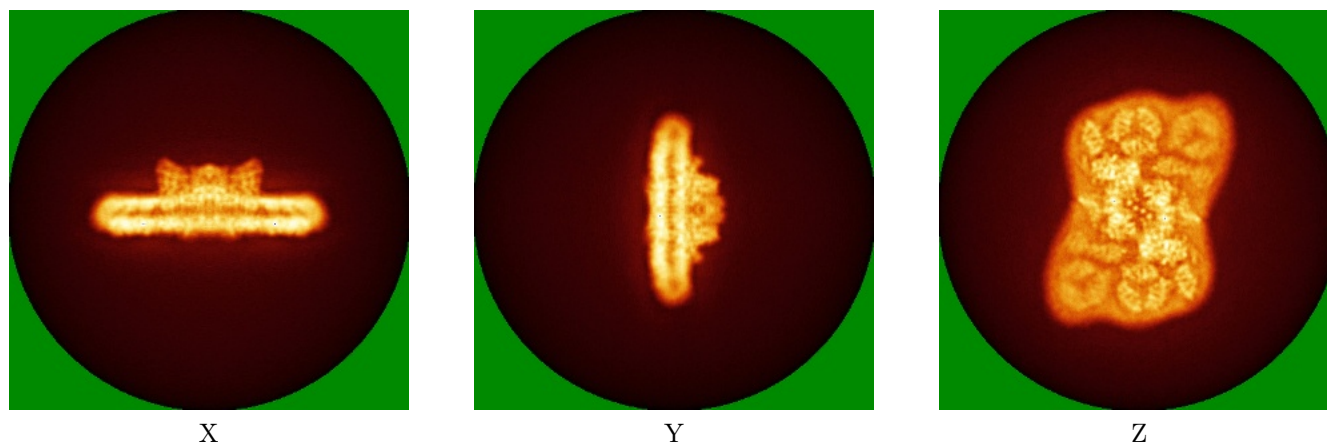
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

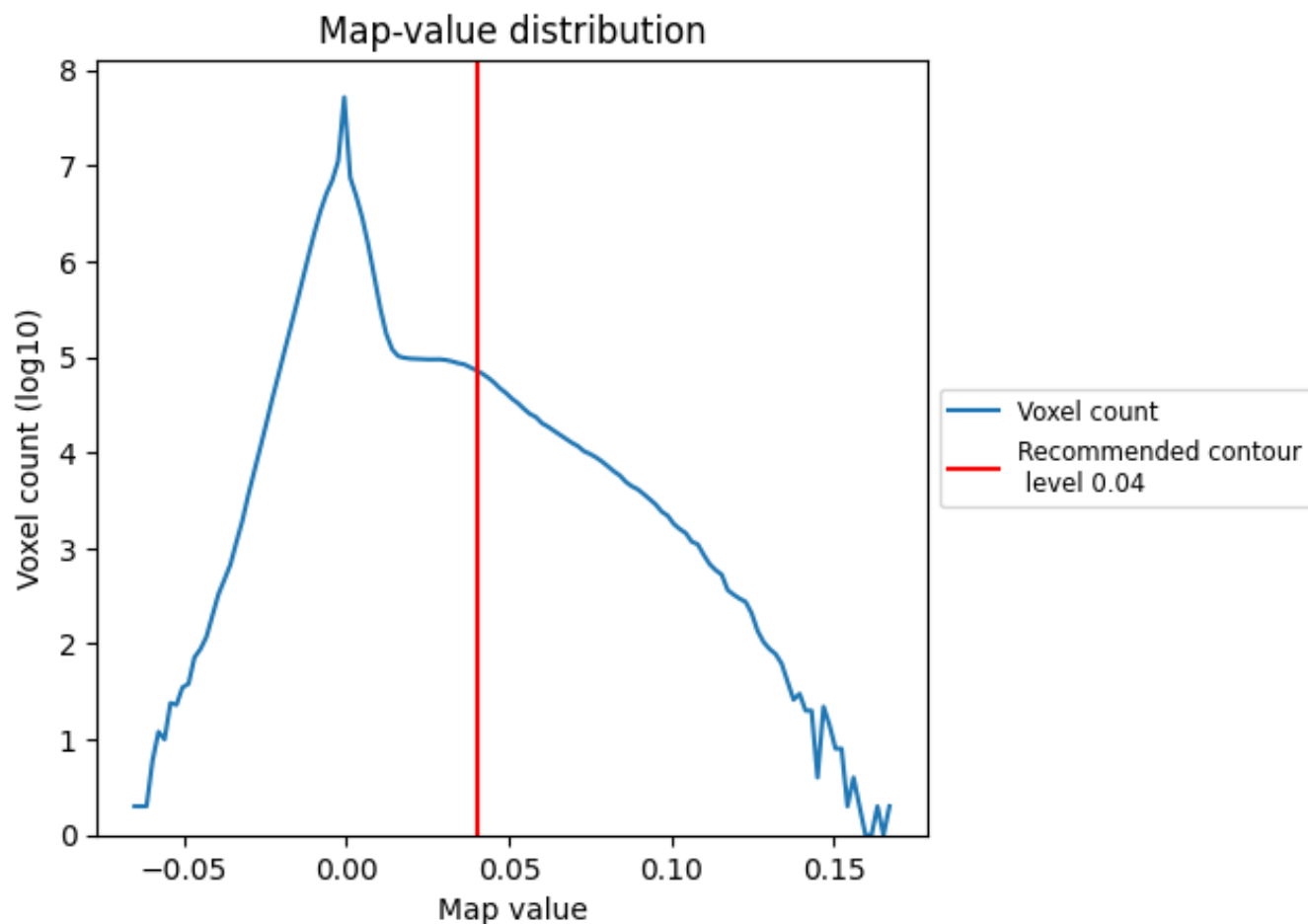
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

