



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:02 AM UTC

PDB ID : 7WZN / pdb_00007wzn
EMDB ID : EMD-32907
Title : PSI-LHCI from Chlamydomonas reinhardtii with bound ferredoxin
Authors : Kurisu, G.; Gerle, C.; Mitsuoka, K.; Kawamoto, A.; Tanaka, H.
Deposited on : 2022-02-18
Resolution : 4.90 Å(reported)
Based on initial model : 6JO5

This is a Full wwPDB EM Validation 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

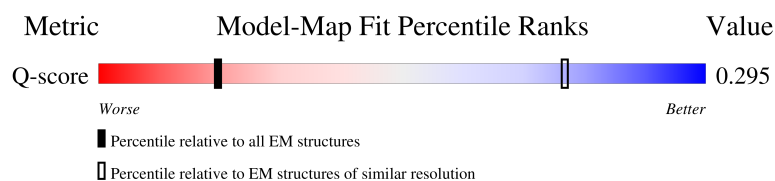
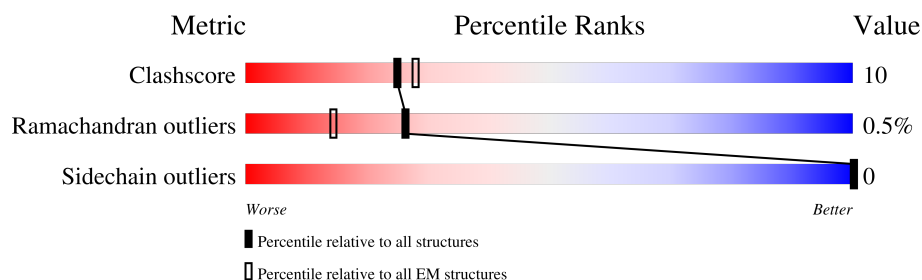
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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	1274 (4.40 - 5.40)

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	751	
2	B	735	
3	C	81	
4	D	196	

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Mol	Chain	Length	Quality of chain
5	E	97	
6	F	227	
7	J	41	
8	1	224	
9	3	298	
10	7	241	
11	8	243	
12	Z	228	
13	4	264	
14	5	257	
15	6	257	
16	G	126	

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
17	CL0	A	801	X	-	-	-
18	CLA	1	602	X	-	-	-
18	CLA	1	603	X	-	-	-
18	CLA	1	604	X	-	-	-
18	CLA	1	605	X	-	-	-
18	CLA	1	607	X	-	-	-
18	CLA	1	608	X	-	-	-
18	CLA	1	609	X	-	-	-
18	CLA	1	610	X	-	-	-
18	CLA	1	611	X	-	-	-
18	CLA	1	612	X	-	-	-
18	CLA	1	613	X	-	-	-
18	CLA	1	614	X	-	-	-
18	CLA	3	301	X	-	-	-
18	CLA	3	302	X	-	-	-
18	CLA	3	303	X	-	-	-
18	CLA	3	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	3	305	X	-	-	-
18	CLA	3	307	X	-	-	-
18	CLA	3	308	X	-	-	-
18	CLA	3	309	X	-	-	-
18	CLA	3	310	X	-	-	-
18	CLA	3	311	X	-	-	-
18	CLA	3	312	X	-	-	-
18	CLA	3	313	X	-	-	-
18	CLA	3	314	X	-	-	-
18	CLA	4	601	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	606	X	-	-	-
18	CLA	4	607	X	-	-	-
18	CLA	4	608	X	-	-	-
18	CLA	4	609	X	-	-	-
18	CLA	4	610	X	-	-	-
18	CLA	4	611	X	-	-	-
18	CLA	4	612	X	-	-	-
18	CLA	5	601	X	-	-	-
18	CLA	5	602	X	-	-	-
18	CLA	5	603	X	-	-	-
18	CLA	5	604	X	-	-	-
18	CLA	5	605	X	-	-	-
18	CLA	5	608	X	-	-	-
18	CLA	5	609	X	-	-	-
18	CLA	5	610	X	-	-	-
18	CLA	5	611	X	-	-	-
18	CLA	5	612	X	-	-	-
18	CLA	5	613	X	-	-	-
18	CLA	5	614	X	-	-	-
18	CLA	5	615	X	-	-	-
18	CLA	5	617	X	-	-	-
18	CLA	6	301	X	-	-	-
18	CLA	6	302	X	-	-	-
18	CLA	6	303	X	-	-	-
18	CLA	6	304	X	-	-	-
18	CLA	6	308	X	-	-	-
18	CLA	6	309	X	-	-	-
18	CLA	6	310	X	-	-	-
18	CLA	6	311	X	-	-	-
18	CLA	6	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	6	313	X	-	-	-
18	CLA	6	314	X	-	-	-
18	CLA	6	315	X	-	-	-
18	CLA	6	317	X	-	-	-
18	CLA	7	601	X	-	-	-
18	CLA	7	602	X	-	-	-
18	CLA	7	603	X	-	-	-
18	CLA	7	604	X	-	-	-
18	CLA	7	605	X	-	-	-
18	CLA	7	607	X	-	-	-
18	CLA	7	608	X	-	-	-
18	CLA	7	609	X	-	-	-
18	CLA	7	610	X	-	-	-
18	CLA	7	611	X	-	-	-
18	CLA	7	612	X	-	-	-
18	CLA	7	613	X	-	-	-
18	CLA	7	614	X	-	-	-
18	CLA	8	601	X	-	-	-
18	CLA	8	602	X	-	-	-
18	CLA	8	603	X	-	-	-
18	CLA	8	604	X	-	-	-
18	CLA	8	605	X	-	-	-
18	CLA	8	607	X	-	-	-
18	CLA	8	608	X	-	-	-
18	CLA	8	609	X	-	-	-
18	CLA	8	610	X	-	-	-
18	CLA	8	611	X	-	-	-
18	CLA	8	612	X	-	-	-
18	CLA	8	613	X	-	-	-
18	CLA	8	614	X	-	-	-
18	CLA	8	615	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	844	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	B	842	X	-	-	-
18	CLA	B	843	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	302	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	Z	602	X	-	-	-
18	CLA	Z	603	X	-	-	-
18	CLA	Z	604	X	-	-	-
18	CLA	Z	606	X	-	-	-
18	CLA	Z	607	X	-	-	-
18	CLA	Z	608	X	-	-	-
18	CLA	Z	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	Z	610	X	-	-	-
18	CLA	Z	611	X	-	-	-
18	CLA	Z	612	X	-	-	-
18	CLA	Z	613	X	-	-	-
20	SF4	C	101	-	-	X	-
21	CHL	1	601	X	-	-	-
21	CHL	1	606	X	-	-	-
21	CHL	3	306	X	-	-	-
21	CHL	4	604	X	-	-	-
21	CHL	4	605	X	-	-	-
21	CHL	5	606	X	-	-	-
21	CHL	5	607	X	-	-	-
21	CHL	5	616	X	-	-	-
21	CHL	6	305	X	-	-	-
21	CHL	6	306	X	-	-	-
21	CHL	6	307	X	-	-	-
21	CHL	6	316	X	-	-	-
21	CHL	7	606	X	-	-	-
21	CHL	8	606	X	-	-	-
21	CHL	Z	601	X	-	-	-
21	CHL	Z	605	X	-	-	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 27190 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 I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	738	Total	C	N	O	0	0
			3628	2151	739	738		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	732	Total	C	N	O	0	0
			3601	2136	733	732		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	80	Total	C	N	O	0	0
			395	235	80	80		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	144	Total	C	N	O	0	0
			706	418	144	144		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			300	178	61	61		

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	165	Total	C	N	O	0	0
			810	480	165	165		

- Molecule 7 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	39	Total	C	N	O	0	0
			194	116	39	39		

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	1	194	Total	C	N	O	0	0
			942	554	194	194		

- Molecule 9 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	3	202	Total	C	N	O	0	0
			985	581	202	202		

- Molecule 10 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	7	212	Total	C	N	O	0	0
			1033	609	212	212		

- Molecule 11 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	8	217	Total	C	N	O	0	0
			1059	625	217	217		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Z	192	Total	C	N	O	0	0
			934	550	192	192		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	4	203	Total	C	N	O	0	0
			992	586	203	203		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	5	223	Total	C	N	O	0	0
			1091	645	223	223		

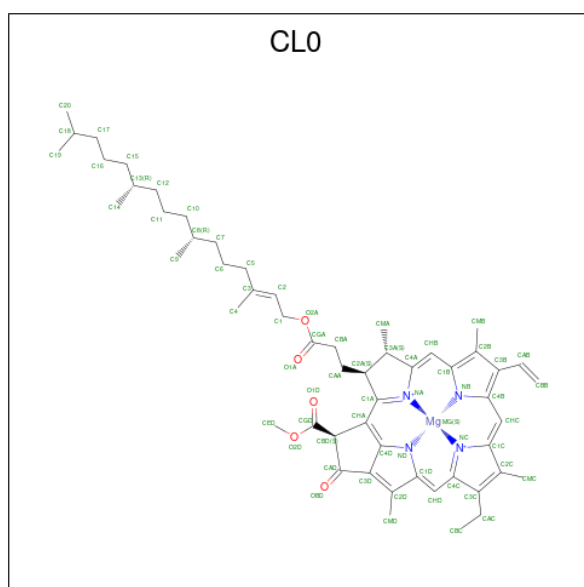
- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	6	229	Total	C	N	O	0	0
			1122	664	229	229		

- Molecule 16 is a protein called Ferredoxin, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	G	95	Total	C	N	O	5	0
			493	293	100	100		

- Molecule 17 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	42	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	Z	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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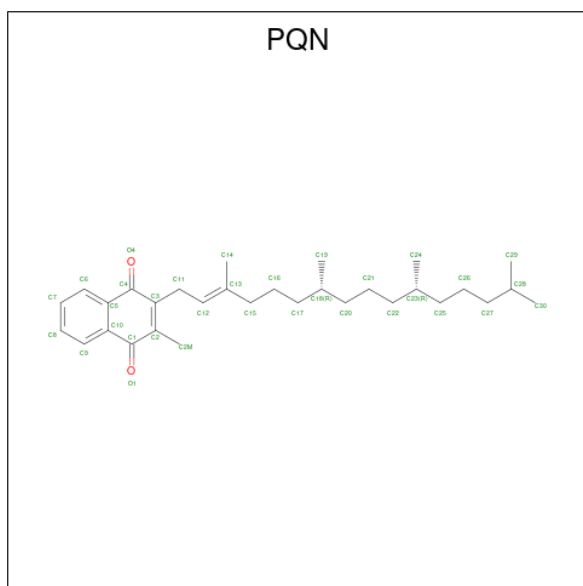
Mol	Chain	Residues	Atoms					AltConf
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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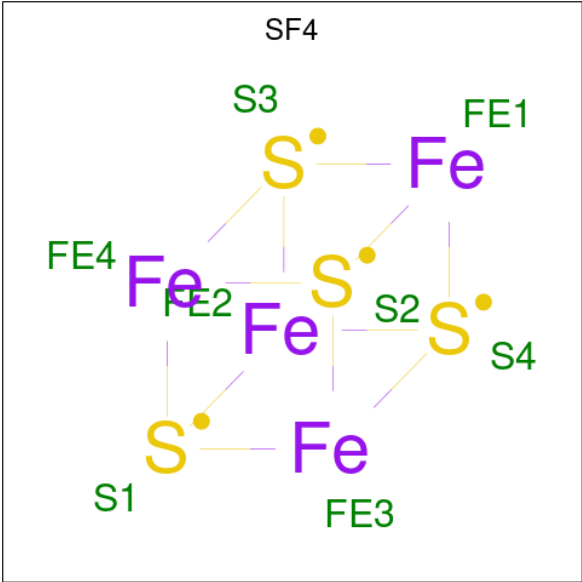
Mol	Chain	Residues	Atoms					AltConf
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



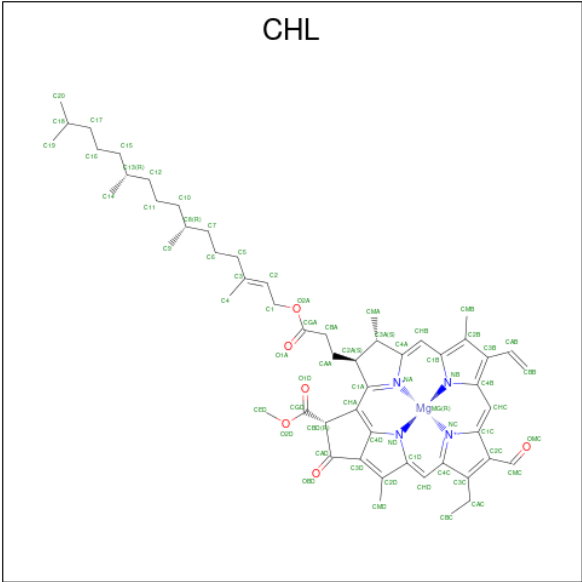
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			33	31	2	
19	B	1	Total	C	O	0
			33	31	2	

- Molecule 20 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



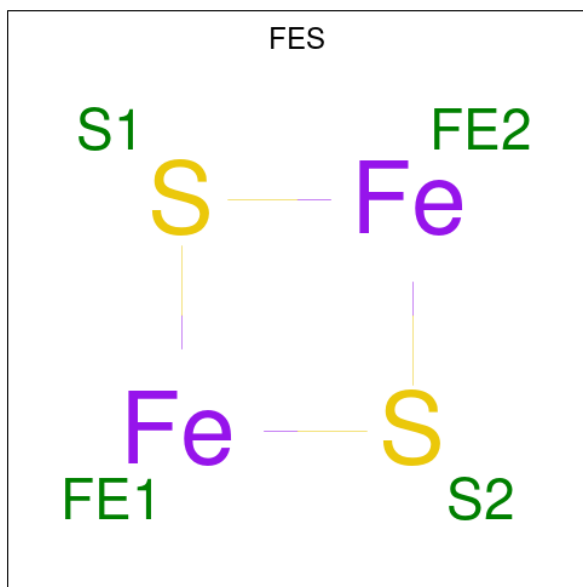
Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	Fe	S	0
			8	4	4	
20	C	1	Total	Fe	S	0
			8	4	4	
20	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 21 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	Z	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	Z	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

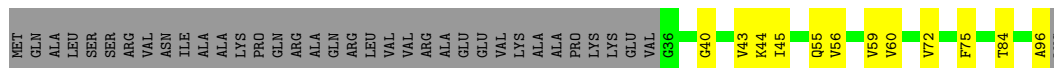


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
22	G	1	4	2	2	0



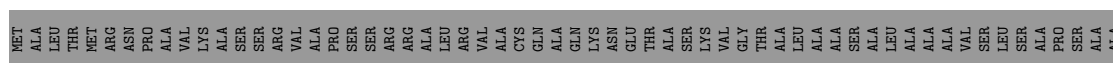
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E: 51% 12% 37%



- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F: 67% 6% 27%



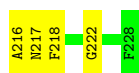
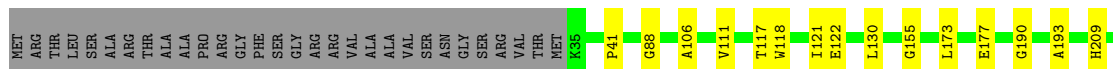
- Molecule 7: Photosystem I reaction center subunit IX

Chain J: 88% 7% 5%



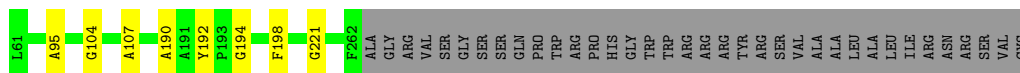
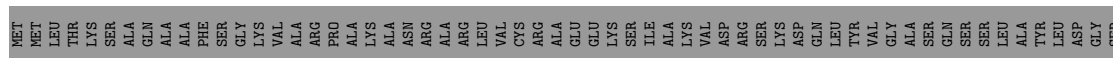
- Molecule 8: Chlorophyll a-b binding protein, chloroplastic

Chain 1: 78% 8% 13%



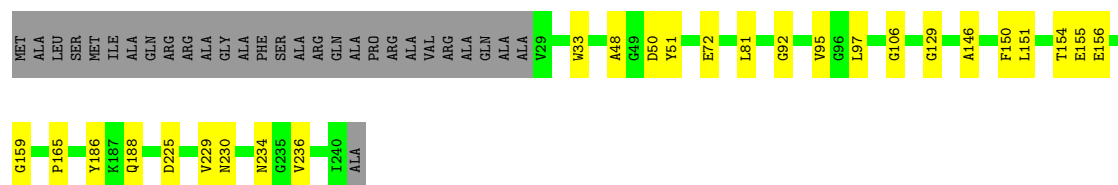
- Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 65% 0% 32%



- Molecule 10: Chlorophyll a-b binding protein, chloroplastic

Chain 7: 77% 11% 12%



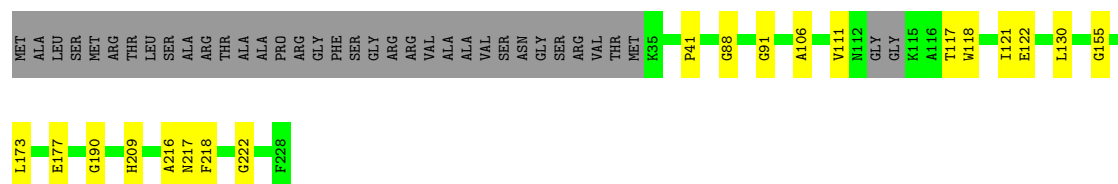
- Molecule 11: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 84% 6% 11%



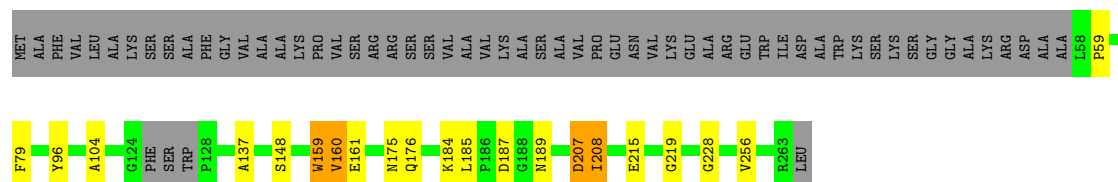
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z: 76% 8% 16%



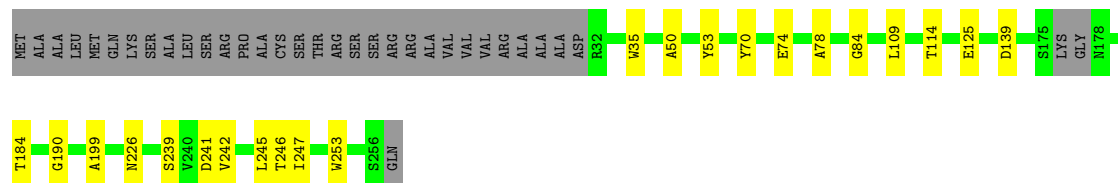
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 69% 6% 23%



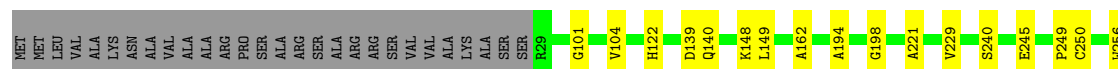
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 5: 78% 9% 13%



- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 6: 82% 7% 11%



MET	ALA	MET	ALA	ALA	MET	ARG	SER	THR	PHE	ALA	ALA	ARG	VAL	GLY	ALA	LYS	PRO	ALA	VAL	ALA	ARG	GLY	ALA	ARG	PRO	ALA	ALA	SER	ARG	MET	SER	CYS	MET	A0	T7	P8	S9	G10	D11	A29	A41	D58	Q59	S60	F61	L62	D63	D64	A65	Q66	M67	G68	V69
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48941	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	91	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	3.579	Depositor
Minimum map value	-0.699	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	431.2, 431.2, 431.2	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, FES, CL0, PQN, CHL, SF4

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	0.32	0/3628	0.51	0/5034
2	B	0.34	0/3602	0.74	9/5001 (0.2%)
3	C	0.37	0/394	0.67	0/547
4	D	0.39	0/705	0.58	1/977 (0.1%)
5	E	0.25	0/299	0.39	0/414
6	F	0.28	0/809	0.45	0/1122
7	J	0.29	0/193	0.53	0/268
8	1	0.30	0/941	0.49	0/1299
9	3	0.32	0/984	0.50	0/1361
10	7	0.32	0/1032	0.51	0/1427
11	8	0.30	0/1058	0.49	0/1464
12	Z	0.29	0/932	0.49	0/1286
13	4	0.32	0/990	0.63	3/1369 (0.2%)
14	5	0.28	0/1089	0.48	0/1507
15	6	0.30	0/1121	0.46	0/1554
16	G	0.46	0/492	0.66	0/683
All	All	0.32	0/18269	0.57	13/25313 (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
4	D	0	1
13	4	0	2
All	All	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	VAL	N-CA-C	-19.95	82.08	109.21
2	B	103	GLU	N-CA-CB	15.49	136.68	110.49
2	B	102	VAL	CB-CA-C	-11.05	95.65	111.34
13	4	160	VAL	N-CA-CB	9.99	121.60	110.51
2	B	113	PRO	CA-C-N	-9.17	109.71	122.92
2	B	113	PRO	C-N-CA	-9.17	109.71	122.92
2	B	105	PHE	N-CA-C	-8.61	102.59	113.43
2	B	106	THR	N-CA-C	-7.93	102.33	110.97
2	B	626	TRP	O-C-N	6.81	129.11	122.03
4	D	148	GLN	O-C-N	6.02	127.45	121.85
2	B	113	PRO	N-CA-CB	-5.62	97.35	103.25
13	4	159	TRP	CA-C-N	-5.32	113.74	120.60
13	4	159	TRP	C-N-CA	-5.32	113.74	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	4	207	ASP	Peptide
13	4	208	ILE	Peptide
4	D	149	TYR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	0	1728	55	0
2	B	3601	0	1713	80	0
3	C	395	0	178	14	0
4	D	706	0	316	12	0
5	E	300	0	135	6	0
6	F	810	0	404	10	0
7	J	194	0	87	4	0
8	1	942	0	489	17	0
9	3	985	0	480	7	0
10	7	1033	0	498	19	0
11	8	1059	0	527	15	0
12	Z	934	0	482	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	4	992	0	471	18	0
14	5	1091	0	504	16	0
15	6	1122	0	524	16	0
16	G	493	0	239	0	0
17	A	42	0	31	7	0
18	1	512	0	376	18	0
18	3	559	0	409	18	0
18	4	423	0	310	7	0
18	5	613	0	458	18	0
18	6	566	0	415	19	0
18	7	565	0	419	20	0
18	8	599	0	440	15	0
18	A	1831	0	1361	67	0
18	B	1782	0	1314	71	0
18	F	110	0	105	12	0
18	J	42	0	31	2	0
18	Z	466	0	345	19	0
19	A	33	0	46	6	0
19	B	33	0	46	5	0
20	B	8	0	0	1	0
20	C	16	0	0	3	0
21	1	96	0	70	4	0
21	3	43	0	29	0	0
21	4	89	0	59	5	0
21	5	129	0	87	2	0
21	6	172	0	116	3	0
21	7	43	0	29	0	0
21	8	43	0	29	3	0
21	Z	86	0	58	3	0
22	G	4	0	0	0	0
All	All	27190	0	15358	447	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 10.

All (447) 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)
2:B:102:VAL:CA	2:B:106:THR:CB	1.79	1.59
2:B:103:GLU:N	2:B:106:THR:CB	1.71	1.51
2:B:102:VAL:C	2:B:106:THR:CB	1.97	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:GLU:CA	2:B:107:ARG:H	1.46	1.25
2:B:103:GLU:C	2:B:107:ARG:H	1.44	1.17
2:B:103:GLU:CA	2:B:107:ARG:N	2.13	1.10
2:B:102:VAL:HA	2:B:106:THR:CB	1.65	1.06
1:A:651:TRP:CE2	2:B:626:TRP:CZ2	2.44	1.06
2:B:103:GLU:C	2:B:107:ARG:N	2.15	0.99
1:A:651:TRP:CH2	2:B:626:TRP:CE2	2.45	0.98
14:5:226:ASN:CB	18:5:613:CLA:HED2	1.94	0.98
1:A:651:TRP:CZ2	2:B:626:TRP:CE2	2.53	0.96
2:B:103:GLU:N	2:B:107:ARG:H	1.65	0.94
12:Z:111:VAL:CB	21:Z:605:CHL:OBD	2.15	0.93
8:1:111:VAL:CB	21:1:606:CHL:OBD	2.15	0.93
1:A:212:ALA:HA	18:A:815:CLA:HBB2	1.53	0.91
2:B:102:VAL:CB	2:B:106:THR:CB	2.48	0.91
10:7:72:GLU:HA	18:7:602:CLA:HBB1	1.56	0.88
4:D:139:TYR:HA	4:D:150:LEU:N	1.65	0.88
1:A:509:THR:HA	1:A:525:PRO:HA	1.55	0.87
11:8:131:GLY:HA2	18:8:608:CLA:HAB	1.55	0.86
2:B:103:GLU:N	2:B:107:ARG:N	2.24	0.85
12:Z:177:GLU:HA	18:Z:608:CLA:HBB1	1.60	0.84
2:B:518:PHE:HA	18:B:839:CLA:HED1	1.57	0.84
8:1:177:GLU:HA	18:1:609:CLA:HBB1	1.60	0.83
15:6:249:PRO:CB	18:6:301:CLA:HBB	2.09	0.82
18:A:835:CLA:HBB1	18:A:837:CLA:HED2	1.61	0.82
17:A:801:CL0:H15	18:A:844:CLA:HED1	1.62	0.81
15:6:249:PRO:CB	18:6:301:CLA:HMA1	2.11	0.81
12:Z:88:GLY:HA2	18:Z:603:CLA:HAB	1.65	0.79
2:B:93:TRP:H	18:B:811:CLA:HED2	1.47	0.79
8:1:88:GLY:HA2	18:1:604:CLA:HAB	1.65	0.78
15:6:101:GLY:HA2	21:6:305:CHL:HAC2	1.65	0.78
18:B:809:CLA:HBB	18:B:810:CLA:HMB3	1.64	0.78
14:5:74:GLU:HA	18:5:602:CLA:HBB1	1.65	0.78
18:F:302:CLA:C1B	18:F:302:CLA:H2	2.14	0.78
18:A:802:CLA:HAA1	18:A:844:CLA:HBB2	1.65	0.77
2:B:103:GLU:N	2:B:106:THR:CA	2.48	0.77
1:A:495:PRO:HA	1:A:499:ALA:HB3	1.67	0.76
14:5:241:ASP:HA	14:5:246:THR:HA	1.69	0.74
9:3:95:ALA:HB1	9:3:221:GLY:HA3	1.69	0.74
18:3:302:CLA:HHC	18:3:302:CLA:HBB1	1.70	0.74
10:7:129:GLY:HA2	18:7:608:CLA:HAB	1.69	0.74
1:A:533:PHE:HA	18:A:838:CLA:HED1	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:GLN:O	4:D:150:LEU:CB	2.38	0.72
18:6:312:CLA:HHC	18:6:312:CLA:HBB1	1.71	0.72
15:6:162:ALA:HB2	18:6:309:CLA:HBD	1.70	0.71
1:A:651:TRP:CZ2	2:B:626:TRP:CZ2	2.75	0.71
18:A:803:CLA:HHC	18:A:803:CLA:HBB1	1.72	0.71
1:A:684:MET:HA	18:A:802:CLA:HBC2	1.73	0.70
2:B:89:ALA:N	2:B:115:ASN:O	2.21	0.70
11:8:188:TRP:O	18:8:609:CLA:HMB3	1.92	0.70
15:6:249:PRO:CB	18:6:301:CLA:CHB	2.69	0.69
4:D:148:GLN:O	4:D:150:LEU:N	2.26	0.69
5:E:40:GLY:N	5:E:59:VAL:O	2.23	0.69
2:B:6:PHE:CB	2:B:14:ALA:HA	2.23	0.69
18:B:821:CLA:HAA2	18:B:826:CLA:HAB	1.73	0.69
2:B:709:VAL:HA	18:B:842:CLA:HED2	1.74	0.69
18:5:611:CLA:HHC	18:5:611:CLA:HBB1	1.74	0.69
8:1:217:ASN:HA	18:1:612:CLA:HAA1	1.74	0.68
4:D:139:TYR:HA	4:D:150:LEU:H	1.57	0.68
18:1:611:CLA:HHC	18:1:611:CLA:HBB1	1.76	0.68
3:C:4:ILE:O	3:C:68:TYR:N	2.27	0.68
2:B:203:SER:HA	2:B:246:GLY:HA2	1.76	0.68
18:A:843:CLA:HHC	18:A:843:CLA:HBB1	1.75	0.68
12:Z:217:ASN:HA	18:Z:611:CLA:HAA1	1.74	0.68
18:Z:610:CLA:HHC	18:Z:610:CLA:HBB1	1.76	0.68
18:A:823:CLA:HBB	18:A:843:CLA:HAC2	1.76	0.67
2:B:103:GLU:HA	2:B:107:ARG:N	2.08	0.67
14:5:242:VAL:N	14:5:245:LEU:O	2.28	0.67
1:A:473:SER:H	1:A:476:ALA:HB3	1.59	0.66
12:Z:130:LEU:HA	18:Z:604:CLA:HED2	1.77	0.66
2:B:92:ILE:N	2:B:113:PRO:O	2.27	0.66
18:A:826:CLA:HAA1	18:A:839:CLA:HED1	1.76	0.66
2:B:563:PRO:HA	2:B:567:GLY:HA2	1.77	0.66
18:8:609:CLA:HMB1	18:8:609:CLA:HBB1	1.78	0.66
1:A:578:PRO:HA	1:A:582:GLY:HA2	1.78	0.66
1:A:300:ALA:HA	18:A:817:CLA:HMC3	1.76	0.65
12:Z:216:ALA:HB1	18:Z:611:CLA:HED1	1.78	0.65
8:1:130:LEU:HA	18:1:605:CLA:HED2	1.77	0.65
18:A:843:CLA:H2	18:A:843:CLA:C4D	2.26	0.65
1:A:389:SER:HA	18:A:828:CLA:HMB3	1.78	0.65
10:7:81:LEU:CB	18:7:604:CLA:HBB2	2.27	0.65
18:F:301:CLA:HHC	18:F:301:CLA:HBB1	1.79	0.65
4:D:84:TYR:N	4:D:115:PHE:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:7:159:GLY:HA2	10:7:165:PRO:HA	1.78	0.65
13:4:215:GLU:HA	18:4:607:CLA:HBB1	1.79	0.64
11:8:88:LEU:O	11:8:92:LEU:N	2.28	0.64
18:5:612:CLA:HHC	18:5:612:CLA:HBB1	1.79	0.64
1:A:329:HIS:HA	18:A:843:CLA:HBC2	1.79	0.64
18:B:829:CLA:O1D	18:B:830:CLA:HBB1	1.98	0.64
8:1:216:ALA:HB1	18:1:612:CLA:HED1	1.78	0.64
18:A:816:CLA:HHC	18:A:816:CLA:HBB1	1.80	0.63
18:8:611:CLA:HHC	18:8:611:CLA:HBB1	1.80	0.63
11:8:69:TYR:O	18:8:602:CLA:HMB3	1.99	0.63
2:B:562:GLY:HA2	20:B:803:SF4:S1	2.39	0.63
10:7:81:LEU:CB	18:7:604:CLA:CBB	2.77	0.63
18:B:805:CLA:HMB1	18:B:805:CLA:HBB1	1.79	0.63
18:B:814:CLA:HHC	18:B:814:CLA:HBB1	1.81	0.62
18:A:806:CLA:H3A	18:A:830:CLA:HAB	1.81	0.62
18:B:842:CLA:HBD	19:B:844:PQN:H28	1.80	0.62
14:5:226:ASN:CB	18:5:613:CLA:CED	2.73	0.62
6:F:70:CYS:CB	6:F:125:CYS:CB	2.78	0.62
18:A:807:CLA:HMB3	18:A:808:CLA:H3A	1.82	0.62
10:7:146:ALA:HB1	10:7:155:GLU:H	1.64	0.62
18:B:806:CLA:HHC	18:B:808:CLA:OBD	2.00	0.61
18:A:812:CLA:HAC2	18:A:813:CLA:HAB	1.81	0.61
3:C:4:ILE:N	3:C:68:TYR:O	2.31	0.61
2:B:263:HIS:N	2:B:268:SER:O	2.23	0.61
18:1:612:CLA:HBB	18:1:613:CLA:HBC3	1.82	0.61
3:C:63:LEU:C	3:C:65:VAL:H	2.07	0.61
15:6:240:SER:HA	15:6:245:GLU:HA	1.82	0.61
1:A:20:ASN:N	1:A:183:LYS:O	2.31	0.61
18:Z:611:CLA:HBB	18:Z:612:CLA:HBC3	1.82	0.61
2:B:4:LYS:C	2:B:6:PHE:H	2.08	0.61
1:A:451:HIS:HA	18:A:834:CLA:HBB2	1.82	0.61
18:B:842:CLA:ND	19:B:844:PQN:H23	2.15	0.61
1:A:651:TRP:CG	2:B:626:TRP:HH2	2.12	0.60
21:5:607:CHL:OMC	21:5:616:CHL:HMC	2.01	0.60
15:6:122:HIS:HA	18:6:308:CLA:HAB	1.84	0.60
19:A:842:PQN:H23	18:A:845:CLA:C1B	2.32	0.59
18:B:814:CLA:HHD	18:B:815:CLA:HAB	1.84	0.59
18:5:610:CLA:H2	18:5:611:CLA:HMD2	1.84	0.59
3:C:53:ARG:N	20:C:101:SF4:S4	2.75	0.59
18:5:610:CLA:HBD	18:5:611:CLA:OBD	2.02	0.59
18:A:845:CLA:ND	18:B:802:CLA:HMC3	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:176:GLN:HA	13:4:184:LYS:HA	1.83	0.59
7:J:25:LEU:HA	18:J:101:CLA:HAB	1.85	0.59
1:A:121:ILE:O	1:A:123:GLY:N	2.35	0.59
2:B:487:PHE:O	2:B:491:GLN:CB	2.51	0.59
10:7:92:GLY:HA3	18:6:301:CLA:HED3	1.84	0.59
18:B:804:CLA:HHC	18:B:804:CLA:HBB1	1.85	0.59
10:7:48:ALA:HB1	10:7:188:GLN:HA	1.85	0.59
14:5:50:ALA:HB1	14:5:184:THR:HA	1.85	0.59
4:D:95:ILE:HA	4:D:105:ILE:HA	1.84	0.58
18:7:604:CLA:HBA1	18:7:605:CLA:C4C	2.33	0.58
4:D:85:VAL:HA	4:D:114:LYS:HA	1.86	0.58
5:E:60:VAL:N	5:E:72:VAL:O	2.35	0.57
1:A:558:ARG:O	1:A:567:ALA:N	2.37	0.57
19:A:842:PQN:H211	18:A:845:CLA:C3B	2.34	0.57
4:D:96:PHE:N	4:D:104:ALA:O	2.27	0.57
21:1:601:CHL:H2	11:8:131:GLY:HA3	1.87	0.57
18:Z:612:CLA:HHC	18:Z:612:CLA:HBB1	1.86	0.57
15:6:140:GLN:HA	15:6:148:LYS:HA	1.87	0.57
18:3:307:CLA:HBB1	18:3:313:CLA:CHC	2.34	0.57
3:C:63:LEU:C	3:C:65:VAL:N	2.61	0.56
18:1:613:CLA:HHC	18:1:613:CLA:HBB1	1.86	0.56
1:A:17:VAL:HA	1:A:186:PRO:HA	1.85	0.56
18:A:844:CLA:HBB1	18:A:844:CLA:HMB1	1.87	0.56
9:3:194:GLY:O	9:3:198:PHE:CB	2.54	0.56
18:A:825:CLA:HAA2	18:A:825:CLA:HBD	1.87	0.56
18:B:807:CLA:HMA3	18:B:831:CLA:HBB2	1.87	0.56
6:F:69:PRO:HA	6:F:124:LEU:HA	1.87	0.56
13:4:137:ALA:HB1	21:4:604:CHL:HAC2	1.87	0.56
18:5:614:CLA:HHC	18:5:614:CLA:HBB1	1.86	0.56
11:8:43:PRO:O	11:8:47:ALA:HB3	2.06	0.56
18:Z:604:CLA:HMC3	21:Z:605:CHL:C1C	2.36	0.56
5:E:75:PHE:N	5:E:84:THR:O	2.38	0.56
18:7:612:CLA:HHC	18:7:612:CLA:HBB1	1.88	0.56
18:3:314:CLA:HHC	18:3:314:CLA:HBB1	1.88	0.56
11:8:43:PRO:O	11:8:47:ALA:CB	2.54	0.55
3:C:31:TRP:N	3:C:37:SER:O	2.39	0.55
8:1:118:TRP:N	8:1:121:ILE:O	2.32	0.55
18:5:605:CLA:HBB1	18:5:605:CLA:HHC	1.88	0.55
18:1:605:CLA:HMC3	21:1:606:CHL:C1C	2.36	0.55
1:A:311:MET:HA	18:A:822:CLA:HAC2	1.88	0.55
9:3:107:ALA:HB2	18:3:303:CLA:HAC2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:TRP:HH2	2:B:626:TRP:O	1.89	0.54
18:3:304:CLA:C2C	18:3:305:CLA:HED2	2.37	0.54
13:4:137:ALA:HB1	21:4:604:CHL:HMC	1.89	0.54
18:3:307:CLA:CBB	18:3:313:CLA:HBB1	2.37	0.54
2:B:545:SER:N	2:B:548:MET:O	2.39	0.54
12:Z:117:THR:HA	12:Z:122:GLU:HA	1.89	0.54
18:A:838:CLA:HHC	18:A:838:CLA:HBB1	1.90	0.54
8:1:117:THR:HA	8:1:122:GLU:HA	1.89	0.54
17:A:801:CL0:H14	18:B:804:CLA:NA	2.23	0.54
5:E:44:LYS:HA	5:E:56:VAL:HA	1.90	0.54
15:6:249:PRO:CB	18:6:301:CLA:CMA	2.86	0.54
2:B:191:TRP:N	18:B:816:CLA:HAB	2.24	0.53
2:B:103:GLU:N	2:B:106:THR:C	2.67	0.53
1:A:651:TRP:CA	2:B:626:TRP:HH2	2.21	0.53
17:A:801:CL0:H14	18:B:804:CLA:C1A	2.38	0.53
18:Z:612:CLA:HED1	13:4:148:SER:HA	1.91	0.53
1:A:297:HIS:HA	18:A:818:CLA:C4B	2.39	0.53
18:A:841:CLA:HMC3	18:B:841:CLA:C1D	2.38	0.53
18:A:845:CLA:C1D	18:B:802:CLA:HMC3	2.39	0.53
4:D:89:GLU:HA	4:D:109:GLY:O	2.09	0.53
19:A:842:PQN:H252	18:A:845:CLA:C4A	2.39	0.52
18:B:801:CLA:HBB1	18:B:801:CLA:HMB1	1.90	0.52
18:F:302:CLA:H2	18:F:302:CLA:NB	2.24	0.52
18:3:313:CLA:HED2	18:7:601:CLA:CHB	2.39	0.52
11:8:239:SER:HA	18:8:614:CLA:O1D	2.09	0.52
12:Z:118:TRP:N	12:Z:121:ILE:O	2.32	0.52
18:B:832:CLA:HMB1	18:B:833:CLA:C3D	2.39	0.52
18:B:842:CLA:CHA	19:B:844:PQN:H261	2.39	0.52
8:1:209:HIS:HA	8:1:216:ALA:HB3	1.92	0.52
13:4:160:VAL:HA	21:4:605:CHL:NB	2.24	0.52
18:4:602:CLA:HBB1	18:4:603:CLA:HAA1	1.90	0.52
1:A:473:SER:N	1:A:476:ALA:HB3	2.25	0.52
2:B:4:LYS:C	2:B:6:PHE:N	2.68	0.52
1:A:651:TRP:HA	2:B:626:TRP:HH2	1.75	0.52
18:A:845:CLA:HED3	6:F:184:GLU:HA	1.92	0.52
2:B:273:ASP:O	18:B:819:CLA:HMB3	2.09	0.52
2:B:162:PHE:HA	18:B:813:CLA:HED2	1.92	0.52
13:4:187:ASP:O	13:4:189:ASN:N	2.40	0.52
18:B:834:CLA:HAB	18:B:835:CLA:HBB1	1.93	0.51
18:7:604:CLA:HMD2	18:6:301:CLA:CHD	2.41	0.51
14:5:70:TYR:O	18:5:602:CLA:HMB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:5:139:ASP:CB	21:5:607:CHL:HAC2	2.40	0.51
18:A:802:CLA:HHC	18:A:802:CLA:HBB1	1.92	0.51
18:6:315:CLA:HHC	18:6:315:CLA:HBB1	1.91	0.51
3:C:12:ILE:N	20:C:102:SF4:S2	2.81	0.51
12:Z:209:HIS:HA	12:Z:216:ALA:HB3	1.92	0.51
1:A:300:ALA:HB1	18:A:817:CLA:HBC2	1.92	0.51
2:B:277:HIS:HA	18:B:819:CLA:C3B	2.41	0.51
13:4:175:ASN:O	13:4:185:LEU:N	2.28	0.50
18:B:826:CLA:HAA2	18:B:826:CLA:HBD	1.93	0.50
18:B:834:CLA:C3B	18:B:835:CLA:HBB1	2.41	0.50
18:1:605:CLA:HAA2	18:1:605:CLA:HBD	1.93	0.50
18:Z:604:CLA:HAA2	18:Z:604:CLA:HBD	1.93	0.50
18:A:824:CLA:HHB	18:A:843:CLA:CBB	2.42	0.50
8:1:218:PHE:O	8:1:222:GLY:N	2.43	0.50
12:Z:218:PHE:O	12:Z:222:GLY:N	2.43	0.50
19:A:842:PQN:H252	18:A:845:CLA:NA	2.27	0.50
15:6:139:ASP:O	15:6:149:LEU:N	2.34	0.50
2:B:235:ALA:HB2	18:B:818:CLA:HMA2	1.93	0.50
3:C:52:LYS:N	20:C:101:SF4:S2	2.78	0.50
18:F:302:CLA:H93	18:F:302:CLA:HBC3	1.93	0.50
2:B:103:GLU:CA	2:B:107:ARG:CA	2.84	0.50
2:B:318:ALA:HB3	2:B:407:ASN:HA	1.92	0.50
13:4:256:VAL:HA	18:4:610:CLA:CAD	2.42	0.50
11:8:131:GLY:CA	18:8:608:CLA:HAB	2.36	0.50
18:B:824:CLA:HMB3	18:B:843:CLA:CHD	2.42	0.50
18:F:302:CLA:H52	18:F:302:CLA:C4B	2.42	0.50
12:Z:155:GLY:N	18:Z:608:CLA:OBD	2.41	0.49
1:A:84:ILE:HA	18:A:806:CLA:HAC2	1.94	0.49
11:8:210:LYS:O	11:8:214:GLY:HA2	2.12	0.49
8:1:155:GLY:N	18:1:609:CLA:OBD	2.41	0.49
18:B:814:CLA:HAC2	18:B:815:CLA:HAB	1.95	0.49
18:8:605:CLA:HMC3	21:8:606:CHL:NC	2.28	0.49
4:D:66:ILE:N	4:D:105:ILE:O	2.38	0.49
18:3:313:CLA:O2A	18:3:313:CLA:HBD	2.13	0.49
3:C:63:LEU:O	3:C:65:VAL:N	2.46	0.49
1:A:651:TRP:O	2:B:626:TRP:CH2	2.65	0.49
1:A:651:TRP:CH2	2:B:626:TRP:CG	2.74	0.48
18:A:841:CLA:HMC3	18:B:841:CLA:ND	2.28	0.48
18:3:304:CLA:HBB1	18:3:305:CLA:OBD	2.13	0.48
10:7:234:ASN:C	10:7:236:VAL:H	2.22	0.48
18:A:808:CLA:HMC3	18:A:809:CLA:HMD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:842:PQN:H211	18:A:845:CLA:C2B	2.43	0.48
2:B:103:GLU:O	2:B:108:GLY:N	2.42	0.48
10:7:50:ASP:HA	18:7:602:CLA:CGD	2.43	0.48
14:5:78:ALA:HB1	14:5:190:GLY:HA3	1.95	0.48
1:A:313:ARG:H	1:A:320:HIS:H	1.62	0.48
18:B:834:CLA:CAB	18:B:835:CLA:HBB1	2.44	0.48
3:C:3:HIS:HA	3:C:70:GLY:N	2.28	0.48
2:B:290:HIS:HA	18:B:822:CLA:HED1	1.96	0.48
14:5:253:TRP:CB	18:5:614:CLA:HMA3	2.43	0.48
21:6:305:CHL:HBC2	21:6:306:CHL:CHD	2.44	0.48
10:7:154:THR:C	10:7:156:GLU:H	2.21	0.47
18:A:803:CLA:HED2	7:J:12:PRO:HA	1.96	0.47
14:5:35:TRP:N	14:5:53:TYR:O	2.45	0.47
18:A:833:CLA:HHC	18:A:833:CLA:HBB1	1.96	0.47
1:A:454:GLY:HA2	18:A:834:CLA:HMC3	1.94	0.47
3:C:51:CYS:O	3:C:53:ARG:N	2.48	0.47
6:F:63:ASP:N	6:F:67:LEU:O	2.47	0.47
6:F:185:ILE:O	7:J:11:ALA:HB2	2.15	0.47
18:3:311:CLA:C4A	18:3:312:CLA:HMD2	2.45	0.47
18:7:604:CLA:HHD	18:6:301:CLA:HMD3	1.96	0.47
18:7:612:CLA:HBA2	18:7:613:CLA:C2D	2.45	0.47
12:Z:41:PRO:O	21:Z:601:CHL:HED1	2.15	0.47
18:B:814:CLA:CHD	18:B:815:CLA:HAB	2.44	0.47
2:B:216:VAL:O	18:B:817:CLA:HED3	2.15	0.47
18:B:802:CLA:C1A	18:B:802:CLA:CGA	2.92	0.47
18:B:825:CLA:HBB1	18:B:832:CLA:HBC2	1.96	0.47
18:B:842:CLA:CHD	19:B:844:PQN:H211	2.45	0.47
2:B:305:ILE:HA	18:B:824:CLA:HED2	1.96	0.47
5:E:43:VAL:HA	5:E:96:ALA:H	1.80	0.46
1:A:215:GLY:HA3	18:A:815:CLA:CAB	2.46	0.46
2:B:99:GLN:O	2:B:100:PRO:C	2.56	0.46
10:7:33:TRP:HA	18:7:601:CLA:C1C	2.45	0.46
1:A:148:TRP:O	1:A:152:GLY:N	2.48	0.46
8:1:41:PRO:O	21:1:601:CHL:HED1	2.15	0.46
2:B:190:ALA:C	18:B:816:CLA:HAB	2.41	0.46
15:6:256:TRP:HA	18:6:317:CLA:O1D	2.16	0.46
15:6:249:PRO:CB	18:6:301:CLA:C3A	2.93	0.46
18:B:810:CLA:HMC3	18:B:811:CLA:C3D	2.45	0.46
1:A:361:GLY:HA2	1:A:398:GLY:HA2	1.98	0.46
13:4:137:ALA:C	21:4:604:CHL:HAC2	2.41	0.46
1:A:118:VAL:HA	18:A:809:CLA:HED2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:7:186:TYR:O	18:7:609:CLA:HMB3	2.16	0.46
1:A:677:PHE:HA	18:A:844:CLA:HAA2	1.98	0.45
15:6:250:CYS:O	18:6:301:CLA:CBA	2.64	0.45
18:6:301:CLA:HAA1	18:6:301:CLA:HBD	1.98	0.45
1:A:651:TRP:CG	2:B:626:TRP:CH2	2.61	0.45
2:B:19:THR:O	2:B:22:ILE:N	2.49	0.45
10:7:225:ASP:O	10:7:229:VAL:N	2.49	0.45
2:B:292:TYR:HA	2:B:300:HIS:H	1.82	0.45
9:3:104:GLY:HA2	18:3:303:CLA:C3C	2.45	0.45
18:3:303:CLA:CHA	18:3:314:CLA:HMB3	2.47	0.45
12:Z:190:GLY:HA2	18:Z:611:CLA:C2C	2.47	0.45
14:5:199:ALA:HB2	18:5:612:CLA:HMC3	1.99	0.45
2:B:29:ALA:O	18:B:806:CLA:HED1	2.16	0.45
1:A:651:TRP:HH2	2:B:626:TRP:CG	2.32	0.45
6:F:69:PRO:O	6:F:73:SER:N	2.48	0.45
6:F:138:GLY:HA3	18:F:302:CLA:C3D	2.47	0.45
18:5:610:CLA:H2	18:5:611:CLA:CMD	2.46	0.45
18:A:812:CLA:HED2	18:A:813:CLA:HBC1	1.98	0.45
2:B:610:PHE:O	2:B:614:SER:CB	2.65	0.45
1:A:676:HIS:HA	17:A:801:CL0:CMA	2.47	0.45
18:A:814:CLA:HHC	18:A:814:CLA:HBB1	1.99	0.45
8:1:190:GLY:HA2	18:1:612:CLA:C2C	2.47	0.45
11:8:83:GLY:HA2	18:8:604:CLA:HAB	1.98	0.45
1:A:330:ARG:O	18:A:843:CLA:HBC3	2.17	0.45
17:A:801:CL0:H7	18:B:804:CLA:HAB	1.99	0.45
18:B:826:CLA:HAA2	18:B:826:CLA:CBD	2.47	0.45
18:B:811:CLA:HHB	18:B:812:CLA:HBB1	1.97	0.44
21:6:307:CHL:HAA1	21:6:307:CHL:HBD	1.98	0.44
18:F:302:CLA:H111	18:F:302:CLA:H72	1.69	0.44
18:A:827:CLA:C2B	18:A:835:CLA:H3A	2.47	0.44
11:8:30:TRP:HA	18:8:601:CLA:C1C	2.47	0.44
18:B:808:CLA:HHB	18:B:831:CLA:HAB	1.99	0.44
18:B:829:CLA:C3D	18:B:830:CLA:HMB3	2.47	0.44
18:F:302:CLA:H52	18:F:302:CLA:C3B	2.47	0.44
18:F:302:CLA:C1C	18:F:302:CLA:H71	2.47	0.44
18:F:302:CLA:CAD	18:F:302:CLA:H152	2.47	0.44
18:8:612:CLA:HBA2	18:8:613:CLA:C2D	2.47	0.44
13:4:96:TYR:O	18:4:602:CLA:HMB3	2.17	0.44
18:A:817:CLA:C1A	18:A:817:CLA:CGA	2.95	0.44
18:B:836:CLA:CHA	18:B:837:CLA:HMB3	2.47	0.44
1:A:270:SER:HA	18:A:817:CLA:HAA2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:842:PQN:H23	18:A:845:CLA:CHB	2.48	0.44
18:B:806:CLA:NA	18:B:806:CLA:HBA2	2.32	0.44
18:A:827:CLA:HBB1	18:A:827:CLA:HMB1	1.99	0.44
5:E:45:ILE:N	5:E:55:GLN:O	2.42	0.44
15:6:104:VAL:HA	18:6:304:CLA:HED1	1.99	0.44
2:B:190:ALA:HA	18:B:817:CLA:HBB2	2.00	0.44
1:A:129:GLY:O	1:A:136:GLN:HA	2.18	0.43
10:7:106:GLY:HA2	18:7:605:CLA:HAC2	2.00	0.43
18:7:614:CLA:HED3	18:7:614:CLA:HMA2	1.99	0.43
18:Z:604:CLA:HAA2	18:Z:604:CLA:CBD	2.47	0.43
1:A:651:TRP:HA	2:B:626:TRP:CH2	2.52	0.43
1:A:651:TRP:O	2:B:626:TRP:HH2	2.01	0.43
2:B:89:ALA:HB3	2:B:115:ASN:CB	2.48	0.43
18:B:825:CLA:HBB	18:B:843:CLA:O1D	2.19	0.43
9:3:190:ALA:C	9:3:192:TYR:H	2.26	0.43
18:8:605:CLA:HBC2	21:8:606:CHL:CHD	2.48	0.43
13:4:160:VAL:O	13:4:161:GLU:C	2.61	0.43
18:A:823:CLA:HMB3	18:A:843:CLA:C3C	2.48	0.43
18:1:605:CLA:HAA2	18:1:605:CLA:CBD	2.47	0.43
13:4:228:GLY:HA2	18:4:610:CLA:HMC2	2.00	0.43
2:B:325:ASP:O	2:B:329:ASN:N	2.51	0.43
18:F:302:CLA:H2	18:F:302:CLA:C2B	2.49	0.43
2:B:93:TRP:H	18:B:811:CLA:CED	2.25	0.43
2:B:291:MET:HA	18:B:823:CLA:HAC2	2.00	0.43
1:A:393:HIS:HA	18:A:828:CLA:CHC	2.49	0.43
2:B:92:ILE:CB	2:B:113:PRO:CB	2.96	0.43
6:F:210:LEU:O	6:F:213:GLY:N	2.49	0.43
14:5:84:GLY:HA2	18:5:604:CLA:HBB1	2.00	0.43
15:6:194:ALA:O	15:6:198:GLY:N	2.40	0.43
13:4:137:ALA:HB1	21:4:604:CHL:CMC	2.49	0.43
3:C:16:GLN:O	3:C:20:ALA:N	2.52	0.43
14:5:109:LEU:CB	14:5:114:THR:HA	2.49	0.43
18:5:610:CLA:H52	18:5:611:CLA:C2D	2.49	0.43
18:A:836:CLA:HHC	18:A:836:CLA:HBB1	1.99	0.43
2:B:153:ALA:HB2	18:B:813:CLA:HBC2	1.99	0.43
11:8:30:TRP:CB	18:8:601:CLA:HBB1	2.49	0.43
2:B:191:TRP:HA	18:B:816:CLA:HAB	2.01	0.42
18:3:302:CLA:HBC1	18:3:307:CLA:HAC1	2.01	0.42
17:A:801:CL0:H14	18:B:804:CLA:HAA2	2.01	0.42
13:4:256:VAL:H	18:4:611:CLA:HED2	1.85	0.42
2:B:11:GLN:HA	2:B:14:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:GLU:O	2:B:459:VAL:N	2.48	0.42
10:7:95:VAL:O	10:7:97:LEU:N	2.52	0.42
2:B:522:HIS:HA	18:B:839:CLA:HMA1	2.01	0.42
18:4:608:CLA:C3D	18:4:609:CLA:HMD3	2.49	0.42
1:A:310:HIS:HA	18:A:820:CLA:HED1	1.99	0.42
18:6:309:CLA:CBB	18:6:311:CLA:H3A	2.50	0.42
1:A:480:GLN:O	1:A:482:VAL:N	2.51	0.42
18:B:827:CLA:HMB2	18:B:840:CLA:CBA	2.49	0.42
18:F:302:CLA:H61	18:F:302:CLA:H41	1.89	0.42
9:3:107:ALA:CB	18:3:303:CLA:HAC2	2.49	0.42
18:8:612:CLA:CGA	18:8:612:CLA:C1A	2.98	0.42
12:Z:106:ALA:HA	18:Z:603:CLA:HED3	2.02	0.42
14:5:239:SER:HA	14:5:247:ILE:O	2.19	0.42
18:6:301:CLA:HAA1	18:6:301:CLA:CBD	2.49	0.42
2:B:486:ALA:HB2	18:B:837:CLA:C3D	2.50	0.42
15:6:221:ALA:HB1	15:6:229:VAL:O	2.20	0.42
1:A:676:HIS:HA	17:A:801:CL0:H6	2.01	0.42
4:D:86:ILE:HA	4:D:138:PHE:CB	2.49	0.42
12:Z:173:LEU:CB	18:Z:608:CLA:HBB	2.50	0.42
13:4:104:ALA:HB1	13:4:219:GLY:HA3	2.02	0.42
18:6:310:CLA:C4D	18:6:311:CLA:HMD3	2.50	0.42
8:1:118:TRP:HA	18:1:604:CLA:OBD	2.20	0.41
18:5:610:CLA:H93	18:5:611:CLA:C1C	2.50	0.41
1:A:119:TRP:N	18:A:809:CLA:O1D	2.54	0.41
2:B:718:TYR:O	18:B:804:CLA:HED2	2.20	0.41
2:B:117:SER:HA	18:B:810:CLA:HMD1	2.03	0.41
3:C:6:LYS:O	3:C:65:VAL:HA	2.19	0.41
18:3:314:CLA:HBD	18:3:314:CLA:HAA1	2.02	0.41
12:Z:118:TRP:HA	18:Z:603:CLA:OBD	2.20	0.41
18:A:806:CLA:H3A	18:A:830:CLA:CAB	2.48	0.41
2:B:191:TRP:CA	18:B:816:CLA:HAB	2.51	0.41
18:7:612:CLA:HBA2	18:7:613:CLA:HMD2	2.02	0.41
13:4:159:TRP:O	13:4:160:VAL:C	2.61	0.41
18:A:845:CLA:CMD	18:B:802:CLA:HBB1	2.50	0.41
9:3:194:GLY:N	18:3:308:CLA:OBD	2.33	0.41
18:7:605:CLA:HHC	18:7:605:CLA:HBB1	2.02	0.41
13:4:59:PRO:O	13:4:79:PHE:HA	2.21	0.41
1:A:311:MET:CA	18:A:822:CLA:HAC2	2.51	0.41
8:1:173:LEU:CB	18:1:609:CLA:HBB	2.50	0.41
18:1:614:CLA:HBA1	18:1:614:CLA:H3A	1.92	0.41
18:3:302:CLA:OBD	18:3:307:CLA:HAA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:637:ASN:C	2:B:639:PHE:H	2.27	0.41
2:B:687:PRO:C	2:B:689:ALA:H	2.29	0.41
10:7:230:ASN:HA	18:7:612:CLA:HAA1	2.02	0.41
1:A:540:ALA:HB1	18:A:838:CLA:HMB3	2.03	0.41
18:B:824:CLA:HMB3	18:B:843:CLA:C1D	2.51	0.41
3:C:15:THR:O	3:C:19:ARG:N	2.36	0.41
10:7:51:TYR:N	18:7:602:CLA:OBD	2.38	0.41
18:7:608:CLA:H3A	18:7:608:CLA:HBA2	1.87	0.41
12:Z:88:GLY:HA2	18:Z:603:CLA:CAB	2.44	0.41
18:5:601:CLA:HAA2	18:5:601:CLA:HBD	2.02	0.41
2:B:288:ALA:C	2:B:290:HIS:H	2.29	0.41
6:F:70:CYS:HA	6:F:73:SER:CB	2.51	0.41
18:3:307:CLA:HBB1	18:3:313:CLA:HHC	2.02	0.41
18:B:814:CLA:HBD	18:B:814:CLA:HAA1	2.02	0.40
11:8:106:ASP:HA	21:8:606:CHL:CED	2.51	0.40
18:B:842:CLA:C1D	19:B:844:PQN:H23	2.51	0.40
8:1:106:ALA:HA	18:1:604:CLA:HED3	2.02	0.40
18:A:818:CLA:O1D	18:A:819:CLA:HHB	2.22	0.40
2:B:375:HIS:HA	18:B:829:CLA:C4B	2.52	0.40
2:B:525:ALA:HB2	18:B:840:CLA:HED2	2.03	0.40
2:B:632:LEU:C	2:B:634:ASN:H	2.29	0.40
11:8:126:GLN:CB	18:8:605:CLA:HMA3	2.51	0.40
12:Z:91:GLY:HA3	18:Z:603:CLA:C1C	2.51	0.40
1:A:501:ASN:CB	18:A:836:CLA:HED2	2.51	0.40
7:J:25:LEU:CA	18:J:101:CLA:HAB	2.49	0.40
8:1:193:ALA:CB	18:1:612:CLA:HAC2	2.52	0.40
10:7:150:PHE:O	10:7:151:LEU:C	2.65	0.40
14:5:125:GLU:HA	18:5:605:CLA:HMA2	2.02	0.40
1:A:25:SER:N	18:A:811:CLA:HMB3	2.37	0.40
1:A:90:GLY:HA3	18:A:807:CLA:CBB	2.51	0.40
18:A:805:CLA:HMB1	18:A:805:CLA:HBB1	2.04	0.40
18:B:822:CLA:CGA	18:B:822:CLA:C4A	2.98	0.40
4:D:138:PHE:O	4:D:149:TYR:C	2.64	0.40
6:F:209:GLU:O	6:F:213:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	734/751 (98%)	670 (91%)	63 (9%)	1 (0%)	48	83
2	B	730/735 (99%)	656 (90%)	68 (9%)	6 (1%)	16	52
3	C	78/81 (96%)	64 (82%)	12 (15%)	2 (3%)	4	25
4	D	142/196 (72%)	120 (84%)	16 (11%)	6 (4%)	2	17
5	E	59/97 (61%)	55 (93%)	4 (7%)	0	100	100
6	F	163/227 (72%)	154 (94%)	9 (6%)	0	100	100
7	J	37/41 (90%)	32 (86%)	5 (14%)	0	100	100
8	1	192/224 (86%)	175 (91%)	17 (9%)	0	100	100
9	3	200/298 (67%)	182 (91%)	18 (9%)	0	100	100
10	7	210/241 (87%)	193 (92%)	17 (8%)	0	100	100
11	8	215/243 (88%)	192 (89%)	23 (11%)	0	100	100
12	Z	188/228 (82%)	172 (92%)	16 (8%)	0	100	100
13	4	199/264 (75%)	175 (88%)	22 (11%)	2 (1%)	12	47
14	5	219/257 (85%)	194 (89%)	25 (11%)	0	100	100
15	6	227/257 (88%)	205 (90%)	22 (10%)	0	100	100
16	G	98/126 (78%)	93 (95%)	5 (5%)	0	100	100
All	All	3691/4266 (86%)	3332 (90%)	342 (9%)	17 (0%)	26	63

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	6	PHE
2	B	7	PRO
2	B	103	GLU
3	C	64	SER
4	D	149	TYR
4	D	151	HIS

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Mol	Chain	Res	Type
1	A	122	VAL
2	B	108	GLY
2	B	110	ALA
4	D	152	PRO
4	D	155	GLY
4	D	156	VAL
13	4	207	ASP
3	C	61	ASP
4	D	153	ALA
13	4	208	ILE
2	B	109	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1/610 (0%)	1 (100%)	0	100	100
2	B	1/597 (0%)	1 (100%)	0	100	100
All	All	2/1207 (0%)	2 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

211 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	823	-	55,59,73	1.95	9 (16%)	64,96,113	1.55	11 (17%)
18	CLA	B	835	-	46,50,73	2.21	9 (19%)	53,85,113	1.65	10 (18%)
18	CLA	3	312	-	49,53,73	2.06	9 (18%)	58,89,113	1.36	8 (13%)
21	CHL	5	616	-	37,51,74	2.52	9 (24%)	30,86,114	1.45	6 (20%)
18	CLA	7	614	10	46,50,73	2.16	10 (21%)	53,85,113	2.02	10 (18%)
18	CLA	1	611	-	46,50,73	2.13	9 (19%)	53,85,113	1.42	7 (13%)
18	CLA	5	614	14	46,50,73	2.03	8 (17%)	53,85,113	1.37	9 (16%)
18	CLA	Z	607	-	46,50,73	2.13	8 (17%)	53,85,113	1.81	11 (20%)
18	CLA	Z	612	-	46,50,73	2.09	9 (19%)	53,85,113	1.47	9 (16%)
18	CLA	4	607	-	46,50,73	2.20	10 (21%)	53,85,113	1.41	7 (13%)
18	CLA	A	838	-	46,50,73	2.05	9 (19%)	53,85,113	1.51	10 (18%)
18	CLA	6	302	-	46,50,73	2.13	10 (21%)	53,85,113	1.48	9 (16%)
18	CLA	B	807	-	53,57,73	2.10	11 (20%)	60,92,113	1.40	8 (13%)
18	CLA	A	818	-	46,50,73	2.15	10 (21%)	53,85,113	1.42	9 (16%)
18	CLA	1	605	-	46,50,73	2.09	12 (26%)	53,85,113	1.43	8 (15%)
18	CLA	B	819	-	46,50,73	2.12	9 (19%)	53,85,113	1.70	9 (16%)
18	CLA	B	809	-	46,50,73	2.07	10 (21%)	53,85,113	1.43	9 (16%)
18	CLA	A	828	-	46,50,73	2.09	11 (23%)	53,85,113	1.36	10 (18%)
21	CHL	7	606	-	37,51,74	2.52	10 (27%)	30,86,114	1.23	4 (13%)
18	CLA	A	821	-	46,50,73	2.10	11 (23%)	53,85,113	1.32	8 (15%)
18	CLA	8	614	-	46,50,73	2.17	10 (21%)	53,85,113	1.57	8 (15%)
20	SF4	C	102	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	837	-	46,50,73	2.03	8 (17%)	53,85,113	1.36	8 (15%)
18	CLA	B	813	-	45,49,73	2.11	10 (22%)	54,84,113	1.40	8 (14%)
18	CLA	A	819	-	46,50,73	2.13	9 (19%)	53,85,113	1.56	9 (16%)
18	CLA	A	820	-	46,50,73	2.12	10 (21%)	53,85,113	1.47	10 (18%)
18	CLA	Z	609	-	46,50,73	2.13	7 (15%)	53,85,113	1.56	9 (16%)
18	CLA	8	612	-	50,54,73	2.05	12 (24%)	59,90,113	1.33	7 (11%)
21	CHL	1	606	-	37,51,74	2.63	10 (27%)	30,86,114	1.28	5 (16%)
18	CLA	A	816	-	46,50,73	2.12	10 (21%)	53,85,113	1.36	8 (15%)
18	CLA	B	808	-	46,50,73	2.14	11 (23%)	53,85,113	1.45	7 (13%)
18	CLA	Z	610	-	46,50,73	2.13	9 (19%)	53,85,113	1.41	7 (13%)
18	CLA	A	831	-	46,50,73	2.13	10 (21%)	53,85,113	1.53	8 (15%)
21	CHL	8	606	-	37,51,74	2.46	9 (24%)	30,86,114	1.38	4 (13%)
18	CLA	F	302	-	69,73,73	1.69	10 (14%)	82,113,113	1.18	10 (12%)
18	CLA	B	840	-	46,50,73	2.12	9 (19%)	53,85,113	1.43	10 (18%)
18	CLA	7	608	-	54,58,73	1.96	9 (16%)	64,95,113	1.37	9 (14%)
18	CLA	Z	602	-	46,50,73	2.10	10 (21%)	53,85,113	1.39	9 (16%)
18	CLA	3	305	9	46,50,73	2.22	10 (21%)	53,85,113	2.00	12 (22%)
18	CLA	A	822	-	46,50,73	2.22	10 (21%)	53,85,113	1.50	8 (15%)
21	CHL	6	307	-	37,51,74	2.52	9 (24%)	30,86,114	1.52	7 (23%)
18	CLA	A	817	-	51,55,73	2.02	12 (23%)	60,91,113	1.37	10 (16%)
18	CLA	A	808	-	46,50,73	2.27	11 (23%)	53,85,113	1.55	8 (15%)
18	CLA	B	830	-	49,53,73	2.04	10 (20%)	58,89,113	1.28	9 (15%)
18	CLA	Z	603	-	46,50,73	2.19	10 (21%)	53,85,113	1.32	8 (15%)
18	CLA	6	314	15	50,54,73	2.09	10 (20%)	59,90,113	1.35	8 (13%)
18	CLA	A	806	-	46,50,73	2.15	10 (21%)	53,85,113	1.45	9 (16%)
18	CLA	1	607	-	46,50,73	2.10	9 (19%)	53,85,113	1.38	8 (15%)
18	CLA	1	612	-	50,54,73	2.02	9 (18%)	59,90,113	1.28	7 (11%)
18	CLA	5	611	-	46,50,73	2.06	10 (21%)	53,85,113	1.49	9 (16%)
22	FES	G	101	-	0,4,4	-	-	-	-	-
18	CLA	A	826	-	46,50,73	2.18	10 (21%)	53,85,113	1.59	8 (15%)
18	CLA	3	311	-	49,53,73	2.10	12 (24%)	58,89,113	1.27	8 (13%)
18	CLA	4	602	-	46,50,73	2.18	11 (23%)	53,85,113	1.46	6 (11%)
21	CHL	Z	605	-	37,51,74	2.62	10 (27%)	30,86,114	1.28	4 (13%)
18	CLA	B	838	-	47,51,73	2.20	9 (19%)	55,86,113	1.33	8 (14%)
18	CLA	B	836	-	46,50,73	2.14	10 (21%)	53,85,113	1.50	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	834	-	46,50,73	2.27	10 (21%)	53,85,113	1.87	12 (22%)
20	SF4	B	803	-	0,12,12	-	-	-		
18	CLA	4	611	-	46,50,73	2.09	8 (17%)	53,85,113	1.36	8 (15%)
18	CLA	4	609	-	46,50,73	2.18	9 (19%)	53,85,113	1.36	9 (16%)
18	CLA	B	825	-	46,50,73	2.11	10 (21%)	53,85,113	1.35	8 (15%)
18	CLA	8	613	-	46,50,73	2.11	10 (21%)	53,85,113	1.41	7 (13%)
18	CLA	B	832	-	46,50,73	2.13	9 (19%)	53,85,113	1.39	7 (13%)
18	CLA	7	602	-	46,50,73	2.12	11 (23%)	53,85,113	1.43	10 (18%)
18	CLA	4	606	-	46,50,73	2.04	9 (19%)	53,85,113	1.35	6 (11%)
18	CLA	6	312	-	49,53,73	2.09	11 (22%)	58,89,113	1.27	8 (13%)
18	CLA	A	809	-	46,50,73	2.12	11 (23%)	53,85,113	1.33	8 (15%)
18	CLA	3	309	-	45,49,73	2.21	10 (22%)	54,84,113	1.85	11 (20%)
18	CLA	3	303	-	46,50,73	2.10	10 (21%)	53,85,113	1.39	8 (15%)
18	CLA	B	812	-	46,50,73	2.21	9 (19%)	53,85,113	1.77	11 (20%)
21	CHL	5	606	-	37,51,74	2.53	10 (27%)	30,86,114	1.21	3 (10%)
18	CLA	A	832	-	46,50,73	2.12	10 (21%)	53,85,113	1.42	8 (15%)
18	CLA	B	829	-	46,50,73	2.16	10 (21%)	53,85,113	1.45	9 (16%)
18	CLA	5	604	-	46,50,73	2.09	9 (19%)	53,85,113	1.41	8 (15%)
18	CLA	1	613	-	46,50,73	2.09	9 (19%)	53,85,113	1.47	9 (16%)
18	CLA	B	834	-	42,46,73	4.18	12 (28%)	40,77,113	1.55	7 (17%)
18	CLA	A	805	-	46,50,73	2.17	11 (23%)	53,85,113	1.50	8 (15%)
18	CLA	8	602	-	46,50,73	2.07	9 (19%)	53,85,113	1.32	9 (16%)
18	CLA	7	604	-	47,51,73	2.29	10 (21%)	55,86,113	1.62	11 (20%)
18	CLA	A	812	-	46,50,73	2.12	12 (26%)	53,85,113	1.45	9 (16%)
18	CLA	A	843	-	56,60,73	1.94	9 (16%)	65,97,113	1.23	8 (12%)
18	CLA	Z	611	-	49,53,73	2.04	9 (18%)	58,89,113	1.30	7 (12%)
18	CLA	1	603	-	46,50,73	2.09	11 (23%)	53,85,113	1.36	8 (15%)
18	CLA	1	604	-	46,50,73	2.19	10 (21%)	53,85,113	1.32	8 (15%)
18	CLA	3	301	-	46,50,73	2.14	9 (19%)	53,85,113	1.46	8 (15%)
18	CLA	B	821	-	46,50,73	2.02	9 (19%)	53,85,113	1.32	9 (16%)
18	CLA	B	826	-	46,50,73	2.11	10 (21%)	53,85,113	1.33	8 (15%)
18	CLA	4	603	-	50,54,73	2.07	12 (24%)	59,90,113	1.34	8 (13%)
18	CLA	A	824	-	46,50,73	2.24	11 (23%)	53,85,113	1.56	8 (15%)
18	CLA	A	841	-	46,50,73	2.20	12 (26%)	53,85,113	1.36	9 (16%)
18	CLA	B	823	-	46,50,73	2.10	11 (23%)	53,85,113	1.44	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	4	601	13	46,50,73	2.24	9 (19%)	53,85,113	1.70	8 (15%)
18	CLA	5	605	-	46,50,73	2.10	11 (23%)	53,85,113	1.38	7 (13%)
18	CLA	5	601	14	46,50,73	2.20	9 (19%)	53,85,113	1.31	8 (15%)
17	CL0	A	801	-	35,50,73	2.53	8 (22%)	32,85,113	1.69	2 (6%)
18	CLA	4	612	-	45,49,73	2.24	8 (17%)	54,84,113	1.24	8 (14%)
18	CLA	8	610	-	50,54,73	2.11	7 (14%)	59,90,113	1.57	11 (18%)
18	CLA	F	301	-	49,53,73	2.07	8 (16%)	58,89,113	1.39	7 (12%)
18	CLA	B	820	-	46,50,73	2.15	7 (15%)	53,85,113	1.73	12 (22%)
18	CLA	8	609	-	46,50,73	2.20	10 (21%)	53,85,113	1.43	7 (13%)
18	CLA	Z	604	-	47,51,73	2.06	12 (25%)	55,86,113	1.41	8 (14%)
18	CLA	B	802	-	50,54,73	2.11	10 (20%)	59,90,113	1.35	8 (13%)
18	CLA	B	816	-	46,50,73	2.12	10 (21%)	53,85,113	1.41	8 (15%)
18	CLA	3	314	-	46,50,73	2.09	11 (23%)	53,85,113	1.36	9 (16%)
18	CLA	7	601	10	46,50,73	2.14	10 (21%)	53,85,113	1.43	9 (16%)
18	CLA	5	608	-	46,50,73	2.13	11 (23%)	53,85,113	1.31	7 (13%)
21	CHL	6	306	-	37,51,74	2.48	9 (24%)	30,86,114	1.44	7 (23%)
18	CLA	3	313	-	50,54,73	2.01	10 (20%)	59,90,113	1.33	9 (15%)
18	CLA	B	801	-	46,50,73	2.13	10 (21%)	53,85,113	1.43	8 (15%)
18	CLA	B	806	-	49,53,73	2.21	9 (18%)	58,89,113	1.67	8 (13%)
18	CLA	8	605	-	46,50,73	2.12	12 (26%)	53,85,113	1.35	7 (13%)
18	CLA	B	814	-	46,50,73	2.14	7 (15%)	53,85,113	1.34	7 (13%)
18	CLA	6	310	-	46,50,73	2.25	7 (15%)	53,85,113	2.13	8 (15%)
18	CLA	3	308	-	46,50,73	2.10	11 (23%)	53,85,113	1.34	9 (16%)
18	CLA	1	610	-	46,50,73	2.13	7 (15%)	53,85,113	1.55	9 (16%)
19	PQN	B	844	-	34,34,34	0.25	0	43,45,45	0.52	1 (2%)
18	CLA	3	307	-	46,50,73	2.19	8 (17%)	53,85,113	1.65	8 (15%)
18	CLA	A	835	-	46,50,73	2.22	10 (21%)	53,85,113	1.39	8 (15%)
18	CLA	J	101	-	46,50,73	2.07	9 (19%)	53,85,113	1.40	8 (15%)
18	CLA	3	304	-	46,50,73	2.07	10 (21%)	53,85,113	1.44	8 (15%)
18	CLA	A	802	-	46,50,73	2.19	9 (19%)	53,85,113	1.72	10 (18%)
18	CLA	8	604	-	46,50,73	2.10	9 (19%)	53,85,113	1.33	7 (13%)
18	CLA	A	845	-	46,50,73	2.19	12 (26%)	53,85,113	1.34	9 (16%)
18	CLA	8	601	11	46,50,73	2.08	9 (19%)	53,85,113	1.34	8 (15%)
18	CLA	A	804	-	46,50,73	2.08	9 (19%)	53,85,113	1.45	7 (13%)
18	CLA	B	839	-	46,50,73	2.08	7 (15%)	53,85,113	1.41	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	4	610	-	46,50,73	2.09	11 (23%)	53,85,113	1.39	5 (9%)
18	CLA	8	603	-	49,53,73	2.06	9 (18%)	58,89,113	1.38	8 (13%)
18	CLA	A	839	-	46,50,73	2.13	12 (26%)	53,85,113	1.42	8 (15%)
18	CLA	A	825	-	46,50,73	2.17	8 (17%)	53,85,113	1.58	10 (18%)
18	CLA	B	843	-	46,50,73	2.07	10 (21%)	53,85,113	1.43	7 (13%)
18	CLA	7	603	-	50,54,73	2.08	10 (20%)	59,90,113	1.33	8 (13%)
18	CLA	3	310	-	50,54,73	2.00	10 (20%)	59,90,113	1.31	8 (13%)
21	CHL	4	605	-	40,54,74	2.60	9 (22%)	34,90,114	1.89	6 (17%)
18	CLA	4	608	-	46,50,73	2.22	8 (17%)	53,85,113	1.78	10 (18%)
18	CLA	A	844	-	46,50,73	2.04	9 (19%)	53,85,113	1.36	9 (16%)
18	CLA	Z	608	-	46,50,73	2.15	10 (21%)	53,85,113	1.34	7 (13%)
21	CHL	6	305	-	37,51,74	2.60	9 (24%)	30,86,114	1.50	7 (23%)
18	CLA	8	607	-	46,50,73	2.19	10 (21%)	53,85,113	1.40	7 (13%)
18	CLA	B	815	-	46,50,73	2.29	10 (21%)	53,85,113	1.79	9 (16%)
18	CLA	B	842	-	46,50,73	2.15	11 (23%)	53,85,113	1.55	9 (16%)
18	CLA	7	609	-	49,53,73	2.04	10 (20%)	58,89,113	1.30	7 (12%)
18	CLA	B	828	-	46,50,73	2.06	9 (19%)	53,85,113	1.36	7 (13%)
18	CLA	A	811	-	47,51,73	2.17	9 (19%)	55,86,113	1.36	7 (12%)
18	CLA	5	615	-	50,54,73	2.16	8 (16%)	59,90,113	1.88	11 (18%)
18	CLA	5	612	-	46,50,73	2.13	11 (23%)	53,85,113	1.39	8 (15%)
18	CLA	6	303	-	50,54,73	1.99	10 (20%)	59,90,113	1.28	8 (13%)
18	CLA	5	610	-	59,63,73	1.79	8 (13%)	70,101,113	1.28	8 (11%)
21	CHL	Z	601	12	37,51,74	2.42	9 (24%)	30,86,114	1.36	5 (16%)
20	SF4	C	101	3	0,12,12	-	-	-	-	-
18	CLA	A	829	-	46,50,73	2.08	10 (21%)	53,85,113	1.43	7 (13%)
18	CLA	A	807	-	46,50,73	2.22	10 (21%)	53,85,113	1.45	10 (18%)
21	CHL	3	306	-	37,51,74	2.85	9 (24%)	30,86,114	1.41	5 (16%)
18	CLA	B	827	-	46,50,73	2.17	9 (19%)	53,85,113	1.70	12 (22%)
18	CLA	8	608	-	46,50,73	2.21	11 (23%)	53,85,113	1.49	9 (16%)
18	CLA	5	609	-	46,50,73	2.12	9 (19%)	53,85,113	1.37	9 (16%)
21	CHL	4	604	-	37,51,74	2.87	9 (24%)	30,86,114	1.78	7 (23%)
19	PQN	A	842	-	34,34,34	0.25	0	43,45,45	0.55	1 (2%)
18	CLA	5	613	-	46,50,73	2.18	9 (19%)	53,85,113	1.47	8 (15%)
18	CLA	B	817	-	46,50,73	2.17	12 (26%)	53,85,113	1.48	9 (16%)
18	CLA	1	602	-	46,50,73	2.09	11 (23%)	53,85,113	1.38	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	6	313	-	46,50,73	2.13	9 (19%)	53,85,113	1.51	11 (20%)
18	CLA	7	611	-	46,50,73	2.14	10 (21%)	53,85,113	1.36	8 (15%)
21	CHL	1	601	8	47,61,74	2.16	9 (19%)	41,98,114	1.18	5 (12%)
18	CLA	1	609	-	46,50,73	2.15	10 (21%)	53,85,113	1.35	7 (13%)
18	CLA	8	615	-	46,50,73	2.08	11 (23%)	53,85,113	1.36	8 (15%)
18	CLA	5	603	-	50,54,73	2.02	11 (22%)	59,90,113	1.29	8 (13%)
18	CLA	A	837	-	46,50,73	2.21	11 (23%)	53,85,113	1.39	8 (15%)
18	CLA	A	813	-	46,50,73	2.17	10 (21%)	53,85,113	1.37	9 (16%)
18	CLA	7	612	-	49,53,73	2.08	12 (24%)	58,89,113	1.33	9 (15%)
18	CLA	6	304	-	46,50,73	2.12	10 (21%)	53,85,113	1.32	7 (13%)
18	CLA	A	830	-	46,50,73	2.13	10 (21%)	53,85,113	1.34	8 (15%)
18	CLA	7	605	-	46,50,73	2.18	11 (23%)	53,85,113	1.48	7 (13%)
18	CLA	6	309	-	49,53,73	2.07	10 (20%)	58,89,113	1.31	5 (8%)
18	CLA	B	811	-	46,50,73	2.12	9 (19%)	53,85,113	1.48	9 (16%)
18	CLA	6	315	-	46,50,73	2.14	8 (17%)	53,85,113	1.61	9 (16%)
18	CLA	B	841	-	46,50,73	2.25	8 (17%)	53,85,113	1.56	10 (18%)
18	CLA	8	611	-	46,50,73	2.20	9 (19%)	53,85,113	1.62	7 (13%)
18	CLA	Z	606	-	46,50,73	2.10	9 (19%)	53,85,113	1.38	8 (15%)
18	CLA	A	836	1	46,50,73	2.14	10 (21%)	53,85,113	1.43	8 (15%)
18	CLA	B	831	-	46,50,73	2.19	10 (21%)	53,85,113	1.43	7 (13%)
18	CLA	1	608	-	46,50,73	2.13	8 (17%)	53,85,113	1.80	11 (20%)
18	CLA	A	827	-	46,50,73	2.16	7 (15%)	53,85,113	1.73	13 (24%)
18	CLA	A	814	-	46,50,73	2.11	9 (19%)	53,85,113	1.43	8 (15%)
18	CLA	A	840	-	46,50,73	2.24	11 (23%)	53,85,113	1.57	7 (13%)
18	CLA	6	317	-	49,53,73	2.01	11 (22%)	58,89,113	1.29	8 (13%)
18	CLA	B	810	-	46,50,73	2.10	9 (19%)	53,85,113	1.37	7 (13%)
18	CLA	3	302	-	46,50,73	2.10	10 (21%)	53,85,113	1.41	8 (15%)
18	CLA	6	308	-	46,50,73	2.10	9 (19%)	53,85,113	1.42	9 (16%)
18	CLA	6	301	-	46,50,73	2.12	12 (26%)	53,85,113	1.32	9 (16%)
18	CLA	Z	613	-	46,50,73	2.12	10 (21%)	53,85,113	1.41	8 (15%)
18	CLA	B	818	-	46,50,73	2.16	8 (17%)	53,85,113	1.44	9 (16%)
18	CLA	B	804	-	46,50,73	2.17	8 (17%)	53,85,113	1.73	11 (20%)
18	CLA	B	833	-	46,50,73	2.14	9 (19%)	53,85,113	1.31	8 (15%)
18	CLA	B	822	-	49,53,73	1.98	8 (16%)	58,89,113	1.45	9 (15%)
21	CHL	6	316	-	37,51,74	2.54	9 (24%)	30,86,114	1.43	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	815	-	46,50,73	2.10	10 (21%)	53,85,113	1.36	8 (15%)
18	CLA	7	610	-	45,49,73	2.49	9 (20%)	54,84,113	1.96	11 (20%)
18	CLA	A	810	-	46,50,73	2.20	9 (19%)	53,85,113	1.35	7 (13%)
18	CLA	7	607	-	46,50,73	2.16	11 (23%)	53,85,113	1.39	9 (16%)
21	CHL	5	607	-	37,51,74	2.58	9 (24%)	30,86,114	1.52	6 (20%)
18	CLA	5	602	-	46,50,73	2.17	11 (23%)	53,85,113	1.45	8 (15%)
18	CLA	5	617	-	50,54,73	2.02	8 (16%)	59,90,113	1.52	11 (18%)
18	CLA	1	614	-	50,54,73	2.04	10 (20%)	59,90,113	1.32	8 (13%)
18	CLA	A	803	-	46,50,73	2.33	11 (23%)	53,85,113	1.62	8 (15%)
18	CLA	A	833	-	46,50,73	2.08	10 (21%)	53,85,113	1.38	8 (15%)
18	CLA	B	824	-	46,50,73	2.09	8 (17%)	53,85,113	1.43	7 (13%)
18	CLA	7	613	-	47,51,73	2.13	8 (17%)	55,86,113	1.46	8 (14%)
18	CLA	B	805	-	46,50,73	2.25	10 (21%)	53,85,113	1.56	10 (18%)
18	CLA	6	311	-	49,53,73	2.05	10 (20%)	58,89,113	1.34	8 (13%)

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
18	CLA	A	823	-	1/1/12/20	3/23/99/115	-
18	CLA	B	835	-	1/1/10/20	2/12/88/115	-
18	CLA	3	312	-	1/1/11/20	4/15/91/115	-
21	CHL	5	616	-	3/3/15/26	0/12/110/137	-
18	CLA	7	614	10	1/1/10/20	3/12/88/115	-
18	CLA	1	611	-	1/1/10/20	2/12/88/115	-
18	CLA	5	614	14	1/1/10/20	1/12/88/115	-
18	CLA	Z	607	-	1/1/10/20	4/12/88/115	-
18	CLA	Z	612	-	1/1/10/20	1/12/88/115	-
18	CLA	4	607	-	1/1/10/20	3/12/88/115	-
18	CLA	A	838	-	1/1/10/20	2/12/88/115	-
18	CLA	6	302	-	1/1/10/20	3/12/88/115	-
18	CLA	B	807	-	1/1/11/20	3/17/93/115	-
18	CLA	A	818	-	1/1/10/20	4/12/88/115	-
18	CLA	1	605	-	1/1/10/20	2/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	819	-	1/1/10/20	3/12/88/115	-
18	CLA	B	809	-	1/1/10/20	3/12/88/115	-
18	CLA	A	828	-	1/1/10/20	2/12/88/115	-
21	CHL	7	606	-	3/3/15/26	3/12/110/137	-
18	CLA	A	821	-	1/1/10/20	1/12/88/115	-
18	CLA	8	614	-	1/1/10/20	2/12/88/115	-
20	SF4	C	102	3	-	-	0/6/5/5
18	CLA	B	837	-	1/1/10/20	0/12/88/115	-
18	CLA	B	813	-	1/1/10/20	1/10/86/115	-
18	CLA	A	819	-	1/1/10/20	4/12/88/115	-
18	CLA	A	820	-	1/1/10/20	5/12/88/115	-
18	CLA	Z	609	-	1/1/10/20	3/12/88/115	-
18	CLA	8	612	-	1/1/11/20	2/17/93/115	-
21	CHL	1	606	-	3/3/15/26	1/12/110/137	-
18	CLA	A	816	-	1/1/10/20	0/12/88/115	-
18	CLA	B	808	-	1/1/10/20	0/12/88/115	-
18	CLA	Z	610	-	1/1/10/20	2/12/88/115	-
18	CLA	A	831	-	1/1/10/20	3/12/88/115	-
21	CHL	8	606	-	3/3/15/26	2/12/110/137	-
18	CLA	F	302	-	1/1/15/20	4/39/115/115	-
18	CLA	B	840	-	1/1/10/20	3/12/88/115	-
18	CLA	7	608	-	1/1/12/20	5/21/97/115	-
18	CLA	Z	602	-	1/1/10/20	5/12/88/115	-
18	CLA	3	305	9	1/1/10/20	3/12/88/115	-
18	CLA	A	822	-	1/1/10/20	7/12/88/115	-
21	CHL	6	307	-	3/3/15/26	2/12/110/137	-
18	CLA	A	817	-	1/1/11/20	1/18/94/115	-
18	CLA	A	808	-	1/1/10/20	2/12/88/115	-
18	CLA	B	830	-	1/1/11/20	5/15/91/115	-
18	CLA	Z	603	-	1/1/10/20	1/12/88/115	-
18	CLA	6	314	15	1/1/11/20	2/17/93/115	-
18	CLA	A	806	-	1/1/10/20	5/12/88/115	-
18	CLA	1	607	-	1/1/10/20	2/12/88/115	-
18	CLA	1	612	-	1/1/11/20	0/17/93/115	-
18	CLA	5	611	-	1/1/10/20	3/12/88/115	-
22	FES	G	101	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	826	-	1/1/10/20	3/12/88/115	-
18	CLA	3	311	-	1/1/11/20	3/15/91/115	-
18	CLA	4	602	-	1/1/10/20	3/12/88/115	-
21	CHL	Z	605	-	3/3/15/26	1/12/110/137	-
18	CLA	B	838	-	1/1/10/20	3/13/89/115	-
18	CLA	B	836	-	1/1/10/20	0/12/88/115	-
18	CLA	A	834	-	1/1/10/20	3/12/88/115	-
20	SF4	B	803	-	-	-	0/6/5/5
18	CLA	4	611	-	1/1/10/20	4/12/88/115	-
18	CLA	4	609	-	1/1/10/20	4/12/88/115	-
18	CLA	B	825	-	1/1/10/20	3/12/88/115	-
18	CLA	8	613	-	1/1/10/20	3/12/88/115	-
18	CLA	B	832	-	1/1/10/20	4/12/88/115	-
18	CLA	7	602	-	1/1/10/20	3/12/88/115	-
18	CLA	4	606	-	1/1/10/20	3/12/88/115	-
18	CLA	6	312	-	1/1/11/20	3/15/91/115	-
18	CLA	A	809	-	1/1/10/20	2/12/88/115	-
18	CLA	3	309	-	1/1/10/20	2/10/86/115	-
18	CLA	3	303	-	1/1/10/20	2/12/88/115	-
18	CLA	B	812	-	1/1/10/20	6/12/88/115	-
21	CHL	5	606	-	3/3/15/26	0/12/110/137	-
18	CLA	A	832	-	1/1/10/20	0/12/88/115	-
18	CLA	B	829	-	1/1/10/20	4/12/88/115	-
18	CLA	5	604	-	1/1/10/20	0/12/88/115	-
18	CLA	1	613	-	1/1/10/20	1/12/88/115	-
18	CLA	B	834	-	1/1/10/20	3/12/85/115	-
18	CLA	A	805	-	1/1/10/20	2/12/88/115	-
18	CLA	8	602	-	1/1/10/20	3/12/88/115	-
18	CLA	7	604	-	1/1/10/20	2/13/89/115	-
18	CLA	A	812	-	1/1/10/20	0/12/88/115	-
18	CLA	A	843	-	1/1/12/20	5/24/100/115	-
18	CLA	Z	611	-	1/1/11/20	2/15/91/115	-
18	CLA	1	603	-	1/1/10/20	4/12/88/115	-
18	CLA	1	604	-	1/1/10/20	1/12/88/115	-
18	CLA	3	301	-	1/1/10/20	3/12/88/115	-
18	CLA	B	821	-	1/1/10/20	1/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	826	-	1/1/10/20	2/12/88/115	-
18	CLA	4	603	-	1/1/11/20	6/17/93/115	-
18	CLA	A	824	-	1/1/10/20	4/12/88/115	-
18	CLA	A	841	-	1/1/10/20	3/12/88/115	-
18	CLA	B	823	-	1/1/10/20	2/12/88/115	-
18	CLA	4	601	13	1/1/10/20	3/12/88/115	-
18	CLA	5	605	-	1/1/10/20	0/12/88/115	-
18	CLA	5	601	14	1/1/10/20	3/12/88/115	-
17	CL0	A	801	-	3/3/15/25	0/10/108/135	-
18	CLA	4	612	-	1/1/10/20	0/10/86/115	-
18	CLA	8	610	-	1/1/11/20	1/17/93/115	-
18	CLA	F	301	-	1/1/11/20	3/15/91/115	-
18	CLA	B	820	-	1/1/10/20	3/12/88/115	-
18	CLA	8	609	-	1/1/10/20	2/12/88/115	-
18	CLA	Z	604	-	1/1/10/20	3/13/89/115	-
18	CLA	B	802	-	1/1/11/20	3/17/93/115	-
18	CLA	B	816	-	1/1/10/20	4/12/88/115	-
18	CLA	3	314	-	1/1/10/20	0/12/88/115	-
18	CLA	7	601	10	1/1/10/20	7/12/88/115	-
18	CLA	5	608	-	1/1/10/20	4/12/88/115	-
21	CHL	6	306	-	3/3/15/26	3/12/110/137	-
18	CLA	3	313	-	1/1/11/20	5/17/93/115	-
18	CLA	B	801	-	1/1/10/20	2/12/88/115	-
18	CLA	B	806	-	1/1/11/20	4/15/91/115	-
18	CLA	8	605	-	1/1/10/20	2/12/88/115	-
18	CLA	B	814	-	1/1/10/20	0/12/88/115	-
18	CLA	6	310	-	1/1/10/20	4/12/88/115	-
18	CLA	3	308	-	1/1/10/20	3/12/88/115	-
18	CLA	1	610	-	1/1/10/20	3/12/88/115	-
19	PQN	B	844	-	-	4/23/43/43	0/2/2/2
18	CLA	3	307	-	1/1/10/20	3/12/88/115	-
18	CLA	A	835	-	1/1/10/20	2/12/88/115	-
18	CLA	J	101	-	1/1/10/20	4/12/88/115	-
18	CLA	3	304	-	1/1/10/20	2/12/88/115	-
18	CLA	A	802	-	1/1/10/20	2/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	8	604	-	1/1/10/20	2/12/88/115	-
18	CLA	A	845	-	1/1/10/20	1/12/88/115	-
18	CLA	8	601	11	1/1/10/20	6/12/88/115	-
18	CLA	A	804	-	1/1/10/20	3/12/88/115	-
18	CLA	B	839	-	1/1/10/20	2/12/88/115	-
18	CLA	4	610	-	1/1/10/20	2/12/88/115	-
18	CLA	8	603	-	1/1/11/20	2/15/91/115	-
18	CLA	A	839	-	1/1/10/20	2/12/88/115	-
18	CLA	A	825	-	1/1/10/20	2/12/88/115	-
18	CLA	B	843	-	1/1/10/20	2/12/88/115	-
18	CLA	7	603	-	1/1/11/20	2/17/93/115	-
18	CLA	3	310	-	1/1/11/20	4/17/93/115	-
21	CHL	4	605	-	3/3/16/26	4/15/113/137	-
18	CLA	4	608	-	1/1/10/20	4/12/88/115	-
18	CLA	A	844	-	1/1/10/20	4/12/88/115	-
18	CLA	Z	608	-	1/1/10/20	3/12/88/115	-
21	CHL	6	305	-	3/3/15/26	0/12/110/137	-
18	CLA	8	607	-	1/1/10/20	3/12/88/115	-
18	CLA	B	815	-	1/1/10/20	6/12/88/115	-
18	CLA	B	842	-	1/1/10/20	2/12/88/115	-
18	CLA	7	609	-	1/1/11/20	0/15/91/115	-
18	CLA	B	828	-	1/1/10/20	4/12/88/115	-
18	CLA	A	811	-	1/1/10/20	3/13/89/115	-
18	CLA	5	615	-	1/1/11/20	3/17/93/115	-
18	CLA	5	612	-	1/1/10/20	0/12/88/115	-
18	CLA	6	303	-	1/1/11/20	7/17/93/115	-
18	CLA	5	610	-	1/1/13/20	4/27/103/115	-
21	CHL	Z	601	12	3/3/15/26	0/12/110/137	-
20	SF4	C	101	3	-	-	0/6/5/5
18	CLA	A	829	-	1/1/10/20	2/12/88/115	-
18	CLA	A	807	-	1/1/10/20	4/12/88/115	-
21	CHL	3	306	-	3/3/15/26	1/12/110/137	-
18	CLA	B	827	-	1/1/10/20	3/12/88/115	-
18	CLA	8	608	-	1/1/10/20	2/12/88/115	-
18	CLA	5	609	-	1/1/10/20	3/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	4	604	-	3/3/15/26	3/12/110/137	-
19	PQN	A	842	-	-	6/23/43/43	0/2/2/2
18	CLA	5	613	-	1/1/10/20	3/12/88/115	-
18	CLA	B	817	-	1/1/10/20	5/12/88/115	-
18	CLA	1	602	-	1/1/10/20	5/12/88/115	-
18	CLA	6	313	-	1/1/10/20	5/12/88/115	-
18	CLA	7	611	-	1/1/10/20	2/12/88/115	-
21	CHL	1	601	8	3/3/17/26	3/24/122/137	-
18	CLA	1	609	-	1/1/10/20	3/12/88/115	-
18	CLA	8	615	-	1/1/10/20	4/12/88/115	-
18	CLA	5	603	-	1/1/11/20	7/17/93/115	-
18	CLA	A	837	-	1/1/10/20	2/12/88/115	-
18	CLA	A	813	-	1/1/10/20	8/12/88/115	-
18	CLA	7	612	-	1/1/11/20	2/15/91/115	-
18	CLA	6	304	-	1/1/10/20	0/12/88/115	-
18	CLA	A	830	-	1/1/10/20	4/12/88/115	-
18	CLA	7	605	-	1/1/10/20	1/12/88/115	-
18	CLA	6	309	-	1/1/11/20	3/15/91/115	-
18	CLA	B	811	-	1/1/10/20	4/12/88/115	-
18	CLA	6	315	-	1/1/10/20	2/12/88/115	-
18	CLA	B	841	-	1/1/10/20	2/12/88/115	-
18	CLA	8	611	-	1/1/10/20	2/12/88/115	-
18	CLA	Z	606	-	1/1/10/20	2/12/88/115	-
18	CLA	A	836	1	1/1/10/20	1/12/88/115	-
18	CLA	B	831	-	1/1/10/20	1/12/88/115	-
18	CLA	1	608	-	1/1/10/20	4/12/88/115	-
18	CLA	A	827	-	1/1/10/20	3/12/88/115	-
18	CLA	A	814	-	1/1/10/20	2/12/88/115	-
18	CLA	A	840	-	1/1/10/20	1/12/88/115	-
18	CLA	6	317	-	1/1/11/20	2/15/91/115	-
18	CLA	B	810	-	1/1/10/20	3/12/88/115	-
18	CLA	3	302	-	1/1/10/20	1/12/88/115	-
18	CLA	6	308	-	1/1/10/20	1/12/88/115	-
18	CLA	6	301	-	1/1/10/20	5/12/88/115	-
18	CLA	Z	613	-	1/1/10/20	2/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	818	-	1/1/10/20	3/12/88/115	-
18	CLA	B	804	-	1/1/10/20	1/12/88/115	-
18	CLA	B	833	-	1/1/10/20	1/12/88/115	-
18	CLA	B	822	-	1/1/11/20	5/15/91/115	-
21	CHL	6	316	-	3/3/15/26	2/12/110/137	-
18	CLA	A	815	-	1/1/10/20	1/12/88/115	-
18	CLA	7	610	-	1/1/10/20	0/10/86/115	-
18	CLA	A	810	-	1/1/10/20	2/12/88/115	-
18	CLA	7	607	-	1/1/10/20	3/12/88/115	-
21	CHL	5	607	-	3/3/15/26	2/12/110/137	-
18	CLA	5	602	-	1/1/10/20	4/12/88/115	-
18	CLA	5	617	-	1/1/11/20	8/17/93/115	-
18	CLA	1	614	-	1/1/11/20	3/17/93/115	-
18	CLA	A	803	-	1/1/10/20	4/12/88/115	-
18	CLA	A	833	-	1/1/10/20	2/12/88/115	-
18	CLA	B	824	-	1/1/10/20	3/12/88/115	-
18	CLA	7	613	-	1/1/10/20	5/13/89/115	-
18	CLA	B	805	-	1/1/10/20	2/12/88/115	-
18	CLA	6	311	-	1/1/11/20	7/15/91/115	-

