Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2026 – 05:56 AM JST

PDB ID	:	8H2U / pdb_00008h2u
Title	:	X-ray Structure of photosystem I-LHCI super complex from Chlamydomonas reinhardtii.
Authors	:	Tanaka, H.; Kubota-Kawai, H.; Misumi, Y.; Kurisu, G.
Deposited on	:	2022-10-07
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

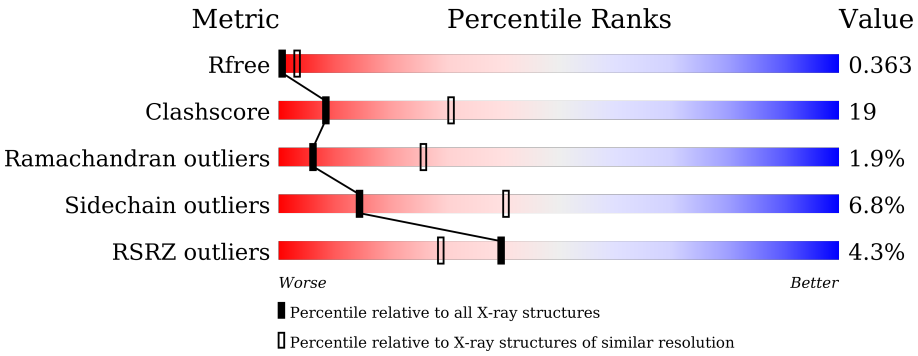
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	4% 69% 26%
2	B	735	4% 67% 28%
3	C	81	9% 68% 28%
4	D	196	2% 63% 8% 28%
5	E	97	54% 9% 37%
6	F	227	3% 56% 9% 34%

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Mol	Chain	Length	Quality of chain
7	G	126	5% 52% 13% 33%
8	H	130	2% 64% 5% 31%
9	I	106	2% 23% 5% 73%
10	J	41	2% 66% 27% 5%
11	K	113	5% 32% 6% 61%
12	L	196	4% 60% 16% 23%
13	0	228	6% 51% 24% 20%
13	1	228	6% 45% 27% 8% 20%
14	8	243	4% 50% 23% 6% 21%
15	7	241	5% 52% 29% 6% 13%
16	3	298	% 48% 18% 33%
17	4	264	3% 52% 22% 23%
18	6	257	2% 42% 25% 28%
19	5	257	3% 37% 31% 5% 25%

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
21	SF4	C	1002	-	-	X	-
27	LMG	0	303	-	-	X	-
27	LMG	4	318	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 42070 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	0	0
			5799	3792	989	996	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	728	Total	C	N	O	S	0	0	0
			5786	3801	969	998	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			600	369	103	116	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1101	703	196	195	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	61	Total	C	N	O	0	0	0
			480	306	85	89			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	150	Total	C	N	O	S	0	0	0
			1150	745	192	210	3			

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	85	Total	C	N	O	0	0	0
			620	398	108	114			

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	90	Total	C	N	O	S	0	0	0
			694	433	120	139	2			

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			221	153	31	36	1			

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	39	Total	C	N	O	S	0	0	0
			320	219	45	55	1			

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	44	Total	C	N	O	S	0	0	0
			295	191	47	55	2			

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	150	Total	C	N	O	S	0	0	0
			1082	703	178	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	0	182	Total	C	N	O	S	0	0	0
			1361	887	226	245	3			
13	1	182	Total	C	N	O	S	0	0	0
			1362	886	226	247	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	8	193	Total	C	N	O	S	0	0	0
			1466	953	251	258	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	7	209	Total	C	N	O	S	0	0	0
			1622	1051	271	294	6			

- Molecule 16 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	201	Total	C	N	O	S	0	0	0
			1542	1008	250	276	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	202	Total	C	N	O	S	0	0	0
			1571	1031	254	281	5			

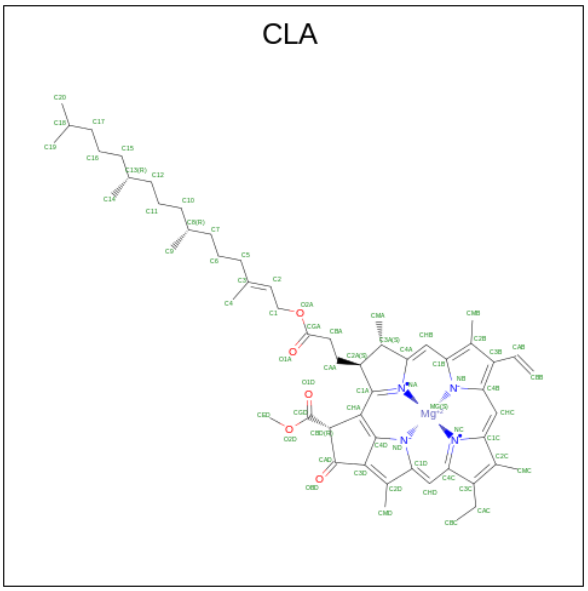
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	6	184	Total	C	N	O	S	0	0	0
			1431	945	235	247	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	5	193	Total	C	N	O	S	0	0	0
			1510	984	255	264	7			

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			40	32	1	4	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
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			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
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			43	33	1	4	5		
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			44	34	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	K	1	Total	C	Mg	N		0	0
			27	22	1	4			
20	L	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	0	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	8	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	8	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	8	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	8	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	8	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	8	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	8	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	8	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	8	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	8	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	7	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	7	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	7	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	7	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	7	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	7	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	7	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	7	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	7	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			40	32	1	4	3		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	4	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

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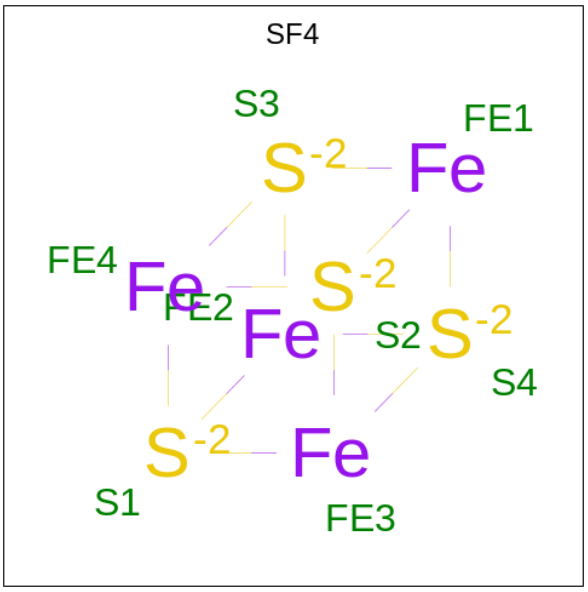
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	6	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

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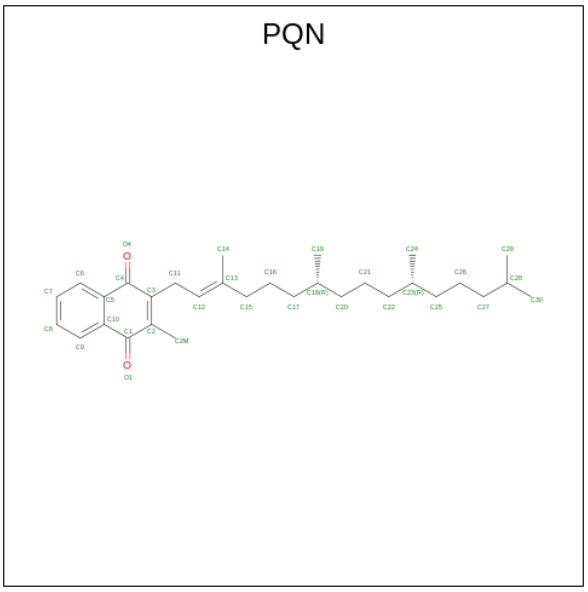
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



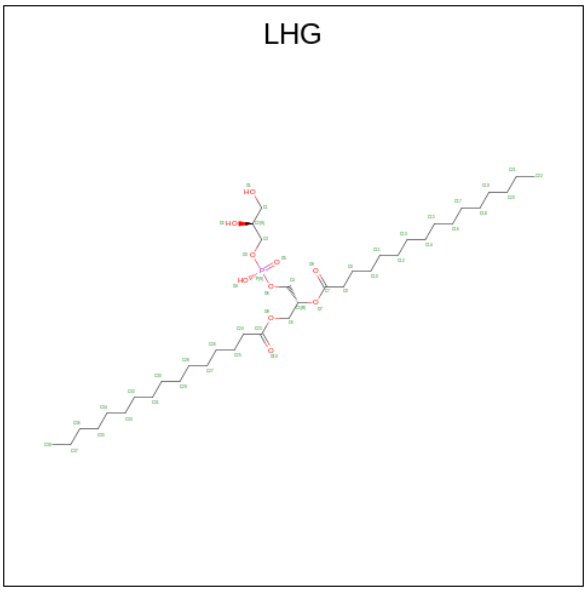
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Fe	S		0	0
			8	4	4			
21	C	1	Total	Fe	S		0	0
			8	4	4			
21	C	1	Total	Fe	S		0	0
			8	4	4			

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



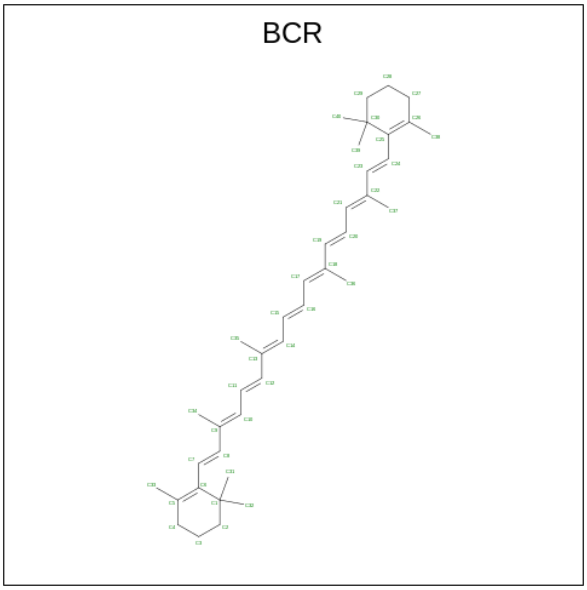
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O P 40 29 10 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O	P	0	0
			49	38	10	1		
23	0	1	Total	C	O	P	0	0
			21	10	10	1		
23	8	1	Total	C	O	P	0	0
			49	38	10	1		
23	7	1	Total	C	O	P	0	0
			35	24	10	1		
23	3	1	Total	C	O	P	0	0
			20	10	9	1		
23	4	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1	Total	C	0	0
			40	40		
24	A	1	Total	C	0	0
			40	40		
24	A	1	Total	C	0	0
			40	40		
24	A	1	Total	C	0	0
			40	40		
24	A	1	Total	C	0	0
			40	40		

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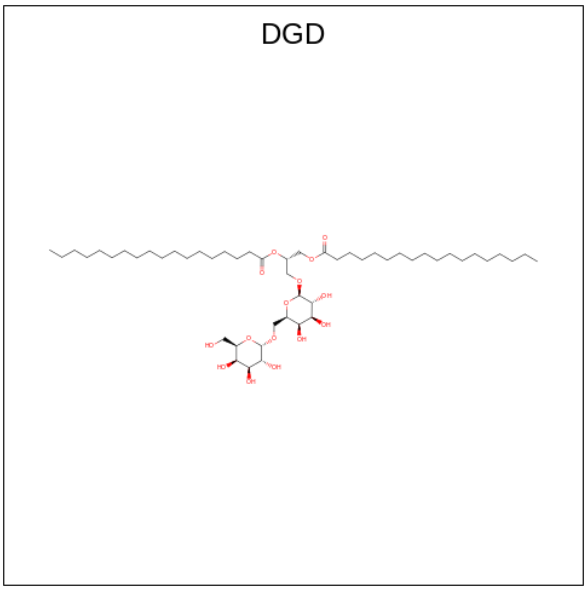
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	G	1	Total C 40 40	0	0
24	G	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	I	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	8	1	Total C 40 40	0	0
24	7	1	Total C 40 40	0	0
24	3	1	Total C 40 40	0	0
24	3	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	4	1	Total C 40 40	0	0
24	6	1	Total C 40 40	0	0

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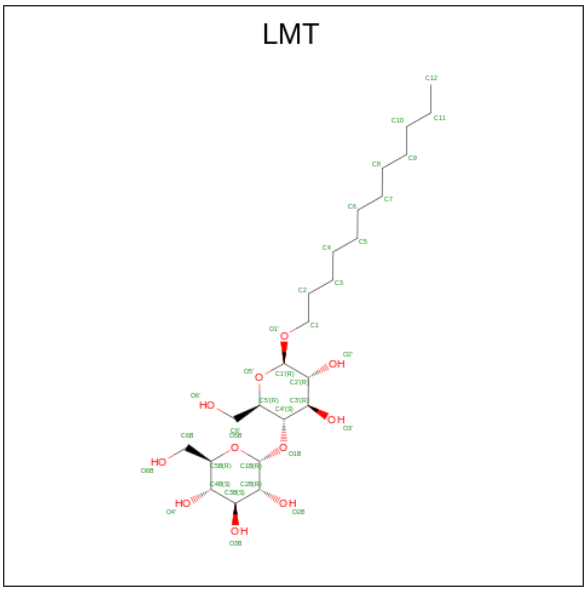
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	5	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



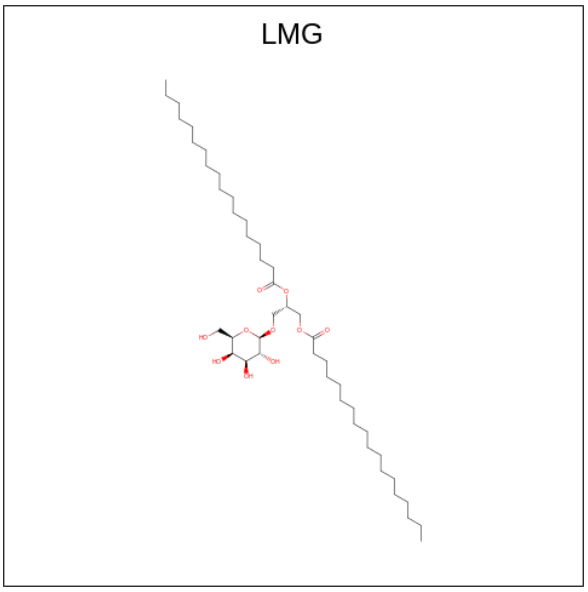
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 61 46 15	0	0
25	5	1	Total C O 51 36 15	0	0

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	B	1	Total C O 31 20 11	0	0
26	3	1	Total C O 31 20 11	0	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



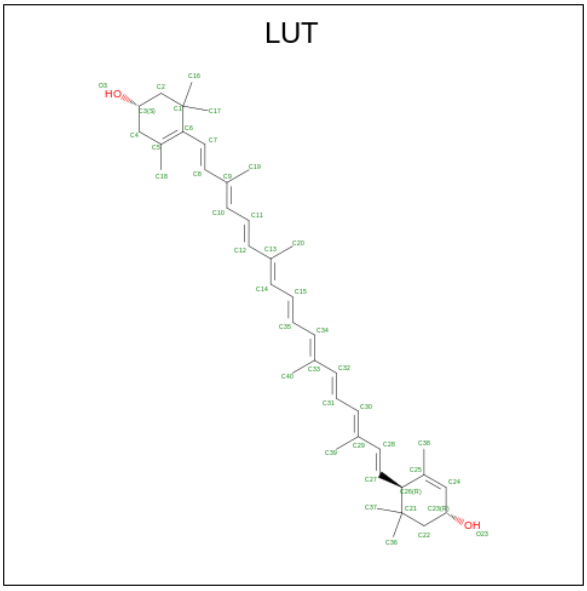
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	J	1	Total C O 30 20 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	0	1	Total C O 50 40 10	0	0
27	8	1	Total C O 28 18 10	0	0
27	8	1	Total C O 44 34 10	0	0
27	4	1	Total C O 34 24 10	0	0
27	6	1	Total C O 44 34 10	0	0
27	5	1	Total C O 45 35 10	0	0

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



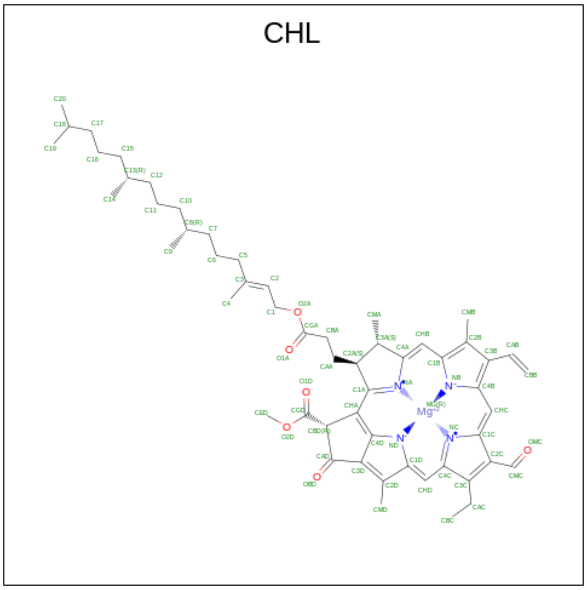
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	J	1	Total C O 42 40 2	0	0
28	0	1	Total C O 42 40 2	0	0
28	0	1	Total C O 42 40 2	0	0
28	8	1	Total C O 42 40 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	7	1	Total C O 42 40 2	0	0
28	3	1	Total C O 42 40 2	0	0
28	3	1	Total C O 42 40 2	0	0
28	1	1	Total C O 42 40 2	0	0
28	1	1	Total C O 42 40 2	0	0
28	4	1	Total C O 42 40 2	0	0
28	6	1	Total C O 42 40 2	0	0
28	5	1	Total C O 42 40 2	0	0

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	0	1	Total C Mg N O 47 36 1 4 6	0	0
29	0	1	Total C Mg N O 51 40 1 4 6	0	0
29	0	1	Total C Mg N O 61 50 1 4 6	0	0

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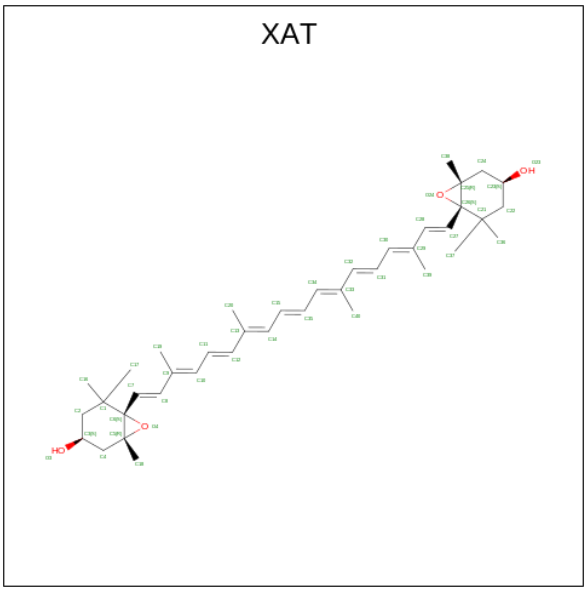
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	8	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	8	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
29	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	1	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
29	6	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	6	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	6	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	6	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
29	5	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	5	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	5	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	5	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 30 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	8	1	Total	C	O	0	0
			44	40	4		
30	7	1	Total	C	O	0	0
			44	40	4		
30	4	1	Total	C	O	0	0
			44	40	4		
30	6	1	Total	C	O	0	0
			44	40	4		
30	5	1	Total	C	O	0	0
			44	40	4		

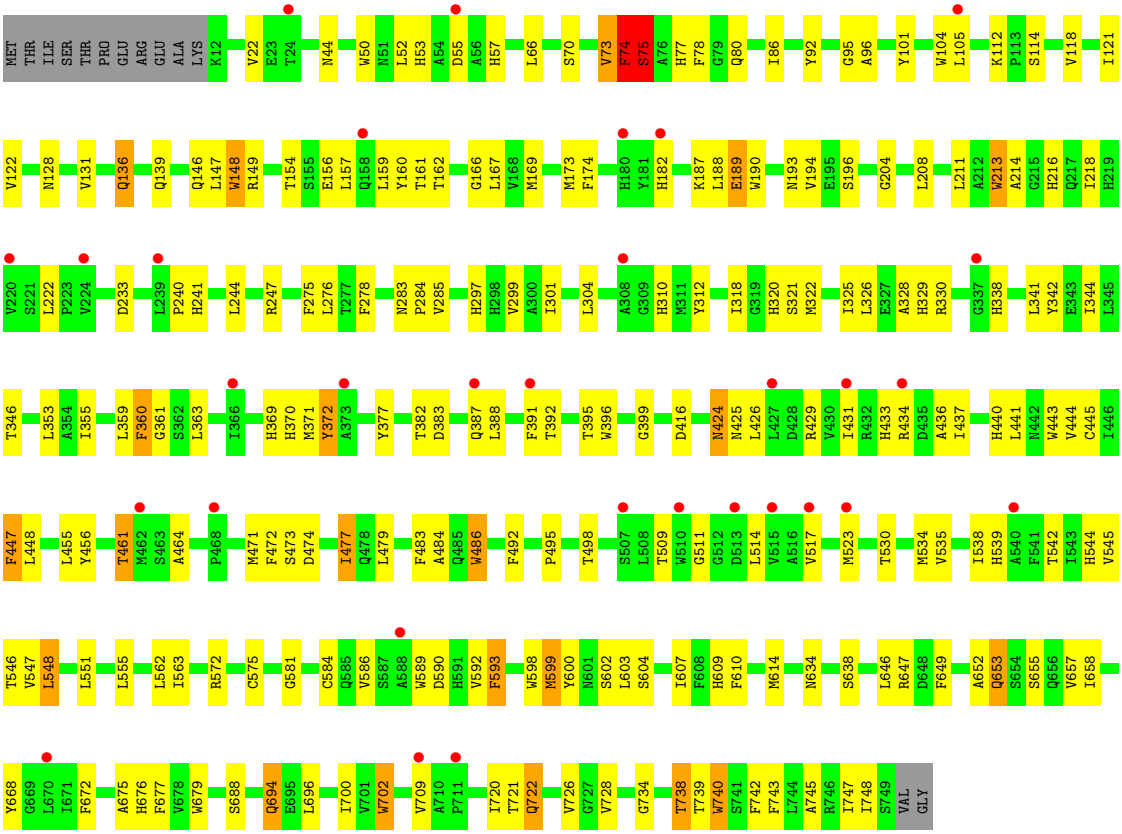
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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:

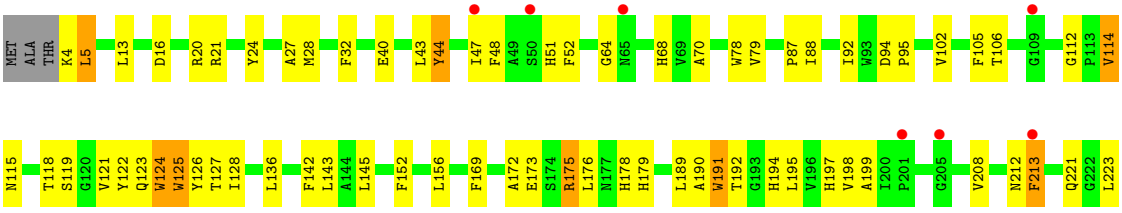


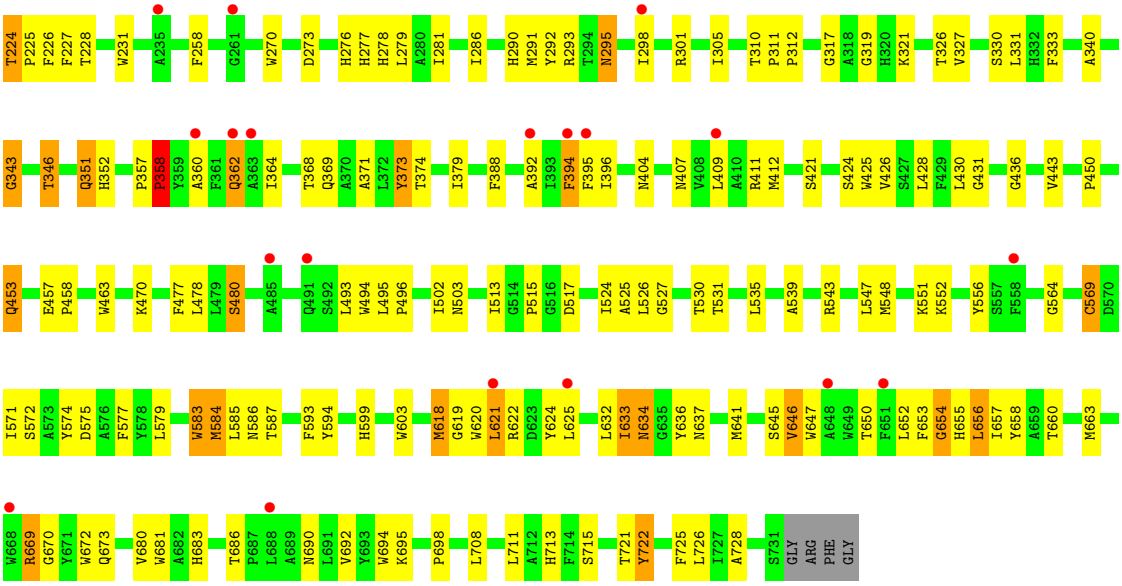


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

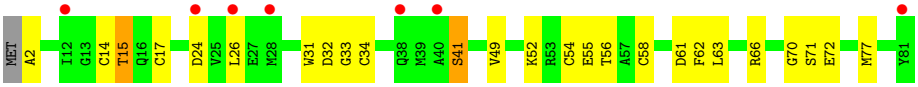






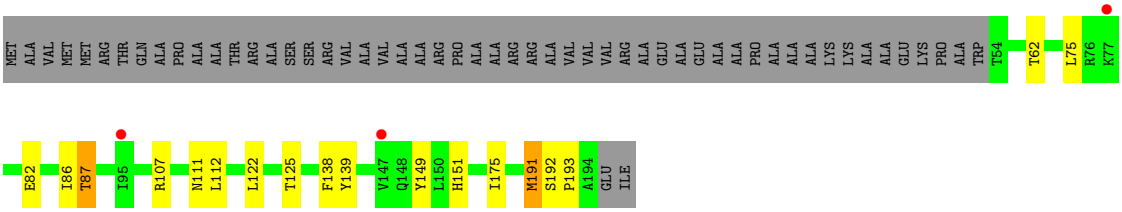
• Molecule 3: Photosystem I iron-sulfur center





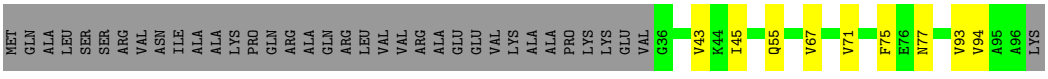
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic





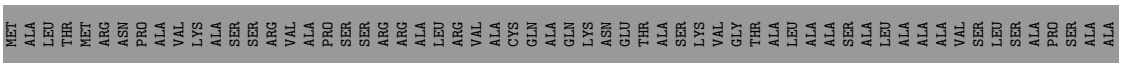
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

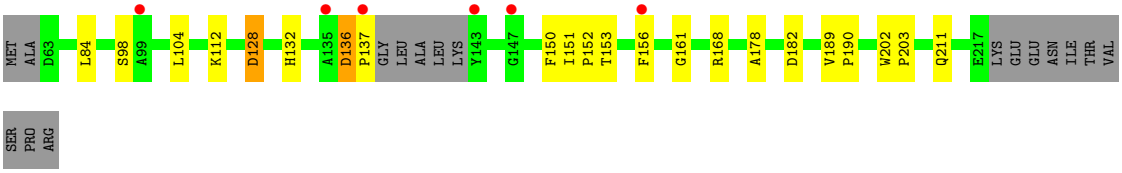




• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

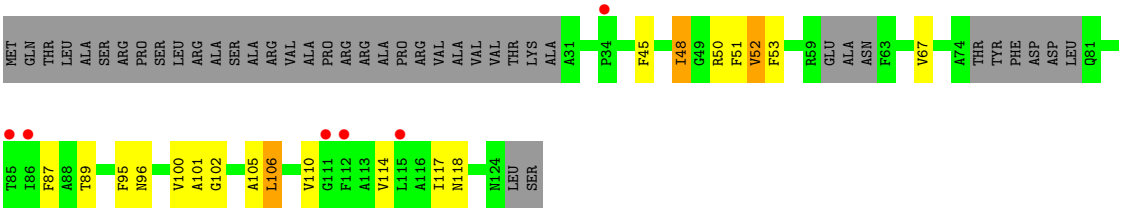






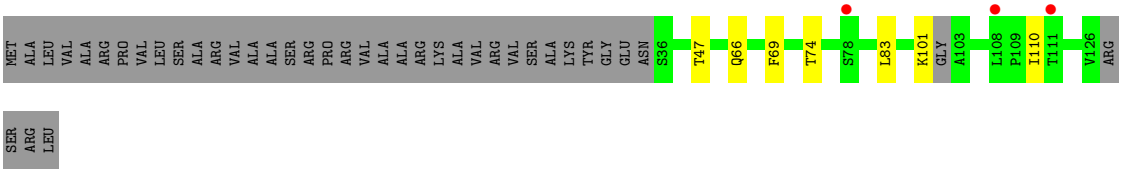
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic





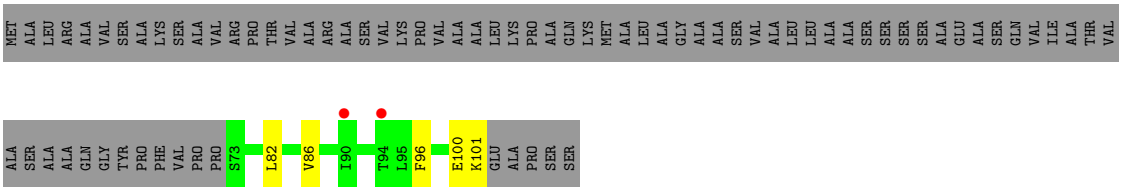
• Molecule 8: Photosystem I reaction center subunit VI, chloroplastic





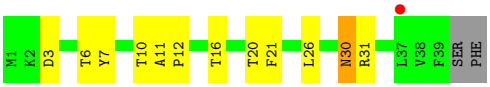
• Molecule 9: Photosystem I reaction center subunit VIII





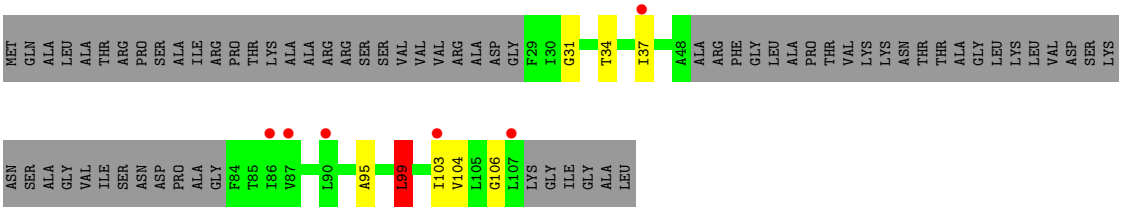
• Molecule 10: Photosystem I reaction center subunit IX





• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

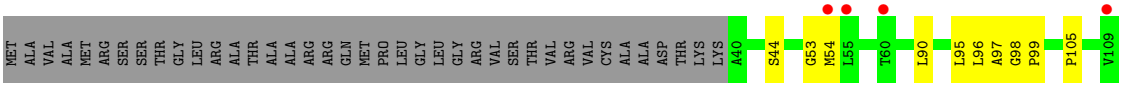


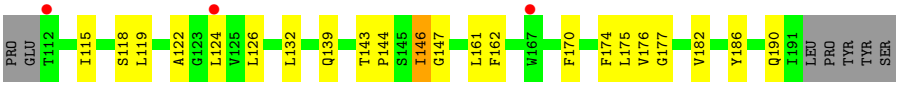


• Molecule 12: PSI subunit V

Chain L:



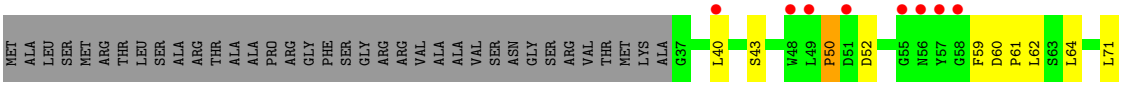


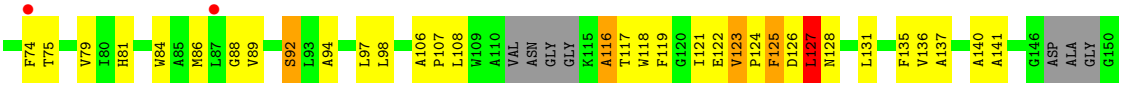


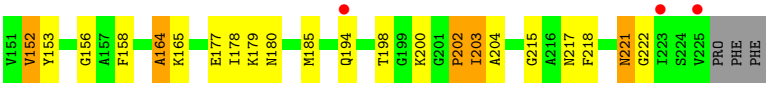
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 0:







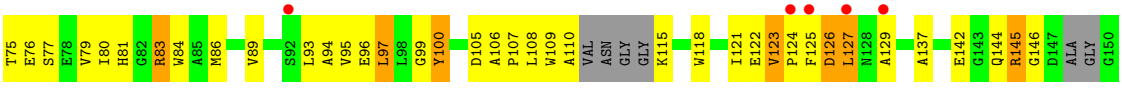


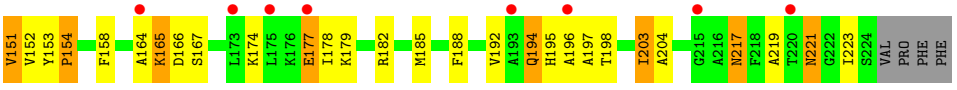
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 1:





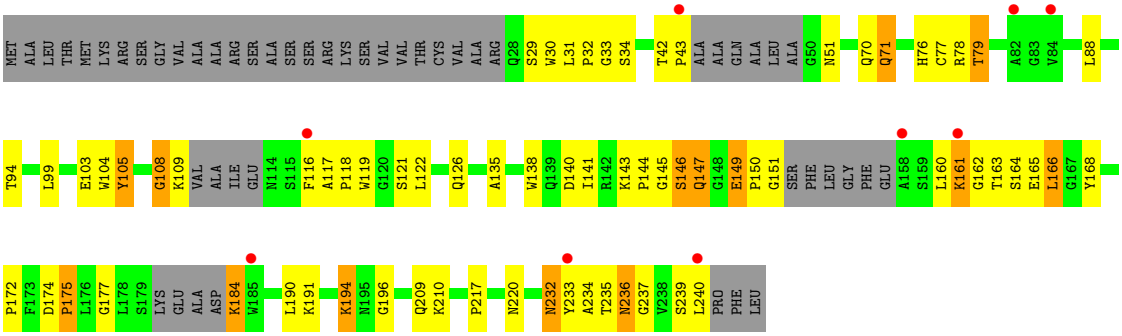




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 8:

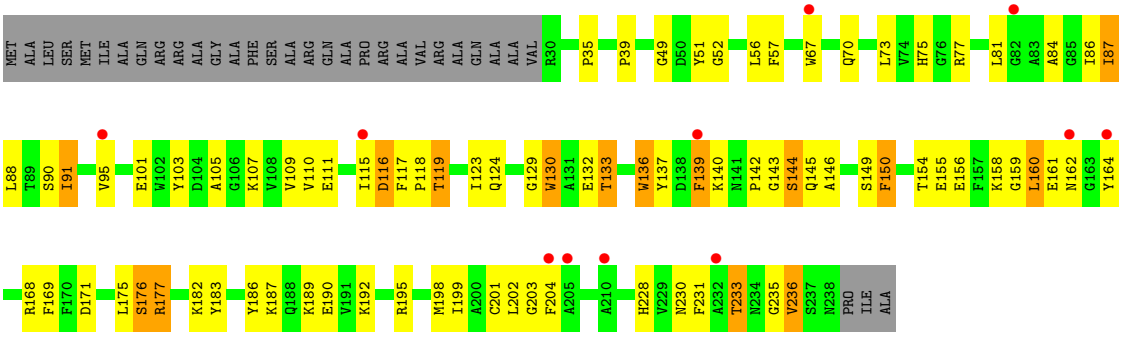




• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 7:

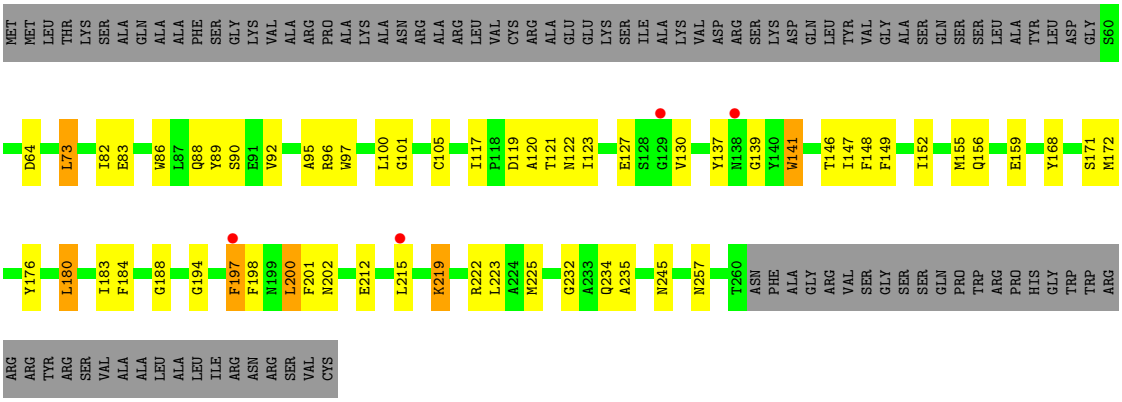




• Molecule 16: Lhca3

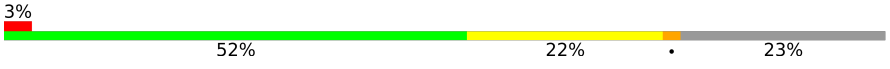
Chain 3:

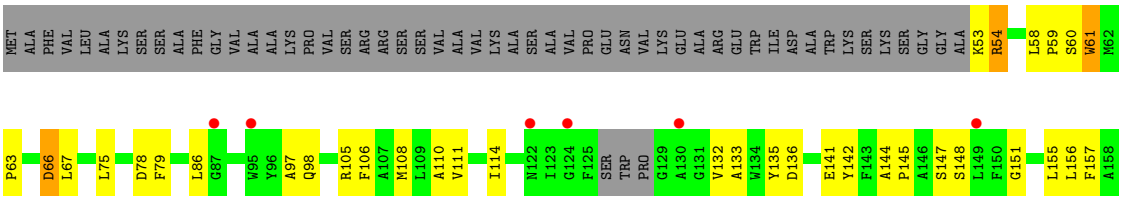


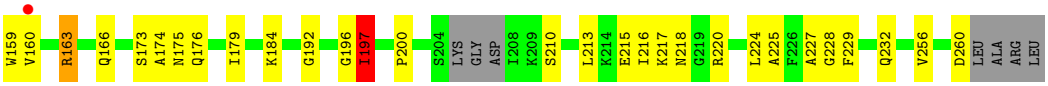


• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 4:

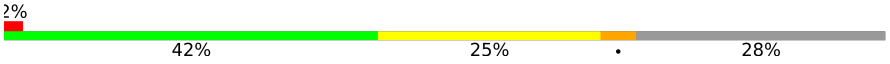


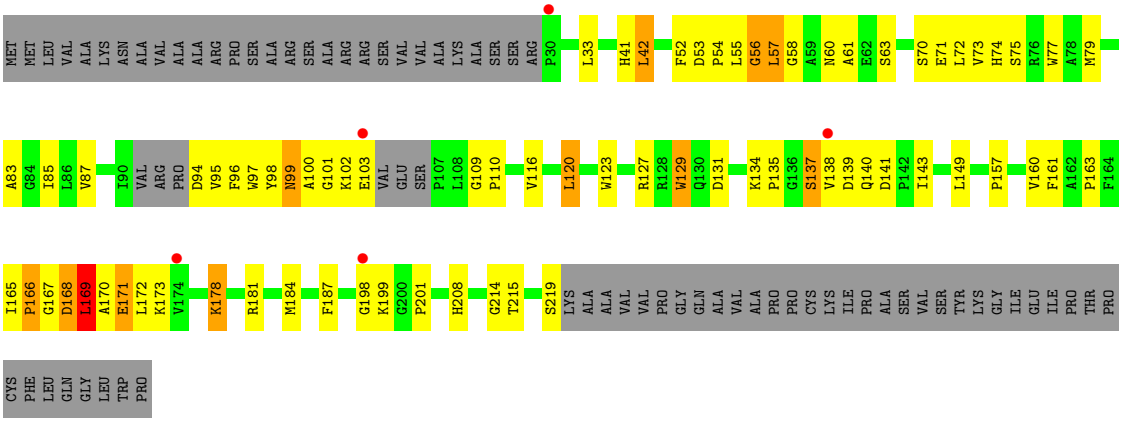




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

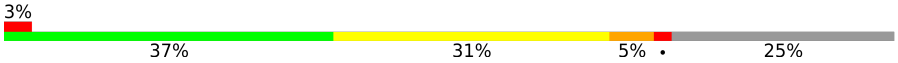
Chain 6:

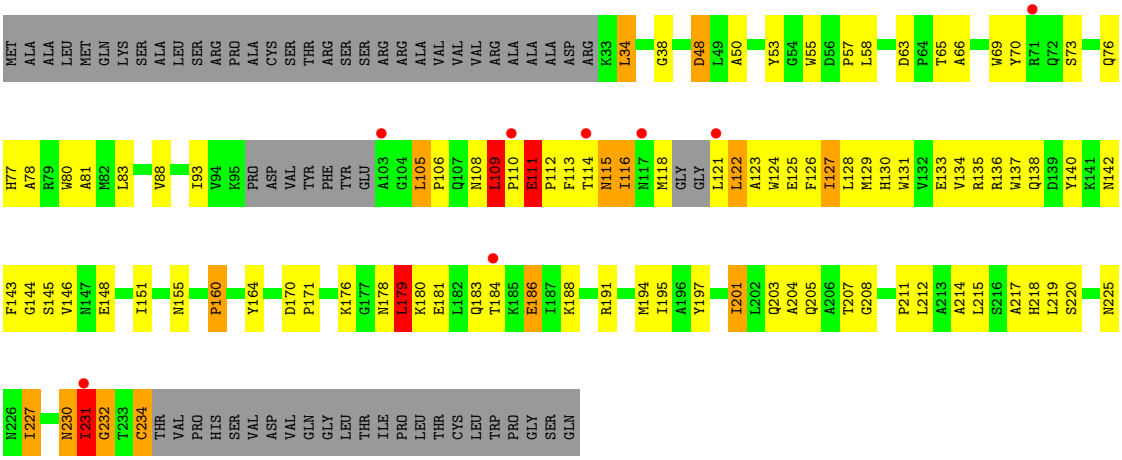




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 5:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	194.57Å 98.12Å 210.13Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	47.74 – 3.40 47.74 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.74-3.40) 99.1 (47.74-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.291 , 0.359 0.300 , 0.363	Depositor DCC
R_{free} test set	5416 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	108.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 121.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	42070	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, CLA, SF4, XAT, LUT, LHG, CHL, BCR, LMG, PQN, DGD

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	0.94	10/5995 (0.2%)	1.16	15/8175 (0.2%)
2	B	0.91	9/5997 (0.2%)	1.16	14/8190 (0.2%)
3	C	0.83	0/610	1.04	0/826
4	D	1.03	0/1127	1.33	0/1521
5	E	1.05	0/490	1.26	0/667
6	F	0.99	0/1174	1.53	2/1588 (0.1%)
7	G	1.04	0/631	1.55	2/855 (0.2%)
8	H	1.06	0/704	1.47	0/947
9	I	1.05	0/228	1.53	0/314
10	J	0.98	0/331	1.44	0/454
11	K	1.09	0/296	1.77	2/401 (0.5%)
12	L	1.08	0/1106	1.55	0/1512
13	0	1.00	0/1402	1.53	1/1906 (0.1%)
13	1	0.99	0/1403	1.47	0/1907
14	8	0.99	0/1509	1.51	4/2050 (0.2%)
15	7	1.00	0/1673	1.49	6/2270 (0.3%)
16	3	0.99	0/1587	1.52	0/2154
17	4	0.97	0/1621	1.47	2/2206 (0.1%)
18	6	0.98	0/1479	1.53	2/2012 (0.1%)
19	5	0.97	0/1553	1.41	2/2107 (0.1%)
All	All	0.97	19/30916 (0.1%)	1.36	52/42062 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
13	0	0	3
13	1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	8	0	1
19	5	0	2
All	All	0	8

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	TYR	C-O	7.60	1.32	1.24
1	A	652	ALA	C-O	7.22	1.32	1.24
2	B	583	TRP	C-O	-7.19	1.15	1.24
1	A	589	TRP	C-O	6.82	1.31	1.24
1	A	148	TRP	C-O	6.68	1.31	1.24
1	A	486	TRP	C-O	6.58	1.31	1.24
2	B	52	PHE	C-O	6.36	1.31	1.24
1	A	189	GLU	C-O	6.10	1.31	1.24
2	B	680	VAL	C-O	-6.10	1.16	1.24
2	B	44	TYR	C-O	5.87	1.30	1.24
1	A	740	TRP	C-O	-5.72	1.17	1.24
1	A	240	PRO	C-O	-5.51	1.16	1.24
1	A	328	ALA	C-O	5.51	1.30	1.24
2	B	656	LEU	C-O	-5.38	1.18	1.24
2	B	654	GLY	C-O	-5.27	1.17	1.23
2	B	584	MET	C-O	-5.22	1.18	1.24
2	B	327	VAL	C-O	5.18	1.29	1.23
2	B	425	TRP	C-O	-5.16	1.18	1.24
1	A	361	GLY	C-O	-5.03	1.17	1.23

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	SER	N-CA-C	-8.48	101.07	111.33
2	B	152	PHE	N-CA-C	-8.25	100.95	111.02
2	B	191	TRP	N-CA-C	-7.78	102.49	110.97
14	8	88	LEU	CA-C-N	7.77	125.14	120.24
14	8	88	LEU	C-N-CA	7.77	125.14	120.24
1	A	360	PHE	N-CA-C	-6.71	103.66	110.97
1	A	738	THR	N-CA-CB	6.44	119.41	110.07
1	A	213	TRP	N-CA-C	-6.39	104.00	110.97
2	B	221	GLN	CA-C-N	6.30	126.09	120.10
2	B	221	GLN	C-N-CA	6.30	126.09	120.10
1	A	548	LEU	CB-CA-C	-6.16	101.47	110.96
1	A	92	TYR	N-CA-C	-5.97	104.47	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	604	SER	CA-C-O	-5.95	114.24	120.55
2	B	669	ARG	N-CA-C	5.81	117.30	110.97
2	B	394	PHE	N-CA-C	-5.79	104.66	110.97
11	K	99	LEU	CA-C-N	5.69	126.40	120.03
11	K	99	LEU	C-N-CA	5.69	126.40	120.03
2	B	343	GLY	O-C-N	5.68	127.70	122.19
2	B	426	VAL	CA-C-O	-5.67	115.15	121.05
14	8	30	TRP	CA-C-N	5.64	128.09	122.00
14	8	30	TRP	C-N-CA	5.64	128.09	122.00
1	A	74	PHE	CA-CB-CG	5.58	119.38	113.80
2	B	175	ARG	CB-CA-C	-5.58	101.52	110.79
6	F	98	SER	CA-C-N	5.51	125.95	119.83
6	F	98	SER	C-N-CA	5.51	125.95	119.83
15	7	75	HIS	CA-C-N	5.50	126.08	119.98
15	7	75	HIS	C-N-CA	5.50	126.08	119.98
2	B	373	TYR	CB-CA-C	5.49	120.18	110.85
1	A	73	VAL	CA-C-O	-5.40	115.33	120.95
1	A	299	VAL	CA-C-O	-5.38	115.47	121.17
2	B	722	TYR	CA-C-O	-5.37	115.18	120.82
15	7	84	ALA	CA-C-N	5.36	125.92	119.98
15	7	84	ALA	C-N-CA	5.36	125.92	119.98
1	A	702	TRP	N-CA-C	-5.34	104.50	111.02
2	B	213	PHE	N-CA-C	-5.33	104.72	111.11
7	G	106	LEU	CA-C-N	5.30	125.96	120.03
7	G	106	LEU	C-N-CA	5.30	125.96	120.03
2	B	647	TRP	N-CA-C	-5.27	105.45	111.14
17	4	218	ASN	CA-C-N	5.25	125.66	119.94
17	4	218	ASN	C-N-CA	5.25	125.66	119.94
19	5	122	LEU	CA-C-N	5.19	127.69	120.63
19	5	122	LEU	C-N-CA	5.19	127.69	120.63
2	B	436	GLY	CA-C-O	-5.18	115.73	120.80
1	A	722	GLN	CB-CA-C	-5.12	102.28	110.79
1	A	44	ASN	N-CA-C	-5.11	106.74	113.12
13	0	50	PRO	N-CA-C	5.11	120.31	114.03
18	6	168	ASP	CA-C-N	5.07	131.23	121.54
18	6	168	ASP	C-N-CA	5.07	131.23	121.54
1	A	609	HIS	N-CA-C	-5.05	104.86	111.02
1	A	672	PHE	CA-C-O	-5.02	115.54	121.07
15	7	130	TRP	CA-C-N	5.01	126.99	120.28
15	7	130	TRP	C-N-CA	5.01	126.99	120.28

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	0	125	PHE	Peptide
13	0	164	ALA	Peptide
13	0	198	THR	Peptide
13	1	164	ALA	Peptide
19	5	160	PRO	Peptide
19	5	231	ILE	Peptide
14	8	232	ASN	Peptide
1	A	447	PHE	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5799	0	5646	194	0
2	B	5786	0	5542	223	0
3	C	600	0	583	21	0
4	D	1101	0	1123	11	0
5	E	480	0	476	7	0
6	F	1150	0	1174	17	0
7	G	620	0	612	44	0
8	H	694	0	682	6	0
9	I	221	0	234	3	0
10	J	320	0	322	10	0
11	K	295	0	312	10	0
12	L	1082	0	1103	27	0
13	0	1361	0	1318	65	0
13	1	1362	0	1313	89	0
14	8	1466	0	1444	78	0
15	7	1622	0	1552	92	0
16	3	1542	0	1511	74	0
17	4	1571	0	1529	83	0
18	6	1431	0	1415	66	0
19	5	1510	0	1499	116	0
20	0	484	0	330	22	0
20	1	484	0	330	35	0
20	3	524	0	356	19	0
20	4	396	0	270	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	5	660	0	450	57	0
20	6	528	0	360	33	0
20	7	396	0	270	27	0
20	8	440	0	300	26	0
20	A	1844	0	1256	97	0
20	B	1803	0	1225	105	0
20	F	132	0	90	6	0
20	G	132	0	90	13	0
20	J	44	0	30	3	0
20	K	71	0	33	5	0
20	L	176	0	120	11	0
21	A	8	0	0	1	0
21	C	16	0	0	2	0
22	A	33	0	46	3	0
22	B	33	0	46	3	0
23	0	21	0	12	3	0
23	3	20	0	14	5	0
23	4	49	0	74	15	0
23	7	35	0	40	6	0
23	8	49	0	74	0	0
23	A	89	0	127	4	0
24	1	40	0	56	7	0
24	3	80	0	112	5	0
24	4	40	0	56	4	0
24	5	40	0	56	16	0
24	6	40	0	56	14	0
24	7	40	0	56	2	0
24	8	40	0	56	5	0
24	A	240	0	336	25	0
24	B	240	0	336	31	0
24	F	80	0	112	7	0
24	G	80	0	112	25	0
24	H	40	0	56	2	0
24	I	40	0	56	17	0
24	J	40	0	56	0	0
25	5	51	0	60	16	0
25	B	61	0	83	4	0
26	3	31	0	35	8	0
26	B	31	0	35	3	0
27	0	50	0	70	27	0
27	4	34	0	38	38	0
27	5	45	0	60	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	6	44	0	61	9	0
27	8	72	0	86	10	0
27	J	30	0	30	0	0
28	0	84	0	112	13	0
28	1	84	0	112	18	0
28	3	84	0	112	5	0
28	4	42	0	56	2	0
28	5	42	0	56	6	0
28	6	42	0	56	3	0
28	7	42	0	56	4	0
28	8	42	0	56	4	0
28	J	42	0	56	10	0
29	0	159	0	124	15	0
29	1	159	0	124	15	0
29	3	47	0	31	1	0
29	4	202	0	153	15	0
29	5	202	0	153	16	0
29	6	202	0	154	12	0
29	7	207	0	164	16	0
29	8	159	0	124	8	0
30	4	44	0	56	2	0
30	5	44	0	56	6	0
30	6	44	0	56	10	0
30	7	44	0	56	0	0
30	8	44	0	56	1	0
All	All	42070	0	39382	1552	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 19.

All (1552) 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)
1:A:738:THR:OG1	20:A:801:CLA:O2D	1.57	1.22
17:4:54:ARG:HB3	17:4:67:LEU:O	1.45	1.17
1:A:473:SER:O	1:A:477:ILE:O	1.64	1.14
20:1:1007:CLA:HBC1	20:1:1014:CLA:HBC2	1.26	1.14
20:4:307:CLA:HAC1	27:4:318:LMG:H151	1.22	1.14
2:B:371:ALA:HB1	20:B:829:CLA:HMA1	1.29	1.10
20:A:813:CLA:HBA2	20:A:815:CLA:HMB3	1.31	1.10
7:G:51:PHE:CD1	24:G:205:BCR:HC21	1.88	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:0:309:CLA:HBC1	20:0:316:CLA:HBC2	1.34	1.05
17:4:224:LEU:HG	27:4:318:LMG:H152	1.40	1.03
15:7:87:ILE:HD11	15:7:204:PHE:CZ	1.93	1.03
20:4:307:CLA:CAC	27:4:318:LMG:H151	1.87	1.02
19:5:179:LEU:HD13	19:5:180:LYS:H	1.24	1.02
7:G:51:PHE:CG	24:G:205:BCR:HC21	1.94	1.01
28:1:1002:LUT:H28	28:1:1002:LUT:H361	1.42	1.01
13:1:123:VAL:HG12	13:1:124:PRO:HD2	1.42	1.01
16:3:123:ILE:HD11	16:3:137:TYR:CE1	2.00	0.96
20:4:307:CLA:HAC1	27:4:318:LMG:C15	1.96	0.95
20:A:813:CLA:CBA	20:A:815:CLA:HMB3	1.95	0.95
18:6:123:TRP:CZ3	24:6:302:BCR:H322	2.02	0.94
19:5:131:TRP:CZ3	24:5:320:BCR:C33	2.50	0.94
13:1:59:PHE:CD2	28:1:1002:LUT:H383	2.03	0.93
19:5:109:LEU:HB2	19:5:110:PRO:CD	1.99	0.93
7:G:51:PHE:HB3	24:G:205:BCR:H323	1.51	0.91
7:G:114:VAL:HG22	27:0:303:LMG:H122	1.52	0.91
13:0:131:LEU:HB3	27:0:303:LMG:H141	1.50	0.91
19:5:109:LEU:HB2	19:5:110:PRO:HD2	1.51	0.91
3:C:17:CYS:SG	21:C:1002:SF4:FE2	1.64	0.90
14:8:147:GLN:HE21	14:8:147:GLN:HA	1.36	0.90
13:1:152:VAL:HG13	13:1:153:TYR:CD2	2.05	0.90
14:8:161:LYS:HG2	14:8:172:PRO:HG3	1.54	0.90
17:4:54:ARG:CB	17:4:67:LEU:O	2.20	0.89
2:B:655:HIS:HB3	20:B:801:CLA:HBD	1.54	0.89
20:B:817:CLA:HAA2	24:B:845:BCR:H392	1.54	0.88
15:7:199:ILE:O	15:7:202:LEU:HG	1.73	0.88
15:7:202:LEU:HD12	15:7:203:GLY:N	1.89	0.86
2:B:301:ARG:HB2	7:G:67:VAL:HG13	1.58	0.86
13:0:127:LEU:HD12	27:0:303:LMG:HC1	1.57	0.86
1:A:471:MET:O	1:A:477:ILE:HB	1.76	0.85
28:0:304:LUT:H28	28:0:304:LUT:H361	1.57	0.85
15:7:171:ASP:CG	15:7:176:SER:OG	2.19	0.85
20:4:307:CLA:HBC1	27:4:318:LMG:H142	1.59	0.85
24:4:302:BCR:H403	24:4:302:BCR:H23C	1.57	0.85
2:B:226:PHE:CZ	24:B:843:BCR:H321	2.11	0.85
15:7:105:ALA:O	15:7:109:VAL:HG23	1.77	0.85
2:B:125:TRP:CZ3	24:B:845:BCR:H282	2.12	0.84
1:A:434:ARG:CZ	1:A:555:LEU:O	2.26	0.83
1:A:441:LEU:HB3	1:A:548:LEU:HD22	1.59	0.83
20:1:1007:CLA:HBC1	20:1:1014:CLA:CBC	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:208:HIS:HA	18:6:215:THR:OG1	1.77	0.83
19:5:131:TRP:CZ3	24:5:320:BCR:H332	2.13	0.83
15:7:202:LEU:HD11	20:7:1006:CLA:HMC1	1.60	0.83
15:7:171:ASP:CG	15:7:176:SER:HG	1.86	0.83
19:5:131:TRP:CH2	24:5:320:BCR:H332	2.14	0.82
7:G:51:PHE:CB	24:G:205:BCR:H323	2.09	0.82
1:A:472:PHE:CD1	1:A:477:ILE:HG21	2.15	0.82
1:A:658:ILE:HD11	20:A:801:CLA:HBC1	1.61	0.82
19:5:186:GLU:HG2	20:5:304:CLA:C1B	2.09	0.82
6:F:156:PHE:CZ	24:F:301:BCR:H402	2.14	0.81
24:A:844:BCR:C22	24:A:850:BCR:H10C	2.10	0.81
13:1:192:VAL:O	13:1:196:ALA:N	2.13	0.81
1:A:74:PHE:O	1:A:77:HIS:N	2.14	0.81
29:6:317:CHL:HHC	29:6:317:CHL:HBB1	1.62	0.81
6:F:156:PHE:CE2	24:F:301:BCR:H402	2.16	0.81
24:G:205:BCR:H403	24:G:205:BCR:H23C	1.64	0.80
24:1:1001:BCR:H403	24:1:1001:BCR:H23C	1.64	0.80
19:5:105:LEU:HG	19:5:106:PRO:HD3	1.62	0.80
1:A:575:CYS:SG	21:A:841:SF4:S4	2.79	0.79
20:6:312:CLA:HBC1	27:6:319:LMG:O4	1.82	0.79
28:J:104:LUT:H28	28:J:104:LUT:H361	1.64	0.79
7:G:51:PHE:HB3	24:G:205:BCR:C32	2.13	0.79
29:1:1015:CHL:HHC	29:1:1015:CHL:HBB1	1.63	0.79
17:4:106:PHE:CE2	29:4:313:CHL:HED2	2.18	0.79
1:A:600:TYR:OH	20:A:801:CLA:O1D	2.00	0.78
17:4:224:LEU:CD1	27:4:318:LMG:C13	2.61	0.78
15:7:110:VAL:HG21	29:7:1012:CHL:HMD1	1.66	0.78
24:G:205:BCR:H363	13:0:137:ALA:HB1	1.64	0.78
19:5:131:TRP:CZ3	24:5:320:BCR:H331	2.18	0.78
20:1:1017:CLA:HAC1	23:4:301:LHG:H211	1.64	0.78
17:4:59:PRO:HB3	17:4:79:PHE:HD2	1.46	0.78
16:3:176:TYR:CZ	26:3:1018:LMT:H6E	2.19	0.77
14:8:232:ASN:HD22	14:8:235:THR:HG23	1.49	0.77
20:B:813:CLA:CHC	24:I:201:BCR:H313	2.14	0.77
20:0:310:CLA:HBA1	29:0:317:CHL:HMD2	1.64	0.77
19:5:234:CYS:O	19:5:234:CYS:SG	2.43	0.77
13:0:131:LEU:HB3	27:0:303:LMG:C14	2.13	0.77
1:A:118:VAL:H	1:A:128:ASN:HD21	1.33	0.76
7:G:45:PHE:CE1	7:G:110:VAL:HG21	2.20	0.76
17:4:217:LYS:NZ	27:4:318:LMG:C10	2.48	0.76
24:A:844:BCR:H392	24:A:850:BCR:C11	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:813:CLA:C1C	24:I:201:BCR:H313	2.14	0.76
17:4:155:LEU:HD23	23:4:301:LHG:C18	2.14	0.76
7:G:50:ARG:HG3	7:G:51:PHE:CE1	2.21	0.76
15:7:202:LEU:HD12	15:7:202:LEU:C	2.09	0.76
29:1:1012:CHL:CAB	29:1:1015:CHL:HBB2	2.16	0.76
20:B:850:CLA:CAC	20:B:850:CLA:C4C	2.64	0.76
17:4:105:ARG:HA	17:4:108:MET:HE2	1.69	0.75
13:1:152:VAL:CG1	13:1:153:TYR:CD2	2.69	0.75
14:8:175:PRO:HA	13:1:62:LEU:HD21	1.67	0.75
19:5:179:LEU:HD13	19:5:180:LYS:N	2.01	0.75
17:4:224:LEU:HD12	27:4:318:LMG:H132	1.70	0.74
19:5:179:LEU:O	19:5:183:GLN:HG3	1.86	0.74
16:3:219:LYS:NZ	23:3:1019:LHG:C23	2.50	0.74
1:A:679:TRP:CE3	20:A:801:CLA:HMA3	2.23	0.74
16:3:183:ILE:HG23	16:3:197:PHE:CD1	2.22	0.74
17:4:224:LEU:CD1	27:4:318:LMG:H132	2.17	0.74
17:4:224:LEU:HD12	27:4:318:LMG:C13	2.18	0.74
20:4:311:CLA:HBC1	27:4:318:LMG:O4	1.88	0.73
24:A:850:BCR:H402	11:K:95:ALA:HB2	1.71	0.73
20:0:309:CLA:HBC1	20:0:316:CLA:CBC	2.15	0.73
2:B:191:TRP:O	2:B:194:HIS:N	2.21	0.73
2:B:371:ALA:CB	20:B:829:CLA:HMA1	2.14	0.73
17:4:155:LEU:HD23	23:4:301:LHG:H181	1.71	0.73
17:4:224:LEU:HD11	27:4:318:LMG:H141	1.70	0.73
14:8:172:PRO:HA	13:1:62:LEU:HD22	1.70	0.73
14:8:209:GLN:HE21	14:8:220:ASN:HD22	1.33	0.73
17:4:224:LEU:HD11	27:4:318:LMG:C14	2.18	0.73
1:A:581:GLY:O	2:B:669:ARG:NH1	2.22	0.73
24:A:844:BCR:C23	24:A:850:BCR:H10C	2.19	0.73
2:B:189:LEU:O	2:B:192:THR:OG1	2.07	0.73
7:G:51:PHE:CZ	24:G:205:BCR:HC41	2.24	0.72
29:7:1017:CHL:O1A	16:3:156:GLN:HB3	1.89	0.72
16:3:130:VAL:HG21	28:3:1002:LUT:H22	1.71	0.72
13:1:137:ALA:HB1	24:1:1001:BCR:H363	1.70	0.72
14:8:119:TRP:CZ2	27:8:319:LMG:H202	2.23	0.72
1:A:679:TRP:CD2	20:A:801:CLA:HMA3	2.24	0.72
1:A:461:THR:HG21	20:L:201:CLA:CBC	2.19	0.72
20:G:203:CLA:HBC1	29:0:314:CHL:CAD	2.19	0.72
16:3:141:TRP:CD1	16:3:147:ILE:HD11	2.25	0.72
1:A:73:VAL:O	1:A:77:HIS:ND1	2.22	0.72
19:5:131:TRP:HZ3	24:5:320:BCR:C33	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:CYS:HG	21:C:1002:SF4:FE2	0.48	0.71
13:1:192:VAL:O	13:1:196:ALA:HB2	1.90	0.71
13:0:118:TRP:HD1	13:0:119:PHE:HB2	1.56	0.70
30:4:303:XAT:H32	20:4:307:CLA:HAB	1.73	0.70
20:A:831:CLA:HAA1	24:I:201:BCR:C17	2.20	0.70
24:3:1004:BCR:H403	24:3:1004:BCR:H23C	1.73	0.70
19:5:109:LEU:HD12	19:5:110:PRO:HD2	1.73	0.70
7:G:51:PHE:CD1	24:G:205:BCR:C2	2.72	0.70
17:4:224:LEU:CG	27:4:318:LMG:H152	2.20	0.70
19:5:188:LYS:NZ	25:5:319:DGD:O3D	2.17	0.70
1:A:545:VAL:HA	1:A:548:LEU:HG	1.73	0.69
1:A:694:GLN:HB3	2:B:547:LEU:HD11	1.75	0.69
7:G:114:VAL:HG22	27:0:303:LMG:C12	2.20	0.69
15:7:204:PHE:CE1	28:7:1001:LUT:H26	2.28	0.69
18:6:55:LEU:O	18:6:56:GLY:C	2.34	0.69
8:H:66:GLN:HA	8:H:69:PHE:HD2	1.58	0.69
1:A:370:HIS:ND1	20:A:817:CLA:OBD	2.25	0.69
13:0:127:LEU:CD1	27:0:303:LMG:HC1	2.23	0.69
1:A:147:LEU:HD23	1:A:377:TYR:CE2	2.27	0.69
11:K:37:ILE:HG21	11:K:103:ILE:HG21	1.74	0.69
13:1:106:ALA:HB3	13:1:107:PRO:HD3	1.74	0.69
27:5:324:LMG:O7	27:5:324:LMG:HC1	1.93	0.69
24:B:843:BCR:H382	7:G:102:GLY:HA3	1.75	0.69
20:5:312:CLA:HHC	20:5:312:CLA:HBB1	1.74	0.69
24:8:302:BCR:H23C	24:8:302:BCR:H403	1.74	0.68
16:3:176:TYR:CZ	26:3:1018:LMT:C6'	2.76	0.68
17:4:200:PRO:HD2	28:4:317:LUT:C23	2.23	0.68
19:5:69:TRP:CD2	20:5:323:CLA:HMA3	2.29	0.68
19:5:115:ASN:O	19:5:116:ILE:HG23	1.92	0.68
14:8:118:PRO:HG2	14:8:121:SER:HB3	1.76	0.68
1:A:456:TYR:CE1	1:A:538:ILE:HD11	2.28	0.68
2:B:392:ALA:HB2	2:B:539:ALA:HA	1.74	0.68
20:A:852:CLA:HBB1	24:I:201:BCR:H403	1.74	0.68
20:4:307:CLA:CBC	27:4:318:LMG:H151	2.23	0.68
17:4:59:PRO:HB3	17:4:79:PHE:CD2	2.28	0.68
19:5:146:VAL:HG12	19:5:146:VAL:O	1.94	0.68
2:B:124:TRP:CE3	2:B:125:TRP:CZ3	2.81	0.68
20:B:830:CLA:ND	24:B:844:BCR:H282	2.09	0.68
14:8:71:GLN:HE22	14:8:166:LEU:CD1	2.07	0.68
19:5:217:ALA:O	19:5:225:ASN:ND2	2.27	0.68
1:A:329:HIS:HA	20:A:840:CLA:HAC1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:THR:O	20:B:829:CLA:HMA2	1.93	0.68
7:G:50:ARG:HG3	7:G:51:PHE:CZ	2.29	0.68
20:1:1017:CLA:HAC2	23:4:301:LHG:H221	1.76	0.68
1:A:190:TRP:CZ2	20:A:812:CLA:HBC3	2.29	0.68
20:A:840:CLA:HMB3	23:A:843:LHG:HC62	1.75	0.68
2:B:583:TRP:O	2:B:587:THR:HG23	1.95	0.67
1:A:464:ALA:HA	2:B:636:TYR:CE2	2.30	0.67
20:1:1008:CLA:HBA1	29:1:1015:CHL:HMD2	1.75	0.67
18:6:120:LEU:HB3	24:6:302:BCR:H16C	1.74	0.67
16:3:82:ILE:HG22	16:3:82:ILE:O	1.92	0.67
1:A:441:LEU:HB3	1:A:548:LEU:CD2	2.24	0.67
16:3:130:VAL:HG22	20:3:1016:CLA:CMC	2.23	0.67
3:C:52:LYS:O	3:C:56:THR:HG23	1.93	0.67
1:A:387:GLN:O	1:A:391:PHE:CD2	2.47	0.67
27:0:303:LMG:H411	29:0:314:CHL:HMB2	1.75	0.67
13:1:48:TRP:CE3	13:1:66:LYS:HD2	2.30	0.67
2:B:586:ASN:HB2	20:B:802:CLA:HBC2	1.76	0.67
13:1:152:VAL:HG13	13:1:153:TYR:CG	2.29	0.67
13:0:153:TYR:HB3	20:0:305:CLA:O1D	1.94	0.66
15:7:129:GLY:O	15:7:133:THR:OG1	2.07	0.66
2:B:669:ARG:HG2	22:B:842:PQN:H7	1.78	0.66
7:G:106:LEU:O	7:G:110:VAL:HG23	1.96	0.66
10:J:31:ARG:CZ	28:J:104:LUT:H173	2.26	0.66
13:1:125:PHE:HB3	13:1:129:ALA:HB3	1.76	0.66
29:5:317:CHL:HBB2	24:5:320:BCR:HC8	1.77	0.66
1:A:121:ILE:HG13	1:A:122:VAL:HG23	1.77	0.66
15:7:202:LEU:HD11	20:7:1006:CLA:CMC	2.26	0.66
2:B:191:TRP:HD1	2:B:278:HIS:HD1	1.43	0.66
20:A:833:CLA:HHC	20:A:833:CLA:HBB1	1.78	0.65
13:0:127:LEU:HD12	27:0:303:LMG:C1	2.26	0.65
19:5:105:LEU:CG	19:5:106:PRO:HD3	2.26	0.65
15:7:182:LYS:NZ	15:7:186:TYR:OH	2.30	0.65
16:3:120:ALA:C	16:3:137:TYR:OH	2.39	0.65
20:J:102:CLA:HBC2	20:J:102:CLA:HMC3	1.79	0.65
13:0:106:ALA:HB3	13:0:107:PRO:HD3	1.78	0.65
24:A:846:BCR:H333	24:A:847:BCR:H381	1.78	0.65
2:B:20:ARG:NH1	3:C:77:MET:SD	2.70	0.65
14:8:194:LYS:HE2	20:8:311:CLA:HMD3	1.79	0.65
15:7:164:TYR:HB3	20:7:1004:CLA:O1D	1.97	0.65
20:5:310:CLA:C4A	25:5:319:DGD:O4D	2.45	0.65
1:A:657:VAL:HG21	1:A:742:PHE:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:7:171:ASP:OD2	15:7:176:SER:OG	2.11	0.64
1:A:593:PHE:HD1	1:A:728:VAL:HG21	1.63	0.64
1:A:675:ALA:HB3	1:A:738:THR:HG22	1.78	0.64
13:1:60:ASP:OD1	28:1:1002:LUT:O23	2.16	0.64
13:1:80:ILE:CD1	13:1:145:ARG:HH21	2.11	0.64
13:1:93:LEU:C	13:1:97:LEU:HD11	2.21	0.64
20:B:813:CLA:C4B	24:I:201:BCR:H313	2.28	0.64
20:1:1007:CLA:CBC	20:1:1014:CLA:HBC2	2.17	0.64
1:A:734:GLY:O	1:A:738:THR:HG23	1.97	0.64
2:B:143:LEU:HD11	24:B:845:BCR:H402	1.79	0.64
2:B:176:LEU:HB3	2:B:292:TYR:CE2	2.32	0.64
20:1:1017:CLA:CAC	23:4:301:LHG:C21	2.75	0.64
19:5:126:PHE:O	19:5:130:HIS:HB2	1.97	0.64
1:A:213:TRP:O	1:A:216:HIS:N	2.31	0.64
20:A:852:CLA:CBB	24:I:201:BCR:H403	2.28	0.64
20:B:823:CLA:C2B	24:B:843:BCR:H362	2.27	0.64
7:G:51:PHE:CB	24:G:205:BCR:HC21	2.28	0.64
20:8:309:CLA:NB	27:8:319:LMG:HC62	2.13	0.64
17:4:217:LYS:HZ1	27:4:318:LMG:C10	2.09	0.64
13:0:64:LEU:HD22	20:0:301:CLA:CBB	2.27	0.64
13:0:81:HIS:HD2	28:0:304:LUT:H35	1.62	0.64
20:A:821:CLA:HMA1	20:A:840:CLA:CBC	2.28	0.64
17:4:224:LEU:HD11	27:4:318:LMG:C13	2.28	0.64
20:A:825:CLA:HAB	24:A:847:BCR:H392	1.79	0.63
11:K:106:GLY:CA	20:K:201:CLA:HMA3	2.28	0.63
20:5:312:CLA:NB	25:5:319:DGD:HB51	2.13	0.63
20:B:813:CLA:HBC2	20:L:201:CLA:HAC1	1.79	0.63
17:4:200:PRO:HD2	28:4:317:LUT:H23	1.80	0.63
19:5:179:LEU:HD22	19:5:180:LYS:N	2.14	0.63
24:6:302:BCR:H403	24:6:302:BCR:H23C	1.81	0.63
2:B:371:ALA:HB1	20:B:829:CLA:CMA	2.19	0.63
12:L:132:LEU:HD13	12:L:174:PHE:CD2	2.34	0.63
14:8:160:LEU:HD11	13:1:66:LYS:HB3	1.80	0.63
29:5:313:CHL:HBB2	20:5:315:CLA:HBC1	1.79	0.63
2:B:583:TRP:O	2:B:584:MET:C	2.40	0.63
28:1:1002:LUT:H361	28:1:1002:LUT:C28	2.25	0.63
18:6:41:HIS:CD2	18:6:42:LEU:HD13	2.34	0.63
19:5:69:TRP:CE2	20:5:323:CLA:HMA3	2.34	0.63
16:3:176:TYR:CE1	26:3:1018:LMT:H6D	2.34	0.63
16:3:219:LYS:HZ1	23:3:1019:LHG:C23	2.12	0.63
20:4:311:CLA:OBD	18:6:127:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:96:PHE:CZ	18:6:198:GLY:O	2.52	0.62
19:5:109:LEU:CD1	19:5:110:PRO:HD2	2.29	0.62
1:A:676:HIS:O	1:A:677:PHE:C	2.41	0.62
12:L:146:ILE:HD11	12:L:162:PHE:CD1	2.34	0.62
17:4:217:LYS:HZ3	27:4:318:LMG:C10	2.11	0.62
20:G:203:CLA:HBC1	29:0:314:CHL:C3D	2.29	0.62
13:0:131:LEU:HD12	27:0:303:LMG:H121	1.80	0.62
14:8:147:GLN:HE21	14:8:147:GLN:CA	2.09	0.62
20:5:309:CLA:CHC	24:5:320:BCR:H393	2.30	0.62
2:B:123:GLN:O	2:B:127:THR:HG23	1.99	0.62
2:B:652:LEU:HB3	20:B:801:CLA:O2A	2.00	0.62
14:8:163:THR:HG22	14:8:164:SER:H	1.65	0.62
1:A:388:LEU:HD13	1:A:747:ILE:HD11	1.81	0.62
2:B:125:TRP:CE3	24:B:845:BCR:H282	2.35	0.62
10:J:7:TYR:O	10:J:10:THR:OG1	2.10	0.62
15:7:91:ILE:O	15:7:95:VAL:HG23	2.00	0.62
2:B:548:MET:HG3	2:B:551:LYS:HG3	1.81	0.62
28:J:104:LUT:H361	28:J:104:LUT:C28	2.26	0.62
15:7:182:LYS:HZ3	15:7:186:TYR:HE2	1.47	0.62
30:5:303:XAT:H183	20:5:309:CLA:C3B	2.29	0.62
15:7:230:ASN:HD22	16:3:146:THR:HG22	1.64	0.62
18:6:33:LEU:HD13	20:6:312:CLA:HMA3	1.81	0.62
18:6:55:LEU:O	18:6:57:LEU:N	2.32	0.62
15:7:101:GLU:O	15:7:105:ALA:HB2	2.00	0.62
1:A:355:ILE:CG1	24:A:846:BCR:H311	2.30	0.61
20:A:831:CLA:HMD2	24:I:201:BCR:H373	1.82	0.61
12:L:146:ILE:HD11	12:L:162:PHE:CG	2.35	0.61
17:4:166:GLN:HG3	17:4:173:SER:OG	2.00	0.61
19:5:170:ASP:OD1	20:5:304:CLA:HBA2	2.00	0.61
1:A:80:GLN:HE21	20:A:804:CLA:HMA1	1.65	0.61
27:0:303:LMG:H392	29:0:314:CHL:CHB	2.30	0.61
14:8:232:ASN:HD22	14:8:235:THR:CG2	2.13	0.61
18:6:123:TRP:CZ3	24:6:302:BCR:C32	2.81	0.61
18:6:181:ARG:HA	18:6:184:MET:HE3	1.81	0.61
20:A:815:CLA:HBC2	20:3:1013:CLA:HAB	1.82	0.61
20:A:833:CLA:HMB1	24:A:847:BCR:HC31	1.83	0.61
2:B:326:THR:HG21	2:B:404:ASN:HD21	1.64	0.61
16:3:234:GLN:HE21	16:3:245:ASN:HD22	1.49	0.61
19:5:181:GLU:O	19:5:184:THR:OG1	2.17	0.61
2:B:358:PRO:HG3	20:B:821:CLA:HBA2	1.83	0.61
14:8:236:ASN:C	14:8:236:ASN:HD22	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:1017:CLA:HAC1	23:4:301:LHG:C21	2.31	0.61
1:A:472:PHE:HA	1:A:477:ILE:CG2	2.31	0.61
2:B:192:THR:HG21	2:B:279:LEU:N	2.16	0.61
2:B:48:PHE:CE2	2:B:169:PHE:CE1	2.89	0.61
16:3:219:LYS:HZ3	23:3:1019:LHG:C23	2.14	0.61
1:A:156:GLU:O	1:A:159:LEU:N	2.34	0.60
1:A:658:ILE:HD11	20:A:801:CLA:CBC	2.30	0.60
20:A:818:CLA:HBA2	20:A:828:CLA:OBD	2.00	0.60
2:B:525:ALA:HB2	20:B:838:CLA:HMA1	1.81	0.60
13:1:179:LYS:HE2	20:1:1009:CLA:C3D	2.31	0.60
2:B:660:THR:O	2:B:663:MET:HB3	2.00	0.60
13:0:158:PHE:O	28:0:318:LUT:H24	2.01	0.60
14:8:210:LYS:HE3	14:8:217:PRO:HD3	1.82	0.60
16:3:194:GLY:O	16:3:197:PHE:CE1	2.54	0.60
16:3:201:PHE:CE1	20:5:312:CLA:HMA1	2.35	0.60
17:4:156:LEU:HB3	24:4:302:BCR:H363	1.83	0.60
13:1:188:PHE:CZ	28:1:1002:LUT:H10	2.36	0.60
1:A:122:VAL:HG12	1:A:122:VAL:O	2.02	0.60
1:A:739:THR:HG22	20:A:801:CLA:OBD	2.01	0.60
13:1:115:LYS:HB3	13:1:122:GLU:OE1	2.02	0.60
1:A:55:ASP:OD2	23:A:849:LHG:O1	2.16	0.60
2:B:88:ILE:HG23	2:B:114:VAL:HG13	1.84	0.60
14:8:78:ARG:HG2	20:8:305:CLA:C4C	2.32	0.60
13:1:81:HIS:HB3	13:1:185:MET:HE3	1.84	0.60
13:1:84:TRP:CE2	29:1:1013:CHL:HED3	2.36	0.60
17:4:155:LEU:HG	23:4:301:LHG:H201	1.83	0.60
20:B:836:CLA:O1A	20:G:203:CLA:CHB	2.50	0.60
20:8:311:CLA:C4B	27:8:318:LMG:O2	2.49	0.60
29:4:315:CHL:H122	29:4:316:CHL:NB	2.15	0.60
18:6:170:ALA:O	18:6:173:LYS:N	2.34	0.60
1:A:114:SER:HB3	1:A:131:VAL:HG11	1.84	0.60
1:A:355:ILE:HG12	24:A:846:BCR:H311	1.84	0.60
1:A:122:VAL:HG13	20:B:834:CLA:OBD	2.02	0.60
1:A:445:CYS:SG	1:A:548:LEU:HD11	2.42	0.60
20:B:821:CLA:CGA	20:B:821:CLA:H3A	2.32	0.60
2:B:291:MET:HB2	20:B:850:CLA:C2C	2.32	0.60
15:7:156:GLU:HG2	15:7:168:ARG:HG2	1.84	0.60
1:A:535:VAL:HG12	1:A:539:HIS:CE1	2.36	0.59
14:8:126:GLN:OE1	29:8:314:CHL:HMC	2.02	0.59
14:8:71:GLN:NE2	14:8:166:LEU:HD12	2.17	0.59
1:A:472:PHE:CD1	1:A:479:LEU:HD11	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:THR:HG22	2:B:583:TRP:HB3	1.85	0.59
2:B:564:GLY:HA3	3:C:56:THR:HG22	1.83	0.59
20:8:313:CLA:HBC3	27:8:318:LMG:HC8	1.84	0.59
30:5:303:XAT:H183	20:5:309:CLA:C2B	2.32	0.59
17:4:224:LEU:O	17:4:227:ALA:N	2.36	0.59
13:0:131:LEU:CB	27:0:303:LMG:H141	2.31	0.59
14:8:31:LEU:HD13	20:8:313:CLA:HMA2	1.84	0.59
14:8:140:ASP:O	14:8:144:PRO:HA	2.03	0.59
14:8:209:GLN:NE2	14:8:220:ASN:HD22	1.99	0.59
15:7:228:HIS:O	15:7:233:THR:HG23	2.02	0.59
16:3:123:ILE:HD11	16:3:137:TYR:CD1	2.37	0.59
2:B:175:ARG:HG3	20:B:816:CLA:HBC2	1.84	0.59
19:5:111:GLU:H	19:5:112:PRO:HD2	1.68	0.59
14:8:147:GLN:HA	14:8:147:GLN:NE2	2.11	0.59
13:1:123:VAL:CG1	13:1:124:PRO:HD2	2.24	0.59
14:8:104:TRP:CZ2	14:8:210:LYS:HD2	2.37	0.58
13:1:97:LEU:HD12	13:1:97:LEU:H	1.68	0.58
20:4:307:CLA:CBC	27:4:318:LMG:H142	2.32	0.58
5:E:55:GLN:HE22	5:E:77:ASN:HD21	1.51	0.58
17:4:155:LEU:CD2	23:4:301:LHG:H201	2.32	0.58
19:5:203:GLN:HE22	28:5:302:LUT:H42	1.68	0.58
15:7:175:LEU:HD22	20:7:1004:CLA:CGA	2.33	0.58
13:1:79:VAL:HG21	13:1:152:VAL:CG2	2.33	0.58
13:1:192:VAL:O	13:1:196:ALA:CB	2.52	0.58
2:B:291:MET:HA	20:B:850:CLA:CAC	2.33	0.58
27:4:318:LMG:O2	24:6:302:BCR:HC42	2.03	0.58
19:5:109:LEU:CB	19:5:110:PRO:HD2	2.28	0.58
19:5:205:GLN:O	19:5:234:CYS:C	2.46	0.58
28:5:302:LUT:H3	20:5:306:CLA:HMA1	1.85	0.58
1:A:391:PHE:O	1:A:395:THR:HG23	2.04	0.58
20:5:310:CLA:CHB	25:5:319:DGD:O4D	2.51	0.58
1:A:657:VAL:HG22	1:A:745:ALA:HB3	1.85	0.58
2:B:197:HIS:CB	20:B:817:CLA:HBC3	2.34	0.58
24:G:205:BCR:H272	13:0:118:TRP:CH2	2.39	0.58
15:7:144:SER:HB3	15:7:145:GLN:OE1	2.03	0.58
2:B:636:TYR:CE2	2:B:645:SER:CB	2.87	0.58
2:B:683:HIS:O	2:B:686:THR:OG1	2.22	0.58
14:8:76:HIS:HE1	20:8:309:CLA:ND	2.01	0.58
15:7:143:GLY:O	15:7:146:ALA:HB3	2.04	0.58
19:5:34:LEU:O	19:5:53:TYR:CD1	2.56	0.58
19:5:127:ILE:HG21	20:5:301:CLA:O2A	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:813:CLA:NC	24:I:201:BCR:H311	2.19	0.58
19:5:140:TYR:HE2	20:5:323:CLA:HMA2	1.68	0.58
1:A:74:PHE:O	1:A:75:SER:C	2.47	0.58
1:A:204:GLY:O	24:A:845:BCR:H352	2.03	0.58
2:B:636:TYR:HE2	2:B:645:SER:HB2	1.69	0.58
3:C:14:CYS:O	3:C:15:THR:HG22	2.04	0.58
15:7:177:ARG:O	18:6:60:ASN:HB2	2.04	0.58
20:A:851:CLA:O1A	2:B:431:GLY:HA3	2.04	0.57
7:G:51:PHE:CE1	24:G:205:BCR:HC41	2.39	0.57
20:1:1017:CLA:CAC	23:4:301:LHG:H211	2.33	0.57
1:A:646:LEU:HD22	2:B:652:LEU:HD21	1.84	0.57
15:7:175:LEU:CB	20:7:1004:CLA:HBA1	2.33	0.57
1:A:464:ALA:HA	2:B:636:TYR:CZ	2.39	0.57
1:A:73:VAL:O	1:A:77:HIS:CE1	2.58	0.57
7:G:51:PHE:HB3	24:G:205:BCR:HC21	1.85	0.57
18:6:123:TRP:CH2	24:6:302:BCR:H322	2.39	0.57
2:B:477:PHE:O	2:B:480:SER:OG	2.23	0.57
7:G:45:PHE:CZ	13:0:135:PHE:CZ	2.92	0.57
13:0:89:VAL:HG11	28:0:318:LUT:H12	1.85	0.57
11:K:106:GLY:HA2	20:K:201:CLA:HMA3	1.85	0.57
13:0:126:ASP:OD1	13:0:127:LEU:N	2.38	0.57
16:3:183:ILE:CG2	16:3:197:PHE:CG	2.88	0.57
12:L:118:SER:HA	12:L:186:TYR:CZ	2.39	0.57
13:1:110:ALA:HB1	13:1:127:LEU:HD11	1.87	0.57
20:6:312:CLA:HBC3	27:6:319:LMG:HC2	1.86	0.57
20:5:312:CLA:HMB3	25:5:319:DGD:HA91	1.87	0.57
27:5:324:LMG:H132	27:5:324:LMG:O9	2.04	0.57
1:A:194:VAL:HG13	20:A:824:CLA:HMD3	1.86	0.57
11:K:37:ILE:HG21	11:K:103:ILE:CG2	2.34	0.57
30:6:304:XAT:H183	20:6:310:CLA:C2B	2.35	0.57
18:6:87:VAL:HB	20:6:310:CLA:HBC3	1.86	0.57
2:B:527:GLY:HA2	2:B:587:THR:HG22	1.87	0.56
2:B:636:TYR:HE2	2:B:645:SER:CB	2.18	0.56
20:A:852:CLA:HBB1	24:I:201:BCR:C40	2.34	0.56
8:H:74:THR:HG22	12:L:176:VAL:HG11	1.87	0.56
17:4:155:LEU:HD23	23:4:301:LHG:C20	2.35	0.56
18:6:57:LEU:HD13	30:6:304:XAT:H23	1.87	0.56
19:5:231:ILE:HG23	19:5:232:GLY:H	1.69	0.56
1:A:147:LEU:HD23	1:A:377:TYR:CZ	2.41	0.56
1:A:562:LEU:HD11	2:B:673:GLN:CG	2.35	0.56
1:A:675:ALA:CB	1:A:738:THR:HG22	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:TYR:HB3	2:B:48:PHE:CE2	2.40	0.56
24:G:205:BCR:HC8	24:G:205:BCR:H311	1.86	0.56
16:3:96:ARG:HB3	20:3:1005:CLA:HBC3	1.86	0.56
2:B:127:THR:HG21	2:B:360:ALA:H	1.70	0.56
20:B:823:CLA:C1B	24:B:843:BCR:H362	2.35	0.56
19:5:93:ILE:HG13	19:5:212:LEU:HD11	1.86	0.56
1:A:479:LEU:H	1:A:530:THR:HG22	1.71	0.56
2:B:312:PRO:O	23:0:302:LHG:O4	2.23	0.56
24:G:205:BCR:H321	24:G:205:BCR:C8	2.36	0.56
20:5:312:CLA:HBC1	25:5:319:DGD:O5D	2.06	0.56
1:A:396:TRP:CD1	20:A:827:CLA:HAB	2.40	0.56
20:A:823:CLA:HMB3	20:A:840:CLA:CAB	2.36	0.56
20:7:1010:CLA:HMB2	26:3:1018:LMT:H11	1.87	0.56
20:4:307:CLA:HAC1	27:4:318:LMG:C14	2.35	0.56
23:7:1016:LHG:HC42	24:3:1003:BCR:HC31	1.88	0.56
16:3:183:ILE:HG23	16:3:197:PHE:CG	2.39	0.56
13:0:116:ALA:O	13:0:117:THR:HG23	2.05	0.56
20:4:310:CLA:CAB	24:6:302:BCR:H333	2.36	0.56
20:B:808:CLA:C4B	20:B:831:CLA:HMB2	2.36	0.56
11:K:99:LEU:HA	20:K:201:CLA:HAC1	1.88	0.56
15:7:230:ASN:HD22	16:3:146:THR:CG2	2.19	0.56
16:3:180:LEU:HB3	16:3:184:PHE:CE2	2.41	0.56
24:A:844:BCR:H372	24:A:845:BCR:H332	1.87	0.55
12:L:115:ILE:HG13	12:L:190:GLN:HE22	1.70	0.55
14:8:71:GLN:HE22	14:8:166:LEU:HD11	1.71	0.55
15:7:171:ASP:O	15:7:177:ARG:NH2	2.39	0.55
17:4:58:LEU:HD22	17:4:59:PRO:HD2	1.88	0.55
29:5:317:CHL:CBB	29:5:317:CHL:HHC	2.35	0.55
7:G:50:ARG:HD2	7:G:95:PHE:CZ	2.42	0.55
12:L:118:SER:HA	12:L:186:TYR:CE1	2.40	0.55
16:3:222:ARG:HA	16:3:225:MET:HE3	1.87	0.55
19:5:197:TYR:OH	30:5:303:XAT:H171	2.05	0.55
20:5:318:CLA:HAC2	20:5:323:CLA:HMB3	1.88	0.55
7:G:114:VAL:HG13	13:0:128:ASN:OD1	2.07	0.55
14:8:184:LYS:O	14:8:184:LYS:HG3	2.06	0.55
17:4:78:ASP:HA	20:4:307:CLA:O1D	2.05	0.55
24:6:302:BCR:H393	20:6:310:CLA:CHC	2.36	0.55
17:4:197:ILE:O	17:4:200:PRO:HD3	2.06	0.55
18:6:99:ASN:HA	29:6:313:CHL:HED3	1.89	0.55
2:B:321:LYS:O	2:B:407:ASN:ND2	2.40	0.55
14:8:119:TRP:CZ3	27:8:319:LMG:H182	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:7:130:TRP:CH2	24:7:1003:BCR:H321	2.42	0.55
15:7:175:LEU:HB2	20:7:1004:CLA:HBA1	1.88	0.55
1:A:112:LYS:O	1:A:131:VAL:CG1	2.55	0.55
1:A:360:PHE:O	1:A:363:LEU:HB3	2.06	0.55
20:B:813:CLA:C1C	24:I:201:BCR:C31	2.83	0.55
13:1:188:PHE:CD2	28:1:1002:LUT:H12	2.42	0.55
20:B:813:CLA:CBC	20:L:201:CLA:HAC1	2.36	0.55
18:6:120:LEU:HD13	24:6:302:BCR:H351	1.89	0.55
27:5:324:LMG:O7	27:5:324:LMG:C1	2.55	0.55
1:A:509:THR:CG2	1:A:523:MET:HE2	2.36	0.55
1:A:593:PHE:HD1	1:A:728:VAL:CG2	2.19	0.55
13:0:116:ALA:HB3	13:0:123:VAL:HG11	1.88	0.55
15:7:51:TYR:OH	15:7:192:LYS:HE2	2.07	0.55
2:B:106:THR:HG22	2:B:112:GLY:C	2.32	0.55
2:B:197:HIS:CG	20:B:817:CLA:HBC3	2.41	0.55
2:B:593:PHE:O	2:B:594:TYR:C	2.50	0.55
15:7:228:HIS:O	15:7:233:THR:CG2	2.55	0.55
19:5:191:ARG:HA	19:5:194:MET:HE3	1.87	0.55
20:A:831:CLA:CHB	24:I:201:BCR:H351	2.37	0.55
2:B:102:VAL:O	2:B:106:THR:HG23	2.06	0.55
14:8:147:GLN:CA	14:8:147:GLN:NE2	2.70	0.55
20:1:1008:CLA:HBA1	29:1:1015:CHL:C2D	2.37	0.55
20:4:310:CLA:C1B	27:4:318:LMG:HC3	2.37	0.55
2:B:326:THR:O	2:B:330:SER:OG	2.18	0.54
20:B:836:CLA:O1A	20:G:203:CLA:C1B	2.55	0.54
24:B:843:BCR:C12	24:G:204:BCR:H271	2.38	0.54
6:F:156:PHE:CE1	24:F:301:BCR:H24C	2.42	0.54
24:I:201:BCR:H392	24:I:201:BCR:H23C	1.88	0.54
20:1:1017:CLA:HAC2	23:4:301:LHG:C21	2.37	0.54
20:4:307:CLA:CBC	27:4:318:LMG:C15	2.85	0.54
2:B:115:ASN:HD21	20:B:812:CLA:HMD3	1.72	0.54
20:6:311:CLA:HBB2	24:5:320:BCR:H322	1.90	0.54
20:B:808:CLA:C1C	20:B:831:CLA:HMB3	2.37	0.54
13:0:127:LEU:CD1	27:0:303:LMG:HC5	2.36	0.54
17:4:132:VAL:HG22	17:4:133:ALA:H	1.72	0.54
1:A:429:ARG:O	1:A:433:HIS:ND1	2.41	0.54
20:B:818:CLA:O1D	26:B:849:LMT:O4'	2.22	0.54
3:C:54:CYS:SG	3:C:55:GLU:N	2.80	0.54
17:4:256:VAL:HG23	20:4:306:CLA:O1A	2.08	0.54
18:6:53:ASP:OD2	18:6:58:GLY:N	2.33	0.54
19:5:170:ASP:HA	28:5:302:LUT:O23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:7:1017:CHL:H91	16:3:149:PHE:CE2	2.43	0.54
13:1:89:VAL:HG11	28:1:1016:LUT:H12	1.88	0.54
17:4:197:ILE:HD13	29:4:315:CHL:H91	1.88	0.54
18:6:71:GLU:HG3	20:6:308:CLA:NB	2.23	0.54
2:B:443:VAL:HG11	20:B:834:CLA:HMD3	1.90	0.54
7:G:101:ALA:HA	24:G:204:BCR:H363	1.90	0.54
12:L:99:PRO:HA	20:L:204:CLA:HMB3	1.90	0.54
14:8:163:THR:HG22	14:8:164:SER:N	2.22	0.54
16:3:197:PHE:HD1	16:3:197:PHE:H	1.56	0.54
13:1:198:THR:HG21	13:1:221:ASN:CB	2.38	0.54
19:5:211:PRO:HA	19:5:214:ALA:HB3	1.90	0.54
1:A:563:ILE:HD12	1:A:586:VAL:HG11	1.88	0.54
1:A:572:ARG:HD3	23:A:849:LHG:HC61	1.90	0.54
15:7:87:ILE:HD11	15:7:204:PHE:HZ	1.62	0.54
15:7:202:LEU:C	15:7:202:LEU:CD1	2.80	0.54
16:3:176:TYR:CE1	26:3:1018:LMT:C6'	2.90	0.54
18:6:168:ASP:O	18:6:169:LEU:HD22	2.08	0.54
2:B:48:PHE:CE2	2:B:169:PHE:CD1	2.95	0.54
20:8:309:CLA:C1B	27:8:319:LMG:HC62	2.37	0.54
13:1:73:ARG:O	13:1:76:GLU:HB3	2.07	0.54
18:6:57:LEU:CD1	30:6:304:XAT:H23	2.38	0.54
20:6:312:CLA:HBC3	27:6:319:LMG:O6	2.08	0.54
20:B:808:CLA:C4B	20:B:831:CLA:CMB	2.85	0.54
28:J:104:LUT:H28	28:J:104:LUT:H371	1.90	0.54
13:0:116:ALA:CB	13:0:123:VAL:HG11	2.38	0.54
1:A:50:TRP:CZ2	20:A:838:CLA:HBB1	2.42	0.54
2:B:463:TRP:CE3	20:F:303:CLA:HMC2	2.44	0.54
14:8:161:LYS:CG	14:8:172:PRO:HG3	2.34	0.54
15:7:91:ILE:O	15:7:95:VAL:N	2.41	0.54
13:1:152:VAL:CG1	13:1:153:TYR:CE2	2.91	0.54
19:5:133:GLU:OE2	19:5:136:ARG:CZ	2.56	0.54
19:5:231:ILE:HG23	19:5:232:GLY:N	2.23	0.54
12:L:95:LEU:HD22	20:L:204:CLA:HBC2	1.90	0.53
28:3:1001:LUT:H3	20:3:1007:CLA:CHB	2.39	0.53
13:1:80:ILE:HD13	13:1:145:ARG:HH21	1.72	0.53
29:6:314:CHL:HBB2	29:6:317:CHL:OMC	2.08	0.53
19:5:88:VAL:HG22	19:5:105:LEU:HD22	1.90	0.53
19:5:128:LEU:HD22	24:5:320:BCR:C14	2.38	0.53
1:A:679:TRP:CD2	20:A:801:CLA:CMA	2.90	0.53
20:B:822:CLA:HMD3	20:B:824:CLA:HHD	1.88	0.53
15:7:136:TRP:CD1	20:7:1014:CLA:HMA1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:201:PHE:CE1	20:5:312:CLA:CMA	2.90	0.53
27:0:303:LMG:H392	29:0:314:CHL:C1B	2.38	0.53
15:7:171:ASP:CB	15:7:176:SER:OG	2.55	0.53
13:1:59:PHE:CE2	28:1:1002:LUT:H383	2.42	0.53
20:A:808:CLA:HBB1	20:A:808:CLA:HMB1	1.89	0.53
13:0:164:ALA:HB2	20:0:305:CLA:HAA2	1.90	0.53
14:8:145:GLY:O	14:8:147:GLN:N	2.41	0.53
29:7:1015:CHL:HBA2	29:7:1015:CHL:CGD	2.38	0.53
18:6:55:LEU:HD12	18:6:55:LEU:N	2.23	0.53
19:5:135:ARG:CZ	19:5:146:VAL:HG13	2.39	0.53
19:5:212:LEU:O	19:5:215:LEU:HB3	2.08	0.53
7:G:52:VAL:HG11	13:0:140:ALA:HA	1.88	0.53
15:7:189:LYS:HD3	20:7:1005:CLA:HAA2	1.90	0.53
13:1:59:PHE:CD2	20:1:1011:CLA:CBB	2.92	0.53
13:1:151:VAL:HG11	13:1:154:PRO:HB3	1.91	0.53
20:6:320:CLA:HBC3	20:5:321:CLA:CHC	2.38	0.53
1:A:740:TRP:CG	24:A:848:BCR:HC41	2.44	0.53
13:1:93:LEU:C	13:1:97:LEU:CD1	2.81	0.53
4:D:192:SER:N	4:D:193:PRO:CD	2.72	0.53
19:5:76:GLN:NE2	29:5:314:CHL:OBD	2.33	0.53
2:B:495:LEU:N	2:B:496:PRO:CD	2.71	0.53
2:B:531:THR:CG2	2:B:583:TRP:HB3	2.39	0.53
17:4:155:LEU:CD2	23:4:301:LHG:C20	2.87	0.53
18:6:166:PRO:HD2	20:6:305:CLA:O1A	2.09	0.53
1:A:369:HIS:O	1:A:372:TYR:N	2.42	0.53
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.91	0.53
1:A:455:LEU:HB3	1:A:534:MET:HE1	1.90	0.53
1:A:593:PHE:CD1	1:A:728:VAL:CG2	2.91	0.53
29:0:314:CHL:CAB	29:0:317:CHL:HBB2	2.39	0.53
13:1:59:PHE:HD2	28:1:1002:LUT:H383	1.69	0.53
20:A:831:CLA:HMD2	24:I:201:BCR:C37	2.39	0.53
2:B:125:TRP:CH2	24:B:845:BCR:H282	2.44	0.53
17:4:61:TRP:CD1	20:4:311:CLA:C1B	2.92	0.53
17:4:155:LEU:HD23	23:4:301:LHG:C19	2.38	0.53
20:A:821:CLA:HMA1	20:A:840:CLA:HBC2	1.89	0.52
6:F:128:ASP:OD1	6:F:128:ASP:N	2.42	0.52
11:K:99:LEU:HD22	20:K:201:CLA:HMC3	1.91	0.52
16:3:120:ALA:HB1	16:3:137:TYR:OH	2.09	0.52
19:5:48:ASP:N	19:5:48:ASP:OD1	2.42	0.52
7:G:100:VAL:HG22	20:G:202:CLA:HMB2	1.91	0.52
15:7:204:PHE:CZ	28:7:1001:LUT:H26	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:158:PHE:O	28:1:1016:LUT:H24	2.09	0.52
2:B:369:GLN:O	2:B:373:TYR:CD2	2.62	0.52
2:B:652:LEU:O	20:B:801:CLA:HBA1	2.10	0.52
24:B:804:BCR:H271	22:B:842:PQN:H142	1.90	0.52
14:8:105:TYR:CD2	14:8:210:LYS:HD3	2.44	0.52
29:7:1013:CHL:HHC	29:7:1013:CHL:HBB1	1.92	0.52
13:1:182:ARG:O	13:1:185:MET:N	2.41	0.52
14:8:77:CYS:HB3	14:8:196:GLY:HA3	1.90	0.52
20:7:1011:CLA:HAA1	20:7:1011:CLA:HBD	1.91	0.52
16:3:123:ILE:CD1	16:3:137:TYR:CE1	2.87	0.52
20:A:804:CLA:C1C	20:A:829:CLA:HMB3	2.40	0.52
4:D:191:MET:HE2	4:D:191:MET:HA	1.91	0.52
6:F:161:GLY:HA3	6:F:202:TRP:CZ2	2.43	0.52
28:J:104:LUT:C28	28:J:104:LUT:H371	2.39	0.52
18:6:149:LEU:HD21	18:6:157:PRO:O	2.09	0.52
20:A:813:CLA:HBA2	20:A:815:CLA:HHB	1.91	0.52
20:B:813:CLA:NC	24:I:201:BCR:C31	2.73	0.52
15:7:35:PRO:HB2	16:3:172:MET:HE1	1.91	0.52
1:A:473:SER:C	1:A:477:ILE:O	2.47	0.52
2:B:191:TRP:CD1	2:B:278:HIS:HD1	2.24	0.52
2:B:593:PHE:O	2:B:594:TYR:O	2.28	0.52
19:5:186:GLU:HG2	20:5:304:CLA:CHB	2.39	0.52
20:5:310:CLA:HBC3	25:5:319:DGD:HG12	1.92	0.52
20:5:312:CLA:HBC1	25:5:319:DGD:O6D	2.09	0.52
1:A:388:LEU:HD13	1:A:747:ILE:CD1	2.39	0.52
2:B:310:THR:HG22	2:B:319:GLY:HA3	1.92	0.52
2:B:620:TRP:O	2:B:624:TYR:HB3	2.10	0.52
12:L:122:ALA:HB2	12:L:182:VAL:HG11	1.92	0.52
15:7:156:GLU:HB2	15:7:168:ARG:CZ	2.39	0.52
18:6:161:PHE:O	28:6:303:LUT:H24	2.08	0.52
2:B:654:GLY:HA3	2:B:721:THR:HG23	1.91	0.52
20:B:831:CLA:HMB1	20:B:831:CLA:HBB1	1.92	0.52
28:3:1002:LUT:C28	28:3:1002:LUT:H381	2.39	0.52
28:5:302:LUT:H183	20:5:306:CLA:C3B	2.40	0.52
25:B:848:DGD:O2E	3:C:70:GLY:C	2.53	0.52
13:0:127:LEU:HD11	27:0:303:LMG:HC5	1.92	0.52
29:7:1017:CHL:H91	16:3:149:PHE:CZ	2.43	0.52
13:1:79:VAL:HG21	13:1:152:VAL:HG21	1.92	0.52
20:1:1008:CLA:HBA1	29:1:1015:CHL:CMD	2.39	0.52
20:A:833:CLA:HAB	24:A:847:BCR:C3	2.40	0.51
2:B:190:ALA:HB3	20:B:817:CLA:HBB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:122:LEU:HA	4:D:125:THR:OG1	2.10	0.51
7:G:114:VAL:HG13	13:0:128:ASN:CG	2.34	0.51
14:8:162:GLY:O	14:8:163:THR:OG1	2.26	0.51
16:3:148:PHE:CE2	16:3:152:ILE:HD11	2.45	0.51
20:4:307:CLA:HAC2	27:4:318:LMG:H122	1.91	0.51
18:6:85:ILE:HD11	30:6:304:XAT:O4	2.10	0.51
20:A:831:CLA:CMD	24:I:201:BCR:H373	2.40	0.51
8:H:69:PHE:CE1	24:H:201:BCR:H332	2.45	0.51
12:L:96:LEU:HD22	12:L:124:LEU:HD12	1.91	0.51
19:5:146:VAL:O	19:5:146:VAL:CG1	2.58	0.51
2:B:124:TRP:NE1	2:B:128:ILE:HD11	2.25	0.51
5:E:45:ILE:HD11	5:E:75:PHE:CZ	2.45	0.51
18:6:127:ARG:HD3	18:6:138:VAL:HG11	1.92	0.51
19:5:57:PRO:C	19:5:58:LEU:HD12	2.35	0.51
27:5:324:LMG:H381	27:5:324:LMG:H342	1.92	0.51
1:A:74:PHE:C	1:A:77:HIS:H	2.19	0.51
2:B:223:LEU:HB2	20:B:818:CLA:CAD	2.41	0.51
2:B:636:TYR:CE2	2:B:645:SER:HB2	2.45	0.51
14:8:104:TRP:CD1	14:8:210:LYS:HZ1	2.28	0.51
24:3:1004:BCR:C8	24:3:1004:BCR:H321	2.40	0.51
13:1:68:PRO:O	13:1:71:LEU:N	2.44	0.51
2:B:64:GLY:O	2:B:68:HIS:ND1	2.44	0.51
2:B:340:ALA:HB2	24:B:847:BCR:H372	1.92	0.51
5:E:55:GLN:HE22	5:E:77:ASN:ND2	2.08	0.51
8:H:83:LEU:HD22	12:L:175:LEU:CD1	2.41	0.51
14:8:42:THR:HA	14:8:51:ASN:HD22	1.75	0.51
20:6:309:CLA:HBB1	20:6:309:CLA:HMB3	1.91	0.51
19:5:137:TRP:CZ3	20:5:323:CLA:HMA1	2.45	0.51
1:A:388:LEU:HD22	1:A:743:PHE:HB3	1.92	0.51
2:B:127:THR:HG21	2:B:360:ALA:N	2.26	0.51
2:B:572:SER:OG	2:B:575:ASP:OD2	2.25	0.51
2:B:574:TYR:OH	2:B:708:LEU:HG	2.11	0.51
6:F:150:PHE:O	6:F:153:THR:OG1	2.28	0.51
13:0:64:LEU:HA	23:0:302:LHG:HC12	1.92	0.51
13:1:153:TYR:CE2	13:1:174:LYS:HD3	2.45	0.51
20:5:312:CLA:C3B	25:5:319:DGD:HA71	2.41	0.51
20:A:802:CLA:CHC	28:J:104:LUT:H23	2.40	0.51
2:B:409:LEU:O	2:B:412:MET:HB2	2.10	0.51
13:0:74:PHE:HZ	20:0:301:CLA:HMC1	1.76	0.51
13:0:218:PHE:HA	13:0:221:ASN:HD21	1.75	0.51
20:8:306:CLA:C1D	20:8:311:CLA:HMD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:HIS:HB2	20:A:817:CLA:CHB	2.41	0.51
1:A:483:PHE:O	1:A:486:TRP:N	2.44	0.51
13:0:127:LEU:HD11	27:0:303:LMG:C5	2.40	0.51
14:8:194:LYS:HE2	20:8:311:CLA:CMD	2.40	0.51
15:7:110:VAL:HG21	29:7:1012:CHL:CMD	2.39	0.51
16:3:130:VAL:HG22	20:3:1016:CLA:HMC2	1.92	0.51
13:1:109:TRP:O	13:1:109:TRP:CE3	2.64	0.51
20:0:313:CLA:O1D	14:8:135:ALA:HB1	2.11	0.51
15:7:160:LEU:HD13	15:7:161:GLU:HB2	1.93	0.51
16:3:219:LYS:HE2	23:3:1019:LHG:HC42	1.93	0.51
29:4:315:CHL:H13	29:4:316:CHL:CHB	2.41	0.51
19:5:138:GLN:O	19:5:142:ASN:N	2.41	0.51
20:5:312:CLA:C1B	25:5:319:DGD:HB51	2.40	0.51
1:A:649:PHE:O	1:A:653:GLN:HB2	2.11	0.51
20:A:813:CLA:HBA1	20:A:815:CLA:HMB3	1.86	0.51
20:A:835:CLA:HHC	20:A:835:CLA:CBB	2.40	0.51
6:F:202:TRP:CG	6:F:203:PRO:HD3	2.46	0.51
13:1:64:LEU:HD12	28:1:1002:LUT:C22	2.41	0.51
13:1:194:GLN:HE21	13:1:194:GLN:C	2.19	0.51
17:4:224:LEU:HD11	27:4:318:LMG:H132	1.89	0.51
1:A:431:ILE:HG12	1:A:434:ARG:CZ	2.42	0.50
20:A:840:CLA:HMB3	23:A:843:LHG:C6	2.41	0.50
2:B:291:MET:CB	20:B:850:CLA:HMC1	2.41	0.50
15:7:124:GLN:HE22	29:7:1012:CHL:CMC	2.24	0.50
14:8:31:LEU:HD21	15:7:137:TYR:CE2	2.45	0.50
20:8:312:CLA:HAA2	15:7:123:ILE:HG12	1.93	0.50
18:6:79:MET:SD	20:6:305:CLA:HAB	2.51	0.50
19:5:80:TRP:CE2	29:5:314:CHL:HED3	2.46	0.50
19:5:138:GLN:HB3	19:5:146:VAL:HG21	1.94	0.50
1:A:136:GLN:HE22	6:F:104:LEU:HD11	1.77	0.50
20:A:809:CLA:O1A	16:3:82:ILE:HD11	2.12	0.50
2:B:458:PRO:CG	2:B:513:ILE:HG22	2.41	0.50
20:1:1011:CLA:OBD	17:4:163:ARG:NH1	2.44	0.50
20:1:1017:CLA:HAC2	23:4:301:LHG:C22	2.41	0.50
18:6:100:ALA:O	18:6:103:GLU:HG3	2.11	0.50
1:A:440:HIS:ND1	20:A:830:CLA:HMB1	2.27	0.50
2:B:124:TRP:CZ3	2:B:125:TRP:CZ3	3.00	0.50
9:I:82:LEU:HD23	9:I:86:VAL:HG21	1.93	0.50
10:J:7:TYR:HA	10:J:10:THR:HG23	1.92	0.50
29:8:314:CHL:HHC	29:8:314:CHL:HBB1	1.93	0.50
20:1:1006:CLA:CGA	20:1:1006:CLA:H3A	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:1007:CLA:OBD	20:1:1014:CLA:CGA	2.60	0.50
17:4:86:LEU:HD12	30:4:303:XAT:H23	1.94	0.50
19:5:186:GLU:CG	20:5:304:CLA:CHB	2.88	0.50
30:5:303:XAT:H403	20:5:308:CLA:CBB	2.40	0.50
20:A:833:CLA:HAB	24:A:847:BCR:HC31	1.93	0.50
2:B:13:LEU:CD1	2:B:28:MET:HG3	2.42	0.50
2:B:352:HIS:CE1	20:B:828:CLA:NB	2.79	0.50
2:B:548:MET:SD	3:C:66:ARG:NH2	2.84	0.50
17:4:224:LEU:HD12	27:4:318:LMG:H131	1.93	0.50
20:B:827:CLA:HMA1	24:B:847:BCR:H14C	1.94	0.50
3:C:24:ASP:HB3	4:D:151:HIS:CE1	2.47	0.50
11:K:34:THR:HG22	11:K:104:VAL:HG13	1.92	0.50
14:8:78:ARG:HG2	20:8:305:CLA:C3C	2.42	0.50
19:5:55:TRP:HH2	25:5:319:DGD:CDA	2.24	0.50
24:A:844:BCR:H392	24:A:850:BCR:C10	2.42	0.50
6:F:136:ASP:HB3	6:F:137:PRO:HD3	1.94	0.50
14:8:194:LYS:CE	20:8:311:CLA:HMD3	2.40	0.50
13:1:83:ARG:O	13:1:86:MET:HB2	2.12	0.50
1:A:187:LYS:O	1:A:190:TRP:N	2.43	0.50
2:B:374:THR:HG21	2:B:726:LEU:CD1	2.41	0.50
5:E:45:ILE:HD11	5:E:75:PHE:CE1	2.47	0.50
14:8:118:PRO:HG2	14:8:121:SER:CB	2.42	0.50
29:7:1017:CHL:C9	16:3:149:PHE:CZ	2.95	0.50
13:1:154:PRO:HG3	29:1:1013:CHL:HMD2	1.93	0.50
20:1:1003:CLA:HBB1	20:1:1003:CLA:HMB1	1.93	0.50
29:1:1012:CHL:CHC	29:1:1015:CHL:CBB	2.90	0.50
17:4:61:TRP:CD1	20:4:311:CLA:NB	2.79	0.50
19:5:131:TRP:CH2	24:5:320:BCR:C33	2.87	0.50
1:A:204:GLY:O	1:A:208:LEU:HB2	2.11	0.50
13:1:152:VAL:HG13	13:1:153:TYR:CE2	2.44	0.50
19:5:80:TRP:O	19:5:83:LEU:N	2.45	0.50
1:A:86:ILE:HD11	1:A:174:PHE:HE2	1.77	0.49
1:A:700:ILE:HD13	20:A:837:CLA:HMD1	1.94	0.49
2:B:695:LYS:HE3	12:L:139:GLN:HA	1.94	0.49
20:B:820:CLA:O1D	20:B:821:CLA:HMA1	2.11	0.49
14:8:118:PRO:O	14:8:121:SER:OG	2.27	0.49
13:1:57:TYR:CD2	20:1:1011:CLA:HMC1	2.47	0.49
13:1:137:ALA:CB	24:1:1001:BCR:H363	2.42	0.49
20:1:1006:CLA:HMB1	20:1:1006:CLA:HBB1	1.93	0.49
19:5:125:GLU:OE2	29:5:313:CHL:HMC	2.11	0.49
19:5:178:ASN:O	19:5:179:LEU:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:0:128:ASN:OD1	27:0:303:LMG:C10	2.60	0.49
14:8:194:LYS:HZ3	27:8:318:LMG:C10	2.25	0.49
29:5:313:CHL:HBB2	20:5:315:CLA:CBC	2.40	0.49
1:A:547:VAL:O	1:A:551:LEU:HB2	2.12	0.49
16:3:100:LEU:HD11	20:3:1005:CLA:HBC1	1.94	0.49
17:4:217:LYS:HZ1	27:4:318:LMG:C8	2.24	0.49
20:6:312:CLA:O2A	19:5:130:HIS:ND1	2.44	0.49
1:A:156:GLU:O	1:A:157:LEU:C	2.55	0.49
1:A:169:MET:O	1:A:173:MET:HG2	2.12	0.49
2:B:513:ILE:HG23	2:B:517:ASP:CB	2.41	0.49
2:B:646:VAL:HG22	20:B:812:CLA:HAC1	1.95	0.49
28:1:1002:LUT:H163	29:1:1015:CHL:CBB	2.43	0.49
18:6:214:GLY:HA2	19:5:118:MET:SD	2.53	0.49
1:A:50:TRP:HZ2	20:A:838:CLA:HBB1	1.78	0.49
2:B:231:TRP:HB2	20:B:819:CLA:HBA2	1.94	0.49
2:B:636:TYR:CE1	2:B:641:MET:HB2	2.48	0.49
13:0:179:LYS:HE2	20:0:311:CLA:C3D	2.42	0.49
15:7:204:PHE:HE1	28:7:1001:LUT:H26	1.78	0.49
1:A:353:LEU:HD13	20:A:804:CLA:C2D	2.42	0.49
2:B:178:HIS:CD2	20:B:816:CLA:HMC1	2.47	0.49
20:B:818:CLA:HBA2	24:B:843:BCR:HC22	1.93	0.49
20:0:309:CLA:CBC	20:0:316:CLA:HBC2	2.24	0.49
14:8:233:TYR:OH	14:8:240:LEU:C	2.55	0.49
17:4:61:TRP:CD1	17:4:61:TRP:C	2.90	0.49
19:5:58:LEU:HD13	30:5:303:XAT:H221	1.95	0.49
19:5:77:HIS:HE1	20:5:308:CLA:NC	2.10	0.49
1:A:431:ILE:HG12	1:A:434:ARG:NH2	2.28	0.49
3:C:31:TRP:CG	3:C:32:ASP:H	2.31	0.49
13:0:131:LEU:HD12	27:0:303:LMG:O9	2.12	0.49
28:8:303:LUT:C24	29:8:315:CHL:H43	2.42	0.49
16:3:176:TYR:CZ	26:3:1018:LMT:H6D	2.48	0.49
30:6:304:XAT:H403	20:6:309:CLA:CBB	2.43	0.49
8:H:69:PHE:CE1	24:H:201:BCR:C33	2.95	0.49
28:1:1002:LUT:C16	29:1:1015:CHL:CBB	2.90	0.49
1:A:146:GLN:OE1	1:A:146:GLN:N	2.42	0.49
2:B:305:ILE:HA	20:B:824:CLA:O1D	2.13	0.49
2:B:527:GLY:CA	2:B:587:THR:HG22	2.43	0.49
14:8:191:LYS:HD3	20:8:306:CLA:HAA2	1.93	0.49
15:7:105:ALA:O	15:7:109:VAL:CG2	2.57	0.49
1:A:726:VAL:HG22	20:A:839:CLA:CAD	2.42	0.49
13:0:84:TRP:CE2	29:0:315:CHL:HED3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:302:BCR:H393	20:6:310:CLA:C4B	2.43	0.49
20:6:312:CLA:CBC	27:6:319:LMG:HC2	2.42	0.49
29:5:317:CHL:CBB	24:5:320:BCR:HC8	2.43	0.49
1:A:162:THR:HG22	20:A:813:CLA:CGA	2.43	0.48
20:A:820:CLA:HMB2	20:A:824:CLA:HMA3	1.95	0.48
2:B:142:PHE:O	2:B:145:LEU:N	2.46	0.48
1:A:114:SER:CB	1:A:131:VAL:HG11	2.44	0.48
1:A:360:PHE:CE2	20:A:828:CLA:HBC3	2.48	0.48
20:B:817:CLA:CAA	24:B:845:BCR:H392	2.37	0.48
20:B:825:CLA:HBA2	24:B:846:BCR:H14C	1.95	0.48
20:B:834:CLA:O1A	10:J:30:ASN:ND2	2.46	0.48
12:L:146:ILE:HD11	12:L:162:PHE:HB2	1.93	0.48
15:7:156:GLU:CD	15:7:169:PHE:HB2	2.38	0.48
16:3:123:ILE:CD1	16:3:137:TYR:CD1	2.96	0.48
16:3:200:LEU:HD13	16:3:201:PHE:CE1	2.48	0.48
13:1:59:PHE:CD1	13:1:61:PRO:HD3	2.47	0.48
13:1:80:ILE:HD13	13:1:145:ARG:NH2	2.28	0.48
18:6:54:PRO:HD2	30:6:304:XAT:O23	2.12	0.48
18:6:116:VAL:O	18:6:120:LEU:HG	2.13	0.48
1:A:388:LEU:HD22	1:A:747:ILE:CD1	2.44	0.48
1:A:472:PHE:HA	1:A:477:ILE:HB	1.94	0.48
2:B:13:LEU:HD11	2:B:28:MET:HG3	1.95	0.48
12:L:126:LEU:HD23	12:L:175:LEU:CD2	2.43	0.48
14:8:103:GLU:CB	14:8:105:TYR:CE1	2.96	0.48
15:7:150:PHE:HE2	29:7:1013:CHL:HBB2	1.79	0.48
16:3:119:ASP:O	16:3:122:ASN:OD1	2.32	0.48
16:3:183:ILE:HG13	19:5:58:LEU:C	2.38	0.48
13:1:95:VAL:O	13:1:99:GLY:O	2.31	0.48
18:6:123:TRP:HE1	29:6:314:CHL:CBB	2.26	0.48
20:6:320:CLA:HAA2	20:6:320:CLA:HBD	1.95	0.48
1:A:392:THR:HG21	20:A:827:CLA:HMB1	1.95	0.48
13:0:153:TYR:CB	20:0:305:CLA:O1D	2.59	0.48
20:4:310:CLA:NB	27:4:318:LMG:HC3	2.29	0.48
19:5:207:THR:OG1	19:5:208:GLY:N	2.47	0.48
1:A:187:LYS:O	1:A:188:LEU:C	2.55	0.48
11:K:103:ILE:HG12	20:K:201:CLA:CHC	2.44	0.48
14:8:164:SER:HB3	14:8:168:TYR:O	2.13	0.48
1:A:194:VAL:HG11	20:A:824:CLA:HAC2	1.94	0.48
1:A:562:LEU:HD11	2:B:673:GLN:HG2	1.96	0.48
2:B:258:PHE:O	2:B:494:TRP:HB3	2.13	0.48
7:G:48:ILE:HD11	13:0:136:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:8:317:CHL:HHC	29:8:317:CHL:HBB1	1.95	0.48
17:4:59:PRO:CB	17:4:79:PHE:CD2	2.95	0.48
19:5:34:LEU:O	19:5:53:TYR:HD1	1.96	0.48
19:5:88:VAL:HG13	19:5:105:LEU:CD2	2.44	0.48
20:5:312:CLA:HBC1	25:5:319:DGD:C5D	2.43	0.48
29:5:313:CHL:CBB	29:5:316:CHL:HBB2	2.43	0.48
15:7:70:GLN:CB	15:7:139:PHE:CZ	2.97	0.48
15:7:195:ARG:O	15:7:199:ILE:HG12	2.14	0.48
1:A:434:ARG:HA	1:A:437:ILE:HD12	1.96	0.48
1:A:668:TYR:CE1	20:A:807:CLA:HBC1	2.47	0.48
2:B:127:THR:CG2	2:B:360:ALA:H	2.26	0.48
2:B:548:MET:HG3	2:B:551:LYS:CG	2.44	0.48
2:B:621:LEU:HD23	2:B:625:LEU:HD12	1.95	0.48
15:7:175:LEU:HD22	20:7:1004:CLA:O1A	2.13	0.48
1:A:359:LEU:HD22	20:A:824:CLA:HMB3	1.96	0.48
1:A:584:CYS:O	2:B:670:GLY:N	2.46	0.48
20:A:831:CLA:HAA1	24:I:201:BCR:C16	2.43	0.48
2:B:421:SER:O	2:B:424:SER:OG	2.26	0.48
28:0:304:LUT:H371	29:0:314:CHL:HMB3	1.94	0.48
15:7:67:TRP:HA	15:7:139:PHE:CZ	2.49	0.48
19:5:151:ILE:HD11	24:5:320:BCR:H323	1.96	0.48
1:A:436:ALA:O	1:A:440:HIS:ND1	2.47	0.48
1:A:445:CYS:CB	1:A:548:LEU:HD11	2.44	0.48
20:A:819:CLA:HMC2	24:A:850:BCR:H14C	1.96	0.48
2:B:722:TYR:CD2	2:B:726:LEU:HD11	2.48	0.48
15:7:231:PHE:HB2	15:7:235:GLY:O	2.14	0.48
1:A:188:LEU:O	1:A:189:GLU:C	2.57	0.47
2:B:173:GLU:HG2	2:B:292:TYR:HB3	1.95	0.47
13:0:131:LEU:CD1	27:0:303:LMG:H121	2.42	0.47
14:8:33:GLY:HA2	15:7:144:SER:OG	2.14	0.47
15:7:86:ILE:O	15:7:90:SER:OG	2.25	0.47
13:1:188:PHE:CE2	28:1:1002:LUT:H12	2.49	0.47
17:4:155:LEU:CG	23:4:301:LHG:H201	2.43	0.47
19:5:105:LEU:CD1	19:5:106:PRO:HD3	2.44	0.47
19:5:155:ASN:HB3	29:5:317:CHL:C3D	2.44	0.47
20:5:310:CLA:HBD	20:5:310:CLA:HAA1	1.95	0.47
1:A:161:THR:HG21	20:A:815:CLA:HAA2	1.96	0.47
1:A:310:HIS:CE1	20:A:819:CLA:CHD	2.97	0.47
20:0:311:CLA:CAB	24:8:302:BCR:H333	2.44	0.47
16:3:101:GLY:O	16:3:105:CYS:SG	2.73	0.47
16:3:257:ASN:HA	20:3:1007:CLA:O1A	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:317:CHL:HBB2	24:5:320:BCR:H10C	1.95	0.47
1:A:392:THR:CG2	20:A:827:CLA:HMB1	2.44	0.47
7:G:50:ARG:CG	7:G:51:PHE:CZ	2.97	0.47
15:7:87:ILE:O	15:7:91:ILE:HG23	2.15	0.47
20:4:310:CLA:C4B	27:4:318:LMG:O2	2.63	0.47
18:6:103:GLU:OE2	20:6:310:CLA:H2A	2.14	0.47
19:5:121:LEU:HD23	19:5:121:LEU:C	2.39	0.47
2:B:722:TYR:CE2	2:B:726:LEU:HD11	2.49	0.47
20:7:1010:CLA:C2C	23:7:1016:LHG:HC5	2.45	0.47
1:A:372:TYR:CZ	20:A:834:CLA:HBC3	2.50	0.47
2:B:24:TYR:O	2:B:27:ALA:N	2.47	0.47
2:B:663:MET:HE2	22:B:842:PQN:H2M2	1.96	0.47
15:7:201:CYS:O	15:7:204:PHE:HB2	2.15	0.47
13:1:203:ILE:HD12	13:1:204:ALA:N	2.29	0.47
24:1:1001:BCR:H393	20:1:1008:CLA:CHC	2.44	0.47
18:6:55:LEU:HD13	30:6:304:XAT:H221	1.96	0.47
19:5:203:GLN:HE22	28:5:302:LUT:C4	2.27	0.47
1:A:247:ARG:NH1	20:A:814:CLA:OBD	2.48	0.47
2:B:524:ILE:HG21	20:B:837:CLA:HAB	1.96	0.47
6:F:189:VAL:N	6:F:190:PRO:HD2	2.29	0.47
14:8:232:ASN:HB2	14:8:234:ALA:H	1.80	0.47
16:3:92:VAL:O	16:3:95:ALA:HB3	2.15	0.47
13:1:93:LEU:O	13:1:97:LEU:HD12	2.15	0.47
17:4:111:VAL:HG23	17:4:229:PHE:CE2	2.50	0.47
17:4:157:PHE:CE1	29:4:315:CHL:HMB1	2.49	0.47
18:6:178:LYS:HE2	27:6:319:LMG:HC5	1.97	0.47
27:5:324:LMG:H381	27:5:324:LMG:C34	2.43	0.47
1:A:50:TRP:CZ2	20:A:838:CLA:CBB	2.98	0.47
1:A:50:TRP:CD1	1:A:722:GLN:HE22	2.33	0.47
1:A:74:PHE:O	1:A:78:PHE:N	2.40	0.47
1:A:112:LYS:O	1:A:131:VAL:HG13	2.14	0.47
1:A:218:ILE:HA	1:A:222:LEU:HD12	1.95	0.47
20:B:830:CLA:C4D	24:B:844:BCR:H282	2.43	0.47
7:G:105:ALA:N	24:G:204:BCR:H362	2.29	0.47
13:0:131:LEU:CB	27:0:303:LMG:C14	2.90	0.47
14:8:71:GLN:CD	14:8:166:LEU:HD12	2.40	0.47
14:8:108:GLY:HA3	29:8:314:CHL:O1D	2.15	0.47
15:7:116:ASP:OD1	15:7:116:ASP:C	2.57	0.47
15:7:182:LYS:CE	15:7:186:TYR:OH	2.62	0.47
16:3:88:GLN:O	16:3:92:VAL:HG23	2.15	0.47
17:4:61:TRP:HD1	20:4:311:CLA:NB	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:129:MET:HE2	20:5:315:CLA:HMC1	1.95	0.47
19:5:135:ARG:NE	19:5:146:VAL:HG13	2.29	0.47
1:A:101:TYR:O	1:A:105:LEU:N	2.48	0.47
12:L:122:ALA:HA	12:L:182:VAL:HG21	1.96	0.47
13:0:81:HIS:CD2	28:0:304:LUT:H401	2.49	0.47
16:3:197:PHE:CE2	16:3:198:PHE:CE2	3.03	0.47
29:5:317:CHL:HAB	24:5:320:BCR:C10	2.45	0.47
1:A:688:SER:HG	22:A:842:PQN:H9	1.80	0.47
2:B:226:PHE:CE1	24:B:843:BCR:H321	2.47	0.47
15:7:67:TRP:HA	15:7:139:PHE:CE1	2.50	0.47
17:4:215:GLU:OE2	20:4:304:CLA:NB	2.48	0.47
20:4:307:CLA:HBC2	20:4:307:CLA:CHD	2.45	0.47
29:5:316:CHL:H142	29:5:317:CHL:HMA3	1.96	0.47
24:B:804:BCR:H20C	24:B:804:BCR:H361	1.57	0.47
20:B:822:CLA:OBD	20:B:824:CLA:HMD3	2.14	0.47
7:G:118:ASN:OD1	27:0:303:LMG:HC2	2.15	0.47
12:L:90:LEU:HB3	20:L:202:CLA:HMA1	1.97	0.47
12:L:161:LEU:HD23	12:L:170:PHE:CZ	2.50	0.47
15:7:49:GLY:O	15:7:195:ARG:NH2	2.34	0.47
20:1:1006:CLA:HMD1	20:1:1011:CLA:CBB	2.45	0.47
17:4:110:ALA:O	17:4:114:ILE:HG12	2.14	0.47
1:A:456:TYR:CE1	1:A:534:MET:HB3	2.50	0.46
2:B:270:TRP:O	2:B:273:ASP:N	2.48	0.46
2:B:632:LEU:HD21	2:B:725:PHE:HA	1.97	0.46
20:B:808:CLA:CHC	20:B:831:CLA:HMB3	2.46	0.46
20:B:817:CLA:HMA2	24:B:845:BCR:H393	1.97	0.46
20:B:833:CLA:HBC2	20:B:839:CLA:HMC2	1.97	0.46
20:J:102:CLA:HBC2	20:J:102:CLA:CMC	2.44	0.46
15:7:164:TYR:CD1	15:7:164:TYR:N	2.83	0.46
23:7:1016:LHG:HC82	29:7:1017:CHL:CHC	2.45	0.46
29:1:1012:CHL:CHC	29:1:1015:CHL:HBB1	2.45	0.46
20:6:308:CLA:HMD2	20:6:312:CLA:CBB	2.44	0.46
19:5:69:TRP:CE3	20:5:323:CLA:HMA3	2.50	0.46
19:5:129:MET:HE2	20:5:315:CLA:CMC	2.45	0.46
1:A:434:ARG:NH1	1:A:555:LEU:O	2.48	0.46
1:A:720:ILE:HG12	2:B:569:CYS:SG	2.56	0.46
2:B:585:LEU:HD21	2:B:715:SER:HA	1.98	0.46
20:B:810:CLA:CHB	20:B:811:CLA:HMA1	2.45	0.46
1:A:461:THR:HG21	20:L:201:CLA:HBC1	1.96	0.46
20:A:817:CLA:HBB1	20:A:817:CLA:HMB3	1.97	0.46
6:F:84:LEU:HD21	6:F:112:LYS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:8:103:GLU:HB2	14:8:105:TYR:CE1	2.50	0.46
15:7:81:LEU:HD11	20:7:1004:CLA:HBC1	1.98	0.46
13:1:217:ASN:HD22	13:1:219:ALA:H	1.62	0.46
24:1:1001:BCR:H383	29:1:1015:CHL:HAA1	1.97	0.46
2:B:388:PHE:HB3	2:B:535:LEU:HB3	1.97	0.46
30:8:304:XAT:H382	20:8:308:CLA:HBA1	1.97	0.46
20:A:815:CLA:HBD	20:A:815:CLA:HAA1	1.98	0.46
20:A:823:CLA:CMB	20:A:840:CLA:CAB	2.93	0.46
2:B:70:ALA:HB2	2:B:136:LEU:HB2	1.96	0.46
2:B:105:PHE:CZ	20:B:812:CLA:HBC1	2.51	0.46
2:B:277:HIS:HB2	20:B:820:CLA:CHB	2.45	0.46
2:B:470:LYS:HA	2:B:503:ASN:OD1	2.15	0.46
2:B:632:LEU:HG	2:B:728:ALA:HB3	1.97	0.46
2:B:658:TYR:CD2	20:B:805:CLA:HMA1	2.50	0.46
15:7:39:PRO:HB3	15:7:52:GLY:HA3	1.98	0.46
16:3:123:ILE:HG22	16:3:127:GLU:HB2	1.96	0.46
16:3:232:GLY:O	16:3:235:ALA:N	2.48	0.46
13:1:219:ALA:HB1	17:4:147:SER:HB2	1.97	0.46
2:B:343:GLY:O	2:B:346:THR:OG1	2.33	0.46
4:D:107:ARG:O	4:D:111:ASN:ND2	2.48	0.46
16:3:64:ASP:HA	20:3:1008:CLA:CGD	2.45	0.46
16:3:130:VAL:HG22	20:3:1016:CLA:HMC1	1.96	0.46
18:6:85:ILE:CD1	30:6:304:XAT:O4	2.64	0.46
20:6:308:CLA:CGA	20:6:308:CLA:H3A	2.46	0.46
19:5:134:VAL:O	19:5:137:TRP:HB3	2.16	0.46
24:B:843:BCR:H20C	24:B:843:BCR:H361	1.52	0.46
29:0:317:CHL:H62	29:0:317:CHL:H41	1.77	0.46
14:8:210:LYS:HE3	14:8:217:PRO:CD	2.44	0.46
15:7:171:ASP:HA	28:7:1001:LUT:H42	1.97	0.46
29:4:315:CHL:H62	29:4:315:CHL:H41	1.78	0.46
19:5:195:ILE:HD11	20:5:307:CLA:CBC	2.46	0.46
1:A:139:GLN:HE22	1:A:748:ILE:HG23	1.81	0.46
1:A:610:PHE:O	1:A:614:MET:HG2	2.16	0.46
4:D:86:ILE:O	4:D:112:LEU:HA	2.16	0.46
7:G:45:PHE:CZ	13:0:135:PHE:CE1	3.04	0.46
20:G:201:CLA:HMC2	24:G:204:BCR:H383	1.98	0.46
17:4:196:GLY:O	17:4:197:ILE:C	2.59	0.46
2:B:225:PRO:HA	2:B:228:THR:OG1	2.16	0.46
2:B:657:ILE:HG22	2:B:713:HIS:O	2.15	0.46
20:8:307:CLA:HAA1	20:8:307:CLA:HBD	1.98	0.46
17:4:142:TYR:CE2	29:4:315:CHL:HBC1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:179:LEU:HD22	19:5:180:LYS:CA	2.45	0.46
20:5:305:CLA:HMD3	20:5:310:CLA:C4D	2.46	0.46
1:A:204:GLY:O	24:A:845:BCR:C35	2.64	0.46
20:A:835:CLA:HHC	20:A:835:CLA:HBB1	1.98	0.46
13:0:203:ILE:HD12	13:0:204:ALA:N	2.30	0.46
20:A:833:CLA:HMB1	24:A:847:BCR:C3	2.45	0.45
2:B:281:ILE:HD13	20:B:821:CLA:CBB	2.46	0.45
2:B:351:GLN:OE1	20:B:827:CLA:OBD	2.34	0.45
20:B:816:CLA:HBC3	20:B:816:CLA:HMC3	1.97	0.45
13:0:86:MET:HE3	13:0:180:ASN:HB3	1.97	0.45
13:0:127:LEU:CD1	27:0:303:LMG:C5	2.94	0.45
20:0:310:CLA:HBD	20:0:310:CLA:HAA1	1.98	0.45
14:8:70:GLN:HA	20:8:308:CLA:CMA	2.46	0.45
17:4:63:PRO:HG2	20:4:311:CLA:O2D	2.16	0.45
18:6:187:PHE:CE1	30:6:304:XAT:H10	2.50	0.45
19:5:179:LEU:CD1	19:5:180:LYS:H	2.12	0.45
20:5:312:CLA:HHC	20:5:312:CLA:CBB	2.39	0.45
1:A:530:THR:O	1:A:534:MET:HG2	2.17	0.45
3:C:72:GLU:HB2	3:C:77:MET:SD	2.56	0.45
13:0:116:ALA:HB3	13:0:123:VAL:HG21	1.98	0.45
15:7:156:GLU:CG	15:7:168:ARG:HG2	2.46	0.45
15:7:164:TYR:HB3	20:7:1004:CLA:CGD	2.46	0.45
13:1:198:THR:HG21	13:1:221:ASN:HB2	1.99	0.45
2:B:119:SER:HB3	20:B:829:CLA:O2D	2.17	0.45
2:B:169:PHE:O	2:B:175:ARG:NH2	2.49	0.45
2:B:223:LEU:HD23	2:B:223:LEU:O	2.16	0.45
3:C:61:ASP:HA	3:C:62:PHE:HA	1.80	0.45
12:L:99:PRO:HA	20:L:204:CLA:CMB	2.46	0.45
14:8:174:ASP:OD1	28:8:303:LUT:O23	2.33	0.45
13:1:166:ASP:HA	13:1:167:SER:HA	1.65	0.45
18:6:98:TYR:OH	29:6:313:CHL:C1	2.64	0.45
29:5:316:CHL:H122	29:5:317:CHL:NA	2.32	0.45
1:A:440:HIS:O	1:A:444:VAL:HG23	2.17	0.45
2:B:636:TYR:CE1	2:B:641:MET:CB	2.99	0.45
6:F:156:PHE:CE1	20:F:302:CLA:C4B	2.99	0.45
7:G:89:THR:HG21	7:G:96:ASN:HA	1.98	0.45
13:1:64:LEU:HD12	28:1:1002:LUT:H221	1.97	0.45
17:4:98:GLN:HE22	17:4:192:GLY:HA3	1.81	0.45
18:6:83:ALA:HB2	28:6:303:LUT:H401	1.98	0.45
19:5:164:TYR:CE2	19:5:183:GLN:NE2	2.81	0.45
22:A:842:PQN:H141	22:A:842:PQN:H161	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:LEU:CD2	26:B:849:LMT:H3'	2.47	0.45
2:B:458:PRO:HG3	2:B:513:ILE:HG22	1.99	0.45
13:0:62:LEU:HD12	28:0:304:LUT:H21	1.99	0.45
16:3:123:ILE:CG2	16:3:127:GLU:HB2	2.47	0.45
20:5:310:CLA:CHB	25:5:319:DGD:HO4D	2.29	0.45
1:A:443:TRP:CE2	20:A:852:CLA:HBB2	2.52	0.45
1:A:544:HIS:O	1:A:548:LEU:HG	2.17	0.45
1:A:599:MET:HG3	1:A:600:TYR:N	2.30	0.45
20:B:801:CLA:O1A	20:B:801:CLA:H3A	2.17	0.45
20:B:810:CLA:HHB	20:B:811:CLA:HMA1	1.97	0.45
3:C:63:LEU:O	4:D:175:ILE:HD11	2.16	0.45
15:7:70:GLN:HB2	15:7:139:PHE:CZ	2.51	0.45
15:7:117:PHE:O	15:7:118:PRO:C	2.60	0.45
20:7:1007:CLA:CGA	20:7:1007:CLA:H3A	2.46	0.45
29:7:1017:CHL:OMC	29:7:1017:CHL:HHC	2.15	0.45
13:1:142:GLU:O	13:1:145:ARG:HB3	2.17	0.45
17:4:179:ILE:HD11	24:4:302:BCR:H311	1.97	0.45
29:4:315:CHL:C15	29:4:315:CHL:H101	2.46	0.45
1:A:50:TRP:HZ2	20:A:838:CLA:CBB	2.29	0.45
1:A:278:PHE:CZ	20:A:817:CLA:HBB1	2.52	0.45
2:B:70:ALA:HB2	2:B:136:LEU:CB	2.47	0.45
2:B:212:ASN:O	2:B:213:PHE:C	2.59	0.45
2:B:632:LEU:HG	2:B:728:ALA:CB	2.46	0.45
7:G:50:ARG:NH1	7:G:51:PHE:CE1	2.84	0.45
20:0:313:CLA:HMD1	24:8:302:BCR:HC22	1.99	0.45
17:4:224:LEU:O	17:4:225:ALA:C	2.60	0.45
29:4:315:CHL:OMC	29:4:315:CHL:HBC3	2.17	0.45
29:5:316:CHL:HBA1	29:5:316:CHL:H3A	1.76	0.45
20:B:831:CLA:C2D	25:B:848:DGD:HB71	2.47	0.45
7:G:50:ARG:HG3	7:G:51:PHE:CD1	2.52	0.45
20:8:306:CLA:HMD3	20:8:311:CLA:C4D	2.47	0.45
13:1:83:ARG:O	13:1:84:TRP:C	2.59	0.45
29:1:1015:CHL:H62	29:1:1015:CHL:H41	1.77	0.45
19:5:133:GLU:HG3	20:5:315:CLA:C4B	2.47	0.45
27:5:324:LMG:HC91	27:5:324:LMG:H291	1.78	0.45
1:A:607:ILE:HG22	1:A:743:PHE:CZ	2.52	0.45
2:B:291:MET:HB2	20:B:850:CLA:HMC1	1.99	0.45
20:B:808:CLA:CGA	20:B:808:CLA:H3A	2.47	0.45
5:E:71:VAL:HG11	5:E:93:VAL:HG11	1.98	0.45
7:G:51:PHE:HB3	24:G:205:BCR:C2	2.46	0.45
16:3:88:GLN:HG3	16:3:89:TYR:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:192:VAL:O	13:1:196:ALA:CA	2.65	0.45
1:A:545:VAL:HG11	1:A:598:TRP:CE2	2.52	0.44
20:0:309:CLA:OBD	20:0:316:CLA:CGA	2.66	0.44
20:7:1008:CLA:HAC1	29:7:1012:CHL:HBB2	1.99	0.44
19:5:128:LEU:HD22	24:5:320:BCR:C15	2.46	0.44
19:5:214:ALA:O	19:5:218:HIS:CD2	2.70	0.44
2:B:51:HIS:ND1	20:B:816:CLA:OBD	2.50	0.44
2:B:124:TRP:HE1	2:B:128:ILE:HD11	1.82	0.44
14:8:71:GLN:NE2	14:8:166:LEU:CD1	2.75	0.44
28:8:303:LUT:H24	29:8:315:CHL:H43	2.00	0.44
24:7:1003:BCR:H321	24:7:1003:BCR:HC8	1.99	0.44
19:5:57:PRO:O	19:5:58:LEU:HD12	2.17	0.44
19:5:109:LEU:HB2	19:5:110:PRO:HD3	1.95	0.44
20:5:301:CLA:HAA1	20:5:301:CLA:HBD	1.99	0.44
1:A:104:TRP:O	1:A:104:TRP:CG	2.71	0.44
1:A:372:TYR:HA	1:A:391:PHE:CZ	2.52	0.44
1:A:539:HIS:O	1:A:542:THR:N	2.50	0.44
20:A:851:CLA:HBA2	2:B:428:LEU:HD23	1.99	0.44
7:G:45:PHE:CD2	7:G:106:LEU:HB3	2.52	0.44
13:1:100:TYR:CD1	13:1:100:TYR:N	2.85	0.44
18:6:73:VAL:HG22	18:6:77:TRP:CD1	2.52	0.44
20:5:312:CLA:HBB1	20:5:312:CLA:CHC	2.47	0.44
20:A:802:CLA:C3B	28:J:104:LUT:H362	2.47	0.44
2:B:127:THR:HG22	2:B:360:ALA:HB3	1.99	0.44
2:B:191:TRP:O	2:B:192:THR:C	2.59	0.44
2:B:346:THR:HG23	20:B:830:CLA:HMC1	1.99	0.44
20:7:1010:CLA:C1B	23:7:1016:LHG:O4	2.64	0.44
16:3:86:TRP:O	16:3:89:TYR:HB3	2.17	0.44
24:3:1004:BCR:HC8	24:3:1004:BCR:H311	2.00	0.44
13:1:125:PHE:HB3	13:1:129:ALA:CB	2.43	0.44
17:4:136:ASP:HA	29:4:312:CHL:HED2	2.00	0.44
17:4:157:PHE:O	17:4:160:VAL:N	2.50	0.44
17:4:176:GLN:HA	17:4:184:LYS:HA	1.99	0.44
19:5:63:ASP:OD1	19:5:65:THR:N	2.49	0.44
19:5:111:GLU:N	19:5:112:PRO:HD2	2.33	0.44
20:5:312:CLA:HAC1	25:5:319:DGD:HD5	1.99	0.44
1:A:166:GLY:HA2	24:A:844:BCR:HC22	1.98	0.44
2:B:227:PHE:CE1	20:G:201:CLA:HBC3	2.52	0.44
2:B:312:PRO:HD2	23:0:302:LHG:O5	2.18	0.44
3:C:33:GLY:O	5:E:67:VAL:HA	2.18	0.44
28:J:104:LUT:H27	28:J:104:LUT:H381	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:129:TRP:HB2	20:6:315:CLA:HMA2	1.99	0.44
18:6:134:LYS:O	18:6:137:SER:OG	2.35	0.44
24:6:302:BCR:H10C	29:6:317:CHL:HBB2	1.99	0.44
30:5:303:XAT:H183	20:5:309:CLA:C4B	2.48	0.44
15:7:156:GLU:HB2	15:7:168:ARG:NH1	2.31	0.44
20:7:1010:CLA:C2B	26:3:1018:LMT:H31	2.48	0.44
13:1:118:TRP:O	13:1:121:ILE:N	2.50	0.44
13:1:177:GLU:HG3	20:1:1003:CLA:CHB	2.47	0.44
13:1:223:ILE:HD11	20:1:1017:CLA:HBC3	2.00	0.44
17:4:220:ARG:HD3	20:4:307:CLA:CHD	2.48	0.44
18:6:97:TRP:CZ2	18:6:98:TYR:HD1	2.36	0.44
2:B:79:VAL:HG22	2:B:126:TYR:CE1	2.53	0.44
2:B:192:THR:CG2	2:B:278:HIS:HB2	2.48	0.44
10:J:11:ALA:N	10:J:12:PRO:HD2	2.32	0.44
20:8:312:CLA:HAA1	20:8:312:CLA:HBD	2.00	0.44
28:1:1002:LUT:C31	20:1:1006:CLA:HMC2	2.48	0.44
17:4:197:ILE:HG21	29:4:315:CHL:C9	2.48	0.44
18:6:55:LEU:HD12	18:6:55:LEU:H	1.82	0.44
20:5:309:CLA:H3A	20:5:309:CLA:HBA2	1.73	0.44
1:A:121:ILE:HD11	10:J:31:ARG:HA	1.99	0.44
2:B:575:ASP:O	2:B:579:LEU:HG	2.17	0.44
4:D:86:ILE:HG23	4:D:138:PHE:HB3	1.99	0.44
12:L:90:LEU:HD23	12:L:177:GLY:O	2.18	0.44
29:8:317:CHL:H41	29:8:317:CHL:H62	1.74	0.44
15:7:160:LEU:CD1	15:7:161:GLU:HB2	2.48	0.44
20:1:1005:CLA:HAA1	20:1:1005:CLA:HBD	1.99	0.44
18:6:178:LYS:NZ	27:6:319:LMG:HC5	2.33	0.44
19:5:230:ASN:O	19:5:231:ILE:C	2.60	0.44
22:A:842:PQN:H172	24:F:301:BCR:H333	2.00	0.44
2:B:281:ILE:CD1	20:B:821:CLA:CBB	2.96	0.44
2:B:326:THR:HG21	2:B:404:ASN:ND2	2.30	0.44
2:B:618:MET:O	2:B:619:GLY:C	2.61	0.44
14:8:236:ASN:C	14:8:236:ASN:ND2	2.76	0.44
16:3:141:TRP:HE1	16:3:147:ILE:HD13	1.83	0.44
1:A:22:VAL:HG13	1:A:182:HIS:ND1	2.33	0.43
1:A:50:TRP:CH2	20:A:839:CLA:HMD3	2.53	0.43
20:A:825:CLA:HBA1	20:A:826:CLA:OBD	2.17	0.43
2:B:118:THR:HA	2:B:368:THR:HG22	2.00	0.43
2:B:634:ASN:N	2:B:634:ASN:HD22	2.16	0.43
2:B:692:VAL:HG11	20:B:803:CLA:CBB	2.48	0.43
24:B:843:BCR:H12C	24:G:204:BCR:H271	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:203:CLA:HBC2	20:G:203:CLA:CHD	2.48	0.43
20:8:309:CLA:HAC1	27:8:319:LMG:HC72	2.00	0.43
20:7:1004:CLA:H3A	20:7:1004:CLA:HBA2	1.66	0.43
16:3:197:PHE:CE2	16:3:198:PHE:CD2	3.06	0.43
16:3:219:LYS:HE2	23:3:1019:LHG:C4	2.48	0.43
29:4:315:CHL:H62	29:4:315:CHL:H101	1.80	0.43
19:5:201:ILE:O	19:5:204:ALA:N	2.51	0.43
20:A:820:CLA:HMA2	20:A:824:CLA:C1C	2.48	0.43
2:B:40:GLU:HA	2:B:43:LEU:HD12	2.01	0.43
24:F:304:BCR:H20C	24:F:304:BCR:H361	1.88	0.43
7:G:51:PHE:CD1	24:G:205:BCR:C3	3.01	0.43
20:G:203:CLA:ND	27:0:303:LMG:H302	2.33	0.43
13:0:152:VAL:HB	13:0:153:TYR:CD2	2.52	0.43
20:8:311:CLA:CHB	27:8:318:LMG:HC3	2.48	0.43
15:7:123:ILE:O	15:7:124:GLN:C	2.60	0.43
16:3:73:LEU:HG	20:3:1008:CLA:HAA2	2.00	0.43
16:3:97:TRP:CE2	20:3:1015:CLA:HBC3	2.53	0.43
13:1:94:ALA:HA	13:1:97:LEU:CD1	2.48	0.43
13:1:100:TYR:N	13:1:100:TYR:HD1	2.16	0.43
13:1:106:ALA:HB3	13:1:107:PRO:CD	2.44	0.43
28:6:303:LUT:H183	20:6:307:CLA:C4B	2.48	0.43
19:5:197:TYR:CE2	19:5:201:ILE:HD12	2.53	0.43
2:B:95:PRO:HA	8:H:110:ILE:HD13	1.99	0.43
24:G:205:BCR:H363	13:0:137:ALA:CB	2.40	0.43
14:8:117:ALA:HB1	14:8:118:PRO:HD2	2.00	0.43
28:3:1001:LUT:C31	20:3:1005:CLA:HMC1	2.48	0.43
18:6:165:ILE:N	18:6:166:PRO:HD3	2.32	0.43
1:A:285:VAL:HG12	1:A:285:VAL:O	2.18	0.43
1:A:658:ILE:CG2	2:B:622:ARG:HB2	2.49	0.43
20:A:823:CLA:HAC1	24:A:846:BCR:H323	1.99	0.43
2:B:172:ALA:HB1	20:B:826:CLA:HHD	2.01	0.43
2:B:478:LEU:HD21	20:B:836:CLA:HBC2	2.01	0.43
13:0:59:PHE:CD2	20:0:313:CLA:CBB	3.01	0.43
20:8:307:CLA:C1A	20:8:307:CLA:CGA	2.96	0.43
15:7:56:LEU:O	15:7:57:PHE:CG	2.72	0.43
15:7:101:GLU:OE1	15:7:103:TYR:HB3	2.18	0.43
16:3:176:TYR:CD1	26:3:1018:LMT:H6D	2.53	0.43
13:1:142:GLU:CD	13:1:145:ARG:HH12	2.26	0.43
17:4:59:PRO:CB	17:4:79:PHE:HD2	2.22	0.43
17:4:217:LYS:NZ	27:4:318:LMG:O7	2.37	0.43
24:6:302:BCR:H373	29:6:316:CHL:CHB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:124:TRP:CE3	20:5:301:CLA:HBA1	2.53	0.43
24:A:846:BCR:H20C	24:A:846:BCR:H361	1.88	0.43
2:B:20:ARG:HB3	2:B:24:TYR:CE2	2.53	0.43
2:B:564:GLY:CA	3:C:56:THR:HG22	2.48	0.43
28:0:304:LUT:H361	29:0:317:CHL:CBB	2.48	0.43
16:3:141:TRP:NE1	16:3:147:ILE:HD11	2.34	0.43
16:3:234:GLN:HE21	16:3:245:ASN:ND2	2.15	0.43
20:3:1009:CLA:HMD3	20:3:1015:CLA:C4D	2.48	0.43
17:4:174:ALA:C	17:4:175:ASN:ND2	2.77	0.43
18:6:160:VAL:O	18:6:163:PRO:HD3	2.18	0.43
19:5:77:HIS:O	19:5:78:ALA:C	2.62	0.43
19:5:113:PHE:O	19:5:114:THR:HG23	2.18	0.43
19:5:143:PHE:CD1	19:5:144:GLY:N	2.86	0.43
1:A:392:THR:O	1:A:395:THR:OG1	2.35	0.43
2:B:121:VAL:CG1	2:B:125:TRP:CE2	3.01	0.43
20:B:850:CLA:CAC	20:B:850:CLA:C2C	2.97	0.43
3:C:58:CYS:HB3	3:C:63:LEU:HD22	2.01	0.43
15:7:175:LEU:HB3	20:7:1004:CLA:HBA1	1.99	0.43
15:7:198:MET:HE1	20:7:1007:CLA:HHC	2.00	0.43
20:4:310:CLA:CHC	27:4:318:LMG:O2	2.66	0.43
30:6:304:XAT:H183	20:6:310:CLA:C1B	2.48	0.43
20:6:312:CLA:HBC3	27:6:319:LMG:C2	2.48	0.43
2:B:192:THR:HG22	2:B:278:HIS:HB2	1.98	0.43
2:B:291:MET:HB3	20:B:850:CLA:HMC1	2.01	0.43
2:B:362:GLN:C	2:B:364:ILE:H	2.26	0.43
2:B:458:PRO:HG2	2:B:513:ILE:HG22	2.01	0.43
20:0:310:CLA:HBA2	20:0:310:CLA:H3A	1.81	0.43
16:3:202:ASN:HB3	19:5:38:GLY:O	2.18	0.43
17:4:224:LEU:CD1	27:4:318:LMG:C14	2.90	0.43
19:5:115:ASN:C	19:5:116:ILE:HG13	2.44	0.43
1:A:341:LEU:N	1:A:424:ASN:HD21	2.17	0.43
1:A:360:PHE:O	1:A:363:LEU:N	2.52	0.43
15:7:87:ILE:HD13	15:7:87:ILE:N	2.33	0.43
15:7:150:PHE:CE2	29:7:1013:CHL:HBB2	2.54	0.43
13:1:93:LEU:O	13:1:97:LEU:CD1	2.67	0.43
20:6:308:CLA:HHD	20:6:312:CLA:HBB2	2.00	0.43
1:A:312:TYR:CE1	1:A:322:MET:SD	3.12	0.43
1:A:448:LEU:HD21	20:A:835:CLA:HAB	2.00	0.43
20:A:851:CLA:O1D	24:F:301:BCR:H322	2.18	0.43
2:B:388:PHE:CD2	2:B:535:LEU:HD13	2.53	0.43
10:J:21:PHE:HA	20:J:102:CLA:HBB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:0:304:LUT:C36	29:0:317:CHL:HBB1	2.49	0.43
20:0:311:CLA:CBB	24:8:302:BCR:H333	2.49	0.43
16:3:141:TRP:HE1	16:3:147:ILE:CD1	2.31	0.43
17:4:197:ILE:O	17:4:200:PRO:CD	2.67	0.43
18:6:54:PRO:HB2	18:6:55:LEU:HD12	2.00	0.43
1:A:95:GLY:HA3	1:A:148:TRP:CH2	2.54	0.43
1:A:101:TYR:HA	1:A:104:TRP:HB3	2.01	0.43
2:B:672:TRP:CZ3	24:B:804:BCR:H391	2.54	0.43
20:B:819:CLA:C1A	20:B:819:CLA:CGA	2.97	0.43
7:G:48:ILE:HG23	7:G:53:PHE:CE1	2.54	0.43
15:7:77:ARG:NE	15:7:190:GLU:OE2	2.45	0.43
13:1:142:GLU:CD	13:1:145:ARG:NH1	2.77	0.43
19:5:69:TRP:O	19:5:70:TYR:C	2.61	0.43
1:A:213:TRP:O	1:A:214:ALA:C	2.61	0.42
1:A:647:ARG:HB3	2:B:633:ILE:HG22	1.99	0.42
20:A:817:CLA:HBA2	20:A:817:CLA:H3A	1.87	0.42
2:B:333:PHE:CE2	24:B:847:BCR:H291	2.54	0.42
6:F:156:PHE:CE1	20:F:302:CLA:CHC	3.01	0.42
24:I:201:BCR:H361	24:I:201:BCR:H20C	1.83	0.42
15:7:70:GLN:CB	15:7:139:PHE:HZ	2.32	0.42
15:7:171:ASP:O	15:7:171:ASP:OD1	2.37	0.42
13:1:95:VAL:HG22	20:1:1008:CLA:C3D	2.49	0.42
13:1:151:VAL:HG11	13:1:154:PRO:CB	2.49	0.42
24:1:1001:BCR:H403	24:1:1001:BCR:C23	2.41	0.42
18:6:120:LEU:HB3	24:6:302:BCR:H363	2.01	0.42
19:5:179:LEU:CD1	19:5:180:LYS:N	2.79	0.42
1:A:474:ASP:OD1	1:A:530:THR:HG23	2.18	0.42
20:A:815:CLA:C4C	20:3:1013:CLA:HBB2	2.49	0.42
2:B:47:ILE:HG12	20:B:808:CLA:HMC2	2.01	0.42
2:B:450:PRO:O	2:B:453:GLN:HB2	2.19	0.42
13:0:116:ALA:CA	13:0:123:VAL:HG21	2.49	0.42
14:8:108:GLY:O	14:8:109:LYS:C	2.62	0.42
20:7:1010:CLA:C3C	23:7:1016:LHG:HC5	2.49	0.42
17:4:148:SER:O	17:4:151:GLY:N	2.51	0.42
20:4:307:CLA:CAC	27:4:318:LMG:C14	2.97	0.42
19:5:66:ALA:HB1	19:5:70:TYR:CE2	2.54	0.42
19:5:137:TRP:HZ3	20:5:323:CLA:HMA1	1.85	0.42
1:A:241:HIS:O	1:A:244:LEU:HB2	2.19	0.42
1:A:592:VAL:O	1:A:593:PHE:O	2.37	0.42
2:B:276:HIS:CG	20:B:820:CLA:HMB1	2.54	0.42
20:B:823:CLA:C3B	24:B:843:BCR:H362	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:845:BCR:H361	24:B:845:BCR:H21C	2.00	0.42
13:0:79:VAL:HG22	13:0:178:ILE:HD13	2.00	0.42
13:0:88:GLY:O	13:0:92:SER:OG	2.37	0.42
28:0:304:LUT:H372	29:0:314:CHL:CHB	2.48	0.42
14:8:150:PRO:O	14:8:151:GLY:C	2.62	0.42
17:4:144:ALA:HB1	17:4:145:PRO:HD2	2.02	0.42
19:5:179:LEU:CD2	19:5:180:LYS:HB2	2.49	0.42
20:5:308:CLA:OBD	20:5:315:CLA:CGA	2.67	0.42
1:A:483:PHE:O	1:A:484:ALA:C	2.63	0.42
20:A:835:CLA:HBB2	20:A:836:CLA:HBC1	2.02	0.42
20:A:837:CLA:HAA2	20:B:833:CLA:HMB1	2.00	0.42
2:B:286:ILE:O	2:B:290:HIS:NE2	2.53	0.42
13:0:60:ASP:N	13:0:61:PRO:HD3	2.34	0.42
14:8:190:LEU:O	14:8:191:LYS:C	2.62	0.42
16:3:168:TYR:HB2	16:3:171:SER:OG	2.19	0.42
17:4:228:GLY:HA2	20:4:306:CLA:C3C	2.48	0.42
18:6:60:ASN:OD1	18:6:61:ALA:N	2.52	0.42
18:6:141:ASP:OD2	29:6:317:CHL:ND	2.52	0.42
20:5:310:CLA:C1B	25:5:319:DGD:HO4D	2.32	0.42
1:A:53:HIS:HE1	20:A:802:CLA:NC	2.17	0.42
1:A:283:ASN:OD1	1:A:284:PRO:HD2	2.19	0.42
2:B:28:MET:HE2	2:B:28:MET:HA	2.02	0.42
2:B:621:LEU:HD23	2:B:621:LEU:HA	1.89	0.42
2:B:650:THR:HA	2:B:653:PHE:HB3	2.01	0.42
2:B:694:TRP:HB3	20:B:840:CLA:C2D	2.49	0.42
7:G:100:VAL:HG22	20:G:202:CLA:CMB	2.50	0.42
24:G:204:BCR:H20C	24:G:204:BCR:H361	1.90	0.42
13:0:118:TRP:CD1	13:0:119:PHE:HB2	2.46	0.42
28:0:304:LUT:H372	29:0:314:CHL:C1B	2.49	0.42
16:3:117:ILE:CG2	16:3:121:THR:HB	2.50	0.42
16:3:180:LEU:O	16:3:183:ILE:N	2.51	0.42
20:1:1014:CLA:HMC1	20:1:1014:CLA:HBC3	2.01	0.42
29:4:315:CHL:C12	29:4:316:CHL:NB	2.82	0.42
1:A:320:HIS:HB3	1:A:325:ILE:HD11	2.02	0.42
1:A:330:ARG:O	20:A:840:CLA:HAC2	2.19	0.42
1:A:677:PHE:CG	24:A:848:BCR:H363	2.55	0.42
25:B:848:DGD:HO2E	3:C:70:GLY:C	2.28	0.42
13:1:197:ALA:O	13:1:198:THR:HG23	2.20	0.42
28:1:1002:LUT:H28	28:1:1002:LUT:C36	2.23	0.42
24:6:302:BCR:H403	24:6:302:BCR:C23	2.45	0.42
20:6:308:CLA:HAA1	20:6:308:CLA:HBD	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5:307:CLA:HMD2	20:5:312:CLA:CBB	2.49	0.42
20:5:312:CLA:CAB	25:5:319:DGD:HA71	2.49	0.42
1:A:472:PHE:HA	1:A:477:ILE:HG22	2.00	0.42
1:A:602:SER:OG	1:A:603:LEU:N	2.52	0.42
2:B:87:PRO:HB3	2:B:122:TYR:CD2	2.55	0.42
6:F:153:THR:HA	20:F:302:CLA:HBC3	2.01	0.42
11:K:95:ALA:O	11:K:99:LEU:N	2.47	0.42
16:3:82:ILE:O	16:3:82:ILE:CG2	2.62	0.42
20:1:1006:CLA:HBC2	20:1:1011:CLA:HAB	2.01	0.42
17:4:224:LEU:HD21	27:4:318:LMG:H161	2.02	0.42
27:5:324:LMG:C1	27:5:324:LMG:HO4	2.31	0.42
1:A:396:TRP:HA	1:A:603:LEU:HD13	2.00	0.42
2:B:290:HIS:NE2	24:B:843:BCR:H363	2.35	0.42
2:B:311:PRO:HA	2:B:312:PRO:HD3	1.93	0.42
2:B:317:GLY:HA3	2:B:411:ARG:HD2	2.01	0.42
2:B:478:LEU:CD2	20:B:836:CLA:HBC2	2.49	0.42
20:B:819:CLA:HAA1	20:B:819:CLA:HBD	2.01	0.42
17:4:66:ASP:OD1	17:4:66:ASP:N	2.53	0.42
1:A:443:TRP:CZ2	20:A:852:CLA:HBB2	2.55	0.42
2:B:291:MET:HB2	20:B:850:CLA:CMC	2.49	0.42
20:B:825:CLA:HMB1	20:0:301:CLA:O2D	2.20	0.42
14:8:138:TRP:CE3	20:8:316:CLA:HMA1	2.55	0.42
14:8:143:LYS:O	14:8:144:PRO:C	2.63	0.42
20:7:1010:CLA:HBC3	23:7:1016:LHG:H252	2.01	0.42
13:1:192:VAL:C	13:1:196:ALA:HB2	2.45	0.42
17:4:220:ARG:HG2	20:4:307:CLA:C4C	2.49	0.42
20:4:311:CLA:HBD	18:6:123:TRP:CZ3	2.54	0.42
1:A:509:THR:HG23	1:A:523:MET:HE2	2.01	0.42
20:A:811:CLA:C1A	20:A:811:CLA:CGA	2.98	0.42
2:B:223:LEU:HD21	2:B:227:PHE:CE2	2.55	0.42
2:B:293:ARG:NH2	7:G:67:VAL:O	2.53	0.42
24:F:301:BCR:C8	24:F:301:BCR:H331	2.50	0.42
9:I:100:GLU:O	9:I:101:LYS:C	2.63	0.42
14:8:94:THR:HA	14:8:99:LEU:O	2.20	0.42
14:8:103:GLU:HB2	14:8:105:TYR:HE1	1.85	0.42
18:6:33:LEU:CD1	20:6:312:CLA:HMA3	2.49	0.42
18:6:71:GLU:OE2	18:6:181:ARG:NE	2.49	0.42
18:6:199:LYS:HA	18:6:199:LYS:HD3	1.88	0.42
20:6:308:CLA:HMB1	20:6:308:CLA:HBB1	2.01	0.42
1:A:372:TYR:HA	1:A:391:PHE:CE2	2.55	0.41
1:A:575:CYS:SG	1:A:584:CYS:HA	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:ALA:HB1	1:A:734:GLY:O	2.19	0.41
2:B:78:TRP:CE3	2:B:126:TYR:CE2	3.07	0.41
2:B:515:PRO:HG3	6:F:132:HIS:CE1	2.54	0.41
7:G:50:ARG:HD2	7:G:95:PHE:CE2	2.54	0.41
20:G:203:CLA:C4D	27:0:303:LMG:H302	2.49	0.41
13:0:127:LEU:CD1	27:0:303:LMG:C1	2.93	0.41
17:4:217:LYS:NZ	27:4:318:LMG:O9	2.53	0.41
29:4:315:CHL:H13	29:4:316:CHL:C1B	2.50	0.41
18:6:77:TRP:NE1	29:6:314:CHL:HED2	2.34	0.41
19:5:121:LEU:C	19:5:123:ALA:H	2.28	0.41
2:B:175:ARG:O	2:B:179:HIS:ND1	2.52	0.41
2:B:279:LEU:HD11	20:B:818:CLA:HAC1	2.02	0.41
2:B:394:PHE:O	2:B:395:PHE:C	2.61	0.41
2:B:478:LEU:HD13	20:B:835:CLA:HMD2	2.02	0.41
2:B:530:THR:HG21	2:B:583:TRP:CZ2	2.55	0.41
2:B:636:TYR:CD1	2:B:641:MET:HB3	2.55	0.41
14:8:119:TRP:CH2	27:8:319:LMG:H182	2.55	0.41
29:3:1014:CHL:CHA	29:3:1014:CHL:HBA1	2.49	0.41
18:6:129:TRP:HB2	20:6:315:CLA:CMA	2.51	0.41
1:A:472:PHE:HA	1:A:477:ILE:CB	2.50	0.41
1:A:498:THR:O	20:A:833:CLA:ND	2.53	0.41
1:A:546:THR:HG23	1:A:598:TRP:HB3	2.01	0.41
2:B:295:ASN:OD1	2:B:295:ASN:N	2.54	0.41
20:F:305:CLA:HMB2	10:J:26:LEU:HD11	2.02	0.41
20:G:203:CLA:HBC2	20:G:203:CLA:HHD	2.01	0.41
14:8:71:GLN:NE2	14:8:141:ILE:HG12	2.35	0.41
14:8:121:SER:OG	14:8:122:LEU:N	2.54	0.41
13:1:153:TYR:HB3	20:1:1003:CLA:O1D	2.21	0.41
13:1:165:LYS:HE2	13:1:166:ASP:OD1	2.20	0.41
29:6:316:CHL:H91	29:6:316:CHL:H111	1.81	0.41
19:5:164:TYR:HB3	20:5:304:CLA:O1D	2.20	0.41
20:A:802:CLA:C2B	28:J:104:LUT:C36	2.98	0.41
2:B:190:ALA:HB1	20:B:817:CLA:HAB	2.02	0.41
4:D:139:TYR:HB3	4:D:149:TYR:HA	2.02	0.41
13:0:94:ALA:HA	13:0:97:LEU:HB2	2.03	0.41
14:8:175:PRO:HA	13:1:62:LEU:CD2	2.41	0.41
17:4:142:TYR:CE1	20:4:309:CLA:HAA2	2.56	0.41
20:4:307:CLA:CBC	27:4:318:LMG:C14	2.96	0.41
19:5:69:TRP:CE3	19:5:140:TYR:CD2	3.07	0.41
19:5:171:PRO:HD2	28:5:302:LUT:H23	2.03	0.41
19:5:218:HIS:CE1	19:5:225:ASN:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:218:HIS:C	19:5:220:SER:N	2.78	0.41
20:5:318:CLA:HAA2	20:5:318:CLA:HBD	2.02	0.41
1:A:492:PHE:O	1:A:495:PRO:HD2	2.21	0.41
1:A:634:ASN:O	1:A:638:SER:OG	2.30	0.41
2:B:16:ASP:HB2	2:B:21:ARG:HB2	2.03	0.41
3:C:2:ALA:N	3:C:71:SER:O	2.53	0.41
13:0:116:ALA:C	13:0:123:VAL:HG21	2.45	0.41
20:0:307:CLA:C4B	28:0:318:LUT:H183	2.50	0.41
14:8:79:THR:HG23	29:8:315:CHL:CED	2.50	0.41
15:7:186:TYR:HB3	20:7:1004:CLA:HMA1	2.02	0.41
16:3:200:LEU:HD12	28:3:1001:LUT:H23	2.02	0.41
13:1:79:VAL:HG22	13:1:178:ILE:HD13	2.01	0.41
13:1:96:GLU:HB3	13:1:203:ILE:HD11	2.02	0.41
29:6:316:CHL:H143	29:6:316:CHL:H112	1.89	0.41
20:A:812:CLA:CGA	20:A:812:CLA:H3A	2.51	0.41
2:B:543:ARG:HG2	2:B:552:LYS:HD3	2.02	0.41
2:B:698:PRO:HB3	20:B:840:CLA:C2C	2.50	0.41
4:D:87:THR:HA	4:D:112:LEU:HD23	2.03	0.41
6:F:151:ILE:O	6:F:152:PRO:C	2.64	0.41
20:G:201:CLA:H3A	24:G:204:BCR:H351	2.03	0.41
13:0:50:PRO:C	13:0:52:ASP:H	2.28	0.41
15:7:73:LEU:HD12	15:7:73:LEU:HA	1.90	0.41
20:3:1006:CLA:OBD	20:3:1011:CLA:HBD	2.20	0.41
20:1:1003:CLA:HBB1	20:1:1003:CLA:CMB	2.50	0.41
17:4:67:LEU:N	17:4:67:LEU:HD23	2.35	0.41
17:4:256:VAL:O	17:4:260:ASP:N	2.51	0.41
20:5:308:CLA:HBA2	20:5:308:CLA:HBD	2.03	0.41
1:A:492:PHE:CD1	1:A:511:GLY:HA2	2.56	0.41
1:A:653:GLN:C	1:A:655:SER:H	2.28	0.41
20:B:813:CLA:HMD3	20:L:201:CLA:C4D	2.51	0.41
7:G:48:ILE:CD1	13:0:135:PHE:CE1	3.04	0.41
14:8:32:PRO:HD2	20:8:313:CLA:O2D	2.20	0.41
14:8:194:LYS:HE2	20:8:311:CLA:C2D	2.51	0.41
15:7:117:PHE:HB3	15:7:118:PRO:HD3	2.02	0.41
15:7:136:TRP:CG	20:7:1014:CLA:HMA1	2.55	0.41
18:6:33:LEU:HD21	19:5:138:GLN:HE22	1.85	0.41
18:6:170:ALA:O	18:6:171:GLU:C	2.63	0.41
20:6:312:CLA:HBC2	20:6:312:CLA:HHD	2.03	0.41
20:5:308:CLA:OBD	20:5:315:CLA:O1A	2.39	0.41
2:B:694:TRP:HB3	20:B:840:CLA:C1D	2.50	0.41
10:J:3:ASP:O	10:J:6:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:212:GLU:O	16:3:215:LEU:HB2	2.20	0.41
20:3:1005:CLA:HBA2	20:3:1005:CLA:H3A	1.87	0.41
13:1:203:ILE:HD12	13:1:204:ALA:H	1.85	0.41
20:6:311:CLA:C4B	27:6:319:LMG:O2	2.68	0.41
1:A:425:ASN:O	1:A:426:LEU:C	2.63	0.41
20:A:821:CLA:HMA1	20:A:840:CLA:HBC1	2.01	0.41
20:A:826:CLA:HBA1	24:A:847:BCR:H14C	2.03	0.41
2:B:32:PHE:CB	2:B:43:LEU:HD23	2.50	0.41
2:B:374:THR:HG21	2:B:726:LEU:HD11	2.03	0.41
2:B:478:LEU:HD13	20:B:835:CLA:CMD	2.51	0.41
2:B:531:THR:HG22	2:B:583:TRP:CB	2.50	0.41
2:B:599:HIS:HB3	2:B:603:TRP:CZ2	2.56	0.41
2:B:681:TRP:CD1	4:D:75:LEU:HD21	2.56	0.41
24:B:804:BCR:H351	24:B:804:BCR:H15C	1.80	0.41
3:C:62:PHE:CG	3:C:63:LEU:N	2.89	0.41
5:E:94:VAL:O	5:E:94:VAL:HG13	2.21	0.41
6:F:202:TRP:N	6:F:203:PRO:CD	2.84	0.41
7:G:45:PHE:CE2	13:0:135:PHE:CZ	3.08	0.41
9:I:96:PHE:CD1	9:I:96:PHE:C	2.98	0.41
12:L:95:LEU:N	12:L:95:LEU:HD23	2.36	0.41
12:L:96:LEU:HD22	12:L:124:LEU:CD1	2.51	0.41
12:L:143:THR:HB	12:L:144:PRO:HD2	2.03	0.41
12:L:146:ILE:CD1	12:L:162:PHE:HB2	2.50	0.41
14:8:217:PRO:O	28:8:303:LUT:O3	2.36	0.41
20:8:310:CLA:H3A	20:8:310:CLA:HBA2	1.81	0.41
13:1:40:LEU:HD23	13:1:41:PRO:O	2.21	0.41
13:1:195:HIS:HA	13:1:198:THR:O	2.21	0.41
20:1:1008:CLA:HBD	20:1:1008:CLA:HAA1	2.03	0.41
18:6:131:ASP:O	18:6:135:PRO:HA	2.20	0.41
19:5:105:LEU:O	19:5:106:PRO:C	2.63	0.41
1:A:326:LEU:O	1:A:338:HIS:HB2	2.21	0.41
2:B:197:HIS:HB2	20:B:817:CLA:HBC3	2.03	0.41
2:B:208:VAL:HG13	2:B:213:PHE:HA	2.02	0.41
2:B:430:LEU:HD21	20:B:838:CLA:CMB	2.50	0.41
2:B:672:TRP:HZ3	24:B:804:BCR:H391	1.86	0.41
20:7:1005:CLA:HHC	20:7:1005:CLA:CBB	2.51	0.41
29:7:1017:CHL:HMA3	20:3:1017:CLA:OBD	2.21	0.41
28:1:1002:LUT:C28	28:1:1002:LUT:C36	2.93	0.41
17:4:75:LEU:HD21	17:4:97:ALA:HB2	2.03	0.41
18:6:70:SER:O	18:6:74:HIS:HB2	2.21	0.41
18:6:127:ARG:HD3	29:6:314:CHL:OMC	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:178:LYS:CE	27:6:319:LMG:HC5	2.52	0.41
19:5:88:VAL:HG13	19:5:105:LEU:HD23	2.02	0.41
19:5:131:TRP:HH2	24:5:320:BCR:H332	1.80	0.41
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.91	0.40
1:A:96:ALA:HB1	1:A:160:TYR:CD2	2.56	0.40
1:A:464:ALA:O	2:B:636:TYR:OH	2.10	0.40
1:A:590:ASP:HA	1:A:593:PHE:HB3	2.03	0.40
2:B:28:MET:HE3	25:B:848:DGD:HG31	2.02	0.40
2:B:169:PHE:O	2:B:175:ARG:CZ	2.69	0.40
2:B:223:LEU:HD22	26:B:849:LMT:O1B	2.21	0.40
2:B:331:LEU:HB3	20:B:808:CLA:HAC1	2.03	0.40
20:F:302:CLA:HBC2	20:F:302:CLA:HHD	2.02	0.40
20:0:301:CLA:HBB1	20:0:301:CLA:HMB1	2.03	0.40
14:8:149:GLU:O	14:8:150:PRO:C	2.64	0.40
24:8:302:BCR:H403	24:8:302:BCR:C23	2.41	0.40
20:1:1007:CLA:HBA2	20:1:1007:CLA:HBD	2.03	0.40
17:4:197:ILE:HG21	29:4:315:CHL:H93	2.02	0.40
17:4:224:LEU:CD1	27:4:318:LMG:H131	2.48	0.40
20:4:307:CLA:CAC	27:4:318:LMG:C15	2.71	0.40
19:5:164:TYR:CZ	19:5:183:GLN:NE2	2.89	0.40
29:5:317:CHL:CBB	29:5:317:CHL:CHC	2.99	0.40
15:7:182:LYS:NZ	15:7:186:TYR:CE2	2.89	0.40
15:7:183:TYR:CE1	15:7:187:LYS:HD2	2.56	0.40
24:1:1001:BCR:C21	29:1:1015:CHL:HBA2	2.51	0.40
17:4:159:TRP:CH2	24:4:302:BCR:H322	2.55	0.40
1:A:275:PHE:CD2	1:A:276:LEU:HG	2.56	0.40
1:A:551:LEU:HD22	1:A:555:LEU:HD11	2.04	0.40
2:B:4:LYS:O	2:B:5:LEU:HD22	2.22	0.40
3:C:26:LEU:HA	3:C:41:SER:O	2.21	0.40
12:L:105:PRO:HA	20:L:201:CLA:O1D	2.21	0.40
13:0:141:ALA:HB1	29:0:315:CHL:C1B	2.52	0.40
24:3:1003:BCR:C20	20:3:1016:CLA:H3A	2.51	0.40
1:A:634:ASN:C	1:A:638:SER:HG	2.27	0.40
20:A:802:CLA:C2B	28:J:104:LUT:H362	2.51	0.40
24:A:848:BCR:H24C	20:B:834:CLA:HMC1	2.02	0.40
2:B:198:VAL:HG21	20:B:817:CLA:C1D	2.52	0.40
2:B:357:PRO:HA	2:B:358:PRO:HD3	1.86	0.40
2:B:556:TYR:O	2:B:574:TYR:HB2	2.21	0.40
20:B:825:CLA:HMA1	20:0:301:CLA:O1D	2.21	0.40
7:G:110:VAL:HG22	27:0:303:LMG:H231	2.03	0.40
7:G:117:ILE:CG2	27:0:303:LMG:HC71	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:97:ALA:HA	12:L:186:TYR:OH	2.21	0.40
12:L:98:GLY:N	12:L:99:PRO:HD2	2.36	0.40
20:L:203:CLA:HMB1	20:L:203:CLA:HBB1	2.02	0.40
13:0:61:PRO:HD2	28:0:304:LUT:H3	2.04	0.40
13:0:81:HIS:HB3	13:0:185:MET:HE3	2.03	0.40
13:0:116:ALA:N	13:0:123:VAL:HG21	2.36	0.40
13:1:152:VAL:HG11	13:1:153:TYR:CE2	2.56	0.40
20:1:1007:CLA:HAC1	29:1:1012:CHL:CBB	2.52	0.40
1:A:193:ASN:HB3	1:A:196:SER:OG	2.21	0.40
1:A:472:PHE:HD1	1:A:479:LEU:HD11	1.85	0.40
20:A:816:CLA:HBD	20:A:816:CLA:HAA1	2.03	0.40
24:A:844:BCR:H361	24:A:844:BCR:H20C	1.83	0.40
2:B:195:LEU:HA	2:B:199:ALA:HB3	2.04	0.40
20:B:818:CLA:HBA1	24:B:843:BCR:HC31	2.03	0.40
10:J:16:THR:O	10:J:20:THR:HG23	2.21	0.40
13:0:127:LEU:HD12	27:0:303:LMG:HC5	2.03	0.40
14:8:42:THR:N	14:8:43:PRO:CD	2.84	0.40
14:8:42:THR:N	14:8:43:PRO:HD3	2.37	0.40
15:7:116:ASP:OD1	15:7:119:THR:HG23	2.21	0.40
15:7:124:GLN:OE1	29:7:1012:CHL:HMC	2.22	0.40
15:7:132:GLU:OE1	20:7:1014:CLA:NA	2.54	0.40
16:3:155:MET:O	16:3:159:GLU:HB2	2.21	0.40
16:3:223:LEU:HD21	20:3:1006:CLA:HAC2	2.03	0.40
17:4:232:GLN:NE2	20:4:306:CLA:NA	2.69	0.40
18:6:52:PHE:CD2	20:6:312:CLA:HBB1	2.56	0.40
19:5:50:ALA:CB	19:5:183:GLN:HB2	2.52	0.40
19:5:121:LEU:C	19:5:123:ALA:N	2.80	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 X-ray entries followed by that with respect to entries of similar resolution.