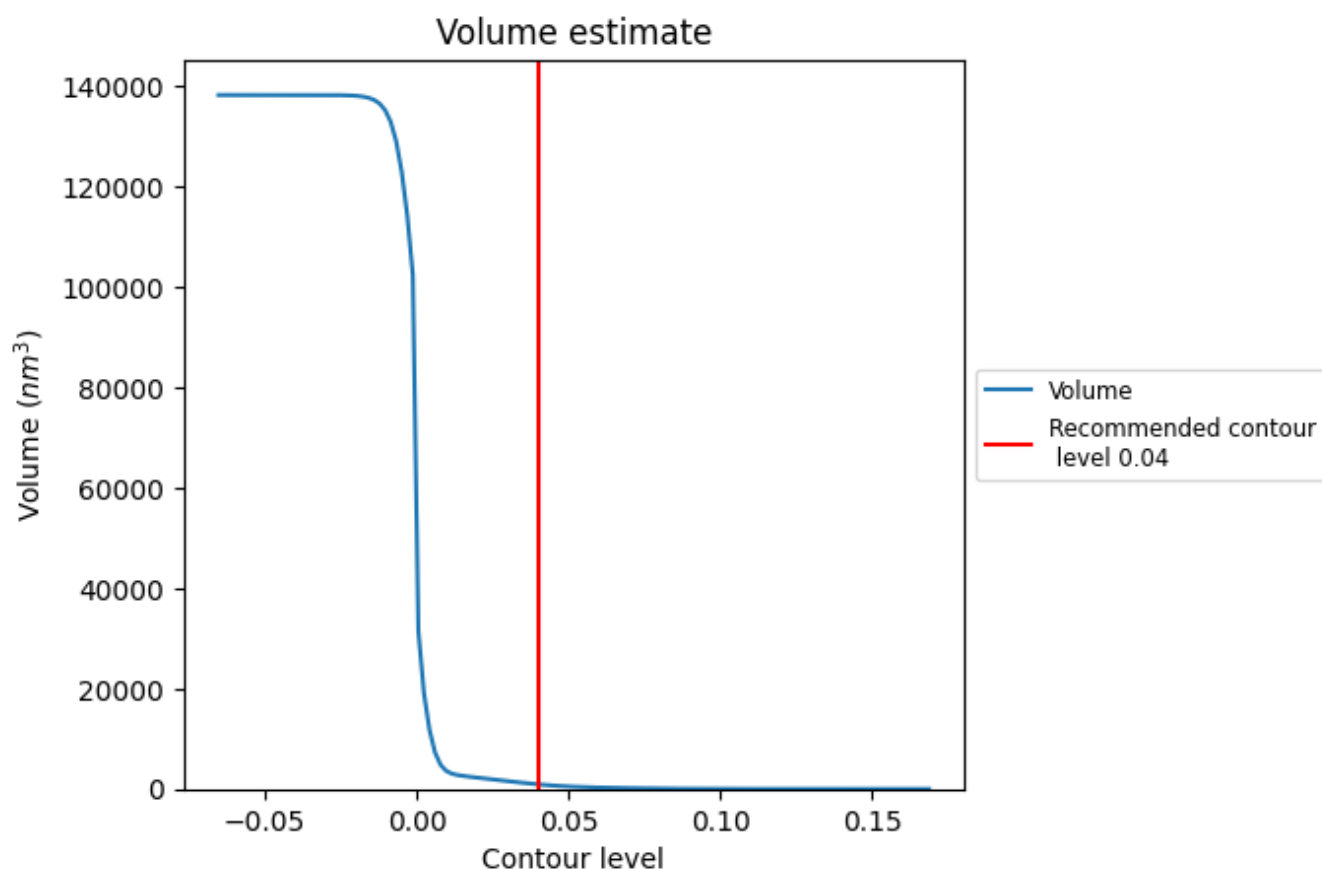
This section contains the results of statistical analysis of the map.