All (1983) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	834	CLA	C4C-NC	22.91	1.47	1.30
21	4	604	CHL	C3A-C2A	-10.08	1.46	1.54
21	3	306	CHL	C3A-C2A	-9.32	1.46	1.54
17	A	801	CL0	C3A-C2A	-9.22	1.46	1.54
21	4	605	CHL	C1A-CHA	8.79	1.50	1.40
18	7	604	CLA	C4B-NB	8.61	1.49	1.37
18	6	310	CLA	MG-NB	-8.49	1.89	2.05
18	7	610	CLA	C3A-C2A	-8.44	1.47	1.54
18	B	823	CLA	C4B-NB	8.18	1.48	1.37
18	6	301	CLA	C4B-NB	7.95	1.48	1.37
18	A	833	CLA	C4B-NB	7.90	1.48	1.37
21	7	606	CHL	MG-NB	-7.74	1.90	2.05
21	4	604	CHL	MG-NB	-7.74	1.90	2.05
18	B	814	CLA	C4B-NB	7.72	1.48	1.37
18	A	808	CLA	C4B-NB	7.67	1.47	1.37
18	A	843	CLA	C4B-NB	7.65	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	606	CHL	MG-NB	-7.64	1.90	2.05
21	5	606	CHL	MG-NB	-7.62	1.90	2.05
18	8	610	CLA	MG-NB	-7.61	1.90	2.05
18	3	302	CLA	C4B-NB	7.58	1.47	1.37
18	5	605	CLA	C4B-NB	7.52	1.47	1.37
18	B	825	CLA	C4B-NB	7.49	1.47	1.37
18	Z	604	CLA	C4B-NB	7.49	1.47	1.37
18	8	605	CLA	C4B-NB	7.48	1.47	1.37
18	1	605	CLA	C4B-NB	7.46	1.47	1.37
18	4	602	CLA	C4B-NB	7.45	1.47	1.37
18	Z	612	CLA	C4B-NB	7.41	1.47	1.37
18	Z	602	CLA	C4B-NB	7.40	1.47	1.37
21	5	607	CHL	MG-NB	-7.39	1.91	2.05
18	1	603	CLA	C4B-NB	7.38	1.47	1.37
18	A	836	CLA	C4B-NB	7.38	1.47	1.37
18	1	613	CLA	C4B-NB	7.37	1.47	1.37
18	1	602	CLA	C4B-NB	7.32	1.47	1.37
18	8	615	CLA	C4B-NB	7.31	1.47	1.37
18	5	603	CLA	C4B-NB	7.29	1.47	1.37
21	1	606	CHL	MG-NB	-7.29	1.91	2.05
18	8	612	CLA	C4B-NB	7.29	1.47	1.37
21	Z	605	CHL	MG-NB	-7.29	1.91	2.05
18	B	824	CLA	C4B-NB	7.28	1.47	1.37
18	7	612	CLA	C4B-NB	7.28	1.47	1.37
18	8	610	CLA	MG-ND	-7.27	1.91	2.05
18	6	310	CLA	MG-ND	-7.27	1.91	2.05
18	Z	610	CLA	C4B-NB	7.26	1.47	1.37
18	6	317	CLA	C4B-NB	7.25	1.47	1.37
18	1	611	CLA	C4B-NB	7.24	1.47	1.37
18	Z	613	CLA	C4B-NB	7.24	1.47	1.37
21	6	305	CHL	MG-NB	-7.23	1.91	2.05
18	1	609	CLA	C4B-NB	7.23	1.47	1.37
18	1	614	CLA	C4B-NB	7.23	1.47	1.37
18	Z	608	CLA	C4B-NB	7.22	1.47	1.37
18	J	101	CLA	C4B-NB	7.21	1.47	1.37
18	6	304	CLA	C4B-NB	7.20	1.47	1.37
18	7	604	CLA	MG-ND	-7.20	1.91	2.05
18	6	309	CLA	C4B-NB	7.19	1.47	1.37
18	4	609	CLA	C4B-NB	7.18	1.47	1.37
21	3	306	CHL	MG-NB	-7.18	1.91	2.05
21	6	306	CHL	MG-NB	-7.16	1.91	2.05
18	6	303	CLA	C4B-NB	7.15	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	606	CHL	MG-ND	-7.14	1.91	2.05
18	5	608	CLA	C4B-NB	7.13	1.47	1.37
18	B	838	CLA	MG-NB	-7.13	1.91	2.05
18	A	804	CLA	C4B-NB	7.12	1.47	1.37
18	8	602	CLA	C4B-NB	7.10	1.47	1.37
18	6	312	CLA	C4B-NB	7.10	1.47	1.37
18	1	604	CLA	C4B-NB	7.09	1.47	1.37
18	A	834	CLA	C4B-NB	7.09	1.47	1.37
18	4	606	CLA	C4B-NB	7.08	1.47	1.37
18	B	816	CLA	C4B-NB	7.08	1.47	1.37
18	Z	603	CLA	C4B-NB	7.08	1.47	1.37
18	5	615	CLA	MG-NB	-7.07	1.91	2.05
21	6	307	CHL	MG-NB	-7.06	1.91	2.05
18	3	312	CLA	C4B-NB	7.06	1.47	1.37
18	7	609	CLA	C4B-NB	7.06	1.47	1.37
18	A	817	CLA	C4B-NB	7.06	1.47	1.37
18	A	803	CLA	C4B-NB	7.05	1.47	1.37
18	B	834	CLA	C4B-NB	7.05	1.47	1.37
21	5	606	CHL	MG-ND	-7.05	1.91	2.05
18	B	809	CLA	C4B-NB	7.05	1.47	1.37
21	7	606	CHL	MG-ND	-7.04	1.91	2.05
18	8	604	CLA	C4B-NB	7.04	1.47	1.37
18	A	831	CLA	C4B-NB	7.02	1.47	1.37
18	A	814	CLA	C4B-NB	7.01	1.47	1.37
18	A	845	CLA	C4B-NB	7.01	1.47	1.37
18	A	816	CLA	C4B-NB	7.01	1.47	1.37
18	B	815	CLA	MG-NB	-7.00	1.91	2.05
18	A	824	CLA	MG-NB	-6.99	1.91	2.05
18	B	826	CLA	C4B-NB	6.98	1.47	1.37
18	8	601	CLA	C4B-NB	6.98	1.47	1.37
18	A	826	CLA	C4B-NB	6.98	1.47	1.37
18	4	601	CLA	C4B-NB	6.97	1.47	1.37
18	B	819	CLA	C4B-NB	6.97	1.47	1.37
18	A	812	CLA	C4B-NB	6.96	1.47	1.37
21	4	605	CHL	MG-NB	-6.95	1.92	2.05
18	4	610	CLA	C4B-NB	6.95	1.47	1.37
21	6	316	CHL	MG-NB	-6.95	1.92	2.05
21	5	616	CHL	MG-NB	-6.94	1.92	2.05
18	A	815	CLA	C4B-NB	6.93	1.47	1.37
18	A	835	CLA	C4B-NB	6.93	1.47	1.37
18	6	311	CLA	C4B-NB	6.93	1.47	1.37
18	B	804	CLA	C4B-NB	6.93	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Z	606	CLA	C4B-NB	6.93	1.47	1.37
18	A	813	CLA	C4B-NB	6.93	1.47	1.37
18	1	607	CLA	C4B-NB	6.92	1.47	1.37
18	B	837	CLA	C4B-NB	6.92	1.46	1.37
21	4	604	CHL	MG-ND	-6.91	1.92	2.05
18	4	603	CLA	C4B-NB	6.90	1.46	1.37
18	A	805	CLA	C4B-NB	6.90	1.46	1.37
18	B	832	CLA	C4B-NB	6.90	1.46	1.37
18	3	311	CLA	C4B-NB	6.90	1.46	1.37
18	A	810	CLA	C4B-NB	6.89	1.46	1.37
18	B	817	CLA	C4B-NB	6.89	1.46	1.37
18	B	835	CLA	C4B-NB	6.88	1.46	1.37
18	B	831	CLA	C4B-NB	6.88	1.46	1.37
18	5	601	CLA	C4B-NB	6.88	1.46	1.37
21	1	606	CHL	MG-ND	-6.88	1.92	2.05
18	7	605	CLA	C4B-NB	6.87	1.46	1.37
18	8	603	CLA	C4B-NB	6.87	1.46	1.37
18	B	833	CLA	C4B-NB	6.87	1.46	1.37
21	Z	605	CHL	MG-ND	-6.87	1.92	2.05
18	5	604	CLA	C4B-NB	6.86	1.46	1.37
18	7	611	CLA	C4B-NB	6.85	1.46	1.37
18	4	607	CLA	C4B-NB	6.84	1.46	1.37
18	A	809	CLA	C4B-NB	6.84	1.46	1.37
18	B	830	CLA	C4B-NB	6.83	1.46	1.37
18	6	314	CLA	C4B-NB	6.83	1.46	1.37
18	A	802	CLA	MG-NB	-6.83	1.92	2.05
18	A	830	CLA	C4B-NB	6.82	1.46	1.37
18	Z	603	CLA	MG-NB	-6.80	1.92	2.05
21	1	601	CHL	MG-ND	-6.80	1.92	2.05
18	7	610	CLA	MG-NB	-6.80	1.92	2.05
18	A	818	CLA	C4B-NB	6.80	1.46	1.37
18	B	818	CLA	C4B-NB	6.79	1.46	1.37
18	7	602	CLA	C4B-NB	6.79	1.46	1.37
18	7	603	CLA	C4B-NB	6.79	1.46	1.37
18	1	604	CLA	MG-NB	-6.79	1.92	2.05
18	7	607	CLA	C4B-NB	6.79	1.46	1.37
18	5	601	CLA	MG-NB	-6.78	1.92	2.05
21	Z	601	CHL	MG-ND	-6.78	1.92	2.05
18	5	602	CLA	C4B-NB	6.77	1.46	1.37
18	B	828	CLA	C4B-NB	6.77	1.46	1.37
18	5	611	CLA	C4B-NB	6.77	1.46	1.37
18	B	815	CLA	C4B-NB	6.77	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	822	CLA	C4B-NB	6.77	1.46	1.37
18	B	829	CLA	MG-NB	-6.76	1.92	2.05
18	F	301	CLA	C4B-NB	6.76	1.46	1.37
18	B	805	CLA	MG-ND	-6.76	1.92	2.05
18	B	821	CLA	C4B-NB	6.75	1.46	1.37
18	A	827	CLA	MG-NB	-6.75	1.92	2.05
18	A	834	CLA	MG-NB	-6.75	1.92	2.05
18	B	820	CLA	MG-NB	-6.75	1.92	2.05
18	6	308	CLA	C4B-NB	6.74	1.46	1.37
18	A	840	CLA	C4B-NB	6.74	1.46	1.37
18	B	836	CLA	C4B-NB	6.72	1.46	1.37
18	8	607	CLA	C4B-NB	6.71	1.46	1.37
21	3	306	CHL	MG-ND	-6.71	1.92	2.05
18	8	609	CLA	C4B-NB	6.70	1.46	1.37
18	B	815	CLA	MG-ND	-6.69	1.92	2.05
21	5	607	CHL	MG-ND	-6.69	1.92	2.05
18	A	837	CLA	C4B-NB	6.69	1.46	1.37
18	Z	609	CLA	MG-NB	-6.69	1.92	2.05
18	A	825	CLA	C4B-NB	6.69	1.46	1.37
18	3	308	CLA	C4B-NB	6.68	1.46	1.37
18	8	611	CLA	C4B-NB	6.68	1.46	1.37
21	4	605	CHL	CHB-C4A	-6.67	1.30	1.38
18	1	610	CLA	MG-NB	-6.67	1.92	2.05
21	5	607	CHL	CHB-C4A	-6.67	1.30	1.38
18	5	610	CLA	MG-NB	-6.66	1.92	2.05
18	3	310	CLA	C4B-NB	6.66	1.46	1.37
18	6	313	CLA	C4B-NB	6.66	1.46	1.37
18	A	819	CLA	C4B-NB	6.65	1.46	1.37
18	A	839	CLA	C4B-NB	6.65	1.46	1.37
18	4	608	CLA	MG-NB	-6.65	1.92	2.05
18	B	802	CLA	MG-NB	-6.64	1.92	2.05
21	6	307	CHL	CHB-C4A	-6.63	1.30	1.38
18	B	811	CLA	MG-NB	-6.63	1.92	2.05
18	A	824	CLA	MG-ND	-6.62	1.92	2.05
18	B	841	CLA	MG-NB	-6.62	1.92	2.05
18	7	601	CLA	C4B-NB	6.62	1.46	1.37
18	B	806	CLA	C4B-NB	6.62	1.46	1.37
21	6	305	CHL	C3A-C2A	-6.62	1.49	1.54
18	A	807	CLA	C4B-NB	6.61	1.46	1.37
18	4	612	CLA	C4B-NB	6.61	1.46	1.37
21	6	316	CHL	MG-ND	-6.61	1.92	2.05
18	B	805	CLA	MG-NB	-6.60	1.92	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	806	CLA	C4B-NB	6.60	1.46	1.37
18	A	822	CLA	MG-ND	-6.59	1.92	2.05
18	A	837	CLA	MG-NB	-6.59	1.92	2.05
18	3	314	CLA	C4B-NB	6.59	1.46	1.37
21	Z	601	CHL	MG-NB	-6.58	1.92	2.05
18	Z	611	CLA	C4B-NB	6.58	1.46	1.37
18	3	313	CLA	C4B-NB	6.57	1.46	1.37
21	1	601	CHL	MG-NB	-6.57	1.92	2.05
18	B	802	CLA	C4B-NB	6.57	1.46	1.37
18	8	608	CLA	C4B-NB	6.55	1.46	1.37
18	7	614	CLA	MG-NB	-6.54	1.92	2.05
18	F	302	CLA	C4B-NB	6.54	1.46	1.37
18	8	613	CLA	C4B-NB	6.54	1.46	1.37
18	A	821	CLA	C4B-NB	6.54	1.46	1.37
18	8	614	CLA	C4B-NB	6.54	1.46	1.37
18	5	615	CLA	MG-ND	-6.53	1.92	2.05
18	B	807	CLA	C4B-NB	6.53	1.46	1.37
18	A	840	CLA	MG-ND	-6.53	1.92	2.05
17	A	801	CL0	MG-ND	-6.53	1.92	2.05
18	1	612	CLA	C4B-NB	6.52	1.46	1.37
18	4	611	CLA	C4B-NB	6.52	1.46	1.37
18	A	828	CLA	C4B-NB	6.52	1.46	1.37
18	8	608	CLA	MG-ND	-6.52	1.92	2.05
18	4	612	CLA	MG-NB	-6.51	1.92	2.05
21	6	306	CHL	CHB-C4A	-6.50	1.30	1.38
18	7	603	CLA	MG-NB	-6.49	1.92	2.05
18	3	305	CLA	MG-NB	-6.49	1.92	2.05
18	5	617	CLA	MG-NB	-6.48	1.92	2.05
18	A	811	CLA	MG-ND	-6.47	1.93	2.05
18	6	315	CLA	MG-NB	-6.47	1.93	2.05
18	7	608	CLA	C4B-NB	6.46	1.46	1.37
21	5	616	CHL	MG-ND	-6.46	1.93	2.05
18	B	843	CLA	C4B-NB	6.46	1.46	1.37
21	6	306	CHL	MG-ND	-6.46	1.93	2.05
18	4	612	CLA	MG-ND	-6.45	1.93	2.05
21	6	307	CHL	MG-ND	-6.45	1.93	2.05
18	B	811	CLA	MG-ND	-6.45	1.93	2.05
18	B	838	CLA	MG-ND	-6.44	1.93	2.05
18	A	820	CLA	MG-NB	-6.43	1.93	2.05
18	A	811	CLA	MG-NB	-6.42	1.93	2.05
18	7	613	CLA	C4B-NB	6.42	1.46	1.37
21	6	305	CHL	MG-ND	-6.42	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	609	CLA	C4B-NB	6.41	1.46	1.37
18	5	613	CLA	C4B-NB	6.41	1.46	1.37
18	A	832	CLA	C4B-NB	6.41	1.46	1.37
18	4	608	CLA	MG-ND	-6.41	1.93	2.05
18	A	841	CLA	MG-NB	-6.40	1.93	2.05
18	8	608	CLA	MG-NB	-6.39	1.93	2.05
18	B	806	CLA	MG-ND	-6.39	1.93	2.05
18	A	840	CLA	MG-NB	-6.39	1.93	2.05
18	6	314	CLA	MG-NB	-6.39	1.93	2.05
18	Z	607	CLA	MG-NB	-6.38	1.93	2.05
18	Z	607	CLA	C4B-NB	6.37	1.46	1.37
18	A	841	CLA	MG-ND	-6.37	1.93	2.05
18	1	608	CLA	MG-NB	-6.37	1.93	2.05
18	B	808	CLA	MG-NB	-6.37	1.93	2.05
18	A	841	CLA	C4B-NB	6.37	1.46	1.37
18	1	608	CLA	C4B-NB	6.37	1.46	1.37
18	A	835	CLA	MG-NB	-6.37	1.93	2.05
18	A	822	CLA	MG-NB	-6.36	1.93	2.05
18	A	807	CLA	MG-NB	-6.35	1.93	2.05
18	A	818	CLA	MG-NB	-6.35	1.93	2.05
18	6	302	CLA	MG-NB	-6.35	1.93	2.05
18	B	840	CLA	C4B-NB	6.34	1.46	1.37
18	B	802	CLA	MG-ND	-6.33	1.93	2.05
17	A	801	CL0	MG-NB	-6.33	1.93	2.05
18	A	802	CLA	MG-ND	-6.33	1.93	2.05
18	Z	609	CLA	MG-ND	-6.33	1.93	2.05
18	B	840	CLA	MG-NB	-6.32	1.93	2.05
21	1	606	CHL	C3A-C2A	-6.32	1.49	1.54
18	1	610	CLA	MG-ND	-6.31	1.93	2.05
18	A	844	CLA	C4B-NB	6.31	1.46	1.37
18	B	840	CLA	MG-ND	-6.30	1.93	2.05
18	B	829	CLA	MG-ND	-6.30	1.93	2.05
18	3	304	CLA	C4B-NB	6.30	1.46	1.37
18	5	614	CLA	C4B-NB	6.30	1.46	1.37
21	3	306	CHL	CHB-C4A	-6.30	1.31	1.38
18	B	812	CLA	MG-NB	-6.30	1.93	2.05
18	6	315	CLA	MG-ND	-6.29	1.93	2.05
18	5	612	CLA	C4B-NB	6.29	1.46	1.37
18	4	603	CLA	MG-ND	-6.29	1.93	2.05
18	B	806	CLA	MG-NB	-6.29	1.93	2.05
18	3	301	CLA	C4B-NB	6.29	1.46	1.37
18	B	839	CLA	MG-NB	-6.29	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	305	CHL	CHB-C4A	-6.28	1.31	1.38
18	B	827	CLA	MG-NB	-6.28	1.93	2.05
18	B	841	CLA	MG-ND	-6.28	1.93	2.05
18	6	302	CLA	C4B-NB	6.28	1.46	1.37
18	B	807	CLA	MG-NB	-6.28	1.93	2.05
18	7	604	CLA	MG-NB	-6.27	1.93	2.05
18	B	801	CLA	MG-ND	-6.27	1.93	2.05
18	8	607	CLA	MG-ND	-6.27	1.93	2.05
21	Z	605	CHL	C3A-C2A	-6.26	1.49	1.54
18	A	813	CLA	MG-ND	-6.26	1.93	2.05
18	1	608	CLA	MG-ND	-6.26	1.93	2.05
18	Z	607	CLA	MG-ND	-6.25	1.93	2.05
18	A	834	CLA	MG-ND	-6.25	1.93	2.05
18	A	803	CLA	MG-ND	-6.24	1.93	2.05
18	A	827	CLA	MG-ND	-6.24	1.93	2.05
18	3	309	CLA	MG-NB	-6.24	1.93	2.05
18	7	605	CLA	MG-ND	-6.24	1.93	2.05
18	B	842	CLA	C4B-NB	6.23	1.46	1.37
18	3	307	CLA	C4B-NB	6.23	1.46	1.37
18	B	808	CLA	MG-ND	-6.22	1.93	2.05
18	A	803	CLA	MG-NB	-6.22	1.93	2.05
18	3	307	CLA	MG-NB	-6.22	1.93	2.05
18	B	842	CLA	MG-NB	-6.22	1.93	2.05
18	B	822	CLA	C4B-NB	6.22	1.46	1.37
18	A	828	CLA	MG-ND	-6.22	1.93	2.05
18	B	835	CLA	MG-ND	-6.21	1.93	2.05
18	A	844	CLA	MG-ND	-6.21	1.93	2.05
18	B	839	CLA	MG-ND	-6.21	1.93	2.05
18	6	314	CLA	MG-ND	-6.21	1.93	2.05
18	5	612	CLA	MG-NB	-6.21	1.93	2.05
18	3	303	CLA	MG-ND	-6.20	1.93	2.05
18	5	615	CLA	MG-NA	-6.20	1.91	2.06
18	A	837	CLA	MG-ND	-6.20	1.93	2.05
18	5	612	CLA	MG-ND	-6.20	1.93	2.05
18	B	804	CLA	MG-ND	-6.19	1.93	2.05
18	B	831	CLA	MG-ND	-6.19	1.93	2.05
18	4	608	CLA	C4B-NB	6.19	1.46	1.37
18	A	844	CLA	MG-NB	-6.19	1.93	2.05
18	3	303	CLA	C4B-NB	6.19	1.46	1.37
18	3	305	CLA	MG-ND	-6.19	1.93	2.05
18	A	823	CLA	C4B-NB	6.19	1.46	1.37
18	A	838	CLA	MG-NB	-6.18	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	832	CLA	MG-NB	-6.18	1.93	2.05
18	5	613	CLA	MG-NB	-6.18	1.93	2.05
18	B	801	CLA	MG-NB	-6.18	1.93	2.05
18	8	614	CLA	MG-NB	-6.18	1.93	2.05
18	B	835	CLA	MG-NB	-6.18	1.93	2.05
21	Z	605	CHL	CHB-C4A	-6.17	1.31	1.38
18	B	830	CLA	MG-NB	-6.17	1.93	2.05
18	A	805	CLA	MG-NB	-6.17	1.93	2.05
18	B	820	CLA	MG-ND	-6.16	1.93	2.05
18	A	820	CLA	MG-ND	-6.16	1.93	2.05
18	A	807	CLA	MG-ND	-6.16	1.93	2.05
18	5	609	CLA	MG-NB	-6.15	1.93	2.05
18	4	601	CLA	MG-NB	-6.15	1.93	2.05
18	A	823	CLA	MG-NB	-6.13	1.93	2.05
18	A	845	CLA	MG-ND	-6.13	1.93	2.05
18	A	820	CLA	C4B-NB	6.13	1.45	1.37
18	7	614	CLA	C4B-NB	6.13	1.45	1.37
18	B	808	CLA	C4B-NB	6.13	1.45	1.37
18	B	806	CLA	MG-NA	-6.12	1.91	2.06
21	1	606	CHL	CHB-C4A	-6.12	1.31	1.38
18	A	811	CLA	C4B-NB	6.12	1.45	1.37
18	7	601	CLA	MG-ND	-6.12	1.93	2.05
18	B	813	CLA	C4B-NB	6.12	1.45	1.37
18	B	811	CLA	C4B-NB	6.12	1.45	1.37
18	B	804	CLA	MG-NB	-6.11	1.93	2.05
18	B	801	CLA	C4B-NB	6.11	1.45	1.37
18	3	309	CLA	C4B-NB	6.11	1.45	1.37
18	8	614	CLA	MG-ND	-6.11	1.93	2.05
18	B	834	CLA	MG-NB	-6.10	1.93	2.05
18	B	810	CLA	MG-NB	-6.10	1.93	2.05
18	B	838	CLA	C4B-NB	6.10	1.45	1.37
18	8	609	CLA	MG-NA	-6.10	1.91	2.06
18	B	818	CLA	MG-NB	-6.10	1.93	2.05
18	4	601	CLA	MG-ND	-6.10	1.93	2.05
18	1	612	CLA	MG-NB	-6.09	1.93	2.05
18	7	605	CLA	MG-NB	-6.09	1.93	2.05
18	B	839	CLA	C4B-NB	6.08	1.45	1.37
18	Z	611	CLA	MG-NB	-6.08	1.93	2.05
18	3	311	CLA	MG-ND	-6.08	1.93	2.05
18	3	301	CLA	MG-NB	-6.08	1.93	2.05
18	B	812	CLA	MG-NA	-6.07	1.91	2.06
18	3	311	CLA	MG-NB	-6.07	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	833	CLA	MG-NB	-6.07	1.93	2.05
18	4	603	CLA	MG-NB	-6.07	1.93	2.05
18	B	817	CLA	MG-NB	-6.06	1.93	2.05
18	6	315	CLA	C4B-NB	6.06	1.45	1.37
18	3	304	CLA	MG-NB	-6.05	1.93	2.05
18	A	835	CLA	MG-ND	-6.05	1.93	2.05
18	A	830	CLA	MG-ND	-6.05	1.93	2.05
18	7	613	CLA	MG-NB	-6.05	1.93	2.05
18	A	831	CLA	MG-NB	-6.05	1.93	2.05
18	5	602	CLA	MG-NB	-6.05	1.93	2.05
21	7	606	CHL	CHB-C4A	-6.04	1.31	1.38
18	F	301	CLA	MG-NB	-6.03	1.93	2.05
18	B	831	CLA	MG-NB	-6.03	1.93	2.05
18	6	310	CLA	MG-NA	-6.03	1.91	2.06
18	5	610	CLA	MG-ND	-6.02	1.93	2.05
21	6	316	CHL	C1B-C2B	6.02	1.46	1.39
18	A	829	CLA	C4B-NB	6.02	1.45	1.37
18	4	607	CLA	MG-NB	-6.02	1.93	2.05
18	3	307	CLA	MG-ND	-6.01	1.93	2.05
21	5	606	CHL	CHB-C4A	-6.01	1.31	1.38
18	7	607	CLA	MG-NB	-6.01	1.93	2.05
18	B	817	CLA	MG-ND	-6.01	1.93	2.05
18	8	609	CLA	MG-NB	-6.01	1.93	2.05
18	F	301	CLA	MG-ND	-6.00	1.93	2.05
18	7	610	CLA	MG-ND	-6.00	1.93	2.05
21	8	606	CHL	C1B-C2B	6.00	1.46	1.39
18	B	827	CLA	MG-ND	-5.99	1.93	2.05
18	A	828	CLA	MG-NB	-5.99	1.93	2.05
18	B	807	CLA	MG-ND	-5.99	1.93	2.05
18	A	813	CLA	MG-NB	-5.99	1.93	2.05
18	8	601	CLA	MG-ND	-5.98	1.93	2.05
18	A	806	CLA	MG-NB	-5.98	1.93	2.05
18	Z	608	CLA	MG-NB	-5.98	1.93	2.05
18	5	613	CLA	MG-ND	-5.97	1.93	2.05
18	8	611	CLA	MG-NB	-5.97	1.94	2.05
18	4	609	CLA	MG-NB	-5.97	1.94	2.05
18	3	305	CLA	MG-NA	-5.97	1.92	2.06
18	7	614	CLA	MG-ND	-5.97	1.94	2.05
18	B	841	CLA	MG-NA	-5.97	1.92	2.06
18	B	812	CLA	C4B-NB	5.97	1.45	1.37
18	A	810	CLA	MG-NB	-5.97	1.94	2.05
18	6	302	CLA	MG-ND	-5.97	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	821	CLA	MG-ND	-5.96	1.94	2.05
18	5	602	CLA	MG-ND	-5.96	1.94	2.05
18	A	829	CLA	MG-NB	-5.96	1.94	2.05
18	B	833	CLA	MG-ND	-5.95	1.94	2.05
18	B	812	CLA	MG-ND	-5.95	1.94	2.05
18	3	303	CLA	MG-NB	-5.95	1.94	2.05
18	1	609	CLA	MG-NB	-5.95	1.94	2.05
18	A	839	CLA	MG-ND	-5.94	1.94	2.05
18	B	836	CLA	MG-NB	-5.94	1.94	2.05
18	7	613	CLA	MG-ND	-5.93	1.94	2.05
18	A	810	CLA	MG-ND	-5.93	1.94	2.05
18	A	818	CLA	MG-ND	-5.93	1.94	2.05
18	B	827	CLA	C4B-NB	5.93	1.45	1.37
18	B	836	CLA	MG-ND	-5.92	1.94	2.05
18	A	819	CLA	MG-NB	-5.92	1.94	2.05
18	B	816	CLA	MG-ND	-5.92	1.94	2.05
18	B	829	CLA	C4B-NB	5.92	1.45	1.37
18	8	613	CLA	MG-NB	-5.92	1.94	2.05
18	4	611	CLA	MG-NB	-5.92	1.94	2.05
18	A	809	CLA	MG-ND	-5.91	1.94	2.05
18	Z	609	CLA	C4B-NB	5.91	1.45	1.37
18	A	839	CLA	MG-NB	-5.90	1.94	2.05
18	Z	606	CLA	MG-NB	-5.90	1.94	2.05
21	5	616	CHL	C1B-C2B	5.90	1.46	1.39
18	1	607	CLA	MG-NB	-5.90	1.94	2.05
18	7	607	CLA	MG-ND	-5.90	1.94	2.05
18	A	808	CLA	MG-ND	-5.90	1.94	2.05
18	3	313	CLA	MG-NB	-5.89	1.94	2.05
18	A	808	CLA	MG-NB	-5.89	1.94	2.05
18	A	823	CLA	MG-ND	-5.89	1.94	2.05
18	B	810	CLA	C4B-NB	5.89	1.45	1.37
18	B	841	CLA	C4B-NB	5.88	1.45	1.37
18	4	602	CLA	MG-NB	-5.88	1.94	2.05
18	1	605	CLA	MG-ND	-5.88	1.94	2.05
18	7	612	CLA	MG-ND	-5.88	1.94	2.05
18	1	610	CLA	C4B-NB	5.87	1.45	1.37
18	B	818	CLA	MG-ND	-5.87	1.94	2.05
18	F	302	CLA	MG-NB	-5.87	1.94	2.05
18	A	805	CLA	MG-ND	-5.87	1.94	2.05
18	8	605	CLA	MG-NB	-5.87	1.94	2.05
18	A	819	CLA	MG-ND	-5.87	1.94	2.05
18	5	603	CLA	MG-ND	-5.86	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	813	CLA	MG-NB	-5.86	1.94	2.05
21	5	616	CHL	CHB-C4A	-5.86	1.31	1.38
18	8	603	CLA	MG-ND	-5.86	1.94	2.05
18	8	603	CLA	MG-NB	-5.85	1.94	2.05
18	A	838	CLA	C4B-NB	5.85	1.45	1.37
18	1	609	CLA	MG-ND	-5.85	1.94	2.05
18	5	614	CLA	MG-ND	-5.85	1.94	2.05
18	B	842	CLA	MG-ND	-5.85	1.94	2.05
18	A	817	CLA	MG-ND	-5.85	1.94	2.05
18	A	827	CLA	MG-NA	-5.84	1.92	2.06
18	6	313	CLA	MG-NB	-5.84	1.94	2.05
18	4	608	CLA	MG-NA	-5.84	1.92	2.06
18	7	610	CLA	C4B-NB	5.84	1.45	1.37
18	3	304	CLA	MG-ND	-5.84	1.94	2.05
18	5	603	CLA	MG-NB	-5.84	1.94	2.05
18	A	804	CLA	MG-NB	-5.84	1.94	2.05
18	B	822	CLA	MG-NB	-5.84	1.94	2.05
18	B	805	CLA	C4B-NB	5.83	1.45	1.37
18	Z	604	CLA	MG-ND	-5.83	1.94	2.05
18	A	832	CLA	MG-ND	-5.83	1.94	2.05
18	B	805	CLA	MG-NA	-5.83	1.92	2.06
18	A	829	CLA	MG-ND	-5.83	1.94	2.05
18	6	312	CLA	MG-NB	-5.83	1.94	2.05
18	8	605	CLA	MG-ND	-5.83	1.94	2.05
18	B	843	CLA	MG-NB	-5.83	1.94	2.05
18	A	804	CLA	MG-ND	-5.82	1.94	2.05
18	4	611	CLA	MG-ND	-5.82	1.94	2.05
18	B	834	CLA	MG-ND	-5.82	1.94	2.05
18	A	845	CLA	MG-NB	-5.82	1.94	2.05
18	B	828	CLA	MG-NB	-5.81	1.94	2.05
18	A	826	CLA	MG-ND	-5.80	1.94	2.05
18	A	809	CLA	MG-NB	-5.80	1.94	2.05
18	8	611	CLA	MG-ND	-5.80	1.94	2.05
18	Z	608	CLA	MG-ND	-5.80	1.94	2.05
18	B	810	CLA	MG-ND	-5.80	1.94	2.05
18	6	313	CLA	MG-ND	-5.80	1.94	2.05
18	5	617	CLA	MG-ND	-5.80	1.94	2.05
18	A	817	CLA	MG-NB	-5.80	1.94	2.05
18	3	305	CLA	C4B-NB	5.79	1.45	1.37
18	4	607	CLA	MG-ND	-5.79	1.94	2.05
18	A	843	CLA	MG-NB	-5.79	1.94	2.05
18	4	610	CLA	MG-NB	-5.79	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	843	CLA	MG-ND	-5.79	1.94	2.05
18	5	614	CLA	MG-NB	-5.78	1.94	2.05
18	A	806	CLA	MG-ND	-5.78	1.94	2.05
18	A	812	CLA	MG-NB	-5.78	1.94	2.05
18	5	617	CLA	C4B-NB	5.78	1.45	1.37
18	1	612	CLA	MG-ND	-5.78	1.94	2.05
18	7	602	CLA	MG-NB	-5.78	1.94	2.05
18	6	308	CLA	MG-NB	-5.78	1.94	2.05
18	5	608	CLA	MG-ND	-5.77	1.94	2.05
18	4	601	CLA	MG-NA	-5.77	1.92	2.06
18	A	814	CLA	MG-ND	-5.77	1.94	2.05
18	Z	611	CLA	MG-ND	-5.77	1.94	2.05
18	B	832	CLA	MG-NB	-5.76	1.94	2.05
18	A	824	CLA	C4B-NB	5.76	1.45	1.37
18	7	603	CLA	MG-ND	-5.75	1.94	2.05
18	3	313	CLA	MG-ND	-5.75	1.94	2.05
18	B	820	CLA	C4B-NB	5.75	1.45	1.37
18	3	309	CLA	MG-ND	-5.75	1.94	2.05
18	3	312	CLA	MG-NB	-5.74	1.94	2.05
18	5	601	CLA	MG-ND	-5.73	1.94	2.05
18	5	609	CLA	MG-ND	-5.73	1.94	2.05
18	A	825	CLA	MG-NB	-5.73	1.94	2.05
18	8	612	CLA	MG-NB	-5.72	1.94	2.05
18	3	314	CLA	MG-ND	-5.72	1.94	2.05
21	1	601	CHL	CHB-C4A	-5.72	1.31	1.38
18	B	830	CLA	MG-ND	-5.71	1.94	2.05
18	8	612	CLA	MG-ND	-5.71	1.94	2.05
18	A	826	CLA	MG-NB	-5.71	1.94	2.05
18	8	613	CLA	MG-ND	-5.71	1.94	2.05
18	3	314	CLA	MG-NB	-5.70	1.94	2.05
18	A	830	CLA	MG-NB	-5.70	1.94	2.05
18	3	302	CLA	MG-NB	-5.70	1.94	2.05
21	Z	601	CHL	CHB-C4A	-5.70	1.31	1.38
18	8	604	CLA	MG-NB	-5.70	1.94	2.05
18	B	825	CLA	MG-ND	-5.68	1.94	2.05
18	8	607	CLA	MG-NB	-5.68	1.94	2.05
18	6	309	CLA	MG-NB	-5.68	1.94	2.05
18	A	802	CLA	C4B-NB	5.68	1.45	1.37
18	A	831	CLA	MG-ND	-5.68	1.94	2.05
18	4	610	CLA	MG-ND	-5.67	1.94	2.05
18	7	612	CLA	MG-NB	-5.67	1.94	2.05
18	B	837	CLA	MG-ND	-5.67	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	311	CLA	MG-NB	-5.67	1.94	2.05
18	3	307	CLA	MG-NA	-5.67	1.92	2.06
18	B	813	CLA	MG-ND	-5.67	1.94	2.05
18	F	302	CLA	MG-ND	-5.67	1.94	2.05
18	8	604	CLA	MG-ND	-5.66	1.94	2.05
18	6	303	CLA	MG-NB	-5.66	1.94	2.05
18	1	603	CLA	MG-NB	-5.66	1.94	2.05
18	B	819	CLA	MG-NB	-5.66	1.94	2.05
18	B	832	CLA	MG-ND	-5.65	1.94	2.05
18	6	312	CLA	MG-ND	-5.65	1.94	2.05
18	8	615	CLA	MG-NB	-5.65	1.94	2.05
18	B	820	CLA	MG-NA	-5.65	1.92	2.06
18	3	308	CLA	MG-NB	-5.65	1.94	2.05
18	B	816	CLA	MG-NB	-5.64	1.94	2.05
18	7	608	CLA	MG-NB	-5.64	1.94	2.05
18	5	605	CLA	MG-ND	-5.64	1.94	2.05
18	B	815	CLA	MG-NA	-5.63	1.92	2.06
18	4	612	CLA	MG-NA	-5.63	1.92	2.06
18	7	609	CLA	MG-NB	-5.63	1.94	2.05
18	7	610	CLA	MG-NA	-5.62	1.92	2.06
18	B	826	CLA	MG-ND	-5.62	1.94	2.05
18	Z	603	CLA	MG-ND	-5.62	1.94	2.05
18	7	601	CLA	MG-NB	-5.62	1.94	2.05
18	Z	606	CLA	MG-ND	-5.61	1.94	2.05
18	7	602	CLA	MG-ND	-5.61	1.94	2.05
18	B	837	CLA	MG-NB	-5.61	1.94	2.05
18	A	821	CLA	MG-NB	-5.61	1.94	2.05
18	1	604	CLA	MG-ND	-5.61	1.94	2.05
18	1	607	CLA	MG-ND	-5.60	1.94	2.05
18	A	814	CLA	MG-NB	-5.60	1.94	2.05
18	Z	604	CLA	MG-NB	-5.59	1.94	2.05
18	B	819	CLA	MG-NA	-5.59	1.93	2.06
18	A	803	CLA	MG-NA	-5.59	1.93	2.06
18	6	301	CLA	MG-ND	-5.59	1.94	2.05
18	A	824	CLA	MG-NA	-5.59	1.93	2.06
18	A	816	CLA	MG-NB	-5.58	1.94	2.05
18	A	816	CLA	MG-ND	-5.58	1.94	2.05
18	5	605	CLA	MG-NB	-5.58	1.94	2.05
18	Z	613	CLA	MG-ND	-5.58	1.94	2.05
18	3	310	CLA	MG-NB	-5.58	1.94	2.05
21	6	316	CHL	CHB-C4A	-5.57	1.31	1.38
18	B	843	CLA	MG-ND	-5.57	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	308	CLA	MG-ND	-5.56	1.94	2.05
18	1	614	CLA	MG-ND	-5.56	1.94	2.05
18	7	611	CLA	MG-ND	-5.56	1.94	2.05
18	5	604	CLA	MG-NB	-5.55	1.94	2.05
18	4	609	CLA	MG-ND	-5.54	1.94	2.05
18	1	605	CLA	MG-NB	-5.54	1.94	2.05
18	B	821	CLA	MG-NB	-5.54	1.94	2.05
18	A	815	CLA	MG-ND	-5.53	1.94	2.05
18	6	308	CLA	MG-ND	-5.53	1.94	2.05
18	7	611	CLA	MG-NB	-5.53	1.94	2.05
18	7	608	CLA	MG-ND	-5.53	1.94	2.05
18	1	614	CLA	MG-NB	-5.52	1.94	2.05
18	A	825	CLA	MG-NA	-5.52	1.93	2.06
18	Z	613	CLA	MG-NB	-5.52	1.94	2.05
18	B	826	CLA	MG-NB	-5.52	1.94	2.05
18	3	301	CLA	MG-ND	-5.51	1.94	2.05
18	B	827	CLA	MG-NA	-5.50	1.93	2.06
18	A	815	CLA	MG-NB	-5.50	1.94	2.05
18	A	825	CLA	MG-ND	-5.50	1.94	2.05
18	A	808	CLA	MG-NA	-5.49	1.93	2.06
18	8	611	CLA	MG-NA	-5.49	1.93	2.06
18	4	602	CLA	MG-ND	-5.49	1.94	2.05
18	5	615	CLA	C4B-NB	5.48	1.45	1.37
18	6	304	CLA	MG-ND	-5.47	1.94	2.05
18	B	822	CLA	MG-ND	-5.47	1.94	2.05
18	5	604	CLA	MG-ND	-5.46	1.95	2.05
18	B	809	CLA	MG-NB	-5.46	1.95	2.05
18	A	810	CLA	MG-NA	-5.45	1.93	2.06
18	Z	610	CLA	MG-NB	-5.44	1.95	2.05
18	1	611	CLA	MG-NB	-5.44	1.95	2.05
18	B	814	CLA	MG-NB	-5.44	1.95	2.05
18	8	615	CLA	MG-ND	-5.44	1.95	2.05
18	5	608	CLA	MG-NB	-5.44	1.95	2.05
18	A	812	CLA	MG-ND	-5.43	1.95	2.05
18	B	824	CLA	MG-ND	-5.43	1.95	2.05
18	5	611	CLA	MG-NB	-5.43	1.95	2.05
18	1	603	CLA	MG-ND	-5.43	1.95	2.05
21	6	316	CHL	C3A-C2A	-5.43	1.50	1.54
18	7	608	CLA	MG-NA	-5.43	1.93	2.06
18	6	309	CLA	MG-ND	-5.43	1.95	2.05
18	B	821	CLA	MG-ND	-5.42	1.95	2.05
18	Z	610	CLA	MG-ND	-5.42	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	611	CLA	MG-ND	-5.41	1.95	2.05
18	8	610	CLA	MG-NA	-5.41	1.93	2.06
18	3	301	CLA	MG-NA	-5.41	1.93	2.06
18	8	602	CLA	MG-NB	-5.40	1.95	2.05
18	4	607	CLA	MG-NA	-5.40	1.93	2.06
18	A	836	CLA	MG-NB	-5.40	1.95	2.05
18	A	827	CLA	C4B-NB	5.40	1.44	1.37
18	A	827	CLA	MG-NC	-5.38	1.93	2.06
18	B	824	CLA	MG-NB	-5.37	1.95	2.05
18	B	823	CLA	MG-NB	-5.37	1.95	2.05
18	B	828	CLA	MG-ND	-5.37	1.95	2.05
21	4	604	CHL	C1B-C2B	5.37	1.45	1.39
18	A	838	CLA	MG-ND	-5.37	1.95	2.05
18	5	613	CLA	MG-NA	-5.36	1.93	2.06
18	6	317	CLA	MG-NB	-5.35	1.95	2.05
21	Z	601	CHL	C1B-C2B	5.34	1.45	1.39
18	B	825	CLA	MG-NB	-5.33	1.95	2.05
18	8	601	CLA	MG-NB	-5.33	1.95	2.05
18	3	312	CLA	MG-ND	-5.33	1.95	2.05
18	A	833	CLA	MG-ND	-5.33	1.95	2.05
18	J	101	CLA	MG-NB	-5.32	1.95	2.05
18	A	802	CLA	MG-NA	-5.32	1.93	2.06
18	A	811	CLA	MG-NA	-5.32	1.93	2.06
18	6	311	CLA	MG-ND	-5.31	1.95	2.05
18	A	825	CLA	MG-NC	-5.31	1.93	2.06
18	B	809	CLA	MG-ND	-5.30	1.95	2.05
18	7	614	CLA	MG-NA	-5.30	1.93	2.06
18	3	310	CLA	MG-ND	-5.29	1.95	2.05
18	7	609	CLA	MG-ND	-5.29	1.95	2.05
18	6	301	CLA	MG-NB	-5.29	1.95	2.05
18	6	304	CLA	MG-NB	-5.28	1.95	2.05
18	5	617	CLA	MG-NA	-5.28	1.93	2.06
18	A	836	CLA	MG-ND	-5.28	1.95	2.05
18	B	814	CLA	MG-ND	-5.28	1.95	2.05
18	4	612	CLA	MG-NC	-5.27	1.93	2.06
18	1	613	CLA	MG-NB	-5.27	1.95	2.05
18	6	303	CLA	MG-ND	-5.26	1.95	2.05
18	B	835	CLA	MG-NA	-5.26	1.93	2.06
18	6	317	CLA	MG-ND	-5.26	1.95	2.05
18	7	613	CLA	MG-NA	-5.26	1.93	2.06
18	3	309	CLA	C3A-C2A	-5.25	1.49	1.54
18	A	813	CLA	MG-NA	-5.25	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	8	609	CLA	MG-ND	-5.25	1.95	2.05
18	Z	612	CLA	MG-NB	-5.25	1.95	2.05
18	B	804	CLA	MG-NA	-5.25	1.93	2.06
21	1	601	CHL	C1B-C2B	5.25	1.45	1.39
18	3	302	CLA	MG-ND	-5.24	1.95	2.05
18	A	834	CLA	MG-NA	-5.24	1.93	2.06
18	Z	602	CLA	MG-NB	-5.23	1.95	2.05
18	Z	607	CLA	MG-NA	-5.23	1.93	2.06
18	4	606	CLA	MG-NB	-5.23	1.95	2.05
18	1	608	CLA	MG-NA	-5.22	1.93	2.06
18	1	602	CLA	MG-ND	-5.21	1.95	2.05
18	Z	602	CLA	MG-ND	-5.21	1.95	2.05
18	5	610	CLA	C4B-NB	5.21	1.44	1.37
18	1	602	CLA	MG-NB	-5.21	1.95	2.05
18	3	309	CLA	MG-NA	-5.20	1.93	2.06
18	1	613	CLA	MG-ND	-5.20	1.95	2.05
18	Z	612	CLA	MG-ND	-5.20	1.95	2.05
18	6	313	CLA	MG-NA	-5.19	1.93	2.06
18	A	803	CLA	MG-NC	-5.19	1.93	2.06
18	8	614	CLA	MG-NA	-5.18	1.94	2.06
18	B	819	CLA	MG-ND	-5.18	1.95	2.05
21	5	616	CHL	C3A-C2A	-5.17	1.50	1.54
18	8	602	CLA	MG-ND	-5.16	1.95	2.05
18	B	805	CLA	MG-NC	-5.15	1.94	2.06
21	6	305	CHL	C1B-C2B	5.15	1.45	1.39
18	4	611	CLA	MG-NA	-5.14	1.94	2.06
18	5	615	CLA	MG-NC	-5.14	1.94	2.06
18	A	838	CLA	MG-NA	-5.13	1.94	2.06
18	B	818	CLA	MG-NA	-5.13	1.94	2.06
18	A	807	CLA	MG-NC	-5.12	1.94	2.06
18	5	602	CLA	MG-NA	-5.12	1.94	2.06
18	B	824	CLA	MG-NA	-5.12	1.94	2.06
18	7	611	CLA	MG-NA	-5.11	1.94	2.06
18	5	611	CLA	MG-ND	-5.10	1.95	2.05
18	B	810	CLA	MG-NA	-5.10	1.94	2.06
18	A	819	CLA	MG-NA	-5.10	1.94	2.06
21	3	306	CHL	C1B-C2B	5.09	1.45	1.39
18	B	838	CLA	MG-NA	-5.08	1.94	2.06
18	A	807	CLA	MG-NA	-5.07	1.94	2.06
18	A	823	CLA	MG-NA	-5.07	1.94	2.06
18	B	841	CLA	MG-NC	-5.07	1.94	2.06
18	B	817	CLA	MG-NA	-5.06	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	606	CHL	C3A-C2A	-5.06	1.50	1.54
18	4	609	CLA	MG-NA	-5.05	1.94	2.06
18	4	602	CLA	MG-NA	-5.05	1.94	2.06
18	7	601	CLA	MG-NA	-5.04	1.94	2.06
18	B	807	CLA	MG-NA	-5.04	1.94	2.06
18	A	840	CLA	MG-NA	-5.03	1.94	2.06
18	5	601	CLA	MG-NA	-5.03	1.94	2.06
18	B	822	CLA	MG-NA	-5.03	1.94	2.06
18	6	315	CLA	MG-NA	-5.02	1.94	2.06
18	7	603	CLA	MG-NA	-5.01	1.94	2.06
18	A	830	CLA	MG-NA	-5.01	1.94	2.06
18	6	309	CLA	MG-NA	-5.01	1.94	2.06
18	A	808	CLA	MG-NC	-5.01	1.94	2.06
18	B	802	CLA	MG-NA	-5.01	1.94	2.06
18	F	301	CLA	MG-NA	-5.00	1.94	2.06
18	A	836	CLA	MG-NA	-4.99	1.94	2.06
18	5	613	CLA	MG-NC	-4.99	1.94	2.06
18	B	832	CLA	MG-NA	-4.99	1.94	2.06
18	6	308	CLA	MG-NA	-4.99	1.94	2.06
18	A	826	CLA	MG-NA	-4.98	1.94	2.06
18	B	842	CLA	MG-NA	-4.98	1.94	2.06
18	5	610	CLA	MG-NA	-4.97	1.94	2.06
18	8	613	CLA	MG-NA	-4.97	1.94	2.06
18	4	601	CLA	MG-NC	-4.97	1.94	2.06
18	A	805	CLA	MG-NA	-4.97	1.94	2.06
18	J	101	CLA	MG-ND	-4.96	1.96	2.05
18	A	835	CLA	MG-NA	-4.95	1.94	2.06
18	B	829	CLA	MG-NA	-4.95	1.94	2.06
18	8	603	CLA	MG-NA	-4.95	1.94	2.06
21	5	607	CHL	C1B-C2B	4.95	1.45	1.39
18	8	607	CLA	MG-NA	-4.95	1.94	2.06
18	4	606	CLA	MG-ND	-4.94	1.96	2.05
18	1	609	CLA	MG-NA	-4.93	1.94	2.06
18	3	305	CLA	MG-NC	-4.93	1.94	2.06
18	A	836	CLA	MG-NC	-4.92	1.94	2.06
18	A	815	CLA	MG-NA	-4.92	1.94	2.06
18	6	310	CLA	MG-NC	-4.91	1.94	2.06
18	A	806	CLA	MG-NA	-4.91	1.94	2.06
18	Z	608	CLA	MG-NA	-4.91	1.94	2.06
21	7	606	CHL	C1B-C2B	4.90	1.45	1.39
18	6	312	CLA	MG-NA	-4.90	1.94	2.06
21	8	606	CHL	CHB-C4A	-4.90	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	606	CLA	MG-NA	-4.90	1.94	2.06
18	B	830	CLA	MG-NA	-4.89	1.94	2.06
18	Z	611	CLA	MG-NA	-4.89	1.94	2.06
21	6	307	CHL	C1B-C2B	4.89	1.45	1.39
21	6	306	CHL	C1B-C2B	4.89	1.45	1.39
18	A	821	CLA	MG-NA	-4.88	1.94	2.06
18	5	611	CLA	MG-NA	-4.88	1.94	2.06
21	5	607	CHL	C3A-C2A	-4.88	1.50	1.54
18	1	612	CLA	MG-NA	-4.87	1.94	2.06
18	A	833	CLA	MG-NB	-4.87	1.96	2.05
18	1	607	CLA	MG-NA	-4.87	1.94	2.06
18	B	835	CLA	MG-NC	-4.87	1.94	2.06
18	3	310	CLA	MG-NA	-4.86	1.94	2.06
18	3	308	CLA	MG-NA	-4.86	1.94	2.06
18	4	609	CLA	MG-NC	-4.86	1.94	2.06
18	7	602	CLA	MG-NA	-4.86	1.94	2.06
18	8	609	CLA	MG-NC	-4.86	1.94	2.06
18	B	827	CLA	MG-NC	-4.85	1.94	2.06
18	B	813	CLA	MG-NA	-4.84	1.94	2.06
18	Z	606	CLA	MG-NA	-4.84	1.94	2.06
18	B	821	CLA	MG-NA	-4.84	1.94	2.06
18	A	841	CLA	MG-NA	-4.83	1.94	2.06
18	5	609	CLA	MG-NA	-4.81	1.94	2.06
18	B	838	CLA	MG-NC	-4.81	1.94	2.06
18	Z	602	CLA	MG-NA	-4.80	1.94	2.06
18	4	607	CLA	MG-NC	-4.80	1.94	2.06
18	1	611	CLA	MG-NA	-4.80	1.94	2.06
18	B	839	CLA	MG-NA	-4.80	1.94	2.06
18	8	602	CLA	MG-NA	-4.80	1.94	2.06
18	8	604	CLA	MG-NA	-4.80	1.94	2.06
18	B	826	CLA	MG-NA	-4.80	1.94	2.06
18	A	802	CLA	MG-NC	-4.80	1.94	2.06
18	B	806	CLA	MG-NC	-4.80	1.94	2.06
18	7	609	CLA	MG-NA	-4.79	1.94	2.06
18	B	801	CLA	MG-NA	-4.78	1.94	2.06
21	4	604	CHL	CHB-C4A	-4.78	1.32	1.38
18	A	816	CLA	MG-NA	-4.78	1.94	2.06
18	B	834	CLA	MG-NA	-4.78	1.94	2.06
18	1	602	CLA	MG-NA	-4.78	1.94	2.06
18	7	607	CLA	MG-NA	-4.77	1.94	2.06
18	A	824	CLA	MG-NC	-4.77	1.94	2.06
18	A	832	CLA	MG-NA	-4.77	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	604	CLA	MG-NA	-4.77	1.94	2.06
18	1	610	CLA	MG-NA	-4.77	1.94	2.06
18	A	845	CLA	MG-NA	-4.77	1.94	2.06
18	6	311	CLA	MG-NA	-4.76	1.95	2.06
18	A	814	CLA	MG-NA	-4.76	1.95	2.06
18	7	611	CLA	MG-NC	-4.76	1.95	2.06
18	Z	610	CLA	MG-NA	-4.76	1.95	2.06
18	Z	603	CLA	MG-NA	-4.76	1.95	2.06
18	8	607	CLA	MG-NC	-4.76	1.95	2.06
18	Z	603	CLA	MG-NC	-4.76	1.95	2.06
18	8	608	CLA	MG-NA	-4.75	1.95	2.06
18	B	833	CLA	MG-NA	-4.75	1.95	2.06
18	B	831	CLA	MG-NA	-4.75	1.95	2.06
18	4	608	CLA	MG-NC	-4.75	1.95	2.06
18	1	604	CLA	MG-NC	-4.74	1.95	2.06
18	8	610	CLA	C4B-NB	4.74	1.44	1.37
18	3	301	CLA	MG-NC	-4.74	1.95	2.06
18	B	809	CLA	MG-NA	-4.74	1.95	2.06
18	B	804	CLA	MG-NC	-4.74	1.95	2.06
18	A	818	CLA	MG-NA	-4.74	1.95	2.06
18	Z	609	CLA	MG-NA	-4.73	1.95	2.06
18	8	611	CLA	MG-NC	-4.73	1.95	2.06
18	B	812	CLA	MG-NC	-4.73	1.95	2.06
18	A	816	CLA	MG-NC	-4.73	1.95	2.06
18	1	613	CLA	MG-NA	-4.73	1.95	2.06
18	3	312	CLA	MG-NA	-4.73	1.95	2.06
18	6	302	CLA	MG-NA	-4.73	1.95	2.06
18	B	828	CLA	MG-NA	-4.73	1.95	2.06
18	Z	612	CLA	MG-NA	-4.73	1.95	2.06
18	A	837	CLA	MG-NA	-4.72	1.95	2.06
18	8	601	CLA	MG-NA	-4.71	1.95	2.06
18	A	831	CLA	MG-NA	-4.70	1.95	2.06
18	3	307	CLA	MG-NC	-4.70	1.95	2.06
18	B	814	CLA	MG-NC	-4.70	1.95	2.06
18	3	303	CLA	MG-NA	-4.70	1.95	2.06
18	8	610	CLA	MG-NC	-4.68	1.95	2.06
18	A	823	CLA	MG-NC	-4.68	1.95	2.06
18	A	809	CLA	MG-NA	-4.68	1.95	2.06
18	6	304	CLA	MG-NA	-4.67	1.95	2.06
18	7	605	CLA	MG-NA	-4.67	1.95	2.06
18	8	614	CLA	MG-NC	-4.66	1.95	2.06
21	6	307	CHL	C3A-C2A	-4.66	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	101	CLA	MG-NA	-4.66	1.95	2.06
18	B	840	CLA	MG-NA	-4.65	1.95	2.06
18	B	814	CLA	MG-NA	-4.65	1.95	2.06
18	A	812	CLA	MG-NA	-4.64	1.95	2.06
18	7	612	CLA	MG-NA	-4.64	1.95	2.06
18	7	614	CLA	MG-NC	-4.64	1.95	2.06
18	7	608	CLA	MG-NC	-4.63	1.95	2.06
18	A	818	CLA	MG-NC	-4.63	1.95	2.06
18	5	604	CLA	MG-NA	-4.62	1.95	2.06
18	5	612	CLA	MG-NA	-4.62	1.95	2.06
18	B	819	CLA	MG-NC	-4.61	1.95	2.06
18	B	836	CLA	MG-NA	-4.60	1.95	2.06
18	5	608	CLA	MG-NA	-4.60	1.95	2.06
18	B	823	CLA	MG-NA	-4.60	1.95	2.06
18	1	614	CLA	MG-NA	-4.59	1.95	2.06
18	B	815	CLA	MG-NC	-4.59	1.95	2.06
18	A	845	CLA	MG-NC	-4.58	1.95	2.06
18	A	820	CLA	MG-NA	-4.58	1.95	2.06
18	B	816	CLA	MG-NA	-4.58	1.95	2.06
18	3	313	CLA	MG-NA	-4.58	1.95	2.06
18	Z	613	CLA	MG-NA	-4.58	1.95	2.06
18	7	607	CLA	MG-NC	-4.58	1.95	2.06
18	7	613	CLA	MG-NC	-4.58	1.95	2.06
18	Z	613	CLA	MG-NC	-4.58	1.95	2.06
18	3	314	CLA	MG-NA	-4.58	1.95	2.06
18	A	840	CLA	MG-NC	-4.57	1.95	2.06
18	A	829	CLA	MG-NA	-4.57	1.95	2.06
18	A	835	CLA	MG-NC	-4.57	1.95	2.06
18	A	810	CLA	MG-NC	-4.57	1.95	2.06
18	6	314	CLA	MG-NA	-4.57	1.95	2.06
18	A	839	CLA	MG-NA	-4.55	1.95	2.06
18	5	614	CLA	MG-NA	-4.55	1.95	2.06
18	A	812	CLA	MG-NC	-4.55	1.95	2.06
18	1	614	CLA	MG-NC	-4.55	1.95	2.06
18	A	826	CLA	MG-NC	-4.55	1.95	2.06
18	A	819	CLA	MG-NC	-4.53	1.95	2.06
18	A	830	CLA	MG-NC	-4.52	1.95	2.06
18	5	601	CLA	MG-NC	-4.51	1.95	2.06
18	A	843	CLA	MG-NA	-4.51	1.95	2.06
18	3	302	CLA	MG-NA	-4.51	1.95	2.06
18	8	603	CLA	MG-NC	-4.51	1.95	2.06
18	3	312	CLA	MG-NC	-4.51	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	828	CLA	MG-NA	-4.50	1.95	2.06
18	A	817	CLA	MG-NA	-4.50	1.95	2.06
18	A	806	CLA	MG-NC	-4.50	1.95	2.06
18	B	831	CLA	MG-NC	-4.50	1.95	2.06
18	B	807	CLA	MG-NC	-4.49	1.95	2.06
18	B	842	CLA	MG-NC	-4.49	1.95	2.06
18	3	311	CLA	MG-NA	-4.48	1.95	2.06
18	7	610	CLA	MG-NC	-4.48	1.95	2.06
18	B	829	CLA	MG-NC	-4.48	1.95	2.06
18	B	818	CLA	MG-NC	-4.48	1.95	2.06
18	3	310	CLA	MG-NC	-4.47	1.95	2.06
18	6	313	CLA	MG-NC	-4.47	1.95	2.06
18	7	601	CLA	MG-NC	-4.47	1.95	2.06
21	1	606	CHL	C1B-C2B	4.46	1.44	1.39
18	6	315	CLA	MG-NC	-4.46	1.95	2.06
18	B	820	CLA	MG-NC	-4.46	1.95	2.06
18	F	302	CLA	MG-NA	-4.46	1.95	2.06
18	A	822	CLA	MG-NA	-4.46	1.95	2.06
18	A	815	CLA	MG-NC	-4.45	1.95	2.06
21	6	306	CHL	C3A-C2A	-4.45	1.50	1.54
18	A	838	CLA	MG-NC	-4.45	1.95	2.06
18	6	303	CLA	MG-NA	-4.44	1.95	2.06
18	A	834	CLA	MG-NC	-4.43	1.95	2.06
18	3	308	CLA	MG-NC	-4.43	1.95	2.06
18	A	805	CLA	MG-NC	-4.43	1.95	2.06
18	J	101	CLA	MG-NC	-4.43	1.95	2.06
18	4	603	CLA	MG-NA	-4.42	1.95	2.06
18	6	311	CLA	MG-NC	-4.41	1.95	2.06
18	5	602	CLA	MG-NC	-4.41	1.95	2.06
18	A	820	CLA	MG-NC	-4.40	1.95	2.06
18	A	833	CLA	MG-NA	-4.40	1.95	2.06
18	B	825	CLA	MG-NA	-4.39	1.95	2.06
18	7	602	CLA	MG-NC	-4.38	1.95	2.06
18	F	301	CLA	MG-NC	-4.38	1.95	2.06
18	3	304	CLA	MG-NA	-4.37	1.95	2.06
21	Z	605	CHL	C1B-C2B	4.37	1.44	1.39
18	B	837	CLA	MG-NA	-4.37	1.95	2.06
18	B	833	CLA	MG-NC	-4.36	1.95	2.06
18	A	822	CLA	MG-NC	-4.36	1.95	2.06
18	6	317	CLA	MG-NA	-4.36	1.95	2.06
18	5	617	CLA	MG-NC	-4.35	1.95	2.06
18	A	814	CLA	MG-NC	-4.35	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	844	CLA	MG-NA	-4.35	1.95	2.06
18	B	801	CLA	MG-NC	-4.35	1.95	2.06
18	7	609	CLA	MG-NC	-4.35	1.95	2.06
18	B	826	CLA	MG-NC	-4.35	1.95	2.06
18	7	603	CLA	MG-NC	-4.34	1.96	2.06
18	3	314	CLA	MG-NC	-4.34	1.96	2.06
18	8	612	CLA	MG-NA	-4.34	1.96	2.06
18	A	837	CLA	MG-NC	-4.33	1.96	2.06
18	B	843	CLA	MG-NA	-4.33	1.96	2.06
18	5	603	CLA	MG-NA	-4.32	1.96	2.06
18	B	816	CLA	MG-NC	-4.32	1.96	2.06
18	B	810	CLA	MG-NC	-4.32	1.96	2.06
18	5	611	CLA	MG-NC	-4.32	1.96	2.06
18	1	608	CLA	MG-NC	-4.31	1.96	2.06
18	4	610	CLA	MG-NA	-4.30	1.96	2.06
18	6	304	CLA	MG-NC	-4.30	1.96	2.06
18	Z	607	CLA	MG-NC	-4.30	1.96	2.06
18	1	602	CLA	MG-NC	-4.30	1.96	2.06
18	B	808	CLA	MG-NA	-4.29	1.96	2.06
21	4	605	CHL	C3B-C2B	-4.29	1.34	1.40
18	1	603	CLA	MG-NA	-4.29	1.96	2.06
18	3	309	CLA	MG-NC	-4.29	1.96	2.06
18	A	817	CLA	MG-NC	-4.28	1.96	2.06
18	B	822	CLA	MG-NC	-4.28	1.96	2.06
18	Z	602	CLA	MG-NC	-4.28	1.96	2.06
18	8	608	CLA	MG-NC	-4.28	1.96	2.06
18	A	811	CLA	MG-NC	-4.27	1.96	2.06
18	B	824	CLA	MG-NC	-4.27	1.96	2.06
18	B	802	CLA	MG-NC	-4.27	1.96	2.06
18	8	615	CLA	MG-NA	-4.27	1.96	2.06
18	A	841	CLA	MG-NC	-4.27	1.96	2.06
18	4	602	CLA	MG-NC	-4.26	1.96	2.06
18	1	613	CLA	MG-NC	-4.25	1.96	2.06
18	6	301	CLA	MG-NA	-4.25	1.96	2.06
18	A	809	CLA	MG-NC	-4.25	1.96	2.06
18	Z	612	CLA	MG-NC	-4.24	1.96	2.06
18	B	813	CLA	MG-NC	-4.24	1.96	2.06
18	B	817	CLA	MG-NC	-4.23	1.96	2.06
18	6	302	CLA	MG-NC	-4.23	1.96	2.06
18	A	832	CLA	MG-NC	-4.23	1.96	2.06
18	A	804	CLA	MG-NA	-4.23	1.96	2.06
18	3	313	CLA	MG-NC	-4.22	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	843	CLA	MG-NC	-4.22	1.96	2.06
18	4	603	CLA	MG-NC	-4.22	1.96	2.06
18	B	811	CLA	MG-NA	-4.21	1.96	2.06
18	8	613	CLA	MG-NC	-4.21	1.96	2.06
18	3	303	CLA	MG-NC	-4.21	1.96	2.06
18	6	308	CLA	MG-NC	-4.21	1.96	2.06
18	A	831	CLA	MG-NC	-4.20	1.96	2.06
18	5	609	CLA	MG-NC	-4.20	1.96	2.06
18	B	809	CLA	MG-NC	-4.20	1.96	2.06
18	8	605	CLA	MG-NA	-4.20	1.96	2.06
18	5	612	CLA	MG-NC	-4.20	1.96	2.06
18	4	611	CLA	MG-NC	-4.20	1.96	2.06
18	Z	610	CLA	MG-NC	-4.19	1.96	2.06
18	6	312	CLA	MG-NC	-4.19	1.96	2.06
18	A	829	CLA	MG-NC	-4.18	1.96	2.06
18	Z	609	CLA	MG-NC	-4.18	1.96	2.06
18	B	832	CLA	MG-NC	-4.18	1.96	2.06
18	B	839	CLA	MG-NC	-4.17	1.96	2.06
18	8	602	CLA	MG-NC	-4.16	1.96	2.06
18	1	611	CLA	MG-NC	-4.16	1.96	2.06
18	B	836	CLA	MG-NC	-4.16	1.96	2.06
18	5	608	CLA	MG-NC	-4.16	1.96	2.06
18	8	604	CLA	MG-NC	-4.15	1.96	2.06
18	1	610	CLA	MG-NC	-4.15	1.96	2.06
18	7	605	CLA	MG-NC	-4.15	1.96	2.06
18	A	821	CLA	MG-NC	-4.14	1.96	2.06
18	3	311	CLA	MG-NC	-4.13	1.96	2.06
18	B	808	CLA	MG-NC	-4.12	1.96	2.06
18	B	823	CLA	MG-ND	-4.12	1.97	2.05
18	5	605	CLA	MG-NA	-4.12	1.96	2.06
18	Z	608	CLA	MG-NC	-4.11	1.96	2.06
18	6	309	CLA	MG-NC	-4.11	1.96	2.06
18	1	609	CLA	MG-NC	-4.10	1.96	2.06
18	6	303	CLA	MG-NC	-4.10	1.96	2.06
18	3	304	CLA	MG-NC	-4.10	1.96	2.06
18	B	828	CLA	MG-NC	-4.09	1.96	2.06
18	8	612	CLA	MG-NC	-4.09	1.96	2.06
18	B	825	CLA	MG-NC	-4.08	1.96	2.06
18	5	604	CLA	MG-NC	-4.08	1.96	2.06
21	1	601	CHL	C3A-C2A	-4.08	1.51	1.54
18	A	839	CLA	MG-NC	-4.07	1.96	2.06
18	8	601	CLA	MG-NC	-4.06	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	813	CLA	MG-NC	-4.05	1.96	2.06
18	7	612	CLA	MG-NC	-4.05	1.96	2.06
18	3	302	CLA	MG-NC	-4.05	1.96	2.06
18	B	840	CLA	MG-NC	-4.03	1.96	2.06
18	A	843	CLA	MG-NC	-4.02	1.96	2.06
18	A	828	CLA	MG-NC	-4.01	1.96	2.06
21	Z	601	CHL	C3A-C2A	-3.99	1.51	1.54
18	1	607	CLA	MG-NC	-3.99	1.96	2.06
18	B	830	CLA	MG-NC	-3.99	1.96	2.06
18	F	302	CLA	MG-NC	-3.99	1.96	2.06
18	6	317	CLA	MG-NC	-3.98	1.96	2.06
21	5	606	CHL	C1B-C2B	3.98	1.44	1.39
18	Z	606	CLA	MG-NC	-3.97	1.96	2.06
18	A	833	CLA	MG-NC	-3.96	1.96	2.06
18	5	610	CLA	MG-NC	-3.96	1.96	2.06
18	B	821	CLA	MG-NC	-3.96	1.96	2.06
18	B	834	CLA	MG-NC	-3.94	1.96	2.06
18	1	605	CLA	MG-NA	-3.92	1.97	2.06
18	Z	604	CLA	MG-NA	-3.91	1.97	2.06
18	1	612	CLA	MG-NC	-3.91	1.97	2.06
18	6	314	CLA	MG-NC	-3.91	1.97	2.06
18	4	606	CLA	MG-NC	-3.91	1.97	2.06
18	Z	611	CLA	MG-NC	-3.91	1.97	2.06
18	8	615	CLA	MG-NC	-3.90	1.97	2.06
18	7	604	CLA	MG-NA	-3.90	1.97	2.06
18	5	614	CLA	MG-NC	-3.89	1.97	2.06
18	1	603	CLA	MG-NC	-3.88	1.97	2.06
21	4	605	CHL	MG-ND	-3.86	1.98	2.05
18	8	605	CLA	MG-NC	-3.82	1.97	2.06
18	A	844	CLA	MG-NC	-3.82	1.97	2.06
18	B	837	CLA	MG-NC	-3.75	1.97	2.06
18	5	603	CLA	MG-NC	-3.75	1.97	2.06
21	4	605	CHL	C1B-C2B	3.73	1.43	1.39
18	A	804	CLA	MG-NC	-3.71	1.97	2.06
18	A	825	CLA	C3A-C2A	-3.71	1.44	1.54
18	B	807	CLA	C2-C3	3.68	1.52	1.29
18	4	610	CLA	MG-NC	-3.67	1.97	2.06
18	6	301	CLA	MG-NC	-3.65	1.97	2.06
18	B	811	CLA	MG-NC	-3.64	1.97	2.06
18	B	823	CLA	MG-NC	-3.63	1.97	2.06
21	3	306	CHL	C3B-C2B	-3.62	1.35	1.40
21	6	316	CHL	C3B-C4B	3.56	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	605	CLA	MG-NC	-3.55	1.97	2.06
18	Z	604	CLA	MG-NC	-3.53	1.97	2.06
18	1	605	CLA	MG-NC	-3.52	1.97	2.06
18	5	601	CLA	C1D-ND	3.43	1.42	1.37
18	6	301	CLA	C1D-ND	3.42	1.42	1.37
21	1	601	CHL	C3B-C2B	-3.42	1.35	1.40
18	7	604	CLA	C1D-ND	3.41	1.42	1.37
18	6	304	CLA	C1D-ND	3.41	1.42	1.37
21	6	307	CHL	C3B-C2B	-3.41	1.35	1.40
18	Z	612	CLA	C1D-ND	3.41	1.42	1.37
18	J	101	CLA	C1D-ND	3.40	1.42	1.37
18	8	608	CLA	C1D-ND	3.39	1.42	1.37
21	Z	601	CHL	C3B-C2B	-3.39	1.35	1.40
18	1	613	CLA	C1D-ND	3.38	1.42	1.37
18	1	611	CLA	C1D-ND	3.36	1.42	1.37
18	B	843	CLA	C1D-ND	3.35	1.42	1.37
18	Z	610	CLA	C1D-ND	3.34	1.42	1.37
21	Z	605	CHL	C3B-C2B	-3.32	1.35	1.40
18	3	312	CLA	C1D-ND	3.29	1.42	1.37
18	A	834	CLA	C3A-C2A	-3.29	1.45	1.54
21	1	606	CHL	C3B-C2B	-3.29	1.35	1.40
21	5	606	CHL	C3B-C2B	-3.27	1.35	1.40
17	A	801	CL0	C3B-C2B	-3.25	1.36	1.40
21	7	606	CHL	C3B-C2B	-3.24	1.36	1.40
18	1	604	CLA	C1D-ND	3.23	1.42	1.37
18	5	604	CLA	C1D-ND	3.21	1.42	1.37
18	4	606	CLA	C1D-ND	3.20	1.42	1.37
21	6	306	CHL	C3B-C2B	-3.20	1.36	1.40
18	A	803	CLA	C3A-C2A	-3.19	1.45	1.54
18	Z	603	CLA	C1D-ND	3.17	1.42	1.37
21	6	306	CHL	C3B-C4B	3.17	1.44	1.41
18	8	609	CLA	C1D-ND	3.17	1.42	1.37
21	7	606	CHL	C3A-C2A	-3.17	1.52	1.54
18	B	814	CLA	C1D-ND	3.16	1.42	1.37
18	7	604	CLA	MG-NC	-3.15	1.98	2.06
21	5	607	CHL	C3B-C2B	-3.15	1.36	1.40
21	7	606	CHL	C3B-C4B	3.11	1.44	1.41
21	4	605	CHL	CHB-C1B	-3.11	1.34	1.39
21	5	616	CHL	C3B-C2B	-3.11	1.36	1.40
18	A	833	CLA	C1D-ND	3.11	1.41	1.37
18	8	607	CLA	C3A-C2A	-3.10	1.46	1.54
21	5	616	CHL	C3B-C4B	3.09	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	605	CHL	C3B-C4B	3.08	1.44	1.41
18	6	312	CLA	C1D-ND	3.06	1.41	1.37
18	5	614	CLA	C1D-ND	3.05	1.41	1.37
18	6	317	CLA	C1D-ND	3.04	1.41	1.37
18	1	603	CLA	C1D-ND	3.03	1.41	1.37
18	8	615	CLA	C1D-ND	3.02	1.41	1.37
21	4	605	CHL	CHC-C4B	-3.02	1.34	1.39
18	B	808	CLA	C1D-ND	3.01	1.41	1.37
18	B	828	CLA	C1D-ND	3.00	1.41	1.37
21	5	606	CHL	C3B-C4B	3.00	1.44	1.41
21	1	601	CHL	CHC-C4B	-2.99	1.34	1.39
21	6	307	CHL	CHB-C1B	-2.99	1.34	1.39
21	1	606	CHL	C3B-C4B	2.99	1.44	1.41
18	8	611	CLA	C3A-C2A	-2.99	1.46	1.54
21	Z	601	CHL	CHC-C4B	-2.98	1.34	1.39
18	6	310	CLA	C4B-NB	2.98	1.41	1.37
21	8	606	CHL	CHC-C4B	-2.98	1.34	1.39
18	5	605	CLA	C1D-ND	2.98	1.41	1.37
18	5	609	CLA	C1D-ND	2.98	1.41	1.37
18	B	823	CLA	C1D-ND	2.98	1.41	1.37
18	A	822	CLA	C1D-ND	2.97	1.41	1.37
18	A	832	CLA	C1D-ND	2.97	1.41	1.37
18	A	829	CLA	C1D-ND	2.97	1.41	1.37
17	A	801	CL0	CHB-C4A	-2.97	1.35	1.38
18	3	313	CLA	C1D-ND	2.96	1.41	1.37
18	B	811	CLA	C3A-C2A	-2.96	1.46	1.54
21	4	605	CHL	C3B-C4B	2.96	1.44	1.41
18	A	839	CLA	C1D-ND	2.95	1.41	1.37
18	A	816	CLA	C1D-ND	2.95	1.41	1.37
18	B	810	CLA	C1D-ND	2.94	1.41	1.37
18	5	603	CLA	C1D-ND	2.93	1.41	1.37
18	6	311	CLA	C1D-ND	2.93	1.41	1.37
18	B	826	CLA	C1D-ND	2.93	1.41	1.37
18	3	314	CLA	C1D-ND	2.93	1.41	1.37
18	7	613	CLA	C1D-ND	2.92	1.41	1.37
18	6	309	CLA	C1D-ND	2.92	1.41	1.37
18	B	825	CLA	C1D-ND	2.92	1.41	1.37
18	A	837	CLA	C3A-C2A	-2.92	1.46	1.54
21	5	607	CHL	CHB-C1B	-2.91	1.34	1.39
18	1	614	CLA	C1D-ND	2.90	1.41	1.37
18	4	609	CLA	C1D-ND	2.90	1.41	1.37
18	B	831	CLA	C1D-ND	2.90	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	8	612	CLA	C1D-ND	2.88	1.41	1.37
18	A	839	CLA	C3A-C2A	-2.88	1.46	1.54
18	7	609	CLA	C1D-ND	2.87	1.41	1.37
18	4	610	CLA	C1D-ND	2.87	1.41	1.37
18	B	823	CLA	C1C-C2C	2.87	1.50	1.44
18	Z	613	CLA	C1D-ND	2.86	1.41	1.37
18	3	310	CLA	C1D-ND	2.86	1.41	1.37
18	8	605	CLA	C1D-ND	2.86	1.41	1.37
18	A	806	CLA	C3A-C2A	-2.86	1.46	1.54
18	Z	602	CLA	C1D-ND	2.86	1.41	1.37
21	8	606	CHL	C3B-C2B	-2.86	1.36	1.40
18	1	609	CLA	C1D-ND	2.85	1.41	1.37
21	6	316	CHL	C3B-C2B	-2.85	1.36	1.40
18	3	311	CLA	C1D-ND	2.85	1.41	1.37
18	B	812	CLA	C1D-ND	2.84	1.41	1.37
18	Z	608	CLA	C1D-ND	2.84	1.41	1.37
21	6	307	CHL	CHC-C4B	-2.84	1.35	1.39
18	8	602	CLA	C1D-ND	2.84	1.41	1.37
18	Z	606	CLA	C1D-ND	2.84	1.41	1.37
18	6	313	CLA	C1D-ND	2.83	1.41	1.37
18	4	606	CLA	C1B-NB	2.83	1.41	1.37
21	Z	601	CHL	CHB-C1B	-2.83	1.35	1.39
21	5	607	CHL	CHC-C4B	-2.82	1.35	1.39
18	1	602	CLA	C1D-ND	2.82	1.41	1.37
18	8	613	CLA	C1D-ND	2.81	1.41	1.37
18	1	607	CLA	C1D-ND	2.81	1.41	1.37
18	A	826	CLA	C3A-C2A	-2.80	1.46	1.54
18	4	603	CLA	C1D-C2D	-2.80	1.39	1.45
21	1	606	CHL	C3D-C4D	-2.79	1.37	1.41
21	8	606	CHL	C3A-C2A	-2.79	1.52	1.54
21	1	601	CHL	CHB-C1B	-2.79	1.35	1.39
21	3	306	CHL	CHB-C1B	-2.79	1.35	1.39
21	Z	605	CHL	C3D-C4D	-2.78	1.37	1.41
18	B	825	CLA	C3A-C2A	-2.78	1.46	1.54
18	1	612	CLA	C1D-ND	2.78	1.41	1.37
18	3	308	CLA	C1D-ND	2.78	1.41	1.37
18	4	607	CLA	C1D-ND	2.77	1.41	1.37
18	A	812	CLA	C1D-ND	2.77	1.41	1.37
21	6	307	CHL	C3B-C4B	2.77	1.44	1.41
18	A	845	CLA	C1D-ND	2.77	1.41	1.37
18	7	614	CLA	C1D-ND	2.77	1.41	1.37
18	5	605	CLA	C3A-C2A	-2.76	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	604	CHL	C3B-C2B	-2.76	1.36	1.40
18	A	823	CLA	C1D-ND	2.75	1.41	1.37
18	7	611	CLA	C1D-ND	2.75	1.41	1.37
17	A	801	CL0	C1A-CHA	-2.75	1.36	1.40
18	B	836	CLA	C1D-ND	2.75	1.41	1.37
18	B	812	CLA	C3A-C2A	-2.75	1.47	1.54
18	B	837	CLA	C1D-ND	2.75	1.41	1.37
18	B	832	CLA	C1D-ND	2.74	1.41	1.37
18	A	835	CLA	C1B-NB	2.74	1.41	1.37
18	B	807	CLA	C3A-C2A	-2.74	1.47	1.54
21	6	305	CHL	C3B-C2B	-2.73	1.36	1.40
21	5	616	CHL	CHC-C4B	-2.73	1.35	1.39
18	5	608	CLA	C1D-ND	2.72	1.41	1.37
18	8	607	CLA	C1D-ND	2.71	1.41	1.37
21	1	606	CHL	CHB-C1B	-2.71	1.35	1.39
18	5	608	CLA	C1D-C2D	-2.70	1.40	1.45
18	6	303	CLA	C1D-ND	2.70	1.41	1.37
18	A	845	CLA	C1D-C2D	-2.70	1.40	1.45
18	1	605	CLA	C1D-ND	2.70	1.41	1.37
21	3	306	CHL	C3B-C4B	2.69	1.44	1.41
18	B	821	CLA	C1D-ND	2.69	1.41	1.37
18	Z	611	CLA	C1D-ND	2.69	1.41	1.37
18	7	608	CLA	C1D-ND	2.69	1.41	1.37
18	B	824	CLA	C1D-ND	2.68	1.41	1.37
18	A	806	CLA	C1D-ND	2.68	1.41	1.37
18	6	304	CLA	C1D-C2D	-2.68	1.40	1.45
21	6	305	CHL	C3B-C4B	2.68	1.44	1.41
18	5	603	CLA	C1D-C2D	-2.68	1.40	1.45
18	A	820	CLA	C1D-ND	2.68	1.41	1.37
21	4	604	CHL	CHC-C4B	-2.68	1.35	1.39
18	B	829	CLA	C1D-C2D	-2.68	1.40	1.45
18	4	607	CLA	C1C-C2C	2.67	1.49	1.44
18	Z	604	CLA	C1D-ND	2.67	1.41	1.37
18	B	834	CLA	C1D-ND	2.67	1.41	1.37
18	B	822	CLA	C1D-ND	2.67	1.41	1.37
18	3	302	CLA	C1D-ND	2.67	1.41	1.37
18	B	816	CLA	C1D-ND	2.66	1.41	1.37
18	8	608	CLA	C1D-C2D	-2.66	1.40	1.45
18	6	314	CLA	C1D-ND	2.66	1.41	1.37
21	6	305	CHL	CHC-C4B	-2.66	1.35	1.39
21	6	306	CHL	CHB-C1B	-2.66	1.35	1.39
18	A	835	CLA	C1D-C2D	-2.65	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	606	CHL	CHC-C4B	-2.65	1.35	1.39
21	Z	605	CHL	CHB-C1B	-2.65	1.35	1.39
18	8	615	CLA	C1D-C2D	-2.65	1.40	1.45
21	7	606	CHL	C1A-CHA	-2.65	1.37	1.40
18	B	808	CLA	C1D-C2D	-2.64	1.40	1.45
18	6	308	CLA	C1D-ND	2.64	1.41	1.37
18	A	821	CLA	C1D-C2D	-2.64	1.40	1.45
18	1	603	CLA	C1D-C2D	-2.64	1.40	1.45
18	B	817	CLA	C1D-ND	2.64	1.41	1.37
18	B	838	CLA	C1D-ND	2.64	1.41	1.37
21	Z	605	CHL	CHC-C4B	-2.64	1.35	1.39
18	5	601	CLA	C1D-C2D	-2.64	1.40	1.45
18	B	813	CLA	C1D-ND	2.63	1.41	1.37
21	3	306	CHL	CHC-C4B	-2.63	1.35	1.39
18	8	604	CLA	C1D-ND	2.63	1.41	1.37
18	A	807	CLA	C1D-ND	2.62	1.41	1.37
18	8	607	CLA	C1D-C2D	-2.62	1.40	1.45
18	A	830	CLA	C1D-ND	2.62	1.41	1.37
18	A	839	CLA	C1D-C2D	-2.62	1.40	1.45
18	B	833	CLA	C1D-C2D	-2.62	1.40	1.45
18	A	835	CLA	C1D-ND	2.62	1.41	1.37
18	A	843	CLA	C1D-ND	2.62	1.41	1.37
18	6	301	CLA	C1B-NB	2.62	1.41	1.37
21	5	616	CHL	CHB-C1B	-2.61	1.35	1.39
18	5	602	CLA	C1D-C2D	-2.61	1.40	1.45
18	A	809	CLA	C1D-C2D	-2.61	1.40	1.45
18	A	841	CLA	C1D-C2D	-2.61	1.40	1.45
18	3	311	CLA	C1D-C2D	-2.61	1.40	1.45
18	6	317	CLA	C1D-C2D	-2.60	1.40	1.45
18	7	607	CLA	C1D-ND	2.60	1.41	1.37
18	6	303	CLA	C1D-C2D	-2.60	1.40	1.45
18	5	612	CLA	C1D-C2D	-2.60	1.40	1.45
21	6	305	CHL	CHB-C1B	-2.60	1.35	1.39
18	3	314	CLA	C1D-C2D	-2.59	1.40	1.45
18	A	841	CLA	C1D-ND	2.59	1.41	1.37
18	7	603	CLA	C1D-ND	2.59	1.41	1.37
18	4	611	CLA	C1D-C2D	-2.59	1.40	1.45
18	6	314	CLA	C3A-C2A	-2.59	1.47	1.54
21	5	606	CHL	CHB-C1B	-2.59	1.35	1.39
18	B	836	CLA	C3A-C2A	-2.59	1.47	1.54
18	1	614	CLA	C1D-C2D	-2.59	1.40	1.45
18	A	804	CLA	C1D-ND	2.58	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	613	CLA	C1D-C2D	-2.58	1.40	1.45
21	7	606	CHL	CHB-C1B	-2.58	1.35	1.39
18	6	301	CLA	C1D-C2D	-2.58	1.40	1.45
18	7	603	CLA	C1D-C2D	-2.58	1.40	1.45
18	7	604	CLA	C3D-C4D	-2.57	1.38	1.44
18	A	818	CLA	C1D-C2D	-2.57	1.40	1.45
18	8	602	CLA	C1D-C2D	-2.57	1.40	1.45
18	A	821	CLA	C1D-ND	2.57	1.41	1.37
18	Z	613	CLA	C1D-C2D	-2.57	1.40	1.45
18	B	838	CLA	C1D-C2D	-2.57	1.40	1.45
18	8	612	CLA	C1D-C2D	-2.57	1.40	1.45
21	1	601	CHL	C3B-C4B	2.57	1.43	1.41
21	8	606	CHL	C3B-C4B	2.57	1.43	1.41
18	A	805	CLA	C3A-C2A	-2.56	1.47	1.54
18	7	607	CLA	C1D-C2D	-2.56	1.40	1.45
18	B	840	CLA	C1D-ND	2.56	1.41	1.37
18	7	605	CLA	C3A-C2A	-2.56	1.47	1.54
21	Z	601	CHL	C3B-C4B	2.56	1.43	1.41
18	A	828	CLA	C1D-C2D	-2.56	1.40	1.45
18	B	815	CLA	C3A-C2A	-2.56	1.47	1.54
18	6	309	CLA	C1B-NB	2.56	1.41	1.37
18	5	612	CLA	C1D-ND	2.55	1.41	1.37
18	F	302	CLA	C1D-C2D	-2.55	1.40	1.45
18	A	836	CLA	C1D-ND	2.55	1.41	1.37
18	B	823	CLA	C1B-NB	2.55	1.41	1.37
18	4	608	CLA	C1D-C2D	-2.54	1.40	1.45
18	F	302	CLA	C1D-ND	2.54	1.41	1.37
18	B	804	CLA	C3A-C2A	-2.54	1.47	1.54
18	B	802	CLA	C1D-C2D	-2.54	1.40	1.45
18	8	601	CLA	C1D-C2D	-2.54	1.40	1.45
18	A	811	CLA	C1D-C2D	-2.54	1.40	1.45
18	A	815	CLA	C1D-C2D	-2.54	1.40	1.45
18	Z	607	CLA	C1D-C2D	-2.54	1.40	1.45
18	Z	610	CLA	C3A-C2A	-2.53	1.47	1.54
18	A	833	CLA	C1D-C2D	-2.53	1.40	1.45
18	7	602	CLA	C1D-C2D	-2.53	1.40	1.45
18	B	809	CLA	C1D-C2D	-2.53	1.40	1.45
18	6	302	CLA	C1D-C2D	-2.53	1.40	1.45
18	6	311	CLA	C3A-C2A	-2.53	1.47	1.54
18	A	830	CLA	C1D-C2D	-2.53	1.40	1.45
18	A	836	CLA	C1D-C2D	-2.53	1.40	1.45
18	7	608	CLA	C1D-C2D	-2.53	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	302	CLA	C1D-C2D	-2.53	1.40	1.45
18	A	841	CLA	C3A-C2A	-2.53	1.47	1.54
18	3	308	CLA	C1D-C2D	-2.52	1.40	1.45
18	6	312	CLA	C1D-C2D	-2.52	1.40	1.45
18	A	834	CLA	C3D-C4D	-2.52	1.38	1.44
18	B	825	CLA	C1D-C2D	-2.52	1.40	1.45
18	8	603	CLA	C1D-C2D	-2.52	1.40	1.45
21	6	306	CHL	CHC-C4B	-2.52	1.35	1.39
18	A	804	CLA	C1D-C2D	-2.51	1.40	1.45
18	A	811	CLA	C1D-ND	2.51	1.41	1.37
18	A	817	CLA	C1D-C2D	-2.51	1.40	1.45
18	A	837	CLA	C1D-C2D	-2.51	1.40	1.45
18	B	840	CLA	C1D-C2D	-2.51	1.40	1.45
18	B	830	CLA	C1D-ND	2.51	1.41	1.37
18	A	808	CLA	C1D-C2D	-2.51	1.40	1.45
18	3	307	CLA	C1D-C2D	-2.51	1.40	1.45
18	8	614	CLA	C1D-C2D	-2.51	1.40	1.45
18	1	608	CLA	C1D-C2D	-2.51	1.40	1.45
18	1	611	CLA	C3A-C2A	-2.50	1.47	1.54
18	3	304	CLA	C1D-ND	2.50	1.41	1.37
18	B	811	CLA	C1D-C2D	-2.50	1.40	1.45
18	B	826	CLA	C1D-C2D	-2.50	1.40	1.45
18	B	806	CLA	C1D-C2D	-2.50	1.40	1.45
18	4	602	CLA	C1D-C2D	-2.50	1.40	1.45
18	A	816	CLA	C1D-C2D	-2.50	1.40	1.45
18	3	303	CLA	C1D-ND	2.49	1.41	1.37
18	1	612	CLA	C1D-C2D	-2.49	1.40	1.45
18	8	610	CLA	C3D-C4D	-2.49	1.38	1.44
18	4	612	CLA	C1D-C2D	-2.49	1.40	1.45
18	3	312	CLA	C1B-NB	2.49	1.41	1.37
18	A	810	CLA	C1D-C2D	-2.49	1.40	1.45
18	B	823	CLA	C1D-C2D	-2.49	1.40	1.45
18	Z	603	CLA	C1D-C2D	-2.49	1.40	1.45
18	Z	604	CLA	C1D-C2D	-2.49	1.40	1.45
18	4	610	CLA	C3A-C2A	-2.49	1.47	1.54
18	A	806	CLA	C1D-C2D	-2.49	1.40	1.45
18	5	609	CLA	C1D-C2D	-2.49	1.40	1.45
18	Z	602	CLA	C1D-C2D	-2.49	1.40	1.45
18	7	614	CLA	C3A-C2A	-2.49	1.47	1.54
18	A	809	CLA	C1D-ND	2.49	1.41	1.37
18	3	309	CLA	C1D-ND	2.49	1.41	1.37
18	B	805	CLA	C1D-C2D	-2.49	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	833	CLA	C1D-ND	2.49	1.41	1.37
18	B	836	CLA	C1D-C2D	-2.49	1.40	1.45
18	1	602	CLA	C1D-C2D	-2.49	1.40	1.45
21	7	606	CHL	CHC-C4B	-2.48	1.35	1.39
18	5	604	CLA	C1D-C2D	-2.48	1.40	1.45
18	B	819	CLA	C3A-C2A	-2.48	1.47	1.54
21	5	607	CHL	C3B-C4B	2.48	1.43	1.41
18	B	811	CLA	C1D-ND	2.48	1.41	1.37
18	B	831	CLA	C1D-C2D	-2.48	1.40	1.45
18	3	304	CLA	C1D-C2D	-2.48	1.40	1.45
18	B	818	CLA	C1D-C2D	-2.48	1.40	1.45
18	B	842	CLA	C1D-C2D	-2.48	1.40	1.45
18	5	604	CLA	C1B-NB	2.47	1.41	1.37
18	B	806	CLA	C3A-C2A	-2.47	1.47	1.54
18	1	611	CLA	C1D-C2D	-2.47	1.40	1.45
18	Z	608	CLA	C1D-C2D	-2.47	1.40	1.45
18	B	841	CLA	C1D-C2D	-2.47	1.40	1.45
18	6	304	CLA	C3A-C2A	-2.47	1.47	1.54
21	6	316	CHL	CHB-C1B	-2.47	1.35	1.39
18	B	801	CLA	C3A-C2A	-2.47	1.47	1.54
18	A	817	CLA	C3D-C4D	-2.47	1.38	1.44
18	A	843	CLA	C1D-C2D	-2.47	1.40	1.45
18	7	611	CLA	C1D-C2D	-2.47	1.40	1.45
18	1	605	CLA	C1D-C2D	-2.47	1.40	1.45
18	A	805	CLA	C1D-C2D	-2.47	1.40	1.45
18	A	844	CLA	C1D-C2D	-2.47	1.40	1.45
18	8	609	CLA	C1D-C2D	-2.47	1.40	1.45
18	6	309	CLA	C1D-C2D	-2.47	1.40	1.45
18	4	601	CLA	C1D-C2D	-2.46	1.40	1.45
18	A	841	CLA	CHC-C1C	-2.46	1.33	1.38
18	8	613	CLA	C1D-C2D	-2.46	1.40	1.45
18	7	609	CLA	C1D-C2D	-2.46	1.40	1.45
18	A	829	CLA	C1D-C2D	-2.46	1.40	1.45
18	B	837	CLA	C1D-C2D	-2.46	1.40	1.45
18	A	810	CLA	C1D-ND	2.46	1.41	1.37
18	B	819	CLA	C1D-ND	2.46	1.41	1.37
18	6	302	CLA	C1D-ND	2.46	1.41	1.37
18	B	830	CLA	C1D-C2D	-2.46	1.40	1.45
18	Z	609	CLA	C1D-C2D	-2.46	1.40	1.45
18	3	305	CLA	C3A-C2A	-2.45	1.47	1.54
18	7	612	CLA	C1D-C2D	-2.45	1.40	1.45
18	4	611	CLA	C1D-ND	2.45	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Z	612	CLA	C1D-C2D	-2.45	1.40	1.45
21	6	316	CHL	CHC-C4B	-2.45	1.35	1.39
18	1	609	CLA	C1D-C2D	-2.45	1.40	1.45
18	A	828	CLA	C1D-ND	2.45	1.41	1.37
18	B	814	CLA	C1D-C2D	-2.45	1.40	1.45
18	4	607	CLA	C1D-C2D	-2.45	1.40	1.45
18	A	826	CLA	C1D-ND	2.45	1.41	1.37
18	1	604	CLA	C1D-C2D	-2.45	1.40	1.45
18	F	301	CLA	C1D-C2D	-2.45	1.40	1.45
18	6	308	CLA	C1D-C2D	-2.45	1.40	1.45
18	4	602	CLA	C1D-ND	2.44	1.41	1.37
18	B	808	CLA	C3A-C2A	-2.44	1.47	1.54
18	A	814	CLA	C1D-C2D	-2.44	1.40	1.45
18	A	807	CLA	C1D-C2D	-2.44	1.40	1.45
18	Z	611	CLA	C1D-C2D	-2.44	1.40	1.45
18	B	832	CLA	C1D-C2D	-2.44	1.40	1.45
18	3	313	CLA	C1D-C2D	-2.44	1.40	1.45
18	A	831	CLA	C3D-C4D	-2.43	1.38	1.44
18	3	305	CLA	C1D-C2D	-2.43	1.40	1.45
18	A	832	CLA	C3A-C2A	-2.43	1.47	1.54
18	8	603	CLA	C1D-ND	2.43	1.41	1.37
18	5	611	CLA	C1D-ND	2.43	1.41	1.37
18	B	831	CLA	C3A-C2A	-2.43	1.47	1.54
18	B	834	CLA	C1D-C2D	-2.43	1.40	1.45
18	B	812	CLA	C1D-C2D	-2.43	1.40	1.45
18	B	839	CLA	C1D-C2D	-2.43	1.40	1.45
18	6	314	CLA	C1D-C2D	-2.43	1.40	1.45
18	A	840	CLA	C3D-C4D	-2.43	1.38	1.44
18	3	307	CLA	C3D-C4D	-2.43	1.38	1.44
18	A	838	CLA	C1D-ND	2.43	1.41	1.37
18	8	605	CLA	C1D-C2D	-2.43	1.40	1.45
18	A	802	CLA	C1D-C2D	-2.43	1.40	1.45
18	7	613	CLA	C1D-C2D	-2.43	1.40	1.45
18	Z	610	CLA	C1D-C2D	-2.43	1.40	1.45
18	B	805	CLA	C3A-C2A	-2.43	1.47	1.54
18	7	604	CLA	C1D-C2D	-2.42	1.40	1.45
18	B	821	CLA	C1D-C2D	-2.42	1.40	1.45
18	B	809	CLA	C1B-NB	2.42	1.41	1.37
18	B	813	CLA	C1D-C2D	-2.42	1.40	1.45
18	1	610	CLA	C1D-C2D	-2.42	1.40	1.45
18	A	823	CLA	C1D-C2D	-2.42	1.40	1.45
18	4	607	CLA	C1B-NB	2.42	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	313	CLA	C3D-C4D	-2.42	1.38	1.44
18	A	812	CLA	C1D-C2D	-2.42	1.40	1.45
18	8	604	CLA	C1D-C2D	-2.42	1.40	1.45
18	8	612	CLA	C3A-C2A	-2.42	1.47	1.54
18	A	826	CLA	C1D-C2D	-2.42	1.40	1.45
18	4	608	CLA	C1B-NB	2.41	1.41	1.37
18	B	804	CLA	C1D-C2D	-2.41	1.40	1.45
18	8	614	CLA	C1B-NB	2.41	1.41	1.37
18	B	824	CLA	C1D-C2D	-2.41	1.40	1.45
18	6	315	CLA	C1D-C2D	-2.41	1.40	1.45
18	7	612	CLA	C1D-ND	2.41	1.41	1.37
18	7	607	CLA	C3A-C2A	-2.41	1.48	1.54
18	7	602	CLA	C1D-ND	2.41	1.41	1.37
18	B	843	CLA	C1D-C2D	-2.41	1.40	1.45
18	6	310	CLA	C1D-C2D	-2.41	1.40	1.45
18	3	303	CLA	C1D-C2D	-2.40	1.40	1.45
18	A	832	CLA	C1D-C2D	-2.40	1.40	1.45
18	A	840	CLA	C1D-C2D	-2.40	1.40	1.45
18	B	841	CLA	C1D-ND	2.40	1.41	1.37
18	1	613	CLA	C1D-C2D	-2.40	1.40	1.45
18	5	614	CLA	C1D-C2D	-2.40	1.40	1.45
18	A	803	CLA	C3D-C4D	-2.40	1.38	1.44
18	B	807	CLA	C1D-ND	2.40	1.41	1.37
18	A	813	CLA	C1D-ND	2.40	1.41	1.37
18	5	615	CLA	C1D-C2D	-2.39	1.40	1.45
18	B	842	CLA	C1D-ND	2.39	1.41	1.37
18	A	824	CLA	C1D-C2D	-2.39	1.40	1.45
18	3	301	CLA	C1D-C2D	-2.39	1.40	1.45
18	7	605	CLA	C1D-C2D	-2.39	1.40	1.45
18	B	805	CLA	C3D-C4D	-2.39	1.38	1.44
18	Z	604	CLA	CHC-C1C	-2.39	1.33	1.38
18	4	610	CLA	C1D-C2D	-2.39	1.40	1.45
18	A	813	CLA	C1D-C2D	-2.39	1.40	1.45
18	A	820	CLA	C1D-C2D	-2.39	1.40	1.45
18	8	611	CLA	C1D-C2D	-2.38	1.40	1.45
18	A	815	CLA	C1D-ND	2.38	1.41	1.37
18	4	601	CLA	C1B-NB	2.38	1.41	1.37
18	A	802	CLA	C3A-C2A	-2.38	1.48	1.54
18	7	601	CLA	C1D-C2D	-2.38	1.40	1.45
18	B	835	CLA	C1D-C2D	-2.38	1.40	1.45
18	B	815	CLA	C3D-C4D	-2.38	1.38	1.44
18	A	822	CLA	C1D-C2D	-2.38	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	822	CLA	C1D-C2D	-2.38	1.40	1.45
18	7	601	CLA	C1D-ND	2.38	1.41	1.37
18	3	303	CLA	C3D-C4D	-2.37	1.38	1.44
18	5	611	CLA	C1D-C2D	-2.37	1.40	1.45
18	1	605	CLA	CHC-C1C	-2.37	1.33	1.38
18	Z	606	CLA	C1D-C2D	-2.37	1.40	1.45
18	B	820	CLA	C3D-C4D	-2.36	1.38	1.44
18	Z	613	CLA	C1B-NB	2.36	1.41	1.37
18	B	835	CLA	C3D-C4D	-2.36	1.38	1.44
18	5	610	CLA	C1D-ND	2.36	1.41	1.37
18	5	605	CLA	C1D-C2D	-2.36	1.40	1.45
18	B	836	CLA	C3D-C4D	-2.36	1.38	1.44
18	3	310	CLA	C1B-NB	2.36	1.41	1.37
18	4	609	CLA	C1D-C2D	-2.36	1.40	1.45
18	8	614	CLA	C1D-ND	2.36	1.41	1.37
18	5	617	CLA	C1D-C2D	-2.36	1.40	1.45
18	B	808	CLA	C3D-C4D	-2.36	1.38	1.44
18	4	603	CLA	C3A-C2A	-2.36	1.48	1.54
18	A	811	CLA	C3D-C4D	-2.36	1.38	1.44
18	5	617	CLA	C3D-C4D	-2.36	1.38	1.44
18	J	101	CLA	C1D-C2D	-2.35	1.40	1.45
21	4	604	CHL	C3B-C4B	2.35	1.43	1.41
18	5	608	CLA	CHD-C4C	-2.35	1.33	1.39
18	A	824	CLA	C3A-C2A	-2.35	1.48	1.54
18	3	312	CLA	C1D-C2D	-2.35	1.40	1.45
18	3	303	CLA	C3A-C2A	-2.35	1.48	1.54
18	B	828	CLA	C1D-C2D	-2.35	1.40	1.45
18	1	614	CLA	C1B-NB	2.35	1.40	1.37
18	B	807	CLA	C1D-C2D	-2.35	1.40	1.45
18	A	831	CLA	C1D-C2D	-2.34	1.40	1.45
18	A	817	CLA	C1D-ND	2.34	1.40	1.37
18	A	834	CLA	C1D-ND	2.34	1.40	1.37
18	6	311	CLA	C1D-C2D	-2.34	1.40	1.45
18	A	804	CLA	C3A-C2A	-2.34	1.48	1.54
18	7	612	CLA	CBD-CAD	-2.34	1.46	1.56
18	1	608	CLA	C3D-C4D	-2.34	1.38	1.44
18	6	315	CLA	C1D-ND	2.34	1.40	1.37
18	1	607	CLA	C1D-C2D	-2.34	1.40	1.45
18	A	819	CLA	C1D-C2D	-2.34	1.40	1.45
18	B	810	CLA	CHC-C1C	-2.34	1.33	1.38
18	Z	609	CLA	C3D-C4D	-2.34	1.38	1.44
18	8	601	CLA	C1D-ND	2.33	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Z	607	CLA	C3D-C4D	-2.33	1.38	1.44
18	B	834	CLA	C3D-C4D	-2.33	1.38	1.44
18	6	312	CLA	C3A-C2A	-2.33	1.48	1.54
18	8	610	CLA	C1D-C2D	-2.33	1.40	1.45
18	B	834	CLA	C2C-C1C	-2.33	1.46	1.51
18	B	834	CLA	CBD-CAD	-2.33	1.46	1.56
18	1	605	CLA	C1B-NB	2.33	1.40	1.37
18	5	610	CLA	C1D-C2D	-2.32	1.40	1.45
18	A	803	CLA	C4D-CHA	-2.32	1.30	1.38
18	A	819	CLA	C3D-C4D	-2.32	1.39	1.44
18	7	601	CLA	CBD-CAD	-2.32	1.46	1.56
18	4	606	CLA	C1D-C2D	-2.32	1.40	1.45
18	B	810	CLA	C1D-C2D	-2.32	1.40	1.45
18	B	827	CLA	C1D-C2D	-2.32	1.40	1.45
18	3	305	CLA	C3D-C4D	-2.32	1.39	1.44
18	B	816	CLA	C1D-C2D	-2.31	1.40	1.45
18	B	802	CLA	C3D-C4D	-2.31	1.39	1.44
18	8	603	CLA	C3D-C4D	-2.31	1.39	1.44
18	A	805	CLA	C3D-C4D	-2.31	1.39	1.44
21	5	606	CHL	C1A-CHA	-2.31	1.37	1.40
18	A	826	CLA	C3D-C4D	-2.31	1.39	1.44
18	A	818	CLA	C1D-ND	2.31	1.40	1.37
18	B	801	CLA	C1D-C2D	-2.31	1.40	1.45
18	A	822	CLA	C1B-NB	2.31	1.40	1.37
18	A	808	CLA	C1D-ND	2.31	1.40	1.37
18	B	809	CLA	C1D-ND	2.31	1.40	1.37
18	7	605	CLA	C3D-C4D	-2.31	1.39	1.44
18	B	817	CLA	C1D-C2D	-2.30	1.40	1.45
18	B	818	CLA	C1D-ND	2.30	1.40	1.37
18	A	824	CLA	CHC-C1C	-2.30	1.33	1.38
18	B	820	CLA	C1D-C2D	-2.30	1.40	1.45
18	Z	604	CLA	C1B-NB	2.30	1.40	1.37
18	A	814	CLA	C3D-C4D	-2.30	1.39	1.44
18	B	806	CLA	C3D-C4D	-2.30	1.39	1.44
18	6	310	CLA	C3D-C4D	-2.30	1.39	1.44
18	B	841	CLA	C3D-C4D	-2.30	1.39	1.44
18	6	304	CLA	C1B-NB	2.30	1.40	1.37
18	A	803	CLA	C1A-CHA	-2.29	1.33	1.43
18	4	603	CLA	C1D-ND	2.29	1.40	1.37
18	A	802	CLA	C3D-C4D	-2.29	1.39	1.44
17	A	801	CL0	CHD-C4C	-2.29	1.34	1.39
18	B	801	CLA	C1D-ND	2.29	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	814	CLA	CHC-C1C	-2.29	1.33	1.38
18	3	310	CLA	C1D-C2D	-2.29	1.40	1.45
18	J	101	CLA	C1B-NB	2.29	1.40	1.37
18	A	843	CLA	C3D-C4D	-2.28	1.39	1.44
18	B	842	CLA	C3D-C4D	-2.28	1.39	1.44
18	3	301	CLA	C1D-ND	2.28	1.40	1.37
18	A	819	CLA	C1D-ND	2.28	1.40	1.37
18	A	827	CLA	C1D-C2D	-2.28	1.40	1.45
18	3	311	CLA	C3A-C2A	-2.28	1.48	1.54
18	B	813	CLA	C1B-NB	2.28	1.40	1.37
17	A	801	CL0	CHC-C1C	-2.27	1.34	1.39
18	7	609	CLA	C1B-NB	2.27	1.40	1.37
18	B	801	CLA	C3D-C4D	-2.27	1.39	1.44
18	1	610	CLA	C3D-C4D	-2.27	1.39	1.44
18	5	602	CLA	C3D-C4D	-2.27	1.39	1.44
18	Z	604	CLA	C3A-C2A	-2.27	1.48	1.54
18	A	813	CLA	C3A-C2A	-2.27	1.48	1.54
18	6	313	CLA	C1D-C2D	-2.27	1.40	1.45
18	5	608	CLA	C3D-C4D	-2.26	1.39	1.44
18	A	839	CLA	CBD-CAD	-2.26	1.46	1.56
18	A	835	CLA	C3D-C4D	-2.26	1.39	1.44
18	A	813	CLA	C3D-C4D	-2.26	1.39	1.44
18	1	605	CLA	C3A-C2A	-2.26	1.48	1.54
18	A	822	CLA	C3D-C4D	-2.26	1.39	1.44
18	B	815	CLA	C1D-C2D	-2.26	1.40	1.45
18	7	610	CLA	C1D-C2D	-2.26	1.40	1.45
18	A	818	CLA	C3D-C4D	-2.26	1.39	1.44
18	A	821	CLA	C1B-NB	2.26	1.40	1.37
21	5	606	CHL	CHC-C4B	-2.26	1.36	1.39
18	3	304	CLA	C3A-C2A	-2.26	1.48	1.54
18	A	843	CLA	C1B-NB	2.25	1.40	1.37
18	8	604	CLA	C1B-NB	2.25	1.40	1.37
18	B	827	CLA	C3D-C4D	-2.25	1.39	1.44
18	8	611	CLA	C3D-C4D	-2.25	1.39	1.44
18	F	301	CLA	C1D-ND	2.25	1.40	1.37
18	7	614	CLA	C1B-NB	2.25	1.40	1.37
18	5	613	CLA	C3D-C4D	-2.25	1.39	1.44
18	A	803	CLA	C1D-C2D	-2.24	1.40	1.45
18	3	309	CLA	C1D-C2D	-2.24	1.40	1.45
18	8	611	CLA	C1D-ND	2.24	1.40	1.37
18	4	603	CLA	CHD-C4C	-2.24	1.34	1.39
18	A	825	CLA	C1D-C2D	-2.24	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	831	CLA	C1D-ND	2.24	1.40	1.37
18	5	617	CLA	C3A-C2A	-2.24	1.48	1.54
18	1	605	CLA	CBD-CAD	-2.24	1.46	1.56
18	A	810	CLA	C3D-C4D	-2.24	1.39	1.44
18	7	601	CLA	C3D-C4D	-2.24	1.39	1.44
18	B	840	CLA	C3A-C2A	-2.24	1.48	1.54
18	Z	604	CLA	CBD-CAD	-2.23	1.46	1.56
18	B	808	CLA	CHC-C1C	-2.23	1.34	1.38
18	5	608	CLA	C1B-NB	2.23	1.40	1.37
18	4	608	CLA	C3D-C4D	-2.23	1.39	1.44
18	7	605	CLA	C1D-ND	2.23	1.40	1.37
18	8	615	CLA	C3A-C2A	-2.23	1.48	1.54
18	B	819	CLA	C1D-C2D	-2.23	1.40	1.45
18	A	820	CLA	C3A-C2A	-2.23	1.48	1.54
18	5	604	CLA	C3D-C4D	-2.23	1.39	1.44
18	8	612	CLA	C1B-NB	2.23	1.40	1.37
18	B	832	CLA	C3D-C4D	-2.23	1.39	1.44
18	F	302	CLA	CBD-CAD	-2.23	1.46	1.56
18	A	844	CLA	C3D-C4D	-2.23	1.39	1.44
18	B	802	CLA	CBD-CAD	-2.23	1.46	1.56
18	5	615	CLA	C3D-C4D	-2.22	1.39	1.44
18	F	301	CLA	C3D-C4D	-2.22	1.39	1.44
18	5	613	CLA	C1B-NB	2.22	1.40	1.37
18	4	603	CLA	C3D-C4D	-2.22	1.39	1.44
18	4	602	CLA	C1B-NB	2.22	1.40	1.37
18	A	837	CLA	C3D-C4D	-2.22	1.39	1.44
18	B	832	CLA	C1B-NB	2.22	1.40	1.37
18	A	815	CLA	C3D-C4D	-2.22	1.39	1.44
18	A	817	CLA	CBD-CAD	-2.22	1.46	1.56
18	B	801	CLA	CBD-CAD	-2.22	1.46	1.56
18	B	813	CLA	C3D-C4D	-2.22	1.39	1.44
18	1	603	CLA	C3A-C2A	-2.22	1.48	1.54
18	8	601	CLA	C3D-C4D	-2.22	1.39	1.44
18	3	301	CLA	C3D-C4D	-2.22	1.39	1.44
18	3	309	CLA	C1B-NB	2.22	1.40	1.37
18	A	828	CLA	C3A-C2A	-2.22	1.48	1.54
18	1	609	CLA	C1B-NB	2.22	1.40	1.37
18	B	809	CLA	C3D-C4D	-2.22	1.39	1.44
18	B	827	CLA	CBD-CAD	-2.22	1.46	1.56
18	A	840	CLA	C4D-CHA	-2.22	1.31	1.38
18	4	601	CLA	C3D-C4D	-2.21	1.39	1.44
18	A	824	CLA	C3D-C4D	-2.21	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	605	CLA	CHC-C1C	-2.21	1.34	1.38
18	A	808	CLA	C3A-C2A	-2.21	1.48	1.54
18	A	829	CLA	C3D-C4D	-2.21	1.39	1.44
18	Z	608	CLA	C1B-NB	2.21	1.40	1.37
18	8	608	CLA	CHD-C4C	-2.21	1.34	1.39
18	A	821	CLA	C3D-C4D	-2.21	1.39	1.44
18	6	308	CLA	C3D-C4D	-2.21	1.39	1.44
18	6	315	CLA	C3D-C4D	-2.21	1.39	1.44
18	B	818	CLA	C3D-C4D	-2.21	1.39	1.44
18	A	817	CLA	C3A-C2A	-2.21	1.48	1.54
18	7	613	CLA	C3D-C4D	-2.20	1.39	1.44
18	3	310	CLA	C3A-C2A	-2.20	1.48	1.54
18	A	837	CLA	CBD-CAD	-2.20	1.46	1.56
18	B	842	CLA	C3A-C2A	-2.20	1.48	1.54
18	7	607	CLA	CHD-C4C	-2.20	1.34	1.39
18	B	840	CLA	C3D-C4D	-2.20	1.39	1.44
18	7	614	CLA	C3D-C4D	-2.20	1.39	1.44
18	A	808	CLA	C3D-C4D	-2.20	1.39	1.44
18	A	810	CLA	C3A-C2A	-2.20	1.48	1.54
18	A	845	CLA	CHD-C4C	-2.20	1.34	1.39
18	A	834	CLA	C1D-C2D	-2.20	1.41	1.45
18	B	825	CLA	C1B-NB	2.20	1.40	1.37
18	A	821	CLA	C3A-C2A	-2.20	1.48	1.54
18	B	811	CLA	C3D-C4D	-2.20	1.39	1.44
18	4	609	CLA	C1B-NB	2.20	1.40	1.37
18	8	604	CLA	C3D-C4D	-2.20	1.39	1.44
18	B	807	CLA	C3D-C4D	-2.19	1.39	1.44
18	B	830	CLA	C3D-C4D	-2.19	1.39	1.44
18	8	605	CLA	C3A-C2A	-2.19	1.48	1.54
18	B	835	CLA	C1D-ND	2.19	1.40	1.37
18	B	839	CLA	C3D-C4D	-2.19	1.39	1.44
18	7	612	CLA	C3D-C4D	-2.19	1.39	1.44
18	A	844	CLA	C1D-ND	2.19	1.40	1.37
18	4	610	CLA	C1C-C2C	2.19	1.49	1.44
18	B	816	CLA	C3D-C4D	-2.19	1.39	1.44
18	B	838	CLA	C3D-C4D	-2.19	1.39	1.44
18	A	820	CLA	CHC-C1C	-2.19	1.34	1.38
18	8	614	CLA	C3D-C4D	-2.19	1.39	1.44
18	A	841	CLA	CHD-C4C	-2.19	1.34	1.39
18	8	608	CLA	C1B-NB	2.18	1.40	1.37
18	B	829	CLA	C3D-C4D	-2.18	1.39	1.44
18	7	603	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	302	CLA	C3D-C4D	-2.18	1.39	1.44
18	B	830	CLA	CBD-CAD	-2.18	1.46	1.56
18	B	831	CLA	C3D-C4D	-2.18	1.39	1.44
18	A	807	CLA	C3A-C2A	-2.18	1.48	1.54
18	5	612	CLA	C3D-C4D	-2.18	1.39	1.44
18	B	815	CLA	C1B-NB	2.18	1.40	1.37
18	8	613	CLA	C3D-C4D	-2.18	1.39	1.44
18	7	602	CLA	CBD-CAD	-2.18	1.46	1.56
18	B	829	CLA	CHD-C4C	-2.18	1.34	1.39
18	B	834	CLA	C3A-C2A	-2.18	1.48	1.54
18	B	806	CLA	C1C-C2C	2.18	1.48	1.44
18	4	612	CLA	C3D-C4D	-2.18	1.39	1.44
18	A	837	CLA	C1D-ND	2.18	1.40	1.37
18	B	817	CLA	C3D-C4D	-2.18	1.39	1.44
18	5	611	CLA	C3A-C2A	-2.17	1.48	1.54
18	B	824	CLA	C3D-C4D	-2.17	1.39	1.44
18	A	845	CLA	CBD-CAD	-2.17	1.46	1.56
18	6	317	CLA	C3A-C2A	-2.17	1.48	1.54
18	6	309	CLA	C1C-C2C	2.17	1.48	1.44
18	B	802	CLA	C3A-C2A	-2.17	1.48	1.54
18	7	611	CLA	C3D-C4D	-2.17	1.39	1.44
18	A	822	CLA	C3A-C2A	-2.17	1.48	1.54
18	B	826	CLA	C3A-C2A	-2.17	1.48	1.54
18	A	804	CLA	C3D-C4D	-2.17	1.39	1.44
18	6	317	CLA	C1B-NB	2.17	1.40	1.37
18	1	614	CLA	CHD-C4C	-2.17	1.34	1.39
18	A	812	CLA	C3D-C4D	-2.17	1.39	1.44
18	B	828	CLA	C3A-C2A	-2.16	1.48	1.54
18	4	602	CLA	C3D-C4D	-2.16	1.39	1.44
18	8	607	CLA	CHD-C4C	-2.16	1.34	1.39
18	4	601	CLA	C1D-ND	2.16	1.40	1.37
18	3	304	CLA	C3D-C4D	-2.16	1.39	1.44
18	7	610	CLA	C3D-C4D	-2.16	1.39	1.44
18	A	829	CLA	C3A-C2A	-2.16	1.48	1.54
18	3	314	CLA	C3D-C4D	-2.16	1.39	1.44
18	7	612	CLA	C3A-C2A	-2.16	1.48	1.54
18	A	839	CLA	CHC-C1C	-2.16	1.34	1.38
18	7	604	CLA	CBD-CAD	-2.16	1.46	1.56
18	3	308	CLA	CBD-CAD	-2.16	1.46	1.56
18	5	603	CLA	CHC-C1C	-2.16	1.34	1.38
18	Z	602	CLA	C1B-NB	2.16	1.40	1.37
18	A	809	CLA	C3A-C2A	-2.16	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	823	CLA	C3D-C4D	-2.16	1.39	1.44
18	1	602	CLA	C1B-NB	2.16	1.40	1.37
18	5	601	CLA	CHD-C4C	-2.16	1.34	1.39
18	A	832	CLA	C3D-C4D	-2.15	1.39	1.44
18	A	845	CLA	C3D-C4D	-2.15	1.39	1.44
18	8	613	CLA	C3A-C2A	-2.15	1.48	1.54
18	8	612	CLA	C3D-C4D	-2.15	1.39	1.44
18	A	841	CLA	CBD-CAD	-2.15	1.46	1.56
18	A	838	CLA	C1D-C2D	-2.15	1.41	1.45
18	5	602	CLA	C1D-ND	2.15	1.40	1.37
18	A	809	CLA	C3D-C4D	-2.15	1.39	1.44
18	7	611	CLA	C3A-C2A	-2.15	1.48	1.54
18	A	807	CLA	C3D-C4D	-2.15	1.39	1.44
18	5	610	CLA	C3D-C4D	-2.15	1.39	1.44
18	5	613	CLA	C1D-ND	2.14	1.40	1.37
18	3	301	CLA	CBD-CAD	-2.14	1.46	1.56
18	4	611	CLA	C3D-C4D	-2.14	1.39	1.44
21	8	606	CHL	CHB-C1B	-2.14	1.36	1.39
18	A	826	CLA	CBD-CAD	-2.14	1.46	1.56
18	Z	613	CLA	CHD-C4C	-2.14	1.34	1.39
18	3	312	CLA	C3D-C4D	-2.14	1.39	1.44
18	A	806	CLA	C3D-C4D	-2.14	1.39	1.44
18	1	604	CLA	C3A-C2A	-2.14	1.48	1.54
18	3	311	CLA	C3D-C4D	-2.14	1.39	1.44
18	B	808	CLA	CHD-C4C	-2.14	1.34	1.39
18	4	607	CLA	C3D-C4D	-2.14	1.39	1.44
18	A	805	CLA	C1C-C2C	2.14	1.48	1.44
18	A	818	CLA	CHC-C1C	-2.13	1.34	1.38
18	A	839	CLA	C3D-C4D	-2.13	1.39	1.44
18	3	311	CLA	CHC-C1C	-2.13	1.34	1.38
18	Z	611	CLA	CHC-C1C	-2.13	1.34	1.38
18	5	601	CLA	CHC-C1C	-2.13	1.34	1.38
18	Z	602	CLA	CBD-CAD	-2.13	1.46	1.56
18	5	605	CLA	C3D-C4D	-2.13	1.39	1.44
18	A	830	CLA	C3D-C4D	-2.13	1.39	1.44
18	1	612	CLA	CHC-C1C	-2.13	1.34	1.38
18	Z	607	CLA	C1D-ND	2.13	1.40	1.37
18	1	607	CLA	C3D-C4D	-2.13	1.39	1.44
18	A	820	CLA	C3D-C4D	-2.13	1.39	1.44
18	A	829	CLA	CBD-CAD	-2.13	1.46	1.56
18	A	824	CLA	C1C-NC	-2.13	1.34	1.37
18	Z	603	CLA	C3A-C2A	-2.13	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	835	CLA	C1B-NB	2.13	1.40	1.37
18	A	836	CLA	C3D-C4D	-2.13	1.39	1.44
18	6	314	CLA	C1B-NB	2.13	1.40	1.37
18	1	611	CLA	C3D-C4D	-2.13	1.39	1.44
18	3	307	CLA	C3A-C2A	-2.13	1.48	1.54
18	8	609	CLA	CHD-C4C	-2.12	1.34	1.39
18	7	614	CLA	C1D-C2D	-2.12	1.41	1.45
18	3	311	CLA	CHD-C4C	-2.12	1.34	1.39
18	1	602	CLA	CBD-CAD	-2.12	1.47	1.56
18	A	812	CLA	C3A-C2A	-2.12	1.48	1.54
18	A	809	CLA	CHD-C4C	-2.12	1.34	1.39
18	B	823	CLA	C3D-C4D	-2.12	1.39	1.44
18	8	608	CLA	CHC-C1C	-2.12	1.34	1.38
18	B	826	CLA	CBD-CAD	-2.12	1.47	1.56
18	8	609	CLA	C1B-NB	2.12	1.40	1.37
18	6	304	CLA	CHD-C4C	-2.12	1.34	1.39
18	A	815	CLA	CHC-C1C	-2.12	1.34	1.38
18	B	827	CLA	C1D-ND	2.12	1.40	1.37
18	6	313	CLA	C3A-C2A	-2.12	1.48	1.54
18	5	602	CLA	CBD-CAD	-2.12	1.47	1.56
18	3	309	CLA	C3D-C4D	-2.12	1.39	1.44
18	3	305	CLA	CBD-CAD	-2.12	1.47	1.56
18	8	605	CLA	C3D-C4D	-2.12	1.39	1.44
18	6	314	CLA	C3D-C4D	-2.12	1.39	1.44
18	4	606	CLA	C3D-C4D	-2.12	1.39	1.44
18	A	827	CLA	C3D-C4D	-2.12	1.39	1.44
18	F	302	CLA	C3D-C4D	-2.11	1.39	1.44
18	5	611	CLA	C3D-C4D	-2.11	1.39	1.44
18	3	302	CLA	C3A-C2A	-2.11	1.48	1.54
18	A	821	CLA	CHD-C4C	-2.11	1.34	1.39
18	A	814	CLA	C1D-ND	2.11	1.40	1.37
18	3	303	CLA	C1B-NB	2.11	1.40	1.37
18	4	602	CLA	CHD-C4C	-2.11	1.34	1.39
18	B	833	CLA	C3D-C4D	-2.11	1.39	1.44
18	7	602	CLA	C3D-C4D	-2.11	1.39	1.44
18	A	816	CLA	CHC-C1C	-2.11	1.34	1.38
18	A	836	CLA	CHD-C4C	-2.11	1.34	1.39
18	Z	610	CLA	C3D-C4D	-2.11	1.39	1.44
18	B	810	CLA	C3A-C2A	-2.11	1.48	1.54
18	7	603	CLA	CHC-C1C	-2.11	1.34	1.38
18	A	834	CLA	C1A-CHA	-2.11	1.34	1.43
18	A	841	CLA	C3D-C4D	-2.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	613	CLA	CHC-C1C	-2.11	1.34	1.38
18	B	838	CLA	CHD-C4C	-2.10	1.34	1.39
18	A	831	CLA	CBD-CAD	-2.10	1.47	1.56
18	B	804	CLA	C3D-C4D	-2.10	1.39	1.44
18	7	603	CLA	CHD-C4C	-2.10	1.34	1.39
18	Z	612	CLA	CHC-C1C	-2.10	1.34	1.38
18	A	840	CLA	CBD-CAD	-2.10	1.47	1.56
18	A	844	CLA	CHC-C1C	-2.10	1.34	1.38
18	6	312	CLA	CHC-C1C	-2.10	1.34	1.38
18	5	611	CLA	CBD-CAD	-2.10	1.47	1.56
18	A	828	CLA	C3D-C4D	-2.10	1.39	1.44
18	Z	606	CLA	C3D-C4D	-2.10	1.39	1.44
18	B	837	CLA	C3D-C4D	-2.10	1.39	1.44
18	4	610	CLA	C3D-C4D	-2.10	1.39	1.44
18	7	602	CLA	CHD-C4C	-2.10	1.34	1.39
18	B	843	CLA	C3A-C2A	-2.10	1.48	1.54
18	3	313	CLA	C3D-C4D	-2.10	1.39	1.44
18	B	816	CLA	C1B-NB	2.10	1.40	1.37
18	A	828	CLA	CHC-C1C	-2.09	1.34	1.38
18	8	605	CLA	CHC-C1C	-2.09	1.34	1.38
18	B	817	CLA	CHC-C1C	-2.09	1.34	1.38
18	6	303	CLA	C3D-C4D	-2.09	1.39	1.44
18	B	825	CLA	C3D-C4D	-2.09	1.39	1.44
18	5	608	CLA	CBD-CAD	-2.09	1.47	1.56
18	B	829	CLA	C1D-ND	2.09	1.40	1.37
18	B	843	CLA	CHC-C1C	-2.09	1.34	1.38
18	5	602	CLA	CHD-C4C	-2.09	1.34	1.39
18	A	838	CLA	C3D-C4D	-2.09	1.39	1.44
18	1	614	CLA	C3D-C4D	-2.09	1.39	1.44
18	A	840	CLA	C3A-C2A	-2.09	1.48	1.54
18	B	812	CLA	C3D-C4D	-2.09	1.39	1.44
18	1	603	CLA	CHD-C4C	-2.09	1.34	1.39
18	B	843	CLA	C3D-C4D	-2.09	1.39	1.44
18	A	823	CLA	CHD-C4C	-2.09	1.34	1.39
18	A	813	CLA	CHC-C1C	-2.09	1.34	1.38
18	B	821	CLA	C1B-NB	2.09	1.40	1.37
18	1	605	CLA	C3D-C4D	-2.08	1.39	1.44
18	Z	602	CLA	C3D-C4D	-2.08	1.39	1.44
18	7	604	CLA	CBB-CAB	2.08	1.40	1.30
18	7	601	CLA	CHC-C1C	-2.08	1.34	1.38
18	5	609	CLA	C3D-C4D	-2.08	1.39	1.44
18	J	101	CLA	C3D-C4D	-2.08	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	609	CLA	C3D-C4D	-2.08	1.39	1.44
18	F	302	CLA	CHD-C4C	-2.08	1.34	1.39
18	7	611	CLA	CBD-CAD	-2.08	1.47	1.56
18	B	826	CLA	C3D-C4D	-2.08	1.39	1.44
18	6	301	CLA	CHD-C4C	-2.08	1.34	1.39
18	7	602	CLA	C3A-C2A	-2.08	1.48	1.54
18	6	312	CLA	C3D-C4D	-2.08	1.39	1.44
18	A	807	CLA	CHC-C1C	-2.08	1.34	1.38
18	1	608	CLA	C1D-ND	2.08	1.40	1.37
18	1	602	CLA	C3D-C4D	-2.08	1.39	1.44
18	8	602	CLA	CHC-C1C	-2.08	1.34	1.38
18	5	603	CLA	CHD-C4C	-2.08	1.34	1.39
18	8	608	CLA	C3D-C4D	-2.08	1.39	1.44
18	3	314	CLA	CHD-C4C	-2.08	1.34	1.39
18	A	819	CLA	C4D-CHA	-2.08	1.31	1.38
18	8	612	CLA	CBD-CAD	-2.07	1.47	1.56
18	Z	608	CLA	C3D-C4D	-2.07	1.39	1.44
18	6	302	CLA	CBD-CAD	-2.07	1.47	1.56
18	B	822	CLA	C3D-C4D	-2.07	1.39	1.44
18	A	828	CLA	CHD-C4C	-2.07	1.34	1.39
18	Z	612	CLA	C3D-C4D	-2.07	1.39	1.44
18	Z	603	CLA	C1B-NB	2.07	1.40	1.37
18	Z	604	CLA	C3D-C4D	-2.07	1.39	1.44
18	A	812	CLA	CHD-C4C	-2.07	1.34	1.39
18	A	808	CLA	C1B-NB	2.07	1.40	1.37
18	B	805	CLA	CHD-C4C	-2.07	1.34	1.39
18	A	812	CLA	CHC-C1C	-2.07	1.34	1.38
18	1	607	CLA	CHC-C1C	-2.07	1.34	1.38
18	A	837	CLA	CHD-C4C	-2.07	1.34	1.39
18	3	310	CLA	C3D-C4D	-2.07	1.39	1.44
18	7	609	CLA	C3D-C4D	-2.07	1.39	1.44
18	6	317	CLA	CHD-C4C	-2.07	1.34	1.39
18	4	603	CLA	C1B-NB	2.07	1.40	1.37
18	7	608	CLA	C3D-C4D	-2.06	1.39	1.44
18	4	610	CLA	C1B-NB	2.06	1.40	1.37
18	7	608	CLA	CHC-C1C	-2.06	1.34	1.38
18	1	612	CLA	C3D-C4D	-2.06	1.39	1.44
18	Z	611	CLA	C3D-C4D	-2.06	1.39	1.44
18	8	609	CLA	C3D-C4D	-2.06	1.39	1.44
18	7	605	CLA	CBD-CAD	-2.06	1.47	1.56
18	6	309	CLA	C3D-C4D	-2.06	1.39	1.44
18	3	302	CLA	CHC-C1C	-2.06	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	817	CLA	CBD-CAD	-2.06	1.47	1.56
18	B	823	CLA	CBD-CAD	-2.06	1.47	1.56
18	A	835	CLA	CHD-C4C	-2.06	1.34	1.39
18	5	602	CLA	C4D-CHA	-2.06	1.31	1.38
18	5	612	CLA	CHC-C1C	-2.06	1.34	1.38
18	A	805	CLA	C1D-ND	2.06	1.40	1.37
18	A	818	CLA	CHD-C4C	-2.06	1.34	1.39
18	B	829	CLA	CBD-CAD	-2.06	1.47	1.56
18	A	811	CLA	CBD-CAD	-2.06	1.47	1.56
18	A	830	CLA	CHC-C1C	-2.06	1.34	1.38
18	B	813	CLA	CAB-C3B	-2.06	1.46	1.50
18	A	808	CLA	CHD-C4C	-2.06	1.34	1.39
18	3	305	CLA	C1D-ND	2.05	1.40	1.37
18	Z	613	CLA	C3D-C4D	-2.05	1.39	1.44
21	4	604	CHL	CHB-C1B	-2.05	1.36	1.39
18	3	313	CLA	CBD-CAD	-2.05	1.47	1.56
18	A	812	CLA	CBD-CAD	-2.05	1.47	1.56
18	A	833	CLA	C3D-C4D	-2.05	1.39	1.44
18	A	803	CLA	C1D-ND	2.05	1.40	1.37
18	7	610	CLA	C1D-ND	2.05	1.40	1.37
18	5	603	CLA	C3D-C4D	-2.05	1.39	1.44
18	6	302	CLA	CHD-C4C	-2.05	1.34	1.39
18	A	833	CLA	CHD-C4C	-2.05	1.34	1.39
18	B	802	CLA	CHD-C4C	-2.05	1.34	1.39
18	A	838	CLA	C3A-C2A	-2.05	1.48	1.54
18	B	836	CLA	CBD-CAD	-2.05	1.47	1.56
18	6	308	CLA	C1B-NB	2.05	1.40	1.37
18	3	311	CLA	CBD-CAD	-2.05	1.47	1.56
18	3	314	CLA	CBD-CAD	-2.05	1.47	1.56
18	6	317	CLA	C3D-C4D	-2.05	1.39	1.44
18	8	615	CLA	CHD-C4C	-2.05	1.34	1.39
18	7	609	CLA	CHD-C4C	-2.05	1.34	1.39
18	1	613	CLA	C3D-C4D	-2.04	1.39	1.44
18	B	805	CLA	CBD-CAD	-2.04	1.47	1.56
18	8	605	CLA	C1B-NB	2.04	1.40	1.37
18	A	830	CLA	CHD-C4C	-2.04	1.34	1.39
18	8	603	CLA	C1B-NB	2.04	1.40	1.37
18	5	612	CLA	CHD-C4C	-2.04	1.34	1.39
18	B	828	CLA	C3D-C4D	-2.04	1.39	1.44
18	3	308	CLA	C3D-C4D	-2.04	1.39	1.44
18	A	836	CLA	C1B-NB	2.04	1.40	1.37
18	7	612	CLA	C1B-NB	2.04	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	821	CLA	C3D-C4D	-2.04	1.39	1.44
18	3	302	CLA	C3D-C4D	-2.04	1.39	1.44
18	B	817	CLA	C1B-NB	2.04	1.40	1.37
18	7	605	CLA	CHC-C1C	-2.04	1.34	1.38
18	B	830	CLA	CHC-C1C	-2.04	1.34	1.38
18	8	602	CLA	CBD-CAD	-2.04	1.47	1.56
18	5	612	CLA	C3A-C2A	-2.04	1.49	1.54
18	7	607	CLA	C3D-C4D	-2.04	1.39	1.44
18	A	805	CLA	CBD-CAD	-2.03	1.47	1.56
18	8	615	CLA	C1B-NB	2.03	1.40	1.37
18	B	816	CLA	CHC-C1C	-2.03	1.34	1.38
18	Z	606	CLA	CHC-C1C	-2.03	1.34	1.38
18	B	809	CLA	CHD-C4C	-2.03	1.34	1.39
18	1	609	CLA	C1C-C2C	2.03	1.48	1.44
18	A	839	CLA	CHD-C4C	-2.03	1.34	1.39
18	A	824	CLA	CHD-C4C	-2.03	1.34	1.39
18	A	802	CLA	CHD-C4C	-2.03	1.34	1.39
18	8	614	CLA	C3A-C2A	-2.03	1.49	1.54
18	A	816	CLA	C3D-C4D	-2.03	1.39	1.44
18	4	603	CLA	CHC-C1C	-2.03	1.34	1.38
18	B	833	CLA	CHD-C4C	-2.03	1.34	1.39
18	3	308	CLA	CHD-C4C	-2.03	1.34	1.39
18	6	301	CLA	C1C-C2C	2.03	1.48	1.44
18	6	311	CLA	CBD-CAD	-2.03	1.47	1.56
18	5	603	CLA	C3A-C2A	-2.03	1.49	1.54
18	A	815	CLA	C3A-C2A	-2.03	1.49	1.54
18	A	806	CLA	CHC-C1C	-2.03	1.34	1.38
18	3	308	CLA	C1B-NB	2.03	1.40	1.37
18	6	303	CLA	CHD-C4C	-2.02	1.34	1.39
18	1	604	CLA	C3D-C4D	-2.02	1.39	1.44
18	7	607	CLA	CHC-C1C	-2.02	1.34	1.38
18	3	304	CLA	CHC-C1C	-2.02	1.34	1.38
18	A	825	CLA	C3D-C4D	-2.02	1.39	1.44
18	B	817	CLA	C3A-C2A	-2.02	1.49	1.54
18	Z	608	CLA	C1C-C2C	2.02	1.48	1.44
18	8	612	CLA	CHD-C4C	-2.02	1.34	1.39
18	6	311	CLA	C3D-C4D	-2.02	1.39	1.44
18	4	602	CLA	C1C-C2C	2.02	1.48	1.44
18	8	615	CLA	C3D-C4D	-2.02	1.39	1.44
18	A	840	CLA	CHC-C1C	-2.02	1.34	1.38
18	5	609	CLA	CBD-CAD	-2.02	1.47	1.56
18	8	605	CLA	CBD-CAD	-2.02	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	314	CLA	CHC-C1C	-2.02	1.34	1.38
18	A	845	CLA	C3A-C2A	-2.02	1.49	1.54
18	6	303	CLA	C1B-NB	2.02	1.40	1.37
18	A	833	CLA	CBD-CAD	-2.02	1.47	1.56
18	A	817	CLA	CHC-C1C	-2.02	1.34	1.38
18	B	819	CLA	C3D-C4D	-2.02	1.39	1.44
18	B	831	CLA	CHD-C4C	-2.02	1.34	1.39
18	A	809	CLA	CHC-C1C	-2.02	1.34	1.38
18	1	602	CLA	CHD-C4C	-2.01	1.34	1.39
18	A	816	CLA	CHD-C4C	-2.01	1.34	1.39
18	1	604	CLA	C1B-NB	2.01	1.40	1.37
18	B	842	CLA	CHD-C4C	-2.01	1.34	1.39
18	4	612	CLA	C1D-ND	2.01	1.40	1.37
18	7	612	CLA	CHD-C4C	-2.01	1.34	1.39
18	4	609	CLA	C3A-C2A	-2.01	1.49	1.54
18	1	603	CLA	C1B-NB	2.01	1.40	1.37
18	8	613	CLA	CBD-CAD	-2.01	1.47	1.56
18	1	603	CLA	C3D-C4D	-2.01	1.39	1.44
18	8	601	CLA	CHC-C1C	-2.01	1.34	1.38
18	6	312	CLA	CHD-C4C	-2.01	1.34	1.39
18	Z	603	CLA	C3D-C4D	-2.01	1.39	1.44
18	A	845	CLA	C1B-NB	2.01	1.40	1.37
18	B	807	CLA	CBD-CAD	-2.01	1.47	1.56
18	8	607	CLA	CHC-C1C	-2.01	1.34	1.38
18	B	815	CLA	C1D-ND	2.00	1.40	1.37
18	5	615	CLA	C3A-C2A	-2.00	1.49	1.54
18	5	614	CLA	C3D-C4D	-2.00	1.39	1.44
18	A	817	CLA	CHD-C4C	-2.00	1.34	1.39
18	6	301	CLA	CBD-CAD	-2.00	1.47	1.56
18	3	313	CLA	C3A-C2A	-2.00	1.49	1.54
18	5	605	CLA	C1B-NB	2.00	1.40	1.37
18	A	832	CLA	CHC-C1C	-2.00	1.34	1.38
18	B	842	CLA	CBD-CAD	-2.00	1.47	1.56
18	A	831	CLA	C3A-C2A	-2.00	1.49	1.54
18	6	301	CLA	C3D-C4D	-2.00	1.39	1.44

All (1676) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	7	614	CLA	C4A-NA-C1A	-10.73	101.78	106.68
18	7	610	CLA	C4A-NA-C1A	-9.85	102.18	106.68
18	A	834	CLA	C4A-NA-C1A	-9.69	102.26	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	305	CLA	C4A-NA-C1A	-9.56	102.32	106.68
18	5	615	CLA	C4A-NA-C1A	-9.25	102.46	106.68
18	6	310	CLA	C4A-NA-C1A	-9.07	102.54	106.68
18	3	309	CLA	C4A-NA-C1A	-8.72	102.70	106.68
18	B	815	CLA	C4A-NA-C1A	-8.68	102.72	106.68
18	4	608	CLA	C4A-NA-C1A	-8.53	102.79	106.68
18	B	804	CLA	C4A-NA-C1A	-8.29	102.90	106.68
18	B	806	CLA	C4A-NA-C1A	-8.02	103.02	106.68
18	A	802	CLA	C4A-NA-C1A	-8.01	103.03	106.68
18	Z	607	CLA	C4A-NA-C1A	-7.99	103.03	106.68
18	1	608	CLA	C4A-NA-C1A	-7.93	103.06	106.68
18	4	601	CLA	C4A-NA-C1A	-7.70	103.17	106.68
18	8	611	CLA	C4A-NA-C1A	-7.63	103.20	106.68
18	8	614	CLA	C4A-NA-C1A	-7.42	103.30	106.68
18	B	835	CLA	C4A-NA-C1A	-7.31	103.34	106.68
18	3	307	CLA	C4A-NA-C1A	-7.28	103.36	106.68
18	B	827	CLA	C4A-NA-C1A	-7.22	103.38	106.68
18	6	310	CLA	C3B-C4B-NB	-7.14	104.15	110.53
18	B	812	CLA	C4A-NA-C1A	-7.13	103.42	106.68
18	A	824	CLA	C4A-NA-C1A	-7.10	103.44	106.68
18	A	805	CLA	C4A-NA-C1A	-7.07	103.45	106.68
18	A	840	CLA	C4A-NA-C1A	-7.04	103.47	106.68
18	6	315	CLA	C4A-NA-C1A	-7.00	103.48	106.68
18	Z	609	CLA	C4A-NA-C1A	-6.95	103.51	106.68
17	A	801	CL0	C1B-CHB-C4A	6.93	125.78	121.32
18	1	610	CLA	C4A-NA-C1A	-6.91	103.53	106.68
18	B	820	CLA	C4A-NA-C1A	-6.85	103.55	106.68
18	5	617	CLA	C4A-NA-C1A	-6.78	103.58	106.68
18	B	836	CLA	C4A-NA-C1A	-6.77	103.59	106.68
18	A	822	CLA	C4A-NA-C1A	-6.76	103.60	106.68
18	A	823	CLA	C4A-NA-C1A	-6.66	103.64	106.68
18	B	819	CLA	C4A-NA-C1A	-6.65	103.64	106.68
18	B	841	CLA	C4A-NA-C1A	-6.65	103.64	106.68
18	A	804	CLA	C4A-NA-C1A	-6.57	103.68	106.68
18	A	803	CLA	C4A-NA-C1A	-6.54	103.69	106.68
18	8	610	CLA	C4A-NA-C1A	-6.42	103.75	106.68
18	B	808	CLA	C4A-NA-C1A	-6.40	103.76	106.68
18	B	822	CLA	C4A-NA-C1A	-6.39	103.77	106.68
18	7	613	CLA	C4A-NA-C1A	-6.36	103.78	106.68
18	7	605	CLA	C4A-NA-C1A	-6.33	103.79	106.68
18	B	805	CLA	C4A-NA-C1A	-6.32	103.79	106.68
18	A	806	CLA	C4A-NA-C1A	-6.30	103.81	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	831	CLA	C4A-NA-C1A	-6.23	103.83	106.68
18	F	301	CLA	C4A-NA-C1A	-6.22	103.84	106.68
18	A	831	CLA	C4A-NA-C1A	-6.21	103.84	106.68
18	B	807	CLA	C4A-NA-C1A	-6.16	103.87	106.68
18	5	613	CLA	C4A-NA-C1A	-6.13	103.88	106.68
18	B	811	CLA	C4A-NA-C1A	-6.13	103.88	106.68
18	B	842	CLA	C4A-NA-C1A	-6.07	103.91	106.68
18	A	838	CLA	C4A-NA-C1A	-6.02	103.93	106.68
18	3	304	CLA	C4A-NA-C1A	-6.01	103.94	106.68
18	A	826	CLA	C4A-NA-C1A	-6.01	103.94	106.68
18	6	314	CLA	C4A-NA-C1A	-5.99	103.95	106.68
18	5	610	CLA	C4A-NA-C1A	-5.99	103.95	106.68
18	6	308	CLA	C4A-NA-C1A	-5.98	103.95	106.68
18	B	832	CLA	C4A-NA-C1A	-5.95	103.97	106.68
18	B	840	CLA	C4A-NA-C1A	-5.91	103.98	106.68
18	B	843	CLA	C4A-NA-C1A	-5.90	103.99	106.68
18	4	610	CLA	C4A-NA-C1A	-5.90	103.99	106.68
18	A	808	CLA	C4A-NA-C1A	-5.89	103.99	106.68
18	4	603	CLA	C4A-NA-C1A	-5.89	103.99	106.68
18	6	302	CLA	C4A-NA-C1A	-5.88	104.00	106.68
18	8	603	CLA	C4A-NA-C1A	-5.83	104.02	106.68
18	B	802	CLA	C4A-NA-C1A	-5.83	104.02	106.68
18	A	827	CLA	C4A-NA-C1A	-5.82	104.03	106.68
18	4	602	CLA	C4A-NA-C1A	-5.81	104.03	106.68
18	1	605	CLA	C4A-NA-C1A	-5.81	104.03	106.68
21	4	605	CHL	CHA-C1A-C2A	-5.78	119.73	133.31
18	A	825	CLA	C4A-NA-C1A	-5.77	104.05	106.68
18	Z	604	CLA	C4A-NA-C1A	-5.77	104.05	106.68
18	6	313	CLA	C4A-NA-C1A	-5.75	104.05	106.68
18	4	607	CLA	C4A-NA-C1A	-5.75	104.06	106.68
18	B	817	CLA	C4A-NA-C1A	-5.75	104.06	106.68
18	5	602	CLA	C4A-NA-C1A	-5.75	104.06	106.68
18	B	819	CLA	CAA-C2A-C1A	-5.68	99.58	112.14
18	6	309	CLA	C4A-NA-C1A	-5.66	104.10	106.68
18	5	605	CLA	C4A-NA-C1A	-5.66	104.10	106.68
18	B	818	CLA	C4A-NA-C1A	-5.63	104.11	106.68
18	3	303	CLA	C4A-NA-C1A	-5.62	104.12	106.68
18	A	811	CLA	C4A-NA-C1A	-5.61	104.12	106.68
18	A	819	CLA	C4A-NA-C1A	-5.60	104.12	106.68
18	5	612	CLA	C4A-NA-C1A	-5.59	104.13	106.68
18	A	832	CLA	C4A-NA-C1A	-5.59	104.13	106.68
18	A	829	CLA	C4A-NA-C1A	-5.59	104.13	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	839	CLA	C4A-NA-C1A	-5.50	104.17	106.68
21	4	605	CHL	C1B-CHB-C4A	5.44	124.82	121.32
18	8	615	CLA	C4A-NA-C1A	-5.42	104.20	106.68
18	8	605	CLA	C4A-NA-C1A	-5.41	104.21	106.68
18	3	302	CLA	C4A-NA-C1A	-5.40	104.22	106.68
18	6	310	CLA	C3A-C2A-C1A	-5.38	93.28	101.34
18	1	603	CLA	C4A-NA-C1A	-5.38	104.22	106.68
18	8	612	CLA	C4A-NA-C1A	-5.36	104.23	106.68
18	1	611	CLA	C4A-NA-C1A	-5.34	104.24	106.68
18	B	824	CLA	C4A-NA-C1A	-5.30	104.26	106.68
18	Z	610	CLA	C4A-NA-C1A	-5.30	104.26	106.68
18	6	311	CLA	C4A-NA-C1A	-5.30	104.26	106.68
18	1	609	CLA	C4A-NA-C1A	-5.28	104.27	106.68
18	A	807	CLA	C4A-NA-C1A	-5.27	104.27	106.68
18	7	604	CLA	C3B-C4B-NB	-5.26	105.83	110.53
18	B	812	CLA	CAA-C2A-C1A	-5.26	100.50	112.14
18	B	801	CLA	C4A-NA-C1A	-5.25	104.28	106.68
18	5	611	CLA	C4A-NA-C1A	-5.24	104.29	106.68
18	A	835	CLA	C4A-NA-C1A	-5.24	104.29	106.68
18	Z	613	CLA	C4A-NA-C1A	-5.24	104.29	106.68
18	3	301	CLA	C4A-NA-C1A	-5.23	104.29	106.68
18	Z	608	CLA	C4A-NA-C1A	-5.23	104.29	106.68
18	8	608	CLA	C4A-NA-C1A	-5.23	104.29	106.68
18	3	312	CLA	C4A-NA-C1A	-5.21	104.30	106.68
18	3	313	CLA	C4A-NA-C1A	-5.20	104.31	106.68
18	7	603	CLA	C4A-NA-C1A	-5.18	104.31	106.68
18	B	813	CLA	C4A-NA-C1A	-5.17	104.32	106.68
18	1	613	CLA	C4A-NA-C1A	-5.17	104.32	106.68
18	1	614	CLA	C4A-NA-C1A	-5.16	104.33	106.68
18	A	839	CLA	C4A-NA-C1A	-5.16	104.33	106.68
18	A	812	CLA	C4A-NA-C1A	-5.15	104.33	106.68
18	Z	612	CLA	C4A-NA-C1A	-5.15	104.33	106.68
18	7	608	CLA	C4A-NA-C1A	-5.14	104.34	106.68
18	A	820	CLA	C4A-NA-C1A	-5.13	104.34	106.68
18	7	612	CLA	C4A-NA-C1A	-5.13	104.34	106.68
18	A	836	CLA	C4A-NA-C1A	-5.12	104.34	106.68
18	A	837	CLA	C4A-NA-C1A	-5.11	104.35	106.68
18	3	310	CLA	C4A-NA-C1A	-5.10	104.35	106.68
18	B	837	CLA	C4A-NA-C1A	-5.10	104.35	106.68
18	8	604	CLA	C4A-NA-C1A	-5.10	104.35	106.68
18	B	809	CLA	C4A-NA-C1A	-5.09	104.36	106.68
18	A	826	CLA	CAA-C2A-C1A	-5.08	100.89	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	7	602	CLA	C4A-NA-C1A	-5.04	104.38	106.68
18	A	814	CLA	C4A-NA-C1A	-5.02	104.39	106.68
18	B	834	CLA	C4A-NA-C1A	-5.01	104.39	106.68
18	8	613	CLA	C4A-NA-C1A	-5.00	104.40	106.68
18	5	604	CLA	C4A-NA-C1A	-5.00	104.40	106.68
18	5	615	CLA	C3A-C2A-C1A	-4.98	93.88	101.34
18	5	609	CLA	C4A-NA-C1A	-4.97	104.41	106.68
18	4	606	CLA	C4A-NA-C1A	-4.97	104.41	106.68
18	5	603	CLA	C4A-NA-C1A	-4.97	104.41	106.68
18	B	816	CLA	C4A-NA-C1A	-4.97	104.41	106.68
18	B	825	CLA	C4A-NA-C1A	-4.96	104.41	106.68
18	Z	611	CLA	C4A-NA-C1A	-4.96	104.42	106.68
18	A	810	CLA	C4A-NA-C1A	-4.94	104.42	106.68
18	4	608	CLA	C3A-C2A-C1A	-4.94	93.94	101.34
18	B	823	CLA	C4A-NA-C1A	-4.93	104.43	106.68
18	B	828	CLA	C4A-NA-C1A	-4.92	104.43	106.68
18	A	830	CLA	C4A-NA-C1A	-4.91	104.44	106.68
18	7	604	CLA	C4A-NA-C1A	-4.89	104.45	106.68
18	Z	606	CLA	C4A-NA-C1A	-4.88	104.45	106.68
18	1	612	CLA	C4A-NA-C1A	-4.87	104.45	106.68
18	1	607	CLA	C4A-NA-C1A	-4.87	104.46	106.68
18	6	301	CLA	C4A-NA-C1A	-4.87	104.46	106.68
18	A	821	CLA	C4A-NA-C1A	-4.84	104.47	106.68
18	A	809	CLA	C4A-NA-C1A	-4.84	104.47	106.68
18	7	601	CLA	C4A-NA-C1A	-4.84	104.47	106.68
18	4	611	CLA	C4A-NA-C1A	-4.84	104.47	106.68
18	3	311	CLA	C4A-NA-C1A	-4.82	104.48	106.68
18	8	610	CLA	C3B-C4B-NB	-4.81	106.23	110.53
18	7	607	CLA	C4A-NA-C1A	-4.81	104.49	106.68
18	7	614	CLA	C3A-C2A-C1A	-4.80	94.15	101.34
18	B	838	CLA	C4A-NA-C1A	-4.78	104.50	106.68
18	F	302	CLA	C4A-NA-C1A	-4.77	104.50	106.68
21	4	604	CHL	CAA-C2A-C1A	4.76	122.78	113.35
18	B	833	CLA	C4A-NA-C1A	-4.73	104.52	106.68
18	6	317	CLA	C4A-NA-C1A	-4.72	104.53	106.68
18	A	827	CLA	CAA-C2A-C1A	-4.71	101.71	112.14
18	B	806	CLA	C3A-C2A-C1A	-4.69	94.31	101.34
18	J	101	CLA	C4A-NA-C1A	-4.68	104.54	106.68
18	8	601	CLA	C4A-NA-C1A	-4.68	104.55	106.68
18	B	826	CLA	C4A-NA-C1A	-4.67	104.55	106.68
18	A	816	CLA	C4A-NA-C1A	-4.67	104.55	106.68
18	A	843	CLA	C4A-NA-C1A	-4.66	104.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	817	CLA	C4A-NA-C1A	-4.62	104.57	106.68
18	A	808	CLA	CAA-C2A-C1A	-4.61	101.93	112.14
18	A	841	CLA	C4A-NA-C1A	-4.61	104.58	106.68
18	B	829	CLA	C4A-NA-C1A	-4.59	104.59	106.68
18	7	609	CLA	C4A-NA-C1A	-4.58	104.59	106.68
18	A	813	CLA	C4A-NA-C1A	-4.53	104.61	106.68
18	1	604	CLA	C4A-NA-C1A	-4.51	104.62	106.68
18	B	823	CLA	C1D-ND-C4D	-4.50	103.15	106.31
18	A	833	CLA	C4A-NA-C1A	-4.49	104.63	106.68
18	Z	603	CLA	C4A-NA-C1A	-4.49	104.63	106.68
18	B	821	CLA	C4A-NA-C1A	-4.48	104.64	106.68
18	A	845	CLA	C4A-NA-C1A	-4.48	104.64	106.68
18	8	607	CLA	C4A-NA-C1A	-4.47	104.64	106.68
18	A	803	CLA	CAA-C2A-C1A	-4.46	102.28	112.14
18	5	614	CLA	C4A-NA-C1A	-4.45	104.65	106.68
18	A	828	CLA	C4A-NA-C1A	-4.45	104.65	106.68
18	3	314	CLA	C4A-NA-C1A	-4.42	104.66	106.68
18	6	303	CLA	C4A-NA-C1A	-4.41	104.67	106.68
18	A	815	CLA	C4A-NA-C1A	-4.38	104.68	106.68
18	A	818	CLA	C4A-NA-C1A	-4.33	104.70	106.68
18	Z	602	CLA	C4A-NA-C1A	-4.32	104.71	106.68
18	4	609	CLA	C4A-NA-C1A	-4.31	104.71	106.68
18	B	814	CLA	C4A-NA-C1A	-4.29	104.72	106.68
18	A	844	CLA	C4A-NA-C1A	-4.29	104.72	106.68
18	B	810	CLA	C4A-NA-C1A	-4.27	104.73	106.68
18	8	609	CLA	C4A-NA-C1A	-4.25	104.74	106.68
18	1	602	CLA	C4A-NA-C1A	-4.25	104.74	106.68
18	B	834	CLA	CMC-C2C-C1C	4.21	126.06	113.33
18	A	819	CLA	CAA-C2A-C1A	-4.20	102.84	112.14
21	4	604	CHL	CMA-C3A-C4A	-4.19	105.58	114.61
18	5	608	CLA	C4A-NA-C1A	-4.18	104.77	106.68
18	1	608	CLA	CAA-C2A-C1A	-4.15	102.94	112.14
18	3	305	CLA	C3A-C2A-C1A	-4.15	95.12	101.34
18	Z	607	CLA	CAA-C2A-C1A	-4.15	102.96	112.14
18	B	815	CLA	C3A-C2A-C1A	-4.15	95.13	101.34
18	7	610	CLA	C3A-C2A-C1A	-4.14	94.63	101.64
21	6	307	CHL	C1B-CHB-C4A	4.13	123.98	121.32
18	3	307	CLA	CAA-C2A-C1A	-4.13	103.00	112.14
18	3	305	CLA	CAA-C2A-C1A	-4.13	103.00	112.14
18	7	611	CLA	C4A-NA-C1A	-4.10	104.81	106.68
18	3	308	CLA	C4A-NA-C1A	-4.09	104.81	106.68
18	5	601	CLA	C4A-NA-C1A	-4.07	104.82	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	829	CLA	CAA-C2A-C1A	-4.01	103.27	112.14
18	A	825	CLA	CAA-C2A-C1A	-3.99	103.30	112.14
18	6	312	CLA	C4A-NA-C1A	-3.97	104.87	106.68
18	1	602	CLA	C1D-ND-C4D	-3.93	103.56	106.31
18	B	842	CLA	CAA-C2A-C1A	-3.90	103.50	112.14
18	Z	602	CLA	C1D-ND-C4D	-3.90	103.57	106.31
18	6	304	CLA	C4A-NA-C1A	-3.86	104.92	106.68
21	5	607	CHL	CAA-C2A-C1A	3.86	120.98	113.35
18	5	610	CLA	C3B-C4B-NB	-3.84	107.11	110.53
18	B	820	CLA	C3A-C2A-C1A	-3.83	95.60	101.34
18	B	830	CLA	C4A-NA-C1A	-3.83	104.93	106.68
18	8	609	CLA	C1D-ND-C4D	-3.81	103.64	106.31
18	3	309	CLA	C3A-C2A-C1A	-3.80	95.21	101.64
18	8	608	CLA	C1D-ND-C4D	-3.80	103.65	106.31
17	A	801	CL0	CHA-C1A-C2A	-3.75	124.50	133.31
18	5	611	CLA	C1D-ND-C4D	-3.75	103.68	106.31
18	7	602	CLA	C1D-ND-C4D	-3.74	103.69	106.31
18	A	825	CLA	CHD-C1D-ND	-3.74	119.54	124.80
21	5	616	CHL	CHA-C1A-C2A	-3.74	124.53	133.31
18	4	601	CLA	C3A-C2A-C1A	-3.74	95.74	101.34
18	A	836	CLA	C1D-ND-C4D	-3.74	103.69	106.31
18	B	809	CLA	C1D-ND-C4D	-3.73	103.70	106.31
18	3	301	CLA	C1D-ND-C4D	-3.73	103.70	106.31
18	B	801	CLA	CAA-C2A-C1A	-3.70	103.94	112.14
18	A	817	CLA	C1D-ND-C4D	-3.69	103.72	106.31
18	6	302	CLA	C1D-ND-C4D	-3.68	103.73	106.31
18	5	602	CLA	C1D-ND-C4D	-3.67	103.74	106.31
18	4	602	CLA	C1D-ND-C4D	-3.66	103.74	106.31
18	5	615	CLA	C2A-C3A-C4A	-3.63	96.01	101.87
18	4	609	CLA	C1D-ND-C4D	-3.62	103.77	106.31
21	6	316	CHL	C1B-CHB-C4A	3.61	123.64	121.32
18	5	615	CLA	C3B-C4B-NB	-3.60	107.32	110.53
18	5	617	CLA	C3B-C4B-NB	-3.60	107.32	110.53
21	4	605	CHL	C4D-CHA-CBD	-3.58	105.36	108.97
18	B	842	CLA	C1D-ND-C4D	-3.57	103.81	106.31
18	A	812	CLA	C1D-ND-C4D	-3.56	103.81	106.31
18	6	311	CLA	C1D-ND-C4D	-3.56	103.81	106.31
18	B	805	CLA	CAA-C2A-C1A	-3.56	104.26	112.14
18	A	808	CLA	C1D-ND-C4D	-3.54	103.83	106.31
18	8	611	CLA	C1D-ND-C4D	-3.54	103.83	106.31
21	6	316	CHL	CHA-C1A-C2A	-3.53	125.03	133.31
18	A	814	CLA	C1D-ND-C4D	-3.51	103.85	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	818	CLA	C1D-ND-C4D	-3.51	103.85	106.31
18	7	603	CLA	C1D-ND-C4D	-3.51	103.85	106.31
18	A	819	CLA	C1D-ND-C4D	-3.51	103.85	106.31
21	4	604	CHL	CHA-C1A-C2A	-3.50	125.09	133.31
18	7	611	CLA	C1D-ND-C4D	-3.49	103.86	106.31
18	6	315	CLA	C3B-C4B-NB	-3.48	107.42	110.53
21	6	305	CHL	CHA-C1A-C2A	-3.48	125.14	133.31
18	6	315	CLA	CAA-C2A-C1A	-3.48	104.44	112.14
18	7	604	CLA	CHA-C1A-NA	-3.47	118.54	126.39
18	B	820	CLA	CAA-C2A-C1A	-3.46	104.48	112.14
18	A	815	CLA	C1D-ND-C4D	-3.46	103.89	106.31
18	6	303	CLA	C1D-ND-C4D	-3.45	103.89	106.31
18	8	602	CLA	C4A-NA-C1A	-3.44	105.11	106.68
18	1	605	CLA	C2C-C1C-NC	3.44	113.59	109.98
18	A	803	CLA	C1D-ND-C4D	-3.43	103.90	106.31
18	6	310	CLA	C2B-C1B-NB	-3.43	106.77	110.33
21	Z	601	CHL	CHA-C1A-C2A	-3.42	125.27	133.31
18	5	613	CLA	C1D-ND-C4D	-3.42	103.91	106.31
18	5	614	CLA	CAA-C2A-C1A	-3.42	104.57	112.14
18	B	817	CLA	CAA-C2A-C1A	-3.42	104.57	112.14
18	7	609	CLA	C1D-ND-C4D	-3.41	103.92	106.31
21	1	601	CHL	CHA-C1A-C2A	-3.41	125.29	133.31
18	B	822	CLA	C1D-ND-C4D	-3.41	103.92	106.31
18	Z	604	CLA	C2C-C1C-NC	3.41	113.56	109.98
18	A	826	CLA	C1D-ND-C4D	-3.40	103.92	106.31
18	8	602	CLA	C1D-ND-C4D	-3.40	103.92	106.31
18	1	608	CLA	C3A-C2A-C1A	-3.40	96.24	101.34
18	Z	607	CLA	C3A-C2A-C1A	-3.40	96.25	101.34
18	B	811	CLA	C3B-C4B-NB	-3.39	107.50	110.53
18	B	829	CLA	C3B-C4B-NB	-3.39	107.50	110.53
21	3	306	CHL	CHA-C1A-C2A	-3.39	125.34	133.31
18	8	609	CLA	CHD-C1D-ND	-3.39	120.04	124.80
18	J	101	CLA	C1D-ND-C4D	-3.38	103.94	106.31
18	3	310	CLA	C1D-ND-C4D	-3.38	103.94	106.31
21	5	616	CHL	C1B-CHB-C4A	3.38	123.50	121.32
18	B	814	CLA	C1D-ND-C4D	-3.36	103.95	106.31
18	B	819	CLA	C1D-ND-C4D	-3.36	103.95	106.31
21	8	606	CHL	CAA-C2A-C1A	3.35	119.99	113.35
18	8	612	CLA	C1D-ND-C4D	-3.34	103.97	106.31
18	A	835	CLA	C1D-ND-C4D	-3.34	103.97	106.31
18	3	302	CLA	C1D-ND-C4D	-3.34	103.97	106.31
18	5	604	CLA	C1D-ND-C4D	-3.32	103.98	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	313	CLA	C1D-ND-C4D	-3.32	103.98	106.31
18	B	832	CLA	C1D-ND-C4D	-3.32	103.98	106.31
18	1	611	CLA	C1D-ND-C4D	-3.32	103.99	106.31
18	7	608	CLA	C1D-ND-C4D	-3.32	103.99	106.31
18	F	302	CLA	C1D-ND-C4D	-3.31	103.99	106.31
21	Z	605	CHL	CHA-C1A-C2A	-3.31	125.53	133.31
18	B	828	CLA	C1D-ND-C4D	-3.31	103.99	106.31
21	1	606	CHL	CHA-C1A-C2A	-3.31	125.54	133.31
18	B	824	CLA	C1D-ND-C4D	-3.30	103.99	106.31
18	4	601	CLA	C1D-ND-C4D	-3.30	103.99	106.31
18	B	820	CLA	C3B-C4B-NB	-3.30	107.58	110.53
18	3	308	CLA	C1D-ND-C4D	-3.30	104.00	106.31
18	A	823	CLA	C1D-ND-C4D	-3.29	104.00	106.31
18	5	608	CLA	C1D-ND-C4D	-3.29	104.00	106.31
18	A	827	CLA	C3B-C4B-NB	-3.28	107.60	110.53
18	A	831	CLA	C1D-ND-C4D	-3.28	104.01	106.31
18	3	312	CLA	C1D-ND-C4D	-3.28	104.01	106.31
18	A	827	CLA	CHD-C1D-ND	-3.28	120.19	124.80
18	Z	610	CLA	C1D-ND-C4D	-3.28	104.01	106.31
18	7	612	CLA	C1D-ND-C4D	-3.27	104.02	106.31
18	B	827	CLA	C3A-C2A-C1A	-3.25	96.47	101.34
18	A	818	CLA	C1D-ND-C4D	-3.25	104.03	106.31
18	Z	612	CLA	C1D-ND-C4D	-3.23	104.04	106.31
18	5	611	CLA	CAA-C2A-C1A	-3.23	104.99	112.14
18	8	613	CLA	C1D-ND-C4D	-3.23	104.05	106.31
18	1	613	CLA	C1D-ND-C4D	-3.22	104.05	106.31
18	B	802	CLA	C3B-C4B-NB	-3.22	107.66	110.53
21	6	305	CHL	C1B-CHB-C4A	3.21	123.39	121.32
18	B	834	CLA	C1D-ND-C4D	-3.20	104.06	106.31
18	B	823	CLA	CHD-C1D-ND	-3.20	120.30	124.80
18	6	309	CLA	C1D-ND-C4D	-3.20	104.07	106.31
18	6	313	CLA	CHD-C1D-ND	-3.19	120.31	124.80
18	B	804	CLA	C3A-C2A-C1A	-3.19	96.56	101.34
18	B	808	CLA	C2C-C1C-NC	3.19	113.33	109.98
18	B	807	CLA	CAA-C2A-C1A	-3.19	105.08	112.14
18	7	607	CLA	CAA-C2A-C1A	-3.19	105.08	112.14
18	Z	604	CLA	CHC-C1C-C2C	-3.19	117.89	126.95
18	Z	613	CLA	C1D-ND-C4D	-3.18	104.08	106.31
18	8	603	CLA	C1D-ND-C4D	-3.18	104.08	106.31
18	3	314	CLA	C1D-ND-C4D	-3.18	104.08	106.31
18	1	605	CLA	CHC-C1C-C2C	-3.18	117.92	126.95
18	A	833	CLA	C1D-ND-C4D	-3.18	104.08	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	307	CHL	CHA-C1A-C2A	-3.17	125.86	133.31
18	1	614	CLA	C1D-ND-C4D	-3.17	104.09	106.31
18	5	603	CLA	C2C-C1C-NC	3.16	113.30	109.98
18	A	838	CLA	CHD-C1D-ND	-3.16	120.35	124.80
18	7	608	CLA	C1-C2-C3	-3.16	121.66	126.76
18	3	309	CLA	C3B-C4B-NB	-3.14	107.72	110.53
21	6	305	CHL	CAA-C2A-C1A	3.14	119.57	113.35
18	A	825	CLA	C1D-ND-C4D	-3.14	104.11	106.31
18	6	308	CLA	C1D-ND-C4D	-3.14	104.11	106.31
18	B	827	CLA	CAA-C2A-C1A	-3.13	105.20	112.14
18	B	816	CLA	CHC-C1C-C2C	-3.13	118.04	126.95
18	4	606	CLA	C1D-ND-C4D	-3.13	104.11	106.31
18	B	827	CLA	C1D-ND-C4D	-3.13	104.12	106.31
18	A	816	CLA	C1D-ND-C4D	-3.13	104.12	106.31
18	4	610	CLA	C1D-ND-C4D	-3.13	104.12	106.31
18	B	835	CLA	C1D-ND-C4D	-3.13	104.12	106.31
18	B	841	CLA	C1D-ND-C4D	-3.13	104.12	106.31
18	B	820	CLA	CHD-C1D-ND	-3.12	120.41	124.80
18	A	819	CLA	CHD-C1D-ND	-3.12	120.41	124.80
18	B	843	CLA	C1D-ND-C4D	-3.12	104.12	106.31
18	A	834	CLA	CAA-C2A-C1A	-3.11	105.25	112.14
18	A	803	CLA	CHD-C1D-ND	-3.11	120.43	124.80
18	1	613	CLA	CHC-C1C-C2C	-3.11	118.12	126.95
18	A	814	CLA	CHC-C1C-C2C	-3.10	118.13	126.95
18	7	614	CLA	CHD-C1D-ND	-3.10	120.44	124.80
18	3	309	CLA	C2A-C3A-C4A	-3.10	97.96	101.59
18	B	835	CLA	CHC-C1C-NC	3.09	128.97	124.31
18	B	810	CLA	CHC-C1C-C2C	-3.09	118.16	126.95
18	J	101	CLA	CAA-C2A-C1A	-3.09	105.30	112.14
18	Z	612	CLA	CHC-C1C-C2C	-3.09	118.17	126.95
21	7	606	CHL	CHA-C1A-C2A	-3.09	126.06	133.31
18	7	601	CLA	CHC-C1C-C2C	-3.09	118.18	126.95
18	F	302	CLA	C1-C2-C3	-3.08	121.14	126.20
18	4	612	CLA	CHD-C1D-ND	-3.08	120.46	124.80
18	B	816	CLA	C1D-ND-C4D	-3.07	104.16	106.31
18	A	814	CLA	C2C-C1C-NC	3.07	113.21	109.98
18	B	835	CLA	CAA-C2A-C1A	-3.07	105.34	112.14
21	6	306	CHL	CHA-C1A-C2A	-3.07	126.09	133.31
18	B	839	CLA	C3B-C4B-NB	-3.07	107.79	110.53
18	A	825	CLA	CHC-C1C-NC	3.07	128.94	124.31
18	A	805	CLA	C1D-ND-C4D	-3.07	104.16	106.31
18	5	617	CLA	C1D-ND-C4D	-3.07	104.16	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	816	CLA	CHC-C1C-NC	3.06	128.93	124.31
18	8	611	CLA	CHD-C1D-ND	-3.06	120.50	124.80
18	5	611	CLA	CHD-C1D-ND	-3.06	120.50	124.80
18	A	807	CLA	C1D-ND-C4D	-3.06	104.17	106.31
18	B	812	CLA	C2A-C1A-CHA	3.06	129.17	123.87
18	4	601	CLA	CHD-C1D-ND	-3.06	120.50	124.80
18	B	813	CLA	C1D-ND-C4D	-3.05	104.17	106.31
18	3	301	CLA	CHD-C1D-ND	-3.05	120.51	124.80
18	3	305	CLA	C2A-C3A-C4A	-3.05	96.94	101.87
18	5	609	CLA	C1D-ND-C4D	-3.05	104.17	106.31
18	B	838	CLA	C1D-ND-C4D	-3.05	104.17	106.31
18	A	840	CLA	C1D-ND-C4D	-3.05	104.17	106.31
18	B	808	CLA	CHC-C1C-C2C	-3.04	118.30	126.95
18	4	611	CLA	C1D-ND-C4D	-3.04	104.18	106.31
18	5	603	CLA	CHC-C1C-C2C	-3.04	118.31	126.95
18	4	607	CLA	CHD-C1D-ND	-3.04	120.53	124.80
18	1	613	CLA	CHC-C1C-NC	3.04	128.88	124.31
18	A	813	CLA	CHC-C1C-C2C	-3.04	118.32	126.95
18	A	838	CLA	C1D-ND-C4D	-3.03	104.18	106.31
18	Z	612	CLA	CHC-C1C-NC	3.03	128.88	124.31
18	7	601	CLA	C1D-ND-C4D	-3.03	104.19	106.31
18	5	605	CLA	C2C-C1C-NC	3.03	113.16	109.98
18	1	607	CLA	C1D-ND-C4D	-3.02	104.19	106.31
18	A	820	CLA	C1D-ND-C4D	-3.02	104.19	106.31
18	B	810	CLA	C1D-ND-C4D	-3.02	104.20	106.31
18	A	827	CLA	C3A-C2A-C1A	-3.02	96.82	101.34
18	Z	606	CLA	C1D-ND-C4D	-3.01	104.20	106.31
18	5	615	CLA	CHD-C1D-ND	-3.01	120.56	124.80
18	A	844	CLA	C2C-C1C-NC	3.01	113.14	109.98
18	B	817	CLA	C2C-C1C-NC	3.01	113.14	109.98
18	B	836	CLA	C1D-ND-C4D	-3.01	104.20	106.31
18	8	604	CLA	C1D-ND-C4D	-3.01	104.20	106.31
18	4	609	CLA	CHD-C1D-ND	-3.00	120.58	124.80
18	B	827	CLA	CHD-C1D-ND	-3.00	120.58	124.80
18	A	833	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
18	7	601	CLA	CHC-C1C-NC	3.00	128.83	124.31
18	A	841	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
18	B	807	CLA	CHD-C1D-ND	-3.00	120.58	124.80
18	6	311	CLA	CHD-C1D-ND	-2.99	120.59	124.80
18	3	304	CLA	C2C-C1C-NC	2.99	113.12	109.98
21	3	306	CHL	C1B-CHB-C4A	2.99	123.25	121.32
18	A	828	CLA	CHC-C1C-C2C	-2.99	118.45	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	806	CLA	C1D-ND-C4D	-2.99	104.22	106.31
18	5	617	CLA	CHD-C1D-ND	-2.99	120.60	124.80
18	7	603	CLA	C2C-C1C-NC	2.98	113.11	109.98
18	B	828	CLA	CHD-C1D-ND	-2.98	120.61	124.80
18	B	819	CLA	CHD-C1D-ND	-2.97	120.62	124.80
18	A	839	CLA	CHC-C1C-C2C	-2.97	118.51	126.95
18	A	829	CLA	C1D-ND-C4D	-2.97	104.23	106.31
18	A	807	CLA	CHD-C1D-ND	-2.97	120.63	124.80
18	3	310	CLA	CHD-C1D-ND	-2.96	120.63	124.80
18	B	815	CLA	CAA-C2A-C1A	-2.96	105.59	112.14
18	B	807	CLA	C1D-ND-C4D	-2.96	104.23	106.31
18	7	610	CLA	CHD-C1D-ND	-2.96	120.64	124.80
18	B	804	CLA	CHD-C1D-ND	-2.95	120.64	124.80
18	F	301	CLA	C1D-ND-C4D	-2.95	104.24	106.31
18	8	608	CLA	CHD-C1D-ND	-2.95	120.65	124.80
18	A	816	CLA	CHC-C1C-C2C	-2.95	118.56	126.95
18	A	827	CLA	C2A-C3A-C4A	-2.95	97.11	101.87
18	7	613	CLA	C1D-ND-C4D	-2.95	104.24	106.31
18	Z	603	CLA	C1D-ND-C4D	-2.94	104.25	106.31
18	6	303	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
18	A	832	CLA	C1D-ND-C4D	-2.94	104.25	106.31
18	B	817	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
18	A	820	CLA	CHD-C1D-ND	-2.94	120.67	124.80
18	4	606	CLA	CHD-C1D-ND	-2.94	120.67	124.80
18	A	831	CLA	CAA-C2A-C1A	-2.94	105.64	112.14
18	4	603	CLA	C1D-ND-C4D	-2.94	104.25	106.31
18	A	810	CLA	C1D-ND-C4D	-2.93	104.25	106.31
18	A	813	CLA	CHC-C1C-NC	2.93	128.73	124.31
18	3	307	CLA	C1D-ND-C4D	-2.93	104.25	106.31
18	B	805	CLA	CHD-C1D-ND	-2.93	120.67	124.80
18	A	825	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
18	7	610	CLA	C3B-C4B-NB	-2.93	107.92	110.53
18	B	822	CLA	CHD-C1D-ND	-2.93	120.68	124.80
18	Z	609	CLA	CAA-C2A-C1A	-2.93	105.66	112.14
18	B	841	CLA	CHD-C1D-ND	-2.93	120.68	124.80
18	A	820	CLA	CHC-C1C-C2C	-2.93	118.63	126.95
18	6	317	CLA	C1D-ND-C4D	-2.92	104.26	106.31
18	A	815	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
18	J	101	CLA	CHD-C1D-ND	-2.92	120.69	124.80
18	5	613	CLA	CHD-C1D-ND	-2.92	120.69	124.80
18	A	816	CLA	CHC-C1C-NC	2.92	128.71	124.31
18	A	844	CLA	CHC-C1C-C2C	-2.92	118.65	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	839	CLA	C2C-C1C-NC	2.92	113.05	109.98
18	5	605	CLA	CHC-C1C-C2C	-2.92	118.66	126.95
18	7	610	CLA	CAA-C2A-C1A	-2.92	104.61	111.81
21	5	607	CHL	C1B-CHB-C4A	2.92	123.20	121.32
18	5	601	CLA	CHC-C1C-C2C	-2.91	118.66	126.95
18	1	613	CLA	CGD-CBD-CAD	-2.91	101.41	110.85
18	7	602	CLA	CHD-C1D-ND	-2.91	120.70	124.80
18	8	603	CLA	CHD-C1D-ND	-2.91	120.70	124.80
18	Z	606	CLA	C2C-C1C-NC	2.91	113.04	109.98
18	3	314	CLA	CHC-C1C-NC	2.91	128.69	124.31
18	6	312	CLA	C1D-ND-C4D	-2.91	104.27	106.31
18	B	826	CLA	C1D-ND-C4D	-2.91	104.27	106.31
18	B	816	CLA	C2C-C1C-NC	2.90	113.03	109.98
18	Z	612	CLA	CGD-CBD-CAD	-2.90	101.46	110.85
18	A	808	CLA	CHD-C1D-ND	-2.90	120.72	124.80
18	B	806	CLA	CHD-C1D-ND	-2.90	120.72	124.80
18	A	836	CLA	CHD-C1D-ND	-2.90	120.73	124.80
18	1	610	CLA	CAA-C2A-C1A	-2.90	105.73	112.14
21	5	607	CHL	C3D-C4D-CHA	2.89	112.94	108.54
18	3	311	CLA	C2C-C1C-NC	2.89	113.02	109.98
18	1	604	CLA	C1D-ND-C4D	-2.89	104.28	106.31
18	3	312	CLA	CHD-C1D-ND	-2.89	120.73	124.80
18	5	617	CLA	CGD-CBD-CAD	-2.89	101.49	110.85
18	B	830	CLA	C1D-ND-C4D	-2.89	104.29	106.31
18	6	312	CLA	CHC-C1C-C2C	-2.89	118.75	126.95
18	7	611	CLA	CHD-C1D-ND	-2.88	120.75	124.80
18	5	614	CLA	C3B-C4B-NB	-2.88	107.96	110.53
18	Z	611	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
18	3	309	CLA	CHD-C1D-ND	-2.88	120.75	124.80
18	7	609	CLA	CHD-C1D-ND	-2.88	120.75	124.80
18	1	607	CLA	C2C-C1C-NC	2.88	113.01	109.98
18	B	813	CLA	CHD-C1D-ND	-2.88	120.75	124.80
18	B	843	CLA	C2C-C1C-NC	2.88	113.00	109.98
18	8	601	CLA	C1D-ND-C4D	-2.88	104.29	106.31
18	7	614	CLA	CHA-C1A-NA	-2.88	119.88	126.39
18	A	836	CLA	CHC-C1C-NC	2.88	128.64	124.31
18	3	314	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
18	1	612	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
18	6	317	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
18	A	803	CLA	CHC-C1C-NC	2.87	128.64	124.31
18	B	835	CLA	CHD-C1D-ND	-2.87	120.76	124.80
18	A	823	CLA	C1-C2-C3	-2.87	121.50	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	310	CLA	C2A-C3A-C4A	-2.87	97.23	101.87
18	8	607	CLA	CHC-C1C-NC	2.87	128.63	124.31
18	A	826	CLA	CHD-C1D-ND	-2.87	120.77	124.80
18	8	601	CLA	CHC-C1C-C2C	-2.87	118.80	126.95
18	A	802	CLA	CHD-C1D-ND	-2.87	120.77	124.80
18	B	809	CLA	CHC-C1C-C2C	-2.87	118.80	126.95
18	A	812	CLA	CHC-C1C-C2C	-2.87	118.80	126.95
18	B	830	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
18	A	814	CLA	CHD-C1D-ND	-2.86	120.77	124.80
18	3	304	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
18	7	601	CLA	C2C-C1C-NC	2.86	112.99	109.98
18	7	610	CLA	C2A-C3A-C4A	-2.86	98.24	101.59
18	B	817	CLA	C1D-ND-C4D	-2.86	104.30	106.31
18	6	302	CLA	CHD-C1D-ND	-2.86	120.78	124.80
18	7	613	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
18	A	833	CLA	C2C-C1C-NC	2.85	112.98	109.98
18	A	828	CLA	CHC-C1C-NC	2.85	128.61	124.31
18	B	810	CLA	CHC-C1C-NC	2.85	128.61	124.31
18	7	603	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
18	A	823	CLA	CHD-C1D-ND	-2.85	120.79	124.80
18	A	835	CLA	CAA-C2A-C1A	-2.85	105.82	112.14
18	3	313	CLA	C1D-ND-C4D	-2.85	104.31	106.31
18	3	310	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
18	B	816	CLA	CHD-C1D-ND	-2.85	120.79	124.80
18	3	302	CLA	C2C-C1C-NC	2.85	112.98	109.98
18	7	604	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
18	A	815	CLA	CHD-C1D-ND	-2.85	120.79	124.80
18	A	812	CLA	CHD-C1D-ND	-2.85	120.79	124.80
18	A	830	CLA	CHC-C1C-NC	2.85	128.60	124.31
18	3	312	CLA	CAA-C2A-C1A	-2.85	102.64	111.97
18	A	830	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
18	3	302	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
18	5	601	CLA	CHA-C1A-NA	-2.85	119.94	126.39
18	8	615	CLA	C1D-ND-C4D	-2.85	104.31	106.31
18	4	607	CLA	C1D-ND-C4D	-2.85	104.31	106.31
18	B	842	CLA	CHD-C1D-ND	-2.85	120.80	124.80
18	A	824	CLA	CHC-C1C-C2C	-2.84	118.86	126.95
18	B	831	CLA	C1D-ND-C4D	-2.84	104.32	106.31
18	A	833	CLA	CHC-C1C-NC	2.84	128.59	124.31
18	3	307	CLA	CHD-C1D-ND	-2.84	120.80	124.80
18	B	840	CLA	CHC-C1C-C2C	-2.84	118.87	126.95
18	J	101	CLA	CHC-C1C-NC	2.84	128.59	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	802	CLA	C1D-ND-C4D	-2.84	104.32	106.31
18	A	809	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
18	A	832	CLA	CHC-C1C-C2C	-2.84	118.89	126.95
18	7	611	CLA	CHC-C1C-NC	2.84	128.58	124.31
18	B	843	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
18	7	613	CLA	CHD-C1D-ND	-2.83	120.82	124.80
18	F	301	CLA	CHD-C1D-ND	-2.83	120.82	124.80
18	8	610	CLA	CHD-C1D-ND	-2.83	120.82	124.80
18	7	614	CLA	C1D-ND-C4D	-2.83	104.33	106.31
18	A	830	CLA	CHD-C1D-ND	-2.83	120.82	124.80
18	1	607	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
18	A	815	CLA	C2C-C1C-NC	2.83	112.95	109.98
18	B	837	CLA	C3B-C4B-NB	-2.83	108.01	110.53
18	3	303	CLA	CHC-C1C-C2C	-2.82	118.92	126.95
18	6	304	CLA	C1D-ND-C4D	-2.82	104.33	106.31
18	Z	613	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
18	5	604	CLA	CHD-C1D-ND	-2.82	120.83	124.80
18	7	611	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
18	B	833	CLA	C1D-ND-C4D	-2.82	104.33	106.31
18	1	603	CLA	C1D-ND-C4D	-2.82	104.33	106.31
18	4	603	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
18	A	817	CLA	CHD-C1D-ND	-2.82	120.84	124.80
18	Z	606	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
18	1	602	CLA	CHD-C1D-ND	-2.82	120.84	124.80
18	A	814	CLA	CHC-C1C-NC	2.82	128.55	124.31
18	8	602	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
18	1	603	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
18	Z	602	CLA	CHD-C1D-ND	-2.81	120.85	124.80
18	4	611	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
18	8	612	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
18	1	614	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
18	B	842	CLA	C2C-C1C-NC	2.81	112.93	109.98
21	1	601	CHL	C1B-CHB-C4A	2.81	123.13	121.32
18	A	820	CLA	CHC-C1C-NC	2.81	128.54	124.31
18	A	824	CLA	CHD-C1D-ND	-2.81	120.85	124.80
18	Z	607	CLA	C3B-C4B-NB	-2.80	108.03	110.53
18	8	615	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
18	A	810	CLA	CHD-C1D-ND	-2.80	120.86	124.80
18	B	825	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
21	Z	601	CHL	C1B-CHB-C4A	2.80	123.12	121.32
18	8	612	CLA	C2C-C1C-NC	2.80	112.92	109.98
18	A	809	CLA	C1D-ND-C4D	-2.80	104.35	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	826	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
18	A	841	CLA	CHC-C1C-NC	2.80	128.52	124.31
18	8	607	CLA	CAA-C2A-C1A	-2.79	105.95	112.14
18	A	822	CLA	CHC-C1C-C2C	-2.79	119.00	126.95
18	8	607	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
18	7	605	CLA	C2C-C1C-NC	2.79	112.92	109.98
18	B	801	CLA	CHD-C1D-ND	-2.79	120.88	124.80
18	A	803	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
18	B	835	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
18	3	307	CLA	C3A-C2A-C1A	-2.79	97.16	101.34
18	8	613	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
18	B	809	CLA	CHD-C1D-ND	-2.79	120.88	124.80
18	B	843	CLA	CHD-C1D-ND	-2.79	120.88	124.80
18	A	830	CLA	C1D-ND-C4D	-2.79	104.36	106.31
18	5	611	CLA	CHC-C1C-C2C	-2.79	119.03	126.95
18	6	303	CLA	C2C-C1C-NC	2.78	112.91	109.98
18	A	805	CLA	CHD-C1D-ND	-2.78	120.89	124.80
18	8	615	CLA	C2C-C1C-NC	2.78	112.91	109.98
18	6	308	CLA	CHD-C1D-ND	-2.78	120.89	124.80
18	B	830	CLA	C2C-C1C-NC	2.78	112.90	109.98
18	1	603	CLA	C2C-C1C-NC	2.78	112.90	109.98
18	A	812	CLA	CHC-C1C-NC	2.78	128.50	124.31
18	6	313	CLA	CHC-C1C-NC	2.78	128.50	124.31
18	4	602	CLA	CHD-C1D-ND	-2.78	120.89	124.80
18	A	824	CLA	C2C-C1C-NC	2.78	112.90	109.98
18	B	818	CLA	CHD-C1D-ND	-2.78	120.89	124.80
18	6	303	CLA	CHC-C1C-NC	2.78	128.50	124.31
18	6	314	CLA	CAA-C2A-C1A	-2.77	102.88	111.97
18	A	827	CLA	CHC-C1C-NC	2.77	128.49	124.31
18	A	802	CLA	C3A-C2A-C1A	-2.77	97.18	101.34
18	B	824	CLA	CHD-C1D-ND	-2.77	120.90	124.80
18	A	806	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
18	8	608	CLA	CHA-C1A-NA	-2.77	120.12	126.39
18	Z	610	CLA	CAA-C2A-C1A	-2.77	106.01	112.14
18	5	602	CLA	CHD-C1D-ND	-2.77	120.91	124.80
18	Z	611	CLA	C2C-C1C-NC	2.77	112.89	109.98
21	6	306	CHL	C3D-C4D-CHA	2.77	112.74	108.54
18	B	823	CLA	CAA-C2A-C1A	-2.77	106.02	112.14
18	A	813	CLA	C2C-C1C-NC	2.76	112.89	109.98
21	8	606	CHL	C3D-C4D-CHA	2.76	112.74	108.54
18	1	611	CLA	CAA-C2A-C1A	-2.76	106.02	112.14
18	B	842	CLA	CHC-C1C-C2C	-2.76	119.09	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	304	CLA	C1D-ND-C4D	-2.76	104.37	106.31
18	A	831	CLA	CHD-C1D-ND	-2.76	120.91	124.80
18	A	807	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
18	6	304	CLA	CHC-C1C-NC	2.76	128.47	124.31
18	4	610	CLA	CHD-C1D-ND	-2.76	120.92	124.80
21	1	601	CHL	C3D-C4D-CHA	2.76	112.73	108.54
18	5	601	CLA	C2C-C1C-NC	2.76	112.88	109.98
18	A	817	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
18	3	308	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
18	A	816	CLA	CHD-C1D-ND	-2.76	120.92	124.80
18	8	601	CLA	CHC-C1C-NC	2.76	128.46	124.31
18	A	836	CLA	CHC-C1C-C2C	-2.75	119.12	126.95
18	Z	613	CLA	CHC-C1C-NC	2.75	128.46	124.31
18	B	832	CLA	CHD-C1D-ND	-2.75	120.93	124.80
18	7	607	CLA	C1D-ND-C4D	-2.75	104.38	106.31
18	Z	609	CLA	C1D-ND-C4D	-2.75	104.38	106.31
18	5	612	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
18	6	301	CLA	CHA-C1A-NA	-2.75	120.16	126.39
18	1	614	CLA	CHC-C1C-NC	2.75	128.45	124.31
18	3	301	CLA	CAA-C2A-C1A	-2.75	106.05	112.14
18	8	602	CLA	CHD-C1D-ND	-2.75	120.93	124.80
18	1	608	CLA	C3B-C4B-NB	-2.75	108.08	110.53
18	B	815	CLA	CHA-C1A-NA	-2.75	120.17	126.39
18	7	613	CLA	CHC-C1C-NC	2.75	128.45	124.31
18	B	814	CLA	CHD-C1D-ND	-2.75	120.94	124.80
18	1	613	CLA	C2C-C1C-NC	2.74	112.86	109.98
18	4	601	CLA	CHA-C1A-NA	-2.74	120.18	126.39
18	5	613	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
18	A	843	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
18	A	829	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
18	6	304	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
18	4	611	CLA	C2C-C1C-NC	2.74	112.86	109.98
18	B	822	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
18	B	833	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
18	8	603	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
18	3	302	CLA	CHD-C1D-ND	-2.74	120.95	124.80
18	8	604	CLA	CHD-C1D-ND	-2.74	120.95	124.80
18	6	309	CLA	CHD-C1D-ND	-2.74	120.95	124.80
18	1	612	CLA	C2C-C1C-NC	2.73	112.85	109.98
18	Z	604	CLA	CHC-C1C-NC	2.73	128.43	124.31
18	5	612	CLA	C1D-ND-C4D	-2.73	104.39	106.31
18	Z	610	CLA	CHC-C1C-C2C	-2.73	119.18	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	802	CLA	C3B-C4B-NB	-2.73	108.09	110.53
18	A	804	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
18	B	809	CLA	CHC-C1C-NC	2.73	128.42	124.31
18	A	845	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
18	3	311	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
18	8	608	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
18	3	305	CLA	CHD-C1D-ND	-2.73	120.96	124.80
18	3	310	CLA	CHC-C1C-NC	2.73	128.42	124.31
18	3	305	CLA	C1D-ND-C4D	-2.73	104.40	106.31
18	8	605	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
18	7	605	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
18	A	827	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
18	B	838	CLA	CHA-C1A-NA	-2.73	120.22	126.39
18	1	611	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
18	7	608	CLA	CHD-C1D-ND	-2.72	120.97	124.80
18	A	840	CLA	CHD-C1D-ND	-2.72	120.97	124.80
18	1	609	CLA	C1D-ND-C4D	-2.72	104.40	106.31
18	3	313	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
18	4	612	CLA	CAA-C2A-C1A	-2.72	105.09	111.81
18	Z	608	CLA	C1D-ND-C4D	-2.72	104.41	106.31
18	A	818	CLA	CHC-C1C-C2C	-2.72	119.23	126.95
18	Z	612	CLA	C2C-C1C-NC	2.72	112.83	109.98
18	6	315	CLA	CHD-C1D-ND	-2.72	120.98	124.80
18	B	825	CLA	CHC-C1C-NC	2.72	128.40	124.31
18	4	603	CLA	C2C-C1C-NC	2.71	112.83	109.98
18	5	614	CLA	CHD-C1D-ND	-2.71	120.98	124.80
18	B	821	CLA	C1D-ND-C4D	-2.71	104.41	106.31
18	A	843	CLA	C2C-C1C-NC	2.71	112.83	109.98
18	1	610	CLA	C2C-C1C-NC	2.71	112.83	109.98
18	6	313	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
18	B	838	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
18	7	612	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
18	F	302	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
18	A	829	CLA	CHC-C1C-NC	2.71	128.39	124.31
18	A	818	CLA	CHD-C1D-ND	-2.71	120.99	124.80
18	3	303	CLA	CHC-C1C-NC	2.71	128.39	124.31
18	5	603	CLA	C1D-ND-C4D	-2.71	104.41	106.31
18	Z	612	CLA	CHD-C1D-ND	-2.71	121.00	124.80
18	A	829	CLA	CHD-C1D-ND	-2.70	121.00	124.80
18	8	613	CLA	CHD-C1D-ND	-2.70	121.00	124.80
18	B	839	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
18	7	604	CLA	CHC-C1C-NC	2.70	128.38	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	101	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
18	3	313	CLA	CHD-C1D-ND	-2.70	121.00	124.80
18	A	838	CLA	C3B-C4B-NB	-2.70	108.12	110.53
18	A	840	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
18	A	811	CLA	CGD-CBD-CAD	-2.70	102.11	110.85
18	1	605	CLA	CHC-C1C-NC	2.70	128.37	124.31
18	A	838	CLA	CHC-C1C-C2C	-2.69	119.29	126.95
18	5	609	CLA	CHD-C1D-ND	-2.69	121.01	124.80
18	8	610	CLA	CHA-C1A-NA	-2.69	120.29	126.39
18	5	604	CLA	CHC-C1C-C2C	-2.69	119.29	126.95
18	F	302	CLA	C2C-C1C-NC	2.69	112.81	109.98
18	8	614	CLA	CHC-C1C-C2C	-2.69	119.29	126.95
21	Z	601	CHL	C3D-C4D-CHA	2.69	112.63	108.54
18	A	832	CLA	CHC-C1C-NC	2.69	128.37	124.31
18	A	808	CLA	CHC-C1C-NC	2.69	128.36	124.31
18	A	815	CLA	CHC-C1C-NC	2.69	128.36	124.31
18	A	817	CLA	CHC-C1C-NC	2.69	128.36	124.31
18	A	845	CLA	CHC-C1C-NC	2.69	128.36	124.31
18	B	815	CLA	CHD-C1D-ND	-2.69	121.02	124.80
18	1	612	CLA	C1D-ND-C4D	-2.69	104.42	106.31
18	Z	609	CLA	C2C-C1C-NC	2.69	112.81	109.98
18	1	602	CLA	CHC-C1C-NC	2.69	128.36	124.31
18	B	828	CLA	CHC-C1C-C2C	-2.68	119.32	126.95
18	6	317	CLA	C2C-C1C-NC	2.68	112.80	109.98
18	A	823	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
18	B	822	CLA	CHC-C1C-NC	2.68	128.35	124.31
18	A	837	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
18	A	813	CLA	CAA-C2A-C1A	-2.68	106.20	112.14
18	A	843	CLA	C1-C2-C3	-2.68	121.80	126.20
18	B	840	CLA	C2C-C1C-NC	2.68	112.80	109.98
21	3	306	CHL	C3D-C4D-CHA	2.68	112.61	108.54
18	A	832	CLA	CHD-C1D-ND	-2.68	121.03	124.80
18	B	817	CLA	CHD-C1D-ND	-2.68	121.03	124.80
18	A	809	CLA	CHC-C1C-NC	2.68	128.34	124.31
18	A	821	CLA	C1D-ND-C4D	-2.68	104.43	106.31
18	7	605	CLA	CAA-C2A-C1A	-2.68	106.22	112.14
18	6	311	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
18	1	613	CLA	CHD-C1D-ND	-2.68	121.04	124.80
18	1	609	CLA	CAA-C2A-C1A	-2.67	106.22	112.14
18	A	818	CLA	CAA-C2A-C1A	-2.67	106.22	112.14
18	A	804	CLA	C2C-C1C-NC	2.67	112.79	109.98
18	A	804	CLA	C1D-ND-C4D	-2.67	104.44	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	602	CLA	CHC-C1C-NC	2.67	128.34	124.31
18	6	312	CLA	CHC-C1C-NC	2.67	128.34	124.31
18	5	603	CLA	CHC-C1C-NC	2.67	128.33	124.31
18	1	605	CLA	CHA-C1A-NA	-2.67	120.34	126.39
21	4	604	CHL	CMA-C3A-C2A	-2.67	103.83	114.13
18	6	314	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
18	B	810	CLA	CHD-C1D-ND	-2.67	121.05	124.80
18	1	614	CLA	CHD-C1D-ND	-2.67	121.05	124.80
18	Z	613	CLA	CHD-C1D-ND	-2.67	121.05	124.80
21	6	307	CHL	C3D-C4D-CHA	2.67	112.59	108.54
18	B	821	CLA	CHD-C1D-ND	-2.66	121.05	124.80
18	B	839	CLA	CHD-C1D-ND	-2.66	121.05	124.80
18	8	602	CLA	CHC-C1C-NC	2.66	128.32	124.31
18	7	601	CLA	CHD-C1D-ND	-2.66	121.06	124.80
18	6	301	CLA	C1D-ND-C4D	-2.66	104.44	106.31
18	3	308	CLA	CHC-C1C-NC	2.66	128.32	124.31
18	6	303	CLA	CHD-C1D-ND	-2.66	121.06	124.80
18	6	310	CLA	CHD-C1D-ND	-2.66	121.06	124.80
18	B	826	CLA	CHC-C1C-NC	2.66	128.31	124.31
18	Z	604	CLA	CHA-C1A-NA	-2.66	120.38	126.39
21	5	616	CHL	C3D-C4D-CHA	2.66	112.58	108.54
18	8	605	CLA	C2C-C1C-NC	2.66	112.77	109.98
18	5	615	CLA	C1D-ND-C4D	-2.66	104.45	106.31
18	A	822	CLA	CHC-C1C-NC	2.65	128.31	124.31
18	Z	608	CLA	CAA-C2A-C1A	-2.65	106.28	112.14
18	3	308	CLA	CHD-C1D-ND	-2.65	121.07	124.80
18	A	833	CLA	CHB-C1B-NB	-2.65	120.08	124.05
18	B	810	CLA	C2C-C1C-NC	2.65	112.76	109.98
18	Z	602	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
18	1	602	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
18	B	820	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
18	B	804	CLA	C3B-C4B-NB	-2.65	108.17	110.53
18	Z	603	CLA	CAA-C2A-C1A	-2.65	106.28	112.14
18	F	302	CLA	CHD-C1D-ND	-2.65	121.08	124.80
18	6	317	CLA	CHC-C1C-NC	2.65	128.30	124.31
18	A	823	CLA	CHC-C1C-NC	2.65	128.30	124.31
18	A	841	CLA	C1D-ND-C4D	-2.65	104.46	106.31
18	A	807	CLA	CHC-C1C-NC	2.64	128.29	124.31
18	B	820	CLA	C1D-ND-C4D	-2.64	104.46	106.31
18	B	818	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
18	1	604	CLA	CAA-C2A-C1A	-2.64	106.29	112.14
18	B	814	CLA	CHC-C1C-NC	2.64	128.29	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	810	CLA	CHC-C1C-NC	2.64	128.29	124.31
18	B	829	CLA	CHD-C1D-ND	-2.64	121.09	124.80
18	A	819	CLA	CHC-C1C-NC	2.64	128.28	124.31
18	Z	606	CLA	CHD-C1D-ND	-2.64	121.09	124.80
18	A	802	CLA	CHC-C1C-C2C	-2.63	119.46	126.95
18	1	610	CLA	C1D-ND-C4D	-2.63	104.46	106.31
18	8	614	CLA	C1D-ND-C4D	-2.63	104.46	106.31
18	4	612	CLA	C3B-C4B-NB	-2.63	108.18	110.53
18	A	802	CLA	C2C-C1C-NC	2.63	112.75	109.98
18	B	808	CLA	CHC-C1C-NC	2.63	128.28	124.31
18	A	835	CLA	CHD-C1D-ND	-2.63	121.10	124.80
18	A	834	CLA	CHD-C1D-ND	-2.63	121.10	124.80
18	B	802	CLA	CHD-C1D-ND	-2.63	121.10	124.80
18	4	601	CLA	CHC-C1C-NC	2.63	128.27	124.31
18	8	601	CLA	C2C-C1C-NC	2.63	112.74	109.98
18	5	610	CLA	CHD-C1D-ND	-2.63	121.10	124.80
18	A	837	CLA	CHD-C1D-ND	-2.63	121.11	124.80
18	B	817	CLA	CHC-C1C-NC	2.62	128.26	124.31
18	A	821	CLA	CHC-C1C-C2C	-2.62	119.49	126.95
18	1	607	CLA	CHD-C1D-ND	-2.62	121.11	124.80
18	8	614	CLA	CHD-C1D-ND	-2.62	121.11	124.80
18	1	608	CLA	CHD-C1D-ND	-2.62	121.11	124.80
18	B	825	CLA	C1D-ND-C4D	-2.62	104.47	106.31
18	7	603	CLA	CHD-C1D-ND	-2.62	121.12	124.80
18	B	831	CLA	CHD-C1D-ND	-2.61	121.12	124.80
18	7	604	CLA	CHB-C1B-NB	-2.61	120.13	124.05
21	4	604	CHL	C3C-C4C-NC	-2.61	108.26	114.65
18	4	611	CLA	CHD-C1D-ND	-2.61	121.13	124.80
18	1	611	CLA	CHD-C1D-ND	-2.61	121.13	124.80
18	Z	603	CLA	CHD-C1D-ND	-2.61	121.13	124.80
18	1	608	CLA	CHA-C1A-NA	-2.61	120.48	126.39
18	3	312	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
18	A	834	CLA	C1D-ND-C4D	-2.61	104.48	106.31
18	B	819	CLA	CHC-C1C-NC	2.61	128.24	124.31
18	8	607	CLA	CHA-C1A-NA	-2.61	120.49	126.39
18	Z	607	CLA	CHA-C1A-NA	-2.61	120.49	126.39
18	5	611	CLA	C2C-C1C-NC	2.60	112.72	109.98
18	A	839	CLA	CHC-C1C-NC	2.60	128.23	124.31
18	6	302	CLA	C2C-C1C-NC	2.60	112.72	109.98
18	5	611	CLA	CHC-C1C-NC	2.60	128.23	124.31
18	Z	607	CLA	CHD-C1D-ND	-2.60	121.14	124.80
18	B	809	CLA	C2C-C1C-NC	2.60	112.72	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	838	CLA	CHD-C1D-ND	-2.60	121.14	124.80
18	A	818	CLA	CHC-C1C-NC	2.60	128.23	124.31
18	8	613	CLA	C2C-C1C-NC	2.60	112.71	109.98
18	A	811	CLA	C1D-ND-C4D	-2.60	104.49	106.31
18	8	613	CLA	CHC-C1C-NC	2.60	128.23	124.31
18	Z	608	CLA	CHD-C1D-ND	-2.60	121.14	124.80
18	Z	611	CLA	C1D-ND-C4D	-2.60	104.49	106.31
18	B	824	CLA	CHC-C1C-NC	2.60	128.23	124.31
18	3	309	CLA	CAA-C2A-C1A	-2.60	105.39	111.81
18	B	812	CLA	CHD-C1D-ND	-2.60	121.14	124.80
18	A	831	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
18	F	301	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
18	B	830	CLA	CHC-C1C-NC	2.60	128.22	124.31
18	5	613	CLA	CHC-C1C-NC	2.60	128.22	124.31
18	7	602	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
18	1	609	CLA	CHD-C1D-ND	-2.60	121.15	124.80
18	7	608	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
18	B	821	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
18	8	603	CLA	CHC-C1C-NC	2.59	128.22	124.31
18	1	612	CLA	CHD-C1D-ND	-2.59	121.15	124.80
18	B	829	CLA	C1D-ND-C4D	-2.59	104.49	106.31
18	7	605	CLA	CHD-C1D-ND	-2.59	121.16	124.80
18	7	613	CLA	C2C-C1C-NC	2.59	112.70	109.98
19	A	842	PQN	C11-C3-C2	-2.59	120.45	124.89
18	7	607	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
18	1	604	CLA	CHD-C1D-ND	-2.59	121.16	124.80
18	B	838	CLA	CHC-C1C-NC	2.59	128.21	124.31
18	B	812	CLA	C3A-C2A-C1A	-2.59	97.46	101.34
18	8	612	CLA	CHD-C1D-ND	-2.59	121.16	124.80
18	7	604	CLA	CGD-CBD-CAD	-2.59	102.47	110.85
18	Z	610	CLA	CHD-C1D-ND	-2.59	121.16	124.80
18	B	836	CLA	CHD-C1D-ND	-2.59	121.16	124.80
18	8	602	CLA	C2C-C1C-NC	2.58	112.70	109.98
18	B	814	CLA	CHC-C1C-C2C	-2.58	119.60	126.95
18	3	303	CLA	CHD-C1D-ND	-2.58	121.17	124.80
18	4	603	CLA	CHC-C1C-NC	2.58	128.20	124.31
18	A	806	CLA	CHD-C1D-ND	-2.58	121.17	124.80
18	B	825	CLA	CHD-C1D-ND	-2.58	121.17	124.80
18	7	605	CLA	C1D-ND-C4D	-2.58	104.50	106.31
18	B	804	CLA	CHA-C1A-NA	-2.58	120.54	126.39
18	F	301	CLA	C3B-C4B-NB	-2.58	108.23	110.53
18	B	841	CLA	CHC-C1C-C2C	-2.58	119.61	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	304	CLA	CHA-C1A-NA	-2.58	120.55	126.39
18	B	830	CLA	CHD-C1D-ND	-2.58	121.17	124.80
18	8	611	CLA	CHC-C1C-NC	2.58	128.20	124.31
18	A	808	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
18	A	845	CLA	C1D-ND-C4D	-2.58	104.50	106.31
18	7	612	CLA	CHC-C1C-NC	2.58	128.19	124.31
18	4	609	CLA	CHC-C1C-C2C	-2.58	119.63	126.95
18	Z	609	CLA	CHD-C1D-ND	-2.58	121.18	124.80
18	6	310	CLA	CHA-C1A-NA	-2.58	120.56	126.39
18	A	838	CLA	C2C-C1C-NC	2.58	112.69	109.98
18	B	820	CLA	C2C-C1C-NC	2.58	112.69	109.98
18	8	601	CLA	CHD-C1D-ND	-2.57	121.18	124.80
18	A	822	CLA	C1D-ND-C4D	-2.57	104.51	106.31
18	B	840	CLA	CHC-C1C-NC	2.57	128.19	124.31
18	7	608	CLA	CHC-C1C-NC	2.57	128.19	124.31
18	8	608	CLA	CAA-C2A-C1A	-2.57	106.45	112.14
18	5	601	CLA	CHC-C1C-NC	2.57	128.19	124.31
21	4	605	CHL	C3D-C4D-CHA	2.57	112.45	108.54
18	A	845	CLA	CHD-C1D-ND	-2.57	121.19	124.80
18	A	844	CLA	CHC-C1C-NC	2.57	128.18	124.31
18	1	610	CLA	CHC-C1C-C2C	-2.57	119.65	126.95
21	6	306	CHL	CMA-C3A-C4A	-2.57	109.08	114.61
18	B	801	CLA	CHC-C1C-C2C	-2.57	119.65	126.95
18	A	839	CLA	CHA-C1A-NA	-2.57	120.58	126.39
18	4	611	CLA	CHC-C1C-NC	2.57	128.18	124.31
18	B	827	CLA	CHC-C1C-C2C	-2.57	119.65	126.95
18	7	604	CLA	C2C-C1C-NC	2.57	112.68	109.98
18	B	833	CLA	CHC-C1C-NC	2.57	128.18	124.31
18	A	819	CLA	CHC-C1C-C2C	-2.57	119.66	126.95
18	A	811	CLA	CHD-C1D-ND	-2.57	121.19	124.80
18	5	602	CLA	CHC-C1C-C2C	-2.57	119.66	126.95
21	6	306	CHL	CAA-C2A-C1A	2.56	118.43	113.35
18	1	612	CLA	CHC-C1C-NC	2.56	128.17	124.31
18	A	837	CLA	C2C-C1C-NC	2.56	112.67	109.98
18	A	806	CLA	CHC-C1C-NC	2.56	128.17	124.31
18	A	828	CLA	C2C-C1C-NC	2.56	112.67	109.98
18	B	826	CLA	C2C-C1C-NC	2.56	112.67	109.98
18	Z	609	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
18	Z	611	CLA	CHC-C1C-NC	2.56	128.16	124.31
18	B	826	CLA	CHD-C1D-ND	-2.56	121.21	124.80
18	3	302	CLA	CHC-C1C-NC	2.56	128.16	124.31
18	B	837	CLA	CHC-C1C-C2C	-2.55	119.70	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	314	CLA	C2C-C1C-NC	2.55	112.66	109.98
18	1	610	CLA	CHD-C1D-ND	-2.55	121.21	124.80
18	3	311	CLA	CHA-C1A-NA	-2.55	120.62	126.39
18	6	315	CLA	CHC-C1C-C2C	-2.55	119.70	126.95
18	3	303	CLA	C2C-C1C-NC	2.55	112.66	109.98
18	6	314	CLA	C1D-ND-C4D	-2.55	104.52	106.31
18	B	819	CLA	CHC-C1C-C2C	-2.55	119.71	126.95
18	B	811	CLA	C2C-C1C-NC	2.54	112.65	109.98
18	8	611	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
18	5	601	CLA	C1D-ND-C4D	-2.54	104.53	106.31
18	A	817	CLA	CGD-CBD-CAD	-2.54	102.62	110.85
18	A	824	CLA	C1D-ND-C4D	-2.54	104.53	106.31
18	B	837	CLA	C1D-ND-C4D	-2.54	104.53	106.31
18	Z	613	CLA	CHA-C1A-NA	-2.54	120.64	126.39
18	8	614	CLA	CHC-C1C-NC	2.54	128.14	124.31
18	A	844	CLA	CHA-C1A-NA	-2.54	120.64	126.39
18	7	607	CLA	CHD-C1D-ND	-2.54	121.23	124.80
18	8	607	CLA	CHD-C1D-ND	-2.54	121.23	124.80
18	A	835	CLA	CHC-C1C-C2C	-2.54	119.73	126.95
18	1	614	CLA	CHA-C1A-NA	-2.54	120.64	126.39
18	B	820	CLA	CHA-C1A-NA	-2.54	120.65	126.39
18	8	609	CLA	CHC-C1C-C2C	-2.54	119.74	126.95
18	A	841	CLA	CAA-C2A-C1A	-2.54	106.53	112.14
18	6	304	CLA	CHD-C1D-ND	-2.53	121.23	124.80
18	B	811	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
18	Z	610	CLA	CHC-C1C-NC	2.53	128.13	124.31
18	6	302	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
18	B	805	CLA	CHC-C1C-NC	2.53	128.13	124.31
18	Z	611	CLA	CHD-C1D-ND	-2.53	121.24	124.80
18	6	317	CLA	CHD-C1D-ND	-2.53	121.24	124.80
18	A	813	CLA	CHD-C1D-ND	-2.53	121.24	124.80
18	3	314	CLA	CHD-C1D-ND	-2.53	121.25	124.80
18	6	314	CLA	CHD-C1D-ND	-2.53	121.25	124.80
18	6	311	CLA	CHC-C1C-NC	2.53	128.12	124.31
18	6	308	CLA	CHC-C1C-C2C	-2.53	119.77	126.95
18	A	834	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
18	1	603	CLA	CHC-C1C-NC	2.52	128.11	124.31
18	5	608	CLA	CHD-C1D-ND	-2.52	121.25	124.80
18	B	809	CLA	CAA-C2A-C1A	-2.52	106.56	112.14
18	A	828	CLA	CHA-C1A-NA	-2.52	120.68	126.39
18	7	612	CLA	CHD-C1D-ND	-2.52	121.26	124.80
18	8	608	CLA	CHC-C1C-NC	2.52	128.10	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	828	CLA	CHC-C1C-NC	2.52	128.10	124.31
18	3	312	CLA	CHC-C1C-NC	2.52	128.10	124.31
18	1	611	CLA	CHC-C1C-NC	2.51	128.10	124.31
18	B	806	CLA	C1D-ND-C4D	-2.51	104.55	106.31
18	8	610	CLA	C3A-C2A-C1A	-2.51	97.57	101.34
18	5	614	CLA	C1D-ND-C4D	-2.51	104.55	106.31
18	8	615	CLA	CHC-C1C-NC	2.51	128.09	124.31
18	3	304	CLA	CHD-C1D-ND	-2.51	121.28	124.80
18	8	603	CLA	C2C-C1C-NC	2.50	112.61	109.98
18	A	826	CLA	CHC-C1C-NC	2.50	128.08	124.31
18	8	612	CLA	CHC-C1C-NC	2.50	128.08	124.31
18	B	833	CLA	CHA-C1A-NA	-2.50	120.72	126.39
18	A	833	CLA	CHD-C1D-ND	-2.50	121.28	124.80
18	8	605	CLA	C1D-ND-C4D	-2.50	104.56	106.31
18	4	609	CLA	CHC-C1C-NC	2.50	128.08	124.31
18	A	823	CLA	C3A-C2A-C1A	-2.50	97.59	101.34
18	5	603	CLA	CHA-C1A-NA	-2.50	120.73	126.39
18	A	840	CLA	C2C-C1C-NC	2.50	112.61	109.98
18	B	836	CLA	CHC-C1C-C2C	-2.50	119.85	126.95
18	B	839	CLA	C2C-C1C-NC	2.50	112.60	109.98
18	8	609	CLA	CAA-C2A-C1A	-2.49	106.62	112.14
18	A	807	CLA	CAA-C2A-C1A	-2.49	106.62	112.14
18	5	612	CLA	CHC-C1C-NC	2.49	128.07	124.31
18	5	614	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
18	1	607	CLA	CHC-C1C-NC	2.49	128.06	124.31
18	B	837	CLA	CHD-C1D-ND	-2.49	121.30	124.80
18	1	604	CLA	CHA-C1A-NA	-2.49	120.76	126.39
18	A	810	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
21	5	606	CHL	C3D-C4D-CHA	2.49	112.32	108.54
18	1	611	CLA	C2C-C1C-NC	2.49	112.59	109.98
18	3	301	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
18	5	609	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
18	5	604	CLA	CHC-C1C-NC	2.48	128.05	124.31
18	A	839	CLA	C1D-ND-C4D	-2.48	104.57	106.31
18	3	313	CLA	CHC-C1C-NC	2.48	128.05	124.31
18	Z	606	CLA	CAA-C2A-C1A	-2.48	106.65	112.14
18	7	603	CLA	CHC-C1C-NC	2.48	128.05	124.31
18	B	812	CLA	CHC-C1C-C2C	-2.48	119.90	126.95
18	3	313	CLA	C2C-C1C-NC	2.48	112.59	109.98
18	B	813	CLA	CHB-C1B-NB	-2.48	120.33	124.05
18	B	841	CLA	CHC-C1C-NC	2.48	128.05	124.31
18	7	614	CLA	CHC-C1C-C2C	-2.48	119.90	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	603	CLA	CHA-C1A-NA	-2.48	120.78	126.39
18	B	804	CLA	CHC-C1C-NC	2.48	128.04	124.31
18	B	843	CLA	CHC-C1C-NC	2.48	128.04	124.31
18	4	608	CLA	CHA-C1A-NA	-2.48	120.78	126.39
18	B	813	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
18	Z	610	CLA	C2C-C1C-NC	2.47	112.58	109.98
18	7	608	CLA	CHB-C1B-NB	-2.47	120.34	124.05
18	6	301	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
18	7	604	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	1	603	CLA	CHA-C1A-NA	-2.47	120.80	126.39
18	B	827	CLA	CHC-C1C-NC	2.47	128.03	124.31
18	B	821	CLA	CAA-C2A-C1A	-2.47	106.67	112.14
18	4	601	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
18	B	814	CLA	CHA-C1A-NA	-2.47	120.80	126.39
18	B	825	CLA	C2C-C1C-NC	2.47	112.58	109.98
18	3	303	CLA	C1D-ND-C4D	-2.47	104.58	106.31
18	7	609	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
18	8	615	CLA	CHA-C1A-NA	-2.47	120.81	126.39
21	6	305	CHL	C3D-C4D-CHA	2.47	112.29	108.54
18	1	607	CLA	CAA-C2A-C1A	-2.47	106.68	112.14
18	8	614	CLA	C2C-C1C-NC	2.46	112.57	109.98
18	4	612	CLA	CHC-C1C-NC	2.46	128.01	124.31
18	A	821	CLA	CHD-C1D-ND	-2.46	121.34	124.80
18	4	608	CLA	CHD-C1D-ND	-2.46	121.34	124.80
18	8	609	CLA	CHB-C1B-NB	-2.46	120.36	124.05
18	A	820	CLA	C3B-C4B-NB	-2.46	108.34	110.53
18	5	614	CLA	C2C-C1C-NC	2.46	112.56	109.98
18	A	820	CLA	C4B-CHC-C1C	-2.46	120.47	126.25
18	A	843	CLA	CHD-C1D-ND	-2.46	121.35	124.80
18	A	831	CLA	CHC-C1C-NC	2.46	128.01	124.31
18	3	304	CLA	CHC-C1C-NC	2.46	128.01	124.31
18	B	828	CLA	C2C-C1C-NC	2.46	112.56	109.98
18	A	804	CLA	CHC-C1C-NC	2.45	128.01	124.31
18	B	818	CLA	CHC-C1C-NC	2.45	128.01	124.31
18	6	310	CLA	C4B-CHC-C1C	-2.45	120.48	126.25
18	8	604	CLA	CHC-C1C-C2C	-2.45	119.98	126.95
18	Z	606	CLA	CHC-C1C-NC	2.45	128.00	124.31
18	A	841	CLA	CHD-C1D-ND	-2.45	121.36	124.80
18	B	840	CLA	CHD-C1D-ND	-2.45	121.36	124.80
18	5	605	CLA	CHC-C1C-NC	2.45	128.00	124.31
18	B	833	CLA	C2C-C1C-NC	2.45	112.55	109.98
18	B	833	CLA	CHD-C1D-ND	-2.45	121.36	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	824	CLA	CHC-C1C-NC	2.44	127.99	124.31
21	4	605	CHL	CMA-C3A-C4A	2.44	119.88	114.61
18	A	843	CLA	C1D-ND-C4D	-2.44	104.60	106.31
18	A	838	CLA	CHC-C1C-NC	2.44	127.99	124.31
18	1	608	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
18	B	838	CLA	C2C-C1C-NC	2.44	112.55	109.98
18	3	305	CLA	CGD-CBD-CAD	-2.44	102.95	110.85
18	5	612	CLA	CHD-C1D-ND	-2.44	121.37	124.80
18	5	605	CLA	CHA-C1A-NA	-2.44	120.87	126.39
18	B	831	CLA	CHC-C1C-C2C	-2.44	120.02	126.95
18	B	841	CLA	C3A-C2A-C1A	-2.44	97.69	101.34
18	A	844	CLA	CHD-C1D-ND	-2.44	121.37	124.80
18	A	823	CLA	CHA-C1A-NA	-2.44	120.87	126.39
18	1	610	CLA	C3B-C4B-NB	-2.44	108.35	110.53
18	3	305	CLA	CHC-C1C-C2C	-2.44	120.02	126.95
18	B	812	CLA	C2A-C3A-C4A	-2.44	97.93	101.87
18	1	608	CLA	CHC-C1C-NC	2.44	127.98	124.31
18	A	821	CLA	CHC-C1C-NC	2.43	127.98	124.31
18	A	828	CLA	CHD-C1D-ND	-2.43	121.38	124.80
18	A	837	CLA	C1D-ND-C4D	-2.43	104.61	106.31
18	6	312	CLA	CHD-C1D-ND	-2.43	121.38	124.80
18	A	811	CLA	CHC-C1C-C2C	-2.43	120.04	126.95
18	5	613	CLA	C2C-C1C-NC	2.43	112.54	109.98
18	5	617	CLA	CHC-C1C-C2C	-2.43	120.04	126.95
18	A	804	CLA	CHA-C1A-NA	-2.43	120.89	126.39
18	B	824	CLA	CHC-C1C-C2C	-2.43	120.04	126.95
18	7	610	CLA	CHC-C1C-C2C	-2.43	120.04	126.95
18	A	817	CLA	CHA-C1A-NA	-2.43	120.89	126.39
18	8	614	CLA	CHA-C1A-NA	-2.43	120.89	126.39
18	A	826	CLA	CHC-C1C-C2C	-2.43	120.04	126.95
18	7	602	CLA	C2C-C1C-NC	2.43	112.53	109.98
18	8	609	CLA	CHC-C1C-NC	2.43	127.97	124.31
18	Z	607	CLA	CHC-C1C-C2C	-2.43	120.05	126.95
18	B	842	CLA	CHC-C1C-NC	2.43	127.96	124.31
18	A	821	CLA	CHA-C1A-NA	-2.43	120.90	126.39
18	A	834	CLA	CHA-C1A-NA	-2.43	120.90	126.39
18	Z	613	CLA	C2C-C1C-NC	2.42	112.53	109.98
18	B	805	CLA	CHC-C1C-C2C	-2.42	120.06	126.95
18	A	833	CLA	CHA-C1A-NA	-2.42	120.91	126.39
18	5	615	CLA	CAA-C2A-C1A	-2.42	104.04	111.97
18	B	824	CLA	CHB-C1B-NB	-2.42	120.42	124.05
18	8	612	CLA	CHA-C1A-NA	-2.42	120.91	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	607	CLA	C2A-C3A-C4A	-2.42	97.96	101.87
18	3	307	CLA	CHC-C1C-NC	2.42	127.95	124.31
18	B	827	CLA	CGD-CBD-CAD	-2.42	103.02	110.85
18	1	604	CLA	CHC-C1C-NC	2.42	127.95	124.31
18	B	843	CLA	CHA-C1A-NA	-2.42	120.92	126.39
18	B	839	CLA	CHC-C1C-NC	2.41	127.95	124.31
18	A	827	CLA	C2A-C1A-CHA	2.41	128.06	123.87
18	A	840	CLA	CHC-C1C-NC	2.41	127.95	124.31
18	Z	609	CLA	C3B-C4B-NB	-2.41	108.38	110.53
18	B	821	CLA	CHC-C1C-NC	2.41	127.94	124.31
21	5	616	CHL	C3C-C4C-NC	-2.41	108.75	114.65
21	5	606	CHL	CMA-C3A-C4A	-2.41	109.42	114.61
18	A	821	CLA	C2C-C1C-NC	2.41	112.51	109.98
18	B	808	CLA	C1D-ND-C4D	-2.41	104.62	106.31
18	7	604	CLA	C1D-ND-C4D	-2.41	104.62	106.31
18	5	608	CLA	CHC-C1C-C2C	-2.41	120.10	126.95
18	1	608	CLA	C2A-C3A-C4A	-2.41	97.98	101.87
18	Z	607	CLA	CHC-C1C-NC	2.41	127.94	124.31
18	A	839	CLA	CHD-C1D-ND	-2.41	121.42	124.80
18	B	837	CLA	CHC-C1C-NC	2.41	127.94	124.31
18	3	305	CLA	CHC-C1C-NC	2.41	127.94	124.31
18	3	307	CLA	CHC-C1C-C2C	-2.40	120.12	126.95
18	3	309	CLA	C1D-ND-C4D	-2.40	104.63	106.31
18	B	808	CLA	CHA-C1A-NA	-2.40	120.95	126.39
18	F	302	CLA	CHC-C1C-NC	2.40	127.92	124.31
18	Z	603	CLA	CHC-C1C-NC	2.40	127.92	124.31
18	A	822	CLA	CHA-C1A-NA	-2.40	120.96	126.39
18	1	614	CLA	C2C-C1C-NC	2.40	112.50	109.98
18	3	310	CLA	C2C-C1C-NC	2.39	112.50	109.98
18	5	608	CLA	CHC-C1C-NC	2.39	127.92	124.31
21	7	606	CHL	C3D-C4D-CHA	2.39	112.17	108.54
18	3	309	CLA	CHC-C1C-C2C	-2.39	120.16	126.95
18	A	806	CLA	C2C-C1C-NC	2.39	112.49	109.98
18	3	305	CLA	C2A-C1A-CHA	2.39	128.01	123.87
18	A	804	CLA	CHD-C1D-ND	-2.39	121.44	124.80
18	B	813	CLA	CHC-C1C-NC	2.39	127.91	124.31
18	A	809	CLA	C2C-C1C-NC	2.39	112.49	109.98
18	8	602	CLA	CHB-C1B-NB	-2.39	120.47	124.05
18	A	802	CLA	CAA-C2A-C1A	-2.38	106.86	112.14
18	F	301	CLA	CHC-C1C-NC	2.38	127.90	124.31
18	B	801	CLA	CHC-C1C-NC	2.38	127.90	124.31
18	7	602	CLA	CHC-C1C-NC	2.38	127.89	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	827	CLA	CHA-C1A-NA	-2.38	121.00	126.39
18	B	815	CLA	CHC-C1C-C2C	-2.38	120.19	126.95
18	8	608	CLA	C2C-C1C-NC	2.38	112.48	109.98
18	A	835	CLA	CHC-C1C-NC	2.38	127.89	124.31
18	B	826	CLA	CHA-C1A-NA	-2.37	121.01	126.39
18	B	820	CLA	CHC-C1C-NC	2.37	127.89	124.31
18	B	829	CLA	CHC-C1C-C2C	-2.37	120.20	126.95
18	A	805	CLA	CAA-C2A-C1A	-2.37	106.89	112.14
18	Z	602	CLA	CHB-C1B-NB	-2.37	120.49	124.05
18	A	806	CLA	CAA-C2A-C1A	-2.37	106.89	112.14
18	5	602	CLA	CHC-C1C-NC	2.37	127.88	124.31
18	A	822	CLA	C2C-C1C-NC	2.37	112.47	109.98
18	A	809	CLA	CHD-C1D-ND	-2.37	121.47	124.80
21	8	606	CHL	C3C-C4C-NC	-2.37	108.86	114.65
18	3	309	CLA	CHA-C1A-NA	-2.37	121.03	126.39
18	A	832	CLA	C2C-C1C-NC	2.37	112.47	109.98
18	3	311	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	8	610	CLA	CHC-C1C-C2C	-2.36	120.23	126.95
18	B	830	CLA	C3B-C4B-NB	-2.36	108.42	110.53
18	A	837	CLA	CHC-C1C-NC	2.36	127.87	124.31
18	6	308	CLA	CHC-C1C-NC	2.36	127.87	124.31
18	F	302	CLA	C3B-C4B-NB	-2.36	108.42	110.53
18	B	823	CLA	C3D-C4D-ND	2.36	113.83	109.99
18	A	815	CLA	CHB-C1B-NB	-2.36	120.51	124.05
18	7	610	CLA	C1D-ND-C4D	-2.36	104.66	106.31
18	5	609	CLA	C2C-C1C-NC	2.36	112.46	109.98
21	6	307	CHL	CAA-C2A-C1A	2.36	118.02	113.35
18	A	834	CLA	C3B-C4B-NB	-2.36	108.43	110.53
18	5	608	CLA	CHB-C1B-NB	-2.36	120.52	124.05
18	B	829	CLA	CHC-C1C-NC	2.35	127.86	124.31
18	7	610	CLA	CHA-C1A-NA	-2.35	121.06	126.39
18	8	610	CLA	C2B-C1B-NB	-2.35	107.89	110.33
21	7	606	CHL	C3C-C4C-NC	-2.35	108.90	114.65
18	B	815	CLA	CHC-C1C-NC	2.35	127.85	124.31
18	A	823	CLA	O2A-C1-C2	2.35	117.15	108.11
18	5	604	CLA	CAA-C2A-C1A	-2.35	106.94	112.14
18	A	827	CLA	CHB-C1B-NB	-2.35	120.53	124.05
18	B	801	CLA	C2C-C1C-NC	2.35	112.45	109.98
18	4	607	CLA	CHA-C1A-NA	-2.35	121.08	126.39
18	B	840	CLA	C1D-ND-C4D	-2.34	104.67	106.31
18	A	834	CLA	CHC-C1C-NC	2.34	127.84	124.31
18	B	818	CLA	C2C-C1C-NC	2.34	112.44	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	840	CLA	CHA-C1A-NA	-2.34	121.09	126.39
18	7	601	CLA	CHB-C1B-NB	-2.34	120.54	124.05
18	5	605	CLA	CHD-C1D-ND	-2.34	121.51	124.80
21	4	604	CHL	C3D-C4D-CHA	2.34	112.10	108.54
21	5	606	CHL	C3C-C4C-NC	-2.34	108.93	114.65
18	3	311	CLA	C1D-ND-C4D	-2.34	104.67	106.31
18	3	309	CLA	CHC-C1C-NC	2.34	127.83	124.31
18	6	309	CLA	CHC-C1C-C2C	-2.33	120.31	126.95
18	A	822	CLA	CHD-C1D-ND	-2.33	121.52	124.80
18	5	617	CLA	CHC-C1C-NC	2.33	127.83	124.31
18	8	615	CLA	CHD-C1D-ND	-2.33	121.52	124.80
18	5	601	CLA	CHB-C1B-NB	-2.33	120.55	124.05
18	A	820	CLA	CHA-C1A-NA	-2.33	121.11	126.39
18	A	824	CLA	CHA-C1A-NA	-2.33	121.11	126.39
18	3	314	CLA	CHA-C1A-NA	-2.33	121.11	126.39
18	A	843	CLA	CHC-C1C-NC	2.33	127.82	124.31
18	A	821	CLA	CHB-C1B-NB	-2.33	120.56	124.05
18	8	610	CLA	CHB-C1B-NB	-2.33	120.56	124.05
18	B	835	CLA	C3A-C2A-C1A	-2.33	97.86	101.34
18	B	804	CLA	CHC-C1C-C2C	-2.33	120.34	126.95
18	8	604	CLA	CHC-C1C-NC	2.33	127.81	124.31
18	A	803	CLA	C3D-C4D-ND	2.32	113.76	109.99
18	8	605	CLA	CHA-C1A-NA	-2.32	121.13	126.39
18	8	605	CLA	CHD-C1D-ND	-2.32	121.53	124.80
18	B	836	CLA	CHC-C1C-NC	2.32	127.81	124.31
18	1	603	CLA	CHD-C1D-ND	-2.32	121.54	124.80
18	B	807	CLA	CHC-C1C-C2C	-2.32	120.36	126.95
18	A	831	CLA	C2C-C1C-NC	2.32	112.42	109.98
18	A	809	CLA	CHA-C1A-NA	-2.32	121.14	126.39
18	6	312	CLA	C2C-C1C-NC	2.32	112.42	109.98
18	B	834	CLA	C2C-C1C-CHC	-2.32	118.78	125.05
18	1	602	CLA	CHB-C1B-NB	-2.32	120.57	124.05
18	3	305	CLA	CHA-C1A-NA	-2.32	121.15	126.39
18	7	605	CLA	CHC-C1C-NC	2.32	127.80	124.31
18	3	308	CLA	CHB-C1B-NB	-2.32	120.58	124.05
18	4	612	CLA	CHB-C1B-NB	-2.32	120.58	124.05
18	5	602	CLA	C2C-C1C-NC	2.31	112.41	109.98
18	6	301	CLA	CHB-C1B-NB	-2.31	120.58	124.05
18	A	818	CLA	CHB-C1B-NB	-2.31	120.58	124.05
18	B	826	CLA	CHB-C1B-NB	-2.31	120.58	124.05
18	6	311	CLA	C2C-C1C-NC	2.31	112.41	109.98
18	5	615	CLA	CHA-C1A-NA	-2.31	121.16	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	303	CLA	CHA-C1A-NA	-2.31	121.16	126.39
18	B	802	CLA	C1D-ND-C4D	-2.31	104.69	106.31
18	5	613	CLA	CHA-C1A-NA	-2.31	121.16	126.39
18	5	612	CLA	C3B-C4B-NB	-2.31	108.47	110.53
18	5	604	CLA	C2C-C1C-NC	2.31	112.41	109.98
18	B	812	CLA	CHC-C1C-NC	2.31	127.79	124.31
18	B	811	CLA	CHA-C1A-NA	-2.31	121.16	126.39
18	B	802	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
18	A	802	CLA	CHC-C1C-NC	2.31	127.79	124.31
18	A	828	CLA	C3B-C4B-NB	-2.31	108.47	110.53
21	6	305	CHL	C3C-C4C-NC	-2.31	109.02	114.65
18	A	811	CLA	CHC-C1C-NC	2.30	127.78	124.31
18	F	301	CLA	C2C-C1C-NC	2.30	112.40	109.98
18	B	841	CLA	CBA-CAA-C2A	2.30	118.30	113.41
18	3	301	CLA	CHC-C1C-NC	2.30	127.78	124.31
18	A	825	CLA	C2C-C1C-NC	2.30	112.40	109.98
18	A	831	CLA	C3D-C4D-ND	2.30	113.72	109.99
18	A	810	CLA	CAA-C2A-C1A	-2.30	107.06	112.14
18	7	611	CLA	CHB-C1B-NB	-2.30	120.61	124.05
18	5	615	CLA	C2A-C1A-CHA	2.30	127.85	123.87
18	7	607	CLA	CHC-C1C-NC	2.30	127.77	124.31
18	B	833	CLA	CHB-C1B-NB	-2.30	120.61	124.05
21	5	607	CHL	CMA-C3A-C4A	-2.29	109.67	114.61
18	4	607	CLA	C1D-CHD-C4C	-2.29	121.14	126.02
18	B	831	CLA	CHC-C1C-NC	2.29	127.77	124.31
18	B	807	CLA	CGD-CBD-CAD	-2.29	103.43	110.85
18	8	605	CLA	CHC-C1C-NC	2.29	127.76	124.31
18	3	308	CLA	CAA-C2A-C1A	-2.29	107.07	112.14
18	F	302	CLA	CHB-C1B-NB	-2.29	120.61	124.05
18	6	315	CLA	CHC-C1C-NC	2.29	127.76	124.31
18	5	612	CLA	C2C-C1C-NC	2.29	112.39	109.98
18	8	607	CLA	CHB-C1B-NB	-2.29	120.62	124.05
21	6	316	CHL	C3D-C4D-CHA	2.29	112.02	108.54
18	B	825	CLA	CHA-C1A-NA	-2.29	121.22	126.39
18	A	834	CLA	CGD-CBD-CAD	-2.29	103.45	110.85
18	7	607	CLA	C2C-C1C-NC	2.29	112.38	109.98
18	B	811	CLA	C1D-ND-C4D	-2.28	104.71	106.31
18	6	303	CLA	CHB-C1B-NB	-2.28	120.62	124.05
18	8	610	CLA	CHC-C1C-NC	2.28	127.75	124.31
18	7	609	CLA	CHB-C1B-NB	-2.28	120.63	124.05
18	B	832	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
18	3	308	CLA	C2C-C1C-NC	2.28	112.38	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	605	CHL	C3C-C4C-NC	-2.28	109.08	114.65
18	A	813	CLA	C1D-ND-C4D	-2.28	104.71	106.31
18	3	301	CLA	C3D-C4D-ND	2.28	113.69	109.99
18	5	610	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
18	A	818	CLA	CHA-C1A-NA	-2.28	121.23	126.39
18	A	823	CLA	C2C-C1C-NC	2.28	112.37	109.98
18	6	314	CLA	CHC-C1C-NC	2.28	127.74	124.31
18	4	608	CLA	C2A-C3A-C4A	-2.28	98.19	101.87
18	B	810	CLA	CHB-C1B-NB	-2.28	120.64	124.05
18	4	610	CLA	CHC-C1C-C2C	-2.27	120.48	126.95
18	B	828	CLA	CHB-C1B-NB	-2.27	120.64	124.05
18	B	806	CLA	CGD-CBD-CAD	-2.27	103.48	110.85
18	A	832	CLA	CHA-C1A-NA	-2.27	121.24	126.39
18	7	601	CLA	CGD-CBD-CAD	-2.27	103.48	110.85
18	B	802	CLA	CHA-C1A-NA	-2.27	121.24	126.39
18	A	817	CLA	CHB-C1B-NB	-2.27	120.64	124.05
18	6	317	CLA	CHB-C1B-NB	-2.27	120.64	124.05
18	A	820	CLA	C2C-C1C-NC	2.27	112.37	109.98
18	Z	604	CLA	C1D-ND-C4D	-2.27	104.72	106.31
18	7	609	CLA	CGD-CBD-CAD	-2.27	103.49	110.85
18	Z	607	CLA	C2A-C1A-CHA	2.27	127.81	123.87
18	B	825	CLA	CHB-C1B-NB	-2.27	120.64	124.05
18	8	614	CLA	C3A-C2A-C1A	-2.27	97.94	101.34
18	7	614	CLA	CHC-C1C-NC	2.27	127.72	124.31
18	B	821	CLA	CHB-C1B-NB	-2.27	120.65	124.05
18	4	611	CLA	CHB-C1B-NB	-2.26	120.65	124.05
18	B	808	CLA	CHD-C1D-ND	-2.26	121.62	124.80
18	A	835	CLA	C2C-C1C-NC	2.26	112.36	109.98
18	7	609	CLA	CHC-C1C-NC	2.26	127.72	124.31
18	A	844	CLA	CHB-C1B-NB	-2.26	120.66	124.05
18	A	802	CLA	CHA-C1A-NA	-2.26	121.28	126.39
18	8	604	CLA	CHA-C1A-NA	-2.26	121.28	126.39
18	4	612	CLA	CHA-C1A-NA	-2.26	121.28	126.39
18	6	301	CLA	CHC-C1C-NC	2.26	127.71	124.31
18	B	822	CLA	C2C-C1C-NC	2.26	112.35	109.98
21	6	307	CHL	C3C-C4C-NC	-2.26	109.14	114.65
21	5	607	CHL	C3C-C4C-NC	-2.25	109.14	114.65
18	B	818	CLA	CAA-C2A-C1A	-2.25	107.15	112.14
18	B	811	CLA	CHD-C1D-ND	-2.25	121.63	124.80
18	5	614	CLA	CHA-C1A-NA	-2.25	121.29	126.39
18	1	605	CLA	C1D-ND-C4D	-2.25	104.73	106.31
21	3	306	CHL	CMA-C3A-C4A	-2.25	109.76	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	601	CLA	CHD-C1D-ND	-2.25	121.63	124.80
18	A	830	CLA	CHA-C1A-NA	-2.25	121.29	126.39
18	4	608	CLA	CHC-C1C-C2C	-2.25	120.55	126.95
18	1	608	CLA	C2A-C1A-CHA	2.25	127.77	123.87
18	A	816	CLA	CHB-C1B-NB	-2.25	120.68	124.05
18	B	814	CLA	CHB-C1B-NB	-2.25	120.68	124.05
18	4	602	CLA	CAA-C2A-C1A	-2.24	107.17	112.14
18	A	839	CLA	CHB-C1B-NB	-2.24	120.69	124.05
18	A	829	CLA	CHA-C1A-NA	-2.24	121.31	126.39
18	3	313	CLA	CHA-C1A-NA	-2.24	121.31	126.39
18	7	614	CLA	C2A-C3A-C4A	-2.24	98.25	101.87
18	5	615	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
18	1	604	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
18	8	611	CLA	C3D-C4D-ND	2.24	113.62	109.99
18	3	311	CLA	CHC-C1C-NC	2.23	127.68	124.31
18	A	813	CLA	CHB-C1B-NB	-2.23	120.70	124.05
18	A	844	CLA	CAA-C2A-C1A	-2.23	107.19	112.14
18	A	835	CLA	CHA-C1A-NA	-2.23	121.33	126.39
18	B	821	CLA	C2C-C1C-NC	2.23	112.33	109.98
18	7	610	CLA	CHC-C1C-NC	2.23	127.67	124.31
18	6	315	CLA	C2C-C1C-NC	2.23	112.33	109.98
18	5	602	CLA	CAA-C2A-C1A	-2.23	107.20	112.14
18	4	606	CLA	CHC-C1C-NC	2.23	127.67	124.31
18	7	608	CLA	CHA-C1A-NA	-2.23	121.34	126.39
18	6	301	CLA	C2C-C1C-NC	2.23	112.32	109.98
18	4	606	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
18	B	806	CLA	CHA-C1A-NA	-2.23	121.34	126.39
19	B	844	PQN	C11-C3-C2	-2.23	121.07	124.89
18	5	611	CLA	C3D-C4D-ND	2.23	113.61	109.99
18	1	614	CLA	CHB-C1B-NB	-2.23	120.71	124.05
18	B	835	CLA	CHA-C1A-NA	-2.23	121.34	126.39
18	B	840	CLA	C3B-C4B-NB	-2.23	108.54	110.53
18	7	614	CLA	C3B-C4B-NB	-2.23	108.54	110.53
18	5	609	CLA	CAA-C2A-C1A	-2.23	107.21	112.14
18	3	305	CLA	C3B-C4B-NB	-2.23	108.54	110.53
18	4	610	CLA	CHA-C1A-NA	-2.23	121.35	126.39
18	6	301	CLA	C2A-C1A-CHA	2.23	127.73	123.87
18	B	819	CLA	C3A-C2A-C1A	-2.22	98.01	101.34
18	B	829	CLA	C4B-CHC-C1C	-2.22	121.02	126.25
18	5	611	CLA	CGD-CBD-CAD	-2.22	103.65	110.85
18	A	830	CLA	CHB-C1B-NB	-2.22	120.72	124.05
18	6	304	CLA	CHB-C1B-NB	-2.22	120.72	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	812	CLA	CHB-C1B-NB	-2.22	120.72	124.05
18	Z	612	CLA	CHB-C1B-NB	-2.22	120.72	124.05
18	B	816	CLA	CHA-C1A-NA	-2.22	121.36	126.39
18	6	313	CLA	CAA-C2A-C1A	-2.22	107.23	112.14
18	7	613	CLA	CHA-C1A-NA	-2.22	121.36	126.39
18	B	807	CLA	CHC-C1C-NC	2.22	127.65	124.31
18	1	613	CLA	CHB-C1B-NB	-2.22	120.72	124.05
18	A	845	CLA	CHA-C1A-NA	-2.22	121.37	126.39
18	4	602	CLA	CHC-C1C-C2C	-2.22	120.65	126.95
18	A	841	CLA	CHA-C1A-NA	-2.22	121.37	126.39
18	A	829	CLA	C3B-C4B-NB	-2.22	108.55	110.53
18	B	834	CLA	CHD-C1D-ND	-2.22	121.13	124.67
18	Z	613	CLA	CHB-C1B-NB	-2.22	120.72	124.05
18	5	604	CLA	CHA-C1A-NA	-2.22	121.37	126.39
18	Z	603	CLA	CHC-C1C-C2C	-2.21	120.65	126.95
18	A	803	CLA	C2C-C1C-NC	2.21	112.31	109.98
18	A	818	CLA	C2C-C1C-NC	2.21	112.31	109.98
18	A	814	CLA	CHB-C1B-NB	-2.21	120.73	124.05
18	A	826	CLA	C3D-C4D-ND	2.21	113.58	109.99
21	4	604	CHL	C4C-CHD-C1D	2.21	123.98	116.07
18	5	605	CLA	C1D-ND-C4D	-2.21	104.76	106.31
18	B	820	CLA	CHB-C1B-NB	-2.21	120.73	124.05
18	4	607	CLA	C3A-C2A-C1A	-2.21	98.03	101.34
18	B	830	CLA	CHB-C1B-NB	-2.21	120.74	124.05
18	B	805	CLA	C3B-C4B-NB	-2.21	108.56	110.53
18	5	610	CLA	CHA-C1A-NA	-2.21	121.40	126.39
18	3	307	CLA	CHB-C1B-NB	-2.20	120.74	124.05
18	5	603	CLA	CHB-C1B-NB	-2.20	120.74	124.05
18	1	609	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
18	A	805	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
18	B	805	CLA	C3A-C2A-C1A	-2.20	98.04	101.34
18	6	317	CLA	CHA-C1A-NA	-2.20	121.41	126.39
18	6	315	CLA	C1D-ND-C4D	-2.20	104.77	106.31
18	B	834	CLA	CHA-C1A-NA	-2.20	121.41	126.39
21	6	316	CHL	C3C-C4C-NC	-2.20	109.28	114.65
18	B	831	CLA	CHA-C1A-NA	-2.20	121.41	126.39
18	B	806	CLA	C3B-C4B-NB	-2.20	108.57	110.53
18	4	609	CLA	CHB-C1B-NB	-2.20	120.75	124.05
18	4	603	CLA	CHA-C1A-NA	-2.20	121.42	126.39
18	Z	604	CLA	CHD-C1D-ND	-2.20	121.71	124.80
18	B	831	CLA	CAA-C2A-C1A	-2.20	107.28	112.14
18	B	801	CLA	CGD-CBD-CAD	-2.20	103.74	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	603	CLA	CHD-C1D-ND	-2.20	121.71	124.80
21	1	606	CHL	C3C-C4C-NC	-2.20	109.28	114.65
18	Z	608	CLA	CHC-C1C-C2C	-2.20	120.71	126.95
18	B	822	CLA	C3B-C4B-NB	-2.20	108.57	110.53
18	B	832	CLA	CHB-C1B-NB	-2.19	120.76	124.05
18	A	827	CLA	CHA-C1A-NA	-2.19	121.42	126.39
18	5	612	CLA	CHA-C1A-NA	-2.19	121.43	126.39
18	1	604	CLA	C3B-C4B-NB	-2.19	108.57	110.53
18	B	836	CLA	C3B-C4B-NB	-2.19	108.57	110.53
18	B	837	CLA	C2C-C1C-NC	2.19	112.28	109.98
21	Z	605	CHL	C3C-C4C-NC	-2.19	109.30	114.65
18	4	606	CLA	CHA-C1A-NA	-2.19	121.43	126.39
18	B	813	CLA	CHA-C1A-NA	-2.19	121.44	126.39
18	A	832	CLA	CHB-C1B-NB	-2.19	120.77	124.05
18	A	836	CLA	CHB-C1B-NB	-2.19	120.77	124.05
18	B	838	CLA	CHB-C1B-NB	-2.19	120.77	124.05
18	6	312	CLA	CHB-C1B-NB	-2.19	120.77	124.05
18	B	841	CLA	CHA-C1A-NA	-2.18	121.44	126.39
18	A	826	CLA	CHB-C1B-NB	-2.18	120.77	124.05
18	B	819	CLA	C3D-C4D-ND	2.18	113.54	109.99
18	A	809	CLA	CHB-C1B-NB	-2.18	120.77	124.05
18	Z	606	CLA	CHB-C1B-NB	-2.18	120.77	124.05
18	A	828	CLA	CHB-C1B-NB	-2.18	120.78	124.05
21	3	306	CHL	C3C-C4C-NC	-2.18	109.32	114.65
18	B	801	CLA	C1D-ND-C4D	-2.18	104.78	106.31
18	4	608	CLA	C3B-C4B-NB	-2.18	108.59	110.53
18	A	816	CLA	CHA-C1A-NA	-2.18	121.46	126.39
18	1	608	CLA	C1D-ND-C4D	-2.18	104.78	106.31
18	Z	607	CLA	C1D-ND-C4D	-2.18	104.78	106.31
18	5	609	CLA	CHA-C1A-NA	-2.18	121.46	126.39
18	B	827	CLA	CHB-C1B-NB	-2.18	120.78	124.05
18	1	607	CLA	CHB-C1B-NB	-2.18	120.78	124.05
21	6	307	CHL	CMA-C3A-C4A	-2.18	109.92	114.61
18	Z	603	CLA	C3B-C4B-NB	-2.18	108.59	110.53
18	1	605	CLA	CHD-C1D-ND	-2.17	121.74	124.80
18	4	611	CLA	CAA-C2A-C1A	-2.17	107.33	112.14
18	B	839	CLA	CHA-C1A-NA	-2.17	121.47	126.39
18	1	613	CLA	CHA-C1A-NA	-2.17	121.47	126.39
18	B	805	CLA	C1D-ND-C4D	-2.17	104.79	106.31
18	B	821	CLA	C3B-C4B-NB	-2.17	108.59	110.53
18	A	816	CLA	C2C-C1C-NC	2.17	112.26	109.98
18	8	601	CLA	CHB-C1B-NB	-2.17	120.79	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	834	CLA	C3A-C2A-C1A	-2.17	98.09	101.34
18	4	602	CLA	C3D-C4D-ND	2.17	113.51	109.99
18	5	610	CLA	CHB-C1B-NB	-2.17	120.79	124.05
18	7	612	CLA	CHA-C1A-NA	-2.17	121.48	126.39
21	8	606	CHL	CHA-C1A-C2A	-2.17	128.21	133.31
18	5	617	CLA	C3D-C4D-ND	2.17	113.51	109.99
18	6	302	CLA	CAA-C2A-C1A	-2.17	107.34	112.14
18	1	603	CLA	CHB-C1B-NB	-2.17	120.80	124.05
18	7	602	CLA	CAA-C2A-C1A	-2.17	107.35	112.14
18	6	313	CLA	CHD-C1D-C2D	2.17	129.99	125.49
18	8	601	CLA	CHA-C1A-NA	-2.16	121.49	126.39
18	4	608	CLA	CAA-C2A-C1A	-2.16	107.35	112.14
18	A	807	CLA	C2C-C1C-NC	2.16	112.25	109.98
18	B	827	CLA	C2C-C1C-NC	2.16	112.25	109.98
18	B	816	CLA	CHB-C1B-NB	-2.16	120.80	124.05
18	Z	612	CLA	CHA-C1A-NA	-2.16	121.49	126.39
18	A	838	CLA	CHB-C1B-NB	-2.16	120.81	124.05
18	5	609	CLA	CHC-C1C-NC	2.16	127.57	124.31
18	A	845	CLA	CHB-C1B-NB	-2.16	120.81	124.05
18	3	314	CLA	CHB-C1B-NB	-2.16	120.81	124.05
18	A	808	CLA	C3D-C4D-ND	2.16	113.50	109.99
18	A	830	CLA	C2C-C1C-NC	2.16	112.25	109.98
18	B	837	CLA	CHA-C1A-NA	-2.16	121.51	126.39
18	5	614	CLA	CHC-C1C-NC	2.16	127.56	124.31
21	6	306	CHL	C3C-C4C-NC	-2.16	109.38	114.65
21	1	606	CHL	CMB-C2B-C3B	2.16	128.99	124.68
18	B	836	CLA	C2C-C1C-NC	2.15	112.24	109.98
18	7	614	CLA	C2C-C1C-NC	2.15	112.24	109.98
18	B	805	CLA	CHB-C1B-NB	-2.15	120.82	124.05
18	7	607	CLA	CHA-C1A-NA	-2.15	121.52	126.39
18	1	610	CLA	CHA-C1A-NA	-2.15	121.52	126.39
18	Z	609	CLA	CHA-C1A-NA	-2.15	121.52	126.39
18	B	819	CLA	CHB-C1B-NB	-2.15	120.82	124.05
18	Z	602	CLA	C3D-C4D-ND	2.15	113.48	109.99
18	6	311	CLA	C3D-C4D-ND	2.15	113.48	109.99
18	7	604	CLA	C1D-CHD-C4C	-2.15	121.46	126.02
18	A	810	CLA	CHB-C1B-NB	-2.15	120.83	124.05
18	8	615	CLA	CHB-C1B-NB	-2.15	120.83	124.05
18	A	845	CLA	CAA-C2A-C1A	-2.15	107.39	112.14
18	6	313	CLA	CHB-C1B-NB	-2.15	120.83	124.05
18	4	608	CLA	C1D-ND-C4D	-2.14	104.81	106.31
21	Z	605	CHL	CMB-C2B-C3B	2.14	128.97	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	804	CLA	CHB-C1B-NB	-2.14	120.83	124.05
18	6	302	CLA	CHA-C1A-NA	-2.14	121.54	126.39
18	A	823	CLA	CGD-CBD-CAD	-2.14	103.91	110.85
18	B	805	CLA	CHA-C1A-NA	-2.14	121.54	126.39
18	4	609	CLA	C2C-C1C-NC	2.14	112.23	109.98
18	B	842	CLA	CHB-C1B-NB	-2.14	120.84	124.05
18	B	807	CLA	C5-C3-C2	-2.14	111.04	126.65
18	A	836	CLA	C2C-C1C-NC	2.14	112.23	109.98
18	B	840	CLA	CHB-C1B-NB	-2.14	120.84	124.05
21	5	616	CHL	CMA-C3A-C4A	-2.14	110.00	114.61
18	A	834	CLA	C3D-C4D-ND	2.14	113.46	109.99
18	3	313	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
18	6	315	CLA	CHA-C1A-NA	-2.14	121.55	126.39
18	6	313	CLA	C2C-C1C-NC	2.14	112.22	109.98
18	B	802	CLA	CHC-C1C-NC	2.13	127.53	124.31
18	3	314	CLA	C3B-C4B-NB	-2.13	108.62	110.53
18	B	842	CLA	C3D-C4D-ND	2.13	113.45	109.99
18	3	314	CLA	C2C-C1C-NC	2.13	112.22	109.98
18	6	311	CLA	CHB-C1B-NB	-2.13	120.85	124.05
21	5	607	CHL	C4C-CHD-C1D	2.13	123.68	116.07
18	7	612	CLA	CHB-C1B-NB	-2.13	120.86	124.05
18	A	814	CLA	C3D-C4D-ND	2.13	113.44	109.99
18	6	302	CLA	C3D-C4D-ND	2.13	113.44	109.99
18	8	610	CLA	CHD-C1D-C2D	2.13	129.91	125.49
18	6	312	CLA	CHA-C1A-NA	-2.13	121.58	126.39
18	A	824	CLA	C3A-C2A-C1A	-2.12	98.16	101.34
21	Z	601	CHL	CAA-C2A-C1A	2.12	117.56	113.35
18	A	819	CLA	CHB-C1B-NB	-2.12	120.86	124.05
18	B	830	CLA	CGD-CBD-CAD	-2.12	103.97	110.85
18	1	602	CLA	C3D-C4D-ND	2.12	113.44	109.99
18	4	609	CLA	C3D-C4D-ND	2.12	113.44	109.99
18	B	832	CLA	CHC-C1C-NC	2.12	127.51	124.31
18	6	314	CLA	CHA-C1A-NA	-2.12	121.59	126.39
18	A	828	CLA	C1D-ND-C4D	-2.12	104.83	106.31
18	B	836	CLA	CHA-C1A-NA	-2.12	121.60	126.39
18	A	827	CLA	CHD-C1D-C2D	2.11	129.88	125.49
18	B	812	CLA	C3B-C4B-NB	-2.11	108.64	110.53
18	A	805	CLA	CHC-C1C-NC	2.11	127.49	124.31
18	6	309	CLA	CHC-C1C-NC	2.11	127.49	124.31
18	B	834	CLA	CHB-C1B-NB	-2.11	120.88	124.05
18	3	310	CLA	CHB-C1B-NB	-2.11	120.88	124.05
18	B	809	CLA	CHB-C1B-NB	-2.11	120.88	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	609	CLA	CHC-C1C-NC	2.11	127.49	124.31
18	B	817	CLA	CHB-C1B-NB	-2.11	120.89	124.05
18	1	610	CLA	CHC-C1C-NC	2.11	127.48	124.31
18	B	841	CLA	C3B-C4B-NB	-2.11	108.65	110.53
18	7	607	CLA	CHB-C1B-NB	-2.11	120.89	124.05
18	8	603	CLA	CHB-C1B-NB	-2.11	120.89	124.05
18	F	302	CLA	CHA-C1A-NA	-2.11	121.62	126.39
18	6	302	CLA	CHC-C1C-NC	2.10	127.48	124.31
18	A	834	CLA	C2C-C1C-NC	2.10	112.19	109.98
18	3	304	CLA	CAA-C2A-C1A	-2.10	107.49	112.14
18	A	825	CLA	CHD-C1D-C2D	2.10	129.86	125.49
18	4	603	CLA	CHB-C1B-NB	-2.10	120.90	124.05
18	J	101	CLA	CHA-C1A-NA	-2.10	121.64	126.39
18	A	819	CLA	C3B-C4B-NB	-2.10	108.66	110.53
18	5	608	CLA	CHA-C1A-NA	-2.10	121.64	126.39
18	8	610	CLA	C4B-CHC-C1C	-2.10	121.31	126.25
18	8	604	CLA	C2C-C1C-NC	2.10	112.19	109.98
18	A	807	CLA	CHA-C1A-NA	-2.09	121.65	126.39
18	B	818	CLA	CHB-C1B-NB	-2.09	120.91	124.05
18	A	817	CLA	C3D-C4D-ND	2.09	113.39	109.99
18	A	812	CLA	CHA-C1A-NA	-2.09	121.65	126.39
18	8	608	CLA	CHB-C1B-NB	-2.09	120.91	124.05
18	5	615	CLA	CHC-C1C-NC	2.09	127.46	124.31
18	7	611	CLA	C2C-C1C-NC	2.09	112.18	109.98
18	A	819	CLA	C3D-C4D-ND	2.09	113.39	109.99
18	B	813	CLA	C2C-C1C-NC	2.09	112.18	109.98
18	3	303	CLA	CHB-C1B-NB	-2.09	120.91	124.05
18	8	613	CLA	CHB-C1B-NB	-2.09	120.91	124.05
21	7	606	CHL	CMA-C3A-C4A	-2.09	110.11	114.61
18	B	804	CLA	C2A-C3A-C4A	-2.09	98.50	101.87
18	A	812	CLA	CGD-CBD-CAD	-2.09	104.09	110.85
21	6	306	CHL	C1B-CHB-C4A	2.08	122.66	121.32
18	3	304	CLA	CHA-C1A-NA	-2.08	121.67	126.39
18	B	811	CLA	CHC-C1C-NC	2.08	127.45	124.31
18	8	602	CLA	CAA-C2A-C1A	-2.08	107.53	112.14
18	B	818	CLA	C3D-C4D-ND	2.08	113.37	109.99
18	3	310	CLA	C3D-C4D-ND	2.08	113.37	109.99
18	A	844	CLA	C3B-C4B-NB	-2.08	108.67	110.53
18	B	836	CLA	CAA-C2A-C1A	-2.08	107.54	112.14
18	6	308	CLA	C3D-C4D-ND	2.08	113.37	109.99
18	6	308	CLA	CHB-C1B-NB	-2.08	120.93	124.05
18	A	843	CLA	CHA-C1A-NA	-2.08	121.69	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	805	CLA	C3B-C4B-NB	-2.08	108.68	110.53
18	B	804	CLA	C2A-C1A-CHA	2.08	127.47	123.87
18	A	822	CLA	CAC-C3C-C4C	2.08	127.49	124.79
18	A	840	CLA	C3D-C4D-ND	2.08	113.36	109.99
18	3	311	CLA	CHB-C1B-NB	-2.08	120.94	124.05
18	5	602	CLA	C3D-C4D-ND	2.07	113.36	109.99
18	B	835	CLA	CHB-C1B-NB	-2.07	120.94	124.05
18	A	811	CLA	CHB-C1B-NB	-2.07	120.94	124.05
18	8	611	CLA	C3B-C4B-NB	-2.07	108.68	110.53
18	Z	602	CLA	CHA-C1A-NA	-2.07	121.70	126.39
18	7	602	CLA	CHB-C1B-NB	-2.07	120.95	124.05
21	Z	601	CHL	C3C-C4C-NC	-2.07	109.60	114.65
18	B	827	CLA	C3D-C4D-ND	2.07	113.35	109.99
21	6	305	CHL	C4C-CHD-C1D	2.07	123.46	116.07
18	A	841	CLA	CHB-C1B-NB	-2.07	120.95	124.05
18	7	603	CLA	CHB-C1B-NB	-2.07	120.95	124.05
21	6	305	CHL	CMB-C2B-C3B	2.07	128.81	124.68
18	A	836	CLA	CAA-C2A-C1A	-2.06	107.57	112.14
18	5	610	CLA	CHC-C1C-NC	2.06	127.42	124.31
18	B	822	CLA	CHA-C1A-NA	-2.06	121.72	126.39
18	B	835	CLA	C3D-C4D-ND	2.06	113.34	109.99
18	Z	602	CLA	C2C-C1C-NC	2.06	112.15	109.98
18	1	602	CLA	CHA-C1A-NA	-2.06	121.72	126.39
18	1	609	CLA	CHB-C1B-NB	-2.06	120.96	124.05
18	6	313	CLA	C3D-C4D-ND	2.06	113.34	109.99
18	7	612	CLA	C3D-C4D-ND	2.06	113.34	109.99
18	4	603	CLA	CHD-C1D-ND	-2.06	121.90	124.80
18	B	832	CLA	C3D-C4D-ND	2.06	113.33	109.99
21	1	601	CHL	C3C-C4C-NC	-2.06	109.62	114.65
18	B	840	CLA	CAA-C2A-C1A	-2.06	107.59	112.14
18	A	845	CLA	C1D-CHD-C4C	-2.06	121.65	126.02
18	A	812	CLA	C2C-C1C-NC	2.06	112.14	109.98
18	A	815	CLA	CHA-C1A-NA	-2.06	121.73	126.39
18	6	308	CLA	CHA-C1A-NA	-2.06	121.74	126.39
18	1	605	CLA	CHB-C1B-NB	-2.06	120.97	124.05
18	3	309	CLA	CHB-C1B-NB	-2.06	120.97	124.05
18	7	602	CLA	C3D-C4D-ND	2.06	113.33	109.99
18	A	825	CLA	CHA-C1A-NA	-2.05	121.74	126.39
18	B	841	CLA	C2C-C1C-NC	2.05	112.14	109.98
18	3	302	CLA	CAA-C2A-C1A	-2.05	107.60	112.14
18	3	312	CLA	C2C-C1C-NC	2.05	112.14	109.98
21	6	307	CHL	C4C-CHD-C1D	2.05	123.40	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	617	CLA	C2C-C1C-NC	2.05	112.14	109.98
18	4	612	CLA	C1D-ND-C4D	-2.05	104.87	106.31
18	Z	604	CLA	CHB-C1B-NB	-2.05	120.98	124.05
18	B	829	CLA	CHA-C1A-NA	-2.05	121.76	126.39
18	B	815	CLA	CHD-C1D-C2D	2.05	129.74	125.49
18	3	308	CLA	CHA-C1A-NA	-2.05	121.76	126.39
18	6	301	CLA	CHD-C1D-ND	-2.05	121.92	124.80
18	B	802	CLA	CHB-C1B-NB	-2.05	120.98	124.05
18	B	812	CLA	CHB-C4A-NA	2.04	127.35	124.40
18	B	822	CLA	C3D-C4D-ND	2.04	113.31	109.99
18	B	812	CLA	C1D-ND-C4D	-2.04	104.88	106.31
18	4	607	CLA	CHC-C1C-NC	2.04	127.39	124.31
18	7	608	CLA	CAA-C2A-C1A	-2.04	105.28	111.97
18	B	806	CLA	CHB-C1B-NB	-2.04	120.99	124.05
21	1	606	CHL	C3D-C4D-CHA	2.04	111.64	108.54
18	A	838	CLA	CHD-C1D-C2D	2.04	129.73	125.49
18	B	815	CLA	C1D-ND-C4D	-2.04	104.88	106.31
18	1	602	CLA	C2C-C1C-NC	2.04	112.12	109.98
18	1	612	CLA	CHA-C1A-NA	-2.04	121.78	126.39
18	3	301	CLA	C2C-C1C-NC	2.03	112.12	109.98
18	Z	611	CLA	CHA-C1A-NA	-2.03	121.79	126.39
18	A	838	CLA	CAA-C2A-C1A	-2.03	107.64	112.14
18	Z	608	CLA	CHB-C1B-NB	-2.03	121.00	124.05
18	7	613	CLA	CHB-C1B-NB	-2.03	121.00	124.05
18	B	809	CLA	C3D-C4D-ND	2.03	113.29	109.99
18	6	313	CLA	CHA-C1A-NA	-2.03	121.80	126.39
18	5	617	CLA	CHB-C1B-NB	-2.03	121.00	124.05
18	5	617	CLA	C4B-CHC-C1C	-2.03	121.48	126.25
18	7	601	CLA	CAA-C2A-C1A	-2.03	107.65	112.14
18	A	837	CLA	CHA-C1A-NA	-2.03	121.80	126.39
18	7	602	CLA	CHA-C1A-NA	-2.03	121.80	126.39
21	5	616	CHL	C4C-CHD-C1D	2.03	123.32	116.07
18	4	612	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
18	J	101	CLA	CHB-C1B-NB	-2.03	121.01	124.05
18	3	313	CLA	CHB-C1B-NB	-2.03	121.01	124.05
18	8	603	CLA	CHA-C1A-NA	-2.03	121.80	126.39
18	B	804	CLA	C1D-ND-C4D	-2.03	104.89	106.31
21	1	606	CHL	C4C-CHD-C1D	2.03	123.32	116.07
18	5	609	CLA	CHB-C1B-NB	-2.03	121.01	124.05
18	A	827	CLA	C2C-C1C-NC	2.03	112.11	109.98
18	A	813	CLA	C4B-CHC-C1C	-2.02	121.49	126.25
18	A	820	CLA	CAA-C2A-C1A	-2.02	107.67	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	807	CLA	CHB-C1B-NB	-2.02	121.02	124.05
18	6	308	CLA	C2C-C1C-NC	2.02	112.10	109.98
18	B	820	CLA	CHD-C1D-C2D	2.02	129.69	125.49
18	A	837	CLA	CGD-CBD-CAD	-2.02	104.31	110.85
18	A	805	CLA	CHB-C1B-NB	-2.02	121.02	124.05
18	4	601	CLA	CHB-C1B-NB	-2.02	121.02	124.05
21	6	306	CHL	C4C-CHD-C1D	2.02	123.29	116.07
18	A	808	CLA	CHB-C1B-NB	-2.02	121.02	124.05
18	B	839	CLA	CHB-C1B-NB	-2.02	121.02	124.05
18	5	610	CLA	C2C-C1C-NC	2.02	112.10	109.98
18	7	611	CLA	CAA-C2A-C1A	-2.02	107.68	112.14
18	A	841	CLA	C2C-C1C-NC	2.02	112.10	109.98
21	1	601	CHL	C1-C2-C3	2.02	129.50	126.20
18	6	303	CLA	CHA-C1A-NA	-2.01	121.83	126.39
21	Z	605	CHL	C4C-CHD-C1D	2.01	123.28	116.07
18	7	603	CLA	CHA-C1A-NA	-2.01	121.83	126.39
18	Z	608	CLA	CHA-C1A-NA	-2.01	121.83	126.39
18	3	312	CLA	C3D-C4D-ND	2.01	113.26	109.99
18	1	609	CLA	CHA-C1A-NA	-2.01	121.83	126.39
18	A	825	CLA	CHB-C1B-NB	-2.01	121.03	124.05
18	3	302	CLA	CHA-C1A-NA	-2.01	121.84	126.39
18	A	807	CLA	C1D-CHD-C4C	-2.01	121.75	126.02
18	7	610	CLA	CHB-C1B-NB	-2.01	121.03	124.05
18	4	608	CLA	CHC-C1C-NC	2.01	127.34	124.31
18	A	817	CLA	C2C-C1C-NC	2.01	112.09	109.98
18	7	612	CLA	C2C-C1C-NC	2.01	112.09	109.98
18	B	811	CLA	C4B-CHC-C1C	-2.01	121.52	126.25
18	5	613	CLA	CHB-C1B-NB	-2.01	121.04	124.05
18	A	806	CLA	CHA-C1A-NA	-2.01	121.84	126.39
18	8	602	CLA	CHA-C1A-NA	-2.00	121.86	126.39
18	A	806	CLA	CHB-C1B-NB	-2.00	121.05	124.05
18	A	828	CLA	C4B-CHC-C1C	-2.00	121.54	126.25
18	4	609	CLA	CHA-C1A-NA	-2.00	121.86	126.39
18	B	817	CLA	CHA-C1A-NA	-2.00	121.86	126.39
18	B	824	CLA	CAA-C2A-C1A	-2.00	107.71	112.14