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	736/751 (98%)	683 (93%)	51 (7%)	2 (0%)	36 65
2	B	726/735 (99%)	668 (92%)	54 (7%)	4 (1%)	21 50
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100 100
4	D	139/196 (71%)	121 (87%)	18 (13%)	0	100 100
5	E	59/97 (61%)	52 (88%)	7 (12%)	0	100 100
6	F	146/227 (64%)	128 (88%)	15 (10%)	3 (2%)	5 24
7	G	79/126 (63%)	69 (87%)	9 (11%)	1 (1%)	9 33
8	H	86/130 (66%)	74 (86%)	12 (14%)	0	100 100
9	I	27/106 (26%)	23 (85%)	4 (15%)	0	100 100
10	J	37/41 (90%)	34 (92%)	3 (8%)	0	100 100
11	K	40/113 (35%)	34 (85%)	5 (12%)	1 (2%)	4 21
12	L	146/196 (74%)	125 (86%)	19 (13%)	2 (1%)	9 31
13	0	176/228 (77%)	136 (77%)	28 (16%)	12 (7%)	1 6
13	1	176/228 (77%)	133 (76%)	37 (21%)	6 (3%)	3 17
14	8	183/243 (75%)	142 (78%)	34 (19%)	7 (4%)	2 15
15	7	207/241 (86%)	168 (81%)	31 (15%)	8 (4%)	2 15
16	3	199/298 (67%)	165 (83%)	32 (16%)	2 (1%)	12 40
17	4	196/264 (74%)	159 (81%)	35 (18%)	2 (1%)	12 40
18	6	178/257 (69%)	152 (85%)	14 (8%)	12 (7%)	1 6
19	5	187/257 (73%)	134 (72%)	42 (22%)	11 (6%)	1 8
All	All	3801/4815 (79%)	3276 (86%)	452 (12%)	73 (2%)	6 26

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	136	ASP
13	0	165	LYS
14	8	146	SER
15	7	150	PHE
13	1	165	LYS
18	6	166	PRO
18	6	169	LEU
19	5	109	LEU
19	5	111	GLU
19	5	116	ILE
19	5	232	GLY

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Mol	Chain	Res	Type
6	F	178	ALA
13	0	43	SER
13	0	125	PHE
13	0	127	LEU
14	8	108	GLY
14	8	161	LYS
14	8	237	GLY
15	7	149	SER
15	7	233	THR
15	7	236	VAL
16	3	139	GLY
13	1	83	ARG
18	6	56	GLY
19	5	219	LEU
2	B	224	THR
13	0	116	ALA
13	0	222	GLY
15	7	160	LEU
18	6	72	LEU
18	6	167	GLY
18	6	201	PRO
19	5	179	LEU
19	5	231	ILE
2	B	124	TRP
6	F	211	GLN
13	0	108	LEU
13	0	122	GLU
14	8	177	GLY
15	7	162	ASN
13	1	108	LEU
13	1	126	ASP
18	6	171	GLU
18	6	178	LYS
19	5	122	LEU
1	A	593	PHE
12	L	147	GLY
13	0	124	PRO
13	0	202	PRO
14	8	116	PHE
15	7	142	PRO
16	3	188	GLY
17	4	197	ILE

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Mol	Chain	Res	Type
17	4	210	SER
18	6	139	ASP
19	5	81	ALA
19	5	160	PRO
1	A	447	PHE
18	6	110	PRO
19	5	227	ILE
2	B	396	ILE
11	K	31	GLY
12	L	53	GLY
2	B	358	PRO
7	G	52	VAL
15	7	159	GLY
18	6	101	GLY
13	0	156	GLY
14	8	175	PRO
18	6	109	GLY
13	0	215	GLY
13	1	154	PRO
13	1	146	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 X-ray entries followed by that with respect to entries of similar resolution.

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	599/610 (98%)	565 (94%)	34 (6%)	18	45
2	B	593/597 (99%)	561 (95%)	32 (5%)	20	47
3	C	69/70 (99%)	65 (94%)	4 (6%)	18	45
4	D	118/152 (78%)	114 (97%)	4 (3%)	32	57
5	E	52/81 (64%)	51 (98%)	1 (2%)	50	66
6	F	114/169 (68%)	111 (97%)	3 (3%)	40	61
7	G	61/94 (65%)	59 (97%)	2 (3%)	33	57
8	H	73/102 (72%)	71 (97%)	2 (3%)	39	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	I	24/76 (32%)	24 (100%)	0	100 100
10	J	35/37 (95%)	34 (97%)	1 (3%)	37 60
11	K	30/80 (38%)	29 (97%)	1 (3%)	33 57
12	L	112/148 (76%)	108 (96%)	4 (4%)	31 56
13	0	130/162 (80%)	114 (88%)	16 (12%)	4 18
13	1	130/162 (80%)	111 (85%)	19 (15%)	3 12
14	8	146/183 (80%)	132 (90%)	14 (10%)	8 28
15	7	161/181 (89%)	142 (88%)	19 (12%)	5 20
16	3	154/230 (67%)	146 (95%)	8 (5%)	21 48
17	4	159/205 (78%)	148 (93%)	11 (7%)	14 40
18	6	146/203 (72%)	130 (89%)	16 (11%)	6 22
19	5	154/206 (75%)	136 (88%)	18 (12%)	5 20
All	All	3060/3748 (82%)	2851 (93%)	209 (7%)	14 40

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	57	HIS
1	A	70	SER
1	A	74	PHE
1	A	75	SER
1	A	136	GLN
1	A	149	ARG
1	A	154	THR
1	A	167	LEU
1	A	211	LEU
1	A	233	ASP
1	A	301	ILE
1	A	304	LEU
1	A	318	ILE
1	A	321	SER
1	A	344	ILE
1	A	346	THR
1	A	371	MET
1	A	372	TYR
1	A	382	THR
1	A	383	ASP

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Mol	Chain	Res	Type
1	A	416	ASP
1	A	424	ASN
1	A	461	THR
1	A	477	ILE
1	A	514	LEU
1	A	517	VAL
1	A	599	MET
1	A	653	GLN
1	A	694	GLN
1	A	696	LEU
1	A	702	TRP
1	A	709	VAL
1	A	721	THR
2	B	5	LEU
2	B	92	ILE
2	B	94	ASP
2	B	114	VAL
2	B	125	TRP
2	B	156	LEU
2	B	224	THR
2	B	295	ASN
2	B	298	ILE
2	B	346	THR
2	B	351	GLN
2	B	358	PRO
2	B	362	GLN
2	B	379	ILE
2	B	453	GLN
2	B	457	GLU
2	B	480	SER
2	B	493	LEU
2	B	502	ILE
2	B	526	LEU
2	B	569	CYS
2	B	571	ILE
2	B	577	PHE
2	B	618	MET
2	B	621	LEU
2	B	633	ILE
2	B	634	ASN
2	B	637	ASN
2	B	646	VAL

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Mol	Chain	Res	Type
2	B	656	LEU
2	B	690	ASN
2	B	711	LEU
3	C	15	THR
3	C	34	CYS
3	C	41	SER
3	C	49	VAL
4	D	62	THR
4	D	82	GLU
4	D	87	THR
4	D	191	MET
5	E	43	VAL
6	F	128	ASP
6	F	168	ARG
6	F	182	ASP
7	G	48	ILE
7	G	87	PHE
8	H	47	THR
8	H	101	LYS
10	J	30	ASN
11	K	99	LEU
12	L	44	SER
12	L	54	MET
12	L	119	LEU
12	L	146	ILE
13	0	40	LEU
13	0	71	LEU
13	0	75	THR
13	0	92	SER
13	0	98	LEU
13	0	121	ILE
13	0	123	VAL
13	0	127	LEU
13	0	152	VAL
13	0	177	GLU
13	0	194	GLN
13	0	200	LYS
13	0	202	PRO
13	0	203	ILE
13	0	217	ASN
13	0	221	ASN
14	8	29	SER

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Mol	Chain	Res	Type
14	8	34	SER
14	8	71	GLN
14	8	79	THR
14	8	105	TYR
14	8	146	SER
14	8	147	GLN
14	8	149	GLU
14	8	165	GLU
14	8	166	LEU
14	8	184	LYS
14	8	194	LYS
14	8	236	ASN
14	8	239	SER
15	7	87	ILE
15	7	88	LEU
15	7	91	ILE
15	7	107	LYS
15	7	111	GLU
15	7	115	ILE
15	7	116	ASP
15	7	119	THR
15	7	133	THR
15	7	136	TRP
15	7	139	PHE
15	7	140	LYS
15	7	144	SER
15	7	154	THR
15	7	155	GLU
15	7	158	LYS
15	7	176	SER
15	7	177	ARG
15	7	236	VAL
16	3	73	LEU
16	3	83	GLU
16	3	90	SER
16	3	141	TRP
16	3	180	LEU
16	3	197	PHE
16	3	200	LEU
16	3	219	LYS
13	1	40	LEU
13	1	64	LEU

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Mol	Chain	Res	Type
13	1	71	LEU
13	1	75	THR
13	1	77	SER
13	1	97	LEU
13	1	100	TYR
13	1	105	ASP
13	1	123	VAL
13	1	126	ASP
13	1	127	LEU
13	1	144	GLN
13	1	145	ARG
13	1	151	VAL
13	1	177	GLU
13	1	194	GLN
13	1	203	ILE
13	1	217	ASN
13	1	221	ASN
17	4	53	LYS
17	4	54	ARG
17	4	60	SER
17	4	61	TRP
17	4	66	ASP
17	4	135	TYR
17	4	141	GLU
17	4	163	ARG
17	4	197	ILE
17	4	213	LEU
17	4	216	ILE
18	6	42	LEU
18	6	57	LEU
18	6	63	SER
18	6	75	SER
18	6	94	ASP
18	6	95	VAL
18	6	99	ASN
18	6	102	LYS
18	6	120	LEU
18	6	129	TRP
18	6	137	SER
18	6	140	GLN
18	6	143	ILE
18	6	169	LEU

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Mol	Chain	Res	Type
18	6	172	LEU
18	6	219	SER
19	5	34	LEU
19	5	48	ASP
19	5	73	SER
19	5	105	LEU
19	5	108	ASN
19	5	109	LEU
19	5	111	GLU
19	5	115	ASN
19	5	127	ILE
19	5	145	SER
19	5	148	GLU
19	5	176	LYS
19	5	179	LEU
19	5	186	GLU
19	5	201	ILE
19	5	227	ILE
19	5	230	ASN
19	5	234	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	53	HIS
1	A	57	HIS
1	A	80	GLN
1	A	110	HIS
1	A	128	ASN
1	A	136	GLN
1	A	139	GLN
1	A	200	HIS
1	A	217	GLN
1	A	387	GLN
1	A	424	ASN
1	A	451	HIS
1	A	485	GLN
1	A	609	HIS
1	A	629	HIS
1	A	640	ASN
1	A	653	GLN

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Mol	Chain	Res	Type
1	A	694	GLN
1	A	714	GLN
1	A	730	HIS
2	B	54	GLN
2	B	115	ASN
2	B	133	ASN
2	B	159	GLN
2	B	178	HIS
2	B	197	HIS
2	B	219	HIS
2	B	267	GLN
2	B	351	GLN
2	B	376	HIS
2	B	390	HIS
2	B	407	ASN
2	B	507	ASN
2	B	586	ASN
2	B	628	ASN
2	B	634	ASN
2	B	637	ASN
2	B	690	ASN
4	D	151	HIS
4	D	180	ASN
5	E	55	GLN
6	F	208	GLN
10	J	30	ASN
12	L	139	GLN
12	L	190	GLN
13	0	56	ASN
13	0	81	HIS
13	0	144	GLN
13	0	221	ASN
14	8	51	ASN
14	8	71	GLN
14	8	76	HIS
14	8	139	GLN
14	8	147	GLN
14	8	195	ASN
14	8	209	GLN
14	8	232	ASN
14	8	236	ASN
15	7	113	ASN

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Mol	Chain	Res	Type
15	7	207	GLN
15	7	230	ASN
15	7	234	ASN
16	3	88	GLN
16	3	138	ASN
16	3	156	GLN
16	3	245	ASN
13	1	56	ASN
13	1	194	GLN
13	1	195	HIS
13	1	217	ASN
17	4	98	GLN
17	4	175	ASN
17	4	189	ASN
17	4	258	GLN
19	5	72	GLN
19	5	77	HIS
19	5	115	ASN
19	5	138	GLN
19	5	155	ASN
19	5	203	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

278 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	$\#\|Z\| > 2$
20	CLA	5	311	-	47,52,73	2.23	8 (17%)	56,88,113	1.50	8 (14%)
20	CLA	A	836	-	47,52,73	1.95	9 (19%)	56,88,113	1.44	8 (14%)
24	BCR	J	103	-	41,41,41	0.32	0	56,56,56	0.41	0
20	CLA	A	830	-	47,52,73	2.05	9 (19%)	56,88,113	1.34	8 (14%)
28	LUT	8	303	-	42,43,43	0.31	0	51,60,60	0.48	0
24	BCR	G	205	-	41,41,41	0.50	1 (2%)	56,56,56	1.20	4 (7%)
20	CLA	1	1008	-	47,52,73	2.02	10 (21%)	56,88,113	1.41	9 (16%)
30	XAT	6	304	-	39,47,47	0.31	0	54,74,74	0.89	2 (3%)
29	CHL	6	316	-	65,69,74	1.82	9 (13%)	74,108,114	1.24	6 (8%)
24	BCR	3	1003	-	41,41,41	0.60	0	56,56,56	0.90	2 (3%)
20	CLA	0	310	-	47,52,73	2.23	9 (19%)	56,88,113	1.36	8 (14%)
23	LHG	8	301	20	48,48,48	0.27	0	51,54,54	0.29	0
29	CHL	5	313	-	51,55,74	2.16	10 (19%)	57,91,114	1.69	8 (14%)
29	CHL	7	1017	15	70,74,74	1.63	8 (11%)	80,114,114	1.37	8 (10%)
20	CLA	0	308	13	47,52,73	1.96	8 (17%)	56,88,113	1.40	7 (12%)
28	LUT	0	318	-	42,43,43	0.41	0	51,60,60	0.53	0
20	CLA	F	302	-	47,52,73	2.04	10 (21%)	56,88,113	1.39	10 (17%)
24	BCR	5	320	-	41,41,41	0.37	0	56,56,56	0.67	1 (1%)
20	CLA	1	1010	-	47,52,73	1.98	9 (19%)	56,88,113	1.37	8 (14%)
23	LHG	0	302	20	20,20,48	0.34	0	23,26,54	1.79	4 (17%)
24	BCR	A	846	-	41,41,41	0.64	0	56,56,56	0.89	2 (3%)
24	BCR	H	201	-	41,41,41	0.86	3 (7%)	56,56,56	1.22	6 (10%)
29	CHL	4	316	17	47,51,74	1.89	10 (21%)	52,86,114	1.49	5 (9%)
20	CLA	6	315	18	47,52,73	1.95	8 (17%)	56,88,113	1.48	8 (14%)
24	BCR	8	302	-	41,41,41	0.52	0	56,56,56	1.28	5 (8%)
20	CLA	3	1009	16	47,52,73	2.04	10 (21%)	56,88,113	1.39	7 (12%)
28	LUT	J	104	-	42,43,43	0.48	0	51,60,60	0.62	0
29	CHL	0	314	-	51,55,74	1.93	10 (19%)	57,91,114	1.36	6 (10%)
20	CLA	1	1017	-	47,52,73	2.03	8 (17%)	56,88,113	1.48	9 (16%)
20	CLA	4	307	17	47,52,73	2.21	9 (19%)	56,88,113	1.97	11 (19%)
29	CHL	6	313	-	51,55,74	1.98	8 (15%)	57,91,114	1.35	5 (8%)
20	CLA	6	308	-	47,52,73	2.19	8 (17%)	56,88,113	1.52	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	DGD	5	319	-	52,52,67	1.07	3 (5%)	66,66,81	1.44	8 (12%)
20	CLA	A	815	-	47,52,73	2.06	9 (19%)	56,88,113	1.48	7 (12%)
20	CLA	B	827	-	47,52,73	2.08	10 (21%)	56,88,113	1.41	8 (14%)
20	CLA	A	818	-	47,52,73	1.97	9 (19%)	56,88,113	1.37	9 (16%)
20	CLA	B	812	2	47,52,73	2.03	8 (17%)	56,88,113	1.35	7 (12%)
20	CLA	3	1013	16	47,52,73	2.02	8 (17%)	56,88,113	1.46	8 (14%)
20	CLA	1	1005	-	47,52,73	2.07	9 (19%)	56,88,113	1.36	8 (14%)
20	CLA	8	306	14	47,52,73	2.07	11 (23%)	56,88,113	1.50	8 (14%)
20	CLA	B	810	2	47,52,73	1.97	9 (19%)	56,88,113	1.47	8 (14%)
20	CLA	6	320	-	47,52,73	2.02	7 (14%)	56,88,113	1.64	12 (21%)
20	CLA	5	318	19	47,52,73	2.17	9 (19%)	56,88,113	1.45	11 (19%)
29	CHL	7	1015	-	50,54,74	2.09	10 (20%)	56,90,114	1.57	8 (14%)
30	XAT	4	303	-	39,47,47	0.19	0	54,74,74	0.85	3 (5%)
20	CLA	L	202	-	47,52,73	1.99	9 (19%)	56,88,113	1.36	7 (12%)
20	CLA	1	1004	13	47,52,73	2.06	9 (19%)	56,88,113	1.42	8 (14%)
20	CLA	A	821	-	47,52,73	2.13	10 (21%)	56,88,113	1.51	9 (16%)
20	CLA	6	301	-	47,52,73	1.94	10 (21%)	56,88,113	1.36	9 (16%)
20	CLA	A	803	20	47,52,73	1.96	9 (19%)	56,88,113	1.40	8 (14%)
20	CLA	1	1014	-	47,52,73	2.09	8 (17%)	56,88,113	1.46	9 (16%)
20	CLA	A	809	-	47,52,73	1.97	10 (21%)	56,88,113	1.29	8 (14%)
20	CLA	B	828	2	47,52,73	1.96	10 (21%)	56,88,113	1.43	8 (14%)
23	LHG	4	301	20	48,48,48	0.31	0	51,54,54	0.48	0
20	CLA	L	201	-	47,52,73	1.96	9 (19%)	56,88,113	1.33	7 (12%)
20	CLA	L	204	-	47,52,73	2.09	9 (19%)	56,88,113	1.35	7 (12%)
20	CLA	A	832	-	47,52,73	1.92	9 (19%)	56,88,113	1.35	8 (14%)
20	CLA	8	307	14	47,52,73	1.93	8 (17%)	56,88,113	1.34	6 (10%)
20	CLA	A	831	-	47,52,73	2.18	9 (19%)	56,88,113	1.31	8 (14%)
20	CLA	7	1004	15	47,52,73	1.83	9 (19%)	56,88,113	1.42	11 (19%)
20	CLA	6	312	18	47,52,73	1.99	9 (19%)	56,88,113	1.59	10 (17%)
20	CLA	B	818	-	47,52,73	1.98	9 (19%)	56,88,113	1.26	8 (14%)
20	CLA	J	102	-	47,52,73	2.02	10 (21%)	56,88,113	1.27	8 (14%)
29	CHL	8	315	-	55,59,74	1.89	9 (16%)	62,96,114	1.62	10 (16%)
20	CLA	1	1003	-	47,52,73	2.01	9 (19%)	56,88,113	1.33	7 (12%)
24	BCR	A	847	-	41,41,41	0.40	0	56,56,56	0.78	2 (3%)
20	CLA	0	301	23	47,52,73	2.07	9 (19%)	56,88,113	1.35	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	F	304	-	41,41,41	0.32	0	56,56,56	0.64	0
20	CLA	A	812	1	47,52,73	1.99	9 (19%)	56,88,113	1.28	7 (12%)
20	CLA	B	805	-	47,52,73	2.02	7 (14%)	56,88,113	1.32	8 (14%)
20	CLA	3	1012	-	47,52,73	2.08	9 (19%)	56,88,113	1.31	8 (14%)
20	CLA	8	313	14	47,52,73	2.08	7 (14%)	56,88,113	1.54	10 (17%)
29	CHL	0	315	-	55,59,74	1.84	9 (16%)	62,96,114	1.42	5 (8%)
29	CHL	4	313	-	55,59,74	1.78	8 (14%)	62,96,114	1.59	11 (17%)
20	CLA	A	839	1	47,52,73	2.10	10 (21%)	56,88,113	1.28	6 (10%)
27	LMG	8	318	-	28,28,55	0.30	0	36,36,63	0.49	0
20	CLA	B	834	2	47,52,73	1.94	10 (21%)	56,88,113	1.23	7 (12%)
20	CLA	B	809	2	47,52,73	2.08	9 (19%)	56,88,113	1.37	8 (14%)
27	LMG	6	319	-	44,44,55	0.37	0	52,52,63	0.61	1 (1%)
20	CLA	K	202	-	28,35,73	2.31	10 (35%)	32,60,113	2.55	12 (37%)
20	CLA	B	837	2	47,52,73	2.13	8 (17%)	56,88,113	1.44	9 (16%)
27	LMG	4	318	-	34,34,55	0.32	0	42,42,63	0.95	3 (7%)
20	CLA	5	321	-	47,52,73	2.06	9 (19%)	56,88,113	1.40	8 (14%)
20	CLA	G	202	-	47,52,73	2.05	9 (19%)	56,88,113	1.36	8 (14%)
20	CLA	B	820	-	47,52,73	2.05	9 (19%)	56,88,113	1.49	8 (14%)
20	CLA	0	312	13	47,52,73	2.08	7 (14%)	56,88,113	1.46	9 (16%)
20	CLA	B	850	-	44,49,73	3.91	9 (20%)	43,80,113	1.46	6 (13%)
24	BCR	A	848	-	41,41,41	0.20	0	56,56,56	0.55	0
20	CLA	4	306	17	47,52,73	2.00	9 (19%)	56,88,113	1.34	8 (14%)
20	CLA	3	1016	-	47,52,73	2.06	9 (19%)	56,88,113	1.49	9 (16%)
20	CLA	A	827	-	47,52,73	1.91	8 (17%)	56,88,113	1.38	7 (12%)
30	XAT	7	1002	-	39,47,47	1.77	7 (17%)	54,74,74	1.80	12 (22%)
20	CLA	B	826	-	47,52,73	2.07	9 (19%)	56,88,113	1.45	8 (14%)
20	CLA	7	1005	15	47,52,73	2.16	10 (21%)	56,88,113	1.59	7 (12%)
20	CLA	6	310	-	47,52,73	1.88	9 (19%)	56,88,113	1.46	10 (17%)
20	CLA	B	801	-	47,52,73	1.94	8 (17%)	56,88,113	1.33	8 (14%)
20	CLA	5	323	-	47,52,73	2.05	8 (17%)	56,88,113	1.34	8 (14%)
20	CLA	5	308	-	47,52,73	1.98	9 (19%)	56,88,113	1.52	11 (19%)
21	SF4	C	1001	3	0,12,12	-	-	-		
25	DGD	B	848	-	62,62,67	0.86	2 (3%)	76,76,81	1.13	6 (7%)
20	CLA	A	825	-	47,52,73	2.04	9 (19%)	56,88,113	1.39	7 (12%)
29	CHL	8	317	-	65,69,74	1.83	9 (13%)	74,108,114	1.40	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	7	1008	15	47,52,73	1.97	9 (19%)	56,88,113	1.36	7 (12%)
24	BCR	B	844	-	41,41,41	0.42	0	56,56,56	0.56	0
20	CLA	F	305	-	47,52,73	2.07	9 (19%)	56,88,113	1.39	9 (16%)
24	BCR	3	1004	-	41,41,41	0.65	1 (2%)	56,56,56	1.02	3 (5%)
20	CLA	A	822	1	47,52,73	2.04	9 (19%)	56,88,113	1.41	8 (14%)
20	CLA	G	201	-	47,52,73	2.03	8 (17%)	56,88,113	1.39	9 (16%)
20	CLA	B	824	-	47,52,73	2.00	9 (19%)	56,88,113	1.49	9 (16%)
20	CLA	B	838	2	47,52,73	2.01	9 (19%)	56,88,113	1.43	7 (12%)
20	CLA	0	309	13	47,52,73	2.05	9 (19%)	56,88,113	1.47	7 (12%)
20	CLA	8	310	-	47,52,73	2.07	9 (19%)	56,88,113	1.35	7 (12%)
20	CLA	1	1011	13	47,52,73	2.05	8 (17%)	56,88,113	1.46	10 (17%)
20	CLA	6	305	18	47,52,73	1.98	10 (21%)	56,88,113	1.39	8 (14%)
29	CHL	1	1015	-	65,69,74	1.74	10 (15%)	74,108,114	1.59	11 (14%)
28	LUT	1	1016	-	42,43,43	0.24	0	51,60,60	0.52	0
29	CHL	8	314	-	51,55,74	1.97	9 (17%)	57,91,114	1.51	8 (14%)
20	CLA	5	307	19	47,52,73	2.01	10 (21%)	56,88,113	1.57	10 (17%)
20	CLA	5	309	19	47,52,73	1.97	8 (17%)	56,88,113	1.56	9 (16%)
20	CLA	8	308	14	47,52,73	2.08	9 (19%)	56,88,113	1.54	11 (19%)
20	CLA	3	1008	16	47,52,73	2.09	9 (19%)	56,88,113	1.53	9 (16%)
20	CLA	5	301	18	47,52,73	2.33	9 (19%)	56,88,113	1.62	12 (21%)
23	LHG	A	849	-	48,48,48	0.25	0	51,54,54	0.33	0
28	LUT	3	1001	-	42,43,43	0.26	0	51,60,60	0.44	0
29	CHL	7	1013	-	52,56,74	1.99	9 (17%)	58,92,114	1.85	8 (13%)
27	LMG	0	303	-	50,50,55	0.30	0	58,58,63	0.53	1 (1%)
30	XAT	8	304	-	39,47,47	1.75	6 (15%)	54,74,74	1.71	11 (20%)
20	CLA	A	806	1	47,52,73	1.93	9 (19%)	56,88,113	1.45	9 (16%)
20	CLA	5	322	-	47,52,73	1.98	9 (19%)	56,88,113	1.40	9 (16%)
29	CHL	6	317	18	47,51,74	2.11	8 (17%)	52,86,114	1.41	5 (9%)
20	CLA	5	312	19	47,52,73	2.09	8 (17%)	56,88,113	1.50	11 (19%)
29	CHL	4	312	-	51,55,74	1.93	9 (17%)	57,91,114	1.64	9 (15%)
20	CLA	A	826	1	47,52,73	2.13	9 (19%)	56,88,113	1.29	8 (14%)
24	BCR	B	846	-	41,41,41	0.34	0	56,56,56	0.47	0
20	CLA	G	203	-	47,52,73	2.06	9 (19%)	56,88,113	1.30	8 (14%)
20	CLA	6	311	-	47,52,73	1.91	10 (21%)	56,88,113	1.22	6 (10%)
20	CLA	B	817	2	47,52,73	2.02	9 (19%)	56,88,113	1.43	9 (16%)
20	CLA	5	315	19	47,52,73	1.91	9 (19%)	56,88,113	1.40	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	6	306	18	47,52,73	1.90	9 (19%)	56,88,113	1.35	10 (17%)
29	CHL	6	314	-	55,59,74	1.82	9 (16%)	62,96,114	1.67	8 (12%)
24	BCR	7	1003	-	41,41,41	0.69	1 (2%)	56,56,56	1.56	6 (10%)
20	CLA	B	839	2	47,52,73	1.97	9 (19%)	56,88,113	1.39	8 (14%)
24	BCR	B	804	-	41,41,41	0.56	1 (2%)	56,56,56	1.88	12 (21%)
20	CLA	4	305	17	47,52,73	2.20	10 (21%)	56,88,113	1.35	8 (14%)
20	CLA	5	304	19	47,52,73	2.13	9 (19%)	56,88,113	1.34	8 (14%)
28	LUT	5	302	-	42,43,43	0.34	0	51,60,60	0.56	0
20	CLA	A	824	-	47,52,73	2.10	8 (17%)	56,88,113	1.53	9 (16%)
20	CLA	3	1011	23	43,48,73	2.17	10 (23%)	51,83,113	1.47	8 (15%)
23	LHG	A	843	-	39,39,48	0.29	0	42,45,54	0.26	0
20	CLA	A	828	1	47,52,73	1.94	10 (21%)	56,88,113	1.42	9 (16%)
21	SF4	A	841	2,1	0,12,12	-	-	-		
20	CLA	B	808	2	47,52,73	2.04	8 (17%)	56,88,113	1.43	8 (14%)
20	CLA	4	311	17	47,52,73	1.96	8 (17%)	56,88,113	1.45	8 (14%)
20	CLA	B	814	-	47,52,73	2.03	9 (19%)	56,88,113	1.34	9 (16%)
28	LUT	7	1001	-	42,43,43	0.46	0	51,60,60	0.75	2 (3%)
20	CLA	A	804	1	47,52,73	2.04	10 (21%)	56,88,113	1.52	8 (14%)
20	CLA	0	306	13	47,52,73	1.94	8 (17%)	56,88,113	1.46	9 (16%)
20	CLA	F	303	6	47,52,73	2.10	9 (19%)	56,88,113	1.39	8 (14%)
28	LUT	6	303	-	42,43,43	0.33	0	51,60,60	0.51	0
20	CLA	A	852	-	47,52,73	2.03	8 (17%)	56,88,113	1.38	8 (14%)
20	CLA	B	840	-	47,52,73	1.98	9 (19%)	56,88,113	1.33	6 (10%)
20	CLA	5	310	-	47,52,73	1.93	10 (21%)	56,88,113	1.33	5 (8%)
20	CLA	B	813	2	47,52,73	2.24	9 (19%)	56,88,113	1.45	9 (16%)
23	LHG	7	1016	20	34,34,48	0.42	0	37,40,54	0.52	0
20	CLA	A	801	-	47,52,73	2.03	7 (14%)	56,88,113	1.59	10 (17%)
20	CLA	A	816	-	47,52,73	2.05	9 (19%)	56,88,113	1.34	7 (12%)
29	CHL	7	1012	-	51,55,74	2.02	8 (15%)	57,91,114	1.56	5 (8%)
20	CLA	7	1009	-	47,52,73	1.97	8 (17%)	56,88,113	1.42	6 (10%)
20	CLA	K	201	-	47,52,73	2.03	8 (17%)	56,88,113	1.36	7 (12%)
20	CLA	A	817	-	47,52,73	2.05	7 (14%)	56,88,113	1.45	9 (16%)
20	CLA	1	1006	13	47,52,73	2.07	7 (14%)	56,88,113	1.46	7 (12%)
20	CLA	3	1015	16	47,52,73	2.03	10 (21%)	56,88,113	1.35	8 (14%)
20	CLA	0	305	-	47,52,73	2.00	10 (21%)	56,88,113	1.39	10 (17%)
20	CLA	A	834	-	47,52,73	2.12	9 (19%)	56,88,113	1.49	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	3	1007	-	47,52,73	2.02	10 (21%)	56,88,113	1.41	9 (16%)
20	CLA	B	836	-	47,52,73	2.04	9 (19%)	56,88,113	1.35	10 (17%)
20	CLA	A	823	-	47,52,73	2.03	8 (17%)	56,88,113	1.44	7 (12%)
20	CLA	8	312	14	47,52,73	1.97	10 (21%)	56,88,113	1.45	9 (16%)
20	CLA	5	305	19	47,52,73	2.17	8 (17%)	56,88,113	1.37	8 (14%)
20	CLA	A	833	1	47,52,73	1.99	10 (21%)	56,88,113	1.48	8 (14%)
20	CLA	B	833	2	47,52,73	1.86	8 (17%)	56,88,113	1.38	11 (19%)
20	CLA	3	1006	16	47,52,73	2.08	9 (19%)	56,88,113	1.51	10 (17%)
20	CLA	B	821	-	47,52,73	2.03	9 (19%)	56,88,113	1.43	8 (14%)
24	BCR	A	844	-	41,41,41	0.34	0	56,56,56	0.55	0
20	CLA	A	802	-	47,52,73	2.04	10 (21%)	56,88,113	1.41	9 (16%)
20	CLA	B	807	-	47,52,73	2.01	9 (19%)	56,88,113	1.32	8 (14%)
20	CLA	B	819	-	47,52,73	2.02	10 (21%)	56,88,113	1.34	8 (14%)
20	CLA	6	307	-	47,52,73	2.09	8 (17%)	56,88,113	1.39	8 (14%)
22	PQN	A	842	-	34,34,34	0.32	0	42,45,45	0.50	1 (2%)
24	BCR	I	201	-	41,41,41	0.58	0	56,56,56	0.93	3 (5%)
26	LMT	B	849	-	32,32,36	0.20	0	43,43,47	0.47	0
30	XAT	5	303	-	39,47,47	0.26	0	54,74,74	1.11	3 (5%)
20	CLA	A	810	1,20	47,52,73	2.05	8 (17%)	56,88,113	1.42	7 (12%)
20	CLA	8	316	14	47,52,73	1.87	8 (17%)	56,88,113	1.36	6 (10%)
20	CLA	B	822	-	47,52,73	2.03	10 (21%)	56,88,113	1.38	7 (12%)
20	CLA	8	305	14	47,52,73	1.87	7 (14%)	56,88,113	1.31	7 (12%)
20	CLA	0	307	-	47,52,73	2.15	10 (21%)	56,88,113	1.32	9 (16%)
20	CLA	7	1006	15	47,52,73	1.88	8 (17%)	56,88,113	1.42	8 (14%)
24	BCR	A	845	-	41,41,41	0.65	0	56,56,56	1.61	9 (16%)
24	BCR	1	1001	-	41,41,41	0.52	1 (2%)	56,56,56	1.08	5 (8%)
29	CHL	4	315	-	65,69,74	1.72	9 (13%)	74,108,114	1.26	6 (8%)
20	CLA	3	1010	-	47,52,73	2.00	8 (17%)	56,88,113	1.38	8 (14%)
20	CLA	3	1005	16	47,52,73	1.92	10 (21%)	56,88,113	1.28	7 (12%)
20	CLA	A	851	-	47,52,73	2.00	9 (19%)	56,88,113	1.31	7 (12%)
20	CLA	B	830	2	47,52,73	1.84	8 (17%)	56,88,113	1.37	8 (14%)
20	CLA	B	815	-	47,52,73	2.17	9 (19%)	56,88,113	1.45	8 (14%)
20	CLA	4	314	17	47,52,73	2.02	7 (14%)	56,88,113	1.37	9 (16%)
20	CLA	0	316	-	47,52,73	2.01	8 (17%)	56,88,113	1.45	8 (14%)
29	CHL	3	1014	-	51,55,74	1.95	9 (17%)	57,91,114	1.65	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	LMT	3	1018	-	32,32,36	0.30	0	43,43,47	0.69	1 (2%)
20	CLA	4	309	-	47,52,73	1.89	9 (19%)	56,88,113	1.42	8 (14%)
20	CLA	A	808	-	47,52,73	2.05	9 (19%)	56,88,113	1.40	7 (12%)
20	CLA	B	835	-	47,52,73	2.01	9 (19%)	56,88,113	1.40	7 (12%)
24	BCR	B	843	-	41,41,41	1.04	3 (7%)	56,56,56	1.48	9 (16%)
20	CLA	0	313	13	47,52,73	2.05	8 (17%)	56,88,113	1.35	10 (17%)
28	LUT	3	1002	-	42,43,43	0.41	0	51,60,60	0.64	1 (1%)
29	CHL	5	316	-	65,69,74	1.83	11 (16%)	74,108,114	1.54	12 (16%)
20	CLA	B	823	-	47,52,73	2.10	9 (19%)	56,88,113	1.38	8 (14%)
28	LUT	1	1002	-	42,43,43	0.36	0	51,60,60	0.59	0
20	CLA	B	832	-	47,52,73	1.98	10 (21%)	56,88,113	1.32	8 (14%)
24	BCR	4	302	-	41,41,41	0.49	1 (2%)	56,56,56	1.14	5 (8%)
29	CHL	1	1012	-	51,55,74	1.88	10 (19%)	57,91,114	1.53	6 (10%)
20	CLA	A	837	-	47,52,73	1.98	10 (21%)	56,88,113	1.42	7 (12%)
20	CLA	1	1009	23	47,52,73	1.84	9 (19%)	56,88,113	1.25	6 (10%)
28	LUT	0	304	-	42,43,43	0.25	0	51,60,60	0.56	1 (1%)
21	SF4	C	1002	3	0,12,12	-	-	-		
29	CHL	1	1013	-	55,59,74	1.88	7 (12%)	62,96,114	1.44	8 (12%)
20	CLA	7	1011	15	47,52,73	2.17	9 (19%)	56,88,113	1.32	10 (17%)
24	BCR	6	302	-	41,41,41	0.52	1 (2%)	56,56,56	1.23	3 (5%)
20	CLA	7	1014	15	47,52,73	1.98	10 (21%)	56,88,113	1.44	7 (12%)
20	CLA	B	831	-	47,52,73	2.14	9 (19%)	56,88,113	1.45	8 (14%)
20	CLA	A	829	1	47,52,73	1.98	10 (21%)	56,88,113	1.37	9 (16%)
24	BCR	F	301	-	41,41,41	0.54	1 (2%)	56,56,56	0.63	1 (1%)
20	CLA	A	840	-	47,52,73	1.94	8 (17%)	56,88,113	1.41	6 (10%)
20	CLA	B	811	-	47,52,73	2.13	9 (19%)	56,88,113	1.38	7 (12%)
20	CLA	7	1007	15	47,52,73	2.17	10 (21%)	56,88,113	1.62	10 (17%)
20	CLA	1	1007	13	47,52,73	2.02	9 (19%)	56,88,113	1.57	9 (16%)
20	CLA	8	309	27	47,52,73	2.15	10 (21%)	56,88,113	1.58	10 (17%)
20	CLA	B	816	2	47,52,73	2.03	9 (19%)	56,88,113	1.34	7 (12%)
20	CLA	A	838	-	47,52,73	2.02	8 (17%)	56,88,113	1.42	7 (12%)
24	BCR	A	850	-	41,41,41	0.39	0	56,56,56	0.79	1 (1%)
24	BCR	B	845	-	41,41,41	0.54	0	56,56,56	0.94	3 (5%)
28	LUT	4	317	-	42,43,43	0.35	0	51,60,60	0.53	1 (1%)
22	PQN	B	842	-	34,34,34	0.31	0	42,45,45	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LMG	8	319	20	44,44,55	0.29	0	52,52,63	0.83	1 (1%)
20	CLA	4	304	17	47,52,73	1.87	9 (19%)	56,88,113	1.43	9 (16%)
20	CLA	6	318	18	47,52,73	2.14	10 (21%)	56,88,113	1.48	9 (16%)
20	CLA	7	1010	23	47,52,73	1.98	9 (19%)	56,88,113	1.29	7 (12%)
29	CHL	0	317	-	65,69,74	1.71	10 (15%)	74,108,114	1.46	9 (12%)
20	CLA	8	311	-	47,52,73	1.96	7 (14%)	56,88,113	1.33	9 (16%)
20	CLA	B	803	-	47,52,73	2.06	9 (19%)	56,88,113	1.49	9 (16%)
24	BCR	G	204	-	41,41,41	0.60	0	56,56,56	1.03	4 (7%)
20	CLA	A	835	-	47,52,73	1.99	9 (19%)	56,88,113	1.43	7 (12%)
20	CLA	3	1017	16	47,52,73	2.08	10 (21%)	56,88,113	1.38	8 (14%)
20	CLA	A	805	1	47,52,73	2.04	9 (19%)	56,88,113	1.32	8 (14%)
20	CLA	A	819	-	47,52,73	2.04	9 (19%)	56,88,113	1.32	8 (14%)
20	CLA	6	309	18	47,52,73	2.00	9 (19%)	56,88,113	1.47	9 (16%)
24	BCR	B	847	-	41,41,41	0.17	0	56,56,56	0.63	0
27	LMG	J	101	-	30,30,55	0.24	0	38,38,63	0.24	0
29	CHL	5	317	19	47,51,74	1.88	8 (17%)	52,86,114	1.38	4 (7%)
20	CLA	A	820	-	47,52,73	2.04	9 (19%)	56,88,113	1.42	7 (12%)
23	LHG	3	1019	20	19,19,48	0.71	1 (5%)	21,24,54	0.51	0
27	LMG	5	324	-	45,45,55	0.44	0	53,53,63	0.64	1 (1%)
20	CLA	4	308	17	47,52,73	2.07	8 (17%)	56,88,113	1.47	9 (16%)
20	CLA	B	802	-	47,52,73	1.99	10 (21%)	56,88,113	1.44	11 (19%)
20	CLA	B	829	-	47,52,73	2.00	9 (19%)	56,88,113	1.41	8 (14%)
20	CLA	A	813	1	47,52,73	2.10	8 (17%)	56,88,113	1.40	9 (16%)
20	CLA	B	841	-	47,52,73	2.07	8 (17%)	56,88,113	1.45	8 (14%)
20	CLA	A	807	-	47,52,73	1.96	10 (21%)	56,88,113	1.40	8 (14%)
20	CLA	A	811	-	47,52,73	2.04	8 (17%)	56,88,113	1.47	9 (16%)
20	CLA	B	806	-	47,52,73	1.97	9 (19%)	56,88,113	1.31	6 (10%)
20	CLA	A	814	-	43,48,73	2.19	10 (23%)	51,83,113	1.49	9 (17%)
20	CLA	4	310	-	47,52,73	2.08	7 (14%)	56,88,113	1.45	7 (12%)
20	CLA	0	311	23	47,52,73	2.01	9 (19%)	56,88,113	1.24	7 (12%)
20	CLA	5	306	-	47,52,73	2.02	9 (19%)	56,88,113	1.38	9 (16%)
29	CHL	5	314	-	55,59,74	1.96	9 (16%)	62,96,114	1.44	6 (9%)
20	CLA	B	825	-	47,52,73	2.04	10 (21%)	56,88,113	1.37	9 (16%)
20	CLA	L	203	-	47,52,73	2.11	9 (19%)	56,88,113	1.34	8 (14%)

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
20	CLA	5	311	-	-	5/13/89/115	-
20	CLA	A	836	-	-	6/13/89/115	-
24	BCR	J	103	-	-	4/29/63/63	0/2/2/2
20	CLA	A	830	-	-	3/13/89/115	-
28	LUT	8	303	-	-	2/29/67/67	0/2/2/2
24	BCR	G	205	-	-	7/29/63/63	0/2/2/2
20	CLA	1	1008	-	-	9/13/89/115	-
30	XAT	6	304	-	-	5/31/93/93	0/4/4/4
29	CHL	6	316	-	-	15/35/111/117	-
24	BCR	3	1003	-	-	11/29/63/63	0/2/2/2
20	CLA	0	310	-	-	7/13/89/115	-
23	LHG	8	301	20	-	17/53/53/53	-
29	CHL	5	313	-	-	6/19/95/117	-
29	CHL	7	1017	15	-	9/41/117/117	-
20	CLA	0	308	13	-	3/13/89/115	-
28	LUT	0	318	-	-	2/29/67/67	0/2/2/2
20	CLA	F	302	-	-	2/13/89/115	-
24	BCR	5	320	-	-	5/29/63/63	0/2/2/2
20	CLA	1	1010	-	-	8/13/89/115	-
23	LHG	0	302	20	-	9/23/23/53	-
24	BCR	A	846	-	-	6/29/63/63	0/2/2/2
24	BCR	H	201	-	-	12/29/63/63	0/2/2/2
29	CHL	4	316	17	-	2/14/90/117	-
20	CLA	6	315	18	-	1/13/89/115	-
24	BCR	8	302	-	-	7/29/63/63	0/2/2/2
20	CLA	3	1009	16	-	9/13/89/115	-
28	LUT	J	104	-	-	7/29/67/67	0/2/2/2
29	CHL	0	314	-	-	2/19/95/117	-
20	CLA	1	1017	-	-	3/13/89/115	-
20	CLA	4	307	17	-	4/13/89/115	-
29	CHL	6	313	-	-	5/19/95/117	-
20	CLA	6	308	-	-	2/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	5	319	-	-	19/40/80/95	0/2/2/2
20	CLA	A	815	-	-	5/13/89/115	-
20	CLA	B	827	-	-	3/13/89/115	-
20	CLA	A	818	-	-	4/13/89/115	-
20	CLA	B	812	2	-	3/13/89/115	-
20	CLA	3	1013	16	-	4/13/89/115	-
20	CLA	1	1005	-	-	3/13/89/115	-
20	CLA	8	306	14	-	3/13/89/115	-
20	CLA	B	810	2	-	4/13/89/115	-
20	CLA	6	320	-	-	3/13/89/115	-
20	CLA	5	318	19	-	1/13/89/115	-
29	CHL	7	1015	-	-	8/17/93/117	-
30	XAT	4	303	-	-	2/31/93/93	0/4/4/4
20	CLA	L	202	-	-	3/13/89/115	-
20	CLA	1	1004	13	-	4/13/89/115	-
20	CLA	A	821	-	-	2/13/89/115	-
20	CLA	6	301	-	-	8/13/89/115	-
20	CLA	A	803	20	-	8/13/89/115	-
20	CLA	1	1014	-	-	3/13/89/115	-
20	CLA	A	809	-	-	2/13/89/115	-
20	CLA	B	828	2	-	3/13/89/115	-
23	LHG	4	301	20	-	21/53/53/53	-
20	CLA	L	201	-	-	5/13/89/115	-
20	CLA	L	204	-	-	4/13/89/115	-
20	CLA	A	832	-	-	2/13/89/115	-
20	CLA	8	307	14	-	3/13/89/115	-
20	CLA	A	831	-	-	3/13/89/115	-
20	CLA	7	1004	15	-	6/13/89/115	-
20	CLA	6	312	18	-	2/13/89/115	-
20	CLA	B	818	-	-	4/13/89/115	-
20	CLA	J	102	-	-	6/13/89/115	-
29	CHL	8	315	-	-	3/23/99/117	-
20	CLA	1	1003	-	-	3/13/89/115	-
24	BCR	A	847	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	0	301	23	-	2/13/89/115	-
24	BCR	F	304	-	-	4/29/63/63	0/2/2/2
20	CLA	A	812	1	-	4/13/89/115	-
20	CLA	B	805	-	-	2/13/89/115	-
20	CLA	3	1012	-	-	5/13/89/115	-
20	CLA	8	313	14	-	4/13/89/115	-
29	CHL	0	315	-	-	4/23/99/117	-
29	CHL	4	313	-	-	5/23/99/117	-
20	CLA	A	839	1	-	4/13/89/115	-
27	LMG	8	318	-	-	5/22/42/70	0/1/1/1
20	CLA	B	834	2	-	2/13/89/115	-
20	CLA	B	809	2	-	3/13/89/115	-
27	LMG	6	319	-	-	11/39/59/70	0/1/1/1
20	CLA	B	837	2	-	6/13/89/115	-
27	LMG	4	318	-	-	10/29/49/70	0/1/1/1
20	CLA	5	321	-	-	4/13/89/115	-
20	CLA	G	202	-	-	4/13/89/115	-
20	CLA	B	820	-	-	3/13/89/115	-
20	CLA	0	312	13	-	5/13/89/115	-
20	CLA	B	850	-	-	6/13/86/115	-
24	BCR	A	848	-	-	9/29/63/63	0/2/2/2
20	CLA	4	306	17	-	4/13/89/115	-
20	CLA	3	1016	-	-	10/13/89/115	-
20	CLA	A	827	-	-	3/13/89/115	-
30	XAT	7	1002	-	-	6/31/93/93	0/4/4/4
20	CLA	B	826	-	-	6/13/89/115	-
20	CLA	7	1005	15	-	2/13/89/115	-
20	CLA	6	310	-	-	7/13/89/115	-
20	CLA	B	801	-	-	3/13/89/115	-
20	CLA	5	323	-	-	7/13/89/115	-
20	CLA	5	308	-	-	3/13/89/115	-
25	DGD	B	848	-	-	18/50/90/95	0/2/2/2
21	SF4	C	1001	3	-	-	0/6/5/5
20	CLA	A	825	-	-	1/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	8	317	-	-	17/35/111/117	-
20	CLA	7	1008	15	-	4/13/89/115	-
24	BCR	B	844	-	-	10/29/63/63	0/2/2/2
20	CLA	F	305	-	-	0/13/89/115	-
24	BCR	3	1004	-	-	8/29/63/63	0/2/2/2
20	CLA	A	822	1	-	4/13/89/115	-
20	CLA	G	201	-	-	3/13/89/115	-
20	CLA	B	824	-	-	1/13/89/115	-
20	CLA	B	838	2	-	5/13/89/115	-
20	CLA	0	309	13	-	5/13/89/115	-
20	CLA	8	310	-	-	4/13/89/115	-
20	CLA	1	1011	13	-	4/13/89/115	-
20	CLA	6	305	18	-	2/13/89/115	-
29	CHL	1	1015	-	-	12/35/111/117	-
28	LUT	1	1016	-	-	1/29/67/67	0/2/2/2
29	CHL	8	314	-	-	4/19/95/117	-
20	CLA	5	307	19	-	2/13/89/115	-
20	CLA	5	309	19	-	9/13/89/115	-
20	CLA	8	308	14	-	2/13/89/115	-
20	CLA	3	1008	16	-	3/13/89/115	-
20	CLA	5	301	18	-	9/13/89/115	-
23	LHG	A	849	-	-	20/53/53/53	-
28	LUT	3	1001	-	-	3/29/67/67	0/2/2/2
29	CHL	7	1013	-	-	3/20/96/117	-
27	LMG	0	303	-	-	21/45/65/70	0/1/1/1
30	XAT	8	304	-	-	12/31/93/93	0/4/4/4
20	CLA	A	806	1	-	5/13/89/115	-
20	CLA	5	322	-	-	3/13/89/115	-
29	CHL	6	317	18	-	4/14/90/117	-
20	CLA	5	312	19	-	2/13/89/115	-
29	CHL	4	312	-	-	3/19/95/117	-
20	CLA	A	826	1	-	0/13/89/115	-
24	BCR	B	846	-	-	2/29/63/63	0/2/2/2
20	CLA	G	203	-	-	8/13/89/115	-
20	CLA	6	311	-	-	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	817	2	-	2/13/89/115	-
20	CLA	5	315	19	-	0/13/89/115	-
20	CLA	6	306	18	-	4/13/89/115	-
29	CHL	6	314	-	-	7/23/99/117	-
24	BCR	7	1003	-	-	16/29/63/63	0/2/2/2
20	CLA	B	839	2	-	4/13/89/115	-
24	BCR	B	804	-	-	6/29/63/63	0/2/2/2
20	CLA	4	305	17	-	5/13/89/115	-
20	CLA	5	304	19	-	2/13/89/115	-
28	LUT	5	302	-	-	3/29/67/67	0/2/2/2
20	CLA	A	824	-	-	4/13/89/115	-
20	CLA	3	1011	23	-	2/8/84/115	-
23	LHG	A	843	-	-	21/44/44/53	-
20	CLA	A	828	1	-	4/13/89/115	-
21	SF4	A	841	2,1	-	-	0/6/5/5
20	CLA	B	808	2	-	4/13/89/115	-
20	CLA	4	311	17	-	4/13/89/115	-
20	CLA	B	814	-	-	0/13/89/115	-
28	LUT	7	1001	-	-	5/29/67/67	0/2/2/2
20	CLA	A	804	1	-	4/13/89/115	-
20	CLA	0	306	13	-	4/13/89/115	-
20	CLA	F	303	6	-	5/13/89/115	-
28	LUT	6	303	-	-	2/29/67/67	0/2/2/2
20	CLA	A	852	-	-	2/13/89/115	-
20	CLA	B	840	-	-	6/13/89/115	-
20	CLA	5	310	-	-	6/13/89/115	-
20	CLA	B	813	2	-	2/13/89/115	-
23	LHG	7	1016	20	-	13/39/39/53	-
20	CLA	A	801	-	-	3/13/89/115	-
20	CLA	A	816	-	-	0/13/89/115	-
29	CHL	7	1012	-	-	4/19/95/117	-
20	CLA	7	1009	-	-	3/13/89/115	-
20	CLA	K	201	-	-	6/13/89/115	-
20	CLA	A	817	-	-	4/13/89/115	-
20	CLA	1	1006	13	-	2/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	1015	16	-	2/13/89/115	-
20	CLA	0	305	-	-	3/13/89/115	-
20	CLA	A	834	-	-	2/13/89/115	-
20	CLA	3	1007	-	-	5/13/89/115	-
20	CLA	B	836	-	-	0/13/89/115	-
20	CLA	A	823	-	-	3/13/89/115	-
20	CLA	8	312	14	-	5/13/89/115	-
20	CLA	5	305	19	-	6/13/89/115	-
20	CLA	A	833	1	-	3/13/89/115	-
20	CLA	B	833	2	-	3/13/89/115	-
20	CLA	3	1006	16	-	4/13/89/115	-
20	CLA	B	821	-	-	3/13/89/115	-
24	BCR	A	844	-	-	2/29/63/63	0/2/2/2
20	CLA	A	802	-	-	2/13/89/115	-
20	CLA	B	807	-	-	4/13/89/115	-
20	CLA	B	819	-	-	4/13/89/115	-
20	CLA	6	307	-	-	3/13/89/115	-
22	PQN	A	842	-	-	6/23/43/43	0/2/2/2
24	BCR	I	201	-	-	11/29/63/63	0/2/2/2
26	LMT	B	849	-	-	5/17/57/61	0/2/2/2
30	XAT	5	303	-	-	2/31/93/93	0/4/4/4
20	CLA	A	810	1,20	-	5/13/89/115	-
20	CLA	8	316	14	-	3/13/89/115	-
20	CLA	B	822	-	-	2/13/89/115	-
20	CLA	8	305	14	-	3/13/89/115	-
20	CLA	0	307	-	-	3/13/89/115	-
20	CLA	7	1006	15	-	5/13/89/115	-
24	BCR	A	845	-	-	9/29/63/63	0/2/2/2
24	BCR	1	1001	-	-	8/29/63/63	0/2/2/2
29	CHL	4	315	-	-	17/35/111/117	-
20	CLA	3	1010	-	-	5/13/89/115	-
20	CLA	3	1005	16	-	8/13/89/115	-
20	CLA	A	851	-	-	2/13/89/115	-
20	CLA	B	830	2	-	3/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	815	-	-	3/13/89/115	-
20	CLA	4	314	17	-	4/13/89/115	-
20	CLA	0	316	-	-	4/13/89/115	-
29	CHL	3	1014	-	-	7/19/95/117	-
26	LMT	3	1018	-	-	4/17/57/61	0/2/2/2
20	CLA	4	309	-	-	9/13/89/115	-
20	CLA	A	808	-	-	3/13/89/115	-
20	CLA	B	835	-	-	0/13/89/115	-
24	BCR	B	843	-	-	9/29/63/63	0/2/2/2
20	CLA	0	313	13	-	4/13/89/115	-
28	LUT	3	1002	-	-	8/29/67/67	0/2/2/2
29	CHL	5	316	-	-	15/35/111/117	-
20	CLA	B	823	-	-	5/13/89/115	-
28	LUT	1	1002	-	-	5/29/67/67	0/2/2/2
20	CLA	B	832	-	-	1/13/89/115	-
24	BCR	4	302	-	-	7/29/63/63	0/2/2/2
29	CHL	1	1012	-	-	5/19/95/117	-
20	CLA	A	837	-	-	4/13/89/115	-
20	CLA	1	1009	23	-	4/13/89/115	-
28	LUT	0	304	-	-	6/29/67/67	0/2/2/2
29	CHL	1	1013	-	-	1/23/99/117	-
21	SF4	C	1002	3	-	-	0/6/5/5
20	CLA	7	1011	15	-	7/13/89/115	-
24	BCR	6	302	-	-	7/29/63/63	0/2/2/2
20	CLA	7	1014	15	-	0/13/89/115	-
20	CLA	B	831	-	-	1/13/89/115	-
20	CLA	A	829	1	-	4/13/89/115	-
24	BCR	F	301	-	-	5/29/63/63	0/2/2/2
20	CLA	A	840	-	-	3/13/89/115	-
20	CLA	B	811	-	-	0/13/89/115	-
20	CLA	7	1007	15	-	3/13/89/115	-
20	CLA	1	1007	13	-	5/13/89/115	-
20	CLA	8	309	27	-	7/13/89/115	-
20	CLA	B	816	2	-	7/13/89/115	-
20	CLA	A	838	-	-	1/13/89/115	-
24	BCR	A	850	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	845	-	-	10/29/63/63	0/2/2/2
28	LUT	4	317	-	-	0/29/67/67	0/2/2/2
22	PQN	B	842	-	-	9/23/43/43	0/2/2/2
27	LMG	8	319	20	-	12/39/59/70	0/1/1/1
20	CLA	4	304	17	-	3/13/89/115	-
20	CLA	6	318	18	-	5/13/89/115	-
20	CLA	7	1010	23	-	0/13/89/115	-
29	CHL	0	317	-	-	14/35/111/117	-
20	CLA	8	311	-	-	5/13/89/115	-
20	CLA	B	803	-	-	5/13/89/115	-
24	BCR	G	204	-	-	2/29/63/63	0/2/2/2
20	CLA	A	835	-	-	2/13/89/115	-
20	CLA	3	1017	16	-	5/13/89/115	-
20	CLA	A	805	1	-	6/13/89/115	-
20	CLA	A	819	-	-	7/13/89/115	-
20	CLA	6	309	18	-	7/13/89/115	-
24	BCR	B	847	-	-	5/29/63/63	0/2/2/2
27	LMG	J	101	-	-	6/25/45/70	0/1/1/1
29	CHL	5	317	19	-	3/14/90/117	-
20	CLA	A	820	-	-	5/13/89/115	-
23	LHG	3	1019	20	-	12/23/23/53	-
27	LMG	5	324	-	-	26/40/60/70	0/1/1/1
20	CLA	4	308	17	-	5/13/89/115	-
20	CLA	B	802	-	-	4/13/89/115	-
20	CLA	B	829	-	-	6/13/89/115	-
20	CLA	A	813	1	-	4/13/89/115	-
20	CLA	B	841	-	-	8/13/89/115	-
20	CLA	A	807	-	-	5/13/89/115	-
20	CLA	A	811	-	-	6/13/89/115	-
20	CLA	B	806	-	-	2/13/89/115	-
20	CLA	A	814	-	-	3/8/84/115	-
20	CLA	4	310	-	-	6/13/89/115	-
20	CLA	0	311	23	-	4/13/89/115	-
20	CLA	5	306	-	-	5/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	5	314	-	-	3/23/99/117	-
20	CLA	B	825	-	-	6/13/89/115	-
20	CLA	L	203	-	-	3/13/89/115	-