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.

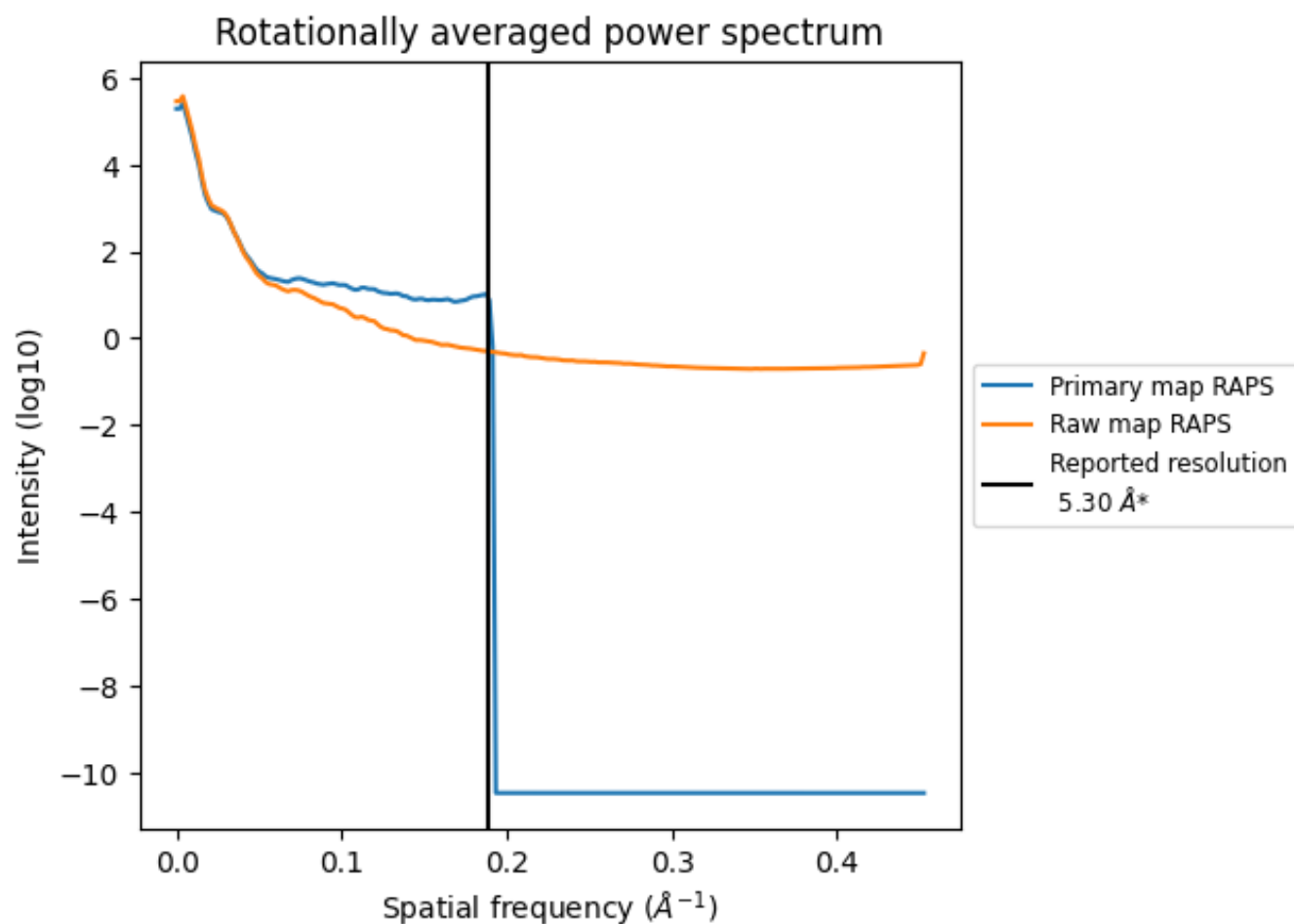
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

