Full wwPDB EM Validation Report (i)

Jun 20, 2024 – 06:20 AM JST

PDB ID	:	7WYI
EMDB ID	:	EMD-32892
Title	:	Native Photosystem I of Chlamydomonas reinhardtii
Authors	:	Kurisu, G.; Gerle, C.; Mitsuoka, K.; Kawamoto, A.; Tanaka, H.
Deposited on	:	2022-02-16
Resolution	:	3.90 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 (i) 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 (1)) were used in the production of this report:

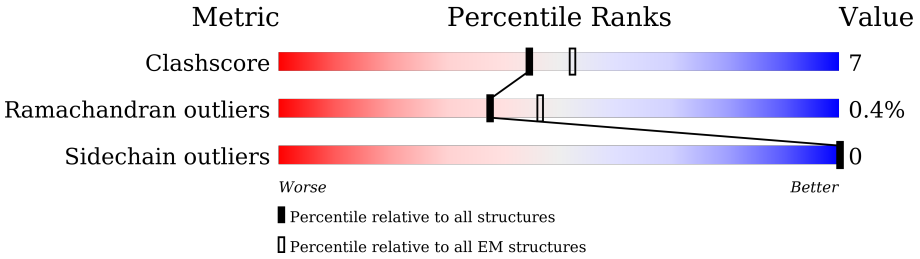
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	94% 5% •
2	B	735	94% 5%
3	C	81	75% 22% ••
4	D	196	5% 66% 7% • 27%
5	E	97	51% 12% 37%
6	F	227	71% • 27%
7	J	41	93% • 5%
8	1	224	81% 5% 13%

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Mol	Chain	Length	Quality of chain
9	3	298	64% • 32%
10	7	241	86% • 12%
11	8	243	84% 5% 11%
12	Z	228	81% • 16%
13	4	264	73% • 23%
14	5	257	81% 5% 13%
15	6	257	84% 5% 11%

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
16	CL0	A	801	X	-	-	-
17	CLA	1	602	X	-	-	-
17	CLA	1	603	X	-	-	-
17	CLA	1	604	X	-	-	-
17	CLA	1	605	X	-	-	-
17	CLA	1	606	X	-	-	-
17	CLA	1	607	X	-	-	-
17	CLA	1	608	X	-	-	-
17	CLA	1	609	X	-	-	-
17	CLA	1	610	X	-	-	-
17	CLA	3	301	X	-	-	-
17	CLA	3	302	X	-	-	-
17	CLA	3	303	X	-	-	-
17	CLA	3	304	X	-	-	-
17	CLA	3	305	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	309	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	-
17	CLA	4	601	X	-	-	-
17	CLA	4	602	X	-	-	-
17	CLA	4	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	4	604	X	-	-	-
17	CLA	4	605	X	-	-	-
17	CLA	5	301	X	-	-	-
17	CLA	5	302	X	-	-	-
17	CLA	5	303	X	-	-	-
17	CLA	5	304	X	-	-	-
17	CLA	5	306	X	-	-	-
17	CLA	5	307	X	-	-	-
17	CLA	5	308	X	-	-	-
17	CLA	5	309	X	-	-	-
17	CLA	5	310	X	-	-	-
17	CLA	5	311	X	-	-	-
17	CLA	5	312	X	-	-	-
17	CLA	5	314	X	-	-	-
17	CLA	5	315	X	-	-	-
17	CLA	6	601	X	-	-	-
17	CLA	6	602	X	-	-	-
17	CLA	6	603	X	-	-	-
17	CLA	6	604	X	-	-	-
17	CLA	6	608	X	-	-	-
17	CLA	6	609	X	-	-	-
17	CLA	6	610	X	-	-	-
17	CLA	7	601	X	-	-	-
17	CLA	7	602	X	-	-	-
17	CLA	7	603	X	-	-	-
17	CLA	7	604	X	-	-	-
17	CLA	7	605	X	-	-	-
17	CLA	7	607	X	-	-	-
17	CLA	7	608	X	-	-	-
17	CLA	7	609	X	-	-	-
17	CLA	7	610	X	-	-	-
17	CLA	7	611	X	-	-	-
17	CLA	7	612	X	-	-	-
17	CLA	7	613	X	-	-	-
17	CLA	7	614	X	-	-	-
17	CLA	8	601	X	-	-	-
17	CLA	8	602	X	-	-	-
17	CLA	8	603	X	-	-	-
17	CLA	8	604	X	-	-	-
17	CLA	8	605	X	-	-	-
17	CLA	8	607	X	-	-	-
17	CLA	8	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	8	609	X	-	-	-
17	CLA	8	610	X	-	-	-
17	CLA	8	611	X	-	-	-
17	CLA	8	612	X	-	-	-
17	CLA	8	613	X	-	-	-
17	CLA	8	614	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	841	X	-	-	-
17	CLA	A	842	X	-	-	-
17	CLA	A	843	X	-	-	-
17	CLA	B	801	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	839	X	-	-	-
17	CLA	F	301	X	-	-	-
17	CLA	F	302	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	J	102	X	-	-	-
19	SF4	C	102	-	-	X	-
20	CHL	1	601	X	-	-	-
20	CHL	3	307	X	-	-	-
20	CHL	5	305	X	-	-	-
20	CHL	5	313	X	-	-	-
20	CHL	6	605	X	-	-	-
20	CHL	6	606	X	-	-	-
20	CHL	6	607	X	-	-	-
20	CHL	7	606	X	-	-	-
20	CHL	8	606	X	-	-	-
20	CHL	Z	601	X	-	-	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 25007 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
			Total	C	N	O		
1	A	738	3628	2151	739	738	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	732	3601	2137	733	731	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

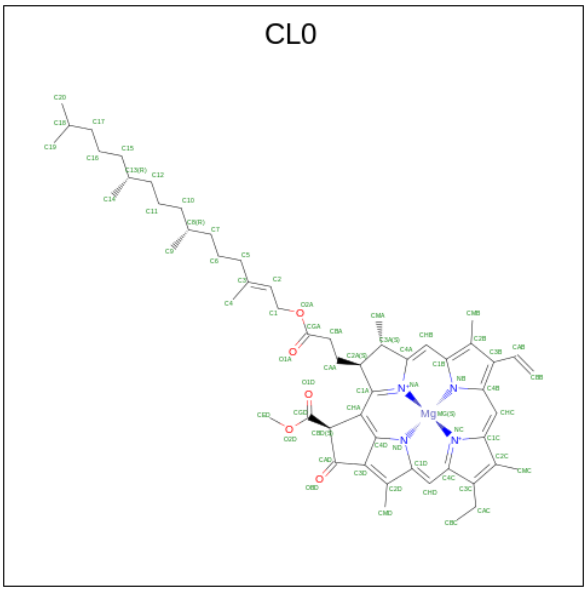
- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

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

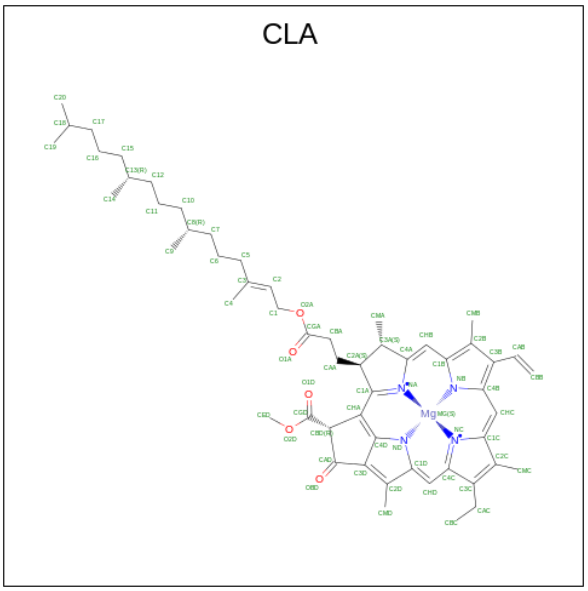
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	6	229	1122	664	229	229	0	0

- Molecule 16 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (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 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0

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Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 45 35 1 4 5	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 51 41 1 4 5	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 43 34 1 4 4	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 40 32 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0
17	A	1	Total C Mg N O 42 34 1 4 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	A	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	A	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	A	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	A	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
17	A	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	A	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
17	B	1	39	33	1	4	1	0
			Total	C	Mg	N	O	
17	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
17	B	1	42	34	1	4	3	0

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

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Mol	Chain	Residues	Atoms	AltConf
17	B	1	Total C Mg N O 42 34 1 4 3	0
17	B	1	Total C Mg N O 42 34 1 4 3	0
17	F	1	Total C Mg N O 42 34 1 4 3	0
17	F	1	Total C Mg N O 62 52 1 4 5	0
17	J	1	Total C Mg N O 43 35 1 4 3	0
17	J	1	Total C Mg N O 42 34 1 4 3	0
17	1	1	Total C Mg N O 43 35 1 4 3	0
17	1	1	Total C Mg N O 42 34 1 4 3	0
17	1	1	Total C Mg N O 42 34 1 4 3	0
17	1	1	Total C Mg N O 42 34 1 4 3	0
17	1	1	Total C Mg N O 42 34 1 4 3	0
17	1	1	Total C Mg N O 42 34 1 4 3	0
17	1	1	Total C Mg N O 42 34 1 4 3	0
17	1	1	Total C Mg N O 42 34 1 4 3	0
17	1	1	Total C Mg N O 42 34 1 4 3	0
17	3	1	Total C Mg N O 42 34 1 4 3	0
17	3	1	Total C Mg N O 42 34 1 4 3	0
17	3	1	Total C Mg N O 42 34 1 4 3	0
17	3	1	Total C Mg N O 45 35 1 4 5	0
17	3	1	Total C Mg N O 42 34 1 4 3	0
17	3	1	Total C Mg N O 42 34 1 4 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	3	1	42	34	1	4	3	0
17	3	1	46	36	1	4	5	0
17	3	1	41	33	1	4	3	0
17	3	1	42	34	1	4	3	0
17	3	1	42	34	1	4	3	0
17	3	1	42	34	1	4	3	0
17	7	1	42	34	1	4	3	0
17	7	1	42	34	1	4	3	0
17	7	1	42	34	1	4	3	0
17	7	1	42	34	1	4	3	0
17	7	1	42	34	1	4	3	0
17	7	1	42	34	1	4	3	0
17	7	1	42	34	1	4	3	0
17	7	1	42	34	1	4	3	0
17	7	1	41	33	1	4	3	0
17	7	1	42	34	1	4	3	0
17	7	1	45	35	1	4	5	0
17	7	1	43	35	1	4	3	0
17	7	1	42	34	1	4	3	0
17	8	1	42	34	1	4	3	0
17	8	1	42	34	1	4	3	0

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Mol	Chain	Residues	Atoms	AltConf
17	8	1	Total C Mg N O 45 35 1 4 5	0
17	8	1	Total C Mg N O 42 34 1 4 3	0
17	8	1	Total C Mg N O 42 34 1 4 3	0
17	8	1	Total C Mg N O 42 34 1 4 3	0
17	8	1	Total C Mg N O 42 34 1 4 3	0
17	8	1	Total C Mg N O 42 34 1 4 3	0
17	8	1	Total C Mg N O 42 34 1 4 3	0
17	8	1	Total C Mg N O 42 34 1 4 3	0
17	8	1	Total C Mg N O 46 36 1 4 5	0
17	8	1	Total C Mg N O 42 34 1 4 3	0
17	8	1	Total C Mg N O 42 34 1 4 3	0
17	4	1	Total C Mg N O 42 34 1 4 3	0
17	4	1	Total C Mg N O 45 35 1 4 5	0
17	4	1	Total C Mg N O 42 34 1 4 3	0
17	4	1	Total C Mg N O 42 34 1 4 3	0
17	4	1	Total C Mg N O 45 35 1 4 5	0
17	5	1	Total C Mg N O 42 34 1 4 3	0
17	5	1	Total C Mg N O 42 34 1 4 3	0
17	5	1	Total C Mg N O 48 38 1 4 5	0
17	5	1	Total C Mg N O 42 34 1 4 3	0
17	5	1	Total C Mg N O 50 40 1 4 5	0

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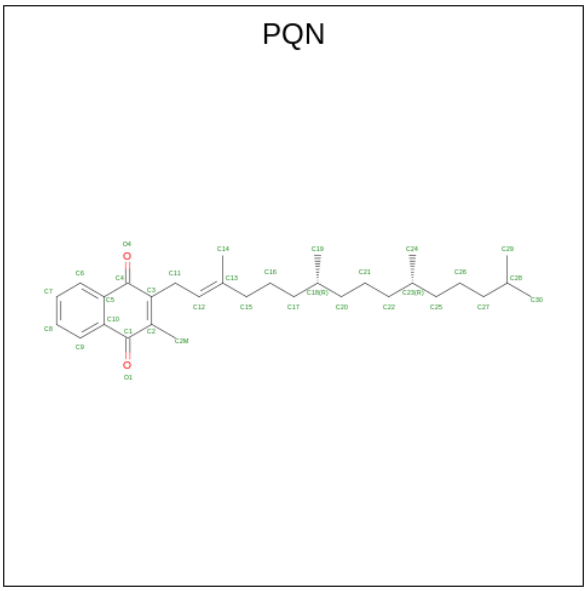
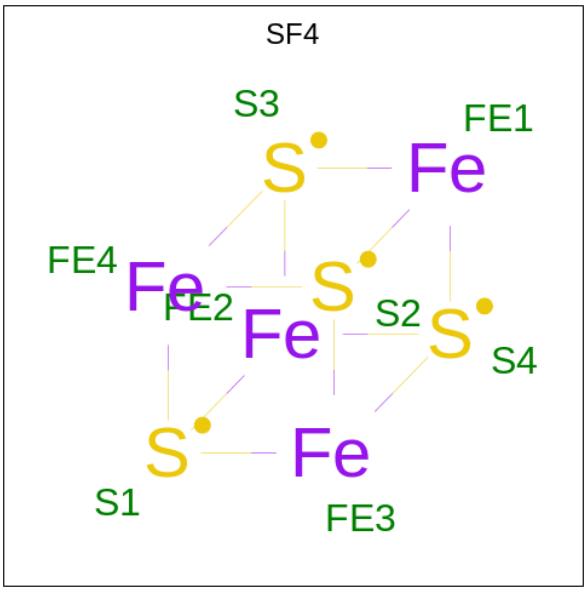
Mol	Chain	Residues	Atoms	AltConf
17	5	1	Total C Mg N O 42 34 1 4 3	0
17	5	1	Total C Mg N O 42 34 1 4 3	0
17	5	1	Total C Mg N O 42 34 1 4 3	0
17	5	1	Total C Mg N O 42 34 1 4 3	0
17	5	1	Total C Mg N O 42 34 1 4 3	0
17	5	1	Total C Mg N O 42 34 1 4 3	0
17	5	1	Total C Mg N O 46 36 1 4 5	0
17	5	1	Total C Mg N O 45 35 1 4 5	0
17	6	1	Total C Mg N O 42 34 1 4 3	0
17	6	1	Total C Mg N O 42 34 1 4 3	0
17	6	1	Total C Mg N O 42 34 1 4 3	0
17	6	1	Total C Mg N O 42 34 1 4 3	0
17	6	1	Total C Mg N O 42 34 1 4 3	0
17	6	1	Total C Mg N O 46 36 1 4 5	0
17	6	1	Total C Mg N O 45 35 1 4 5	0

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

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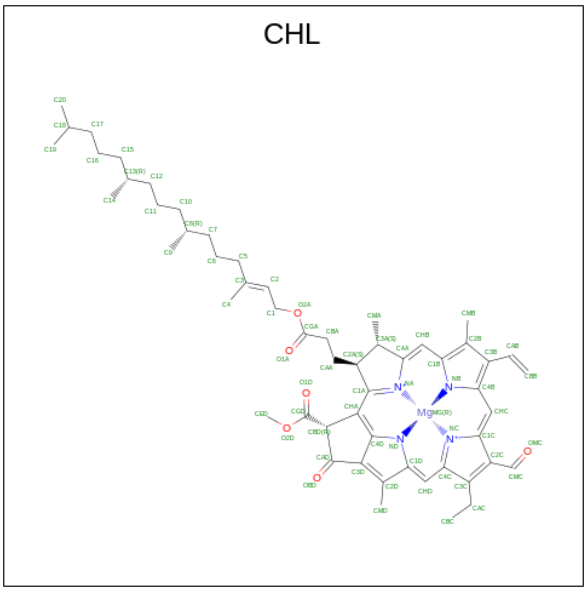
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
19	C	1	8	4	4	0
			Total	Fe	S	
19	C	1	8	4	4	0

- Molecule 20 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	1	1	53	42	1	4	6	0
			Total	C	Mg	N	O	
20	3	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
20	7	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
20	8	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
20	Z	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
20	5	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
20	5	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
20	6	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
20	6	1	43	34	1	4	4	0

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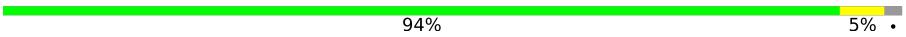
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	6	1	43	34	1	4	4	0

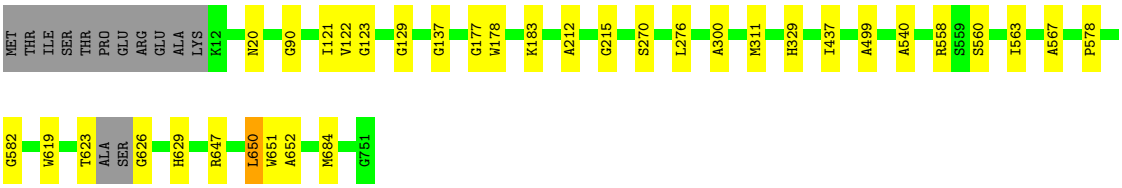
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

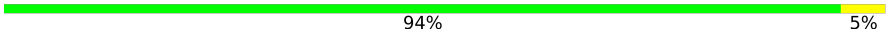
Chain A:

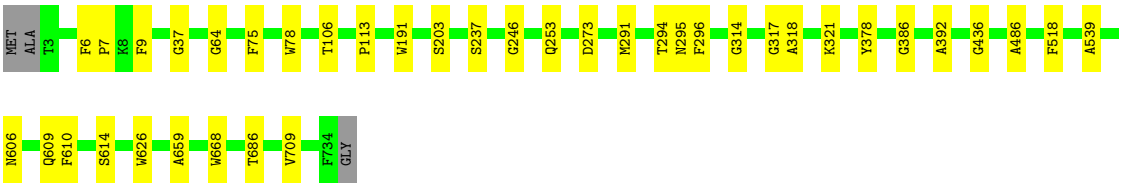




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

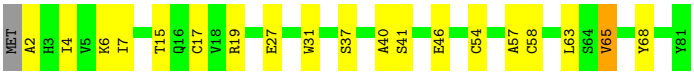
Chain B:





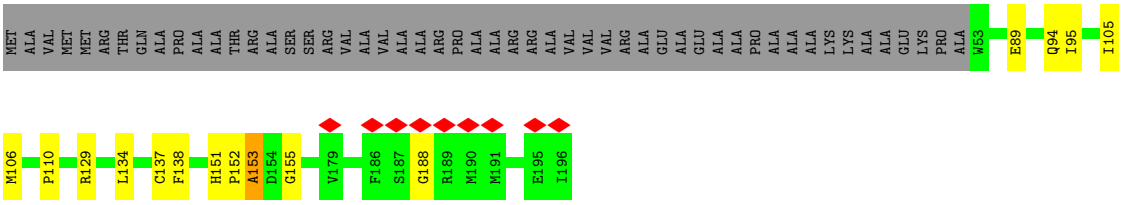
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



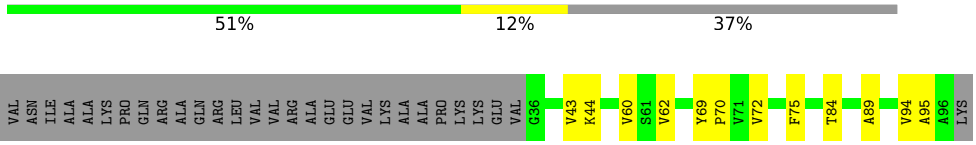
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



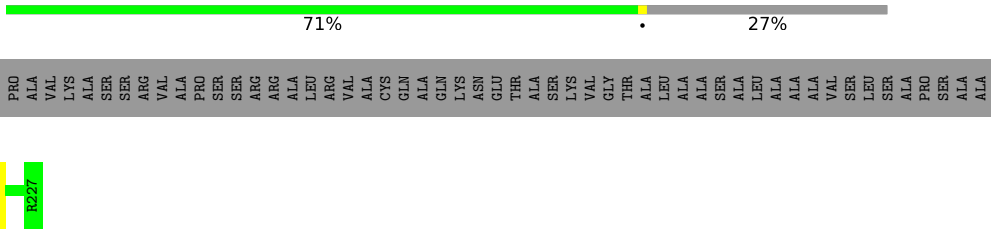
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



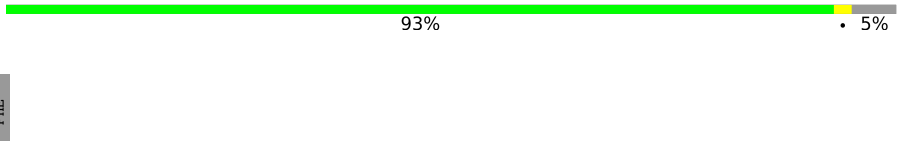
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:



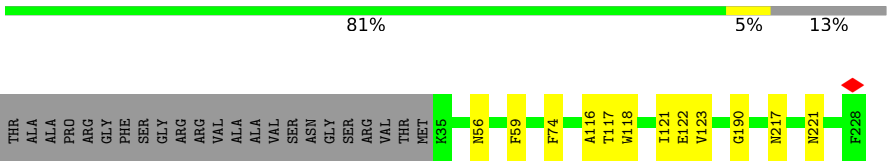
• Molecule 7: Photosystem I reaction center subunit IX

Chain J:



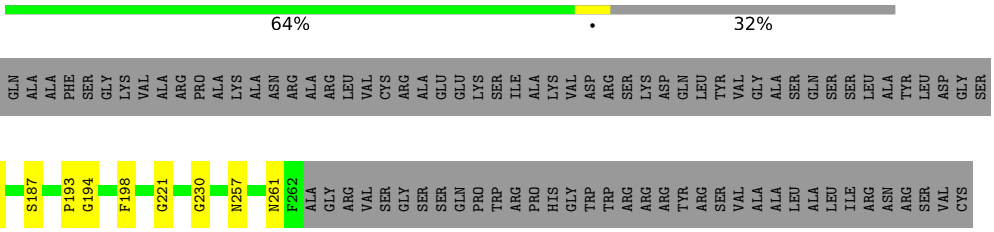
• Molecule 8: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



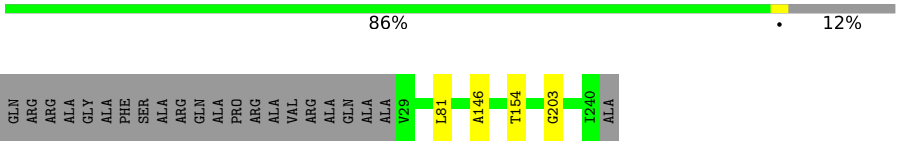
• Molecule 9: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



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

Chain 7:



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

Chain 8: 84% 5% 11%

MET ALA LEU THR MET LYS ARG SER GLY VAL ALA ALA ARG SER ALA SER SER ARG LYS SER VAL VAL THR CYS VAL ALA R27 A49 G50 N51 Q71 C77 L88 L92 Q126 W188 G196 K210 G214 L243

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

Chain Z: 81% • 16%

MET ALA LEU SER MET ARG THR LEU SER ALA ARG THR ALA ALA PRO ARG GLY PHE SER GLY ARG ARG VAL ALA ALA VAL SER ASN GLY SER ARG VAL THR MET K35 N112 GLY GLY K115 A116 T117 W118 I121 E122 V123 N217 N221 F228

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

Chain 4: 73% • 23%

MET ALA PHE VAL LEU ALA LYS SER SER ALA PHE GLY VAL ALA ALA LYS PRO VAL SER ARG ARG SER SER VAL ALA ALA VAL LYS ALA SER ALA VAL PRO GLU ASN VAL LYS GLU ALA ARG GLU TRP ILE ASP ALA TRP LYS SER LYS SER GLY GLY ALA LYS ARG ASP ALA ALA L58 Y96

A104 G124 PHE SER TRP P128 F157 E161 N175 Q176 K184 L185 G206 D207 G219 R263 LEU

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

Chain 5: 81% 5% 13%

MET ALA ALA LEU MET GLN LYS SER ALA LEU SER ARG PRO ALA CYS SER THR ARG SER SER ARG ARG ALA VAL VAL VAL ARG ALA ALA ALA ASP R32 A50 Y53 E102 A103 G104 L105 P106 Q107 N108 H130 S175 LYS GLY N178 T184 N226 D241 V242 L245

T246 S256 GLN

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

Chain 6: 84% 5% 11%

MET MET LEU VAL ALA LYS ASN ALA VAL ALA ALA ARG PRO SER ALA ARG SER ALA ARG ARG SER VAL VAL ALA LYS ALA SER SER R29 D49 F96 N99 A100 G101 R128 A221 A222 V229 P236 S240 Y241 K242 G243 I244 E245 P257

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47618	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 ($e^-/Å^2$)	45.5	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	3.382	Depositor
Minimum map value	-0.724	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	431.2, 431.2, 431.2	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.34	0/3628	0.51	0/5034
2	B	0.35	0/3602	0.50	0/5001
3	C	0.43	0/394	0.72	0/547
4	D	0.37	0/705	0.54	0/977
5	E	0.30	0/299	0.51	0/414
6	F	0.32	0/809	0.47	0/1122
7	J	0.30	0/193	0.44	0/268
8	1	0.30	0/941	0.47	0/1299
9	3	0.34	0/984	0.49	0/1361
10	7	0.34	0/1032	0.48	0/1427
11	8	0.33	0/1058	0.47	0/1464
12	Z	0.31	0/932	0.46	0/1286
13	4	0.34	0/990	0.48	0/1369
14	5	0.33	0/1089	0.51	0/1507
15	6	0.32	0/1121	0.47	0/1554
All	All	0.34	0/17777	0.50	0/24630

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
13	4	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	4	206	GLY	Peptide

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	30	0
2	B	3601	0	1715	29	0
3	C	395	0	178	11	0
4	D	706	0	316	11	0
5	E	300	0	135	6	0
6	F	810	0	404	2	0
7	J	194	0	87	1	0
8	1	942	0	489	9	0
9	3	985	0	480	7	0
10	7	1033	0	498	4	0
11	8	1059	0	527	8	0
12	Z	934	0	482	4	0
13	4	992	0	471	5	0
14	5	1091	0	504	13	0
15	6	1122	0	524	9	0
16	A	42	0	31	4	0
17	1	379	0	279	12	0
17	3	510	0	374	10	0
17	4	216	0	159	4	0
17	5	567	0	416	10	0
17	6	301	0	221	5	0
17	7	549	0	405	7	0
17	8	553	0	407	14	0
17	A	1743	0	1290	52	0
17	B	1630	0	1223	50	0
17	F	104	0	94	4	0
17	J	85	0	62	2	0
18	A	33	0	46	0	0
18	B	33	0	46	3	0
19	B	8	0	0	0	0
19	C	16	0	0	2	0
20	1	53	0	41	0	0
20	3	46	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	5	89	0	60	1	0
20	6	129	0	87	5	0
20	7	43	0	29	2	0
20	8	43	0	29	2	0
20	Z	43	0	29	0	0
All	All	25007	0	13897	264	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 7.

All (264) 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)
10:7:81:LEU:CB	17:7:604:CLA:HBB2	1.90	1.01
4:D:138:PHE:H	4:D:151:HIS:CB	1.83	0.90
15:6:240:SER:HA	15:6:245:GLU:HA	1.56	0.86
14:5:105:LEU:CB	14:5:108:ASN:CB	2.53	0.86
14:5:226:ASN:CB	17:5:311:CLA:HED3	2.07	0.84
2:B:64:GLY:HA2	17:B:809:CLA:HMC3	1.60	0.84
4:D:137:CYS:HA	4:D:151:HIS:CB	2.09	0.82
3:C:6:LYS:O	3:C:65:VAL:HA	1.83	0.78
13:4:104:ALA:HB1	13:4:219:GLY:HA3	1.67	0.77
17:B:809:CLA:HHB	17:B:810:CLA:HMB3	1.69	0.75
17:A:824:CLA:HBB1	17:A:837:CLA:HHB	1.69	0.75
12:Z:117:THR:HA	12:Z:122:GLU:HA	1.71	0.73
8:1:117:THR:HA	8:1:122:GLU:HA	1.71	0.72
17:B:808:CLA:HMC3	17:B:827:CLA:HBB1	1.71	0.71
14:5:241:ASP:HA	14:5:246:THR:HA	1.70	0.71
1:A:300:ALA:HA	17:A:815:CLA:HMC3	1.74	0.70
17:A:825:CLA:O1A	17:A:825:CLA:CBA	2.40	0.69
17:B:814:CLA:HHC	17:B:814:CLA:HBB1	1.75	0.68
17:A:802:CLA:HHC	17:A:802:CLA:HBB1	1.75	0.68
17:B:822:CLA:HHB	17:B:839:CLA:O1D	1.95	0.67
9:3:95:ALA:HB1	9:3:221:GLY:HA3	1.77	0.66
1:A:121:ILE:O	1:A:123:GLY:N	2.29	0.66
17:1:608:CLA:HHC	17:1:608:CLA:HBB1	1.77	0.66
4:D:138:PHE:N	4:D:151:HIS:CB	2.56	0.66
17:A:807:CLA:HMC3	17:A:808:CLA:HMD2	1.77	0.66
1:A:212:ALA:HA	17:A:813:CLA:HBB2	1.76	0.65
17:A:819:CLA:HMD3	17:A:820:CLA:HMC3	1.77	0.64
15:6:101:GLY:HA2	20:6:605:CHL:HAC2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:CYS:CA	4:D:151:HIS:CB	2.75	0.64
17:J:101:CLA:HBB1	17:J:101:CLA:HHC	1.78	0.64
17:A:823:CLA:HHC	17:A:823:CLA:HBB1	1.80	0.64
17:7:611:CLA:HHC	17:7:611:CLA:HBB1	1.80	0.63
5:E:44:LYS:N	5:E:94:VAL:O	2.29	0.63
10:7:81:LEU:CB	17:7:604:CLA:CBB	2.73	0.63
17:A:824:CLA:HBB1	17:A:837:CLA:HMA1	1.81	0.62
2:B:37:GLY:H	4:D:188:GLY:HA2	1.66	0.61
2:B:237:SER:O	2:B:253:GLN:N	2.33	0.61
14:5:53:TYR:N	17:5:303:CLA:OBD	2.32	0.61
17:B:801:CLA:HBB1	17:B:801:CLA:HMB1	1.82	0.61
2:B:709:VAL:HA	17:B:838:CLA:HED2	1.81	0.61
3:C:17:CYS:N	19:C:102:SF4:S4	2.72	0.61
17:A:841:CLA:HHC	17:A:841:CLA:HBB1	1.82	0.60
4:D:95:ILE:HA	4:D:105:ILE:HA	1.82	0.60
17:B:809:CLA:HMA1	17:B:810:CLA:HMB3	1.83	0.60
1:A:311:MET:HA	17:A:820:CLA:HAC2	1.82	0.60
17:8:603:CLA:HHC	17:8:603:CLA:HBB1	1.84	0.59
14:5:226:ASN:HA	17:5:310:CLA:HAA1	1.85	0.59
17:5:304:CLA:HBC1	17:5:306:CLA:HAC1	1.83	0.59
2:B:294:THR:O	2:B:296:PHE:N	2.35	0.59
2:B:610:PHE:O	2:B:614:SER:CB	2.51	0.59
15:6:222:ALA:HA	17:6:609:CLA:HBB1	1.85	0.59
1:A:578:PRO:HA	1:A:582:GLY:HA2	1.85	0.58
2:B:486:ALA:HB2	17:B:833:CLA:C1D	2.34	0.57
14:5:242:VAL:N	14:5:245:LEU:O	2.38	0.57
4:D:94:GLN:O	4:D:106:MET:N	2.38	0.57
2:B:436:GLY:HA3	17:B:831:CLA:HBB2	1.85	0.57
17:A:834:CLA:HHC	17:A:834:CLA:HBB1	1.87	0.57
17:7:605:CLA:HMC3	20:7:606:CHL:C1C	2.33	0.57
17:B:810:CLA:HHC	17:B:810:CLA:HBB1	1.88	0.56
17:3:311:CLA:CHB	17:3:312:CLA:HMD3	2.35	0.56
5:E:43:VAL:HA	5:E:95:ALA:HA	1.87	0.56
13:4:175:ASN:O	13:4:185:LEU:N	2.32	0.56
1:A:129:GLY:N	1:A:137:GLY:O	2.37	0.56
17:8:608:CLA:HHC	17:8:608:CLA:HBB1	1.86	0.56
17:8:604:CLA:HHC	17:8:604:CLA:HBB1	1.88	0.56
17:A:812:CLA:C1D	17:A:814:CLA:HAB	2.37	0.55
3:C:31:TRP:N	3:C:37:SER:O	2.34	0.55
17:B:807:CLA:HBC2	17:B:828:CLA:HMA1	1.88	0.55
6:F:138:GLY:HA3	17:F:302:CLA:C3D	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:THR:N	1:A:626:GLY:O	2.32	0.55
13:4:176:GLN:HA	13:4:184:LYS:HA	1.89	0.55
2:B:291:MET:HA	17:B:821:CLA:HHD	1.89	0.54
17:B:833:CLA:HHC	17:B:833:CLA:HBB1	1.89	0.54
20:6:605:CHL:HBB2	20:6:606:CHL:HAB	1.88	0.54
14:5:105:LEU:CB	14:5:108:ASN:H	2.20	0.54
1:A:90:GLY:HA2	17:A:806:CLA:HMC3	1.88	0.54
20:3:307:CHL:CAD	17:3:309:CLA:HMD3	2.38	0.54
3:C:15:THR:O	3:C:19:ARG:N	2.31	0.54
8:1:217:ASN:HA	17:1:609:CLA:HAA1	1.90	0.54
2:B:203:SER:HA	2:B:246:GLY:HA2	1.89	0.53
17:B:804:CLA:HHC	17:B:804:CLA:HBB1	1.90	0.53
17:A:815:CLA:HMD1	17:A:834:CLA:HED1	1.90	0.53
4:D:89:GLU:HA	4:D:110:PRO:HA	1.91	0.53
17:B:822:CLA:H3A	17:B:839:CLA:HED3	1.90	0.53
17:B:809:CLA:HBC2	17:B:809:CLA:HHD	1.90	0.53
9:3:187:SER:H	9:3:193:PRO:HA	1.74	0.53
8:1:74:PHE:O	17:1:602:CLA:HMB3	2.10	0.52
12:Z:116:ALA:O	12:Z:123:VAL:N	2.37	0.52
1:A:558:ARG:O	1:A:567:ALA:N	2.42	0.52
9:3:151:GLU:HA	17:3:305:CLA:HMA1	1.91	0.52
17:4:604:CLA:HMB2	17:4:605:CLA:HHD	1.91	0.52
17:3:303:CLA:HHC	17:3:303:CLA:HBB1	1.91	0.52
17:3:311:CLA:C4A	17:3:312:CLA:HMD3	2.40	0.52
1:A:437:ILE:HA	17:A:829:CLA:HAB	1.92	0.52
9:3:257:ASN:O	9:3:261:ASN:N	2.41	0.52
17:A:806:CLA:HMA1	17:A:807:CLA:HMB3	1.92	0.52
17:5:309:CLA:HHC	17:5:309:CLA:HBB1	1.91	0.52
13:4:157:PHE:O	13:4:161:GLU:CB	2.58	0.52
14:5:102:GLU:O	14:5:104:GLY:N	2.43	0.51
17:1:605:CLA:HAA2	17:1:605:CLA:HBD	1.93	0.51
2:B:106:THR:HA	2:B:113:PRO:HA	1.93	0.51
17:1:603:CLA:HBC1	17:1:606:CLA:HAC1	1.91	0.51
10:7:146:ALA:HB1	10:7:154:THR:HA	1.92	0.51
17:A:823:CLA:HBD	17:A:823:CLA:HAA2	1.91	0.51
2:B:75:PHE:O	2:B:78:TRP:N	2.44	0.51
17:8:610:CLA:HHC	17:8:610:CLA:HBB1	1.92	0.51
17:A:838:CLA:HHC	17:A:838:CLA:HBB1	1.93	0.50
17:B:811:CLA:HHB	17:B:812:CLA:HBB1	1.93	0.50
3:C:54:CYS:O	3:C:57:ALA:N	2.42	0.50
17:1:609:CLA:CHB	17:1:610:CLA:HMD3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:821:CLA:HAB	17:A:841:CLA:CBB	2.41	0.50
16:A:801:CL0:H11	17:B:804:CLA:HAA2	1.93	0.50
1:A:619:TRP:O	1:A:629:HIS:HA	2.12	0.50
8:1:116:ALA:O	8:1:123:VAL:N	2.37	0.50
17:A:836:CLA:HHC	17:A:836:CLA:HBB1	1.93	0.49
17:A:811:CLA:HMA3	17:3:301:CLA:HBB2	1.94	0.49
11:8:49:ALA:O	11:8:51:ASN:N	2.46	0.49
14:5:50:ALA:HB1	14:5:184:THR:HA	1.93	0.49
11:8:71:GLN:C	17:8:608:CLA:HED1	2.33	0.49
17:A:807:CLA:HBB1	17:A:808:CLA:C3D	2.43	0.49
2:B:518:PHE:HA	17:B:835:CLA:HED1	1.94	0.49
17:B:810:CLA:HMC3	17:B:811:CLA:C3D	2.42	0.48
17:B:826:CLA:O1D	17:B:827:CLA:HHB	2.13	0.48
17:B:836:CLA:HHC	17:B:836:CLA:HBB1	1.95	0.48
2:B:273:ASP:O	17:B:818:CLA:HMB3	2.13	0.48
1:A:215:GLY:HA3	17:A:813:CLA:CAB	2.44	0.48
1:A:90:GLY:CA	17:A:806:CLA:HMC3	2.43	0.48
15:6:99:ASN:HA	20:6:606:CHL:O1D	2.13	0.48
17:B:810:CLA:HMC3	17:B:811:CLA:CAD	2.43	0.48
17:B:825:CLA:HBB1	17:B:832:CLA:HAA2	1.96	0.48
16:A:801:CL0:H8	16:A:801:CL0:O2D	2.14	0.48
17:A:830:CLA:H3A	2:B:686:THR:HA	1.94	0.48
17:A:836:CLA:HMB2	17:A:837:CLA:C3D	2.44	0.48
5:E:75:PHE:N	5:E:84:THR:O	2.47	0.48
17:B:835:CLA:C1A	17:B:835:CLA:CGA	2.92	0.48
11:8:126:GLN:CB	17:8:605:CLA:HMA3	2.44	0.48
17:B:805:CLA:HMB1	17:B:805:CLA:HBB1	1.96	0.47
3:C:2:ALA:HB2	3:C:46:GLU:HA	1.96	0.47
17:A:821:CLA:HMB3	17:A:841:CLA:C3C	2.44	0.47
14:5:102:GLU:C	14:5:104:GLY:H	2.17	0.47
5:E:60:VAL:N	5:E:72:VAL:O	2.43	0.47
1:A:651:TRP:O	1:A:651:TRP:CD2	2.67	0.47
2:B:386:GLY:HA3	17:B:828:CLA:C2C	2.44	0.47
9:3:194:GLY:O	9:3:198:PHE:CB	2.63	0.47
17:5:310:CLA:CHB	17:5:311:CLA:HMD3	2.44	0.47
1:A:276:LEU:O	17:A:815:CLA:HED1	2.14	0.47
14:5:102:GLU:C	14:5:104:GLY:N	2.67	0.47
17:A:822:CLA:H3A	17:A:841:CLA:HBB2	1.97	0.47
13:4:96:TYR:O	17:4:602:CLA:HMB3	2.15	0.46
15:6:241:TYR:O	15:6:243:GLY:N	2.47	0.46
17:F:302:CLA:H61	17:F:302:CLA:H41	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:823:CLA:HAA2	17:B:823:CLA:HBD	1.97	0.46
17:6:610:CLA:HBA1	17:6:610:CLA:H3A	1.68	0.46
15:6:96:PHE:O	15:6:99:ASN:N	2.39	0.46
17:1:603:CLA:HMD2	17:1:606:CLA:C1D	2.45	0.46
17:1:605:CLA:HAA2	17:1:605:CLA:CBD	2.46	0.46
17:B:810:CLA:HBA2	17:B:810:CLA:C4A	2.46	0.46
4:D:129:ARG:HA	4:D:134:LEU:O	2.16	0.46
11:8:210:LYS:O	11:8:214:GLY:HA2	2.16	0.46
11:8:49:ALA:O	17:8:602:CLA:HED3	2.15	0.46
16:A:801:CL0:H22	2:B:626:TRP:CD1	2.51	0.45
12:Z:118:TRP:N	12:Z:121:ILE:O	2.44	0.45
3:C:4:ILE:N	3:C:68:TYR:O	2.45	0.45
17:8:612:CLA:C1A	17:8:612:CLA:CGA	2.94	0.45
17:8:612:CLA:CHB	17:8:613:CLA:HMD3	2.46	0.45
17:B:801:CLA:OBD	17:B:804:CLA:HMB3	2.16	0.45
8:1:118:TRP:N	8:1:121:ILE:O	2.44	0.45
1:A:540:ALA:HB1	17:A:836:CLA:HMB3	1.97	0.45
1:A:560:SER:N	1:A:563:ILE:O	2.49	0.45
17:A:839:CLA:HMC3	17:B:837:CLA:ND	2.31	0.45
12:Z:217:ASN:O	12:Z:221:ASN:N	2.43	0.45
17:B:822:CLA:HBB1	17:B:822:CLA:HHC	1.97	0.45
3:C:7:ILE:HA	3:C:65:VAL:HA	1.97	0.45
20:5:305:CHL:HBB2	20:5:313:CHL:CHC	2.47	0.44
17:A:833:CLA:HMD2	17:A:834:CLA:CBB	2.47	0.44
2:B:486:ALA:HB2	17:B:833:CLA:C2D	2.48	0.44
17:B:837:CLA:HBB2	18:B:840:PQN:H141	2.00	0.44
16:A:801:CL0:H21	2:B:626:TRP:HD1	1.82	0.44
17:A:831:CLA:HAA2	17:A:831:CLA:HBD	1.98	0.44
1:A:300:ALA:HB1	17:A:815:CLA:HBC2	1.98	0.44
1:A:651:TRP:O	1:A:651:TRP:CG	2.70	0.44
1:A:651:TRP:CD2	1:A:651:TRP:C	2.91	0.44
17:B:824:CLA:CAD	17:B:834:CLA:HBB1	2.48	0.44
17:3:304:CLA:CHA	17:5:301:CLA:HMB3	2.47	0.44
17:8:605:CLA:HBC2	20:8:606:CHL:CHD	2.48	0.44
17:4:604:CLA:C1B	17:4:605:CLA:HMD3	2.47	0.44
2:B:386:GLY:HA3	17:B:828:CLA:C3C	2.48	0.43
2:B:606:ASN:O	2:B:609:GLN:N	2.50	0.43
17:F:302:CLA:C2C	17:F:302:CLA:H93	2.48	0.43
10:7:203:GLY:HA2	17:7:612:CLA:C2C	2.47	0.43
14:5:105:LEU:C	14:5:107:GLN:N	2.70	0.43
2:B:318:ALA:HB1	2:B:321:LYS:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:ALA:HB2	19:C:102:SF4:S1	2.58	0.43
17:4:604:CLA:H2A	17:4:604:CLA:O2D	2.18	0.43
17:A:815:CLA:HMD1	17:A:834:CLA:CED	2.48	0.43
2:B:314:GLY:C	2:B:317:GLY:H	2.22	0.43
7:J:25:LEU:N	17:J:102:CLA:HAB	2.33	0.43
2:B:191:TRP:HA	17:B:816:CLA:HAB	2.00	0.43
17:B:815:CLA:H171	17:B:827:CLA:C3D	2.49	0.43
1:A:329:HIS:HA	17:A:841:CLA:HBC2	2.00	0.43
5:E:62:VAL:HA	5:E:70:PRO:O	2.18	0.43
8:1:56:ASN:HA	17:1:602:CLA:HED3	1.99	0.43
5:E:69:TYR:HA	5:E:89:ALA:HA	1.99	0.43
17:8:605:CLA:HMC3	20:8:606:CHL:C1C	2.49	0.43
17:A:825:CLA:C4A	17:A:833:CLA:HMB2	2.49	0.43
17:B:815:CLA:H193	17:B:827:CLA:OBD	2.18	0.43
11:8:77:CYS:CB	11:8:196:GLY:HA3	2.49	0.42
17:6:609:CLA:HAA2	17:6:609:CLA:O2D	2.18	0.42
1:A:270:SER:HA	17:A:815:CLA:HAA2	2.01	0.42
17:A:807:CLA:HBB1	17:A:808:CLA:C2D	2.48	0.42
17:B:823:CLA:HMB1	17:B:823:CLA:HBB1	2.02	0.42
8:1:217:ASN:O	8:1:221:ASN:N	2.43	0.42
9:3:230:GLY:HA2	17:3:311:CLA:C2C	2.49	0.42
17:B:815:CLA:H62	17:B:815:CLA:H102	1.79	0.42
1:A:651:TRP:CD1	2:B:626:TRP:NE1	2.87	0.42
17:A:831:CLA:CAB	17:A:832:CLA:HMB2	2.49	0.42
2:B:378:TYR:CB	17:B:826:CLA:HMC3	2.49	0.42
8:1:59:PHE:H	17:1:602:CLA:CAD	2.25	0.42
17:3:305:CLA:C2C	17:3:306:CLA:HED2	2.49	0.42
17:A:812:CLA:CHA	17:A:814:CLA:HMB3	2.50	0.42
17:B:815:CLA:H62	17:B:815:CLA:H41	1.76	0.42
1:A:650:LEU:C	1:A:652:ALA:N	2.70	0.42
17:A:806:CLA:CGD	17:A:808:CLA:HED1	2.50	0.42
4:D:153:ALA:C	4:D:155:GLY:N	2.73	0.42
1:A:20:ASN:N	1:A:183:LYS:O	2.48	0.42
1:A:647:ARG:HA	1:A:651:TRP:HB3	2.02	0.42
2:B:392:ALA:HB2	2:B:539:ALA:HA	2.02	0.42
9:3:79:GLY:C	17:3:301:CLA:HED1	2.40	0.42
17:8:601:CLA:HAA1	17:8:601:CLA:HBD	2.02	0.42
15:6:221:ALA:HB1	15:6:229:VAL:O	2.20	0.42
17:A:803:CLA:HED1	17:A:809:CLA:CAD	2.50	0.42
17:B:807:CLA:HED2	17:B:828:CLA:HBB2	2.02	0.42
17:F:302:CLA:HMB2	17:F:302:CLA:H2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:6:128:ARG:HA	20:6:607:CHL:HAC2	2.02	0.42
2:B:659:ALA:O	17:B:805:CLA:HAB	2.19	0.41
2:B:668:TRP:HA	18:B:840:PQN:H8	2.00	0.41
1:A:178:TRP:CB	17:A:809:CLA:HMC3	2.51	0.41
17:A:841:CLA:C4A	17:A:841:CLA:HBA2	2.50	0.41
17:7:605:CLA:HMC3	20:7:606:CHL:C2C	2.50	0.41
17:5:301:CLA:HAA1	17:5:301:CLA:HBD	2.02	0.41
1:A:177:GLY:C	17:A:809:CLA:HAC1	2.41	0.41
3:C:27:GLU:O	3:C:41:SER:N	2.53	0.41
11:8:88:LEU:O	11:8:92:LEU:N	2.45	0.41
17:B:814:CLA:CHD	17:B:815:CLA:HAB	2.51	0.41
6:F:63:ASP:N	6:F:67:LEU:O	2.54	0.41
17:1:609:CLA:HMB2	17:1:610:CLA:HAC1	2.01	0.41
20:6:605:CHL:HBB2	20:6:606:CHL:CAB	2.50	0.41
17:A:843:CLA:C1D	17:B:802:CLA:HMC3	2.51	0.41
3:C:27:GLU:N	3:C:41:SER:O	2.54	0.41
1:A:684:MET:HA	17:A:802:CLA:HBC2	2.02	0.41
11:8:188:TRP:O	17:8:609:CLA:HMB3	2.19	0.41
17:6:609:CLA:HAA2	17:6:609:CLA:CGD	2.51	0.41
18:B:840:PQN:H111	18:B:840:PQN:H2M1	1.90	0.40
8:1:190:GLY:HA2	17:1:609:CLA:C2C	2.51	0.40
17:7:612:CLA:C4A	17:7:613:CLA:HMD3	2.51	0.40
17:B:826:CLA:O1D	17:B:827:CLA:HMA1	2.20	0.40
4:D:153:ALA:C	4:D:155:GLY:H	2.24	0.40
17:8:604:CLA:CMB	17:8:605:CLA:HBB1	2.50	0.40
17:5:304:CLA:HAA2	17:5:304:CLA:HBD	2.02	0.40
1:A:499:ALA:HB2	17:A:834:CLA:HMA3	2.03	0.40
17:A:821:CLA:HMB3	17:A:841:CLA:C2C	2.52	0.40
17:A:806:CLA:HHB	17:A:807:CLA:HMB3	2.02	0.40
15:6:49:ASP:HA	17:6:602:CLA:O1D	2.21	0.40
14:5:130:HIS:HA	17:5:306:CLA:HMB1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	734/751 (98%)	671 (91%)	61 (8%)	2 (0%)	41	75
2	B	730/735 (99%)	660 (90%)	66 (9%)	4 (0%)	29	67
3	C	78/81 (96%)	62 (80%)	13 (17%)	3 (4%)	3	28
4	D	142/196 (72%)	122 (86%)	18 (13%)	2 (1%)	11	46
5	E	59/97 (61%)	53 (90%)	6 (10%)	0	100	100
6	F	163/227 (72%)	156 (96%)	7 (4%)	0	100	100
7	J	37/41 (90%)	34 (92%)	3 (8%)	0	100	100
8	1	192/224 (86%)	175 (91%)	17 (9%)	0	100	100
9	3	200/298 (67%)	183 (92%)	17 (8%)	0	100	100
10	7	210/241 (87%)	186 (89%)	24 (11%)	0	100	100
11	8	215/243 (88%)	202 (94%)	12 (6%)	1 (0%)	29	67
12	Z	188/228 (82%)	172 (92%)	16 (8%)	0	100	100
13	4	199/264 (75%)	181 (91%)	17 (8%)	1 (0%)	29	67
14	5	219/257 (85%)	195 (89%)	24 (11%)	0	100	100
15	6	227/257 (88%)	213 (94%)	13 (6%)	1 (0%)	34	71
All	All	3593/4140 (87%)	3265 (91%)	314 (9%)	14 (0%)	38	71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
2	B	6	PHE
4	D	152	PRO
2	B	9	PHE
1	A	650	LEU
4	D	153	ALA
3	C	63	LEU
13	4	207	ASP
2	B	295	ASN
3	C	65	VAL
2	B	7	PRO
3	C	58	CYS
15	6	236	PRO
11	8	50	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

171 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
17	CLA	B	838	-	42,50,73	2.68	11 (26%)	48,85,113	1.53	8 (16%)
17	CLA	5	314	-	46,54,73	2.35	10 (21%)	53,90,113	1.57	8 (15%)
17	CLA	A	839	-	42,50,73	2.69	11 (26%)	48,85,113	1.54	10 (20%)
20	CHL	6	607	-	43,51,74	2.49	10 (23%)	45,86,114	1.73	9 (20%)
17	CLA	B	807	-	42,50,73	2.70	10 (23%)	48,85,113	1.89	9 (18%)
17	CLA	4	605	-	45,53,73	2.56	10 (22%)	52,89,113	1.38	8 (15%)
17	CLA	8	610	-	42,50,73	2.54	9 (21%)	48,85,113	1.55	8 (16%)
17	CLA	8	604	-	42,50,73	2.84	10 (23%)	48,85,113	1.47	8 (16%)
17	CLA	A	829	-	42,50,73	2.69	9 (21%)	48,85,113	1.59	9 (18%)
17	CLA	B	816	-	42,50,73	2.83	10 (23%)	48,85,113	1.54	7 (14%)
17	CLA	B	813	-	41,49,73	2.62	9 (21%)	51,84,113	1.50	8 (15%)
17	CLA	B	828	-	43,51,73	2.77	9 (20%)	49,86,113	1.46	7 (14%)
17	CLA	3	308	-	42,50,73	2.67	9 (21%)	48,85,113	1.90	8 (16%)
17	CLA	A	816	-	42,50,73	2.62	9 (21%)	48,85,113	1.44	9 (18%)
19	SF4	C	102	-	0,12,12	-	-	-		
17	CLA	1	603	-	42,50,73	2.76	11 (26%)	48,85,113	1.43	7 (14%)
17	CLA	7	601	10	42,50,73	2.73	10 (23%)	48,85,113	1.55	8 (16%)
17	CLA	A	809	-	42,50,73	2.73	9 (21%)	48,85,113	1.56	9 (18%)
20	CHL	3	307	-	46,54,74	2.38	11 (23%)	49,90,114	1.76	9 (18%)
17	CLA	B	804	-	42,50,73	2.69	9 (21%)	48,85,113	1.69	7 (14%)
17	CLA	B	814	-	38,47,73	3.00	8 (21%)	45,81,113	1.49	8 (17%)
17	CLA	B	832	-	42,50,73	2.81	11 (26%)	48,85,113	1.52	8 (16%)
17	CLA	7	613	-	43,51,73	2.71	10 (23%)	49,86,113	1.45	8 (16%)
20	CHL	5	313	-	43,51,74	2.47	10 (23%)	45,86,114	1.79	8 (17%)
17	CLA	A	806	-	42,50,73	2.85	11 (26%)	48,85,113	1.48	7 (14%)
17	CLA	6	610	-	45,53,73	2.73	11 (24%)	52,89,113	1.43	8 (15%)
17	CLA	A	808	-	42,50,73	2.74	11 (26%)	48,85,113	1.47	7 (14%)
17	CLA	7	604	-	42,50,73	2.87	9 (21%)	48,85,113	1.57	11 (22%)
17	CLA	F	302	-	62,70,73	2.17	8 (12%)	72,109,113	1.22	8 (11%)
17	CLA	J	102	-	42,50,73	2.82	9 (21%)	48,85,113	1.60	9 (18%)
17	CLA	7	609	-	42,50,73	2.75	9 (21%)	48,85,113	1.52	9 (18%)
17	CLA	A	810	-	42,50,73	2.84	10 (23%)	48,85,113	1.52	9 (18%)
17	CLA	A	823	-	42,50,73	2.83	10 (23%)	48,85,113	1.58	9 (18%)
17	CLA	7	605	-	42,50,73	2.79	11 (26%)	48,85,113	1.47	10 (20%)
18	PQN	B	840	-	34,34,34	0.23	0	42,45,45	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CLA	B	810	-	46,54,73	2.52	9 (19%)	52,89,113	1.54	8 (15%)
17	CLA	3	310	-	41,49,73	2.73	9 (21%)	47,84,113	2.12	13 (27%)
17	CLA	B	830	-	42,50,73	2.67	9 (21%)	48,85,113	1.57	8 (16%)
17	CLA	8	602	-	42,50,73	2.72	9 (21%)	48,85,113	1.49	7 (14%)
17	CLA	B	802	-	45,53,73	2.47	7 (15%)	52,89,113	1.69	7 (13%)
17	CLA	8	605	-	42,50,73	2.75	10 (23%)	48,85,113	1.44	8 (16%)
17	CLA	A	815	-	42,50,73	2.91	10 (23%)	48,85,113	1.52	7 (14%)
20	CHL	8	606	-	43,51,74	2.49	10 (23%)	45,86,114	1.82	7 (15%)
17	CLA	B	827	-	42,50,73	2.67	10 (23%)	48,85,113	1.45	7 (14%)
17	CLA	1	604	-	42,50,73	2.77	7 (16%)	48,85,113	1.42	9 (18%)
17	CLA	3	305	-	42,50,73	2.58	8 (19%)	48,85,113	1.62	8 (16%)
19	SF4	C	101	-	0,12,12	-	-	-		
17	CLA	A	802	-	42,50,73	2.77	10 (23%)	48,85,113	1.74	9 (18%)
17	CLA	A	807	-	42,50,73	2.80	9 (21%)	48,85,113	1.77	10 (20%)
16	CL0	A	801	-	42,50,73	2.68	10 (23%)	48,85,113	1.61	8 (16%)
17	CLA	3	301	-	42,50,73	2.76	10 (23%)	48,85,113	1.60	9 (18%)
17	CLA	B	817	-	42,50,73	2.79	9 (21%)	48,85,113	1.56	9 (18%)
17	CLA	A	831	-	42,50,73	2.83	10 (23%)	48,85,113	1.47	9 (18%)
17	CLA	6	604	-	42,50,73	2.75	10 (23%)	48,85,113	1.44	9 (18%)
17	CLA	5	301	-	42,50,73	2.72	10 (23%)	48,85,113	1.46	7 (14%)
17	CLA	B	811	-	42,50,73	2.73	10 (23%)	48,85,113	1.50	10 (20%)
17	CLA	1	602	-	42,50,73	2.67	9 (21%)	48,85,113	1.54	8 (16%)
17	CLA	A	830	-	42,50,73	2.72	10 (23%)	48,85,113	1.59	9 (18%)
17	CLA	4	604	-	42,50,73	2.84	9 (21%)	48,85,113	1.46	8 (16%)
17	CLA	8	609	-	42,50,73	2.67	9 (21%)	48,85,113	1.46	8 (16%)
17	CLA	8	608	-	42,50,73	2.80	9 (21%)	48,85,113	1.65	11 (22%)
17	CLA	B	837	-	42,50,73	2.74	9 (21%)	48,85,113	1.61	8 (16%)
17	CLA	A	832	-	41,48,73	2.93	11 (26%)	46,82,113	2.12	11 (23%)
17	CLA	A	819	-	42,50,73	2.72	9 (21%)	48,85,113	1.46	9 (18%)
17	CLA	7	607	-	42,50,73	2.74	10 (23%)	48,85,113	1.45	8 (16%)
17	CLA	7	612	-	45,53,73	2.71	10 (22%)	52,89,113	1.36	7 (13%)
17	CLA	A	804	-	42,50,73	2.59	9 (21%)	48,85,113	2.01	10 (20%)
17	CLA	A	811	-	42,50,73	2.77	11 (26%)	48,85,113	1.49	7 (14%)
17	CLA	B	834	-	42,50,73	2.69	10 (23%)	48,85,113	1.62	8 (16%)
17	CLA	6	602	-	42,50,73	2.74	9 (21%)	48,85,113	1.50	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CLA	6	603	-	42,50,73	2.71	10 (23%)	48,85,113	1.59	7 (14%)
17	CLA	1	606	-	42,50,73	2.78	7 (16%)	48,85,113	1.76	9 (18%)
20	CHL	7	606	-	43,51,74	2.48	10 (23%)	45,86,114	1.86	8 (17%)
17	CLA	1	608	-	42,50,73	2.96	9 (21%)	48,85,113	1.49	9 (18%)
17	CLA	A	834	1	42,50,73	2.71	9 (21%)	48,85,113	1.54	7 (14%)
17	CLA	7	611	-	42,50,73	2.85	10 (23%)	48,85,113	1.53	8 (16%)
17	CLA	8	603	-	45,53,73	2.79	11 (24%)	52,89,113	1.47	8 (15%)
17	CLA	B	824	-	41,49,73	2.82	9 (21%)	47,84,113	1.74	10 (21%)
17	CLA	5	304	-	42,50,73	2.80	10 (23%)	48,85,113	1.38	7 (14%)
17	CLA	3	303	-	42,50,73	2.82	10 (23%)	48,85,113	1.48	8 (16%)
17	CLA	B	821	-	46,54,73	2.76	10 (21%)	53,90,113	1.37	7 (13%)
17	CLA	A	826	-	42,50,73	2.59	9 (21%)	48,85,113	1.44	7 (14%)
17	CLA	A	841	-	52,60,73	2.49	9 (17%)	60,97,113	1.48	10 (16%)
17	CLA	8	601	11	42,50,73	2.75	11 (26%)	48,85,113	1.51	7 (14%)
17	CLA	B	822	-	42,50,73	2.68	10 (23%)	48,85,113	1.47	8 (16%)
17	CLA	6	608	-	42,50,73	2.54	8 (19%)	48,85,113	1.53	9 (18%)
17	CLA	B	819	-	42,50,73	2.79	9 (21%)	48,85,113	1.71	10 (20%)
17	CLA	A	821	-	51,59,73	2.46	9 (17%)	59,96,113	1.58	10 (16%)
17	CLA	B	835	-	43,51,73	2.64	9 (20%)	49,86,113	1.47	8 (16%)
17	CLA	B	808	-	42,50,73	2.69	10 (23%)	48,85,113	1.53	8 (16%)
17	CLA	A	813	-	42,50,73	2.80	11 (26%)	48,85,113	1.54	10 (20%)
17	CLA	B	809	-	42,50,73	2.82	10 (23%)	48,85,113	1.57	7 (14%)
19	SF4	B	803	-	0,12,12	-	-	-		
17	CLA	A	822	-	42,50,73	2.71	10 (23%)	48,85,113	1.64	9 (18%)
17	CLA	B	825	-	42,50,73	2.79	10 (23%)	48,85,113	1.43	8 (16%)
17	CLA	B	815	-	65,73,73	2.29	8 (12%)	76,113,113	1.62	14 (18%)
17	CLA	A	837	-	42,50,73	2.73	11 (26%)	48,85,113	1.49	7 (14%)
17	CLA	A	825	-	42,50,73	2.60	10 (23%)	48,85,113	1.67	9 (18%)
17	CLA	1	610	-	42,50,73	2.80	9 (21%)	48,85,113	1.46	8 (16%)
17	CLA	B	831	-	42,50,73	2.84	10 (23%)	48,85,113	1.78	9 (18%)
17	CLA	5	307	-	42,50,73	2.75	9 (21%)	48,85,113	1.48	8 (16%)
17	CLA	3	311	-	42,50,73	2.83	9 (21%)	48,85,113	1.45	8 (16%)
20	CHL	6	605	-	43,51,74	2.53	10 (23%)	45,86,114	1.78	9 (20%)
17	CLA	A	836	-	42,50,73	2.75	10 (23%)	48,85,113	1.53	8 (16%)
17	CLA	B	812	-	42,50,73	2.72	10 (23%)	48,85,113	2.04	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CHL	Z	601	12	43,51,74	2.50	10 (23%)	45,86,114	1.74	7 (15%)
17	CLA	A	833	-	42,50,73	2.74	10 (23%)	48,85,113	1.61	8 (16%)
17	CLA	A	828	-	42,50,73	2.74	10 (23%)	48,85,113	1.41	8 (16%)
17	CLA	5	312	-	42,50,73	2.71	10 (23%)	48,85,113	1.45	8 (16%)
17	CLA	A	803	-	42,50,73	2.75	10 (23%)	48,85,113	1.61	7 (14%)
17	CLA	7	614	10	42,50,73	2.72	9 (21%)	48,85,113	1.90	11 (22%)
17	CLA	B	839	-	42,50,73	2.67	9 (21%)	48,85,113	1.50	8 (16%)
17	CLA	B	829	-	43,51,73	2.55	9 (20%)	49,86,113	1.59	9 (18%)
20	CHL	5	305	-	46,54,74	2.33	11 (23%)	49,90,114	1.85	9 (18%)
20	CHL	6	606	-	43,51,74	2.45	11 (25%)	45,86,114	1.86	8 (17%)
20	CHL	1	601	8	53,61,74	2.25	10 (18%)	57,98,114	1.54	7 (12%)
17	CLA	3	306	-	42,50,73	2.69	9 (21%)	48,85,113	1.95	13 (27%)
17	CLA	B	826	-	42,50,73	2.62	9 (21%)	48,85,113	1.79	7 (14%)
17	CLA	5	311	-	42,50,73	2.74	9 (21%)	48,85,113	1.50	8 (16%)
17	CLA	A	843	-	42,50,73	2.73	11 (26%)	48,85,113	1.39	7 (14%)
17	CLA	4	601	-	42,50,73	2.73	10 (23%)	48,85,113	1.53	8 (16%)
17	CLA	5	308	-	42,50,73	2.49	8 (19%)	48,85,113	1.46	7 (14%)
17	CLA	3	309	-	45,53,73	2.54	8 (17%)	52,89,113	1.47	7 (13%)
17	CLA	3	302	-	42,50,73	2.78	10 (23%)	48,85,113	1.45	8 (16%)
17	CLA	5	309	-	42,50,73	2.69	10 (23%)	48,85,113	1.64	8 (16%)
17	CLA	8	607	-	42,50,73	2.71	11 (26%)	48,85,113	1.54	8 (16%)
17	CLA	B	806	-	42,50,73	2.81	10 (23%)	48,85,113	2.02	12 (25%)
18	PQN	A	840	-	34,34,34	0.21	0	42,45,45	0.26	0
17	CLA	7	603	-	42,50,73	2.77	9 (21%)	48,85,113	1.74	10 (20%)
17	CLA	A	814	-	42,50,73	2.70	11 (26%)	48,85,113	1.46	7 (14%)
17	CLA	A	817	-	42,50,73	2.75	9 (21%)	48,85,113	1.73	10 (20%)
17	CLA	F	301	-	42,50,73	2.67	9 (21%)	48,85,113	1.61	9 (18%)
17	CLA	B	833	-	42,50,73	2.67	9 (21%)	48,85,113	1.53	8 (16%)
17	CLA	1	607	-	42,50,73	2.83	8 (19%)	48,85,113	1.94	9 (18%)
17	CLA	1	609	-	42,50,73	2.90	8 (19%)	48,85,113	1.39	7 (14%)
17	CLA	5	310	-	42,50,73	2.82	11 (26%)	48,85,113	1.42	8 (16%)
17	CLA	8	611	-	42,50,73	2.79	10 (23%)	48,85,113	1.59	7 (14%)
17	CLA	8	613	-	42,50,73	2.67	10 (23%)	48,85,113	1.51	8 (16%)
17	CLA	B	823	-	42,50,73	2.78	10 (23%)	48,85,113	1.58	10 (20%)
17	CLA	B	801	-	42,50,73	2.49	8 (19%)	48,85,113	1.72	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	CLA	J	101	-	42,50,73	2.83	11 (26%)	48,85,113	1.62	9 (18%)
17	CLA	B	805	-	42,50,73	2.66	7 (16%)	48,85,113	1.55	8 (16%)
17	CLA	5	302	14	42,50,73	2.76	10 (23%)	48,85,113	1.48	8 (16%)
17	CLA	5	306	-	50,58,73	2.55	9 (18%)	58,95,113	1.36	7 (12%)
17	CLA	5	315	-	45,53,73	2.63	10 (22%)	52,89,113	1.53	8 (15%)
17	CLA	3	313	-	42,50,73	2.73	10 (23%)	48,85,113	1.77	10 (20%)
17	CLA	A	824	-	42,50,73	2.62	10 (23%)	48,85,113	1.73	9 (18%)
17	CLA	A	842	-	42,50,73	2.64	7 (16%)	48,85,113	1.34	9 (18%)
17	CLA	A	838	-	42,50,73	2.76	9 (21%)	48,85,113	1.67	10 (20%)
17	CLA	B	820	-	42,50,73	2.65	8 (19%)	48,85,113	1.62	9 (18%)
17	CLA	B	818	-	42,50,73	2.72	9 (21%)	48,85,113	1.66	10 (20%)
17	CLA	B	836	-	42,50,73	2.74	10 (23%)	48,85,113	1.61	7 (14%)
17	CLA	A	818	-	45,53,73	2.65	10 (22%)	52,89,113	1.48	9 (17%)
17	CLA	8	612	-	46,54,73	2.68	10 (21%)	53,90,113	1.39	7 (13%)
17	CLA	A	835	-	42,50,73	2.69	11 (26%)	48,85,113	1.46	9 (18%)
17	CLA	7	610	-	41,49,73	2.88	10 (24%)	47,84,113	2.00	11 (23%)
17	CLA	7	602	-	42,50,73	2.71	10 (23%)	48,85,113	1.51	8 (16%)
17	CLA	A	812	-	42,50,73	2.76	11 (26%)	48,85,113	1.49	8 (16%)
17	CLA	3	312	-	42,50,73	2.67	9 (21%)	48,85,113	1.63	8 (16%)
17	CLA	7	608	-	42,50,73	2.76	8 (19%)	48,85,113	1.59	8 (16%)
17	CLA	8	614	11	42,50,73	2.79	10 (23%)	48,85,113	1.65	8 (16%)
17	CLA	6	609	15	46,54,73	2.73	10 (21%)	53,90,113	1.42	8 (15%)
17	CLA	4	602	-	45,53,73	2.69	7 (15%)	52,89,113	1.45	8 (15%)
17	CLA	6	601	15	42,50,73	2.80	10 (23%)	48,85,113	1.47	8 (16%)
17	CLA	5	303	-	48,56,73	2.49	9 (18%)	55,92,113	1.33	8 (14%)
17	CLA	A	805	-	42,50,73	2.80	10 (23%)	48,85,113	1.69	9 (18%)
17	CLA	A	827	-	42,50,73	2.66	11 (26%)	48,85,113	1.49	9 (18%)
17	CLA	3	304	-	45,53,73	2.60	9 (20%)	52,89,113	1.39	8 (15%)
17	CLA	4	603	-	42,50,73	2.82	8 (19%)	48,85,113	1.94	10 (20%)
17	CLA	A	820	-	42,50,73	2.90	10 (23%)	48,85,113	1.50	6 (12%)
17	CLA	1	605	-	42,50,73	2.85	9 (21%)	48,85,113	1.52	9 (18%)

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
17	CLA	B	838	-	1/1/10/20	2/10/88/115	-
17	CLA	5	314	-	1/1/11/20	7/15/93/115	-
17	CLA	A	839	-	1/1/10/20	1/10/88/115	-
20	CHL	6	607	-	3/3/15/26	2/12/110/137	-
17	CLA	B	807	-	1/1/10/20	4/10/88/115	-
17	CLA	4	605	-	1/1/11/20	1/13/91/115	-
17	CLA	8	610	-	1/1/10/20	3/10/88/115	-
17	CLA	8	604	-	1/1/10/20	0/10/88/115	-
17	CLA	A	829	-	1/1/10/20	3/10/88/115	-
17	CLA	B	816	-	1/1/10/20	3/10/88/115	-
17	CLA	B	813	-	1/1/10/20	1/10/86/115	-
17	CLA	B	828	-	1/1/10/20	1/11/89/115	-
17	CLA	3	308	-	1/1/10/20	1/10/88/115	-
17	CLA	A	816	-	1/1/10/20	3/10/88/115	-
19	SF4	C	102	-	-	-	0/6/5/5
17	CLA	1	603	-	1/1/10/20	2/10/88/115	-
17	CLA	7	601	10	1/1/10/20	3/10/88/115	-
17	CLA	A	809	-	1/1/10/20	2/10/88/115	-
20	CHL	3	307	-	3/3/16/26	5/15/113/137	-
17	CLA	B	804	-	1/1/10/20	1/10/88/115	-
17	CLA	B	814	-	1/1/9/20	0/4/82/115	-
17	CLA	B	832	-	1/1/10/20	2/10/88/115	-
17	CLA	7	613	-	1/1/10/20	1/11/89/115	-
20	CHL	5	313	-	3/3/15/26	2/12/110/137	-
17	CLA	A	806	-	1/1/10/20	1/10/88/115	-
17	CLA	6	610	-	1/1/11/20	3/13/91/115	-
17	CLA	A	808	-	1/1/10/20	0/10/88/115	-
17	CLA	7	604	-	1/1/10/20	0/10/88/115	-
17	CLA	F	302	-	1/1/14/20	8/34/112/115	-
17	CLA	J	102	-	1/1/10/20	2/10/88/115	-
17	CLA	7	609	-	1/1/10/20	1/10/88/115	-
17	CLA	A	810	-	1/1/10/20	1/10/88/115	-
17	CLA	A	823	-	1/1/10/20	3/10/88/115	-
17	CLA	7	605	-	1/1/10/20	3/10/88/115	-
18	PQN	B	840	-	-	4/23/43/43	0/2/2/2
17	CLA	B	810	-	1/1/11/20	5/13/91/115	-
17	CLA	3	310	-	1/1/10/20	2/8/86/115	-
17	CLA	B	830	-	1/1/10/20	2/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	8	602	-	1/1/10/20	3/10/88/115	-
17	CLA	B	802	-	1/1/11/20	5/13/91/115	-
17	CLA	8	605	-	1/1/10/20	2/10/88/115	-
17	CLA	A	815	-	1/1/10/20	0/10/88/115	-
20	CHL	8	606	-	3/3/15/26	0/12/110/137	-
17	CLA	B	827	-	1/1/10/20	4/10/88/115	-
17	CLA	1	604	-	1/1/10/20	1/10/88/115	-
17	CLA	3	305	-	1/1/10/20	1/10/88/115	-
19	SF4	C	101	-	-	-	0/6/5/5
17	CLA	A	802	-	1/1/10/20	4/10/88/115	-
17	CLA	A	807	-	1/1/10/20	2/10/88/115	-
16	CL0	A	801	-	3/3/15/25	3/10/108/135	-
17	CLA	3	301	-	1/1/10/20	3/10/88/115	-
17	CLA	B	817	-	1/1/10/20	3/10/88/115	-
17	CLA	A	831	-	1/1/10/20	3/10/88/115	-
17	CLA	6	604	-	1/1/10/20	0/10/88/115	-
17	CLA	5	301	-	1/1/10/20	2/10/88/115	-
17	CLA	B	811	-	1/1/10/20	0/10/88/115	-
17	CLA	1	602	-	1/1/10/20	3/10/88/115	-
17	CLA	A	830	-	1/1/10/20	1/10/88/115	-
17	CLA	4	604	-	1/1/10/20	1/10/88/115	-
17	CLA	8	609	-	1/1/10/20	1/10/88/115	-
17	CLA	8	608	-	1/1/10/20	0/10/88/115	-
17	CLA	B	837	-	1/1/10/20	1/10/88/115	-
17	CLA	A	832	-	1/1/10/20	4/8/86/115	-
17	CLA	A	819	-	1/1/10/20	2/10/88/115	-
17	CLA	7	607	-	1/1/10/20	3/10/88/115	-
17	CLA	7	612	-	1/1/11/20	4/13/91/115	-
17	CLA	A	804	-	1/1/10/20	3/10/88/115	-
17	CLA	A	811	-	1/1/10/20	2/10/88/115	-
17	CLA	B	834	-	1/1/10/20	5/10/88/115	-
17	CLA	6	602	-	1/1/10/20	3/10/88/115	-
17	CLA	6	603	-	1/1/10/20	3/10/88/115	-
17	CLA	1	606	-	1/1/10/20	0/10/88/115	-
20	CHL	7	606	-	3/3/15/26	0/12/110/137	-
17	CLA	1	608	-	1/1/10/20	3/10/88/115	-
17	CLA	A	834	1	1/1/10/20	0/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	7	611	-	1/1/10/20	3/10/88/115	-
17	CLA	8	603	-	1/1/11/20	2/13/91/115	-
17	CLA	B	824	-	1/1/10/20	1/8/86/115	-
17	CLA	5	304	-	1/1/10/20	2/10/88/115	-
17	CLA	3	303	-	1/1/10/20	0/10/88/115	-
17	CLA	B	821	-	1/1/11/20	3/15/93/115	-
17	CLA	A	826	-	1/1/10/20	0/10/88/115	-
17	CLA	A	841	-	1/1/12/20	9/22/100/115	-
17	CLA	8	601	11	1/1/10/20	1/10/88/115	-
17	CLA	B	822	-	1/1/10/20	3/10/88/115	-
17	CLA	6	608	-	1/1/10/20	2/10/88/115	-
17	CLA	B	819	-	1/1/10/20	3/10/88/115	-
17	CLA	A	821	-	1/1/12/20	5/21/99/115	-
17	CLA	B	835	-	1/1/10/20	3/11/89/115	-
17	CLA	B	808	-	1/1/10/20	1/10/88/115	-
17	CLA	A	813	-	1/1/10/20	3/10/88/115	-
17	CLA	B	809	-	1/1/10/20	4/10/88/115	-
19	SF4	B	803	-	-	-	0/6/5/5
17	CLA	A	822	-	1/1/10/20	2/10/88/115	-
17	CLA	B	825	-	1/1/10/20	4/10/88/115	-
17	CLA	B	815	-	1/1/15/20	10/37/115/115	-
17	CLA	A	837	-	1/1/10/20	3/10/88/115	-
17	CLA	A	825	-	1/1/10/20	2/10/88/115	-
17	CLA	1	610	-	1/1/10/20	3/10/88/115	-
17	CLA	B	831	-	1/1/10/20	0/10/88/115	-
17	CLA	5	307	-	1/1/10/20	3/10/88/115	-
17	CLA	3	311	-	1/1/10/20	3/10/88/115	-
20	CHL	6	605	-	3/3/15/26	1/12/110/137	-
17	CLA	A	836	-	1/1/10/20	2/10/88/115	-
17	CLA	B	812	-	1/1/10/20	4/10/88/115	-
20	CHL	Z	601	12	3/3/15/26	3/12/110/137	-
17	CLA	A	833	-	1/1/10/20	1/10/88/115	-
17	CLA	A	828	-	1/1/10/20	1/10/88/115	-
17	CLA	5	312	-	1/1/10/20	1/10/88/115	-
17	CLA	A	803	-	1/1/10/20	2/10/88/115	-
17	CLA	7	614	10	1/1/10/20	2/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	839	-	1/1/10/20	1/10/88/115	-
17	CLA	B	829	-	1/1/10/20	5/11/89/115	-
20	CHL	5	305	-	3/3/16/26	3/15/113/137	-
20	CHL	6	606	-	3/3/15/26	3/12/110/137	-
20	CHL	1	601	8	3/3/17/26	6/24/122/137	-
17	CLA	3	306	-	1/1/10/20	2/10/88/115	-
17	CLA	B	826	-	1/1/10/20	2/10/88/115	-
17	CLA	5	311	-	1/1/10/20	3/10/88/115	-
17	CLA	A	843	-	1/1/10/20	2/10/88/115	-
17	CLA	4	601	-	1/1/10/20	2/10/88/115	-
17	CLA	5	308	-	1/1/10/20	3/10/88/115	-
17	CLA	3	309	-	1/1/11/20	0/13/91/115	-
17	CLA	3	302	-	1/1/10/20	2/10/88/115	-
17	CLA	5	309	-	1/1/10/20	3/10/88/115	-
17	CLA	8	607	-	1/1/10/20	2/10/88/115	-
17	CLA	B	806	-	1/1/10/20	2/10/88/115	-
18	PQN	A	840	-	-	5/23/43/43	0/2/2/2
17	CLA	7	603	-	1/1/10/20	2/10/88/115	-
17	CLA	A	814	-	1/1/10/20	1/10/88/115	-
17	CLA	A	817	-	1/1/10/20	2/10/88/115	-
17	CLA	F	301	-	1/1/10/20	2/10/88/115	-
17	CLA	B	833	-	1/1/10/20	1/10/88/115	-
17	CLA	1	607	-	1/1/10/20	3/10/88/115	-
17	CLA	1	609	-	1/1/10/20	2/10/88/115	-
17	CLA	5	310	-	1/1/10/20	0/10/88/115	-
17	CLA	8	611	-	1/1/10/20	3/10/88/115	-
17	CLA	8	613	-	1/1/10/20	3/10/88/115	-
17	CLA	B	823	-	1/1/10/20	4/10/88/115	-
17	CLA	B	801	-	1/1/10/20	3/10/88/115	-
17	CLA	J	101	-	1/1/10/20	4/10/88/115	-
17	CLA	B	805	-	1/1/10/20	0/10/88/115	-
17	CLA	5	302	14	1/1/10/20	2/10/88/115	-
17	CLA	5	306	-	1/1/12/20	3/19/97/115	-
17	CLA	5	315	-	1/1/11/20	4/13/91/115	-
17	CLA	3	313	-	1/1/10/20	1/10/88/115	-
17	CLA	A	824	-	1/1/10/20	0/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	842	-	1/1/10/20	3/10/88/115	-
17	CLA	A	838	-	1/1/10/20	2/10/88/115	-
17	CLA	B	820	-	1/1/10/20	3/10/88/115	-
17	CLA	B	818	-	1/1/10/20	3/10/88/115	-
17	CLA	B	836	-	1/1/10/20	2/10/88/115	-
17	CLA	A	818	-	1/1/11/20	3/13/91/115	-
17	CLA	8	612	-	1/1/11/20	0/15/93/115	-
17	CLA	A	835	-	1/1/10/20	4/10/88/115	-
17	CLA	7	610	-	1/1/10/20	3/8/86/115	-
17	CLA	7	602	-	1/1/10/20	3/10/88/115	-
17	CLA	A	812	-	1/1/10/20	2/10/88/115	-
17	CLA	3	312	-	1/1/10/20	1/10/88/115	-
17	CLA	7	608	-	1/1/10/20	1/10/88/115	-
17	CLA	8	614	11	1/1/10/20	1/10/88/115	-
17	CLA	6	609	15	1/1/11/20	1/15/93/115	-
17	CLA	4	602	-	1/1/11/20	4/13/91/115	-
17	CLA	6	601	15	1/1/10/20	3/10/88/115	-
17	CLA	5	303	-	1/1/11/20	5/17/95/115	-
17	CLA	A	805	-	1/1/10/20	2/10/88/115	-
17	CLA	A	827	-	1/1/10/20	0/10/88/115	-
17	CLA	3	304	-	1/1/11/20	2/13/91/115	-
17	CLA	4	603	-	1/1/10/20	4/10/88/115	-
17	CLA	A	820	-	1/1/10/20	4/10/88/115	-
17	CLA	1	605	-	1/1/10/20	2/10/88/115	-