All (1915) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	850	CLA	C4C-NC	21.89	1.46	1.30
20	5	301	CLA	C4B-NB	10.33	1.50	1.37
20	6	308	CLA	C4B-NB	10.12	1.50	1.37
20	B	837	CLA	C4B-NB	10.02	1.50	1.37
20	8	309	CLA	C4B-NB	9.99	1.50	1.37
20	B	813	CLA	C4B-NB	9.91	1.50	1.37
20	4	307	CLA	C4B-NB	9.90	1.50	1.37
20	4	305	CLA	C4B-NB	9.80	1.49	1.37
20	G	203	CLA	C4B-NB	9.64	1.49	1.37
20	L	204	CLA	C4B-NB	9.63	1.49	1.37
29	5	313	CHL	C4B-NB	9.62	1.49	1.37
20	7	1007	CLA	C4B-NB	9.58	1.49	1.37
20	B	815	CLA	C4B-NB	9.52	1.49	1.37
20	A	813	CLA	C4B-NB	9.45	1.49	1.37
20	6	320	CLA	C4B-NB	9.44	1.49	1.37
20	B	812	CLA	C4B-NB	9.44	1.49	1.37
20	A	808	CLA	C4B-NB	9.43	1.49	1.37
20	B	823	CLA	C4B-NB	9.43	1.49	1.37
20	5	311	CLA	C4B-NB	9.37	1.49	1.37
20	A	831	CLA	C4B-NB	9.32	1.49	1.37
20	7	1011	CLA	C4B-NB	9.31	1.49	1.37
20	A	821	CLA	C4B-NB	9.29	1.49	1.37
20	B	808	CLA	C4B-NB	9.26	1.49	1.37
20	B	831	CLA	C4B-NB	9.24	1.49	1.37
20	3	1009	CLA	C4B-NB	9.24	1.49	1.37
20	3	1015	CLA	C4B-NB	9.20	1.49	1.37
20	B	826	CLA	C4B-NB	9.19	1.49	1.37
20	5	305	CLA	C4B-NB	9.19	1.49	1.37
20	A	801	CLA	C4B-NB	9.15	1.49	1.37
20	8	313	CLA	C4B-NB	9.14	1.49	1.37
20	K	201	CLA	C4B-NB	9.14	1.49	1.37
20	3	1006	CLA	C4B-NB	9.10	1.49	1.37
20	A	826	CLA	C4B-NB	9.08	1.48	1.37
20	7	1005	CLA	C4B-NB	9.07	1.48	1.37
20	3	1008	CLA	C4B-NB	9.05	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	811	CLA	C4B-NB	9.05	1.48	1.37
20	B	814	CLA	C4B-NB	9.05	1.48	1.37
20	A	830	CLA	C4B-NB	9.01	1.48	1.37
20	4	311	CLA	C4B-NB	9.00	1.48	1.37
20	B	816	CLA	C4B-NB	8.99	1.48	1.37
20	B	809	CLA	C4B-NB	8.97	1.48	1.37
20	G	202	CLA	C4B-NB	8.96	1.48	1.37
20	A	824	CLA	C4B-NB	8.94	1.48	1.37
20	A	814	CLA	C4B-NB	8.94	1.48	1.37
20	A	825	CLA	C4B-NB	8.94	1.48	1.37
20	A	822	CLA	C4B-NB	8.93	1.48	1.37
20	A	810	CLA	C4B-NB	8.92	1.48	1.37
20	6	309	CLA	C4B-NB	8.91	1.48	1.37
20	0	301	CLA	C4B-NB	8.89	1.48	1.37
20	A	804	CLA	C4B-NB	8.88	1.48	1.37
20	A	803	CLA	C4B-NB	8.87	1.48	1.37
20	3	1017	CLA	C4B-NB	8.86	1.48	1.37
20	3	1011	CLA	C4B-NB	8.85	1.48	1.37
20	1	1014	CLA	C4B-NB	8.84	1.48	1.37
20	0	310	CLA	C4B-NB	8.84	1.48	1.37
20	8	308	CLA	C4B-NB	8.80	1.48	1.37
20	A	852	CLA	C4B-NB	8.79	1.48	1.37
20	L	203	CLA	C4B-NB	8.78	1.48	1.37
20	G	201	CLA	C4B-NB	8.77	1.48	1.37
20	5	304	CLA	C4B-NB	8.76	1.48	1.37
20	F	305	CLA	C4B-NB	8.75	1.48	1.37
20	B	817	CLA	C4B-NB	8.75	1.48	1.37
20	B	841	CLA	C4B-NB	8.74	1.48	1.37
20	A	834	CLA	C4B-NB	8.72	1.48	1.37
20	B	820	CLA	C4B-NB	8.70	1.48	1.37
20	A	833	CLA	C4B-NB	8.69	1.48	1.37
20	6	315	CLA	C4B-NB	8.67	1.48	1.37
20	B	821	CLA	C4B-NB	8.67	1.48	1.37
20	A	812	CLA	C4B-NB	8.67	1.48	1.37
20	B	850	CLA	C4B-NB	8.65	1.48	1.37
29	7	1015	CHL	C4B-NB	8.63	1.48	1.37
20	0	312	CLA	C4B-NB	8.56	1.48	1.37
20	B	840	CLA	C4B-NB	8.51	1.48	1.37
20	7	1009	CLA	C4B-NB	8.50	1.48	1.37
20	A	817	CLA	C4B-NB	8.50	1.48	1.37
20	0	313	CLA	C4B-NB	8.50	1.48	1.37
20	3	1012	CLA	C4B-NB	8.48	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	805	CLA	C4B-NB	8.48	1.48	1.37
20	0	307	CLA	C4B-NB	8.47	1.48	1.37
20	5	322	CLA	C4B-NB	8.47	1.48	1.37
20	1	1005	CLA	C4B-NB	8.45	1.48	1.37
20	A	816	CLA	C4B-NB	8.43	1.48	1.37
20	1	1004	CLA	C4B-NB	8.43	1.48	1.37
20	3	1010	CLA	C4B-NB	8.42	1.48	1.37
20	B	811	CLA	C4B-NB	8.41	1.48	1.37
20	L	202	CLA	C4B-NB	8.41	1.48	1.37
20	J	102	CLA	C4B-NB	8.41	1.48	1.37
20	7	1014	CLA	C4B-NB	8.40	1.48	1.37
20	5	309	CLA	C4B-NB	8.40	1.48	1.37
20	0	311	CLA	C4B-NB	8.40	1.48	1.37
20	B	819	CLA	C4B-NB	8.38	1.48	1.37
20	5	312	CLA	C4B-NB	8.38	1.48	1.37
20	B	838	CLA	C4B-NB	8.37	1.48	1.37
20	B	835	CLA	C4B-NB	8.36	1.48	1.37
20	6	318	CLA	C4B-NB	8.35	1.48	1.37
20	0	306	CLA	C4B-NB	8.34	1.48	1.37
20	5	306	CLA	C4B-NB	8.33	1.48	1.37
20	A	820	CLA	C4B-NB	8.28	1.48	1.37
20	5	310	CLA	C4B-NB	8.26	1.47	1.37
20	A	828	CLA	C4B-NB	8.25	1.47	1.37
20	3	1007	CLA	C4B-NB	8.25	1.47	1.37
20	A	806	CLA	C4B-NB	8.23	1.47	1.37
20	1	1011	CLA	C4B-NB	8.20	1.47	1.37
20	A	819	CLA	C4B-NB	8.17	1.47	1.37
20	B	803	CLA	C4B-NB	8.17	1.47	1.37
20	5	307	CLA	C4B-NB	8.17	1.47	1.37
20	A	809	CLA	C4B-NB	8.13	1.47	1.37
20	1	1007	CLA	C4B-NB	8.12	1.47	1.37
29	6	313	CHL	C4B-NB	8.11	1.47	1.37
20	4	309	CLA	C4B-NB	8.11	1.47	1.37
20	5	323	CLA	C4B-NB	8.10	1.47	1.37
20	A	851	CLA	C4B-NB	8.09	1.47	1.37
20	0	309	CLA	C4B-NB	8.09	1.47	1.37
20	B	806	CLA	C4B-NB	8.08	1.47	1.37
20	6	301	CLA	C4B-NB	8.07	1.47	1.37
20	A	839	CLA	C4B-NB	8.07	1.47	1.37
20	7	1008	CLA	C4B-NB	8.06	1.47	1.37
20	B	807	CLA	C4B-NB	8.05	1.47	1.37
20	B	832	CLA	C4B-NB	8.04	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	835	CLA	C4B-NB	8.04	1.47	1.37
20	6	312	CLA	C4B-NB	8.03	1.47	1.37
20	4	308	CLA	C4B-NB	8.03	1.47	1.37
20	B	836	CLA	C4B-NB	8.01	1.47	1.37
20	B	801	CLA	C4B-NB	8.01	1.47	1.37
20	B	833	CLA	C4B-NB	8.00	1.47	1.37
20	A	837	CLA	C4B-NB	7.98	1.47	1.37
20	B	825	CLA	C4B-NB	7.94	1.47	1.37
20	5	308	CLA	C4B-NB	7.93	1.47	1.37
20	A	836	CLA	C4B-NB	7.92	1.47	1.37
20	B	805	CLA	C4B-NB	7.91	1.47	1.37
20	B	828	CLA	C4B-NB	7.89	1.47	1.37
20	1	1017	CLA	C4B-NB	7.89	1.47	1.37
20	A	802	CLA	C4B-NB	7.88	1.47	1.37
20	8	312	CLA	C4B-NB	7.85	1.47	1.37
20	A	832	CLA	C4B-NB	7.83	1.47	1.37
20	A	823	CLA	C4B-NB	7.82	1.47	1.37
20	0	316	CLA	C4B-NB	7.81	1.47	1.37
20	3	1005	CLA	C4B-NB	7.81	1.47	1.37
20	6	307	CLA	C4B-NB	7.78	1.47	1.37
29	8	317	CHL	C4B-NB	7.78	1.47	1.37
20	B	802	CLA	C4B-NB	7.78	1.47	1.37
20	0	308	CLA	C4B-NB	7.75	1.47	1.37
29	8	314	CHL	C4B-NB	7.75	1.47	1.37
20	B	810	CLA	C4B-NB	7.73	1.47	1.37
20	B	818	CLA	C4B-NB	7.72	1.47	1.37
20	5	321	CLA	C4B-NB	7.72	1.47	1.37
20	B	827	CLA	C4B-NB	7.71	1.47	1.37
20	F	303	CLA	C4B-NB	7.70	1.47	1.37
20	A	818	CLA	C4B-NB	7.65	1.47	1.37
20	4	306	CLA	C4B-NB	7.65	1.47	1.37
20	K	202	CLA	C4C-NC	7.62	1.49	1.37
20	8	306	CLA	C4B-NB	7.61	1.47	1.37
20	B	839	CLA	C4B-NB	7.61	1.47	1.37
29	6	317	CHL	C4B-NB	7.60	1.47	1.37
20	1	1010	CLA	C4B-NB	7.60	1.47	1.37
20	A	829	CLA	C4B-NB	7.59	1.47	1.37
20	8	310	CLA	C4B-NB	7.59	1.47	1.37
20	5	318	CLA	C4B-NB	7.58	1.47	1.37
20	6	306	CLA	C4B-NB	7.54	1.47	1.37
20	B	824	CLA	C4B-NB	7.53	1.47	1.37
29	1	1013	CHL	C4B-NB	7.49	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	201	CLA	C4B-NB	7.49	1.47	1.37
20	1	1003	CLA	C4B-NB	7.46	1.47	1.37
20	3	1013	CLA	C4B-NB	7.46	1.47	1.37
20	0	305	CLA	C4B-NB	7.45	1.46	1.37
20	1	1009	CLA	C4B-NB	7.42	1.46	1.37
20	8	311	CLA	C4B-NB	7.40	1.46	1.37
29	0	315	CHL	C4B-NB	7.37	1.46	1.37
20	4	304	CLA	C4B-NB	7.37	1.46	1.37
20	1	1008	CLA	C4B-NB	7.37	1.46	1.37
20	7	1006	CLA	C4B-NB	7.35	1.46	1.37
20	4	310	CLA	C4B-NB	7.33	1.46	1.37
29	0	314	CHL	C4B-NB	7.32	1.46	1.37
20	A	807	CLA	C4B-NB	7.28	1.46	1.37
20	F	302	CLA	C4B-NB	7.27	1.46	1.37
20	A	827	CLA	C4B-NB	7.27	1.46	1.37
20	6	311	CLA	C4B-NB	7.26	1.46	1.37
29	1	1015	CHL	MG-NB	-7.23	1.91	2.05
29	4	312	CHL	C4B-NB	7.23	1.46	1.37
20	4	314	CLA	C4B-NB	7.18	1.46	1.37
29	6	316	CHL	MG-NB	-7.18	1.91	2.05
20	8	305	CLA	C4B-NB	7.17	1.46	1.37
20	3	1016	CLA	C4B-NB	7.16	1.46	1.37
29	4	315	CHL	C4B-NB	7.12	1.46	1.37
29	8	317	CHL	MG-NB	-7.10	1.91	2.05
29	5	316	CHL	C4B-NB	7.06	1.46	1.37
20	B	829	CLA	C4B-NB	7.05	1.46	1.37
20	1	1006	CLA	C4B-NB	7.03	1.46	1.37
29	5	314	CHL	C4B-NB	7.00	1.46	1.37
20	B	834	CLA	C4B-NB	6.99	1.46	1.37
20	B	822	CLA	C4B-NB	6.98	1.46	1.37
20	5	315	CLA	C4B-NB	6.90	1.46	1.37
20	7	1010	CLA	C4B-NB	6.88	1.46	1.37
20	A	838	CLA	C4B-NB	6.87	1.46	1.37
20	6	305	CLA	C4B-NB	6.86	1.46	1.37
20	A	840	CLA	C4B-NB	6.84	1.46	1.37
29	7	1012	CHL	C4B-NB	6.81	1.46	1.37
29	3	1014	CHL	MG-NB	-6.78	1.92	2.05
20	5	321	CLA	MG-NB	-6.78	1.92	2.05
29	7	1012	CHL	MG-NB	-6.76	1.92	2.05
29	0	317	CHL	C4B-NB	6.71	1.46	1.37
29	5	317	CHL	MG-ND	-6.71	1.92	2.05
29	7	1017	CHL	C4B-NB	6.70	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	815	CLA	C4B-NB	6.69	1.46	1.37
29	6	313	CHL	MG-ND	-6.67	1.92	2.05
29	8	315	CHL	C4B-NB	6.67	1.46	1.37
20	5	318	CLA	MG-NB	-6.61	1.92	2.05
20	5	301	CLA	MG-NB	-6.60	1.92	2.05
20	8	316	CLA	C4B-NB	6.57	1.45	1.37
20	5	311	CLA	MG-NB	-6.57	1.92	2.05
20	7	1007	CLA	MG-NB	-6.55	1.92	2.05
29	6	316	CHL	MG-ND	-6.48	1.92	2.05
29	7	1013	CHL	C4B-NB	6.47	1.45	1.37
29	6	314	CHL	MG-NB	-6.42	1.93	2.05
20	7	1004	CLA	C4B-NB	6.42	1.45	1.37
29	7	1017	CHL	MG-NB	-6.42	1.93	2.05
29	0	317	CHL	MG-NB	-6.40	1.93	2.05
20	6	310	CLA	C4B-NB	6.37	1.45	1.37
20	4	314	CLA	MG-NB	-6.31	1.93	2.05
29	6	317	CHL	MG-ND	-6.30	1.93	2.05
29	5	316	CHL	MG-NB	-6.29	1.93	2.05
29	3	1014	CHL	C4B-NB	6.29	1.45	1.37
29	4	313	CHL	C4B-NB	6.26	1.45	1.37
20	5	305	CLA	C1D-ND	6.25	1.45	1.37
20	B	830	CLA	C4B-NB	6.25	1.45	1.37
20	7	1010	CLA	MG-NB	-6.23	1.93	2.05
29	3	1014	CHL	MG-ND	-6.23	1.93	2.05
20	A	838	CLA	MG-ND	-6.22	1.93	2.05
20	B	805	CLA	MG-NB	-6.22	1.93	2.05
29	7	1013	CHL	MG-ND	-6.14	1.93	2.05
20	6	305	CLA	MG-NB	-6.11	1.93	2.05
29	5	317	CHL	C4B-NB	6.07	1.45	1.37
29	1	1012	CHL	C4B-NB	6.05	1.45	1.37
20	3	1013	CLA	MG-NB	-6.02	1.93	2.05
20	4	308	CLA	C1D-ND	6.01	1.45	1.37
20	4	314	CLA	C1D-ND	6.01	1.45	1.37
20	4	310	CLA	MG-NB	-6.01	1.93	2.05
29	7	1013	CHL	MG-NB	-5.98	1.93	2.05
20	B	831	CLA	MG-NB	-5.96	1.94	2.05
20	8	307	CLA	MG-NB	-5.95	1.94	2.05
29	5	314	CHL	MG-NC	-5.95	1.92	2.06
29	8	314	CHL	MG-NB	-5.93	1.94	2.05
20	A	839	CLA	C1D-ND	5.92	1.45	1.37
20	3	1016	CLA	MG-ND	-5.88	1.94	2.05
20	6	311	CLA	MG-NB	-5.88	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	1005	CLA	MG-NB	-5.87	1.94	2.05
29	6	316	CHL	C4B-NB	5.85	1.45	1.37
29	4	316	CHL	MG-ND	-5.81	1.94	2.05
20	6	318	CLA	MG-NB	-5.81	1.94	2.05
20	3	1012	CLA	MG-NB	-5.79	1.94	2.05
20	B	822	CLA	MG-NB	-5.76	1.94	2.05
29	5	314	CHL	MG-ND	-5.74	1.94	2.05
29	4	316	CHL	C4B-NB	5.73	1.44	1.37
20	8	308	CLA	MG-NB	-5.73	1.94	2.05
20	1	1006	CLA	MG-NB	-5.70	1.94	2.05
20	4	306	CLA	C1D-ND	5.69	1.44	1.37
29	4	315	CHL	MG-NB	-5.69	1.94	2.05
20	B	825	CLA	MG-NB	-5.68	1.94	2.05
20	B	815	CLA	C1D-ND	5.67	1.44	1.37
29	0	315	CHL	MG-NB	-5.67	1.94	2.05
29	5	313	CHL	MG-ND	-5.66	1.94	2.05
29	7	1015	CHL	MG-ND	-5.66	1.94	2.05
29	4	312	CHL	MG-ND	-5.65	1.94	2.05
20	8	316	CLA	MG-NB	-5.64	1.94	2.05
29	0	314	CHL	MG-NB	-5.64	1.94	2.05
20	8	309	CLA	C1D-ND	5.64	1.44	1.37
20	0	305	CLA	MG-NB	-5.63	1.94	2.05
20	A	837	CLA	MG-ND	-5.63	1.94	2.05
29	8	315	CHL	MG-NB	-5.63	1.94	2.05
20	A	827	CLA	MG-ND	-5.63	1.94	2.05
20	5	312	CLA	MG-ND	-5.61	1.94	2.05
29	7	1015	CHL	MG-NB	-5.61	1.94	2.05
20	5	315	CLA	MG-ND	-5.60	1.94	2.05
20	B	836	CLA	MG-NB	-5.60	1.94	2.05
20	6	308	CLA	MG-NB	-5.60	1.94	2.05
29	1	1015	CHL	MG-ND	-5.60	1.94	2.05
20	A	838	CLA	MG-NB	-5.59	1.94	2.05
20	7	1011	CLA	MG-NB	-5.59	1.94	2.05
20	8	310	CLA	MG-NB	-5.57	1.94	2.05
20	1	1003	CLA	MG-NB	-5.55	1.94	2.05
20	B	802	CLA	MG-NB	-5.55	1.94	2.05
29	6	314	CHL	MG-ND	-5.55	1.94	2.05
20	B	827	CLA	MG-NB	-5.54	1.94	2.05
20	6	310	CLA	MG-NB	-5.54	1.94	2.05
20	F	303	CLA	MG-NB	-5.53	1.94	2.05
29	1	1012	CHL	MG-NB	-5.53	1.94	2.05
29	6	317	CHL	MG-NB	-5.52	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	316	CHL	MG-NB	-5.52	1.94	2.05
29	7	1012	CHL	MG-ND	-5.51	1.94	2.05
20	4	310	CLA	MG-NA	-5.51	1.93	2.06
20	8	311	CLA	MG-NB	-5.49	1.94	2.05
20	A	815	CLA	MG-ND	-5.48	1.94	2.05
20	A	815	CLA	MG-NB	-5.46	1.95	2.05
20	6	318	CLA	C1D-ND	5.46	1.44	1.37
20	A	834	CLA	MG-NB	-5.46	1.95	2.05
29	0	314	CHL	MG-ND	-5.44	1.95	2.05
20	5	323	CLA	C1D-ND	5.44	1.44	1.37
20	1	1006	CLA	MG-ND	-5.44	1.95	2.05
29	0	317	CHL	MG-ND	-5.44	1.95	2.05
29	4	315	CHL	MG-ND	-5.43	1.95	2.05
20	0	310	CLA	C1B-NB	5.43	1.44	1.37
20	A	826	CLA	MG-ND	-5.43	1.95	2.05
20	6	307	CLA	MG-NB	-5.43	1.95	2.05
20	1	1005	CLA	MG-NB	-5.42	1.95	2.05
20	B	830	CLA	MG-NA	-5.42	1.93	2.06
20	A	839	CLA	MG-NB	-5.41	1.95	2.05
20	B	834	CLA	MG-NB	-5.41	1.95	2.05
20	0	308	CLA	MG-NB	-5.41	1.95	2.05
20	5	318	CLA	C1D-ND	5.41	1.44	1.37
20	A	802	CLA	MG-NB	-5.41	1.95	2.05
20	7	1009	CLA	MG-NB	-5.40	1.95	2.05
29	4	312	CHL	MG-NB	-5.39	1.95	2.05
20	6	312	CLA	MG-NB	-5.38	1.95	2.05
20	B	822	CLA	MG-ND	-5.38	1.95	2.05
20	0	307	CLA	C1D-ND	5.38	1.44	1.37
29	1	1012	CHL	MG-ND	-5.37	1.95	2.05
29	1	1015	CHL	C4B-NB	5.36	1.44	1.37
20	0	311	CLA	C1D-ND	5.35	1.44	1.37
20	B	813	CLA	C1D-ND	5.35	1.44	1.37
20	B	802	CLA	MG-ND	-5.34	1.95	2.05
20	B	829	CLA	MG-NB	-5.34	1.95	2.05
20	3	1008	CLA	MG-NB	-5.34	1.95	2.05
29	5	314	CHL	MG-NB	-5.34	1.95	2.05
20	6	320	CLA	MG-ND	-5.34	1.95	2.05
20	1	1010	CLA	MG-NB	-5.33	1.95	2.05
20	B	807	CLA	C1D-ND	5.33	1.44	1.37
20	L	203	CLA	C1D-ND	5.32	1.44	1.37
20	A	831	CLA	MG-NB	-5.32	1.95	2.05
20	5	308	CLA	MG-NB	-5.32	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	818	CLA	MG-NB	-5.31	1.95	2.05
20	K	201	CLA	C1D-ND	5.30	1.44	1.37
20	L	204	CLA	C1D-ND	5.30	1.44	1.37
20	B	803	CLA	MG-NB	-5.30	1.95	2.05
20	4	305	CLA	C1D-ND	5.30	1.44	1.37
20	6	307	CLA	C1D-ND	5.29	1.44	1.37
20	A	817	CLA	MG-NB	-5.29	1.95	2.05
20	A	810	CLA	MG-NB	-5.29	1.95	2.05
20	B	803	CLA	MG-ND	-5.28	1.95	2.05
20	A	806	CLA	MG-NB	-5.28	1.95	2.05
20	5	305	CLA	MG-NB	-5.27	1.95	2.05
29	0	315	CHL	MG-ND	-5.27	1.95	2.05
20	8	306	CLA	C1D-ND	5.27	1.44	1.37
29	5	316	CHL	MG-ND	-5.26	1.95	2.05
20	A	823	CLA	MG-NB	-5.25	1.95	2.05
20	B	811	CLA	MG-NB	-5.25	1.95	2.05
20	B	839	CLA	MG-NB	-5.25	1.95	2.05
20	1	1014	CLA	MG-NB	-5.25	1.95	2.05
20	0	316	CLA	MG-NB	-5.24	1.95	2.05
20	A	821	CLA	MG-NB	-5.24	1.95	2.05
20	A	833	CLA	MG-ND	-5.23	1.95	2.05
20	1	1004	CLA	MG-ND	-5.23	1.95	2.05
20	F	305	CLA	MG-NB	-5.22	1.95	2.05
29	7	1017	CHL	MG-ND	-5.22	1.95	2.05
20	F	303	CLA	C1D-ND	5.21	1.44	1.37
20	B	828	CLA	MG-NB	-5.21	1.95	2.05
20	8	307	CLA	MG-ND	-5.21	1.95	2.05
20	B	824	CLA	MG-NB	-5.20	1.95	2.05
20	1	1008	CLA	C1D-ND	5.19	1.44	1.37
29	1	1013	CHL	MG-NB	-5.19	1.95	2.05
20	3	1016	CLA	MG-NB	-5.18	1.95	2.05
20	F	302	CLA	MG-ND	-5.18	1.95	2.05
20	0	313	CLA	C1D-ND	5.17	1.44	1.37
29	7	1012	CHL	C1D-ND	5.17	1.44	1.37
20	B	841	CLA	MG-ND	-5.16	1.95	2.05
20	1	1007	CLA	MG-ND	-5.16	1.95	2.05
20	8	313	CLA	C1D-ND	5.15	1.44	1.37
20	1	1011	CLA	MG-NB	-5.15	1.95	2.05
20	L	203	CLA	MG-NB	-5.14	1.95	2.05
20	A	820	CLA	MG-NB	-5.14	1.95	2.05
29	8	317	CHL	MG-ND	-5.14	1.95	2.05
20	4	307	CLA	MG-NB	-5.14	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	304	CLA	MG-ND	-5.14	1.95	2.05
29	6	314	CHL	C4B-NB	5.13	1.44	1.37
20	B	807	CLA	MG-NB	-5.13	1.95	2.05
20	3	1005	CLA	MG-NB	-5.11	1.95	2.05
20	7	1006	CLA	C1D-ND	5.11	1.44	1.37
20	5	323	CLA	MG-NB	-5.10	1.95	2.05
20	B	832	CLA	MG-ND	-5.09	1.95	2.05
20	A	814	CLA	MG-NB	-5.09	1.95	2.05
20	B	810	CLA	MG-NB	-5.09	1.95	2.05
20	B	827	CLA	C1D-ND	5.08	1.44	1.37
20	A	813	CLA	C1D-ND	5.08	1.44	1.37
20	0	301	CLA	C1D-ND	5.07	1.44	1.37
20	0	309	CLA	MG-NB	-5.07	1.95	2.05
29	4	313	CHL	MG-NB	-5.07	1.95	2.05
20	5	311	CLA	MG-ND	-5.06	1.95	2.05
29	1	1013	CHL	MG-ND	-5.06	1.95	2.05
20	0	312	CLA	MG-NB	-5.06	1.95	2.05
20	5	307	CLA	MG-NB	-5.06	1.95	2.05
20	8	310	CLA	C1D-ND	5.06	1.44	1.37
20	8	313	CLA	MG-NB	-5.05	1.95	2.05
20	8	310	CLA	MG-ND	-5.05	1.95	2.05
20	4	304	CLA	MG-NA	-5.05	1.94	2.06
20	0	310	CLA	C1D-ND	5.05	1.44	1.37
20	L	201	CLA	C1D-ND	5.04	1.44	1.37
20	8	307	CLA	C4B-NB	5.04	1.44	1.37
20	6	306	CLA	MG-NB	-5.04	1.95	2.05
20	1	1008	CLA	C1B-NB	5.03	1.44	1.37
20	7	1006	CLA	MG-NB	-5.02	1.95	2.05
20	5	309	CLA	MG-NB	-5.02	1.95	2.05
20	B	809	CLA	MG-NB	-5.02	1.95	2.05
20	B	836	CLA	MG-ND	-5.01	1.95	2.05
20	B	823	CLA	C1D-ND	5.01	1.43	1.37
20	7	1004	CLA	MG-ND	-5.01	1.95	2.05
20	3	1006	CLA	C1D-ND	5.01	1.43	1.37
20	B	809	CLA	C1D-ND	5.00	1.43	1.37
20	5	309	CLA	MG-ND	-5.00	1.95	2.05
20	0	312	CLA	C1D-ND	5.00	1.43	1.37
20	B	819	CLA	MG-NB	-4.99	1.95	2.05
20	6	312	CLA	MG-NC	-4.99	1.94	2.06
29	4	313	CHL	MG-ND	-4.98	1.95	2.05
20	B	805	CLA	MG-NA	-4.97	1.94	2.06
20	A	816	CLA	MG-NB	-4.97	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	305	CLA	MG-NB	-4.97	1.95	2.05
20	B	840	CLA	C1D-ND	4.96	1.43	1.37
20	8	312	CLA	MG-ND	-4.95	1.96	2.05
20	3	1010	CLA	MG-NB	-4.95	1.96	2.05
20	7	1011	CLA	MG-ND	-4.94	1.96	2.05
20	B	801	CLA	MG-NB	-4.94	1.96	2.05
20	1	1014	CLA	MG-ND	-4.94	1.96	2.05
20	7	1005	CLA	C1D-ND	4.94	1.43	1.37
20	B	821	CLA	MG-NB	-4.93	1.96	2.05
29	8	315	CHL	C1D-ND	4.93	1.43	1.37
20	5	304	CLA	C1D-ND	4.93	1.43	1.37
20	A	829	CLA	MG-NB	-4.92	1.96	2.05
20	B	830	CLA	C1D-ND	4.92	1.43	1.37
20	A	831	CLA	MG-ND	-4.92	1.96	2.05
20	7	1007	CLA	MG-ND	-4.92	1.96	2.05
20	B	850	CLA	MG-NB	-4.92	1.96	2.05
20	0	307	CLA	MG-NB	-4.90	1.96	2.05
20	0	313	CLA	MG-NB	-4.90	1.96	2.05
20	A	832	CLA	MG-ND	-4.90	1.96	2.05
20	A	836	CLA	MG-NB	-4.89	1.96	2.05
20	1	1003	CLA	C1D-ND	4.89	1.43	1.37
20	B	821	CLA	MG-ND	-4.89	1.96	2.05
20	3	1010	CLA	MG-ND	-4.89	1.96	2.05
20	B	834	CLA	C1D-ND	4.88	1.43	1.37
29	5	317	CHL	MG-NB	-4.88	1.96	2.05
20	4	305	CLA	C1B-NB	4.88	1.43	1.37
20	4	307	CLA	MG-NA	-4.87	1.94	2.06
20	1	1017	CLA	C1D-ND	4.87	1.43	1.37
20	B	835	CLA	MG-ND	-4.87	1.96	2.05
29	4	313	CHL	MG-NC	-4.86	1.94	2.06
20	A	807	CLA	MG-NB	-4.86	1.96	2.05
20	A	837	CLA	MG-NB	-4.85	1.96	2.05
20	5	301	CLA	MG-ND	-4.85	1.96	2.05
20	A	814	CLA	MG-ND	-4.85	1.96	2.05
20	G	203	CLA	C1D-ND	4.84	1.43	1.37
20	A	834	CLA	MG-ND	-4.84	1.96	2.05
20	1	1006	CLA	MG-NC	-4.84	1.94	2.06
20	3	1007	CLA	MG-NB	-4.84	1.96	2.05
20	B	806	CLA	MG-NB	-4.83	1.96	2.05
20	1	1004	CLA	MG-NB	-4.83	1.96	2.05
20	G	202	CLA	MG-NB	-4.82	1.96	2.05
20	A	824	CLA	MG-ND	-4.81	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	1013	CHL	MG-NC	-4.81	1.94	2.06
20	3	1006	CLA	MG-NB	-4.80	1.96	2.05
20	4	306	CLA	MG-NB	-4.80	1.96	2.05
20	7	1010	CLA	MG-NA	-4.80	1.94	2.06
20	A	818	CLA	MG-NB	-4.79	1.96	2.05
20	3	1011	CLA	MG-NB	-4.79	1.96	2.05
20	A	819	CLA	MG-NB	-4.79	1.96	2.05
20	3	1013	CLA	C1D-ND	4.79	1.43	1.37
20	8	316	CLA	MG-ND	-4.79	1.96	2.05
20	0	310	CLA	MG-ND	-4.79	1.96	2.05
20	B	825	CLA	MG-ND	-4.78	1.96	2.05
20	5	322	CLA	MG-NB	-4.77	1.96	2.05
20	B	837	CLA	C1D-ND	4.77	1.43	1.37
20	B	831	CLA	MG-ND	-4.77	1.96	2.05
20	B	826	CLA	MG-NB	-4.77	1.96	2.05
20	B	841	CLA	MG-NB	-4.76	1.96	2.05
20	B	840	CLA	MG-NB	-4.76	1.96	2.05
20	5	304	CLA	MG-NA	-4.76	1.95	2.06
29	6	313	CHL	MG-NB	-4.75	1.96	2.05
20	A	827	CLA	MG-NB	-4.75	1.96	2.05
20	0	308	CLA	MG-ND	-4.75	1.96	2.05
20	6	301	CLA	MG-NB	-4.75	1.96	2.05
20	A	826	CLA	C1D-ND	4.75	1.43	1.37
20	6	305	CLA	MG-ND	-4.75	1.96	2.05
30	7	1002	XAT	C34-C33	4.75	1.42	1.35
20	A	812	CLA	C1D-ND	4.74	1.43	1.37
20	B	820	CLA	MG-NB	-4.74	1.96	2.05
20	L	202	CLA	MG-NB	-4.74	1.96	2.05
20	A	816	CLA	C1D-ND	4.74	1.43	1.37
20	A	805	CLA	MG-NB	-4.74	1.96	2.05
20	A	824	CLA	MG-NB	-4.74	1.96	2.05
20	0	311	CLA	MG-NB	-4.73	1.96	2.05
20	6	309	CLA	MG-ND	-4.73	1.96	2.05
20	A	852	CLA	MG-NB	-4.73	1.96	2.05
20	B	801	CLA	MG-ND	-4.73	1.96	2.05
20	A	809	CLA	MG-NB	-4.73	1.96	2.05
20	B	820	CLA	MG-ND	-4.72	1.96	2.05
20	3	1017	CLA	MG-NB	-4.71	1.96	2.05
20	4	310	CLA	C1B-NB	4.71	1.43	1.37
20	4	308	CLA	MG-NB	-4.71	1.96	2.05
20	G	201	CLA	MG-NB	-4.71	1.96	2.05
20	1	1010	CLA	MG-ND	-4.71	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	827	CLA	MG-ND	-4.70	1.96	2.05
20	0	310	CLA	MG-NB	-4.70	1.96	2.05
20	G	202	CLA	C1D-ND	4.69	1.43	1.37
20	A	831	CLA	C1D-ND	4.69	1.43	1.37
20	F	303	CLA	MG-ND	-4.68	1.96	2.05
20	1	1017	CLA	MG-ND	-4.68	1.96	2.05
20	8	311	CLA	MG-NA	-4.68	1.95	2.06
20	B	823	CLA	C1B-NB	4.68	1.43	1.37
20	A	851	CLA	MG-NB	-4.67	1.96	2.05
20	A	828	CLA	MG-NB	-4.67	1.96	2.05
20	B	814	CLA	C1D-ND	4.67	1.43	1.37
20	B	817	CLA	MG-NB	-4.67	1.96	2.05
20	5	307	CLA	MG-ND	-4.67	1.96	2.05
20	A	801	CLA	MG-NA	-4.67	1.95	2.06
20	A	812	CLA	MG-NB	-4.66	1.96	2.05
20	B	810	CLA	C1D-ND	4.66	1.43	1.37
20	B	828	CLA	C1D-ND	4.66	1.43	1.37
20	A	852	CLA	C1D-ND	4.66	1.43	1.37
20	B	814	CLA	MG-NB	-4.66	1.96	2.05
20	0	309	CLA	MG-ND	-4.65	1.96	2.05
20	A	829	CLA	MG-ND	-4.65	1.96	2.05
20	8	306	CLA	MG-NB	-4.65	1.96	2.05
20	A	821	CLA	MG-ND	-4.65	1.96	2.05
20	A	851	CLA	MG-ND	-4.65	1.96	2.05
20	3	1009	CLA	MG-NB	-4.64	1.96	2.05
20	G	201	CLA	C1D-ND	4.64	1.43	1.37
20	B	824	CLA	C1D-ND	4.63	1.43	1.37
20	B	824	CLA	MG-ND	-4.63	1.96	2.05
20	0	316	CLA	MG-ND	-4.63	1.96	2.05
20	A	813	CLA	MG-ND	-4.63	1.96	2.05
20	5	301	CLA	MG-NA	-4.62	1.95	2.06
20	A	834	CLA	C1D-ND	4.61	1.43	1.37
29	8	315	CHL	MG-ND	-4.61	1.96	2.05
20	4	310	CLA	C1D-ND	4.61	1.43	1.37
20	6	307	CLA	MG-ND	-4.61	1.96	2.05
20	F	302	CLA	MG-NB	-4.61	1.96	2.05
20	5	306	CLA	MG-NB	-4.61	1.96	2.05
20	A	822	CLA	MG-NB	-4.60	1.96	2.05
20	J	102	CLA	C1D-ND	4.60	1.43	1.37
20	1	1005	CLA	C1D-ND	4.60	1.43	1.37
20	3	1007	CLA	MG-ND	-4.59	1.96	2.05
20	8	305	CLA	MG-NA	-4.58	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	840	CLA	MG-NB	-4.58	1.96	2.05
20	A	817	CLA	C1D-ND	4.58	1.43	1.37
20	A	830	CLA	C1D-ND	4.58	1.43	1.37
20	J	102	CLA	MG-ND	-4.58	1.96	2.05
20	A	828	CLA	MG-ND	-4.57	1.96	2.05
20	4	304	CLA	MG-ND	-4.57	1.96	2.05
20	B	811	CLA	MG-ND	-4.57	1.96	2.05
20	A	810	CLA	C1D-ND	4.57	1.43	1.37
20	6	309	CLA	MG-NB	-4.56	1.96	2.05
20	B	829	CLA	C1D-ND	4.56	1.43	1.37
20	A	835	CLA	MG-NB	-4.56	1.96	2.05
20	F	305	CLA	MG-ND	-4.55	1.96	2.05
20	1	1008	CLA	MG-ND	-4.55	1.96	2.05
20	8	308	CLA	MG-ND	-4.55	1.96	2.05
29	6	314	CHL	MG-NC	-4.55	1.95	2.06
20	A	840	CLA	MG-NC	-4.55	1.95	2.06
20	0	301	CLA	MG-NB	-4.55	1.96	2.05
20	L	201	CLA	MG-NB	-4.54	1.96	2.05
20	A	808	CLA	MG-NB	-4.54	1.96	2.05
20	A	804	CLA	MG-NB	-4.54	1.96	2.05
29	1	1013	CHL	MG-NA	-4.54	1.95	2.06
20	B	835	CLA	MG-NB	-4.54	1.96	2.05
25	5	319	DGD	O2G-C1B	4.53	1.47	1.34
20	A	824	CLA	C1D-ND	4.53	1.43	1.37
20	B	813	CLA	C1B-NB	4.53	1.43	1.37
20	A	809	CLA	C1D-ND	4.53	1.43	1.37
20	K	201	CLA	C1B-NB	4.53	1.43	1.37
20	0	316	CLA	C1D-ND	4.52	1.43	1.37
20	1	1011	CLA	C1D-ND	4.52	1.43	1.37
20	5	310	CLA	MG-ND	-4.52	1.96	2.05
20	6	305	CLA	MG-NA	-4.51	1.95	2.06
20	6	308	CLA	MG-ND	-4.51	1.96	2.05
20	5	308	CLA	MG-ND	-4.50	1.96	2.05
20	A	823	CLA	C1D-ND	4.50	1.43	1.37
20	B	811	CLA	MG-NA	-4.50	1.95	2.06
20	A	818	CLA	C1D-ND	4.50	1.43	1.37
20	7	1008	CLA	MG-ND	-4.50	1.96	2.05
20	A	815	CLA	MG-NA	-4.50	1.95	2.06
20	B	816	CLA	MG-ND	-4.49	1.96	2.05
29	8	315	CHL	MG-NA	-4.49	1.95	2.06
20	A	829	CLA	C1D-ND	4.49	1.43	1.37
20	3	1017	CLA	MG-ND	-4.49	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	816	CLA	C1D-ND	4.49	1.43	1.37
20	7	1014	CLA	MG-NB	-4.49	1.96	2.05
20	B	815	CLA	MG-NB	-4.48	1.96	2.05
20	A	802	CLA	C1D-ND	4.48	1.43	1.37
20	5	312	CLA	MG-NB	-4.48	1.96	2.05
20	K	202	CLA	MG-NB	-4.47	1.96	2.05
29	1	1015	CHL	C1D-ND	4.47	1.43	1.37
30	7	1002	XAT	C14-C13	4.47	1.41	1.35
20	8	311	CLA	C1D-ND	4.47	1.43	1.37
20	3	1011	CLA	C1D-ND	4.47	1.43	1.37
20	A	813	CLA	MG-NB	-4.46	1.96	2.05
29	5	313	CHL	MG-NB	-4.46	1.96	2.05
20	8	309	CLA	C1B-NB	4.46	1.43	1.37
20	A	804	CLA	MG-ND	-4.46	1.96	2.05
20	B	838	CLA	C1D-ND	4.45	1.43	1.37
20	6	308	CLA	MG-NA	-4.45	1.95	2.06
20	F	302	CLA	C1D-ND	4.45	1.43	1.37
20	6	315	CLA	MG-NB	-4.45	1.97	2.05
20	7	1005	CLA	MG-NA	-4.45	1.95	2.06
20	5	322	CLA	C1D-ND	4.44	1.43	1.37
29	5	313	CHL	C1D-ND	4.44	1.43	1.37
20	5	304	CLA	MG-NB	-4.43	1.97	2.05
20	B	812	CLA	MG-NB	-4.43	1.97	2.05
20	B	806	CLA	MG-ND	-4.43	1.97	2.05
20	F	302	CLA	C1C-C2C	4.43	1.53	1.44
20	A	830	CLA	MG-ND	-4.43	1.97	2.05
20	B	818	CLA	C1D-ND	4.42	1.43	1.37
20	5	321	CLA	MG-NC	-4.42	1.95	2.06
20	6	311	CLA	C1D-ND	4.42	1.43	1.37
20	A	815	CLA	MG-NC	-4.42	1.95	2.06
20	A	811	CLA	MG-ND	-4.42	1.97	2.05
20	6	320	CLA	MG-NB	-4.42	1.97	2.05
30	8	304	XAT	C10-C9	4.41	1.41	1.35
20	3	1017	CLA	C1D-ND	4.41	1.43	1.37
20	6	318	CLA	C1B-NB	4.40	1.43	1.37
20	A	836	CLA	MG-ND	-4.40	1.97	2.05
20	1	1006	CLA	MG-NA	-4.40	1.95	2.06
29	8	314	CHL	MG-ND	-4.40	1.97	2.05
20	B	803	CLA	C1D-ND	4.39	1.43	1.37
20	B	812	CLA	MG-ND	-4.39	1.97	2.05
20	J	102	CLA	C1B-NB	4.39	1.43	1.37
20	L	202	CLA	C1D-ND	4.39	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	837	CLA	MG-ND	-4.38	1.97	2.05
20	5	306	CLA	C1D-ND	4.38	1.43	1.37
20	A	825	CLA	MG-ND	-4.38	1.97	2.05
20	A	807	CLA	MG-ND	-4.38	1.97	2.05
20	A	830	CLA	MG-NB	-4.38	1.97	2.05
20	3	1015	CLA	C1D-ND	4.38	1.43	1.37
20	A	823	CLA	MG-ND	-4.37	1.97	2.05
20	1	1014	CLA	MG-NC	-4.37	1.95	2.06
20	B	826	CLA	MG-ND	-4.37	1.97	2.05
20	0	306	CLA	MG-ND	-4.37	1.97	2.05
20	1	1017	CLA	MG-NB	-4.36	1.97	2.05
30	8	304	XAT	C14-C13	4.36	1.41	1.35
20	4	306	CLA	MG-ND	-4.36	1.97	2.05
20	3	1016	CLA	MG-NC	-4.36	1.95	2.06
20	0	307	CLA	MG-ND	-4.36	1.97	2.05
29	6	316	CHL	MG-NA	-4.36	1.95	2.06
29	8	317	CHL	C1D-ND	4.36	1.43	1.37
20	6	306	CLA	C1D-ND	4.35	1.43	1.37
20	B	813	CLA	MG-ND	-4.35	1.97	2.05
20	B	825	CLA	C1D-ND	4.34	1.43	1.37
20	B	829	CLA	MG-ND	-4.34	1.97	2.05
20	8	306	CLA	MG-ND	-4.34	1.97	2.05
20	A	805	CLA	MG-ND	-4.34	1.97	2.05
20	6	310	CLA	MG-ND	-4.34	1.97	2.05
20	5	312	CLA	MG-NA	-4.34	1.96	2.06
25	5	319	DGD	O1G-C1A	4.34	1.46	1.33
20	0	305	CLA	MG-ND	-4.33	1.97	2.05
20	3	1015	CLA	MG-NB	-4.33	1.97	2.05
20	A	806	CLA	MG-ND	-4.33	1.97	2.05
20	A	852	CLA	MG-ND	-4.33	1.97	2.05
20	0	309	CLA	MG-NA	-4.33	1.96	2.06
20	8	309	CLA	MG-NB	-4.32	1.97	2.05
20	3	1012	CLA	MG-ND	-4.32	1.97	2.05
20	B	832	CLA	MG-NB	-4.32	1.97	2.05
29	6	316	CHL	MG-NC	-4.32	1.96	2.06
20	5	315	CLA	MG-NA	-4.32	1.96	2.06
30	8	304	XAT	C34-C33	4.32	1.41	1.35
20	A	820	CLA	MG-ND	-4.32	1.97	2.05
20	B	835	CLA	C1D-ND	4.32	1.43	1.37
20	1	1017	CLA	MG-NA	-4.32	1.96	2.06
20	A	835	CLA	MG-ND	-4.31	1.97	2.05
20	A	840	CLA	C1D-ND	4.31	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	1008	CLA	MG-NB	-4.31	1.97	2.05
20	6	315	CLA	MG-NA	-4.31	1.96	2.06
20	A	816	CLA	MG-ND	-4.30	1.97	2.05
20	B	813	CLA	MG-NB	-4.30	1.97	2.05
20	B	820	CLA	C1D-ND	4.30	1.43	1.37
20	3	1012	CLA	C1D-ND	4.30	1.43	1.37
20	A	825	CLA	MG-NB	-4.30	1.97	2.05
20	B	833	CLA	C1D-ND	4.29	1.43	1.37
20	A	805	CLA	C1D-ND	4.29	1.43	1.37
20	3	1013	CLA	MG-ND	-4.29	1.97	2.05
20	A	835	CLA	C1D-ND	4.29	1.43	1.37
20	B	837	CLA	MG-NB	-4.29	1.97	2.05
20	5	311	CLA	C1D-ND	4.29	1.43	1.37
20	5	312	CLA	MG-NC	-4.28	1.96	2.06
20	B	838	CLA	MG-NB	-4.28	1.97	2.05
20	B	819	CLA	MG-ND	-4.27	1.97	2.05
20	A	801	CLA	C1D-ND	4.27	1.43	1.37
20	B	826	CLA	C1D-ND	4.27	1.43	1.37
20	1	1010	CLA	C1D-ND	4.27	1.43	1.37
20	8	305	CLA	MG-ND	-4.26	1.97	2.05
25	B	848	DGD	O1G-C1A	4.26	1.45	1.33
20	5	306	CLA	MG-NA	-4.26	1.96	2.06
20	A	840	CLA	MG-NA	-4.26	1.96	2.06
30	8	304	XAT	C30-C29	4.26	1.41	1.35
20	5	315	CLA	MG-NB	-4.25	1.97	2.05
20	A	821	CLA	C1D-ND	4.25	1.43	1.37
20	B	829	CLA	MG-NA	-4.25	1.96	2.06
20	A	817	CLA	C1B-NB	4.25	1.43	1.37
20	L	204	CLA	C1B-NB	4.24	1.43	1.37
20	5	311	CLA	C1B-NB	4.24	1.43	1.37
20	A	822	CLA	C1D-ND	4.24	1.43	1.37
20	B	818	CLA	MG-ND	-4.23	1.97	2.05
20	B	808	CLA	MG-NB	-4.23	1.97	2.05
20	B	839	CLA	MG-NC	-4.23	1.96	2.06
29	4	315	CHL	MG-NA	-4.23	1.96	2.06
20	A	806	CLA	C1D-ND	4.22	1.43	1.37
20	7	1014	CLA	MG-ND	-4.22	1.97	2.05
20	8	312	CLA	MG-NB	-4.22	1.97	2.05
20	6	310	CLA	MG-NC	-4.22	1.96	2.06
20	0	306	CLA	MG-NB	-4.22	1.97	2.05
20	1	1011	CLA	MG-NA	-4.21	1.96	2.06
20	A	817	CLA	MG-ND	-4.21	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	314	CHL	C1D-ND	4.21	1.43	1.37
20	3	1008	CLA	MG-ND	-4.21	1.97	2.05
20	4	311	CLA	MG-ND	-4.21	1.97	2.05
20	4	304	CLA	MG-NB	-4.21	1.97	2.05
20	B	810	CLA	MG-ND	-4.21	1.97	2.05
20	3	1010	CLA	MG-NC	-4.20	1.96	2.06
20	3	1009	CLA	C1D-ND	4.20	1.42	1.37
20	3	1016	CLA	MG-NA	-4.20	1.96	2.06
20	J	102	CLA	MG-NB	-4.20	1.97	2.05
20	B	816	CLA	MG-NB	-4.20	1.97	2.05
20	A	819	CLA	MG-ND	-4.18	1.97	2.05
30	7	1002	XAT	C30-C29	4.18	1.41	1.35
20	A	808	CLA	MG-ND	-4.18	1.97	2.05
20	4	308	CLA	MG-ND	-4.18	1.97	2.05
20	B	827	CLA	MG-NA	-4.18	1.96	2.06
20	A	826	CLA	MG-NB	-4.18	1.97	2.05
20	A	819	CLA	C1D-ND	4.18	1.42	1.37
20	1	1007	CLA	MG-NC	-4.17	1.96	2.06
20	A	832	CLA	MG-NA	-4.17	1.96	2.06
20	5	315	CLA	MG-NC	-4.16	1.96	2.06
20	A	822	CLA	MG-ND	-4.16	1.97	2.05
29	4	312	CHL	C1D-ND	4.16	1.42	1.37
30	7	1002	XAT	C10-C9	4.16	1.41	1.35
20	B	838	CLA	MG-ND	-4.16	1.97	2.05
20	3	1009	CLA	MG-ND	-4.15	1.97	2.05
20	B	828	CLA	MG-ND	-4.15	1.97	2.05
20	7	1010	CLA	MG-ND	-4.15	1.97	2.05
20	1	1009	CLA	MG-NB	-4.15	1.97	2.05
20	4	305	CLA	MG-ND	-4.15	1.97	2.05
20	3	1007	CLA	C1D-ND	4.15	1.42	1.37
20	A	833	CLA	MG-NB	-4.14	1.97	2.05
20	A	811	CLA	C1D-ND	4.14	1.42	1.37
20	7	1011	CLA	MG-NA	-4.14	1.96	2.06
20	B	839	CLA	MG-ND	-4.13	1.97	2.05
20	6	301	CLA	MG-ND	-4.13	1.97	2.05
20	5	307	CLA	C1D-ND	4.13	1.42	1.37
20	B	850	CLA	C1D-ND	4.13	1.42	1.37
20	5	305	CLA	C1B-NB	4.13	1.42	1.37
20	A	840	CLA	MG-ND	-4.13	1.97	2.05
20	0	309	CLA	C1D-ND	4.12	1.42	1.37
20	A	802	CLA	MG-ND	-4.12	1.97	2.05
20	B	811	CLA	MG-NC	-4.12	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	836	CLA	C1D-ND	4.12	1.42	1.37
20	0	306	CLA	C1D-ND	4.11	1.42	1.37
20	6	307	CLA	MG-NA	-4.11	1.96	2.06
20	B	817	CLA	MG-ND	-4.10	1.97	2.05
20	A	801	CLA	MG-NC	-4.10	1.96	2.06
20	A	851	CLA	MG-NA	-4.10	1.96	2.06
20	G	202	CLA	C1B-NB	4.09	1.42	1.37
20	A	816	CLA	MG-NA	-4.09	1.96	2.06
20	B	819	CLA	C1D-ND	4.08	1.42	1.37
20	4	307	CLA	MG-NC	-4.08	1.96	2.06
20	B	832	CLA	C1D-ND	4.08	1.42	1.37
20	4	309	CLA	MG-NB	-4.07	1.97	2.05
20	1	1017	CLA	MG-NC	-4.07	1.96	2.06
20	F	305	CLA	MG-NA	-4.07	1.96	2.06
20	B	807	CLA	MG-ND	-4.07	1.97	2.05
20	3	1005	CLA	MG-ND	-4.07	1.97	2.05
20	3	1011	CLA	C1B-NB	4.07	1.42	1.37
29	5	316	CHL	C1D-ND	4.07	1.42	1.37
20	B	822	CLA	MG-NA	-4.07	1.96	2.06
20	6	306	CLA	MG-ND	-4.06	1.97	2.05
20	F	303	CLA	MG-NA	-4.06	1.96	2.06
20	A	803	CLA	MG-NB	-4.06	1.97	2.05
20	B	817	CLA	MG-NA	-4.05	1.96	2.06
20	A	832	CLA	MG-NB	-4.05	1.97	2.05
20	B	823	CLA	MG-NB	-4.05	1.97	2.05
20	7	1009	CLA	MG-ND	-4.05	1.97	2.05
20	B	850	CLA	MG-ND	-4.05	1.97	2.05
20	4	308	CLA	C1B-NB	4.05	1.42	1.37
20	6	320	CLA	MG-NA	-4.05	1.96	2.06
29	0	317	CHL	C1D-ND	4.04	1.42	1.37
20	A	807	CLA	C1D-ND	4.04	1.42	1.37
20	1	1004	CLA	C1D-ND	4.04	1.42	1.37
20	L	203	CLA	C1B-NB	4.04	1.42	1.37
20	A	819	CLA	MG-NA	-4.04	1.96	2.06
20	0	307	CLA	MG-NA	-4.03	1.96	2.06
20	B	808	CLA	C1D-ND	4.03	1.42	1.37
20	8	311	CLA	MG-ND	-4.03	1.97	2.05
20	0	309	CLA	MG-NC	-4.03	1.96	2.06
20	1	1003	CLA	C1B-NB	4.02	1.42	1.37
29	0	315	CHL	C1D-ND	4.02	1.42	1.37
29	1	1012	CHL	C2C-C1C	4.02	1.52	1.44
20	7	1009	CLA	MG-NC	-4.02	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	1013	CHL	C1D-ND	4.01	1.42	1.37
20	1	1009	CLA	C1D-ND	4.01	1.42	1.37
20	0	305	CLA	MG-NC	-4.01	1.96	2.06
20	B	812	CLA	C1D-ND	4.00	1.42	1.37
20	A	811	CLA	C1B-NB	4.00	1.42	1.37
20	8	313	CLA	MG-NA	-4.00	1.96	2.06
20	A	809	CLA	MG-ND	-4.00	1.97	2.05
20	B	830	CLA	MG-ND	-3.99	1.97	2.05
20	G	202	CLA	MG-ND	-3.99	1.97	2.05
20	A	823	CLA	MG-NA	-3.99	1.96	2.06
29	6	317	CHL	MG-NA	-3.99	1.96	2.06
20	B	834	CLA	MG-ND	-3.98	1.97	2.05
20	1	1008	CLA	MG-NB	-3.98	1.97	2.05
20	0	301	CLA	MG-ND	-3.97	1.97	2.05
20	B	821	CLA	MG-NC	-3.97	1.96	2.06
20	8	307	CLA	C1D-ND	3.97	1.42	1.37
20	B	817	CLA	C1D-ND	3.97	1.42	1.37
20	4	311	CLA	MG-NB	-3.97	1.97	2.05
20	5	318	CLA	MG-NC	-3.96	1.96	2.06
29	1	1012	CHL	C1D-ND	3.96	1.42	1.37
20	0	308	CLA	MG-NA	-3.96	1.96	2.06
20	B	833	CLA	MG-ND	-3.95	1.98	2.05
20	A	825	CLA	C1D-ND	3.95	1.42	1.37
20	A	801	CLA	MG-NB	-3.94	1.98	2.05
20	6	318	CLA	MG-ND	-3.94	1.98	2.05
20	6	307	CLA	MG-NC	-3.94	1.96	2.06
20	B	809	CLA	MG-ND	-3.94	1.98	2.05
20	A	808	CLA	MG-NA	-3.93	1.96	2.06
20	B	850	CLA	MG-NA	-3.93	1.96	2.06
20	A	820	CLA	MG-NA	-3.93	1.96	2.06
20	B	805	CLA	MG-ND	-3.93	1.98	2.05
20	5	312	CLA	C1D-ND	3.92	1.42	1.37
20	5	306	CLA	MG-ND	-3.92	1.98	2.05
20	A	839	CLA	MG-NA	-3.92	1.97	2.06
20	7	1014	CLA	MG-NA	-3.92	1.97	2.06
20	A	829	CLA	MG-NA	-3.91	1.97	2.06
20	1	1014	CLA	C1D-ND	3.91	1.42	1.37
29	6	317	CHL	MG-NC	-3.91	1.97	2.06
20	A	833	CLA	C1D-ND	3.91	1.42	1.37
20	0	305	CLA	C1D-ND	3.90	1.42	1.37
20	B	808	CLA	MG-ND	-3.90	1.98	2.05
20	B	830	CLA	C1B-NB	3.90	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	819	CLA	MG-NC	-3.90	1.97	2.06
20	A	805	CLA	MG-NA	-3.90	1.97	2.06
20	4	310	CLA	MG-ND	-3.89	1.98	2.05
29	4	312	CHL	MG-NC	-3.88	1.97	2.06
20	7	1008	CLA	C1D-ND	3.88	1.42	1.37
20	3	1011	CLA	MG-ND	-3.88	1.98	2.05
20	A	836	CLA	C1D-ND	3.88	1.42	1.37
20	4	314	CLA	MG-NA	-3.88	1.97	2.06
20	7	1006	CLA	MG-NA	-3.88	1.97	2.06
20	A	820	CLA	MG-NC	-3.87	1.97	2.06
20	A	804	CLA	C1D-ND	3.87	1.42	1.37
20	1	1007	CLA	MG-NA	-3.87	1.97	2.06
29	6	313	CHL	MG-NC	-3.86	1.97	2.06
20	A	818	CLA	MG-ND	-3.86	1.98	2.05
20	G	201	CLA	MG-ND	-3.86	1.98	2.05
20	B	841	CLA	MG-NC	-3.86	1.97	2.06
25	B	848	DGD	O2G-C1B	3.86	1.45	1.34
20	B	813	CLA	C1C-C2C	3.86	1.52	1.44
20	1	1011	CLA	MG-NC	-3.85	1.97	2.06
20	B	811	CLA	C1D-ND	3.85	1.42	1.37
20	A	818	CLA	MG-NC	-3.85	1.97	2.06
20	A	811	CLA	MG-NC	-3.84	1.97	2.06
20	7	1014	CLA	C1D-ND	3.84	1.42	1.37
20	6	312	CLA	MG-ND	-3.84	1.98	2.05
20	1	1011	CLA	MG-ND	-3.84	1.98	2.05
20	1	1005	CLA	MG-ND	-3.84	1.98	2.05
20	3	1007	CLA	MG-NC	-3.84	1.97	2.06
29	7	1013	CHL	MG-NA	-3.84	1.97	2.06
20	A	807	CLA	MG-NC	-3.84	1.97	2.06
20	A	825	CLA	MG-NA	-3.83	1.97	2.06
20	A	823	CLA	MG-NC	-3.83	1.97	2.06
20	0	312	CLA	MG-ND	-3.83	1.98	2.05
20	A	826	CLA	MG-NA	-3.83	1.97	2.06
20	B	814	CLA	MG-ND	-3.83	1.98	2.05
20	7	1004	CLA	MG-NA	-3.83	1.97	2.06
29	1	1013	CHL	MG-NC	-3.82	1.97	2.06
20	0	312	CLA	MG-NC	-3.82	1.97	2.06
20	F	305	CLA	C1D-ND	3.82	1.42	1.37
20	A	851	CLA	C1D-ND	3.82	1.42	1.37
20	A	835	CLA	MG-NA	-3.82	1.97	2.06
29	5	316	CHL	MG-NA	-3.82	1.97	2.06
20	A	839	CLA	MG-ND	-3.82	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	808	CLA	C1D-ND	3.82	1.42	1.37
20	8	310	CLA	MG-NA	-3.82	1.97	2.06
29	5	317	CHL	MG-NC	-3.82	1.97	2.06
20	A	803	CLA	C1B-NB	3.81	1.42	1.37
20	5	308	CLA	MG-NA	-3.81	1.97	2.06
20	A	811	CLA	MG-NB	-3.81	1.98	2.05
20	5	323	CLA	MG-NC	-3.81	1.97	2.06
20	L	204	CLA	MG-NB	-3.81	1.98	2.05
29	0	314	CHL	C1D-ND	3.81	1.42	1.37
29	8	314	CHL	MG-NC	-3.80	1.97	2.06
20	A	820	CLA	C1D-ND	3.80	1.42	1.37
20	8	307	CLA	C1C-NC	-3.79	1.32	1.37
20	B	820	CLA	MG-NC	-3.79	1.97	2.06
20	F	303	CLA	MG-NC	-3.79	1.97	2.06
20	L	202	CLA	MG-ND	-3.79	1.98	2.05
20	7	1008	CLA	MG-NA	-3.78	1.97	2.06
20	5	322	CLA	MG-ND	-3.78	1.98	2.05
20	8	308	CLA	MG-NA	-3.78	1.97	2.06
20	B	831	CLA	MG-NC	-3.78	1.97	2.06
20	1	1009	CLA	MG-ND	-3.78	1.98	2.05
29	4	316	CHL	MG-NC	-3.78	1.97	2.06
20	3	1010	CLA	MG-NA	-3.78	1.97	2.06
20	B	822	CLA	MG-NC	-3.77	1.97	2.06
20	L	201	CLA	MG-NA	-3.77	1.97	2.06
20	B	850	CLA	MG-NC	-3.77	1.97	2.06
20	B	834	CLA	MG-NA	-3.77	1.97	2.06
29	6	317	CHL	C1D-ND	3.77	1.42	1.37
20	1	1007	CLA	MG-NB	-3.77	1.98	2.05
29	4	315	CHL	MG-NC	-3.77	1.97	2.06
20	0	313	CLA	MG-NA	-3.77	1.97	2.06
20	L	201	CLA	C1B-NB	3.77	1.42	1.37
20	5	323	CLA	MG-ND	-3.77	1.98	2.05
20	0	316	CLA	MG-NC	-3.76	1.97	2.06
20	B	836	CLA	MG-NA	-3.76	1.97	2.06
20	A	838	CLA	MG-NC	-3.76	1.97	2.06
20	A	824	CLA	MG-NA	-3.76	1.97	2.06
20	4	311	CLA	MG-NC	-3.76	1.97	2.06
20	0	312	CLA	MG-NA	-3.75	1.97	2.06
20	8	307	CLA	MG-NA	-3.75	1.97	2.06
20	5	301	CLA	C1D-ND	3.75	1.42	1.37
29	7	1012	CHL	MG-NA	-3.75	1.97	2.06
20	A	810	CLA	MG-NA	-3.75	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	815	CLA	C1D-ND	3.75	1.42	1.37
20	B	815	CLA	C1B-NB	3.75	1.42	1.37
20	3	1008	CLA	MG-NC	-3.75	1.97	2.06
20	4	305	CLA	MG-NB	-3.74	1.98	2.05
20	A	803	CLA	MG-ND	-3.74	1.98	2.05
20	6	301	CLA	C1D-ND	3.73	1.42	1.37
20	8	306	CLA	C1C-C2C	3.73	1.51	1.44
20	3	1016	CLA	C1D-ND	3.73	1.42	1.37
20	A	802	CLA	MG-NC	-3.73	1.97	2.06
20	B	806	CLA	C1D-ND	3.73	1.42	1.37
20	4	309	CLA	C1B-NB	3.72	1.42	1.37
20	5	307	CLA	MG-NC	-3.71	1.97	2.06
20	B	838	CLA	C1B-NB	3.71	1.42	1.37
20	B	808	CLA	MG-NA	-3.71	1.97	2.06
20	5	310	CLA	C1B-NB	3.71	1.42	1.37
20	0	308	CLA	MG-NC	-3.70	1.97	2.06
20	8	306	CLA	MG-NC	-3.70	1.97	2.06
20	1	1005	CLA	MG-NA	-3.70	1.97	2.06
20	0	313	CLA	MG-ND	-3.70	1.98	2.05
20	3	1006	CLA	MG-ND	-3.70	1.98	2.05
20	8	308	CLA	C1D-ND	3.70	1.42	1.37
20	5	322	CLA	MG-NA	-3.70	1.97	2.06
20	A	803	CLA	C1D-ND	3.70	1.42	1.37
20	A	812	CLA	MG-ND	-3.70	1.98	2.05
20	8	313	CLA	MG-ND	-3.69	1.98	2.05
20	3	1012	CLA	MG-NA	-3.69	1.97	2.06
20	5	310	CLA	MG-NB	-3.69	1.98	2.05
20	B	833	CLA	MG-NB	-3.69	1.98	2.05
20	L	203	CLA	MG-ND	-3.69	1.98	2.05
20	B	821	CLA	MG-NA	-3.69	1.97	2.06
20	B	841	CLA	C1B-NB	3.69	1.42	1.37
20	B	827	CLA	MG-NC	-3.68	1.97	2.06
20	0	305	CLA	C1B-NB	3.68	1.42	1.37
20	A	810	CLA	MG-NC	-3.67	1.97	2.06
20	6	311	CLA	C1B-NB	3.67	1.42	1.37
20	G	203	CLA	MG-NB	-3.67	1.98	2.05
20	5	310	CLA	MG-NA	-3.67	1.97	2.06
20	A	836	CLA	MG-NA	-3.67	1.97	2.06
20	K	202	CLA	MG-ND	-3.67	1.98	2.05
20	5	308	CLA	MG-NC	-3.66	1.97	2.06
20	3	1017	CLA	MG-NA	-3.66	1.97	2.06
20	A	802	CLA	MG-NA	-3.65	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	807	CLA	MG-NA	-3.65	1.97	2.06
20	1	1005	CLA	MG-NC	-3.65	1.97	2.06
20	4	309	CLA	MG-ND	-3.64	1.98	2.05
20	1	1009	CLA	MG-NA	-3.64	1.97	2.06
20	B	831	CLA	MG-NA	-3.64	1.97	2.06
20	B	809	CLA	MG-NA	-3.64	1.97	2.06
20	B	840	CLA	MG-NA	-3.64	1.97	2.06
20	0	310	CLA	MG-NA	-3.63	1.97	2.06
20	A	831	CLA	C1B-NB	3.63	1.42	1.37
20	3	1015	CLA	MG-ND	-3.63	1.98	2.05
20	5	318	CLA	MG-ND	-3.63	1.98	2.05
20	3	1009	CLA	MG-NA	-3.62	1.97	2.06
29	8	315	CHL	MG-NC	-3.62	1.97	2.06
20	B	824	CLA	MG-NC	-3.62	1.97	2.06
20	B	815	CLA	MG-NC	-3.62	1.97	2.06
20	A	822	CLA	MG-NC	-3.62	1.97	2.06
20	B	806	CLA	MG-NC	-3.61	1.97	2.06
20	0	307	CLA	C1B-NB	3.61	1.42	1.37
20	L	201	CLA	MG-NC	-3.61	1.97	2.06
20	B	816	CLA	C1B-NB	3.60	1.42	1.37
20	L	201	CLA	MG-ND	-3.60	1.98	2.05
20	G	201	CLA	C1B-NB	3.60	1.42	1.37
20	K	201	CLA	MG-NB	-3.59	1.98	2.05
20	0	306	CLA	MG-NC	-3.59	1.97	2.06
20	3	1005	CLA	MG-NA	-3.59	1.97	2.06
20	A	835	CLA	C1B-NB	3.59	1.42	1.37
20	6	315	CLA	MG-ND	-3.58	1.98	2.05
20	3	1008	CLA	MG-NA	-3.58	1.97	2.06
20	3	1008	CLA	C1D-ND	3.58	1.42	1.37
20	A	826	CLA	C1B-NB	3.58	1.42	1.37
20	0	307	CLA	MG-NC	-3.57	1.97	2.06
20	8	313	CLA	MG-NC	-3.57	1.97	2.06
20	B	829	CLA	MG-NC	-3.57	1.97	2.06
20	A	824	CLA	MG-NC	-3.57	1.97	2.06
20	B	815	CLA	MG-ND	-3.57	1.98	2.05
20	7	1004	CLA	MG-NB	-3.57	1.98	2.05
20	A	830	CLA	C1B-NB	3.56	1.42	1.37
29	4	313	CHL	MG-NA	-3.56	1.97	2.06
20	A	813	CLA	C1B-NB	3.56	1.42	1.37
20	B	841	CLA	C1D-ND	3.56	1.42	1.37
20	B	824	CLA	MG-NA	-3.56	1.97	2.06
20	B	835	CLA	MG-NA	-3.55	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	838	CLA	MG-NA	-3.55	1.97	2.06
20	A	837	CLA	MG-NC	-3.55	1.97	2.06
20	A	818	CLA	MG-NA	-3.55	1.97	2.06
20	5	321	CLA	C1D-ND	3.55	1.42	1.37
20	B	825	CLA	MG-NA	-3.55	1.97	2.06
20	A	814	CLA	C1D-ND	3.54	1.42	1.37
20	G	201	CLA	MG-NC	-3.54	1.97	2.06
20	5	323	CLA	MG-NA	-3.53	1.97	2.06
20	B	806	CLA	MG-NA	-3.53	1.97	2.06
20	A	822	CLA	C1B-NB	3.53	1.42	1.37
20	3	1005	CLA	C1D-ND	3.53	1.42	1.37
20	B	818	CLA	MG-NC	-3.52	1.97	2.06
20	8	312	CLA	MG-NC	-3.52	1.97	2.06
20	7	1011	CLA	C1D-ND	3.52	1.42	1.37
20	1	1004	CLA	MG-NC	-3.52	1.97	2.06
29	7	1015	CHL	MG-NC	-3.52	1.97	2.06
29	0	314	CHL	MG-NC	-3.51	1.97	2.06
20	5	321	CLA	MG-ND	-3.51	1.98	2.05
20	B	823	CLA	MG-NC	-3.51	1.97	2.06
20	B	803	CLA	MG-NC	-3.51	1.97	2.06
20	1	1007	CLA	C1D-ND	3.50	1.42	1.37
29	7	1017	CHL	MG-NA	-3.50	1.98	2.06
20	0	310	CLA	C1C-C2C	3.50	1.51	1.44
20	B	818	CLA	MG-NA	-3.50	1.98	2.06
20	6	309	CLA	MG-NA	-3.49	1.98	2.06
29	5	313	CHL	MG-NA	-3.49	1.98	2.06
20	A	836	CLA	MG-NC	-3.49	1.98	2.06
29	5	313	CHL	MG-NC	-3.49	1.98	2.06
20	4	311	CLA	MG-NA	-3.49	1.98	2.06
20	A	832	CLA	C1D-ND	3.49	1.42	1.37
20	B	819	CLA	MG-NC	-3.49	1.98	2.06
20	A	827	CLA	C1D-ND	3.48	1.42	1.37
20	1	1003	CLA	MG-ND	-3.48	1.98	2.05
20	L	202	CLA	MG-NA	-3.48	1.98	2.06
20	6	318	CLA	C1C-C2C	3.48	1.51	1.44
20	B	832	CLA	MG-NA	-3.48	1.98	2.06
20	0	311	CLA	MG-NA	-3.48	1.98	2.06
20	B	808	CLA	MG-NC	-3.47	1.98	2.06
20	6	305	CLA	C1D-ND	3.47	1.42	1.37
20	0	316	CLA	C1B-NB	3.47	1.42	1.37
20	3	1011	CLA	MG-NA	-3.46	1.98	2.06
20	1	1010	CLA	MG-NC	-3.46	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	0	313	CLA	C1B-NB	3.46	1.42	1.37
20	5	322	CLA	MG-NC	-3.46	1.98	2.06
20	7	1008	CLA	MG-NC	-3.46	1.98	2.06
20	A	809	CLA	MG-NA	-3.46	1.98	2.06
20	A	828	CLA	C1D-ND	3.46	1.42	1.37
20	A	804	CLA	MG-NC	-3.45	1.98	2.06
20	1	1003	CLA	C1C-C2C	3.45	1.51	1.44
20	4	309	CLA	MG-NC	-3.45	1.98	2.06
20	7	1004	CLA	C1B-NB	3.45	1.42	1.37
20	8	312	CLA	MG-NA	-3.45	1.98	2.06
20	1	1007	CLA	C1B-NB	3.45	1.42	1.37
20	1	1003	CLA	MG-NC	-3.44	1.98	2.06
20	A	801	CLA	MG-ND	-3.44	1.99	2.05
20	L	202	CLA	C1B-NB	3.44	1.42	1.37
20	3	1015	CLA	C1B-NB	3.44	1.42	1.37
29	7	1017	CHL	MG-NC	-3.44	1.98	2.06
20	0	311	CLA	MG-ND	-3.44	1.99	2.05
20	L	204	CLA	MG-ND	-3.44	1.99	2.05
20	L	202	CLA	MG-NC	-3.44	1.98	2.06
20	3	1013	CLA	MG-NA	-3.44	1.98	2.06
20	B	837	CLA	MG-NA	-3.43	1.98	2.06
20	3	1012	CLA	C1B-NB	3.43	1.42	1.37
20	7	1009	CLA	MG-NA	-3.43	1.98	2.06
20	3	1006	CLA	MG-NA	-3.43	1.98	2.06
20	4	306	CLA	MG-NA	-3.43	1.98	2.06
20	B	839	CLA	C1B-NB	3.42	1.42	1.37
20	4	309	CLA	C1D-ND	3.42	1.42	1.37
20	B	801	CLA	MG-NA	-3.42	1.98	2.06
20	A	812	CLA	C1B-NB	3.42	1.42	1.37
20	8	305	CLA	MG-NC	-3.41	1.98	2.06
20	B	838	CLA	MG-NA	-3.41	1.98	2.06
20	7	1005	CLA	MG-NC	-3.41	1.98	2.06
20	5	318	CLA	MG-NA	-3.41	1.98	2.06
20	K	201	CLA	MG-NA	-3.41	1.98	2.06
20	B	817	CLA	MG-NC	-3.41	1.98	2.06
29	0	314	CHL	MG-NA	-3.41	1.98	2.06
20	6	310	CLA	C1D-ND	3.41	1.42	1.37
20	A	814	CLA	MG-NC	-3.41	1.98	2.06
20	6	315	CLA	MG-NC	-3.41	1.98	2.06
20	A	804	CLA	MG-NA	-3.41	1.98	2.06
20	5	321	CLA	C1B-NB	3.40	1.42	1.37
29	0	315	CHL	MG-NC	-3.40	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	835	CLA	MG-NC	-3.39	1.98	2.06
20	F	305	CLA	MG-NC	-3.39	1.98	2.06
20	B	803	CLA	C1B-NB	3.38	1.41	1.37
20	B	831	CLA	C1D-ND	3.38	1.41	1.37
29	7	1015	CHL	C1D-ND	3.38	1.41	1.37
20	6	309	CLA	MG-NC	-3.38	1.98	2.06
20	7	1014	CLA	MG-NC	-3.38	1.98	2.06
20	G	203	CLA	C1B-NB	3.38	1.41	1.37
20	A	814	CLA	MG-NA	-3.38	1.98	2.06
20	0	310	CLA	MG-NC	-3.38	1.98	2.06
20	B	810	CLA	C1B-NB	3.38	1.41	1.37
29	8	317	CHL	MG-NA	-3.38	1.98	2.06
29	1	1015	CHL	MG-NC	-3.37	1.98	2.06
20	0	311	CLA	C1B-NB	3.37	1.41	1.37
29	5	316	CHL	MG-NC	-3.37	1.98	2.06
20	7	1010	CLA	C1B-NB	3.37	1.41	1.37
20	B	808	CLA	C1B-NB	3.37	1.41	1.37
20	F	302	CLA	C1B-NB	3.37	1.41	1.37
20	A	834	CLA	MG-NA	-3.36	1.98	2.06
20	A	827	CLA	MG-NC	-3.36	1.98	2.06
20	B	814	CLA	MG-NA	-3.36	1.98	2.06
20	B	802	CLA	C1D-ND	3.35	1.41	1.37
20	A	804	CLA	C1B-NB	3.35	1.41	1.37
29	6	313	CHL	MG-NA	-3.35	1.98	2.06
20	B	823	CLA	MG-ND	-3.34	1.99	2.05
20	7	1004	CLA	MG-NC	-3.34	1.98	2.06
20	7	1011	CLA	MG-NC	-3.34	1.98	2.06
20	4	307	CLA	C1D-ND	3.34	1.41	1.37
20	3	1013	CLA	C1B-NB	3.34	1.41	1.37
20	3	1007	CLA	C1B-NB	3.34	1.41	1.37
20	4	314	CLA	MG-ND	-3.34	1.99	2.05
20	G	203	CLA	MG-ND	-3.33	1.99	2.05
20	8	307	CLA	MG-NC	-3.32	1.98	2.06
20	3	1015	CLA	MG-NA	-3.32	1.98	2.06
20	A	831	CLA	C1C-C2C	3.32	1.51	1.44
20	3	1017	CLA	MG-NC	-3.32	1.98	2.06
20	B	819	CLA	MG-NA	-3.32	1.98	2.06
20	G	201	CLA	MG-NA	-3.32	1.98	2.06
20	L	203	CLA	MG-NC	-3.32	1.98	2.06
29	8	314	CHL	MG-NA	-3.32	1.98	2.06
20	5	318	CLA	C1C-C2C	3.31	1.51	1.44
20	1	1008	CLA	MG-NA	-3.31	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	0	312	CLA	C1B-NB	3.31	1.41	1.37
20	5	308	CLA	C1D-ND	3.31	1.41	1.37
20	B	833	CLA	MG-NA	-3.31	1.98	2.06
20	F	302	CLA	MG-NA	-3.31	1.98	2.06
20	B	826	CLA	C1B-NB	3.31	1.41	1.37
20	5	309	CLA	C1D-ND	3.31	1.41	1.37
20	6	320	CLA	MG-NC	-3.31	1.98	2.06
20	B	836	CLA	MG-NC	-3.30	1.98	2.06
20	F	302	CLA	MG-NC	-3.30	1.98	2.06
29	4	315	CHL	C1D-ND	3.30	1.41	1.37
20	A	852	CLA	C1B-NB	3.30	1.41	1.37
20	5	306	CLA	MG-NC	-3.29	1.98	2.06
20	A	808	CLA	MG-NC	-3.29	1.98	2.06
29	3	1014	CHL	MG-NC	-3.29	1.98	2.06
20	G	203	CLA	C1C-C2C	3.29	1.50	1.44
20	A	822	CLA	MG-NA	-3.29	1.98	2.06
20	6	301	CLA	MG-NC	-3.29	1.98	2.06
29	4	316	CHL	C2C-C1C	3.29	1.51	1.44
20	A	819	CLA	C1B-NB	3.29	1.41	1.37
20	A	828	CLA	MG-NA	-3.29	1.98	2.06
20	B	815	CLA	MG-NA	-3.28	1.98	2.06
29	1	1012	CHL	MG-NC	-3.28	1.98	2.06
20	B	803	CLA	MG-NA	-3.28	1.98	2.06
20	6	308	CLA	MG-NC	-3.27	1.98	2.06
20	1	1008	CLA	MG-NC	-3.27	1.98	2.06
20	3	1006	CLA	C1B-NB	3.27	1.41	1.37
20	A	829	CLA	C1B-NB	3.27	1.41	1.37
20	A	814	CLA	C1B-NB	3.27	1.41	1.37
20	8	316	CLA	MG-NC	-3.27	1.98	2.06
20	A	809	CLA	MG-NC	-3.26	1.98	2.06
20	1	1005	CLA	C1B-NB	3.26	1.41	1.37
20	A	805	CLA	MG-NC	-3.26	1.98	2.06
20	B	820	CLA	C1B-NB	3.25	1.41	1.37
20	6	318	CLA	MG-NC	-3.25	1.98	2.06
20	A	805	CLA	C1B-NB	3.25	1.41	1.37
29	7	1015	CHL	C2C-C1C	3.25	1.51	1.44
20	K	202	CLA	C4D-C3D	-3.25	1.39	1.46
20	5	305	CLA	MG-ND	-3.25	1.99	2.05
20	1	1004	CLA	MG-NA	-3.24	1.98	2.06
20	A	834	CLA	C1B-NB	3.23	1.41	1.37
20	6	310	CLA	C1B-NB	3.23	1.41	1.37
29	0	317	CHL	MG-NC	-3.23	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	801	CLA	C1D-ND	3.23	1.41	1.37
20	4	304	CLA	MG-NC	-3.22	1.98	2.06
20	B	815	CLA	C1C-C2C	3.22	1.50	1.44
20	B	805	CLA	C1D-ND	3.22	1.41	1.37
29	7	1017	CHL	C1D-ND	3.22	1.41	1.37
20	5	301	CLA	MG-NC	-3.22	1.98	2.06
20	K	202	CLA	MG-NA	-3.22	1.98	2.06
20	8	316	CLA	MG-NA	-3.22	1.98	2.06
20	8	306	CLA	C1B-NB	3.22	1.41	1.37
20	A	834	CLA	MG-NC	-3.21	1.98	2.06
20	A	802	CLA	C1B-NB	3.21	1.41	1.37
20	A	816	CLA	MG-NC	-3.21	1.98	2.06
20	B	833	CLA	C1B-NB	3.21	1.41	1.37
20	A	810	CLA	MG-ND	-3.21	1.99	2.05
20	A	851	CLA	MG-NC	-3.21	1.98	2.06
20	1	1014	CLA	MG-NA	-3.21	1.98	2.06
29	3	1014	CHL	MG-NA	-3.21	1.98	2.06
20	5	310	CLA	C1D-ND	3.21	1.41	1.37
20	A	821	CLA	MG-NC	-3.20	1.98	2.06
20	A	828	CLA	MG-NC	-3.20	1.98	2.06
20	B	805	CLA	MG-NC	-3.20	1.98	2.06
20	B	839	CLA	C1D-ND	3.19	1.41	1.37
20	A	825	CLA	MG-NC	-3.18	1.98	2.06
20	A	827	CLA	MG-NA	-3.18	1.98	2.06
20	3	1015	CLA	MG-NC	-3.17	1.98	2.06
20	5	304	CLA	C1B-NB	3.17	1.41	1.37
20	B	828	CLA	MG-NC	-3.17	1.98	2.06
20	B	810	CLA	MG-NA	-3.17	1.98	2.06
29	0	315	CHL	MG-NA	-3.17	1.98	2.06
20	7	1007	CLA	C1D-ND	3.17	1.41	1.37
20	B	838	CLA	MG-NC	-3.16	1.98	2.06
20	A	852	CLA	MG-NA	-3.16	1.98	2.06
20	B	825	CLA	MG-NC	-3.16	1.98	2.06
20	A	830	CLA	MG-NC	-3.16	1.98	2.06
20	3	1011	CLA	MG-NC	-3.15	1.98	2.06
20	0	313	CLA	MG-NC	-3.14	1.98	2.06
20	B	832	CLA	C1B-NB	3.14	1.41	1.37
20	K	202	CLA	MG-NC	-3.14	1.98	2.06
20	4	305	CLA	MG-NC	-3.14	1.98	2.06
20	0	301	CLA	C1C-C2C	3.13	1.50	1.44
20	0	308	CLA	C1D-ND	3.13	1.41	1.37
20	1	1010	CLA	MG-NA	-3.13	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	812	CLA	C1B-NB	3.12	1.41	1.37
20	B	814	CLA	C1B-NB	3.12	1.41	1.37
20	3	1017	CLA	C1B-NB	3.12	1.41	1.37
20	A	837	CLA	C1D-ND	3.12	1.41	1.37
20	G	203	CLA	MG-NA	-3.11	1.98	2.06
20	A	806	CLA	MG-NC	-3.11	1.98	2.06
20	8	310	CLA	MG-NC	-3.11	1.98	2.06
20	B	807	CLA	MG-NA	-3.11	1.98	2.06
29	8	317	CHL	MG-NC	-3.11	1.98	2.06
20	7	1005	CLA	MG-ND	-3.11	1.99	2.05
20	B	841	CLA	MG-NA	-3.11	1.98	2.06
20	6	301	CLA	MG-NA	-3.11	1.98	2.06
20	A	826	CLA	MG-NC	-3.10	1.98	2.06
20	3	1008	CLA	C1B-NB	3.10	1.41	1.37
20	B	835	CLA	MG-NC	-3.10	1.98	2.06
20	5	307	CLA	C1B-NB	3.10	1.41	1.37
20	A	812	CLA	MG-NC	-3.10	1.98	2.06
20	1	1017	CLA	C1B-NB	3.09	1.41	1.37
20	A	821	CLA	C1B-NB	3.09	1.41	1.37
20	3	1006	CLA	MG-NC	-3.09	1.98	2.06
29	8	314	CHL	C2C-C1C	3.09	1.51	1.44
20	3	1013	CLA	MG-NC	-3.09	1.98	2.06
29	5	316	CHL	C2C-C1C	3.09	1.51	1.44
20	8	310	CLA	C1B-NB	3.09	1.41	1.37
20	0	301	CLA	MG-NC	-3.08	1.98	2.06
20	B	837	CLA	MG-NC	-3.08	1.98	2.06
29	0	317	CHL	CHB-C4A	-3.08	1.30	1.37
20	0	305	CLA	MG-NA	-3.07	1.99	2.06
20	3	1007	CLA	MG-NA	-3.07	1.99	2.06
20	8	312	CLA	C1D-ND	3.07	1.41	1.37
20	B	811	CLA	C1B-NB	3.07	1.41	1.37
29	1	1015	CHL	CHB-C4A	-3.07	1.30	1.37
20	B	837	CLA	C1B-NB	3.06	1.41	1.37
20	A	838	CLA	C1B-NB	3.06	1.41	1.37
20	5	309	CLA	MG-NA	-3.06	1.99	2.06
20	0	301	CLA	MG-NA	-3.06	1.99	2.06
20	7	1010	CLA	MG-NC	-3.06	1.99	2.06
20	B	819	CLA	C1B-NB	3.06	1.41	1.37
20	0	316	CLA	MG-NA	-3.05	1.99	2.06
20	8	309	CLA	MG-ND	-3.05	1.99	2.05
20	B	801	CLA	MG-NC	-3.05	1.99	2.06
20	A	839	CLA	MG-NC	-3.05	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	313	CHL	C1D-ND	3.05	1.41	1.37
20	4	305	CLA	MG-NA	-3.05	1.99	2.06
29	3	1014	CHL	CHB-C4A	-3.05	1.30	1.37
20	A	811	CLA	MG-NA	-3.04	1.99	2.06
20	4	306	CLA	MG-NC	-3.04	1.99	2.06
20	B	840	CLA	MG-NC	-3.04	1.99	2.06
20	7	1006	CLA	MG-ND	-3.04	1.99	2.05
29	3	1014	CHL	C1D-ND	3.04	1.41	1.37
20	1	1009	CLA	MG-NC	-3.04	1.99	2.06
20	B	802	CLA	MG-NC	-3.04	1.99	2.06
20	B	822	CLA	C1D-ND	3.04	1.41	1.37
20	B	839	CLA	C1C-C2C	3.04	1.50	1.44
20	J	102	CLA	MG-NA	-3.03	1.99	2.06
20	A	825	CLA	C1C-C2C	3.03	1.50	1.44
20	6	312	CLA	MG-NA	-3.03	1.99	2.06
29	6	314	CHL	MG-NA	-3.02	1.99	2.06
20	B	826	CLA	MG-NA	-3.02	1.99	2.06
20	A	839	CLA	C1C-C2C	3.02	1.50	1.44
20	B	810	CLA	MG-NC	-3.02	1.99	2.06
29	5	314	CHL	C2C-C1C	3.01	1.50	1.44
20	B	814	CLA	MG-NC	-3.01	1.99	2.06
20	0	301	CLA	C1B-NB	3.01	1.41	1.37
20	A	830	CLA	MG-NA	-3.01	1.99	2.06
20	B	840	CLA	MG-ND	-3.00	1.99	2.05
20	3	1012	CLA	MG-NC	-3.00	1.99	2.06
20	1	1006	CLA	C1D-ND	3.00	1.41	1.37
29	1	1015	CHL	MG-NA	-3.00	1.99	2.06
20	4	307	CLA	C1D-C2D	-3.00	1.39	1.45
20	B	826	CLA	C1C-C2C	2.99	1.50	1.44
20	8	308	CLA	MG-NC	-2.99	1.99	2.06
20	A	852	CLA	MG-NC	-2.99	1.99	2.06
20	4	309	CLA	MG-NA	-2.99	1.99	2.06
20	B	809	CLA	MG-NC	-2.98	1.99	2.06
20	1	1011	CLA	C1B-NB	2.98	1.41	1.37
20	4	307	CLA	MG-ND	-2.98	1.99	2.05
20	6	306	CLA	MG-NC	-2.98	1.99	2.06
20	6	311	CLA	MG-ND	-2.98	1.99	2.05
20	L	203	CLA	MG-NA	-2.98	1.99	2.06
20	B	807	CLA	C1B-NB	2.98	1.41	1.37
20	8	312	CLA	C1B-NB	2.98	1.41	1.37
29	6	314	CHL	C3A-C2A	-2.98	1.46	1.54
20	A	833	CLA	MG-NA	-2.98	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	813	CLA	MG-NA	-2.98	1.99	2.06
20	B	832	CLA	MG-NC	-2.97	1.99	2.06
20	L	204	CLA	MG-NA	-2.97	1.99	2.06
20	B	801	CLA	C1B-NB	2.97	1.41	1.37
20	B	839	CLA	MG-NA	-2.96	1.99	2.06
20	0	311	CLA	MG-NC	-2.96	1.99	2.06
20	8	305	CLA	C1D-ND	2.96	1.41	1.37
20	7	1006	CLA	MG-NC	-2.96	1.99	2.06
20	6	305	CLA	C1B-NB	2.95	1.41	1.37
20	A	832	CLA	MG-NC	-2.95	1.99	2.06
20	8	316	CLA	C1D-ND	2.95	1.41	1.37
20	1	1014	CLA	C1B-NB	2.95	1.41	1.37
20	A	803	CLA	C1C-C2C	2.93	1.50	1.44
29	7	1012	CHL	MG-NC	-2.93	1.99	2.06
20	A	820	CLA	C1B-NB	2.93	1.41	1.37
20	0	306	CLA	MG-NA	-2.92	1.99	2.06
20	0	307	CLA	C1C-C2C	2.92	1.50	1.44
20	B	822	CLA	C1B-NB	2.92	1.41	1.37
20	L	204	CLA	MG-NC	-2.92	1.99	2.06
20	B	812	CLA	MG-NC	-2.92	1.99	2.06
20	6	310	CLA	MG-NA	-2.92	1.99	2.06
20	A	813	CLA	MG-NC	-2.91	1.99	2.06
20	B	829	CLA	C1B-NB	2.91	1.41	1.37
29	1	1012	CHL	MG-NA	-2.91	1.99	2.06
20	5	305	CLA	MG-NA	-2.91	1.99	2.06
20	B	826	CLA	MG-NC	-2.91	1.99	2.06
20	B	809	CLA	C1B-NB	2.90	1.41	1.37
20	A	833	CLA	MG-NC	-2.90	1.99	2.06
20	B	816	CLA	MG-NC	-2.90	1.99	2.06
20	A	817	CLA	MG-NA	-2.90	1.99	2.06
29	5	314	CHL	MG-NA	-2.90	1.99	2.06
20	5	318	CLA	C1B-NB	2.89	1.41	1.37
20	A	832	CLA	C1B-NB	2.89	1.41	1.37
20	A	816	CLA	C1B-NB	2.88	1.41	1.37
20	5	311	CLA	MG-NC	-2.88	1.99	2.06
20	K	201	CLA	MG-NC	-2.88	1.99	2.06
20	B	824	CLA	C1B-NB	2.88	1.41	1.37
20	A	821	CLA	C1C-C2C	2.88	1.50	1.44
20	B	835	CLA	C1B-NB	2.88	1.41	1.37
20	6	311	CLA	MG-NA	-2.87	1.99	2.06
29	5	317	CHL	MG-NA	-2.87	1.99	2.06
20	A	825	CLA	C1B-NB	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	303	CLA	C1B-NB	2.86	1.41	1.37
20	3	1005	CLA	MG-NC	-2.86	1.99	2.06
20	A	807	CLA	C1C-C2C	2.85	1.50	1.44
20	A	824	CLA	C1B-NB	2.85	1.41	1.37
20	B	816	CLA	MG-NA	-2.84	1.99	2.06
20	A	851	CLA	C1B-NB	2.84	1.41	1.37
20	7	1011	CLA	C1C-C2C	2.83	1.50	1.44
20	3	1005	CLA	C1C-C2C	2.83	1.50	1.44
20	G	202	CLA	MG-NC	-2.83	1.99	2.06
20	B	802	CLA	MG-NA	-2.83	1.99	2.06
20	B	825	CLA	C1B-NB	2.83	1.41	1.37
20	A	817	CLA	MG-NC	-2.83	1.99	2.06
20	4	308	CLA	MG-NA	-2.82	1.99	2.06
20	B	807	CLA	C1C-C2C	2.82	1.50	1.44
20	B	834	CLA	C1C-C2C	2.81	1.50	1.44
20	A	831	CLA	MG-NC	-2.81	1.99	2.06
20	5	311	CLA	MG-NA	-2.81	1.99	2.06
20	1	1004	CLA	C1C-C2C	2.81	1.50	1.44
20	A	839	CLA	C1B-NB	2.81	1.41	1.37
29	8	317	CHL	C2C-C1C	2.80	1.50	1.44
20	B	832	CLA	C1C-C2C	2.80	1.50	1.44
20	L	203	CLA	C1C-C2C	2.80	1.50	1.44
20	B	834	CLA	MG-NC	-2.80	1.99	2.06
20	7	1010	CLA	C1D-C2D	-2.80	1.39	1.45
20	B	840	CLA	C1B-NB	2.80	1.41	1.37
20	A	821	CLA	MG-NA	-2.80	1.99	2.06
20	B	807	CLA	MG-NC	-2.80	1.99	2.06
20	A	814	CLA	C3A-C2A	-2.79	1.51	1.54
20	B	828	CLA	C1C-C2C	2.79	1.50	1.44
20	A	813	CLA	MG-NA	-2.79	1.99	2.06
20	4	311	CLA	C1B-NB	2.78	1.41	1.37
29	0	317	CHL	MG-NA	-2.78	1.99	2.06
20	7	1007	CLA	MG-NA	-2.77	1.99	2.06
29	6	316	CHL	C1D-ND	2.77	1.41	1.37
20	5	309	CLA	MG-NC	-2.77	1.99	2.06
29	4	312	CHL	MG-NA	-2.77	1.99	2.06
20	A	818	CLA	C1B-NB	2.77	1.41	1.37
29	4	316	CHL	C1D-ND	2.76	1.41	1.37
29	7	1013	CHL	CHB-C4A	-2.76	1.31	1.37
20	8	309	CLA	MG-NA	-2.76	1.99	2.06
20	7	1005	CLA	C1B-NB	2.76	1.41	1.37
20	7	1007	CLA	C1B-NB	2.76	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	305	CLA	C1C-C2C	2.75	1.49	1.44
20	A	837	CLA	MG-NA	-2.75	1.99	2.06
20	7	1004	CLA	C3A-C2A	-2.75	1.46	1.54
20	6	308	CLA	C1D-C2D	-2.75	1.39	1.45
20	K	201	CLA	MG-ND	-2.75	2.00	2.05
20	6	309	CLA	C1D-ND	2.75	1.41	1.37
20	B	819	CLA	C1C-C2C	2.75	1.49	1.44
20	B	821	CLA	C1D-ND	2.74	1.41	1.37
20	B	828	CLA	C1B-NB	2.74	1.41	1.37
20	B	850	CLA	C1B-NB	2.74	1.41	1.37
20	B	821	CLA	C1B-NB	2.74	1.41	1.37
20	6	315	CLA	C1D-C2D	-2.74	1.39	1.45
20	4	308	CLA	MG-NC	-2.73	1.99	2.06
20	A	809	CLA	C1C-C2C	2.73	1.49	1.44
20	A	803	CLA	MG-NA	-2.73	1.99	2.06
20	3	1009	CLA	C1B-NB	2.72	1.41	1.37
20	5	310	CLA	MG-NC	-2.72	1.99	2.06
20	G	202	CLA	MG-NA	-2.71	1.99	2.06
29	6	317	CHL	C1D-C2D	-2.71	1.40	1.45
20	5	323	CLA	C1D-C2D	-2.71	1.40	1.45
29	7	1013	CHL	C3A-C2A	-2.70	1.46	1.54
20	B	811	CLA	C1C-C2C	2.70	1.49	1.44
29	1	1013	CHL	CHB-C4A	-2.70	1.31	1.37
20	J	102	CLA	MG-NC	-2.70	1.99	2.06
20	B	833	CLA	MG-NC	-2.70	1.99	2.06
20	4	314	CLA	MG-NC	-2.70	1.99	2.06
20	B	802	CLA	C1B-NB	2.69	1.41	1.37
20	G	203	CLA	MG-NC	-2.69	1.99	2.06
20	5	321	CLA	C1D-C2D	-2.69	1.40	1.45
20	A	834	CLA	C1C-C2C	2.69	1.49	1.44
20	A	807	CLA	C1B-NB	2.68	1.41	1.37
29	8	315	CHL	C3A-C2A	-2.68	1.47	1.54
24	3	1004	BCR	C24-C25	2.68	1.54	1.45
20	B	825	CLA	C1C-C2C	2.68	1.49	1.44
29	7	1015	CHL	MG-NA	-2.68	1.99	2.06
20	B	820	CLA	MG-NA	-2.68	1.99	2.06
24	B	843	BCR	C15-C14	2.68	1.51	1.43
20	8	310	CLA	C1C-C2C	2.67	1.49	1.44
20	A	820	CLA	C1C-C2C	2.67	1.49	1.44
20	A	831	CLA	MG-NA	-2.67	1.99	2.06
29	5	317	CHL	C1D-C2D	-2.67	1.40	1.45
20	6	306	CLA	MG-NA	-2.67	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	1003	CLA	MG-NA	-2.67	1.99	2.06
29	1	1015	CHL	C2C-C1C	2.66	1.50	1.44
20	A	809	CLA	C1B-NB	2.65	1.41	1.37
20	A	805	CLA	C1D-C2D	-2.65	1.40	1.45
20	3	1017	CLA	C1C-C2C	2.65	1.49	1.44
20	5	306	CLA	C1C-C2C	2.65	1.49	1.44
20	B	823	CLA	MG-NA	-2.65	2.00	2.06
20	6	301	CLA	C1C-C2C	2.64	1.49	1.44
20	8	308	CLA	C1C-C2C	2.64	1.49	1.44
29	5	314	CHL	C1D-C2D	-2.64	1.40	1.45
20	A	819	CLA	C1C-C2C	2.64	1.49	1.44
20	5	323	CLA	C1B-NB	2.64	1.41	1.37
20	7	1008	CLA	C1B-NB	2.64	1.41	1.37
29	5	314	CHL	C1B-NB	2.63	1.41	1.37
20	4	307	CLA	C4C-C3C	-2.63	1.40	1.45
20	6	311	CLA	MG-NC	-2.63	2.00	2.06
29	5	316	CHL	C1D-C2D	-2.63	1.40	1.45
20	6	308	CLA	C1C-C2C	2.63	1.49	1.44
20	B	802	CLA	C1C-C2C	2.63	1.49	1.44
29	6	314	CHL	C2C-C1C	2.62	1.50	1.44
20	A	828	CLA	C1B-NB	2.62	1.41	1.37
20	B	806	CLA	C1B-NB	2.62	1.41	1.37
20	8	312	CLA	C1C-C2C	2.62	1.49	1.44
20	A	836	CLA	C1B-NB	2.61	1.41	1.37
20	5	318	CLA	C1C-NC	-2.60	1.33	1.37
20	6	301	CLA	C1B-NB	2.60	1.41	1.37
20	B	831	CLA	C1B-NB	2.59	1.41	1.37
20	5	308	CLA	C1D-C2D	-2.59	1.40	1.45
20	B	822	CLA	C1D-C2D	-2.59	1.40	1.45
20	A	838	CLA	C1D-ND	2.59	1.41	1.37
20	B	830	CLA	MG-NB	-2.59	2.00	2.05
20	8	306	CLA	MG-NA	-2.59	2.00	2.06
20	4	311	CLA	C1D-ND	2.58	1.41	1.37
20	5	305	CLA	C1D-C2D	-2.58	1.40	1.45
20	A	824	CLA	C1D-C2D	-2.58	1.40	1.45
20	A	803	CLA	MG-NC	-2.57	2.00	2.06
20	6	307	CLA	C1C-C2C	2.57	1.49	1.44
20	3	1016	CLA	C1D-C2D	-2.57	1.40	1.45
20	A	823	CLA	C1B-NB	2.57	1.40	1.37
20	1	1010	CLA	C1B-NB	2.57	1.40	1.37
20	5	305	CLA	MG-NC	-2.56	2.00	2.06
20	6	308	CLA	C3D-C4D	-2.56	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	1010	CLA	C1D-ND	2.56	1.40	1.37
20	1	1009	CLA	C1D-C2D	-2.56	1.40	1.45
20	A	812	CLA	MG-NA	-2.55	2.00	2.06
20	A	815	CLA	C1B-NB	2.55	1.40	1.37
20	B	818	CLA	C1D-C2D	-2.55	1.40	1.45
20	6	312	CLA	C1D-C2D	-2.55	1.40	1.45
29	8	315	CHL	CHB-C4A	-2.55	1.31	1.37
20	4	306	CLA	C1D-C2D	-2.55	1.40	1.45
20	A	838	CLA	C1D-C2D	-2.54	1.40	1.45
20	7	1009	CLA	C1D-C2D	-2.54	1.40	1.45
20	B	812	CLA	MG-NA	-2.54	2.00	2.06
20	A	802	CLA	C1C-C2C	2.54	1.49	1.44
20	0	309	CLA	C1D-C2D	-2.53	1.40	1.45
24	B	843	BCR	C16-C15	2.53	1.42	1.36
20	F	302	CLA	C1D-C2D	-2.53	1.40	1.45
20	B	840	CLA	C1C-C2C	2.53	1.49	1.44
20	B	828	CLA	MG-NA	-2.53	2.00	2.06
20	4	309	CLA	C1D-C2D	-2.53	1.40	1.45
20	7	1004	CLA	C1D-C2D	-2.52	1.40	1.45
20	B	816	CLA	C1C-C2C	2.52	1.49	1.44
20	8	311	CLA	C1B-NB	2.52	1.40	1.37
29	5	316	CHL	CHB-C4A	-2.52	1.31	1.37
20	B	818	CLA	C1B-NB	2.52	1.40	1.37
20	A	837	CLA	C1B-NB	2.51	1.40	1.37
20	1	1004	CLA	C1D-C2D	-2.51	1.40	1.45
20	0	311	CLA	C1C-C2C	2.51	1.49	1.44
20	8	310	CLA	C1D-C2D	-2.51	1.40	1.45
29	5	316	CHL	C3D-C4D	-2.51	1.38	1.44
20	3	1005	CLA	C1D-C2D	-2.51	1.40	1.45
20	A	812	CLA	C1D-C2D	-2.51	1.40	1.45
20	A	815	CLA	C1D-C2D	-2.51	1.40	1.45
20	5	312	CLA	C1D-C2D	-2.51	1.40	1.45
20	A	816	CLA	C1C-C2C	2.50	1.49	1.44
20	B	827	CLA	C1C-C2C	2.50	1.49	1.44
20	B	838	CLA	C1D-C2D	-2.50	1.40	1.45
29	0	317	CHL	C2C-C1C	2.50	1.49	1.44
20	5	322	CLA	C1B-NB	2.50	1.40	1.37
20	A	831	CLA	C1D-C2D	-2.49	1.40	1.45
20	A	818	CLA	C1D-C2D	-2.49	1.40	1.45
20	B	809	CLA	C1C-C2C	2.49	1.49	1.44
29	8	314	CHL	CHB-C4A	-2.49	1.31	1.37
20	3	1012	CLA	C1C-C2C	2.49	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	313	CHL	C1D-C2D	-2.49	1.40	1.45
20	5	310	CLA	C1D-C2D	-2.48	1.40	1.45
20	A	806	CLA	C1B-NB	2.48	1.40	1.37
29	6	313	CHL	C1D-C2D	-2.48	1.40	1.45
29	4	316	CHL	MG-NA	-2.48	2.00	2.06
25	5	319	DGD	O5D-C1E	2.48	1.44	1.40
20	0	306	CLA	C1D-C2D	-2.48	1.40	1.45
20	B	829	CLA	C1C-C2C	2.48	1.49	1.44
20	A	819	CLA	C1D-C2D	-2.48	1.40	1.45
20	6	301	CLA	C1D-C2D	-2.48	1.40	1.45
20	5	306	CLA	C1B-NB	2.47	1.40	1.37
20	B	834	CLA	C1B-NB	2.47	1.40	1.37
20	B	836	CLA	C1C-C2C	2.47	1.49	1.44
20	0	307	CLA	C1D-C2D	-2.46	1.40	1.45
20	8	305	CLA	C1D-C2D	-2.46	1.40	1.45
20	B	809	CLA	C1D-C2D	-2.46	1.40	1.45
20	5	307	CLA	C1D-C2D	-2.46	1.40	1.45
29	6	314	CHL	C1D-ND	2.46	1.40	1.37
20	B	823	CLA	C1C-C2C	2.46	1.49	1.44
20	1	1009	CLA	C1B-NB	2.46	1.40	1.37
29	6	316	CHL	CHB-C4A	-2.46	1.31	1.37
20	A	805	CLA	C1C-C2C	2.46	1.49	1.44
20	6	311	CLA	C1D-C2D	-2.45	1.40	1.45
20	5	315	CLA	C1D-ND	2.45	1.40	1.37
20	G	202	CLA	C1C-C2C	2.45	1.49	1.44
20	7	1004	CLA	C3D-C4D	-2.45	1.38	1.44
20	7	1011	CLA	C1D-C2D	-2.45	1.40	1.45
20	A	829	CLA	MG-NC	-2.44	2.00	2.06
20	5	301	CLA	C1C-C2C	2.44	1.49	1.44
20	5	307	CLA	C1C-C2C	2.44	1.49	1.44
29	4	313	CHL	CHB-C4A	-2.44	1.31	1.37
20	B	817	CLA	C1C-C2C	2.44	1.49	1.44
20	A	827	CLA	C1C-C2C	2.44	1.49	1.44
20	B	835	CLA	C1C-C2C	2.44	1.49	1.44
20	0	301	CLA	C1D-C2D	-2.44	1.40	1.45
20	0	311	CLA	C1D-C2D	-2.44	1.40	1.45
20	A	804	CLA	C1C-C2C	2.43	1.49	1.44
20	A	815	CLA	CHC-C1C	-2.43	1.33	1.38
20	B	816	CLA	C1D-C2D	-2.43	1.40	1.45
20	B	812	CLA	C1D-C2D	-2.43	1.40	1.45
20	A	851	CLA	C1C-C2C	2.43	1.49	1.44
29	5	313	CHL	C3D-C4D	-2.43	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	834	CLA	C1D-C2D	-2.43	1.40	1.45
20	6	309	CLA	C1D-C2D	-2.43	1.40	1.45
20	8	307	CLA	C1D-C2D	-2.42	1.40	1.45
29	4	316	CHL	C1D-C2D	-2.42	1.40	1.45
20	7	1008	CLA	C1D-C2D	-2.42	1.40	1.45
20	3	1007	CLA	C1C-C2C	2.42	1.49	1.44
20	0	306	CLA	C1B-NB	2.42	1.40	1.37
24	B	843	BCR	C24-C25	2.41	1.53	1.45
20	B	850	CLA	C1D-C2D	-2.41	1.40	1.45
20	B	813	CLA	MG-NC	-2.41	2.00	2.06
20	7	1005	CLA	C1D-C2D	-2.41	1.40	1.45
20	K	202	CLA	C2C-C1C	2.41	1.48	1.43
20	5	309	CLA	C3D-C4D	-2.41	1.38	1.44
20	7	1007	CLA	C1C-C2C	2.41	1.49	1.44
20	B	811	CLA	C1D-C2D	-2.41	1.40	1.45
29	5	313	CHL	CHB-C4A	-2.40	1.32	1.37
20	A	821	CLA	C1D-C2D	-2.40	1.40	1.45
20	1	1010	CLA	C1D-C2D	-2.40	1.40	1.45
24	B	804	BCR	C7-C6	2.40	1.53	1.45
20	5	321	CLA	MG-NA	-2.40	2.00	2.06
20	F	303	CLA	C1D-C2D	-2.40	1.40	1.45
20	1	1005	CLA	C1C-C2C	2.40	1.49	1.44
20	1	1005	CLA	C1D-C2D	-2.40	1.40	1.45
29	6	316	CHL	C1D-C2D	-2.39	1.40	1.45
20	B	801	CLA	C1D-C2D	-2.39	1.40	1.45
29	8	317	CHL	C3D-C4D	-2.39	1.38	1.44
20	4	304	CLA	C1D-ND	2.39	1.40	1.37
20	K	202	CLA	CAD-C3D	-2.39	1.46	1.50
20	J	102	CLA	C1C-C2C	2.39	1.49	1.44
20	6	310	CLA	C1D-C2D	-2.38	1.40	1.45
20	L	204	CLA	C1C-C2C	2.38	1.49	1.44
20	B	827	CLA	C1B-NB	2.38	1.40	1.37
20	1	1009	CLA	C1C-C2C	2.38	1.49	1.44
29	7	1015	CHL	C1D-C2D	-2.38	1.40	1.45
20	0	313	CLA	C1D-C2D	-2.38	1.40	1.45
20	1	1007	CLA	C1D-C2D	-2.38	1.40	1.45
20	A	829	CLA	C1D-C2D	-2.37	1.40	1.45
20	A	820	CLA	C1D-C2D	-2.37	1.40	1.45
20	3	1015	CLA	C1D-C2D	-2.37	1.40	1.45
20	A	830	CLA	C1D-C2D	-2.37	1.40	1.45
20	B	806	CLA	C1D-C2D	-2.37	1.40	1.45
20	6	309	CLA	C3D-C4D	-2.37	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	305	CLA	MG-NC	-2.37	2.00	2.06
20	A	837	CLA	C1D-C2D	-2.36	1.40	1.45
20	7	1010	CLA	C3D-C4D	-2.36	1.38	1.44
20	A	814	CLA	C1D-C2D	-2.36	1.40	1.45
29	0	315	CHL	C2C-C1C	2.36	1.49	1.44
20	6	306	CLA	C1C-C2C	2.36	1.49	1.44
20	F	305	CLA	C1B-NB	2.36	1.40	1.37
29	7	1015	CHL	C3D-C4D	-2.36	1.38	1.44
20	7	1006	CLA	C1D-C2D	-2.36	1.40	1.45
20	7	1007	CLA	MG-NC	-2.35	2.00	2.06
20	3	1011	CLA	C1C-C2C	2.35	1.49	1.44
20	B	802	CLA	C3D-C4D	-2.35	1.38	1.44
29	7	1017	CHL	C1D-C2D	-2.35	1.40	1.45
20	3	1010	CLA	C1D-C2D	-2.35	1.40	1.45
20	0	308	CLA	C1D-C2D	-2.35	1.40	1.45
20	3	1006	CLA	C1D-C2D	-2.35	1.40	1.45
20	A	833	CLA	C1C-C2C	2.34	1.49	1.44
20	3	1006	CLA	C1C-C2C	2.34	1.49	1.44
20	B	839	CLA	C1D-C2D	-2.34	1.40	1.45
20	5	307	CLA	MG-NA	-2.34	2.00	2.06
20	A	826	CLA	C1D-C2D	-2.34	1.40	1.45
20	6	315	CLA	C1D-ND	2.34	1.40	1.37
20	A	828	CLA	C1C-C2C	2.34	1.49	1.44
20	A	823	CLA	C1D-C2D	-2.33	1.40	1.45
20	8	312	CLA	C1D-C2D	-2.33	1.40	1.45
20	B	814	CLA	C1C-C2C	2.33	1.49	1.44
20	A	851	CLA	C1D-C2D	-2.33	1.40	1.45
20	A	832	CLA	C1D-C2D	-2.33	1.40	1.45
20	B	806	CLA	C1C-C2C	2.33	1.49	1.44
20	B	805	CLA	C1D-C2D	-2.33	1.40	1.45
20	3	1016	CLA	C3D-C4D	-2.32	1.38	1.44
20	B	822	CLA	C1C-C2C	2.32	1.49	1.44
29	1	1012	CHL	C1D-C2D	-2.32	1.40	1.45
20	F	305	CLA	C1D-C2D	-2.32	1.40	1.45
20	1	1006	CLA	C1B-NB	2.32	1.40	1.37
20	B	836	CLA	C1D-C2D	-2.32	1.40	1.45
20	A	837	CLA	C1C-C2C	2.32	1.49	1.44
24	G	205	BCR	C24-C25	2.32	1.53	1.45
29	6	314	CHL	C1D-C2D	-2.32	1.40	1.45
24	4	302	BCR	C24-C25	2.32	1.53	1.45
20	4	304	CLA	C1B-NB	2.32	1.40	1.37
20	6	315	CLA	C3D-C4D	-2.32	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	821	CLA	C1D-C2D	-2.32	1.40	1.45
20	7	1007	CLA	C3D-C4D	-2.31	1.39	1.44
29	0	314	CHL	C2C-C1C	2.31	1.49	1.44
29	4	312	CHL	C1D-C2D	-2.31	1.40	1.45
20	3	1012	CLA	C1D-C2D	-2.31	1.40	1.45
20	B	819	CLA	C1D-C2D	-2.31	1.40	1.45
29	7	1017	CHL	C3D-C4D	-2.31	1.39	1.44
20	4	308	CLA	C1D-C2D	-2.31	1.40	1.45
20	A	829	CLA	C1C-C2C	2.31	1.49	1.44
29	6	313	CHL	C3D-C4D	-2.31	1.39	1.44
20	0	309	CLA	C1B-NB	2.30	1.40	1.37
20	4	311	CLA	C1D-C2D	-2.30	1.40	1.45
20	0	305	CLA	C1C-C2C	2.30	1.49	1.44
20	A	833	CLA	C1D-C2D	-2.30	1.40	1.45
20	6	306	CLA	C1D-C2D	-2.30	1.40	1.45
20	B	829	CLA	C1D-C2D	-2.29	1.40	1.45
20	0	309	CLA	C3D-C4D	-2.29	1.39	1.44
20	A	840	CLA	C1D-C2D	-2.29	1.40	1.45
20	6	305	CLA	C1D-C2D	-2.29	1.40	1.45
29	1	1012	CHL	CHB-C4A	-2.29	1.32	1.37
20	4	309	CLA	C3D-C4D	-2.29	1.39	1.44
20	G	203	CLA	C1D-C2D	-2.29	1.40	1.45
20	F	305	CLA	C1C-C2C	2.29	1.49	1.44
20	7	1014	CLA	C1B-NB	2.29	1.40	1.37
20	A	826	CLA	C3D-C4D	-2.29	1.39	1.44
20	K	202	CLA	C4D-CHA	-2.29	1.37	1.44
20	0	310	CLA	C1D-C2D	-2.29	1.40	1.45
20	B	828	CLA	C1D-C2D	-2.28	1.40	1.45
20	8	311	CLA	C3D-C4D	-2.28	1.39	1.44
20	3	1009	CLA	C3D-C4D	-2.28	1.39	1.44
20	L	201	CLA	C1C-C2C	2.28	1.49	1.44
20	A	816	CLA	C1D-C2D	-2.28	1.40	1.45
24	H	201	BCR	C7-C6	2.28	1.53	1.45
20	A	818	CLA	C1C-C2C	2.27	1.49	1.44
29	5	317	CHL	C1D-ND	2.27	1.40	1.37
24	F	301	BCR	C24-C25	2.27	1.53	1.45
20	5	311	CLA	C1D-C2D	-2.27	1.40	1.45
20	B	824	CLA	C1C-C2C	2.27	1.49	1.44
20	5	304	CLA	C1D-C2D	-2.27	1.40	1.45
24	H	201	BCR	C24-C25	2.27	1.53	1.45
20	A	837	CLA	C3D-C4D	-2.26	1.39	1.44
20	B	820	CLA	C1D-C2D	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	309	CLA	C1D-C2D	-2.26	1.40	1.45
20	4	305	CLA	C1D-C2D	-2.26	1.40	1.45
20	L	203	CLA	C1D-C2D	-2.26	1.40	1.45
29	5	314	CHL	C3D-C4D	-2.26	1.39	1.44
29	4	316	CHL	CHB-C4A	-2.26	1.32	1.37
20	3	1011	CLA	C3A-C2A	-2.26	1.52	1.54
20	A	806	CLA	MG-NA	-2.26	2.00	2.06
20	B	827	CLA	C1D-C2D	-2.26	1.40	1.45
20	B	841	CLA	C1D-C2D	-2.26	1.40	1.45
20	4	306	CLA	C1B-NB	2.26	1.40	1.37
20	G	202	CLA	C1D-C2D	-2.26	1.40	1.45
20	B	803	CLA	C1D-C2D	-2.26	1.40	1.45
20	6	312	CLA	C1B-NB	2.26	1.40	1.37
20	A	830	CLA	C1C-C2C	2.25	1.48	1.44
20	4	305	CLA	C3D-C4D	-2.25	1.39	1.44
20	8	316	CLA	C1D-C2D	-2.25	1.40	1.45
20	B	823	CLA	C1D-C2D	-2.25	1.40	1.45
20	5	306	CLA	C1D-C2D	-2.25	1.40	1.45
20	3	1009	CLA	C1D-C2D	-2.25	1.40	1.45
20	B	820	CLA	C1C-C2C	2.25	1.48	1.44
20	5	301	CLA	C1B-NB	2.25	1.40	1.37
20	8	306	CLA	C3A-C2A	-2.25	1.48	1.54
29	7	1012	CHL	C1D-C2D	-2.25	1.40	1.45
20	6	320	CLA	C1D-C2D	-2.25	1.40	1.45
20	B	832	CLA	C1D-C2D	-2.24	1.40	1.45
20	3	1007	CLA	C1D-C2D	-2.24	1.40	1.45
20	1	1014	CLA	C1D-C2D	-2.24	1.40	1.45
20	A	825	CLA	C1D-C2D	-2.24	1.40	1.45
20	8	306	CLA	C1D-C2D	-2.24	1.40	1.45
30	8	304	XAT	C32-C33	-2.24	1.41	1.45
20	K	202	CLA	C2D-C3D	2.24	1.42	1.36
20	8	312	CLA	C3D-C4D	-2.24	1.39	1.44
29	4	316	CHL	C3D-C4D	-2.24	1.39	1.44
20	A	827	CLA	C1D-C2D	-2.24	1.40	1.45
29	3	1014	CHL	C1D-C2D	-2.24	1.40	1.45
29	0	315	CHL	CHB-C4A	-2.24	1.32	1.37
20	B	810	CLA	C1C-C2C	2.24	1.48	1.44
29	0	314	CHL	C1D-C2D	-2.24	1.40	1.45
20	A	806	CLA	C1D-C2D	-2.24	1.40	1.45
20	7	1011	CLA	C3D-C4D	-2.24	1.39	1.44
20	7	1009	CLA	C1D-ND	2.24	1.40	1.37
20	5	309	CLA	C1B-NB	2.24	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	309	CLA	C1B-NB	2.23	1.40	1.37
20	K	201	CLA	C1D-C2D	-2.22	1.40	1.45
20	L	204	CLA	C1D-C2D	-2.22	1.40	1.45
20	A	822	CLA	C1D-C2D	-2.22	1.40	1.45
20	1	1010	CLA	C3D-C4D	-2.22	1.39	1.44
20	6	305	CLA	C1C-C2C	2.22	1.48	1.44
20	A	811	CLA	C1D-C2D	-2.22	1.40	1.45
20	A	834	CLA	C1D-C2D	-2.22	1.40	1.45
20	5	321	CLA	C3D-C4D	-2.22	1.39	1.44
20	1	1003	CLA	C1D-C2D	-2.22	1.41	1.45
20	5	308	CLA	C1C-C2C	2.21	1.48	1.44
20	A	802	CLA	C1D-C2D	-2.21	1.41	1.45
20	1	1007	CLA	C3D-C4D	-2.21	1.39	1.44
29	4	315	CHL	C1D-C2D	-2.21	1.41	1.45
20	8	316	CLA	C3D-C4D	-2.21	1.39	1.44
20	5	315	CLA	C1D-C2D	-2.21	1.41	1.45
20	B	821	CLA	C3D-C4D	-2.20	1.39	1.44
20	6	311	CLA	C3D-C4D	-2.20	1.39	1.44
20	4	314	CLA	C1D-C2D	-2.20	1.41	1.45
20	A	810	CLA	C1D-C2D	-2.20	1.41	1.45
20	A	833	CLA	C1B-NB	2.20	1.40	1.37
20	A	808	CLA	C1D-C2D	-2.20	1.41	1.45
20	3	1011	CLA	C1D-C2D	-2.20	1.41	1.45
20	1	1011	CLA	C1D-C2D	-2.20	1.41	1.45
20	3	1016	CLA	C1B-NB	2.20	1.40	1.37
20	J	102	CLA	C1D-C2D	-2.20	1.41	1.45
20	A	812	CLA	C1C-C2C	2.20	1.48	1.44
24	6	302	BCR	C24-C25	2.19	1.52	1.45
20	B	826	CLA	C1D-C2D	-2.19	1.41	1.45
20	5	310	CLA	C3D-C4D	-2.19	1.39	1.44
20	A	832	CLA	C1C-C2C	2.19	1.48	1.44
20	3	1005	CLA	C3D-C4D	-2.19	1.39	1.44
20	1	1017	CLA	C1D-C2D	-2.19	1.41	1.45
20	3	1015	CLA	C3D-C4D	-2.19	1.39	1.44
20	5	304	CLA	C1C-C2C	2.19	1.48	1.44
29	6	317	CHL	C3D-C4D	-2.19	1.39	1.44
20	0	305	CLA	C1D-C2D	-2.19	1.41	1.45
20	A	852	CLA	C1D-C2D	-2.18	1.41	1.45
30	8	304	XAT	C28-C29	-2.18	1.41	1.45
20	4	307	CLA	C1C-C2C	2.18	1.48	1.44
20	0	308	CLA	C3D-C4D	-2.18	1.39	1.44
20	B	802	CLA	C1D-C2D	-2.18	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	301	CLA	C3D-C4D	-2.18	1.39	1.44
20	B	830	CLA	C1C-C2C	2.18	1.48	1.44
20	B	838	CLA	C1C-C2C	2.18	1.48	1.44
20	4	310	CLA	C1D-C2D	-2.18	1.41	1.45
20	B	837	CLA	C1D-C2D	-2.18	1.41	1.45
20	B	830	CLA	C1D-C2D	-2.18	1.41	1.45
20	B	822	CLA	C3D-C4D	-2.18	1.39	1.44
29	6	316	CHL	C3D-C4D	-2.18	1.39	1.44
20	B	815	CLA	C1D-C2D	-2.18	1.41	1.45
30	7	1002	XAT	C28-C29	-2.18	1.41	1.45
20	A	810	CLA	C1B-NB	2.18	1.40	1.37
20	A	836	CLA	C1D-C2D	-2.17	1.41	1.45
20	A	835	CLA	C1D-C2D	-2.17	1.41	1.45
20	B	808	CLA	C1D-C2D	-2.17	1.41	1.45
29	4	315	CHL	CHB-C4A	-2.17	1.32	1.37
20	A	807	CLA	C1D-C2D	-2.17	1.41	1.45
20	A	804	CLA	C1D-C2D	-2.17	1.41	1.45
20	G	201	CLA	C1D-C2D	-2.17	1.41	1.45
20	B	814	CLA	C1D-C2D	-2.17	1.41	1.45
20	1	1004	CLA	C1B-NB	2.17	1.40	1.37
20	7	1007	CLA	C1D-C2D	-2.17	1.41	1.45
20	8	309	CLA	MG-NC	-2.16	2.01	2.06
20	A	813	CLA	C1D-C2D	-2.16	1.41	1.45
20	L	202	CLA	C1D-C2D	-2.16	1.41	1.45
20	B	813	CLA	C1D-C2D	-2.16	1.41	1.45
20	L	201	CLA	C1D-C2D	-2.16	1.41	1.45
20	3	1005	CLA	C1B-NB	2.16	1.40	1.37
20	0	307	CLA	CHD-C4C	-2.16	1.34	1.39
20	B	807	CLA	C1D-C2D	-2.16	1.41	1.45
20	A	802	CLA	C3D-C4D	-2.16	1.39	1.44
20	B	827	CLA	C3D-C4D	-2.16	1.39	1.44
29	4	315	CHL	C3D-C4D	-2.16	1.39	1.44
29	5	316	CHL	C3B-C2B	-2.15	1.33	1.41
20	6	318	CLA	MG-NA	-2.15	2.01	2.06
20	B	825	CLA	C1D-C2D	-2.15	1.41	1.45
20	7	1006	CLA	C1B-NB	2.15	1.40	1.37
20	A	808	CLA	C3D-C4D	-2.15	1.39	1.44
29	7	1013	CHL	C3D-C4D	-2.15	1.39	1.44
29	0	315	CHL	C1D-C2D	-2.15	1.41	1.45
29	4	313	CHL	C1D-C2D	-2.15	1.41	1.45
20	3	1017	CLA	C3D-C4D	-2.15	1.39	1.44
20	6	306	CLA	C1B-NB	2.14	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	832	CLA	C3D-C4D	-2.14	1.39	1.44
24	7	1003	BCR	C16-C17	2.14	1.50	1.43
20	5	315	CLA	C3D-C4D	-2.14	1.39	1.44
20	B	831	CLA	C1D-C2D	-2.14	1.41	1.45
29	8	314	CHL	C1D-C2D	-2.14	1.41	1.45
20	5	308	CLA	C3D-C4D	-2.13	1.39	1.44
20	A	840	CLA	C1B-NB	2.13	1.40	1.37
29	4	312	CHL	CHB-C4A	-2.13	1.32	1.37
20	8	306	CLA	CHD-C4C	-2.13	1.34	1.39
20	3	1010	CLA	C1B-NB	2.13	1.40	1.37
20	8	308	CLA	C3D-C4D	-2.13	1.39	1.44
29	5	313	CHL	C3A-C2A	-2.13	1.48	1.54
20	8	308	CLA	C1D-C2D	-2.13	1.41	1.45
20	A	828	CLA	C3D-C4D	-2.13	1.39	1.44
20	3	1017	CLA	C1D-C2D	-2.12	1.41	1.45
20	3	1009	CLA	MG-NC	-2.12	2.01	2.06
20	5	322	CLA	C1D-C2D	-2.12	1.41	1.45
29	3	1014	CHL	C3D-C4D	-2.12	1.39	1.44
23	3	1019	LHG	O7-C7	-2.12	1.34	1.42
20	A	808	CLA	C1B-NB	2.12	1.40	1.37
20	4	306	CLA	C1C-C2C	2.11	1.48	1.44
20	A	839	CLA	C1D-C2D	-2.11	1.41	1.45
20	3	1015	CLA	C1C-C2C	2.11	1.48	1.44
20	7	1005	CLA	C3D-C4D	-2.11	1.39	1.44
20	B	834	CLA	C3D-C4D	-2.11	1.39	1.44
20	5	301	CLA	C3D-C4D	-2.11	1.39	1.44
20	B	835	CLA	C1D-C2D	-2.11	1.41	1.45
20	3	1008	CLA	C1D-C2D	-2.11	1.41	1.45
20	7	1014	CLA	C1D-C2D	-2.11	1.41	1.45
20	7	1008	CLA	C3D-C4D	-2.11	1.39	1.44
20	3	1009	CLA	C1C-C2C	2.11	1.48	1.44
20	6	310	CLA	C1C-C2C	2.10	1.48	1.44
20	A	803	CLA	C1D-C2D	-2.10	1.41	1.45
20	6	307	CLA	C1B-NB	2.10	1.40	1.37
20	6	318	CLA	C1D-C2D	-2.10	1.41	1.45
20	A	835	CLA	C3D-C4D	-2.10	1.39	1.44
29	7	1013	CHL	C3B-C2B	-2.10	1.34	1.41
29	8	317	CHL	C1D-C2D	-2.10	1.41	1.45
20	7	1005	CLA	CHC-C1C	-2.10	1.34	1.38
29	0	314	CHL	CHB-C4A	-2.10	1.32	1.37
20	F	302	CLA	C3D-C4D	-2.10	1.39	1.44
20	B	836	CLA	C3D-C4D	-2.09	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	304	CLA	MG-NC	-2.09	2.01	2.06
20	B	828	CLA	C3D-C4D	-2.09	1.39	1.44
20	4	304	CLA	C1D-C2D	-2.09	1.41	1.45
20	F	303	CLA	CHD-C4C	-2.09	1.34	1.39
24	1	1001	BCR	C24-C25	2.09	1.52	1.45
20	A	804	CLA	C3D-C4D	-2.09	1.39	1.44
20	B	803	CLA	C3D-C4D	-2.09	1.39	1.44
20	7	1014	CLA	C3D-C4D	-2.09	1.39	1.44
20	6	312	CLA	C3D-C4D	-2.08	1.39	1.44
20	A	828	CLA	C1D-C2D	-2.08	1.41	1.45
20	0	316	CLA	C1D-C2D	-2.08	1.41	1.45
20	5	312	CLA	C3D-C4D	-2.08	1.39	1.44
29	1	1015	CHL	C3D-C4D	-2.08	1.39	1.44
20	B	825	CLA	C3D-C4D	-2.08	1.39	1.44
29	7	1012	CHL	C3D-C4D	-2.08	1.39	1.44
20	A	833	CLA	C3D-C4D	-2.08	1.39	1.44
20	6	311	CLA	C1C-C2C	2.08	1.48	1.44
24	H	201	BCR	C15-C14	2.08	1.49	1.43
20	A	836	CLA	C3D-C4D	-2.07	1.39	1.44
30	7	1002	XAT	C32-C33	-2.07	1.41	1.45
20	6	312	CLA	C1D-ND	2.07	1.40	1.37
29	0	314	CHL	C3D-C4D	-2.07	1.39	1.44
20	A	814	CLA	C3D-C4D	-2.07	1.39	1.44
20	A	801	CLA	C1D-C2D	-2.06	1.41	1.45
20	B	818	CLA	C1C-C2C	2.06	1.48	1.44
20	B	810	CLA	C1D-C2D	-2.06	1.41	1.45
29	4	312	CHL	C2C-C1C	2.06	1.49	1.44
29	0	317	CHL	C1D-C2D	-2.06	1.41	1.45
20	1	1008	CLA	C3D-C4D	-2.06	1.39	1.44
20	3	1007	CLA	C3D-C4D	-2.06	1.39	1.44
20	1	1008	CLA	C1D-C2D	-2.05	1.41	1.45
20	1	1008	CLA	C1C-C2C	2.05	1.48	1.44
20	7	1009	CLA	C3D-C4D	-2.05	1.39	1.44
30	7	1002	XAT	C12-C13	-2.05	1.41	1.45
29	0	317	CHL	C3D-C4D	-2.05	1.39	1.44
20	J	102	CLA	C3D-C4D	-2.05	1.39	1.44
20	4	304	CLA	C3D-C4D	-2.05	1.39	1.44
20	3	1010	CLA	C1D-ND	2.05	1.40	1.37
20	A	809	CLA	C3D-C4D	-2.05	1.39	1.44
20	A	822	CLA	C1C-C2C	2.05	1.48	1.44
20	A	821	CLA	C3D-C4D	-2.05	1.39	1.44
20	B	840	CLA	C1D-C2D	-2.05	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	315	CHL	C1D-C2D	-2.05	1.41	1.45
20	3	1013	CLA	C1D-C2D	-2.05	1.41	1.45
20	A	809	CLA	C1D-C2D	-2.04	1.41	1.45
29	1	1015	CHL	C1D-C2D	-2.04	1.41	1.45
20	B	833	CLA	C1D-C2D	-2.04	1.41	1.45
20	B	831	CLA	C3D-C4D	-2.04	1.39	1.44
20	8	309	CLA	C3D-C4D	-2.04	1.39	1.44
20	B	817	CLA	C3D-C4D	-2.03	1.39	1.44
29	7	1015	CHL	CHB-C4A	-2.03	1.32	1.37
20	6	320	CLA	C3D-C4D	-2.03	1.39	1.44
20	6	318	CLA	C3D-C4D	-2.03	1.39	1.44
29	6	313	CHL	CHB-C4A	-2.03	1.32	1.37
20	L	202	CLA	C1C-C2C	2.03	1.48	1.44
20	B	817	CLA	C1B-NB	2.03	1.40	1.37
20	5	322	CLA	C3D-C4D	-2.02	1.39	1.44
29	5	317	CHL	C3D-C4D	-2.02	1.39	1.44
20	5	310	CLA	CHD-C4C	-2.02	1.34	1.39
29	1	1012	CHL	C3D-C4D	-2.02	1.39	1.44
20	A	839	CLA	C3D-C4D	-2.02	1.39	1.44
20	0	305	CLA	C3D-C4D	-2.02	1.39	1.44
20	8	309	CLA	C1C-C2C	2.02	1.48	1.44
20	7	1014	CLA	C3A-C2A	-2.02	1.48	1.54
20	3	1008	CLA	C3D-C4D	-2.01	1.39	1.44
20	8	313	CLA	C1D-C2D	-2.01	1.41	1.45
20	B	824	CLA	C3D-C4D	-2.01	1.39	1.44
20	A	806	CLA	C3D-C4D	-2.01	1.39	1.44
20	6	305	CLA	C3D-C4D	-2.01	1.39	1.44
20	A	807	CLA	C3D-C4D	-2.01	1.39	1.44
20	B	819	CLA	C3D-C4D	-2.01	1.39	1.44
20	5	307	CLA	C3D-C4D	-2.00	1.39	1.44
20	5	315	CLA	C3B-C2B	-2.00	1.34	1.41
20	A	829	CLA	C3D-C4D	-2.00	1.39	1.44