All (239) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CL0	ND
17	A	801	CL0	NA
17	A	801	CL0	NC

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Mol	Chain	Res	Type	Atom
18	A	802	CLA	ND
18	A	803	CLA	ND
18	A	804	CLA	ND
18	A	805	CLA	ND
18	A	806	CLA	ND
18	A	807	CLA	ND
18	A	808	CLA	ND
18	A	809	CLA	ND
18	A	810	CLA	ND
18	A	811	CLA	ND
18	A	812	CLA	ND
18	A	813	CLA	ND
18	A	814	CLA	ND
18	A	815	CLA	ND
18	A	816	CLA	ND
18	A	817	CLA	ND
18	A	818	CLA	ND
18	A	819	CLA	ND
18	A	820	CLA	ND
18	A	821	CLA	ND
18	A	822	CLA	ND
18	A	823	CLA	ND
18	A	824	CLA	ND
18	A	825	CLA	ND
18	A	826	CLA	ND
18	A	827	CLA	ND
18	A	828	CLA	ND
18	A	829	CLA	ND
18	A	830	CLA	ND
18	A	831	CLA	ND
18	A	832	CLA	ND
18	A	833	CLA	ND
18	A	834	CLA	ND
18	A	835	CLA	ND
18	A	836	CLA	ND
18	A	837	CLA	ND
18	A	838	CLA	ND
18	A	839	CLA	ND
18	A	840	CLA	ND
18	A	841	CLA	ND
18	A	843	CLA	ND
18	A	844	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	845	CLA	ND
18	B	801	CLA	ND
18	B	802	CLA	ND
18	B	804	CLA	ND
18	B	805	CLA	ND
18	B	806	CLA	ND
18	B	807	CLA	ND
18	B	808	CLA	ND
18	B	809	CLA	ND
18	B	810	CLA	ND
18	B	811	CLA	ND
18	B	812	CLA	ND
18	B	813	CLA	ND
18	B	814	CLA	ND
18	B	815	CLA	ND
18	B	816	CLA	ND
18	B	817	CLA	ND
18	B	818	CLA	ND
18	B	819	CLA	ND
18	B	820	CLA	ND
18	B	821	CLA	ND
18	B	822	CLA	ND
18	B	823	CLA	ND
18	B	824	CLA	ND
18	B	825	CLA	ND
18	B	826	CLA	ND
18	B	827	CLA	ND
18	B	828	CLA	ND
18	B	829	CLA	ND
18	B	830	CLA	ND
18	B	831	CLA	ND
18	B	832	CLA	ND
18	B	833	CLA	ND
18	B	834	CLA	ND
18	B	835	CLA	ND
18	B	836	CLA	ND
18	B	837	CLA	ND
18	B	838	CLA	ND
18	B	839	CLA	ND
18	B	840	CLA	ND
18	B	841	CLA	ND
18	B	842	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	843	CLA	ND
18	F	301	CLA	ND
18	F	302	CLA	ND
18	J	101	CLA	ND
18	1	602	CLA	ND
18	1	603	CLA	ND
18	1	604	CLA	ND
18	1	605	CLA	ND
18	1	607	CLA	ND
18	1	608	CLA	ND
18	1	609	CLA	ND
18	1	610	CLA	ND
18	1	611	CLA	ND
18	1	612	CLA	ND
18	1	613	CLA	ND
18	1	614	CLA	ND
18	3	301	CLA	ND
18	3	302	CLA	ND
18	3	303	CLA	ND
18	3	304	CLA	ND
18	3	305	CLA	ND
18	3	307	CLA	ND
18	3	308	CLA	ND
18	3	309	CLA	ND
18	3	310	CLA	ND
18	3	311	CLA	ND
18	3	312	CLA	ND
18	3	313	CLA	ND
18	3	314	CLA	ND
18	7	601	CLA	ND
18	7	602	CLA	ND
18	7	603	CLA	ND
18	7	604	CLA	ND
18	7	605	CLA	ND
18	7	607	CLA	ND
18	7	608	CLA	ND
18	7	609	CLA	ND
18	7	610	CLA	ND
18	7	611	CLA	ND
18	7	612	CLA	ND
18	7	613	CLA	ND
18	7	614	CLA	ND

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Mol	Chain	Res	Type	Atom
18	8	601	CLA	ND
18	8	602	CLA	ND
18	8	603	CLA	ND
18	8	604	CLA	ND
18	8	605	CLA	ND
18	8	607	CLA	ND
18	8	608	CLA	ND
18	8	609	CLA	ND
18	8	610	CLA	ND
18	8	611	CLA	ND
18	8	612	CLA	ND
18	8	613	CLA	ND
18	8	614	CLA	ND
18	8	615	CLA	ND
18	Z	602	CLA	ND
18	Z	603	CLA	ND
18	Z	604	CLA	ND
18	Z	606	CLA	ND
18	Z	607	CLA	ND
18	Z	608	CLA	ND
18	Z	609	CLA	ND
18	Z	610	CLA	ND
18	Z	611	CLA	ND
18	Z	612	CLA	ND
18	Z	613	CLA	ND
18	4	601	CLA	ND
18	4	602	CLA	ND
18	4	603	CLA	ND
18	4	606	CLA	ND
18	4	607	CLA	ND
18	4	608	CLA	ND
18	4	609	CLA	ND
18	4	610	CLA	ND
18	4	611	CLA	ND
18	4	612	CLA	ND
18	5	601	CLA	ND
18	5	602	CLA	ND
18	5	603	CLA	ND
18	5	604	CLA	ND
18	5	605	CLA	ND
18	5	608	CLA	ND
18	5	609	CLA	ND

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Mol	Chain	Res	Type	Atom
18	5	610	CLA	ND
18	5	611	CLA	ND
18	5	612	CLA	ND
18	5	613	CLA	ND
18	5	614	CLA	ND
18	5	615	CLA	ND
18	5	617	CLA	ND
18	6	301	CLA	ND
18	6	302	CLA	ND
18	6	303	CLA	ND
18	6	304	CLA	ND
18	6	308	CLA	ND
18	6	309	CLA	ND
18	6	310	CLA	ND
18	6	311	CLA	ND
18	6	312	CLA	ND
18	6	313	CLA	ND
18	6	314	CLA	ND
18	6	315	CLA	ND
18	6	317	CLA	ND
21	1	601	CHL	ND
21	1	601	CHL	NA
21	1	601	CHL	NC
21	1	606	CHL	ND
21	1	606	CHL	NA
21	1	606	CHL	NC
21	3	306	CHL	ND
21	3	306	CHL	NA
21	3	306	CHL	NC
21	7	606	CHL	ND
21	7	606	CHL	NA
21	7	606	CHL	NC
21	8	606	CHL	ND
21	8	606	CHL	NA
21	8	606	CHL	NC
21	Z	601	CHL	ND
21	Z	601	CHL	NA
21	Z	601	CHL	NC
21	Z	605	CHL	ND
21	Z	605	CHL	NA
21	Z	605	CHL	NC
21	4	604	CHL	ND

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Mol	Chain	Res	Type	Atom
21	4	604	CHL	NA
21	4	604	CHL	NC
21	4	605	CHL	NA
21	4	605	CHL	ND
21	4	605	CHL	NC
21	5	606	CHL	ND
21	5	606	CHL	NA
21	5	606	CHL	NC
21	5	607	CHL	ND
21	5	607	CHL	NA
21	5	607	CHL	NC
21	5	616	CHL	ND
21	5	616	CHL	NA
21	5	616	CHL	NC
21	6	305	CHL	ND
21	6	305	CHL	NA
21	6	305	CHL	NC
21	6	306	CHL	ND
21	6	306	CHL	NA
21	6	306	CHL	NC
21	6	307	CHL	ND
21	6	307	CHL	NA
21	6	307	CHL	NC
21	6	316	CHL	ND
21	6	316	CHL	NA
21	6	316	CHL	NC

All (560) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	802	CLA	C1A-C2A-CAA-CBA
18	A	802	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	C1A-C2A-CAA-CBA
18	A	803	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	CAD-CBD-CGD-O1D
18	A	803	CLA	CAD-CBD-CGD-O2D
18	A	806	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	808	CLA	CHA-CBD-CGD-O1D
18	A	808	CLA	CHA-CBD-CGD-O2D
18	A	809	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	A	809	CLA	C4B-C3B-CAB-CBB
18	A	813	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C3A-C2A-CAA-CBA
18	A	814	CLA	CHA-CBD-CGD-O1D
18	A	814	CLA	CHA-CBD-CGD-O2D
18	A	818	CLA	C1A-C2A-CAA-CBA
18	A	818	CLA	C3A-C2A-CAA-CBA
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	820	CLA	C2B-C3B-CAB-CBB
18	A	820	CLA	C4B-C3B-CAB-CBB
18	A	820	CLA	CHA-CBD-CGD-O1D
18	A	820	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	C3A-C2A-CAA-CBA
18	A	822	CLA	CHA-CBD-CGD-O1D
18	A	822	CLA	CHA-CBD-CGD-O2D
18	A	823	CLA	C1A-C2A-CAA-CBA
18	A	823	CLA	C3A-C2A-CAA-CBA
18	A	824	CLA	C1A-C2A-CAA-CBA
18	A	824	CLA	C3A-C2A-CAA-CBA
18	A	828	CLA	C2B-C3B-CAB-CBB
18	A	828	CLA	C4B-C3B-CAB-CBB
18	A	829	CLA	C2B-C3B-CAB-CBB
18	A	829	CLA	C4B-C3B-CAB-CBB
18	A	830	CLA	CHA-CBD-CGD-O2D
18	A	831	CLA	C1A-C2A-CAA-CBA
18	A	831	CLA	CHA-CBD-CGD-O1D
18	A	831	CLA	CHA-CBD-CGD-O2D
18	A	833	CLA	C1A-C2A-CAA-CBA
18	A	833	CLA	C3A-C2A-CAA-CBA
18	A	834	CLA	C2B-C3B-CAB-CBB
18	A	834	CLA	C4B-C3B-CAB-CBB
18	A	840	CLA	C1A-C2A-CAA-CBA
18	A	843	CLA	CAD-CBD-CGD-O1D
18	A	843	CLA	CAD-CBD-CGD-O2D
18	A	844	CLA	C1A-C2A-CAA-CBA
18	A	844	CLA	C3A-C2A-CAA-CBA
18	A	844	CLA	CAD-CBD-CGD-O1D
18	A	844	CLA	CAD-CBD-CGD-O2D
18	B	801	CLA	C1A-C2A-CAA-CBA
18	B	801	CLA	C3A-C2A-CAA-CBA
18	B	804	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	806	CLA	C1A-C2A-CAA-CBA
18	B	806	CLA	CHA-CBD-CGD-O1D
18	B	806	CLA	CHA-CBD-CGD-O2D
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	810	CLA	CHA-CBD-CGD-O1D
18	B	810	CLA	CHA-CBD-CGD-O2D
18	B	811	CLA	C1A-C2A-CAA-CBA
18	B	812	CLA	C1A-C2A-CAA-CBA
18	B	812	CLA	C3A-C2A-CAA-CBA
18	B	812	CLA	C2B-C3B-CAB-CBB
18	B	812	CLA	C4B-C3B-CAB-CBB
18	B	815	CLA	C1A-C2A-CAA-CBA
18	B	815	CLA	C2B-C3B-CAB-CBB
18	B	815	CLA	C4B-C3B-CAB-CBB
18	B	815	CLA	CAD-CBD-CGD-O1D
18	B	815	CLA	CAD-CBD-CGD-O2D
18	B	816	CLA	C3A-C2A-CAA-CBA
18	B	816	CLA	C4B-C3B-CAB-CBB
18	B	817	CLA	C1A-C2A-CAA-CBA
18	B	817	CLA	CHA-CBD-CGD-O1D
18	B	817	CLA	CHA-CBD-CGD-O2D
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	823	CLA	CHA-CBD-CGD-O1D
18	B	823	CLA	CHA-CBD-CGD-O2D
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	825	CLA	C2B-C3B-CAB-CBB
18	B	825	CLA	C4B-C3B-CAB-CBB
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C2B-C3B-CAB-CBB
18	B	827	CLA	C4B-C3B-CAB-CBB
18	B	828	CLA	C2B-C3B-CAB-CBB
18	B	828	CLA	C4B-C3B-CAB-CBB
18	B	828	CLA	CAD-CBD-CGD-O1D
18	B	828	CLA	CAD-CBD-CGD-O2D
18	B	829	CLA	C1A-C2A-CAA-CBA
18	B	829	CLA	C3A-C2A-CAA-CBA
18	B	829	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	B	830	CLA	C1A-C2A-CAA-CBA
18	B	830	CLA	C3A-C2A-CAA-CBA
18	B	832	CLA	CHA-CBD-CGD-O1D
18	B	832	CLA	CHA-CBD-CGD-O2D
18	B	840	CLA	C1A-C2A-CAA-CBA
18	B	843	CLA	C3A-C2A-CAA-CBA
18	J	101	CLA	CAD-CBD-CGD-O1D
18	J	101	CLA	CAD-CBD-CGD-O2D
18	1	602	CLA	C1A-C2A-CAA-CBA
18	1	602	CLA	CHA-CBD-CGD-O2D
18	1	603	CLA	CHA-CBD-CGD-O1D
18	1	603	CLA	CHA-CBD-CGD-O2D
18	1	607	CLA	C2B-C3B-CAB-CBB
18	1	607	CLA	C4B-C3B-CAB-CBB
18	1	608	CLA	C1A-C2A-CAA-CBA
18	1	609	CLA	C1A-C2A-CAA-CBA
18	1	609	CLA	C2B-C3B-CAB-CBB
18	1	609	CLA	C4B-C3B-CAB-CBB
18	1	610	CLA	C1A-C2A-CAA-CBA
18	1	611	CLA	C1A-C2A-CAA-CBA
18	3	305	CLA	C3A-C2A-CAA-CBA
18	3	305	CLA	C2B-C3B-CAB-CBB
18	3	305	CLA	C4B-C3B-CAB-CBB
18	3	308	CLA	C1A-C2A-CAA-CBA
18	3	313	CLA	C1A-C2A-CAA-CBA
18	3	313	CLA	C2B-C3B-CAB-CBB
18	3	313	CLA	C4B-C3B-CAB-CBB
18	7	601	CLA	CHA-CBD-CGD-O1D
18	7	601	CLA	CHA-CBD-CGD-O2D
18	7	602	CLA	C1A-C2A-CAA-CBA
18	7	613	CLA	CHA-CBD-CGD-O1D
18	7	613	CLA	CHA-CBD-CGD-O2D
18	8	601	CLA	C3A-C2A-CAA-CBA
18	8	602	CLA	C1A-C2A-CAA-CBA
18	8	605	CLA	CHA-CBD-CGD-O1D
18	8	605	CLA	CHA-CBD-CGD-O2D
18	8	607	CLA	C2B-C3B-CAB-CBB
18	8	607	CLA	C4B-C3B-CAB-CBB
18	8	609	CLA	C1A-C2A-CAA-CBA
18	8	610	CLA	C1A-C2A-CAA-CBA
18	8	611	CLA	C1A-C2A-CAA-CBA
18	8	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	8	615	CLA	CHA-CBD-CGD-O1D
18	8	615	CLA	CHA-CBD-CGD-O2D
18	Z	602	CLA	C1A-C2A-CAA-CBA
18	Z	602	CLA	CHA-CBD-CGD-O2D
18	Z	606	CLA	C2B-C3B-CAB-CBB
18	Z	606	CLA	C4B-C3B-CAB-CBB
18	Z	607	CLA	C1A-C2A-CAA-CBA
18	Z	608	CLA	C1A-C2A-CAA-CBA
18	Z	608	CLA	C2B-C3B-CAB-CBB
18	Z	608	CLA	C4B-C3B-CAB-CBB
18	Z	609	CLA	C1A-C2A-CAA-CBA
18	Z	610	CLA	C1A-C2A-CAA-CBA
18	4	602	CLA	C1A-C2A-CAA-CBA
18	4	602	CLA	CHA-CBD-CGD-O2D
18	4	603	CLA	C2B-C3B-CAB-CBB
18	4	603	CLA	C4B-C3B-CAB-CBB
18	4	606	CLA	C1A-C2A-CAA-CBA
18	4	607	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	609	CLA	C1A-C2A-CAA-CBA
18	4	609	CLA	C3A-C2A-CAA-CBA
18	5	601	CLA	C1A-C2A-CAA-CBA
18	5	601	CLA	C3A-C2A-CAA-CBA
18	5	602	CLA	C4B-C3B-CAB-CBB
18	5	608	CLA	C3A-C2A-CAA-CBA
18	5	609	CLA	C1A-C2A-CAA-CBA
18	5	611	CLA	C1A-C2A-CAA-CBA
18	5	611	CLA	C3A-C2A-CAA-CBA
18	5	613	CLA	C4B-C3B-CAB-CBB
18	5	615	CLA	C2B-C3B-CAB-CBB
18	5	615	CLA	C4B-C3B-CAB-CBB
18	6	301	CLA	CAD-CBD-CGD-O2D
18	6	310	CLA	C1A-C2A-CAA-CBA
18	6	310	CLA	C3A-C2A-CAA-CBA
18	6	310	CLA	C2B-C3B-CAB-CBB
18	6	310	CLA	C4B-C3B-CAB-CBB
18	6	313	CLA	CAD-CBD-CGD-O1D
18	6	313	CLA	CAD-CBD-CGD-O2D
18	6	315	CLA	C1A-C2A-CAA-CBA
18	6	315	CLA	C3A-C2A-CAA-CBA
21	1	601	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	1	601	CHL	C4-C3-C5-C6
21	7	606	CHL	C1A-C2A-CAA-CBA
21	4	604	CHL	C4C-C3C-CAC-CBC
21	5	607	CHL	C3A-C2A-CAA-CBA
21	6	307	CHL	C1A-C2A-CAA-CBA
21	6	307	CHL	C3A-C2A-CAA-CBA
21	6	316	CHL	C1A-C2A-CAA-CBA
18	3	310	CLA	C2A-CAA-CBA-CGA
18	5	617	CLA	C2A-CAA-CBA-CGA
18	4	603	CLA	C2C-C3C-CAC-CBC
19	A	842	PQN	C24-C23-C25-C26
19	B	844	PQN	C24-C23-C25-C26
18	3	313	CLA	C2A-CAA-CBA-CGA
21	4	605	CHL	C2A-CAA-CBA-CGA
18	A	823	CLA	C2-C1-O2A-CGA
18	6	311	CLA	C2A-CAA-CBA-CGA
19	B	844	PQN	C20-C21-C22-C23
18	7	604	CLA	C2A-CAA-CBA-CGA
18	A	811	CLA	C4B-C3B-CAB-CBB
18	A	826	CLA	C4B-C3B-CAB-CBB
18	A	835	CLA	C4B-C3B-CAB-CBB
18	B	802	CLA	C4B-C3B-CAB-CBB
18	B	832	CLA	C4B-C3B-CAB-CBB
18	B	834	CLA	C4B-C3B-CAB-CBB
18	F	302	CLA	C4B-C3B-CAB-CBB
18	3	303	CLA	C4B-C3B-CAB-CBB
18	7	602	CLA	C4B-C3B-CAB-CBB
18	7	607	CLA	C4B-C3B-CAB-CBB
18	7	613	CLA	C4B-C3B-CAB-CBB
18	8	604	CLA	C4B-C3B-CAB-CBB
18	8	613	CLA	C4B-C3B-CAB-CBB
18	5	603	CLA	C4B-C3B-CAB-CBB
18	5	608	CLA	C4B-C3B-CAB-CBB
18	6	311	CLA	C4B-C3B-CAB-CBB
18	B	806	CLA	C3A-C2A-CAA-CBA
18	6	311	CLA	C3A-C2A-CAA-CBA
18	B	802	CLA	C2B-C3B-CAB-CBB
18	B	816	CLA	C2B-C3B-CAB-CBB
18	B	829	CLA	C2B-C3B-CAB-CBB
18	B	834	CLA	C2B-C3B-CAB-CBB
18	F	302	CLA	C2B-C3B-CAB-CBB
18	1	610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	3	303	CLA	C2B-C3B-CAB-CBB
18	7	613	CLA	C2B-C3B-CAB-CBB
18	8	604	CLA	C2B-C3B-CAB-CBB
18	8	613	CLA	C2B-C3B-CAB-CBB
18	Z	609	CLA	C2B-C3B-CAB-CBB
18	5	602	CLA	C2B-C3B-CAB-CBB
18	5	603	CLA	C2B-C3B-CAB-CBB
18	5	613	CLA	C2B-C3B-CAB-CBB
21	6	316	CHL	C3A-C2A-CAA-CBA
18	B	822	CLA	C1A-C2A-CAA-CBA
18	F	302	CLA	C1A-C2A-CAA-CBA
18	5	603	CLA	C2C-C3C-CAC-CBC
18	A	806	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	811	CLA	C3A-C2A-CAA-CBA
18	1	611	CLA	C3A-C2A-CAA-CBA
18	Z	610	CLA	C3A-C2A-CAA-CBA
19	A	842	PQN	C19-C18-C20-C21
21	1	601	CHL	O2A-C1-C2-C3
18	B	807	CLA	C2-C3-C5-C6
18	A	843	CLA	C2A-CAA-CBA-CGA
18	6	303	CLA	C2C-C3C-CAC-CBC
18	A	804	CLA	C4B-C3B-CAB-CBB
18	A	818	CLA	C4B-C3B-CAB-CBB
18	A	830	CLA	C4B-C3B-CAB-CBB
18	B	824	CLA	C4B-C3B-CAB-CBB
18	B	826	CLA	C4B-C3B-CAB-CBB
18	B	835	CLA	C4B-C3B-CAB-CBB
18	B	841	CLA	C4B-C3B-CAB-CBB
18	1	610	CLA	C4B-C3B-CAB-CBB
18	1	614	CLA	C4B-C3B-CAB-CBB
18	3	307	CLA	C4B-C3B-CAB-CBB
18	7	614	CLA	C4B-C3B-CAB-CBB
18	Z	609	CLA	C4B-C3B-CAB-CBB
18	Z	613	CLA	C4B-C3B-CAB-CBB
18	4	601	CLA	C4B-C3B-CAB-CBB
18	4	609	CLA	C4B-C3B-CAB-CBB
18	4	611	CLA	C4B-C3B-CAB-CBB
18	6	302	CLA	C4B-C3B-CAB-CBB
18	6	314	CLA	C4B-C3B-CAB-CBB
19	A	842	PQN	C17-C18-C20-C21
18	3	313	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	1	603	CLA	C2B-C3B-CAB-CBB
18	8	615	CLA	C2B-C3B-CAB-CBB
18	4	609	CLA	C2B-C3B-CAB-CBB
18	4	611	CLA	C2B-C3B-CAB-CBB
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	807	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	826	CLA	C1A-C2A-CAA-CBA
18	A	834	CLA	C1A-C2A-CAA-CBA
18	A	838	CLA	C1A-C2A-CAA-CBA
18	B	816	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	B	821	CLA	C1A-C2A-CAA-CBA
18	B	824	CLA	C1A-C2A-CAA-CBA
18	B	834	CLA	C1A-C2A-CAA-CBA
18	1	613	CLA	C1A-C2A-CAA-CBA
18	3	301	CLA	C1A-C2A-CAA-CBA
18	7	607	CLA	C1A-C2A-CAA-CBA
18	7	614	CLA	C1A-C2A-CAA-CBA
18	8	613	CLA	C1A-C2A-CAA-CBA
18	Z	612	CLA	C1A-C2A-CAA-CBA
18	4	611	CLA	C1A-C2A-CAA-CBA
18	5	602	CLA	C1A-C2A-CAA-CBA
18	5	608	CLA	C1A-C2A-CAA-CBA
18	5	613	CLA	C1A-C2A-CAA-CBA
18	5	614	CLA	C1A-C2A-CAA-CBA
18	6	302	CLA	C1A-C2A-CAA-CBA
18	6	313	CLA	C1A-C2A-CAA-CBA
18	B	807	CLA	C5-C6-C7-C8
19	A	842	PQN	C18-C20-C21-C22
18	4	601	CLA	C2C-C3C-CAC-CBC
18	4	603	CLA	C4C-C3C-CAC-CBC
18	B	831	CLA	C2C-C3C-CAC-CBC
21	6	306	CHL	C4C-C3C-CAC-CBC
18	A	807	CLA	C4B-C3B-CAB-CBB
18	A	810	CLA	C4B-C3B-CAB-CBB
18	A	813	CLA	C4B-C3B-CAB-CBB
18	A	822	CLA	C4B-C3B-CAB-CBB
18	A	839	CLA	C4B-C3B-CAB-CBB
18	B	802	CLA	C1A-C2A-CAA-CBA
18	B	809	CLA	C4B-C3B-CAB-CBB
18	B	811	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	B	818	CLA	C4B-C3B-CAB-CBB
18	B	840	CLA	C4B-C3B-CAB-CBB
18	1	603	CLA	C4B-C3B-CAB-CBB
18	1	608	CLA	C4B-C3B-CAB-CBB
18	3	304	CLA	C4B-C3B-CAB-CBB
18	3	309	CLA	C4B-C3B-CAB-CBB
18	3	310	CLA	C4B-C3B-CAB-CBB
18	3	312	CLA	C4B-C3B-CAB-CBB
18	7	601	CLA	C4B-C3B-CAB-CBB
18	7	603	CLA	C4B-C3B-CAB-CBB
18	7	608	CLA	C1A-C2A-CAA-CBA
18	7	608	CLA	C4B-C3B-CAB-CBB
18	7	611	CLA	C4B-C3B-CAB-CBB
18	7	613	CLA	C1A-C2A-CAA-CBA
18	8	601	CLA	C4B-C3B-CAB-CBB
18	8	603	CLA	C4B-C3B-CAB-CBB
18	8	608	CLA	C4B-C3B-CAB-CBB
18	8	614	CLA	C4B-C3B-CAB-CBB
18	8	615	CLA	C4B-C3B-CAB-CBB
18	Z	607	CLA	C4B-C3B-CAB-CBB
18	4	606	CLA	C4B-C3B-CAB-CBB
18	5	617	CLA	C4B-C3B-CAB-CBB
18	6	301	CLA	C4B-C3B-CAB-CBB
18	6	303	CLA	C4B-C3B-CAB-CBB
18	6	309	CLA	C1A-C2A-CAA-CBA
18	6	311	CLA	C1A-C2A-CAA-CBA
18	6	313	CLA	C4B-C3B-CAB-CBB
18	A	822	CLA	C2C-C3C-CAC-CBC
18	Z	604	CLA	C2C-C3C-CAC-CBC
18	7	601	CLA	C3A-C2A-CAA-CBA
18	6	301	CLA	C3A-C2A-CAA-CBA
18	5	617	CLA	C3A-C2A-CAA-CBA
18	1	605	CLA	C2C-C3C-CAC-CBC
18	Z	604	CLA	C2A-CAA-CBA-CGA
18	A	805	CLA	CAD-CBD-CGD-O2D
18	A	813	CLA	CAD-CBD-CGD-O2D
18	A	825	CLA	CAD-CBD-CGD-O2D
18	B	839	CLA	CAD-CBD-CGD-O2D
18	7	604	CLA	CAD-CBD-CGD-O2D
18	8	601	CLA	CAD-CBD-CGD-O2D
21	1	606	CHL	C1A-C2A-CAA-CBA
21	3	306	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	Z	605	CHL	C1A-C2A-CAA-CBA
21	5	607	CHL	C1A-C2A-CAA-CBA
18	A	805	CLA	CAD-CBD-CGD-O1D
18	A	813	CLA	CAD-CBD-CGD-O1D
18	A	825	CLA	CAD-CBD-CGD-O1D
18	A	827	CLA	CHA-CBD-CGD-O1D
18	A	827	CLA	CHA-CBD-CGD-O2D
18	A	830	CLA	CHA-CBD-CGD-O1D
18	A	838	CLA	CAD-CBD-CGD-O1D
18	B	812	CLA	CHA-CBD-CGD-O1D
18	B	812	CLA	CHA-CBD-CGD-O2D
18	B	839	CLA	CAD-CBD-CGD-O1D
18	1	602	CLA	CHA-CBD-CGD-O1D
18	8	601	CLA	CAD-CBD-CGD-O1D
18	Z	602	CLA	CHA-CBD-CGD-O1D
18	4	602	CLA	CHA-CBD-CGD-O1D
18	4	611	CLA	CHA-CBD-CGD-O1D
18	5	603	CLA	CHA-CBD-CGD-O1D
18	5	603	CLA	CHA-CBD-CGD-O2D
18	6	301	CLA	CAD-CBD-CGD-O1D
18	6	303	CLA	CHA-CBD-CGD-O1D
18	6	303	CLA	CHA-CBD-CGD-O2D
21	7	606	CHL	CHA-CBD-CGD-O2D
21	8	606	CHL	CHA-CBD-CGD-O2D
18	A	811	CLA	C2B-C3B-CAB-CBB
18	A	826	CLA	C2B-C3B-CAB-CBB
18	A	835	CLA	C2B-C3B-CAB-CBB
18	B	809	CLA	C2B-C3B-CAB-CBB
18	B	818	CLA	C2B-C3B-CAB-CBB
18	B	826	CLA	C2B-C3B-CAB-CBB
18	B	832	CLA	C2B-C3B-CAB-CBB
18	B	840	CLA	C2B-C3B-CAB-CBB
18	B	841	CLA	C2B-C3B-CAB-CBB
18	B	842	CLA	C2B-C3B-CAB-CBB
18	J	101	CLA	C2B-C3B-CAB-CBB
18	3	304	CLA	C2B-C3B-CAB-CBB
18	3	310	CLA	C2B-C3B-CAB-CBB
18	7	602	CLA	C2B-C3B-CAB-CBB
18	7	607	CLA	C2B-C3B-CAB-CBB
18	7	614	CLA	C2B-C3B-CAB-CBB
18	8	601	CLA	C2B-C3B-CAB-CBB
18	5	608	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	6	301	CLA	C2B-C3B-CAB-CBB
18	6	311	CLA	C2B-C3B-CAB-CBB
19	B	844	PQN	C14-C13-C15-C16
18	8	612	CLA	C2C-C3C-CAC-CBC
18	7	608	CLA	CAA-CBA-CGA-O2A
18	6	312	CLA	C2C-C3C-CAC-CBC
18	A	819	CLA	C4B-C3B-CAB-CBB
18	A	837	CLA	C4B-C3B-CAB-CBB
18	A	841	CLA	C4B-C3B-CAB-CBB
18	B	842	CLA	C4B-C3B-CAB-CBB
18	3	301	CLA	C4B-C3B-CAB-CBB
18	8	602	CLA	C4B-C3B-CAB-CBB
18	4	610	CLA	C4B-C3B-CAB-CBB
18	B	838	CLA	C2C-C3C-CAC-CBC
18	3	311	CLA	CAA-CBA-CGA-O2A
18	1	604	CLA	C2C-C3C-CAC-CBC
18	Z	603	CLA	C2C-C3C-CAC-CBC
18	7	601	CLA	C2C-C3C-CAC-CBC
18	6	312	CLA	CAA-CBA-CGA-O2A
18	A	824	CLA	C2C-C3C-CAC-CBC
18	Z	604	CLA	C4C-C3C-CAC-CBC
18	6	317	CLA	C2A-CAA-CBA-CGA
18	1	605	CLA	C4C-C3C-CAC-CBC
21	4	605	CHL	CAA-CBA-CGA-O1A
18	3	311	CLA	CAA-CBA-CGA-O1A
18	3	302	CLA	C2C-C3C-CAC-CBC
19	B	844	PQN	C12-C13-C15-C16
18	5	617	CLA	C1A-C2A-CAA-CBA
18	7	601	CLA	C4C-C3C-CAC-CBC
18	A	807	CLA	C2B-C3B-CAB-CBB
18	A	810	CLA	C2B-C3B-CAB-CBB
18	A	813	CLA	C2B-C3B-CAB-CBB
18	A	819	CLA	C2B-C3B-CAB-CBB
18	A	822	CLA	C2B-C3B-CAB-CBB
18	A	830	CLA	C2B-C3B-CAB-CBB
18	A	837	CLA	C2B-C3B-CAB-CBB
18	A	839	CLA	C2B-C3B-CAB-CBB
18	A	841	CLA	C2B-C3B-CAB-CBB
18	B	811	CLA	C2B-C3B-CAB-CBB
18	B	819	CLA	C2B-C3B-CAB-CBB
18	B	835	CLA	C2B-C3B-CAB-CBB
18	B	838	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	1	602	CLA	C2B-C3B-CAB-CBB
18	1	608	CLA	C2B-C3B-CAB-CBB
18	3	301	CLA	C2B-C3B-CAB-CBB
18	3	307	CLA	C2B-C3B-CAB-CBB
18	3	309	CLA	C2B-C3B-CAB-CBB
18	3	312	CLA	C2B-C3B-CAB-CBB
18	7	601	CLA	C2B-C3B-CAB-CBB
18	7	603	CLA	C2B-C3B-CAB-CBB
18	7	608	CLA	C2B-C3B-CAB-CBB
18	7	611	CLA	C2B-C3B-CAB-CBB
18	8	603	CLA	C2B-C3B-CAB-CBB
18	8	608	CLA	C2B-C3B-CAB-CBB
18	8	614	CLA	C2B-C3B-CAB-CBB
18	Z	602	CLA	C2B-C3B-CAB-CBB
18	Z	607	CLA	C2B-C3B-CAB-CBB
18	4	606	CLA	C2B-C3B-CAB-CBB
18	4	608	CLA	C2B-C3B-CAB-CBB
18	5	609	CLA	C2B-C3B-CAB-CBB
18	5	610	CLA	C2B-C3B-CAB-CBB
18	5	617	CLA	C2B-C3B-CAB-CBB
18	6	302	CLA	C2B-C3B-CAB-CBB
18	6	303	CLA	C2B-C3B-CAB-CBB
18	6	313	CLA	C2B-C3B-CAB-CBB
18	6	314	CLA	C2B-C3B-CAB-CBB
21	4	605	CHL	CAA-CBA-CGA-O2A
18	F	302	CLA	C6-C7-C8-C10
18	A	824	CLA	C4C-C3C-CAC-CBC
18	B	815	CLA	C3A-C2A-CAA-CBA
18	7	612	CLA	CAA-CBA-CGA-O2A
18	6	312	CLA	CAA-CBA-CGA-O1A
18	6	311	CLA	CAA-CBA-CGA-O1A
18	A	807	CLA	C2C-C3C-CAC-CBC
18	5	617	CLA	C2C-C3C-CAC-CBC
18	6	311	CLA	CAA-CBA-CGA-O2A
18	Z	611	CLA	CAA-CBA-CGA-O2A
18	6	309	CLA	CAA-CBA-CGA-O2A
18	A	822	CLA	C1A-C2A-CAA-CBA
18	B	843	CLA	C1A-C2A-CAA-CBA
18	8	601	CLA	C1A-C2A-CAA-CBA
18	5	615	CLA	C2A-CAA-CBA-CGA
18	1	602	CLA	C4B-C3B-CAB-CBB
18	3	308	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	3	311	CLA	C4B-C3B-CAB-CBB
18	Z	602	CLA	C4B-C3B-CAB-CBB
18	4	607	CLA	C4B-C3B-CAB-CBB
18	5	609	CLA	C4B-C3B-CAB-CBB
18	5	610	CLA	C4B-C3B-CAB-CBB
18	B	822	CLA	C2C-C3C-CAC-CBC
21	7	606	CHL	CHA-CBD-CGD-O1D
21	4	604	CHL	CHA-CBD-CGD-O1D
21	4	604	CHL	CHA-CBD-CGD-O2D
21	4	605	CHL	CHA-CBD-CGD-O2D
21	6	306	CHL	CHA-CBD-CGD-O1D
21	6	306	CHL	CHA-CBD-CGD-O2D
18	B	830	CLA	CAA-CBA-CGA-O2A
18	3	312	CLA	CAA-CBA-CGA-O2A
18	A	836	CLA	C2C-C3C-CAC-CBC
18	7	612	CLA	CAA-CBA-CGA-O1A
18	7	608	CLA	C3A-C2A-CAA-CBA
18	B	830	CLA	CAA-CBA-CGA-O1A
18	F	301	CLA	CAA-CBA-CGA-O1A
18	3	312	CLA	CAA-CBA-CGA-O1A
18	Z	611	CLA	CAA-CBA-CGA-O1A
18	6	309	CLA	CAA-CBA-CGA-O1A
18	5	602	CLA	C2C-C3C-CAC-CBC
19	A	842	PQN	C22-C23-C25-C26
18	A	804	CLA	C2B-C3B-CAB-CBB
18	A	818	CLA	C2B-C3B-CAB-CBB
18	B	817	CLA	C2B-C3B-CAB-CBB
18	B	824	CLA	C2B-C3B-CAB-CBB
18	1	614	CLA	C2B-C3B-CAB-CBB
18	3	308	CLA	C2B-C3B-CAB-CBB
18	8	602	CLA	C2B-C3B-CAB-CBB
18	Z	613	CLA	C2B-C3B-CAB-CBB
18	4	601	CLA	C2B-C3B-CAB-CBB
18	4	607	CLA	C2B-C3B-CAB-CBB
18	4	610	CLA	C2B-C3B-CAB-CBB
18	6	317	CLA	C2B-C3B-CAB-CBB
18	5	610	CLA	C2A-CAA-CBA-CGA
18	4	603	CLA	CAA-CBA-CGA-O2A
18	A	813	CLA	C2C-C3C-CAC-CBC
18	5	603	CLA	CAA-CBA-CGA-O2A
18	5	617	CLA	CAA-CBA-CGA-O2A
18	A	806	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	A	815	CLA	C4B-C3B-CAB-CBB
18	A	817	CLA	C4B-C3B-CAB-CBB
18	A	821	CLA	C4B-C3B-CAB-CBB
18	A	845	CLA	C4B-C3B-CAB-CBB
18	B	810	CLA	C4B-C3B-CAB-CBB
18	B	817	CLA	C4B-C3B-CAB-CBB
18	B	820	CLA	C4B-C3B-CAB-CBB
18	B	822	CLA	C4B-C3B-CAB-CBB
18	B	830	CLA	C4B-C3B-CAB-CBB
18	B	838	CLA	C4B-C3B-CAB-CBB
18	J	101	CLA	C4B-C3B-CAB-CBB
18	1	614	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C4B-C3B-CAB-CBB
18	5	601	CLA	C4B-C3B-CAB-CBB
18	5	611	CLA	C4B-C3B-CAB-CBB
18	6	308	CLA	C4B-C3B-CAB-CBB
18	A	843	CLA	CAA-CBA-CGA-O2A
18	F	301	CLA	CAA-CBA-CGA-O2A
18	3	310	CLA	CAA-CBA-CGA-O2A
18	6	303	CLA	CAA-CBA-CGA-O2A
18	A	813	CLA	C4C-C3C-CAC-CBC
18	B	819	CLA	C3A-C2A-CAA-CBA
18	1	608	CLA	C3A-C2A-CAA-CBA
18	Z	607	CLA	C3A-C2A-CAA-CBA
18	F	301	CLA	C3A-C2A-CAA-CBA
18	4	603	CLA	CAA-CBA-CGA-O1A
19	A	842	PQN	C23-C25-C26-C27
18	B	807	CLA	C6-C7-C8-C9
18	5	603	CLA	CAA-CBA-CGA-O1A
18	6	303	CLA	CAA-CBA-CGA-O1A
18	5	617	CLA	CAA-CBA-CGA-O1A
18	A	843	CLA	CAA-CBA-CGA-O1A
18	8	612	CLA	CAA-CBA-CGA-O2A
18	B	833	CLA	C2C-C3C-CAC-CBC
18	A	811	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	A	841	CLA	CAD-CBD-CGD-O2D
18	B	813	CLA	CAD-CBD-CGD-O2D
18	3	307	CLA	CAD-CBD-CGD-O2D
18	7	605	CLA	CAD-CBD-CGD-O2D
18	8	607	CLA	CAD-CBD-CGD-O2D
18	8	609	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	8	606	CHL	C1A-C2A-CAA-CBA
18	5	610	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

163 monomers are involved in 300 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	823	CLA	2	0
18	B	835	CLA	3	0
18	3	312	CLA	1	0
21	5	616	CHL	1	0
18	7	614	CLA	1	0
18	1	611	CLA	1	0
18	5	614	CLA	2	0
18	Z	612	CLA	3	0
18	4	607	CLA	1	0
18	A	838	CLA	3	0
18	B	807	CLA	1	0
18	A	818	CLA	2	0
18	1	605	CLA	4	0
18	B	819	CLA	2	0
18	B	809	CLA	1	0
18	A	828	CLA	2	0
18	8	614	CLA	1	0
20	C	102	SF4	1	0
18	B	837	CLA	2	0
18	B	813	CLA	2	0
18	A	819	CLA	1	0
18	A	820	CLA	1	0
18	8	612	CLA	2	0
21	1	606	CHL	2	0
18	A	816	CLA	1	0
18	B	808	CLA	2	0
18	Z	610	CLA	1	0
21	8	606	CHL	3	0
18	F	302	CLA	11	0
18	B	840	CLA	2	0
18	7	608	CLA	2	0
18	3	305	CLA	2	0
18	A	822	CLA	2	0
21	6	307	CHL	1	0
18	A	817	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	808	CLA	2	0
18	B	830	CLA	2	0
18	Z	603	CLA	5	0
18	A	806	CLA	3	0
18	1	612	CLA	5	0
18	5	611	CLA	6	0
18	A	826	CLA	1	0
18	3	311	CLA	1	0
18	4	602	CLA	2	0
21	Z	605	CHL	2	0
18	B	836	CLA	1	0
18	A	834	CLA	2	0
20	B	803	SF4	1	0
18	4	611	CLA	1	0
18	4	609	CLA	1	0
18	B	825	CLA	2	0
18	8	613	CLA	1	0
18	B	832	CLA	2	0
18	7	602	CLA	3	0
18	6	312	CLA	1	0
18	A	809	CLA	3	0
18	3	303	CLA	4	0
18	B	812	CLA	1	0
18	B	829	CLA	3	0
18	5	604	CLA	1	0
18	1	613	CLA	2	0
18	B	834	CLA	3	0
18	A	805	CLA	1	0
18	8	602	CLA	1	0
18	7	604	CLA	5	0
18	A	812	CLA	2	0
18	A	843	CLA	7	0
18	Z	611	CLA	4	0
18	1	604	CLA	3	0
18	B	821	CLA	1	0
18	B	826	CLA	3	0
18	4	603	CLA	1	0
18	A	824	CLA	1	0
18	A	841	CLA	2	0
18	B	823	CLA	1	0
18	5	605	CLA	2	0
18	5	601	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	801	CL0	7	0
18	F	301	CLA	1	0
18	8	609	CLA	2	0
18	Z	604	CLA	4	0
18	B	802	CLA	4	0
18	B	816	CLA	4	0
18	3	314	CLA	3	0
18	7	601	CLA	2	0
21	6	306	CHL	1	0
18	3	313	CLA	5	0
18	B	801	CLA	1	0
18	B	806	CLA	3	0
18	8	605	CLA	3	0
18	B	814	CLA	5	0
18	6	310	CLA	1	0
18	3	308	CLA	1	0
19	B	844	PQN	5	0
18	3	307	CLA	5	0
18	A	835	CLA	2	0
18	J	101	CLA	2	0
18	3	304	CLA	2	0
18	A	802	CLA	3	0
18	8	604	CLA	1	0
18	A	845	CLA	10	0
18	8	601	CLA	2	0
18	B	839	CLA	2	0
18	4	610	CLA	2	0
18	A	839	CLA	1	0
18	A	825	CLA	1	0
18	B	843	CLA	3	0
21	4	605	CHL	1	0
18	4	608	CLA	1	0
18	A	844	CLA	4	0
18	Z	608	CLA	3	0
21	6	305	CHL	2	0
18	B	815	CLA	3	0
18	B	842	CLA	6	0
18	7	609	CLA	1	0
18	A	811	CLA	1	0
18	5	612	CLA	2	0
18	5	610	CLA	5	0
21	Z	601	CHL	1	0

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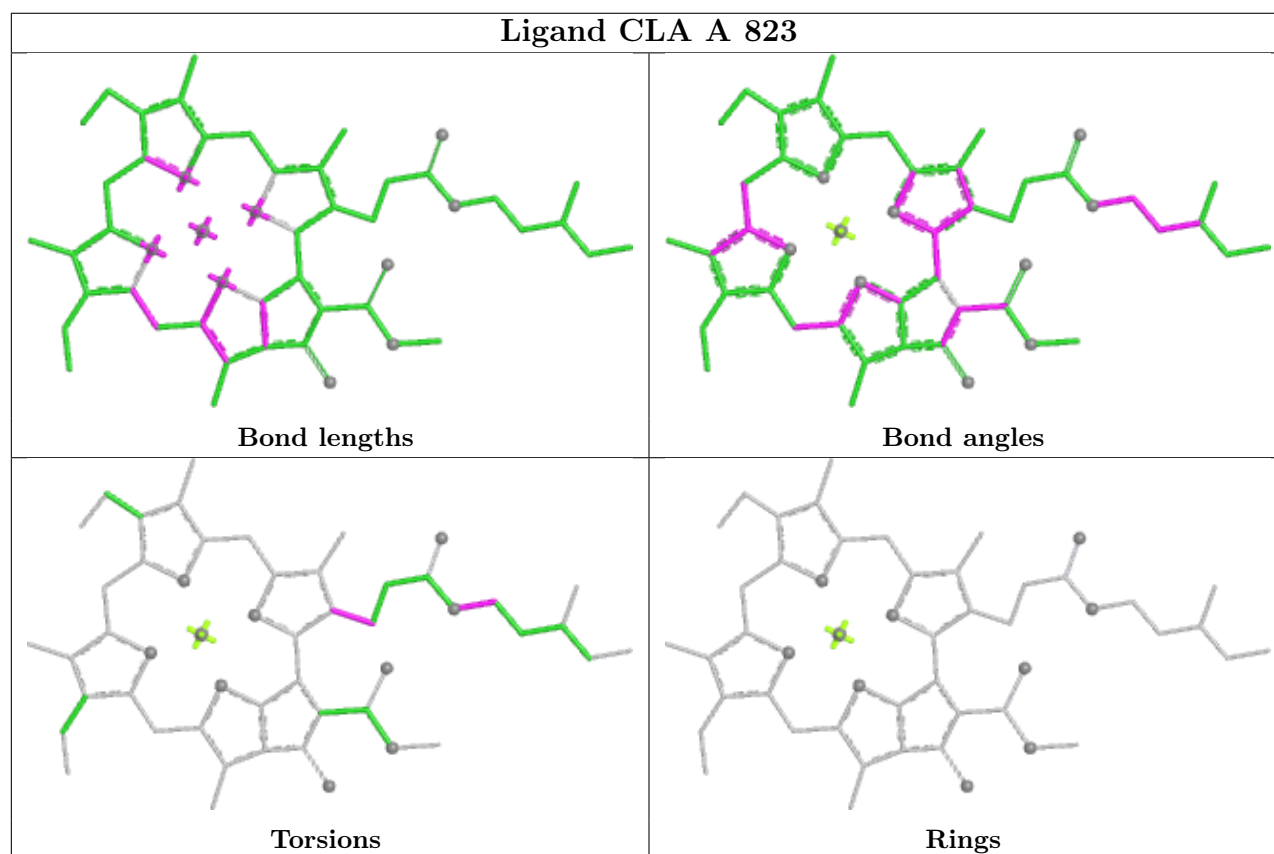
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	101	SF4	2	0
18	A	807	CLA	2	0
18	B	827	CLA	1	0
18	8	608	CLA	2	0
21	4	604	CHL	4	0
19	A	842	PQN	6	0
18	5	613	CLA	2	0
18	B	817	CLA	2	0
21	1	601	CHL	2	0
18	1	609	CLA	3	0
18	A	837	CLA	1	0
18	A	813	CLA	2	0
18	7	612	CLA	4	0
18	6	304	CLA	1	0
18	A	830	CLA	2	0
18	7	605	CLA	3	0
18	6	309	CLA	2	0
18	B	811	CLA	4	0
18	6	315	CLA	1	0
18	B	841	CLA	2	0
18	8	611	CLA	1	0
18	A	836	CLA	2	0
18	B	831	CLA	2	0
18	A	827	CLA	2	0
18	A	814	CLA	1	0
18	6	317	CLA	1	0
18	B	810	CLA	3	0
18	3	302	CLA	3	0
18	6	308	CLA	1	0
18	6	301	CLA	11	0
18	B	818	CLA	1	0
18	B	804	CLA	6	0
18	B	833	CLA	1	0
18	B	822	CLA	2	0
18	A	815	CLA	2	0
21	5	607	CHL	2	0
18	5	602	CLA	2	0
18	1	614	CLA	1	0
18	A	803	CLA	2	0
18	A	833	CLA	1	0
18	B	824	CLA	3	0
18	7	613	CLA	2	0

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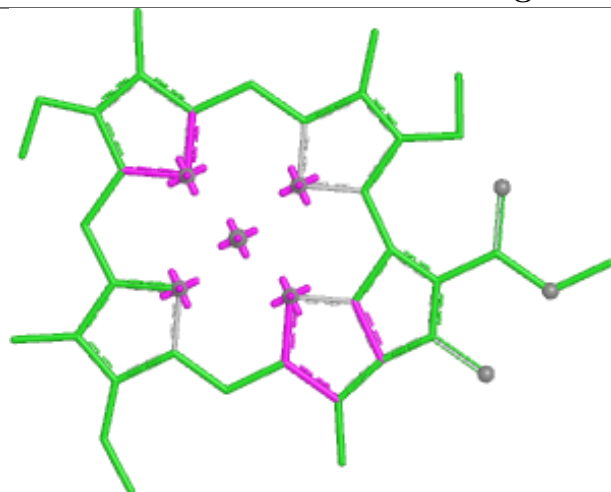
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	805	CLA	1	0
18	6	311	CLA	2	0

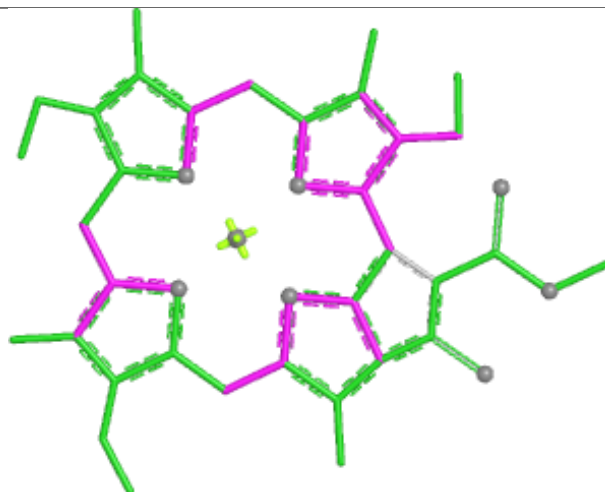
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



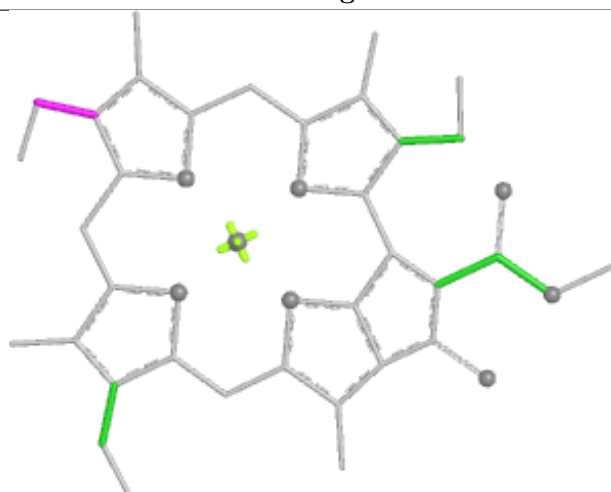
Ligand CLA B 835



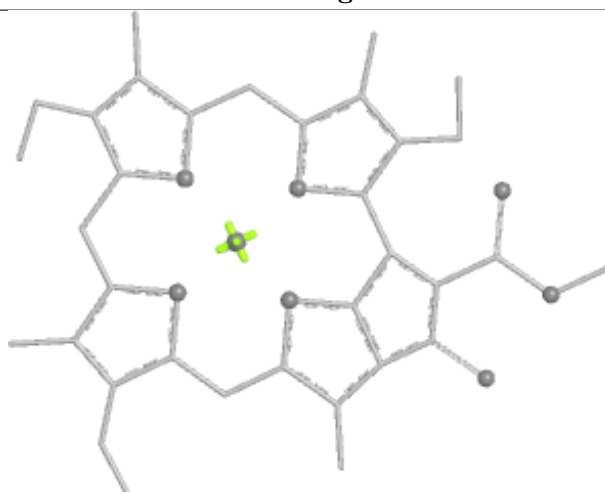
Bond lengths



Bond angles

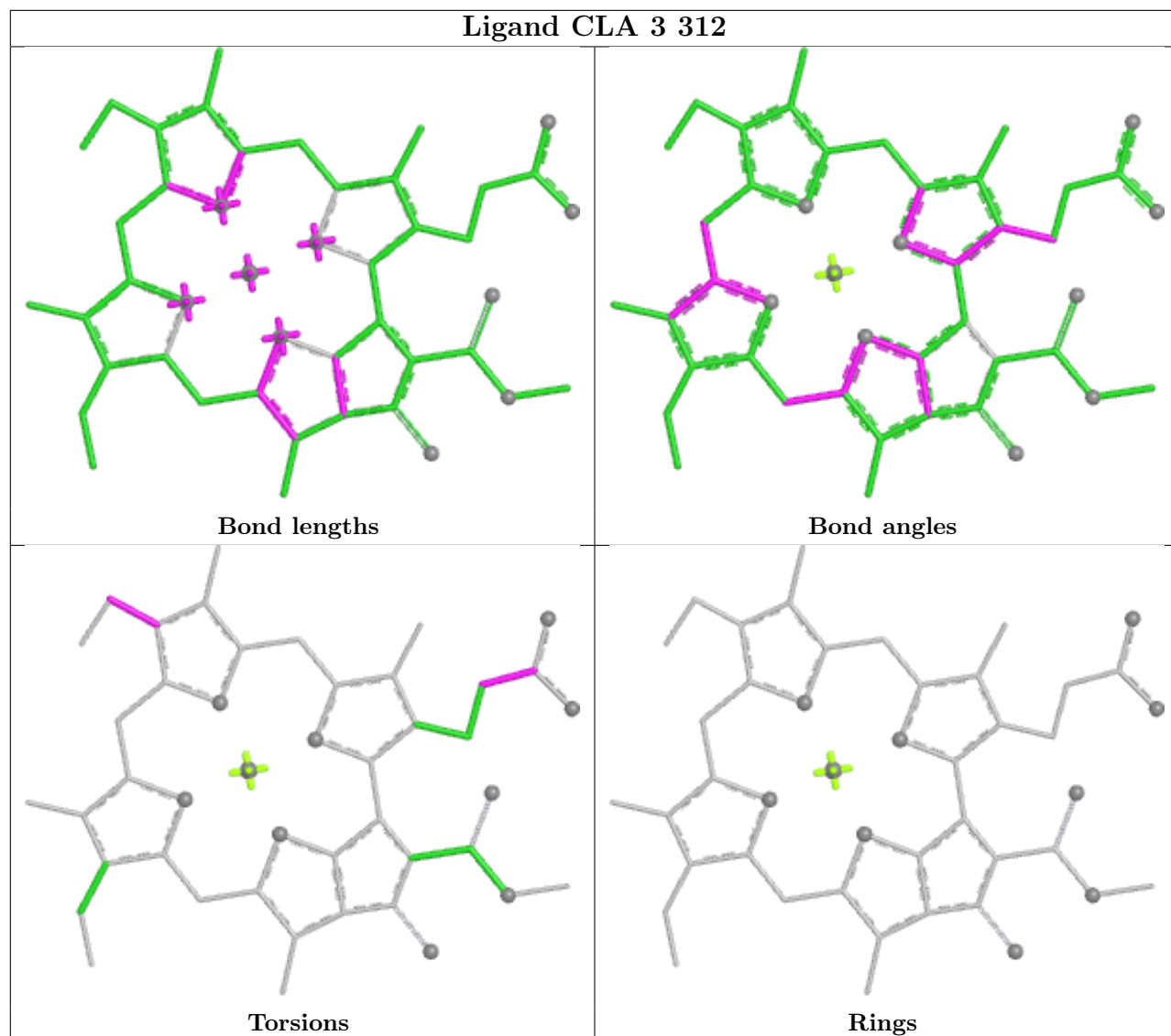


Torsions

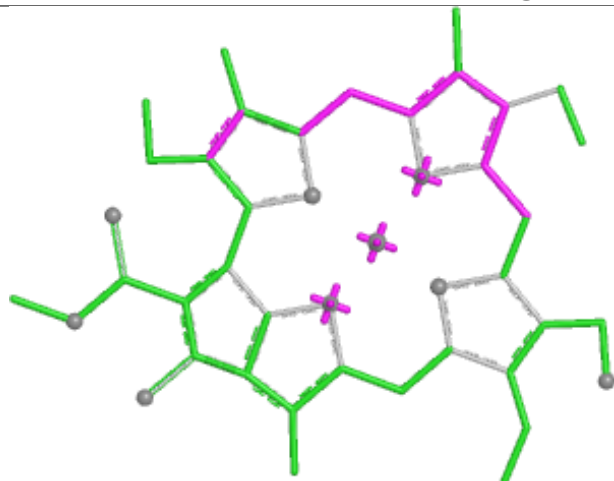


Rings

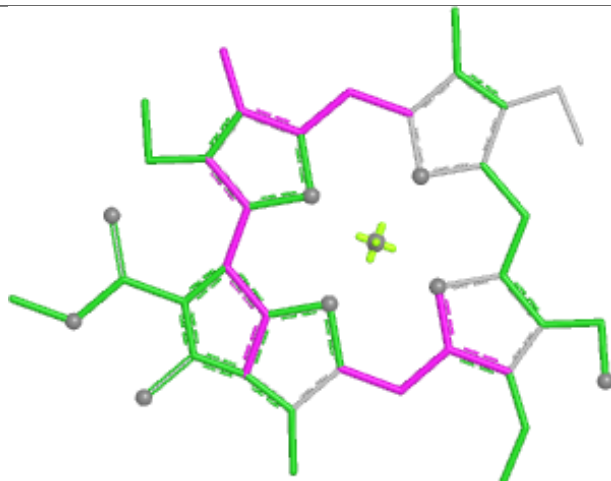
Ligand CLA 3 312



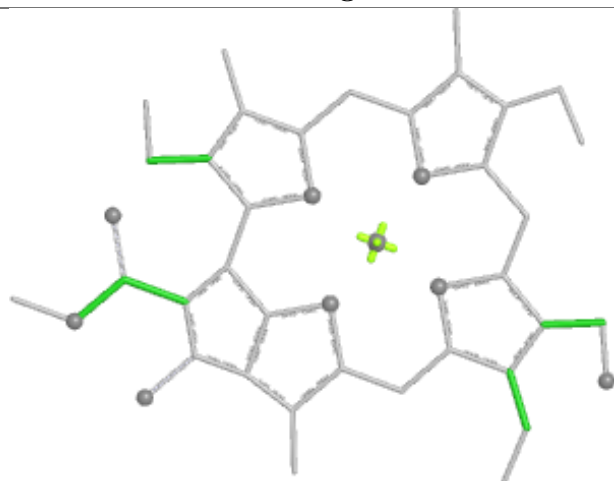
Ligand CHL 5 616



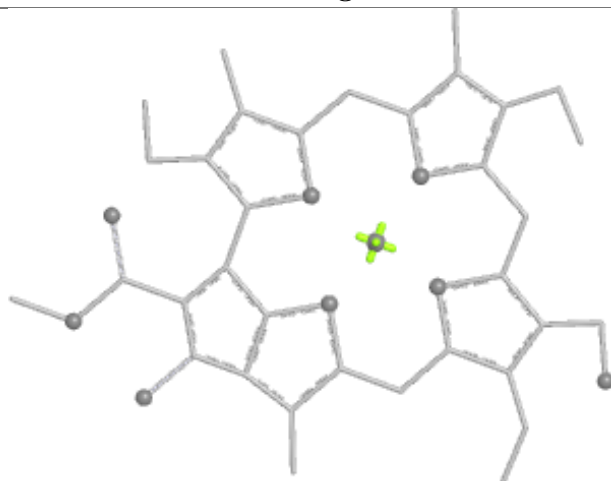
Bond lengths



Bond angles

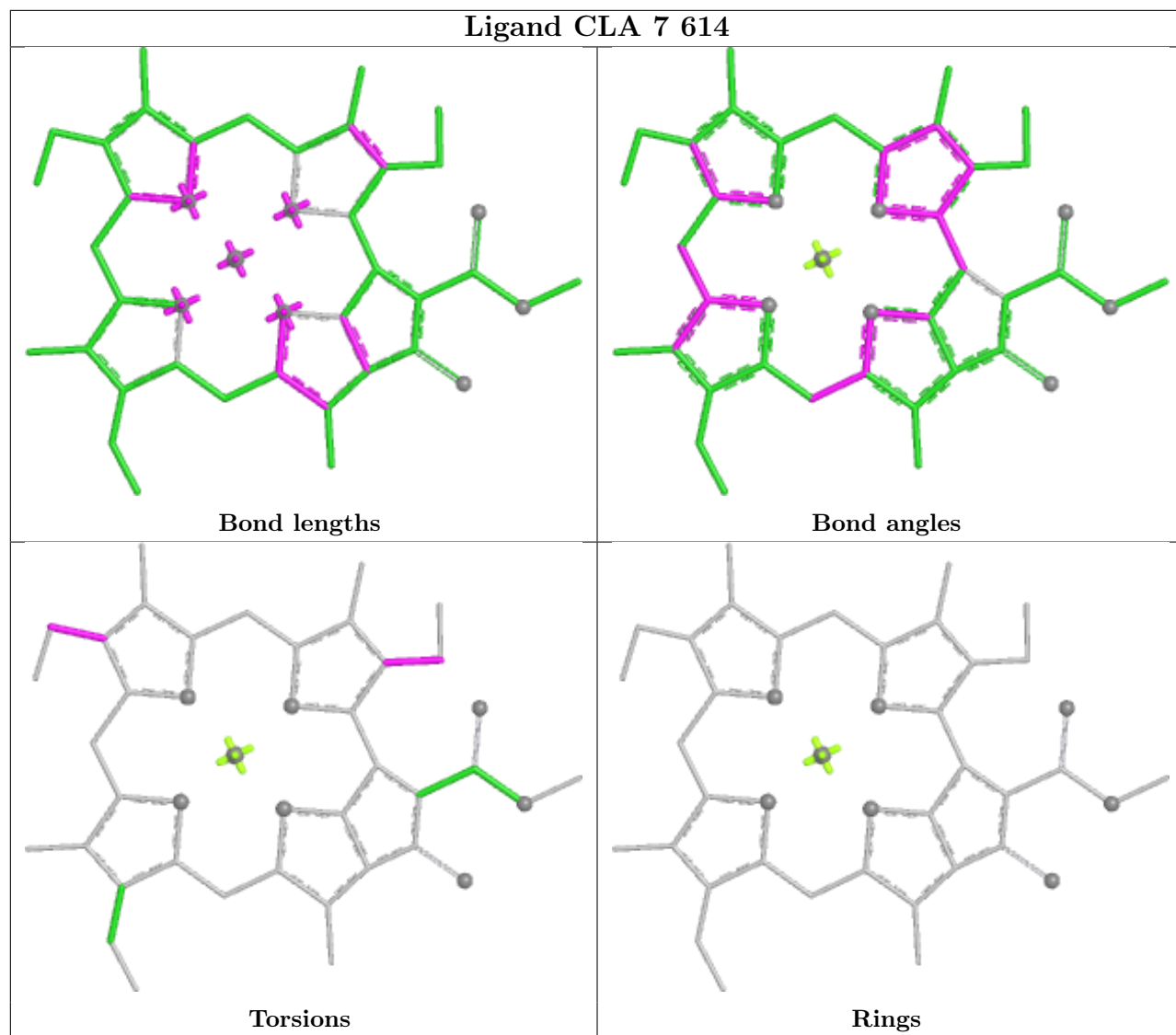


Torsions

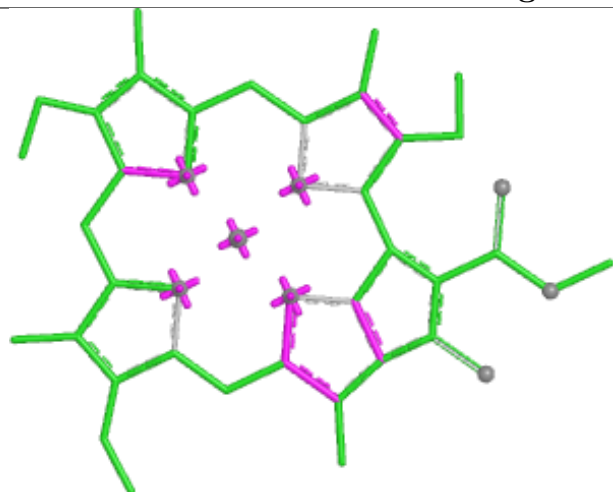


Rings

Ligand CLA 7 614



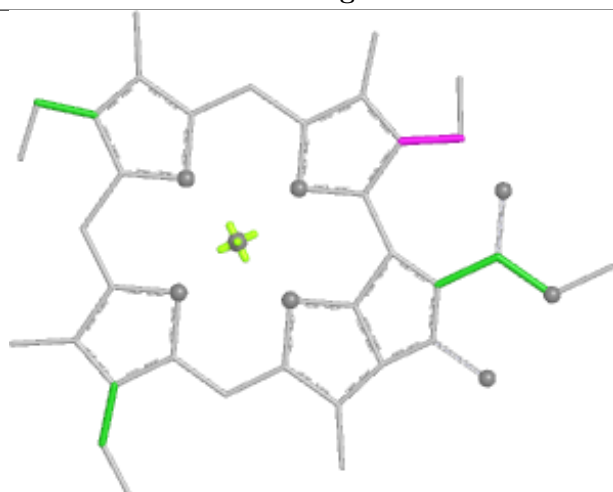
Ligand CLA 1 611



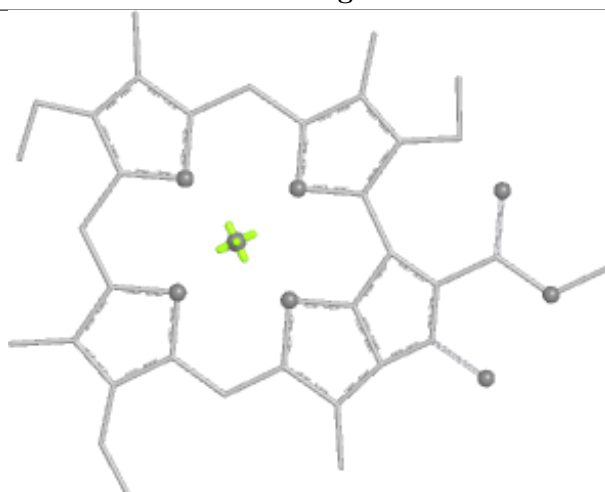
Bond lengths



Bond angles

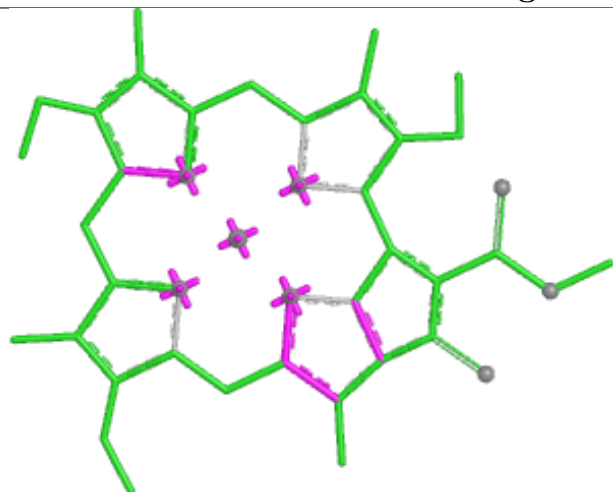


Torsions

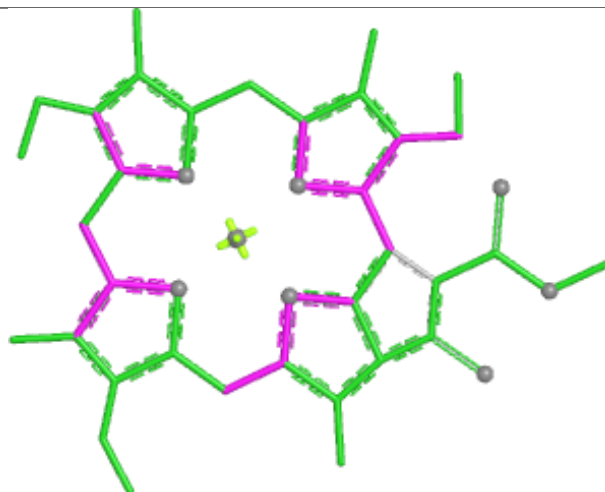


Rings

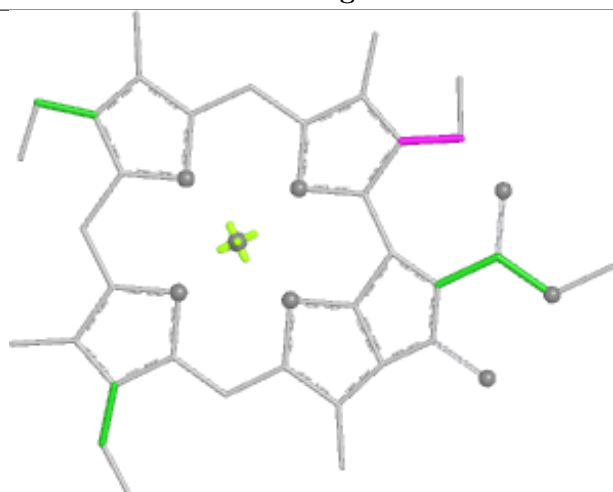
Ligand CLA 5 614



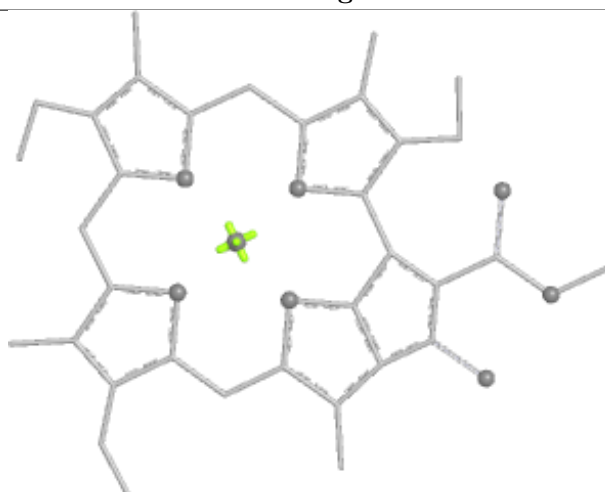
Bond lengths



Bond angles

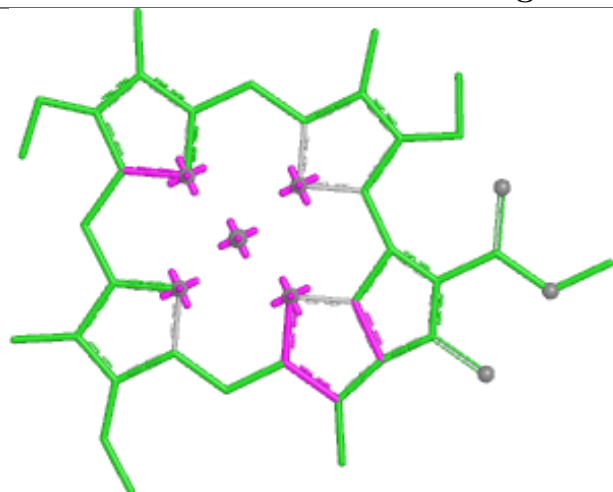


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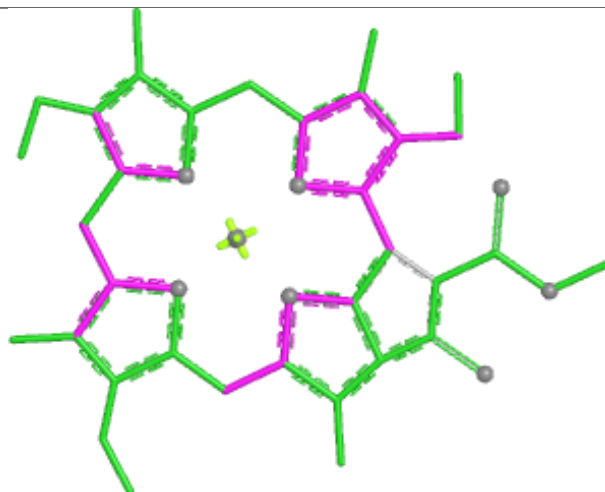


Rings

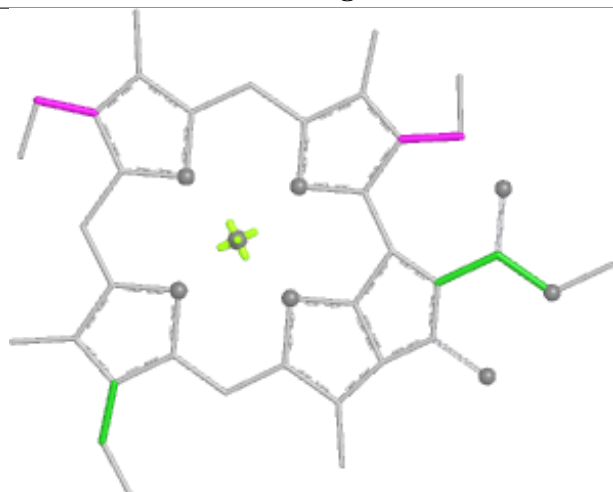
Ligand CLA Z 607



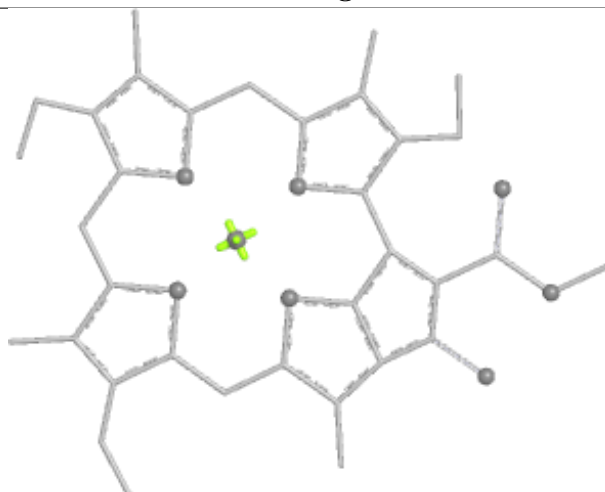
Bond lengths



Bond angles

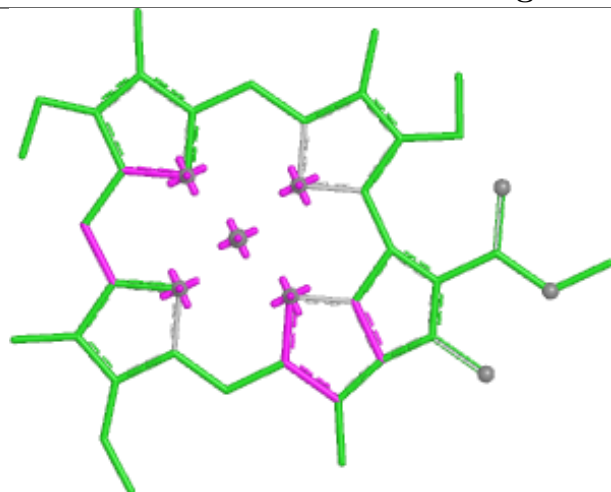


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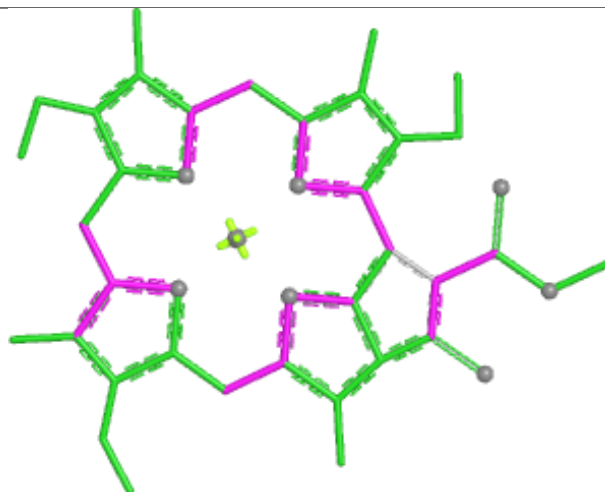


Rings

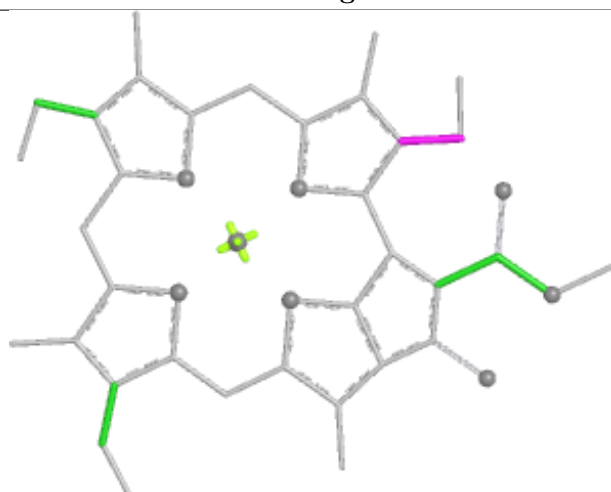
Ligand CLA Z 612



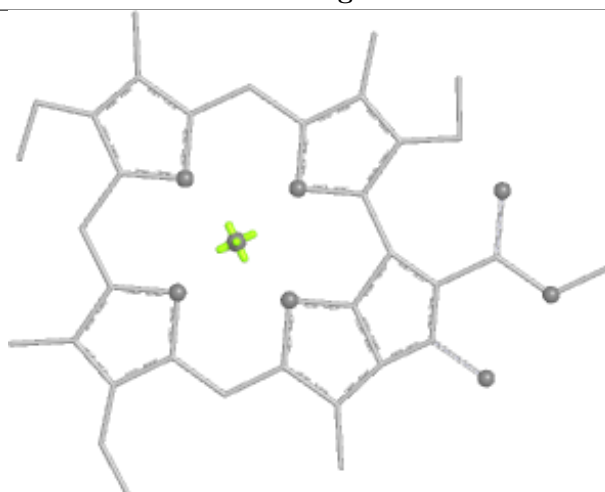
Bond lengths



Bond angles

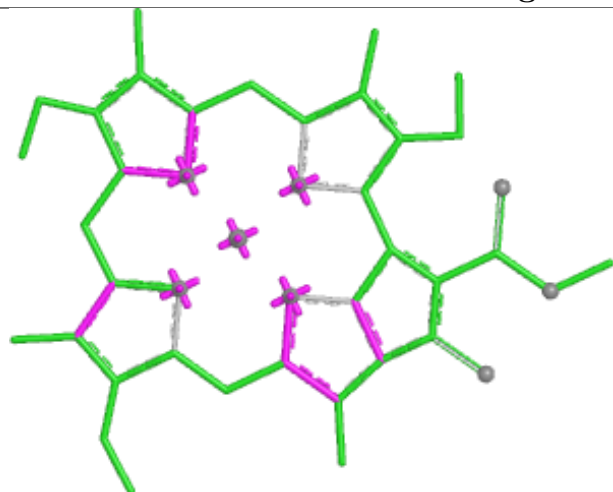


Torsions



Rings

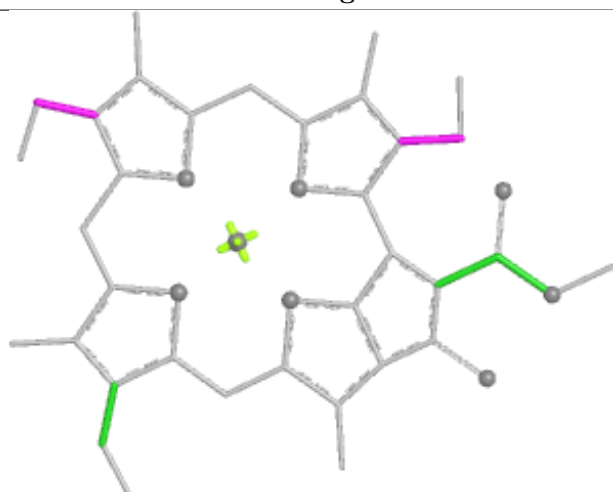
Ligand CLA 4 607



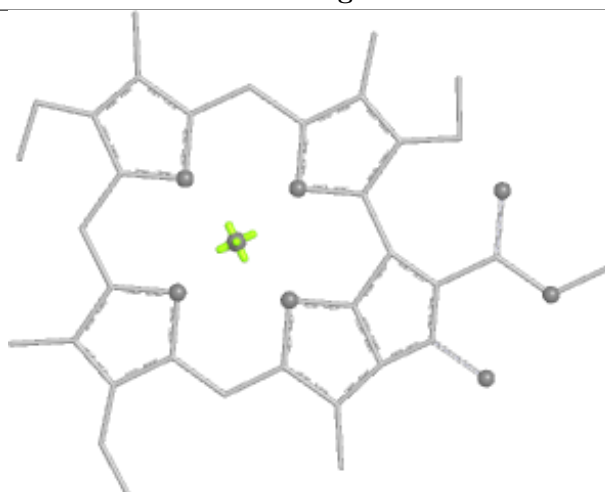
Bond lengths



Bond angles

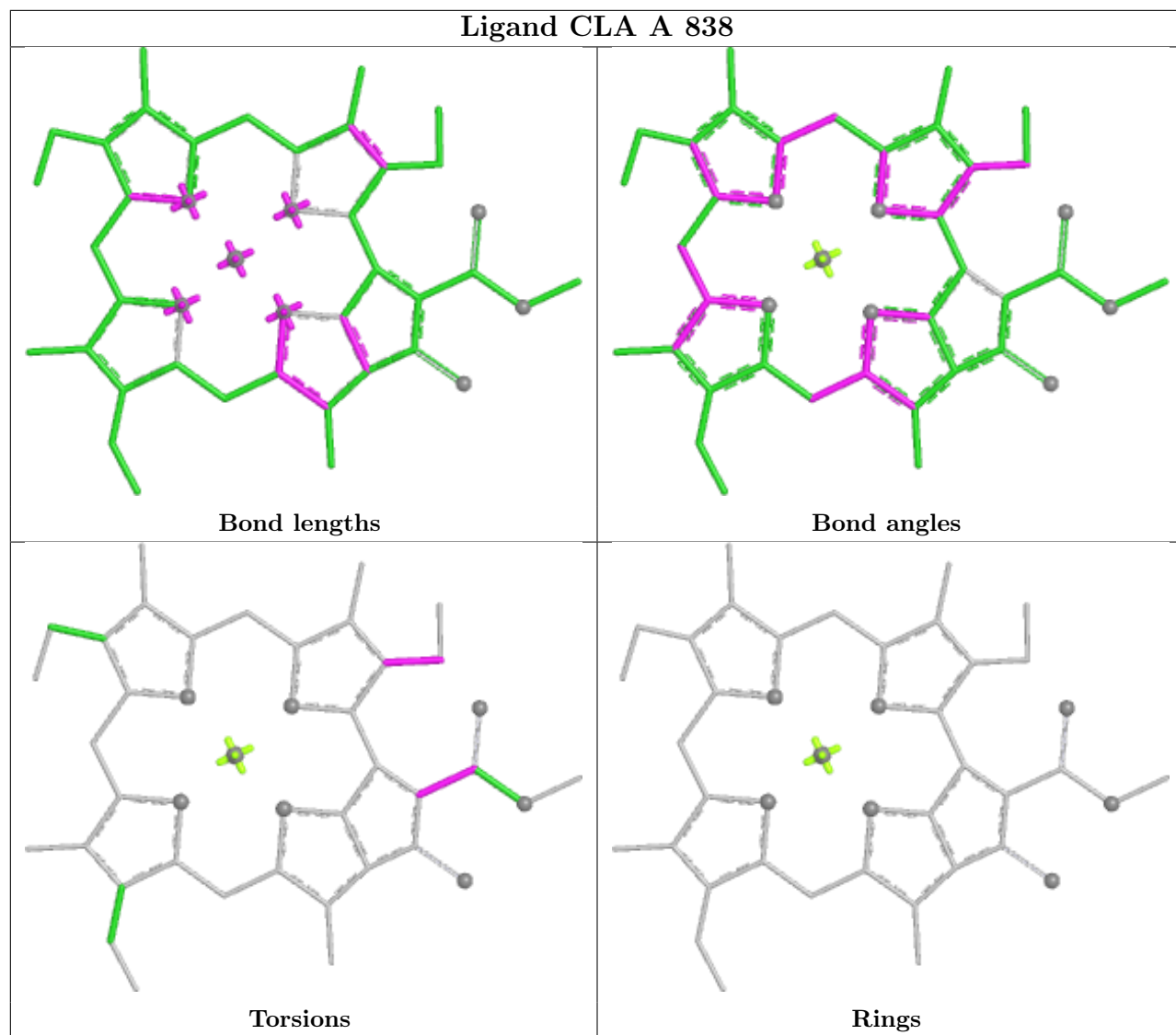


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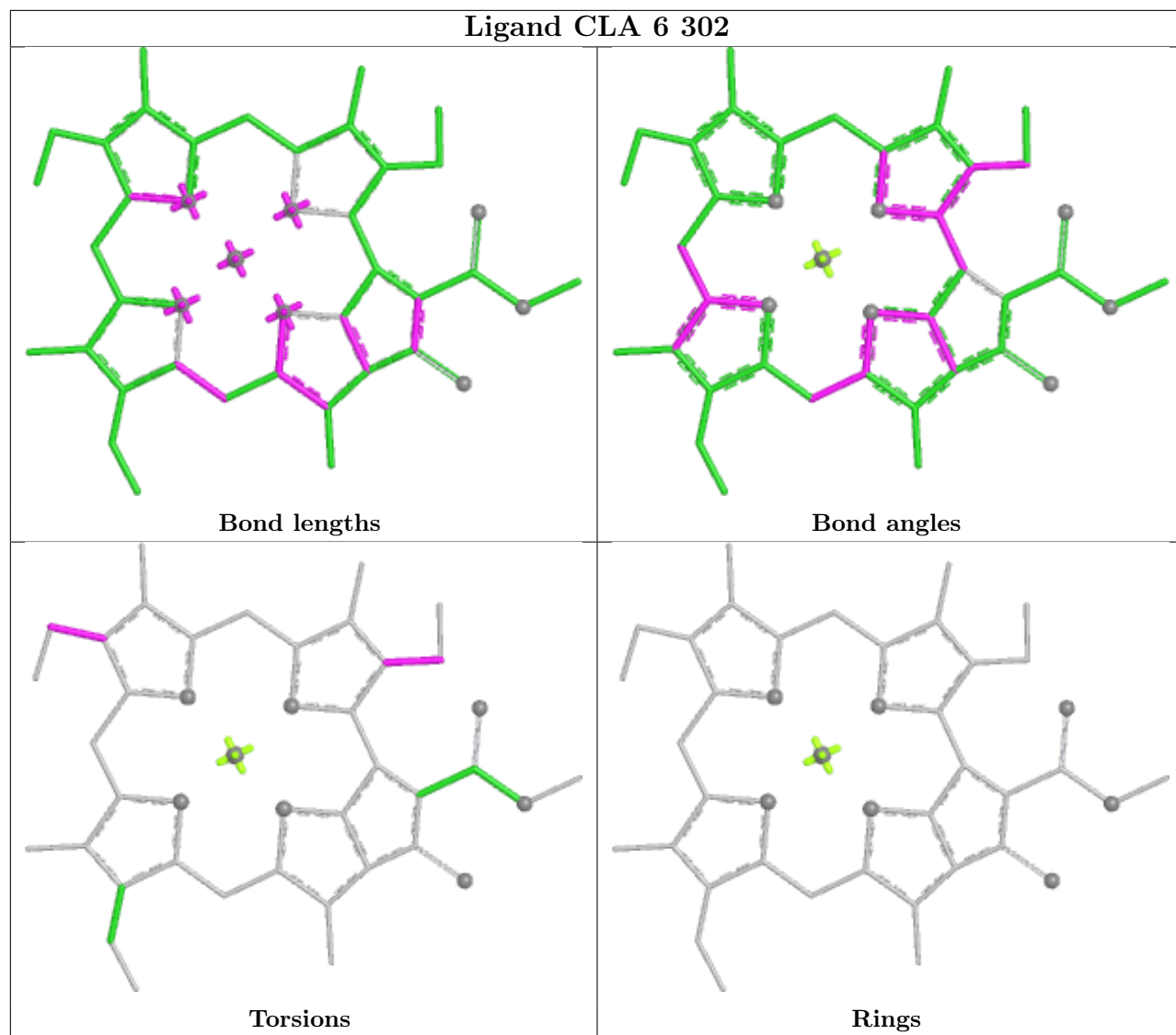