All (1588) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	608	CLA	C4B-NB	14.91	1.48	1.35
17	7	604	CLA	C4B-NB	14.47	1.48	1.35
17	B	821	CLA	C4B-NB	14.31	1.48	1.35
17	B	814	CLA	C4B-NB	14.30	1.48	1.35
17	1	609	CLA	C4B-NB	14.16	1.47	1.35
17	1	605	CLA	C4B-NB	14.01	1.47	1.35
17	8	603	CLA	C4B-NB	13.95	1.47	1.35
17	3	311	CLA	C4B-NB	13.94	1.47	1.35
17	4	604	CLA	C4B-NB	13.94	1.47	1.35
17	6	609	CLA	C4B-NB	13.93	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	815	CLA	C4B-NB	13.86	1.47	1.35
17	8	604	CLA	C4B-NB	13.85	1.47	1.35
17	A	831	CLA	C4B-NB	13.84	1.47	1.35
17	A	820	CLA	C4B-NB	13.84	1.47	1.35
17	A	806	CLA	C4B-NB	13.81	1.47	1.35
17	A	823	CLA	C4B-NB	13.81	1.47	1.35
17	5	304	CLA	C4B-NB	13.79	1.47	1.35
17	3	303	CLA	C4B-NB	13.71	1.47	1.35
17	A	810	CLA	C4B-NB	13.69	1.47	1.35
17	J	101	CLA	C4B-NB	13.64	1.47	1.35
17	7	611	CLA	C4B-NB	13.61	1.47	1.35
17	6	601	CLA	C4B-NB	13.58	1.47	1.35
17	4	602	CLA	C4B-NB	13.53	1.47	1.35
17	7	605	CLA	C4B-NB	13.51	1.47	1.35
17	7	612	CLA	C4B-NB	13.50	1.47	1.35
17	6	610	CLA	C4B-NB	13.49	1.47	1.35
17	8	612	CLA	C4B-NB	13.48	1.47	1.35
17	7	608	CLA	C4B-NB	13.46	1.47	1.35
17	B	809	CLA	C4B-NB	13.44	1.47	1.35
17	J	102	CLA	C4B-NB	13.43	1.47	1.35
17	B	828	CLA	C4B-NB	13.42	1.47	1.35
17	B	817	CLA	C4B-NB	13.38	1.47	1.35
17	8	605	CLA	C4B-NB	13.38	1.47	1.35
17	7	607	CLA	C4B-NB	13.37	1.47	1.35
17	B	816	CLA	C4B-NB	13.36	1.47	1.35
17	1	610	CLA	C4B-NB	13.35	1.47	1.35
17	A	813	CLA	C4B-NB	13.34	1.47	1.35
17	B	823	CLA	C4B-NB	13.34	1.47	1.35
17	1	603	CLA	C4B-NB	13.33	1.47	1.35
17	B	832	CLA	C4B-NB	13.30	1.47	1.35
17	3	302	CLA	C4B-NB	13.30	1.47	1.35
17	A	811	CLA	C4B-NB	13.28	1.47	1.35
17	5	307	CLA	C4B-NB	13.27	1.47	1.35
17	5	310	CLA	C4B-NB	13.22	1.47	1.35
17	B	811	CLA	C4B-NB	13.19	1.47	1.35
17	A	812	CLA	C4B-NB	13.19	1.47	1.35
17	A	807	CLA	C4B-NB	13.18	1.47	1.35
17	A	828	CLA	C4B-NB	13.17	1.47	1.35
17	B	822	CLA	C4B-NB	13.15	1.46	1.35
17	1	606	CLA	C4B-NB	13.15	1.46	1.35
17	B	815	CLA	C4B-NB	13.15	1.46	1.35
17	A	819	CLA	C4B-NB	13.14	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	311	CLA	C4B-NB	13.12	1.46	1.35
17	A	805	CLA	C4B-NB	13.09	1.46	1.35
17	B	825	CLA	C4B-NB	13.09	1.46	1.35
17	7	601	CLA	C4B-NB	13.09	1.46	1.35
17	5	302	CLA	C4B-NB	13.09	1.46	1.35
17	A	836	CLA	C4B-NB	13.05	1.46	1.35
17	6	604	CLA	C4B-NB	13.05	1.46	1.35
17	8	601	CLA	C4B-NB	13.04	1.46	1.35
17	B	836	CLA	C4B-NB	13.03	1.46	1.35
17	8	614	CLA	C4B-NB	13.00	1.46	1.35
17	3	301	CLA	C4B-NB	13.00	1.46	1.35
17	A	834	CLA	C4B-NB	12.98	1.46	1.35
17	8	602	CLA	C4B-NB	12.98	1.46	1.35
17	A	843	CLA	C4B-NB	12.98	1.46	1.35
17	7	609	CLA	C4B-NB	12.98	1.46	1.35
17	8	608	CLA	C4B-NB	12.98	1.46	1.35
17	1	604	CLA	C4B-NB	12.96	1.46	1.35
17	5	306	CLA	C4B-NB	12.96	1.46	1.35
17	6	602	CLA	C4B-NB	12.96	1.46	1.35
17	5	312	CLA	C4B-NB	12.96	1.46	1.35
17	A	803	CLA	C4B-NB	12.95	1.46	1.35
17	6	603	CLA	C4B-NB	12.92	1.46	1.35
17	5	301	CLA	C4B-NB	12.90	1.46	1.35
17	A	808	CLA	C4B-NB	12.89	1.46	1.35
17	8	607	CLA	C4B-NB	12.85	1.46	1.35
17	B	831	CLA	C4B-NB	12.84	1.46	1.35
17	A	829	CLA	C4B-NB	12.82	1.46	1.35
17	B	818	CLA	C4B-NB	12.82	1.46	1.35
17	7	602	CLA	C4B-NB	12.80	1.46	1.35
17	7	603	CLA	C4B-NB	12.78	1.46	1.35
17	8	611	CLA	C4B-NB	12.77	1.46	1.35
17	B	808	CLA	C4B-NB	12.77	1.46	1.35
17	7	613	CLA	C4B-NB	12.77	1.46	1.35
17	B	827	CLA	C4B-NB	12.75	1.46	1.35
17	A	818	CLA	C4B-NB	12.74	1.46	1.35
17	B	830	CLA	C4B-NB	12.74	1.46	1.35
17	A	842	CLA	C4B-NB	12.73	1.46	1.35
17	A	832	CLA	C4B-NB	12.73	1.46	1.35
17	B	839	CLA	C4B-NB	12.72	1.46	1.35
17	4	601	CLA	C4B-NB	12.69	1.46	1.35
17	A	837	CLA	C4B-NB	12.68	1.46	1.35
17	B	838	CLA	C4B-NB	12.67	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	804	CLA	C4B-NB	12.66	1.46	1.35
17	A	838	CLA	C4B-NB	12.65	1.46	1.35
17	A	809	CLA	C4B-NB	12.62	1.46	1.35
17	5	309	CLA	C4B-NB	12.61	1.46	1.35
17	B	833	CLA	C4B-NB	12.59	1.46	1.35
17	A	841	CLA	C4B-NB	12.59	1.46	1.35
17	A	833	CLA	C4B-NB	12.58	1.46	1.35
17	1	602	CLA	C4B-NB	12.58	1.46	1.35
17	1	607	CLA	C4B-NB	12.58	1.46	1.35
17	8	609	CLA	C4B-NB	12.57	1.46	1.35
17	5	315	CLA	C4B-NB	12.56	1.46	1.35
17	A	817	CLA	C4B-NB	12.56	1.46	1.35
17	B	837	CLA	C4B-NB	12.55	1.46	1.35
17	5	303	CLA	C4B-NB	12.54	1.46	1.35
17	A	830	CLA	C4B-NB	12.52	1.46	1.35
17	B	820	CLA	C4B-NB	12.51	1.46	1.35
17	A	816	CLA	C4B-NB	12.49	1.46	1.35
17	4	603	CLA	C4B-NB	12.49	1.46	1.35
16	A	801	CL0	C4B-NB	12.46	1.46	1.35
17	B	824	CLA	C4B-NB	12.44	1.46	1.35
17	A	835	CLA	C4B-NB	12.43	1.46	1.35
17	B	806	CLA	C4B-NB	12.42	1.46	1.35
17	A	826	CLA	C4B-NB	12.41	1.46	1.35
17	F	301	CLA	C4B-NB	12.41	1.46	1.35
17	B	819	CLA	C4B-NB	12.40	1.46	1.35
17	A	802	CLA	C4B-NB	12.39	1.46	1.35
17	B	805	CLA	C4B-NB	12.39	1.46	1.35
17	B	834	CLA	C4B-NB	12.39	1.46	1.35
17	B	835	CLA	C4B-NB	12.38	1.46	1.35
17	3	312	CLA	C4B-NB	12.38	1.46	1.35
17	3	313	CLA	C4B-NB	12.37	1.46	1.35
17	A	822	CLA	C4B-NB	12.36	1.46	1.35
17	A	821	CLA	C4B-NB	12.35	1.46	1.35
17	A	814	CLA	C4B-NB	12.35	1.46	1.35
17	3	309	CLA	C4B-NB	12.33	1.46	1.35
17	3	306	CLA	C4B-NB	12.32	1.46	1.35
17	A	827	CLA	C4B-NB	12.31	1.46	1.35
17	F	302	CLA	C4B-NB	12.29	1.46	1.35
17	8	613	CLA	C4B-NB	12.24	1.46	1.35
17	7	614	CLA	C4B-NB	12.22	1.46	1.35
17	B	813	CLA	C4B-NB	12.20	1.46	1.35
20	6	605	CHL	C4B-NB	12.20	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	308	CLA	C4B-NB	12.19	1.46	1.35
17	3	304	CLA	C4B-NB	12.19	1.46	1.35
17	4	605	CLA	C4B-NB	12.09	1.46	1.35
17	3	305	CLA	C4B-NB	12.07	1.46	1.35
17	A	825	CLA	C4B-NB	12.07	1.46	1.35
17	7	610	CLA	C4B-NB	11.97	1.45	1.35
17	B	807	CLA	C4B-NB	11.96	1.45	1.35
17	A	839	CLA	C4B-NB	11.95	1.45	1.35
17	6	608	CLA	C4B-NB	11.89	1.45	1.35
17	B	812	CLA	C4B-NB	11.79	1.45	1.35
17	B	826	CLA	C4B-NB	11.74	1.45	1.35
17	8	610	CLA	C4B-NB	11.72	1.45	1.35
17	A	824	CLA	C4B-NB	11.67	1.45	1.35
17	5	308	CLA	C4B-NB	11.65	1.45	1.35
17	3	310	CLA	C4B-NB	11.65	1.45	1.35
20	5	313	CHL	C4B-NB	11.61	1.45	1.35
20	8	606	CHL	C4B-NB	11.59	1.45	1.35
17	B	829	CLA	C4B-NB	11.56	1.45	1.35
17	B	802	CLA	C4B-NB	11.41	1.45	1.35
17	B	810	CLA	C4B-NB	11.35	1.45	1.35
20	7	606	CHL	C4B-NB	11.34	1.45	1.35
20	6	607	CHL	C4B-NB	11.28	1.45	1.35
20	Z	601	CHL	C4B-NB	11.22	1.45	1.35
17	B	801	CLA	C4B-NB	11.19	1.45	1.35
20	1	601	CHL	C4B-NB	11.17	1.45	1.35
17	A	804	CLA	C4B-NB	11.14	1.45	1.35
20	3	307	CHL	C4B-NB	11.02	1.45	1.35
20	6	606	CHL	C4B-NB	10.97	1.45	1.35
17	5	314	CLA	C4B-NB	10.89	1.44	1.35
20	5	305	CHL	C4B-NB	10.52	1.44	1.35
17	4	603	CLA	C1B-NB	7.13	1.41	1.35
17	7	610	CLA	C3A-C2A	-6.97	1.48	1.54
17	7	604	CLA	MG-ND	-6.92	1.92	2.05
17	1	607	CLA	C1B-NB	6.75	1.41	1.35
17	A	832	CLA	C4C-NC	6.73	1.48	1.37
20	Z	601	CHL	MG-ND	-6.72	1.92	2.05
20	1	601	CHL	MG-ND	-6.70	1.92	2.05
17	A	820	CLA	C1B-NB	6.68	1.41	1.35
17	B	821	CLA	C1B-NB	6.62	1.41	1.35
17	1	606	CLA	C1B-NB	6.60	1.41	1.35
20	5	305	CHL	MG-ND	-6.60	1.92	2.05
17	1	605	CLA	C1B-NB	6.60	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	805	CLA	MG-ND	-6.58	1.92	2.05
20	7	606	CHL	MG-ND	-6.54	1.92	2.05
20	3	307	CHL	MG-ND	-6.49	1.92	2.05
17	B	816	CLA	C1B-NB	6.48	1.41	1.35
17	8	611	CLA	C1B-NB	6.47	1.41	1.35
17	A	842	CLA	MG-ND	-6.46	1.93	2.05
20	8	606	CHL	MG-ND	-6.43	1.93	2.05
17	B	802	CLA	MG-ND	-6.43	1.93	2.05
20	6	607	CHL	MG-ND	-6.42	1.93	2.05
17	B	801	CLA	MG-ND	-6.39	1.93	2.05
17	A	839	CLA	MG-ND	-6.37	1.93	2.05
17	B	831	CLA	MG-ND	-6.36	1.93	2.05
17	1	608	CLA	C1B-NB	6.36	1.40	1.35
20	6	606	CHL	MG-ND	-6.33	1.93	2.05
17	B	809	CLA	MG-ND	-6.33	1.93	2.05
17	A	841	CLA	MG-ND	-6.32	1.93	2.05
17	1	604	CLA	C1B-NB	6.30	1.40	1.35
20	5	313	CHL	MG-ND	-6.29	1.93	2.05
17	A	838	CLA	MG-ND	-6.27	1.93	2.05
20	6	605	CHL	MG-ND	-6.26	1.93	2.05
17	5	314	CLA	MG-ND	-6.25	1.93	2.05
17	4	602	CLA	C1B-NB	6.24	1.40	1.35
17	A	833	CLA	C1B-NB	6.23	1.40	1.35
17	3	313	CLA	MG-ND	-6.23	1.93	2.05
17	A	812	CLA	MG-ND	-6.22	1.93	2.05
17	A	822	CLA	MG-ND	-6.21	1.93	2.05
17	1	609	CLA	C1B-NB	6.20	1.40	1.35
17	1	610	CLA	C1B-NB	6.19	1.40	1.35
17	1	607	CLA	MG-NA	-6.19	1.91	2.06
17	B	829	CLA	MG-ND	-6.18	1.93	2.05
17	A	815	CLA	MG-ND	-6.16	1.93	2.05
17	B	807	CLA	MG-ND	-6.16	1.93	2.05
17	B	824	CLA	MG-ND	-6.15	1.93	2.05
17	5	302	CLA	MG-ND	-6.13	1.93	2.05
17	4	605	CLA	MG-ND	-6.13	1.93	2.05
17	B	810	CLA	MG-ND	-6.12	1.93	2.05
17	7	611	CLA	C1B-NB	6.10	1.40	1.35
17	A	821	CLA	MG-ND	-6.09	1.93	2.05
17	J	102	CLA	C1B-NB	6.09	1.40	1.35
17	B	804	CLA	MG-ND	-6.08	1.93	2.05
17	B	812	CLA	MG-ND	-6.08	1.93	2.05
17	8	610	CLA	MG-ND	-6.07	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	837	CLA	MG-ND	-6.07	1.93	2.05
17	6	602	CLA	C1B-NB	6.07	1.40	1.35
17	7	614	CLA	C1B-NB	6.07	1.40	1.35
17	5	304	CLA	MG-ND	-6.07	1.93	2.05
17	3	308	CLA	MG-ND	-6.06	1.93	2.05
17	8	614	CLA	MG-ND	-6.04	1.93	2.05
17	A	803	CLA	MG-ND	-6.04	1.93	2.05
17	3	301	CLA	MG-ND	-6.03	1.93	2.05
17	8	601	CLA	MG-ND	-6.03	1.93	2.05
17	A	831	CLA	C1B-NB	6.03	1.40	1.35
17	7	605	CLA	MG-ND	-6.02	1.93	2.05
17	B	806	CLA	MG-NA	-6.02	1.92	2.06
17	B	806	CLA	C1B-NB	6.02	1.40	1.35
17	4	604	CLA	C1B-NB	6.01	1.40	1.35
17	A	809	CLA	MG-ND	-6.01	1.93	2.05
17	B	823	CLA	MG-ND	-6.01	1.93	2.05
17	F	301	CLA	MG-ND	-6.00	1.93	2.05
17	B	809	CLA	C1B-NB	6.00	1.40	1.35
17	1	602	CLA	C1B-NB	6.00	1.40	1.35
17	F	302	CLA	MG-ND	-6.00	1.93	2.05
17	A	837	CLA	MG-ND	-6.00	1.93	2.05
17	A	807	CLA	MG-ND	-6.00	1.93	2.05
17	B	817	CLA	C1B-NB	6.00	1.40	1.35
17	6	610	CLA	MG-ND	-5.99	1.93	2.05
17	7	601	CLA	MG-ND	-5.99	1.93	2.05
17	7	610	CLA	MG-ND	-5.98	1.93	2.05
17	8	608	CLA	C1B-NB	5.98	1.40	1.35
17	A	824	CLA	MG-ND	-5.98	1.93	2.05
17	3	305	CLA	MG-ND	-5.97	1.93	2.05
17	A	804	CLA	MG-ND	-5.97	1.93	2.05
17	A	826	CLA	MG-ND	-5.97	1.93	2.05
17	5	315	CLA	C1B-NB	5.97	1.40	1.35
17	A	817	CLA	C1B-NB	5.97	1.40	1.35
17	3	303	CLA	MG-ND	-5.96	1.94	2.05
17	A	835	CLA	MG-ND	-5.96	1.94	2.05
17	5	312	CLA	MG-ND	-5.96	1.94	2.05
17	B	815	CLA	MG-NA	-5.95	1.92	2.06
17	A	807	CLA	C1B-NB	5.95	1.40	1.35
17	5	310	CLA	MG-ND	-5.95	1.94	2.05
17	B	836	CLA	MG-ND	-5.94	1.94	2.05
17	8	608	CLA	MG-ND	-5.94	1.94	2.05
17	B	825	CLA	MG-ND	-5.94	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	826	CLA	MG-ND	-5.93	1.94	2.05
17	A	806	CLA	MG-ND	-5.93	1.94	2.05
17	B	831	CLA	C1B-NB	5.92	1.40	1.35
17	A	802	CLA	MG-ND	-5.91	1.94	2.05
17	B	815	CLA	C1B-NB	5.91	1.40	1.35
17	B	835	CLA	MG-ND	-5.90	1.94	2.05
17	B	812	CLA	MG-NA	-5.90	1.92	2.06
17	8	604	CLA	C1B-NB	5.90	1.40	1.35
17	A	817	CLA	MG-ND	-5.89	1.94	2.05
17	4	601	CLA	MG-ND	-5.88	1.94	2.05
17	7	609	CLA	C1B-NB	5.88	1.40	1.35
17	4	603	CLA	MG-NA	-5.88	1.92	2.06
17	5	310	CLA	C1B-NB	5.87	1.40	1.35
17	8	612	CLA	C1B-NB	5.87	1.40	1.35
17	3	310	CLA	MG-ND	-5.87	1.94	2.05
17	8	613	CLA	MG-ND	-5.86	1.94	2.05
17	J	101	CLA	MG-ND	-5.86	1.94	2.05
17	6	609	CLA	C1B-NB	5.86	1.40	1.35
17	8	614	CLA	C1B-NB	5.86	1.40	1.35
17	A	808	CLA	MG-ND	-5.86	1.94	2.05
17	A	841	CLA	C1B-NB	5.86	1.40	1.35
17	A	836	CLA	C1B-NB	5.85	1.40	1.35
17	B	838	CLA	MG-ND	-5.85	1.94	2.05
17	1	607	CLA	MG-ND	-5.83	1.94	2.05
17	B	812	CLA	C1B-NB	5.83	1.40	1.35
17	B	817	CLA	MG-ND	-5.83	1.94	2.05
17	6	604	CLA	C1B-NB	5.83	1.40	1.35
17	3	304	CLA	MG-ND	-5.83	1.94	2.05
17	A	830	CLA	C1B-NB	5.82	1.40	1.35
17	A	843	CLA	MG-ND	-5.82	1.94	2.05
17	A	813	CLA	C1B-NB	5.82	1.40	1.35
17	7	613	CLA	MG-ND	-5.81	1.94	2.05
17	B	815	CLA	MG-ND	-5.81	1.94	2.05
17	B	818	CLA	C1B-NB	5.79	1.40	1.35
17	5	307	CLA	MG-ND	-5.79	1.94	2.05
17	B	822	CLA	MG-ND	-5.79	1.94	2.05
17	7	602	CLA	MG-ND	-5.79	1.94	2.05
17	3	302	CLA	C1B-NB	5.79	1.40	1.35
17	B	833	CLA	MG-ND	-5.79	1.94	2.05
17	3	306	CLA	MG-ND	-5.79	1.94	2.05
17	5	311	CLA	C1B-NB	5.78	1.40	1.35
17	B	816	CLA	MG-ND	-5.78	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	814	CLA	MG-ND	-5.78	1.94	2.05
17	8	605	CLA	C1B-NB	5.78	1.40	1.35
17	7	614	CLA	MG-ND	-5.78	1.94	2.05
17	7	612	CLA	MG-ND	-5.78	1.94	2.05
17	A	805	CLA	MG-ND	-5.77	1.94	2.05
17	B	814	CLA	C1B-NB	5.77	1.40	1.35
17	8	602	CLA	C1B-NB	5.76	1.40	1.35
17	B	832	CLA	MG-ND	-5.76	1.94	2.05
17	B	828	CLA	MG-ND	-5.76	1.94	2.05
17	6	608	CLA	MG-ND	-5.76	1.94	2.05
17	A	802	CLA	MG-NA	-5.76	1.92	2.06
17	A	823	CLA	MG-ND	-5.74	1.94	2.05
17	3	310	CLA	C3A-C2A	-5.73	1.49	1.54
17	3	302	CLA	MG-ND	-5.71	1.94	2.05
17	A	819	CLA	C1B-NB	5.71	1.40	1.35
17	B	810	CLA	MG-NA	-5.71	1.92	2.06
17	4	603	CLA	MG-ND	-5.71	1.94	2.05
17	7	607	CLA	MG-ND	-5.70	1.94	2.05
17	A	818	CLA	MG-ND	-5.70	1.94	2.05
17	B	819	CLA	MG-NA	-5.69	1.92	2.06
17	B	818	CLA	MG-ND	-5.69	1.94	2.05
17	1	605	CLA	MG-ND	-5.69	1.94	2.05
17	5	311	CLA	MG-ND	-5.68	1.94	2.05
17	7	612	CLA	C1B-NB	5.68	1.40	1.35
17	B	824	CLA	C3A-C2A	-5.68	1.49	1.54
17	3	312	CLA	C1B-NB	5.68	1.40	1.35
17	B	820	CLA	C1B-NB	5.68	1.40	1.35
17	1	603	CLA	C1B-NB	5.67	1.40	1.35
17	3	304	CLA	C1B-NB	5.67	1.40	1.35
17	7	603	CLA	MG-NA	-5.67	1.92	2.06
17	8	603	CLA	MG-ND	-5.67	1.94	2.05
17	A	818	CLA	C1B-NB	5.66	1.40	1.35
17	4	601	CLA	C1B-NB	5.66	1.40	1.35
17	6	602	CLA	MG-ND	-5.66	1.94	2.05
17	8	604	CLA	MG-ND	-5.65	1.94	2.05
17	F	302	CLA	C1B-NB	5.65	1.40	1.35
17	A	830	CLA	MG-ND	-5.65	1.94	2.05
17	B	839	CLA	MG-ND	-5.65	1.94	2.05
17	5	315	CLA	MG-ND	-5.65	1.94	2.05
17	J	102	CLA	MG-ND	-5.65	1.94	2.05
17	4	604	CLA	MG-ND	-5.64	1.94	2.05
17	5	303	CLA	MG-ND	-5.64	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	811	CLA	MG-ND	-5.63	1.94	2.05
17	B	834	CLA	MG-ND	-5.63	1.94	2.05
17	A	810	CLA	MG-ND	-5.63	1.94	2.05
17	A	836	CLA	MG-ND	-5.63	1.94	2.05
17	A	832	CLA	C1B-NB	5.62	1.40	1.35
17	3	311	CLA	C1B-NB	5.62	1.40	1.35
17	7	605	CLA	C1B-NB	5.62	1.40	1.35
17	A	806	CLA	C1B-NB	5.62	1.40	1.35
17	A	827	CLA	MG-ND	-5.62	1.94	2.05
17	B	825	CLA	C1B-NB	5.62	1.40	1.35
16	A	801	CL0	MG-ND	-5.61	1.94	2.05
17	A	813	CLA	MG-ND	-5.61	1.94	2.05
17	5	306	CLA	C1B-NB	5.60	1.40	1.35
17	8	607	CLA	MG-ND	-5.59	1.94	2.05
17	B	819	CLA	MG-ND	-5.59	1.94	2.05
17	B	808	CLA	MG-ND	-5.59	1.94	2.05
17	A	810	CLA	C1B-NB	5.58	1.40	1.35
17	B	834	CLA	C1B-NB	5.58	1.40	1.35
17	3	312	CLA	MG-ND	-5.57	1.94	2.05
17	B	827	CLA	MG-ND	-5.57	1.94	2.05
17	B	820	CLA	MG-ND	-5.57	1.94	2.05
17	A	829	CLA	MG-ND	-5.55	1.94	2.05
17	B	835	CLA	C1B-NB	5.55	1.40	1.35
17	7	603	CLA	C1B-NB	5.55	1.40	1.35
17	3	313	CLA	C1B-NB	5.55	1.40	1.35
17	3	313	CLA	MG-NA	-5.55	1.93	2.06
17	1	603	CLA	MG-ND	-5.55	1.94	2.05
17	A	815	CLA	C1B-NB	5.55	1.40	1.35
17	6	601	CLA	MG-ND	-5.54	1.94	2.05
17	7	602	CLA	C1B-NB	5.54	1.40	1.35
17	6	609	CLA	MG-ND	-5.54	1.94	2.05
17	A	809	CLA	C1B-NB	5.54	1.40	1.35
17	A	834	CLA	MG-ND	-5.54	1.94	2.05
17	A	811	CLA	MG-ND	-5.54	1.94	2.05
17	A	828	CLA	MG-ND	-5.54	1.94	2.05
17	3	311	CLA	MG-ND	-5.53	1.94	2.05
17	5	302	CLA	C1B-NB	5.53	1.40	1.35
17	6	601	CLA	C1B-NB	5.53	1.40	1.35
17	A	819	CLA	MG-ND	-5.53	1.94	2.05
17	A	832	CLA	MG-ND	-5.53	1.94	2.05
17	8	609	CLA	MG-ND	-5.53	1.94	2.05
17	5	306	CLA	MG-ND	-5.53	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	807	CLA	C1B-NB	5.52	1.40	1.35
17	8	603	CLA	C1B-NB	5.52	1.40	1.35
17	8	612	CLA	MG-ND	-5.51	1.94	2.05
17	5	301	CLA	MG-ND	-5.51	1.94	2.05
17	8	609	CLA	C1B-NB	5.51	1.40	1.35
17	A	804	CLA	MG-NA	-5.50	1.93	2.06
17	8	611	CLA	MG-ND	-5.50	1.94	2.05
17	5	308	CLA	MG-ND	-5.50	1.94	2.05
17	A	820	CLA	MG-ND	-5.49	1.94	2.05
17	8	605	CLA	MG-ND	-5.49	1.94	2.05
17	B	819	CLA	C1B-NB	5.49	1.40	1.35
17	1	604	CLA	MG-ND	-5.48	1.94	2.05
17	7	603	CLA	MG-ND	-5.48	1.94	2.05
17	A	833	CLA	MG-ND	-5.48	1.94	2.05
17	8	602	CLA	MG-ND	-5.47	1.94	2.05
17	8	601	CLA	C1B-NB	5.47	1.40	1.35
17	A	811	CLA	C1B-NB	5.46	1.40	1.35
17	7	613	CLA	C1B-NB	5.46	1.40	1.35
17	B	806	CLA	MG-ND	-5.46	1.95	2.05
17	A	831	CLA	MG-ND	-5.44	1.95	2.05
17	5	301	CLA	C1B-NB	5.44	1.40	1.35
17	B	830	CLA	MG-ND	-5.44	1.95	2.05
17	A	821	CLA	MG-NA	-5.43	1.93	2.06
17	B	836	CLA	C1B-NB	5.43	1.40	1.35
17	1	606	CLA	MG-ND	-5.42	1.95	2.05
17	A	835	CLA	C1B-NB	5.42	1.40	1.35
17	A	837	CLA	C1B-NB	5.42	1.40	1.35
17	B	802	CLA	MG-NA	-5.41	1.93	2.06
17	6	603	CLA	MG-ND	-5.41	1.95	2.05
17	A	828	CLA	C1B-NB	5.41	1.40	1.35
17	7	610	CLA	MG-NA	-5.41	1.93	2.06
17	A	805	CLA	C1B-NB	5.41	1.40	1.35
17	A	817	CLA	MG-NA	-5.40	1.93	2.06
17	1	610	CLA	MG-ND	-5.40	1.95	2.05
17	7	608	CLA	C1B-NB	5.40	1.40	1.35
17	3	306	CLA	C1B-NB	5.40	1.40	1.35
17	1	609	CLA	MG-ND	-5.39	1.95	2.05
17	6	604	CLA	MG-ND	-5.38	1.95	2.05
17	A	816	CLA	MG-ND	-5.38	1.95	2.05
17	5	307	CLA	C1B-NB	5.38	1.40	1.35
17	A	825	CLA	MG-ND	-5.37	1.95	2.05
17	B	808	CLA	C1B-NB	5.37	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	832	CLA	C1B-NB	5.37	1.40	1.35
17	3	309	CLA	MG-ND	-5.36	1.95	2.05
17	3	301	CLA	MG-NA	-5.36	1.93	2.06
17	B	828	CLA	C1B-NB	5.35	1.40	1.35
17	3	310	CLA	MG-NA	-5.35	1.93	2.06
17	B	831	CLA	MG-NA	-5.34	1.93	2.06
17	B	826	CLA	MG-NA	-5.34	1.93	2.06
17	A	838	CLA	C1B-NB	5.32	1.40	1.35
17	7	614	CLA	MG-NA	-5.32	1.93	2.06
17	3	306	CLA	MG-NA	-5.32	1.93	2.06
17	3	308	CLA	MG-NA	-5.32	1.93	2.06
17	6	610	CLA	C1B-NB	5.31	1.39	1.35
17	A	803	CLA	C1B-NB	5.30	1.39	1.35
17	B	804	CLA	MG-NA	-5.30	1.93	2.06
17	3	309	CLA	C1B-NB	5.30	1.39	1.35
17	A	822	CLA	MG-NA	-5.29	1.93	2.06
17	B	824	CLA	C1B-NB	5.29	1.39	1.35
17	B	805	CLA	MG-NA	-5.29	1.93	2.06
17	B	813	CLA	MG-ND	-5.28	1.95	2.05
17	5	309	CLA	MG-ND	-5.28	1.95	2.05
17	B	811	CLA	C1B-NB	5.28	1.39	1.35
17	5	303	CLA	C1B-NB	5.27	1.39	1.35
17	J	101	CLA	C1B-NB	5.24	1.39	1.35
17	7	609	CLA	MG-ND	-5.24	1.95	2.05
17	A	827	CLA	C1B-NB	5.23	1.39	1.35
17	A	829	CLA	C1B-NB	5.23	1.39	1.35
17	B	807	CLA	MG-NA	-5.22	1.93	2.06
17	5	309	CLA	MG-NA	-5.22	1.93	2.06
17	3	310	CLA	C1B-NB	5.20	1.39	1.35
17	F	301	CLA	C1B-NB	5.20	1.39	1.35
17	1	606	CLA	MG-NA	-5.19	1.93	2.06
17	B	837	CLA	MG-NA	-5.19	1.93	2.06
17	A	814	CLA	C1B-NB	5.18	1.39	1.35
17	A	809	CLA	MG-NA	-5.18	1.94	2.06
17	8	613	CLA	C1B-NB	5.16	1.39	1.35
17	7	608	CLA	MG-ND	-5.15	1.95	2.05
17	A	823	CLA	C1B-NB	5.15	1.39	1.35
17	B	806	CLA	MG-NC	-5.15	1.94	2.06
17	6	603	CLA	C1B-NB	5.15	1.39	1.35
17	B	838	CLA	C1B-NB	5.14	1.39	1.35
17	1	607	CLA	MG-NC	-5.13	1.94	2.06
17	4	605	CLA	C1B-NB	5.13	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	829	CLA	MG-NA	-5.13	1.94	2.06
17	4	602	CLA	MG-ND	-5.11	1.95	2.05
17	3	303	CLA	C1B-NB	5.11	1.39	1.35
17	A	824	CLA	C1B-NB	5.10	1.39	1.35
17	7	601	CLA	C1B-NB	5.10	1.39	1.35
17	A	834	CLA	C1B-NB	5.10	1.39	1.35
17	5	306	CLA	MG-NA	-5.10	1.94	2.06
17	B	823	CLA	C1B-NB	5.09	1.39	1.35
17	B	839	CLA	C1B-NB	5.09	1.39	1.35
17	B	824	CLA	MG-NA	-5.09	1.94	2.06
17	7	610	CLA	C1B-NB	5.08	1.39	1.35
17	8	607	CLA	C1B-NB	5.08	1.39	1.35
17	A	802	CLA	MG-NC	-5.07	1.94	2.06
17	7	611	CLA	MG-ND	-5.07	1.95	2.05
17	A	812	CLA	C1B-NB	5.07	1.39	1.35
17	5	304	CLA	C1B-NB	5.06	1.39	1.35
17	1	608	CLA	MG-ND	-5.06	1.95	2.05
17	A	825	CLA	C1B-NB	5.06	1.39	1.35
17	B	810	CLA	C1B-NB	5.06	1.39	1.35
17	A	838	CLA	MG-NA	-5.05	1.94	2.06
17	3	305	CLA	C1B-NB	5.05	1.39	1.35
17	A	802	CLA	C1B-NB	5.05	1.39	1.35
17	B	830	CLA	C1B-NB	5.04	1.39	1.35
17	3	303	CLA	MG-NA	-5.04	1.94	2.06
17	4	603	CLA	MG-NC	-5.03	1.94	2.06
17	A	815	CLA	MG-NA	-5.03	1.94	2.06
17	5	312	CLA	C1B-NB	5.03	1.39	1.35
17	5	314	CLA	MG-NA	-5.02	1.94	2.06
17	F	301	CLA	MG-NA	-5.01	1.94	2.06
17	B	827	CLA	MG-NA	-5.00	1.94	2.06
17	A	808	CLA	C1B-NB	5.00	1.39	1.35
17	8	608	CLA	MG-NA	-5.00	1.94	2.06
17	5	309	CLA	C1B-NB	4.98	1.39	1.35
17	A	843	CLA	C1B-NB	4.98	1.39	1.35
17	A	807	CLA	MG-NA	-4.97	1.94	2.06
17	A	821	CLA	C1B-NB	4.94	1.39	1.35
17	A	841	CLA	MG-NA	-4.94	1.94	2.06
17	A	822	CLA	C1B-NB	4.93	1.39	1.35
17	7	608	CLA	MG-NA	-4.93	1.94	2.06
20	Z	601	CHL	MG-NA	-4.92	1.94	2.06
17	7	603	CLA	MG-NC	-4.92	1.94	2.06
17	B	837	CLA	C1B-NB	4.92	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	607	CHL	MG-NC	-4.92	1.94	2.06
17	B	831	CLA	MG-NC	-4.92	1.94	2.06
17	8	610	CLA	MG-NA	-4.91	1.94	2.06
17	B	814	CLA	MG-ND	-4.90	1.96	2.05
17	B	832	CLA	MG-NA	-4.90	1.94	2.06
17	B	804	CLA	MG-NC	-4.89	1.94	2.06
17	1	602	CLA	MG-ND	-4.89	1.96	2.05
17	8	614	CLA	MG-NA	-4.89	1.94	2.06
20	1	601	CHL	MG-NA	-4.89	1.94	2.06
17	A	839	CLA	MG-NA	-4.88	1.94	2.06
17	3	309	CLA	MG-NA	-4.88	1.94	2.06
17	B	821	CLA	MG-ND	-4.87	1.96	2.05
17	A	805	CLA	MG-NA	-4.86	1.94	2.06
17	A	816	CLA	MG-NA	-4.86	1.94	2.06
17	3	301	CLA	C1B-NB	4.86	1.39	1.35
17	B	833	CLA	C1B-NB	4.85	1.39	1.35
17	A	821	CLA	MG-NC	-4.83	1.94	2.06
17	A	804	CLA	MG-NC	-4.82	1.94	2.06
17	B	825	CLA	MG-NA	-4.82	1.94	2.06
17	4	605	CLA	MG-NA	-4.82	1.94	2.06
17	A	825	CLA	MG-NA	-4.81	1.94	2.06
17	B	820	CLA	MG-NA	-4.80	1.94	2.06
17	B	833	CLA	MG-NA	-4.80	1.94	2.06
17	3	302	CLA	MG-NA	-4.80	1.94	2.06
17	A	839	CLA	C1B-NB	4.79	1.39	1.35
17	B	813	CLA	C1B-NB	4.79	1.39	1.35
17	7	609	CLA	MG-NA	-4.78	1.94	2.06
17	5	315	CLA	MG-NA	-4.78	1.94	2.06
17	A	834	CLA	MG-NA	-4.77	1.94	2.06
17	B	818	CLA	MG-NA	-4.77	1.94	2.06
17	B	823	CLA	MG-NA	-4.76	1.95	2.06
17	8	603	CLA	MG-NA	-4.76	1.95	2.06
17	8	613	CLA	MG-NA	-4.76	1.95	2.06
17	5	307	CLA	MG-NA	-4.76	1.95	2.06
17	B	835	CLA	MG-NA	-4.76	1.95	2.06
17	4	601	CLA	MG-NA	-4.76	1.95	2.06
17	B	802	CLA	MG-NC	-4.75	1.95	2.06
17	5	308	CLA	C1B-NB	4.75	1.39	1.35
17	B	828	CLA	MG-NA	-4.74	1.95	2.06
17	7	611	CLA	MG-NA	-4.74	1.95	2.06
17	B	829	CLA	C1B-NB	4.74	1.39	1.35
20	6	607	CHL	MG-NA	-4.73	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	603	CLA	MG-NA	-4.73	1.95	2.06
17	B	801	CLA	MG-NA	-4.72	1.95	2.06
17	B	837	CLA	MG-NC	-4.72	1.95	2.06
17	A	813	CLA	MG-NA	-4.72	1.95	2.06
17	8	603	CLA	MG-NC	-4.71	1.95	2.06
17	5	308	CLA	MG-NA	-4.71	1.95	2.06
20	5	305	CHL	MG-NA	-4.71	1.95	2.06
17	B	810	CLA	MG-NC	-4.71	1.95	2.06
17	7	613	CLA	MG-NA	-4.71	1.95	2.06
17	B	826	CLA	MG-NC	-4.70	1.95	2.06
17	J	102	CLA	MG-NA	-4.70	1.95	2.06
17	A	830	CLA	MG-NA	-4.69	1.95	2.06
17	A	811	CLA	MG-NA	-4.69	1.95	2.06
17	B	830	CLA	MG-NA	-4.69	1.95	2.06
17	B	812	CLA	MG-NC	-4.69	1.95	2.06
17	8	609	CLA	MG-NA	-4.69	1.95	2.06
17	8	611	CLA	MG-NA	-4.68	1.95	2.06
16	A	801	CL0	MG-NA	-4.68	1.95	2.06
17	A	814	CLA	MG-NA	-4.68	1.95	2.06
17	B	805	CLA	MG-NC	-4.68	1.95	2.06
17	1	604	CLA	MG-NA	-4.68	1.95	2.06
17	7	614	CLA	MG-NC	-4.67	1.95	2.06
17	3	301	CLA	MG-NC	-4.67	1.95	2.06
17	A	824	CLA	MG-NA	-4.66	1.95	2.06
17	A	806	CLA	MG-NA	-4.66	1.95	2.06
17	6	610	CLA	MG-NA	-4.66	1.95	2.06
17	B	815	CLA	MG-NC	-4.66	1.95	2.06
17	3	312	CLA	MG-NA	-4.65	1.95	2.06
17	7	610	CLA	MG-NC	-4.65	1.95	2.06
17	A	815	CLA	MG-NC	-4.65	1.95	2.06
17	B	819	CLA	MG-NC	-4.64	1.95	2.06
17	5	310	CLA	MG-NA	-4.64	1.95	2.06
17	A	823	CLA	MG-NA	-4.64	1.95	2.06
17	A	836	CLA	MG-NA	-4.63	1.95	2.06
17	8	612	CLA	MG-NA	-4.63	1.95	2.06
20	1	601	CHL	MG-NC	-4.63	1.95	2.06
17	8	602	CLA	MG-NA	-4.63	1.95	2.06
17	A	829	CLA	MG-NA	-4.63	1.95	2.06
17	A	820	CLA	MG-NA	-4.62	1.95	2.06
20	5	305	CHL	MG-NC	-4.62	1.95	2.06
17	J	101	CLA	MG-NC	-4.61	1.95	2.06
16	A	801	CL0	C1B-NB	4.61	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	818	CLA	MG-NA	-4.61	1.95	2.06
17	A	842	CLA	MG-NA	-4.61	1.95	2.06
17	A	832	CLA	MG-NA	-4.61	1.95	2.06
17	3	304	CLA	MG-NA	-4.60	1.95	2.06
17	6	608	CLA	C1B-NB	4.60	1.39	1.35
17	3	308	CLA	MG-NC	-4.60	1.95	2.06
20	Z	601	CHL	MG-NC	-4.60	1.95	2.06
17	A	826	CLA	MG-NA	-4.59	1.95	2.06
17	A	814	CLA	MG-NC	-4.59	1.95	2.06
17	A	819	CLA	MG-NA	-4.59	1.95	2.06
17	1	609	CLA	MG-NA	-4.59	1.95	2.06
17	B	809	CLA	MG-NA	-4.58	1.95	2.06
20	6	606	CHL	MG-NA	-4.57	1.95	2.06
17	6	601	CLA	MG-NA	-4.57	1.95	2.06
17	A	812	CLA	MG-NA	-4.57	1.95	2.06
17	A	843	CLA	MG-NA	-4.57	1.95	2.06
17	B	834	CLA	MG-NA	-4.56	1.95	2.06
17	3	306	CLA	MG-NC	-4.56	1.95	2.06
17	8	608	CLA	MG-NC	-4.56	1.95	2.06
17	J	101	CLA	MG-NA	-4.55	1.95	2.06
17	3	305	CLA	MG-NA	-4.55	1.95	2.06
17	7	608	CLA	MG-NC	-4.55	1.95	2.06
17	A	827	CLA	MG-NA	-4.55	1.95	2.06
17	B	828	CLA	MG-NC	-4.54	1.95	2.06
17	A	833	CLA	MG-NA	-4.54	1.95	2.06
17	5	303	CLA	MG-NA	-4.54	1.95	2.06
17	A	839	CLA	MG-NC	-4.54	1.95	2.06
17	3	308	CLA	C1B-NB	4.54	1.39	1.35
17	7	607	CLA	C1B-NB	4.53	1.39	1.35
17	5	311	CLA	MG-NA	-4.53	1.95	2.06
17	4	602	CLA	MG-NA	-4.53	1.95	2.06
17	1	602	CLA	MG-NA	-4.53	1.95	2.06
17	1	603	CLA	MG-NA	-4.52	1.95	2.06
17	A	841	CLA	MG-NC	-4.52	1.95	2.06
17	B	839	CLA	MG-NA	-4.52	1.95	2.06
17	B	813	CLA	MG-NA	-4.52	1.95	2.06
17	6	602	CLA	MG-NA	-4.51	1.95	2.06
17	7	607	CLA	MG-NA	-4.51	1.95	2.06
17	B	811	CLA	MG-NA	-4.51	1.95	2.06
17	5	301	CLA	MG-NA	-4.50	1.95	2.06
17	3	313	CLA	MG-NC	-4.50	1.95	2.06
17	7	602	CLA	MG-NA	-4.49	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	606	CHL	MG-NC	-4.49	1.95	2.06
17	4	604	CLA	MG-NA	-4.49	1.95	2.06
17	5	306	CLA	MG-NC	-4.49	1.95	2.06
17	A	810	CLA	MG-NA	-4.49	1.95	2.06
17	B	829	CLA	MG-NC	-4.48	1.95	2.06
17	A	822	CLA	MG-NC	-4.47	1.95	2.06
17	A	808	CLA	MG-NA	-4.47	1.95	2.06
17	F	302	CLA	MG-NA	-4.45	1.95	2.06
17	A	835	CLA	MG-NA	-4.44	1.95	2.06
17	A	834	CLA	MG-NC	-4.44	1.95	2.06
17	B	816	CLA	MG-NA	-4.44	1.95	2.06
20	7	606	CHL	MG-NC	-4.43	1.95	2.06
17	1	610	CLA	MG-NA	-4.43	1.95	2.06
17	3	303	CLA	MG-NC	-4.43	1.95	2.06
17	A	820	CLA	MG-NC	-4.42	1.95	2.06
17	8	607	CLA	MG-NA	-4.42	1.95	2.06
17	A	823	CLA	MG-NC	-4.41	1.95	2.06
17	5	312	CLA	MG-NA	-4.41	1.95	2.06
20	3	307	CHL	MG-NA	-4.41	1.95	2.06
17	A	817	CLA	MG-NC	-4.40	1.95	2.06
17	6	604	CLA	MG-NA	-4.40	1.95	2.06
17	6	608	CLA	MG-NA	-4.40	1.95	2.06
17	8	601	CLA	MG-NA	-4.39	1.95	2.06
17	B	817	CLA	MG-NA	-4.39	1.95	2.06
17	B	823	CLA	MG-NC	-4.39	1.95	2.06
20	8	606	CHL	MG-NA	-4.39	1.95	2.06
17	A	837	CLA	MG-NA	-4.39	1.95	2.06
17	A	825	CLA	MG-NC	-4.39	1.95	2.06
17	A	828	CLA	MG-NA	-4.38	1.95	2.06
20	3	307	CHL	MG-NC	-4.38	1.95	2.06
17	A	831	CLA	MG-NA	-4.38	1.95	2.06
17	B	822	CLA	MG-NA	-4.38	1.95	2.06
17	4	601	CLA	MG-NC	-4.38	1.95	2.06
17	3	312	CLA	MG-NC	-4.38	1.95	2.06
17	5	309	CLA	MG-NC	-4.38	1.95	2.06
17	A	803	CLA	MG-NA	-4.38	1.95	2.06
17	B	822	CLA	C1B-NB	4.38	1.39	1.35
17	1	609	CLA	MG-NC	-4.37	1.95	2.06
17	A	805	CLA	MG-NC	-4.37	1.95	2.06
17	A	804	CLA	C1B-NB	4.36	1.39	1.35
17	7	612	CLA	MG-NA	-4.36	1.95	2.06
17	B	836	CLA	MG-NA	-4.36	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	808	CLA	MG-NA	-4.36	1.95	2.06
17	A	818	CLA	MG-NC	-4.36	1.95	2.06
17	A	810	CLA	MG-NC	-4.35	1.95	2.06
17	B	814	CLA	MG-NA	-4.35	1.95	2.06
17	6	609	CLA	MG-NA	-4.35	1.95	2.06
17	3	311	CLA	MG-NA	-4.34	1.95	2.06
17	5	304	CLA	MG-NA	-4.34	1.96	2.06
17	5	302	CLA	MG-NA	-4.34	1.96	2.06
17	7	613	CLA	MG-NC	-4.34	1.96	2.06
17	J	102	CLA	MG-NC	-4.34	1.96	2.06
16	A	801	CL0	MG-NC	-4.33	1.96	2.06
17	5	314	CLA	MG-NC	-4.33	1.96	2.06
17	A	838	CLA	MG-NC	-4.33	1.96	2.06
17	1	604	CLA	MG-NC	-4.32	1.96	2.06
20	5	313	CHL	MG-NC	-4.32	1.96	2.06
17	7	605	CLA	MG-NA	-4.32	1.96	2.06
17	8	614	CLA	MG-NC	-4.31	1.96	2.06
17	6	603	CLA	MG-NC	-4.31	1.96	2.06
20	5	313	CHL	MG-NA	-4.31	1.96	2.06
17	3	304	CLA	MG-NC	-4.30	1.96	2.06
17	A	816	CLA	C1B-NB	4.30	1.39	1.35
17	8	604	CLA	MG-NA	-4.30	1.96	2.06
17	B	825	CLA	MG-NC	-4.30	1.96	2.06
17	A	808	CLA	MG-NC	-4.29	1.96	2.06
17	B	834	CLA	MG-NC	-4.29	1.96	2.06
17	3	302	CLA	MG-NC	-4.28	1.96	2.06
20	7	606	CHL	MG-NA	-4.28	1.96	2.06
17	8	611	CLA	MG-NC	-4.27	1.96	2.06
17	A	809	CLA	MG-NC	-4.27	1.96	2.06
17	B	816	CLA	MG-NC	-4.27	1.96	2.06
17	B	805	CLA	C1B-NB	4.26	1.39	1.35
17	3	310	CLA	MG-NC	-4.26	1.96	2.06
17	7	601	CLA	MG-NA	-4.26	1.96	2.06
17	A	830	CLA	MG-NC	-4.26	1.96	2.06
17	8	610	CLA	C1B-NB	4.26	1.39	1.35
17	A	813	CLA	MG-NC	-4.24	1.96	2.06
17	A	811	CLA	MG-NC	-4.24	1.96	2.06
17	7	611	CLA	MG-NC	-4.24	1.96	2.06
17	1	608	CLA	MG-NA	-4.24	1.96	2.06
17	A	807	CLA	MG-NC	-4.23	1.96	2.06
17	4	602	CLA	MG-NC	-4.23	1.96	2.06
17	B	807	CLA	MG-NC	-4.23	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	311	CLA	MG-NC	-4.23	1.96	2.06
20	8	606	CHL	MG-NC	-4.22	1.96	2.06
17	F	301	CLA	MG-NC	-4.22	1.96	2.06
17	7	607	CLA	MG-NC	-4.21	1.96	2.06
17	8	605	CLA	MG-NA	-4.21	1.96	2.06
17	A	816	CLA	MG-NC	-4.21	1.96	2.06
17	B	830	CLA	MG-NC	-4.20	1.96	2.06
17	B	813	CLA	MG-NC	-4.20	1.96	2.06
17	5	315	CLA	MG-NC	-4.19	1.96	2.06
17	5	302	CLA	MG-NC	-4.19	1.96	2.06
17	A	829	CLA	MG-NC	-4.19	1.96	2.06
17	5	310	CLA	MG-NC	-4.18	1.96	2.06
17	A	837	CLA	MG-NC	-4.18	1.96	2.06
17	8	607	CLA	MG-NC	-4.17	1.96	2.06
17	8	610	CLA	MG-NC	-4.16	1.96	2.06
17	B	814	CLA	MG-NC	-4.16	1.96	2.06
17	4	605	CLA	MG-NC	-4.16	1.96	2.06
17	1	606	CLA	MG-NC	-4.15	1.96	2.06
17	A	806	CLA	MG-NC	-4.15	1.96	2.06
17	A	832	CLA	MG-NC	-4.15	1.96	2.06
17	B	820	CLA	MG-NC	-4.15	1.96	2.06
17	A	833	CLA	MG-NC	-4.14	1.96	2.06
17	B	832	CLA	MG-NC	-4.14	1.96	2.06
17	5	301	CLA	MG-NC	-4.14	1.96	2.06
17	B	801	CLA	C1B-NB	4.13	1.38	1.35
17	7	602	CLA	MG-NC	-4.13	1.96	2.06
17	A	836	CLA	MG-NC	-4.12	1.96	2.06
17	B	821	CLA	MG-NA	-4.12	1.96	2.06
17	B	833	CLA	MG-NC	-4.11	1.96	2.06
20	6	605	CHL	MG-NC	-4.11	1.96	2.06
17	1	602	CLA	MG-NC	-4.11	1.96	2.06
17	A	842	CLA	MG-NC	-4.11	1.96	2.06
17	8	601	CLA	MG-NC	-4.10	1.96	2.06
17	8	602	CLA	MG-NC	-4.10	1.96	2.06
20	6	605	CHL	MG-NA	-4.09	1.96	2.06
17	A	842	CLA	C1B-NB	4.09	1.38	1.35
17	3	309	CLA	MG-NC	-4.09	1.96	2.06
17	6	608	CLA	MG-NC	-4.07	1.96	2.06
17	B	826	CLA	C1B-NB	4.07	1.38	1.35
17	B	817	CLA	MG-NC	-4.07	1.96	2.06
17	8	613	CLA	MG-NC	-4.06	1.96	2.06
17	B	824	CLA	MG-NC	-4.06	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	605	CLA	MG-NA	-4.06	1.96	2.06
17	6	610	CLA	MG-NC	-4.06	1.96	2.06
17	6	609	CLA	MG-NC	-4.06	1.96	2.06
17	6	602	CLA	MG-NC	-4.04	1.96	2.06
17	B	835	CLA	MG-NC	-4.04	1.96	2.06
17	5	307	CLA	MG-NC	-4.04	1.96	2.06
17	B	838	CLA	MG-NA	-4.04	1.96	2.06
17	5	311	CLA	MG-NC	-4.03	1.96	2.06
17	A	826	CLA	MG-NC	-4.03	1.96	2.06
17	B	839	CLA	MG-NC	-4.03	1.96	2.06
17	A	819	CLA	MG-NC	-4.01	1.96	2.06
17	A	827	CLA	MG-NC	-4.01	1.96	2.06
17	8	612	CLA	MG-NC	-4.00	1.96	2.06
17	6	601	CLA	MG-NC	-4.00	1.96	2.06
17	A	843	CLA	MG-NC	-3.99	1.96	2.06
17	1	610	CLA	MG-NC	-3.99	1.96	2.06
17	B	827	CLA	MG-NC	-3.96	1.96	2.06
17	7	609	CLA	MG-NC	-3.96	1.96	2.06
17	8	604	CLA	MG-NC	-3.96	1.96	2.06
17	B	801	CLA	MG-NC	-3.96	1.96	2.06
17	7	604	CLA	MG-NA	-3.95	1.96	2.06
17	5	308	CLA	MG-NC	-3.95	1.96	2.06
17	B	822	CLA	MG-NC	-3.94	1.96	2.06
17	B	827	CLA	C1B-NB	3.94	1.38	1.35
17	A	826	CLA	C1B-NB	3.94	1.38	1.35
17	A	831	CLA	MG-NC	-3.94	1.96	2.06
17	A	828	CLA	MG-NC	-3.93	1.96	2.06
17	8	609	CLA	MG-NC	-3.92	1.97	2.06
17	A	803	CLA	MG-NC	-3.90	1.97	2.06
17	5	303	CLA	MG-NC	-3.90	1.97	2.06
17	5	304	CLA	MG-NC	-3.89	1.97	2.06
17	7	612	CLA	MG-NC	-3.89	1.97	2.06
17	B	818	CLA	MG-NC	-3.88	1.97	2.06
17	B	808	CLA	MG-NC	-3.88	1.97	2.06
17	B	811	CLA	MG-NC	-3.88	1.97	2.06
17	1	610	CLA	C1D-ND	3.87	1.42	1.37
17	7	601	CLA	MG-NC	-3.85	1.97	2.06
17	B	836	CLA	MG-NC	-3.85	1.97	2.06
17	A	835	CLA	MG-NC	-3.84	1.97	2.06
17	A	812	CLA	MG-NC	-3.84	1.97	2.06
17	7	604	CLA	C1B-NB	3.84	1.38	1.35
17	1	605	CLA	MG-NC	-3.83	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	605	CLA	MG-NC	-3.83	1.97	2.06
17	A	824	CLA	MG-NC	-3.83	1.97	2.06
17	F	302	CLA	MG-NC	-3.82	1.97	2.06
17	B	809	CLA	MG-NC	-3.81	1.97	2.06
17	1	608	CLA	MG-NC	-3.80	1.97	2.06
17	1	603	CLA	MG-NC	-3.78	1.97	2.06
17	B	838	CLA	MG-NC	-3.78	1.97	2.06
17	1	608	CLA	C1D-ND	3.77	1.42	1.37
17	3	305	CLA	MG-NC	-3.75	1.97	2.06
20	3	307	CHL	C3B-C2B	-3.73	1.35	1.40
17	5	312	CLA	MG-NC	-3.71	1.97	2.06
17	B	821	CLA	C1D-ND	3.71	1.42	1.37
17	6	604	CLA	MG-NC	-3.71	1.97	2.06
17	7	604	CLA	MG-NC	-3.68	1.97	2.06
17	B	802	CLA	C1B-NB	3.66	1.38	1.35
17	4	604	CLA	MG-NC	-3.61	1.97	2.06
17	6	604	CLA	C1D-ND	3.61	1.42	1.37
17	1	604	CLA	C1D-ND	3.58	1.42	1.37
17	8	605	CLA	MG-NC	-3.58	1.97	2.06
17	B	819	CLA	C3B-C2B	-3.52	1.35	1.40
17	B	821	CLA	MG-NC	-3.51	1.97	2.06
20	6	606	CHL	C3B-C2B	-3.51	1.35	1.40
20	5	305	CHL	C3B-C2B	-3.47	1.35	1.40
17	A	816	CLA	C3B-C2B	-3.39	1.35	1.40
16	A	801	CL0	C3B-C2B	-3.36	1.35	1.40
17	A	804	CLA	C3A-C2A	-3.36	1.45	1.54
17	5	306	CLA	C1D-ND	3.35	1.41	1.37
17	B	814	CLA	C1D-ND	3.30	1.41	1.37
20	8	606	CHL	C3B-C2B	-3.29	1.35	1.40
17	6	609	CLA	C1D-ND	3.26	1.41	1.37
17	3	311	CLA	C1D-ND	3.26	1.41	1.37
17	B	828	CLA	C1D-ND	3.26	1.41	1.37
17	A	833	CLA	C1D-ND	3.25	1.41	1.37
17	B	838	CLA	C3B-C2B	-3.25	1.35	1.40
17	A	831	CLA	C1D-ND	3.24	1.41	1.37
20	6	607	CHL	C3B-C2B	-3.23	1.35	1.40
17	B	804	CLA	C3B-C2B	-3.23	1.35	1.40
20	7	606	CHL	C3B-C2B	-3.22	1.35	1.40
17	B	815	CLA	C3A-C2A	-3.22	1.45	1.54
17	A	803	CLA	C3B-C2B	-3.21	1.35	1.40
17	1	605	CLA	C1D-ND	3.20	1.41	1.37
17	8	605	CLA	C1D-ND	3.19	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	614	CLA	C1D-ND	3.18	1.41	1.37
17	8	604	CLA	C1D-ND	3.18	1.41	1.37
17	5	314	CLA	C1B-NB	3.18	1.38	1.35
17	A	814	CLA	C3B-C2B	-3.17	1.36	1.40
17	B	804	CLA	C1B-NB	3.17	1.38	1.35
16	A	801	CL0	C1D-ND	3.17	1.41	1.37
17	4	602	CLA	C1D-ND	3.16	1.41	1.37
17	8	609	CLA	C1D-ND	3.14	1.41	1.37
17	7	611	CLA	C1D-ND	3.13	1.41	1.37
17	1	609	CLA	C1D-ND	3.12	1.41	1.37
17	5	301	CLA	C1D-ND	3.12	1.41	1.37
17	4	604	CLA	C1D-ND	3.12	1.41	1.37
17	A	820	CLA	C1D-ND	3.12	1.41	1.37
17	5	310	CLA	C1D-ND	3.11	1.41	1.37
17	6	604	CLA	C3B-C2B	-3.10	1.36	1.40
17	8	612	CLA	C1D-ND	3.09	1.41	1.37
17	B	808	CLA	C1D-ND	3.09	1.41	1.37
20	5	313	CHL	C3B-C2B	-3.07	1.36	1.40
17	3	304	CLA	C3B-C2B	-3.07	1.36	1.40
17	A	818	CLA	C1D-ND	3.07	1.41	1.37
20	1	601	CHL	C3B-C2B	-3.06	1.36	1.40
17	A	843	CLA	C3B-C2B	-3.06	1.36	1.40
17	B	834	CLA	C1D-ND	3.05	1.41	1.37
17	B	836	CLA	C1D-ND	3.04	1.41	1.37
17	A	830	CLA	C1D-ND	3.04	1.41	1.37
17	8	607	CLA	C1D-ND	3.04	1.41	1.37
17	B	827	CLA	C3B-C2B	-3.03	1.36	1.40
17	6	601	CLA	C1D-ND	3.03	1.41	1.37
17	A	814	CLA	C1D-ND	3.03	1.41	1.37
20	Z	601	CHL	C3B-C2B	-3.02	1.36	1.40
17	1	603	CLA	C1D-ND	3.01	1.41	1.37
17	B	807	CLA	C1D-ND	3.01	1.41	1.37
17	A	811	CLA	C3B-C2B	-3.01	1.36	1.40
17	A	839	CLA	C3B-C2B	-2.99	1.36	1.40
17	A	828	CLA	C1D-ND	2.99	1.41	1.37
17	3	312	CLA	C1D-ND	2.99	1.41	1.37
17	7	609	CLA	C1D-ND	2.99	1.41	1.37
17	B	832	CLA	C1D-ND	2.98	1.41	1.37
17	5	315	CLA	C1D-ND	2.98	1.41	1.37
17	7	613	CLA	C1D-ND	2.98	1.41	1.37
17	B	839	CLA	C1D-ND	2.97	1.41	1.37
17	8	613	CLA	C1D-ND	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	612	CLA	C1D-ND	2.97	1.41	1.37
17	5	309	CLA	C1D-ND	2.95	1.41	1.37
17	7	609	CLA	C3B-C2B	-2.94	1.36	1.40
17	A	805	CLA	C3A-C2A	-2.94	1.46	1.54
17	A	810	CLA	C1D-ND	2.93	1.41	1.37
17	B	833	CLA	C1D-ND	2.93	1.41	1.37
17	A	827	CLA	C3B-C2B	-2.91	1.36	1.40
17	8	611	CLA	C3A-C2A	-2.90	1.46	1.54
17	1	602	CLA	C1D-ND	2.89	1.41	1.37
17	5	302	CLA	C1D-ND	2.89	1.41	1.37
17	A	808	CLA	C3B-C2B	-2.89	1.36	1.40
17	A	824	CLA	C3A-C2A	-2.88	1.46	1.54
17	B	819	CLA	C1D-C2D	-2.88	1.39	1.45
17	B	837	CLA	C3B-C2B	-2.87	1.36	1.40
17	B	808	CLA	C3B-C2B	-2.87	1.36	1.40
17	6	610	CLA	C1D-C2D	-2.87	1.39	1.45
17	7	604	CLA	C1D-ND	2.87	1.41	1.37
17	A	828	CLA	C3B-C2B	-2.86	1.36	1.40
17	1	602	CLA	C3B-C2B	-2.85	1.36	1.40
17	8	601	CLA	C3B-C2B	-2.84	1.36	1.40
17	J	102	CLA	C1D-ND	2.84	1.41	1.37
17	A	805	CLA	C1D-ND	2.83	1.41	1.37
17	8	603	CLA	C1D-ND	2.83	1.41	1.37
17	B	818	CLA	C3B-C2B	-2.83	1.36	1.40
17	B	833	CLA	C3B-C2B	-2.83	1.36	1.40
17	A	805	CLA	C3B-C2B	-2.83	1.36	1.40
20	6	605	CHL	C3B-C2B	-2.83	1.36	1.40
17	A	835	CLA	C1D-ND	2.82	1.41	1.37
17	A	823	CLA	C1D-ND	2.82	1.41	1.37
17	5	308	CLA	C1D-ND	2.82	1.41	1.37
17	3	309	CLA	C1D-ND	2.82	1.41	1.37
17	B	813	CLA	C1D-ND	2.81	1.41	1.37
17	A	824	CLA	C1D-ND	2.81	1.41	1.37
17	A	823	CLA	C3B-C2B	-2.81	1.36	1.40
17	A	838	CLA	C3B-C2B	-2.81	1.36	1.40
17	A	837	CLA	C3A-C2A	-2.80	1.46	1.54
17	8	611	CLA	C1D-ND	2.80	1.41	1.37
17	A	808	CLA	C1D-ND	2.80	1.41	1.37
17	B	838	CLA	C1D-C2D	-2.79	1.39	1.45
17	B	825	CLA	C1D-ND	2.79	1.41	1.37
17	A	836	CLA	C1D-ND	2.78	1.41	1.37
17	7	601	CLA	C3B-C2B	-2.78	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	603	CLA	C1D-ND	2.77	1.41	1.37
17	B	816	CLA	C1D-ND	2.77	1.41	1.37
17	5	304	CLA	C1D-ND	2.77	1.41	1.37
17	6	610	CLA	C3A-C2A	-2.76	1.46	1.54
17	A	837	CLA	C1D-ND	2.75	1.41	1.37
17	B	811	CLA	C1D-ND	2.75	1.41	1.37
17	A	813	CLA	C1D-ND	2.75	1.41	1.37
17	7	611	CLA	C3B-C2B	-2.75	1.36	1.40
17	B	817	CLA	C1D-ND	2.75	1.41	1.37
17	8	607	CLA	C3A-C2A	-2.75	1.46	1.54
17	A	833	CLA	C3B-C2B	-2.74	1.36	1.40
17	5	307	CLA	C1D-ND	2.74	1.41	1.37
17	A	808	CLA	C1D-C2D	-2.74	1.39	1.45
17	4	605	CLA	C1D-C2D	-2.74	1.39	1.45
17	5	303	CLA	C3B-C2B	-2.74	1.36	1.40
17	A	824	CLA	C3B-C2B	-2.74	1.36	1.40
17	A	841	CLA	C1D-ND	2.73	1.41	1.37
17	5	303	CLA	C1D-ND	2.73	1.41	1.37
17	A	843	CLA	C1D-C2D	-2.72	1.39	1.45
17	A	815	CLA	C1D-C2D	-2.72	1.40	1.45
17	B	812	CLA	C1D-ND	2.72	1.41	1.37
17	B	829	CLA	C3B-C2B	-2.72	1.36	1.40
17	8	601	CLA	C1D-ND	2.71	1.41	1.37
17	B	823	CLA	C1D-ND	2.71	1.41	1.37
17	A	827	CLA	C3A-C2A	-2.70	1.46	1.54
17	6	602	CLA	C1D-ND	2.70	1.41	1.37
17	5	304	CLA	C1D-C2D	-2.70	1.40	1.45
17	A	803	CLA	C3A-C2A	-2.70	1.46	1.54
17	A	837	CLA	C1D-C2D	-2.69	1.40	1.45
17	7	607	CLA	C1D-ND	2.68	1.41	1.37
17	A	830	CLA	C3B-C2B	-2.67	1.36	1.40
17	5	312	CLA	C1D-ND	2.67	1.41	1.37
17	A	843	CLA	C1D-ND	2.67	1.41	1.37
17	6	610	CLA	C1D-ND	2.66	1.41	1.37
17	A	827	CLA	C1D-C2D	-2.66	1.40	1.45
17	8	607	CLA	C3B-C2B	-2.66	1.36	1.40
17	A	838	CLA	C1D-ND	2.66	1.41	1.37
17	4	601	CLA	C1D-ND	2.66	1.41	1.37
17	B	810	CLA	C3B-C2B	-2.66	1.36	1.40
17	7	611	CLA	C3A-C2A	-2.66	1.47	1.54
17	B	834	CLA	C3B-C2B	-2.65	1.36	1.40
17	6	609	CLA	C1D-C2D	-2.65	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	839	CLA	C1D-ND	2.65	1.41	1.37
17	A	827	CLA	C1D-ND	2.65	1.41	1.37
17	1	603	CLA	C1D-C2D	-2.65	1.40	1.45
17	1	609	CLA	C1D-C2D	-2.65	1.40	1.45
17	A	832	CLA	C1D-ND	2.64	1.41	1.37
17	7	612	CLA	C1D-C2D	-2.64	1.40	1.45
17	5	312	CLA	C1D-C2D	-2.64	1.40	1.45
20	6	605	CHL	C1B-NB	2.64	1.37	1.35
17	A	814	CLA	C1D-C2D	-2.64	1.40	1.45
17	7	604	CLA	C3D-C4D	-2.64	1.38	1.44
17	5	310	CLA	C1D-C2D	-2.63	1.40	1.45
17	A	831	CLA	C1D-C2D	-2.63	1.40	1.45
17	6	601	CLA	C3B-C2B	-2.63	1.36	1.40
17	A	835	CLA	C1D-C2D	-2.63	1.40	1.45
17	A	812	CLA	C3B-C2B	-2.63	1.36	1.40
17	1	605	CLA	C1D-C2D	-2.63	1.40	1.45
17	J	101	CLA	C1D-C2D	-2.62	1.40	1.45
17	A	839	CLA	C1D-C2D	-2.62	1.40	1.45
17	B	806	CLA	C1D-ND	2.62	1.41	1.37
17	8	602	CLA	C1D-ND	2.62	1.41	1.37
17	J	101	CLA	C3A-C2A	-2.62	1.47	1.54
17	A	803	CLA	C1D-C2D	-2.62	1.40	1.45
17	A	802	CLA	C1D-C2D	-2.62	1.40	1.45
17	A	834	CLA	C1D-ND	2.62	1.41	1.37
17	5	301	CLA	C3B-C2B	-2.61	1.36	1.40
17	B	835	CLA	C3B-C2B	-2.61	1.36	1.40
17	7	601	CLA	C3A-C2A	-2.61	1.47	1.54
17	A	828	CLA	C1D-C2D	-2.61	1.40	1.45
17	7	612	CLA	C3A-C2A	-2.61	1.47	1.54
17	A	806	CLA	C1D-C2D	-2.61	1.40	1.45
17	A	810	CLA	C3B-C2B	-2.61	1.36	1.40
17	A	837	CLA	C3B-C2B	-2.61	1.36	1.40
17	3	302	CLA	C1D-C2D	-2.60	1.40	1.45
17	3	308	CLA	C3A-C2A	-2.60	1.47	1.54
17	A	818	CLA	C3B-C2B	-2.60	1.36	1.40
17	6	602	CLA	C1D-C2D	-2.60	1.40	1.45
17	A	821	CLA	C1D-ND	2.59	1.41	1.37
17	A	835	CLA	C3B-C2B	-2.59	1.36	1.40
20	6	605	CHL	C1D-ND	2.59	1.41	1.37
17	B	823	CLA	C3A-C2A	-2.59	1.47	1.54
17	B	832	CLA	C1D-C2D	-2.59	1.40	1.45
17	A	826	CLA	C1D-C2D	-2.59	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	802	CLA	C3B-C2B	-2.59	1.36	1.40
17	1	610	CLA	C1D-C2D	-2.58	1.40	1.45
17	8	613	CLA	C3B-C2B	-2.58	1.36	1.40
17	7	601	CLA	C1D-ND	2.58	1.41	1.37
17	A	823	CLA	C3A-C2A	-2.58	1.47	1.54
17	5	302	CLA	C1D-C2D	-2.58	1.40	1.45
17	6	604	CLA	C1D-C2D	-2.58	1.40	1.45
17	5	311	CLA	C1D-C2D	-2.58	1.40	1.45
17	A	807	CLA	C1D-C2D	-2.57	1.40	1.45
17	A	816	CLA	C1D-C2D	-2.57	1.40	1.45
17	5	303	CLA	C1D-C2D	-2.57	1.40	1.45
20	6	606	CHL	C1D-ND	2.57	1.40	1.37
17	B	814	CLA	C3B-C2B	-2.57	1.36	1.40
17	A	810	CLA	C1D-C2D	-2.57	1.40	1.45
17	A	813	CLA	C1D-C2D	-2.57	1.40	1.45
17	7	605	CLA	C1D-C2D	-2.57	1.40	1.45
17	1	608	CLA	C1D-C2D	-2.56	1.40	1.45
17	6	601	CLA	C1D-C2D	-2.56	1.40	1.45
17	A	812	CLA	C1D-C2D	-2.56	1.40	1.45
17	4	604	CLA	C1D-C2D	-2.56	1.40	1.45
17	7	607	CLA	C1D-C2D	-2.56	1.40	1.45
17	7	603	CLA	C1D-ND	2.56	1.40	1.37
17	7	613	CLA	C1D-C2D	-2.56	1.40	1.45
17	F	302	CLA	C1D-ND	2.56	1.40	1.37
17	A	829	CLA	C1D-C2D	-2.56	1.40	1.45
17	B	835	CLA	C1D-C2D	-2.56	1.40	1.45
17	B	834	CLA	C1D-C2D	-2.55	1.40	1.45
17	A	842	CLA	C1D-C2D	-2.55	1.40	1.45
17	B	822	CLA	C1D-C2D	-2.55	1.40	1.45
17	7	604	CLA	C1D-C2D	-2.55	1.40	1.45
17	A	803	CLA	C1D-ND	2.55	1.40	1.37
17	8	601	CLA	C1D-C2D	-2.55	1.40	1.45
17	8	604	CLA	C1D-C2D	-2.55	1.40	1.45
20	7	606	CHL	C1B-NB	2.55	1.37	1.35
17	8	605	CLA	C3B-C2B	-2.54	1.36	1.40
17	4	603	CLA	C1D-ND	2.54	1.40	1.37
20	6	607	CHL	C1D-ND	2.54	1.40	1.37
17	8	613	CLA	C1D-C2D	-2.54	1.40	1.45
17	B	821	CLA	C1D-C2D	-2.54	1.40	1.45
17	8	607	CLA	C1D-C2D	-2.54	1.40	1.45
17	A	806	CLA	C1D-ND	2.54	1.40	1.37
17	7	601	CLA	C1D-C2D	-2.53	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	306	CLA	C1D-ND	2.53	1.40	1.37
17	5	311	CLA	C1D-ND	2.53	1.40	1.37
17	1	602	CLA	C1D-C2D	-2.53	1.40	1.45
17	4	601	CLA	C1D-C2D	-2.53	1.40	1.45
17	B	816	CLA	C3A-C2A	-2.53	1.47	1.54
17	7	609	CLA	C1D-C2D	-2.53	1.40	1.45
17	A	836	CLA	C1D-C2D	-2.53	1.40	1.45
17	4	605	CLA	C3B-C2B	-2.53	1.36	1.40
17	B	818	CLA	C1D-C2D	-2.53	1.40	1.45
17	B	830	CLA	C1D-ND	2.52	1.40	1.37
17	8	612	CLA	C1D-C2D	-2.52	1.40	1.45
17	1	606	CLA	C3D-C4D	-2.52	1.38	1.44
17	B	822	CLA	C1D-ND	2.52	1.40	1.37
17	B	805	CLA	C1D-C2D	-2.52	1.40	1.45
17	B	813	CLA	CAB-C3B	-2.52	1.46	1.51
17	B	808	CLA	C1D-C2D	-2.52	1.40	1.45
17	7	608	CLA	C1D-ND	2.52	1.40	1.37
17	3	304	CLA	C1D-C2D	-2.52	1.40	1.45
17	6	610	CLA	C3B-C2B	-2.52	1.36	1.40
17	3	303	CLA	C1D-ND	2.52	1.40	1.37
17	3	311	CLA	C1D-C2D	-2.52	1.40	1.45
17	B	823	CLA	C1D-C2D	-2.51	1.40	1.45
17	5	301	CLA	C1D-C2D	-2.51	1.40	1.45
17	B	830	CLA	C1D-C2D	-2.51	1.40	1.45
17	B	825	CLA	C3B-C2B	-2.51	1.36	1.40
17	A	833	CLA	C1D-C2D	-2.51	1.40	1.45
17	B	825	CLA	C1D-C2D	-2.51	1.40	1.45
17	A	822	CLA	C1D-C2D	-2.51	1.40	1.45
17	8	614	CLA	C1D-C2D	-2.51	1.40	1.45
20	5	313	CHL	C1D-ND	2.51	1.40	1.37
17	A	830	CLA	C1D-C2D	-2.51	1.40	1.45
17	B	809	CLA	C3B-C2B	-2.51	1.36	1.40
17	7	602	CLA	C1D-C2D	-2.51	1.40	1.45
17	A	811	CLA	C1D-ND	2.51	1.40	1.37
17	A	810	CLA	C3A-C2A	-2.50	1.47	1.54
17	7	602	CLA	C3B-C2B	-2.50	1.36	1.40
17	B	809	CLA	C1D-C2D	-2.50	1.40	1.45
17	B	804	CLA	C1D-C2D	-2.50	1.40	1.45
17	A	832	CLA	C1D-C2D	-2.50	1.40	1.45
17	A	835	CLA	C3A-C2A	-2.50	1.47	1.54
17	8	609	CLA	C1D-C2D	-2.50	1.40	1.45
20	8	606	CHL	C1D-C2D	-2.49	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	810	CLA	C1D-ND	2.49	1.40	1.37
17	B	819	CLA	C3D-C4D	-2.49	1.38	1.44
17	A	820	CLA	C3B-C2B	-2.49	1.36	1.40
17	8	611	CLA	C1D-C2D	-2.49	1.40	1.45
17	3	302	CLA	C1D-ND	2.49	1.40	1.37
17	F	302	CLA	C1D-C2D	-2.49	1.40	1.45
17	7	613	CLA	C3B-C2B	-2.49	1.36	1.40
17	5	307	CLA	C1D-C2D	-2.49	1.40	1.45
17	B	839	CLA	C1D-C2D	-2.49	1.40	1.45
17	8	605	CLA	C1D-C2D	-2.49	1.40	1.45
17	B	831	CLA	C3A-C2A	-2.49	1.47	1.54
17	A	813	CLA	C3B-C2B	-2.49	1.36	1.40
17	8	608	CLA	C1D-C2D	-2.49	1.40	1.45
17	7	611	CLA	C1D-C2D	-2.49	1.40	1.45
17	B	826	CLA	C1D-C2D	-2.49	1.40	1.45
17	5	312	CLA	C3B-C2B	-2.48	1.36	1.40
17	3	310	CLA	C1D-ND	2.48	1.40	1.37
17	A	809	CLA	C1D-C2D	-2.48	1.40	1.45
17	A	818	CLA	C1D-C2D	-2.48	1.40	1.45
20	5	305	CHL	C1D-C2D	-2.48	1.40	1.45
17	A	817	CLA	C1D-C2D	-2.48	1.40	1.45
17	B	816	CLA	C1D-C2D	-2.48	1.40	1.45
20	3	307	CHL	C1D-C2D	-2.48	1.40	1.45
17	B	827	CLA	C1D-C2D	-2.48	1.40	1.45
17	A	805	CLA	C1D-C2D	-2.48	1.40	1.45
17	3	305	CLA	C1D-C2D	-2.48	1.40	1.45
17	3	308	CLA	C1D-ND	2.48	1.40	1.37
17	A	823	CLA	C1D-C2D	-2.48	1.40	1.45
17	3	304	CLA	C1D-ND	2.48	1.40	1.37
17	B	827	CLA	C1D-ND	2.47	1.40	1.37
17	3	306	CLA	C1D-C2D	-2.47	1.40	1.45
17	B	817	CLA	C1D-C2D	-2.47	1.40	1.45
17	5	307	CLA	C3B-C2B	-2.47	1.36	1.40
17	B	820	CLA	C1D-C2D	-2.47	1.40	1.45
17	1	609	CLA	C3B-C2B	-2.46	1.36	1.40
17	A	807	CLA	C3A-C2A	-2.46	1.47	1.54
17	3	308	CLA	C1D-C2D	-2.46	1.40	1.45
17	A	838	CLA	C1D-C2D	-2.46	1.40	1.45
17	5	304	CLA	C3B-C2B	-2.46	1.37	1.40
17	A	822	CLA	C3B-C2B	-2.46	1.37	1.40
17	8	603	CLA	C3B-C2B	-2.46	1.37	1.40
17	B	806	CLA	C3A-C2A	-2.45	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	801	CLA	C3D-C4D	-2.45	1.38	1.44
17	J	102	CLA	C1D-C2D	-2.45	1.40	1.45
17	B	831	CLA	C1D-C2D	-2.45	1.40	1.45
17	8	603	CLA	C1D-C2D	-2.45	1.40	1.45
17	B	832	CLA	C3A-C2A	-2.45	1.47	1.54
17	8	602	CLA	C1D-C2D	-2.45	1.40	1.45
17	B	802	CLA	C1D-C2D	-2.45	1.40	1.45
17	F	301	CLA	C1D-C2D	-2.45	1.40	1.45
17	A	815	CLA	C3B-C2B	-2.45	1.37	1.40
17	5	314	CLA	C1D-C2D	-2.45	1.40	1.45
17	8	612	CLA	C3B-C2B	-2.45	1.37	1.40
17	B	828	CLA	C1D-C2D	-2.44	1.40	1.45
17	A	824	CLA	C1D-C2D	-2.44	1.40	1.45
17	A	819	CLA	C1D-C2D	-2.44	1.40	1.45
17	7	607	CLA	C3A-C2A	-2.44	1.47	1.54
17	B	811	CLA	C1D-C2D	-2.44	1.40	1.45
17	B	836	CLA	C1D-C2D	-2.44	1.40	1.45
17	B	814	CLA	C1D-C2D	-2.44	1.40	1.45
17	A	838	CLA	C3D-C4D	-2.44	1.38	1.44
17	A	820	CLA	C1D-C2D	-2.44	1.40	1.45
17	6	608	CLA	C1D-ND	2.43	1.40	1.37
17	A	821	CLA	C1D-C2D	-2.43	1.40	1.45
20	7	606	CHL	C1D-C2D	-2.43	1.40	1.45
20	3	307	CHL	C3A-C2A	-2.43	1.47	1.54
20	6	607	CHL	C1D-C2D	-2.43	1.40	1.45
17	3	313	CLA	C1D-C2D	-2.43	1.40	1.45
17	A	841	CLA	C1D-C2D	-2.43	1.40	1.45
17	A	809	CLA	C1D-ND	2.43	1.40	1.37
17	B	837	CLA	C1D-C2D	-2.42	1.40	1.45
17	1	604	CLA	C1D-C2D	-2.42	1.40	1.45
17	B	829	CLA	C1D-C2D	-2.42	1.40	1.45
17	7	605	CLA	C3A-C2A	-2.42	1.47	1.54
17	B	810	CLA	C1D-C2D	-2.42	1.40	1.45
20	8	606	CHL	C1B-NB	2.42	1.37	1.35
17	B	813	CLA	C1D-C2D	-2.42	1.40	1.45
17	4	604	CLA	C3A-C2A	-2.41	1.47	1.54
17	5	306	CLA	C1D-C2D	-2.41	1.40	1.45
17	A	808	CLA	C3A-C2A	-2.41	1.47	1.54
17	A	825	CLA	C1D-ND	2.41	1.40	1.37
17	A	818	CLA	C3A-C2A	-2.41	1.47	1.54
17	3	309	CLA	C1D-C2D	-2.41	1.40	1.45
17	A	825	CLA	C1D-C2D	-2.41	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	834	CLA	C1D-C2D	-2.41	1.40	1.45
17	B	821	CLA	C1C-C2C	2.40	1.49	1.44
20	8	606	CHL	C1D-ND	2.40	1.40	1.37
17	8	610	CLA	C1D-C2D	-2.40	1.40	1.45
17	8	613	CLA	C3A-C2A	-2.39	1.47	1.54
17	B	829	CLA	C3D-C4D	-2.39	1.38	1.44
17	7	602	CLA	C1D-ND	2.39	1.40	1.37
20	5	313	CHL	C1D-C2D	-2.39	1.40	1.45
17	8	608	CLA	C1D-ND	2.38	1.40	1.37
17	7	610	CLA	C1D-C2D	-2.38	1.40	1.45
17	A	816	CLA	C1D-ND	2.38	1.40	1.37
20	1	601	CHL	C1D-C2D	-2.38	1.40	1.45
17	A	811	CLA	C1D-C2D	-2.38	1.40	1.45
20	Z	601	CHL	C1D-C2D	-2.38	1.40	1.45
20	6	605	CHL	C1D-C2D	-2.37	1.40	1.45
17	6	609	CLA	C3A-C2A	-2.37	1.47	1.54
17	B	806	CLA	C1D-C2D	-2.37	1.40	1.45
17	5	312	CLA	C3A-C2A	-2.37	1.47	1.54
17	B	836	CLA	C3B-C2B	-2.37	1.37	1.40
17	B	833	CLA	C1D-C2D	-2.37	1.40	1.45
17	B	824	CLA	C1D-C2D	-2.37	1.40	1.45
17	3	303	CLA	C1D-C2D	-2.37	1.40	1.45
17	A	804	CLA	C1D-C2D	-2.37	1.40	1.45
17	B	811	CLA	C3A-C2A	-2.36	1.47	1.54
17	A	819	CLA	C1D-ND	2.36	1.40	1.37
17	B	838	CLA	C3A-C2A	-2.36	1.47	1.54
17	A	812	CLA	C1D-ND	2.36	1.40	1.37
17	B	807	CLA	C3B-C2B	-2.36	1.37	1.40
17	A	836	CLA	C3A-C2A	-2.36	1.47	1.54
17	7	610	CLA	C3D-C4D	-2.36	1.38	1.44
17	B	824	CLA	C3D-C4D	-2.36	1.38	1.44
17	8	614	CLA	C1D-ND	2.36	1.40	1.37
17	6	608	CLA	C1D-C2D	-2.35	1.40	1.45
17	5	315	CLA	C1D-C2D	-2.35	1.40	1.45
17	A	812	CLA	C3D-C4D	-2.35	1.38	1.44
17	B	839	CLA	C3A-C2A	-2.35	1.47	1.54
17	3	301	CLA	C1D-C2D	-2.35	1.40	1.45
17	A	804	CLA	C3B-C2B	-2.35	1.37	1.40
17	8	614	CLA	C3A-C2A	-2.35	1.47	1.54
20	1	601	CHL	C1D-ND	2.35	1.40	1.37
17	6	609	CLA	C3B-C2B	-2.35	1.37	1.40
17	3	301	CLA	C3D-C4D	-2.34	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	608	CLA	C1D-C2D	-2.34	1.40	1.45
17	3	312	CLA	C1D-C2D	-2.34	1.40	1.45
17	7	610	CLA	C3B-C2B	-2.34	1.37	1.40
17	A	825	CLA	C3B-C2B	-2.34	1.37	1.40
17	A	815	CLA	CHD-C4C	-2.34	1.33	1.39
17	4	602	CLA	C1D-C2D	-2.34	1.40	1.45
17	1	607	CLA	C1D-C2D	-2.34	1.40	1.45
17	8	612	CLA	C3A-C2A	-2.34	1.47	1.54
17	B	837	CLA	C3D-C4D	-2.34	1.38	1.44
17	8	614	CLA	C3D-C4D	-2.34	1.38	1.44
17	A	826	CLA	C3B-C2B	-2.33	1.37	1.40
17	B	820	CLA	C1D-ND	2.33	1.40	1.37
17	5	310	CLA	C3B-C2B	-2.33	1.37	1.40
17	6	603	CLA	C1D-C2D	-2.33	1.40	1.45
17	B	806	CLA	C3D-C4D	-2.33	1.38	1.44
17	A	829	CLA	C1D-ND	2.32	1.40	1.37
17	A	824	CLA	C3D-C4D	-2.32	1.38	1.44
17	B	826	CLA	C3D-C4D	-2.32	1.38	1.44
17	3	306	CLA	C3A-C2A	-2.32	1.48	1.54
20	1	601	CHL	C3D-C4D	-2.32	1.38	1.44
17	8	608	CLA	C3D-C4D	-2.32	1.38	1.44
17	5	309	CLA	C1D-C2D	-2.32	1.40	1.45
17	A	829	CLA	C3D-C4D	-2.32	1.38	1.44
17	5	314	CLA	C3D-C4D	-2.32	1.38	1.44
17	3	302	CLA	C3B-C2B	-2.32	1.37	1.40
17	A	822	CLA	C3D-C4D	-2.32	1.38	1.44
17	7	603	CLA	C1D-C2D	-2.32	1.40	1.45
17	3	304	CLA	C3D-C4D	-2.32	1.38	1.44
20	6	606	CHL	C1D-C2D	-2.31	1.40	1.45
17	B	831	CLA	C3B-C2B	-2.31	1.37	1.40
20	Z	601	CHL	C3D-C4D	-2.31	1.39	1.44
17	5	306	CLA	C3B-C2B	-2.31	1.37	1.40
17	B	835	CLA	C1D-ND	2.31	1.40	1.37
17	B	826	CLA	C3B-C2B	-2.31	1.37	1.40
17	A	802	CLA	C3A-C2A	-2.31	1.48	1.54
17	6	610	CLA	CHD-C4C	-2.31	1.33	1.39
17	A	804	CLA	C3D-C4D	-2.31	1.39	1.44
17	A	817	CLA	C3D-C4D	-2.31	1.39	1.44
17	B	812	CLA	C1D-C2D	-2.30	1.40	1.45
17	7	605	CLA	C3D-C4D	-2.30	1.39	1.44
17	4	603	CLA	C1D-C2D	-2.30	1.40	1.45
17	6	603	CLA	C3B-C2B	-2.30	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	839	CLA	C3A-C2A	-2.29	1.48	1.54
16	A	801	CL0	C3D-C4D	-2.29	1.39	1.44
17	5	309	CLA	C3A-C2A	-2.29	1.48	1.54
17	A	807	CLA	C3D-C4D	-2.29	1.39	1.44
17	A	829	CLA	C3B-C2B	-2.29	1.37	1.40
20	Z	601	CHL	C1D-ND	2.29	1.40	1.37
17	J	101	CLA	C3D-C4D	-2.29	1.39	1.44
17	7	612	CLA	C3D-C4D	-2.29	1.39	1.44
17	B	838	CLA	C3D-C4D	-2.29	1.39	1.44
17	A	815	CLA	C3D-C4D	-2.29	1.39	1.44
17	B	822	CLA	C3B-C2B	-2.29	1.37	1.40
20	1	601	CHL	C1B-NB	2.28	1.37	1.35
17	5	308	CLA	C1D-C2D	-2.28	1.40	1.45
17	3	305	CLA	C3D-C4D	-2.28	1.39	1.44
17	7	603	CLA	C3A-C2A	-2.28	1.48	1.54
17	A	841	CLA	C3D-C4D	-2.28	1.39	1.44
17	A	833	CLA	C3A-C2A	-2.28	1.48	1.54
17	3	308	CLA	C3D-C4D	-2.28	1.39	1.44
17	B	804	CLA	C3D-C4D	-2.28	1.39	1.44
17	A	842	CLA	C3D-C4D	-2.28	1.39	1.44
17	B	831	CLA	C3D-C4D	-2.28	1.39	1.44
17	B	807	CLA	C1D-C2D	-2.27	1.40	1.45
17	B	831	CLA	C1D-ND	2.27	1.40	1.37
17	A	843	CLA	C3A-C2A	-2.27	1.48	1.54
17	B	808	CLA	C3A-C2A	-2.27	1.48	1.54
17	A	806	CLA	C3A-C2A	-2.27	1.48	1.54
17	1	607	CLA	C1D-ND	2.27	1.40	1.37
17	A	836	CLA	C3B-C2B	-2.27	1.37	1.40
17	A	821	CLA	C3D-C4D	-2.27	1.39	1.44
17	7	614	CLA	C1D-C2D	-2.27	1.40	1.45
20	6	605	CHL	C3D-C4D	-2.26	1.39	1.44
17	5	302	CLA	C3B-C2B	-2.26	1.37	1.40
17	B	830	CLA	C3D-C4D	-2.26	1.39	1.44
17	A	807	CLA	C1D-ND	2.26	1.40	1.37
17	A	831	CLA	C3A-C2A	-2.26	1.48	1.54
17	A	834	CLA	C3D-C4D	-2.25	1.39	1.44
17	5	314	CLA	C3A-C2A	-2.25	1.48	1.54
17	B	818	CLA	C1D-ND	2.25	1.40	1.37
20	Z	601	CHL	C1B-NB	2.25	1.37	1.35
17	A	839	CLA	C3D-C4D	-2.25	1.39	1.44
20	7	606	CHL	C3D-C4D	-2.25	1.39	1.44
17	B	834	CLA	C3A-C2A	-2.25	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	804	CLA	C3A-C2A	-2.25	1.48	1.54
16	A	801	CL0	C1D-C2D	-2.25	1.40	1.45
17	B	826	CLA	C1D-ND	2.24	1.40	1.37
20	7	606	CHL	C1D-ND	2.24	1.40	1.37
17	B	836	CLA	C3A-C2A	-2.24	1.48	1.54
17	8	609	CLA	C3B-C2B	-2.24	1.37	1.40
20	8	606	CHL	C3D-C4D	-2.24	1.39	1.44
17	F	301	CLA	C3D-C4D	-2.24	1.39	1.44
17	3	313	CLA	C3D-C4D	-2.24	1.39	1.44
17	B	827	CLA	C3D-C4D	-2.24	1.39	1.44
17	A	812	CLA	C3A-C2A	-2.24	1.48	1.54
17	B	835	CLA	C3D-C4D	-2.24	1.39	1.44
17	A	806	CLA	C3B-C2B	-2.23	1.37	1.40
17	8	610	CLA	C3D-C4D	-2.23	1.39	1.44
17	7	601	CLA	C3D-C4D	-2.23	1.39	1.44
17	3	310	CLA	C1D-C2D	-2.23	1.40	1.45
17	7	603	CLA	C3D-C4D	-2.23	1.39	1.44
17	1	608	CLA	C3B-C2B	-2.23	1.37	1.40
17	3	306	CLA	C3D-C4D	-2.23	1.39	1.44
17	7	608	CLA	C3D-C4D	-2.23	1.39	1.44
17	8	603	CLA	C3D-C4D	-2.23	1.39	1.44
20	3	307	CHL	C3D-C4D	-2.23	1.39	1.44
17	B	815	CLA	C1D-C2D	-2.23	1.40	1.45
17	B	832	CLA	C3D-C4D	-2.23	1.39	1.44
17	5	308	CLA	C3D-C4D	-2.23	1.39	1.44
17	B	807	CLA	C3D-C4D	-2.23	1.39	1.44
17	A	830	CLA	C3D-C4D	-2.23	1.39	1.44
17	7	610	CLA	C1D-ND	2.23	1.40	1.37
20	6	606	CHL	C3D-C4D	-2.23	1.39	1.44
17	B	832	CLA	C3B-C2B	-2.22	1.37	1.40
17	A	809	CLA	C3D-C4D	-2.22	1.39	1.44
17	8	613	CLA	C3D-C4D	-2.22	1.39	1.44
17	A	803	CLA	C3D-C4D	-2.22	1.39	1.44
20	5	313	CHL	C3D-C4D	-2.22	1.39	1.44
17	4	605	CLA	C3D-C4D	-2.22	1.39	1.44
17	A	839	CLA	CHD-C4C	-2.21	1.34	1.39
17	A	815	CLA	C1D-ND	2.21	1.40	1.37
17	B	817	CLA	C3D-C4D	-2.21	1.39	1.44
17	A	835	CLA	C3D-C4D	-2.21	1.39	1.44
17	4	601	CLA	C3D-C4D	-2.21	1.39	1.44
17	B	801	CLA	C1D-C2D	-2.21	1.41	1.45
17	B	807	CLA	C3A-C2A	-2.21	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	802	CLA	CHD-C4C	-2.21	1.34	1.39
17	5	303	CLA	C3D-C4D	-2.21	1.39	1.44
17	A	837	CLA	C3D-C4D	-2.21	1.39	1.44
17	8	611	CLA	C3D-C4D	-2.21	1.39	1.44
17	3	303	CLA	C3B-C2B	-2.21	1.37	1.40
17	B	832	CLA	CHD-C4C	-2.21	1.34	1.39
17	B	838	CLA	C1D-ND	2.20	1.40	1.37
17	7	605	CLA	C1D-ND	2.20	1.40	1.37
17	B	802	CLA	C3D-C4D	-2.20	1.39	1.44
17	7	613	CLA	C3D-C4D	-2.20	1.39	1.44
17	A	822	CLA	C3A-C2A	-2.20	1.48	1.54
17	F	301	CLA	C1D-ND	2.20	1.40	1.37
17	A	833	CLA	C3D-C4D	-2.20	1.39	1.44
17	F	302	CLA	C3D-C4D	-2.20	1.39	1.44
17	6	603	CLA	C3D-C4D	-2.20	1.39	1.44
17	A	819	CLA	C3B-C2B	-2.20	1.37	1.40
17	A	806	CLA	C3D-C4D	-2.20	1.39	1.44
17	6	602	CLA	C3D-C4D	-2.20	1.39	1.44
17	B	805	CLA	C3D-C4D	-2.20	1.39	1.44
17	5	302	CLA	C3D-C4D	-2.20	1.39	1.44
17	7	607	CLA	C3B-C2B	-2.20	1.37	1.40
17	A	841	CLA	C3B-C2B	-2.20	1.37	1.40
17	8	602	CLA	C3D-C4D	-2.19	1.39	1.44
17	B	819	CLA	C3A-C2A	-2.19	1.48	1.54
17	A	832	CLA	C3C-C4C	2.19	1.43	1.40
17	5	310	CLA	C3A-C2A	-2.19	1.48	1.54
17	7	612	CLA	C3B-C2B	-2.19	1.37	1.40
17	B	810	CLA	C3D-C4D	-2.19	1.39	1.44
17	A	831	CLA	CHD-C4C	-2.19	1.34	1.39
17	A	811	CLA	C3D-C4D	-2.19	1.39	1.44
17	8	609	CLA	C3D-C4D	-2.19	1.39	1.44
17	B	813	CLA	C3D-C4D	-2.19	1.39	1.44
17	B	820	CLA	C3D-C4D	-2.19	1.39	1.44
20	5	313	CHL	C1B-NB	2.19	1.37	1.35
17	8	610	CLA	C3A-C2A	-2.19	1.48	1.54
17	A	832	CLA	C3D-C4D	-2.19	1.39	1.44
17	B	834	CLA	C3D-C4D	-2.19	1.39	1.44
20	6	606	CHL	C1B-CHB	-2.19	1.34	1.41
17	4	605	CLA	CHD-C4C	-2.19	1.34	1.39
17	6	608	CLA	C3D-C4D	-2.18	1.39	1.44
17	5	304	CLA	C3D-C4D	-2.18	1.39	1.44
17	4	605	CLA	C1D-ND	2.18	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	825	CLA	C3D-C4D	-2.18	1.39	1.44
17	B	812	CLA	C3D-C4D	-2.18	1.39	1.44
17	8	602	CLA	C3B-C2B	-2.18	1.37	1.40
17	3	302	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	813	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	808	CLA	CHD-C4C	-2.18	1.34	1.39
17	J	101	CLA	C1D-ND	2.18	1.40	1.37
17	J	102	CLA	C3A-C2A	-2.18	1.48	1.54
17	B	818	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	817	CLA	C1D-ND	2.18	1.40	1.37
17	A	802	CLA	C3D-C4D	-2.18	1.39	1.44
17	B	806	CLA	C3B-C2B	-2.18	1.37	1.40
17	B	811	CLA	C3B-C2B	-2.18	1.37	1.40
17	A	836	CLA	C3D-C4D	-2.18	1.39	1.44
17	7	602	CLA	C3D-C4D	-2.18	1.39	1.44
17	5	315	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	808	CLA	C3D-C4D	-2.18	1.39	1.44
17	B	811	CLA	C3D-C4D	-2.18	1.39	1.44
17	1	607	CLA	C3D-C4D	-2.18	1.39	1.44
17	A	805	CLA	C3D-C4D	-2.18	1.39	1.44
17	3	310	CLA	C3D-C4D	-2.18	1.39	1.44
17	B	808	CLA	C3D-C4D	-2.17	1.39	1.44
17	A	810	CLA	C3D-C4D	-2.17	1.39	1.44
17	J	102	CLA	C3D-C4D	-2.17	1.39	1.44
17	8	608	CLA	C3B-C2B	-2.17	1.37	1.40
17	B	801	CLA	C3A-C2A	-2.17	1.48	1.54
17	B	836	CLA	C3D-C4D	-2.17	1.39	1.44
17	A	809	CLA	C3B-C2B	-2.17	1.37	1.40
17	8	604	CLA	C3A-C2A	-2.17	1.48	1.54
17	7	614	CLA	C3A-C2A	-2.16	1.48	1.54
17	5	309	CLA	C3D-C4D	-2.16	1.39	1.44
17	A	825	CLA	C3A-C2A	-2.16	1.48	1.54
17	5	314	CLA	C1D-ND	2.16	1.40	1.37
17	B	809	CLA	C3D-C4D	-2.16	1.39	1.44
17	3	313	CLA	C3B-C2B	-2.16	1.37	1.40
17	A	819	CLA	C3D-C4D	-2.16	1.39	1.44
20	5	305	CHL	C1D-ND	2.16	1.40	1.37
17	3	309	CLA	C3D-C4D	-2.16	1.39	1.44
17	3	312	CLA	C3D-C4D	-2.16	1.39	1.44
20	1	601	CHL	C4B-CHC	-2.15	1.35	1.41
17	A	826	CLA	C3D-C4D	-2.15	1.39	1.44
17	B	816	CLA	C3B-C2B	-2.15	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	601	CLA	C3B-C2B	-2.15	1.37	1.40
17	7	611	CLA	C3D-C4D	-2.15	1.39	1.44
20	5	305	CHL	C3D-C4D	-2.15	1.39	1.44
17	1	608	CLA	C3A-C2A	-2.15	1.48	1.54
17	5	314	CLA	C3B-C2B	-2.14	1.37	1.40
17	3	303	CLA	C3D-C4D	-2.14	1.39	1.44
17	8	611	CLA	C3B-C2B	-2.14	1.37	1.40
20	Z	601	CHL	C4B-CHC	-2.14	1.35	1.41
17	6	603	CLA	C3A-C2A	-2.14	1.48	1.54
17	A	827	CLA	C3D-C4D	-2.14	1.39	1.44
17	B	833	CLA	C3D-C4D	-2.14	1.39	1.44
17	5	306	CLA	C3D-C4D	-2.14	1.39	1.44
20	7	606	CHL	C4B-CHC	-2.14	1.35	1.41
17	8	612	CLA	C3D-C4D	-2.14	1.39	1.44
17	1	606	CLA	C1D-C2D	-2.14	1.41	1.45
17	B	828	CLA	C3D-C4D	-2.14	1.39	1.44
17	J	101	CLA	C3B-C2B	-2.14	1.37	1.40
17	5	301	CLA	C3D-C4D	-2.13	1.39	1.44
17	3	305	CLA	C3A-C2A	-2.13	1.48	1.54
17	5	310	CLA	C3D-C4D	-2.13	1.39	1.44
17	8	601	CLA	C3D-C4D	-2.13	1.39	1.44
17	B	825	CLA	CHD-C4C	-2.13	1.34	1.39
17	B	812	CLA	C3A-C2A	-2.12	1.48	1.54
17	F	301	CLA	C3A-C2A	-2.12	1.48	1.54
20	5	305	CHL	C1B-NB	2.12	1.37	1.35
20	6	606	CHL	C1B-NB	2.12	1.37	1.35
17	A	811	CLA	C3A-C2A	-2.12	1.48	1.54
17	4	601	CLA	C3A-C2A	-2.12	1.48	1.54
17	B	838	CLA	CHD-C4C	-2.12	1.34	1.39
17	5	315	CLA	C3A-C2A	-2.12	1.48	1.54
17	5	312	CLA	C3D-C4D	-2.12	1.39	1.44
17	4	603	CLA	C3D-C4D	-2.12	1.39	1.44
17	A	828	CLA	C3D-C4D	-2.12	1.39	1.44
20	3	307	CHL	C1B-CHB	-2.12	1.35	1.41
17	A	814	CLA	C3D-C4D	-2.12	1.39	1.44
17	8	604	CLA	C3D-C4D	-2.12	1.39	1.44
17	J	101	CLA	CHD-C4C	-2.12	1.34	1.39
17	5	302	CLA	CHD-C4C	-2.11	1.34	1.39
17	3	301	CLA	C1D-ND	2.11	1.40	1.37
17	A	843	CLA	C3D-C4D	-2.11	1.39	1.44
17	7	605	CLA	C3B-C2B	-2.11	1.37	1.40
17	7	609	CLA	C3D-C4D	-2.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	607	CLA	C3D-C4D	-2.11	1.39	1.44
17	B	809	CLA	C3A-C2A	-2.11	1.48	1.54
17	B	822	CLA	C3D-C4D	-2.11	1.39	1.44
17	6	609	CLA	CHD-C4C	-2.11	1.34	1.39
17	B	816	CLA	C3D-C4D	-2.11	1.39	1.44
17	1	605	CLA	C3A-C2A	-2.11	1.48	1.54
17	5	311	CLA	C3D-C4D	-2.11	1.39	1.44
17	3	313	CLA	C3A-C2A	-2.11	1.48	1.54
17	7	613	CLA	C3A-C2A	-2.11	1.48	1.54
17	1	603	CLA	C3B-C2B	-2.11	1.37	1.40
17	B	812	CLA	C3B-C2B	-2.10	1.37	1.40
17	8	610	CLA	C1D-ND	2.10	1.40	1.37
17	5	307	CLA	C3D-C4D	-2.10	1.39	1.44
17	6	601	CLA	C3D-C4D	-2.10	1.39	1.44
17	A	820	CLA	C3D-C4D	-2.10	1.39	1.44
17	B	815	CLA	C3D-C4D	-2.10	1.39	1.44
17	1	602	CLA	C3D-C4D	-2.09	1.39	1.44
17	7	605	CLA	CHD-C4C	-2.09	1.34	1.39
20	5	305	CHL	C1B-CHB	-2.09	1.35	1.41
17	6	604	CLA	C3A-C2A	-2.09	1.48	1.54
20	6	607	CHL	C1B-CHB	-2.09	1.35	1.41
16	A	801	CL0	C3A-C2A	-2.09	1.48	1.54
17	B	817	CLA	C3B-C2B	-2.09	1.37	1.40
17	5	304	CLA	CHD-C4C	-2.09	1.34	1.39
17	6	601	CLA	C3A-C2A	-2.09	1.48	1.54
17	A	816	CLA	C3D-C4D	-2.09	1.39	1.44
17	3	313	CLA	C1D-ND	2.09	1.40	1.37
17	8	605	CLA	C3A-C2A	-2.09	1.48	1.54
17	B	821	CLA	CHD-C4C	-2.09	1.34	1.39
17	8	601	CLA	C3A-C2A	-2.09	1.48	1.54
20	5	305	CHL	C4B-CHC	-2.09	1.35	1.41
20	6	606	CHL	C4B-CHC	-2.08	1.35	1.41
17	5	309	CLA	C3B-C2B	-2.08	1.37	1.40
17	8	607	CLA	C3D-C4D	-2.08	1.39	1.44
17	3	311	CLA	C3D-C4D	-2.08	1.39	1.44
20	6	607	CHL	C3D-C4D	-2.08	1.39	1.44
17	7	614	CLA	C3D-C4D	-2.08	1.39	1.44
17	4	604	CLA	C3D-C4D	-2.08	1.39	1.44
17	1	603	CLA	C3D-C4D	-2.08	1.39	1.44
20	5	313	CHL	C4B-CHC	-2.08	1.35	1.41
17	A	823	CLA	C3D-C4D	-2.08	1.39	1.44
17	B	825	CLA	C3D-C4D	-2.07	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	607	CLA	CHD-C4C	-2.07	1.34	1.39
17	A	821	CLA	C3B-C2B	-2.07	1.37	1.40
17	A	843	CLA	CHD-C4C	-2.07	1.34	1.39
17	B	827	CLA	C3A-C2A	-2.06	1.48	1.54
17	6	610	CLA	C3D-C4D	-2.06	1.39	1.44
17	A	818	CLA	C3D-C4D	-2.06	1.39	1.44
17	A	811	CLA	CHD-C4C	-2.06	1.34	1.39
17	1	603	CLA	C3A-C2A	-2.06	1.48	1.54
17	1	610	CLA	C3B-C2B	-2.06	1.37	1.40
17	B	839	CLA	C3D-C4D	-2.05	1.39	1.44
17	1	610	CLA	C3D-C4D	-2.05	1.39	1.44
17	A	826	CLA	C3A-C2A	-2.05	1.48	1.54
17	6	604	CLA	C3D-C4D	-2.05	1.39	1.44
17	5	301	CLA	CHD-C4C	-2.05	1.34	1.39
17	3	312	CLA	C3B-C2B	-2.05	1.37	1.40
17	B	837	CLA	C1D-ND	2.05	1.40	1.37
17	5	310	CLA	CHD-C4C	-2.05	1.34	1.39
17	B	822	CLA	C3A-C2A	-2.05	1.48	1.54
17	A	832	CLA	C3A-C2A	-2.05	1.48	1.54
17	A	834	CLA	C3B-C2B	-2.05	1.37	1.40
20	6	605	CHL	C1B-CHB	-2.04	1.35	1.41
20	8	606	CHL	C4B-CHC	-2.04	1.35	1.41
17	A	813	CLA	C3A-C2A	-2.04	1.48	1.54
17	A	828	CLA	C3A-C2A	-2.04	1.48	1.54
17	B	824	CLA	C1D-ND	2.04	1.40	1.37
17	A	837	CLA	CHD-C4C	-2.04	1.34	1.39
17	A	820	CLA	CHD-C4C	-2.04	1.34	1.39
17	B	830	CLA	C3B-C2B	-2.04	1.37	1.40
17	3	301	CLA	C3A-C2A	-2.04	1.48	1.54
17	3	302	CLA	CHD-C4C	-2.03	1.34	1.39
17	8	601	CLA	CHD-C4C	-2.03	1.34	1.39
20	6	607	CHL	C4B-CHC	-2.03	1.35	1.41
17	8	603	CLA	C3A-C2A	-2.03	1.48	1.54
17	A	806	CLA	CHD-C4C	-2.03	1.34	1.39
17	A	817	CLA	C3B-C2B	-2.03	1.37	1.40
17	A	822	CLA	C1D-ND	2.03	1.40	1.37
17	A	835	CLA	CHD-C4C	-2.03	1.34	1.39
17	A	813	CLA	CHD-C4C	-2.02	1.34	1.39
17	8	605	CLA	C3D-C4D	-2.02	1.39	1.44
17	B	829	CLA	C1D-ND	2.02	1.40	1.37
17	5	311	CLA	CHD-C4C	-2.02	1.34	1.39
17	1	605	CLA	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	315	CLA	C3B-C2B	-2.02	1.37	1.40
17	7	604	CLA	C3A-C2A	-2.02	1.48	1.54
17	A	812	CLA	CHD-C4C	-2.02	1.34	1.39
17	A	814	CLA	CHD-C4C	-2.02	1.34	1.39
17	8	604	CLA	CHD-C4C	-2.02	1.34	1.39
17	3	301	CLA	C3B-C2B	-2.01	1.37	1.40
17	3	303	CLA	C3A-C2A	-2.01	1.48	1.54
17	B	809	CLA	C1D-ND	2.01	1.40	1.37
17	B	821	CLA	C3D-C4D	-2.01	1.39	1.44
17	A	831	CLA	C3D-C4D	-2.01	1.39	1.44
17	1	603	CLA	CHD-C4C	-2.01	1.34	1.39
17	B	828	CLA	C3A-C2A	-2.01	1.48	1.54
17	B	823	CLA	C3D-C4D	-2.01	1.39	1.44
20	3	307	CHL	C1D-ND	2.01	1.40	1.37
20	3	307	CHL	C4B-CHC	-2.01	1.35	1.41
17	8	614	CLA	CHD-C4C	-2.01	1.34	1.39
17	6	602	CLA	CHD-C4C	-2.01	1.34	1.39
17	7	602	CLA	CHD-C4C	-2.00	1.34	1.39
17	A	830	CLA	CHD-C4C	-2.00	1.34	1.39
17	B	823	CLA	CHD-C4C	-2.00	1.34	1.39
17	3	311	CLA	C3A-C2A	-2.00	1.48	1.54
17	A	827	CLA	CHD-C4C	-2.00	1.34	1.39
17	8	603	CLA	CHD-C4C	-2.00	1.34	1.39
17	A	814	CLA	C3A-C2A	-2.00	1.48	1.54

All (1401) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	804	CLA	C4A-NA-C1A	-9.73	102.33	106.71
17	3	310	CLA	C4A-NA-C1A	-9.32	102.52	106.71
17	A	832	CLA	C1C-NC-C4C	-9.00	102.66	106.71
17	B	815	CLA	C4A-NA-C1A	-8.93	102.69	106.71
17	B	812	CLA	C4A-NA-C1A	-8.85	102.72	106.71
17	B	807	CLA	C4A-NA-C1A	-8.58	102.85	106.71
17	7	610	CLA	C4A-NA-C1A	-8.47	102.90	106.71
17	7	614	CLA	C4A-NA-C1A	-8.46	102.90	106.71
17	3	306	CLA	C4A-NA-C1A	-8.40	102.93	106.71
17	4	603	CLA	C4A-NA-C1A	-8.17	103.03	106.71
20	6	606	CHL	C4A-NA-C1A	-8.14	103.05	106.71
20	7	606	CHL	C4A-NA-C1A	-8.02	103.10	106.71
20	8	606	CHL	C4A-NA-C1A	-7.83	103.19	106.71
17	A	824	CLA	C4A-NA-C1A	-7.81	103.20	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	607	CLA	C4A-NA-C1A	-7.67	103.26	106.71
20	5	313	CHL	C4A-NA-C1A	-7.66	103.26	106.71
20	5	305	CHL	C4A-NA-C1A	-7.60	103.29	106.71
17	3	308	CLA	C4A-NA-C1A	-7.53	103.32	106.71
17	B	802	CLA	C4A-NA-C1A	-7.47	103.35	106.71
17	B	806	CLA	C4A-NA-C1A	-7.42	103.37	106.71
17	B	824	CLA	C4A-NA-C1A	-7.37	103.39	106.71
20	3	307	CHL	C4A-NA-C1A	-7.37	103.39	106.71
17	8	614	CLA	C4A-NA-C1A	-7.28	103.43	106.71
17	B	831	CLA	C4A-NA-C1A	-7.25	103.45	106.71
17	A	807	CLA	C4A-NA-C1A	-7.21	103.47	106.71
17	A	805	CLA	C4A-NA-C1A	-7.18	103.48	106.71
20	Z	601	CHL	C4A-NA-C1A	-7.07	103.53	106.71
17	B	834	CLA	C4A-NA-C1A	-6.98	103.57	106.71
17	3	313	CLA	C4A-NA-C1A	-6.95	103.58	106.71
20	1	601	CHL	C4A-NA-C1A	-6.95	103.58	106.71
20	6	605	CHL	C4A-NA-C1A	-6.87	103.62	106.71
17	F	301	CLA	C4A-NA-C1A	-6.84	103.63	106.71
17	3	305	CLA	C4A-NA-C1A	-6.82	103.64	106.71
17	7	603	CLA	C4A-NA-C1A	-6.80	103.65	106.71
17	A	822	CLA	C4A-NA-C1A	-6.79	103.65	106.71
17	B	820	CLA	C4A-NA-C1A	-6.72	103.69	106.71
17	B	804	CLA	C4A-NA-C1A	-6.70	103.69	106.71
17	A	803	CLA	C4A-NA-C1A	-6.67	103.71	106.71
17	A	838	CLA	C4A-NA-C1A	-6.67	103.71	106.71
17	B	819	CLA	C4A-NA-C1A	-6.65	103.72	106.71
17	A	825	CLA	C4A-NA-C1A	-6.63	103.73	106.71
17	5	314	CLA	C4A-NA-C1A	-6.53	103.77	106.71
17	B	836	CLA	C4A-NA-C1A	-6.43	103.81	106.71
17	A	802	CLA	C4A-NA-C1A	-6.41	103.83	106.71
17	5	309	CLA	C4A-NA-C1A	-6.41	103.83	106.71
17	3	312	CLA	C4A-NA-C1A	-6.39	103.83	106.71
17	A	841	CLA	C4A-NA-C1A	-6.37	103.84	106.71
17	A	809	CLA	C4A-NA-C1A	-6.35	103.85	106.71
17	1	606	CLA	C4A-NA-C1A	-6.34	103.86	106.71
17	B	826	CLA	C4A-NA-C1A	-6.31	103.87	106.71
17	A	821	CLA	C4A-NA-C1A	-6.29	103.88	106.71
17	B	823	CLA	C4A-NA-C1A	-6.27	103.89	106.71
17	J	102	CLA	C4A-NA-C1A	-6.15	103.94	106.71
17	J	101	CLA	C4A-NA-C1A	-6.12	103.95	106.71
17	B	826	CLA	CAA-C2A-C1A	-6.10	98.64	112.14
17	5	315	CLA	C4A-NA-C1A	-6.09	103.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	808	CLA	C4A-NA-C1A	-6.08	103.97	106.71
17	B	801	CLA	C4A-NA-C1A	-6.06	103.98	106.71
17	B	837	CLA	C4A-NA-C1A	-6.06	103.98	106.71
17	B	806	CLA	CAA-C2A-C1A	-6.00	98.86	112.14
17	B	833	CLA	C4A-NA-C1A	-5.99	104.01	106.71
17	8	611	CLA	C4A-NA-C1A	-5.98	104.02	106.71
17	8	608	CLA	C4A-NA-C1A	-5.94	104.03	106.71
17	3	301	CLA	C4A-NA-C1A	-5.91	104.05	106.71
17	4	604	CLA	C4A-NA-C1A	-5.89	104.06	106.71
17	B	829	CLA	C4A-NA-C1A	-5.85	104.08	106.71
17	B	835	CLA	C4A-NA-C1A	-5.84	104.08	106.71
17	6	603	CLA	C4A-NA-C1A	-5.84	104.08	106.71
17	B	830	CLA	C4A-NA-C1A	-5.83	104.08	106.71
17	7	601	CLA	C4A-NA-C1A	-5.82	104.09	106.71
17	A	833	CLA	C4A-NA-C1A	-5.81	104.09	106.71
17	A	817	CLA	C4A-NA-C1A	-5.78	104.11	106.71
17	B	817	CLA	C4A-NA-C1A	-5.78	104.11	106.71
17	B	818	CLA	C4A-NA-C1A	-5.77	104.11	106.71
20	6	607	CHL	C4A-NA-C1A	-5.74	104.12	106.71
17	A	836	CLA	C4A-NA-C1A	-5.73	104.13	106.71
17	5	311	CLA	C4A-NA-C1A	-5.71	104.14	106.71
17	3	309	CLA	C4A-NA-C1A	-5.65	104.17	106.71
17	A	829	CLA	C4A-NA-C1A	-5.63	104.17	106.71
17	A	837	CLA	C4A-NA-C1A	-5.59	104.19	106.71
17	1	605	CLA	C4A-NA-C1A	-5.57	104.20	106.71
17	B	816	CLA	C4A-NA-C1A	-5.57	104.20	106.71
17	B	838	CLA	C4A-NA-C1A	-5.51	104.23	106.71
17	A	806	CLA	C4A-NA-C1A	-5.49	104.24	106.71
17	B	839	CLA	C4A-NA-C1A	-5.49	104.24	106.71
17	3	303	CLA	C4A-NA-C1A	-5.46	104.25	106.71
17	1	607	CLA	C3A-C2A-C1A	-5.43	93.21	101.34
17	A	830	CLA	C4A-NA-C1A	-5.43	104.27	106.71
17	4	605	CLA	C4A-NA-C1A	-5.43	104.27	106.71
17	5	307	CLA	C4A-NA-C1A	-5.43	104.27	106.71
17	8	610	CLA	C4A-NA-C1A	-5.42	104.27	106.71
17	8	604	CLA	C4A-NA-C1A	-5.41	104.27	106.71
17	7	605	CLA	C4A-NA-C1A	-5.40	104.28	106.71
17	A	834	CLA	C4A-NA-C1A	-5.39	104.28	106.71
17	B	809	CLA	C4A-NA-C1A	-5.39	104.28	106.71
17	6	608	CLA	C4A-NA-C1A	-5.39	104.28	106.71
17	B	810	CLA	C4A-NA-C1A	-5.38	104.29	106.71
17	A	812	CLA	C4A-NA-C1A	-5.38	104.29	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	839	CLA	C4A-NA-C1A	-5.38	104.29	106.71
17	6	610	CLA	C4A-NA-C1A	-5.35	104.30	106.71
17	8	613	CLA	C4A-NA-C1A	-5.34	104.31	106.71
17	A	813	CLA	C4A-NA-C1A	-5.32	104.31	106.71
17	F	302	CLA	C4A-NA-C1A	-5.30	104.32	106.71
17	A	810	CLA	C4A-NA-C1A	-5.28	104.33	106.71
17	B	832	CLA	C4A-NA-C1A	-5.27	104.34	106.71
17	A	817	CLA	CAA-C2A-C1A	-5.27	100.48	112.14
17	A	823	CLA	C4A-NA-C1A	-5.26	104.34	106.71
17	7	604	CLA	C4A-NA-C1A	-5.26	104.34	106.71
17	A	818	CLA	C4A-NA-C1A	-5.26	104.34	106.71
17	B	805	CLA	C4A-NA-C1A	-5.26	104.34	106.71
17	5	312	CLA	C4A-NA-C1A	-5.21	104.36	106.71
17	A	811	CLA	C4A-NA-C1A	-5.19	104.37	106.71
17	3	308	CLA	CAA-C2A-C1A	-5.18	100.68	112.14
17	B	828	CLA	C4A-NA-C1A	-5.12	104.41	106.71
17	4	601	CLA	C4A-NA-C1A	-5.12	104.41	106.71
17	B	813	CLA	C4A-NA-C1A	-5.11	104.41	106.71
17	A	832	CLA	C4A-NA-C1A	-5.10	104.41	106.71
17	B	821	CLA	C4A-NA-C1A	-5.09	104.42	106.71
17	B	827	CLA	C4A-NA-C1A	-5.09	104.42	106.71
17	8	601	CLA	C4A-NA-C1A	-5.08	104.42	106.71
17	7	602	CLA	C4A-NA-C1A	-5.06	104.43	106.71
17	1	608	CLA	C4A-NA-C1A	-5.04	104.44	106.71
17	8	609	CLA	C4A-NA-C1A	-5.01	104.45	106.71
17	7	608	CLA	C4A-NA-C1A	-4.97	104.47	106.71
17	8	603	CLA	C4A-NA-C1A	-4.97	104.47	106.71
17	A	826	CLA	C4A-NA-C1A	-4.97	104.47	106.71
17	8	605	CLA	C4A-NA-C1A	-4.96	104.48	106.71
17	A	819	CLA	C4A-NA-C1A	-4.94	104.49	106.71
17	A	814	CLA	C4A-NA-C1A	-4.93	104.49	106.71
17	8	612	CLA	C4A-NA-C1A	-4.90	104.50	106.71
17	8	607	CLA	C4A-NA-C1A	-4.90	104.50	106.71
17	6	609	CLA	C4A-NA-C1A	-4.90	104.50	106.71
17	7	613	CLA	C4A-NA-C1A	-4.89	104.51	106.71
17	B	822	CLA	C4A-NA-C1A	-4.88	104.51	106.71
17	4	602	CLA	C4A-NA-C1A	-4.88	104.51	106.71
17	A	807	CLA	CAA-C2A-C1A	-4.85	101.40	112.14
16	A	801	CL0	C4A-NA-C1A	-4.85	104.53	106.71
17	7	612	CLA	C4A-NA-C1A	-4.83	104.54	106.71
17	6	601	CLA	C4A-NA-C1A	-4.82	104.54	106.71
17	B	811	CLA	C4A-NA-C1A	-4.82	104.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	6	602	CLA	C4A-NA-C1A	-4.82	104.54	106.71
17	B	801	CLA	CAA-C2A-C1A	-4.81	101.49	112.14
17	5	303	CLA	C4A-NA-C1A	-4.80	104.55	106.71
17	A	808	CLA	C4A-NA-C1A	-4.79	104.55	106.71
17	1	610	CLA	C4A-NA-C1A	-4.79	104.55	106.71
17	5	306	CLA	C4A-NA-C1A	-4.77	104.56	106.71
17	7	609	CLA	C4A-NA-C1A	-4.77	104.56	106.71
17	A	827	CLA	C4A-NA-C1A	-4.76	104.57	106.71
17	5	310	CLA	C4A-NA-C1A	-4.76	104.57	106.71
17	3	311	CLA	C4A-NA-C1A	-4.74	104.58	106.71
17	5	304	CLA	C4A-NA-C1A	-4.73	104.58	106.71
17	3	304	CLA	C4A-NA-C1A	-4.72	104.58	106.71
17	A	802	CLA	CAA-C2A-C1A	-4.71	101.71	112.14
17	A	820	CLA	C4A-NA-C1A	-4.71	104.59	106.71
17	1	602	CLA	C4A-NA-C1A	-4.71	104.59	106.71
17	A	828	CLA	C4A-NA-C1A	-4.69	104.60	106.71
17	1	606	CLA	CAA-C2A-C1A	-4.65	101.84	112.14
17	4	603	CLA	C3A-C2A-C1A	-4.64	94.39	101.34
17	A	835	CLA	C4A-NA-C1A	-4.60	104.64	106.71
17	1	603	CLA	C4A-NA-C1A	-4.59	104.64	106.71
17	7	611	CLA	C4A-NA-C1A	-4.55	104.66	106.71
17	7	603	CLA	CHD-C1D-ND	-4.55	120.27	124.45
17	7	614	CLA	CHD-C1D-ND	-4.53	120.29	124.45
17	5	301	CLA	C4A-NA-C1A	-4.52	104.67	106.71
17	A	831	CLA	C4A-NA-C1A	-4.50	104.68	106.71
17	7	608	CLA	CHD-C1D-ND	-4.49	120.33	124.45
17	A	832	CLA	CHC-C1C-C2C	-4.48	119.11	129.77
17	5	302	CLA	C4A-NA-C1A	-4.46	104.70	106.71
17	3	302	CLA	C4A-NA-C1A	-4.46	104.70	106.71
17	A	825	CLA	CHD-C1D-ND	-4.45	120.36	124.45
17	1	606	CLA	CHD-C1D-ND	-4.45	120.37	124.45
17	8	602	CLA	C4A-NA-C1A	-4.42	104.72	106.71
17	B	806	CLA	CHD-C1D-ND	-4.41	120.41	124.45
17	B	814	CLA	C4A-NA-C1A	-4.37	104.74	106.71
17	1	607	CLA	CHD-C1D-ND	-4.36	120.45	124.45
17	3	301	CLA	CHD-C1D-ND	-4.34	120.46	124.45
17	A	815	CLA	C4A-NA-C1A	-4.33	104.76	106.71
17	B	825	CLA	C4A-NA-C1A	-4.32	104.76	106.71
17	6	604	CLA	C4A-NA-C1A	-4.32	104.77	106.71
17	B	818	CLA	CAA-C2A-C1A	-4.30	102.62	112.14
17	4	603	CLA	CHD-C1D-ND	-4.30	120.51	124.45
17	A	804	CLA	CHD-C1D-ND	-4.29	120.51	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	843	CLA	C4A-NA-C1A	-4.29	104.78	106.71
17	B	801	CLA	CHD-C1D-ND	-4.26	120.53	124.45
17	7	610	CLA	CHD-C1D-ND	-4.23	120.56	124.45
17	7	607	CLA	C4A-NA-C1A	-4.22	104.81	106.71
17	3	310	CLA	C3A-C2A-C1A	-4.20	94.53	101.64
17	5	309	CLA	CHD-C1D-ND	-4.19	120.60	124.45
17	B	807	CLA	CHD-C1D-ND	-4.19	120.61	124.45
17	5	308	CLA	CHD-C1D-ND	-4.18	120.61	124.45
17	4	602	CLA	CHD-C1D-ND	-4.18	120.61	124.45
16	A	801	CL0	CHD-C1D-ND	-4.18	120.61	124.45
17	8	608	CLA	CHD-C1D-ND	-4.18	120.61	124.45
17	3	310	CLA	CHD-C1D-ND	-4.17	120.62	124.45
17	5	308	CLA	C4A-NA-C1A	-4.17	104.83	106.71
17	6	603	CLA	CHD-C1D-ND	-4.17	120.63	124.45
17	B	831	CLA	CAA-C2A-C1A	-4.14	102.98	112.14
17	A	802	CLA	CHD-C1D-ND	-4.12	120.67	124.45
17	8	610	CLA	CHD-C1D-ND	-4.10	120.69	124.45
17	B	837	CLA	CHD-C1D-ND	-4.09	120.69	124.45
17	B	805	CLA	CHD-C1D-ND	-4.09	120.69	124.45
20	5	305	CHL	C2A-C1A-CHA	4.08	130.99	123.86
17	B	812	CLA	C3A-C2A-C1A	-4.07	95.24	101.34
17	B	812	CLA	CAA-C2A-C1A	-4.07	103.14	112.14
17	1	604	CLA	C4A-NA-C1A	-4.06	104.88	106.71
17	B	826	CLA	CHD-C1D-ND	-4.05	120.73	124.45
17	B	813	CLA	CHD-C1D-ND	-4.04	120.74	124.45
17	B	831	CLA	CHD-C1D-ND	-4.04	120.75	124.45
17	8	603	CLA	CHD-C1D-ND	-4.03	120.75	124.45
17	3	312	CLA	CHD-C1D-ND	-4.03	120.75	124.45
17	B	829	CLA	CHD-C1D-ND	-4.02	120.76	124.45
17	A	819	CLA	CHD-C1D-ND	-4.02	120.76	124.45
17	B	836	CLA	CHD-C1D-ND	-4.02	120.76	124.45
17	B	804	CLA	CHD-C1D-ND	-4.01	120.77	124.45
17	5	306	CLA	CHD-C1D-ND	-4.01	120.77	124.45
17	7	611	CLA	CHD-C1D-ND	-3.99	120.78	124.45
17	J	102	CLA	CHD-C1D-ND	-3.99	120.79	124.45
17	B	812	CLA	CHD-C1D-ND	-3.97	120.81	124.45
17	A	834	CLA	CHD-C1D-ND	-3.97	120.81	124.45
17	A	805	CLA	CHD-C1D-ND	-3.96	120.81	124.45
17	1	602	CLA	CHD-C1D-ND	-3.96	120.82	124.45
17	3	313	CLA	CAA-C2A-C1A	-3.95	103.39	112.14
17	1	609	CLA	C4A-NA-C1A	-3.95	104.93	106.71
17	B	830	CLA	CHD-C1D-ND	-3.93	120.84	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	304	CLA	CHD-C1D-ND	-3.93	120.84	124.45
17	B	810	CLA	CHD-C1D-ND	-3.92	120.85	124.45
17	3	303	CLA	CHD-C1D-ND	-3.92	120.85	124.45
17	B	824	CLA	CHD-C1D-ND	-3.91	120.86	124.45
17	A	817	CLA	CHD-C1D-ND	-3.89	120.88	124.45
17	A	821	CLA	CHD-C1D-ND	-3.89	120.88	124.45
17	B	802	CLA	CHD-C1D-ND	-3.89	120.88	124.45
17	8	611	CLA	CHD-C1D-ND	-3.89	120.88	124.45
17	B	819	CLA	CHC-C1C-NC	3.88	130.09	124.20
17	3	309	CLA	CHD-C1D-ND	-3.88	120.89	124.45
17	5	314	CLA	CHD-C1D-ND	-3.88	120.89	124.45
17	3	306	CLA	CHD-C1D-ND	-3.86	120.91	124.45
17	6	608	CLA	CHD-C1D-ND	-3.85	120.92	124.45
17	A	809	CLA	CHD-C1D-ND	-3.85	120.92	124.45
17	B	815	CLA	CHD-C1D-ND	-3.84	120.92	124.45
17	A	833	CLA	CHD-C1D-ND	-3.84	120.92	124.45
17	B	828	CLA	CHD-C1D-ND	-3.84	120.93	124.45
17	A	836	CLA	CHD-C1D-ND	-3.84	120.93	124.45
17	A	818	CLA	CHD-C1D-ND	-3.84	120.93	124.45
17	B	810	CLA	C1B-CHB-C4A	-3.83	122.53	130.12
17	7	610	CLA	C3A-C2A-C1A	-3.82	95.18	101.64
17	3	313	CLA	CHD-C1D-ND	-3.82	120.95	124.45
17	5	307	CLA	CHD-C1D-ND	-3.82	120.95	124.45
17	A	824	CLA	CAA-C2A-C1A	-3.82	103.69	112.14
17	F	302	CLA	CHD-C1D-ND	-3.81	120.95	124.45
17	B	827	CLA	CHD-C1D-ND	-3.81	120.96	124.45
17	A	822	CLA	CHD-C1D-ND	-3.80	120.96	124.45
17	3	308	CLA	CHD-C1D-ND	-3.79	120.97	124.45
17	8	607	CLA	CHD-C1D-ND	-3.79	120.97	124.45
17	7	609	CLA	CHD-C1D-ND	-3.79	120.97	124.45
17	8	602	CLA	CHD-C1D-ND	-3.78	120.98	124.45
17	B	816	CLA	CHD-C1D-ND	-3.77	120.98	124.45
17	A	823	CLA	CAA-C2A-C1A	-3.77	103.79	112.14
17	A	829	CLA	CHD-C1D-ND	-3.77	120.99	124.45
17	J	101	CLA	CHD-C1D-ND	-3.77	120.99	124.45
17	8	609	CLA	CHD-C1D-ND	-3.77	120.99	124.45
17	5	315	CLA	CHD-C1D-ND	-3.76	121.00	124.45
17	4	601	CLA	CHD-C1D-ND	-3.76	121.00	124.45
17	B	809	CLA	CHD-C1D-ND	-3.75	121.01	124.45
17	A	806	CLA	CHD-C1D-ND	-3.74	121.02	124.45
17	B	814	CLA	CHD-C1D-ND	-3.74	121.02	124.45
17	B	839	CLA	CHD-C1D-ND	-3.73	121.02	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	310	CLA	C1B-CHB-C4A	-3.73	122.73	130.12
20	6	607	CHL	CAA-C2A-C1A	3.73	120.40	112.14
17	A	823	CLA	CHD-C1D-ND	-3.73	121.03	124.45
17	7	611	CLA	C1D-ND-C4D	-3.72	103.69	106.33
17	6	602	CLA	CHD-C1D-ND	-3.72	121.03	124.45
17	A	820	CLA	CHD-C1D-ND	-3.72	121.03	124.45
17	A	816	CLA	C4A-NA-C1A	-3.72	105.03	106.71
17	3	310	CLA	C2A-C3A-C4A	-3.72	97.04	101.78
17	A	811	CLA	CHD-C1D-ND	-3.71	121.04	124.45
17	7	613	CLA	CHD-C1D-ND	-3.71	121.04	124.45
17	1	604	CLA	CHD-C1D-ND	-3.70	121.06	124.45
20	6	606	CHL	C1B-CHB-C4A	-3.70	122.80	130.12
17	A	841	CLA	CHD-C1D-ND	-3.69	121.06	124.45
17	A	830	CLA	CAA-C2A-C1A	-3.69	103.96	112.14
16	A	801	CL0	CHC-C1C-NC	3.69	129.81	124.20
17	A	816	CLA	CHD-C1D-ND	-3.69	121.06	124.45
17	1	602	CLA	C1D-ND-C4D	-3.68	103.72	106.33
17	A	830	CLA	CHD-C1D-ND	-3.68	121.07	124.45
17	A	838	CLA	CHD-C1D-ND	-3.67	121.08	124.45
17	B	820	CLA	CHD-C1D-ND	-3.67	121.08	124.45
17	7	602	CLA	CHD-C1D-ND	-3.66	121.09	124.45
17	5	301	CLA	CHD-C1D-ND	-3.65	121.10	124.45
20	Z	601	CHL	C1B-CHB-C4A	-3.65	122.89	130.12
17	A	815	CLA	C1D-ND-C4D	-3.65	103.74	106.33
17	B	811	CLA	CHD-C1D-ND	-3.64	121.11	124.45
17	A	813	CLA	CHD-C1D-ND	-3.63	121.12	124.45
17	B	818	CLA	CHD-C1D-ND	-3.61	121.13	124.45
20	1	601	CHL	C1B-CHB-C4A	-3.61	122.96	130.12
17	A	807	CLA	CHD-C1D-ND	-3.61	121.14	124.45
17	7	607	CLA	CHD-C1D-ND	-3.61	121.14	124.45
17	A	814	CLA	CHD-C1D-ND	-3.61	121.14	124.45
17	F	301	CLA	CHD-C1D-ND	-3.61	121.14	124.45
17	A	842	CLA	CHD-C1D-ND	-3.60	121.14	124.45
17	A	824	CLA	CHD-C1D-ND	-3.60	121.14	124.45
17	7	608	CLA	C1D-ND-C4D	-3.59	103.78	106.33
17	1	605	CLA	C2C-C1C-NC	3.59	113.33	109.97
17	B	802	CLA	C3A-C2A-C1A	-3.59	95.97	101.34
20	8	606	CHL	C1B-CHB-C4A	-3.59	123.01	130.12
17	5	302	CLA	C2C-C1C-NC	3.58	113.33	109.97
17	A	810	CLA	CHD-C1D-ND	-3.58	121.16	124.45
17	8	603	CLA	C1D-ND-C4D	-3.58	103.79	106.33
17	A	826	CLA	CHD-C1D-ND	-3.58	121.16	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	8	604	CLA	CHD-C1D-ND	-3.58	121.17	124.45
17	A	803	CLA	CHD-C1D-ND	-3.57	121.17	124.45
17	A	833	CLA	C1D-ND-C4D	-3.57	103.80	106.33
17	B	834	CLA	CHD-C1D-ND	-3.56	121.18	124.45
20	6	605	CHL	C1B-CHB-C4A	-3.56	123.08	130.12
17	A	835	CLA	C2C-C1C-NC	3.54	113.29	109.97
17	A	815	CLA	CHD-C1D-ND	-3.53	121.21	124.45
17	4	602	CLA	C1D-ND-C4D	-3.53	103.83	106.33
17	B	825	CLA	CHD-C1D-ND	-3.53	121.21	124.45
17	B	833	CLA	CHD-C1D-ND	-3.53	121.21	124.45
17	5	303	CLA	CHD-C1D-ND	-3.53	121.21	124.45
17	A	832	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	B	823	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	3	302	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	B	808	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	8	612	CLA	CHD-C1D-ND	-3.52	121.22	124.45
17	A	820	CLA	C1D-ND-C4D	-3.51	103.84	106.33
17	A	837	CLA	CHD-C1D-ND	-3.51	121.22	124.45
17	8	614	CLA	CHD-C1D-ND	-3.51	121.22	124.45
17	3	305	CLA	CHD-C1D-ND	-3.51	121.22	124.45
17	7	604	CLA	CHD-C1D-ND	-3.51	121.23	124.45
17	B	806	CLA	C1D-ND-C4D	-3.51	103.84	106.33
17	8	611	CLA	C1D-ND-C4D	-3.50	103.85	106.33
20	5	305	CHL	CHA-C1A-NA	-3.50	118.39	126.40
17	B	817	CLA	CHD-C1D-ND	-3.49	121.25	124.45
20	6	605	CHL	CMB-C2B-C1B	-3.48	123.12	128.46
17	7	601	CLA	C2C-C1C-NC	3.48	113.23	109.97
17	6	602	CLA	C1D-ND-C4D	-3.48	103.87	106.33
17	6	603	CLA	C1D-ND-C4D	-3.47	103.87	106.33
17	8	601	CLA	C2C-C1C-NC	3.47	113.22	109.97
20	7	606	CHL	C1B-CHB-C4A	-3.47	123.25	130.12
20	5	305	CHL	C1B-CHB-C4A	-3.46	123.26	130.12
17	3	311	CLA	CHD-C1D-ND	-3.46	121.28	124.45
17	6	609	CLA	CHD-C1D-ND	-3.45	121.28	124.45
17	A	828	CLA	CHD-C1D-ND	-3.45	121.28	124.45
17	B	822	CLA	CHD-C1D-ND	-3.44	121.29	124.45
17	5	312	CLA	CHD-C1D-ND	-3.44	121.30	124.45
17	7	603	CLA	C1D-ND-C4D	-3.44	103.89	106.33
17	B	832	CLA	CHD-C1D-ND	-3.43	121.31	124.45
17	1	608	CLA	CHD-C1D-ND	-3.42	121.31	124.45
17	B	835	CLA	CHD-C1D-ND	-3.42	121.31	124.45
17	6	601	CLA	CHD-C1D-ND	-3.41	121.32	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	302	CLA	CHD-C1D-ND	-3.41	121.32	124.45
17	A	812	CLA	CHD-C1D-ND	-3.41	121.32	124.45
20	3	307	CHL	C1B-CHB-C4A	-3.40	123.38	130.12
17	7	609	CLA	CAA-C2A-C1A	-3.40	104.62	112.14
20	5	313	CHL	C1B-CHB-C4A	-3.40	123.39	130.12
17	A	808	CLA	CHD-C1D-ND	-3.39	121.34	124.45
17	B	807	CLA	CAA-C2A-C1A	-3.39	104.64	112.14
17	B	821	CLA	CHD-C1D-ND	-3.38	121.34	124.45
17	A	839	CLA	CHD-C1D-ND	-3.38	121.35	124.45
20	Z	601	CHL	CHD-C1D-ND	-3.38	121.35	124.45
17	6	604	CLA	CHD-C1D-ND	-3.38	121.35	124.45
20	7	606	CHL	CHD-C1D-ND	-3.38	121.35	124.45
20	1	601	CHL	CHD-C1D-ND	-3.38	121.35	124.45
17	B	812	CLA	C1B-CHB-C4A	-3.38	123.43	130.12
17	1	603	CLA	CHD-C1D-ND	-3.36	121.36	124.45
17	8	608	CLA	C1D-ND-C4D	-3.35	103.95	106.33
17	A	803	CLA	C2C-C1C-NC	3.35	113.11	109.97
17	5	314	CLA	C1B-CHB-C4A	-3.34	123.51	130.12
17	A	813	CLA	C1D-ND-C4D	-3.33	103.97	106.33
17	1	609	CLA	CHD-C1D-ND	-3.32	121.40	124.45
17	A	839	CLA	C2C-C1C-NC	3.32	113.08	109.97
17	5	311	CLA	CHD-C1D-ND	-3.32	121.40	124.45
17	B	807	CLA	C1D-ND-C4D	-3.31	103.98	106.33
17	A	829	CLA	C1D-ND-C4D	-3.31	103.98	106.33
17	A	805	CLA	C1D-ND-C4D	-3.31	103.98	106.33
17	J	101	CLA	C1D-ND-C4D	-3.31	103.99	106.33
17	B	814	CLA	C1D-ND-C4D	-3.30	103.99	106.33
17	B	821	CLA	C1D-ND-C4D	-3.30	103.99	106.33
17	5	309	CLA	C1D-ND-C4D	-3.30	103.99	106.33
17	B	836	CLA	C2C-C1C-NC	3.30	113.06	109.97
17	B	815	CLA	C3A-C2A-C1A	-3.30	96.40	101.34
17	8	601	CLA	CHD-C1D-ND	-3.29	121.43	124.45
17	7	605	CLA	CHD-C1D-ND	-3.28	121.44	124.45
17	5	308	CLA	C1B-CHB-C4A	-3.28	123.63	130.12
17	3	301	CLA	C1D-ND-C4D	-3.27	104.01	106.33
17	3	302	CLA	C1D-ND-C4D	-3.27	104.01	106.33
17	8	610	CLA	C1B-CHB-C4A	-3.27	123.63	130.12
17	7	614	CLA	C3A-C2A-C1A	-3.27	96.45	101.34
17	B	811	CLA	CAA-C2A-C1A	-3.26	104.92	112.14
16	A	801	CL0	CHC-C1C-C2C	-3.26	117.69	126.72
17	A	843	CLA	CHD-C1D-ND	-3.26	121.46	124.45
17	4	601	CLA	C2C-C1C-NC	3.26	113.02	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	8	605	CLA	C2C-C1C-NC	3.25	113.02	109.97
17	4	603	CLA	C1B-CHB-C4A	-3.25	123.67	130.12
17	B	838	CLA	CHD-C1D-ND	-3.25	121.47	124.45
17	3	306	CLA	C3A-C2A-C1A	-3.25	96.47	101.34
17	A	825	CLA	C1D-ND-C4D	-3.25	104.03	106.33
17	5	310	CLA	CHD-C1D-ND	-3.25	121.47	124.45
17	8	613	CLA	CHD-C1D-ND	-3.25	121.47	124.45
17	1	610	CLA	CHD-C1D-ND	-3.24	121.47	124.45
20	6	606	CHL	CHD-C1D-ND	-3.24	121.47	124.45
17	5	306	CLA	C1D-ND-C4D	-3.23	104.04	106.33
17	A	804	CLA	C1B-CHB-C4A	-3.23	123.71	130.12
17	B	804	CLA	C1B-CHB-C4A	-3.23	123.71	130.12
17	B	802	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
17	B	806	CLA	C3A-C2A-C1A	-3.22	96.51	101.34
17	3	312	CLA	CAA-C2A-C1A	-3.22	105.00	112.14
20	5	313	CHL	CHD-C1D-ND	-3.22	121.50	124.45
20	6	605	CHL	CHD-C1D-ND	-3.22	121.50	124.45
17	A	827	CLA	CHD-C1D-ND	-3.21	121.50	124.45
20	5	313	CHL	CMB-C2B-C1B	-3.21	123.53	128.46
17	8	602	CLA	C1D-ND-C4D	-3.20	104.06	106.33
17	7	601	CLA	CHD-C1D-ND	-3.19	121.52	124.45
17	3	306	CLA	CAA-C2A-C1A	-3.19	105.08	112.14
17	A	812	CLA	C2C-C1C-NC	3.19	112.96	109.97
17	4	604	CLA	CHD-C1D-ND	-3.19	121.53	124.45
17	8	613	CLA	C2C-C1C-NC	3.19	112.96	109.97
17	B	822	CLA	C2C-C1C-NC	3.18	112.95	109.97
17	B	817	CLA	C2C-C1C-NC	3.18	112.95	109.97
20	6	607	CHL	CHD-C1D-ND	-3.18	121.54	124.45
17	A	831	CLA	CHD-C1D-ND	-3.17	121.54	124.45
17	B	813	CLA	C1D-ND-C4D	-3.17	104.08	106.33
17	3	305	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
17	5	301	CLA	C1D-ND-C4D	-3.16	104.09	106.33
17	B	830	CLA	C1D-ND-C4D	-3.16	104.09	106.33
17	J	101	CLA	CAA-C2A-C1A	-3.16	105.15	112.14
17	A	806	CLA	C1D-ND-C4D	-3.16	104.09	106.33
17	1	608	CLA	C1D-ND-C4D	-3.16	104.09	106.33
17	3	308	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
17	7	612	CLA	CHD-C1D-ND	-3.15	121.56	124.45
20	6	607	CHL	C1B-CHB-C4A	-3.15	123.89	130.12
20	3	307	CHL	CHA-C1A-NA	-3.15	119.19	126.40
20	6	607	CHL	CHA-C1A-NA	-3.14	119.20	126.40
17	B	825	CLA	C1D-ND-C4D	-3.14	104.10	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	609	CLA	C1D-ND-C4D	-3.14	104.10	106.33
17	8	602	CLA	C2C-C1C-NC	3.14	112.91	109.97
17	A	802	CLA	C1D-ND-C4D	-3.13	104.11	106.33
17	1	603	CLA	C1D-ND-C4D	-3.13	104.11	106.33
17	A	818	CLA	C2C-C1C-NC	3.13	112.90	109.97
17	4	605	CLA	C2C-C1C-NC	3.13	112.90	109.97
17	B	832	CLA	C1D-ND-C4D	-3.13	104.11	106.33
20	5	305	CHL	C2C-C3C-C4C	3.13	108.72	106.49
17	B	815	CLA	CAA-C2A-C1A	-3.13	101.73	111.97
17	3	313	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
17	A	835	CLA	CHD-C1D-ND	-3.12	121.59	124.45
17	7	605	CLA	C2C-C1C-NC	3.12	112.89	109.97
17	A	811	CLA	C1D-ND-C4D	-3.11	104.12	106.33
17	B	838	CLA	C2C-C1C-NC	3.11	112.88	109.97
17	B	818	CLA	C2C-C1C-NC	3.11	112.88	109.97
20	1	601	CHL	CMB-C2B-C1B	-3.10	123.69	128.46
17	B	837	CLA	C1D-ND-C4D	-3.10	104.13	106.33
20	Z	601	CHL	CMB-C2B-C1B	-3.10	123.70	128.46
17	J	102	CLA	C1D-ND-C4D	-3.10	104.13	106.33
17	6	609	CLA	C2C-C1C-NC	3.10	112.88	109.97
17	8	607	CLA	C2C-C1C-NC	3.10	112.87	109.97
17	7	608	CLA	CHC-C1C-NC	3.09	128.90	124.20
17	J	102	CLA	CAA-C2A-C1A	-3.09	105.30	112.14
17	A	834	CLA	C1D-ND-C4D	-3.09	104.14	106.33
17	B	826	CLA	C1D-ND-C4D	-3.08	104.14	106.33
17	1	605	CLA	CHD-C1D-ND	-3.08	121.62	124.45
16	A	801	CL0	C1D-ND-C4D	-3.07	104.15	106.33
17	A	838	CLA	C1D-ND-C4D	-3.07	104.15	106.33
17	A	830	CLA	C1D-ND-C4D	-3.07	104.16	106.33
17	6	601	CLA	C2C-C1C-NC	3.07	112.84	109.97
17	5	303	CLA	C1D-ND-C4D	-3.06	104.16	106.33
17	A	827	CLA	C2C-C1C-NC	3.06	112.84	109.97
17	B	809	CLA	CHC-C1C-NC	3.05	128.84	124.20
17	A	829	CLA	C2C-C1C-NC	3.05	112.83	109.97
20	8	606	CHL	CHA-C1A-NA	-3.05	119.41	126.40
17	B	808	CLA	C2C-C1C-NC	3.05	112.83	109.97
17	B	809	CLA	CHC-C1C-C2C	-3.05	118.30	126.72
17	A	833	CLA	C2C-C1C-NC	3.05	112.83	109.97
17	A	821	CLA	C3A-C2A-C1A	-3.04	96.78	101.34
17	A	808	CLA	C2C-C1C-NC	3.04	112.82	109.97
17	8	612	CLA	C1D-ND-C4D	-3.04	104.18	106.33
17	5	302	CLA	CHC-C1C-C2C	-3.04	118.32	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	302	CLA	C2C-C1C-NC	3.03	112.81	109.97
17	B	818	CLA	C1D-ND-C4D	-3.03	104.18	106.33
17	B	805	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
17	7	602	CLA	C1D-ND-C4D	-3.02	104.19	106.33
17	B	831	CLA	C1D-ND-C4D	-3.02	104.19	106.33
17	8	607	CLA	C1D-ND-C4D	-3.02	104.19	106.33
17	7	614	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
17	7	601	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
20	5	305	CHL	CAA-C2A-C1A	3.01	121.84	111.97
17	8	605	CLA	CHD-C1D-ND	-3.01	121.69	124.45
20	6	607	CHL	CMB-C2B-C1B	-3.01	123.84	128.46
17	1	604	CLA	CAA-C2A-C1A	-3.01	105.48	112.14
20	5	305	CHL	CHD-C1D-ND	-3.01	121.69	124.45
17	A	823	CLA	C2C-C1C-NC	3.00	112.79	109.97
17	A	839	CLA	CHC-C1C-C2C	-3.00	118.41	126.72
17	5	309	CLA	CAA-C2A-C1A	-3.00	105.50	112.14
17	B	820	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
17	A	817	CLA	C1D-ND-C4D	-3.00	104.20	106.33
17	B	827	CLA	C1D-ND-C4D	-2.99	104.21	106.33
17	8	612	CLA	C2C-C1C-NC	2.99	112.77	109.97
20	7	606	CHL	CHA-C1A-NA	-2.99	119.55	126.40
17	B	816	CLA	C2C-C1C-NC	2.99	112.77	109.97
17	1	609	CLA	CHC-C1C-NC	2.98	128.73	124.20
17	A	810	CLA	C1D-ND-C4D	-2.98	104.22	106.33
17	8	601	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
17	7	610	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
17	A	813	CLA	C2C-C1C-NC	2.98	112.76	109.97
17	B	834	CLA	C2C-C1C-NC	2.98	112.76	109.97
17	A	821	CLA	C1-C2-C3	-2.98	120.89	126.04
17	A	814	CLA	C1D-ND-C4D	-2.98	104.22	106.33
17	3	312	CLA	C1D-ND-C4D	-2.98	104.22	106.33
20	8	606	CHL	CMB-C2B-C1B	-2.97	123.89	128.46
17	B	801	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
17	4	601	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
17	A	816	CLA	CHC-C1C-NC	2.97	128.70	124.20
17	A	835	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
17	A	825	CLA	CAA-C2A-C1A	-2.96	105.59	112.14
17	B	830	CLA	C2C-C1C-NC	2.96	112.74	109.97
17	1	602	CLA	CAA-C2A-C1A	-2.96	105.60	112.14
17	5	315	CLA	C1D-ND-C4D	-2.95	104.24	106.33
17	B	836	CLA	C1D-ND-C4D	-2.95	104.24	106.33
20	3	307	CHL	CAA-C2A-C1A	2.94	121.62	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	812	CLA	C1D-ND-C4D	-2.94	104.24	106.33
17	7	611	CLA	C2C-C1C-NC	2.94	112.73	109.97
17	F	301	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
20	3	307	CHL	CHD-C1D-ND	-2.94	121.76	124.45
20	6	606	CHL	CHA-C1A-NA	-2.93	119.69	126.40
17	5	315	CLA	C2C-C1C-NC	2.93	112.72	109.97
20	3	307	CHL	CMB-C2B-C1B	-2.93	123.97	128.46
17	7	613	CLA	C2C-C1C-NC	2.92	112.71	109.97
17	1	604	CLA	C1D-ND-C4D	-2.92	104.26	106.33
17	6	609	CLA	C1D-ND-C4D	-2.92	104.26	106.33
17	6	602	CLA	C2C-C1C-NC	2.92	112.71	109.97
17	7	604	CLA	CHA-C1A-NA	-2.92	119.72	126.40
17	7	613	CLA	C1D-ND-C4D	-2.92	104.26	106.33
17	8	603	CLA	CHC-C1C-NC	2.91	128.62	124.20
17	6	609	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
20	6	606	CHL	CMB-C2B-C1B	-2.91	123.99	128.46
17	3	308	CLA	C3A-C2A-C1A	-2.91	96.98	101.34
17	1	607	CLA	C1D-ND-C4D	-2.91	104.27	106.33
17	1	609	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
17	A	823	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
17	8	614	CLA	C1D-ND-C4D	-2.90	104.27	106.33
17	5	312	CLA	C2C-C1C-NC	2.90	112.69	109.97
17	1	603	CLA	C2C-C1C-NC	2.90	112.69	109.97
17	3	305	CLA	CAA-C2A-C1A	-2.90	105.72	112.14
17	A	838	CLA	C2C-C1C-NC	2.90	112.69	109.97
17	3	309	CLA	C1D-ND-C4D	-2.90	104.28	106.33
17	B	816	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
17	1	605	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
17	5	304	CLA	C2C-C1C-NC	2.89	112.68	109.97
17	B	817	CLA	C1D-ND-C4D	-2.89	104.28	106.33
17	6	610	CLA	C2C-C1C-NC	2.88	112.67	109.97
17	A	832	CLA	CHC-C1C-NC	2.88	128.58	124.20
17	A	821	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
17	A	816	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
17	A	827	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
17	1	610	CLA	C1D-ND-C4D	-2.88	104.29	106.33
17	A	804	CLA	C1D-ND-C4D	-2.88	104.29	106.33
17	B	839	CLA	C1D-ND-C4D	-2.87	104.29	106.33
17	A	837	CLA	C2C-C1C-NC	2.87	112.66	109.97
20	6	605	CHL	CAA-C2A-C1A	2.87	118.50	112.14
17	8	609	CLA	C1D-ND-C4D	-2.87	104.30	106.33
17	5	304	CLA	CHD-C1D-ND	-2.87	121.82	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	606	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
17	A	815	CLA	CGD-CBD-CAD	-2.87	101.44	110.73
17	4	601	CLA	C1D-ND-C4D	-2.87	104.30	106.33
17	A	818	CLA	C1D-ND-C4D	-2.87	104.30	106.33
17	4	604	CLA	C2C-C1C-NC	2.86	112.65	109.97
17	B	819	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
17	A	831	CLA	C1D-ND-C4D	-2.86	104.31	106.33
17	7	608	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
20	7	606	CHL	CMB-C2B-C1B	-2.85	124.08	128.46
17	8	607	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
17	A	816	CLA	C1D-ND-C4D	-2.85	104.31	106.33
17	B	817	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
17	8	604	CLA	C1D-ND-C4D	-2.85	104.31	106.33
17	A	804	CLA	C2A-C3A-C4A	-2.85	97.27	101.87
17	8	602	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
17	1	607	CLA	CHA-C1A-NA	-2.85	119.88	126.40
17	B	837	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
17	A	803	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
17	A	818	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
17	1	602	CLA	C2C-C1C-NC	2.84	112.63	109.97
17	3	311	CLA	C1D-ND-C4D	-2.84	104.32	106.33
17	3	305	CLA	C2C-C1C-NC	2.83	112.63	109.97
17	B	822	CLA	CHC-C1C-C2C	-2.83	118.88	126.72
17	3	303	CLA	C2C-C1C-NC	2.83	112.62	109.97
17	B	816	CLA	CHC-C1C-NC	2.83	128.50	124.20
17	6	604	CLA	C1D-ND-C4D	-2.83	104.33	106.33
17	B	837	CLA	C2C-C1C-NC	2.83	112.62	109.97
17	B	836	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
17	5	302	CLA	CHA-C1A-NA	-2.83	119.92	126.40
17	3	304	CLA	CHC-C1C-NC	2.82	128.48	124.20
17	J	101	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
17	A	815	CLA	CHC-C1C-NC	2.82	128.47	124.20
17	A	820	CLA	CHC-C1C-NC	2.82	128.47	124.20
17	B	823	CLA	C2C-C1C-NC	2.81	112.61	109.97
17	B	835	CLA	C2C-C1C-NC	2.81	112.61	109.97
17	7	611	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
17	A	808	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
17	7	602	CLA	C2C-C1C-NC	2.81	112.60	109.97
17	8	612	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
17	6	609	CLA	CHC-C1C-NC	2.80	128.46	124.20
17	3	304	CLA	CHC-C1C-C2C	-2.80	118.96	126.72
17	A	834	CLA	CHC-C1C-NC	2.80	128.46	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	309	CLA	C2C-C1C-NC	2.80	112.60	109.97
17	5	310	CLA	C1D-ND-C4D	-2.80	104.35	106.33
17	B	831	CLA	CHC-C1C-NC	2.80	128.45	124.20
17	A	829	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
17	A	834	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
17	5	314	CLA	C1D-ND-C4D	-2.80	104.35	106.33
17	4	601	CLA	CHC-C1C-NC	2.80	128.45	124.20
17	A	823	CLA	CHC-C1C-NC	2.80	128.45	124.20
17	B	813	CLA	CHC-C1C-NC	2.80	128.44	124.20
20	8	606	CHL	CHD-C1D-ND	-2.79	121.89	124.45
17	A	836	CLA	C1D-ND-C4D	-2.79	104.35	106.33
17	8	608	CLA	C2C-C1C-NC	2.79	112.58	109.97
17	B	815	CLA	C1D-ND-C4D	-2.79	104.36	106.33
17	1	610	CLA	C2C-C1C-NC	2.79	112.58	109.97
20	8	606	CHL	CAA-C2A-C1A	2.79	118.31	112.14
17	8	603	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
17	B	801	CLA	C2C-C1C-NC	2.79	112.58	109.97
17	7	612	CLA	CHC-C1C-C2C	-2.79	119.02	126.72
17	8	613	CLA	CHC-C1C-C2C	-2.79	119.02	126.72
17	B	838	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
17	J	101	CLA	CHC-C1C-NC	2.78	128.43	124.20
17	3	301	CLA	CHC-C1C-NC	2.78	128.42	124.20
17	B	809	CLA	CAC-C3C-C4C	2.78	128.42	124.81
17	B	839	CLA	C2C-C1C-NC	2.78	112.58	109.97
17	1	607	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
17	1	609	CLA	C1D-ND-C4D	-2.78	104.36	106.33
17	6	610	CLA	CHA-C1A-NA	-2.77	120.05	126.40
17	6	601	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
17	7	610	CLA	CAA-C2A-C1A	-2.77	104.96	111.81
17	B	830	CLA	CAA-C2A-C1A	-2.77	106.00	112.14
17	7	607	CLA	C1D-ND-C4D	-2.77	104.37	106.33
17	J	101	CLA	C2C-C1C-NC	2.77	112.57	109.97
20	6	605	CHL	CHA-C1A-NA	-2.77	120.05	126.40
17	A	827	CLA	CHC-C1C-NC	2.77	128.40	124.20
17	A	836	CLA	C2C-C1C-NC	2.77	112.57	109.97
17	B	832	CLA	C2C-C1C-NC	2.77	112.57	109.97
17	B	828	CLA	C1D-ND-C4D	-2.77	104.37	106.33
17	1	610	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
17	8	611	CLA	C2C-C1C-NC	2.76	112.56	109.97
17	6	610	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
17	B	806	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
17	7	603	CLA	CHC-C1C-NC	2.76	128.39	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	822	CLA	CAA-C2A-C1A	-2.76	106.04	112.14
17	A	822	CLA	C1D-ND-C4D	-2.75	104.38	106.33
17	A	805	CLA	C2C-C1C-NC	2.75	112.55	109.97
20	5	313	CHL	CHA-C1A-NA	-2.75	120.10	126.40
17	7	601	CLA	CHC-C1C-NC	2.75	128.38	124.20
17	A	832	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
17	7	613	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
17	4	605	CLA	CHD-C1D-ND	-2.75	121.93	124.45
17	A	803	CLA	C1D-ND-C4D	-2.75	104.38	106.33
17	1	606	CLA	C1D-ND-C4D	-2.75	104.38	106.33
17	B	808	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
17	A	817	CLA	C3A-C2A-C1A	-2.75	97.23	101.34
17	A	808	CLA	C1D-ND-C4D	-2.75	104.38	106.33
17	B	807	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
17	3	303	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
17	B	831	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
17	B	834	CLA	C1D-ND-C4D	-2.74	104.39	106.33
17	A	839	CLA	CHC-C1C-NC	2.74	128.36	124.20
17	6	603	CLA	C2C-C1C-NC	2.74	112.54	109.97
17	5	315	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
17	3	311	CLA	C2C-C1C-NC	2.74	112.53	109.97
17	A	811	CLA	C2C-C1C-NC	2.73	112.53	109.97
17	8	604	CLA	C2C-C1C-NC	2.73	112.53	109.97
17	B	837	CLA	CAA-C2A-C1A	-2.73	106.09	112.14
17	4	603	CLA	C1D-ND-C4D	-2.73	104.39	106.33
17	B	804	CLA	C3A-C2A-C1A	-2.73	97.25	101.34
17	3	311	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
17	A	816	CLA	C2C-C1C-NC	2.73	112.53	109.97
17	A	812	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
17	7	602	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
17	6	608	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
17	7	604	CLA	C2C-C1C-NC	2.73	112.53	109.97
17	A	826	CLA	CHC-C1C-NC	2.73	128.34	124.20
17	4	604	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
17	B	824	CLA	CAA-C2A-C1A	-2.73	105.08	111.81
17	5	302	CLA	CHC-C1C-NC	2.73	128.34	124.20
17	B	816	CLA	C1D-ND-C4D	-2.73	104.40	106.33
17	A	809	CLA	C1D-ND-C4D	-2.72	104.40	106.33
17	4	602	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
17	B	804	CLA	CHC-C1C-NC	2.72	128.33	124.20
17	B	809	CLA	C1D-ND-C4D	-2.72	104.40	106.33
17	A	810	CLA	CHC-C1C-NC	2.72	128.32	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	304	CLA	CHC-C1C-C2C	-2.71	119.21	126.72
17	7	612	CLA	CHC-C1C-NC	2.71	128.32	124.20
17	3	304	CLA	C1D-ND-C4D	-2.71	104.41	106.33
17	B	826	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
17	A	821	CLA	C1D-ND-C4D	-2.71	104.41	106.33
17	7	611	CLA	CHC-C1C-NC	2.71	128.31	124.20
17	A	805	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
17	B	837	CLA	CHC-C1C-NC	2.71	128.31	124.20
17	F	302	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
17	B	833	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
17	A	837	CLA	CHC-C1C-C2C	-2.71	119.24	126.72
17	4	605	CLA	CHC-C1C-C2C	-2.70	119.24	126.72
17	1	606	CLA	C2C-C1C-NC	2.70	112.50	109.97
17	B	829	CLA	CGD-CBD-CAD	-2.70	101.98	110.73
20	5	305	CHL	CMB-C2B-C1B	-2.70	124.31	128.46
17	A	839	CLA	C1D-ND-C4D	-2.70	104.42	106.33
17	A	831	CLA	CHA-C1A-NA	-2.70	120.22	126.40
17	6	604	CLA	CHC-C1C-C2C	-2.70	119.26	126.72
17	A	821	CLA	CHC-C1C-NC	2.69	128.29	124.20
17	8	601	CLA	CHC-C1C-NC	2.69	128.29	124.20
17	A	811	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
17	A	820	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
17	B	824	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
16	A	801	CL0	C2C-C1C-NC	2.69	112.49	109.97
17	4	602	CLA	CHC-C1C-NC	2.69	128.29	124.20
17	A	829	CLA	CAA-C2A-C1A	-2.69	106.18	112.14
17	A	810	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
17	B	834	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
17	1	603	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
17	A	819	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
17	B	820	CLA	C1D-ND-C4D	-2.69	104.43	106.33
17	1	608	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
17	B	835	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
17	6	603	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
17	1	608	CLA	CHC-C1C-NC	2.68	128.27	124.20
17	3	308	CLA	CHC-C1C-NC	2.68	128.27	124.20
17	B	829	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
17	A	838	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
17	B	805	CLA	CAA-C2A-C1A	-2.68	106.21	112.14
17	A	842	CLA	C4A-NA-C1A	-2.68	105.50	106.71
17	B	825	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
17	5	304	CLA	CHA-C1A-NA	-2.68	120.27	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	811	CLA	CHC-C1C-NC	2.67	128.26	124.20
17	B	811	CLA	CHC-C1C-C2C	-2.67	119.32	126.72
17	8	608	CLA	CHC-C1C-C2C	-2.67	119.32	126.72
17	5	307	CLA	C2C-C1C-NC	2.67	112.48	109.97
17	6	604	CLA	CHC-C1C-NC	2.67	128.26	124.20
17	J	102	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
17	8	605	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
17	A	802	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
17	B	823	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
17	B	825	CLA	CHC-C1C-NC	2.67	128.25	124.20
17	8	608	CLA	CAA-C2A-C1A	-2.67	106.24	112.14
17	8	602	CLA	CHC-C1C-NC	2.67	128.25	124.20
17	A	814	CLA	CHC-C1C-C2C	-2.67	119.35	126.72
17	3	310	CLA	CAA-C2A-C1A	-2.66	105.23	111.81
17	A	804	CLA	CAA-C2A-C1A	-2.66	106.24	112.14
17	B	810	CLA	CHC-C1C-NC	2.66	128.24	124.20
17	3	301	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
17	A	831	CLA	C2C-C1C-NC	2.66	112.46	109.97
17	A	819	CLA	C2C-C1C-NC	2.66	112.46	109.97
17	6	610	CLA	CHC-C1C-NC	2.66	128.23	124.20
17	3	303	CLA	CHC-C1C-NC	2.66	128.23	124.20
17	8	611	CLA	CHC-C1C-C2C	-2.66	119.38	126.72
17	A	830	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
17	B	838	CLA	CHA-C1A-NA	-2.65	120.32	126.40
17	8	613	CLA	C1D-ND-C4D	-2.65	104.45	106.33
17	3	306	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
17	A	831	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
17	B	830	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
17	1	605	CLA	CHA-C1A-NA	-2.65	120.33	126.40
17	3	302	CLA	C2C-C1C-NC	2.65	112.45	109.97
17	5	301	CLA	CHC-C1C-NC	2.65	128.22	124.20
17	A	822	CLA	C2C-C1C-NC	2.65	112.45	109.97
17	7	603	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
17	7	604	CLA	C1D-ND-C4D	-2.65	104.45	106.33
17	6	610	CLA	CHD-C1D-ND	-2.65	122.02	124.45
17	A	834	CLA	C2C-C1C-NC	2.65	112.45	109.97
17	A	833	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
17	7	607	CLA	CHC-C1C-C2C	-2.64	119.41	126.72
17	1	610	CLA	CHC-C1C-NC	2.64	128.21	124.20
17	B	817	CLA	CHC-C1C-NC	2.64	128.21	124.20
17	A	813	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
17	J	102	CLA	CHC-C1C-NC	2.64	128.21	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	602	CLA	C2C-C1C-NC	2.64	112.44	109.97
17	8	614	CLA	C2C-C1C-NC	2.64	112.44	109.97
17	A	805	CLA	CHC-C1C-NC	2.64	128.21	124.20
17	B	818	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
17	B	833	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
17	B	819	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
17	A	837	CLA	C1D-ND-C4D	-2.64	104.46	106.33
17	7	602	CLA	CHC-C1C-NC	2.64	128.21	124.20
17	8	607	CLA	CHC-C1C-NC	2.64	128.20	124.20
17	B	839	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
17	6	602	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
17	A	823	CLA	C1D-ND-C4D	-2.64	104.46	106.33
17	F	302	CLA	C1D-ND-C4D	-2.63	104.46	106.33
17	3	306	CLA	CHC-C1C-NC	2.63	128.20	124.20
17	8	604	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
17	B	838	CLA	C1D-ND-C4D	-2.63	104.47	106.33
17	7	610	CLA	C1D-ND-C4D	-2.63	104.47	106.33
17	8	601	CLA	C1D-ND-C4D	-2.63	104.47	106.33
17	A	826	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
17	5	301	CLA	CHC-C1C-C2C	-2.63	119.46	126.72
17	A	819	CLA	CHC-C1C-NC	2.63	128.19	124.20
17	7	605	CLA	CHC-C1C-C2C	-2.63	119.46	126.72
17	7	604	CLA	CHC-C1C-C2C	-2.62	119.46	126.72
17	1	606	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
17	5	311	CLA	C1D-ND-C4D	-2.62	104.47	106.33
17	B	833	CLA	C2C-C1C-NC	2.62	112.43	109.97
17	5	306	CLA	CHC-C1C-NC	2.62	128.17	124.20
17	A	811	CLA	CHC-C1C-NC	2.62	128.17	124.20
17	5	309	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
17	3	313	CLA	C3A-C2A-C1A	-2.62	97.42	101.34
17	7	614	CLA	CHA-C1A-NA	-2.62	120.41	126.40
17	A	829	CLA	CHC-C1C-NC	2.61	128.17	124.20
17	A	841	CLA	CHC-C1C-C2C	-2.61	119.49	126.72
17	6	603	CLA	CHC-C1C-NC	2.61	128.17	124.20
17	B	822	CLA	CHC-C1C-NC	2.61	128.16	124.20
17	A	836	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
17	A	814	CLA	CHC-C1C-NC	2.61	128.16	124.20
20	Z	601	CHL	CHA-C1A-NA	-2.61	120.43	126.40
17	A	808	CLA	CHC-C1C-NC	2.61	128.16	124.20
17	B	823	CLA	CHA-C1A-NA	-2.61	120.43	126.40
17	7	614	CLA	CHC-C1C-C2C	-2.60	119.52	126.72
17	6	608	CLA	CHC-C1C-C2C	-2.60	119.52	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	603	CLA	CHC-C1C-C2C	-2.60	119.53	126.72
17	B	819	CLA	C2D-C1D-ND	-2.60	108.19	110.10
17	A	842	CLA	C2C-C1C-NC	2.60	112.41	109.97
17	5	314	CLA	CGD-CBD-CAD	-2.60	102.31	110.73
17	5	308	CLA	CHC-C1C-NC	2.60	128.15	124.20
17	5	311	CLA	CHC-C1C-NC	2.60	128.15	124.20
17	A	835	CLA	CHC-C1C-NC	2.60	128.14	124.20
17	B	817	CLA	CAA-C2A-C1A	-2.60	106.39	112.14
17	B	812	CLA	C1D-ND-C4D	-2.59	104.49	106.33
17	B	824	CLA	C2C-C1C-NC	2.59	112.40	109.97
17	B	813	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
17	3	311	CLA	CHC-C1C-NC	2.59	128.13	124.20
17	1	602	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
17	B	825	CLA	C2C-C1C-NC	2.59	112.40	109.97
17	A	818	CLA	CHC-C1C-NC	2.59	128.13	124.20
17	A	830	CLA	CHC-C1C-NC	2.59	128.13	124.20
17	A	828	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
20	6	606	CHL	CHC-C1C-NC	2.59	128.13	124.20
17	B	829	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
17	3	302	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
17	A	825	CLA	CHC-C1C-NC	2.58	128.12	124.20
17	8	614	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
20	1	601	CHL	CHC-C1C-NC	2.58	128.12	124.20
17	A	824	CLA	C1D-ND-C4D	-2.58	104.50	106.33
17	7	604	CLA	CGD-CBD-CAD	-2.58	102.37	110.73
17	B	810	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
17	5	315	CLA	CHC-C1C-NC	2.58	128.12	124.20
17	B	832	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
17	5	311	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
17	5	307	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
17	8	601	CLA	CHA-C1A-NA	-2.58	120.49	126.40
17	B	801	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
20	1	601	CHL	CHA-C1A-NA	-2.58	120.49	126.40
17	7	613	CLA	CHC-C1C-NC	2.58	128.11	124.20
17	A	822	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
17	A	828	CLA	C2C-C1C-NC	2.58	112.39	109.97
17	6	608	CLA	C1D-ND-C4D	-2.57	104.51	106.33
17	B	804	CLA	CHA-C1A-NA	-2.57	120.50	126.40
17	8	612	CLA	CHC-C1C-NC	2.57	128.11	124.20
17	B	801	CLA	C1D-ND-C4D	-2.57	104.51	106.33
17	B	815	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
17	B	833	CLA	CHC-C1C-NC	2.57	128.10	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	J	102	CLA	C2C-C1C-NC	2.57	112.38	109.97
17	A	815	CLA	CHC-C1C-C2C	-2.57	119.61	126.72
17	A	828	CLA	C1D-ND-C4D	-2.57	104.51	106.33
17	A	802	CLA	CHC-C1C-NC	2.57	128.10	124.20
17	A	808	CLA	CHA-C1A-NA	-2.57	120.52	126.40
17	7	602	CLA	CAA-C2A-C1A	-2.56	106.46	112.14
17	B	823	CLA	C1D-ND-C4D	-2.56	104.51	106.33
17	A	805	CLA	CAA-C2A-C1A	-2.56	106.47	112.14
17	B	809	CLA	C2C-C1C-NC	2.56	112.37	109.97
17	B	829	CLA	CHC-C1C-NC	2.56	128.09	124.20
17	A	802	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
17	7	601	CLA	CHA-C1A-NA	-2.56	120.54	126.40
17	A	841	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
17	7	612	CLA	C2C-C1C-NC	2.56	112.37	109.97
17	A	819	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
17	7	614	CLA	CHC-C1C-NC	2.56	128.08	124.20
17	A	843	CLA	C1D-ND-C4D	-2.56	104.52	106.33
17	B	838	CLA	CHC-C1C-NC	2.56	128.08	124.20
17	B	839	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
17	A	831	CLA	CHC-C1C-NC	2.55	128.08	124.20
17	6	609	CLA	CHA-C1A-NA	-2.55	120.55	126.40
20	7	606	CHL	C2C-C3C-C4C	2.55	108.31	106.49
17	A	821	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
17	A	830	CLA	C2C-C1C-NC	2.55	112.36	109.97
20	Z	601	CHL	CHC-C1C-NC	2.55	128.07	124.20
17	1	608	CLA	CHA-C1A-NA	-2.55	120.56	126.40
17	5	309	CLA	CHC-C1C-C2C	-2.55	119.68	126.72
17	A	843	CLA	CHC-C1C-C2C	-2.55	119.68	126.72
17	A	841	CLA	C1D-ND-C4D	-2.55	104.53	106.33
17	7	614	CLA	C1D-ND-C4D	-2.55	104.53	106.33
17	3	312	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
17	8	611	CLA	CHC-C1C-NC	2.54	128.06	124.20
17	6	601	CLA	C1D-ND-C4D	-2.54	104.53	106.33
17	A	842	CLA	CHA-C1A-NA	-2.53	120.59	126.40
17	6	604	CLA	C2C-C1C-NC	2.53	112.35	109.97
17	A	816	CLA	CAA-C2A-C1A	-2.53	106.53	112.14
17	B	829	CLA	C2C-C1C-NC	2.53	112.34	109.97
17	B	808	CLA	CHC-C1C-NC	2.53	128.04	124.20
17	3	309	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
20	3	307	CHL	C2A-C1A-CHA	2.53	128.28	123.86
17	A	843	CLA	CHC-C1C-NC	2.53	128.04	124.20
17	1	608	CLA	C2C-C1C-NC	2.53	112.34	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	835	CLA	CHC-C1C-NC	2.53	128.04	124.20
17	7	610	CLA	CHC-C1C-NC	2.53	128.04	124.20
17	A	826	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
17	4	604	CLA	C1D-ND-C4D	-2.53	104.54	106.33
17	6	601	CLA	CHC-C1C-NC	2.53	128.03	124.20
17	B	823	CLA	CHC-C1C-NC	2.53	128.03	124.20
17	A	814	CLA	C2C-C1C-NC	2.52	112.34	109.97
17	A	842	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
17	B	836	CLA	CHC-C1C-NC	2.52	128.03	124.20
17	B	828	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
17	1	603	CLA	CHC-C1C-NC	2.52	128.03	124.20
17	5	302	CLA	C1D-ND-C4D	-2.52	104.55	106.33
17	5	312	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
17	5	309	CLA	CHC-C1C-NC	2.52	128.02	124.20
17	7	603	CLA	CAA-C2A-C1A	-2.52	106.57	112.14
17	3	313	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
17	3	313	CLA	CHC-C1C-NC	2.52	128.02	124.20
17	A	819	CLA	C1D-ND-C4D	-2.51	104.55	106.33
17	1	606	CLA	CHC-C1C-NC	2.51	128.02	124.20
17	B	815	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
17	B	828	CLA	CHC-C1C-NC	2.51	128.01	124.20
17	8	608	CLA	CHC-C1C-NC	2.51	128.01	124.20
17	3	303	CLA	C1D-ND-C4D	-2.51	104.55	106.33
17	F	302	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
17	8	613	CLA	CHC-C1C-NC	2.51	128.01	124.20
17	A	803	CLA	CHC-C1C-NC	2.51	128.01	124.20
17	A	841	CLA	CHC-C1C-NC	2.51	128.01	124.20
17	5	312	CLA	CHA-C1A-NA	-2.51	120.66	126.40
17	B	815	CLA	CHC-C1C-NC	2.51	128.00	124.20
20	3	307	CHL	C2C-C3C-C4C	2.50	108.27	106.49
17	1	607	CLA	CHC-C1C-NC	2.50	128.00	124.20
17	3	306	CLA	CHC-C1C-C2C	-2.50	119.80	126.72
20	5	313	CHL	C2C-C3C-C4C	2.50	108.27	106.49
17	3	306	CLA	C2A-C3A-C4A	-2.50	97.83	101.87
17	3	311	CLA	CHA-C1A-NA	-2.50	120.67	126.40
17	B	827	CLA	CHC-C1C-NC	2.50	127.99	124.20
17	3	306	CLA	C1D-ND-C4D	-2.50	104.56	106.33
17	B	802	CLA	CHC-C1C-NC	2.50	127.99	124.20
17	B	810	CLA	C3A-C2A-C1A	-2.50	97.60	101.34
17	4	605	CLA	C1D-ND-C4D	-2.50	104.56	106.33
17	B	814	CLA	CHC-C1C-NC	2.49	127.99	124.20
17	A	822	CLA	C1B-CHB-C4A	-2.49	125.18	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5	304	CLA	CHC-C1C-NC	2.49	127.98	124.20
17	B	807	CLA	C2C-C1C-NC	2.49	112.31	109.97
17	A	809	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
17	6	610	CLA	C1D-ND-C4D	-2.49	104.57	106.33
17	B	839	CLA	CHC-C1C-NC	2.49	127.98	124.20
17	5	314	CLA	CHC-C1C-C2C	-2.49	119.84	126.72
17	3	308	CLA	CHC-C1C-C2C	-2.48	119.85	126.72
17	4	604	CLA	CHC-C1C-NC	2.48	127.97	124.20
17	3	302	CLA	CAA-C2A-C1A	-2.48	106.65	112.14
17	5	310	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
17	7	607	CLA	CHC-C1C-NC	2.48	127.97	124.20
17	7	609	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
17	A	825	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
17	6	608	CLA	CHC-C1C-NC	2.48	127.97	124.20
17	5	306	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
17	5	308	CLA	C1D-ND-C4D	-2.48	104.58	106.33
17	6	608	CLA	CAA-C2A-C1A	-2.48	106.66	112.14
17	7	610	CLA	C2A-C3A-C4A	-2.48	98.63	101.78
17	7	604	CLA	CHC-C1C-NC	2.48	127.96	124.20
17	8	614	CLA	CHC-C1C-NC	2.47	127.96	124.20
17	6	608	CLA	C2C-C1C-NC	2.47	112.29	109.97
17	8	610	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
17	B	814	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
17	5	314	CLA	C2C-C1C-NC	2.47	112.29	109.97
17	F	301	CLA	CAA-C2A-C1A	-2.47	106.67	112.14
17	1	604	CLA	CHC-C1C-NC	2.47	127.95	124.20
17	A	807	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
17	1	604	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
17	B	827	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
17	1	605	CLA	CHC-C1C-NC	2.47	127.94	124.20
17	8	607	CLA	CHA-C1A-NA	-2.47	120.75	126.40
17	7	607	CLA	C2C-C1C-NC	2.47	112.28	109.97
17	B	811	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
17	7	609	CLA	C2C-C1C-NC	2.46	112.28	109.97
17	A	838	CLA	CHC-C1C-NC	2.46	127.94	124.20
17	B	834	CLA	CHC-C1C-NC	2.46	127.94	124.20
17	F	302	CLA	CHC-C1C-NC	2.46	127.94	124.20
17	5	307	CLA	CHC-C1C-NC	2.46	127.94	124.20
20	7	606	CHL	CHC-C1C-NC	2.46	127.93	124.20
17	8	604	CLA	CHC-C1C-NC	2.46	127.93	124.20
17	A	825	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
17	A	822	CLA	CHC-C1C-NC	2.46	127.93	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	836	CLA	CHC-C1C-NC	2.45	127.93	124.20
17	A	830	CLA	CGD-CBD-CAD	-2.45	102.79	110.73
20	6	607	CHL	CHC-C1C-NC	2.45	127.92	124.20
17	8	603	CLA	C2C-C1C-NC	2.45	112.27	109.97
17	B	826	CLA	CHC-C1C-NC	2.45	127.92	124.20
17	7	614	CLA	C2C-C1C-NC	2.45	112.27	109.97
17	B	822	CLA	CHA-C1A-NA	-2.45	120.79	126.40
17	B	820	CLA	CHC-C1C-NC	2.45	127.92	124.20
17	5	308	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
17	B	834	CLA	CHA-C1A-NA	-2.44	120.80	126.40
17	B	805	CLA	CHA-C1A-NA	-2.44	120.80	126.40
17	B	808	CLA	CHA-C1A-NA	-2.44	120.80	126.40
17	A	802	CLA	C2C-C1C-NC	2.44	112.26	109.97
17	4	603	CLA	CHC-C1C-NC	2.44	127.91	124.20
17	8	605	CLA	CHA-C1A-NA	-2.44	120.81	126.40
17	A	837	CLA	CHC-C1C-NC	2.44	127.90	124.20
17	A	807	CLA	C1D-ND-C4D	-2.44	104.60	106.33
17	A	832	CLA	C2C-C1C-NC	2.44	112.26	109.97
17	A	807	CLA	C2C-C1C-NC	2.44	112.25	109.97
17	5	307	CLA	C1D-ND-C4D	-2.43	104.61	106.33
17	A	828	CLA	CHC-C1C-NC	2.43	127.89	124.20
17	5	312	CLA	CAA-C2A-C1A	-2.43	106.76	112.14
17	3	305	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
17	7	601	CLA	C1D-ND-C4D	-2.42	104.61	106.33
17	B	819	CLA	CAA-C2A-C1A	-2.42	106.78	112.14
17	A	824	CLA	C2C-C1C-NC	2.42	112.24	109.97
17	8	610	CLA	C2C-C1C-NC	2.42	112.24	109.97
17	B	818	CLA	CGD-CBD-CAD	-2.42	102.89	110.73
17	A	817	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
17	7	610	CLA	CHC-C1C-C2C	-2.42	120.04	126.72
17	3	304	CLA	C2C-C1C-NC	2.42	112.23	109.97
17	A	836	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
17	B	833	CLA	C1D-ND-C4D	-2.41	104.62	106.33
17	8	610	CLA	C1D-ND-C4D	-2.41	104.62	106.33
17	A	812	CLA	CHC-C1C-NC	2.41	127.86	124.20
17	5	303	CLA	CHC-C1C-C2C	-2.41	120.05	126.72
17	3	302	CLA	CHC-C1C-NC	2.41	127.86	124.20
17	4	605	CLA	CHC-C1C-NC	2.41	127.86	124.20
17	B	824	CLA	CHC-C1C-C2C	-2.41	120.06	126.72
17	8	610	CLA	CHC-C1C-NC	2.41	127.86	124.20
17	B	829	CLA	C1D-ND-C4D	-2.41	104.62	106.33
17	7	609	CLA	CHC-C1C-NC	2.40	127.85	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	832	CLA	CHC-C1C-NC	2.40	127.85	124.20
17	5	310	CLA	CHC-C1C-NC	2.40	127.85	124.20
17	A	841	CLA	CHA-C1A-NA	-2.40	120.90	126.40
17	B	805	CLA	CHC-C1C-NC	2.40	127.84	124.20
17	4	603	CLA	CHA-C1A-NA	-2.40	120.91	126.40
17	A	810	CLA	C2C-C1C-NC	2.40	112.22	109.97
17	A	842	CLA	CHC-C1C-NC	2.40	127.84	124.20
17	B	806	CLA	CHC-C1C-NC	2.40	127.84	124.20
17	B	802	CLA	CHA-C1A-NA	-2.39	120.92	126.40
17	3	310	CLA	CHA-C1A-NA	-2.39	120.92	126.40
17	5	311	CLA	C2C-C1C-NC	2.39	112.21	109.97
17	1	609	CLA	C2C-C1C-NC	2.39	112.21	109.97
17	B	829	CLA	CHA-C1A-NA	-2.39	120.93	126.40
17	3	313	CLA	C1D-ND-C4D	-2.39	104.64	106.33
20	3	307	CHL	CHC-C1C-NC	2.39	127.82	124.20
17	B	820	CLA	CHC-C1C-C2C	-2.39	120.12	126.72
17	A	838	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
17	B	807	CLA	CHC-C1C-C2C	-2.38	120.13	126.72
20	8	606	CHL	CHC-C1C-NC	2.38	127.82	124.20
17	8	609	CLA	CAA-C2A-C1A	-2.38	106.87	112.14
17	6	610	CLA	C2A-C1A-CHA	2.38	128.02	123.86
17	4	601	CLA	CHA-C1A-NA	-2.38	120.95	126.40
17	A	817	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
17	A	809	CLA	CAA-C2A-C1A	-2.38	106.88	112.14
17	A	841	CLA	C1-C2-C3	-2.38	121.94	126.04
17	6	602	CLA	CHC-C1C-NC	2.37	127.81	124.20
17	A	817	CLA	CHC-C1C-NC	2.37	127.80	124.20
17	1	602	CLA	CHC-C1C-NC	2.37	127.80	124.20
17	7	612	CLA	CHA-C1A-NA	-2.37	120.97	126.40
17	A	820	CLA	C2C-C1C-NC	2.37	112.19	109.97
17	B	830	CLA	CHC-C1C-NC	2.37	127.80	124.20
17	5	314	CLA	CHC-C1C-NC	2.37	127.80	124.20
17	1	607	CLA	CBA-CAA-C2A	2.37	118.74	113.47
17	5	301	CLA	C2C-C1C-NC	2.37	112.19	109.97
17	1	605	CLA	C1D-ND-C4D	-2.37	104.65	106.33
17	B	815	CLA	C2A-C1A-CHA	2.37	128.00	123.86
17	A	814	CLA	CHA-C1A-NA	-2.37	120.98	126.40
20	5	313	CHL	CHC-C1C-NC	2.37	127.79	124.20
17	8	609	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
17	A	806	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
17	3	313	CLA	C2C-C1C-NC	2.36	112.18	109.97
17	A	826	CLA	C2C-C1C-NC	2.35	112.18	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	312	CLA	C2C-C1C-NC	2.35	112.18	109.97
17	F	301	CLA	CHC-C1C-C2C	-2.35	120.21	126.72
17	A	821	CLA	CHA-C1A-NA	-2.35	121.01	126.40
17	B	801	CLA	CHC-C1C-NC	2.35	127.77	124.20
17	A	834	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
17	B	815	CLA	C2C-C1C-NC	2.35	112.17	109.97
17	A	833	CLA	CHC-C1C-NC	2.35	127.77	124.20
17	B	824	CLA	C3A-C2A-C1A	-2.35	97.66	101.64
17	A	831	CLA	CGD-CBD-CAD	-2.35	103.12	110.73
17	A	813	CLA	CHC-C1C-NC	2.35	127.77	124.20
17	4	603	CLA	CHC-C1C-C2C	-2.35	120.23	126.72
17	A	813	CLA	CAA-C2A-C1A	-2.35	106.94	112.14
17	B	804	CLA	CHC-C1C-C2C	-2.35	120.23	126.72
17	B	819	CLA	CHD-C1D-ND	-2.35	122.30	124.45
17	7	608	CLA	C2C-C1C-NC	2.34	112.17	109.97
17	8	607	CLA	CAA-C2A-C3A	-2.34	108.40	114.26
17	3	312	CLA	CHC-C1C-NC	2.34	127.76	124.20
17	7	610	CLA	CHA-C1A-NA	-2.34	121.03	126.40
17	B	818	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
17	7	605	CLA	C1D-ND-C4D	-2.34	104.67	106.33
17	B	802	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
17	5	304	CLA	C1D-ND-C4D	-2.34	104.67	106.33
17	B	805	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
17	1	607	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
17	A	839	CLA	CHA-C1A-NA	-2.34	121.04	126.40
17	A	832	CLA	CHA-C1A-NA	-2.34	121.04	126.40
17	B	811	CLA	C2C-C1C-NC	2.34	112.16	109.97
17	A	807	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
17	B	820	CLA	C3A-C2A-C1A	-2.33	97.84	101.34
17	B	808	CLA	C1D-ND-C4D	-2.33	104.68	106.33
17	A	824	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
17	A	841	CLA	C2C-C1C-NC	2.33	112.16	109.97
17	B	824	CLA	C1D-ND-C4D	-2.33	104.68	106.33
17	A	826	CLA	CHA-C1A-NA	-2.33	121.07	126.40
17	B	812	CLA	CHC-C1C-NC	2.33	127.73	124.20
17	A	806	CLA	CHC-C1C-NC	2.32	127.73	124.20
17	B	816	CLA	CAA-C2A-C1A	-2.32	107.00	112.14
17	F	301	CLA	C1D-ND-C4D	-2.32	104.69	106.33
17	1	609	CLA	CHA-C1A-NA	-2.32	121.08	126.40
17	5	303	CLA	C2C-C1C-NC	2.32	112.15	109.97
17	7	612	CLA	C1D-ND-C4D	-2.32	104.69	106.33
17	A	832	CLA	CAA-C2A-C1A	-2.32	107.01	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	7	606	CHL	CAA-C2A-C1A	2.32	117.27	112.14
17	8	609	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
17	A	807	CLA	CHC-C1C-NC	2.32	127.72	124.20
17	5	311	CLA	CAA-C2A-C1A	-2.32	107.02	112.14
17	6	601	CLA	CAA-C2A-C1A	-2.32	107.02	112.14
17	A	819	CLA	CHA-C1A-NA	-2.31	121.10	126.40
17	A	822	CLA	CHA-C1A-NA	-2.31	121.10	126.40
17	A	803	CLA	CHA-C1A-NA	-2.31	121.11	126.40
17	A	831	CLA	CAA-C2A-C3A	-2.30	108.50	114.26
17	A	843	CLA	C2C-C1C-NC	2.30	112.13	109.97
17	F	301	CLA	CHC-C1C-NC	2.30	127.69	124.20
17	B	821	CLA	CHA-C1A-NA	-2.30	121.13	126.40
17	A	824	CLA	CHC-C1C-C2C	-2.30	120.37	126.72
17	3	310	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
20	5	305	CHL	CHC-C1C-NC	2.29	127.68	124.20
17	A	843	CLA	CHA-C1A-NA	-2.29	121.15	126.40
17	A	816	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
17	3	310	CLA	CHC-C1C-NC	2.29	127.68	124.20
17	A	827	CLA	CHA-C1A-NA	-2.29	121.16	126.40
17	A	804	CLA	C3A-C2A-C1A	-2.28	97.92	101.34
17	B	818	CLA	CHC-C1C-NC	2.28	127.67	124.20
17	A	833	CLA	CHA-C1A-NA	-2.28	121.17	126.40
17	A	810	CLA	CAA-C2A-C1A	-2.28	107.09	112.14
17	8	608	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	3	309	CLA	CHC-C1C-NC	2.28	127.66	124.20
17	B	826	CLA	CHC-C1C-C2C	-2.28	120.43	126.72
17	B	819	CLA	C3D-C2D-C1D	2.27	108.94	105.83
17	7	605	CLA	CHC-C1C-NC	2.27	127.65	124.20
17	4	601	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
17	A	832	CLA	C4C-C3C-C2C	-2.27	106.38	108.89
17	3	306	CLA	C2A-C1A-CHA	2.27	127.83	123.86
17	8	609	CLA	CHC-C1C-NC	2.27	127.64	124.20
17	5	315	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
17	7	607	CLA	CHA-C1A-NA	-2.26	121.22	126.40
17	8	614	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
17	A	835	CLA	C1D-ND-C4D	-2.26	104.73	106.33
17	5	306	CLA	CGD-CBD-CAD	-2.26	103.41	110.73
17	5	309	CLA	C2C-C1C-NC	2.26	112.09	109.97
17	B	813	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
17	3	306	CLA	CHA-C1A-NA	-2.26	121.23	126.40
20	6	605	CHL	C2C-C3C-C4C	2.26	108.10	106.49
17	A	833	CLA	C1B-CHB-C4A	-2.26	125.65	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	835	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
17	B	823	CLA	CAA-C2A-C3A	-2.25	108.63	114.26
17	A	838	CLA	CHA-C1A-NA	-2.25	121.24	126.40
17	8	605	CLA	CHC-C1C-NC	2.25	127.62	124.20
17	A	828	CLA	CHA-C1A-NA	-2.25	121.25	126.40
17	5	303	CLA	CHC-C1C-NC	2.25	127.62	124.20
17	A	832	CLA	C1D-ND-C4D	-2.25	104.74	106.33
17	B	813	CLA	CAB-C3B-C4B	-2.25	125.01	128.46
17	B	827	CLA	C2C-C1C-NC	2.25	112.08	109.97
17	A	827	CLA	C1D-ND-C4D	-2.25	104.74	106.33
17	B	819	CLA	C1D-CHD-C4C	-2.24	121.22	126.06
17	B	812	CLA	CHC-C1C-C2C	-2.24	120.51	126.72
17	B	812	CLA	CHA-C1A-NA	-2.24	121.26	126.40
17	F	301	CLA	C2C-C1C-NC	2.24	112.07	109.97
17	A	842	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
17	B	815	CLA	C3D-C4D-ND	2.24	113.86	110.24
16	A	801	CL0	CGD-CBD-CAD	-2.24	103.48	110.73
17	7	611	CLA	C3A-C2A-C1A	2.24	104.69	101.34
17	8	604	CLA	CHA-C1A-NA	-2.23	121.28	126.40
17	A	809	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
17	B	815	CLA	CHA-C1A-NA	-2.23	121.29	126.40
17	B	812	CLA	C2A-C3A-C4A	-2.23	98.27	101.87
17	B	806	CLA	CGD-CBD-CAD	-2.23	103.52	110.73
17	B	835	CLA	C1D-ND-C4D	-2.23	104.75	106.33
17	3	310	CLA	C1D-ND-C4D	-2.23	104.75	106.33
17	A	804	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
17	B	831	CLA	C2C-C1C-NC	2.23	112.06	109.97
17	3	306	CLA	CGD-CBD-CAD	-2.22	103.53	110.73
17	B	820	CLA	CHA-C1A-NA	-2.22	121.31	126.40
17	5	307	CLA	CHA-C1A-NA	-2.22	121.31	126.40
17	B	810	CLA	C1D-ND-C4D	-2.22	104.76	106.33
17	7	603	CLA	C3A-C2A-C1A	-2.22	98.02	101.34
17	B	819	CLA	C3C-C4C-NC	-2.22	108.08	110.57
16	A	801	CL0	CHA-C1A-NA	-2.22	121.32	126.40
17	8	603	CLA	CHA-C1A-NA	-2.21	121.33	126.40
20	6	605	CHL	CHC-C1C-NC	2.21	127.56	124.20
17	8	608	CLA	CHA-C1A-NA	-2.21	121.33	126.40
17	B	807	CLA	CHC-C1C-NC	2.21	127.56	124.20
17	B	832	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
17	6	604	CLA	CHA-C1A-NA	-2.21	121.33	126.40
17	A	837	CLA	CHA-C1A-NA	-2.21	121.34	126.40
17	1	604	CLA	CHA-C1A-NA	-2.21	121.34	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	604	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
17	A	828	CLA	CAA-C2A-C1A	-2.21	107.26	112.14
17	B	806	CLA	C2A-C3A-C4A	-2.21	98.31	101.87
17	5	312	CLA	CHC-C1C-NC	2.20	127.55	124.20
17	8	605	CLA	C1D-ND-C4D	-2.20	104.77	106.33
17	5	303	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
17	3	303	CLA	CHA-C1A-NA	-2.20	121.36	126.40
17	6	601	CLA	CHA-C1A-NA	-2.20	121.36	126.40
17	8	613	CLA	CHA-C1A-NA	-2.20	121.37	126.40
17	1	604	CLA	C2C-C1C-NC	2.20	112.03	109.97
17	8	610	CLA	CHA-C1A-NA	-2.20	121.37	126.40
17	A	809	CLA	CHA-C1A-NA	-2.19	121.38	126.40
17	B	836	CLA	CHA-C1A-NA	-2.19	121.38	126.40
17	8	611	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
17	7	613	CLA	CHA-C1A-NA	-2.19	121.39	126.40
17	5	311	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
17	B	839	CLA	CHA-C1A-NA	-2.18	121.40	126.40
17	A	818	CLA	CHA-C1A-NA	-2.18	121.41	126.40
17	A	806	CLA	CAA-C2A-C1A	-2.18	107.32	112.14
17	A	827	CLA	CAA-C2A-C1A	-2.18	107.32	112.14
17	5	301	CLA	CHA-C1A-NA	-2.18	121.41	126.40
17	B	821	CLA	CMB-C2B-C1B	-2.18	125.12	128.46
17	A	804	CLA	CHC-C1C-NC	2.17	127.50	124.20
17	1	608	CLA	CAA-C2A-C3A	-2.17	108.83	114.26
17	1	610	CLA	CHA-C1A-NA	-2.17	121.42	126.40
17	7	608	CLA	CAA-C2A-C1A	-2.17	107.33	112.14
17	A	817	CLA	C2C-C1C-NC	2.17	112.00	109.97
17	4	603	CLA	CBA-CAA-C2A	2.17	118.29	113.47
17	B	831	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
17	A	835	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
17	1	603	CLA	CHA-C1A-NA	-2.16	121.44	126.40
17	B	827	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
17	A	818	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
17	B	817	CLA	CHA-C1A-NA	-2.16	121.45	126.40
17	A	825	CLA	C2C-C1C-NC	2.16	112.00	109.97
17	5	310	CLA	CHA-C1A-NA	-2.16	121.45	126.40
17	5	303	CLA	CHA-C1A-NA	-2.16	121.46	126.40
17	3	309	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
17	7	603	CLA	C2C-C1C-NC	2.16	111.99	109.97
17	B	821	CLA	CHC-C1C-NC	2.16	127.47	124.20
17	3	308	CLA	C1D-ND-C4D	-2.16	104.80	106.33
17	B	821	CLA	CHC-C1C-C2C	-2.16	120.76	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	807	CLA	CHA-C1A-NA	-2.15	121.47	126.40
17	6	604	CLA	CAA-C2A-C1A	-2.15	107.37	112.14
17	B	823	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
17	3	306	CLA	C2C-C1C-NC	2.15	111.98	109.97
17	A	829	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
17	B	824	CLA	CHC-C1C-NC	2.15	127.46	124.20
17	B	806	CLA	CHC-C1C-C2C	-2.15	120.79	126.72
17	3	313	CLA	CHA-C1A-NA	-2.14	121.50	126.40
20	6	607	CHL	C2C-C3C-C4C	2.14	108.02	106.49
17	4	605	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
17	A	827	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
17	A	809	CLA	CHC-C1C-NC	2.14	127.45	124.20
17	B	823	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
17	1	602	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
17	A	835	CLA	CHA-C1A-NA	-2.13	121.52	126.40
17	7	609	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
17	J	101	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
17	B	813	CLA	CHA-C1A-NA	-2.13	121.53	126.40
17	B	811	CLA	CHA-C1A-NA	-2.12	121.53	126.40
17	A	829	CLA	CHA-C1A-NA	-2.12	121.54	126.40
17	B	814	CLA	C2C-C1C-NC	2.12	111.96	109.97
17	3	310	CLA	C2A-C1A-CHA	2.12	127.56	123.85
17	7	605	CLA	CHA-C1A-NA	-2.12	121.54	126.40
17	8	609	CLA	C2C-C1C-NC	2.12	111.96	109.97
17	5	310	CLA	C2C-C1C-NC	2.12	111.96	109.97
20	6	605	CHL	CMB-C2B-C3B	2.12	128.64	124.68
17	A	824	CLA	CHA-C1A-NA	-2.12	121.55	126.40
17	3	301	CLA	CAA-C2A-C1A	-2.11	107.47	112.14
17	A	838	CLA	CGD-CBD-CAD	-2.11	103.90	110.73
17	B	833	CLA	CHA-C1A-NA	-2.11	121.57	126.40
17	7	605	CLA	CAA-C2A-C1A	-2.11	107.47	112.14
17	3	312	CLA	C1B-CHB-C4A	-2.11	125.95	130.12
17	7	607	CLA	C1B-CHB-C4A	-2.11	125.95	130.12
17	8	608	CLA	CGD-CBD-CAD	-2.10	103.92	110.73
17	A	842	CLA	CAA-C2A-C1A	-2.10	107.49	112.14
17	5	315	CLA	CHA-C1A-NA	-2.10	121.59	126.40
17	B	835	CLA	CHA-C1A-NA	-2.10	121.59	126.40
17	8	613	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
17	B	825	CLA	CHA-C1A-NA	-2.10	121.59	126.40
17	6	602	CLA	CHA-C1A-NA	-2.10	121.60	126.40
17	B	814	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
17	A	825	CLA	CHA-C1A-NA	-2.10	121.60	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	605	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
17	A	810	CLA	CHA-C1A-NA	-2.09	121.61	126.40
17	3	310	CLA	C2C-C1C-NC	2.09	111.93	109.97
17	4	605	CLA	CHA-C1A-NA	-2.09	121.61	126.40
17	3	301	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
17	8	605	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
17	B	801	CLA	CHD-C1D-C2D	2.09	129.86	125.48
17	3	310	CLA	CHD-C1D-C2D	2.09	129.86	125.48
17	B	806	CLA	C3D-C4D-ND	2.08	113.61	110.24
17	7	603	CLA	C3D-C4D-ND	2.08	113.61	110.24
17	7	608	CLA	C3D-C4D-ND	2.08	113.61	110.24
17	A	813	CLA	CHA-C1A-NA	-2.08	121.63	126.40
17	7	614	CLA	C2A-C3A-C4A	-2.08	98.51	101.87
17	5	312	CLA	C1D-ND-C4D	-2.08	104.86	106.33
17	A	824	CLA	CHC-C1C-NC	2.08	127.35	124.20
17	B	831	CLA	CHA-C1A-NA	-2.08	121.64	126.40
17	A	842	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
17	B	825	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
17	A	815	CLA	CHA-C1A-NA	-2.07	121.65	126.40
17	3	304	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
17	A	807	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
17	8	608	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
17	A	839	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
17	A	804	CLA	C2C-C1C-NC	2.07	111.91	109.97
17	8	614	CLA	CHA-C1A-NA	-2.07	121.66	126.40
17	A	812	CLA	CHA-C1A-NA	-2.07	121.66	126.40
17	3	301	CLA	C2C-C1C-NC	2.07	111.91	109.97
17	5	306	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
17	8	612	CLA	CHA-C1A-NA	-2.07	121.66	126.40
17	5	307	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
17	3	303	CLA	CMB-C2B-C1B	-2.07	125.29	128.46
17	5	308	CLA	CHD-C1D-C2D	2.07	129.81	125.48
17	F	302	CLA	CHA-C1A-NA	-2.07	121.67	126.40
17	7	602	CLA	CHA-C1A-NA	-2.07	121.67	126.40
17	B	838	CLA	C1B-CHB-C4A	-2.07	126.03	130.12
17	B	806	CLA	C2A-C1A-CHA	2.07	127.47	123.86
17	4	604	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
17	B	808	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
17	3	311	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
17	4	602	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
17	B	805	CLA	C2C-C1C-NC	2.06	111.90	109.97
17	1	605	CLA	CMB-C2B-C1B	-2.06	125.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	6	608	CLA	CHA-C1A-NA	-2.06	121.68	126.40
17	A	805	CLA	CHA-C1A-NA	-2.06	121.68	126.40
17	6	603	CLA	CGD-CBD-CAD	-2.06	104.06	110.73
20	6	606	CHL	CMB-C2B-C3B	2.06	128.53	124.68
17	6	602	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
17	1	604	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
17	8	604	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
17	B	810	CLA	CHA-C1A-NA	-2.06	121.69	126.40
17	A	809	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
17	7	601	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
17	7	613	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
17	B	828	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
20	Z	601	CHL	C2C-C3C-C4C	2.05	107.95	106.49
17	A	823	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
17	1	605	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
17	A	806	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
17	4	602	CLA	CHA-C1A-NA	-2.05	121.70	126.40
17	3	305	CLA	CHC-C1C-NC	2.05	127.31	124.20
17	A	841	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
17	B	832	CLA	CHA-C1A-NA	-2.05	121.71	126.40
17	A	823	CLA	CHA-C1A-NA	-2.05	121.71	126.40
17	8	602	CLA	CHA-C1A-NA	-2.05	121.71	126.40
17	3	305	CLA	C1D-ND-C4D	-2.05	104.88	106.33
20	1	601	CHL	C2C-C3C-C4C	2.05	107.95	106.49
17	1	606	CLA	CHD-C1D-C2D	2.04	129.77	125.48
17	3	302	CLA	CHA-C1A-NA	-2.04	121.72	126.40
17	4	603	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
17	4	604	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
17	B	817	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
17	A	836	CLA	CHA-C1A-NA	-2.04	121.73	126.40
17	B	815	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
17	A	839	CLA	CAA-C2A-C1A	-2.04	107.63	112.14
17	B	814	CLA	CHA-C1A-NA	-2.04	121.73	126.40
17	8	603	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
17	B	811	CLA	C1D-ND-C4D	-2.04	104.89	106.33
17	J	102	CLA	CHA-C1A-NA	-2.04	121.74	126.40
17	B	834	CLA	C1B-CHB-C4A	-2.04	126.09	130.12
17	7	609	CLA	CGD-CBD-CAD	-2.03	104.14	110.73
17	B	811	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
17	7	605	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
17	A	821	CLA	C2C-C1C-NC	2.03	111.88	109.97
17	B	818	CLA	CMB-C2B-C1B	-2.03	125.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	614	CLA	CHD-C1D-C2D	2.03	129.74	125.48
17	J	102	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
17	B	828	CLA	CHA-C1A-NA	-2.03	121.75	126.40
20	6	607	CHL	C2A-C1A-CHA	2.03	127.41	123.86
17	6	609	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
17	1	608	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
17	B	824	CLA	CHA-C1A-NA	-2.03	121.76	126.40
17	B	822	CLA	C1D-ND-C4D	-2.03	104.90	106.33
20	6	606	CHL	C2C-C3C-C4C	2.02	107.93	106.49
17	7	604	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
17	F	301	CLA	CHA-C1A-NA	-2.02	121.77	126.40
17	3	301	CLA	CHA-C1A-NA	-2.02	121.77	126.40
17	B	837	CLA	CHA-C1A-NA	-2.02	121.77	126.40
17	A	805	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
17	A	838	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
20	5	313	CHL	CMB-C2B-C3B	2.02	128.46	124.68
17	7	611	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
17	A	835	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
17	A	818	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
17	A	816	CLA	CHA-C1A-NA	-2.02	121.78	126.40
17	A	810	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
17	A	813	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
17	1	610	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
17	A	811	CLA	CAA-C2A-C1A	-2.02	107.68	112.14
17	A	817	CLA	CHA-C1A-NA	-2.01	121.78	126.40
17	A	822	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
17	3	304	CLA	CHA-C1A-NA	-2.01	121.79	126.40
17	A	812	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
17	A	807	CLA	CHA-C1A-NA	-2.01	121.79	126.40
17	A	802	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
17	5	310	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
17	J	101	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
17	5	302	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
17	A	813	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
17	A	830	CLA	CHA-C1A-NA	-2.01	121.80	126.40
17	B	815	CLA	C1-C2-C3	-2.01	122.57	126.04
17	B	830	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
17	7	604	CLA	C1D-CHD-C4C	-2.01	121.73	126.06
17	6	604	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
17	A	839	CLA	CMB-C2B-C1B	-2.00	125.38	128.46
17	7	610	CLA	C2C-C1C-NC	2.00	111.85	109.97
17	A	819	CLA	CMB-C2B-C1B	-2.00	125.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	820	CLA	C2C-C1C-NC	2.00	111.85	109.97