All (1866) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	1013	CHL	C4A-NA-C1A	-9.89	102.26	106.71
29	6	314	CHL	C4A-NA-C1A	-9.07	102.63	106.71
29	1	1015	CHL	C4A-NA-C1A	-9.04	102.64	106.71
20	K	202	CLA	C1C-NC-C4C	-8.95	102.68	106.71
29	5	313	CHL	C4A-NA-C1A	-8.26	102.99	106.71
29	3	1014	CHL	C4A-NA-C1A	-8.25	103.00	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	1012	CHL	C4A-NA-C1A	-7.95	103.13	106.71
29	1	1012	CHL	C4A-NA-C1A	-7.70	103.24	106.71
29	7	1015	CHL	C4A-NA-C1A	-7.69	103.25	106.71
29	0	317	CHL	C4A-NA-C1A	-7.56	103.31	106.71
24	6	302	BCR	C16-C15-C14	7.49	138.82	123.47
29	8	317	CHL	C4A-NA-C1A	-7.47	103.35	106.71
29	7	1017	CHL	C4A-NA-C1A	-7.38	103.39	106.71
29	4	312	CHL	C4A-NA-C1A	-7.20	103.47	106.71
29	5	316	CHL	C4A-NA-C1A	-7.12	103.51	106.71
29	0	315	CHL	C4A-NA-C1A	-6.98	103.57	106.71
24	8	302	BCR	C16-C15-C14	6.97	137.76	123.47
24	7	1003	BCR	C16-C15-C14	6.78	137.36	123.47
24	B	804	BCR	C16-C15-C14	6.64	137.07	123.47
20	8	306	CLA	C4A-NA-C1A	-6.63	103.72	106.71
23	0	302	LHG	O3-P-O5	-6.56	83.44	109.07
29	8	315	CHL	C4A-NA-C1A	-6.55	103.76	106.71
20	5	307	CLA	C4A-NA-C1A	-6.49	103.79	106.71
29	8	314	CHL	C4A-NA-C1A	-6.46	103.80	106.71
20	4	307	CLA	CAC-C3C-C4C	-6.41	116.49	124.81
29	6	316	CHL	C4A-NA-C1A	-6.40	103.83	106.71
24	B	804	BCR	C15-C16-C17	-6.29	110.58	123.47
29	4	313	CHL	C4A-NA-C1A	-6.26	103.89	106.71
20	8	309	CLA	C4A-NA-C1A	-6.23	103.91	106.71
29	6	313	CHL	C4A-NA-C1A	-6.18	103.93	106.71
24	4	302	BCR	C16-C15-C14	6.07	135.91	123.47
20	7	1007	CLA	C4A-NA-C1A	-6.03	104.00	106.71
20	B	820	CLA	C4A-NA-C1A	-6.00	104.01	106.71
29	6	317	CHL	C4A-NA-C1A	-5.99	104.01	106.71
29	5	314	CHL	C4A-NA-C1A	-5.97	104.02	106.71
25	5	319	DGD	O5D-C1E-C2E	5.97	117.62	108.30
20	A	837	CLA	C4A-NA-C1A	-5.93	104.04	106.71
20	5	311	CLA	C4A-NA-C1A	-5.91	104.05	106.71
29	0	314	CHL	C4A-NA-C1A	-5.87	104.07	106.71
20	B	803	CLA	C4A-NA-C1A	-5.86	104.07	106.71
20	8	308	CLA	C4A-NA-C1A	-5.84	104.08	106.71
20	A	804	CLA	C4A-NA-C1A	-5.72	104.13	106.71
20	B	813	CLA	C4A-NA-C1A	-5.71	104.14	106.71
29	4	316	CHL	C4A-NA-C1A	-5.67	104.16	106.71
20	A	834	CLA	C4A-NA-C1A	-5.65	104.17	106.71
29	5	317	CHL	C4A-NA-C1A	-5.58	104.20	106.71
24	G	205	BCR	C16-C15-C14	5.55	134.85	123.47
20	A	833	CLA	C4A-NA-C1A	-5.54	104.21	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	318	CLA	C4A-NA-C1A	-5.44	104.26	106.71
20	5	309	CLA	C4A-NA-C1A	-5.41	104.27	106.71
29	1	1013	CHL	C4A-NA-C1A	-5.41	104.28	106.71
24	1	1001	BCR	C16-C15-C14	5.40	134.54	123.47
20	1	1004	CLA	C4A-NA-C1A	-5.38	104.29	106.71
20	3	1008	CLA	C4A-NA-C1A	-5.38	104.29	106.71
20	3	1006	CLA	C4A-NA-C1A	-5.36	104.30	106.71
20	A	821	CLA	C4A-NA-C1A	-5.33	104.31	106.71
20	6	312	CLA	CHD-C1D-ND	-5.32	119.57	124.45
20	B	827	CLA	C4A-NA-C1A	-5.28	104.33	106.71
20	3	1013	CLA	C4A-NA-C1A	-5.28	104.33	106.71
20	B	822	CLA	C4A-NA-C1A	-5.28	104.33	106.71
20	7	1009	CLA	C4A-NA-C1A	-5.22	104.36	106.71
20	B	824	CLA	C4A-NA-C1A	-5.18	104.38	106.71
20	B	828	CLA	C4A-NA-C1A	-5.17	104.38	106.71
20	B	815	CLA	C4A-NA-C1A	-5.14	104.39	106.71
20	B	826	CLA	C4A-NA-C1A	-5.13	104.40	106.71
20	1	1010	CLA	C4A-NA-C1A	-5.13	104.40	106.71
20	A	828	CLA	C4A-NA-C1A	-5.12	104.41	106.71
20	4	308	CLA	C4A-NA-C1A	-5.08	104.42	106.71
24	A	845	BCR	C8-C7-C6	5.06	141.41	127.20
20	B	810	CLA	C4A-NA-C1A	-5.05	104.44	106.71
20	8	316	CLA	C4A-NA-C1A	-5.00	104.46	106.71
20	A	806	CLA	C4A-NA-C1A	-4.99	104.46	106.71
20	5	301	CLA	C4A-NA-C1A	-4.97	104.47	106.71
20	A	814	CLA	C4A-NA-C1A	-4.95	104.48	106.71
20	A	820	CLA	C4A-NA-C1A	-4.94	104.48	106.71
20	A	831	CLA	C4A-NA-C1A	-4.94	104.48	106.71
20	A	801	CLA	CHD-C1D-ND	-4.84	120.01	124.45
27	8	319	LMG	C7-O1-C1	4.83	123.17	113.74
20	B	821	CLA	C4A-NA-C1A	-4.82	104.54	106.71
29	4	315	CHL	C4A-NA-C1A	-4.81	104.54	106.71
20	4	307	CLA	CHD-C1D-ND	-4.80	120.04	124.45
20	5	305	CLA	C4A-NA-C1A	-4.78	104.56	106.71
30	5	303	XAT	O24-C25-C24	4.77	116.97	113.38
20	A	802	CLA	C4A-NA-C1A	-4.76	104.56	106.71
24	A	845	BCR	C7-C8-C9	-4.75	119.05	126.23
20	A	825	CLA	C4A-NA-C1A	-4.75	104.57	106.71
20	6	320	CLA	CHB-C1B-NB	-4.71	119.27	124.26
20	A	827	CLA	C4A-NA-C1A	-4.70	104.59	106.71
20	A	803	CLA	C4A-NA-C1A	-4.68	104.60	106.71
20	7	1005	CLA	C4A-NA-C1A	-4.67	104.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	321	CLA	C4A-NA-C1A	-4.66	104.61	106.71
20	5	318	CLA	CHD-C1D-ND	-4.62	120.20	124.45
20	G	202	CLA	C4A-NA-C1A	-4.62	104.63	106.71
20	A	840	CLA	CHD-C1D-ND	-4.61	120.22	124.45
29	5	314	CHL	CHD-C1D-ND	-4.60	120.22	124.45
24	B	843	BCR	C19-C18-C17	4.60	126.00	118.94
20	4	307	CLA	CHB-C1B-NB	-4.59	119.39	124.26
20	B	811	CLA	C4A-NA-C1A	-4.59	104.64	106.71
24	7	1003	BCR	C21-C20-C19	4.59	137.53	123.22
20	B	836	CLA	C4A-NA-C1A	-4.58	104.65	106.71
20	0	306	CLA	C4A-NA-C1A	-4.58	104.65	106.71
20	3	1009	CLA	C4A-NA-C1A	-4.58	104.65	106.71
20	8	310	CLA	C4A-NA-C1A	-4.57	104.65	106.71
20	0	301	CLA	C4A-NA-C1A	-4.57	104.65	106.71
20	0	305	CLA	C4A-NA-C1A	-4.56	104.66	106.71
20	A	830	CLA	C4A-NA-C1A	-4.55	104.66	106.71
24	B	843	BCR	C21-C20-C19	4.52	137.33	123.22
20	B	835	CLA	C4A-NA-C1A	-4.52	104.67	106.71
20	8	313	CLA	CHB-C1B-NB	-4.50	119.49	124.26
20	8	313	CLA	C4A-NA-C1A	-4.49	104.69	106.71
20	3	1008	CLA	CHD-C1D-ND	-4.48	120.34	124.45
20	A	817	CLA	C4A-NA-C1A	-4.48	104.69	106.71
20	4	307	CLA	C1D-ND-C4D	-4.47	103.16	106.33
20	B	802	CLA	C4A-NA-C1A	-4.46	104.70	106.71
20	A	823	CLA	CHB-C1B-NB	-4.46	119.53	124.26
20	B	838	CLA	C4A-NA-C1A	-4.45	104.70	106.71
20	A	852	CLA	C4A-NA-C1A	-4.45	104.71	106.71
20	B	824	CLA	CHD-C1D-ND	-4.45	120.37	124.45
20	B	809	CLA	C4A-NA-C1A	-4.44	104.71	106.71
20	4	307	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
20	B	816	CLA	C4A-NA-C1A	-4.42	104.72	106.71
30	7	1002	XAT	C19-C9-C10	-4.42	116.73	122.92
20	A	824	CLA	CHB-C1B-NB	-4.42	119.58	124.26
20	A	807	CLA	C4A-NA-C1A	-4.39	104.73	106.71
20	A	838	CLA	C4A-NA-C1A	-4.39	104.73	106.71
20	3	1007	CLA	C4A-NA-C1A	-4.38	104.73	106.71
20	K	202	CLA	C4A-NA-C1A	-4.38	104.74	106.71
20	F	302	CLA	C4A-NA-C1A	-4.37	104.74	106.71
20	A	822	CLA	C4A-NA-C1A	-4.37	104.74	106.71
20	A	815	CLA	CHB-C1B-NB	-4.35	119.65	124.26
20	0	309	CLA	CHB-C1B-NB	-4.35	119.65	124.26
20	A	813	CLA	C4A-NA-C1A	-4.35	104.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	815	CLA	C2C-C1C-NC	4.34	114.04	109.97
24	G	204	BCR	C16-C15-C14	4.33	132.35	123.47
20	A	808	CLA	CHB-C1B-NB	-4.33	119.67	124.26
20	6	310	CLA	C4A-NA-C1A	-4.33	104.76	106.71
20	A	836	CLA	C4A-NA-C1A	-4.31	104.77	106.71
20	B	825	CLA	C4A-NA-C1A	-4.31	104.77	106.71
29	4	313	CHL	CHD-C1D-ND	-4.29	120.51	124.45
20	7	1014	CLA	C4A-NA-C1A	-4.29	104.78	106.71
20	B	819	CLA	C4A-NA-C1A	-4.29	104.78	106.71
20	6	315	CLA	CHB-C1B-NB	-4.29	119.72	124.26
20	B	839	CLA	C4A-NA-C1A	-4.28	104.78	106.71
24	3	1003	BCR	C16-C15-C14	4.28	132.25	123.47
20	6	306	CLA	C4A-NA-C1A	-4.28	104.78	106.71
20	6	312	CLA	C4A-NA-C1A	-4.27	104.79	106.71
20	6	320	CLA	CHD-C1D-ND	-4.25	120.55	124.45
20	1	1006	CLA	CHD-C1D-ND	-4.25	120.55	124.45
20	7	1007	CLA	CHB-C1B-NB	-4.24	119.77	124.26
20	B	823	CLA	C4A-NA-C1A	-4.23	104.81	106.71
20	4	310	CLA	CHD-C1D-ND	-4.22	120.57	124.45
30	8	304	XAT	C19-C9-C10	-4.22	117.01	122.92
20	B	817	CLA	C4A-NA-C1A	-4.22	104.81	106.71
20	0	312	CLA	C4A-NA-C1A	-4.22	104.81	106.71
20	4	305	CLA	C4A-NA-C1A	-4.22	104.81	106.71
20	B	832	CLA	C4A-NA-C1A	-4.20	104.82	106.71
20	1	1008	CLA	C4A-NA-C1A	-4.20	104.82	106.71
20	7	1005	CLA	CHB-C1B-NB	-4.20	119.81	124.26
20	L	203	CLA	C4A-NA-C1A	-4.20	104.82	106.71
20	0	316	CLA	C4A-NA-C1A	-4.19	104.82	106.71
20	A	801	CLA	CHB-C1B-NB	-4.18	119.83	124.26
20	1	1011	CLA	CHD-C1D-ND	-4.17	120.63	124.45
20	6	309	CLA	CHB-C1B-NB	-4.15	119.86	124.26
20	8	312	CLA	C4A-NA-C1A	-4.15	104.84	106.71
20	3	1016	CLA	CHB-C1B-NB	-4.14	119.87	124.26
30	8	304	XAT	C39-C29-C30	-4.13	117.14	122.92
30	7	1002	XAT	C39-C29-C30	-4.12	117.14	122.92
20	1	1017	CLA	CHC-C1C-NC	4.11	130.44	124.20
29	7	1013	CHL	CHD-C1D-ND	-4.10	120.69	124.45
20	1	1007	CLA	CHB-C1B-NB	-4.09	119.93	124.26
20	A	824	CLA	C2C-C1C-NC	4.08	113.80	109.97
24	B	804	BCR	C16-C17-C18	4.08	133.13	127.31
20	6	309	CLA	C4A-NA-C1A	-4.07	104.88	106.71
20	7	1005	CLA	C1D-ND-C4D	-4.06	103.45	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	307	CLA	C4A-NA-C1A	-4.05	104.88	106.71
20	B	807	CLA	C4A-NA-C1A	-4.04	104.89	106.71
30	7	1002	XAT	C35-C15-C14	4.03	131.73	123.47
20	5	308	CLA	CHB-C1B-NB	-4.02	120.00	124.26
20	0	305	CLA	CHD-C1D-ND	-4.02	120.76	124.45
20	7	1008	CLA	CHB-C1B-NB	-4.01	120.01	124.26
20	4	310	CLA	C1D-ND-C4D	-4.01	103.49	106.33
30	8	304	XAT	C35-C15-C14	4.01	131.68	123.47
20	A	810	CLA	CHD-C1D-ND	-4.01	120.77	124.45
20	8	305	CLA	CHD-C1D-ND	-4.00	120.78	124.45
29	8	315	CHL	CHD-C1D-ND	-4.00	120.78	124.45
20	8	311	CLA	CHD-C1D-ND	-4.00	120.78	124.45
20	B	837	CLA	C4A-NA-C1A	-3.99	104.91	106.71
20	5	301	CLA	CHD-C1D-ND	-3.99	120.79	124.45
20	1	1014	CLA	CHC-C1C-NC	3.98	130.25	124.20
20	F	305	CLA	C4A-NA-C1A	-3.98	104.92	106.71
20	B	814	CLA	C4A-NA-C1A	-3.98	104.92	106.71
20	6	301	CLA	C4A-NA-C1A	-3.98	104.92	106.71
20	6	308	CLA	C4A-NA-C1A	-3.98	104.92	106.71
20	B	839	CLA	CHD-C1D-ND	-3.97	120.80	124.45
20	0	312	CLA	CHD-C1D-ND	-3.96	120.82	124.45
20	5	318	CLA	C4A-NA-C1A	-3.96	104.93	106.71
20	0	310	CLA	C4A-NA-C1A	-3.94	104.94	106.71
20	6	315	CLA	C4A-NA-C1A	-3.93	104.94	106.71
20	A	828	CLA	CHD-C1D-ND	-3.93	120.85	124.45
20	3	1011	CLA	C4A-NA-C1A	-3.92	104.94	106.71
20	G	201	CLA	C4A-NA-C1A	-3.90	104.95	106.71
20	1	1017	CLA	CHB-C1B-NB	-3.90	120.12	124.26
20	A	818	CLA	C4A-NA-C1A	-3.89	104.96	106.71
24	B	804	BCR	C19-C18-C17	3.89	124.90	118.94
20	3	1010	CLA	CHB-C1B-NB	-3.89	120.14	124.26
20	4	307	CLA	C4C-C3C-C2C	3.88	112.56	106.90
20	0	308	CLA	C4A-NA-C1A	-3.88	104.96	106.71
20	K	202	CLA	C1B-NB-C4B	-3.88	103.58	106.33
20	5	307	CLA	CHB-C1B-NB	-3.88	120.15	124.26
20	1	1017	CLA	CHD-C1D-ND	-3.88	120.89	124.45
20	4	309	CLA	CHB-C1B-NB	-3.87	120.16	124.26
20	A	805	CLA	CHB-C1B-NB	-3.86	120.17	124.26
24	A	845	BCR	C11-C10-C9	3.86	132.82	127.31
29	4	312	CHL	CHA-C1A-NA	-3.85	117.57	126.40
20	F	303	CLA	CHD-C1D-ND	-3.85	120.91	124.45
20	4	311	CLA	CHD-C1D-ND	-3.85	120.92	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	806	CLA	C4A-NA-C1A	-3.85	104.98	106.71
25	5	319	DGD	O2G-C1B-C2B	3.84	119.78	111.50
20	A	811	CLA	C4A-NA-C1A	-3.84	104.98	106.71
20	5	322	CLA	CHD-C1D-ND	-3.84	120.93	124.45
20	1	1007	CLA	CHC-C1C-NC	3.84	130.02	124.20
20	K	201	CLA	CHB-C1B-NB	-3.83	120.20	124.26
20	3	1015	CLA	CHB-C1B-NB	-3.82	120.22	124.26
20	A	838	CLA	C2C-C1C-NC	3.82	113.55	109.97
20	6	308	CLA	CHB-C1B-NB	-3.81	120.23	124.26
20	L	204	CLA	CHB-C1B-NB	-3.80	120.24	124.26
20	L	201	CLA	CHD-C1D-ND	-3.80	120.97	124.45
20	B	810	CLA	CHB-C1B-NB	-3.78	120.26	124.26
20	A	807	CLA	CHD-C1D-ND	-3.78	120.98	124.45
20	4	304	CLA	CHD-C1D-ND	-3.77	120.99	124.45
20	0	316	CLA	CHD-C1D-ND	-3.77	120.99	124.45
20	A	836	CLA	CHD-C1D-ND	-3.76	121.00	124.45
20	3	1017	CLA	C4A-NA-C1A	-3.76	105.02	106.71
20	A	812	CLA	C4A-NA-C1A	-3.76	105.02	106.71
20	5	315	CLA	CHB-C1B-NB	-3.75	120.28	124.26
20	0	313	CLA	CHB-C1B-NB	-3.75	120.28	124.26
20	A	835	CLA	CHB-C1B-NB	-3.75	120.29	124.26
20	A	835	CLA	C2C-C1C-NC	3.75	113.48	109.97
20	1	1006	CLA	C4A-NA-C1A	-3.74	105.02	106.71
20	4	314	CLA	C4A-NA-C1A	-3.74	105.03	106.71
24	7	1003	BCR	C15-C14-C13	3.74	132.65	127.31
20	A	815	CLA	CHC-C1C-C2C	-3.74	116.35	126.73
20	1	1003	CLA	CHD-C1D-ND	-3.74	121.02	124.45
20	6	320	CLA	CHC-C1C-NC	3.74	129.87	124.20
20	8	307	CLA	C2C-C1C-NC	3.73	113.47	109.97
20	A	816	CLA	C4A-NA-C1A	-3.73	105.03	106.71
20	4	310	CLA	C2C-C1C-NC	3.73	113.47	109.97
20	5	310	CLA	CHC-C1C-NC	3.72	129.85	124.20
29	4	316	CHL	C2C-C3C-C4C	3.72	109.14	106.49
20	5	312	CLA	CHC-C1C-NC	3.71	129.84	124.20
20	A	824	CLA	CHC-C1C-C2C	-3.71	116.42	126.73
29	1	1013	CHL	CHD-C1D-ND	-3.71	121.04	124.45
20	7	1009	CLA	CHB-C1B-NB	-3.70	120.33	124.26
20	B	817	CLA	CHD-C1D-ND	-3.70	121.05	124.45
20	A	851	CLA	C4A-NA-C1A	-3.69	105.05	106.71
25	5	319	DGD	C3G-C2G-C1G	-3.68	103.07	111.79
20	0	308	CLA	CHB-C1B-NB	-3.68	120.36	124.26
20	1	1007	CLA	CHD-C1D-ND	-3.68	121.07	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	1011	CLA	CHD-C1D-ND	-3.68	121.07	124.45
23	0	302	LHG	O4-P-O3	-3.68	90.67	107.75
20	A	801	CLA	CHC-C1C-NC	3.67	129.78	124.20
20	A	840	CLA	CHB-C1B-NB	-3.67	120.37	124.26
20	B	841	CLA	C4A-NA-C1A	-3.67	105.06	106.71
20	7	1005	CLA	C2C-C1C-NC	3.66	113.40	109.97
20	G	203	CLA	CHD-C1D-ND	-3.66	121.09	124.45
20	1	1014	CLA	CHD-C1D-ND	-3.66	121.09	124.45
20	A	823	CLA	C2C-C1C-NC	3.66	113.40	109.97
20	A	817	CLA	CHD-C1D-ND	-3.66	121.09	124.45
20	B	837	CLA	CHB-C1B-NB	-3.65	120.39	124.26
20	K	201	CLA	CHD-C1D-ND	-3.65	121.10	124.45
29	8	315	CHL	C2C-C3C-C4C	3.65	109.09	106.49
20	5	322	CLA	C4A-NA-C1A	-3.64	105.07	106.71
20	7	1014	CLA	CHD-C1D-ND	-3.64	121.11	124.45
20	A	838	CLA	CHB-C1B-NB	-3.64	120.41	124.26
24	3	1004	BCR	C23-C24-C25	3.64	137.42	127.20
20	5	321	CLA	CHD-C1D-ND	-3.64	121.11	124.45
20	4	311	CLA	CHB-C1B-NB	-3.63	120.41	124.26
20	7	1006	CLA	CHC-C1C-NC	3.63	129.72	124.20
20	B	808	CLA	CHD-C1D-ND	-3.63	121.12	124.45
20	7	1014	CLA	CHB-C1B-NB	-3.63	120.41	124.26
24	A	846	BCR	C16-C15-C14	3.63	130.91	123.47
20	G	203	CLA	CHB-C1B-NB	-3.63	120.42	124.26
20	1	1006	CLA	CHB-C1B-NB	-3.63	120.42	124.26
20	4	309	CLA	CHC-C1C-NC	3.63	129.71	124.20
20	A	822	CLA	CHD-C1D-ND	-3.62	121.12	124.45
24	B	804	BCR	C8-C7-C6	3.62	137.38	127.20
20	A	827	CLA	CHB-C1B-NB	-3.62	120.42	124.26
20	3	1012	CLA	C4A-NA-C1A	-3.62	105.08	106.71
29	7	1013	CHL	C2B-C1B-NB	3.62	112.66	110.23
24	A	845	BCR	C8-C9-C10	3.60	124.47	118.94
20	B	830	CLA	CHC-C1C-NC	3.60	129.67	124.20
20	3	1016	CLA	C4A-NA-C1A	-3.60	105.09	106.71
20	1	1017	CLA	CHC-C1C-C2C	-3.60	116.73	126.73
20	0	306	CLA	CHB-C1B-NB	-3.60	120.45	124.26
20	1	1011	CLA	CHB-C1B-NB	-3.60	120.45	124.26
20	3	1016	CLA	CHC-C1C-NC	3.59	129.66	124.20
20	A	817	CLA	C2C-C1C-NC	3.59	113.34	109.97
20	1	1009	CLA	CHB-C1B-NB	-3.59	120.46	124.26
20	4	310	CLA	CHC-C4B-NB	-3.59	120.46	124.26
20	L	202	CLA	C4A-NA-C1A	-3.59	105.09	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	304	CLA	C4A-NA-C1A	-3.59	105.09	106.71
29	5	316	CHL	C2B-C1B-NB	3.58	112.64	110.23
30	8	304	XAT	C15-C35-C34	3.58	130.81	123.47
20	A	818	CLA	CHD-C1D-ND	-3.58	121.16	124.45
20	B	831	CLA	C4A-NA-C1A	-3.57	105.10	106.71
20	A	815	CLA	CHC-C1C-NC	3.56	129.61	124.20
20	B	821	CLA	CHD-C1D-ND	-3.56	121.18	124.45
20	5	306	CLA	C1D-ND-C4D	-3.56	103.81	106.33
20	5	309	CLA	CHD-C1D-ND	-3.56	121.18	124.45
20	8	309	CLA	CHC-C1C-NC	3.56	129.60	124.20
20	3	1017	CLA	CHD-C1D-ND	-3.56	121.19	124.45
20	4	306	CLA	CHB-C1B-NB	-3.55	120.50	124.26
20	A	832	CLA	CHD-C1D-ND	-3.55	121.19	124.45
20	A	811	CLA	CHD-C1D-ND	-3.55	121.19	124.45
20	7	1005	CLA	CHD-C1D-ND	-3.55	121.19	124.45
20	B	808	CLA	CHC-C1C-NC	3.54	129.58	124.20
20	B	805	CLA	CHD-C1D-ND	-3.54	121.20	124.45
20	B	850	CLA	CHD-C1D-ND	-3.54	120.83	124.40
20	A	824	CLA	CHC-C1C-NC	3.54	129.57	124.20
20	A	840	CLA	C1D-ND-C4D	-3.54	103.82	106.33
20	G	201	CLA	CHD-C1D-ND	-3.54	121.20	124.45
20	L	204	CLA	C4A-NA-C1A	-3.53	105.12	106.71
20	L	203	CLA	CHD-C1D-ND	-3.53	121.21	124.45
20	1	1004	CLA	CHB-C1B-NB	-3.52	120.53	124.26
20	F	303	CLA	C1D-ND-C4D	-3.52	103.83	106.33
20	A	819	CLA	CHB-C1B-NB	-3.52	120.53	124.26
20	1	1005	CLA	CHD-C1D-ND	-3.52	121.22	124.45
20	B	815	CLA	CHB-C1B-NB	-3.52	120.53	124.26
20	A	819	CLA	CHD-C1D-ND	-3.52	121.22	124.45
29	5	313	CHL	CHC-C1C-NC	3.52	129.54	124.20
20	0	307	CLA	CHC-C1C-NC	3.51	129.53	124.20
20	B	837	CLA	CHC-C1C-NC	3.51	129.53	124.20
20	6	318	CLA	CHD-C1D-ND	-3.51	121.23	124.45
20	B	829	CLA	C4A-NA-C1A	-3.51	105.13	106.71
20	3	1006	CLA	C1D-ND-C4D	-3.51	103.84	106.33
20	7	1006	CLA	CHB-C1B-NB	-3.50	120.55	124.26
20	A	810	CLA	C1D-ND-C4D	-3.49	103.85	106.33
29	8	314	CHL	C2B-C1B-NB	3.49	112.57	110.23
20	B	833	CLA	CHD-C1D-ND	-3.49	121.25	124.45
20	8	308	CLA	CHD-C1D-ND	-3.49	121.25	124.45
20	B	812	CLA	C4A-NA-C1A	-3.49	105.14	106.71
29	4	312	CHL	CAA-C2A-C1A	3.48	123.38	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	7	1004	CLA	CHC-C1C-NC	3.48	129.48	124.20
20	A	805	CLA	C4A-NA-C1A	-3.48	105.14	106.71
20	A	804	CLA	CHD-C1D-ND	-3.48	121.26	124.45
20	A	816	CLA	CHD-C1D-ND	-3.48	121.26	124.45
20	1	1011	CLA	CHC-C1C-NC	3.47	129.47	124.20
20	B	809	CLA	CHB-C1B-NB	-3.47	120.58	124.26
20	3	1008	CLA	CHB-C1B-NB	-3.47	120.58	124.26
20	3	1010	CLA	CHD-C1D-ND	-3.47	121.27	124.45
24	H	201	BCR	C16-C15-C14	3.47	130.58	123.47
20	B	841	CLA	CHC-C1C-NC	3.46	129.45	124.20
20	A	809	CLA	CHD-C1D-ND	-3.46	121.28	124.45
20	B	823	CLA	CHB-C1B-NB	-3.46	120.59	124.26
20	B	850	CLA	CHB-C1B-NB	-3.46	120.60	124.26
30	7	1002	XAT	C32-C33-C34	3.46	124.25	118.94
20	A	820	CLA	CHB-C1B-NB	-3.46	120.60	124.26
20	A	819	CLA	C1D-ND-C4D	-3.45	103.88	106.33
20	4	304	CLA	CHB-C1B-NB	-3.45	120.60	124.26
20	7	1005	CLA	CHC-C1C-NC	3.45	129.44	124.20
27	4	318	LMG	C4-C3-C2	3.45	116.85	110.82
20	A	825	CLA	CHB-C1B-NB	-3.45	120.61	124.26
20	7	1005	CLA	CHC-C1C-C2C	-3.45	117.15	126.73
20	B	828	CLA	CHB-C1B-NB	-3.45	120.61	124.26
20	6	320	CLA	C4A-NA-C1A	-3.45	105.16	106.71
20	B	810	CLA	CHD-C1D-ND	-3.45	121.29	124.45
24	3	1004	BCR	C16-C15-C14	3.44	130.53	123.47
20	L	202	CLA	CHB-C1B-NB	-3.44	120.61	124.26
20	1	1007	CLA	CHC-C1C-C2C	-3.44	117.17	126.73
24	B	843	BCR	C16-C17-C18	3.44	132.22	127.31
20	A	811	CLA	CHC-C1C-NC	3.43	129.41	124.20
20	F	305	CLA	CHD-C1D-ND	-3.43	121.30	124.45
20	0	308	CLA	CHD-C1D-ND	-3.43	121.31	124.45
20	6	309	CLA	CHD-C1D-ND	-3.43	121.31	124.45
20	4	314	CLA	CHB-C1B-NB	-3.43	120.63	124.26
20	8	313	CLA	CHC-C1C-NC	3.42	129.40	124.20
20	1	1007	CLA	C1D-ND-C4D	-3.42	103.90	106.33
20	A	818	CLA	CHB-C1B-NB	-3.42	120.64	124.26
20	B	828	CLA	CHD-C1D-ND	-3.42	121.31	124.45
20	B	831	CLA	C2C-C1C-NC	3.42	113.17	109.97
20	1	1005	CLA	C4A-NA-C1A	-3.42	105.17	106.71
20	3	1017	CLA	CHB-C1B-NB	-3.42	120.64	124.26
20	6	310	CLA	CHD-C1D-ND	-3.41	121.32	124.45
20	3	1007	CLA	CHD-C1D-ND	-3.41	121.32	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	1002	XAT	C8-C9-C10	3.41	124.17	118.94
20	8	308	CLA	CHB-C1B-NB	-3.41	120.65	124.26
20	A	826	CLA	CHC-C1C-NC	3.41	129.37	124.20
20	8	305	CLA	CHB-C1B-NB	-3.41	120.65	124.26
20	6	315	CLA	CHC-C1C-NC	3.41	129.37	124.20
20	B	837	CLA	CHD-C1D-ND	-3.40	121.33	124.45
20	B	840	CLA	CHB-C1B-NB	-3.40	120.65	124.26
24	I	201	BCR	C16-C15-C14	3.40	130.45	123.47
20	A	816	CLA	CHB-C1B-NB	-3.40	120.65	124.26
30	7	1002	XAT	C40-C33-C34	-3.40	118.16	122.92
20	B	831	CLA	CHD-C1D-ND	-3.40	121.33	124.45
20	A	834	CLA	CHB-C1B-NB	-3.40	120.66	124.26
20	B	850	CLA	C4A-NA-C1A	-3.40	105.18	106.71
20	K	201	CLA	C1D-ND-C4D	-3.40	103.92	106.33
20	0	316	CLA	CHC-C1C-NC	3.40	129.36	124.20
20	K	201	CLA	CHC-C1C-NC	3.40	129.35	124.20
20	B	829	CLA	CHD-C1D-ND	-3.40	121.33	124.45
20	7	1008	CLA	C4A-NA-C1A	-3.39	105.18	106.71
20	A	823	CLA	CHC-C1C-C2C	-3.39	117.31	126.73
20	0	306	CLA	CHC-C1C-NC	3.39	129.34	124.20
20	K	202	CLA	CHD-C1D-ND	-3.39	121.24	124.52
20	0	309	CLA	CHD-C1D-ND	-3.39	121.34	124.45
20	1	1008	CLA	CHB-C1B-NB	-3.39	120.67	124.26
20	5	306	CLA	CHD-C1D-ND	-3.38	121.34	124.45
20	L	201	CLA	C1D-ND-C4D	-3.38	103.93	106.33
30	8	304	XAT	C20-C13-C14	-3.38	118.19	122.92
20	1	1009	CLA	CHD-C1D-ND	-3.38	121.35	124.45
20	0	309	CLA	C1D-ND-C4D	-3.38	103.93	106.33
29	5	317	CHL	CHD-C1D-ND	-3.38	121.35	124.45
20	A	821	CLA	CMA-C3A-C4A	3.38	120.85	111.77
20	B	836	CLA	CHD-C1D-ND	-3.38	121.35	124.45
20	F	303	CLA	CHB-C1B-NB	-3.38	120.68	124.26
20	A	833	CLA	C2C-C1C-NC	3.37	113.13	109.97
20	B	840	CLA	CHD-C1D-ND	-3.37	121.36	124.45
20	7	1010	CLA	CHC-C4B-NB	-3.37	120.69	124.26
29	5	317	CHL	CHA-C1A-NA	-3.36	118.70	126.40
29	8	314	CHL	CHD-C1D-ND	-3.36	121.36	124.45
29	6	314	CHL	CHD-C1D-ND	-3.36	121.37	124.45
20	4	310	CLA	CHC-C1C-C2C	-3.35	117.41	126.73
20	5	312	CLA	CHC-C1C-C2C	-3.35	117.42	126.73
20	A	835	CLA	CHD-C1D-ND	-3.35	121.37	124.45
20	1	1014	CLA	CHC-C1C-C2C	-3.35	117.42	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	0	316	CLA	CHC-C1C-C2C	-3.34	117.44	126.73
29	4	316	CHL	CHA-C1A-NA	-3.34	118.75	126.40
20	J	102	CLA	CHD-C1D-ND	-3.34	121.38	124.45
20	B	818	CLA	CHD-C1D-ND	-3.34	121.39	124.45
20	A	823	CLA	CHC-C1C-NC	3.34	129.26	124.20
20	5	306	CLA	C4A-NA-C1A	-3.33	105.21	106.71
29	4	312	CHL	CHD-C1D-ND	-3.33	121.39	124.45
20	F	303	CLA	CHC-C1C-NC	3.33	129.25	124.20
20	5	323	CLA	CHC-C1C-NC	3.33	129.25	124.20
20	B	825	CLA	CHB-C1B-NB	-3.33	120.74	124.26
29	1	1015	CHL	CHA-C1A-NA	-3.32	118.79	126.40
20	8	307	CLA	CHC-C1C-C2C	-3.32	117.50	126.73
20	3	1010	CLA	C4A-NA-C1A	-3.32	105.21	106.71
24	B	804	BCR	C21-C20-C19	3.32	133.58	123.22
20	A	829	CLA	CHC-C1C-NC	3.31	129.23	124.20
20	1	1008	CLA	CHD-C1D-ND	-3.31	121.41	124.45
20	A	811	CLA	CHB-C1B-NB	-3.31	120.75	124.26
20	8	309	CLA	CHB-C1B-NB	-3.31	120.75	124.26
20	4	304	CLA	CHC-C1C-NC	3.31	129.22	124.20
20	0	313	CLA	CHD-C1D-ND	-3.31	121.42	124.45
24	7	1003	BCR	C15-C16-C17	-3.31	116.70	123.47
20	B	808	CLA	CHB-C1B-NB	-3.31	120.76	124.26
20	5	318	CLA	C1D-ND-C4D	-3.30	103.99	106.33
20	3	1006	CLA	CHB-C1B-NB	-3.30	120.76	124.26
20	A	806	CLA	CHC-C1C-NC	3.30	129.21	124.20
20	B	802	CLA	CHD-C1D-ND	-3.30	121.42	124.45
20	5	308	CLA	C1D-ND-C4D	-3.30	103.99	106.33
20	B	823	CLA	CHD-C1D-ND	-3.29	121.43	124.45
29	1	1012	CHL	CHA-C1A-NA	-3.29	118.86	126.40
30	7	1002	XAT	C20-C13-C14	-3.29	118.31	122.92
20	B	806	CLA	CHD-C1D-ND	-3.29	121.43	124.45
20	A	810	CLA	CHB-C1B-NB	-3.29	120.78	124.26
20	3	1009	CLA	CHB-C1B-NB	-3.29	120.78	124.26
20	5	323	CLA	C4A-NA-C1A	-3.28	105.23	106.71
20	B	815	CLA	CHD-C1D-ND	-3.28	121.44	124.45
20	6	307	CLA	CHD-C1D-ND	-3.28	121.44	124.45
20	B	830	CLA	CHD-C1D-ND	-3.27	121.44	124.45
20	A	804	CLA	CHB-C1B-NB	-3.27	120.79	124.26
20	F	302	CLA	CHB-C1B-NB	-3.27	120.79	124.26
20	B	820	CLA	CHD-C1D-ND	-3.27	121.45	124.45
20	3	1013	CLA	CHD-C1D-ND	-3.27	121.45	124.45
20	A	835	CLA	CHC-C1C-C2C	-3.27	117.65	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	1011	CLA	CHC-C1C-C2C	-3.27	117.65	126.73
20	B	839	CLA	C1D-ND-C4D	-3.27	104.01	106.33
20	6	320	CLA	CHC-C1C-C2C	-3.26	117.67	126.73
29	7	1015	CHL	CHA-C1A-NA	-3.26	118.94	126.40
20	B	814	CLA	CHD-C1D-ND	-3.26	121.46	124.45
20	4	308	CLA	CHB-C1B-NB	-3.25	120.81	124.26
20	G	201	CLA	CHB-C1B-NB	-3.25	120.82	124.26
20	G	202	CLA	CHB-C1B-NB	-3.25	120.82	124.26
20	B	831	CLA	CHC-C1C-C2C	-3.25	117.70	126.73
20	3	1013	CLA	CHB-C1B-NB	-3.25	120.82	124.26
20	A	830	CLA	CHC-C1C-NC	3.25	129.13	124.20
20	7	1008	CLA	CHD-C1D-ND	-3.25	121.47	124.45
29	0	317	CHL	CHA-C1A-NA	-3.25	118.97	126.40
20	B	830	CLA	CHC-C1C-C2C	-3.25	117.72	126.73
20	6	306	CLA	CHD-C1D-ND	-3.24	121.47	124.45
20	3	1011	CLA	CHB-C1B-NB	-3.24	120.82	124.26
20	1	1005	CLA	C1D-ND-C4D	-3.24	104.03	106.33
30	6	304	XAT	O4-C5-C6	-3.24	56.28	58.96
20	B	841	CLA	CHB-C1B-NB	-3.24	120.83	124.26
20	0	309	CLA	CHC-C1C-NC	3.24	129.12	124.20
20	4	311	CLA	CHC-C1C-NC	3.24	129.12	124.20
20	A	834	CLA	CHD-C1D-ND	-3.24	121.48	124.45
20	1	1008	CLA	CHC-C1C-NC	3.24	129.11	124.20
20	5	315	CLA	CHD-C1D-ND	-3.24	121.48	124.45
20	1	1014	CLA	CHB-C1B-NB	-3.24	120.83	124.26
20	6	308	CLA	CHD-C1D-ND	-3.24	121.48	124.45
20	A	836	CLA	CHB-C1B-NB	-3.23	120.83	124.26
20	3	1005	CLA	C4A-NA-C1A	-3.23	105.25	106.71
20	5	311	CLA	CHD-C1D-ND	-3.23	121.48	124.45
20	B	829	CLA	C1D-ND-C4D	-3.23	104.04	106.33
20	A	814	CLA	CHD-C1D-ND	-3.23	121.49	124.45
20	A	852	CLA	CHB-C1B-NB	-3.23	120.84	124.26
20	0	312	CLA	CHC-C1C-NC	3.23	129.10	124.20
20	0	309	CLA	C2C-C1C-NC	3.22	112.99	109.97
20	B	838	CLA	CHB-C1B-NB	-3.22	120.84	124.26
20	4	307	CLA	C2C-C1C-NC	3.22	112.99	109.97
29	4	313	CHL	C3A-C2A-C1A	3.22	106.16	101.34
20	4	305	CLA	CHC-C1C-NC	3.22	129.09	124.20
29	4	312	CHL	C2B-C1B-NB	3.22	112.39	110.23
20	A	811	CLA	CHC-C1C-C2C	-3.22	117.80	126.73
20	A	822	CLA	CHB-C1B-NB	-3.21	120.85	124.26
20	A	829	CLA	CHC-C4B-NB	-3.21	120.86	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	0	312	CLA	CHB-C1B-NB	-3.21	120.86	124.26
20	1	1005	CLA	CHB-C1B-NB	-3.21	120.86	124.26
29	1	1012	CHL	C2B-C1B-NB	3.21	112.38	110.23
20	3	1013	CLA	C2C-C1C-NC	3.21	112.97	109.97
20	4	310	CLA	CHC-C1C-NC	3.21	129.07	124.20
20	6	312	CLA	C1D-ND-C4D	-3.21	104.06	106.33
20	A	809	CLA	CHB-C1B-NB	-3.21	120.86	124.26
20	B	831	CLA	CHC-C1C-NC	3.20	129.06	124.20
30	8	304	XAT	C40-C33-C34	-3.20	118.44	122.92
20	3	1005	CLA	CHD-C1D-ND	-3.20	121.51	124.45
20	A	815	CLA	CHD-C1D-ND	-3.20	121.51	124.45
20	K	202	CLA	CHB-C1B-NB	-3.20	121.04	124.27
20	7	1007	CLA	CHD-C1D-ND	-3.20	121.52	124.45
20	B	833	CLA	C4A-NA-C1A	-3.19	105.27	106.71
20	A	839	CLA	C1D-ND-C4D	-3.19	104.07	106.33
20	A	807	CLA	CHB-C1B-NB	-3.19	120.88	124.26
20	B	821	CLA	CHC-C1C-NC	3.19	129.04	124.20
20	8	311	CLA	CHC-C1C-NC	3.19	129.04	124.20
29	8	317	CHL	CHD-C1D-ND	-3.19	121.52	124.45
20	0	307	CLA	C1D-ND-C4D	-3.19	104.07	106.33
25	B	848	DGD	O2G-C1B-C2B	3.19	118.37	111.50
20	5	301	CLA	CHC-C1C-NC	3.19	129.04	124.20
20	3	1015	CLA	CHD-C1D-ND	-3.19	121.53	124.45
20	0	309	CLA	CHC-C1C-C2C	-3.18	117.89	126.73
20	A	826	CLA	C4A-NA-C1A	-3.18	105.28	106.71
20	8	307	CLA	CHC-C1C-NC	3.18	129.03	124.20
20	3	1006	CLA	CHC-C1C-NC	3.18	129.03	124.20
20	B	819	CLA	CHD-C1D-ND	-3.18	121.53	124.45
20	B	807	CLA	CHD-C1D-ND	-3.18	121.54	124.45
29	4	315	CHL	CHD-C1D-ND	-3.18	121.54	124.45
20	3	1006	CLA	CHD-C1D-ND	-3.17	121.54	124.45
20	A	806	CLA	CHD-C1D-ND	-3.17	121.54	124.45
20	B	833	CLA	CHC-C1C-NC	3.17	129.01	124.20
20	A	817	CLA	CHC-C1C-C2C	-3.17	117.92	126.73
20	5	310	CLA	CHB-C1B-NB	-3.17	120.90	124.26
20	3	1010	CLA	CHC-C1C-NC	3.17	129.01	124.20
20	B	826	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	L	202	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	A	829	CLA	CHC-C1C-C2C	-3.16	117.95	126.73
29	5	314	CHL	C2C-C3C-C4C	3.16	108.74	106.49
20	A	832	CLA	CHB-C1B-NB	-3.16	120.91	124.26
20	4	306	CLA	CHC-C1C-NC	3.16	129.00	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	312	CLA	CHB-C1B-NB	-3.16	120.91	124.26
20	7	1006	CLA	CHC-C1C-C2C	-3.16	117.95	126.73
20	B	805	CLA	CHB-C1B-NB	-3.16	120.91	124.26
20	5	305	CLA	C2C-C1C-NC	3.16	112.93	109.97
20	8	312	CLA	CHB-C1B-NB	-3.15	120.92	124.26
20	A	820	CLA	CHD-C1D-ND	-3.15	121.56	124.45
20	B	820	CLA	CHB-C1B-NB	-3.15	120.92	124.26
20	0	307	CLA	CHB-C1B-NB	-3.15	120.92	124.26
29	3	1014	CHL	CHA-C1A-NA	-3.15	119.19	126.40
20	A	851	CLA	CHB-C1B-NB	-3.15	120.93	124.26
20	B	835	CLA	CHB-C1B-NB	-3.15	120.93	124.26
20	3	1007	CLA	CHC-C1C-NC	3.15	128.98	124.20
20	7	1014	CLA	CHC-C1C-NC	3.14	128.97	124.20
20	5	308	CLA	C4A-NA-C1A	-3.14	105.29	106.71
20	B	840	CLA	CHC-C1C-NC	3.14	128.97	124.20
20	B	823	CLA	CHC-C1C-NC	3.14	128.97	124.20
20	1	1006	CLA	CHC-C1C-NC	3.14	128.97	124.20
20	A	825	CLA	CHD-C1D-ND	-3.14	121.57	124.45
20	1	1006	CLA	C2C-C1C-NC	3.14	112.91	109.97
20	B	808	CLA	CHC-C1C-C2C	-3.14	118.01	126.73
29	4	313	CHL	C2C-C3C-C4C	3.14	108.72	106.49
24	B	845	BCR	C21-C20-C19	3.14	133.00	123.22
20	B	829	CLA	CHB-C1B-NB	-3.13	120.94	124.26
20	6	310	CLA	C1D-ND-C4D	-3.13	104.11	106.33
29	6	317	CHL	CHA-C1A-NA	-3.13	119.23	126.40
20	B	841	CLA	CHD-C1D-ND	-3.13	121.58	124.45
20	L	201	CLA	CHC-C1C-NC	3.13	128.95	124.20
20	3	1015	CLA	C4A-NA-C1A	-3.13	105.30	106.71
20	6	305	CLA	C2C-C1C-NC	3.13	112.90	109.97
20	A	802	CLA	CHC-C1C-NC	3.13	128.95	124.20
20	7	1009	CLA	CHC-C1C-NC	3.13	128.95	124.20
20	B	841	CLA	CHC-C1C-C2C	-3.12	118.05	126.73
20	A	838	CLA	CHC-C1C-C2C	-3.12	118.05	126.73
29	3	1014	CHL	CHD-C1D-ND	-3.12	121.58	124.45
20	5	323	CLA	CHB-C1B-NB	-3.12	120.95	124.26
20	0	311	CLA	CHD-C1D-ND	-3.12	121.59	124.45
20	0	306	CLA	CHC-C1C-C2C	-3.12	118.07	126.73
20	5	322	CLA	CHB-C1B-NB	-3.12	120.96	124.26
20	5	301	CLA	C1D-ND-C4D	-3.12	104.12	106.33
20	A	823	CLA	CHD-C1D-ND	-3.12	121.59	124.45
20	A	833	CLA	CHC-C1C-C2C	-3.12	118.08	126.73
20	0	301	CLA	CHD-C1D-ND	-3.11	121.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	813	CLA	C1D-ND-C4D	-3.11	104.12	106.33
20	B	812	CLA	CHC-C1C-NC	3.11	128.93	124.20
29	8	317	CHL	CHA-C1A-NA	-3.11	119.27	126.40
20	1	1003	CLA	C4A-NA-C1A	-3.11	105.31	106.71
20	5	315	CLA	C4A-NA-C1A	-3.11	105.31	106.71
20	A	852	CLA	C2C-C1C-NC	3.11	112.89	109.97
20	1	1006	CLA	CHC-C1C-C2C	-3.11	118.09	126.73
20	A	808	CLA	CHD-C1D-ND	-3.11	121.60	124.45
20	A	832	CLA	CHC-C1C-NC	3.10	128.91	124.20
20	A	836	CLA	CHC-C1C-NC	3.10	128.91	124.20
20	B	825	CLA	CHD-C1D-ND	-3.10	121.60	124.45
20	5	304	CLA	CHC-C1C-NC	3.10	128.91	124.20
20	L	201	CLA	C4A-NA-C1A	-3.10	105.31	106.71
20	A	818	CLA	CHC-C1C-NC	3.10	128.91	124.20
20	5	308	CLA	CHC-C1C-NC	3.10	128.91	124.20
20	6	301	CLA	CHD-C1D-ND	-3.10	121.61	124.45
29	6	313	CHL	CHD-C1D-ND	-3.10	121.61	124.45
29	0	317	CHL	CHD-C1D-ND	-3.10	121.61	124.45
20	A	826	CLA	CHB-C1B-NB	-3.10	120.98	124.26
20	B	803	CLA	CHC-C1C-NC	3.09	128.90	124.20
20	5	312	CLA	CHD-C1D-ND	-3.09	121.61	124.45
20	K	202	CLA	C3A-C4A-CHB	-3.09	120.13	123.91
20	B	815	CLA	CHC-C1C-NC	3.09	128.89	124.20
20	4	304	CLA	CHC-C1C-C2C	-3.09	118.15	126.73
20	A	838	CLA	CHD-C1D-ND	-3.09	121.61	124.45
20	B	820	CLA	C2C-C1C-NC	3.09	112.86	109.97
20	6	309	CLA	CHC-C1C-NC	3.08	128.88	124.20
29	0	314	CHL	CHD-C1D-ND	-3.08	121.62	124.45
20	A	839	CLA	CHB-C1B-NB	-3.08	121.00	124.26
20	B	802	CLA	CHB-C1B-NB	-3.08	121.00	124.26
20	6	305	CLA	CHC-C1C-NC	3.08	128.88	124.20
20	6	307	CLA	C1D-ND-C4D	-3.08	104.15	106.33
20	7	1010	CLA	C2C-C1C-NC	3.08	112.85	109.97
20	G	201	CLA	CHC-C1C-NC	3.08	128.87	124.20
20	B	850	CLA	C2C-C1C-CHC	-3.08	116.09	124.50
29	5	314	CHL	C1D-ND-C4D	-3.07	104.15	106.33
20	B	803	CLA	CHB-C1B-NB	-3.07	121.00	124.26
20	A	813	CLA	CHD-C1D-ND	-3.07	121.63	124.45
20	6	305	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
20	A	816	CLA	C1D-ND-C4D	-3.07	104.15	106.33
20	B	801	CLA	C2C-C1C-NC	3.07	112.85	109.97
20	L	204	CLA	CHC-C1C-NC	3.07	128.86	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	852	CLA	CHD-C1D-ND	-3.07	121.63	124.45
20	1	1005	CLA	CHC-C1C-NC	3.07	128.86	124.20
24	G	204	BCR	C15-C16-C17	3.07	129.76	123.47
20	B	850	CLA	C1D-ND-C4D	-3.07	104.16	106.33
20	3	1011	CLA	C1D-ND-C4D	-3.07	104.16	106.33
20	K	201	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
29	6	313	CHL	CHA-C1A-NA	-3.07	119.38	126.40
20	5	305	CLA	CHB-C1B-NB	-3.07	121.01	124.26
20	B	850	CLA	CMC-C2C-C1C	3.07	123.83	113.11
29	0	314	CHL	CHA-C1A-NA	-3.06	119.38	126.40
20	A	810	CLA	CHC-C1C-NC	3.06	128.85	124.20
29	1	1013	CHL	C2C-C3C-C4C	3.06	108.67	106.49
20	B	838	CLA	CHC-C1C-NC	3.06	128.85	124.20
20	5	301	CLA	CHC-C4B-NB	-3.06	121.02	124.26
20	4	309	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
20	5	301	CLA	CHB-C1B-NB	-3.06	121.02	124.26
20	A	801	CLA	C4A-NA-C1A	-3.06	105.33	106.71
20	K	202	CLA	CHC-C1C-NC	3.06	128.74	124.23
20	B	817	CLA	CHB-C1B-NB	-3.06	121.02	124.26
20	0	310	CLA	CHD-C1D-ND	-3.06	121.65	124.45
20	A	822	CLA	CHC-C1C-NC	3.05	128.84	124.20
20	L	202	CLA	CHC-C1C-NC	3.05	128.84	124.20
20	7	1004	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
20	0	311	CLA	CHC-C1C-NC	3.05	128.83	124.20
20	0	301	CLA	C1D-ND-C4D	-3.05	104.17	106.33
20	3	1012	CLA	CHB-C1B-NB	-3.05	121.03	124.26
20	7	1010	CLA	CHC-C1C-NC	3.05	128.83	124.20
20	6	310	CLA	CHC-C1C-NC	3.05	128.82	124.20
20	5	311	CLA	CHC-C1C-NC	3.05	128.82	124.20
20	F	303	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
20	A	835	CLA	CHC-C1C-NC	3.04	128.82	124.20
20	A	852	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
20	6	307	CLA	CHC-C1C-NC	3.04	128.82	124.20
20	A	829	CLA	C2C-C1C-NC	3.04	112.82	109.97
29	7	1012	CHL	C1D-ND-C4D	-3.04	104.17	106.33
29	5	316	CHL	C3C-C4C-NC	-3.04	107.16	110.57
20	A	835	CLA	C4A-NA-C1A	-3.04	105.34	106.71
20	0	312	CLA	C1D-ND-C4D	-3.04	104.18	106.33
20	8	313	CLA	CHD-C1D-ND	-3.04	121.66	124.45
29	8	315	CHL	C3A-C2A-C1A	3.04	105.89	101.34
20	A	851	CLA	CHD-C1D-ND	-3.03	121.67	124.45
20	1	1017	CLA	C2C-C1C-NC	3.03	112.81	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	7	1010	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
20	7	1004	CLA	CHD-C1D-ND	-3.03	121.67	124.45
20	7	1009	CLA	CHD-C1D-ND	-3.03	121.67	124.45
20	A	806	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
20	7	1008	CLA	C1D-ND-C4D	-3.03	104.19	106.33
24	A	845	BCR	C16-C15-C14	3.03	129.67	123.47
20	A	811	CLA	C1D-ND-C4D	-3.03	104.19	106.33
29	1	1015	CHL	CHD-C1D-ND	-3.02	121.67	124.45
20	A	813	CLA	CHC-C1C-NC	3.02	128.79	124.20
20	0	310	CLA	CHC-C1C-NC	3.02	128.79	124.20
20	5	315	CLA	CHC-C1C-NC	3.02	128.79	124.20
20	A	804	CLA	CHC-C1C-NC	3.02	128.78	124.20
20	B	814	CLA	CHC-C1C-NC	3.02	128.78	124.20
20	B	805	CLA	CHC-C1C-NC	3.02	128.78	124.20
20	B	827	CLA	CHB-C1B-NB	-3.02	121.06	124.26
20	B	822	CLA	C2C-C1C-NC	3.02	112.80	109.97
20	3	1016	CLA	CHC-C1C-C2C	-3.02	118.35	126.73
20	1	1006	CLA	C1D-ND-C4D	-3.01	104.19	106.33
20	A	833	CLA	CHC-C1C-NC	3.01	128.77	124.20
20	0	316	CLA	CHB-C1B-NB	-3.01	121.07	124.26
20	A	803	CLA	CHD-C1D-ND	-3.01	121.69	124.45
20	B	811	CLA	CHB-C1B-NB	-3.01	121.07	124.26
20	B	819	CLA	CHB-C1B-NB	-3.01	121.07	124.26
20	5	309	CLA	CHB-C1B-NB	-3.01	121.07	124.26
20	1	1009	CLA	CHC-C1C-NC	3.01	128.77	124.20
20	B	830	CLA	C1D-ND-C4D	-3.01	104.20	106.33
20	5	322	CLA	C1D-ND-C4D	-3.01	104.20	106.33
20	8	306	CLA	CHC-C1C-NC	3.00	128.76	124.20
20	B	816	CLA	CHB-C1B-NB	-3.00	121.08	124.26
20	G	202	CLA	CHD-C1D-ND	-3.00	121.69	124.45
29	7	1012	CHL	CHD-C1D-ND	-3.00	121.69	124.45
20	B	815	CLA	C1D-ND-C4D	-3.00	104.20	106.33
20	3	1008	CLA	C1D-ND-C4D	-3.00	104.20	106.33
20	B	812	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
24	H	201	BCR	C8-C7-C6	3.00	135.62	127.20
24	A	845	BCR	C34-C9-C10	-3.00	118.73	122.92
20	0	306	CLA	CHD-C1D-ND	-3.00	121.70	124.45
20	L	203	CLA	C1D-ND-C4D	-2.99	104.21	106.33
20	1	1009	CLA	C1D-ND-C4D	-2.99	104.21	106.33
29	0	315	CHL	CHD-C1D-ND	-2.99	121.70	124.45
20	1	1004	CLA	C1D-ND-C4D	-2.99	104.21	106.33
20	3	1017	CLA	C1D-ND-C4D	-2.99	104.21	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	0	308	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
20	A	814	CLA	CHB-C1B-NB	-2.99	121.09	124.26
20	B	838	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
20	A	814	CLA	CHC-C1C-NC	2.99	128.74	124.20
20	A	817	CLA	CHC-C1C-NC	2.99	128.74	124.20
20	A	819	CLA	CHC-C1C-NC	2.99	128.74	124.20
20	0	308	CLA	CHC-C1C-NC	2.99	128.74	124.20
20	L	204	CLA	CHD-C1D-ND	-2.99	121.71	124.45
20	A	852	CLA	CHC-C1C-NC	2.99	128.73	124.20
20	1	1007	CLA	C2C-C1C-NC	2.99	112.77	109.97
20	6	309	CLA	CHC-C1C-C2C	-2.99	118.44	126.73
20	A	836	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
29	8	314	CHL	C1D-ND-C4D	-2.98	104.22	106.33
20	1	1011	CLA	C2C-C1C-NC	2.98	112.77	109.97
20	5	307	CLA	CHC-C1C-NC	2.98	128.73	124.20
20	5	310	CLA	CHC-C4B-NB	-2.98	121.10	124.26
20	A	830	CLA	CHD-C1D-ND	-2.98	121.72	124.45
20	5	308	CLA	CHD-C1D-ND	-2.98	121.72	124.45
20	7	1007	CLA	C2C-C1C-NC	2.97	112.76	109.97
20	B	801	CLA	CHD-C1D-ND	-2.97	121.72	124.45
20	A	826	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
20	B	830	CLA	CHC-C4B-NB	-2.97	121.11	124.26
20	0	316	CLA	C2C-C1C-NC	2.97	112.75	109.97
20	5	310	CLA	CHC-C1C-C2C	-2.97	118.48	126.73
20	A	811	CLA	C2C-C1C-NC	2.97	112.75	109.97
20	B	816	CLA	CHC-C1C-NC	2.97	128.70	124.20
20	B	820	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
29	0	315	CHL	CHA-C1A-NA	-2.96	119.62	126.40
20	3	1010	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
20	B	832	CLA	CHD-C1D-ND	-2.96	121.73	124.45
20	A	824	CLA	CHD-C1D-ND	-2.96	121.73	124.45
20	B	817	CLA	CHC-C1C-NC	2.96	128.69	124.20
20	A	802	CLA	CHC-C4B-NB	-2.96	121.12	124.26
20	5	321	CLA	C1D-ND-C4D	-2.96	104.23	106.33
20	5	312	CLA	C2C-C1C-NC	2.96	112.74	109.97
23	0	302	LHG	O6-P-O5	2.96	120.62	109.07
20	3	1013	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
20	B	806	CLA	CHB-C1B-NB	-2.95	121.13	124.26
20	7	1004	CLA	C4A-NA-C1A	-2.95	105.38	106.71
20	0	308	CLA	C2C-C1C-NC	2.95	112.74	109.97
20	B	802	CLA	CHA-C1A-NA	-2.95	119.64	126.40
20	8	312	CLA	CHD-C1D-ND	-2.95	121.74	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	818	CLA	C1D-ND-C4D	-2.95	104.24	106.33
20	B	801	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
20	6	311	CLA	CHD-C1D-ND	-2.95	121.74	124.45
20	A	814	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
20	A	812	CLA	CHC-C1C-NC	2.94	128.66	124.20
20	8	316	CLA	CHD-C1D-ND	-2.94	121.75	124.45
20	1	1010	CLA	CHD-C1D-ND	-2.94	121.75	124.45
25	B	848	DGD	O5D-C1E-C2E	-2.94	103.71	108.30
20	A	808	CLA	CHC-C1C-NC	2.94	128.66	124.20
20	5	311	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
20	B	813	CLA	CHD-C1D-ND	-2.94	121.75	124.45
20	8	305	CLA	CHC-C1C-NC	2.94	128.66	124.20
20	G	203	CLA	C1D-ND-C4D	-2.94	104.25	106.33
20	4	308	CLA	CHC-C1C-C2C	-2.94	118.58	126.73
20	5	305	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
20	B	838	CLA	C2C-C1C-NC	2.93	112.72	109.97
20	B	837	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
20	5	311	CLA	CHA-C1A-NA	-2.93	119.68	126.40
20	A	802	CLA	CHC-C1C-C2C	-2.93	118.59	126.73
20	A	828	CLA	CHB-C1B-NB	-2.93	121.15	124.26
20	5	322	CLA	CHC-C1C-NC	2.93	128.65	124.20
20	B	812	CLA	CHB-C1B-NB	-2.93	121.16	124.26
24	G	205	BCR	C23-C24-C25	2.93	135.43	127.20
20	8	313	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
29	7	1017	CHL	CHD-C1D-ND	-2.93	121.76	124.45
20	A	801	CLA	CHB-C4A-NA	2.93	128.56	124.51
20	F	305	CLA	C1D-ND-C4D	-2.93	104.26	106.33
20	B	835	CLA	CHD-C1D-ND	-2.92	121.77	124.45
20	A	823	CLA	C4A-NA-C1A	-2.92	105.39	106.71
20	J	102	CLA	CHB-C1B-NB	-2.92	121.16	124.26
20	A	834	CLA	C2C-C1C-NC	2.92	112.71	109.97
20	B	827	CLA	CHD-C1D-ND	-2.92	121.77	124.45
29	1	1015	CHL	C2B-C1B-NB	2.92	112.19	110.23
20	B	829	CLA	CHC-C1C-NC	2.92	128.63	124.20
29	1	1015	CHL	CHB-C1B-NB	2.92	127.35	124.26
20	A	822	CLA	C1D-ND-C4D	-2.92	104.26	106.33
20	B	803	CLA	CHD-C1D-ND	-2.92	121.77	124.45
20	A	808	CLA	C4A-NA-C1A	-2.92	105.39	106.71
20	A	826	CLA	CHD-C1D-ND	-2.92	121.78	124.45
20	F	305	CLA	CHB-C1B-NB	-2.92	121.17	124.26
20	4	311	CLA	CHC-C1C-C2C	-2.92	118.63	126.73
24	H	201	BCR	C12-C13-C14	2.91	123.41	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	843	BCR	C36-C18-C17	-2.91	118.84	122.92
20	B	823	CLA	C1D-ND-C4D	-2.91	104.27	106.33
20	0	309	CLA	C4A-NA-C1A	-2.91	105.40	106.71
20	B	826	CLA	CHB-C1B-NB	-2.91	121.17	124.26
30	7	1002	XAT	C15-C35-C34	2.91	129.44	123.47
20	L	202	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
20	B	840	CLA	C4A-NA-C1A	-2.91	105.40	106.71
24	H	201	BCR	C11-C10-C9	2.91	131.46	127.31
20	3	1007	CLA	CHC-C1C-C2C	-2.91	118.66	126.73
30	8	304	XAT	C32-C33-C34	2.91	123.40	118.94
20	B	811	CLA	CHD-C1D-ND	-2.91	121.78	124.45
29	5	316	CHL	CHA-C1A-NA	-2.90	119.75	126.40
20	A	831	CLA	CHB-C1B-NB	-2.90	121.18	124.26
20	B	808	CLA	C1D-ND-C4D	-2.90	104.27	106.33
20	3	1005	CLA	CHB-C1B-NB	-2.90	121.19	124.26
20	B	835	CLA	CHC-C1C-NC	2.90	128.60	124.20
20	6	306	CLA	C1D-ND-C4D	-2.90	104.28	106.33
25	5	319	DGD	O1G-C1A-C2A	2.90	121.00	111.91
20	4	308	CLA	C2C-C1C-NC	2.89	112.68	109.97
20	B	833	CLA	CHC-C4B-NB	-2.89	121.19	124.26
20	A	810	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
20	A	804	CLA	C1D-ND-C4D	-2.89	104.28	106.33
20	A	840	CLA	CHC-C1C-NC	2.89	128.59	124.20
20	A	822	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
29	5	313	CHL	CHD-C1D-ND	-2.89	121.80	124.45
20	B	803	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
20	A	814	CLA	C2C-C1C-NC	2.89	112.68	109.97
20	8	312	CLA	CHC-C1C-NC	2.89	128.58	124.20
20	A	833	CLA	CHB-C1B-NB	-2.88	121.20	124.26
20	B	801	CLA	CHC-C1C-NC	2.88	128.58	124.20
20	0	310	CLA	C1D-ND-C4D	-2.88	104.29	106.33
20	B	834	CLA	CHD-C1D-ND	-2.88	121.81	124.45
20	A	840	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
20	A	838	CLA	CHA-C1A-NA	-2.88	119.80	126.40
20	0	311	CLA	CHB-C1B-NB	-2.88	121.21	124.26
20	A	839	CLA	CHD-C1D-ND	-2.88	121.81	124.45
30	7	1002	XAT	C12-C13-C14	2.88	123.35	118.94
20	1	1011	CLA	C1D-ND-C4D	-2.87	104.30	106.33
20	7	1010	CLA	CHB-C1B-NB	-2.87	121.22	124.26
20	G	201	CLA	CHC-C1C-C2C	-2.87	118.76	126.73
20	A	837	CLA	CHC-C1C-NC	2.87	128.56	124.20
20	B	818	CLA	CHB-C1B-NB	-2.87	121.22	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	8	310	CLA	CHB-C1B-NB	-2.87	121.22	124.26
20	6	305	CLA	CHB-C1B-NB	-2.87	121.22	124.26
29	5	316	CHL	C2D-C1D-ND	-2.87	107.99	110.10
20	B	820	CLA	CHC-C1C-NC	2.86	128.55	124.20
20	A	805	CLA	CHC-C1C-NC	2.86	128.55	124.20
20	A	807	CLA	C1D-ND-C4D	-2.86	104.30	106.33
20	5	310	CLA	CGD-CBD-CAD	-2.86	101.46	110.73
20	6	310	CLA	CHB-C1B-NB	-2.86	121.23	124.26
29	1	1013	CHL	C2B-C1B-NB	2.86	112.15	110.23
20	3	1006	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
20	J	102	CLA	C2C-C1C-NC	2.86	112.65	109.97
20	1	1004	CLA	CHC-C1C-NC	2.86	128.54	124.20
20	B	812	CLA	C2C-C1C-NC	2.86	112.65	109.97
20	5	306	CLA	CHB-C1B-NB	-2.86	121.23	124.26
20	7	1006	CLA	CMA-C3A-C4A	2.85	119.44	111.77
20	B	812	CLA	CHA-C1A-NA	-2.85	119.87	126.40
20	A	832	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
20	G	201	CLA	C1D-ND-C4D	-2.85	104.31	106.33
30	8	304	XAT	C12-C13-C14	2.85	123.31	118.94
20	0	313	CLA	CHC-C1C-NC	2.85	128.53	124.20
20	B	805	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
20	B	814	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
20	B	831	CLA	C3B-C2B-C1B	2.85	110.60	107.16
20	5	323	CLA	CHC-C1C-C2C	-2.85	118.83	126.73
20	7	1010	CLA	CHD-C1D-ND	-2.84	121.84	124.45
20	1	1010	CLA	CHB-C1B-NB	-2.84	121.25	124.26
20	B	822	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
20	3	1007	CLA	C1D-ND-C4D	-2.84	104.31	106.33
20	1	1010	CLA	CHC-C1C-NC	2.84	128.52	124.20
20	B	821	CLA	CHB-C1B-NB	-2.84	121.25	124.26
20	3	1007	CLA	CHB-C1B-NB	-2.84	121.25	124.26
20	7	1004	CLA	CHB-C1B-NB	-2.84	121.25	124.26
20	B	810	CLA	C2C-C1C-NC	2.84	112.63	109.97
20	B	808	CLA	C4A-NA-C1A	-2.84	105.43	106.71
20	4	305	CLA	CHD-C1D-ND	-2.84	121.85	124.45
20	5	307	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
20	3	1015	CLA	CHC-C1C-NC	2.84	128.51	124.20
20	4	306	CLA	C2D-C1D-ND	-2.84	108.01	110.10
29	0	317	CHL	CHB-C1B-NB	2.84	127.26	124.26
29	4	313	CHL	C2B-C1B-NB	2.84	112.13	110.23
20	7	1008	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
20	1	1014	CLA	C4A-NA-C1A	-2.83	105.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	8	305	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
20	7	1008	CLA	C2C-C1C-NC	2.83	112.62	109.97
20	A	839	CLA	C4A-NA-C1A	-2.83	105.43	106.71
20	7	1011	CLA	C4A-NA-C1A	-2.83	105.43	106.71
20	A	813	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
20	A	813	CLA	CHB-C1B-NB	-2.83	121.26	124.26
20	6	311	CLA	C2C-C1C-NC	2.83	112.62	109.97
20	5	323	CLA	CHD-C1D-ND	-2.82	121.86	124.45
20	4	306	CLA	CHC-C1C-C2C	-2.82	118.88	126.73
20	5	305	CLA	CHC-C1C-NC	2.82	128.49	124.20
20	6	311	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
20	B	826	CLA	C1D-ND-C4D	-2.82	104.33	106.33
20	A	801	CLA	C1D-ND-C4D	-2.82	104.33	106.33
20	B	810	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
20	B	821	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
20	3	1017	CLA	CHC-C1C-NC	2.82	128.48	124.20
20	3	1012	CLA	CHD-C1D-ND	-2.82	121.86	124.45
25	B	848	DGD	C2G-O2G-C1B	-2.82	110.85	117.79
20	G	202	CLA	CHC-C1C-NC	2.82	128.48	124.20
20	5	308	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
29	1	1013	CHL	CHC-C1C-NC	2.82	128.48	124.20
29	4	315	CHL	CHC-C1C-NC	2.82	128.48	124.20
20	B	818	CLA	C1D-ND-C4D	-2.82	104.33	106.33
20	K	202	CLA	C4D-ND-C1D	-2.82	104.33	106.33
20	B	835	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
20	3	1013	CLA	CHC-C1C-NC	2.81	128.47	124.20
20	A	801	CLA	CHC-C1C-C2C	-2.81	118.91	126.73
20	B	830	CLA	C2C-C1C-NC	2.81	112.61	109.97
20	5	304	CLA	CHB-C1B-NB	-2.81	121.28	124.26
20	B	809	CLA	CHC-C1C-NC	2.81	128.47	124.20
20	5	311	CLA	C2C-C1C-NC	2.81	112.61	109.97
20	3	1008	CLA	CHC-C1C-NC	2.81	128.47	124.20
24	1	1001	BCR	C23-C24-C25	2.81	135.09	127.20
20	B	810	CLA	CHC-C1C-NC	2.81	128.46	124.20
29	8	315	CHL	C3C-C4C-NC	-2.81	107.42	110.57
20	A	830	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
20	L	201	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
20	5	309	CLA	CHA-C1A-NA	-2.81	119.97	126.40
20	B	832	CLA	CHB-C1B-NB	-2.81	121.29	124.26
20	8	311	CLA	CHC-C1C-C2C	-2.80	118.94	126.73
20	B	839	CLA	CHB-C1B-NB	-2.80	121.29	124.26
20	A	821	CLA	CHB-C1B-NB	-2.80	121.29	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	839	CLA	CHC-C1C-NC	2.80	128.45	124.20
24	A	845	BCR	C12-C13-C14	2.80	123.23	118.94
20	A	840	CLA	C2C-C1C-NC	2.80	112.59	109.97
20	B	836	CLA	CHC-C1C-NC	2.80	128.45	124.20
24	B	804	BCR	C36-C18-C17	-2.80	119.00	122.92
20	0	313	CLA	C1D-ND-C4D	-2.79	104.35	106.33
20	5	305	CLA	C1D-ND-C4D	-2.79	104.35	106.33
20	B	824	CLA	CHC-C1C-NC	2.79	128.44	124.20
20	6	311	CLA	CHC-C1C-NC	2.79	128.44	124.20
20	L	204	CLA	C1D-ND-C4D	-2.79	104.35	106.33
29	6	314	CHL	CHA-C1A-NA	-2.79	120.01	126.40
20	A	828	CLA	CHC-C1C-NC	2.79	128.43	124.20
20	4	304	CLA	C2C-C1C-NC	2.79	112.58	109.97
20	A	816	CLA	CHC-C1C-NC	2.79	128.43	124.20
20	A	821	CLA	CHC-C1C-NC	2.79	128.43	124.20
29	6	316	CHL	CHA-C1A-NA	-2.79	120.02	126.40
20	3	1009	CLA	CHC-C1C-NC	2.79	128.43	124.20
20	8	310	CLA	CHC-C1C-NC	2.78	128.42	124.20
20	1	1003	CLA	CHC-C1C-NC	2.78	128.42	124.20
29	8	314	CHL	CHA-C1A-NA	-2.78	120.03	126.40
20	A	827	CLA	CHD-C1D-ND	-2.78	121.90	124.45
30	8	304	XAT	C8-C9-C10	2.78	123.21	118.94
20	A	824	CLA	CGD-CBD-CAD	-2.78	101.73	110.73
20	1	1008	CLA	CHC-C1C-C2C	-2.78	119.01	126.73
20	F	305	CLA	CHC-C1C-NC	2.78	128.42	124.20
20	B	823	CLA	CHC-C1C-C2C	-2.78	119.01	126.73
20	1	1007	CLA	CHC-C4B-NB	-2.78	121.32	124.26
20	A	808	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
20	4	314	CLA	CHD-C1D-ND	-2.78	121.90	124.45
20	6	312	CLA	CHC-C1C-NC	2.78	128.41	124.20
29	1	1012	CHL	CHD-C1D-ND	-2.77	121.90	124.45
20	0	312	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
20	4	309	CLA	C4A-NA-C1A	-2.77	105.46	106.71
29	7	1013	CHL	CHA-C1A-NA	-2.77	120.05	126.40
20	A	834	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
20	3	1011	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
20	3	1009	CLA	CHD-C1D-ND	-2.77	121.91	124.45
20	5	323	CLA	CHA-C1A-NA	-2.77	120.06	126.40
20	6	306	CLA	CHC-C1C-NC	2.77	128.40	124.20
20	K	202	CLA	C2C-C1C-CHC	-2.77	119.04	125.67
20	5	322	CLA	CHC-C1C-C2C	-2.77	119.05	126.73
20	A	821	CLA	CHC-C1C-C2C	-2.76	119.05	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	836	CLA	C2C-C1C-NC	2.76	112.56	109.97
24	8	302	BCR	C15-C16-C17	-2.76	117.81	123.47
20	A	821	CLA	C1D-ND-C4D	-2.76	104.37	106.33
20	A	851	CLA	CHC-C1C-NC	2.76	128.39	124.20
20	3	1012	CLA	C2C-C1C-NC	2.76	112.56	109.97
20	A	812	CLA	CHD-C1D-ND	-2.76	121.92	124.45
20	B	840	CLA	C1D-ND-C4D	-2.76	104.38	106.33
20	A	830	CLA	CHB-C1B-NB	-2.76	121.34	124.26
20	3	1012	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
20	J	102	CLA	CHC-C1C-C2C	-2.76	119.08	126.73
20	L	201	CLA	CHB-C1B-NB	-2.76	121.34	124.26
20	7	1011	CLA	C3B-C4B-NB	-2.76	107.96	110.52
20	0	301	CLA	CHC-C1C-NC	2.75	128.38	124.20
20	A	819	CLA	C4A-NA-C1A	-2.75	105.47	106.71
20	A	817	CLA	CHB-C1B-NB	-2.75	121.34	124.26
20	A	838	CLA	CHC-C1C-NC	2.75	128.38	124.20
24	A	845	BCR	C10-C11-C12	-2.75	114.63	123.22
20	4	308	CLA	CHD-C1D-ND	-2.75	121.92	124.45
29	7	1017	CHL	CHA-C1A-NA	-2.75	120.10	126.40
20	3	1011	CLA	CHC-C1C-NC	2.75	128.38	124.20
20	B	827	CLA	CHC-C1C-NC	2.75	128.38	124.20
20	8	316	CLA	CHB-C1B-NB	-2.75	121.35	124.26
20	B	828	CLA	C2C-C1C-NC	2.75	112.55	109.97
20	B	833	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
20	A	821	CLA	CHD-C1D-ND	-2.75	121.93	124.45
20	A	829	CLA	CHD-C1D-ND	-2.75	121.93	124.45
20	6	315	CLA	CHD-C1D-ND	-2.75	121.93	124.45
20	F	302	CLA	CMC-C2C-C1C	2.75	129.22	125.04
20	7	1011	CLA	CHD-C1D-ND	-2.75	121.93	124.45
29	6	316	CHL	CHD-C1D-ND	-2.75	121.93	124.45
20	G	202	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
20	A	803	CLA	CHC-C1C-NC	2.75	128.37	124.20
20	1	1010	CLA	CHC-C1C-C2C	-2.75	119.11	126.73
20	B	822	CLA	CHC-C1C-NC	2.74	128.37	124.20
20	3	1012	CLA	CHC-C1C-NC	2.74	128.37	124.20
20	4	308	CLA	CHC-C1C-NC	2.74	128.37	124.20
20	F	305	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
20	A	818	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
20	6	309	CLA	C1D-ND-C4D	-2.74	104.39	106.33
29	4	313	CHL	CHC-C1C-NC	2.74	128.36	124.20
20	6	315	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
29	8	315	CHL	CHC-C1C-NC	2.74	128.35	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	818	CLA	CHC-C1C-NC	2.74	128.35	124.20
20	A	809	CLA	CHC-C1C-NC	2.73	128.35	124.20
20	L	203	CLA	CHC-C1C-NC	2.73	128.35	124.20
20	7	1006	CLA	C4A-NA-C1A	-2.73	105.48	106.71
20	7	1008	CLA	CHC-C1C-NC	2.73	128.35	124.20
20	B	824	CLA	CHB-C1B-NB	-2.73	121.37	124.26
20	A	823	CLA	C1D-ND-C4D	-2.73	104.40	106.33
20	A	815	CLA	C1D-ND-C4D	-2.73	104.40	106.33
20	3	1015	CLA	CHC-C1C-C2C	-2.73	119.16	126.73
20	B	827	CLA	CHC-C1C-C2C	-2.72	119.16	126.73
24	1	1001	BCR	C15-C14-C13	2.72	131.20	127.31
20	1	1004	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
20	1	1004	CLA	CHD-C1D-ND	-2.72	121.95	124.45
20	4	309	CLA	CHD-C1D-ND	-2.72	121.95	124.45
20	6	307	CLA	CHB-C1B-NB	-2.72	121.38	124.26
20	B	828	CLA	C1D-ND-C4D	-2.72	104.40	106.33
24	7	1003	BCR	C20-C19-C18	2.72	134.06	126.42
29	3	1014	CHL	CHB-C1B-NB	2.72	127.13	124.26
20	B	826	CLA	CHC-C1C-NC	2.72	128.32	124.20
20	5	321	CLA	CHC-C1C-NC	2.72	128.32	124.20
20	1	1005	CLA	CHC-C1C-C2C	-2.72	119.19	126.73
20	A	813	CLA	CHA-C1A-NA	-2.72	120.18	126.40
20	3	1009	CLA	CHC-C1C-C2C	-2.72	119.19	126.73
20	F	303	CLA	C4A-NA-C1A	-2.72	105.48	106.71
20	3	1011	CLA	CAA-C2A-C1A	-2.71	105.10	111.81
20	B	811	CLA	C1D-ND-C4D	-2.71	104.41	106.33
20	5	304	CLA	CHC-C1C-C2C	-2.71	119.19	126.73
20	B	819	CLA	C1D-ND-C4D	-2.71	104.41	106.33
24	4	302	BCR	C15-C14-C13	2.71	131.18	127.31
20	B	829	CLA	CHC-C1C-C2C	-2.71	119.20	126.73
20	B	818	CLA	CHA-C1A-NA	-2.71	120.19	126.40
20	8	307	CLA	CHD-C1D-ND	-2.71	121.96	124.45
20	B	824	CLA	CHC-C1C-C2C	-2.71	119.20	126.73
20	B	826	CLA	CHC-C1C-C2C	-2.71	119.20	126.73
20	L	202	CLA	C2C-C1C-NC	2.71	112.51	109.97
29	0	317	CHL	C2B-C1B-NB	2.71	112.05	110.23
29	6	314	CHL	C2B-C1B-NB	2.71	112.05	110.23
20	7	1011	CLA	CHC-C1C-NC	2.71	128.31	124.20
20	7	1011	CLA	CHB-C1B-NB	-2.71	121.39	124.26
20	B	811	CLA	CHC-C1C-NC	2.71	128.31	124.20
20	0	301	CLA	CHB-C1B-NB	-2.70	121.39	124.26
20	0	313	CLA	CHC-C1C-C2C	-2.70	119.22	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	321	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
20	3	1017	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
20	5	301	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
20	B	807	CLA	CHB-C1B-NB	-2.70	121.40	124.26
20	A	805	CLA	CHD-C1D-ND	-2.70	121.97	124.45
20	0	305	CLA	CHC-C1C-NC	2.70	128.30	124.20
20	A	803	CLA	CHB-C1B-NB	-2.70	121.40	124.26
24	6	302	BCR	C15-C14-C13	2.70	131.16	127.31
20	8	309	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
29	7	1017	CHL	C3A-C2A-C1A	2.69	105.37	101.34
20	B	841	CLA	C2C-C1C-NC	2.69	112.50	109.97
20	A	837	CLA	CHB-C1B-NB	-2.69	121.41	124.26
20	B	835	CLA	C2C-C1C-NC	2.69	112.49	109.97
24	B	804	BCR	C8-C9-C10	2.69	123.07	118.94
20	4	304	CLA	CHC-C4B-NB	-2.69	121.41	124.26
20	A	812	CLA	CHB-C1B-NB	-2.69	121.41	124.26
20	3	1010	CLA	C2C-C1C-NC	2.69	112.49	109.97
20	B	819	CLA	CHC-C1C-NC	2.69	128.28	124.20
20	A	851	CLA	CHC-C1C-C2C	-2.69	119.27	126.73
20	A	834	CLA	C1D-ND-C4D	-2.68	104.43	106.33
20	3	1008	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
20	A	821	CLA	C2C-C1C-NC	2.68	112.48	109.97
20	6	308	CLA	CHC-C1C-NC	2.68	128.27	124.20
20	A	831	CLA	CHA-C1A-NA	-2.68	120.26	126.40
20	A	820	CLA	CHC-C1C-NC	2.68	128.27	124.20
20	8	308	CLA	C1D-ND-C4D	-2.68	104.43	106.33
20	B	834	CLA	CHB-C1B-NB	-2.68	121.42	124.26
29	5	313	CHL	CHA-C1A-NA	-2.68	120.26	126.40
20	A	804	CLA	CHC-C4B-NB	-2.68	121.42	124.26
29	7	1012	CHL	C3A-C2A-C1A	2.68	105.35	101.34
29	4	315	CHL	CHA-C1A-NA	-2.67	120.27	126.40
20	B	809	CLA	CHD-C1D-ND	-2.67	122.00	124.45
20	B	809	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
20	F	305	CLA	C2C-C1C-NC	2.67	112.47	109.97
20	B	833	CLA	C1D-ND-C4D	-2.67	104.44	106.33
20	A	834	CLA	CHC-C1C-NC	2.67	128.26	124.20
20	B	815	CLA	CHC-C4B-NB	-2.67	121.43	124.26
20	7	1006	CLA	CHD-C1D-ND	-2.67	122.00	124.45
20	6	312	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
20	8	309	CLA	C1C-C2C-C3C	2.67	109.76	106.96
30	5	303	XAT	O4-C5-C4	2.67	115.38	113.38
20	B	836	CLA	CHC-C1C-C2C	-2.66	119.33	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	837	CLA	C1D-ND-C4D	-2.66	104.44	106.33
20	8	305	CLA	C2C-C1C-NC	2.66	112.47	109.97
20	6	312	CLA	CHB-C1B-NB	-2.66	121.44	124.26
30	7	1002	XAT	C28-C29-C30	2.66	123.03	118.94
20	5	309	CLA	CHC-C1C-C2C	-2.66	119.33	126.73
20	7	1011	CLA	C1D-ND-C4D	-2.66	104.44	106.33
29	4	312	CHL	CHC-C1C-NC	2.66	128.24	124.20
20	0	307	CLA	CHC-C1C-C2C	-2.66	119.34	126.73
20	0	301	CLA	CHA-C1A-NA	-2.66	120.31	126.40
20	8	312	CLA	CHC-C4B-NB	-2.66	121.44	124.26
20	B	832	CLA	CHC-C1C-NC	2.66	128.24	124.20
29	4	316	CHL	CHD-C1D-ND	-2.66	122.01	124.45
20	8	307	CLA	CHB-C1B-NB	-2.66	121.44	124.26
20	B	834	CLA	CHC-C1C-NC	2.66	128.24	124.20
20	5	309	CLA	CHC-C1C-NC	2.66	128.23	124.20
20	8	309	CLA	C2D-C1D-ND	-2.66	108.15	110.10
20	A	806	CLA	C2C-C1C-NC	2.66	112.46	109.97
20	5	305	CLA	CHD-C1D-ND	-2.66	122.01	124.45
20	B	815	CLA	CHC-C1C-C2C	-2.66	119.35	126.73
20	6	307	CLA	CHC-C1C-C2C	-2.66	119.35	126.73
20	0	306	CLA	C2C-C1C-NC	2.65	112.46	109.97
29	7	1012	CHL	CHA-C1A-NA	-2.65	120.32	126.40
20	K	202	CLA	C3B-C2B-C1B	2.65	109.62	106.75
20	A	802	CLA	CHB-C1B-NB	-2.65	121.45	124.26
20	7	1004	CLA	CHC-C4B-NB	-2.65	121.45	124.26
20	A	812	CLA	CHA-C1A-NA	-2.65	120.33	126.40
20	5	307	CLA	CHA-C1A-NA	-2.65	120.33	126.40
20	A	837	CLA	CHC-C1C-C2C	-2.65	119.37	126.73
20	3	1012	CLA	C1D-ND-C4D	-2.65	104.45	106.33
20	0	307	CLA	CHC-C4B-NB	-2.65	121.45	124.26
20	B	812	CLA	CHD-C1D-ND	-2.65	122.02	124.45
20	A	802	CLA	C2C-C1C-NC	2.65	112.45	109.97
20	5	315	CLA	CHC-C1C-C2C	-2.64	119.38	126.73
29	4	313	CHL	CHA-C1A-NA	-2.64	120.34	126.40
20	0	311	CLA	C1D-ND-C4D	-2.64	104.46	106.33
20	A	827	CLA	C2C-C1C-NC	2.64	112.45	109.97
20	A	822	CLA	C2C-C1C-NC	2.64	112.44	109.97
20	5	312	CLA	C4A-NA-C1A	-2.64	105.52	106.71
20	A	832	CLA	C1D-ND-C4D	-2.64	104.46	106.33
20	A	825	CLA	CHC-C1C-NC	2.64	128.20	124.20
20	B	827	CLA	C2C-C1C-NC	2.64	112.44	109.97
20	A	805	CLA	CHC-C1C-C2C	-2.64	119.41	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	841	CLA	CHA-C1A-NA	-2.63	120.36	126.40
20	A	827	CLA	CHC-C1C-C2C	-2.63	119.41	126.73
20	A	828	CLA	CHC-C1C-C2C	-2.63	119.42	126.73
20	B	819	CLA	CHC-C1C-C2C	-2.63	119.42	126.73
20	1	1007	CLA	CGD-CBD-CAD	-2.63	102.21	110.73
20	A	837	CLA	CHD-C1D-ND	-2.63	122.04	124.45
20	5	321	CLA	CHA-C1A-NA	-2.63	120.38	126.40
20	B	808	CLA	CHC-C4B-NB	-2.63	121.47	124.26
20	4	305	CLA	C1D-ND-C4D	-2.63	104.47	106.33
20	A	810	CLA	C2C-C1C-NC	2.63	112.43	109.97
20	5	318	CLA	CHC-C1C-NC	2.63	128.19	124.20
20	B	818	CLA	CHC-C1C-C2C	-2.63	119.44	126.73
20	F	302	CLA	CHD-C1D-ND	-2.63	122.04	124.45
24	8	302	BCR	C15-C14-C13	2.62	131.06	127.31
20	6	308	CLA	CHC-C1C-C2C	-2.62	119.45	126.73
20	5	318	CLA	CHC-C1C-C2C	-2.62	119.45	126.73
20	B	801	CLA	C4A-NA-C1A	-2.62	105.53	106.71
20	A	807	CLA	CHC-C1C-NC	2.62	128.18	124.20
20	A	809	CLA	C4A-NA-C1A	-2.62	105.53	106.71
20	5	321	CLA	C2C-C1C-NC	2.62	112.42	109.97
20	J	102	CLA	CHC-C1C-NC	2.61	128.17	124.20
20	7	1009	CLA	CHC-C1C-C2C	-2.61	119.47	126.73
20	B	830	CLA	CHB-C1B-NB	-2.61	121.49	124.26
20	L	204	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
20	L	202	CLA	C1D-ND-C4D	-2.61	104.48	106.33
20	B	839	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
20	B	839	CLA	CHC-C1C-NC	2.61	128.16	124.20
20	A	816	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
29	5	314	CHL	CHC-C1C-NC	2.61	128.16	124.20
20	A	802	CLA	CHD-C1D-ND	-2.61	122.06	124.45
24	A	846	BCR	C15-C16-C17	2.61	128.81	123.47
20	8	306	CLA	CHD-C1D-ND	-2.61	122.06	124.45
20	B	816	CLA	CHC-C1C-C2C	-2.61	119.49	126.73
20	6	318	CLA	CHA-C1A-NA	-2.61	120.43	126.40
20	F	302	CLA	CHC-C4B-NB	-2.61	121.50	124.26
20	A	837	CLA	CHA-C1A-NA	-2.61	120.43	126.40
24	B	843	BCR	C23-C24-C25	2.60	134.51	127.20
20	A	806	CLA	CHA-C1A-NA	-2.60	120.44	126.40
20	0	310	CLA	CHC-C1C-C2C	-2.60	119.51	126.73
24	7	1003	BCR	C16-C17-C18	2.60	131.02	127.31
20	3	1005	CLA	C1D-ND-C4D	-2.60	104.49	106.33
20	0	311	CLA	CHC-C1C-C2C	-2.60	119.52	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	309	CLA	C2C-C1C-NC	2.60	112.40	109.97
20	7	1007	CLA	CHC-C1C-C2C	-2.60	119.52	126.73
20	L	203	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
20	1	1009	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
20	5	307	CLA	C2C-C1C-NC	2.59	112.40	109.97
20	B	828	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
20	6	306	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
29	5	317	CHL	CAA-C2A-C1A	2.59	117.88	112.14
20	A	814	CLA	C1D-ND-C4D	-2.59	104.50	106.33
20	F	303	CLA	C2C-C1C-NC	2.59	112.40	109.97
20	8	306	CLA	CHC-C4B-NB	-2.59	121.52	124.26
20	8	306	CLA	CHB-C1B-NB	-2.59	121.52	124.26
20	K	201	CLA	C2C-C1C-NC	2.59	112.39	109.97
20	B	811	CLA	CHC-C4B-NB	-2.59	121.52	124.26
20	B	806	CLA	CHC-C1C-NC	2.59	128.12	124.20
20	G	202	CLA	C2C-C1C-NC	2.58	112.39	109.97
29	8	317	CHL	C1D-ND-C4D	-2.58	104.50	106.33
20	A	833	CLA	CHA-C1A-NA	-2.58	120.49	126.40
20	A	805	CLA	C1D-ND-C4D	-2.58	104.50	106.33
20	B	814	CLA	C2C-C1C-NC	2.58	112.39	109.97
20	8	311	CLA	CHC-C4B-NB	-2.58	121.53	124.26
20	A	824	CLA	C4A-NA-C1A	-2.58	105.55	106.71
20	B	805	CLA	C2C-C1C-NC	2.58	112.39	109.97
20	G	202	CLA	C1D-ND-C4D	-2.58	104.50	106.33
30	7	1002	XAT	C17-C1-C2	-2.57	104.51	108.98
27	4	318	LMG	C1-C2-C3	2.57	115.36	110.00
20	B	832	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
20	A	832	CLA	CHA-C1A-NA	-2.57	120.50	126.40
20	1	1014	CLA	CHA-C1A-NA	-2.57	120.50	126.40
20	B	841	CLA	C1D-ND-C4D	-2.57	104.51	106.33
20	B	813	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
20	A	827	CLA	CHC-C1C-NC	2.57	128.10	124.20
20	A	813	CLA	CAA-CBA-CGA	2.57	119.33	112.51
20	6	301	CLA	CHC-C1C-NC	2.57	128.10	124.20
20	6	301	CLA	CHB-C1B-NB	-2.57	121.54	124.26
20	6	311	CLA	CHC-C4B-NB	-2.57	121.54	124.26
25	B	848	DGD	O1G-C1A-C2A	2.57	119.97	111.91
20	1	1007	CLA	C4A-NA-C1A	-2.57	105.55	106.71
20	B	809	CLA	C1D-ND-C4D	-2.57	104.51	106.33
20	5	309	CLA	C2C-C1C-NC	2.57	112.38	109.97
20	0	305	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
20	A	835	CLA	C1D-ND-C4D	-2.56	104.51	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	308	CLA	CHC-C4B-NB	-2.56	121.54	124.26
20	4	314	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
24	4	302	BCR	C23-C24-C25	2.56	134.40	127.20
20	8	316	CLA	C2C-C1C-NC	2.56	112.37	109.97
20	7	1014	CLA	C1D-ND-C4D	-2.56	104.52	106.33
20	B	826	CLA	C2C-C1C-NC	2.56	112.37	109.97
20	1	1010	CLA	C2C-C1C-NC	2.56	112.37	109.97
29	6	317	CHL	CHD-C1D-ND	-2.56	122.10	124.45
24	H	201	BCR	C8-C9-C10	2.56	122.87	118.94
20	0	306	CLA	C1D-ND-C4D	-2.56	104.52	106.33
20	3	1007	CLA	C2C-C1C-NC	2.56	112.37	109.97
20	B	828	CLA	CHA-C1A-NA	-2.56	120.54	126.40
20	5	306	CLA	CHC-C1C-NC	2.55	128.08	124.20
20	A	819	CLA	CHC-C1C-C2C	-2.55	119.64	126.73
20	B	837	CLA	CHA-C1A-NA	-2.55	120.55	126.40
20	4	304	CLA	C4D-CHA-C1A	-2.55	118.15	121.25
20	8	316	CLA	CHC-C1C-C2C	-2.55	119.66	126.73
20	8	310	CLA	CHC-C1C-C2C	-2.54	119.66	126.73
24	H	201	BCR	C7-C8-C9	-2.54	122.39	126.23
20	3	1011	CLA	C2C-C1C-NC	2.54	112.36	109.97
20	B	839	CLA	C2C-C1C-NC	2.54	112.35	109.97
20	7	1007	CLA	CMC-C2C-C1C	2.54	128.91	125.04
20	6	310	CLA	CHC-C1C-C2C	-2.54	119.67	126.73
20	5	318	CLA	C2C-C1C-NC	2.54	112.35	109.97
29	6	316	CHL	CHC-C1C-NC	2.54	128.06	124.20
20	B	814	CLA	CHB-C1B-NB	-2.54	121.57	124.26
20	3	1015	CLA	C1D-ND-C4D	-2.54	104.53	106.33
20	B	816	CLA	CHD-C1D-ND	-2.54	122.12	124.45
20	B	803	CLA	C2C-C1C-NC	2.54	112.35	109.97
20	4	307	CLA	CHD-C4C-NC	2.54	128.20	124.20
20	5	304	CLA	C2D-C1D-ND	-2.53	108.24	110.10
30	8	304	XAT	C28-C29-C30	2.53	122.83	118.94
20	4	314	CLA	CHC-C1C-NC	2.53	128.04	124.20
20	5	304	CLA	CHD-C1D-ND	-2.53	122.13	124.45
20	0	313	CLA	C4A-NA-C1A	-2.53	105.57	106.71
20	A	813	CLA	C2C-C1C-NC	2.53	112.34	109.97
20	6	305	CLA	CMC-C2C-C1C	2.53	128.89	125.04
20	B	824	CLA	CHD-C1D-C2D	2.53	130.78	125.48
29	6	313	CHL	CHC-C1C-NC	2.53	128.03	124.20
20	A	833	CLA	CHD-C1D-ND	-2.52	122.14	124.45
20	B	824	CLA	C2C-C1C-NC	2.52	112.34	109.97
20	6	318	CLA	CHC-C1C-NC	2.52	128.03	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	205	BCR	C15-C14-C13	2.52	130.91	127.31
20	A	839	CLA	CHC-C1C-C2C	-2.52	119.74	126.73
20	A	809	CLA	CHC-C1C-C2C	-2.52	119.74	126.73
20	7	1006	CLA	C2C-C1C-NC	2.52	112.33	109.97
29	1	1013	CHL	CHA-C1A-NA	-2.51	120.64	126.40
20	5	301	CLA	C3B-C2B-C1B	2.51	110.20	107.16
20	8	309	CLA	CHA-C1A-NA	-2.51	120.64	126.40
20	8	308	CLA	C2A-C3A-C4A	2.51	105.93	101.87
24	B	843	BCR	C12-C13-C14	2.51	122.79	118.94
20	1	1010	CLA	CHA-C1A-NA	-2.51	120.65	126.40
20	A	820	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
20	A	829	CLA	C4A-NA-C1A	-2.51	105.58	106.71
20	B	840	CLA	CHC-C1C-C2C	-2.51	119.77	126.73
20	8	308	CLA	C2C-C1C-NC	2.51	112.32	109.97
25	5	319	DGD	O3D-C3D-C2D	-2.50	104.56	110.35
20	A	812	CLA	CHC-C1C-C2C	-2.50	119.78	126.73
20	5	307	CLA	CHD-C1D-ND	-2.50	122.15	124.45
29	4	313	CHL	C1D-ND-C4D	-2.50	104.56	106.33
24	B	843	BCR	C15-C14-C13	2.50	130.88	127.31
20	A	836	CLA	C1D-ND-C4D	-2.50	104.56	106.33
20	A	808	CLA	C2C-C1C-NC	2.50	112.31	109.97
20	B	825	CLA	C1D-ND-C4D	-2.50	104.56	106.33
20	B	821	CLA	C1D-ND-C4D	-2.50	104.56	106.33
20	6	305	CLA	CHC-C4B-NB	-2.50	121.61	124.26
20	B	817	CLA	CHC-C1C-C2C	-2.50	119.80	126.73
20	J	102	CLA	C4A-NA-C1A	-2.49	105.58	106.71
20	B	814	CLA	C1D-ND-C4D	-2.49	104.56	106.33
20	8	306	CLA	CHC-C1C-C2C	-2.49	119.81	126.73
20	B	803	CLA	CHA-C1A-NA	-2.49	120.70	126.40
20	F	303	CLA	CHA-C1A-NA	-2.49	120.70	126.40
20	A	808	CLA	C1D-ND-C4D	-2.49	104.57	106.33
20	A	824	CLA	C1D-ND-C4D	-2.49	104.57	106.33
20	B	822	CLA	CHB-C1B-NB	-2.49	121.62	124.26
29	6	314	CHL	CGD-CBD-CAD	-2.49	102.68	110.73
20	B	801	CLA	CHA-C1A-NA	-2.49	120.70	126.40
29	7	1013	CHL	CHC-C1C-NC	2.48	127.97	124.20
20	B	808	CLA	C2C-C1C-NC	2.48	112.30	109.97
20	0	310	CLA	CHB-C1B-NB	-2.48	121.63	124.26
20	7	1007	CLA	CHA-C1A-NA	-2.48	120.72	126.40
20	1	1008	CLA	CHC-C4B-NB	-2.48	121.63	124.26
27	5	324	LMG	C7-O1-C1	2.48	118.58	113.74
20	A	831	CLA	CHC-C1C-NC	2.48	127.96	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	813	CLA	CHC-C1C-NC	2.48	127.96	124.20
20	6	320	CLA	CHA-C1A-NA	-2.48	120.72	126.40
20	B	810	CLA	C1D-ND-C4D	-2.48	104.58	106.33
20	G	203	CLA	CHC-C1C-C2C	-2.48	119.85	126.73
20	1	1017	CLA	C1D-ND-C4D	-2.47	104.58	106.33
20	0	316	CLA	CHA-C1A-NA	-2.47	120.73	126.40
20	7	1010	CLA	C1D-ND-C4D	-2.47	104.58	106.33
20	A	804	CLA	CHA-C1A-NA	-2.47	120.73	126.40
20	0	305	CLA	CHA-C1A-NA	-2.47	120.73	126.40
20	6	310	CLA	CHA-C1A-NA	-2.47	120.74	126.40
25	5	319	DGD	O5D-C6D-C5D	2.47	113.62	109.05
20	5	312	CLA	CAC-C3C-C4C	-2.47	121.60	124.81
20	B	802	CLA	CHC-C1C-C2C	-2.47	119.86	126.73
20	G	203	CLA	CHC-C1C-NC	2.47	127.95	124.20
20	A	804	CLA	CHC-C1C-C2C	-2.47	119.87	126.73
20	3	1013	CLA	C1D-ND-C4D	-2.47	104.58	106.33
20	B	819	CLA	C2C-C1C-NC	2.47	112.28	109.97
20	8	312	CLA	CHC-C1C-C2C	-2.47	119.87	126.73
20	A	825	CLA	CHC-C1C-C2C	-2.47	119.87	126.73
20	3	1016	CLA	CHD-C1D-ND	-2.47	122.19	124.45
20	7	1004	CLA	CHB-C4A-NA	2.47	127.92	124.51
20	7	1014	CLA	CHC-C1C-C2C	-2.47	119.88	126.73
20	A	832	CLA	C4A-NA-C1A	-2.46	105.60	106.71
24	I	201	BCR	C31-C1-C6	-2.46	106.31	110.30
24	G	204	BCR	C12-C13-C14	2.46	122.72	118.94
20	B	827	CLA	C1D-ND-C4D	-2.46	104.59	106.33
20	4	307	CLA	CHC-C1C-C2C	-2.46	119.90	126.73
20	B	807	CLA	C1D-ND-C4D	-2.46	104.59	106.33
29	5	314	CHL	CHA-C1A-NA	-2.46	120.77	126.40
20	A	851	CLA	C2C-C1C-NC	2.46	112.27	109.97
20	A	802	CLA	C1D-ND-C4D	-2.46	104.59	106.33
20	4	305	CLA	CHC-C1C-C2C	-2.46	119.91	126.73
20	8	310	CLA	CHA-C1A-NA	-2.45	120.78	126.40
20	1	1004	CLA	CHA-C1A-NA	-2.45	120.78	126.40
20	B	806	CLA	CHC-C1C-C2C	-2.45	119.91	126.73
20	4	305	CLA	CHB-C1B-NB	-2.45	121.66	124.26
20	8	306	CLA	C1D-ND-C4D	-2.45	104.59	106.33
20	B	834	CLA	C1D-ND-C4D	-2.45	104.59	106.33
20	4	314	CLA	C2C-C1C-NC	2.45	112.27	109.97
29	7	1013	CHL	CHB-C1B-C2B	-2.45	120.31	127.24
20	A	832	CLA	C2C-C1C-NC	2.45	112.27	109.97
20	0	306	CLA	CHC-C4B-NB	-2.45	121.66	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	316	CHL	C2C-C3C-C4C	2.45	108.23	106.49
29	8	315	CHL	C2B-C1B-NB	2.45	111.87	110.23
20	1	1011	CLA	CAA-C2A-C1A	-2.45	103.95	111.97
20	A	810	CLA	CBA-CAA-C2A	2.45	121.09	113.86
20	3	1005	CLA	CHC-C1C-NC	2.45	127.92	124.20
20	0	306	CLA	CHA-C1A-NA	-2.45	120.80	126.40
20	A	812	CLA	C1D-ND-C4D	-2.44	104.60	106.33
20	0	305	CLA	CHB-C1B-NB	-2.44	121.67	124.26
20	G	201	CLA	C2C-C1C-NC	2.44	112.26	109.97
20	A	817	CLA	CHA-C1A-NA	-2.44	120.81	126.40
20	6	309	CLA	CHC-C4B-NB	-2.44	121.67	124.26
20	B	802	CLA	C2C-C1C-NC	2.44	112.26	109.97
29	7	1017	CHL	C2B-C1B-NB	2.44	111.87	110.23
20	5	308	CLA	CHA-C1A-NA	-2.44	120.81	126.40
20	3	1009	CLA	C1D-ND-C4D	-2.44	104.60	106.33
24	B	804	BCR	C12-C13-C14	2.44	122.68	118.94
20	3	1008	CLA	C2C-C1C-NC	2.44	112.25	109.97
20	3	1017	CLA	C2C-C1C-NC	2.44	112.25	109.97
20	A	829	CLA	C1D-ND-C4D	-2.44	104.60	106.33
20	A	820	CLA	C1D-ND-C4D	-2.44	104.61	106.33
20	3	1015	CLA	C2C-C1C-NC	2.43	112.25	109.97
20	A	834	CLA	CHA-C1A-NA	-2.43	120.83	126.40
29	8	315	CHL	CHD-C1D-C2D	2.43	130.58	125.48
20	B	820	CLA	C1D-ND-C4D	-2.43	104.61	106.33
20	6	301	CLA	C1D-ND-C4D	-2.43	104.61	106.33
20	4	306	CLA	C4A-NA-C1A	-2.43	105.61	106.71
20	6	318	CLA	CHB-C1B-NB	-2.43	121.69	124.26
20	B	835	CLA	CHA-C1A-NA	-2.43	120.84	126.40
20	J	102	CLA	C1D-ND-C4D	-2.43	104.61	106.33
20	4	310	CLA	CHB-C1B-NB	-2.42	121.69	124.26
20	8	308	CLA	CHC-C1C-C2C	-2.42	120.00	126.73
20	5	322	CLA	C2C-C1C-NC	2.42	112.24	109.97
20	L	203	CLA	CHB-C1B-NB	-2.42	121.69	124.26
30	4	303	XAT	O4-C5-C6	-2.42	56.96	58.96
20	B	802	CLA	CHC-C1C-NC	2.42	127.87	124.20
20	3	1009	CLA	C2C-C1C-NC	2.42	112.24	109.97
29	6	316	CHL	C4B-CHC-C1C	-2.42	120.60	126.34
20	B	828	CLA	CHC-C1C-NC	2.42	127.87	124.20
29	8	317	CHL	C10-C8-C7	2.41	124.83	112.13
25	B	848	DGD	C3G-O3G-C1D	-2.41	109.02	113.74
20	F	302	CLA	C2C-C1C-NC	2.41	112.23	109.97
20	6	306	CLA	CHA-C1A-NA	-2.41	120.87	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	4	315	CHL	CHD-C4C-C3C	2.41	128.38	124.84
20	B	807	CLA	CHC-C1C-NC	2.41	127.86	124.20
29	7	1015	CHL	CHC-C1C-NC	2.41	127.86	124.20
20	6	318	CLA	CHC-C1C-C2C	-2.41	120.04	126.73
20	4	311	CLA	C2C-C1C-NC	2.41	112.23	109.97
20	6	308	CLA	C3D-C2D-C1D	2.41	109.12	105.83
20	0	307	CLA	C4A-NA-C1A	-2.41	105.62	106.71
20	0	313	CLA	C2C-C1C-NC	2.40	112.22	109.97
27	6	319	LMG	C4-C3-C2	2.40	115.02	110.82
20	8	307	CLA	CAC-C3C-C4C	2.40	127.93	124.81
20	A	831	CLA	CHC-C1C-C2C	-2.40	120.05	126.73
20	4	305	CLA	CHA-C1A-NA	-2.40	120.89	126.40
20	B	825	CLA	CHC-C1C-C2C	-2.40	120.06	126.73
22	A	842	PQN	C12-C11-C3	-2.40	105.57	112.05
29	7	1015	CHL	CHD-C1D-ND	-2.40	122.25	124.45
29	1	1015	CHL	CHB-C1B-C2B	-2.40	120.46	127.24
28	4	317	LUT	C1-C2-C3	2.40	119.06	113.64
20	3	1016	CLA	CHA-C1A-NA	-2.40	120.91	126.40
20	0	305	CLA	CHC-C4B-NB	-2.40	121.72	124.26
20	7	1004	CLA	CHA-C1A-NA	-2.40	120.91	126.40
20	B	817	CLA	C1D-ND-C4D	-2.40	104.63	106.33
29	8	315	CHL	CHA-C1A-NA	-2.39	120.92	126.40
20	7	1004	CLA	C2C-C1C-NC	2.39	112.21	109.97
29	5	316	CHL	CHD-C1D-ND	-2.39	122.26	124.45
20	1	1003	CLA	CHA-C1A-NA	-2.39	120.93	126.40
20	A	803	CLA	CHC-C1C-C2C	-2.39	120.09	126.73
20	B	801	CLA	CHB-C1B-NB	-2.39	121.73	124.26
20	5	306	CLA	CMA-C3A-C4A	2.39	118.19	111.77
30	4	303	XAT	C18-C5-C4	-2.38	111.60	114.28
20	5	311	CLA	CHB-C1B-NB	-2.38	121.73	124.26
20	B	807	CLA	CHC-C1C-C2C	-2.38	120.11	126.73
20	F	302	CLA	C1D-ND-C4D	-2.38	104.64	106.33
20	A	807	CLA	CHC-C1C-C2C	-2.38	120.12	126.73
20	8	306	CLA	CHA-C1A-NA	-2.38	120.95	126.40
20	G	203	CLA	C2C-C1C-NC	2.38	112.20	109.97
29	6	317	CHL	CHC-C1C-NC	2.38	127.81	124.20
20	B	816	CLA	CHA-C1A-NA	-2.38	120.95	126.40
24	A	847	BCR	C7-C8-C9	2.38	129.83	126.23
20	1	1004	CLA	C2C-C1C-NC	2.38	112.20	109.97
20	A	828	CLA	C1D-ND-C4D	-2.37	104.65	106.33
20	A	828	CLA	CHA-C1A-NA	-2.37	120.96	126.40
20	L	203	CLA	CHA-C1A-NA	-2.37	120.97	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	301	CLA	CAA-CBA-CGA	2.37	118.80	112.51
20	B	811	CLA	CHC-C1C-C2C	-2.37	120.14	126.73
28	7	1001	LUT	C7-C8-C9	-2.37	122.66	126.23
20	6	301	CLA	CHC-C4B-NB	-2.37	121.75	124.26
20	B	822	CLA	CHD-C1D-ND	-2.37	122.28	124.45
20	7	1011	CLA	CHC-C1C-C2C	-2.37	120.15	126.73
20	6	308	CLA	C2C-C1C-NC	2.37	112.19	109.97
20	3	1016	CLA	CHB-C4A-NA	2.37	127.78	124.51
20	A	803	CLA	CHA-C1A-NA	-2.37	120.98	126.40
20	B	836	CLA	C2C-C1C-NC	2.37	112.19	109.97
20	B	831	CLA	CHB-C1B-NB	-2.36	121.75	124.26
20	6	315	CLA	CHC-C4B-NB	-2.36	121.75	124.26
20	6	305	CLA	CHD-C1D-ND	-2.36	122.28	124.45
20	B	822	CLA	C1D-ND-C4D	-2.36	104.66	106.33
20	A	817	CLA	C1D-ND-C4D	-2.36	104.66	106.33
24	5	320	BCR	C24-C23-C22	2.36	129.80	126.23
20	A	825	CLA	C1D-ND-C4D	-2.36	104.66	106.33
20	6	308	CLA	C3A-C2A-C1A	-2.36	97.81	101.34
20	6	308	CLA	CMC-C2C-C1C	2.36	128.63	125.04
20	8	316	CLA	CHC-C1C-NC	2.36	127.78	124.20
20	8	311	CLA	C1D-ND-C4D	-2.36	104.66	106.33
20	K	201	CLA	CHC-C4B-NB	-2.35	121.77	124.26
29	0	315	CHL	CHC-C1C-NC	2.35	127.77	124.20
20	B	836	CLA	C1D-ND-C4D	-2.35	104.67	106.33
20	F	302	CLA	CHA-C1A-NA	-2.35	121.02	126.40
29	7	1017	CHL	C1C-C2C-C3C	2.35	108.98	107.11
29	5	316	CHL	C10-C8-C7	2.35	124.47	112.13
20	A	818	CLA	CHC-C4B-NB	-2.34	121.78	124.26
24	8	302	BCR	C23-C24-C25	2.34	133.77	127.20
20	0	311	CLA	C4A-NA-C1A	-2.34	105.65	106.71
20	A	829	CLA	CHA-C1A-NA	-2.34	121.05	126.40
20	5	306	CLA	CHC-C1C-C2C	-2.34	120.24	126.73
29	4	315	CHL	C2C-C3C-C4C	2.34	108.16	106.49
20	3	1005	CLA	CHC-C1C-C2C	-2.34	120.24	126.73
20	A	801	CLA	C2A-C3A-C4A	2.34	105.64	101.87
20	B	829	CLA	C2C-C1C-NC	2.34	112.16	109.97
20	0	307	CLA	CHD-C1D-ND	-2.33	122.31	124.45
20	4	307	CLA	CMC-C2C-C1C	2.33	128.59	125.04
20	B	806	CLA	CHA-C1A-NA	-2.33	121.06	126.40
20	5	312	CLA	CHA-C1A-NA	-2.33	121.06	126.40
29	5	316	CHL	C3D-C2D-C1D	2.33	109.01	105.83
24	I	201	BCR	C15-C16-C17	2.33	128.24	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	1013	CHL	CHB-C1B-NB	2.33	126.72	124.26
20	0	305	CLA	C1D-ND-C4D	-2.33	104.68	106.33
20	4	314	CLA	C2D-C1D-ND	-2.33	108.39	110.10
29	4	316	CHL	CHB-C1B-NB	2.32	126.72	124.26
20	6	315	CLA	CHB-C4A-NA	2.32	127.73	124.51
20	0	312	CLA	CHC-C4B-NB	-2.32	121.80	124.26
20	B	826	CLA	CHA-C1A-NA	-2.32	121.08	126.40
20	A	828	CLA	C2C-C1C-NC	2.32	112.15	109.97
20	B	831	CLA	C1D-ND-C4D	-2.32	104.69	106.33
20	8	309	CLA	CHD-C1D-ND	-2.32	122.32	124.45
20	B	832	CLA	C2C-C1C-NC	2.32	112.15	109.97
29	0	317	CHL	CHB-C1B-C2B	-2.32	120.69	127.24
20	B	825	CLA	CHC-C1C-NC	2.32	127.72	124.20
20	A	826	CLA	C2C-C1C-NC	2.32	112.14	109.97
20	4	304	CLA	C1D-ND-C4D	-2.32	104.69	106.33
24	B	804	BCR	C7-C8-C9	-2.31	122.74	126.23
29	1	1015	CHL	C2D-C1D-ND	-2.31	108.40	110.10
20	A	811	CLA	CHC-C4B-NB	-2.31	121.81	124.26
27	0	303	LMG	O1-C7-C8	2.31	116.48	110.90
20	B	823	CLA	CHC-C4B-NB	-2.31	121.81	124.26
29	5	316	CHL	CHB-C1B-C2B	-2.31	120.71	127.24
30	8	304	XAT	C16-C1-C2	-2.31	104.97	108.98
20	A	809	CLA	C1D-ND-C4D	-2.31	104.69	106.33
20	5	301	CLA	C3B-C4B-NB	-2.31	108.37	110.52
20	4	306	CLA	CHC-C4B-NB	-2.31	121.81	124.26
20	6	312	CLA	C2C-C1C-NC	2.31	112.13	109.97
30	7	1002	XAT	C7-C8-C9	2.30	129.11	125.53
20	8	305	CLA	C1D-ND-C4D	-2.30	104.70	106.33
20	4	311	CLA	C1D-ND-C4D	-2.30	104.70	106.33
20	A	801	CLA	CMA-C3A-C4A	-2.30	105.58	111.77
20	5	308	CLA	C2C-C1C-NC	2.30	112.13	109.97
20	6	309	CLA	CHA-C1A-NA	-2.30	121.13	126.40
20	5	318	CLA	CHB-C1B-NB	-2.30	121.82	124.26
20	F	302	CLA	CHC-C1C-C2C	-2.30	120.34	126.73
29	8	314	CHL	CHC-C1C-NC	2.30	127.69	124.20
20	7	1007	CLA	CHC-C1C-NC	2.30	127.69	124.20
20	8	305	CLA	CGD-CBD-CAD	-2.30	103.30	110.73
20	B	809	CLA	C2C-C1C-NC	2.29	112.12	109.97
20	L	203	CLA	C2C-C1C-NC	2.29	112.12	109.97
20	6	318	CLA	C1D-ND-C4D	-2.29	104.71	106.33
20	B	825	CLA	C2C-C1C-NC	2.29	112.12	109.97
20	5	312	CLA	C3B-C4B-NB	-2.29	108.39	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	314	CHL	C3A-C2A-C1A	2.29	104.77	101.34
20	0	301	CLA	CHC-C4B-NB	-2.29	121.83	124.26
20	A	852	CLA	C1D-ND-C4D	-2.29	104.71	106.33
28	7	1001	LUT	C8-C7-C6	2.29	133.62	127.20
20	L	201	CLA	C2C-C1C-NC	2.29	112.11	109.97
20	B	836	CLA	CHA-C1A-NA	-2.29	121.17	126.40
20	3	1010	CLA	C1D-ND-C4D	-2.28	104.71	106.33
20	1	1005	CLA	CHC-C4B-NB	-2.28	121.84	124.26
28	0	304	LUT	C21-C26-C27	2.28	115.58	112.70
30	5	303	XAT	C7-C8-C9	2.28	129.07	125.53
20	8	308	CLA	CHC-C1C-NC	2.28	127.66	124.20
29	0	314	CHL	CHC-C1C-NC	2.28	127.66	124.20
20	A	829	CLA	C3B-C2B-C1B	2.28	109.91	107.16
29	5	313	CHL	C4B-CHC-C1C	-2.28	120.93	126.34
24	B	804	BCR	C15-C14-C13	-2.28	124.06	127.31
25	B	848	DGD	O6E-C5E-C6E	2.28	112.10	106.44
20	5	311	CLA	C1D-ND-C4D	-2.28	104.72	106.33
20	6	320	CLA	C2C-C1C-NC	2.27	112.10	109.97
20	B	813	CLA	CHC-C4B-NB	-2.27	121.85	124.26
24	B	845	BCR	C20-C19-C18	2.27	132.80	126.42
29	1	1015	CHL	C3B-C4B-NB	-2.27	108.41	110.52
20	7	1011	CLA	CHC-C4B-NB	-2.27	121.86	124.26
20	B	814	CLA	CHC-C4B-NB	-2.27	121.86	124.26
20	6	306	CLA	CHB-C1B-NB	-2.27	121.86	124.26
20	G	202	CLA	CHA-C1A-NA	-2.26	121.21	126.40
20	A	830	CLA	C1D-ND-C4D	-2.26	104.73	106.33
20	8	311	CLA	CHB-C1B-NB	-2.26	121.86	124.26
20	5	318	CLA	CHD-C1D-C2D	2.26	130.23	125.48
29	5	316	CHL	CHB-C1B-NB	2.26	126.65	124.26
20	B	818	CLA	C2C-C1C-NC	2.26	112.09	109.97
20	B	824	CLA	C1D-ND-C4D	-2.26	104.73	106.33
20	6	312	CLA	C3B-C2B-C1B	2.26	109.89	107.16
20	B	829	CLA	C2A-C3A-C4A	2.26	105.52	101.87
20	A	816	CLA	C2C-C1C-NC	2.26	112.09	109.97
20	B	805	CLA	C1D-ND-C4D	-2.26	104.73	106.33
20	6	312	CLA	C3B-C4B-NB	-2.26	108.42	110.52
20	6	307	CLA	CMA-C3A-C4A	2.26	117.83	111.77
20	3	1016	CLA	CGD-CBD-CAD	-2.25	103.43	110.73
20	B	834	CLA	CHA-C1A-NA	-2.25	121.24	126.40
20	4	311	CLA	CAA-C2A-C1A	-2.25	104.59	111.97
20	B	821	CLA	CAA-C2A-C1A	-2.25	104.59	111.97
25	5	319	DGD	O1G-C1A-O1A	-2.25	117.91	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	305	CLA	CHA-C1A-NA	-2.25	121.24	126.40
20	6	301	CLA	CHC-C1C-C2C	-2.25	120.48	126.73
20	B	820	CLA	CHA-C1A-NA	-2.25	121.24	126.40
20	A	836	CLA	CHA-C1A-NA	-2.25	121.25	126.40
20	A	806	CLA	CHB-C1B-NB	-2.25	121.88	124.26
20	0	311	CLA	CHC-C4B-NB	-2.25	121.88	124.26
20	3	1007	CLA	CHA-C1A-NA	-2.25	121.25	126.40
24	A	847	BCR	C8-C9-C10	-2.25	115.49	118.94
20	1	1017	CLA	CHC-C4B-NB	-2.25	121.88	124.26
20	A	830	CLA	CHA-C1A-NA	-2.24	121.26	126.40
24	6	302	BCR	C23-C24-C25	2.24	133.50	127.20
20	A	826	CLA	CHA-C1A-NA	-2.24	121.26	126.40
20	6	310	CLA	CBA-CAA-C2A	2.24	120.48	113.86
29	7	1017	CHL	C10-C8-C7	2.24	123.91	112.13
20	B	832	CLA	CHA-C1A-NA	-2.24	121.27	126.40
20	5	306	CLA	C3B-C2B-C1B	2.24	109.87	107.16
20	B	809	CLA	CHA-C1A-NA	-2.24	121.27	126.40
20	8	308	CLA	CHA-C1A-NA	-2.24	121.27	126.40
20	A	851	CLA	CAA-C2A-C1A	-2.24	104.64	111.97
20	8	311	CLA	CHD-C1D-C2D	2.24	130.17	125.48
20	3	1005	CLA	CHA-C1A-NA	-2.24	121.27	126.40
20	3	1013	CLA	CHA-C1A-NA	-2.24	121.28	126.40
20	5	305	CLA	CHA-C1A-NA	-2.24	121.28	126.40
29	5	313	CHL	C2B-C1B-NB	2.23	111.73	110.23
20	4	309	CLA	C2C-C1C-NC	2.23	112.06	109.97
20	6	320	CLA	C2A-C3A-C4A	2.23	105.47	101.87
20	B	802	CLA	C2D-C1D-ND	-2.23	108.46	110.10
20	B	802	CLA	CHC-C4B-NB	-2.23	121.90	124.26
20	3	1006	CLA	C2C-C1C-NC	2.23	112.06	109.97
29	7	1015	CHL	C1D-ND-C4D	-2.22	104.75	106.33
20	G	201	CLA	CAA-C2A-C1A	-2.22	104.69	111.97
29	1	1013	CHL	C1D-ND-C4D	-2.22	104.76	106.33
20	B	813	CLA	CHB-C1B-NB	-2.22	121.91	124.26
20	1	1003	CLA	CHC-C1C-C2C	-2.22	120.57	126.73
20	8	308	CLA	C3B-C4B-NB	-2.22	108.46	110.52
20	B	821	CLA	C2C-C1C-NC	2.22	112.05	109.97
30	4	303	XAT	C7-C8-C9	2.22	128.97	125.53
20	B	837	CLA	CHC-C4B-NB	-2.21	121.91	124.26
20	0	305	CLA	C2C-C1C-NC	2.21	112.05	109.97
29	8	314	CHL	CHB-C1B-C2B	-2.21	120.99	127.24
20	0	313	CLA	CAA-C2A-C1A	-2.21	104.73	111.97
24	3	1003	BCR	C15-C14-C13	2.21	130.47	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	1011	CLA	C4A-NA-C1A	-2.21	105.71	106.71
20	B	807	CLA	CHA-C1A-NA	-2.21	121.34	126.40
20	B	825	CLA	CHA-C1A-NA	-2.21	121.34	126.40
20	5	318	CLA	CHA-C1A-NA	-2.21	121.34	126.40
20	A	837	CLA	C2C-C1C-NC	2.21	112.04	109.97
29	1	1013	CHL	CHD-C1D-C2D	2.21	130.11	125.48
20	B	802	CLA	CHD-C1D-C2D	2.20	130.10	125.48
24	G	204	BCR	C10-C11-C12	2.20	130.09	123.22
20	A	827	CLA	CHA-C1A-NA	-2.20	121.35	126.40
20	A	819	CLA	CHA-C1A-NA	-2.20	121.36	126.40
20	4	306	CLA	C2C-C1C-NC	2.20	112.03	109.97
29	4	312	CHL	C1D-ND-C4D	-2.20	104.77	106.33
20	4	314	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	0	314	CHL	C2B-C1B-NB	2.20	111.70	110.23
20	6	306	CLA	C2C-C1C-NC	2.20	112.03	109.97
20	B	817	CLA	CHC-C4B-NB	-2.20	121.93	124.26
26	3	1018	LMT	O1B-C4'-C3'	2.19	113.12	107.28
20	A	852	CLA	CHA-C1A-NA	-2.19	121.38	126.40
20	1	1017	CLA	C4A-NA-C1A	-2.19	105.72	106.71
20	4	307	CLA	C2D-C1D-ND	2.19	111.72	110.10
29	7	1017	CHL	CHC-C1C-NC	2.19	127.52	124.20
20	0	301	CLA	CHC-C1C-C2C	-2.19	120.65	126.73
20	8	312	CLA	C1D-ND-C4D	-2.19	104.78	106.33
20	B	836	CLA	C3B-C2B-C1B	2.19	109.80	107.16
20	1	1008	CLA	C1D-ND-C4D	-2.19	104.78	106.33
20	5	309	CLA	CHD-C4C-C3C	2.18	128.05	124.84
20	B	813	CLA	CAA-C2A-C1A	-2.18	104.82	111.97
29	7	1015	CHL	CAA-C2A-C1A	2.18	119.13	111.97
20	A	811	CLA	CHA-C1A-NA	-2.18	121.41	126.40
24	B	843	BCR	C20-C19-C18	-2.18	120.29	126.42
20	5	309	CLA	CHD-C1D-C2D	2.18	130.05	125.48
20	1	1009	CLA	CHA-C1A-NA	-2.18	121.41	126.40
20	6	318	CLA	CHD-C1D-C2D	2.18	130.04	125.48
20	1	1017	CLA	CHA-C1A-NA	-2.17	121.42	126.40
29	6	313	CHL	C1D-ND-C4D	-2.17	104.79	106.33
24	3	1004	BCR	C15-C16-C17	2.17	127.93	123.47
20	A	801	CLA	CHD-C1D-C2D	2.17	130.04	125.48
29	5	313	CHL	C1C-C2C-C3C	2.17	108.84	107.11
20	B	834	CLA	C3B-C4B-NB	-2.17	108.50	110.52
20	8	311	CLA	C2C-C1C-NC	2.17	112.00	109.97
20	7	1004	CLA	CMC-C2C-C1C	2.17	128.34	125.04
20	A	824	CLA	CHA-C1A-NA	-2.16	121.44	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	3	1002	LUT	O23-C23-C24	2.16	115.42	110.53
20	8	313	CLA	CHA-C1A-NA	-2.16	121.44	126.40
20	B	833	CLA	CHA-C1A-NA	-2.16	121.45	126.40
20	B	813	CLA	CHA-C1A-NA	-2.16	121.45	126.40
20	B	839	CLA	CHA-C1A-NA	-2.16	121.45	126.40
20	1	1014	CLA	C1D-ND-C4D	-2.16	104.80	106.33
20	7	1004	CLA	CGD-CBD-CAD	2.16	117.72	110.73
29	0	317	CHL	C10-C8-C7	2.15	123.45	112.13
20	B	807	CLA	C2C-C1C-NC	2.15	111.99	109.97
24	4	302	BCR	C15-C16-C17	-2.15	119.07	123.47
20	B	825	CLA	CAA-C2A-C3A	2.15	118.66	112.78
20	5	307	CLA	C3D-C2D-C1D	2.15	108.76	105.83
29	6	314	CHL	C2C-C3C-C4C	2.15	108.02	106.49
20	5	307	CLA	C2D-C1D-ND	-2.15	108.52	110.10
20	1	1003	CLA	CMC-C2C-C1C	2.14	128.31	125.04
20	B	824	CLA	CHA-C1A-NA	-2.14	121.49	126.40
20	A	818	CLA	C2C-C1C-NC	2.14	111.98	109.97
20	A	805	CLA	C2C-C1C-NC	2.14	111.98	109.97
20	0	316	CLA	CHD-C1D-C2D	2.14	129.97	125.48
20	B	823	CLA	C2C-C1C-NC	2.14	111.98	109.97
20	B	803	CLA	C1D-ND-C4D	-2.14	104.81	106.33
20	B	836	CLA	CHC-C4B-NB	-2.14	121.99	124.26
20	A	826	CLA	C1D-ND-C4D	-2.14	104.81	106.33
24	A	845	BCR	C35-C13-C14	-2.14	119.93	122.92
24	8	302	BCR	C16-C17-C18	2.14	130.36	127.31
20	4	308	CLA	C1D-ND-C4D	-2.14	104.82	106.33
20	A	815	CLA	C4A-NA-C1A	-2.14	105.75	106.71
20	B	827	CLA	CHA-C1A-NA	-2.14	121.50	126.40
20	0	310	CLA	CHA-C1A-NA	-2.14	121.50	126.40
20	7	1007	CLA	C2D-C1D-ND	-2.14	108.53	110.10
20	B	834	CLA	CHC-C1C-C2C	-2.14	120.80	126.73
20	6	312	CLA	CGD-CBD-CAD	2.14	117.65	110.73
29	5	316	CHL	CHD-C4C-C3C	2.13	127.98	124.84
20	5	315	CLA	CHB-C4A-NA	2.13	127.46	124.51
20	8	310	CLA	CBA-CAA-C2A	2.13	120.16	113.86
20	5	323	CLA	C1D-ND-C4D	-2.13	104.82	106.33
24	G	205	BCR	C15-C16-C17	-2.13	119.11	123.47
20	6	320	CLA	CAA-CBA-CGA	2.13	118.16	112.51
29	1	1012	CHL	CHB-C1B-C2B	-2.13	121.22	127.24
24	B	843	BCR	C8-C9-C10	2.13	122.20	118.94
20	A	820	CLA	C2C-C1C-NC	2.13	111.96	109.97
24	1	1001	BCR	C16-C17-C18	2.13	130.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	301	CLA	CHA-C1A-NA	-2.12	121.53	126.40
29	5	313	CHL	CHB-C1B-NB	2.12	126.51	124.26
20	J	102	CLA	CHA-C1A-NA	-2.12	121.53	126.40
20	0	307	CLA	CHA-C1A-NA	-2.12	121.54	126.40
24	1	1001	BCR	C15-C16-C17	-2.12	119.13	123.47
29	4	313	CHL	CHB-C1B-NB	2.12	126.50	124.26
29	7	1015	CHL	CHB-C1B-NB	2.12	126.50	124.26
20	3	1008	CLA	CHD-C1D-C2D	2.12	129.92	125.48
29	1	1015	CHL	CHD-C1D-C2D	2.12	129.92	125.48
20	8	313	CLA	C2C-C1C-NC	2.12	111.95	109.97
29	4	313	CHL	CHB-C1B-C2B	-2.12	121.26	127.24
20	7	1007	CLA	CHD-C1D-C2D	2.11	129.91	125.48
20	B	838	CLA	CHD-C1D-ND	-2.11	122.51	124.45
20	6	310	CLA	CHC-C4B-NB	-2.11	122.02	124.26
20	1	1005	CLA	C2C-C1C-NC	2.11	111.95	109.97
20	B	836	CLA	C3B-C4B-NB	-2.11	108.56	110.52
20	A	833	CLA	CHC-C4B-NB	-2.11	122.02	124.26
20	0	305	CLA	CHD-C1D-C2D	2.11	129.91	125.48
20	3	1006	CLA	CHA-C1A-NA	-2.11	121.57	126.40
20	4	311	CLA	C4A-NA-C1A	-2.11	105.76	106.71
20	6	301	CLA	CHA-C1A-NA	-2.11	121.58	126.40
29	3	1014	CHL	CHB-C1B-C2B	-2.10	121.29	127.24
29	6	316	CHL	CHD-C4C-C3C	2.10	127.93	124.84
30	6	304	XAT	C18-C5-C4	-2.10	111.91	114.28
20	1	1010	CLA	C1D-ND-C4D	-2.10	104.84	106.33
20	A	803	CLA	CHC-C4B-NB	-2.10	122.03	124.26
20	A	819	CLA	CHC-C4B-NB	-2.10	122.03	124.26
20	5	321	CLA	CHB-C1B-NB	-2.10	122.03	124.26
20	B	817	CLA	CHD-C1D-C2D	2.10	129.89	125.48
20	1	1014	CLA	CHD-C1D-C2D	2.10	129.89	125.48
20	5	306	CLA	C3D-C4D-ND	2.10	113.63	110.24
29	7	1013	CHL	C1D-ND-C4D	-2.10	104.84	106.33
20	6	320	CLA	CHD-C1D-C2D	2.10	129.88	125.48
20	1	1011	CLA	CHD-C1D-C2D	2.10	129.88	125.48
20	A	814	CLA	CAA-C2A-C1A	-2.10	106.63	111.81
20	3	1007	CLA	CHC-C4B-NB	-2.10	122.04	124.26
20	6	310	CLA	C3A-C2A-C1A	2.09	104.48	101.34
20	8	313	CLA	C2D-C1D-ND	-2.09	108.56	110.10
29	1	1015	CHL	C9-C8-C10	2.09	118.87	111.29
20	6	308	CLA	C3B-C4B-NB	-2.09	108.57	110.52
20	7	1014	CLA	CHD-C1D-C2D	2.09	129.87	125.48
20	5	307	CLA	CHC-C4B-NB	-2.09	122.04	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	308	CLA	CAA-CBA-CGA	2.09	118.06	112.51
29	3	1014	CHL	C3A-C2A-C1A	2.09	104.47	101.34
24	B	804	BCR	C20-C19-C18	-2.09	120.55	126.42
24	4	302	BCR	C16-C17-C18	2.09	130.29	127.31
20	6	306	CLA	C3B-C2B-C1B	2.09	109.68	107.16
29	4	312	CHL	C2A-C1A-CHA	2.09	127.51	123.86
20	A	821	CLA	CHA-C1A-NA	-2.09	121.62	126.40
20	B	816	CLA	C1D-ND-C4D	-2.08	104.85	106.33
20	8	309	CLA	C1D-ND-C4D	-2.08	104.85	106.33
24	A	850	BCR	C16-C15-C14	2.08	127.74	123.47
20	1	1008	CLA	CHA-C1A-NA	-2.08	121.62	126.40
20	K	202	CLA	C2D-C1D-CHD	2.08	129.37	125.00
20	F	302	CLA	CHC-C1C-NC	2.08	127.36	124.20
20	5	318	CLA	C3B-C4B-NB	-2.08	108.58	110.52
20	G	203	CLA	CHA-C1A-NA	-2.08	121.63	126.40
20	0	308	CLA	CHA-C1A-NA	-2.08	121.63	126.40
20	B	819	CLA	CHA-C1A-NA	-2.08	121.63	126.40
20	B	815	CLA	CHA-C1A-NA	-2.08	121.63	126.40
20	B	805	CLA	C4A-NA-C1A	-2.08	105.77	106.71
20	L	204	CLA	CHA-C1A-NA	-2.08	121.64	126.40
20	3	1010	CLA	CHA-C1A-NA	-2.08	121.64	126.40
20	B	833	CLA	C3D-C4D-ND	2.08	113.60	110.24
20	G	203	CLA	C4A-NA-C1A	-2.08	105.77	106.71
20	6	318	CLA	C2C-C1C-NC	2.08	111.92	109.97
20	5	323	CLA	C2C-C1C-NC	2.08	111.92	109.97
20	B	833	CLA	C3B-C4B-NB	-2.08	108.59	110.52
20	6	315	CLA	C3D-C2D-C1D	2.07	108.66	105.83
20	3	1017	CLA	CHA-C1A-NA	-2.07	121.65	126.40
20	A	831	CLA	C2C-C1C-NC	2.07	111.91	109.97
29	0	317	CHL	C2D-C1D-ND	-2.07	108.58	110.10
20	8	310	CLA	C2C-C1C-NC	2.07	111.91	109.97
20	B	833	CLA	CHB-C1B-NB	-2.07	122.07	124.26
20	F	305	CLA	CHC-C4B-NB	-2.07	122.07	124.26
20	5	315	CLA	CHC-C4B-NB	-2.07	122.07	124.26
20	8	312	CLA	C2A-C3A-C4A	2.07	105.21	101.87
20	0	312	CLA	CHD-C1D-C2D	2.07	129.82	125.48
20	0	307	CLA	CGD-CBD-CAD	-2.07	104.03	110.73
24	B	845	BCR	C16-C15-C14	2.07	127.71	123.47
20	A	830	CLA	C2C-C1C-NC	2.07	111.91	109.97
29	1	1015	CHL	C10-C8-C7	2.07	123.00	112.13
20	6	320	CLA	C1D-ND-C4D	-2.07	104.87	106.33
29	1	1012	CHL	C3B-C4B-NB	-2.06	108.60	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	828	CLA	CHD-C1D-C2D	2.06	129.81	125.48
20	6	305	CLA	C2D-C1D-ND	-2.06	108.58	110.10
20	A	803	CLA	C1D-ND-C4D	-2.06	104.87	106.33
20	A	813	CLA	C1D-ND-C4D	-2.06	104.87	106.33
29	0	315	CHL	C2C-C3C-C4C	2.06	107.96	106.49
20	8	311	CLA	C4A-NA-C1A	-2.06	105.78	106.71
20	6	311	CLA	CHB-C1B-NB	-2.06	122.08	124.26
29	6	314	CHL	C1D-ND-C4D	-2.06	104.87	106.33
20	5	312	CLA	C3B-C2B-C1B	2.06	109.65	107.16
29	0	317	CHL	CHD-C1D-C2D	2.06	129.80	125.48
20	0	310	CLA	CHC-C4B-NB	-2.06	122.08	124.26
29	8	314	CHL	CAA-C2A-C1A	2.06	118.73	111.97
20	3	1006	CLA	C3D-C4D-ND	2.06	113.57	110.24
20	8	309	CLA	C3D-C2D-C1D	2.06	108.64	105.83
20	4	309	CLA	CBA-CAA-C2A	2.06	119.94	113.86
20	A	822	CLA	CHA-C1A-NA	-2.06	121.68	126.40
20	B	802	CLA	C3B-C4B-NB	-2.06	108.61	110.52
20	1	1011	CLA	C3B-C2B-C1B	2.06	109.64	107.16
20	7	1006	CLA	CHD-C4C-C3C	2.05	127.86	124.84
20	6	307	CLA	CHC-C4B-NB	-2.05	122.09	124.26
20	5	322	CLA	CHA-C1A-NA	-2.05	121.71	126.40
20	B	833	CLA	C2C-C1C-NC	2.05	111.89	109.97
20	B	830	CLA	CHA-C1A-NA	-2.05	121.71	126.40
23	0	302	LHG	O4-P-O5	2.05	122.36	112.24
20	B	832	CLA	C1D-ND-C4D	-2.05	104.88	106.33
20	7	1009	CLA	C1D-ND-C4D	-2.04	104.88	106.33
29	4	313	CHL	CHD-C1D-C2D	2.04	129.76	125.48
20	G	201	CLA	CHA-C1A-NA	-2.04	121.72	126.40
20	3	1006	CLA	CHC-C4B-NB	-2.04	122.10	124.26
20	4	308	CLA	CHC-C4B-NB	-2.04	122.10	124.26
20	A	806	CLA	CHD-C1D-C2D	2.04	129.76	125.48
20	A	805	CLA	CHA-C1A-NA	-2.04	121.72	126.40
20	A	809	CLA	CHD-C1D-C2D	2.04	129.76	125.48
20	5	308	CLA	CGD-CBD-CAD	-2.04	104.13	110.73
20	A	809	CLA	C2C-C1C-NC	2.04	111.88	109.97
20	6	320	CLA	CHB-C4A-NA	2.04	127.33	124.51
20	4	305	CLA	C3B-C2B-C1B	2.04	109.62	107.16
20	6	308	CLA	C3B-C2B-C1B	2.04	109.62	107.16
20	8	313	CLA	C1D-ND-C4D	-2.04	104.89	106.33
20	1	1003	CLA	CHD-C1D-C2D	2.04	129.75	125.48
20	8	312	CLA	C3B-C2B-C1B	2.03	109.62	107.16
20	A	825	CLA	C2C-C1C-NC	2.03	111.88	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	8	313	CLA	CHD-C1D-C2D	2.03	129.74	125.48
20	K	202	CLA	CBD-CAD-C3D	2.03	108.58	105.94
20	B	803	CLA	C2D-C1D-ND	-2.03	108.61	110.10
20	1	1008	CLA	C2C-C1C-NC	2.03	111.88	109.97
20	B	810	CLA	CHA-C1A-NA	-2.03	121.75	126.40
20	0	312	CLA	C2C-C1C-NC	2.03	111.87	109.97
20	6	306	CLA	C3D-C4D-ND	2.03	113.52	110.24
20	B	801	CLA	C3B-C2B-C1B	2.03	109.61	107.16
29	4	312	CHL	CHB-C1B-C2B	-2.03	121.51	127.24
20	4	306	CLA	C3D-C2D-C1D	2.03	108.60	105.83
29	8	317	CHL	CHD-C4C-C3C	2.03	127.82	124.84
29	8	315	CHL	C2D-C1D-ND	-2.03	108.61	110.10
20	A	818	CLA	CHA-C1A-NA	-2.03	121.76	126.40
20	B	818	CLA	C4A-NA-C1A	-2.02	105.80	106.71
20	7	1011	CLA	CHA-C1A-NA	-2.02	121.76	126.40
20	6	301	CLA	C3B-C4B-NB	-2.02	108.64	110.52
29	0	314	CHL	CAA-C2A-C1A	2.02	118.60	111.97
20	4	304	CLA	CGD-CBD-CAD	-2.02	104.19	110.73
20	B	837	CLA	C2C-C1C-NC	2.02	111.87	109.97
20	A	807	CLA	CHA-C1A-NA	-2.02	121.77	126.40
20	A	807	CLA	CHC-C4B-NB	-2.02	122.12	124.26
20	5	322	CLA	CHD-C1D-C2D	2.02	129.72	125.48
20	5	301	CLA	CHD-C1D-C2D	2.02	129.72	125.48
20	5	312	CLA	C2A-C3A-C4A	2.02	105.13	101.87
29	7	1015	CHL	C2B-C1B-NB	2.02	111.59	110.23
29	6	317	CHL	C2B-C1B-NB	2.02	111.59	110.23
25	5	319	DGD	O6D-C5D-C4D	-2.02	106.03	109.69
20	5	318	CLA	CAA-C2A-C1A	-2.02	105.36	111.97
20	A	814	CLA	CHA-C1A-NA	-2.02	121.78	126.40
20	5	304	CLA	CHA-C1A-NA	-2.02	121.78	126.40
20	1	1014	CLA	C2C-C1C-NC	2.02	111.86	109.97
20	B	805	CLA	C3B-C2B-C1B	2.02	109.60	107.16
20	3	1015	CLA	CHA-C1A-NA	-2.02	121.78	126.40
27	4	318	LMG	C12-C11-C10	-2.02	106.29	113.62
20	8	308	CLA	C3B-C2B-C1B	2.02	109.60	107.16
20	5	304	CLA	C2C-C1C-NC	2.02	111.86	109.97
20	3	1016	CLA	C1C-C2C-C3C	2.01	109.07	106.96
20	0	313	CLA	CMA-C3A-C4A	2.01	117.19	111.77
20	3	1008	CLA	C3D-C4D-ND	2.01	113.49	110.24
20	A	831	CLA	CHD-C1D-ND	-2.01	122.60	124.45
20	4	309	CLA	C2D-C1D-ND	-2.01	108.62	110.10
20	A	817	CLA	CHD-C1D-C2D	2.01	129.70	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	308	CLA	CHA-C1A-NA	-2.01	121.79	126.40
20	A	806	CLA	C1D-ND-C4D	-2.01	104.91	106.33
20	B	838	CLA	C4D-CHA-C1A	-2.01	118.81	121.25
20	B	814	CLA	CHA-C1A-NA	-2.01	121.80	126.40
20	A	831	CLA	C1D-ND-C4D	-2.01	104.91	106.33
20	4	314	CLA	CHD-C1D-C2D	2.01	129.69	125.48
20	0	313	CLA	CHA-C1A-NA	-2.01	121.80	126.40
20	A	802	CLA	CHA-C1A-NA	-2.00	121.81	126.40
20	7	1011	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	F	301	BCR	C40-C30-C25	2.00	113.55	110.30
20	3	1012	CLA	CHA-C1A-NA	-2.00	121.81	126.40
20	B	817	CLA	C3B-C4B-NB	-2.00	108.66	110.52

There are no chirality outliers.

All (1426) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	803	CLA	C1A-C2A-CAA-CBA
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	807	CLA	C3A-C2A-CAA-CBA
20	A	809	CLA	C2B-C3B-CAB-CBB
20	A	809	CLA	C4B-C3B-CAB-CBB
20	A	810	CLA	C1A-C2A-CAA-CBA
20	A	810	CLA	C3A-C2A-CAA-CBA
20	A	811	CLA	C1A-C2A-CAA-CBA
20	A	814	CLA	CAD-CBD-CGD-O2D
20	A	817	CLA	C3A-C2A-CAA-CBA
20	A	824	CLA	CHA-CBD-CGD-O2D
20	A	840	CLA	C2A-CAA-CBA-CGA
20	B	805	CLA	CHA-CBD-CGD-O2D
20	B	807	CLA	C1A-C2A-CAA-CBA
20	B	807	CLA	C3A-C2A-CAA-CBA
20	B	808	CLA	C3A-C2A-CAA-CBA
20	B	809	CLA	CHA-CBD-CGD-O2D
20	B	818	CLA	CHA-CBD-CGD-O2D
20	B	820	CLA	C2A-CAA-CBA-CGA
20	B	825	CLA	C3A-C2A-CAA-CBA
20	B	827	CLA	CHA-CBD-CGD-O2D
20	B	829	CLA	C3A-C2A-CAA-CBA
20	B	829	CLA	CHA-CBD-CGD-O2D
20	B	830	CLA	C1A-C2A-CAA-CBA
20	B	830	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	B	837	CLA	C2B-C3B-CAB-CBB
20	B	837	CLA	C4B-C3B-CAB-CBB
20	B	841	CLA	C1A-C2A-CAA-CBA
20	B	841	CLA	C3A-C2A-CAA-CBA
20	B	850	CLA	NC-C1C-C2C-CMC
20	F	303	CLA	C4B-C3B-CAB-CBB
20	0	310	CLA	C1A-C2A-CAA-CBA
20	0	310	CLA	C3A-C2A-CAA-CBA
20	0	313	CLA	C2B-C3B-CAB-CBB
20	0	313	CLA	C4B-C3B-CAB-CBB
20	8	310	CLA	C1A-C2A-CAA-CBA
20	8	310	CLA	C3A-C2A-CAA-CBA
20	8	313	CLA	C2B-C3B-CAB-CBB
20	8	313	CLA	C4B-C3B-CAB-CBB
20	7	1004	CLA	C3A-C2A-CAA-CBA
20	7	1007	CLA	C3A-C2A-CAA-CBA
20	7	1011	CLA	CHA-CBD-CGD-O2D
20	3	1005	CLA	C1A-C2A-CAA-CBA
20	3	1005	CLA	C3A-C2A-CAA-CBA
20	3	1005	CLA	C2B-C3B-CAB-CBB
20	3	1005	CLA	C4B-C3B-CAB-CBB
20	3	1009	CLA	C1A-C2A-CAA-CBA
20	3	1009	CLA	C3A-C2A-CAA-CBA
20	3	1010	CLA	C2A-CAA-CBA-CGA
20	3	1016	CLA	C1A-C2A-CAA-CBA
20	3	1016	CLA	CAD-CBD-CGD-O2D
20	3	1017	CLA	C1A-C2A-CAA-CBA
20	3	1017	CLA	C3A-C2A-CAA-CBA
20	1	1007	CLA	CHA-CBD-CGD-O2D
20	1	1008	CLA	C1A-C2A-CAA-CBA
20	1	1008	CLA	C3A-C2A-CAA-CBA
20	1	1011	CLA	C2B-C3B-CAB-CBB
20	1	1011	CLA	C4B-C3B-CAB-CBB
20	4	309	CLA	C1A-C2A-CAA-CBA
20	4	309	CLA	C3A-C2A-CAA-CBA
20	4	311	CLA	C4B-C3B-CAB-CBB
20	6	307	CLA	C4B-C3B-CAB-CBB
20	6	310	CLA	C1A-C2A-CAA-CBA
20	6	310	CLA	C3A-C2A-CAA-CBA
20	5	305	CLA	CHA-CBD-CGD-O2D
20	5	309	CLA	C1A-C2A-CAA-CBA
20	5	309	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	5	310	CLA	C4B-C3B-CAB-CBB
20	5	321	CLA	CHA-CBD-CGD-O2D
22	A	842	PQN	C12-C13-C15-C16
23	A	843	LHG	O1-C1-C2-O2
23	A	843	LHG	O1-C1-C2-C3
23	A	843	LHG	O2-C2-C3-O3
23	A	843	LHG	C4-O6-P-O5
23	A	843	LHG	O6-C4-C5-O7
23	A	849	LHG	C3-O3-P-O5
23	0	302	LHG	O1-C1-C2-O2
23	0	302	LHG	O1-C1-C2-C3
23	0	302	LHG	C4-O6-P-O5
23	0	302	LHG	C8-C7-O7-C5
23	8	301	LHG	C3-O3-P-O4
23	7	1016	LHG	C4-O6-P-O5
23	3	1019	LHG	C3-O3-P-O4
23	3	1019	LHG	C3-O3-P-O5
23	3	1019	LHG	C3-O3-P-O6
23	3	1019	LHG	C4-C5-O7-C7
23	3	1019	LHG	C6-C5-O7-C7
23	4	301	LHG	C3-O3-P-O4
23	4	301	LHG	C4-O6-P-O3
23	4	301	LHG	O10-C23-O8-C6
23	4	301	LHG	C24-C23-O8-C6
24	A	845	BCR	C21-C22-C23-C24
24	A	845	BCR	C37-C22-C23-C24
24	A	846	BCR	C21-C22-C23-C24
24	A	846	BCR	C37-C22-C23-C24
24	A	847	BCR	C7-C8-C9-C10
24	A	847	BCR	C7-C8-C9-C34
24	A	848	BCR	C21-C22-C23-C24
24	A	848	BCR	C37-C22-C23-C24
24	A	850	BCR	C1-C6-C7-C8
24	A	850	BCR	C5-C6-C7-C8
24	A	850	BCR	C7-C8-C9-C34
24	A	850	BCR	C11-C10-C9-C8
24	B	804	BCR	C1-C6-C7-C8
24	B	843	BCR	C23-C24-C25-C26
24	B	843	BCR	C23-C24-C25-C30
24	B	844	BCR	C21-C22-C23-C24
24	B	844	BCR	C37-C22-C23-C24
24	B	845	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
24	B	845	BCR	C7-C8-C9-C34
24	B	845	BCR	C36-C18-C19-C20
24	B	845	BCR	C21-C22-C23-C24
24	B	845	BCR	C37-C22-C23-C24
24	F	301	BCR	C7-C8-C9-C34
24	F	304	BCR	C23-C24-C25-C30
24	G	205	BCR	C1-C6-C7-C8
24	G	205	BCR	C5-C6-C7-C8
24	G	205	BCR	C7-C8-C9-C34
24	H	201	BCR	C7-C8-C9-C10
24	H	201	BCR	C17-C18-C19-C20
24	H	201	BCR	C36-C18-C19-C20
24	H	201	BCR	C21-C22-C23-C24
24	H	201	BCR	C37-C22-C23-C24
24	I	201	BCR	C21-C22-C23-C24
24	I	201	BCR	C23-C24-C25-C26
24	I	201	BCR	C23-C24-C25-C30
24	J	103	BCR	C1-C6-C7-C8
24	J	103	BCR	C7-C8-C9-C34
24	8	302	BCR	C1-C6-C7-C8
24	8	302	BCR	C5-C6-C7-C8
24	8	302	BCR	C7-C8-C9-C34
24	8	302	BCR	C13-C14-C15-C16
24	8	302	BCR	C21-C22-C23-C24
24	8	302	BCR	C37-C22-C23-C24
24	7	1003	BCR	C1-C6-C7-C8
24	7	1003	BCR	C5-C6-C7-C8
24	7	1003	BCR	C7-C8-C9-C10
24	7	1003	BCR	C7-C8-C9-C34
24	7	1003	BCR	C11-C12-C13-C14
24	7	1003	BCR	C36-C18-C19-C20
24	7	1003	BCR	C37-C22-C23-C24
24	3	1003	BCR	C1-C6-C7-C8
24	3	1003	BCR	C5-C6-C7-C8
24	3	1003	BCR	C21-C22-C23-C24
24	3	1003	BCR	C37-C22-C23-C24
24	3	1004	BCR	C21-C22-C23-C24
24	3	1004	BCR	C37-C22-C23-C24
24	1	1001	BCR	C1-C6-C7-C8
24	1	1001	BCR	C5-C6-C7-C8
24	1	1001	BCR	C7-C8-C9-C10
24	1	1001	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
24	4	302	BCR	C1-C6-C7-C8
24	4	302	BCR	C5-C6-C7-C8
24	4	302	BCR	C7-C8-C9-C10
24	4	302	BCR	C7-C8-C9-C34
24	6	302	BCR	C1-C6-C7-C8
24	6	302	BCR	C5-C6-C7-C8
24	6	302	BCR	C7-C8-C9-C10
24	6	302	BCR	C7-C8-C9-C34
24	6	302	BCR	C21-C22-C23-C24
24	5	320	BCR	C11-C12-C13-C14
24	5	320	BCR	C11-C12-C13-C35
25	B	848	DGD	C2B-C1B-O2G-C2G
25	B	848	DGD	O1B-C1B-O2G-C2G
25	5	319	DGD	O6D-C1D-O3G-C3G
26	3	1018	LMT	C2-C1-O1'-C1'
27	J	101	LMG	C11-C10-O7-C8
27	0	303	LMG	C11-C10-O7-C8
27	8	319	LMG	C2-C1-O1-C7
27	8	319	LMG	O7-C8-C9-O8
27	5	324	LMG	O6-C1-O1-C7
27	5	324	LMG	O10-C28-O8-C9
28	J	104	LUT	C1-C6-C7-C8
28	J	104	LUT	C21-C26-C27-C28
28	J	104	LUT	C27-C28-C29-C30
28	J	104	LUT	C27-C28-C29-C39
28	J	104	LUT	C31-C32-C33-C34
28	J	104	LUT	C31-C32-C33-C40
28	0	304	LUT	C21-C26-C27-C28
28	8	303	LUT	C7-C8-C9-C10
28	8	303	LUT	C7-C8-C9-C19
28	7	1001	LUT	C7-C8-C9-C10
28	7	1001	LUT	C7-C8-C9-C19
28	3	1002	LUT	C7-C8-C9-C10
28	3	1002	LUT	C7-C8-C9-C19
28	3	1002	LUT	C25-C26-C27-C28
28	3	1002	LUT	C27-C28-C29-C30
28	3	1002	LUT	C27-C28-C29-C39
28	1	1002	LUT	C21-C26-C27-C28
28	1	1002	LUT	C27-C28-C29-C30
28	1	1002	LUT	C27-C28-C29-C39
28	6	303	LUT	C7-C8-C9-C19
29	0	315	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	0	317	CHL	C1A-C2A-CAA-CBA
29	0	317	CHL	C3A-C2A-CAA-CBA
29	0	317	CHL	C2-C3-C5-C6
29	0	317	CHL	C4-C3-C5-C6
29	0	317	CHL	C11-C10-C8-C9
29	8	317	CHL	C3A-C2A-CAA-CBA
29	8	317	CHL	C11-C10-C8-C9
29	7	1015	CHL	C1A-C2A-CAA-CBA
29	7	1017	CHL	O2A-C1-C2-C3
29	7	1017	CHL	C2-C3-C5-C6
29	7	1017	CHL	C4-C3-C5-C6
29	3	1014	CHL	C1A-C2A-CAA-CBA
29	1	1015	CHL	C1A-C2A-CAA-CBA
29	1	1015	CHL	C3A-C2A-CAA-CBA
29	1	1015	CHL	C2-C3-C5-C6
29	1	1015	CHL	C4-C3-C5-C6
29	1	1015	CHL	C11-C10-C8-C9
29	4	315	CHL	C2-C3-C5-C6
29	4	315	CHL	C4-C3-C5-C6
29	4	315	CHL	C6-C7-C8-C10
29	6	313	CHL	CHA-CBD-CGD-O1D
29	6	313	CHL	CHA-CBD-CGD-O2D
29	6	314	CHL	C2A-CAA-CBA-CGA
29	6	316	CHL	C2-C3-C5-C6
29	6	316	CHL	C4-C3-C5-C6
29	5	313	CHL	CBA-CGA-O2A-C1
29	5	316	CHL	C1A-C2A-CAA-CBA
29	5	316	CHL	C3A-C2A-CAA-CBA
30	8	304	XAT	C6-C7-C8-C9
30	8	304	XAT	C7-C8-C9-C10
30	8	304	XAT	C7-C8-C9-C19
30	8	304	XAT	C11-C10-C9-C8
30	8	304	XAT	C11-C10-C9-C19
30	8	304	XAT	C11-C12-C13-C14
30	8	304	XAT	C11-C12-C13-C20
30	8	304	XAT	C26-C27-C28-C29
30	8	304	XAT	C39-C29-C30-C31
30	8	304	XAT	C29-C30-C31-C32
30	7	1002	XAT	O4-C6-C7-C8
30	7	1002	XAT	C6-C7-C8-C9
30	7	1002	XAT	C7-C8-C9-C10
30	7	1002	XAT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
30	7	1002	XAT	C10-C11-C12-C13
30	4	303	XAT	C27-C28-C29-C30
30	4	303	XAT	C27-C28-C29-C39
30	6	304	XAT	O24-C26-C27-C28
30	6	304	XAT	C27-C28-C29-C30
30	6	304	XAT	C27-C28-C29-C39
30	6	304	XAT	C31-C32-C33-C40
20	J	102	CLA	C4C-C3C-CAC-CBC
27	8	318	LMG	C11-C10-O7-C8
20	J	102	CLA	C2C-C3C-CAC-CBC
23	0	302	LHG	O9-C7-O7-C5
29	6	316	CHL	CBD-CGD-O2D-CED
29	5	313	CHL	O1A-CGA-O2A-C1
25	B	848	DGD	C2G-C1G-O1G-C1A
27	0	303	LMG	C29-C28-O8-C9
29	8	317	CHL	CBD-CGD-O2D-CED
29	7	1015	CHL	CBD-CGD-O2D-CED
29	5	317	CHL	CBD-CGD-O2D-CED
23	8	301	LHG	O10-C23-O8-C6
25	5	319	DGD	O1A-C1A-O1G-C1G
27	0	303	LMG	O10-C28-O8-C9
27	8	318	LMG	O9-C10-O7-C8
27	J	101	LMG	O9-C10-O7-C8
27	0	303	LMG	O9-C10-O7-C8
27	5	324	LMG	C29-C28-O8-C9
20	1	1014	CLA	C4C-C3C-CAC-CBC
22	A	842	PQN	C14-C13-C15-C16
29	8	317	CHL	C4-C3-C5-C6
20	A	833	CLA	C2A-CAA-CBA-CGA
20	B	841	CLA	C2A-CAA-CBA-CGA
20	0	312	CLA	C2A-CAA-CBA-CGA
20	3	1013	CLA	C2A-CAA-CBA-CGA
20	6	310	CLA	C2A-CAA-CBA-CGA
29	8	315	CHL	C2A-CAA-CBA-CGA
29	8	317	CHL	C2A-CAA-CBA-CGA
29	7	1012	CHL	C2A-CAA-CBA-CGA
29	5	316	CHL	C2A-CAA-CBA-CGA
23	8	301	LHG	C24-C23-O8-C6
25	5	319	DGD	C2A-C1A-O1G-C1G
29	6	316	CHL	CBA-CGA-O2A-C1
20	1	1014	CLA	C2C-C3C-CAC-CBC
27	5	324	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
29	0	317	CHL	CBD-CGD-O2D-CED
29	4	313	CHL	CBD-CGD-O2D-CED
29	5	313	CHL	CBD-CGD-O2D-CED
27	0	303	LMG	C35-C36-C37-C38
29	6	316	CHL	O1A-CGA-O2A-C1
24	4	302	BCR	C13-C14-C15-C16
24	6	302	BCR	C13-C14-C15-C16
30	8	304	XAT	C9-C10-C11-C12
27	8	319	LMG	O6-C5-C6-O5
29	7	1013	CHL	CBD-CGD-O2D-CED
29	4	315	CHL	CBD-CGD-O2D-CED
29	4	316	CHL	CBD-CGD-O2D-CED
29	6	314	CHL	CBD-CGD-O2D-CED
27	6	319	LMG	C11-C10-O7-C8
29	5	316	CHL	CBD-CGD-O2D-CED
25	B	848	DGD	C8A-C9A-CAA-CBA
29	6	316	CHL	O1D-CGD-O2D-CED
25	5	319	DGD	C2A-C3A-C4A-C5A
29	5	316	CHL	C4-C3-C5-C6
26	3	1018	LMT	C4'-C5'-C6'-O6'
29	8	317	CHL	C2-C3-C5-C6
29	5	316	CHL	C2-C3-C5-C6
29	5	314	CHL	C2A-CAA-CBA-CGA
25	5	319	DGD	O6E-C5E-C6E-O5E
27	0	303	LMG	O6-C5-C6-O5
27	5	324	LMG	C10-C11-C12-C13
20	5	309	CLA	C2C-C3C-CAC-CBC
29	5	317	CHL	O1D-CGD-O2D-CED
20	0	316	CLA	C2C-C3C-CAC-CBC
27	6	319	LMG	O9-C10-O7-C8
27	8	319	LMG	C29-C28-O8-C9
27	0	303	LMG	C4-C5-C6-O5
29	6	316	CHL	C10-C11-C12-C13
29	8	314	CHL	CBA-CGA-O2A-C1
25	5	319	DGD	C2D-C1D-O3G-C3G
27	8	319	LMG	O10-C28-O8-C9
29	4	315	CHL	C11-C10-C8-C9
20	G	203	CLA	C2A-CAA-CBA-CGA
29	0	317	CHL	C2A-CAA-CBA-CGA
24	A	845	BCR	C11-C12-C13-C35
24	A	847	BCR	C11-C12-C13-C35
24	A	850	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	B	847	BCR	C7-C8-C9-C34
24	B	847	BCR	C37-C22-C23-C24
24	F	301	BCR	C37-C22-C23-C24
24	I	201	BCR	C37-C22-C23-C24
24	7	1003	BCR	C11-C12-C13-C35
24	3	1003	BCR	C11-C12-C13-C35
24	6	302	BCR	C37-C22-C23-C24
24	5	320	BCR	C7-C8-C9-C34
28	0	304	LUT	C27-C28-C29-C39
28	0	318	LUT	C7-C8-C9-C19
28	3	1001	LUT	C31-C32-C33-C40
28	5	302	LUT	C7-C8-C9-C19
30	5	303	XAT	C27-C28-C29-C39
24	A	845	BCR	C11-C12-C13-C14
24	A	850	BCR	C21-C22-C23-C24
24	F	301	BCR	C21-C22-C23-C24
24	G	205	BCR	C7-C8-C9-C10
24	H	201	BCR	C11-C12-C13-C14
24	8	302	BCR	C7-C8-C9-C10
24	1	1001	BCR	C21-C22-C23-C24
24	4	302	BCR	C21-C22-C23-C24
25	5	319	DGD	C4E-C5E-C6E-O5E
22	A	842	PQN	C18-C20-C21-C22
29	7	1015	CHL	O1D-CGD-O2D-CED
22	A	842	PQN	C25-C26-C27-C28
29	8	317	CHL	O1D-CGD-O2D-CED
23	A	849	LHG	C7-C8-C9-C10
23	7	1016	LHG	C23-C24-C25-C26
25	5	319	DGD	C1B-C2B-C3B-C4B
20	0	316	CLA	C4C-C3C-CAC-CBC
20	3	1005	CLA	C4C-C3C-CAC-CBC
23	7	1016	LHG	C7-C8-C9-C10
27	0	303	LMG	C28-C29-C30-C31
27	8	319	LMG	C4-C5-C6-O5
27	8	319	LMG	C11-C10-O7-C8
29	0	317	CHL	C6-C7-C8-C10
29	7	1017	CHL	C11-C10-C8-C7
29	1	1015	CHL	C6-C7-C8-C10
29	6	316	CHL	C6-C7-C8-C10
29	5	316	CHL	C6-C7-C8-C10
20	A	819	CLA	C2A-CAA-CBA-CGA
20	B	830	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	6	301	CLA	C2A-CAA-CBA-CGA
20	5	301	CLA	C2A-CAA-CBA-CGA
20	5	311	CLA	C2A-CAA-CBA-CGA
29	8	314	CHL	C2A-CAA-CBA-CGA
29	7	1015	CHL	C2A-CAA-CBA-CGA
29	5	313	CHL	O1D-CGD-O2D-CED
24	7	1003	BCR	C18-C19-C20-C21
23	A	843	LHG	C4-O6-P-O3
23	8	301	LHG	C3-O3-P-O6
23	7	1016	LHG	C4-O6-P-O3
23	3	1019	LHG	C4-O6-P-O3
23	4	301	LHG	C3-O3-P-O6
29	6	314	CHL	O1D-CGD-O2D-CED
23	A	843	LHG	C1-C2-C3-O3
27	8	319	LMG	O9-C10-O7-C8
20	3	1007	CLA	C2A-CAA-CBA-CGA
20	3	1008	CLA	C2A-CAA-CBA-CGA
29	3	1014	CHL	C2A-CAA-CBA-CGA
29	6	313	CHL	C2A-CAA-CBA-CGA
29	8	317	CHL	C11-C12-C13-C15
27	0	303	LMG	C31-C32-C33-C34
26	B	849	LMT	O1'-C1-C2-C3
24	G	205	BCR	C13-C14-C15-C16
25	5	319	DGD	C7A-C8A-C9A-CAA
23	A	849	LHG	C29-C30-C31-C32
23	4	301	LHG	C11-C10-C9-C8
29	4	313	CHL	O1D-CGD-O2D-CED
25	5	319	DGD	C3B-C4B-C5B-C6B
27	4	318	LMG	C12-C13-C14-C15
27	5	324	LMG	C12-C13-C14-C15
29	0	317	CHL	O1D-CGD-O2D-CED
26	3	1018	LMT	O5'-C5'-C6'-O6'
22	B	842	PQN	C25-C26-C27-C28
25	B	848	DGD	C6A-C7A-C8A-C9A
27	0	303	LMG	C17-C18-C19-C20
27	5	324	LMG	C14-C15-C16-C17
20	1	1009	CLA	C2C-C3C-CAC-CBC
24	A	845	BCR	C11-C10-C9-C8
24	A	845	BCR	C12-C13-C14-C15
24	A	847	BCR	C11-C10-C9-C8
24	H	201	BCR	C11-C10-C9-C8
24	H	201	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	3	1003	BCR	C12-C13-C14-C15
27	4	318	LMG	C2-C1-O1-C7
30	8	304	XAT	C28-C29-C30-C31
27	5	324	LMG	O1-C7-C8-O7
29	4	315	CHL	O1D-CGD-O2D-CED
29	4	316	CHL	O1D-CGD-O2D-CED
23	A	843	LHG	C15-C16-C17-C18
25	B	848	DGD	C2A-C3A-C4A-C5A
29	0	317	CHL	C6-C7-C8-C9
29	6	316	CHL	C11-C10-C8-C9
20	5	309	CLA	C4C-C3C-CAC-CBC
27	6	319	LMG	C12-C13-C14-C15
20	A	811	CLA	C2A-CAA-CBA-CGA
20	B	839	CLA	C2A-CAA-CBA-CGA
20	8	309	CLA	C2A-CAA-CBA-CGA
20	7	1011	CLA	C2A-CAA-CBA-CGA
20	3	1009	CLA	C2A-CAA-CBA-CGA
29	1	1013	CHL	C2A-CAA-CBA-CGA
29	1	1015	CHL	C2A-CAA-CBA-CGA
29	4	313	CHL	C2A-CAA-CBA-CGA
29	4	315	CHL	C2A-CAA-CBA-CGA
24	G	205	BCR	C37-C22-C23-C24
24	H	201	BCR	C11-C12-C13-C35
24	1	1001	BCR	C37-C22-C23-C24
24	4	302	BCR	C37-C22-C23-C24
25	B	848	DGD	C3A-C4A-C5A-C6A
25	B	848	DGD	C4B-C5B-C6B-C7B
23	4	301	LHG	O1-C1-C2-C3
24	G	205	BCR	C21-C22-C23-C24
24	J	103	BCR	C7-C8-C9-C10
24	3	1003	BCR	C11-C12-C13-C14
24	3	1004	BCR	C11-C12-C13-C14
28	0	304	LUT	C27-C28-C29-C30
23	A	843	LHG	C13-C14-C15-C16
27	5	324	LMG	C38-C39-C40-C41
23	8	301	LHG	C7-C8-C9-C10
23	A	843	LHG	C11-C12-C13-C14
23	A	849	LHG	C13-C14-C15-C16
23	4	301	LHG	C17-C18-C19-C20
27	0	303	LMG	C15-C16-C17-C18
25	5	319	DGD	O6D-C5D-C6D-O5D
20	A	803	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	A	819	CLA	C4B-C3B-CAB-CBB
20	A	823	CLA	C4B-C3B-CAB-CBB
20	B	810	CLA	C4B-C3B-CAB-CBB
20	B	825	CLA	C4B-C3B-CAB-CBB
20	B	841	CLA	C4B-C3B-CAB-CBB
20	7	1011	CLA	C4B-C3B-CAB-CBB
20	3	1010	CLA	C4B-C3B-CAB-CBB
20	1	1017	CLA	C4B-C3B-CAB-CBB
20	6	312	CLA	C4B-C3B-CAB-CBB
20	5	301	CLA	C4B-C3B-CAB-CBB
20	5	306	CLA	C4B-C3B-CAB-CBB
20	5	323	CLA	C4B-C3B-CAB-CBB
25	5	319	DGD	C5A-C6A-C7A-C8A
27	0	303	LMG	C14-C15-C16-C17
29	1	1012	CHL	CBD-CGD-O2D-CED
29	1	1015	CHL	CBA-CGA-O2A-C1
29	6	314	CHL	CBA-CGA-O2A-C1
20	A	804	CLA	C3A-C2A-CAA-CBA
20	A	805	CLA	C3A-C2A-CAA-CBA
20	B	826	CLA	C3A-C2A-CAA-CBA
20	G	202	CLA	C3A-C2A-CAA-CBA
20	J	102	CLA	C3A-C2A-CAA-CBA
20	0	309	CLA	C3A-C2A-CAA-CBA
20	8	309	CLA	C3A-C2A-CAA-CBA
20	3	1016	CLA	C3A-C2A-CAA-CBA
20	1	1007	CLA	C3A-C2A-CAA-CBA
20	4	308	CLA	C3A-C2A-CAA-CBA
20	6	309	CLA	C3A-C2A-CAA-CBA
20	5	308	CLA	C3A-C2A-CAA-CBA
29	7	1015	CHL	C3A-C2A-CAA-CBA
29	3	1014	CHL	C3A-C2A-CAA-CBA
24	7	1003	BCR	C13-C14-C15-C16
23	4	301	LHG	C33-C34-C35-C36
29	3	1014	CHL	CBA-CGA-O2A-C1
20	1	1009	CLA	C4C-C3C-CAC-CBC
29	7	1013	CHL	O1D-CGD-O2D-CED
27	4	318	LMG	O6-C5-C6-O5
23	3	1019	LHG	C24-C23-O8-C6
29	8	314	CHL	O1A-CGA-O2A-C1
27	4	318	LMG	C11-C10-O7-C8
20	B	823	CLA	C2A-CAA-CBA-CGA
20	6	309	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	A	819	CLA	C2B-C3B-CAB-CBB
20	A	823	CLA	C2B-C3B-CAB-CBB
20	B	807	CLA	C2B-C3B-CAB-CBB
20	B	810	CLA	C2B-C3B-CAB-CBB
20	B	822	CLA	C2B-C3B-CAB-CBB
20	B	825	CLA	C2B-C3B-CAB-CBB
20	F	303	CLA	C2B-C3B-CAB-CBB
20	7	1011	CLA	C2B-C3B-CAB-CBB
20	3	1010	CLA	C2B-C3B-CAB-CBB
20	1	1009	CLA	C2B-C3B-CAB-CBB
20	1	1017	CLA	C2B-C3B-CAB-CBB
20	4	310	CLA	C2B-C3B-CAB-CBB
20	4	311	CLA	C2B-C3B-CAB-CBB
20	6	307	CLA	C2B-C3B-CAB-CBB
20	6	312	CLA	C2B-C3B-CAB-CBB
20	5	306	CLA	C2B-C3B-CAB-CBB
20	5	310	CLA	C2B-C3B-CAB-CBB
20	5	323	CLA	C2B-C3B-CAB-CBB
20	6	310	CLA	C2C-C3C-CAC-CBC
23	A	843	LHG	C9-C10-C11-C12
27	8	319	LMG	C14-C15-C16-C17
29	6	314	CHL	O1A-CGA-O2A-C1
23	A	849	LHG	C27-C28-C29-C30
24	B	804	BCR	C5-C6-C7-C8
24	B	845	BCR	C1-C6-C7-C8
24	B	845	BCR	C5-C6-C7-C8
24	B	846	BCR	C23-C24-C25-C26
24	B	846	BCR	C23-C24-C25-C30
24	F	304	BCR	C23-C24-C25-C26
24	H	201	BCR	C1-C6-C7-C8
24	J	103	BCR	C5-C6-C7-C8
24	7	1003	BCR	C23-C24-C25-C26
24	7	1003	BCR	C23-C24-C25-C30
24	3	1004	BCR	C1-C6-C7-C8
24	3	1004	BCR	C5-C6-C7-C8
24	5	320	BCR	C23-C24-C25-C30
28	J	104	LUT	C5-C6-C7-C8
28	1	1002	LUT	C5-C6-C7-C8
20	A	836	CLA	C2C-C3C-CAC-CBC
29	6	316	CHL	C8-C10-C11-C12
20	G	203	CLA	C4C-C3C-CAC-CBC
29	8	317	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
29	1	1015	CHL	O1A-CGA-O2A-C1
27	8	318	LMG	O6-C5-C6-O5
27	4	318	LMG	O9-C10-O7-C8
27	5	324	LMG	O9-C10-O7-C8
25	B	848	DGD	C2A-C1A-O1G-C1G
27	4	318	LMG	C29-C28-O8-C9
23	A	849	LHG	C34-C35-C36-C37
27	5	324	LMG	C15-C16-C17-C18
20	B	802	CLA	C2A-CAA-CBA-CGA
29	5	313	CHL	C2A-CAA-CBA-CGA
23	8	301	LHG	C11-C10-C9-C8
27	4	318	LMG	O6-C1-O1-C7
23	A	849	LHG	C8-C7-O7-C5
27	5	324	LMG	C11-C10-O7-C8
27	0	303	LMG	C11-C12-C13-C14
23	A	849	LHG	O9-C7-O7-C5
23	8	301	LHG	C33-C34-C35-C36
23	3	1019	LHG	O7-C5-C6-O8
23	3	1019	LHG	O10-C23-O8-C6
20	F	302	CLA	C2C-C3C-CAC-CBC
29	8	317	CHL	C6-C7-C8-C9
29	1	1015	CHL	C6-C7-C8-C9
29	5	316	CHL	C11-C10-C8-C9
27	5	324	LMG	O6-C5-C6-O5
20	A	807	CLA	C2A-CAA-CBA-CGA
20	A	815	CLA	C2A-CAA-CBA-CGA
20	B	803	CLA	C2A-CAA-CBA-CGA
20	3	1016	CLA	C2A-CAA-CBA-CGA
20	4	309	CLA	C2A-CAA-CBA-CGA
20	6	307	CLA	C2A-CAA-CBA-CGA
28	7	1001	LUT	C11-C12-C13-C20
30	5	303	XAT	C7-C8-C9-C19
20	A	804	CLA	C1A-C2A-CAA-CBA
20	A	805	CLA	C1A-C2A-CAA-CBA
20	A	808	CLA	C1A-C2A-CAA-CBA
20	A	817	CLA	C1A-C2A-CAA-CBA
20	B	808	CLA	C1A-C2A-CAA-CBA
20	B	821	CLA	C1A-C2A-CAA-CBA
20	B	825	CLA	C1A-C2A-CAA-CBA
20	B	826	CLA	C1A-C2A-CAA-CBA
20	B	829	CLA	C1A-C2A-CAA-CBA
20	B	839	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	G	202	CLA	C1A-C2A-CAA-CBA
20	J	102	CLA	C1A-C2A-CAA-CBA
20	K	201	CLA	C1A-C2A-CAA-CBA
20	L	202	CLA	C1A-C2A-CAA-CBA
20	L	204	CLA	C1A-C2A-CAA-CBA
20	0	305	CLA	C1A-C2A-CAA-CBA
20	0	309	CLA	C1A-C2A-CAA-CBA
20	8	309	CLA	C1A-C2A-CAA-CBA
20	7	1004	CLA	C1A-C2A-CAA-CBA
20	7	1007	CLA	C1A-C2A-CAA-CBA
20	7	1009	CLA	C1A-C2A-CAA-CBA
20	3	1008	CLA	C1A-C2A-CAA-CBA
20	3	1012	CLA	C1A-C2A-CAA-CBA
20	3	1013	CLA	C1A-C2A-CAA-CBA
20	1	1007	CLA	C1A-C2A-CAA-CBA
20	4	308	CLA	C1A-C2A-CAA-CBA
20	6	309	CLA	C1A-C2A-CAA-CBA
20	5	308	CLA	C1A-C2A-CAA-CBA
29	4	312	CHL	C1A-C2A-CAA-CBA
29	8	317	CHL	C11-C12-C13-C14
24	1	1001	BCR	C13-C14-C15-C16
20	B	850	CLA	CHC-C1C-C2C-CMC
25	B	848	DGD	C1B-C2B-C3B-C4B
26	B	849	LMT	O5'-C5'-C6'-O6'
27	6	319	LMG	O6-C5-C6-O5
27	5	324	LMG	C33-C34-C35-C36
23	A	843	LHG	C11-C10-C9-C8
23	A	849	LHG	C24-C25-C26-C27
25	B	848	DGD	O1A-C1A-O1G-C1G
27	4	318	LMG	O10-C28-O8-C9
23	A	849	LHG	C11-C12-C13-C14
25	5	319	DGD	C1G-C2G-C3G-O3G
27	5	324	LMG	C8-C7-O1-C1
27	5	324	LMG	C16-C17-C18-C19
20	3	1009	CLA	C2C-C3C-CAC-CBC
20	5	310	CLA	C4C-C3C-CAC-CBC
29	8	317	CHL	CBA-CGA-O2A-C1
23	A	849	LHG	C35-C36-C37-C38
20	B	833	CLA	C2A-CAA-CBA-CGA
20	K	201	CLA	C2A-CAA-CBA-CGA
29	5	316	CHL	O1D-CGD-O2D-CED
26	3	1018	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
20	A	812	CLA	C4C-C3C-CAC-CBC
24	7	1003	BCR	C20-C21-C22-C23
27	5	324	LMG	C2-C1-O1-C7
27	4	318	LMG	O1-C7-C8-O7
23	4	301	LHG	C18-C19-C20-C21
22	B	842	PQN	C22-C23-C25-C26
29	7	1017	CHL	C6-C7-C8-C10
20	0	311	CLA	C4C-C3C-CAC-CBC
23	4	301	LHG	C25-C26-C27-C28
24	3	1003	BCR	C13-C14-C15-C16
27	6	319	LMG	C29-C28-O8-C9
29	0	314	CHL	C2A-CAA-CBA-CGA
24	A	848	BCR	C7-C8-C9-C34
28	6	303	LUT	C7-C8-C9-C10
29	0	315	CHL	CBA-CGA-O2A-C1
29	4	315	CHL	CBA-CGA-O2A-C1
23	A	849	LHG	C33-C34-C35-C36
20	A	839	CLA	C4B-C3B-CAB-CBB
20	B	801	CLA	C4B-C3B-CAB-CBB
20	B	803	CLA	C4B-C3B-CAB-CBB
20	B	822	CLA	C4B-C3B-CAB-CBB
20	B	823	CLA	C4B-C3B-CAB-CBB
20	G	203	CLA	C4B-C3B-CAB-CBB
20	L	201	CLA	C4B-C3B-CAB-CBB
20	0	316	CLA	C4B-C3B-CAB-CBB
20	8	311	CLA	C4B-C3B-CAB-CBB
20	8	312	CLA	C4B-C3B-CAB-CBB
20	3	1009	CLA	C4B-C3B-CAB-CBB
20	1	1009	CLA	C4B-C3B-CAB-CBB
20	4	310	CLA	C4B-C3B-CAB-CBB
20	6	301	CLA	C4B-C3B-CAB-CBB
20	6	318	CLA	C4B-C3B-CAB-CBB
20	5	305	CLA	C4B-C3B-CAB-CBB
20	5	311	CLA	C4B-C3B-CAB-CBB
27	5	324	LMG	C8-C9-O8-C28
23	A	843	LHG	O6-C4-C5-C6
27	J	101	LMG	C11-C12-C13-C14
20	3	1006	CLA	C2C-C3C-CAC-CBC
29	0	317	CHL	CBA-CGA-O2A-C1
20	1	1007	CLA	C2C-C3C-CAC-CBC
23	A	849	LHG	C12-C13-C14-C15
20	A	803	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	B	821	CLA	C3A-C2A-CAA-CBA
20	8	316	CLA	C3A-C2A-CAA-CBA
29	4	315	CHL	C3A-C2A-CAA-CBA
29	8	317	CHL	C10-C11-C12-C13
25	5	319	DGD	C4A-C5A-C6A-C7A
23	A	843	LHG	C26-C27-C28-C29
27	5	324	LMG	C28-C29-C30-C31
25	B	848	DGD	O1G-C1G-C2G-C3G
27	8	319	LMG	C7-C8-C9-O8
27	5	324	LMG	O1-C7-C8-C9
23	A	849	LHG	C3-O3-P-O6
27	6	319	LMG	O10-C28-O8-C9
29	8	317	CHL	O1A-CGA-O2A-C1
23	A	849	LHG	C28-C29-C30-C31
23	8	301	LHG	C9-C10-C11-C12
29	0	317	CHL	C11-C12-C13-C15
25	5	319	DGD	C5B-C6B-C7B-C8B
20	A	803	CLA	C2B-C3B-CAB-CBB
20	A	839	CLA	C2B-C3B-CAB-CBB
20	B	841	CLA	C2B-C3B-CAB-CBB
23	7	1016	LHG	C8-C7-O7-C5
23	8	301	LHG	C28-C29-C30-C31
29	6	316	CHL	C2-C1-O2A-CGA
29	6	316	CHL	C6-C7-C8-C9
20	3	1005	CLA	C2C-C3C-CAC-CBC
20	A	820	CLA	C2A-CAA-CBA-CGA
29	6	316	CHL	C2A-CAA-CBA-CGA
29	3	1014	CHL	O1A-CGA-O2A-C1
24	A	844	BCR	C1-C6-C7-C8
24	A	844	BCR	C5-C6-C7-C8
24	A	847	BCR	C1-C6-C7-C8
24	A	847	BCR	C5-C6-C7-C8
24	B	844	BCR	C1-C6-C7-C8
24	B	847	BCR	C1-C6-C7-C8
24	H	201	BCR	C5-C6-C7-C8
24	3	1003	BCR	C23-C24-C25-C30
24	5	320	BCR	C23-C24-C25-C26
28	0	304	LUT	C1-C6-C7-C8
28	0	304	LUT	C5-C6-C7-C8
28	3	1002	LUT	C1-C6-C7-C8
28	3	1002	LUT	C5-C6-C7-C8
28	1	1002	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	8	301	LHG	C15-C16-C17-C18
24	B	847	BCR	C21-C22-C23-C24
24	7	1003	BCR	C17-C18-C19-C20
24	7	1003	BCR	C21-C22-C23-C24
23	A	849	LHG	C17-C18-C19-C20
20	0	309	CLA	C2C-C3C-CAC-CBC
22	B	842	PQN	C16-C17-C18-C20
20	A	823	CLA	C2A-CAA-CBA-CGA
20	8	312	CLA	C2A-CAA-CBA-CGA
24	A	847	BCR	C11-C10-C9-C34
24	A	850	BCR	C11-C10-C9-C34
20	0	311	CLA	C2C-C3C-CAC-CBC
20	1	1008	CLA	C4C-C3C-CAC-CBC
20	6	310	CLA	C4C-C3C-CAC-CBC
29	7	1015	CHL	CAD-CBD-CGD-O2D
29	3	1014	CHL	CAD-CBD-CGD-O2D
29	1	1012	CHL	O1D-CGD-O2D-CED
23	A	849	LHG	C25-C26-C27-C28
29	4	315	CHL	O1A-CGA-O2A-C1
27	0	303	LMG	O6-C1-O1-C7
27	8	319	LMG	O6-C1-O1-C7
23	3	1019	LHG	C4-C5-C6-O8
23	4	301	LHG	C15-C16-C17-C18
29	0	317	CHL	C11-C12-C13-C14
29	6	317	CHL	CHA-CBD-CGD-O1D
20	4	309	CLA	C4C-C3C-CAC-CBC
29	0	315	CHL	O1A-CGA-O2A-C1
29	0	317	CHL	O1A-CGA-O2A-C1
23	8	301	LHG	C17-C18-C19-C20
25	B	848	DGD	O1G-C1G-C2G-O2G
25	5	319	DGD	O2G-C2G-C3G-O3G
25	B	848	DGD	O6D-C5D-C6D-O5D
20	4	309	CLA	C2C-C3C-CAC-CBC
23	7	1016	LHG	O9-C7-O7-C5
29	4	315	CHL	C6-C7-C8-C9
27	5	324	LMG	C40-C41-C42-C43
22	B	842	PQN	C26-C27-C28-C30
20	L	201	CLA	C2A-CAA-CBA-CGA
20	1	1010	CLA	C2A-CAA-CBA-CGA
28	5	302	LUT	C31-C32-C33-C40
28	7	1001	LUT	C11-C12-C13-C14
28	7	1001	LUT	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
20	A	803	CLA	CHA-CBD-CGD-O2D
20	A	807	CLA	CHA-CBD-CGD-O2D
20	A	812	CLA	CHA-CBD-CGD-O2D
20	A	813	CLA	CHA-CBD-CGD-O2D
20	A	815	CLA	CHA-CBD-CGD-O2D
20	A	828	CLA	CHA-CBD-CGD-O2D
20	B	820	CLA	CHA-CBD-CGD-O2D
20	B	831	CLA	C1A-C2A-CAA-CBA
20	B	833	CLA	CHA-CBD-CGD-O2D
20	B	834	CLA	CHA-CBD-CGD-O2D
20	B	840	CLA	CHA-CBD-CGD-O2D
20	G	203	CLA	CHA-CBD-CGD-O2D
20	L	202	CLA	CHA-CBD-CGD-O2D
20	8	308	CLA	CHA-CBD-CGD-O2D
20	8	311	CLA	CHA-CBD-CGD-O2D
20	7	1006	CLA	CHA-CBD-CGD-O2D
20	6	309	CLA	CHA-CBD-CGD-O2D
20	6	311	CLA	CHA-CBD-CGD-O2D
20	5	318	CLA	CHA-CBD-CGD-O2D
29	8	314	CHL	C1A-C2A-CAA-CBA
29	8	317	CHL	C1A-C2A-CAA-CBA
20	F	302	CLA	C4C-C3C-CAC-CBC
25	B	848	DGD	C7A-C8A-C9A-CAA
23	8	301	LHG	C4-O6-P-O3
20	B	816	CLA	C2C-C3C-CAC-CBC
23	4	301	LHG	O2-C2-C3-O3
20	8	309	CLA	C2C-C3C-CAC-CBC
20	A	822	CLA	C4B-C3B-CAB-CBB
20	B	807	CLA	C4B-C3B-CAB-CBB
20	B	840	CLA	C4B-C3B-CAB-CBB
20	0	311	CLA	C4B-C3B-CAB-CBB
20	0	312	CLA	C4B-C3B-CAB-CBB
20	3	1011	CLA	C4B-C3B-CAB-CBB
20	3	1012	CLA	C4B-C3B-CAB-CBB
20	1	1005	CLA	C4B-C3B-CAB-CBB
20	1	1010	CLA	C4B-C3B-CAB-CBB
20	4	305	CLA	C4B-C3B-CAB-CBB
20	6	306	CLA	C4B-C3B-CAB-CBB
20	6	311	CLA	C4B-C3B-CAB-CBB
20	6	320	CLA	C4B-C3B-CAB-CBB
20	5	322	CLA	C4B-C3B-CAB-CBB
23	A	843	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
23	0	302	LHG	C4-O6-P-O4
23	3	1019	LHG	C4-O6-P-O4
23	4	301	LHG	C4-O6-P-O4
29	8	315	CHL	C4B-C3B-CAB-CBB
29	4	313	CHL	C4B-C3B-CAB-CBB
23	8	301	LHG	C27-C28-C29-C30
23	7	1016	LHG	C27-C28-C29-C30
20	A	806	CLA	C2A-CAA-CBA-CGA
27	5	324	LMG	C13-C14-C15-C16
25	5	319	DGD	C1A-C2A-C3A-C4A
25	B	848	DGD	CAA-CBA-CCA-CDA
23	A	843	LHG	C14-C15-C16-C17
22	B	842	PQN	C26-C27-C28-C29
20	A	818	CLA	CAD-CBD-CGD-O2D
20	A	824	CLA	CHA-CBD-CGD-O1D
20	A	837	CLA	CAD-CBD-CGD-O2D
20	B	826	CLA	CHA-CBD-CGD-O1D
20	B	827	CLA	CHA-CBD-CGD-O1D
20	B	834	CLA	CHA-CBD-CGD-O1D
20	B	838	CLA	CAD-CBD-CGD-O2D
20	K	201	CLA	CAD-CBD-CGD-O2D
20	0	306	CLA	CHA-CBD-CGD-O1D
20	8	313	CLA	CAD-CBD-CGD-O2D
20	7	1008	CLA	CAD-CBD-CGD-O2D
20	3	1008	CLA	CAD-CBD-CGD-O2D
20	1	1008	CLA	CAD-CBD-CGD-O2D
20	4	306	CLA	CAD-CBD-CGD-O2D
20	4	309	CLA	CAD-CBD-CGD-O2D
20	4	310	CLA	CHA-CBD-CGD-O1D
20	4	310	CLA	CAD-CBD-CGD-O2D
20	6	318	CLA	CAD-CBD-CGD-O2D
20	5	301	CLA	CAD-CBD-CGD-O2D
20	5	309	CLA	CAD-CBD-CGD-O2D
20	5	310	CLA	CAD-CBD-CGD-O2D
29	4	315	CHL	C11-C10-C8-C7
29	5	316	CHL	C11-C10-C8-C7
20	8	311	CLA	C4C-C3C-CAC-CBC
20	3	1006	CLA	C4C-C3C-CAC-CBC
25	B	848	DGD	C4A-C5A-C6A-C7A
20	G	203	CLA	C2C-C3C-CAC-CBC
20	A	801	CLA	CAD-CBD-CGD-O1D
20	A	804	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	A	819	CLA	CAD-CBD-CGD-O1D
20	A	834	CLA	CAD-CBD-CGD-O1D
20	B	816	CLA	CAD-CBD-CGD-O1D
20	0	313	CLA	CAD-CBD-CGD-O1D
20	8	313	CLA	CAD-CBD-CGD-O1D
20	1	1011	CLA	CAD-CBD-CGD-O1D
20	4	311	CLA	CAD-CBD-CGD-O1D
20	5	312	CLA	CAD-CBD-CGD-O1D
20	5	323	CLA	CAD-CBD-CGD-O1D
27	6	319	LMG	C22-C23-C24-C25
20	4	310	CLA	C4C-C3C-CAC-CBC
27	0	303	LMG	C8-C7-O1-C1
22	B	842	PQN	C24-C23-C25-C26
23	8	301	LHG	C25-C26-C27-C28
26	B	849	LMT	O5'-C1'-O1'-C1
27	5	324	LMG	C29-C30-C31-C32
24	B	845	BCR	C18-C19-C20-C21
20	1	1008	CLA	C2C-C3C-CAC-CBC
30	6	304	XAT	C31-C32-C33-C34
20	A	822	CLA	C2B-C3B-CAB-CBB
20	B	803	CLA	C2B-C3B-CAB-CBB
20	B	823	CLA	C2B-C3B-CAB-CBB
20	B	850	CLA	C2B-C3B-CAB-CBB
20	G	203	CLA	C2B-C3B-CAB-CBB
20	0	311	CLA	C2B-C3B-CAB-CBB
20	0	316	CLA	C2B-C3B-CAB-CBB
20	8	311	CLA	C2B-C3B-CAB-CBB
20	7	1006	CLA	C2B-C3B-CAB-CBB
20	3	1009	CLA	C2B-C3B-CAB-CBB
20	3	1011	CLA	C2B-C3B-CAB-CBB
20	3	1012	CLA	C2B-C3B-CAB-CBB
20	6	306	CLA	C2B-C3B-CAB-CBB
20	6	311	CLA	C2B-C3B-CAB-CBB
20	6	318	CLA	C2B-C3B-CAB-CBB
20	6	320	CLA	C2B-C3B-CAB-CBB
20	5	301	CLA	C2B-C3B-CAB-CBB
20	5	311	CLA	C2B-C3B-CAB-CBB
29	6	316	CHL	C2B-C3B-CAB-CBB
20	B	816	CLA	C4C-C3C-CAC-CBC
23	A	843	LHG	C16-C17-C18-C19
27	0	303	LMG	C13-C14-C15-C16
29	1	1012	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	A	843	LHG	C19-C20-C21-C22
29	7	1017	CHL	C2C-C3C-CAC-CBC
20	0	307	CLA	C2A-CAA-CBA-CGA
20	8	310	CLA	C2A-CAA-CBA-CGA
20	7	1006	CLA	C2A-CAA-CBA-CGA
20	4	308	CLA	C2A-CAA-CBA-CGA
29	1	1012	CHL	C2A-CAA-CBA-CGA
20	4	310	CLA	C2C-C3C-CAC-CBC
24	I	201	BCR	C1-C6-C7-C8
24	I	201	BCR	C5-C6-C7-C8
20	A	828	CLA	C2A-CAA-CBA-CGA
20	7	1009	CLA	C2A-CAA-CBA-CGA
20	5	323	CLA	C2A-CAA-CBA-CGA
24	7	1003	BCR	C16-C17-C18-C19
23	A	843	LHG	C3-O3-P-O6
23	0	302	LHG	C3-O3-P-O6
23	0	302	LHG	C4-O6-P-O3
23	7	1016	LHG	C3-O3-P-O6
20	8	309	CLA	C4C-C3C-CAC-CBC
27	0	303	LMG	O1-C7-C8-C9
27	4	318	LMG	O1-C7-C8-C9
22	B	842	PQN	C16-C17-C18-C19
29	5	316	CHL	C6-C7-C8-C9
24	B	844	BCR	C36-C18-C19-C20
29	5	316	CHL	C11-C12-C13-C15
23	7	1016	LHG	C2-C3-O3-P
20	A	822	CLA	CAA-CBA-CGA-O1A
22	A	842	PQN	C15-C16-C17-C18
20	3	1009	CLA	C4C-C3C-CAC-CBC
20	A	828	CLA	CAA-CBA-CGA-O2A
20	4	305	CLA	CAA-CBA-CGA-O2A
20	A	805	CLA	C4B-C3B-CAB-CBB
20	A	831	CLA	C4B-C3B-CAB-CBB
20	B	818	CLA	C4B-C3B-CAB-CBB
20	B	819	CLA	C4B-C3B-CAB-CBB
20	B	824	CLA	C4B-C3B-CAB-CBB
20	B	829	CLA	C4B-C3B-CAB-CBB
20	J	102	CLA	C4B-C3B-CAB-CBB
20	L	202	CLA	C4B-C3B-CAB-CBB
20	3	1007	CLA	C4B-C3B-CAB-CBB
20	3	1016	CLA	C4B-C3B-CAB-CBB
20	4	314	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	6	315	CLA	C4B-C3B-CAB-CBB
29	6	314	CHL	C4B-C3B-CAB-CBB
29	6	316	CHL	C4B-C3B-CAB-CBB
30	7	1002	XAT	C9-C10-C11-C12
27	6	319	LMG	C15-C16-C17-C18
20	5	310	CLA	C2C-C3C-CAC-CBC
29	1	1015	CHL	C11-C12-C13-C14
20	A	802	CLA	CAA-CBA-CGA-O2A
20	A	827	CLA	CAA-CBA-CGA-O1A
23	4	301	LHG	C16-C17-C18-C19
27	6	319	LMG	C30-C31-C32-C33
20	B	802	CLA	C2C-C3C-CAC-CBC
27	5	324	LMG	C37-C38-C39-C40
20	B	819	CLA	CAA-CBA-CGA-O1A
20	0	306	CLA	CAA-CBA-CGA-O1A
29	8	317	CHL	C2-C1-O2A-CGA
20	A	813	CLA	CAA-CBA-CGA-O1A
20	B	815	CLA	CAA-CBA-CGA-O1A
20	A	810	CLA	C2A-CAA-CBA-CGA
20	B	810	CLA	C2A-CAA-CBA-CGA
20	7	1004	CLA	C2A-CAA-CBA-CGA
20	1	1008	CLA	C2A-CAA-CBA-CGA
20	5	306	CLA	C2A-CAA-CBA-CGA
27	0	303	LMG	O1-C7-C8-O7
20	5	301	CLA	C3A-C2A-CAA-CBA
20	A	802	CLA	CAA-CBA-CGA-O1A
20	A	815	CLA	CAA-CBA-CGA-O2A
20	A	827	CLA	CAA-CBA-CGA-O2A
20	B	816	CLA	CAA-CBA-CGA-O1A
20	B	839	CLA	CAA-CBA-CGA-O1A
20	3	1013	CLA	CAA-CBA-CGA-O1A
20	1	1004	CLA	CAA-CBA-CGA-O1A
20	A	806	CLA	C4C-C3C-CAC-CBC
25	B	848	DGD	CCB-CDB-CEB-CFB
20	0	310	CLA	C4C-C3C-CAC-CBC
20	A	819	CLA	CAA-CBA-CGA-O1A
20	A	819	CLA	CAA-CBA-CGA-O2A
20	3	1016	CLA	CAA-CBA-CGA-O1A
20	3	1017	CLA	CAA-CBA-CGA-O2A
29	6	313	CHL	CBA-CGA-O2A-C1
29	1	1015	CHL	C11-C12-C13-C15
29	5	316	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	A	808	CLA	CAA-CBA-CGA-O2A
20	B	839	CLA	CAA-CBA-CGA-O2A
20	4	305	CLA	CAA-CBA-CGA-O1A
20	6	306	CLA	CAA-CBA-CGA-O1A
27	8	318	LMG	O10-C28-O8-C9
24	A	845	BCR	C11-C10-C9-C34
24	A	846	BCR	C16-C17-C18-C36
24	A	848	BCR	C11-C10-C9-C34
24	A	848	BCR	C16-C17-C18-C36
24	B	804	BCR	C11-C10-C9-C34
24	B	804	BCR	C16-C17-C18-C36
24	B	843	BCR	C11-C10-C9-C34
24	B	843	BCR	C35-C13-C14-C15
24	B	843	BCR	C16-C17-C18-C36
24	B	844	BCR	C11-C10-C9-C34
24	B	845	BCR	C11-C10-C9-C34
24	F	304	BCR	C16-C17-C18-C36
24	G	204	BCR	C16-C17-C18-C36
24	I	201	BCR	C16-C17-C18-C36
24	I	201	BCR	C20-C21-C22-C37
24	3	1003	BCR	C35-C13-C14-C15
24	3	1004	BCR	C16-C17-C18-C36
28	3	1002	LUT	C21-C26-C27-C28
25	5	319	DGD	O1B-C1B-O2G-C2G
20	0	312	CLA	CAA-CBA-CGA-O1A
20	7	1004	CLA	CAA-CBA-CGA-O1A
20	5	311	CLA	CAA-CBA-CGA-O1A
20	5	321	CLA	CAA-CBA-CGA-O1A
27	J	101	LMG	C29-C28-O8-C9
20	A	815	CLA	CAA-CBA-CGA-O1A
20	B	840	CLA	CAA-CBA-CGA-O1A
20	1	1010	CLA	CAA-CBA-CGA-O1A
24	A	845	BCR	C36-C18-C19-C20
24	A	846	BCR	C7-C8-C9-C34
24	B	844	BCR	C11-C12-C13-C35
24	3	1004	BCR	C11-C12-C13-C35
28	0	304	LUT	C7-C8-C9-C10
20	A	836	CLA	CAA-CBA-CGA-O1A
20	B	837	CLA	C1A-C2A-CAA-CBA
20	8	316	CLA	C1A-C2A-CAA-CBA
20	1	1003	CLA	C1A-C2A-CAA-CBA
20	4	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	0	314	CHL	C1A-C2A-CAA-CBA
29	6	313	CHL	C1A-C2A-CAA-CBA
29	5	313	CHL	C1A-C2A-CAA-CBA
27	5	324	LMG	C36-C37-C38-C39
29	7	1017	CHL	C5-C6-C7-C8
20	A	808	CLA	CAA-CBA-CGA-O1A
20	B	819	CLA	CAA-CBA-CGA-O2A
20	0	308	CLA	CAA-CBA-CGA-O1A
20	0	312	CLA	CAA-CBA-CGA-O2A
20	7	1011	CLA	CAA-CBA-CGA-O2A
20	3	1006	CLA	CAA-CBA-CGA-O2A
20	1	1004	CLA	CAA-CBA-CGA-O2A
20	0	308	CLA	CAA-CBA-CGA-O2A
20	7	1011	CLA	CAA-CBA-CGA-O1A
20	3	1006	CLA	CAA-CBA-CGA-O1A
20	5	304	CLA	CAA-CBA-CGA-O1A
20	5	304	CLA	CAA-CBA-CGA-O2A
29	7	1017	CHL	C8-C10-C11-C12
26	B	849	LMT	C2-C3-C4-C5
20	4	306	CLA	C2A-CAA-CBA-CGA
23	7	1016	LHG	O6-C4-C5-O7
20	A	836	CLA	CAA-CBA-CGA-O2A
20	B	815	CLA	CAA-CBA-CGA-O2A
20	B	840	CLA	CAA-CBA-CGA-O2A
20	0	306	CLA	CAA-CBA-CGA-O2A
20	8	312	CLA	CAA-CBA-CGA-O1A
20	3	1016	CLA	CAA-CBA-CGA-O2A
20	B	813	CLA	CAA-CBA-CGA-O2A
20	3	1013	CLA	CAA-CBA-CGA-O2A
20	5	309	CLA	CAA-CBA-CGA-O1A
29	7	1015	CHL	CAA-CBA-CGA-O2A
27	5	324	LMG	C32-C33-C34-C35
20	A	805	CLA	C2B-C3B-CAB-CBB
20	B	801	CLA	C2B-C3B-CAB-CBB
20	B	818	CLA	C2B-C3B-CAB-CBB
20	B	829	CLA	C2B-C3B-CAB-CBB
20	B	840	CLA	C2B-C3B-CAB-CBB
20	J	102	CLA	C2B-C3B-CAB-CBB
20	8	312	CLA	C2B-C3B-CAB-CBB
20	3	1016	CLA	C2B-C3B-CAB-CBB
20	1	1005	CLA	C2B-C3B-CAB-CBB
20	1	1010	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	6	301	CLA	C2B-C3B-CAB-CBB
20	5	305	CLA	C2B-C3B-CAB-CBB
20	5	322	CLA	C2B-C3B-CAB-CBB
29	8	315	CHL	C2B-C3B-CAB-CBB
29	4	313	CHL	C2B-C3B-CAB-CBB
29	6	314	CHL	C2B-C3B-CAB-CBB
20	B	817	CLA	C4C-C3C-CAC-CBC
20	A	817	CLA	CAA-CBA-CGA-O1A
20	A	821	CLA	CAA-CBA-CGA-O1A
20	A	821	CLA	CAA-CBA-CGA-O2A
20	B	826	CLA	CAA-CBA-CGA-O1A
20	7	1004	CLA	CAA-CBA-CGA-O2A
24	A	846	BCR	C16-C17-C18-C19
24	A	848	BCR	C11-C10-C9-C8
24	A	848	BCR	C16-C17-C18-C19
24	B	804	BCR	C11-C10-C9-C8
24	B	804	BCR	C16-C17-C18-C19
24	B	843	BCR	C11-C10-C9-C8
24	B	843	BCR	C12-C13-C14-C15
24	B	843	BCR	C16-C17-C18-C19
24	B	844	BCR	C11-C10-C9-C8
24	F	304	BCR	C16-C17-C18-C19
24	G	204	BCR	C16-C17-C18-C19
24	I	201	BCR	C16-C17-C18-C19
24	I	201	BCR	C20-C21-C22-C23
20	A	813	CLA	CAA-CBA-CGA-O2A
20	A	822	CLA	CAA-CBA-CGA-O2A
20	L	204	CLA	CAA-CBA-CGA-O2A
27	J	101	LMG	O10-C28-O8-C9
20	A	817	CLA	CAA-CBA-CGA-O2A
29	7	1015	CHL	CAA-CBA-CGA-O1A
29	8	317	CHL	C5-C6-C7-C8
20	4	308	CLA	C2C-C3C-CAC-CBC
20	A	840	CLA	CAA-CBA-CGA-O1A
20	B	803	CLA	CAA-CBA-CGA-O1A
20	B	816	CLA	CAA-CBA-CGA-O2A
20	5	311	CLA	CAA-CBA-CGA-O2A
29	4	315	CHL	C2-C1-O2A-CGA
20	A	824	CLA	CAA-CBA-CGA-O2A
20	A	828	CLA	CAA-CBA-CGA-O1A
20	B	803	CLA	CAA-CBA-CGA-O2A
20	B	809	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	6	306	CLA	CAA-CBA-CGA-O2A
22	B	842	PQN	C21-C22-C23-C24
20	B	813	CLA	CAA-CBA-CGA-O1A
20	3	1010	CLA	CAA-CBA-CGA-O2A
20	3	1017	CLA	CAA-CBA-CGA-O1A
24	A	847	BCR	C23-C24-C25-C30
24	A	848	BCR	C23-C24-C25-C30
24	B	844	BCR	C5-C6-C7-C8
24	B	844	BCR	C23-C24-C25-C30
28	3	1001	LUT	C1-C6-C7-C8
28	1	1016	LUT	C1-C6-C7-C8
28	5	302	LUT	C1-C6-C7-C8
20	K	201	CLA	CAA-CBA-CGA-O1A
20	3	1007	CLA	CAA-CBA-CGA-O2A
20	5	323	CLA	CAA-CBA-CGA-O1A
23	7	1016	LHG	C28-C29-C30-C31
23	4	301	LHG	C9-C10-C11-C12
24	A	845	BCR	C17-C18-C19-C20
24	F	301	BCR	C7-C8-C9-C10
23	4	301	LHG	C28-C29-C30-C31
22	A	842	PQN	C13-C15-C16-C17
20	A	810	CLA	CAA-CBA-CGA-O2A
20	A	818	CLA	CAA-CBA-CGA-O2A
20	A	839	CLA	CAA-CBA-CGA-O2A
20	A	840	CLA	CAA-CBA-CGA-O2A
20	B	809	CLA	CAA-CBA-CGA-O1A
20	6	305	CLA	CAA-CBA-CGA-O2A
20	5	309	CLA	CAA-CBA-CGA-O2A
20	5	321	CLA	CAA-CBA-CGA-O2A
20	A	811	CLA	CAA-CBA-CGA-O2A
20	7	1006	CLA	CAA-CBA-CGA-O2A
20	1	1003	CLA	CAA-CBA-CGA-O2A
20	4	304	CLA	CAA-CBA-CGA-O2A
20	8	310	CLA	C4C-C3C-CAC-CBC
20	A	812	CLA	CAA-CBA-CGA-O2A
20	A	851	CLA	CAA-CBA-CGA-O2A
20	B	806	CLA	CAA-CBA-CGA-O2A
20	B	850	CLA	CAA-CBA-CGA-O2A
20	3	1010	CLA	CAA-CBA-CGA-O1A
20	3	1012	CLA	CAA-CBA-CGA-O2A
20	1	1006	CLA	CAA-CBA-CGA-O2A
20	A	836	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	A	824	CLA	CAA-CBA-CGA-O1A
20	B	838	CLA	CAA-CBA-CGA-O2A
20	A	814	CLA	C4B-C3B-CAB-CBB
20	A	825	CLA	C4B-C3B-CAB-CBB
20	B	850	CLA	C4B-C3B-CAB-CBB
20	L	204	CLA	C4B-C3B-CAB-CBB
20	8	316	CLA	C4B-C3B-CAB-CBB
20	1	1014	CLA	C4B-C3B-CAB-CBB
27	J	101	LMG	C10-C11-C12-C13
20	0	307	CLA	CAA-CBA-CGA-O2A
23	4	301	LHG	O1-C1-C2-O2
20	0	305	CLA	CAA-CBA-CGA-O2A
20	7	1008	CLA	CAA-CBA-CGA-O1A
20	6	301	CLA	CAA-CBA-CGA-O1A
29	6	317	CHL	O1D-CGD-O2D-CED
20	A	803	CLA	CAA-CBA-CGA-O2A
20	A	829	CLA	CAA-CBA-CGA-O2A
20	A	833	CLA	CAA-CBA-CGA-O2A
20	G	202	CLA	CAA-CBA-CGA-O2A
20	L	204	CLA	CAA-CBA-CGA-O1A
20	8	305	CLA	CAA-CBA-CGA-O2A
27	8	318	LMG	C29-C28-O8-C9
24	H	201	BCR	C11-C10-C9-C34
27	0	303	LMG	C16-C17-C18-C19
29	4	315	CHL	C2C-C3C-CAC-CBC
20	B	812	CLA	CAA-CBA-CGA-O2A
20	B	826	CLA	CAA-CBA-CGA-O2A
20	G	203	CLA	CAA-CBA-CGA-O2A
20	7	1008	CLA	CAA-CBA-CGA-O2A
20	B	850	CLA	CAA-CBA-CGA-O1A
20	8	312	CLA	CAA-CBA-CGA-O2A
20	3	1009	CLA	CAA-CBA-CGA-O2A
20	A	811	CLA	C3A-C2A-CAA-CBA
20	B	837	CLA	C3A-C2A-CAA-CBA
20	L	203	CLA	C3A-C2A-CAA-CBA
29	5	314	CHL	O1A-CGA-O2A-C1
20	A	812	CLA	CAA-CBA-CGA-O1A
29	4	315	CHL	C11-C12-C13-C15
23	8	301	LHG	O9-C7-O7-C5
20	L	203	CLA	CAA-CBA-CGA-O2A
20	3	1005	CLA	CAA-CBA-CGA-O2A
20	1	1008	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	1	1010	CLA	CAA-CBA-CGA-O2A
20	A	831	CLA	CAA-CBA-CGA-O2A
20	B	808	CLA	CAA-CBA-CGA-O1A
20	0	305	CLA	CAA-CBA-CGA-O1A
20	8	306	CLA	CAA-CBA-CGA-O2A
20	1	1003	CLA	CAA-CBA-CGA-O1A
20	1	1006	CLA	CAA-CBA-CGA-O1A
20	5	305	CLA	CAA-CBA-CGA-O2A
24	A	848	BCR	C7-C8-C9-C10
24	B	844	BCR	C11-C12-C13-C14
24	B	847	BCR	C7-C8-C9-C10
24	I	201	BCR	C7-C8-C9-C10
28	0	318	LUT	C7-C8-C9-C10
28	3	1001	LUT	C31-C32-C33-C34
20	A	806	CLA	CAA-CBA-CGA-O2A
20	A	810	CLA	CAA-CBA-CGA-O1A
20	A	818	CLA	CAA-CBA-CGA-O1A
20	B	825	CLA	CAA-CBA-CGA-O1A
20	G	202	CLA	CAA-CBA-CGA-O1A
20	0	310	CLA	CAA-CBA-CGA-O2A
20	7	1006	CLA	CAA-CBA-CGA-O1A
20	3	1007	CLA	CAA-CBA-CGA-O1A
20	6	305	CLA	CAA-CBA-CGA-O1A
20	B	806	CLA	CAA-CBA-CGA-O1A
20	B	841	CLA	CAA-CBA-CGA-O2A
20	L	203	CLA	CAA-CBA-CGA-O1A
20	0	307	CLA	CAA-CBA-CGA-O1A
20	8	306	CLA	CAA-CBA-CGA-O1A
20	8	311	CLA	C2C-C3C-CAC-CBC
27	0	303	LMG	C19-C20-C21-C22
20	A	830	CLA	C2A-CAA-CBA-CGA
20	B	801	CLA	C2A-CAA-CBA-CGA
20	A	806	CLA	CAA-CBA-CGA-O1A
20	A	811	CLA	CAA-CBA-CGA-O1A
20	A	820	CLA	CAA-CBA-CGA-O1A
20	A	820	CLA	CAA-CBA-CGA-O2A
20	A	851	CLA	CAA-CBA-CGA-O1A
20	B	808	CLA	CAA-CBA-CGA-O2A
20	G	203	CLA	CAA-CBA-CGA-O1A
20	K	201	CLA	CAA-CBA-CGA-O2A
20	8	305	CLA	CAA-CBA-CGA-O1A
20	4	304	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
20	5	323	CLA	CAA-CBA-CGA-O2A
27	8	319	LMG	C20-C21-C22-C23
29	1	1012	CHL	O1A-CGA-O2A-C1
29	4	312	CHL	CHA-CBD-CGD-O2D
29	6	317	CHL	CHA-CBD-CGD-O2D
20	A	803	CLA	CAA-CBA-CGA-O1A
20	A	837	CLA	CAA-CBA-CGA-O1A
20	A	837	CLA	CAA-CBA-CGA-O2A
20	A	852	CLA	CAA-CBA-CGA-O2A
20	B	812	CLA	CAA-CBA-CGA-O1A
20	3	1005	CLA	CAA-CBA-CGA-O1A
20	3	1009	CLA	CAA-CBA-CGA-O1A
20	3	1012	CLA	CAA-CBA-CGA-O1A
20	1	1008	CLA	CAA-CBA-CGA-O1A
20	4	307	CLA	CAA-CBA-CGA-O1A
20	4	307	CLA	CAA-CBA-CGA-O2A
23	7	1016	LHG	O6-C4-C5-C6
29	7	1012	CHL	O1D-CGD-O2D-CED
24	B	845	BCR	C11-C10-C9-C8
24	3	1004	BCR	C16-C17-C18-C19
20	A	831	CLA	CAA-CBA-CGA-O1A
20	A	835	CLA	CAA-CBA-CGA-O2A
20	B	841	CLA	CAA-CBA-CGA-O1A
20	0	310	CLA	CAA-CBA-CGA-O1A
20	5	305	CLA	CAA-CBA-CGA-O1A
23	A	849	LHG	O7-C5-C6-O8
27	6	319	LMG	C10-C11-C12-C13
20	B	825	CLA	CAA-CBA-CGA-O2A
23	A	849	LHG	O7-C7-C8-C9
23	4	301	LHG	O8-C23-C24-C25
20	B	840	CLA	C2A-CAA-CBA-CGA
29	4	315	CHL	C11-C12-C13-C14
20	A	839	CLA	CAA-CBA-CGA-O1A
20	A	852	CLA	CAA-CBA-CGA-O1A
20	8	307	CLA	CAA-CBA-CGA-O2A
29	5	314	CHL	CBA-CGA-O2A-C1
20	B	821	CLA	CAA-CBA-CGA-O1A
20	A	836	CLA	C4C-C3C-CAC-CBC
20	L	201	CLA	C2B-C3B-CAB-CBB
20	B	841	CLA	C2C-C3C-CAC-CBC
20	A	833	CLA	CAA-CBA-CGA-O1A
20	6	301	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	6	309	CLA	CAA-CBA-CGA-O2A
20	A	806	CLA	C2C-C3C-CAC-CBC
25	5	319	DGD	C2B-C1B-O2G-C2G
20	A	829	CLA	CAA-CBA-CGA-O1A
20	A	830	CLA	CAA-CBA-CGA-O2A
20	B	838	CLA	CAA-CBA-CGA-O1A
20	1	1005	CLA	C2A-CAA-CBA-CGA
26	B	849	LMT	C3-C4-C5-C6
29	7	1012	CHL	CBD-CGD-O2D-CED
24	A	846	BCR	C7-C8-C9-C10
20	4	314	CLA	C2C-C3C-CAC-CBC
20	A	805	CLA	CHA-CBD-CGD-O2D
20	A	820	CLA	CHA-CBD-CGD-O2D
20	A	829	CLA	CHA-CBD-CGD-O2D
20	A	832	CLA	CHA-CBD-CGD-O2D
20	B	802	CLA	CHA-CBD-CGD-O2D
20	B	810	CLA	CHA-CBD-CGD-O2D
20	B	812	CLA	CHA-CBD-CGD-O2D
20	B	815	CLA	CHA-CBD-CGD-O2D
20	B	816	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	CHA-CBD-CGD-O2D
20	B	826	CLA	CHA-CBD-CGD-O2D
20	B	827	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C1A-C2A-CAA-CBA
20	B	837	CLA	CHA-CBD-CGD-O2D
20	F	303	CLA	CHA-CBD-CGD-O2D
20	G	201	CLA	CHA-CBD-CGD-O2D
20	L	201	CLA	CHA-CBD-CGD-O2D
20	0	306	CLA	CHA-CBD-CGD-O2D
20	0	309	CLA	CHA-CBD-CGD-O2D
20	8	309	CLA	CHA-CBD-CGD-O2D
20	7	1007	CLA	CHA-CBD-CGD-O2D
20	3	1007	CLA	C1A-C2A-CAA-CBA
20	3	1015	CLA	CHA-CBD-CGD-O2D
20	1	1004	CLA	CHA-CBD-CGD-O2D
20	1	1010	CLA	CHA-CBD-CGD-O2D
20	4	305	CLA	CHA-CBD-CGD-O2D
20	4	307	CLA	CHA-CBD-CGD-O2D
20	4	314	CLA	CHA-CBD-CGD-O2D
20	6	301	CLA	CHA-CBD-CGD-O2D
20	6	308	CLA	CHA-CBD-CGD-O2D
20	6	318	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	5	301	CLA	C1A-C2A-CAA-CBA
20	5	306	CLA	C1A-C2A-CAA-CBA
20	5	307	CLA	CHA-CBD-CGD-O2D
29	7	1013	CHL	C1A-C2A-CAA-CBA
29	4	315	CHL	C1A-C2A-CAA-CBA
23	8	301	LHG	C4-C5-C6-O8
20	F	303	CLA	C2A-CAA-CBA-CGA
20	5	309	CLA	C2A-CAA-CBA-CGA
29	5	316	CHL	C10-C11-C12-C13
23	4	301	LHG	C10-C11-C12-C13
23	7	1016	LHG	C26-C27-C28-C29
20	4	309	CLA	CAA-CBA-CGA-O2A
20	5	301	CLA	CAA-CBA-CGA-O2A
20	A	811	CLA	C4B-C3B-CAB-CBB
20	A	836	CLA	C4B-C3B-CAB-CBB
20	B	820	CLA	C4B-C3B-CAB-CBB
20	8	307	CLA	C4B-C3B-CAB-CBB
20	3	1017	CLA	C4B-C3B-CAB-CBB
23	0	302	LHG	C3-O3-P-O5
29	0	315	CHL	C4B-C3B-CAB-CBB
29	3	1014	CHL	C4B-C3B-CAB-CBB
29	5	317	CHL	C4B-C3B-CAB-CBB
23	8	301	LHG	C8-C7-O7-C5
20	7	1005	CLA	CAA-CBA-CGA-O2A
20	6	310	CLA	CAA-CBA-CGA-O2A
24	3	1003	BCR	C23-C24-C25-C26
23	A	849	LHG	O9-C7-C8-C9
20	0	310	CLA	C2C-C3C-CAC-CBC
20	6	311	CLA	C4C-C3C-CAC-CBC
20	A	835	CLA	CAA-CBA-CGA-O1A
20	5	306	CLA	CAA-CBA-CGA-O2A
20	8	307	CLA	CAA-CBA-CGA-O1A
29	7	1012	CHL	CAD-CBD-CGD-O1D
29	4	312	CHL	CAD-CBD-CGD-O1D
29	6	317	CHL	CBD-CGD-O2D-CED
29	5	316	CHL	O1A-CGA-O2A-C1
23	A	843	LHG	O8-C23-C24-C25
20	4	306	CLA	CAA-CBA-CGA-O2A
20	5	301	CLA	CAA-CBA-CGA-O1A
20	3	1016	CLA	C4C-C3C-CAC-CBC
20	A	830	CLA	CAA-CBA-CGA-O1A
20	6	309	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
23	A	843	LHG	C23-C24-C25-C26
27	0	303	LMG	C29-C30-C31-C32
20	B	819	CLA	C2A-CAA-CBA-CGA
20	B	838	CLA	C2A-CAA-CBA-CGA
23	4	301	LHG	O10-C23-C24-C25
24	F	301	BCR	C36-C18-C19-C20
20	A	801	CLA	CAD-CBD-CGD-O2D
20	A	803	CLA	CHA-CBD-CGD-O1D
20	A	804	CLA	CAD-CBD-CGD-O2D
20	A	805	CLA	CAD-CBD-CGD-O2D
20	A	807	CLA	CHA-CBD-CGD-O1D
20	A	813	CLA	CHA-CBD-CGD-O1D
20	A	814	CLA	CHA-CBD-CGD-O1D
20	A	815	CLA	CHA-CBD-CGD-O1D
20	A	818	CLA	CHA-CBD-CGD-O1D
20	A	819	CLA	CAD-CBD-CGD-O2D
20	A	820	CLA	CAD-CBD-CGD-O2D
20	A	827	CLA	CHA-CBD-CGD-O1D
20	A	829	CLA	CHA-CBD-CGD-O1D
20	A	832	CLA	CAD-CBD-CGD-O2D
20	A	834	CLA	CAD-CBD-CGD-O2D
20	A	837	CLA	CHA-CBD-CGD-O1D
20	A	838	CLA	CHA-CBD-CGD-O1D
20	B	802	CLA	CHA-CBD-CGD-O1D
20	B	805	CLA	CAD-CBD-CGD-O2D
20	B	816	CLA	CAD-CBD-CGD-O2D
20	B	817	CLA	CHA-CBD-CGD-O1D
20	B	818	CLA	CHA-CBD-CGD-O1D
20	B	823	CLA	CHA-CBD-CGD-O1D
20	B	828	CLA	C3A-C2A-CAA-CBA
20	B	828	CLA	CAD-CBD-CGD-O2D
20	B	832	CLA	CHA-CBD-CGD-O1D
20	B	833	CLA	CHA-CBD-CGD-O1D
20	B	837	CLA	CHA-CBD-CGD-O1D
20	B	838	CLA	CHA-CBD-CGD-O1D
20	F	303	CLA	CAD-CBD-CGD-O2D
20	G	201	CLA	CHA-CBD-CGD-O1D
20	G	201	CLA	CAD-CBD-CGD-O2D
20	K	201	CLA	CHA-CBD-CGD-O1D
20	L	201	CLA	CHA-CBD-CGD-O1D
20	0	308	CLA	CHA-CBD-CGD-O1D
20	0	309	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	0	310	CLA	CAD-CBD-CGD-O2D
20	0	312	CLA	CAD-CBD-CGD-O2D
20	0	313	CLA	CAD-CBD-CGD-O2D
20	8	305	CLA	CHA-CBD-CGD-O1D
20	8	306	CLA	CHA-CBD-CGD-O1D
20	8	308	CLA	CHA-CBD-CGD-O1D
20	8	309	CLA	CHA-CBD-CGD-O1D
20	7	1004	CLA	CHA-CBD-CGD-O1D
20	7	1008	CLA	CHA-CBD-CGD-O1D
20	7	1009	CLA	CHA-CBD-CGD-O1D
20	7	1011	CLA	CAD-CBD-CGD-O2D
20	3	1015	CLA	CAD-CBD-CGD-O2D
20	3	1016	CLA	CHA-CBD-CGD-O1D
20	1	1004	CLA	CHA-CBD-CGD-O1D
20	1	1007	CLA	CHA-CBD-CGD-O1D
20	1	1008	CLA	CHA-CBD-CGD-O1D
20	1	1010	CLA	CHA-CBD-CGD-O1D
20	1	1010	CLA	CAD-CBD-CGD-O2D
20	1	1011	CLA	CAD-CBD-CGD-O2D
20	4	305	CLA	CHA-CBD-CGD-O1D
20	4	306	CLA	CHA-CBD-CGD-O1D
20	4	307	CLA	CHA-CBD-CGD-O1D
20	4	308	CLA	CHA-CBD-CGD-O1D
20	4	309	CLA	CHA-CBD-CGD-O1D
20	4	311	CLA	CAD-CBD-CGD-O2D
20	4	314	CLA	CAD-CBD-CGD-O2D
20	6	301	CLA	CHA-CBD-CGD-O1D
20	6	301	CLA	CAD-CBD-CGD-O2D
20	6	308	CLA	CHA-CBD-CGD-O1D
20	6	309	CLA	CHA-CBD-CGD-O1D
20	6	318	CLA	CHA-CBD-CGD-O1D
20	6	320	CLA	CAD-CBD-CGD-O2D
20	5	301	CLA	CHA-CBD-CGD-O1D
20	5	305	CLA	CHA-CBD-CGD-O1D
20	5	307	CLA	CHA-CBD-CGD-O1D
20	5	308	CLA	CHA-CBD-CGD-O1D
20	5	309	CLA	CHA-CBD-CGD-O1D
20	5	310	CLA	CHA-CBD-CGD-O1D
20	5	312	CLA	CAD-CBD-CGD-O2D
20	5	321	CLA	CHA-CBD-CGD-O1D
20	5	322	CLA	CHA-CBD-CGD-O1D
20	5	323	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	842	PQN	C21-C22-C23-C25
29	7	1017	CHL	C12-C13-C15-C16
20	0	301	CLA	CAA-CBA-CGA-O1A
20	4	309	CLA	CAA-CBA-CGA-O1A
23	3	1019	LHG	O8-C23-C24-C25
24	A	847	BCR	C11-C12-C13-C14
24	B	843	BCR	C11-C12-C13-C14
24	1	1001	BCR	C11-C12-C13-C14
20	A	801	CLA	CAA-CBA-CGA-O1A
20	0	301	CLA	CAA-CBA-CGA-O2A
20	6	310	CLA	CAA-CBA-CGA-O1A
27	6	319	LMG	C13-C14-C15-C16
20	B	829	CLA	CAA-CBA-CGA-O2A
20	7	1005	CLA	CAA-CBA-CGA-O1A
20	1	1017	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

243 monomers are involved in 819 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	836	CLA	1	0
20	A	830	CLA	1	0
28	8	303	LUT	4	0
24	G	205	BCR	18	0
20	1	1008	CLA	6	0
30	6	304	XAT	10	0
29	6	316	CHL	3	0
24	3	1003	BCR	2	0
20	0	310	CLA	3	0
29	5	313	CHL	4	0
29	7	1017	CHL	7	0
28	0	318	LUT	3	0
20	F	302	CLA	4	0
24	5	320	BCR	16	0
23	0	302	LHG	3	0
24	A	846	BCR	5	0
24	H	201	BCR	2	0
29	4	316	CHL	4	0
20	6	315	CLA	2	0
24	8	302	BCR	5	0
20	3	1009	CLA	1	0
28	J	104	LUT	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	0	314	CHL	9	0
20	1	1017	CLA	8	0
20	4	307	CLA	17	0
29	6	313	CHL	2	0
20	6	308	CLA	6	0
25	5	319	DGD	16	0
20	A	815	CLA	8	0
20	B	827	CLA	2	0
20	A	818	CLA	1	0
20	B	812	CLA	3	0
20	3	1013	CLA	2	0
20	1	1005	CLA	1	0
20	8	306	CLA	3	0
20	B	810	CLA	2	0
20	6	320	CLA	2	0
20	5	318	CLA	2	0
29	7	1015	CHL	1	0
30	4	303	XAT	2	0
20	L	202	CLA	1	0
20	A	821	CLA	3	0
20	1	1014	CLA	5	0
20	A	809	CLA	1	0
20	B	828	CLA	1	0
23	4	301	LHG	15	0
20	L	201	CLA	6	0
20	L	204	CLA	3	0
20	8	307	CLA	2	0
20	A	831	CLA	6	0
20	7	1004	CLA	10	0
20	6	312	CLA	12	0
20	B	818	CLA	5	0
20	J	102	CLA	3	0
29	8	315	CHL	3	0
20	1	1003	CLA	4	0
24	A	847	BCR	7	0
20	0	301	CLA	5	0
24	F	304	BCR	1	0
20	A	812	CLA	2	0
20	B	805	CLA	1	0
20	8	313	CLA	3	0
29	0	315	CHL	2	0
29	4	313	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	839	CLA	2	0
27	8	318	LMG	4	0
20	B	834	CLA	4	0
27	6	319	LMG	9	0
20	B	837	CLA	1	0
27	4	318	LMG	38	0
20	5	321	CLA	1	0
20	G	202	CLA	2	0
20	B	820	CLA	3	0
20	B	850	CLA	8	0
24	A	848	BCR	3	0
20	4	306	CLA	3	0
20	3	1016	CLA	4	0
20	A	827	CLA	3	0
20	B	826	CLA	1	0
20	7	1005	CLA	2	0
20	6	310	CLA	6	0
20	B	801	CLA	4	0
20	5	323	CLA	7	0
20	5	308	CLA	5	0
25	B	848	DGD	4	0
20	A	825	CLA	2	0
29	8	317	CHL	2	0
20	7	1008	CLA	1	0
24	B	844	BCR	2	0
20	F	305	CLA	1	0
24	3	1004	BCR	3	0
20	G	201	CLA	3	0
20	B	824	CLA	3	0
20	B	838	CLA	2	0
20	0	309	CLA	4	0
20	8	310	CLA	1	0
20	1	1011	CLA	5	0
20	6	305	CLA	2	0
29	1	1015	CHL	12	0
28	1	1016	LUT	2	0
29	8	314	CHL	3	0
20	5	307	CLA	2	0
20	5	309	CLA	5	0
20	8	308	CLA	2	0
20	3	1008	CLA	2	0
20	5	301	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	849	LHG	2	0
28	3	1001	LUT	3	0
29	7	1013	CHL	3	0
27	0	303	LMG	27	0
30	8	304	XAT	1	0
29	6	317	CHL	4	0
20	5	312	CLA	15	0
29	4	312	CHL	1	0
20	A	826	CLA	2	0
24	B	846	BCR	1	0
20	G	203	CLA	8	0
20	6	311	CLA	2	0
20	B	817	CLA	9	0
20	5	315	CLA	7	0
29	6	314	CHL	4	0
24	7	1003	BCR	2	0
20	B	839	CLA	1	0
24	B	804	BCR	5	0
20	5	304	CLA	5	0
28	5	302	LUT	6	0
20	A	824	CLA	5	0
20	3	1011	CLA	1	0
23	A	843	LHG	2	0
20	A	828	CLA	2	0
21	A	841	SF4	1	0
20	B	808	CLA	7	0
20	4	311	CLA	7	0
28	7	1001	LUT	4	0
20	A	804	CLA	3	0
20	F	303	CLA	1	0
28	6	303	LUT	3	0
20	A	852	CLA	5	0
20	B	840	CLA	3	0
20	5	310	CLA	7	0
20	B	813	CLA	9	0
23	7	1016	LHG	6	0
20	A	801	CLA	8	0
20	A	816	CLA	1	0
29	7	1012	CHL	5	0
20	K	201	CLA	5	0
20	A	817	CLA	5	0
20	1	1006	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	1015	CLA	2	0
20	0	305	CLA	3	0
20	A	834	CLA	1	0
20	3	1007	CLA	2	0
20	B	836	CLA	4	0
20	A	823	CLA	3	0
20	8	312	CLA	2	0
20	5	305	CLA	1	0
20	A	833	CLA	6	0
20	B	833	CLA	2	0
20	3	1006	CLA	2	0
20	B	821	CLA	5	0
24	A	844	BCR	7	0
20	A	802	CLA	5	0
20	B	819	CLA	3	0
20	6	307	CLA	1	0
22	A	842	PQN	3	0
24	I	201	BCR	17	0
26	B	849	LMT	3	0
30	5	303	XAT	6	0
20	8	316	CLA	1	0
20	B	822	CLA	2	0
20	8	305	CLA	2	0
20	0	307	CLA	1	0
20	7	1006	CLA	2	0
24	A	845	BCR	3	0
24	1	1001	BCR	7	0
29	4	315	CHL	13	0
20	3	1005	CLA	4	0
20	A	851	CLA	3	0
20	B	830	CLA	3	0
20	0	316	CLA	4	0
29	3	1014	CHL	1	0
26	3	1018	LMT	8	0
20	4	309	CLA	1	0
20	A	808	CLA	1	0
20	B	835	CLA	2	0
24	B	843	BCR	12	0
20	0	313	CLA	3	0
28	3	1002	LUT	2	0
29	5	316	CHL	4	0
20	B	823	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	1	1002	LUT	16	0
24	4	302	BCR	4	0
29	1	1012	CHL	4	0
20	A	837	CLA	2	0
20	1	1009	CLA	1	0
28	0	304	LUT	10	0
21	C	1002	SF4	2	0
29	1	1013	CHL	2	0
20	7	1011	CLA	1	0
24	6	302	BCR	14	0
20	7	1014	CLA	3	0
20	B	831	CLA	6	0
20	A	829	CLA	1	0
24	F	301	BCR	6	0
20	A	840	CLA	9	0
20	B	811	CLA	2	0
20	7	1007	CLA	2	0
20	1	1007	CLA	6	0
20	8	309	CLA	4	0
20	B	816	CLA	4	0
20	A	838	CLA	4	0
24	A	850	BCR	6	0
24	B	845	BCR	8	0
28	4	317	LUT	2	0
22	B	842	PQN	3	0
27	8	319	LMG	6	0
20	4	304	CLA	1	0
20	7	1010	CLA	6	0
29	0	317	CHL	5	0
20	8	311	CLA	8	0
20	B	803	CLA	1	0
24	G	204	BCR	7	0
20	A	835	CLA	4	0
20	3	1017	CLA	1	0
20	A	819	CLA	2	0
20	6	309	CLA	2	0
24	B	847	BCR	3	0
29	5	317	CHL	9	0
20	A	820	CLA	2	0
23	3	1019	LHG	5	0
27	5	324	LMG	7	0
20	B	802	CLA	1	0

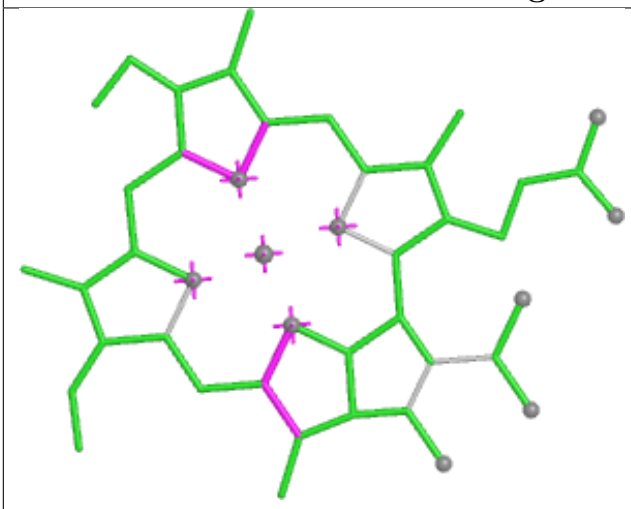
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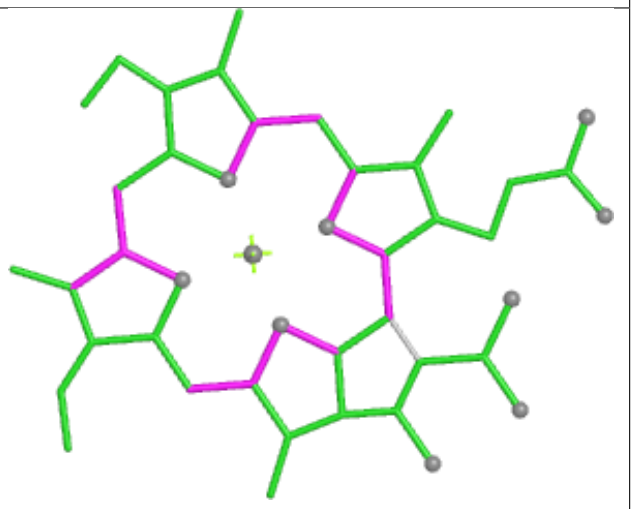
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	829	CLA	5	0
20	A	813	CLA	5	0
20	A	807	CLA	1	0
20	A	811	CLA	1	0
20	A	814	CLA	1	0
20	4	310	CLA	5	0
20	0	311	CLA	3	0
20	5	306	CLA	2	0
29	5	314	CHL	2	0
20	B	825	CLA	3	0
20	L	203	CLA	1	0

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.