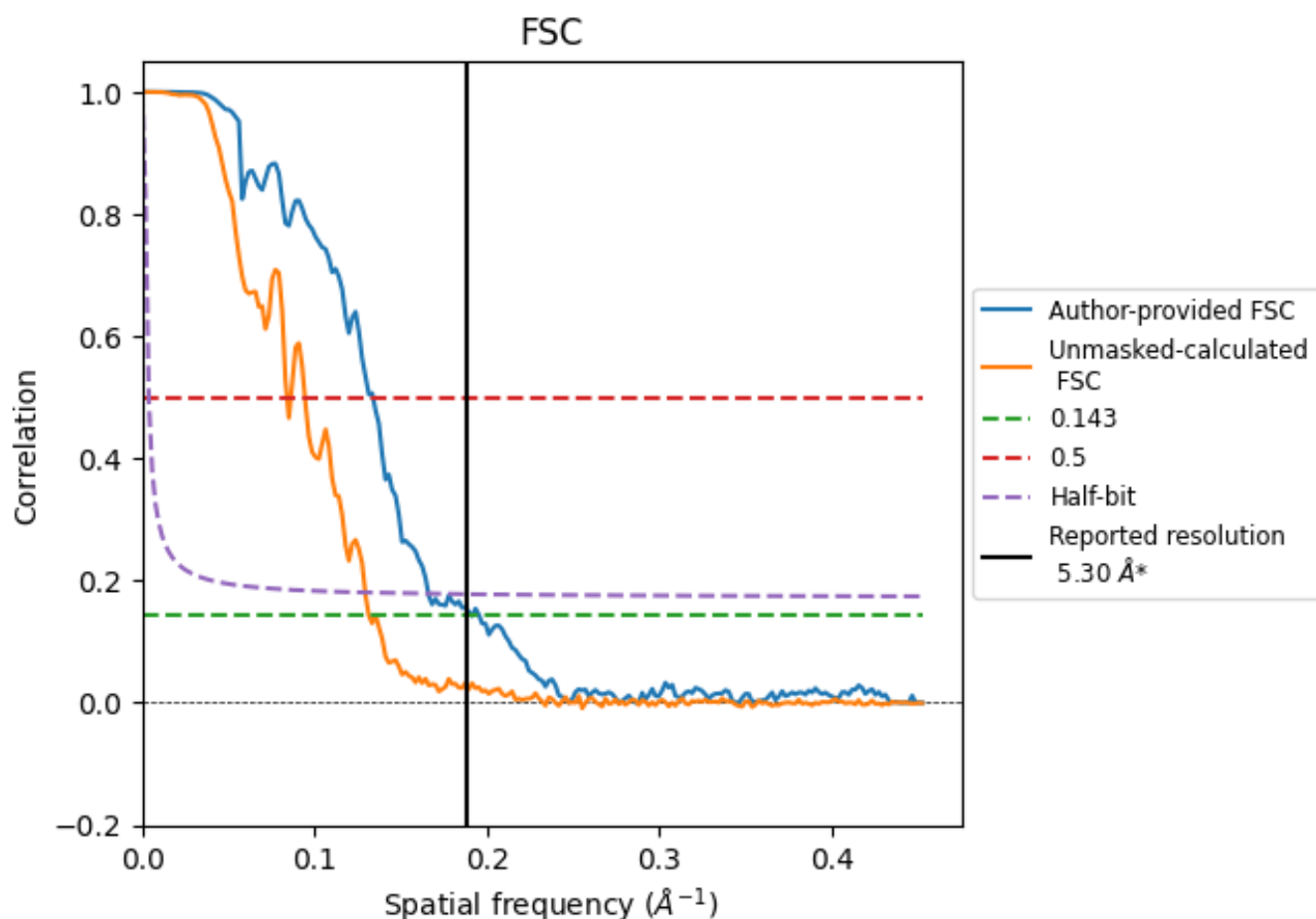


*Reported resolution corresponds to spatial frequency of 0.189 $\text{\AA}^{-1}$

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 $0.189 