All (188) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	801	CL0	NA
16	A	801	CL0	ND
16	A	801	CL0	NC
17	A	802	CLA	ND
17	A	803	CLA	ND
17	A	804	CLA	ND
17	A	805	CLA	ND
17	A	806	CLA	ND
17	A	807	CLA	ND
17	A	808	CLA	ND
17	A	809	CLA	ND
17	A	810	CLA	ND
17	A	811	CLA	ND
17	A	812	CLA	ND
17	A	813	CLA	ND
17	A	814	CLA	ND
17	A	815	CLA	ND
17	A	816	CLA	ND
17	A	817	CLA	ND
17	A	818	CLA	ND
17	A	819	CLA	ND
17	A	820	CLA	ND
17	A	821	CLA	ND
17	A	822	CLA	ND
17	A	823	CLA	ND
17	A	824	CLA	ND
17	A	825	CLA	ND
17	A	826	CLA	ND
17	A	827	CLA	ND
17	A	828	CLA	ND
17	A	829	CLA	ND
17	A	830	CLA	ND
17	A	831	CLA	ND
17	A	832	CLA	ND
17	A	833	CLA	ND
17	A	834	CLA	ND
17	A	835	CLA	ND

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Mol	Chain	Res	Type	Atom
17	A	836	CLA	ND
17	A	837	CLA	ND
17	A	838	CLA	ND
17	A	839	CLA	ND
17	A	841	CLA	ND
17	A	842	CLA	ND
17	A	843	CLA	ND
17	B	801	CLA	ND
17	B	802	CLA	ND
17	B	804	CLA	ND
17	B	805	CLA	ND
17	B	806	CLA	ND
17	B	807	CLA	ND
17	B	808	CLA	ND
17	B	809	CLA	ND
17	B	810	CLA	ND
17	B	811	CLA	ND
17	B	812	CLA	ND
17	B	813	CLA	ND
17	B	814	CLA	ND
17	B	815	CLA	ND
17	B	816	CLA	ND
17	B	817	CLA	ND
17	B	818	CLA	ND
17	B	819	CLA	ND
17	B	820	CLA	ND
17	B	821	CLA	ND
17	B	822	CLA	ND
17	B	823	CLA	ND
17	B	824	CLA	ND
17	B	825	CLA	ND
17	B	826	CLA	ND
17	B	827	CLA	ND
17	B	828	CLA	ND
17	B	829	CLA	ND
17	B	830	CLA	ND
17	B	831	CLA	ND
17	B	832	CLA	ND
17	B	833	CLA	ND
17	B	834	CLA	ND
17	B	835	CLA	ND
17	B	836	CLA	ND

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Mol	Chain	Res	Type	Atom
17	B	837	CLA	ND
17	B	838	CLA	ND
17	B	839	CLA	ND
17	F	301	CLA	ND
17	F	302	CLA	ND
17	J	101	CLA	ND
17	J	102	CLA	ND
17	1	602	CLA	ND
17	1	603	CLA	ND
17	1	604	CLA	ND
17	1	605	CLA	ND
17	1	606	CLA	ND
17	1	607	CLA	ND
17	1	608	CLA	ND
17	1	609	CLA	ND
17	1	610	CLA	ND
17	3	301	CLA	ND
17	3	302	CLA	ND
17	3	303	CLA	ND
17	3	304	CLA	ND
17	3	305	CLA	ND
17	3	306	CLA	ND
17	3	308	CLA	ND
17	3	309	CLA	ND
17	3	310	CLA	ND
17	3	311	CLA	ND
17	3	312	CLA	ND
17	3	313	CLA	ND
17	7	601	CLA	ND
17	7	602	CLA	ND
17	7	603	CLA	ND
17	7	604	CLA	ND
17	7	605	CLA	ND
17	7	607	CLA	ND
17	7	608	CLA	ND
17	7	609	CLA	ND
17	7	610	CLA	ND
17	7	611	CLA	ND
17	7	612	CLA	ND
17	7	613	CLA	ND
17	7	614	CLA	ND
17	8	601	CLA	ND

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Mol	Chain	Res	Type	Atom
17	8	602	CLA	ND
17	8	603	CLA	ND
17	8	604	CLA	ND
17	8	605	CLA	ND
17	8	607	CLA	ND
17	8	608	CLA	ND
17	8	609	CLA	ND
17	8	610	CLA	ND
17	8	611	CLA	ND
17	8	612	CLA	ND
17	8	613	CLA	ND
17	8	614	CLA	ND
17	4	601	CLA	ND
17	4	602	CLA	ND
17	4	603	CLA	ND
17	4	604	CLA	ND
17	4	605	CLA	ND
17	5	301	CLA	ND
17	5	302	CLA	ND
17	5	303	CLA	ND
17	5	304	CLA	ND
17	5	306	CLA	ND
17	5	307	CLA	ND
17	5	308	CLA	ND
17	5	309	CLA	ND
17	5	310	CLA	ND
17	5	311	CLA	ND
17	5	312	CLA	ND
17	5	314	CLA	ND
17	5	315	CLA	ND
17	6	601	CLA	ND
17	6	602	CLA	ND
17	6	603	CLA	ND
17	6	604	CLA	ND
17	6	608	CLA	ND
17	6	609	CLA	ND
17	6	610	CLA	ND
20	1	601	CHL	NA
20	1	601	CHL	ND
20	1	601	CHL	NC
20	3	307	CHL	NA
20	3	307	CHL	ND

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Mol	Chain	Res	Type	Atom
20	3	307	CHL	NC
20	7	606	CHL	NA
20	7	606	CHL	ND
20	7	606	CHL	NC
20	8	606	CHL	NA
20	8	606	CHL	ND
20	8	606	CHL	NC
20	Z	601	CHL	NA
20	Z	601	CHL	ND
20	Z	601	CHL	NC
20	5	305	CHL	NA
20	5	305	CHL	ND
20	5	305	CHL	NC
20	5	313	CHL	NA
20	5	313	CHL	ND
20	5	313	CHL	NC
20	6	605	CHL	NA
20	6	605	CHL	ND
20	6	605	CHL	NC
20	6	606	CHL	NA
20	6	606	CHL	ND
20	6	606	CHL	NC
20	6	607	CHL	NA
20	6	607	CHL	ND
20	6	607	CHL	NC

All (396) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	802	CLA	C1A-C2A-CAA-CBA
17	A	802	CLA	CHA-CBD-CGD-O1D
17	A	802	CLA	CHA-CBD-CGD-O2D
17	A	803	CLA	CHA-CBD-CGD-O1D
17	A	803	CLA	CHA-CBD-CGD-O2D
17	A	805	CLA	C1A-C2A-CAA-CBA
17	A	806	CLA	C1A-C2A-CAA-CBA
17	A	807	CLA	CHA-CBD-CGD-O1D
17	A	807	CLA	CHA-CBD-CGD-O2D
17	A	809	CLA	C1A-C2A-CAA-CBA
17	A	812	CLA	C3A-C2A-CAA-CBA
17	A	814	CLA	C1A-C2A-CAA-CBA
17	A	816	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	A	816	CLA	C3A-C2A-CAA-CBA
17	A	817	CLA	C1A-C2A-CAA-CBA
17	A	817	CLA	C3A-C2A-CAA-CBA
17	A	819	CLA	CHA-CBD-CGD-O1D
17	A	819	CLA	CHA-CBD-CGD-O2D
17	A	820	CLA	C3A-C2A-CAA-CBA
17	A	821	CLA	C1A-C2A-CAA-CBA
17	A	821	CLA	C3A-C2A-CAA-CBA
17	A	821	CLA	C2-C3-C5-C6
17	A	822	CLA	C1A-C2A-CAA-CBA
17	A	829	CLA	C1A-C2A-CAA-CBA
17	A	830	CLA	C1A-C2A-CAA-CBA
17	A	831	CLA	C1A-C2A-CAA-CBA
17	A	832	CLA	C1A-C2A-CAA-CBA
17	A	832	CLA	CHA-CBD-CGD-O1D
17	A	837	CLA	CHA-CBD-CGD-O1D
17	A	837	CLA	CHA-CBD-CGD-O2D
17	A	838	CLA	C1A-C2A-CAA-CBA
17	A	843	CLA	CHA-CBD-CGD-O1D
17	A	843	CLA	CHA-CBD-CGD-O2D
17	B	801	CLA	C1A-C2A-CAA-CBA
17	B	801	CLA	C3A-C2A-CAA-CBA
17	B	802	CLA	CHA-CBD-CGD-O1D
17	B	802	CLA	CHA-CBD-CGD-O2D
17	B	804	CLA	C1A-C2A-CAA-CBA
17	B	807	CLA	CAD-CBD-CGD-O1D
17	B	807	CLA	CAD-CBD-CGD-O2D
17	B	812	CLA	C1A-C2A-CAA-CBA
17	B	812	CLA	CHA-CBD-CGD-O1D
17	B	812	CLA	CHA-CBD-CGD-O2D
17	B	813	CLA	C1A-C2A-CAA-CBA
17	B	815	CLA	C1A-C2A-CAA-CBA
17	B	815	CLA	CHA-CBD-CGD-O1D
17	B	815	CLA	CHA-CBD-CGD-O2D
17	B	815	CLA	CAD-CBD-CGD-O1D
17	B	815	CLA	CAD-CBD-CGD-O2D
17	B	816	CLA	C3A-C2A-CAA-CBA
17	B	817	CLA	C1A-C2A-CAA-CBA
17	B	818	CLA	C1A-C2A-CAA-CBA
17	B	818	CLA	C3A-C2A-CAA-CBA
17	B	819	CLA	C1A-C2A-CAA-CBA
17	B	819	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	B	820	CLA	C1A-C2A-CAA-CBA
17	B	822	CLA	C1A-C2A-CAA-CBA
17	B	823	CLA	CHA-CBD-CGD-O1D
17	B	823	CLA	CHA-CBD-CGD-O2D
17	B	823	CLA	CAD-CBD-CGD-O1D
17	B	825	CLA	C1A-C2A-CAA-CBA
17	B	825	CLA	C3A-C2A-CAA-CBA
17	B	825	CLA	CAD-CBD-CGD-O1D
17	B	825	CLA	CAD-CBD-CGD-O2D
17	B	826	CLA	C1A-C2A-CAA-CBA
17	B	826	CLA	C3A-C2A-CAA-CBA
17	B	827	CLA	C3A-C2A-CAA-CBA
17	B	830	CLA	C1A-C2A-CAA-CBA
17	B	832	CLA	C1A-C2A-CAA-CBA
17	B	836	CLA	C1A-C2A-CAA-CBA
17	B	837	CLA	C1A-C2A-CAA-CBA
17	B	838	CLA	C1A-C2A-CAA-CBA
17	F	301	CLA	C3A-C2A-CAA-CBA
17	F	302	CLA	C2-C3-C5-C6
17	F	302	CLA	C4-C3-C5-C6
17	J	101	CLA	C1A-C2A-CAA-CBA
17	J	101	CLA	C3A-C2A-CAA-CBA
17	J	102	CLA	CAD-CBD-CGD-O1D
17	J	102	CLA	CAD-CBD-CGD-O2D
17	1	602	CLA	C1A-C2A-CAA-CBA
17	1	607	CLA	C1A-C2A-CAA-CBA
17	1	607	CLA	CHA-CBD-CGD-O1D
17	1	607	CLA	CHA-CBD-CGD-O2D
17	1	608	CLA	C1A-C2A-CAA-CBA
17	1	609	CLA	CHA-CBD-CGD-O1D
17	1	609	CLA	CHA-CBD-CGD-O2D
17	1	610	CLA	C3A-C2A-CAA-CBA
17	1	610	CLA	CHA-CBD-CGD-O1D
17	1	610	CLA	CHA-CBD-CGD-O2D
17	3	301	CLA	C1A-C2A-CAA-CBA
17	3	301	CLA	C3A-C2A-CAA-CBA
17	3	306	CLA	C3A-C2A-CAA-CBA
17	3	310	CLA	CHA-CBD-CGD-O1D
17	3	310	CLA	CHA-CBD-CGD-O2D
17	7	603	CLA	CHA-CBD-CGD-O1D
17	7	603	CLA	CHA-CBD-CGD-O2D
17	7	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	7	611	CLA	C3A-C2A-CAA-CBA
17	7	614	CLA	CHA-CBD-CGD-O1D
17	7	614	CLA	CHA-CBD-CGD-O2D
17	8	602	CLA	C1A-C2A-CAA-CBA
17	8	609	CLA	C1A-C2A-CAA-CBA
17	8	610	CLA	C1A-C2A-CAA-CBA
17	8	610	CLA	CHA-CBD-CGD-O1D
17	8	610	CLA	CHA-CBD-CGD-O2D
17	8	611	CLA	C1A-C2A-CAA-CBA
17	4	603	CLA	C1A-C2A-CAA-CBA
17	4	603	CLA	CHA-CBD-CGD-O1D
17	4	603	CLA	CHA-CBD-CGD-O2D
17	5	301	CLA	CHA-CBD-CGD-O1D
17	5	301	CLA	CHA-CBD-CGD-O2D
17	5	302	CLA	C1A-C2A-CAA-CBA
17	5	307	CLA	C1A-C2A-CAA-CBA
17	5	307	CLA	CHA-CBD-CGD-O1D
17	5	307	CLA	CHA-CBD-CGD-O2D
17	5	308	CLA	CHA-CBD-CGD-O1D
17	5	308	CLA	CHA-CBD-CGD-O2D
17	5	309	CLA	C1A-C2A-CAA-CBA
17	5	309	CLA	C3A-C2A-CAA-CBA
17	6	601	CLA	CHA-CBD-CGD-O1D
17	6	602	CLA	CHA-CBD-CGD-O1D
17	6	602	CLA	CHA-CBD-CGD-O2D
20	3	307	CHL	C1A-C2A-CAA-CBA
20	5	305	CHL	C1A-C2A-CAA-CBA
20	5	305	CHL	C3A-C2A-CAA-CBA
20	5	313	CHL	CHA-CBD-CGD-O1D
20	5	313	CHL	CHA-CBD-CGD-O2D
20	6	607	CHL	C3A-C2A-CAA-CBA
17	B	809	CLA	C2C-C3C-CAC-CBC
17	6	609	CLA	C2A-CAA-CBA-CGA
17	B	829	CLA	C2A-CAA-CBA-CGA
17	B	809	CLA	C4C-C3C-CAC-CBC
18	A	840	PQN	C19-C18-C20-C21
20	3	307	CHL	C3A-C2A-CAA-CBA
17	F	302	CLA	O2A-C1-C2-C3
18	B	840	PQN	C18-C20-C21-C22
17	B	815	CLA	C11-C10-C8-C7
17	A	841	CLA	C2A-CAA-CBA-CGA
17	5	314	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
17	B	815	CLA	C11-C10-C8-C9
17	B	828	CLA	C2C-C3C-CAC-CBC
17	B	802	CLA	C1A-C2A-CAA-CBA
17	B	810	CLA	C1A-C2A-CAA-CBA
17	B	829	CLA	C1A-C2A-CAA-CBA
17	4	605	CLA	C1A-C2A-CAA-CBA
17	A	802	CLA	C3A-C2A-CAA-CBA
17	A	805	CLA	C3A-C2A-CAA-CBA
17	A	831	CLA	C3A-C2A-CAA-CBA
17	B	838	CLA	C3A-C2A-CAA-CBA
17	1	608	CLA	C3A-C2A-CAA-CBA
17	8	611	CLA	C3A-C2A-CAA-CBA
17	4	603	CLA	C3A-C2A-CAA-CBA
17	4	604	CLA	C3A-C2A-CAA-CBA
17	5	302	CLA	C3A-C2A-CAA-CBA
17	5	303	CLA	O2A-C1-C2-C3
17	F	302	CLA	C6-C7-C8-C10
17	F	302	CLA	C6-C7-C8-C9
17	A	821	CLA	C2A-CAA-CBA-CGA
20	1	601	CHL	O2A-C1-C2-C3
17	A	841	CLA	C4-C3-C5-C6
17	5	315	CLA	C2A-CAA-CBA-CGA
17	A	841	CLA	C2-C3-C5-C6
18	A	840	PQN	C24-C23-C25-C26
17	A	821	CLA	C4-C3-C5-C6
20	3	307	CHL	C2A-CAA-CBA-CGA
17	A	828	CLA	C1A-C2A-CAA-CBA
17	A	833	CLA	C1A-C2A-CAA-CBA
17	B	816	CLA	C1A-C2A-CAA-CBA
17	B	827	CLA	C1A-C2A-CAA-CBA
17	F	301	CLA	C1A-C2A-CAA-CBA
17	3	302	CLA	C1A-C2A-CAA-CBA
17	3	306	CLA	C1A-C2A-CAA-CBA
17	3	313	CLA	C1A-C2A-CAA-CBA
17	7	602	CLA	C1A-C2A-CAA-CBA
17	7	607	CLA	C1A-C2A-CAA-CBA
17	7	609	CLA	C1A-C2A-CAA-CBA
17	5	312	CLA	C1A-C2A-CAA-CBA
17	6	602	CLA	C1A-C2A-CAA-CBA
17	6	608	CLA	C1A-C2A-CAA-CBA
20	6	606	CHL	C1A-C2A-CAA-CBA
20	6	607	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	A	822	CLA	CAD-CBD-CGD-O2D
17	B	808	CLA	CAD-CBD-CGD-O2D
17	B	820	CLA	CAD-CBD-CGD-O2D
17	B	823	CLA	CAD-CBD-CGD-O2D
17	B	832	CLA	CAD-CBD-CGD-O2D
17	B	836	CLA	CAD-CBD-CGD-O2D
17	3	301	CLA	CAD-CBD-CGD-O2D
17	3	305	CLA	CAD-CBD-CGD-O2D
17	7	608	CLA	CAD-CBD-CGD-O2D
17	7	611	CLA	CAD-CBD-CGD-O2D
17	8	607	CLA	CAD-CBD-CGD-O2D
17	8	611	CLA	CAD-CBD-CGD-O2D
17	8	614	CLA	CAD-CBD-CGD-O2D
17	5	306	CLA	CAD-CBD-CGD-O2D
17	5	309	CLA	CAD-CBD-CGD-O2D
17	6	608	CLA	CAD-CBD-CGD-O2D
16	A	801	CL0	CHA-CBD-CGD-O1D
16	A	801	CL0	CHA-CBD-CGD-O2D
17	A	804	CLA	CHA-CBD-CGD-O1D
17	A	811	CLA	CHA-CBD-CGD-O1D
17	A	811	CLA	CHA-CBD-CGD-O2D
17	A	813	CLA	CHA-CBD-CGD-O1D
17	A	813	CLA	CHA-CBD-CGD-O2D
17	A	818	CLA	CHA-CBD-CGD-O1D
17	A	818	CLA	CHA-CBD-CGD-O2D
17	A	823	CLA	CHA-CBD-CGD-O1D
17	A	823	CLA	CHA-CBD-CGD-O2D
17	A	829	CLA	CHA-CBD-CGD-O1D
17	A	829	CLA	CHA-CBD-CGD-O2D
17	A	832	CLA	CHA-CBD-CGD-O2D
17	A	835	CLA	CHA-CBD-CGD-O1D
17	A	841	CLA	CHA-CBD-CGD-O1D
17	A	842	CLA	CHA-CBD-CGD-O1D
17	A	842	CLA	CHA-CBD-CGD-O2D
17	B	821	CLA	CHA-CBD-CGD-O1D
17	B	821	CLA	CHA-CBD-CGD-O2D
17	B	829	CLA	CHA-CBD-CGD-O1D
17	B	829	CLA	CHA-CBD-CGD-O2D
17	B	834	CLA	CHA-CBD-CGD-O1D
17	B	834	CLA	CHA-CBD-CGD-O2D
17	B	835	CLA	CHA-CBD-CGD-O1D
17	B	835	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	J	101	CLA	CHA-CBD-CGD-O1D
17	7	601	CLA	CHA-CBD-CGD-O1D
17	7	601	CLA	CHA-CBD-CGD-O2D
17	7	602	CLA	CHA-CBD-CGD-O1D
17	7	602	CLA	CHA-CBD-CGD-O2D
17	7	605	CLA	CHA-CBD-CGD-O1D
17	7	610	CLA	CHA-CBD-CGD-O1D
17	8	602	CLA	CHA-CBD-CGD-O1D
17	8	602	CLA	CHA-CBD-CGD-O2D
17	8	613	CLA	CHA-CBD-CGD-O2D
17	4	601	CLA	CHA-CBD-CGD-O1D
17	4	601	CLA	CHA-CBD-CGD-O2D
17	5	304	CLA	CHA-CBD-CGD-O1D
17	5	304	CLA	CHA-CBD-CGD-O2D
17	5	311	CLA	CHA-CBD-CGD-O1D
17	5	311	CLA	CHA-CBD-CGD-O2D
17	6	601	CLA	CHA-CBD-CGD-O2D
20	1	601	CHL	CHA-CBD-CGD-O1D
20	Z	601	CHL	CHA-CBD-CGD-O1D
17	4	602	CLA	C1A-C2A-CAA-CBA
17	5	315	CLA	C1A-C2A-CAA-CBA
17	A	804	CLA	CAD-CBD-CGD-O1D
17	A	813	CLA	CAD-CBD-CGD-O1D
17	A	818	CLA	CAD-CBD-CGD-O1D
17	A	832	CLA	CAD-CBD-CGD-O1D
17	A	835	CLA	CAD-CBD-CGD-O1D
17	A	836	CLA	CAD-CBD-CGD-O1D
17	A	841	CLA	CAD-CBD-CGD-O1D
17	A	842	CLA	CAD-CBD-CGD-O1D
17	B	834	CLA	CAD-CBD-CGD-O1D
17	B	835	CLA	CAD-CBD-CGD-O1D
17	J	101	CLA	CAD-CBD-CGD-O1D
17	1	603	CLA	CAD-CBD-CGD-O1D
17	7	601	CLA	CAD-CBD-CGD-O1D
17	7	605	CLA	CAD-CBD-CGD-O1D
17	6	601	CLA	CAD-CBD-CGD-O1D
20	1	601	CHL	CAD-CBD-CGD-O1D
20	Z	601	CHL	CAD-CBD-CGD-O1D
17	B	834	CLA	C4C-C3C-CAC-CBC
17	A	837	CLA	C3A-C2A-CAA-CBA
17	5	308	CLA	C3A-C2A-CAA-CBA
20	6	606	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
17	5	314	CLA	C2A-CAA-CBA-CGA
17	3	312	CLA	C2C-C3C-CAC-CBC
17	B	834	CLA	C2C-C3C-CAC-CBC
17	5	306	CLA	C2-C1-O2A-CGA
17	A	823	CLA	C2C-C3C-CAC-CBC
17	B	821	CLA	C2C-C3C-CAC-CBC
18	A	840	PQN	C17-C18-C20-C21
18	A	840	PQN	C22-C23-C25-C26
18	B	840	PQN	C17-C18-C20-C21
20	6	606	CHL	C2C-C3C-CAC-CBC
20	1	601	CHL	C4-C3-C5-C6
17	5	315	CLA	CAA-CBA-CGA-O2A
17	B	815	CLA	C4-C3-C5-C6
17	B	815	CLA	C2-C1-O2A-CGA
17	B	815	CLA	C3A-C2A-CAA-CBA
17	5	315	CLA	CAA-CBA-CGA-O1A
17	4	602	CLA	CAA-CBA-CGA-O1A
17	A	841	CLA	C2C-C3C-CAC-CBC
17	A	841	CLA	C1A-C2A-CAA-CBA
17	B	812	CLA	C3A-C2A-CAA-CBA
17	1	605	CLA	C3A-C2A-CAA-CBA
17	4	602	CLA	CAA-CBA-CGA-O2A
17	7	612	CLA	CAA-CBA-CGA-O2A
18	B	840	PQN	C14-C13-C15-C16
17	A	820	CLA	C1A-C2A-CAA-CBA
17	8	613	CLA	C1A-C2A-CAA-CBA
20	6	605	CHL	C1A-C2A-CAA-CBA
17	B	802	CLA	CAA-CBA-CGA-O2A
17	B	810	CLA	CAA-CBA-CGA-O2A
17	6	610	CLA	CAA-CBA-CGA-O2A
17	8	607	CLA	C2C-C3C-CAC-CBC
17	7	612	CLA	CAA-CBA-CGA-O1A
16	A	801	CL0	CAD-CBD-CGD-O2D
17	A	810	CLA	CAD-CBD-CGD-O2D
17	A	816	CLA	CAD-CBD-CGD-O2D
17	A	831	CLA	CAD-CBD-CGD-O2D
17	A	838	CLA	CAD-CBD-CGD-O2D
17	A	839	CLA	CAD-CBD-CGD-O2D
17	B	816	CLA	CAD-CBD-CGD-O2D
17	B	818	CLA	CAD-CBD-CGD-O2D
17	B	819	CLA	CAD-CBD-CGD-O2D
17	B	824	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	B	829	CLA	CAD-CBD-CGD-O2D
17	B	830	CLA	CAD-CBD-CGD-O2D
17	B	833	CLA	CAD-CBD-CGD-O2D
17	1	604	CLA	CAD-CBD-CGD-O2D
17	1	605	CLA	CAD-CBD-CGD-O2D
17	1	608	CLA	CAD-CBD-CGD-O2D
17	3	304	CLA	CAD-CBD-CGD-O2D
17	3	308	CLA	CAD-CBD-CGD-O2D
17	7	607	CLA	CAD-CBD-CGD-O2D
17	7	610	CLA	CAD-CBD-CGD-O2D
17	8	601	CLA	CAD-CBD-CGD-O2D
17	5	311	CLA	CAD-CBD-CGD-O2D
17	6	603	CLA	CAD-CBD-CGD-O2D
20	5	305	CHL	CAD-CBD-CGD-O2D
18	B	840	PQN	C12-C13-C15-C16
17	8	603	CLA	CAA-CBA-CGA-O1A
17	5	306	CLA	O2A-C1-C2-C3
17	5	303	CLA	CAA-CBA-CGA-O2A
17	B	802	CLA	CAA-CBA-CGA-O1A
17	8	603	CLA	CAA-CBA-CGA-O2A
17	A	804	CLA	CHA-CBD-CGD-O2D
17	A	812	CLA	CHA-CBD-CGD-O2D
17	A	820	CLA	CHA-CBD-CGD-O1D
17	A	820	CLA	CHA-CBD-CGD-O2D
17	A	825	CLA	CHA-CBD-CGD-O1D
17	A	825	CLA	CHA-CBD-CGD-O2D
17	A	835	CLA	CHA-CBD-CGD-O2D
17	A	836	CLA	CHA-CBD-CGD-O1D
17	A	841	CLA	CHA-CBD-CGD-O2D
17	B	806	CLA	CHA-CBD-CGD-O1D
17	B	806	CLA	CHA-CBD-CGD-O2D
17	B	807	CLA	CHA-CBD-CGD-O1D
17	B	807	CLA	CHA-CBD-CGD-O2D
17	B	809	CLA	CHA-CBD-CGD-O1D
17	B	809	CLA	CHA-CBD-CGD-O2D
17	B	810	CLA	CHA-CBD-CGD-O1D
17	B	810	CLA	CHA-CBD-CGD-O2D
17	B	817	CLA	CHA-CBD-CGD-O1D
17	B	817	CLA	CHA-CBD-CGD-O2D
17	B	822	CLA	CHA-CBD-CGD-O1D
17	B	822	CLA	CHA-CBD-CGD-O2D
17	B	827	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	F	302	CLA	CHA-CBD-CGD-O1D
17	F	302	CLA	CHA-CBD-CGD-O2D
17	1	602	CLA	CHA-CBD-CGD-O1D
17	1	602	CLA	CHA-CBD-CGD-O2D
17	1	603	CLA	CHA-CBD-CGD-O1D
17	3	302	CLA	CHA-CBD-CGD-O2D
17	3	311	CLA	CHA-CBD-CGD-O1D
17	3	311	CLA	CHA-CBD-CGD-O2D
17	7	605	CLA	CHA-CBD-CGD-O2D
17	7	610	CLA	CHA-CBD-CGD-O2D
17	7	612	CLA	CHA-CBD-CGD-O1D
17	7	612	CLA	CHA-CBD-CGD-O2D
17	7	613	CLA	CHA-CBD-CGD-O1D
17	8	605	CLA	CHA-CBD-CGD-O1D
17	8	605	CLA	CHA-CBD-CGD-O2D
17	8	613	CLA	CHA-CBD-CGD-O1D
17	4	602	CLA	CHA-CBD-CGD-O2D
17	5	303	CLA	CHA-CBD-CGD-O1D
17	5	303	CLA	CHA-CBD-CGD-O2D
17	5	314	CLA	CHA-CBD-CGD-O1D
17	5	314	CLA	CHA-CBD-CGD-O2D
17	6	603	CLA	CHA-CBD-CGD-O1D
17	6	603	CLA	CHA-CBD-CGD-O2D
20	1	601	CHL	CHA-CBD-CGD-O2D
20	Z	601	CHL	CHA-CBD-CGD-O2D
17	B	810	CLA	CAA-CBA-CGA-O1A
17	A	835	CLA	C4C-C3C-CAC-CBC
17	5	314	CLA	CAA-CBA-CGA-O2A
17	A	841	CLA	C4C-C3C-CAC-CBC
17	F	302	CLA	C2C-C3C-CAC-CBC
17	6	610	CLA	CAA-CBA-CGA-O1A
20	3	307	CHL	CAA-CBA-CGA-O2A
20	1	601	CHL	C2-C3-C5-C6
17	7	607	CLA	C4C-C3C-CAC-CBC
17	5	303	CLA	CAA-CBA-CGA-O1A
17	3	304	CLA	CAA-CBA-CGA-O2A
17	A	809	CLA	CAD-CBD-CGD-O1D
17	B	801	CLA	CAD-CBD-CGD-O1D
17	B	827	CLA	CAD-CBD-CGD-O1D
17	B	839	CLA	CAD-CBD-CGD-O1D
17	3	311	CLA	CAD-CBD-CGD-O1D
17	5	314	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	6	610	CLA	CAD-CBD-CGD-O1D
17	B	820	CLA	C3A-C2A-CAA-CBA
20	3	307	CHL	CAA-CBA-CGA-O1A
18	A	840	PQN	C23-C25-C26-C27
17	5	314	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

118 monomers are involved in 179 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	838	CLA	1	0
17	A	839	CLA	1	0
20	6	607	CHL	1	0
17	B	807	CLA	2	0
17	4	605	CLA	2	0
17	8	610	CLA	1	0
17	8	604	CLA	2	0
17	A	829	CLA	1	0
17	B	816	CLA	1	0
17	B	828	CLA	4	0
19	C	102	SF4	2	0
17	1	603	CLA	2	0
17	A	809	CLA	3	0
20	3	307	CHL	1	0
17	B	804	CLA	3	0
17	B	814	CLA	2	0
17	B	832	CLA	1	0
17	7	613	CLA	1	0
20	5	313	CHL	1	0
17	A	806	CLA	5	0
17	6	610	CLA	1	0
17	A	808	CLA	4	0
17	7	604	CLA	2	0
17	F	302	CLA	4	0
17	J	102	CLA	1	0
17	A	823	CLA	2	0
17	7	605	CLA	2	0
18	B	840	PQN	3	0
17	B	810	CLA	6	0
17	8	602	CLA	1	0
17	B	802	CLA	1	0
17	8	605	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	815	CLA	6	0
20	8	606	CHL	2	0
17	B	827	CLA	5	0
17	3	305	CLA	2	0
17	A	802	CLA	2	0
17	A	807	CLA	5	0
16	A	801	CL0	4	0
17	3	301	CLA	2	0
17	A	831	CLA	2	0
17	5	301	CLA	2	0
17	B	811	CLA	3	0
17	1	602	CLA	3	0
17	A	830	CLA	1	0
17	4	604	CLA	3	0
17	8	609	CLA	1	0
17	8	608	CLA	2	0
17	B	837	CLA	2	0
17	A	832	CLA	1	0
17	A	819	CLA	1	0
17	7	612	CLA	2	0
17	A	811	CLA	1	0
17	B	834	CLA	1	0
17	6	602	CLA	1	0
17	1	606	CLA	2	0
20	7	606	CHL	2	0
17	1	608	CLA	1	0
17	A	834	CLA	5	0
17	7	611	CLA	1	0
17	8	603	CLA	1	0
17	B	824	CLA	1	0
17	5	304	CLA	2	0
17	3	303	CLA	1	0
17	B	821	CLA	1	0
17	A	841	CLA	7	0
17	8	601	CLA	1	0
17	B	822	CLA	3	0
17	A	821	CLA	3	0
17	B	835	CLA	2	0
17	B	808	CLA	1	0
17	A	813	CLA	2	0
17	B	809	CLA	4	0
17	A	822	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	825	CLA	1	0
17	B	815	CLA	5	0
17	A	837	CLA	3	0
17	A	825	CLA	2	0
17	1	610	CLA	2	0
17	B	831	CLA	1	0
17	3	311	CLA	3	0
20	6	605	CHL	3	0
17	A	836	CLA	3	0
17	B	812	CLA	1	0
17	A	833	CLA	2	0
17	A	803	CLA	1	0
17	B	839	CLA	2	0
20	5	305	CHL	1	0
20	6	606	CHL	3	0
17	3	306	CLA	1	0
17	B	826	CLA	3	0
17	5	311	CLA	2	0
17	A	843	CLA	1	0
17	3	309	CLA	1	0
17	5	309	CLA	1	0
17	A	814	CLA	2	0
17	B	833	CLA	3	0
17	1	609	CLA	4	0
17	5	310	CLA	2	0
17	8	613	CLA	1	0
17	B	823	CLA	2	0
17	B	801	CLA	2	0
17	J	101	CLA	1	0
17	B	805	CLA	2	0
17	5	306	CLA	2	0
17	A	824	CLA	2	0
17	A	838	CLA	1	0
17	B	818	CLA	1	0
17	B	836	CLA	1	0
17	8	612	CLA	2	0
17	A	812	CLA	2	0
17	3	312	CLA	2	0
17	6	609	CLA	3	0
17	4	602	CLA	1	0
17	5	303	CLA	1	0
17	3	304	CLA	1	0

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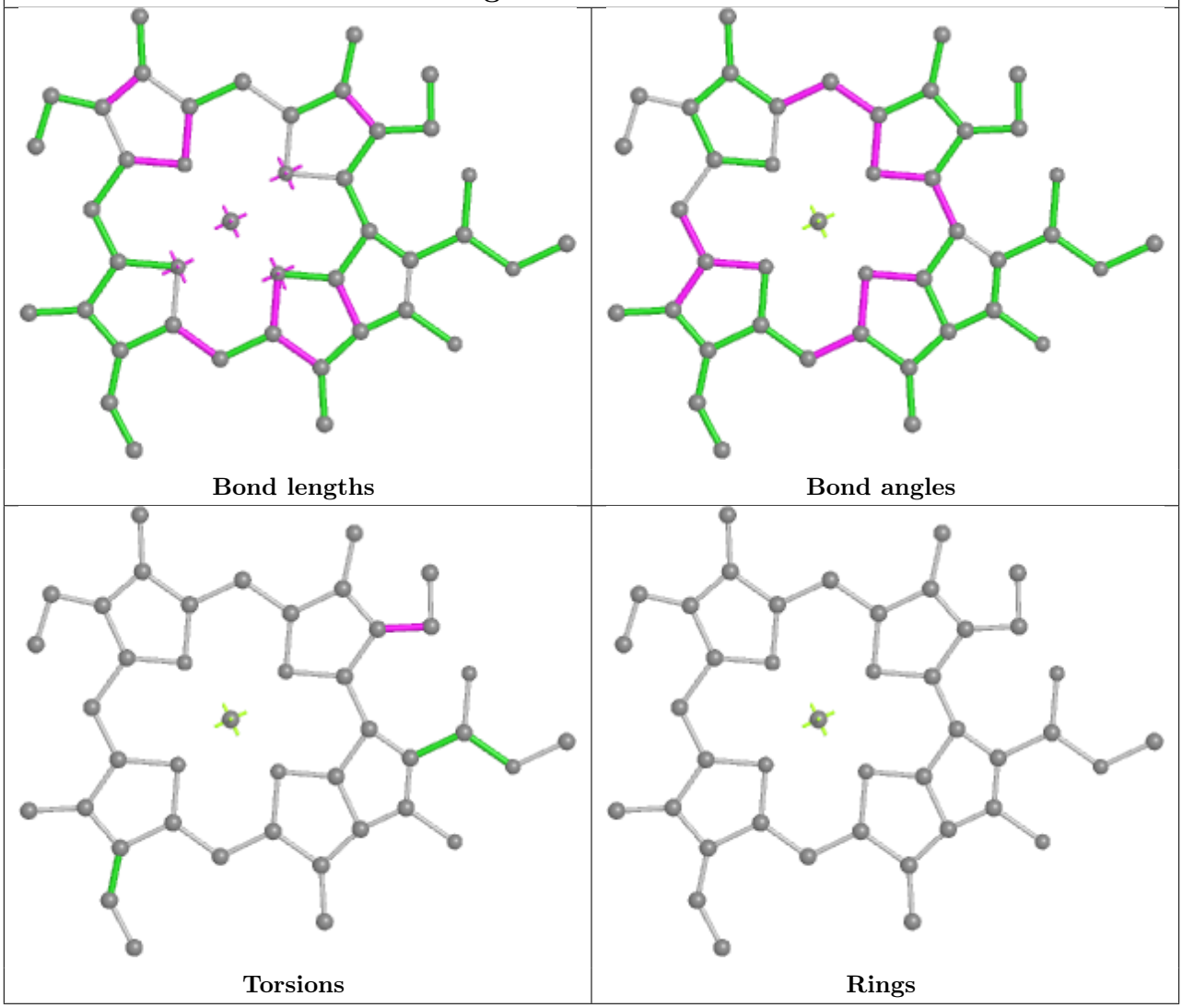
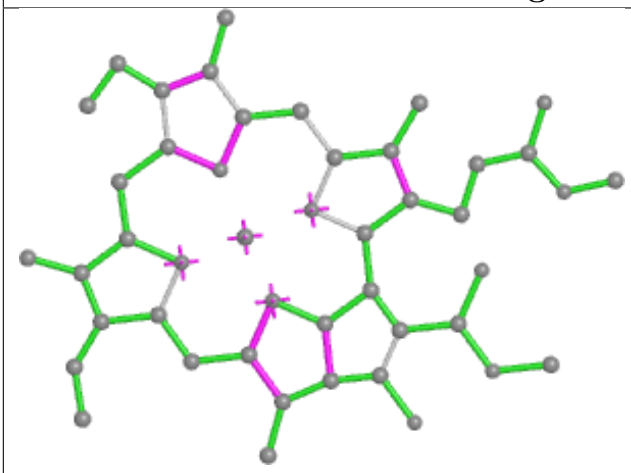
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	820	CLA	2	0
17	1	605	CLA	2	0

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 then 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.

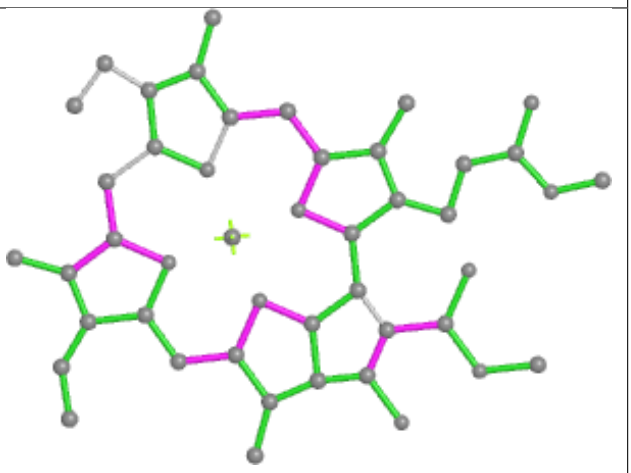
Ligand CLA B 838



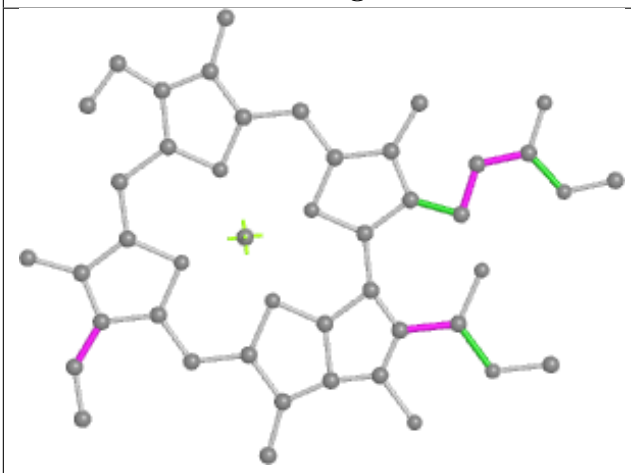
Ligand CLA 5 314



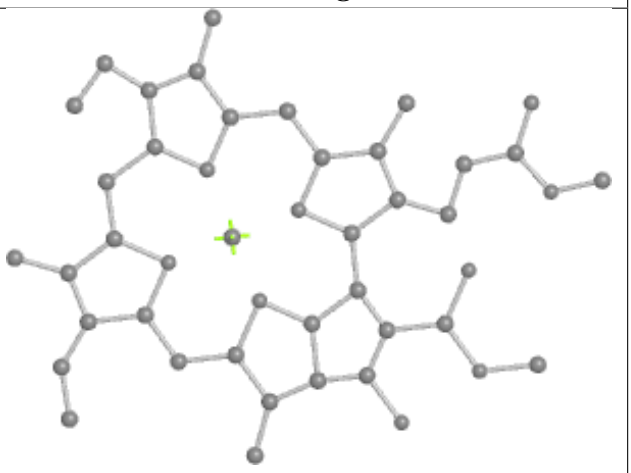
Bond lengths



Bond angles

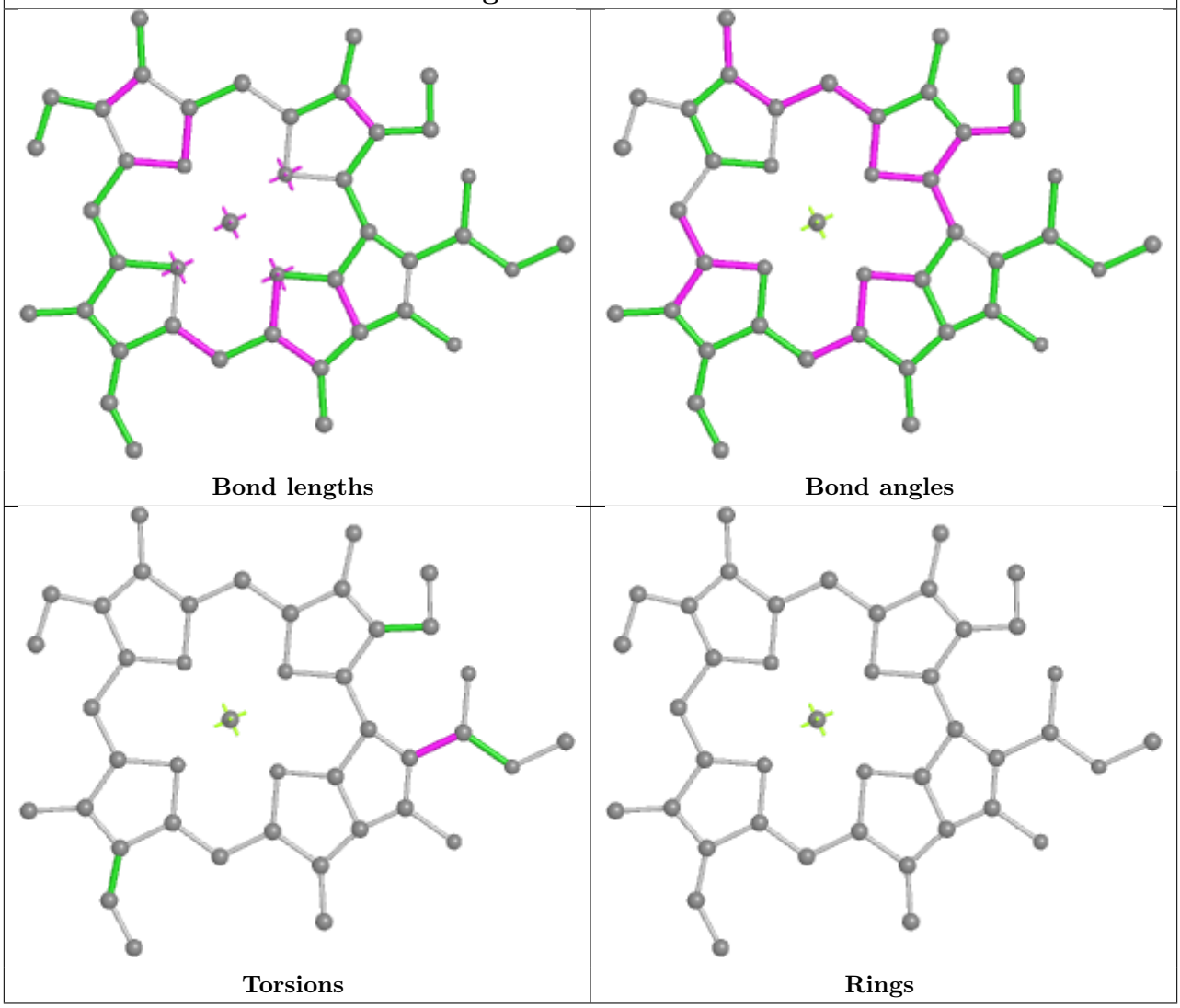


Torsions

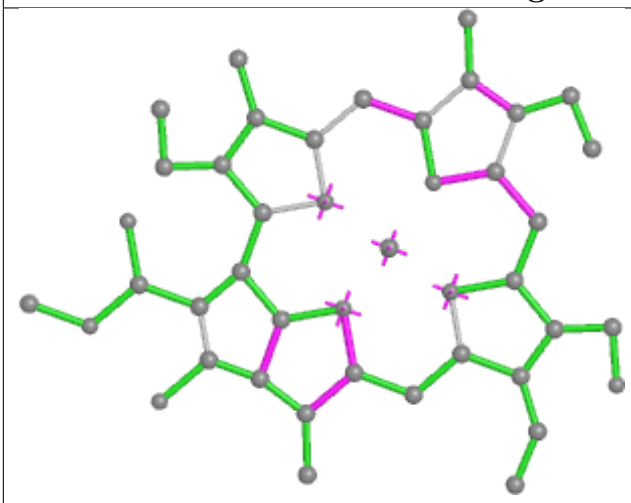


Rings

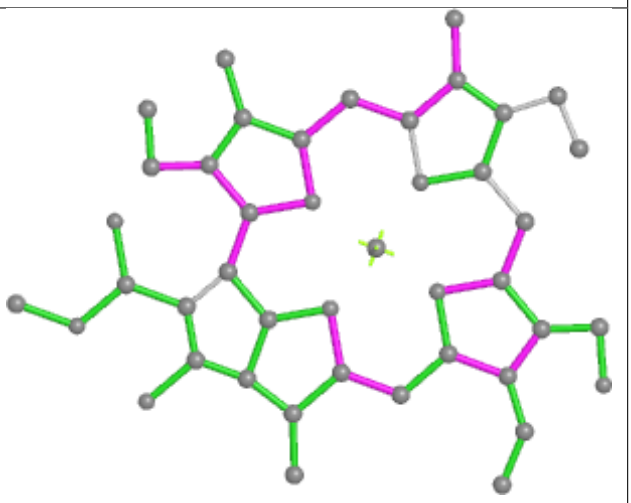
Ligand CLA A 839



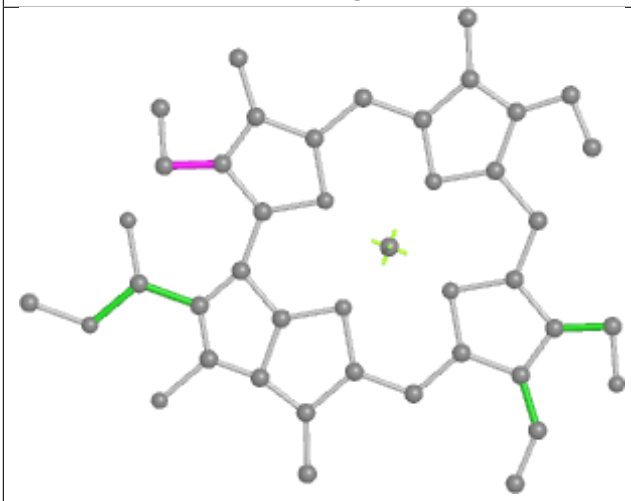
Ligand CHL 6 607



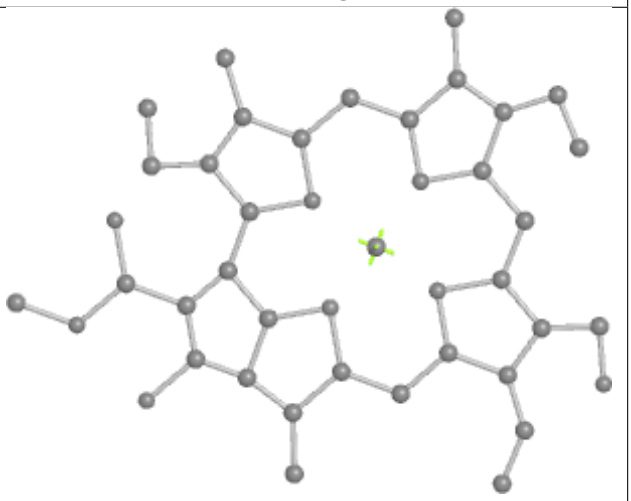
Bond lengths



Bond angles

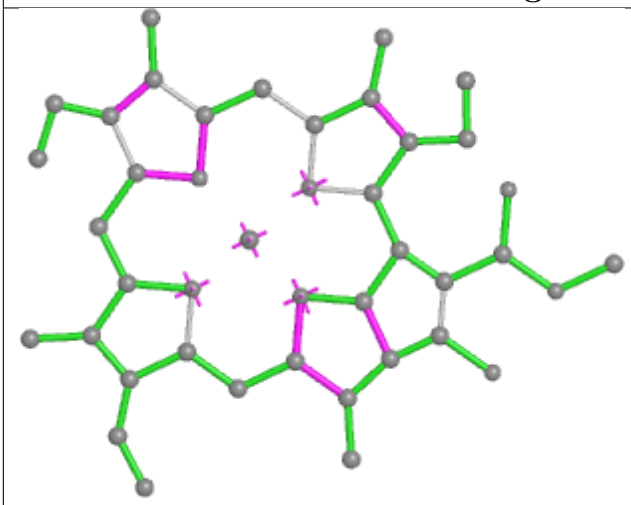


Torsions

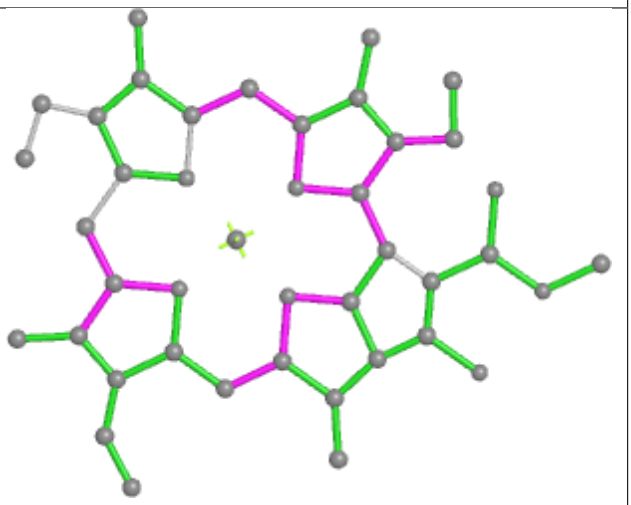


Rings

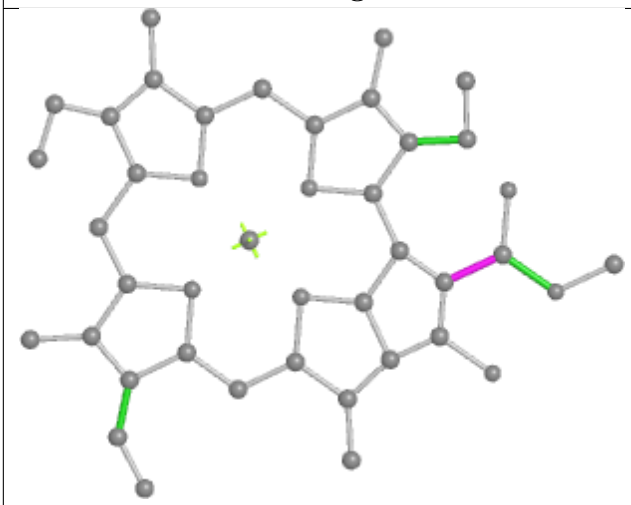
Ligand CLA B 807



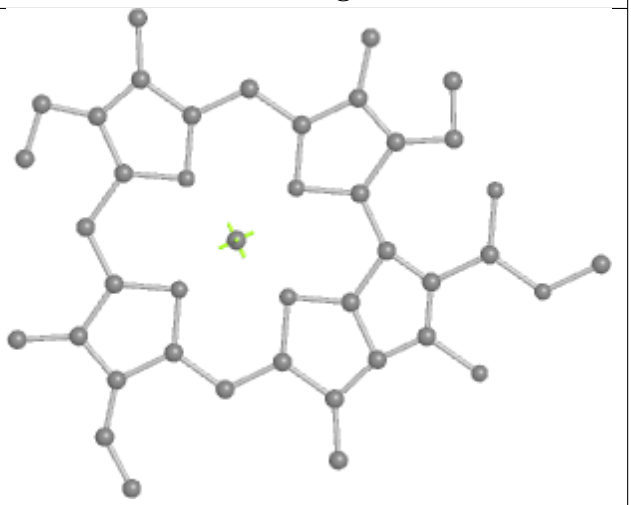
Bond lengths



Bond angles

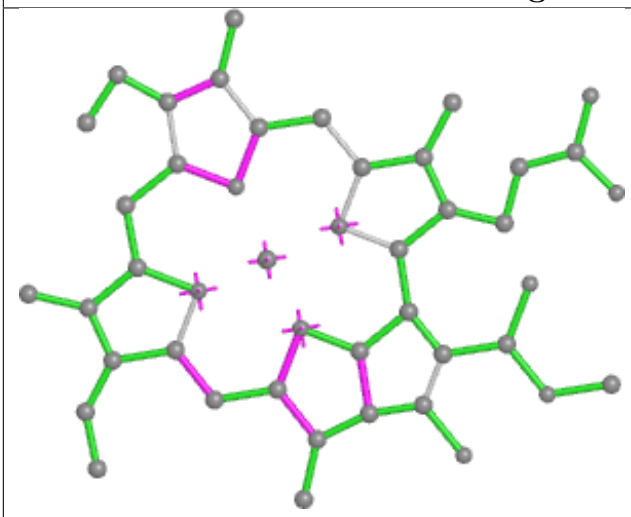


Torsions

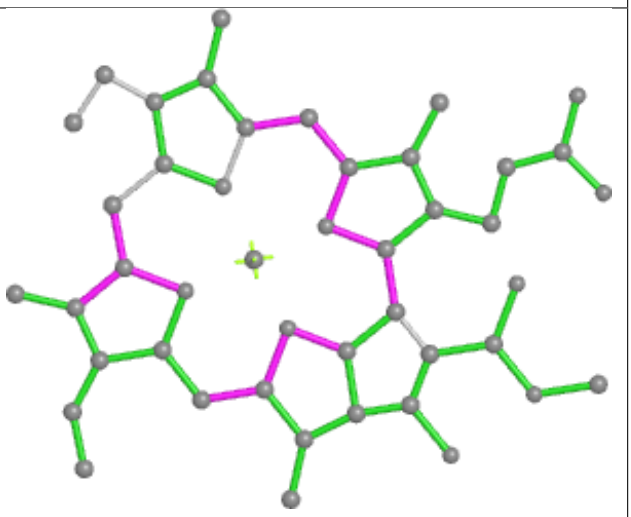


Rings

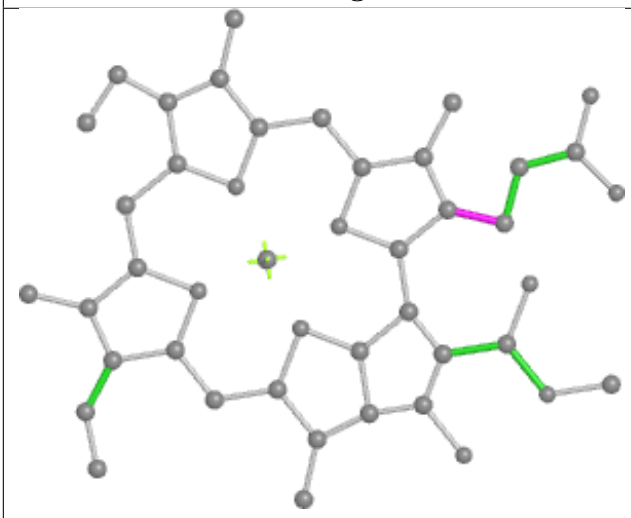
Ligand CLA 4 605



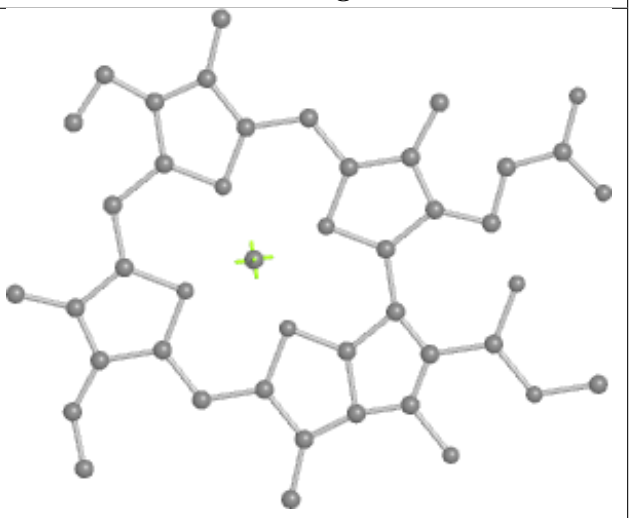
Bond lengths



Bond angles

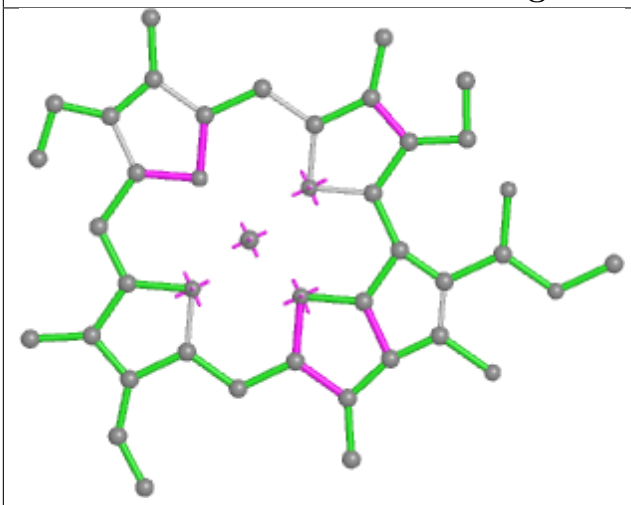


Torsions

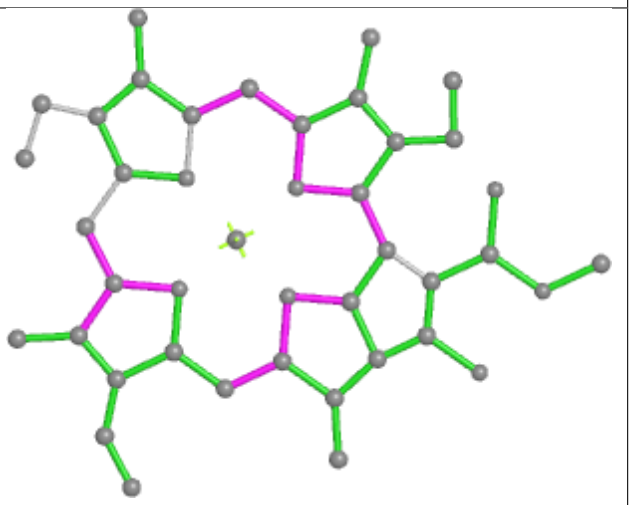


Rings

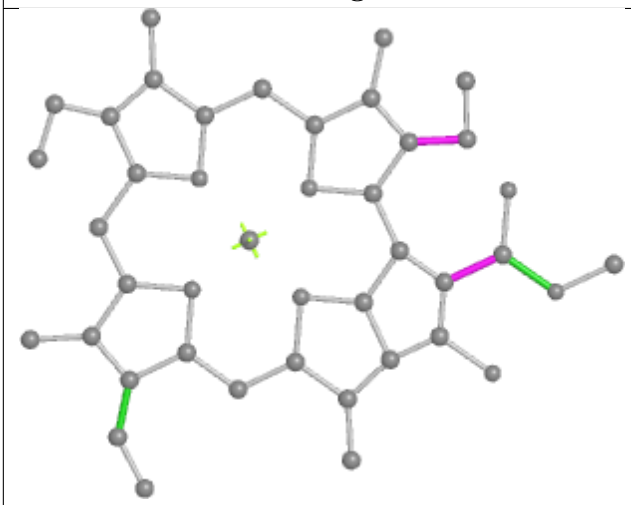
Ligand CLA 8 610



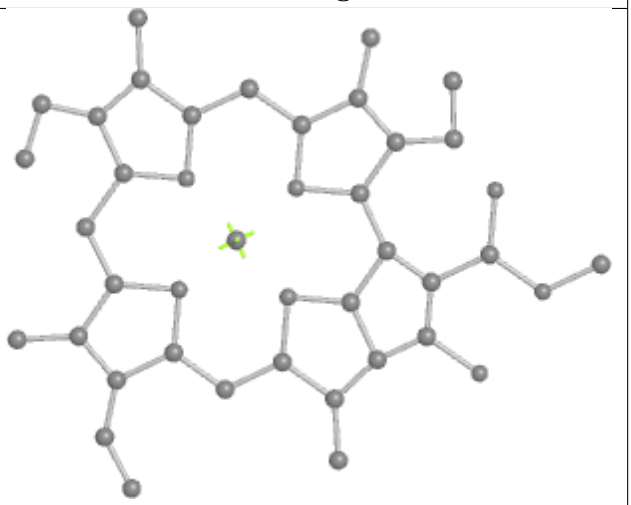
Bond lengths



Bond angles

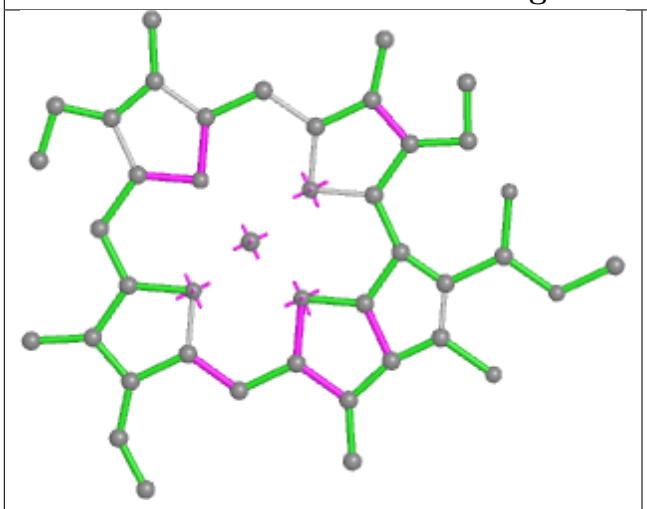


Torsions



Rings

Ligand CLA 8 604



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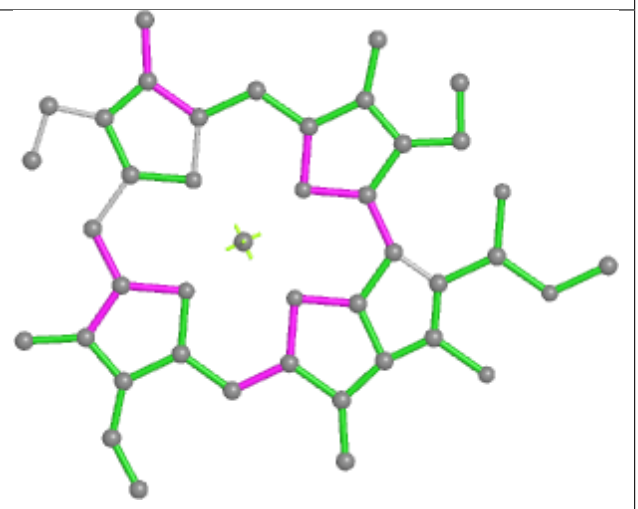
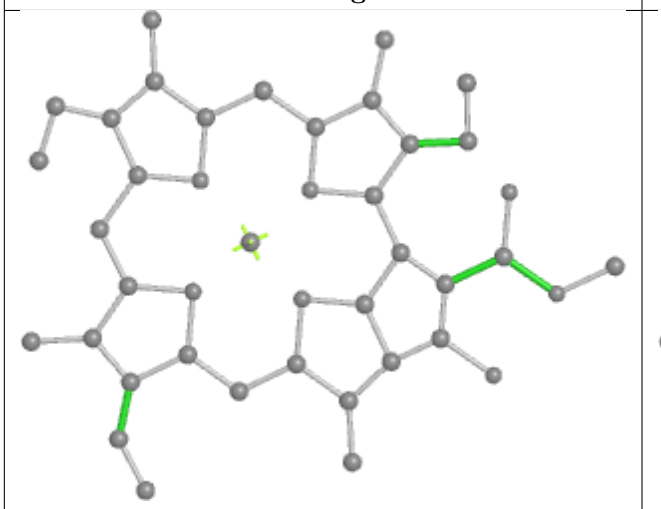


Bond angles



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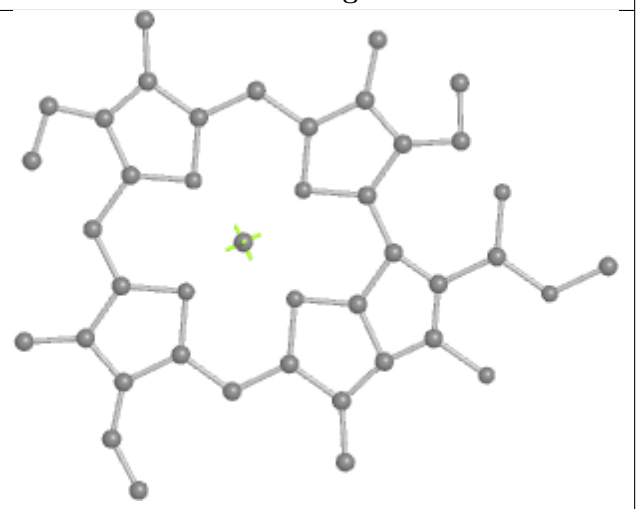
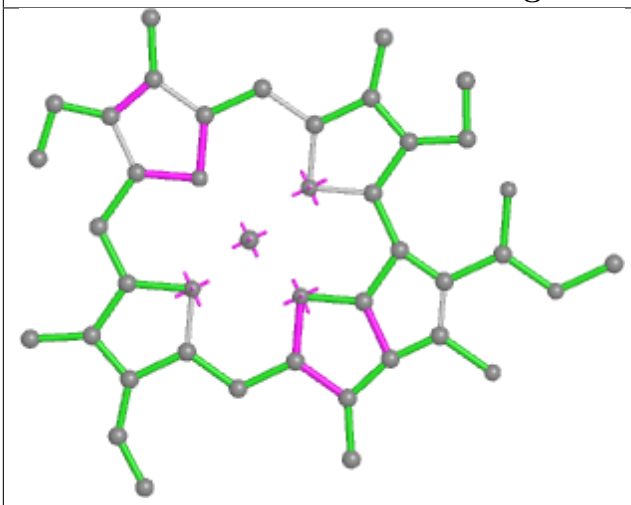


Rings

Ligand CLA A 829



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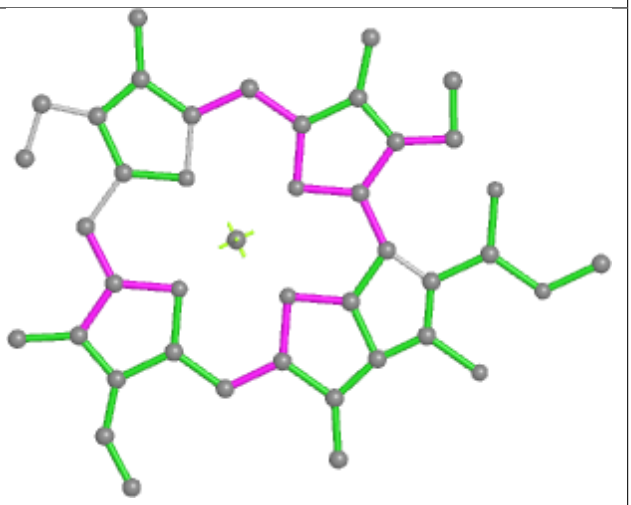
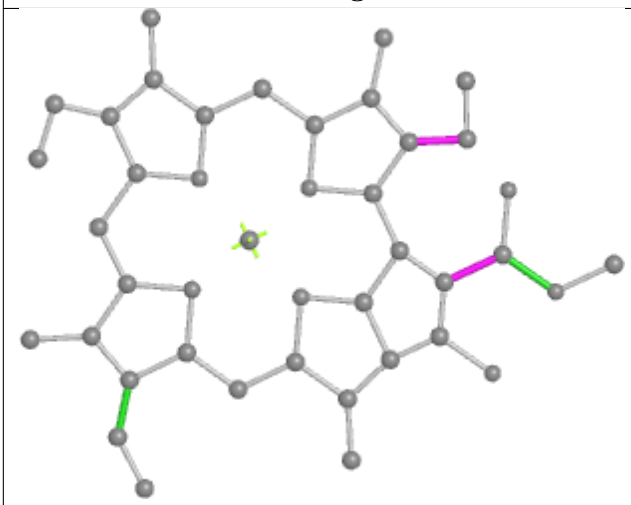


Bond angles



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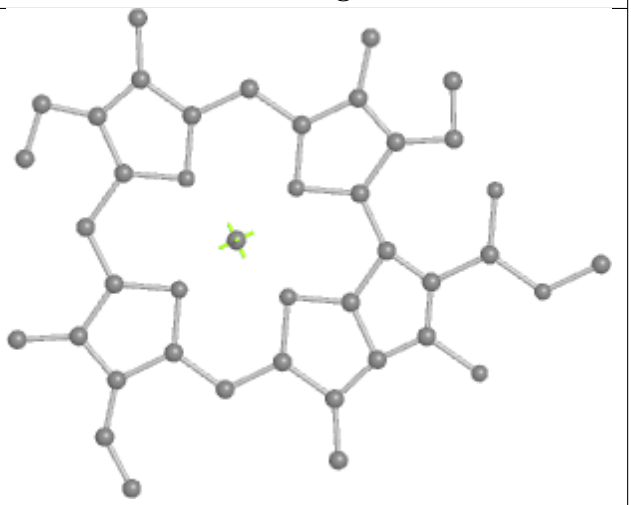
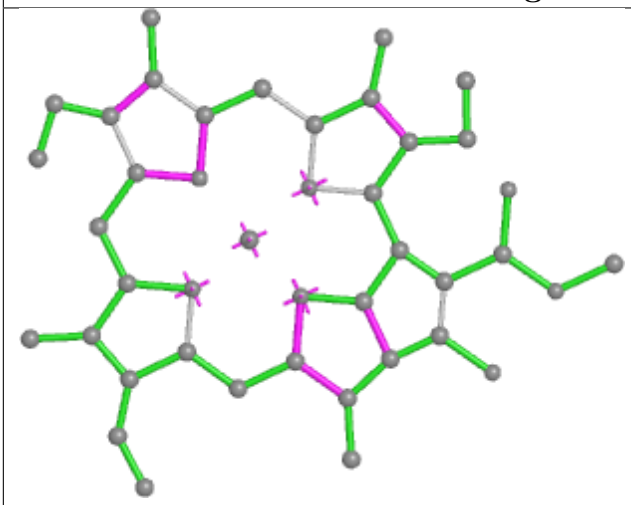


Rings

Ligand CLA B 816



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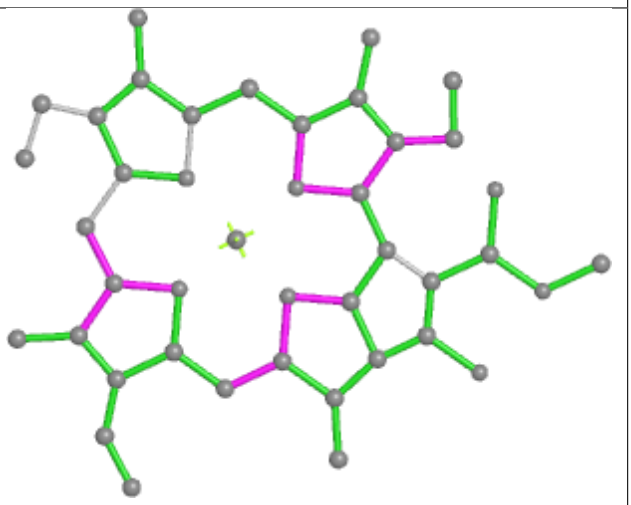

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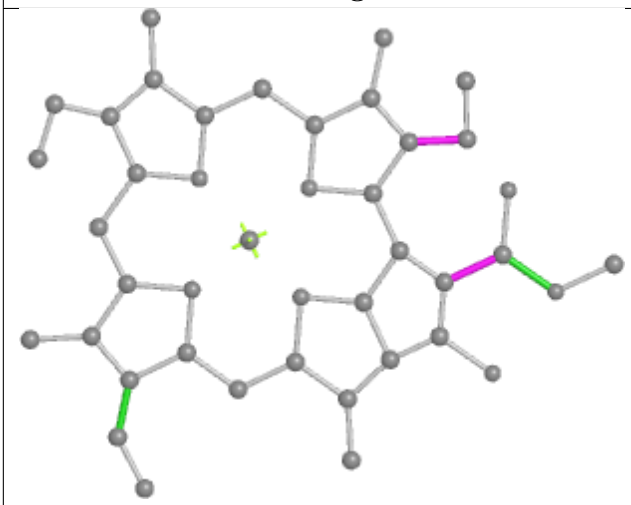

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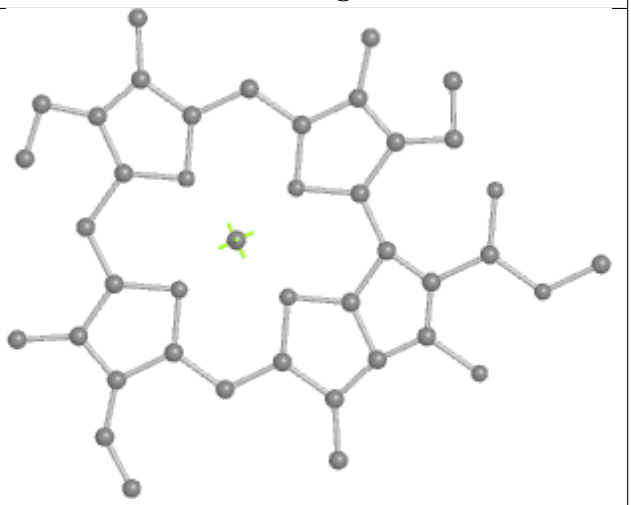
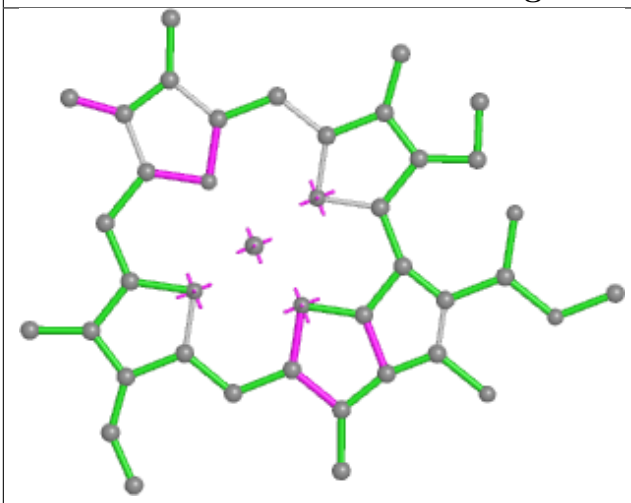
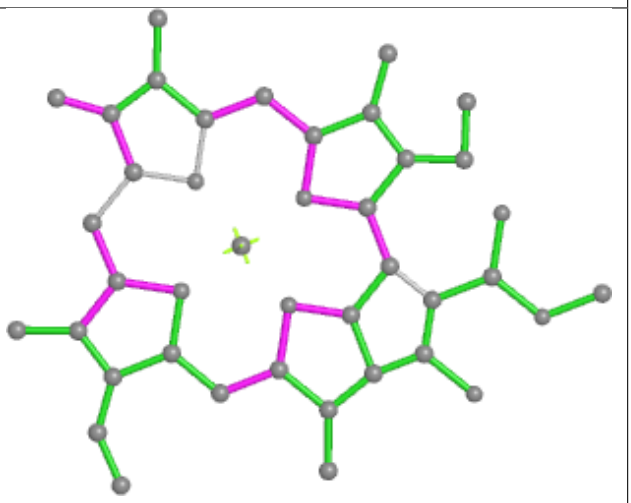


Rings

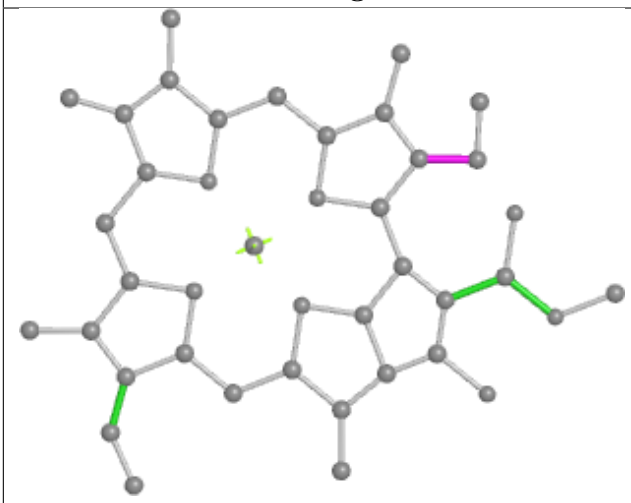
Ligand CLA B 813



Bond lengths



Bond angles



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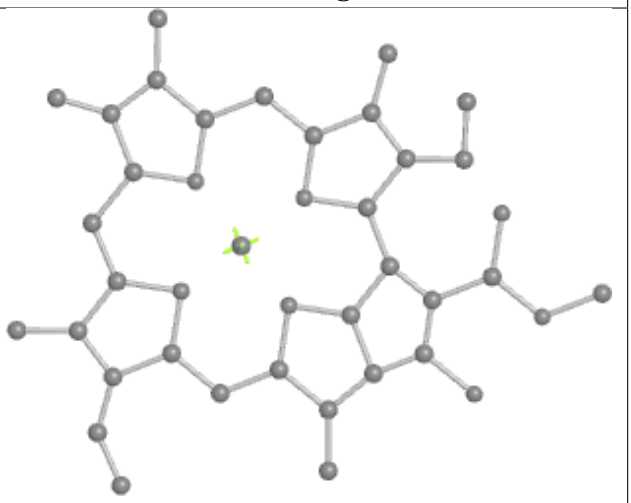
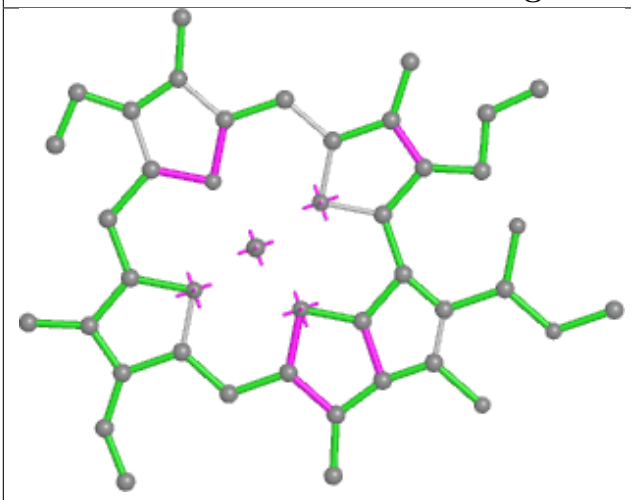


Rings

Ligand CLA B 828



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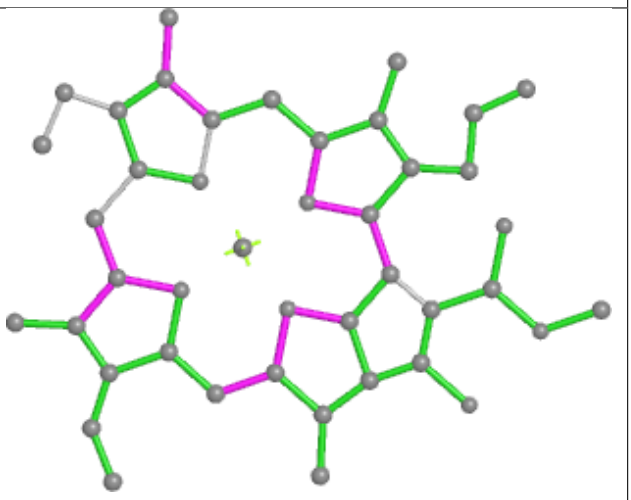

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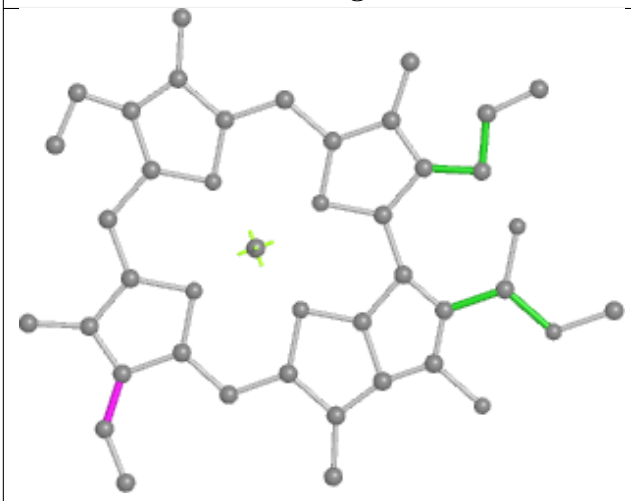

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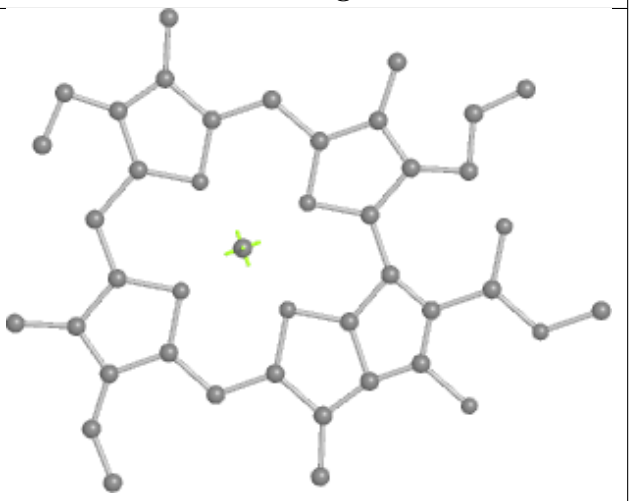
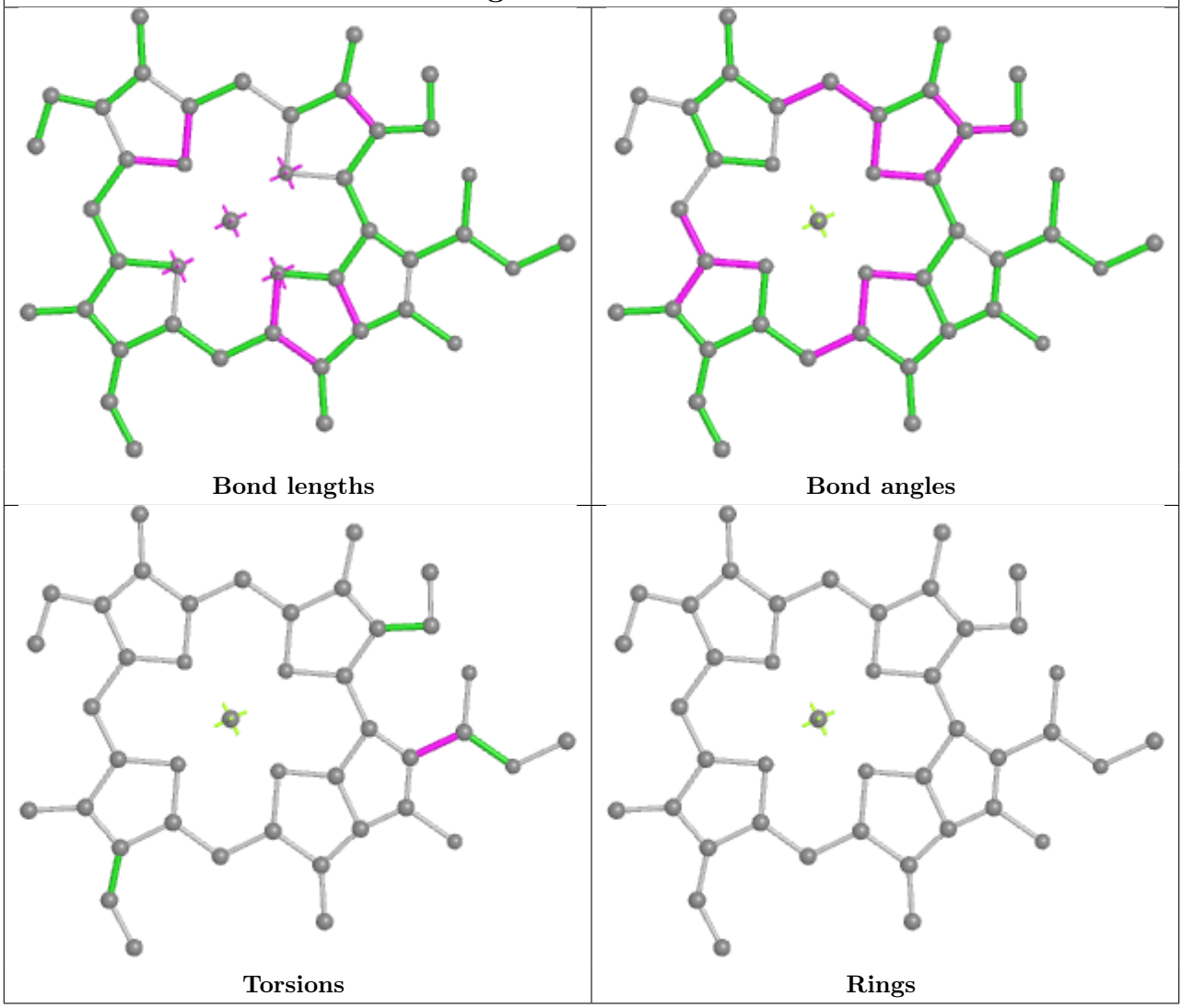
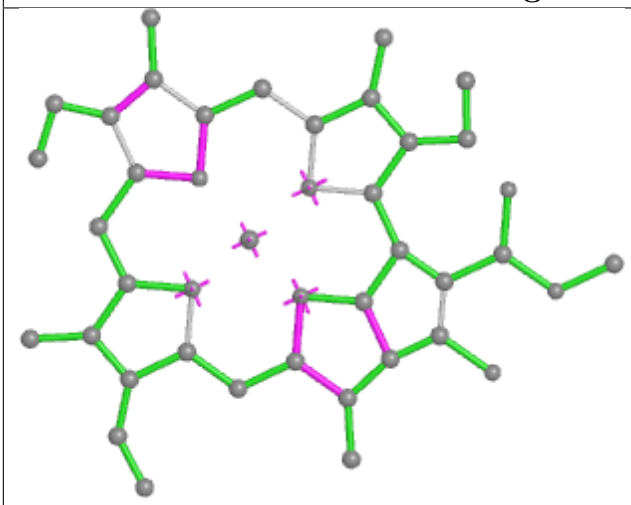


Rings

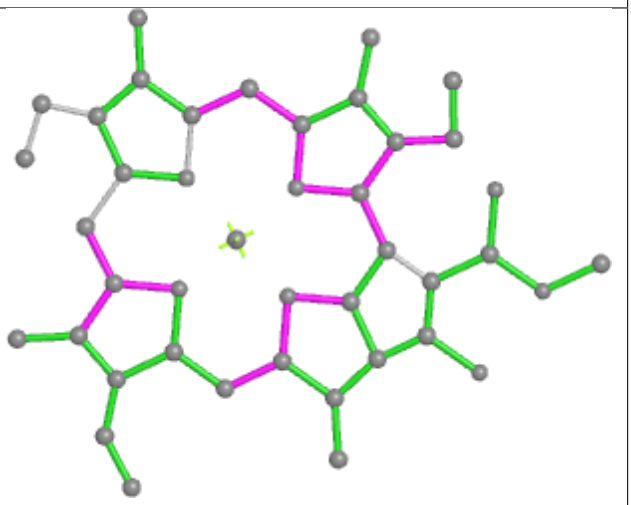
Ligand CLA 3 308



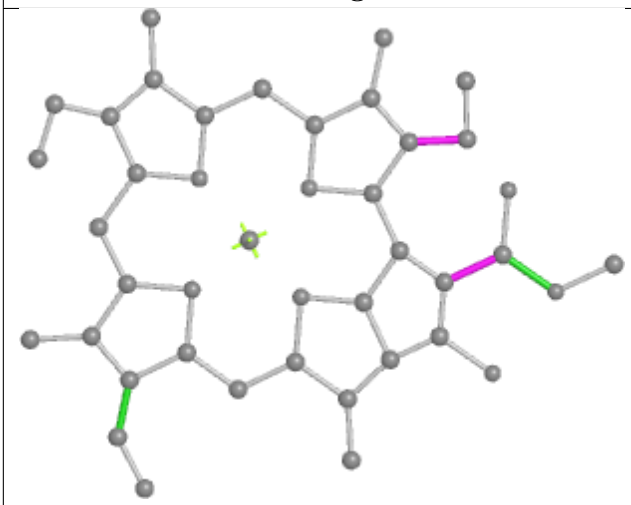
Ligand CLA A 816



Bond lengths



Bond angles



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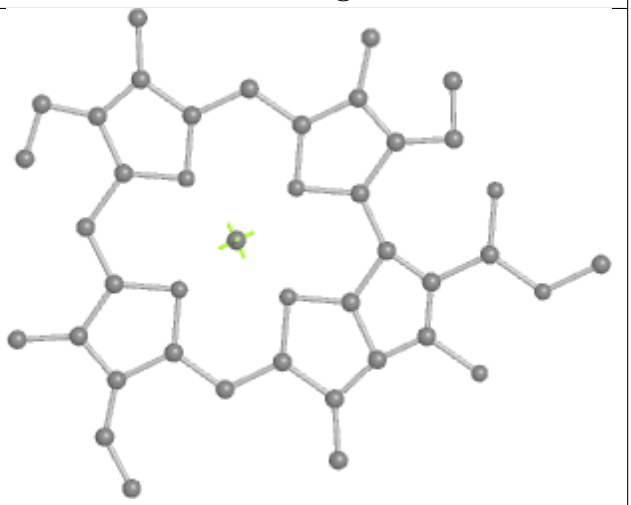
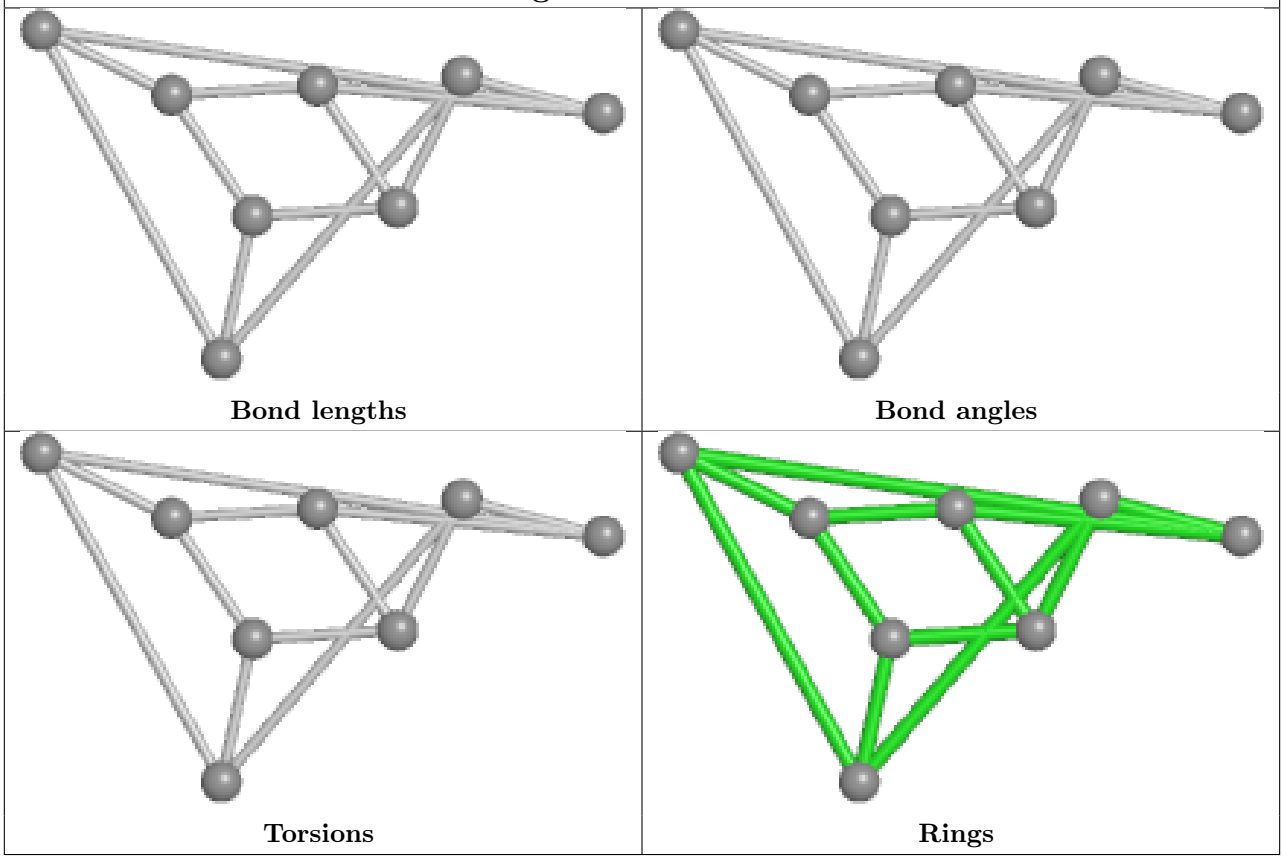
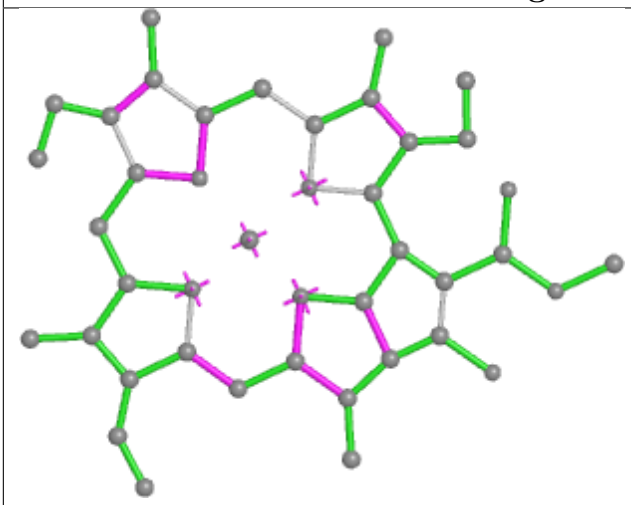


Rings

Ligand SF4 C 102



Ligand CLA 1 603



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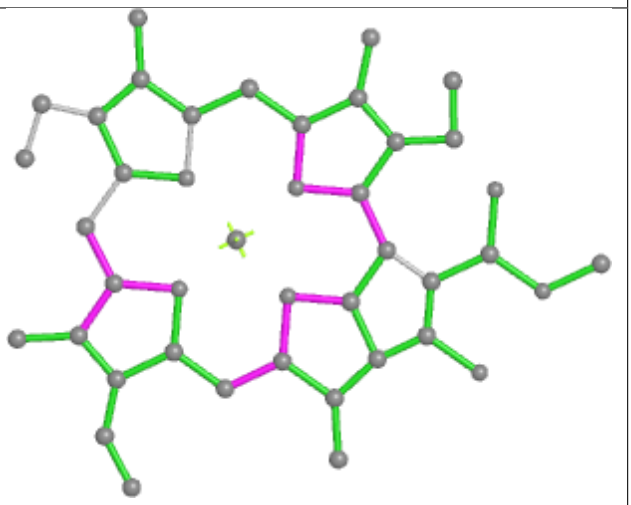
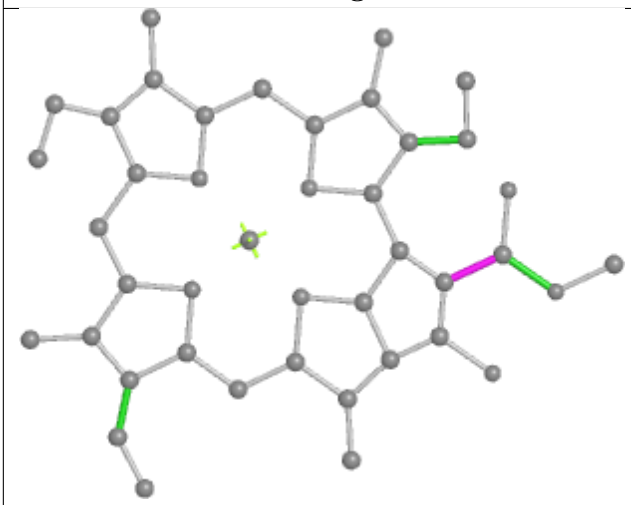


Bond angles



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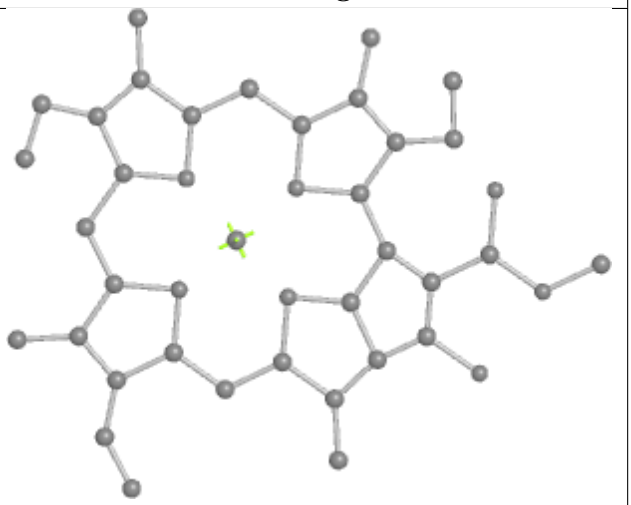
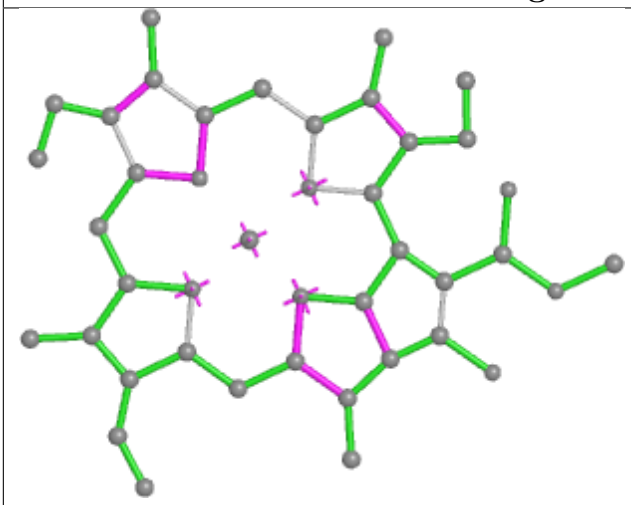
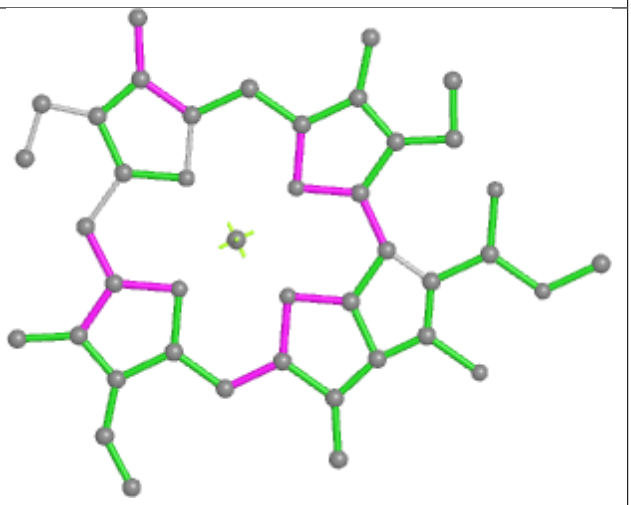