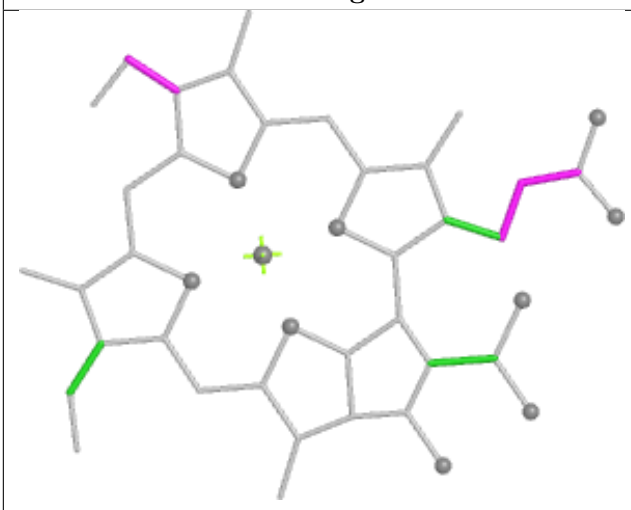
Ligand CLA 5 311



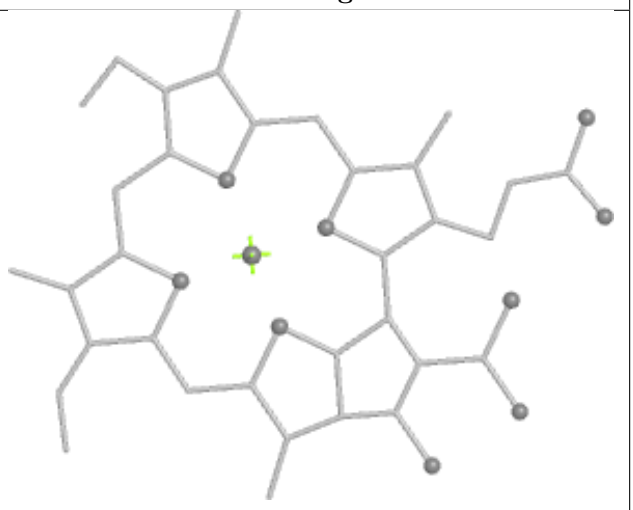
Bond lengths



Bond angles

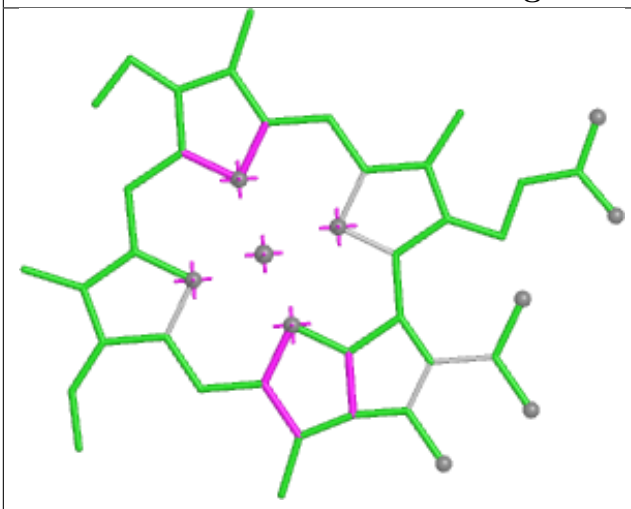


Torsions

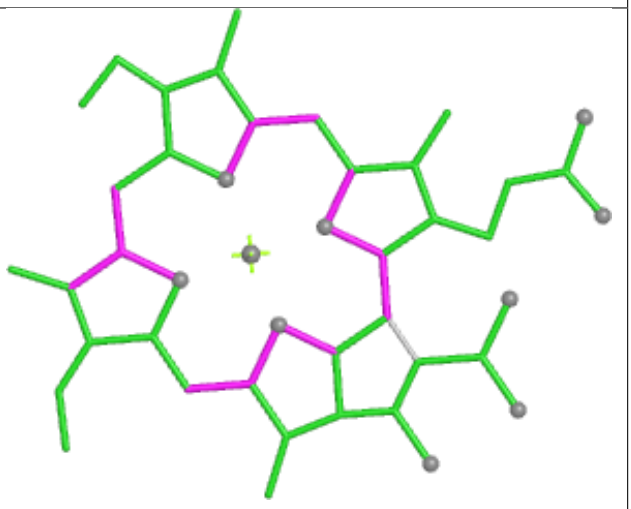


Rings

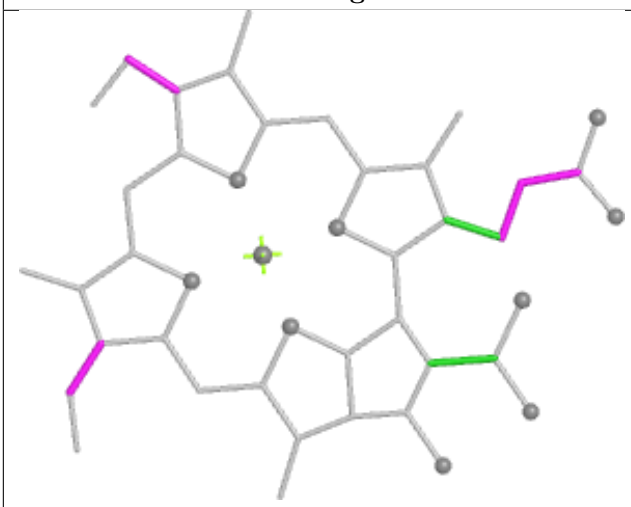
Ligand CLA A 836



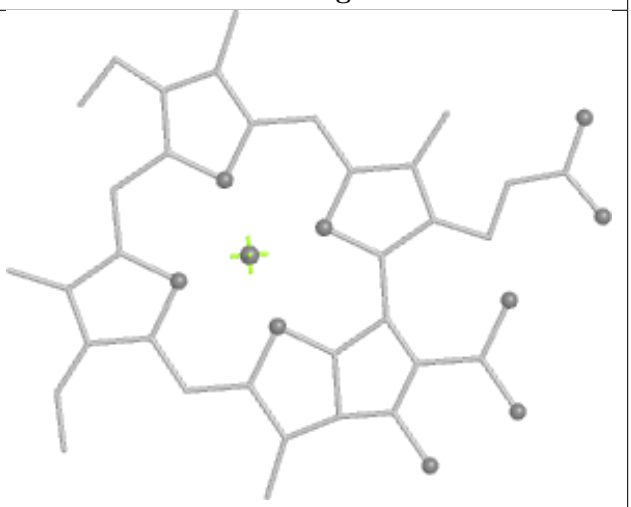
Bond lengths



Bond angles

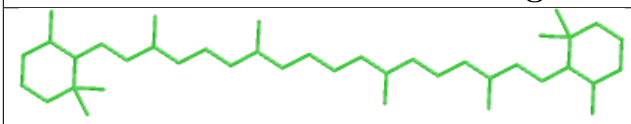


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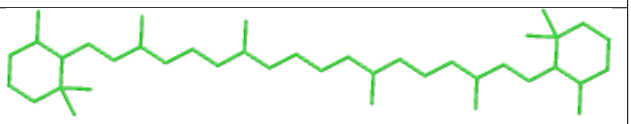


Rings

Ligand BCR J 103



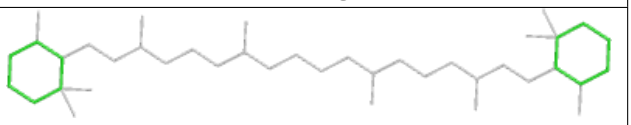
Bond lengths



Bond angles

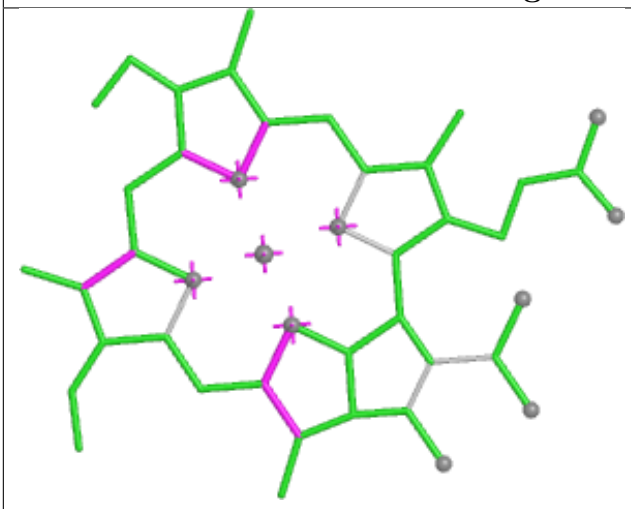


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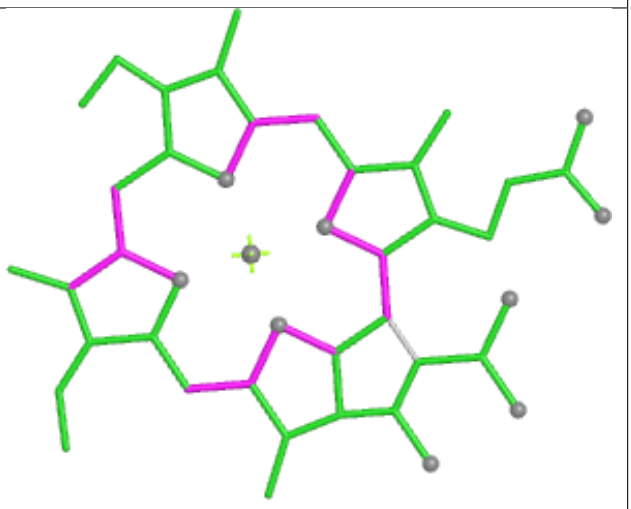


Rings

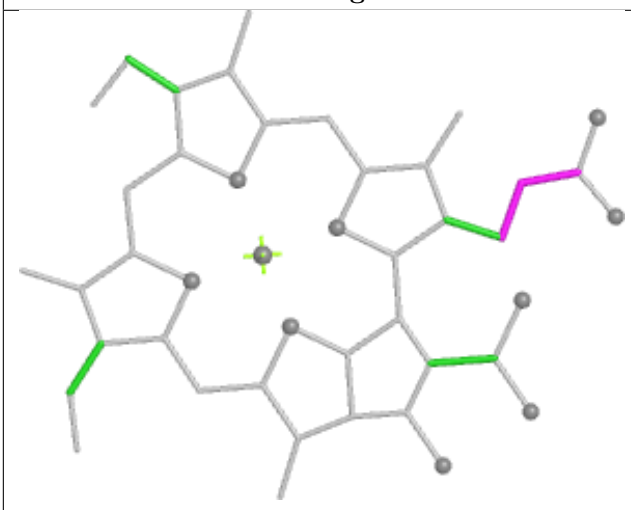
Ligand CLA A 830



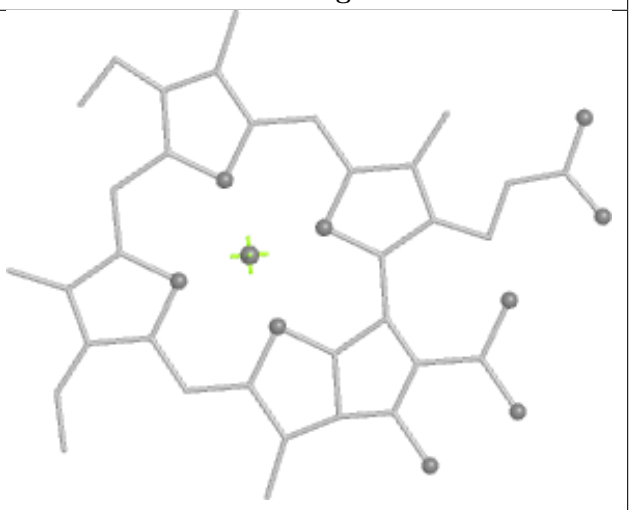
Bond lengths



Bond angles

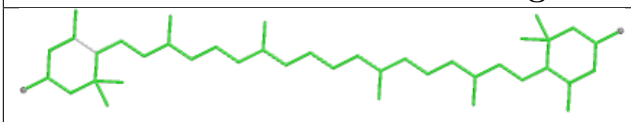


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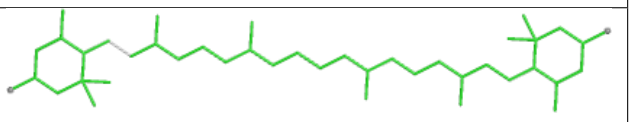


Rings

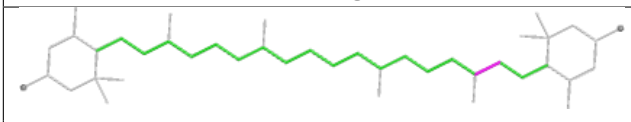
Ligand LUT 8 303



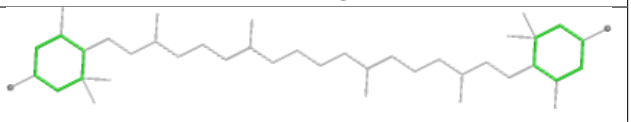
Bond lengths



Bond angles

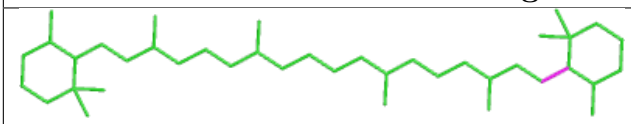


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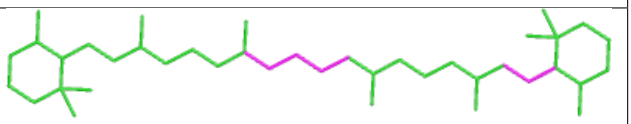


Rings

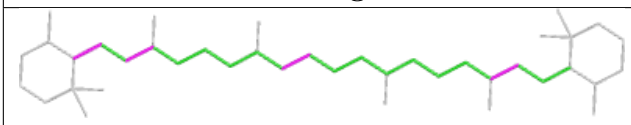
Ligand BCR G 205



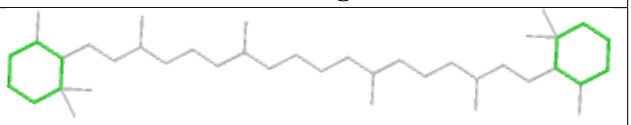
Bond lengths



Bond angles

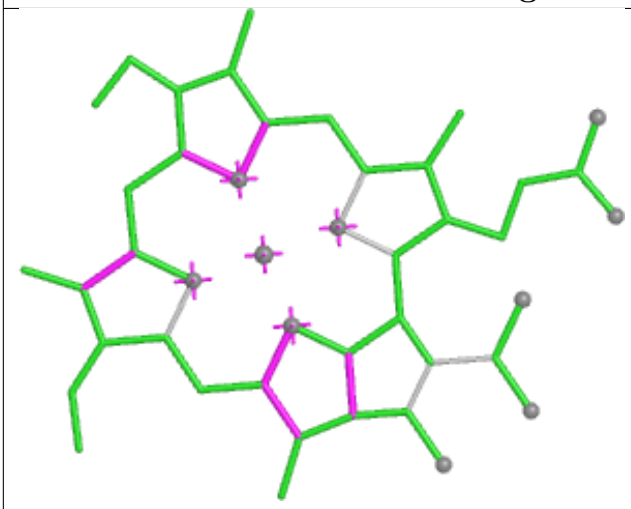


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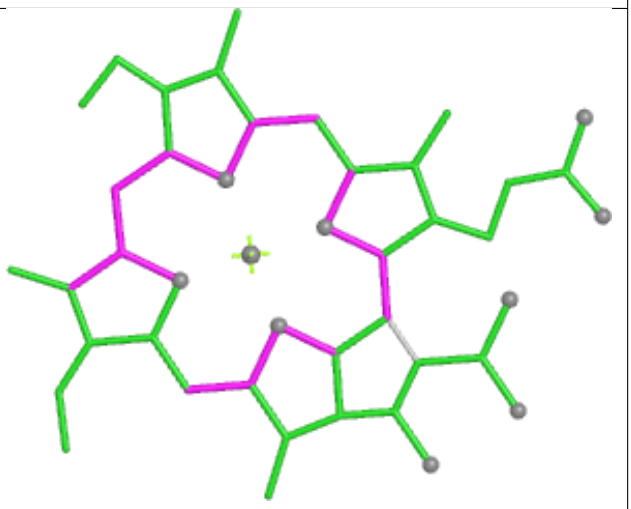


Rings

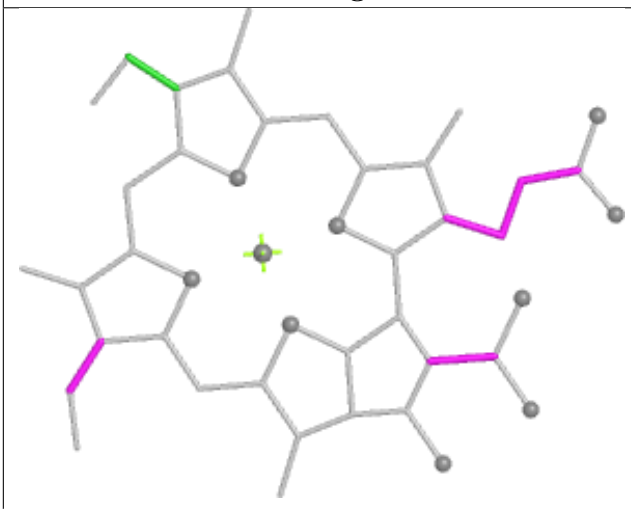
Ligand CLA 1 1008



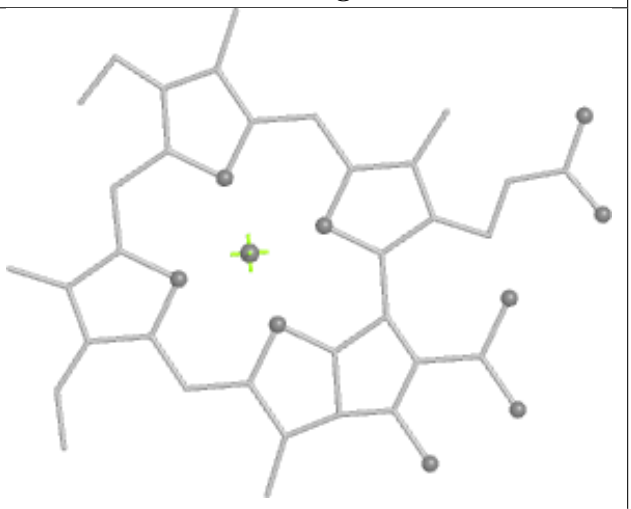
Bond lengths



Bond angles

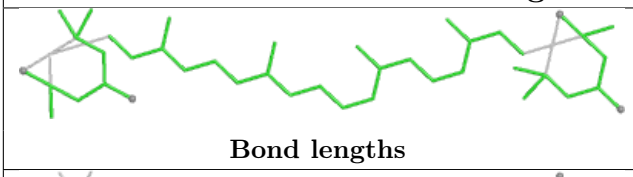


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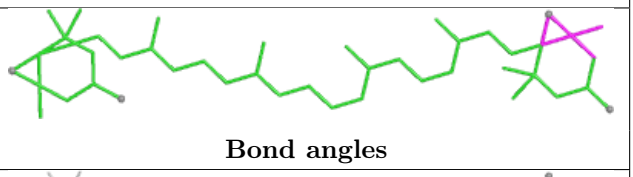


Rings

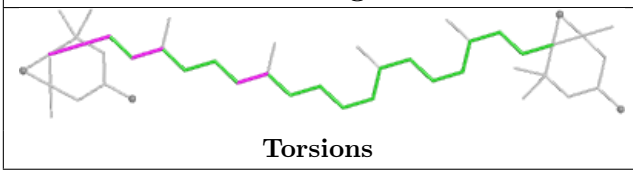
Ligand XAT 6 304



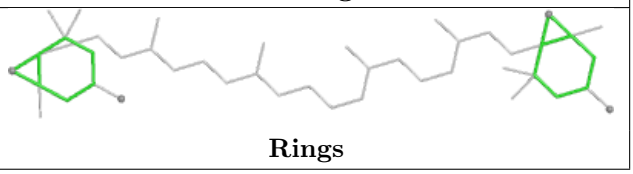
Bond lengths



Bond angles

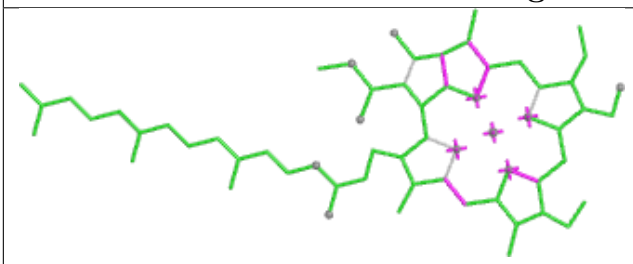


Torsions

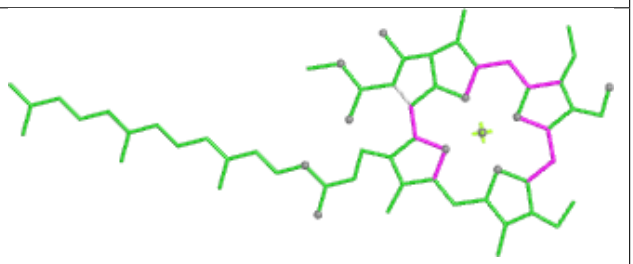


Rings

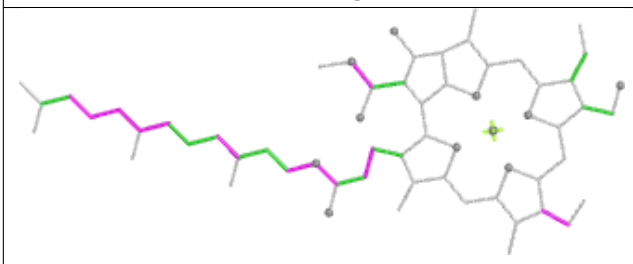
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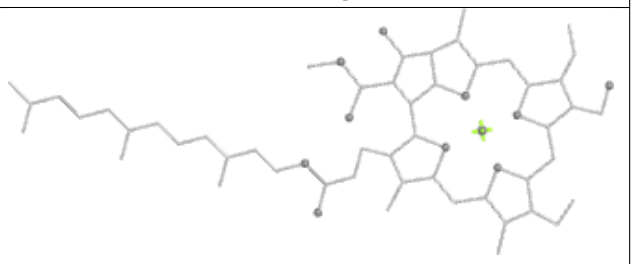
Bond lengths



Bond angles

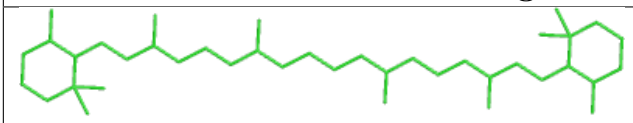


Torsions

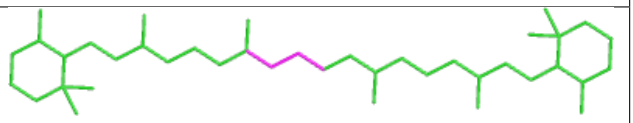


Rings

Ligand BCR 3 1003



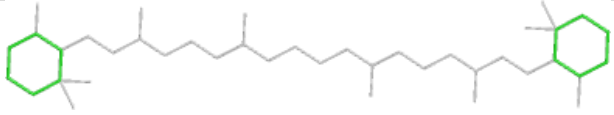
Bond lengths



Bond angles

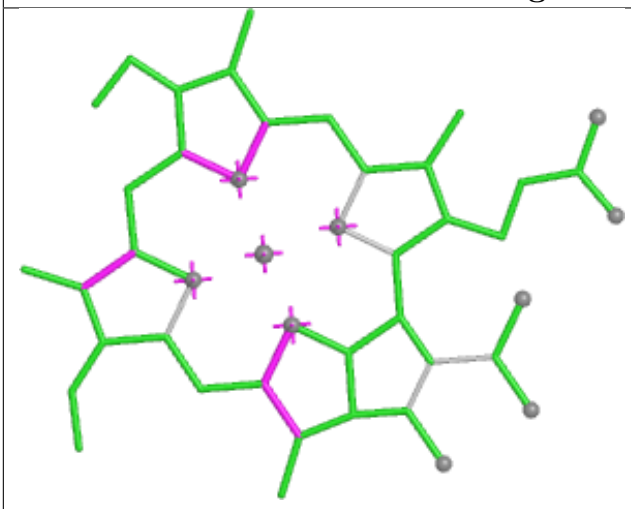


Torsions

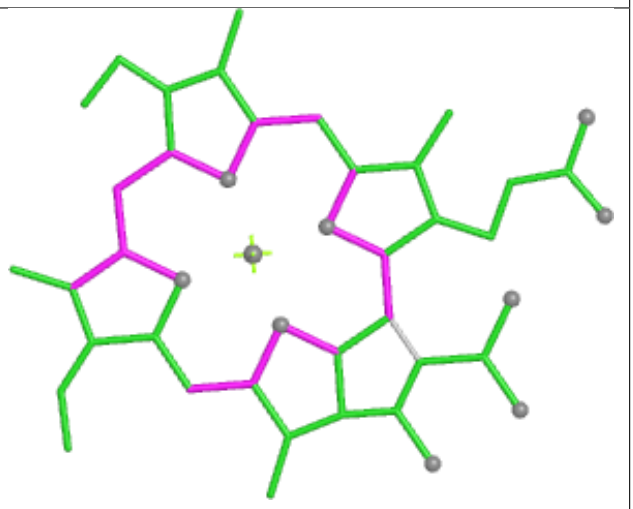


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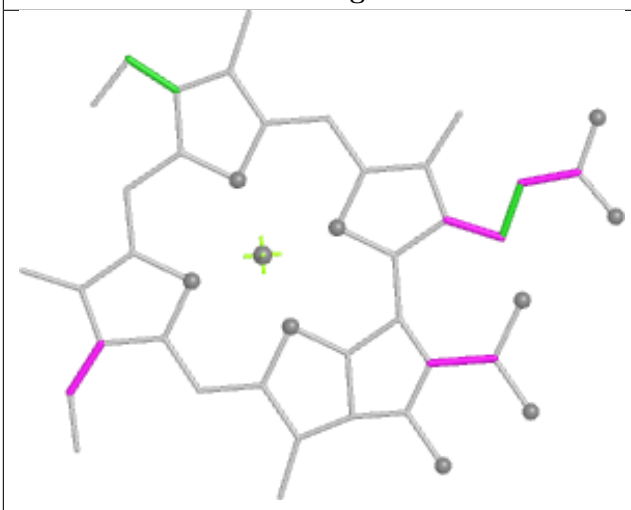
Ligand CLA 0 310



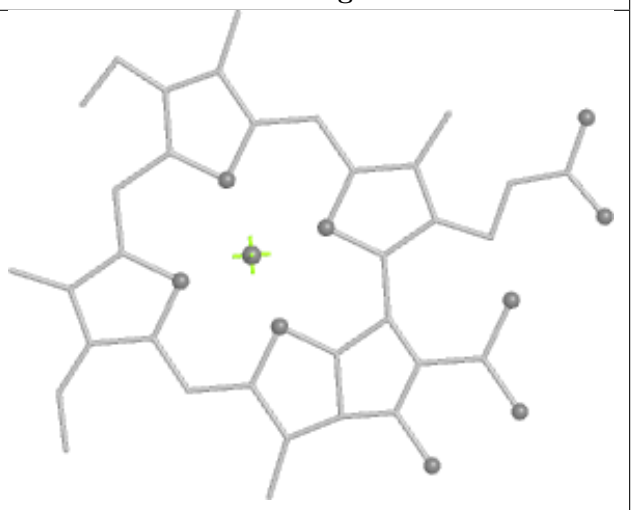
Bond lengths



Bond angles

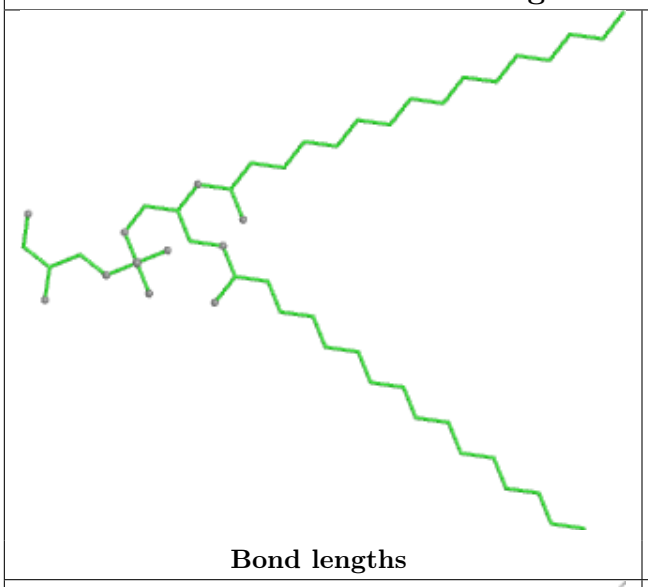


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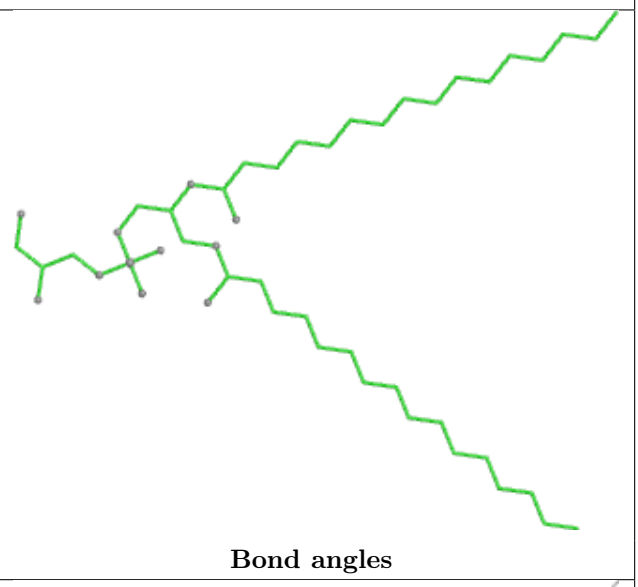


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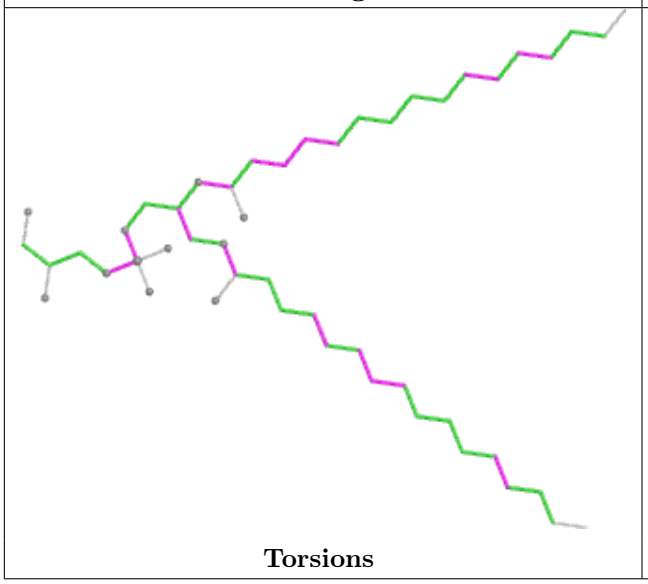
Ligand LHG 8 301



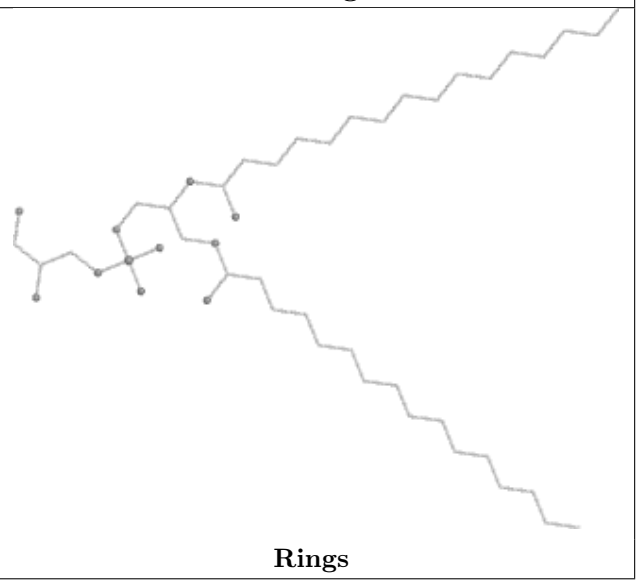
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Bond angles

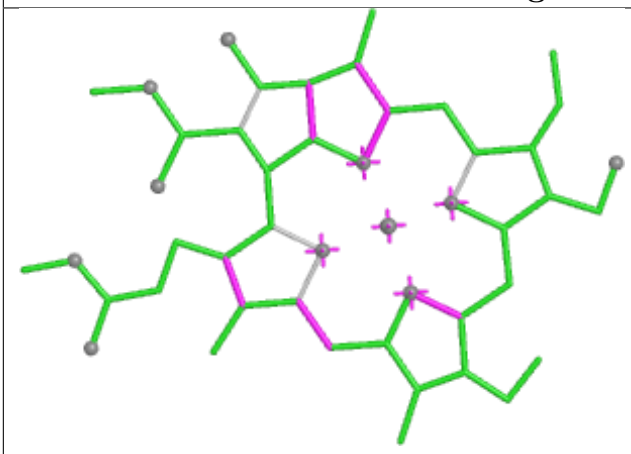


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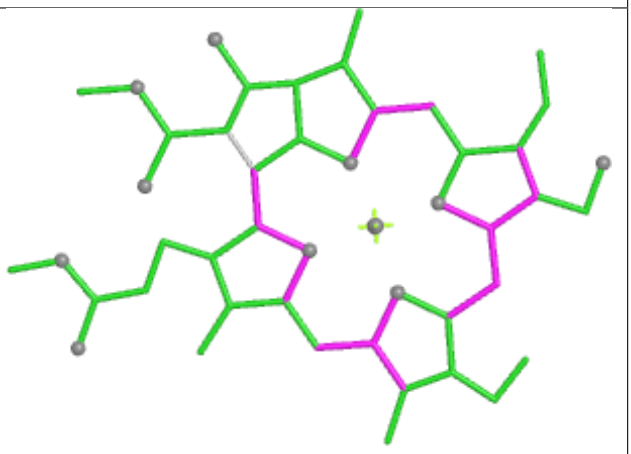


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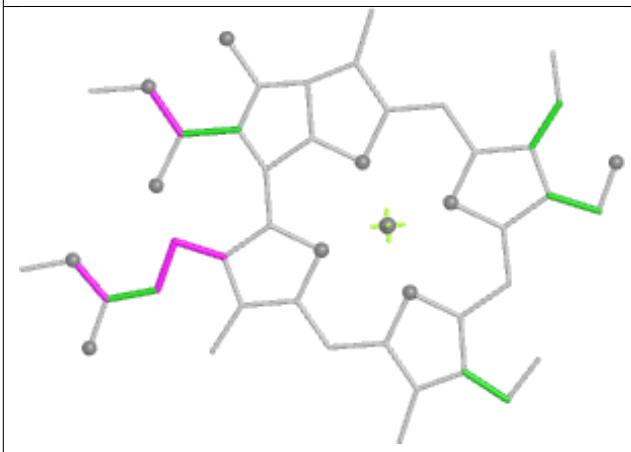
Ligand CHL 5 313



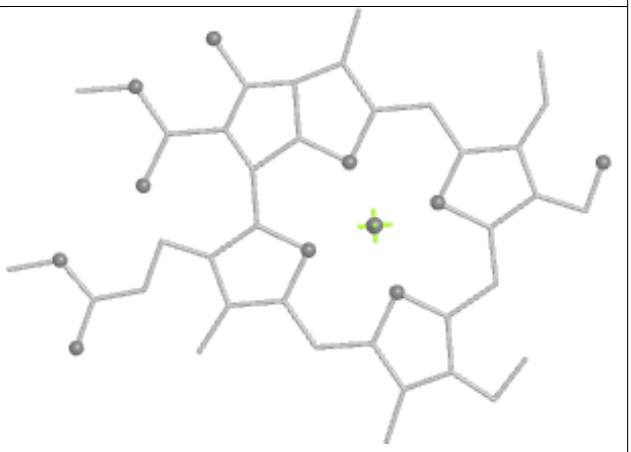
Bond lengths



Bond angles

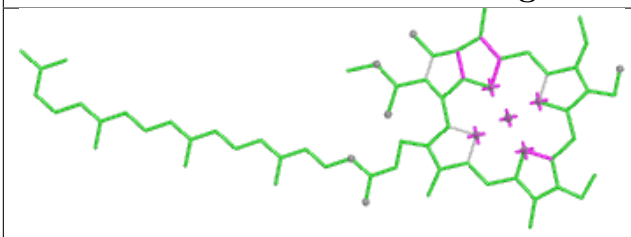


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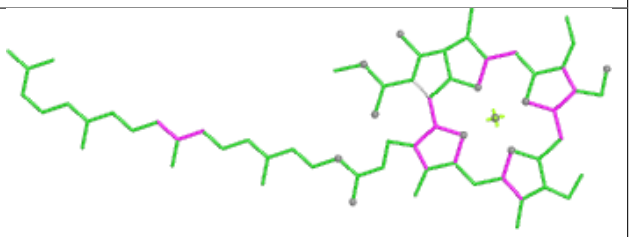


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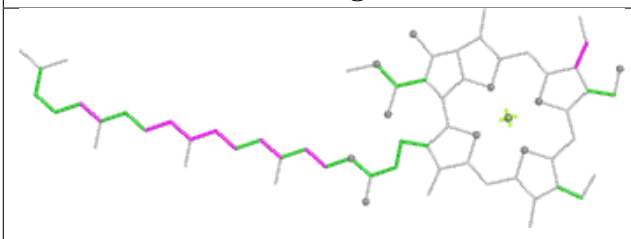
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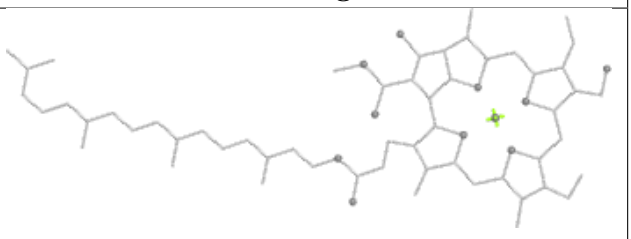
Bond lengths



Bond angles

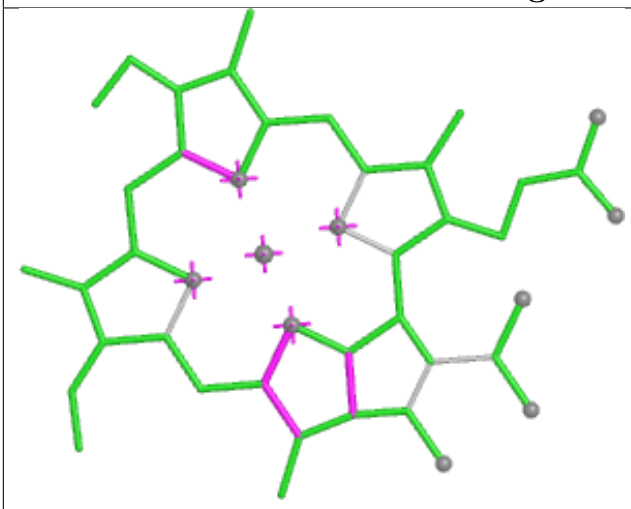


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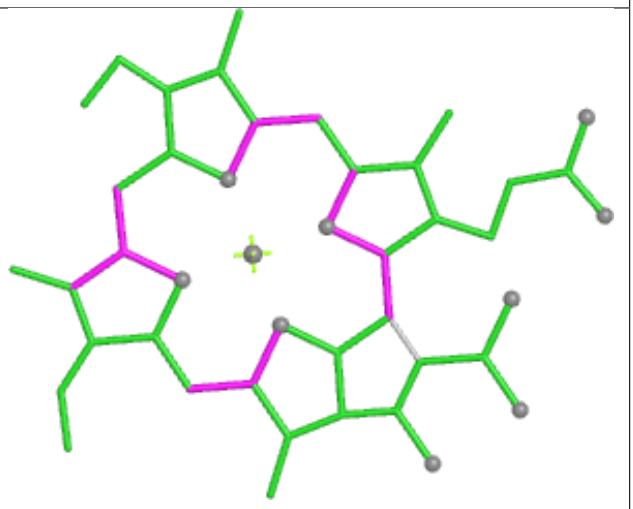


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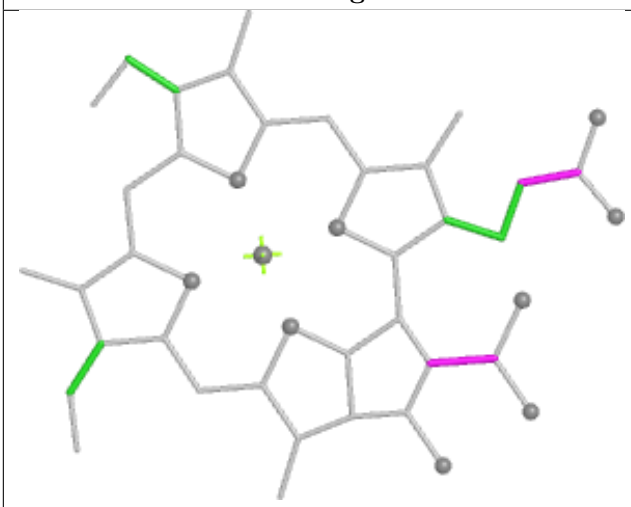
Ligand CLA 0 308



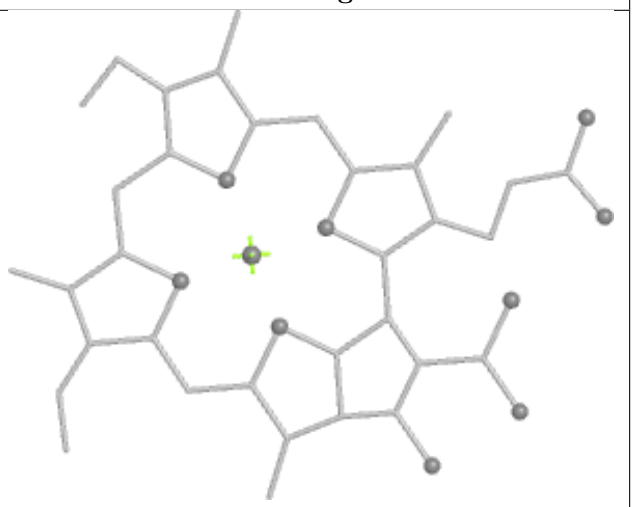
Bond lengths



Bond angles

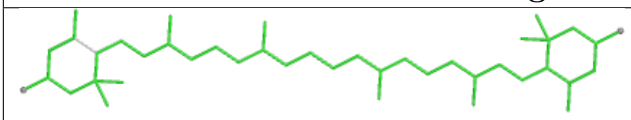


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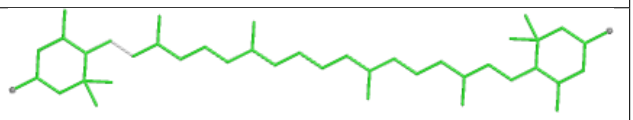


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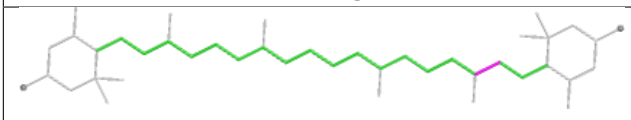
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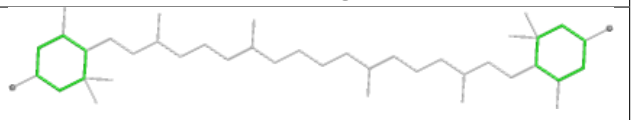
Bond lengths



Bond angles

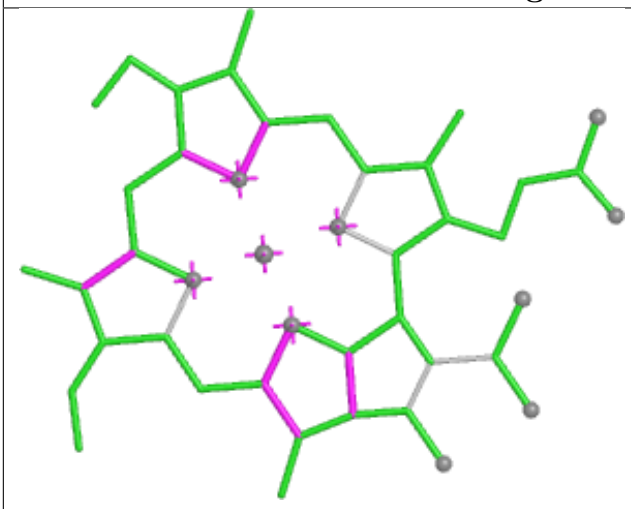


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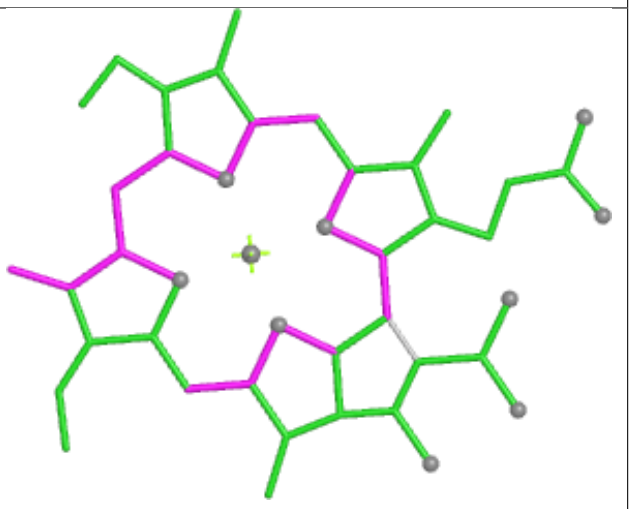


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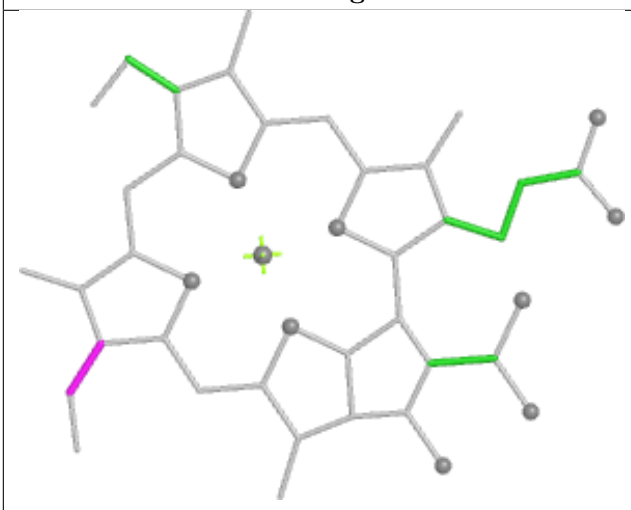
Ligand CLA F 302



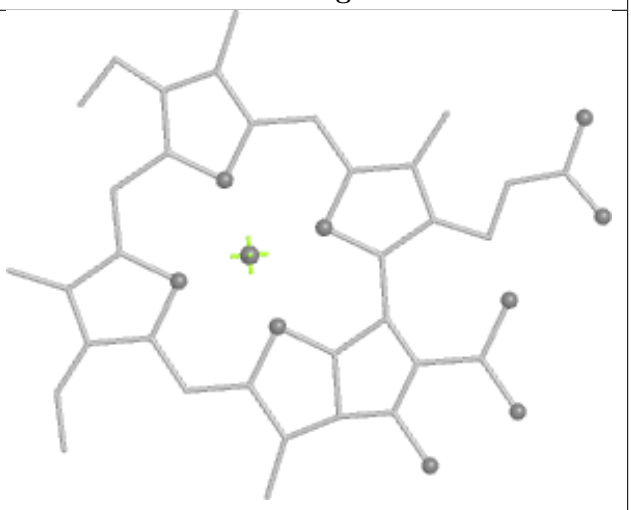
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Bond angles

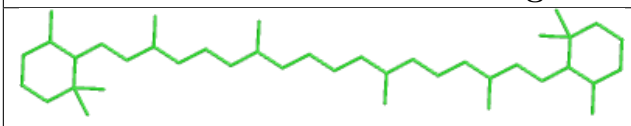


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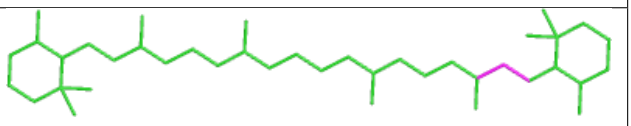


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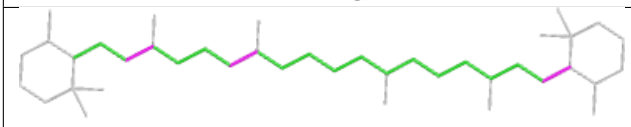
Ligand BCR 5 320



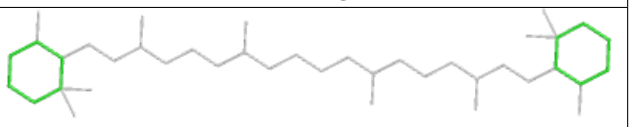
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Bond angles

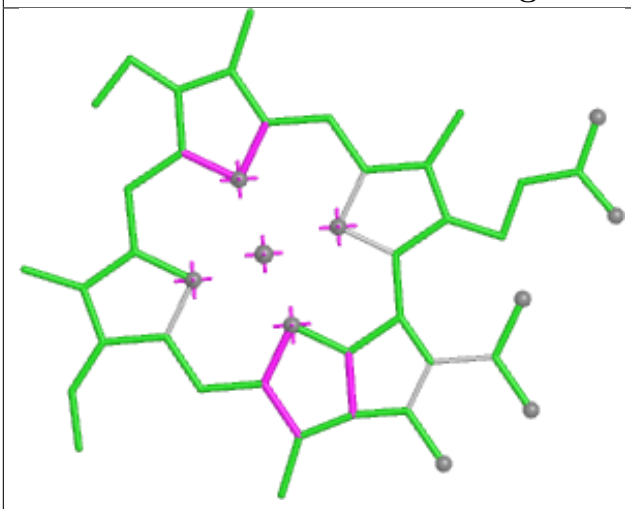


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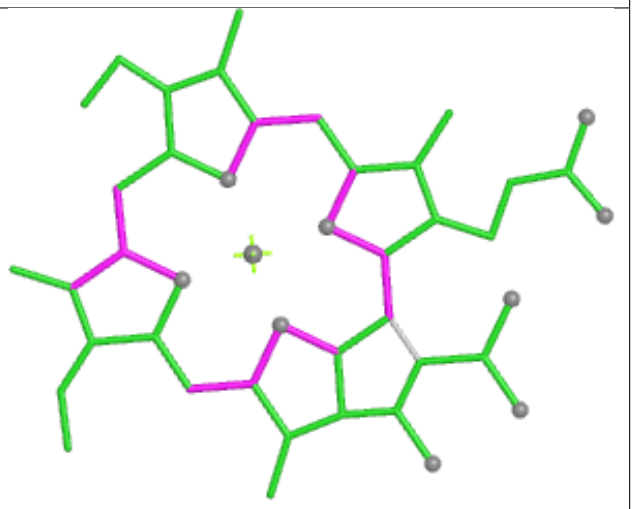


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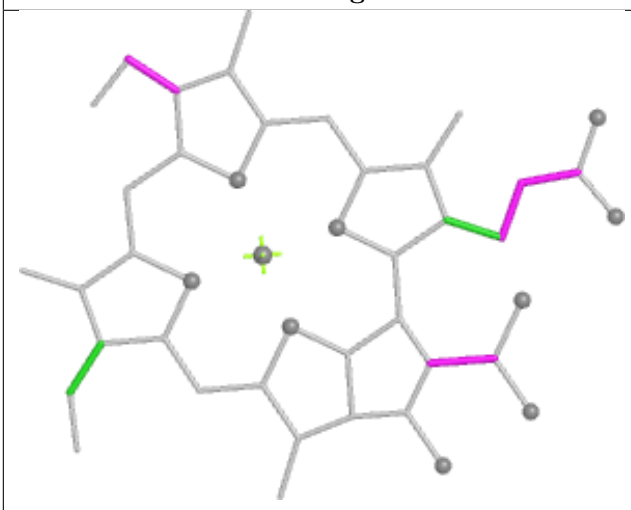
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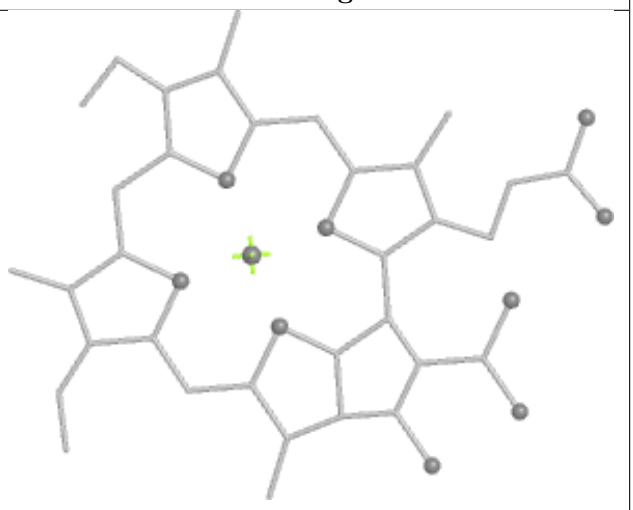
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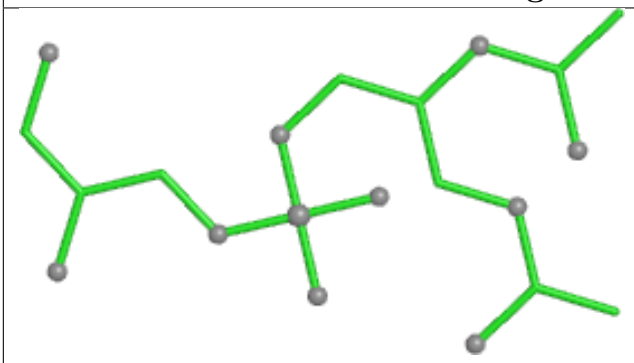


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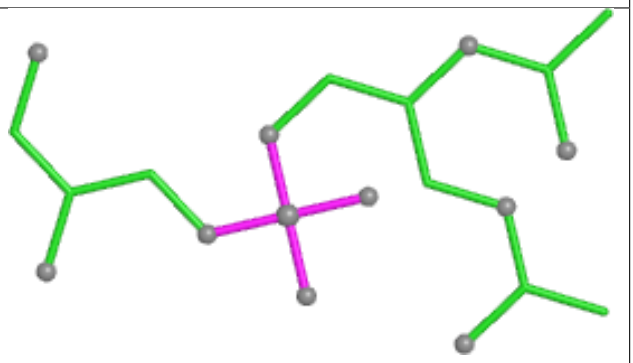


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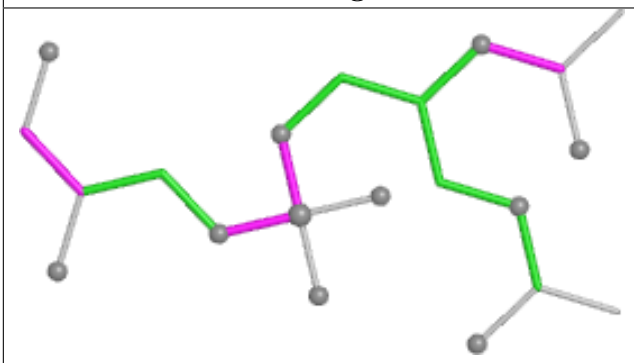
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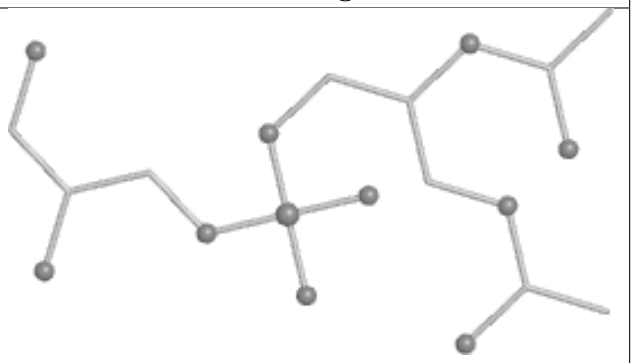
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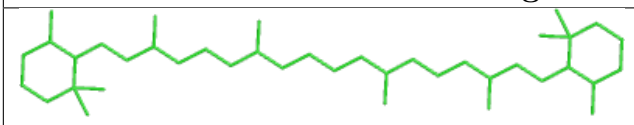


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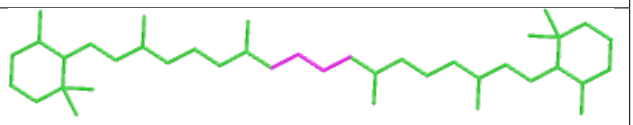


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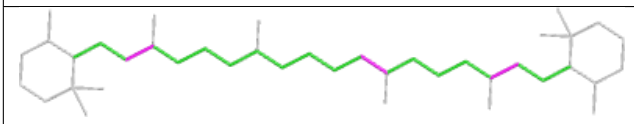
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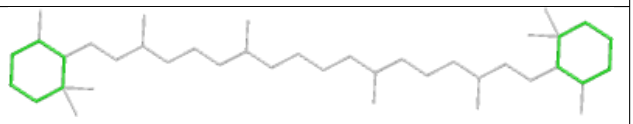
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Bond angles

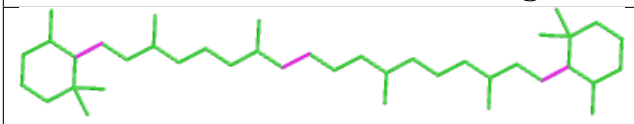


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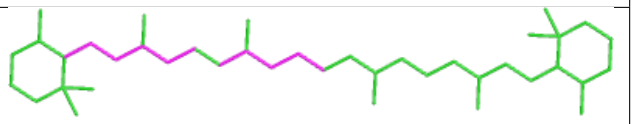


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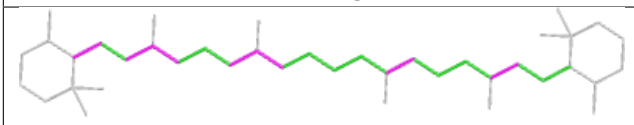
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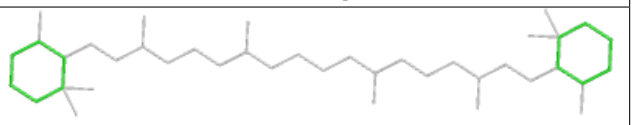
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Bond angles

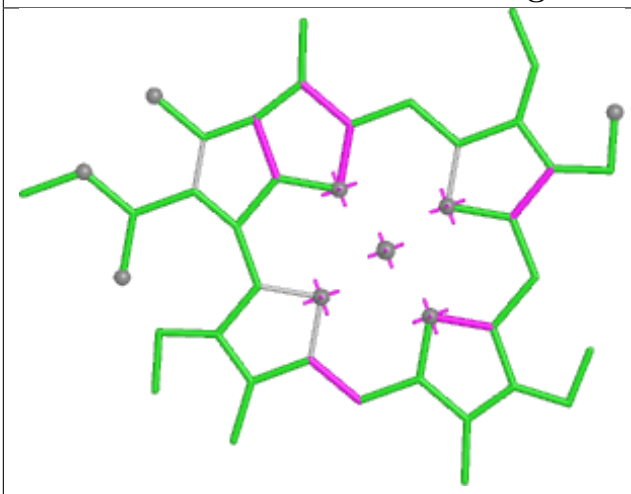


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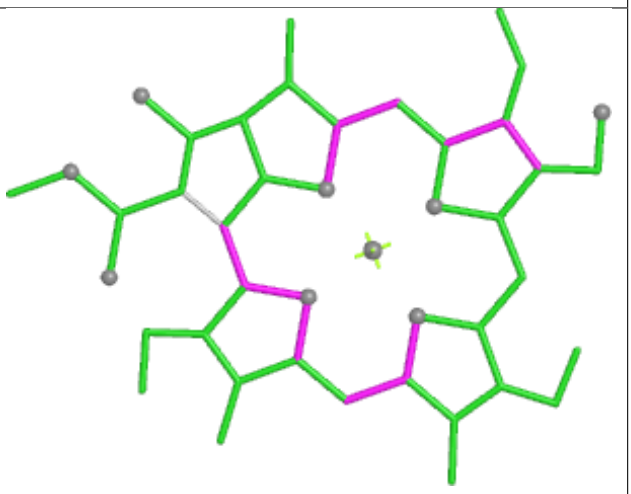


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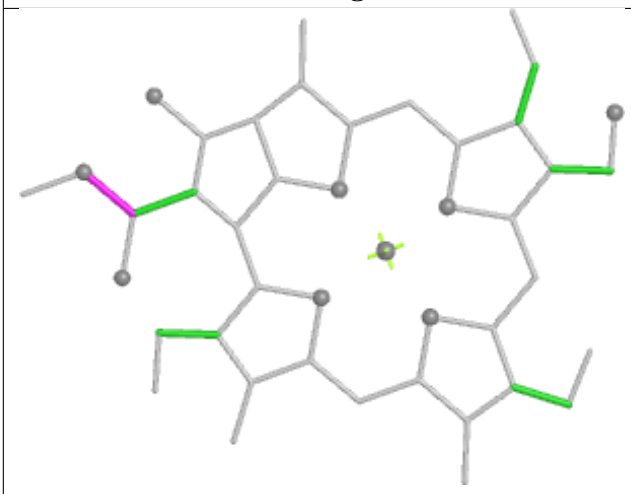
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Bond lengths



Bond angles

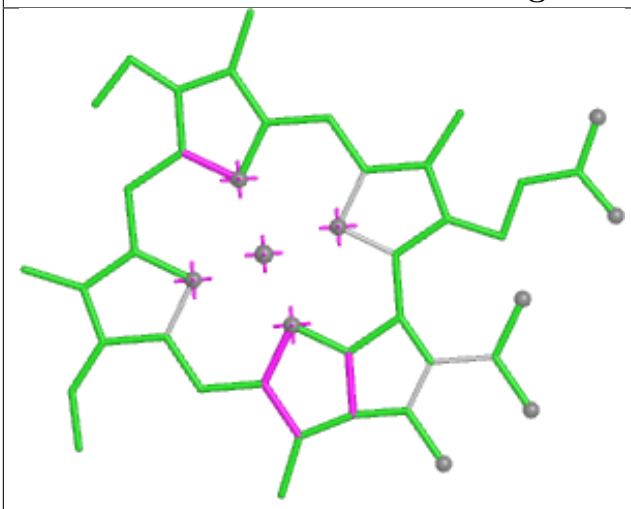


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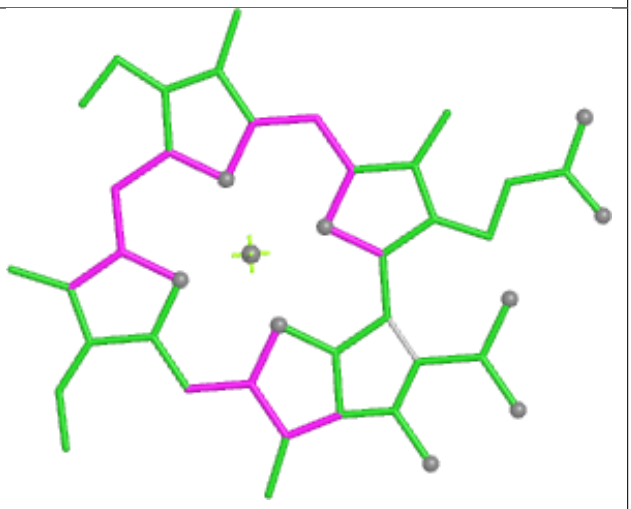


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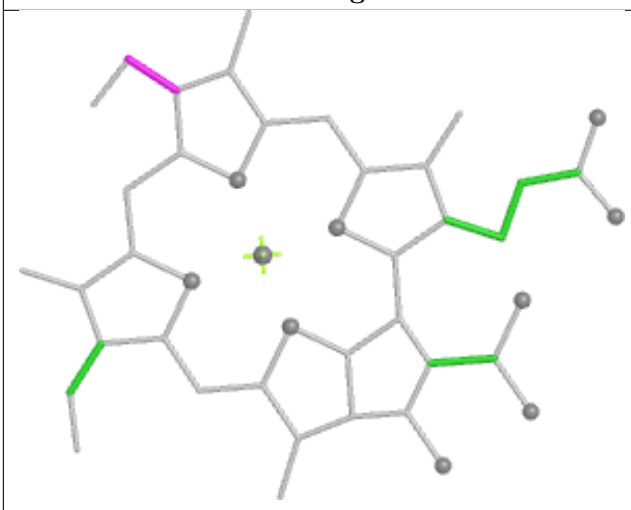
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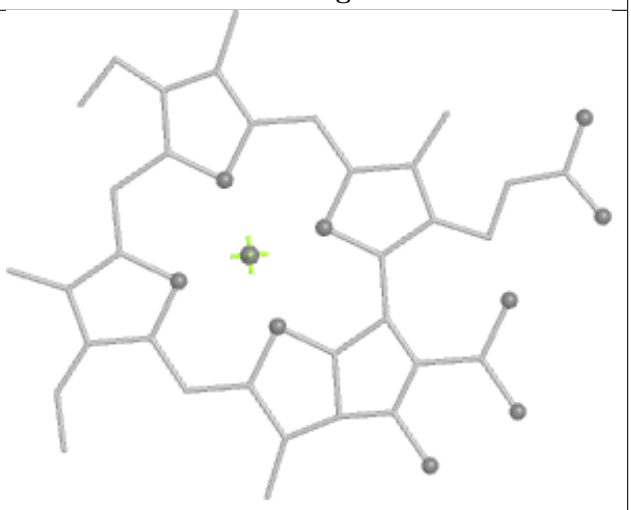
Bond lengths



Bond angles

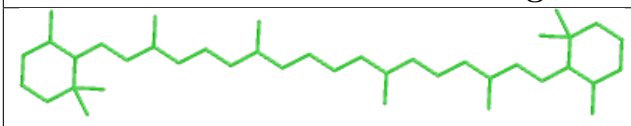


Torsions

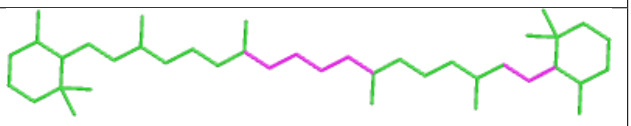


Rings

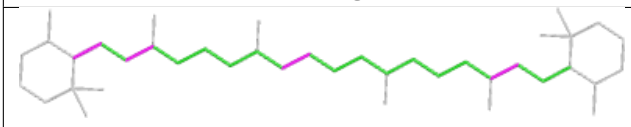
Ligand BCR 8 302



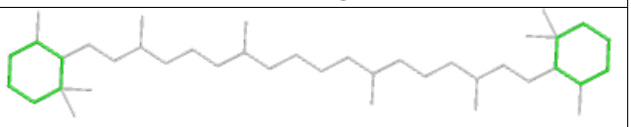
Bond lengths



Bond angles

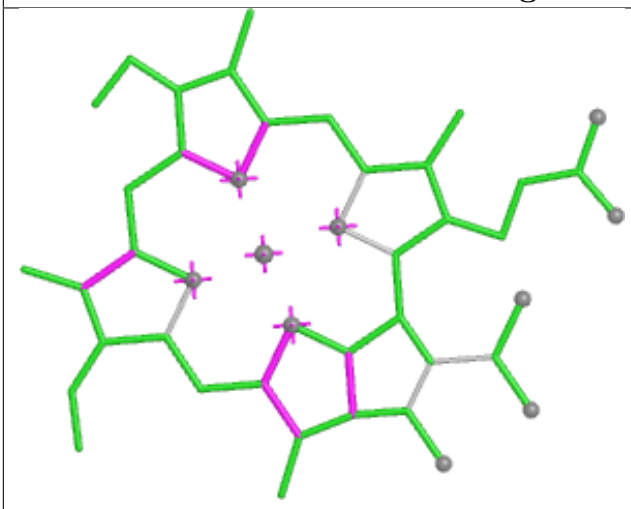


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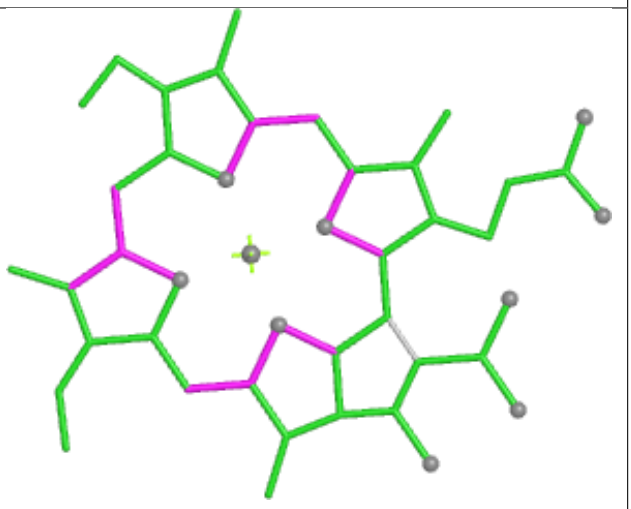


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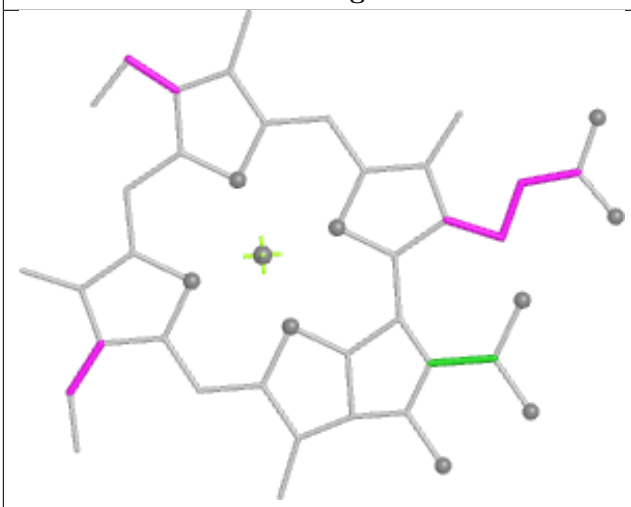
Ligand CLA 3 1009



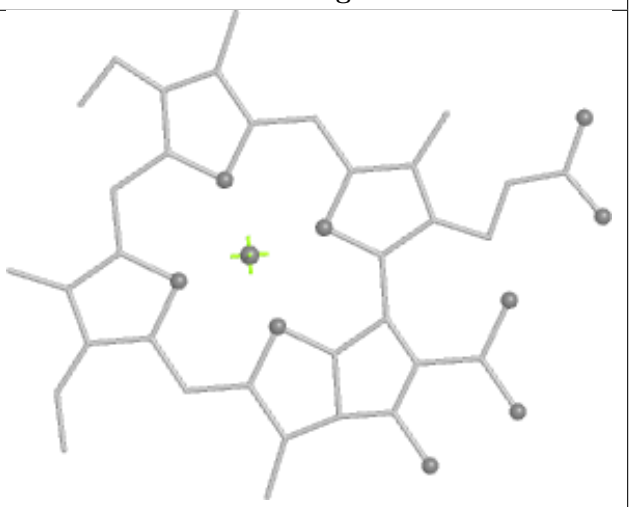
Bond lengths



Bond angles

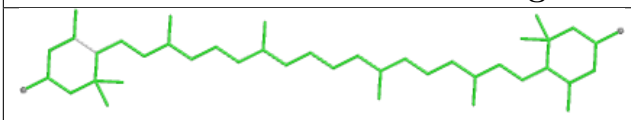


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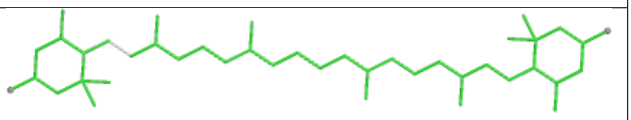


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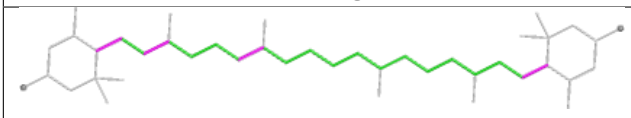
Ligand LUT J 104



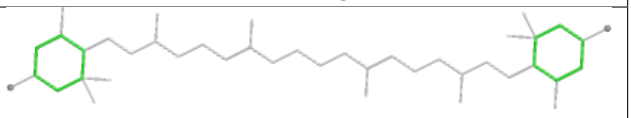
Bond lengths



Bond angles

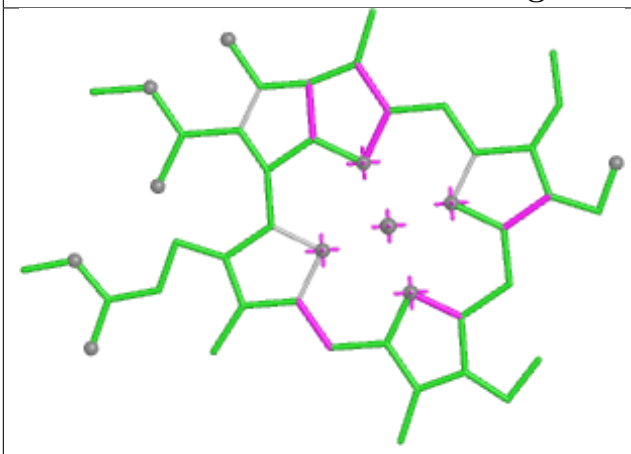


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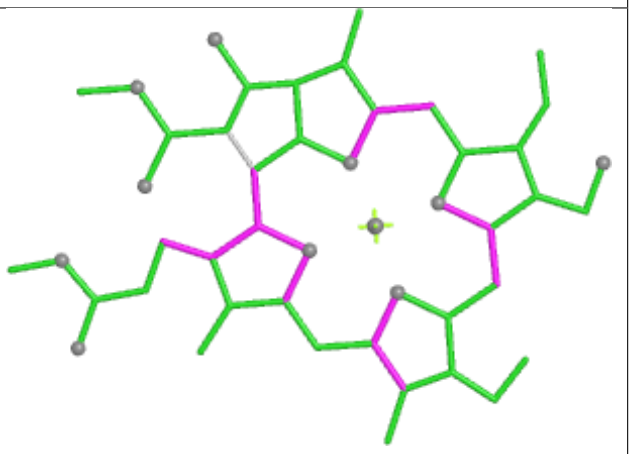


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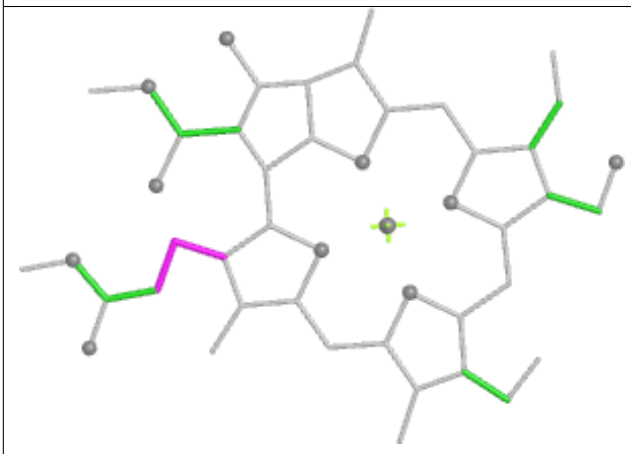
Ligand CHL 0 314



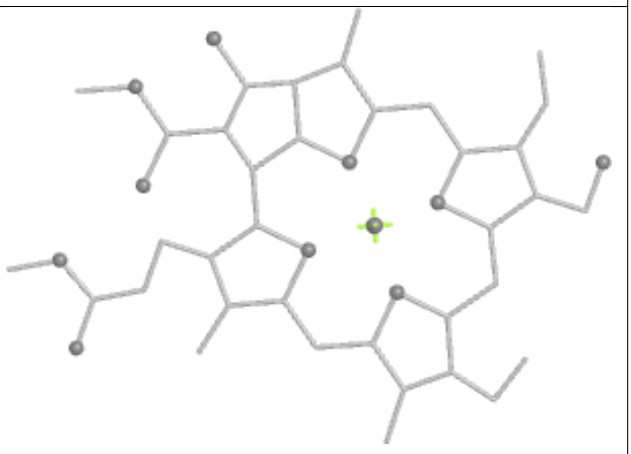
Bond lengths



Bond angles

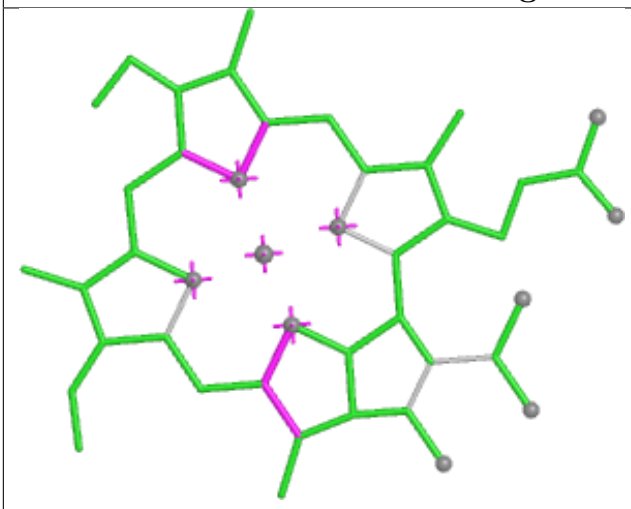


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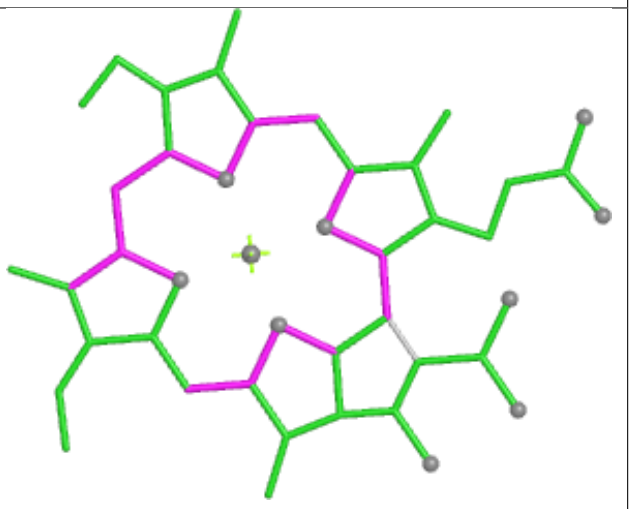


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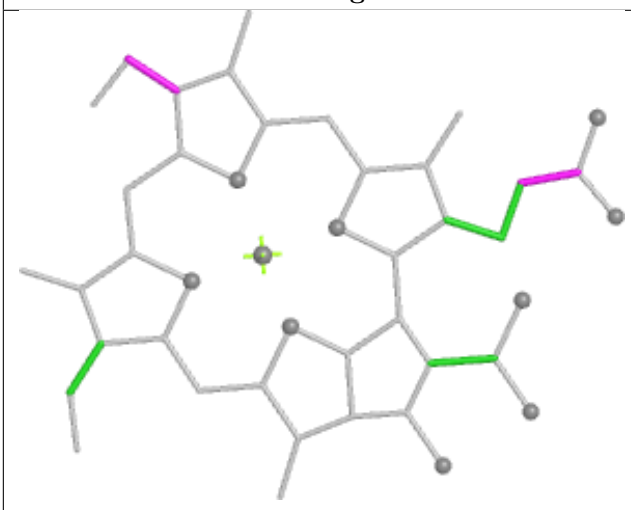
Ligand CLA 1 1017



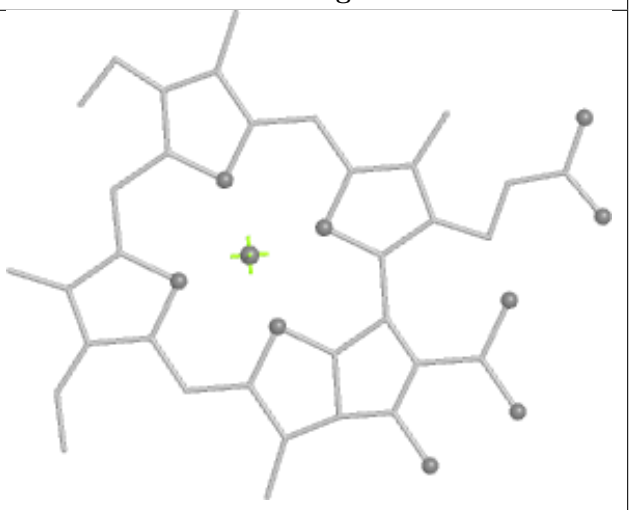
Bond lengths



Bond angles

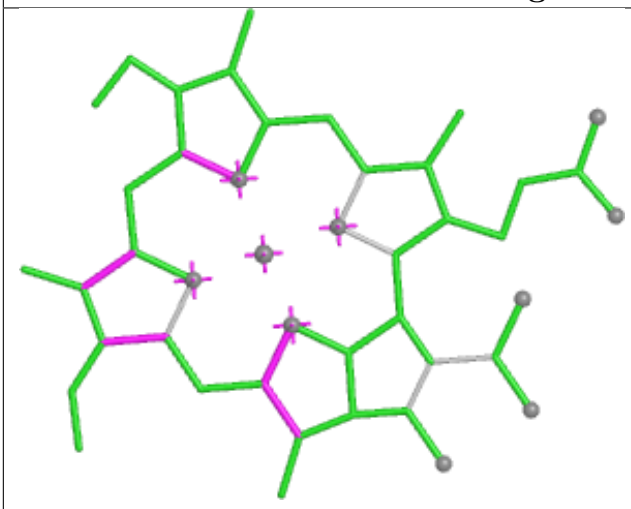


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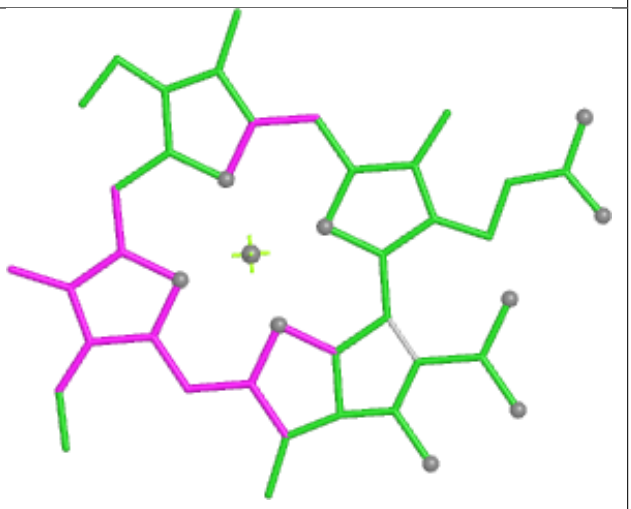


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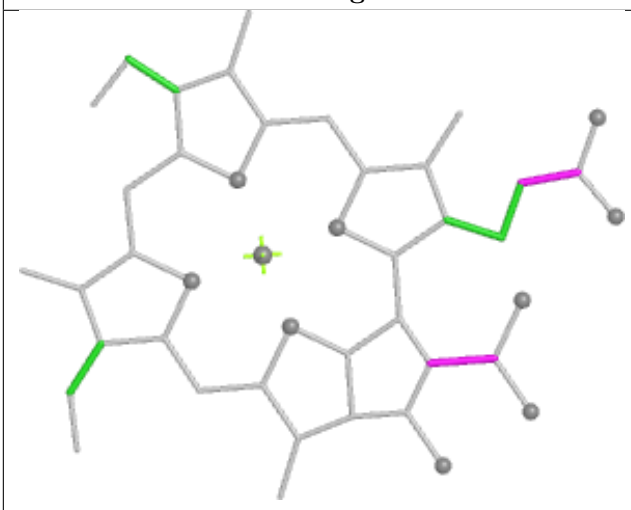
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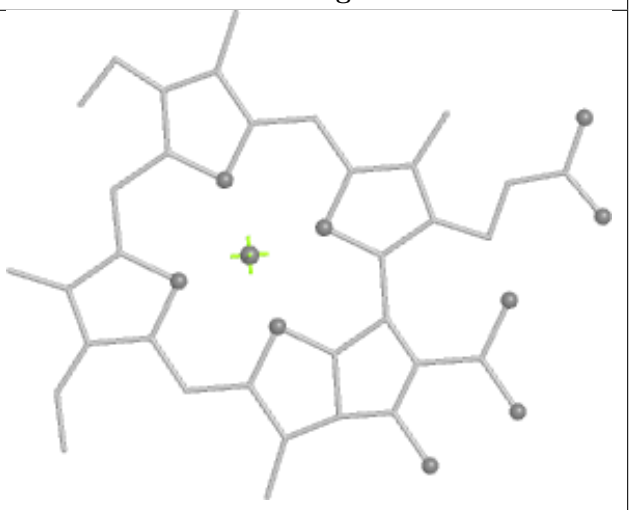
Bond lengths



Bond angles

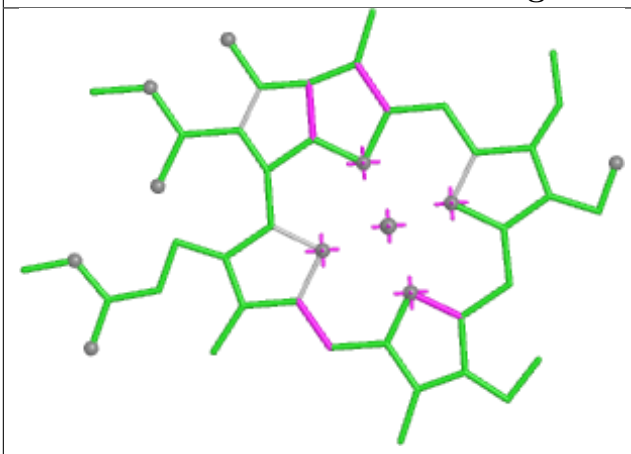


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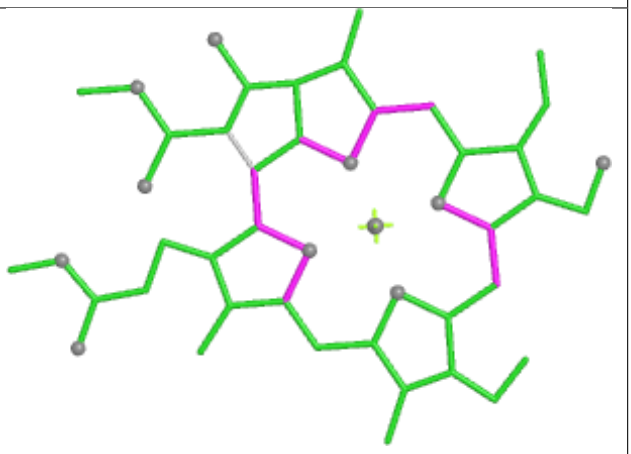


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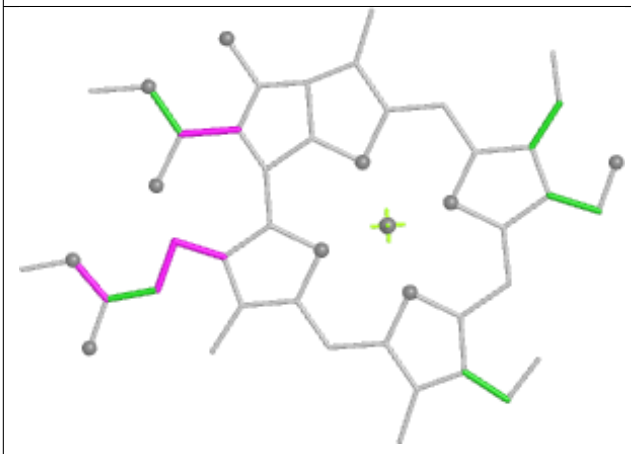
Ligand CHL 6 313



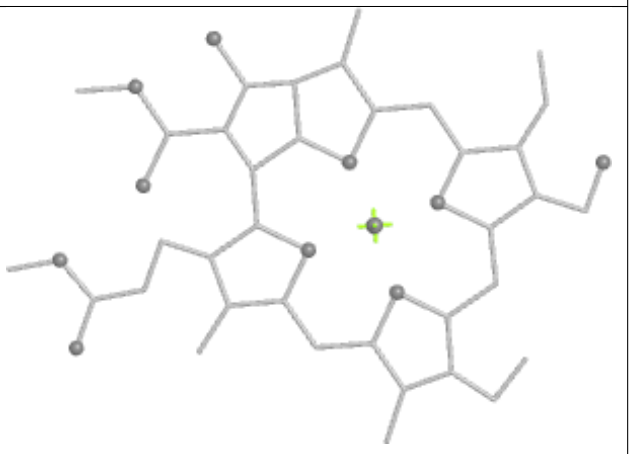
Bond lengths



Bond angles

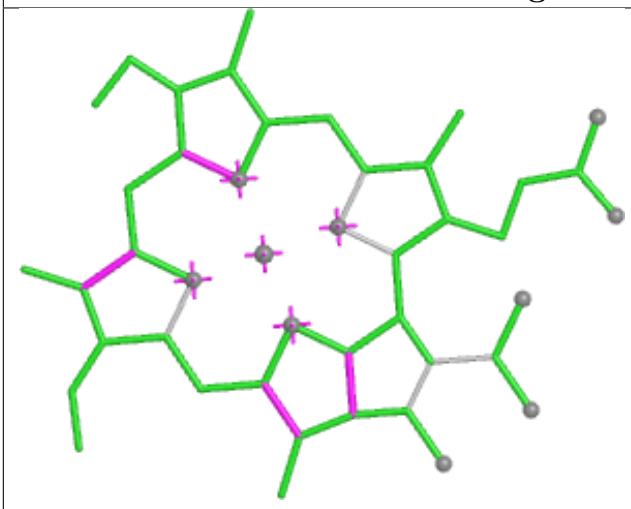


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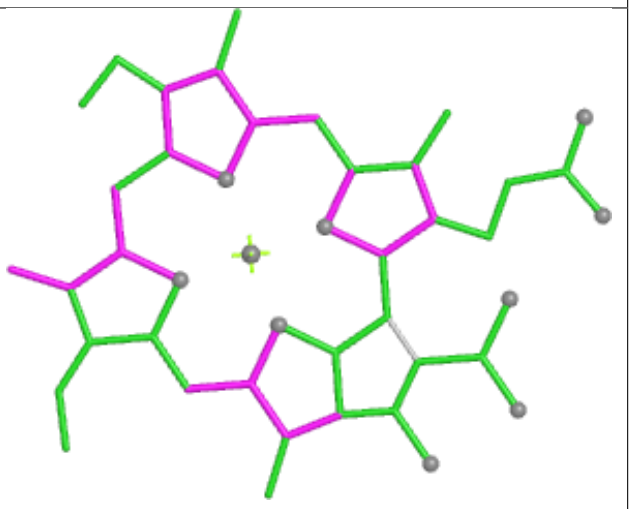


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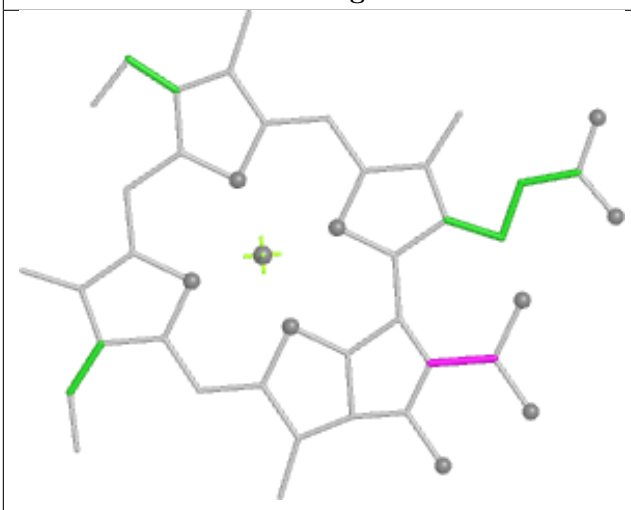
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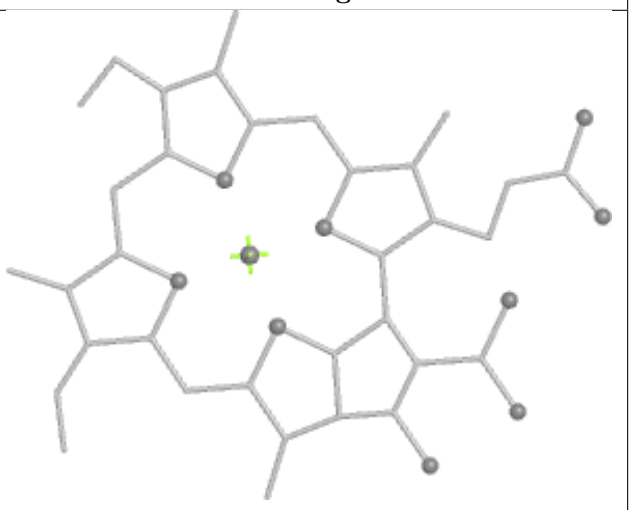
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Bond angles

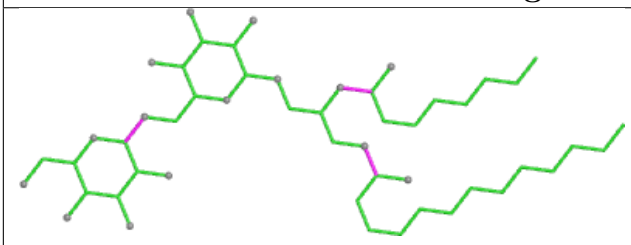


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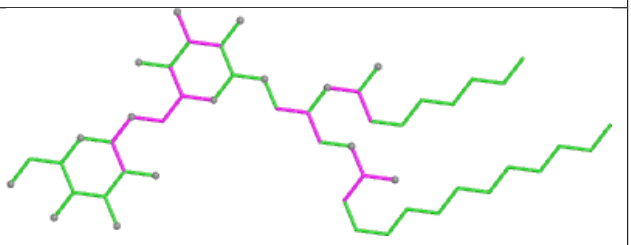


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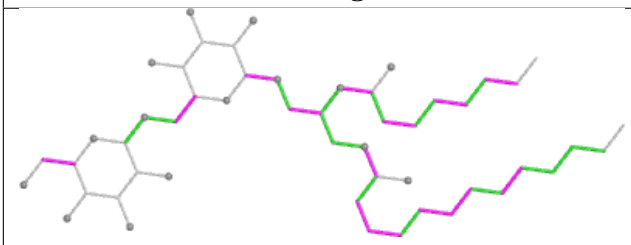
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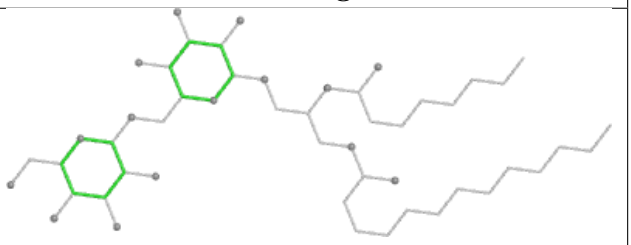
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Bond angles

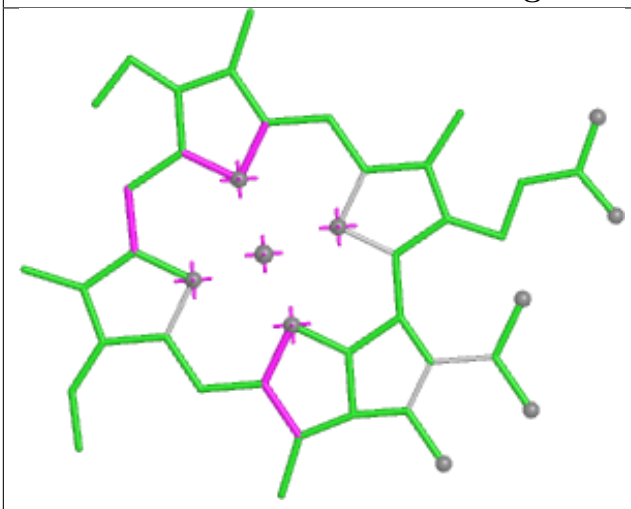


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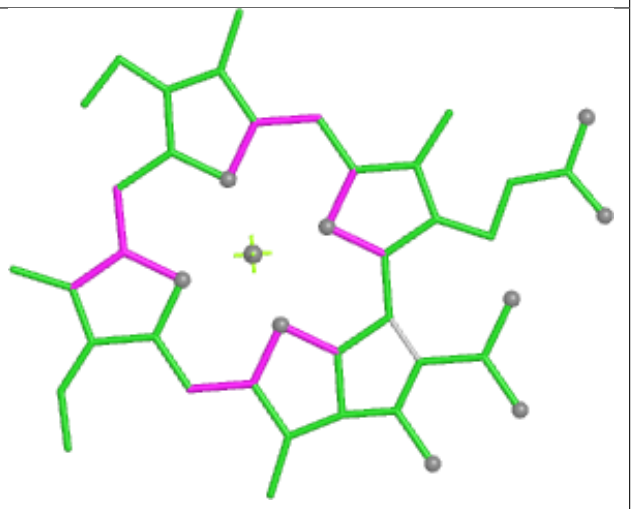


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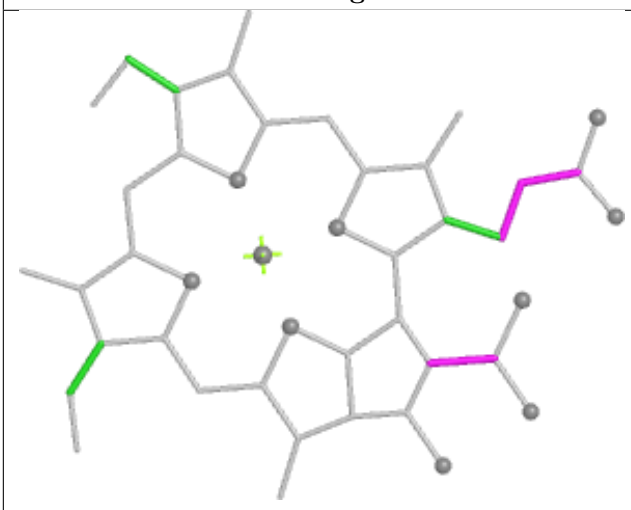
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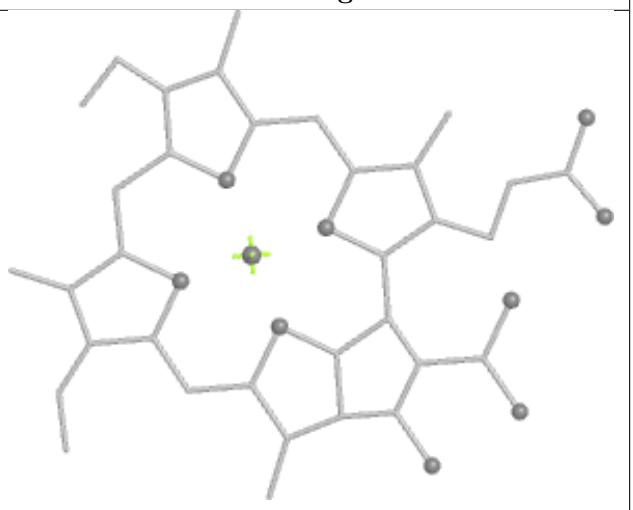
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Bond angles

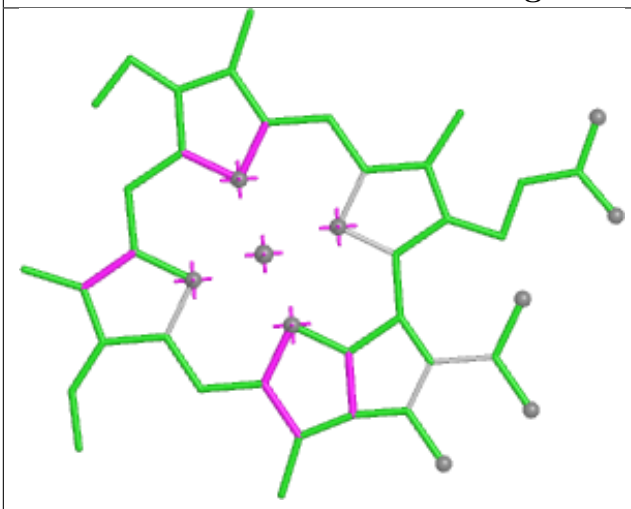


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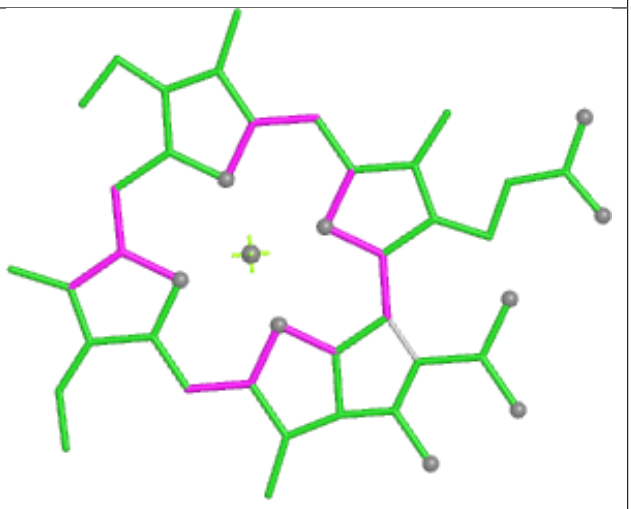


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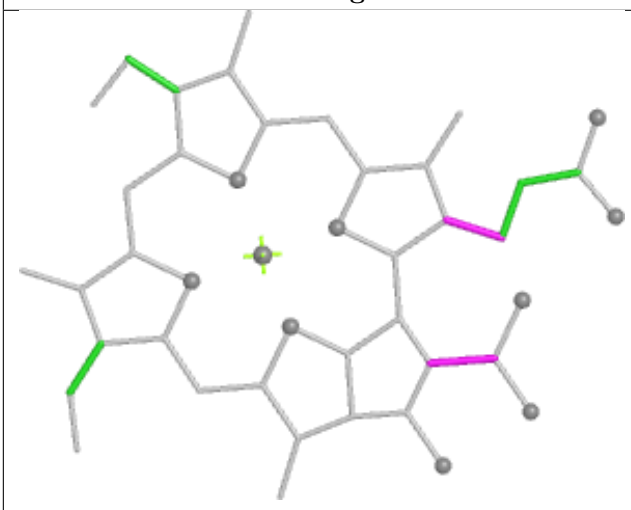
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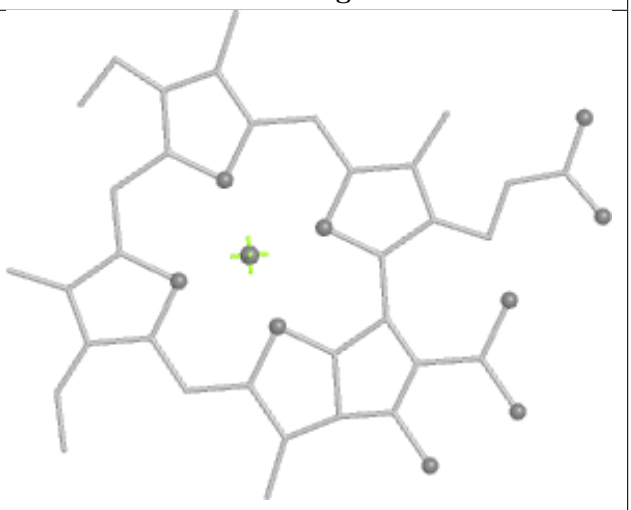
Bond lengths



Bond angles

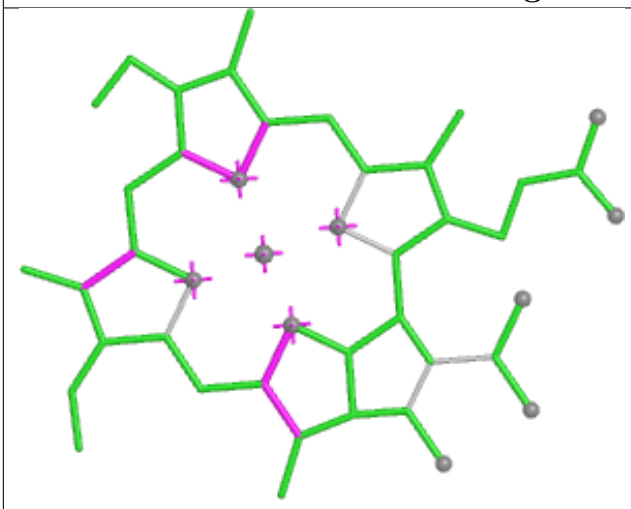


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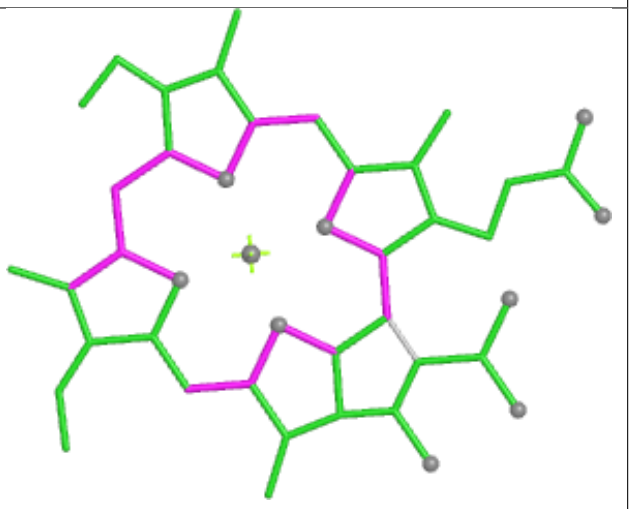


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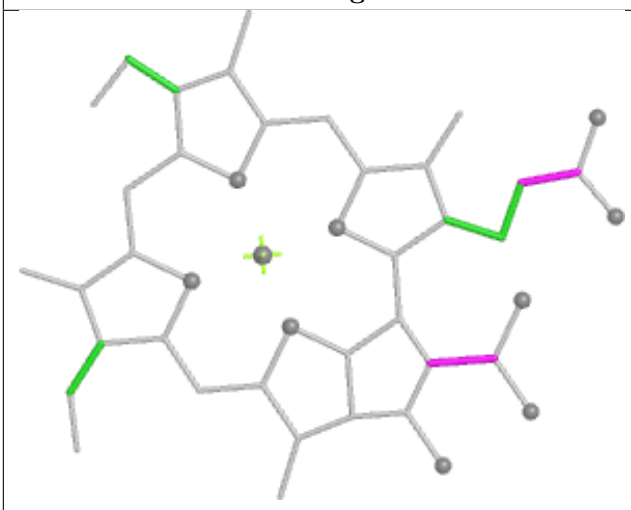
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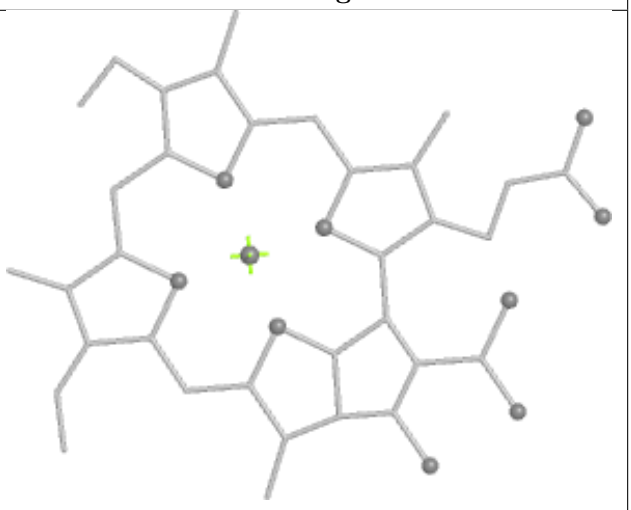
Bond lengths



Bond angles

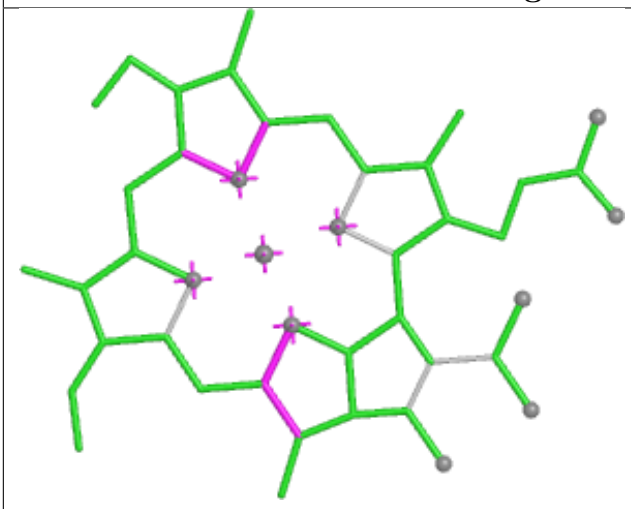


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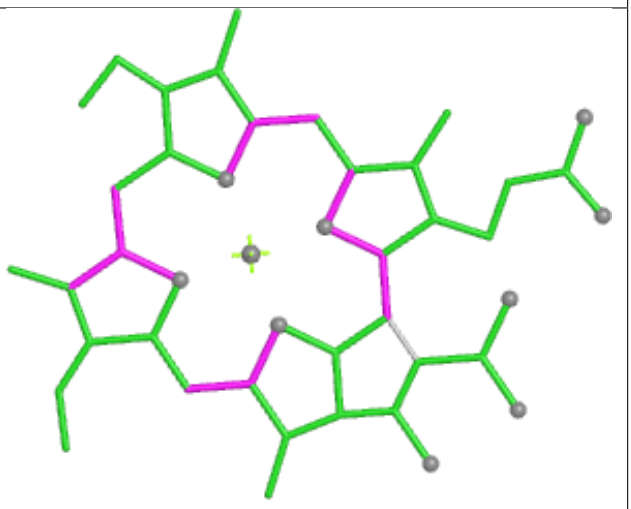


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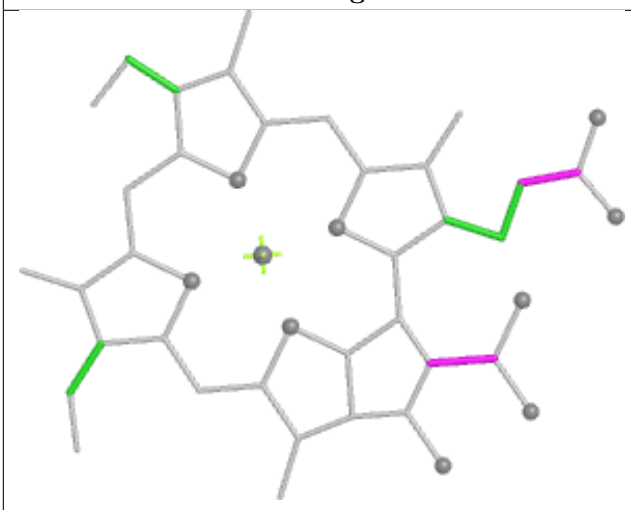
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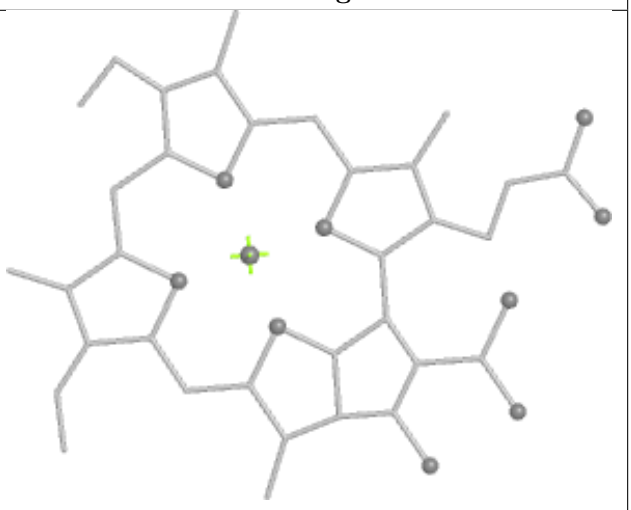
Bond lengths



Bond angles

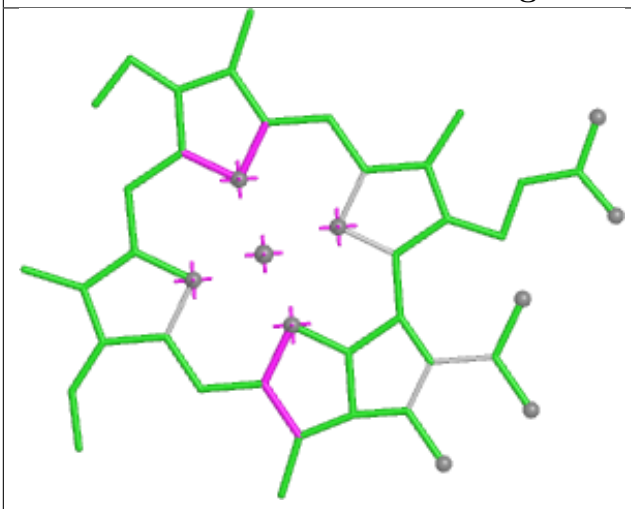


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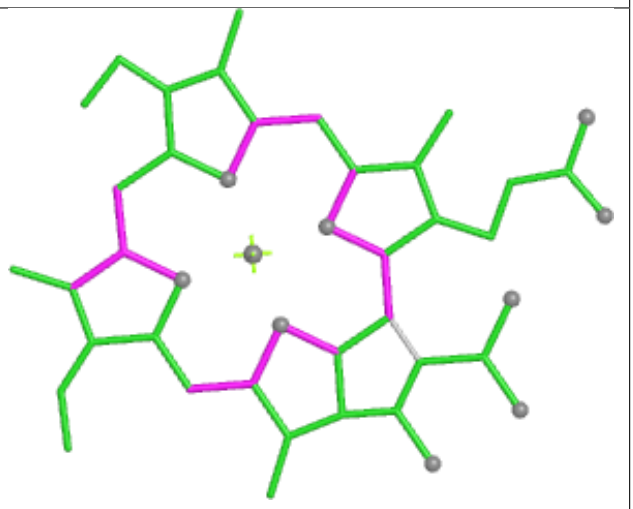


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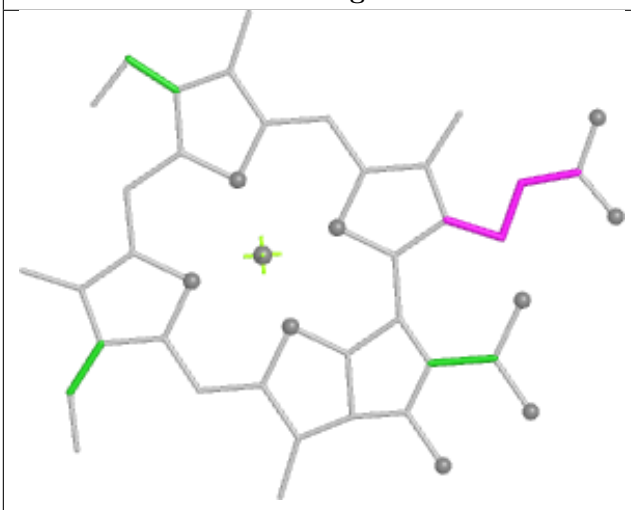
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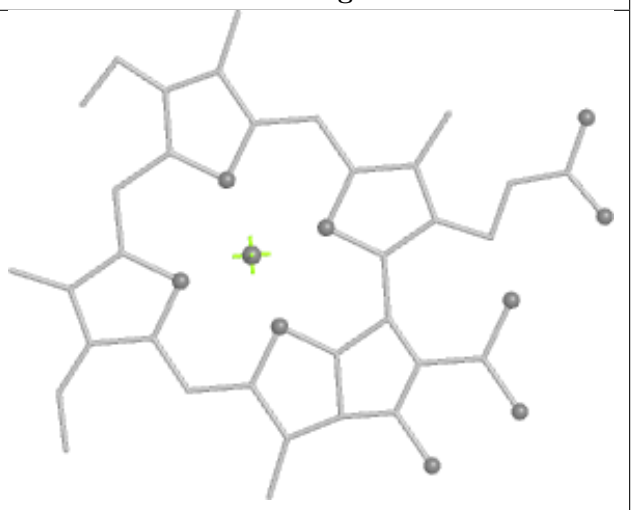
Bond lengths



Bond angles

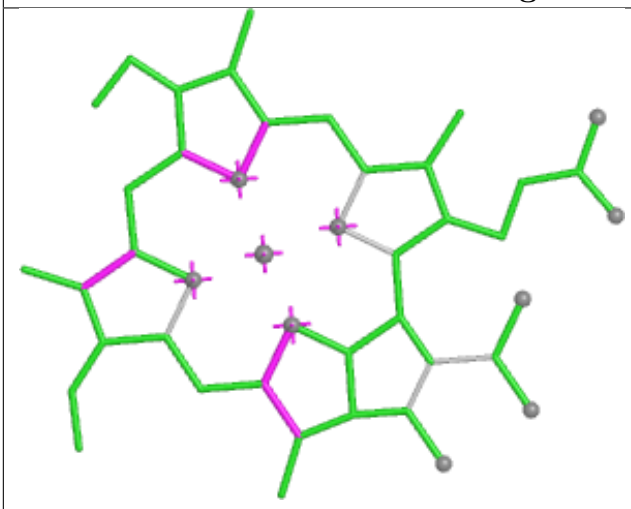


Torsions

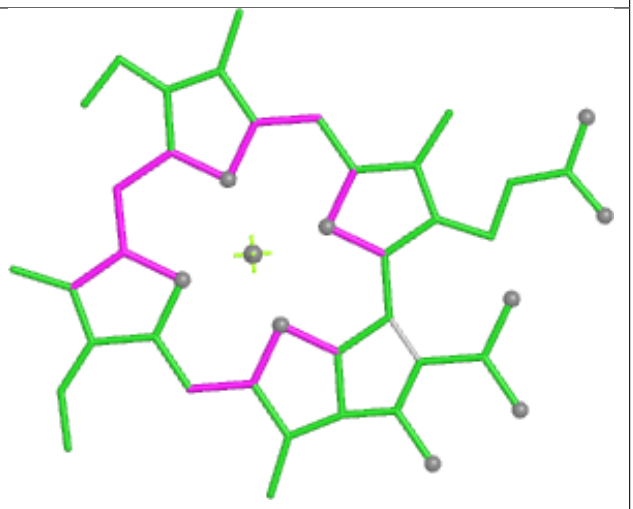


Rings

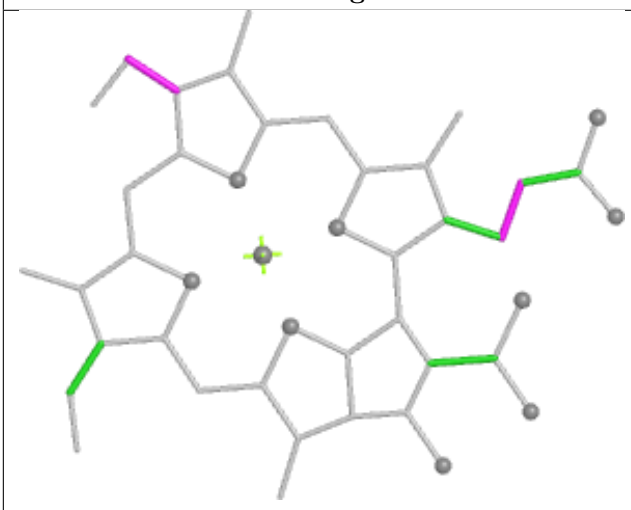
Ligand CLA 1 1005



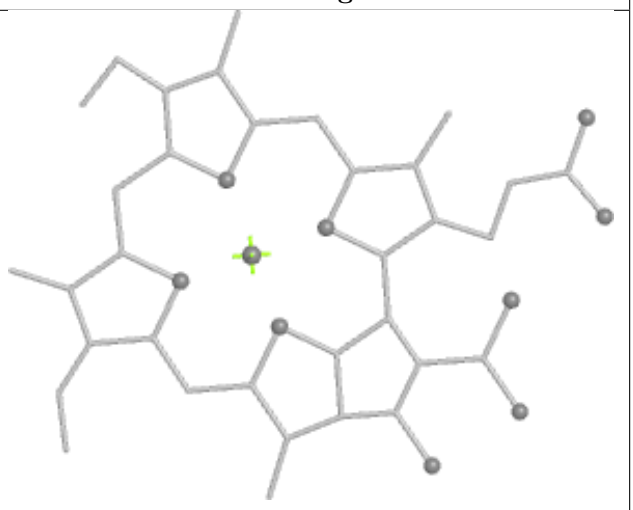
Bond lengths



Bond angles

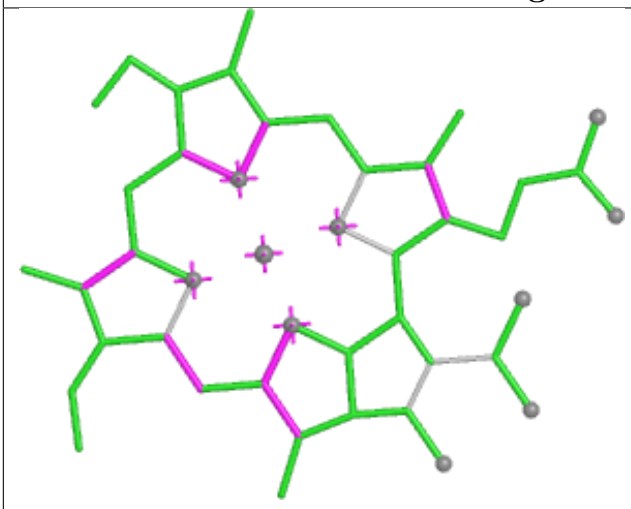


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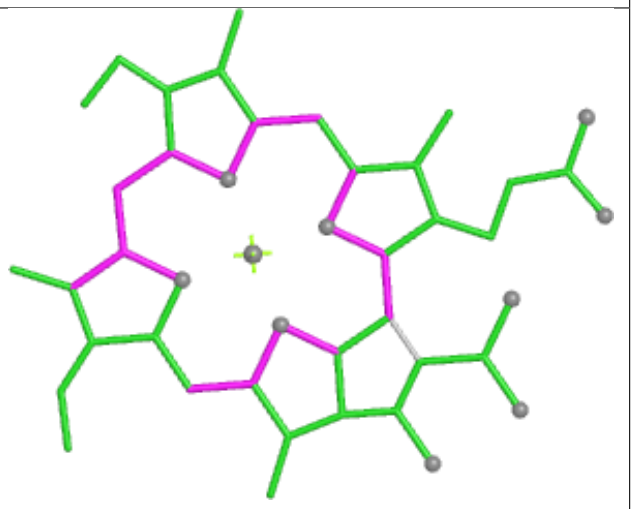


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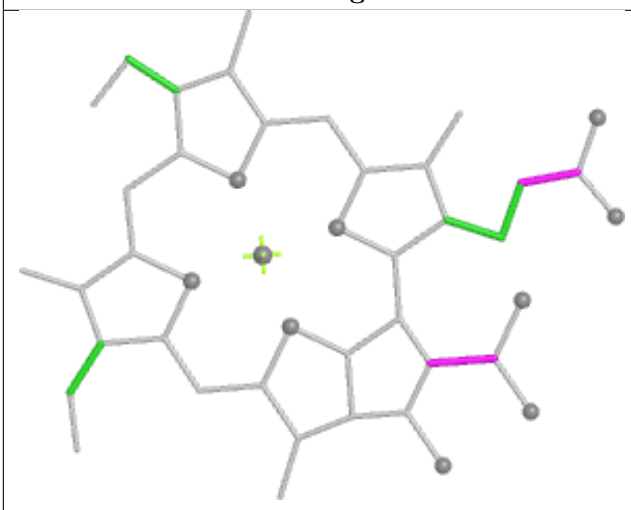
Ligand CLA 8 306



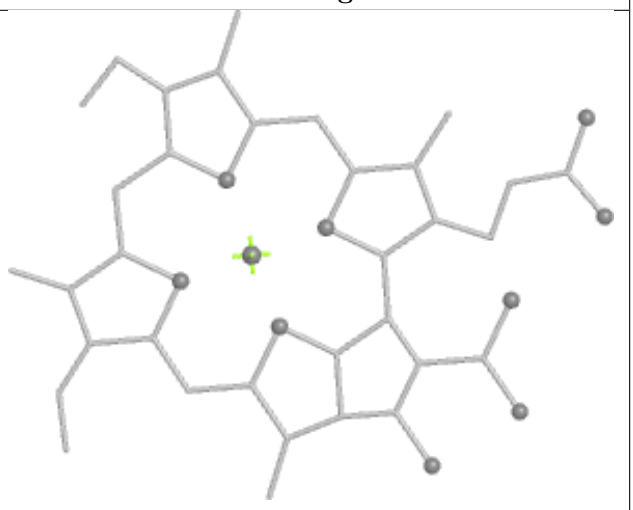
Bond lengths



Bond angles

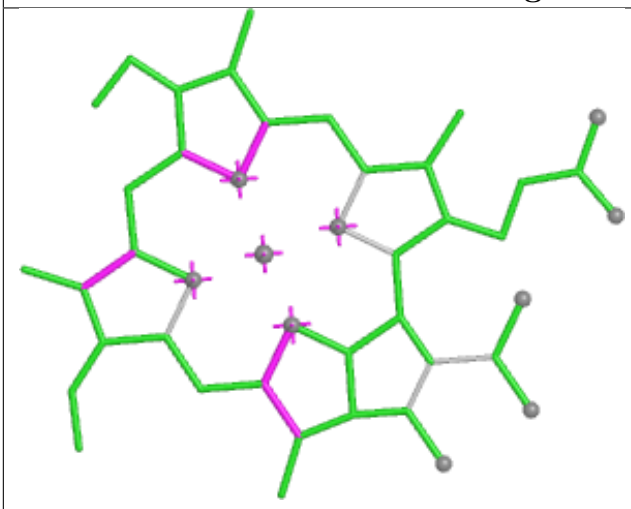


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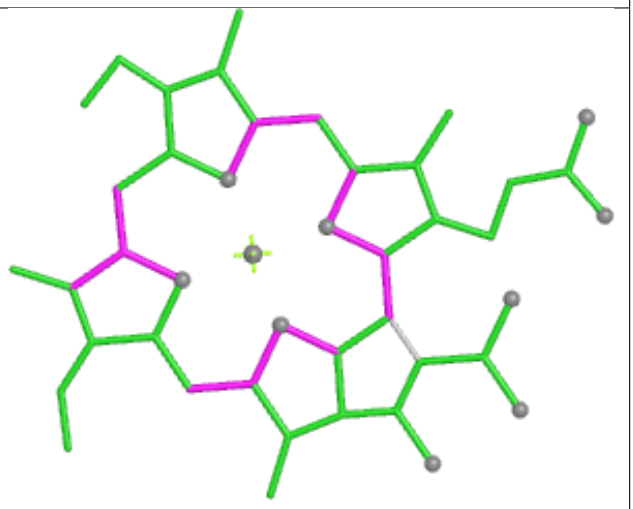


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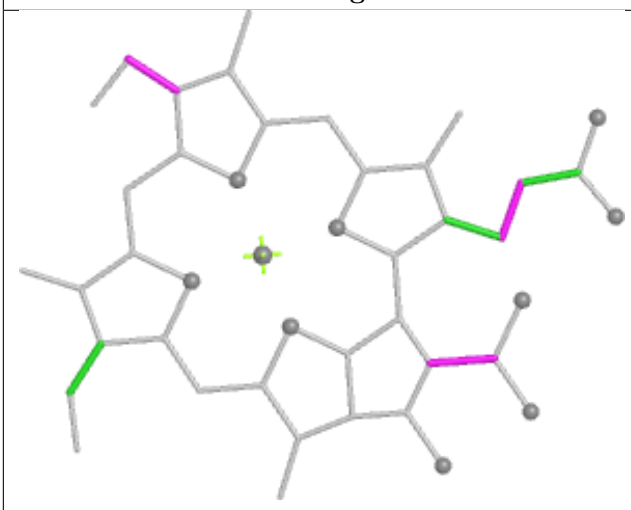
Ligand CLA B 810



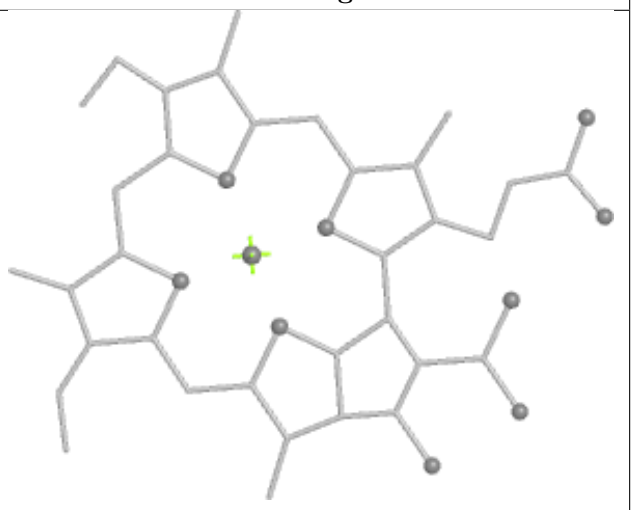
Bond lengths



Bond angles

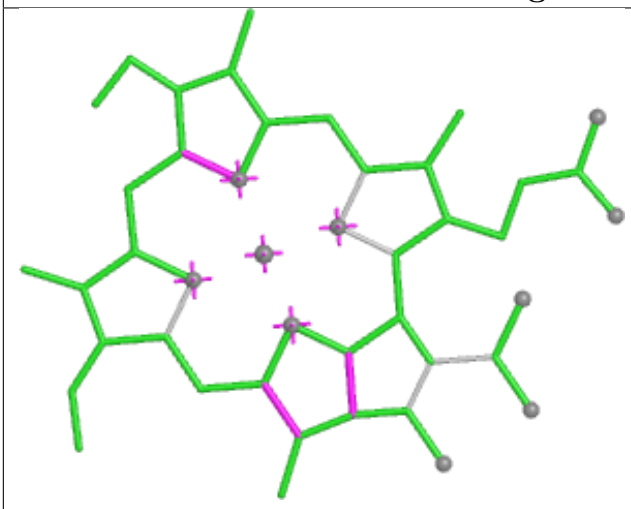


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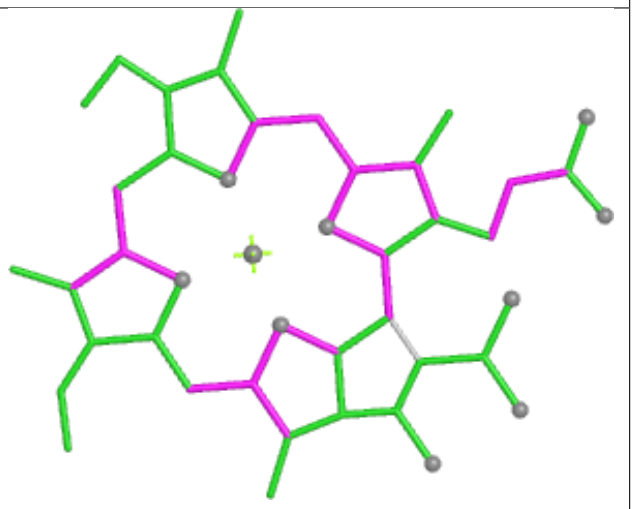


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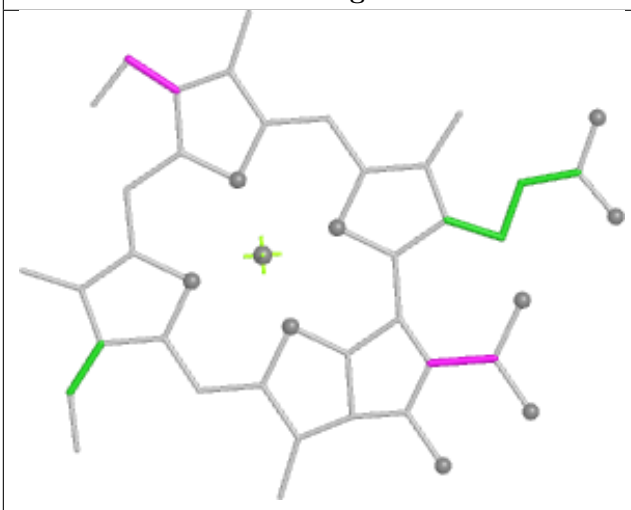
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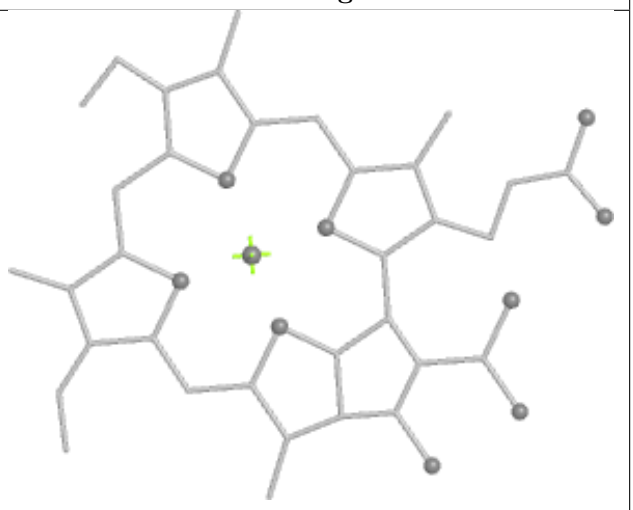
Bond lengths