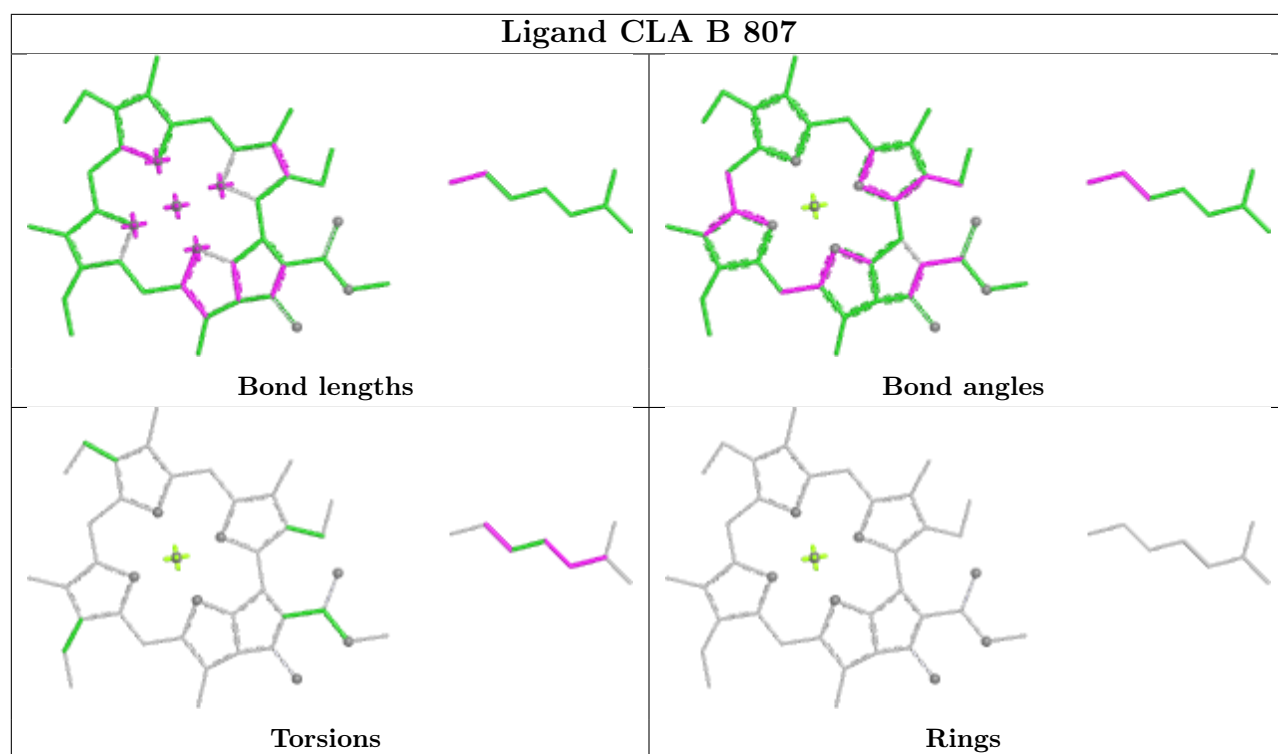
Rings

Ligand CLA A 838

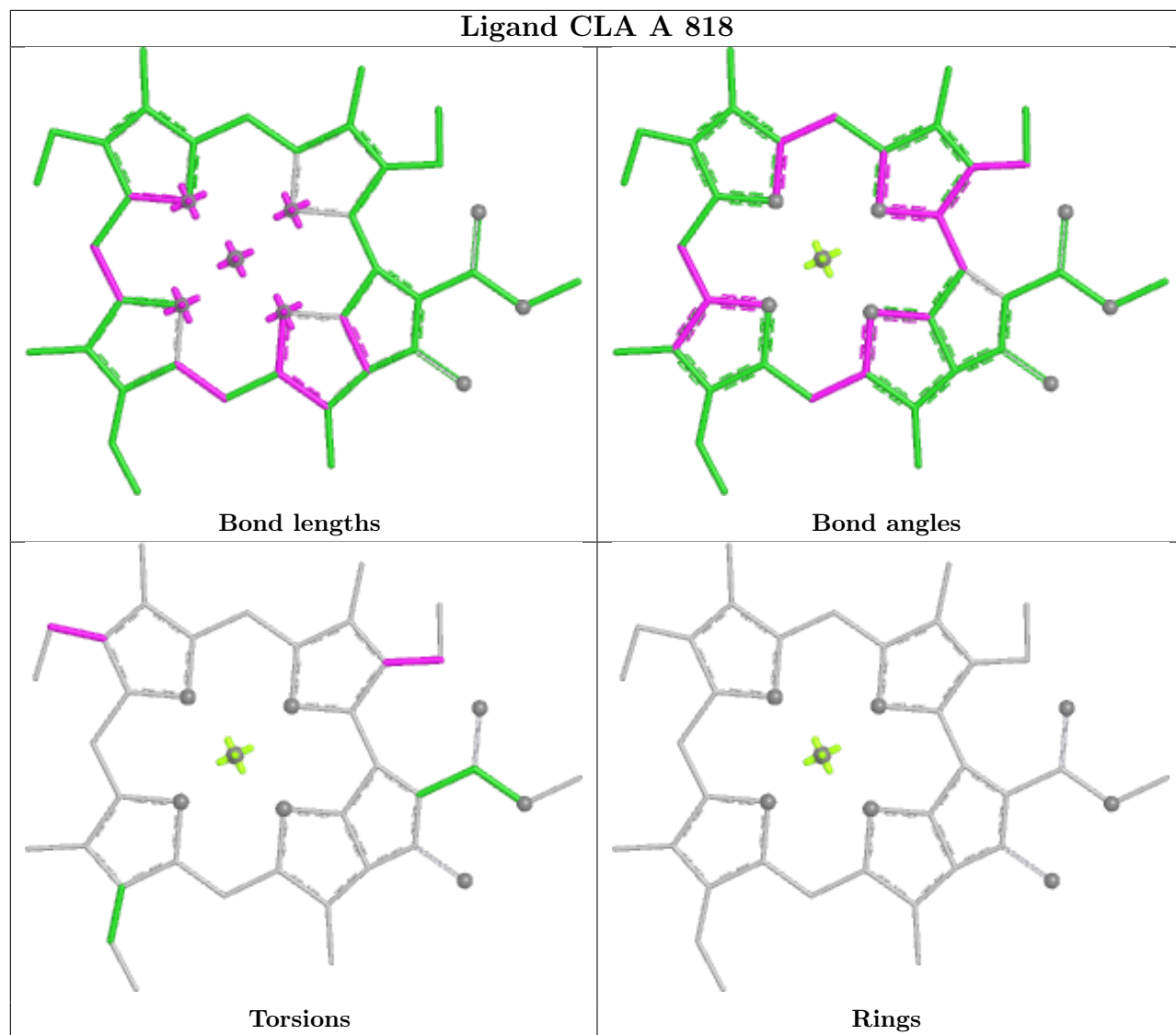


Ligand CLA 6 302

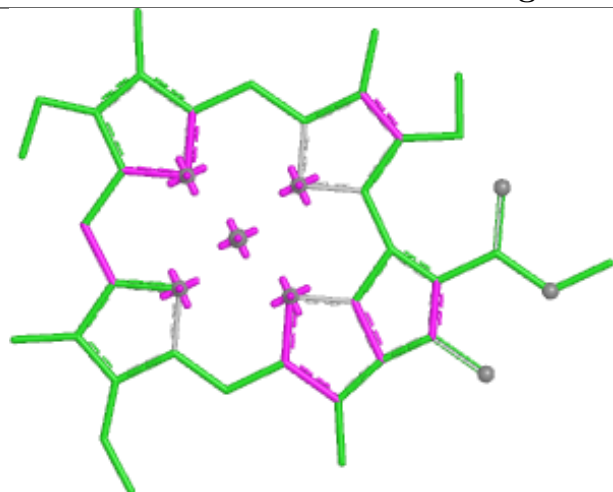




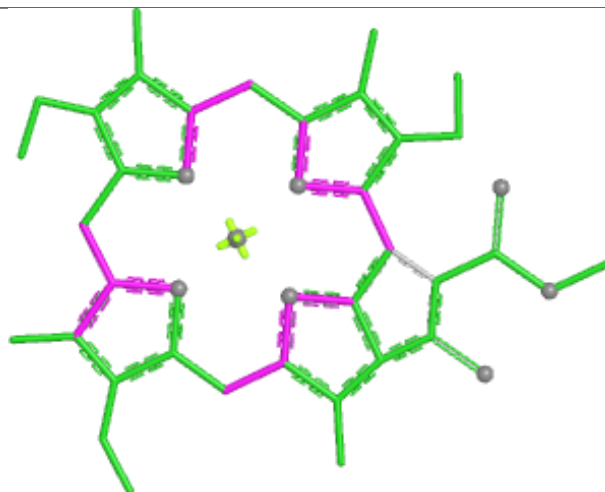
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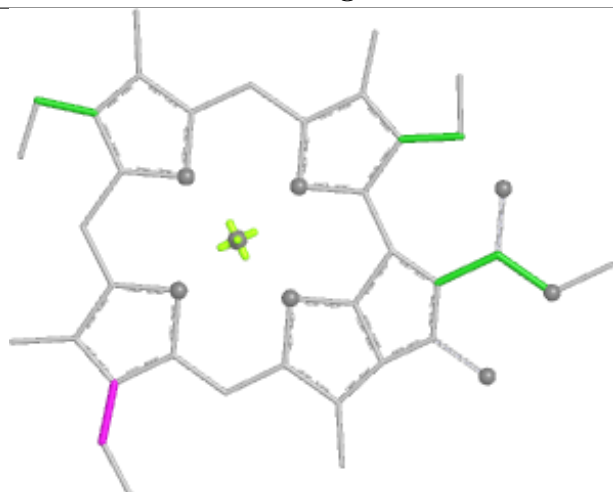
Ligand CLA 1 605



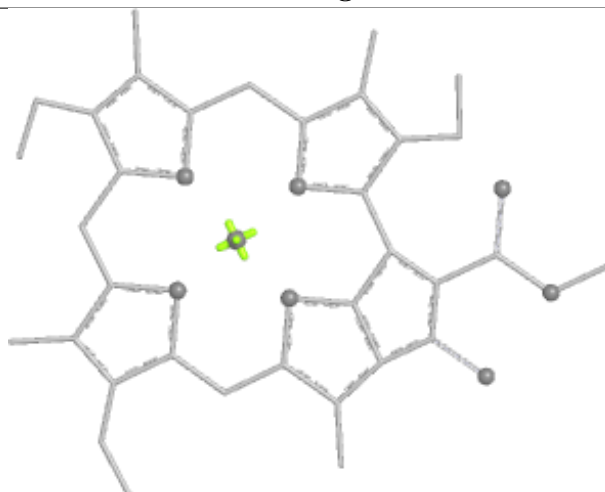
Bond lengths



Bond angles

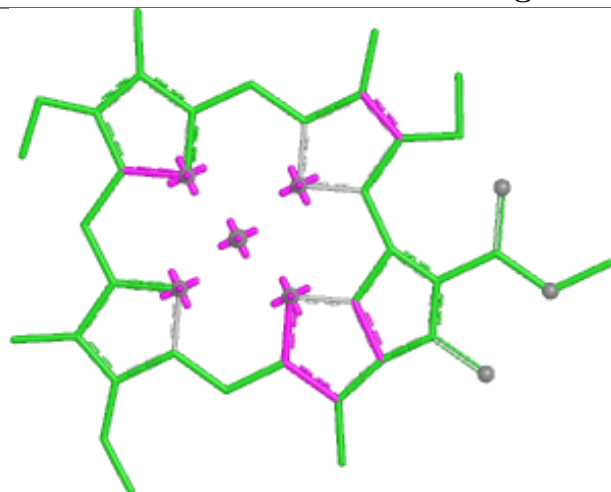


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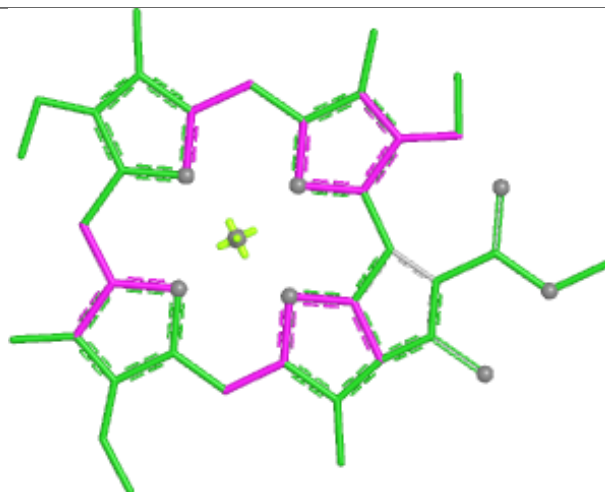


Rings

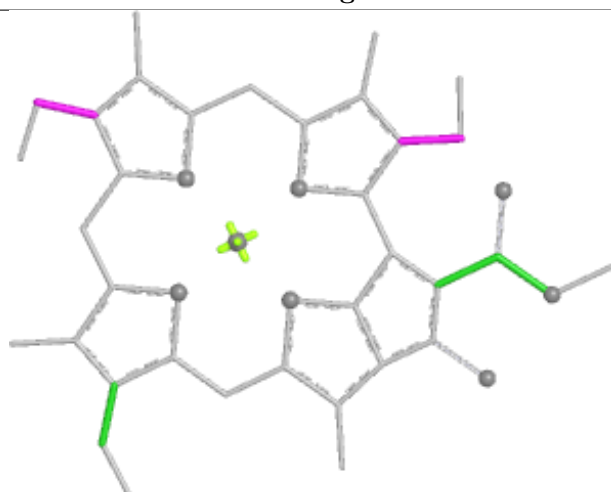
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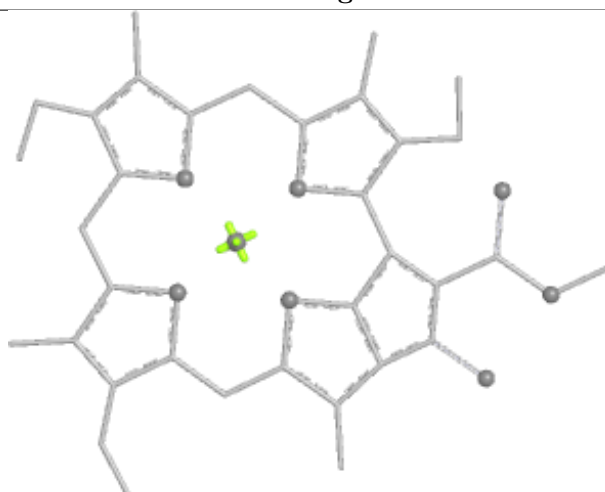
Bond lengths



Bond angles

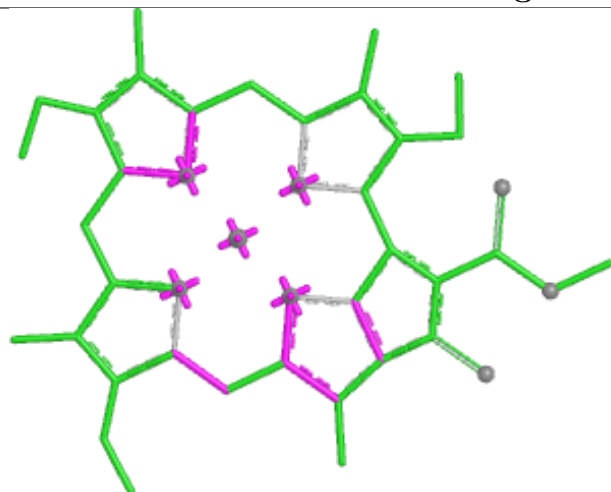


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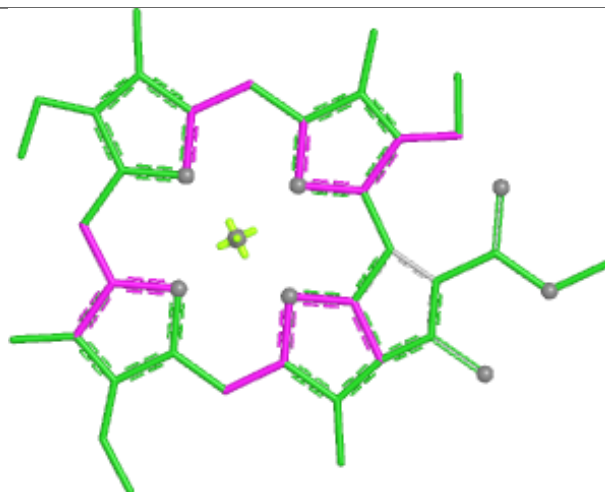


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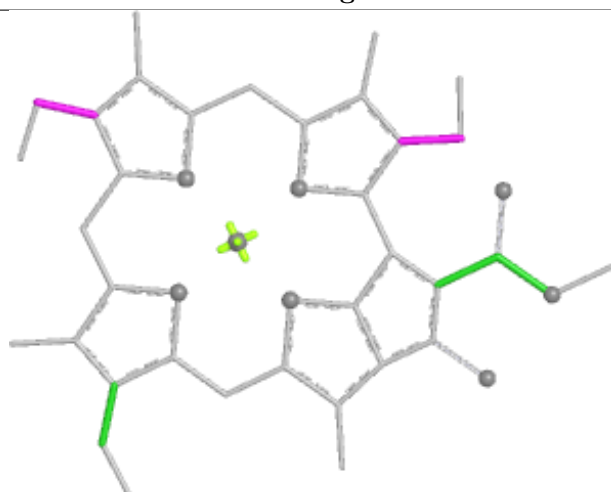
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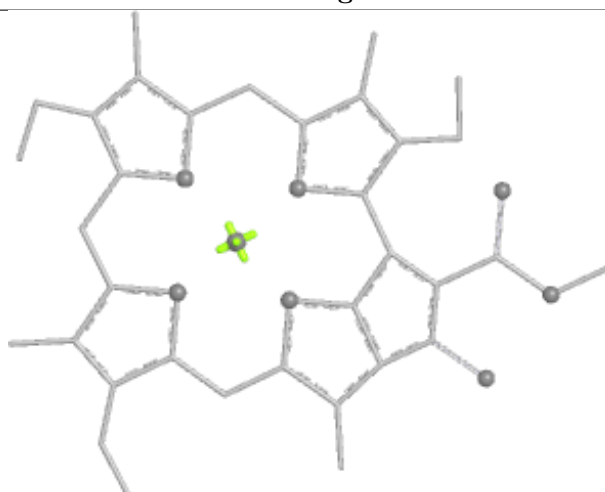
Bond lengths



Bond angles

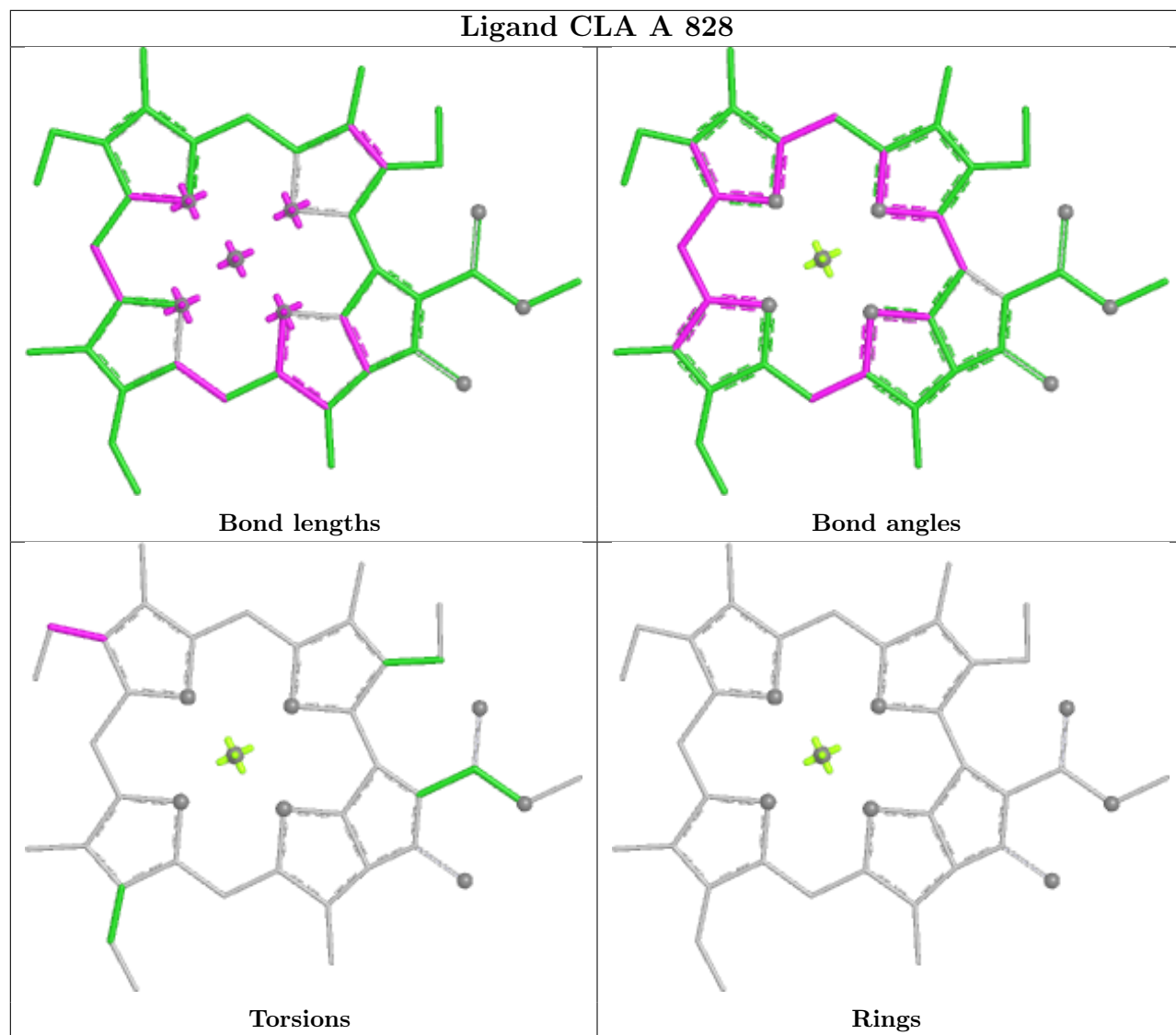


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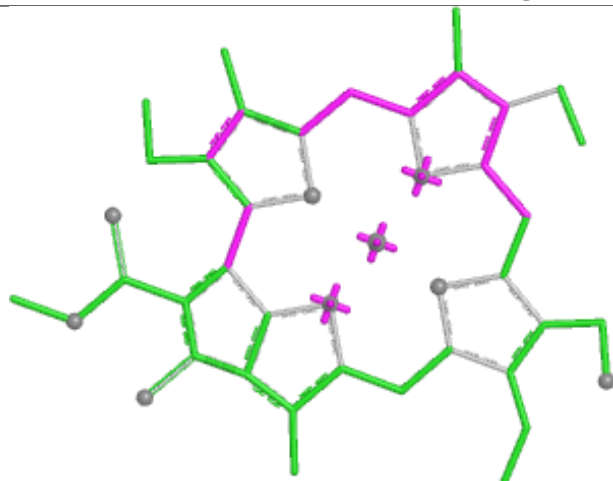


Rings

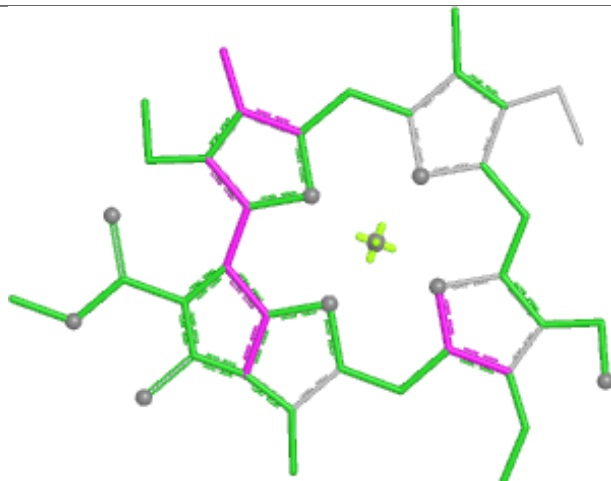
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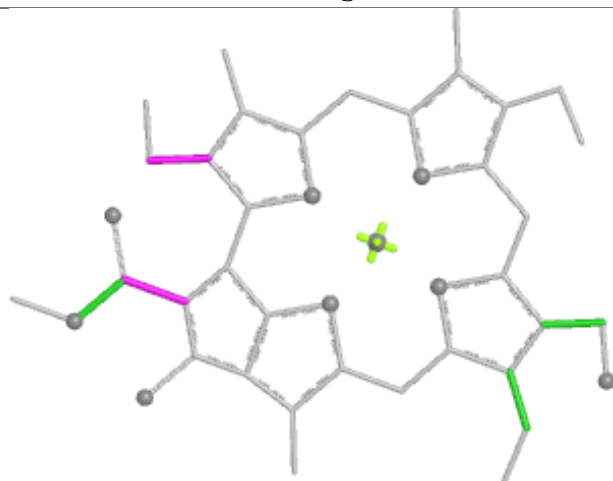
Ligand CHL 7 606



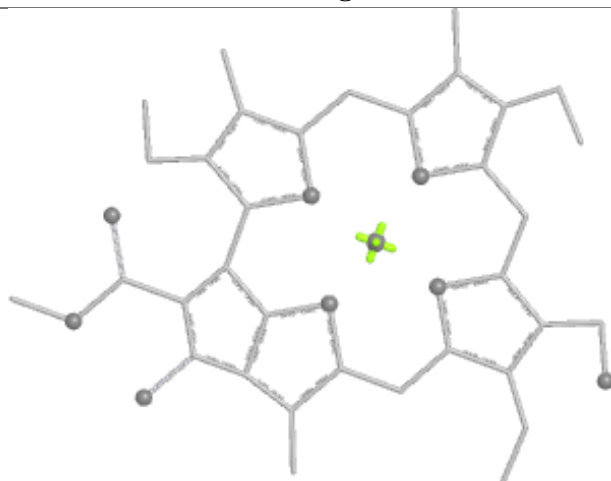
Bond lengths



Bond angles

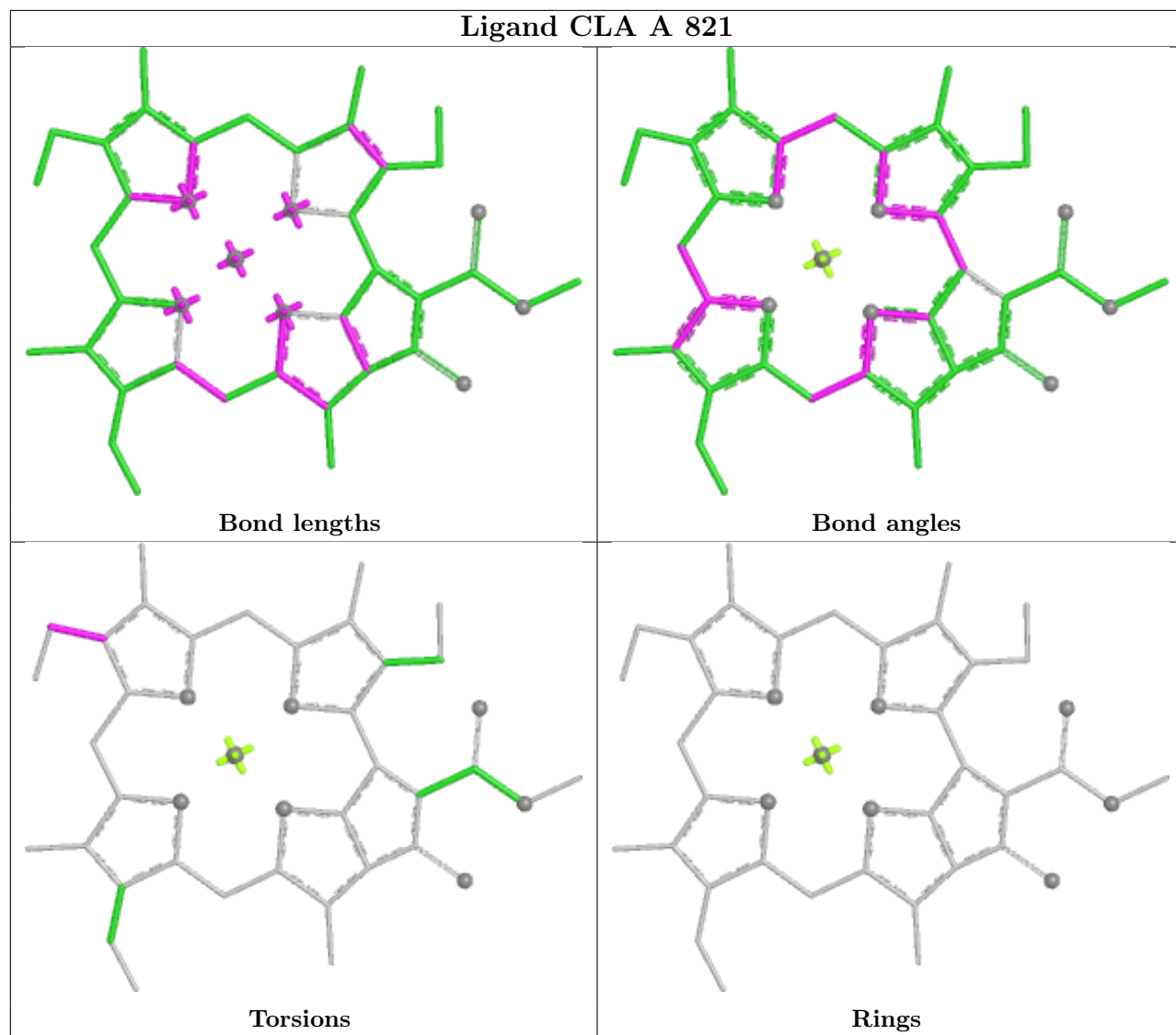


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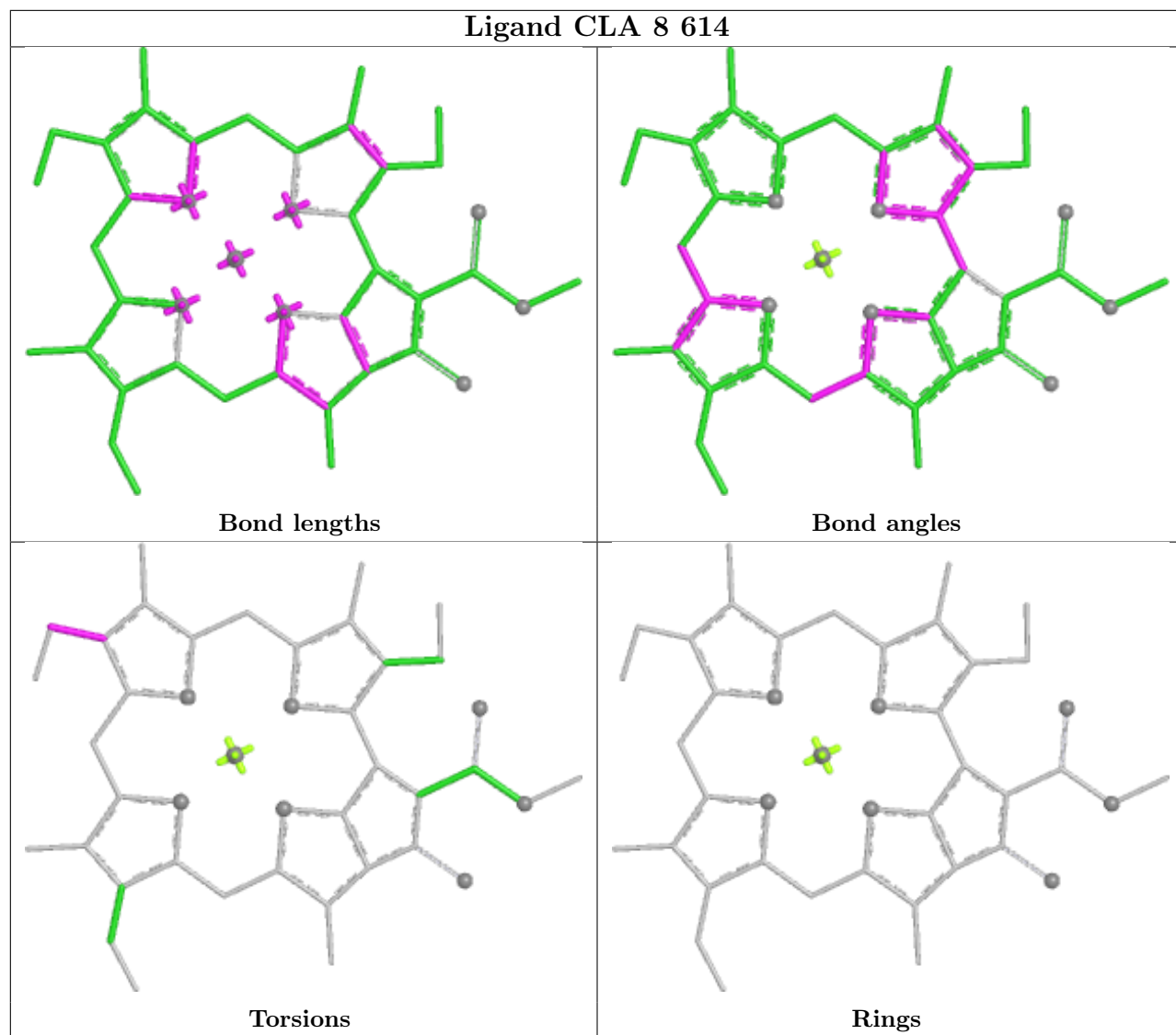


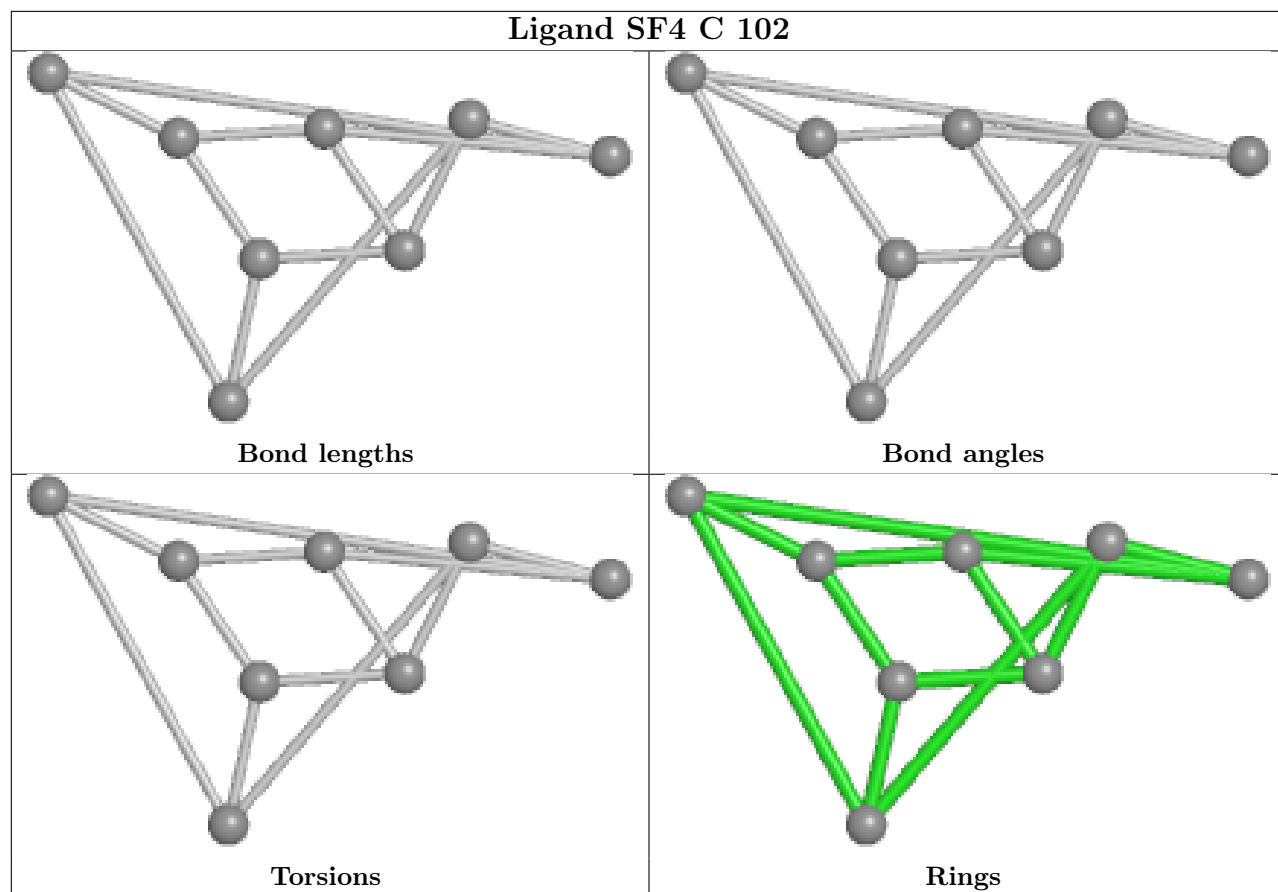
Rings

Ligand CLA A 821

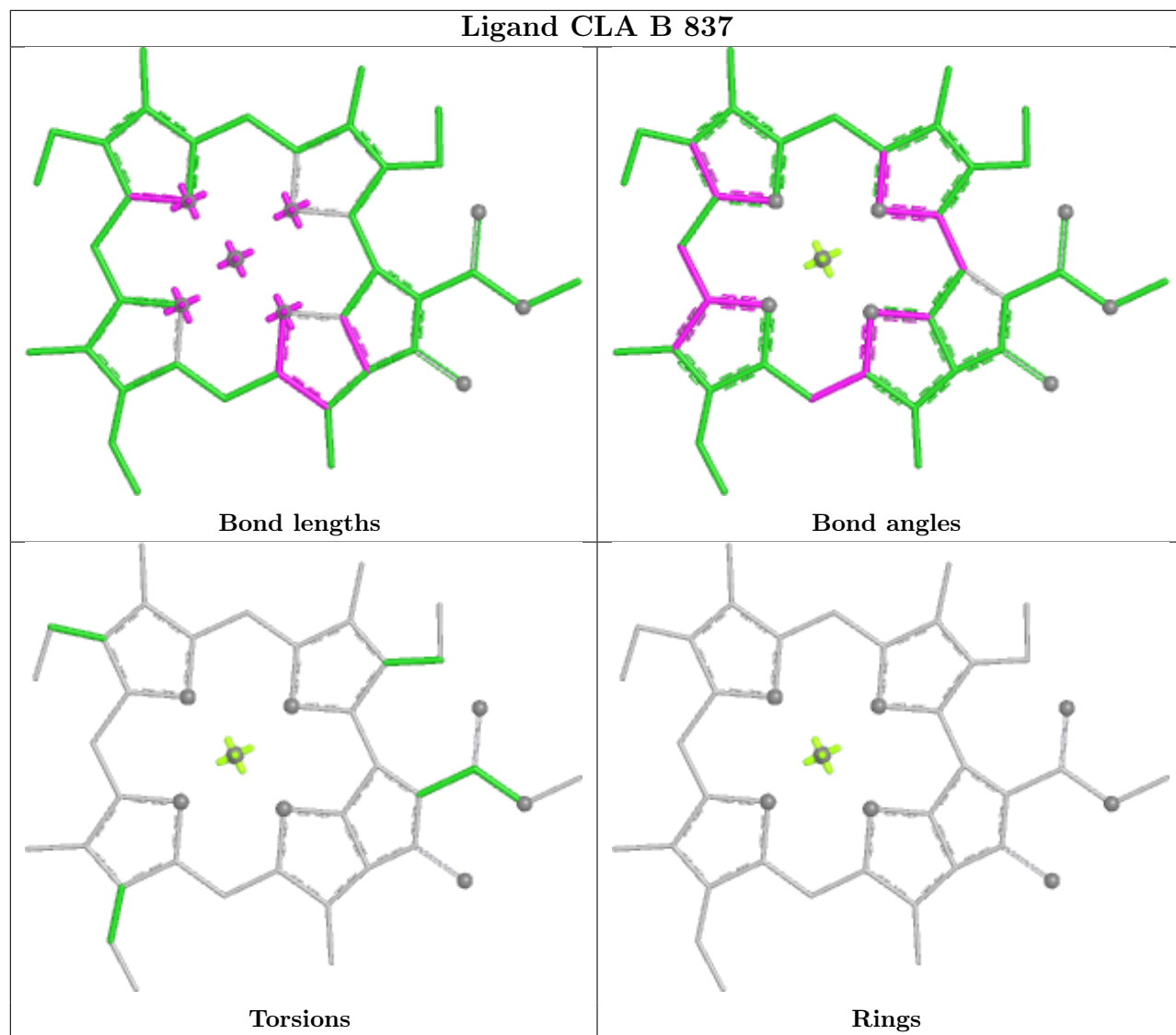


Ligand CLA 8 614

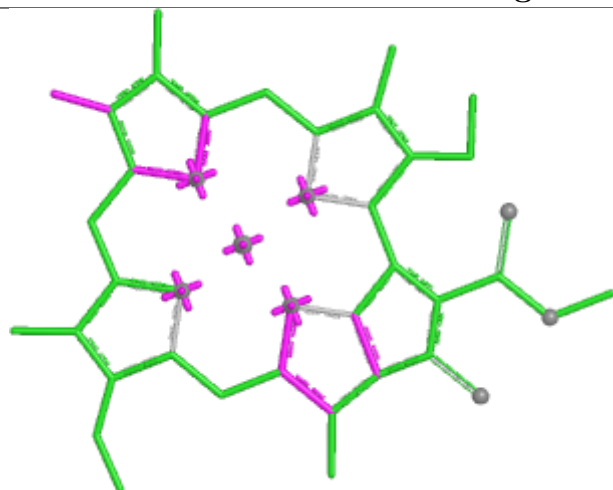




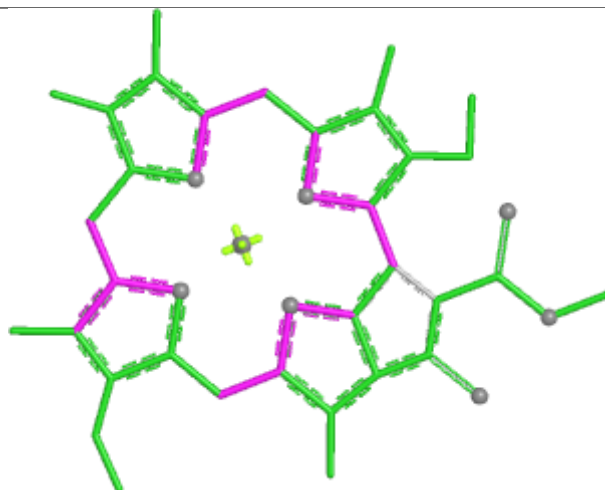
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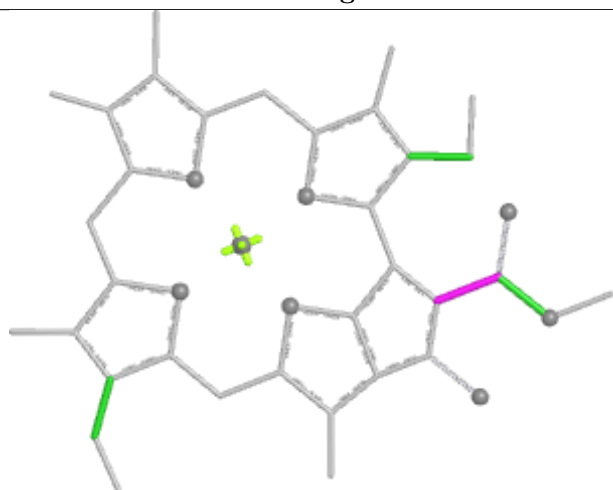
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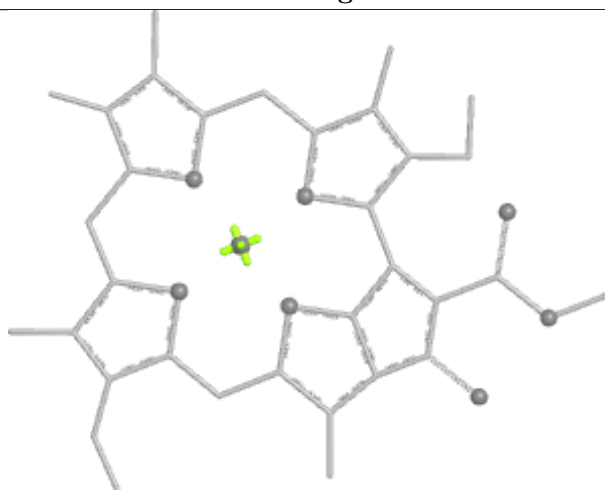
Bond lengths



Bond angles

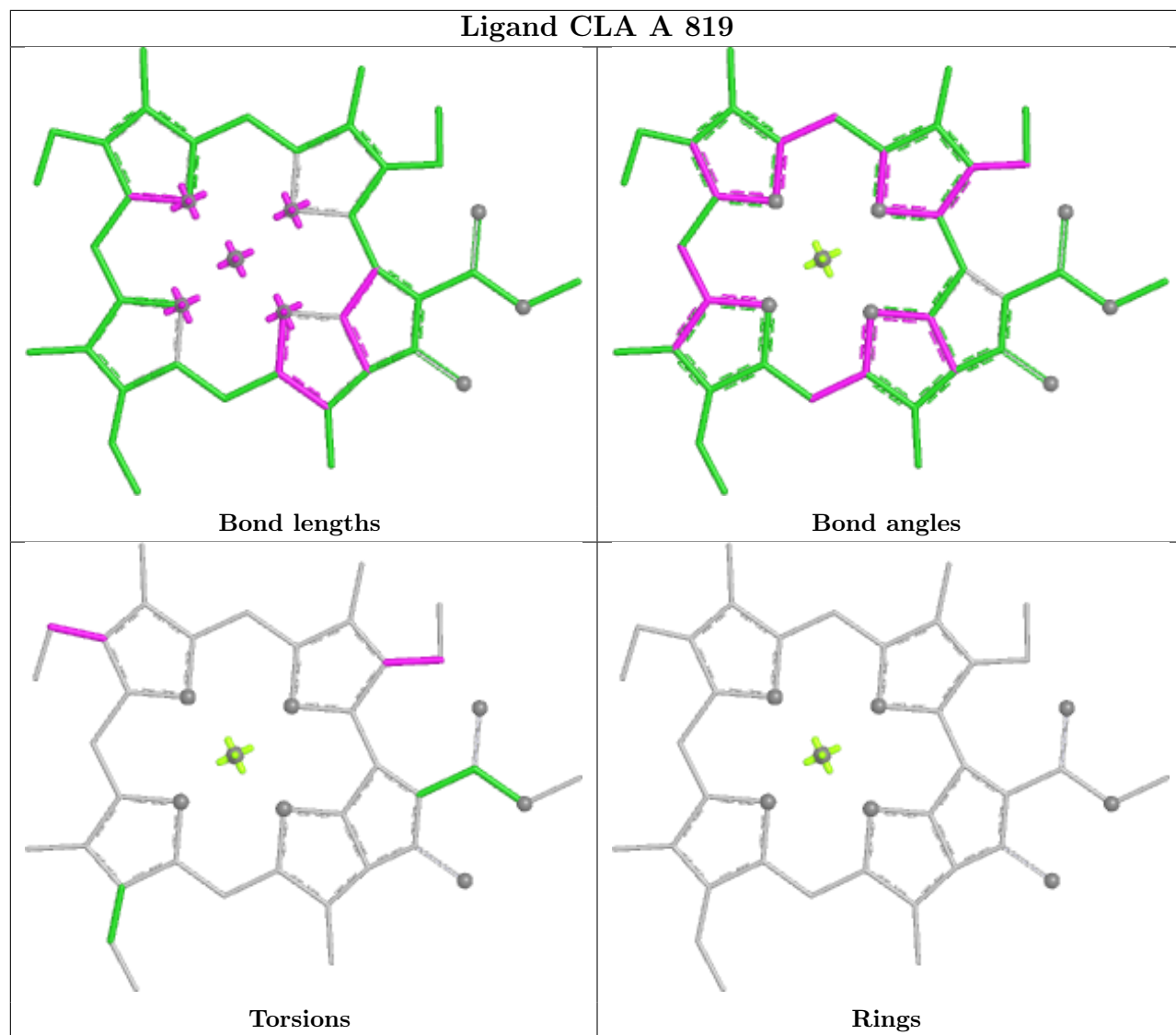


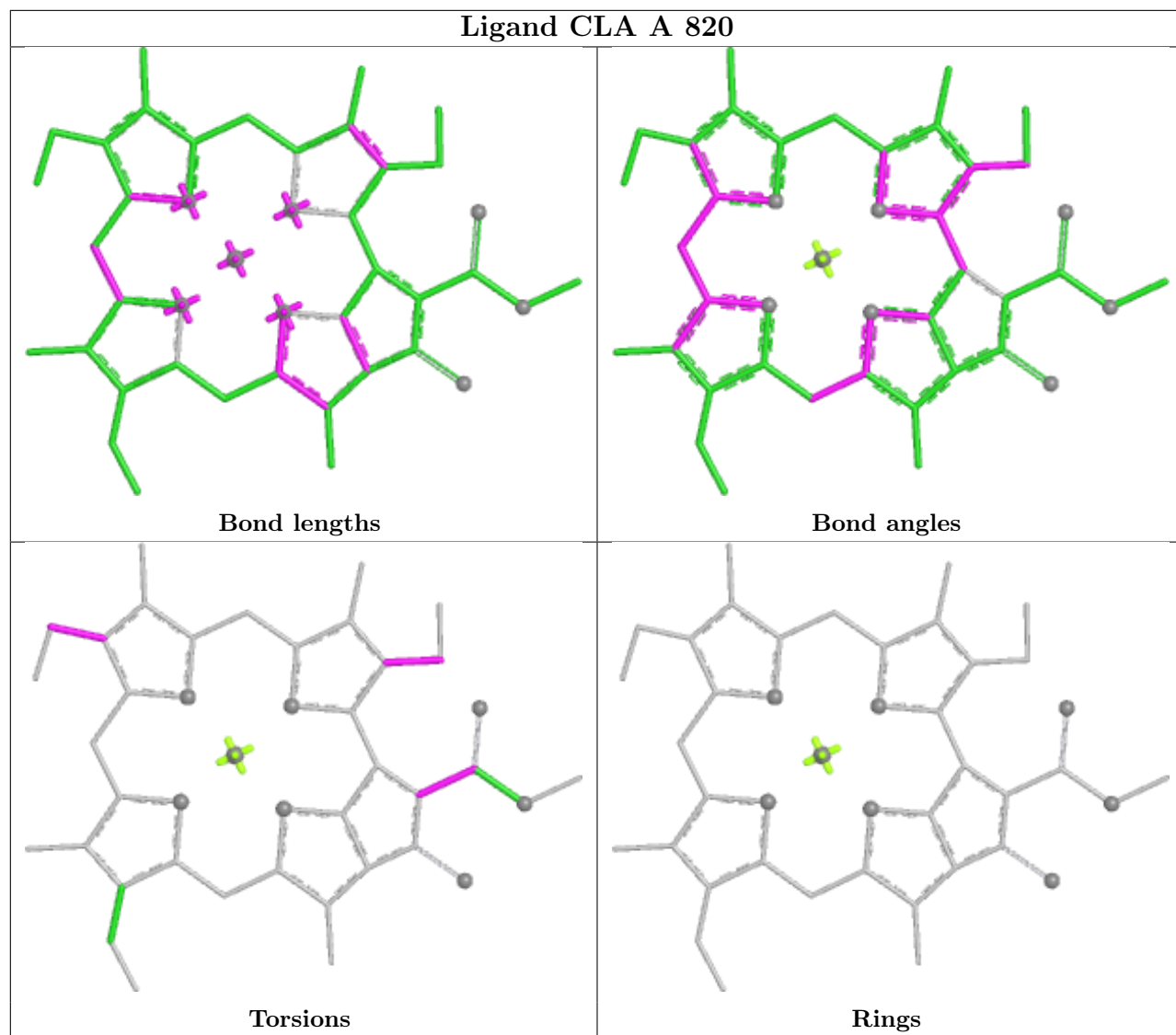
Torsions



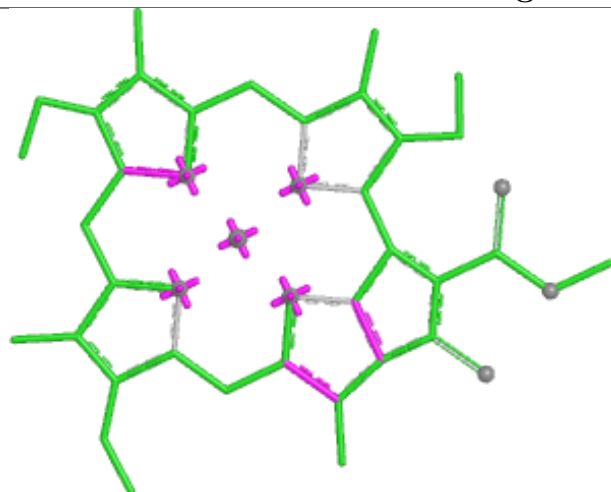
Rings

Ligand CLA A 819

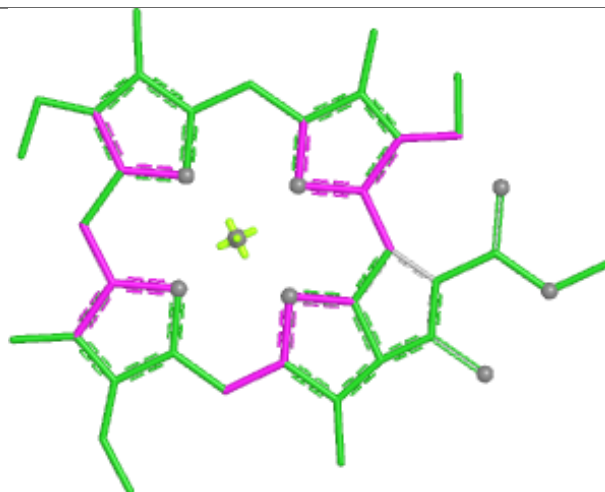




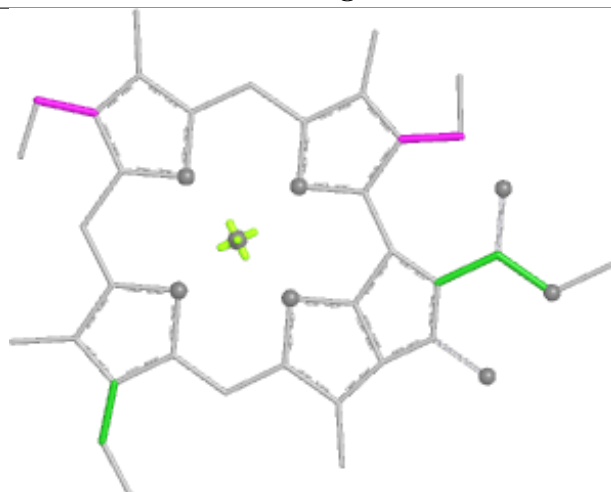
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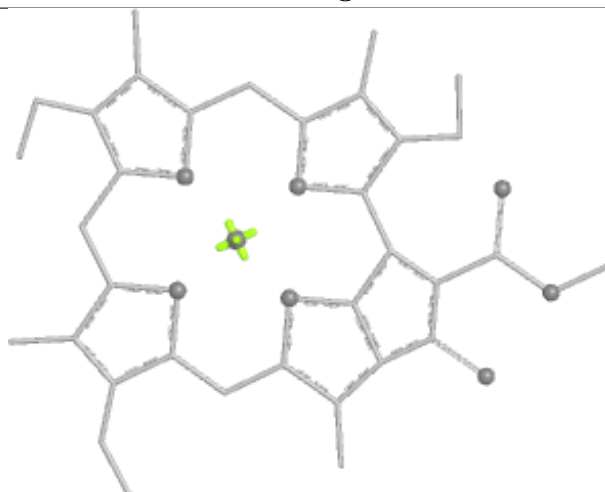
Bond lengths



Bond angles

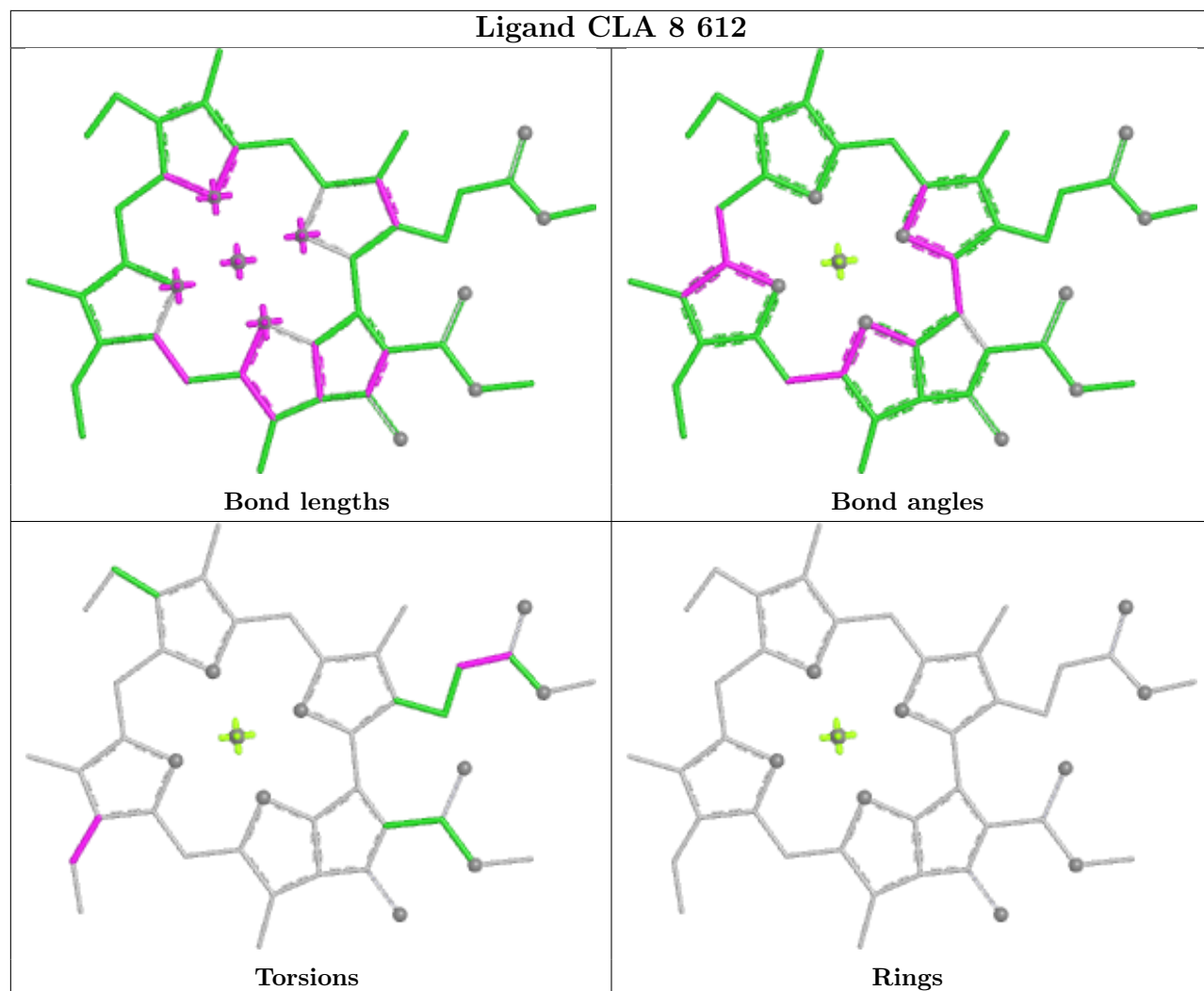


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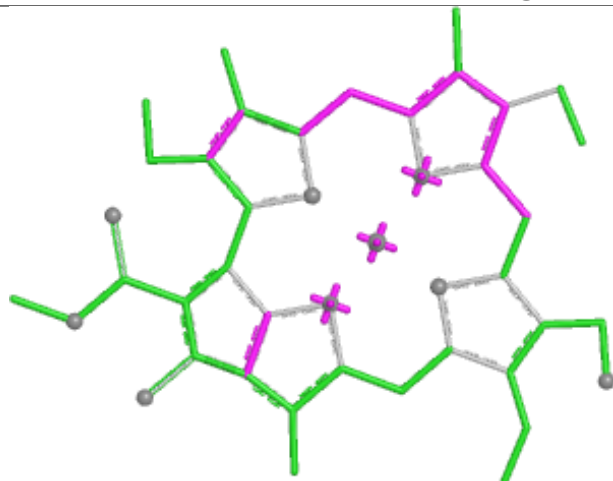


Rings

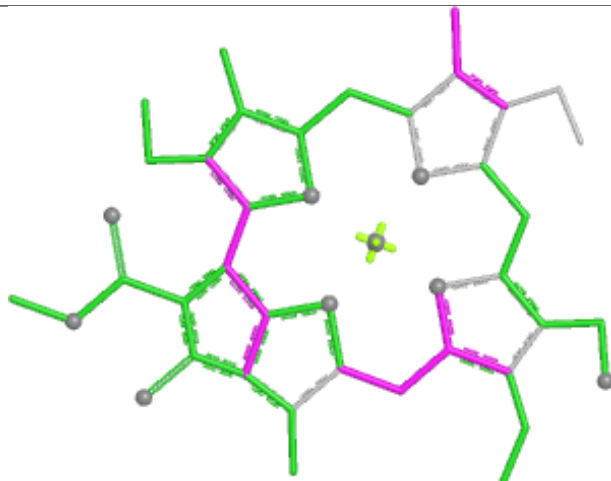
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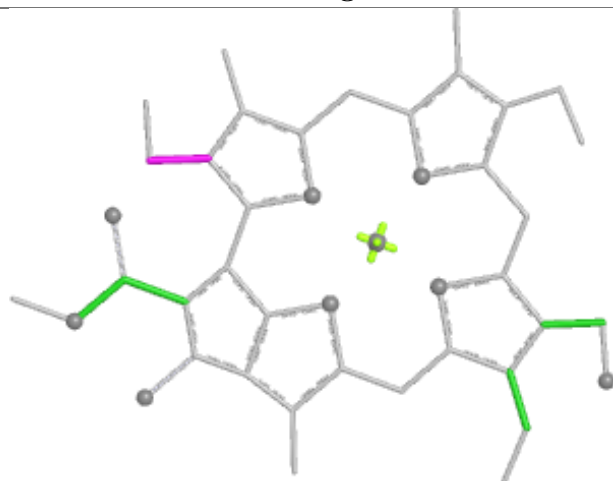
Ligand CHL 1 606



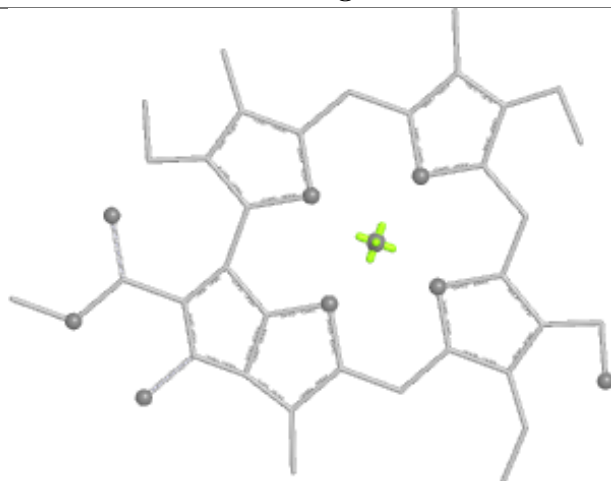
Bond lengths



Bond angles

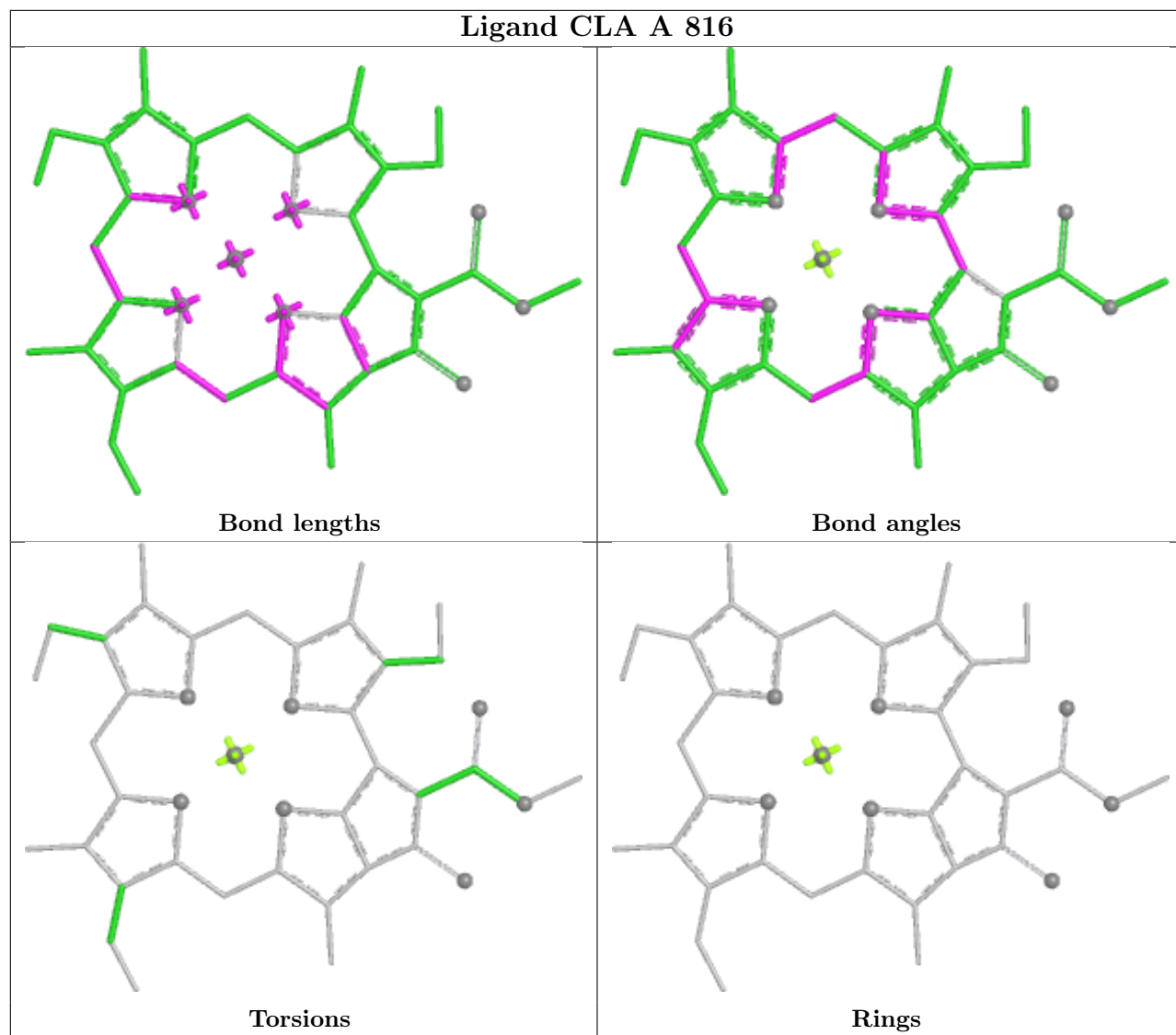


Torsions

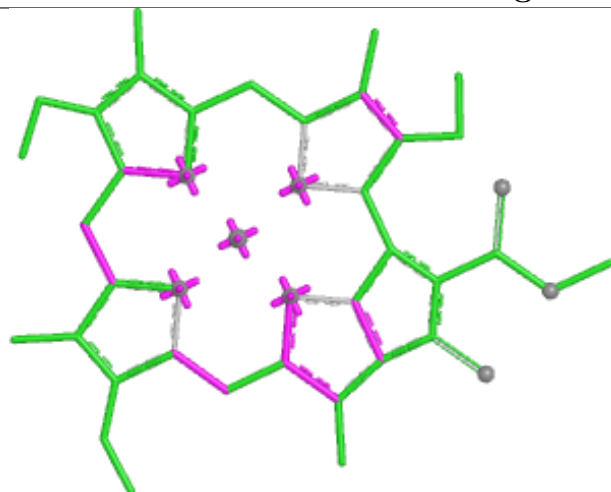


Rings

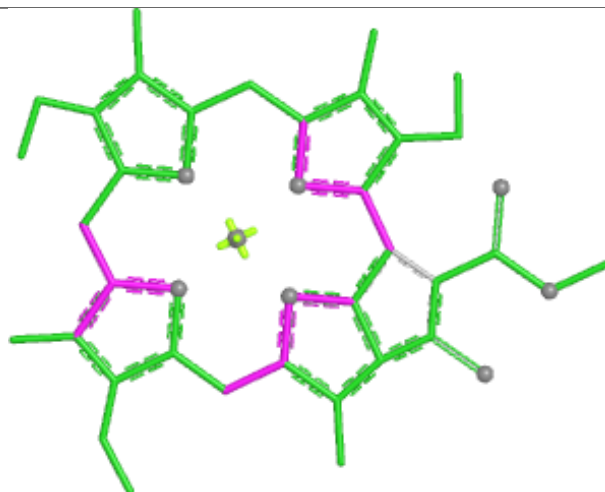
Ligand CLA A 816



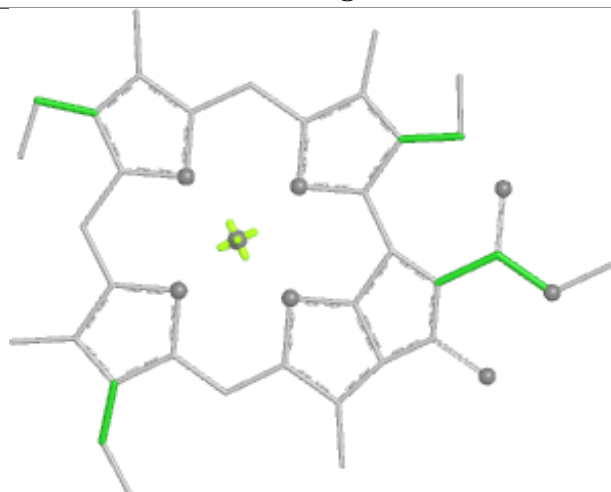
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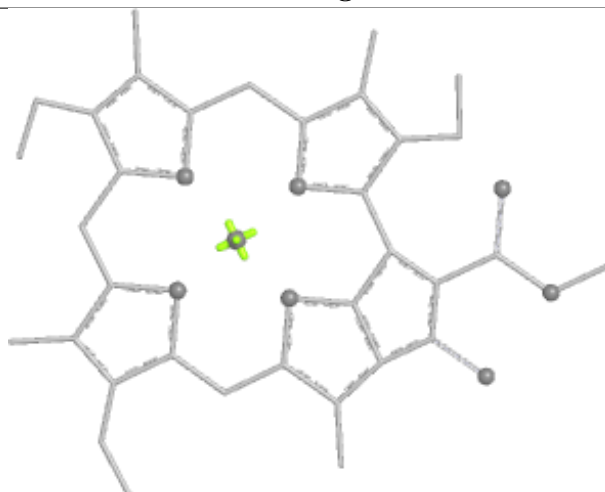
Bond lengths



Bond angles

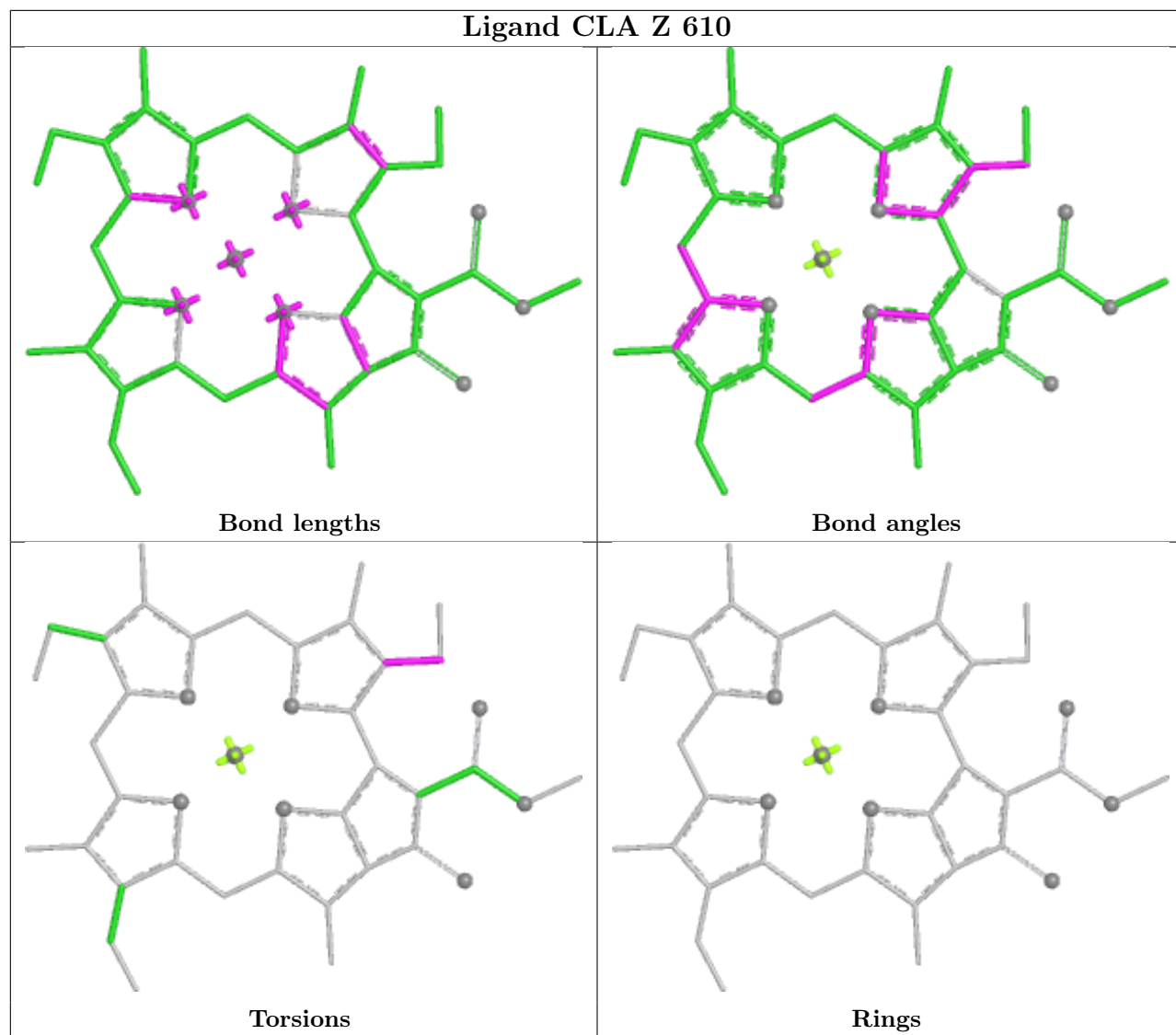


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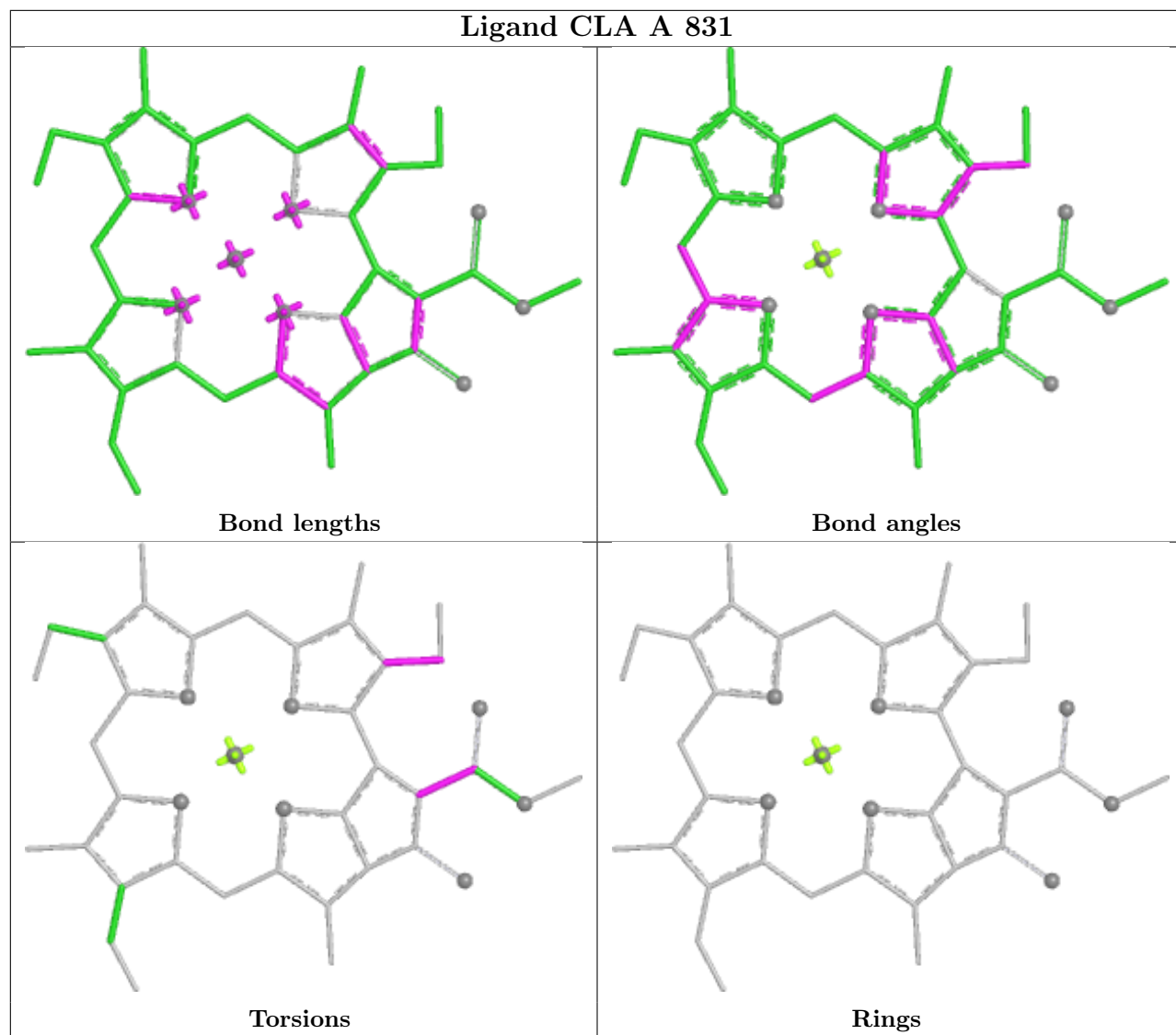


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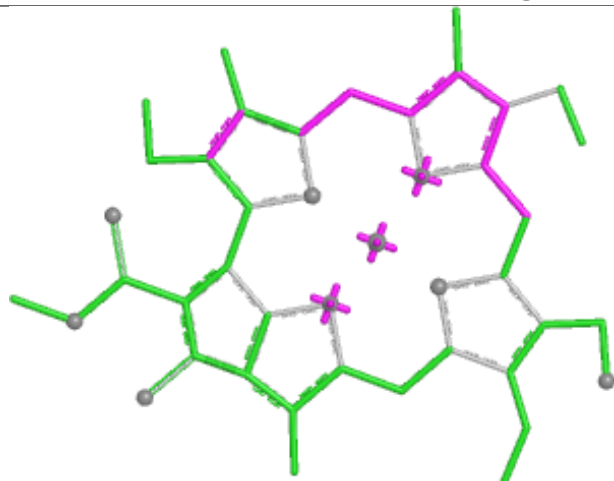
Ligand CLA Z 610



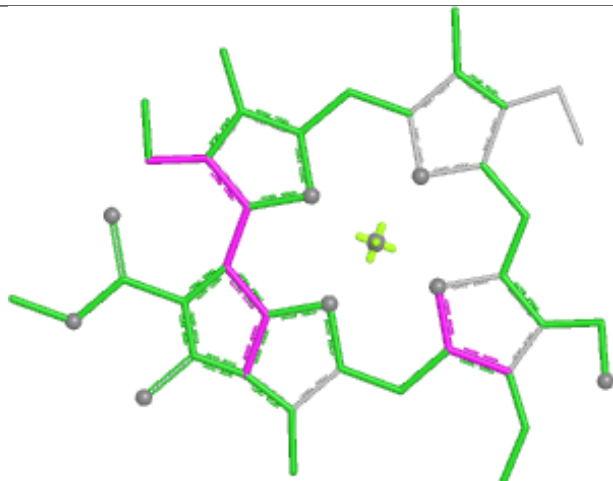
Ligand CLA A 831



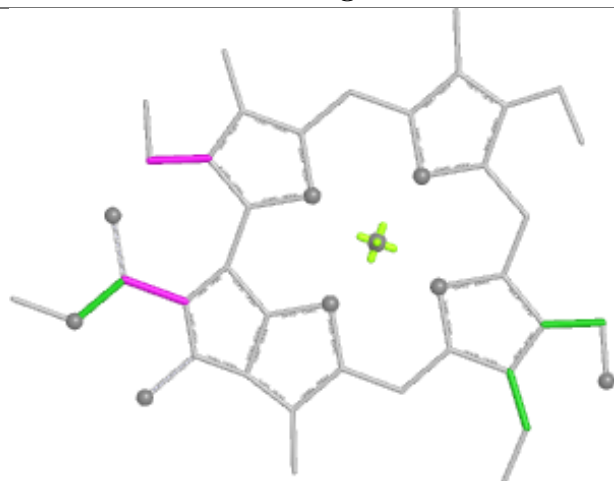
Ligand CHL 8 606



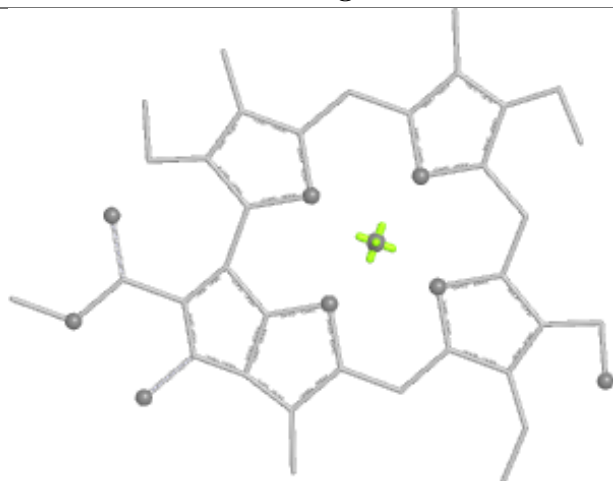
Bond lengths



Bond angles

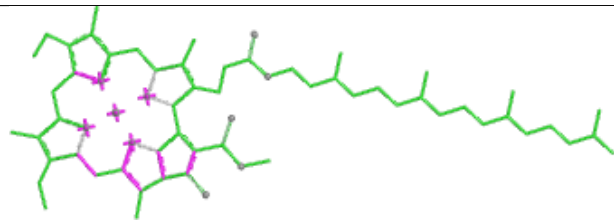


Torsions

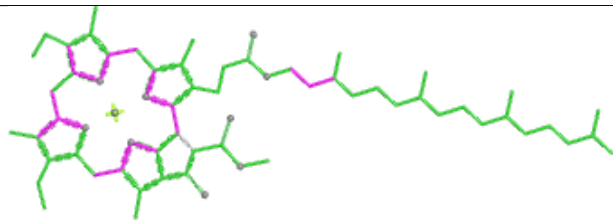


Rings

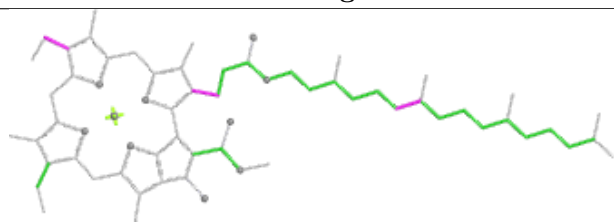
Ligand CLA F 302



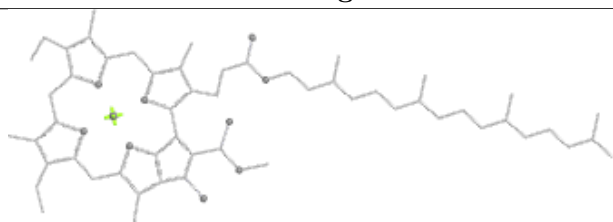
Bond lengths



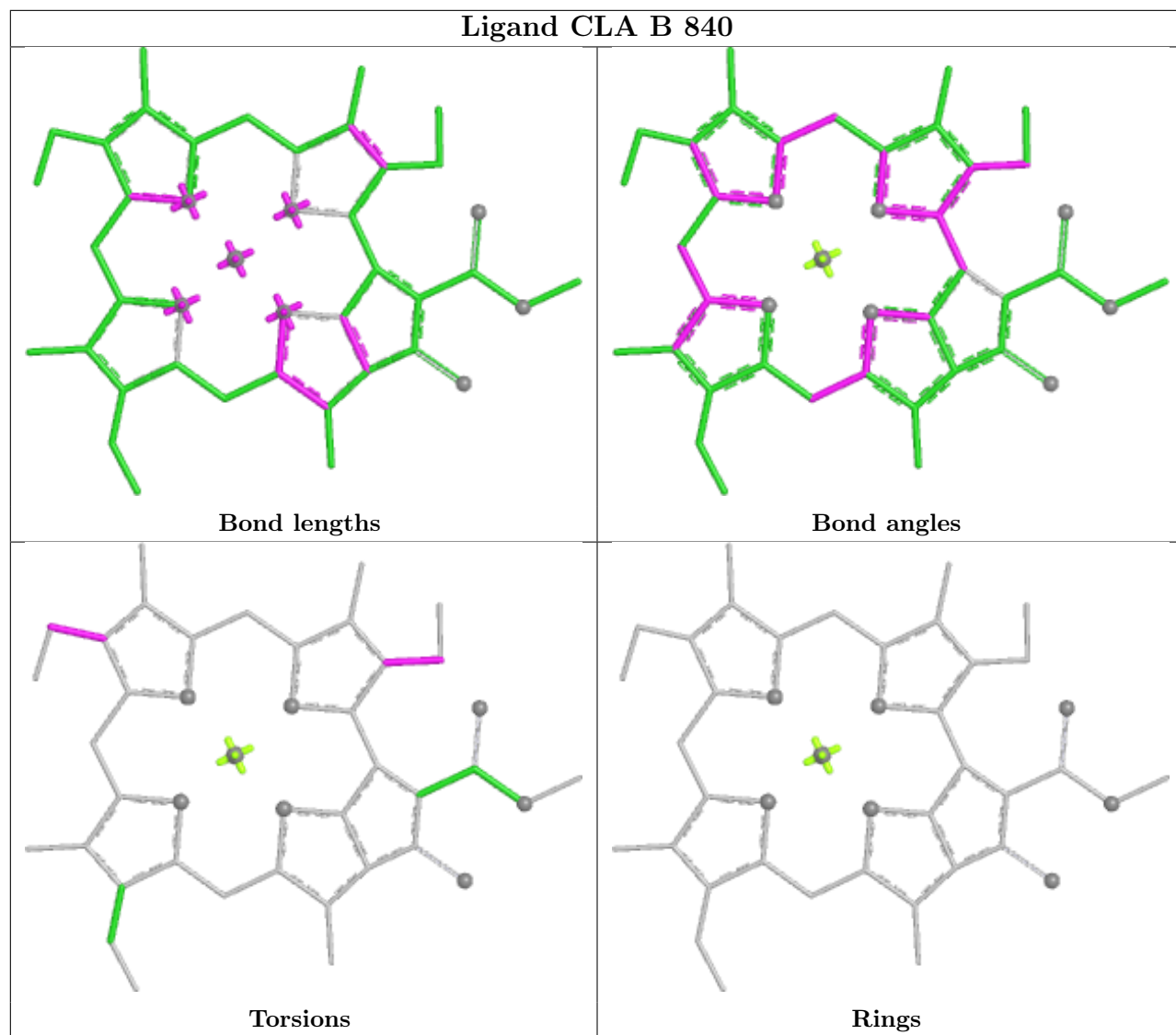
Bond angles

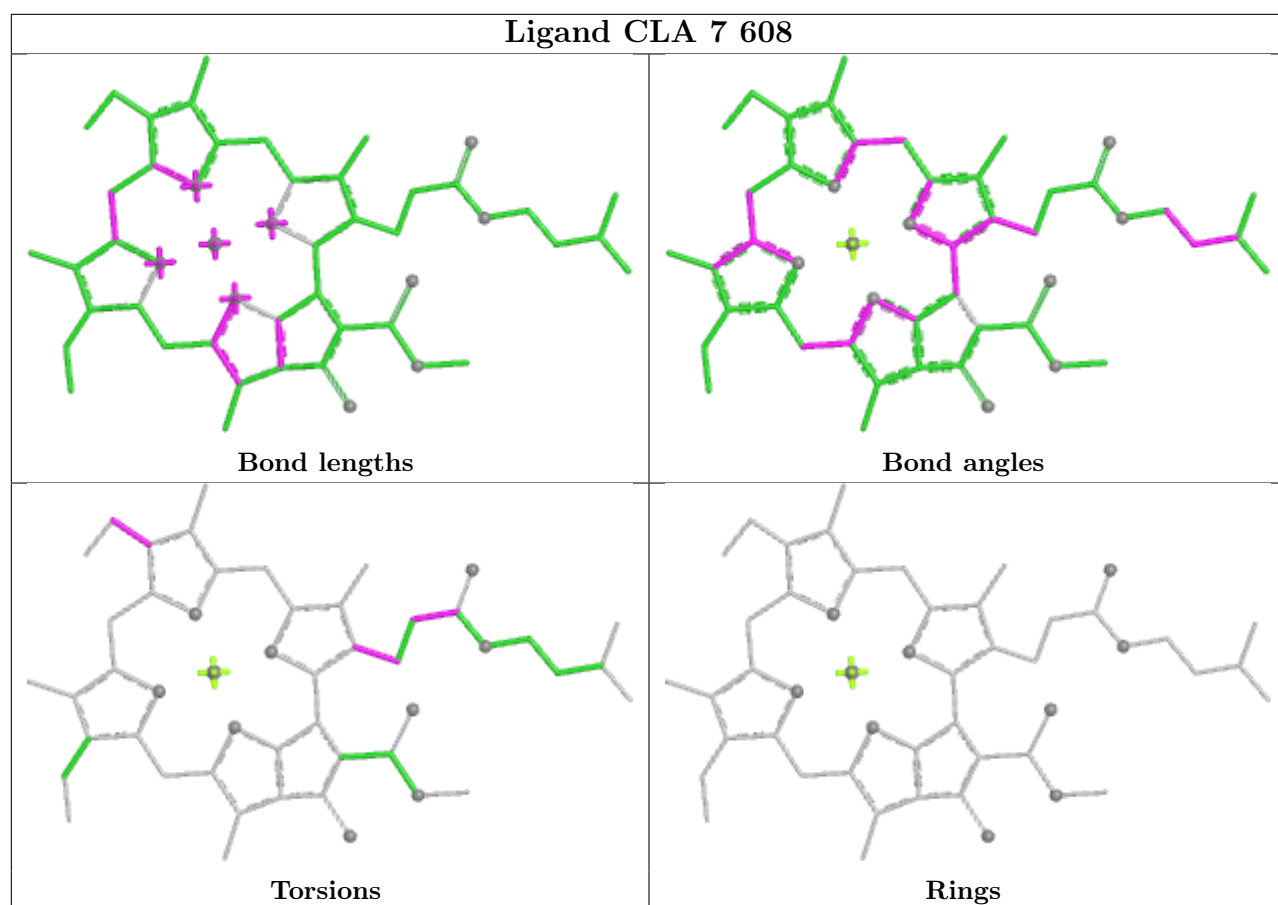


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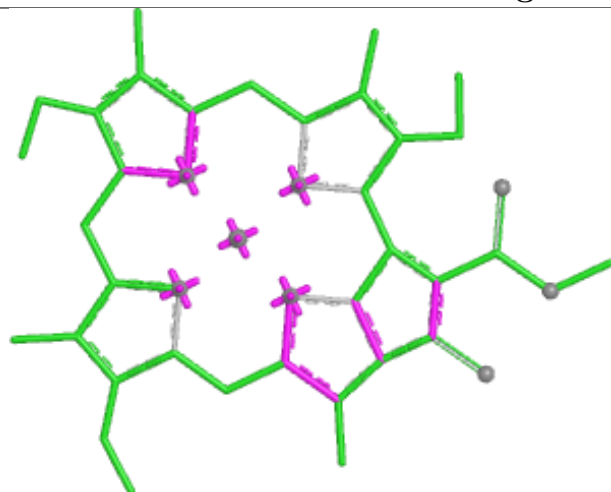


Rings

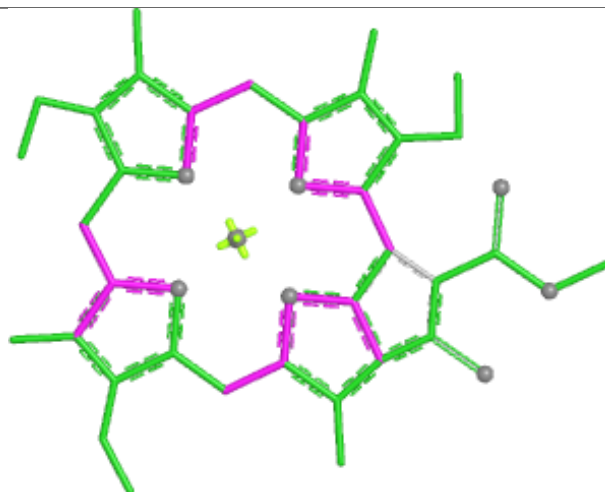




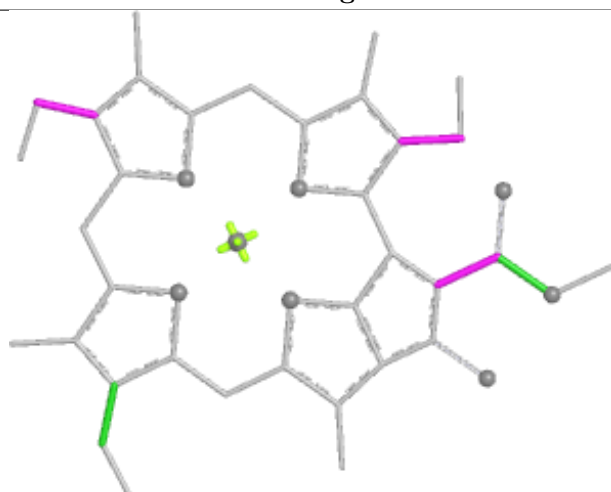
Ligand CLA Z 602



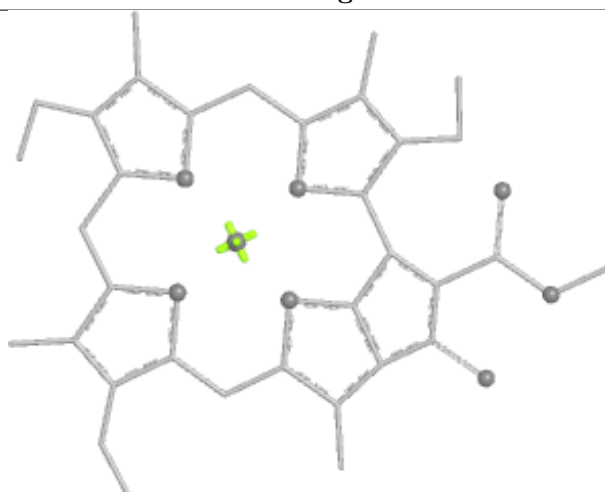
Bond lengths



Bond angles

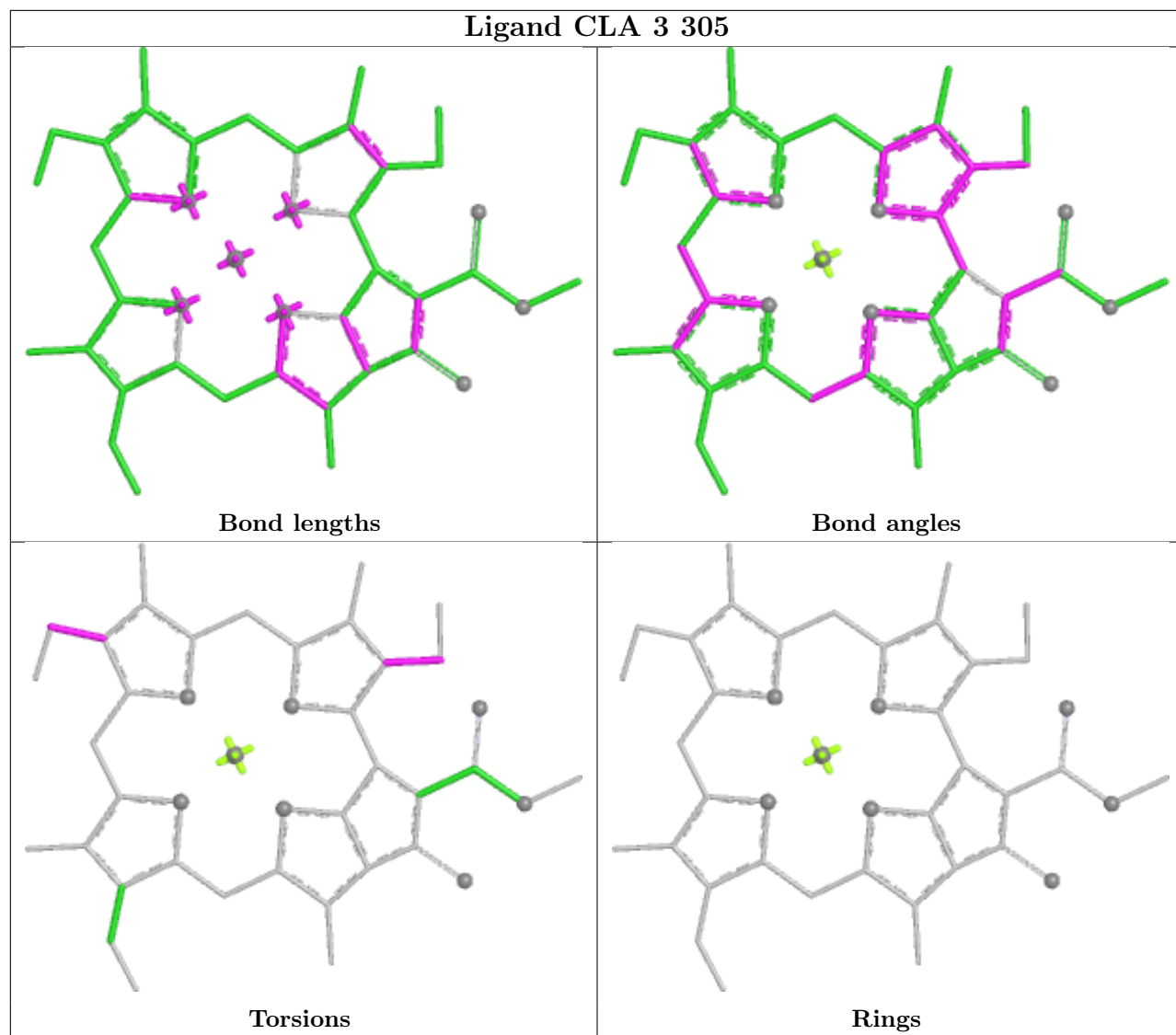


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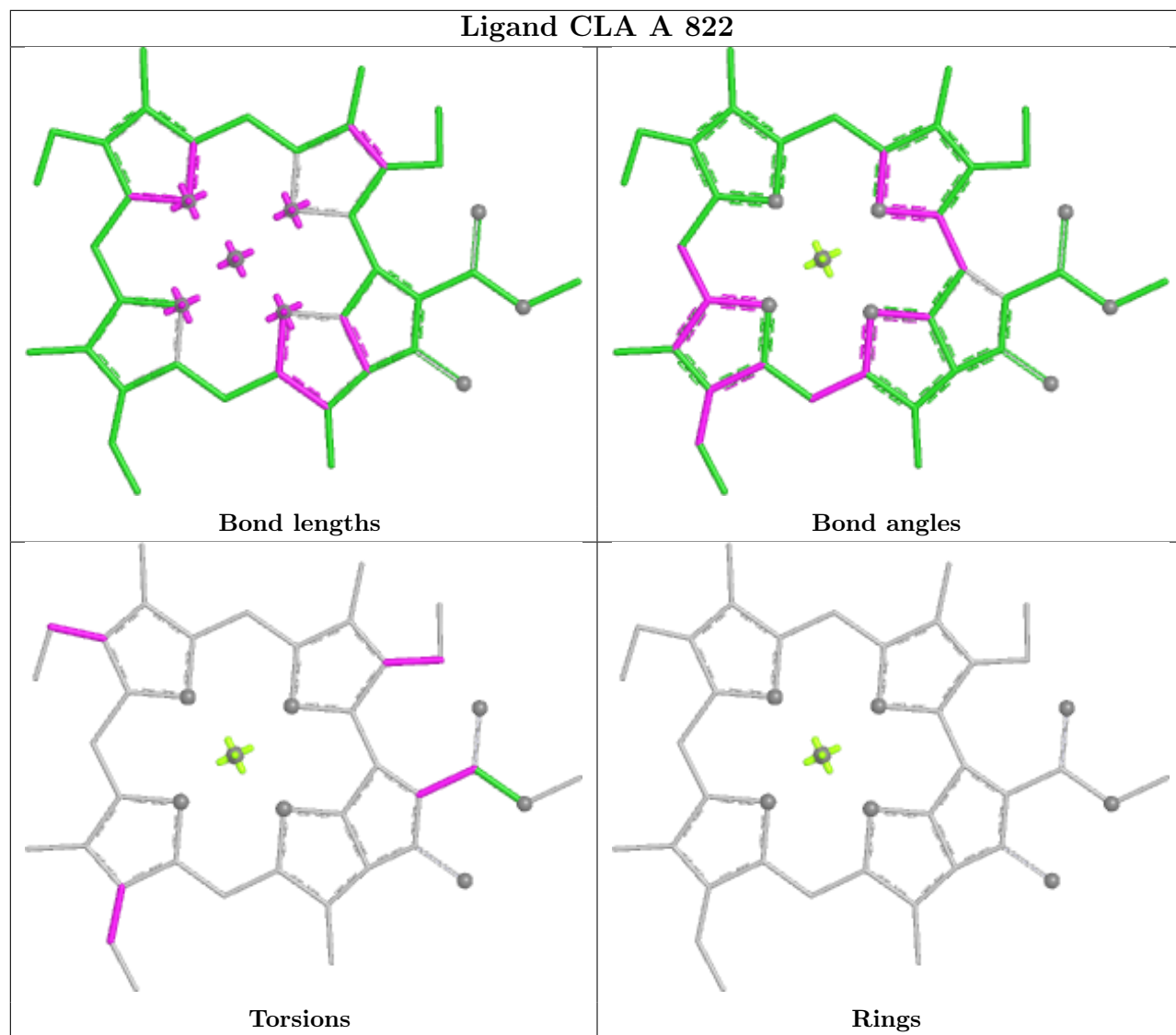


Rings

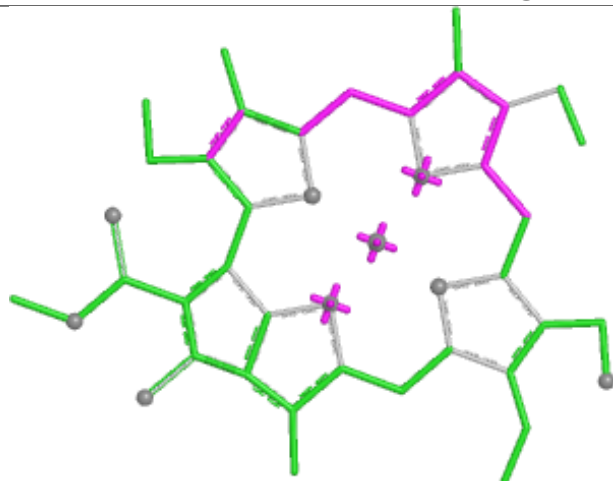
Ligand CLA 3 305



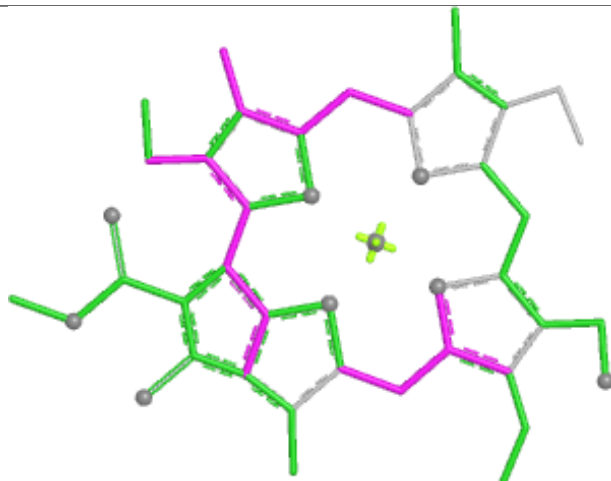
Ligand CLA A 822



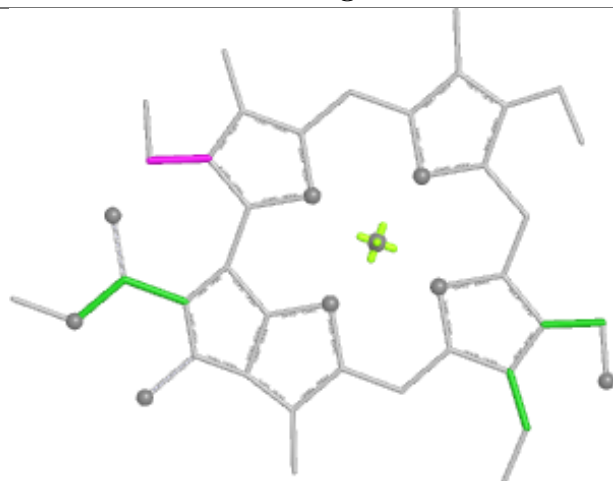
Ligand CHL 6 307



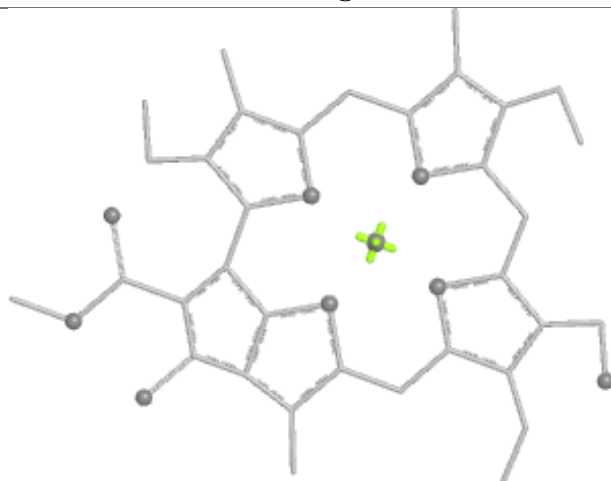
Bond lengths



Bond angles

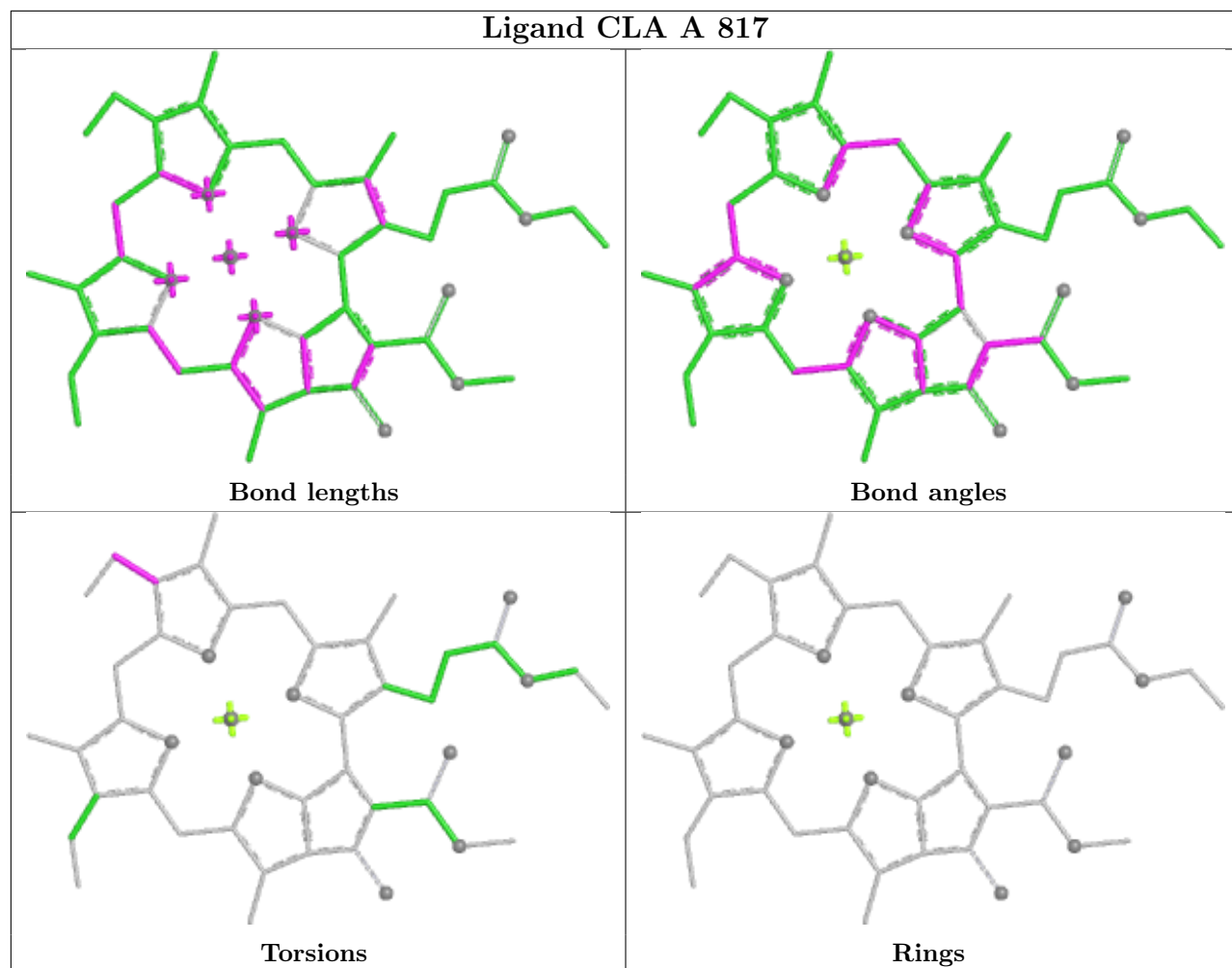


Torsions

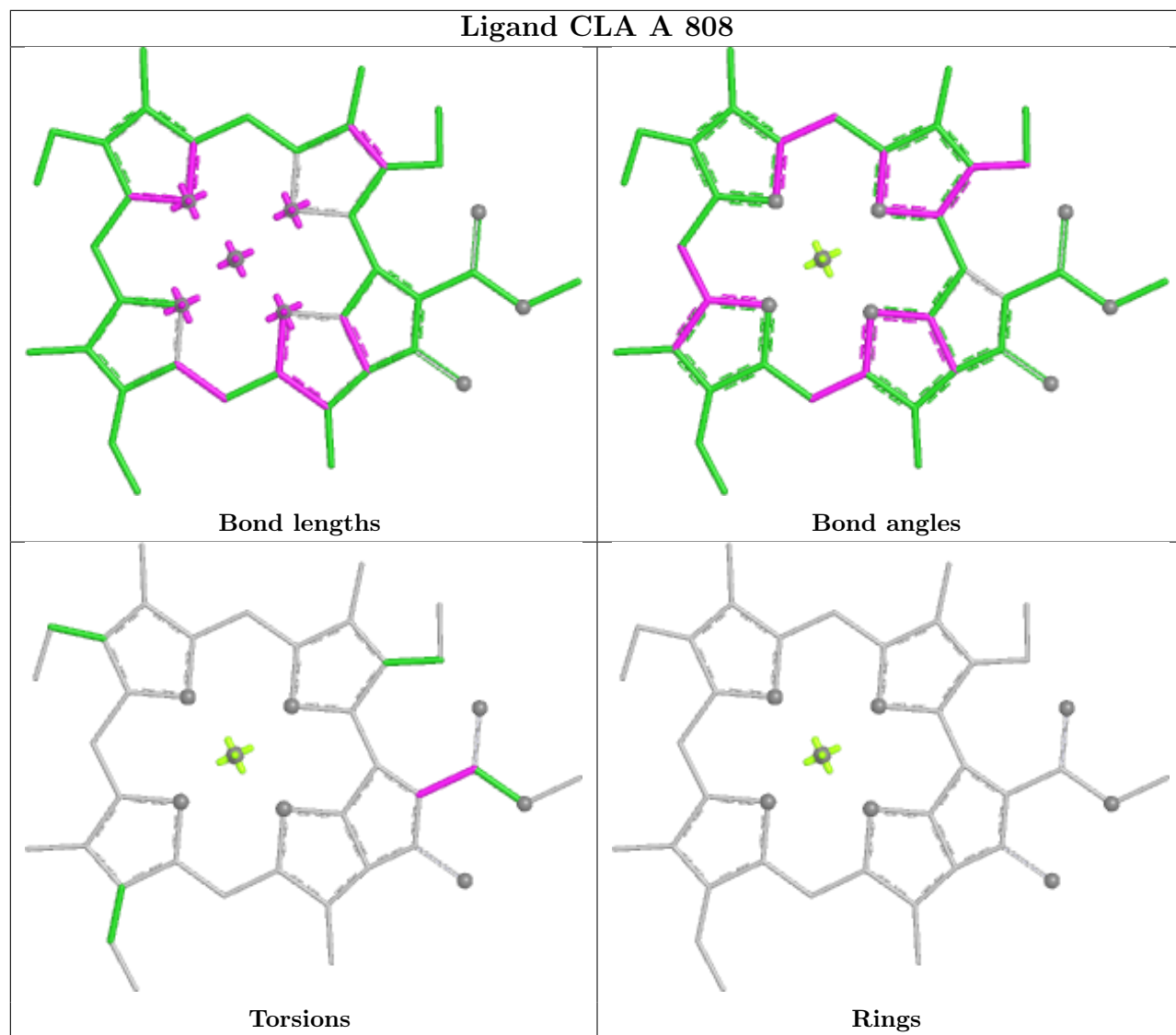


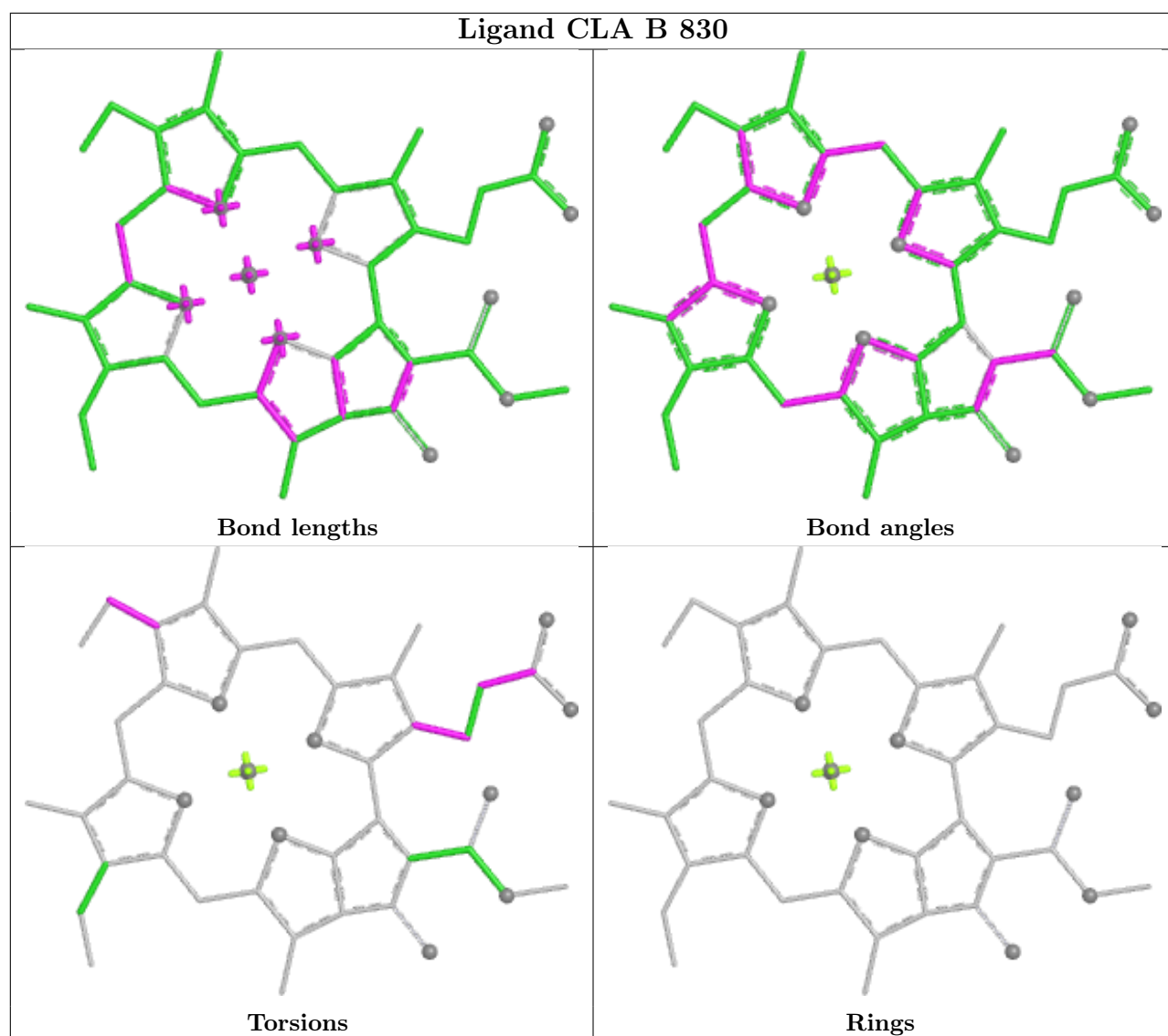
Rings

Ligand CLA A 817

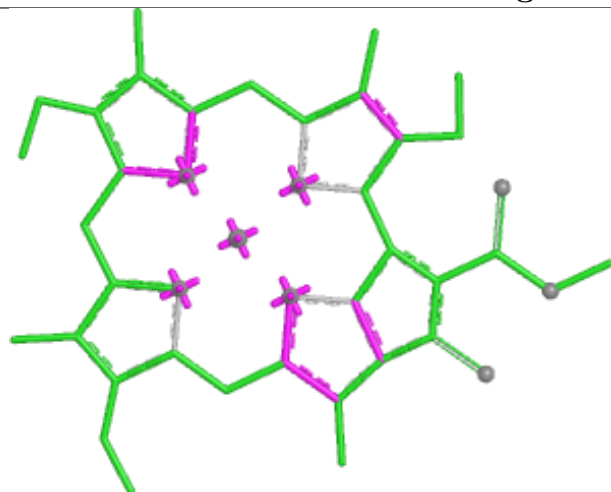


Ligand CLA A 808

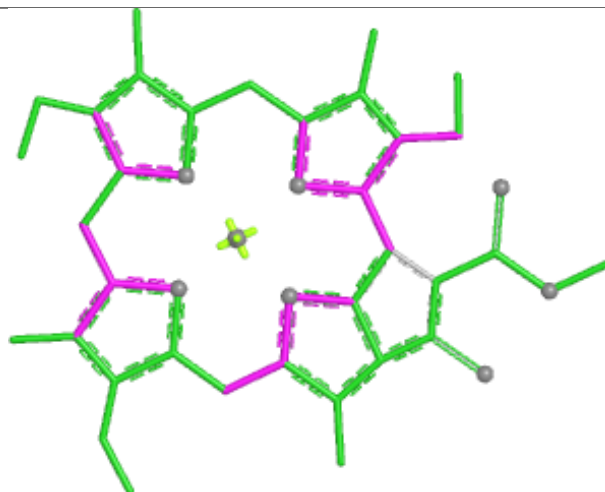




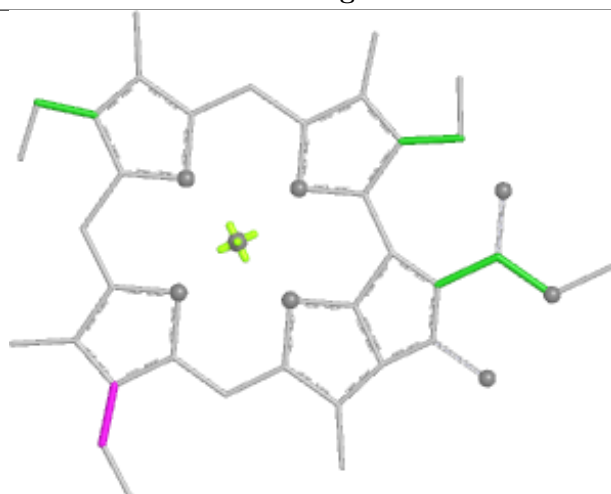
Ligand CLA Z 603



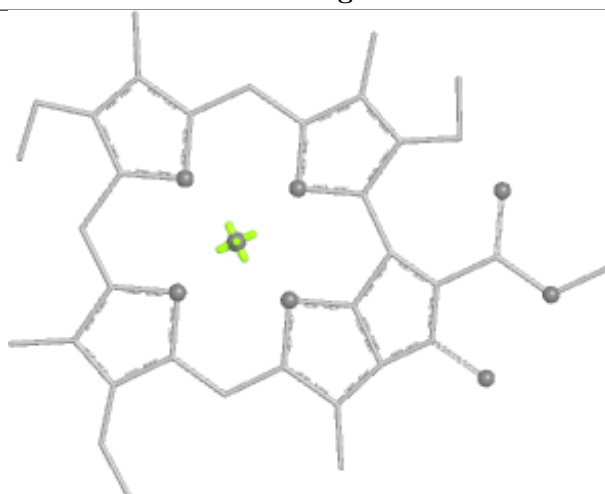
Bond lengths



Bond angles

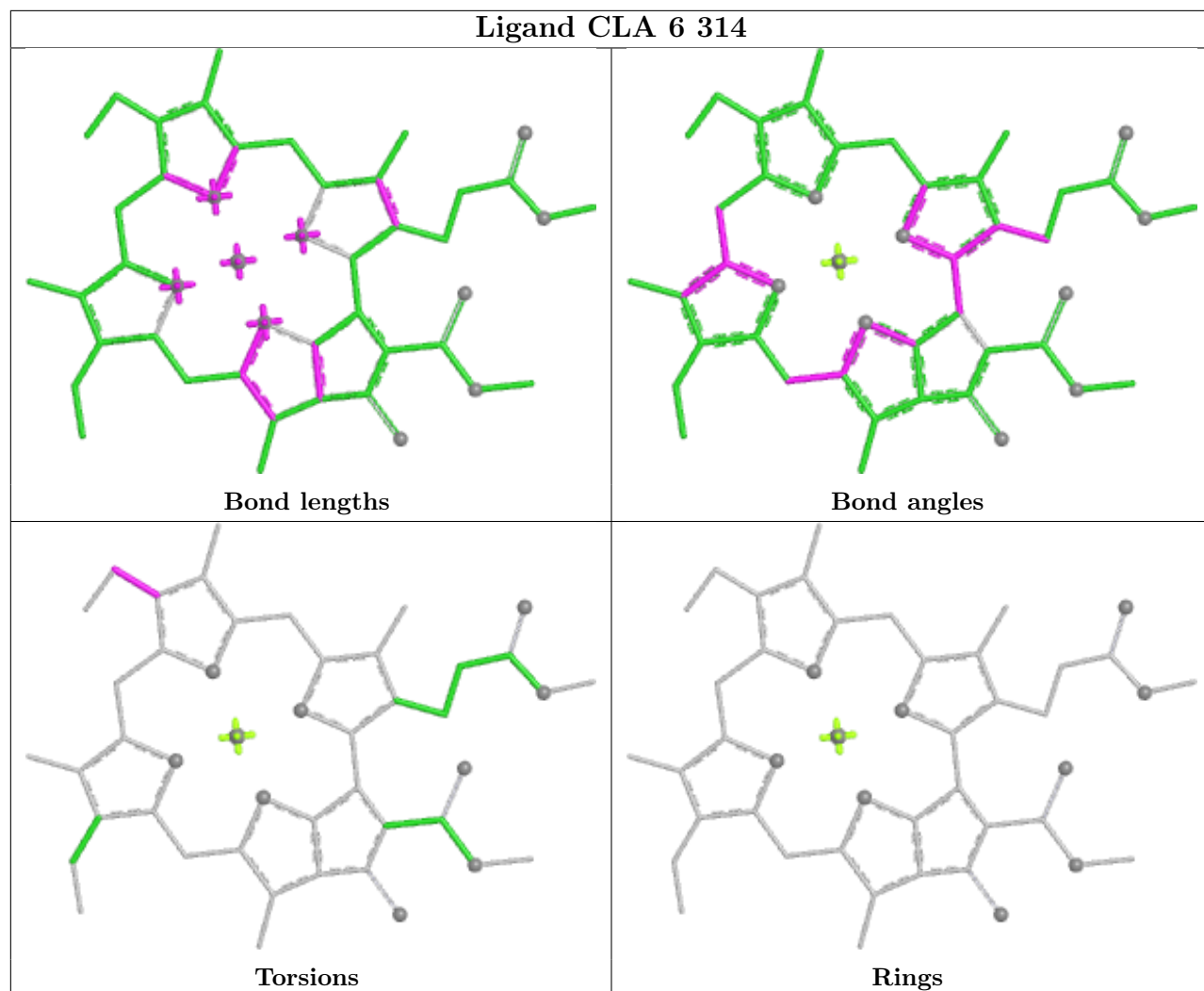


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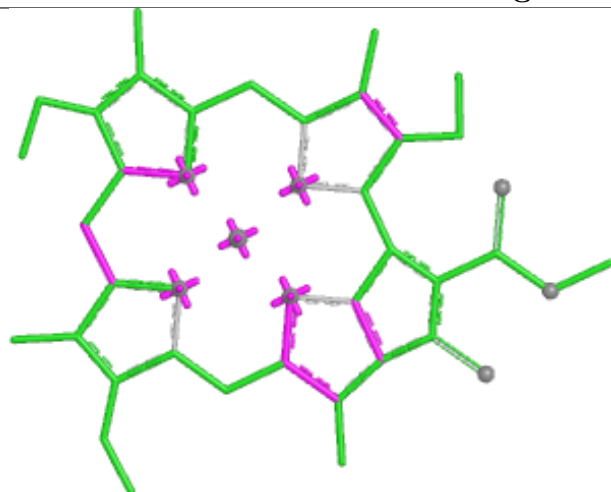


Rings

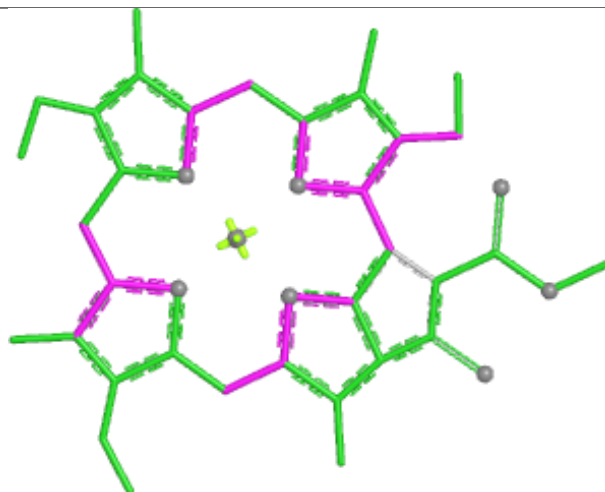
Ligand CLA 6 314



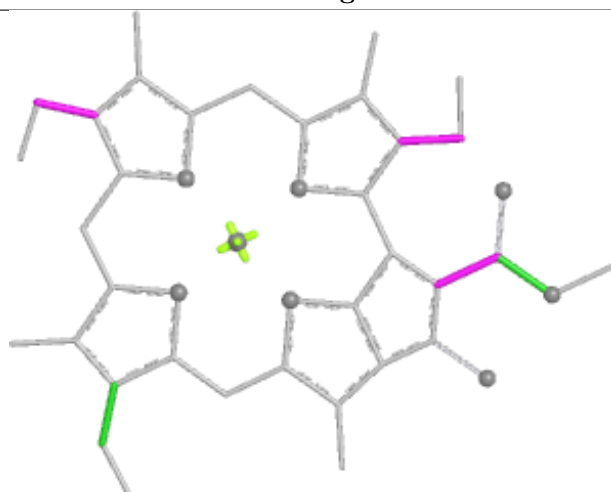
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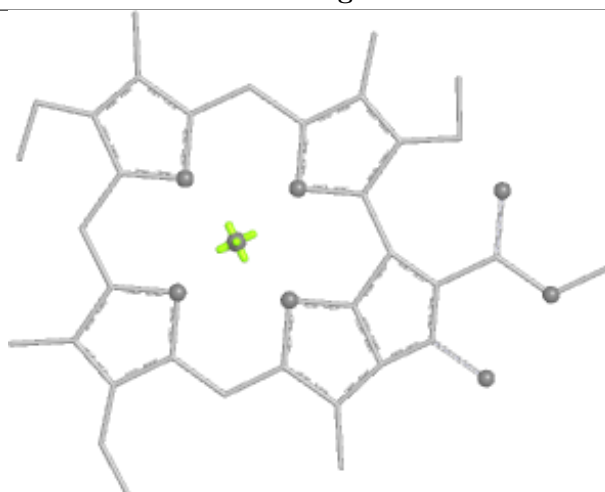
Bond lengths



Bond angles

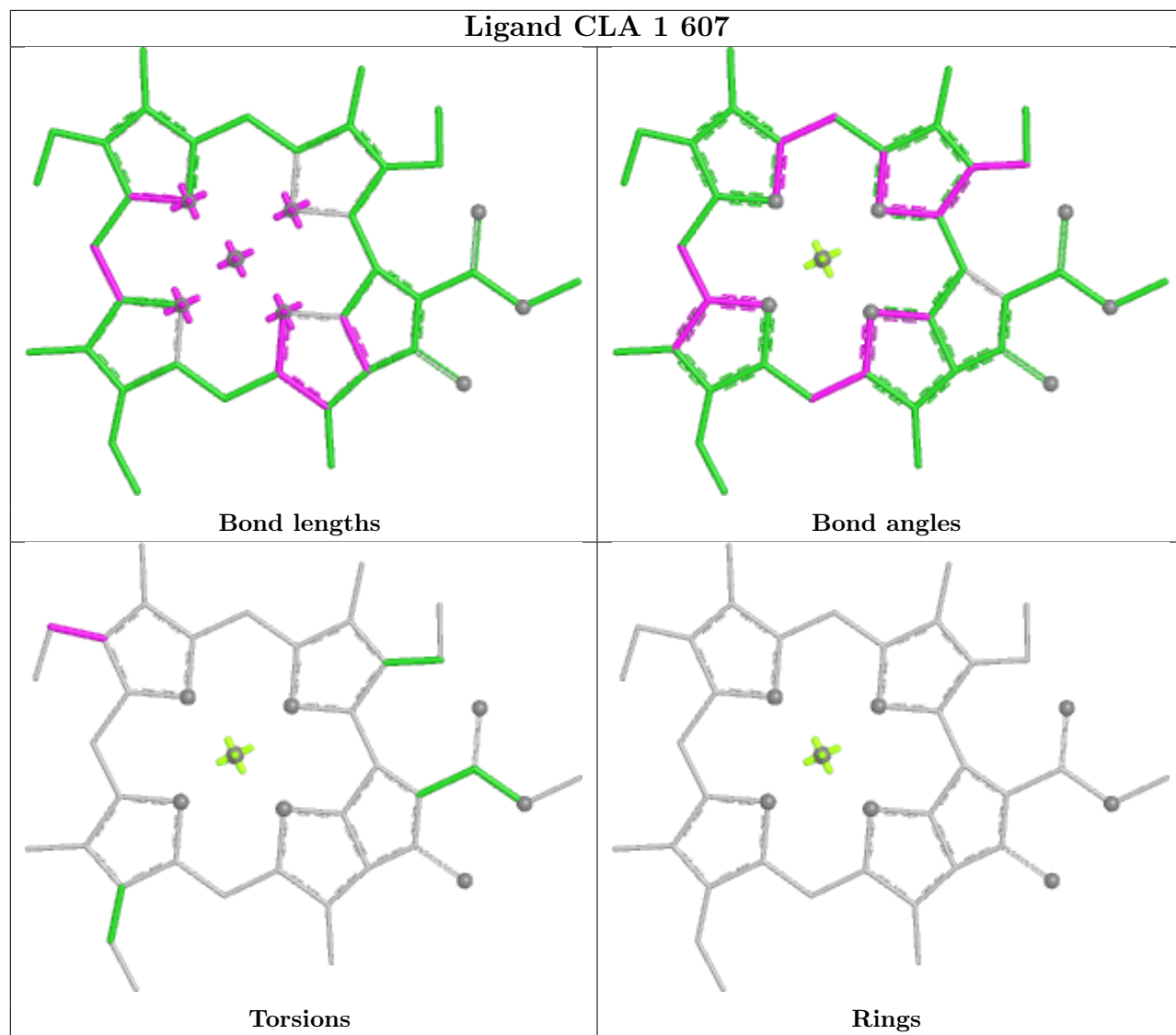


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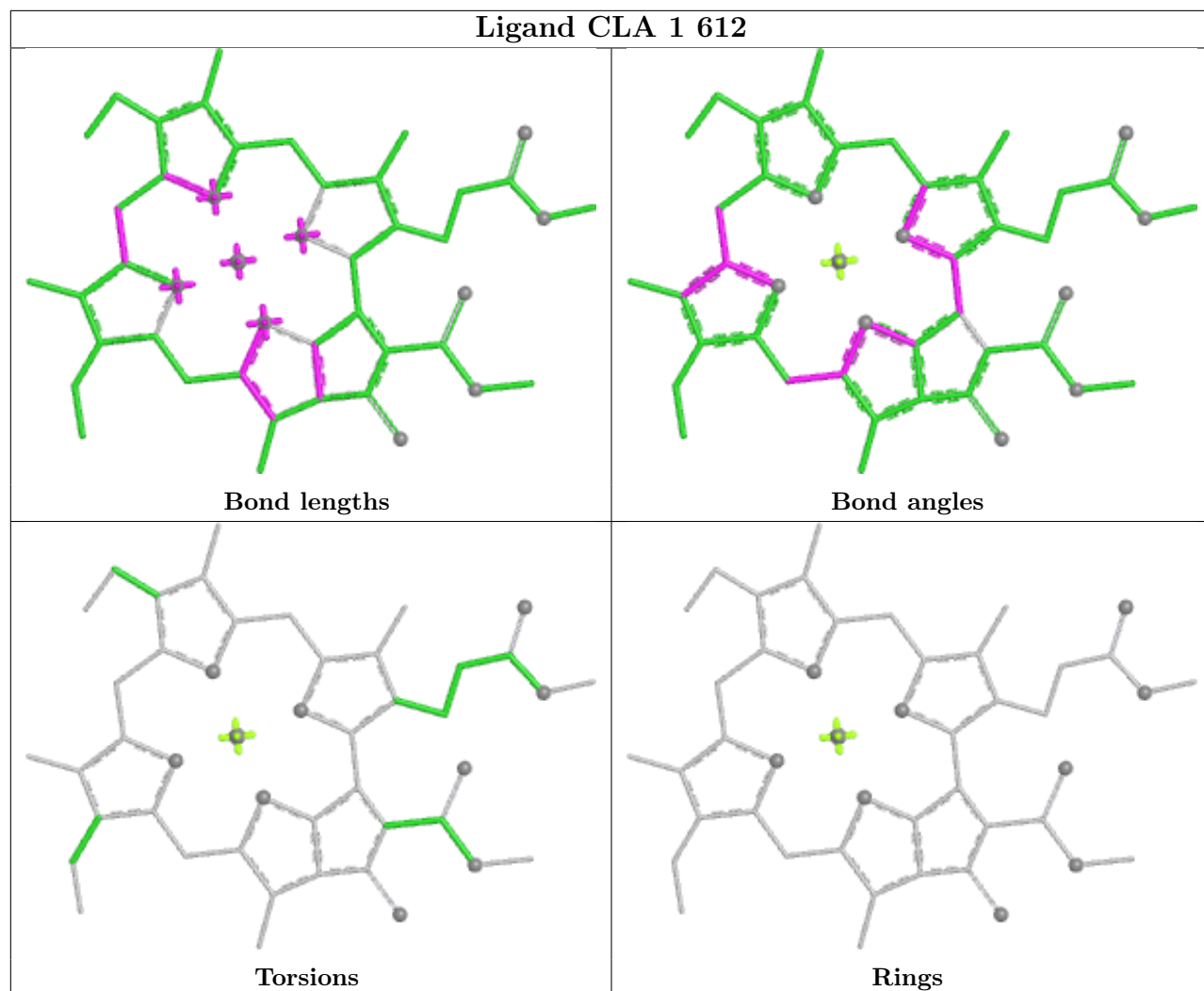


Rings

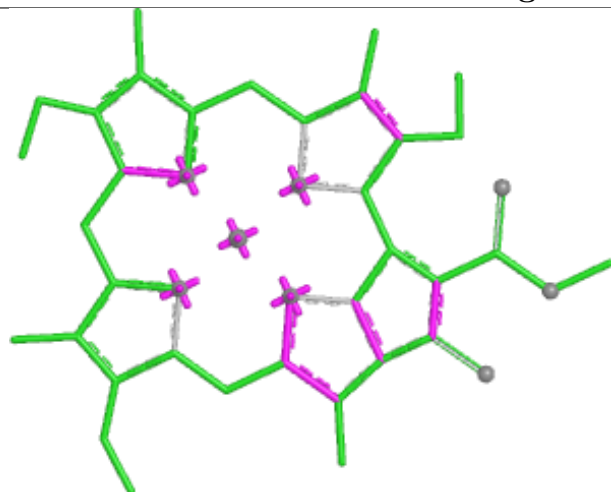
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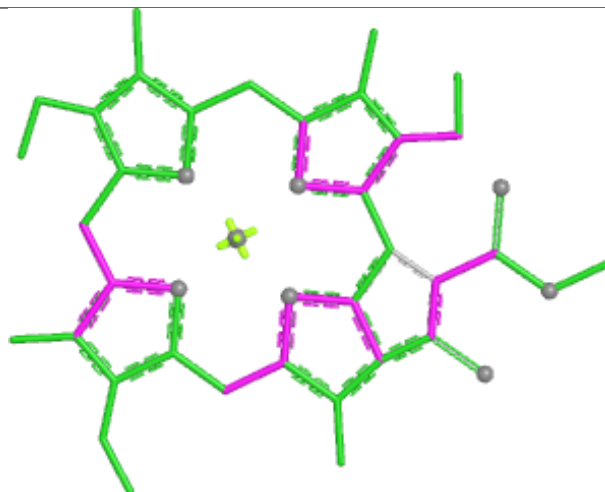
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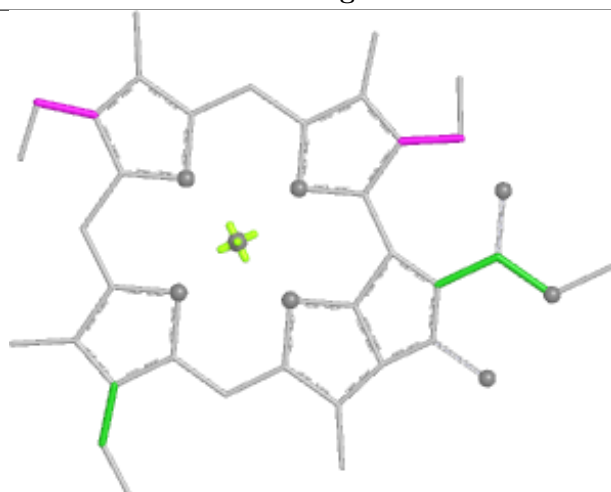
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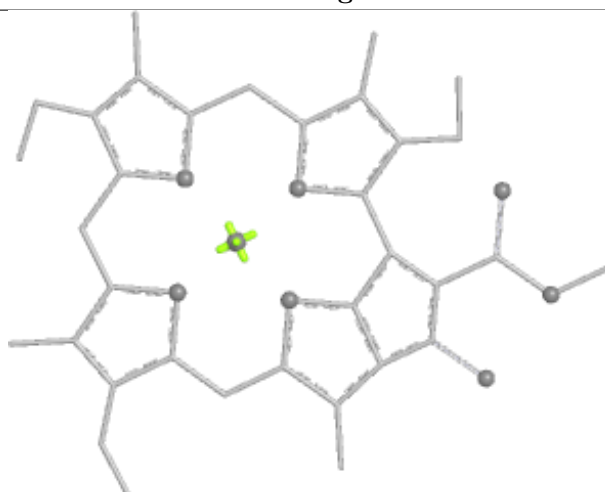
Bond lengths



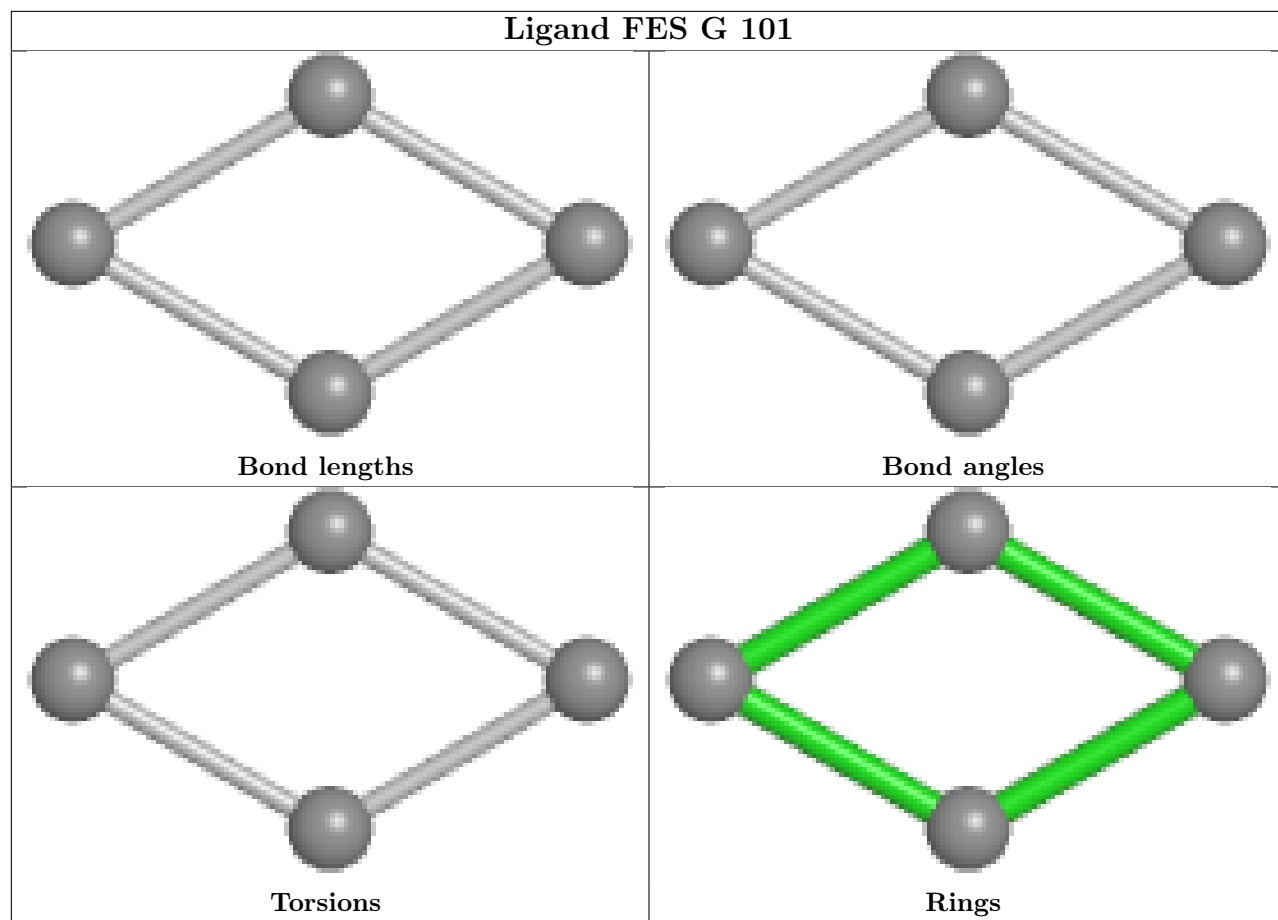
Bond angles



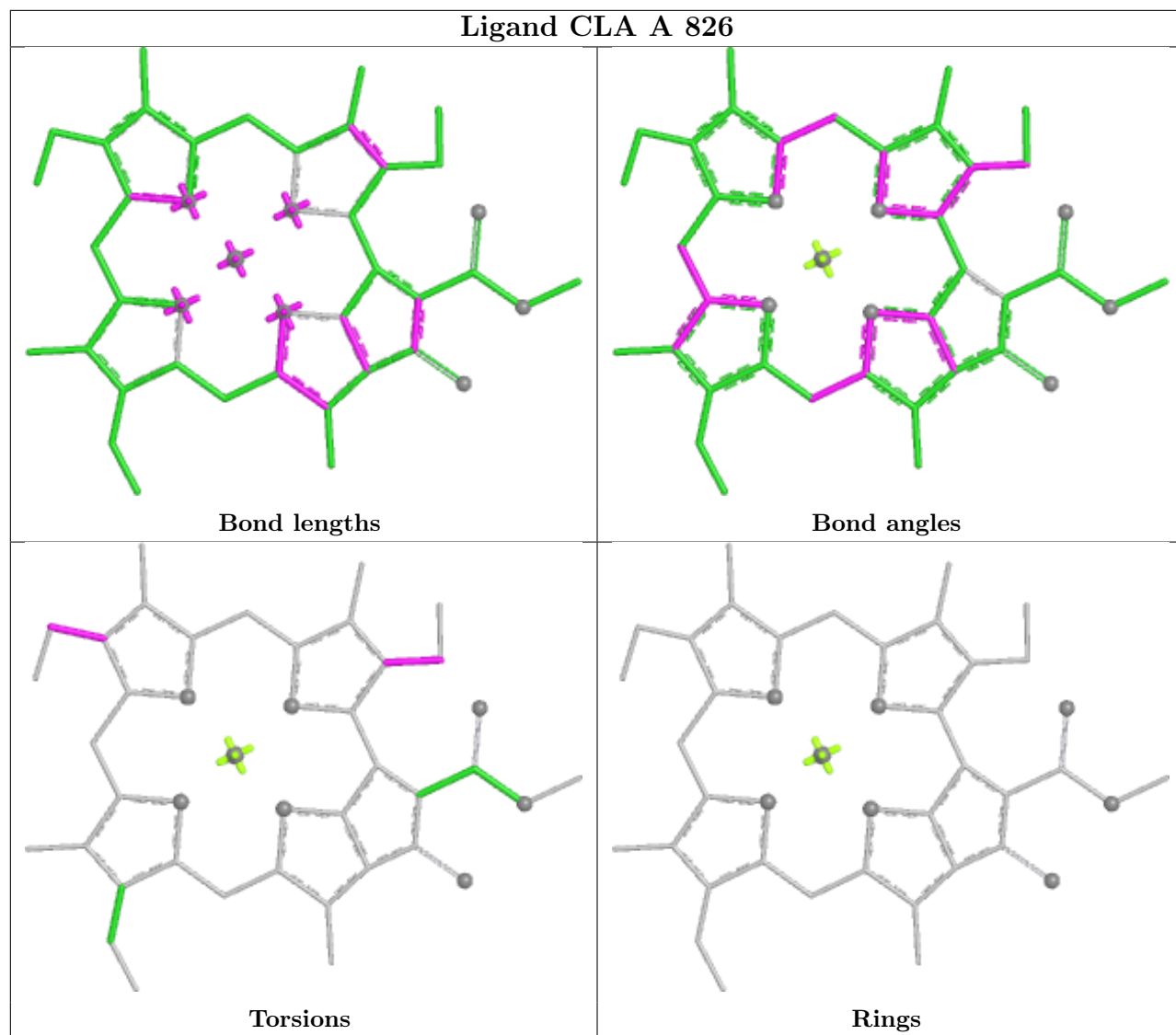
Torsions



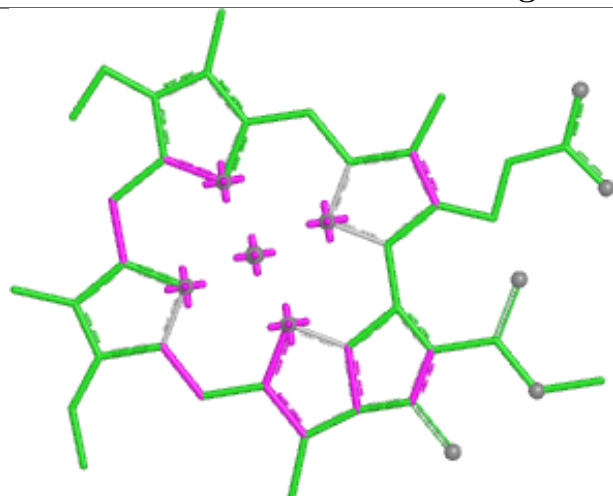
Rings



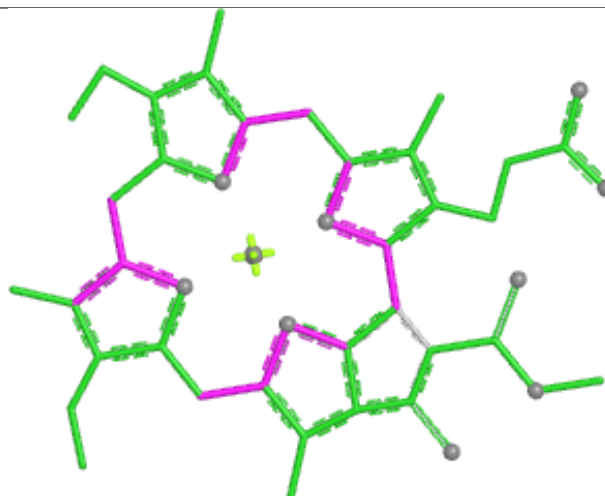
Ligand CLA A 826



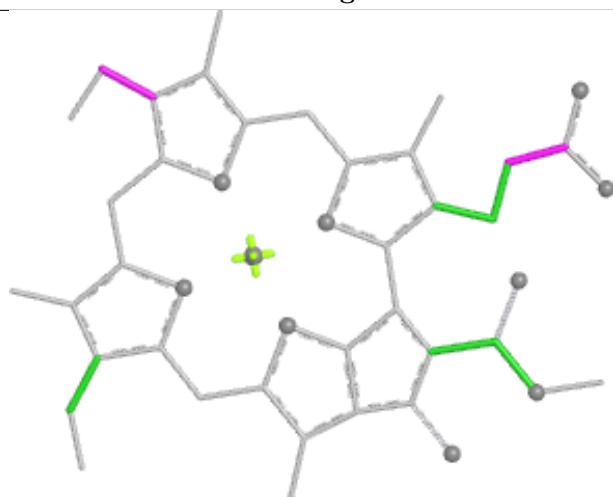
Ligand CLA 3 311



Bond lengths



Bond angles

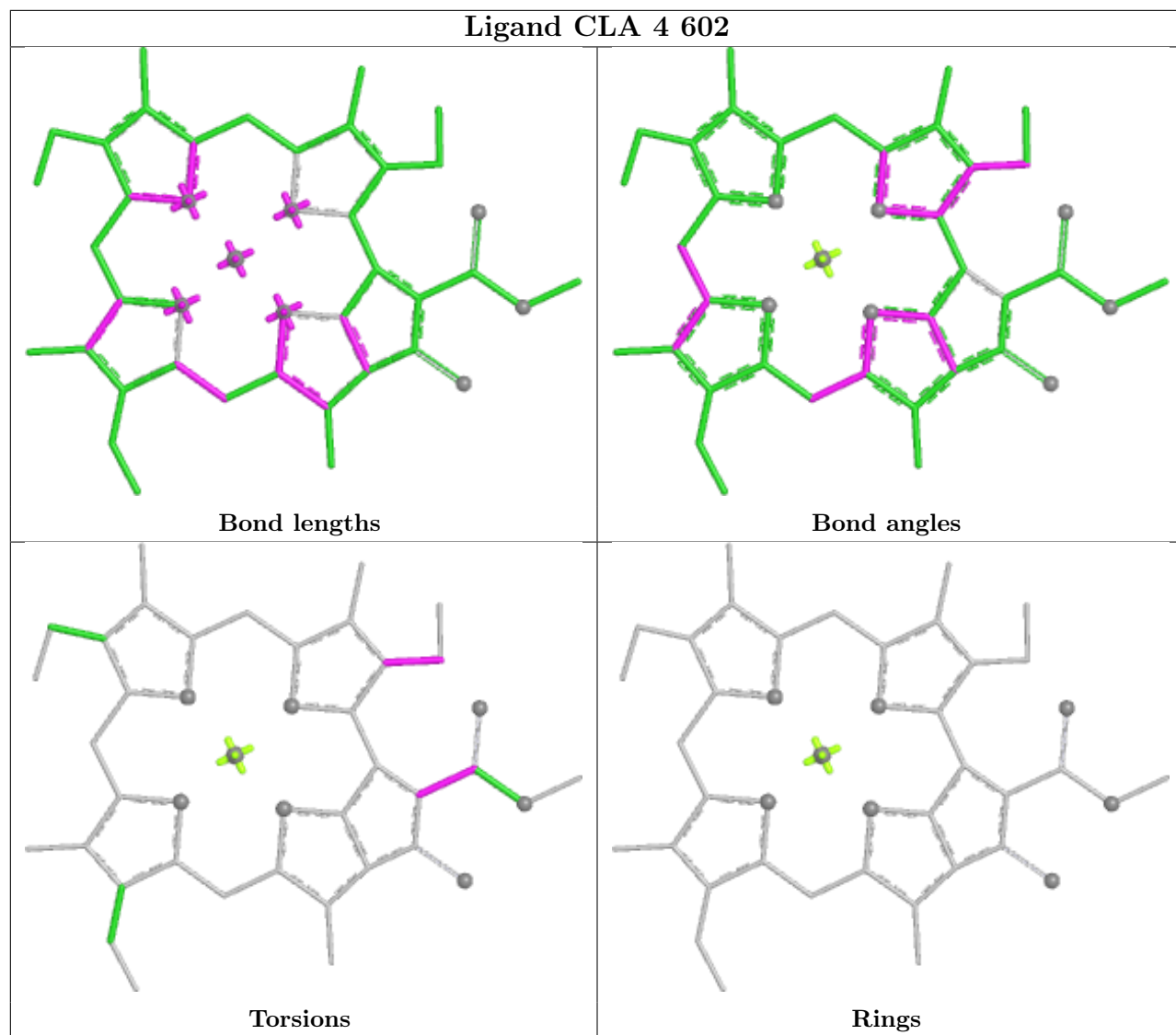


Torsions

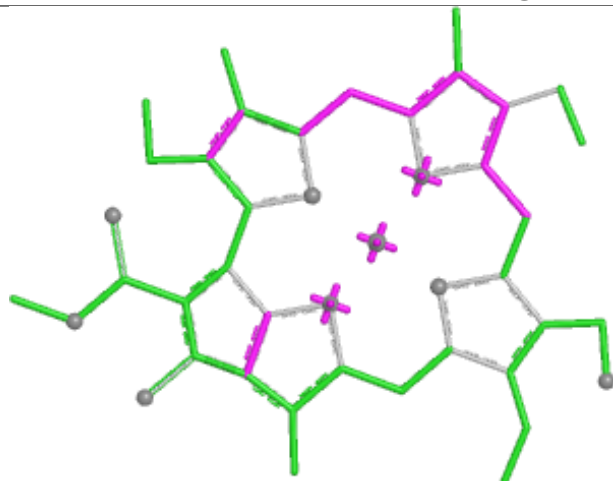


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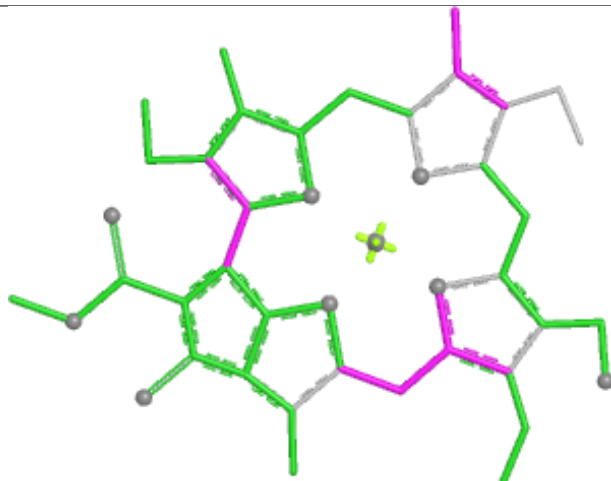
Ligand CLA 4 602