Rings

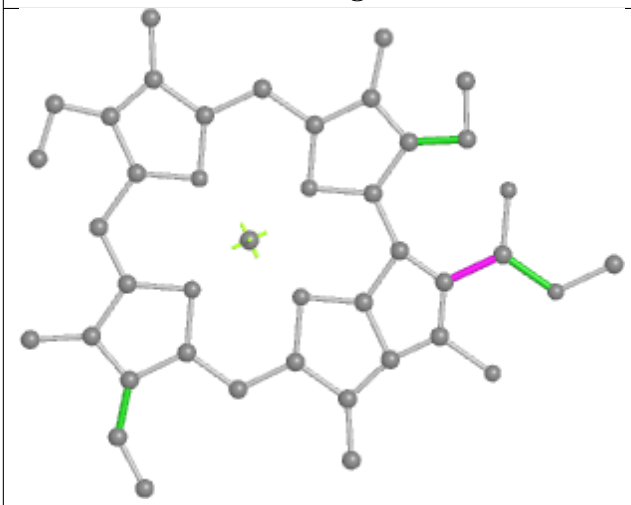
Ligand CLA 7 601



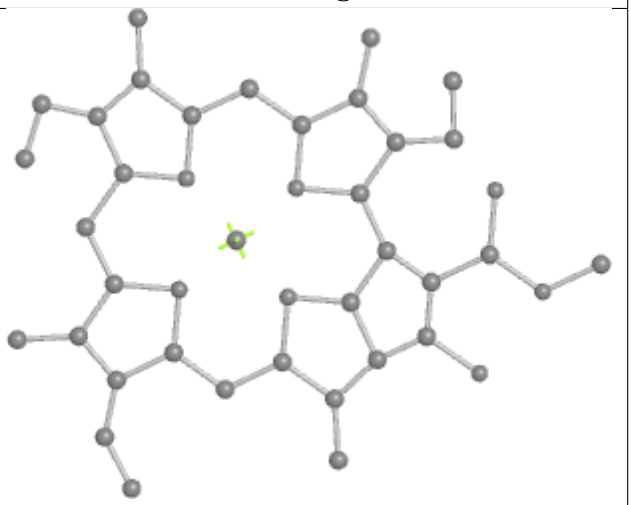
Bond lengths



Bond angles

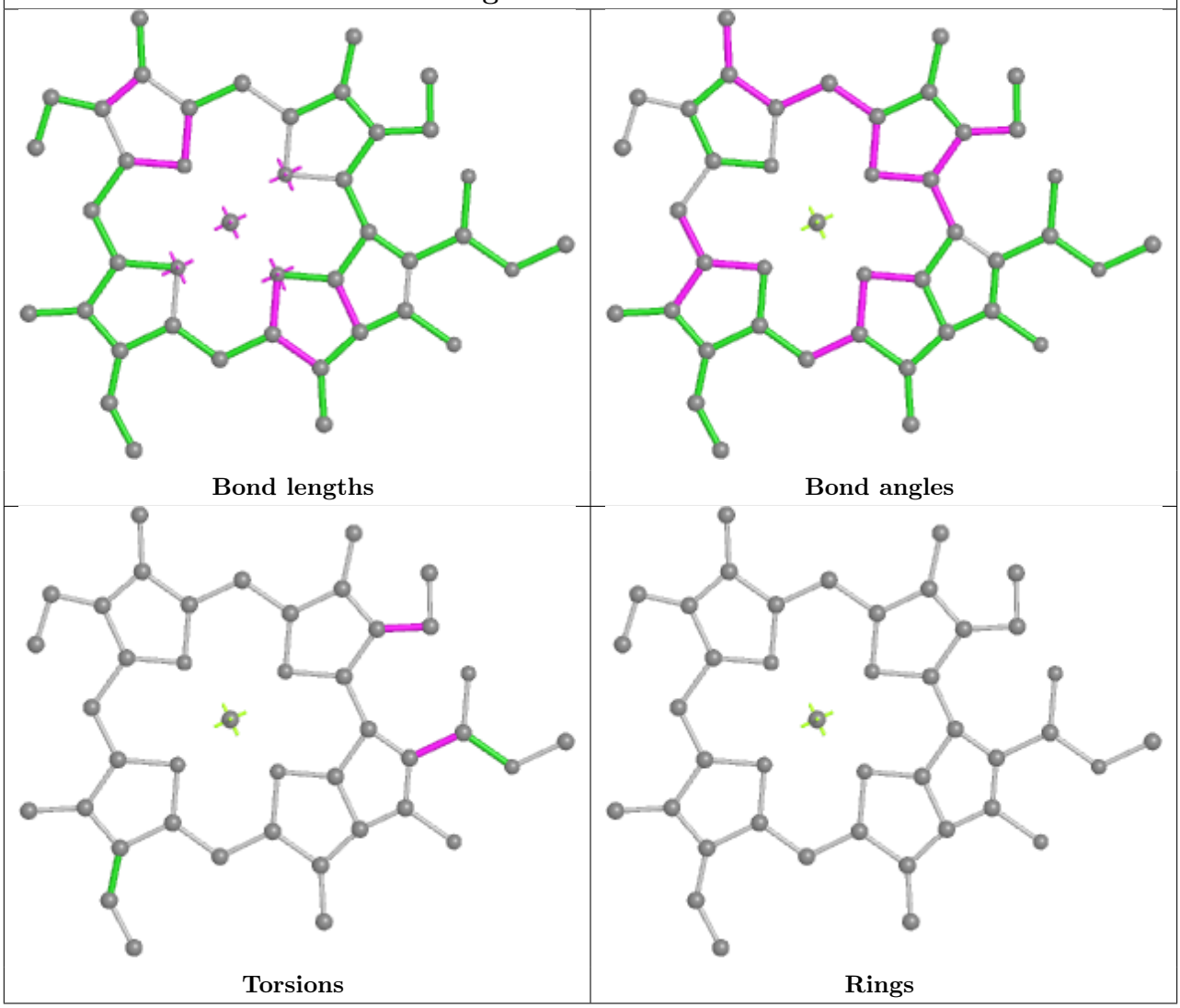


Torsions

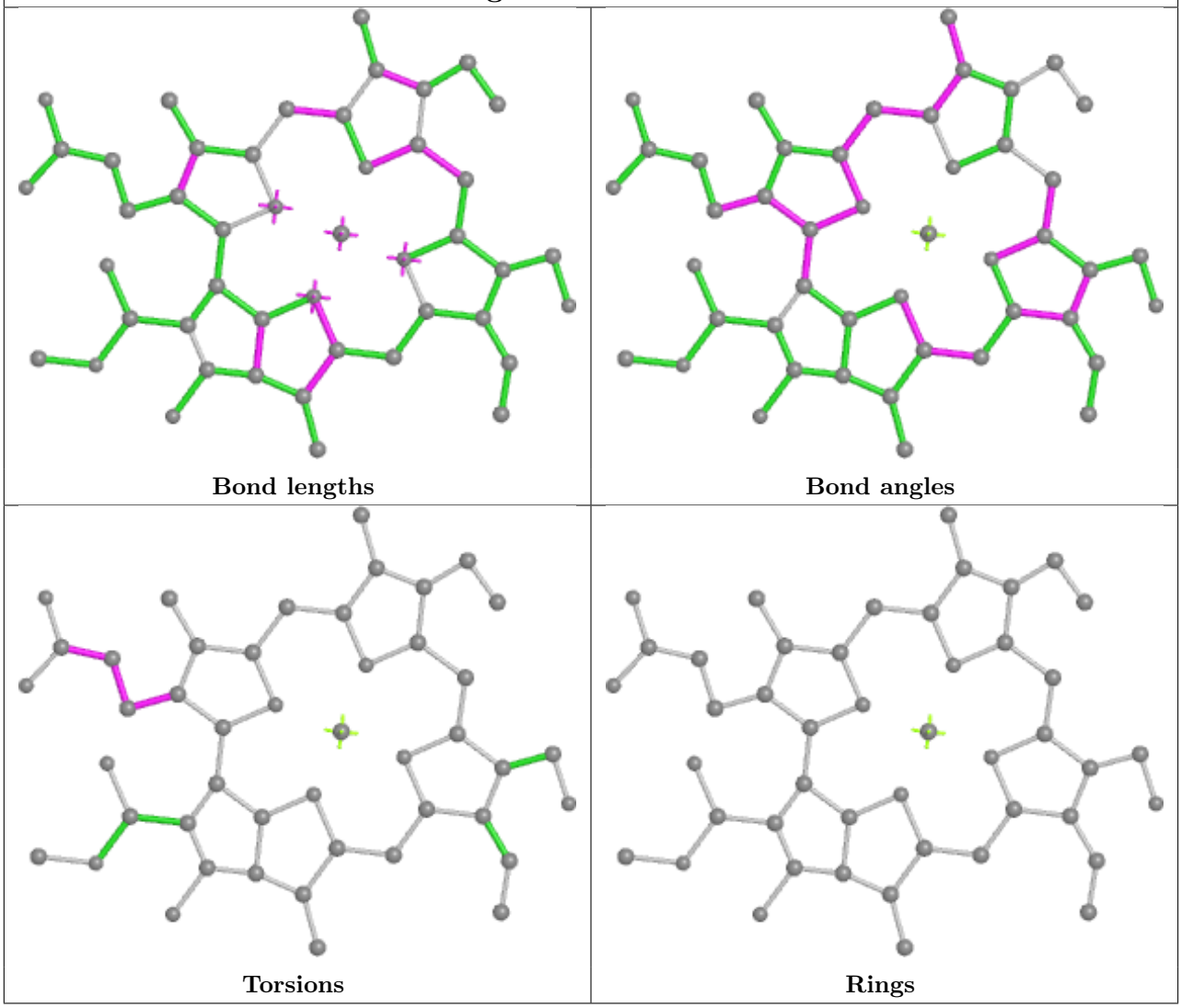


Rings

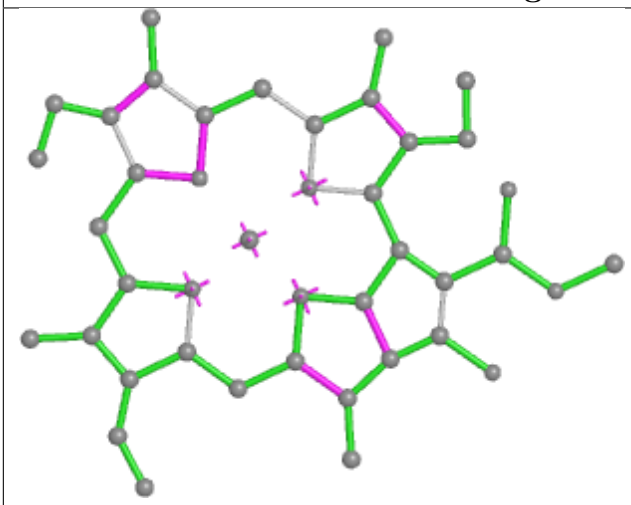
Ligand CLA A 809



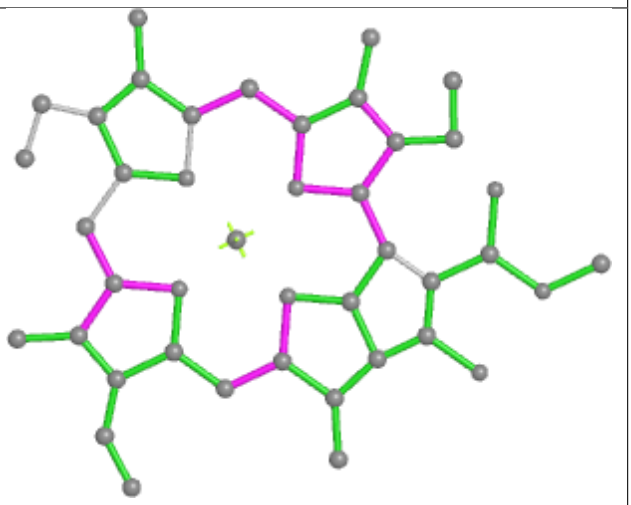
Ligand CHL 3 307



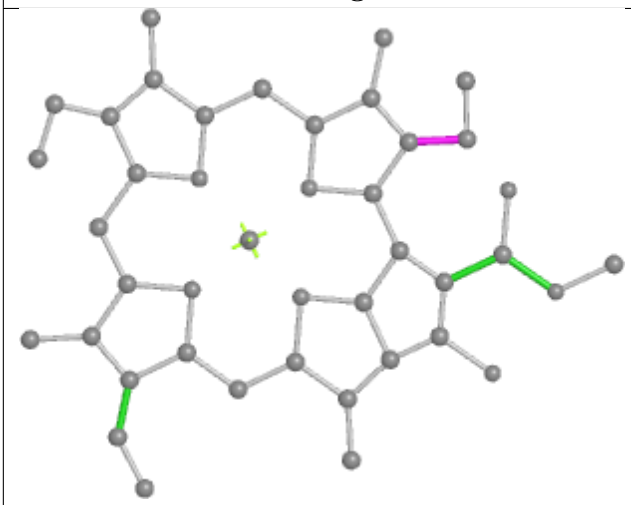
Ligand CLA B 804



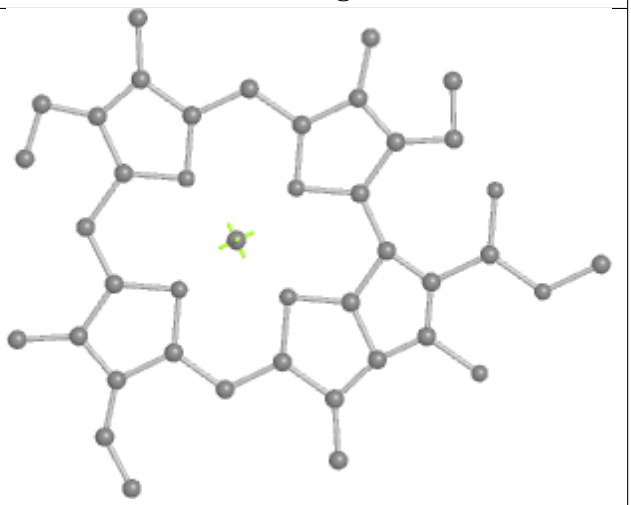
Bond lengths



Bond angles

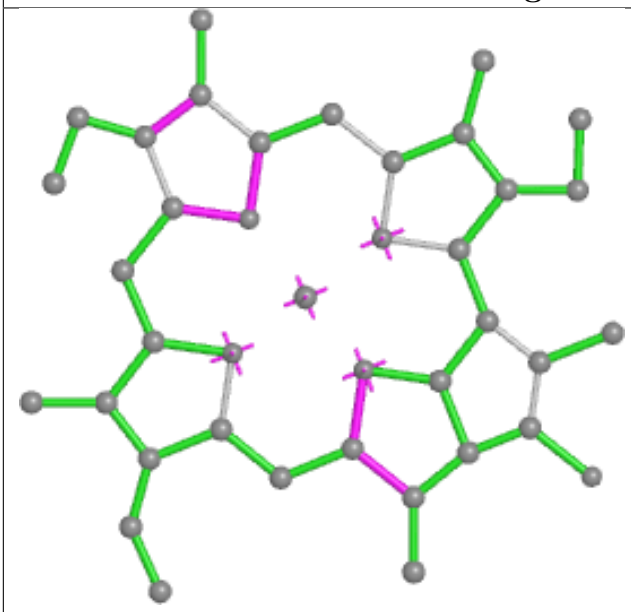


Torsions



Rings

Ligand CLA B 814



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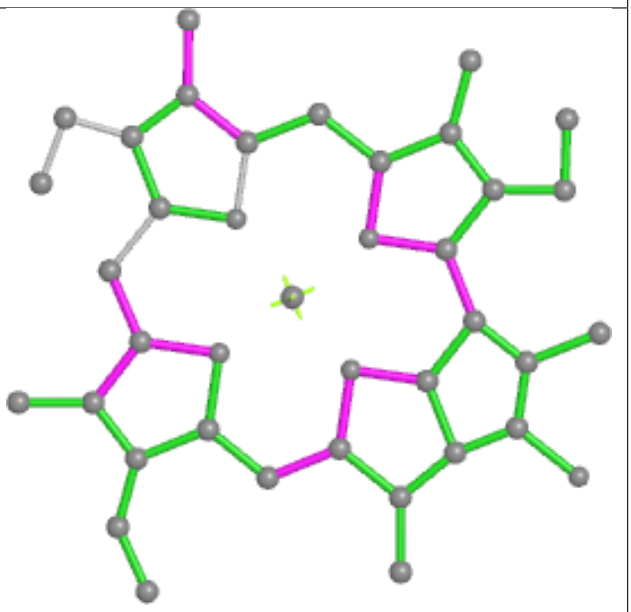
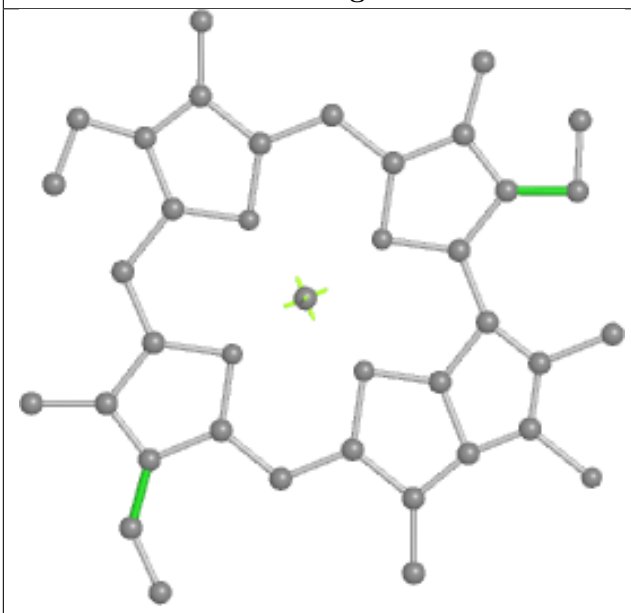


Bond angles



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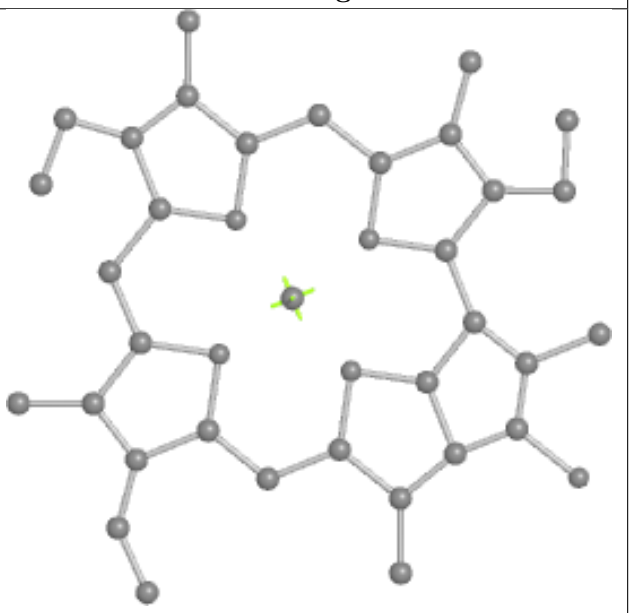
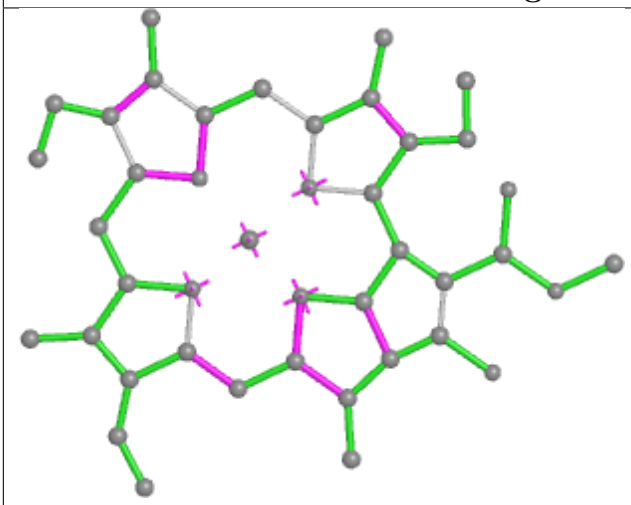
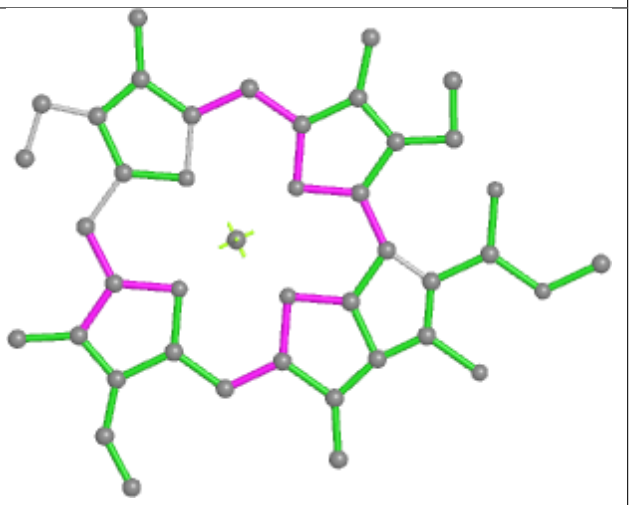


Rings

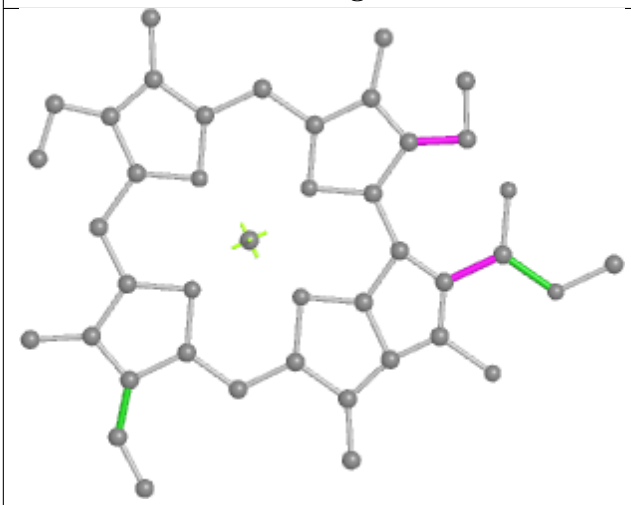
Ligand CLA B 832



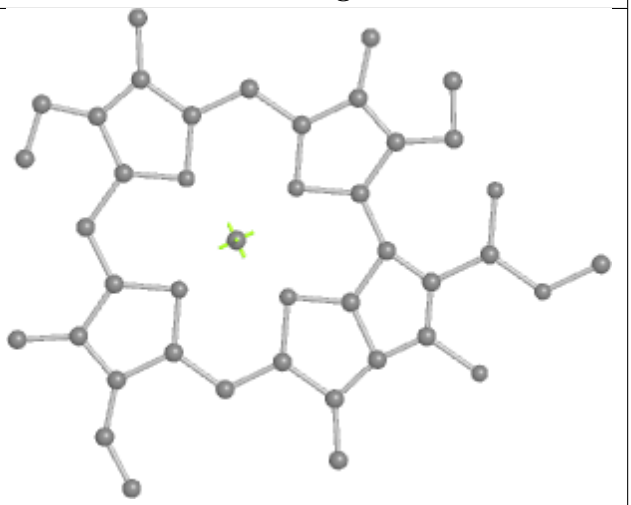
Bond lengths



Bond angles

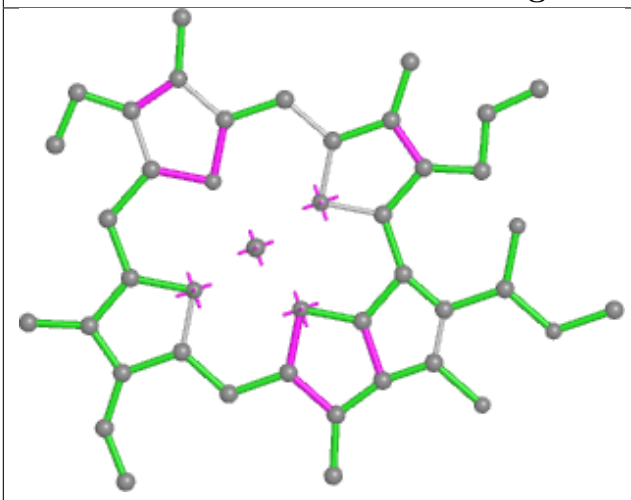


Torsions



Rings

Ligand CLA 7 613



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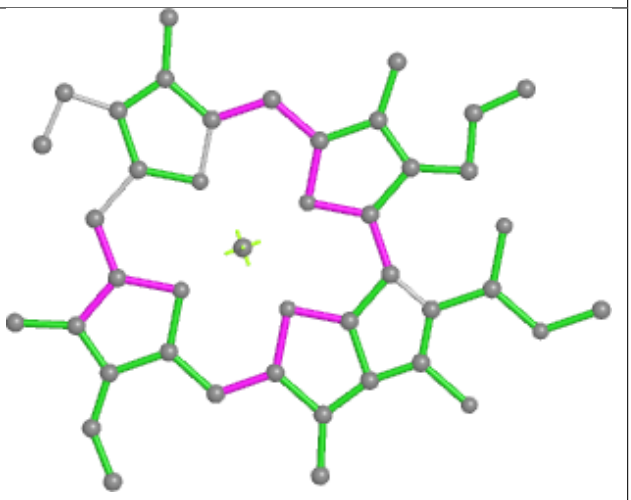
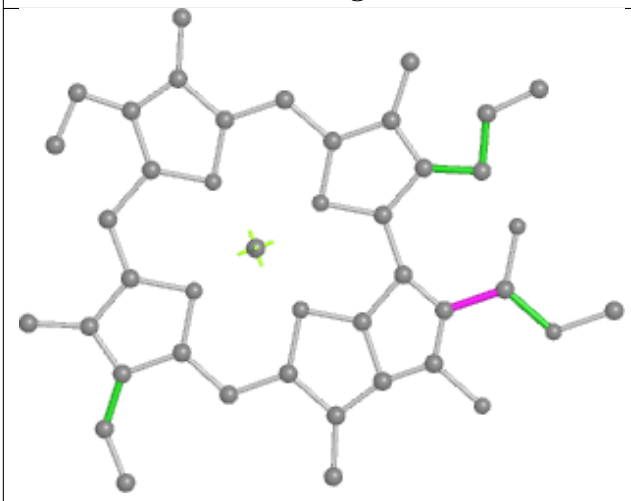
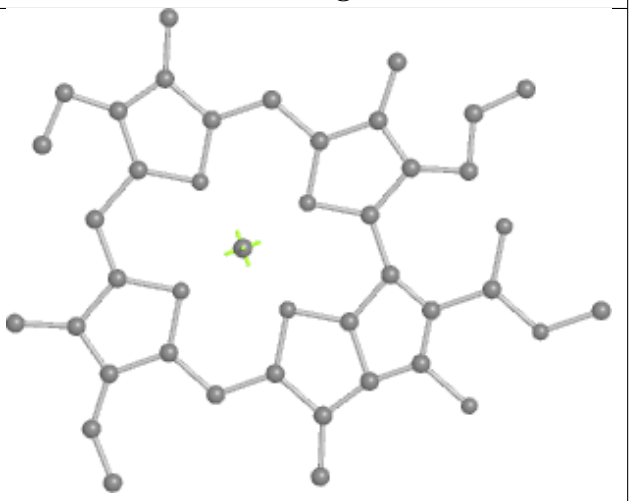


Bond angles

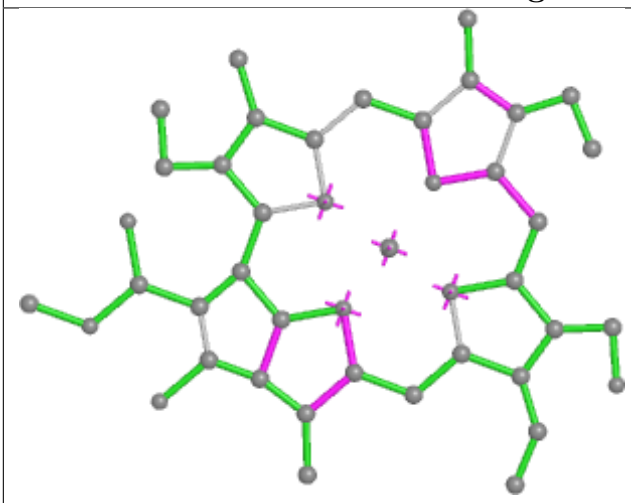


Torsions

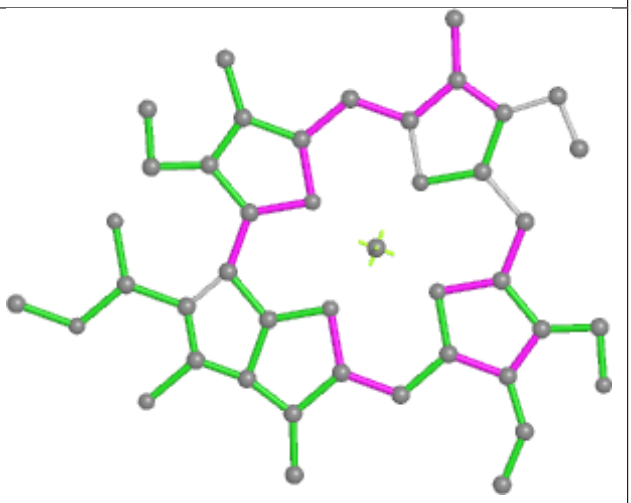


Rings

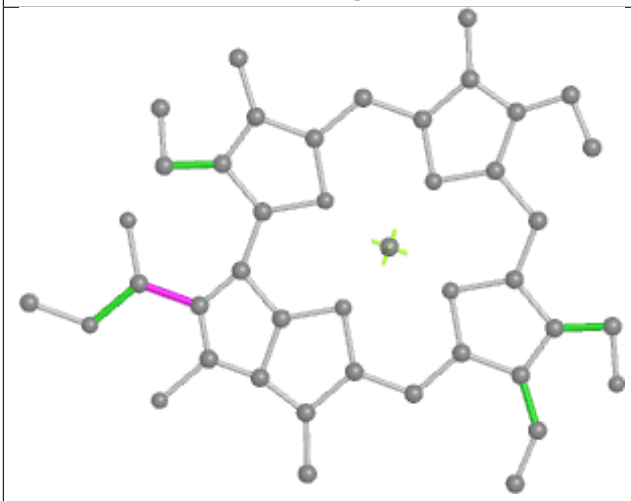
Ligand CHL 5 313



Bond lengths



Bond angles



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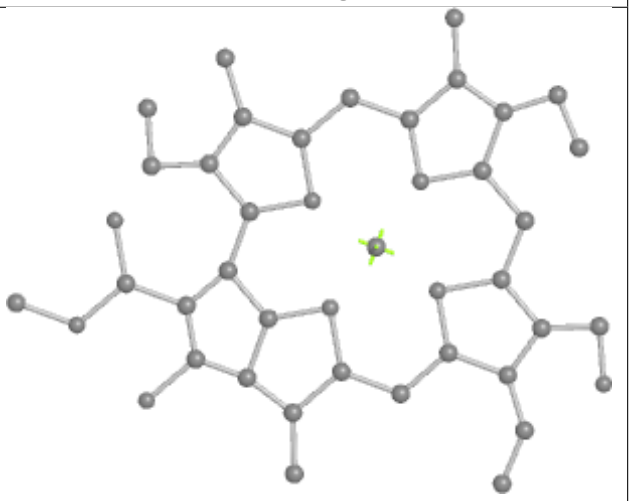
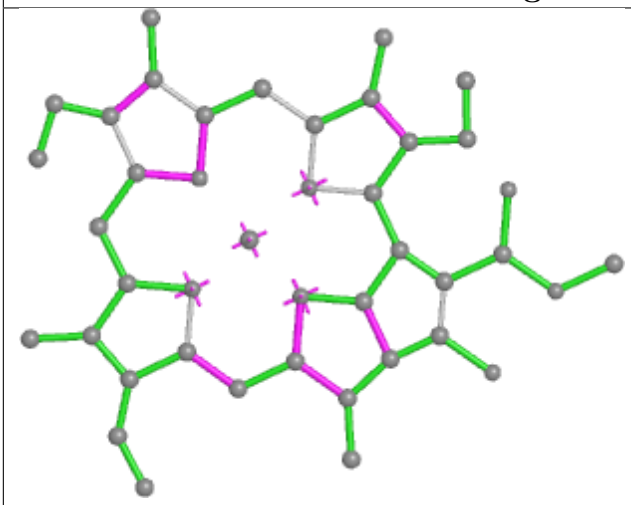
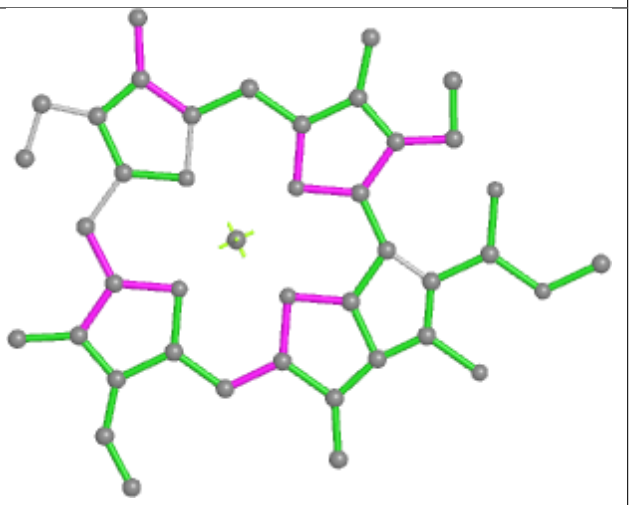


Rings

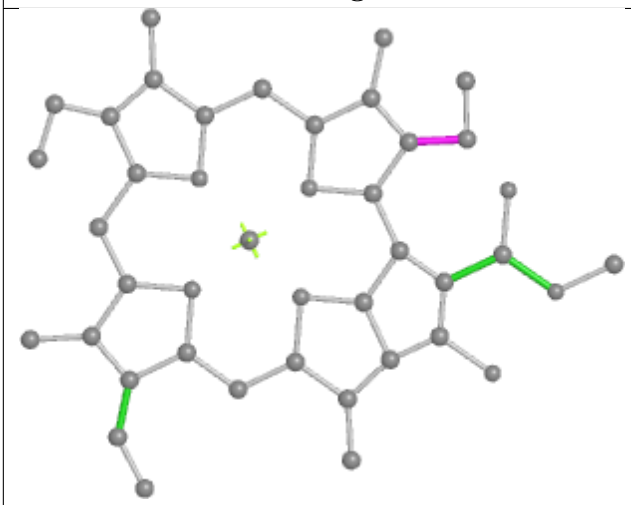
Ligand CLA A 806



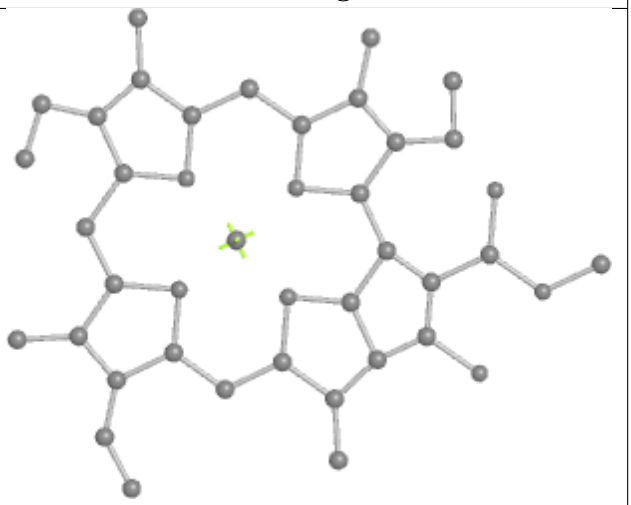
Bond lengths



Bond angles

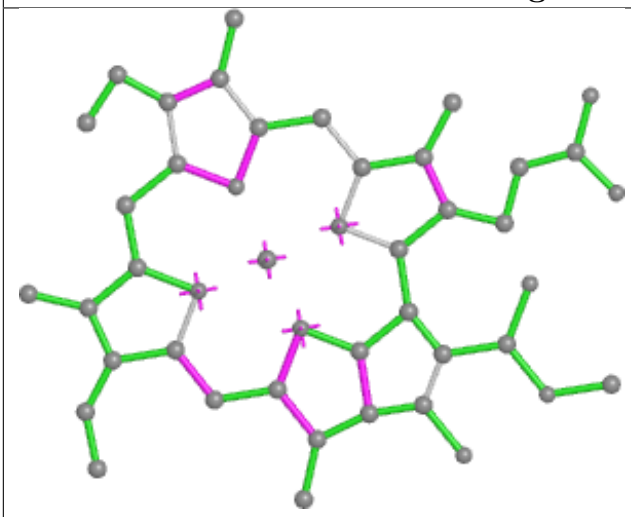


Torsions



Rings

Ligand CLA 6 610



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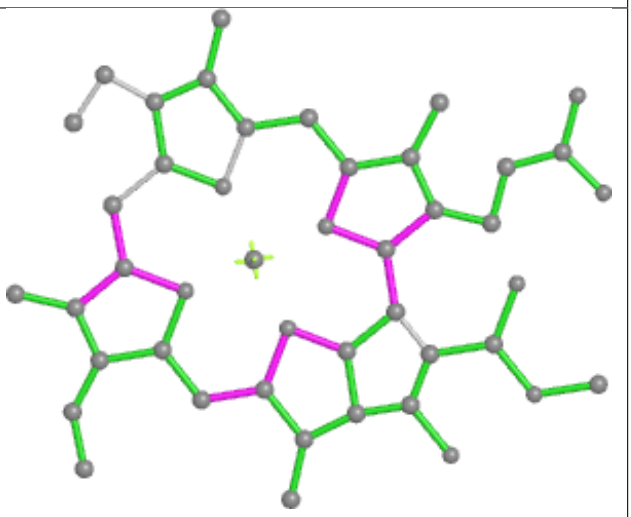

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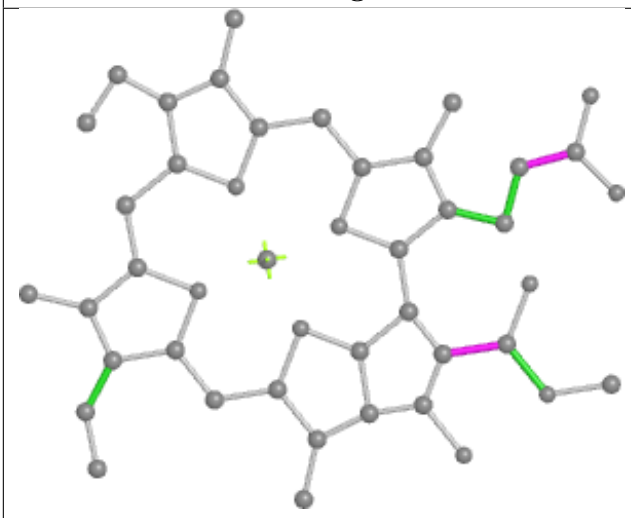

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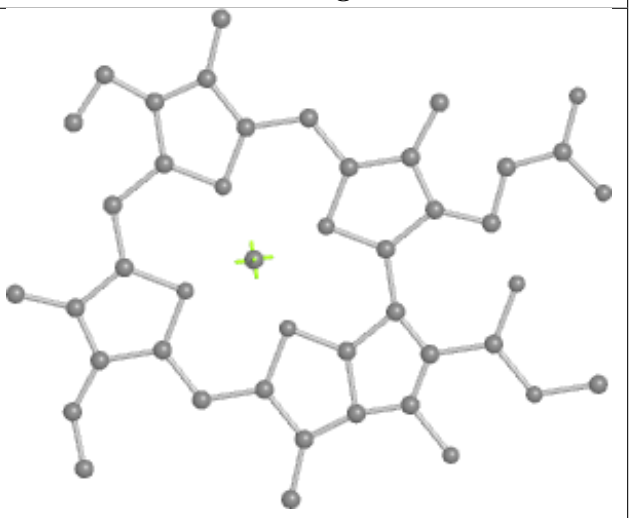
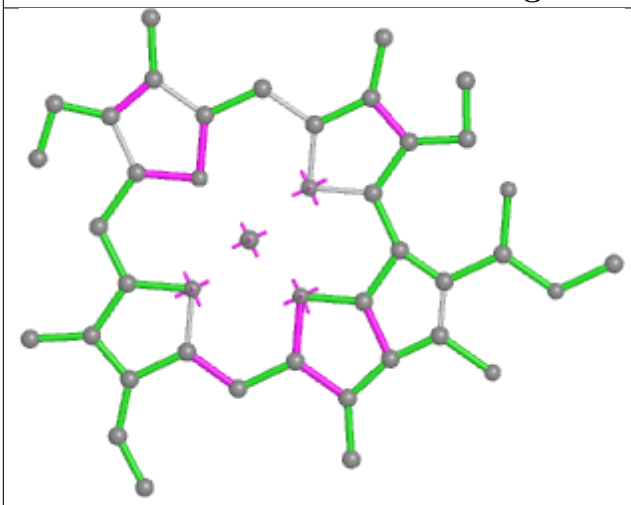


Rings

Ligand CLA A 808



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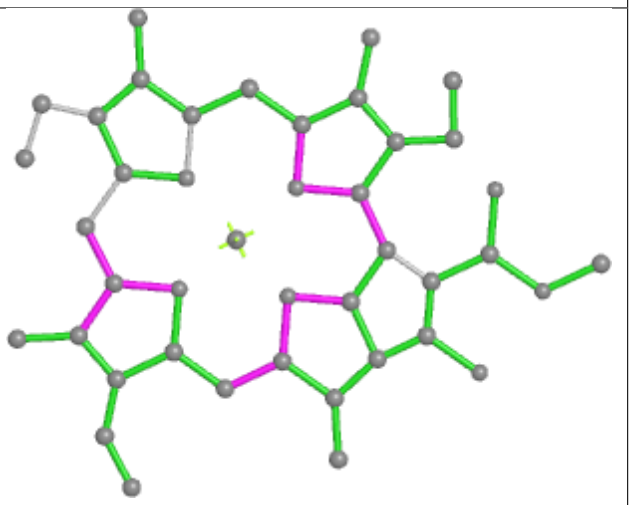
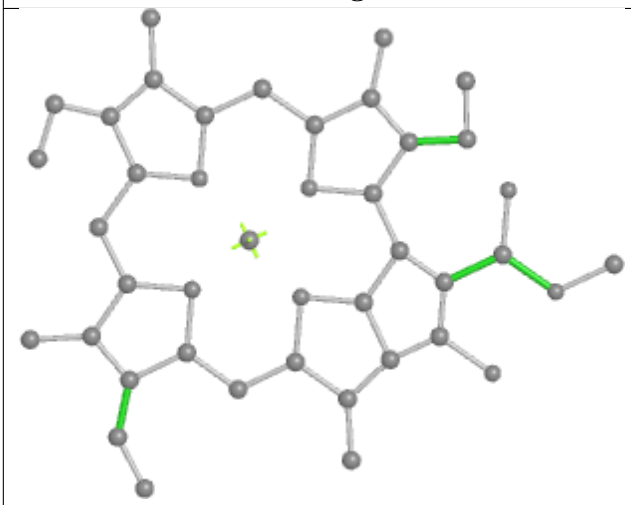


Bond angles



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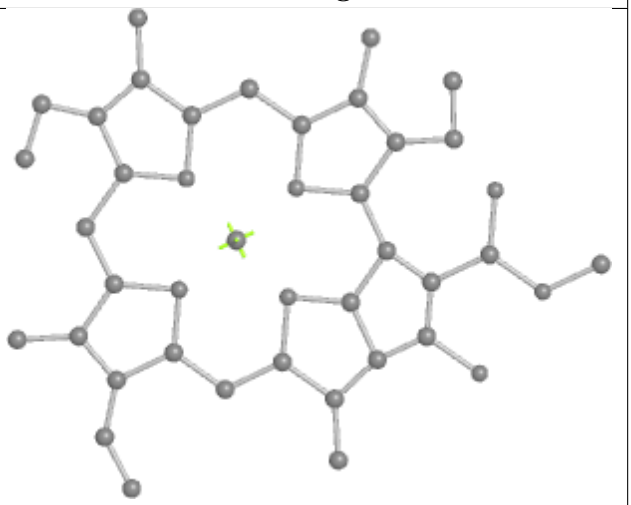
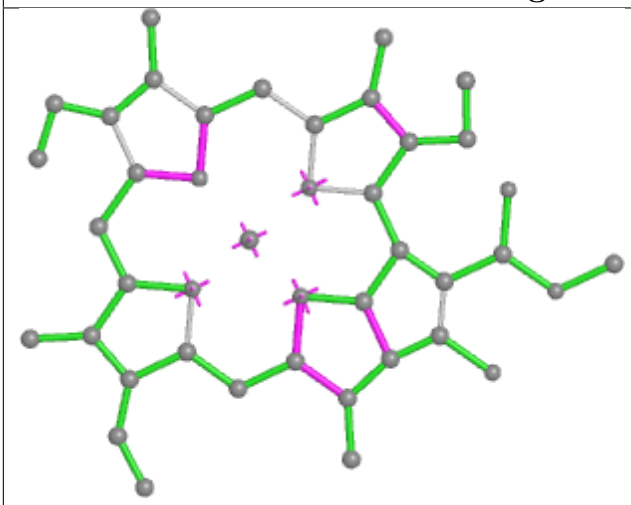


Rings

Ligand CLA 7 604



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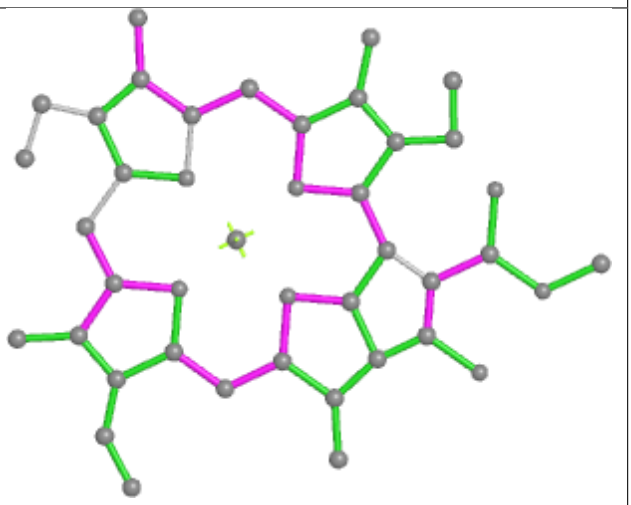
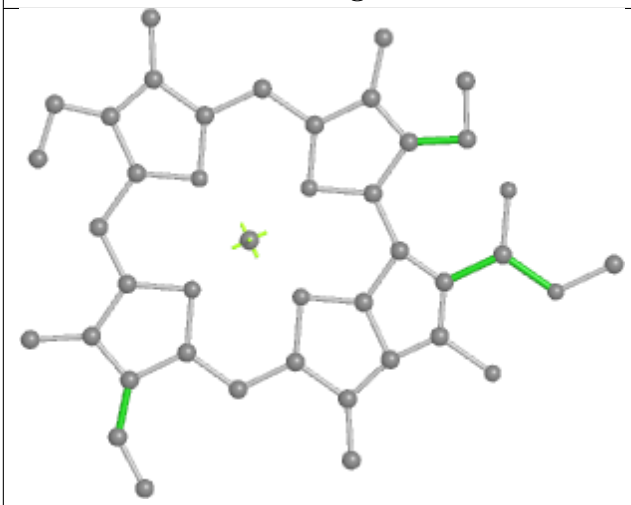


Bond angles



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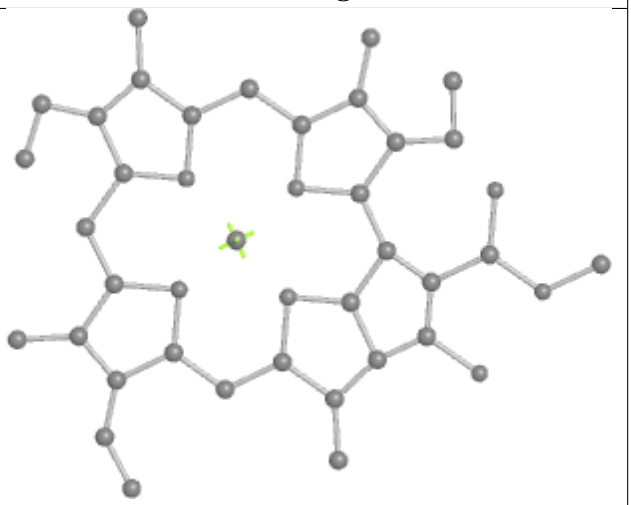
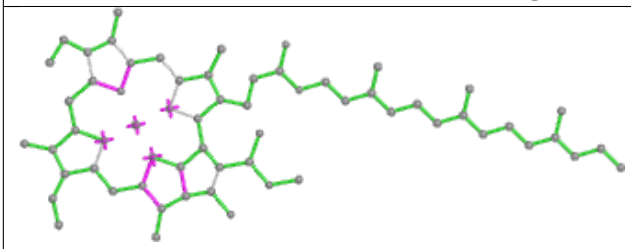


Rings

Ligand CLA F 302



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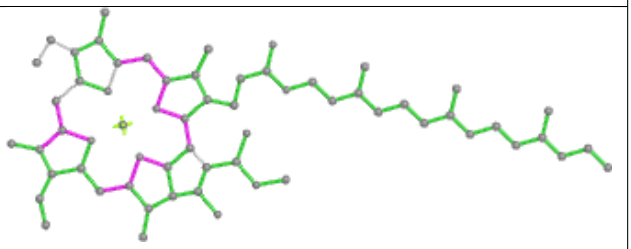
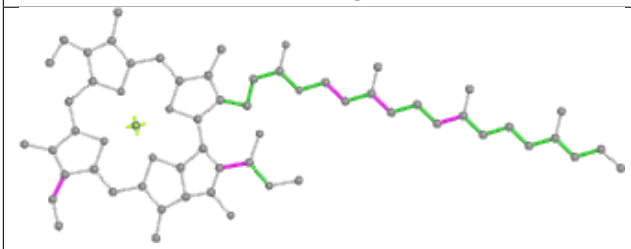


Bond angles



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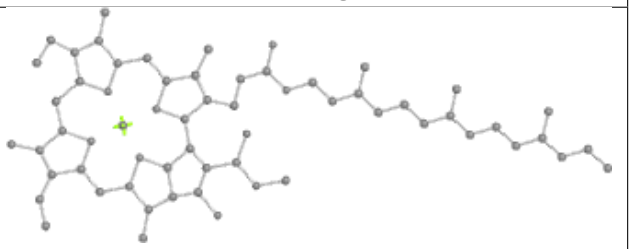
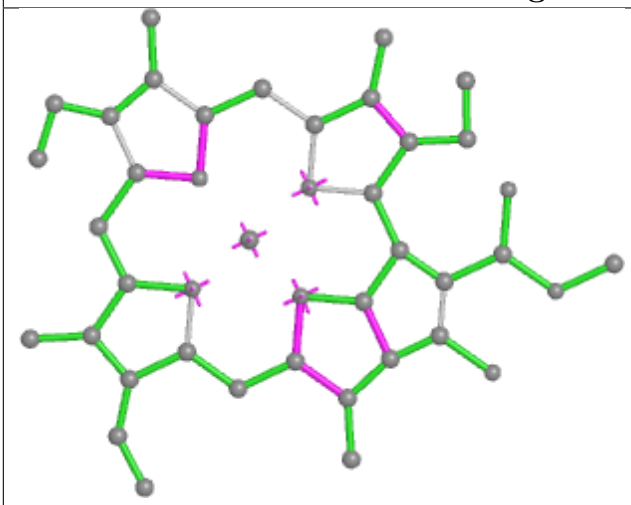


Rings

Ligand CLA J 102



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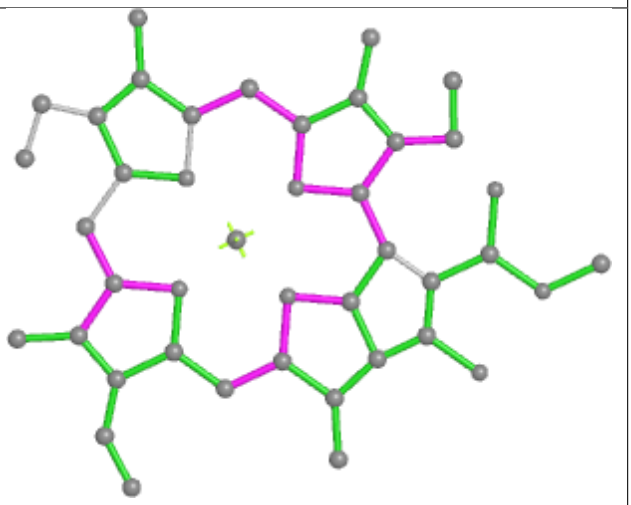
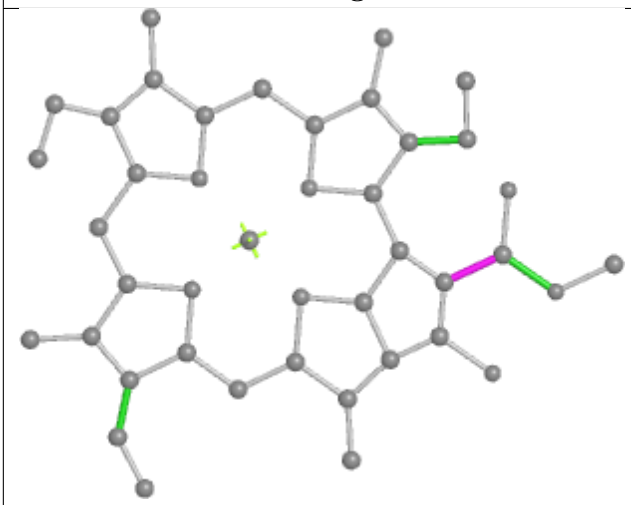


Bond angles



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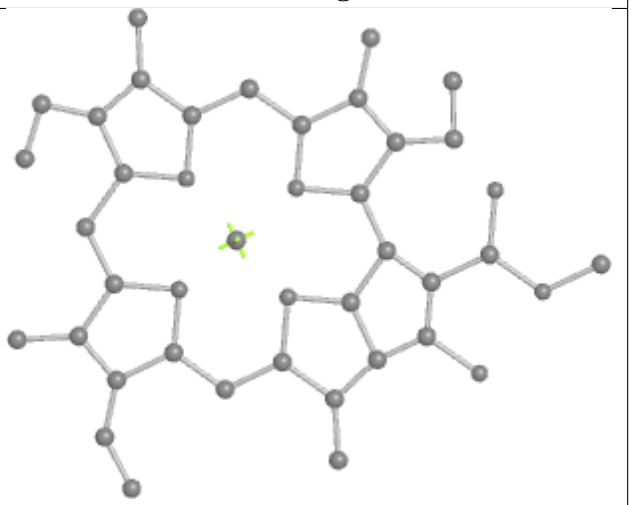
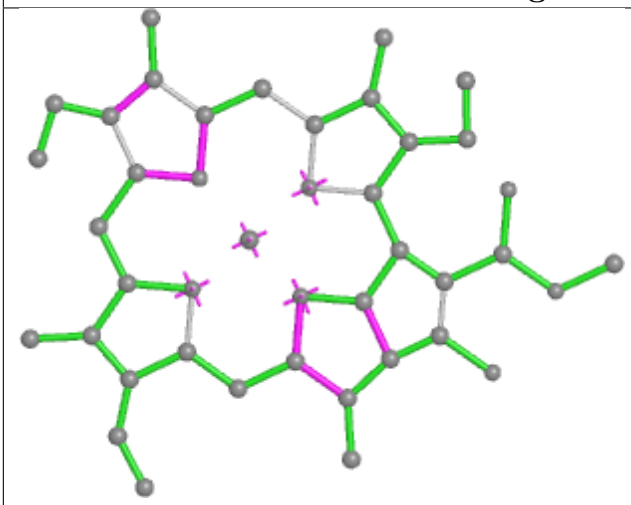


Rings

Ligand CLA 7 609



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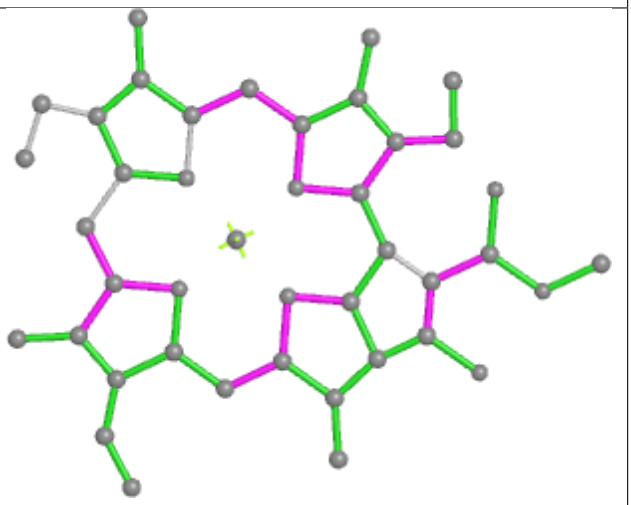

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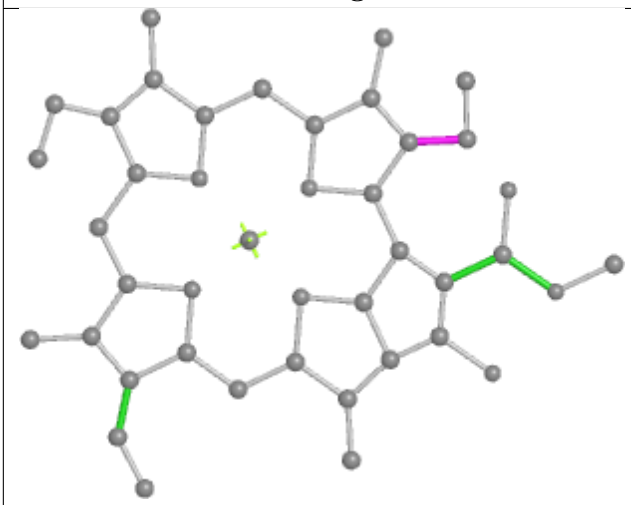

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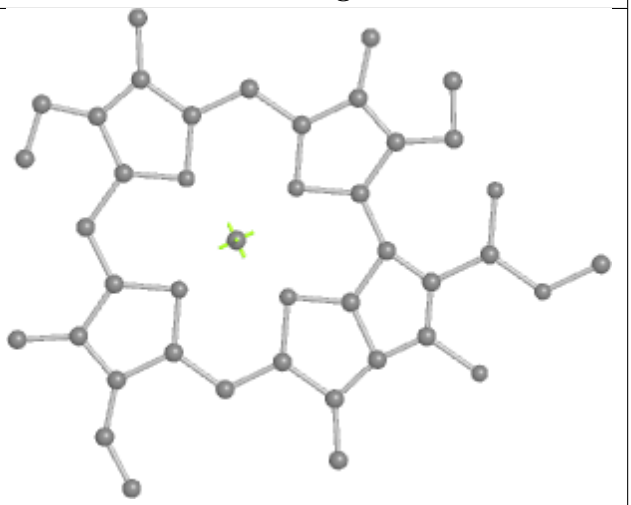
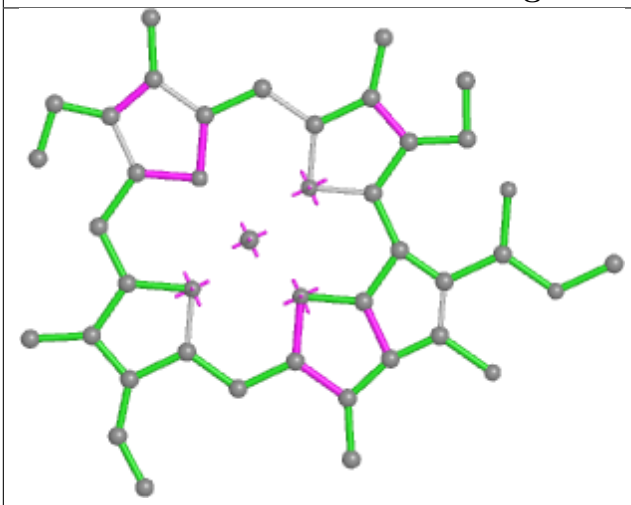


Rings

Ligand CLA A 810



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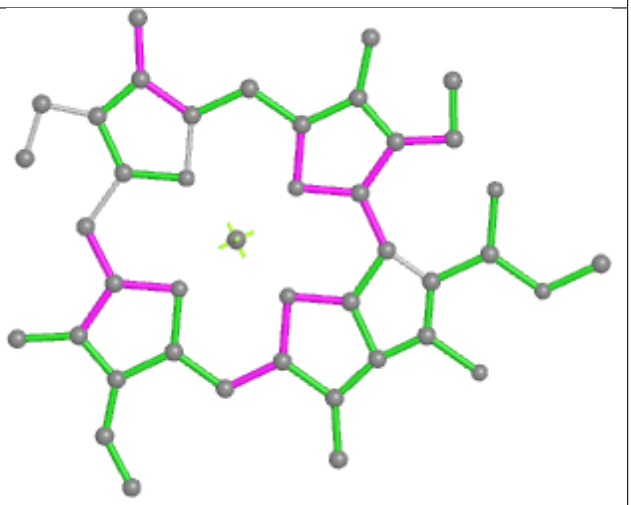
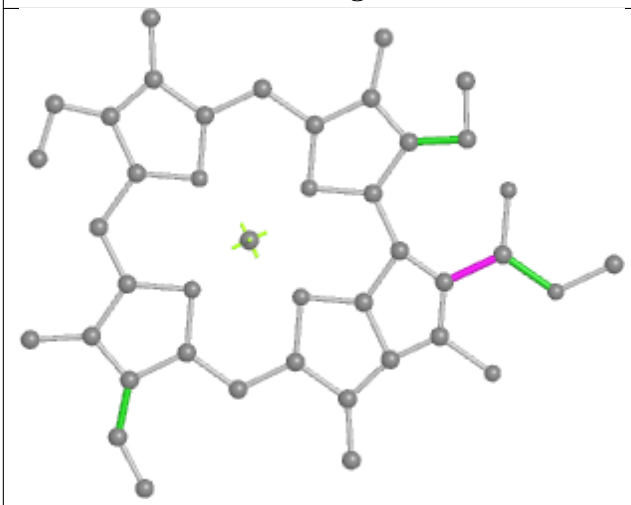


Bond angles



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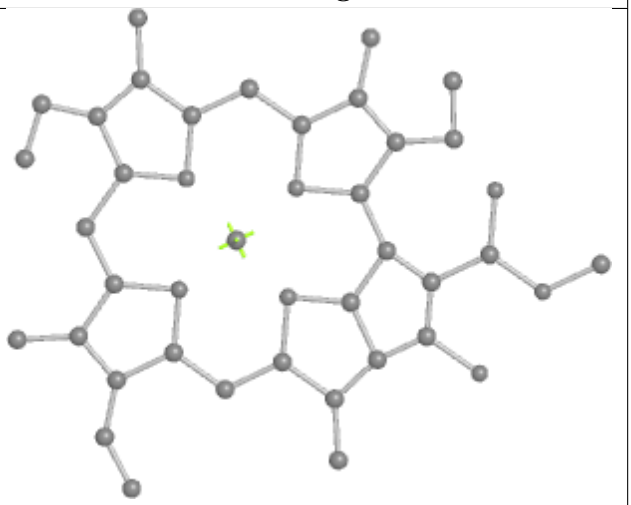
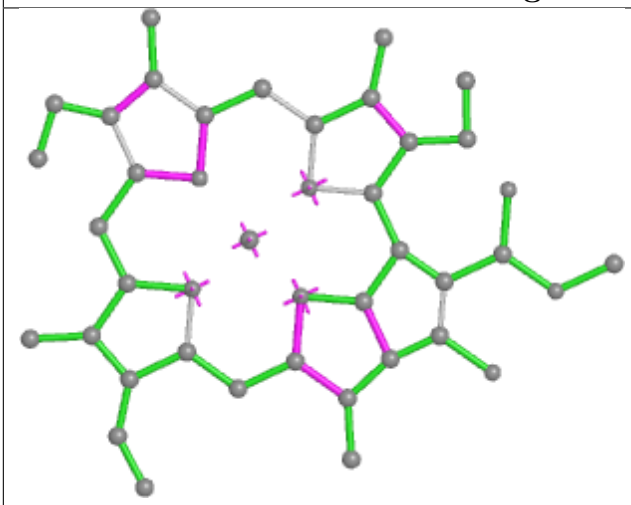


Rings

Ligand CLA A 823



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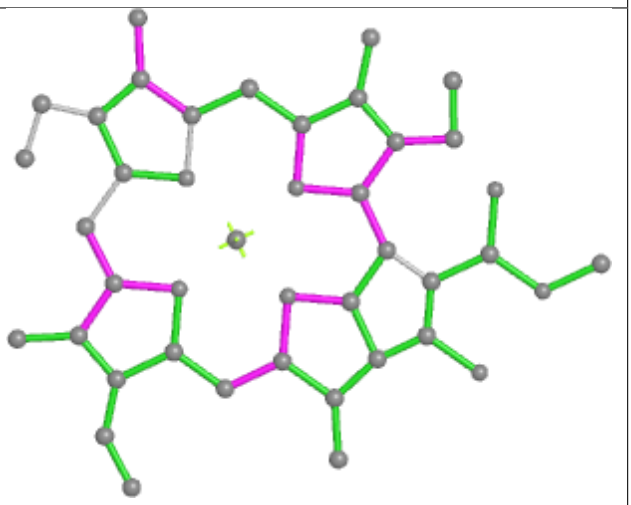
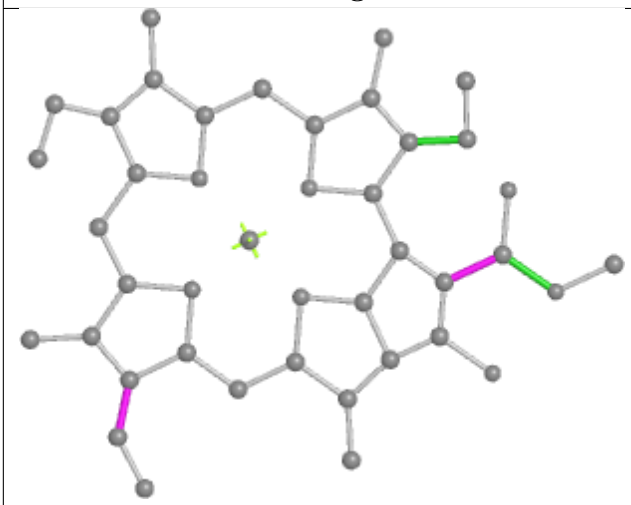


Bond angles



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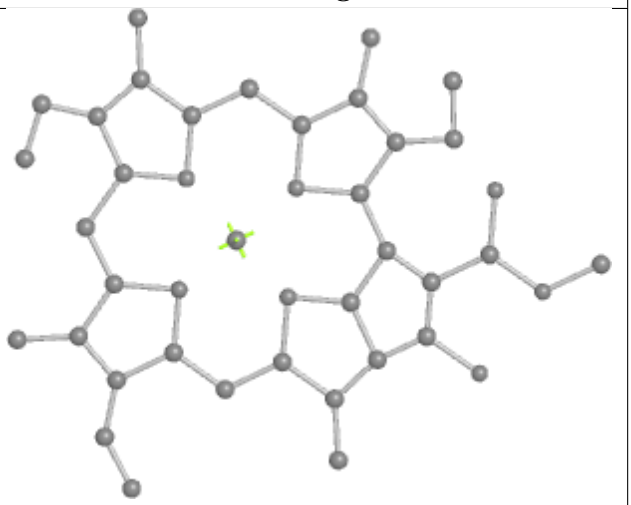
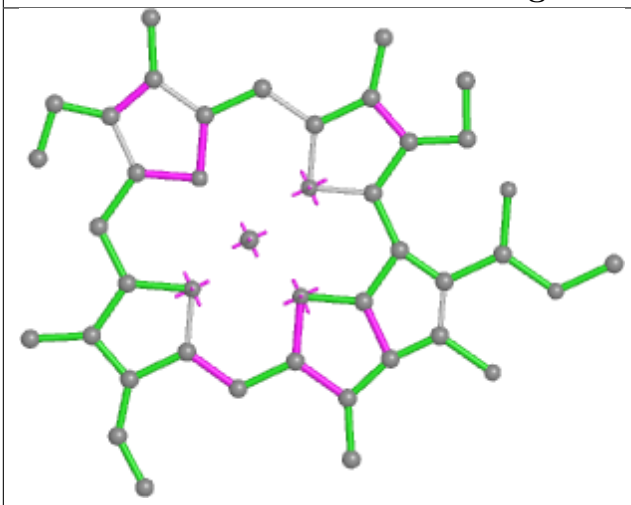
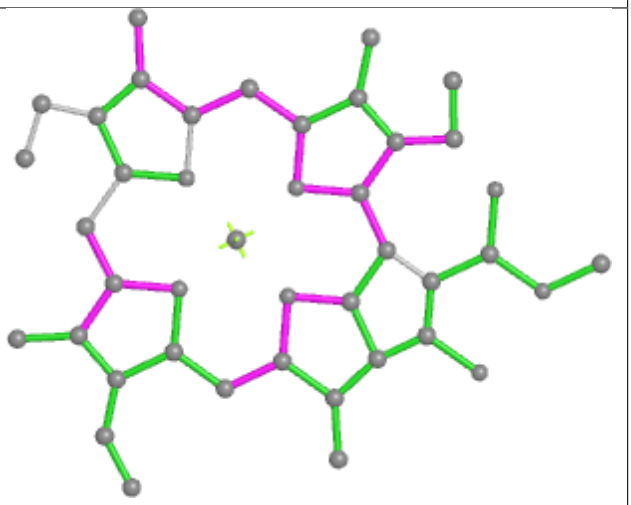


Rings

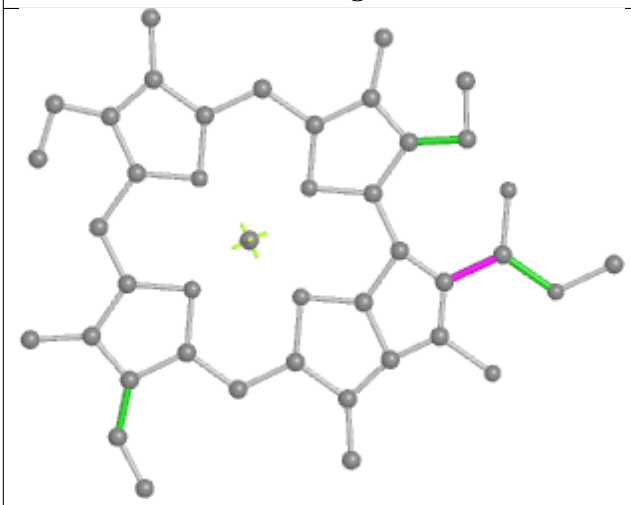
Ligand CLA 7 605



Bond lengths



Bond angles



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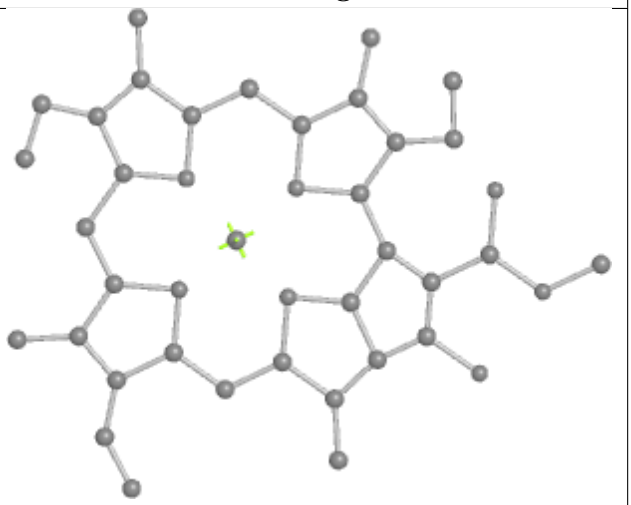
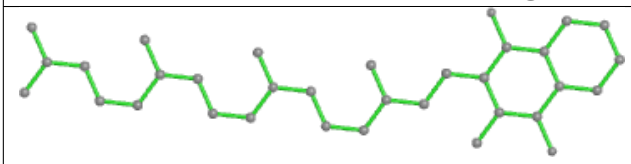


Rings

Ligand PQN B 840



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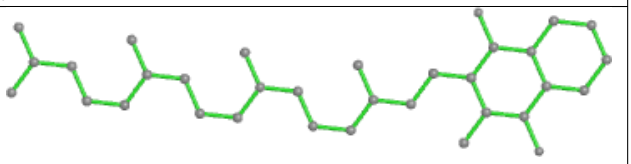
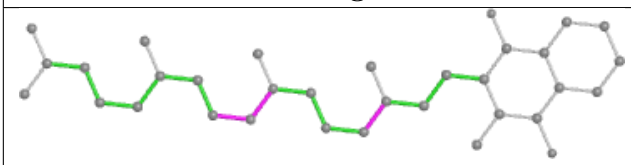


Bond angles



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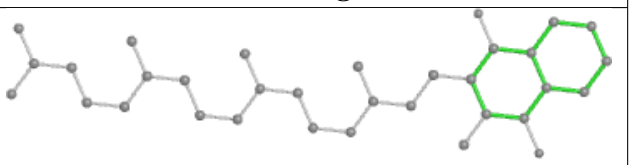
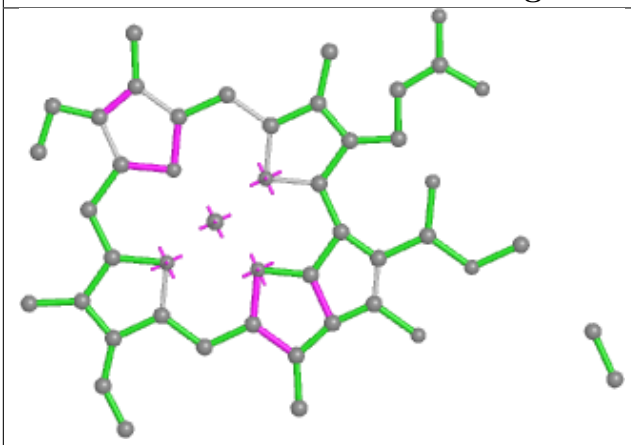
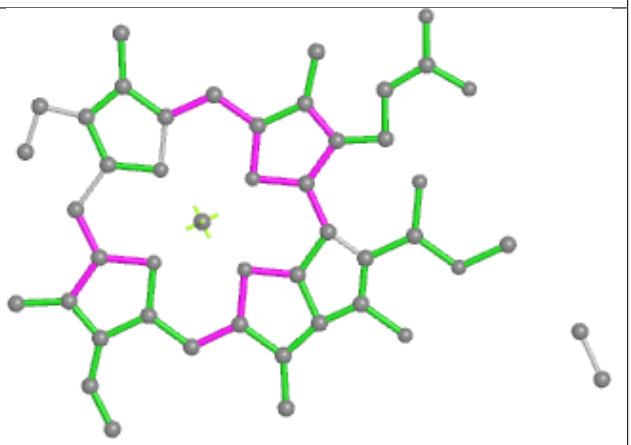
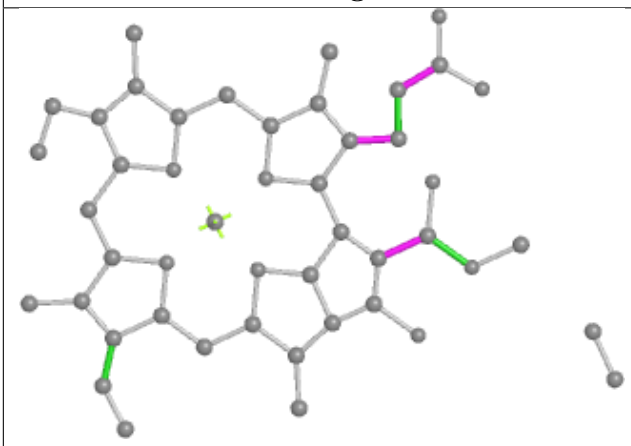
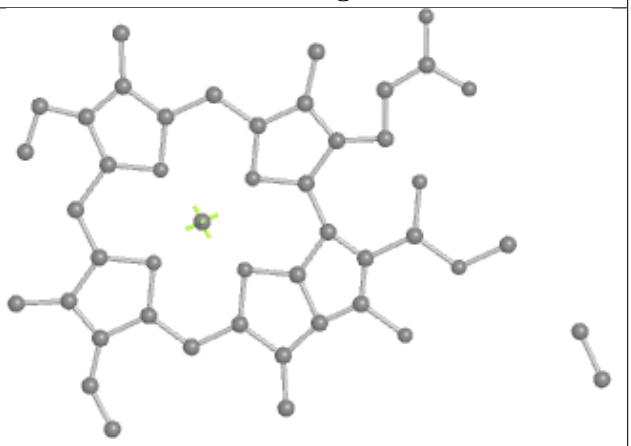
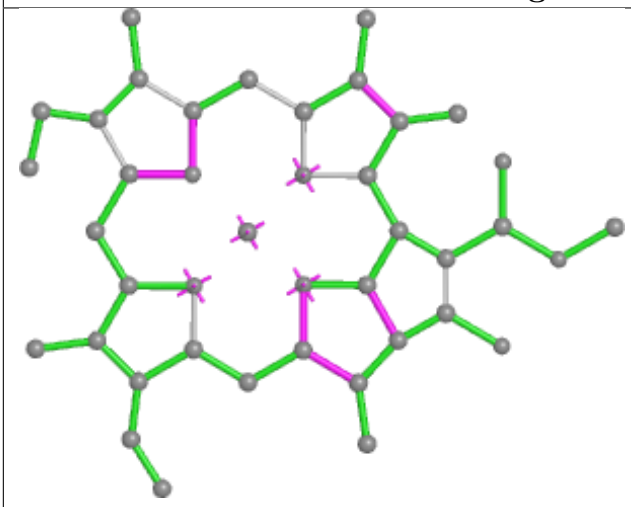
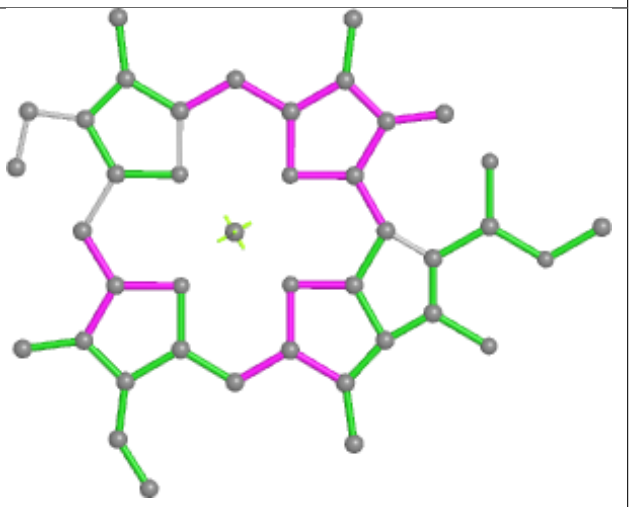
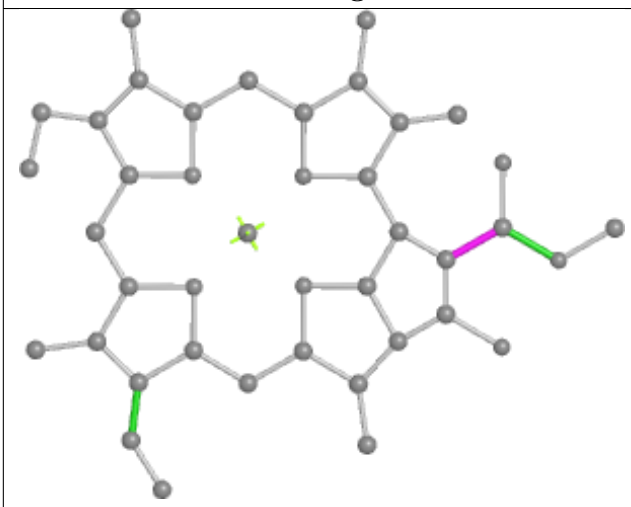
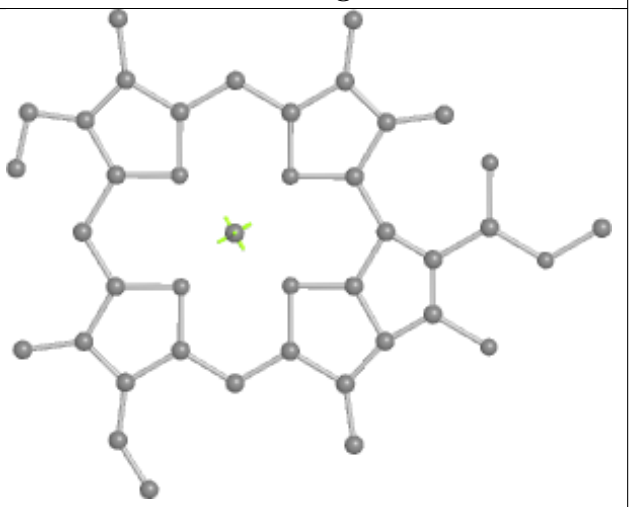
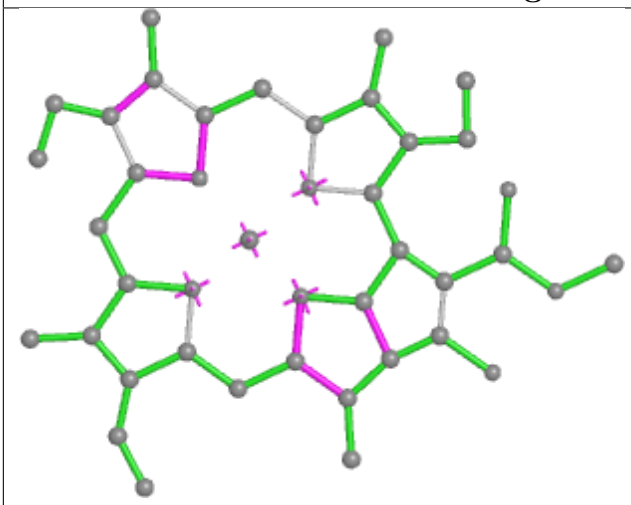


Rings

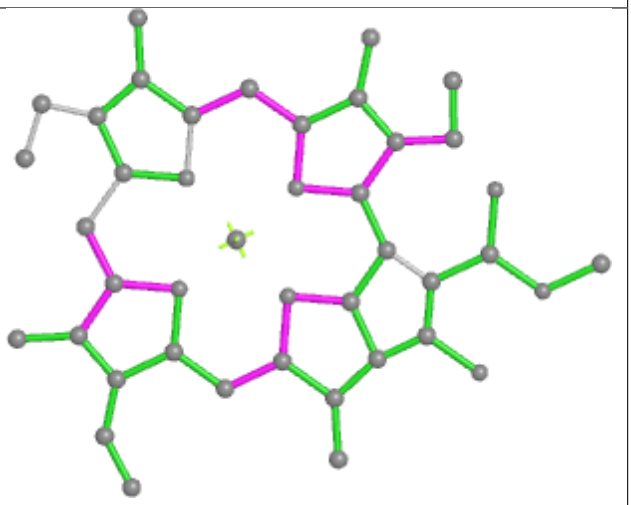
Ligand CLA B 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

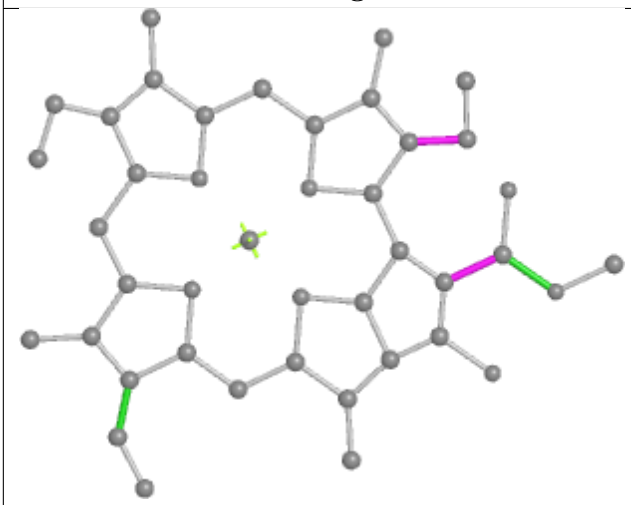
Ligand CLA B 830



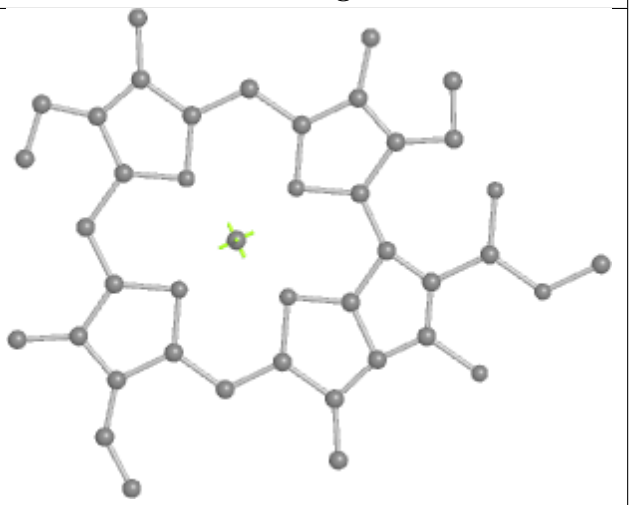
Bond lengths



Bond angles

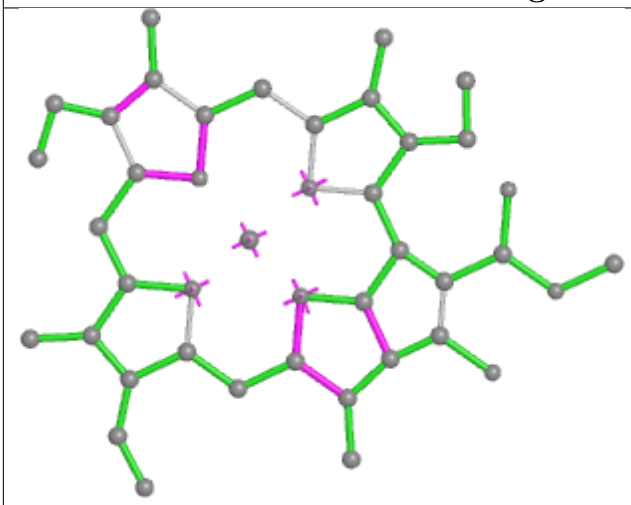


Torsions

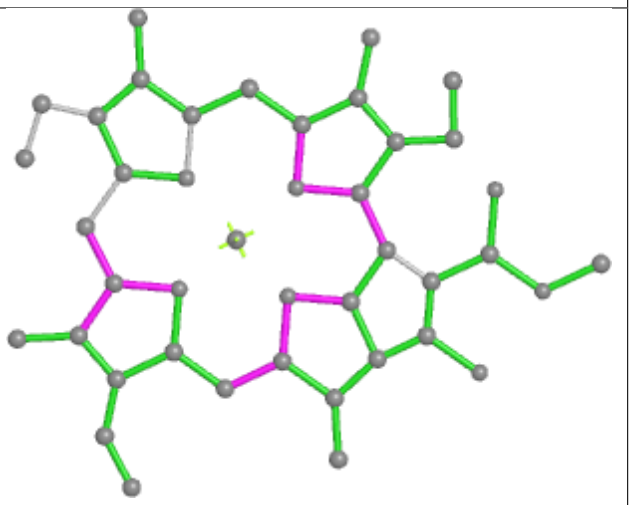


Rings

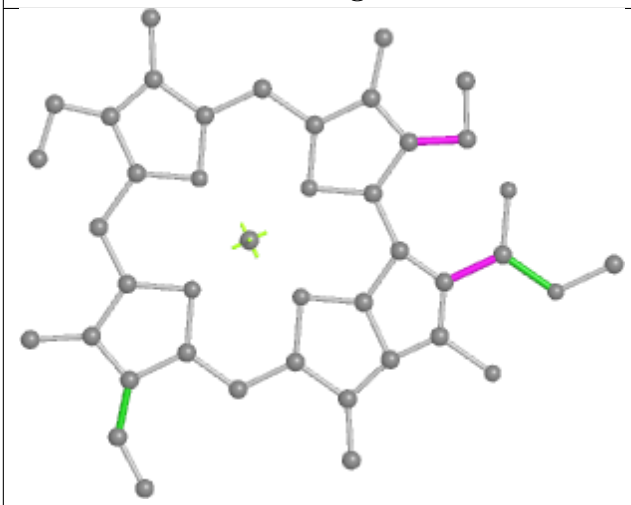
Ligand CLA 8 602



Bond lengths



Bond angles



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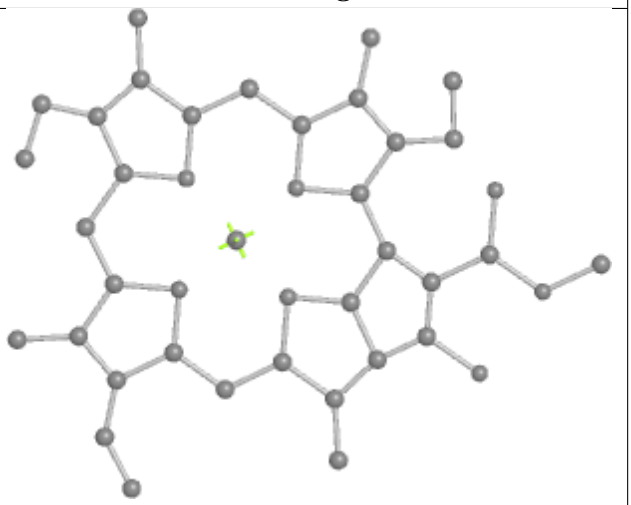
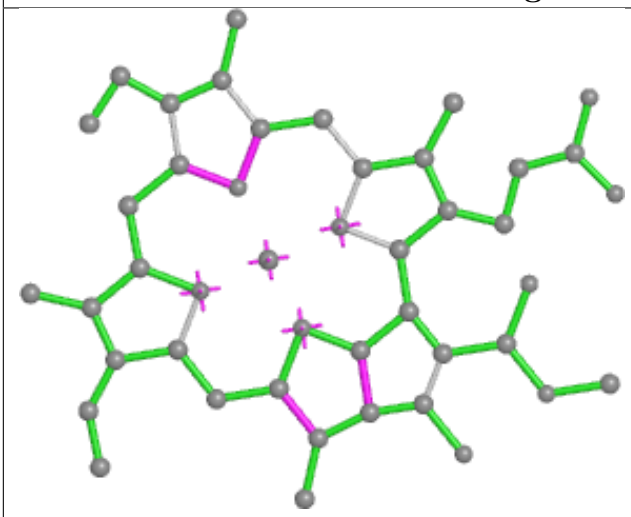
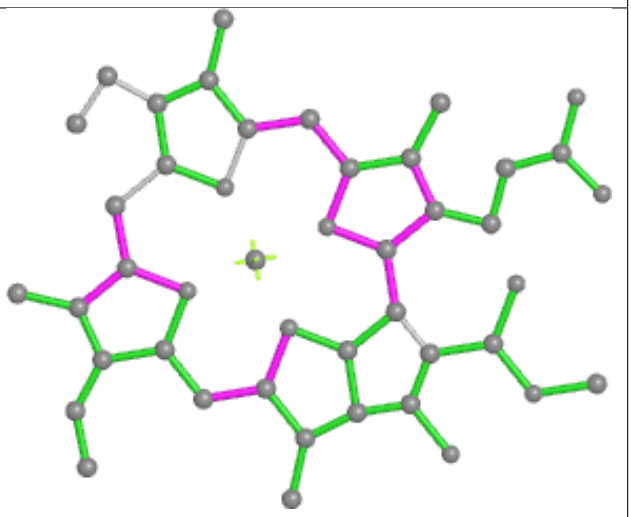
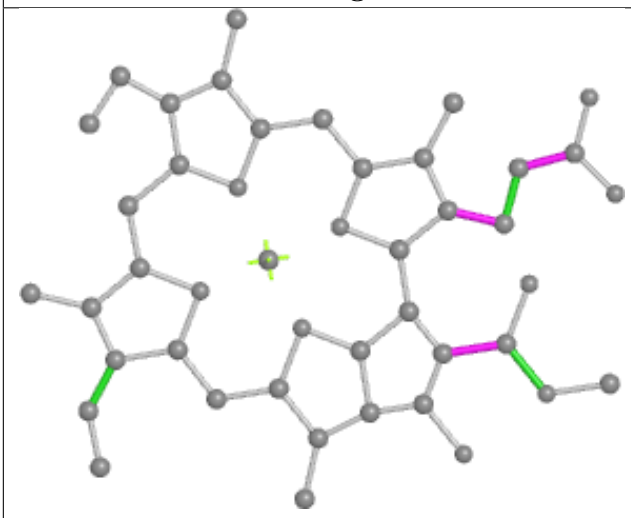
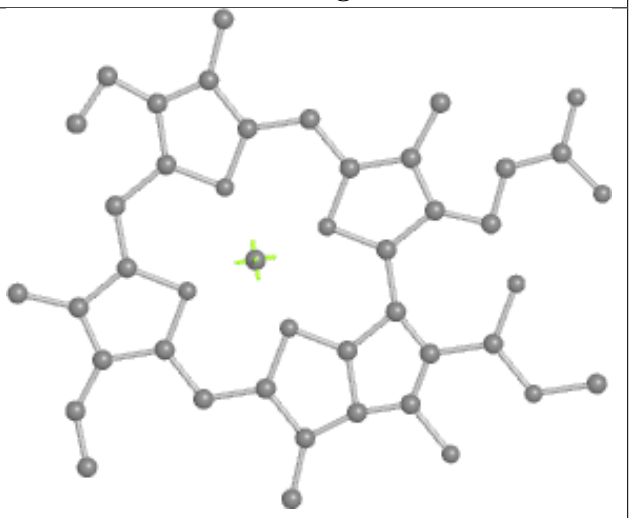
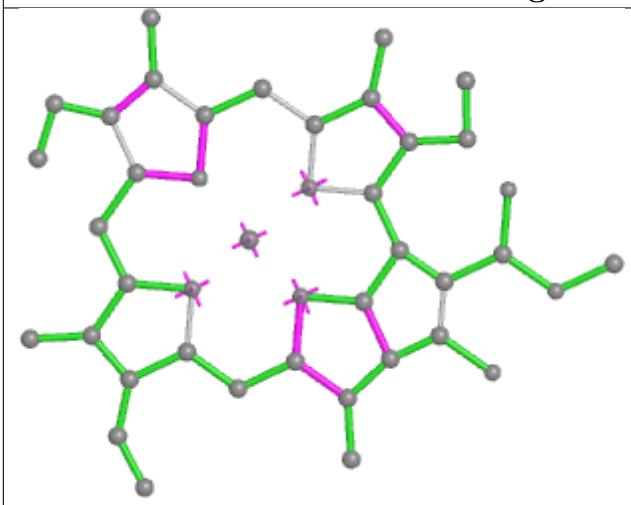


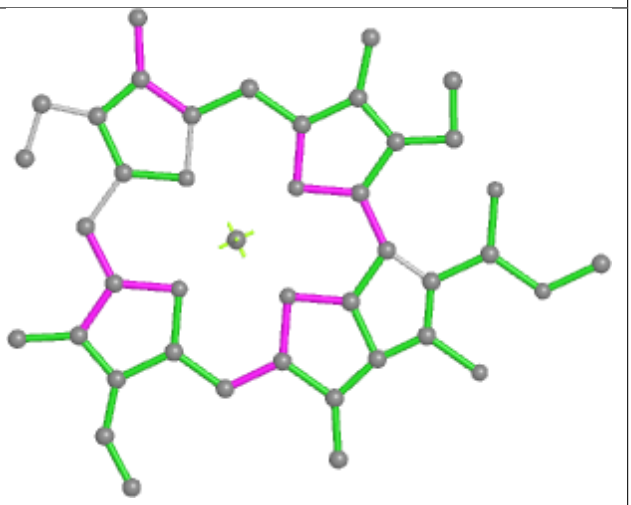
Rings

Ligand CLA B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

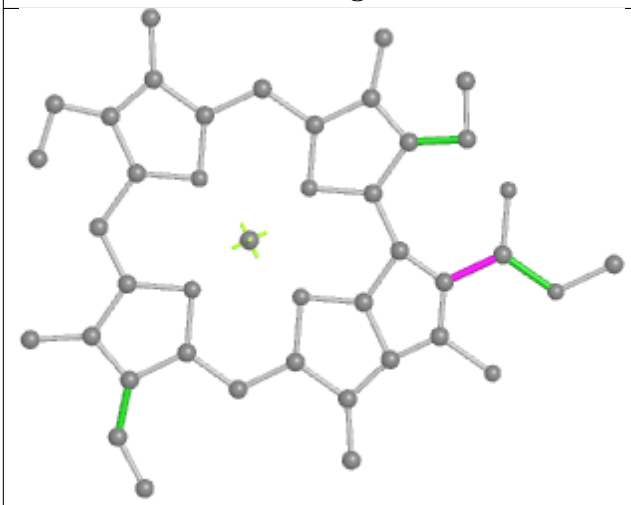
Ligand CLA 8 605



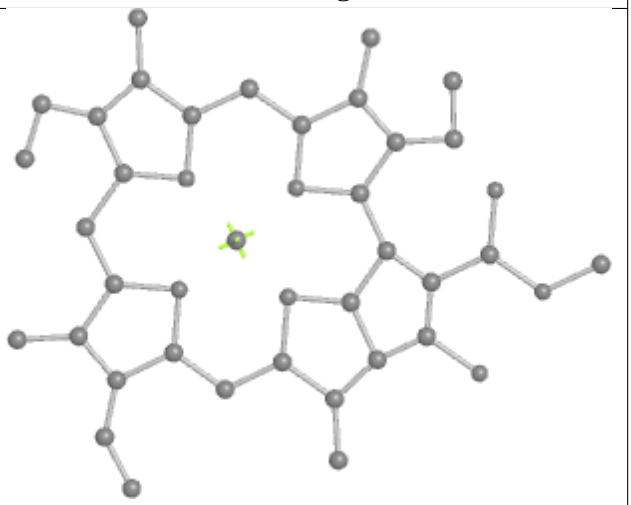
Bond lengths



Bond angles

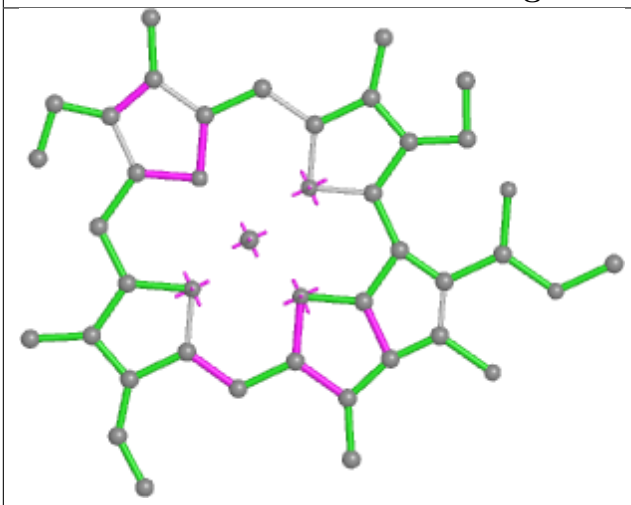


Torsions



Rings

Ligand CLA A 815



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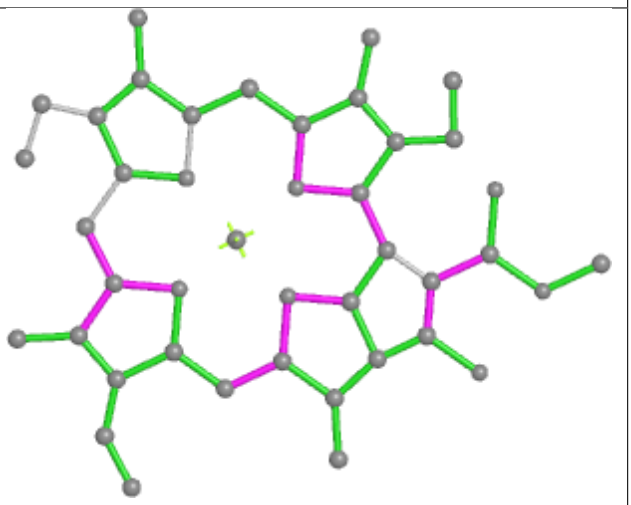
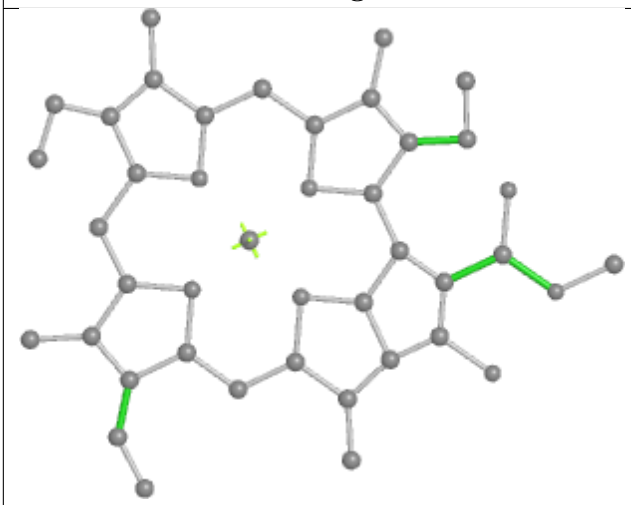


Bond angles



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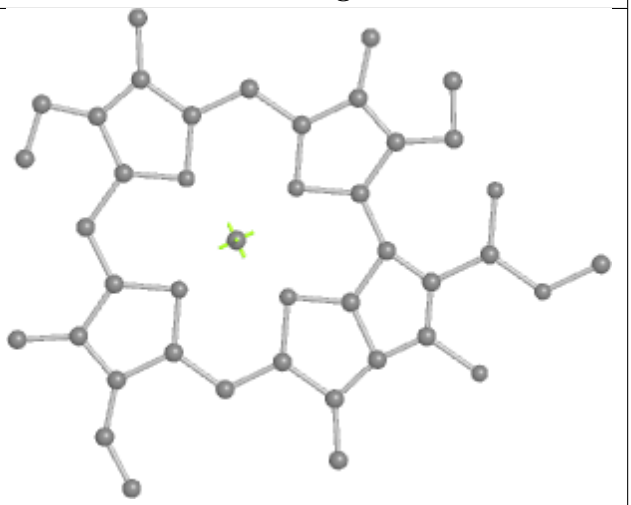
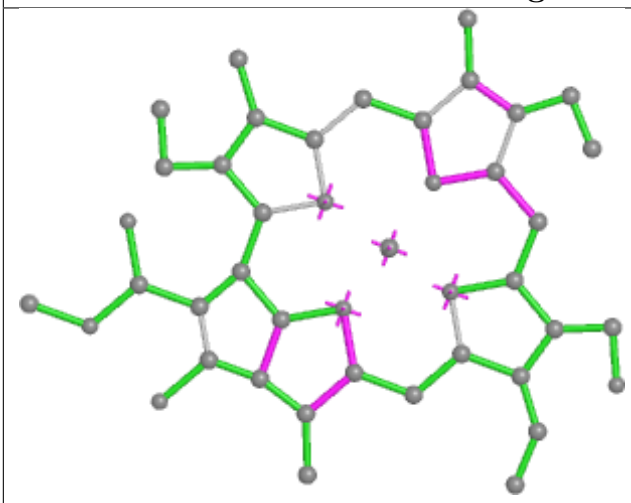
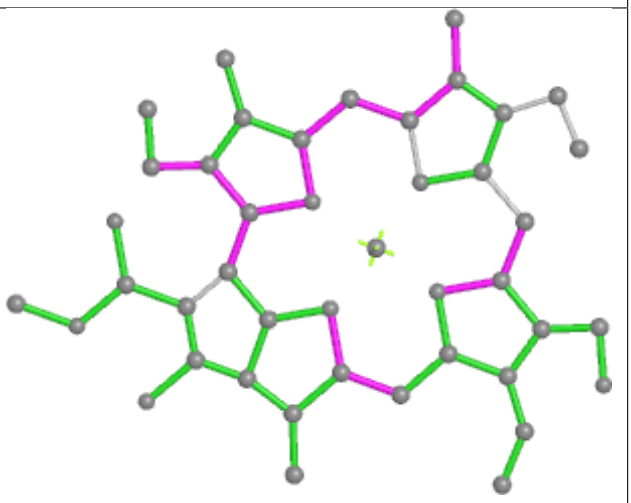


Rings

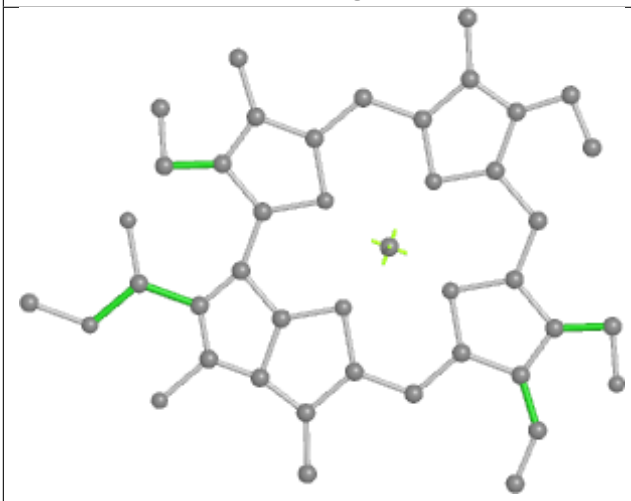
Ligand CHL 8 606



Bond lengths



Bond angles



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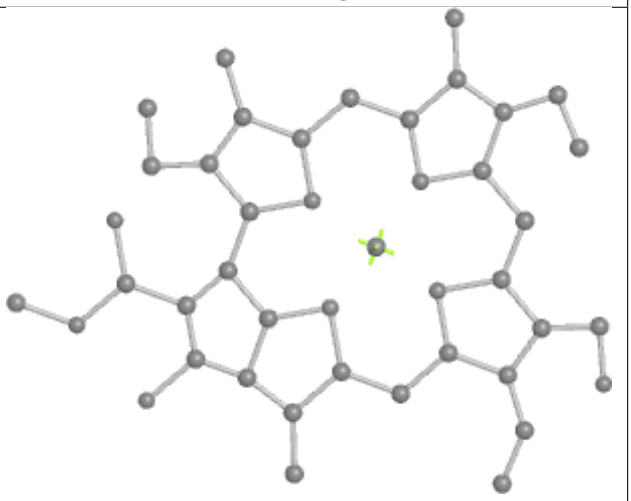
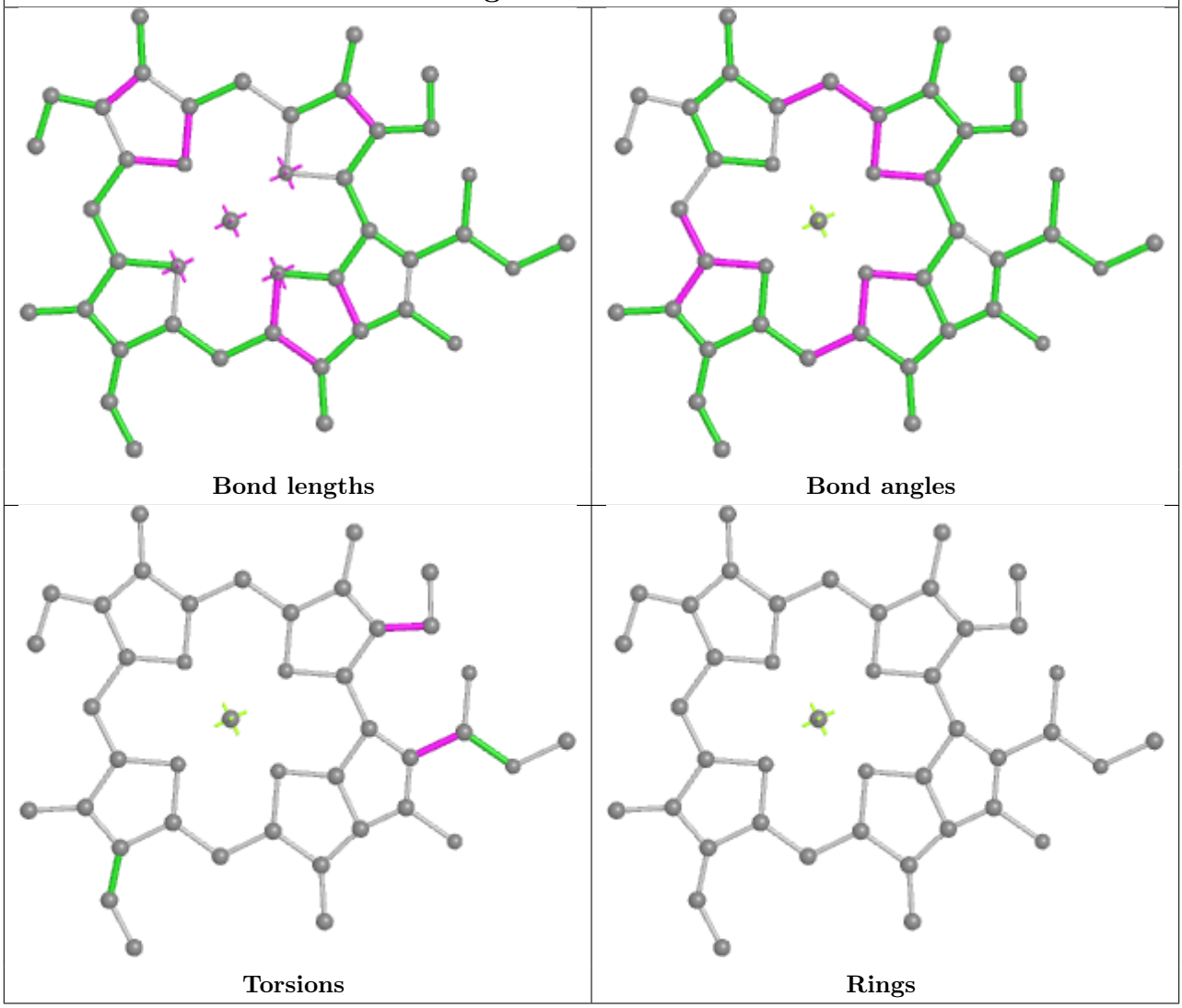
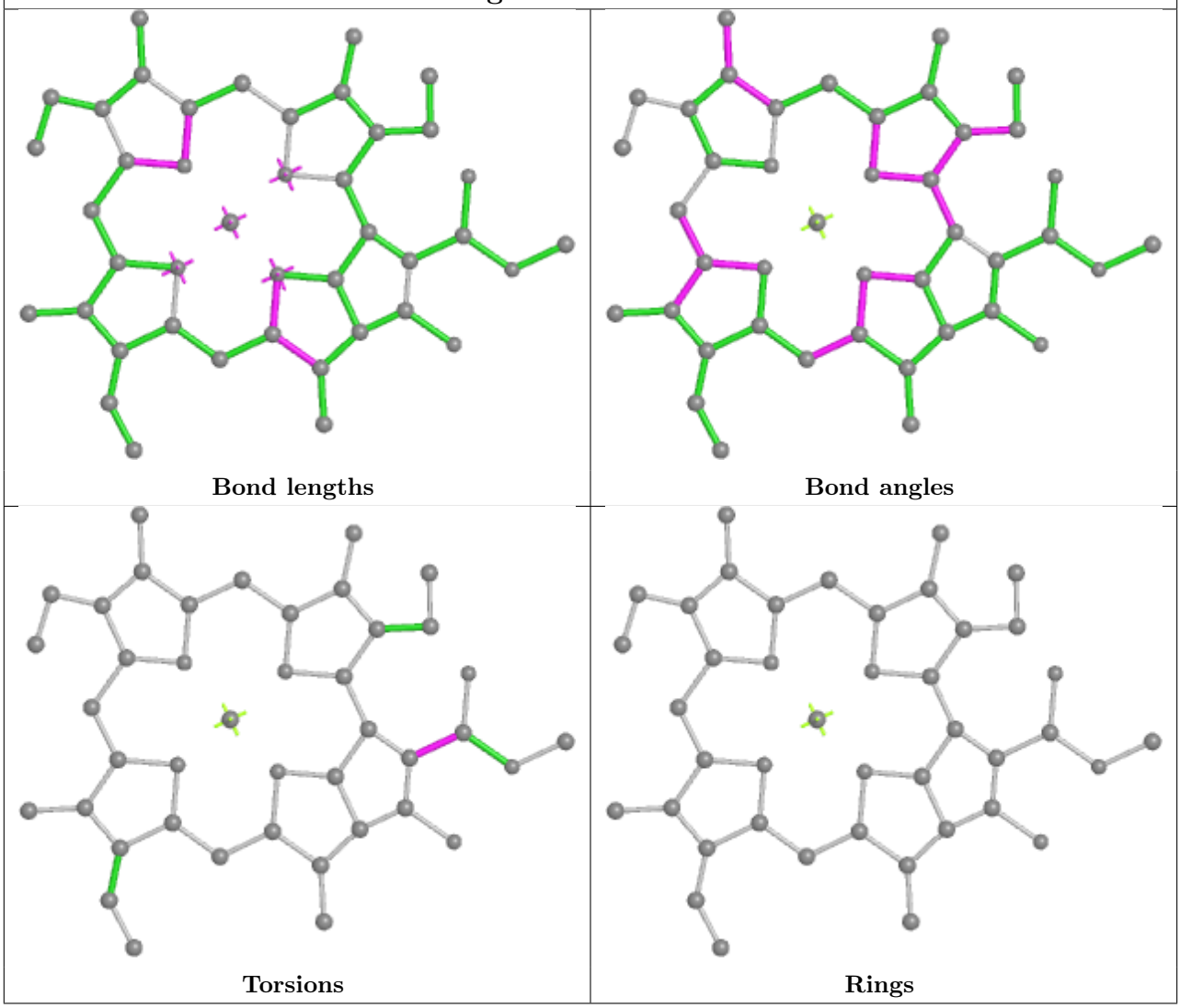


Rings

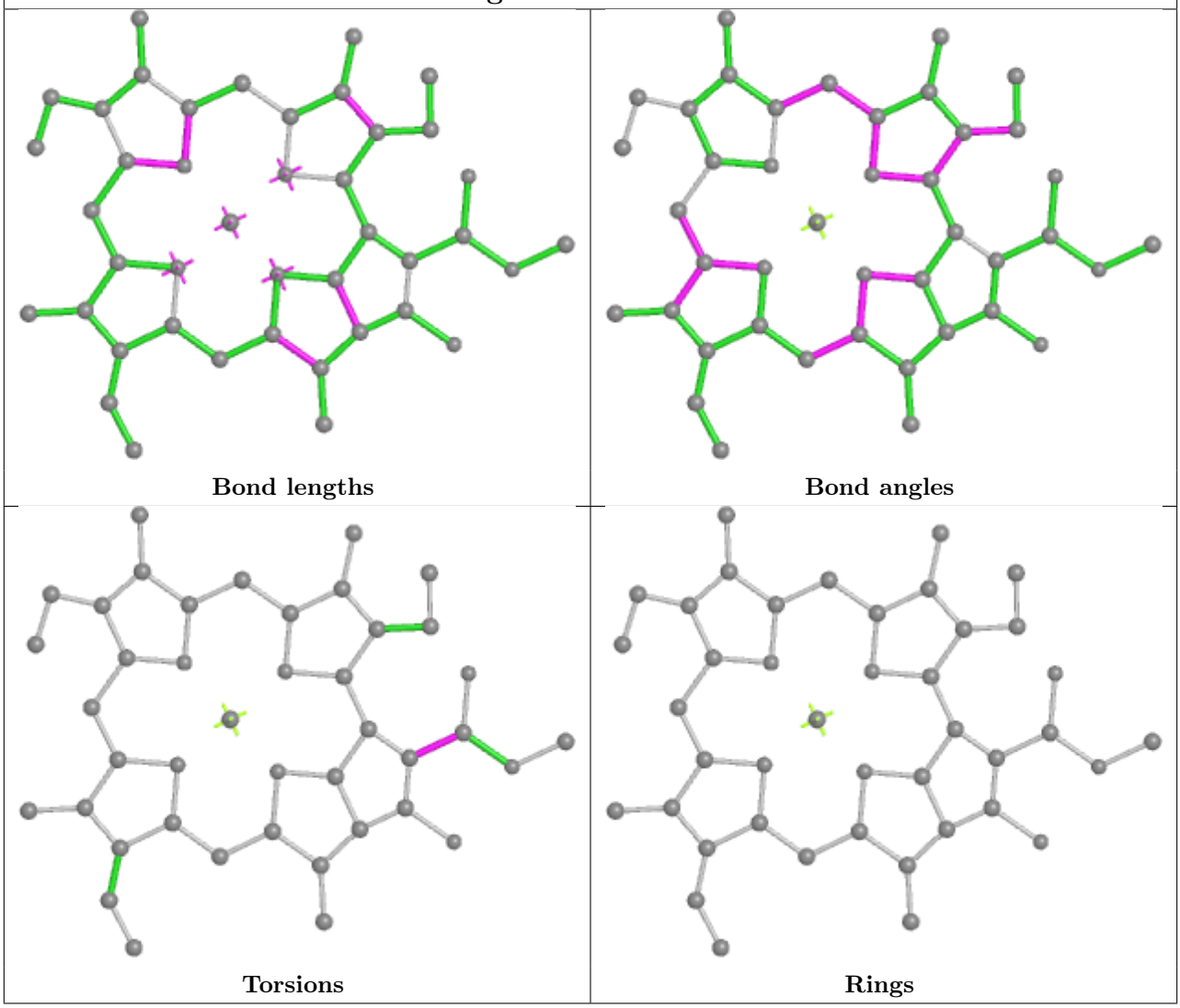
Ligand CLA B 827

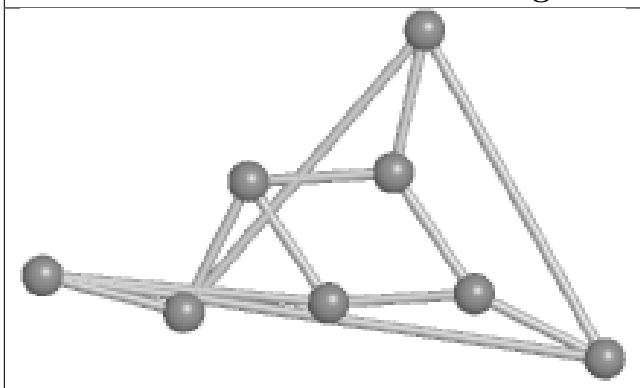
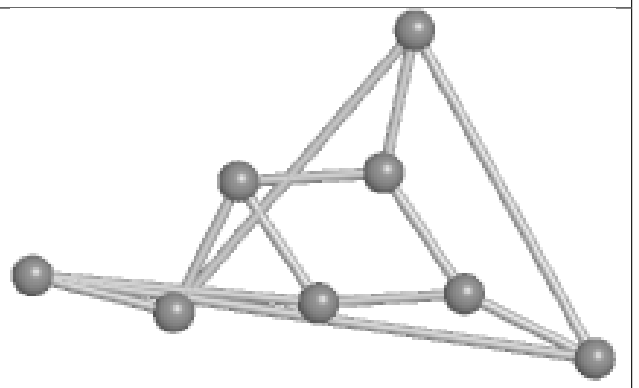
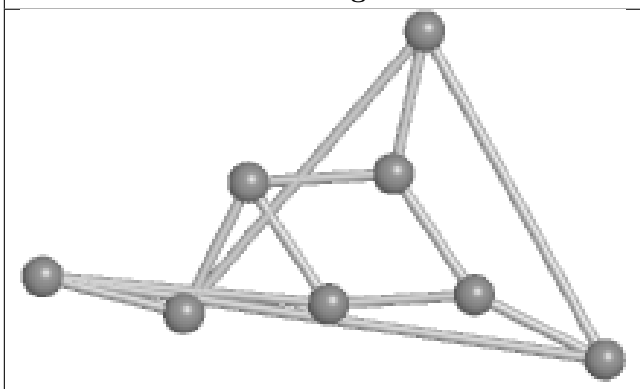
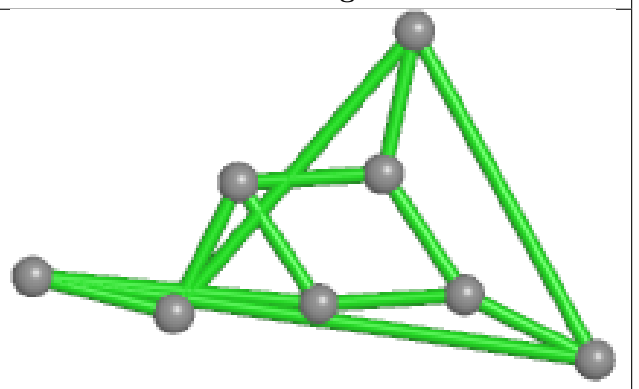


Ligand CLA 1 604

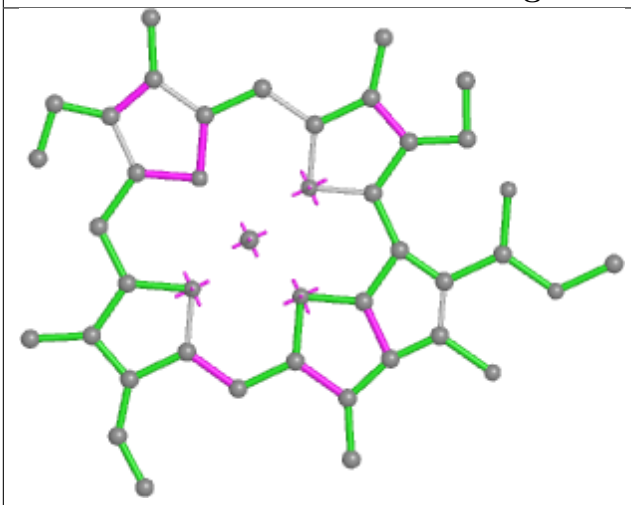


Ligand CLA 3 305



Ligand SF4 C 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 802



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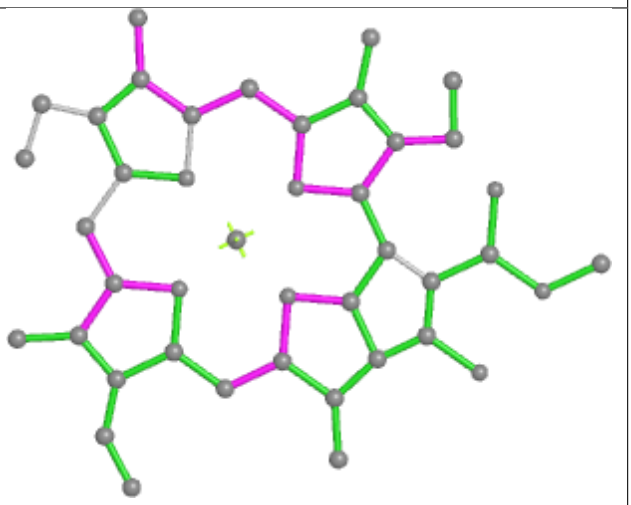
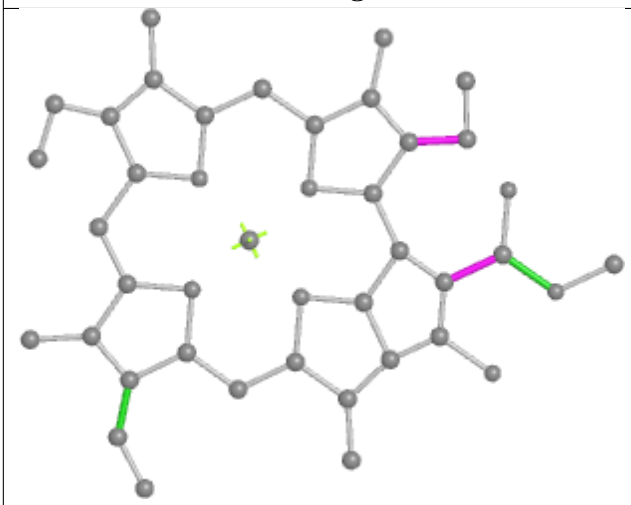


Bond angles



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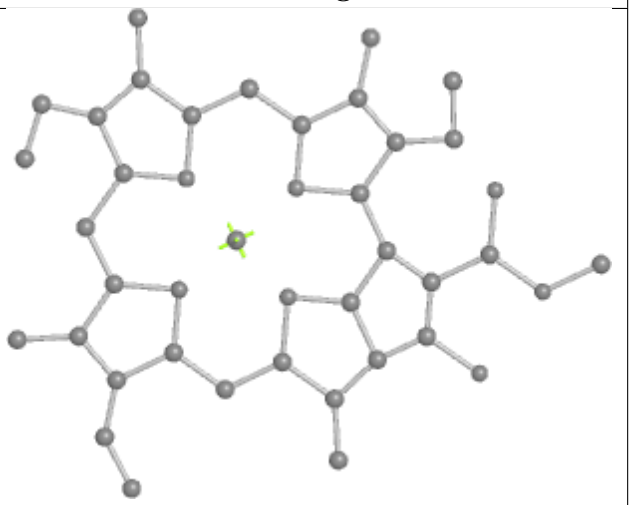
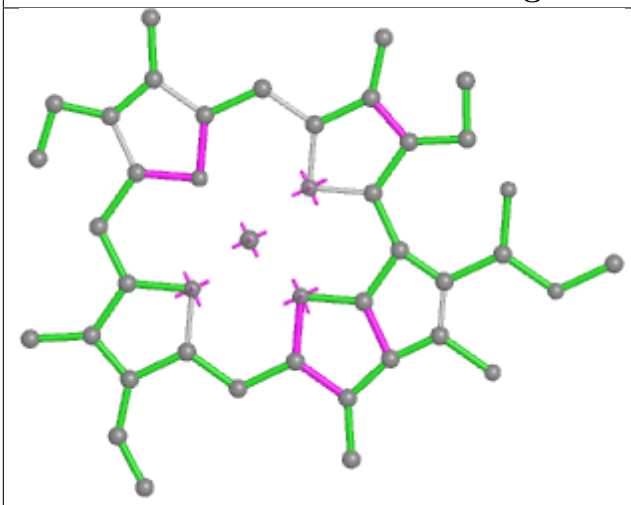


Rings

Ligand CLA A 807



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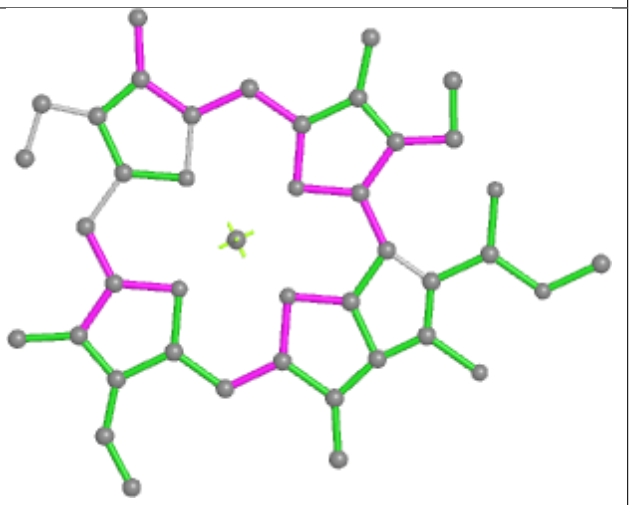
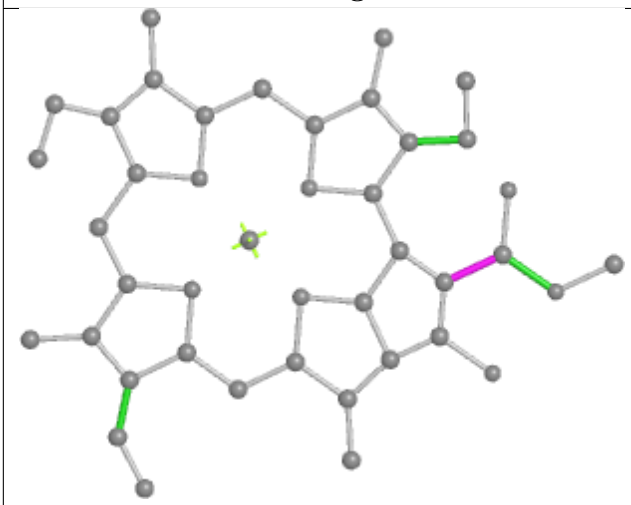


Bond angles



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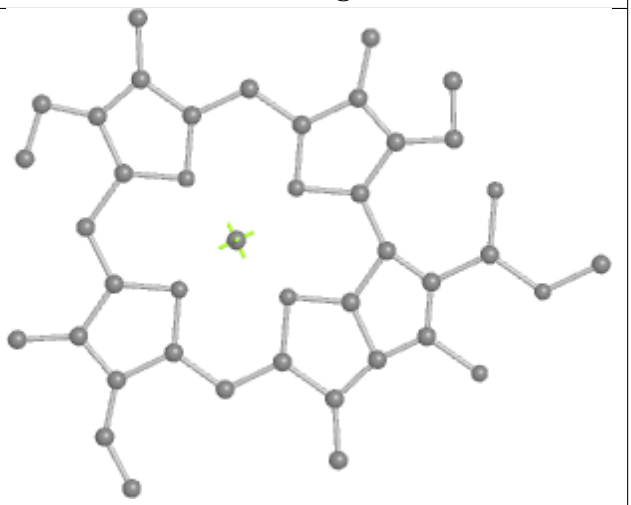
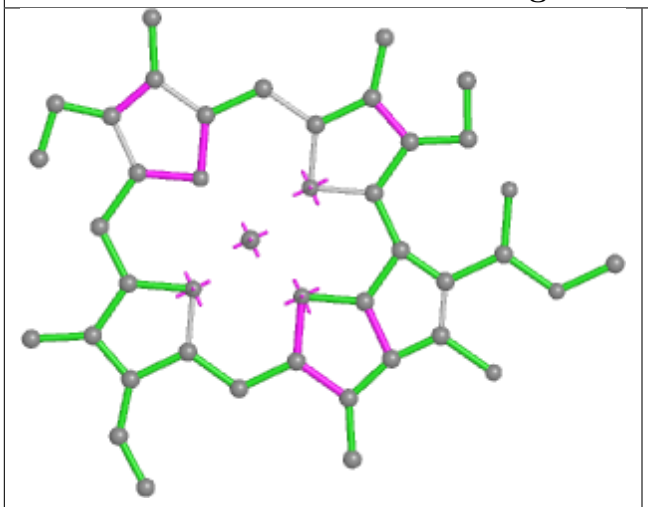