Bond angles

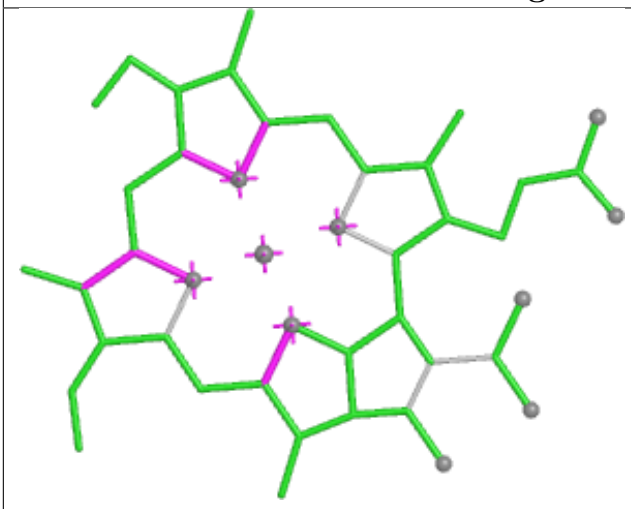


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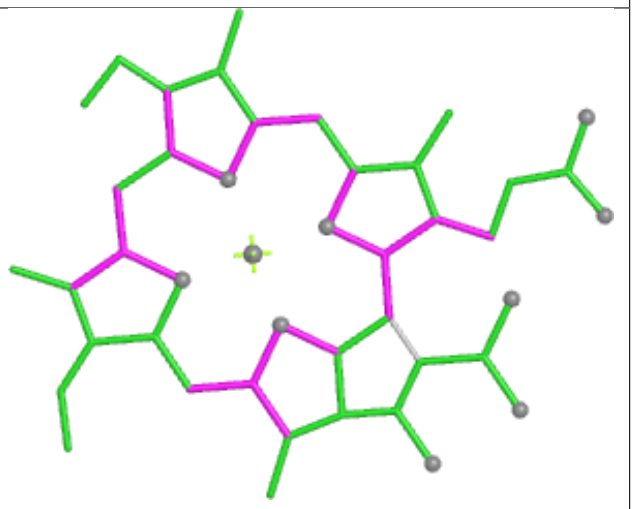


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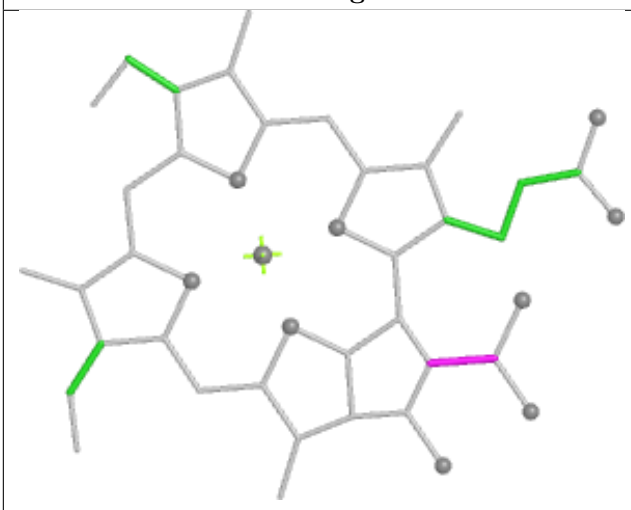
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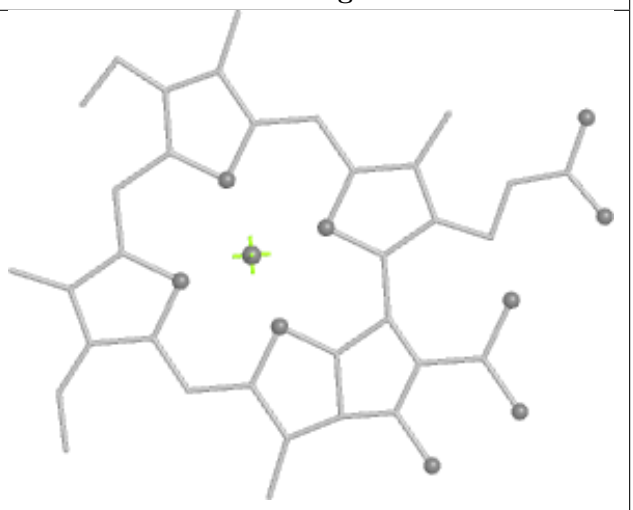
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Bond angles

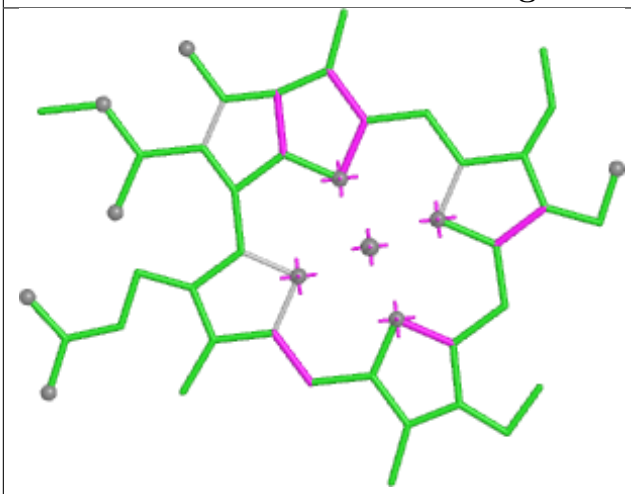


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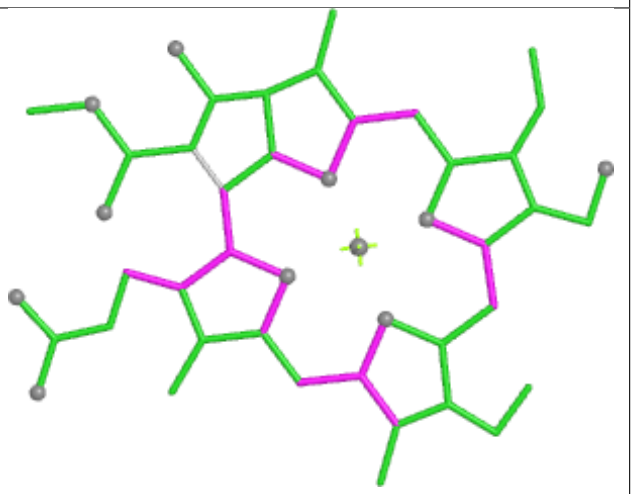


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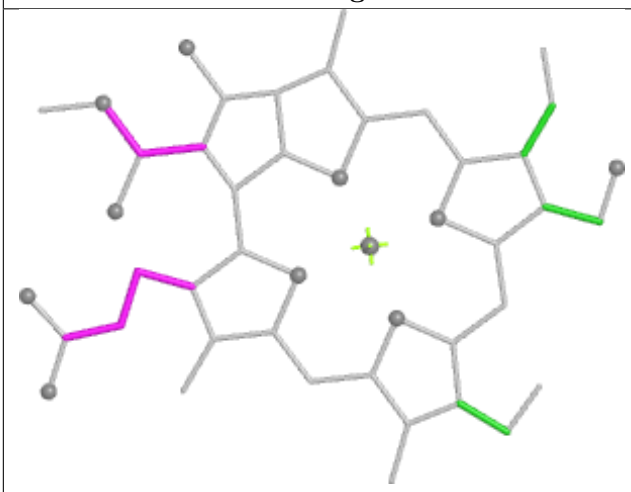
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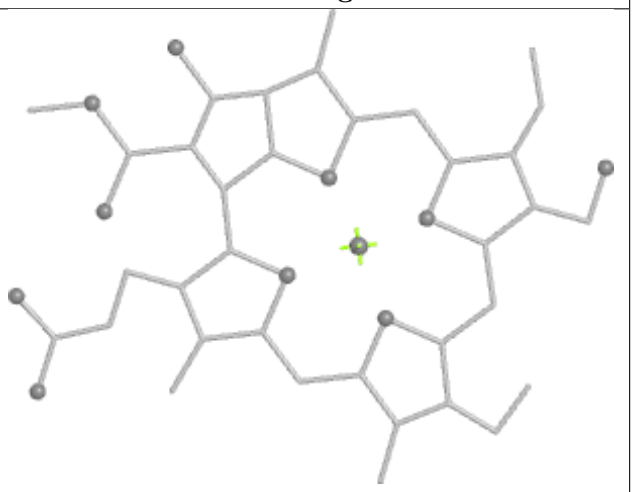
Bond lengths



Bond angles

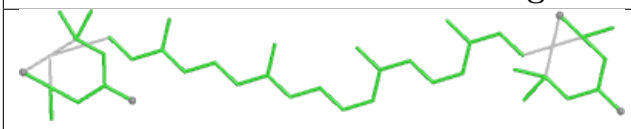


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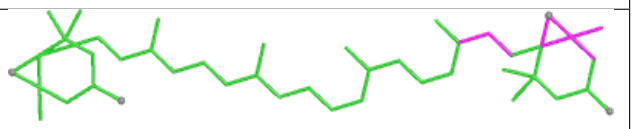


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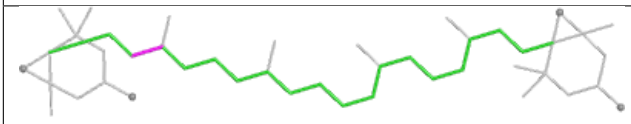
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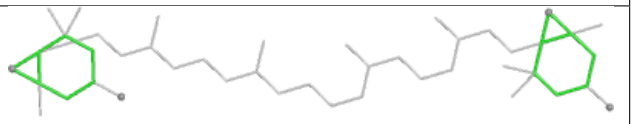
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Bond angles

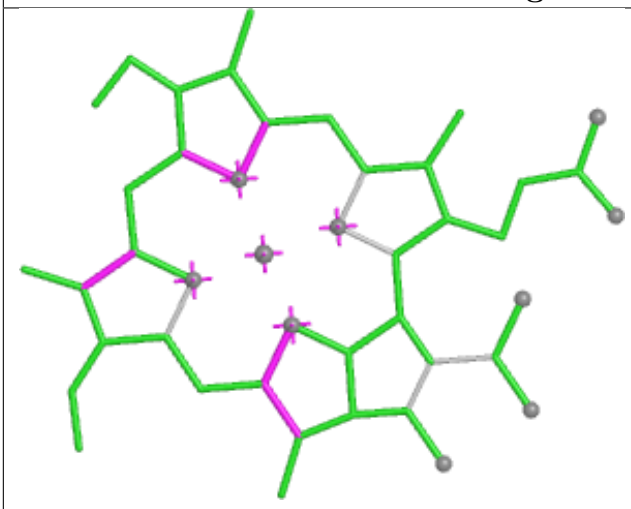


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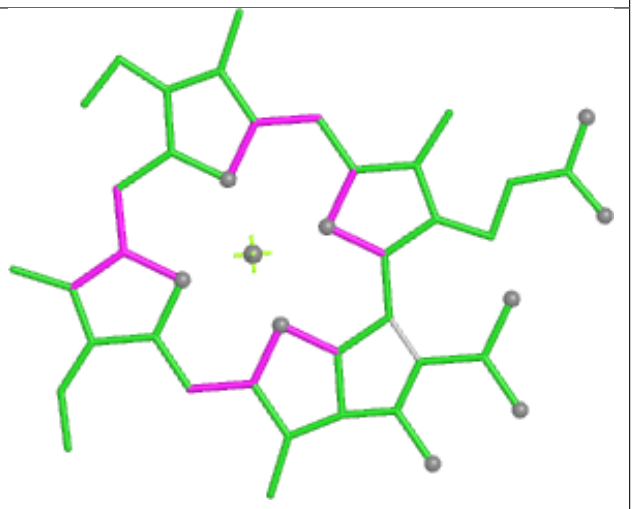


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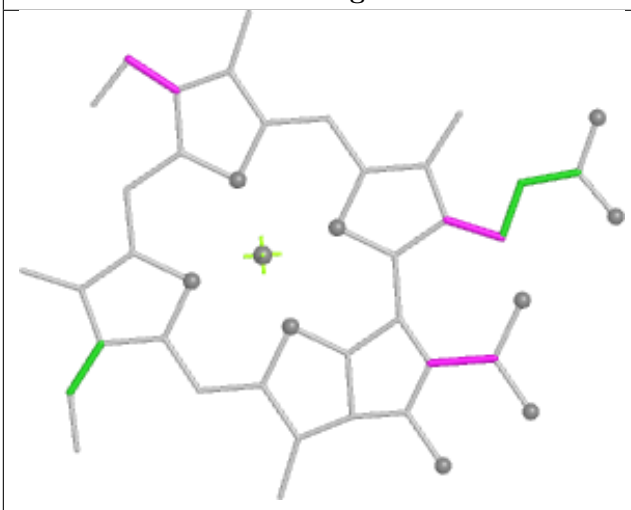
Ligand CLA L 202



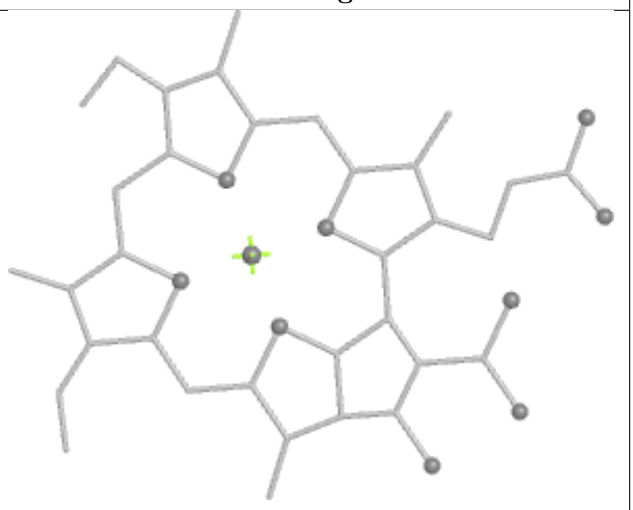
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Bond angles

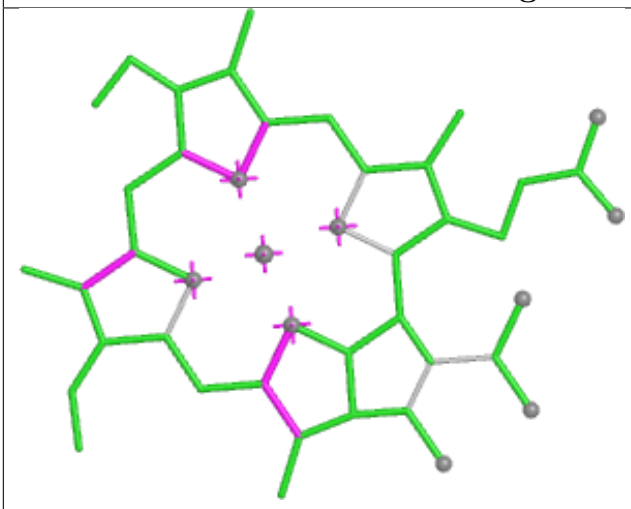


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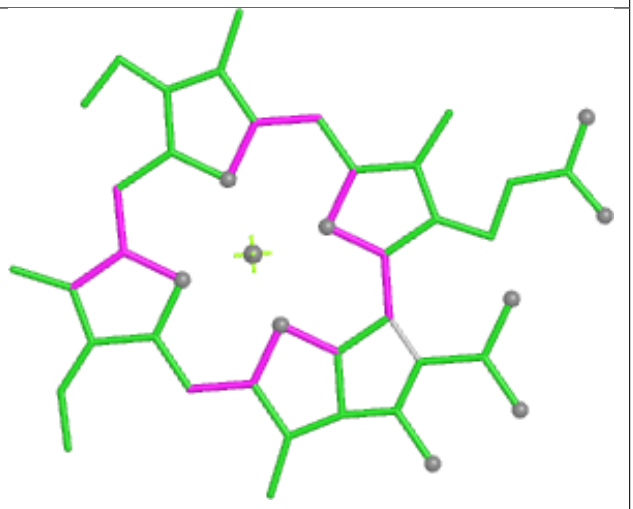


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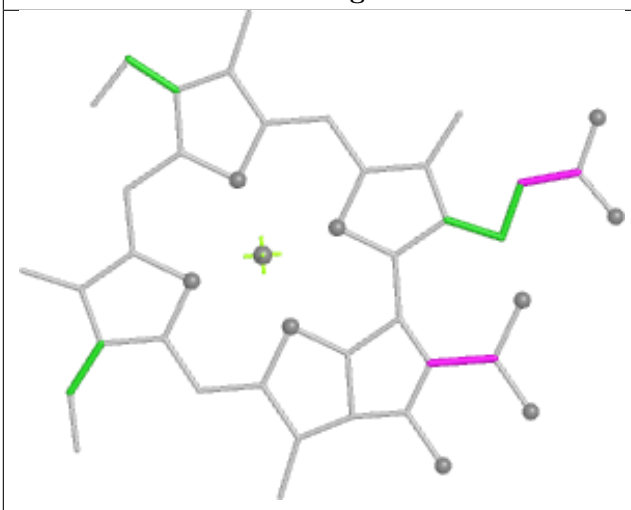
Ligand CLA 1 1004



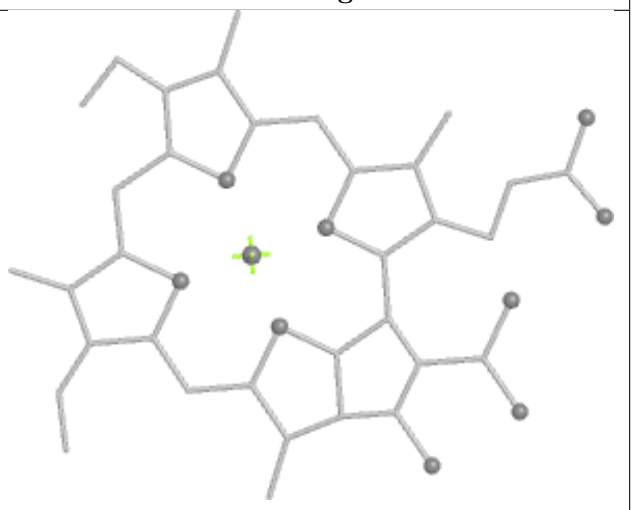
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Bond angles

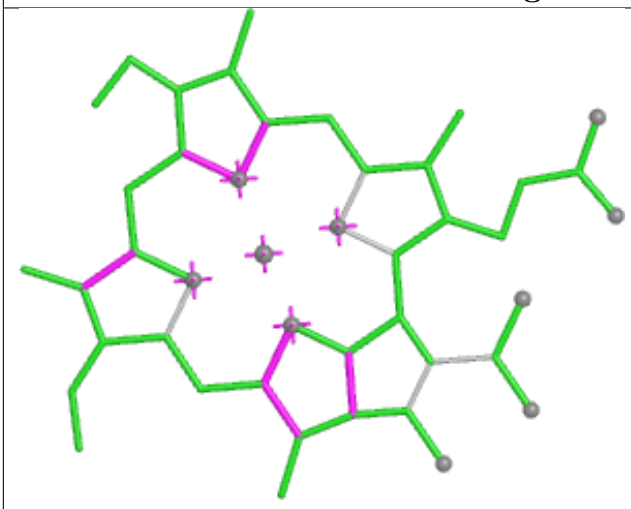


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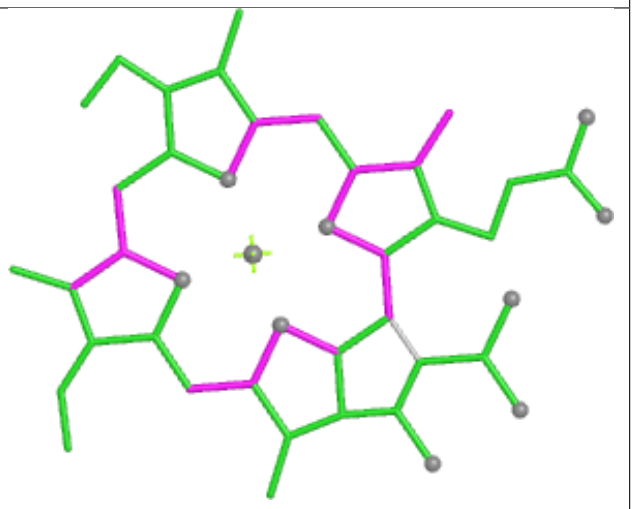


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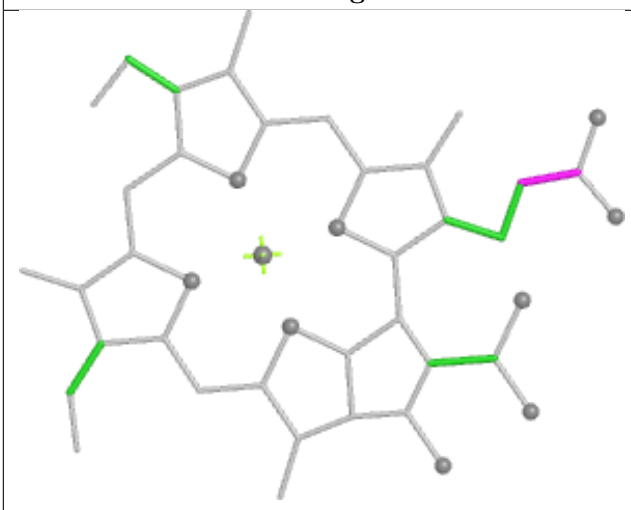
Ligand CLA A 821



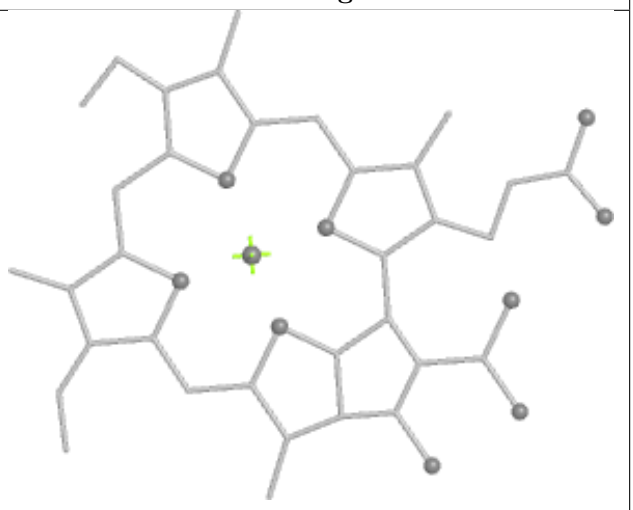
Bond lengths



Bond angles

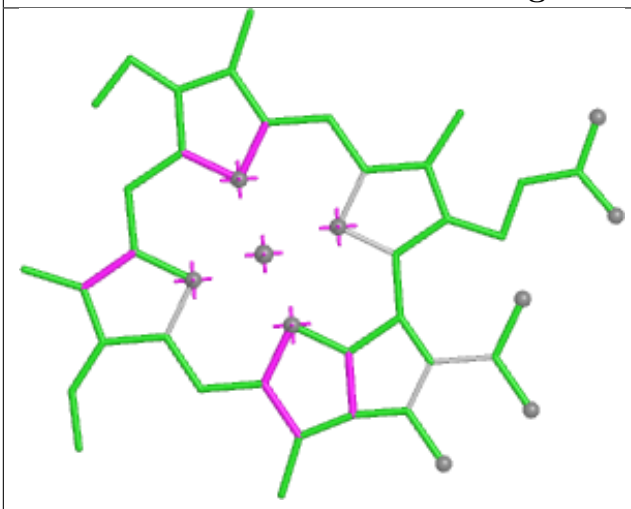


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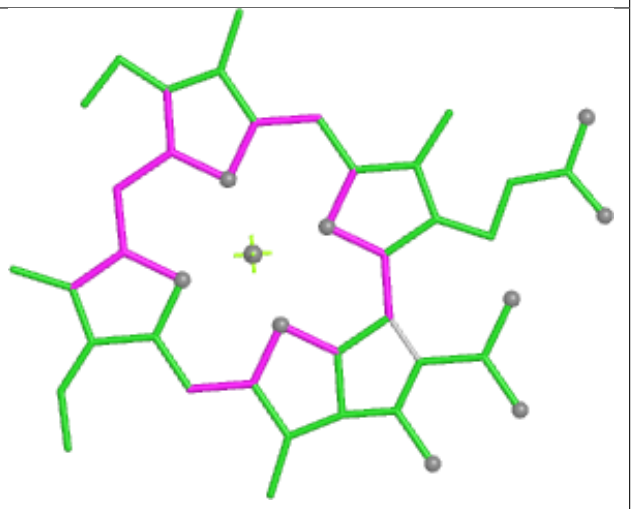


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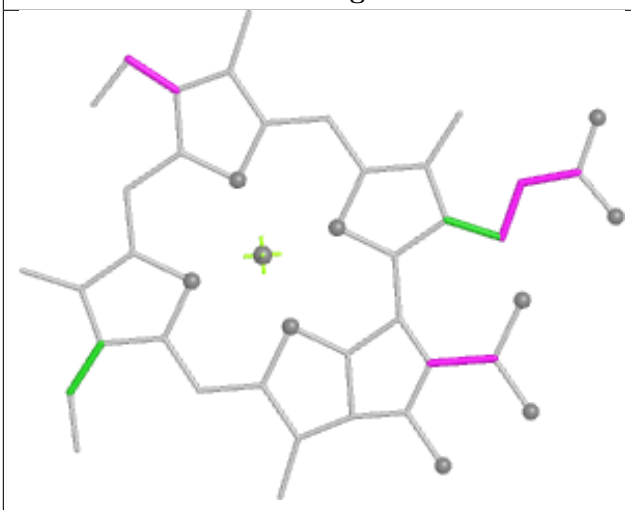
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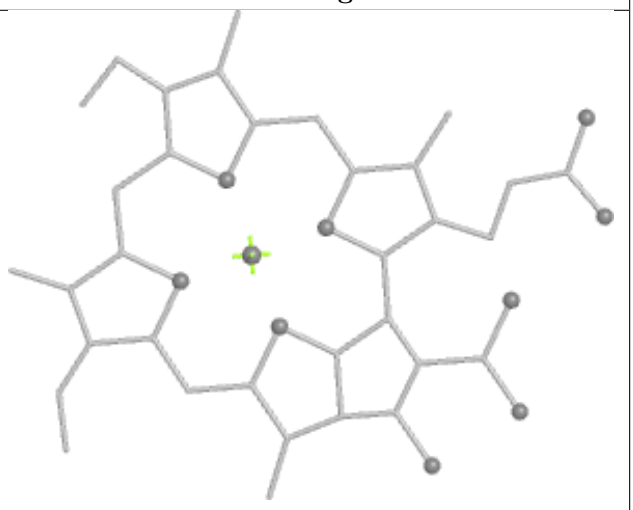
Bond lengths



Bond angles

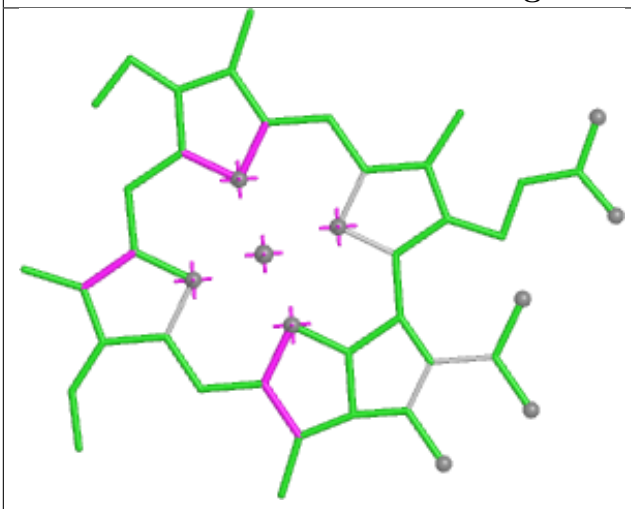


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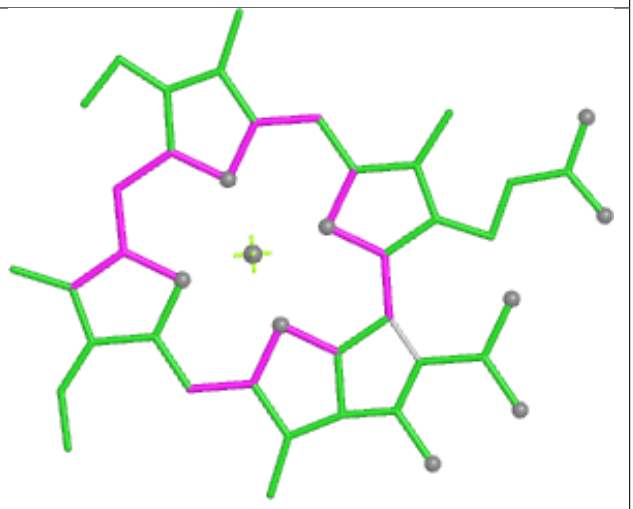


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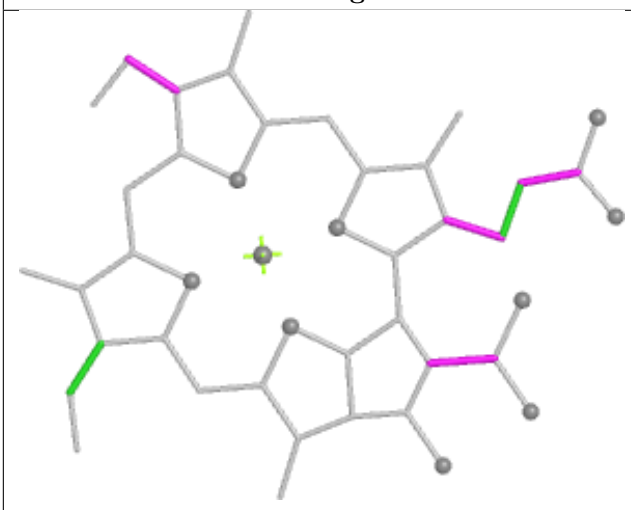
Ligand CLA A 803



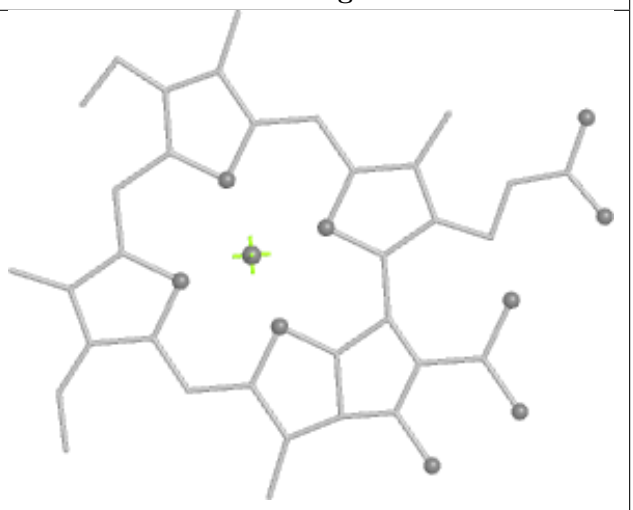
Bond lengths



Bond angles

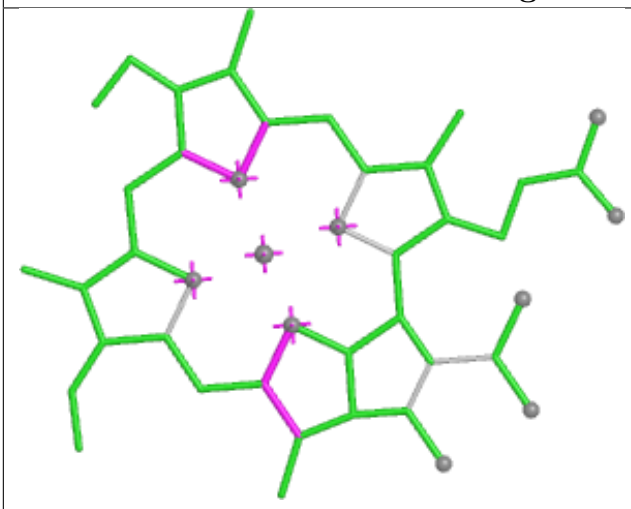


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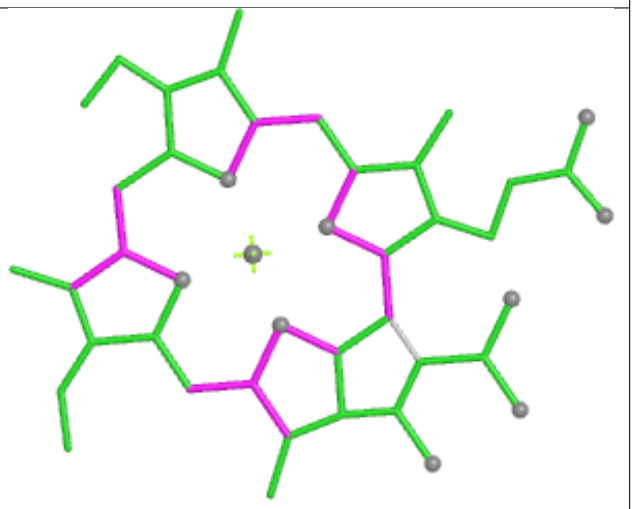


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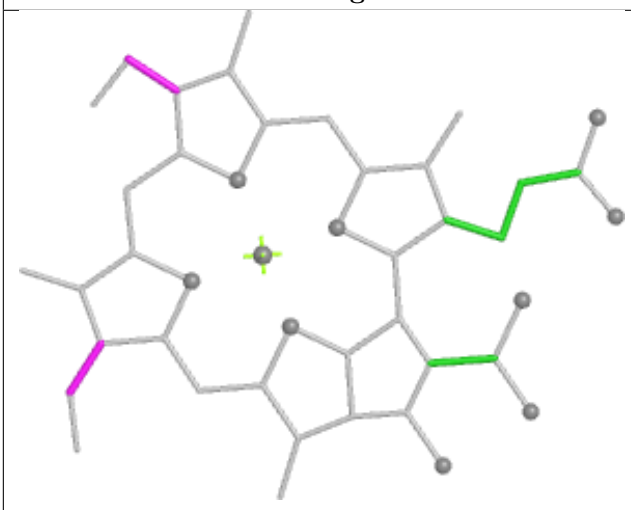
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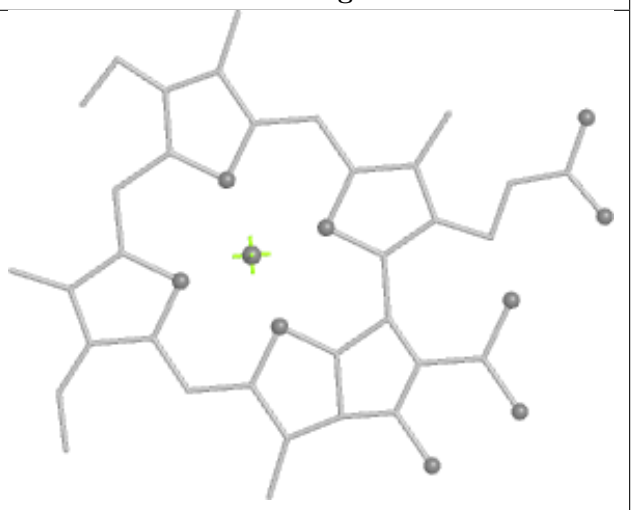
Bond lengths



Bond angles

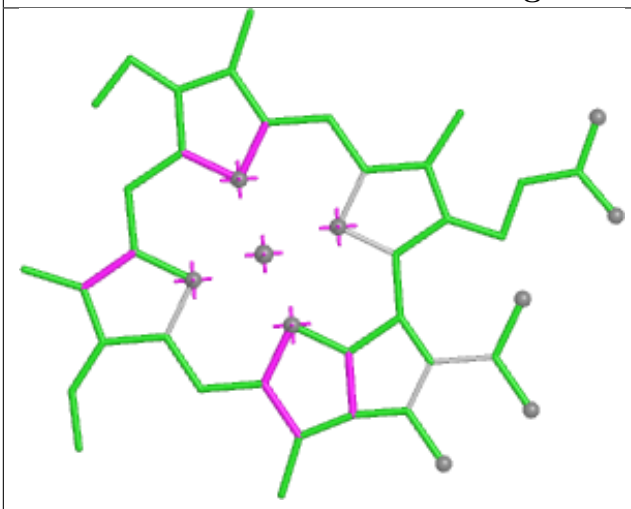


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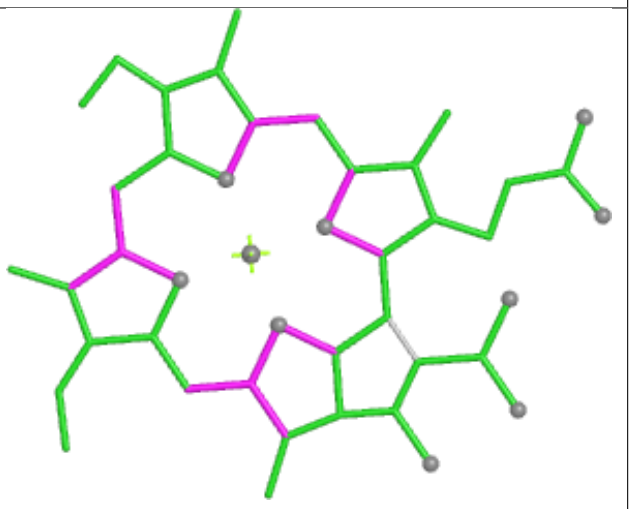


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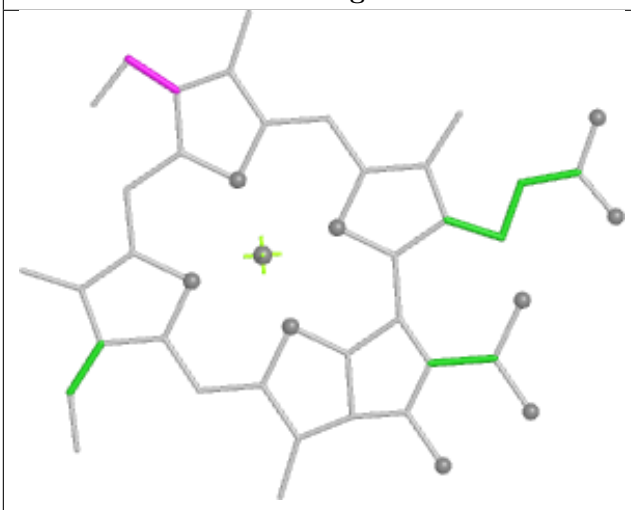
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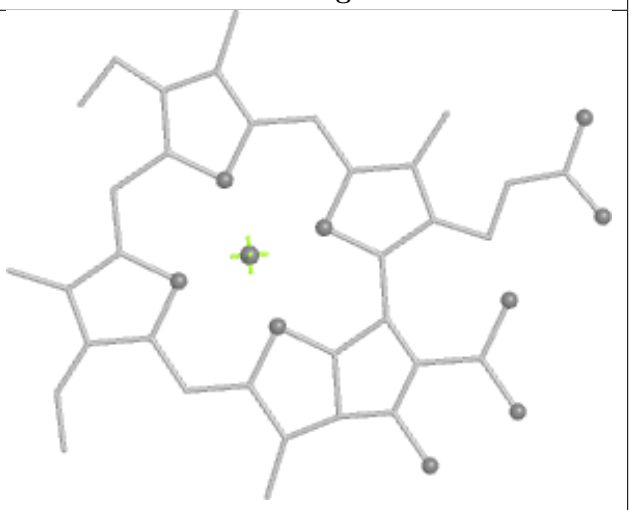
Bond lengths



Bond angles

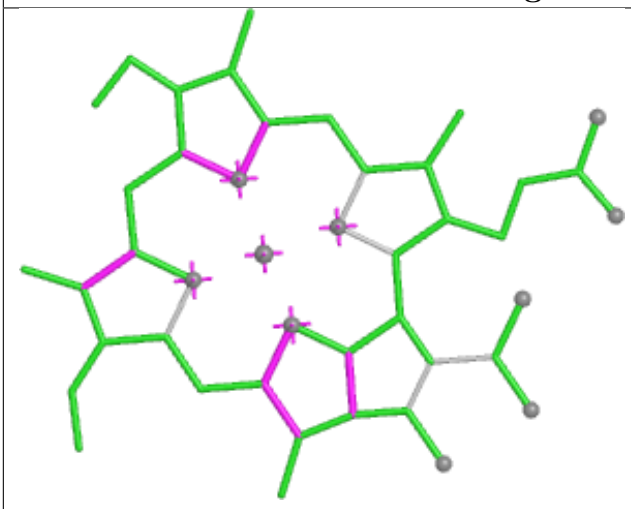


Torsions

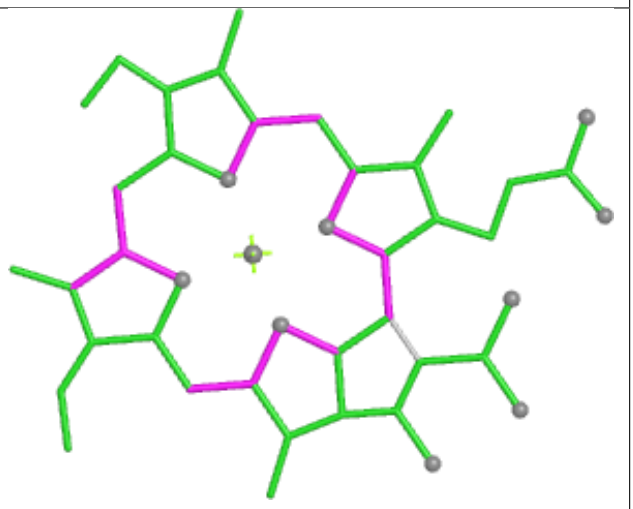


Rings

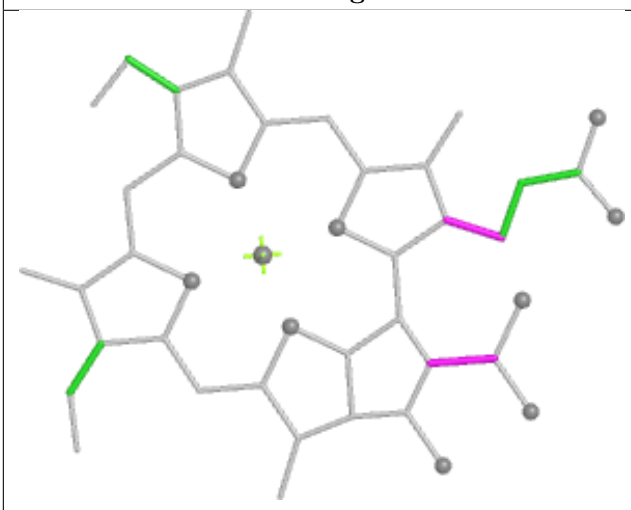
Ligand CLA B 828



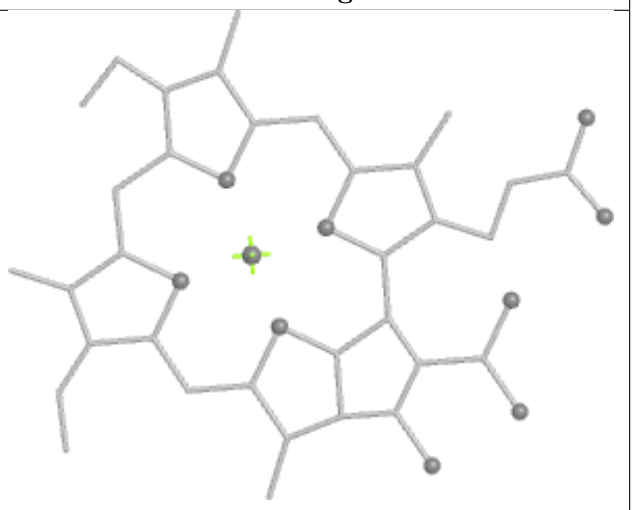
Bond lengths



Bond angles

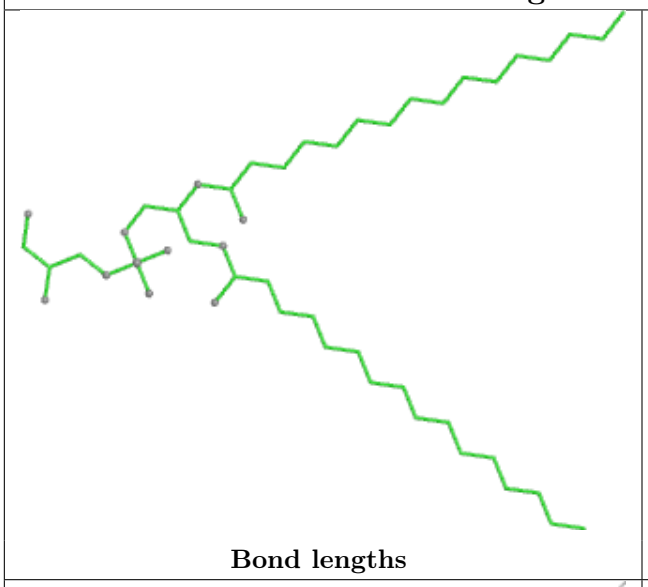


Torsions

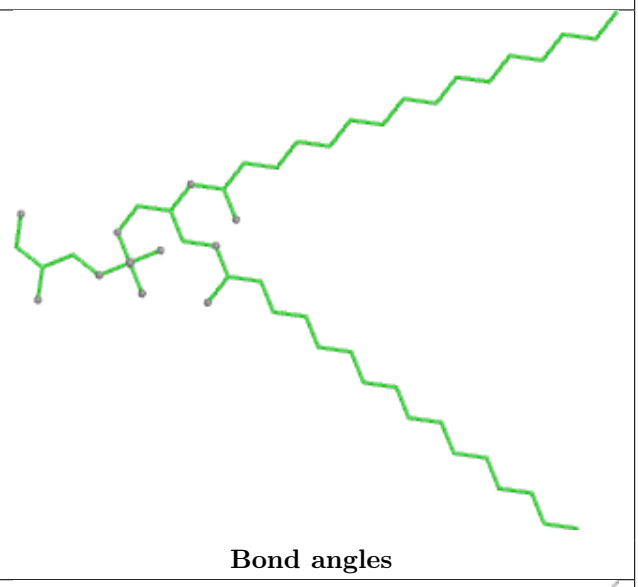


Rings

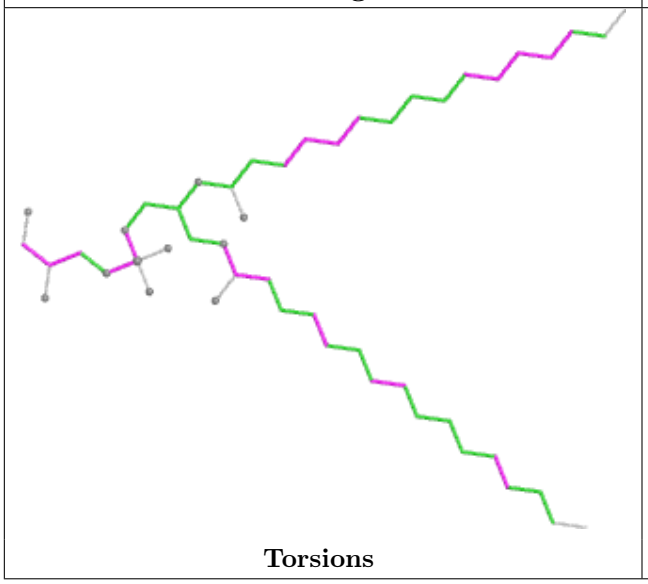
Ligand LHG 4 301



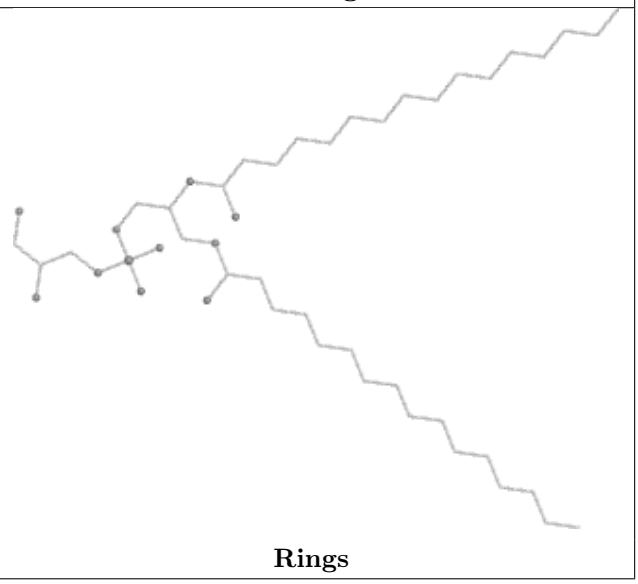
Bond lengths



Bond angles

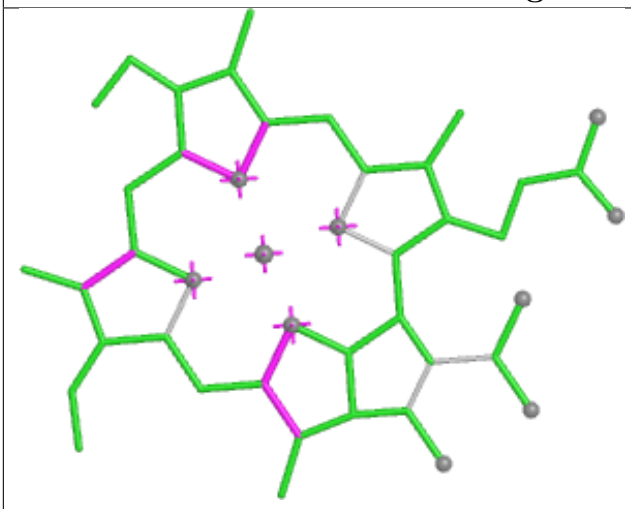


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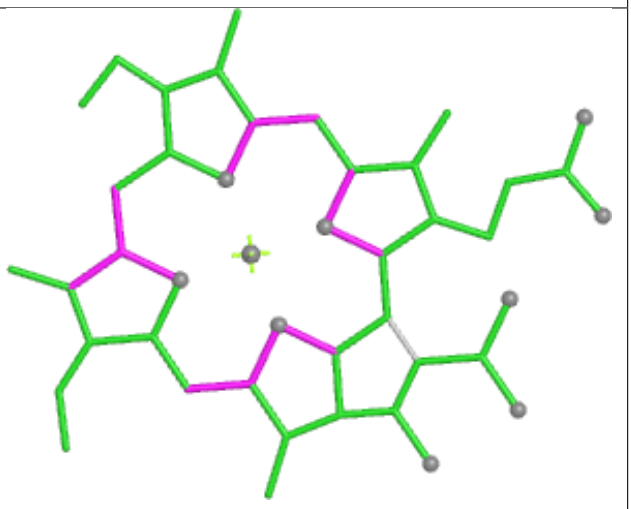


Rings

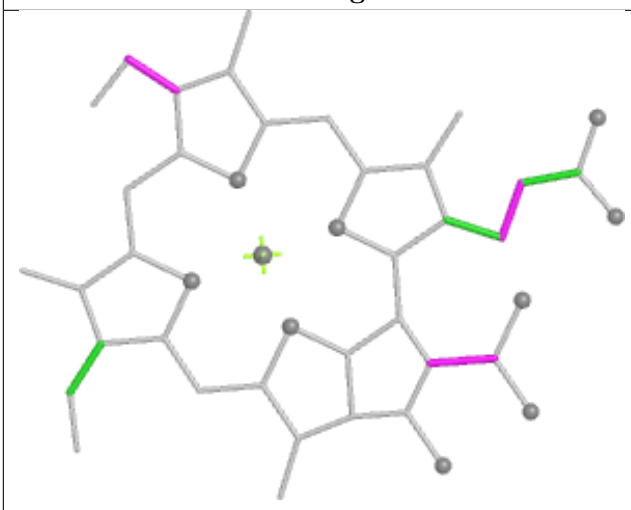
Ligand CLA L 201



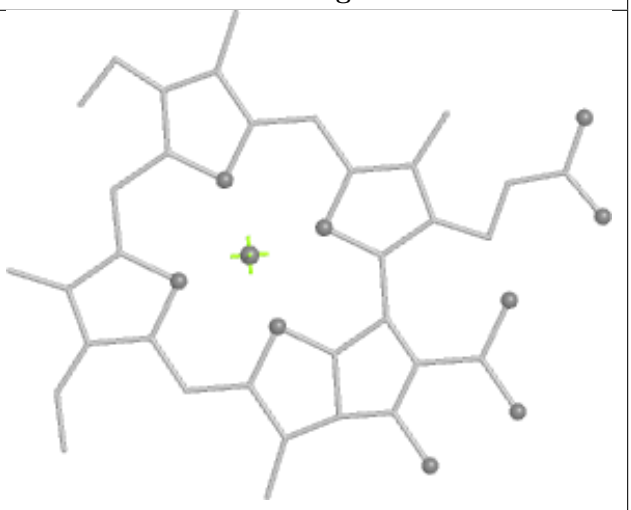
Bond lengths



Bond angles

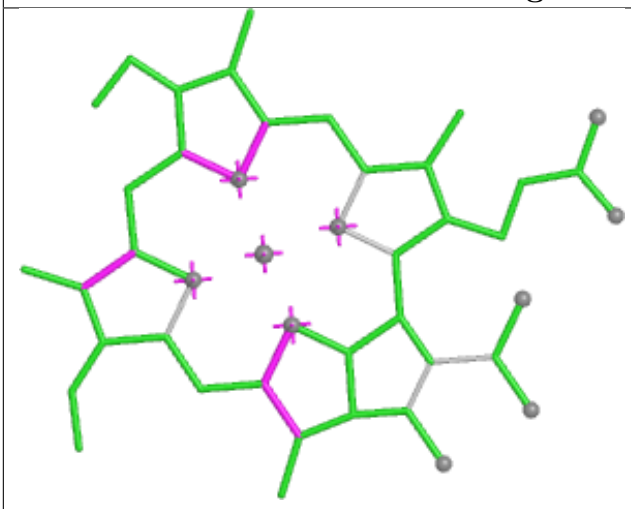


Torsions

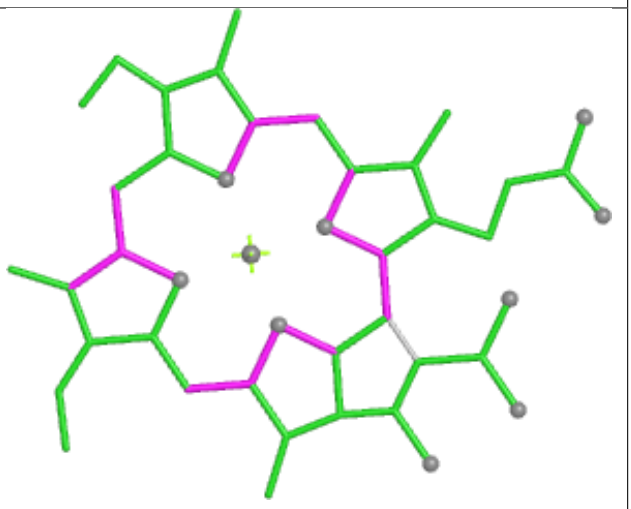


Rings

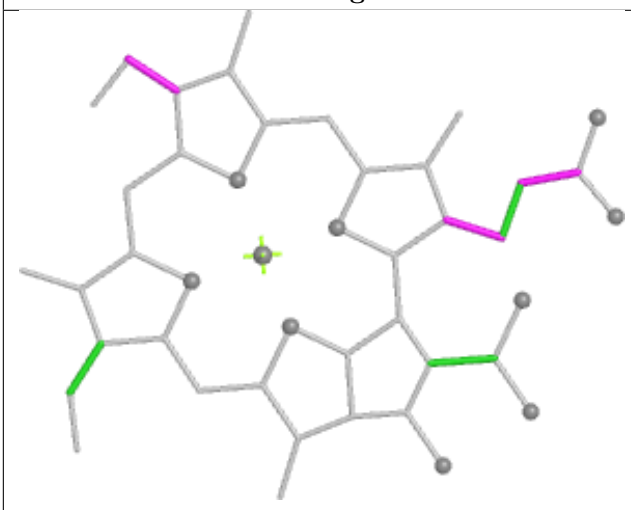
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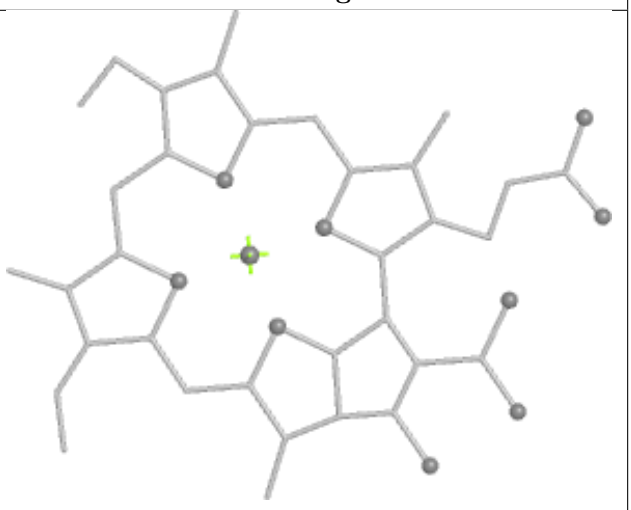
Bond lengths



Bond angles

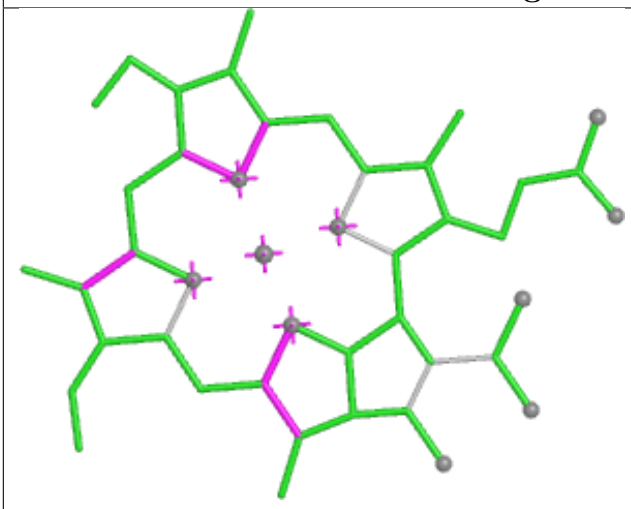


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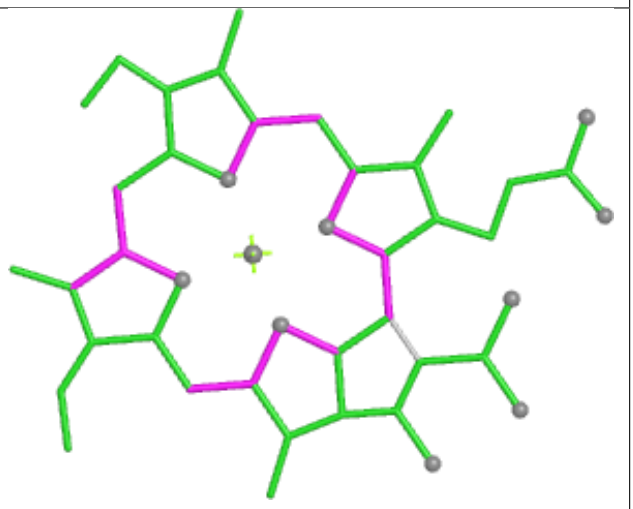


Rings

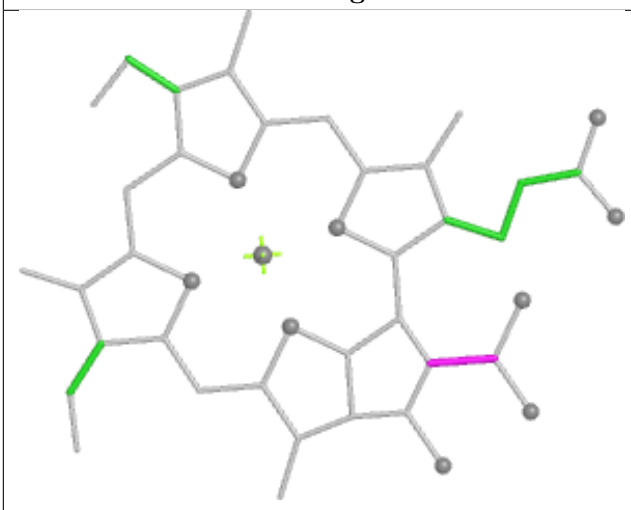
Ligand CLA A 832



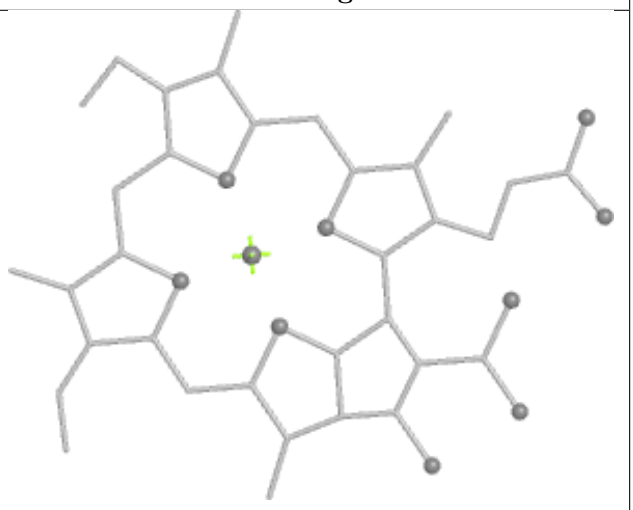
Bond lengths



Bond angles

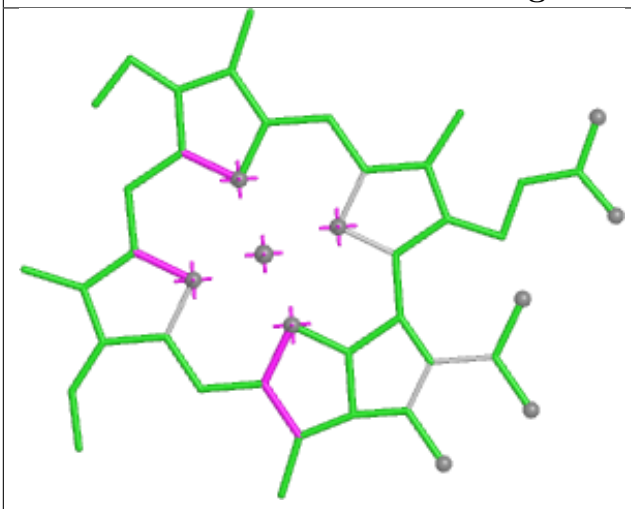


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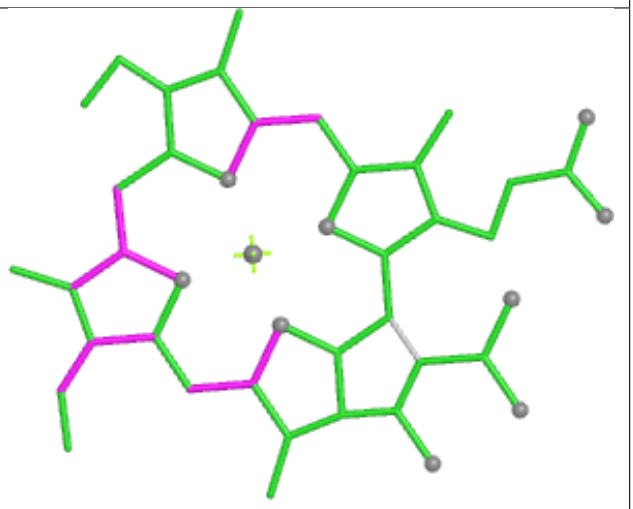


Rings

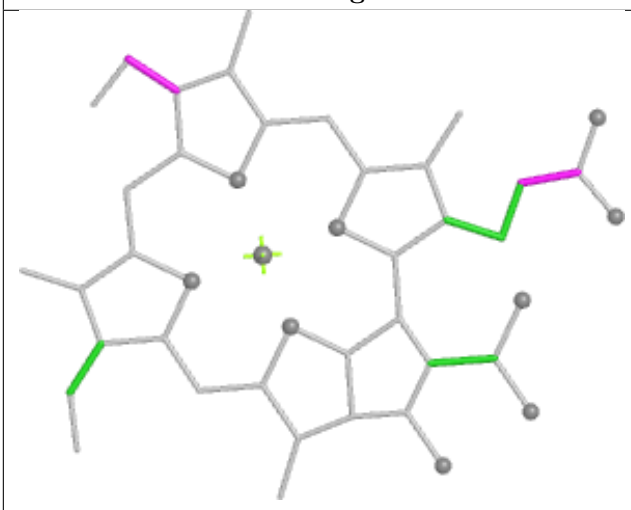
Ligand CLA 8 307



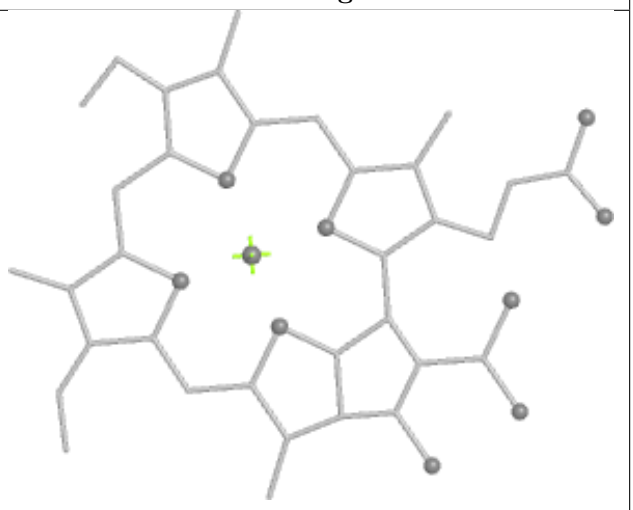
Bond lengths



Bond angles

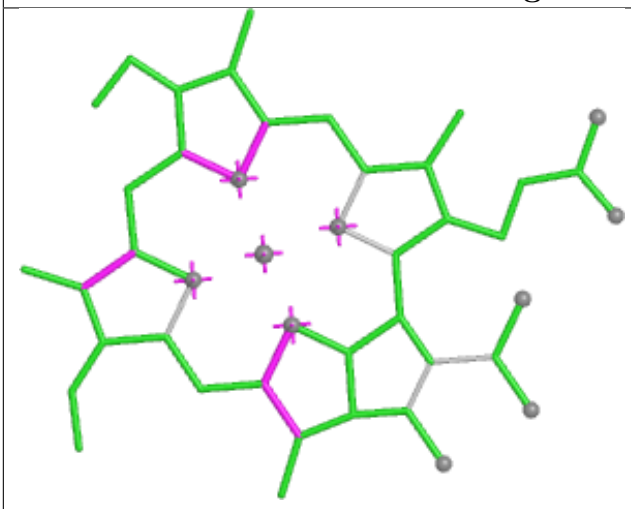


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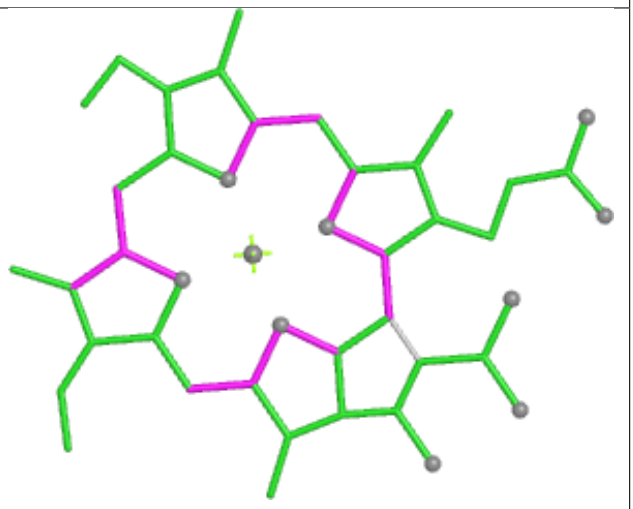


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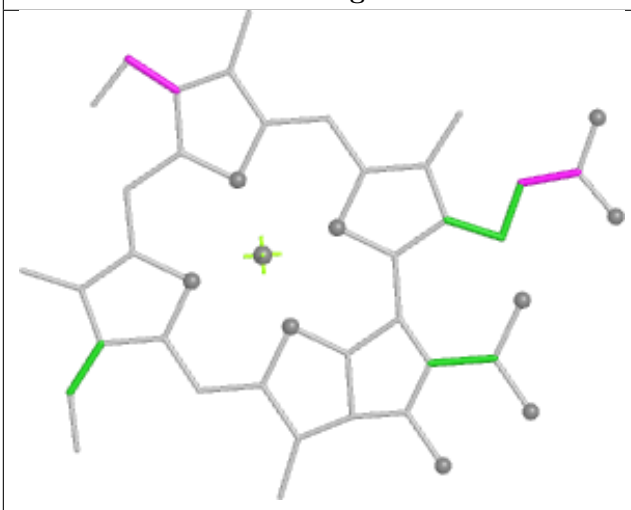
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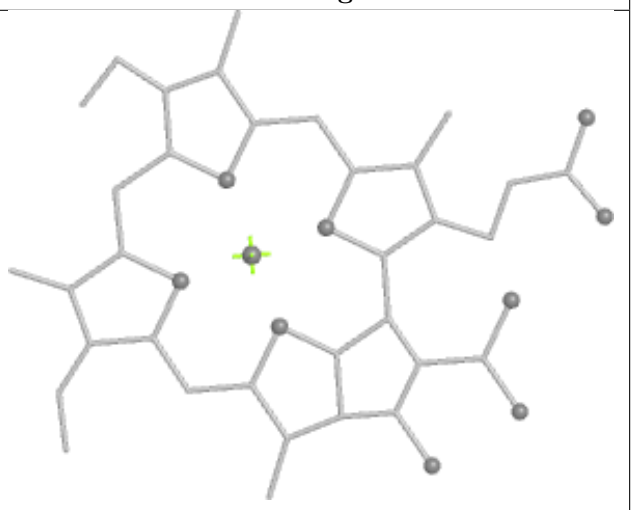
Bond lengths



Bond angles

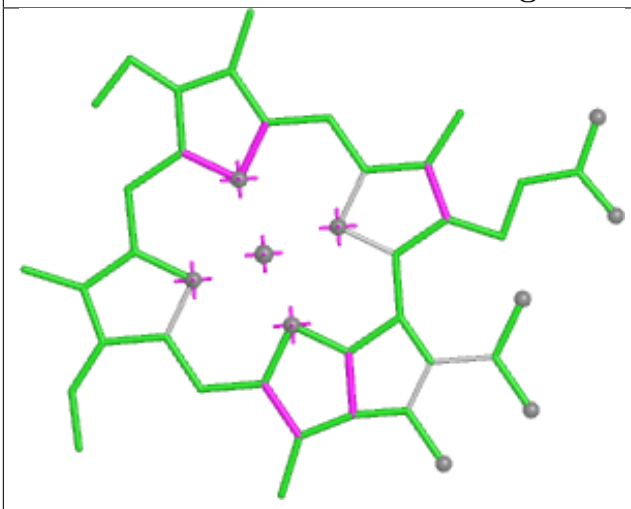


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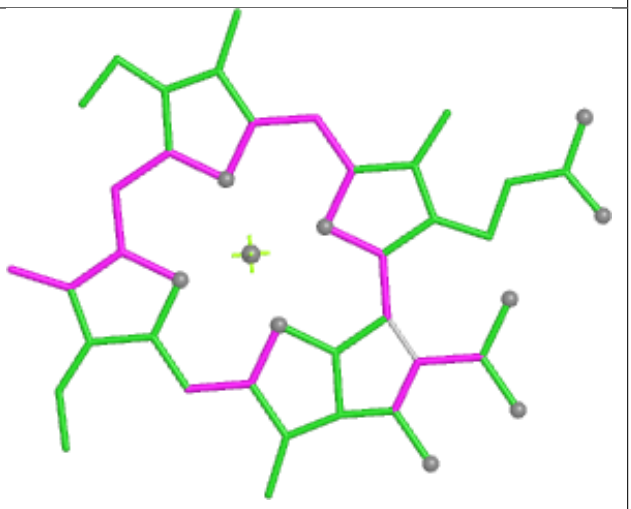


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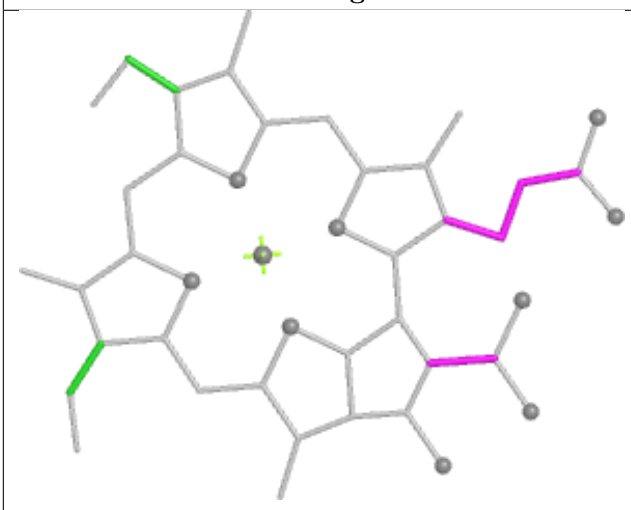
Ligand CLA 7 1004



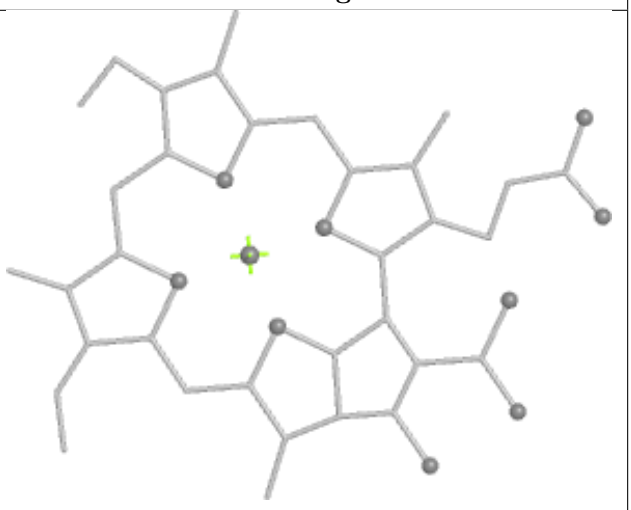
Bond lengths



Bond angles

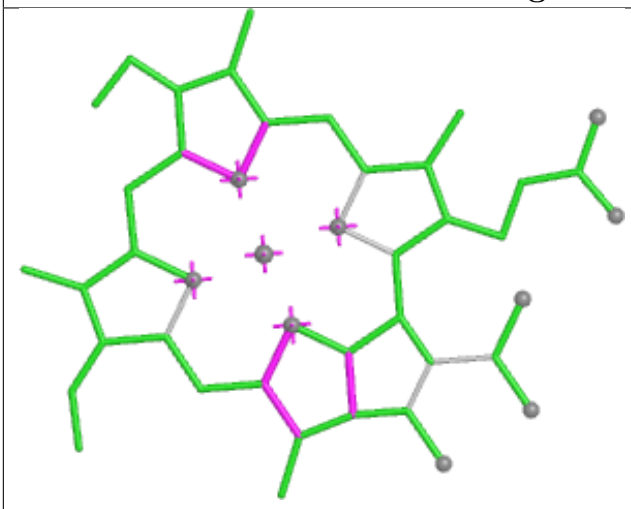


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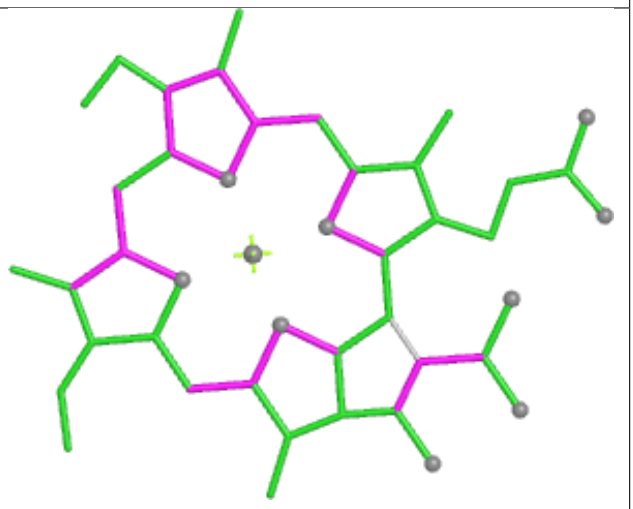


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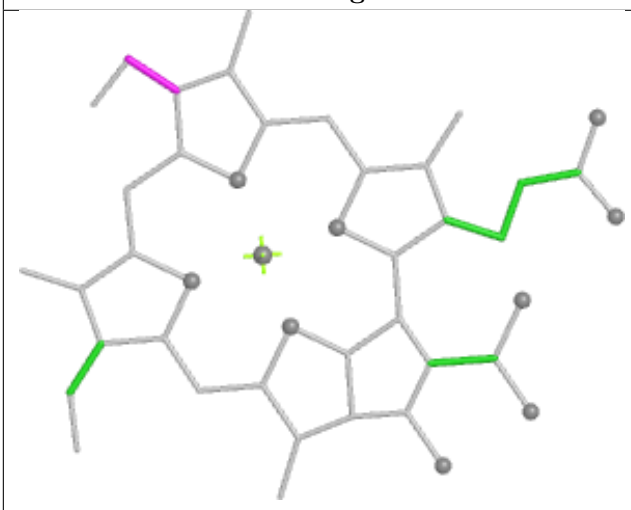
Ligand CLA 6 312



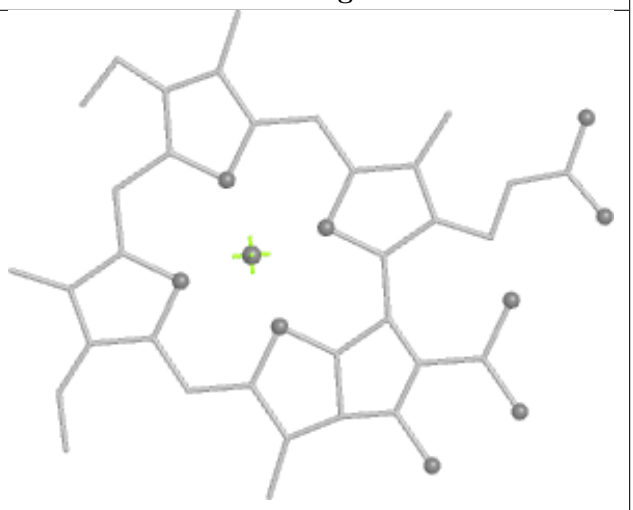
Bond lengths



Bond angles

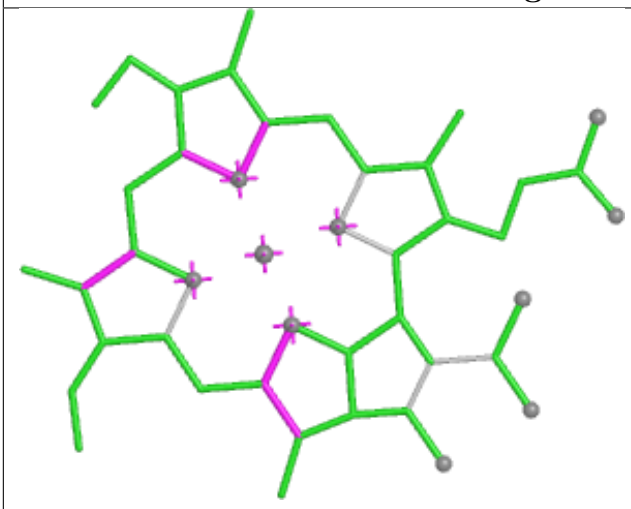


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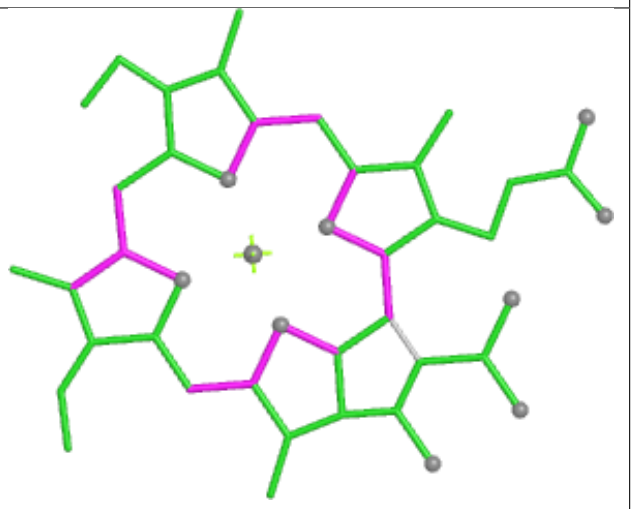


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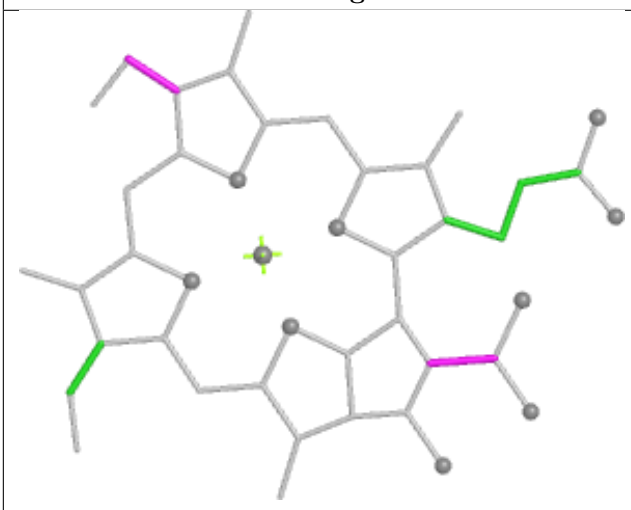
Ligand CLA B 818



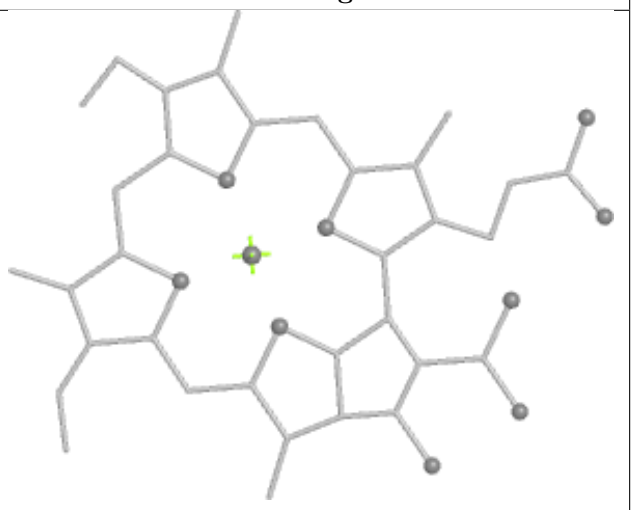
Bond lengths



Bond angles

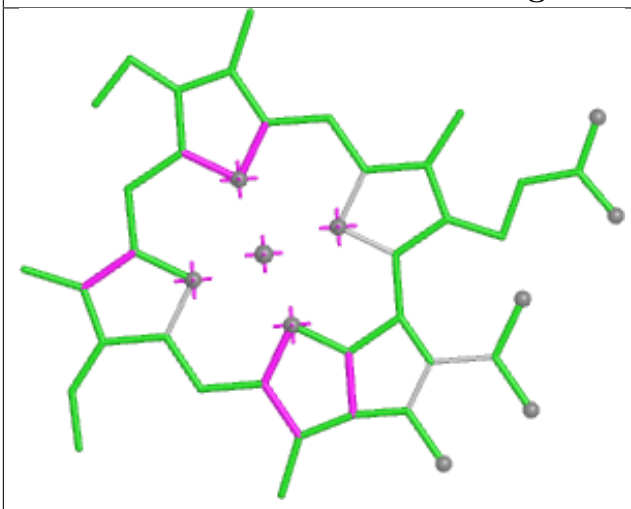


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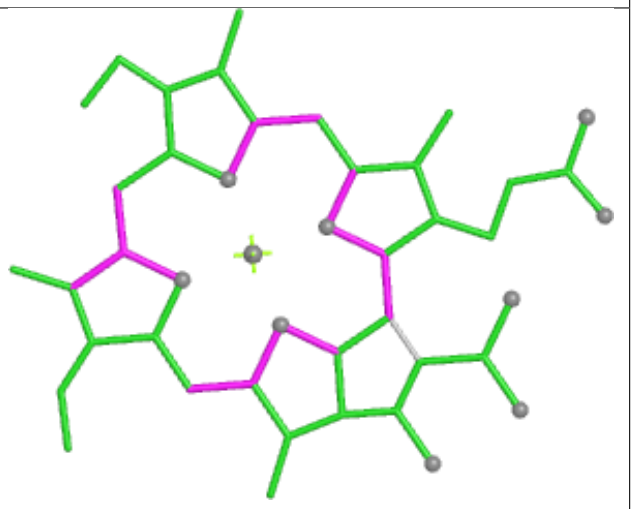


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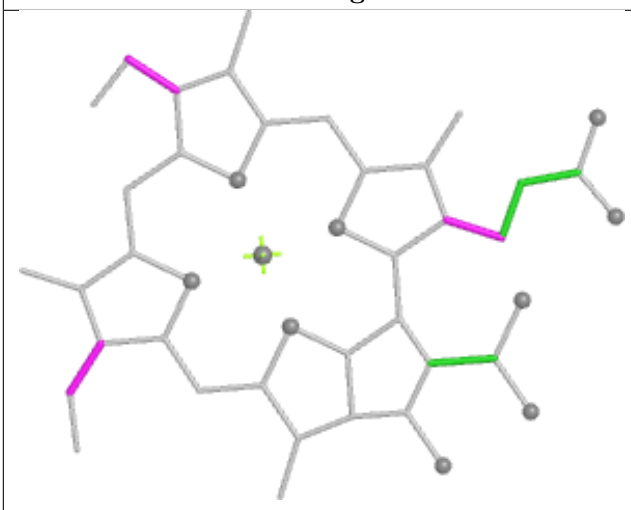
Ligand CLA J 102



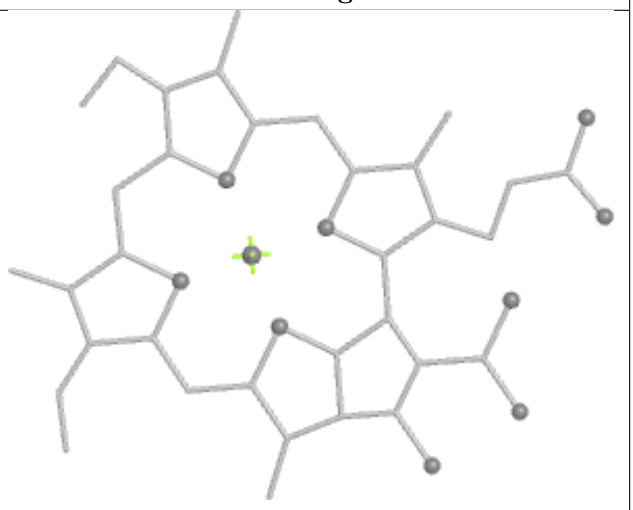
Bond lengths



Bond angles

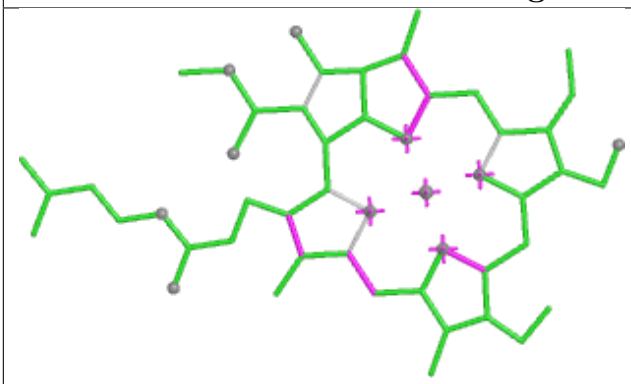


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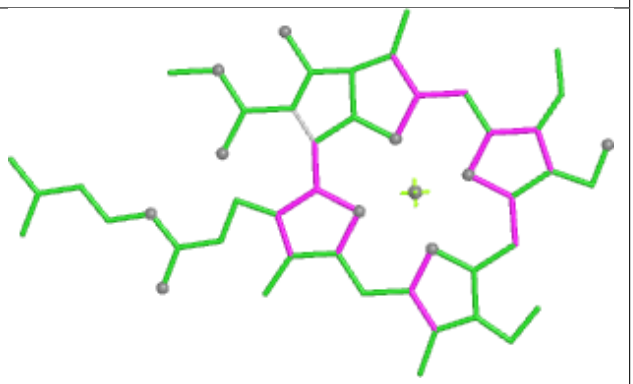


Rings

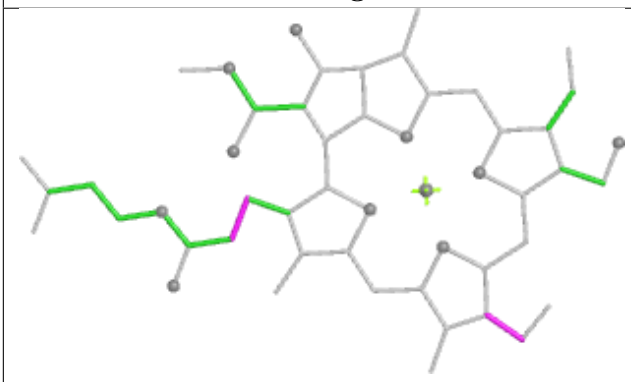
Ligand CHL 8 315



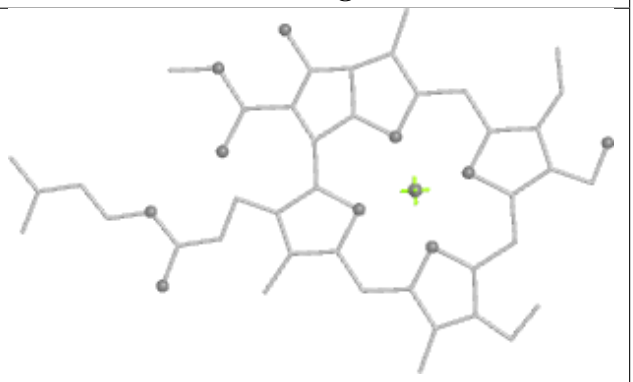
Bond lengths



Bond angles

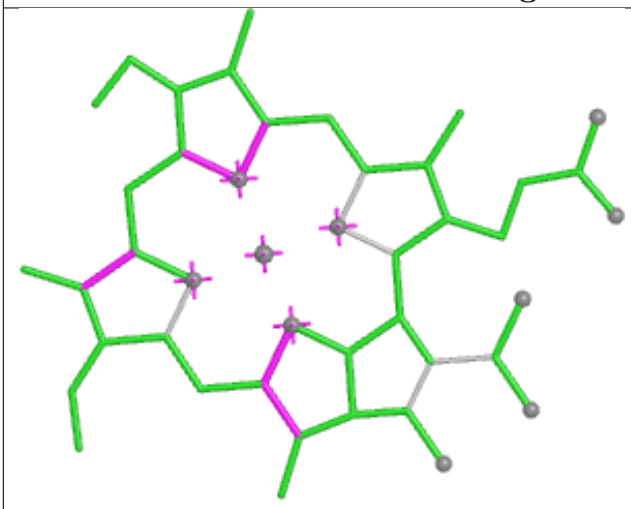


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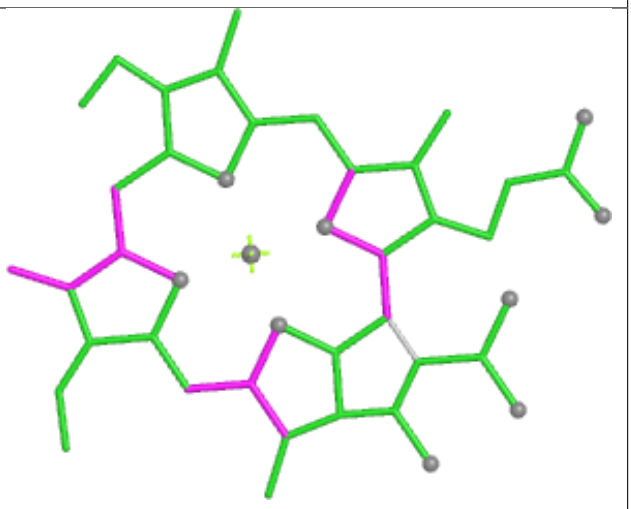


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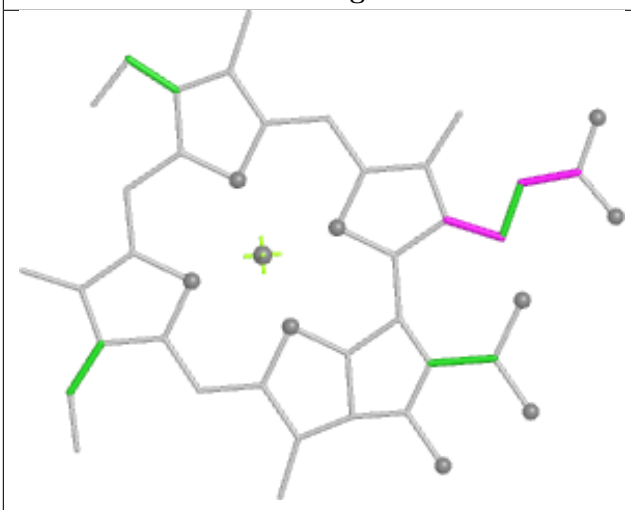
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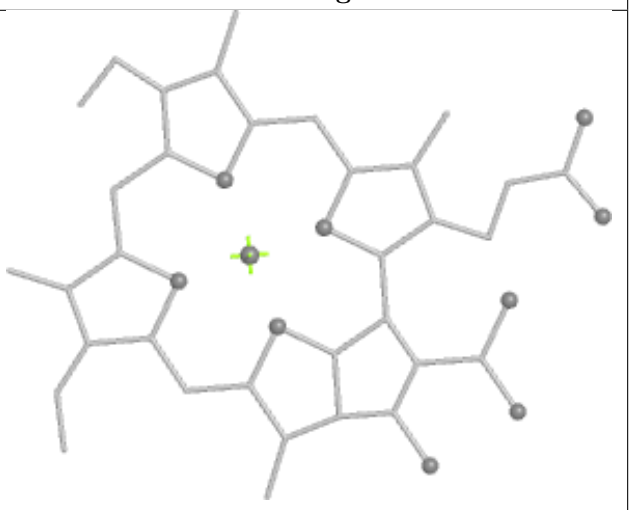
Bond lengths



Bond angles

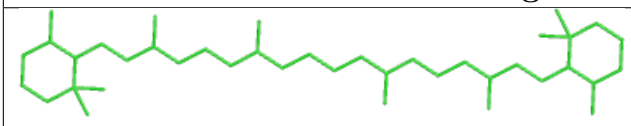


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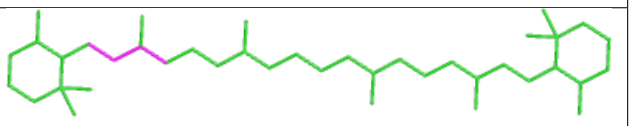


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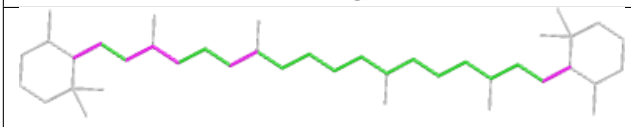
Ligand BCR A 847



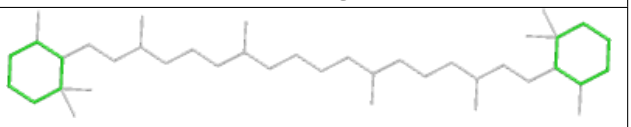
Bond lengths



Bond angles

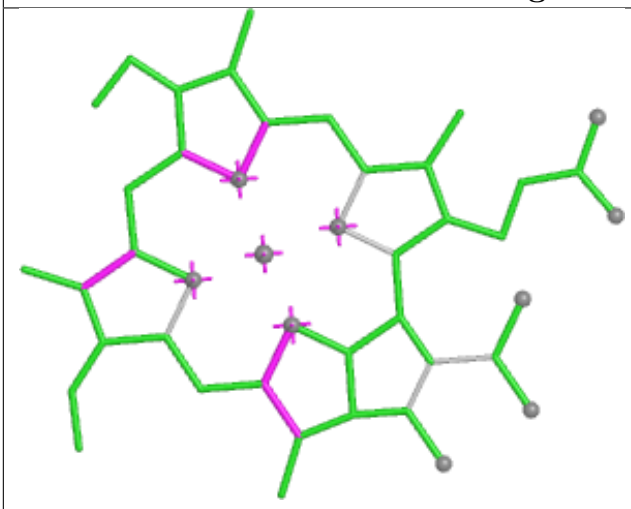


Torsions

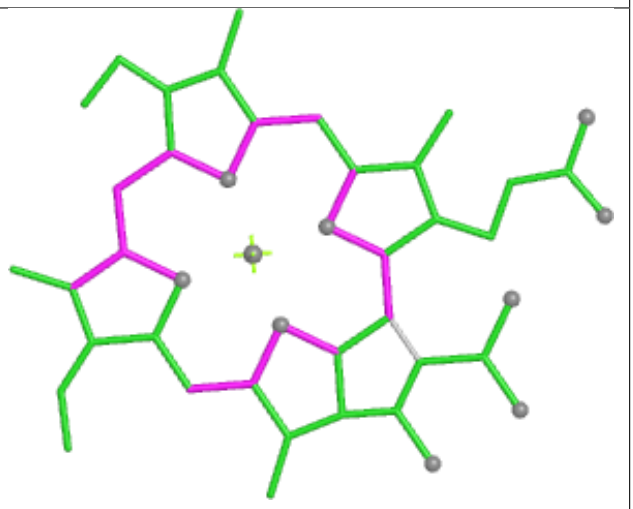


Rings

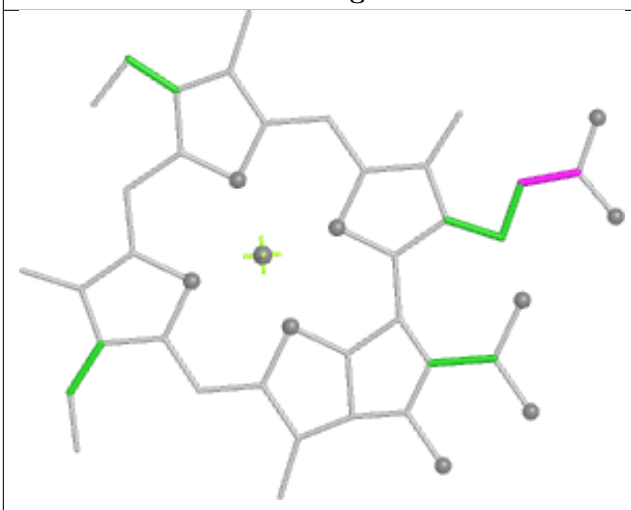
Ligand CLA 0 301



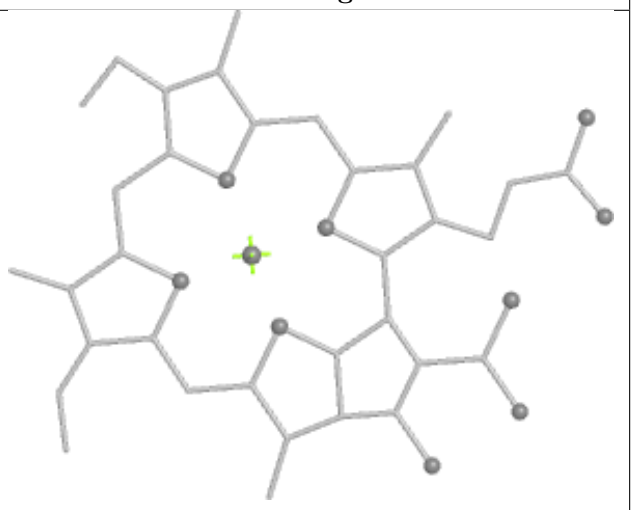
Bond lengths



Bond angles

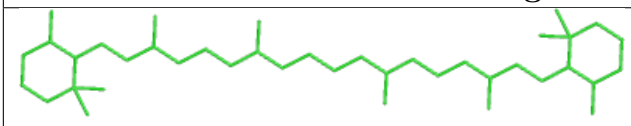


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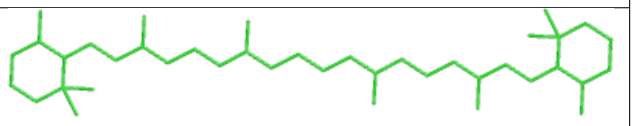


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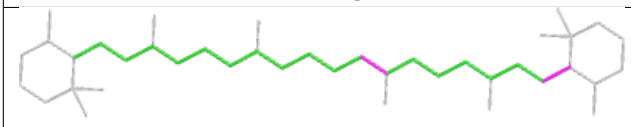
Ligand BCR F 304



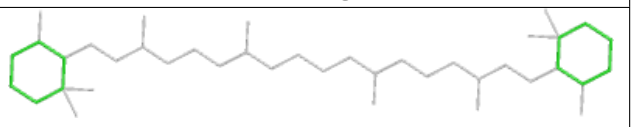
Bond lengths



Bond angles

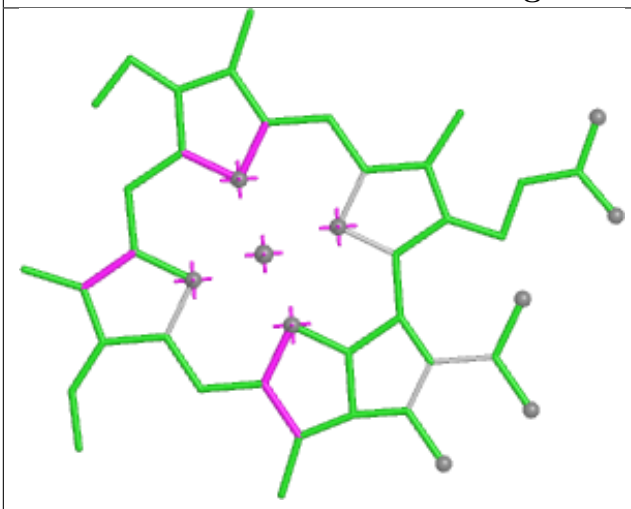


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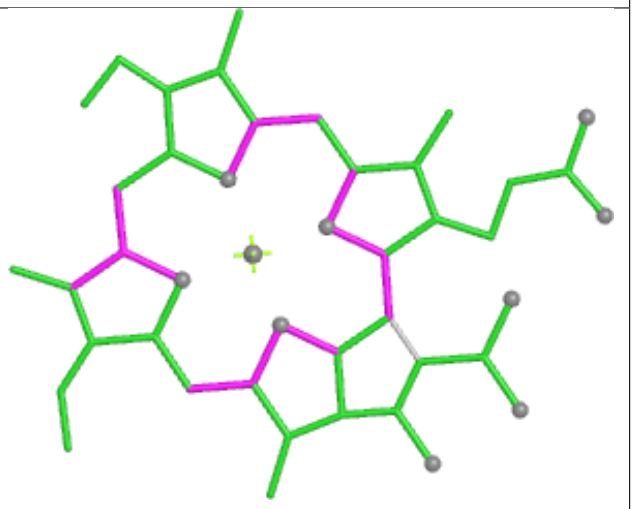


Rings

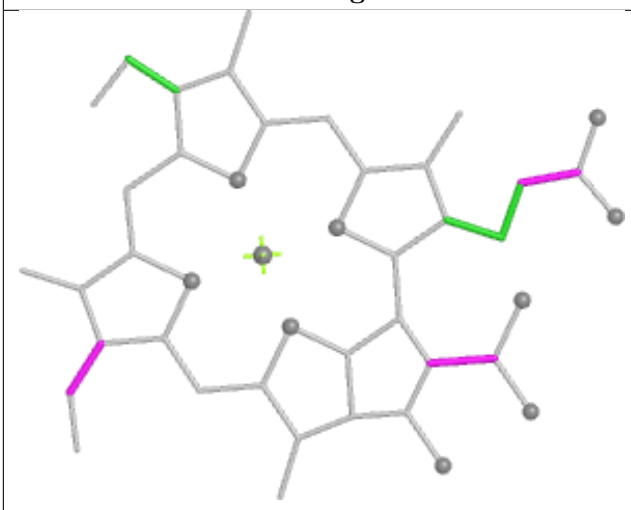
Ligand CLA A 812



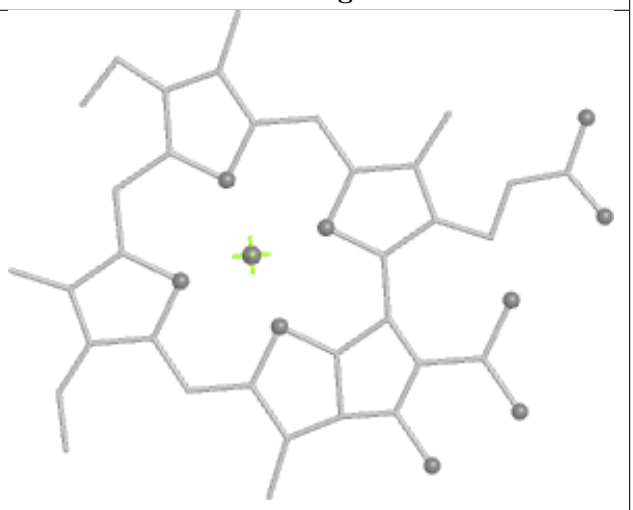
Bond lengths



Bond angles

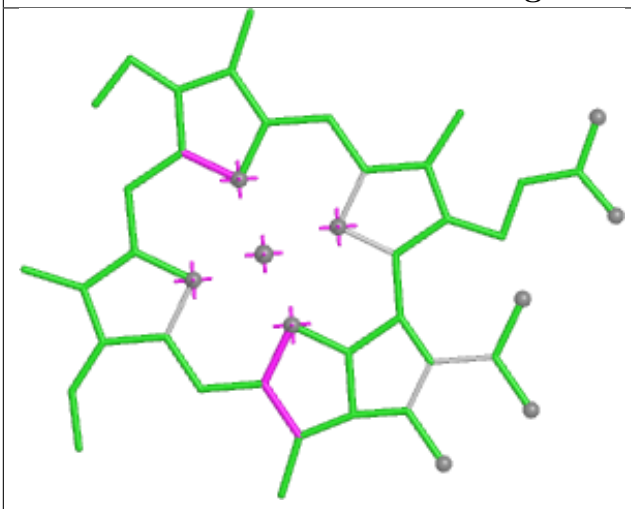


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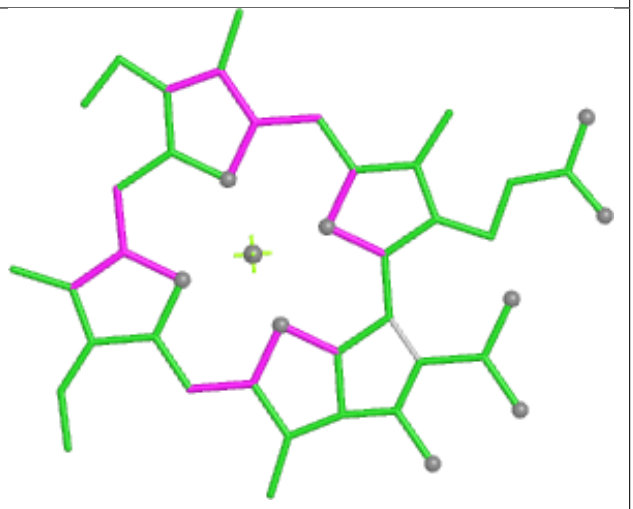


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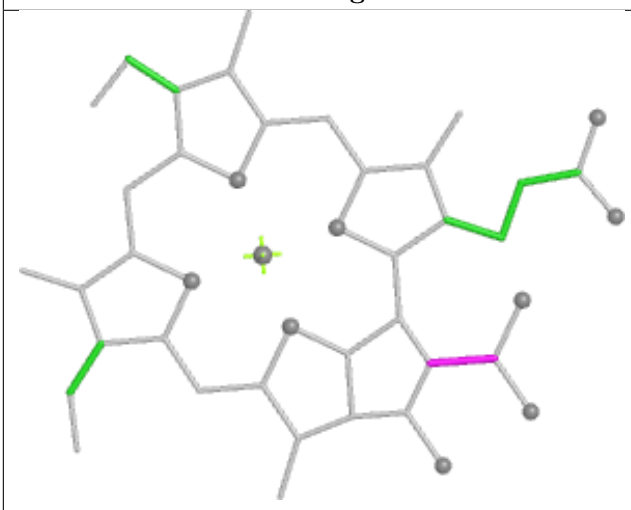
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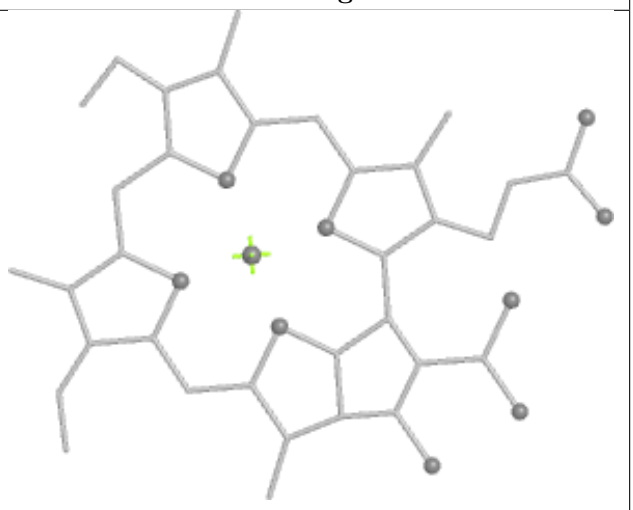
Bond lengths



Bond angles

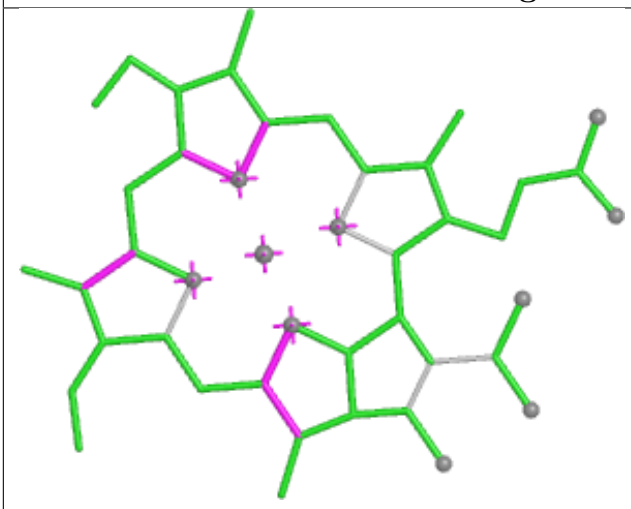


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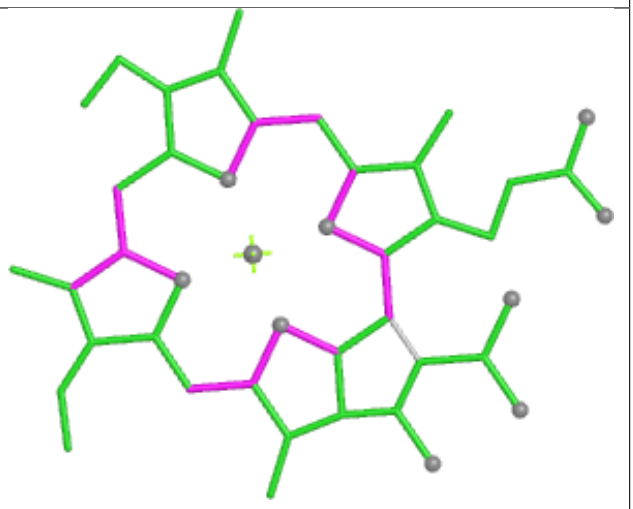


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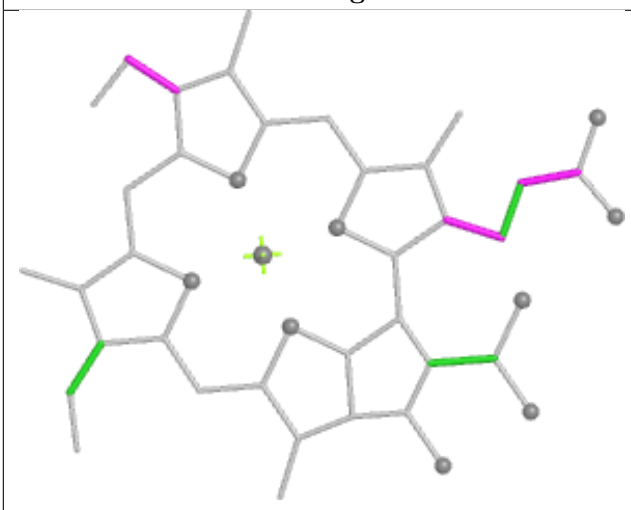
Ligand CLA 3 1012



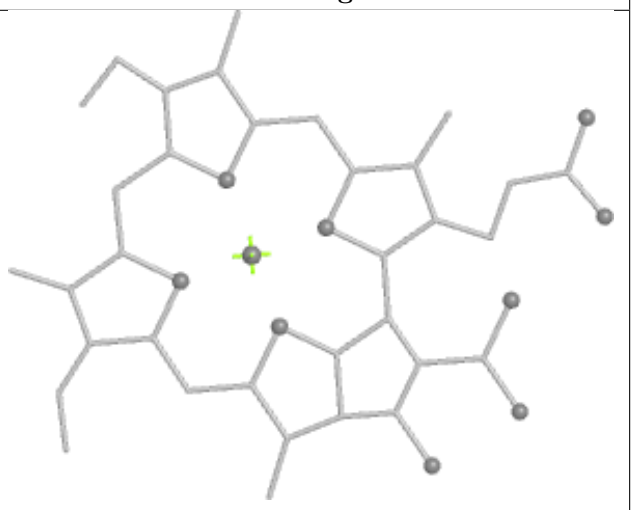
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Bond angles

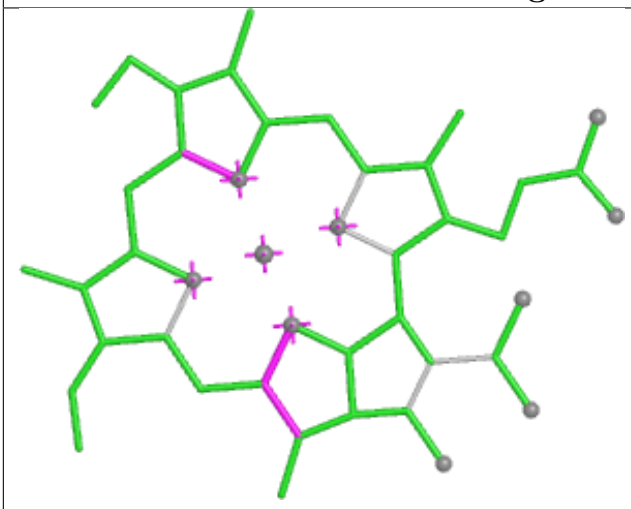


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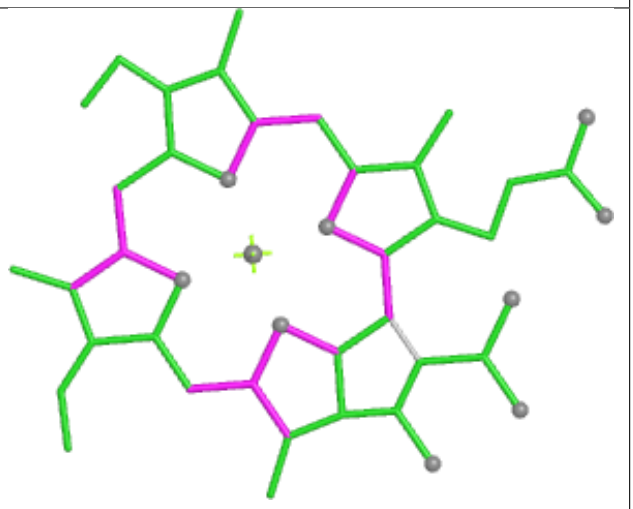


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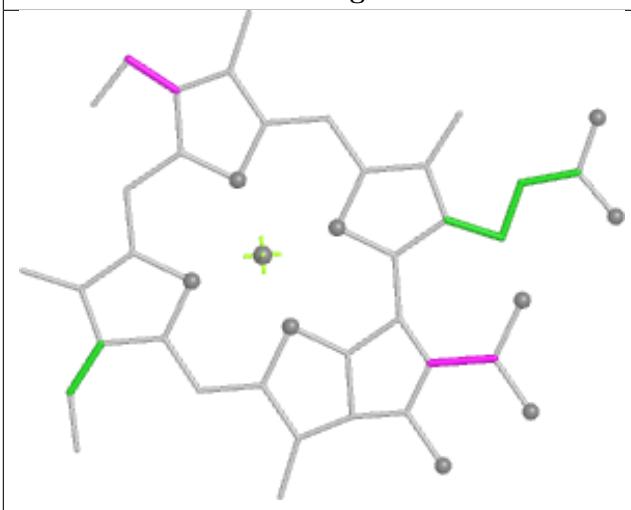
Ligand CLA 8 313



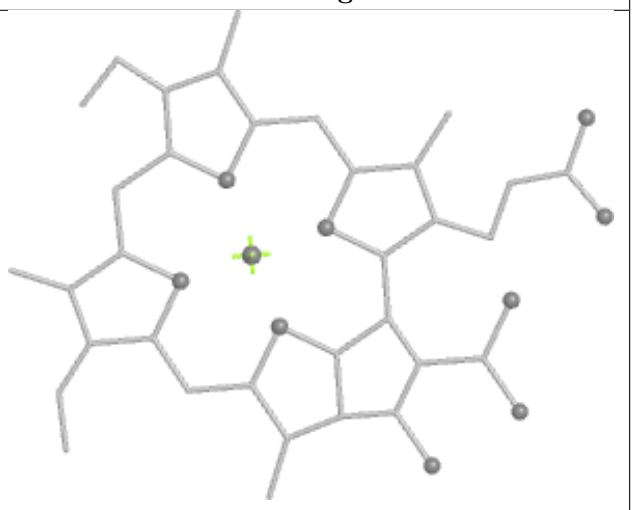
Bond lengths



Bond angles

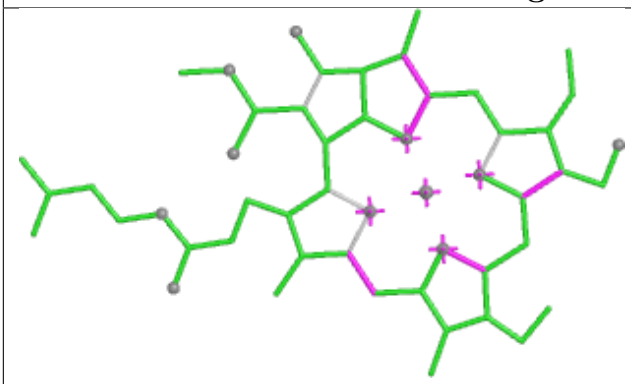


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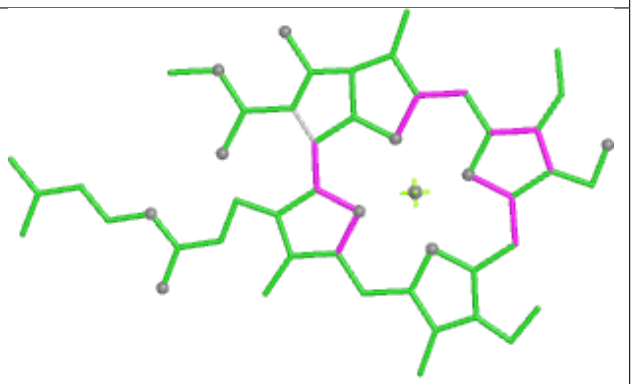


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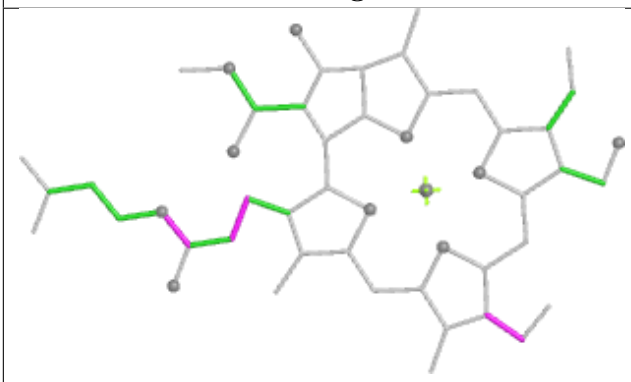
Ligand CHL 0 315



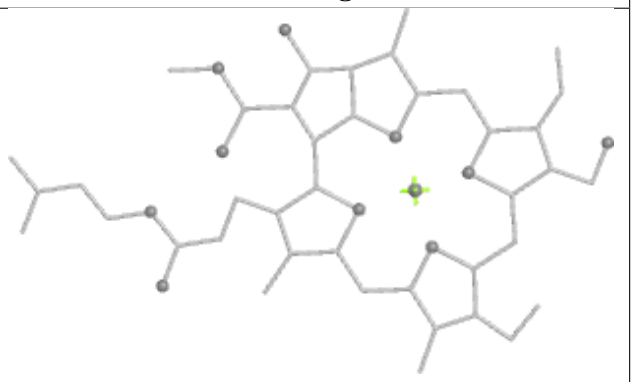
Bond lengths



Bond angles

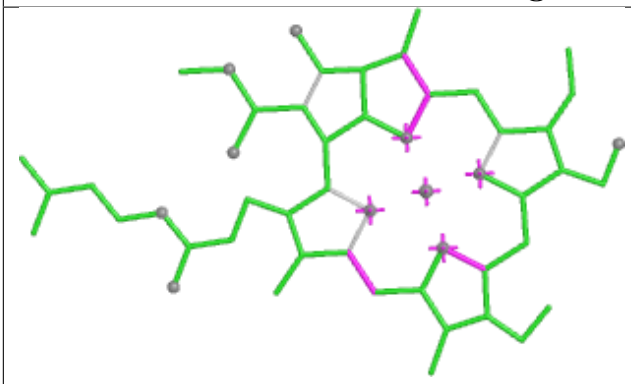


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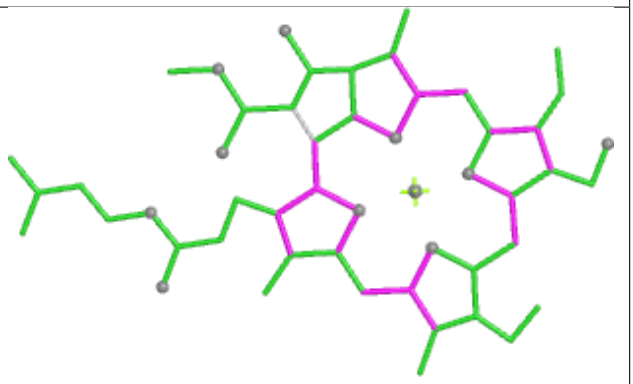


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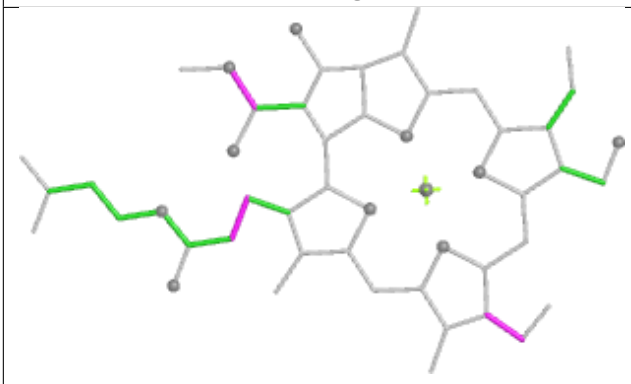
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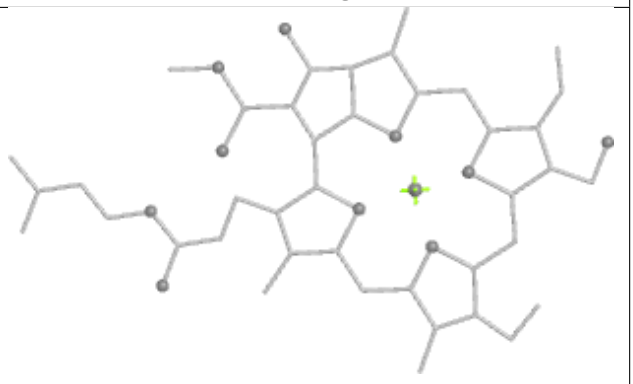
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Bond angles

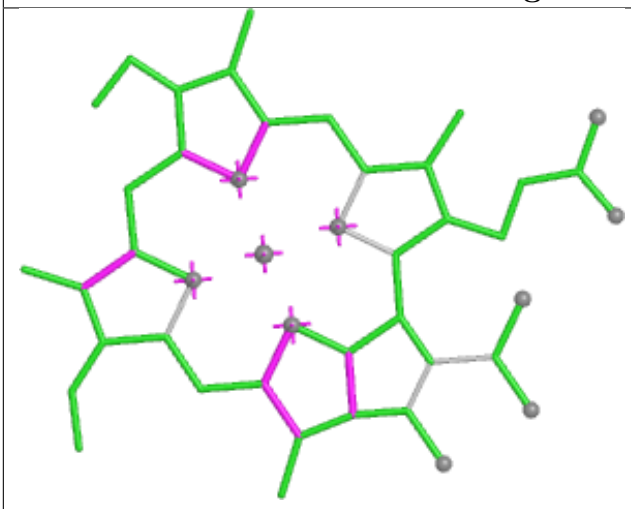


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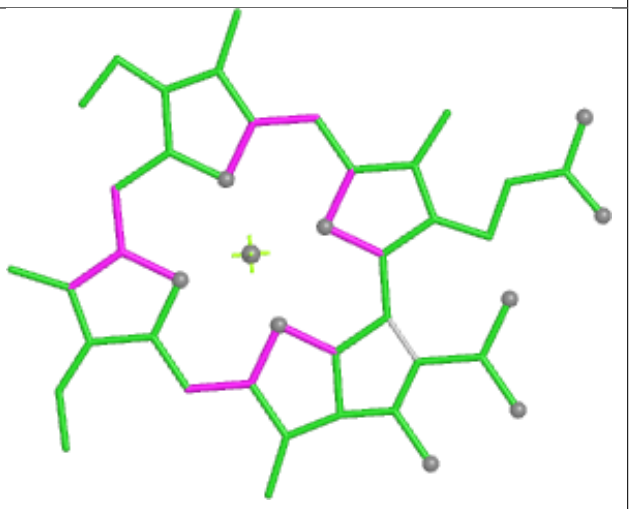


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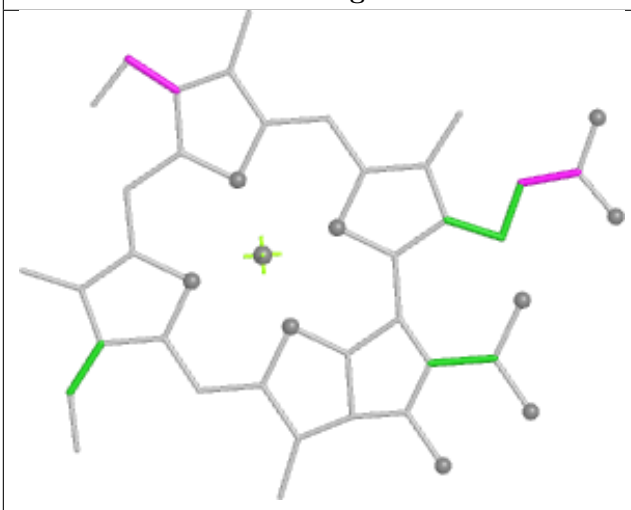
Ligand CLA A 839



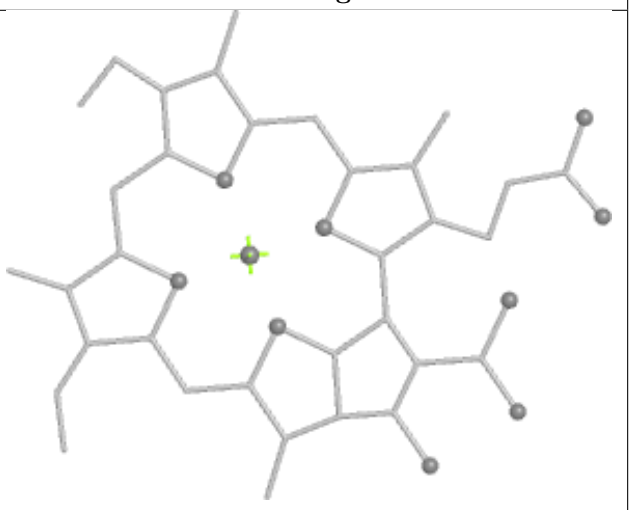
Bond lengths



Bond angles

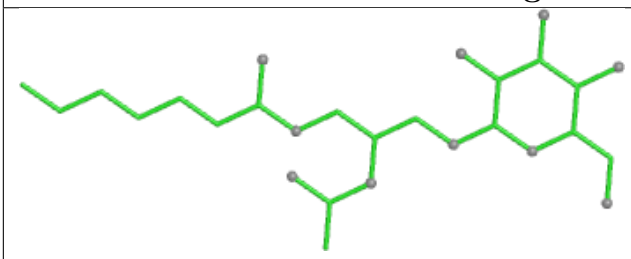


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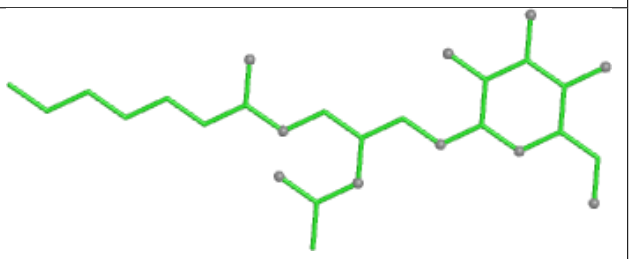


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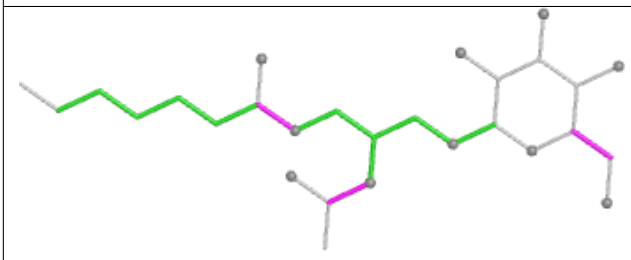
Ligand LMG 8 318



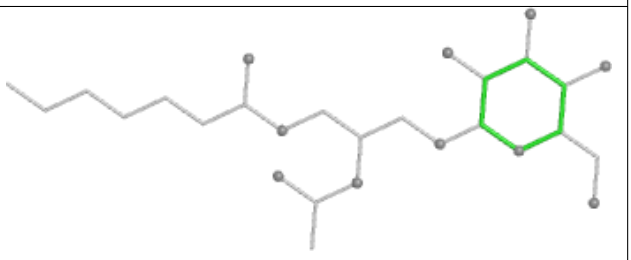
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Bond angles

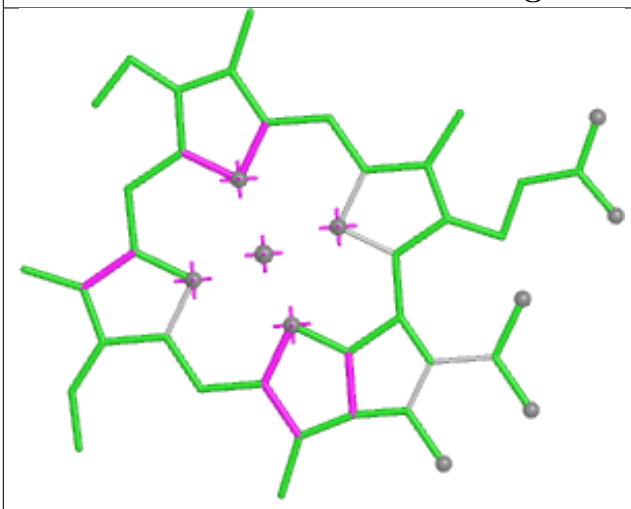


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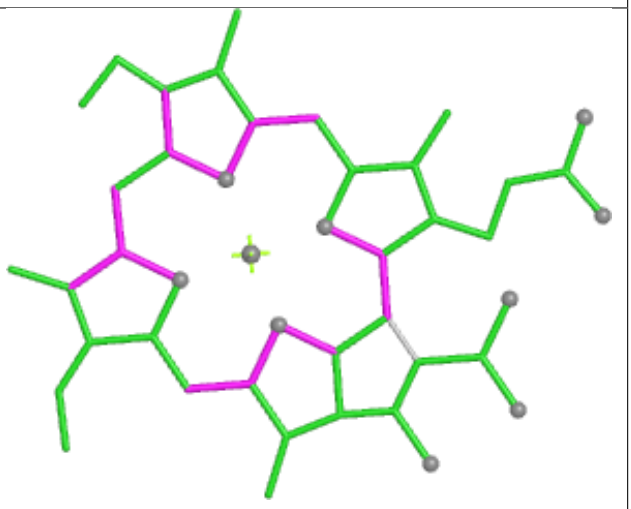


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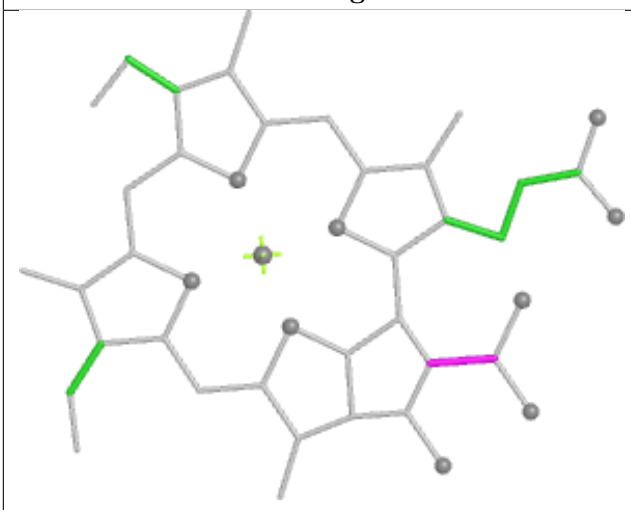
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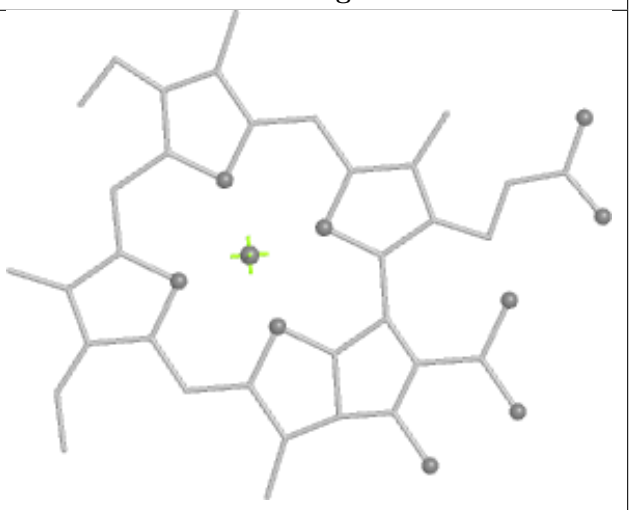
Bond lengths



Bond angles

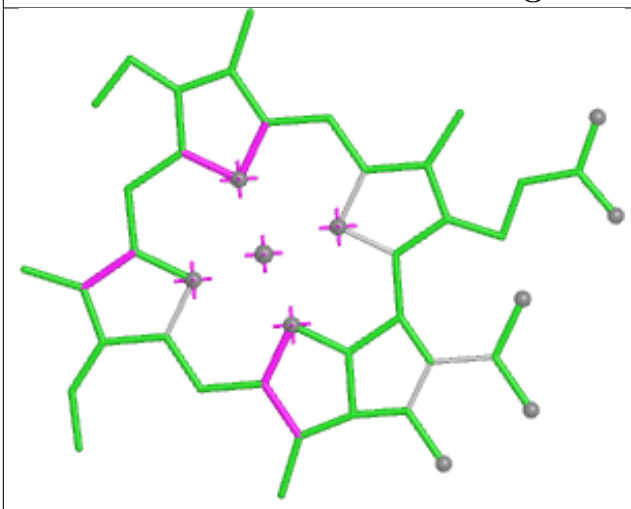


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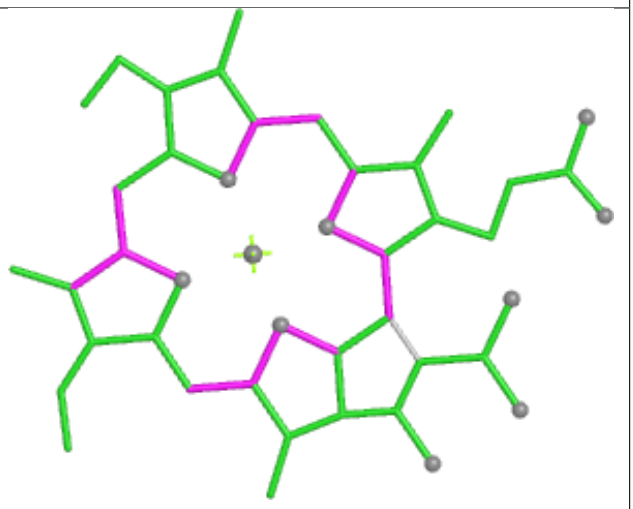


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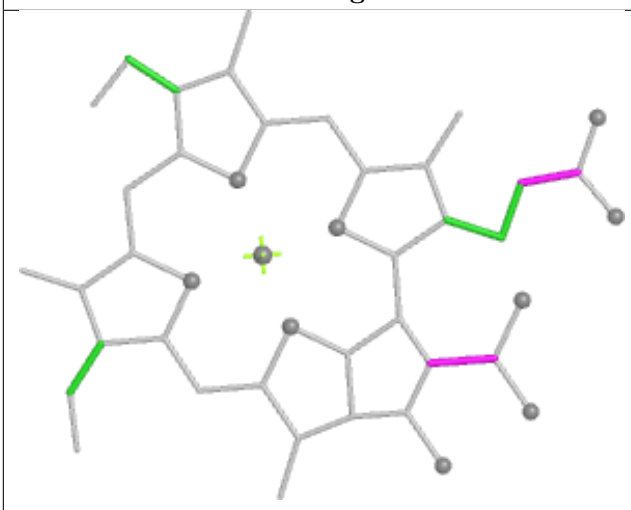
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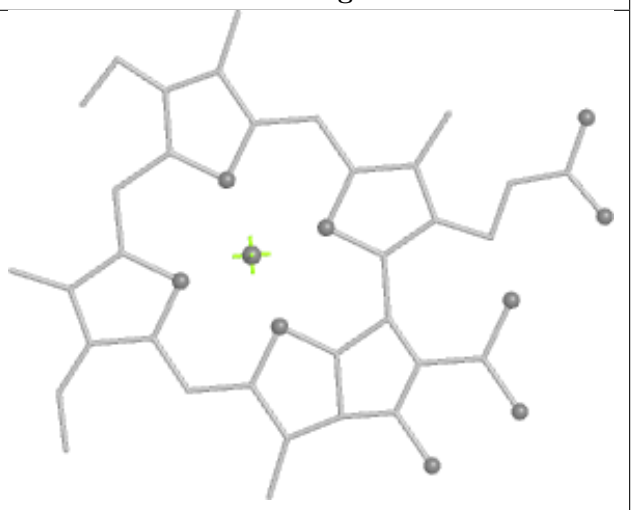
Bond lengths



Bond angles

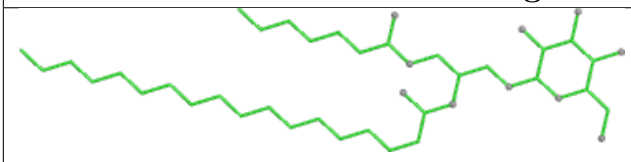


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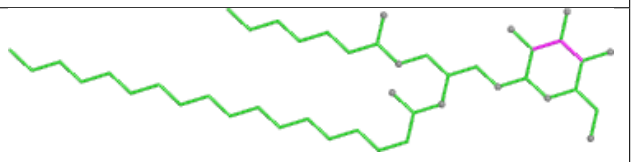


Rings

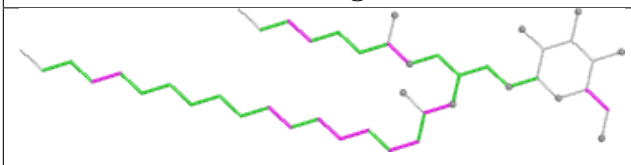
Ligand LMG 6 319



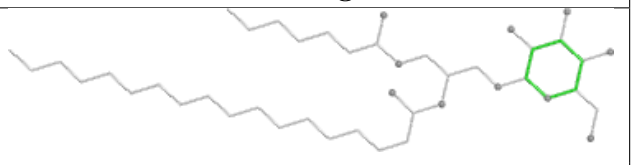
Bond lengths



Bond angles

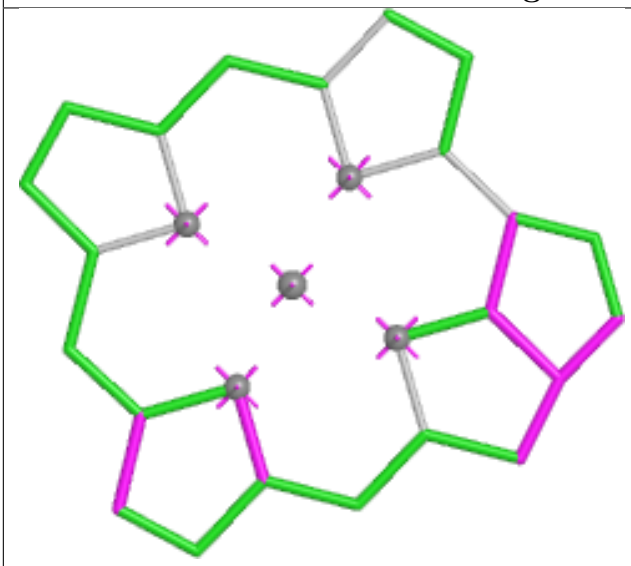


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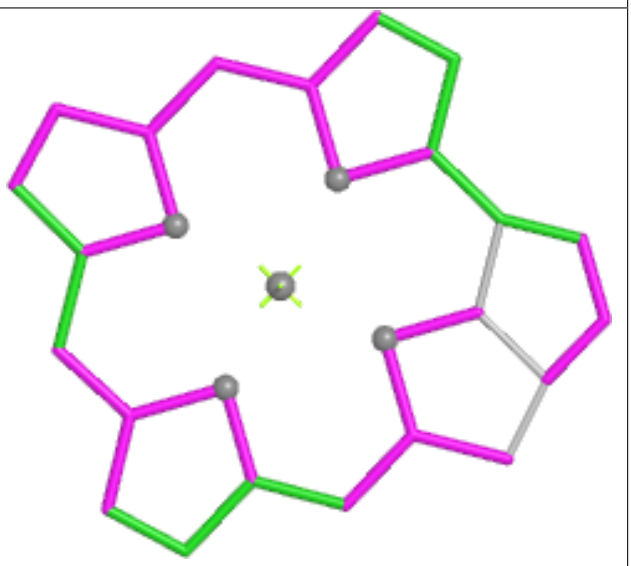


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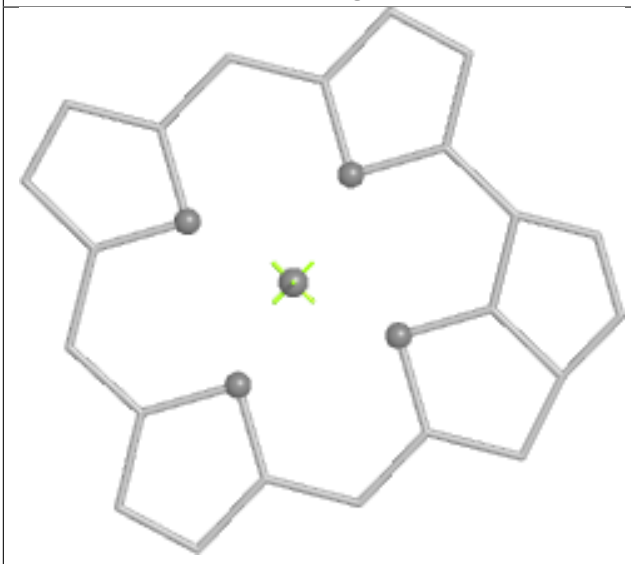
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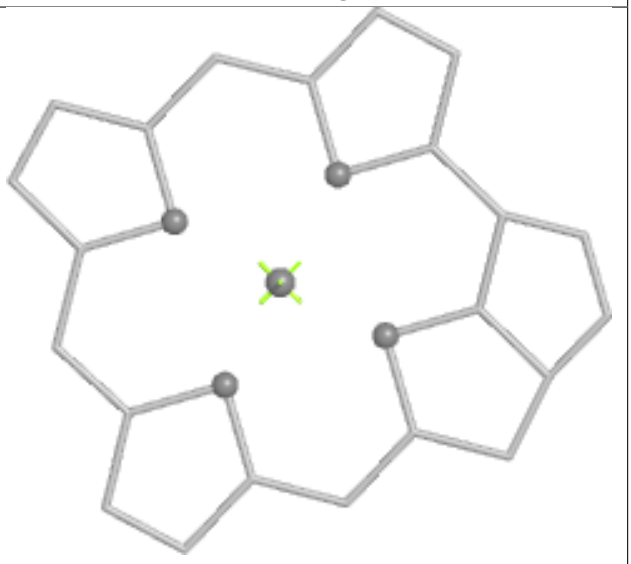
Bond lengths



Bond angles

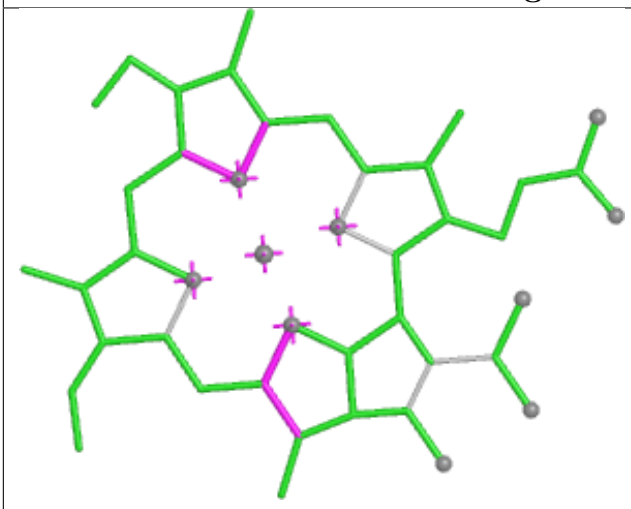


Torsions

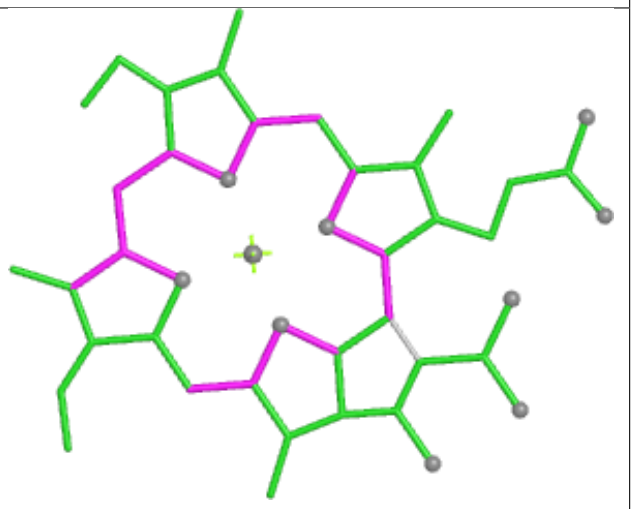


Rings

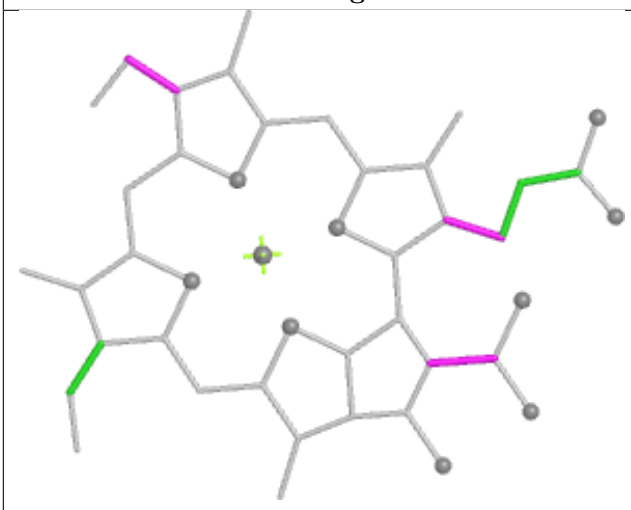
Ligand CLA B 837



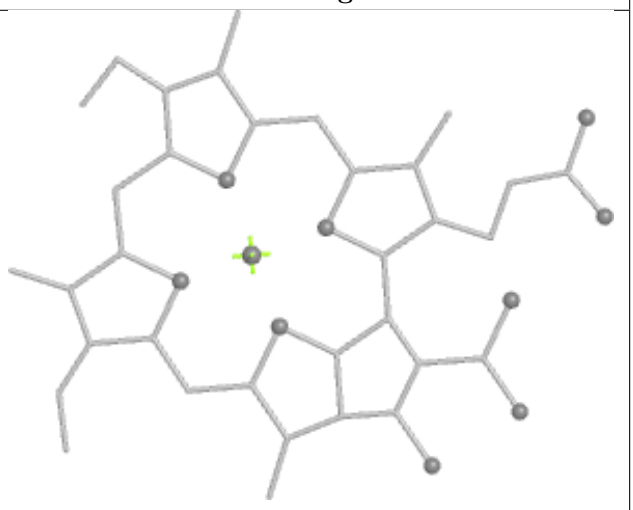
Bond lengths



Bond angles

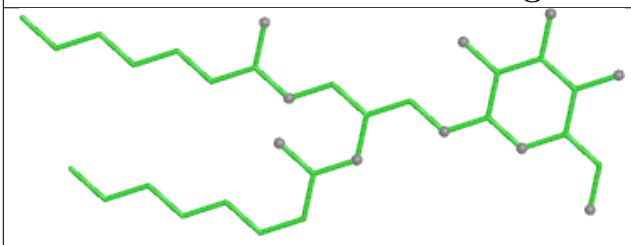


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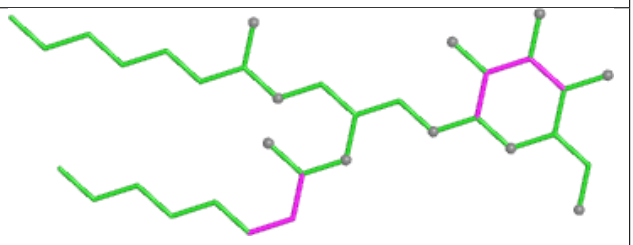