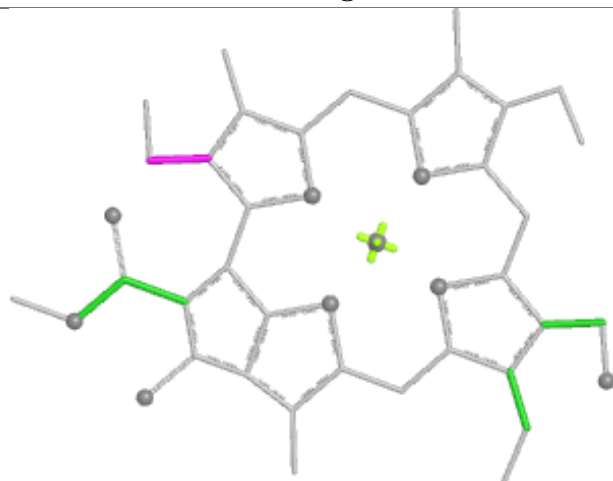
Ligand CHL Z 605



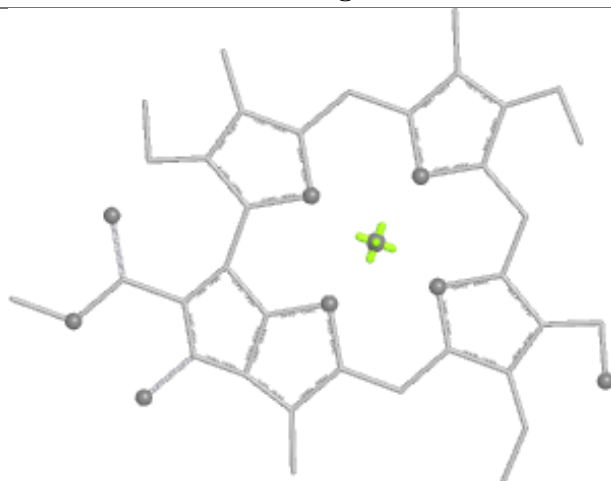
Bond lengths



Bond angles

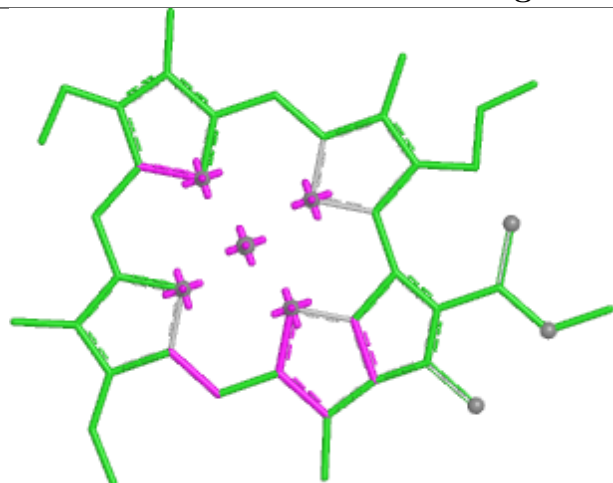


Torsions

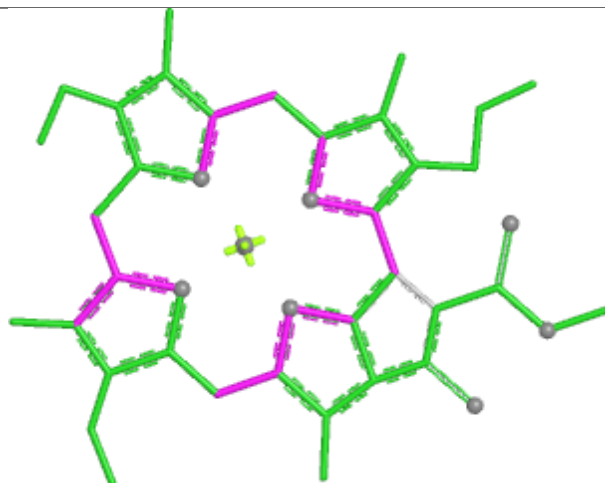


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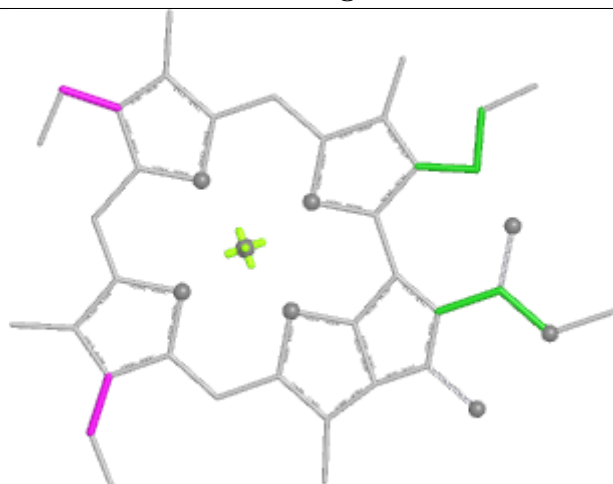
Ligand CLA B 838



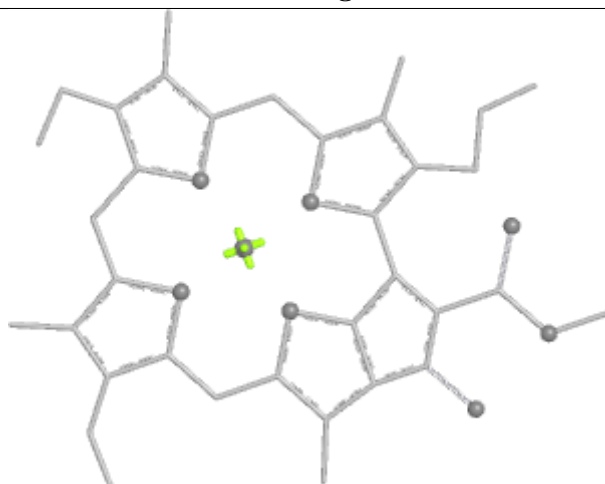
Bond lengths



Bond angles

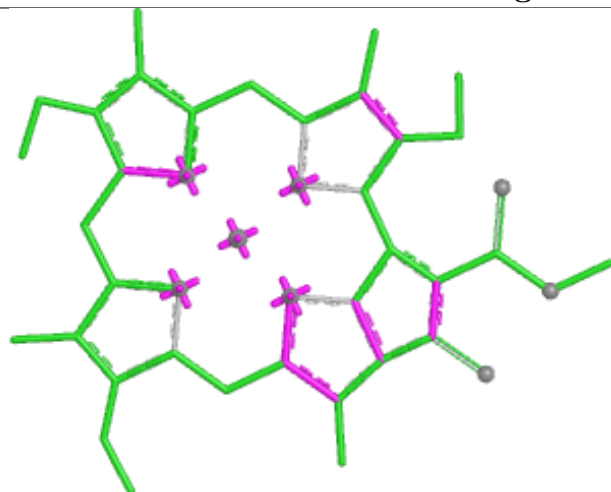


Torsions

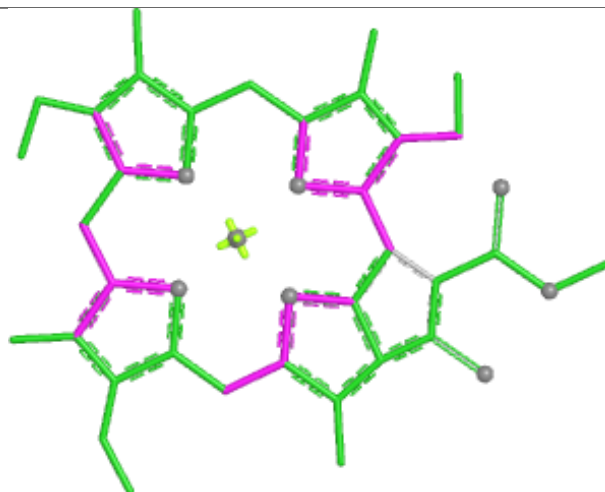


Rings

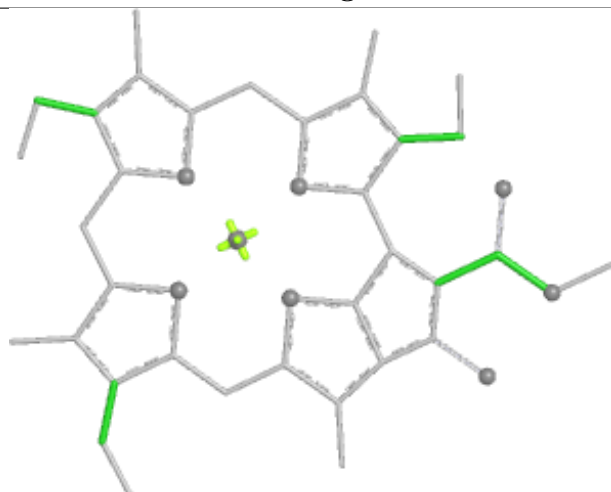
Ligand CLA B 836



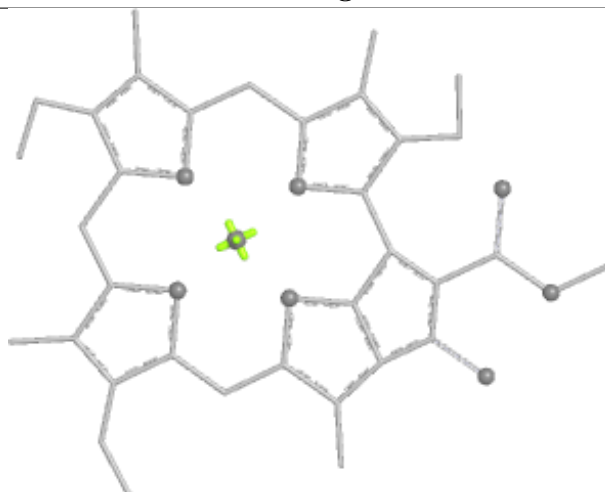
Bond lengths



Bond angles

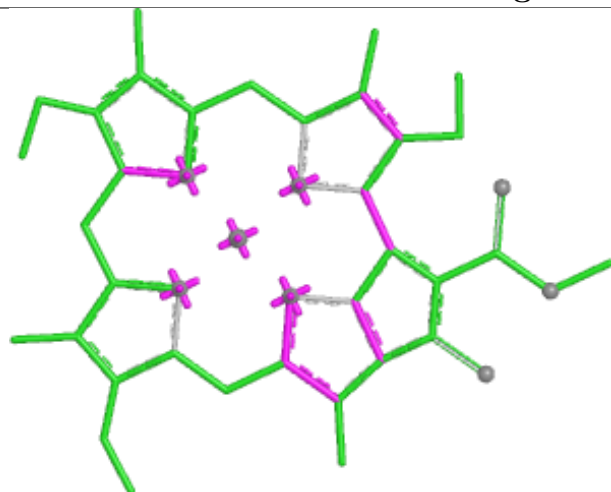


Torsions

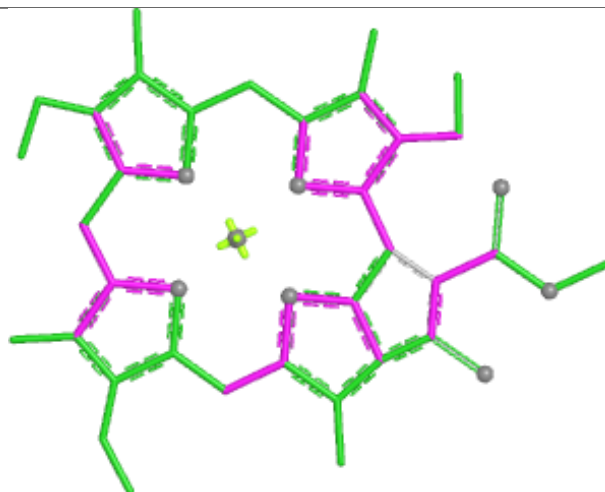


Rings

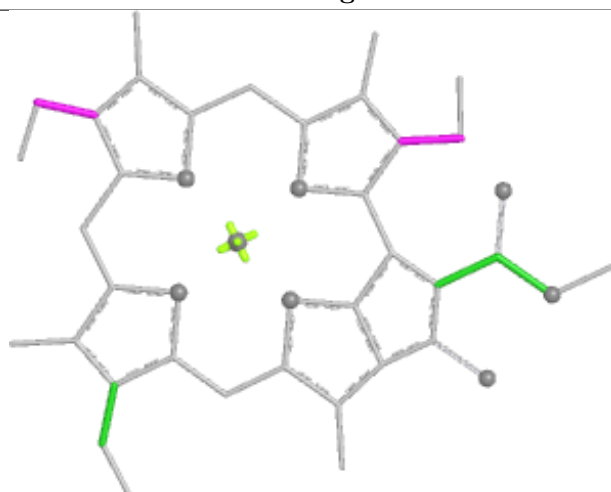
Ligand CLA A 834



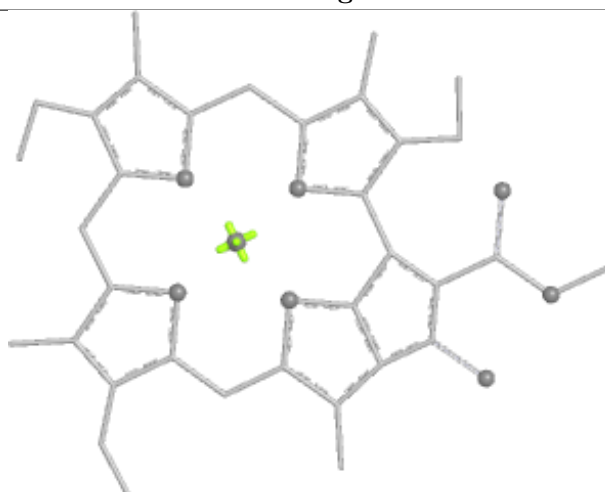
Bond lengths



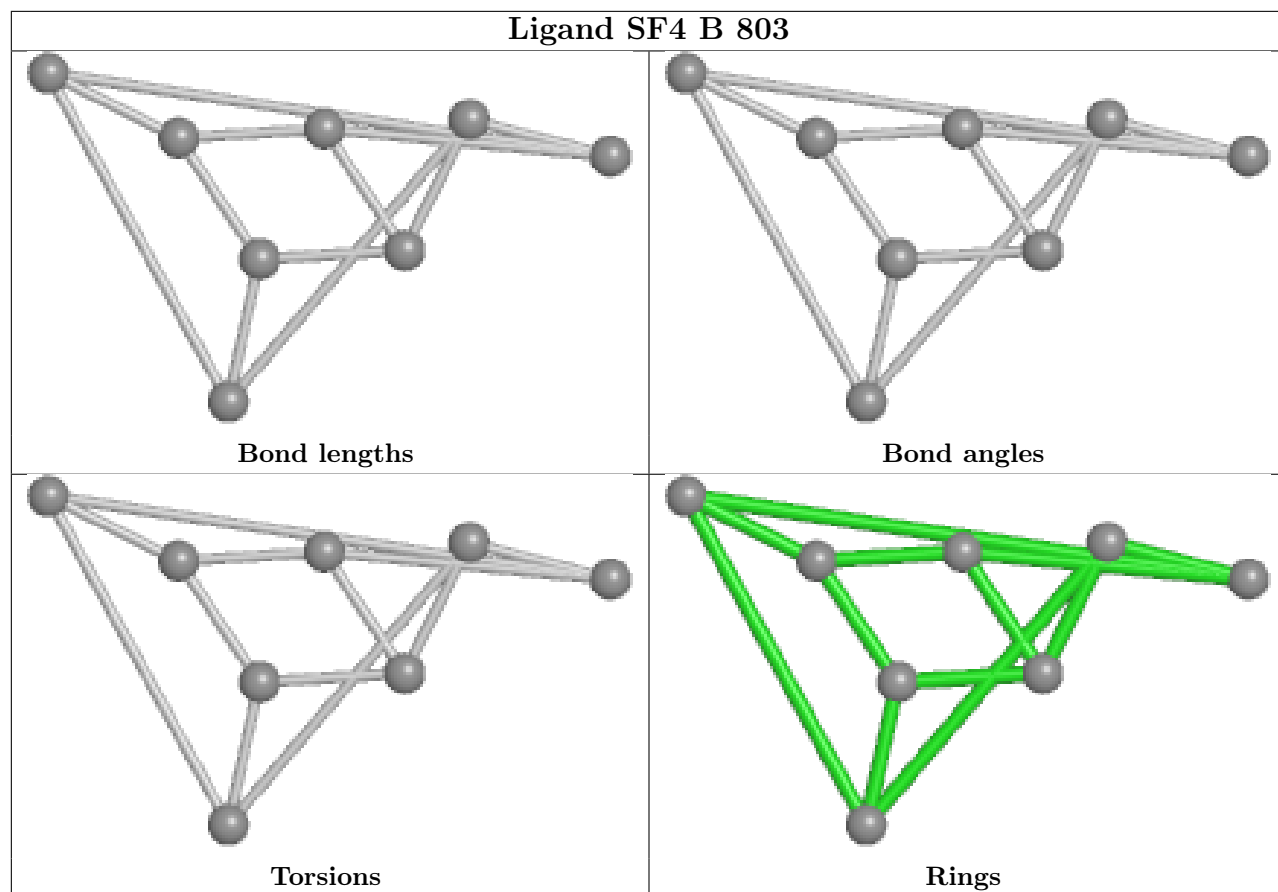
Bond angles



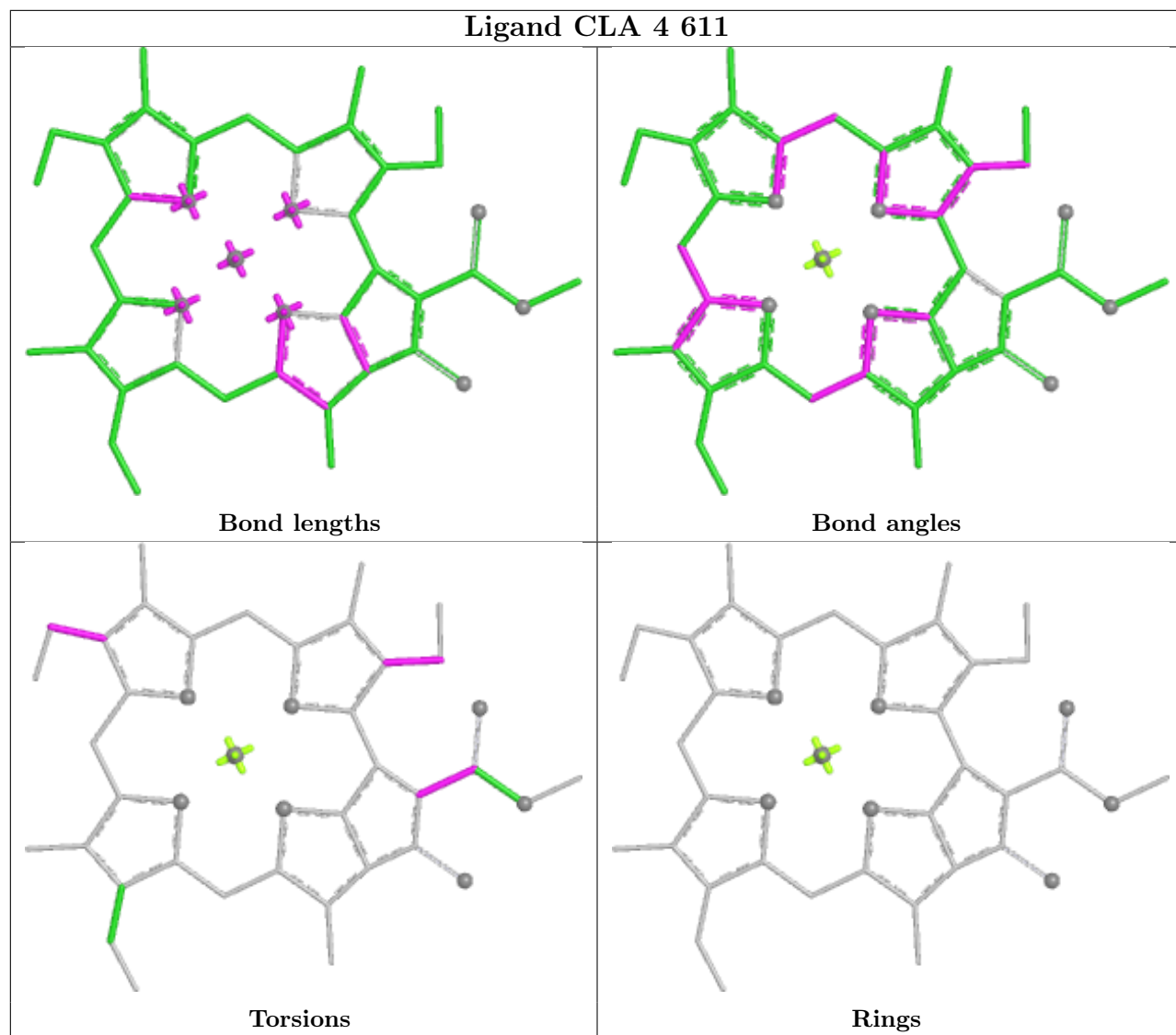
Torsions



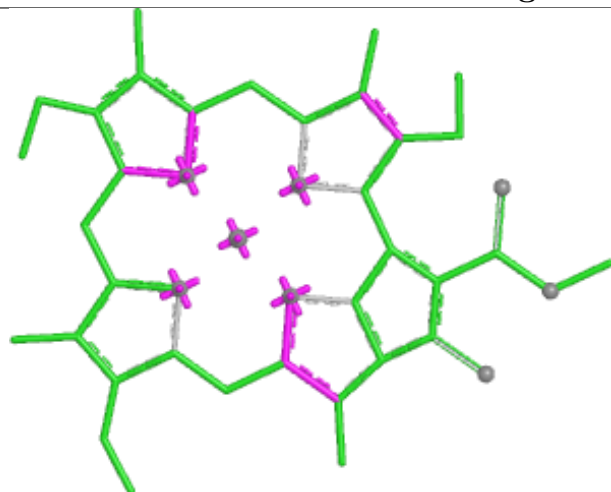
Rings



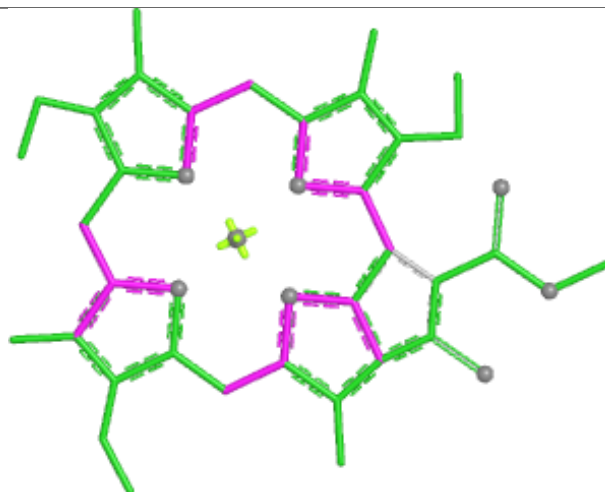
Ligand CLA 4 611



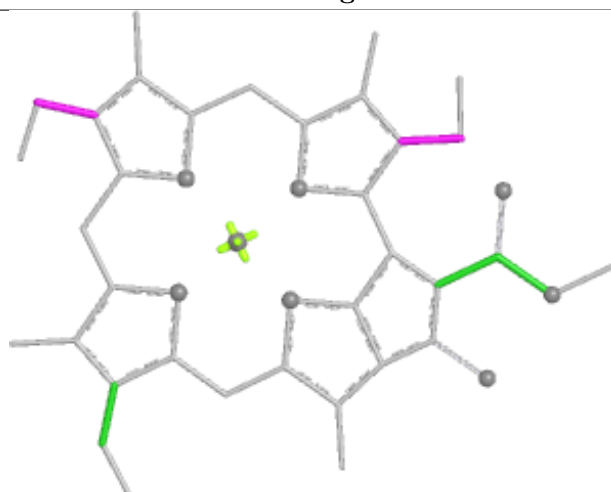
Ligand CLA 4 609



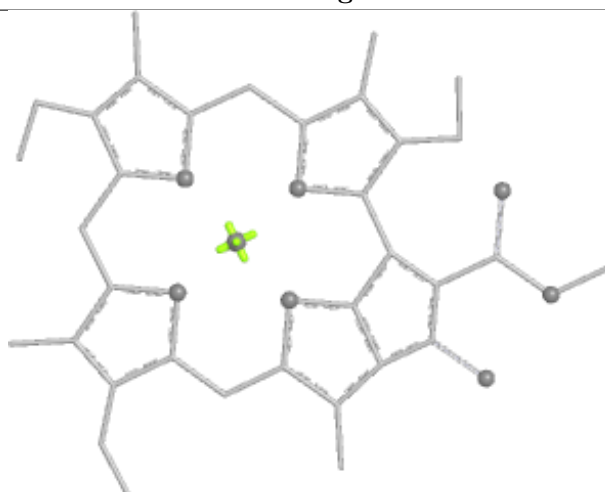
Bond lengths



Bond angles

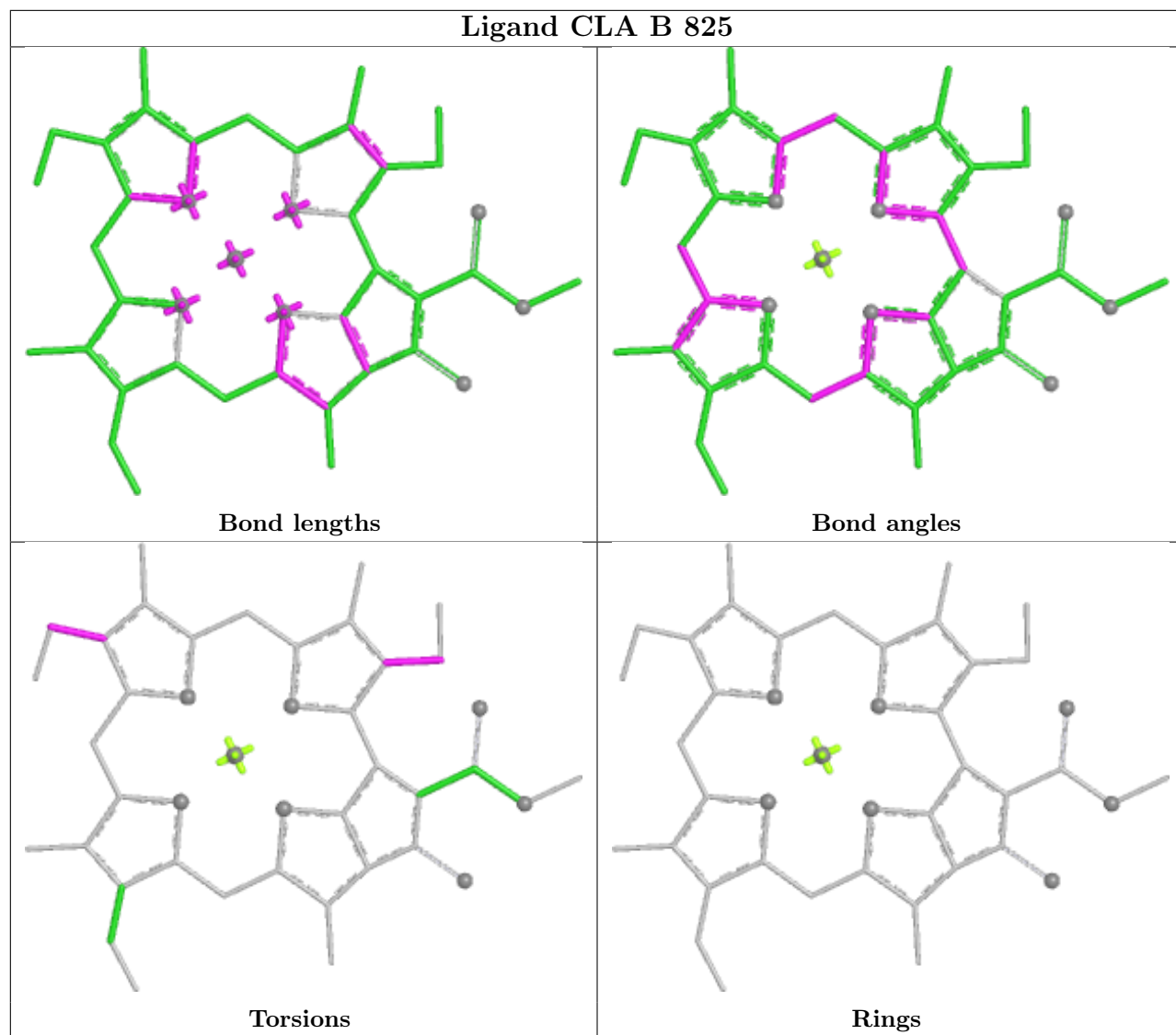


Torsions

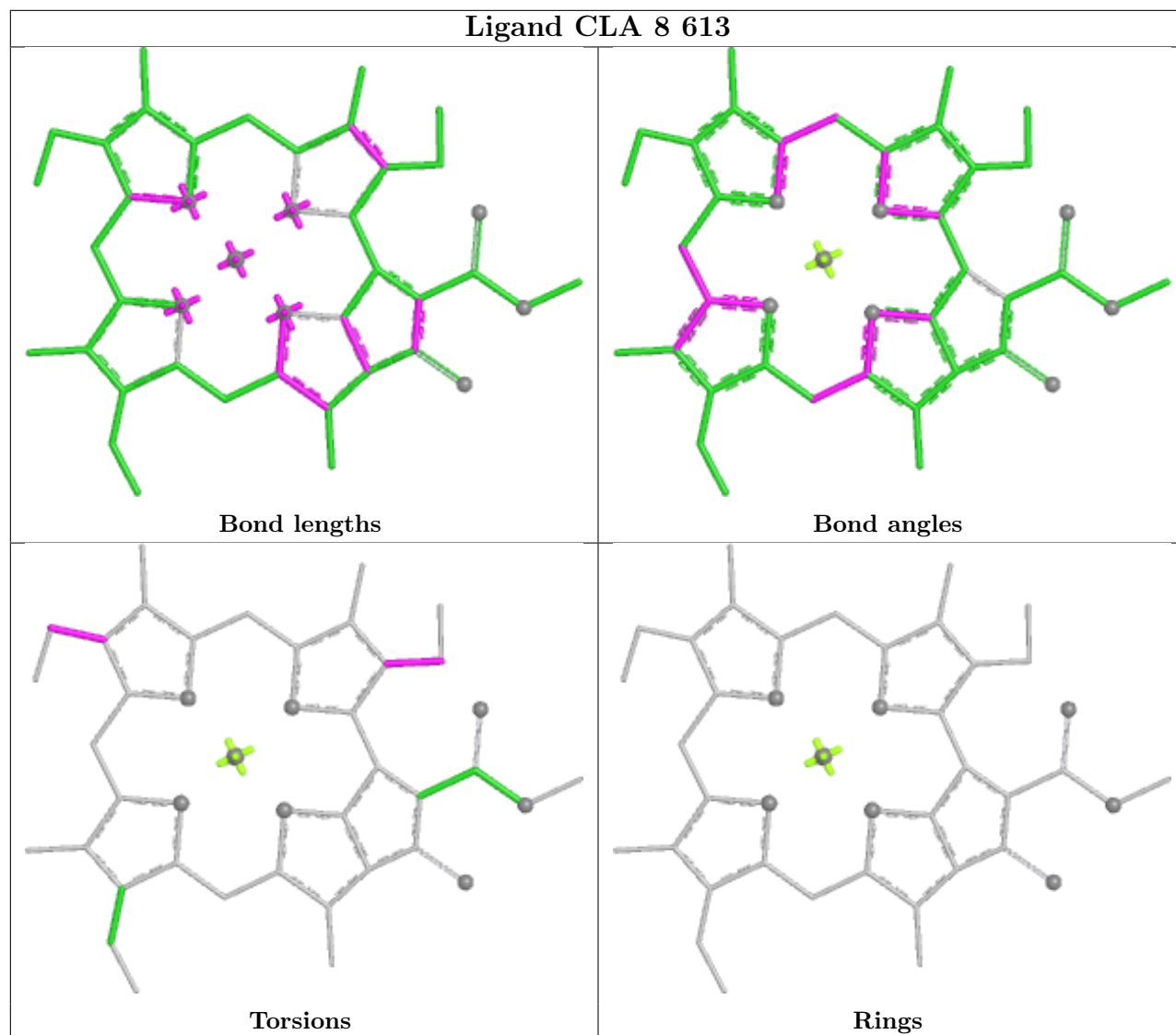


Rings

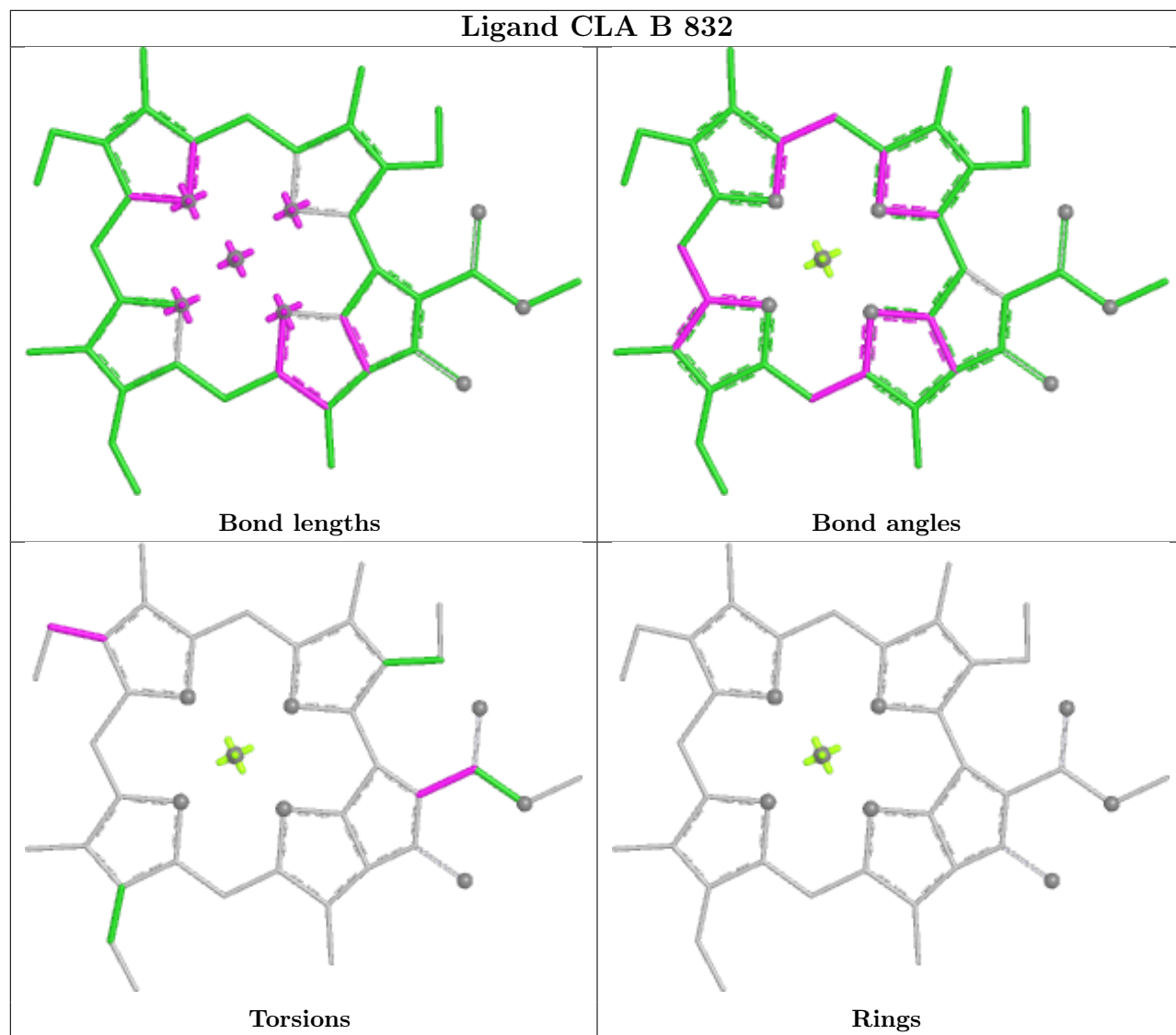
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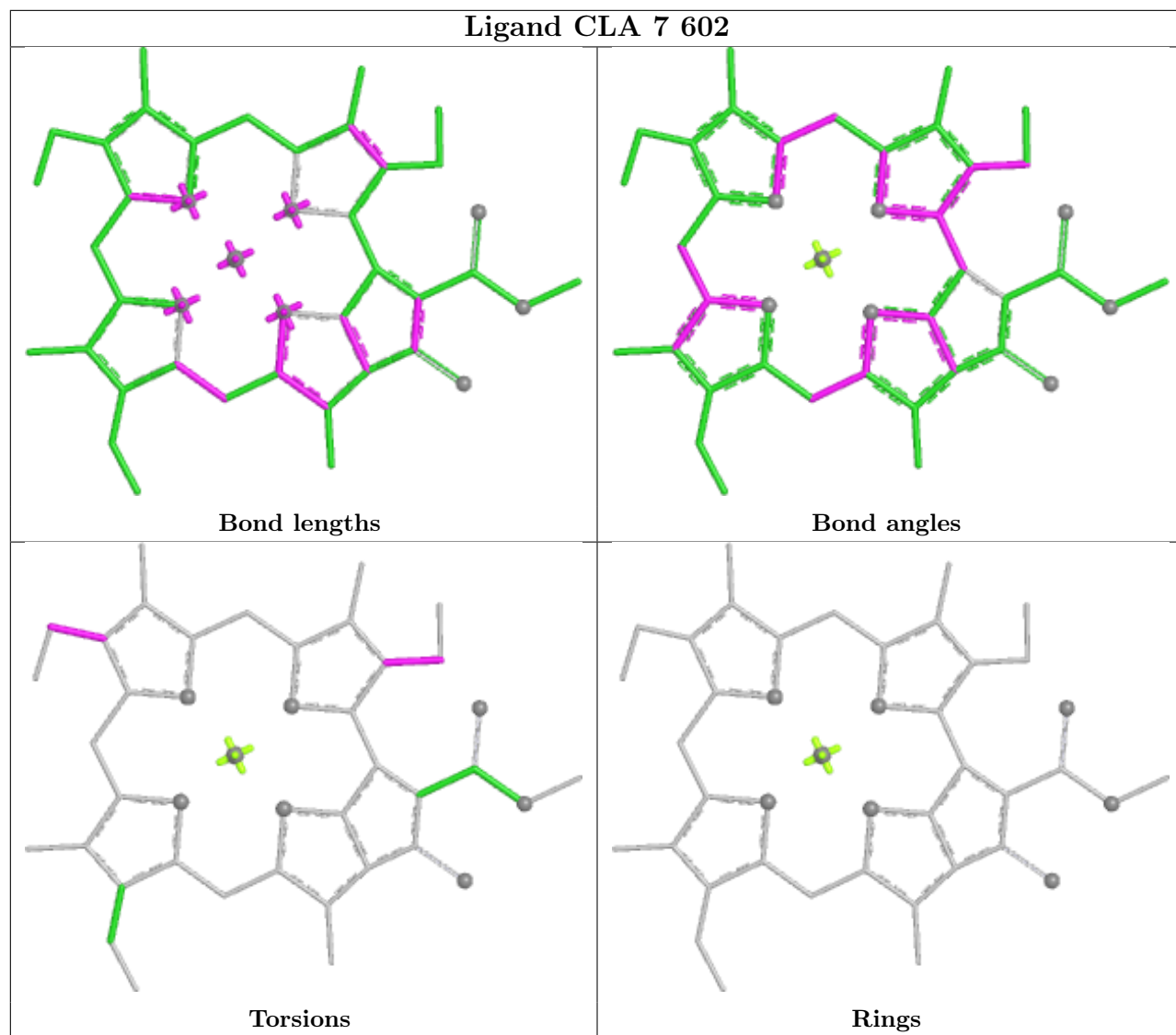
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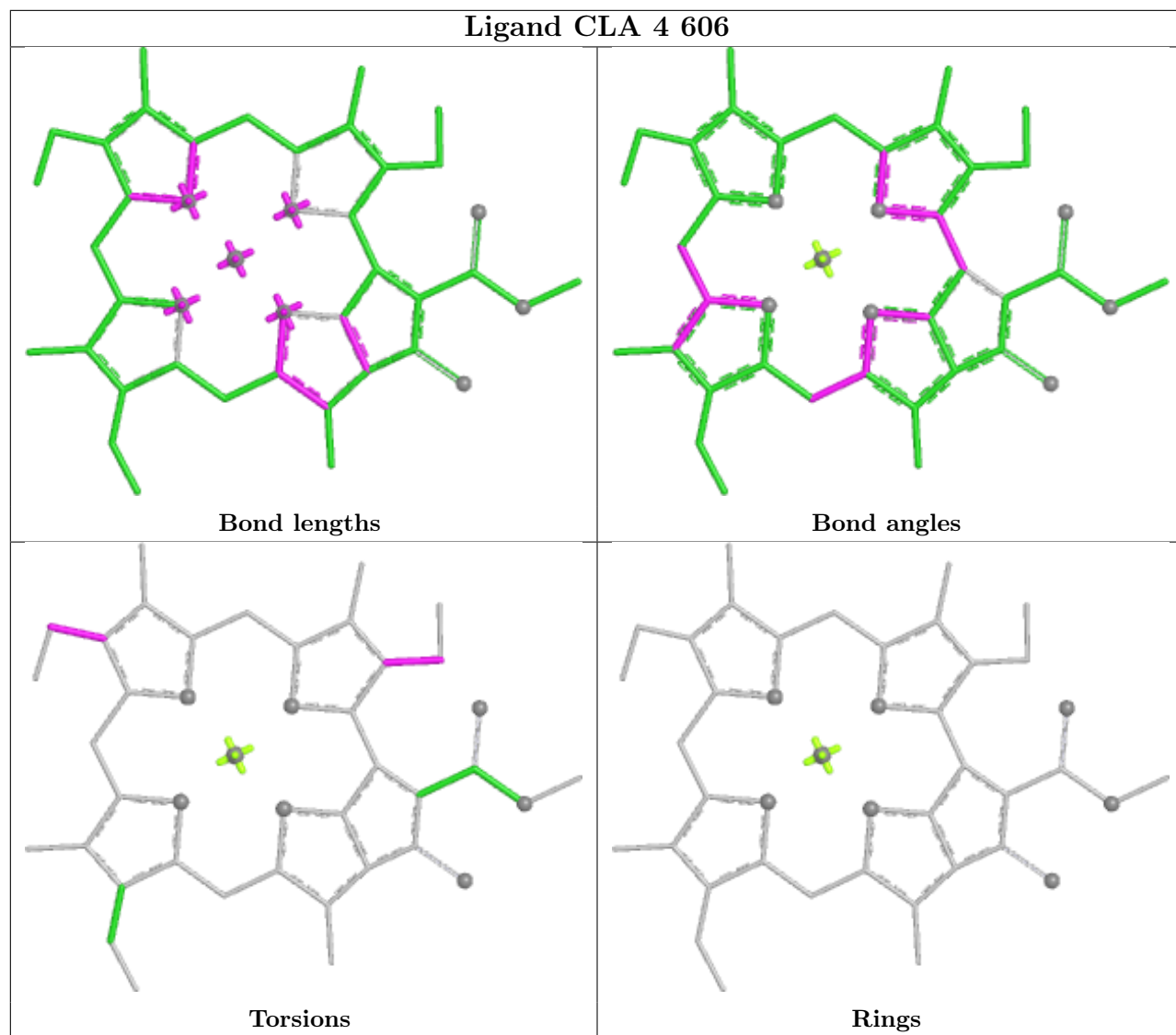
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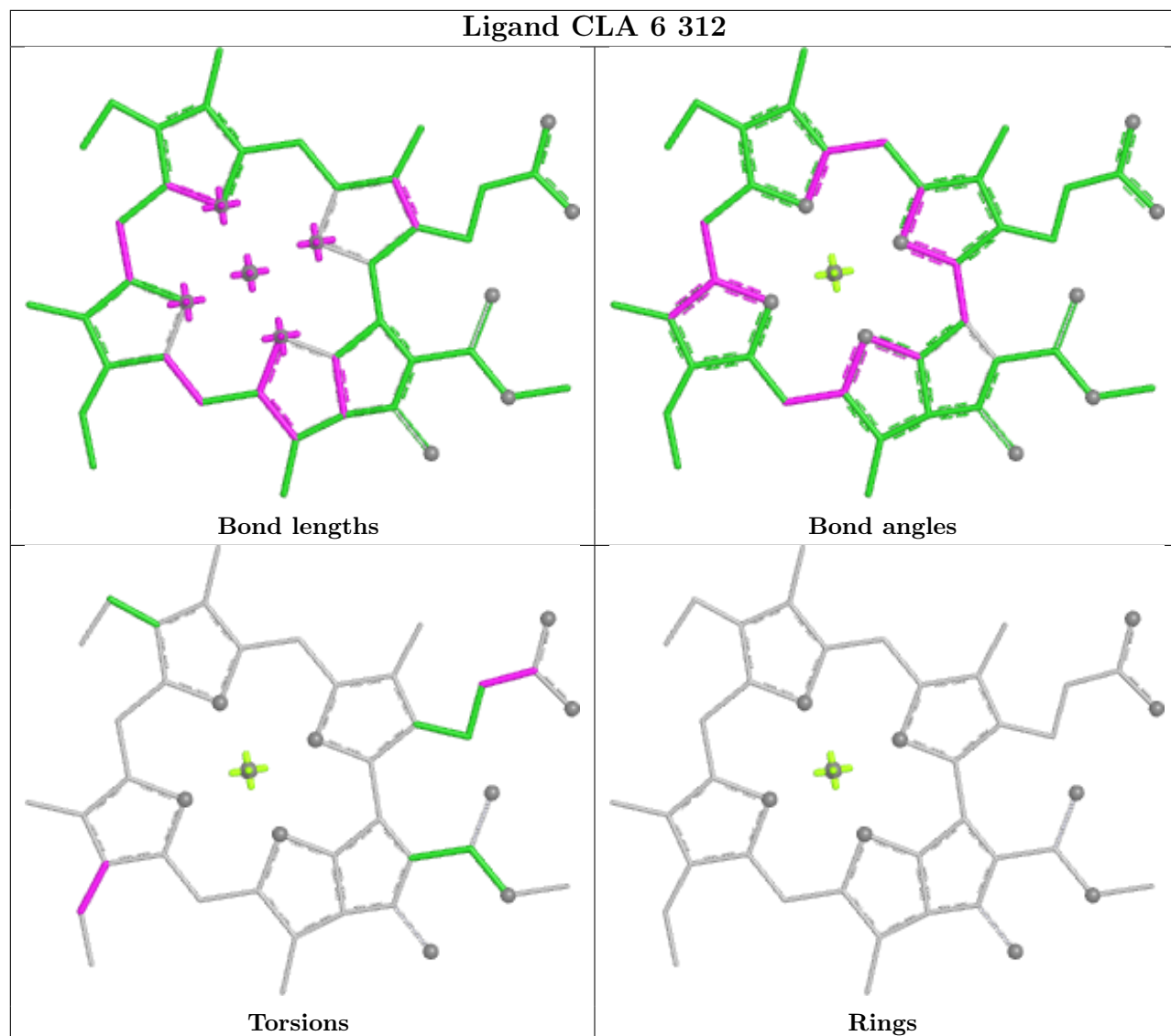
Ligand CLA 7 602



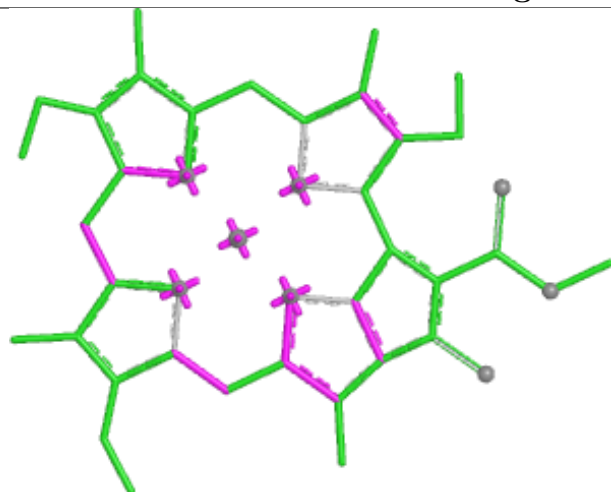
Ligand CLA 4 606



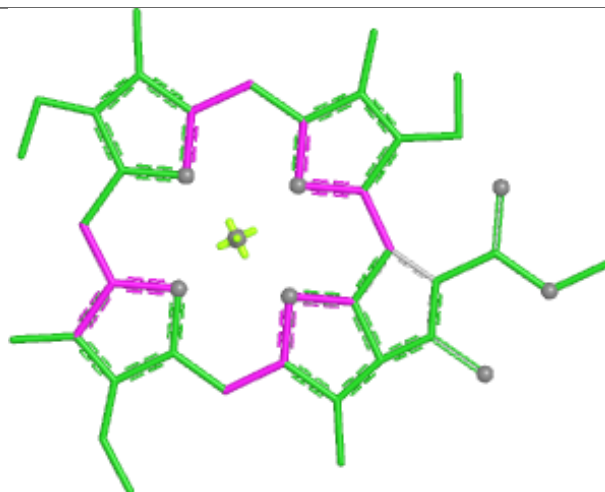
Ligand CLA 6 312



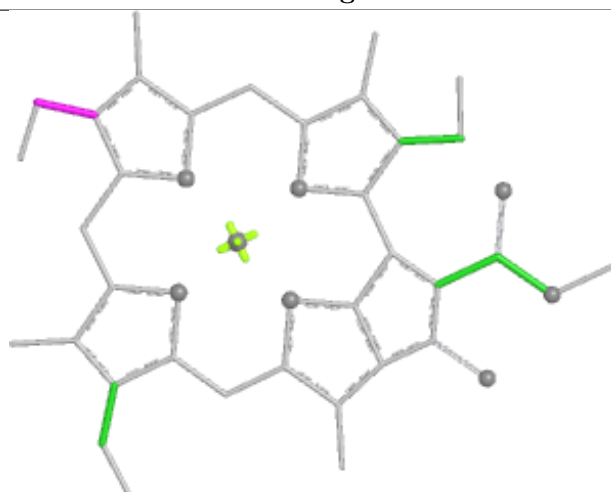
Ligand CLA A 809



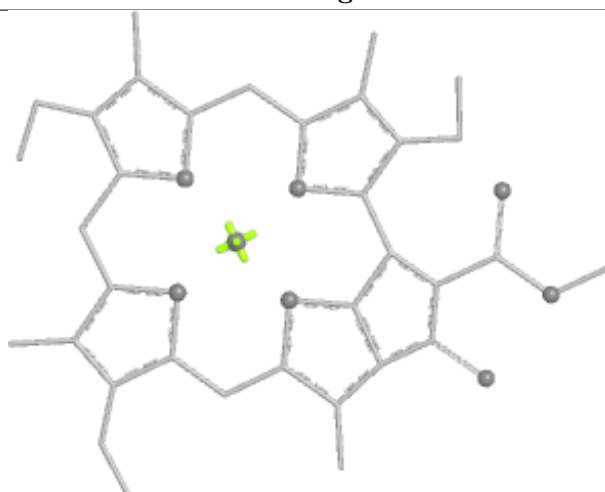
Bond lengths



Bond angles

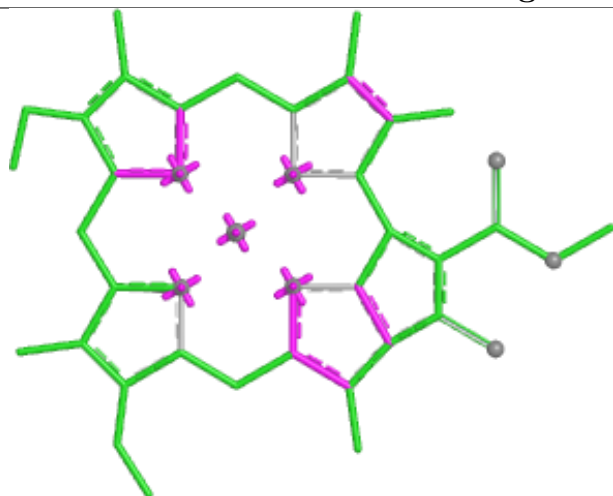


Torsions

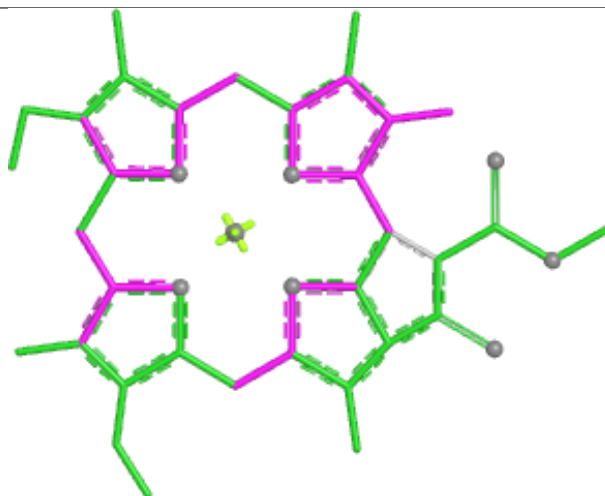


Rings

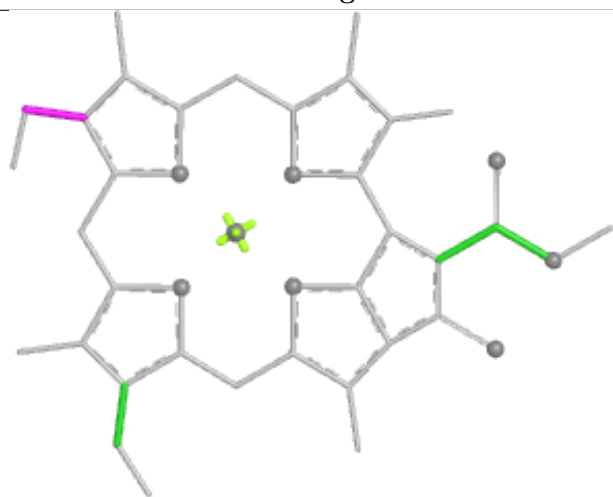
Ligand CLA 3 309



Bond lengths



Bond angles

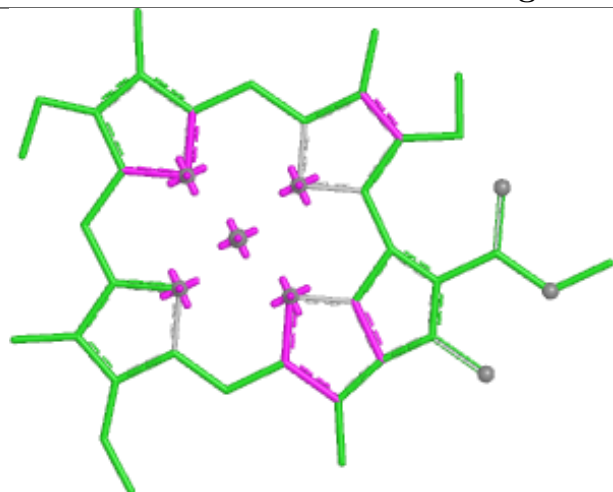


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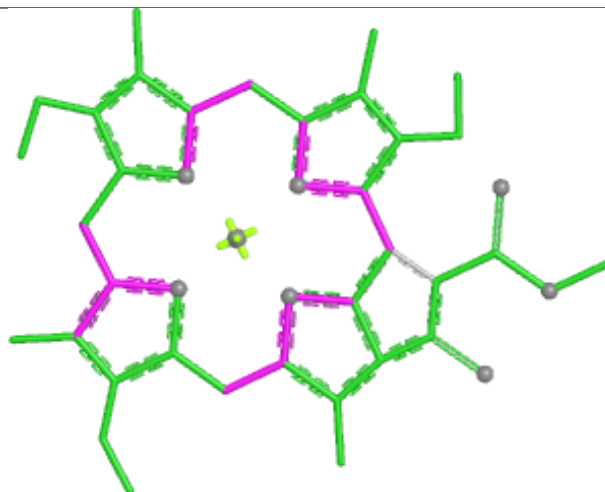


Rings

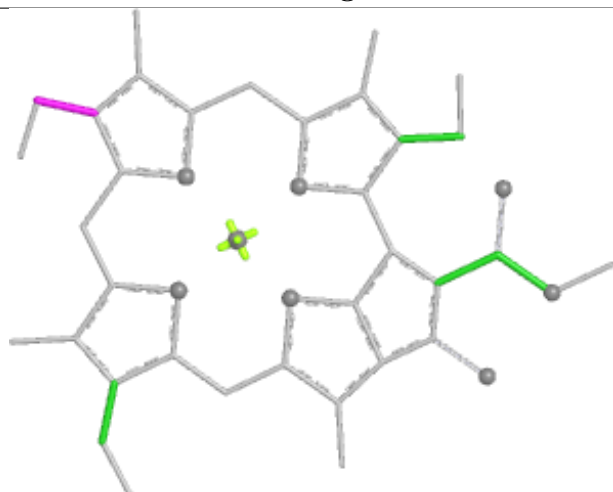
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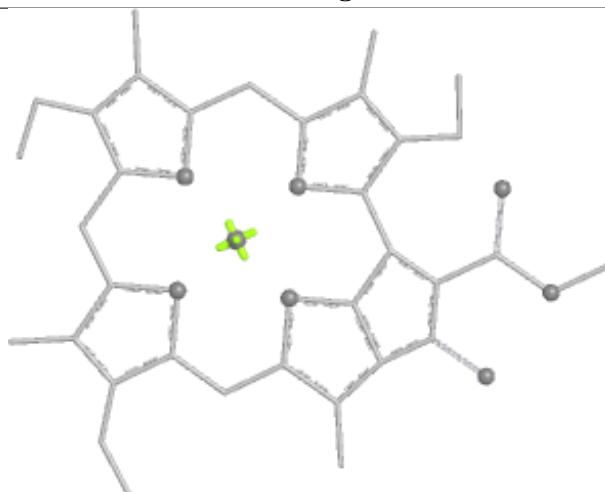
Bond lengths



Bond angles

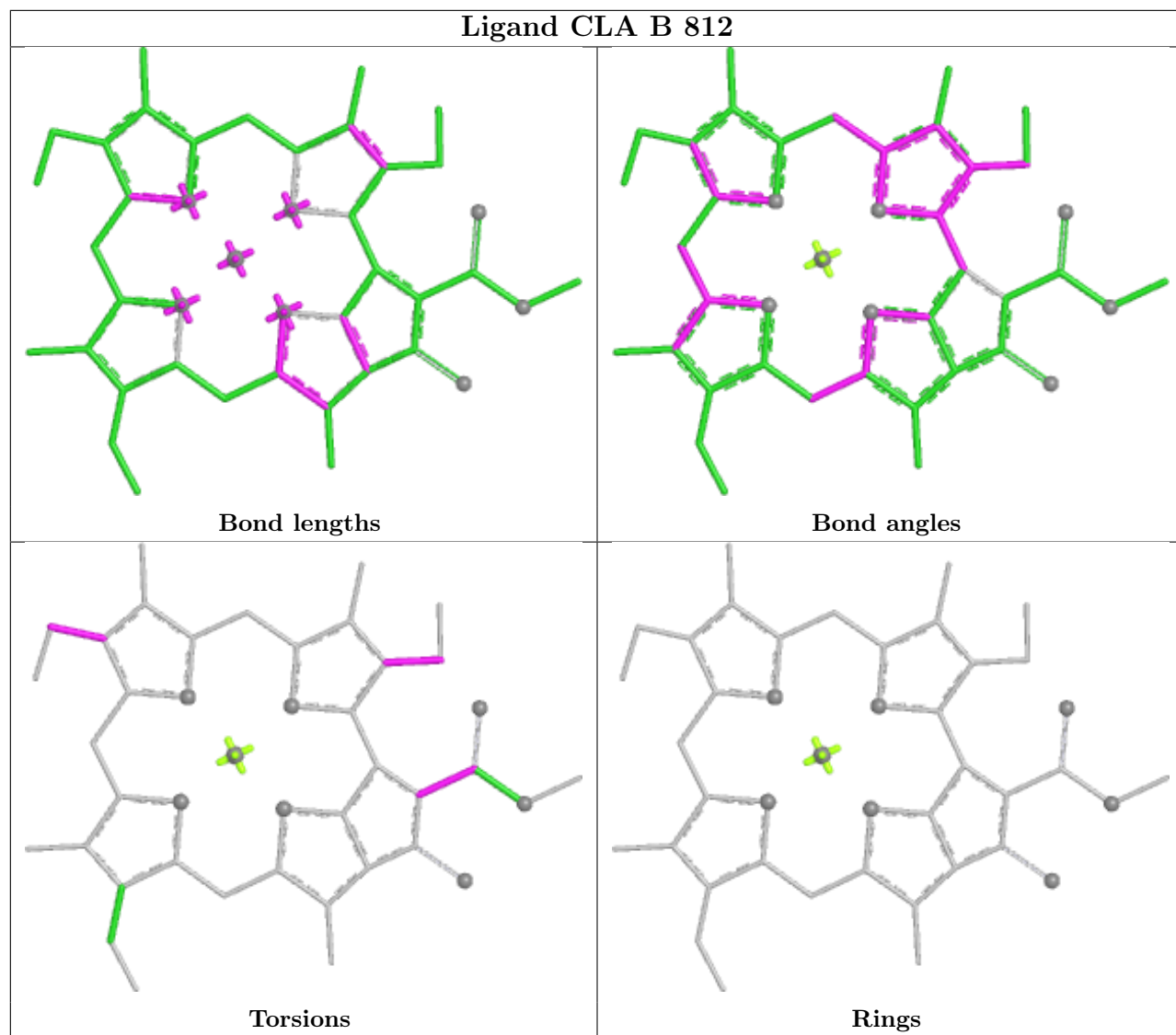


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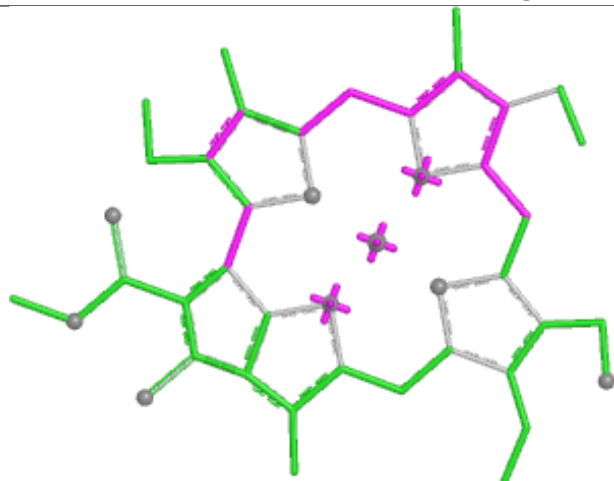


Rings

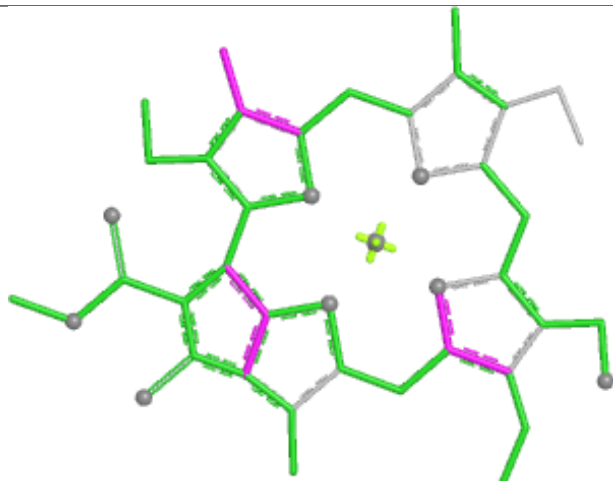
Ligand CLA B 812



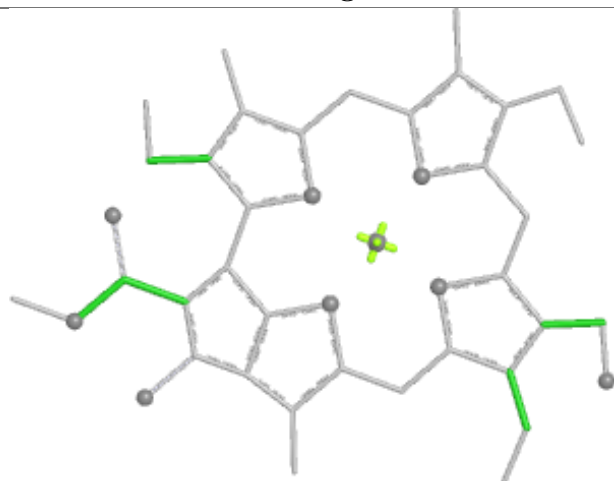
Ligand CHL 5 606



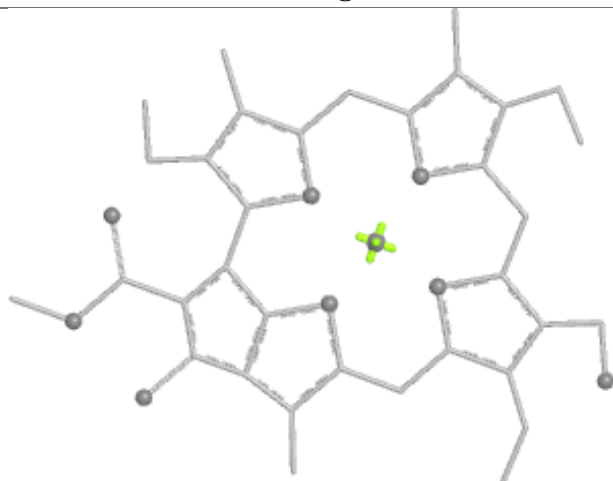
Bond lengths



Bond angles

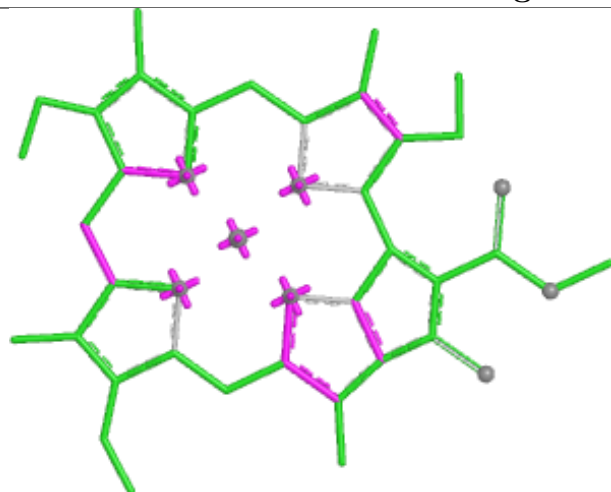


Torsions

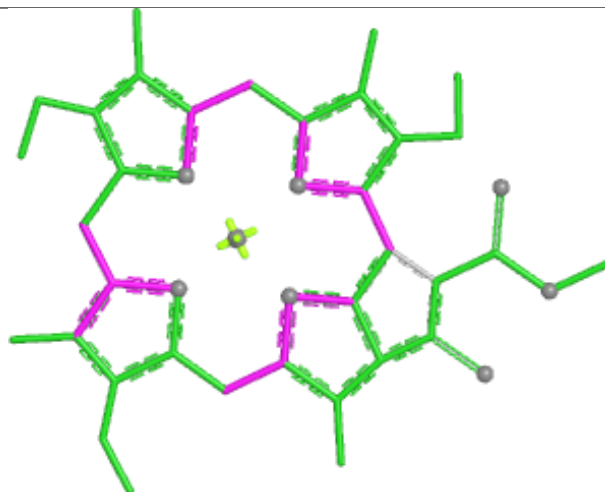


Rings

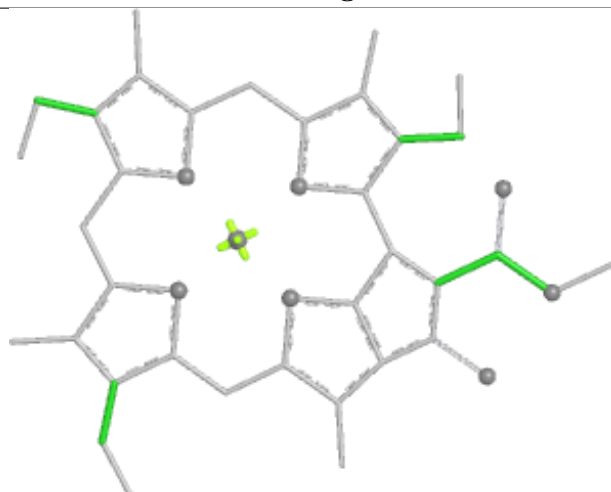
Ligand CLA A 832



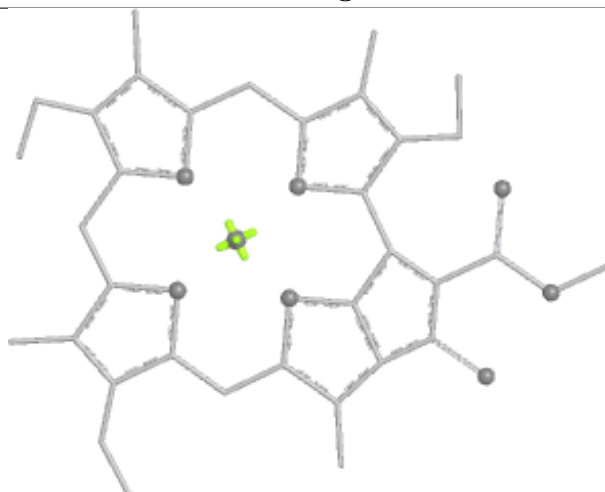
Bond lengths



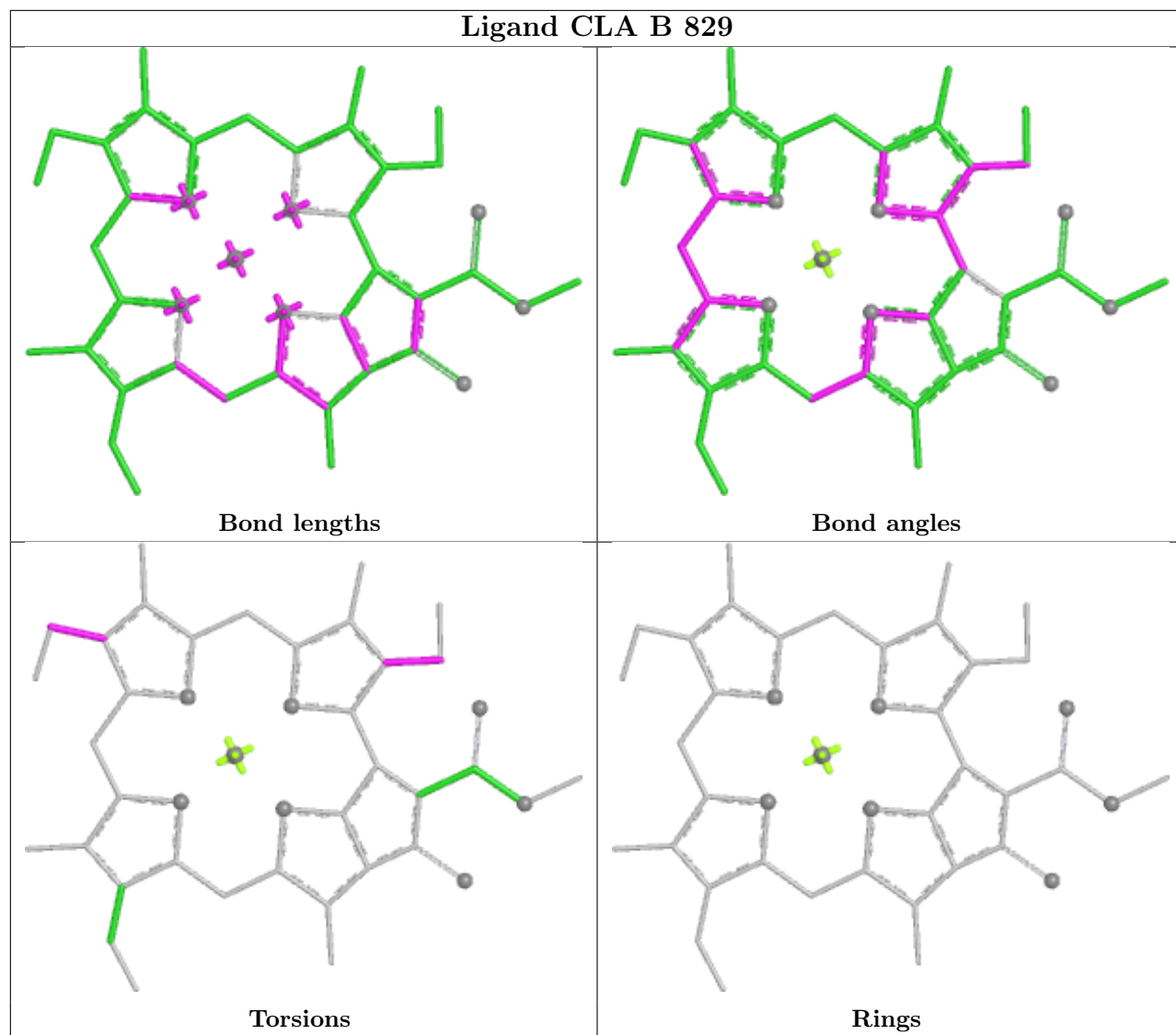
Bond angles



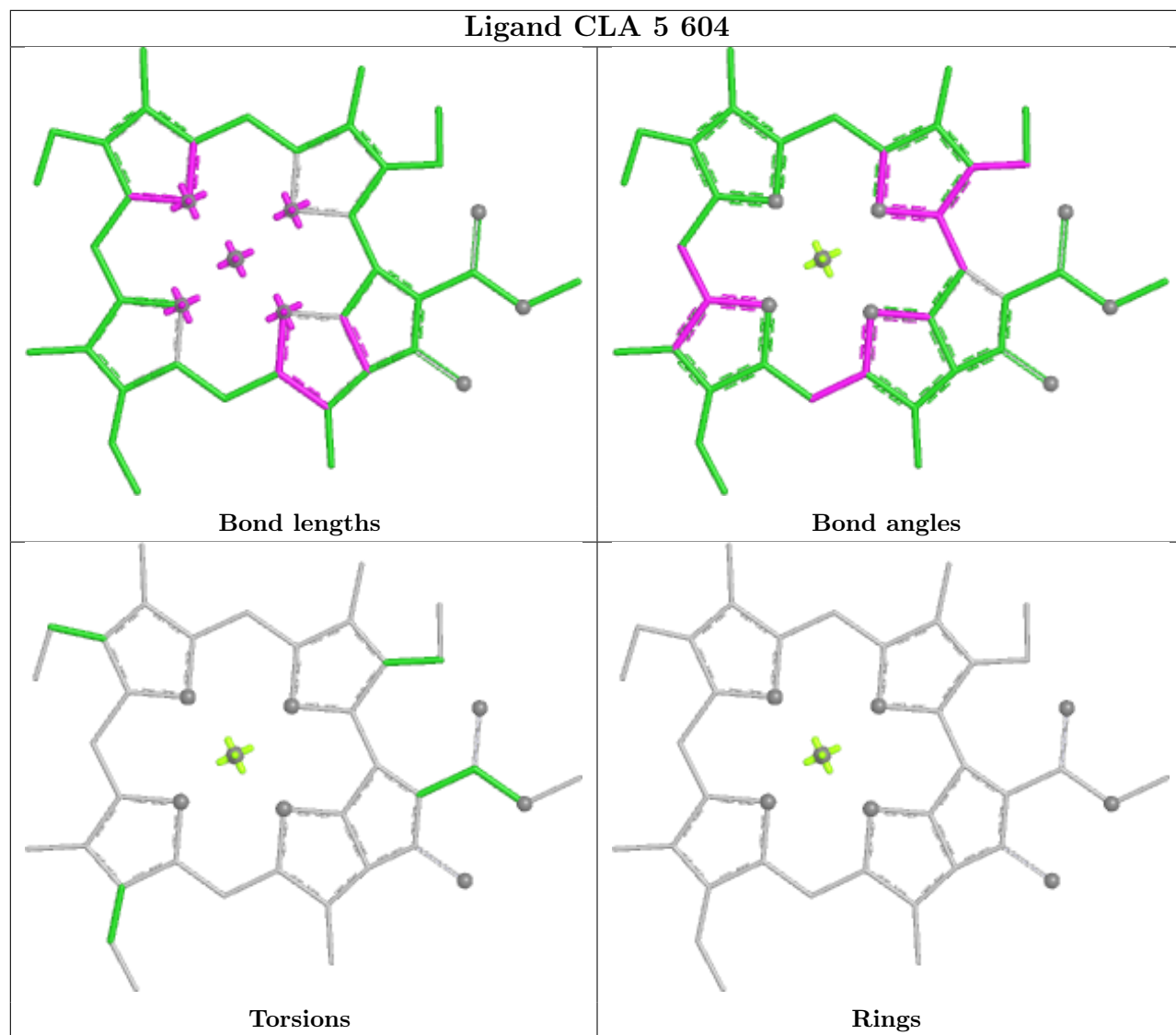
Torsions



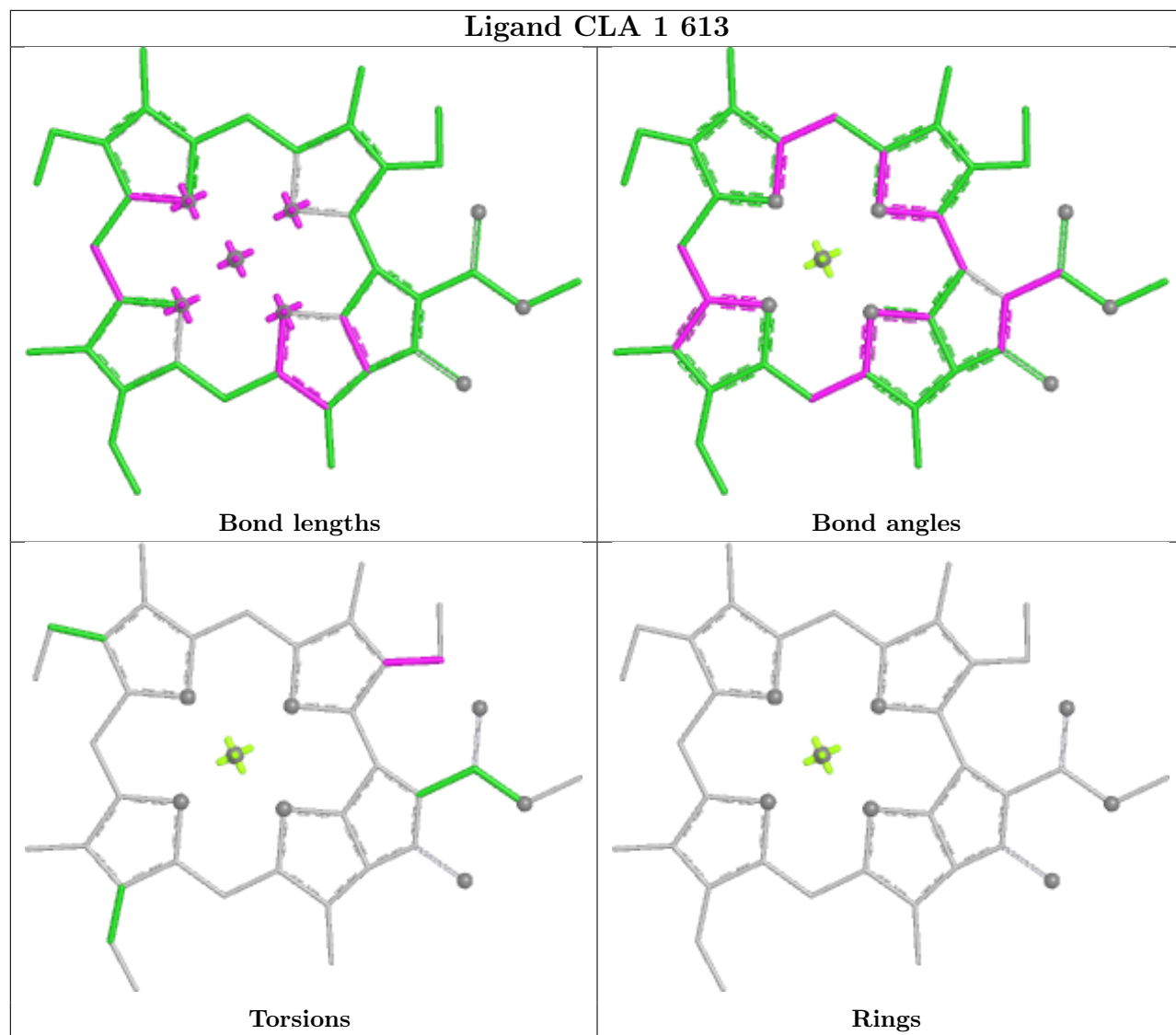
Rings

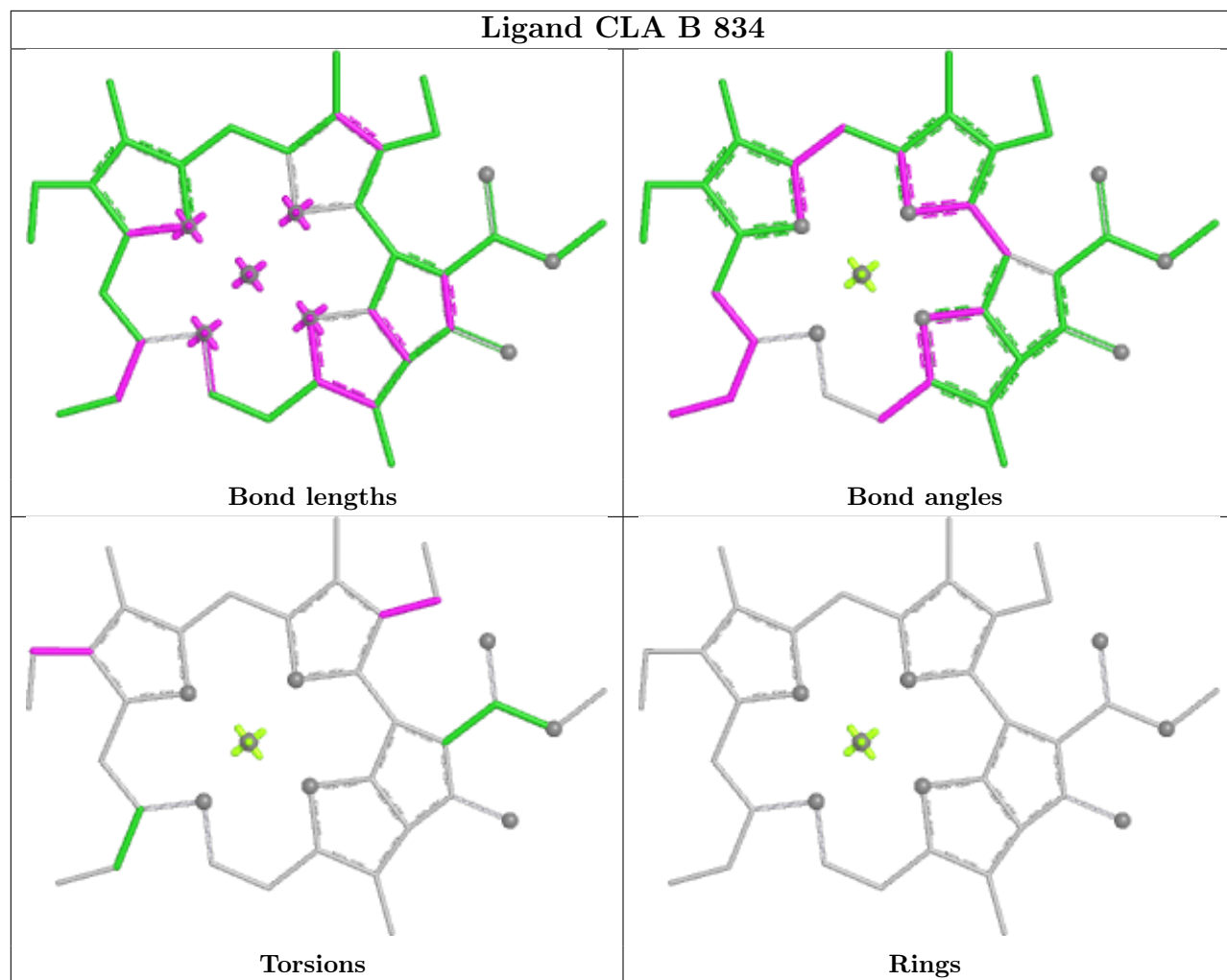


Ligand CLA 5 604

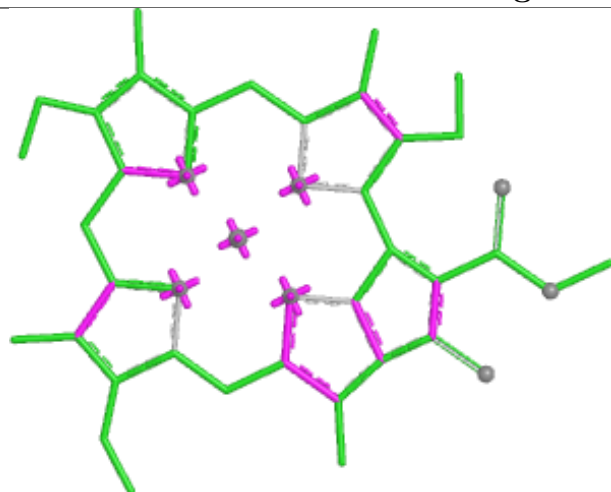


Ligand CLA 1 613

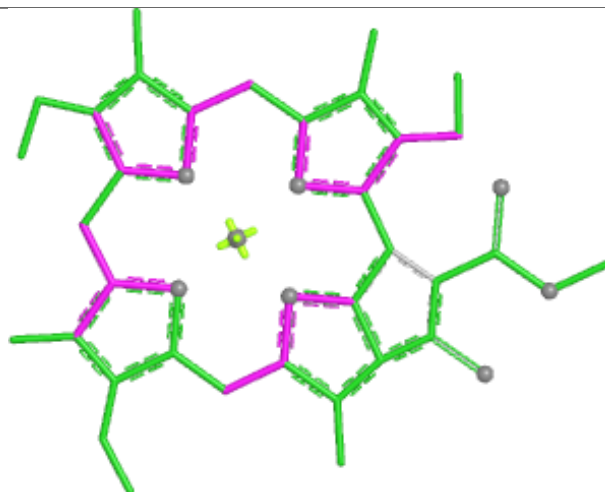




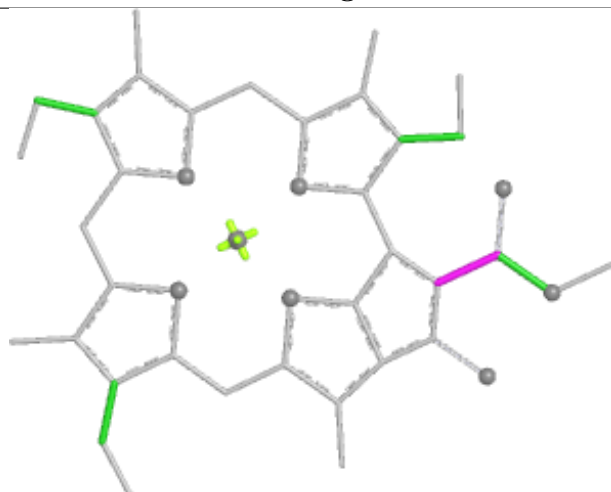
Ligand CLA A 805



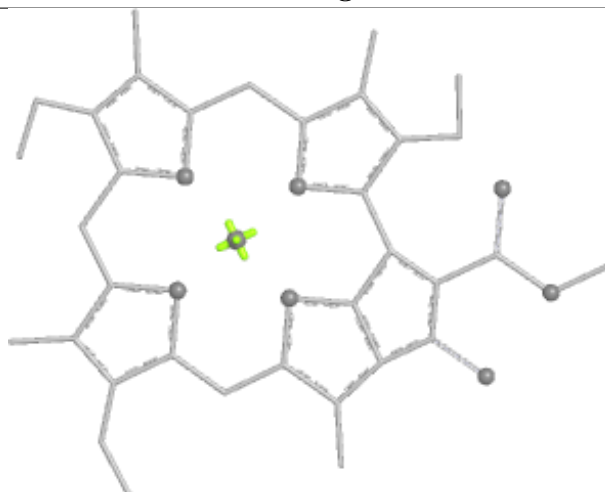
Bond lengths



Bond angles

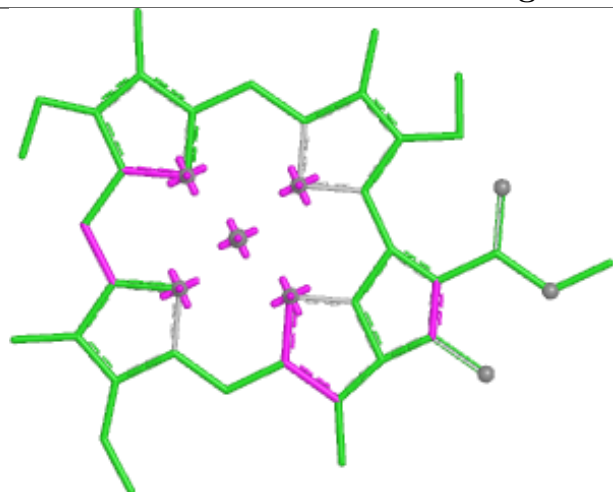


Torsions

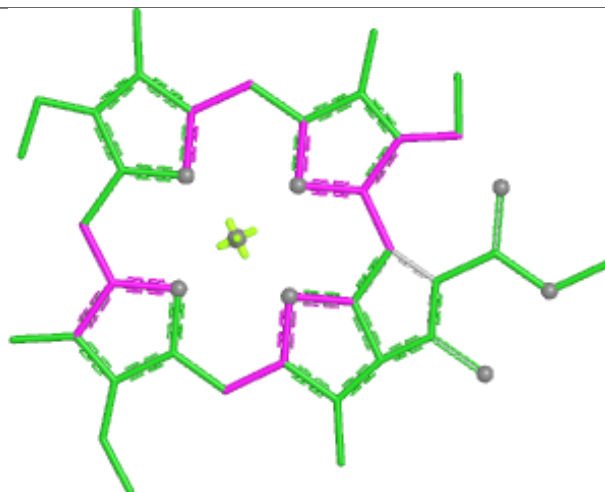


Rings

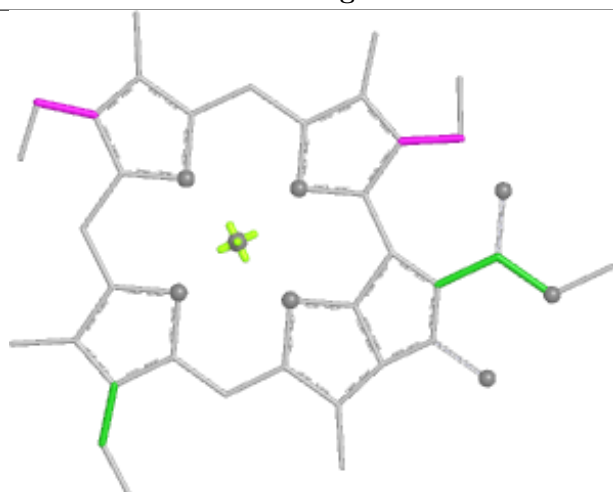
Ligand CLA 8 602



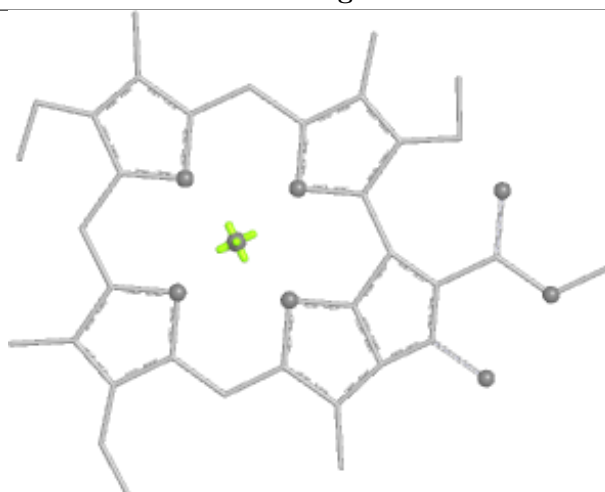
Bond lengths



Bond angles

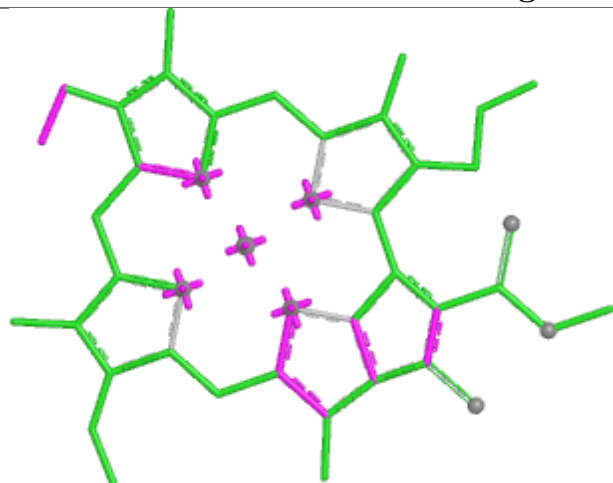


Torsions

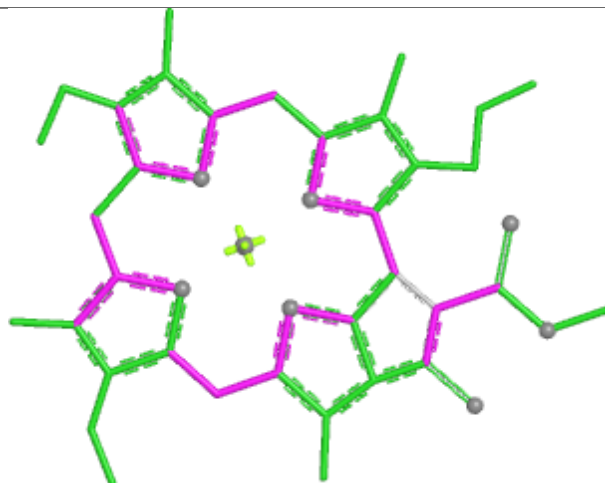


Rings

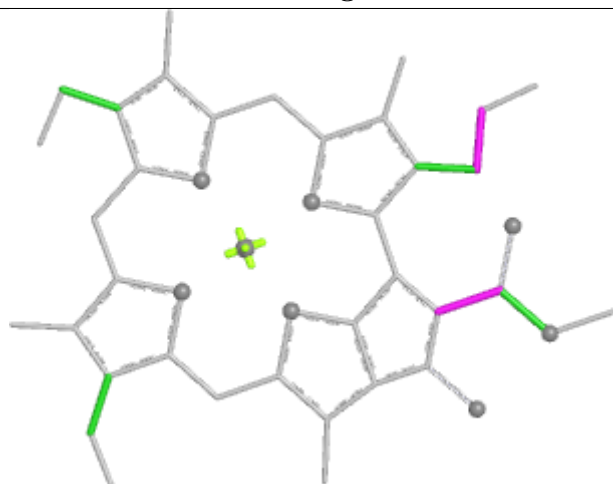
Ligand CLA 7 604



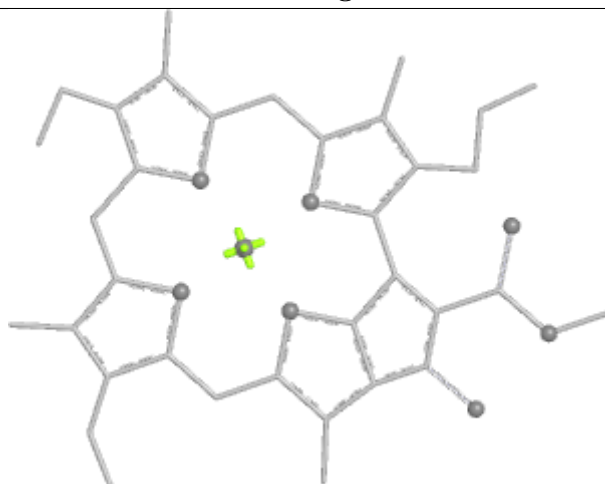
Bond lengths



Bond angles

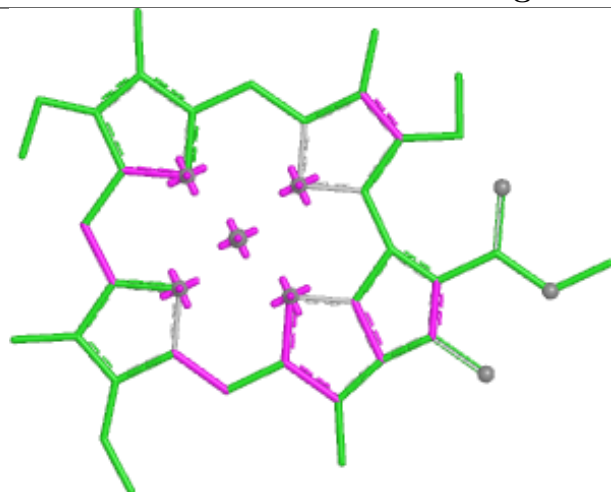


Torsions

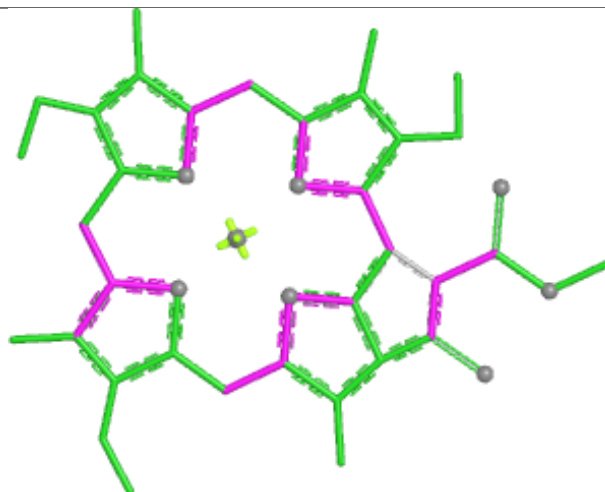


Rings

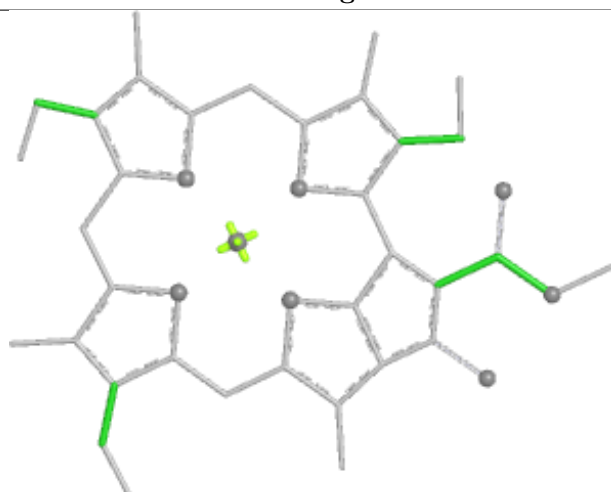
Ligand CLA A 812



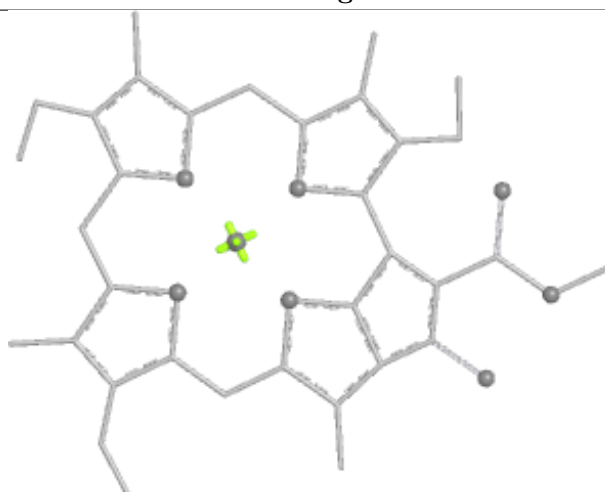
Bond lengths



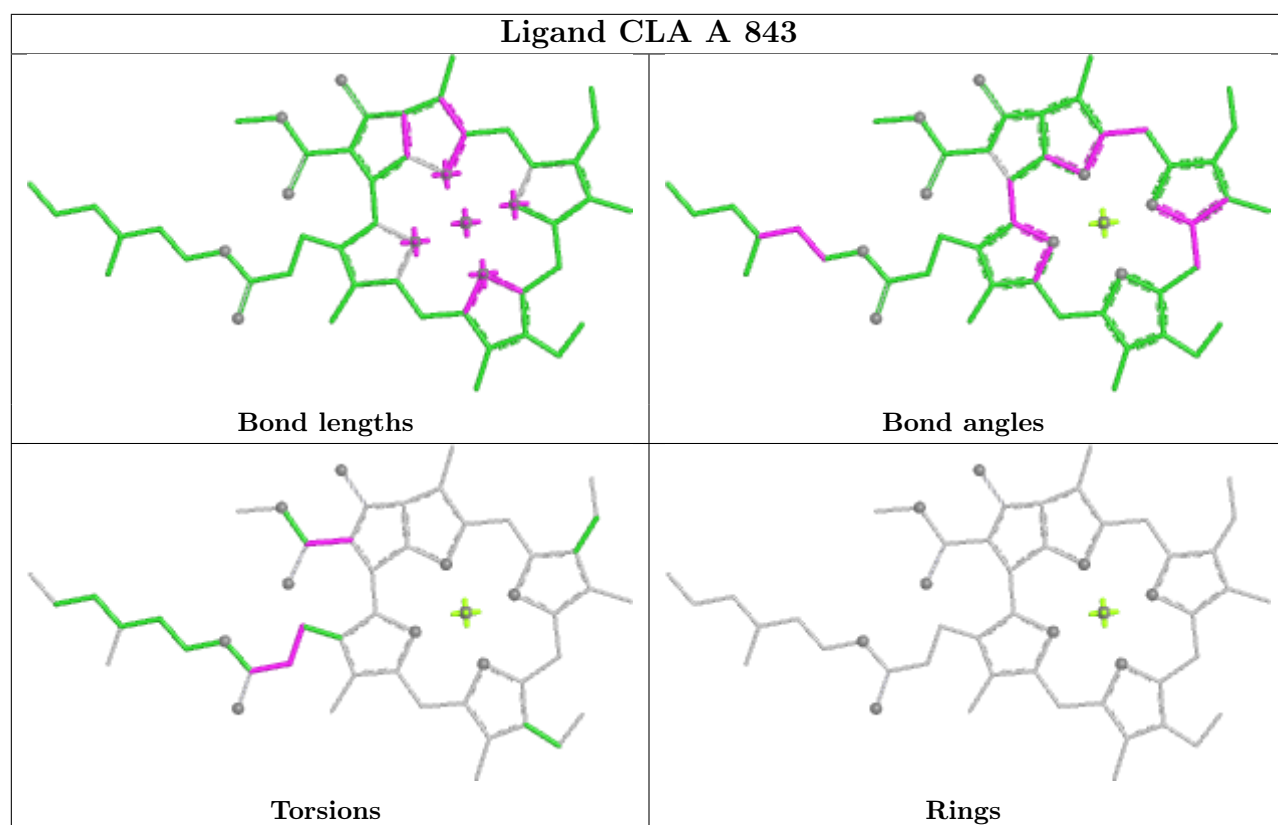
Bond angles



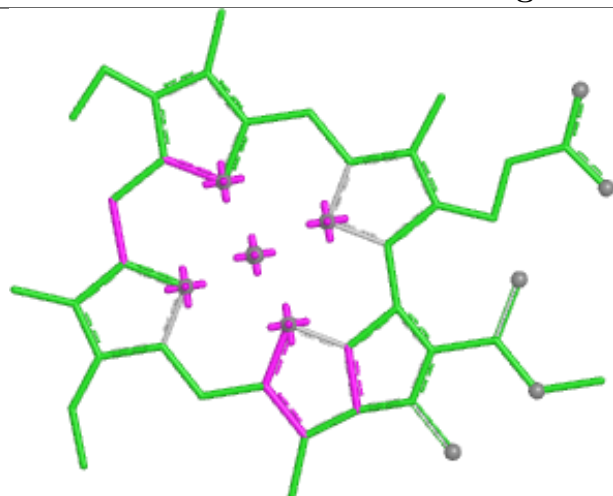
Torsions



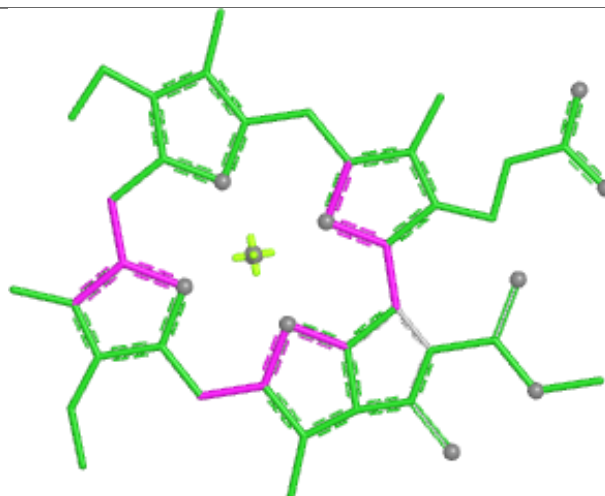
Rings



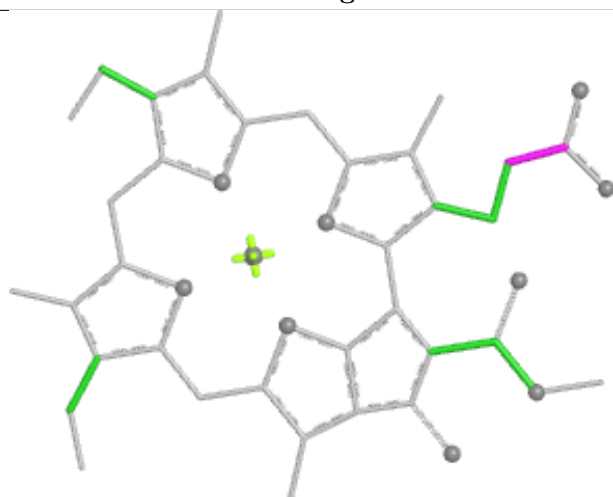
Ligand CLA Z 611



Bond lengths



Bond angles

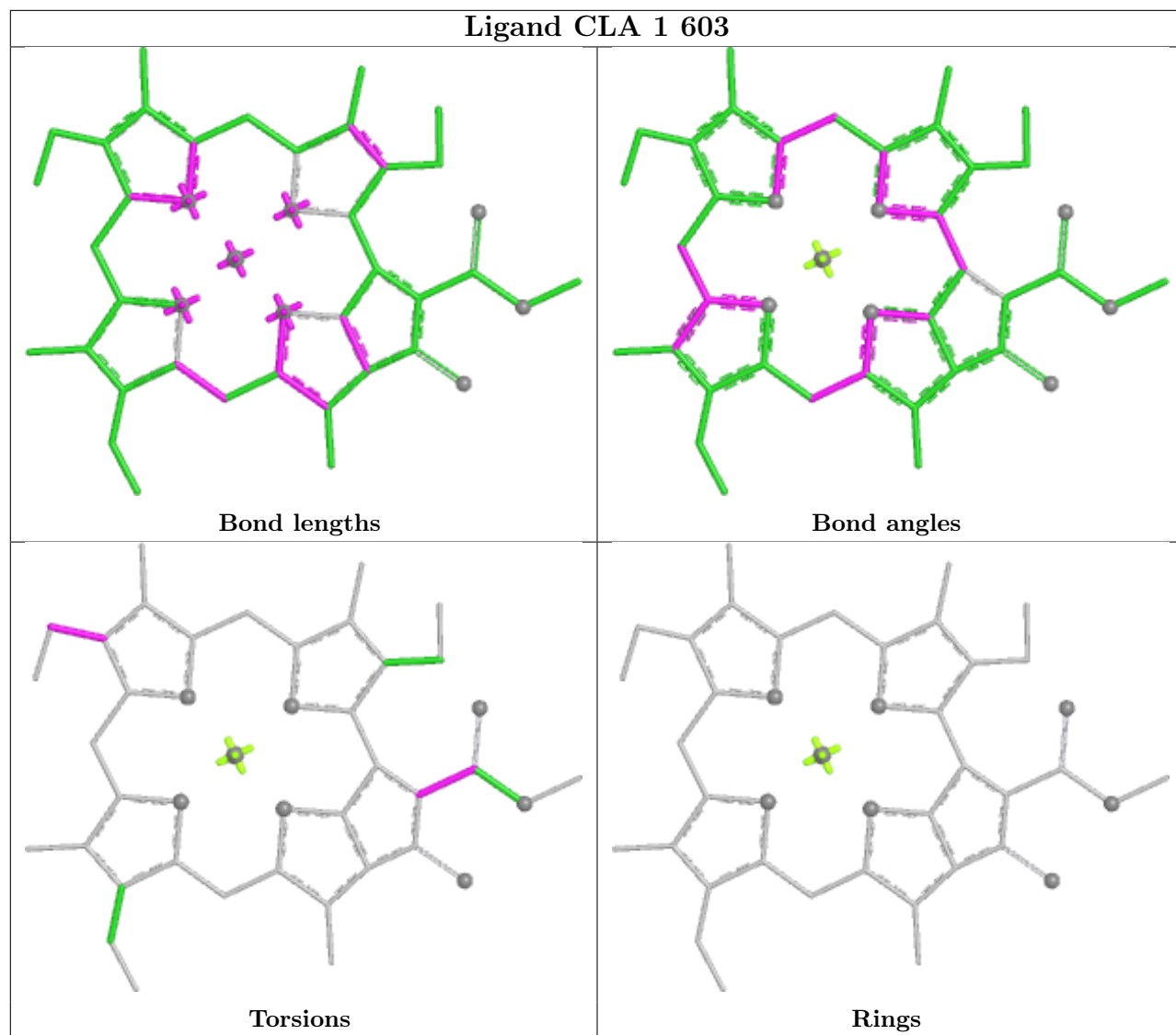


Torsions

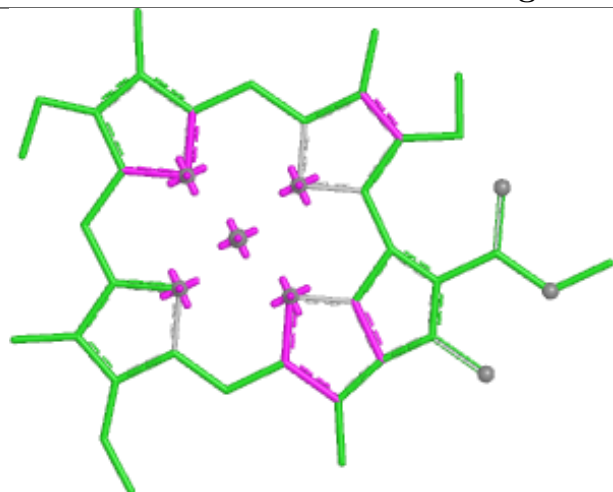


Rings

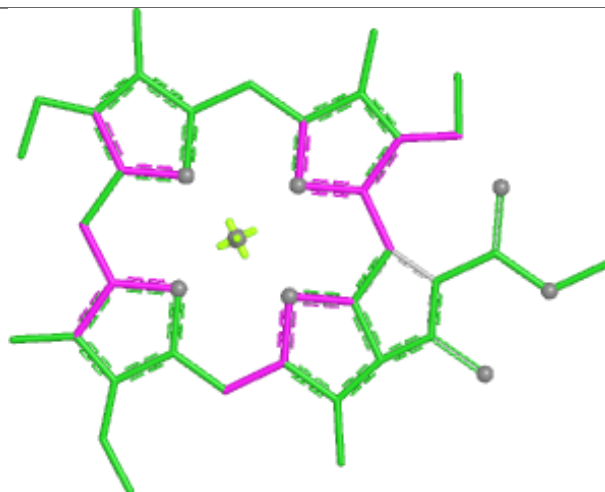
Ligand CLA 1 603



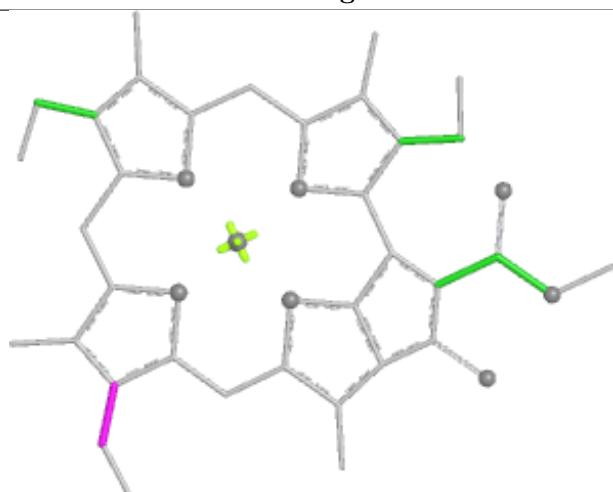
Ligand CLA 1 604



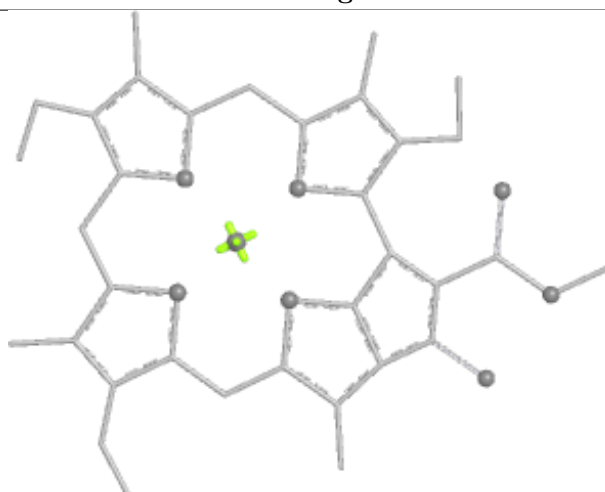
Bond lengths



Bond angles

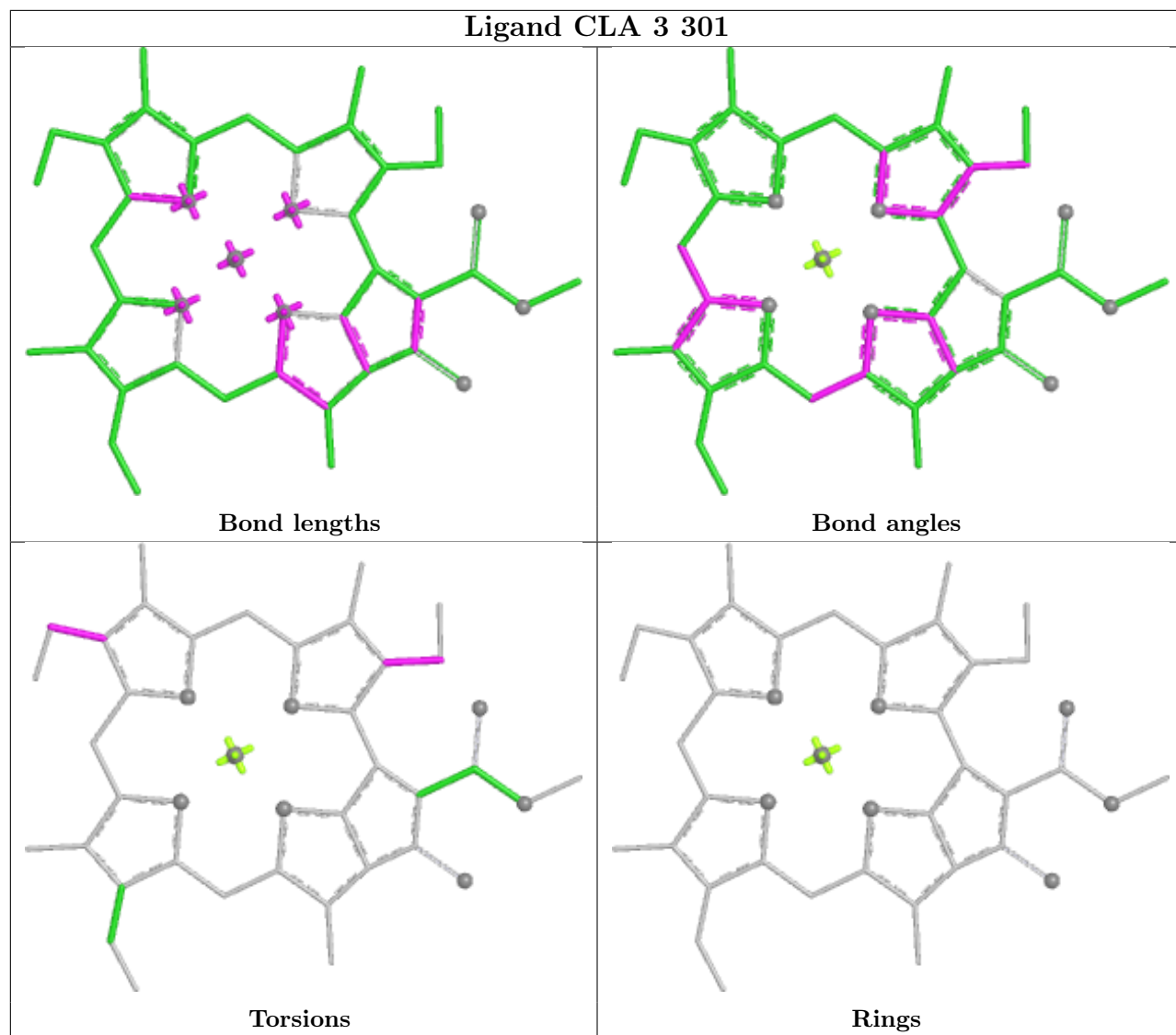


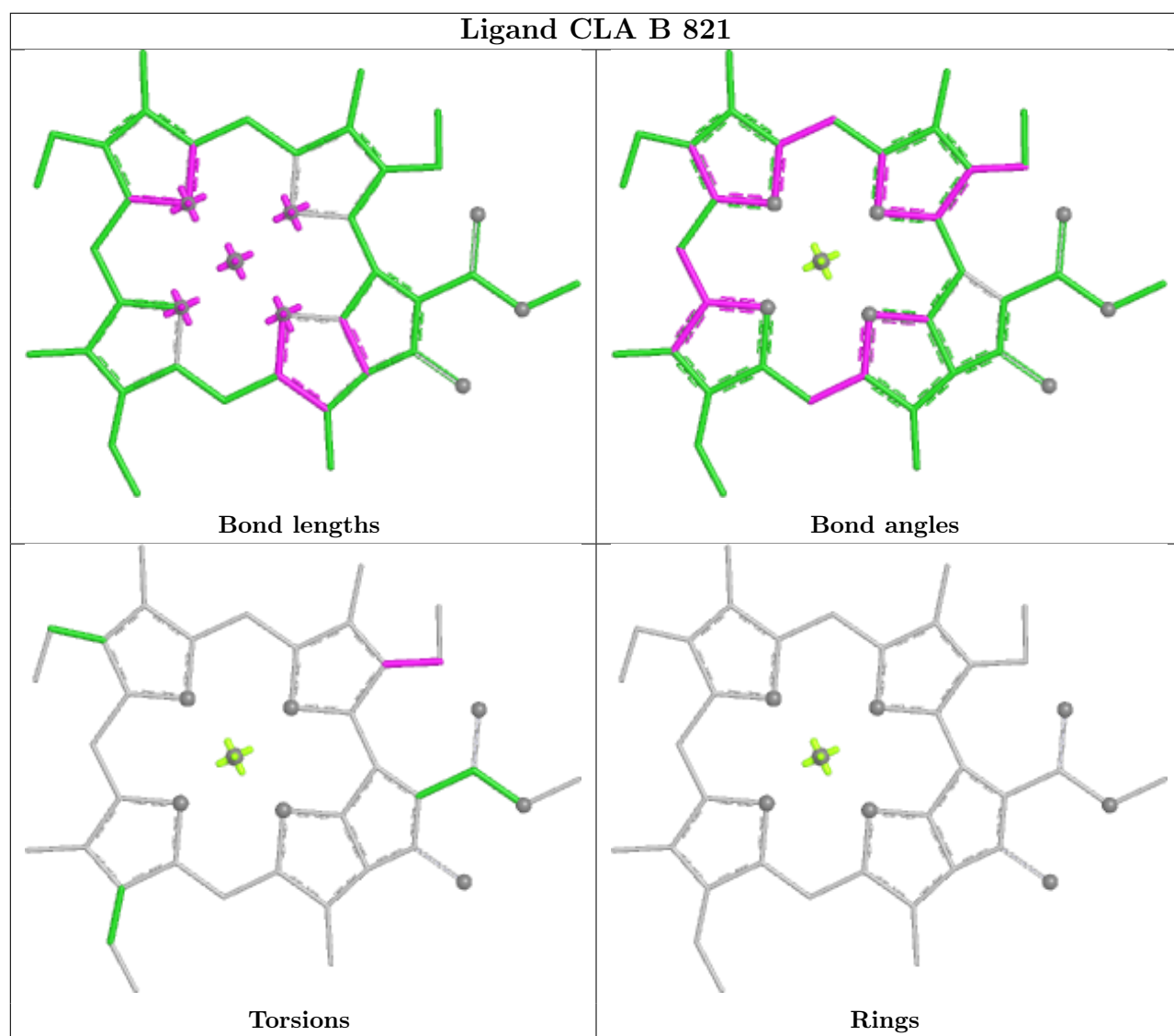
Torsions



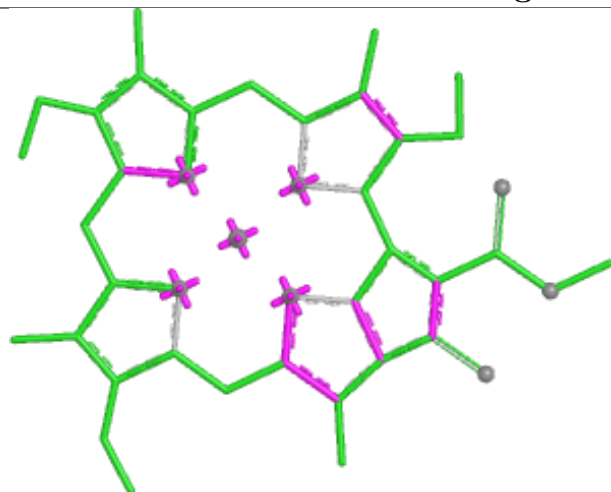
Rings

Ligand CLA 3 301

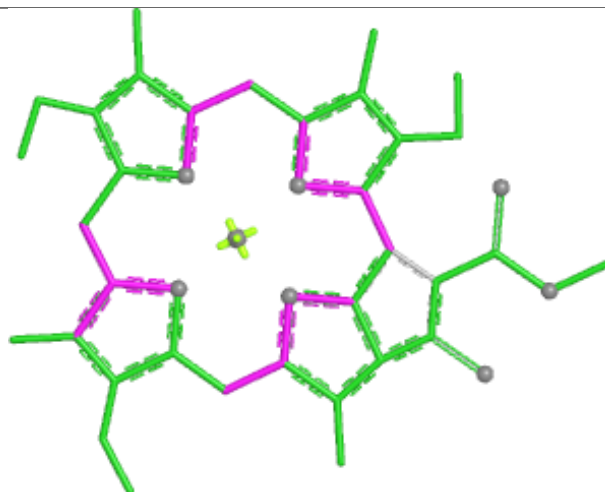




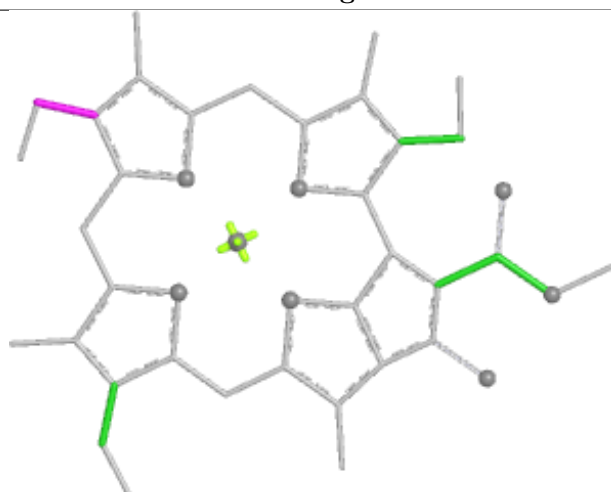
Ligand CLA B 826



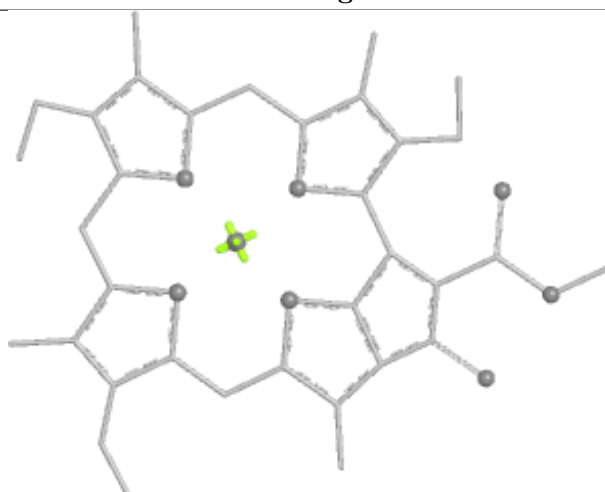
Bond lengths



Bond angles

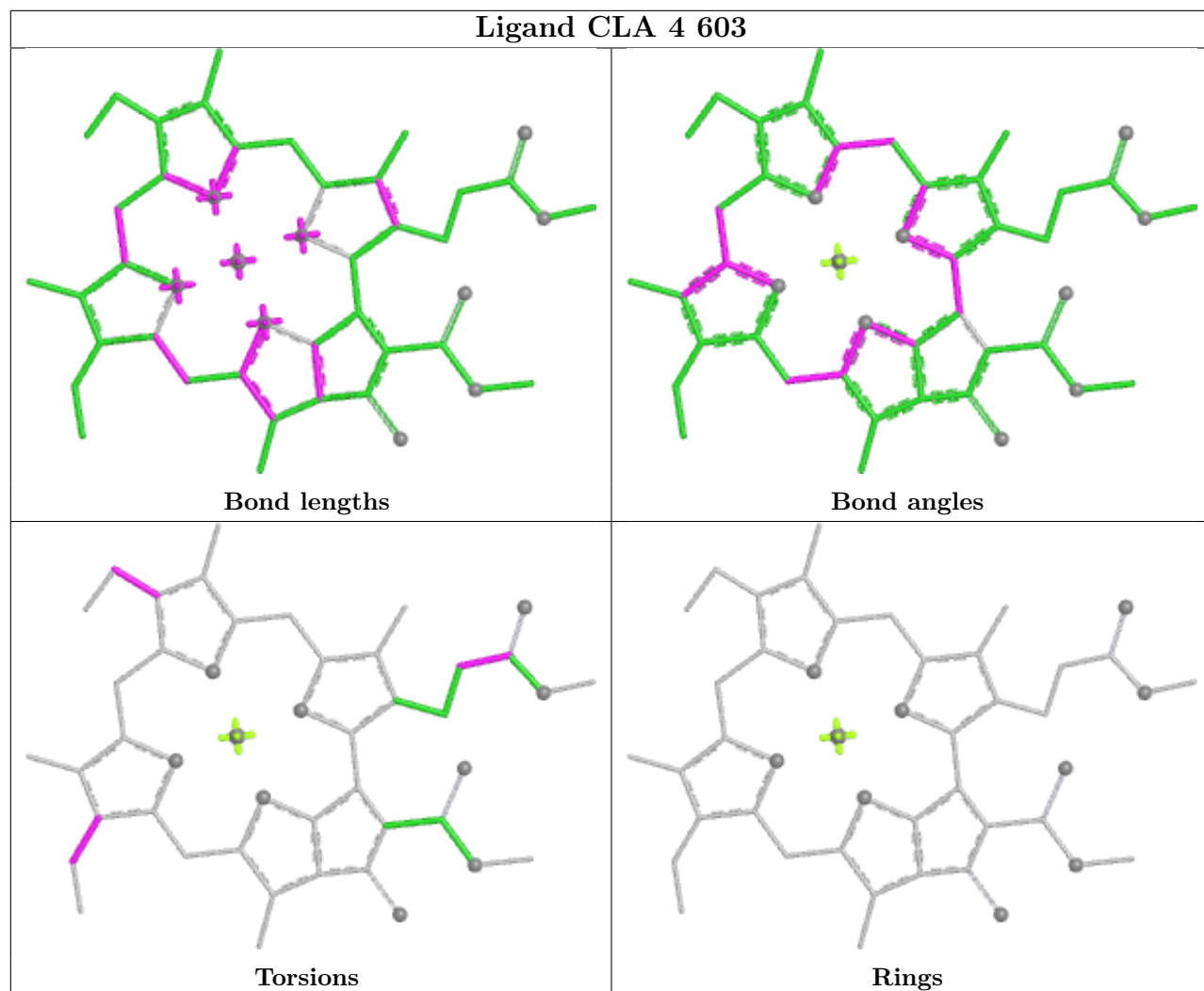


Torsions

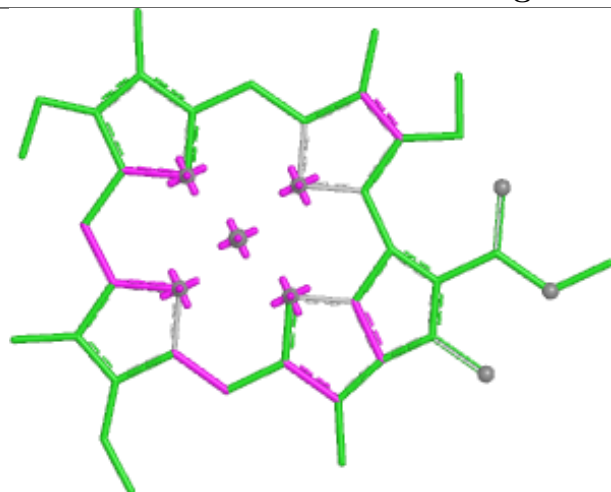


Rings

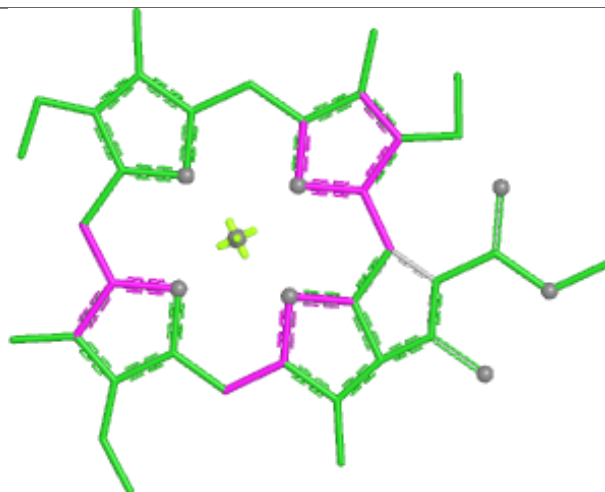
Ligand CLA 4 603



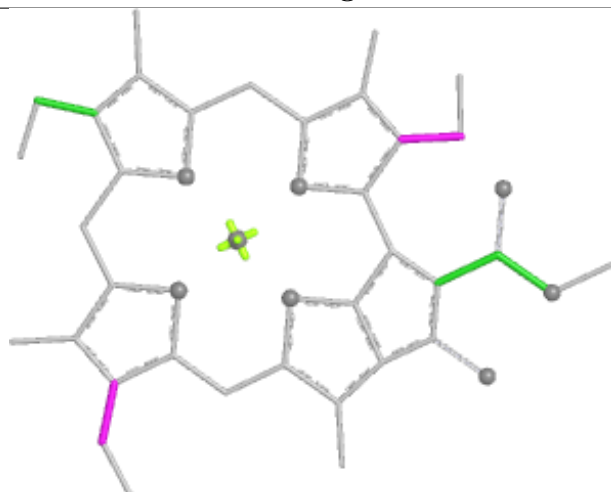
Ligand CLA A 824



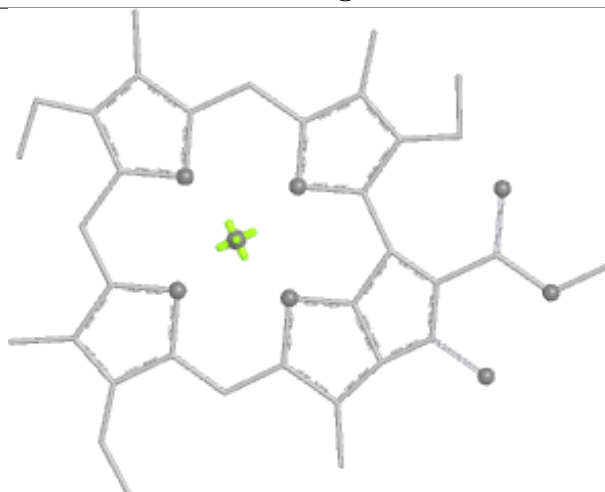
Bond lengths



Bond angles

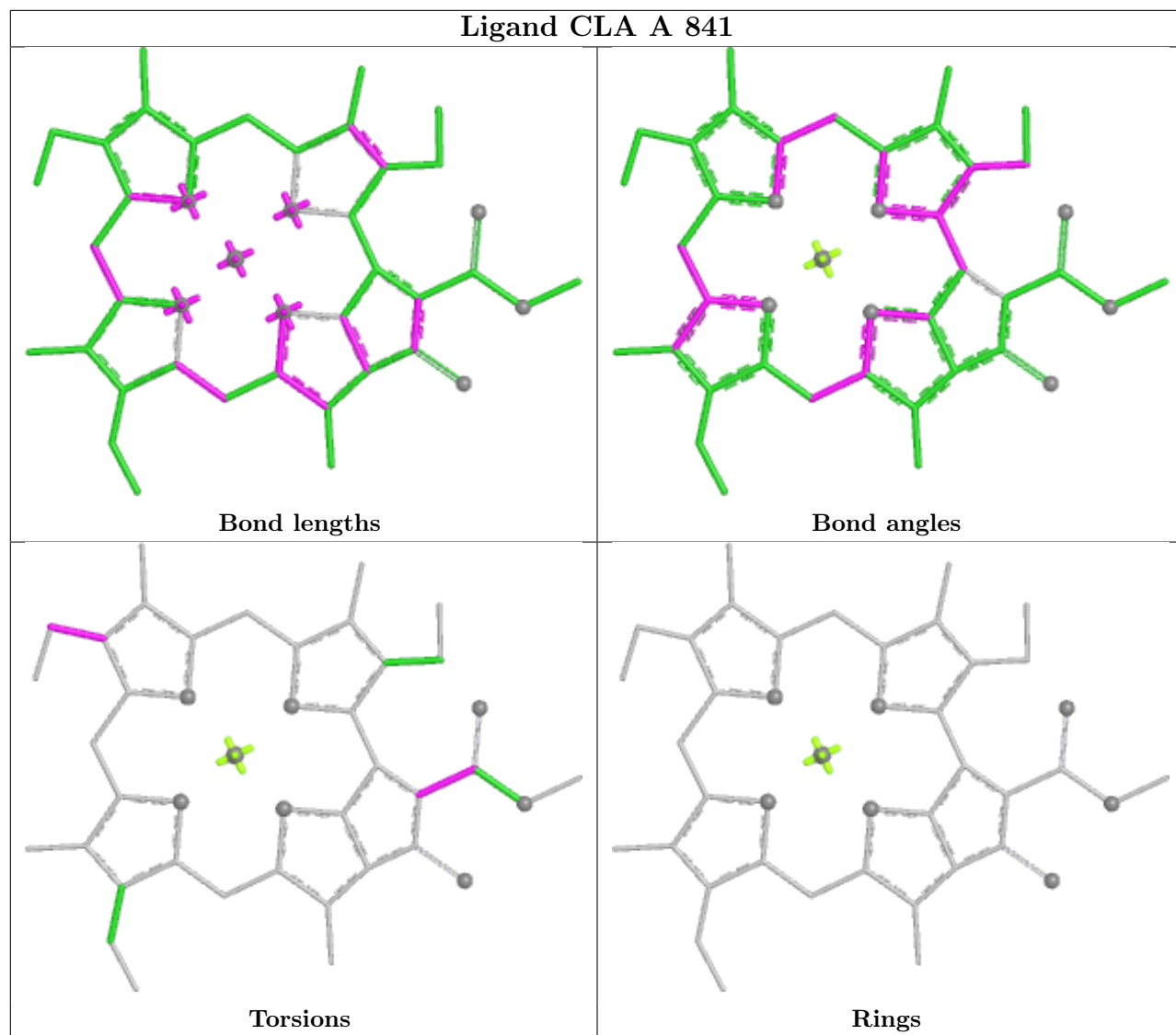


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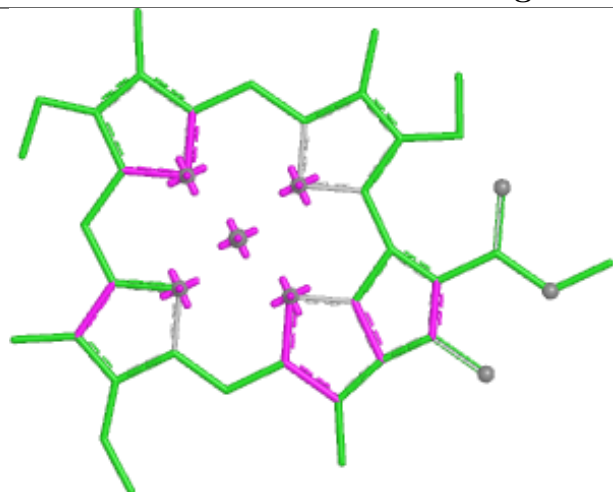