Rings

Ligand CL0 A 801



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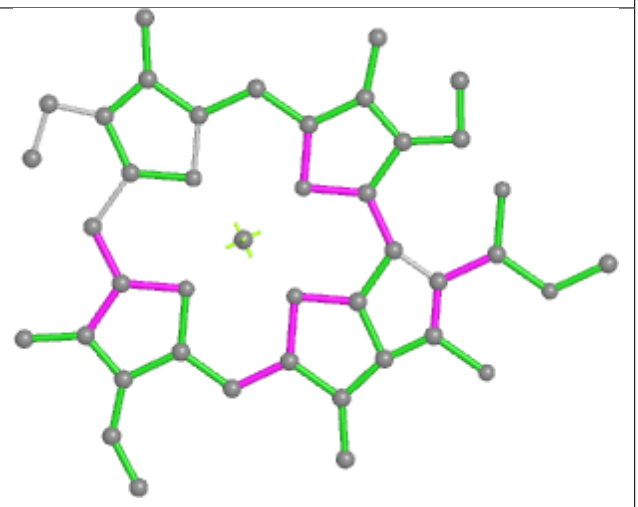
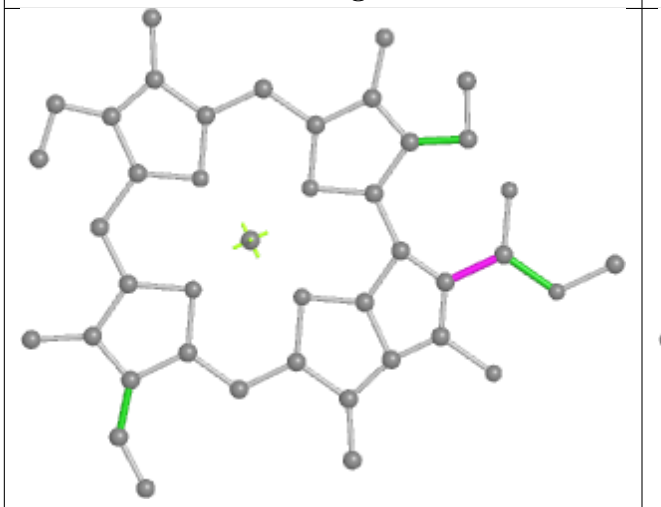
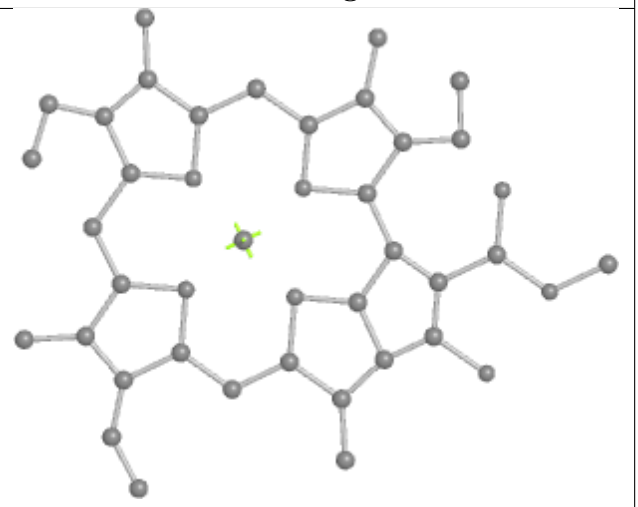


Bond angles

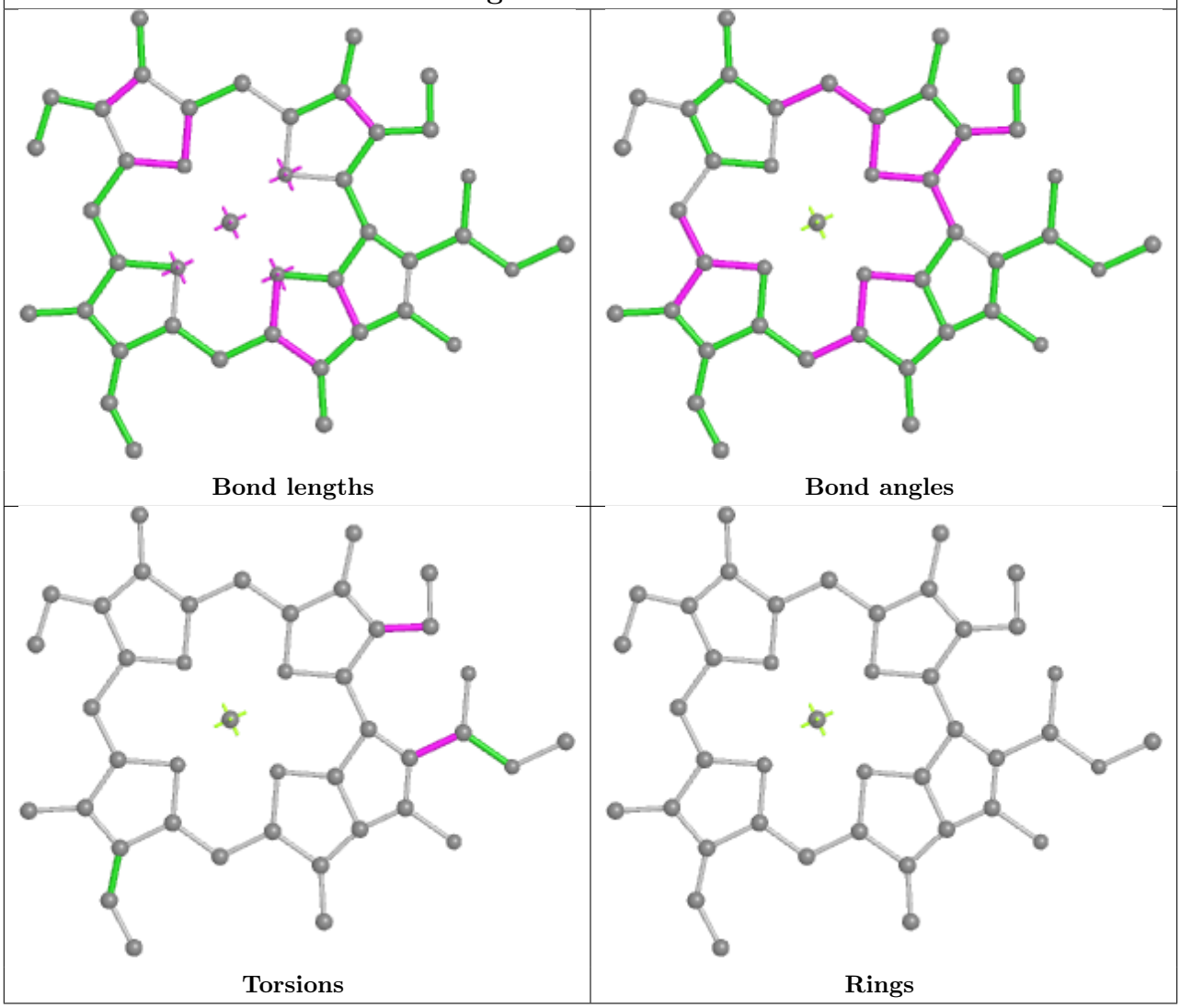


Torsions

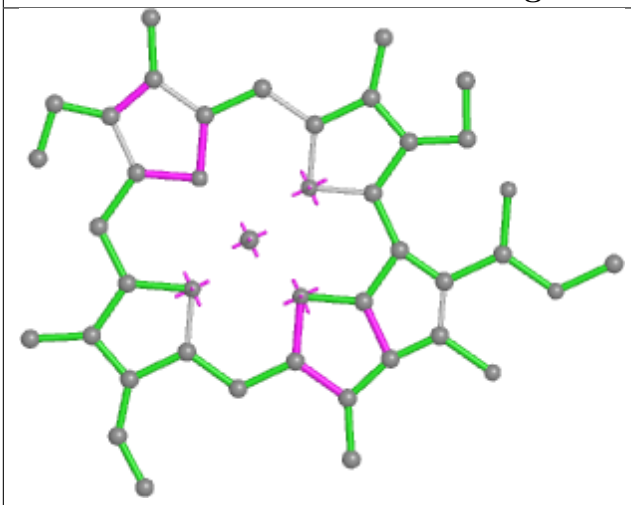


Rings

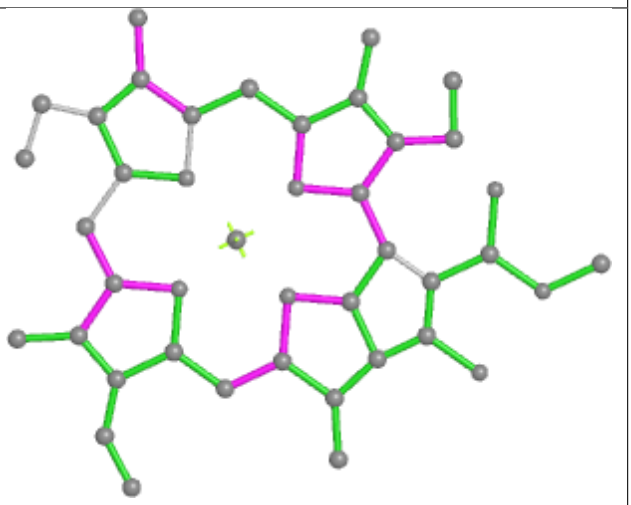
Ligand CLA 3 301



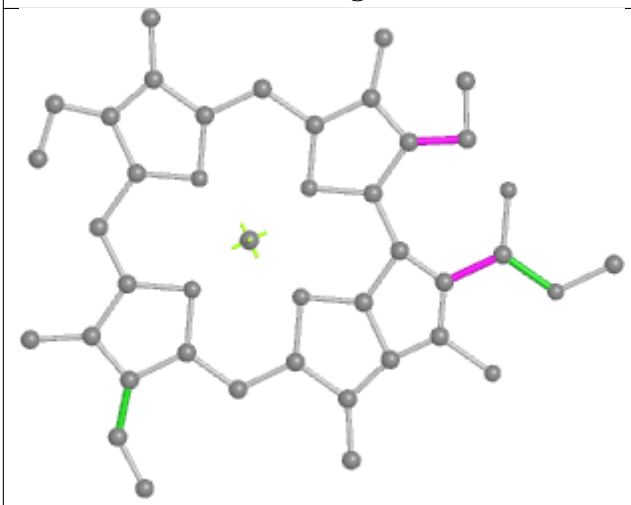
Ligand CLA B 817



Bond lengths



Bond angles



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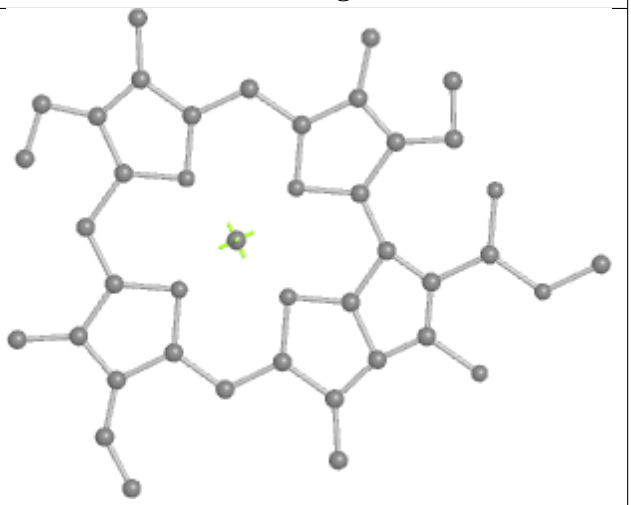
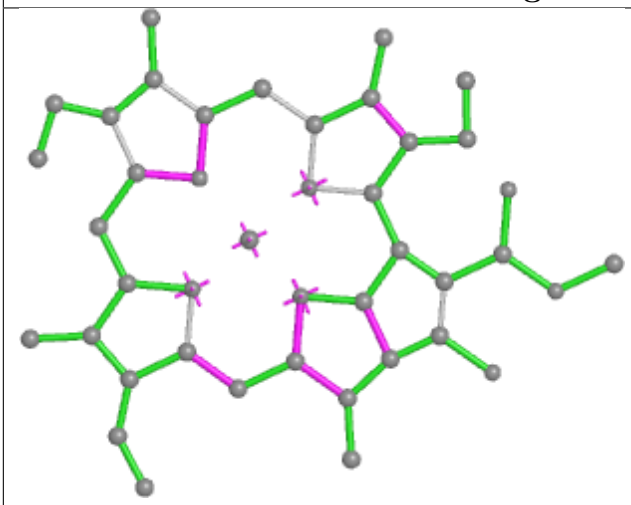
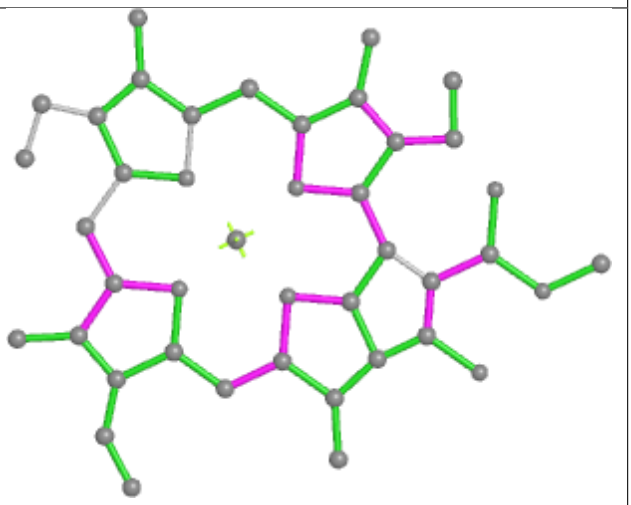


Rings

Ligand CLA A 831



Bond lengths



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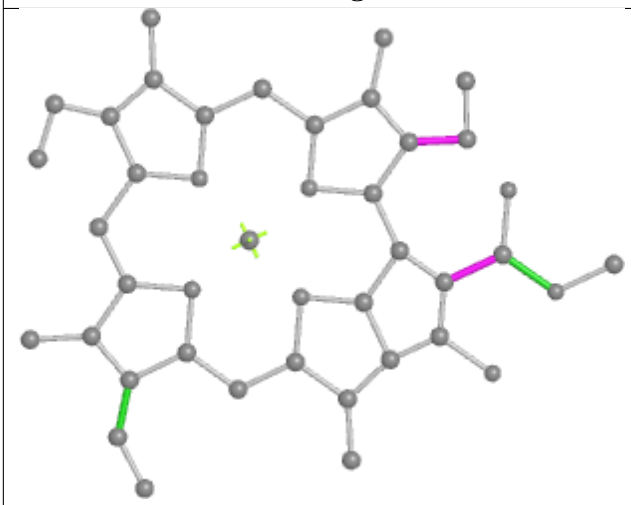

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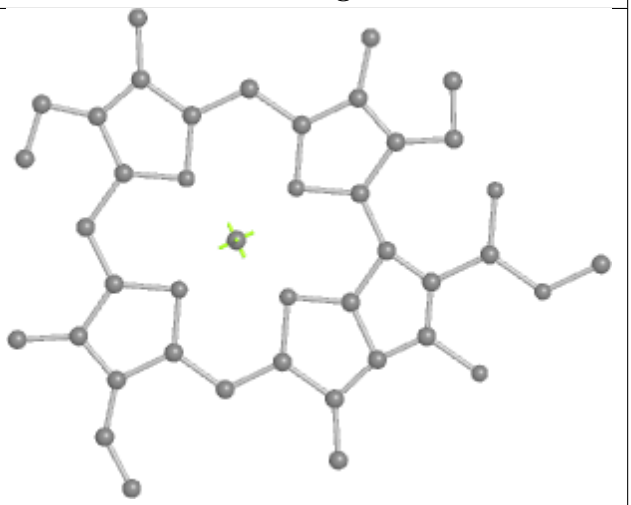
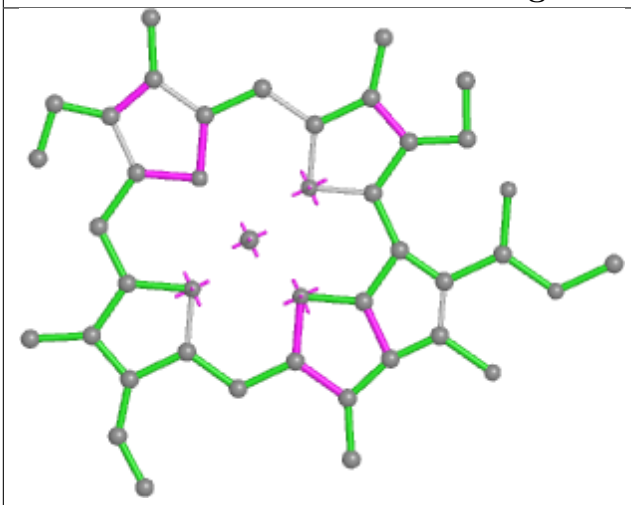
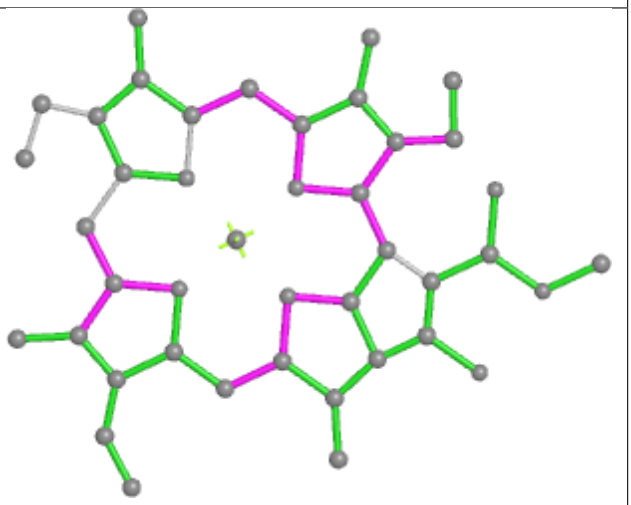


Rings

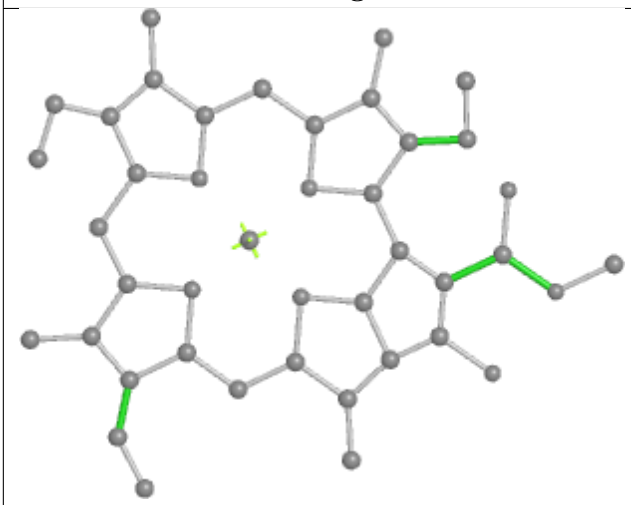
Ligand CLA 6 604



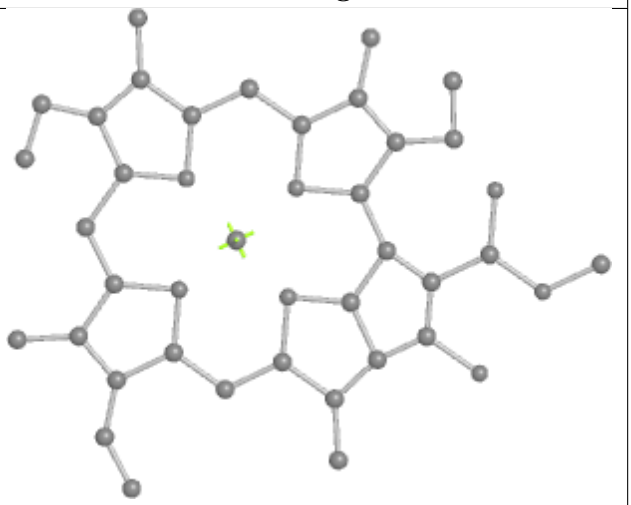
Bond lengths



Bond angles

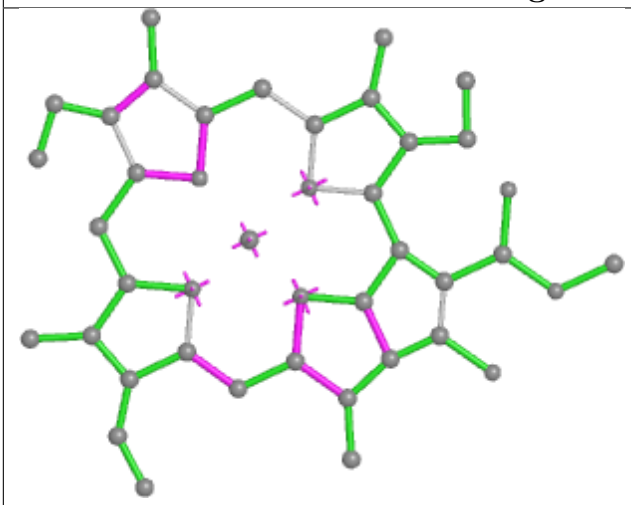


Torsions



Rings

Ligand CLA 5 301



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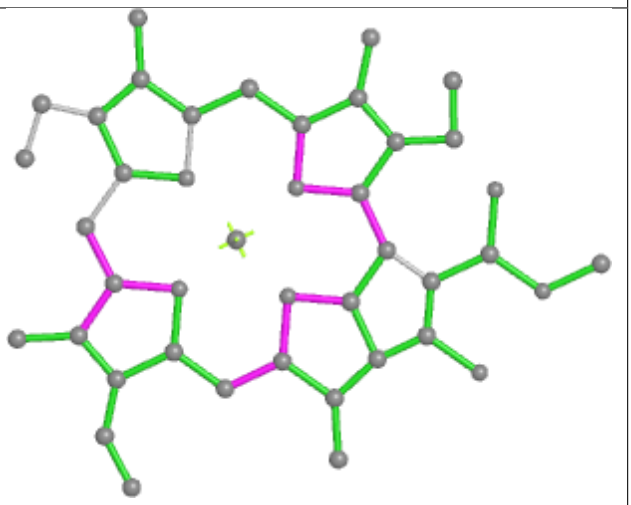
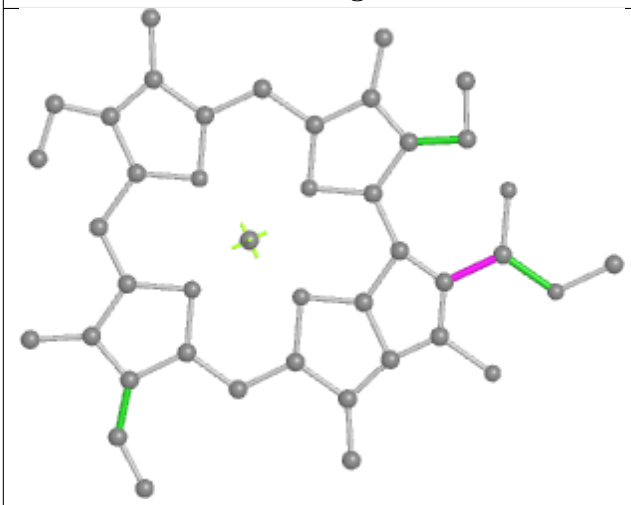
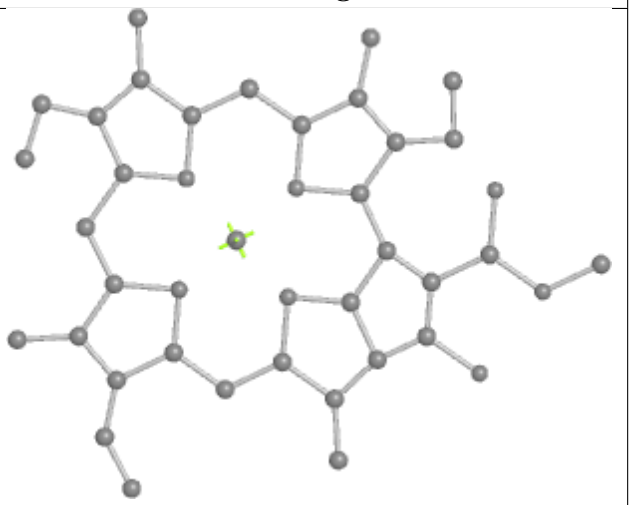


Bond angles

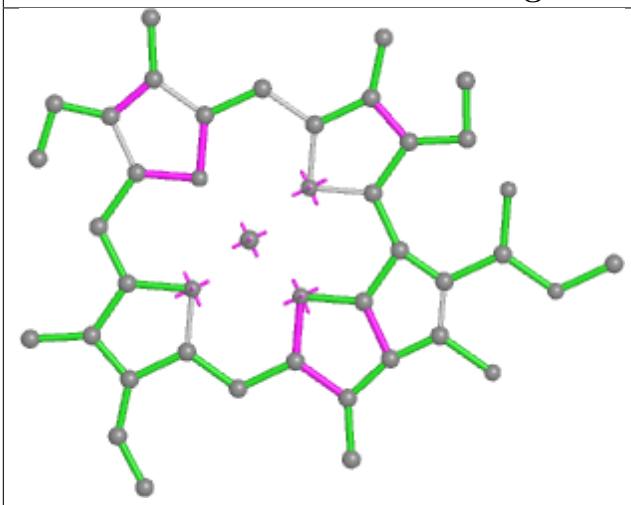


Torsions



Rings

Ligand CLA B 811



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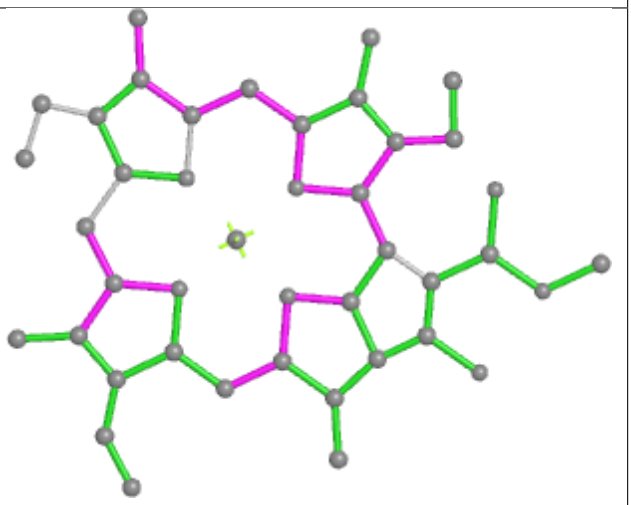
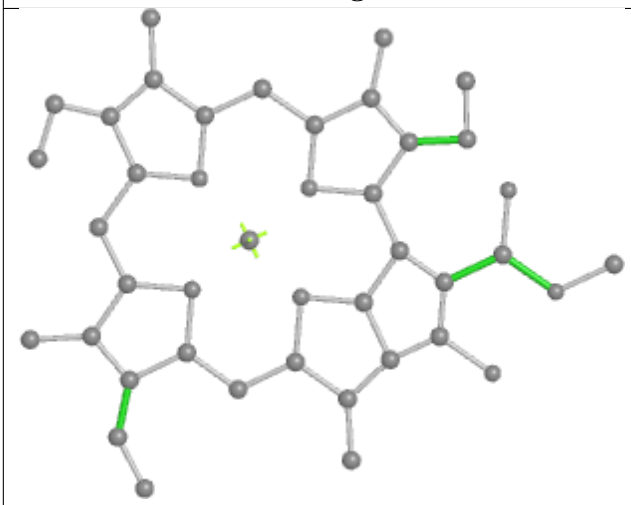
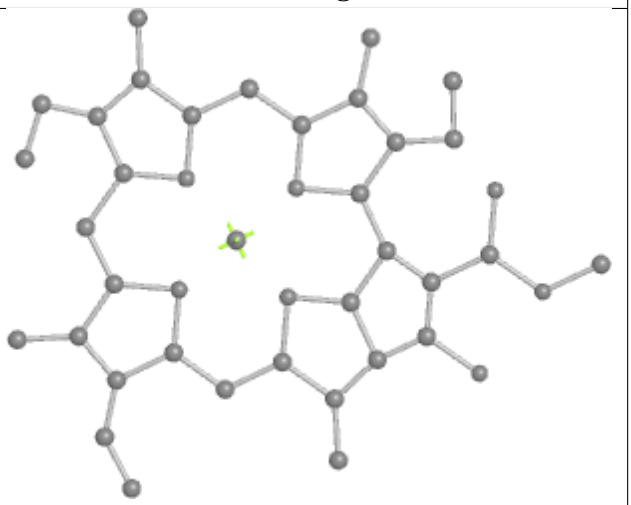


Bond angles

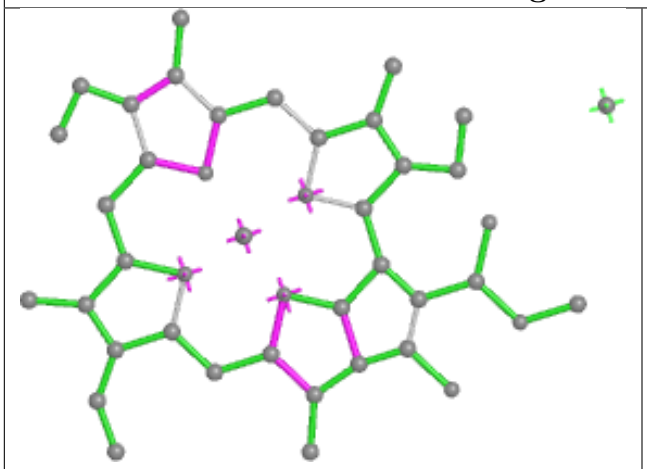


Torsions



Rings

Ligand CLA 1 602



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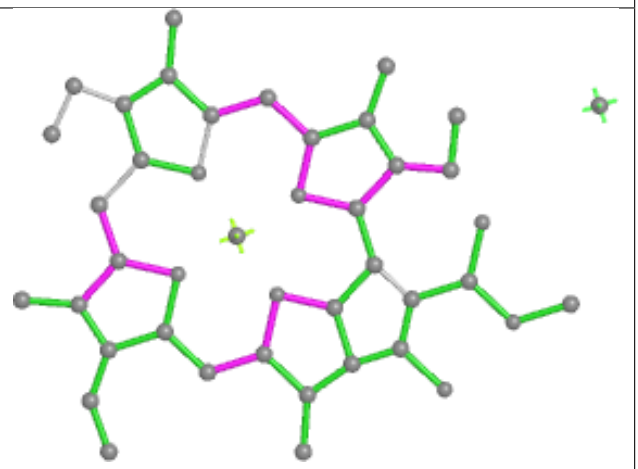
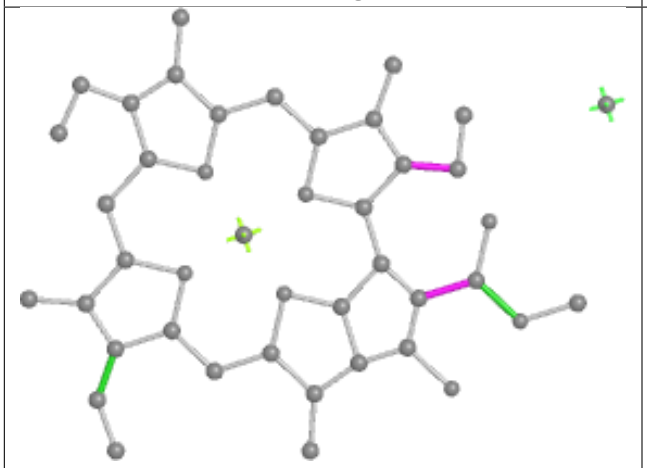
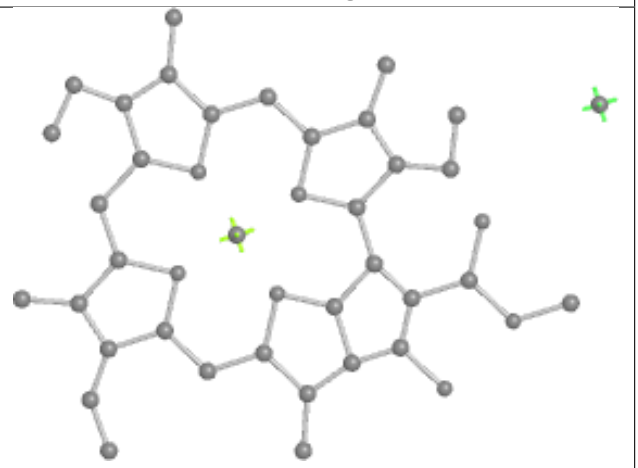


Bond angles

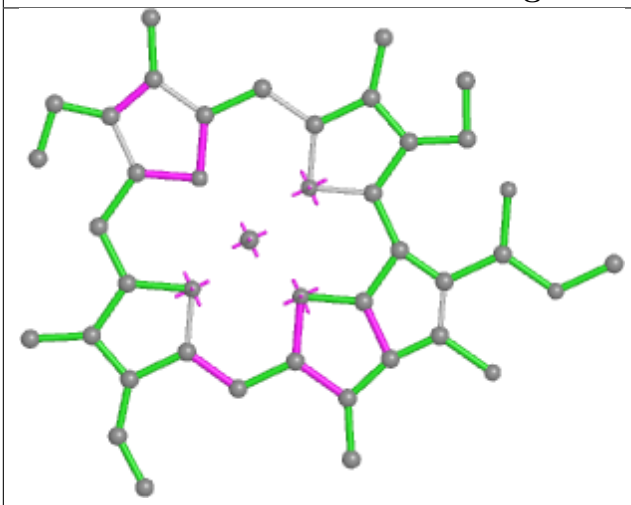


Torsions

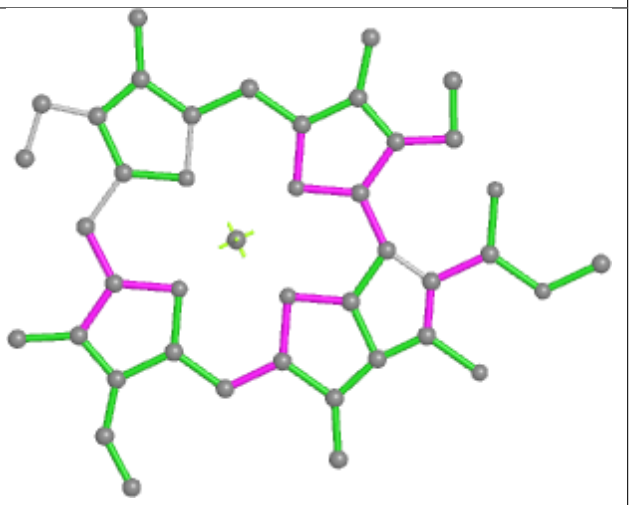


Rings

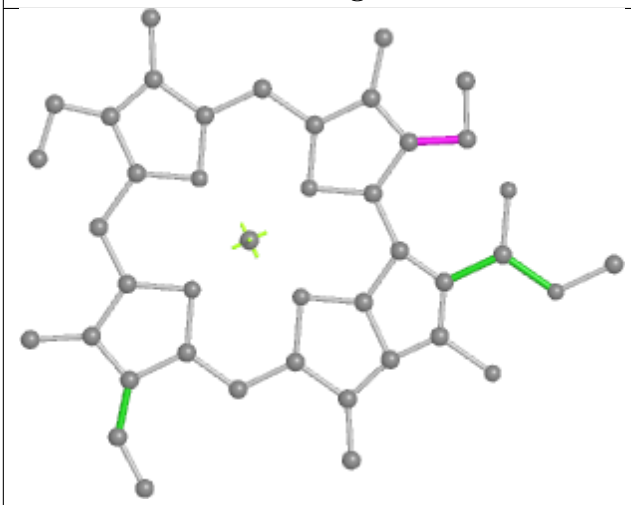
Ligand CLA A 830



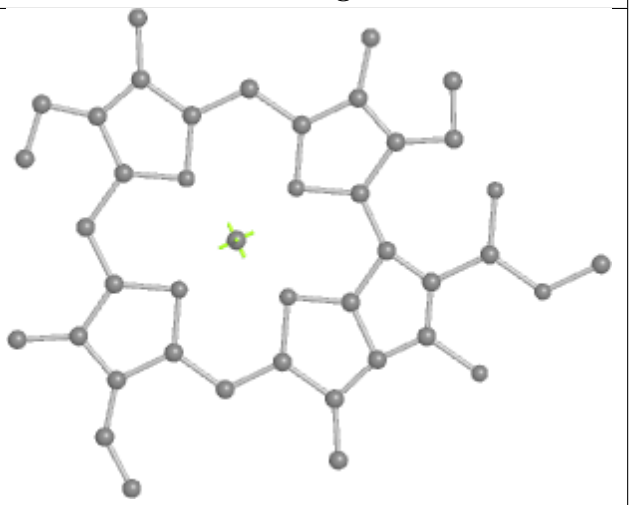
Bond lengths



Bond angles

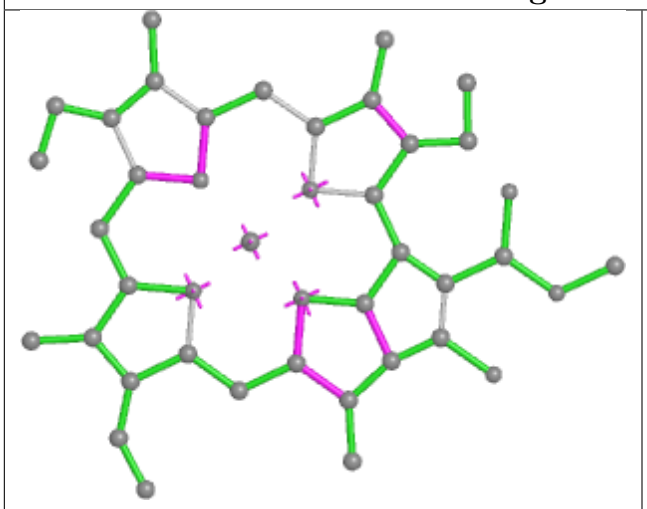


Torsions



Rings

Ligand CLA 4 604



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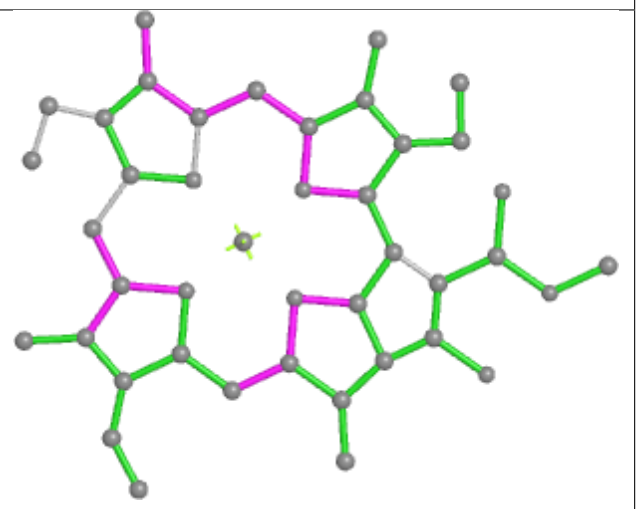

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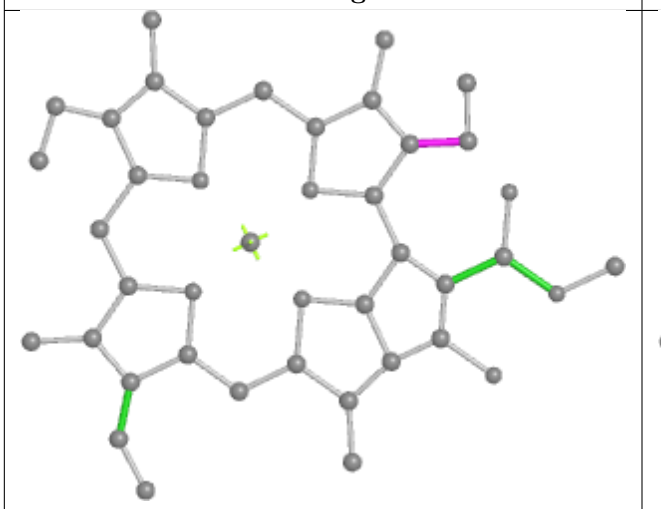

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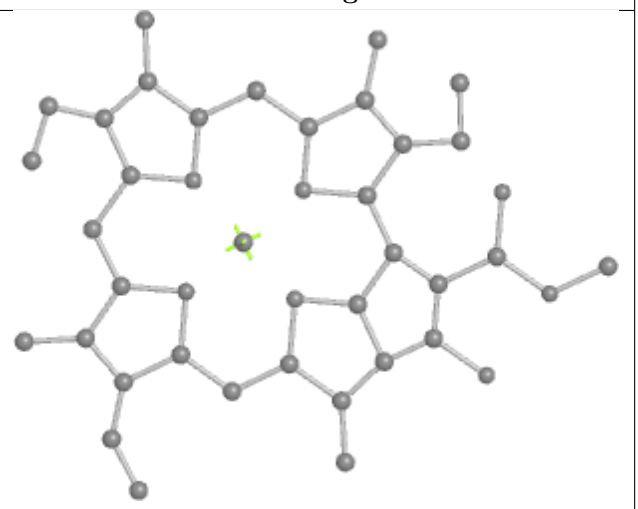
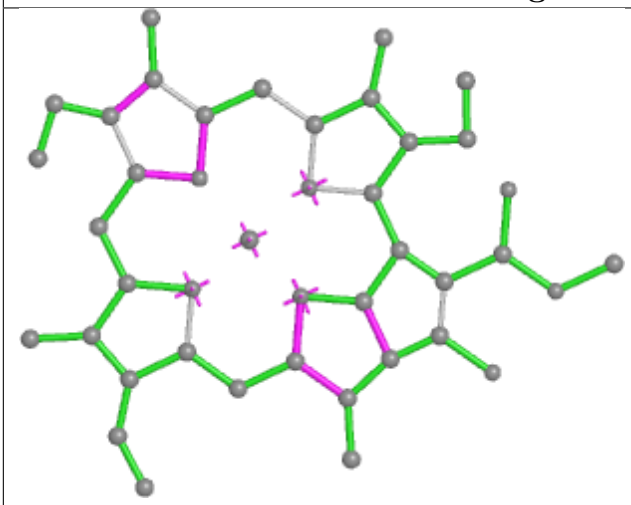


Rings

Ligand CLA 8 609



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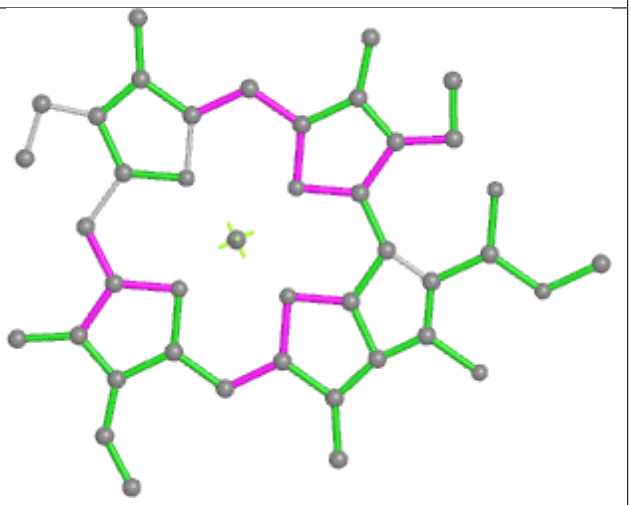

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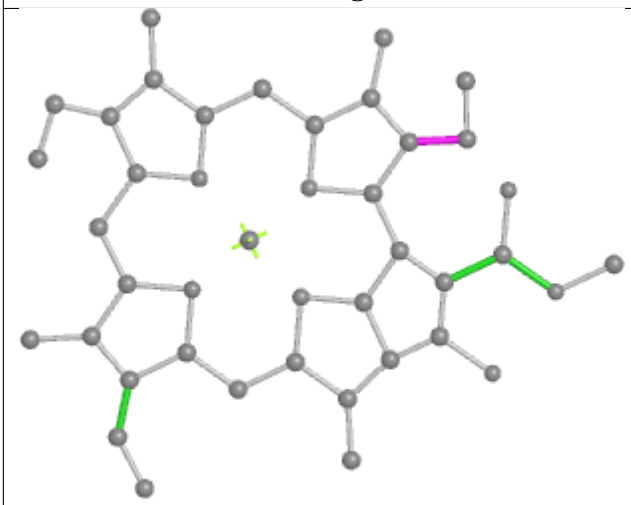

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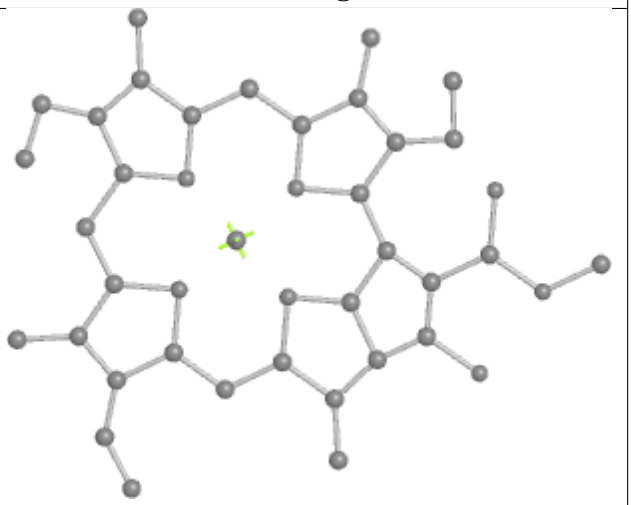

Rings

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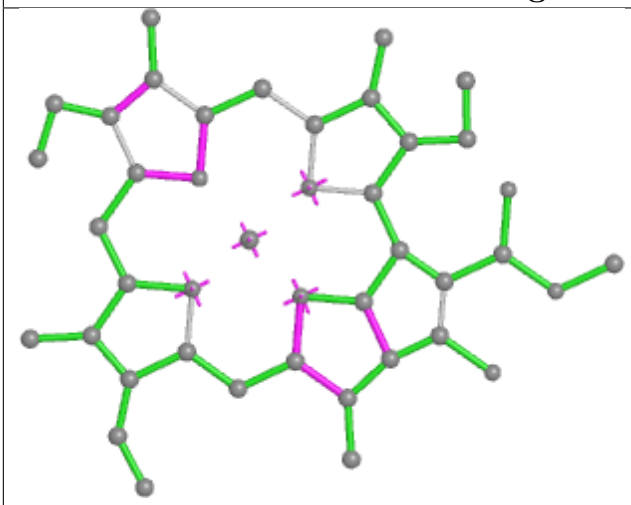

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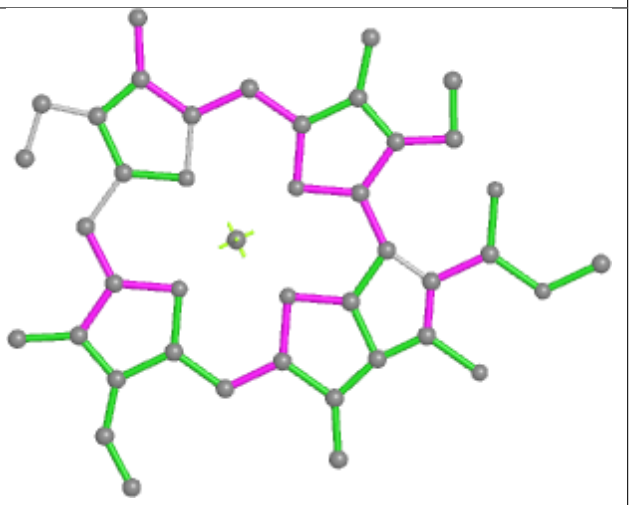

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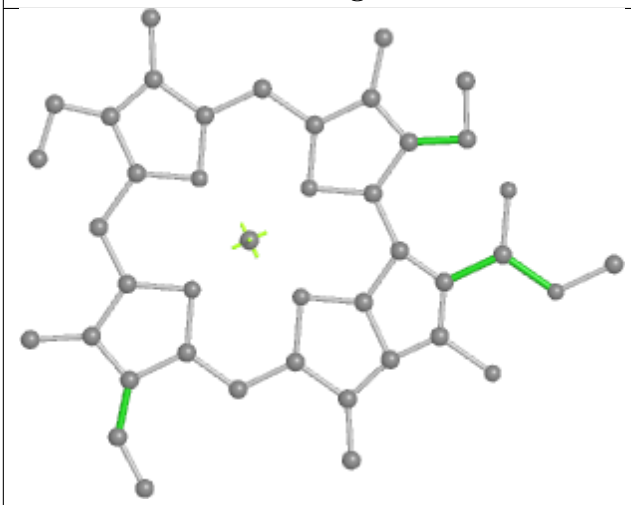

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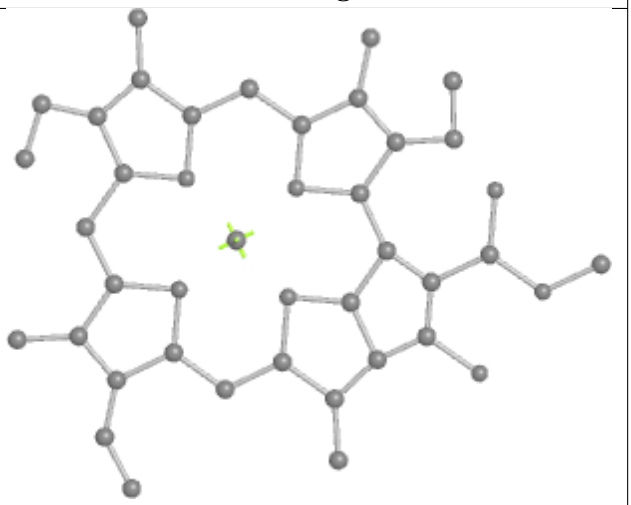
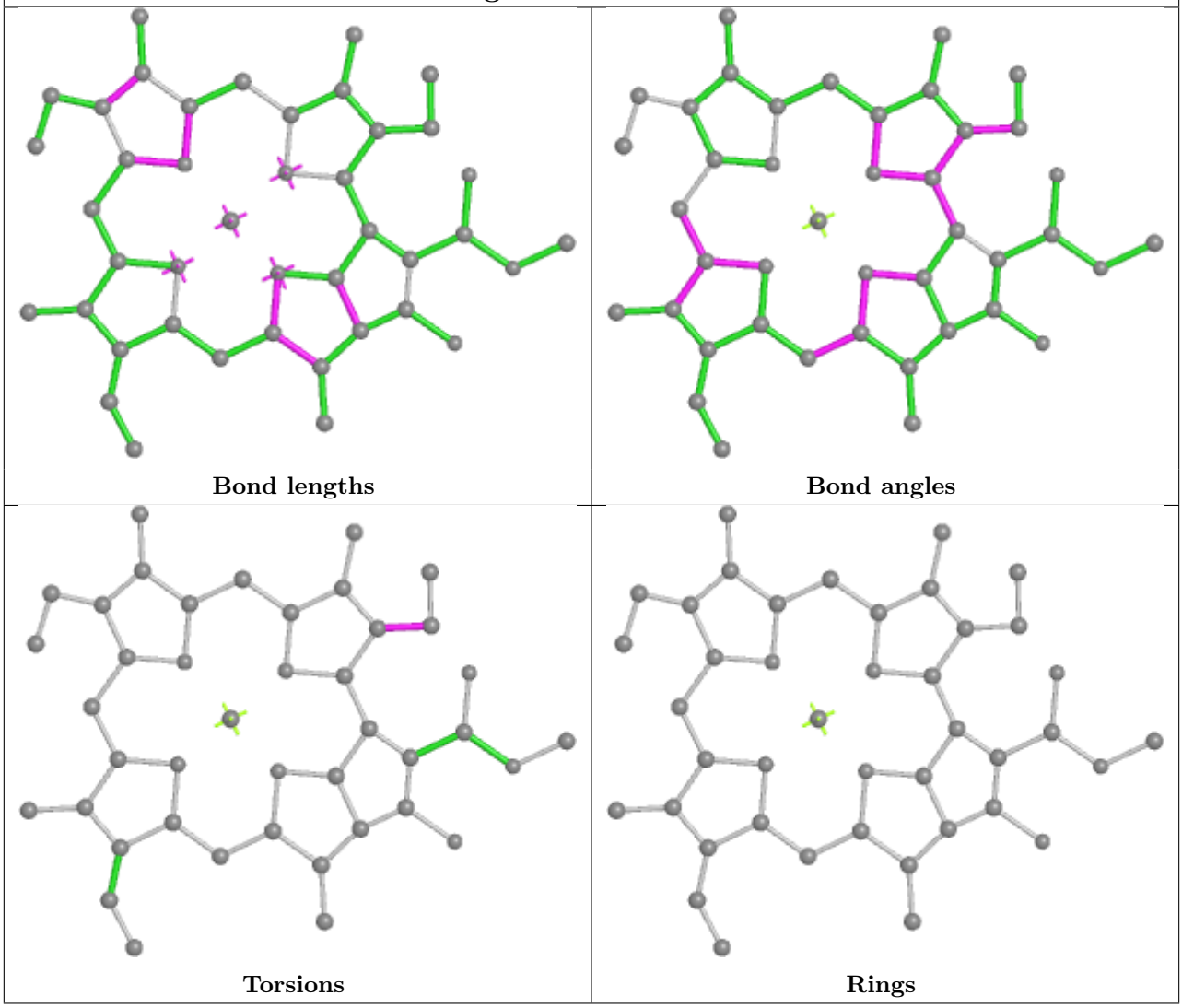
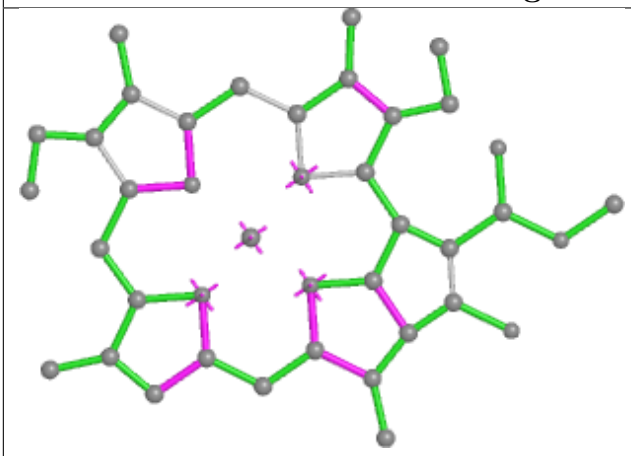


Rings

Ligand CLA B 837



Ligand CLA A 832



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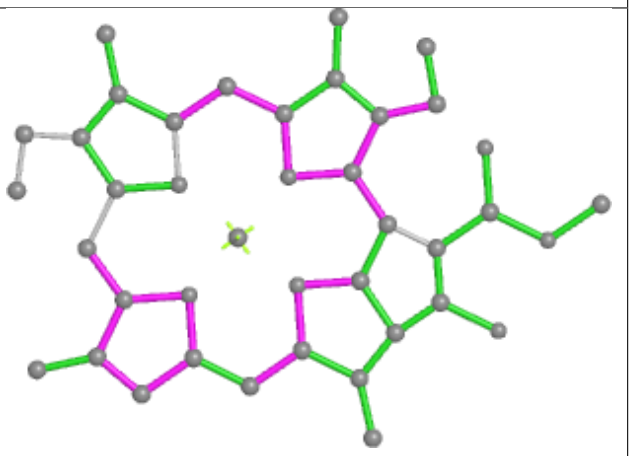

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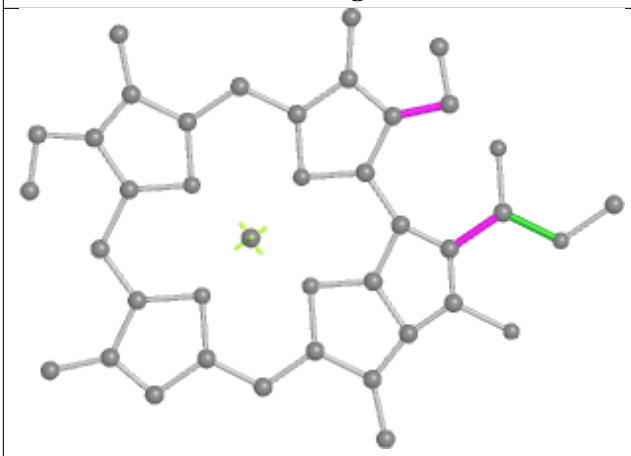

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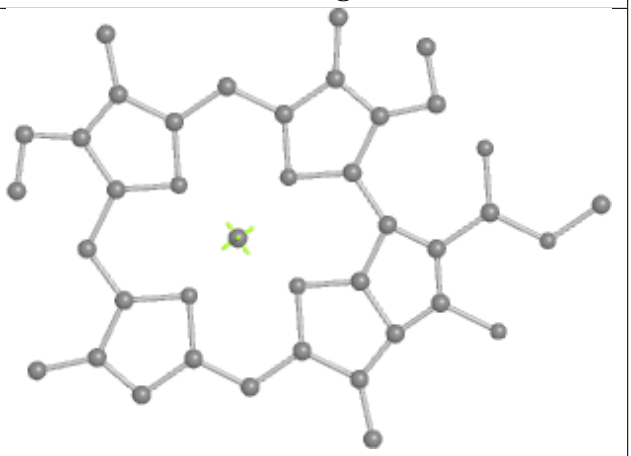
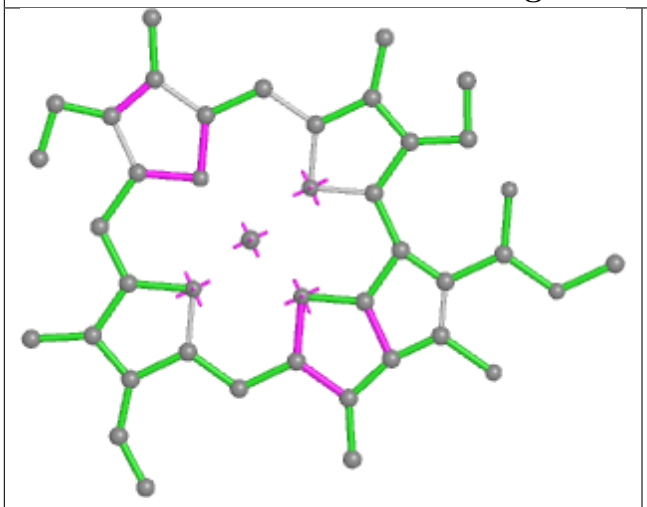


Rings

Ligand CLA A 819



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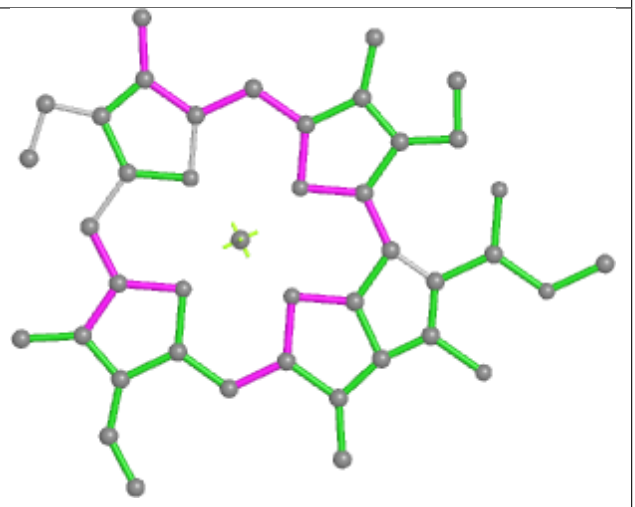
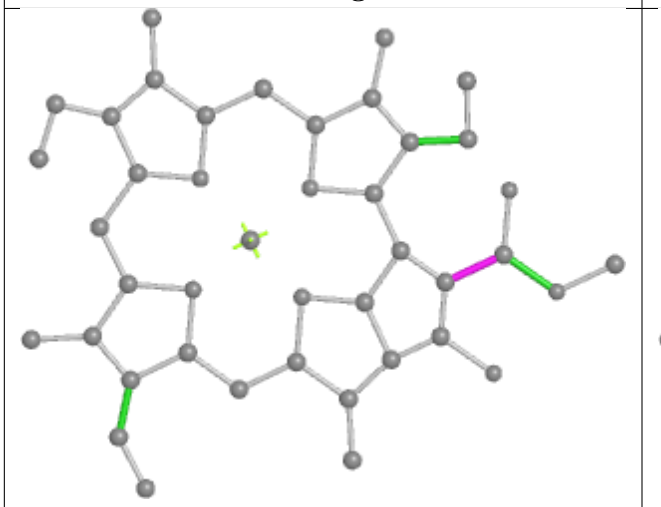


Bond angles



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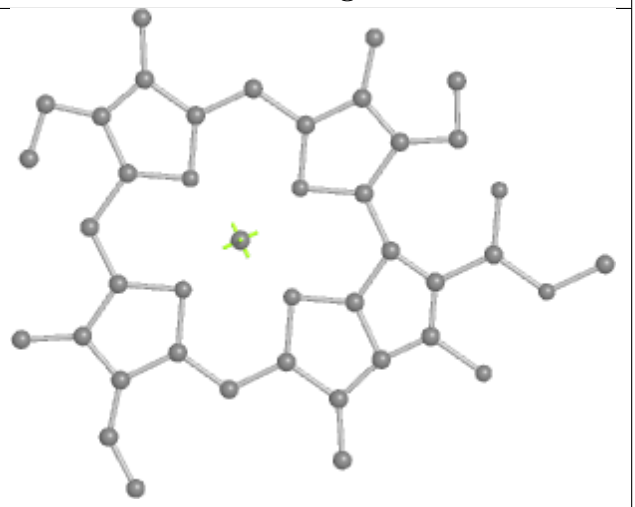
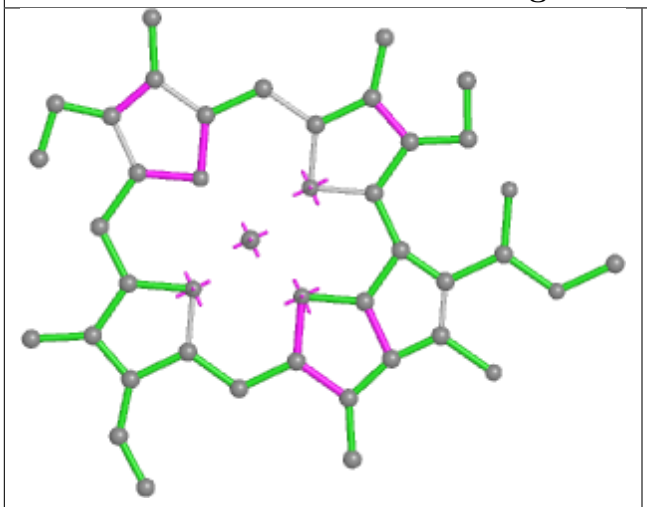


Rings

Ligand CLA 7 607



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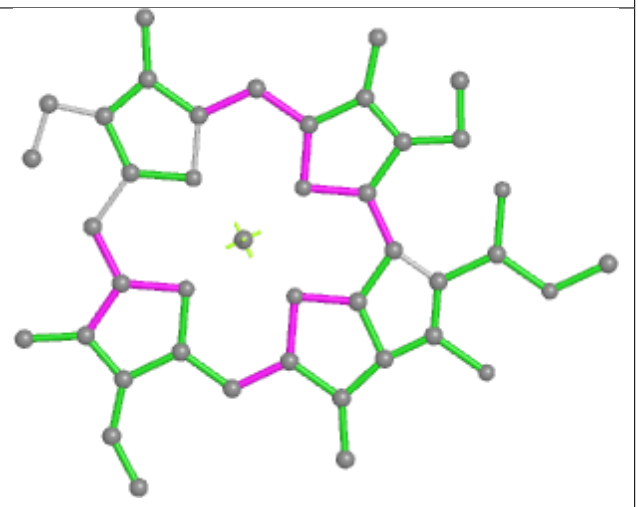

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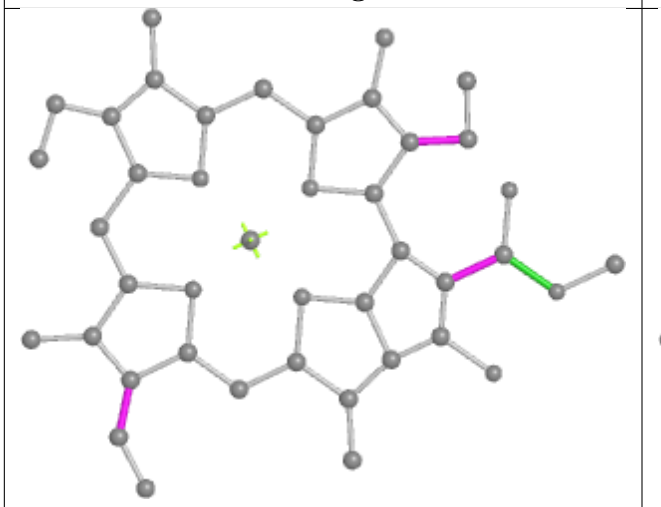

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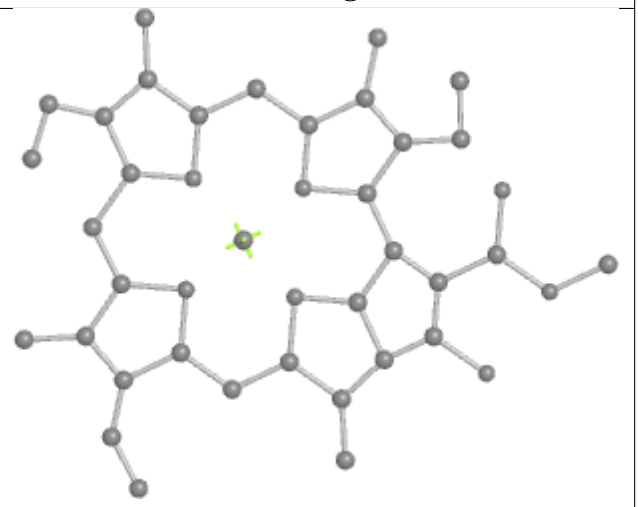
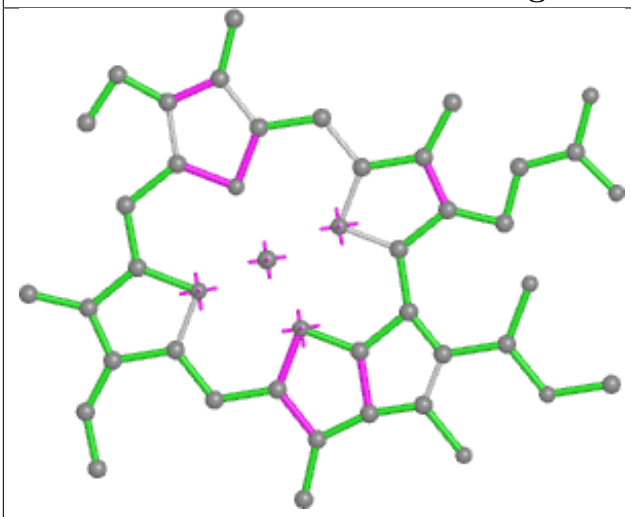


Rings

Ligand CLA 7 612



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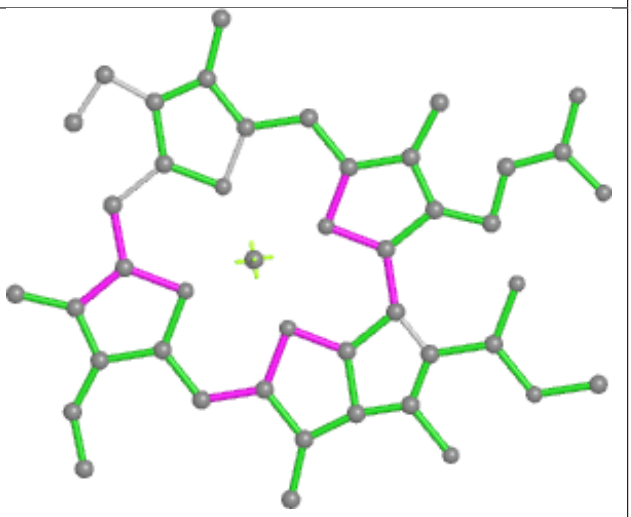
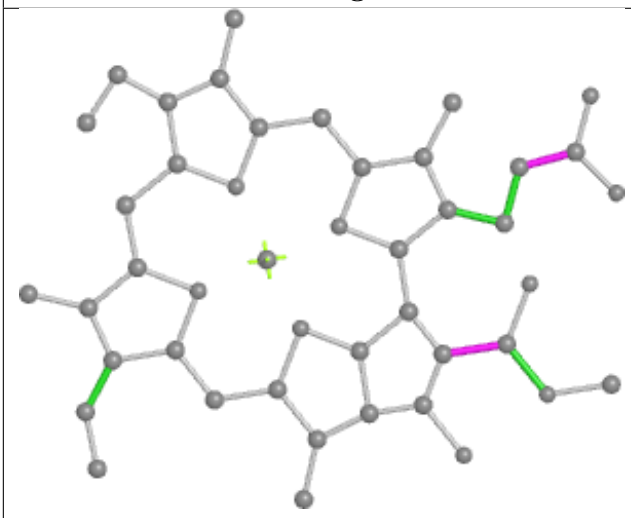


Bond angles



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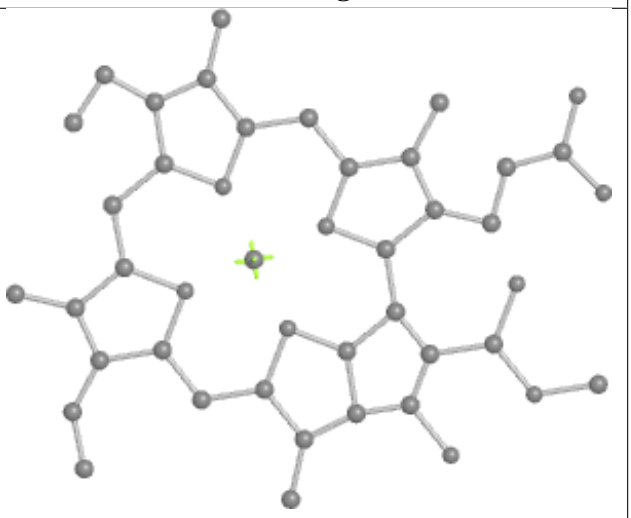
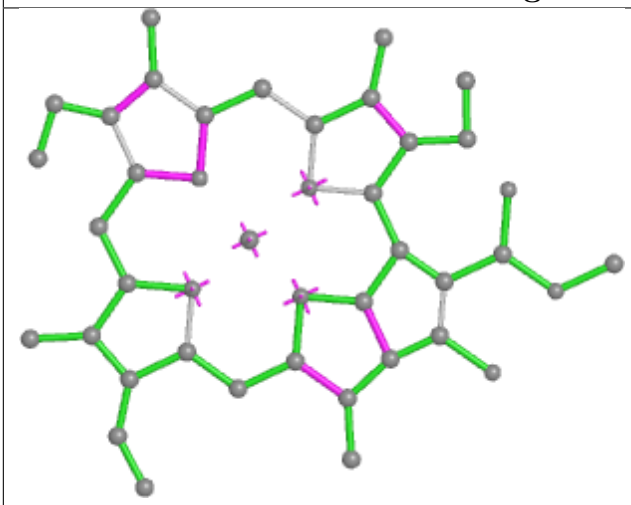


Rings

Ligand CLA A 804



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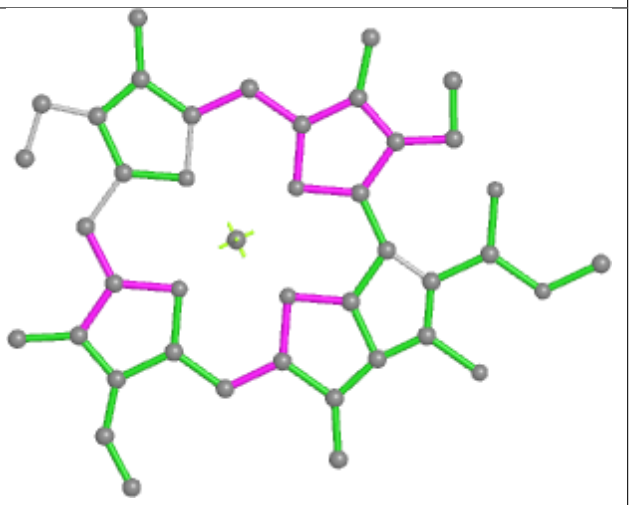
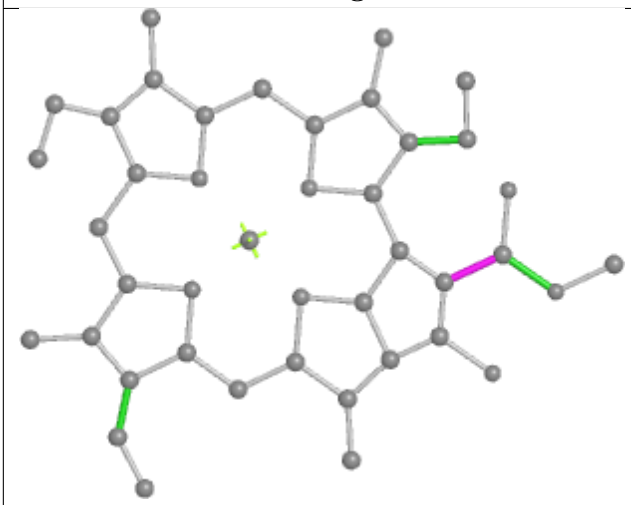


Bond angles



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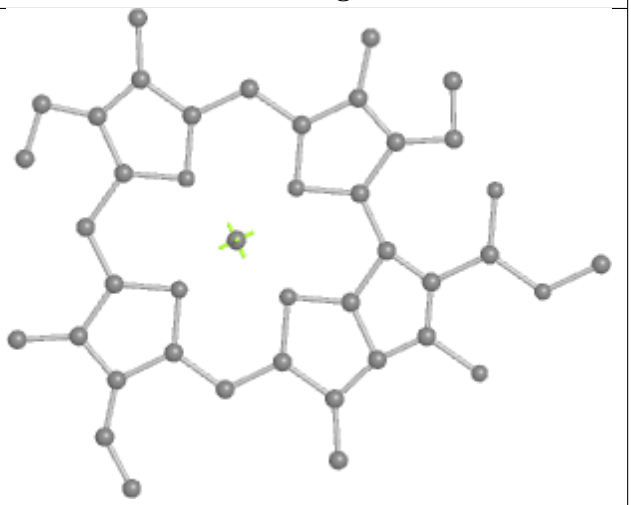
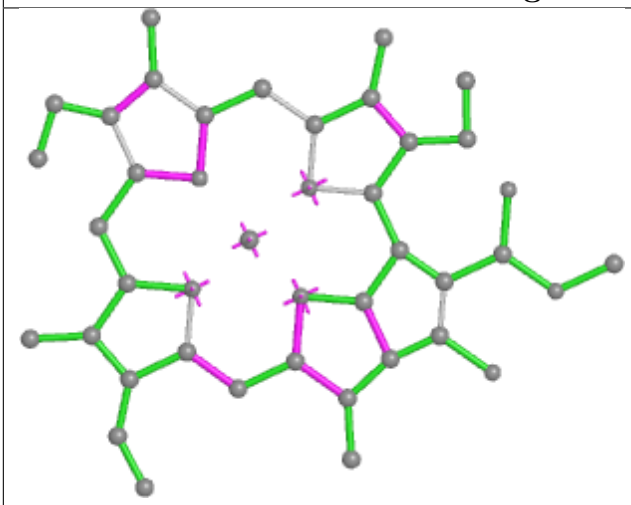


Rings

Ligand CLA A 811



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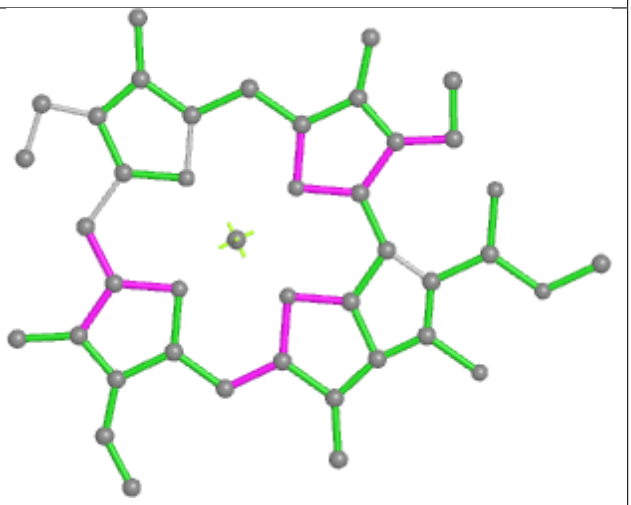
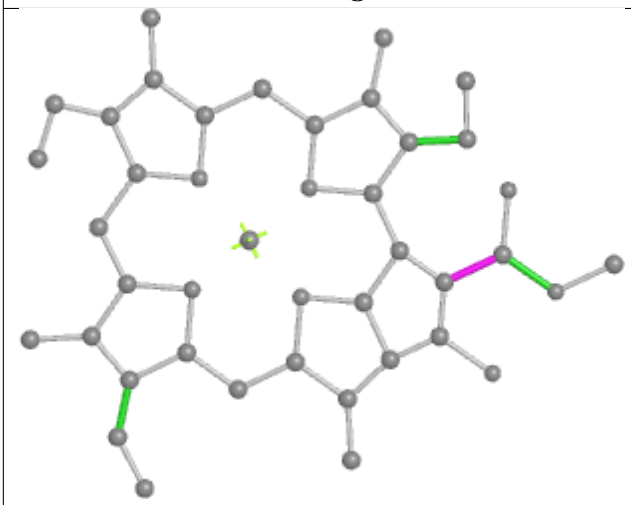


Bond angles



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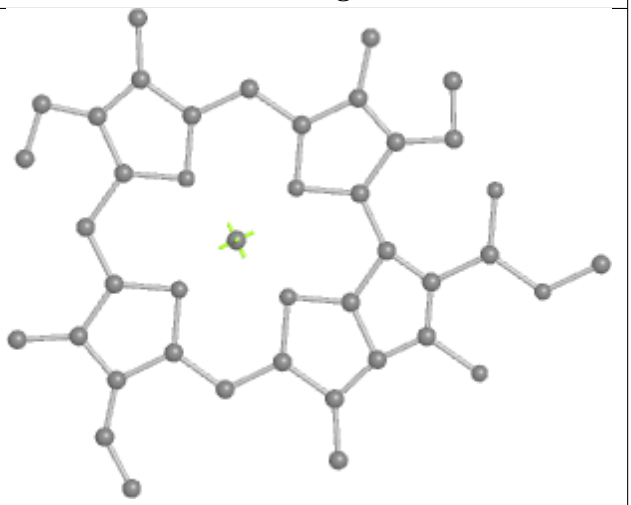
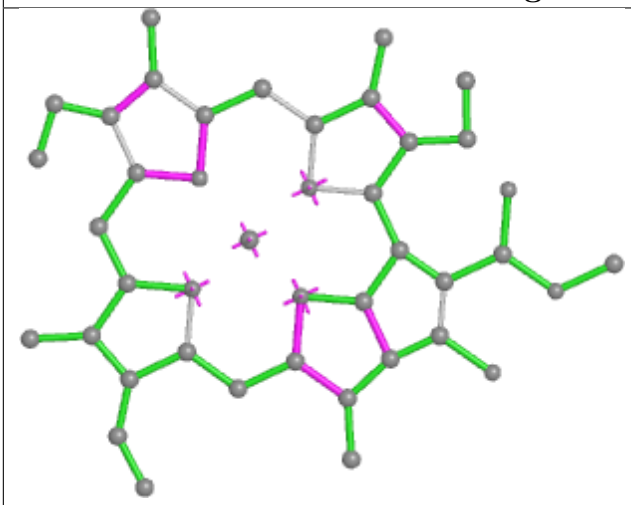


Rings

Ligand CLA B 834



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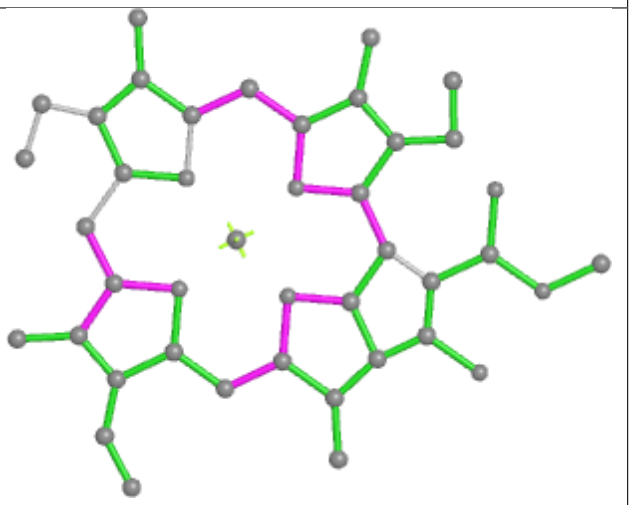

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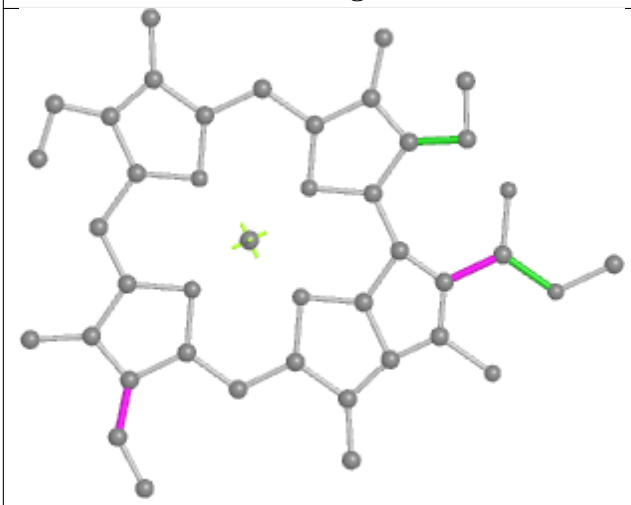

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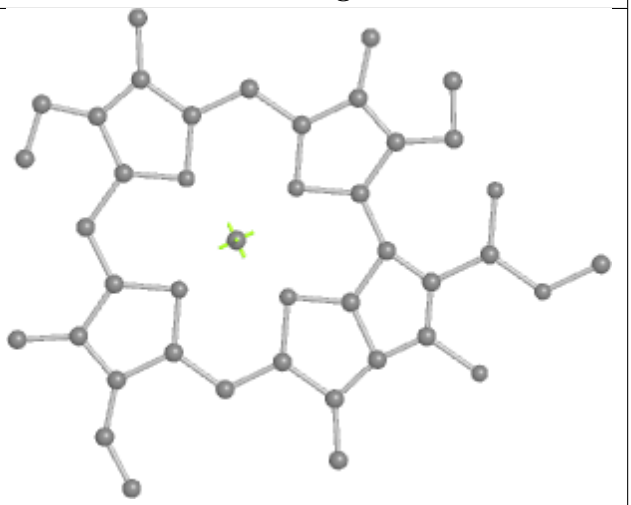
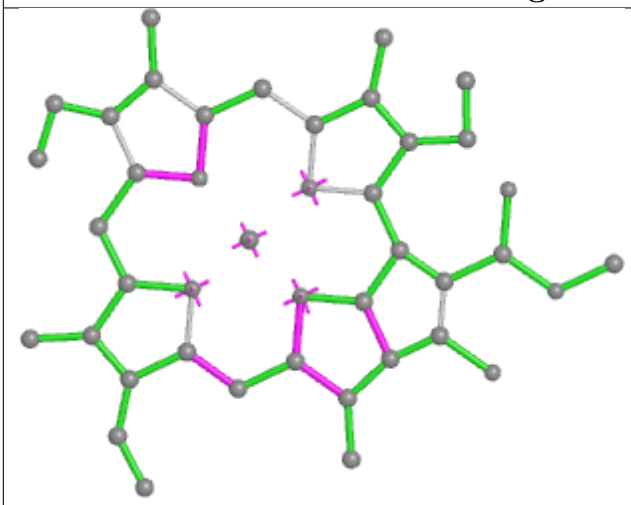


Rings

Ligand CLA 6 602



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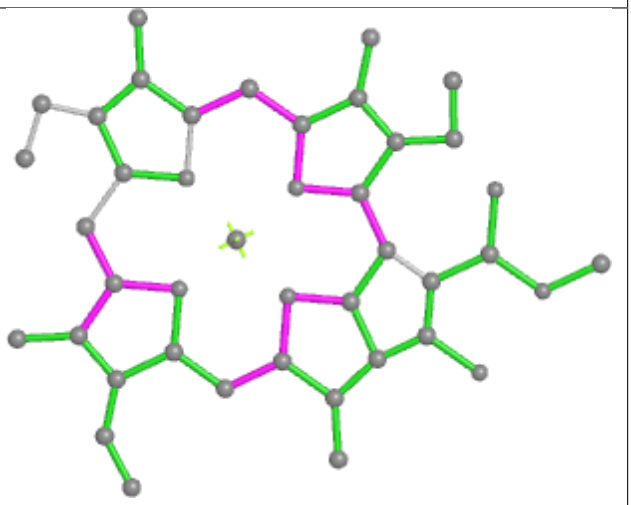
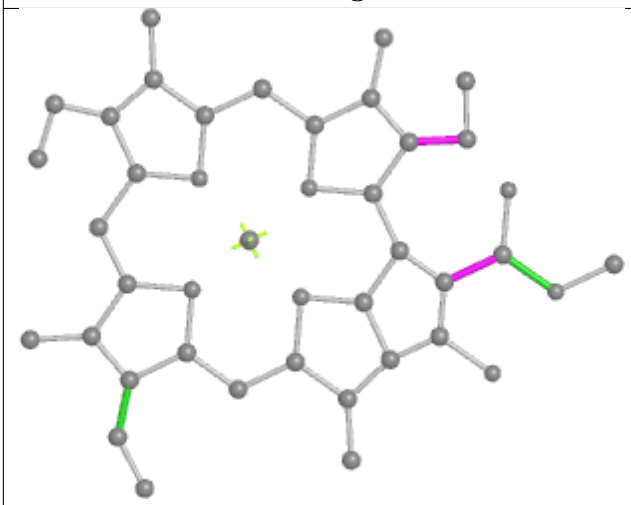


Bond angles



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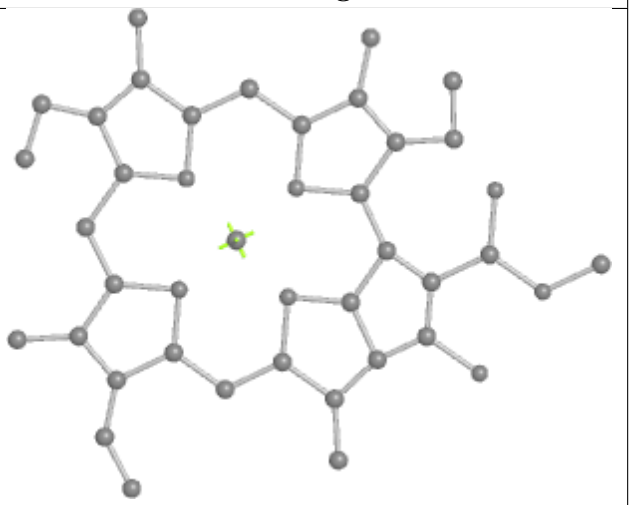

Rings

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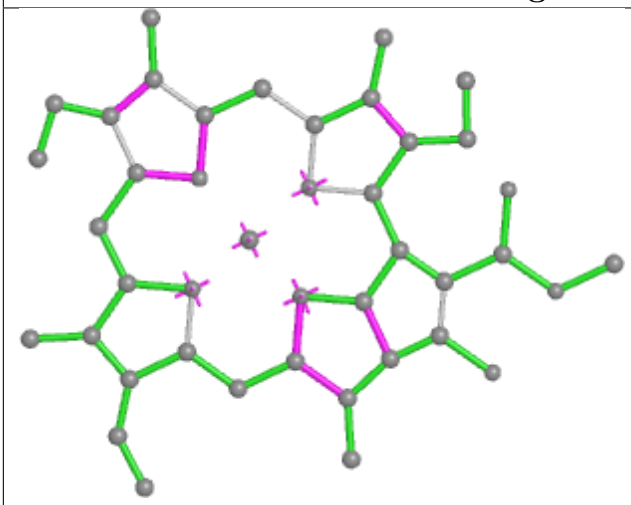

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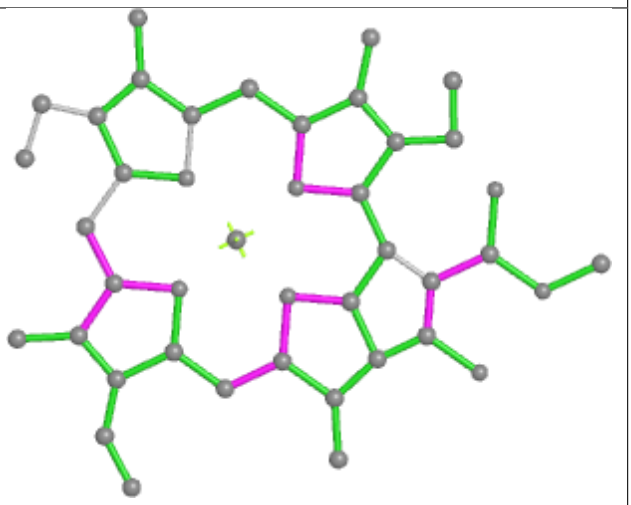
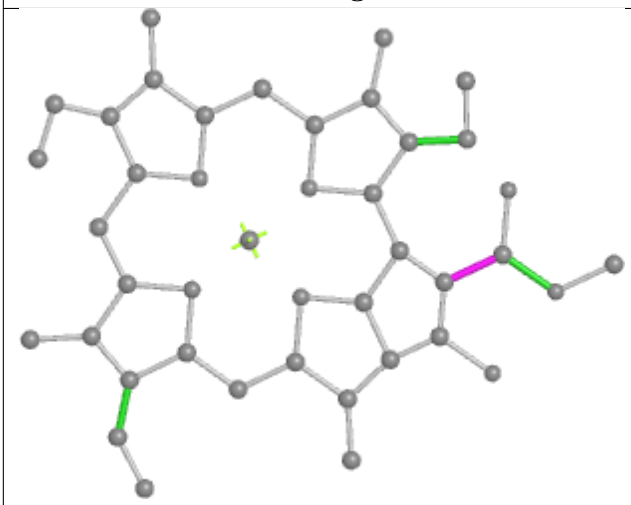


Bond angles



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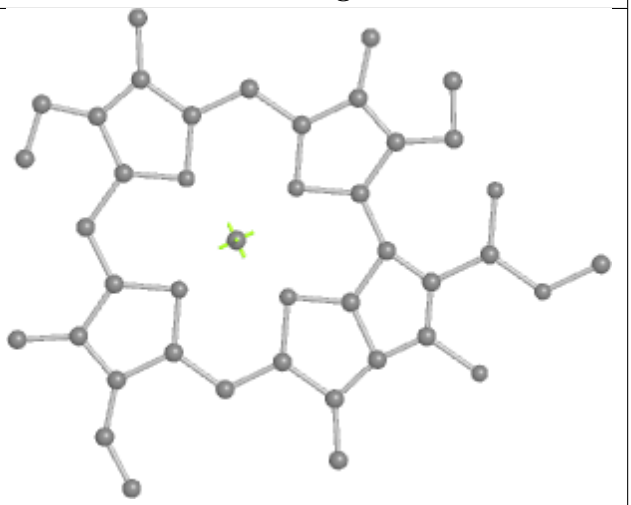
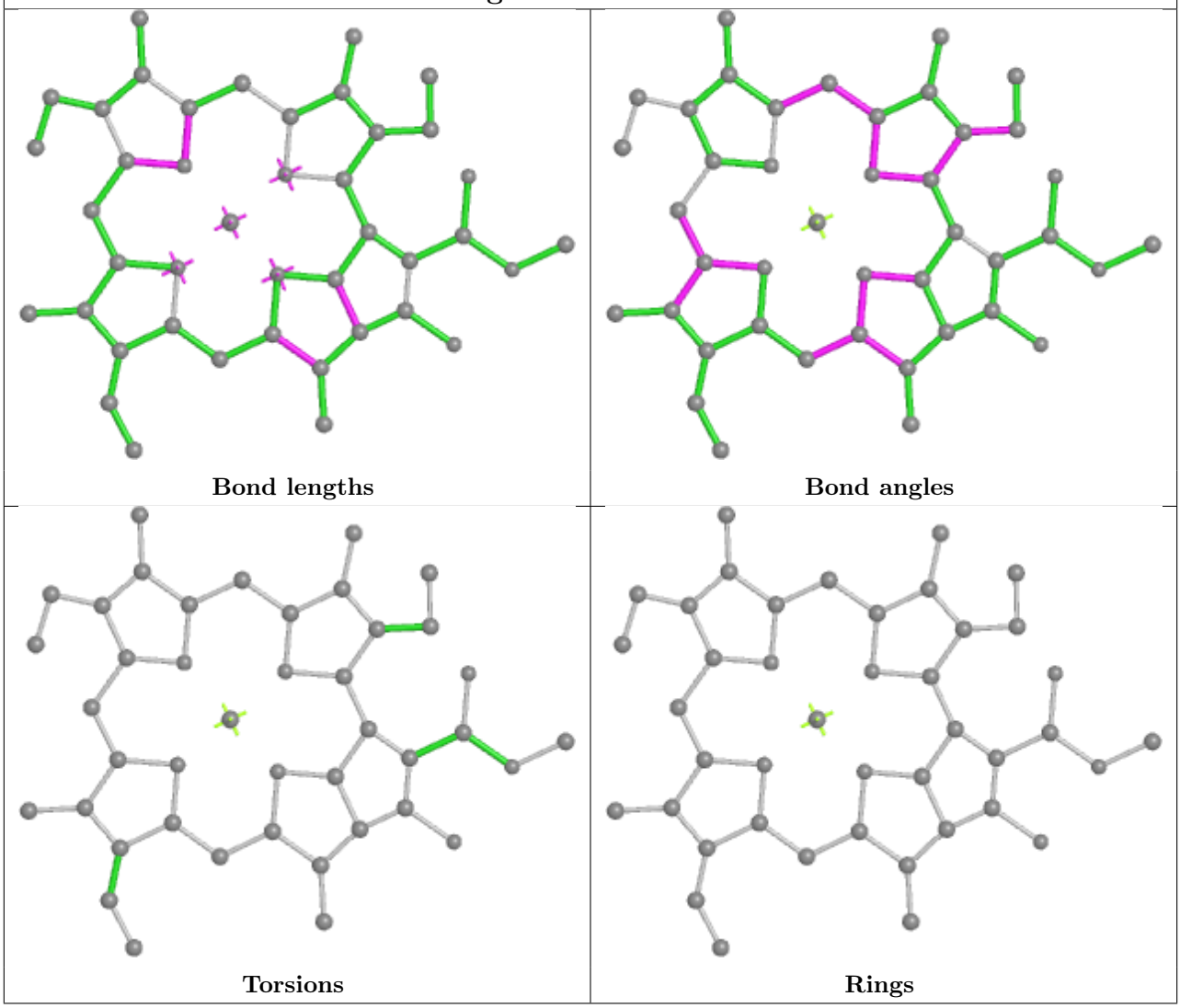
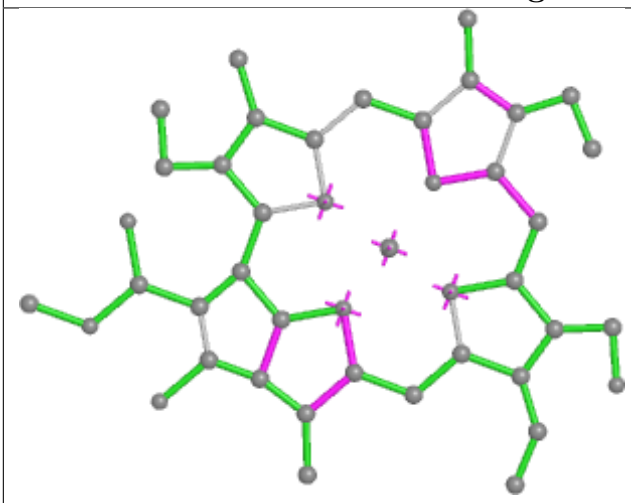


Rings

Ligand CLA 1 606



Ligand CHL 7 606



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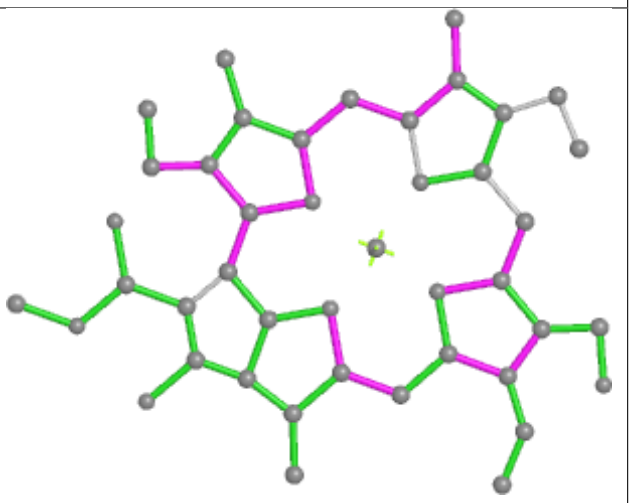
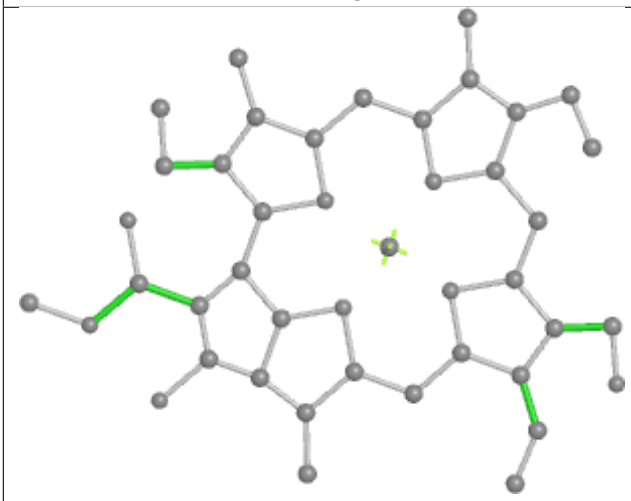


Bond angles



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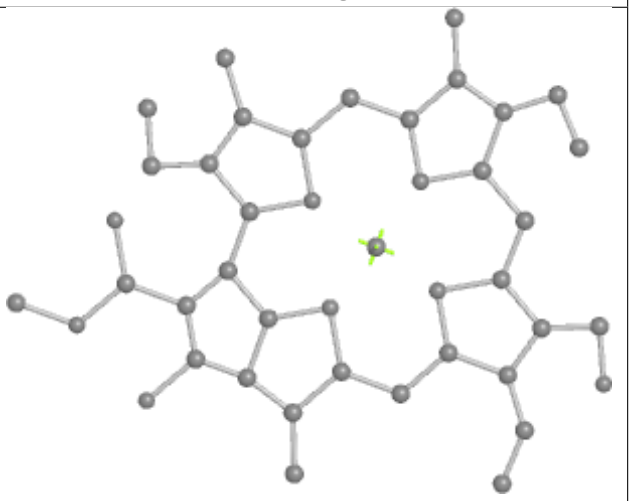

Rings

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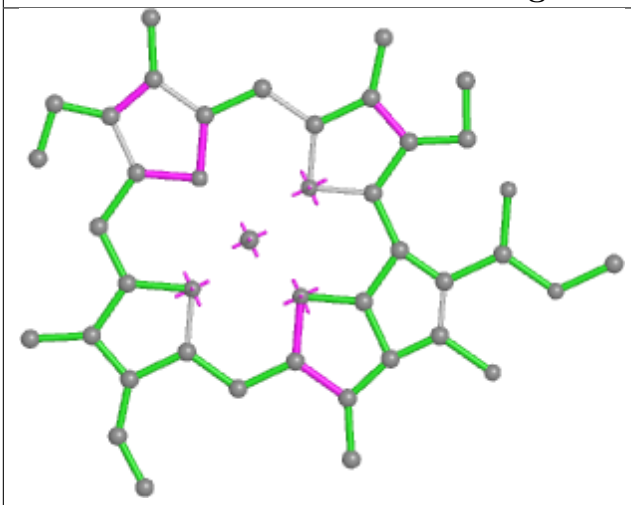

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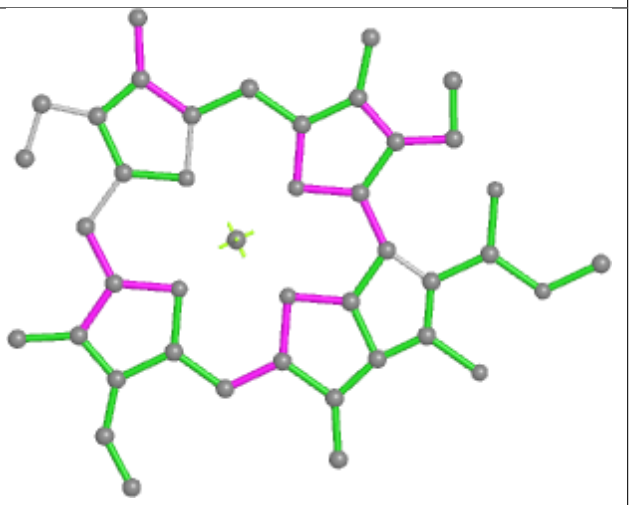
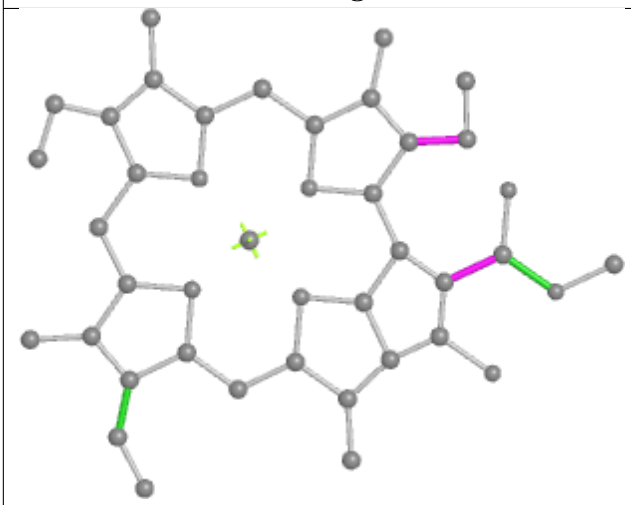
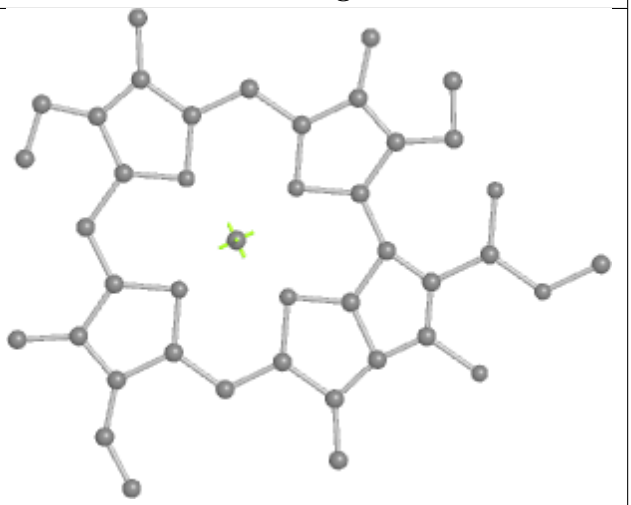


Bond angles

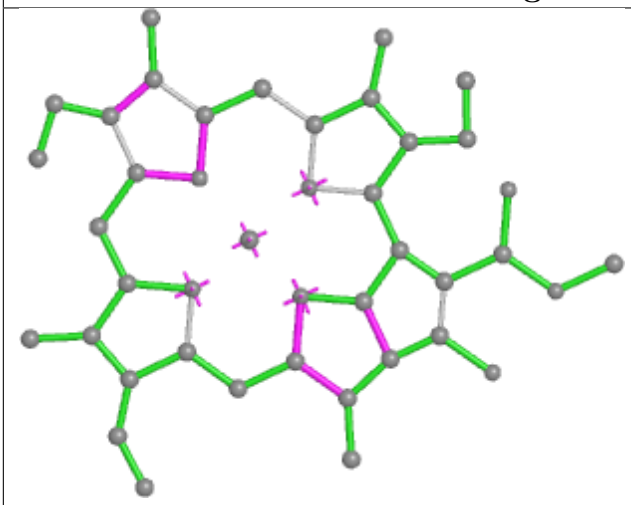


Torsions

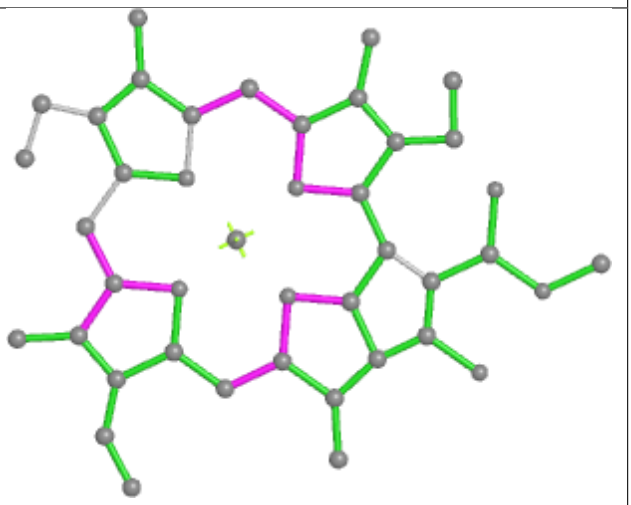


Rings

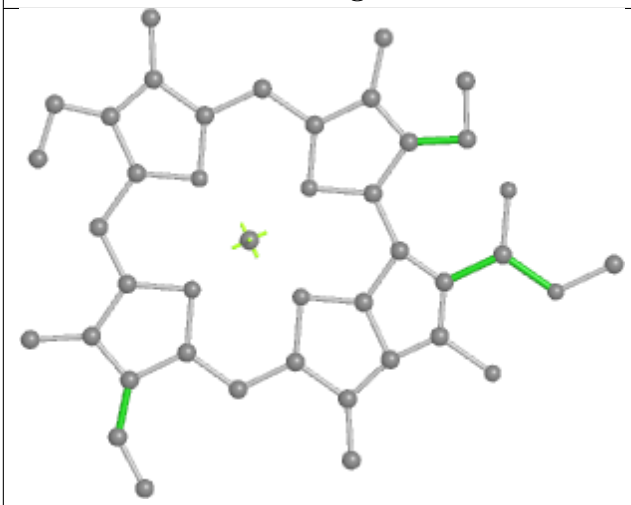
Ligand CLA A 834



Bond lengths



Bond angles



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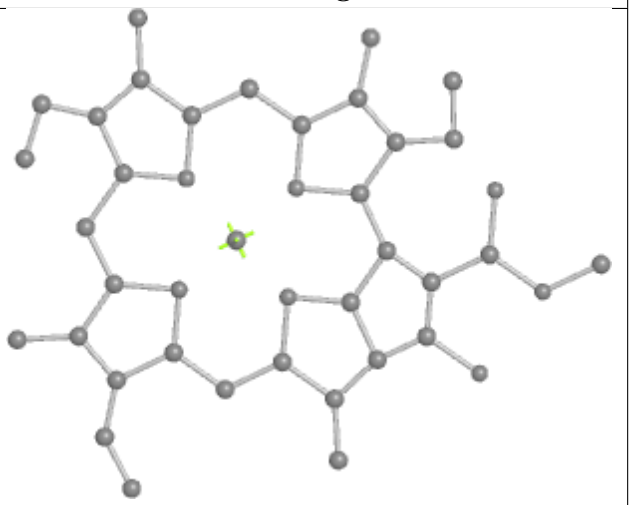
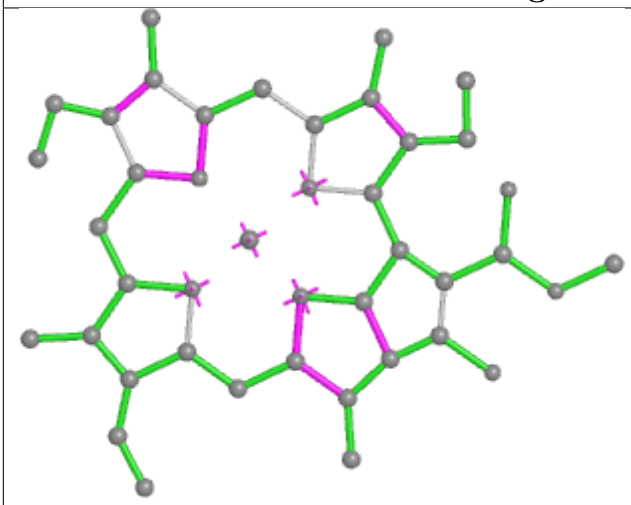


Rings

Ligand CLA 7 611



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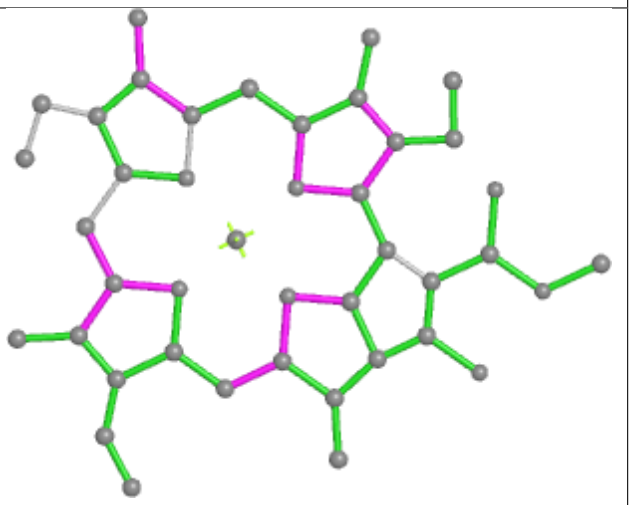
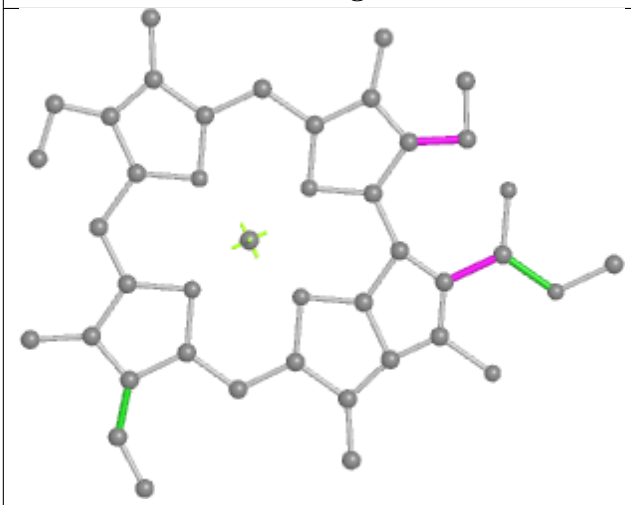
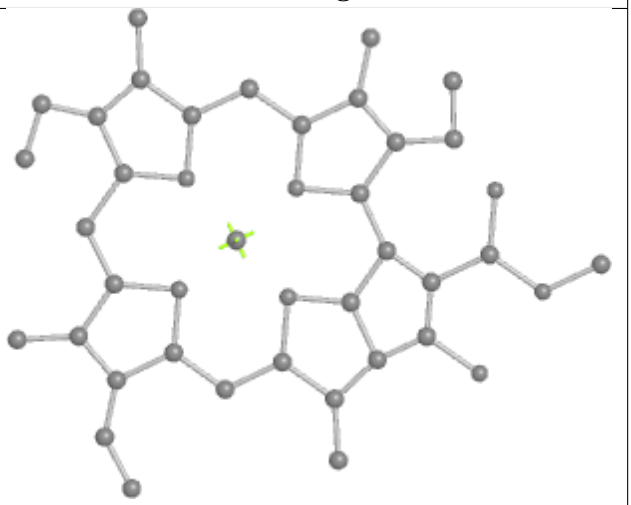


Bond angles

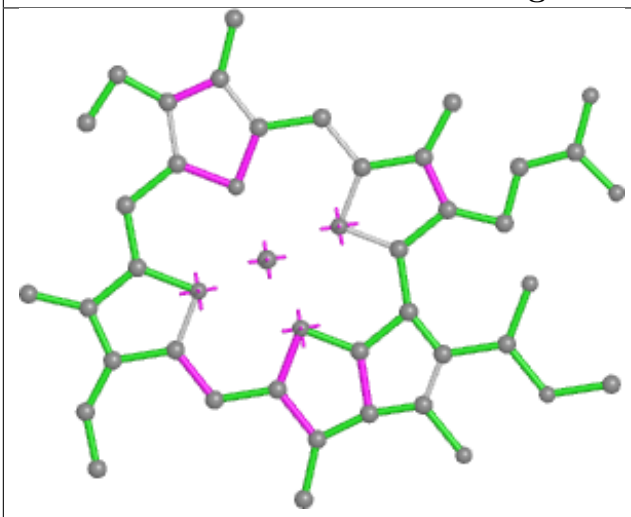


Torsions



Rings

Ligand CLA 8 603



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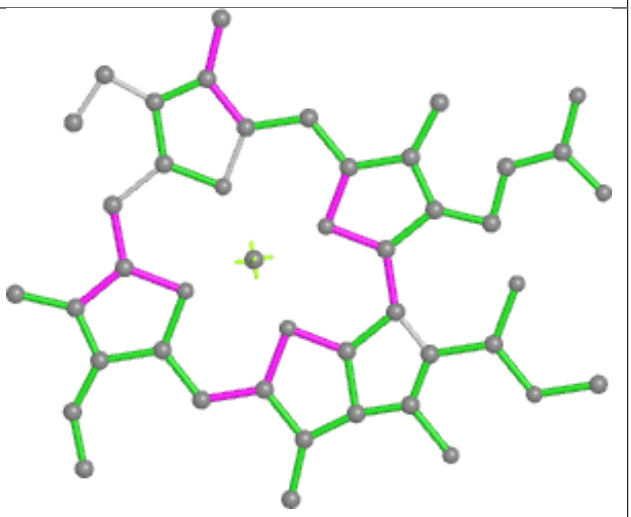
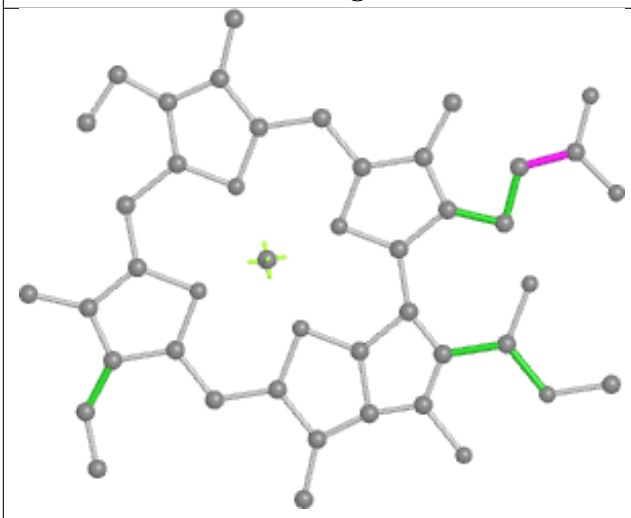
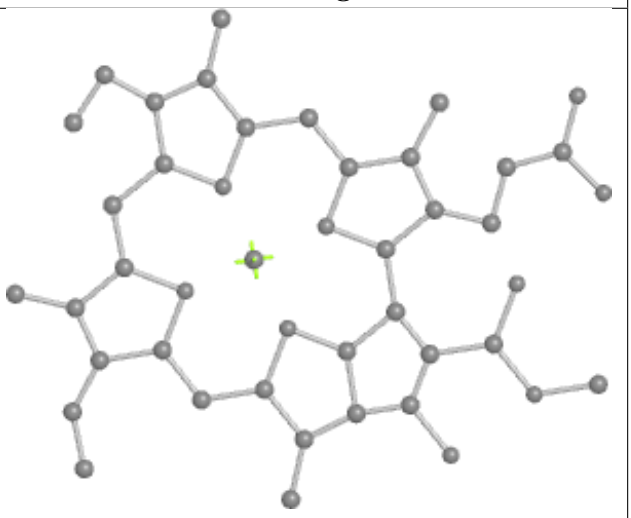


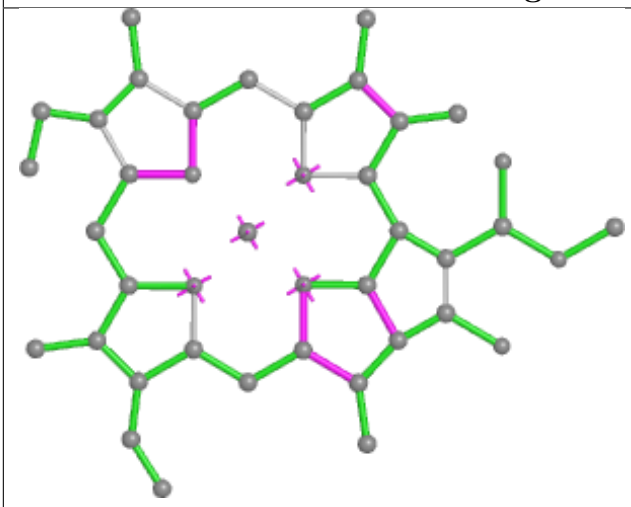
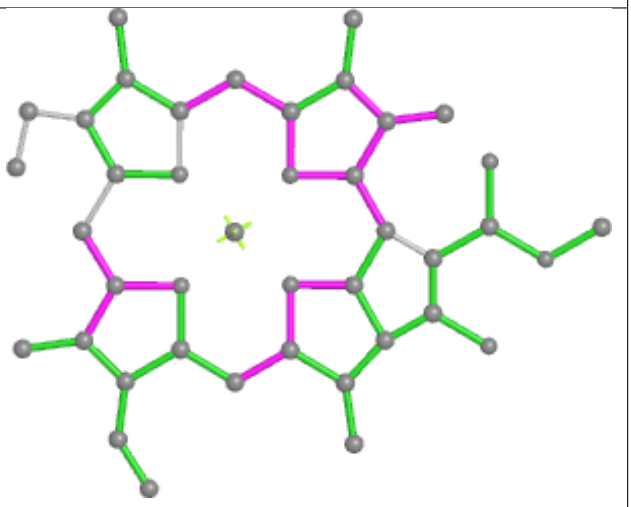
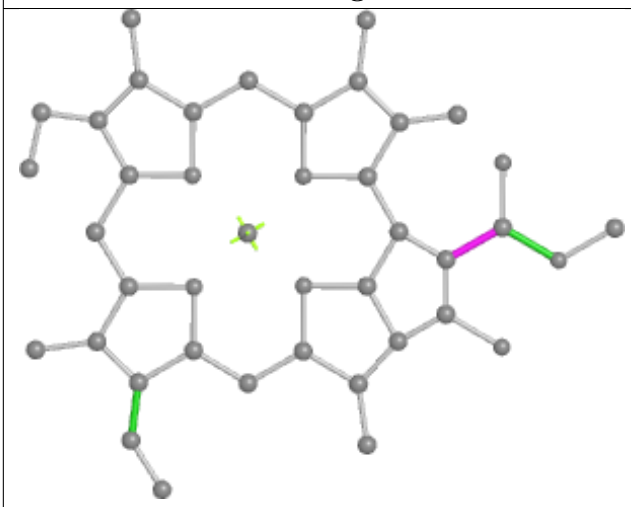
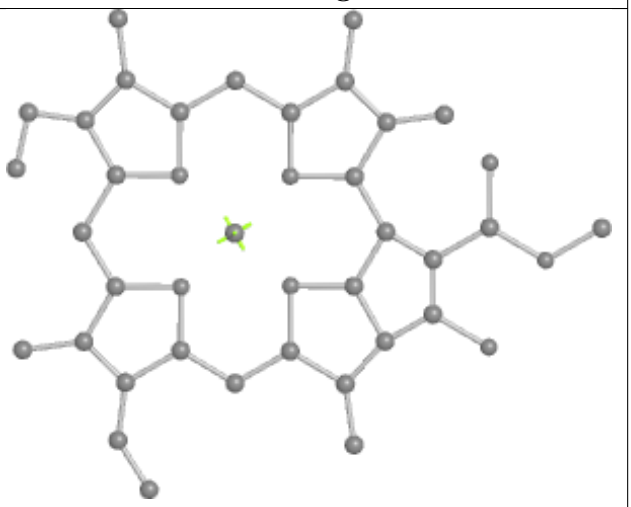
Bond angles



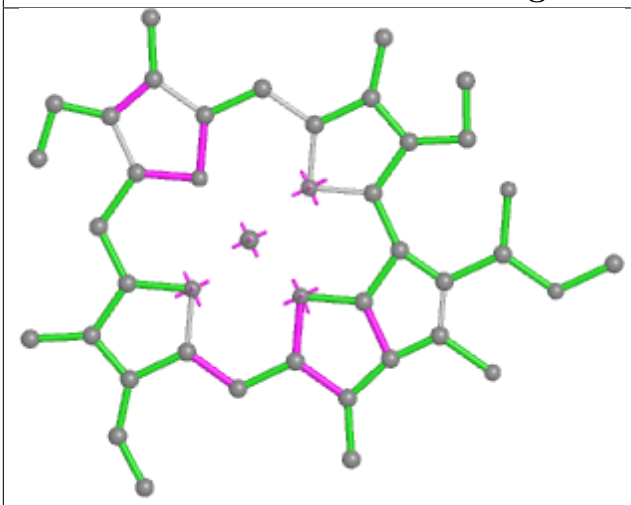
Torsions



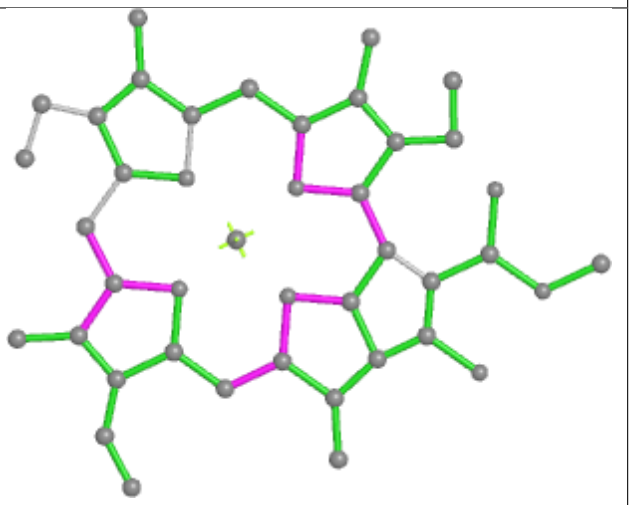
Rings

Ligand CLA B 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

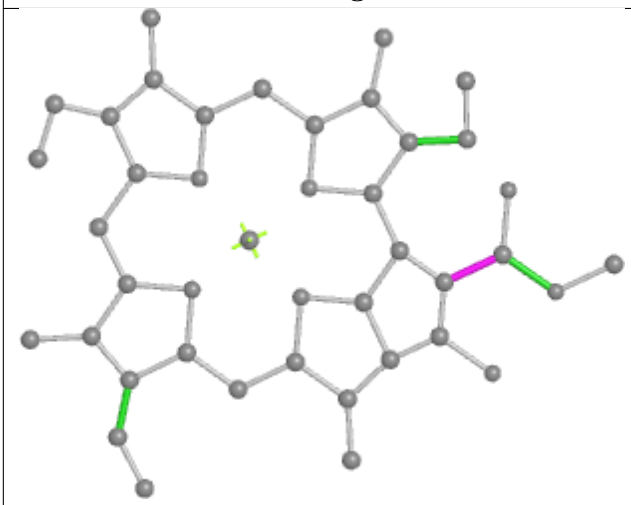
Ligand CLA 5 304



Bond lengths



Bond angles



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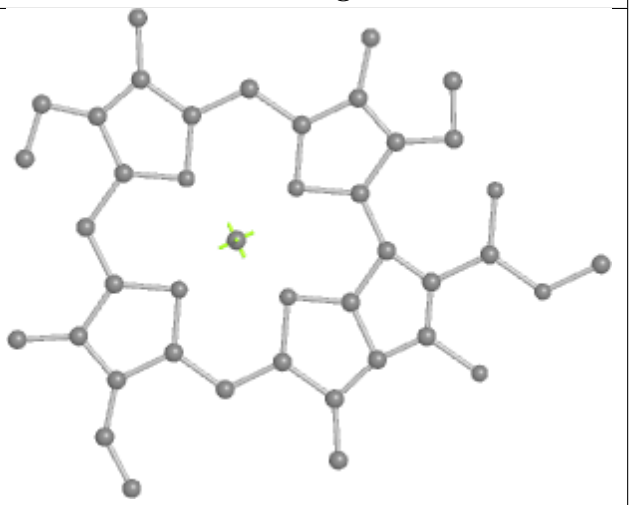
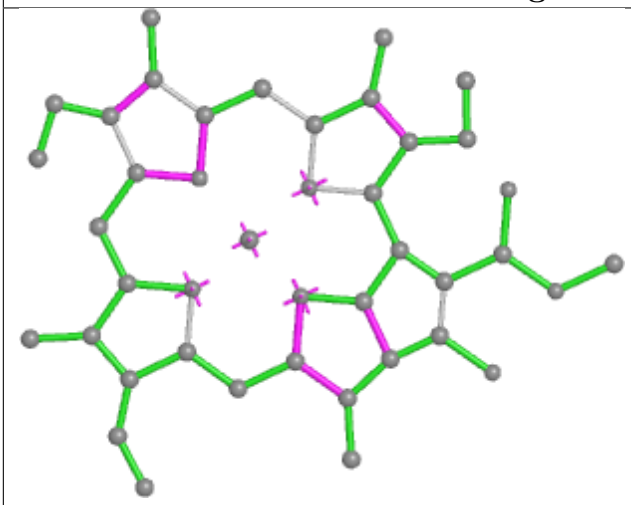


Rings

Ligand CLA 3 303



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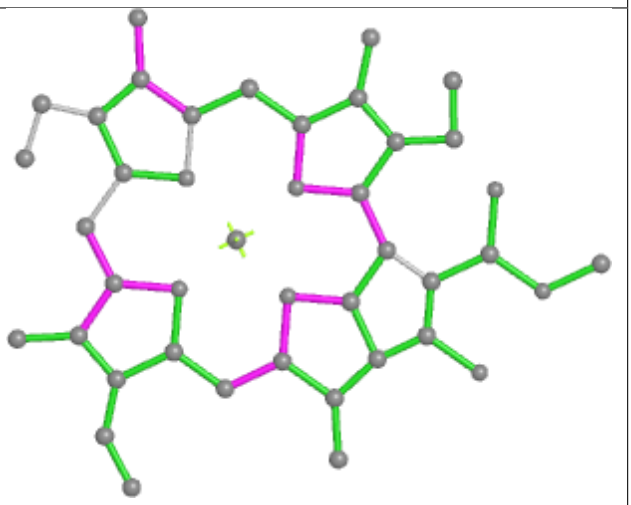
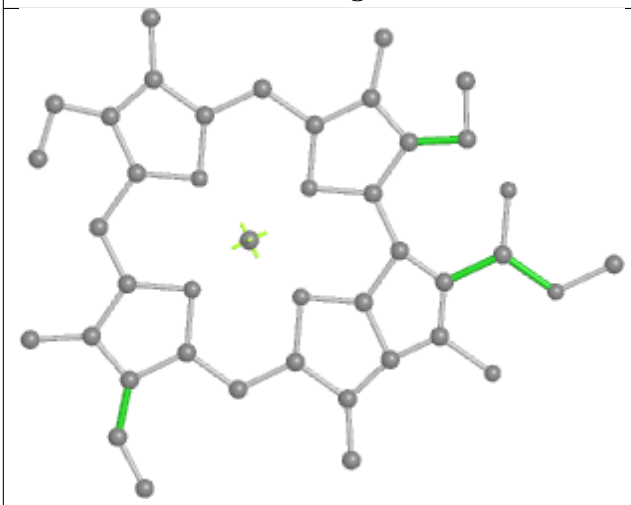


Bond angles



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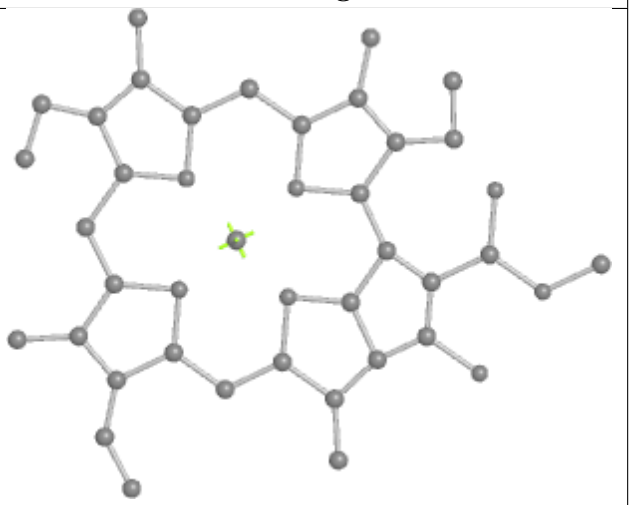
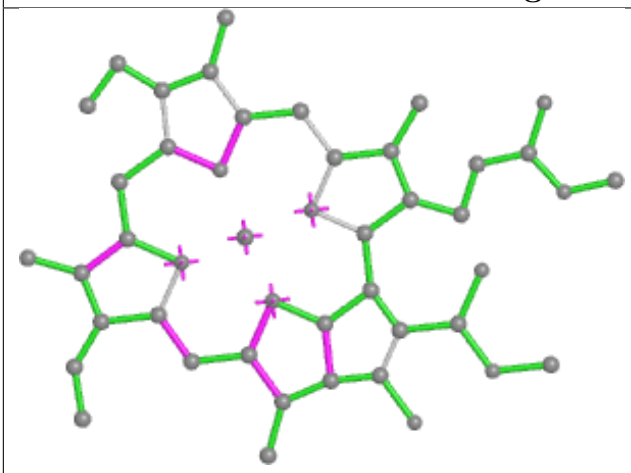
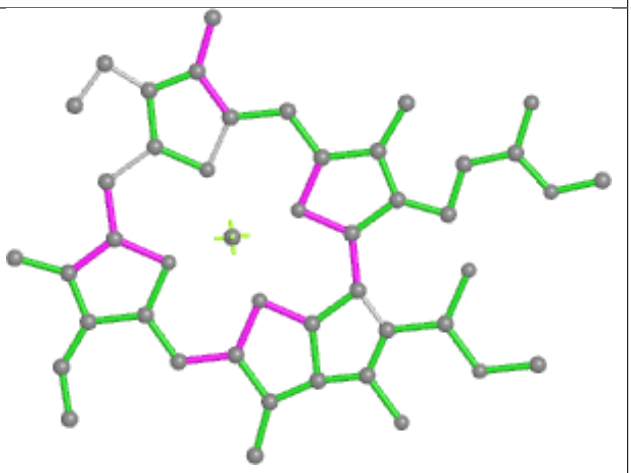