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

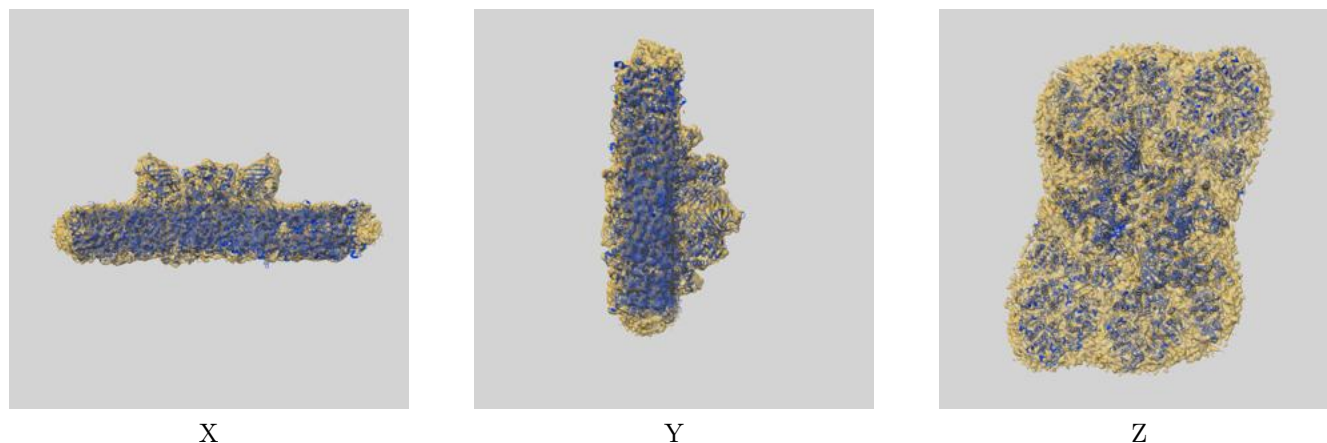
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.23	7.47	6.02
Unmasked-calculated*	7.60	11.90	7.73