Rings

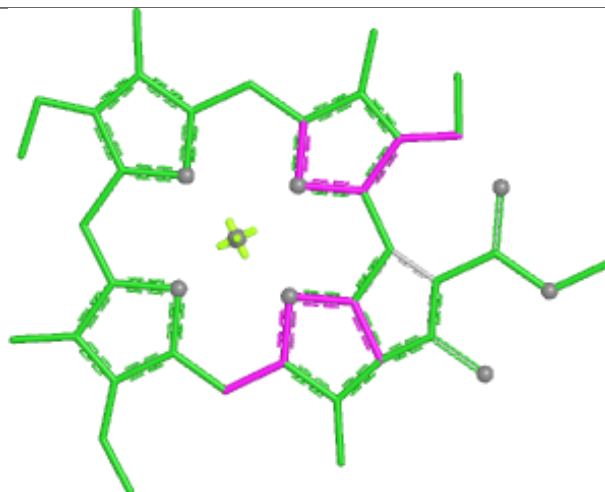
Ligand CLA A 841



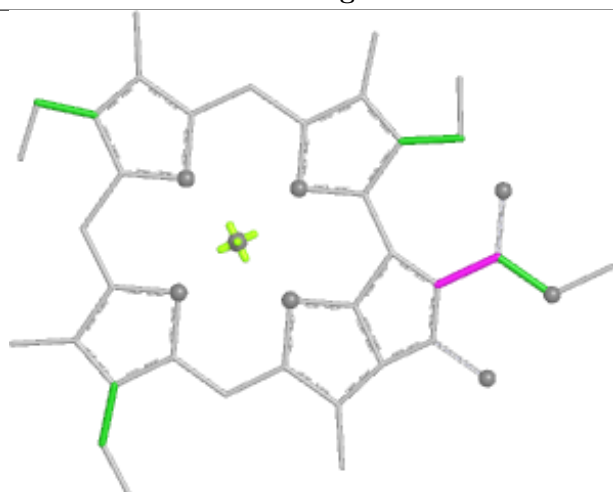
Ligand CLA B 823



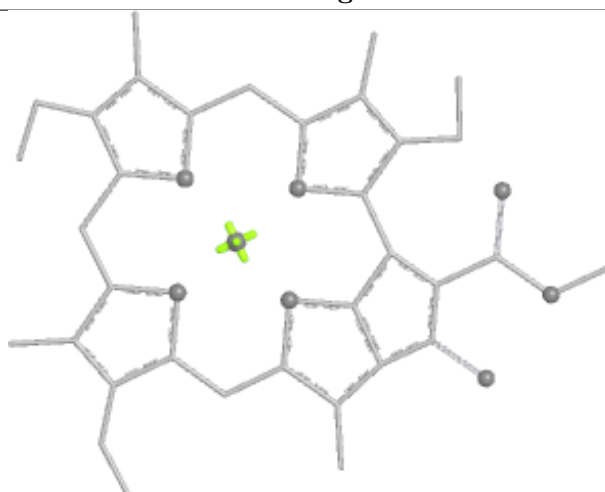
Bond lengths



Bond angles

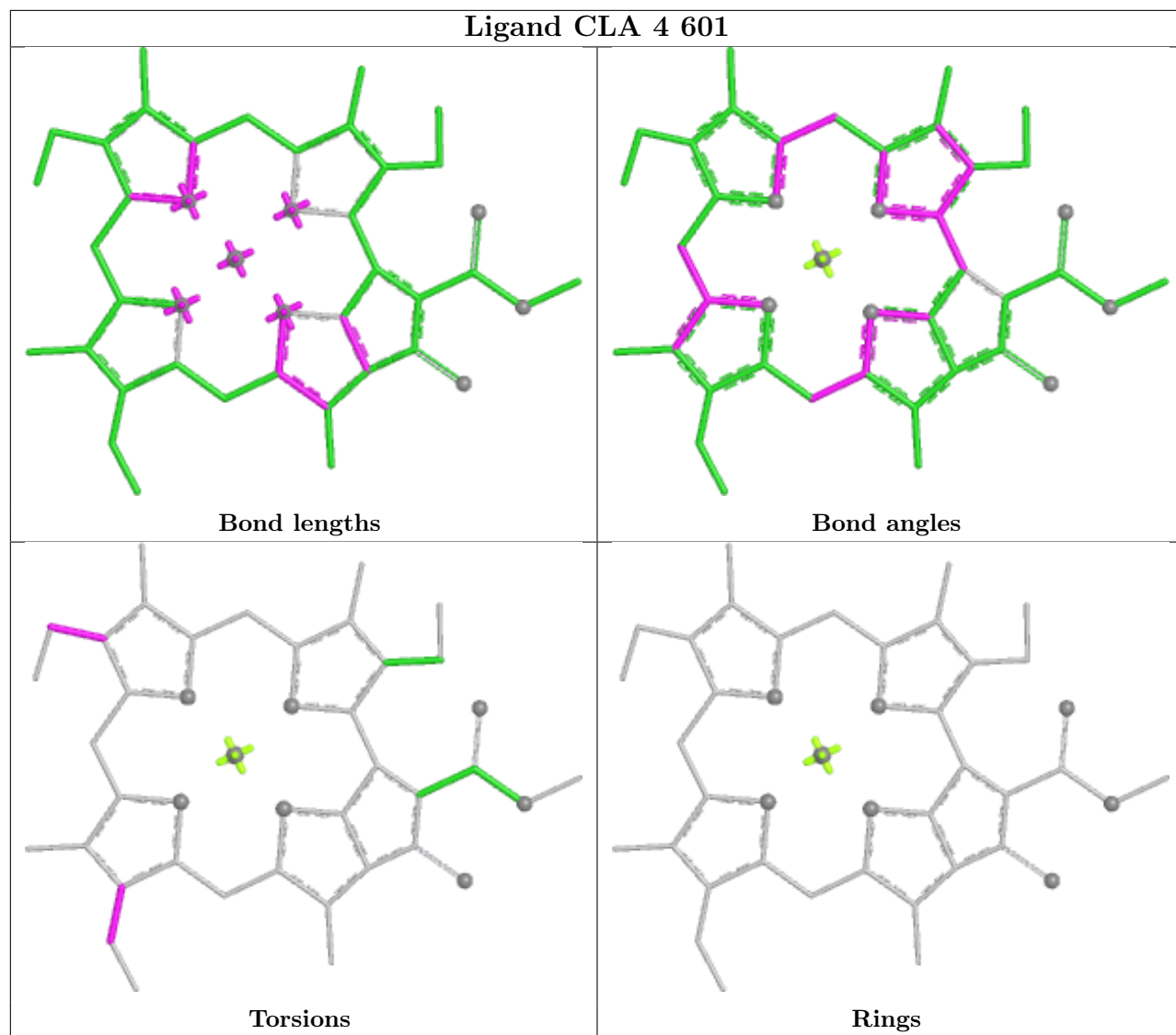


Torsions

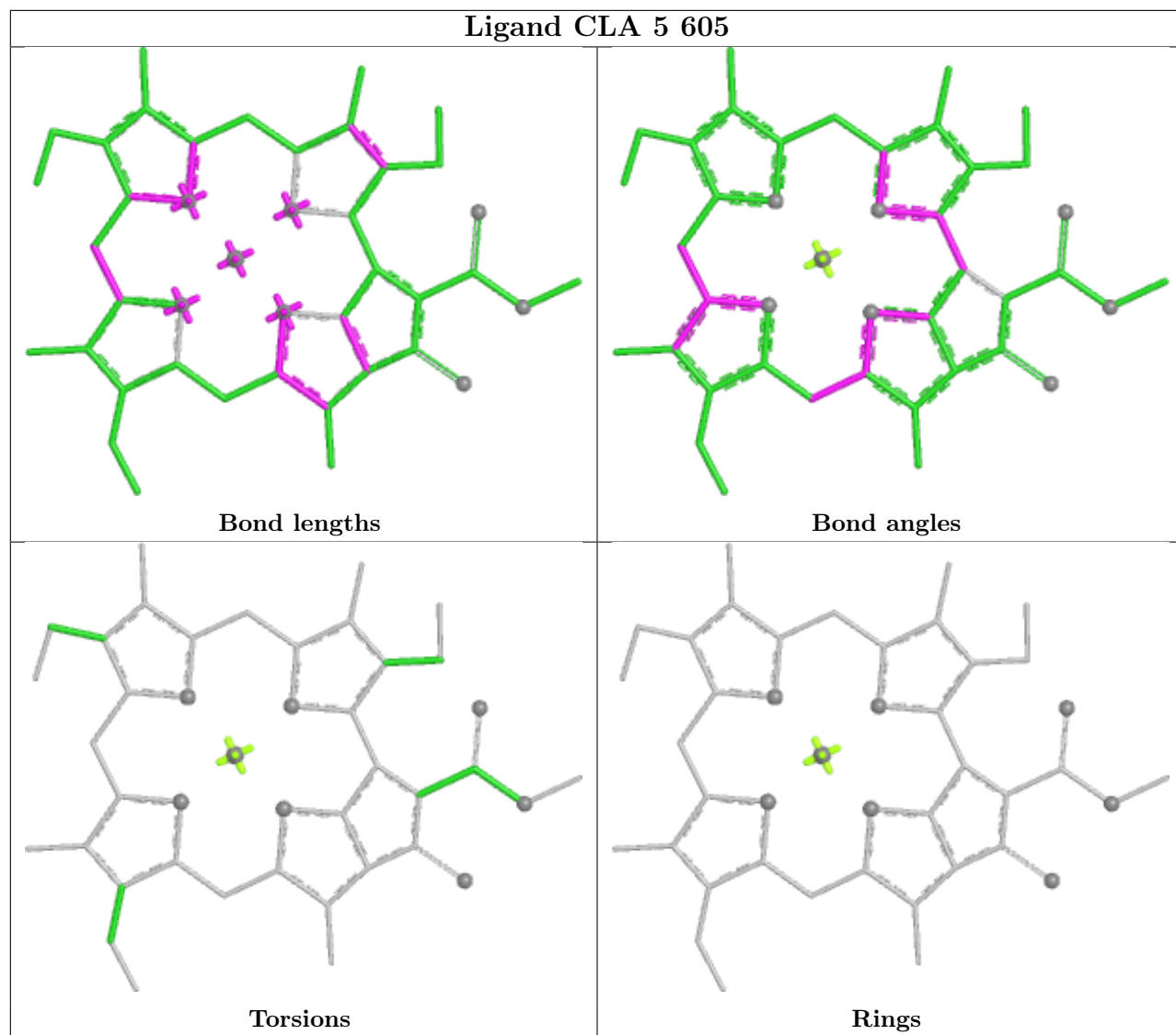


Rings

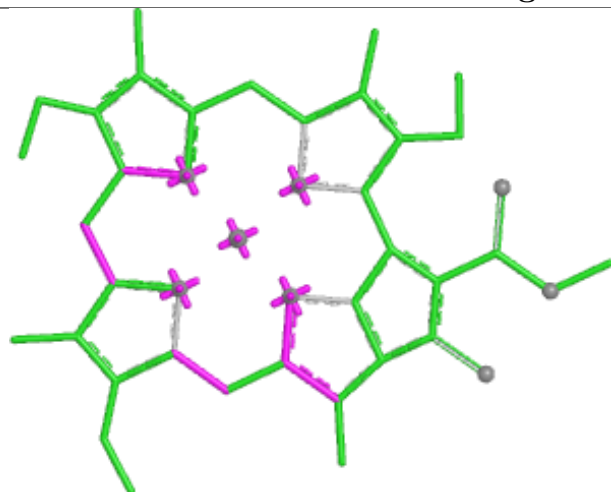
Ligand CLA 4 601



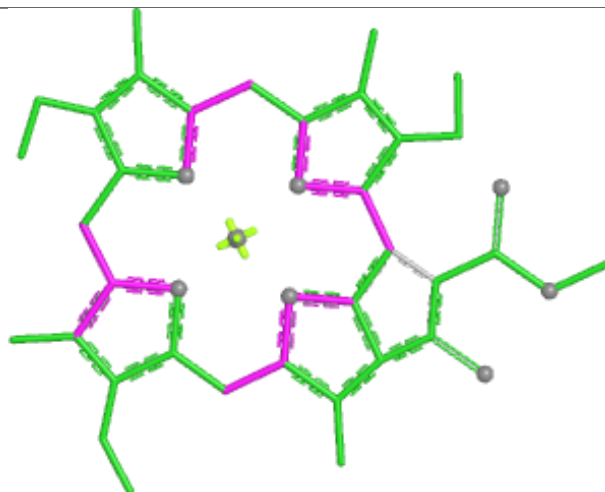
Ligand CLA 5 605



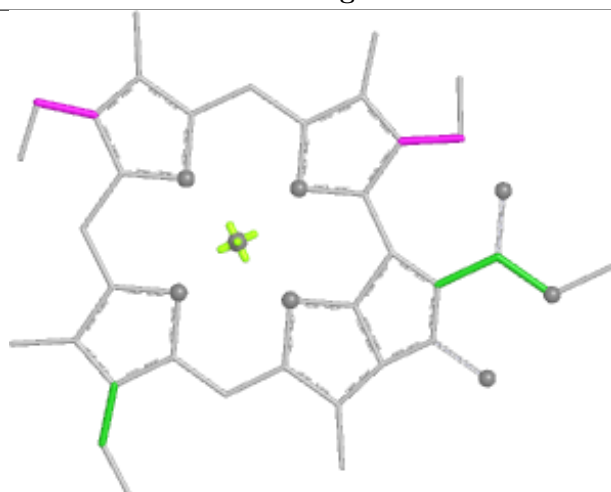
Ligand CLA 5 601



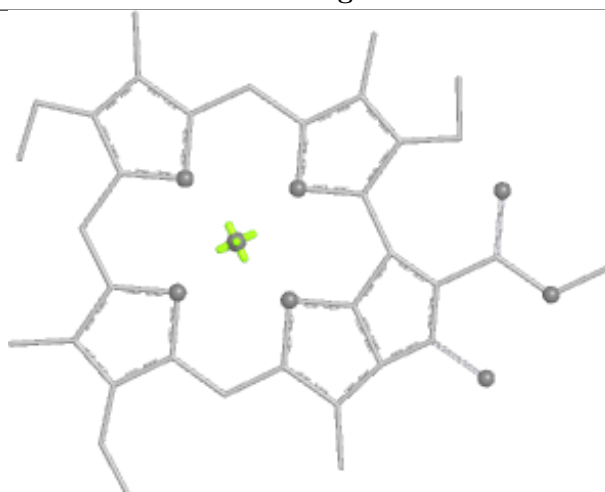
Bond lengths



Bond angles

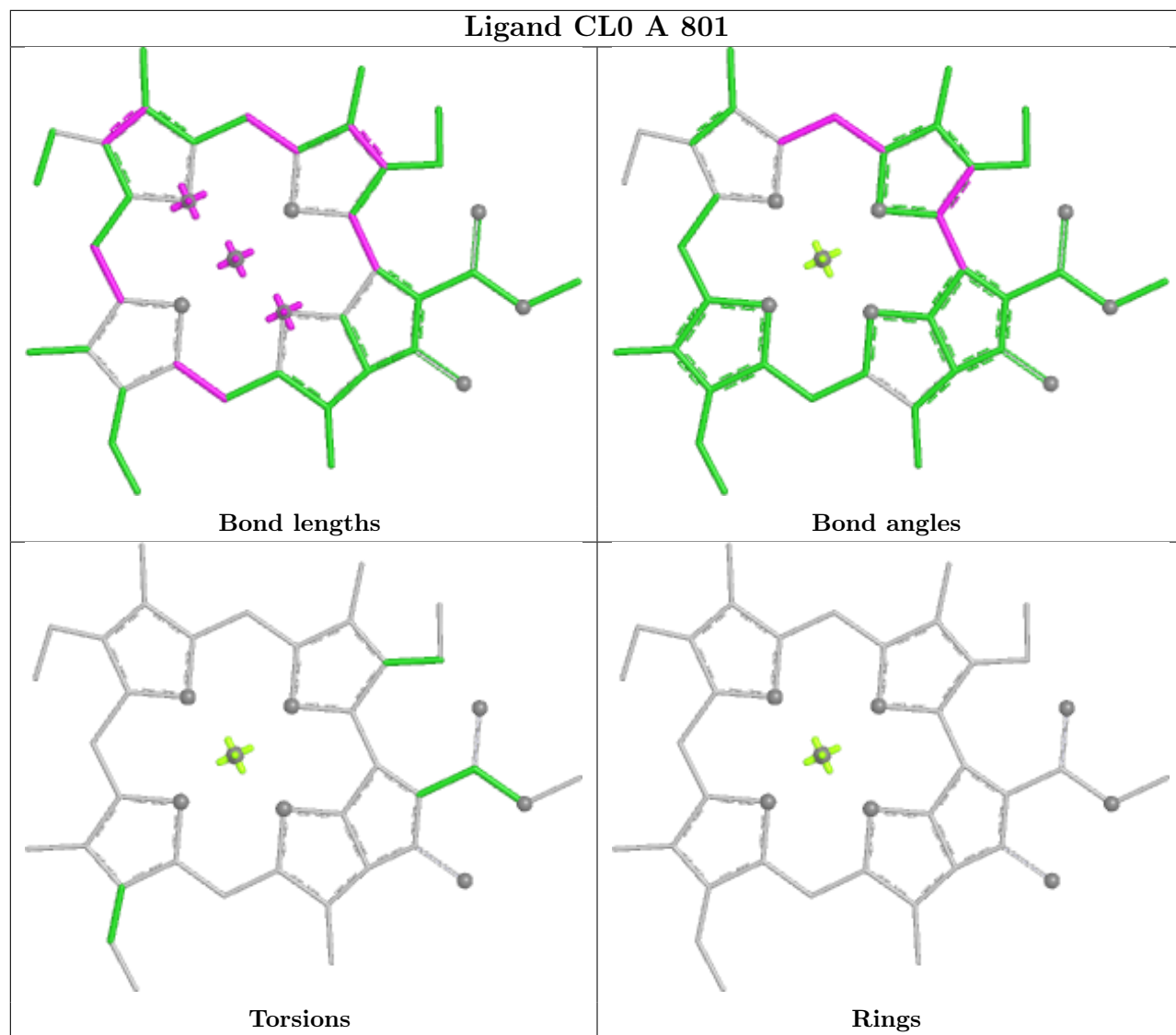


Torsions

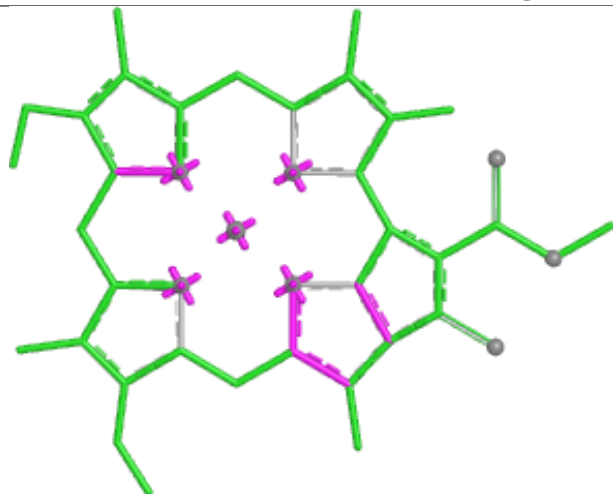


Rings

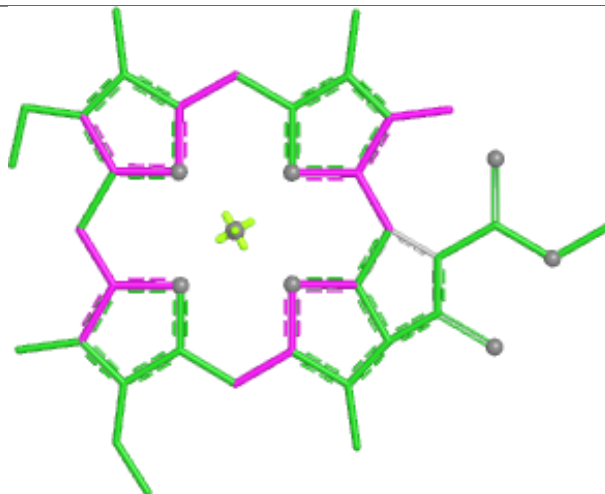
Ligand CL0 A 801



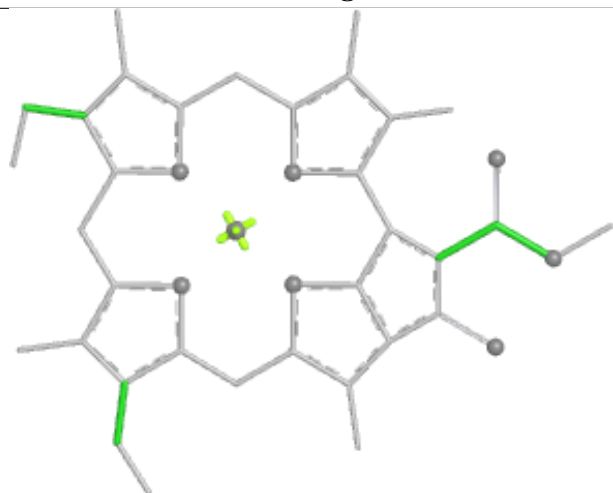
Ligand CLA 4 612



Bond lengths



Bond angles

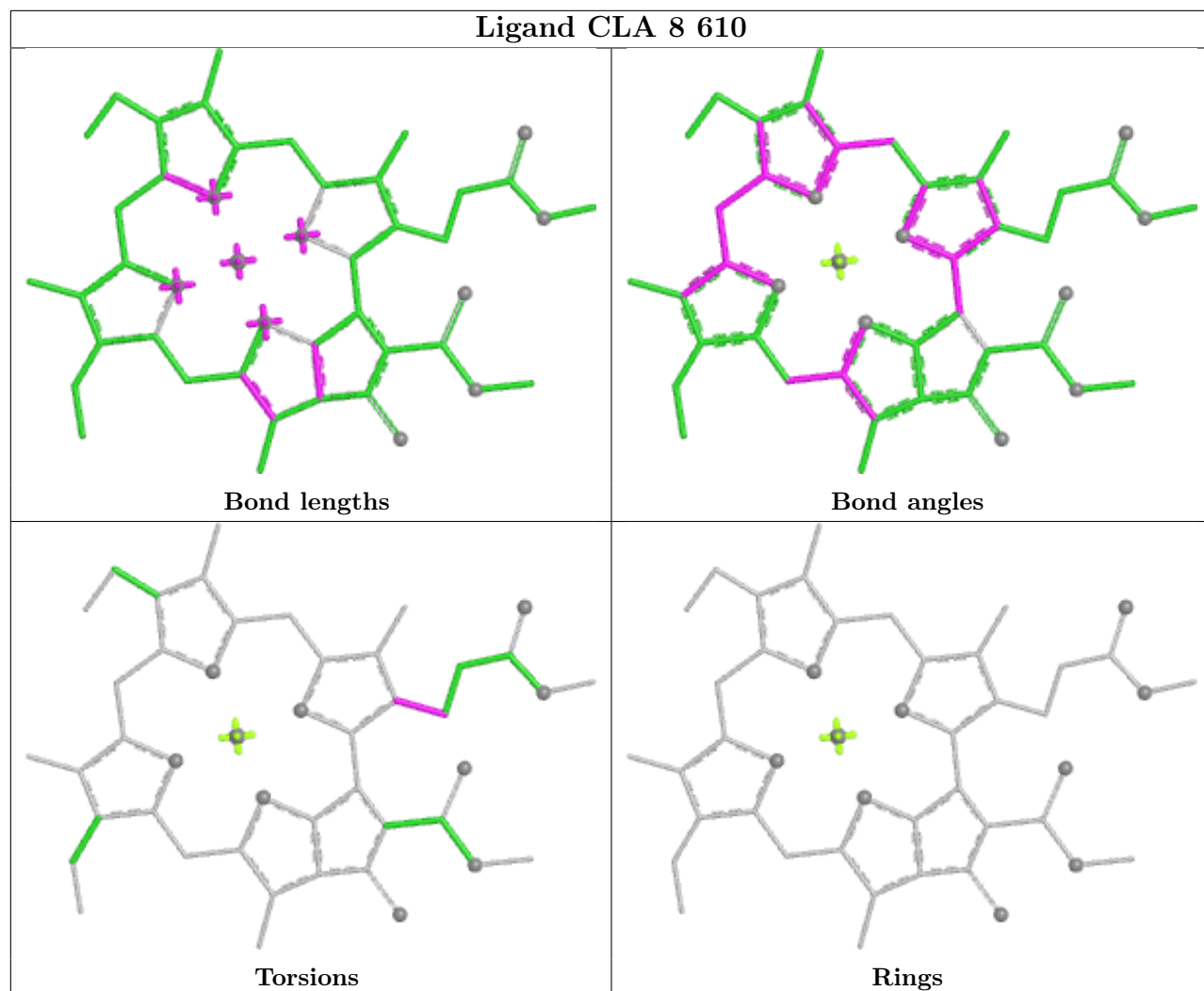


Torsions

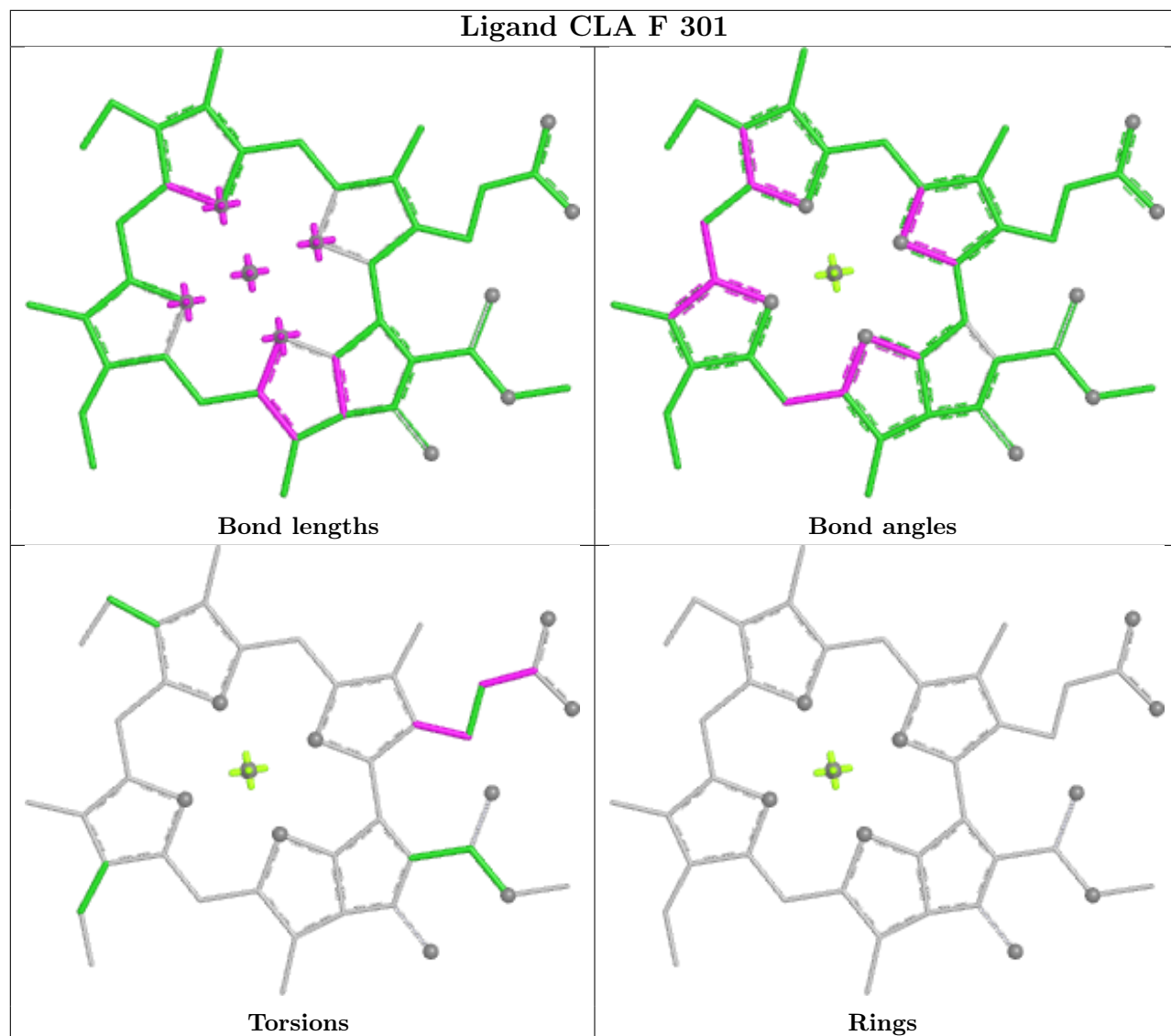


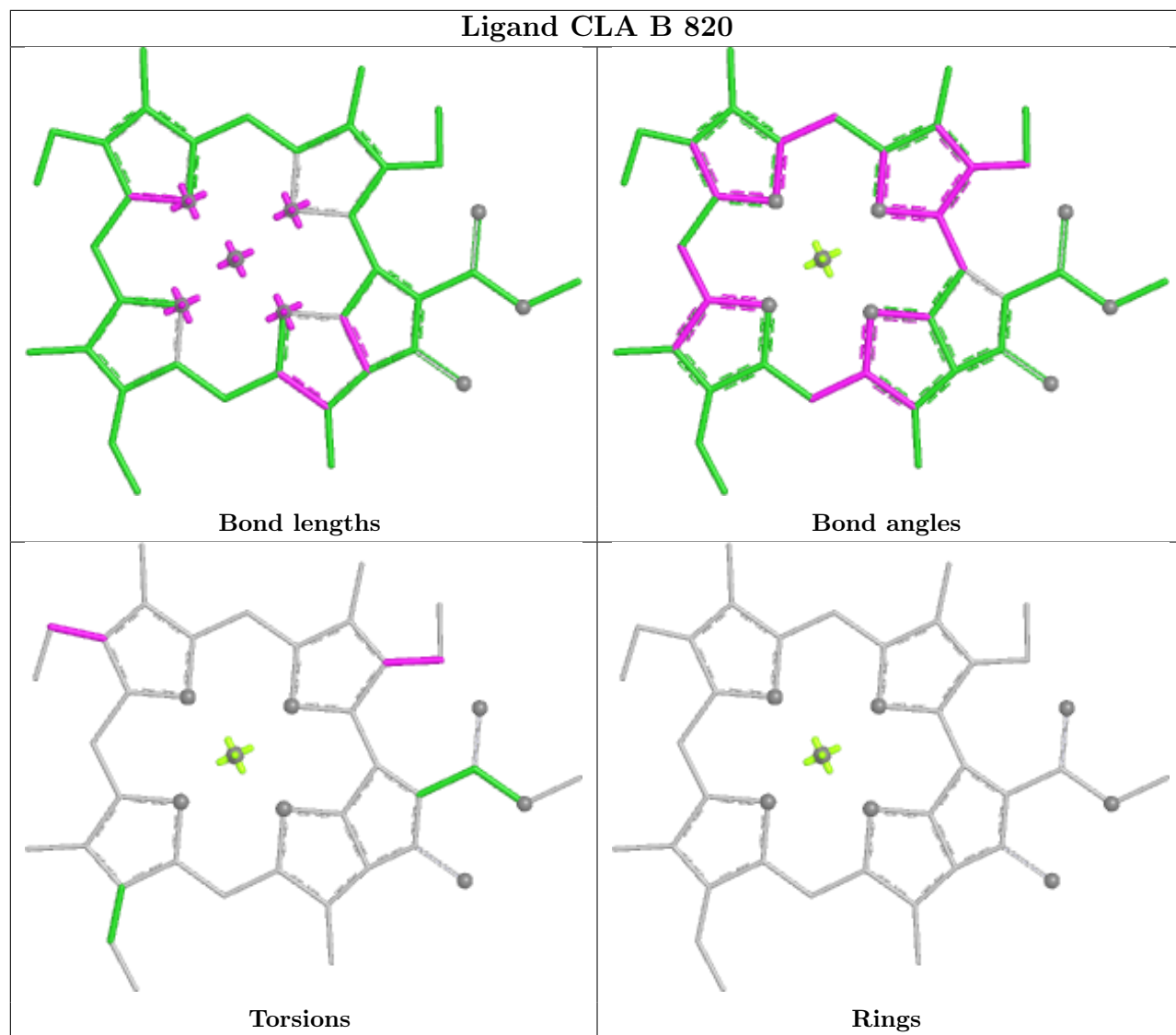
Rings

Ligand CLA 8 610

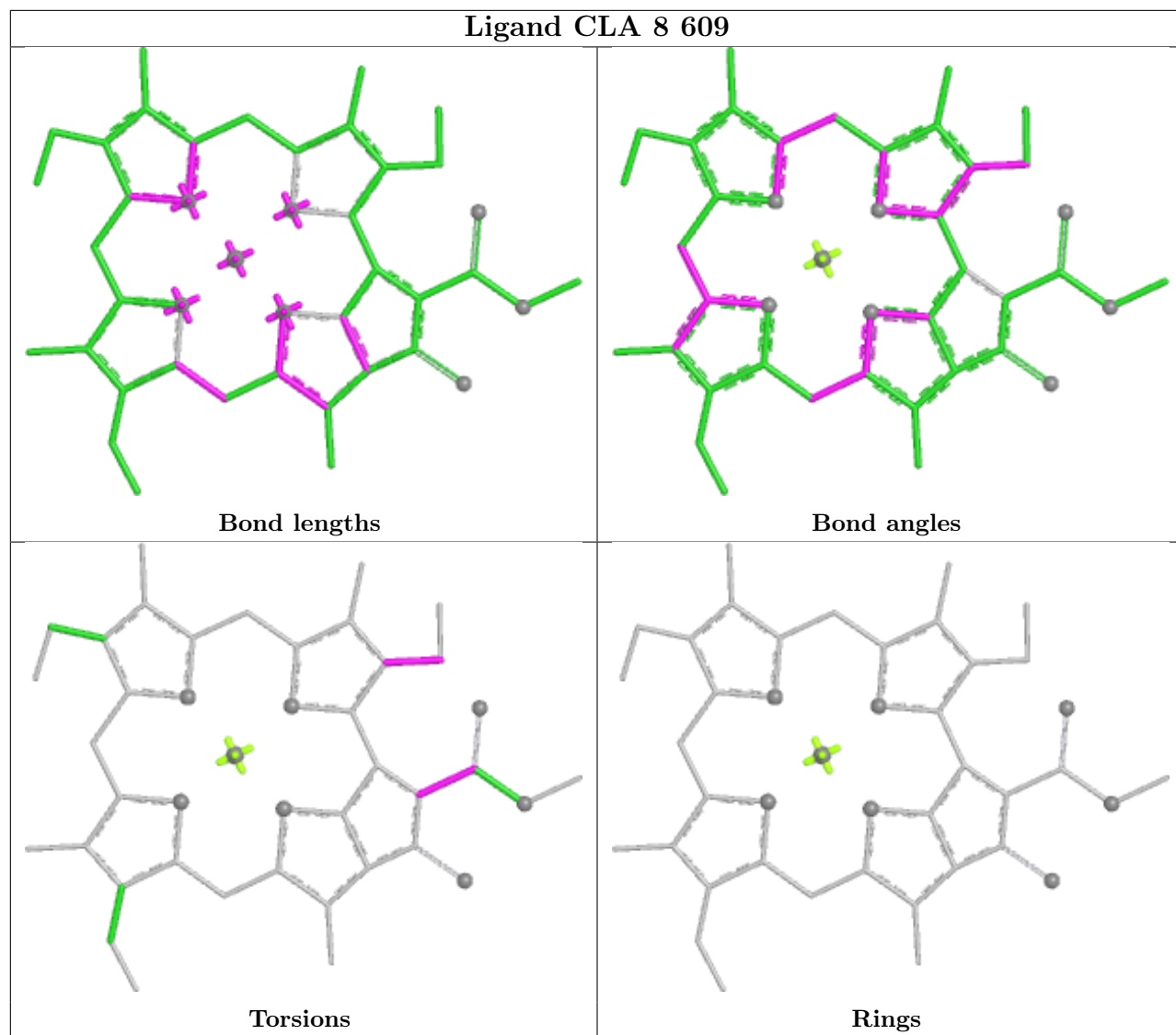


Ligand CLA F 301

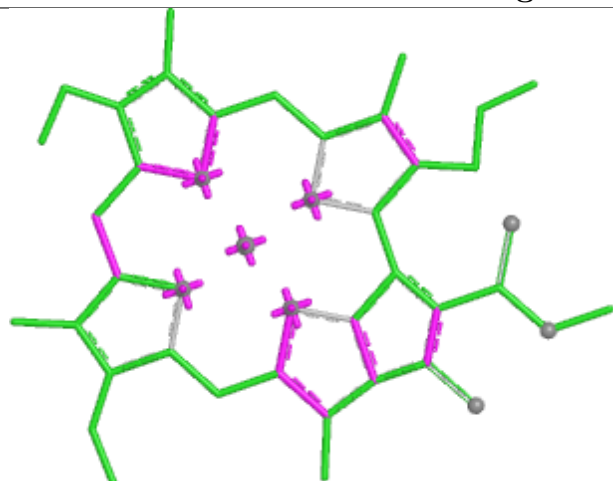




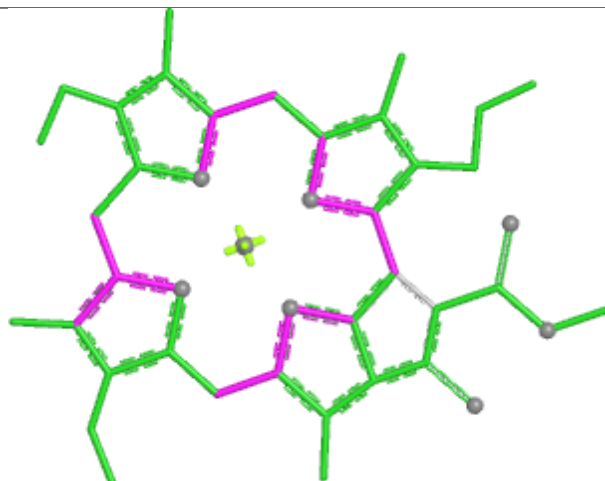
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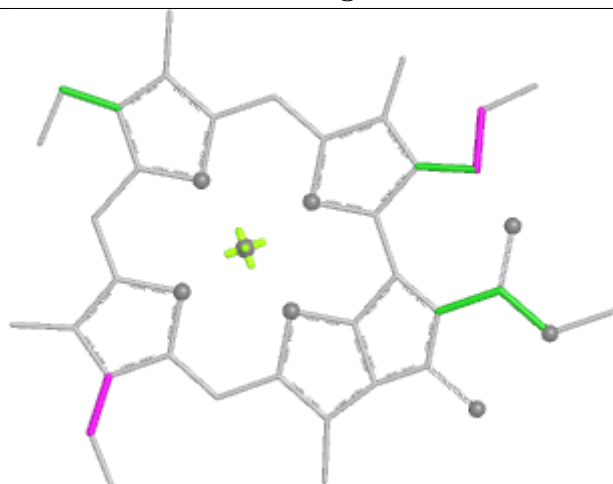
Ligand CLA Z 604



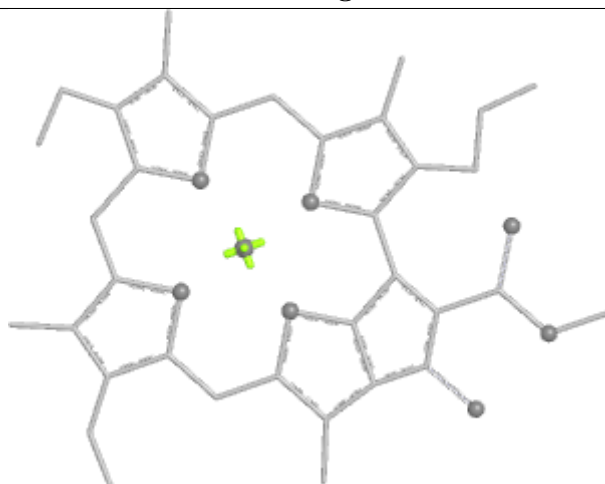
Bond lengths



Bond angles

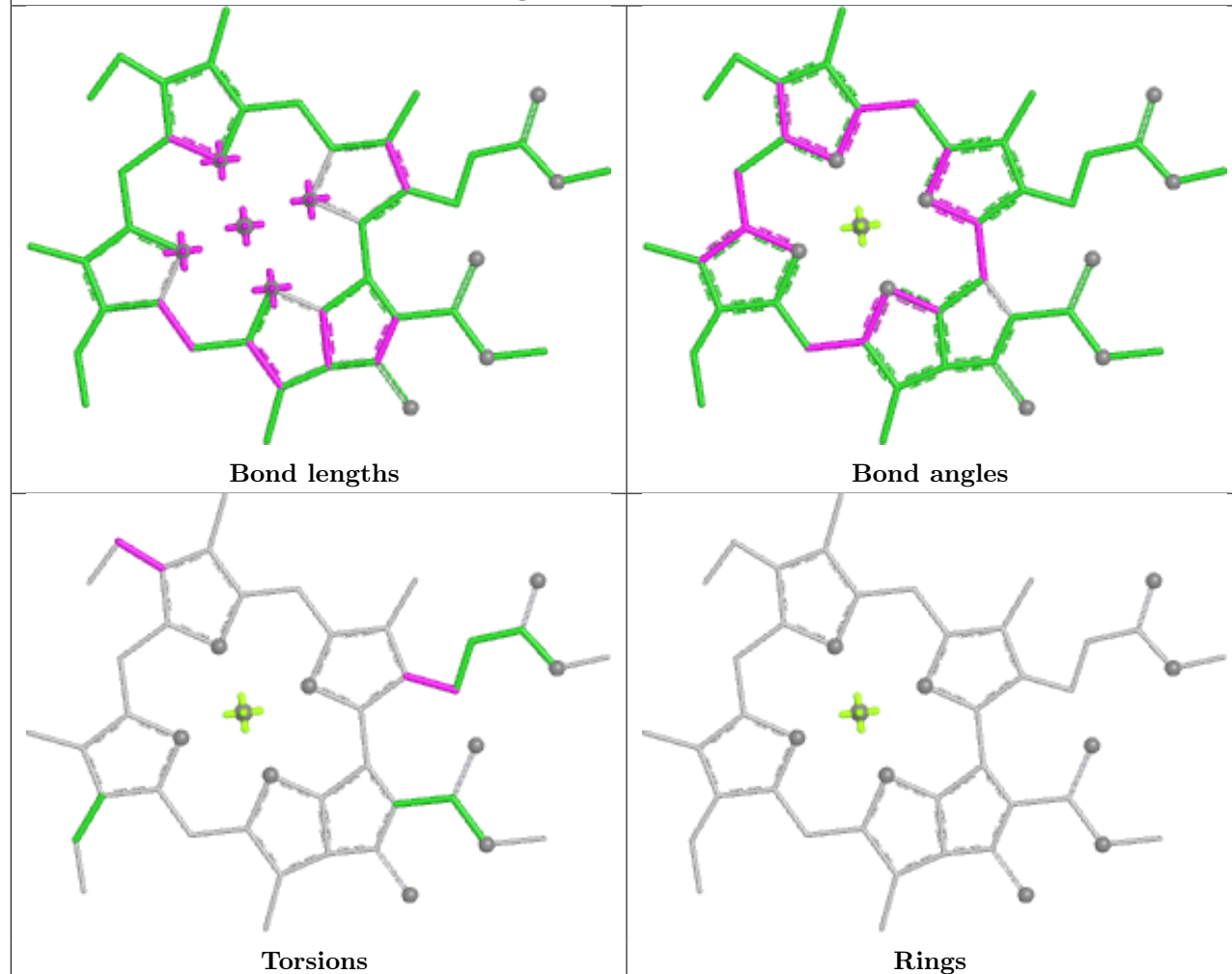


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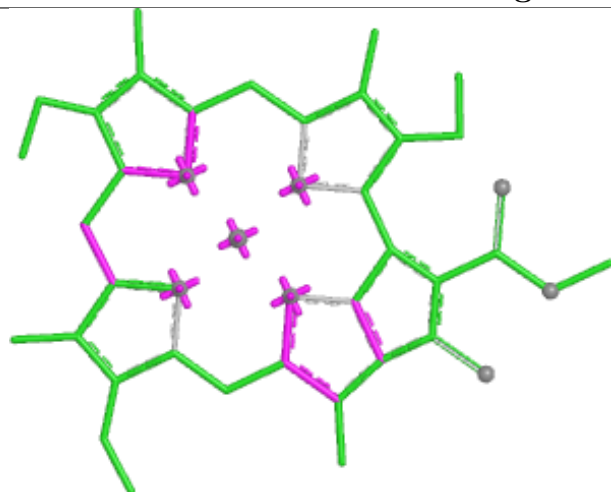


Rings

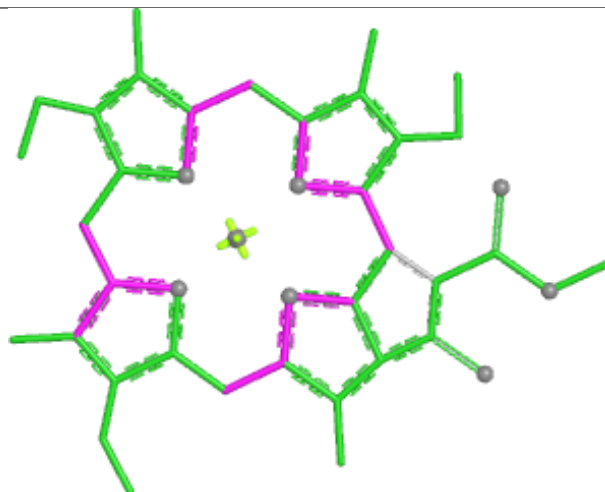
Ligand CLA B 802



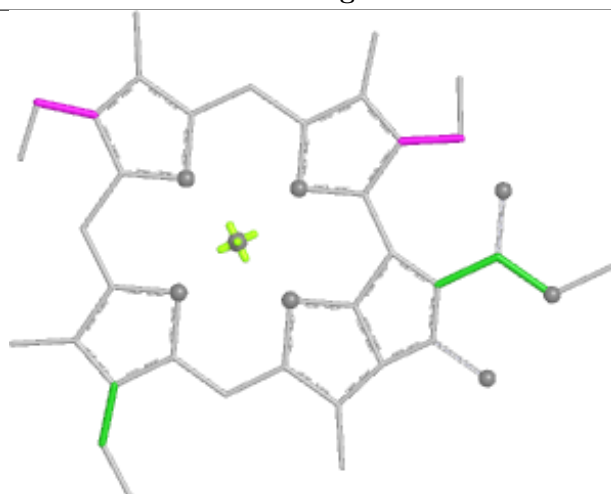
Ligand CLA B 816



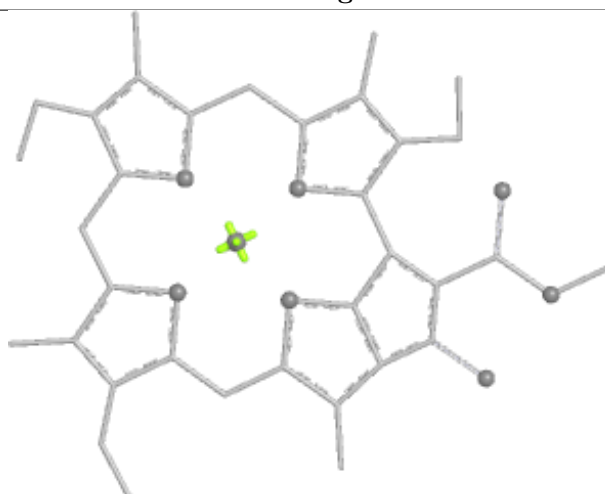
Bond lengths



Bond angles

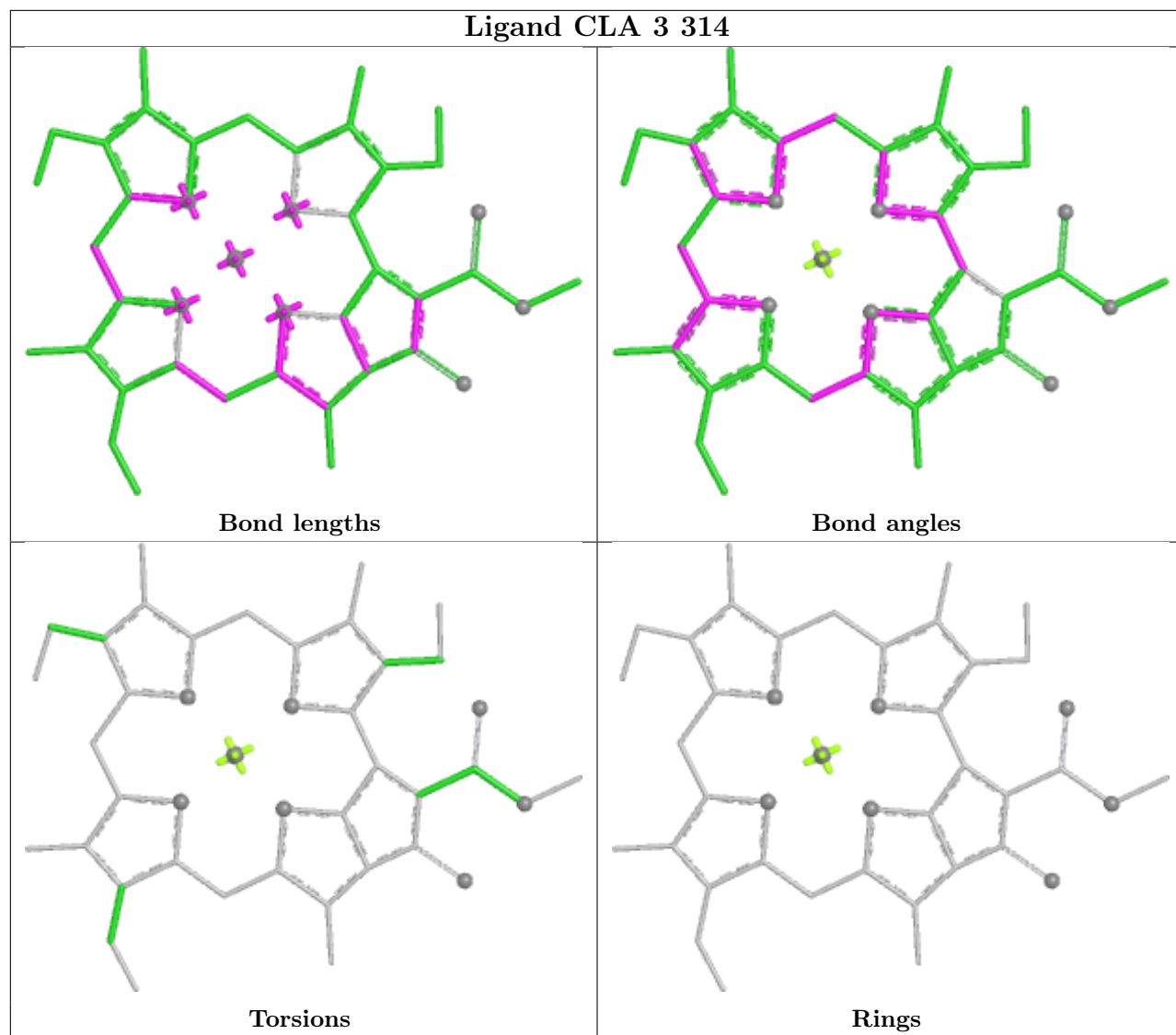


Torsions

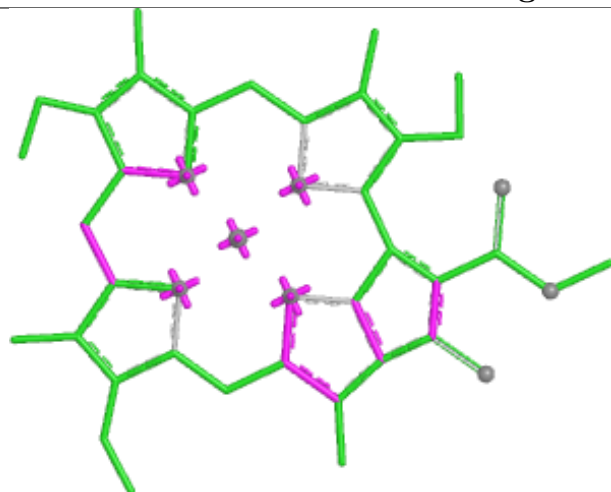


Rings

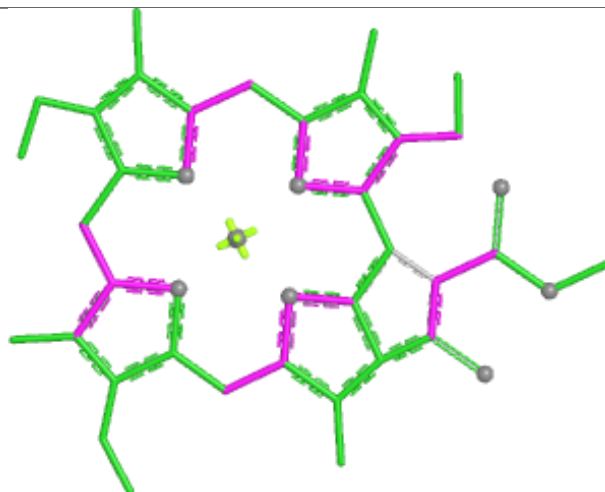
Ligand CLA 3 314



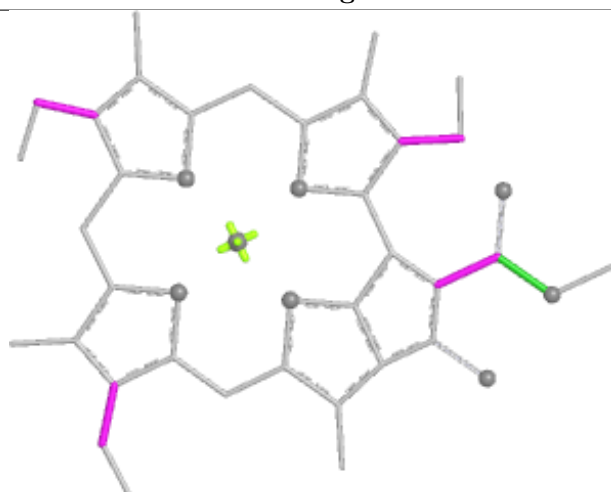
Ligand CLA 7 601



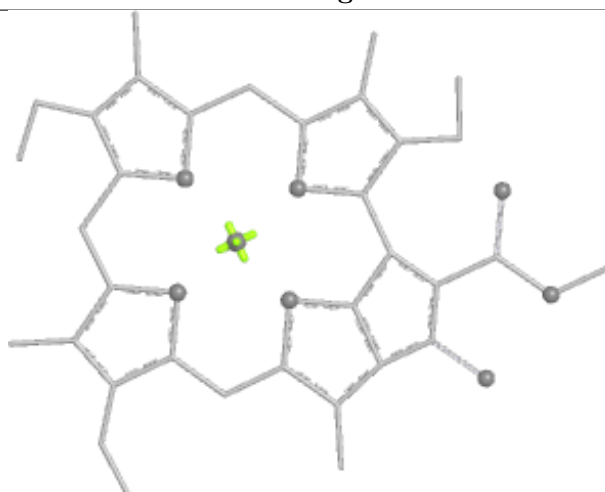
Bond lengths



Bond angles

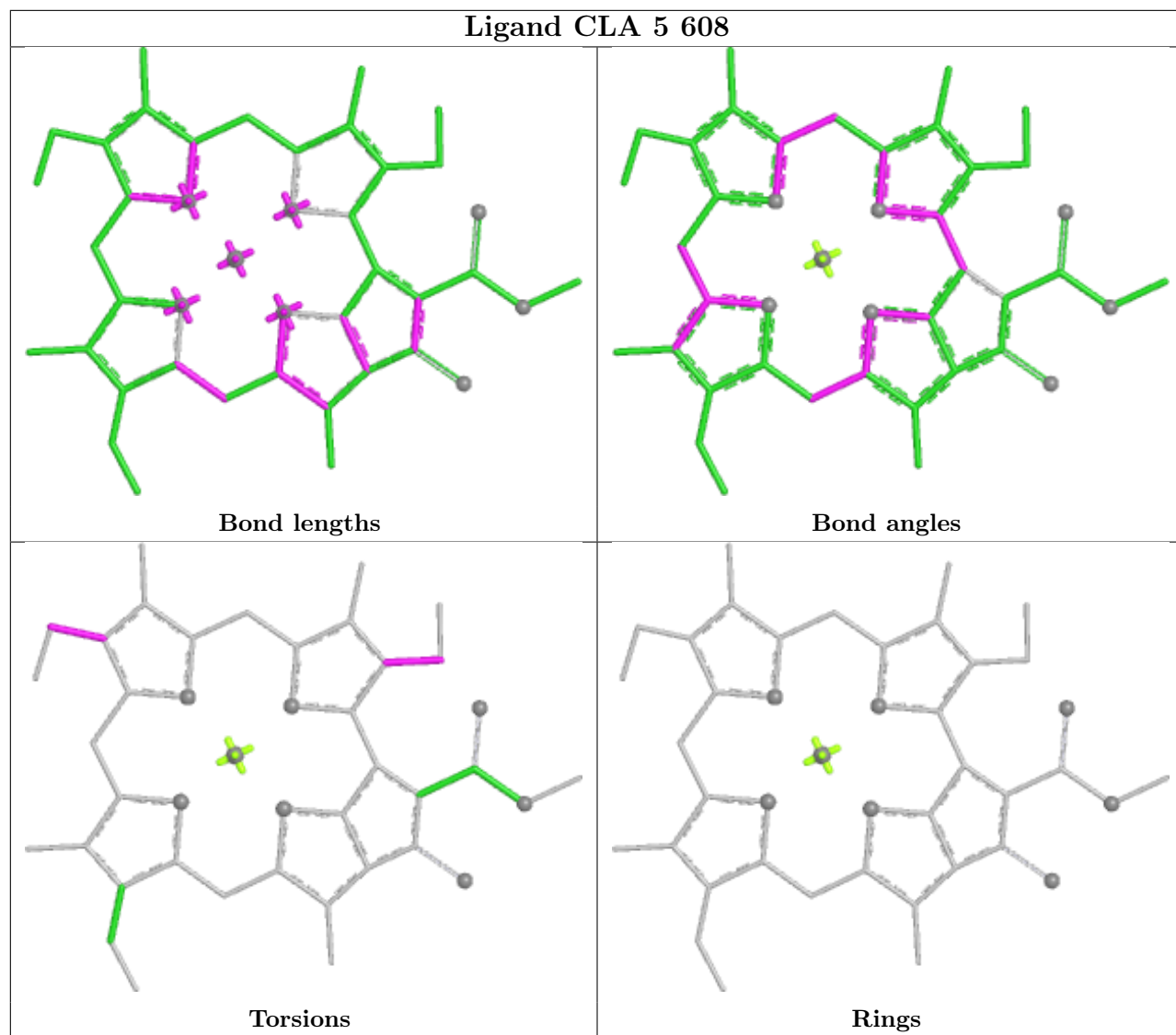


Torsions

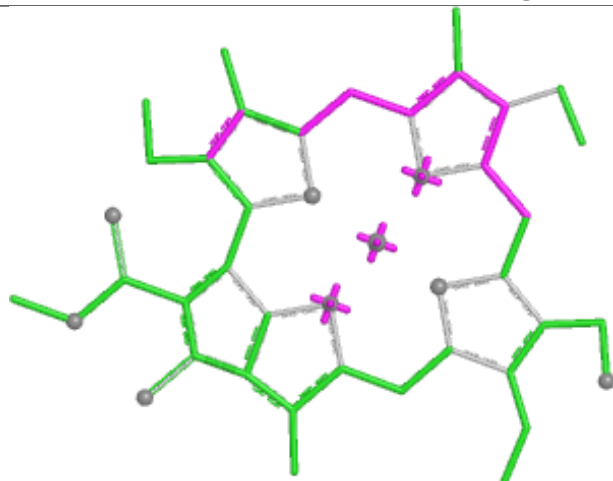


Rings

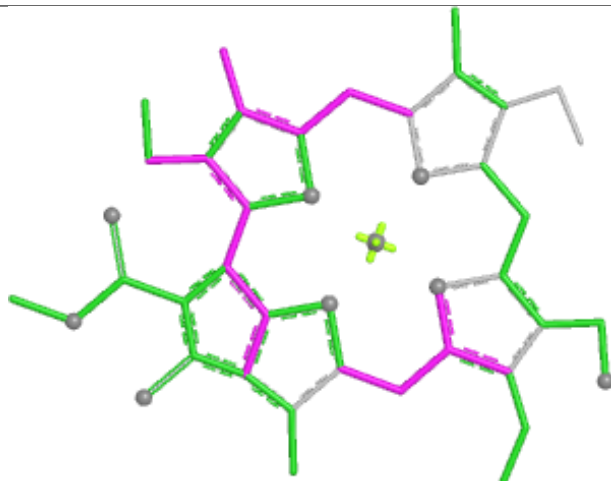
Ligand CLA 5 608



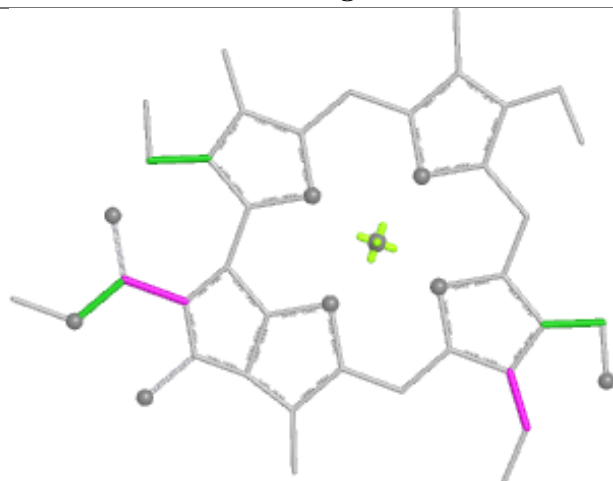
Ligand CHL 6 306



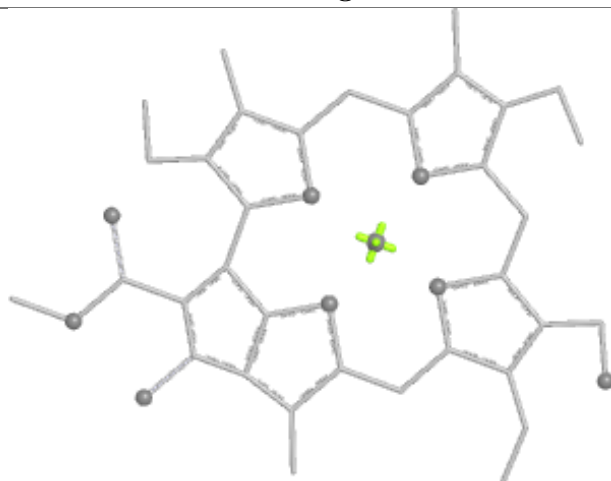
Bond lengths



Bond angles

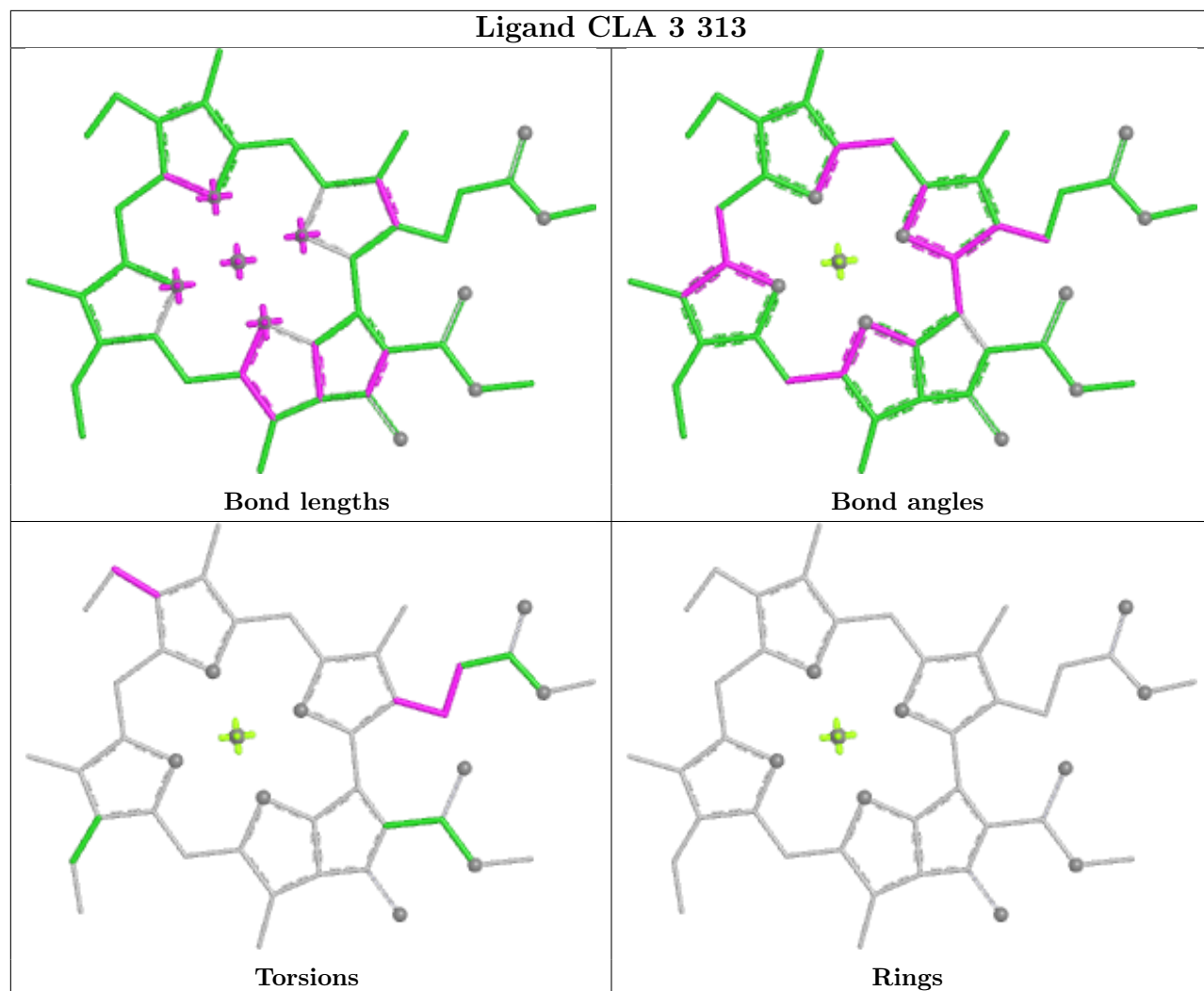


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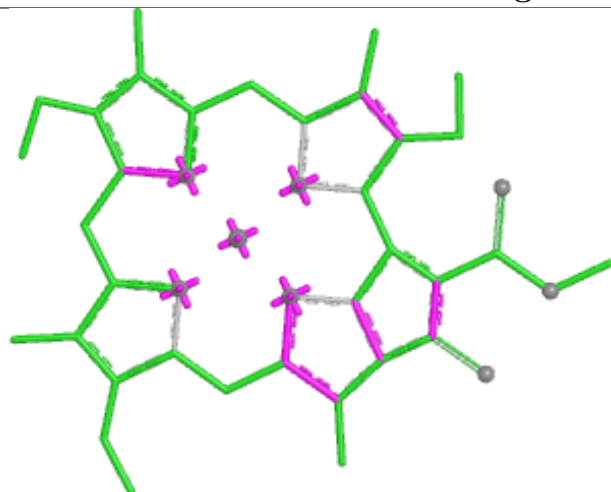


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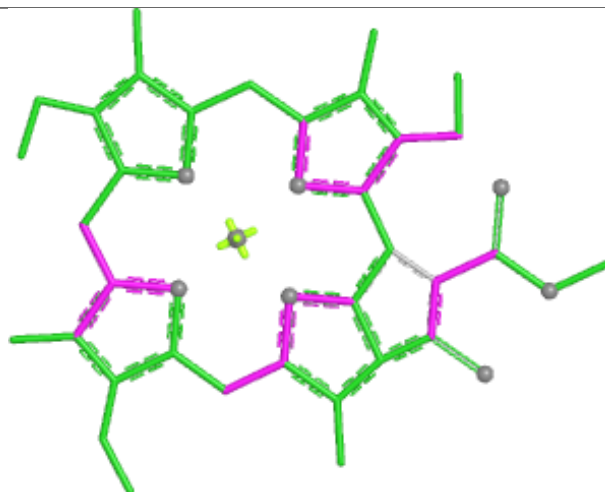
Ligand CLA 3 313



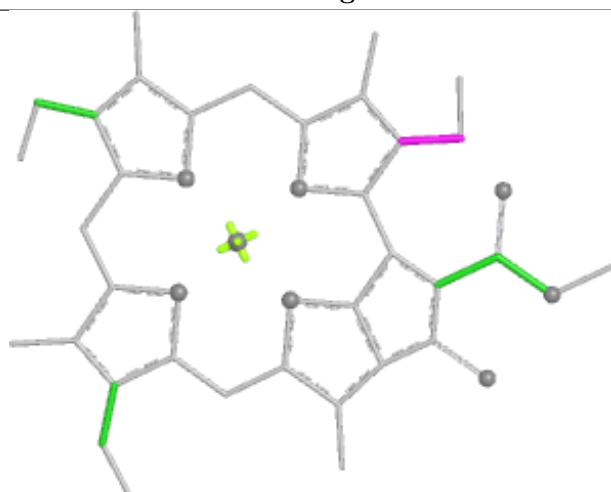
Ligand CLA B 801



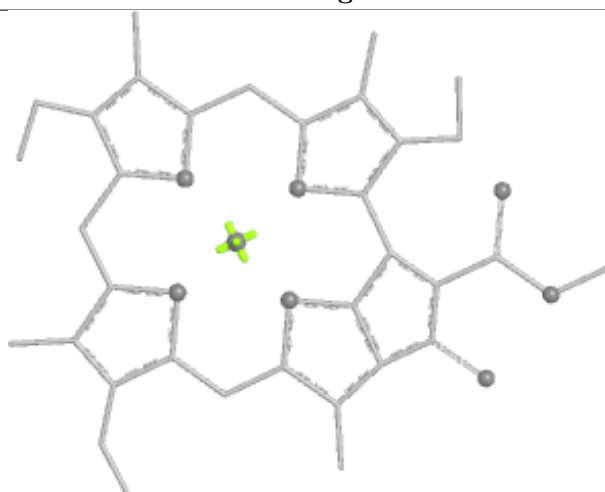
Bond lengths



Bond angles

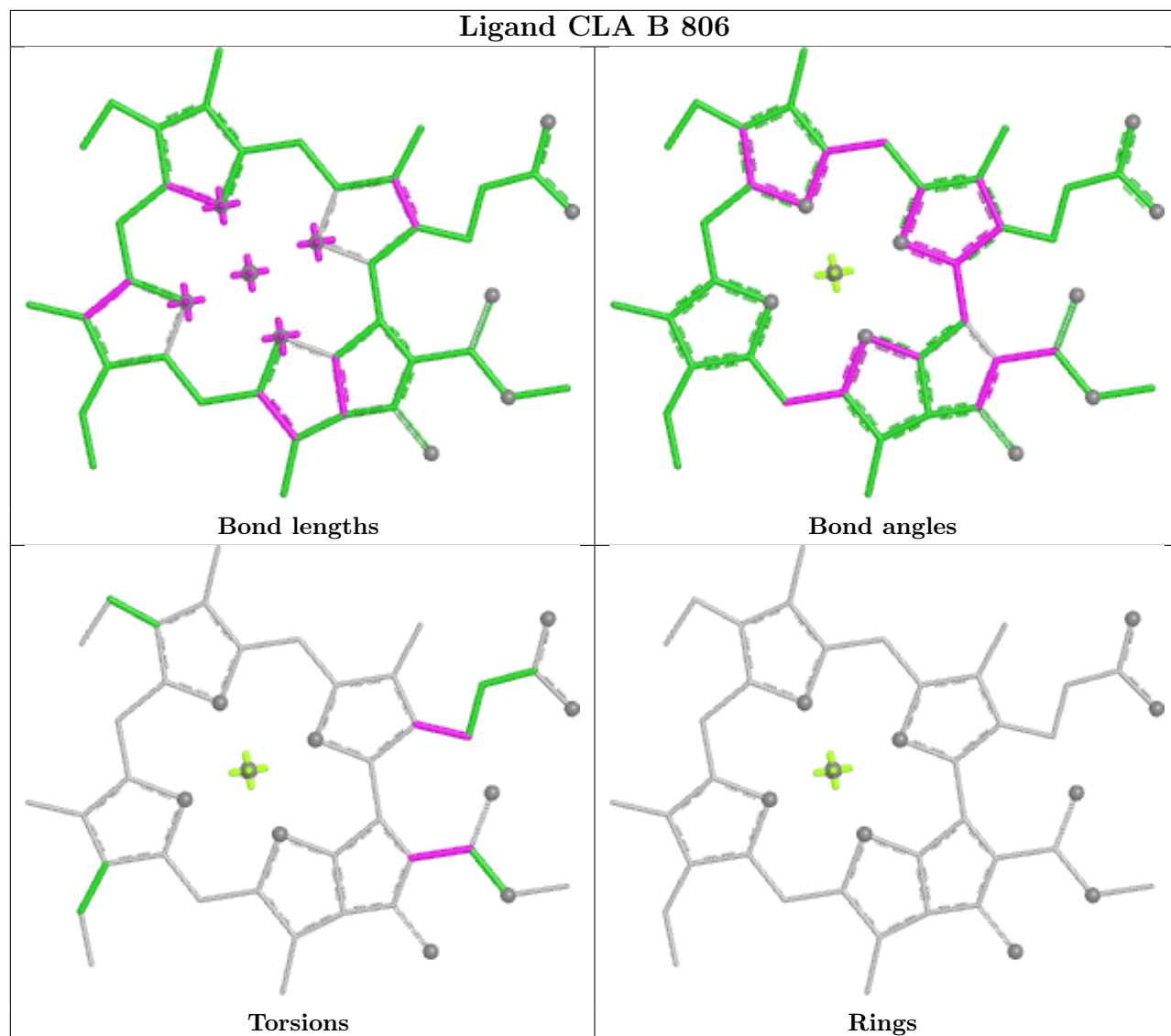


Torsions

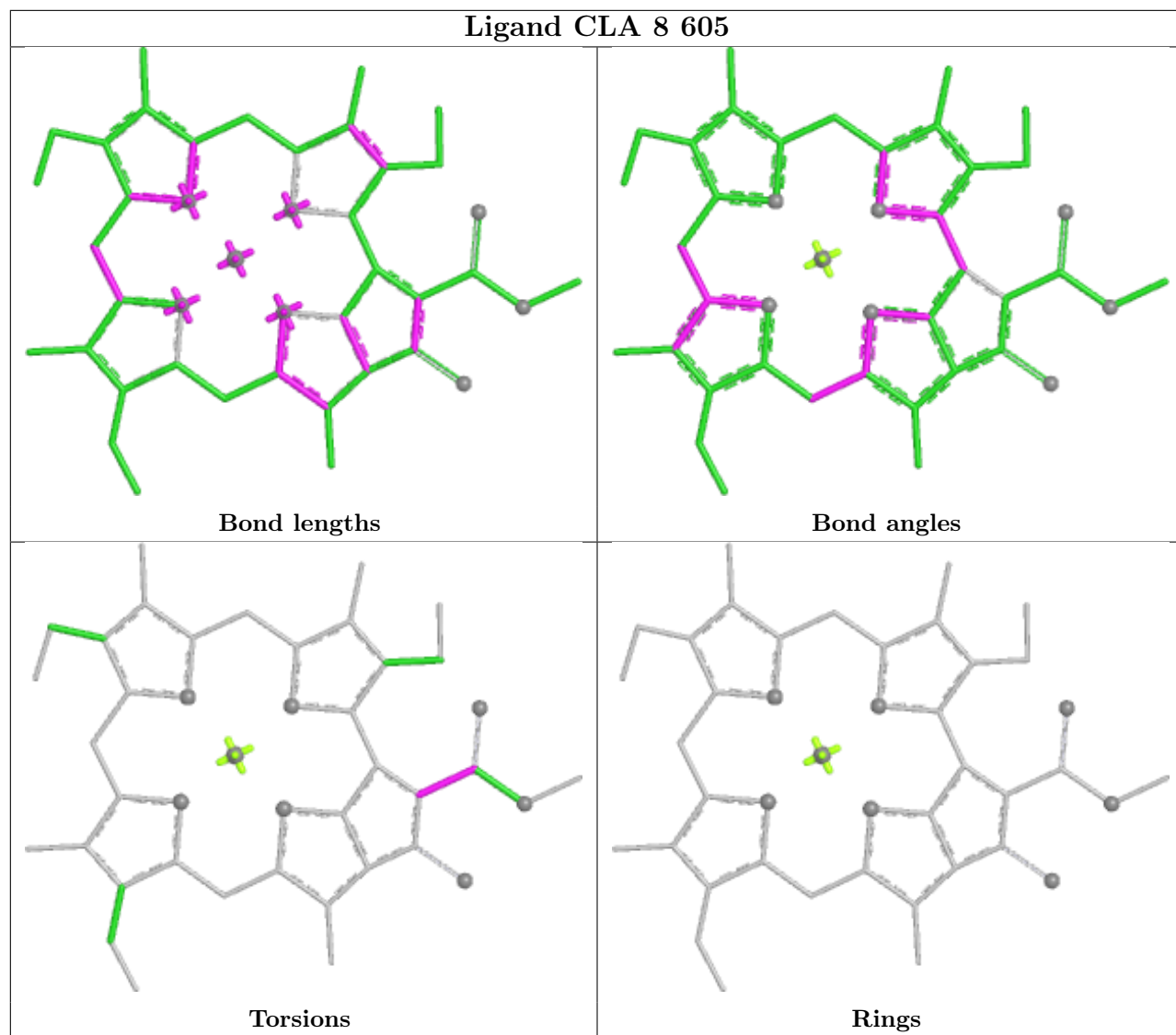


Rings

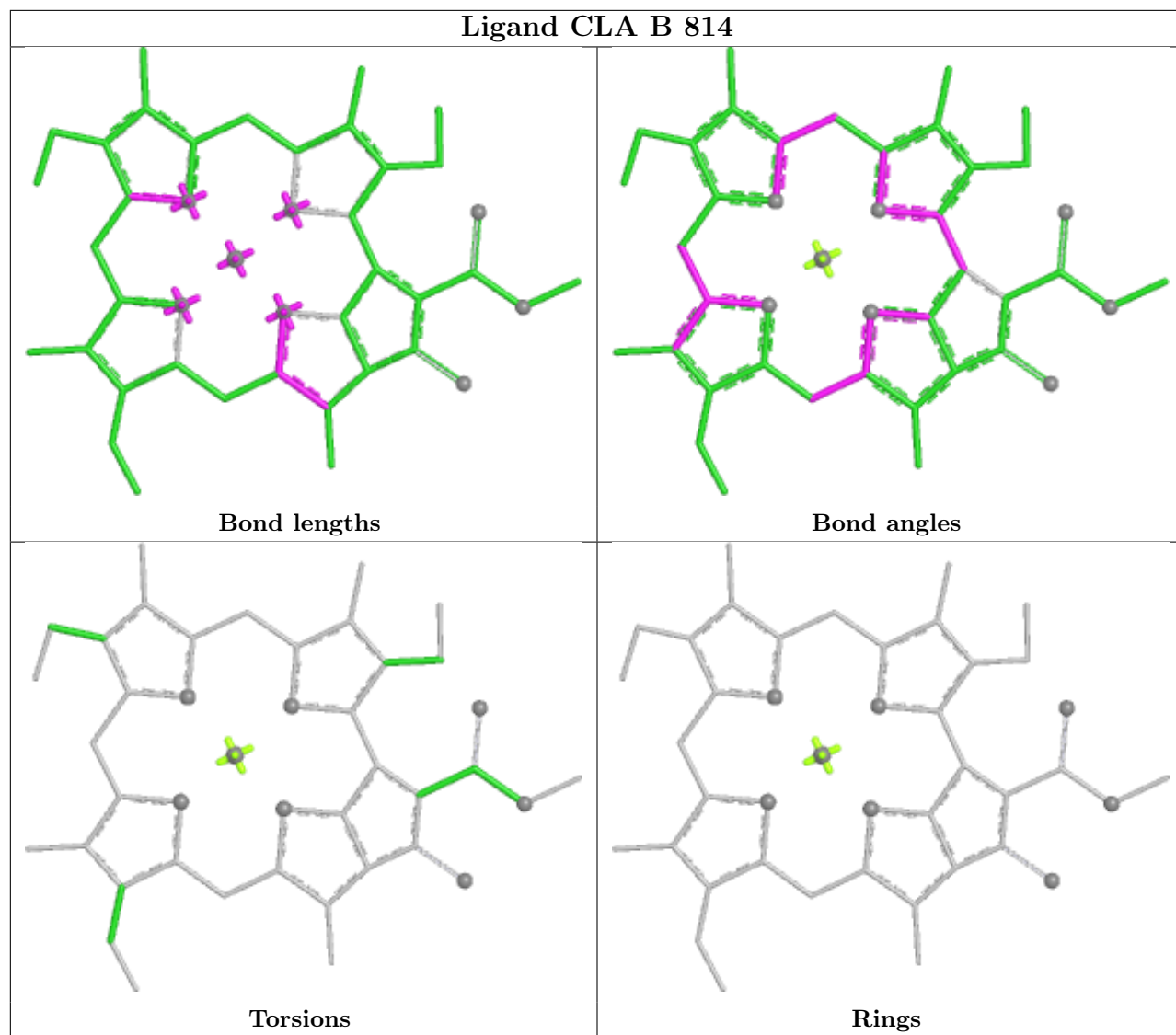
Ligand CLA B 806



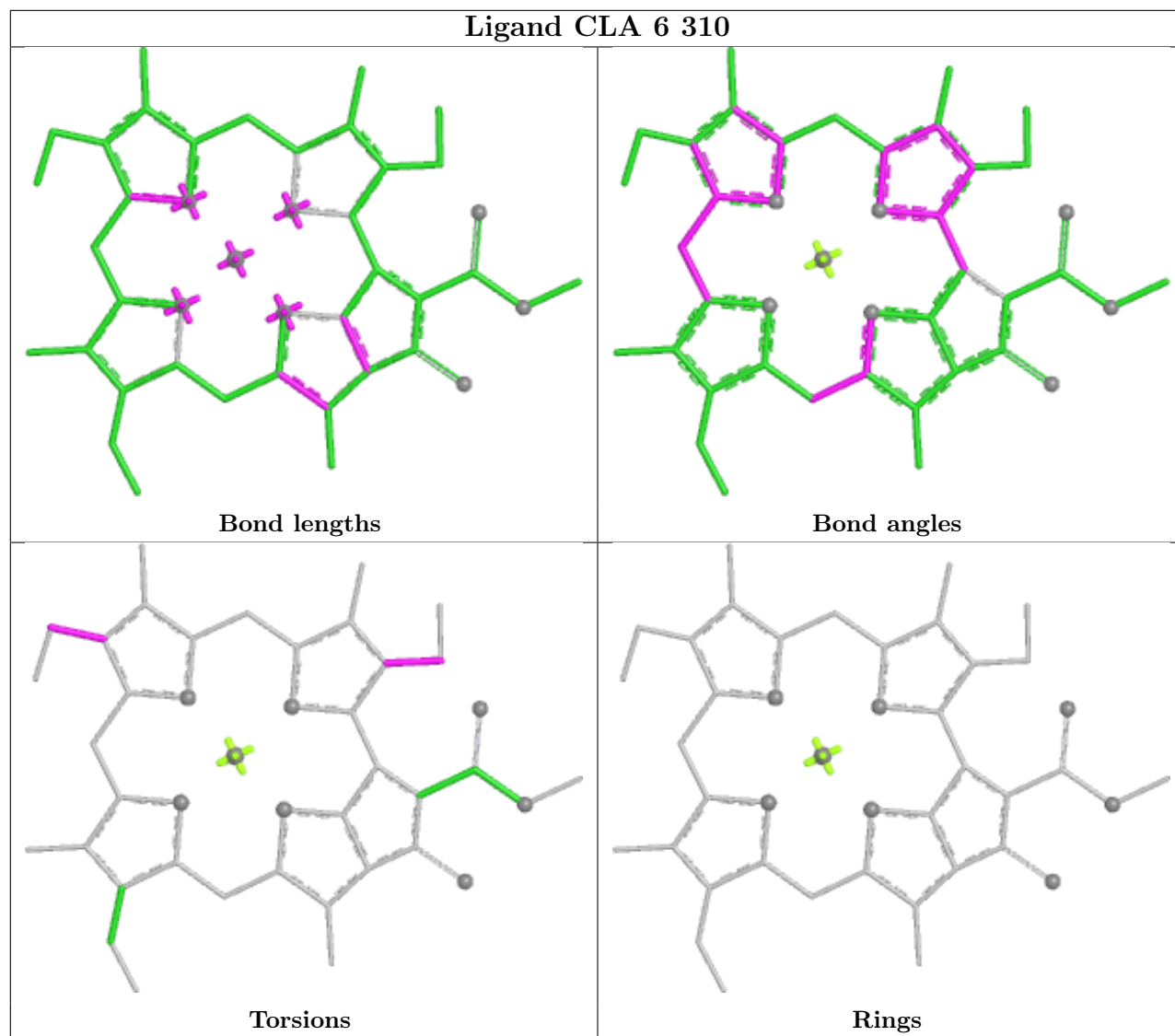
Ligand CLA 8 605



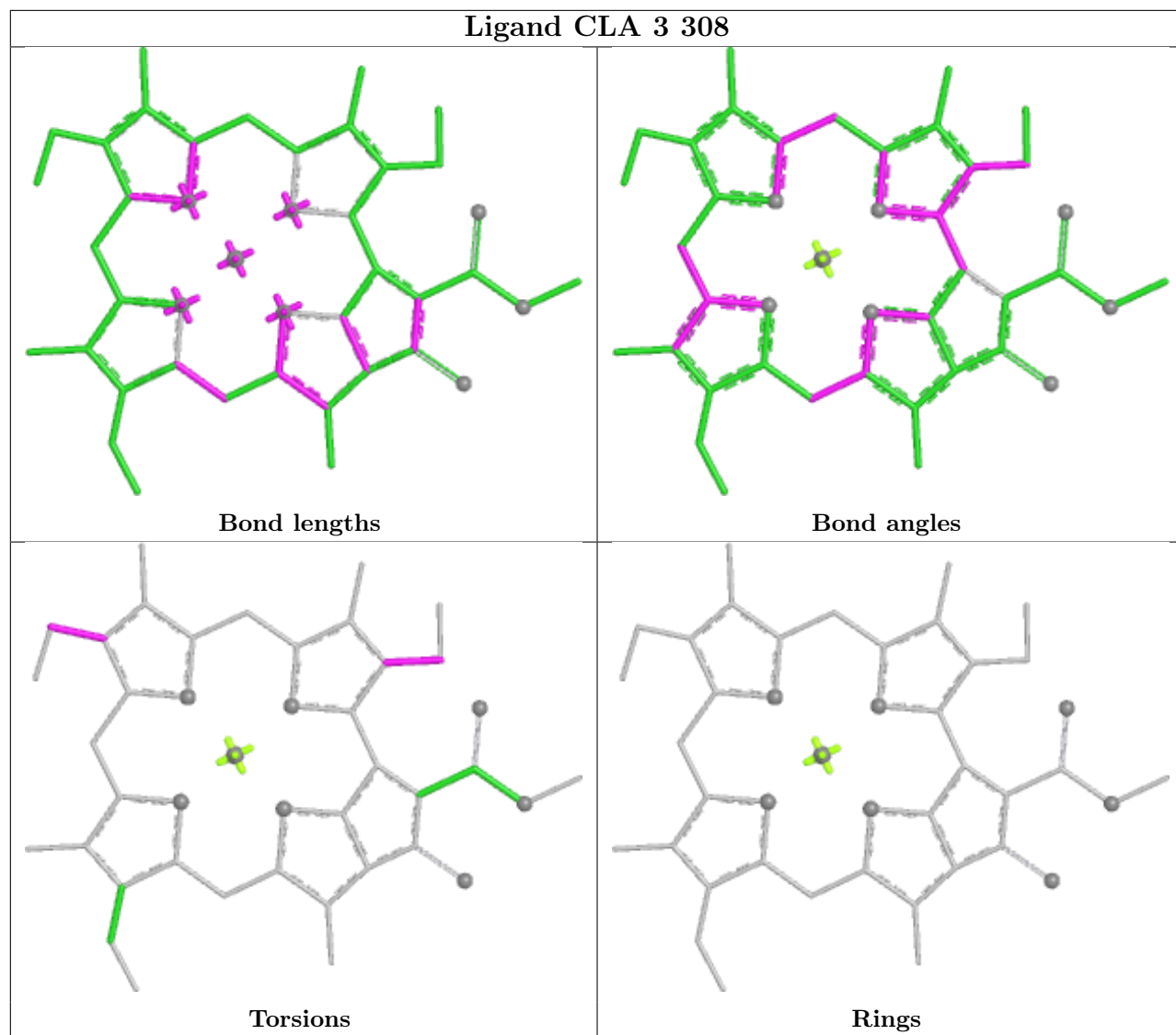
Ligand CLA B 814



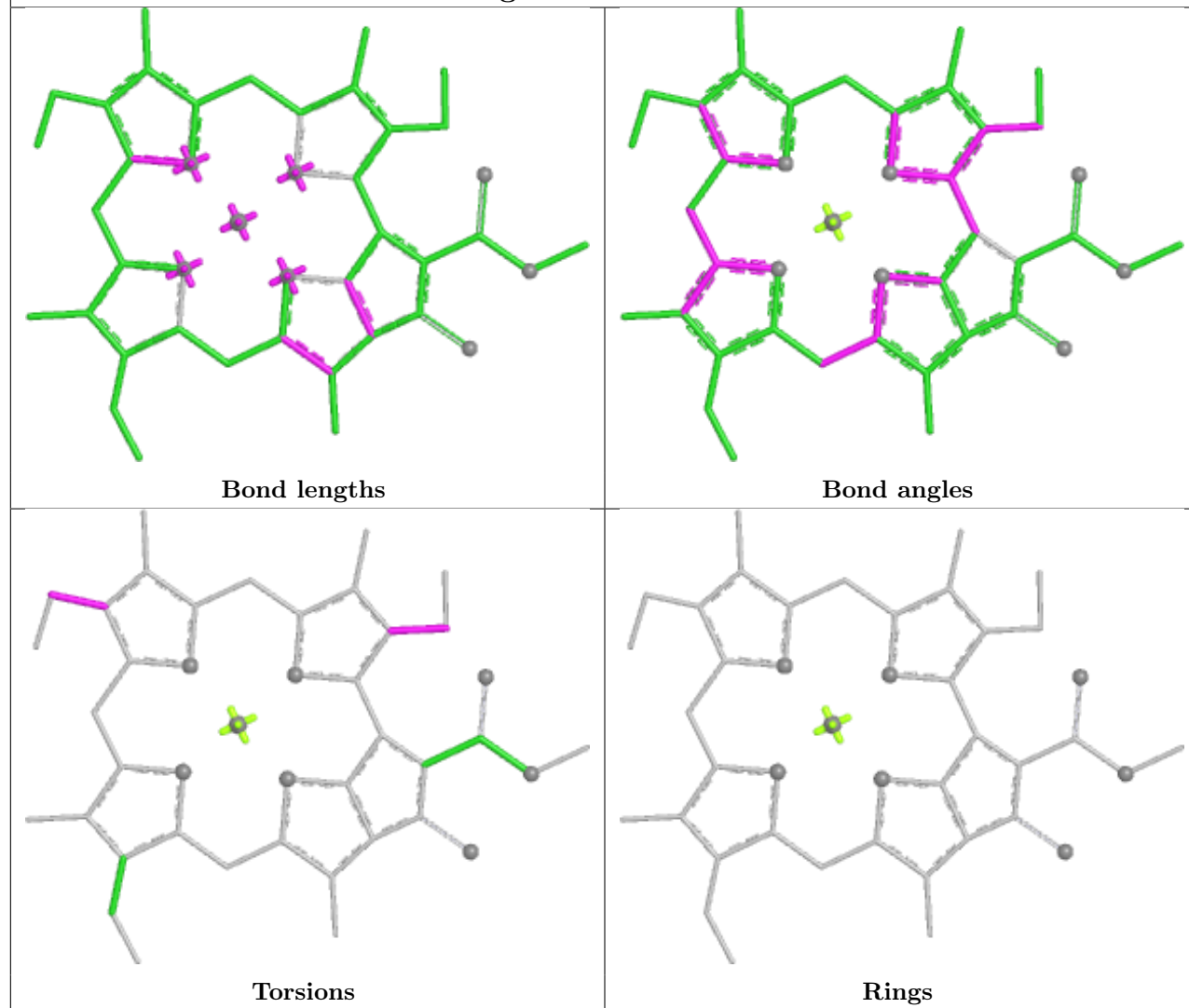
Ligand CLA 6 310



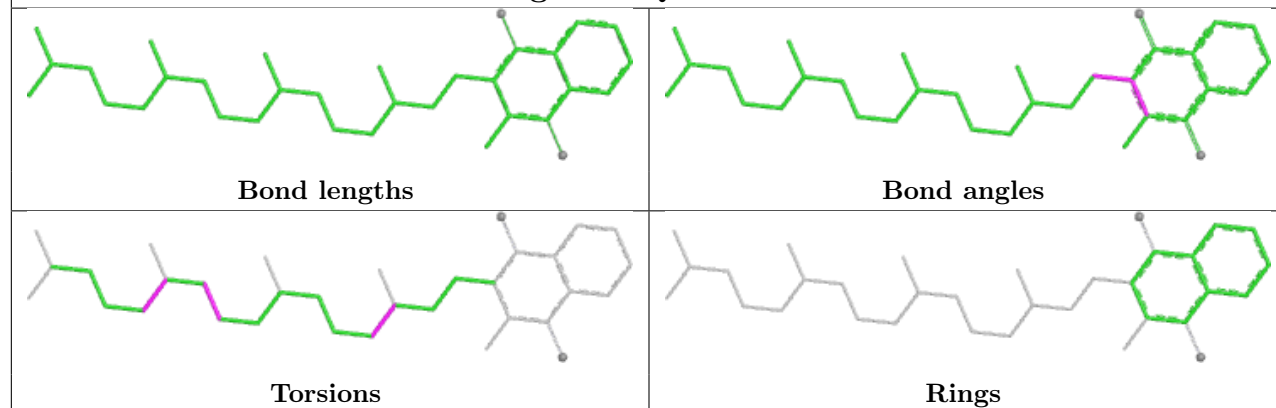
Ligand CLA 3 308



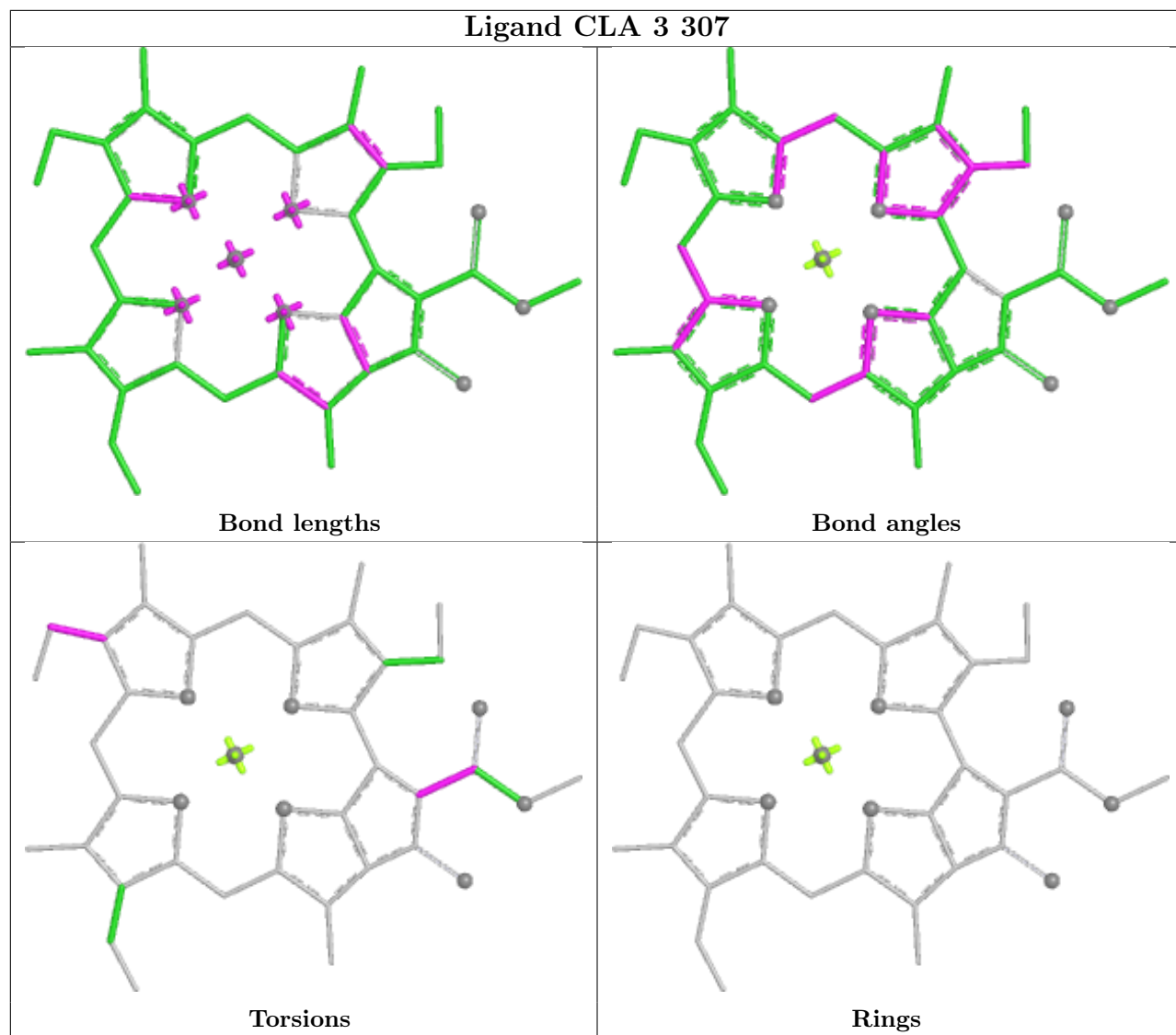
Ligand CLA 1 610



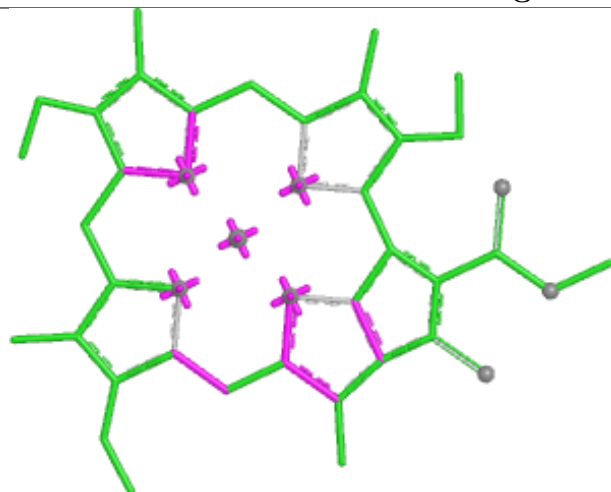
Ligand PQN B 844



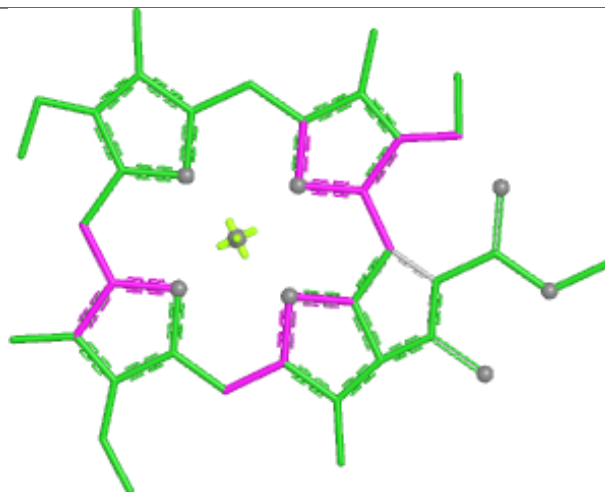
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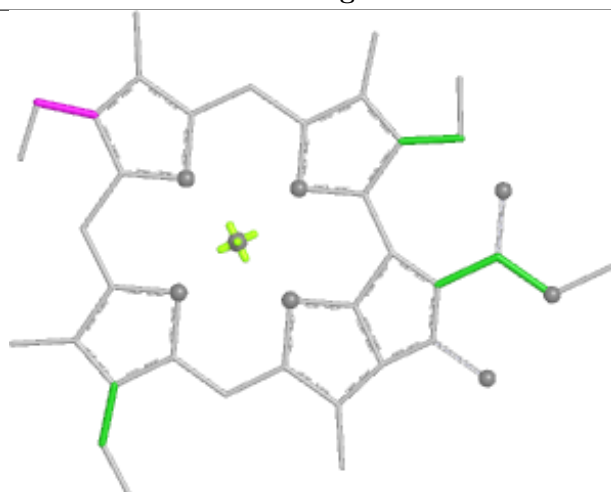
Ligand CLA A 835



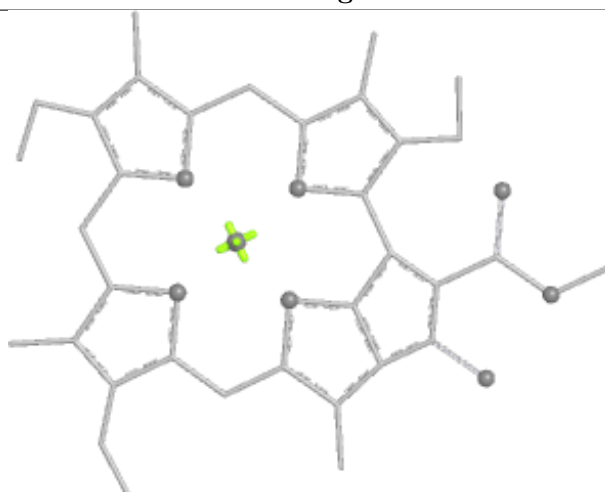
Bond lengths



Bond angles

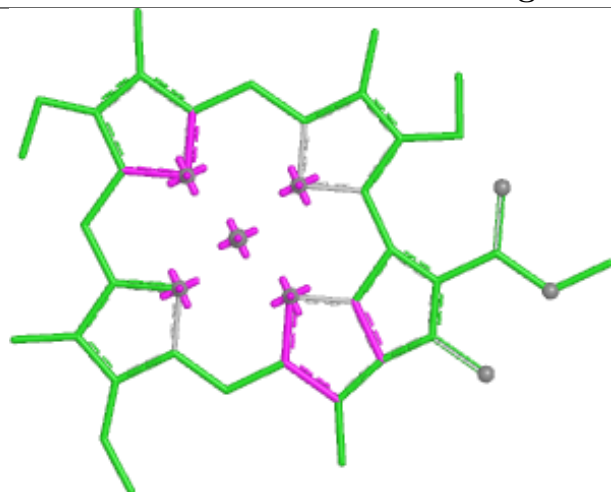


Torsions

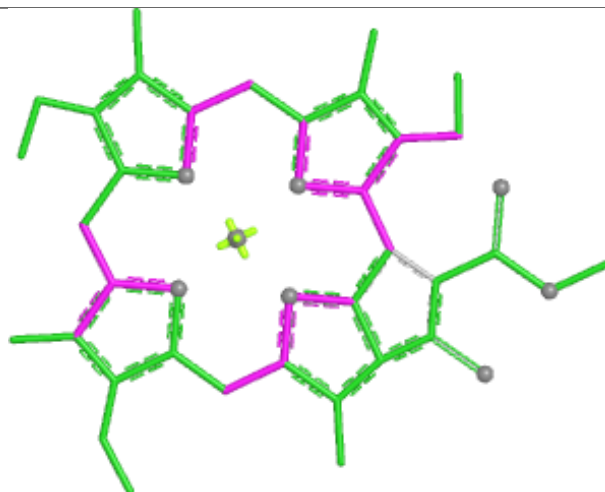


Rings

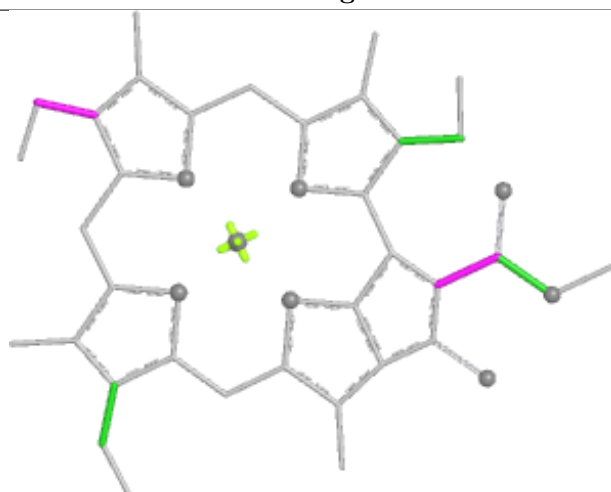
Ligand CLA J 101



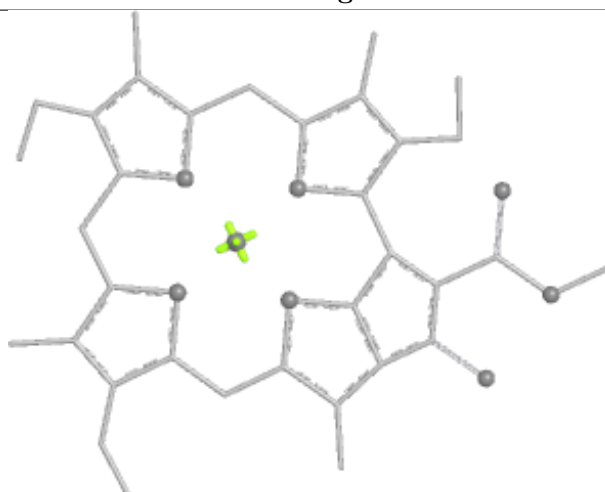
Bond lengths



Bond angles

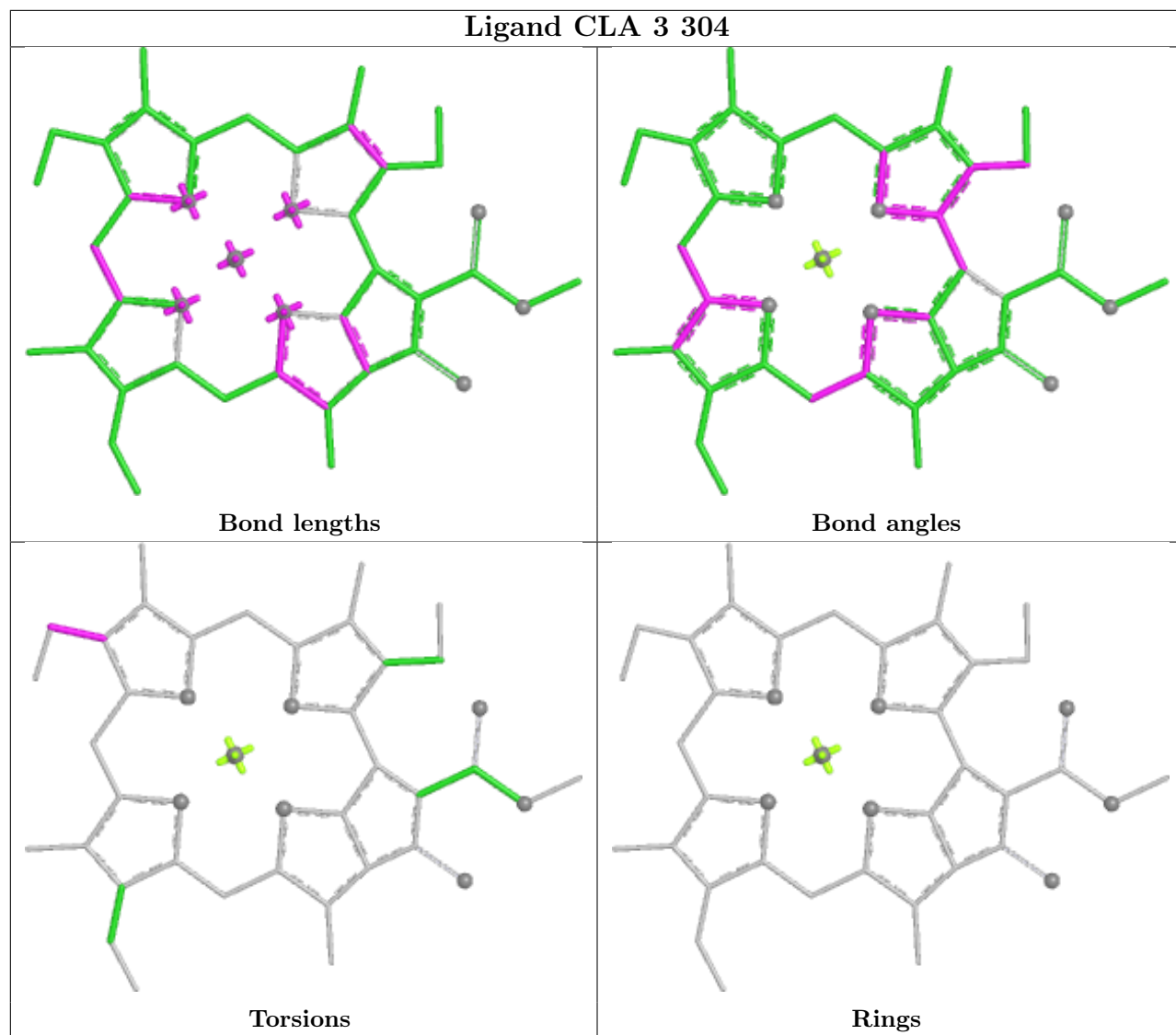


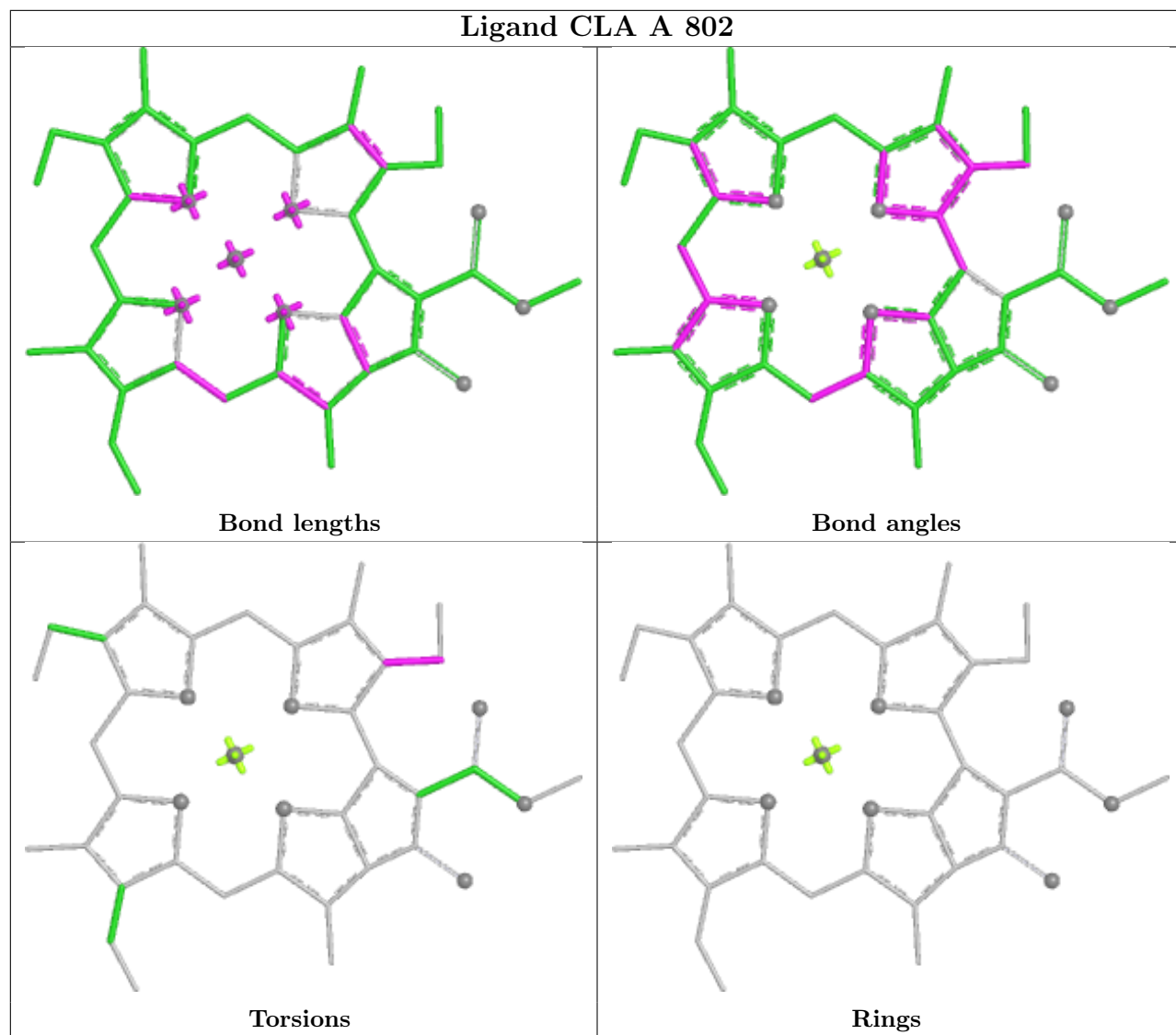
Torsions



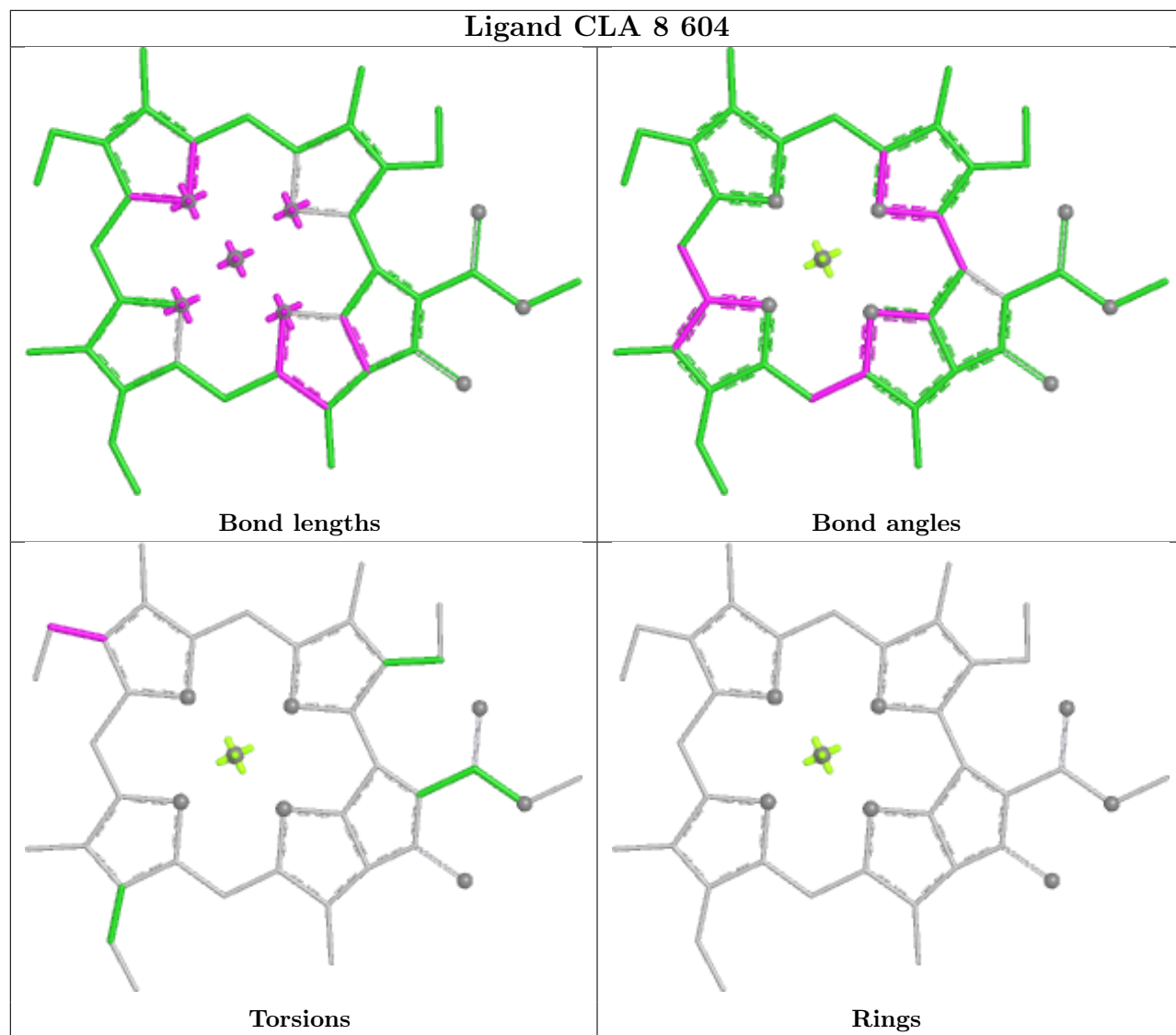
Rings

Ligand CLA 3 304

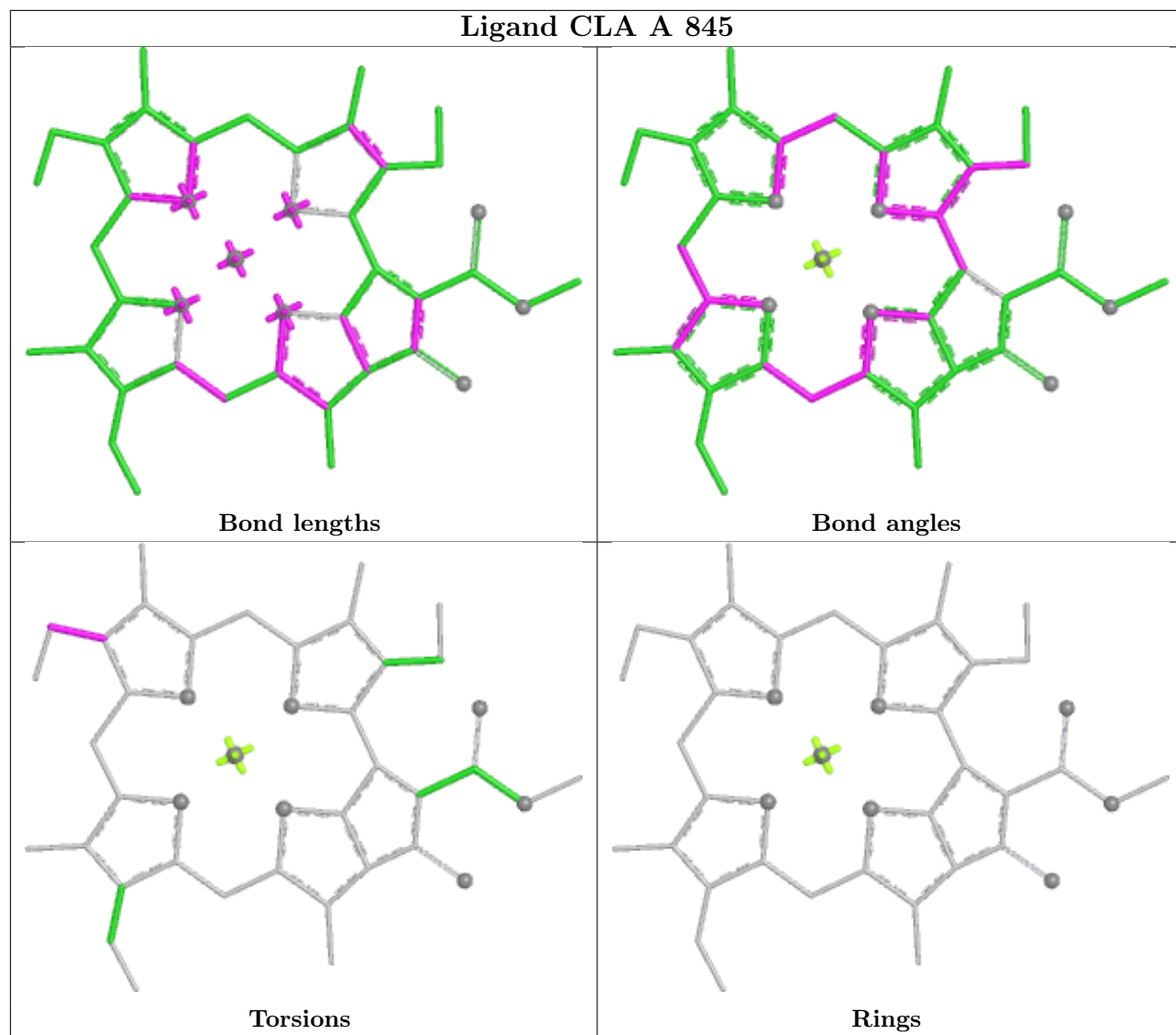




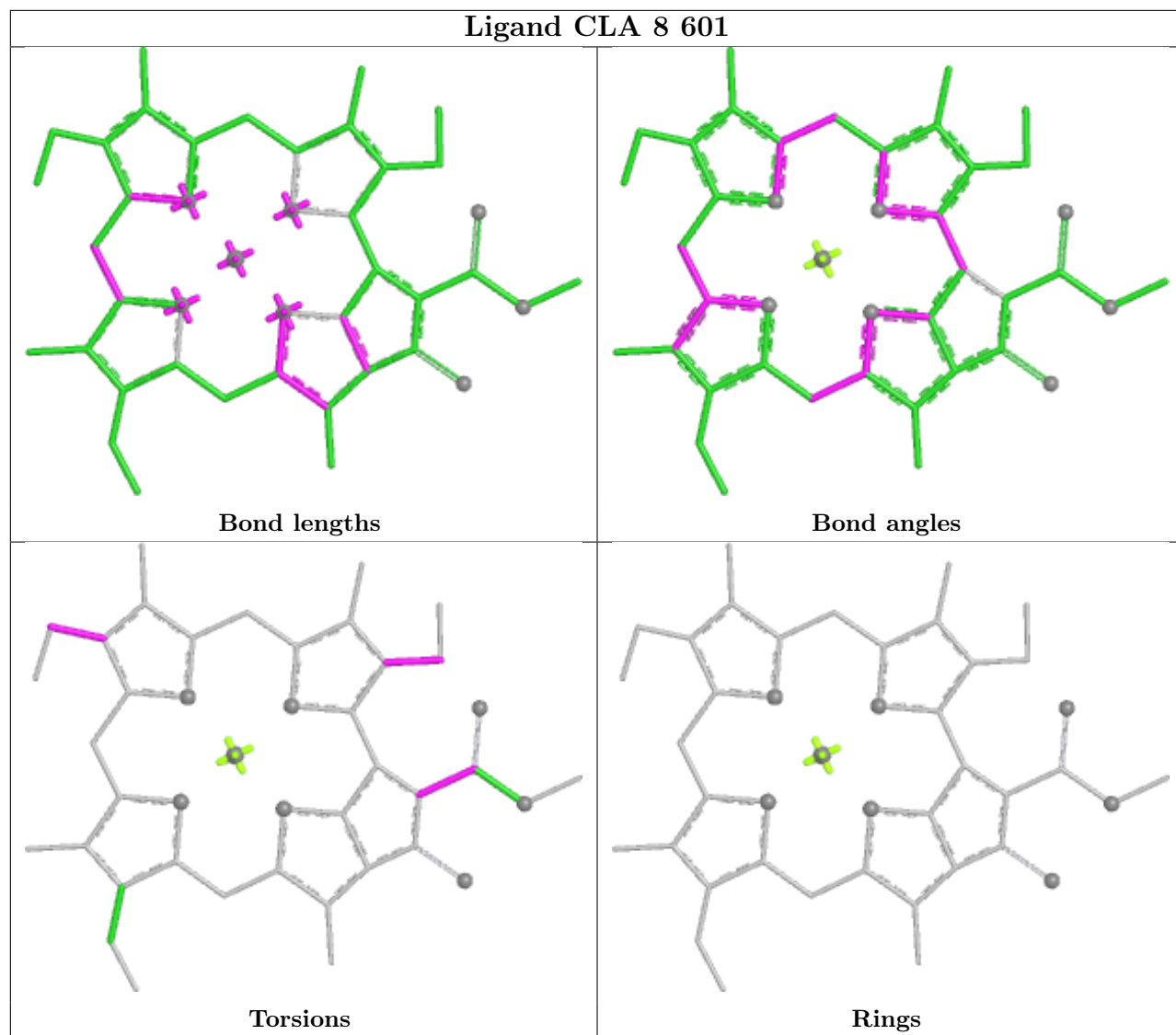
Ligand CLA 8 604

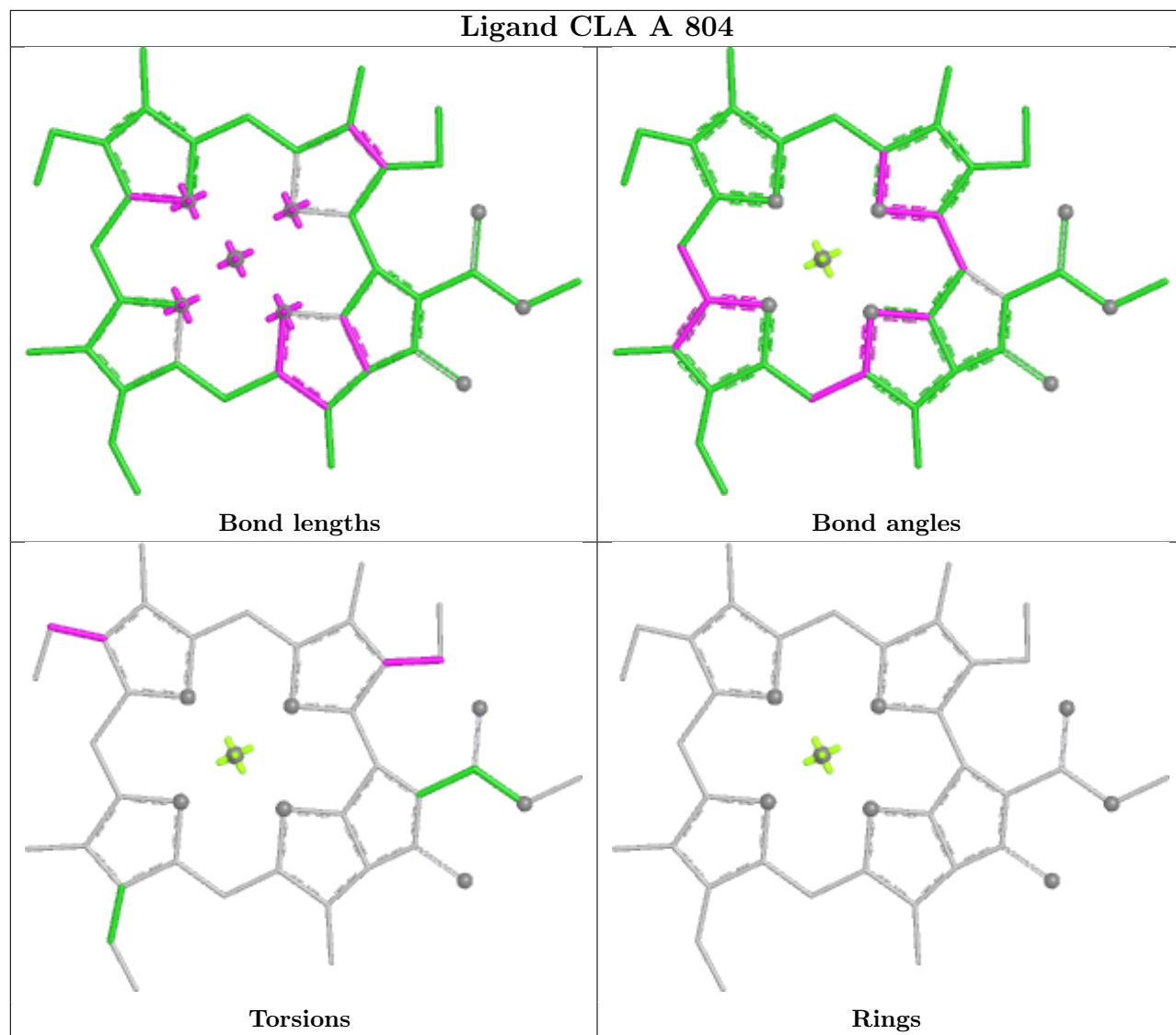


Ligand CLA A 845

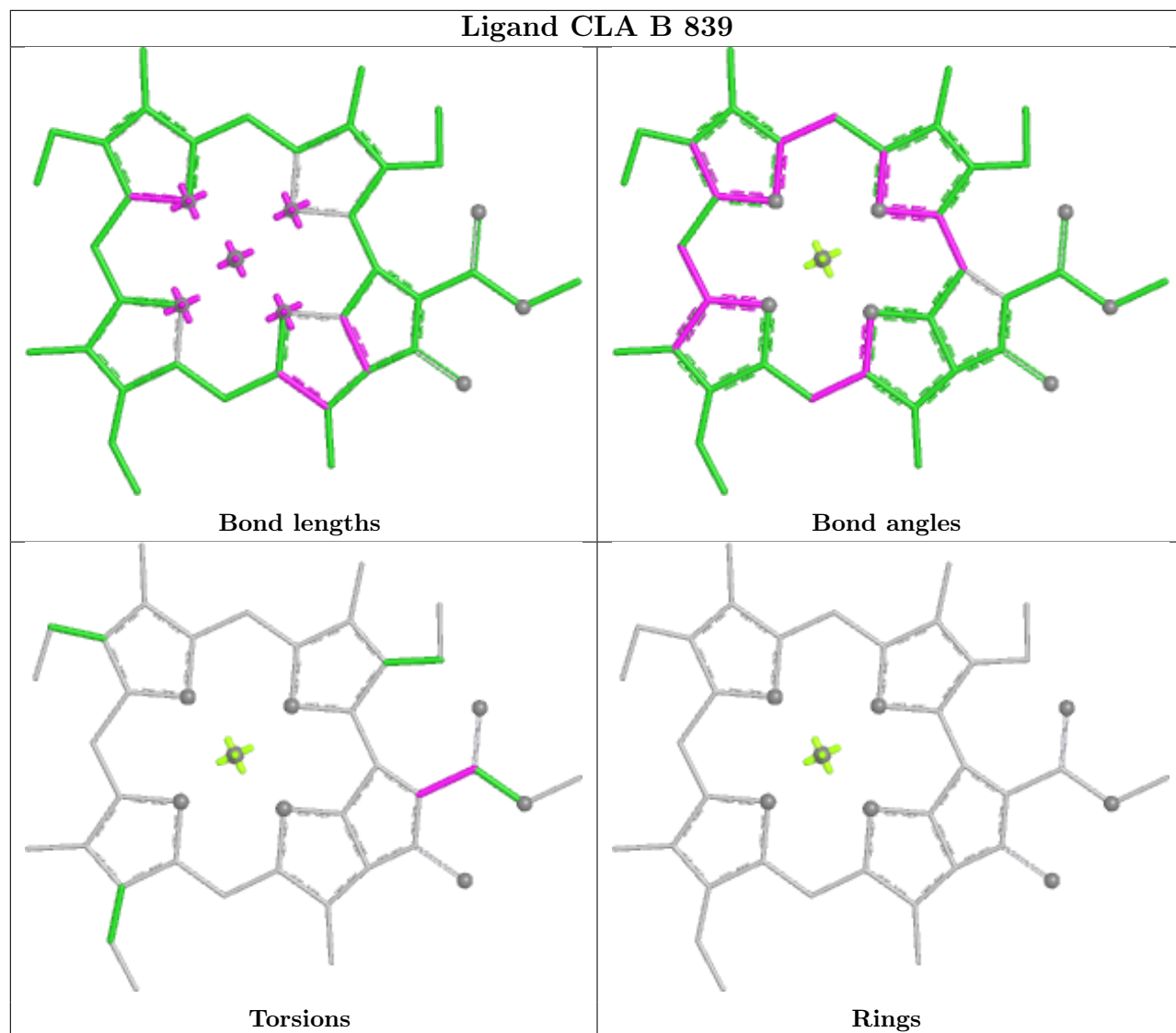


Ligand CLA 8 601

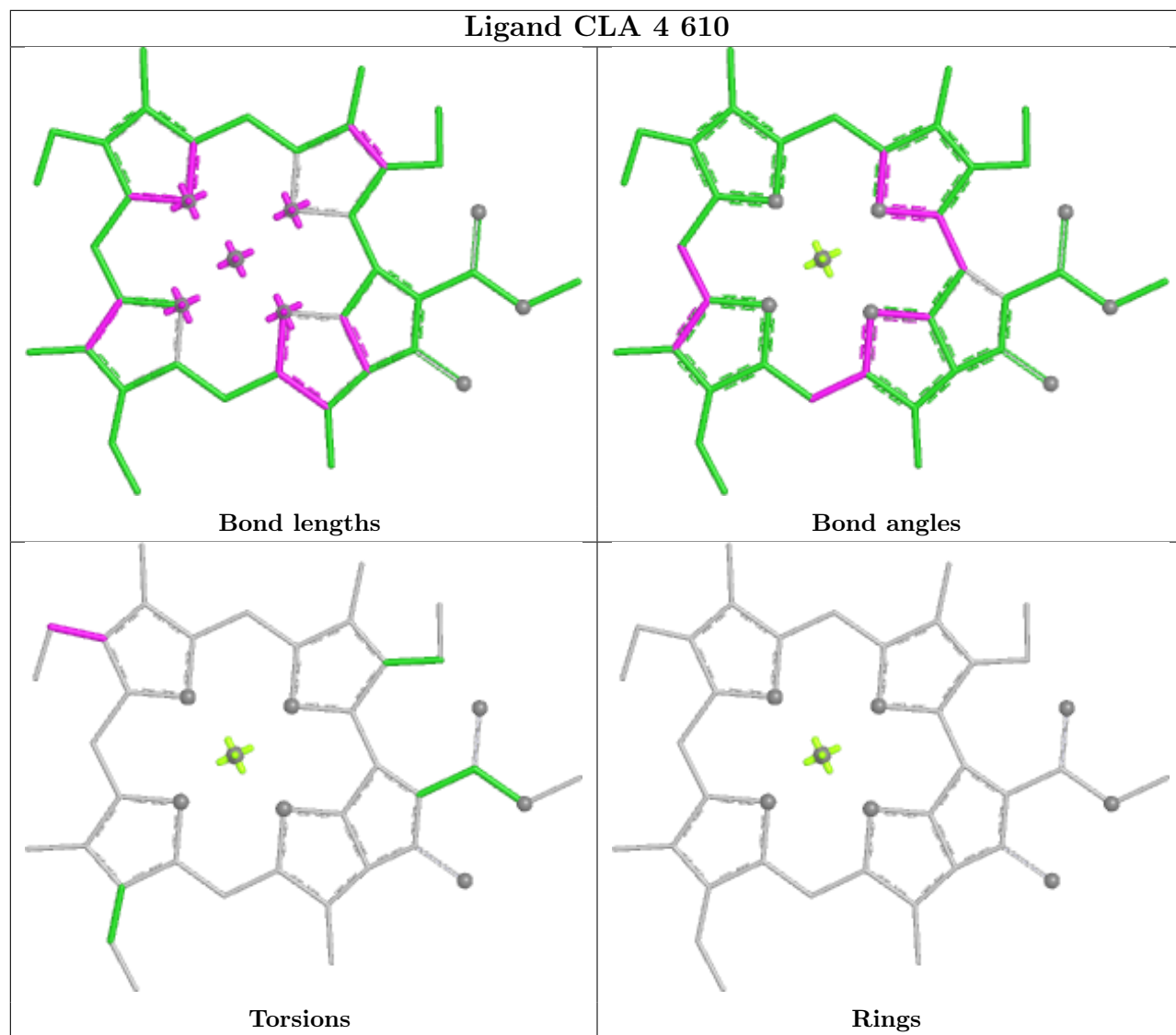




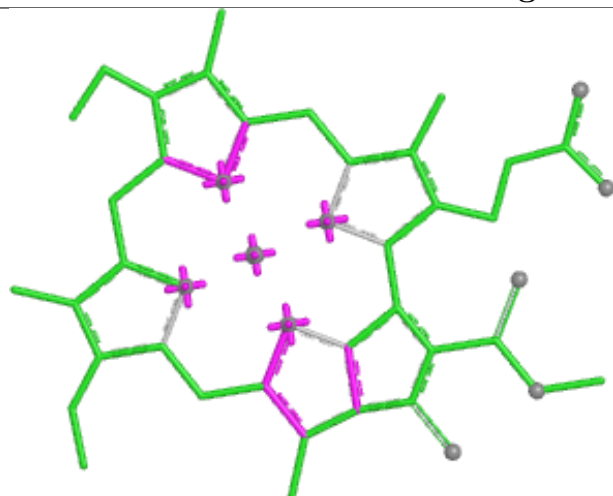
Ligand CLA B 839



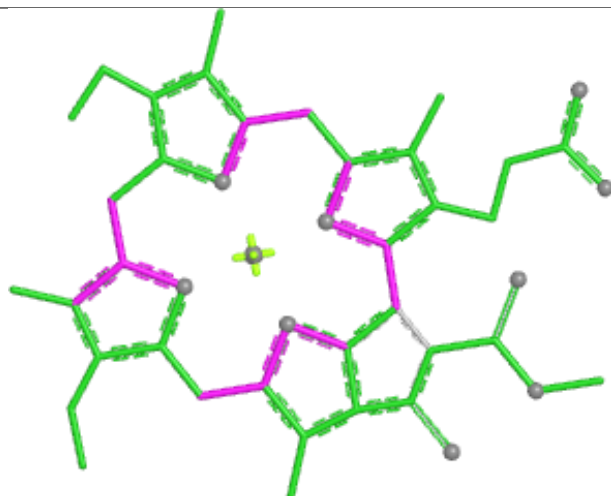
Ligand CLA 4 610



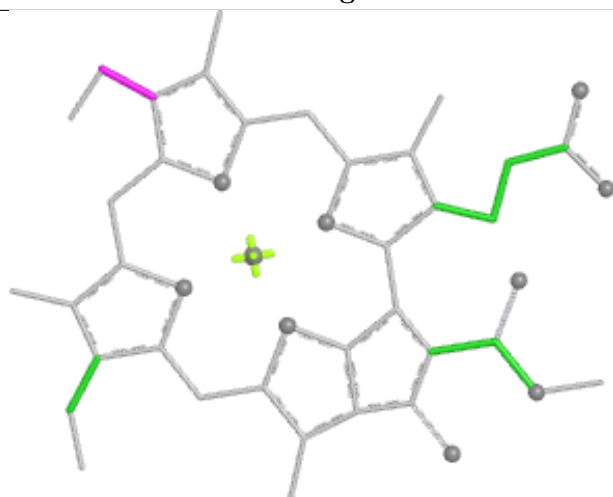
Ligand CLA 8 603



Bond lengths



Bond angles

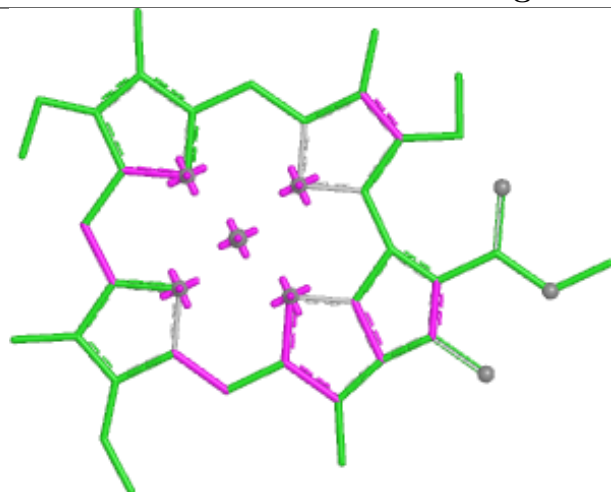


Torsions

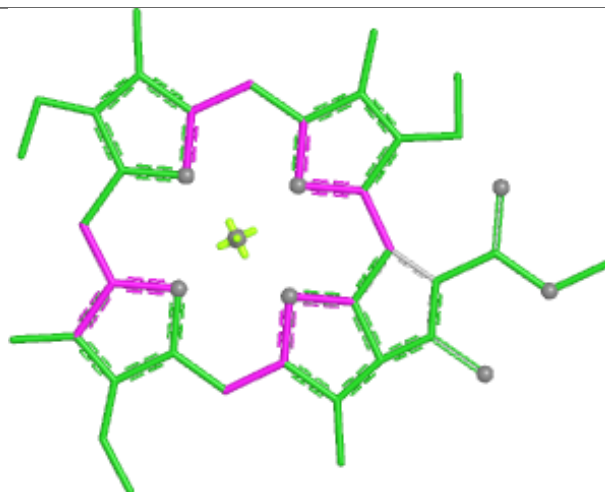


Rings

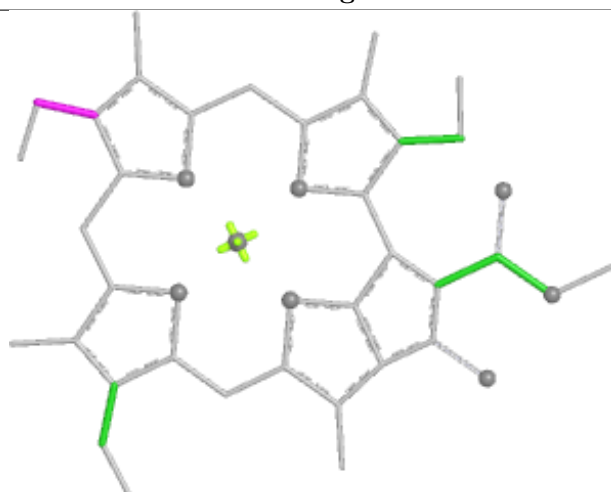
Ligand CLA A 839



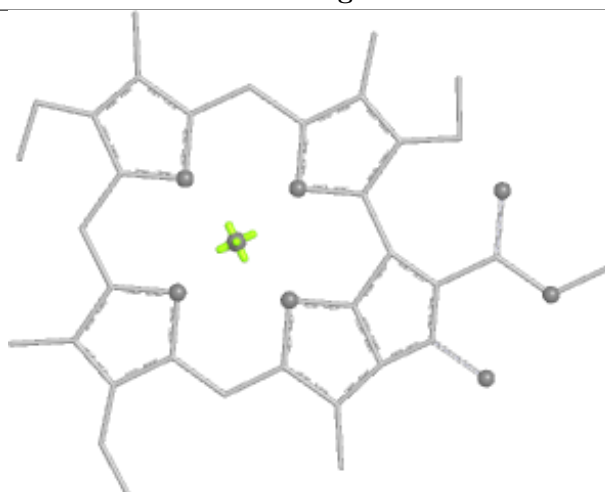
Bond lengths



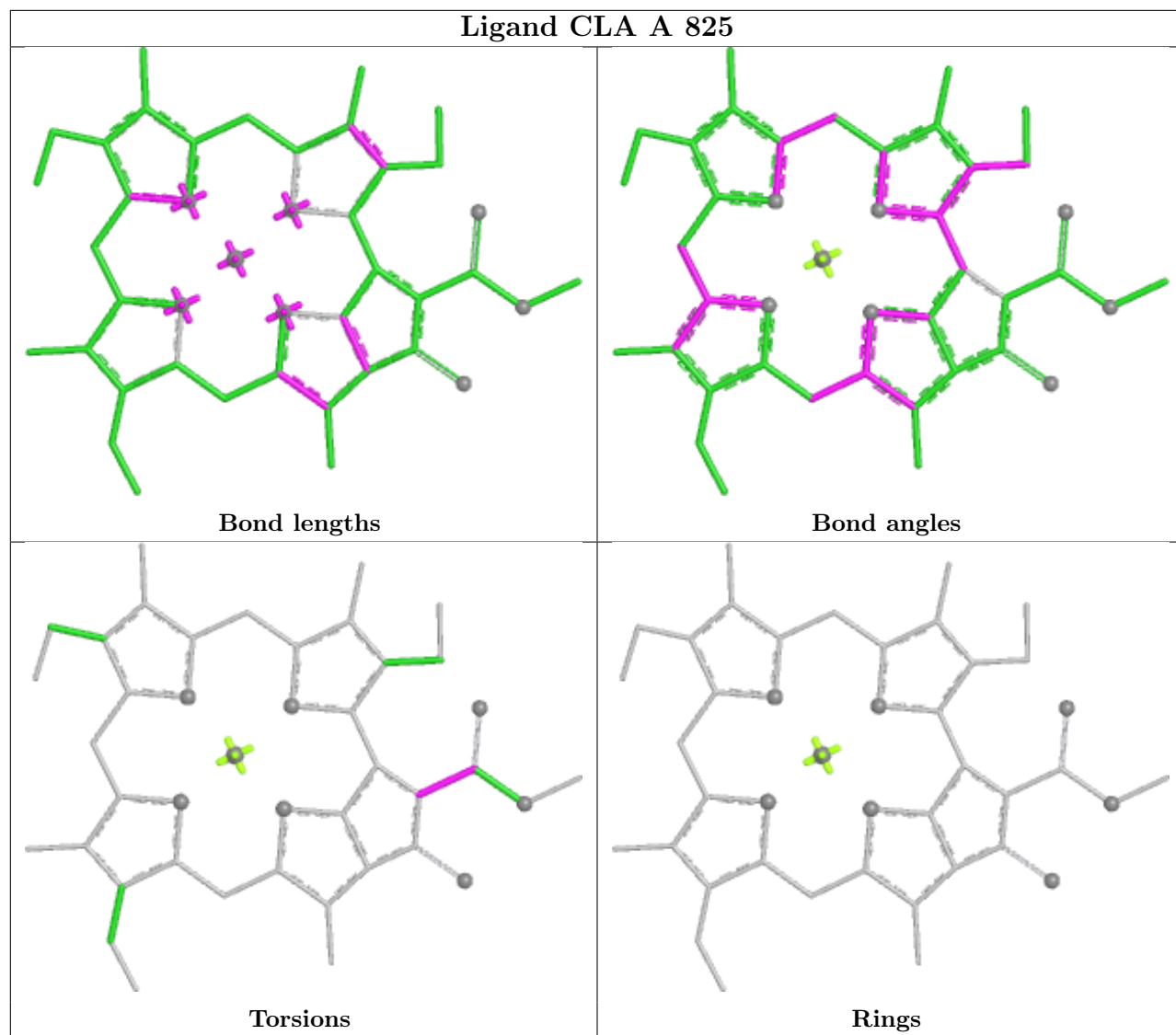
Bond angles



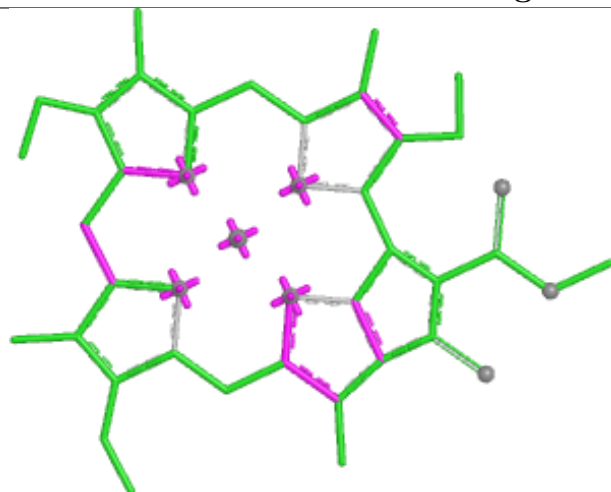
Torsions



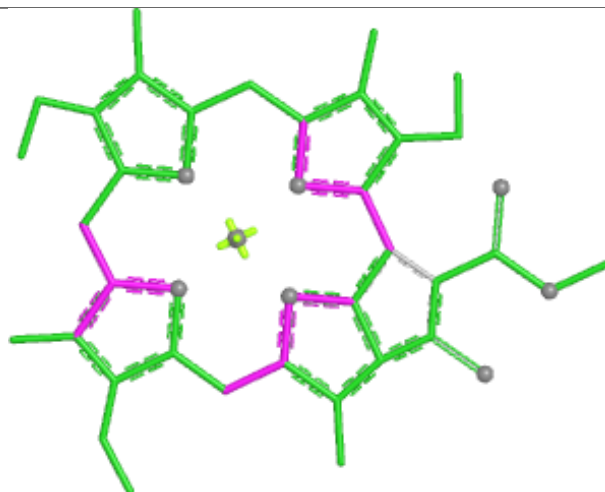
Rings



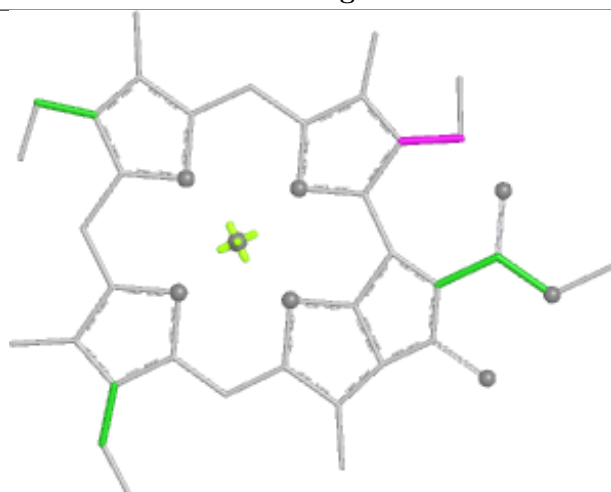
Ligand CLA B 843



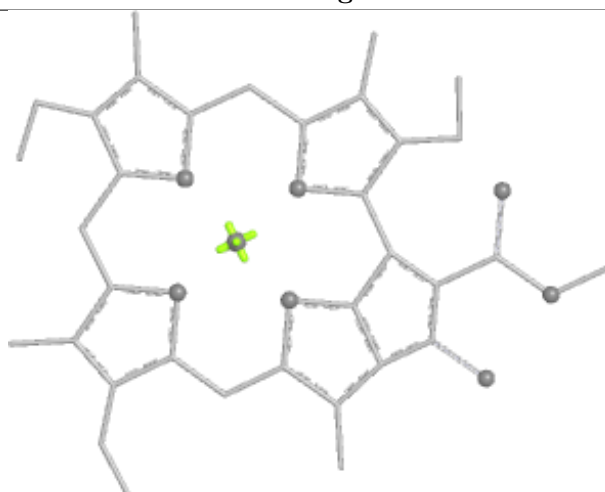
Bond lengths



Bond angles

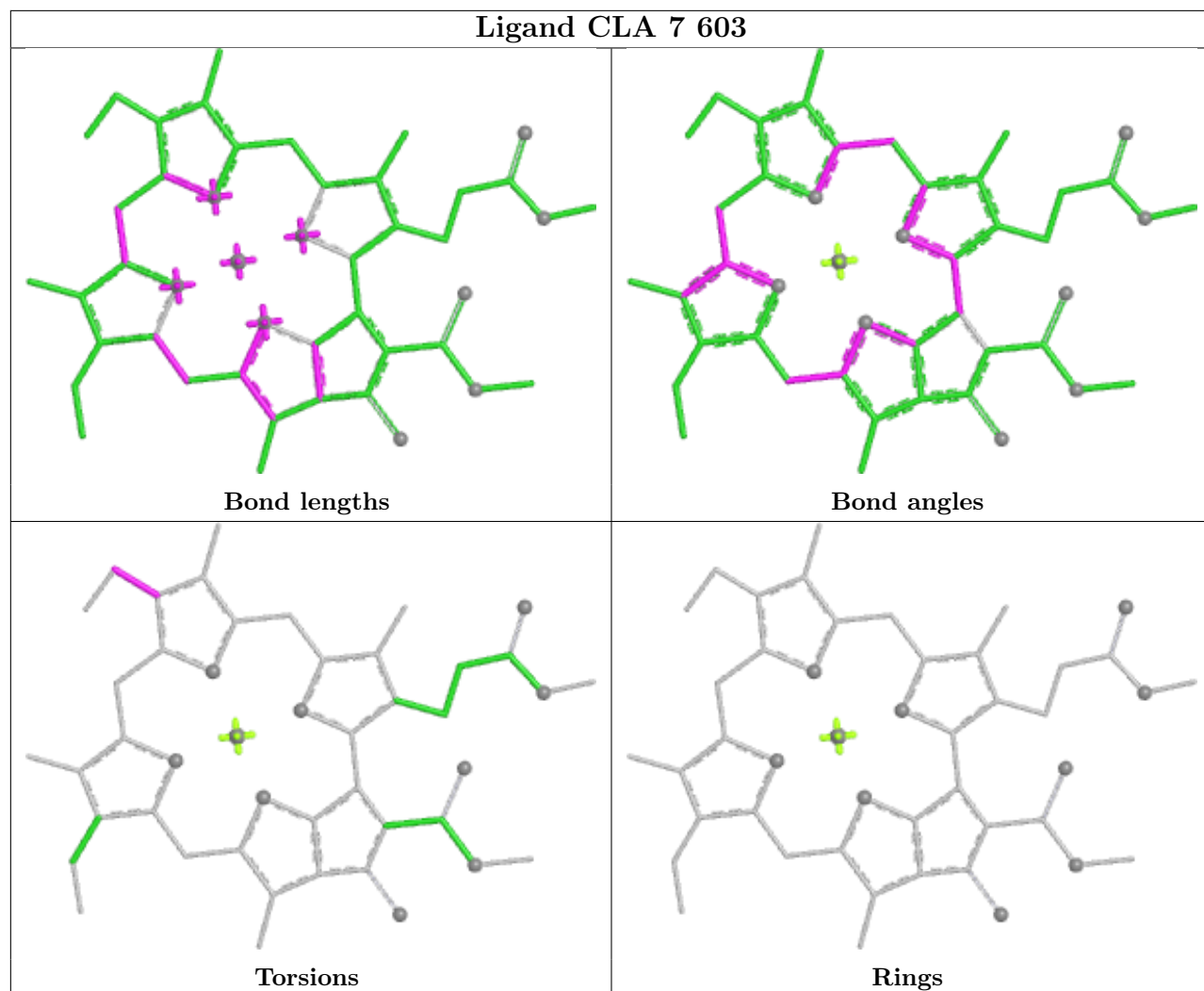


Torsions

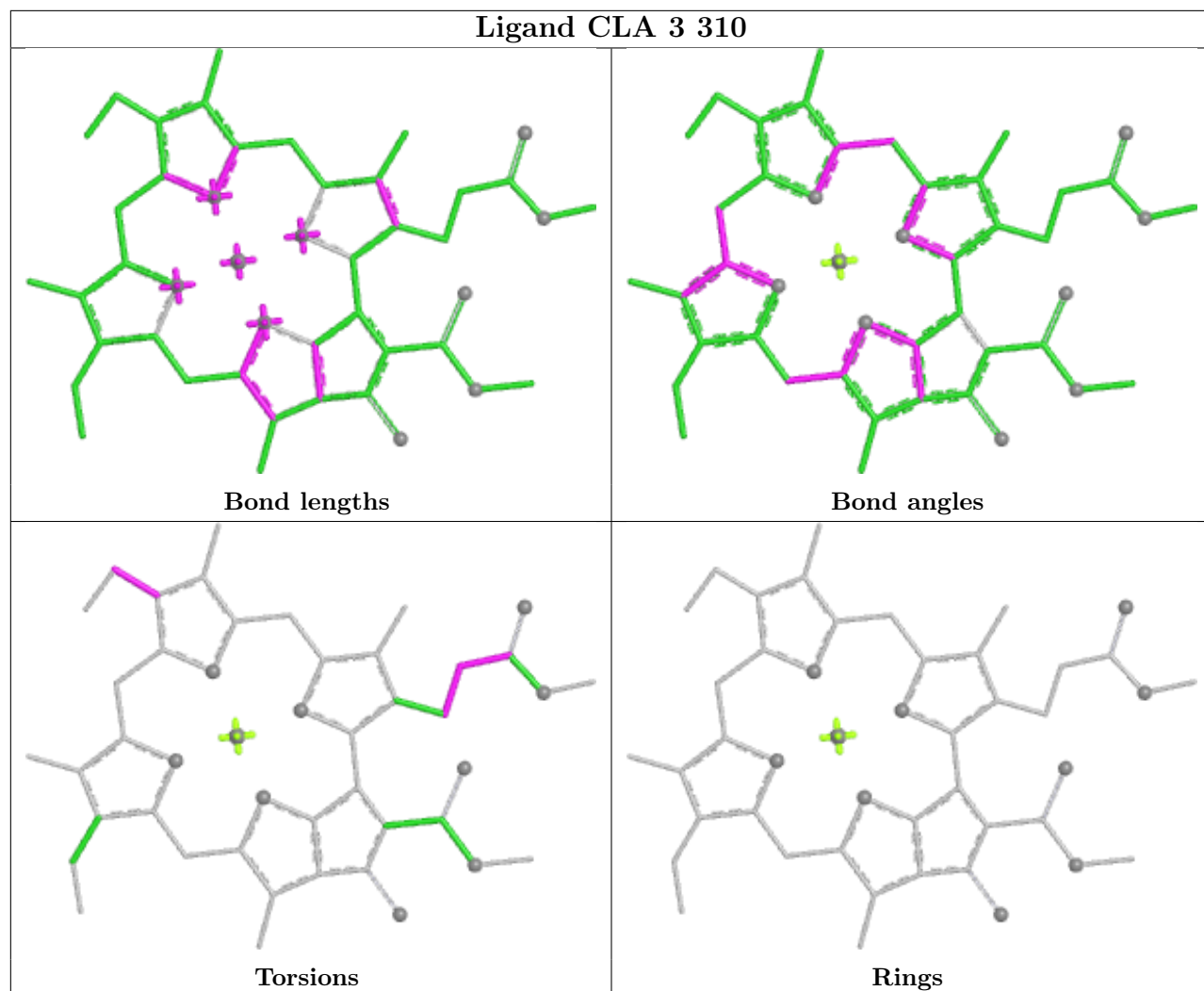


Rings

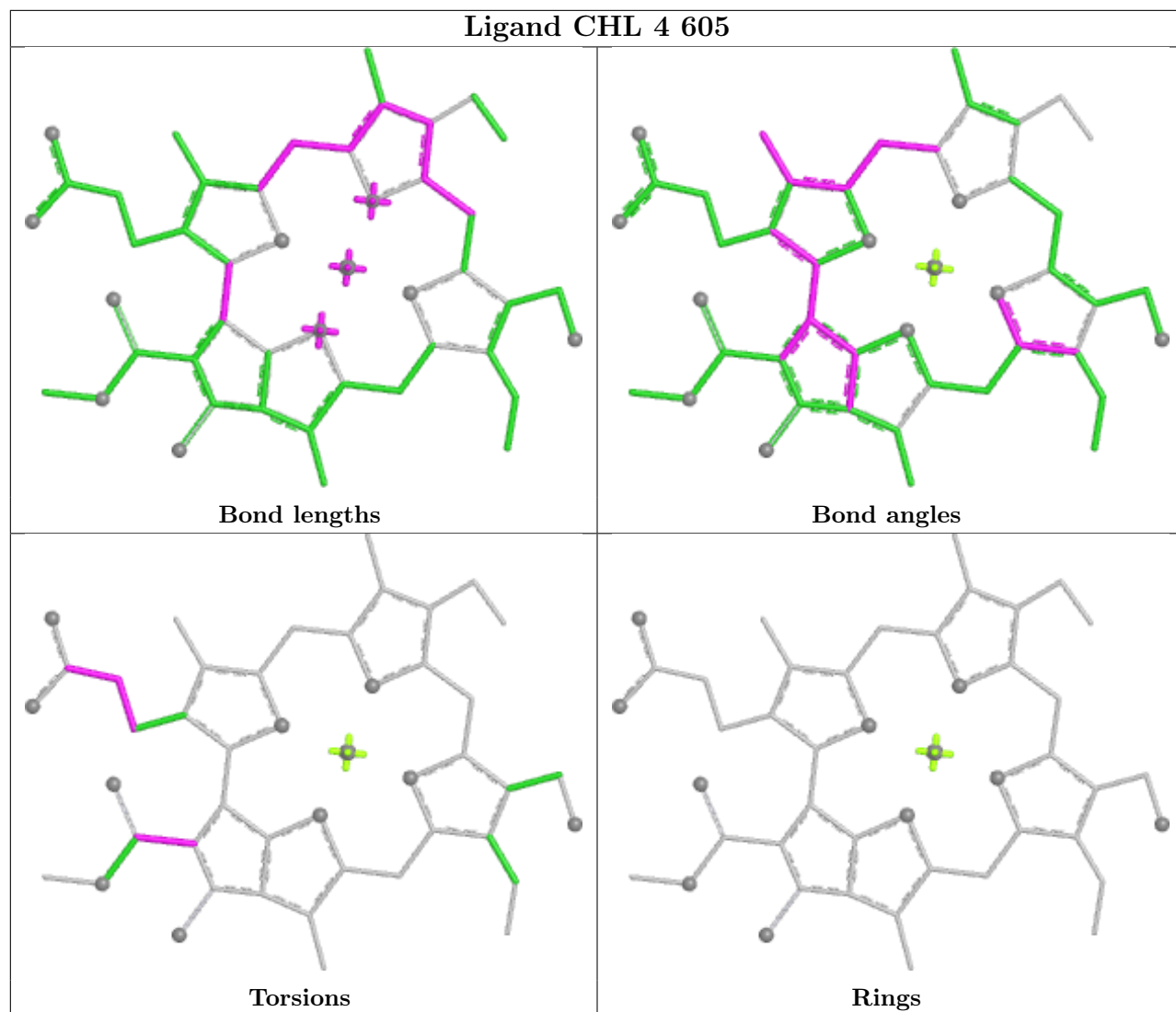
Ligand CLA 7 603



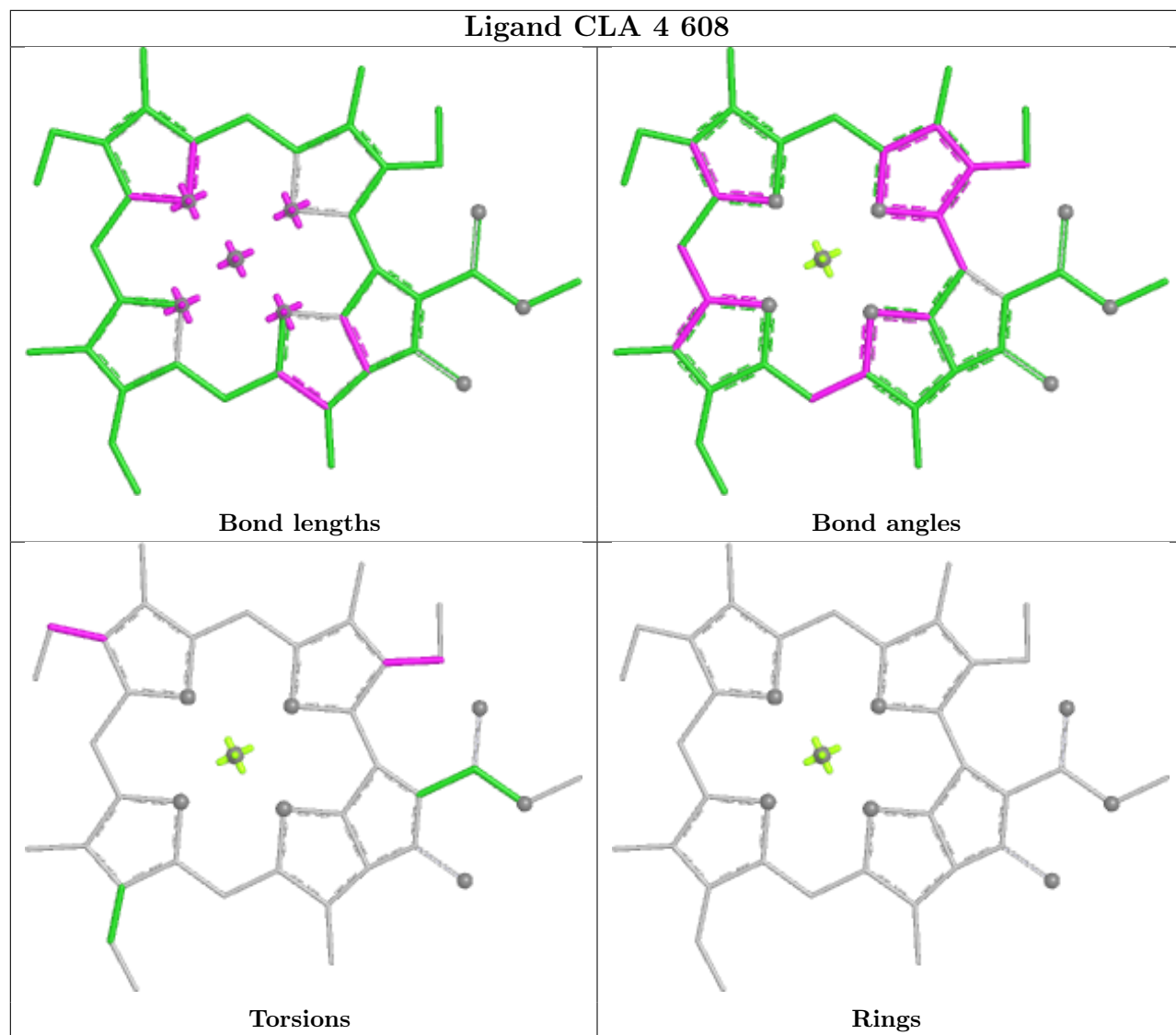
Ligand CLA 3 310



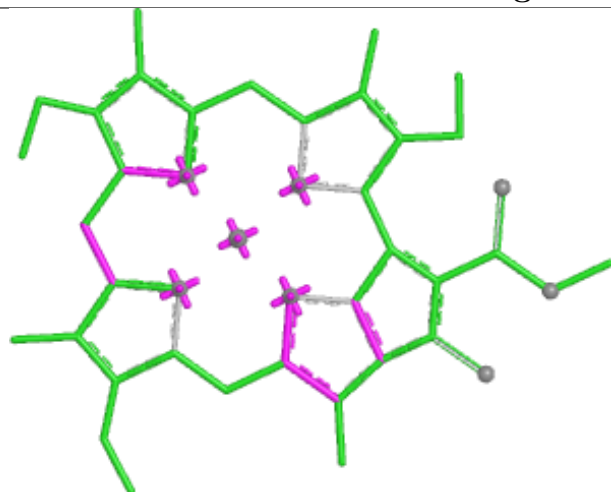
Ligand CHL 4 605



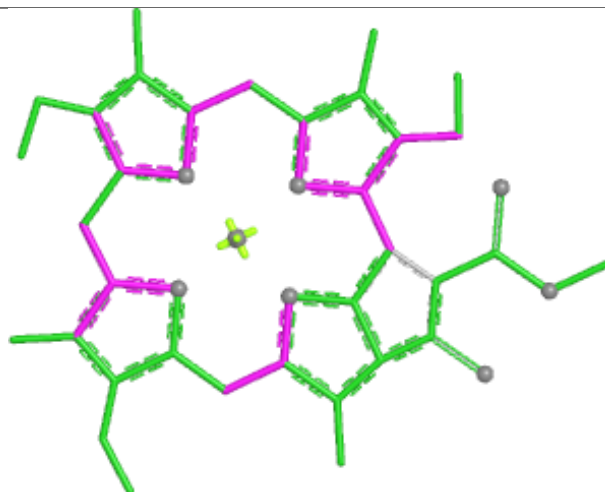
Ligand CLA 4 608



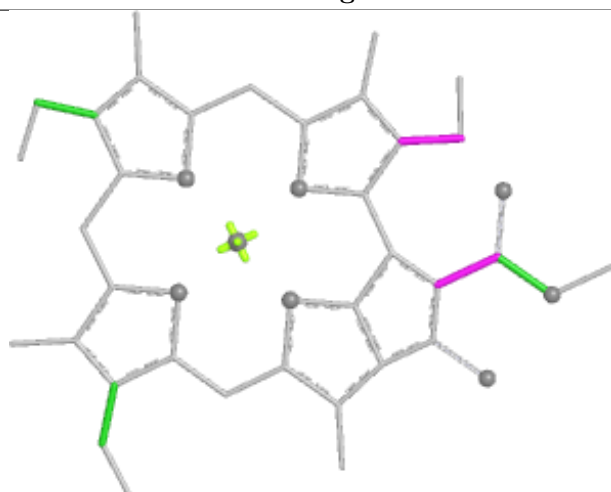
Ligand CLA A 844



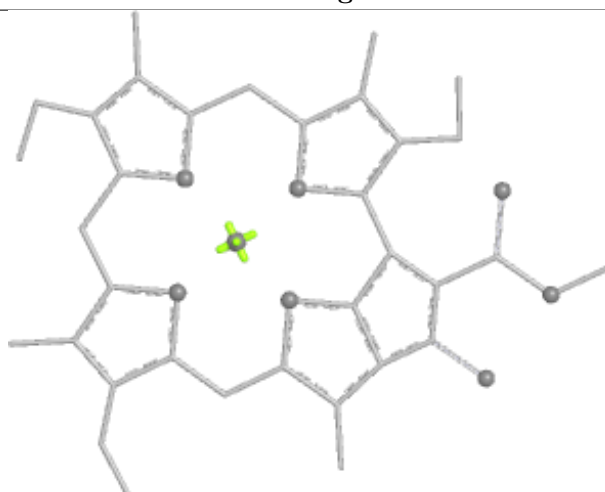
Bond lengths



Bond angles

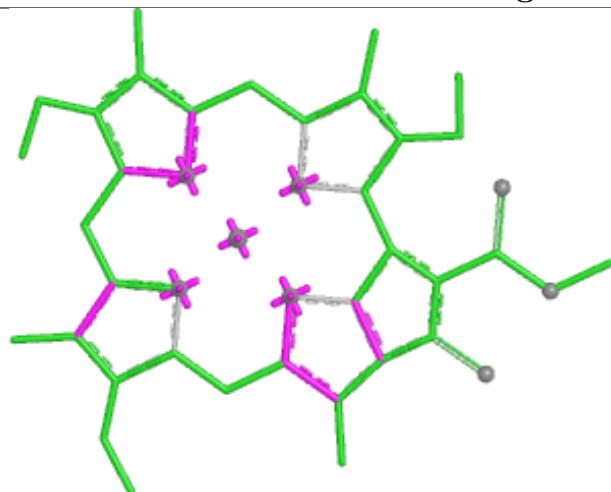


Torsions

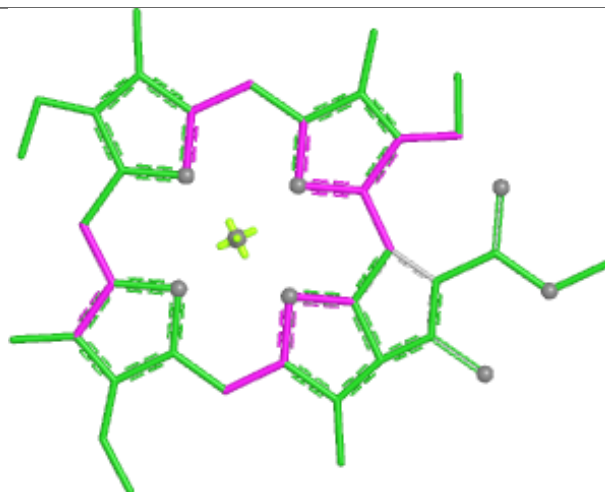


Rings

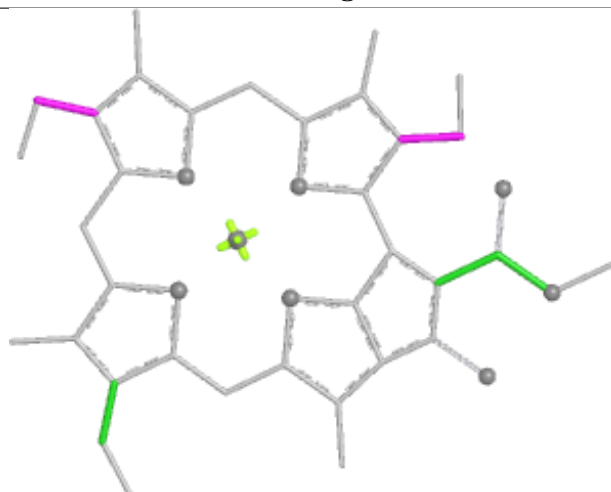
Ligand CLA Z 608



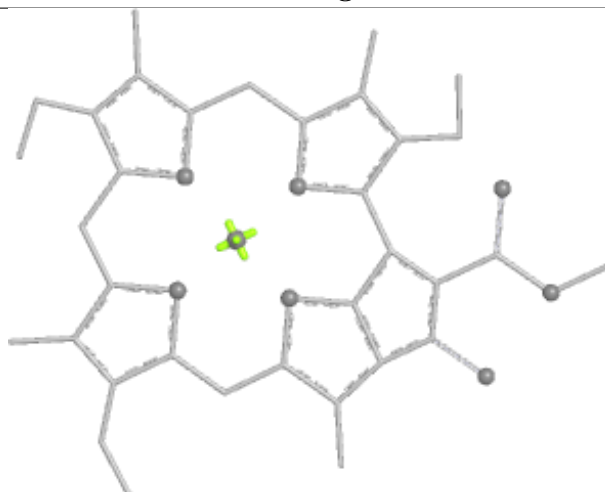
Bond lengths



Bond angles

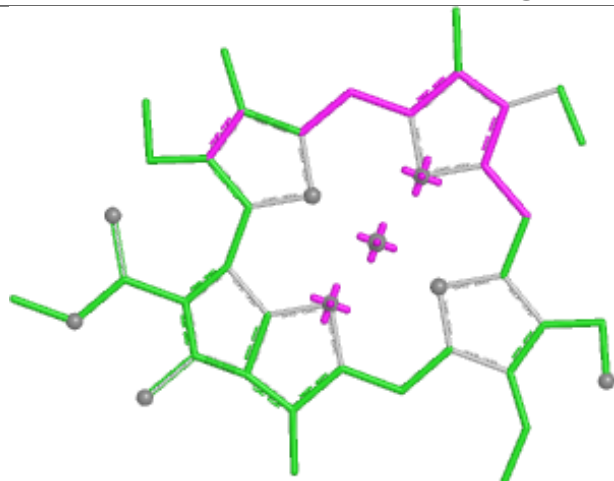


Torsions

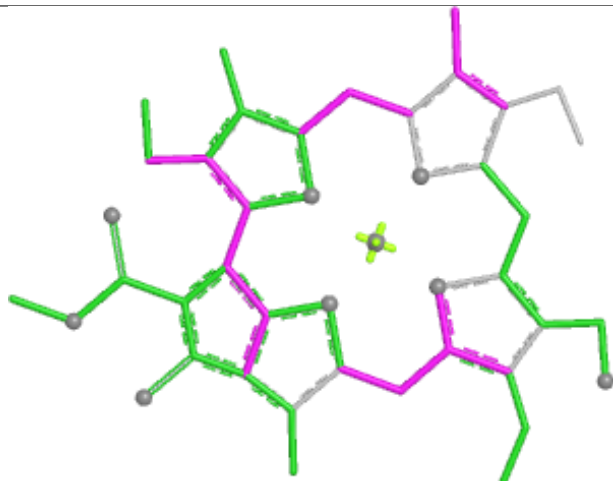


Rings

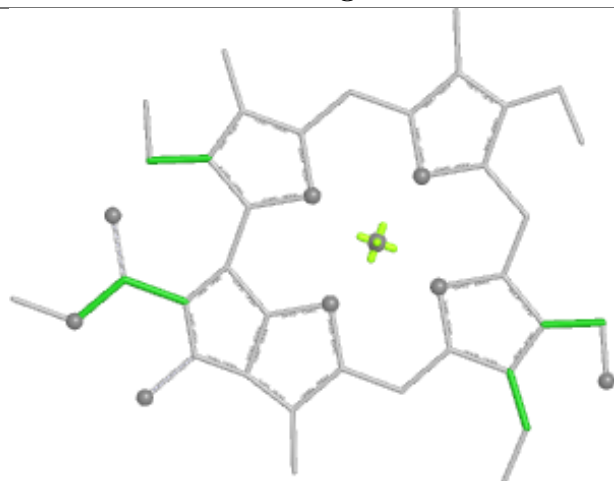
Ligand CHL 6 305



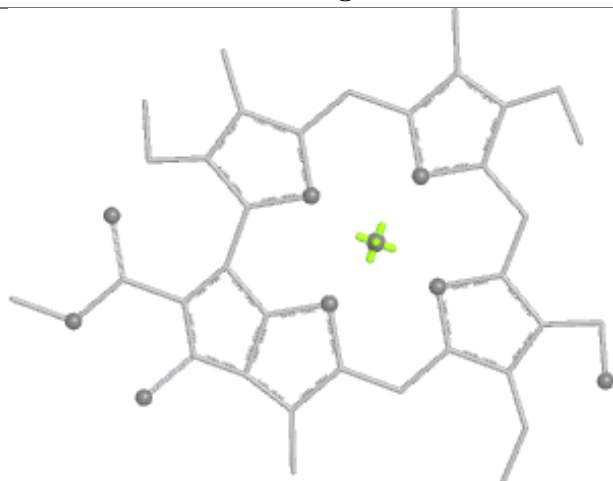
Bond lengths



Bond angles

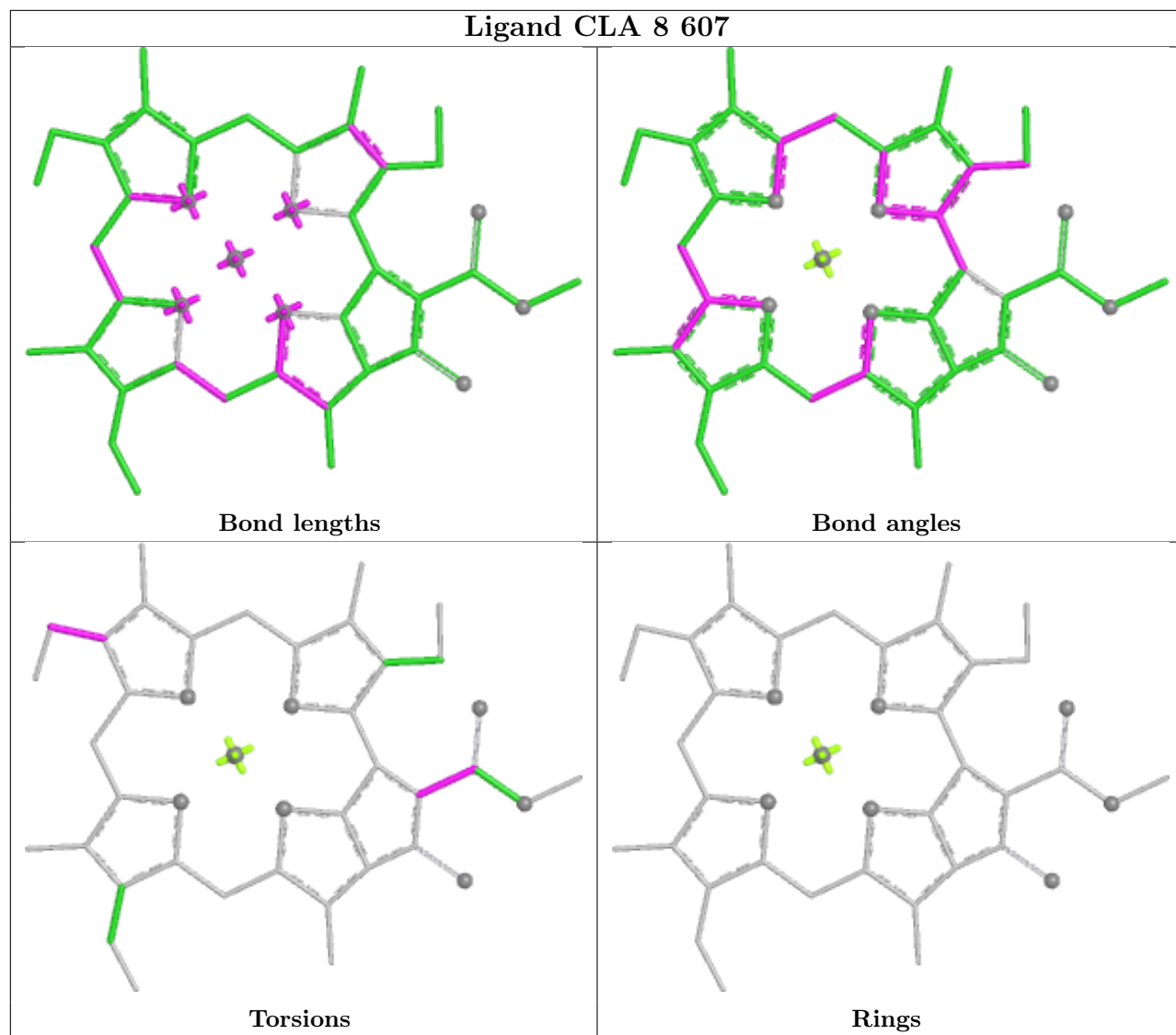


Torsions

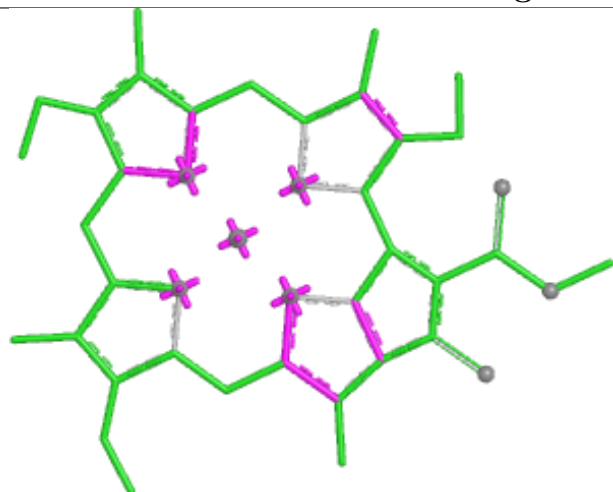


Rings

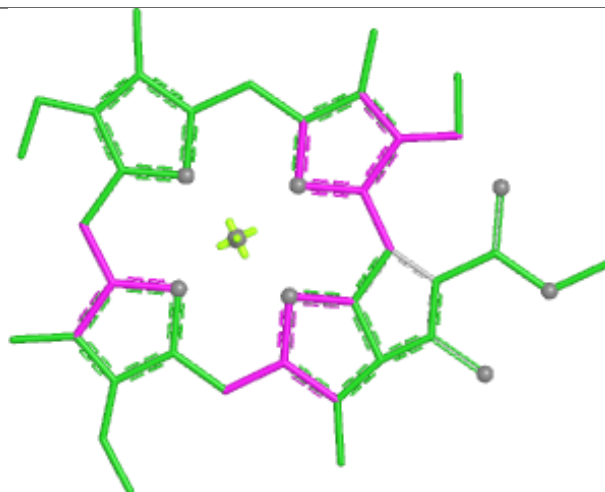
Ligand CLA 8 607



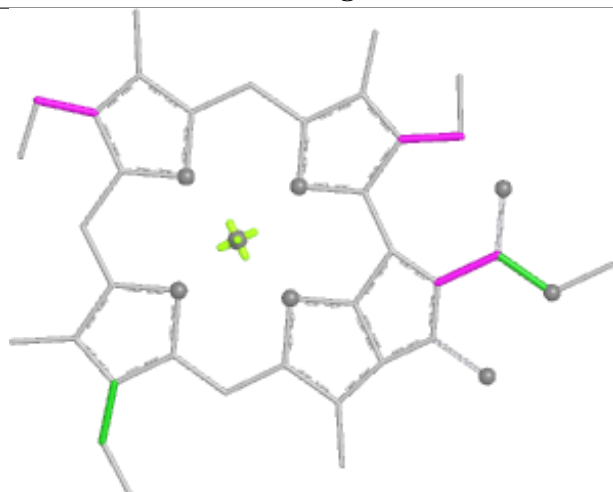
Ligand CLA B 815



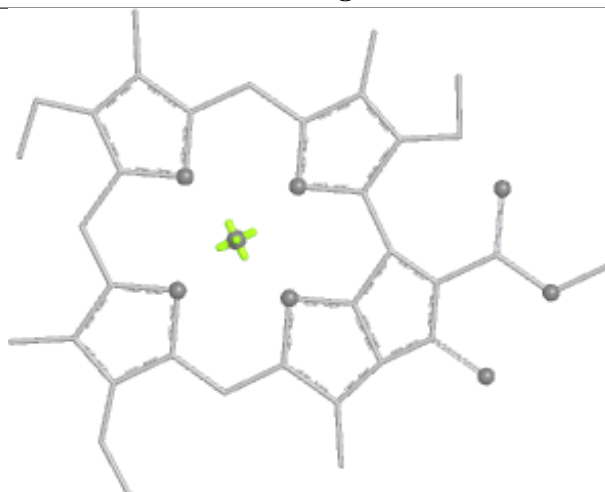
Bond lengths



Bond angles

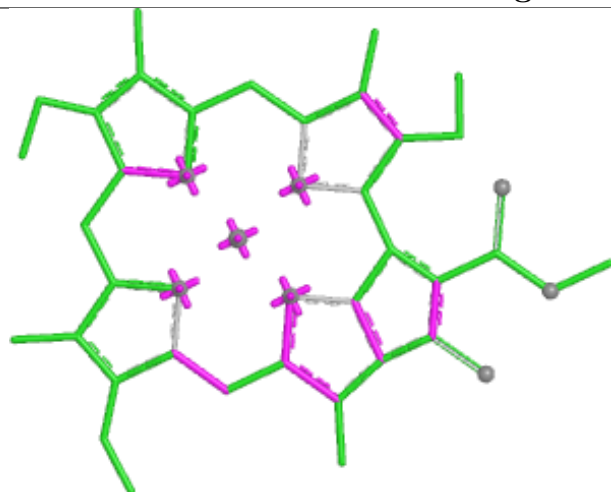


Torsions

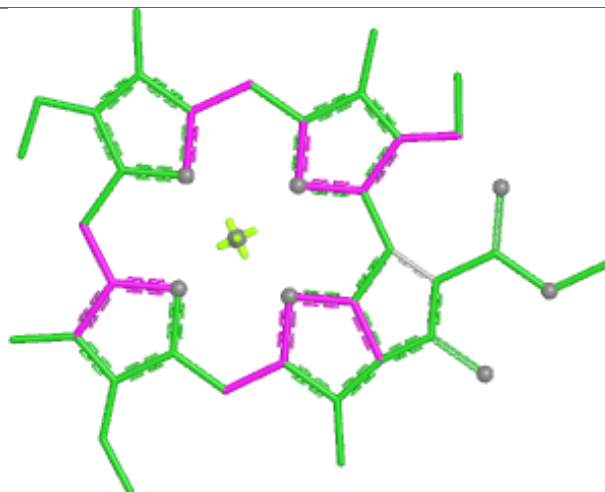


Rings

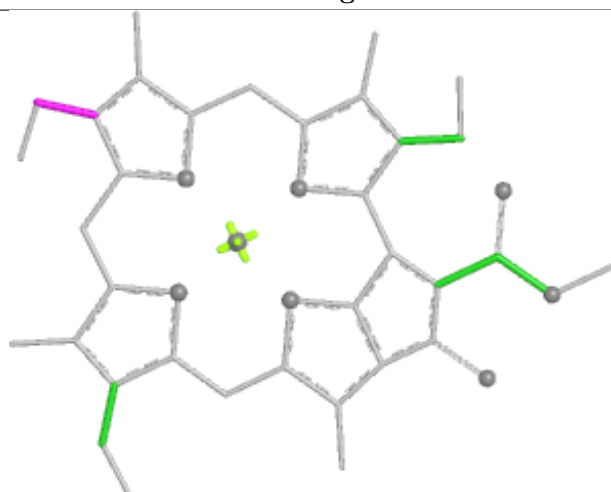
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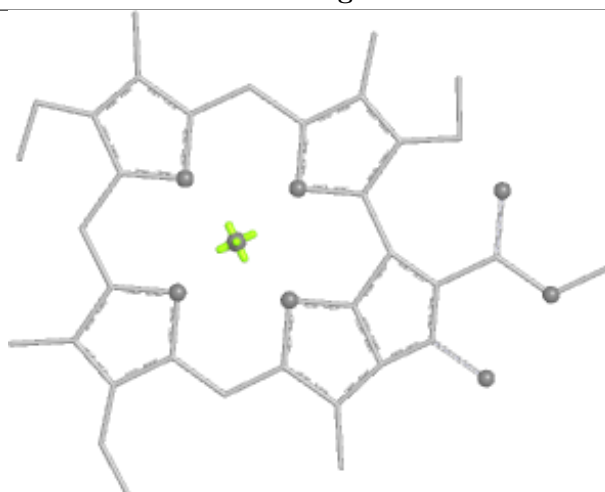
Bond lengths