Rings

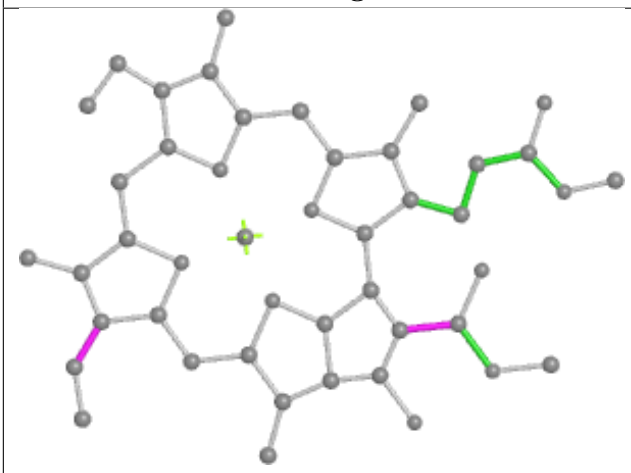
Ligand CLA B 821



Bond lengths



Bond angles



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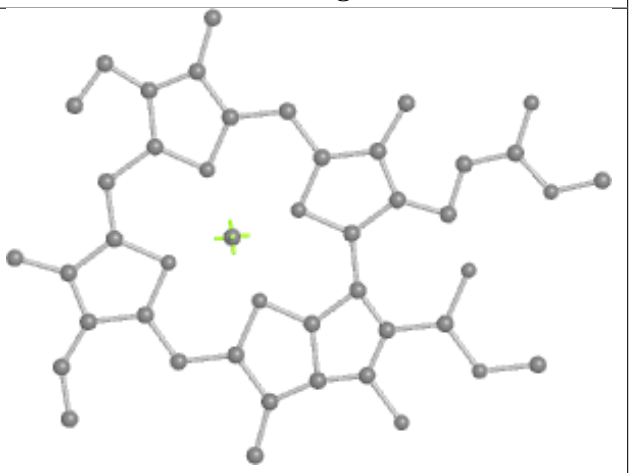
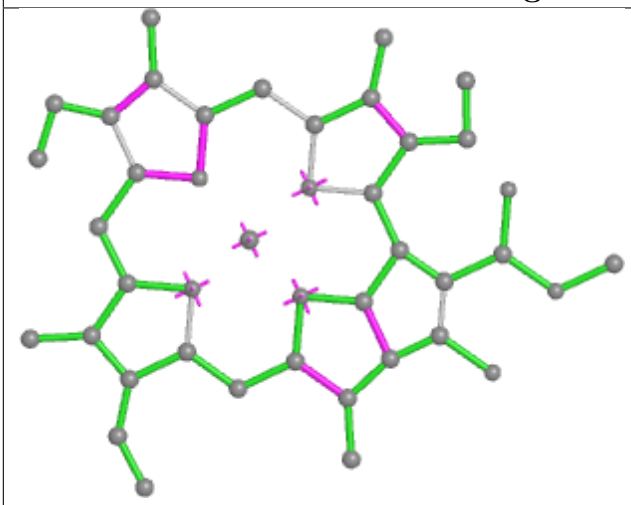
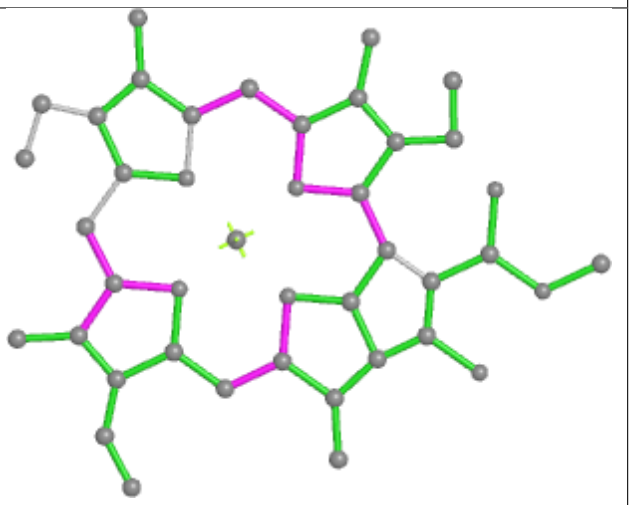


Rings

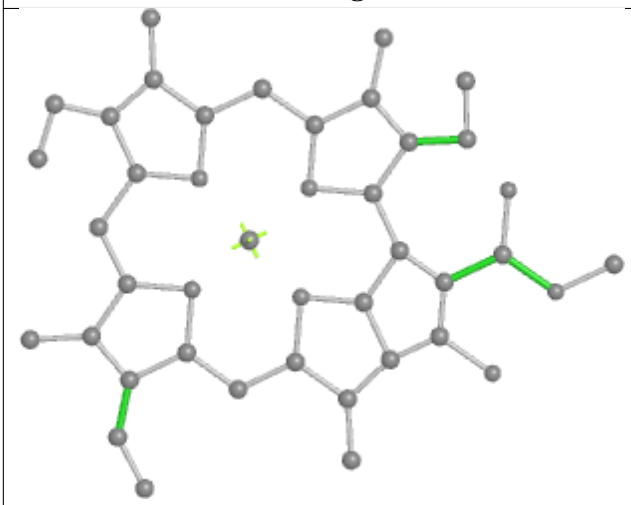
Ligand CLA A 826



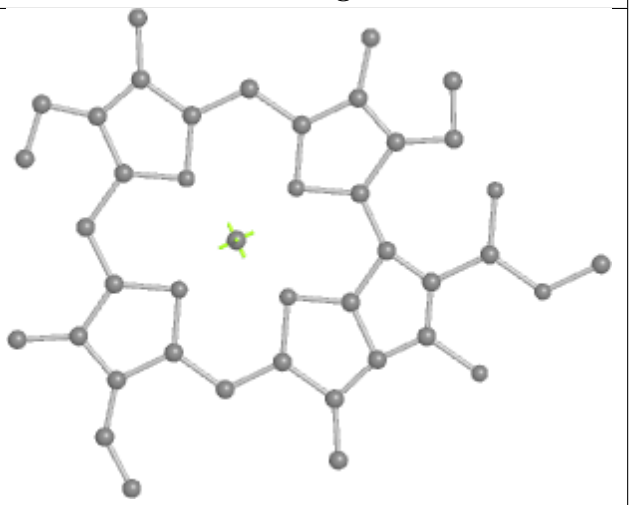
Bond lengths



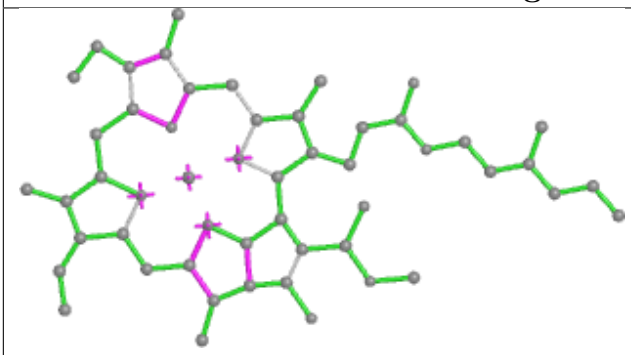
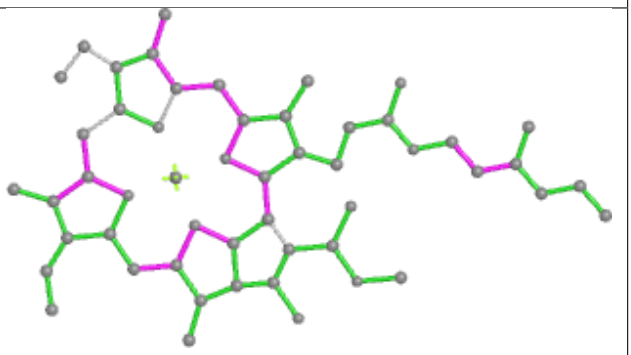
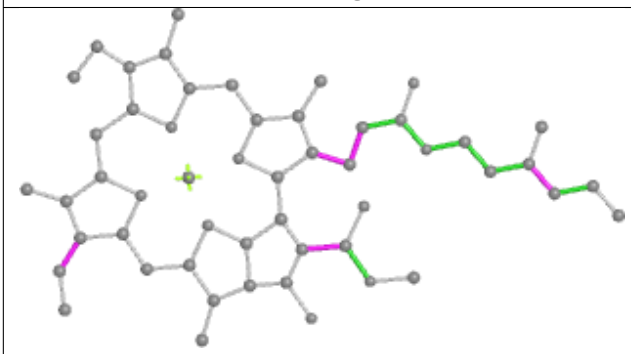
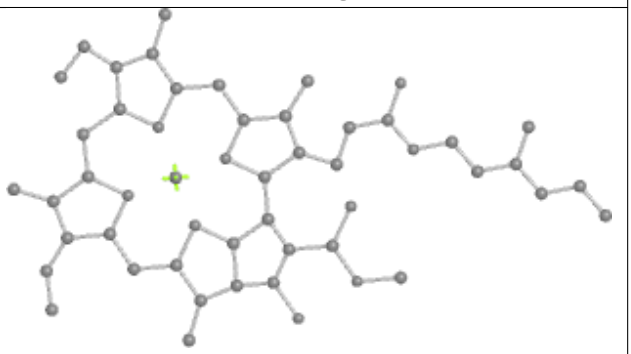
Bond angles



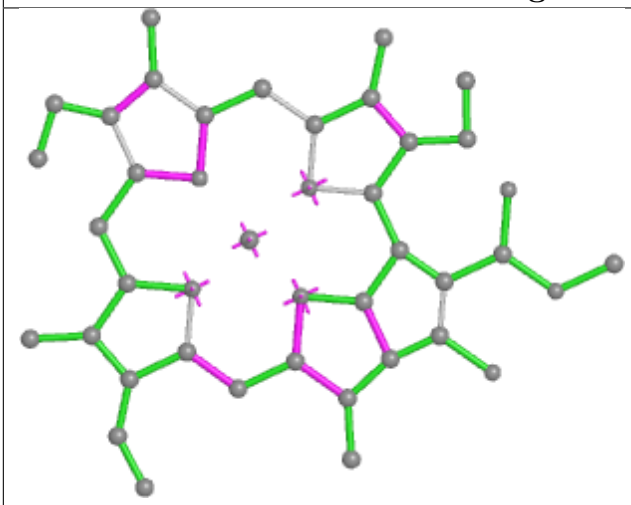
Torsions



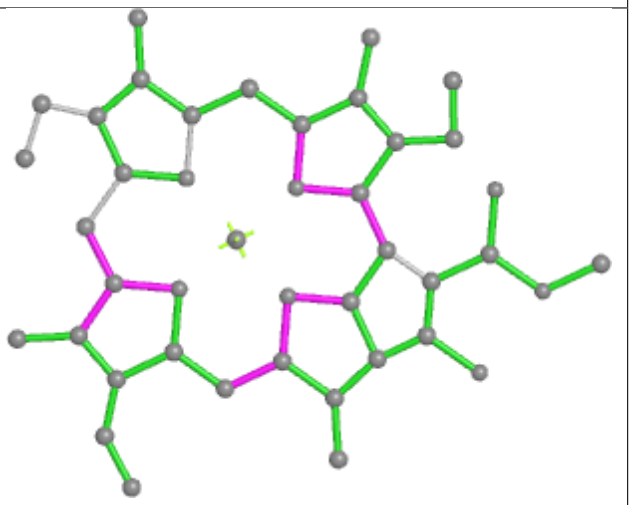
Rings

Ligand CLA A 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

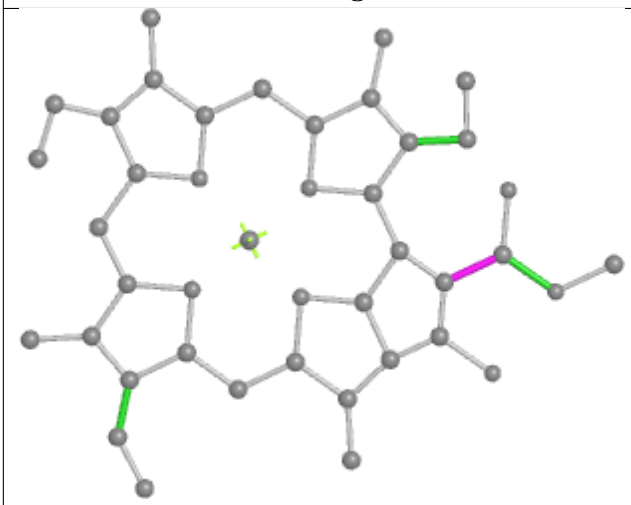
Ligand CLA 8 601



Bond lengths



Bond angles



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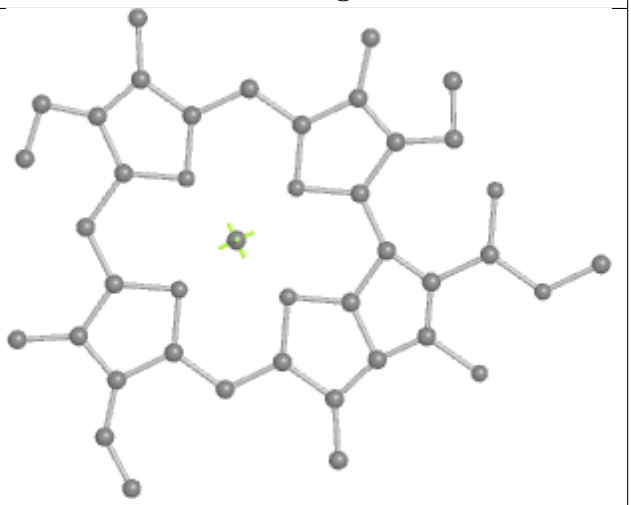
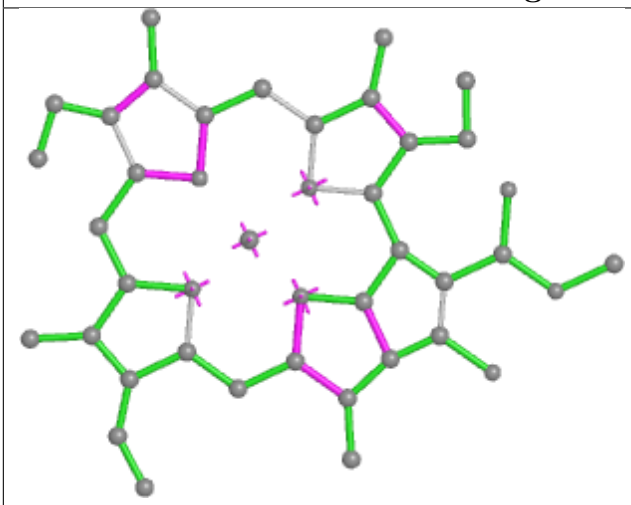


Rings

Ligand CLA B 822



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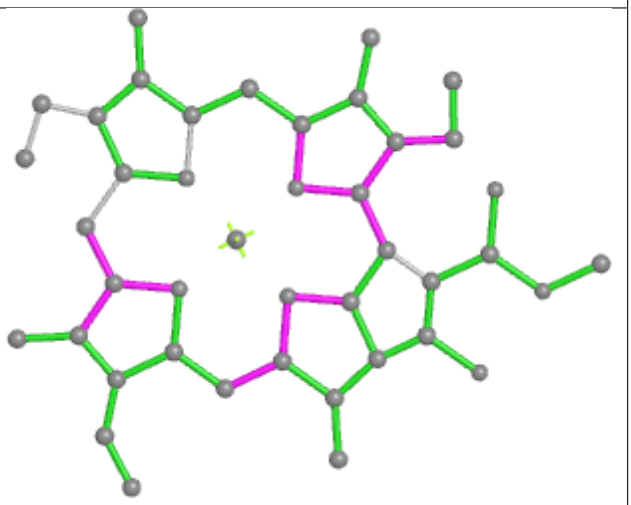
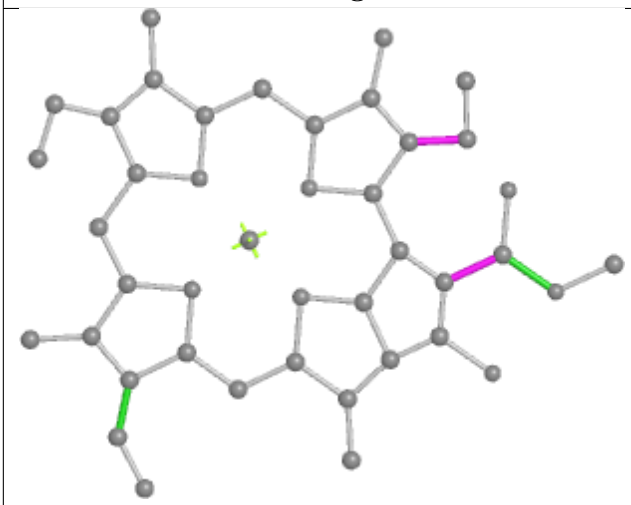
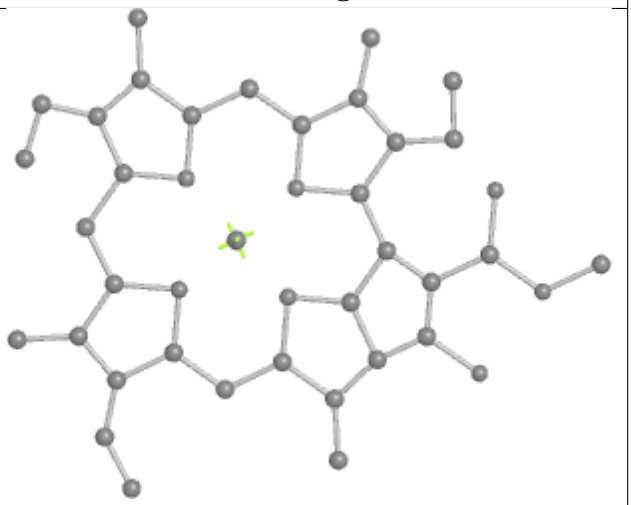


Bond angles

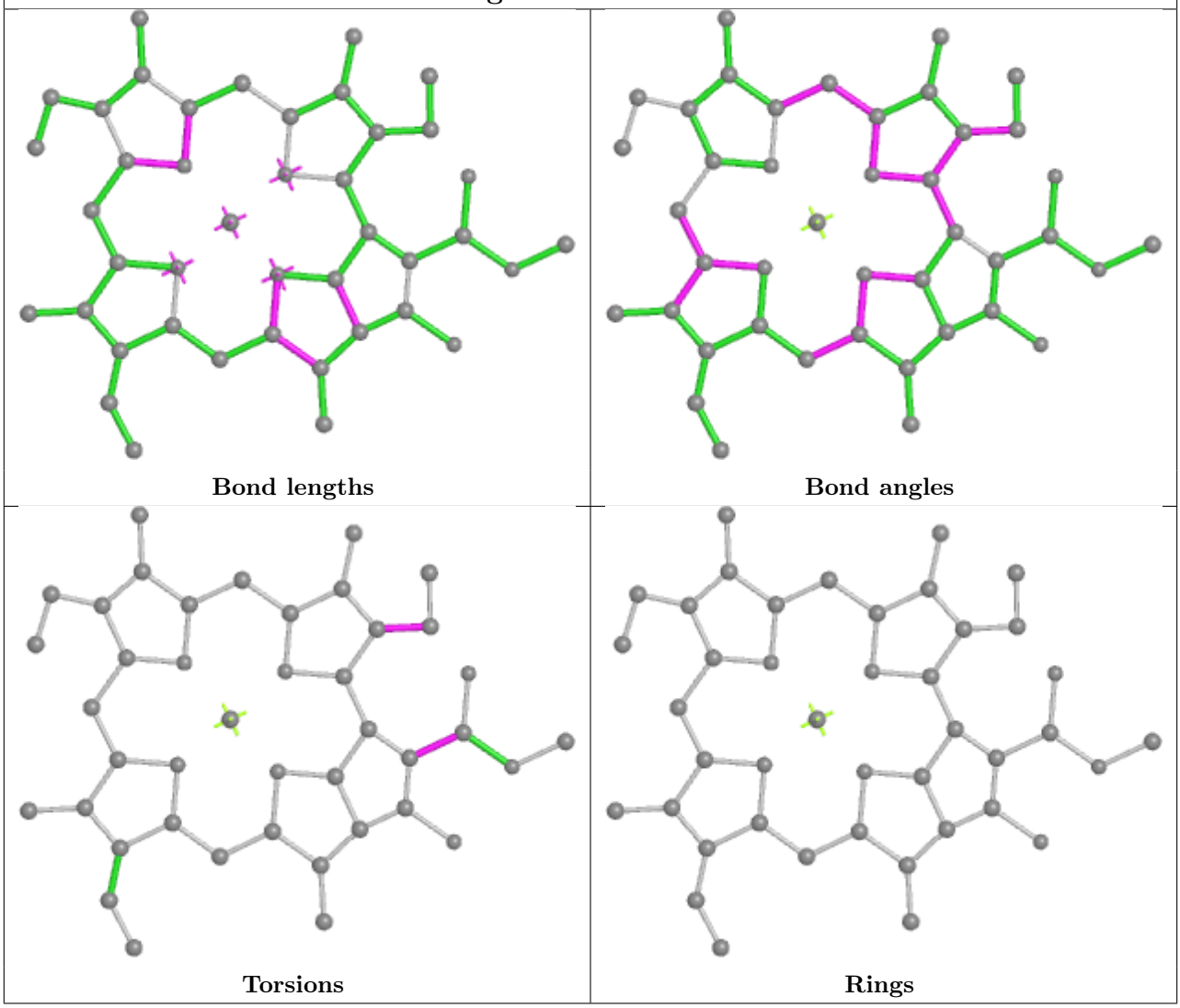


Torsions

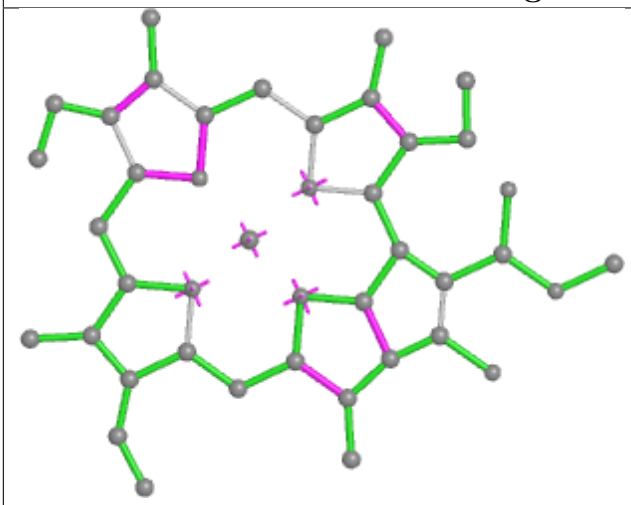


Rings

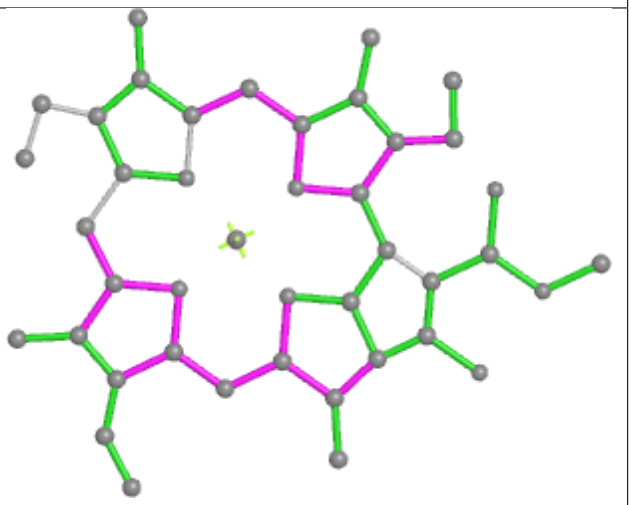
Ligand CLA 6 608



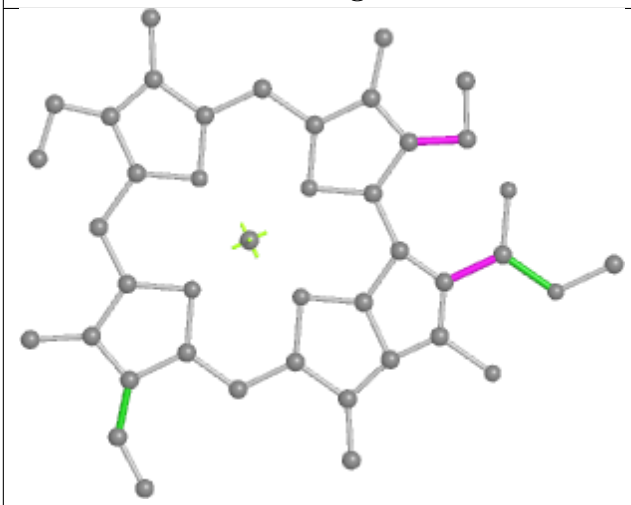
Ligand CLA B 819



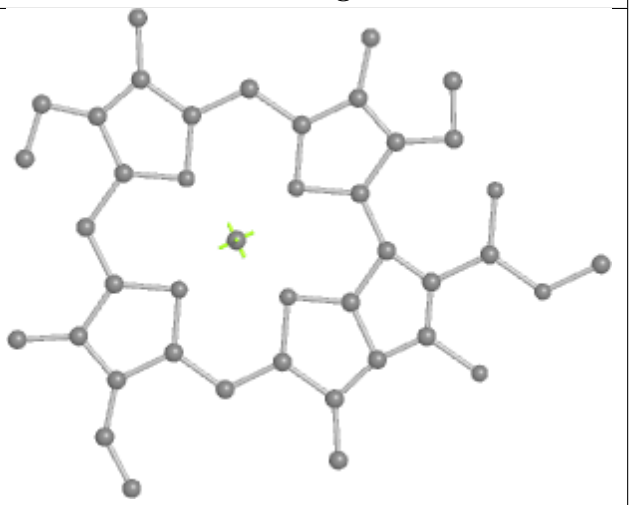
Bond lengths



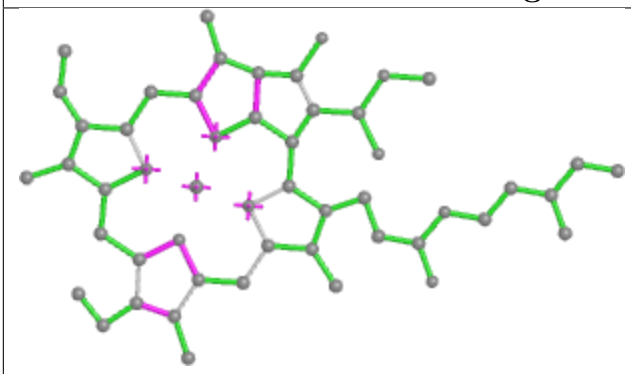
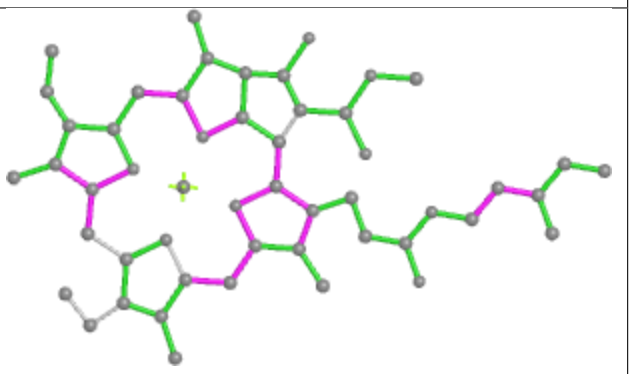
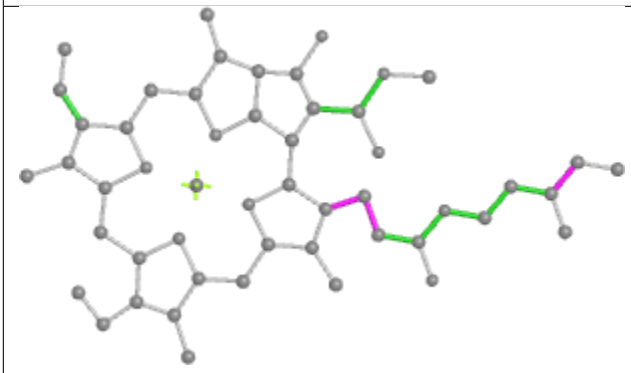
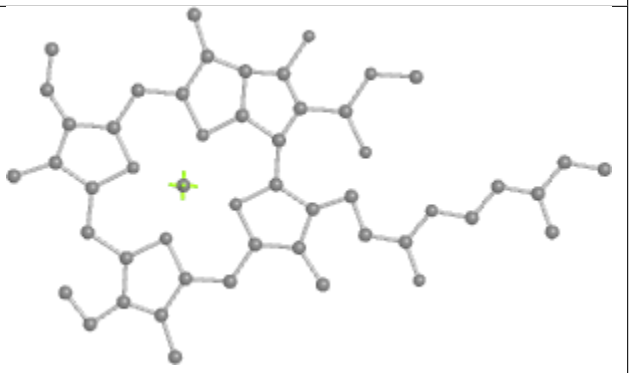
Bond angles



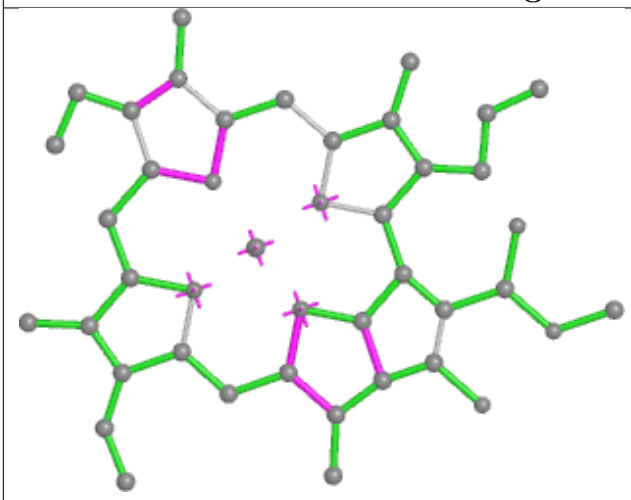
Torsions



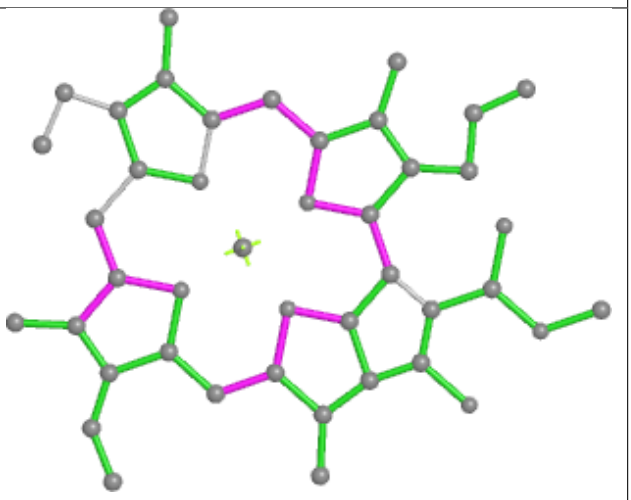
Rings

Ligand CLA A 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

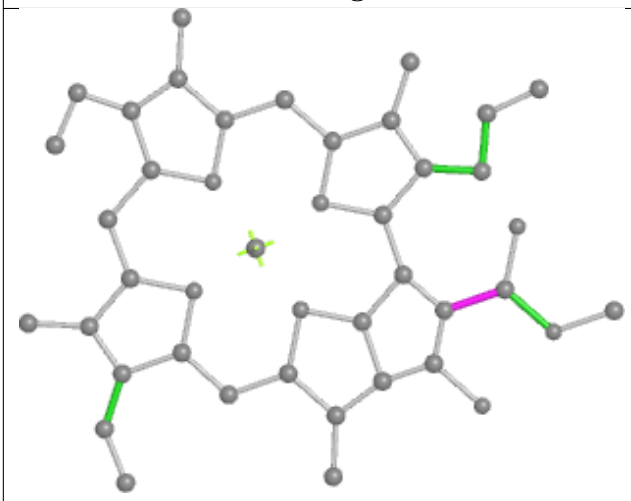
Ligand CLA B 835



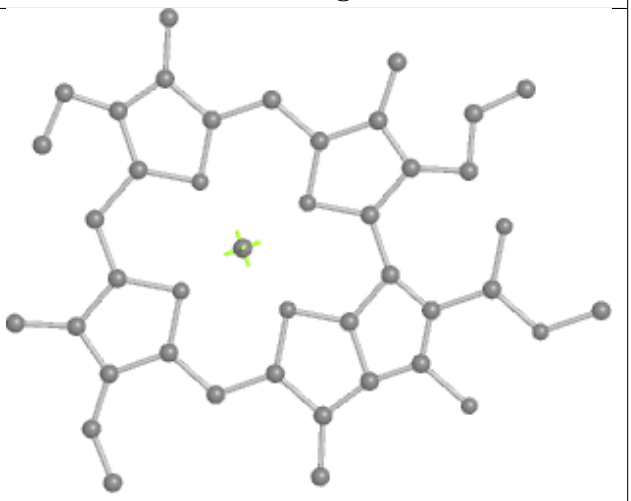
Bond lengths



Bond angles

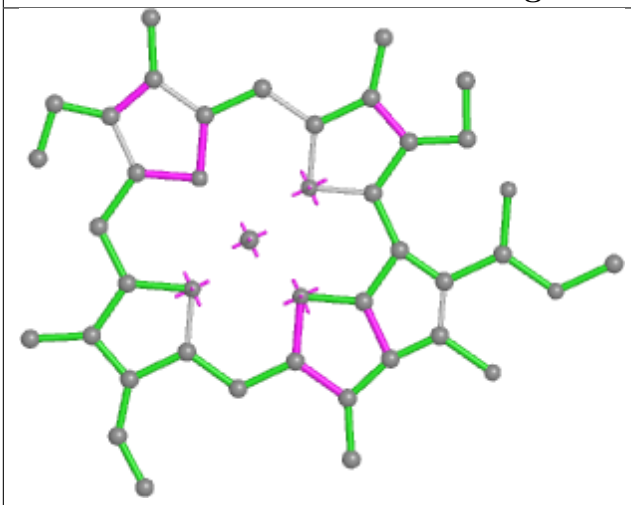


Torsions

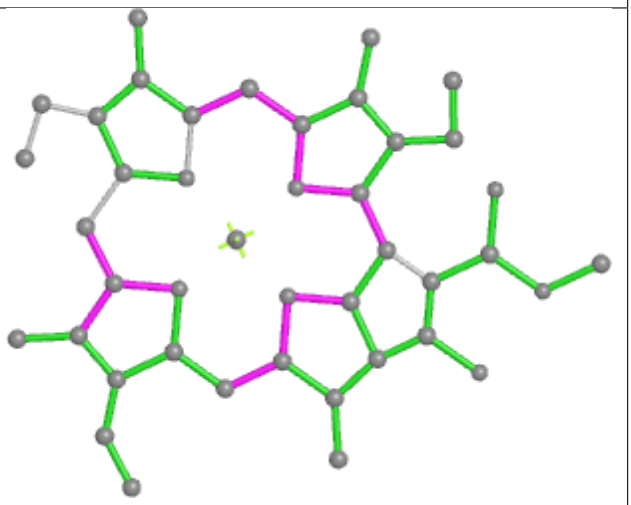


Rings

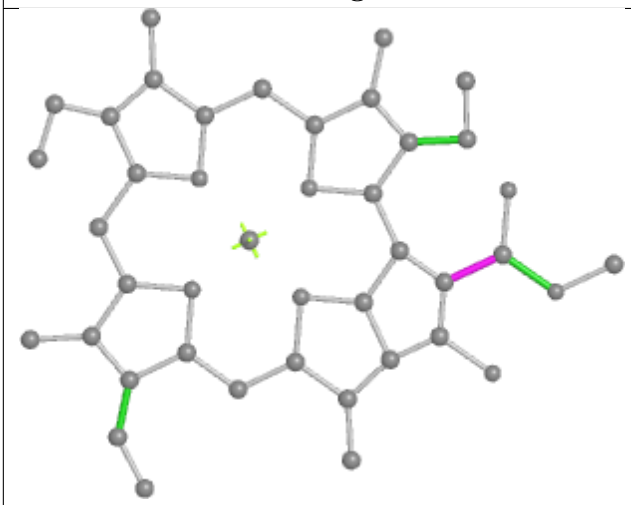
Ligand CLA B 808



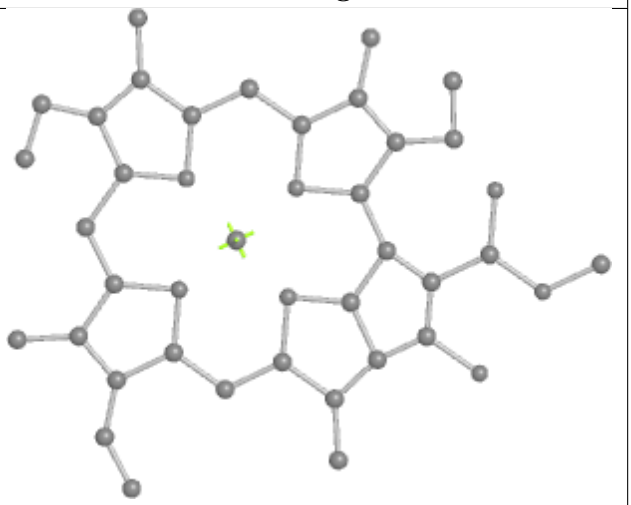
Bond lengths



Bond angles

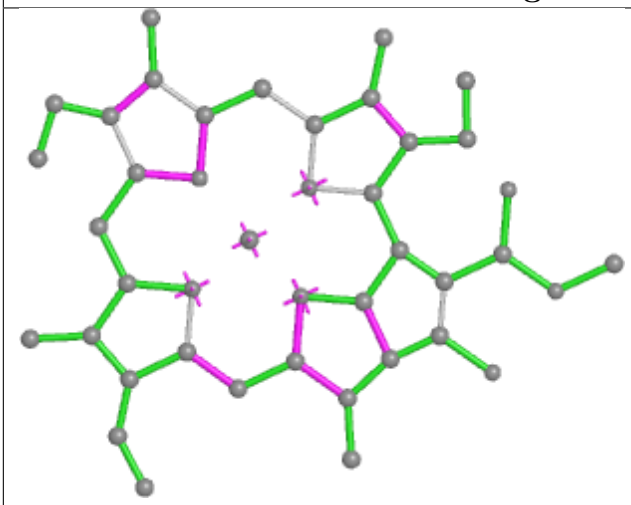


Torsions



Rings

Ligand CLA A 813



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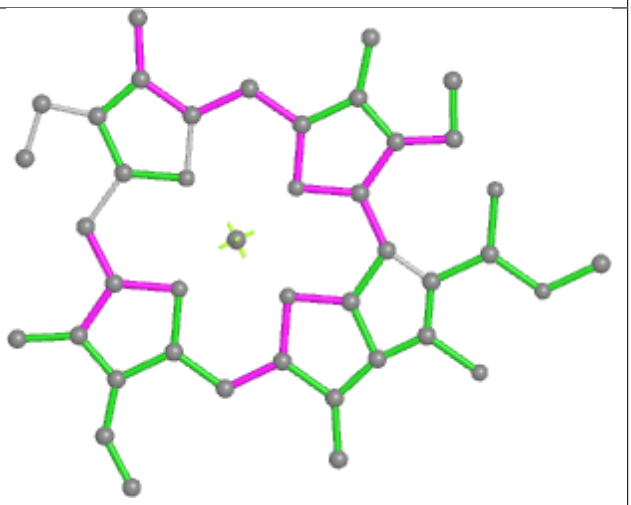
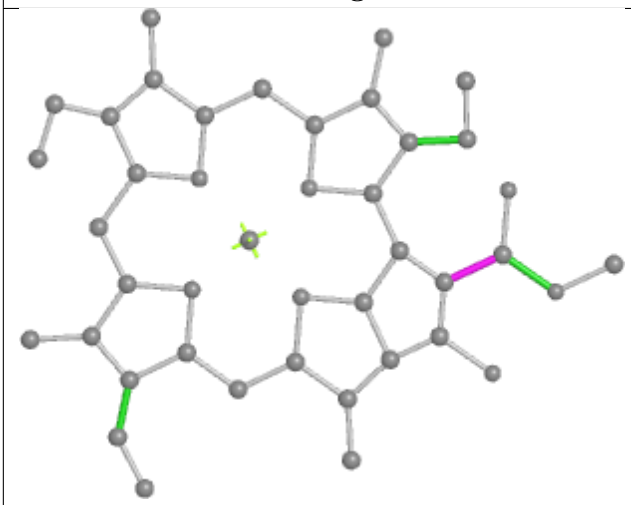


Bond angles



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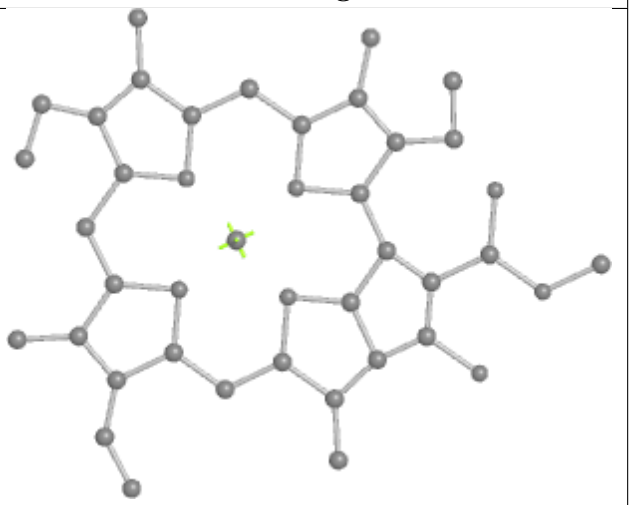
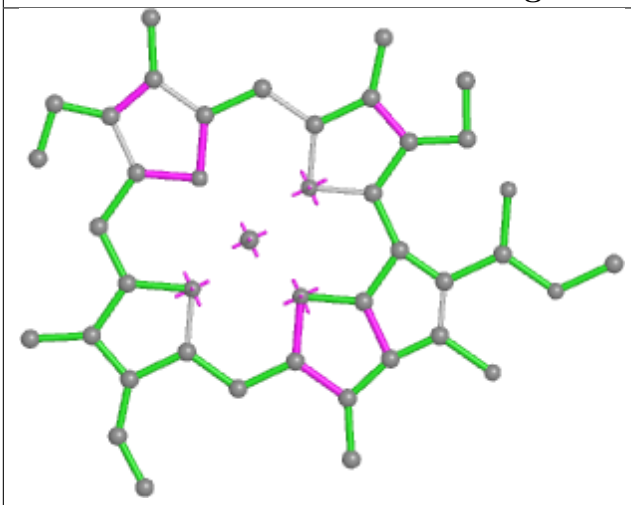


Rings

Ligand CLA B 809



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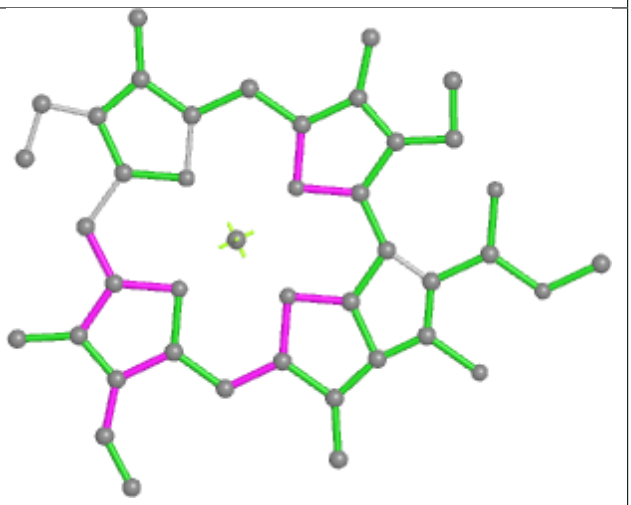
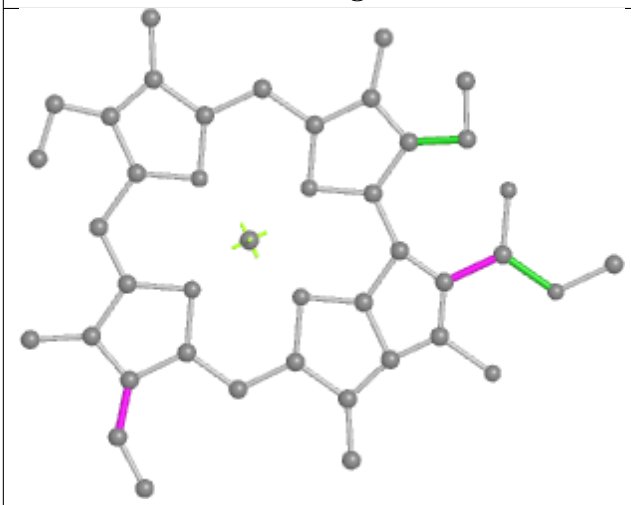


Bond angles



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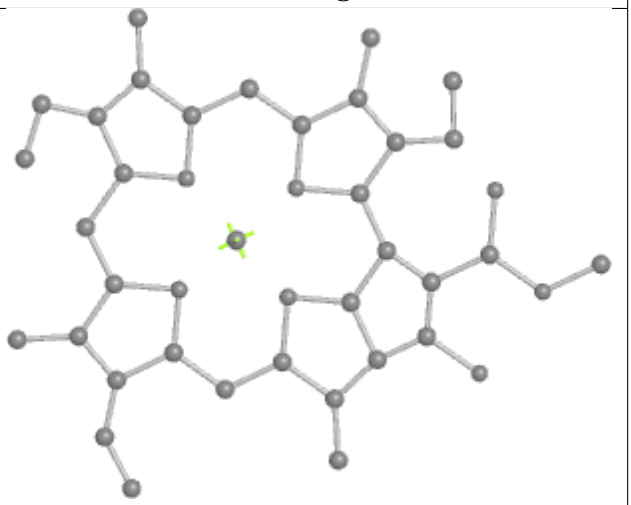
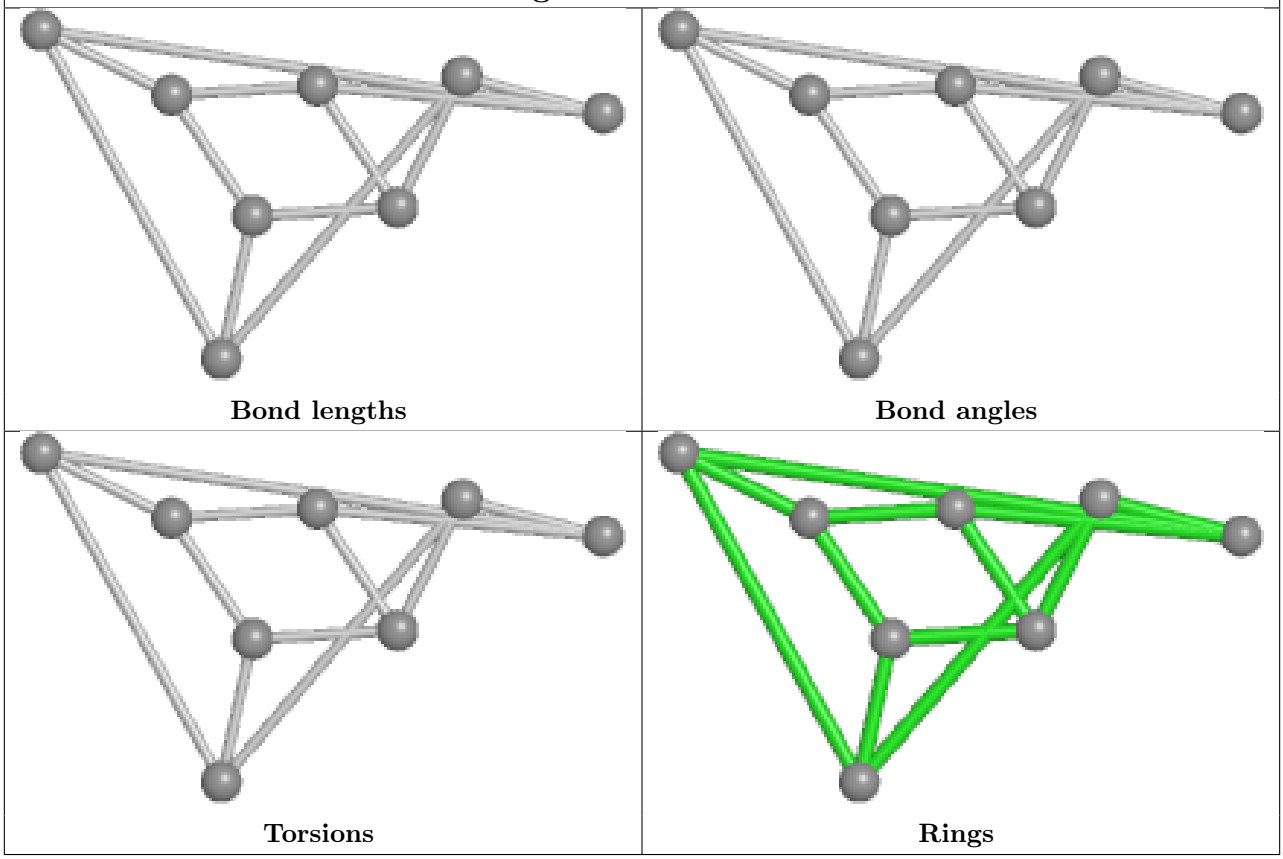
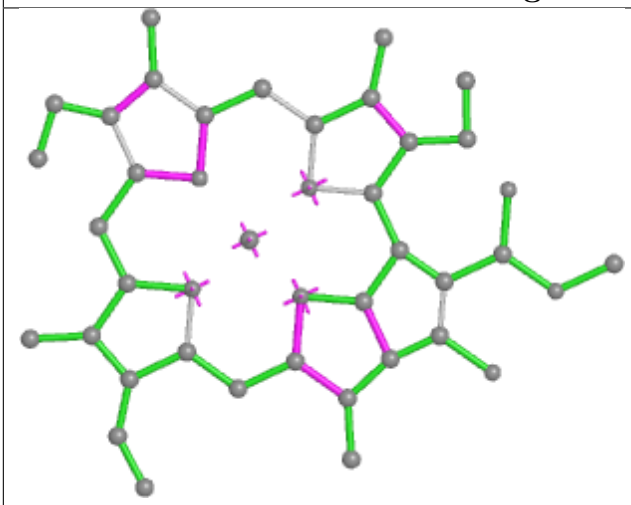


Rings

Ligand SF4 B 803



Ligand CLA A 822



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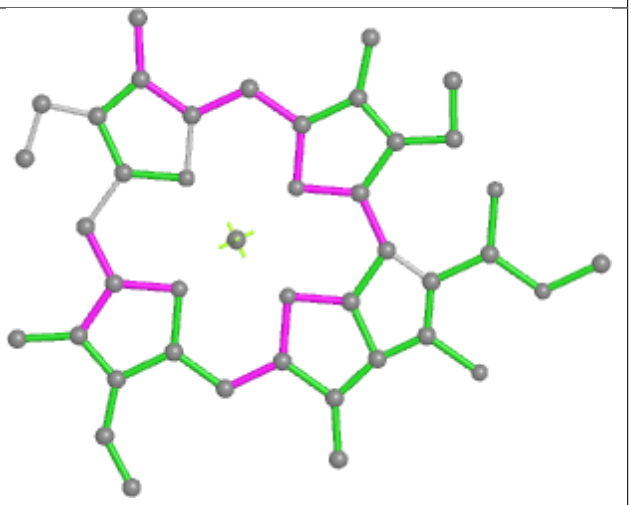
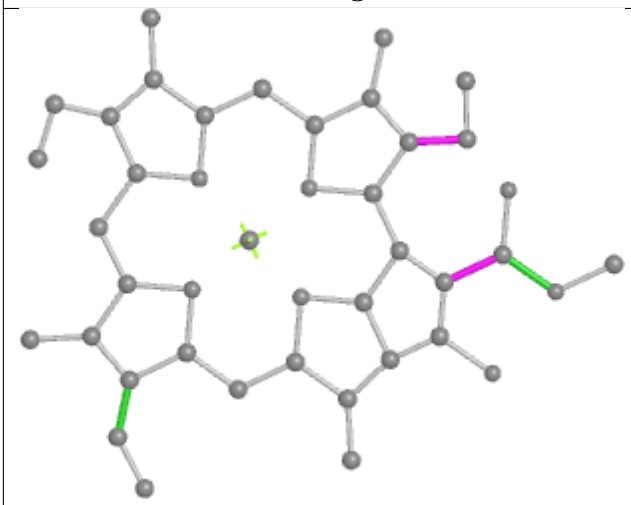


Bond angles



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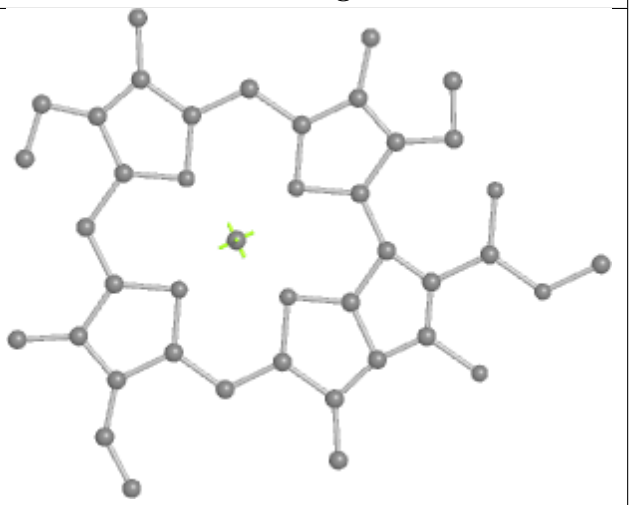
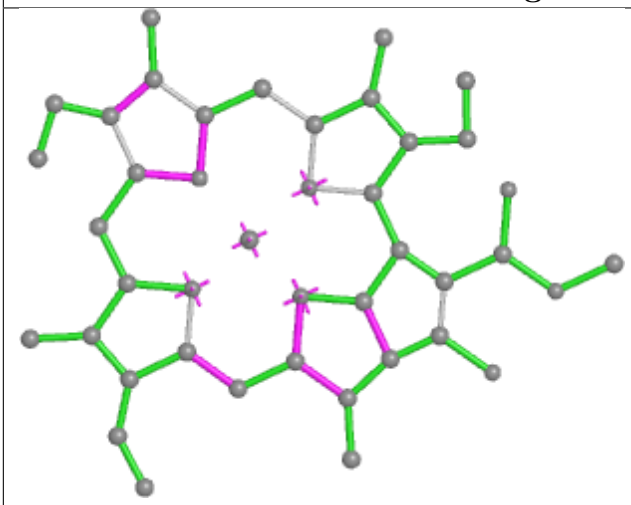


Rings

Ligand CLA B 825



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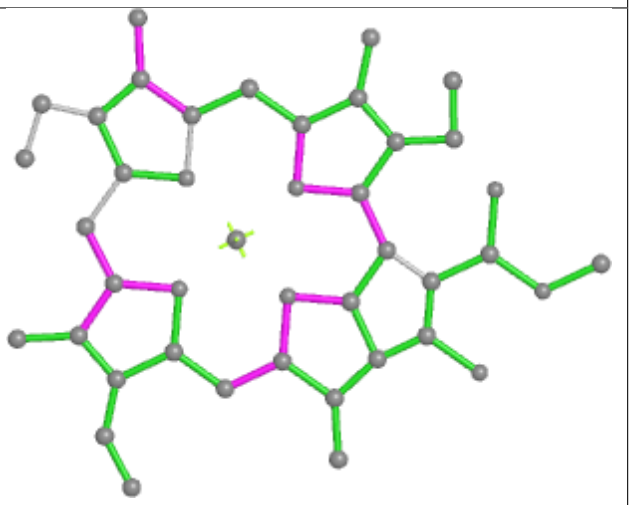
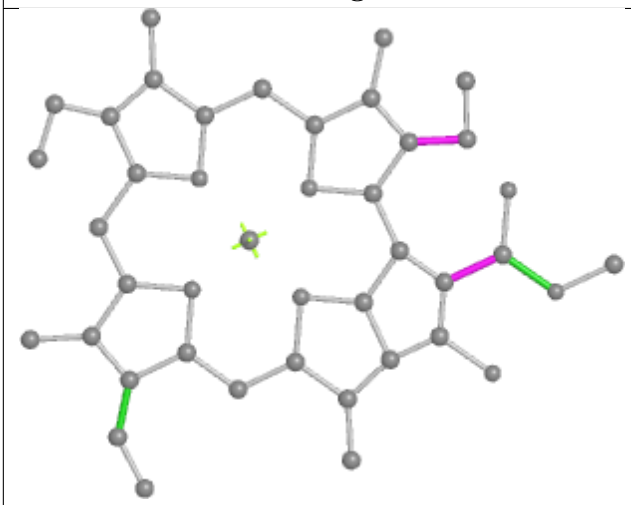


Bond angles



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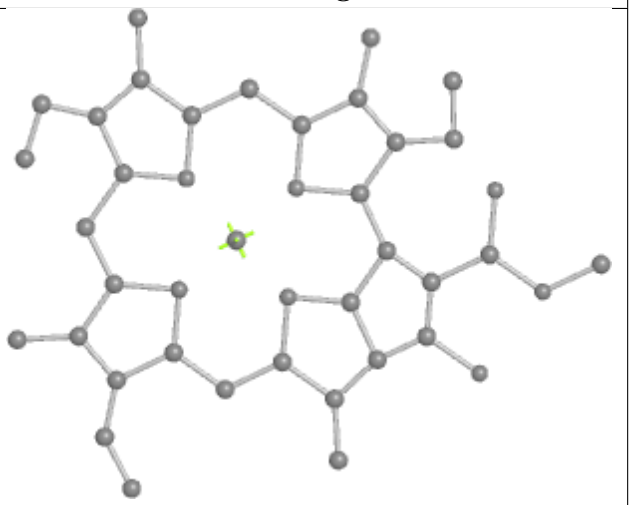
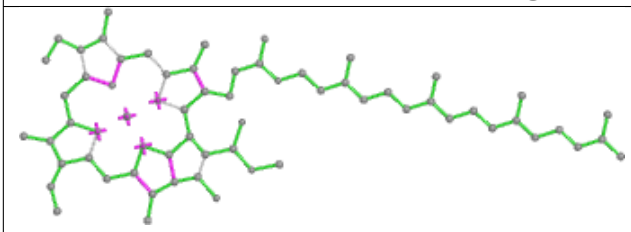


Rings

Ligand CLA B 815



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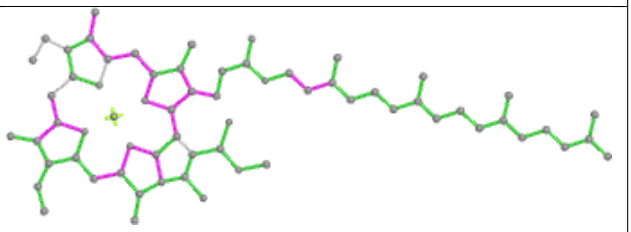
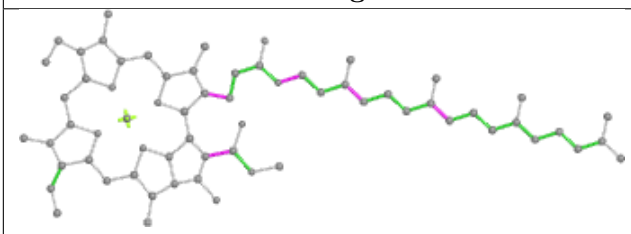


Bond angles



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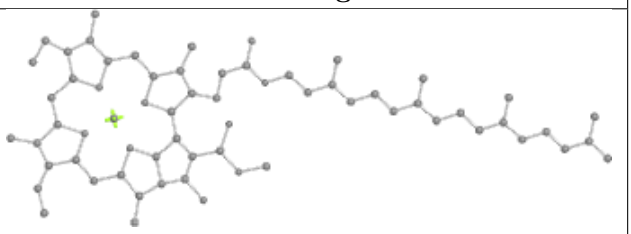
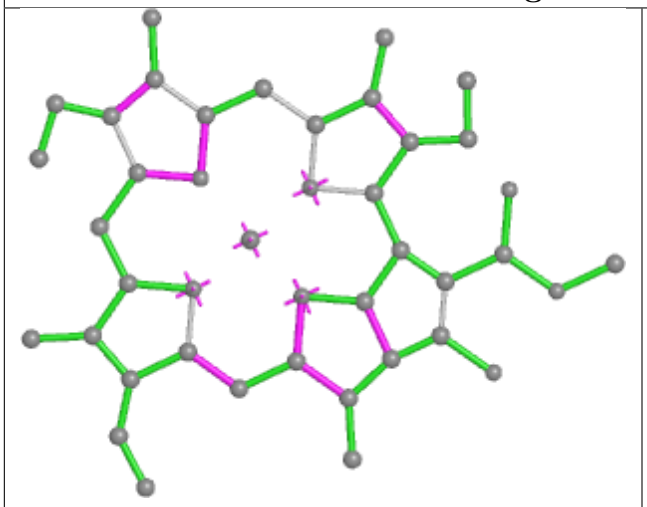


Rings

Ligand CLA A 837



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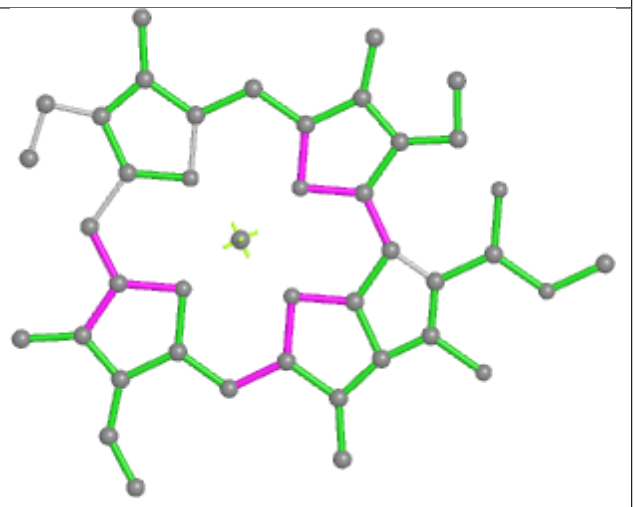
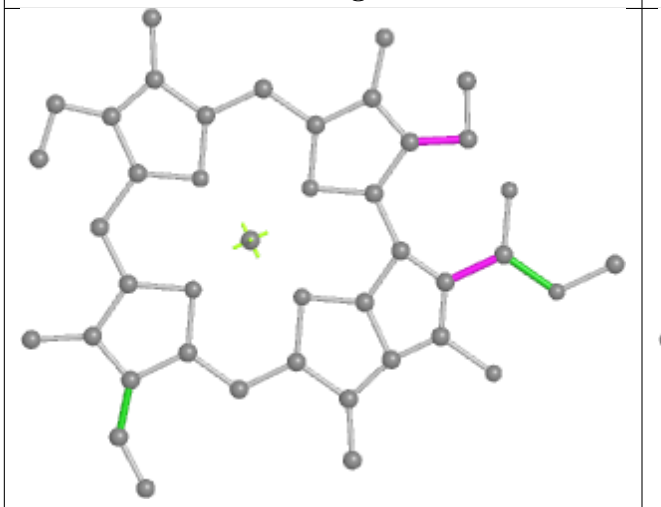


Bond angles



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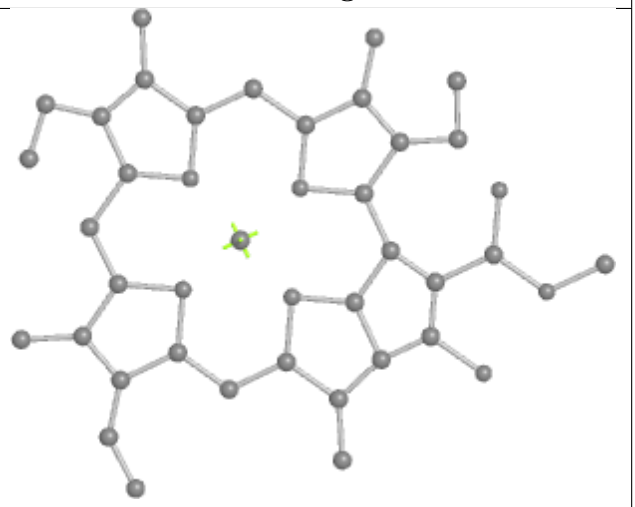
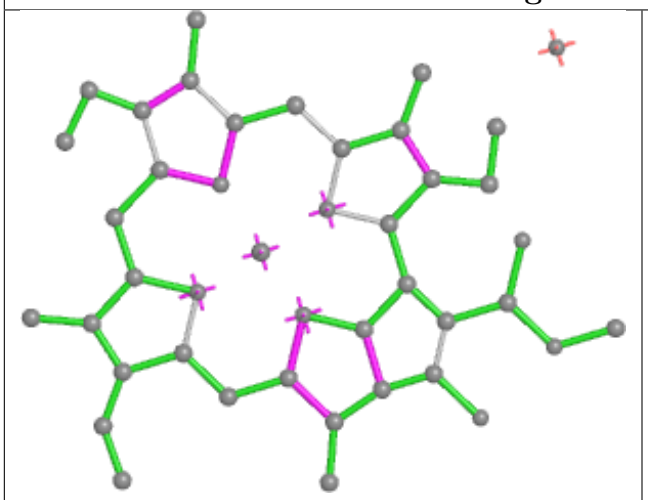


Rings

Ligand CLA A 825



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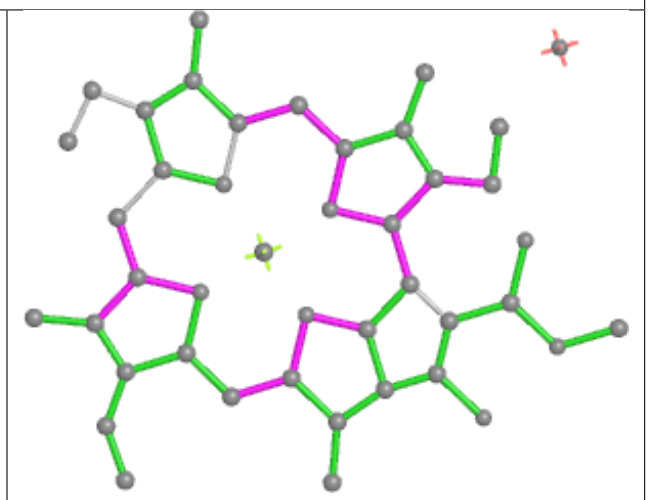
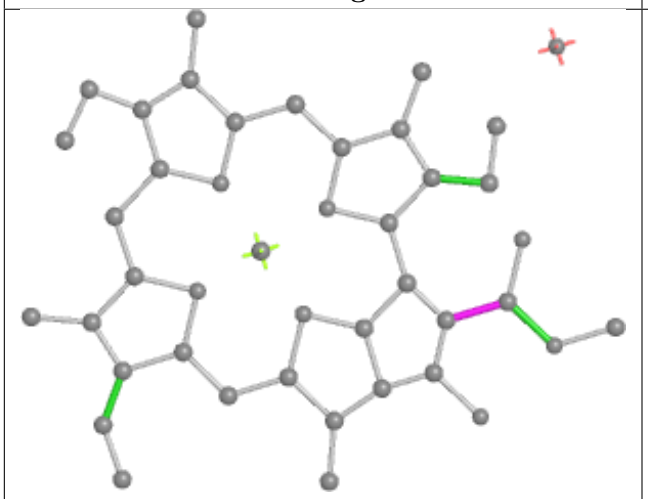


Bond angles



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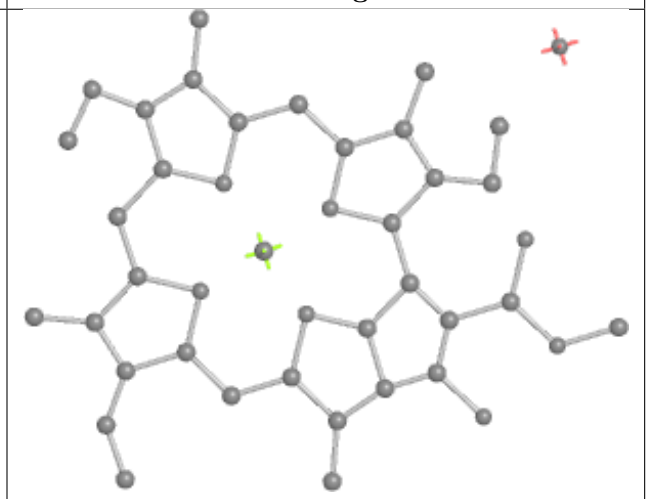
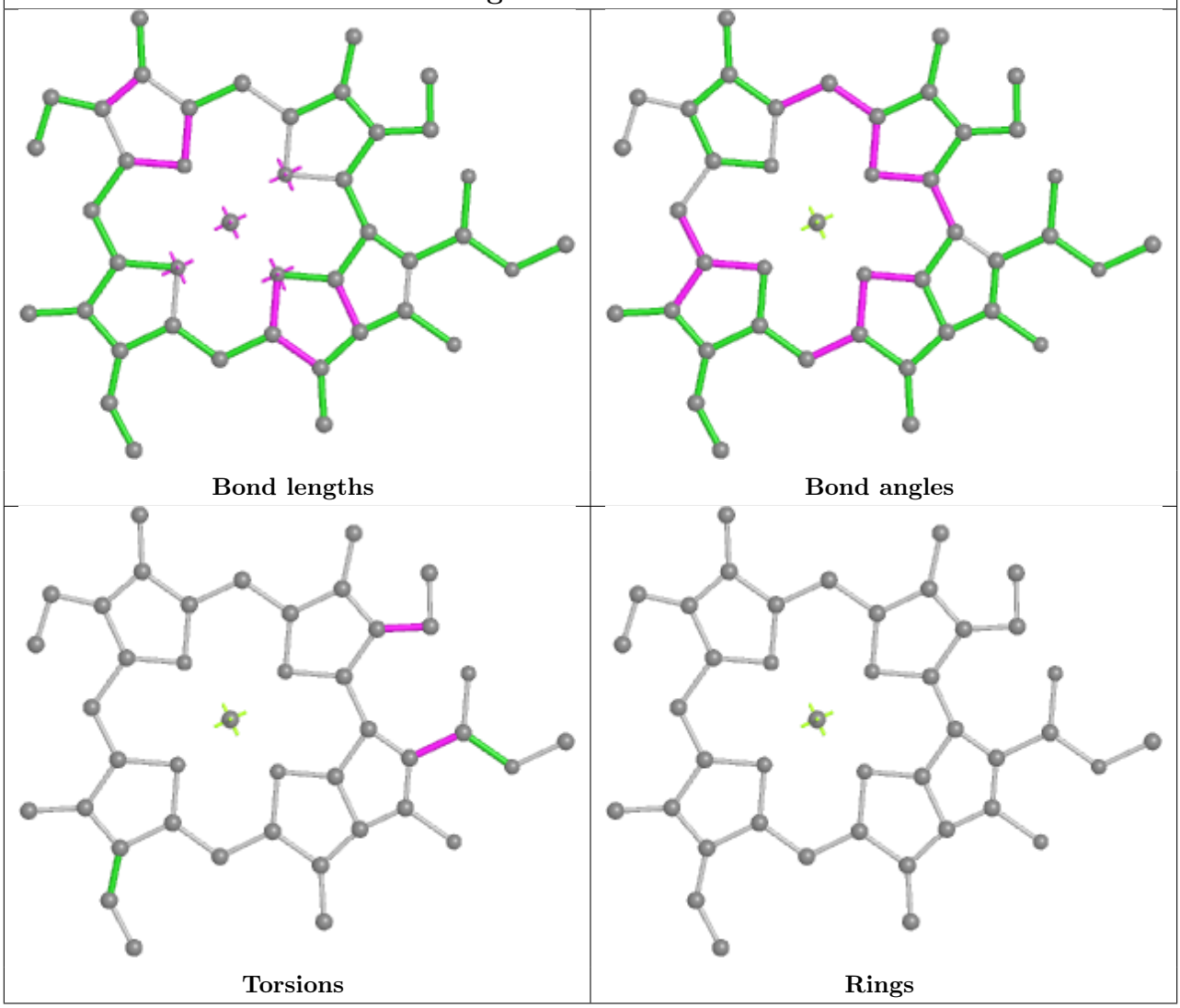
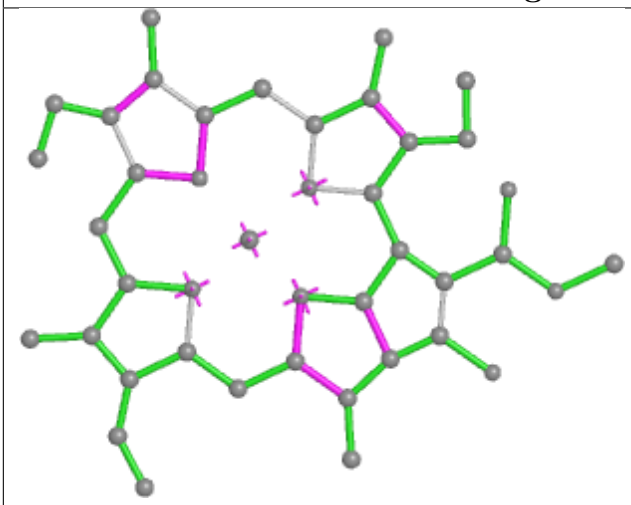


Rings

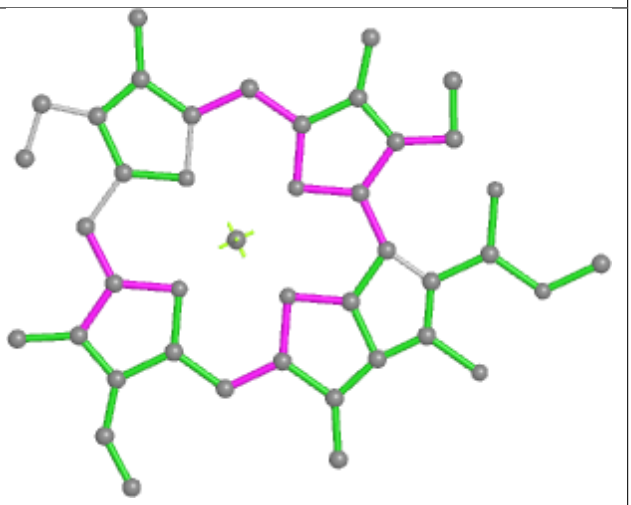
Ligand CLA 1 610



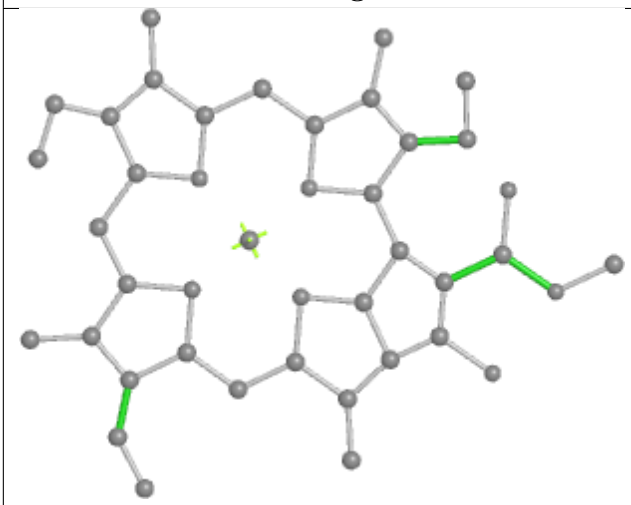
Ligand CLA B 831



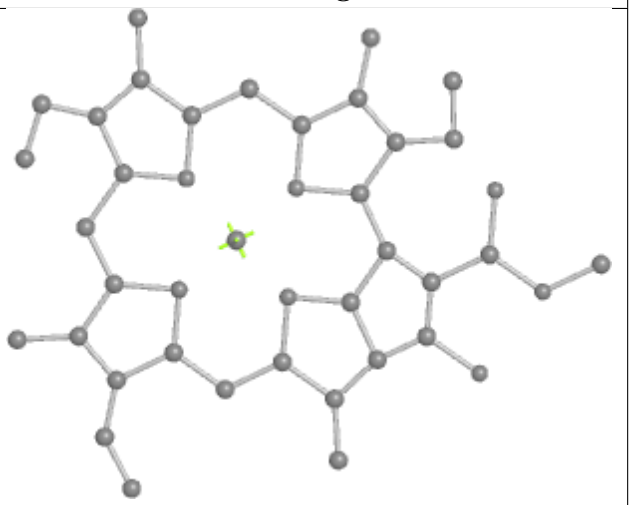
Bond lengths



Bond angles

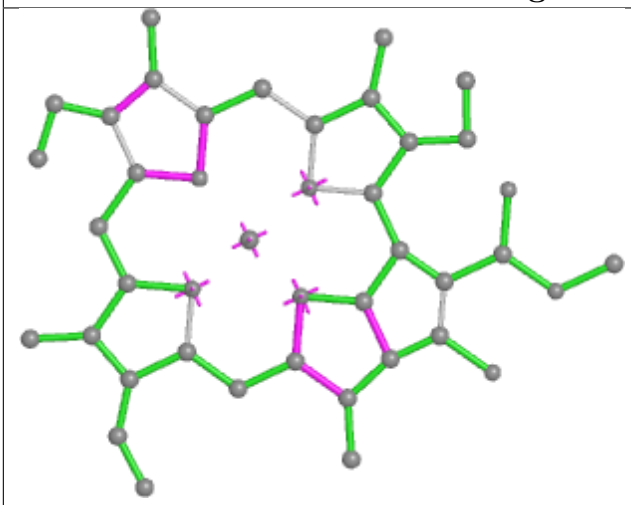


Torsions

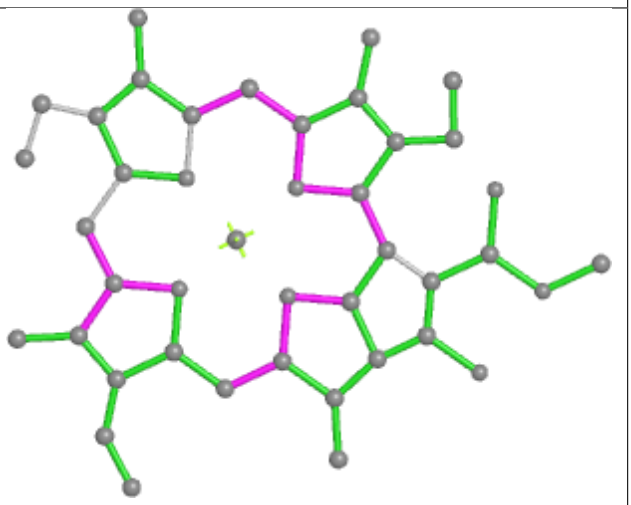


Rings

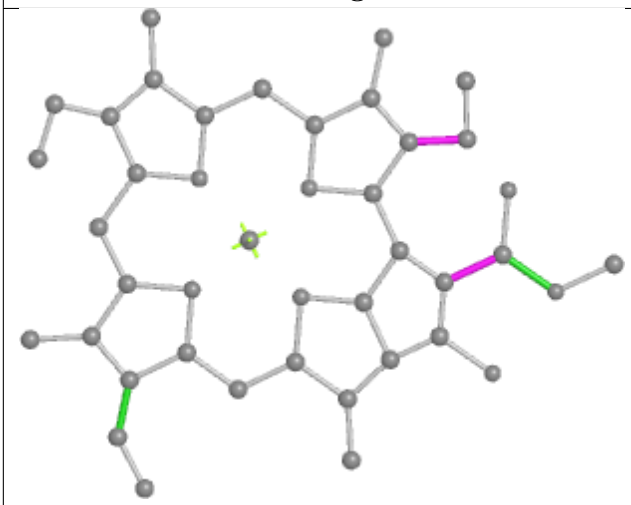
Ligand CLA 5 307



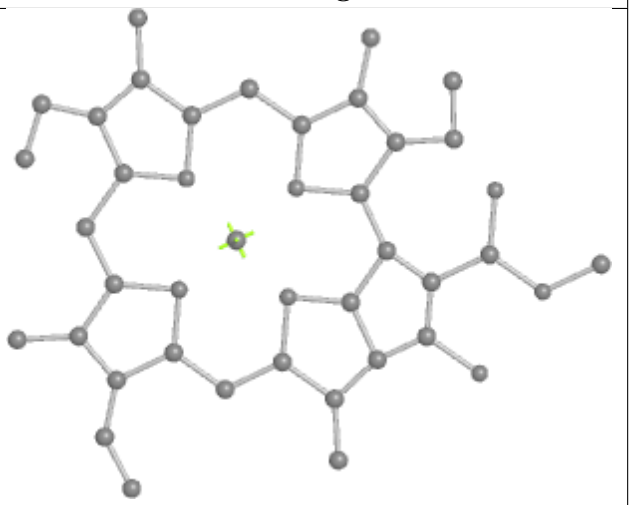
Bond lengths



Bond angles

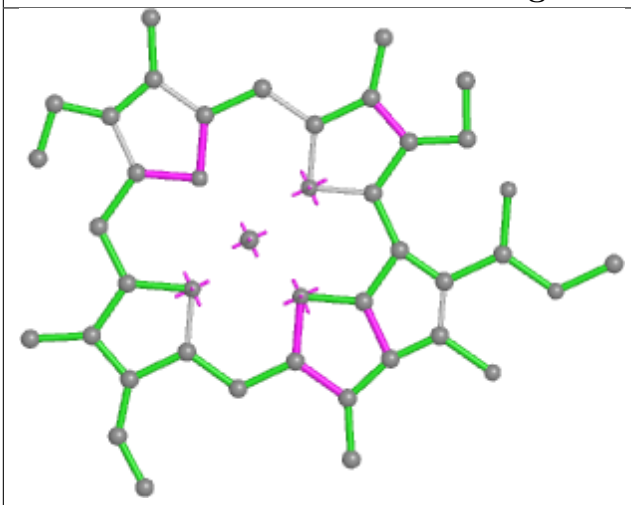


Torsions

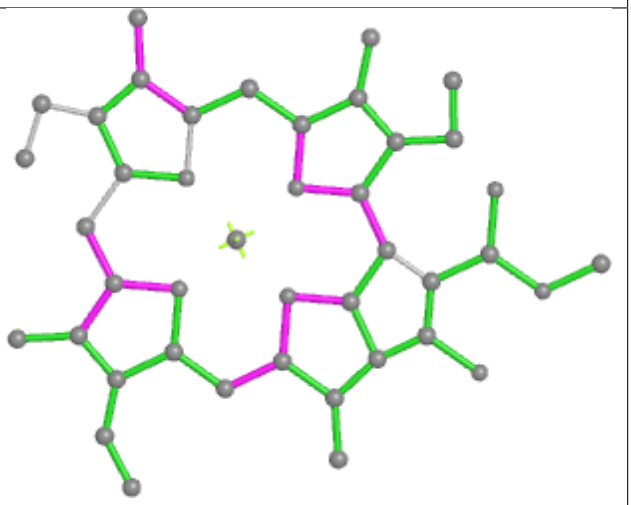


Rings

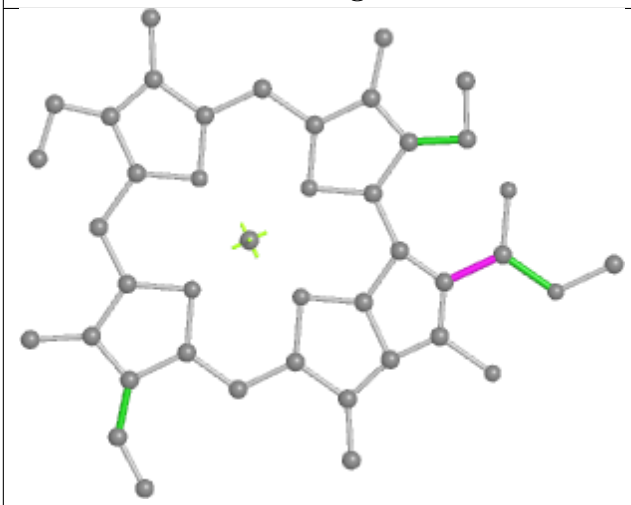
Ligand CLA 3 311



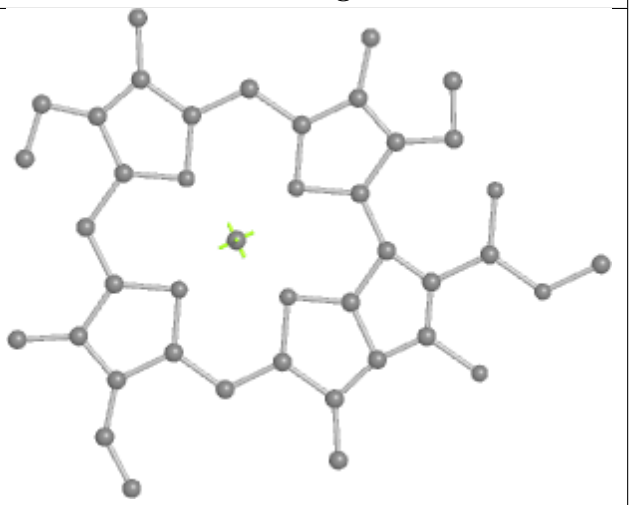
Bond lengths



Bond angles

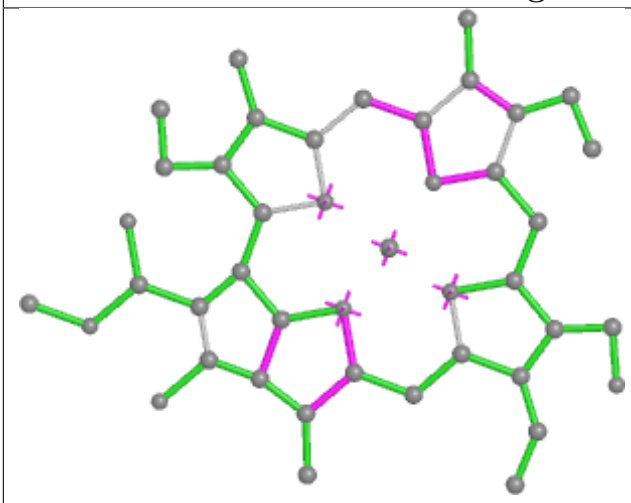


Torsions



Rings

Ligand CHL 6 605



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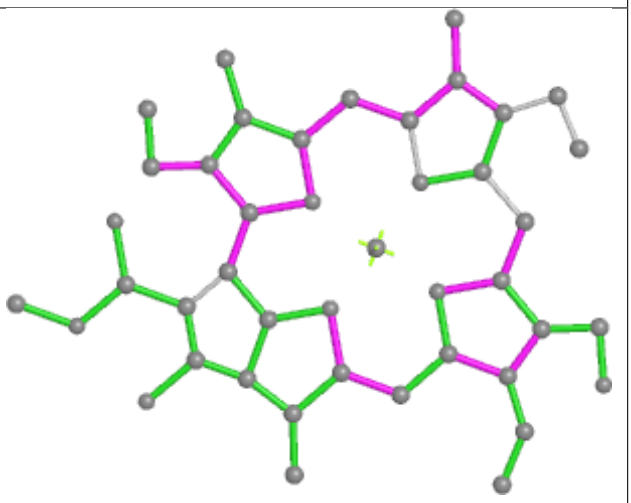
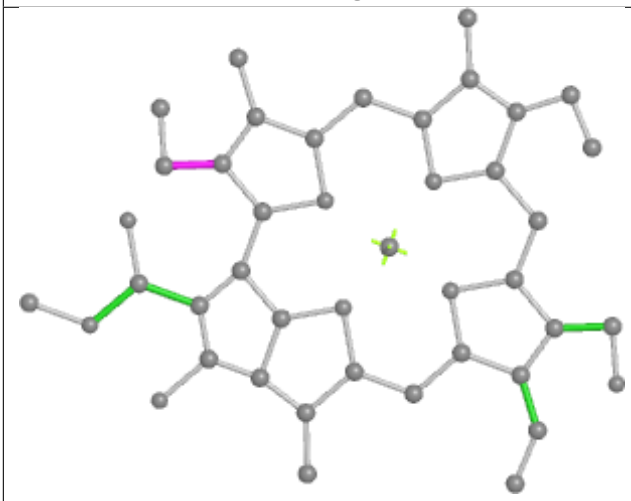
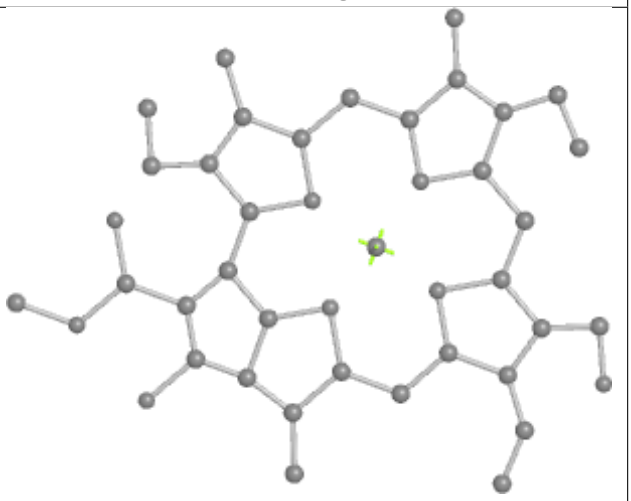


Bond angles

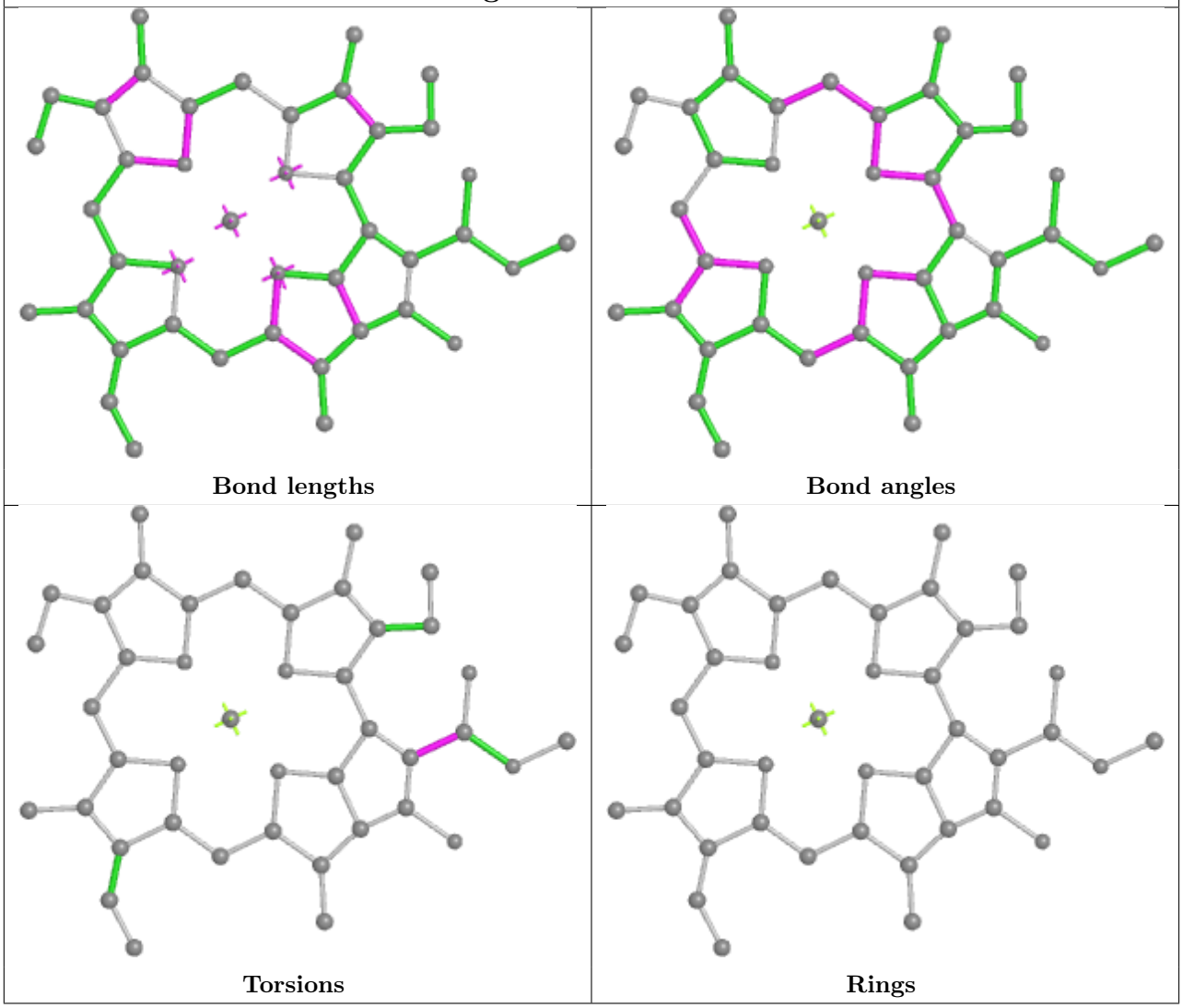


Torsions

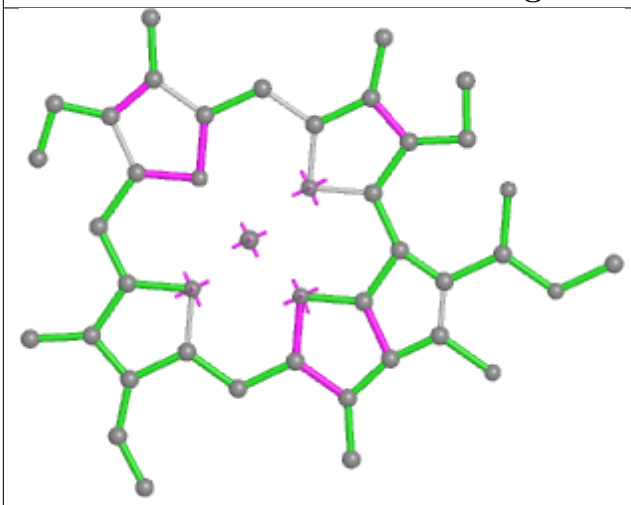


Rings

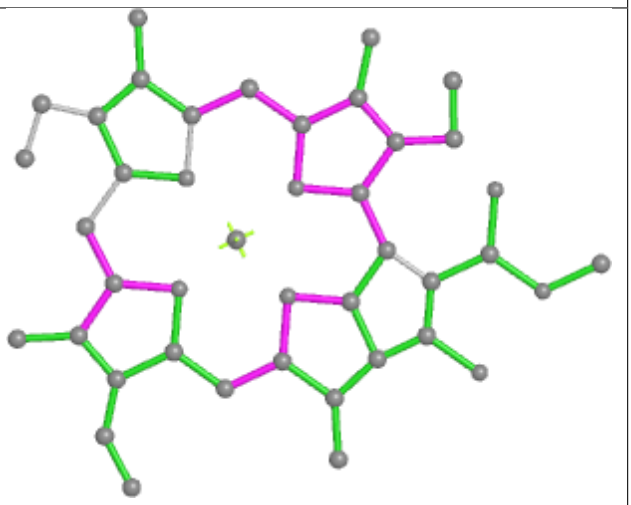
Ligand CLA A 836



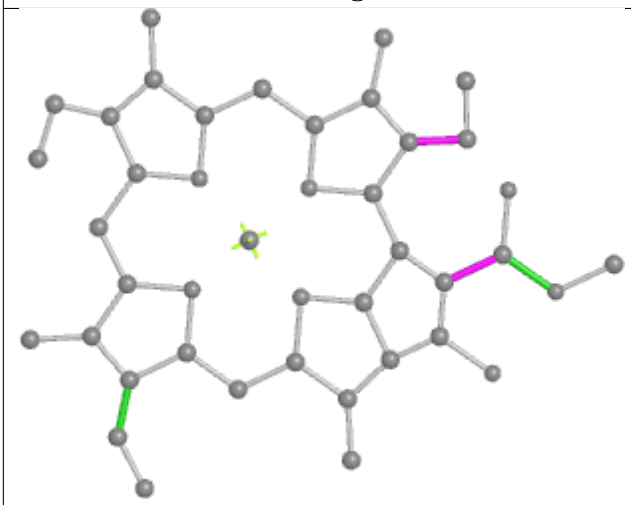
Ligand CLA B 812



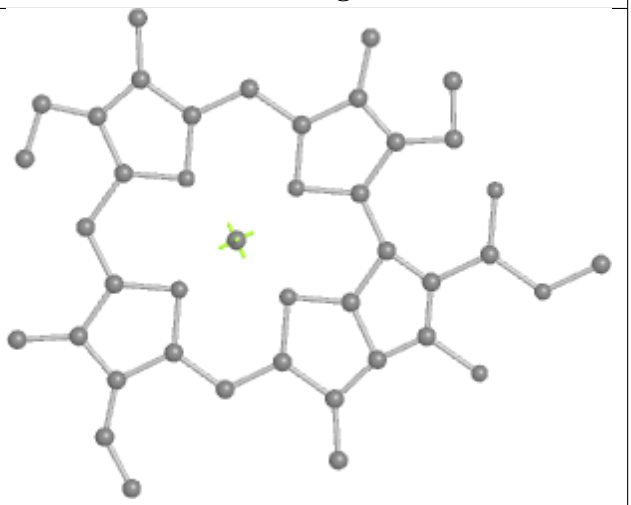
Bond lengths



Bond angles

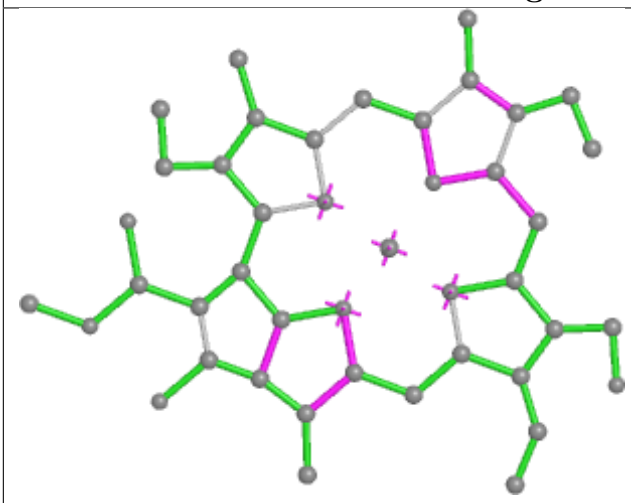


Torsions

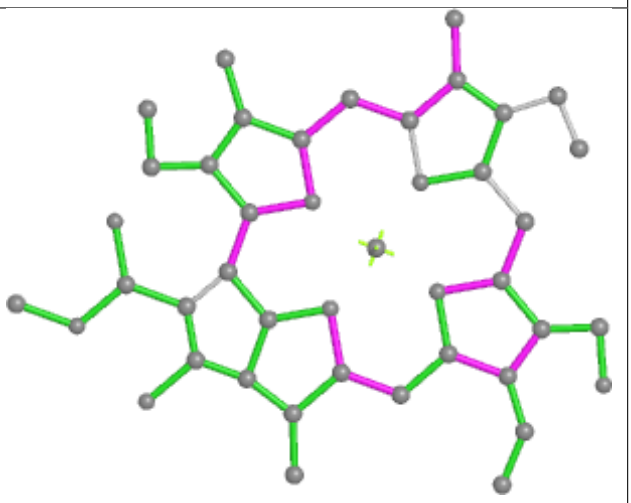


Rings

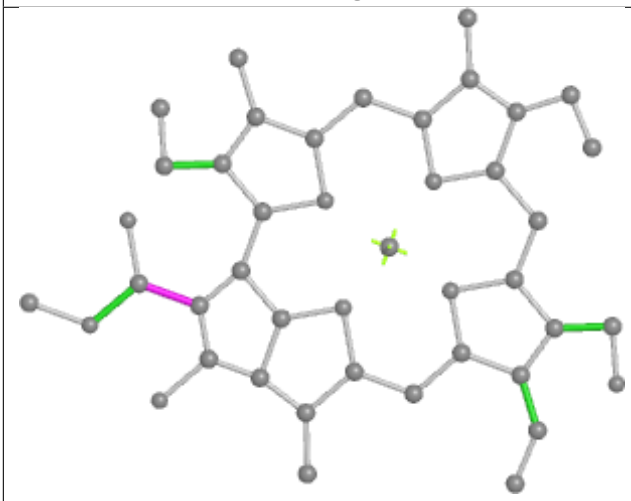
Ligand CHL Z 601



Bond lengths



Bond angles



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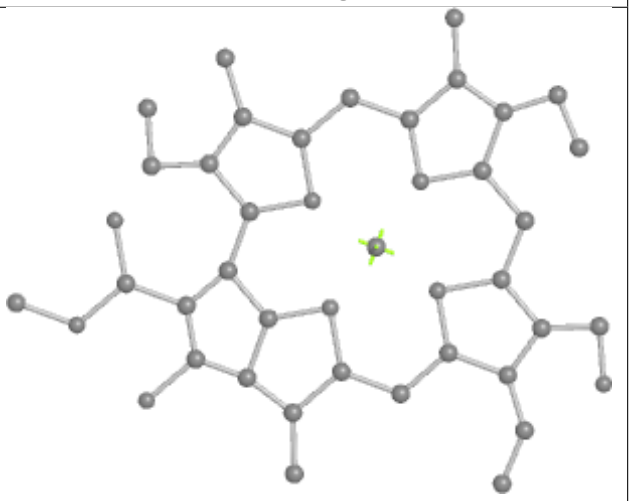
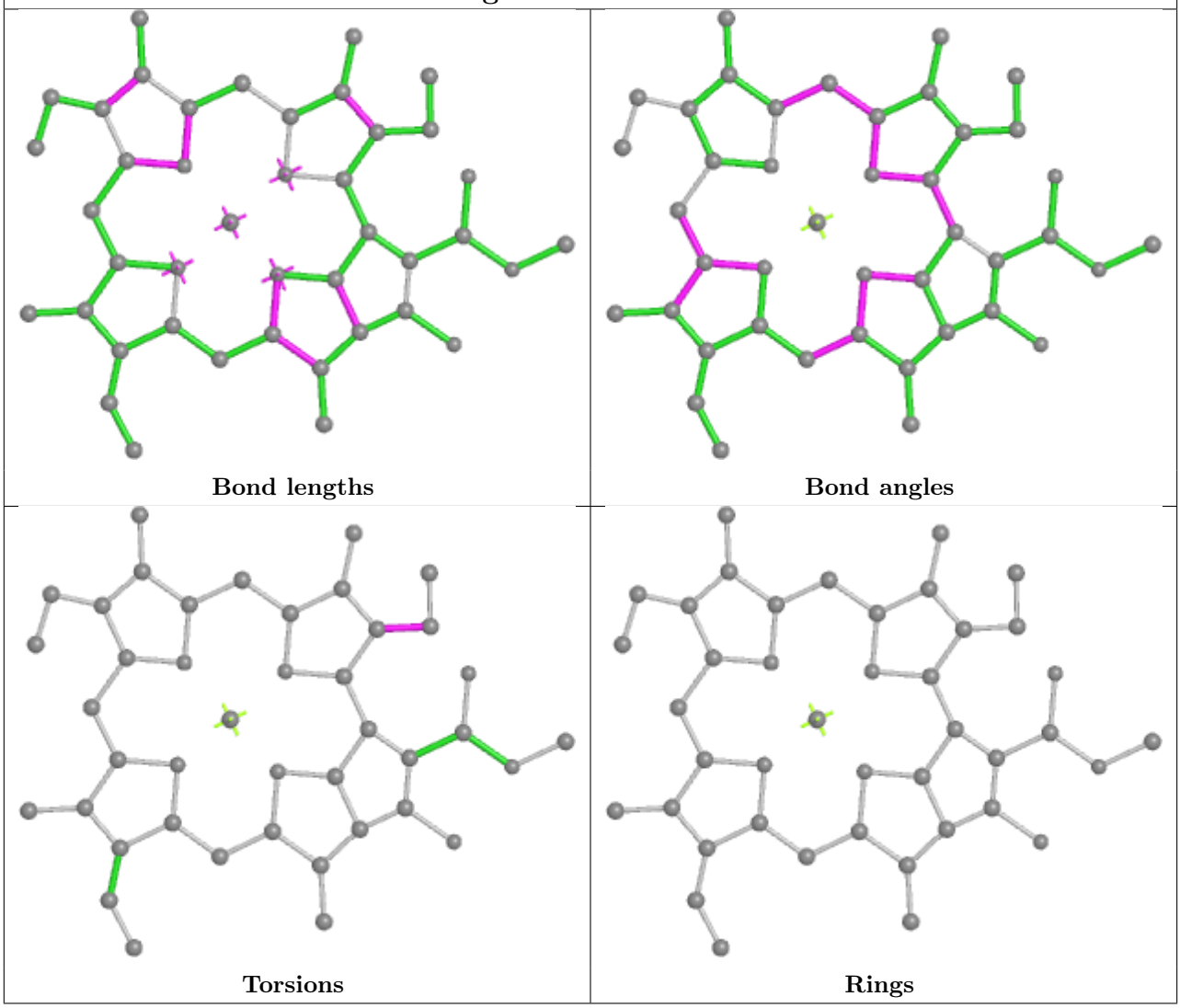
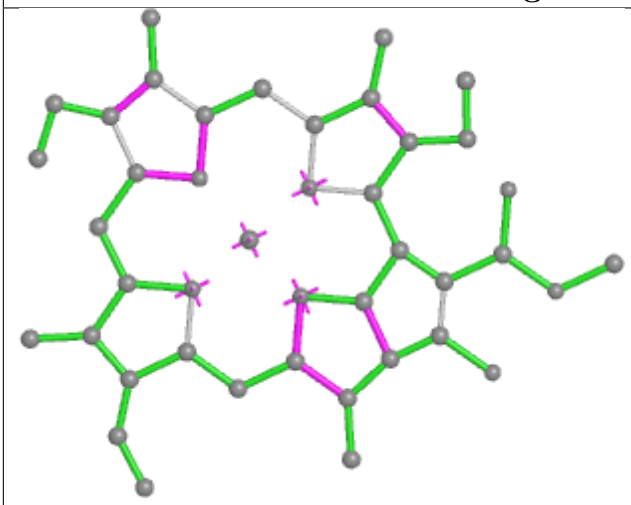


Rings

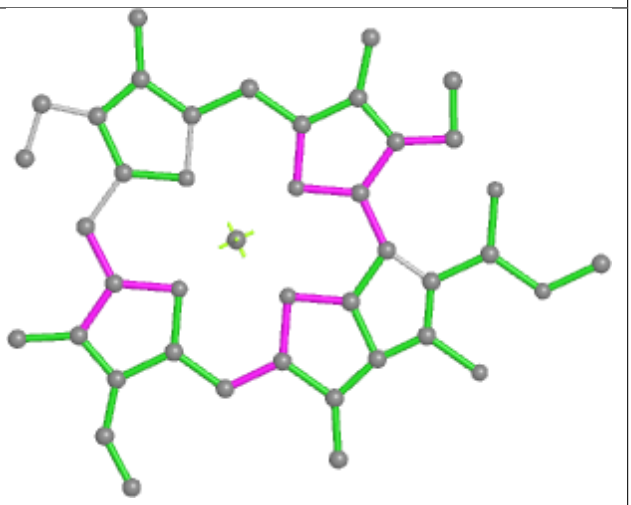
Ligand CLA A 833



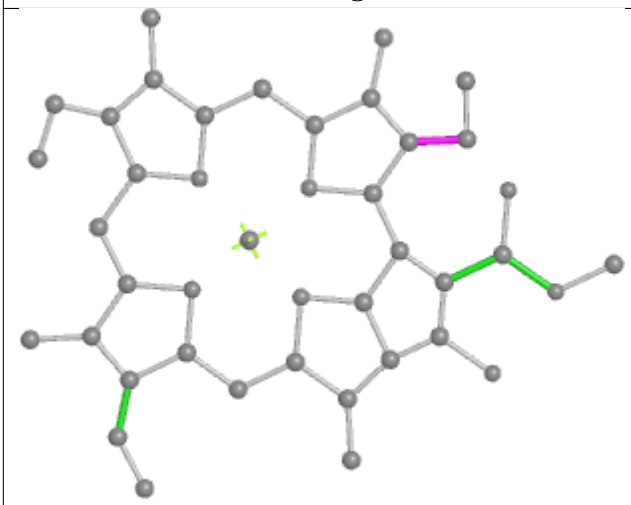
Ligand CLA A 828



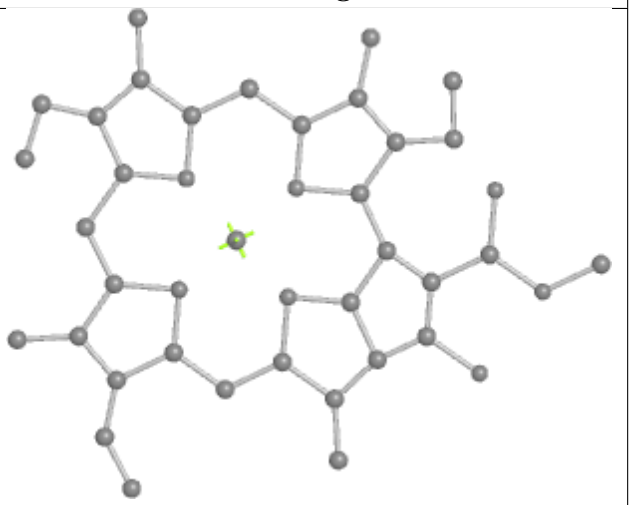
Bond lengths



Bond angles

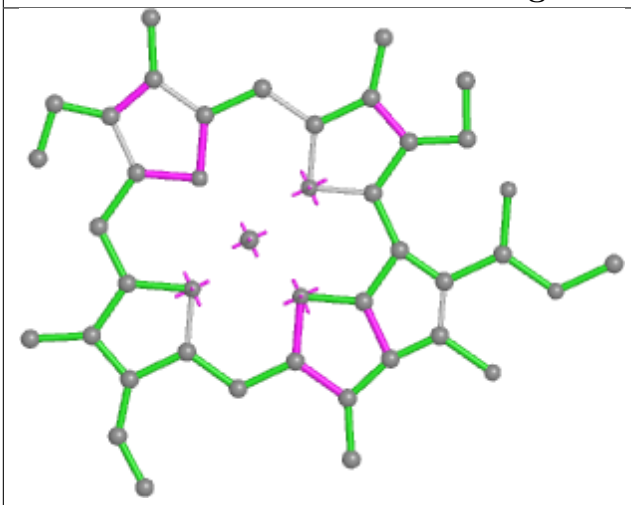


Torsions



Rings

Ligand CLA 5 312



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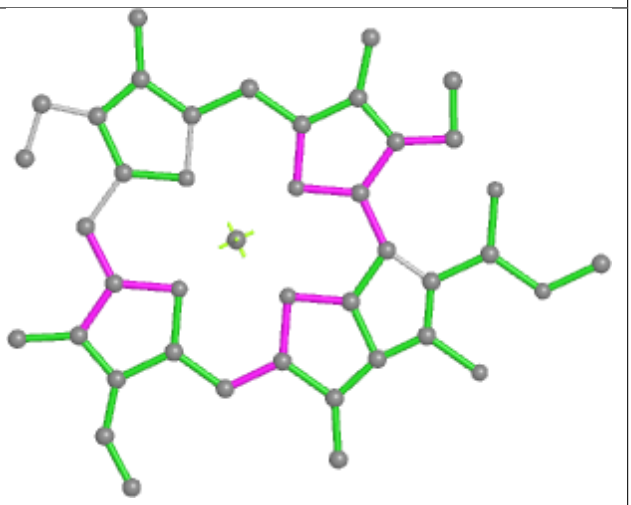
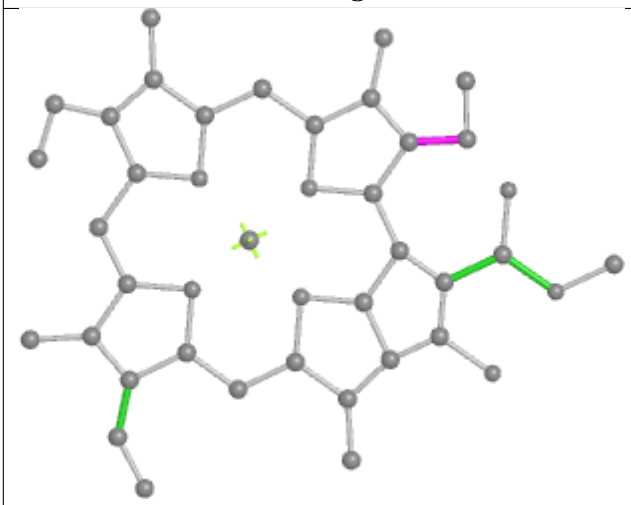


Bond angles



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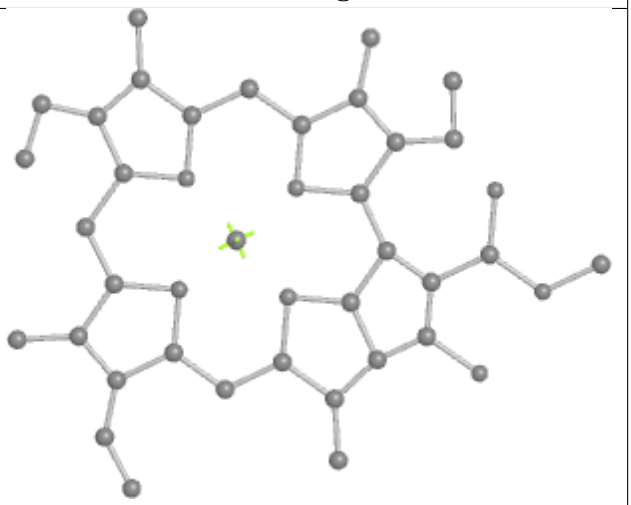
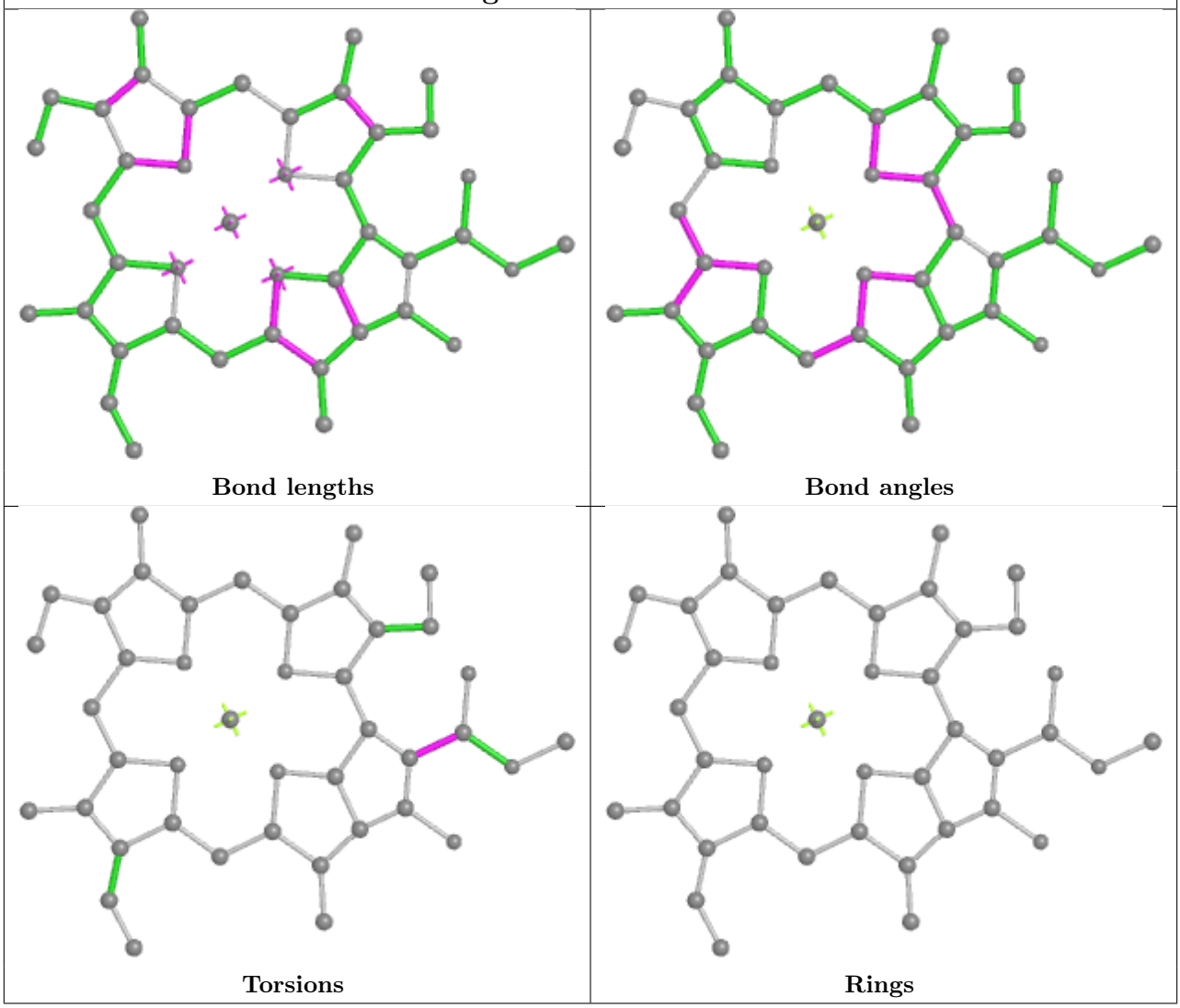
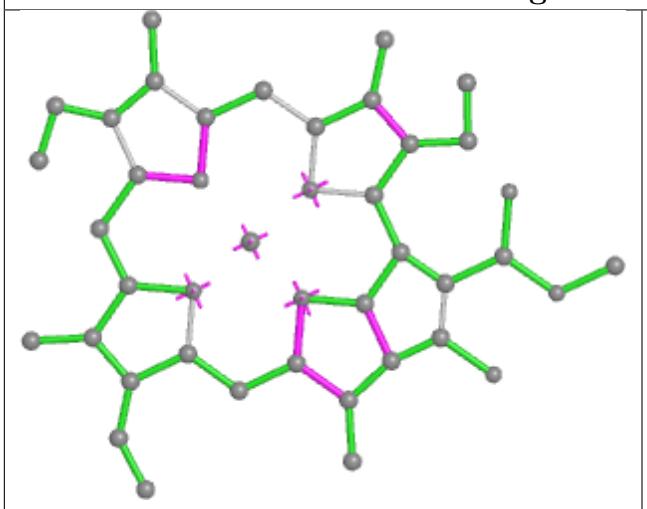


Rings

Ligand CLA A 803



Ligand CLA 7 614



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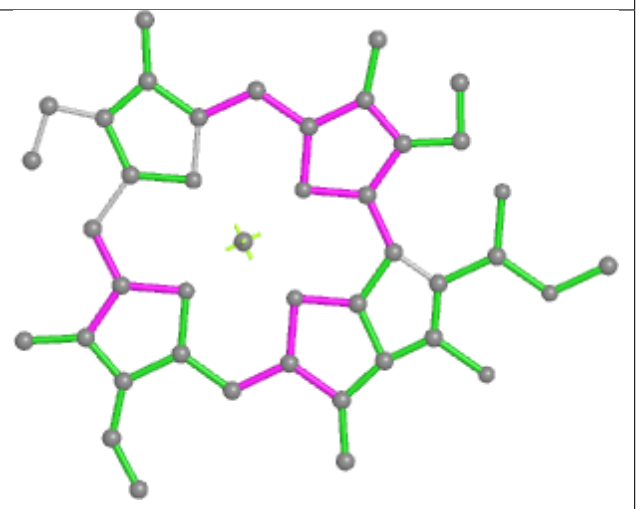
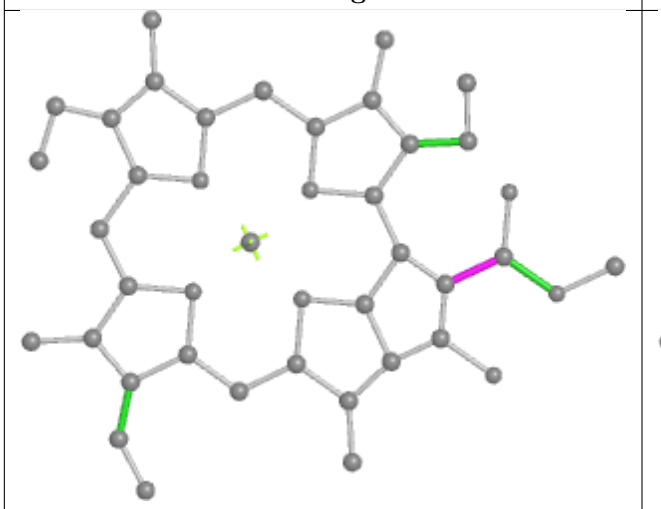


Bond angles



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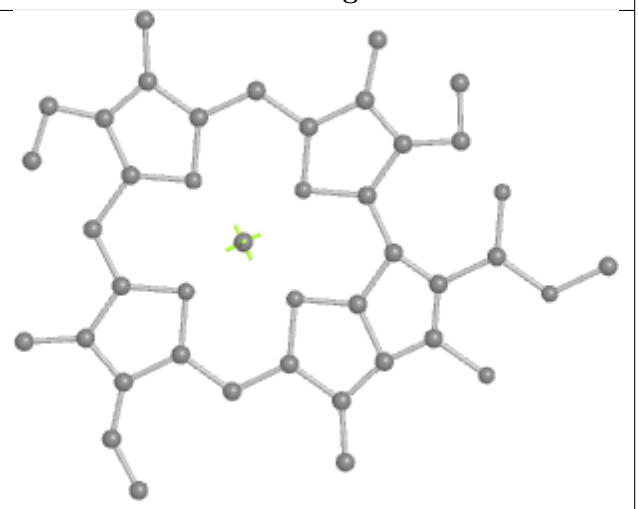
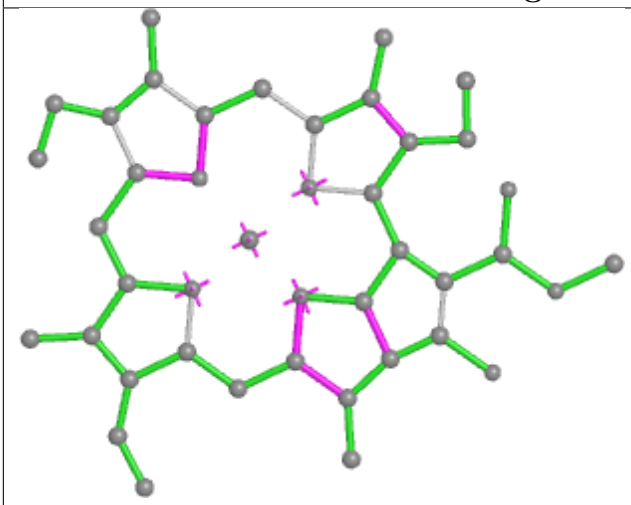
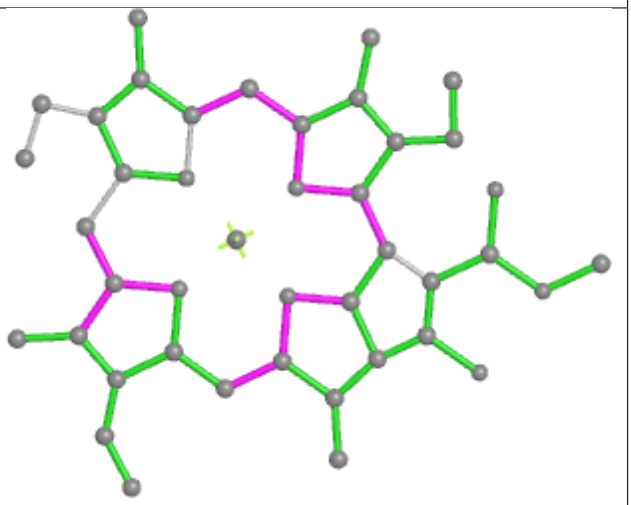


Rings

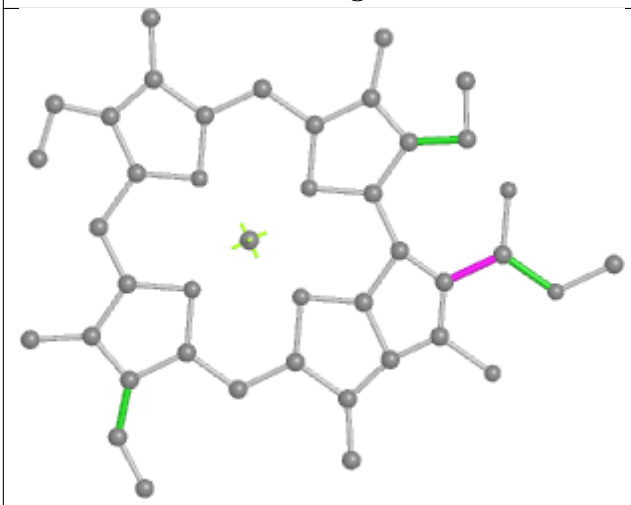
Ligand CLA B 839



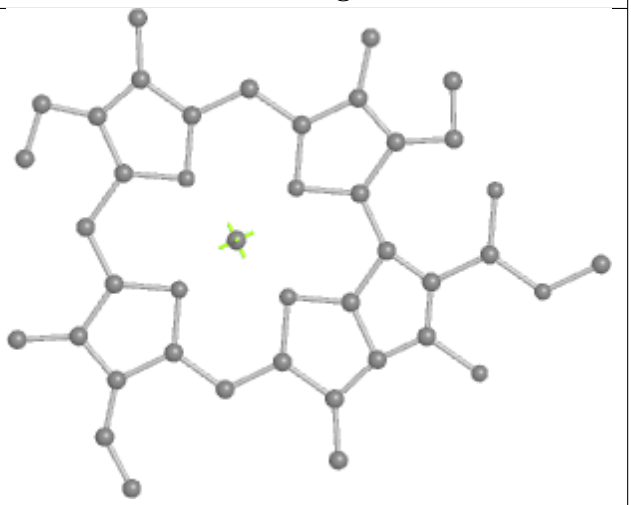
Bond lengths



Bond angles

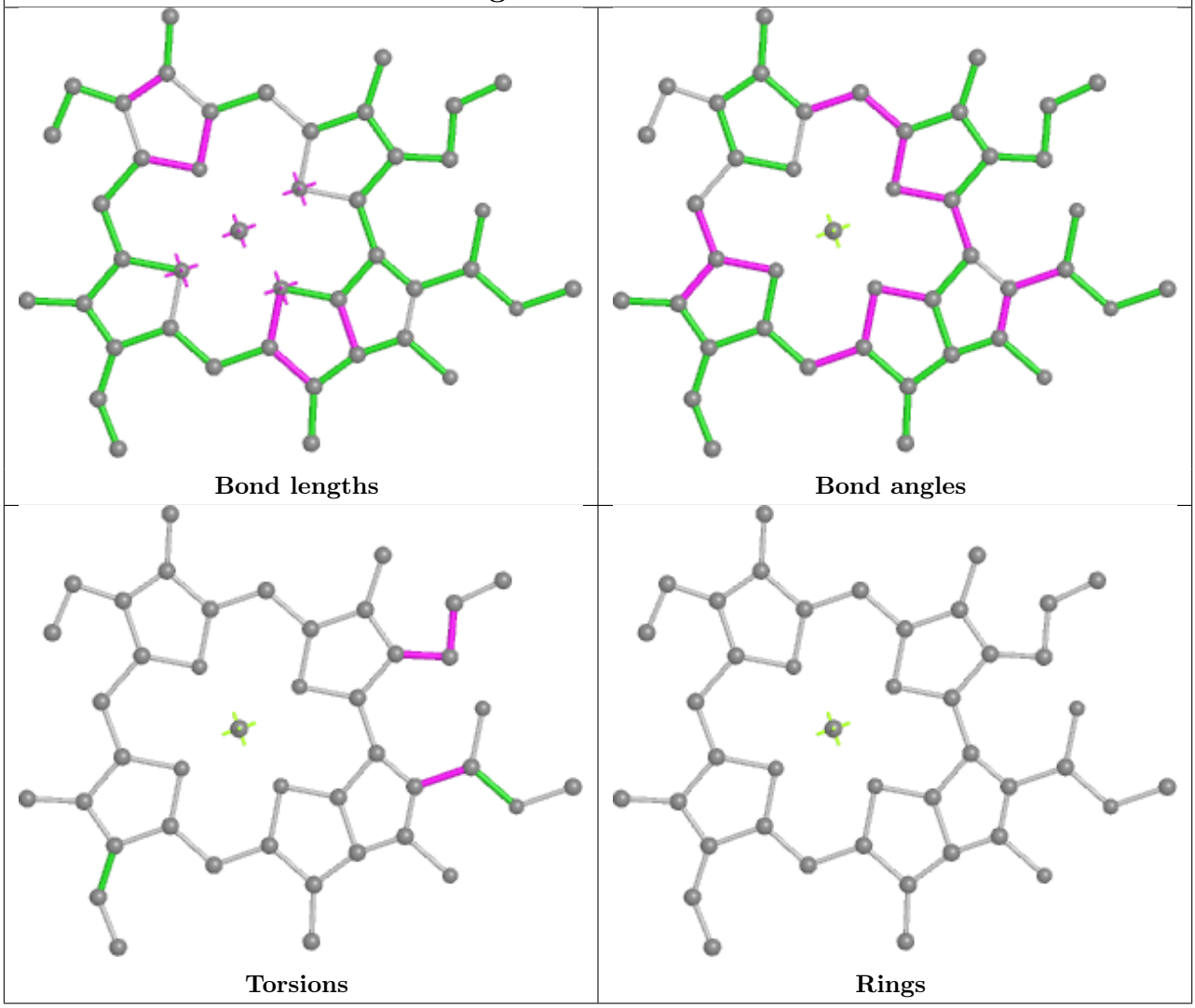


Torsions

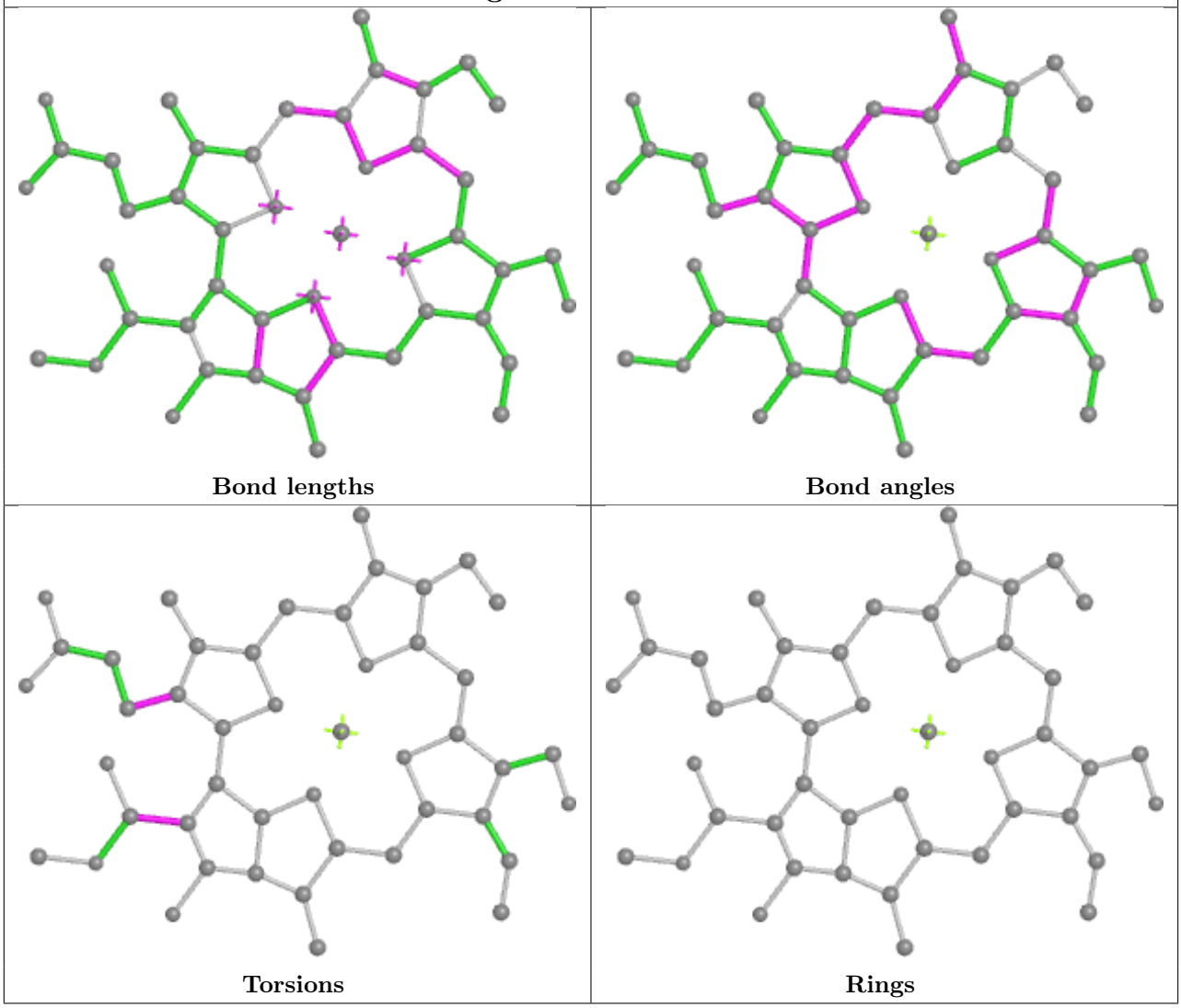


Rings

Ligand CLA B 829



Ligand CHL 5 305



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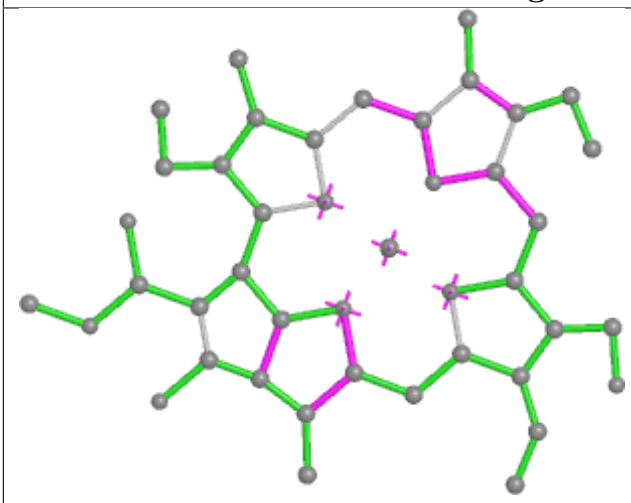
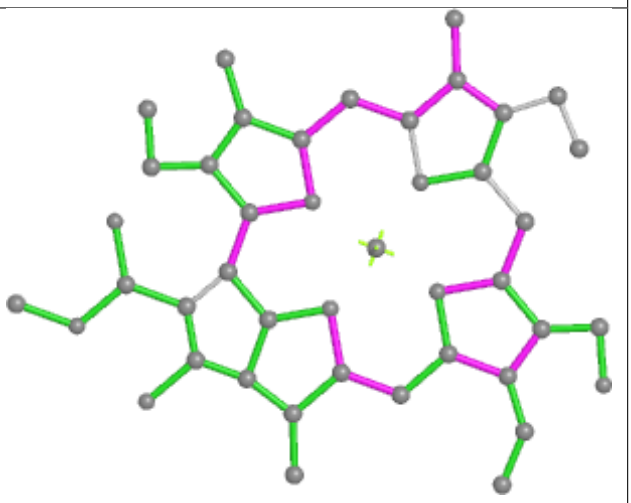
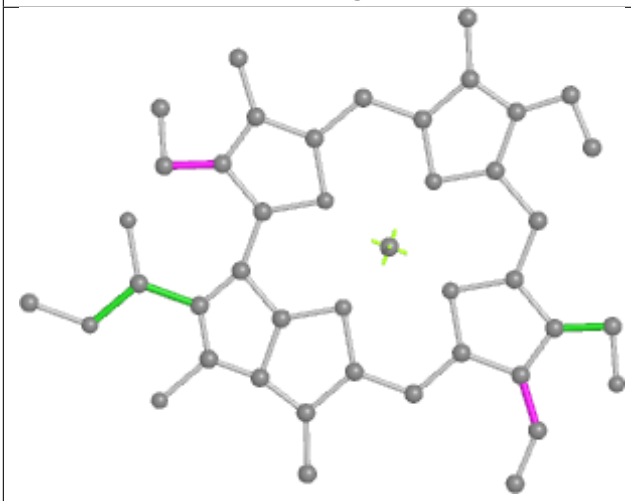