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

9 Map-model fit [i](#)

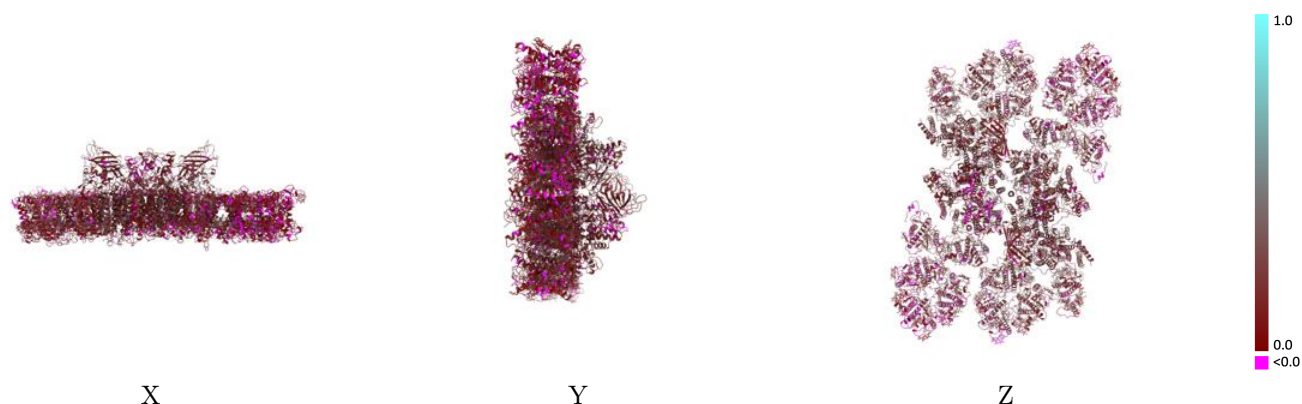
This section contains information regarding the fit between EMDB map EMD-3491 and PDB model 5MDX. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