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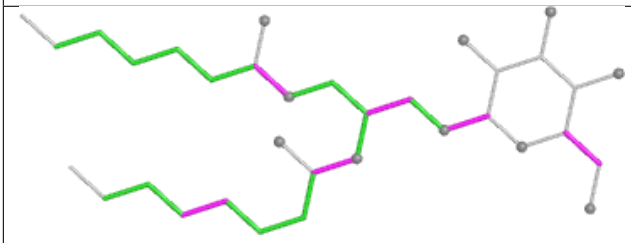
Ligand LMG 4 318



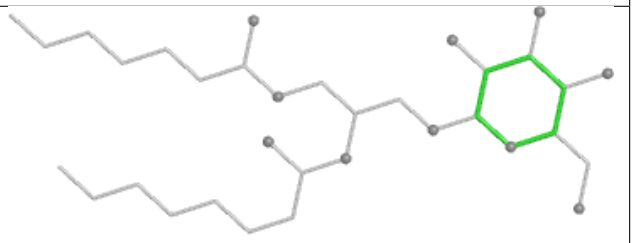
Bond lengths



Bond angles

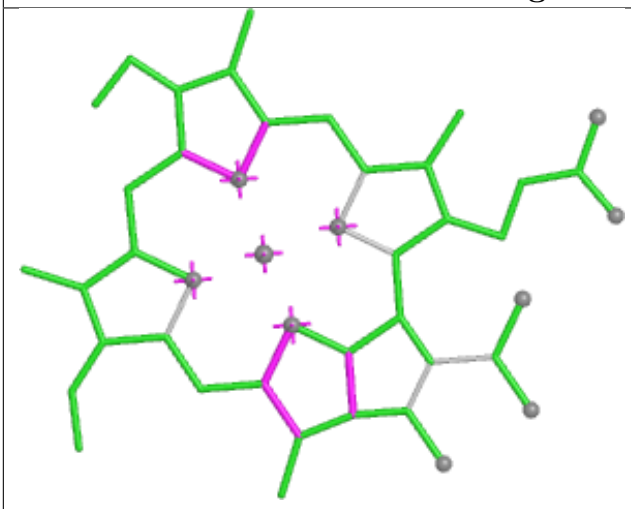


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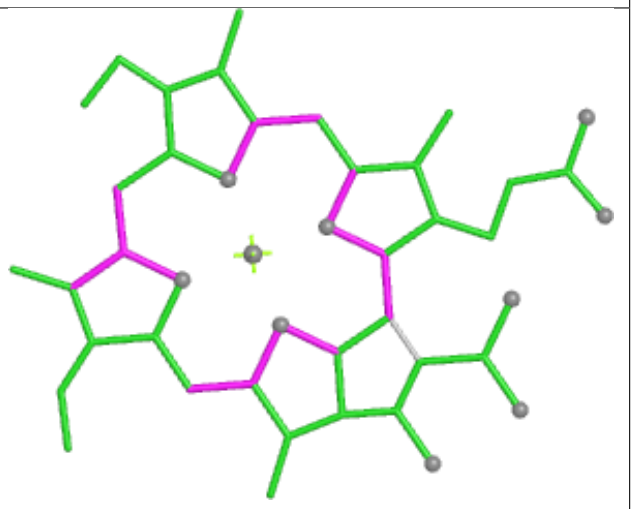


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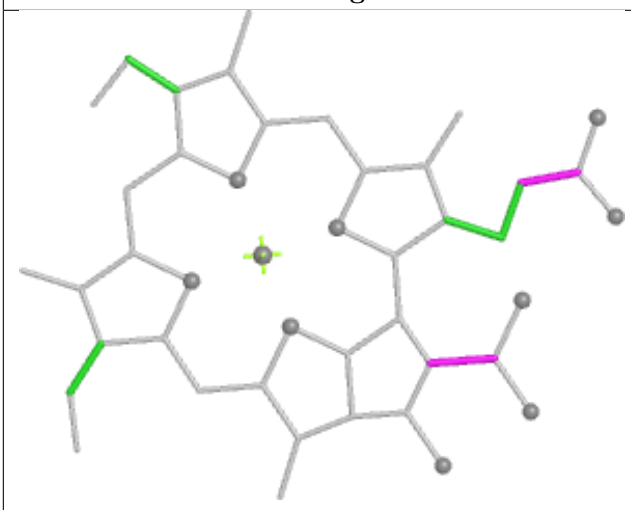
Ligand CLA 5 321



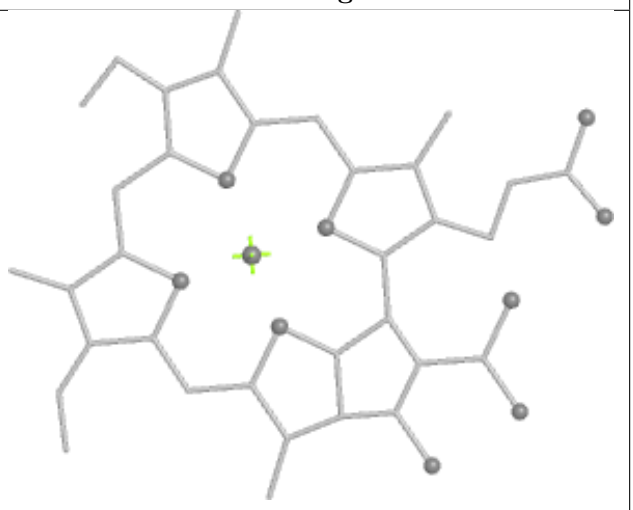
Bond lengths



Bond angles

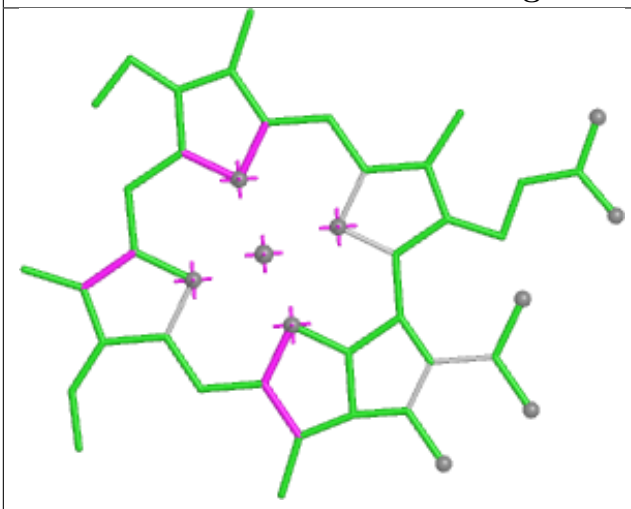


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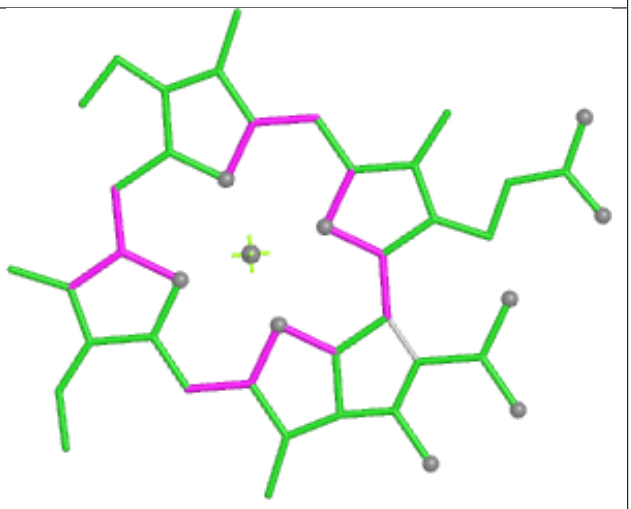


Rings

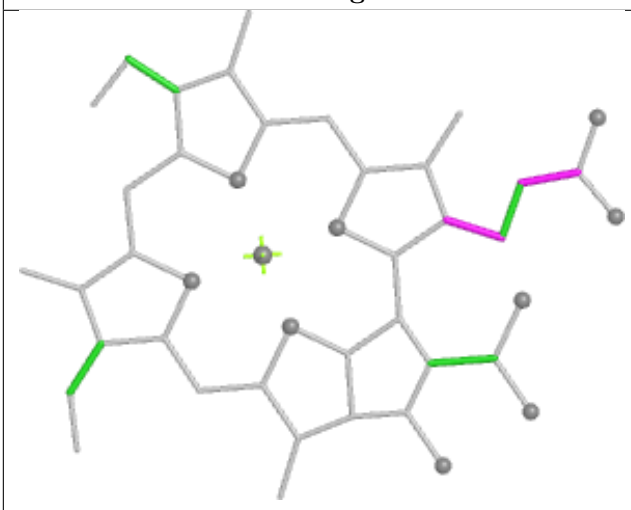
Ligand CLA G 202



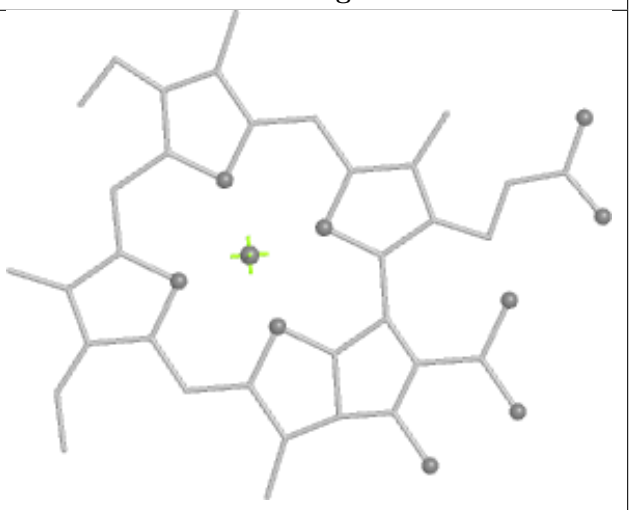
Bond lengths



Bond angles

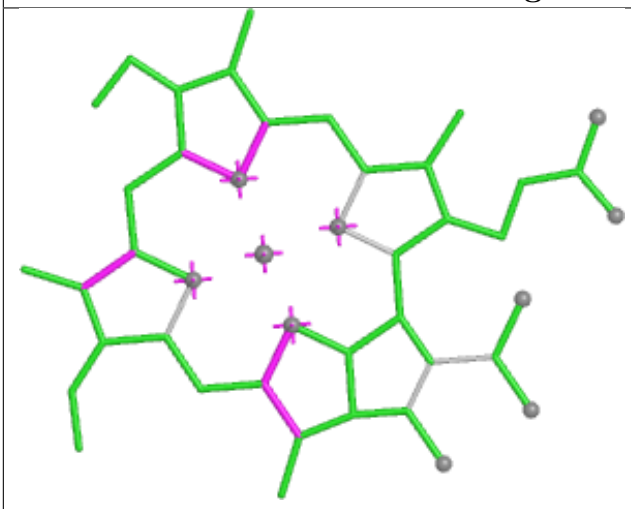


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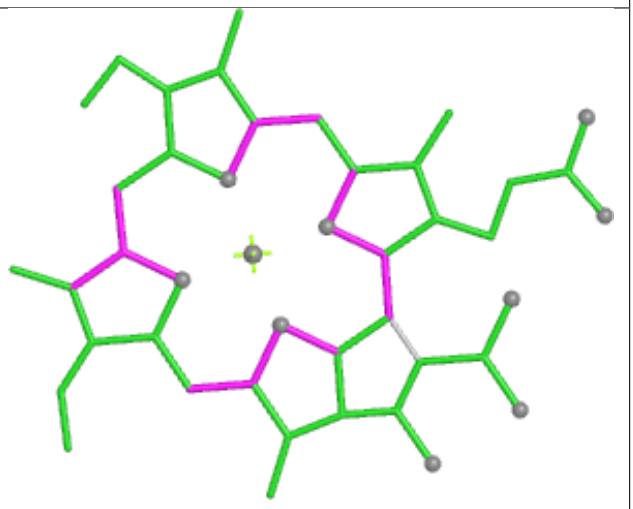


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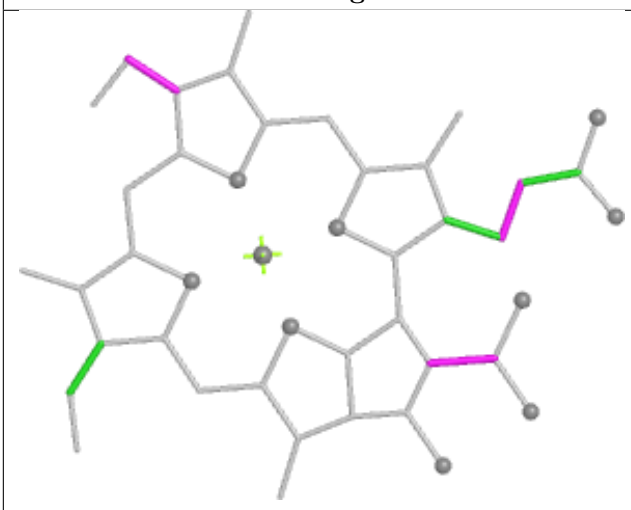
Ligand CLA B 820



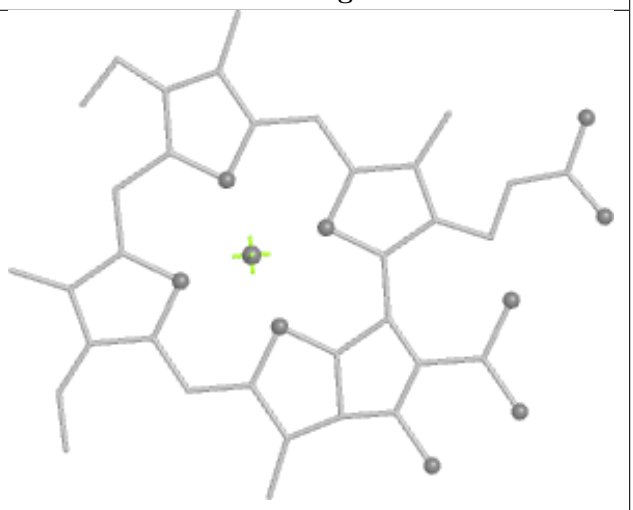
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Bond angles

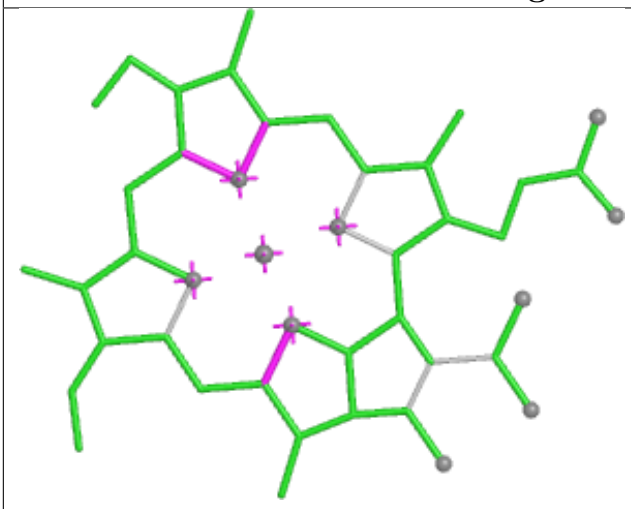


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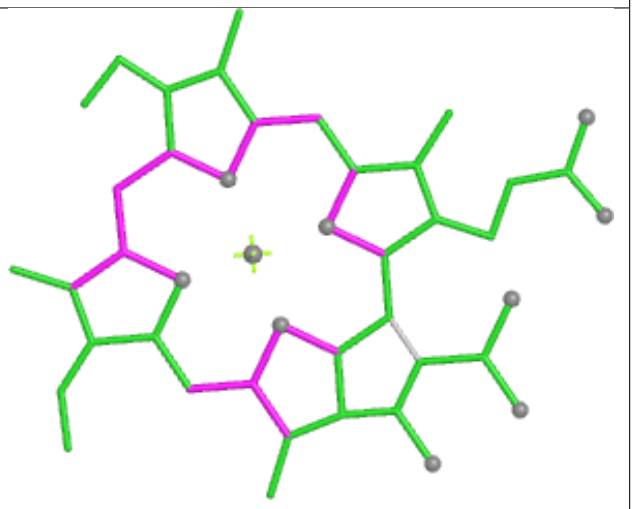


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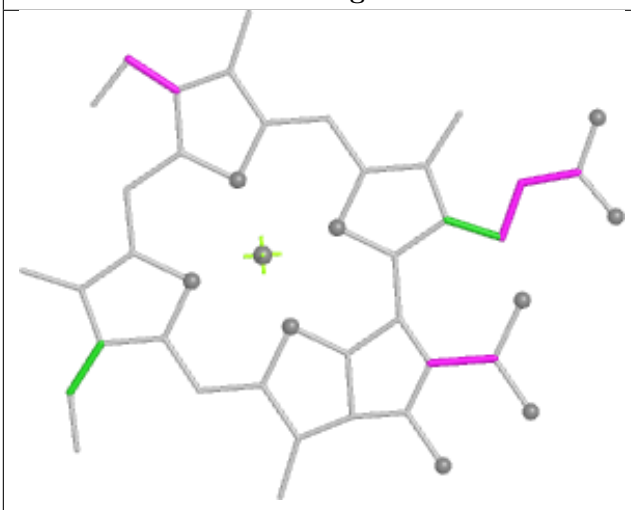
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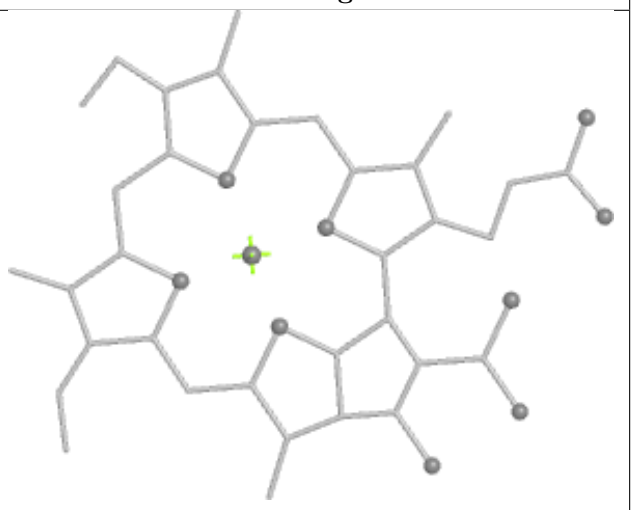
Bond lengths



Bond angles

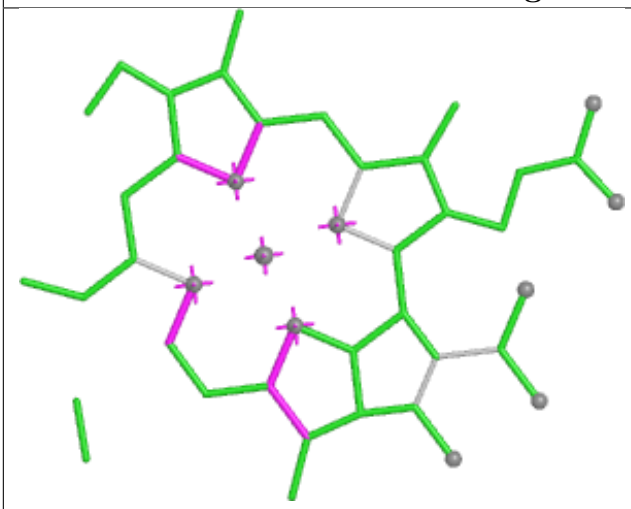


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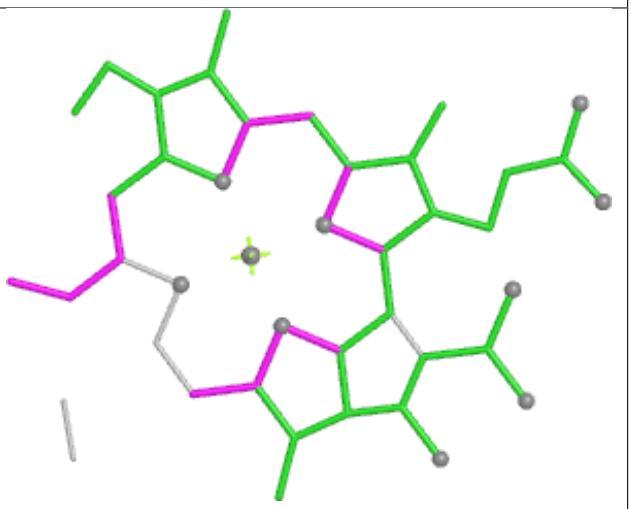


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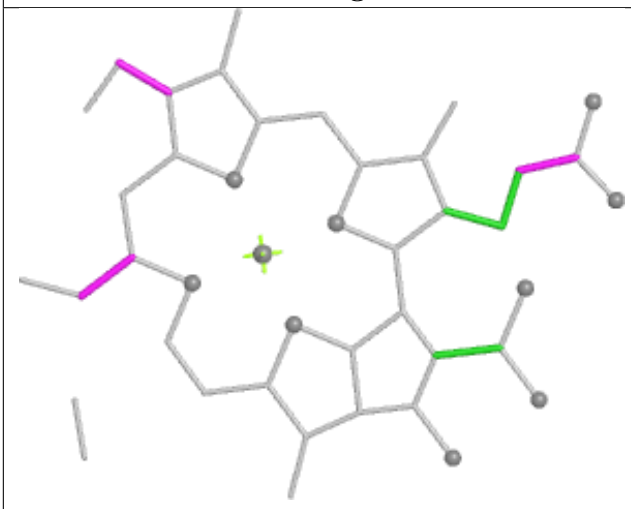
Ligand CLA B 850



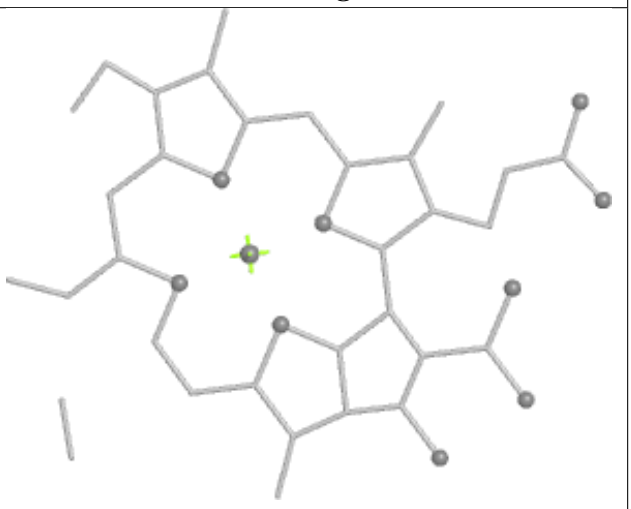
Bond lengths



Bond angles

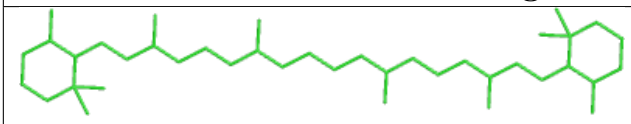


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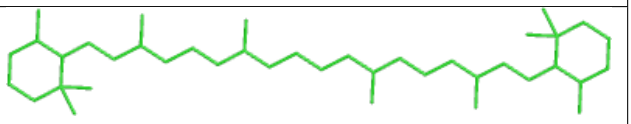


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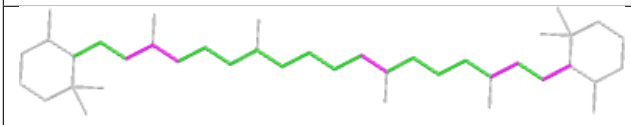
Ligand BCR A 848



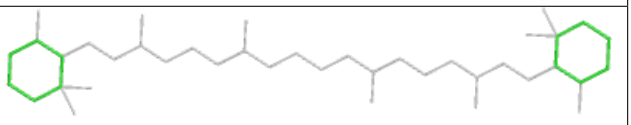
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Bond angles

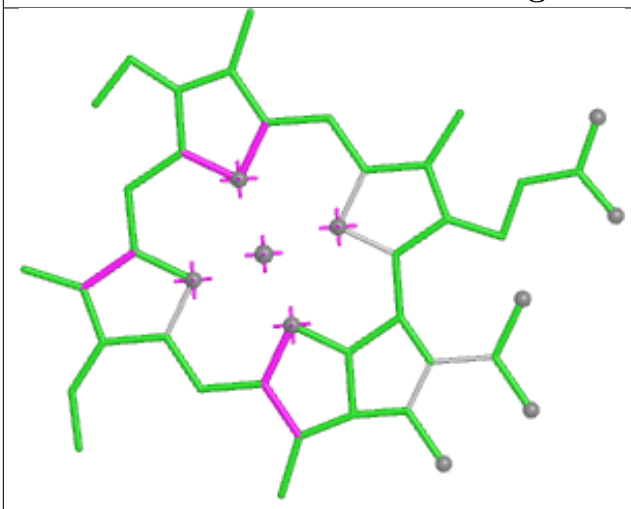


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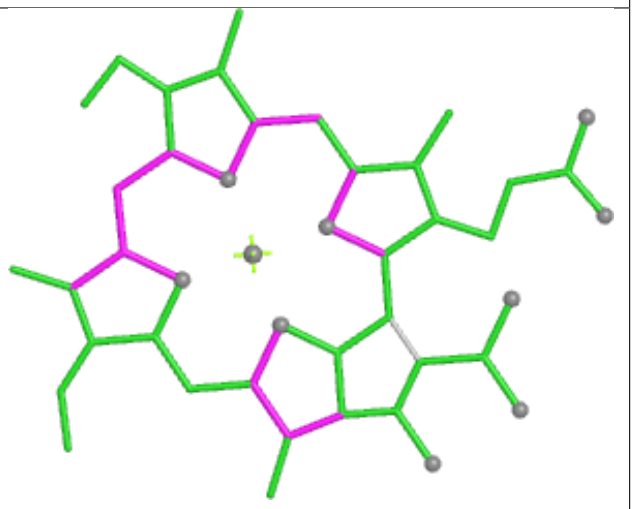


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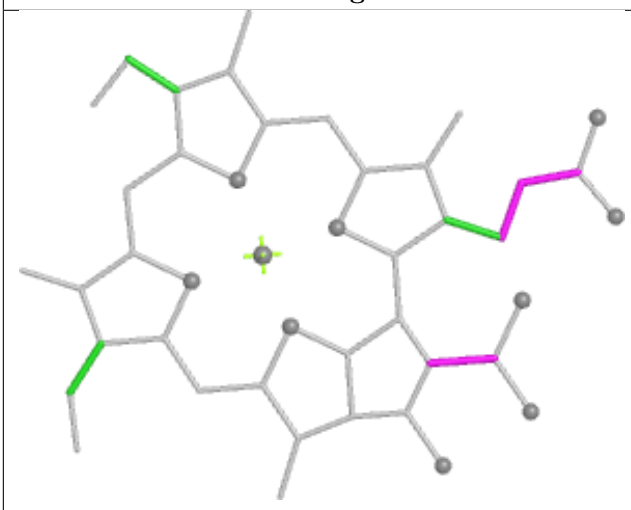
Ligand CLA 4 306



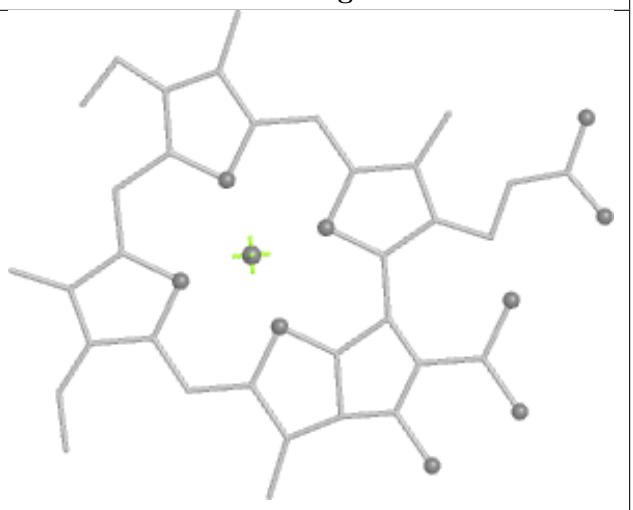
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Bond angles

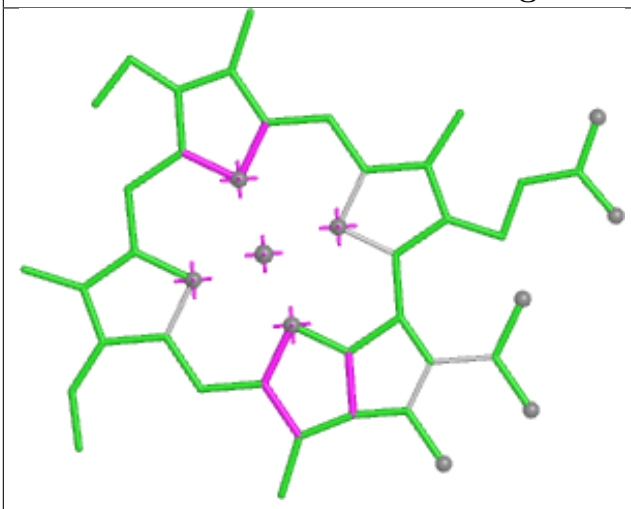


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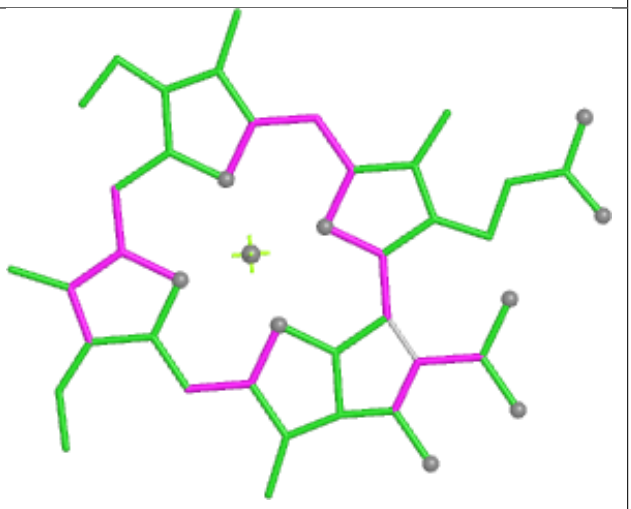


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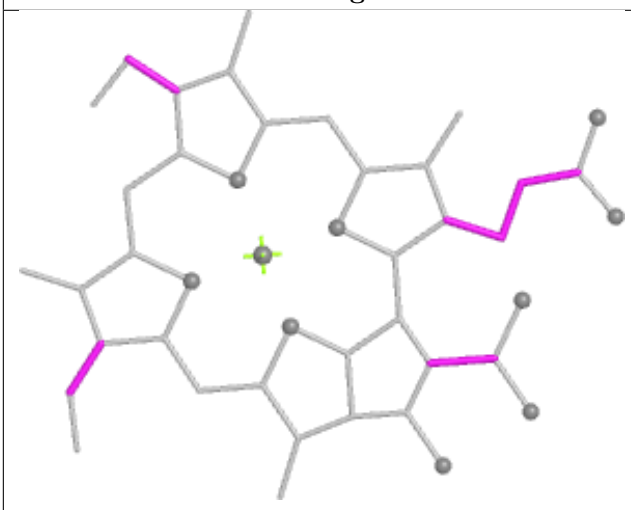
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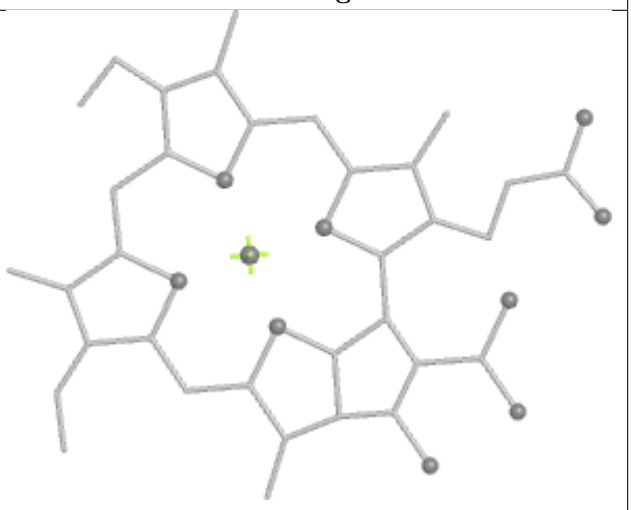
Bond lengths



Bond angles

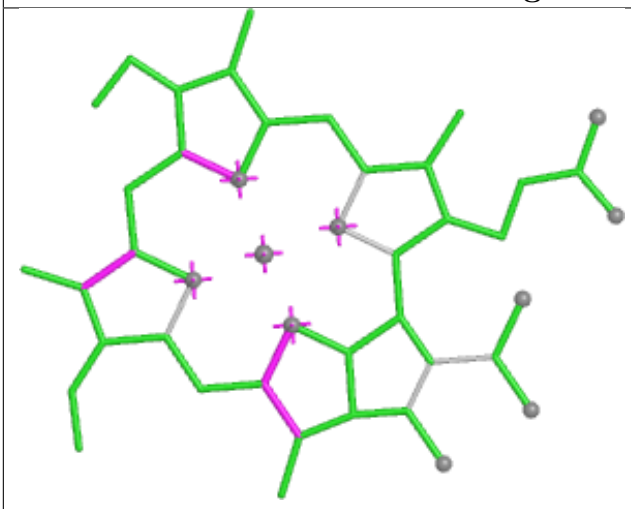


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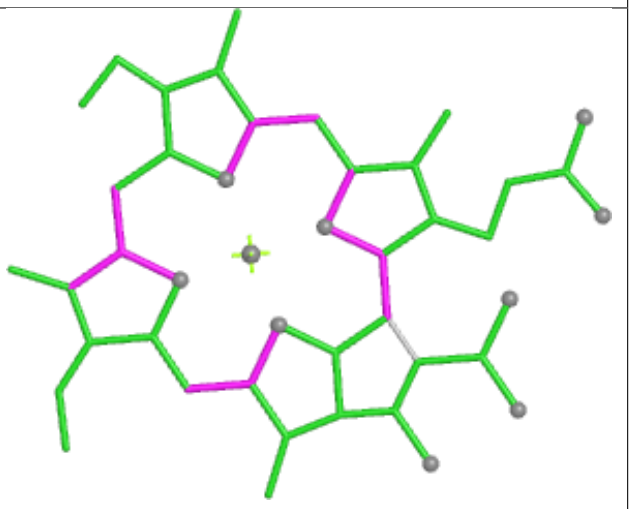


Rings

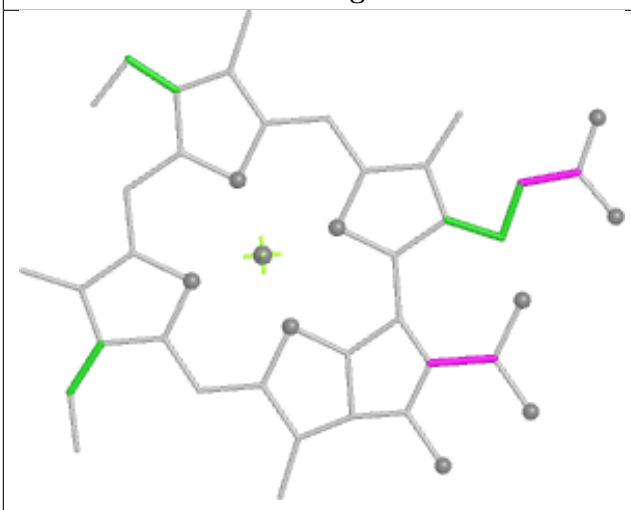
Ligand CLA A 827



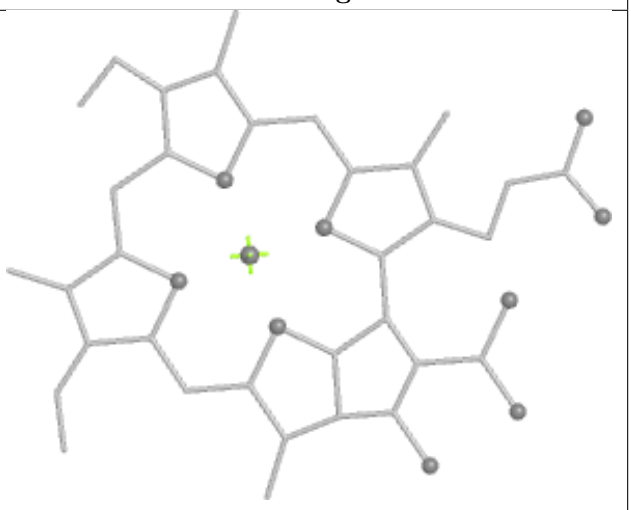
Bond lengths



Bond angles

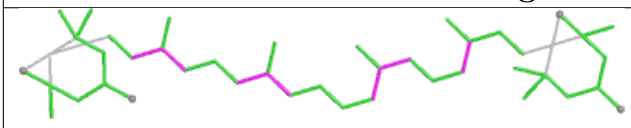


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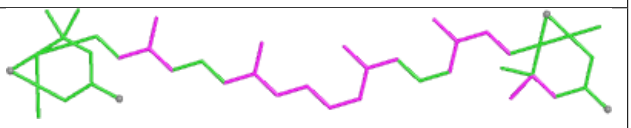


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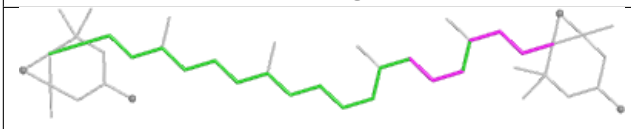
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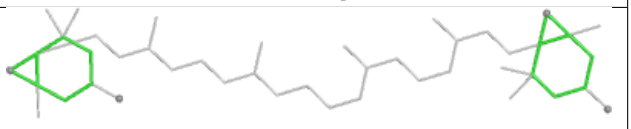
Bond lengths



Bond angles

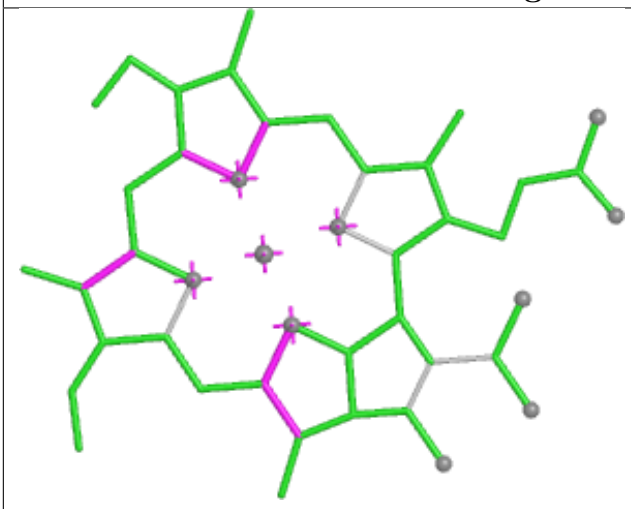


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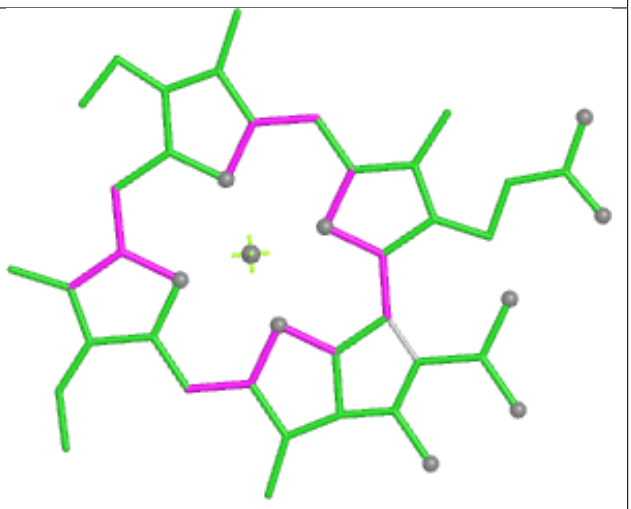


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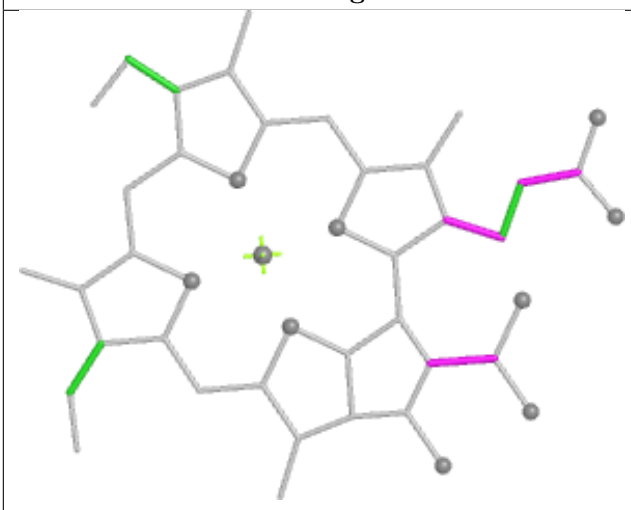
Ligand CLA B 826



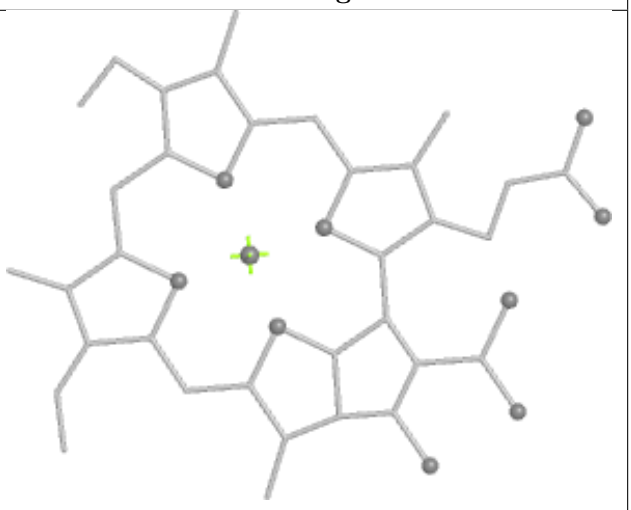
Bond lengths



Bond angles

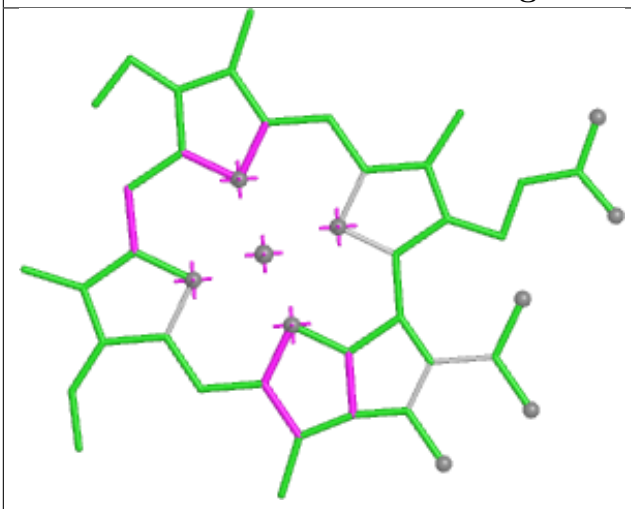


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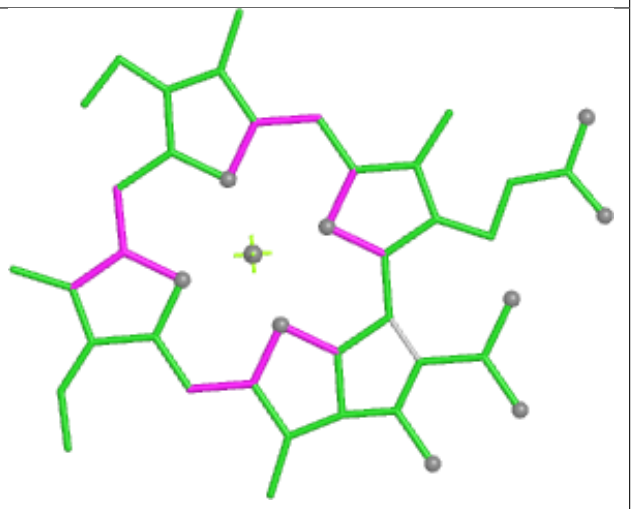


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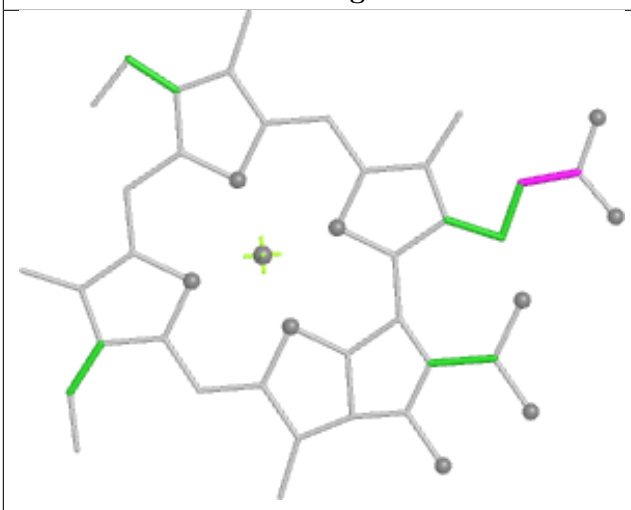
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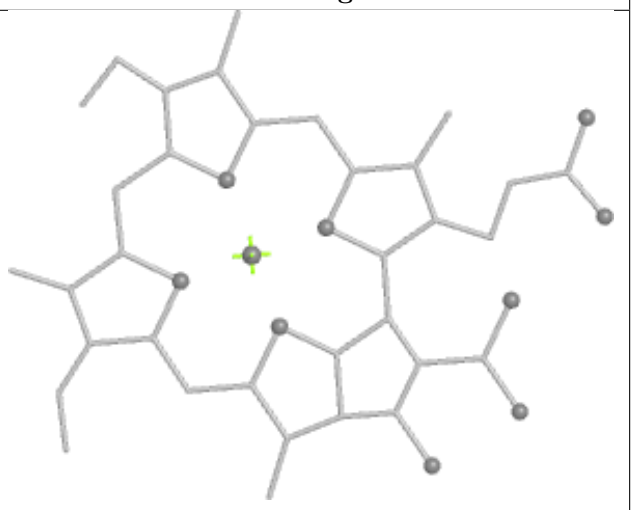
Bond lengths



Bond angles

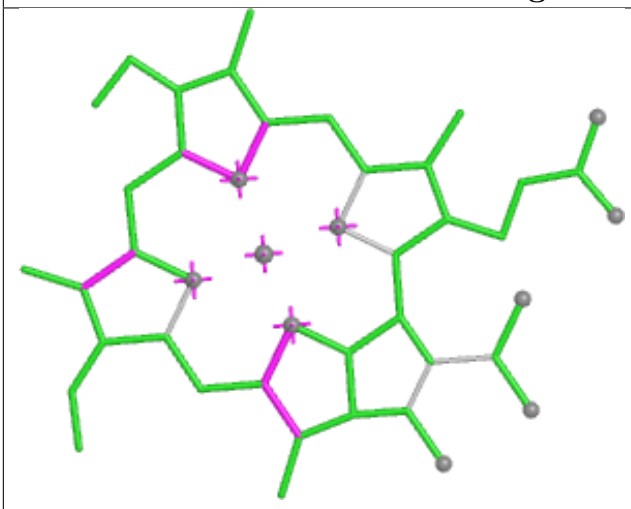


Torsions

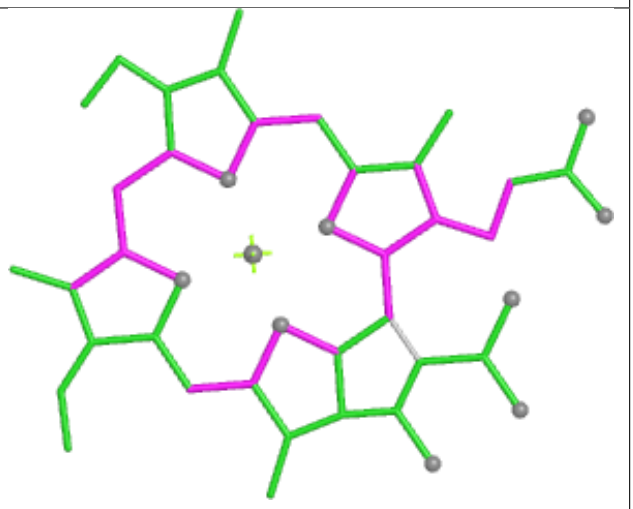


Rings

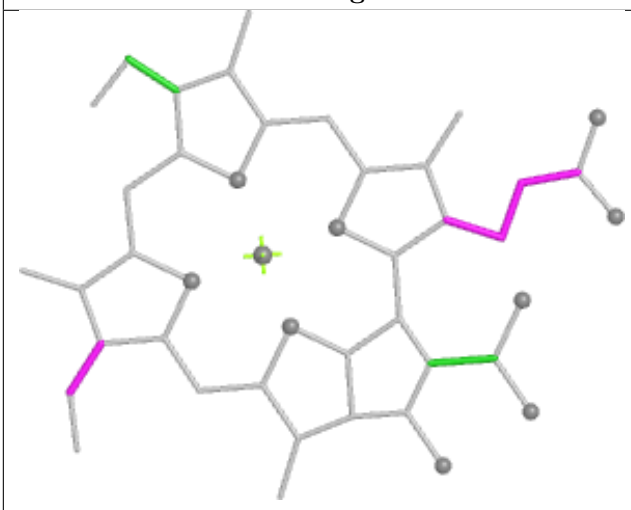
Ligand CLA 6 310



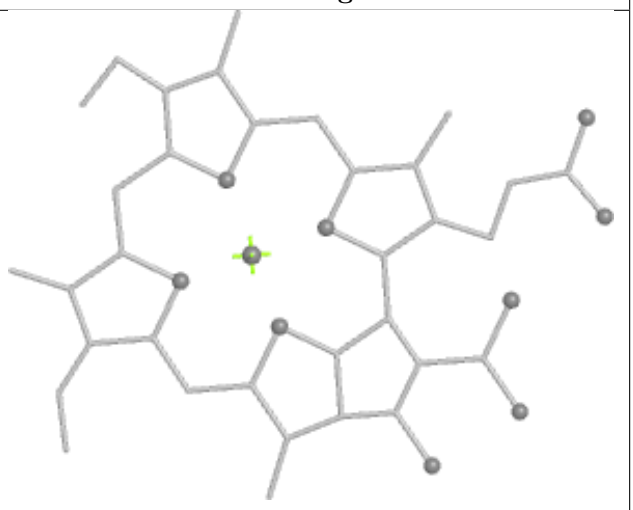
Bond lengths



Bond angles

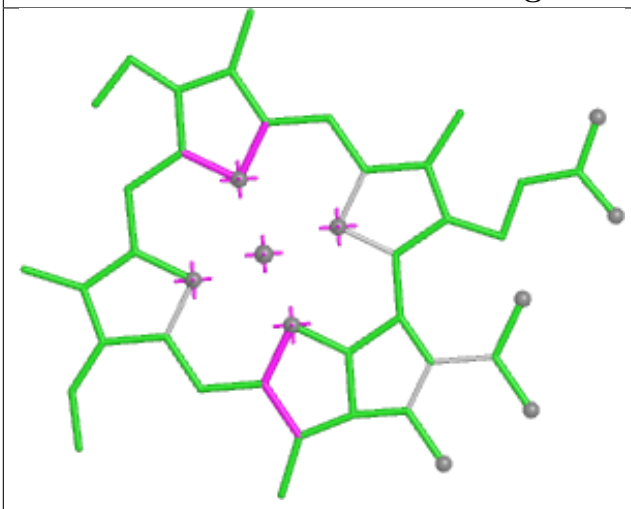


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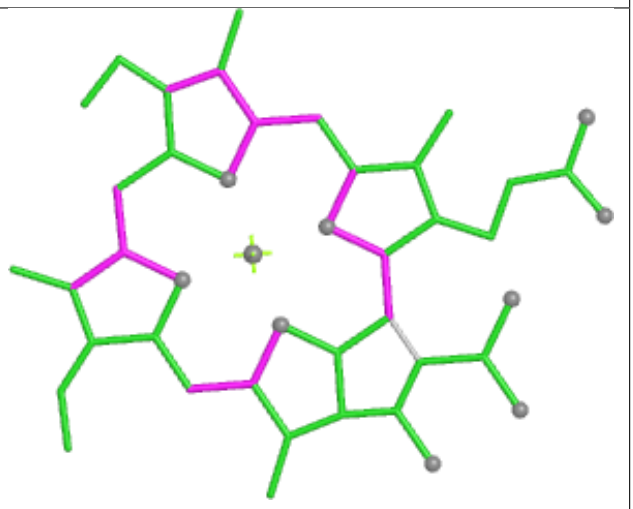


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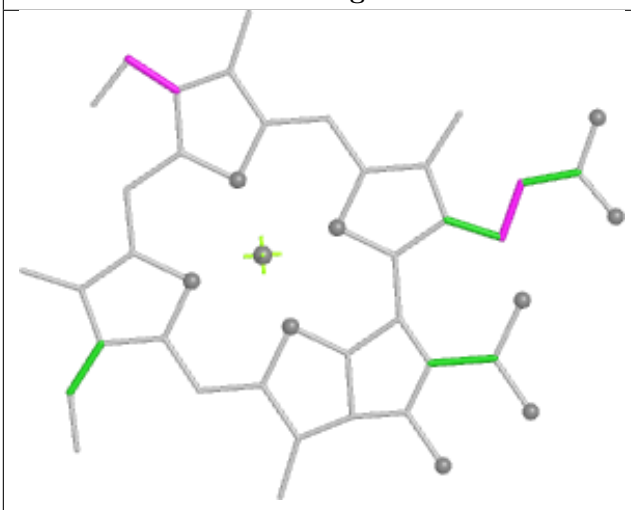
Ligand CLA B 801



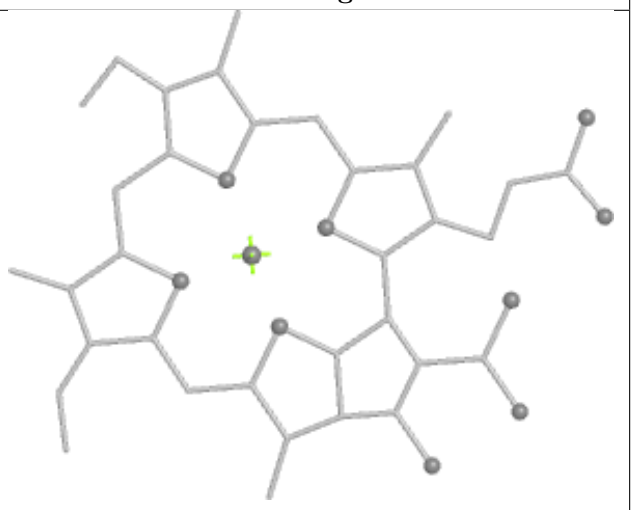
Bond lengths



Bond angles

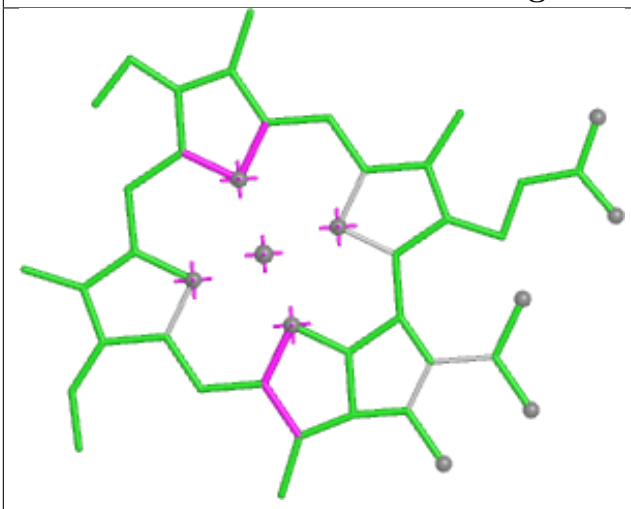


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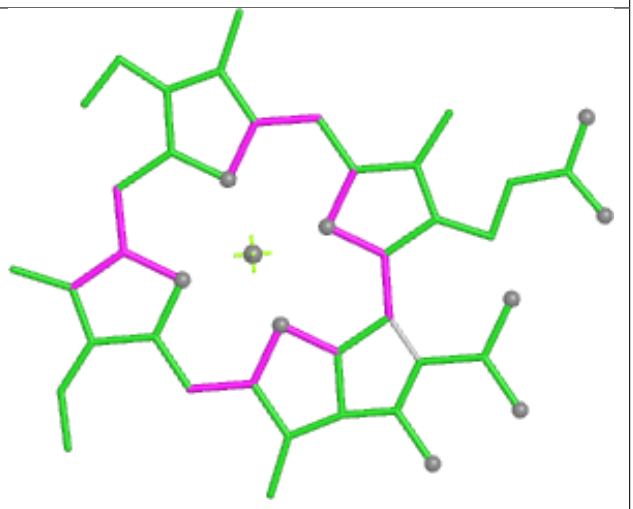


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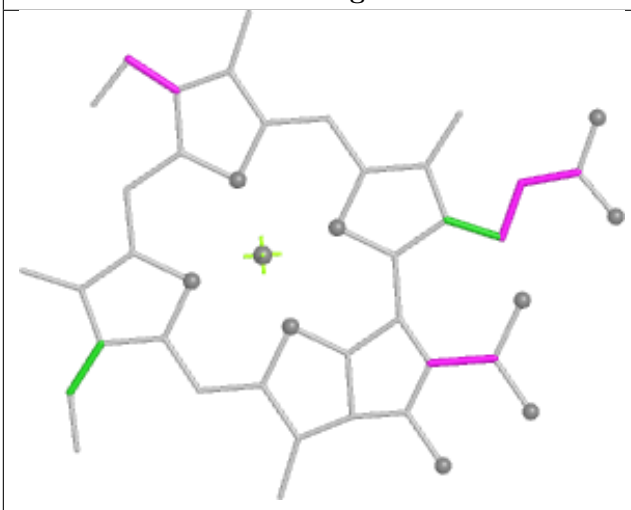
Ligand CLA 5 323



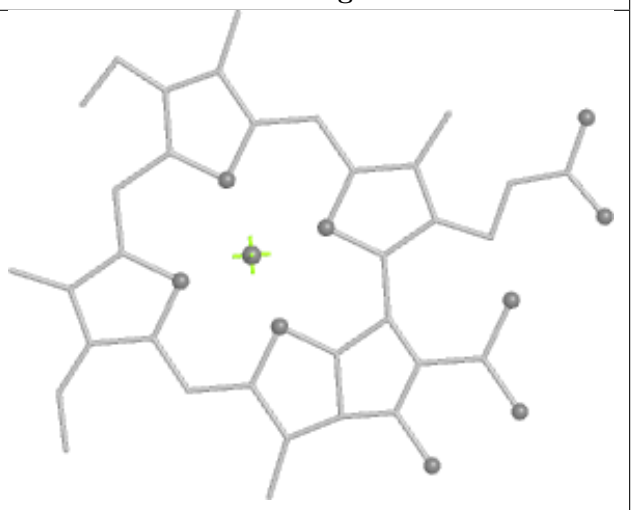
Bond lengths



Bond angles

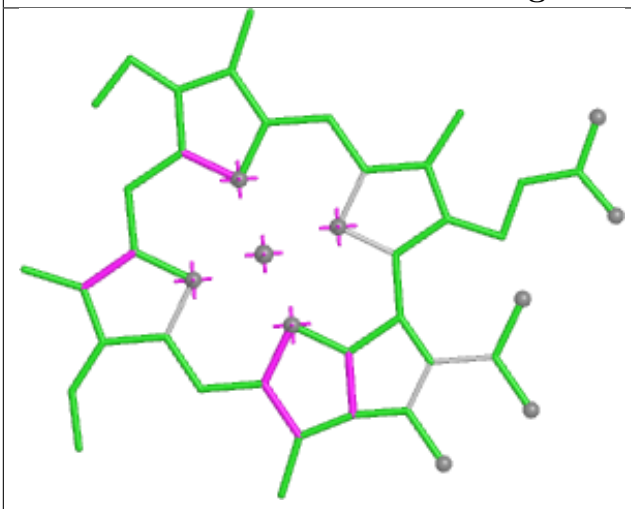


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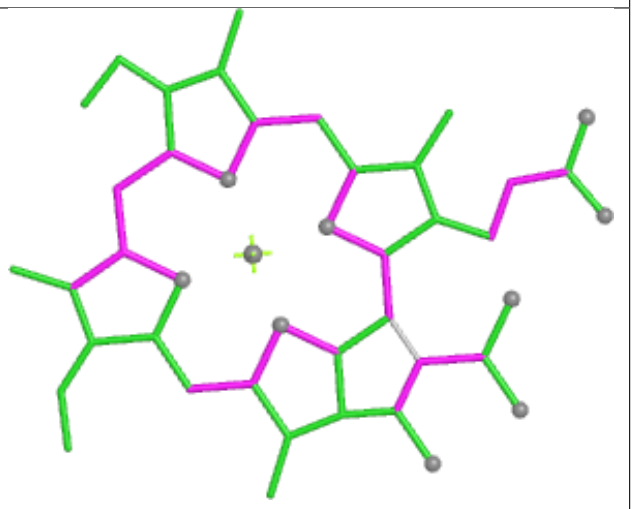


Rings

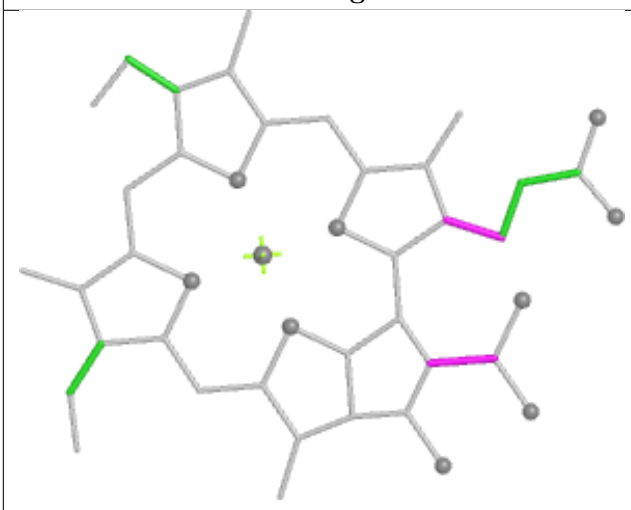
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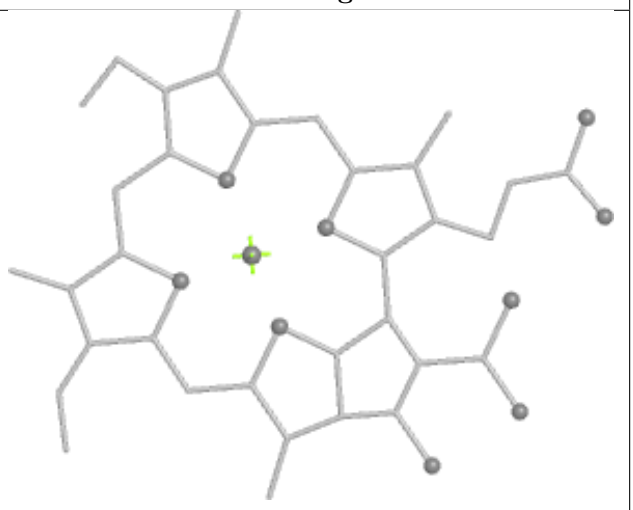
Bond lengths



Bond angles

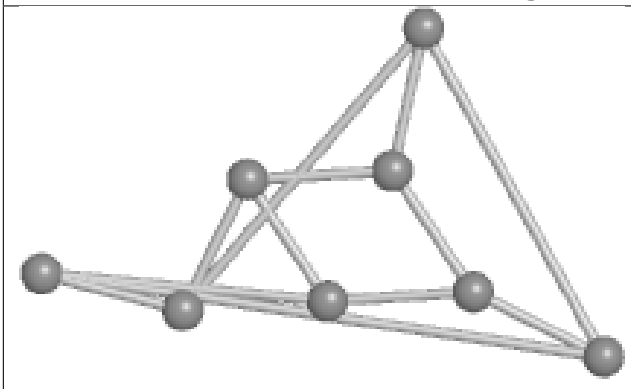


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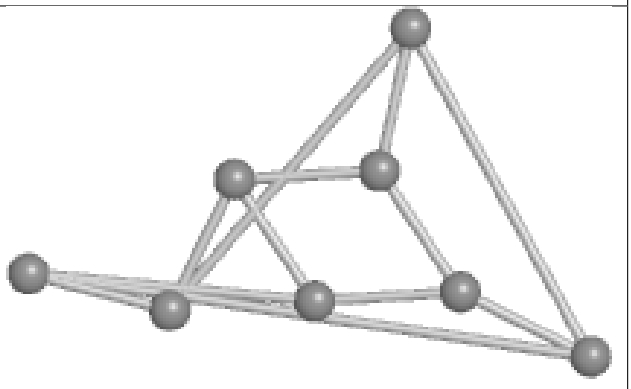


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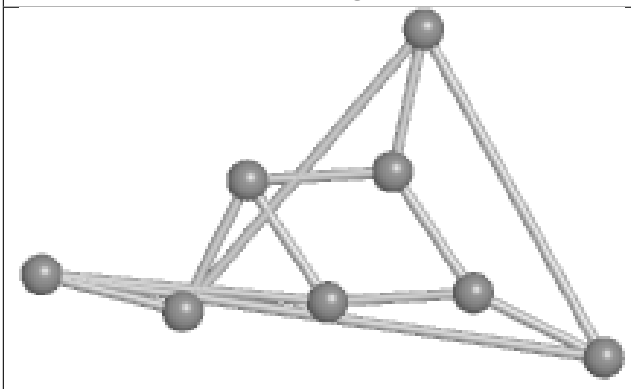
Ligand SF4 C 1001



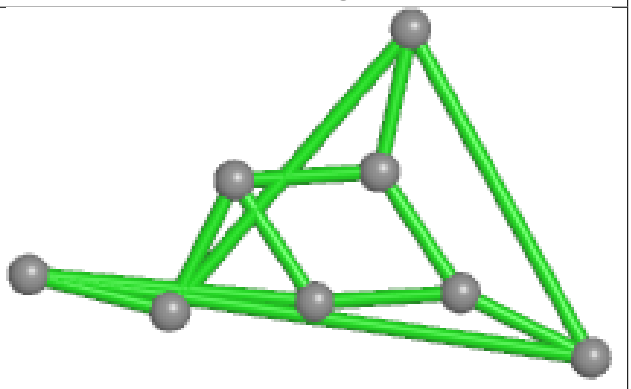
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Bond angles

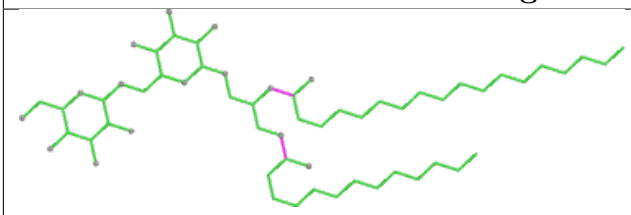


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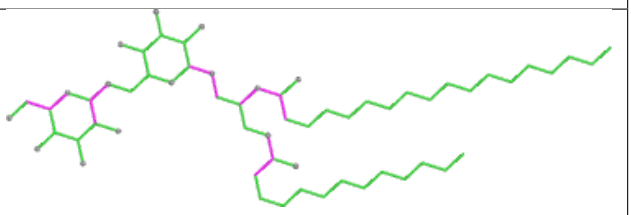


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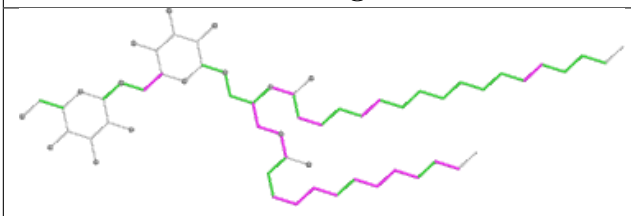
Ligand DGD B 848



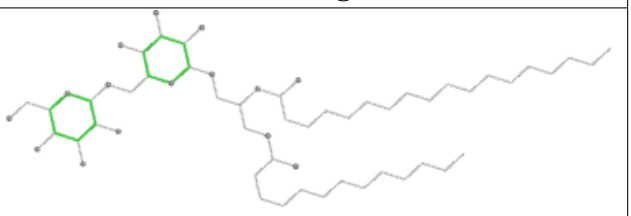
Bond lengths



Bond angles

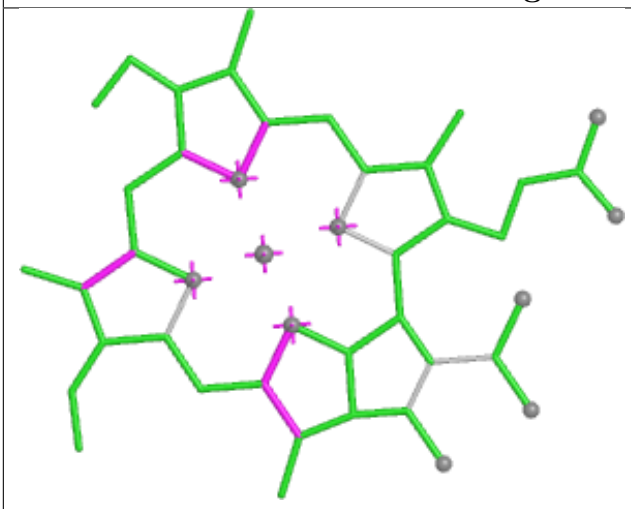


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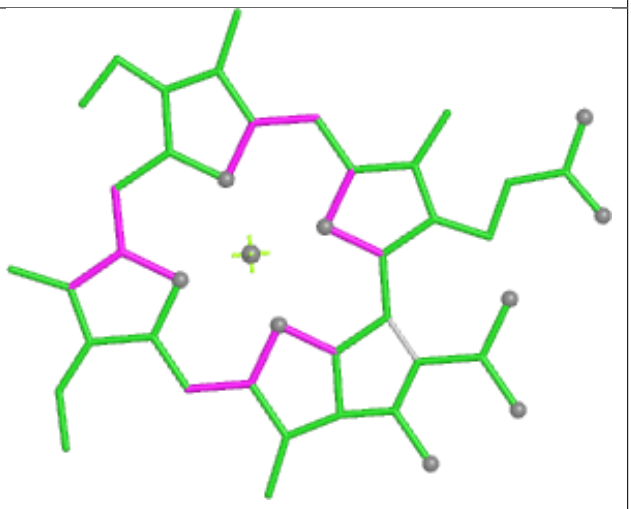


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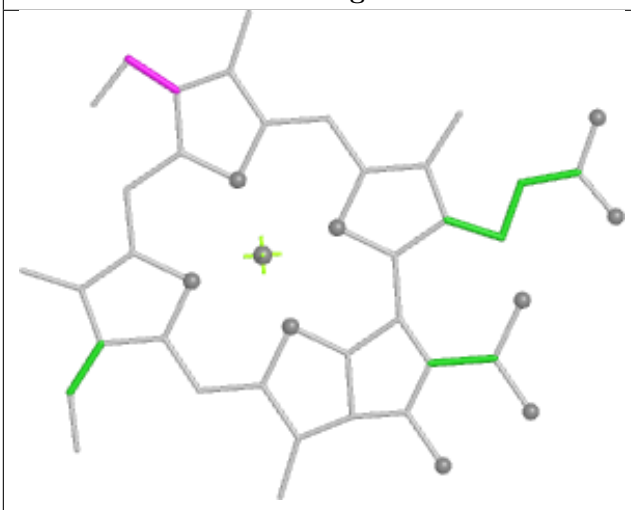
Ligand CLA A 825



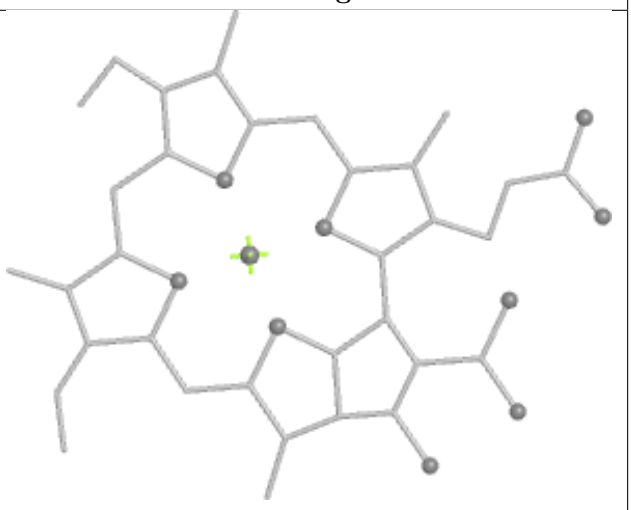
Bond lengths



Bond angles

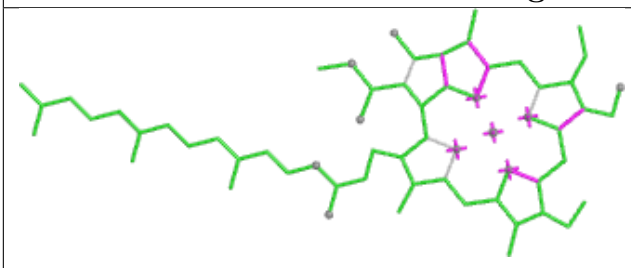


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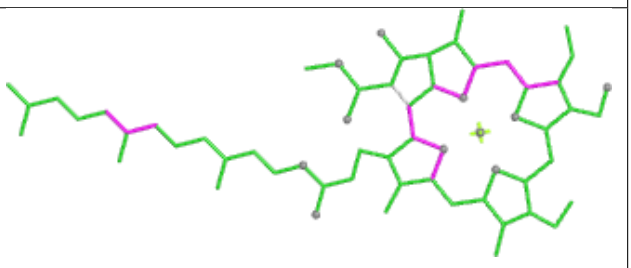


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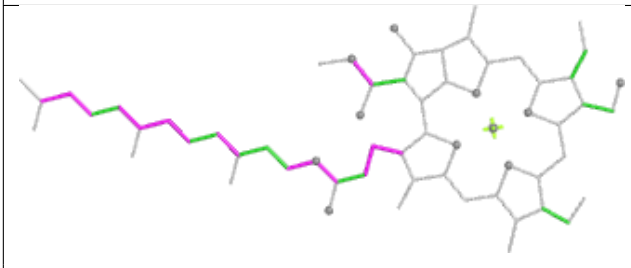
Ligand CHL 8 317



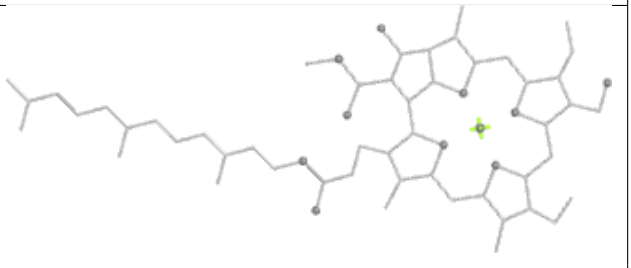
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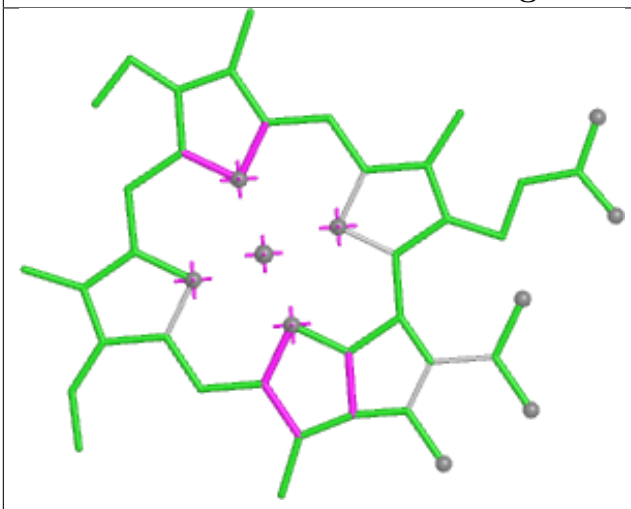


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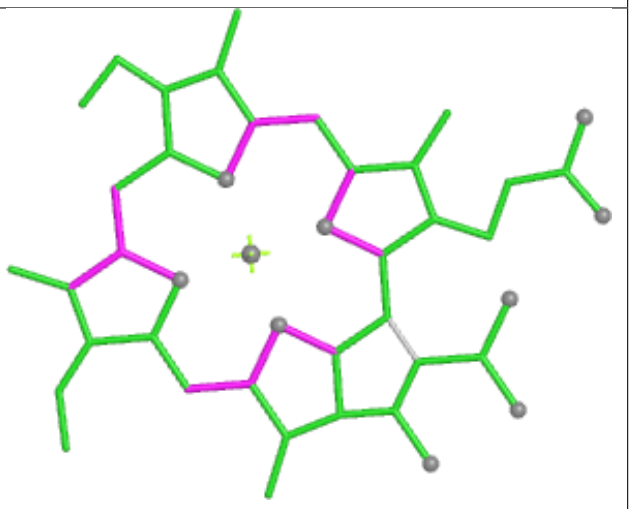


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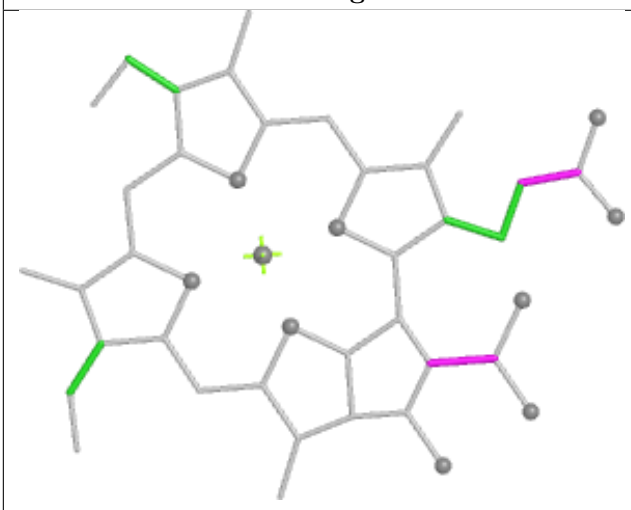
Ligand CLA 7 1008



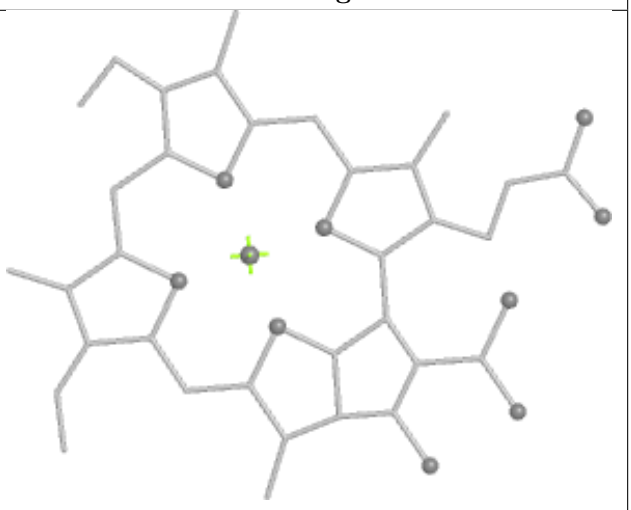
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Bond angles

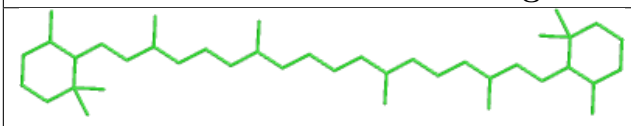


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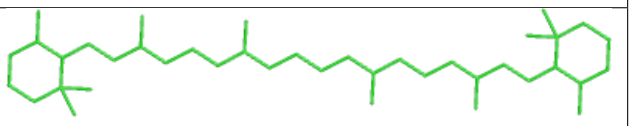


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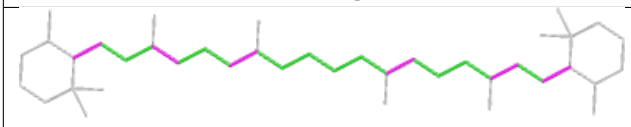
Ligand BCR B 844



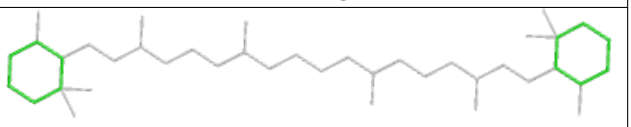
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Bond angles

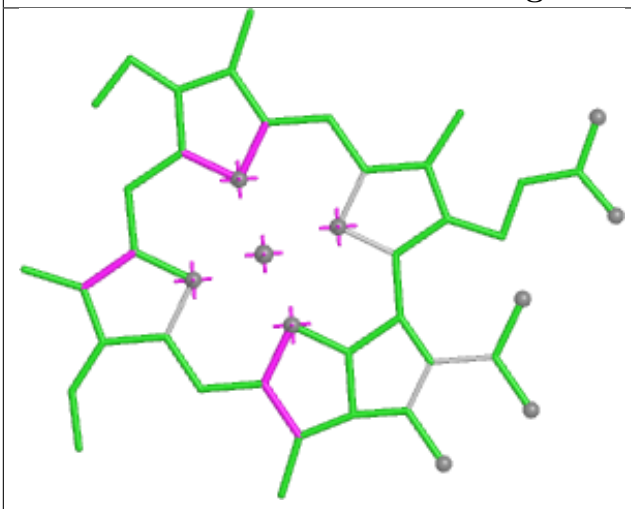


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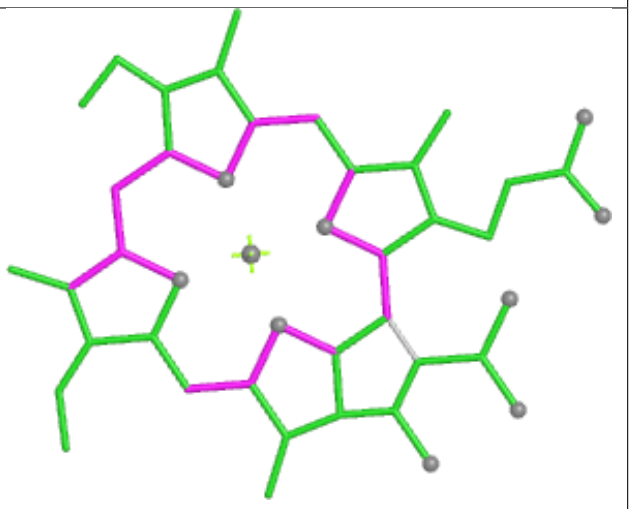


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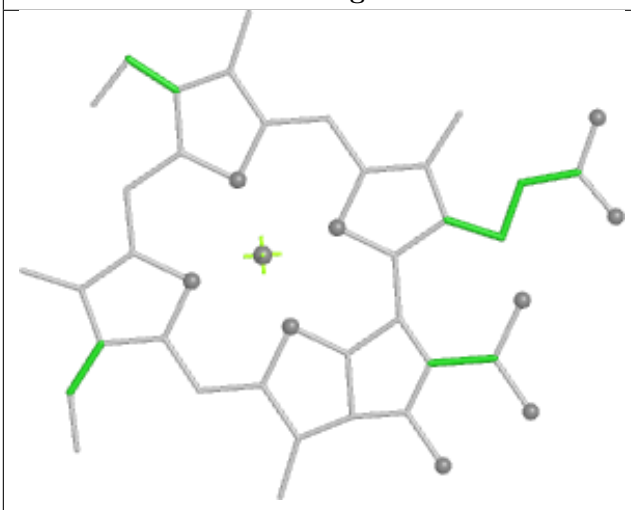
Ligand CLA F 305



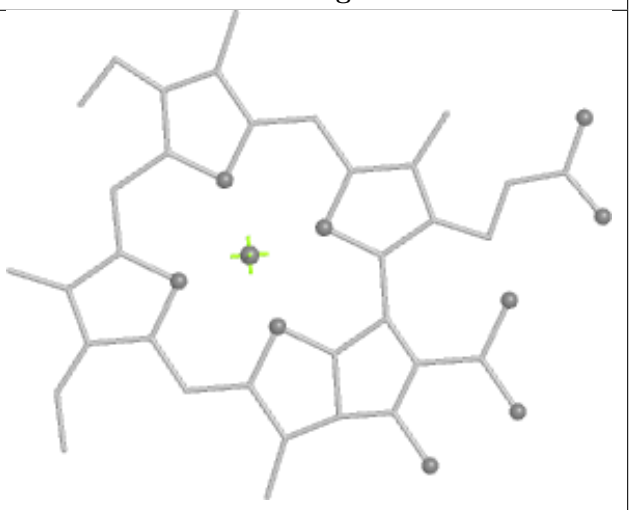
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Bond angles

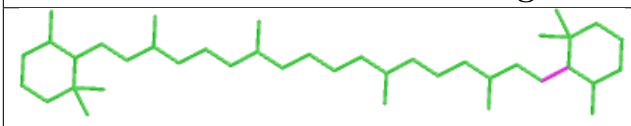


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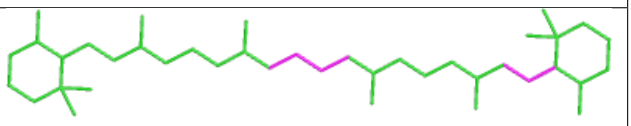


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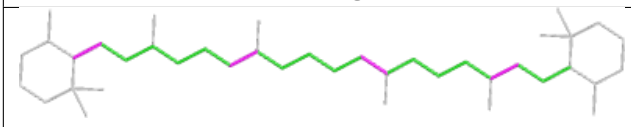
Ligand BCR 3 1004



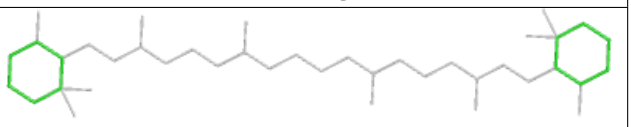
Bond lengths



Bond angles

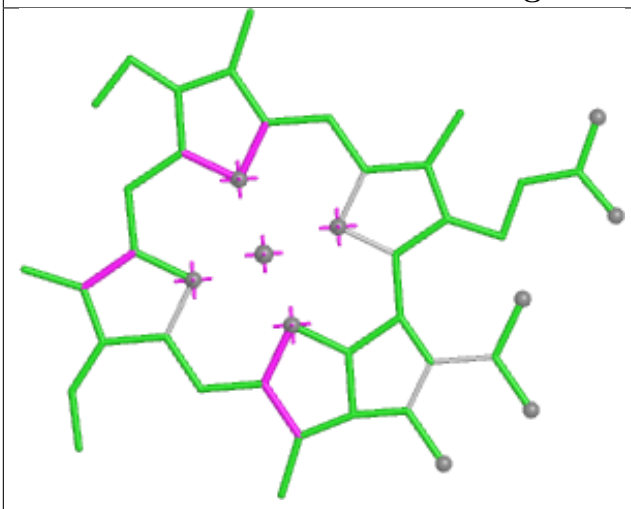


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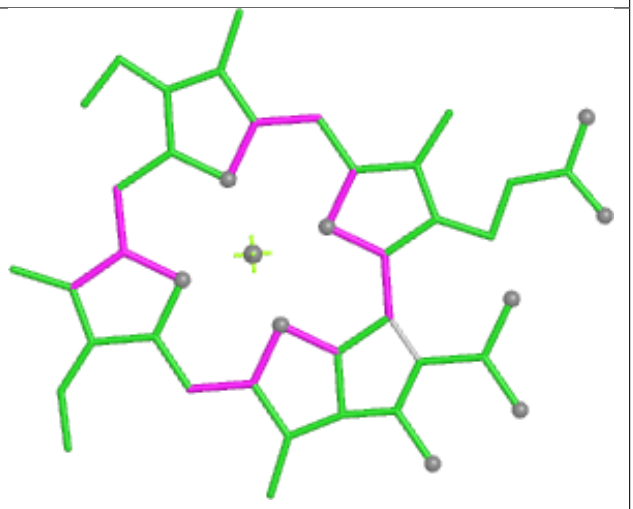


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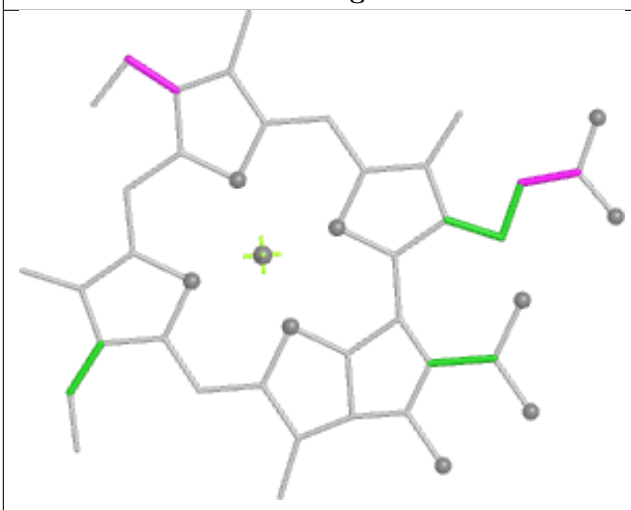
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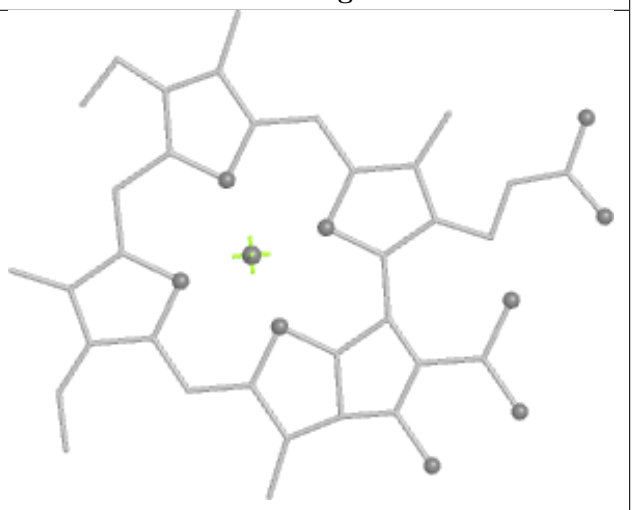
Bond lengths



Bond angles

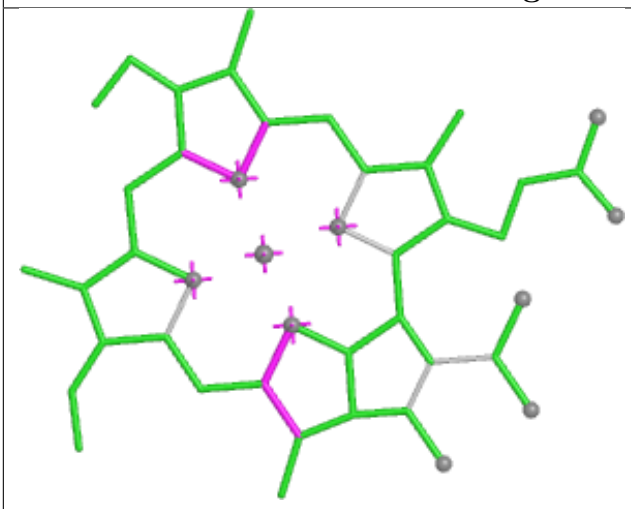


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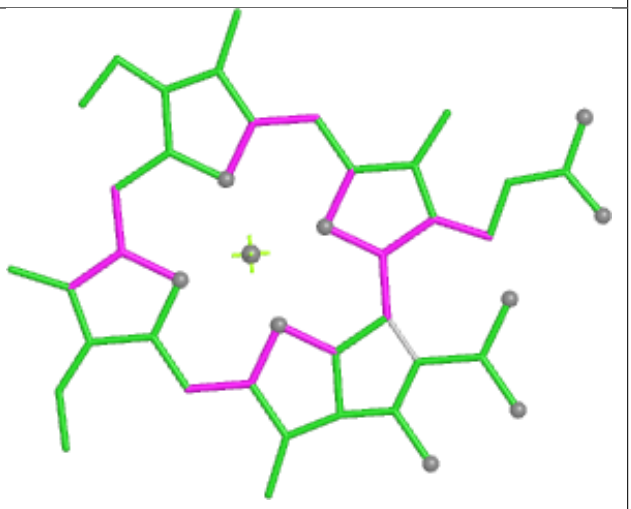


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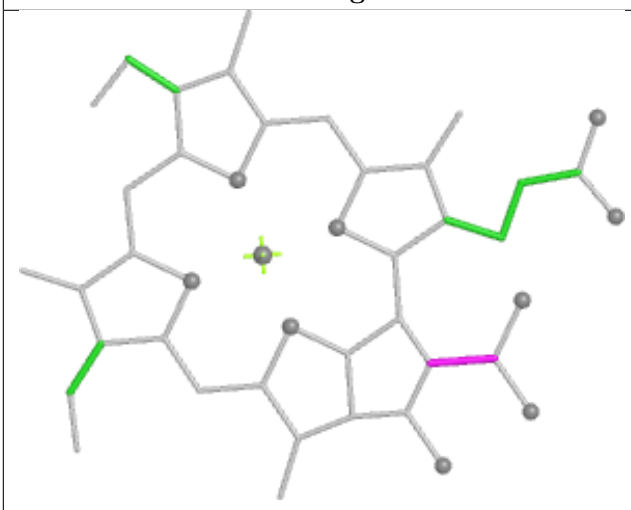
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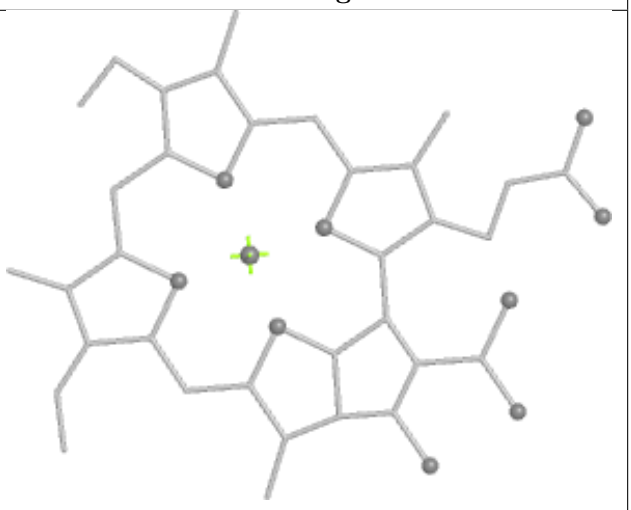
Bond lengths



Bond angles

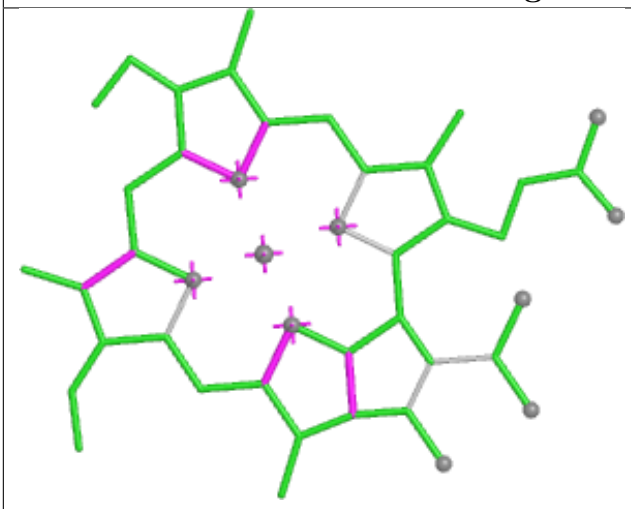


Torsions

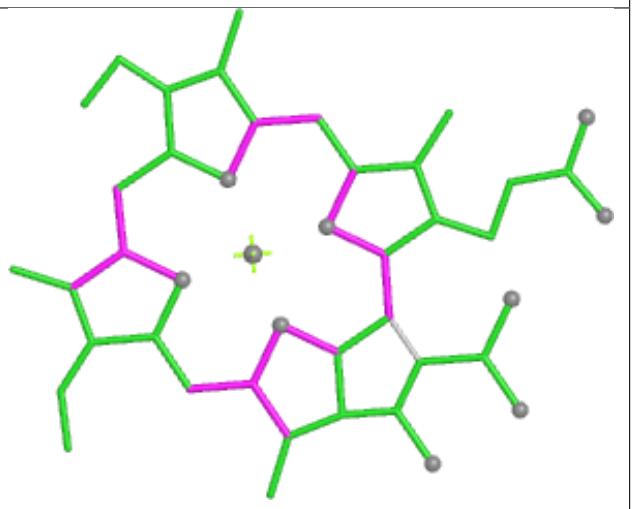


Rings

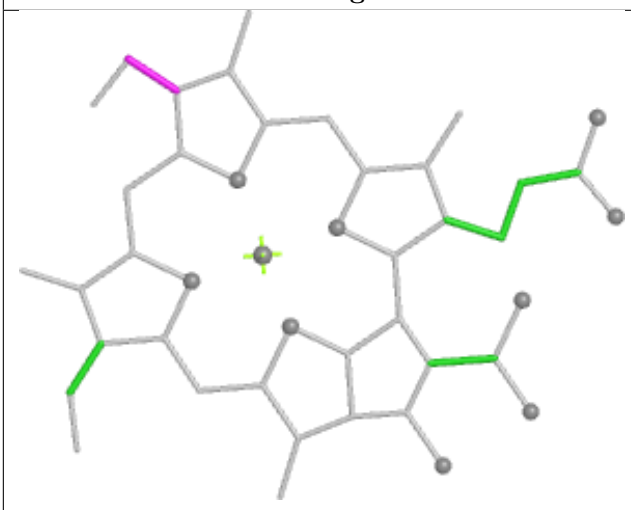
Ligand CLA B 824



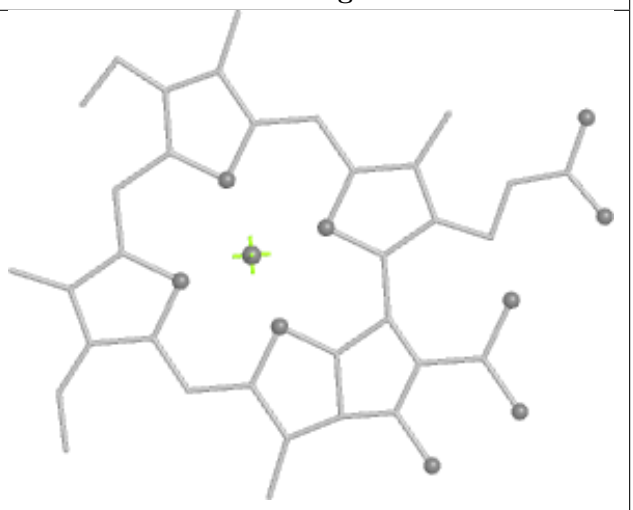
Bond lengths



Bond angles

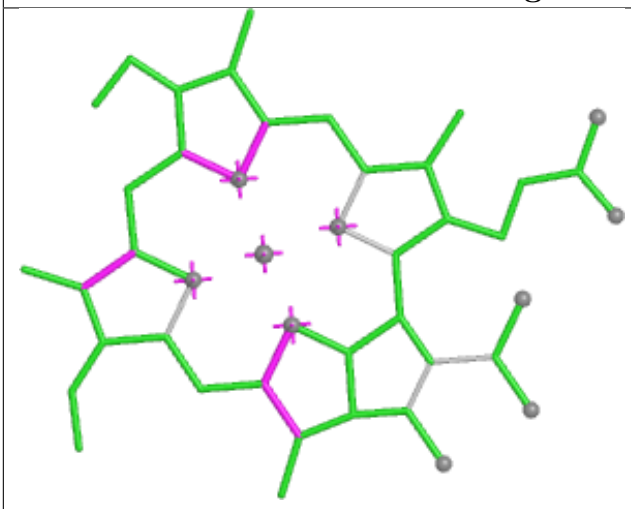


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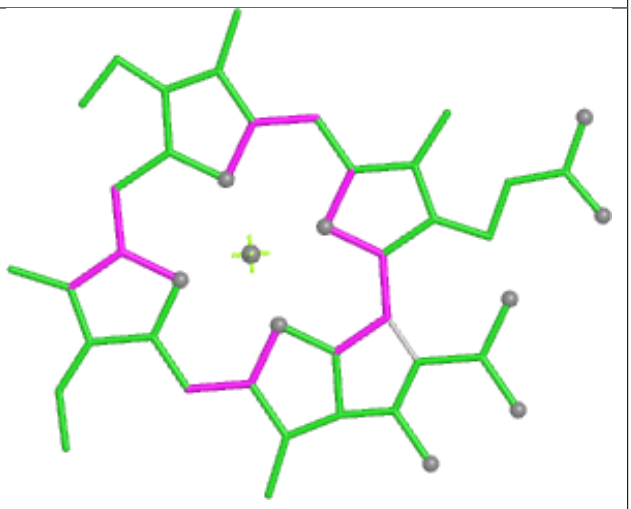


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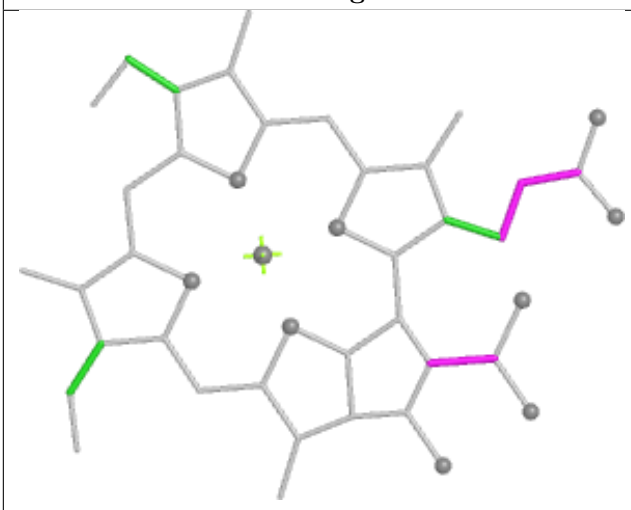
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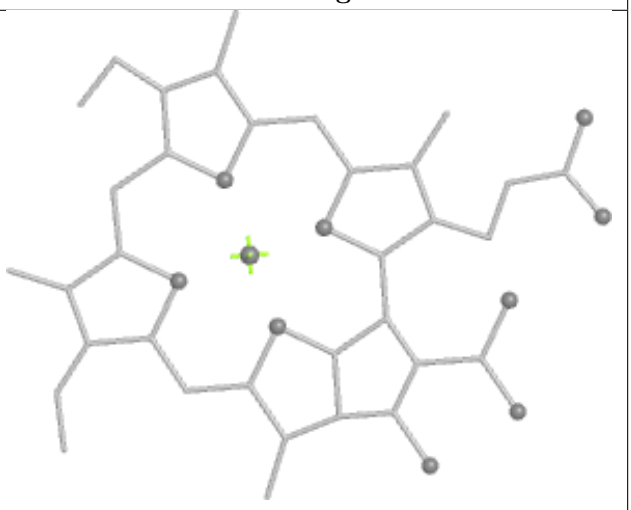
Bond lengths



Bond angles

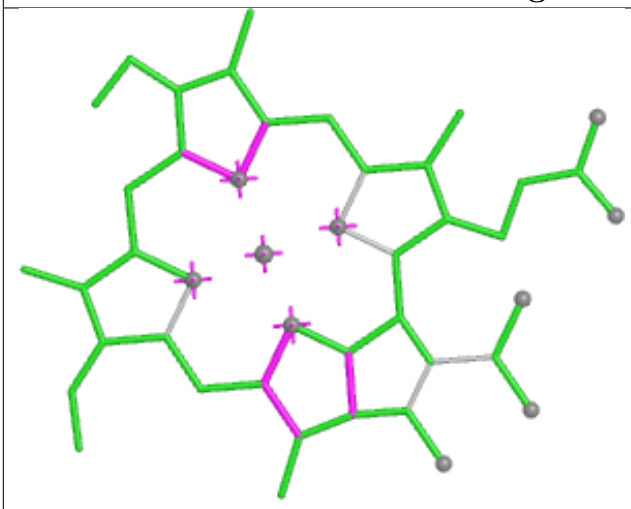


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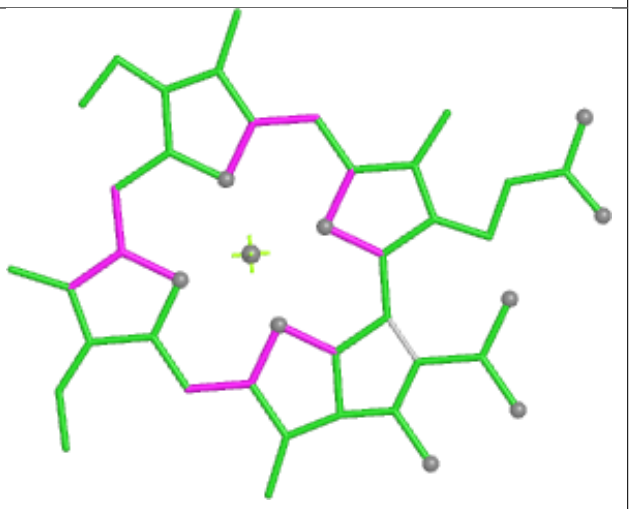


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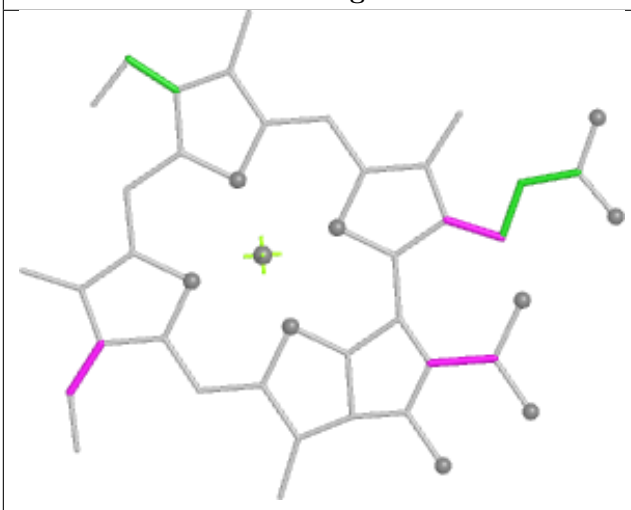
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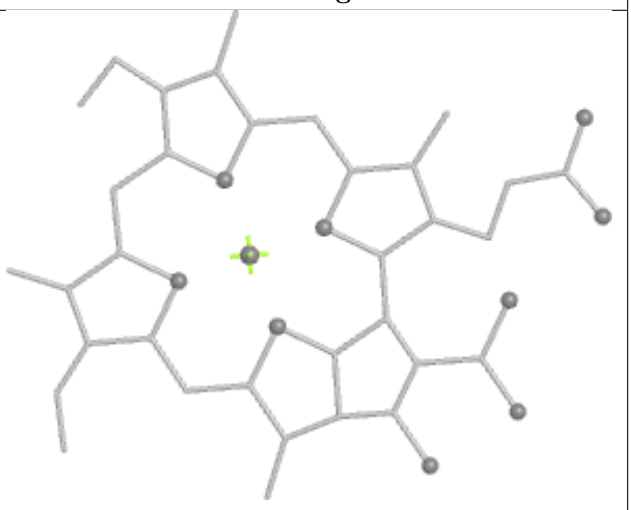
Bond lengths



Bond angles

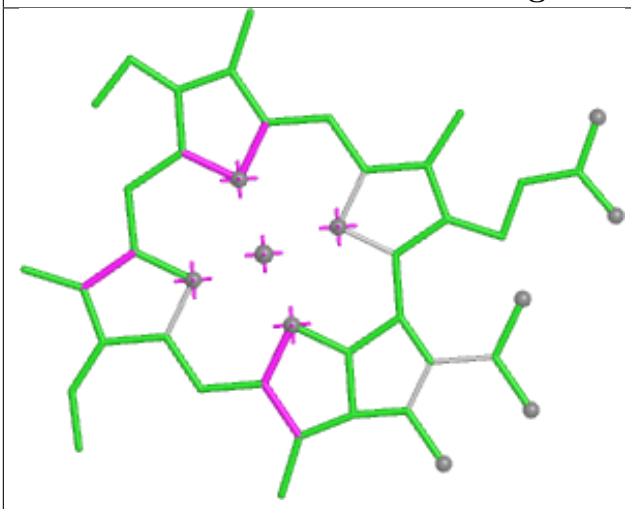


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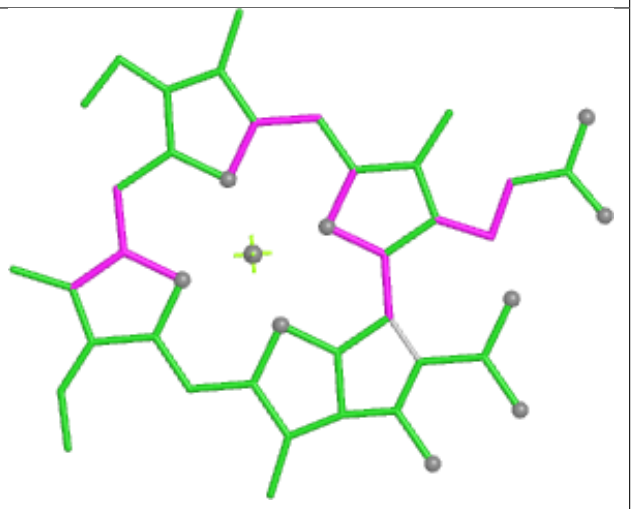


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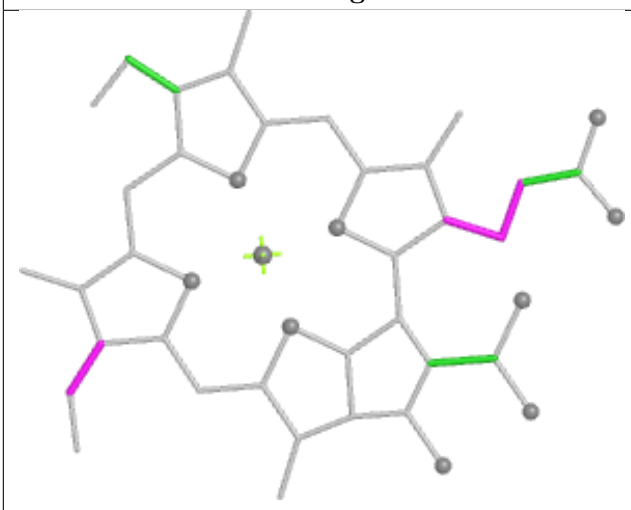
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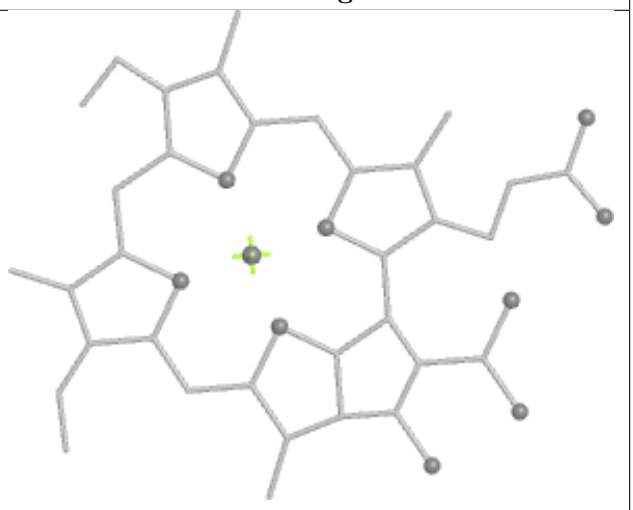
Bond lengths



Bond angles

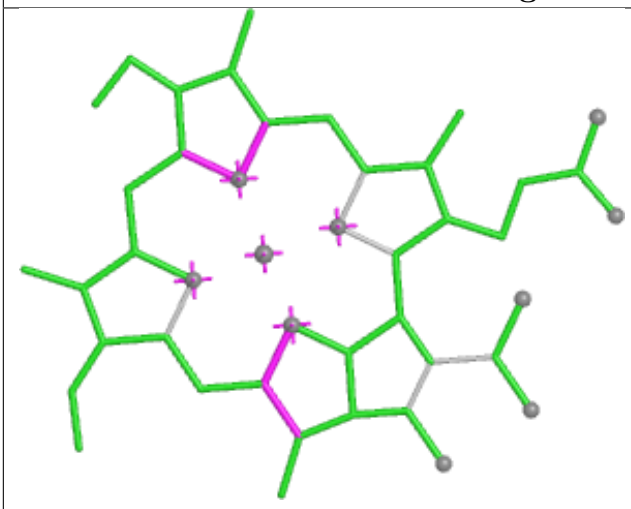


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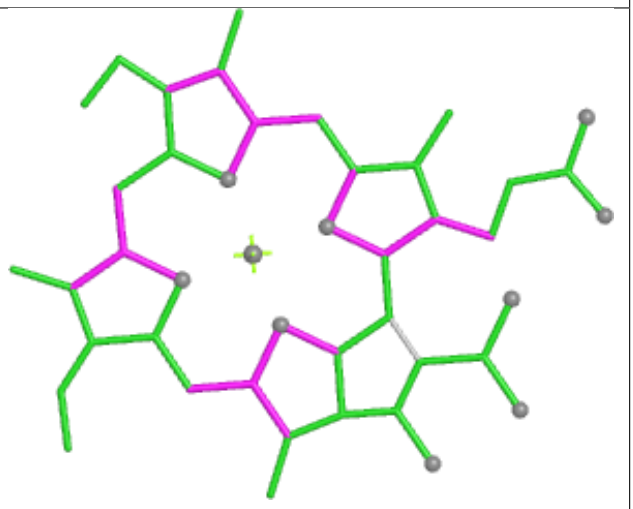


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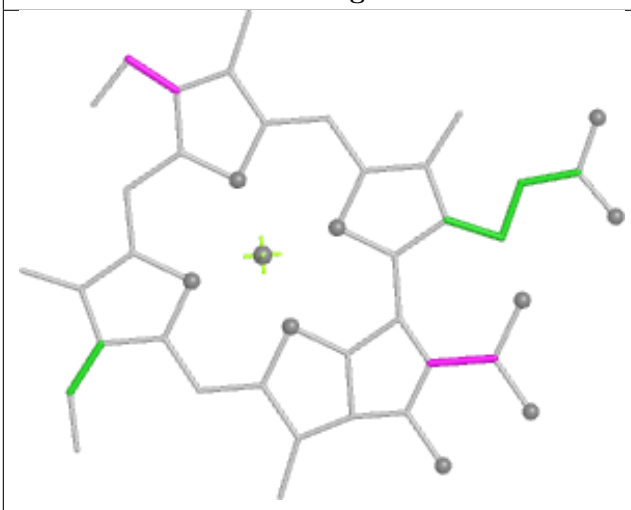
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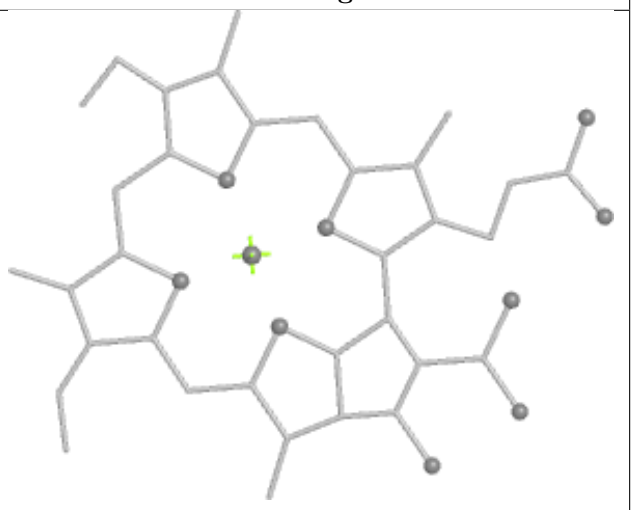
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Bond angles

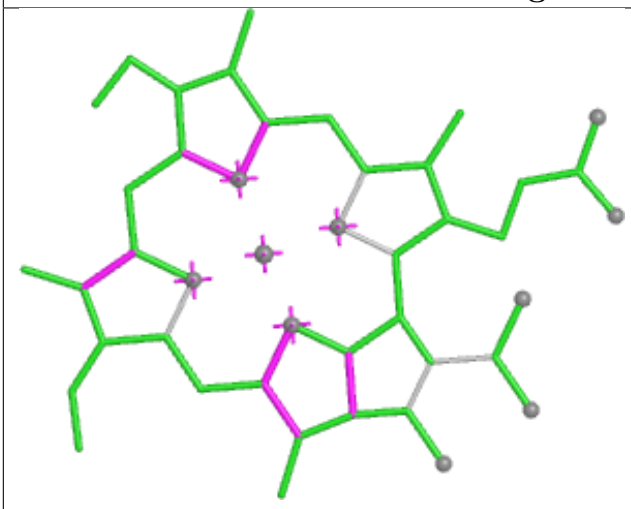


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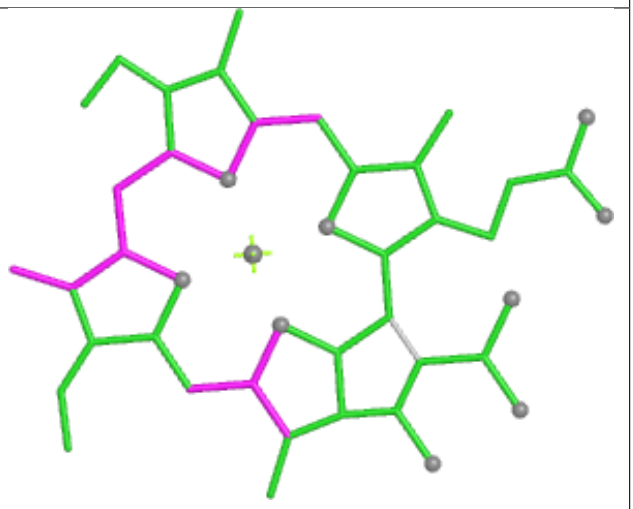


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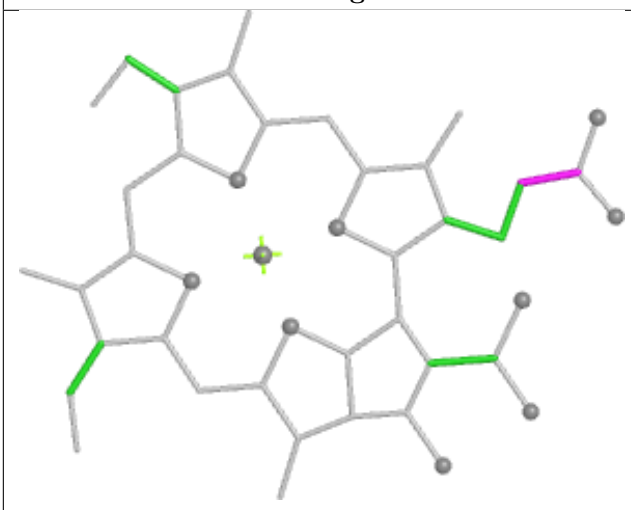
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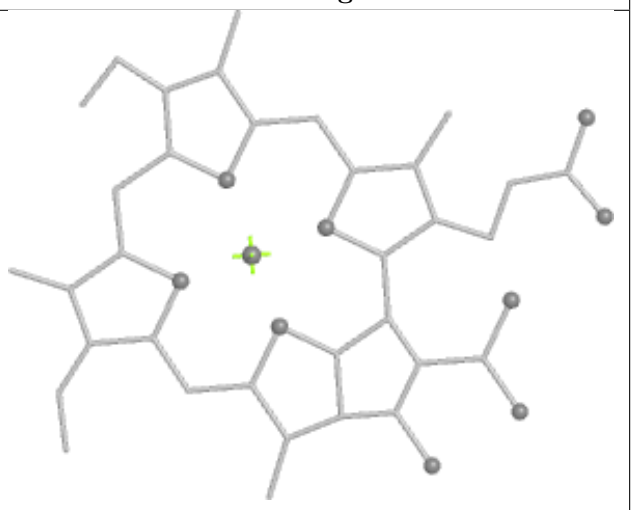
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Bond angles

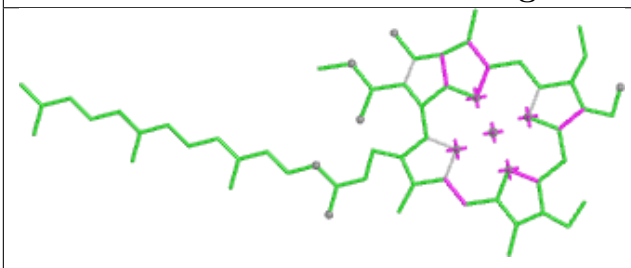


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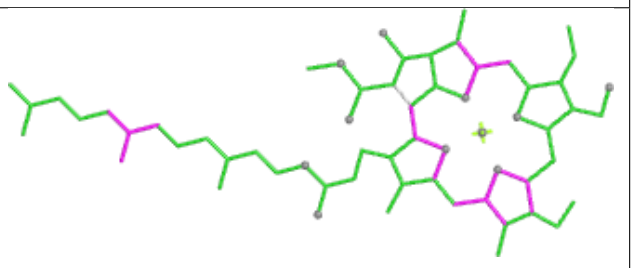


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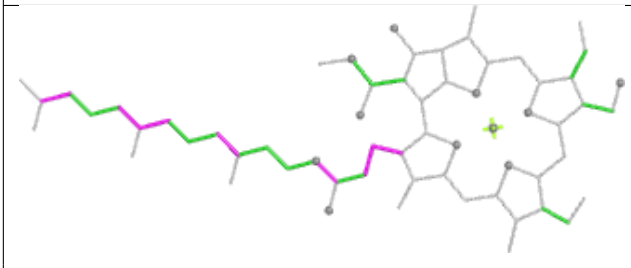
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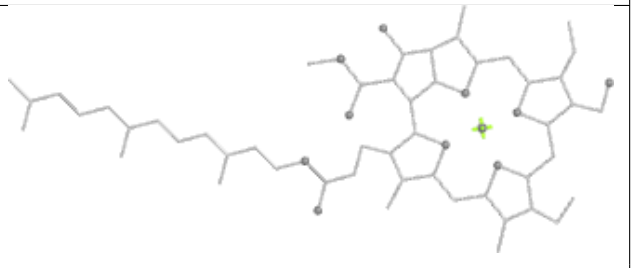
Bond lengths



Bond angles

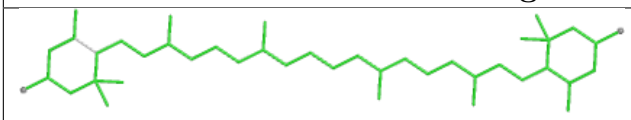


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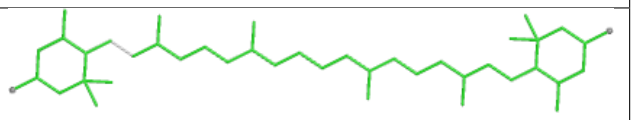


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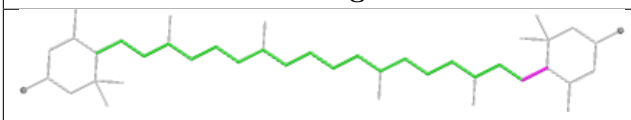
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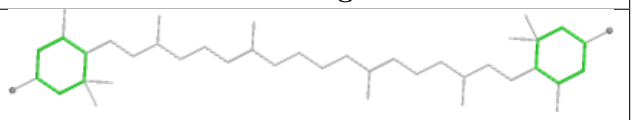
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Bond angles

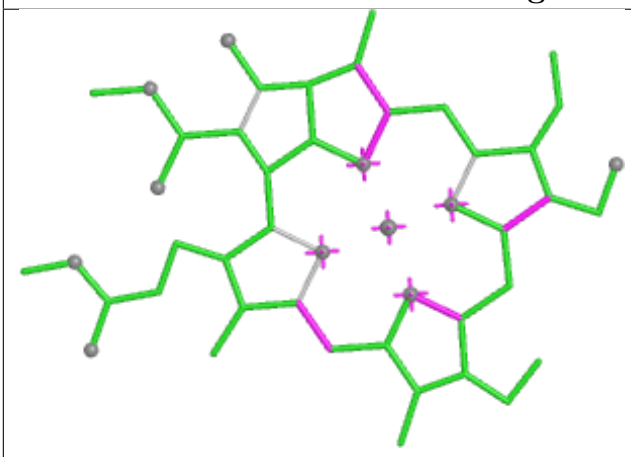


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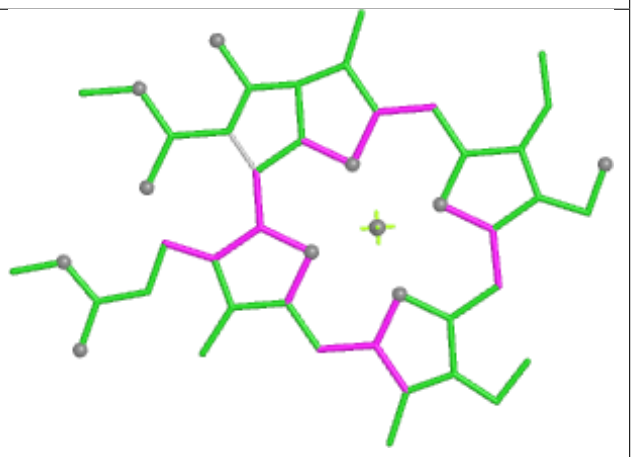


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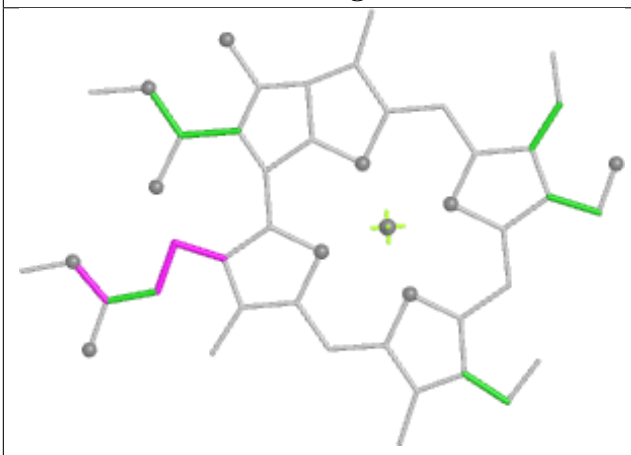
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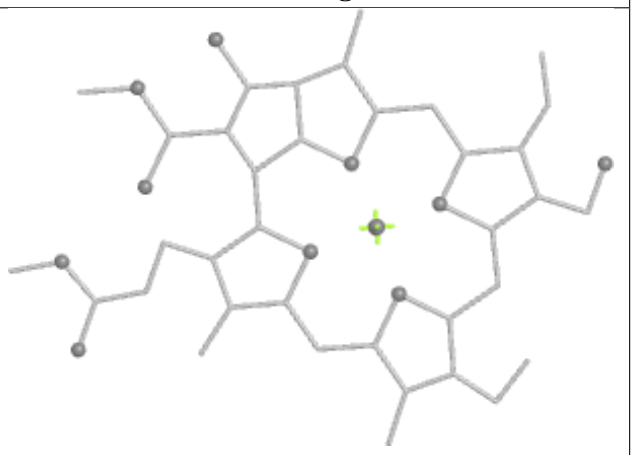
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Bond angles

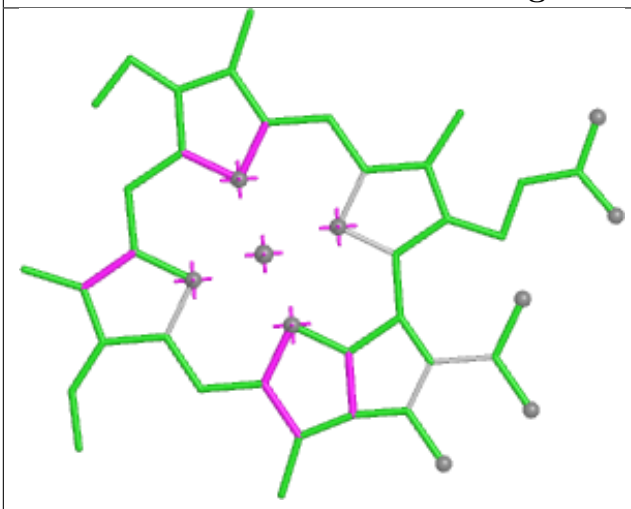


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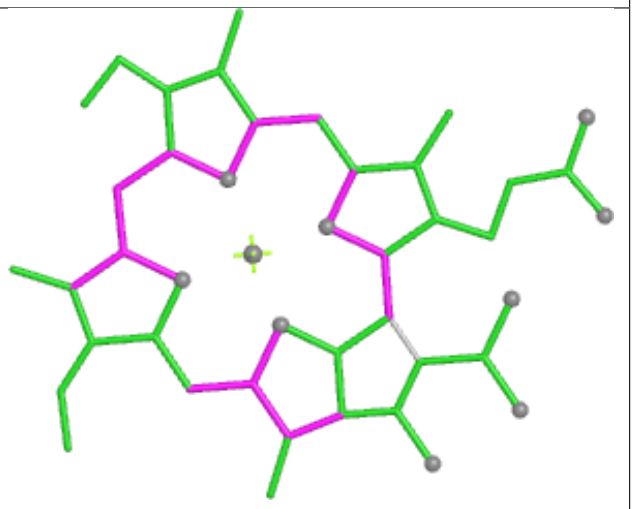


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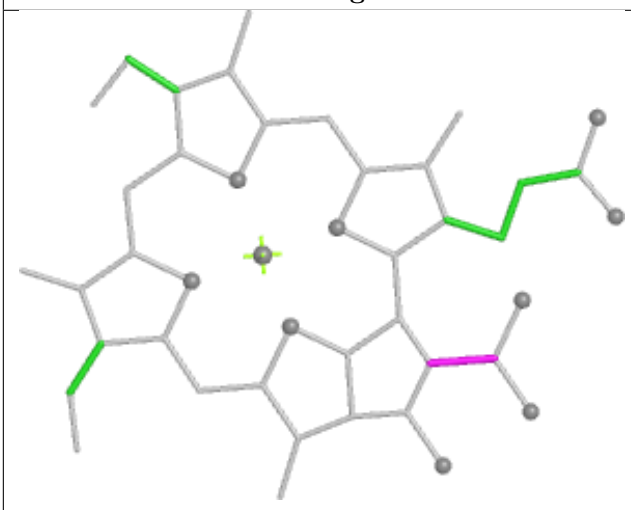
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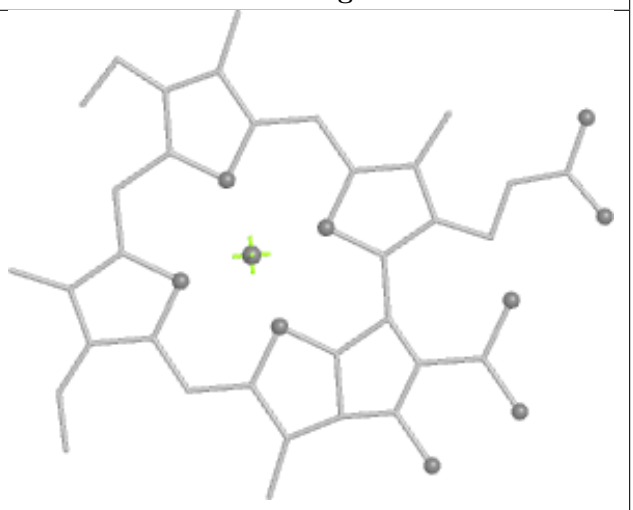
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Bond angles

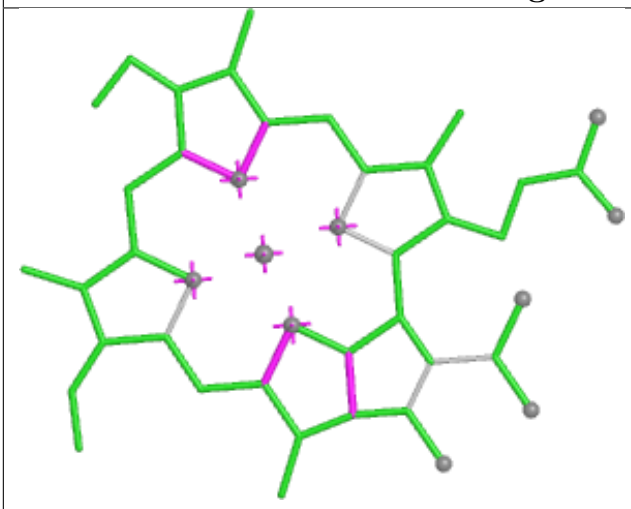


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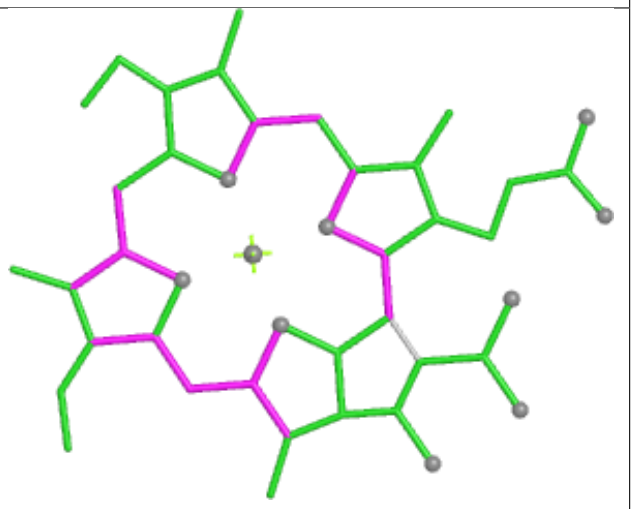


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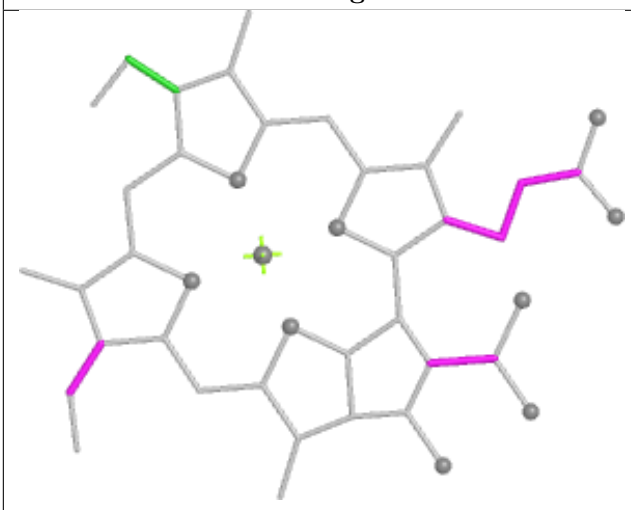
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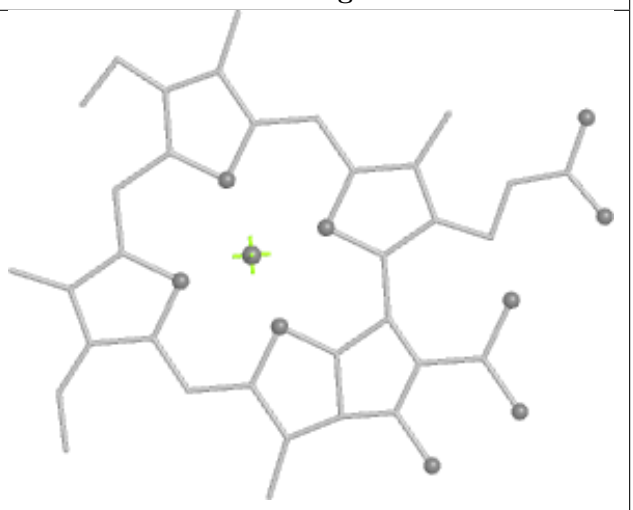
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Bond angles

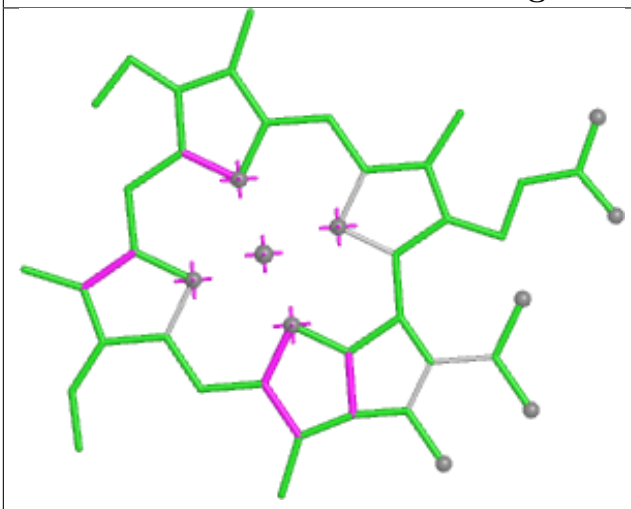


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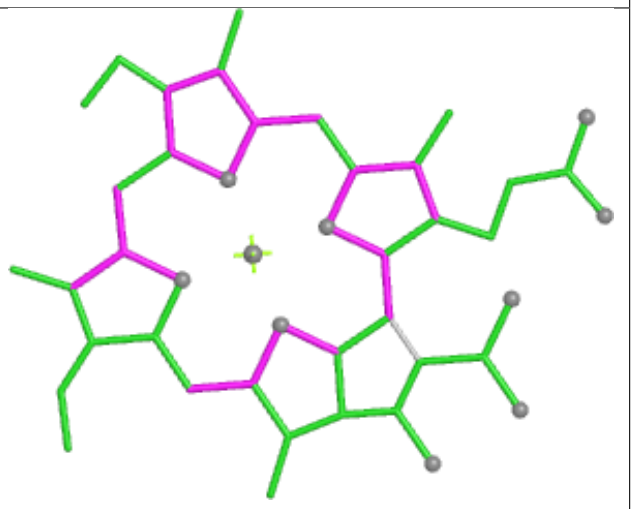


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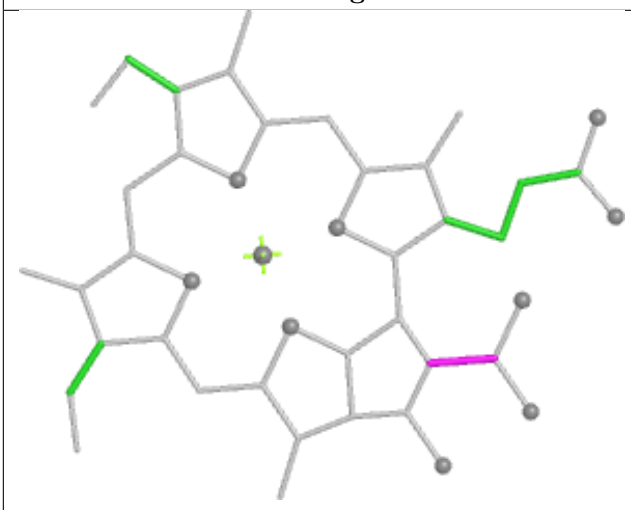
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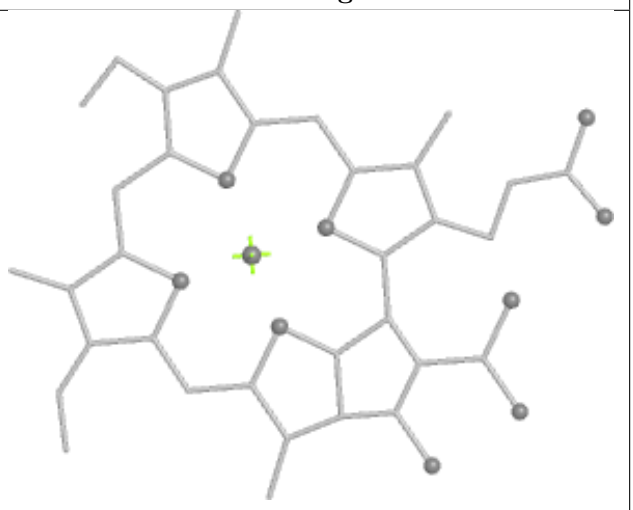
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Bond angles

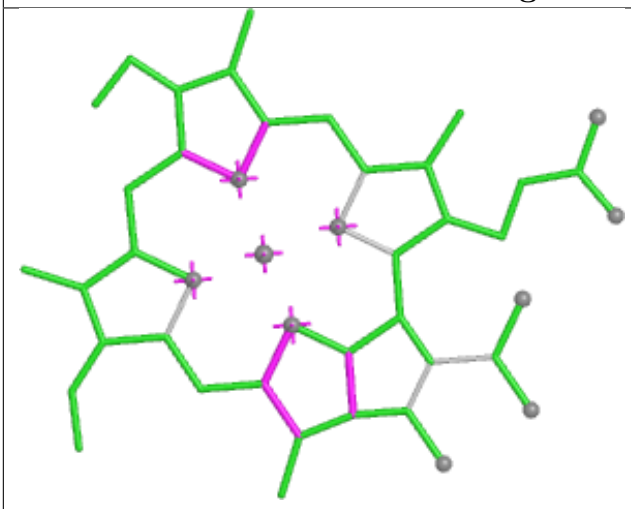


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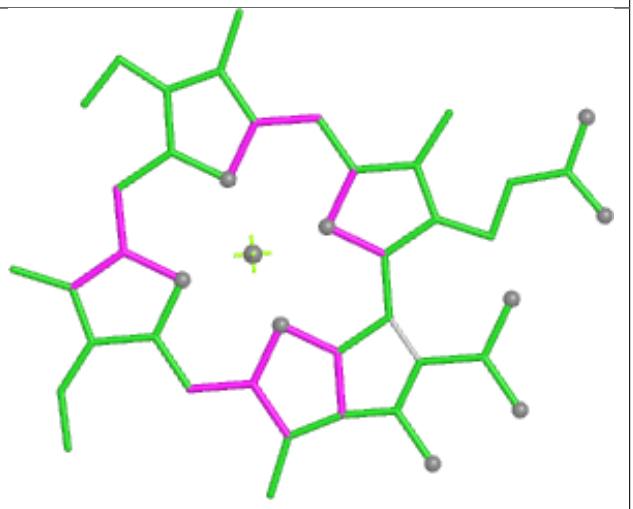


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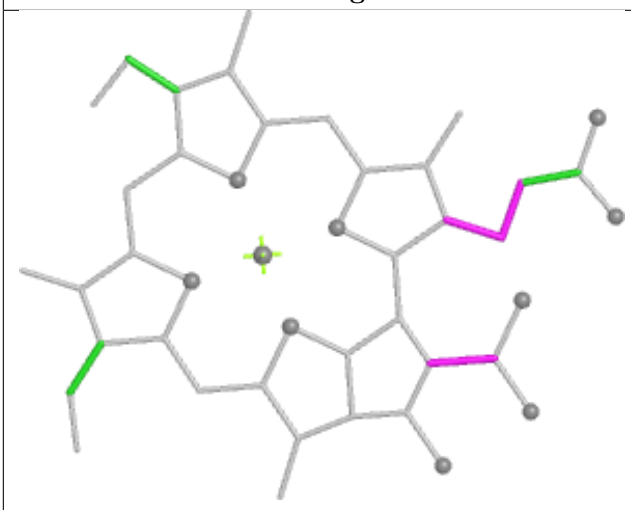
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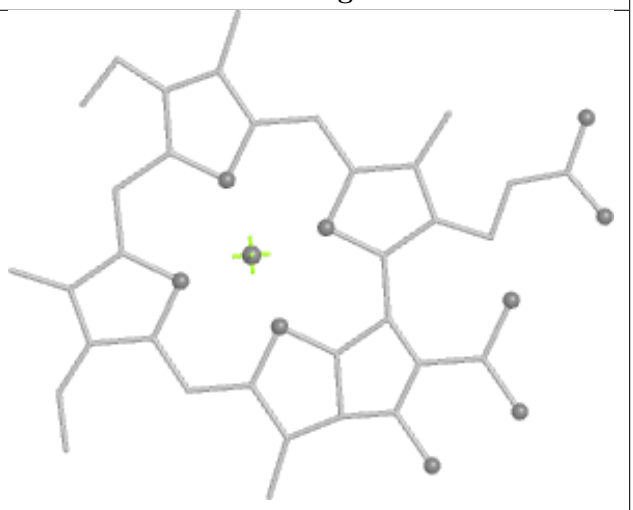
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Bond angles

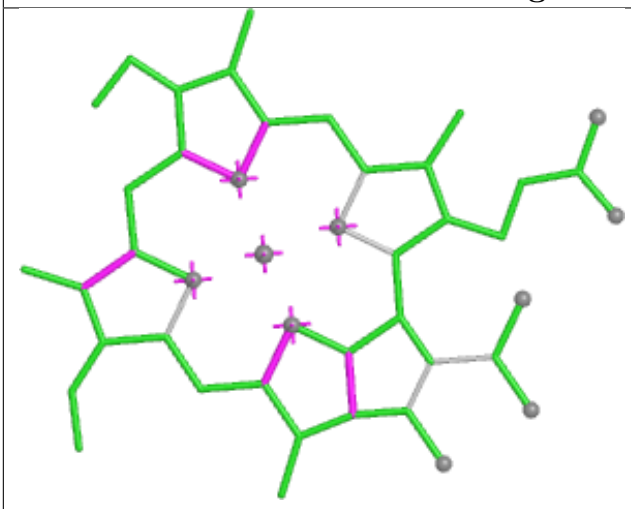


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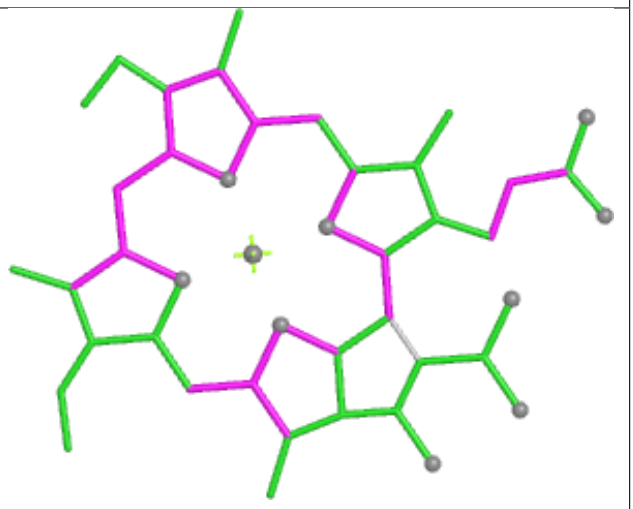