Bond lengths



Bond angles



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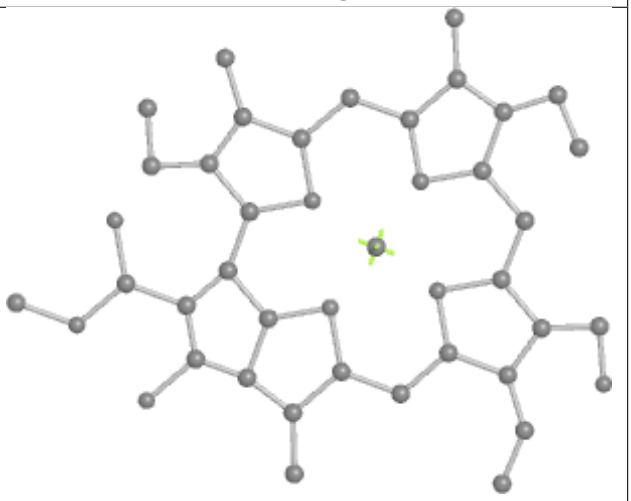
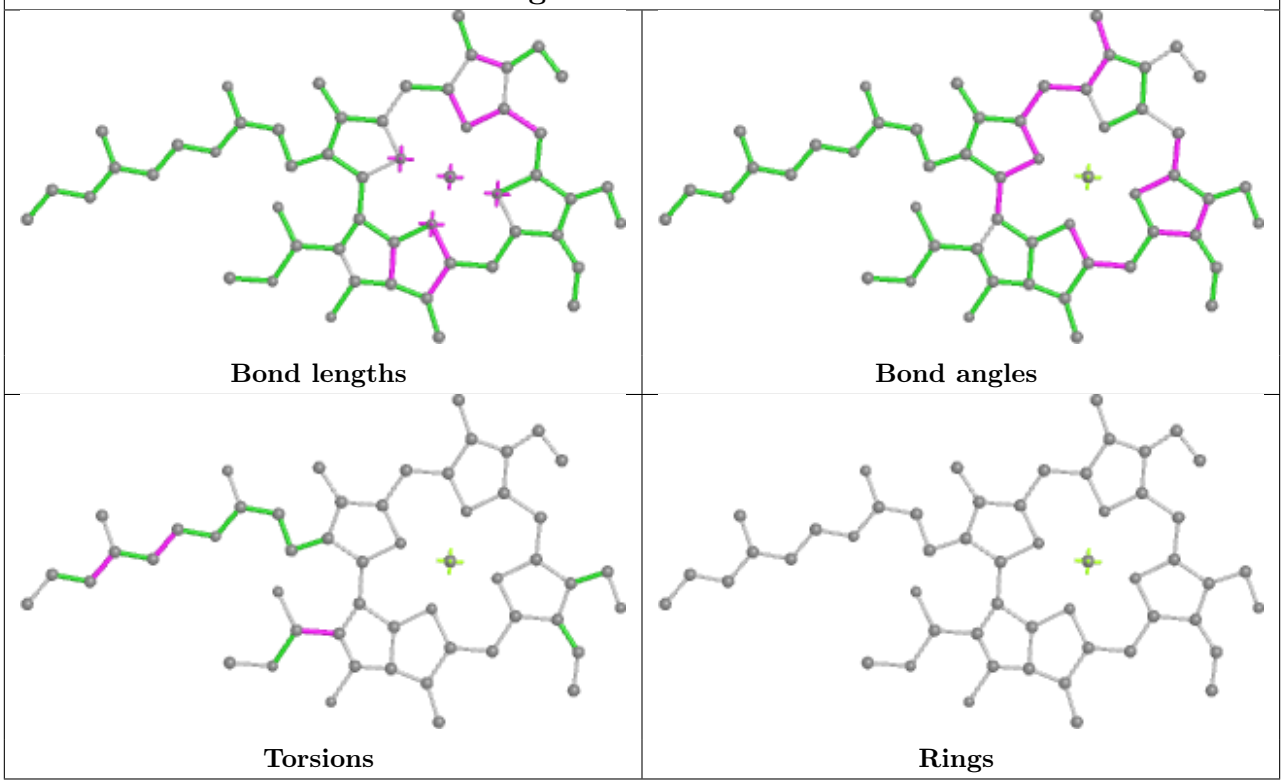
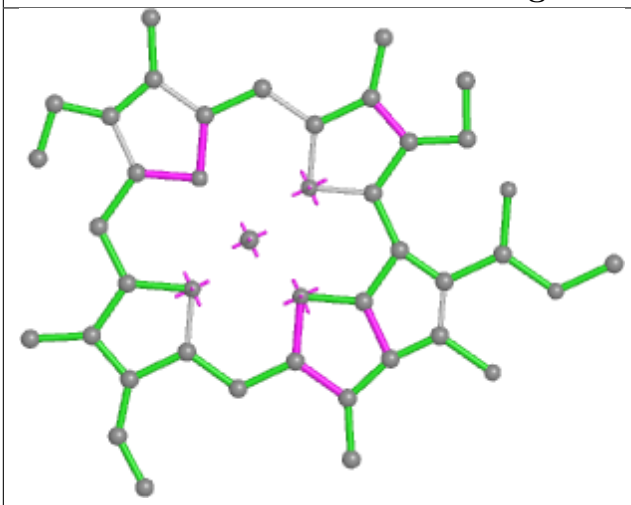


Rings

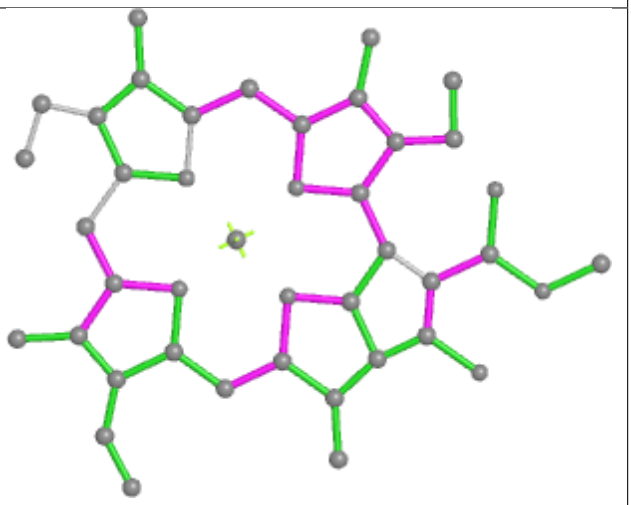
Ligand CHL 1 601



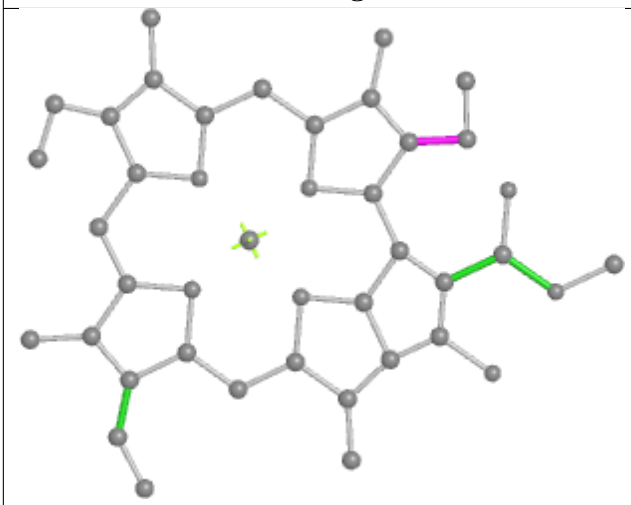
Ligand CLA 3 306



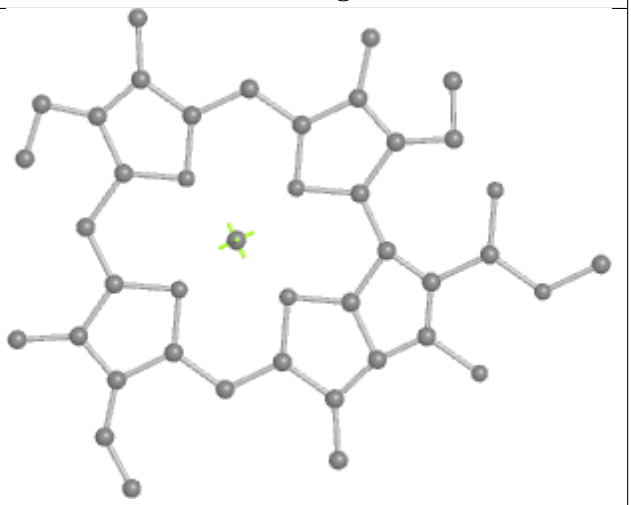
Bond lengths



Bond angles

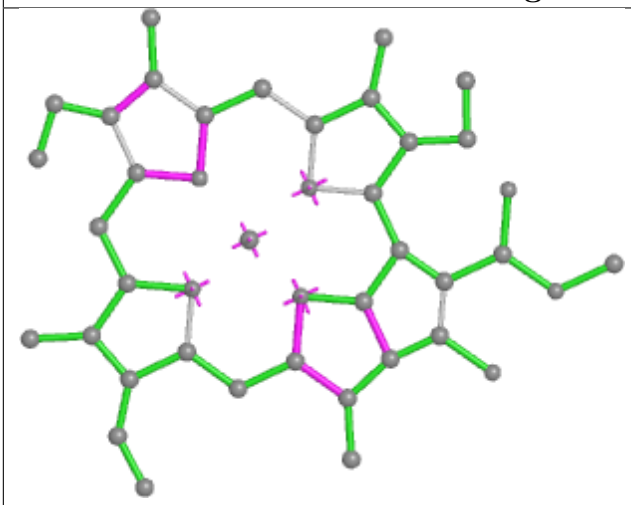


Torsions

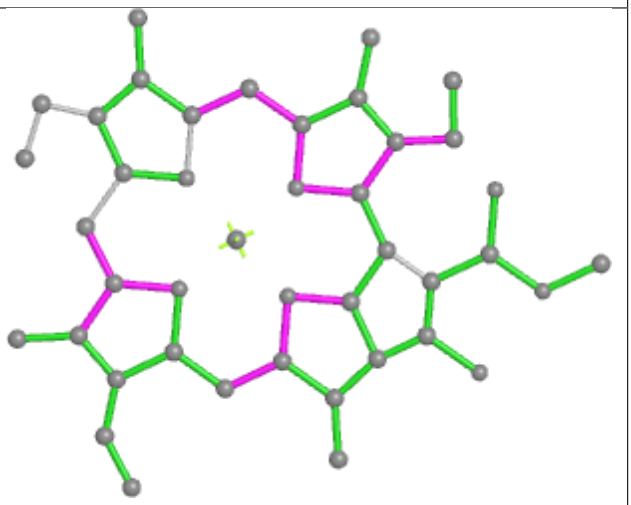


Rings

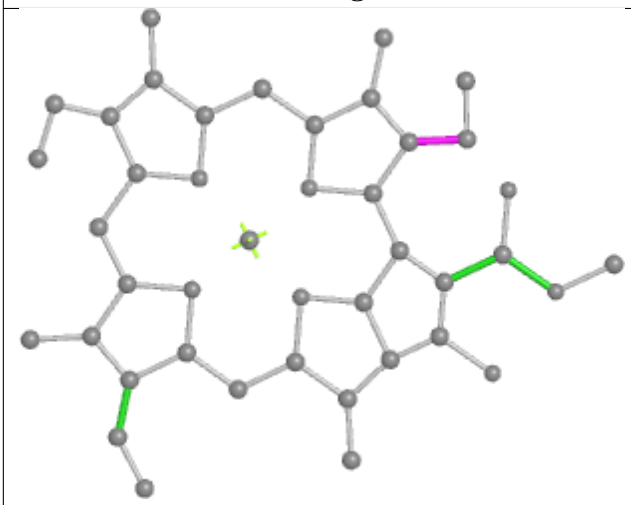
Ligand CLA B 826



Bond lengths



Bond angles



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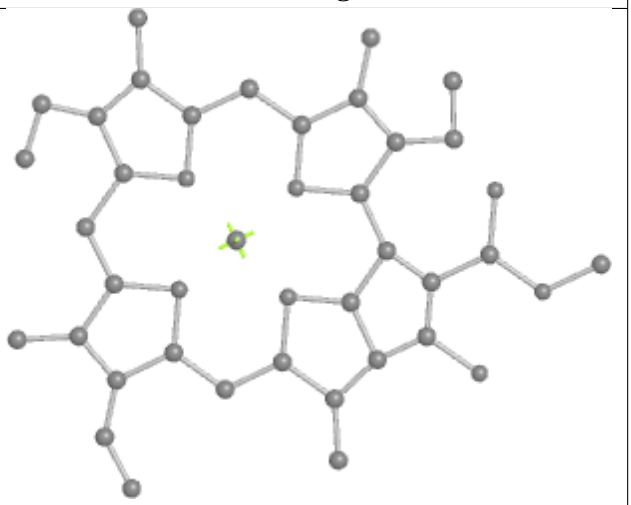
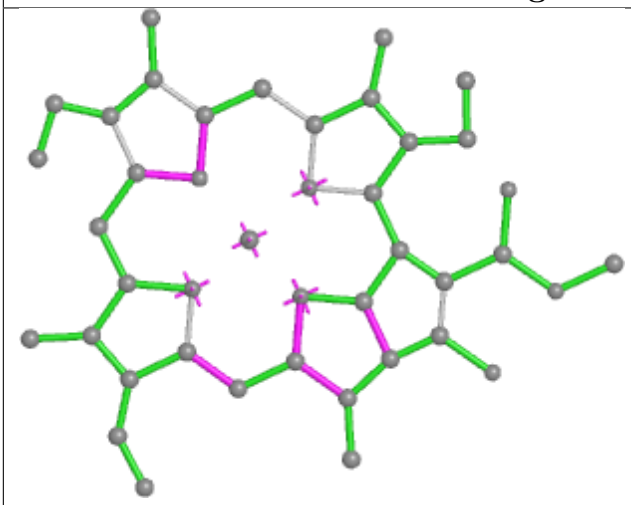


Rings

Ligand CLA 5 311



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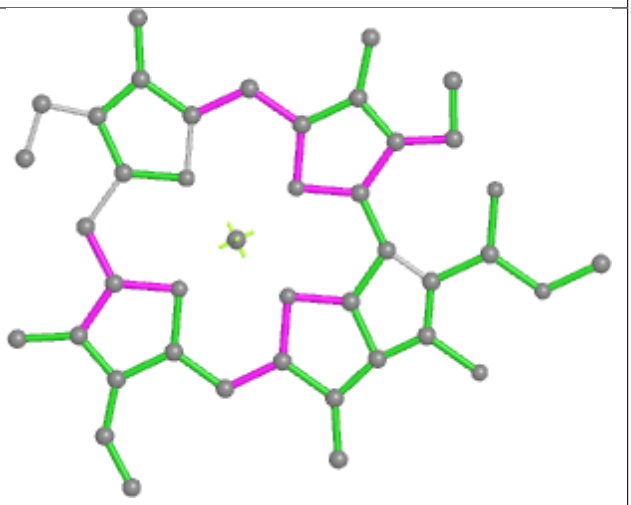
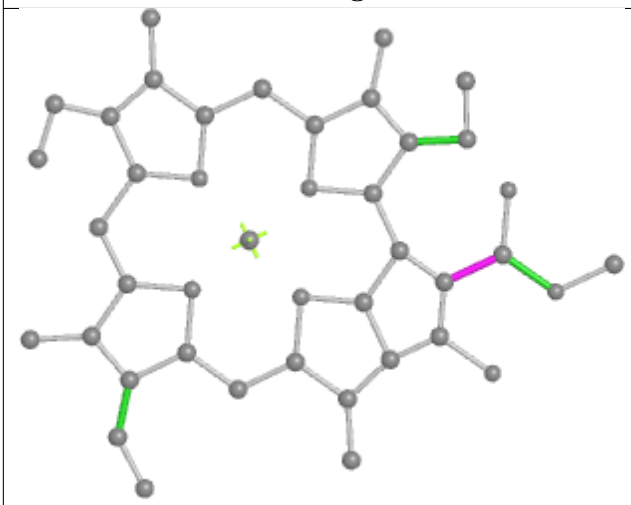
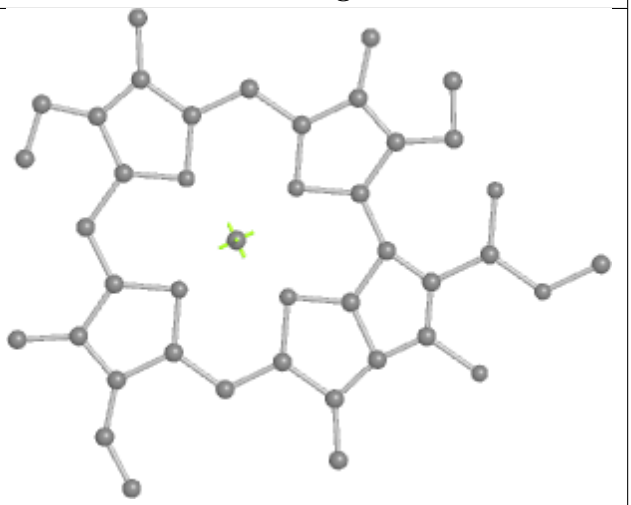


Bond angles

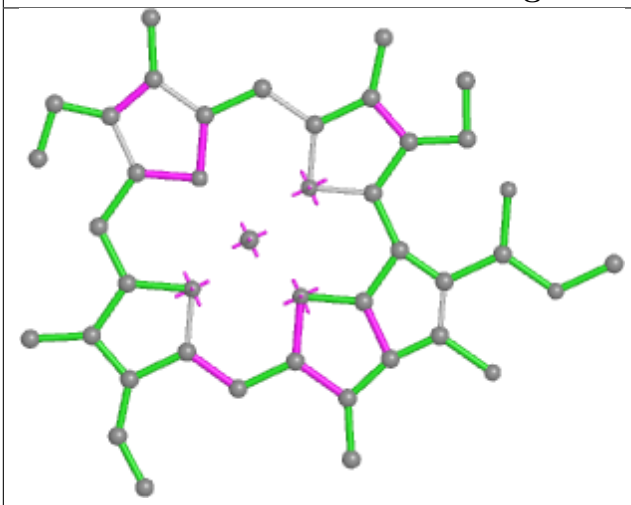


Torsions

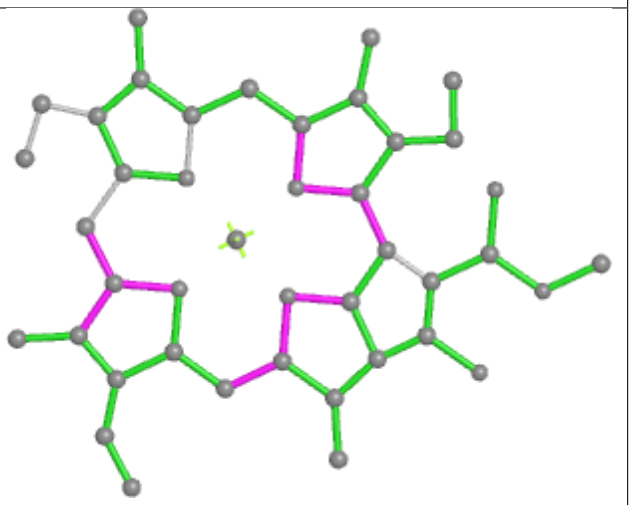


Rings

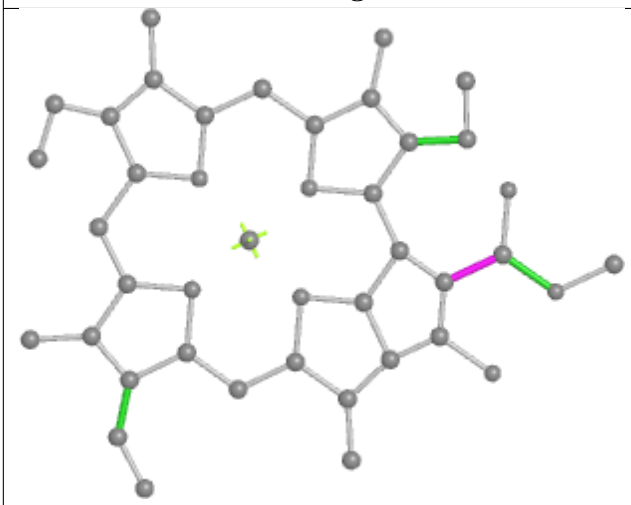
Ligand CLA A 843



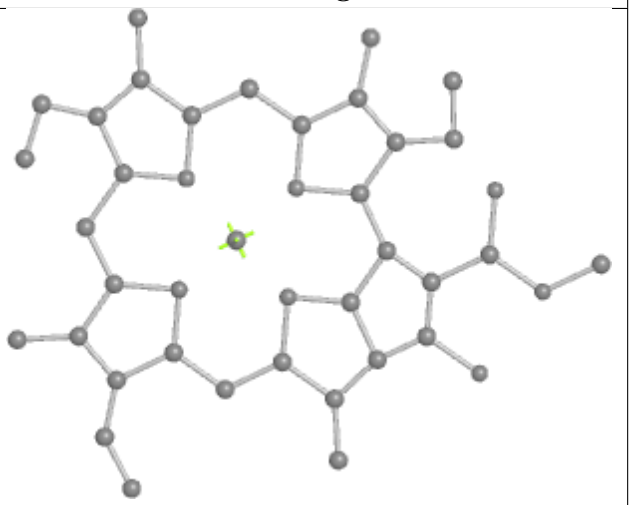
Bond lengths



Bond angles

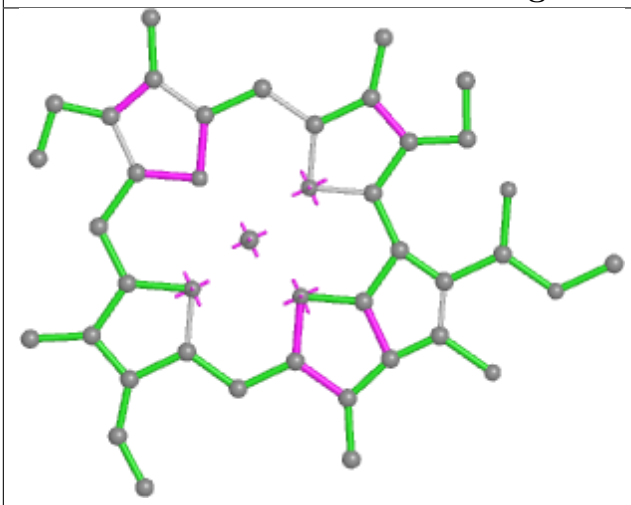


Torsions

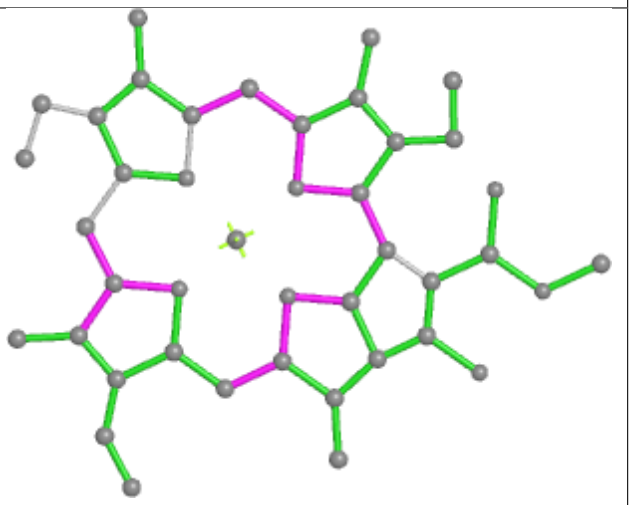


Rings

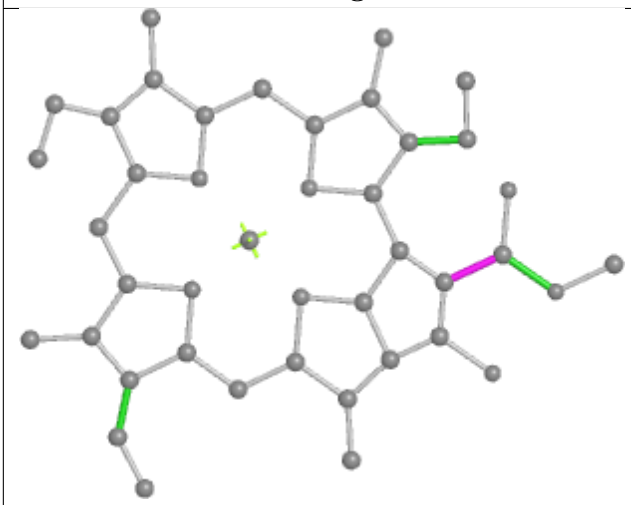
Ligand CLA 4 601



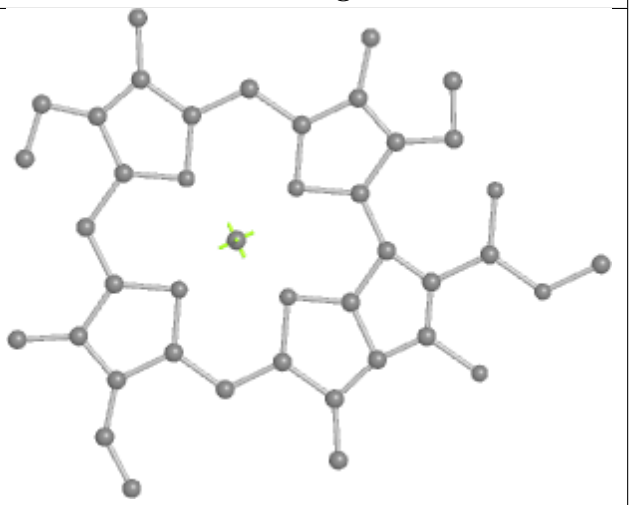
Bond lengths



Bond angles

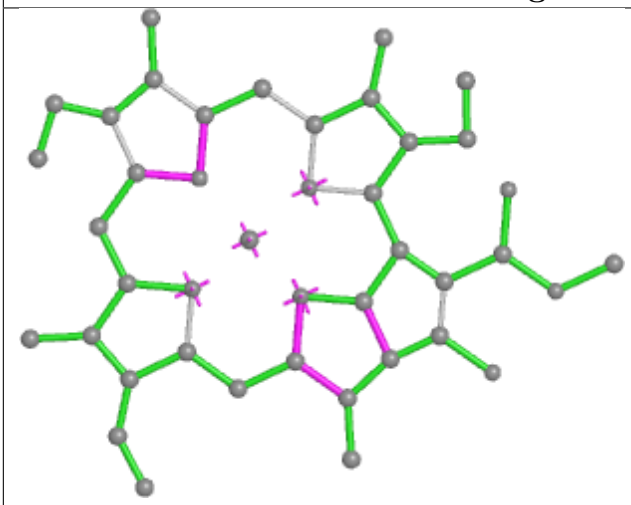


Torsions



Rings

Ligand CLA 5 308



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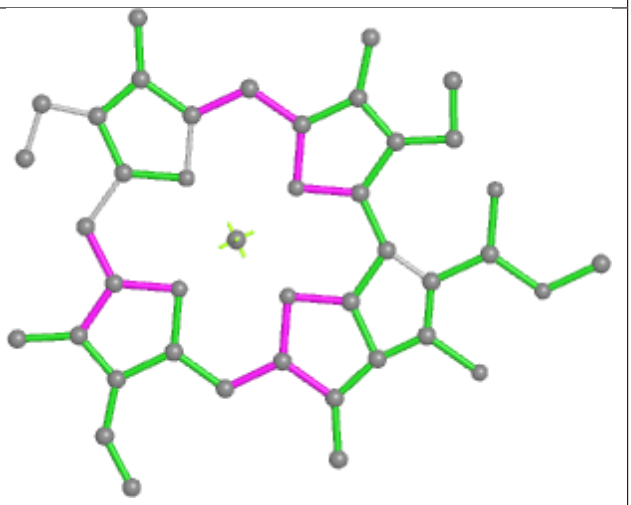
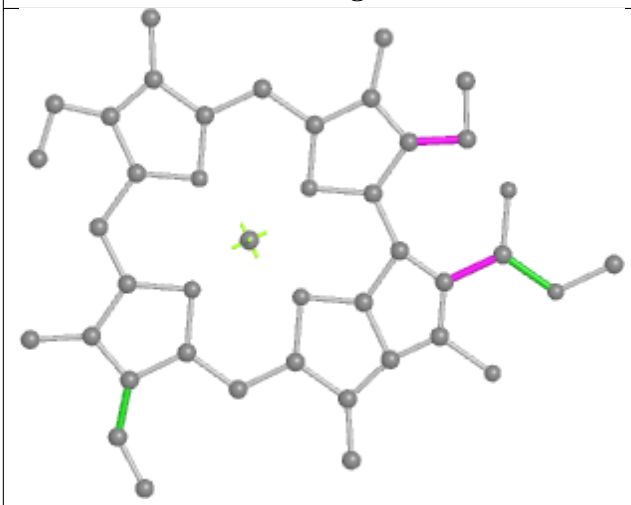


Bond angles



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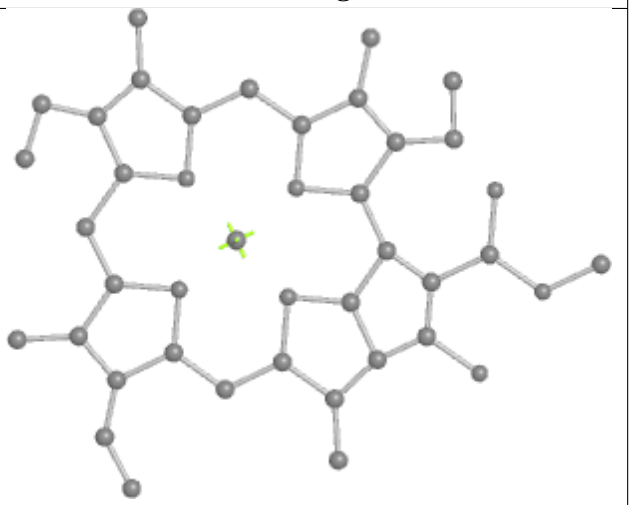
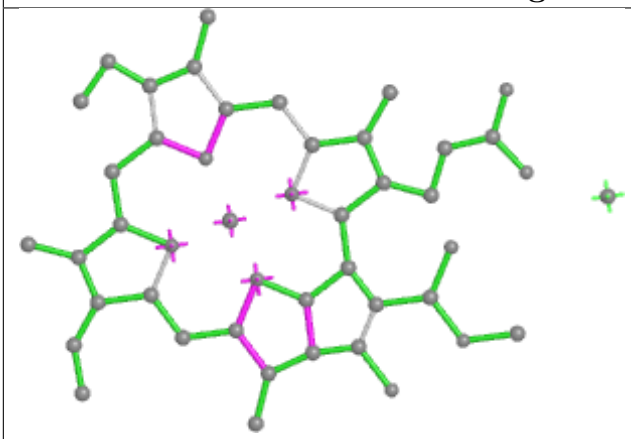
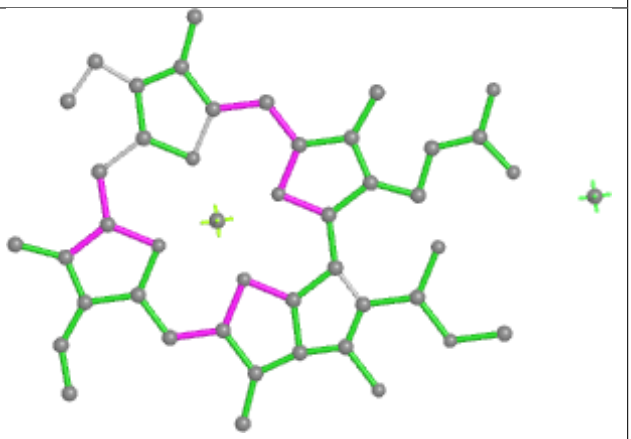
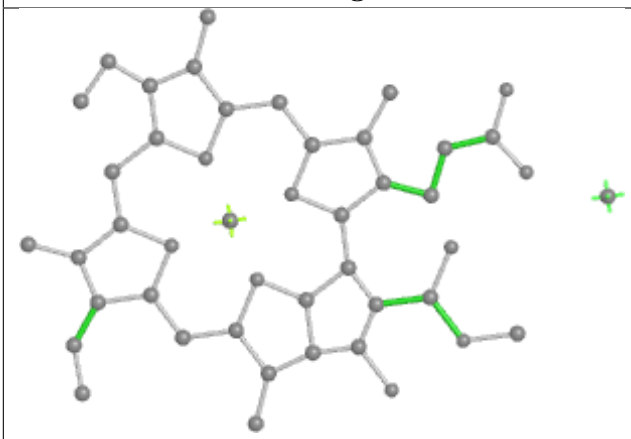
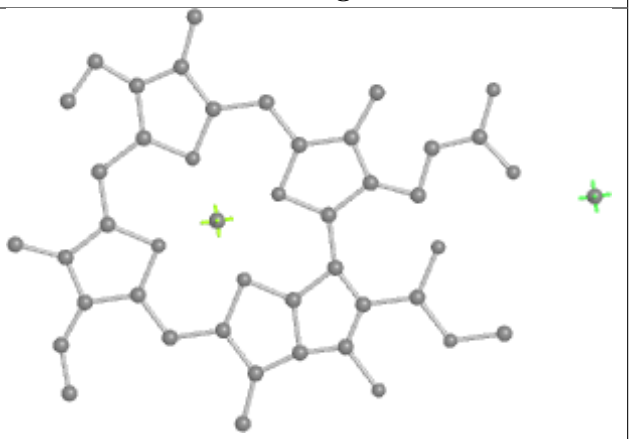
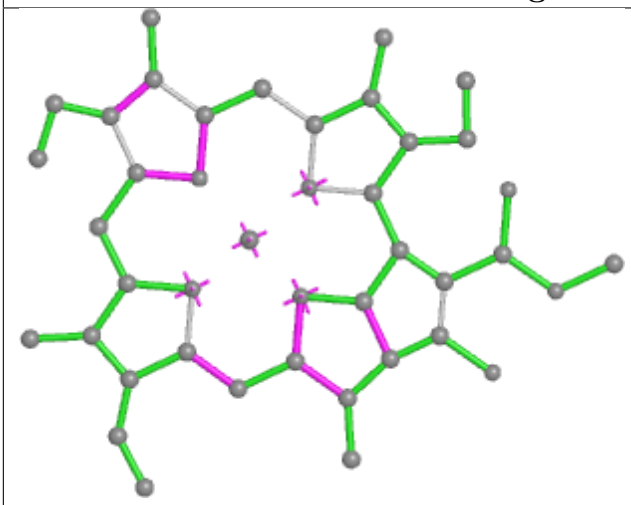


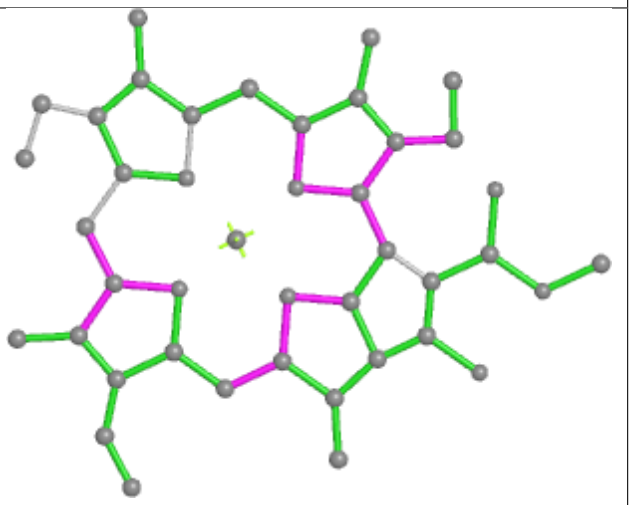
Rings

Ligand CLA 3 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

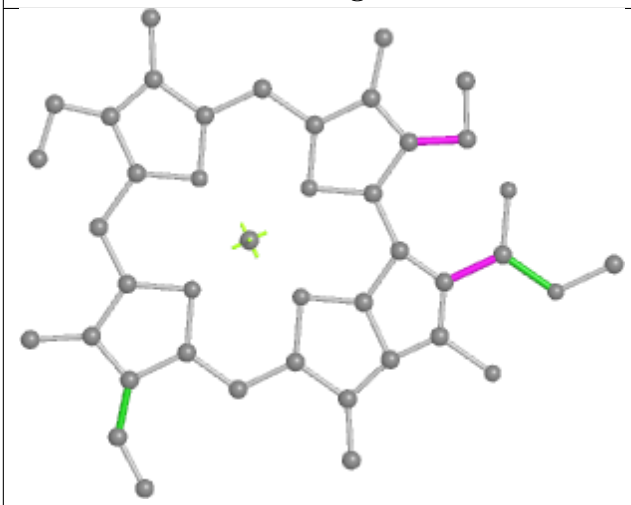
Ligand CLA 3 302



Bond lengths



Bond angles



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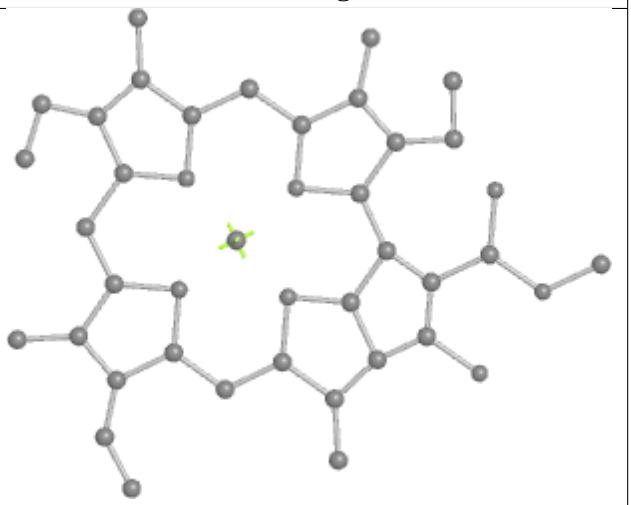
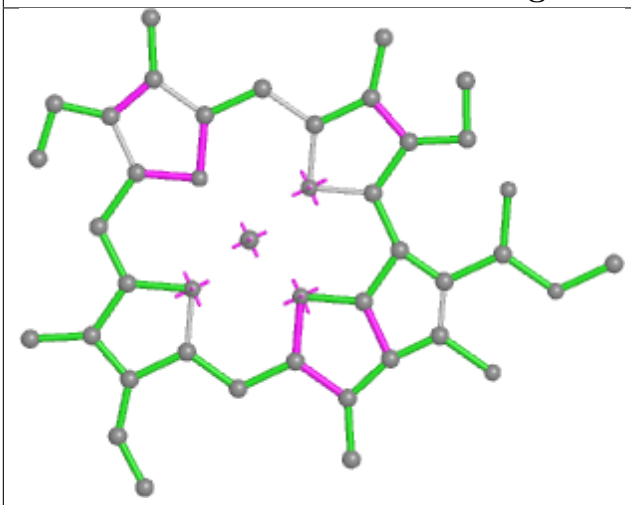


Rings

Ligand CLA 5 309



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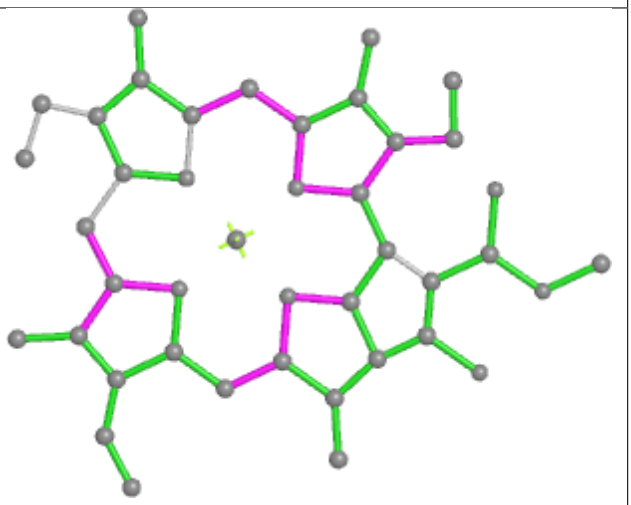
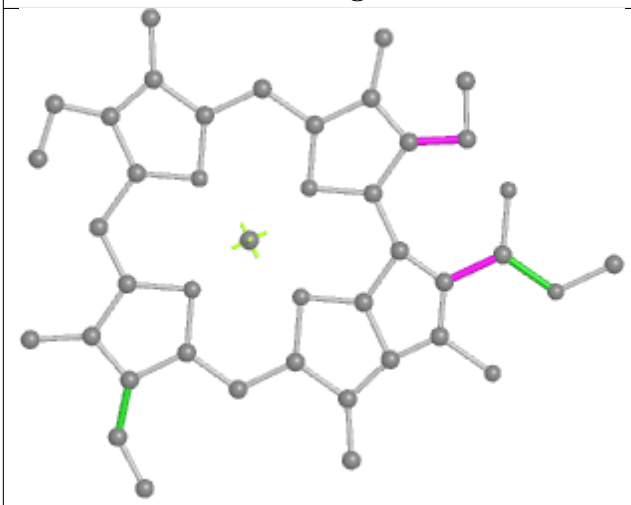


Bond angles



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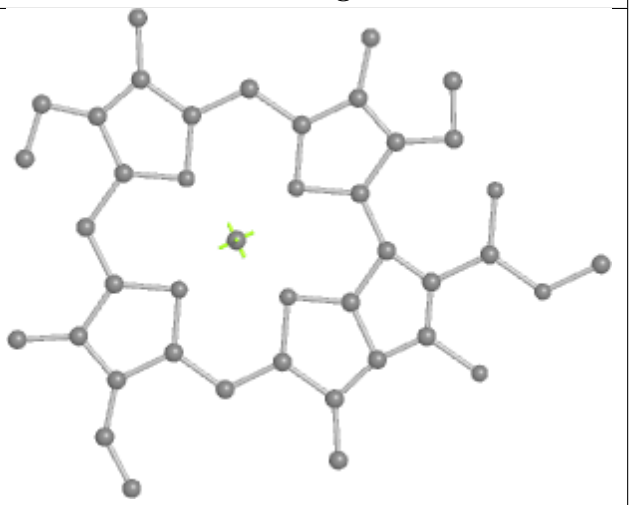
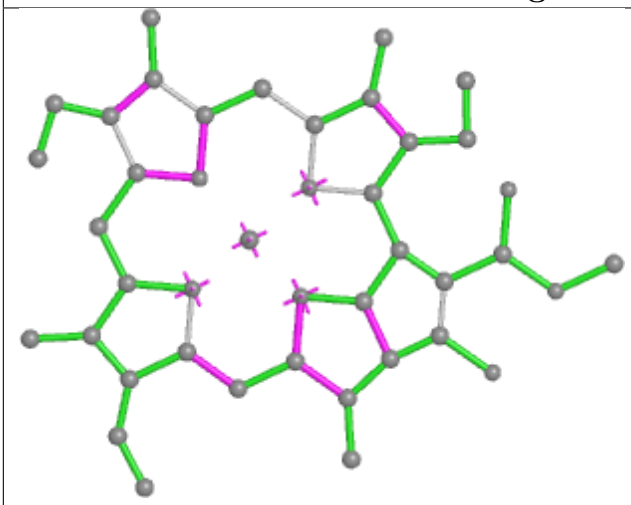
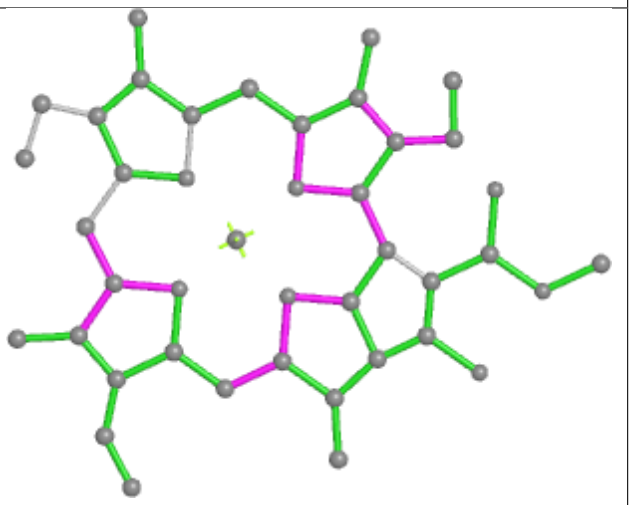


Rings

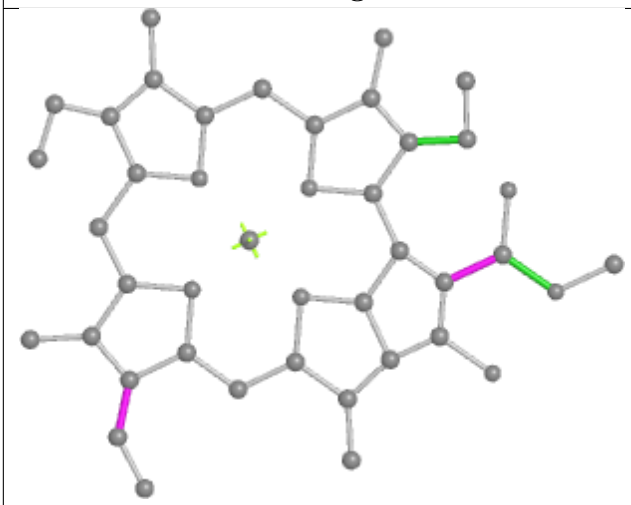
Ligand CLA 8 607



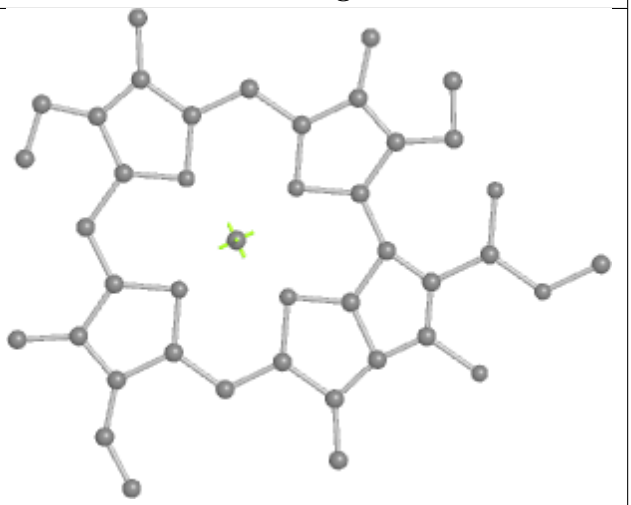
Bond lengths



Bond angles

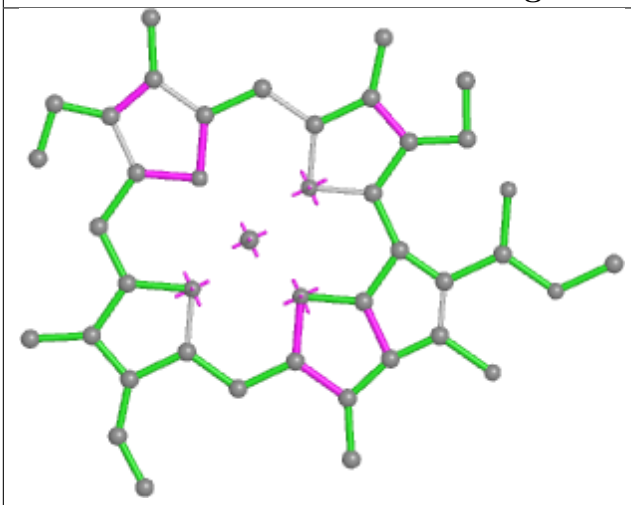


Torsions



Rings

Ligand CLA B 806



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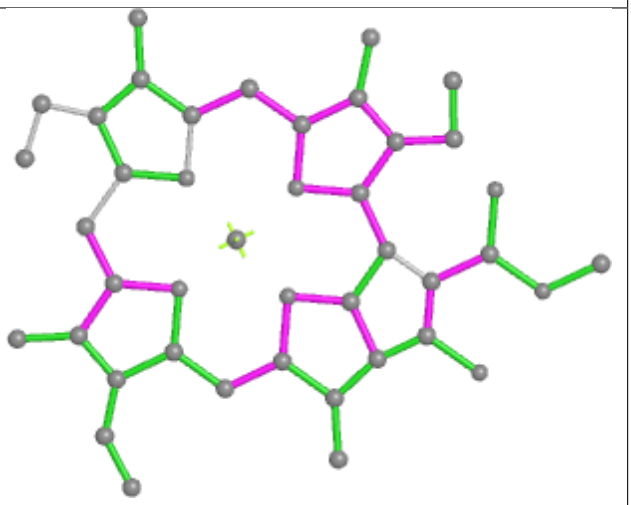

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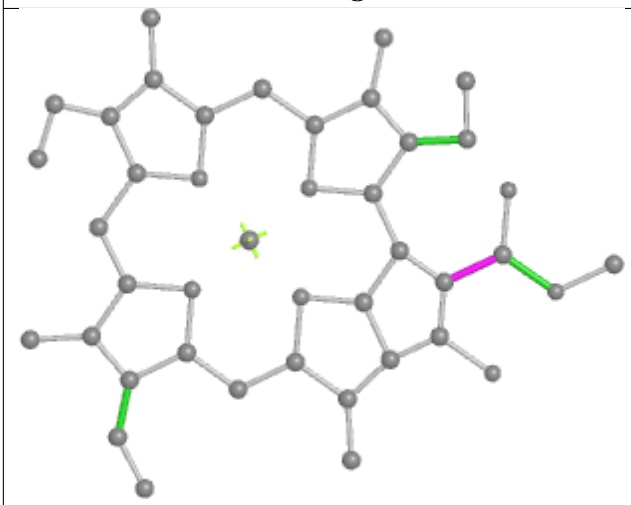
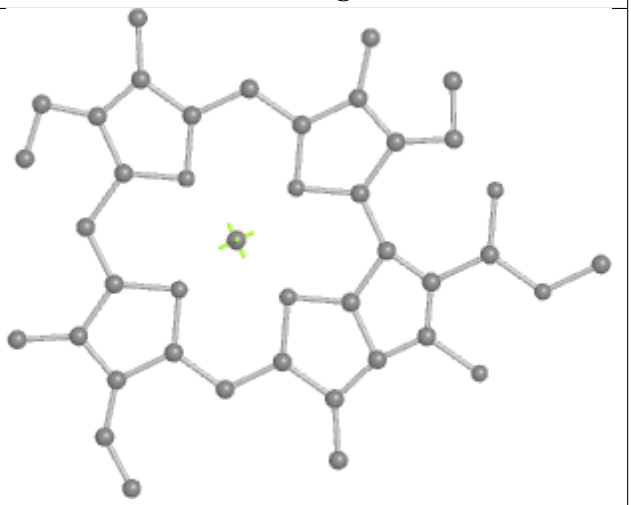
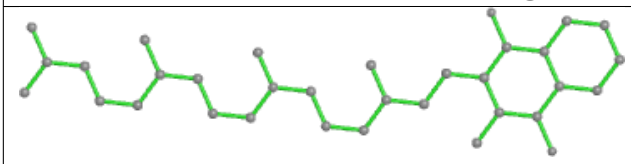


Torsions



Rings

Ligand PQN A 840



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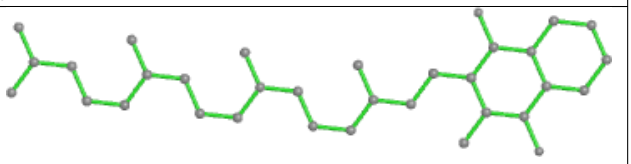

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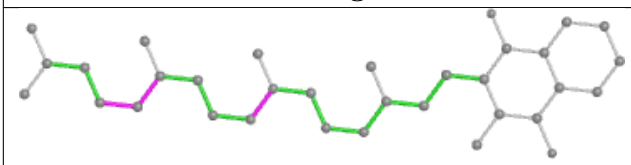
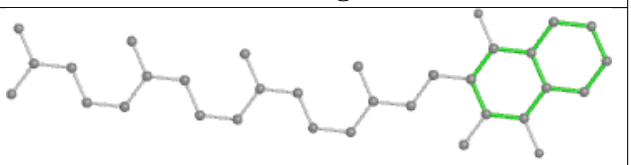
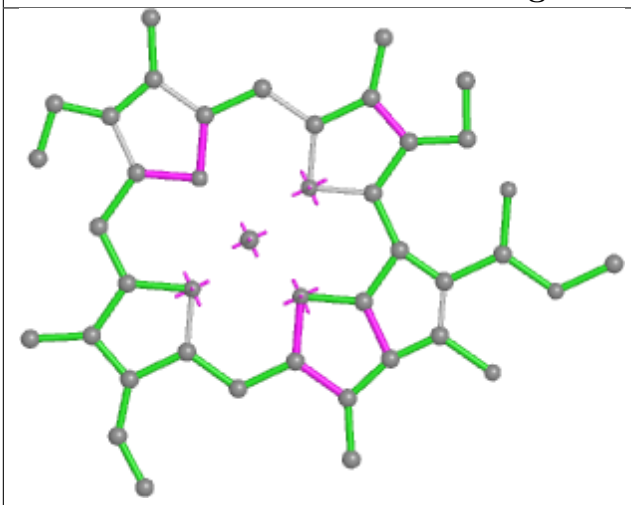


Torsions



Rings

Ligand CLA 7 603



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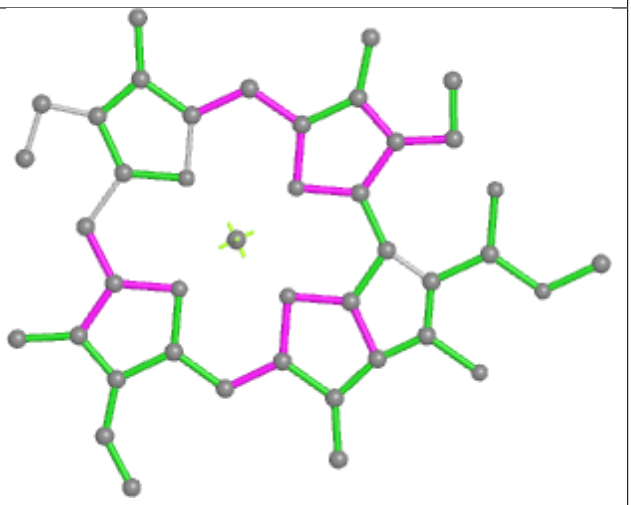

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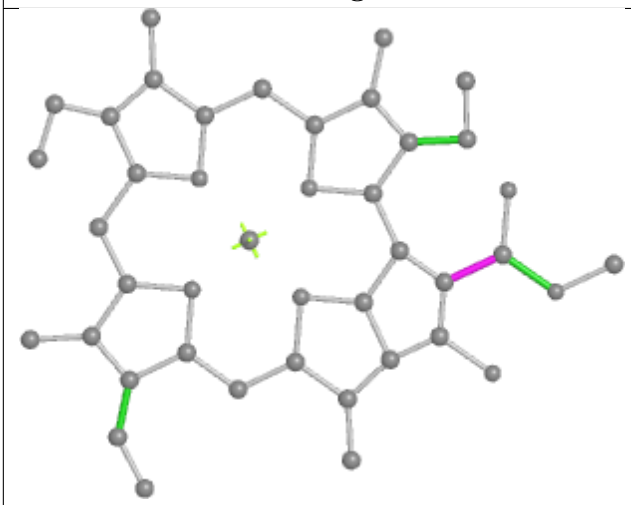

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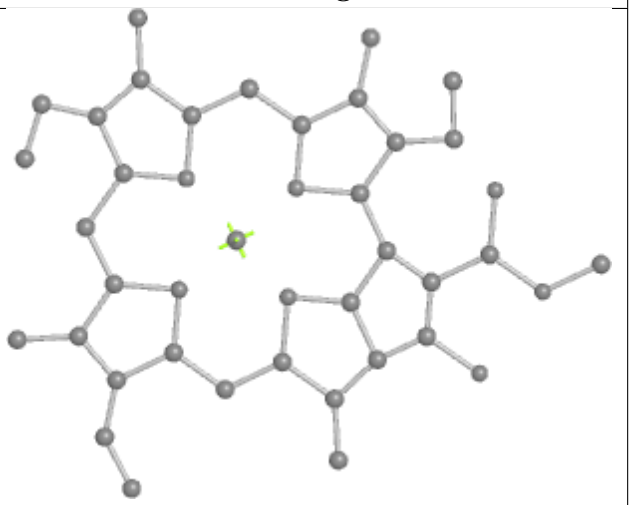
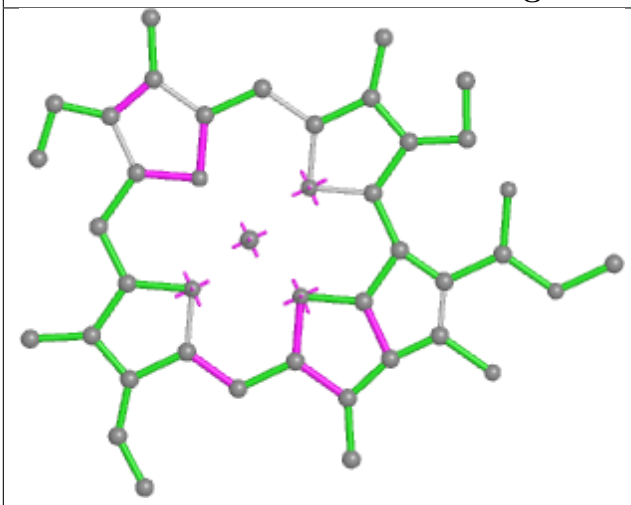


Rings

Ligand CLA A 814



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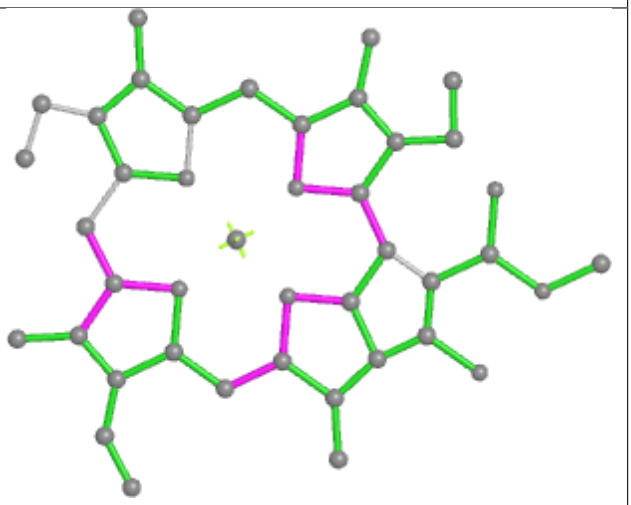

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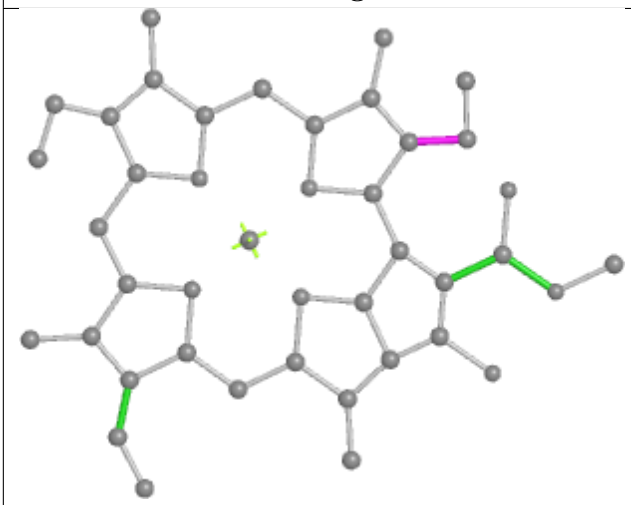

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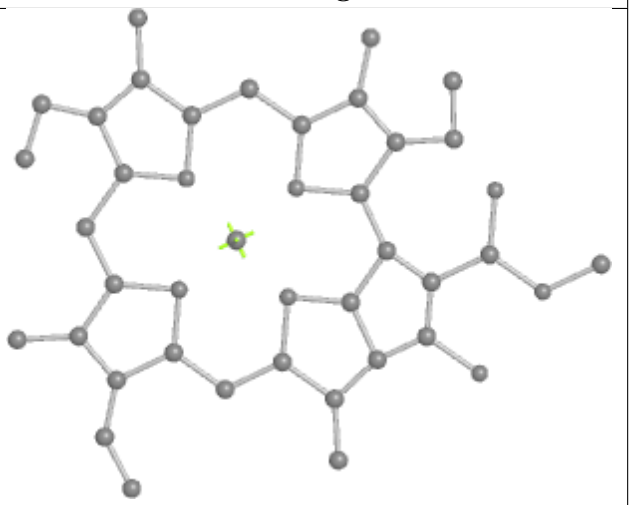
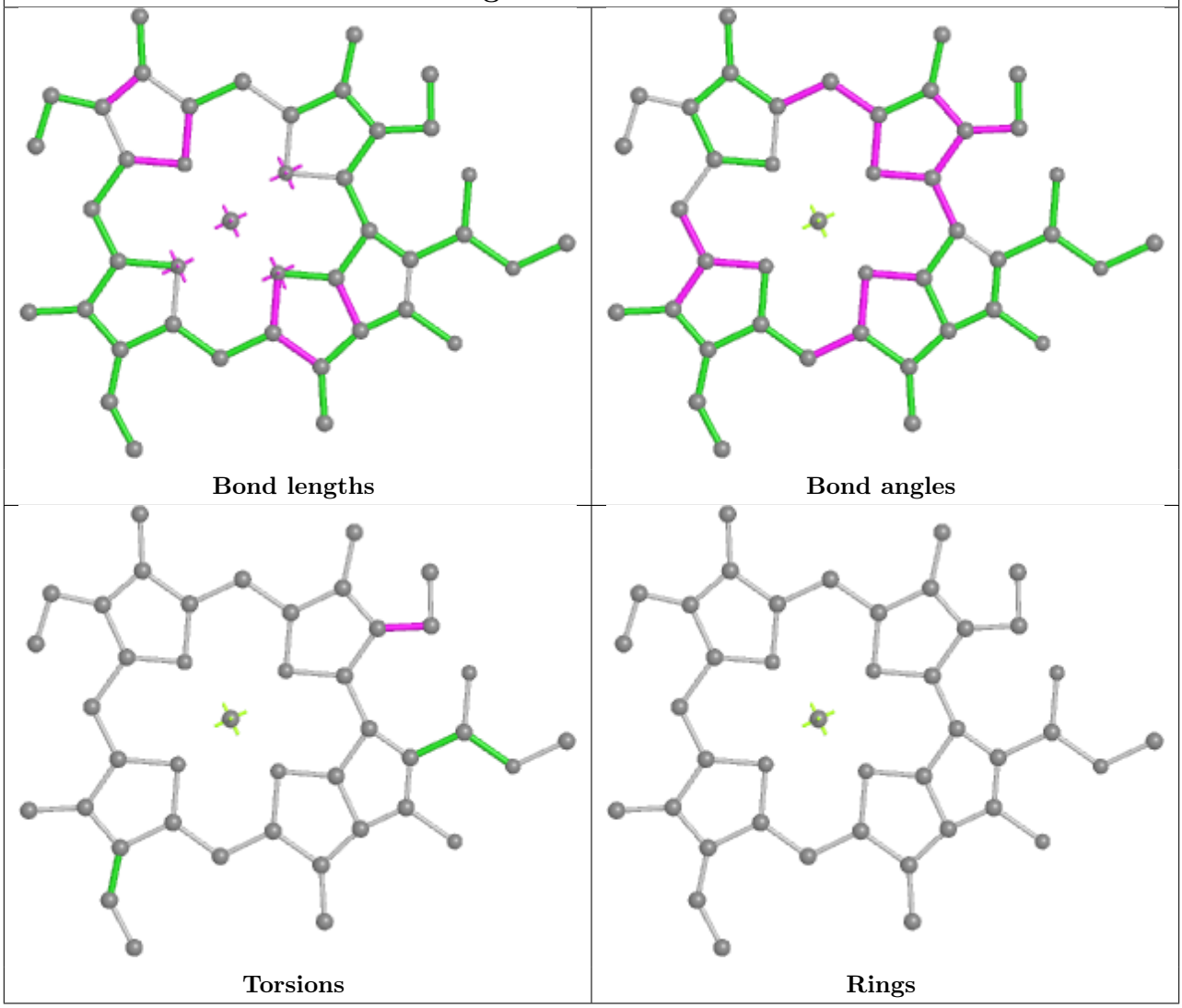
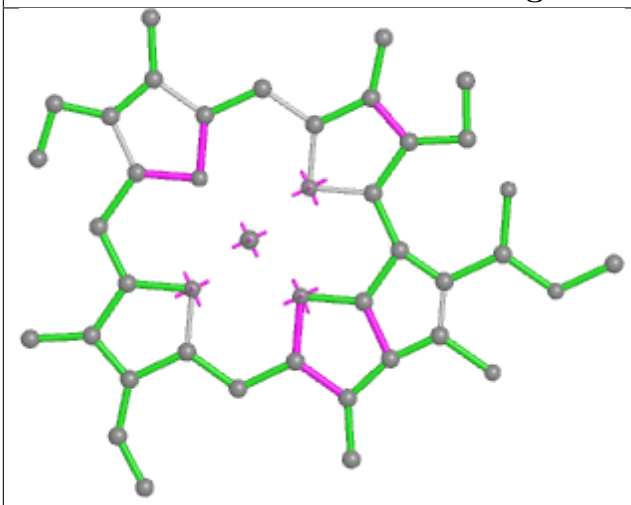


Rings

Ligand CLA A 817



Ligand CLA F 301



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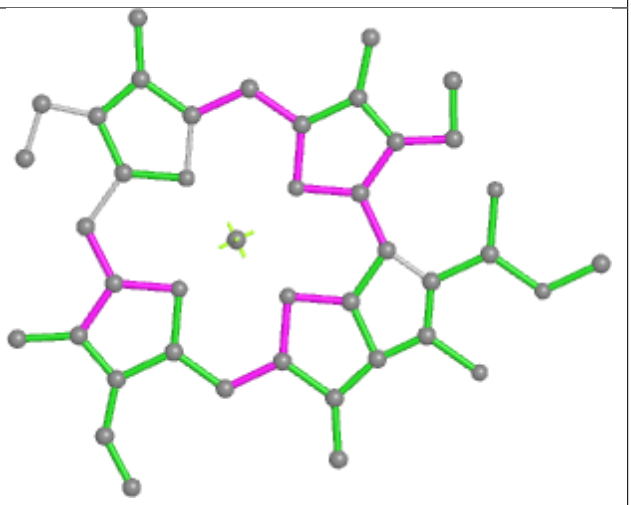

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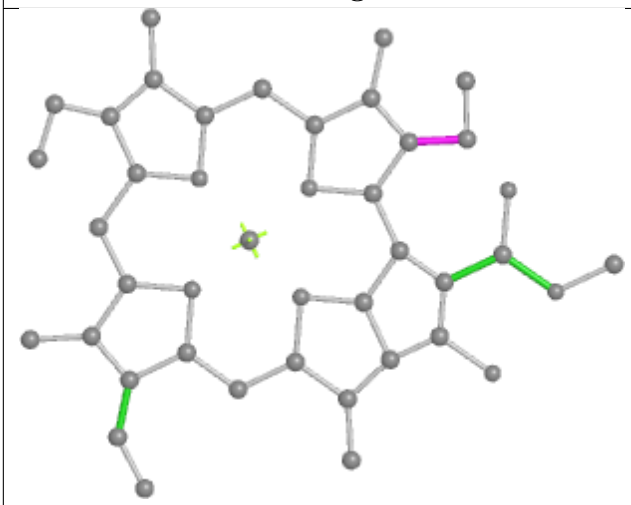

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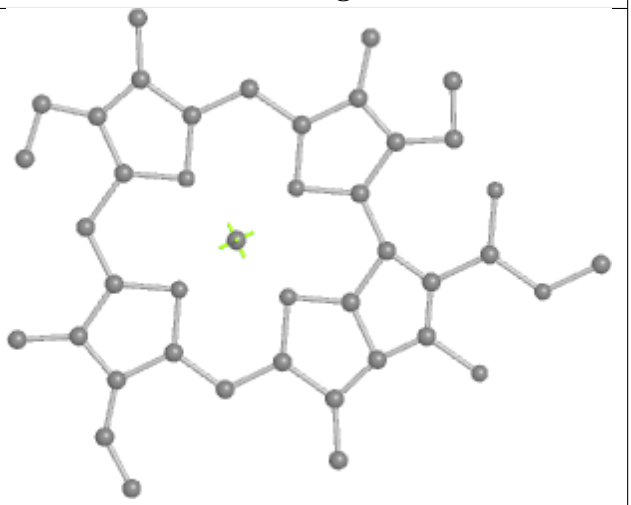
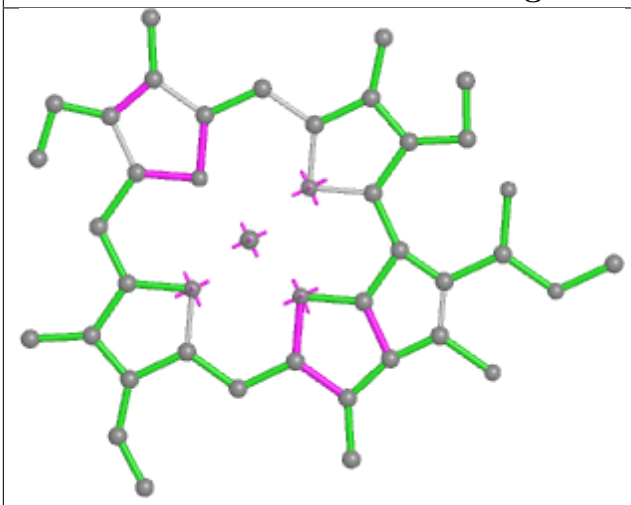


Rings

Ligand CLA B 833



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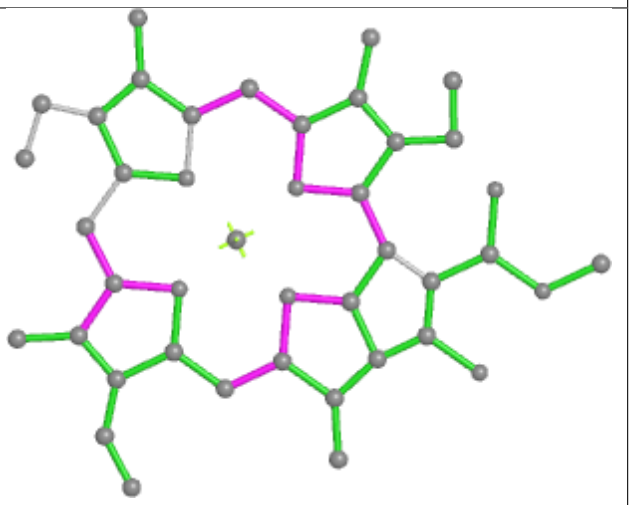

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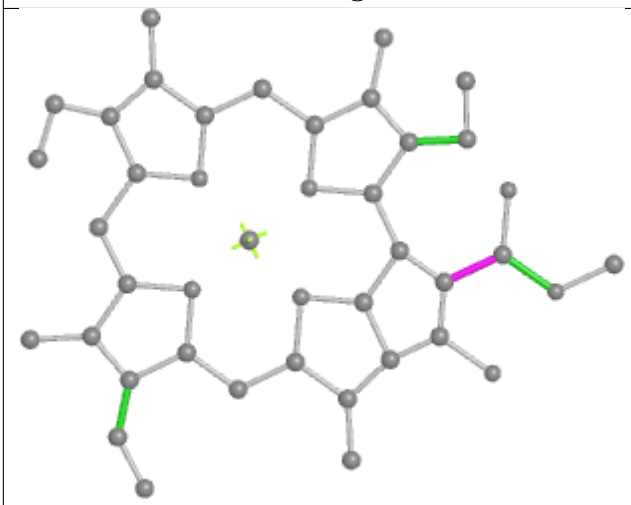

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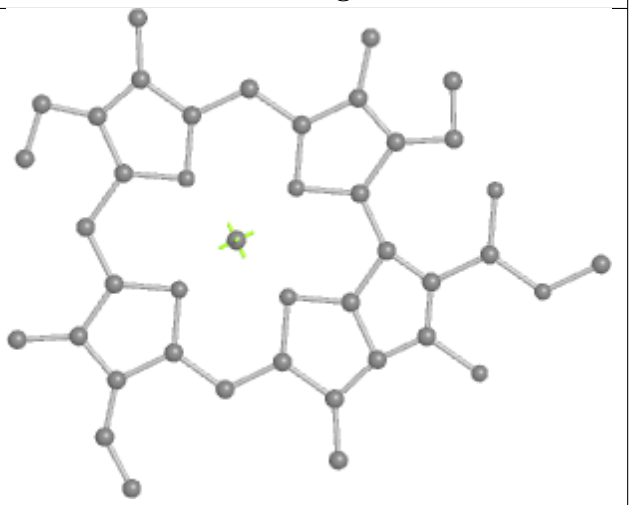
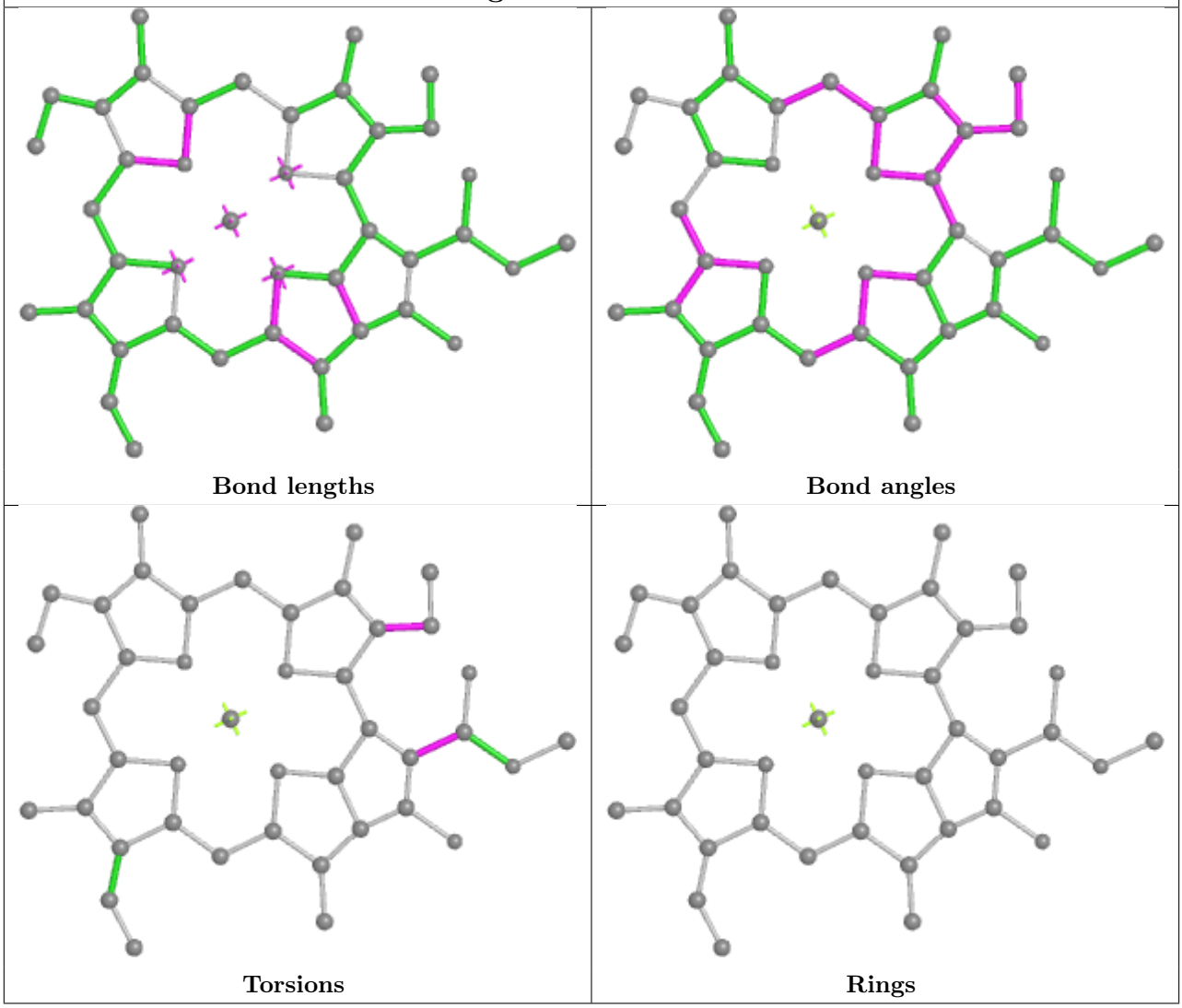


Rings

Ligand CLA 1 607



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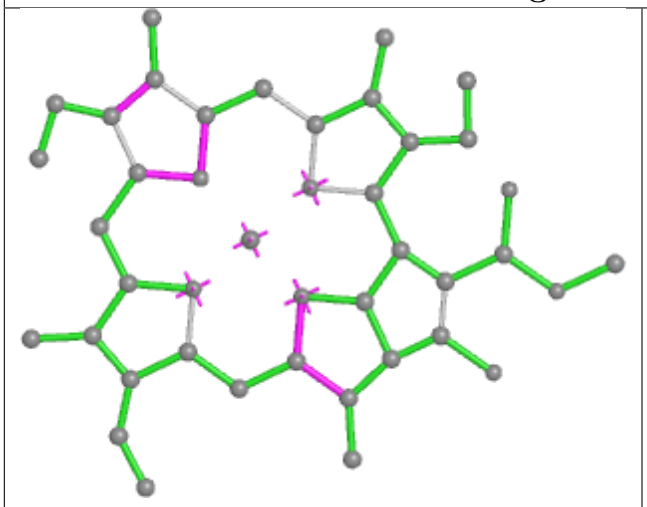

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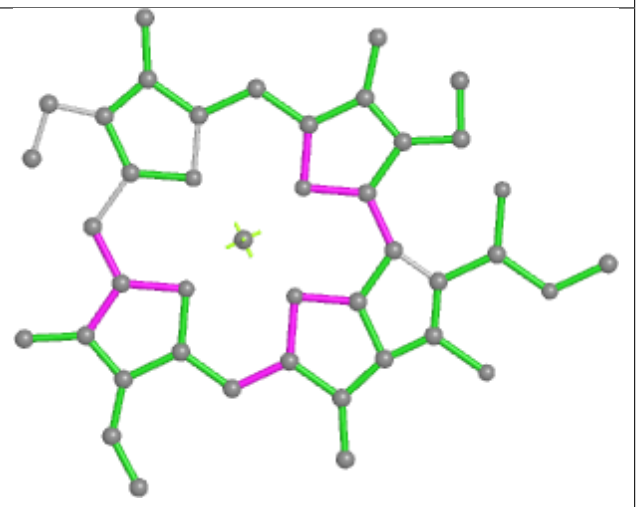
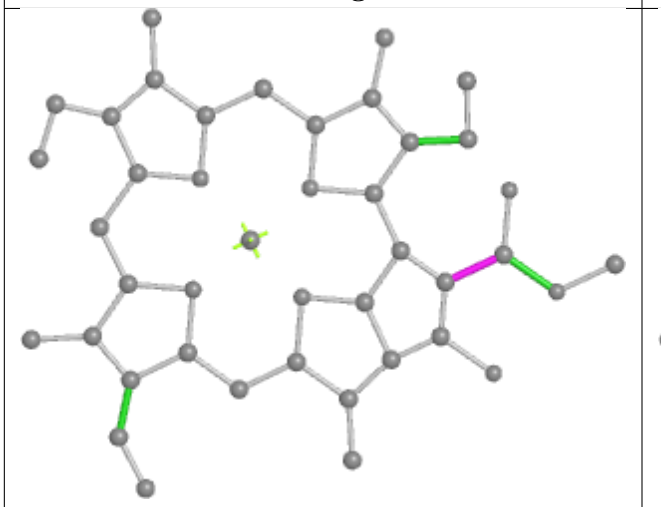


Bond angles



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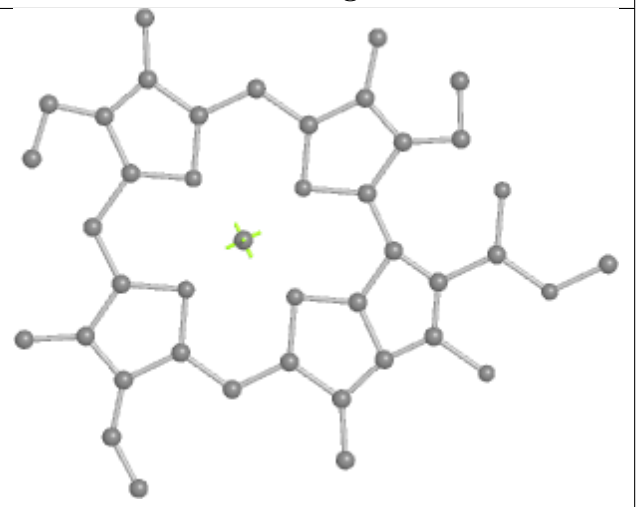
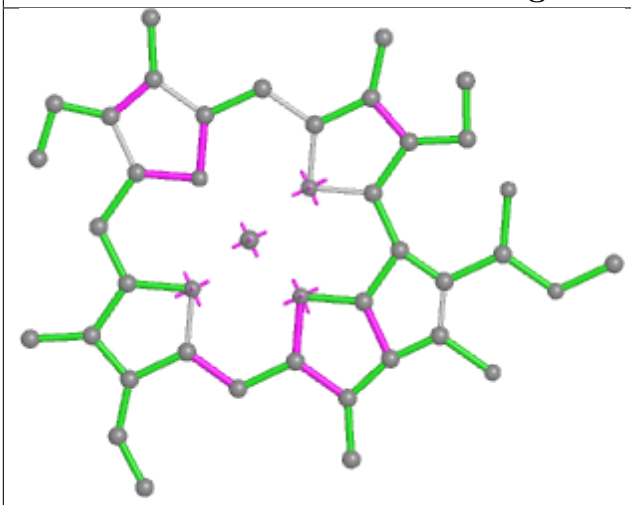
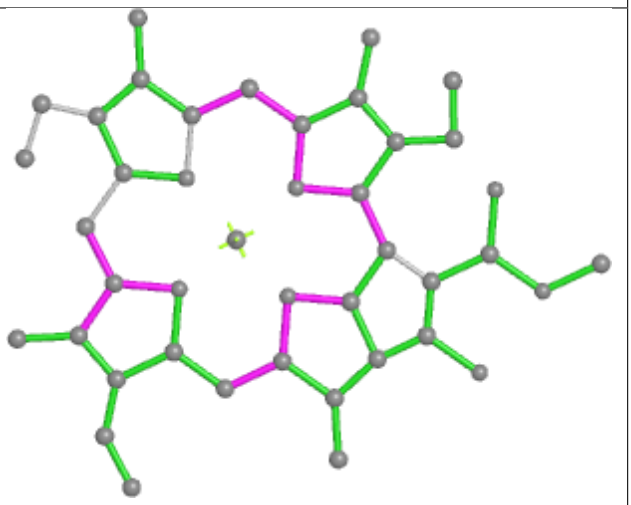


Rings

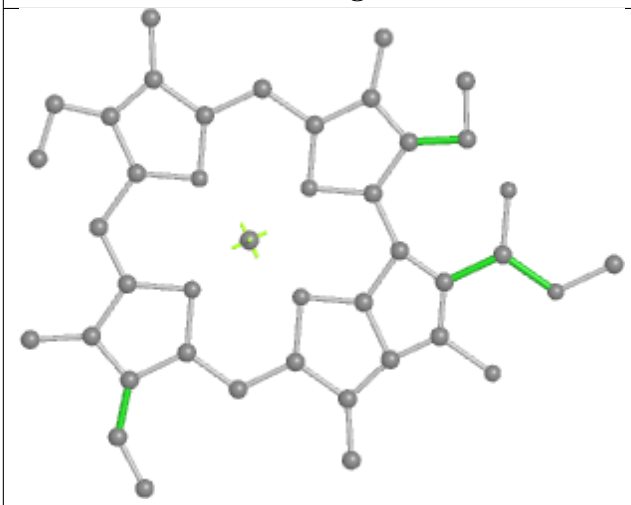
Ligand CLA 5 310



Bond lengths



Bond angles



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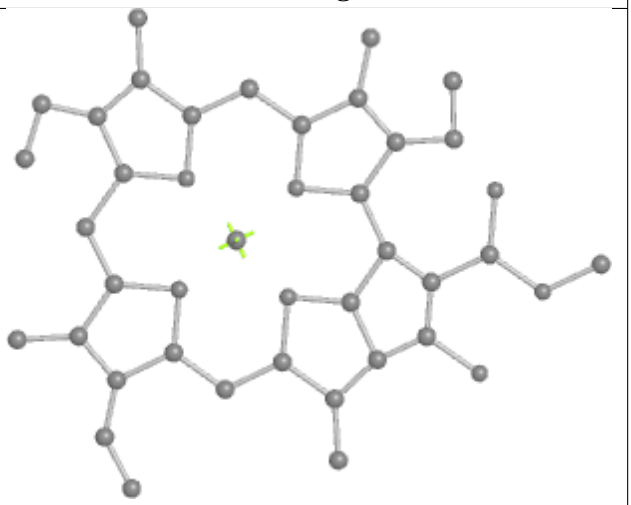
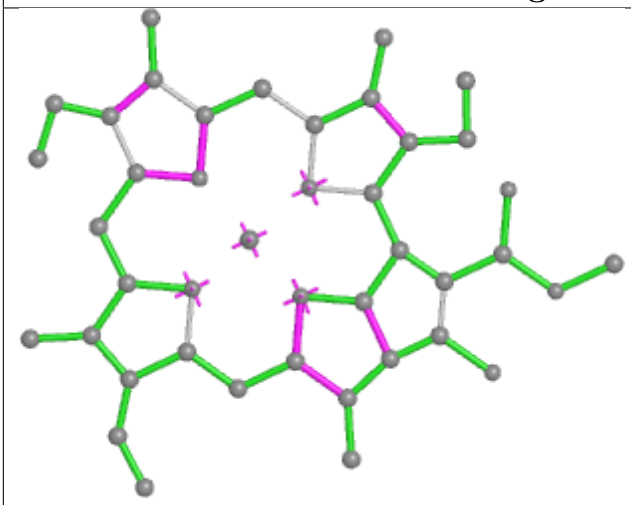


Rings

Ligand CLA 8 611



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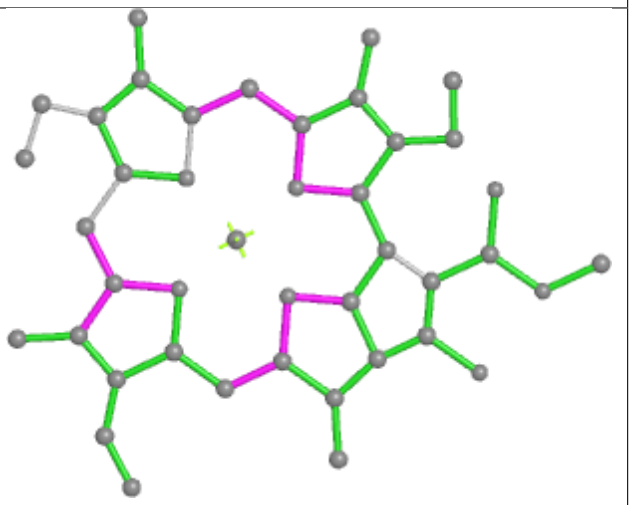
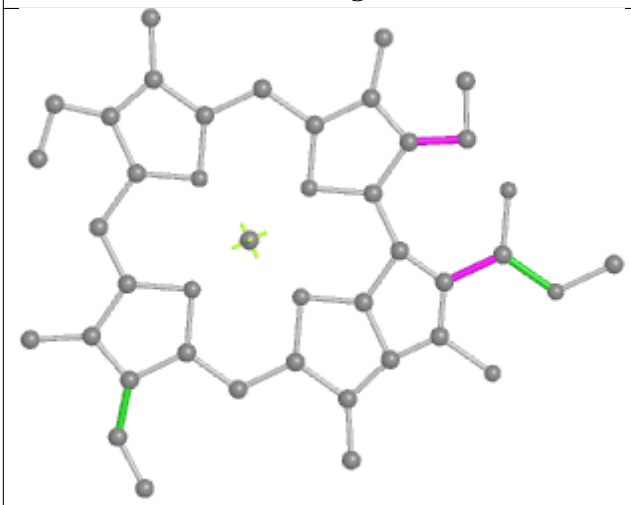


Bond angles



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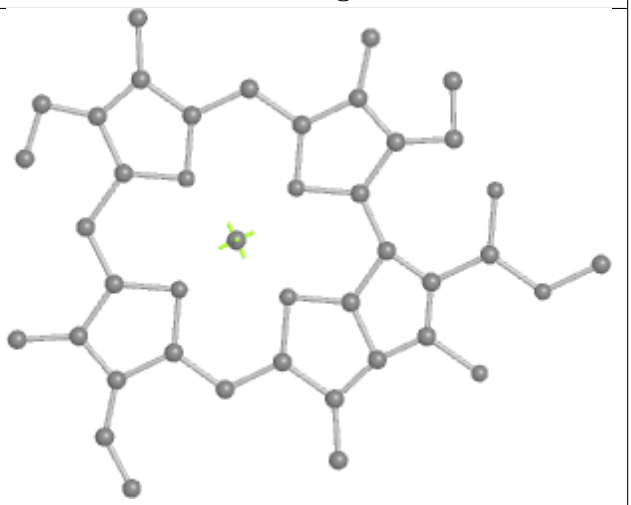
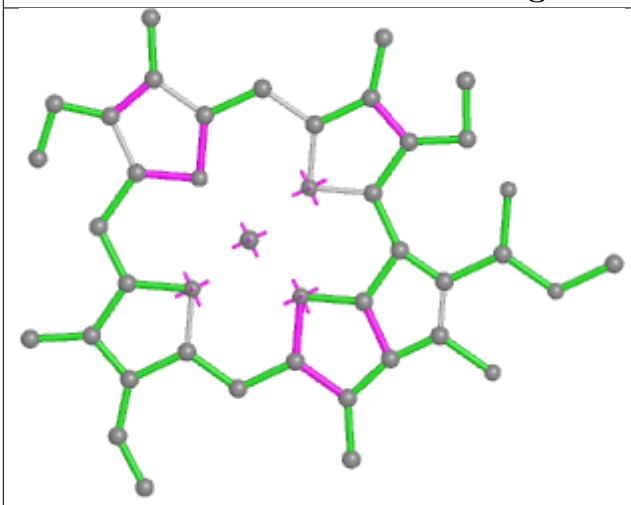


Rings

Ligand CLA 8 613



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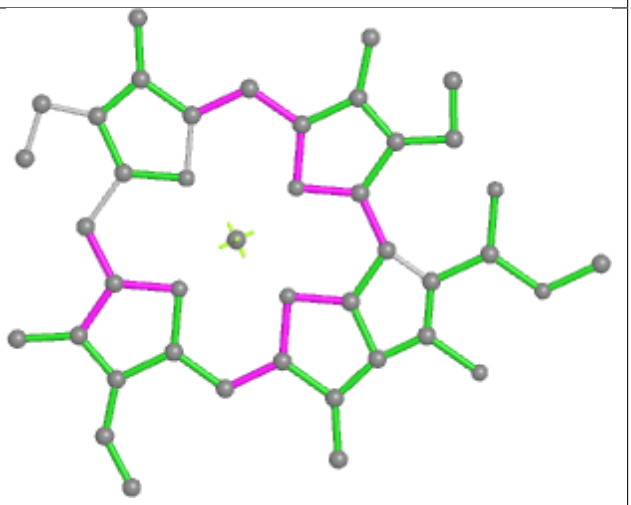

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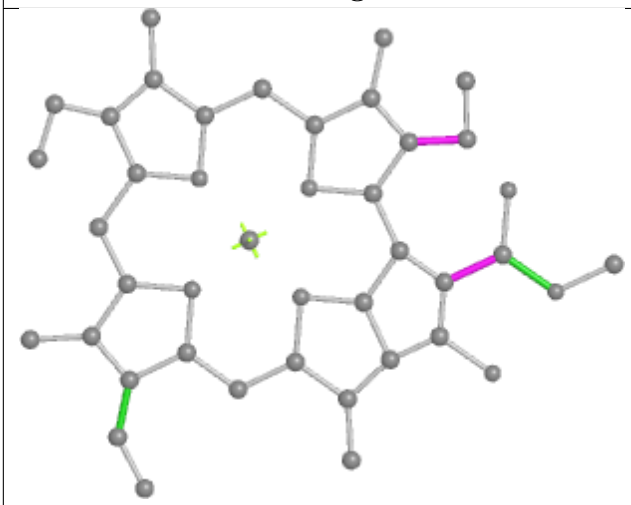

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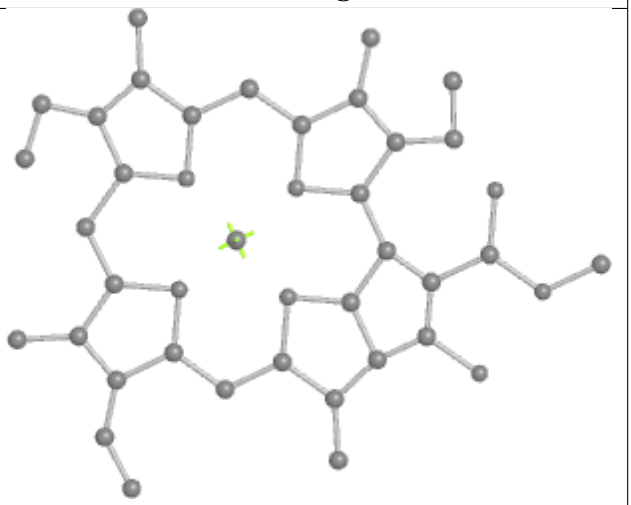
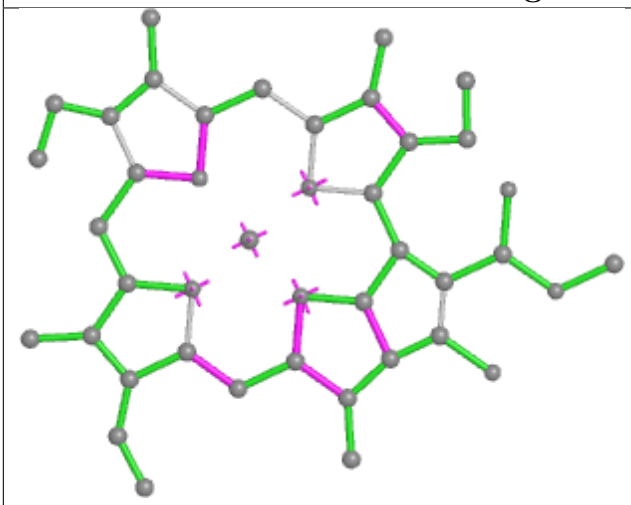


Rings

Ligand CLA B 823



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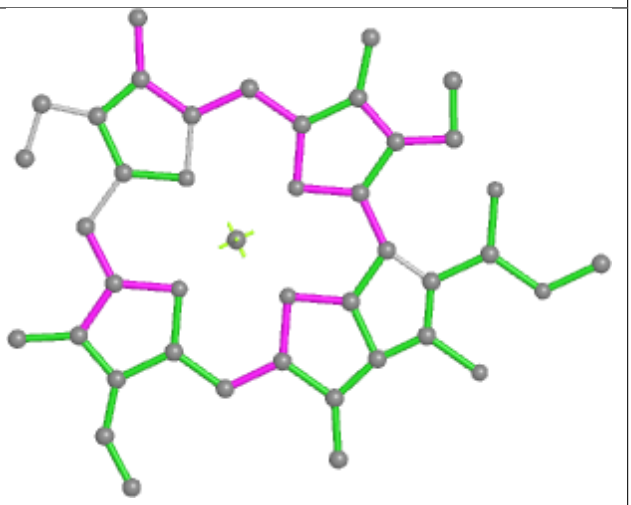
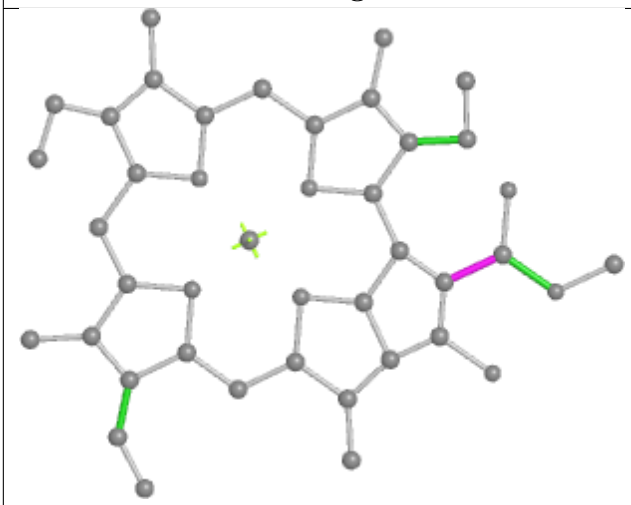


Bond angles



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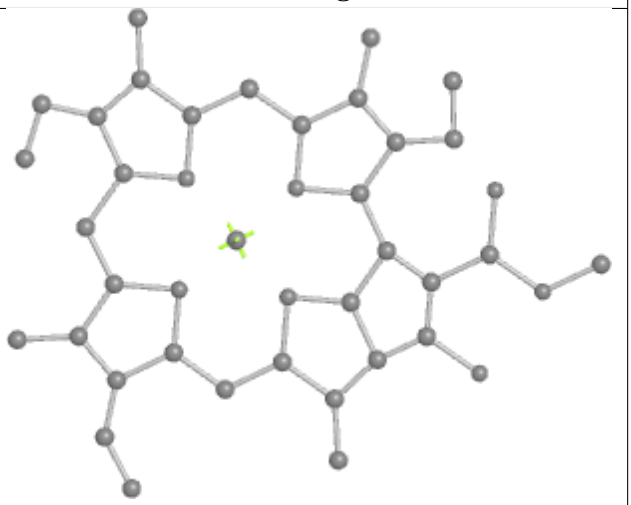
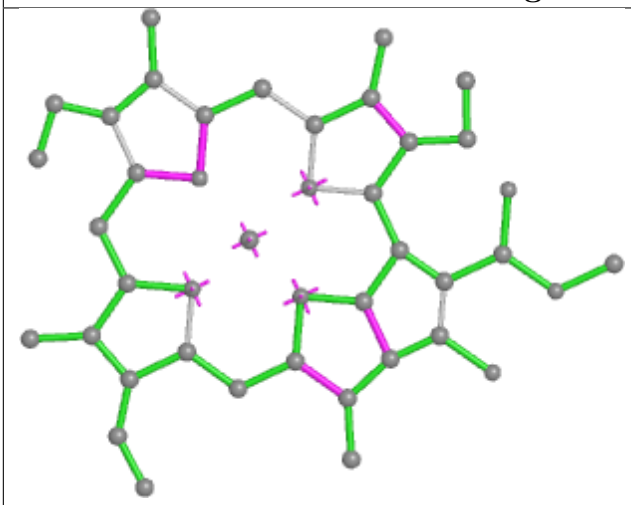


Rings

Ligand CLA B 801



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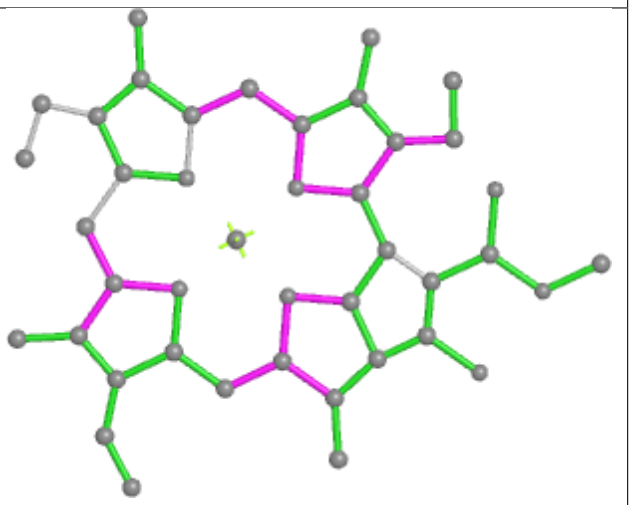
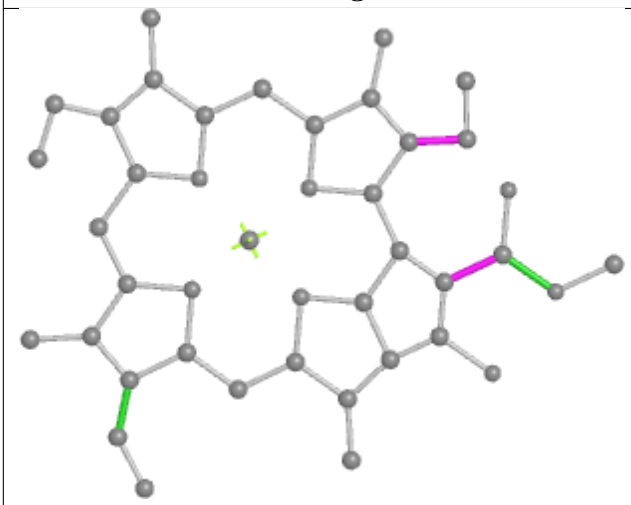


Bond angles



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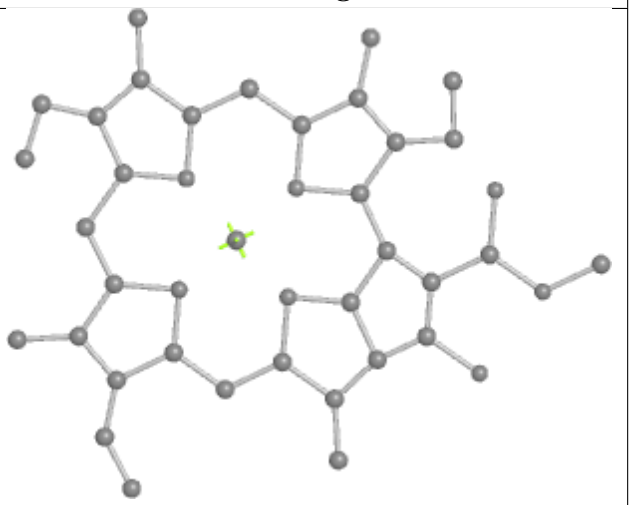
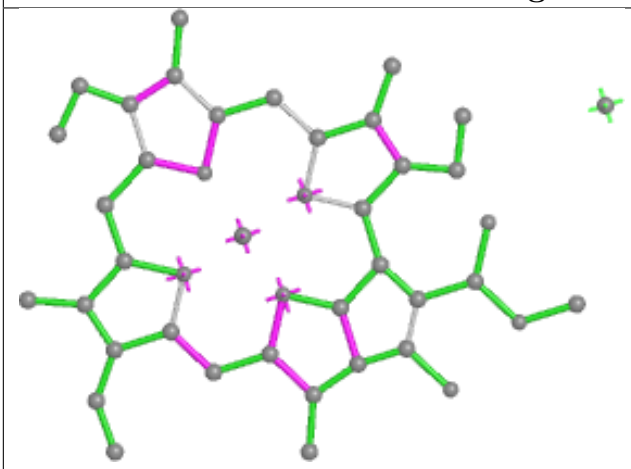
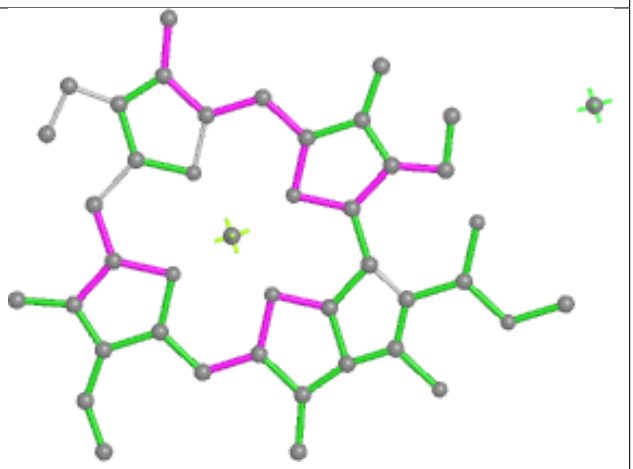
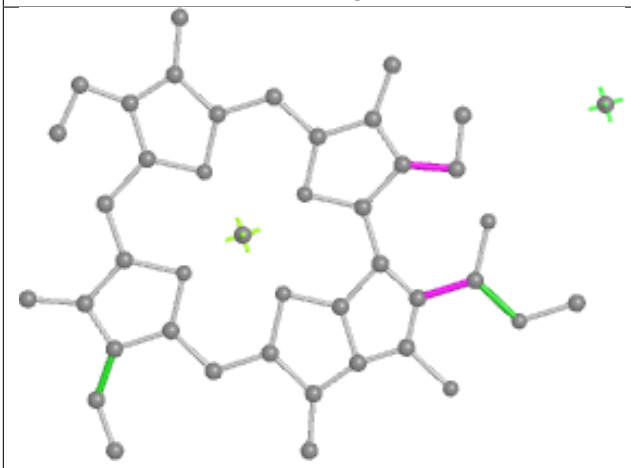
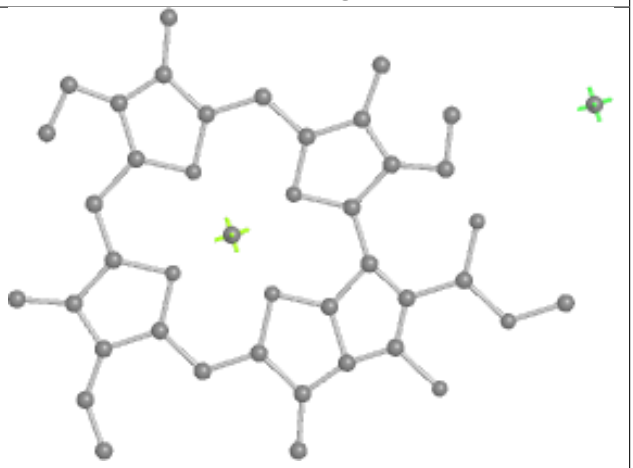
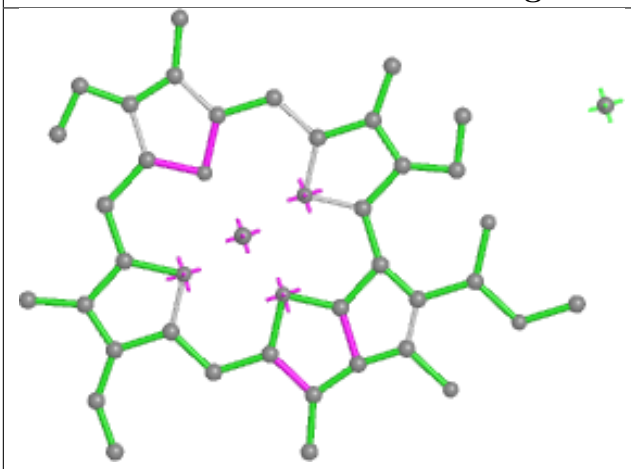
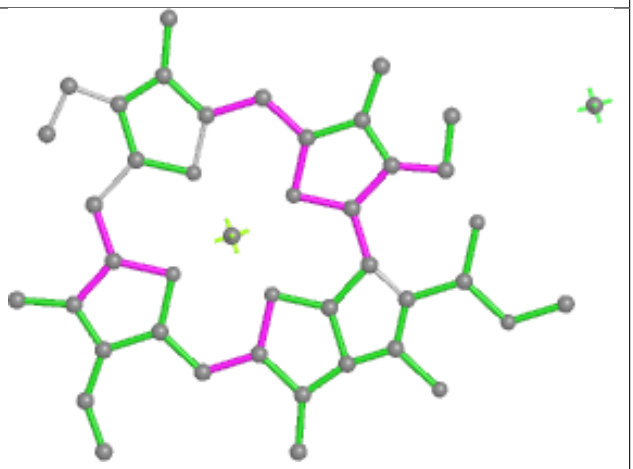
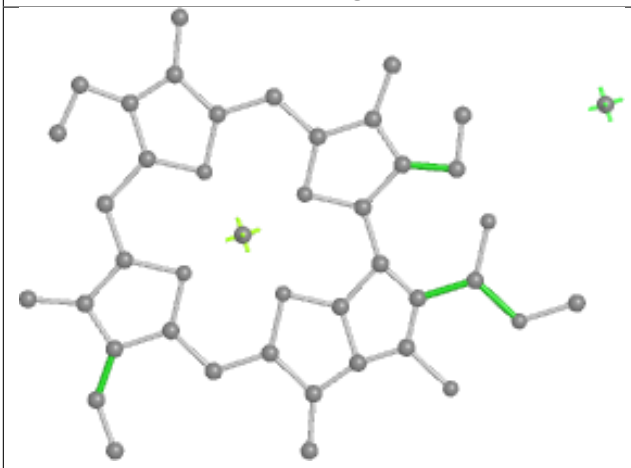
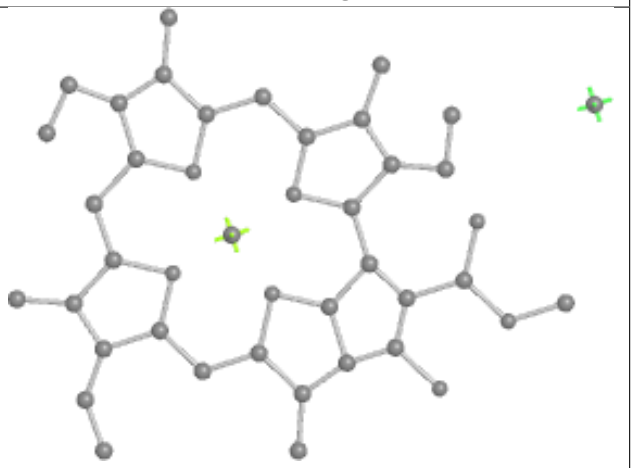
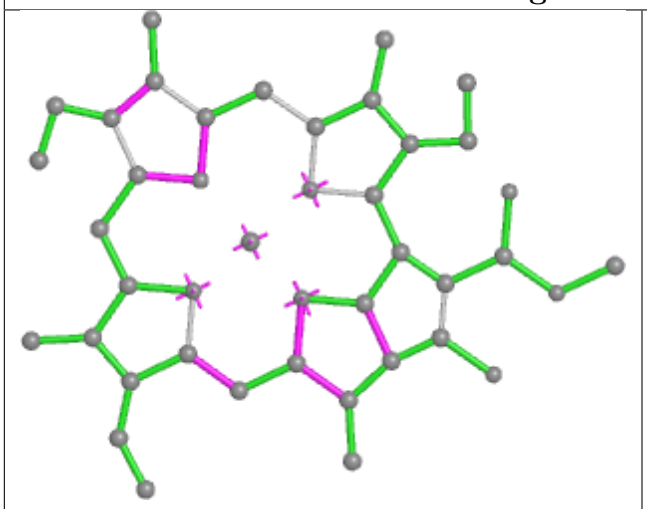


Rings

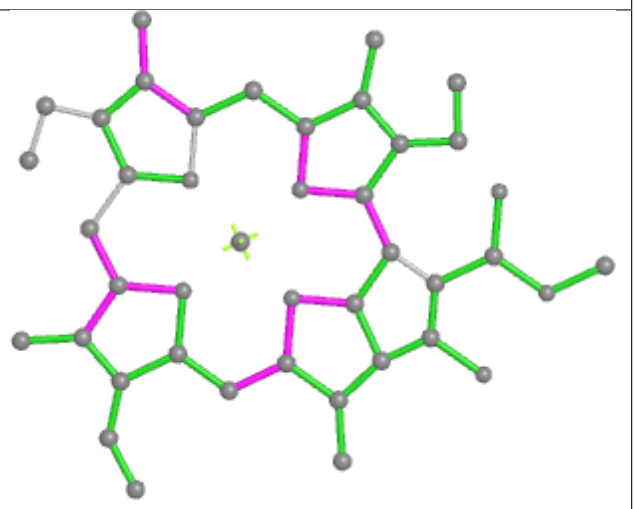
Ligand CLA J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 302



Bond lengths



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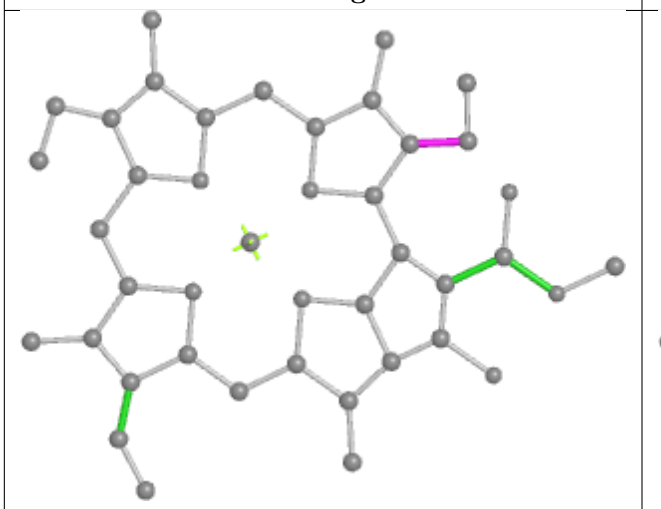

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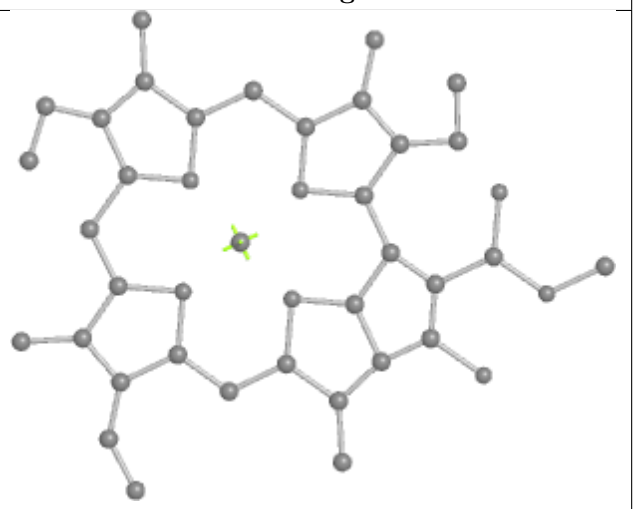

Rings

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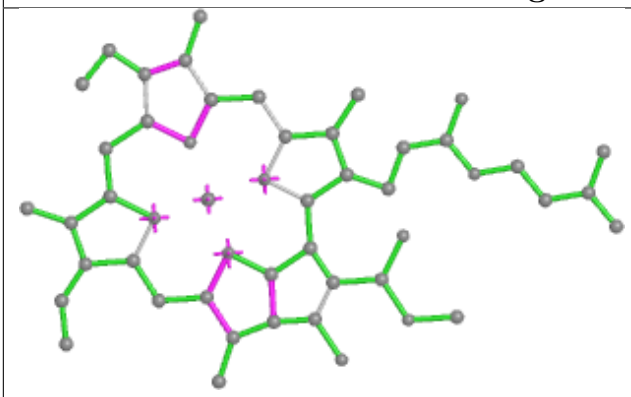
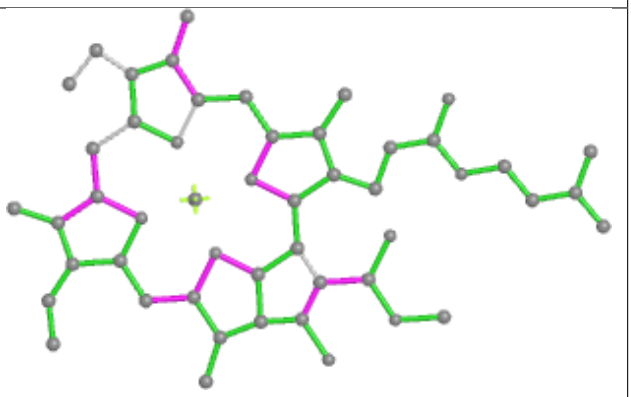
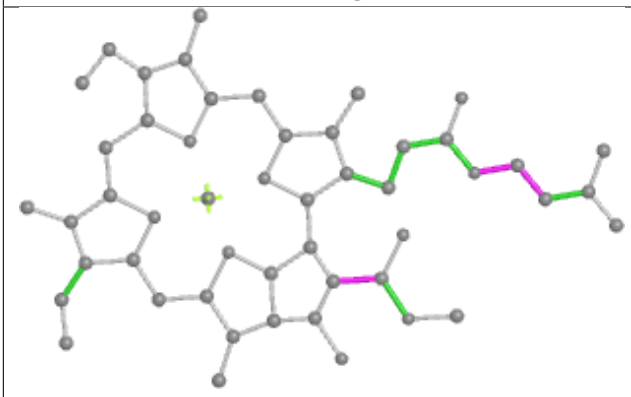
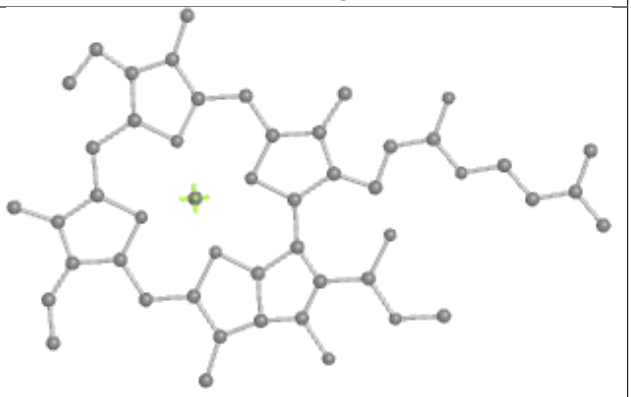
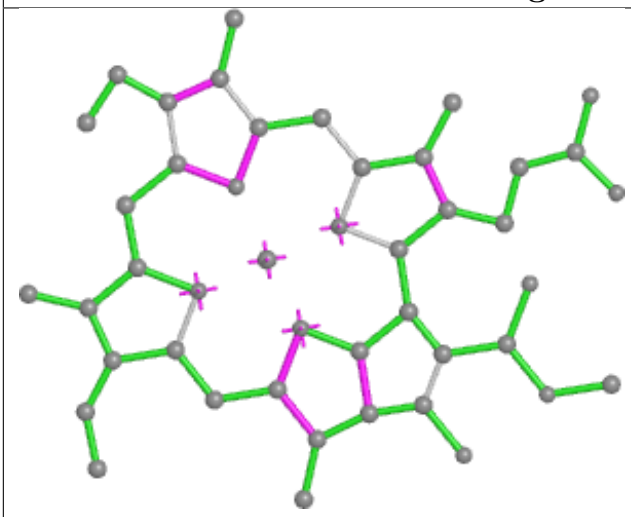
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 315



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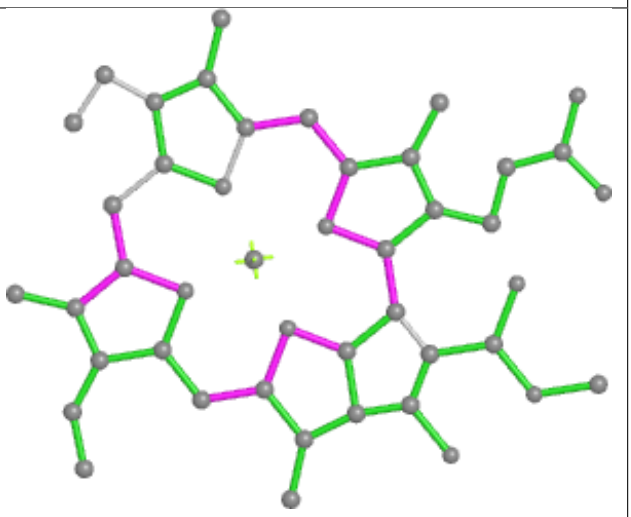

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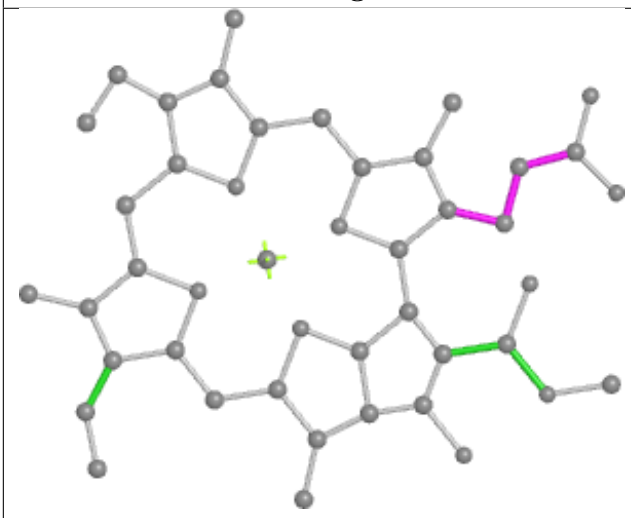

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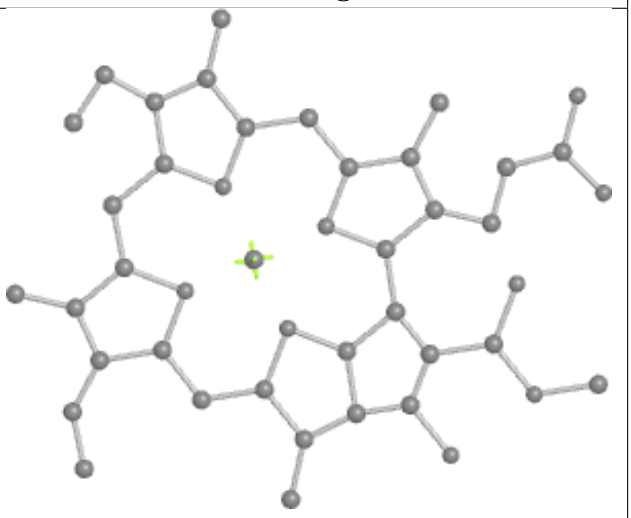
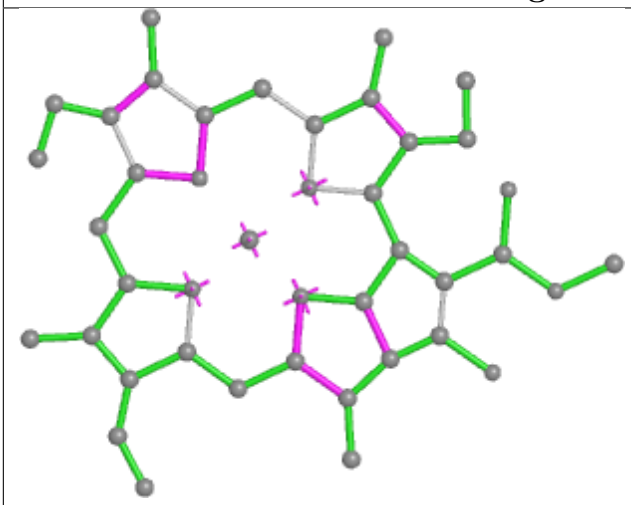


Rings

Ligand CLA 3 313



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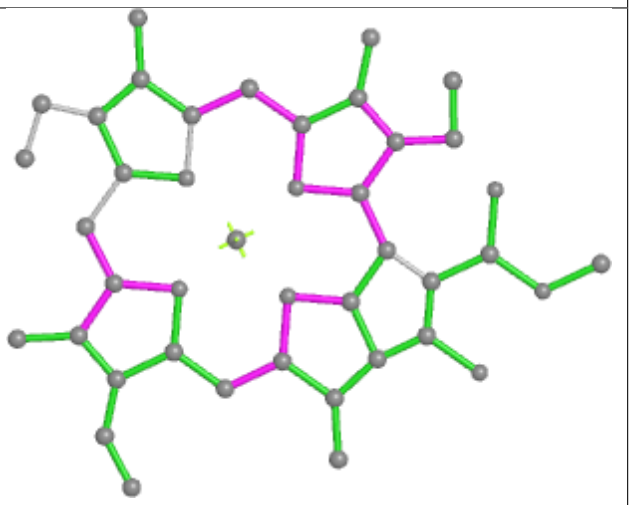

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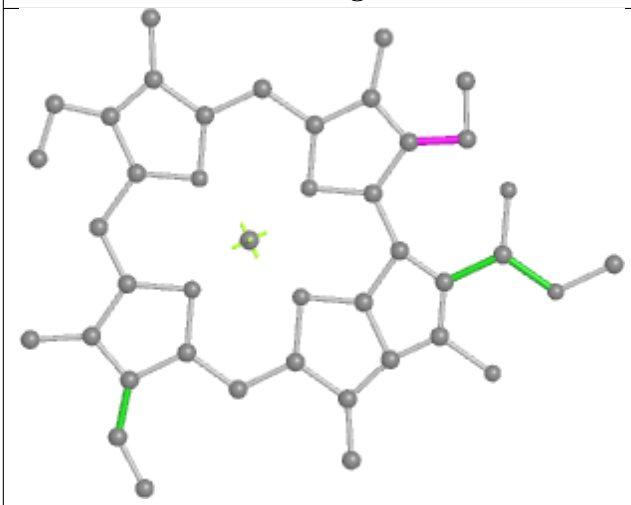

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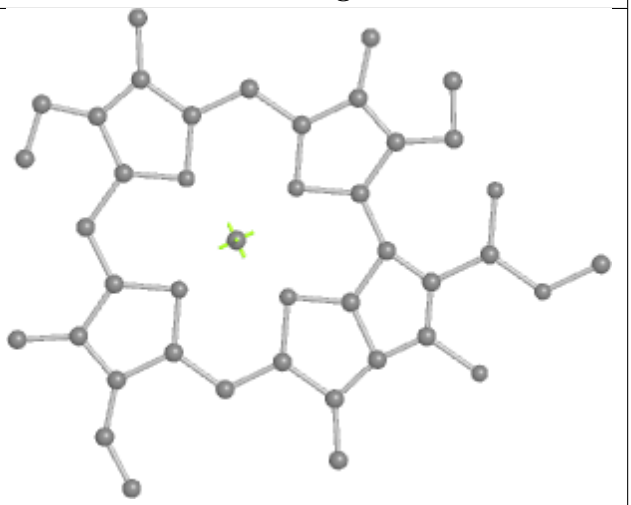
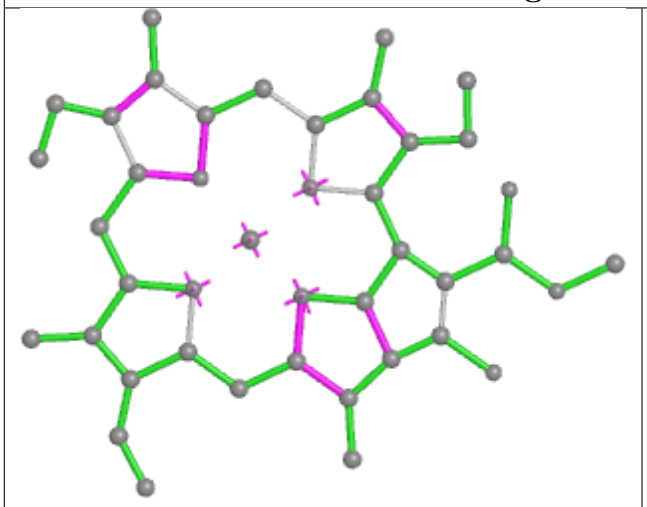


Rings

Ligand CLA A 824



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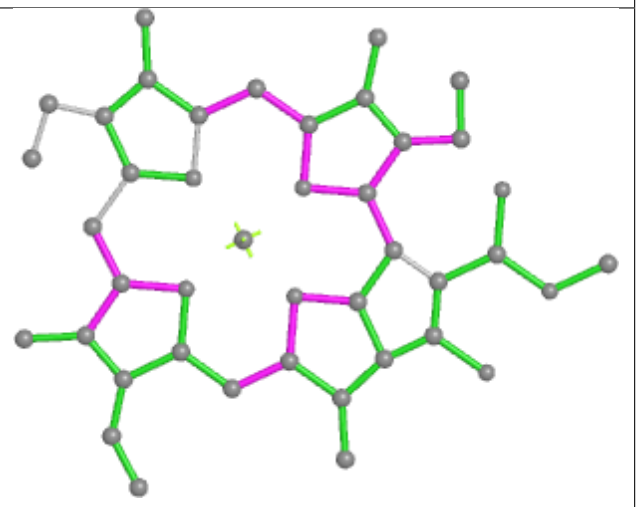