Bond angles

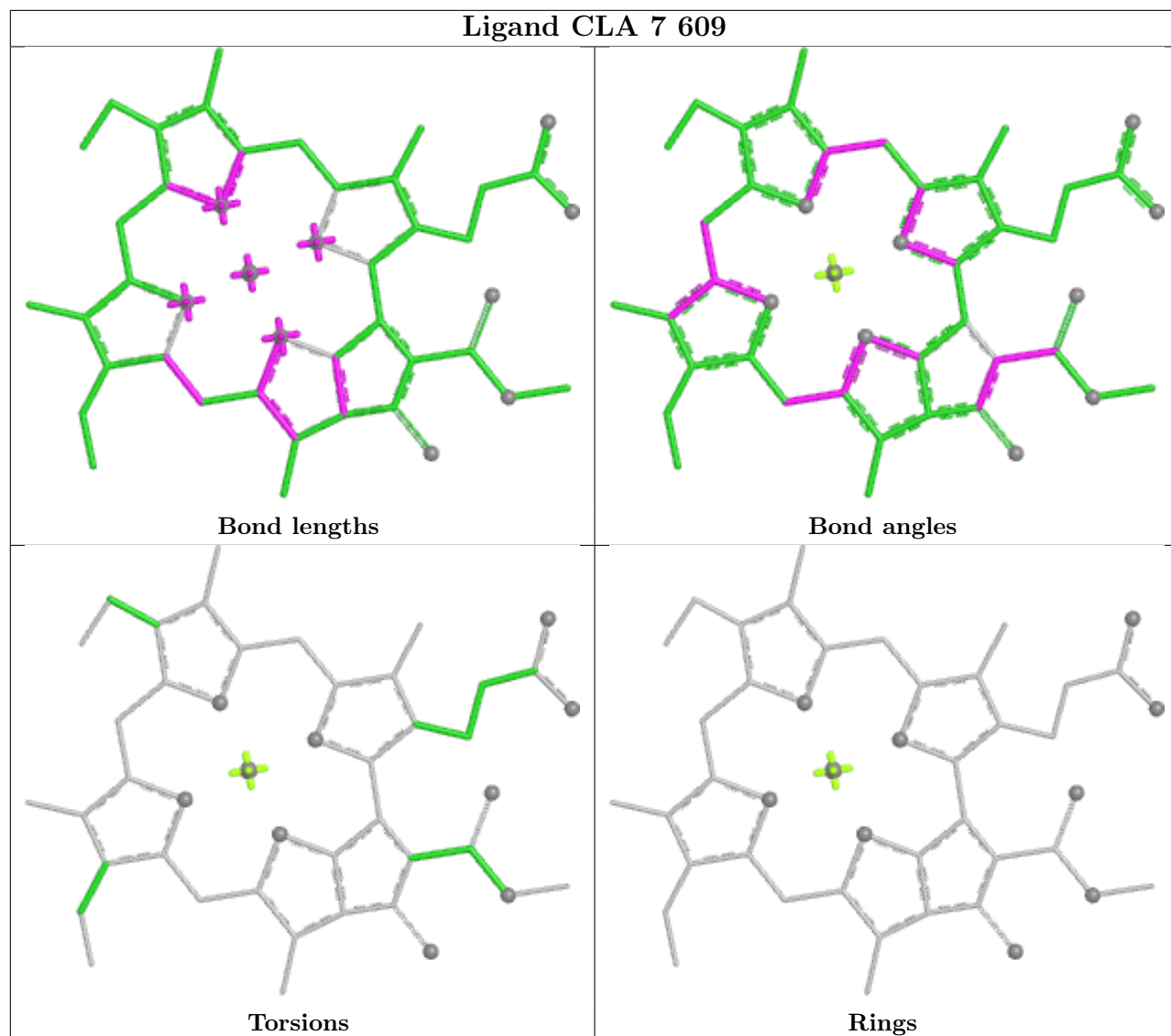


Torsions

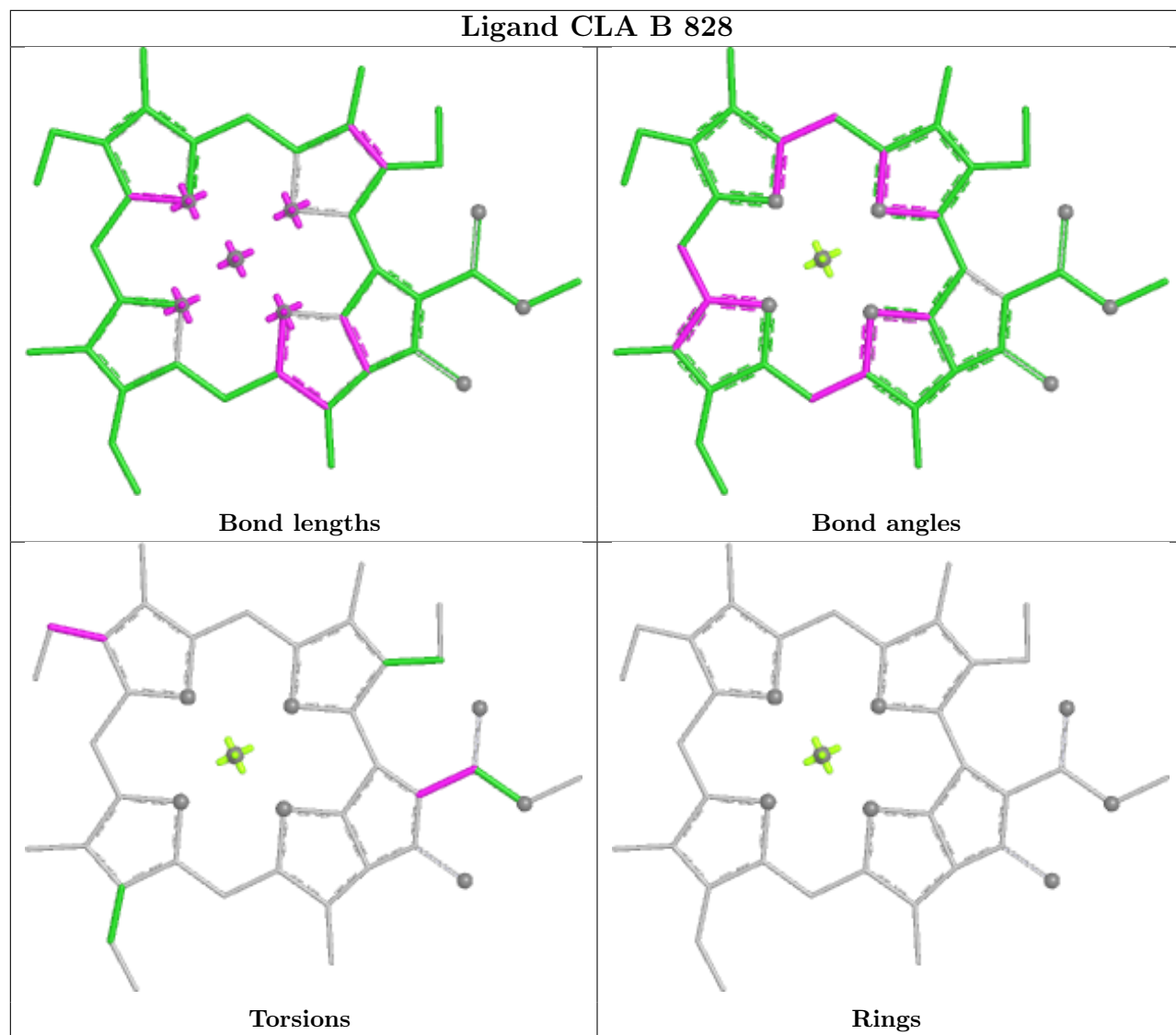


Rings

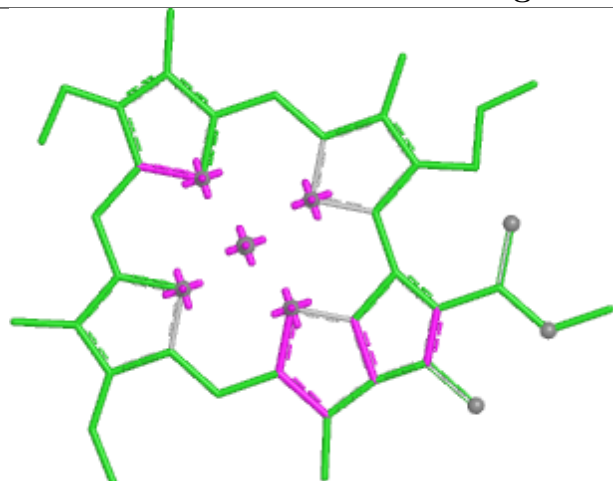
Ligand CLA 7 609



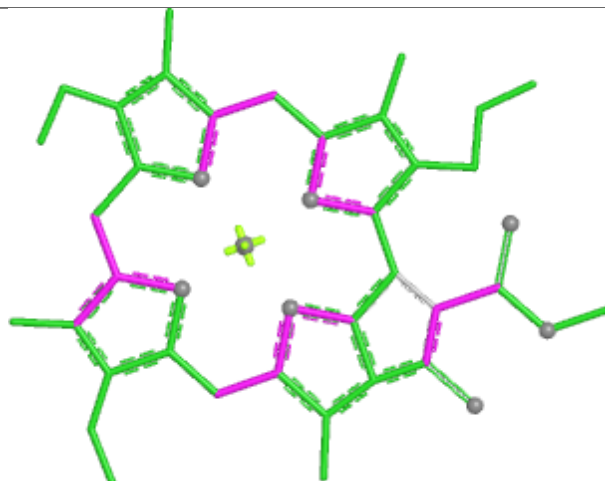
Ligand CLA B 828



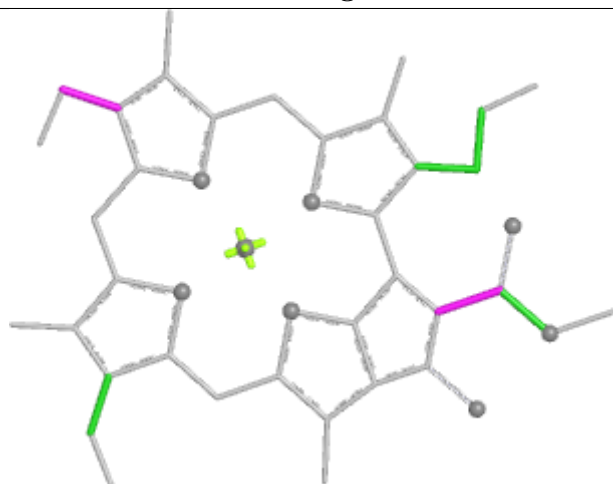
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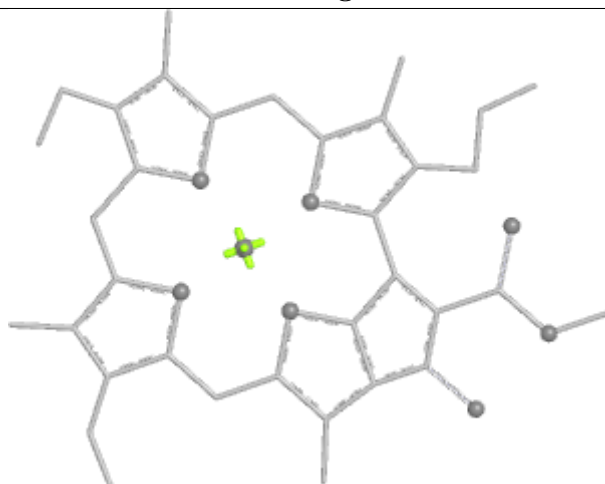
Bond lengths



Bond angles

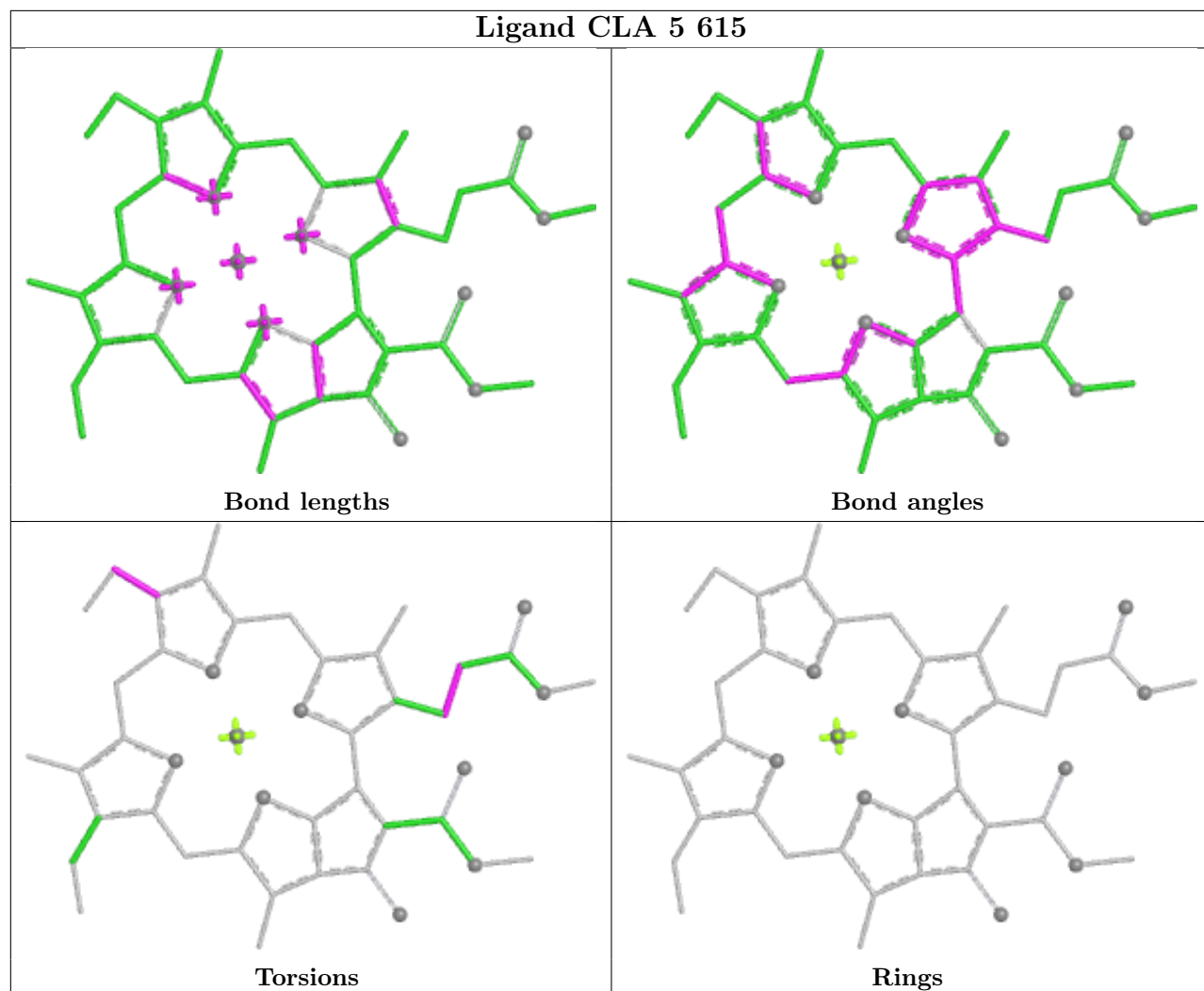


Torsions

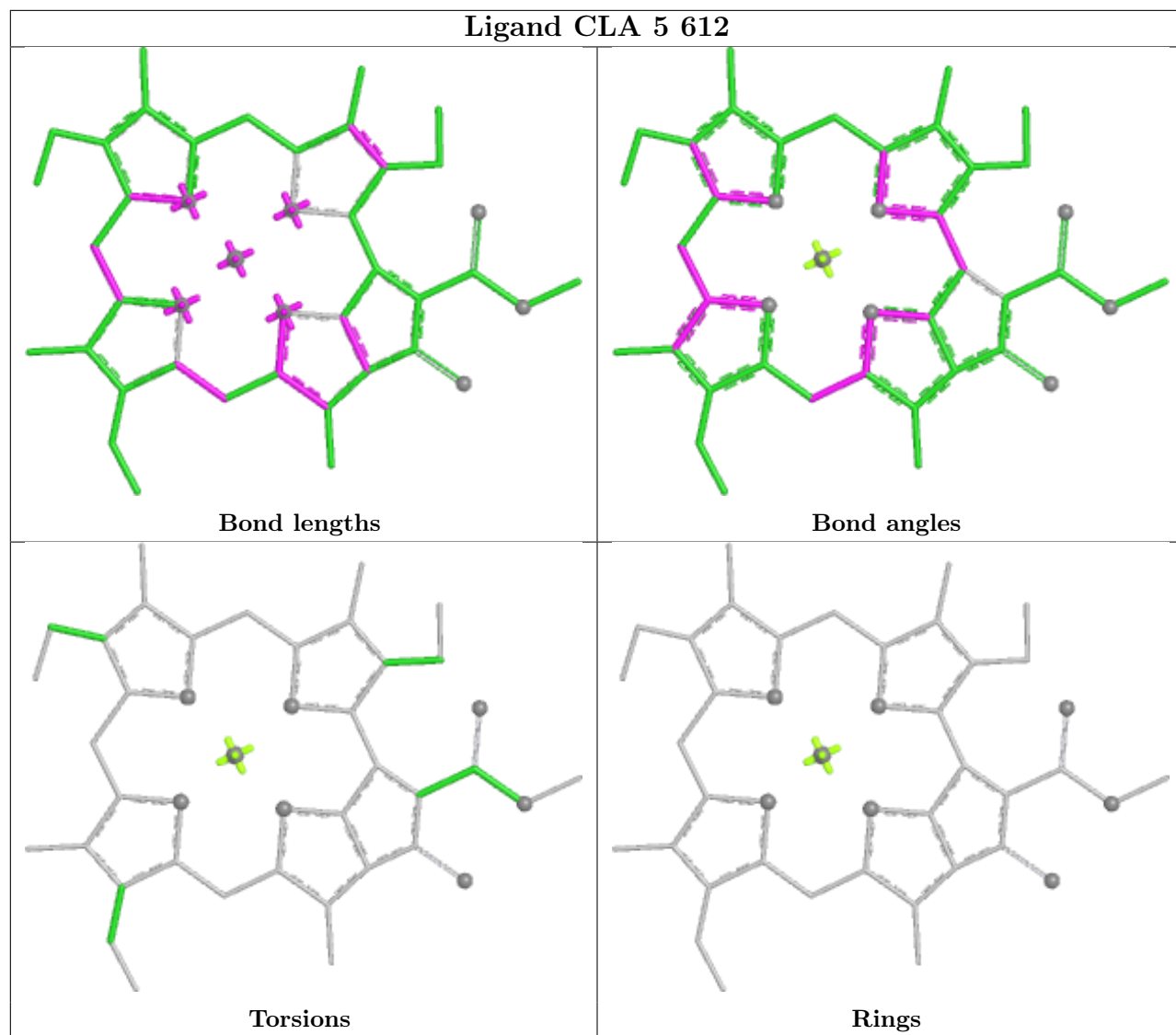


Rings

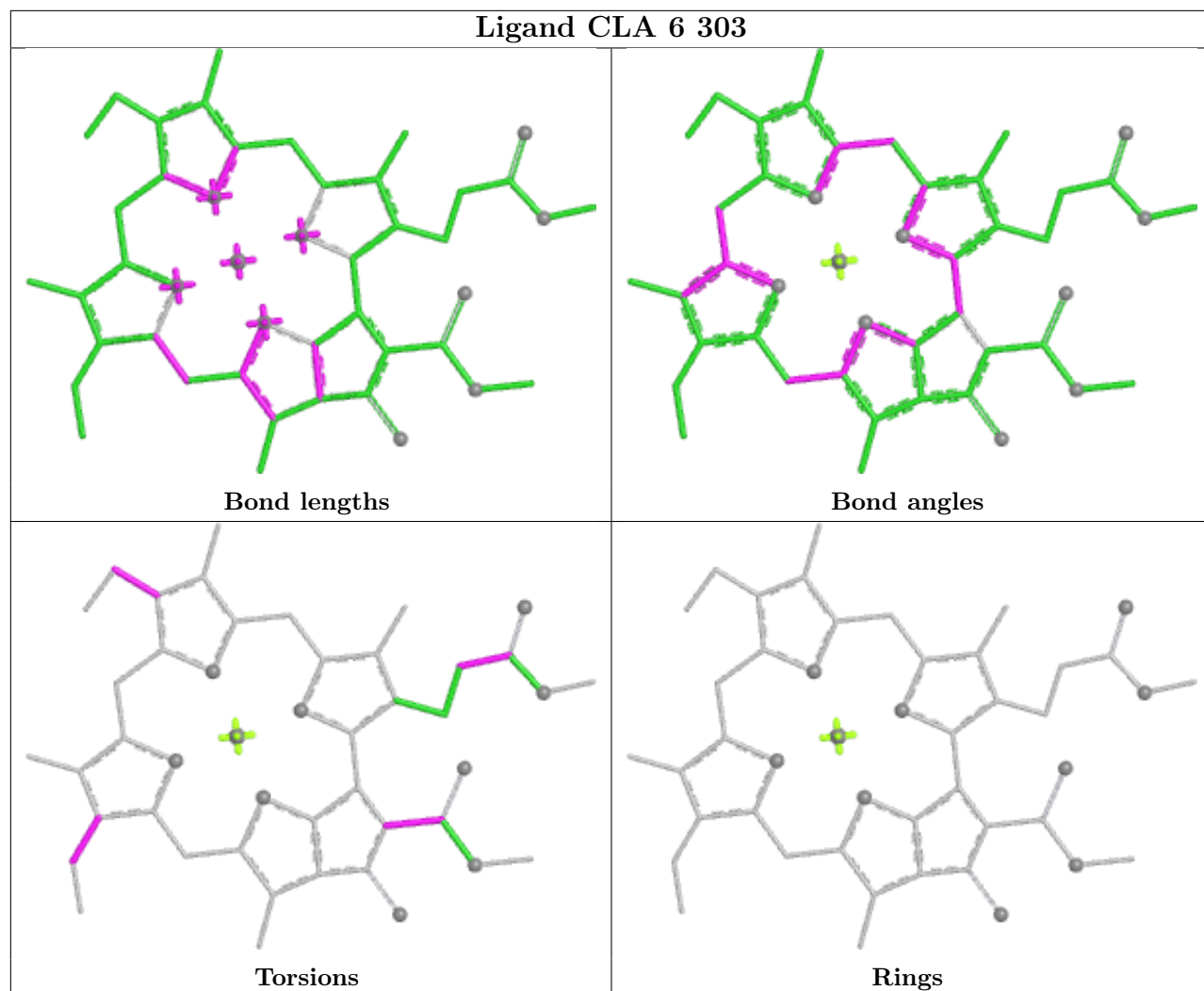
Ligand CLA 5 615

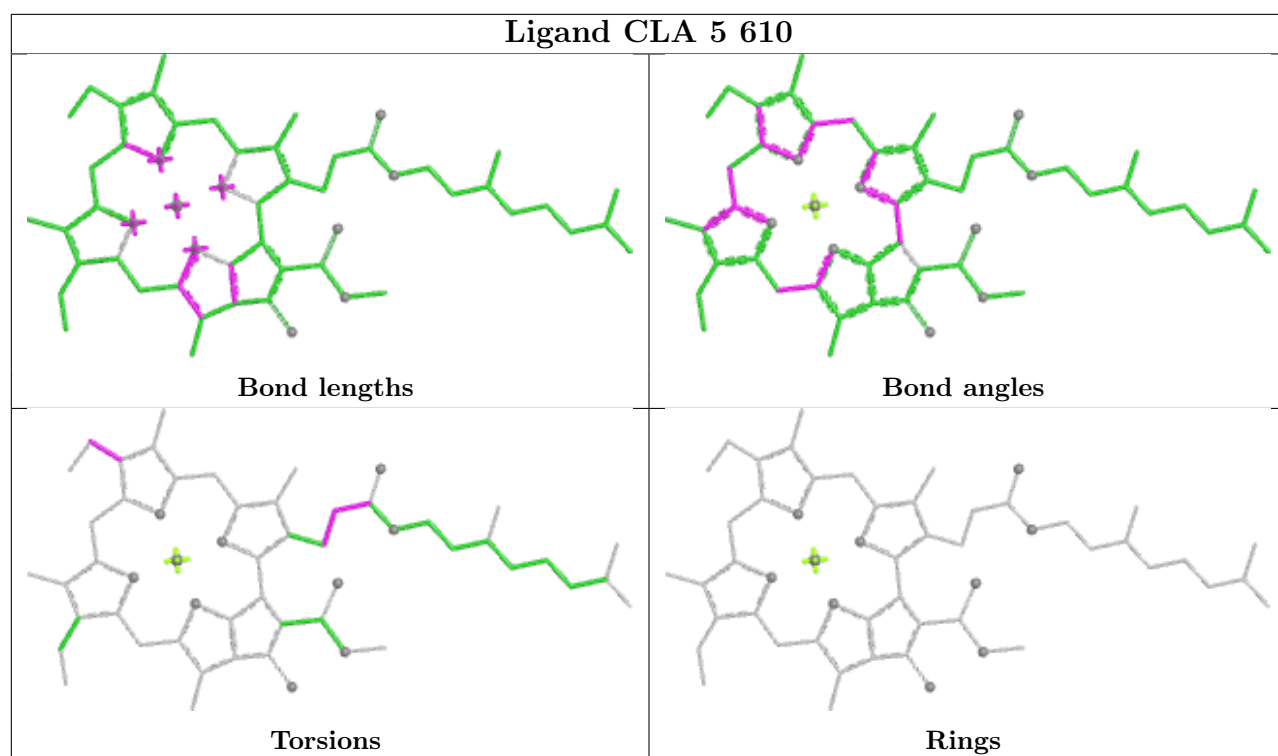


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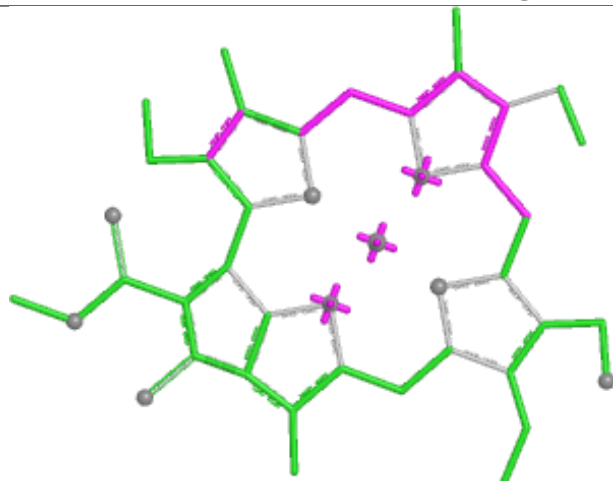


Ligand CLA 6 303

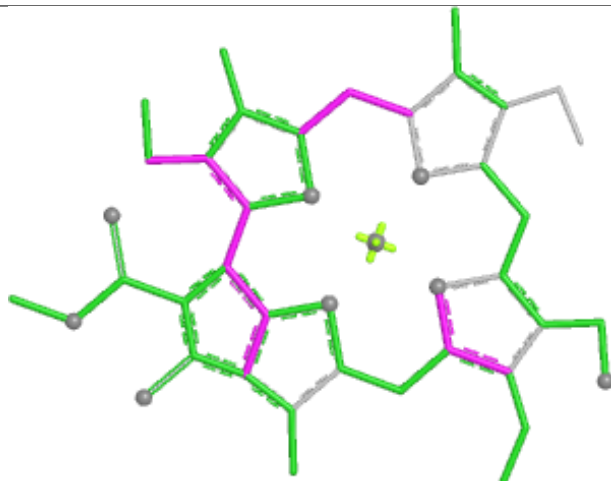




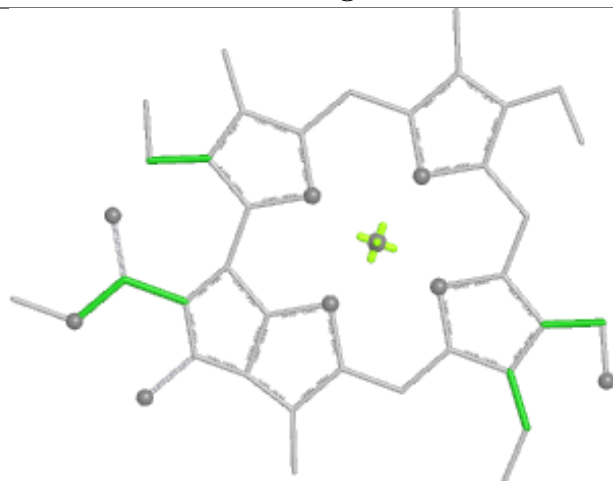
Ligand CHL Z 601



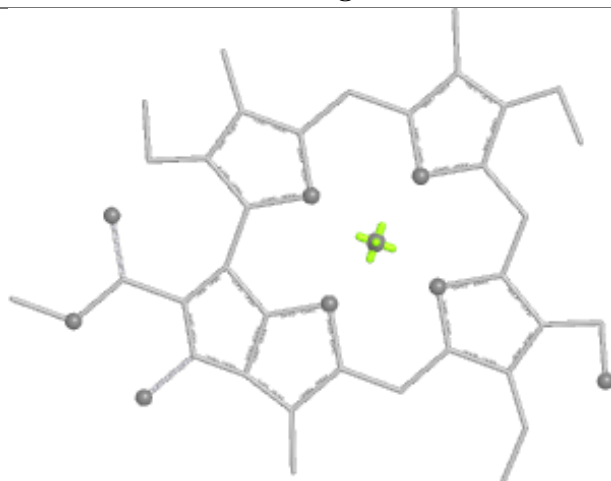
Bond lengths



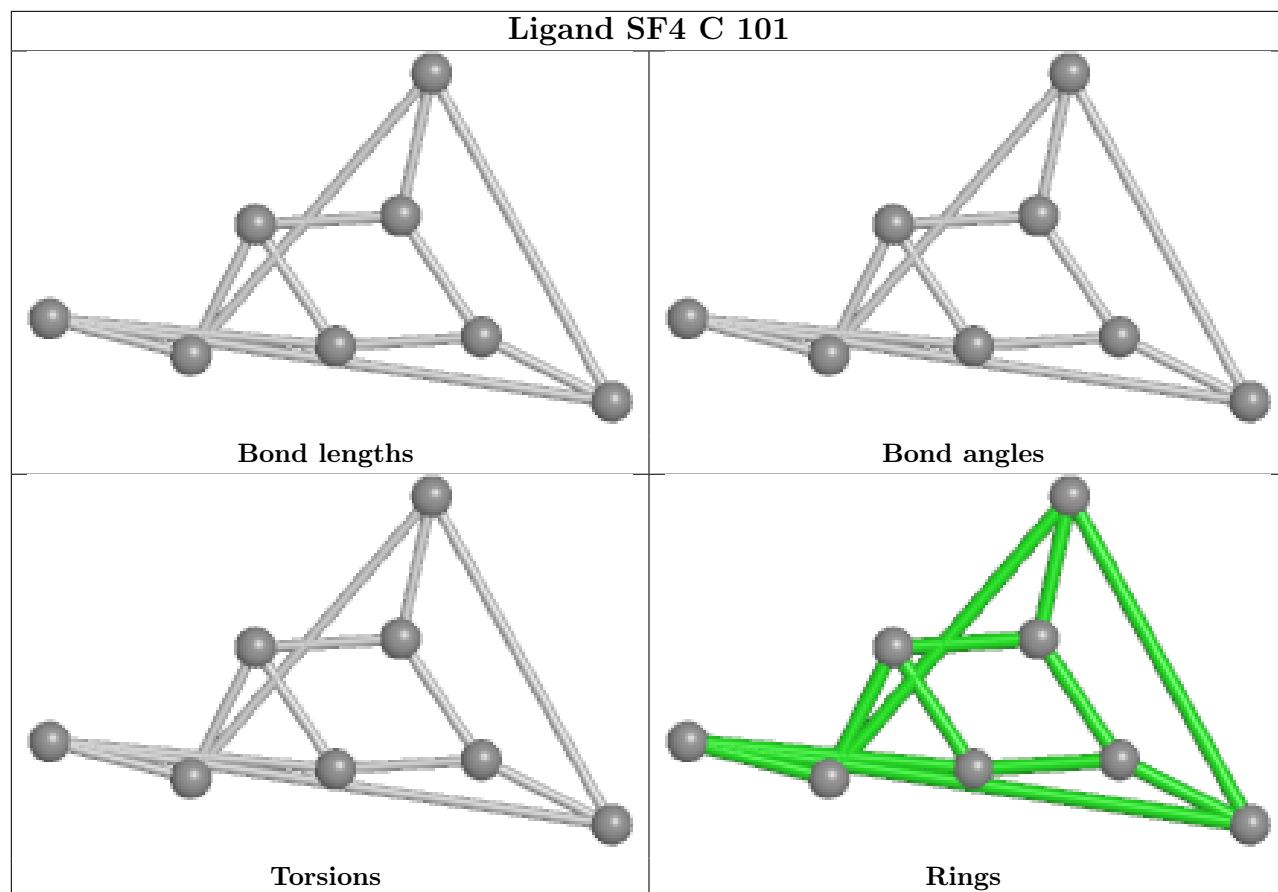
Bond angles



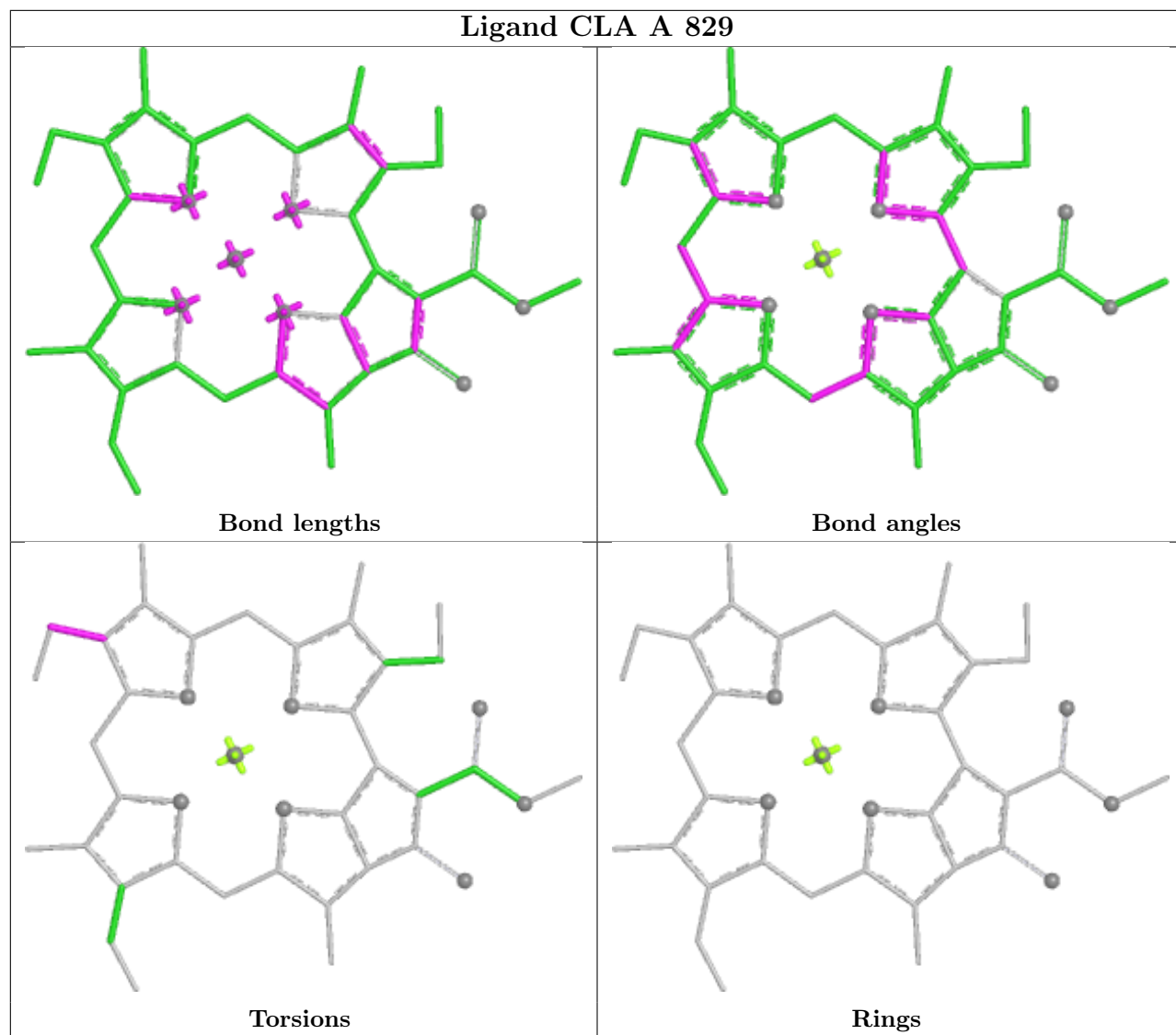
Torsions



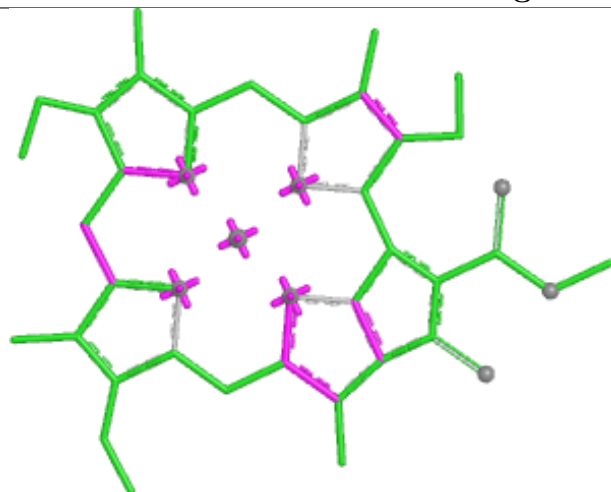
Rings



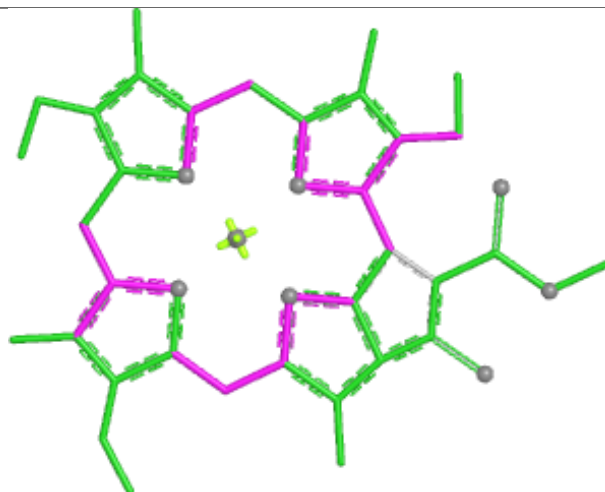
Ligand CLA A 829



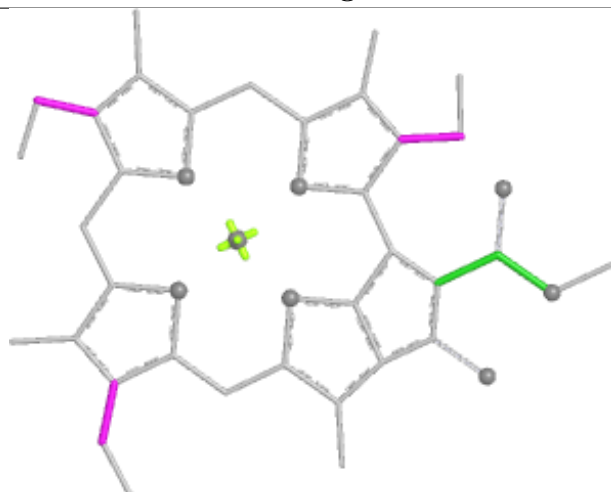
Ligand CLA A 807



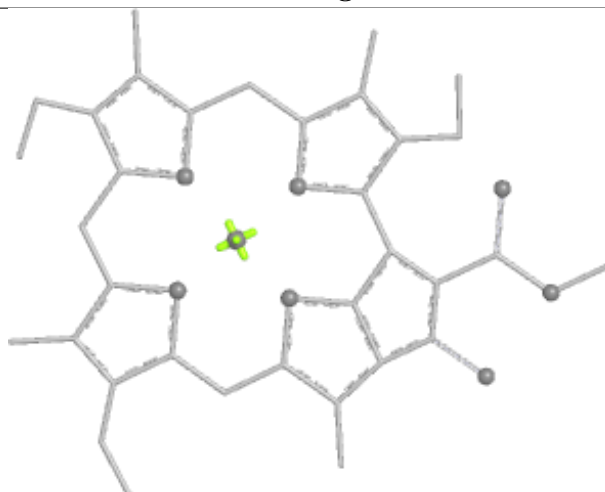
Bond lengths



Bond angles

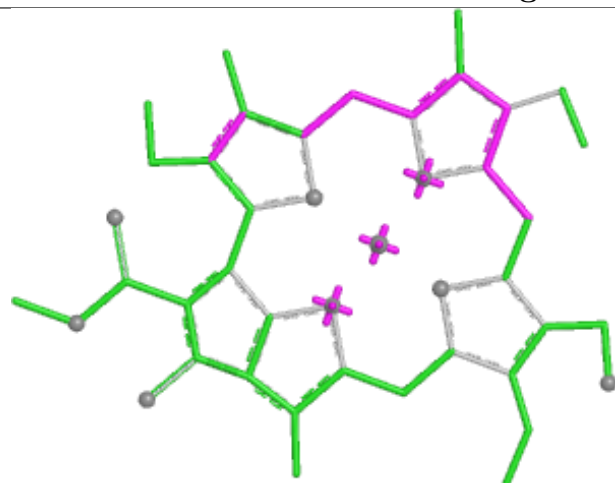


Torsions

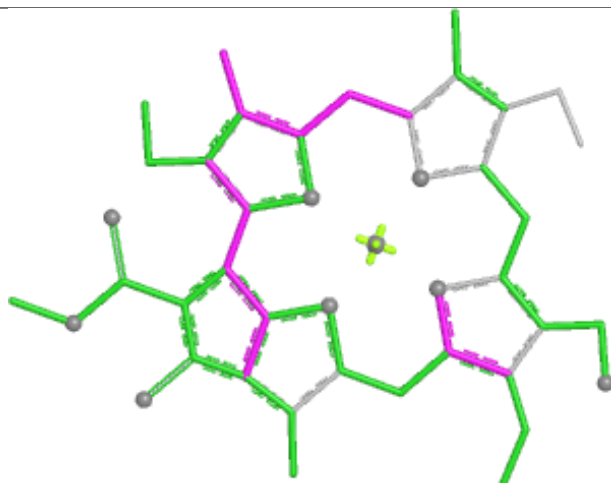


Rings

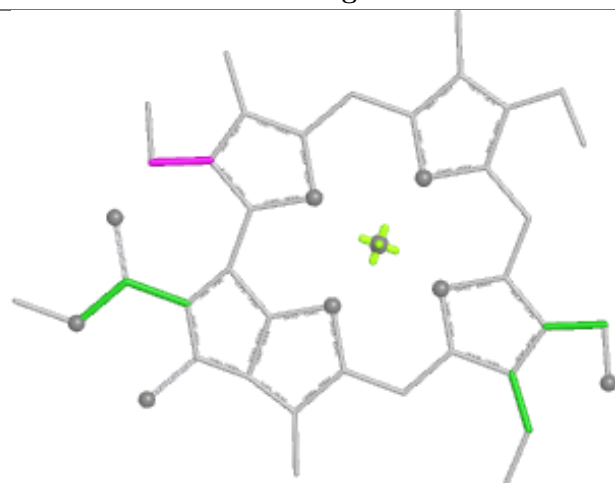
Ligand CHL 3 306



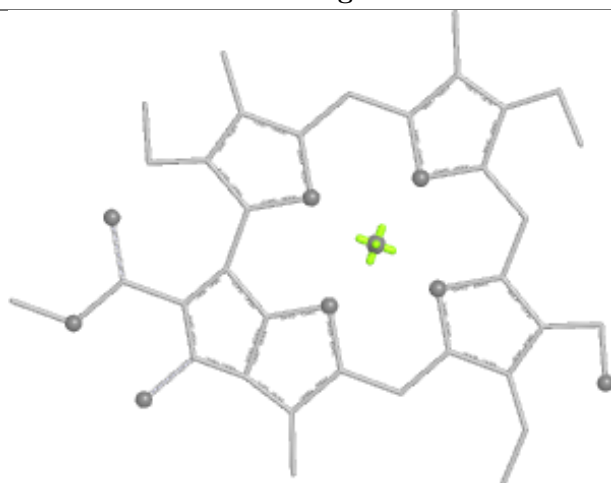
Bond lengths



Bond angles

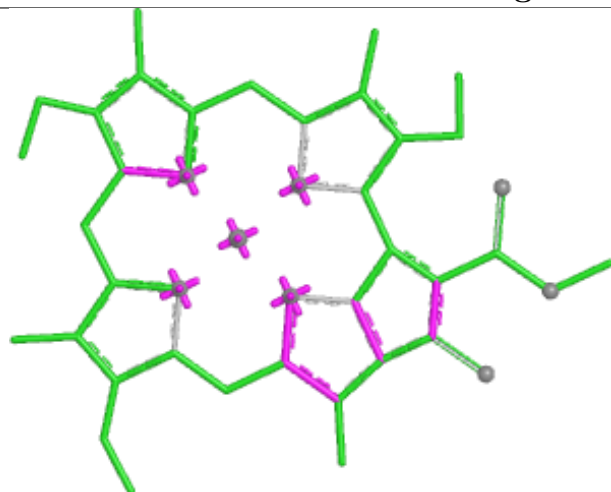


Torsions

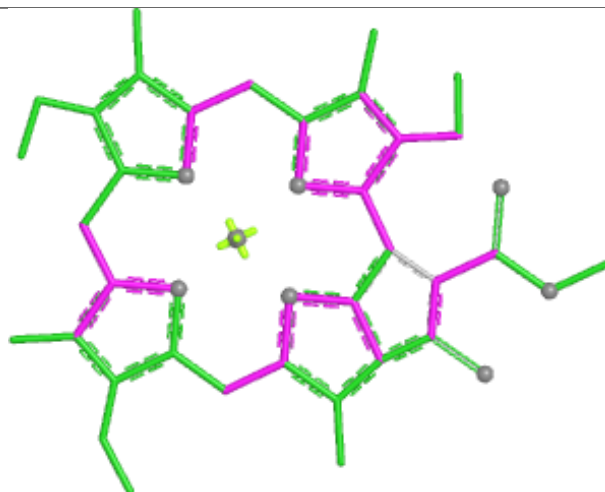


Rings

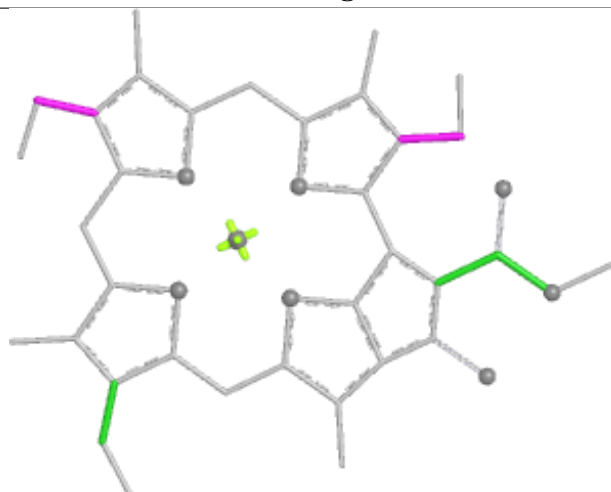
Ligand CLA B 827



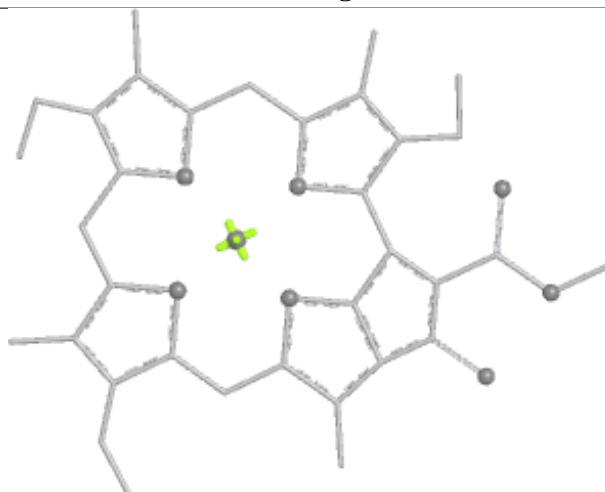
Bond lengths



Bond angles

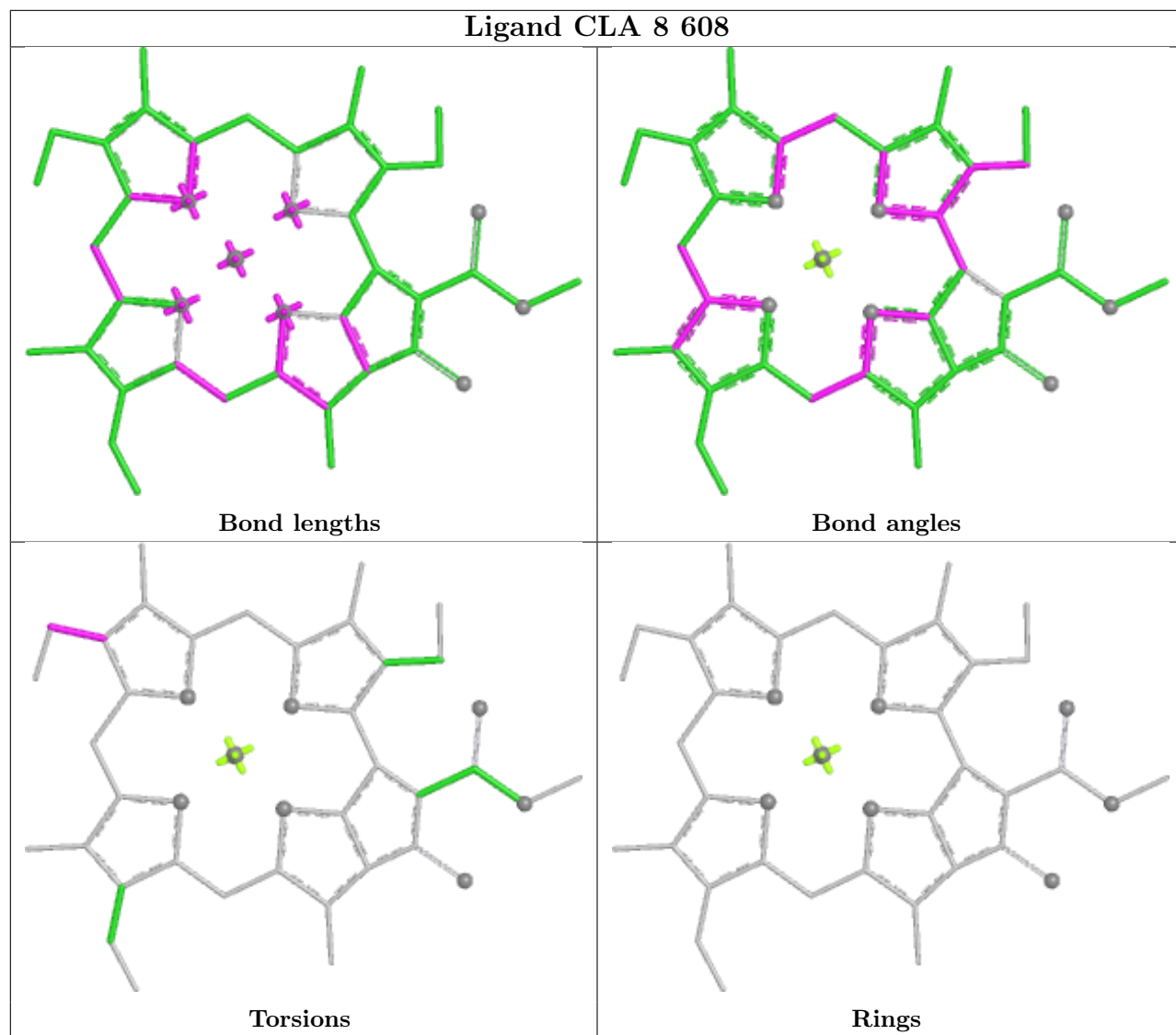


Torsions

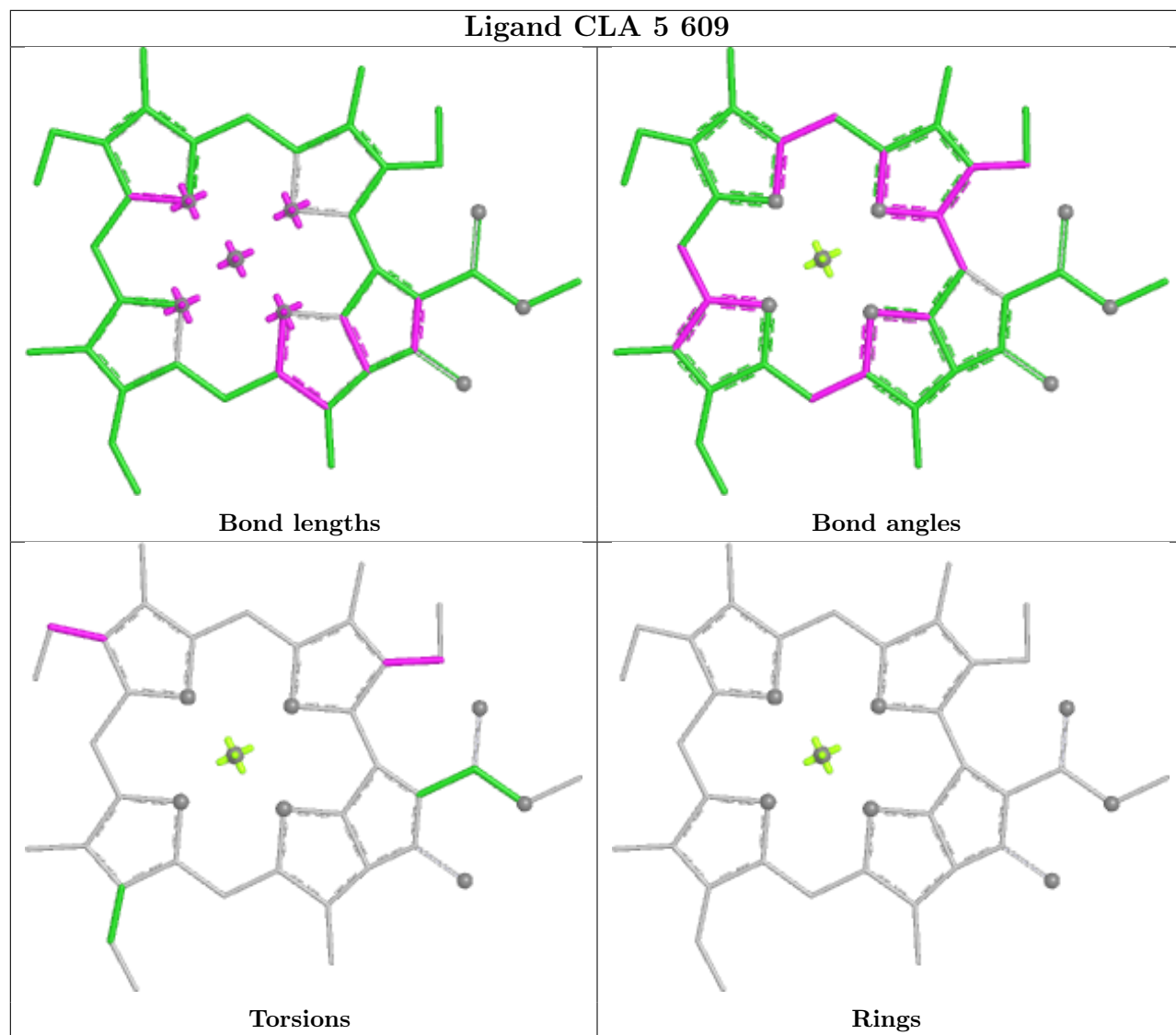


Rings

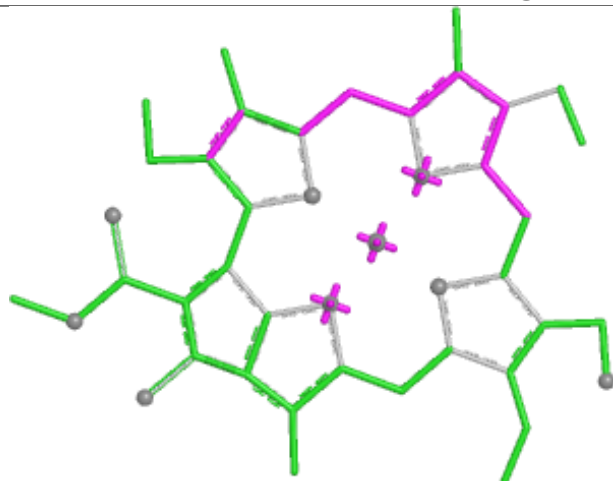
Ligand CLA 8 608



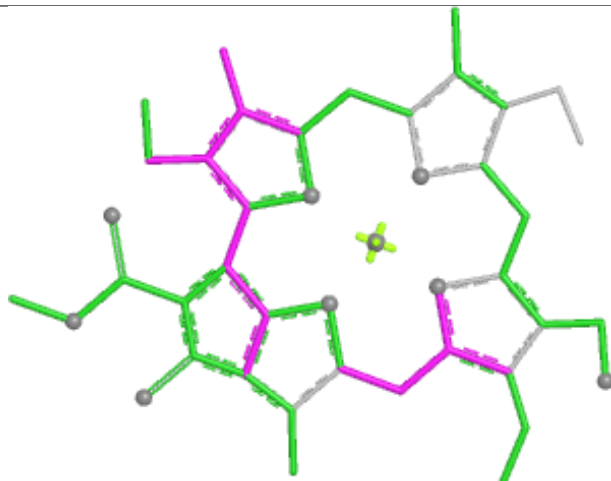
Ligand CLA 5 609



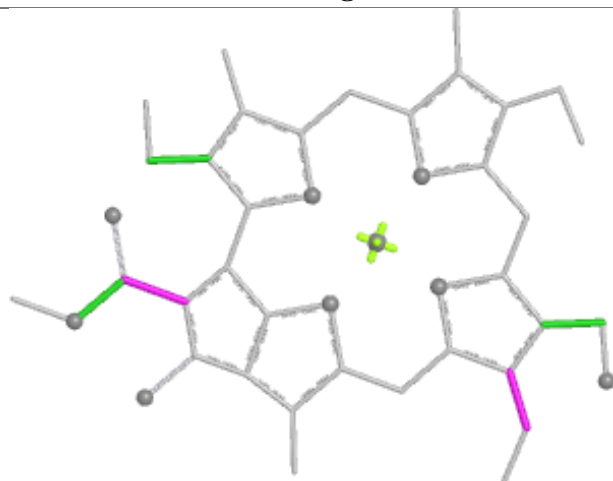
Ligand CHL 4 604



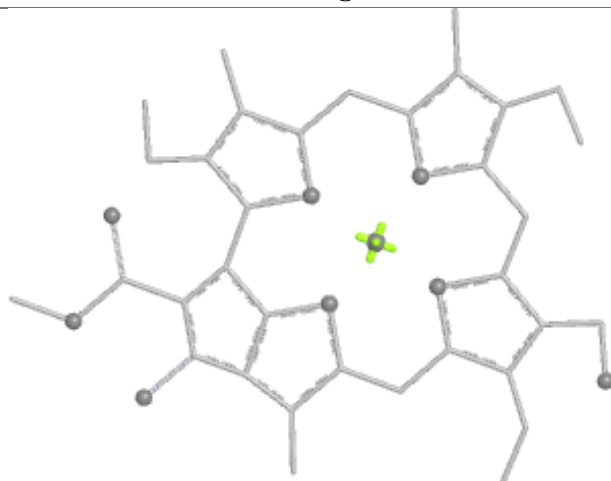
Bond lengths



Bond angles

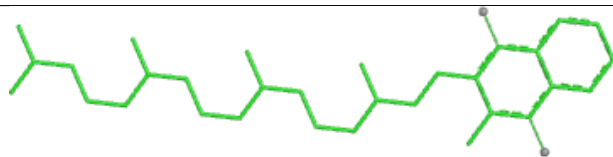


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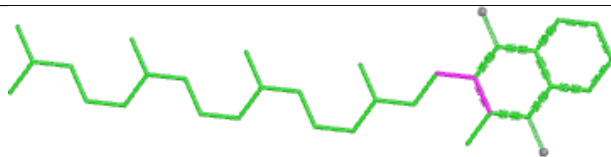


Rings

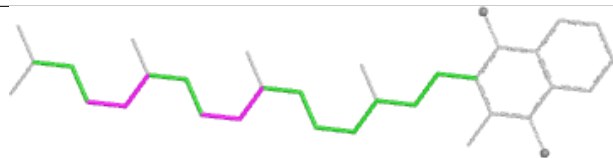
Ligand PQN A 842



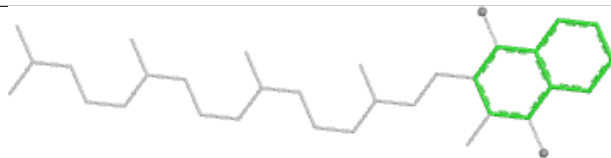
Bond lengths



Bond angles

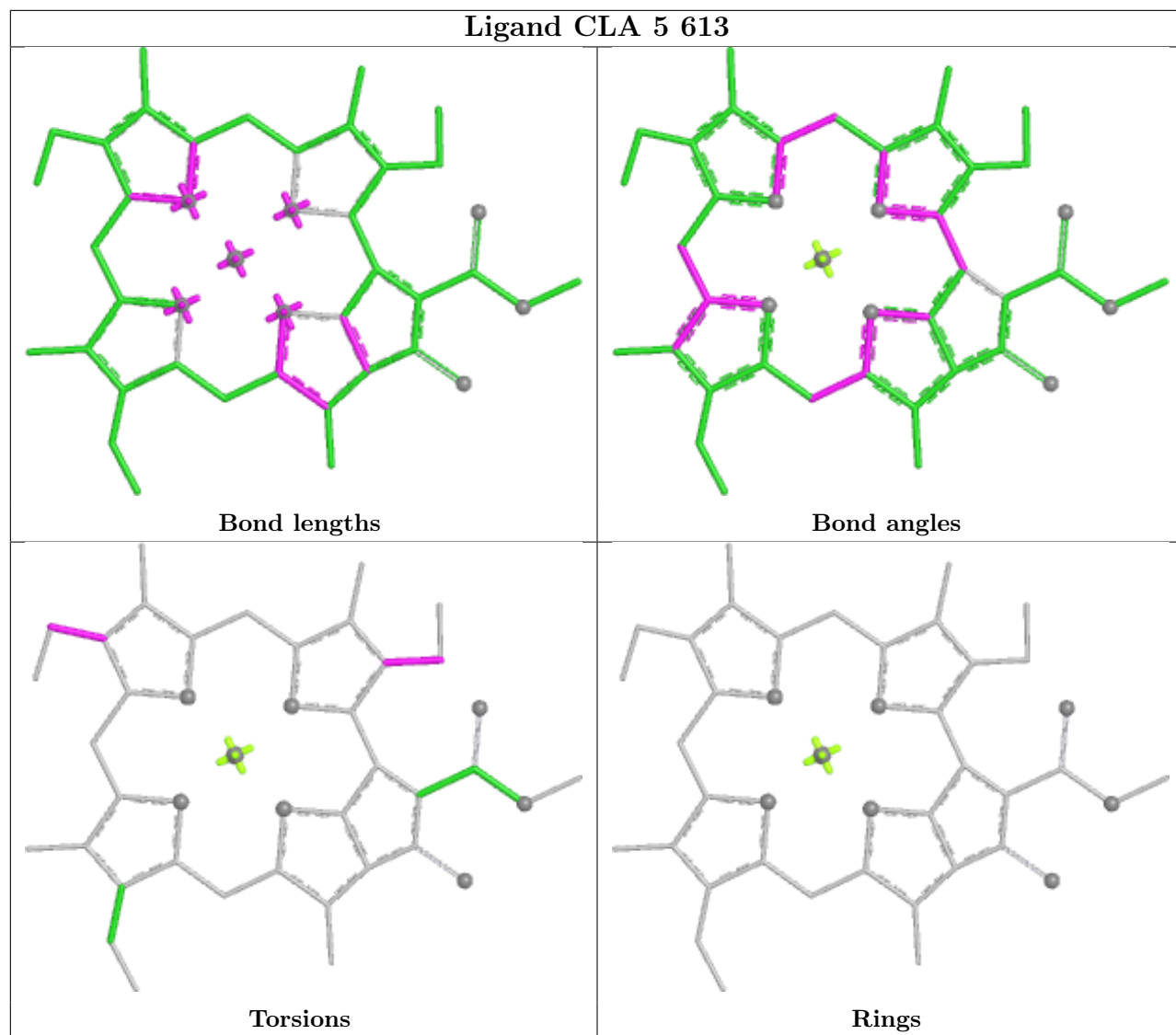


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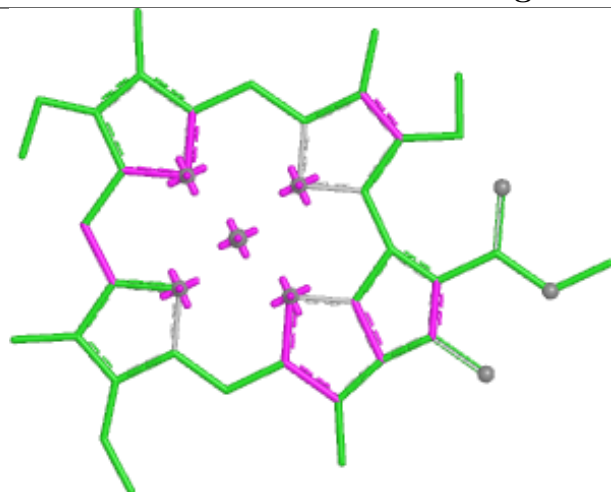


Rings

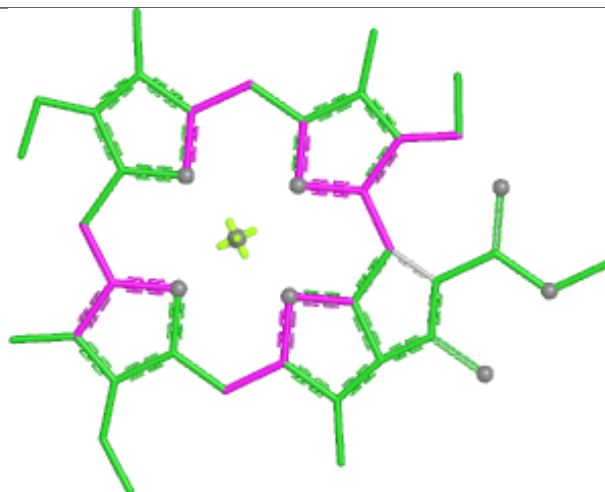
Ligand CLA 5 613



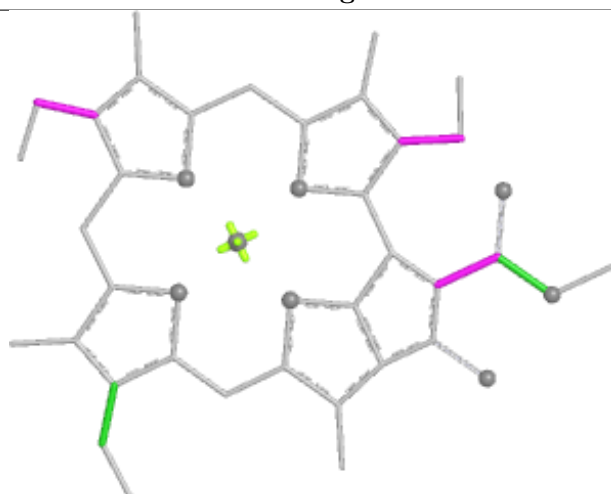
Ligand CLA B 817



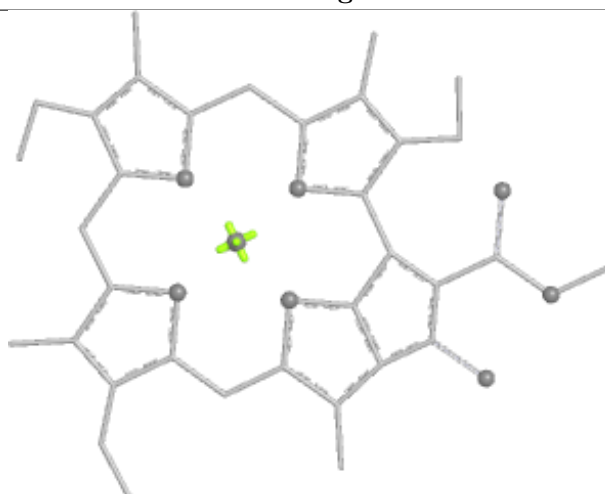
Bond lengths



Bond angles

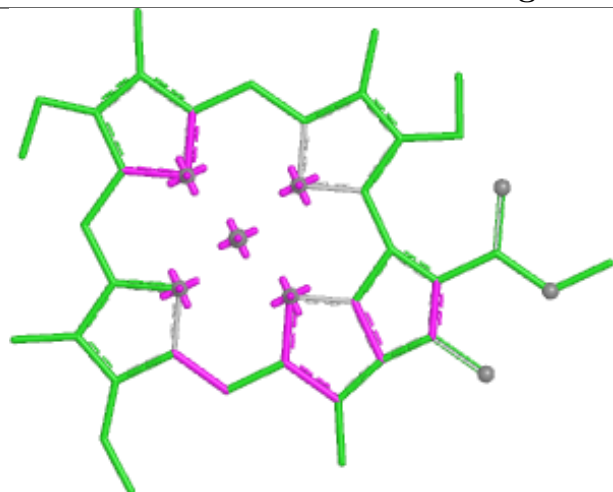


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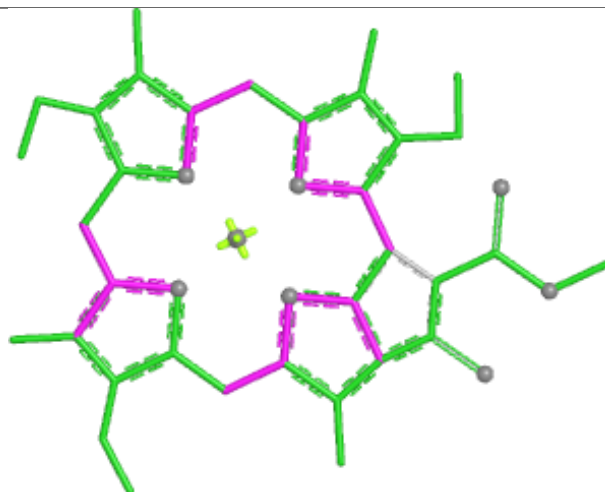


Rings

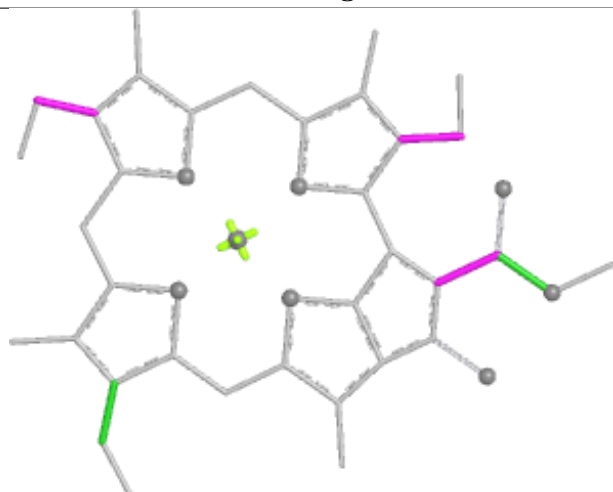
Ligand CLA 1 602



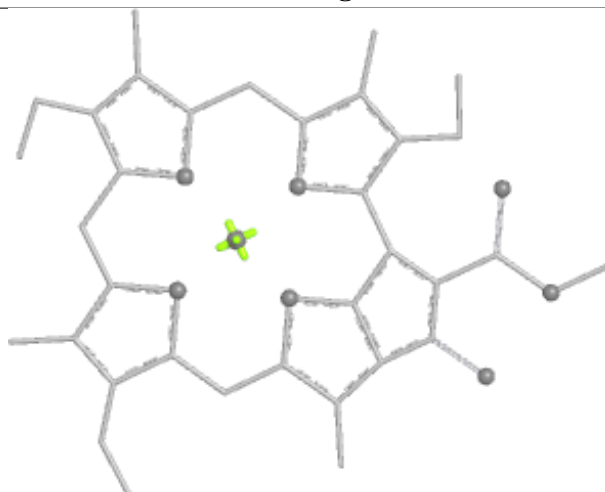
Bond lengths



Bond angles

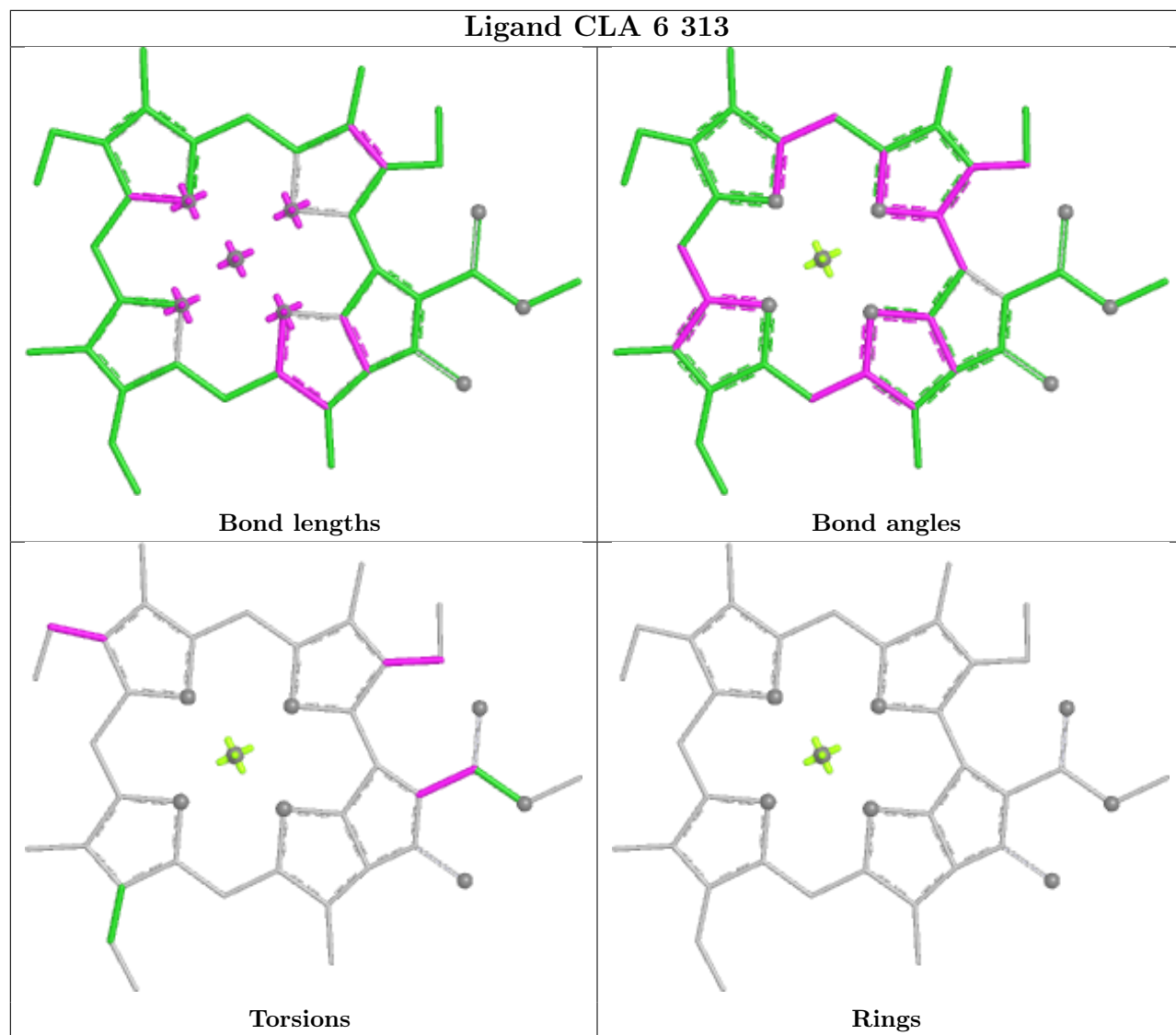


Torsions

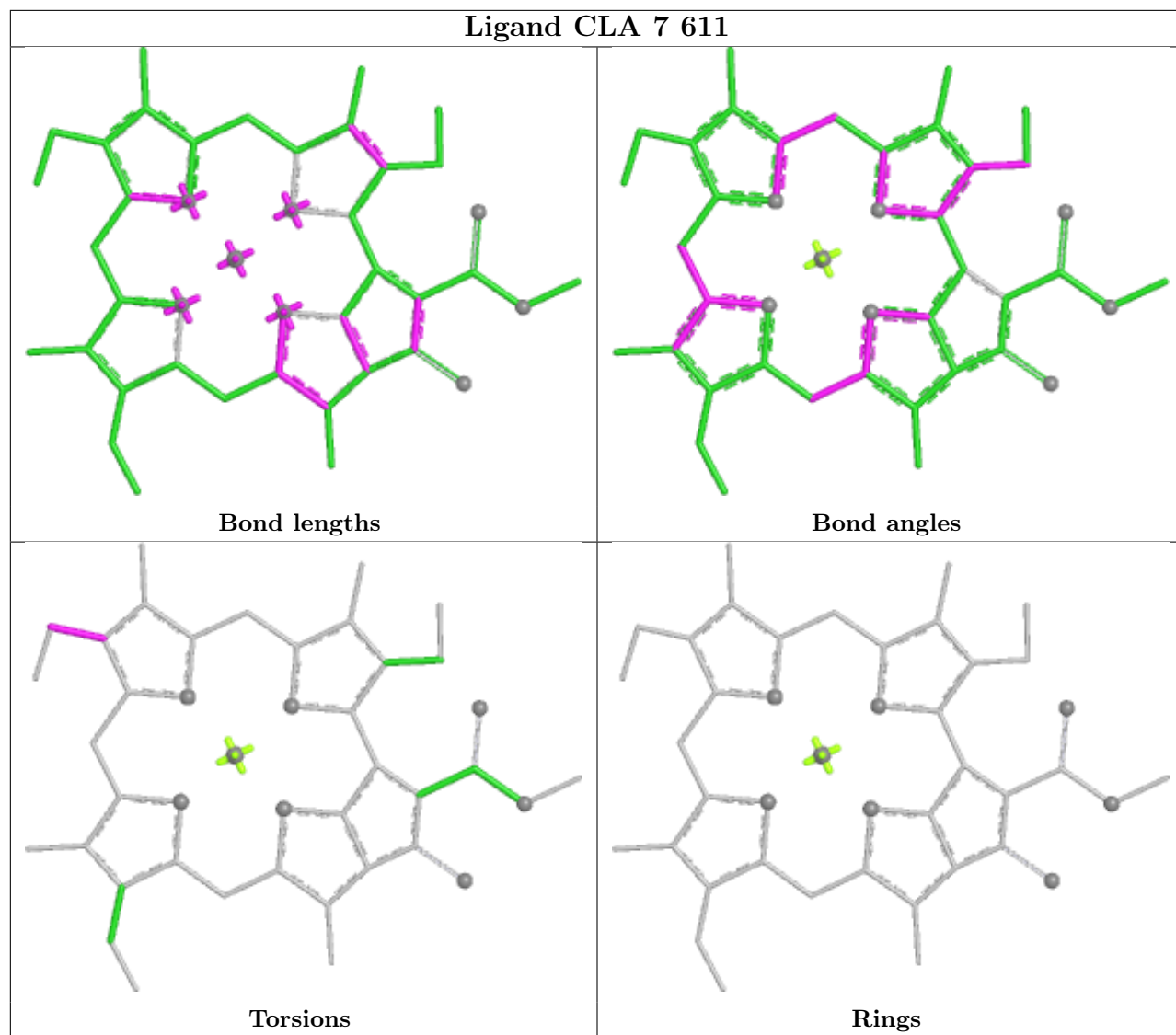


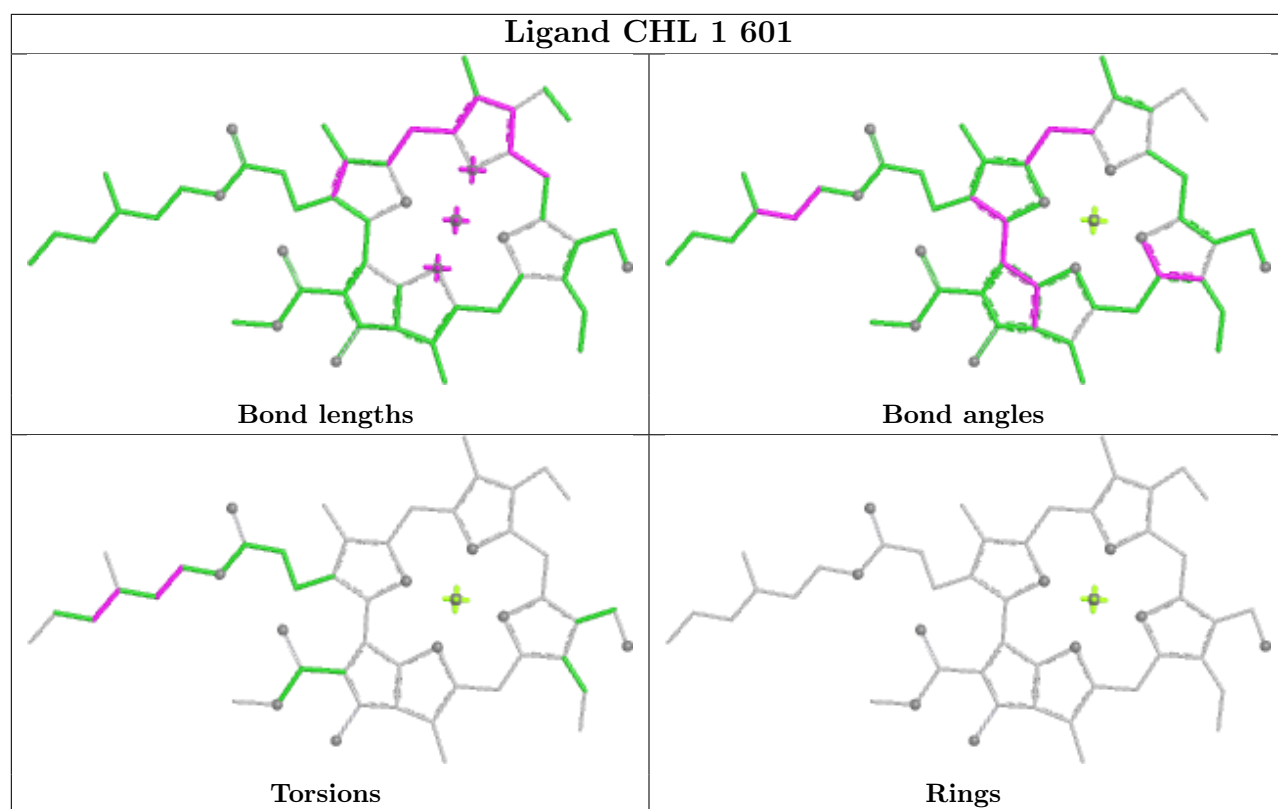
Rings

Ligand CLA 6 313

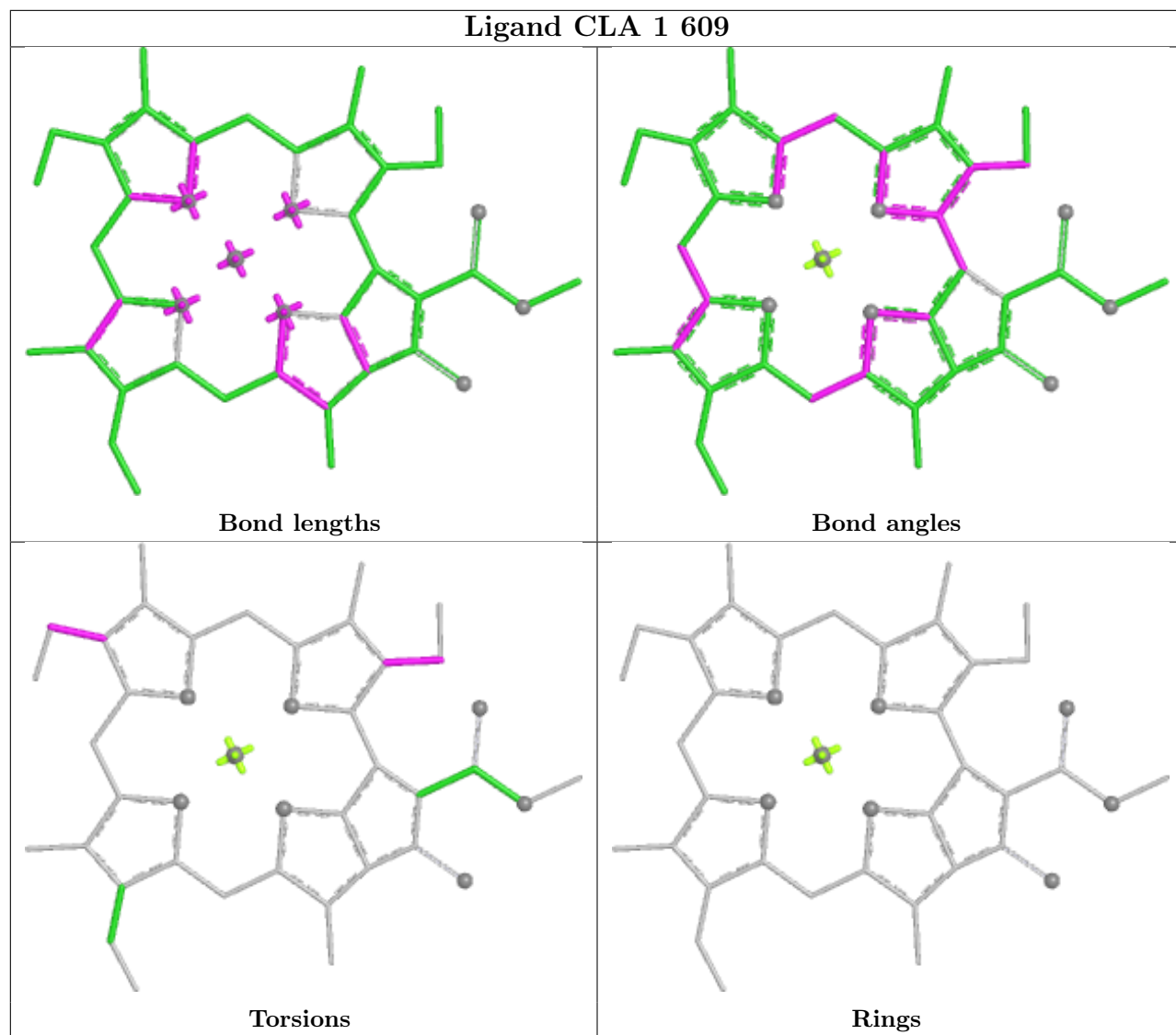


Ligand CLA 7 611

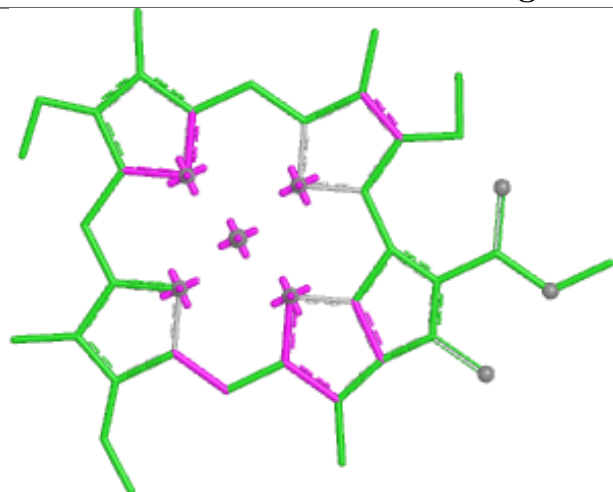




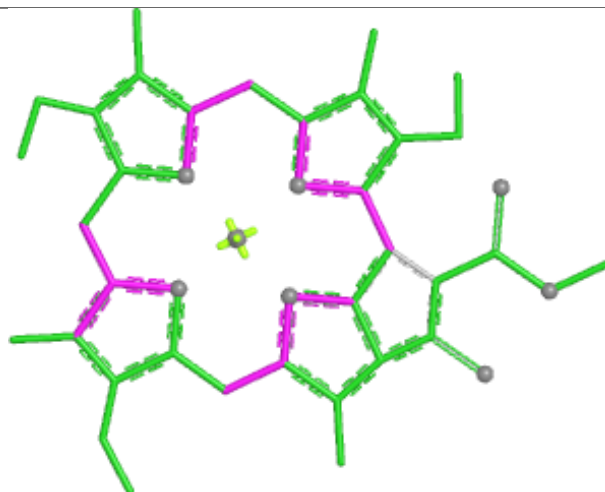
Ligand CLA 1 609



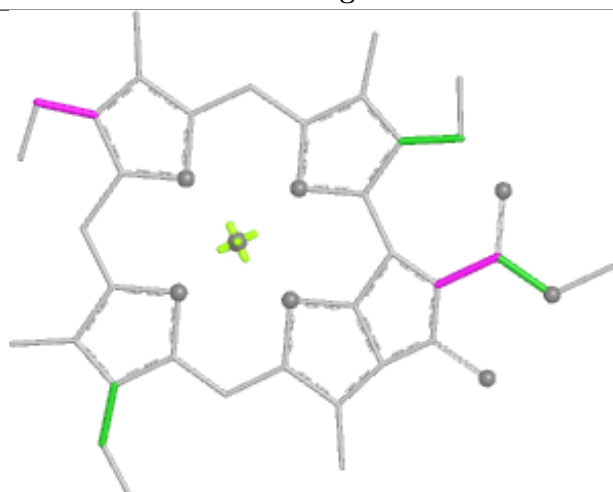
Ligand CLA 8 615



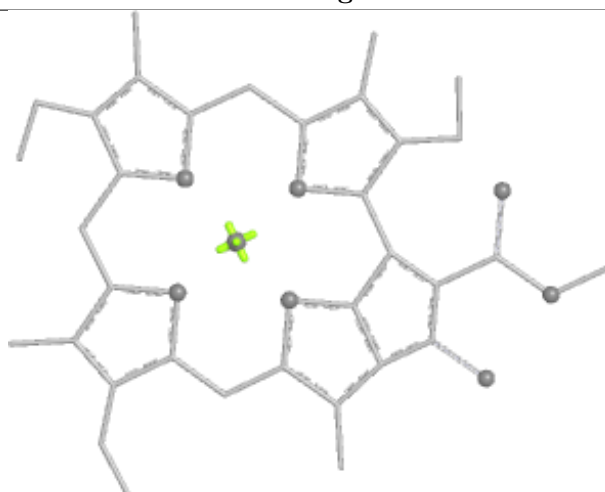
Bond lengths



Bond angles

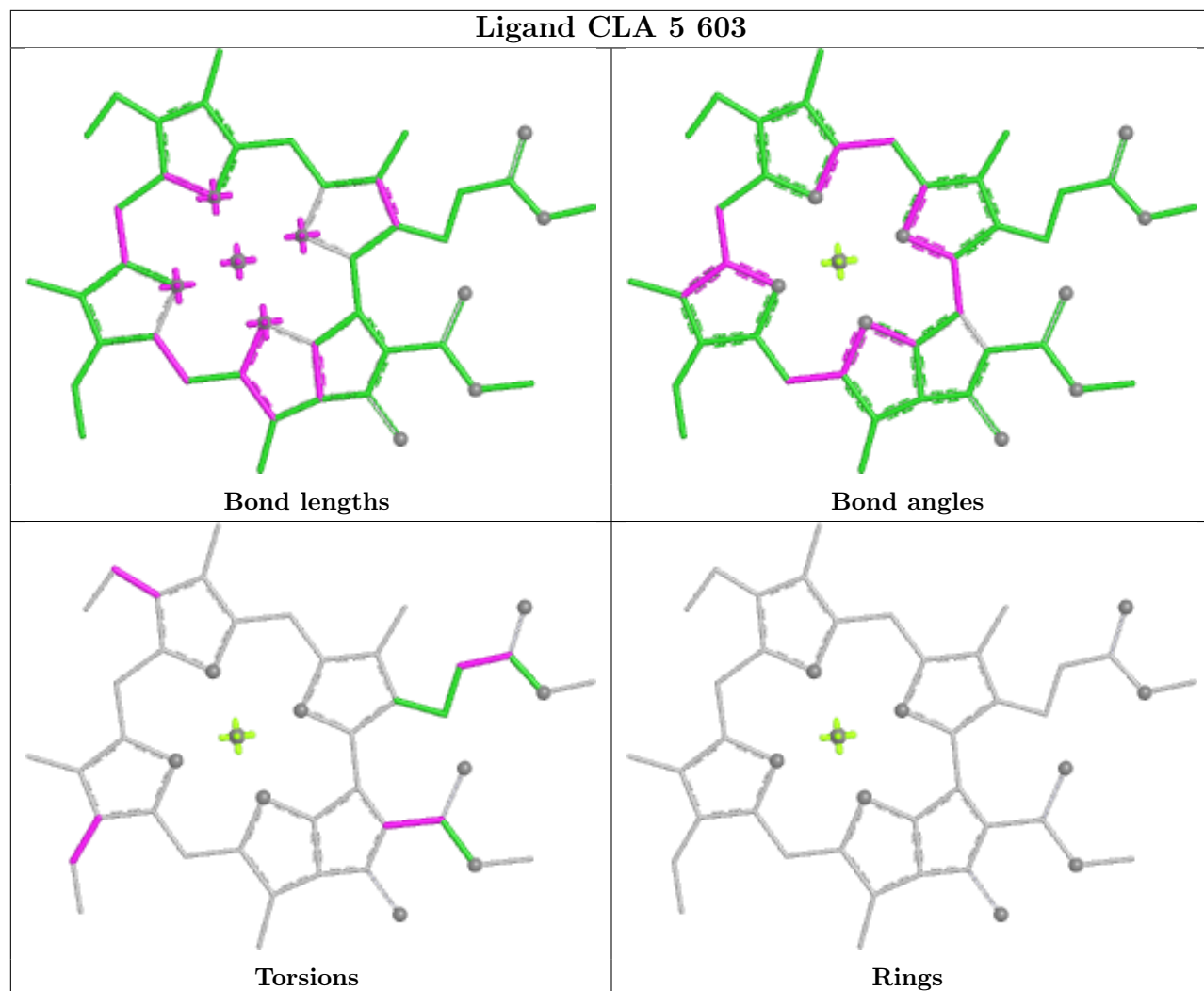


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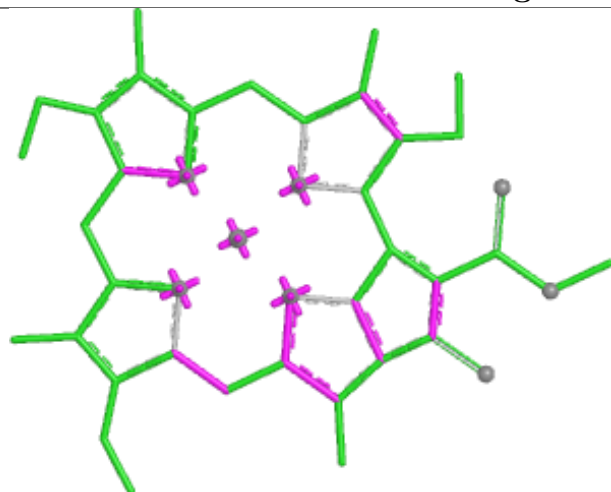


Rings

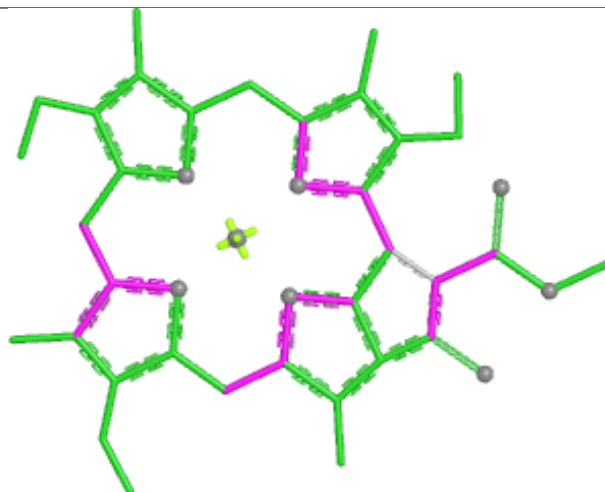
Ligand CLA 5 603



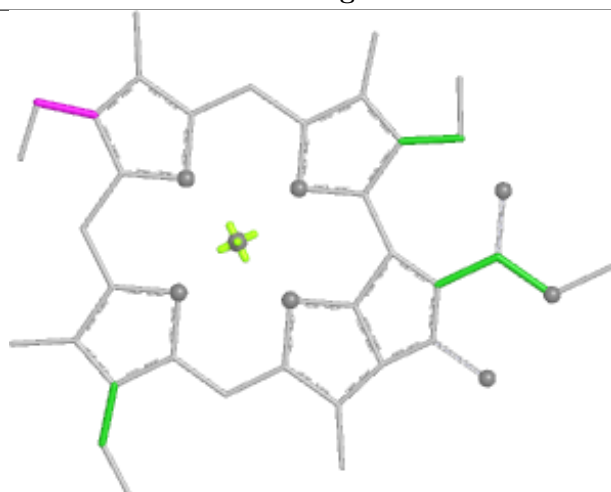
Ligand CLA A 837



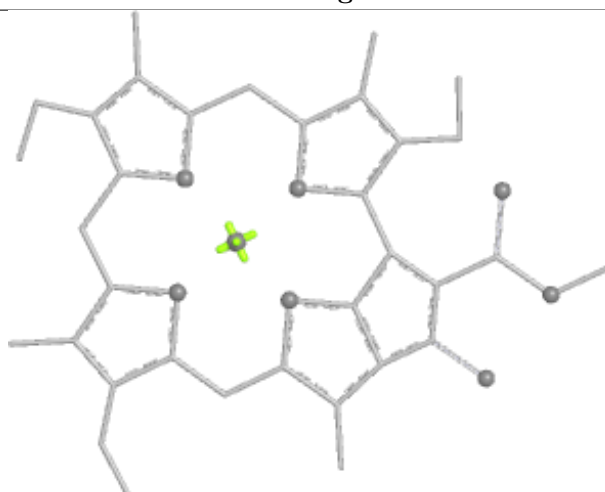
Bond lengths



Bond angles

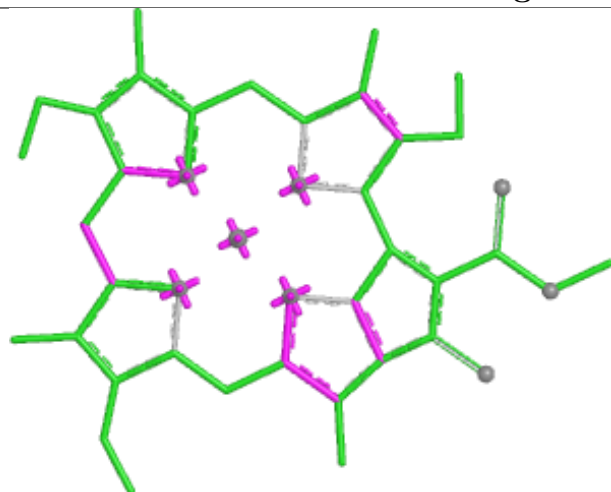


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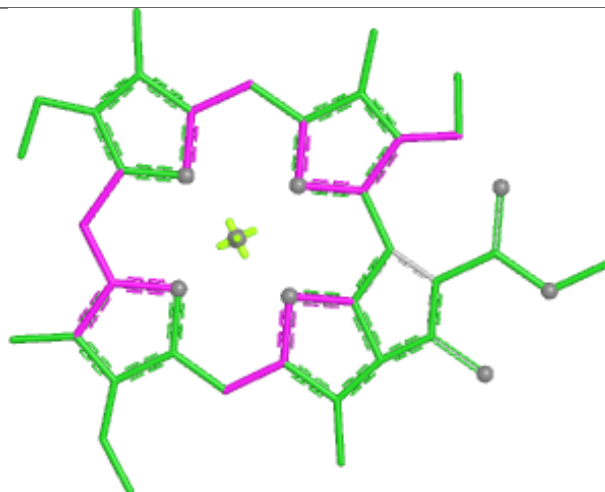


Rings

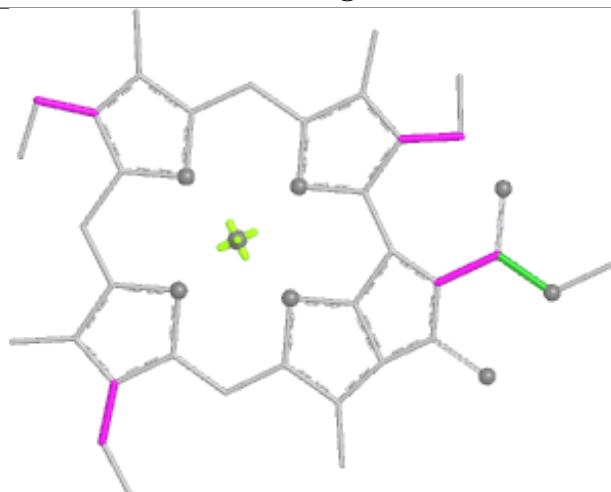
Ligand CLA A 813



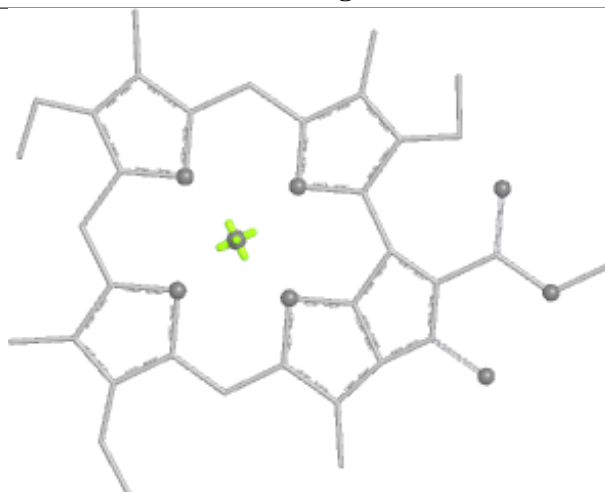
Bond lengths



Bond angles

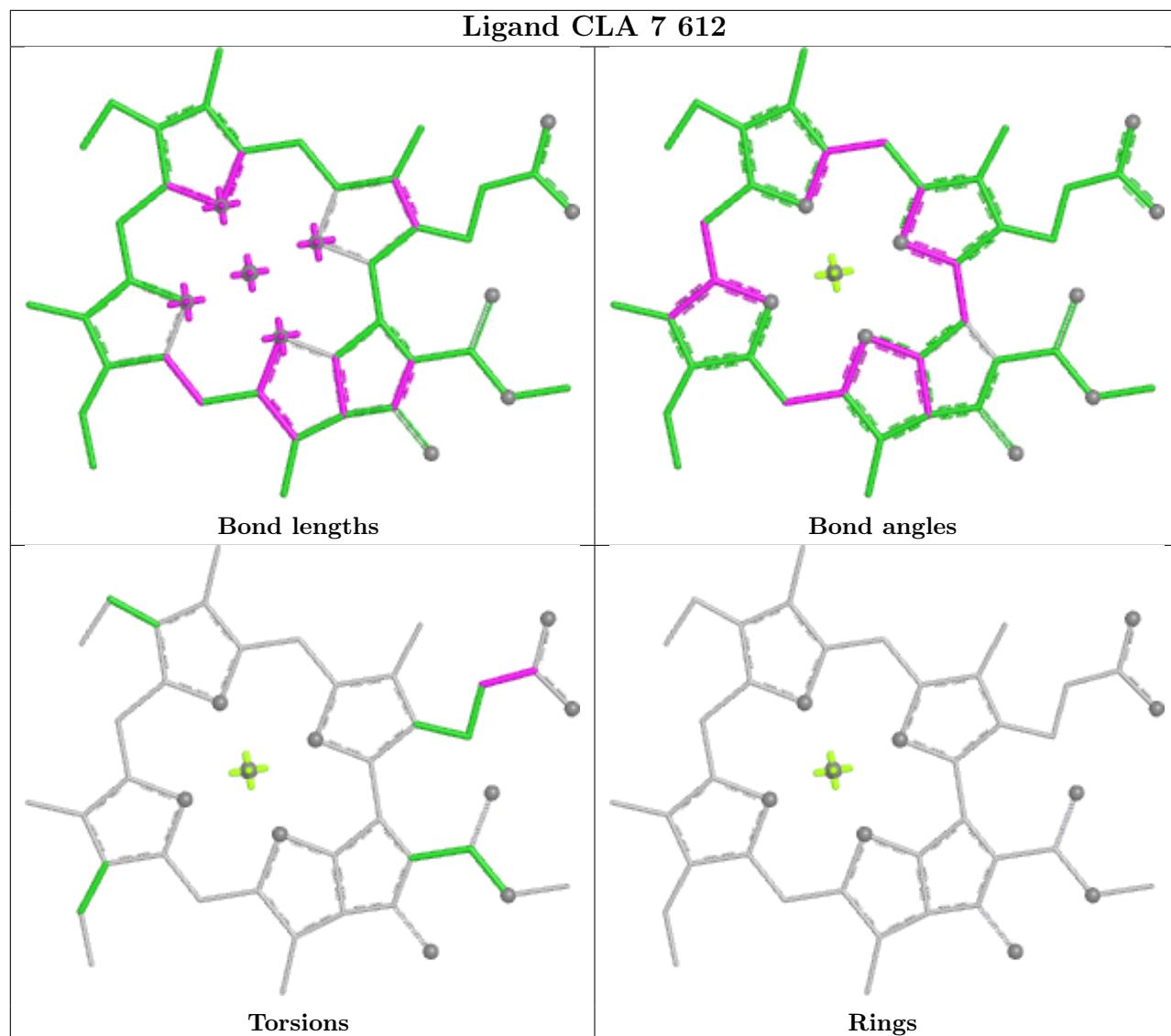


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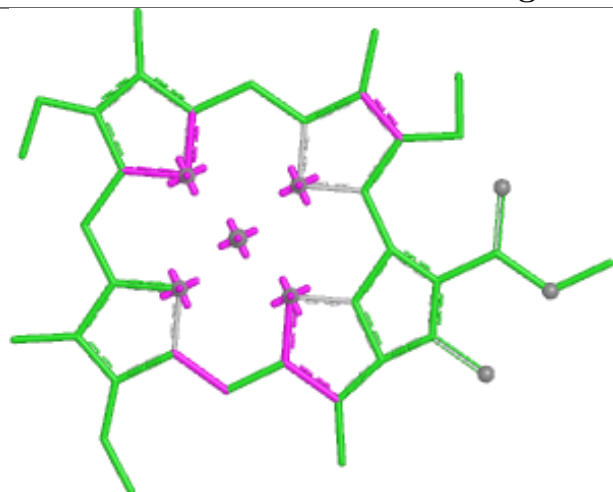


Rings

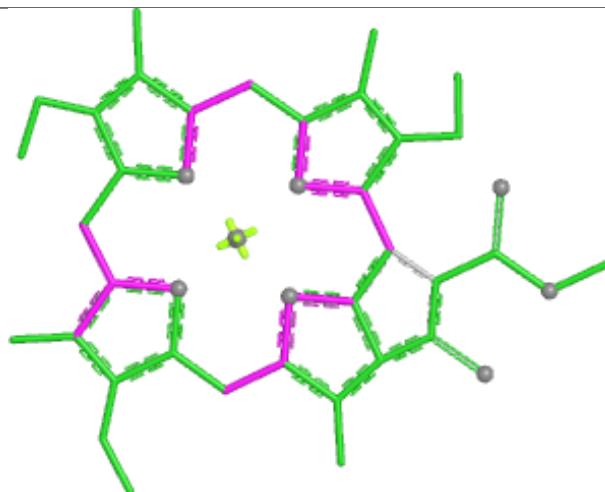
Ligand CLA 7 612



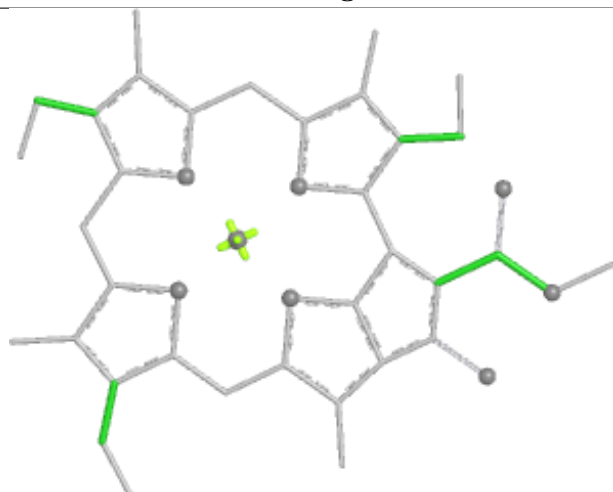
Ligand CLA 6 304



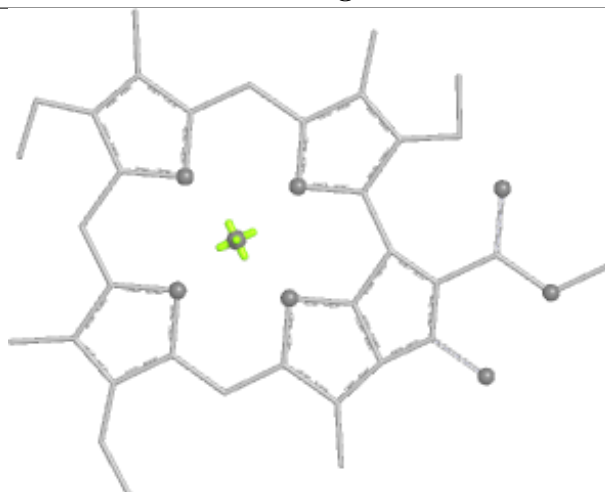
Bond lengths



Bond angles

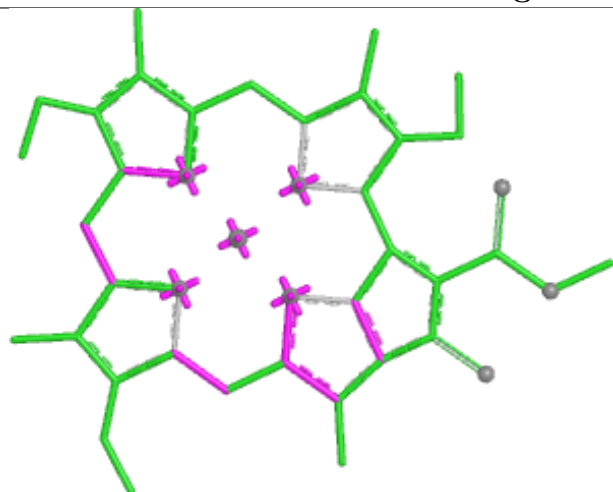


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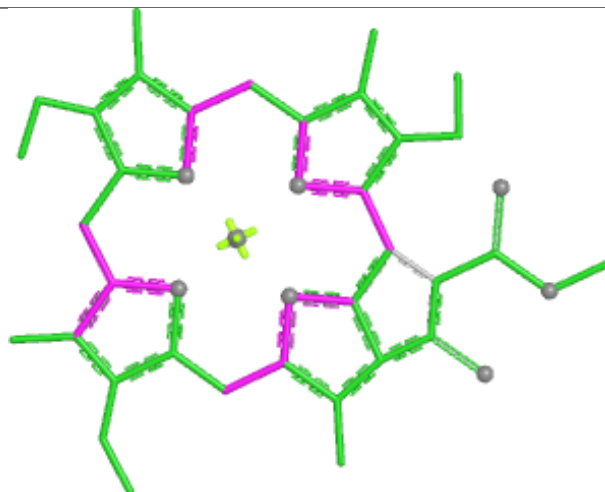


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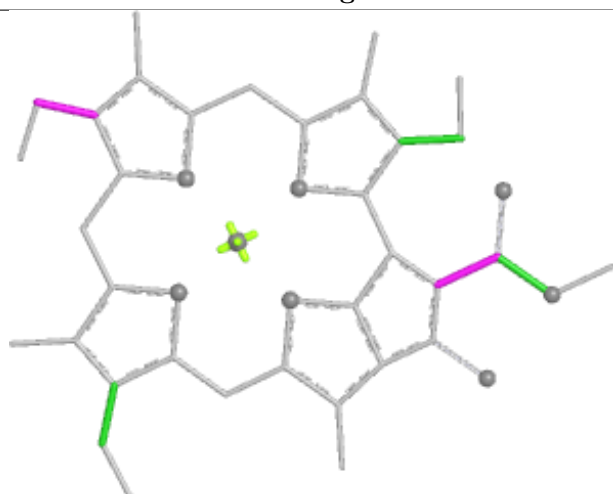
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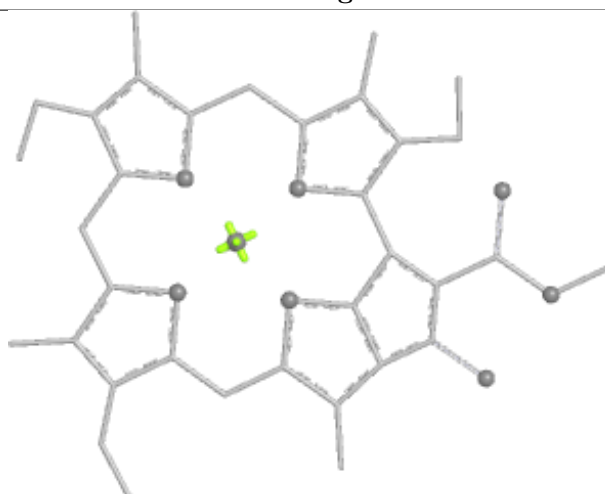
Bond lengths



Bond angles

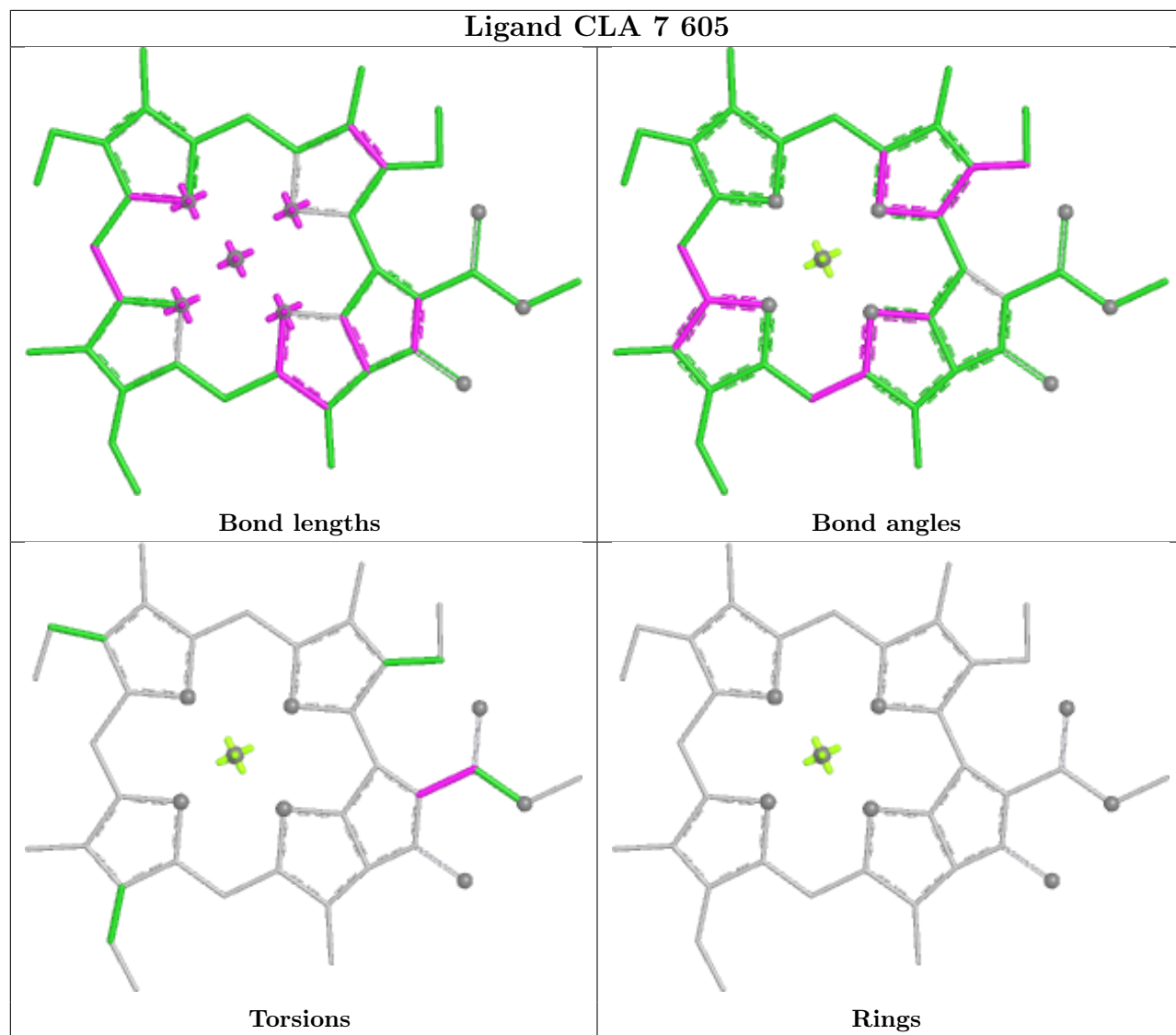


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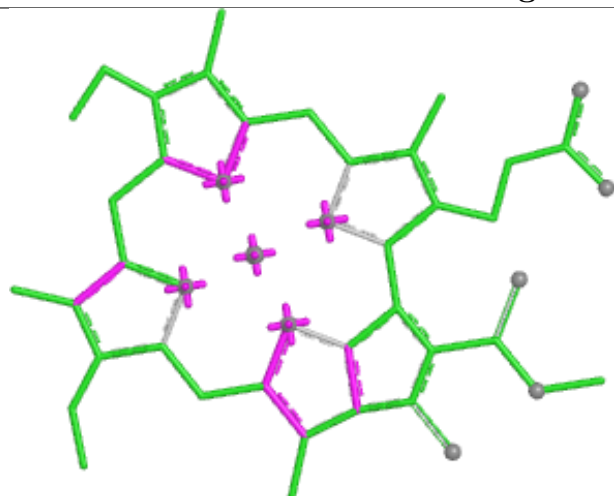


Rings

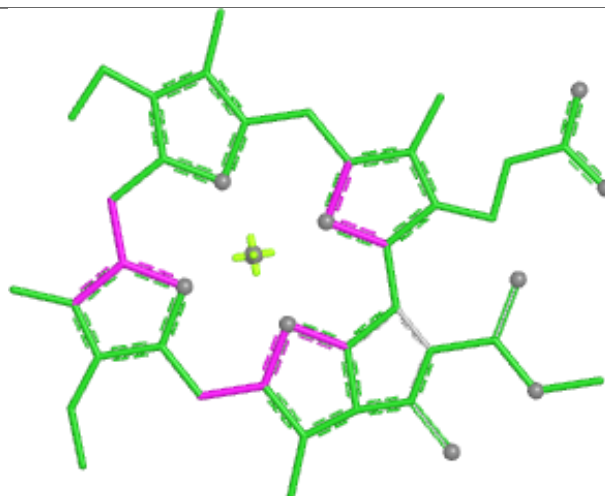
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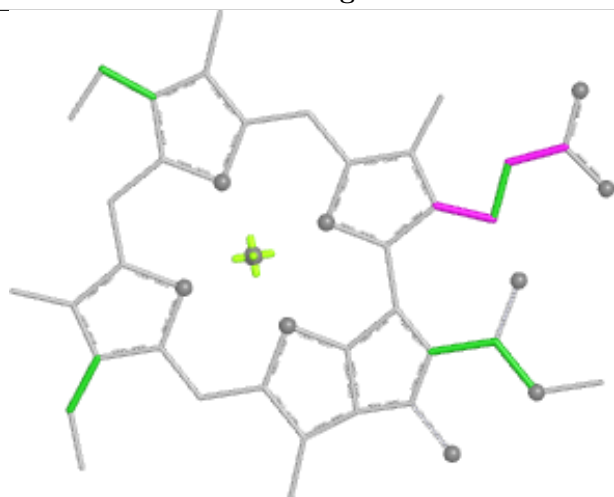
Ligand CLA 6 309



Bond lengths



Bond angles

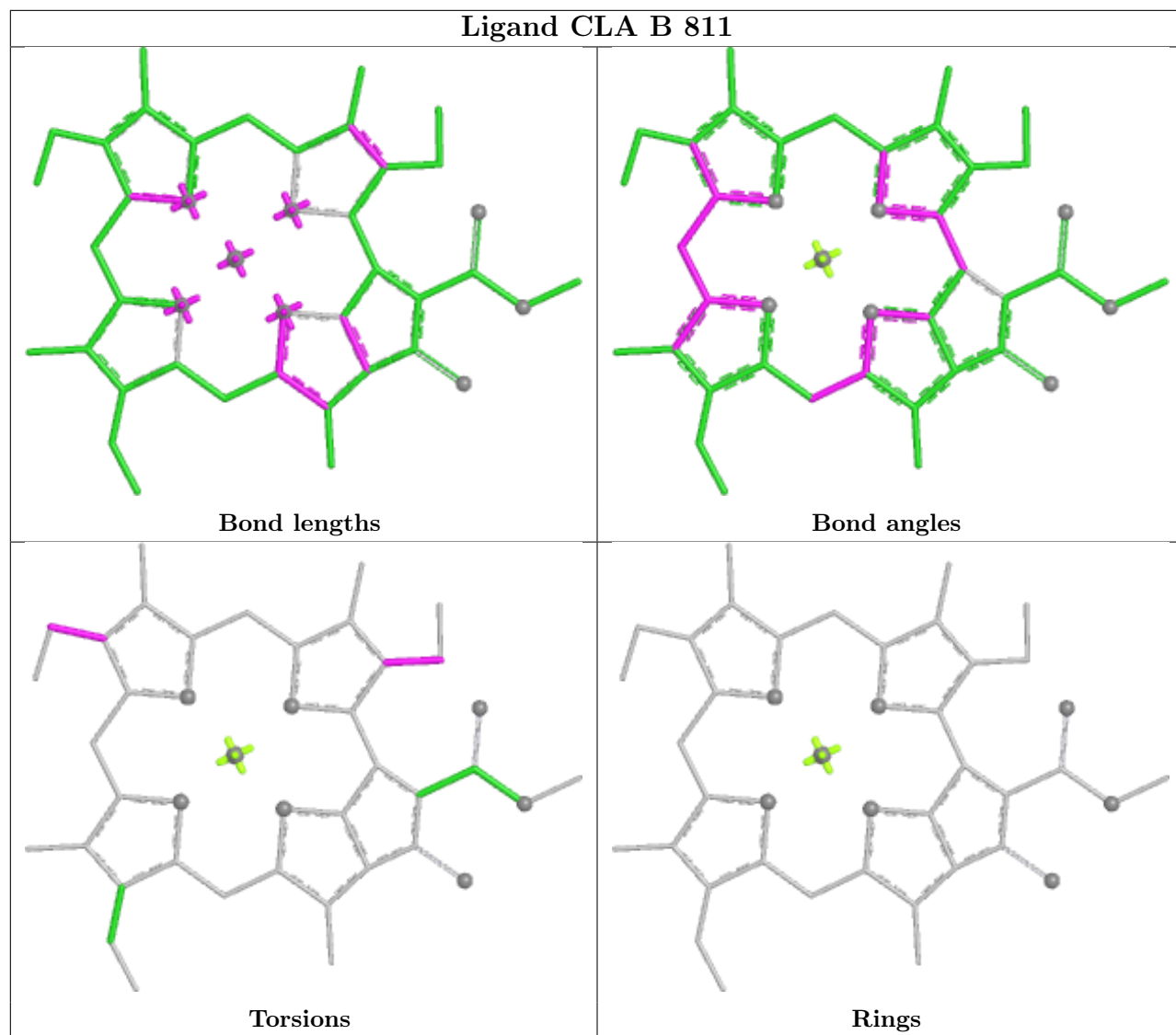


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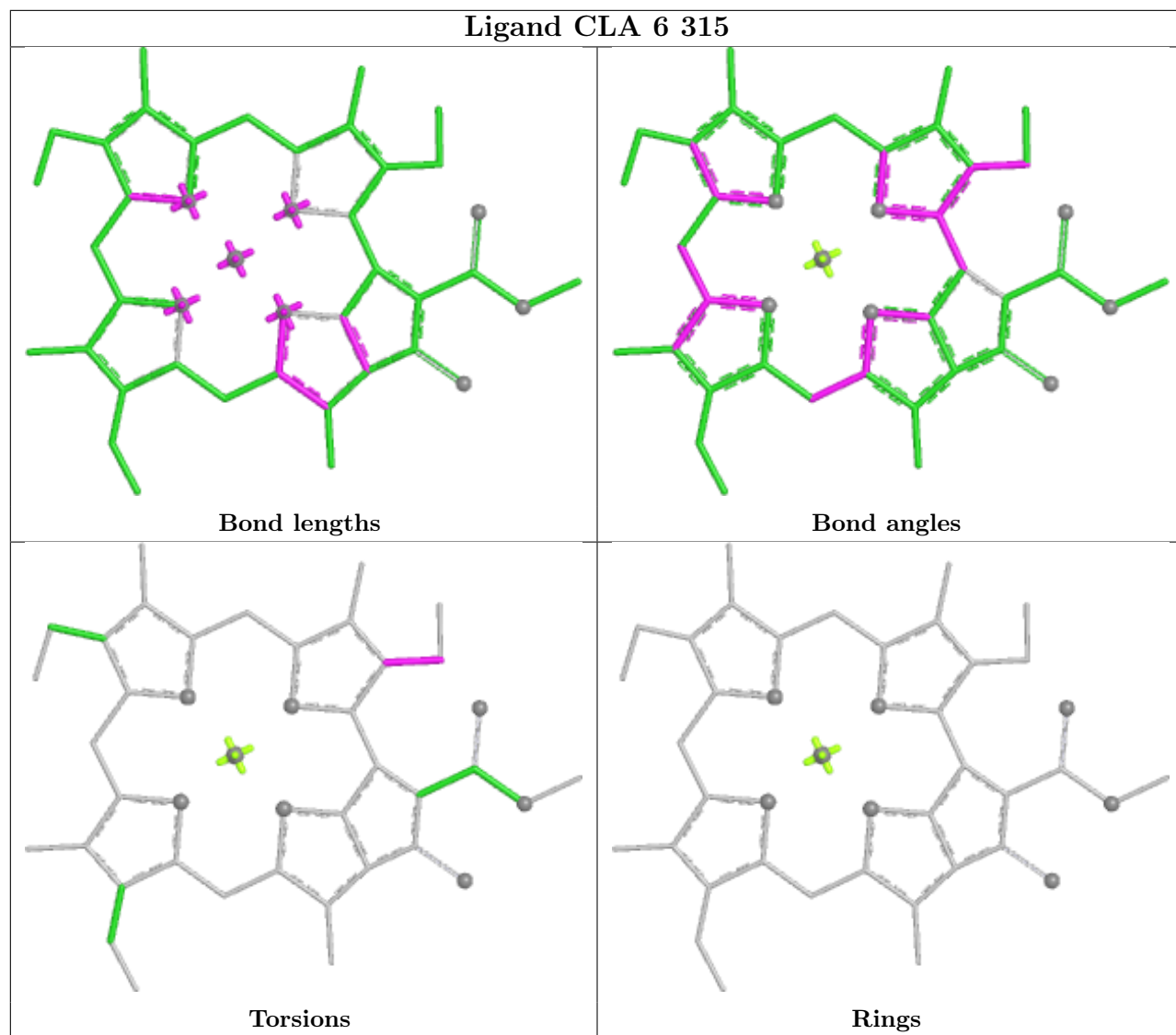


Rings

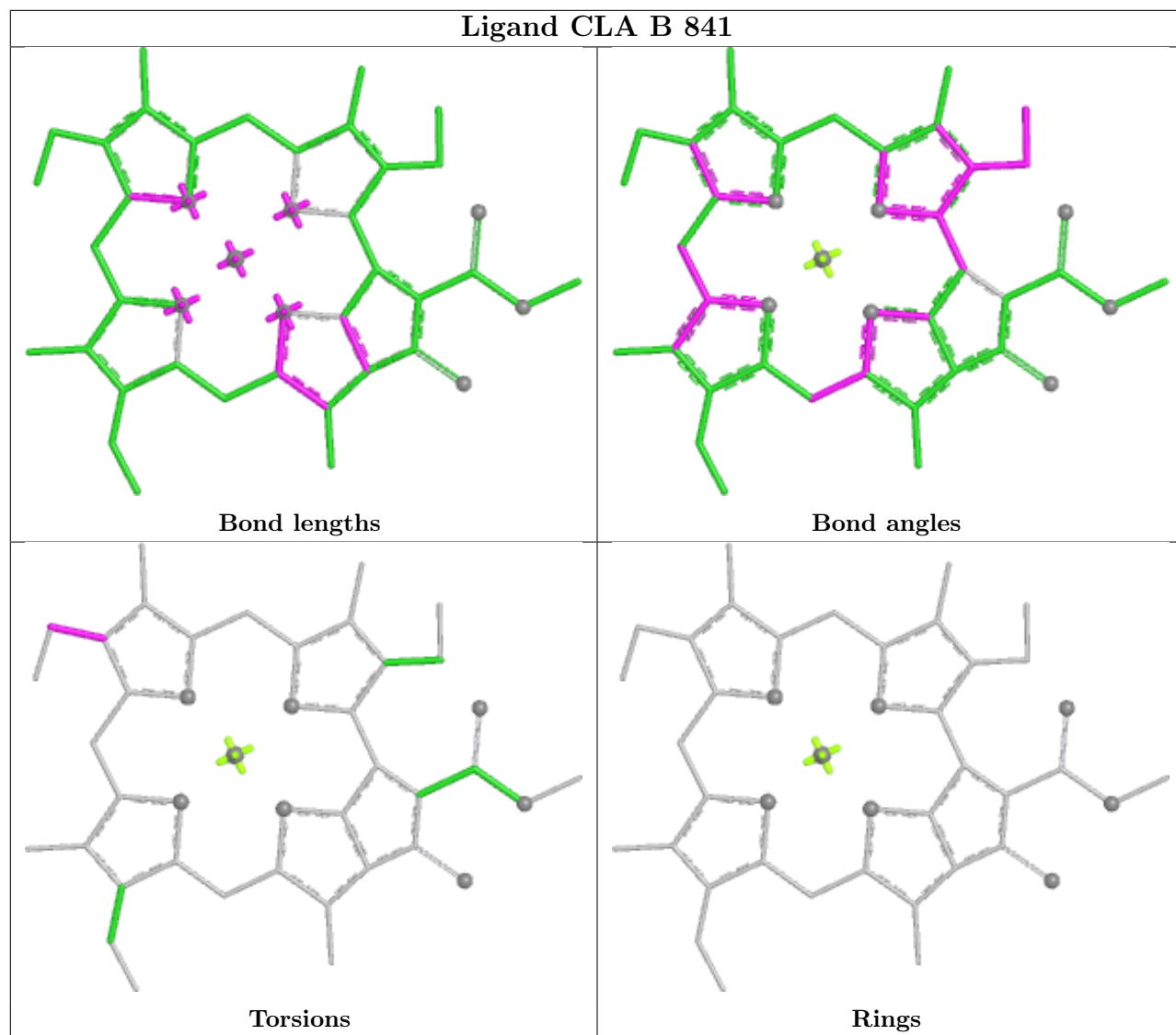
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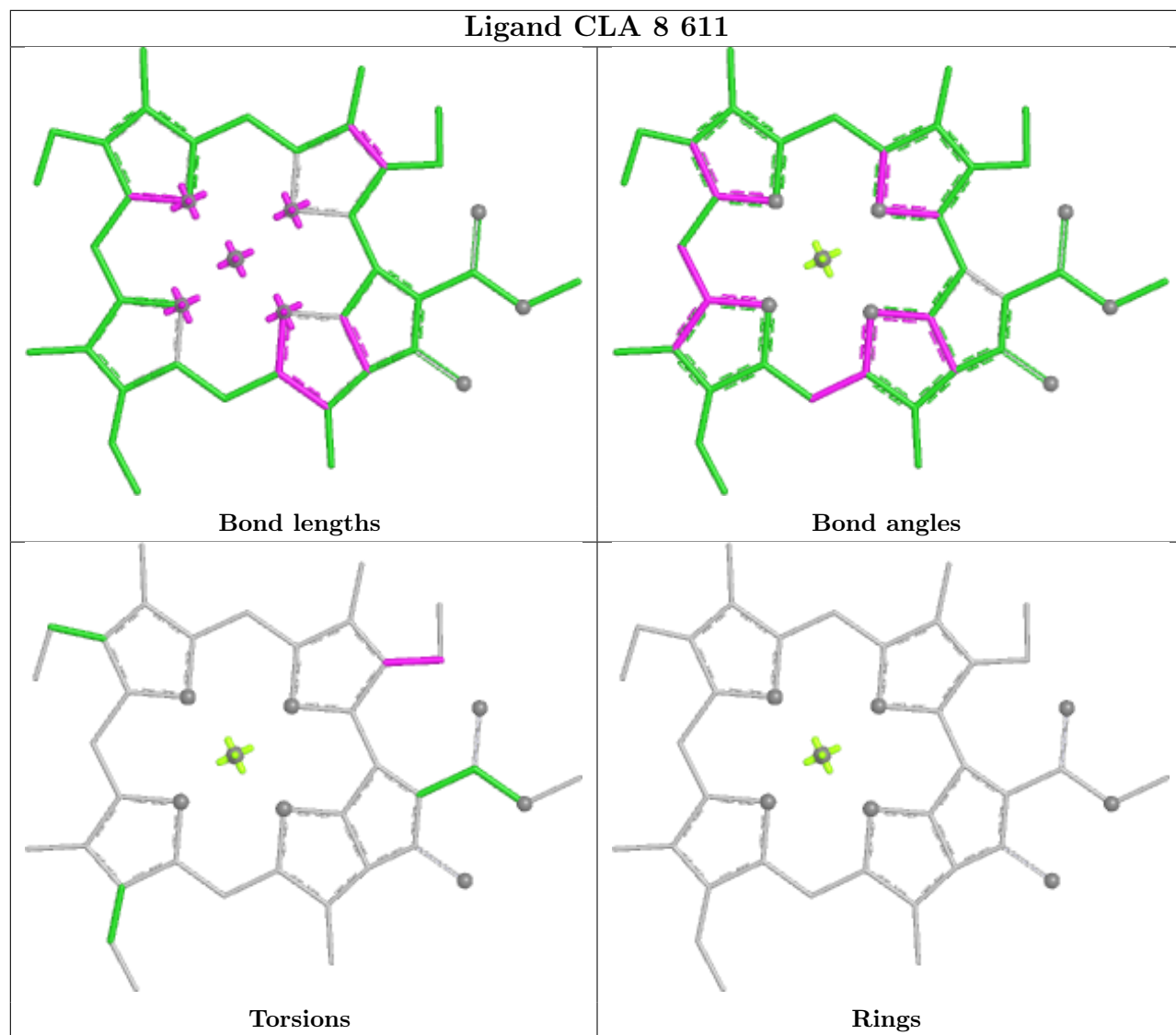
Ligand CLA 6 315