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

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

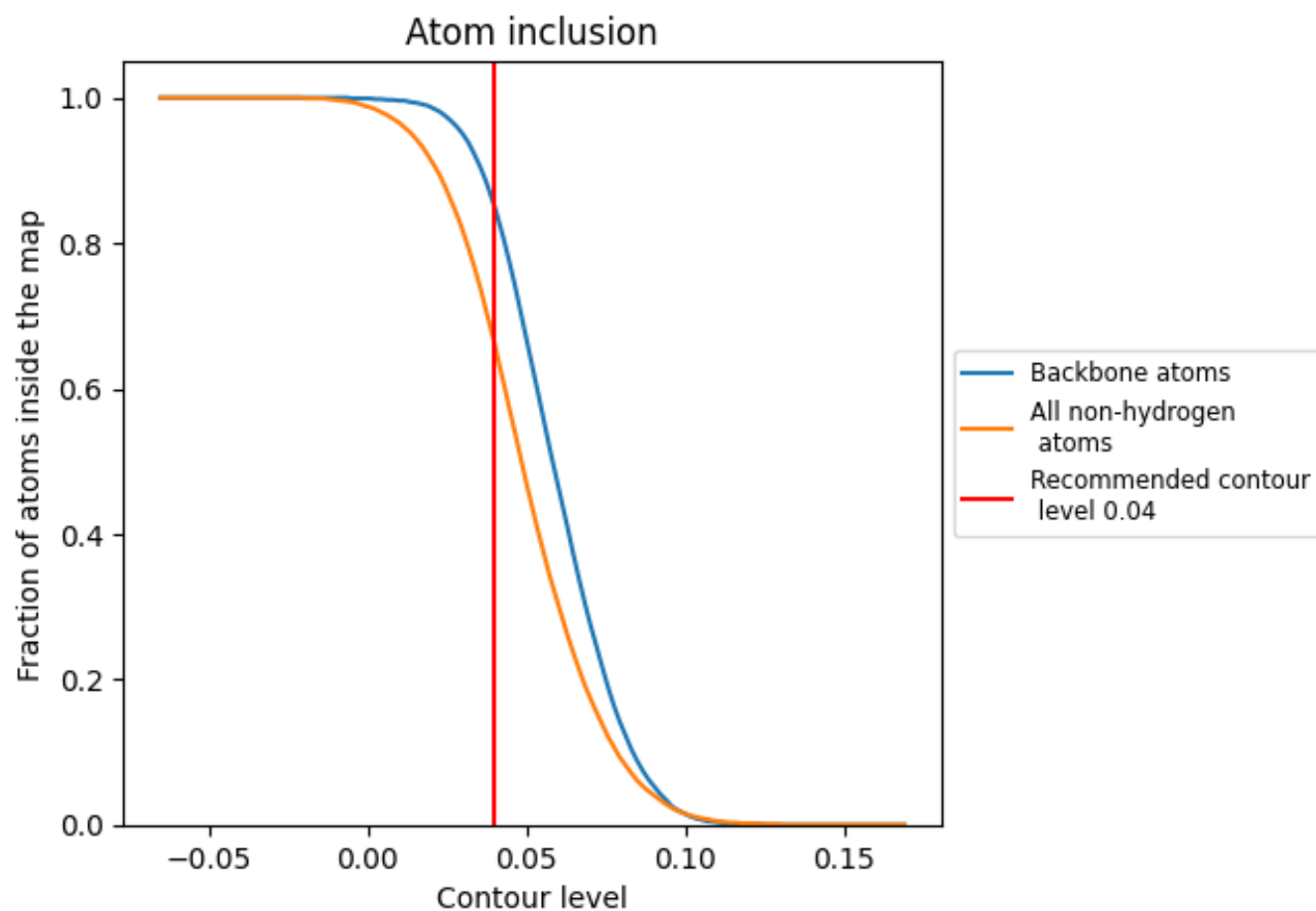


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6600	 0.1630
1	 0.6190	 0.1070
2	 0.5790	 0.1060
3	 0.5530	 0.0770
4	 0.5140	 0.1140
5	 0.6190	 0.1080
6	 0.5790	 0.1060
7	 0.5530	 0.0780
8	 0.5140	 0.1150
A	 0.6300	 0.2030
B	 0.6970	 0.1970
C	 0.7380	 0.2150
D	 0.6570	 0.2030
E	 0.6980	 0.1580
F	 0.7400	 0.1420
G	 0.7100	 0.1470
H	 0.7060	 0.2160
I	 0.5870	 0.1790
K	 0.6740	 0.2180
L	 0.6330	 0.1940
M	 0.5870	 0.1950
N	 0.7540	 0.1700
O	 0.7250	 0.2070
R	 0.6520	 0.1620
S	 0.7370	 0.1660
T	 0.5420	 0.1940
W	 0.6510	 0.2050
X	 0.6060	 0.1600
Y	 0.7030	 0.1760
Z	 0.6690	 0.1580
a	 0.6500	 0.2110
b	 0.5830	 0.1220
c	 0.7460	 0.2260
d	 0.6660	 0.2030
e	 0.7250	 0.1830



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Chain	Atom inclusion	Q-score
f	 0.6850	 0.1790
g	 0.7100	 0.1450
h	 0.6610	 0.1880
i	 0.5800	 0.1780
k	 0.6910	 0.2100
l	 0.6230	 0.1810
m	 0.5560	 0.1770
n	 0.7540	 0.1690
o	 0.7000	 0.1850
r	 0.6520	 0.1610
s	 0.7370	 0.1640
t	 0.5420	 0.2050
w	 0.6270	 0.2140
x	 0.5750	 0.1480
y	 0.7030	 0.1760
z	 0.6730	 0.1730