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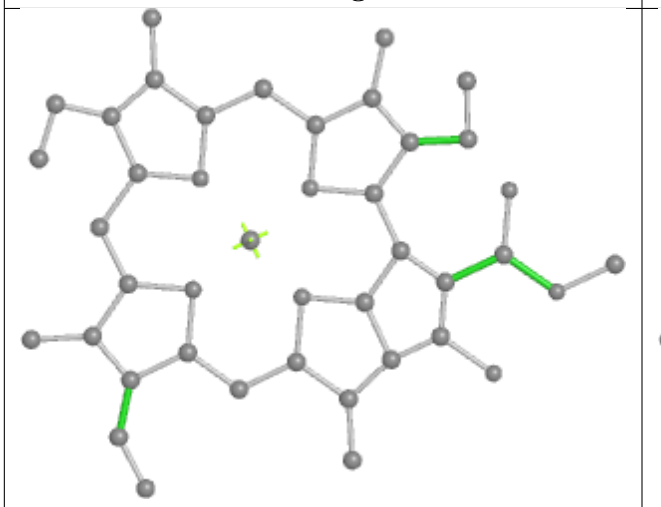

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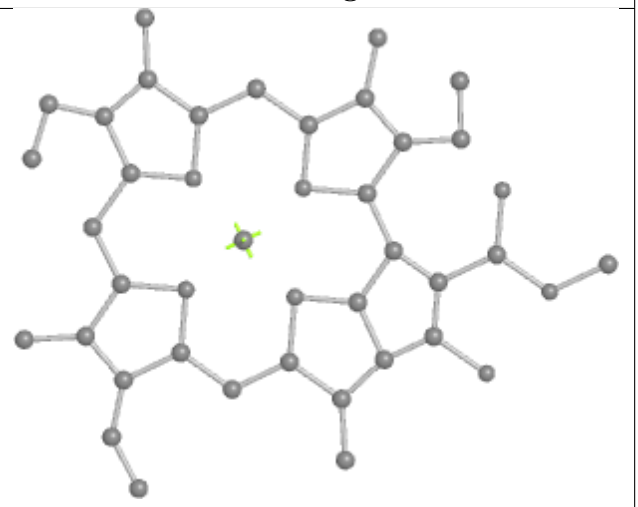
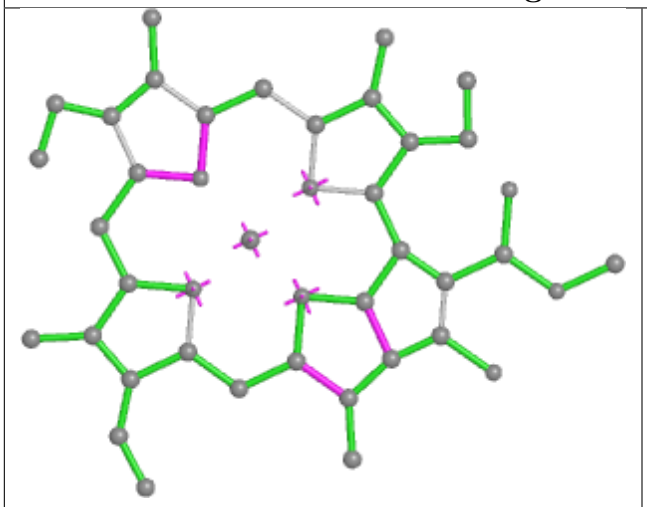


Rings

Ligand CLA A 842



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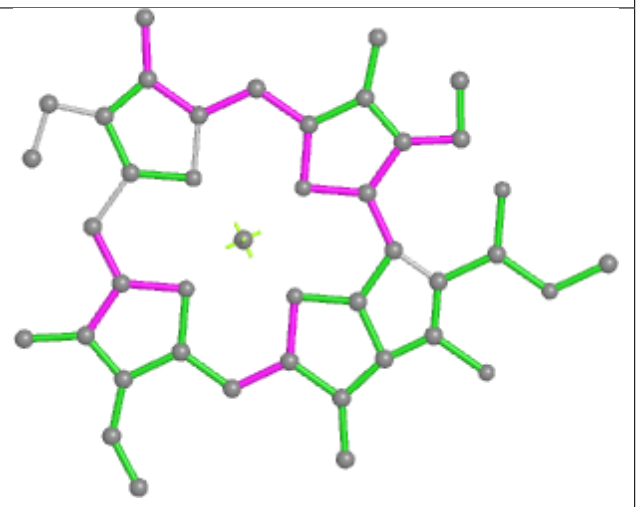
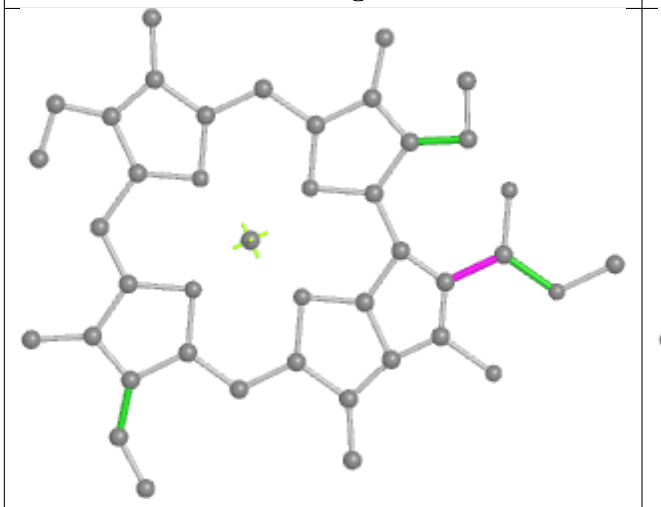


Bond angles



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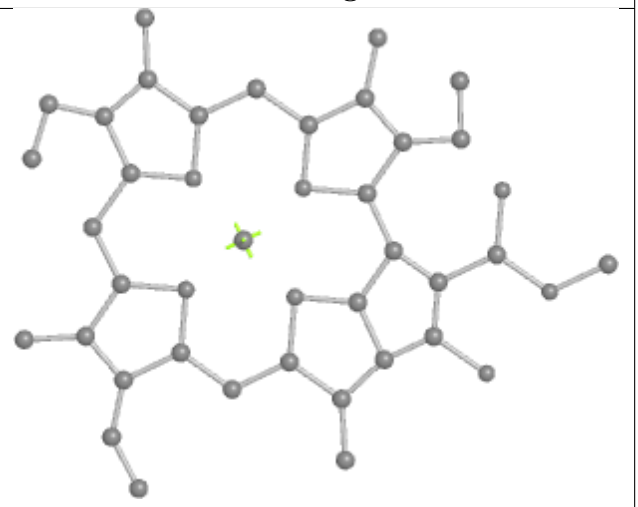
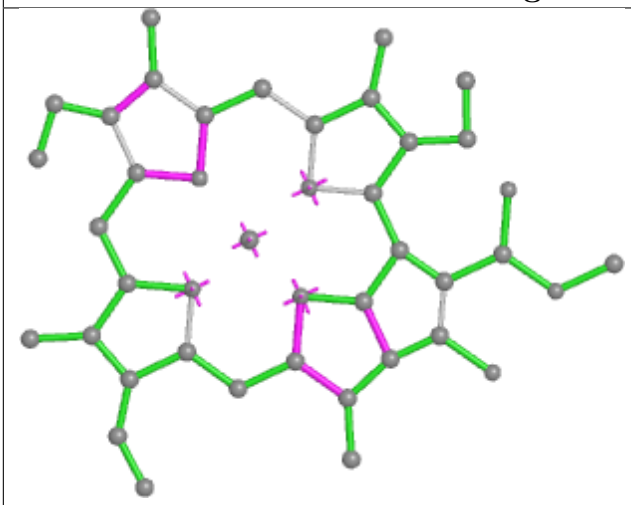


Rings

Ligand CLA A 838



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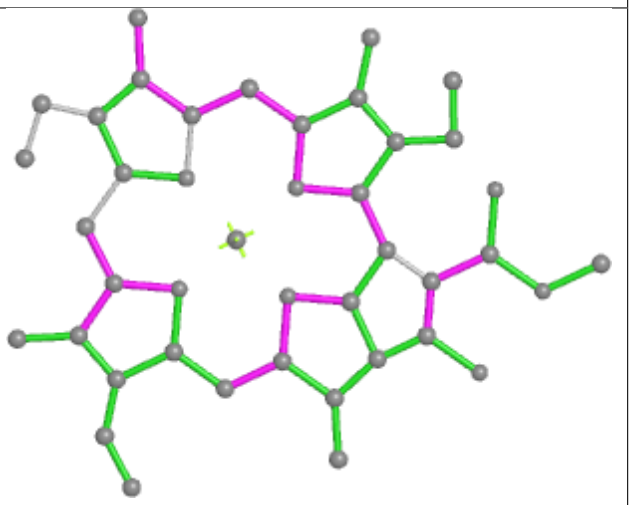

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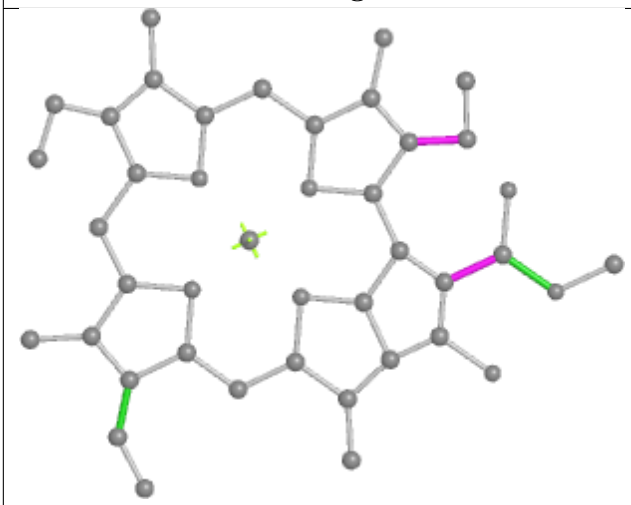

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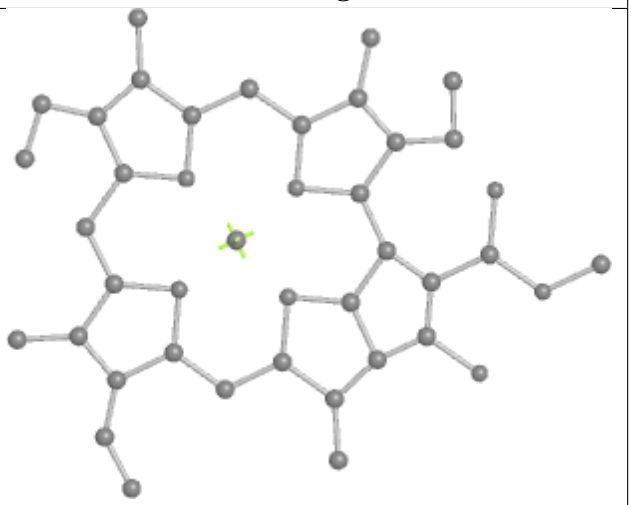
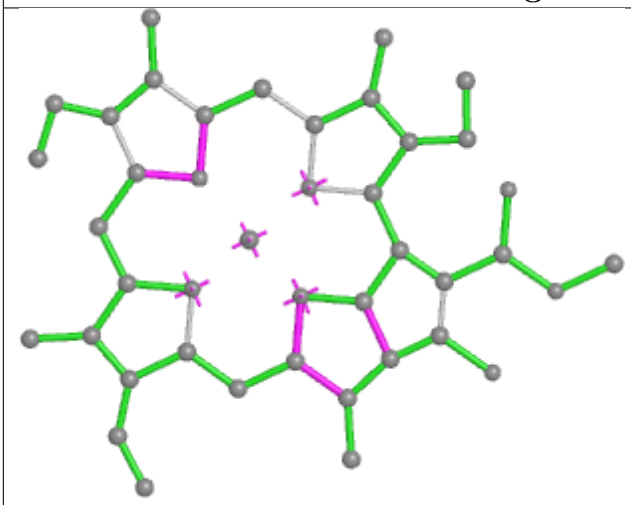


Rings

Ligand CLA B 820



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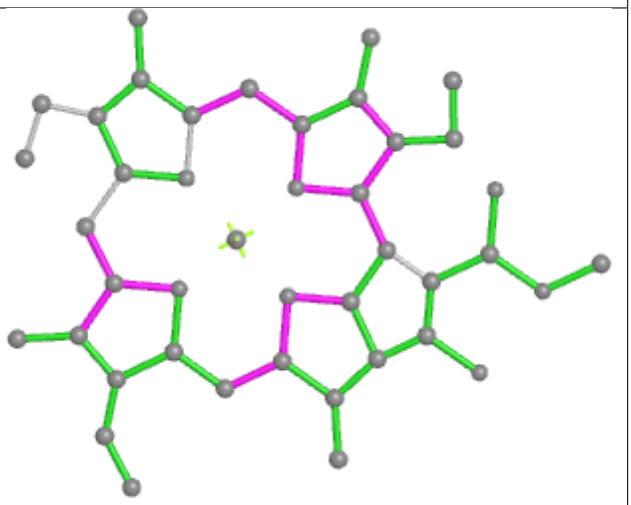

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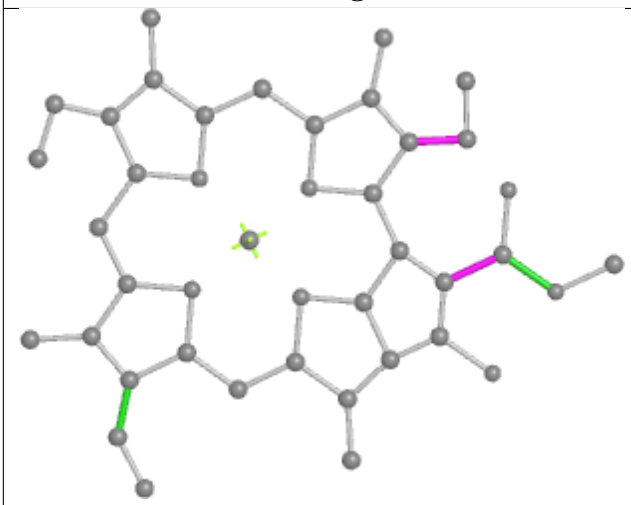

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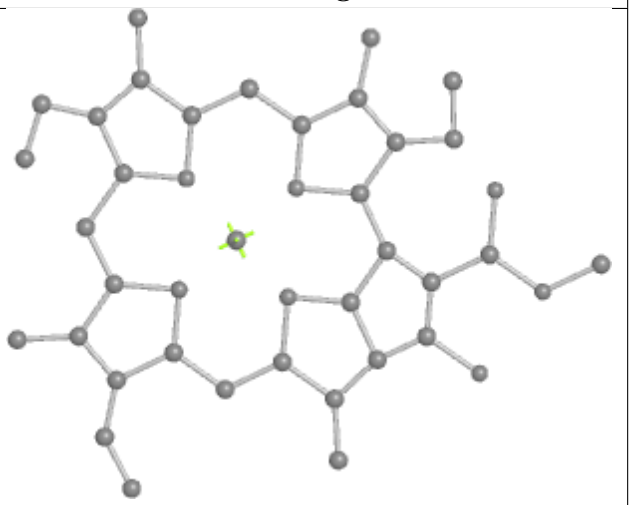
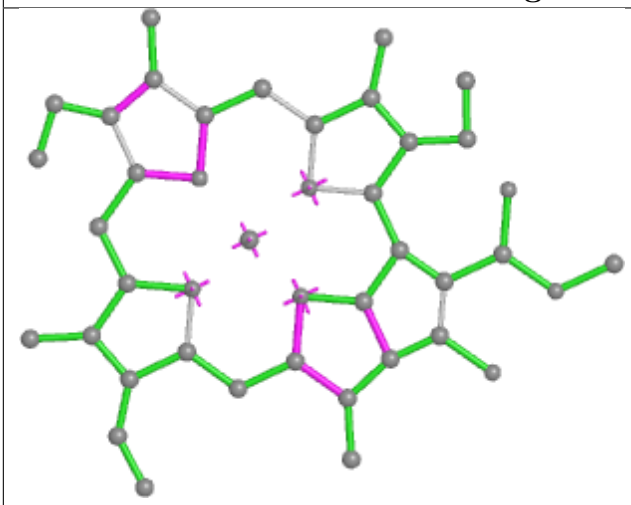


Rings

Ligand CLA B 818



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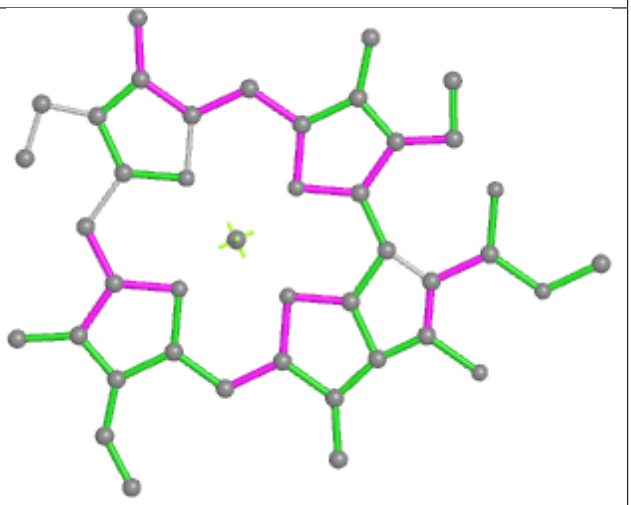

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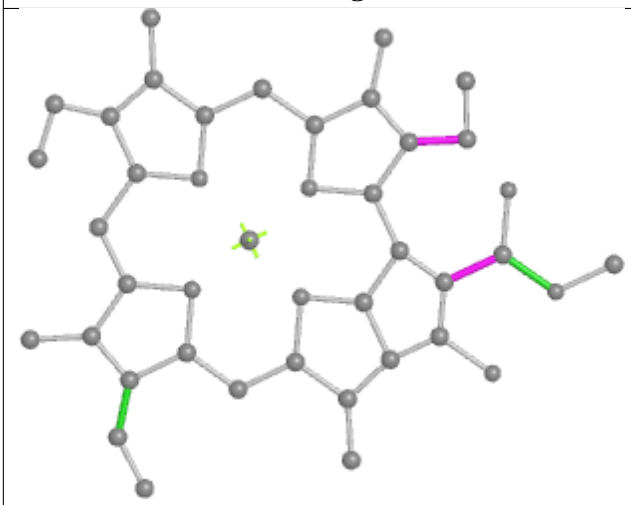

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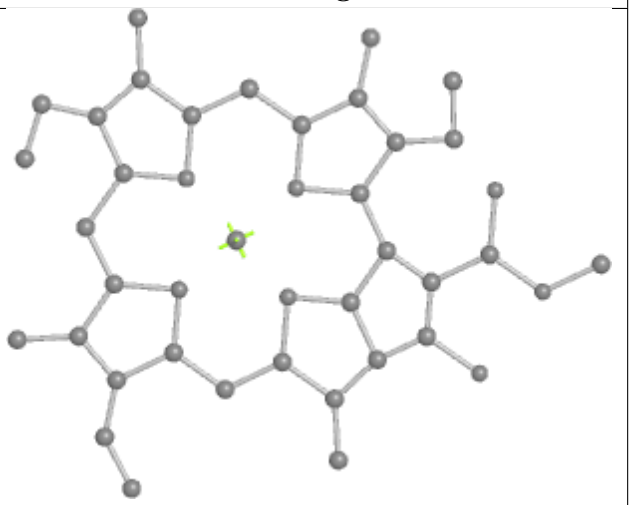
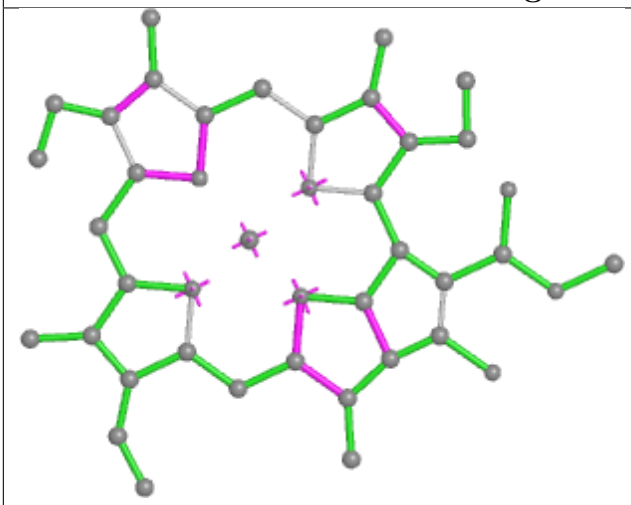
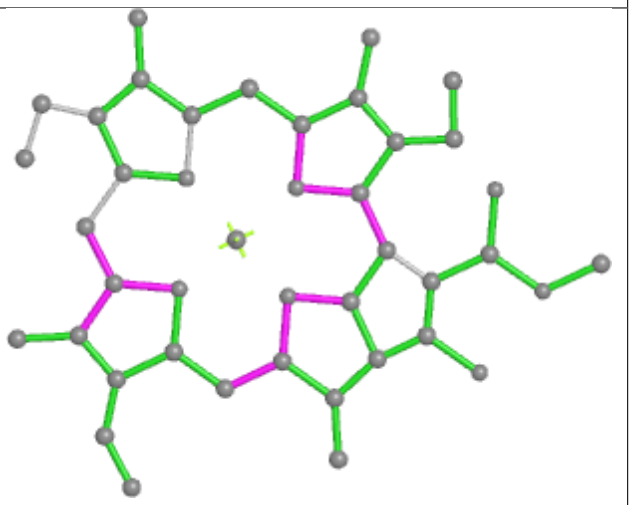


Rings

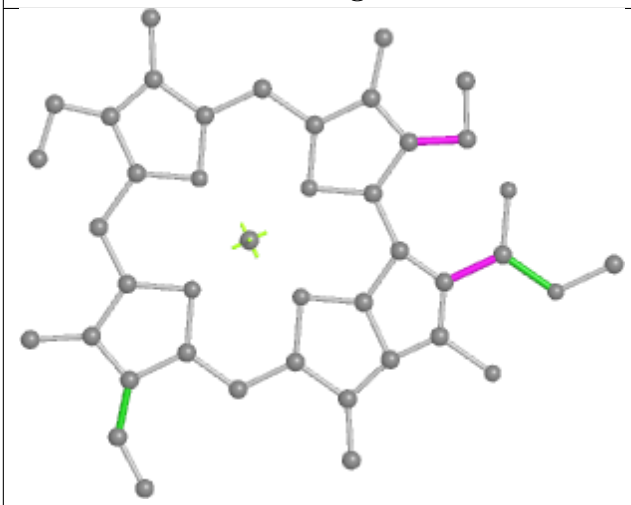
Ligand CLA B 836



Bond lengths



Bond angles



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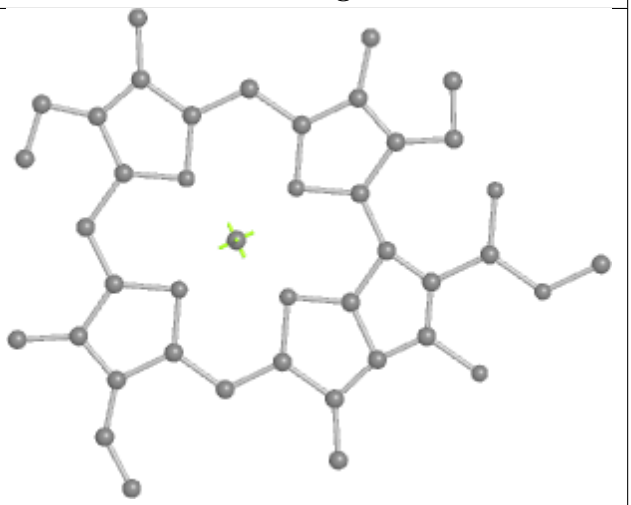
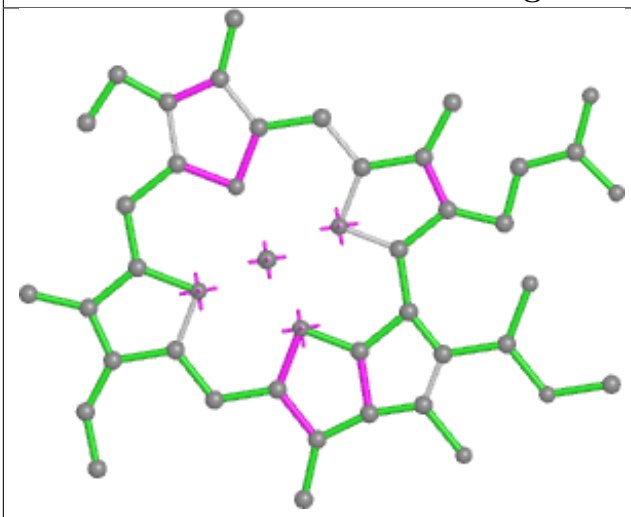


Rings

Ligand CLA A 818



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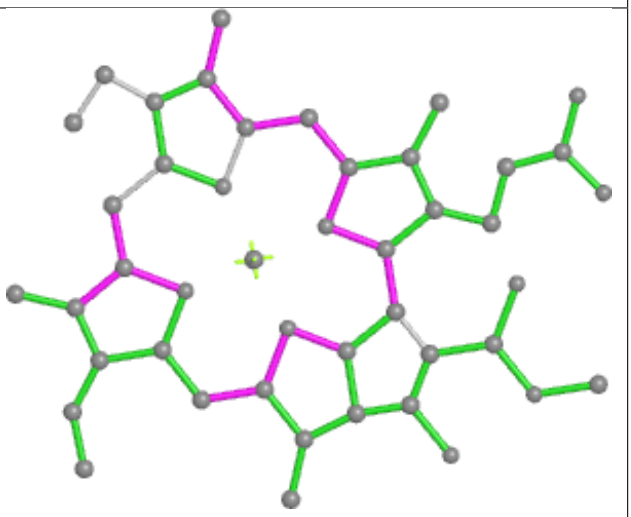

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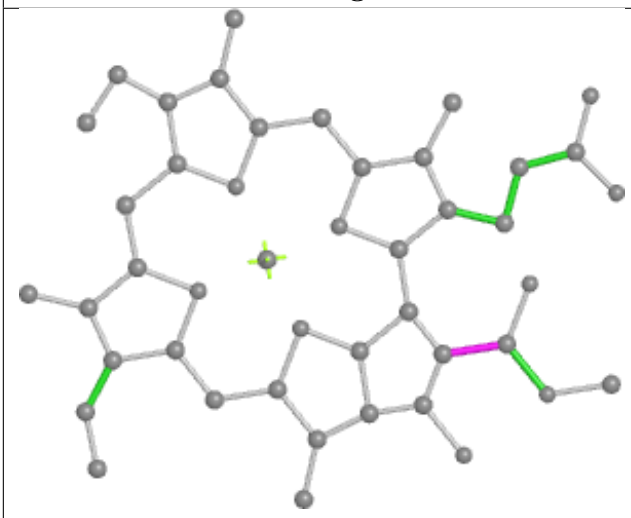

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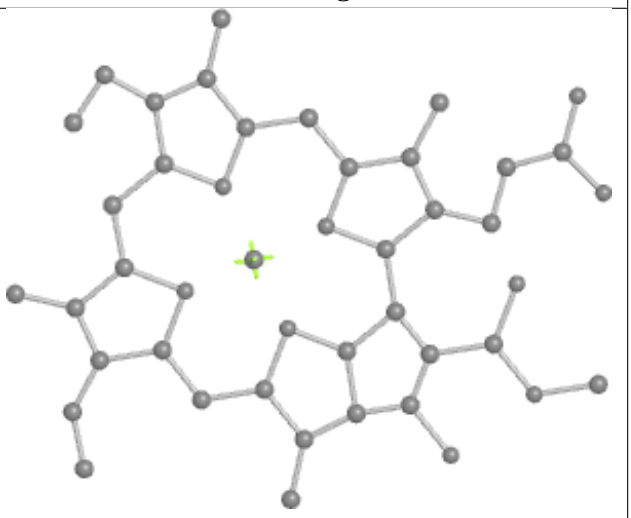
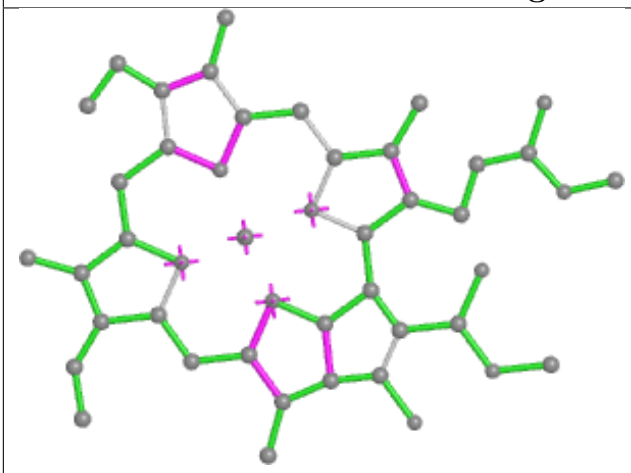
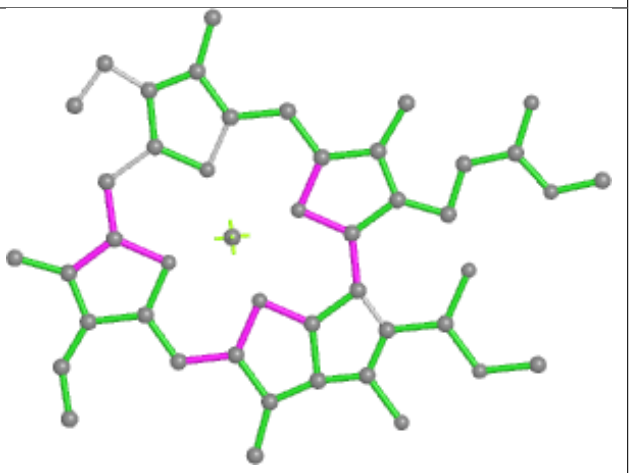
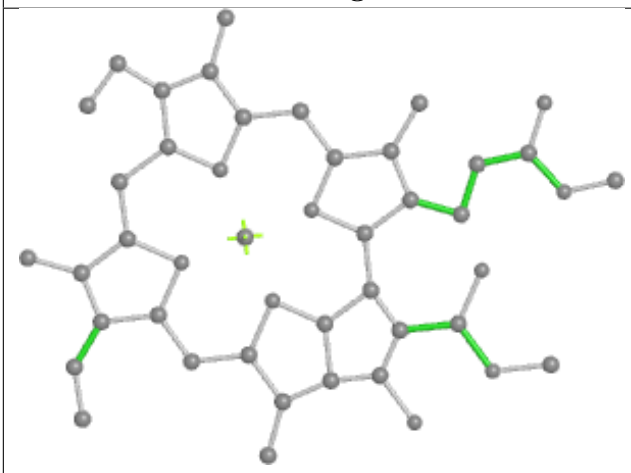
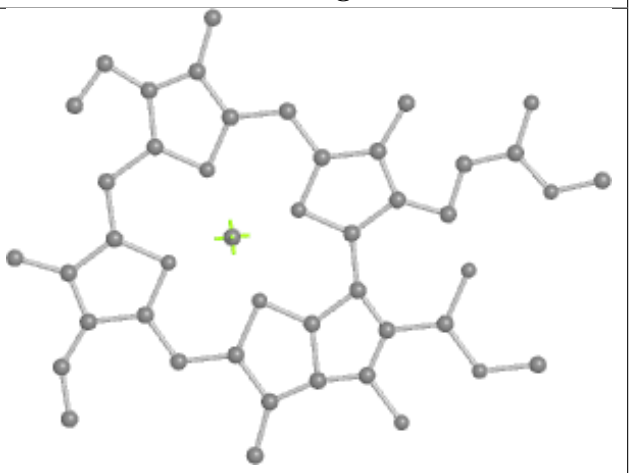
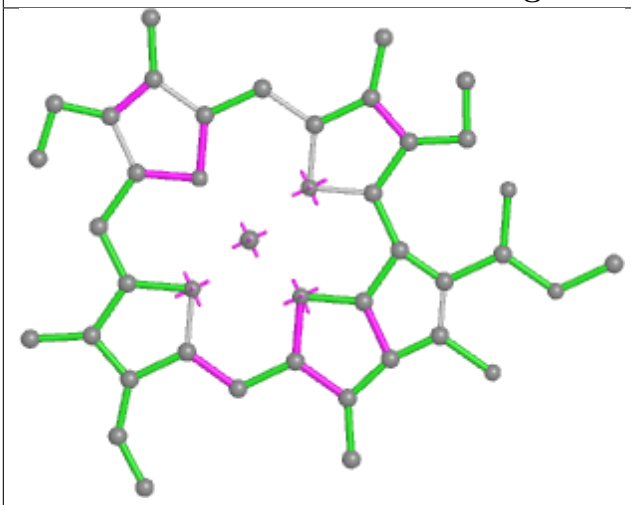


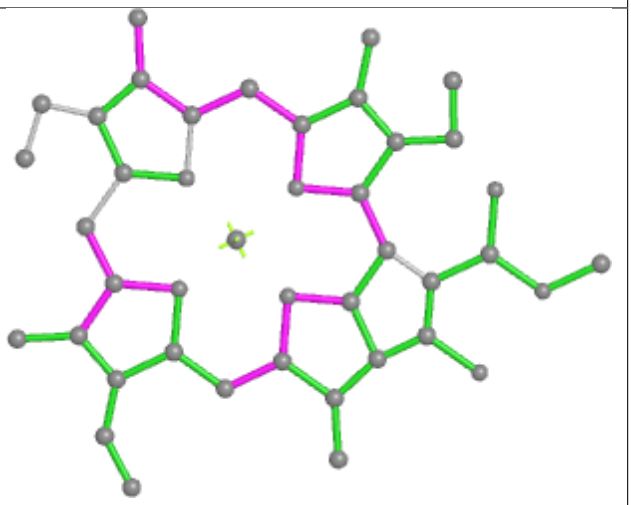
Rings

Ligand CLA 8 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

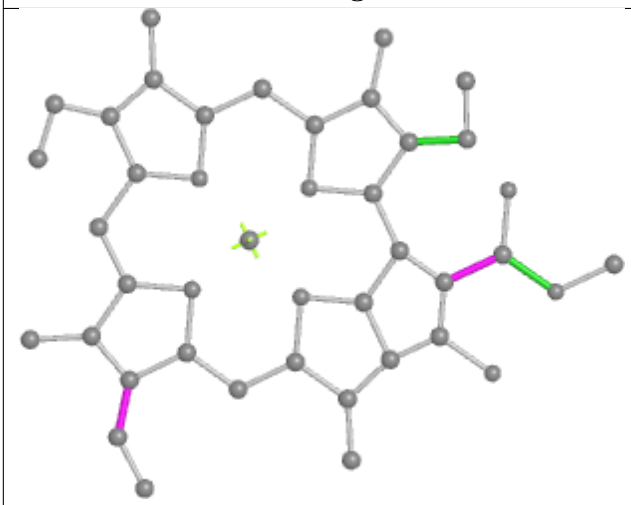
Ligand CLA A 835



Bond lengths



Bond angles



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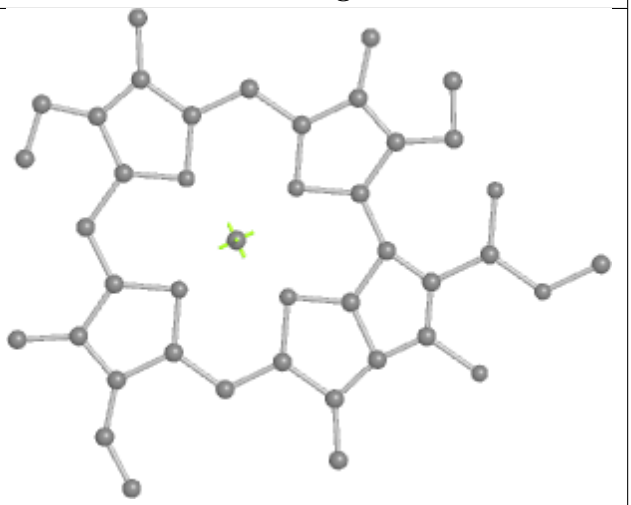
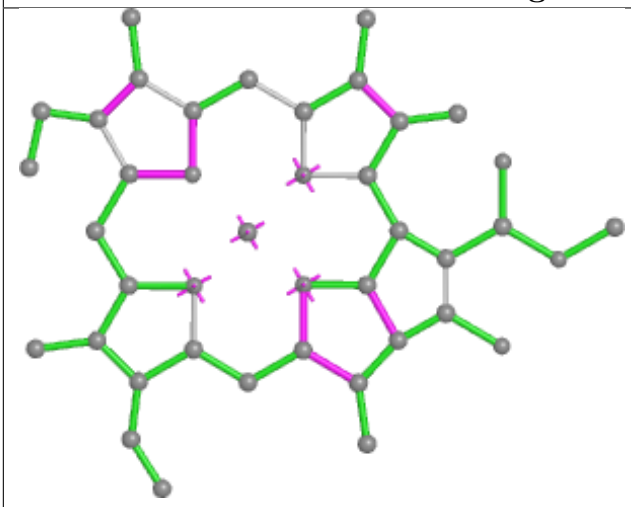
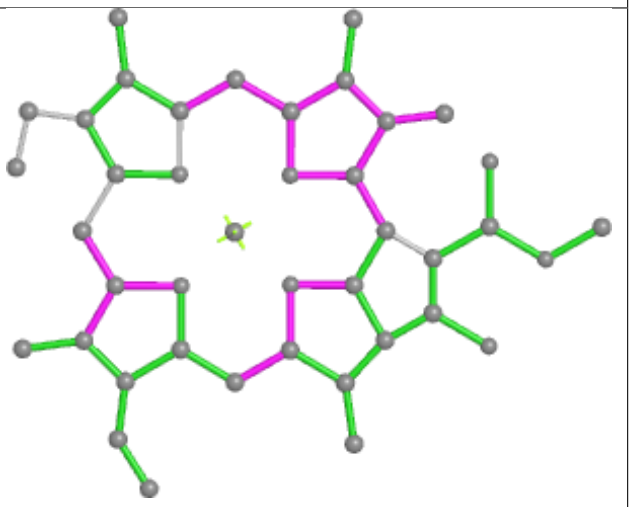
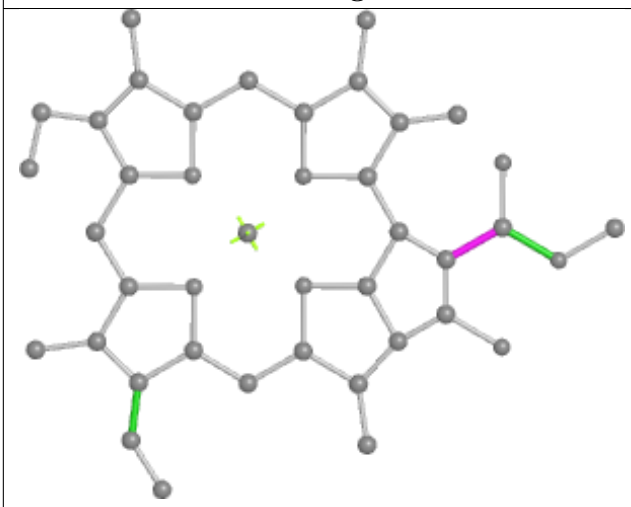
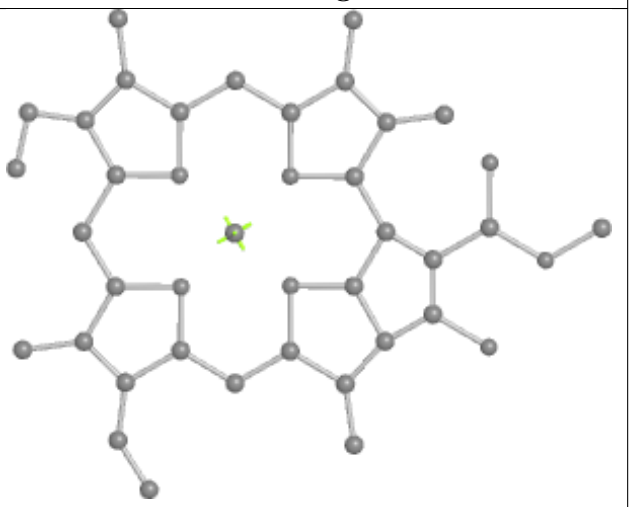
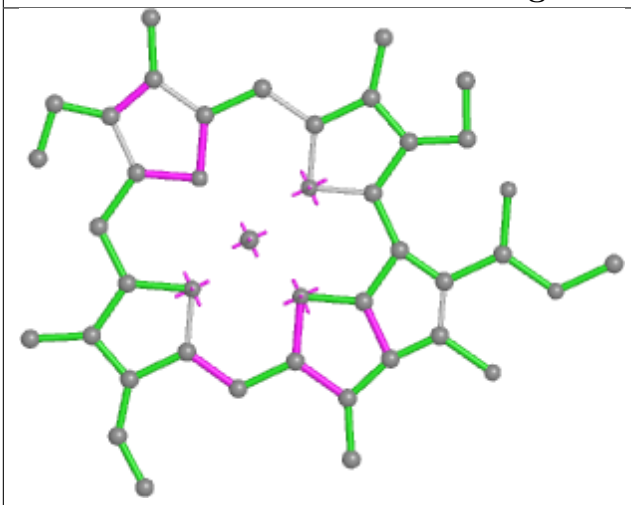


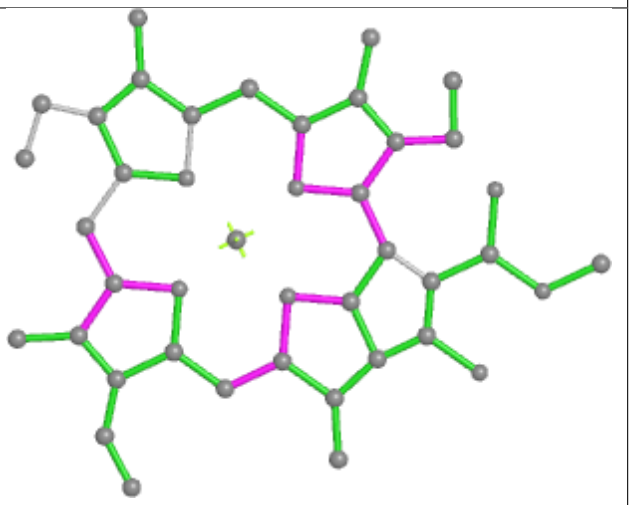
Rings

Ligand CLA 7 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

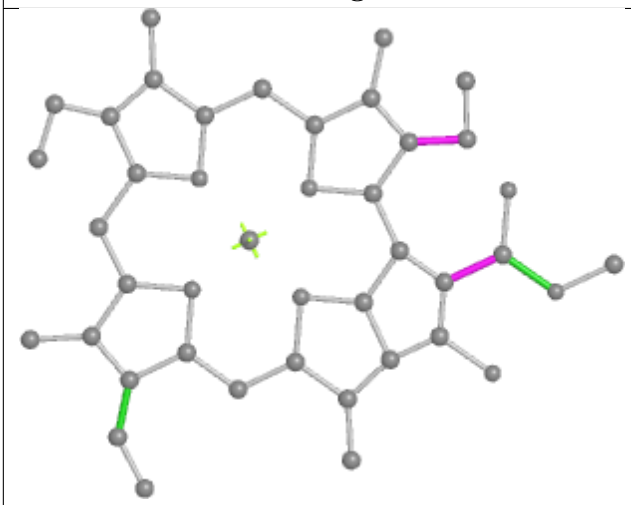
Ligand CLA 7 602



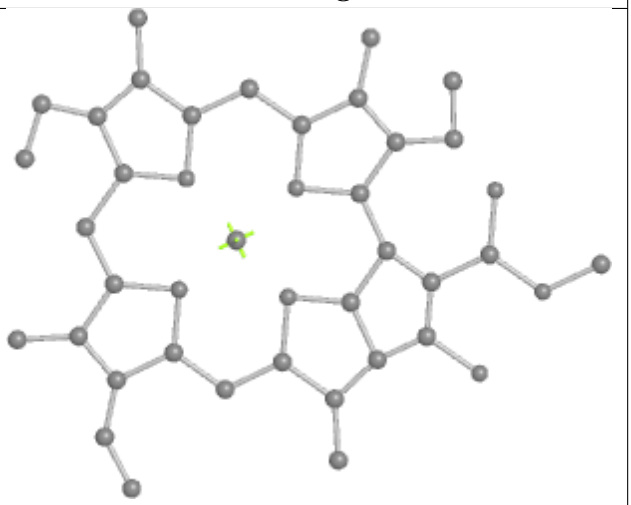
Bond lengths



Bond angles

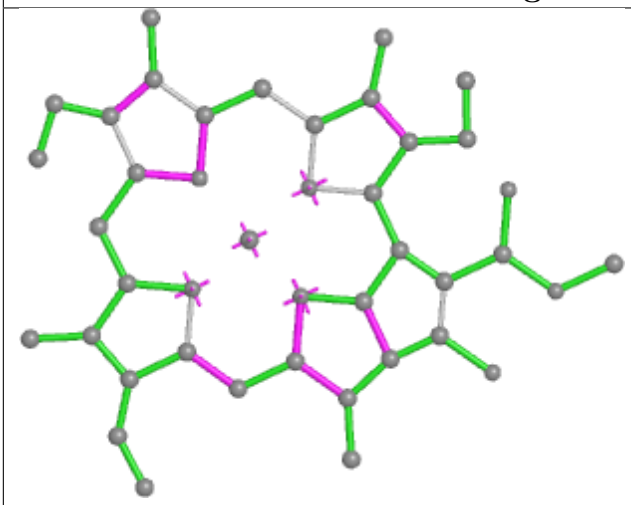


Torsions

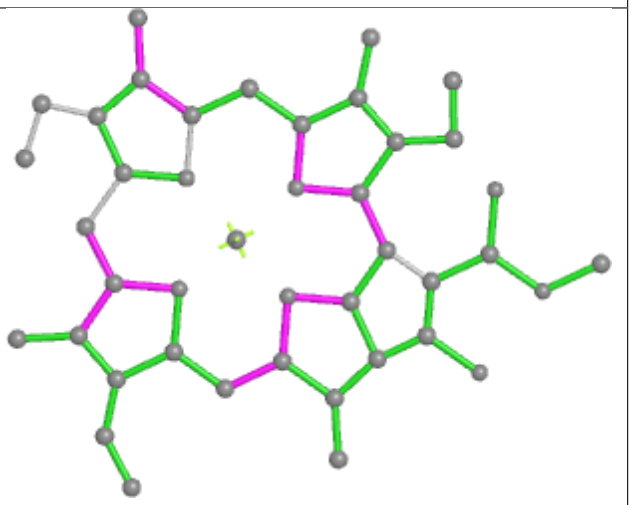


Rings

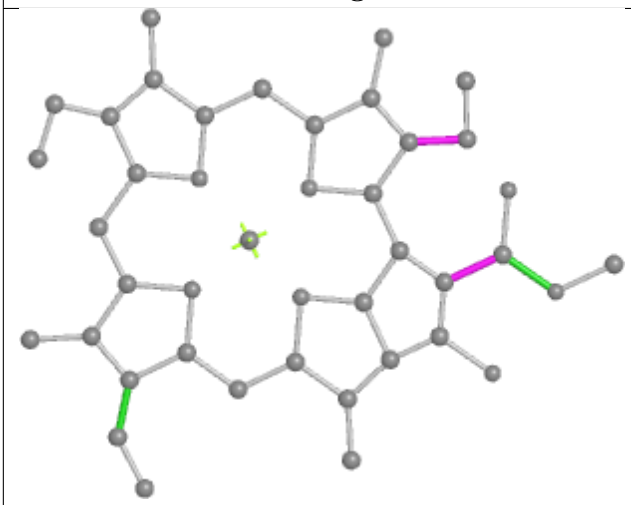
Ligand CLA A 812



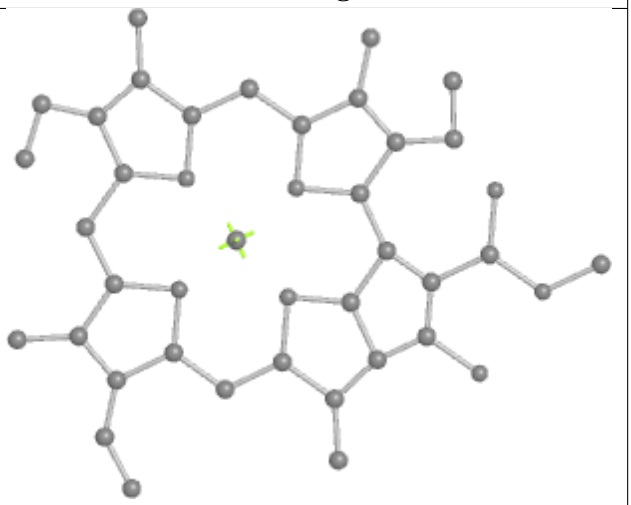
Bond lengths



Bond angles

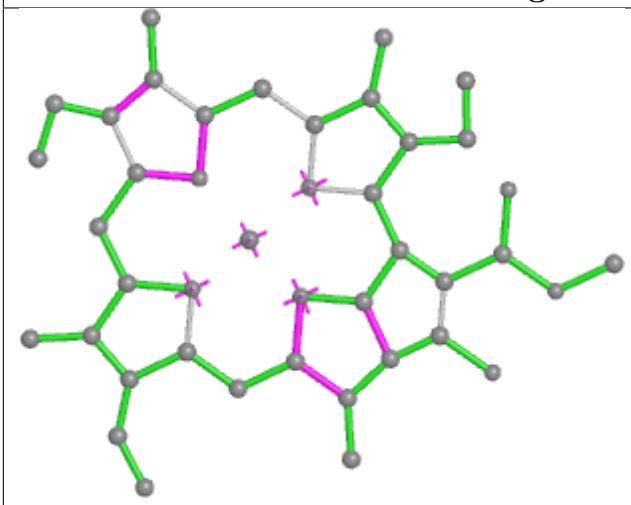


Torsions

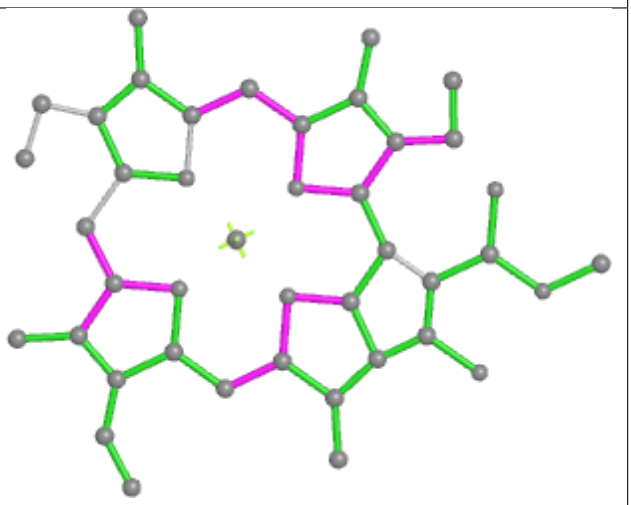


Rings

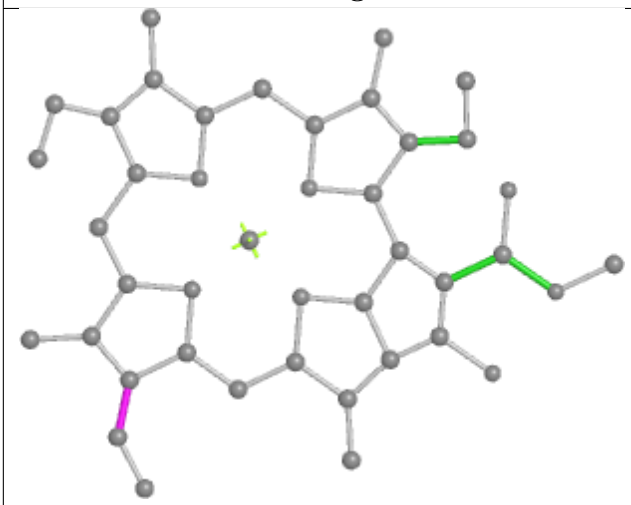
Ligand CLA 3 312



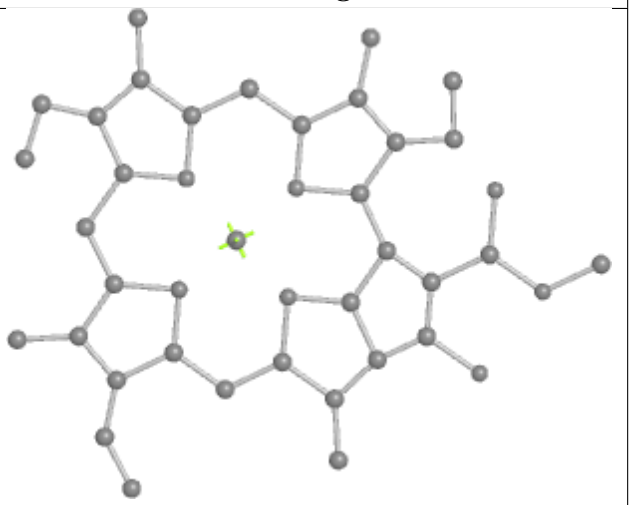
Bond lengths



Bond angles

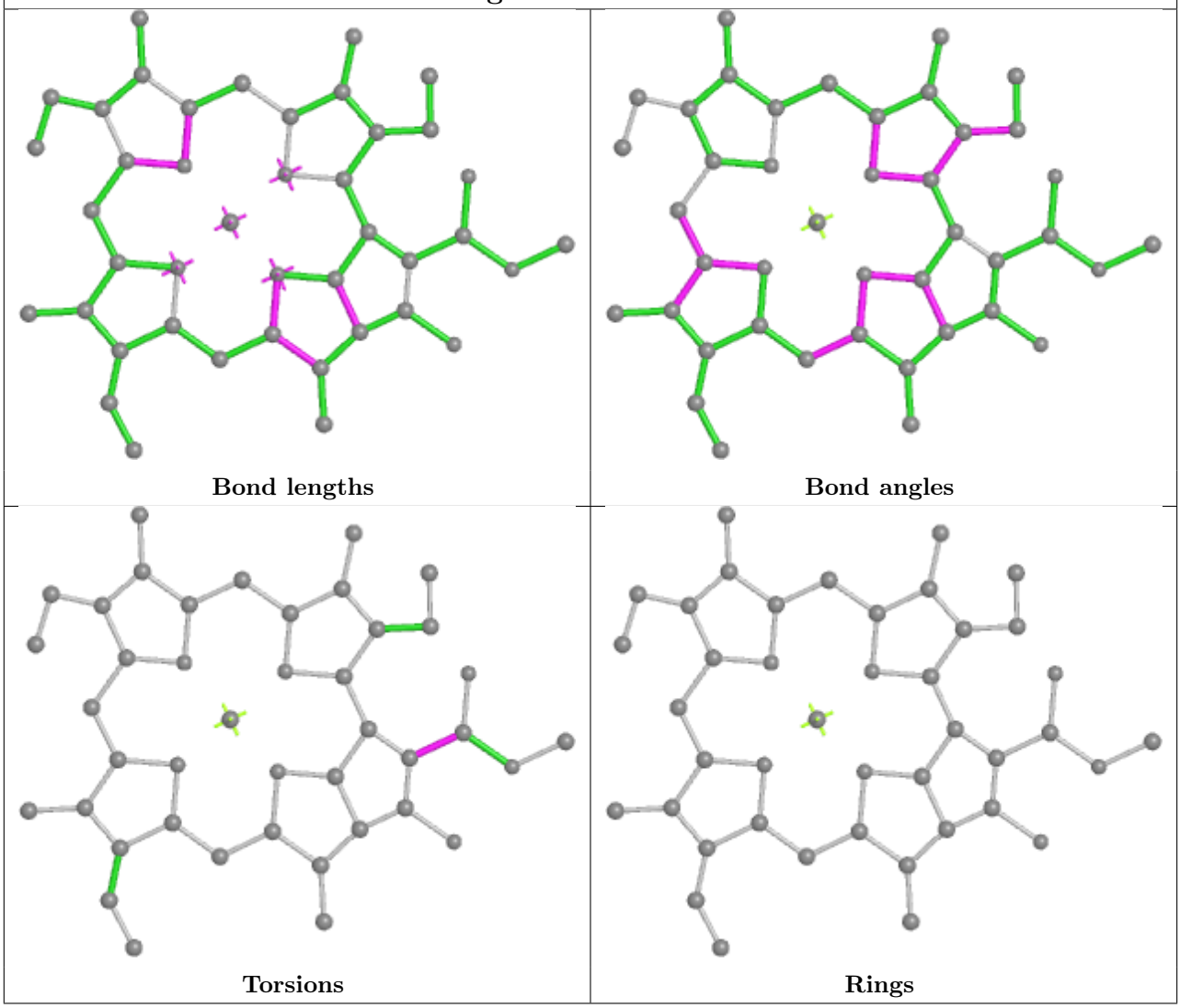


Torsions

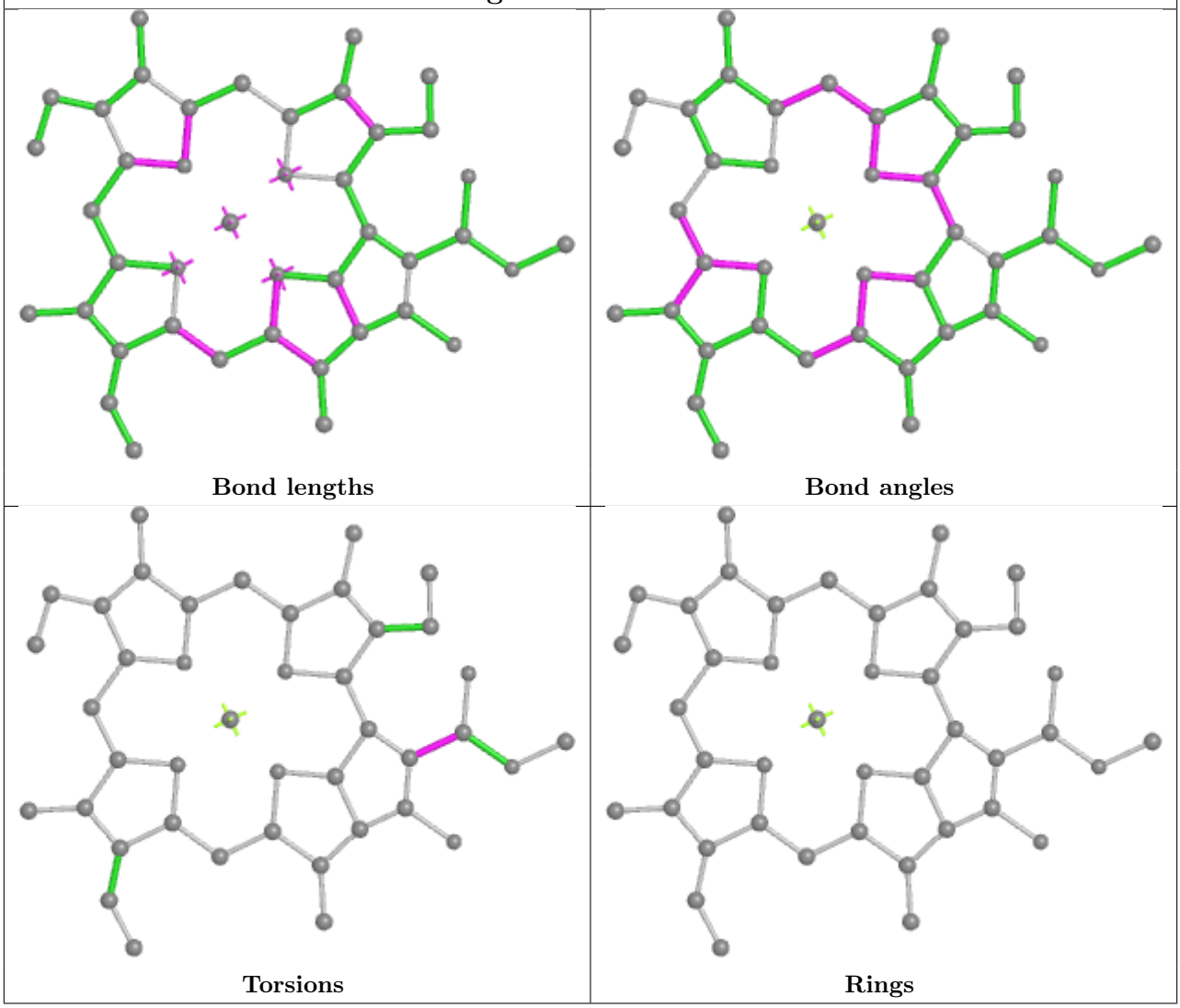


Rings

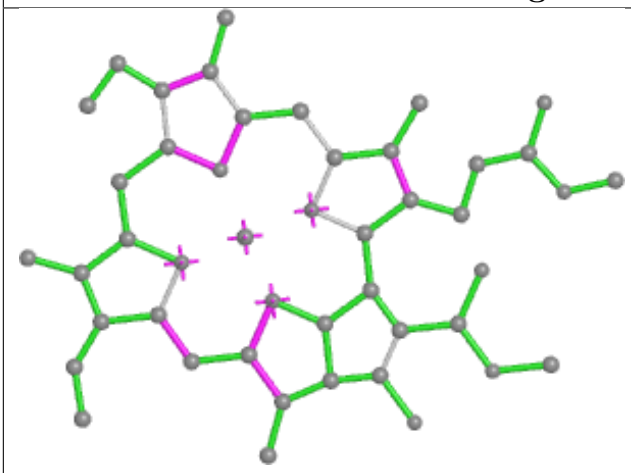
Ligand CLA 7 608



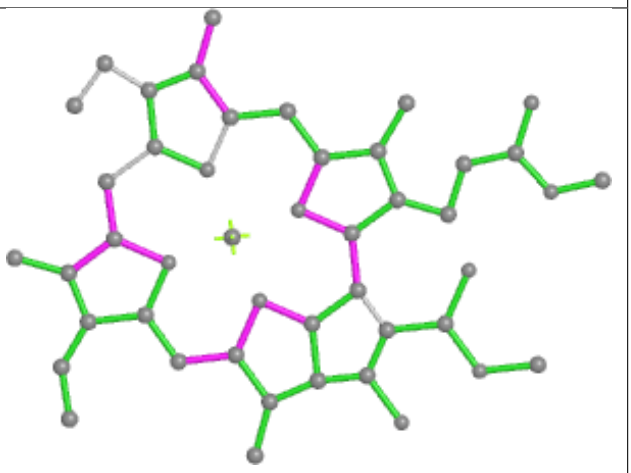
Ligand CLA 8 614



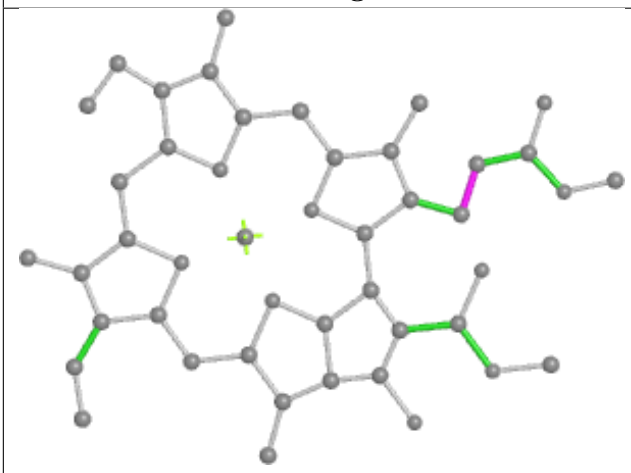
Ligand CLA 6 609



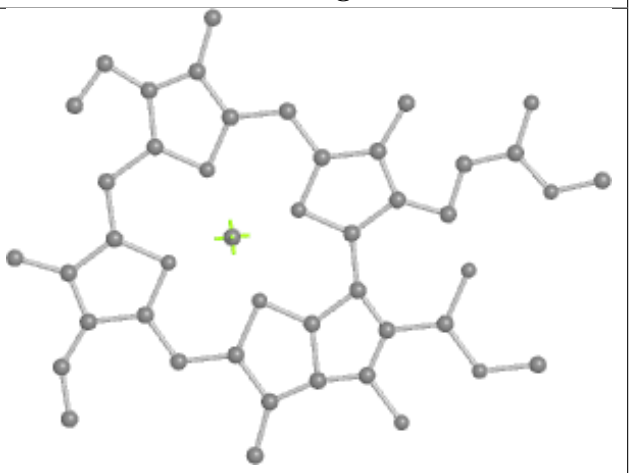
Bond lengths



Bond angles

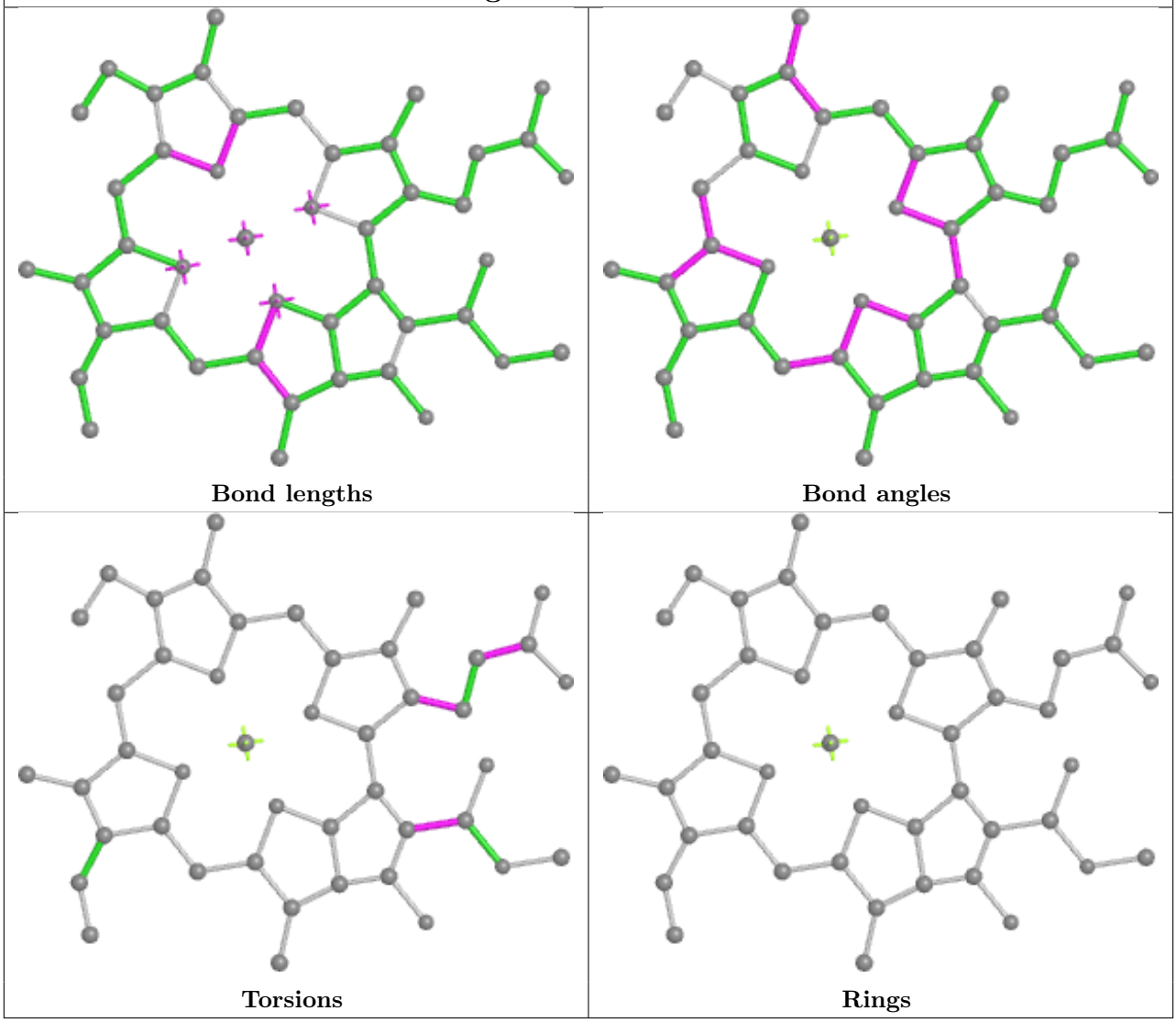


Torsions

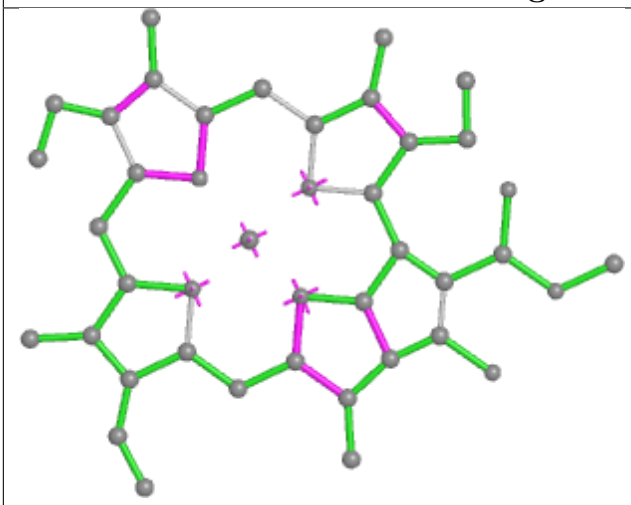


Rings

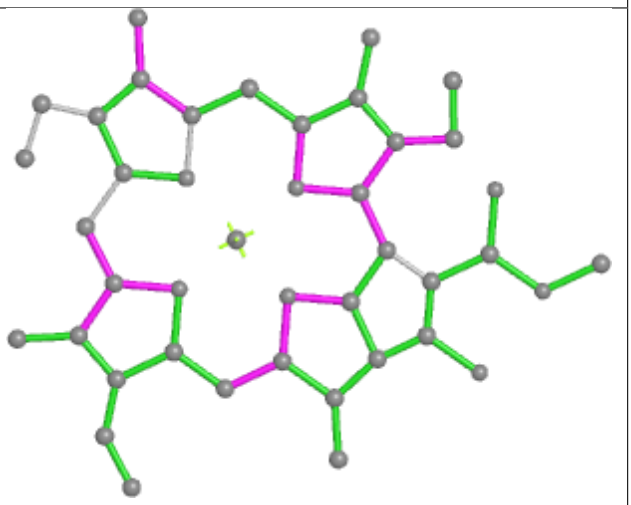
Ligand CLA 4 602



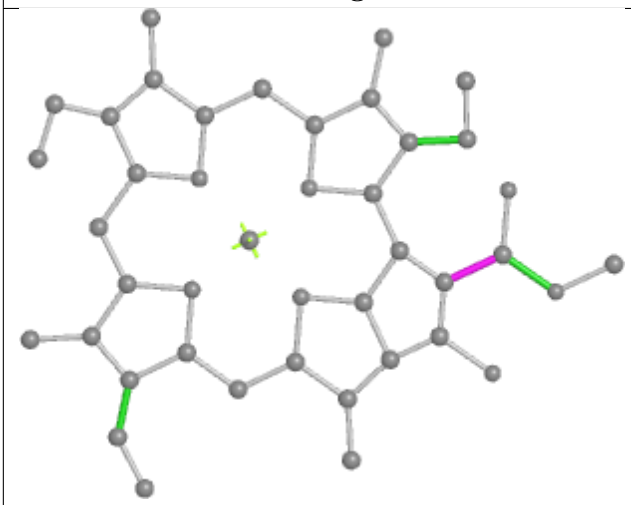
Ligand CLA 6 601



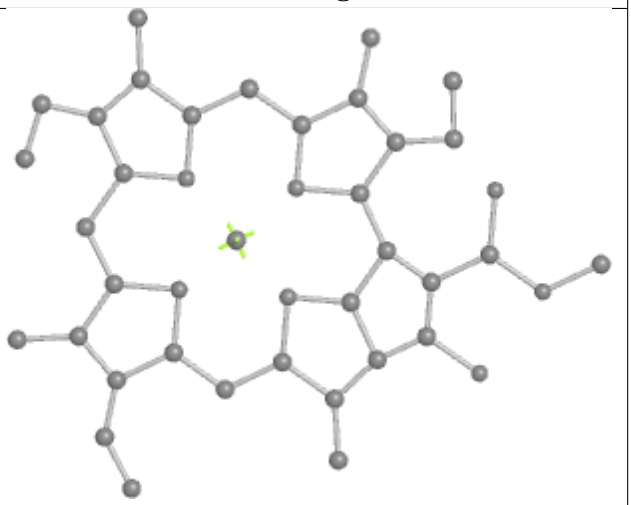
Bond lengths



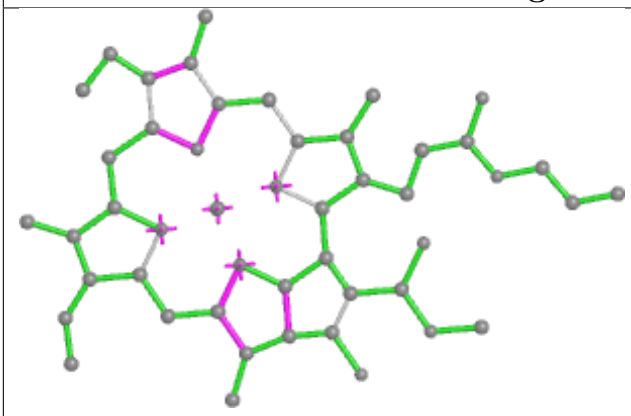
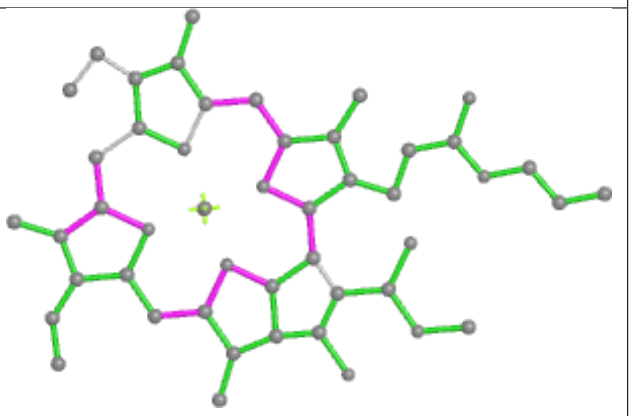
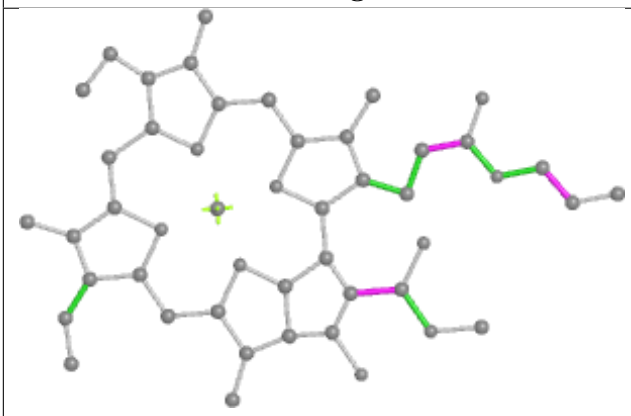
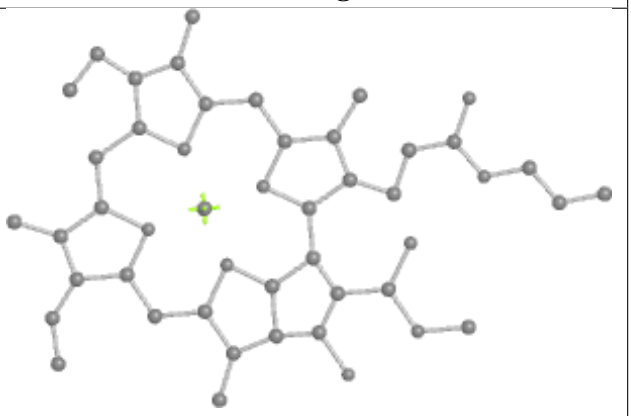
Bond angles



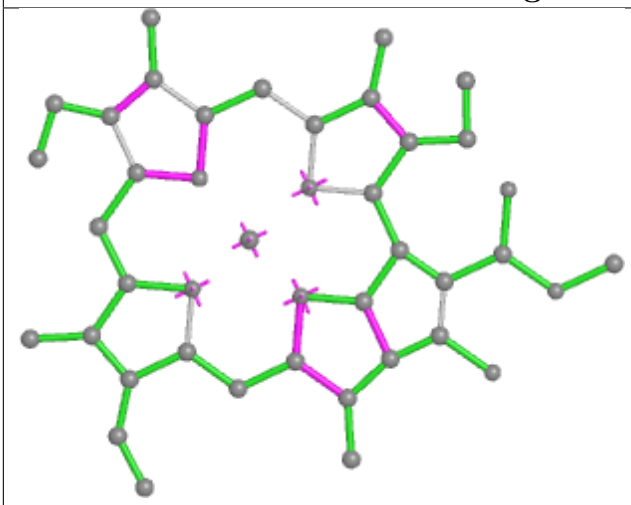
Torsions



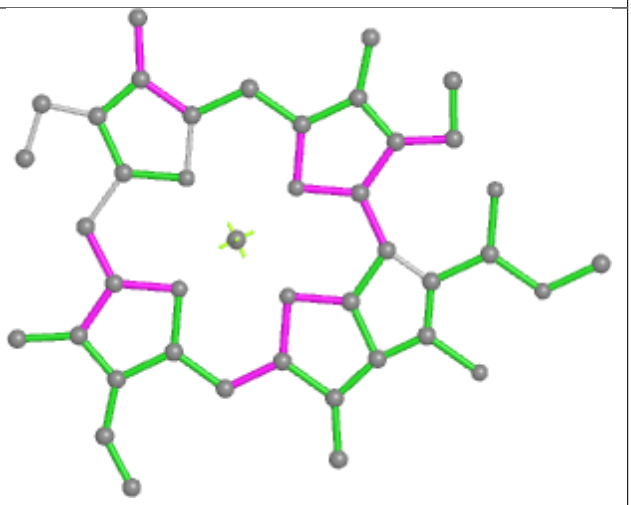
Rings

Ligand CLA 5 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

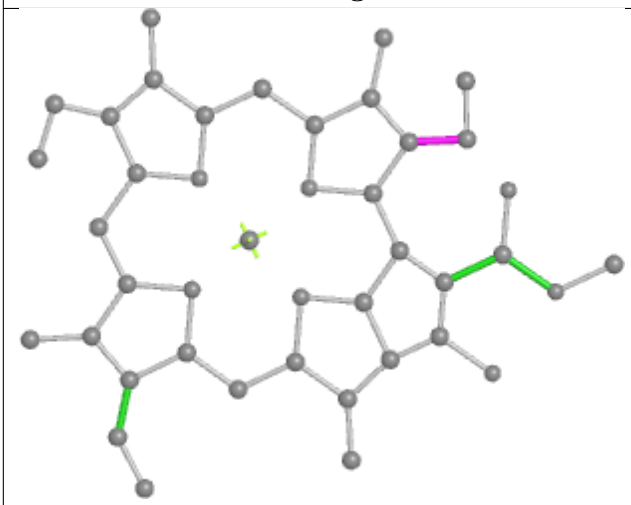
Ligand CLA A 805



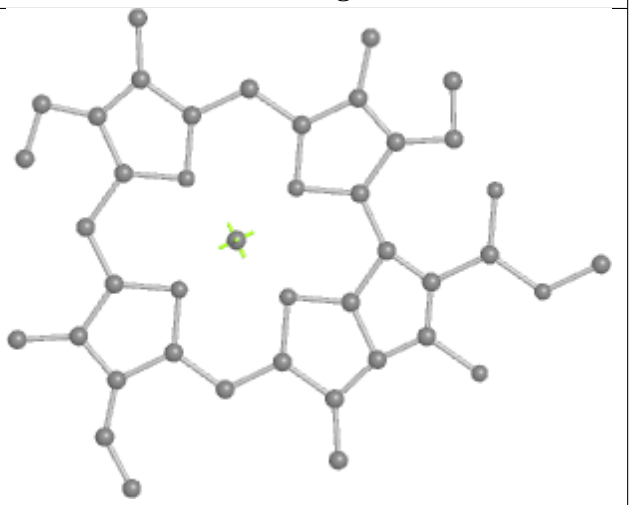
Bond lengths



Bond angles

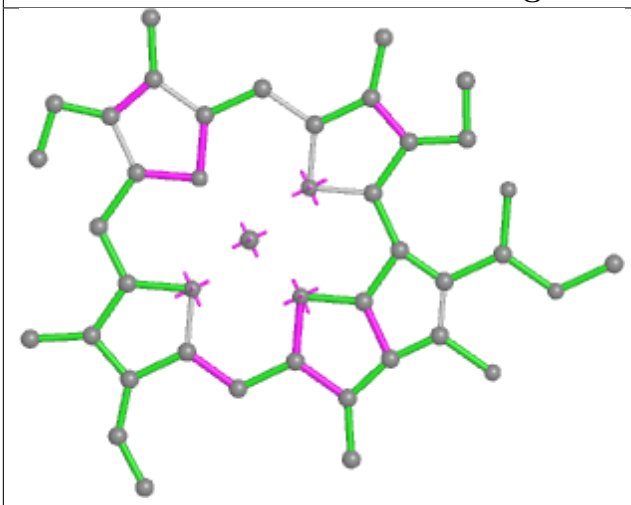


Torsions

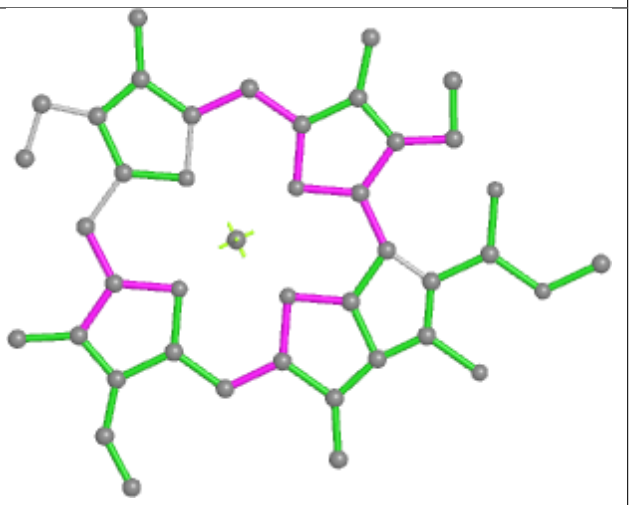


Rings

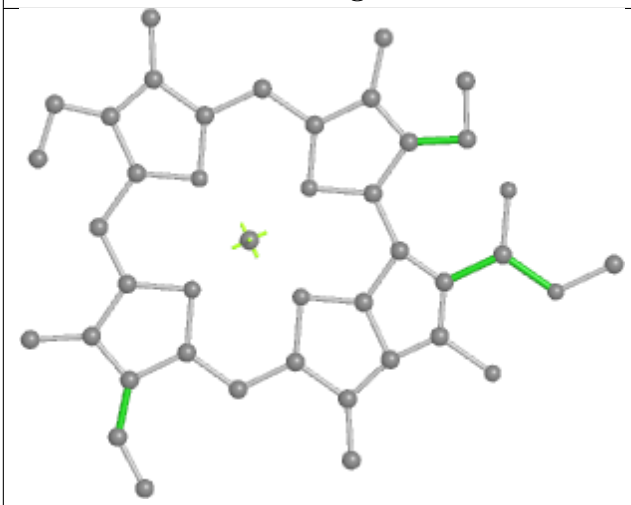
Ligand CLA A 827



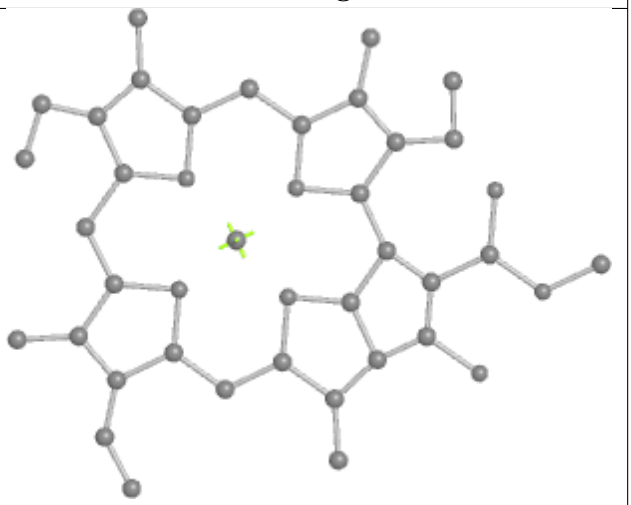
Bond lengths



Bond angles

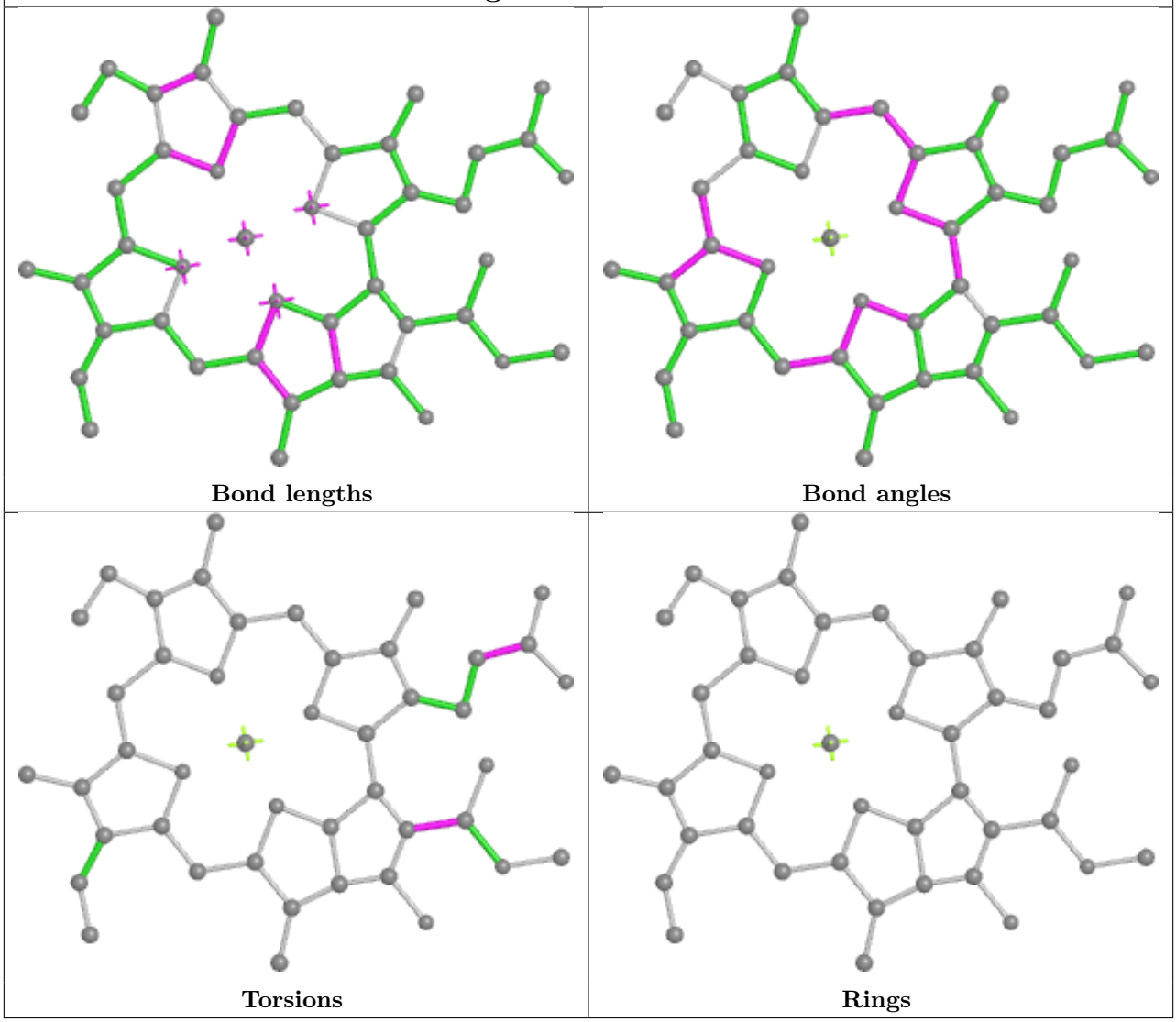


Torsions

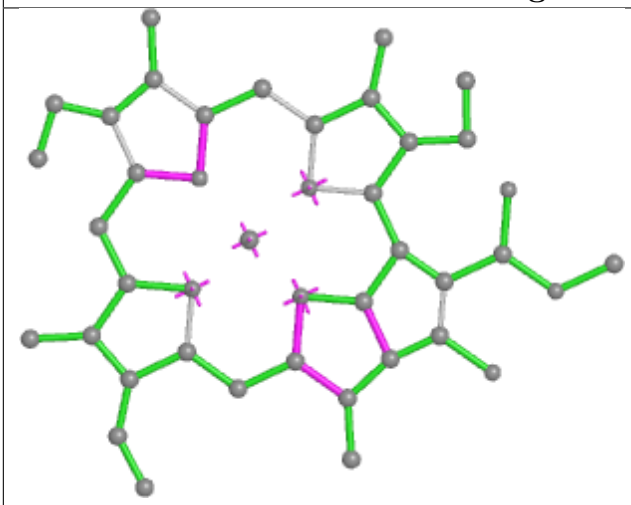


Rings

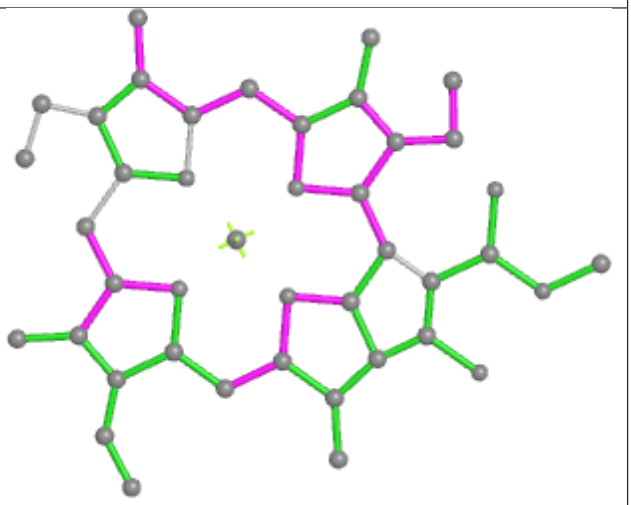
Ligand CLA 3 304



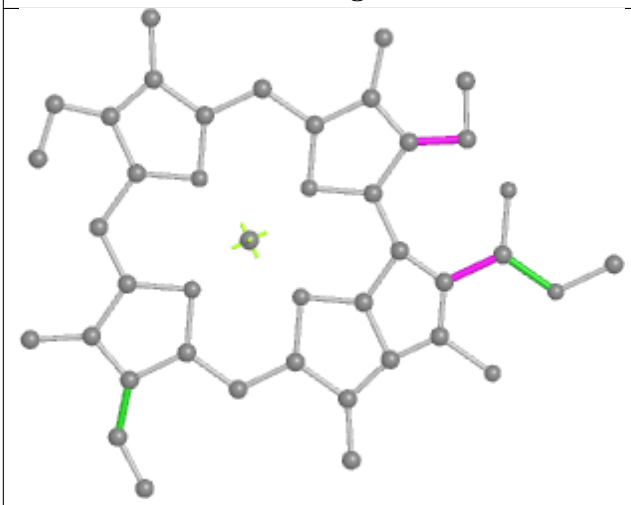
Ligand CLA 4 603



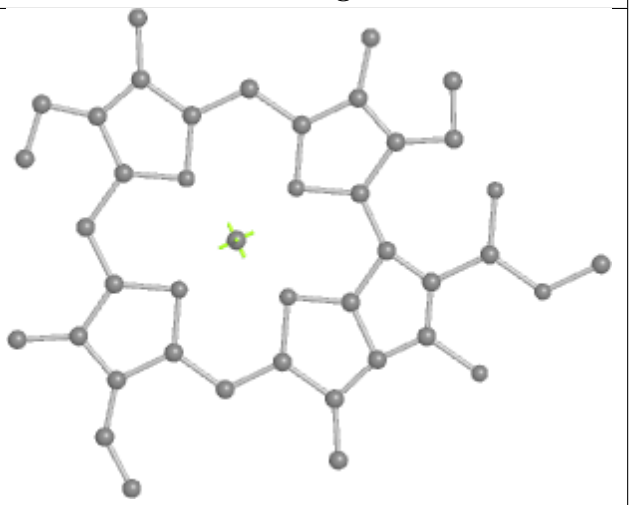
Bond lengths



Bond angles

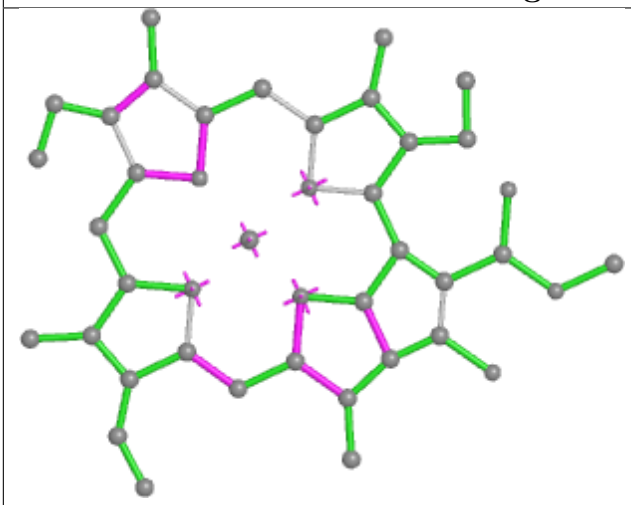


Torsions

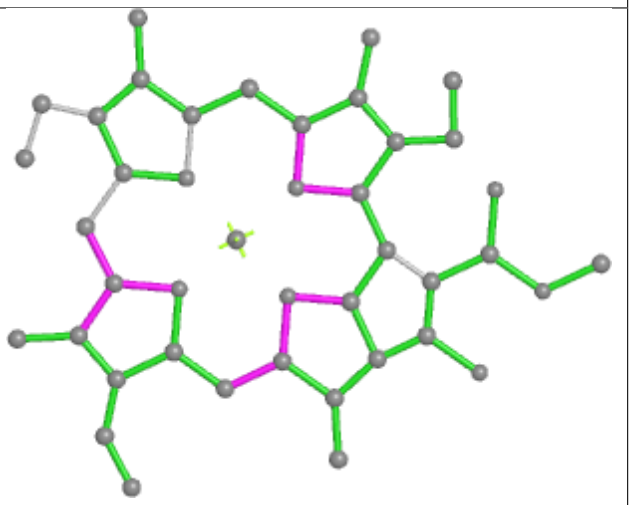


Rings

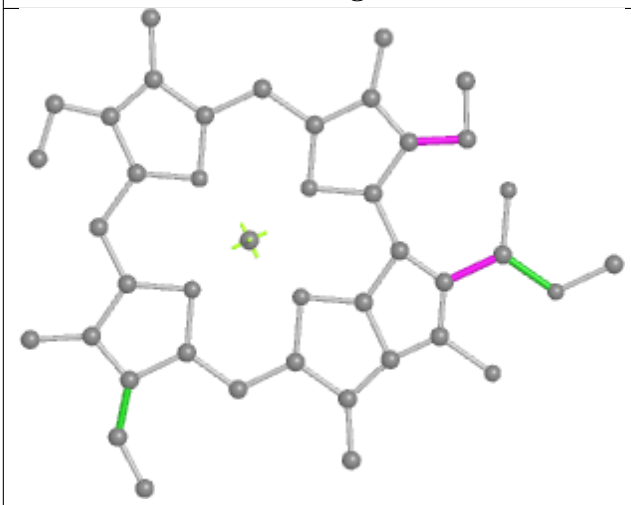
Ligand CLA A 820



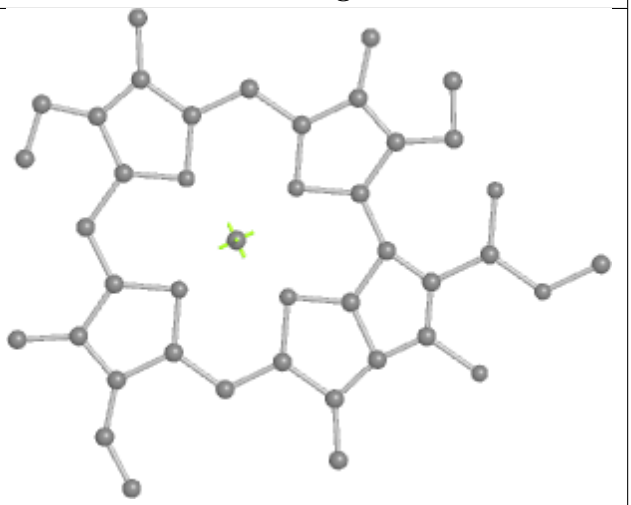
Bond lengths



Bond angles

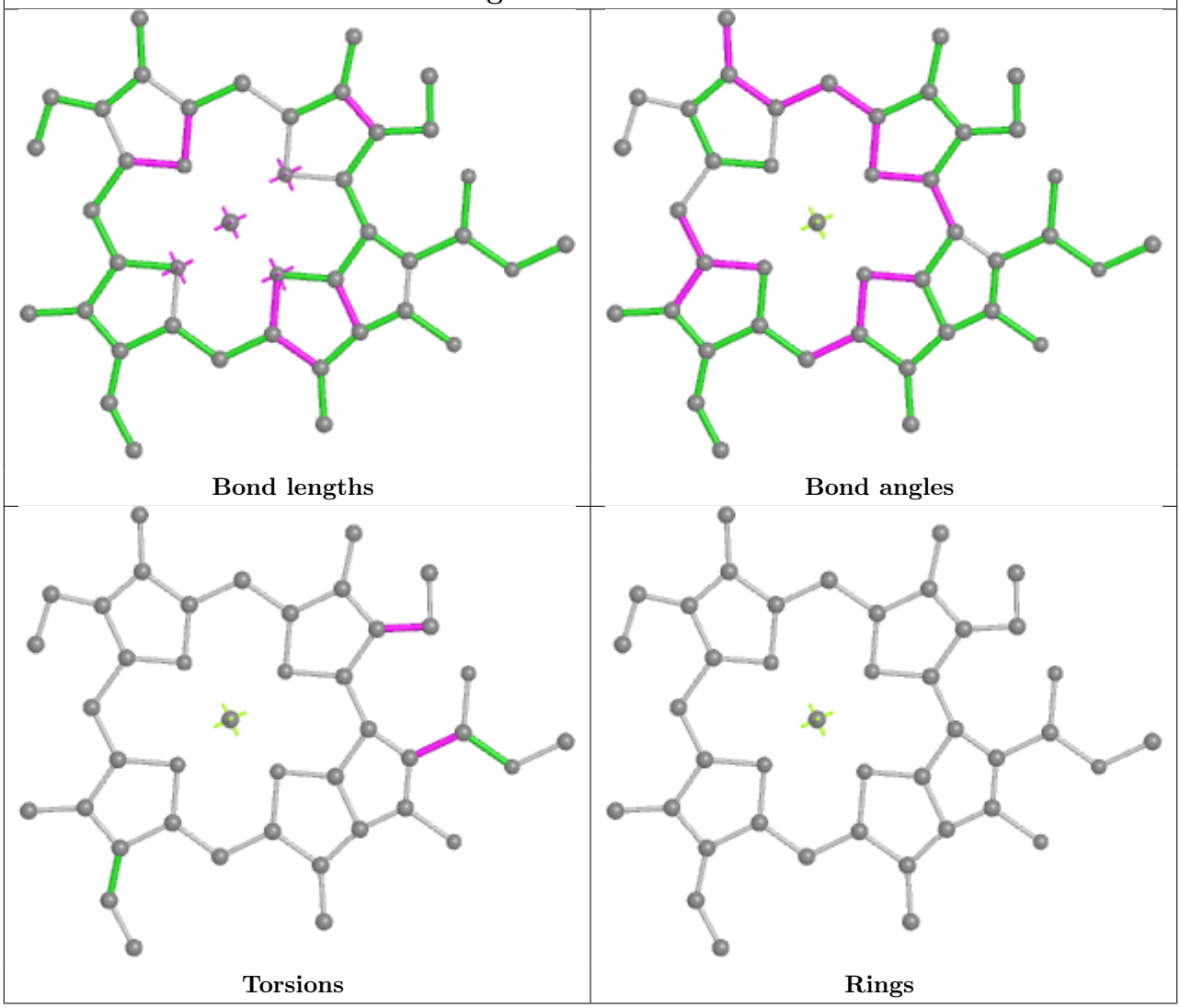


Torsions



Rings

Ligand CLA 1 605



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.

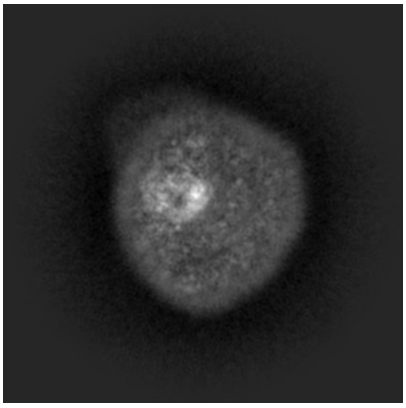
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32892. These allow visual inspection of the internal detail of the map and identification of artifacts.

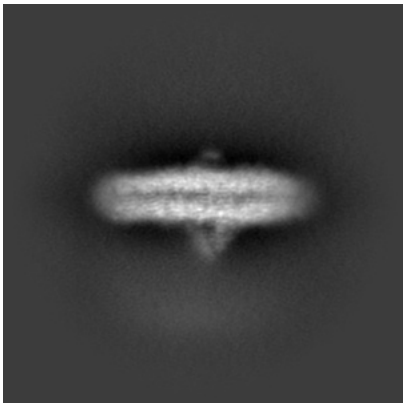
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

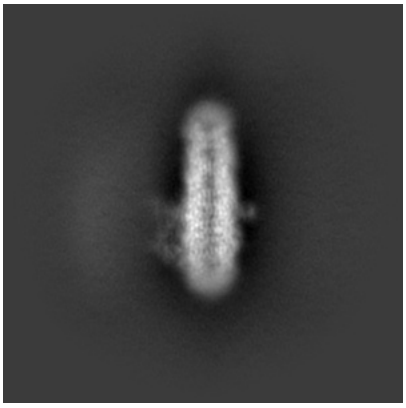
6.1.1 Primary map



X



Y

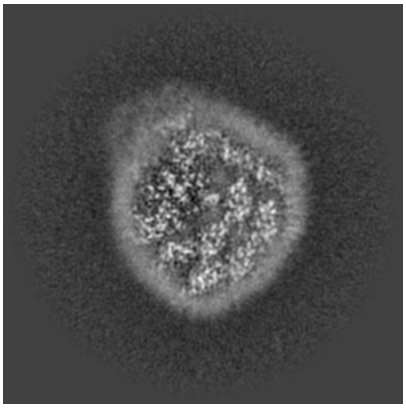


Z

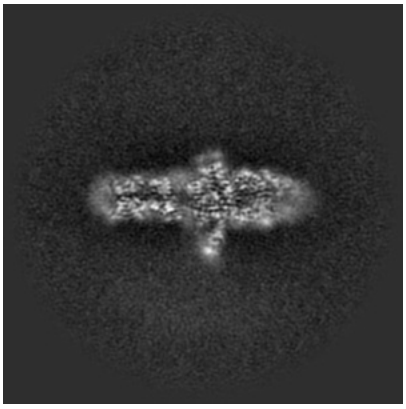
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

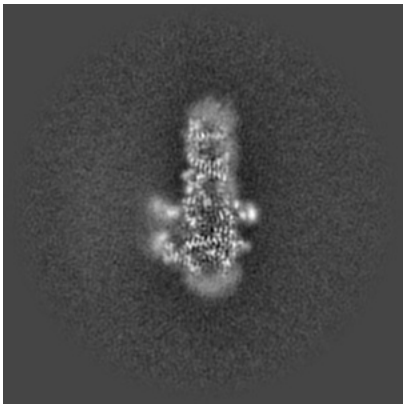
6.2.1 Primary map



X Index: 196



Y Index: 196

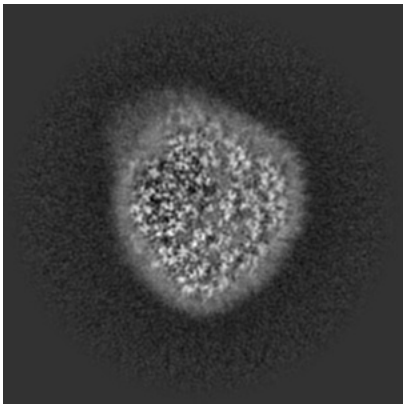


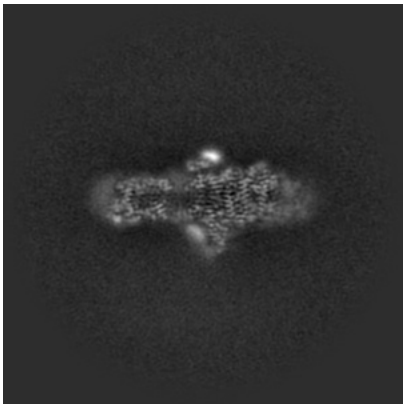
Z Index: 196

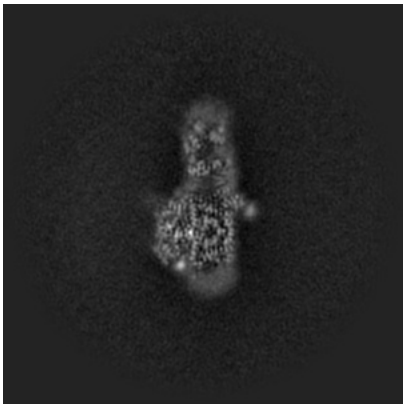
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 190

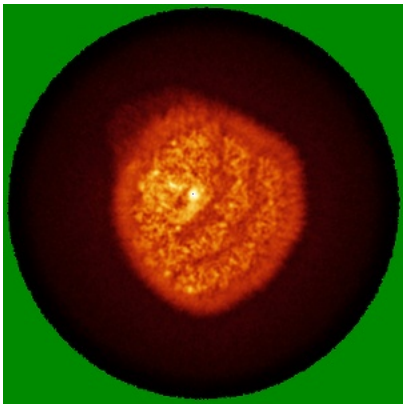

Y Index: 185

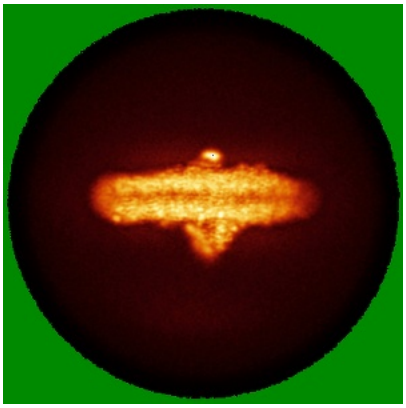

Z Index: 213

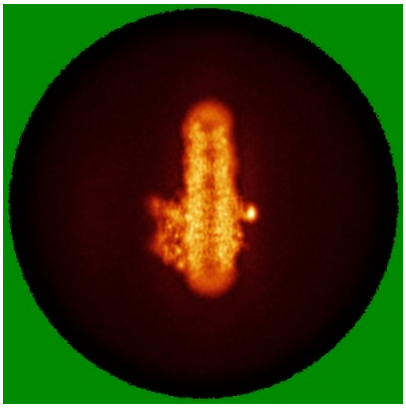
The images above show the largest variance slices of the map in three orthogonal directions.

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

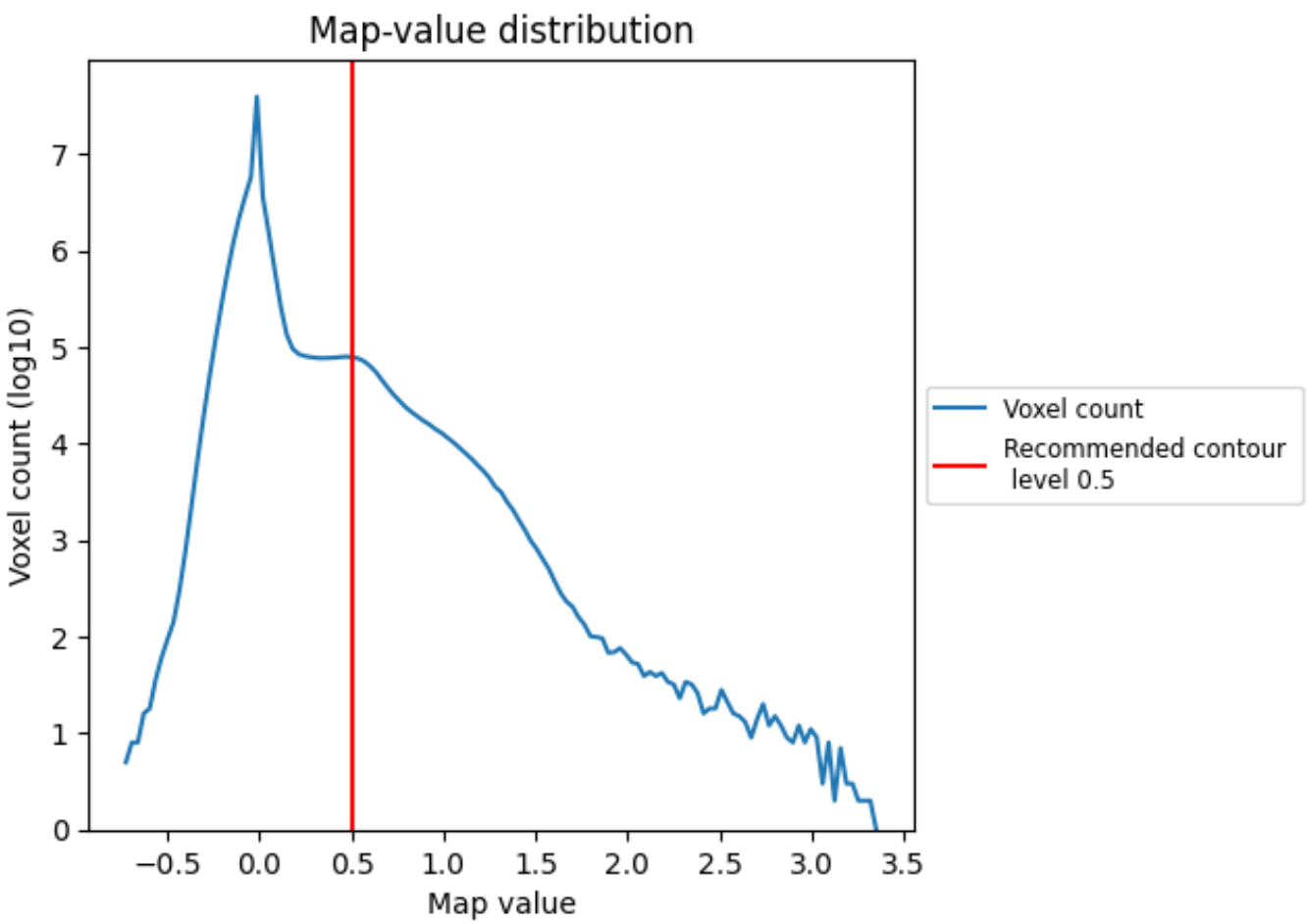
6.6 Mask visualisation (i)

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

7 Map analysis (i)

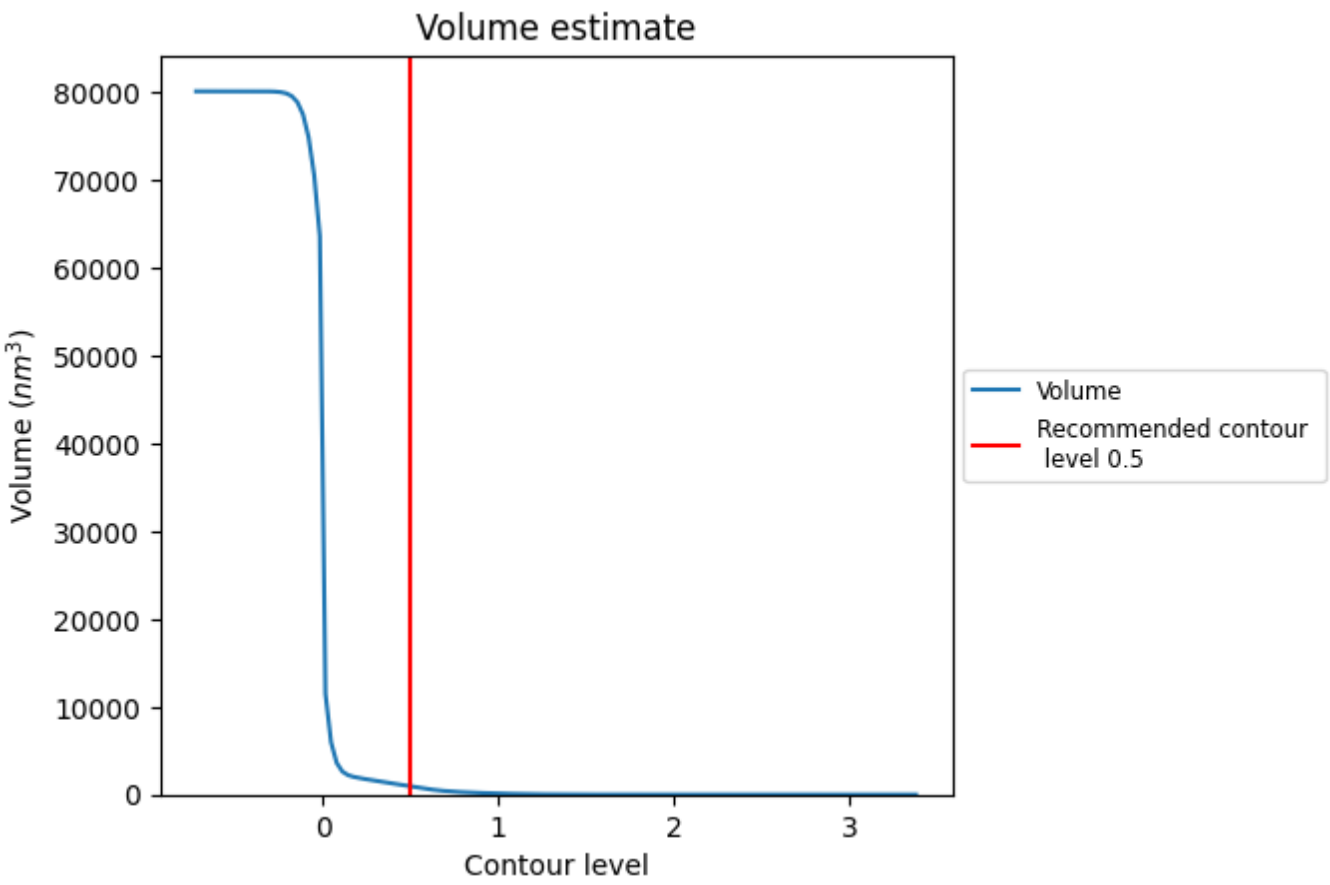
This section contains the results of statistical analysis of the map.

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.

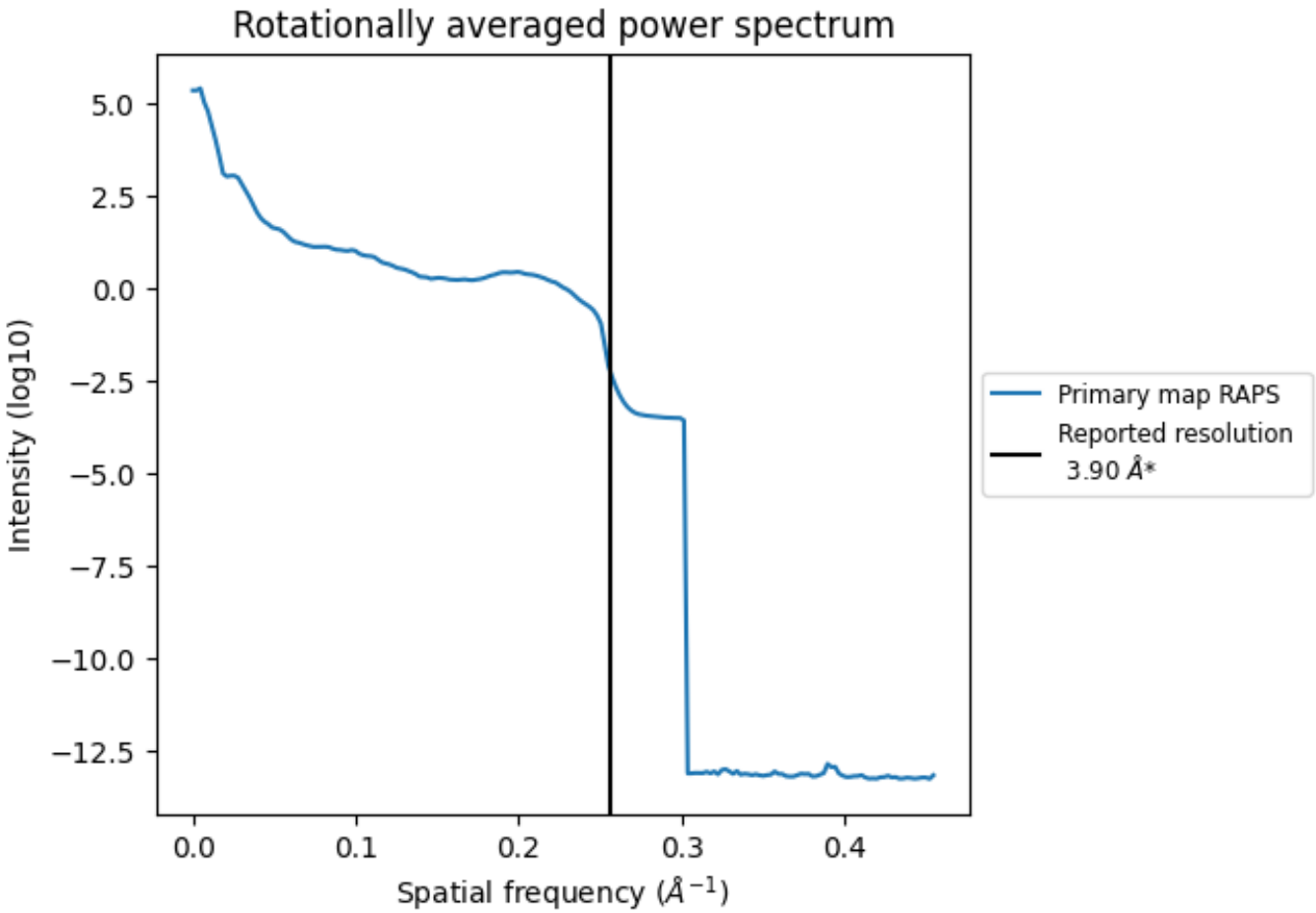
7.2 Volume estimate (i)



The volume at the recommended contour level is 932 nm^3; this corresponds to an approximate mass of 842 kDa.

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

7.3 Rotationally averaged power spectrum (i)

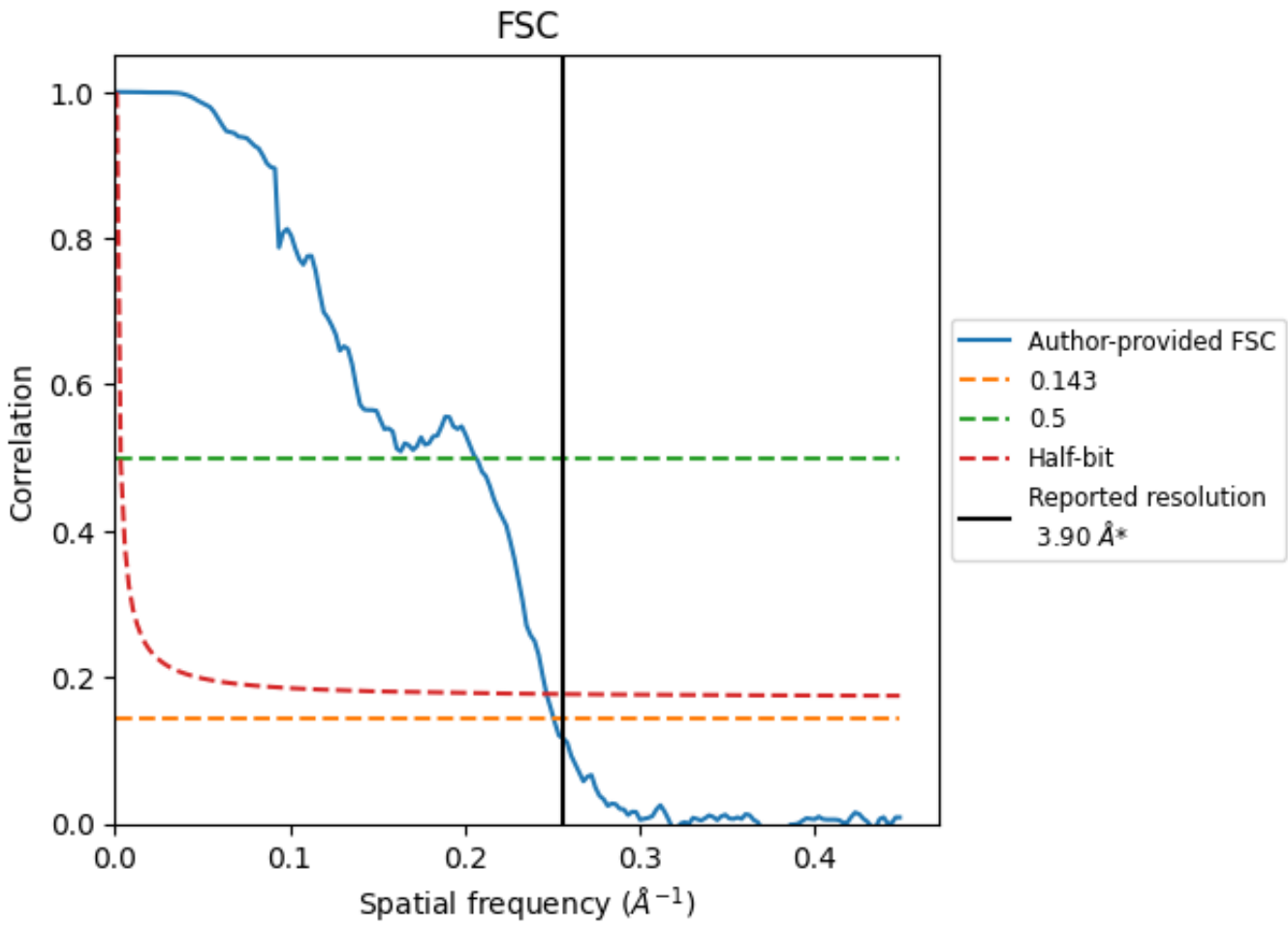


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

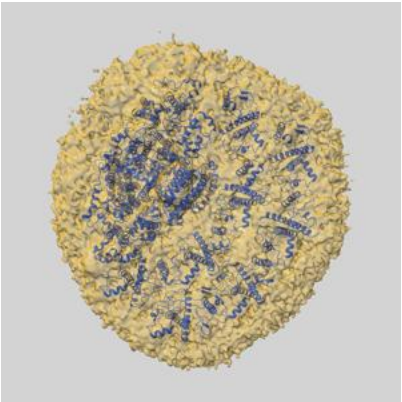
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.98	4.84	4.05
Unmasked-calculated*	-	-	-

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

9 Map-model fit (i)

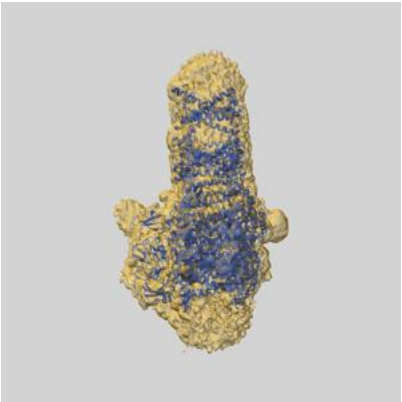
This section contains information regarding the fit between EMDB map EMD-32892 and PDB model 7WYI. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay (i)



X

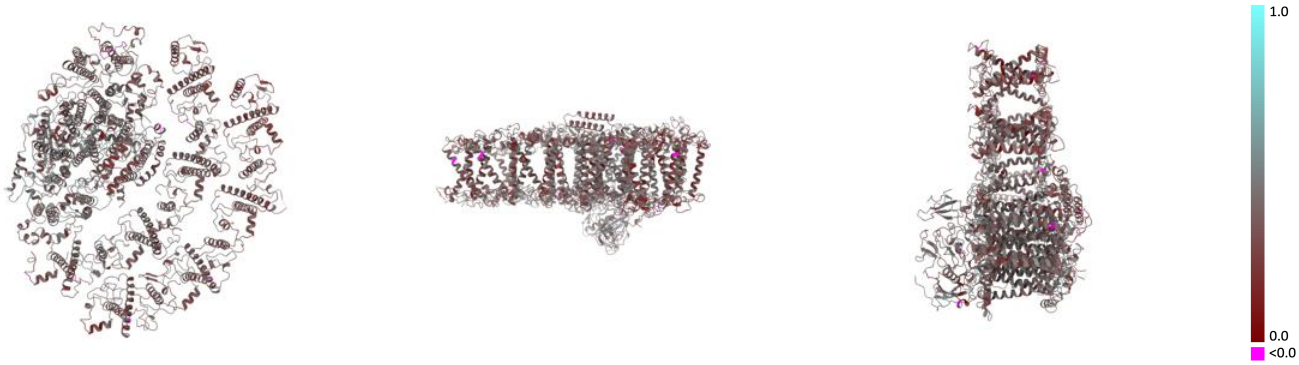
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

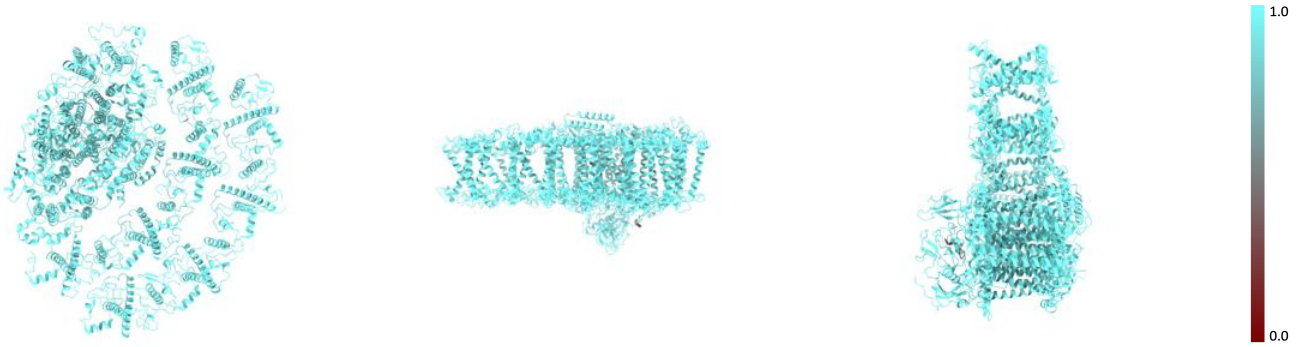
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

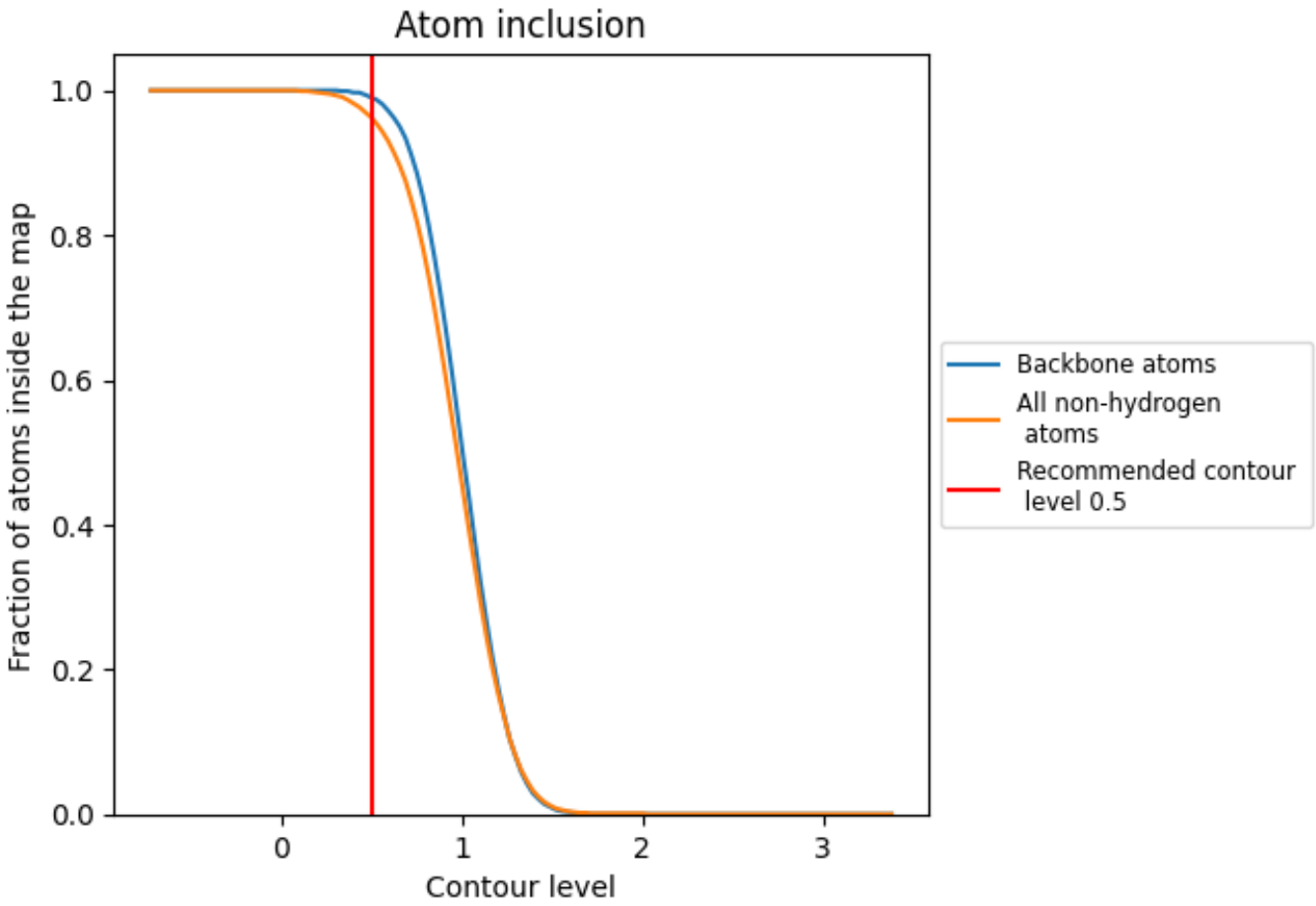
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9620	0.3900
1	0.9600	0.3350
3	0.9640	0.3910
4	0.9760	0.3530
5	0.9670	0.3710
6	0.9670	0.3750
7	0.9710	0.4090
8	0.9670	0.3910
A	0.9600	0.4250
B	0.9480	0.3920
C	0.9900	0.4060
D	0.9320	0.3800
E	0.9970	0.4360
F	0.9670	0.3800
J	0.9590	0.4200
Z	0.9850	0.3180