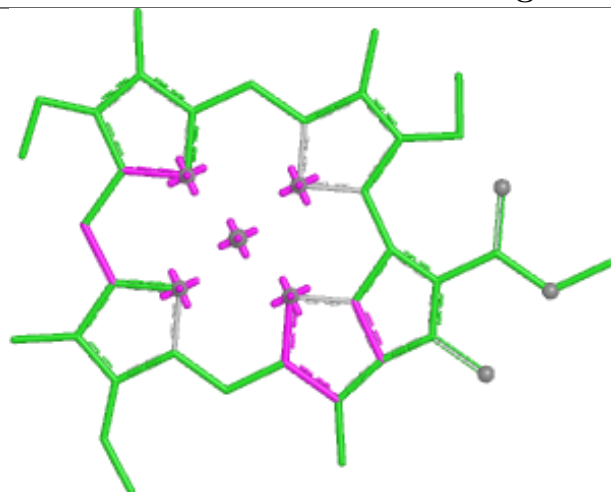
Ligand CLA B 841



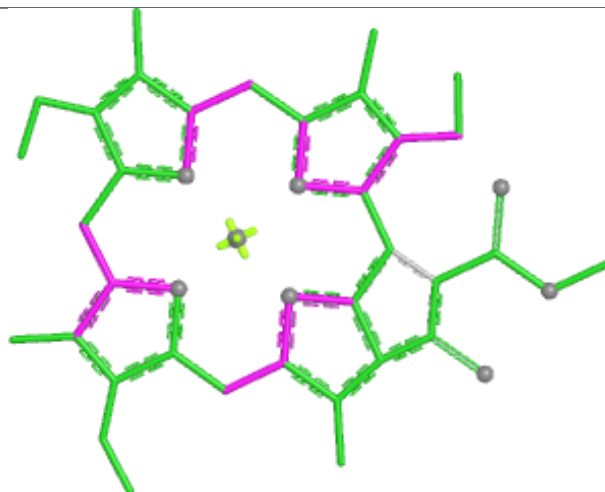
Ligand CLA 8 611



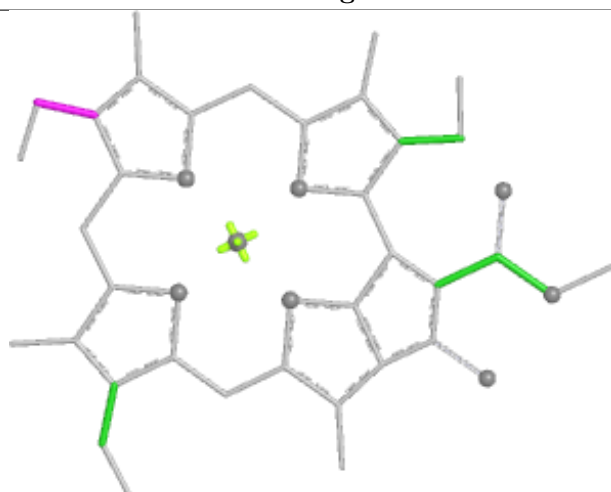
Ligand CLA Z 606



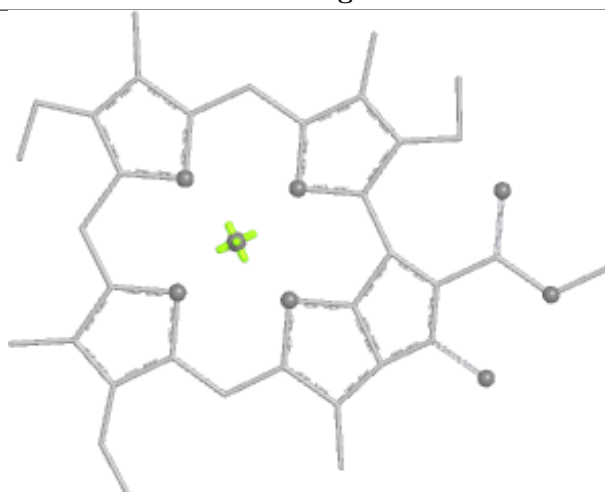
Bond lengths



Bond angles

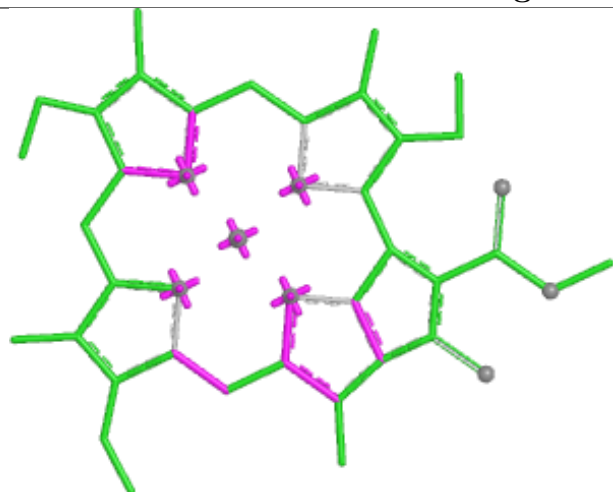


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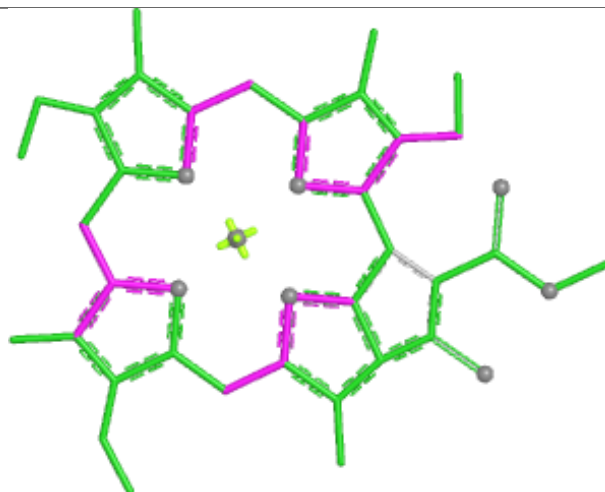


Rings

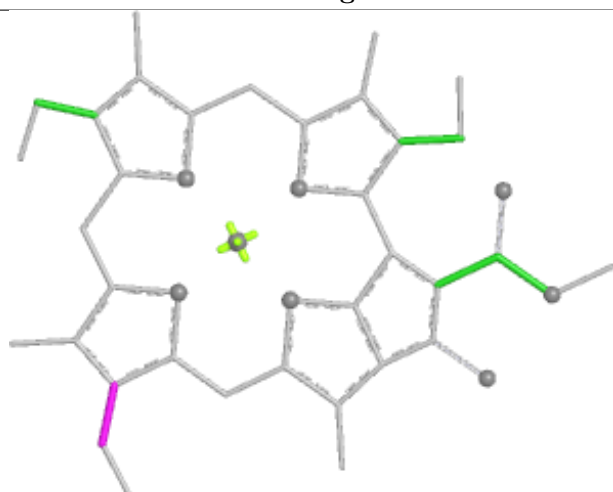
Ligand CLA A 836



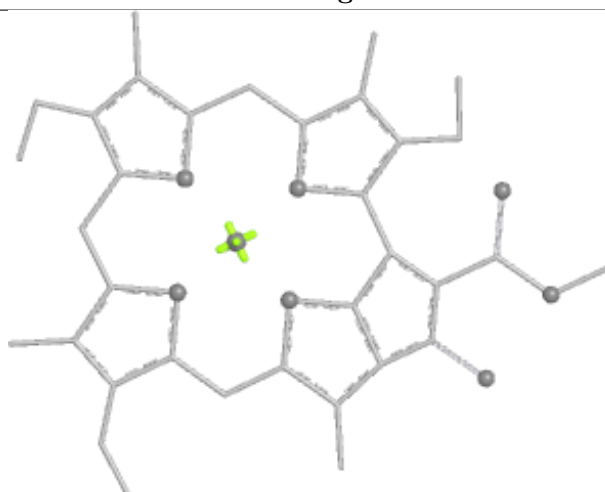
Bond lengths



Bond angles

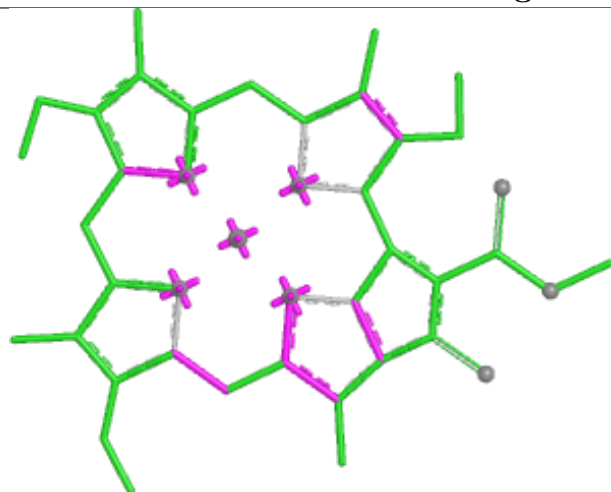


Torsions

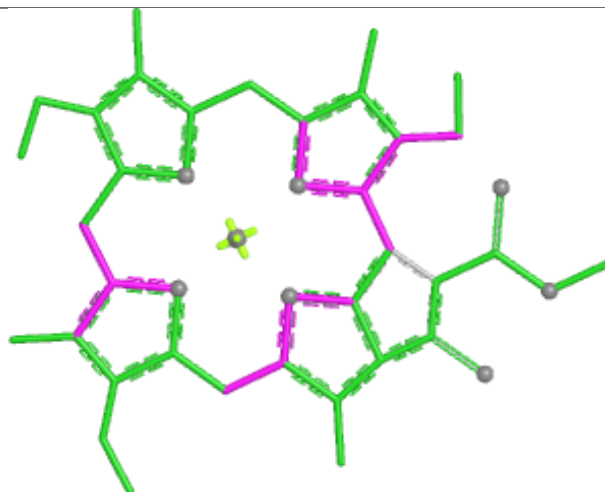


Rings

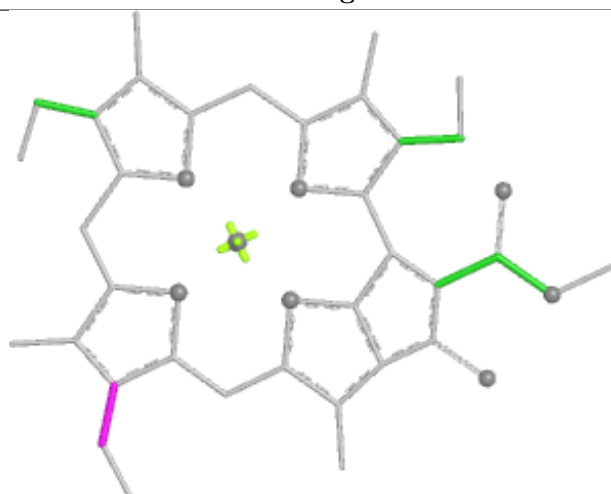
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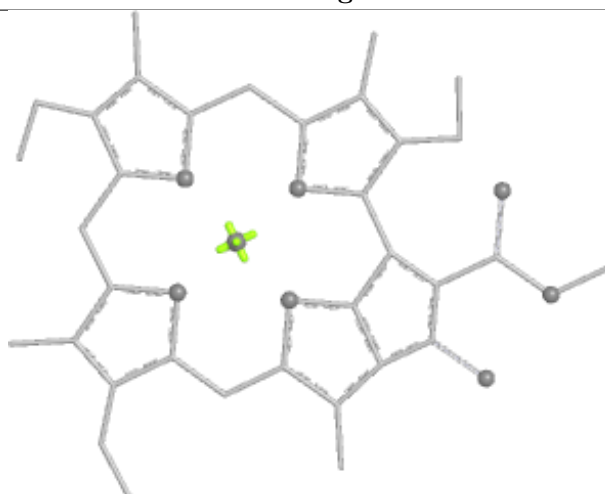
Bond lengths



Bond angles

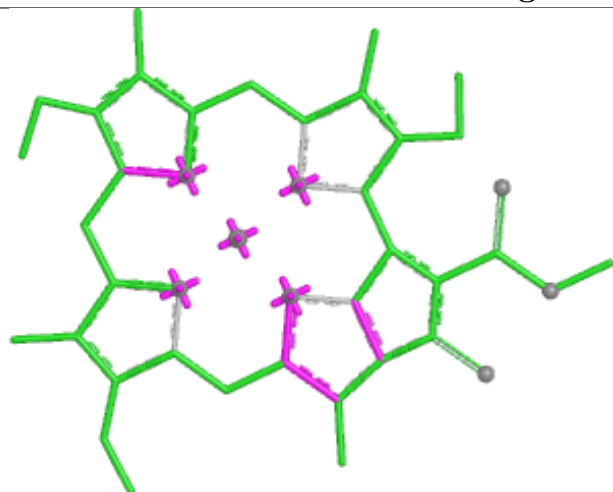


Torsions

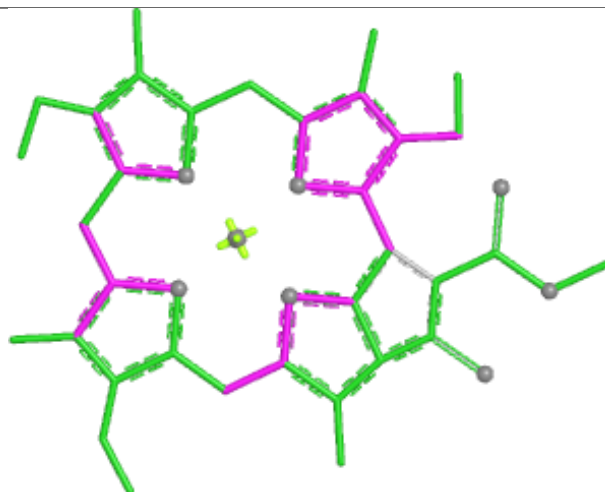


Rings

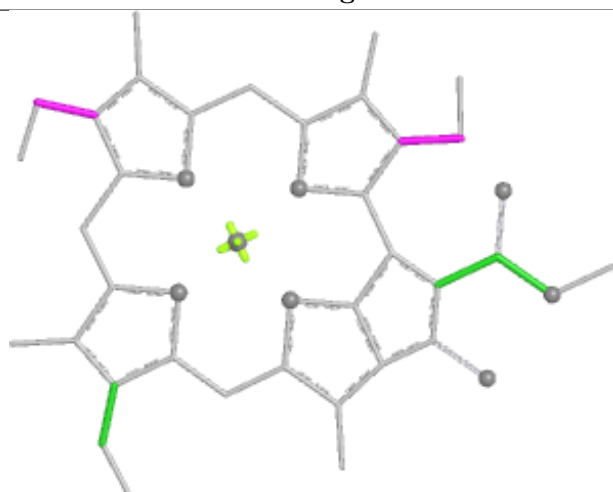
Ligand CLA 1 608



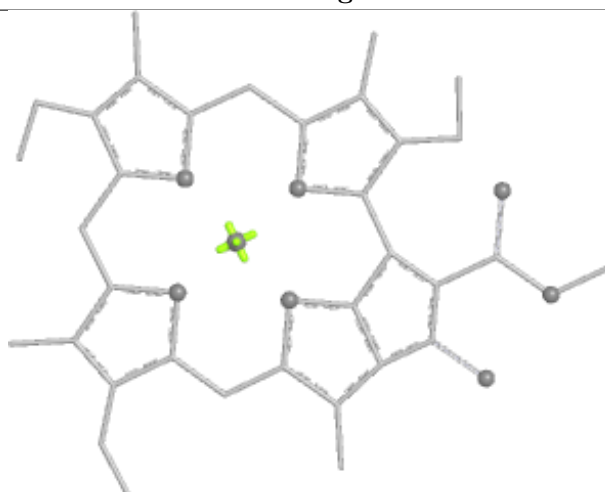
Bond lengths



Bond angles

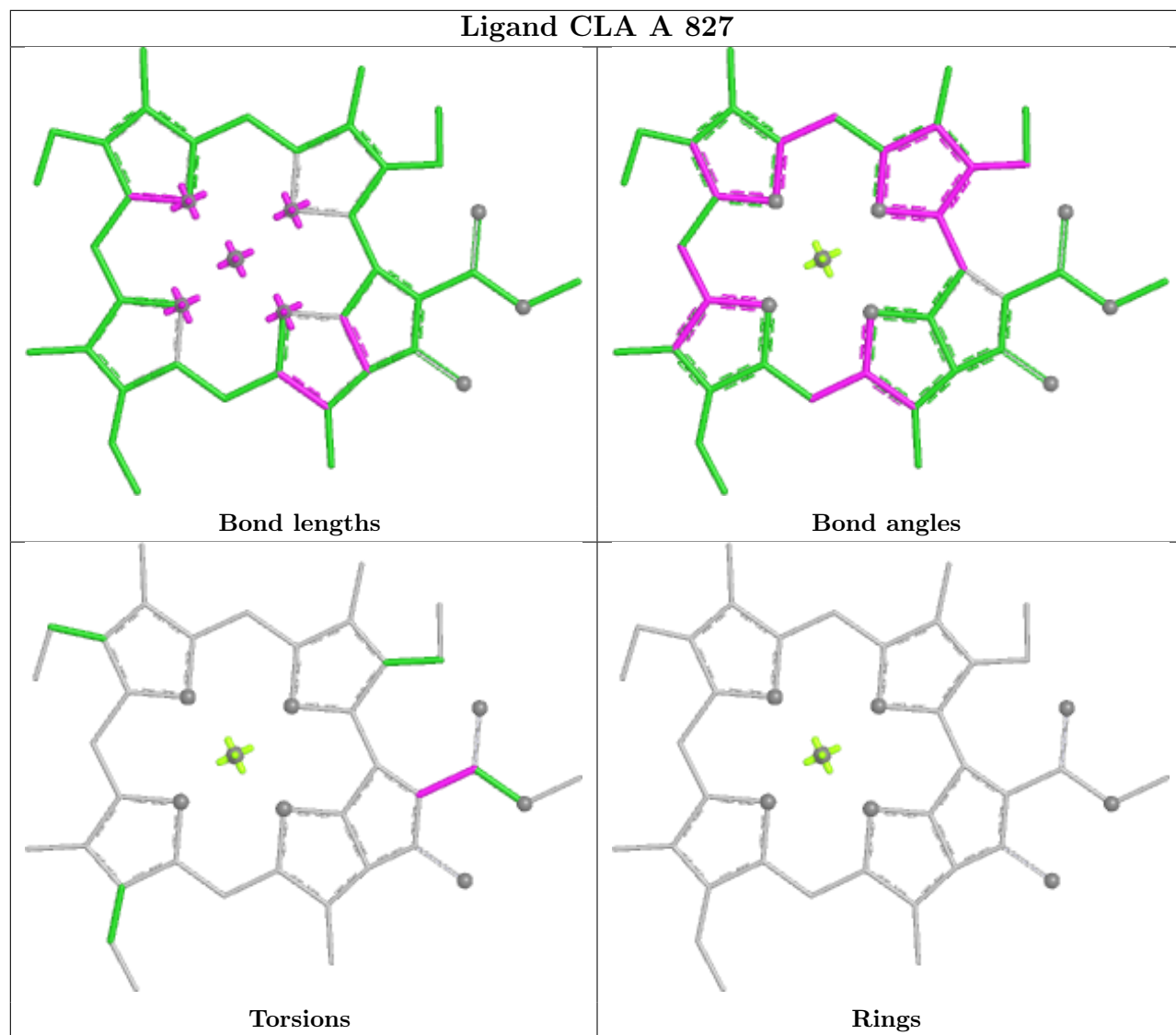


Torsions

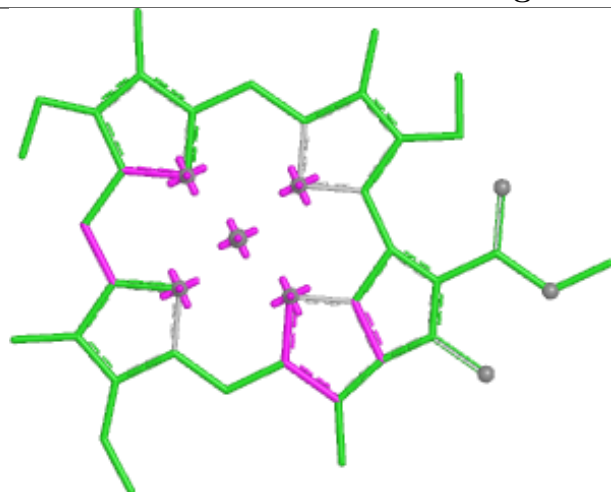


Rings

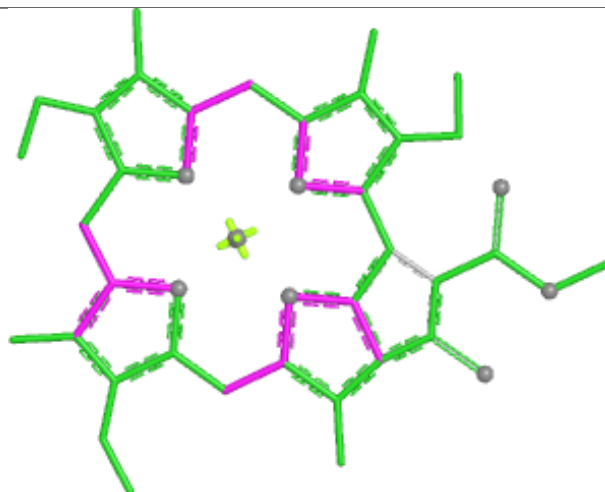
Ligand CLA A 827



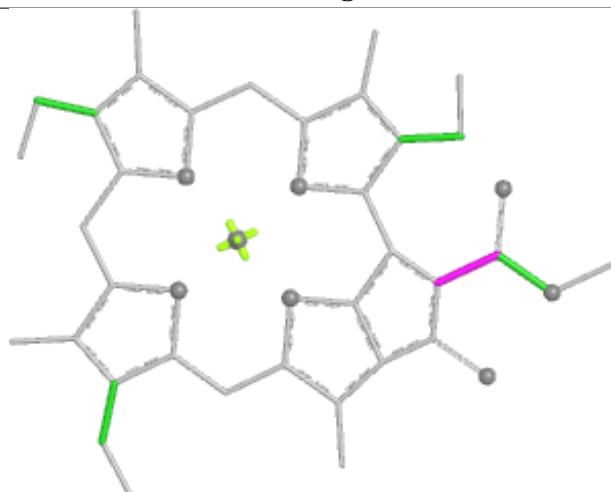
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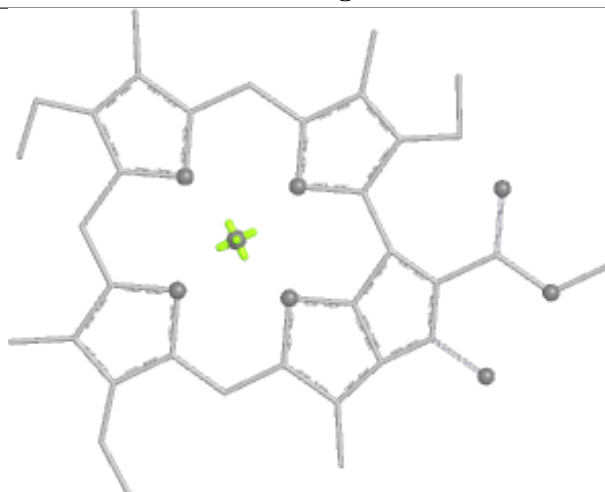
Bond lengths



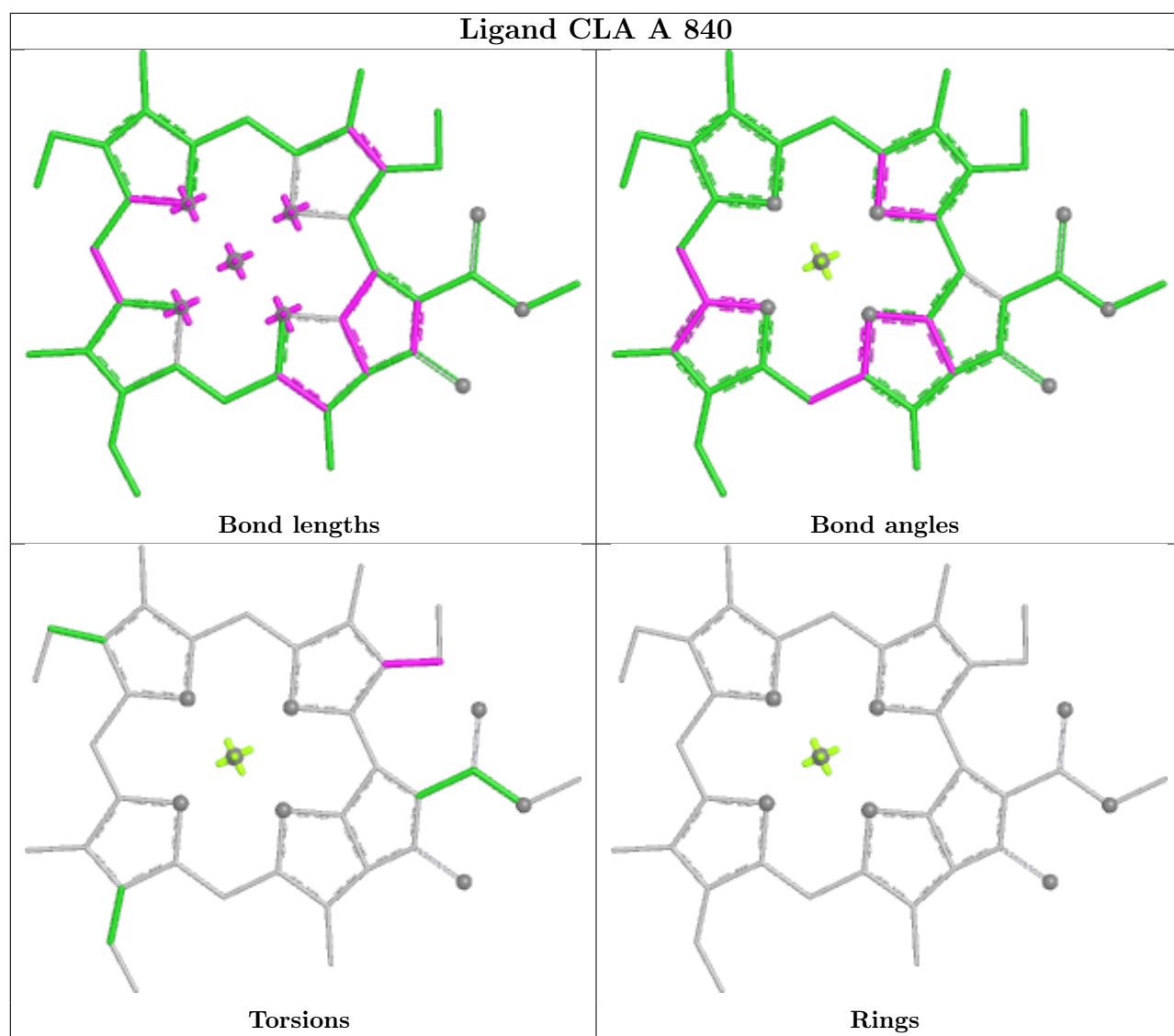
Bond angles



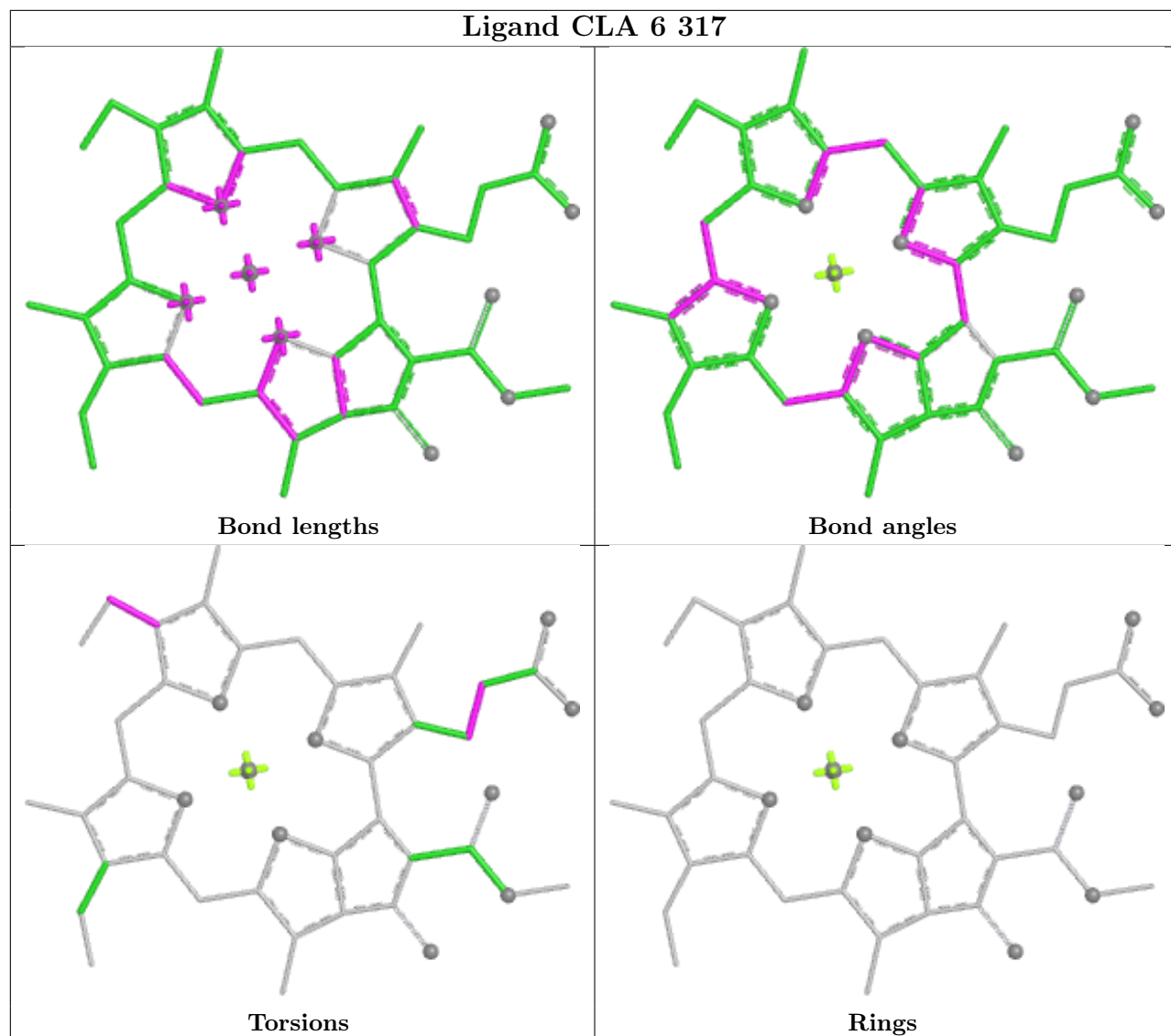
Torsions



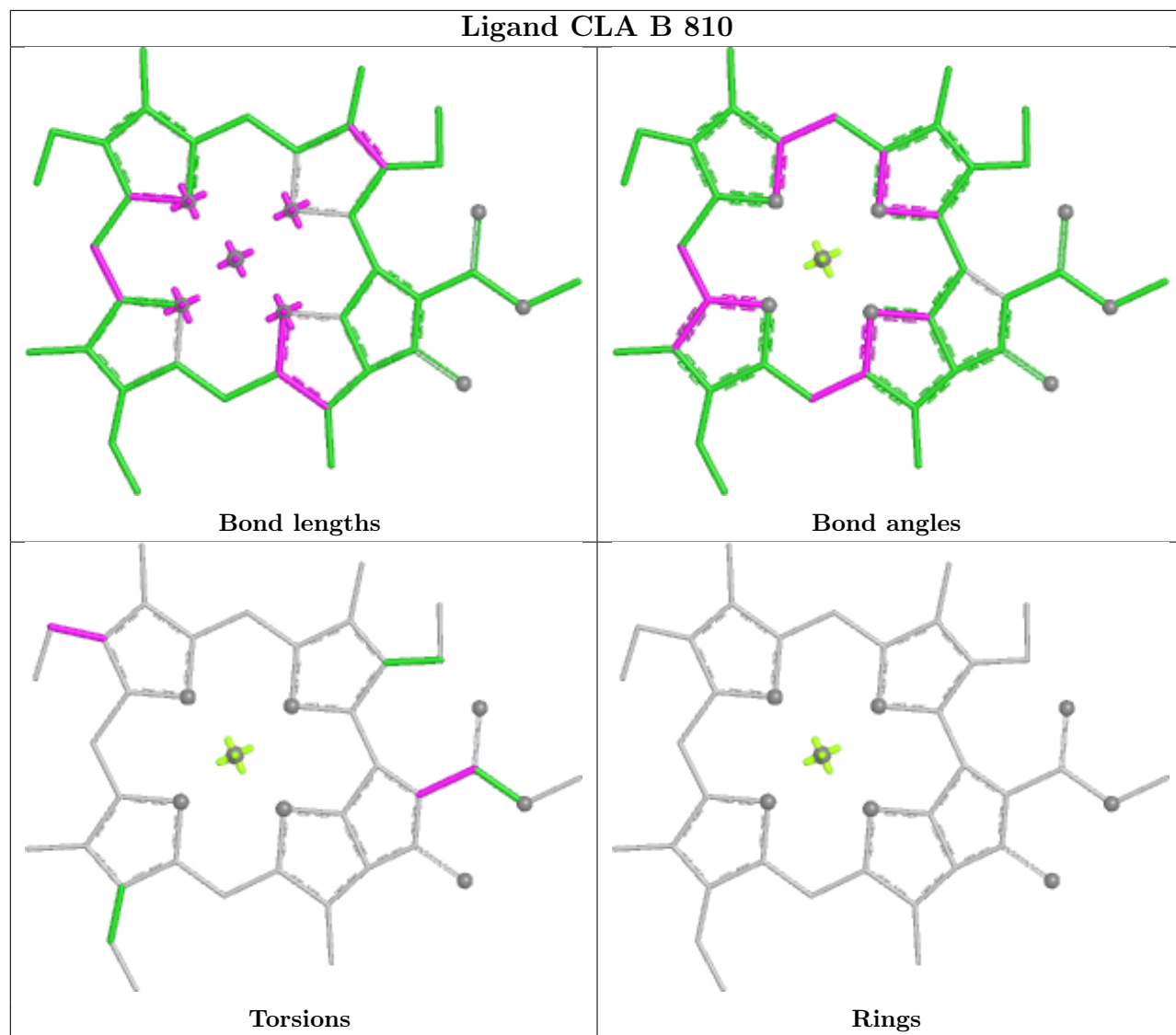
Rings



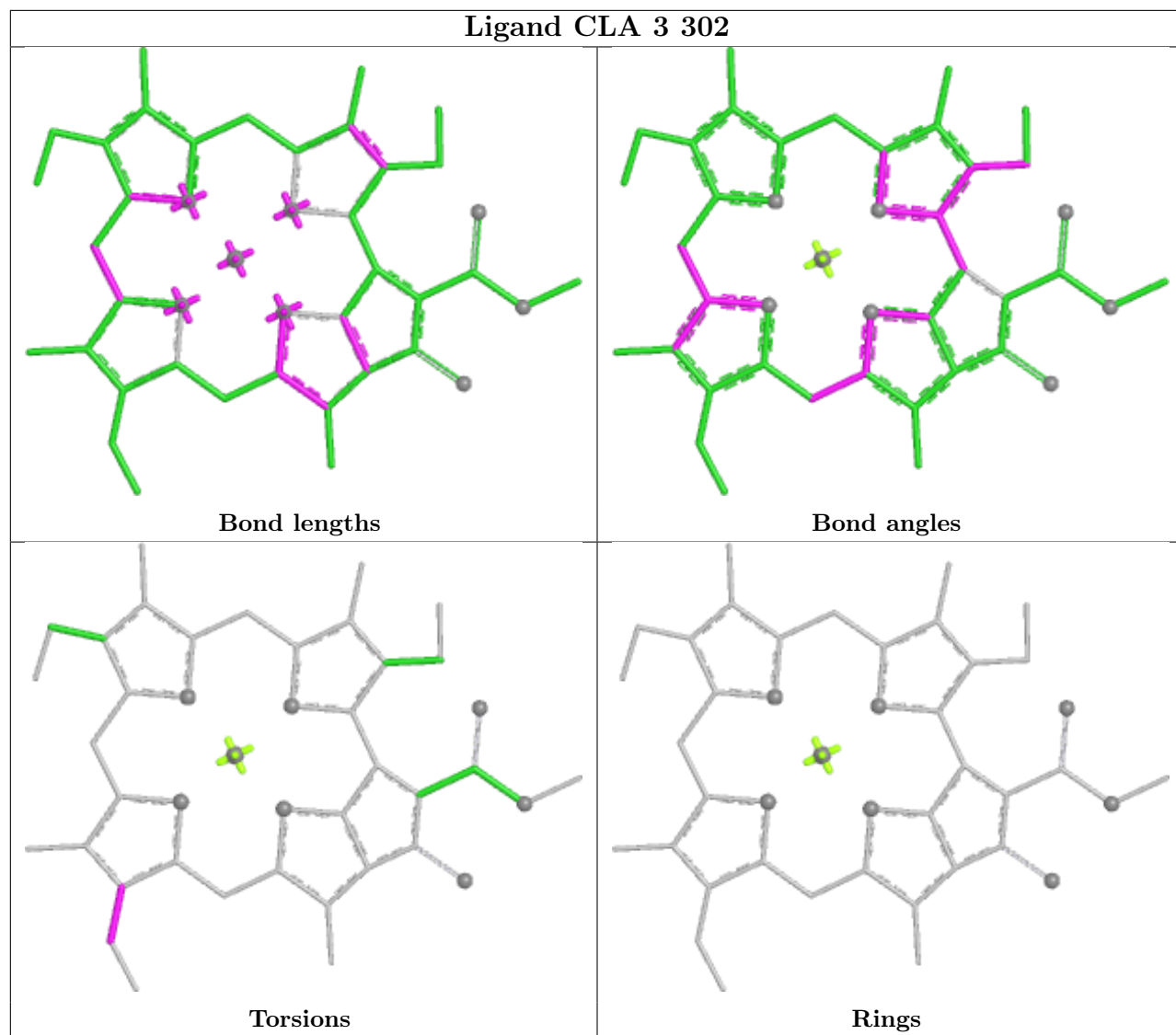
Ligand CLA 6 317



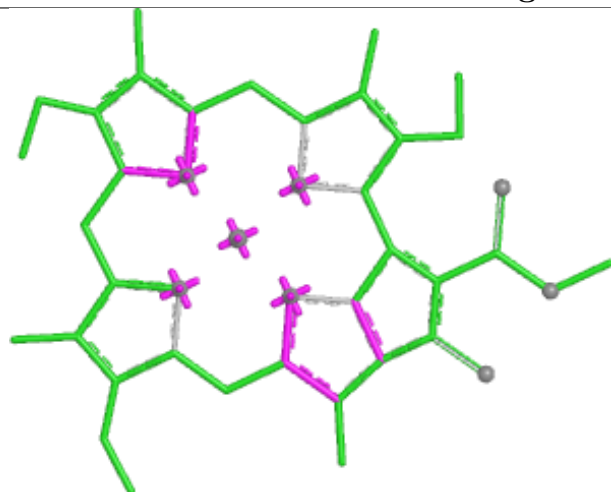
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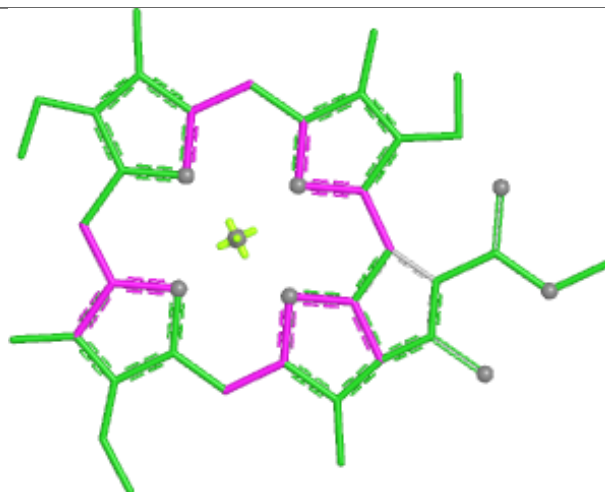
Ligand CLA 3 302



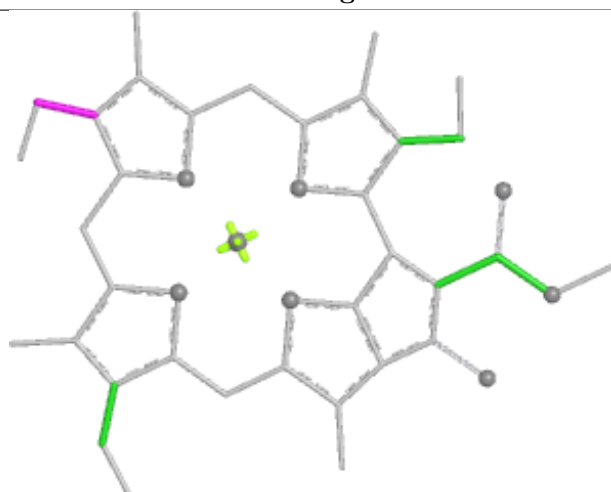
Ligand CLA 6 308



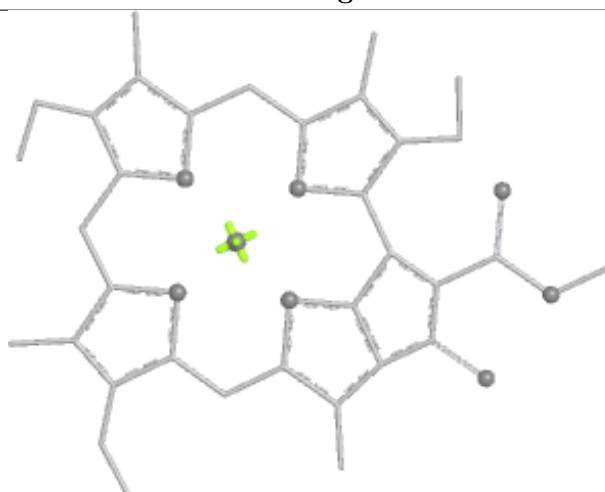
Bond lengths



Bond angles

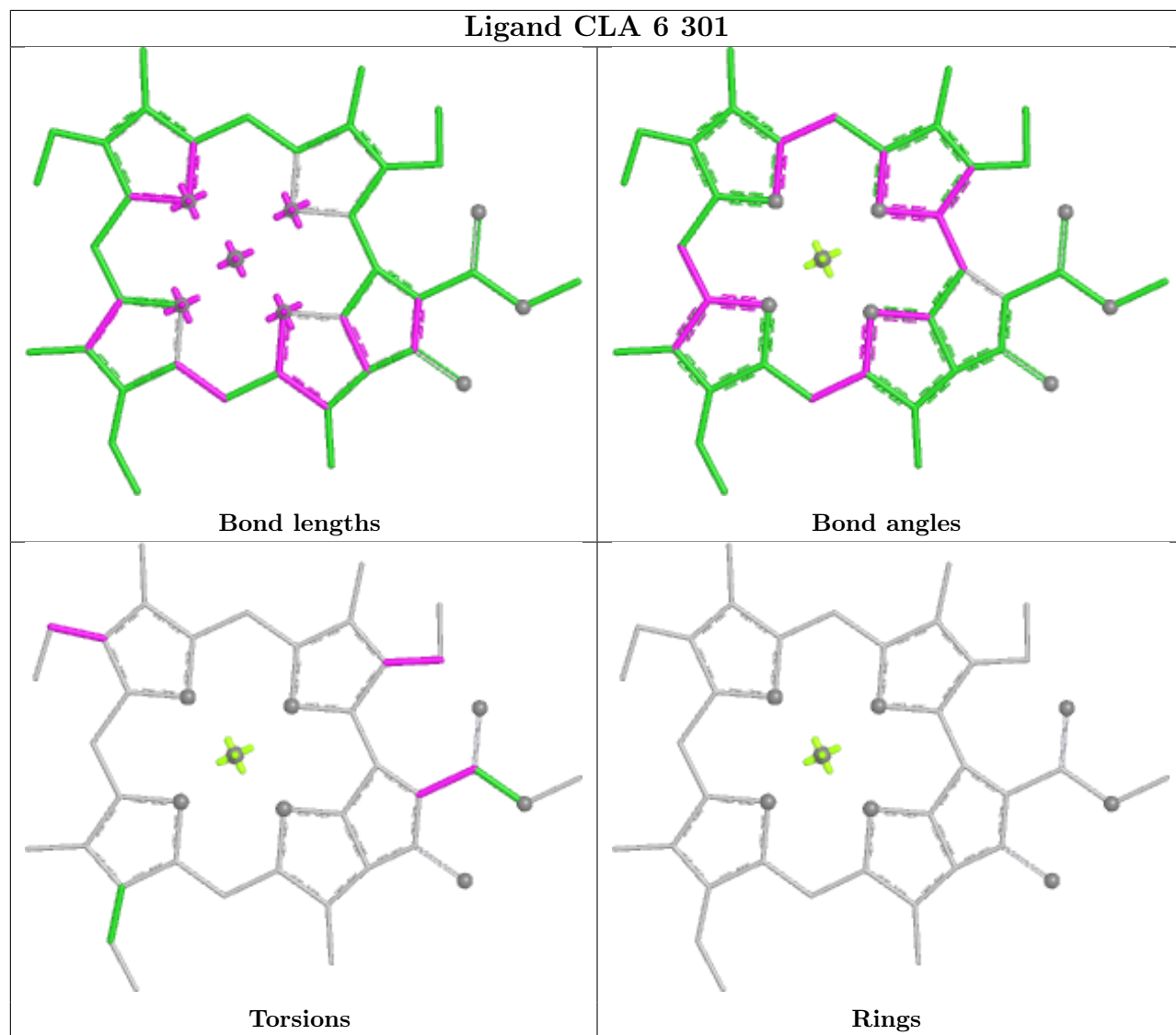


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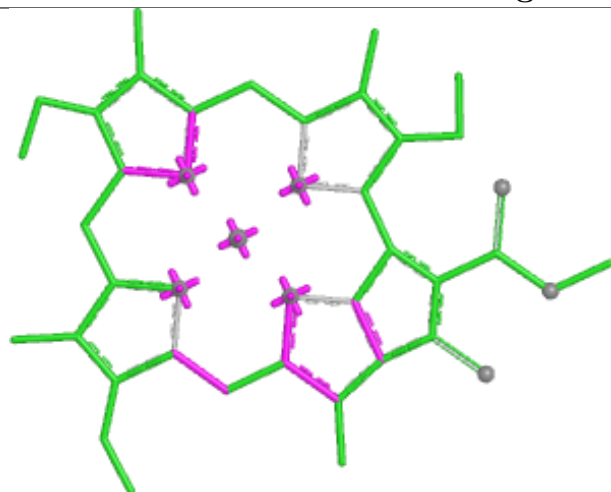


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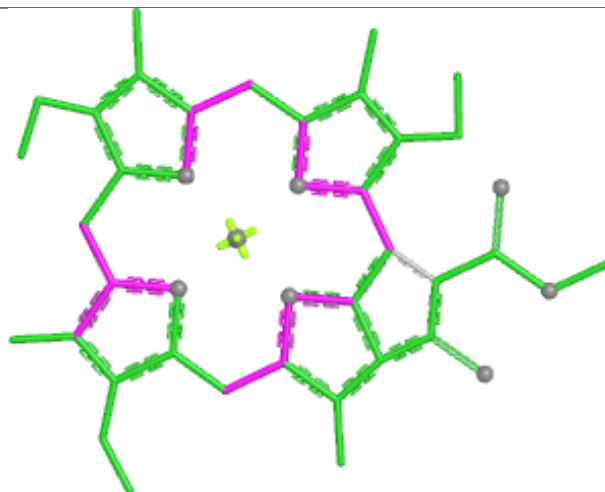
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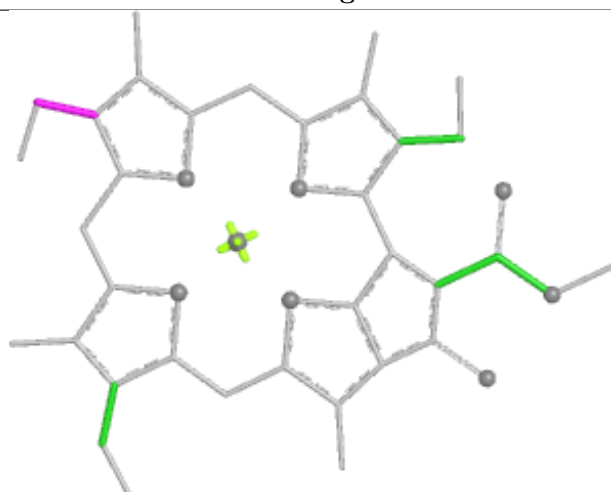
Ligand CLA Z 613



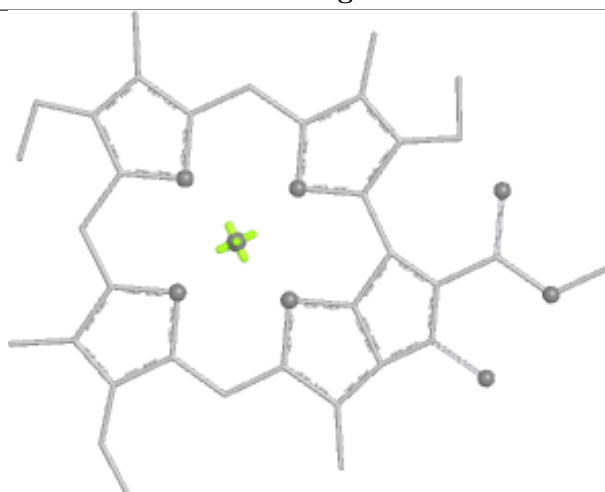
Bond lengths



Bond angles

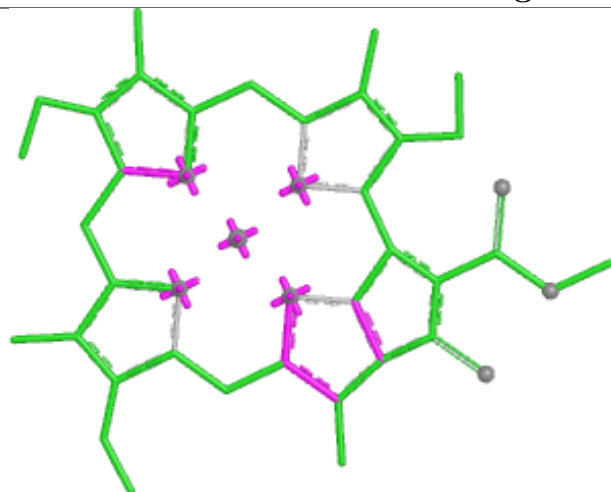


Torsions

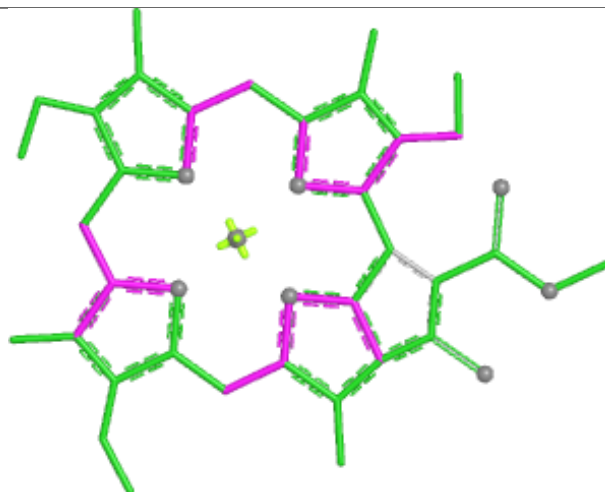


Rings

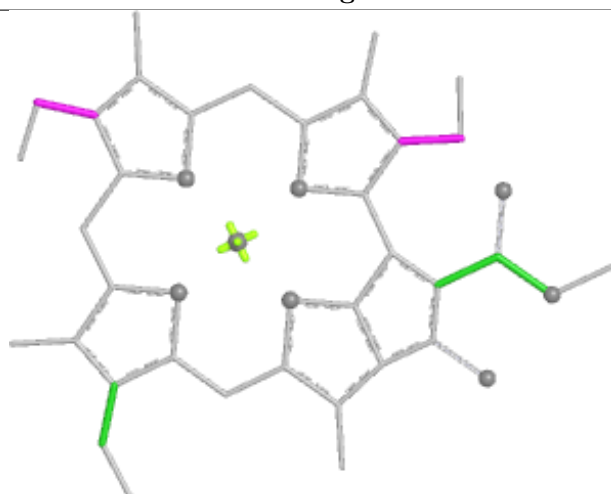
Ligand CLA B 818



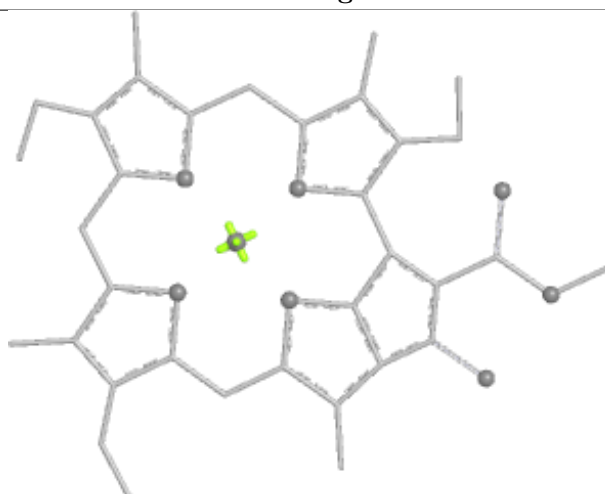
Bond lengths



Bond angles

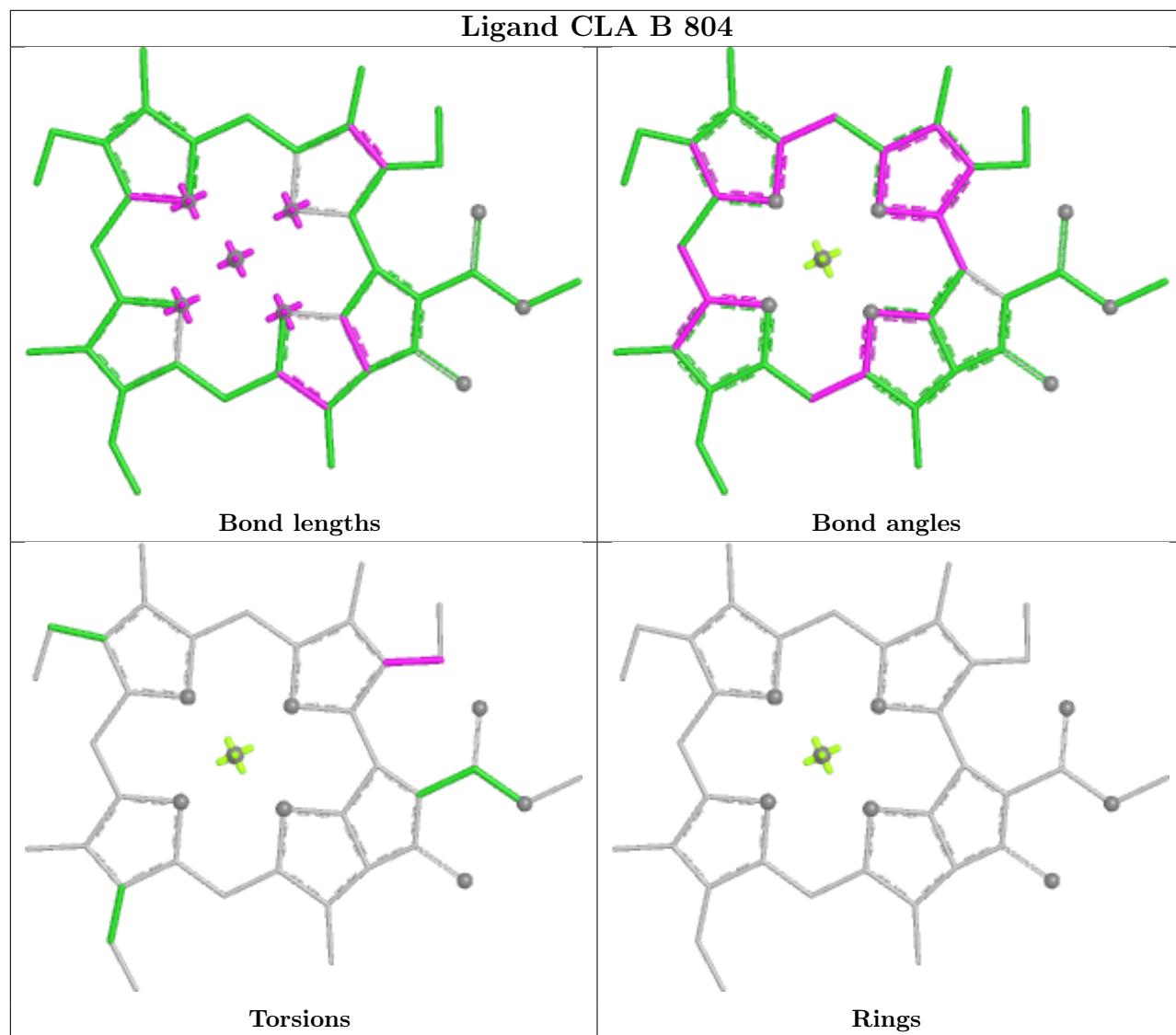


Torsions

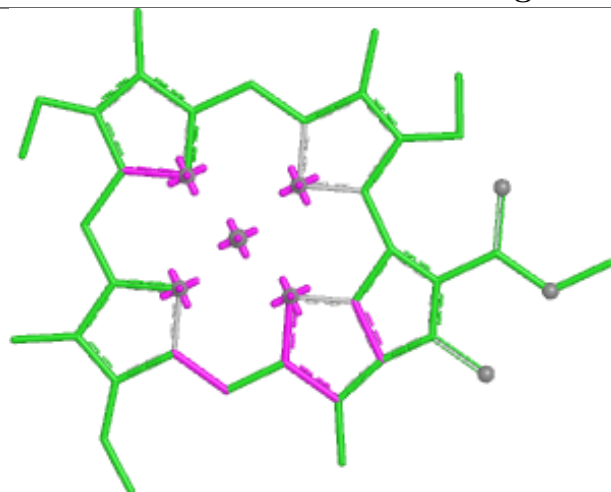


Rings

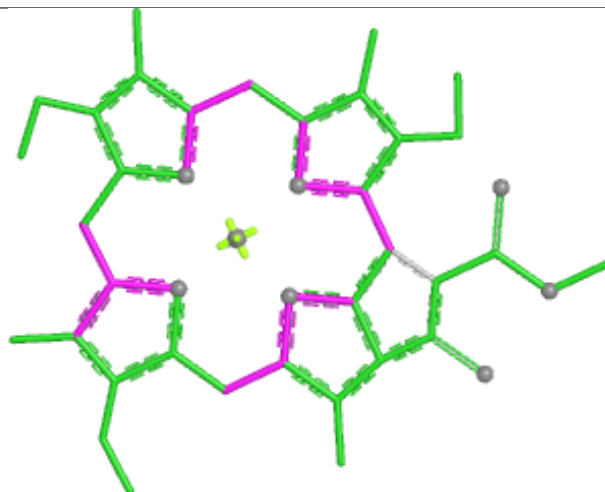
Ligand CLA B 804



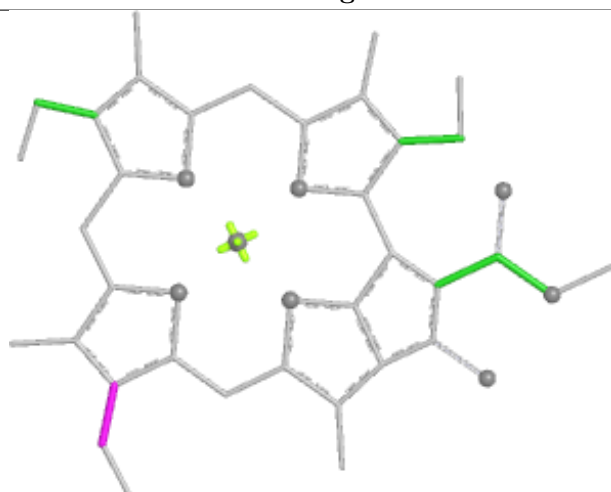
Ligand CLA B 833



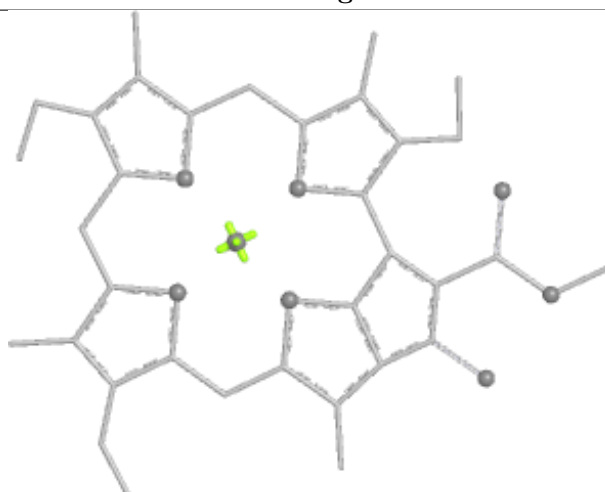
Bond lengths



Bond angles

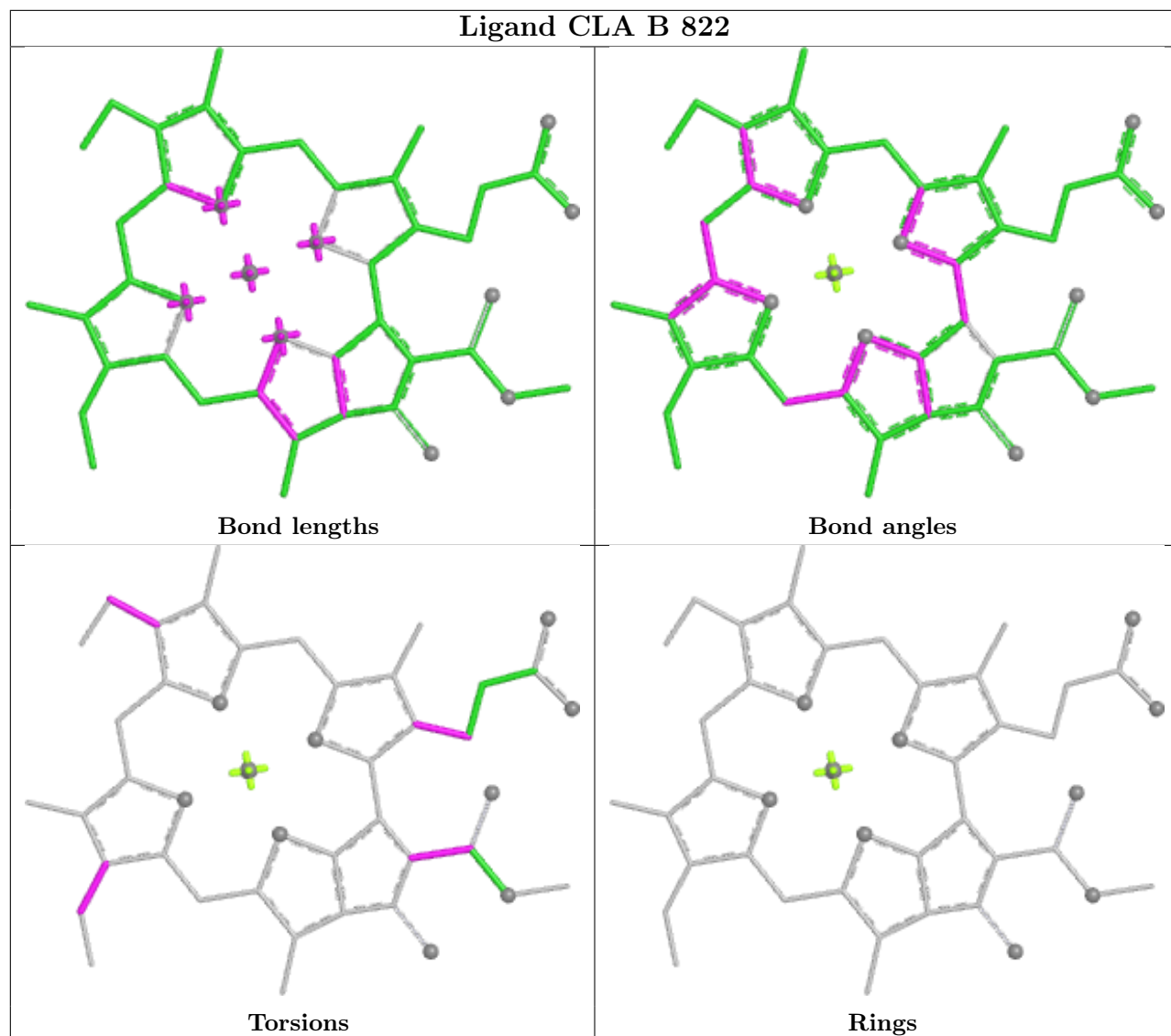


Torsions

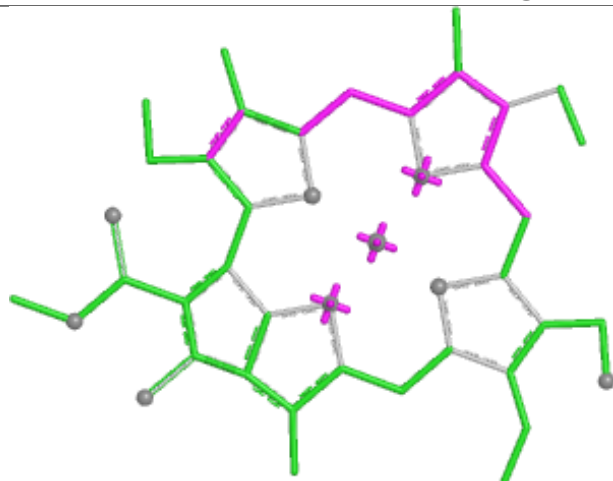


Rings

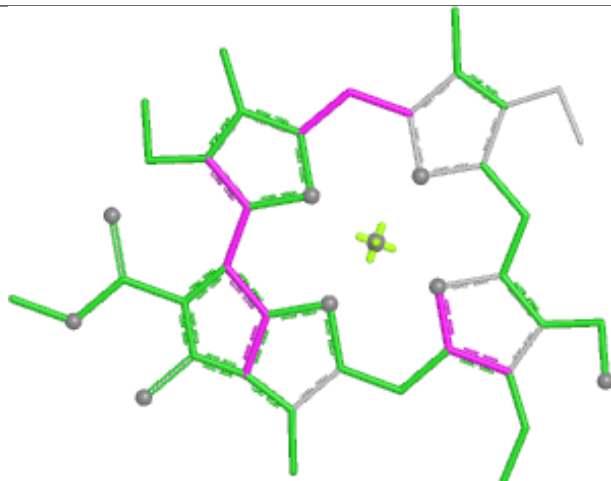
Ligand CLA B 822



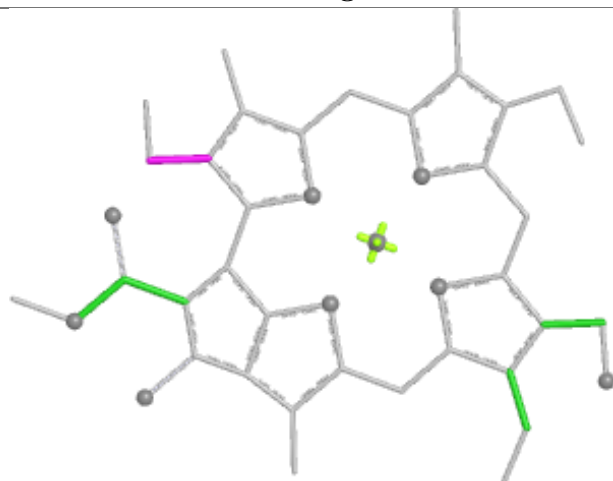
Ligand CHL 6 316



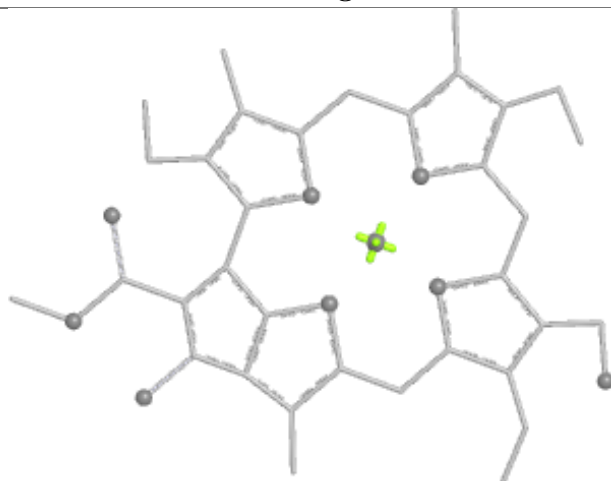
Bond lengths



Bond angles

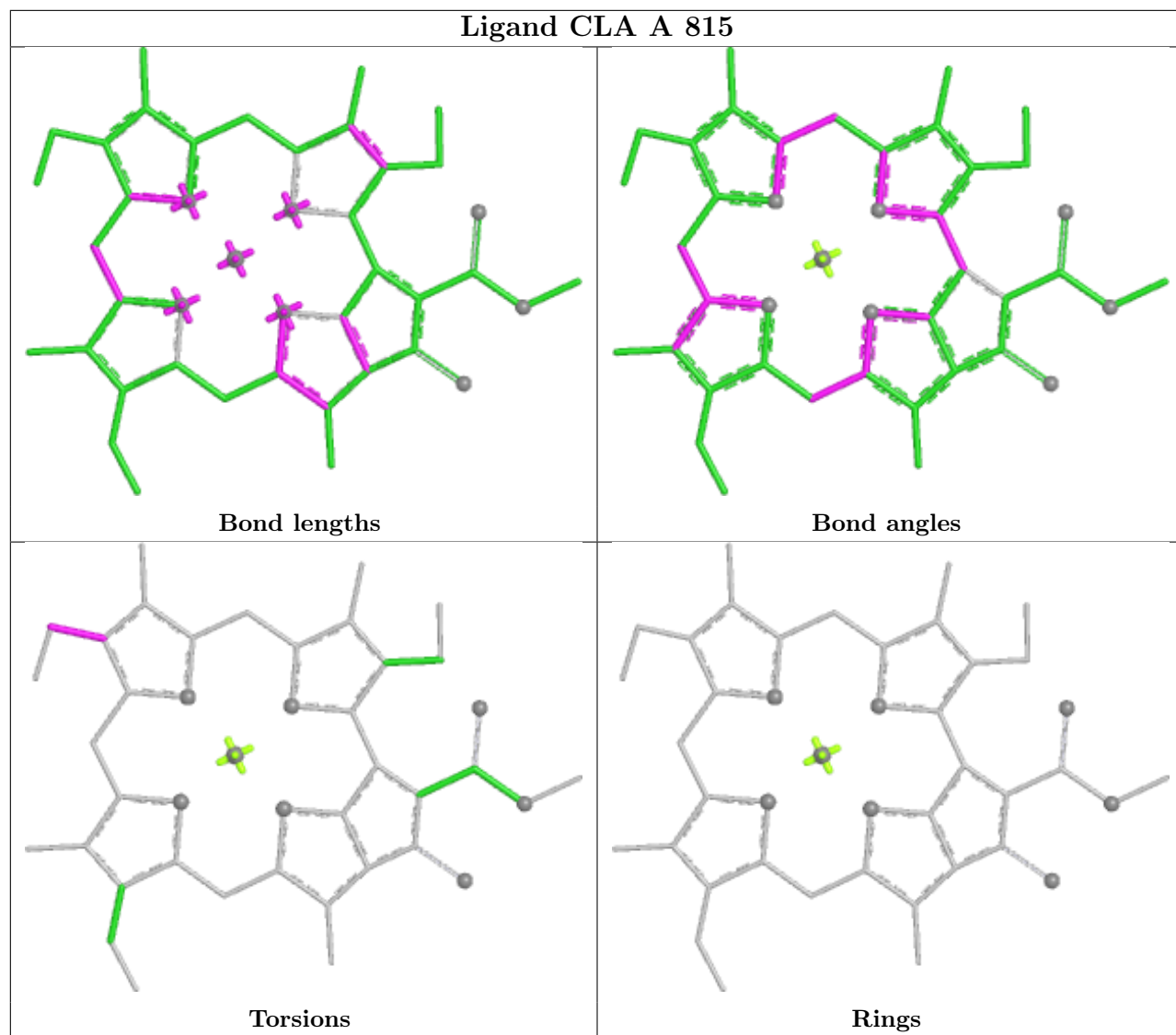


Torsions

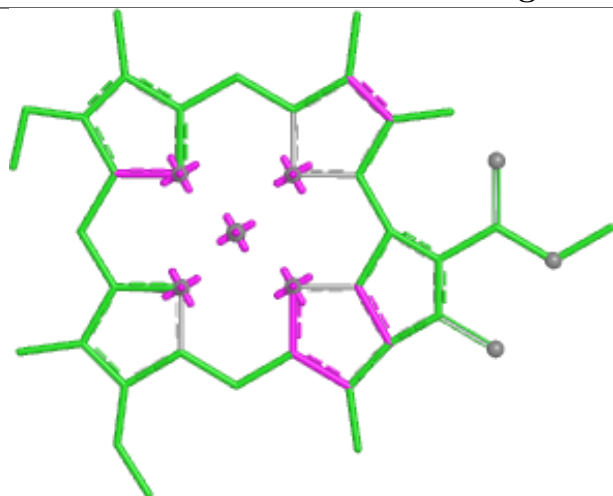


Rings

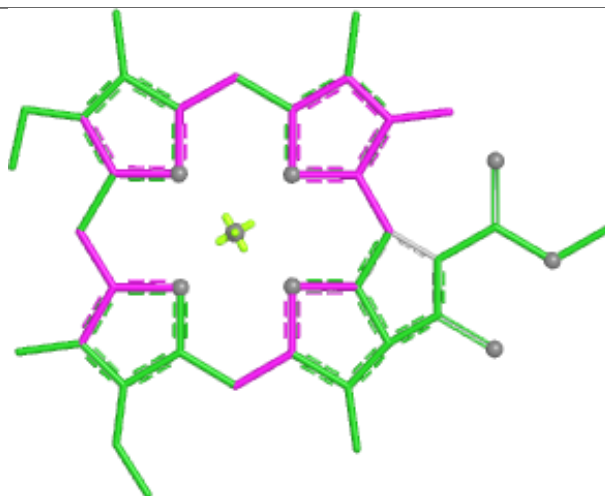
Ligand CLA A 815



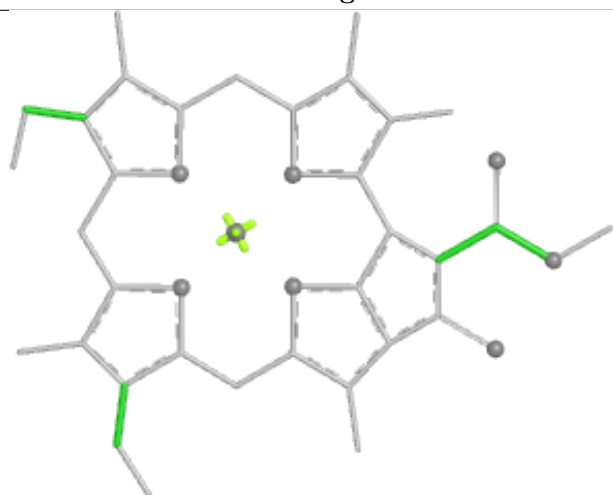
Ligand CLA 7 610



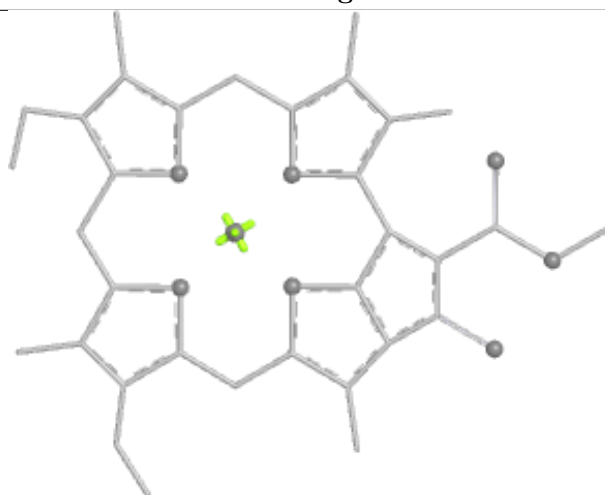
Bond lengths



Bond angles

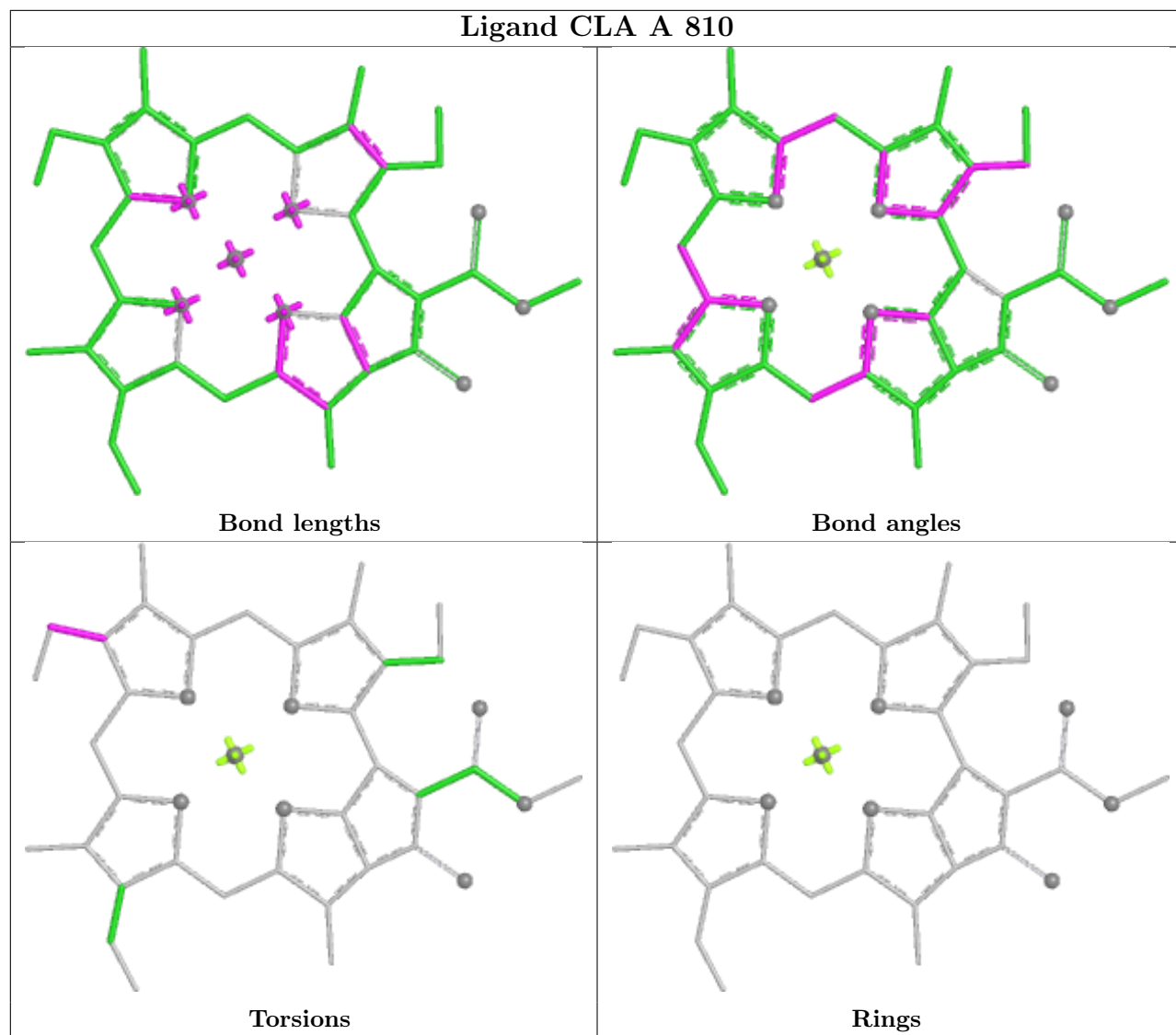


Torsions

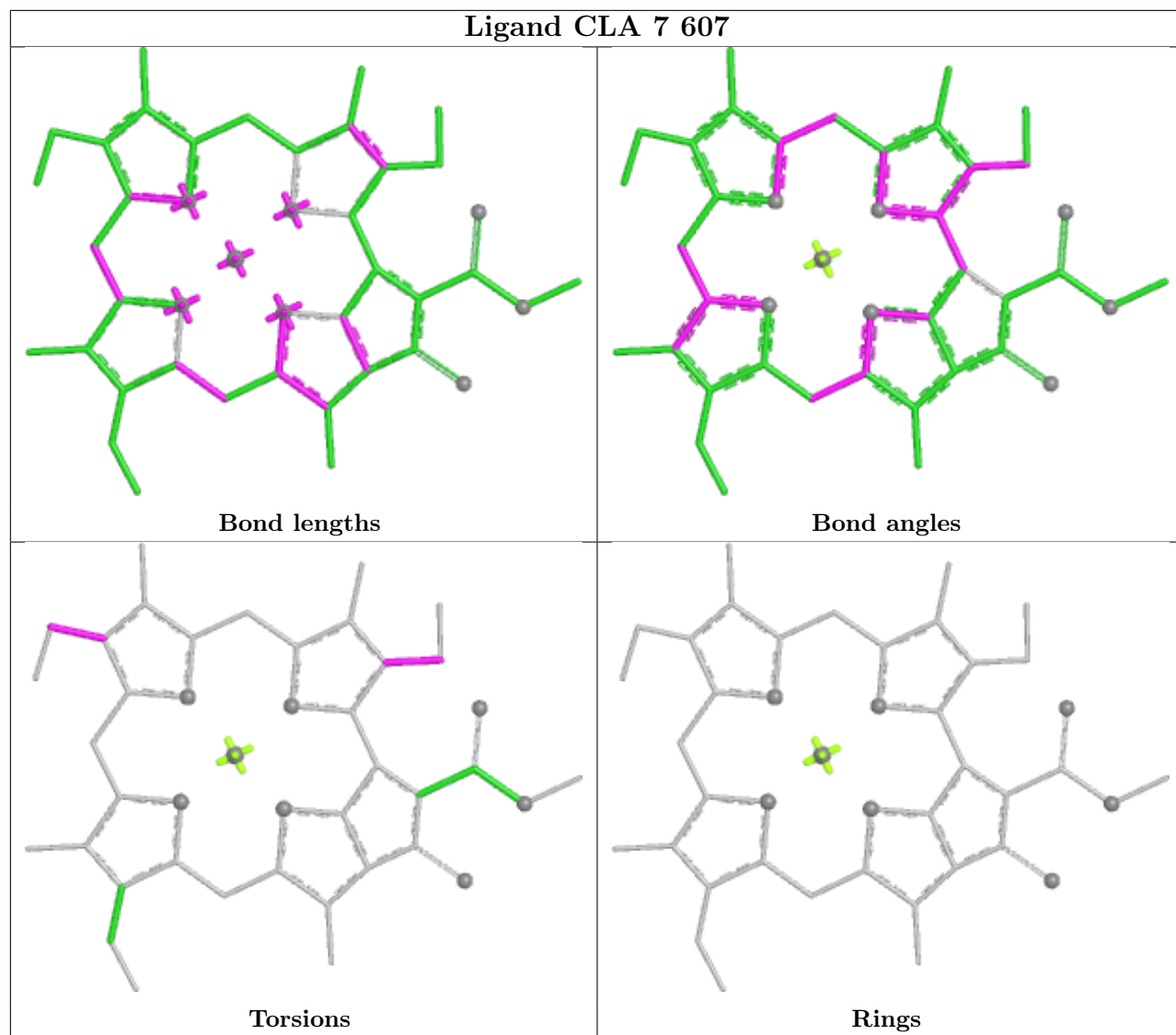


Rings

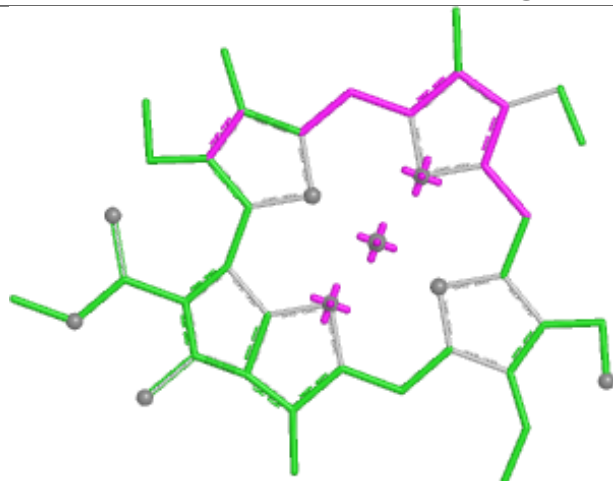
Ligand CLA A 810



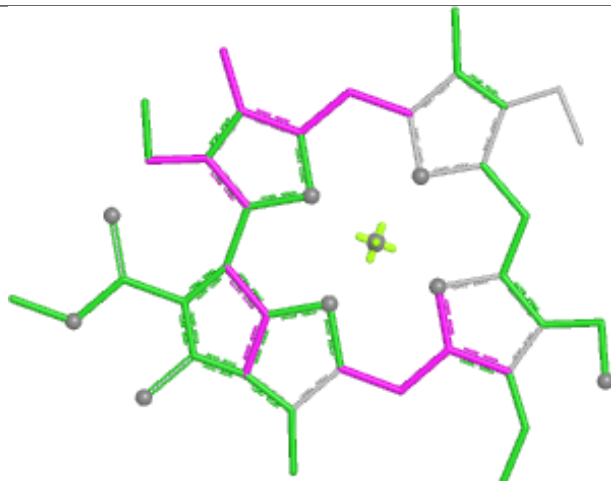
Ligand CLA 7 607



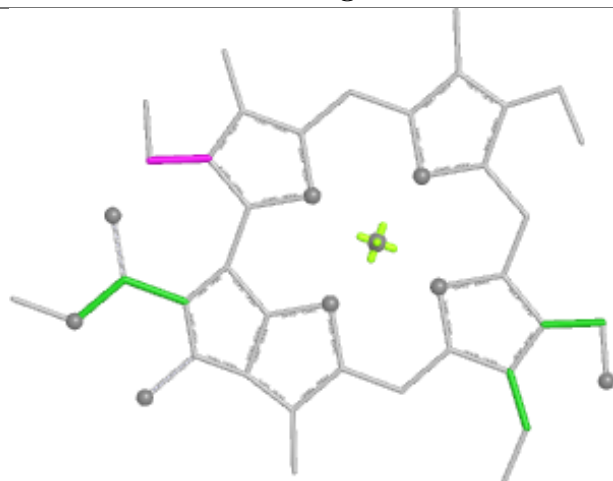
Ligand CHL 5 607



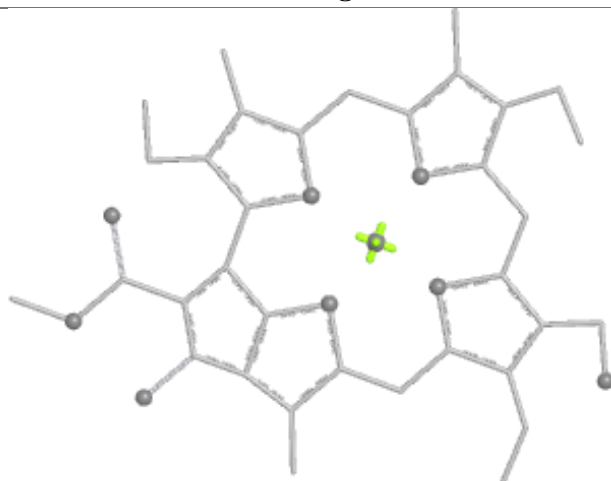
Bond lengths



Bond angles

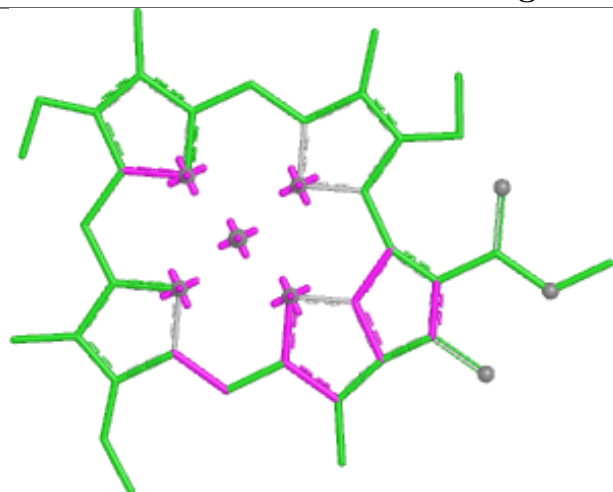


Torsions

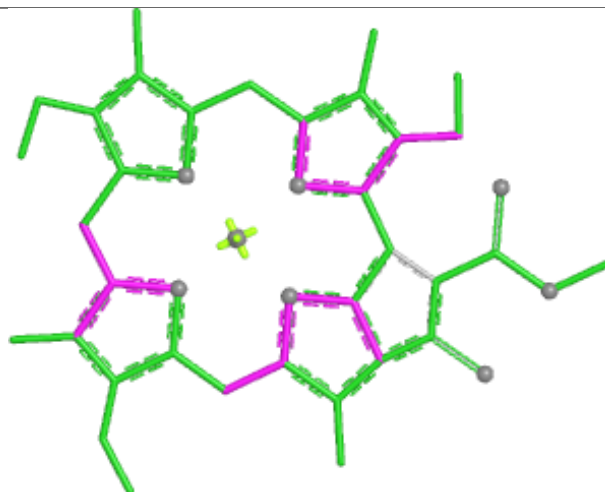


Rings

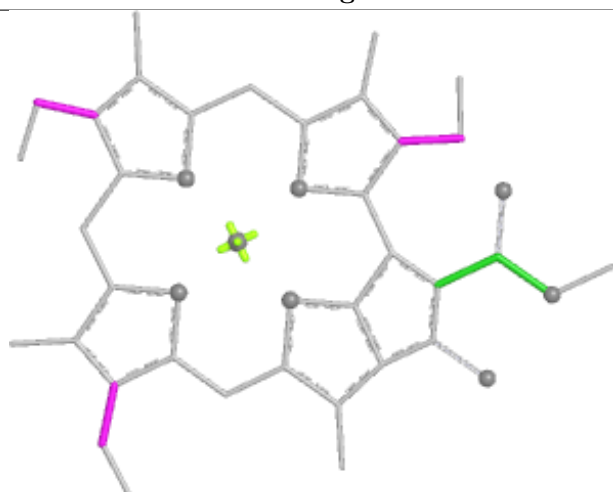
Ligand CLA 5 602



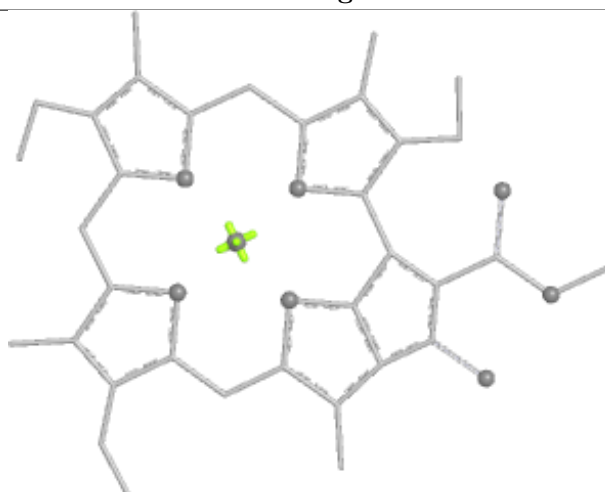
Bond lengths



Bond angles

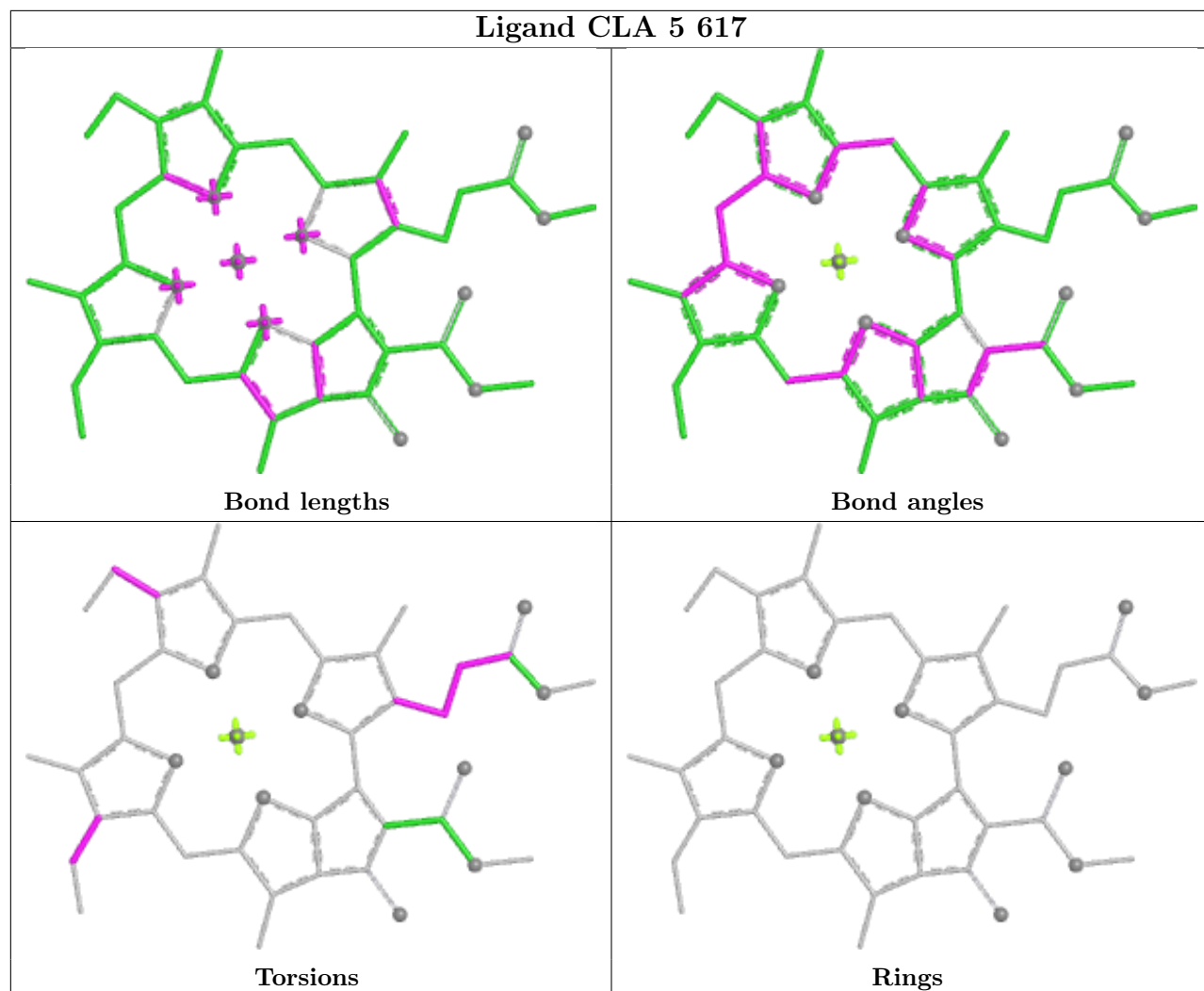


Torsions

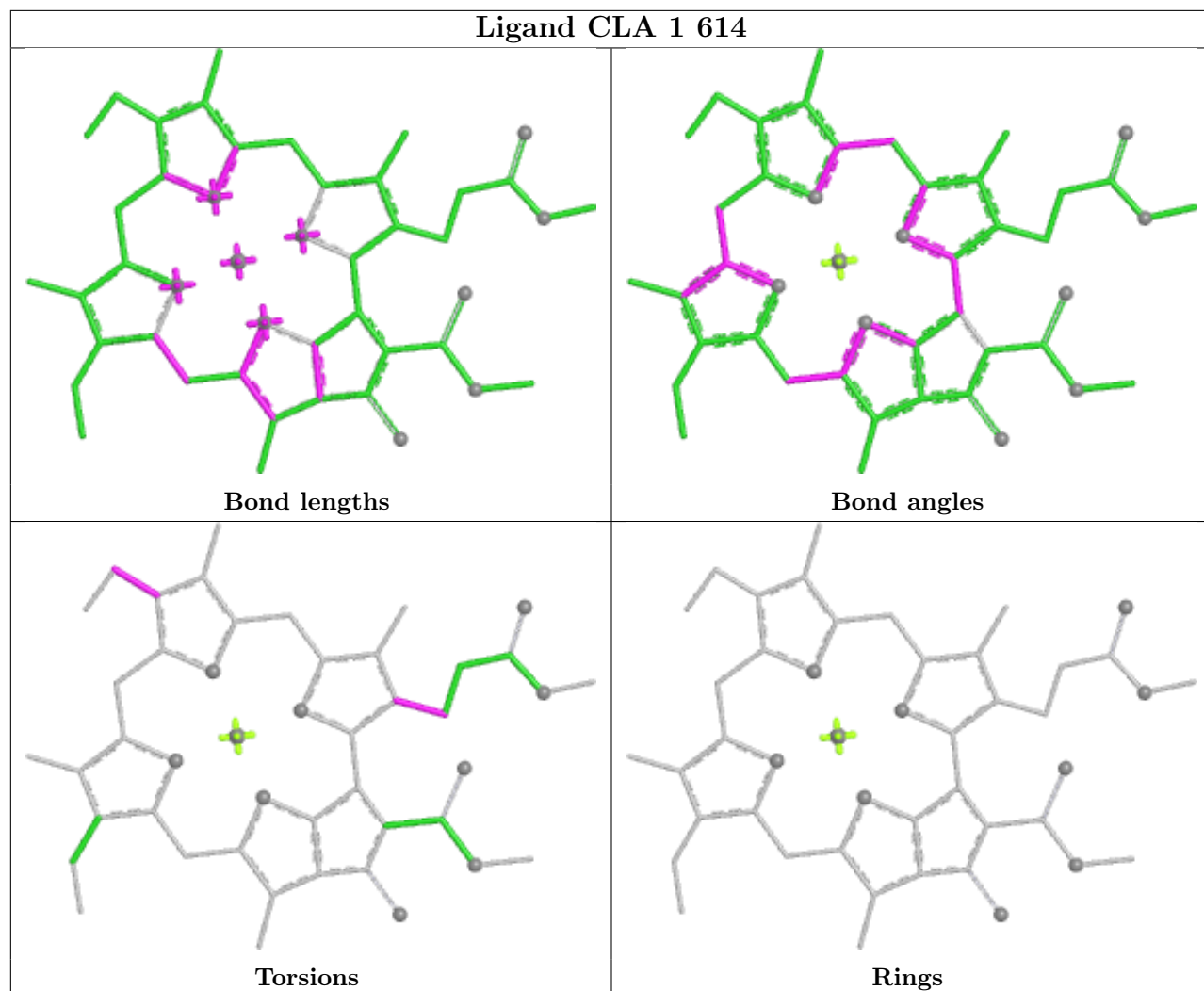


Rings

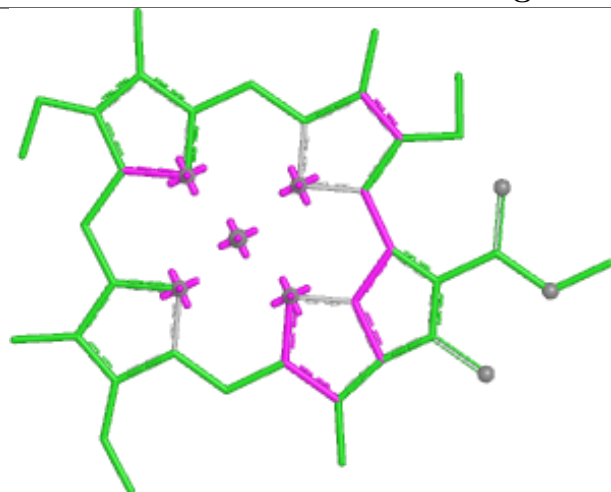
Ligand CLA 5 617



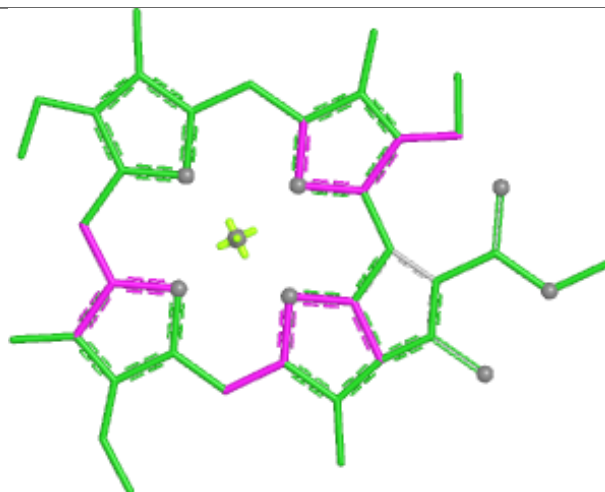
Ligand CLA 1 614



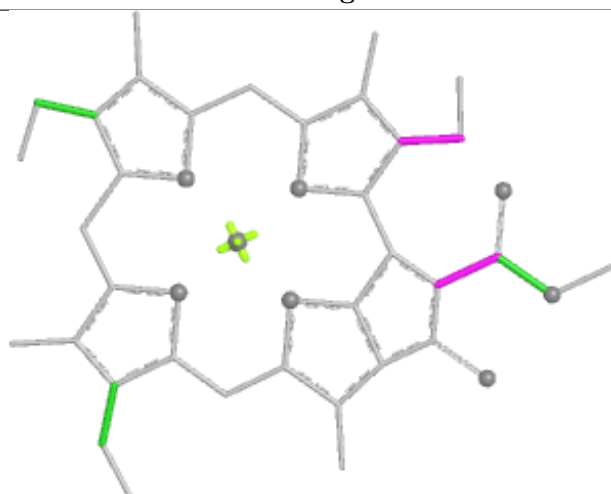
Ligand CLA A 803



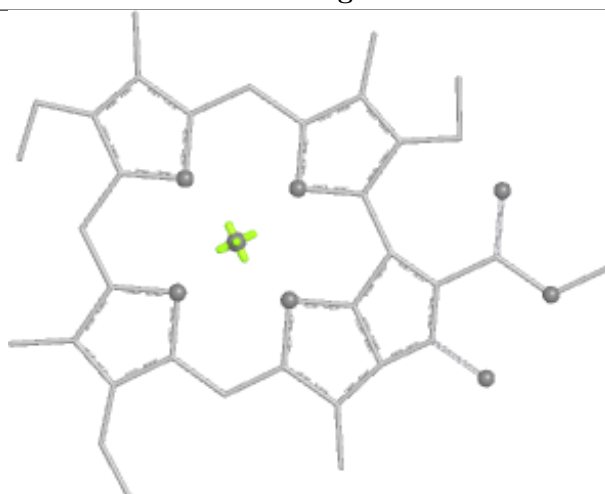
Bond lengths



Bond angles

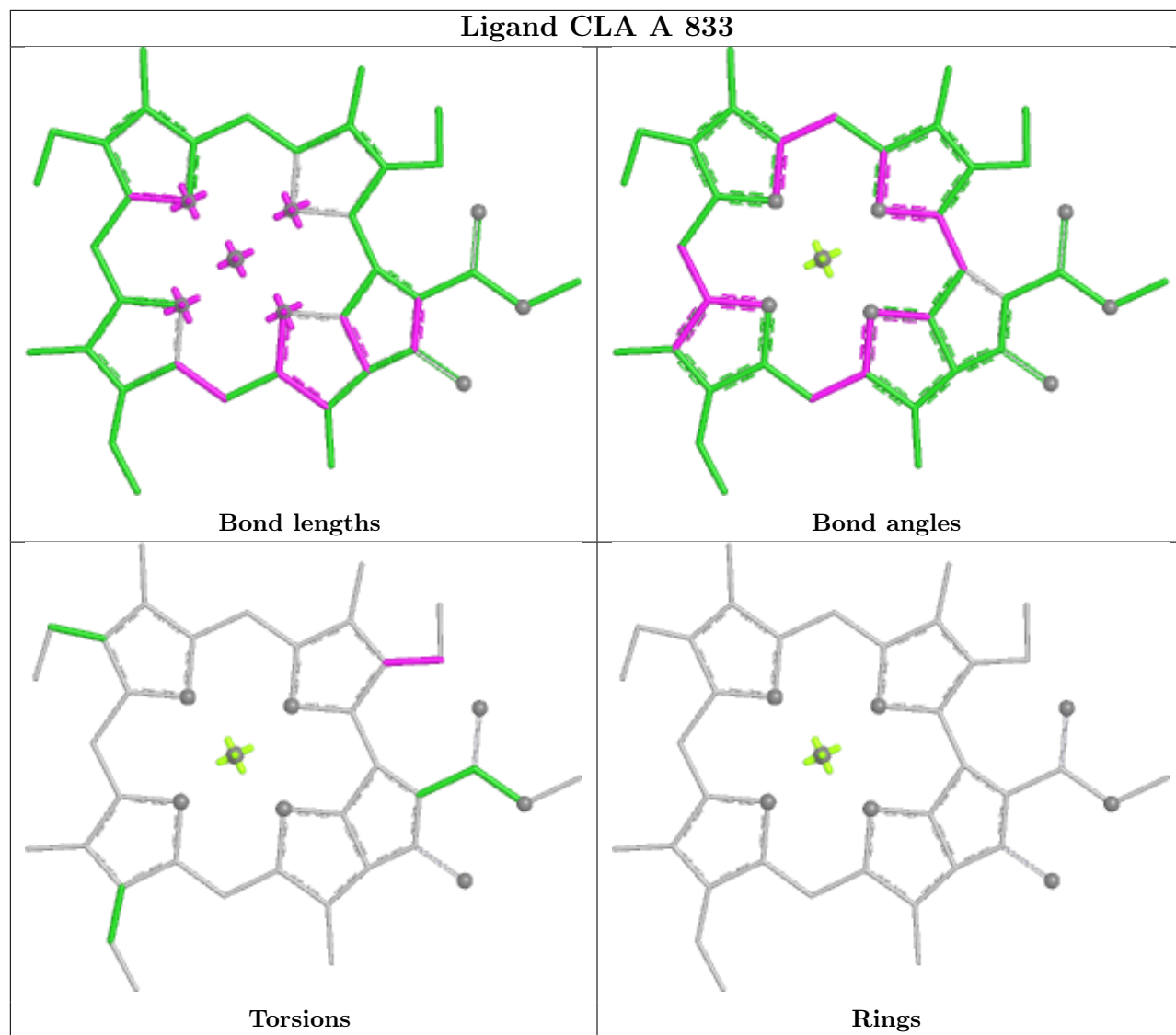


Torsions

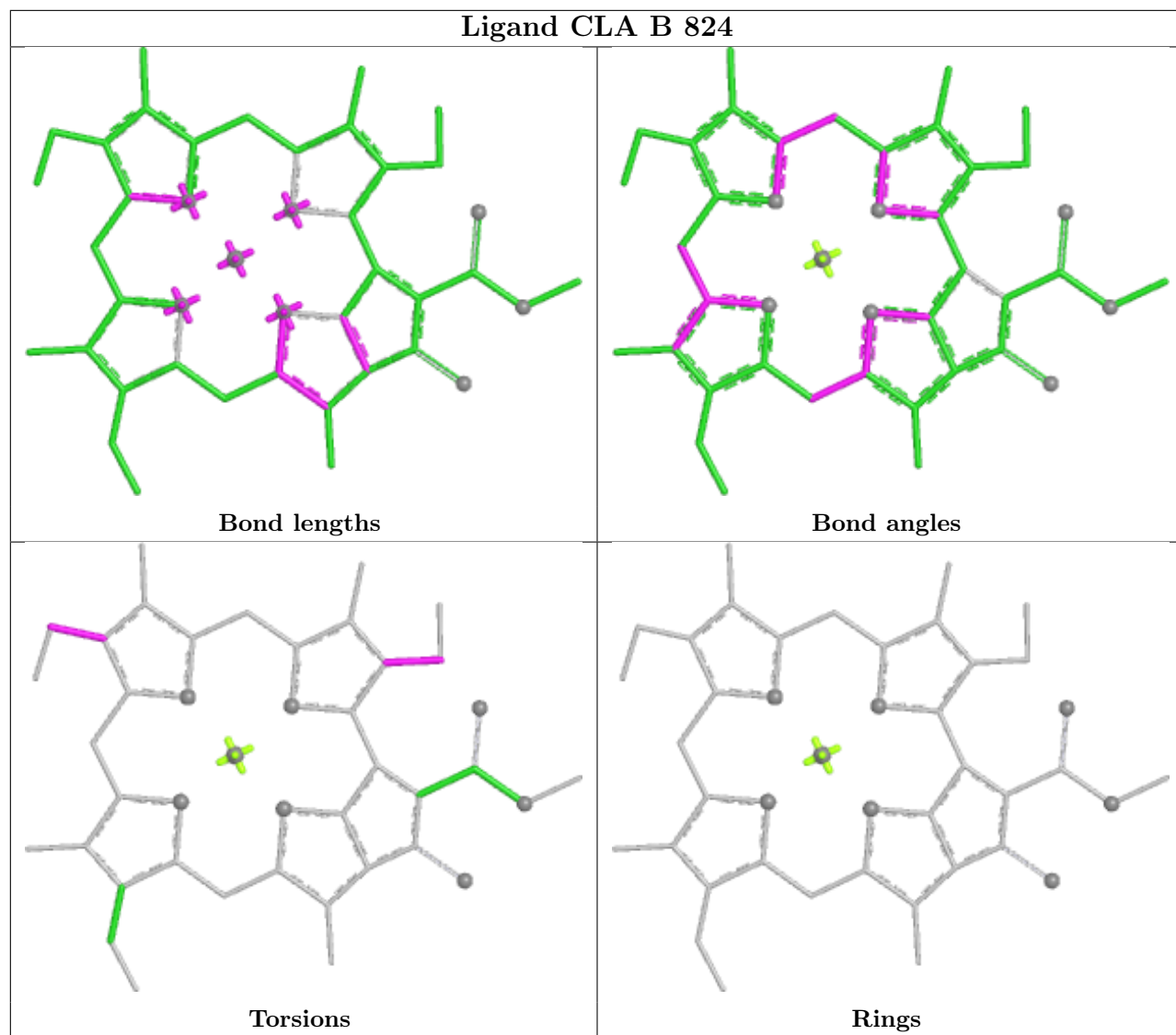


Rings

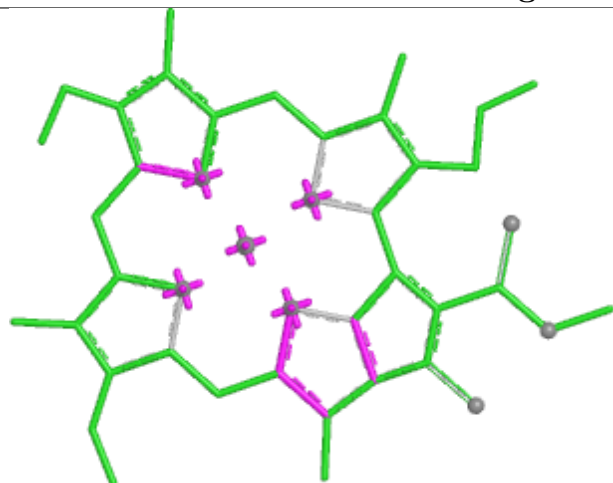
Ligand CLA A 833



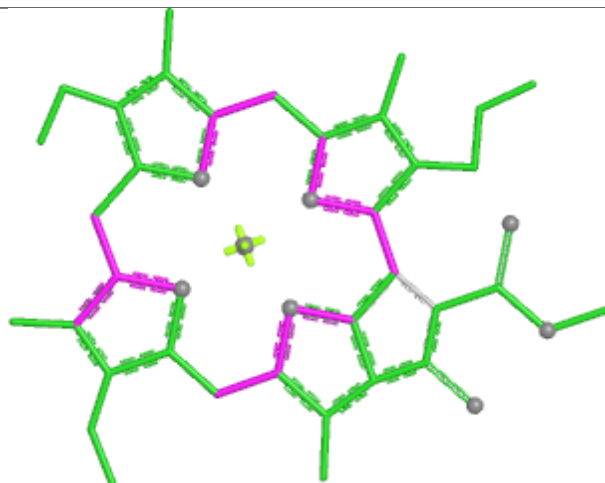
Ligand CLA B 824



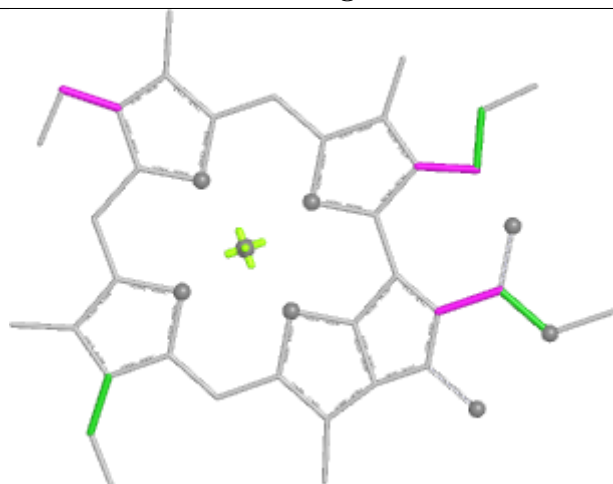
Ligand CLA 7 613



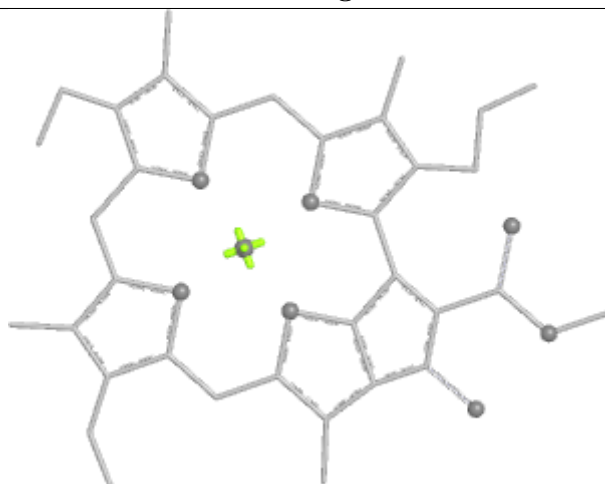
Bond lengths



Bond angles

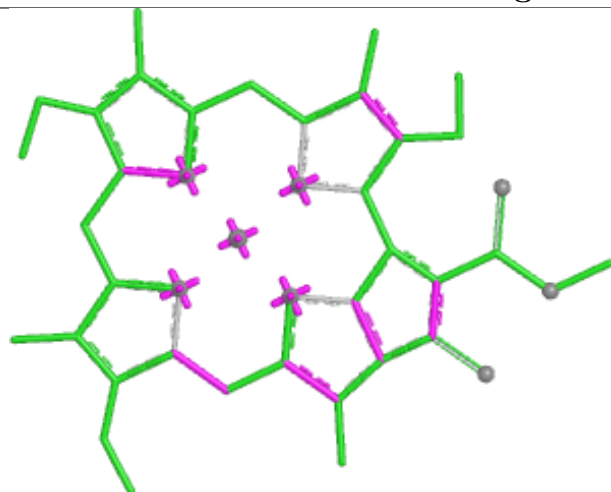


Torsions

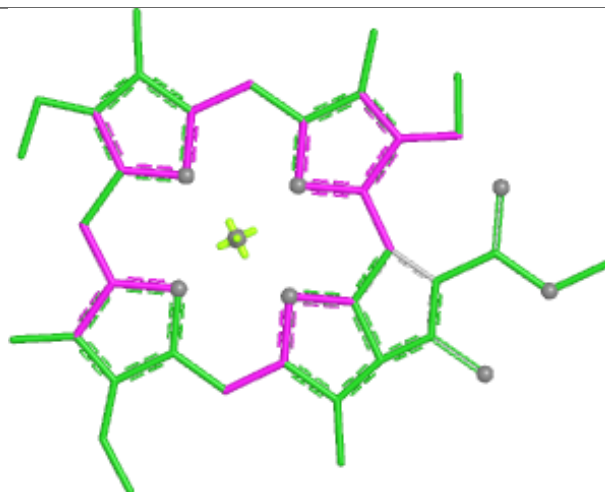


Rings

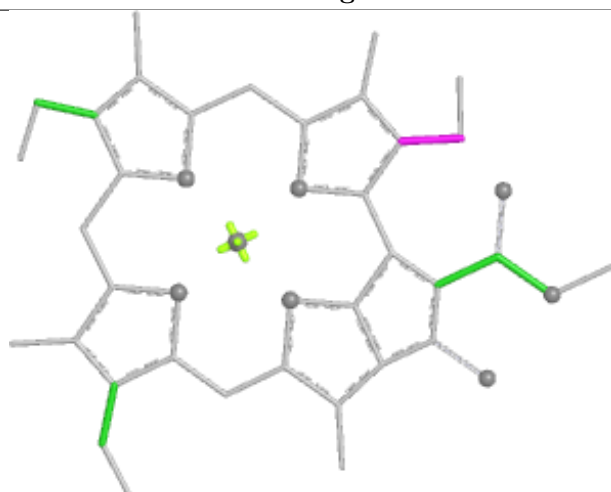
Ligand CLA B 805



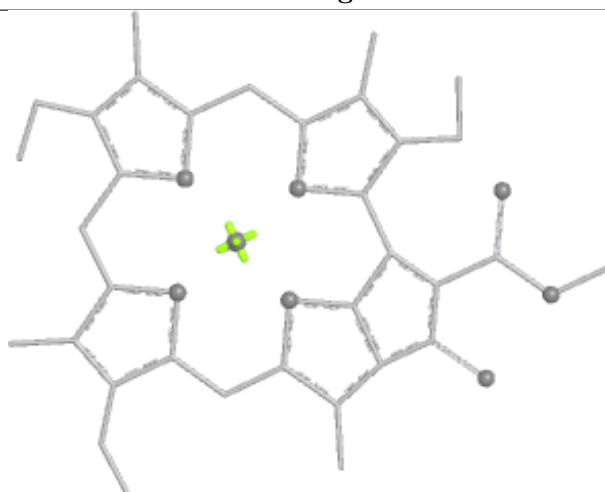
Bond lengths



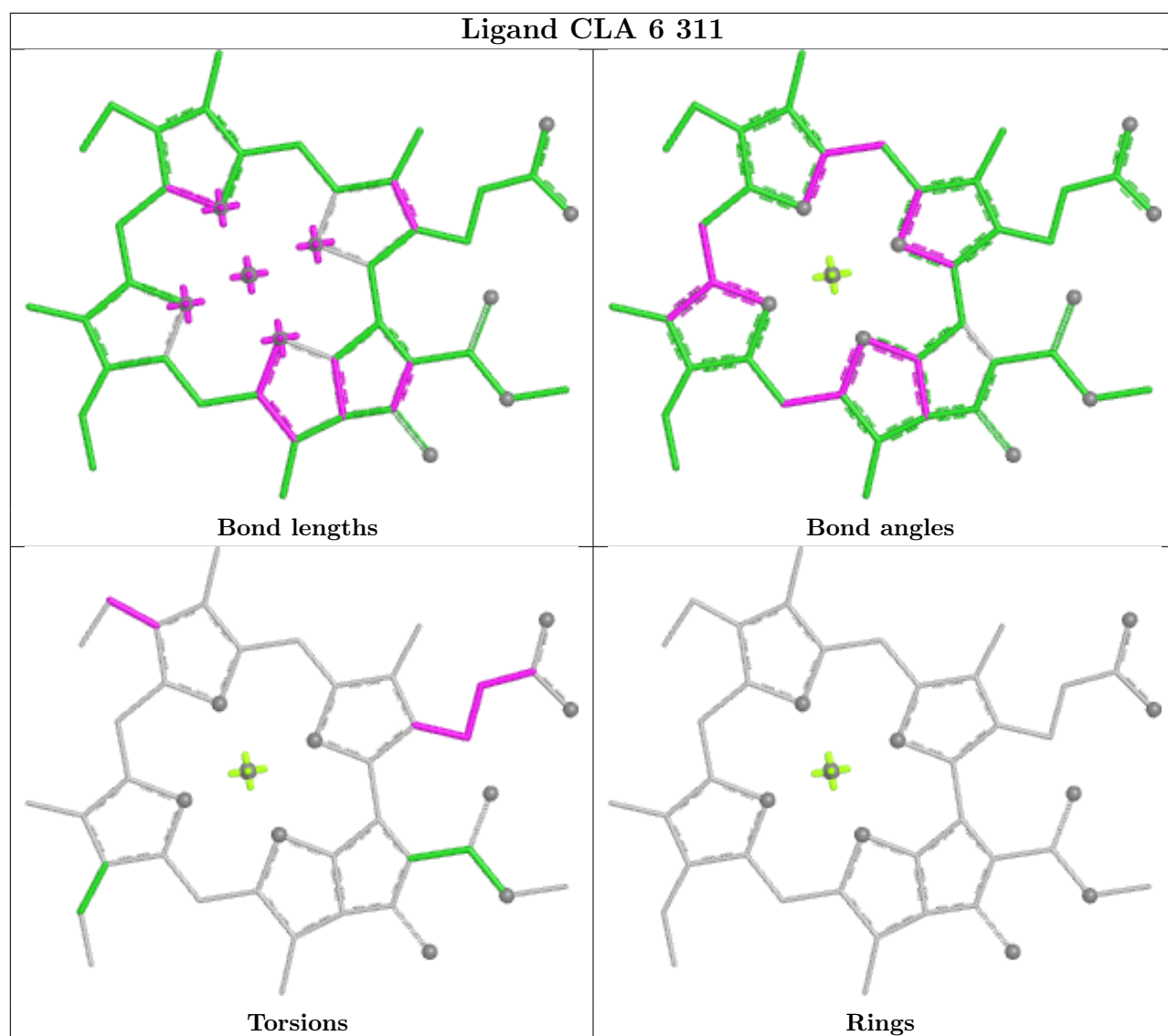
Bond angles



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.

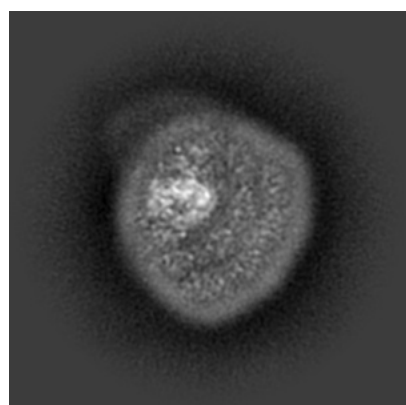
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32907. These allow visual inspection of the internal detail of the map and identification of artifacts.

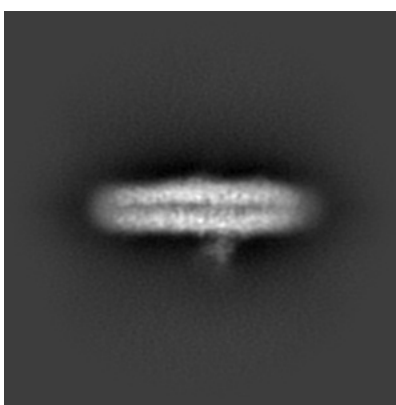
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

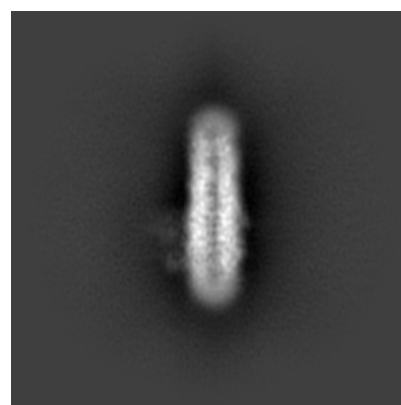
6.1.1 Primary map



X



Y

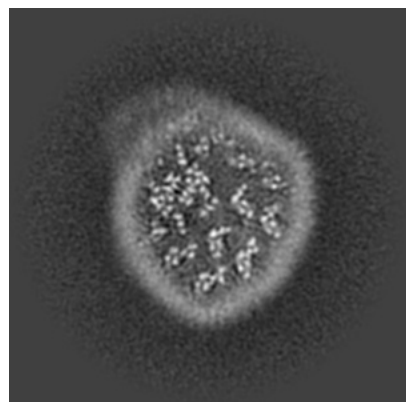


Z

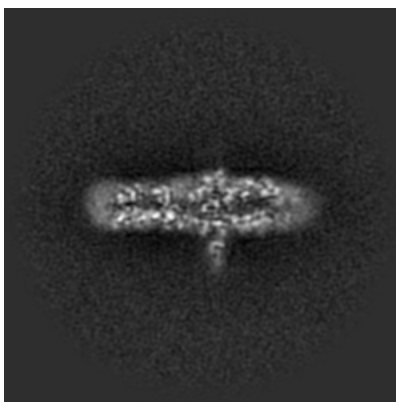
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

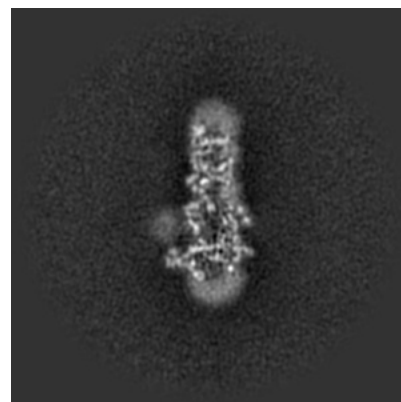
6.2.1 Primary map



X Index: 196



Y Index: 196

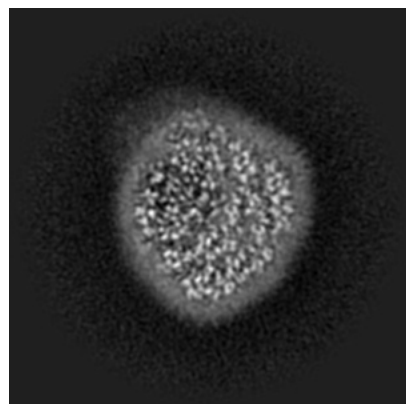


Z Index: 196

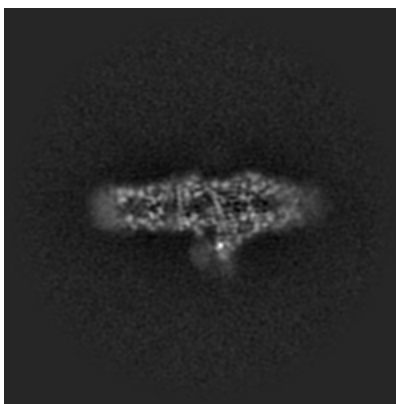
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

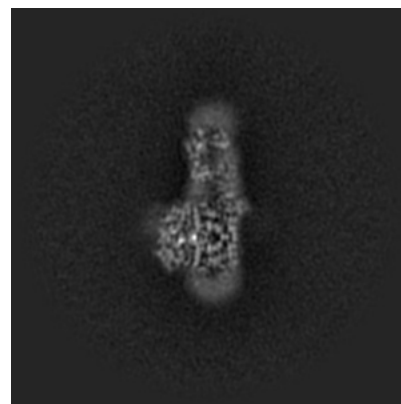
6.3.1 Primary map



X Index: 186



Y Index: 172

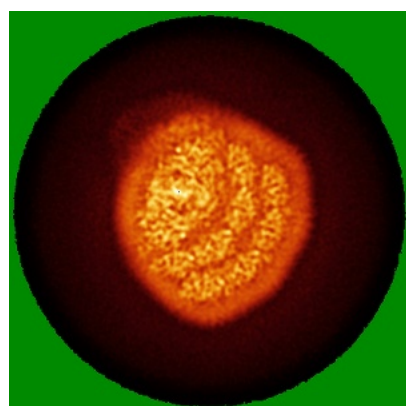


Z Index: 214

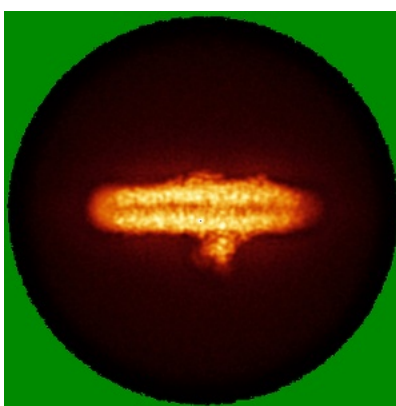
The images above show the largest variance slices of the map in three orthogonal directions.

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

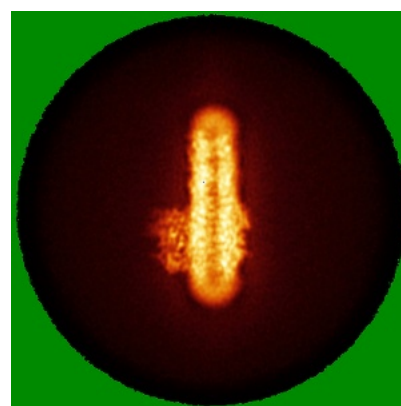
6.4.1 Primary map



X



Y

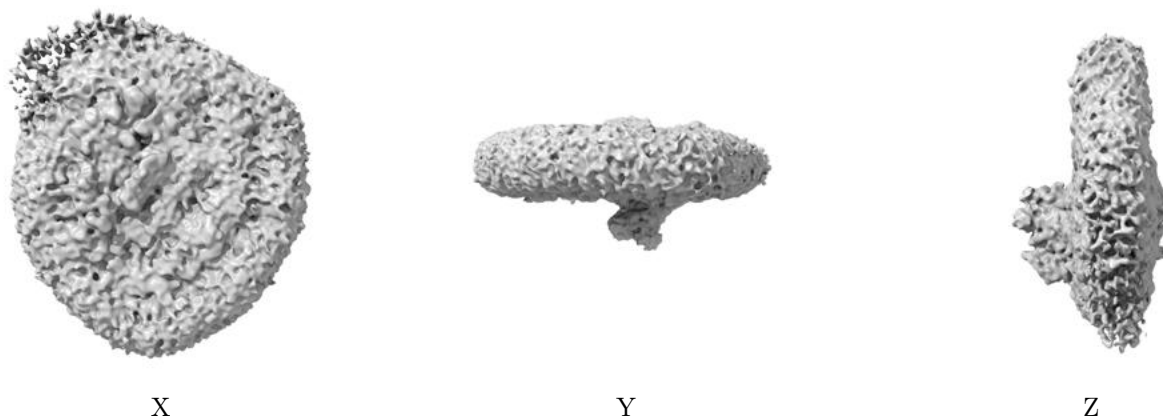


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

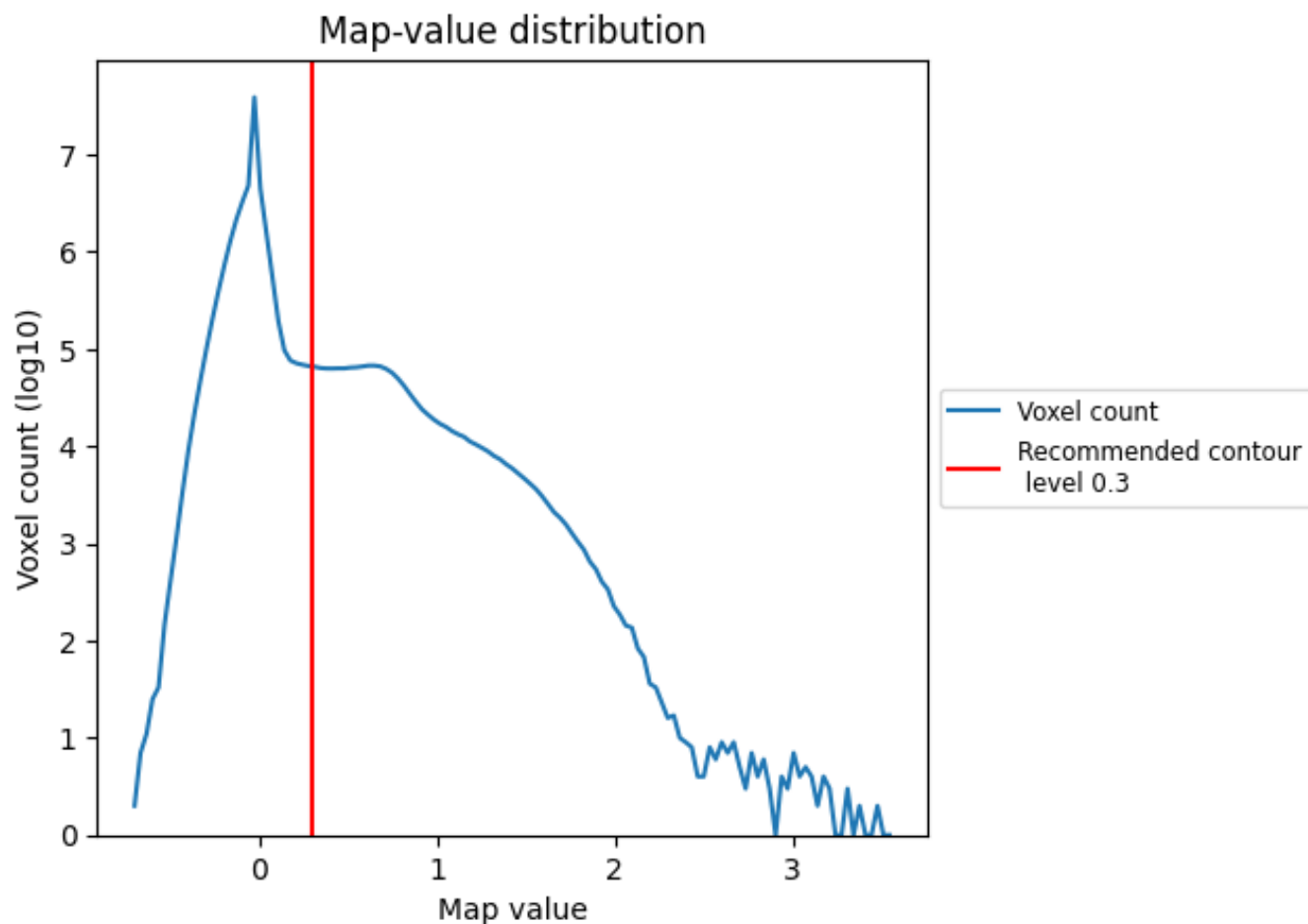
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

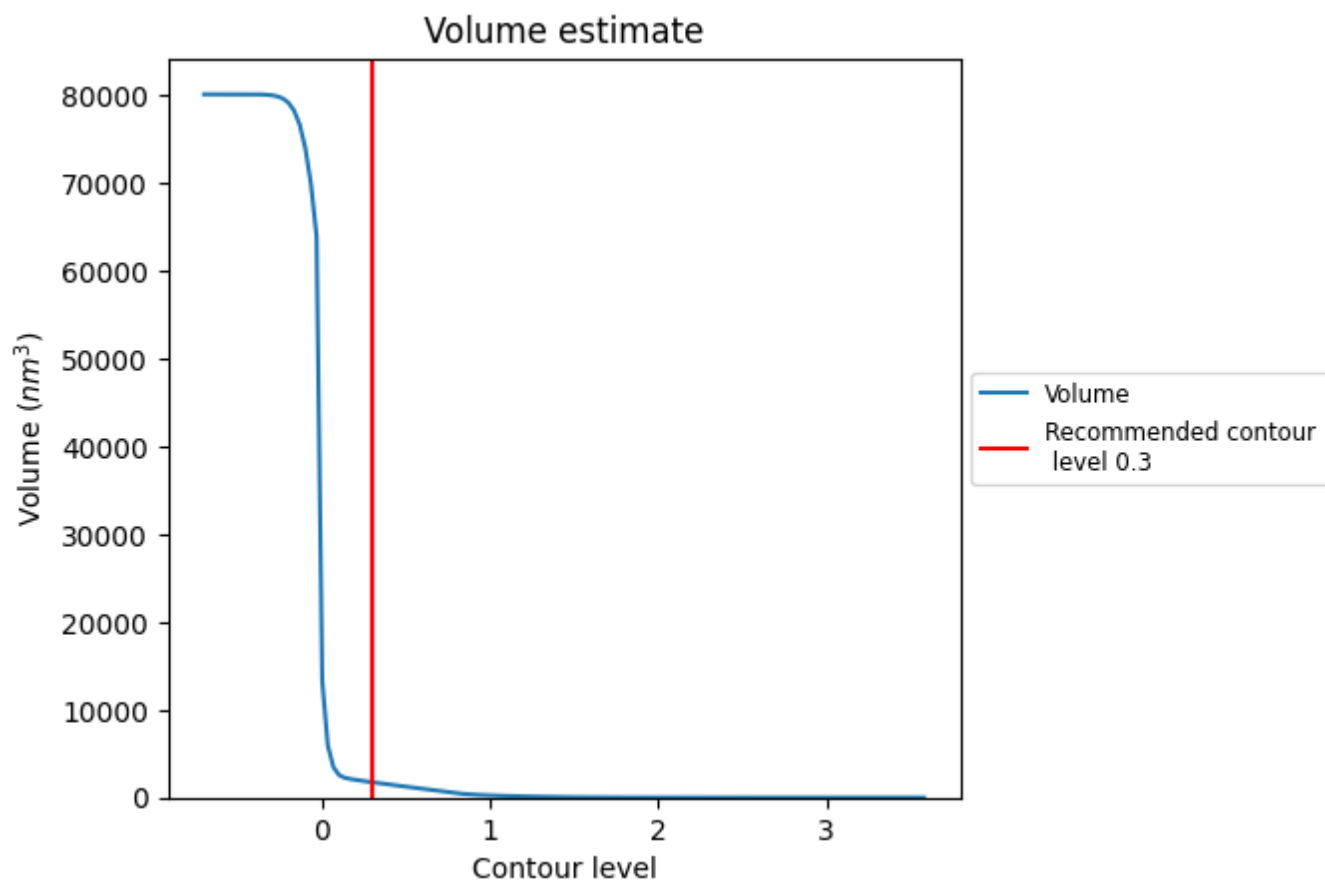
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

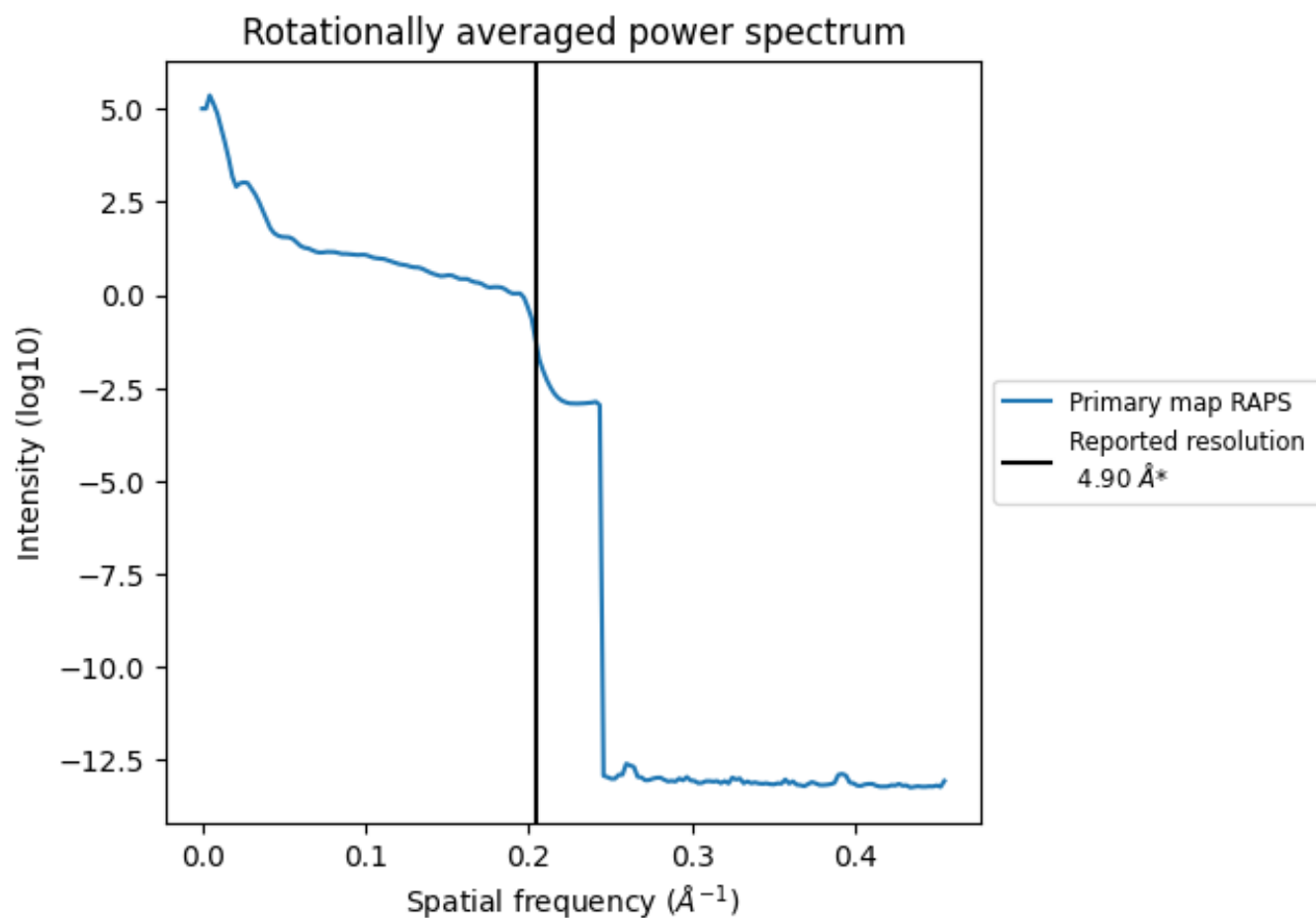
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1747 nm^3 ; this corresponds to an approximate mass of 1578 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 ⓘ

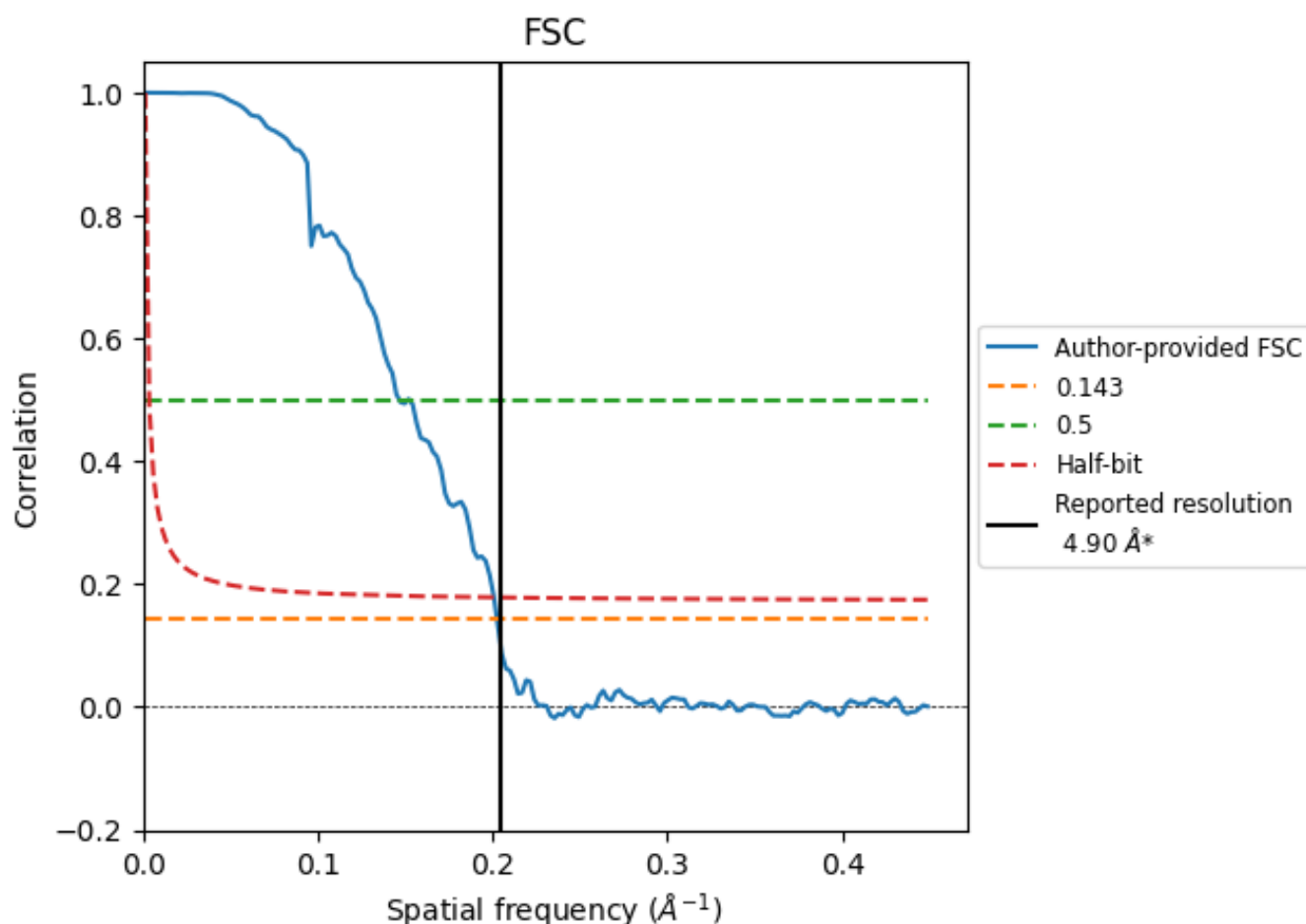


*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

8.2 Resolution estimates [i](#)

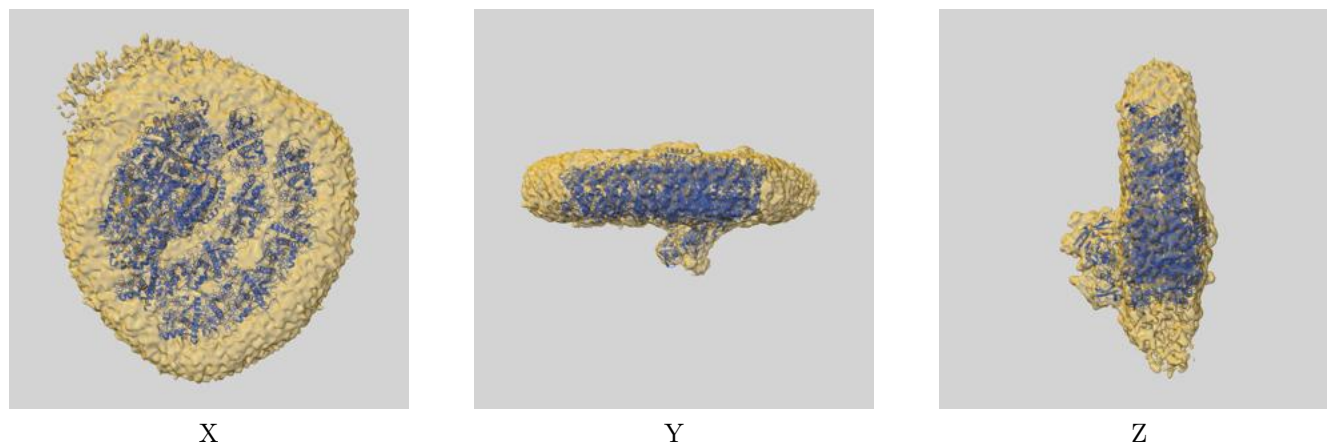
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.94	6.82	4.98
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

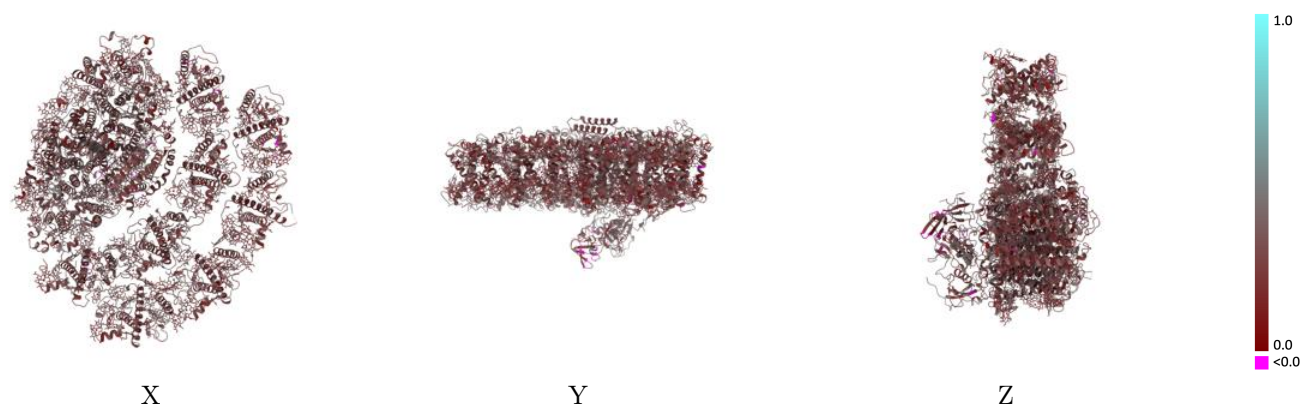
This section contains information regarding the fit between EMDB map EMD-32907 and PDB model 7WZN. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



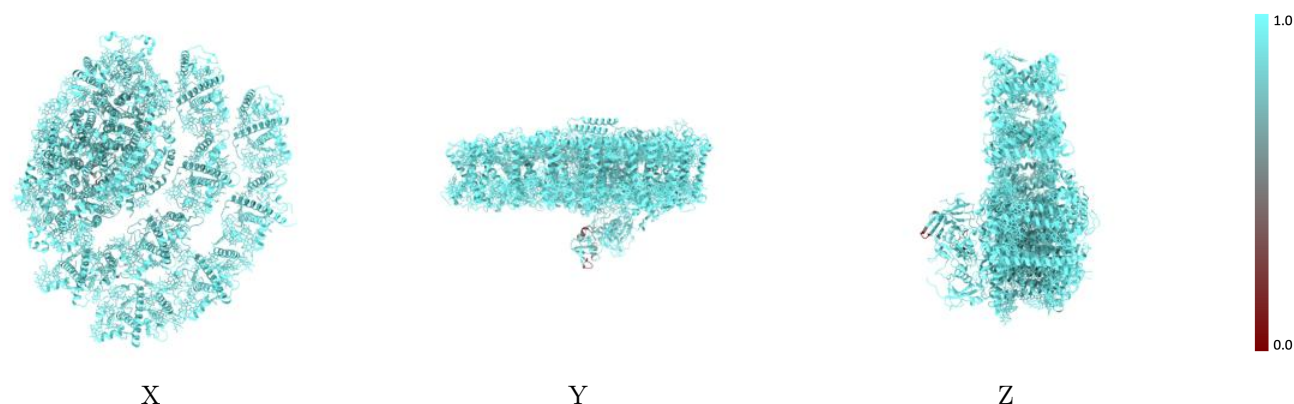
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



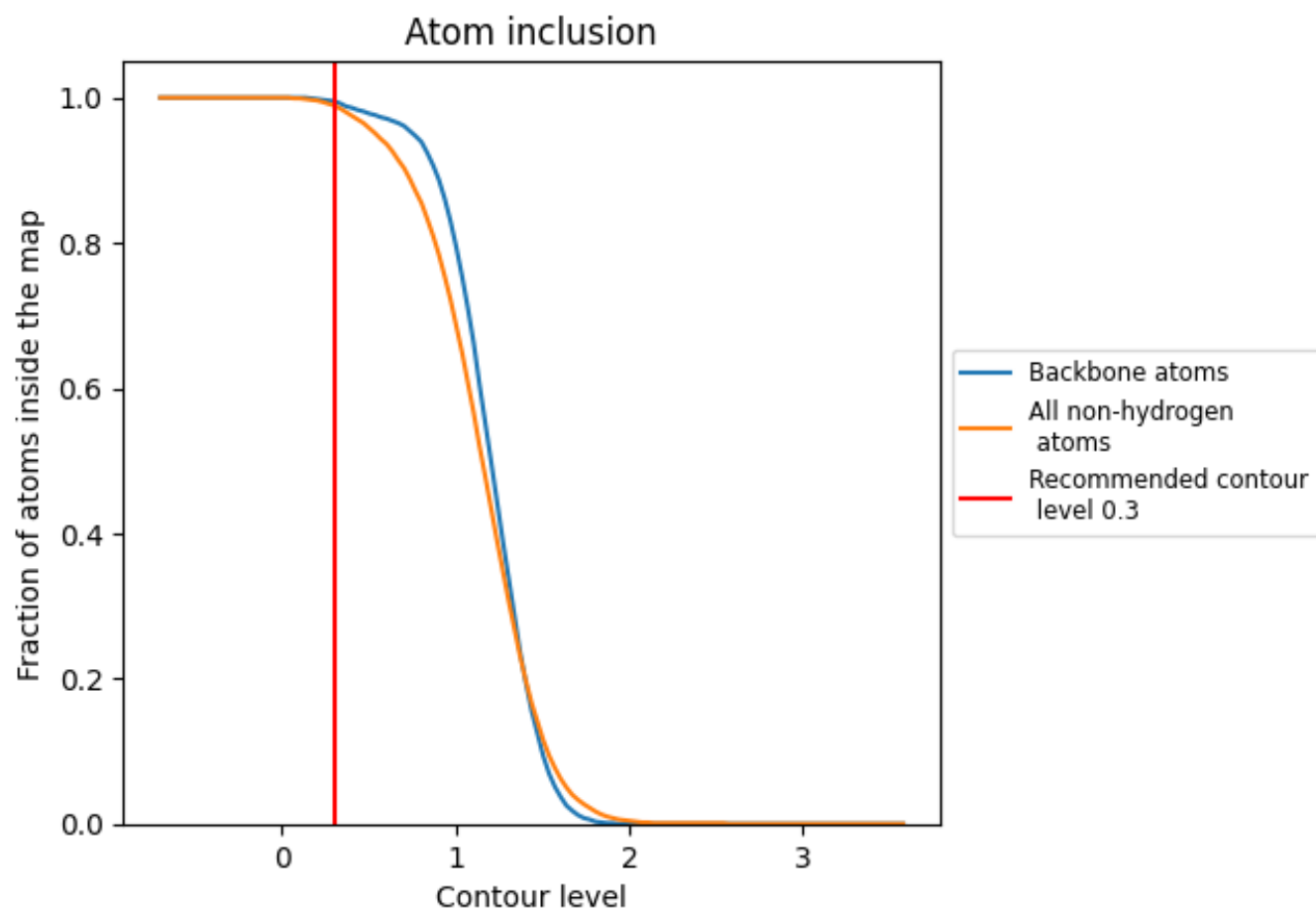
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9890	0.2950
1	0.9930	0.2740
3	0.9970	0.3020
4	0.9920	0.2710
5	0.9970	0.2920
6	0.9960	0.2900
7	0.9930	0.3080
8	0.9960	0.2980
A	0.9920	0.3100
B	0.9890	0.2970
C	1.0000	0.3050
D	1.0000	0.3520
E	1.0000	0.3480
F	0.9960	0.2970
G	0.7650	0.1610
J	1.0000	0.2920
Z	0.9990	0.2560