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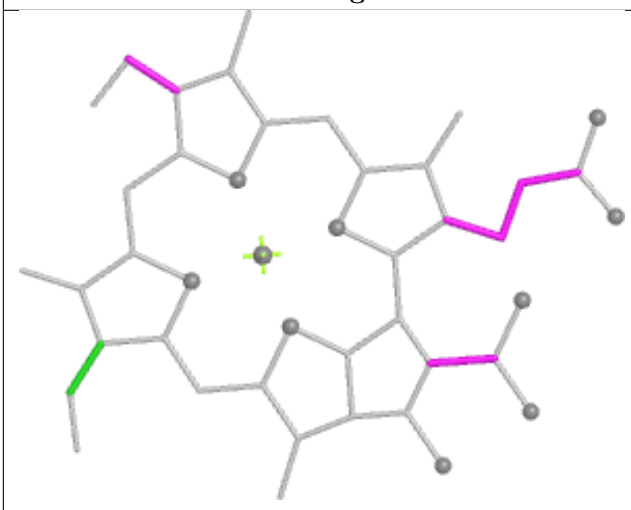
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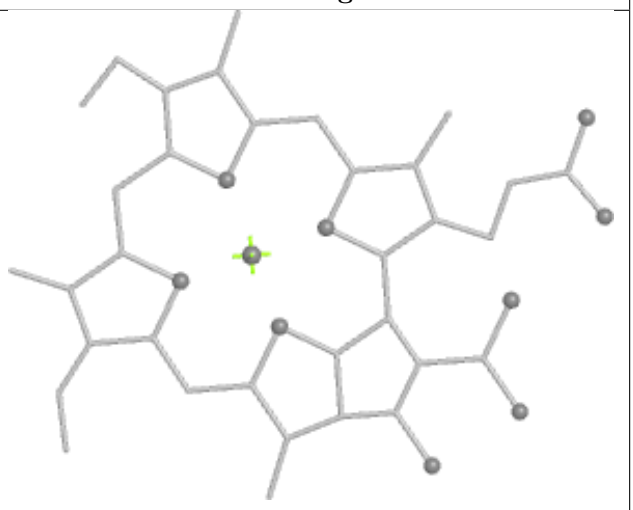
Bond lengths



Bond angles

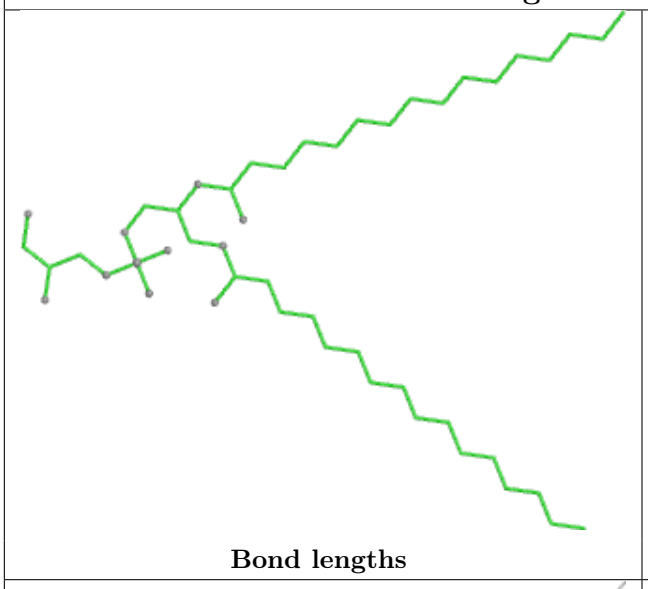


Torsions

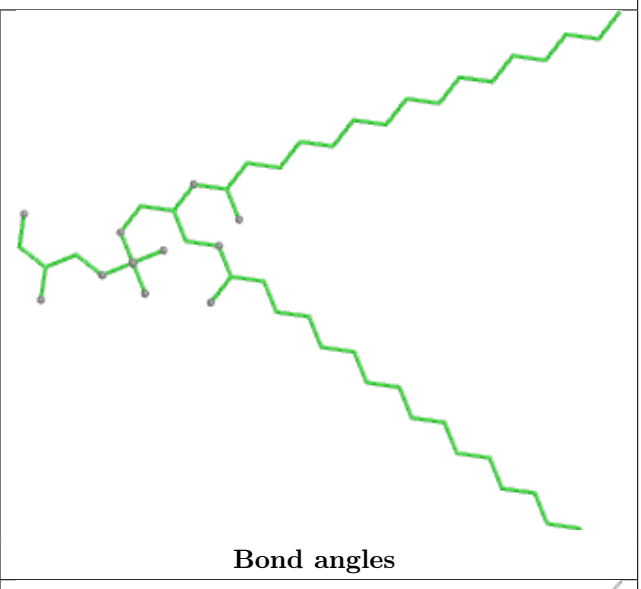


Rings

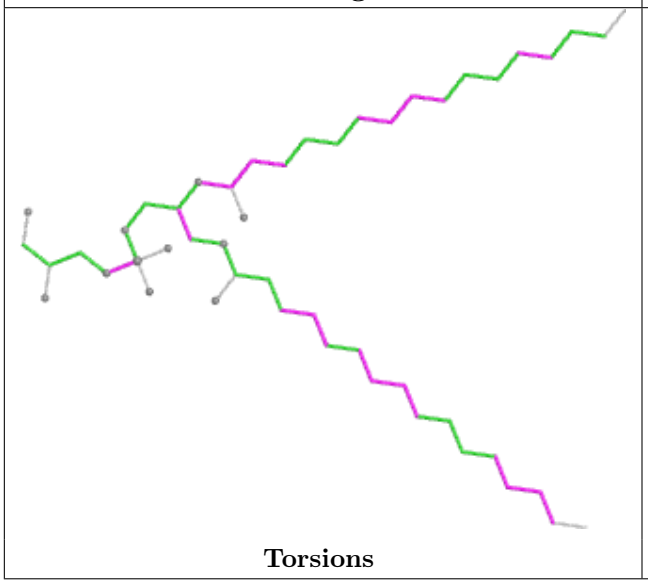
Ligand LHG A 849



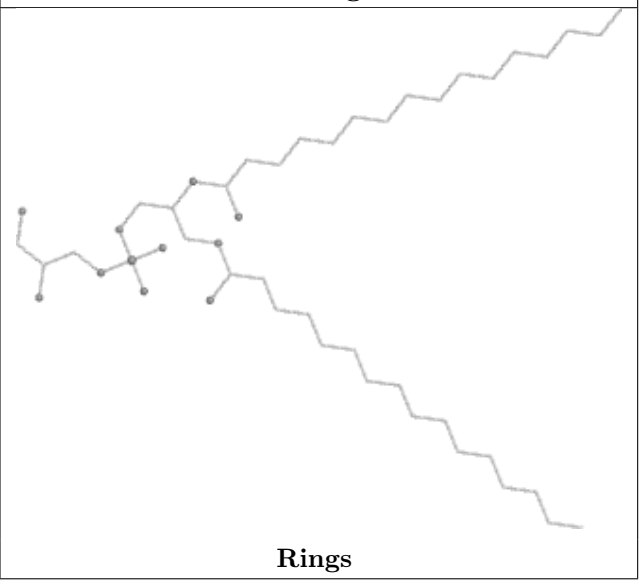
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Bond angles

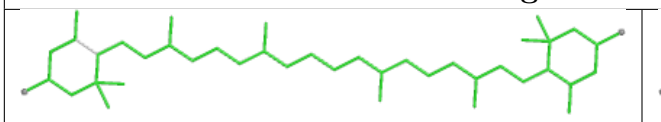


Torsions



Rings

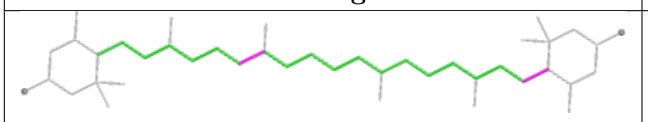
Ligand LUT 3 1001



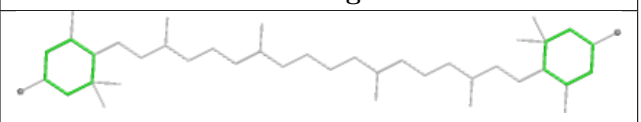
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Bond angles

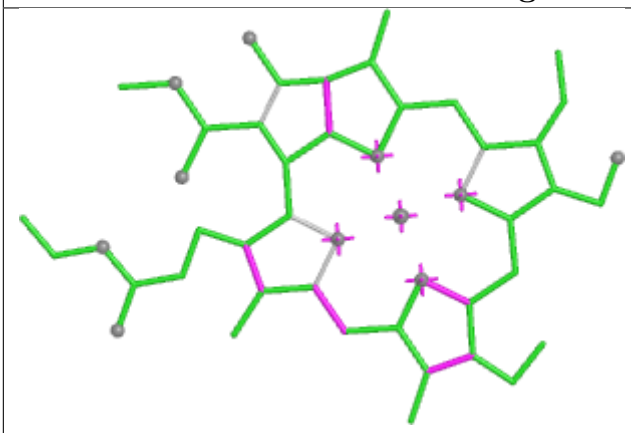


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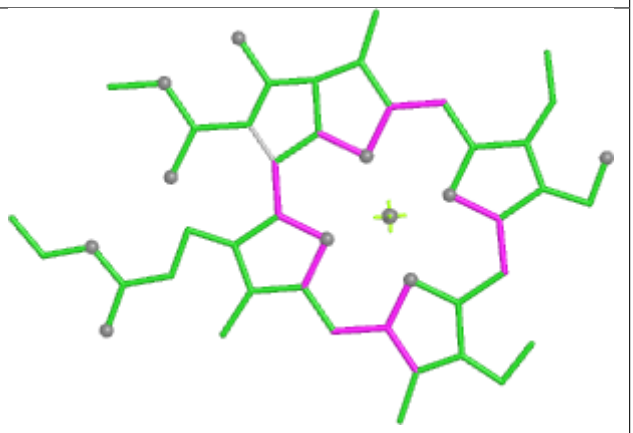


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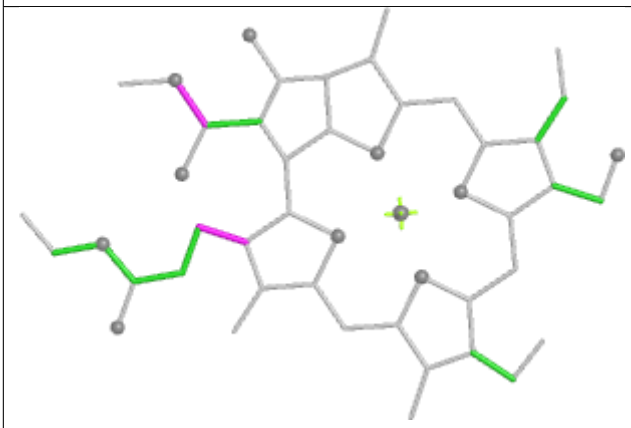
Ligand CHL 7 1013



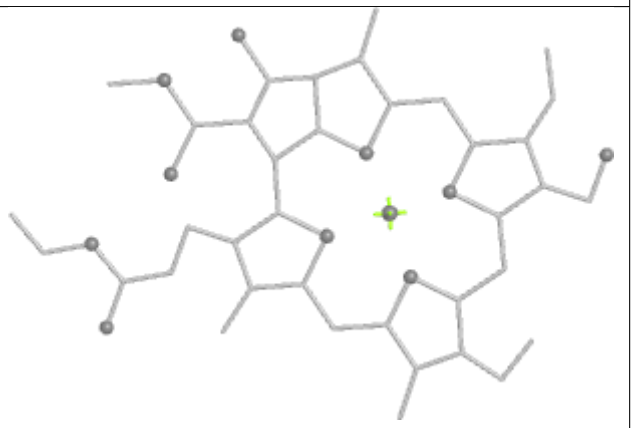
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Bond angles

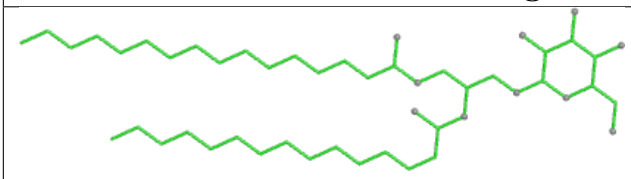


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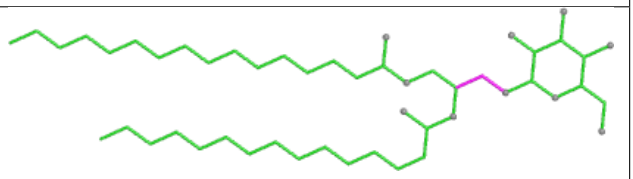


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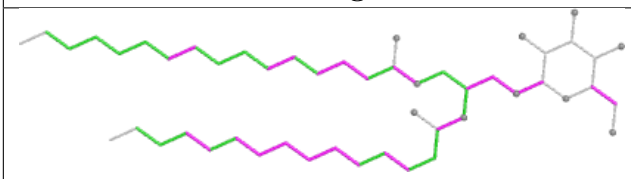
Ligand LMG 0 303



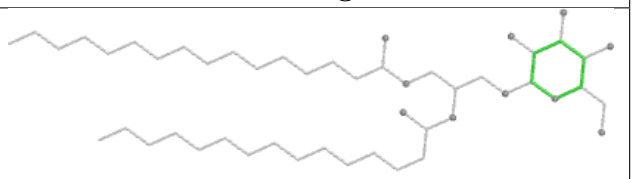
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Bond angles

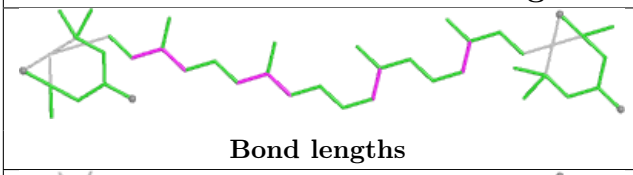


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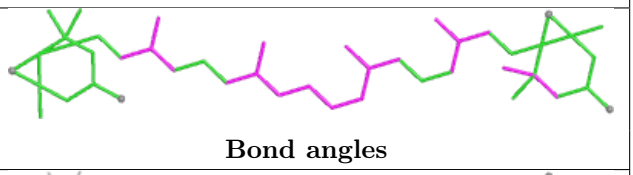


Rings

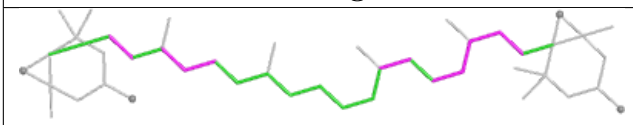
Ligand XAT 8 304



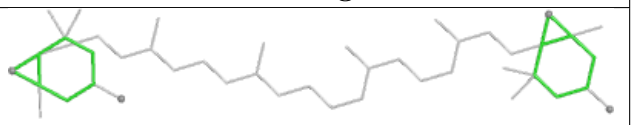
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Bond angles

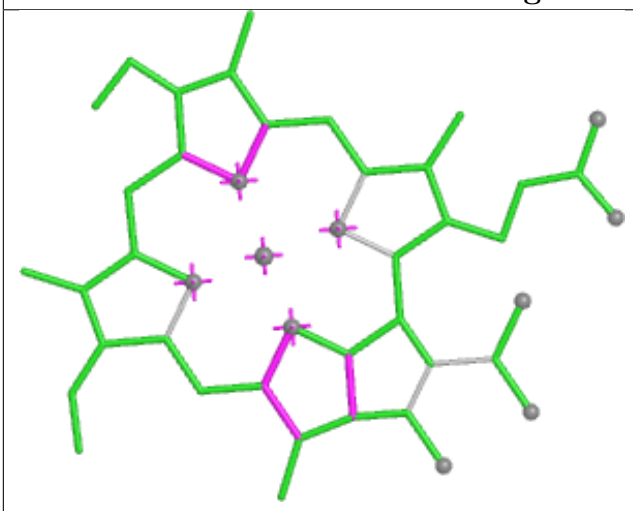


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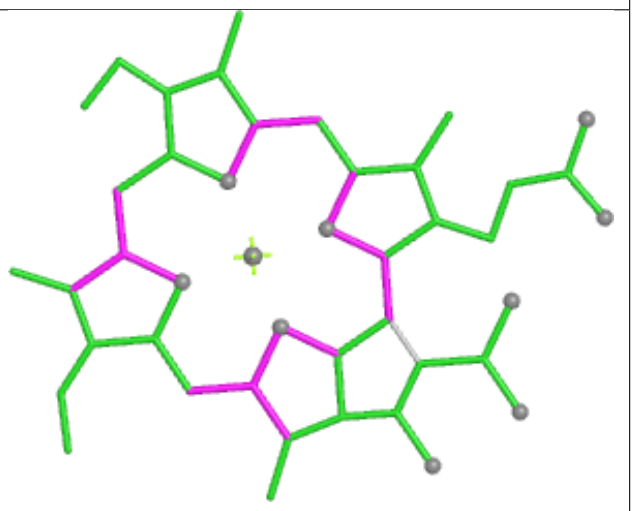


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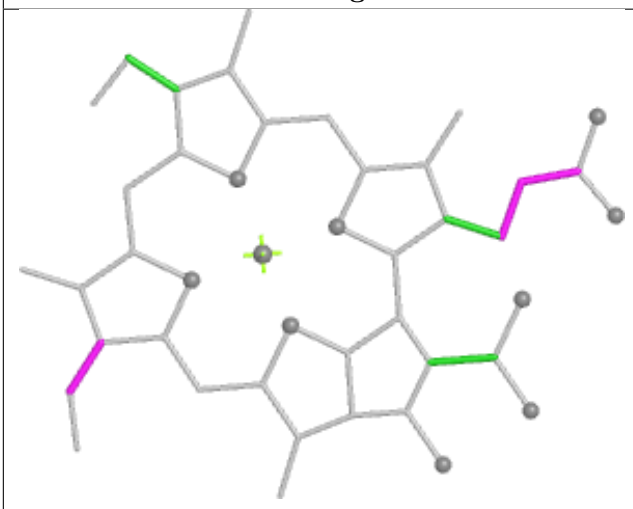
Ligand CLA A 806



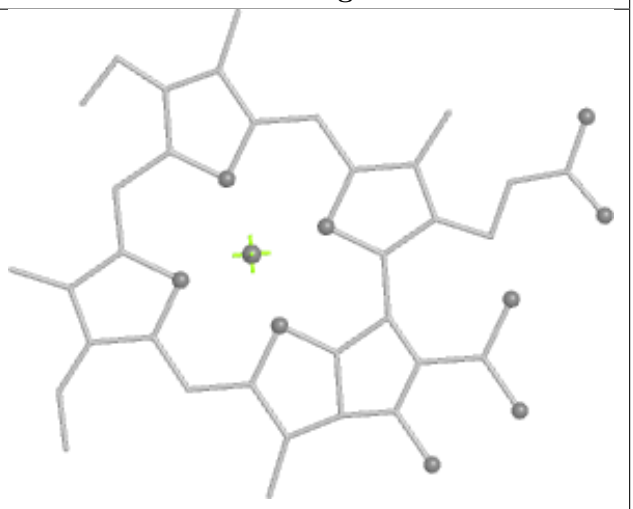
Bond lengths



Bond angles

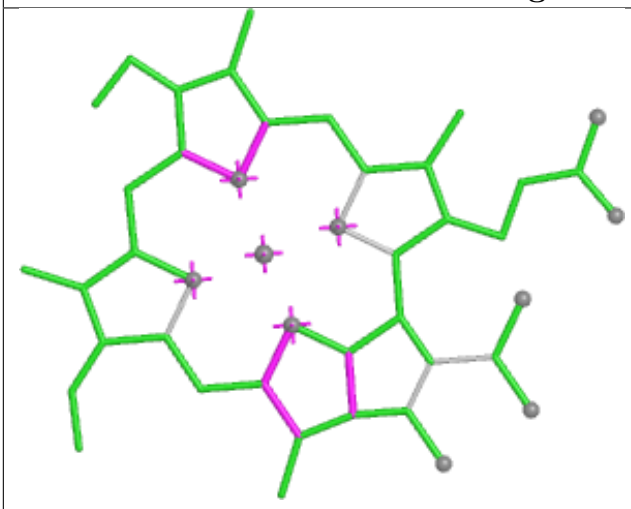


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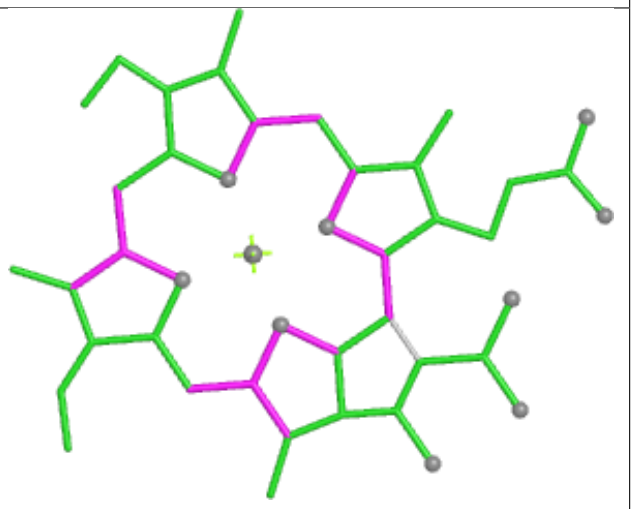


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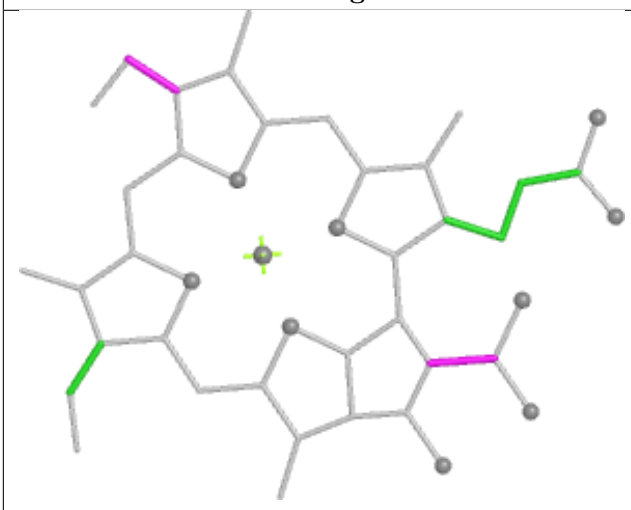
Ligand CLA 5 322



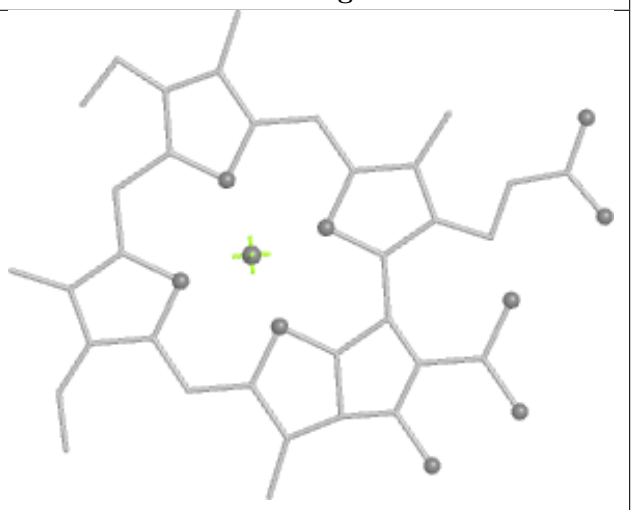
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Bond angles

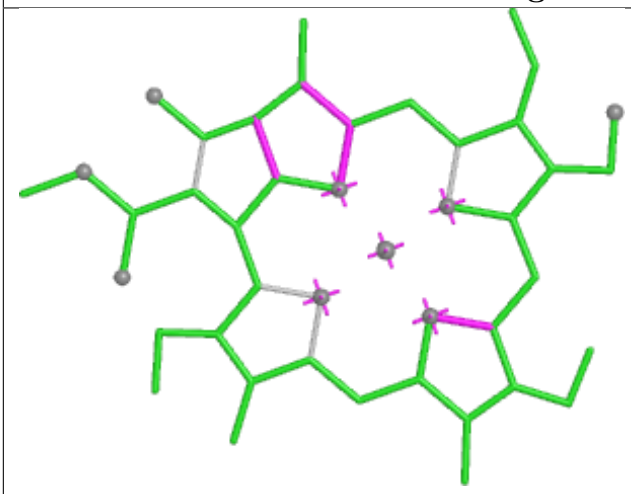


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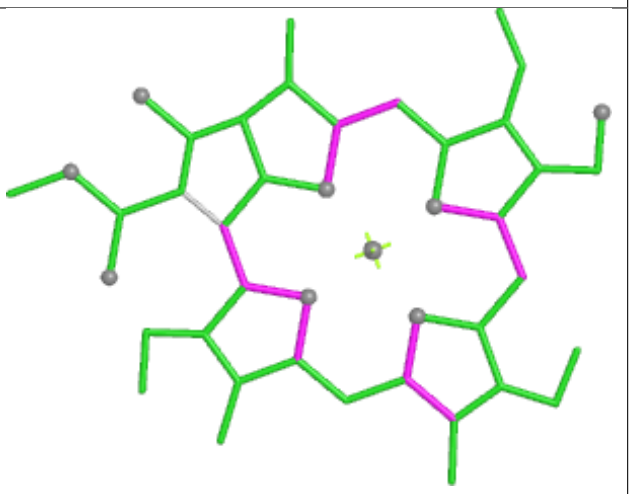


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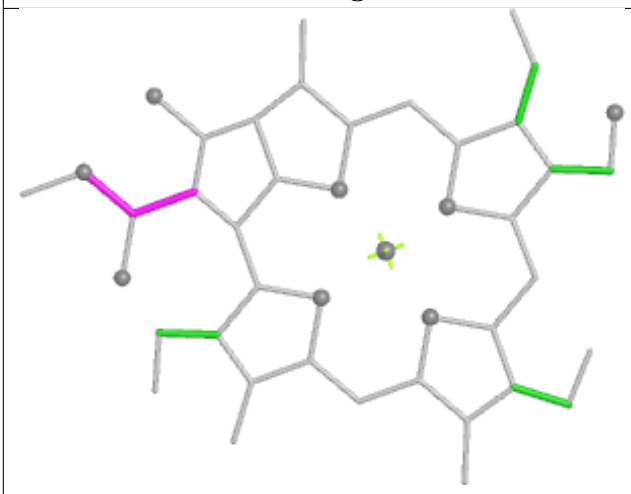
Ligand CHL 6 317



Bond lengths



Bond angles

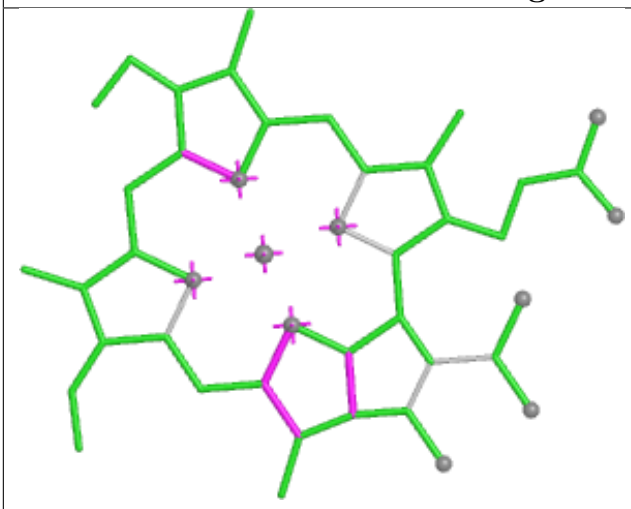


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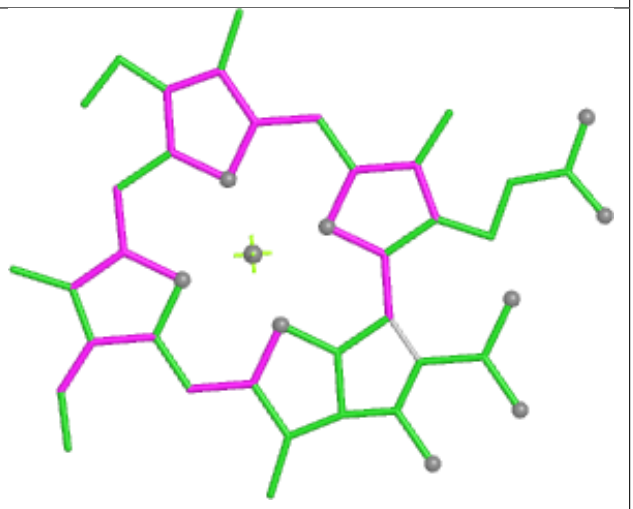


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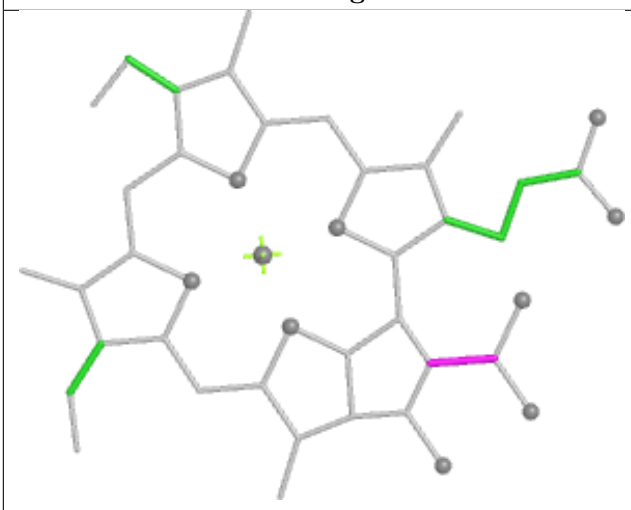
Ligand CLA 5 312



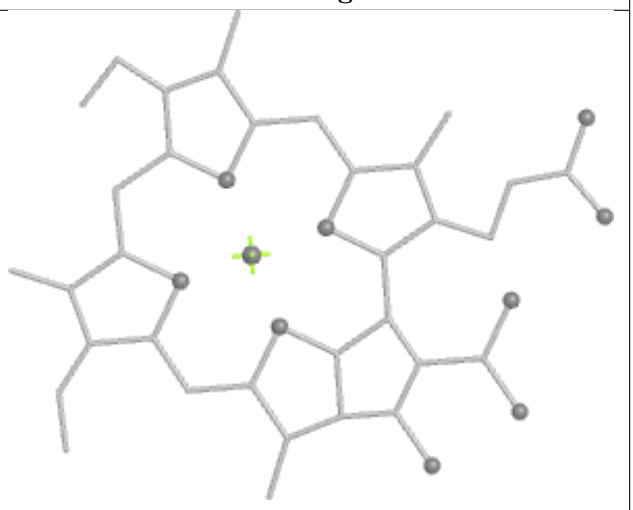
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Bond angles

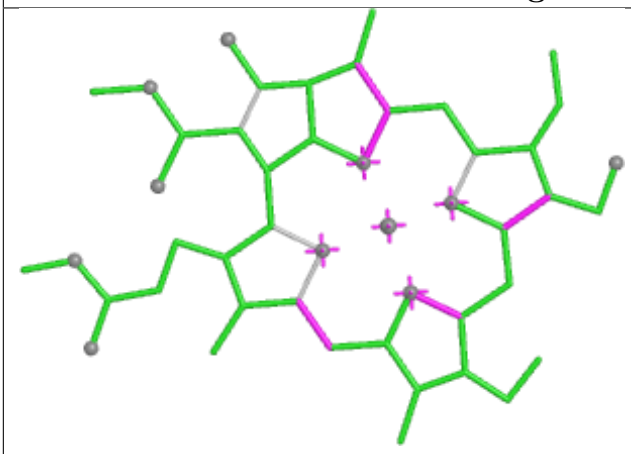


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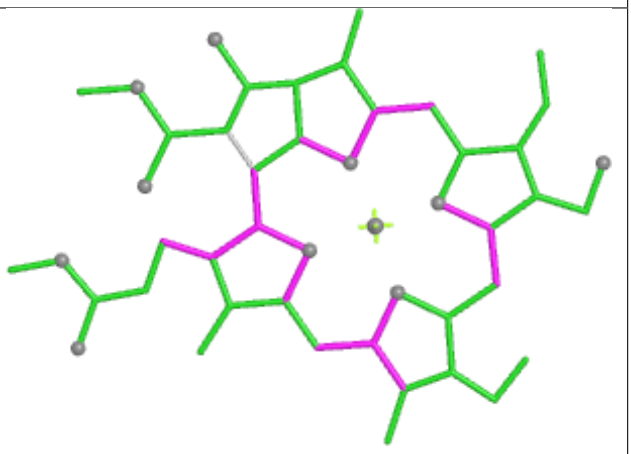


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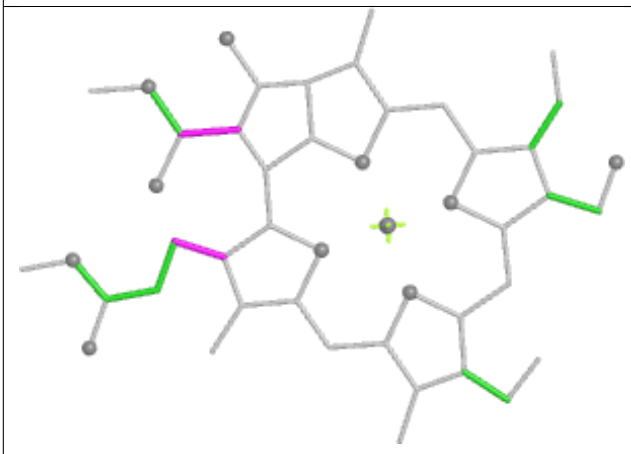
Ligand CHL 4 312



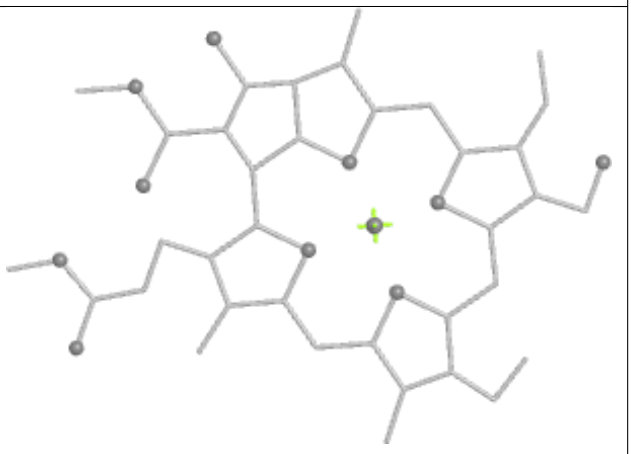
Bond lengths



Bond angles

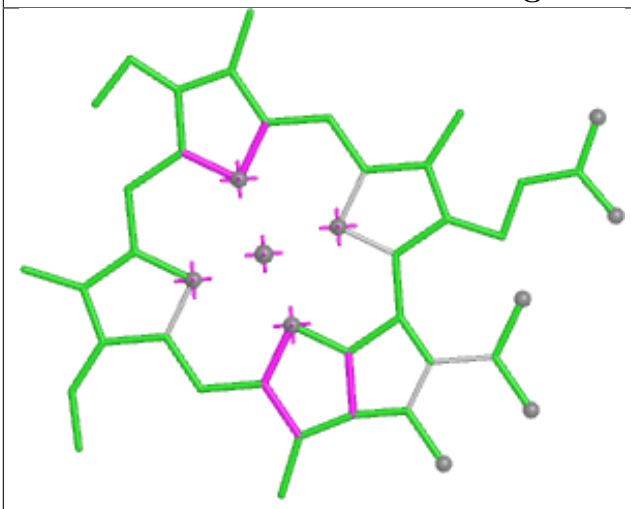


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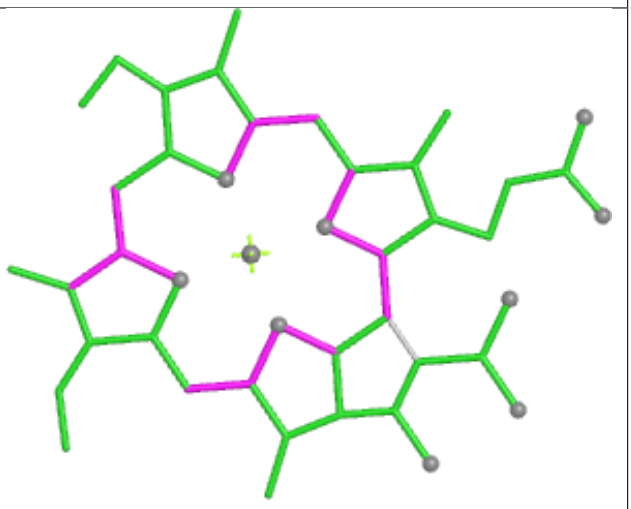


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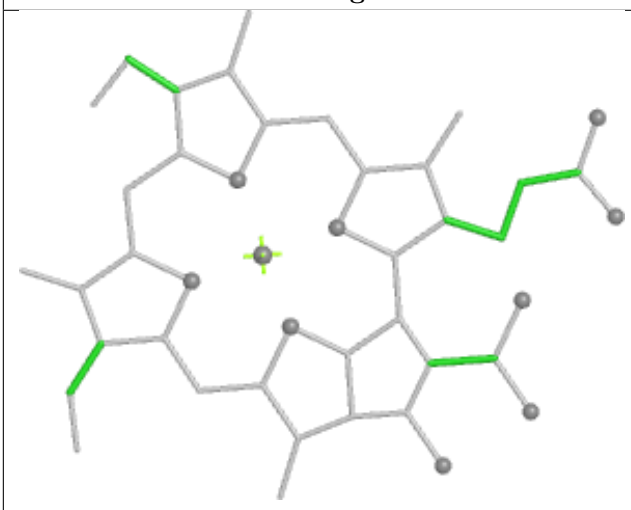
Ligand CLA A 826



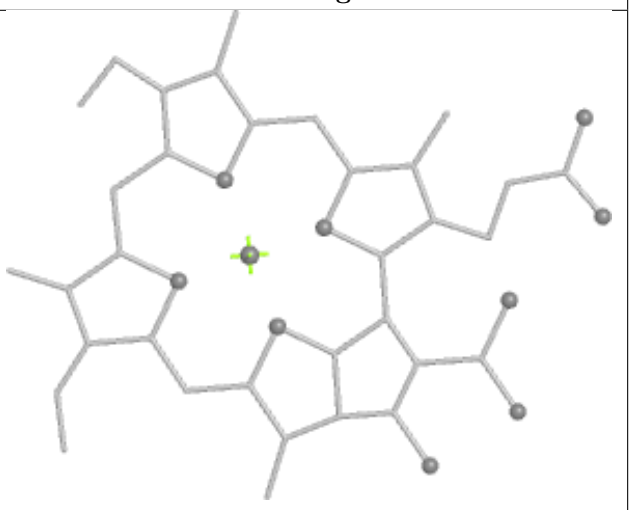
Bond lengths



Bond angles

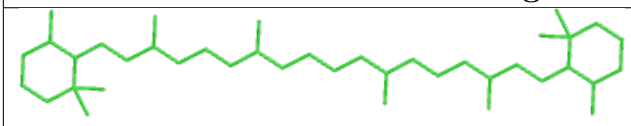


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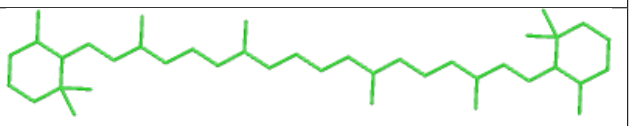


Rings

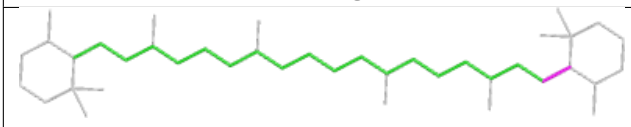
Ligand BCR B 846



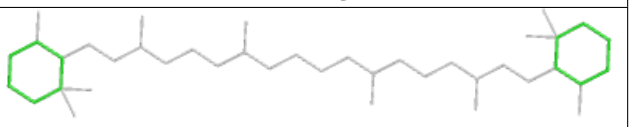
Bond lengths



Bond angles

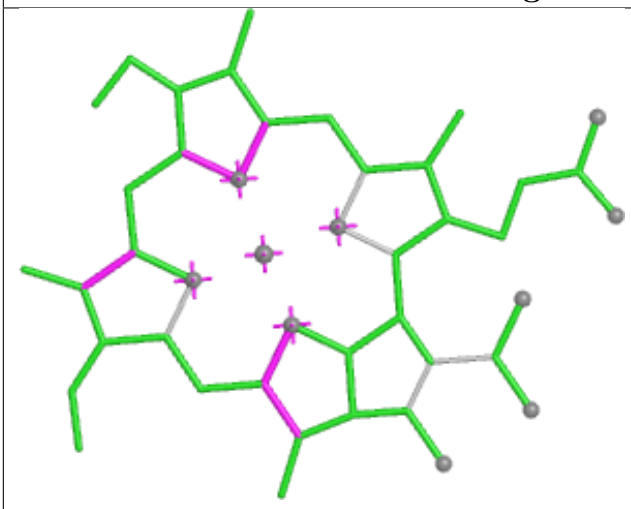


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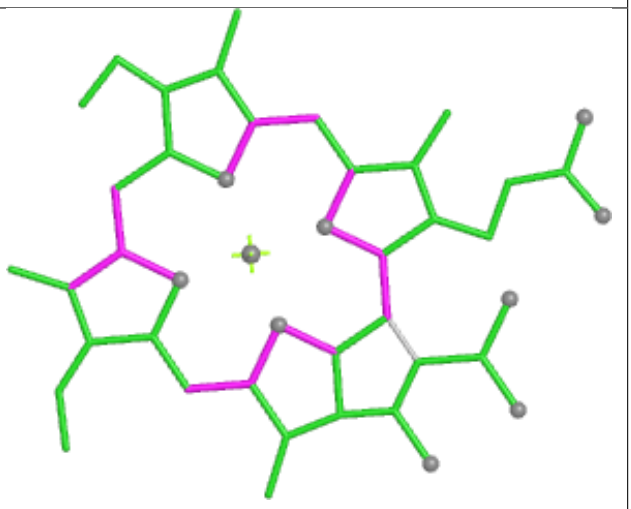


Rings

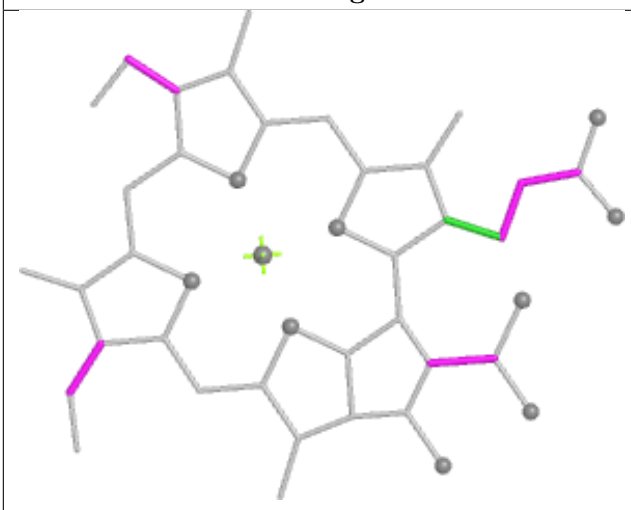
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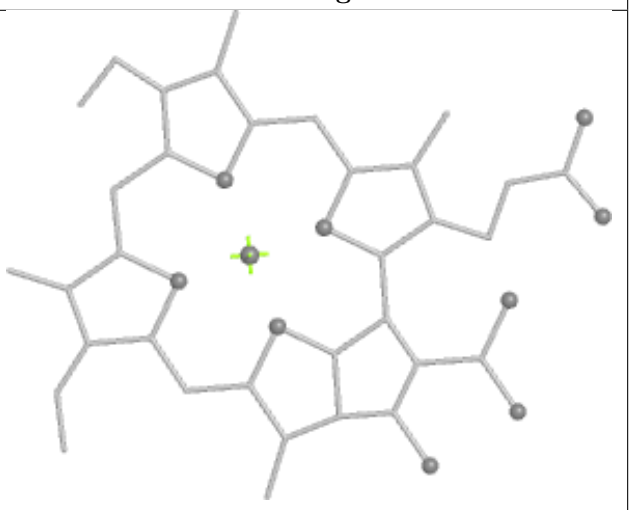
Bond lengths



Bond angles

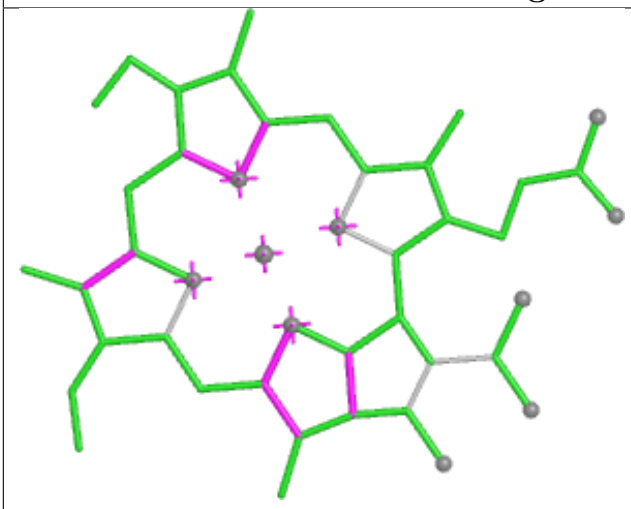


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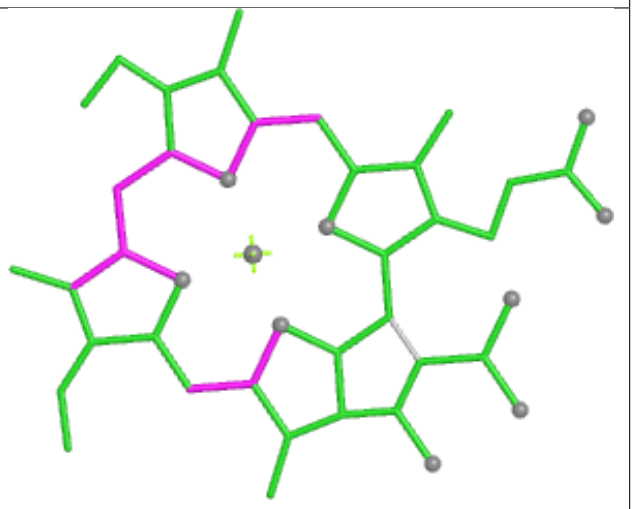


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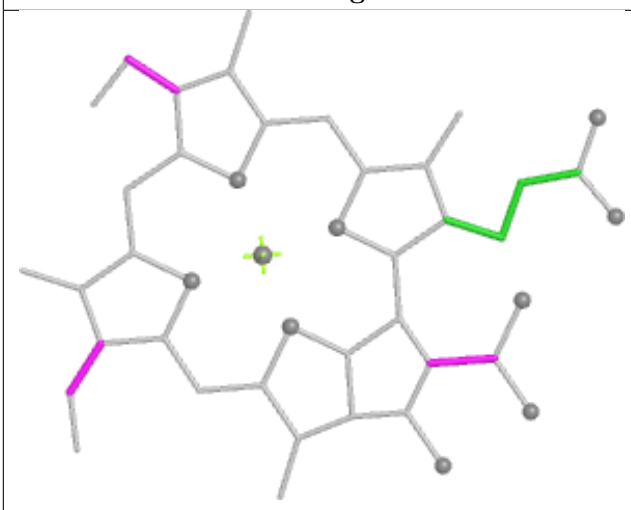
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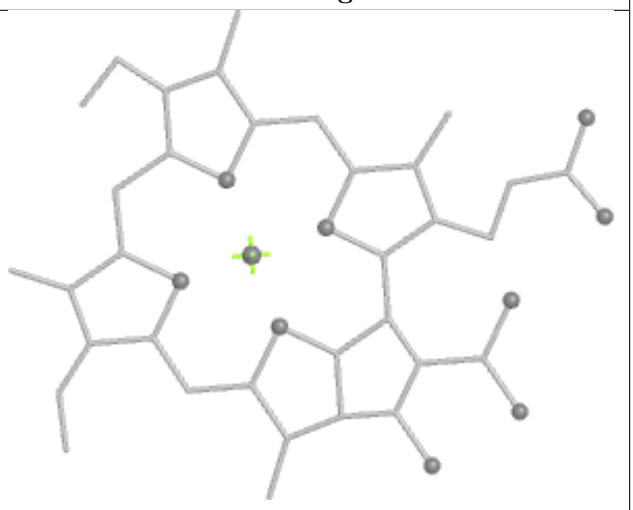
Bond lengths



Bond angles

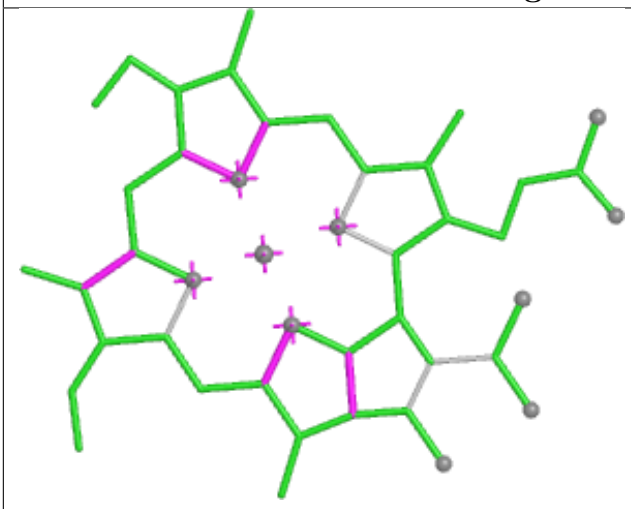


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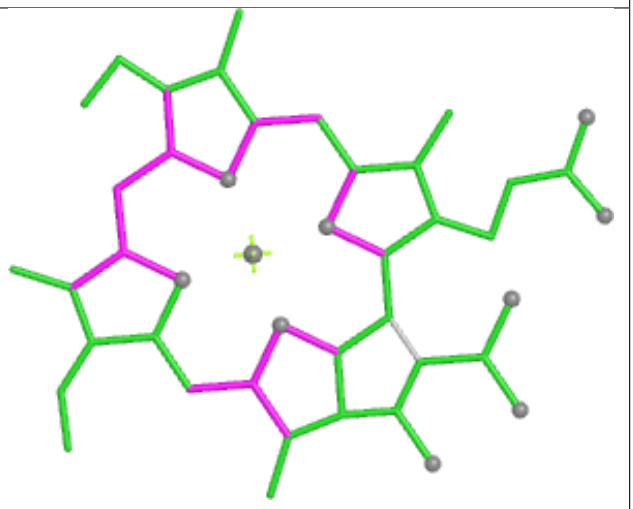


Rings

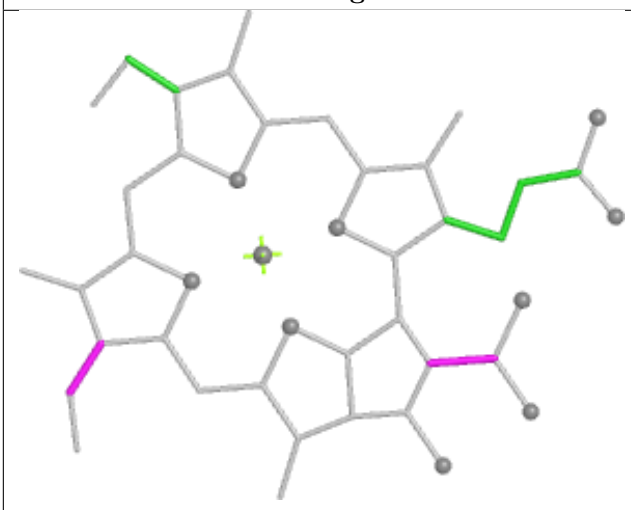
Ligand CLA B 817



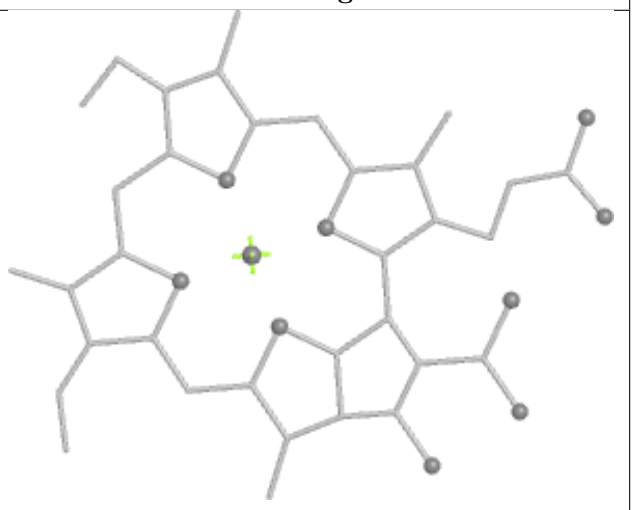
Bond lengths



Bond angles

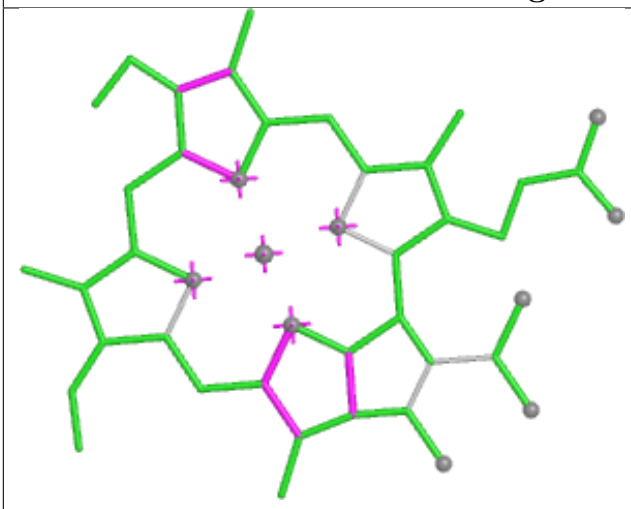


Torsions

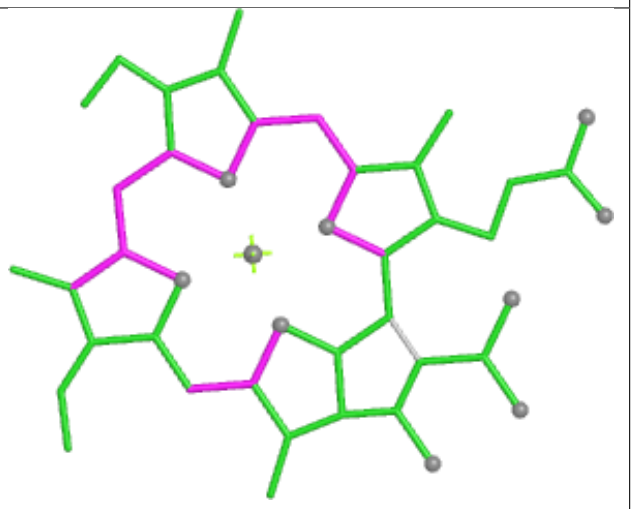


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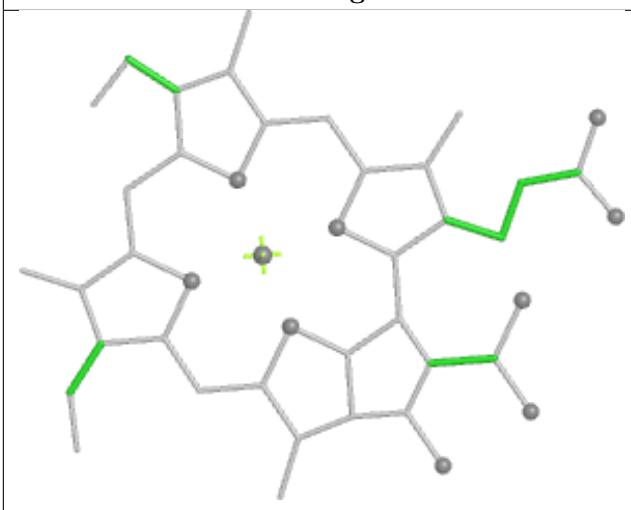
Ligand CLA 5 315



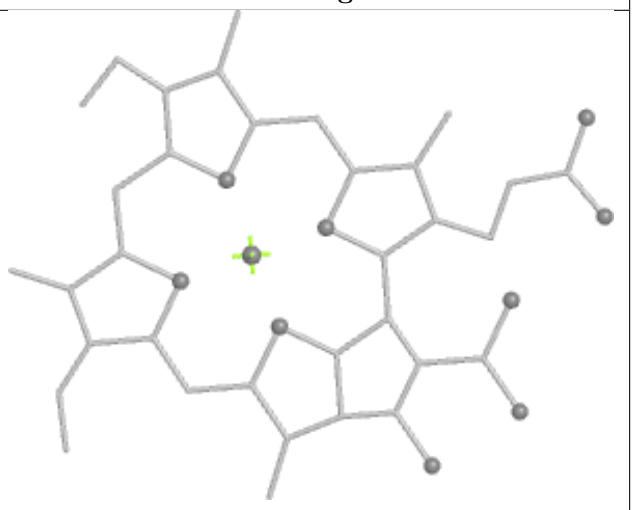
Bond lengths



Bond angles

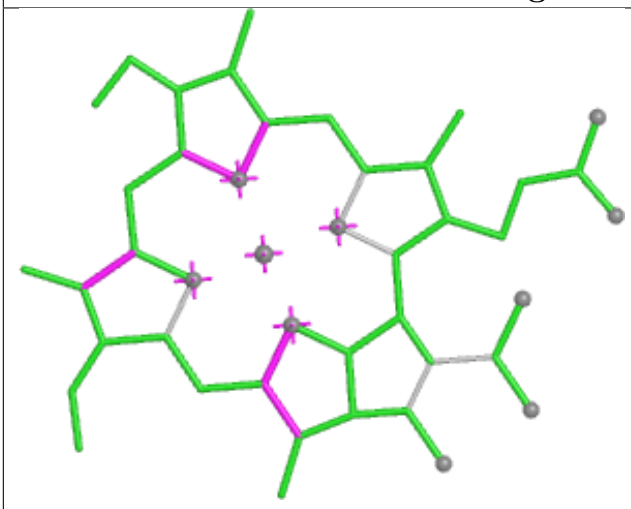


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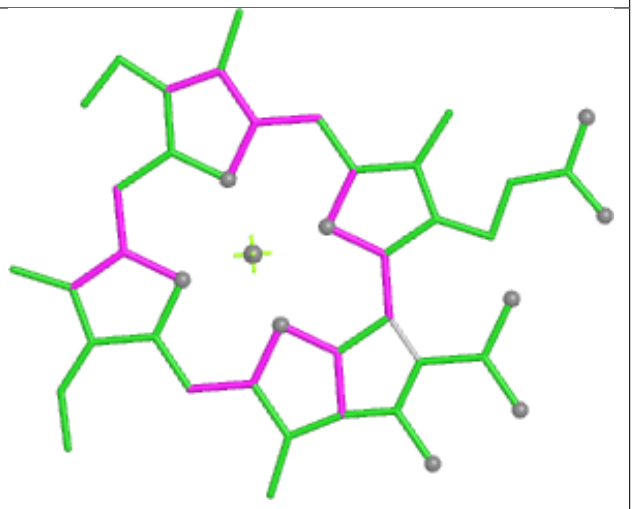


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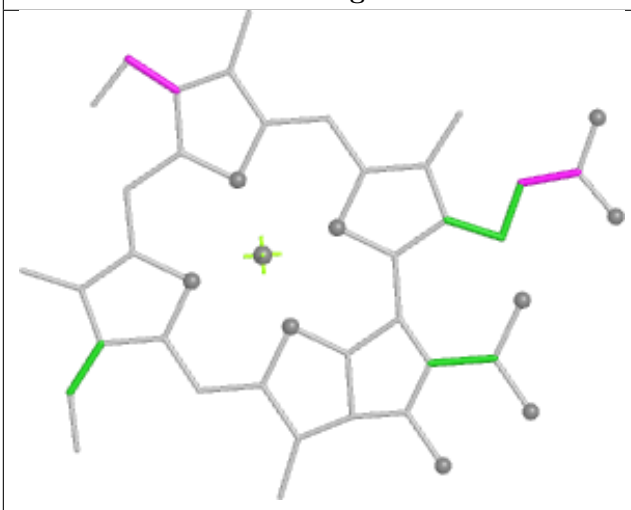
Ligand CLA 6 306



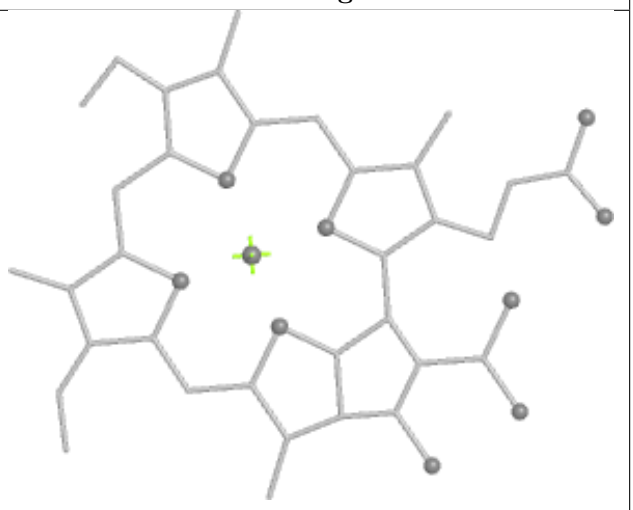
Bond lengths



Bond angles

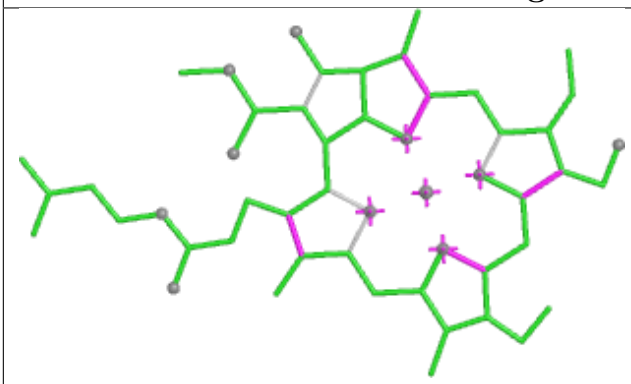


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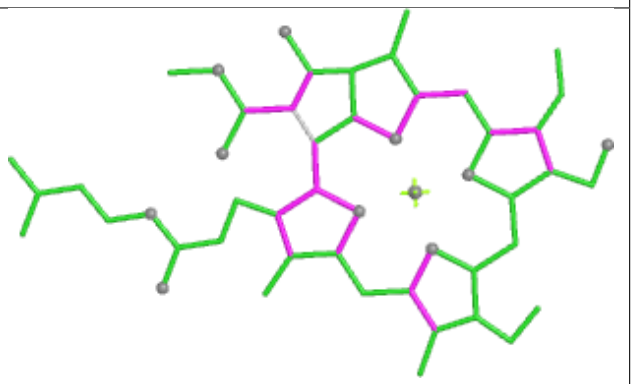


Rings

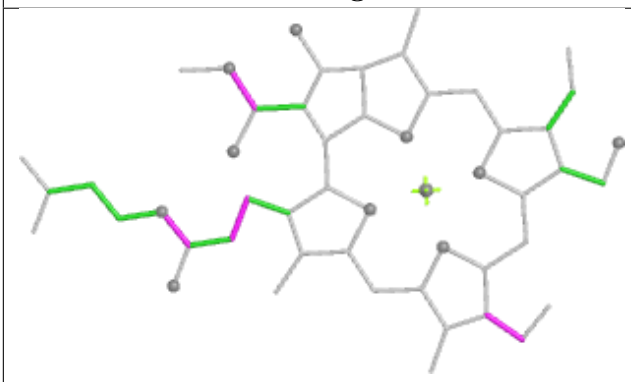
Ligand CHL 6 314



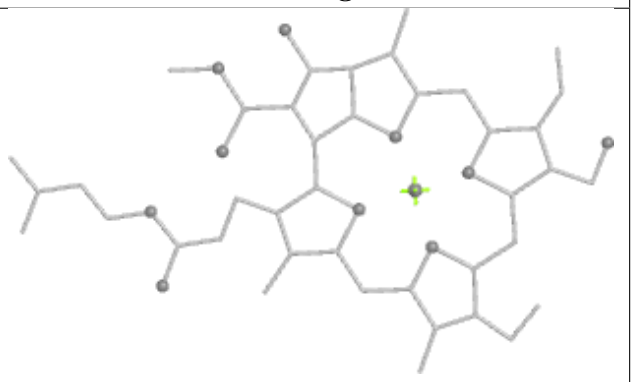
Bond lengths



Bond angles

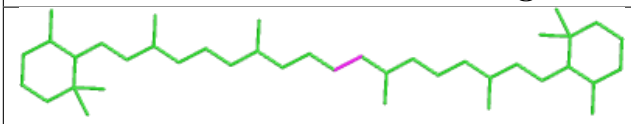


Torsions

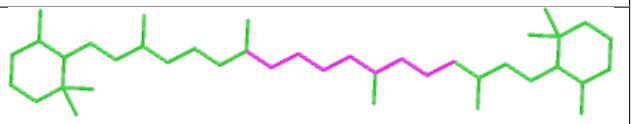


Rings

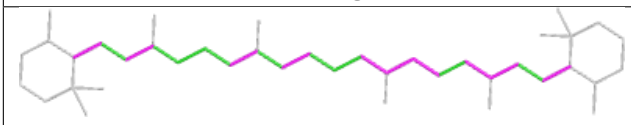
Ligand BCR 7 1003



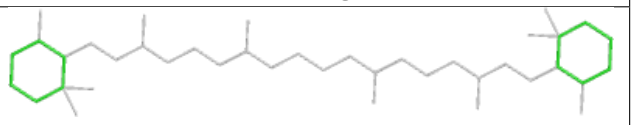
Bond lengths



Bond angles

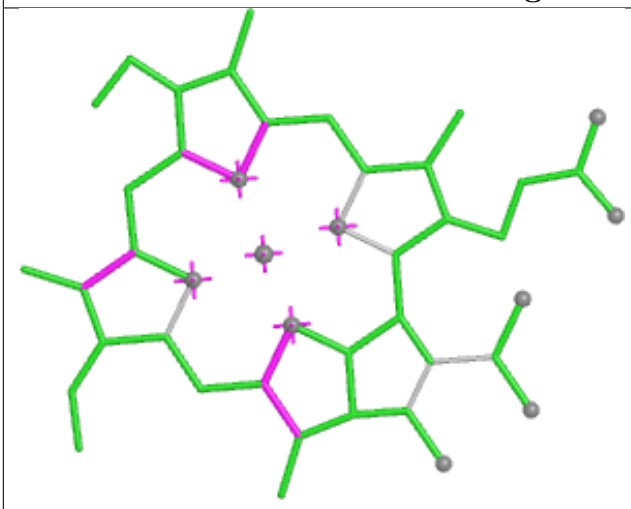


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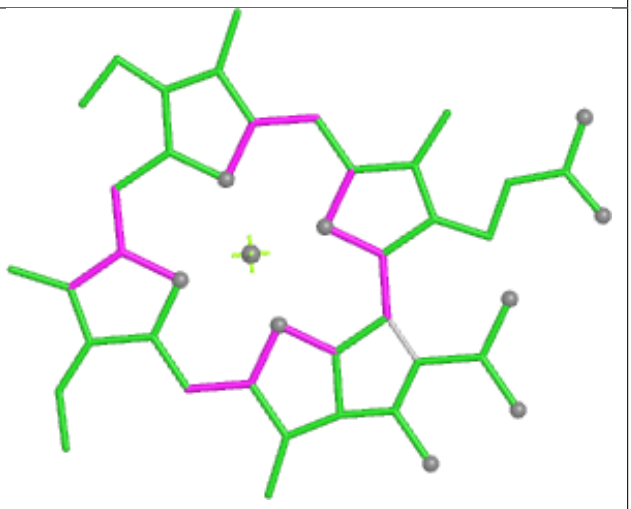


Rings

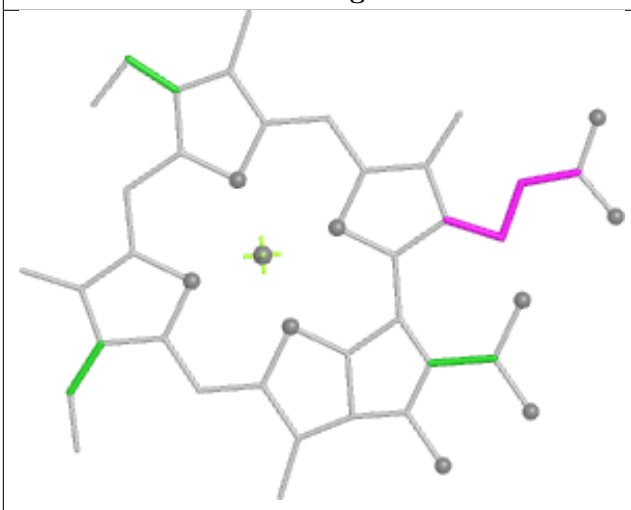
Ligand CLA B 839



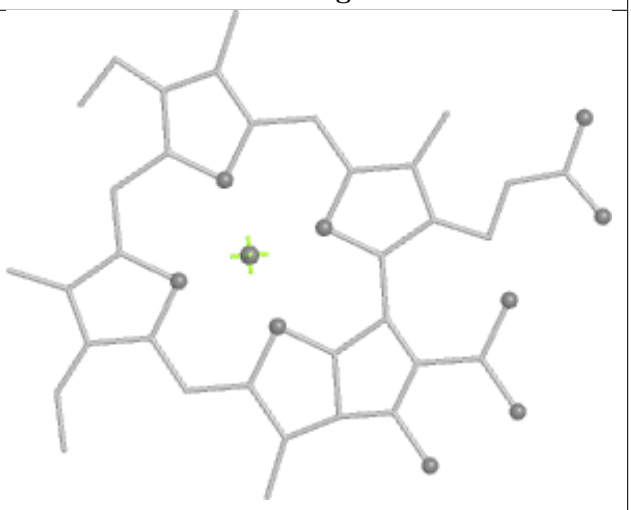
Bond lengths



Bond angles

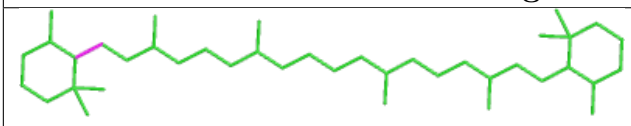


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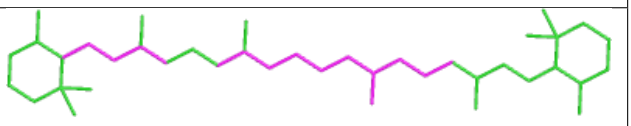


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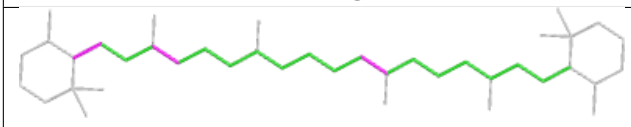
Ligand BCR B 804



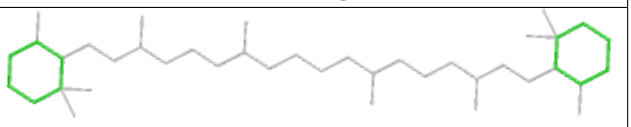
Bond lengths



Bond angles

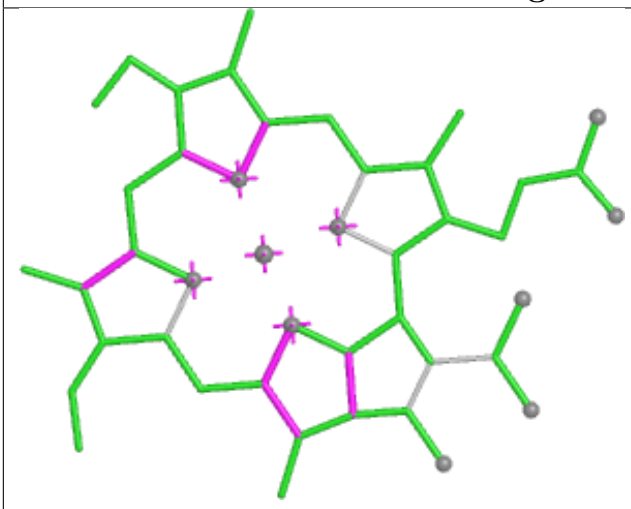


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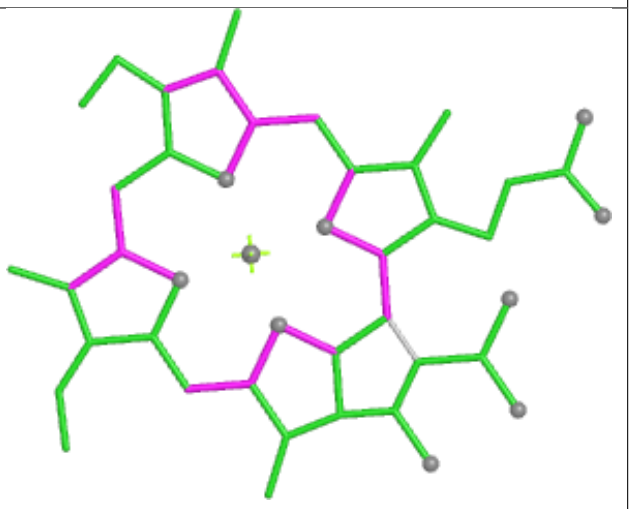


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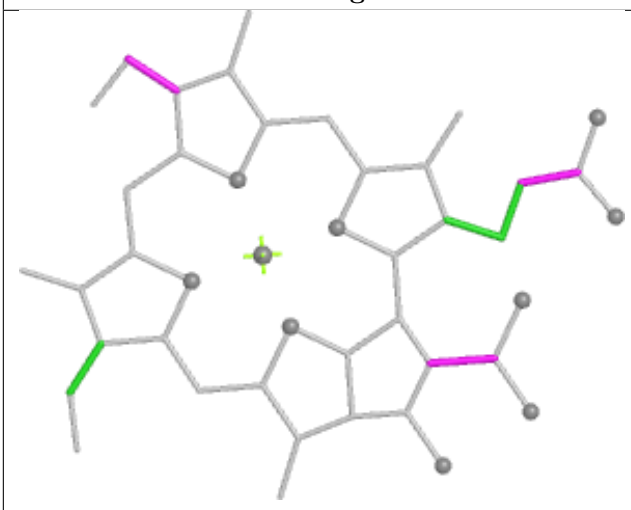
Ligand CLA 4 305



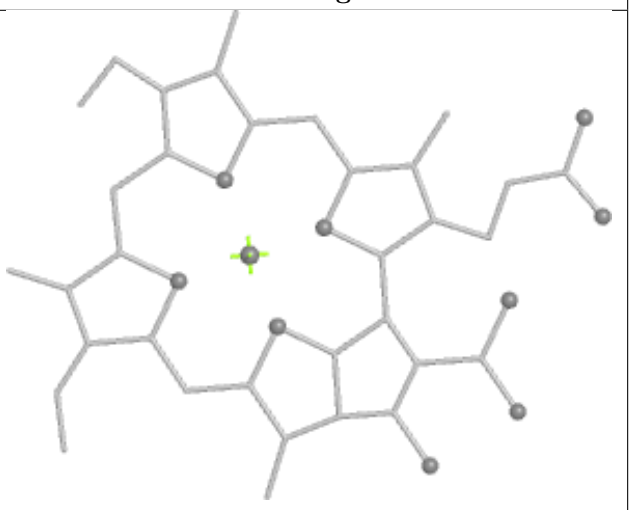
Bond lengths



Bond angles

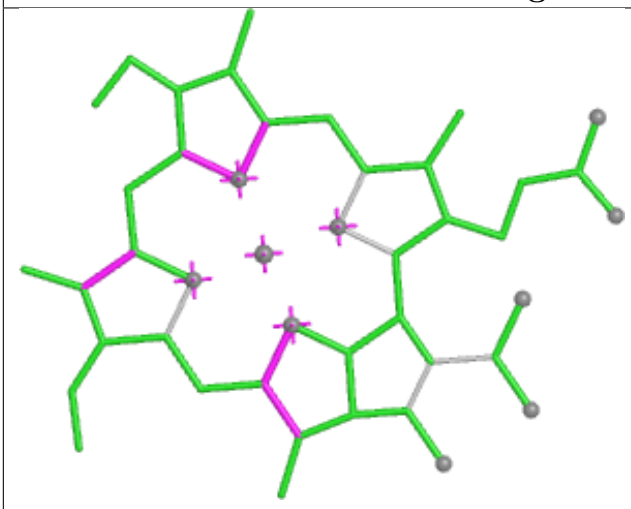


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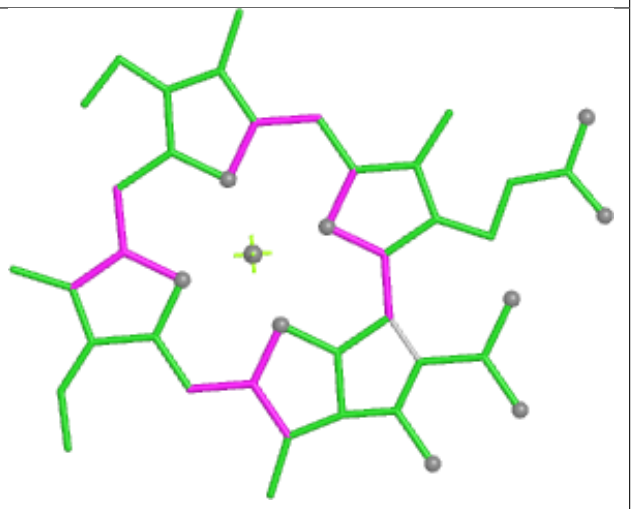


Rings

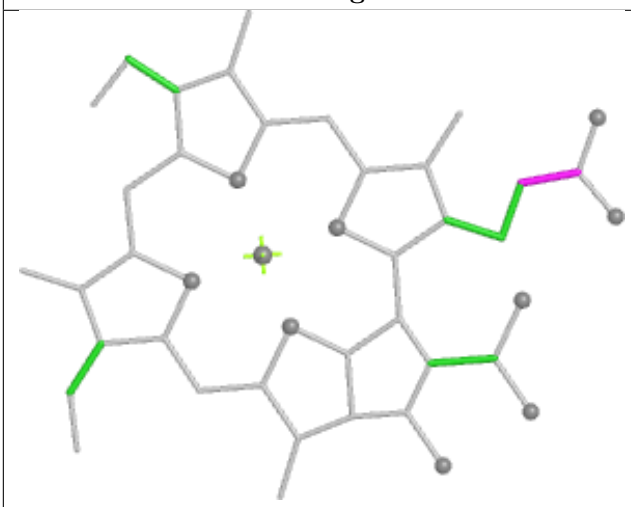
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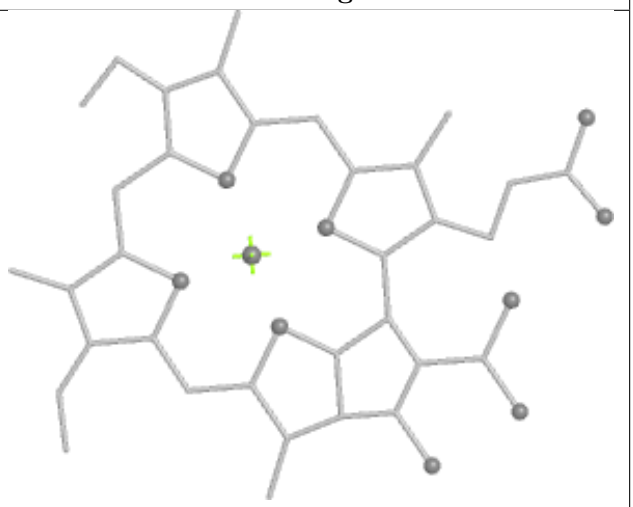
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Bond angles

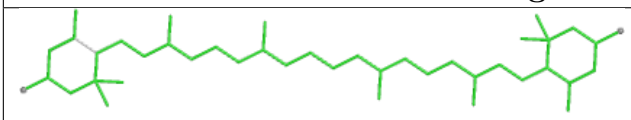


Torsions

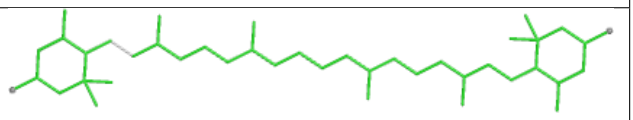


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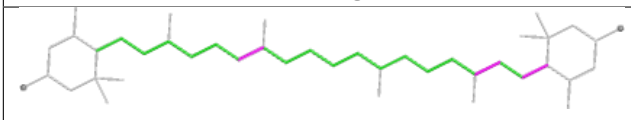
Ligand LUT 5 302



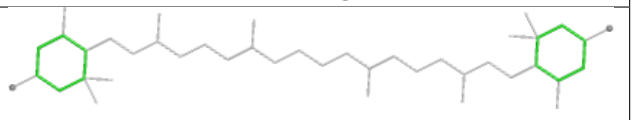
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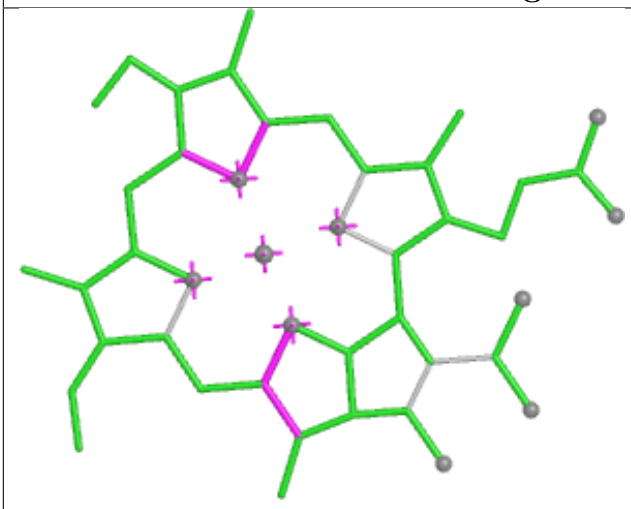


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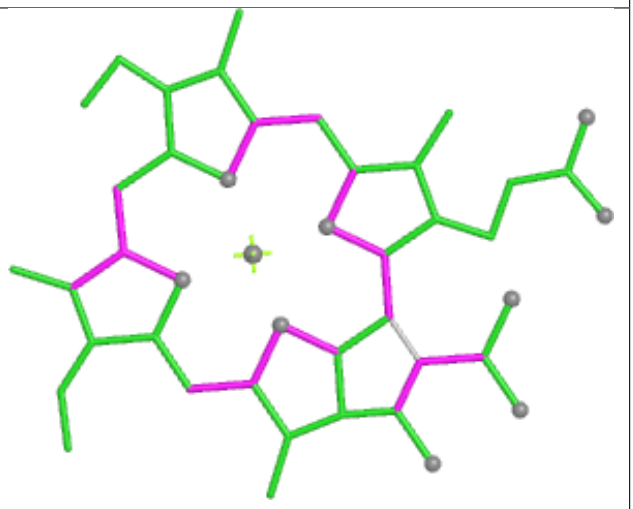


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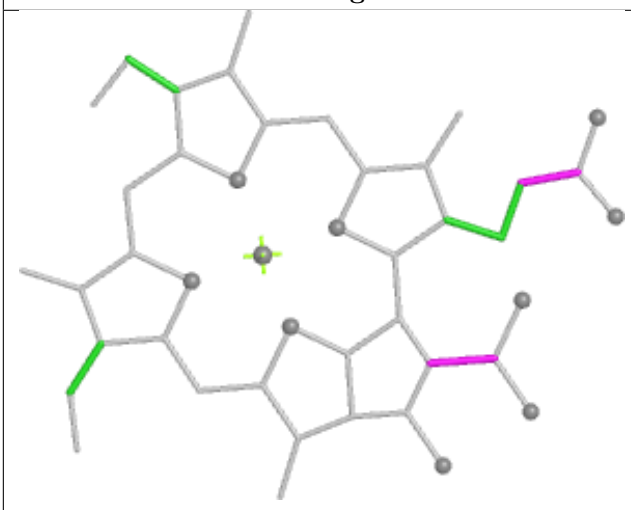
Ligand CLA A 824



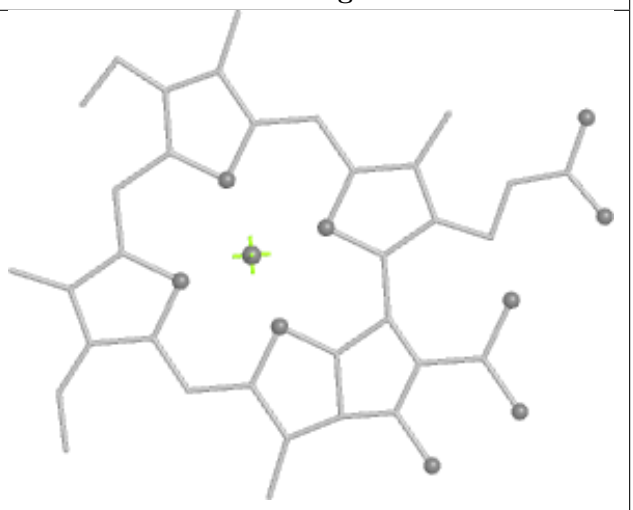
Bond lengths



Bond angles

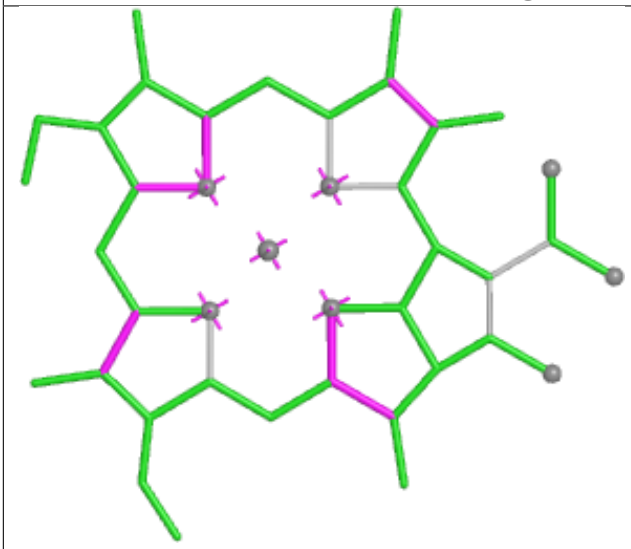


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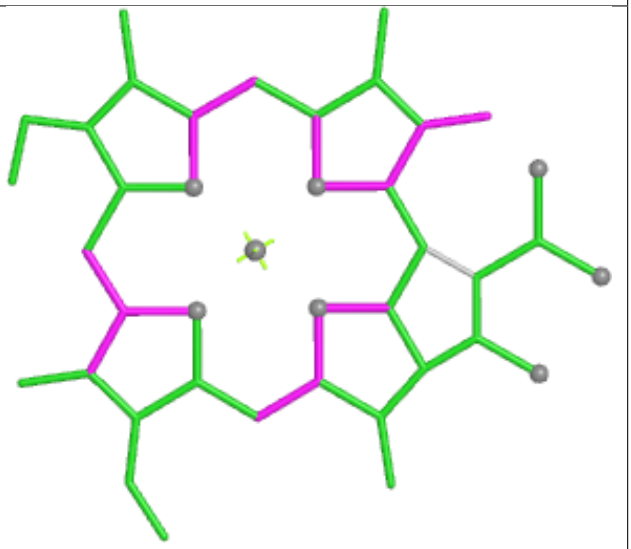


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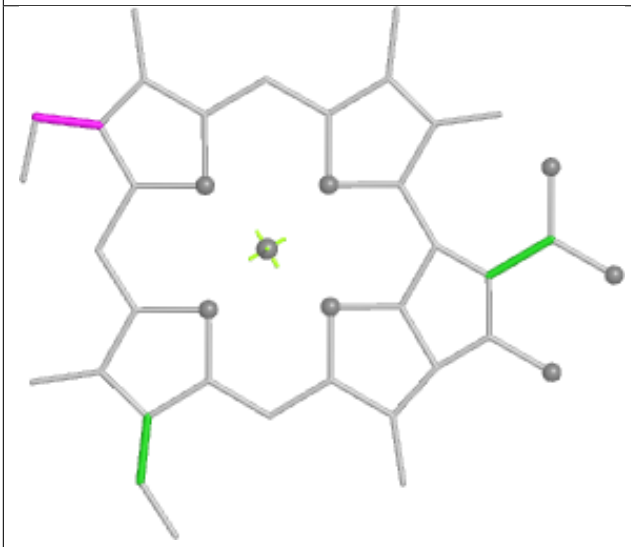
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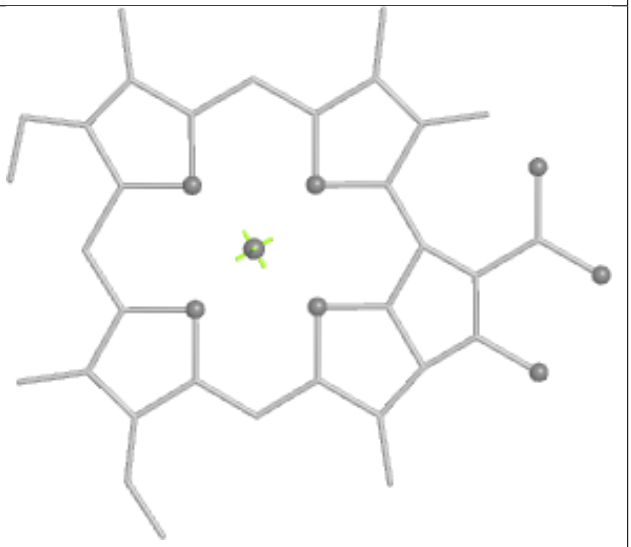
Bond lengths



Bond angles

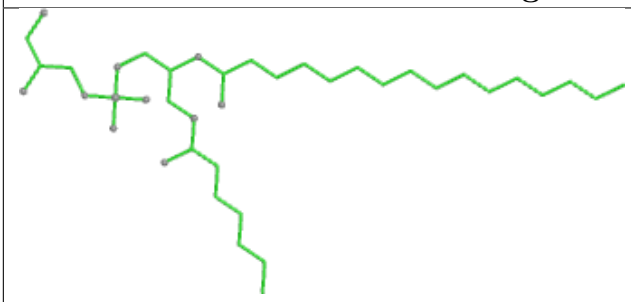


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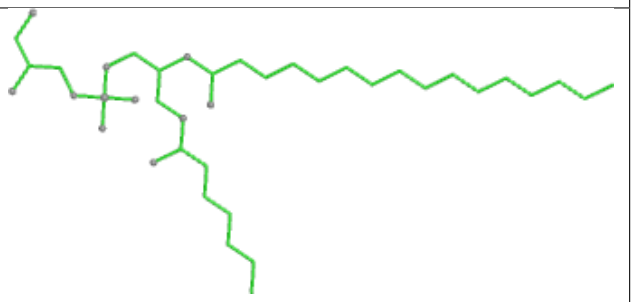


Rings

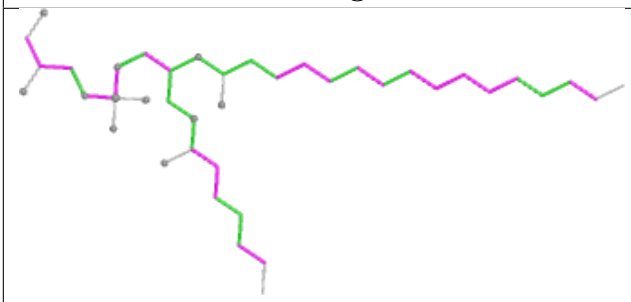
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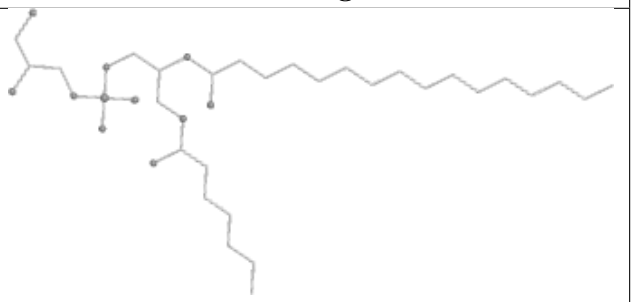
Bond lengths



Bond angles

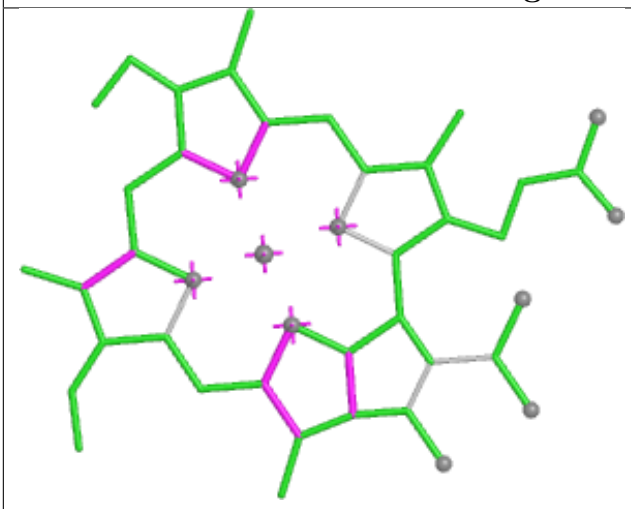


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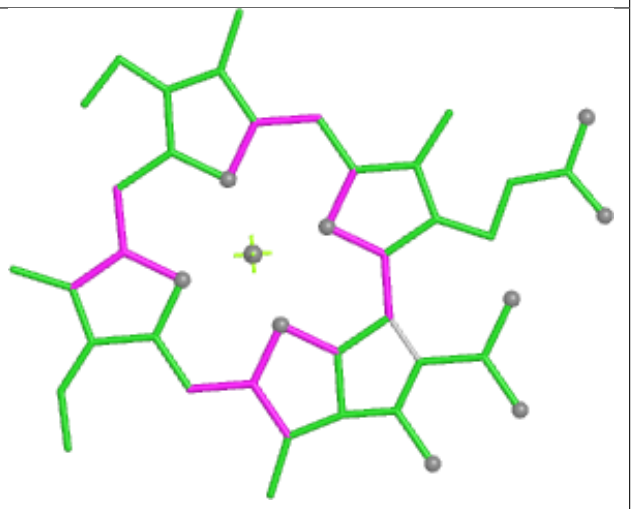


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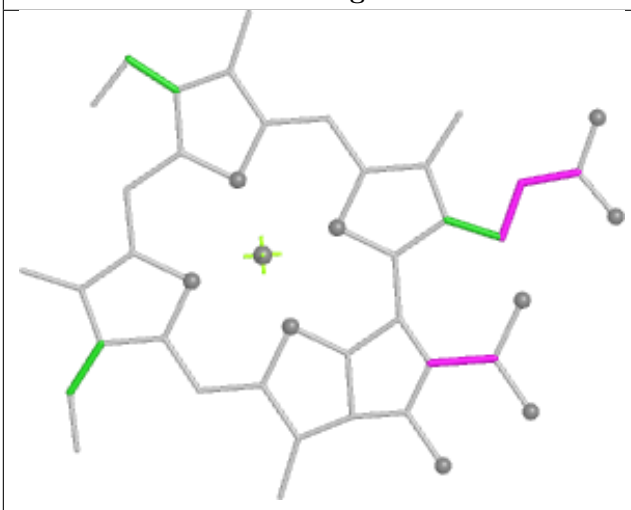
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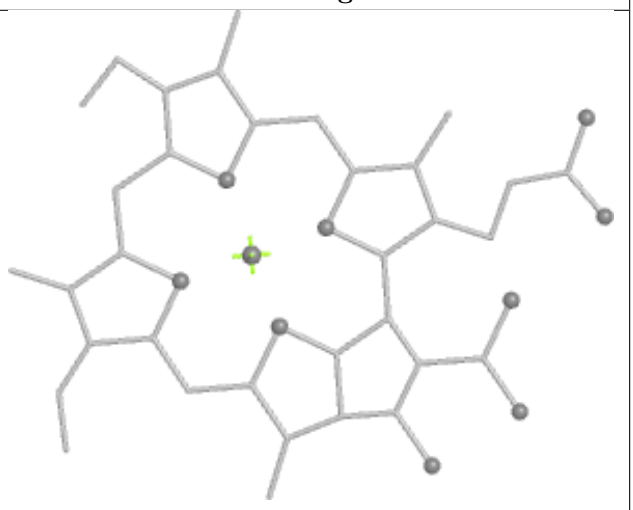
Bond lengths



Bond angles

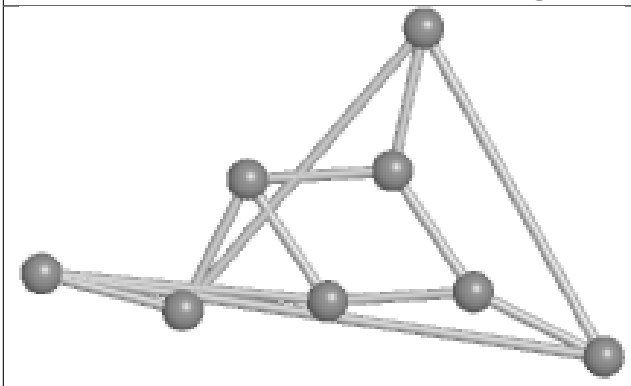


Torsions

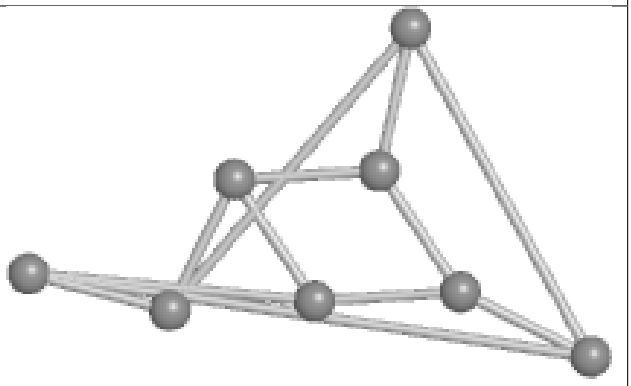


Rings

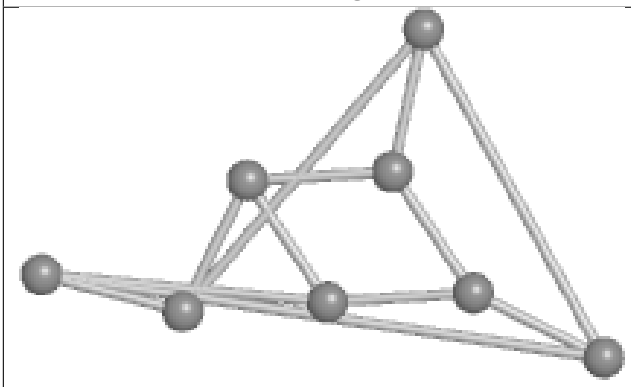
Ligand SF4 A 841



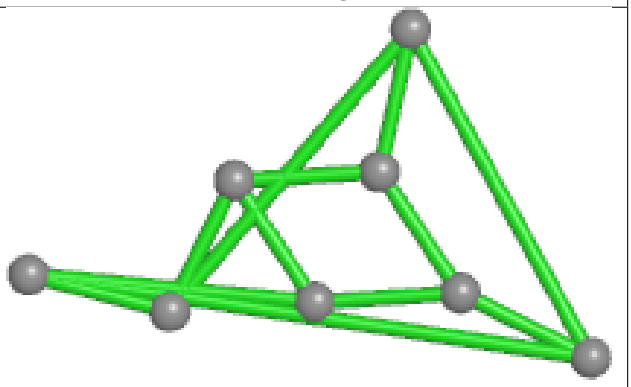
Bond lengths



Bond angles

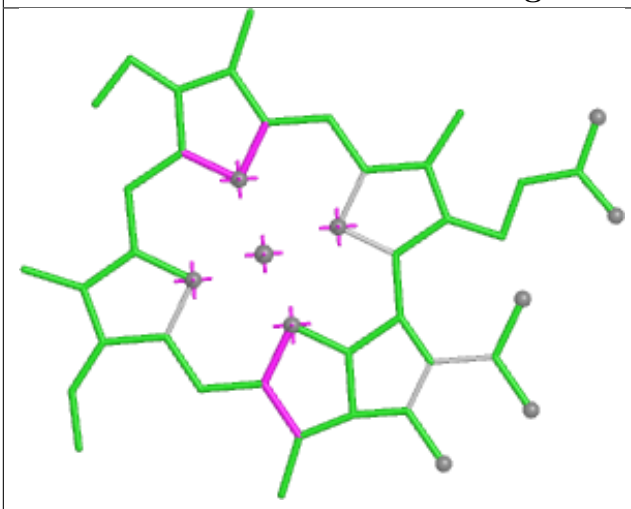


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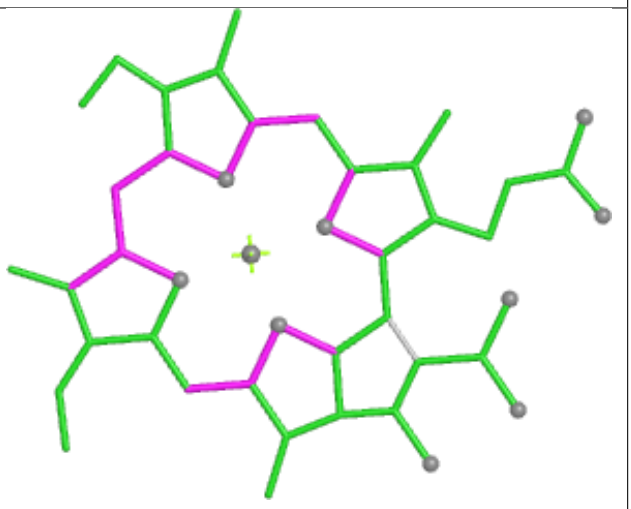


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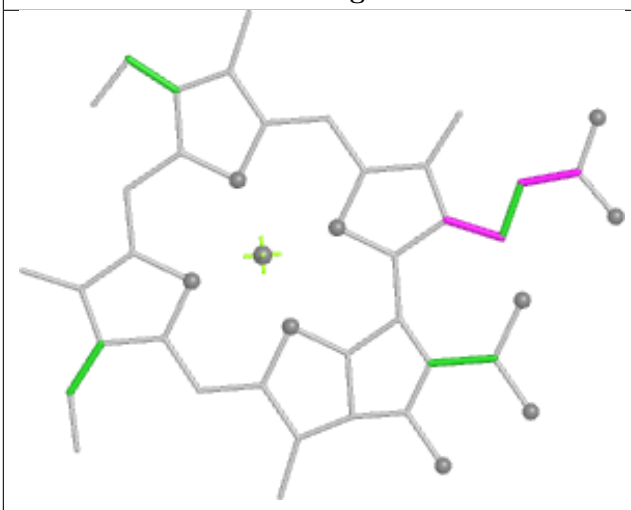
Ligand CLA B 808



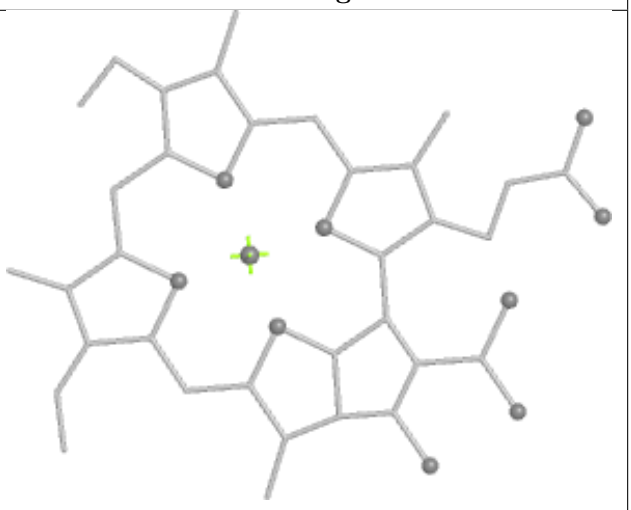
Bond lengths



Bond angles

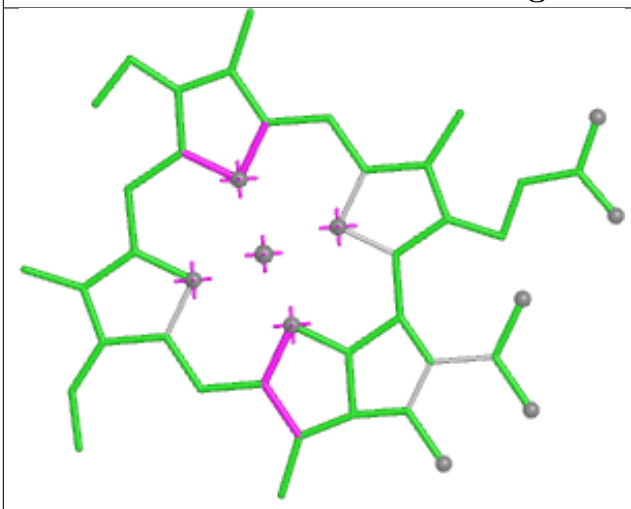


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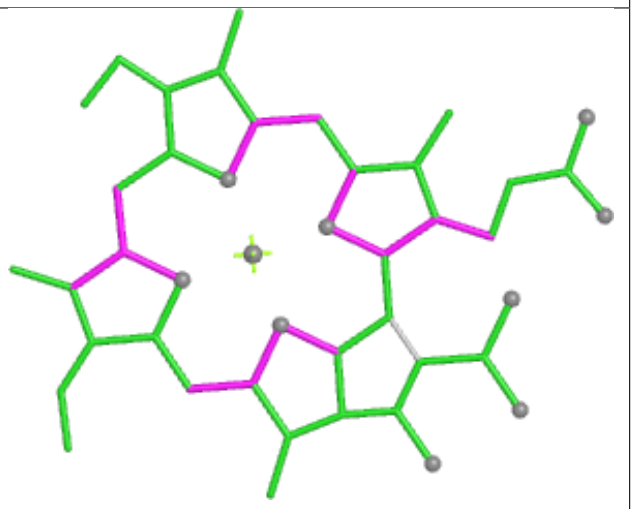


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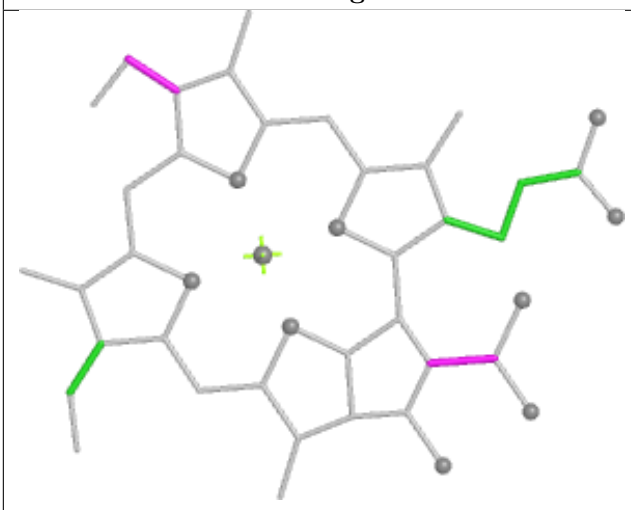
Ligand CLA 4 311



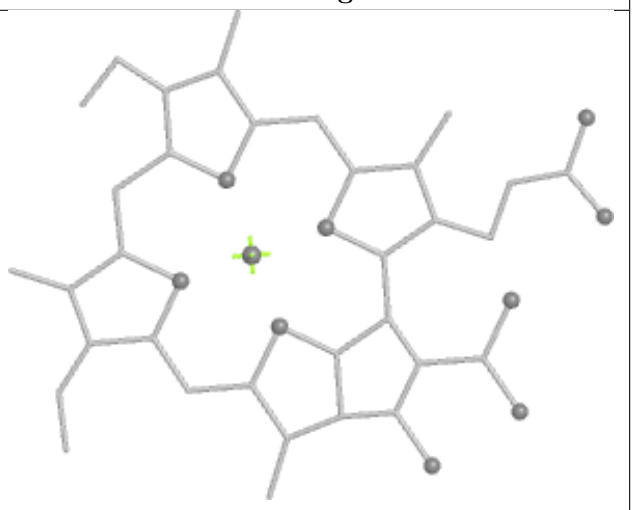
Bond lengths



Bond angles

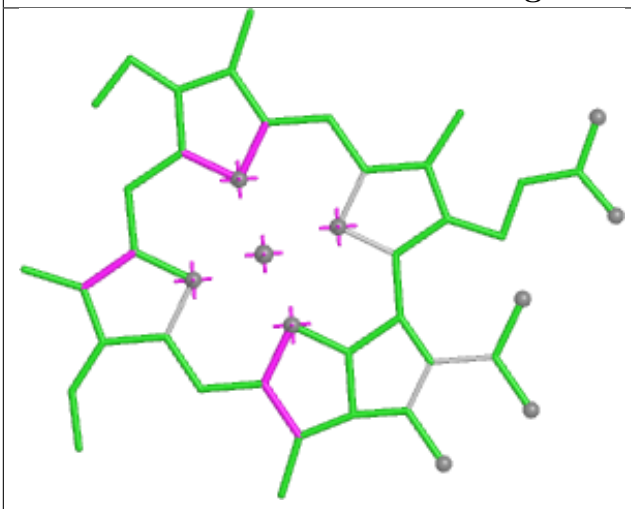


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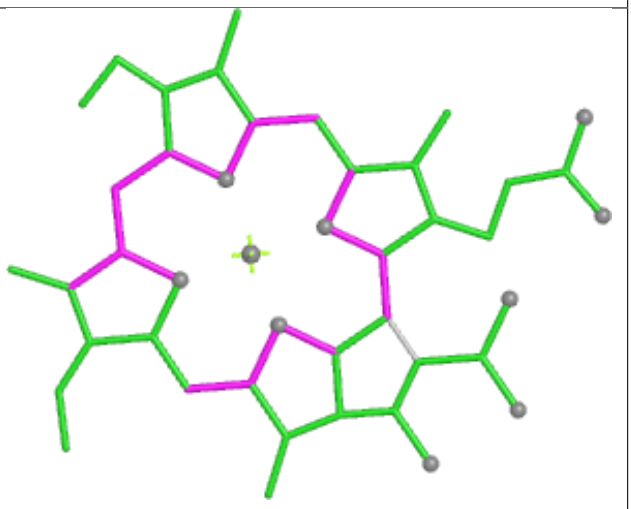


Rings

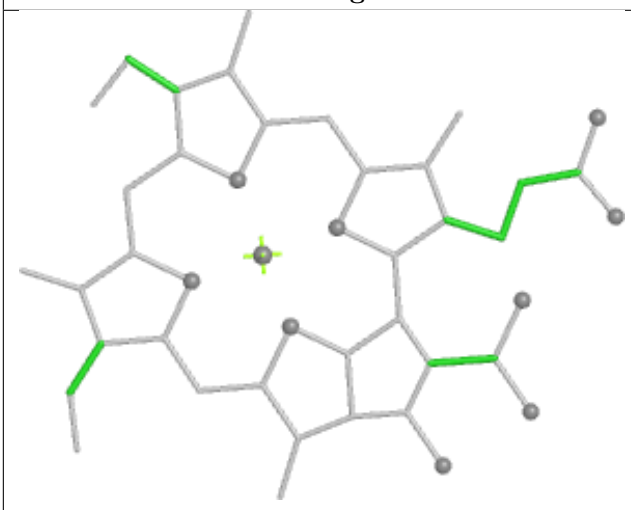
Ligand CLA B 814



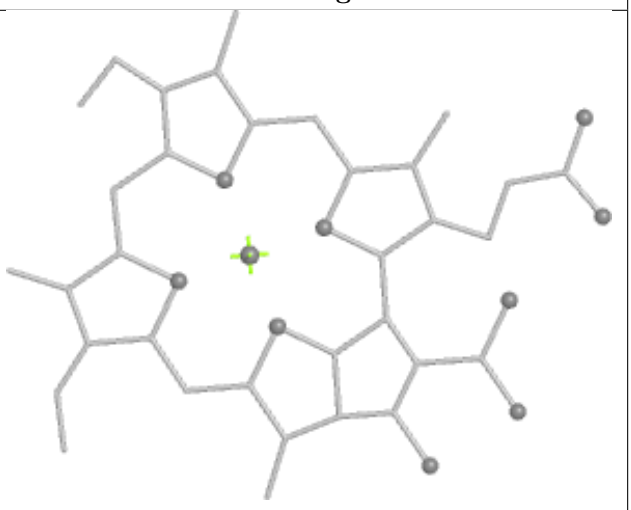
Bond lengths



Bond angles

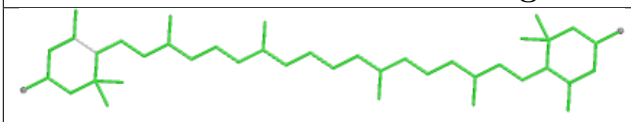


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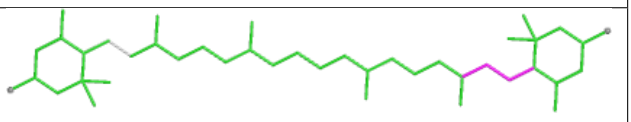


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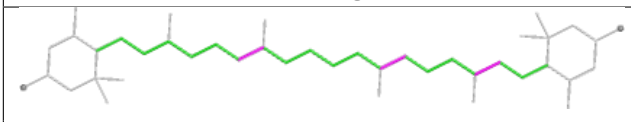
Ligand LUT 7 1001



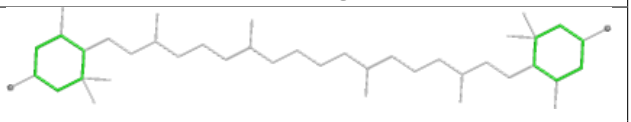
Bond lengths



Bond angles

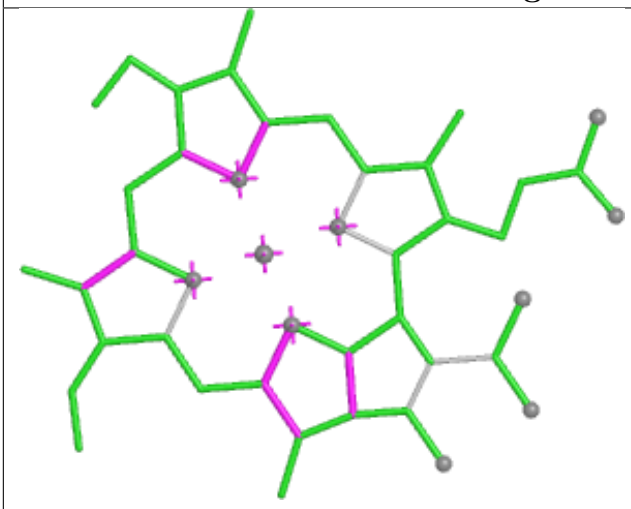


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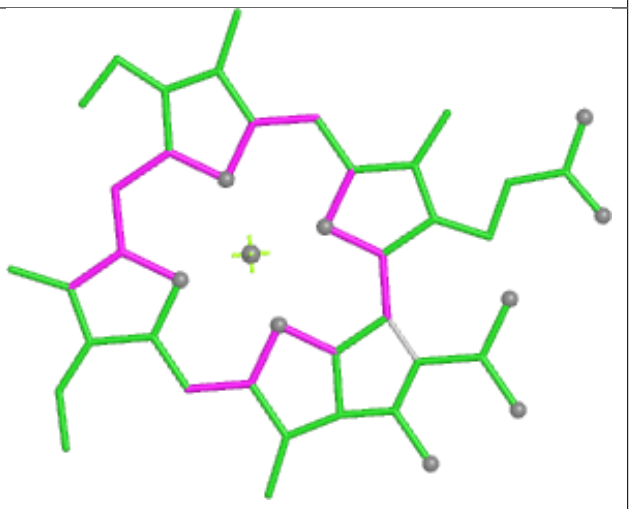


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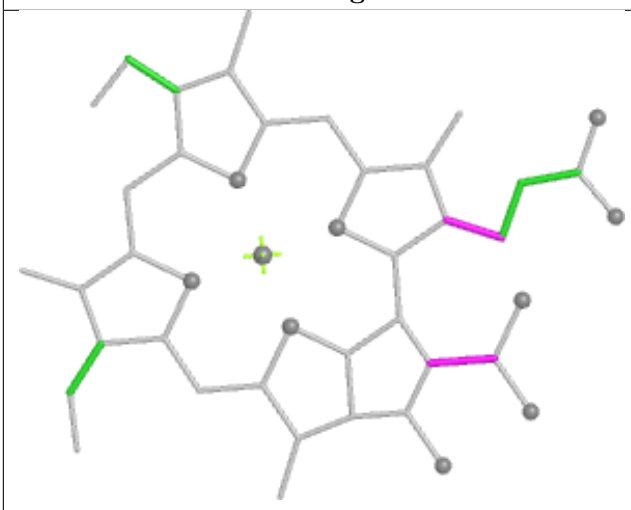
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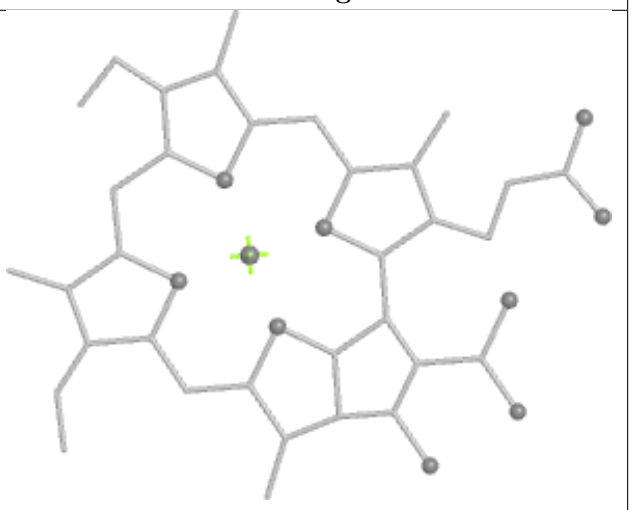
Bond lengths



Bond angles

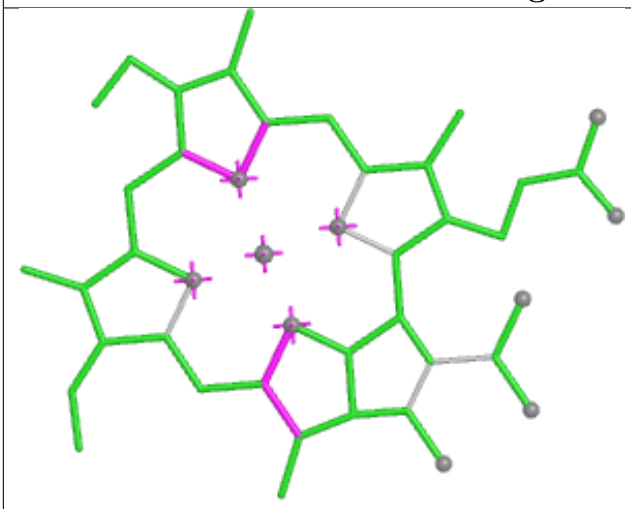


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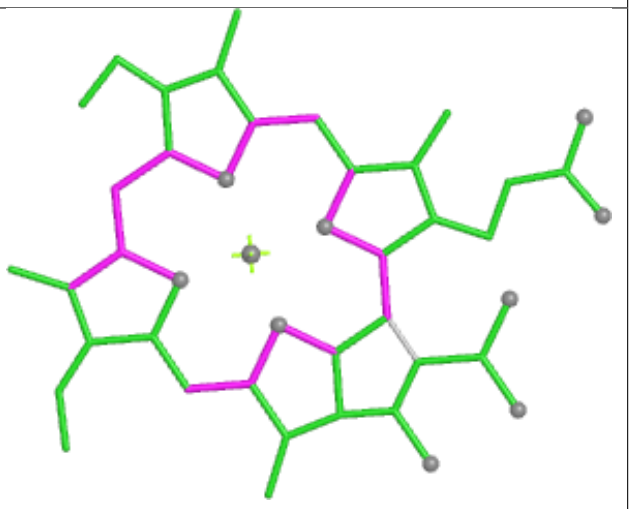


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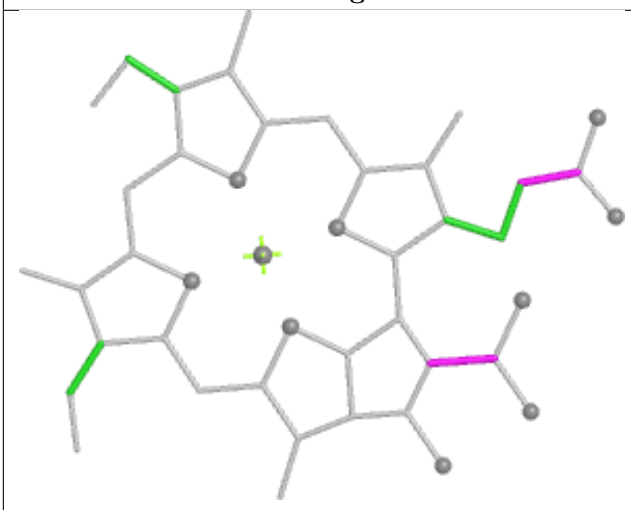
Ligand CLA 0 306



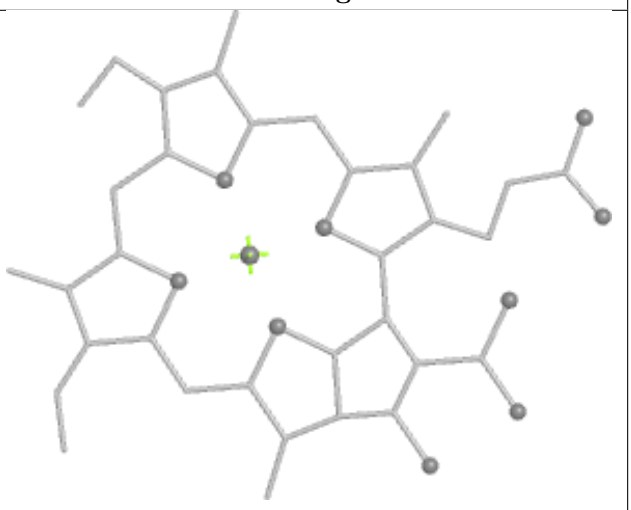
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Bond angles

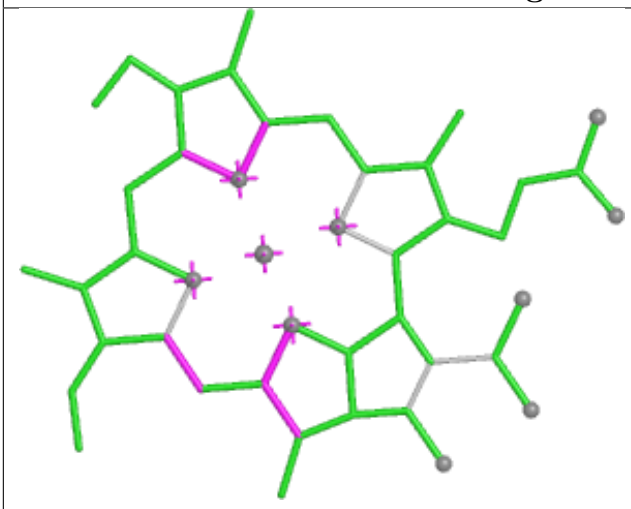


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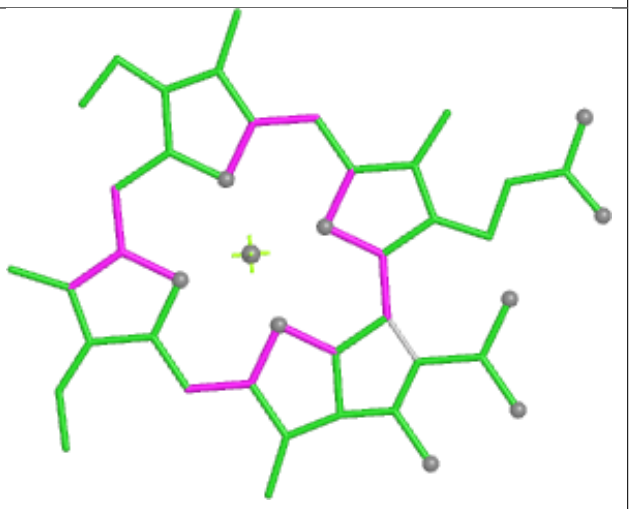


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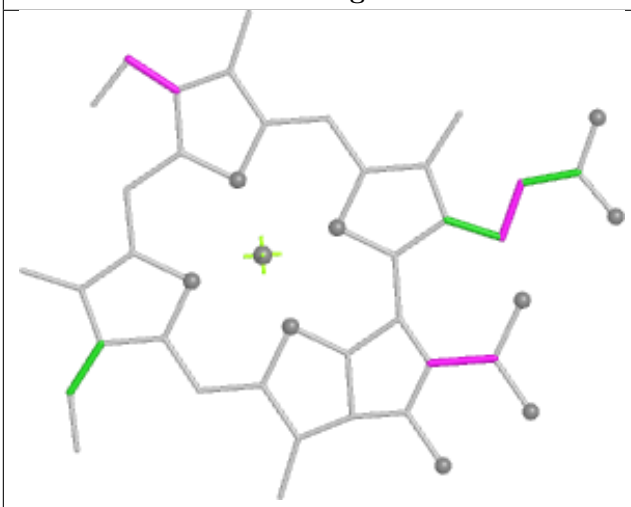
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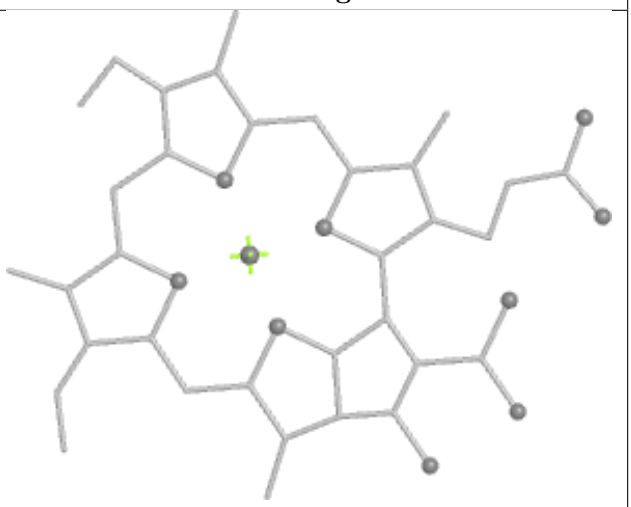
Bond lengths



Bond angles

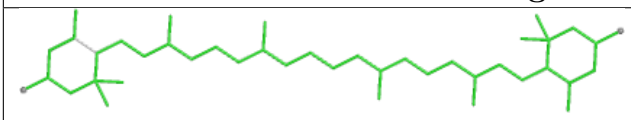


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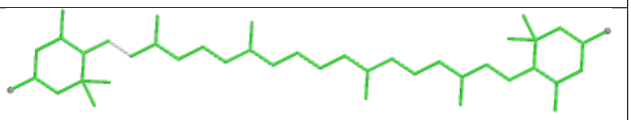


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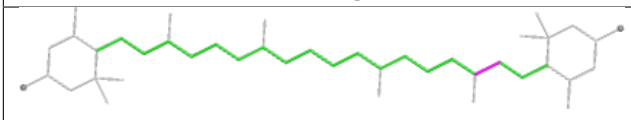
Ligand LUT 6 303



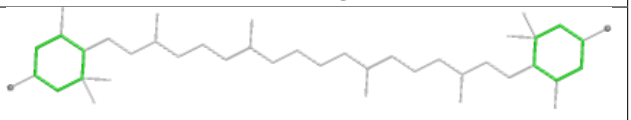
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Bond angles

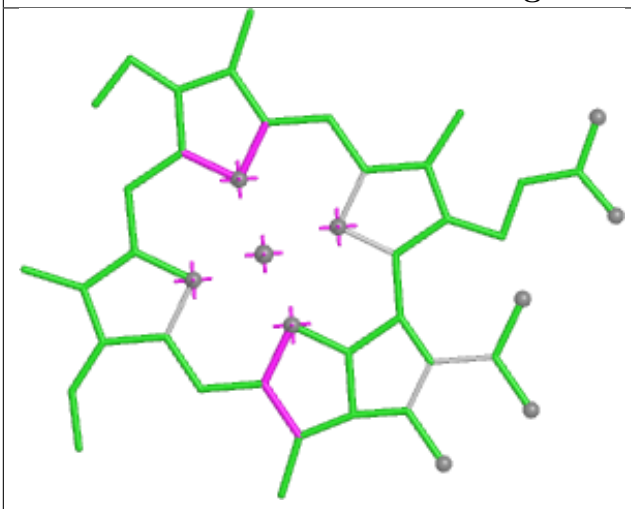


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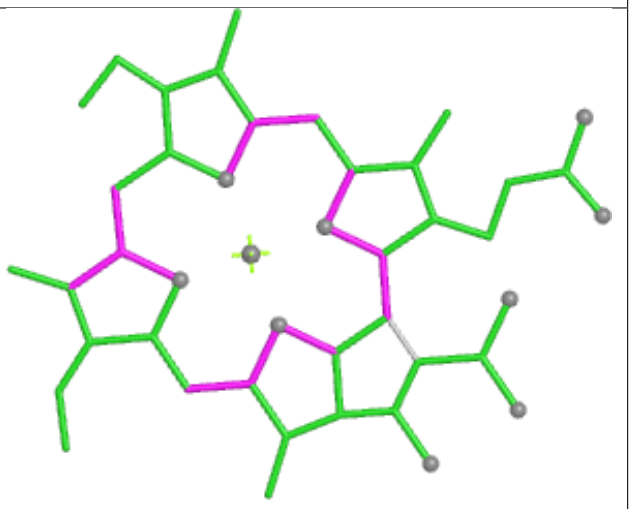


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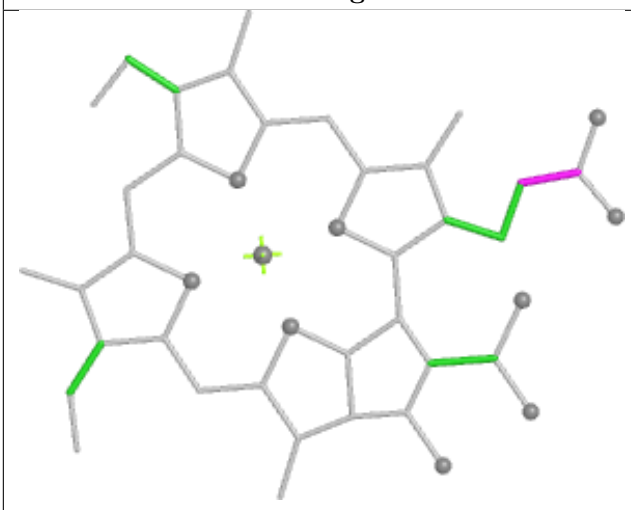
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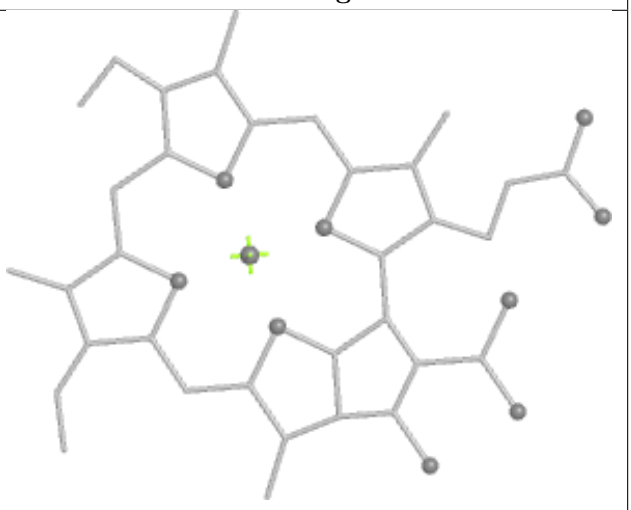
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Bond angles

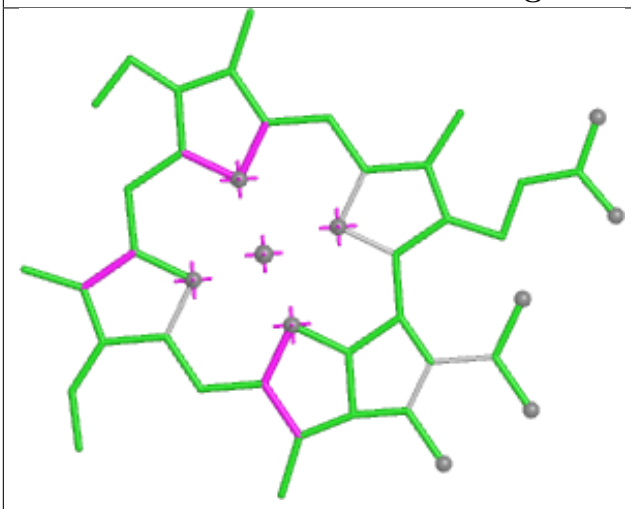


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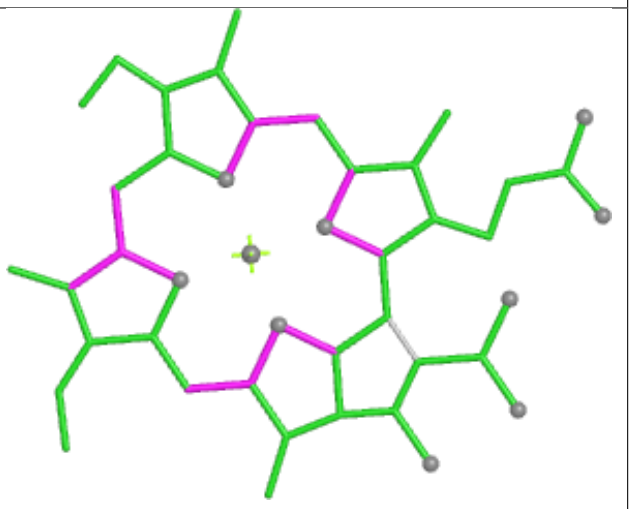


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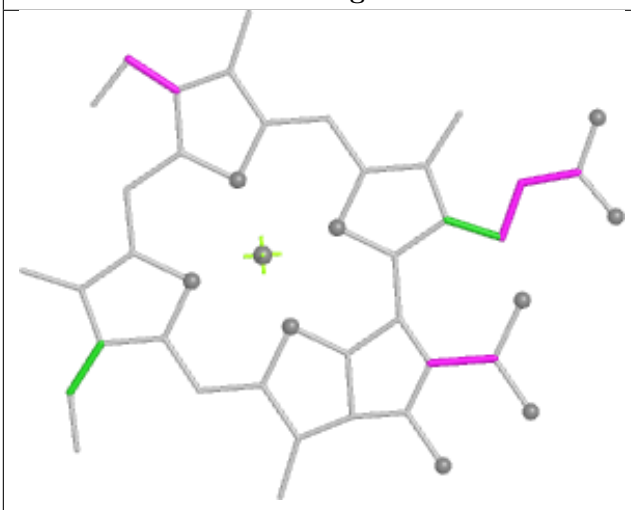
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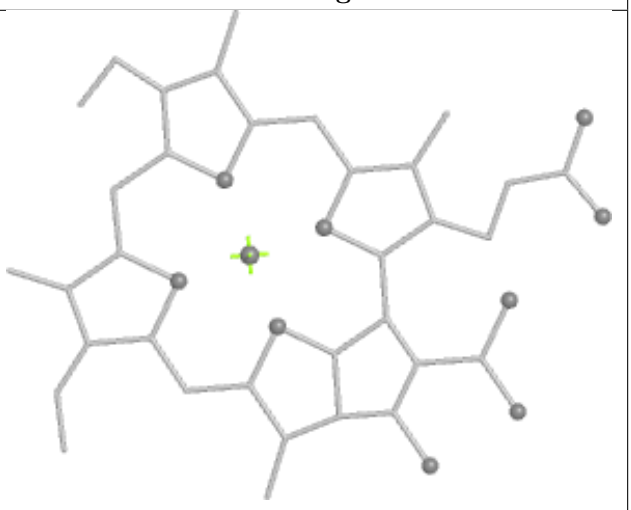
Bond lengths



Bond angles

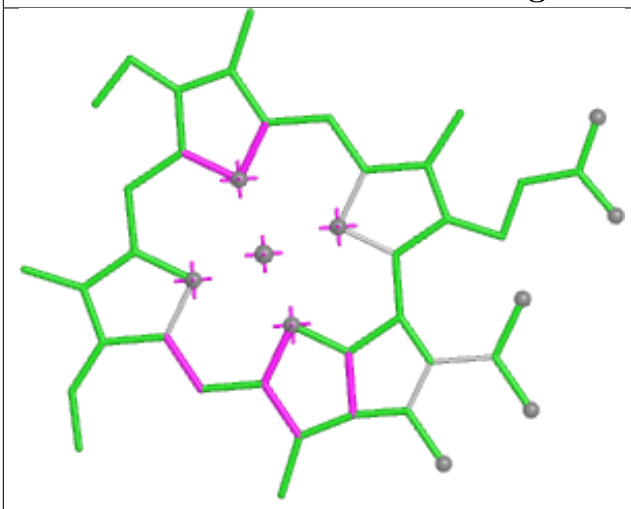


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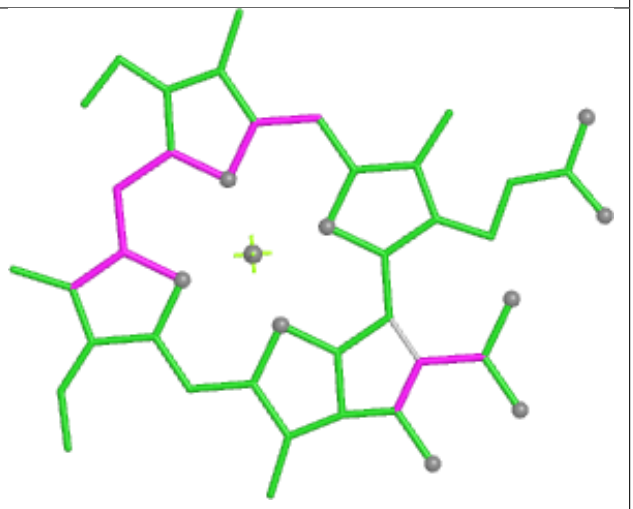


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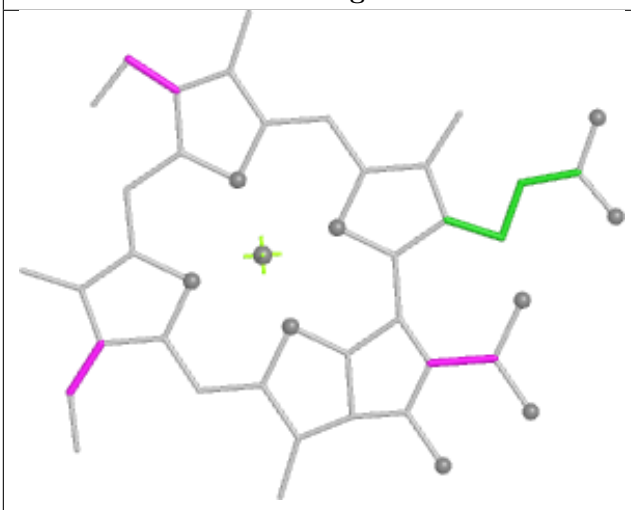
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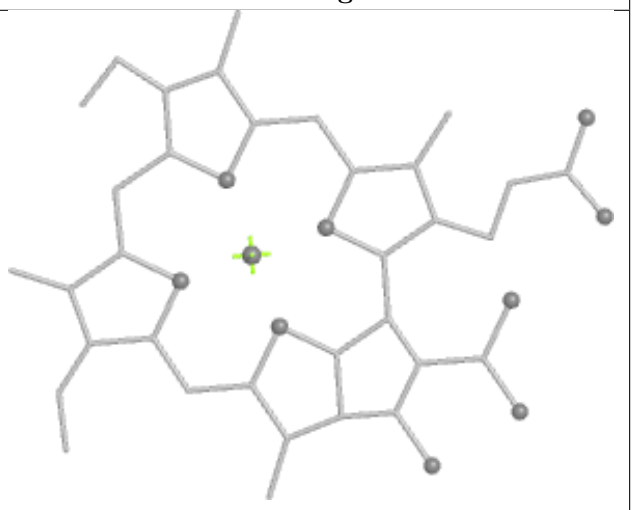
Bond lengths



Bond angles

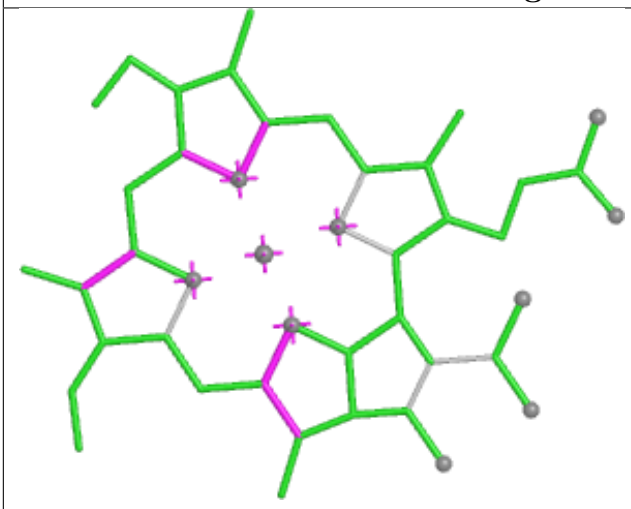


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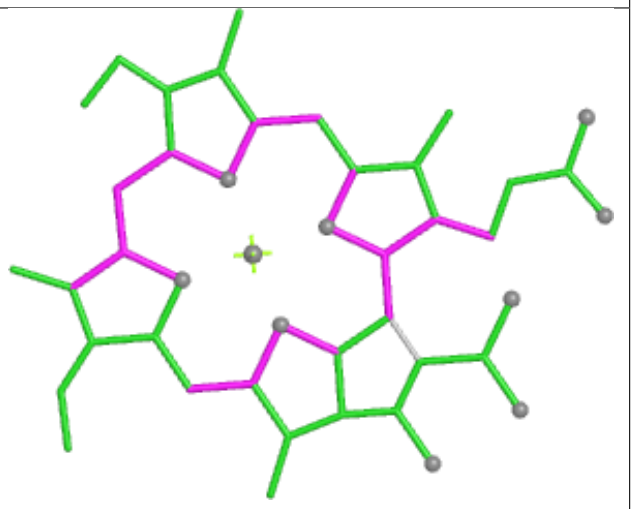


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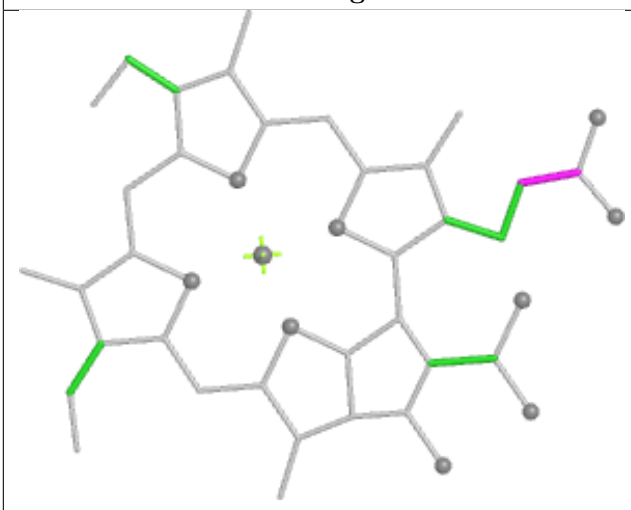
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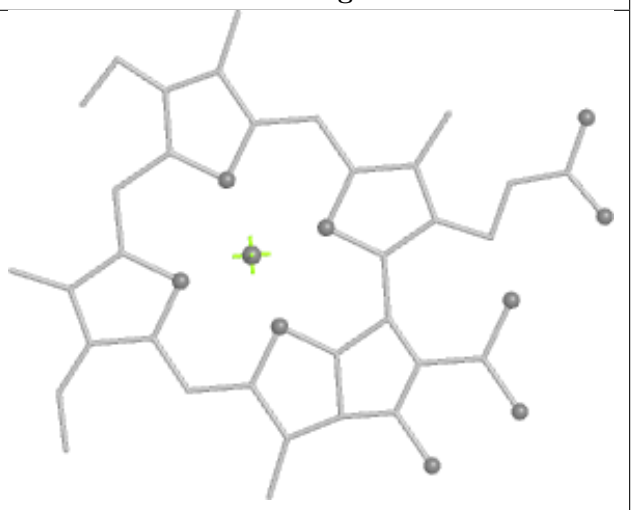
Bond lengths



Bond angles

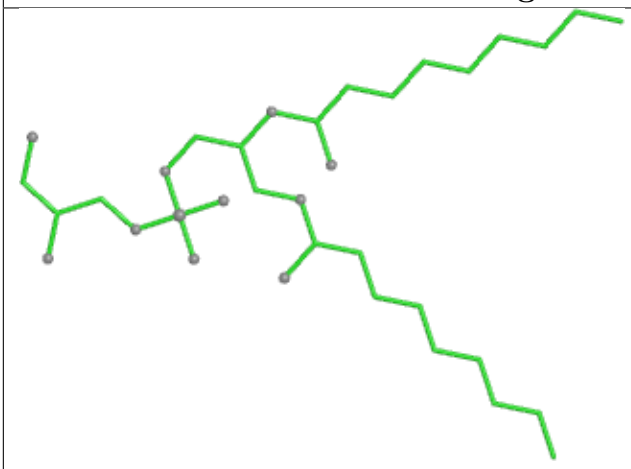


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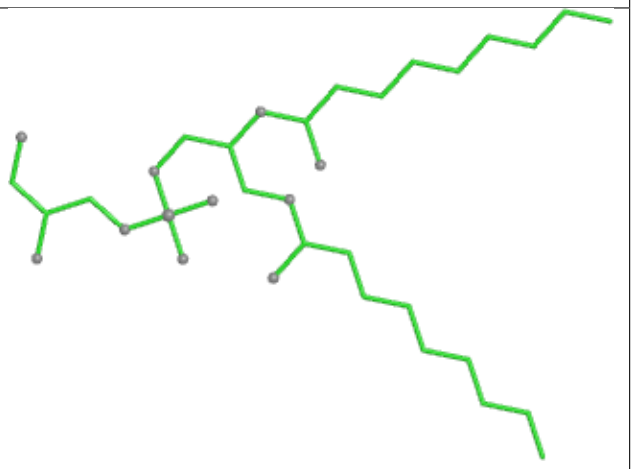


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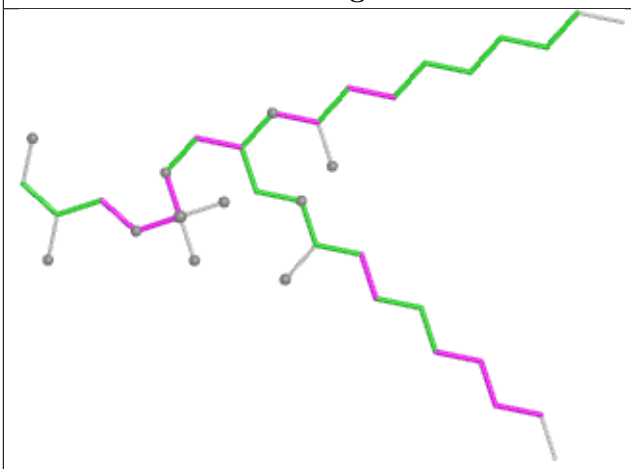
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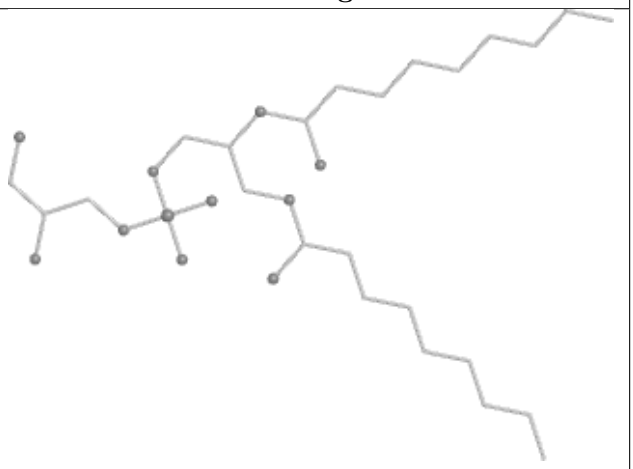
Bond lengths



Bond angles

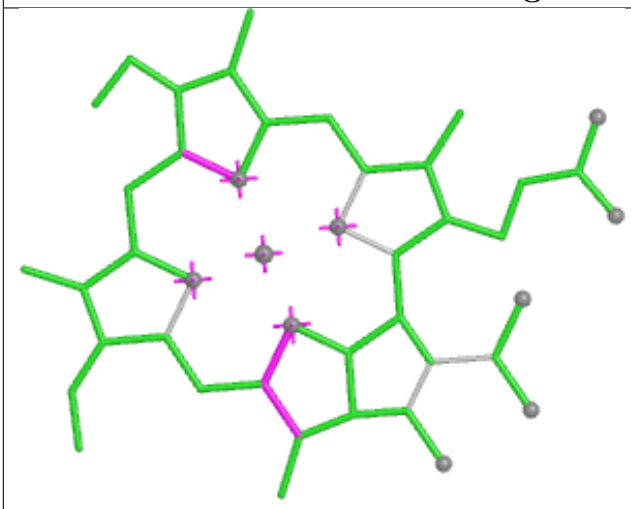


Torsions

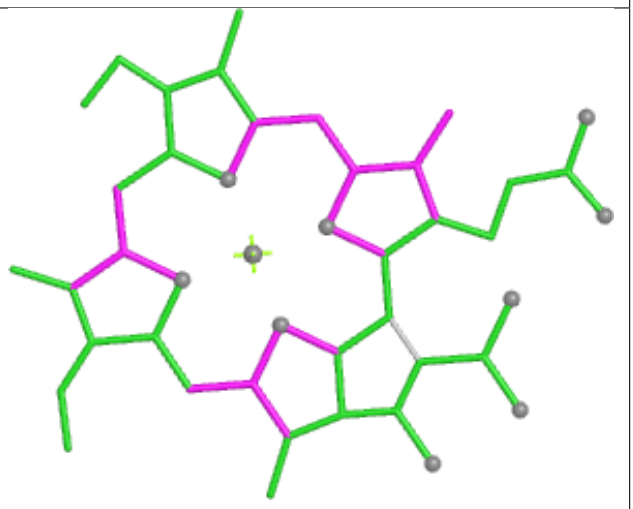


Rings

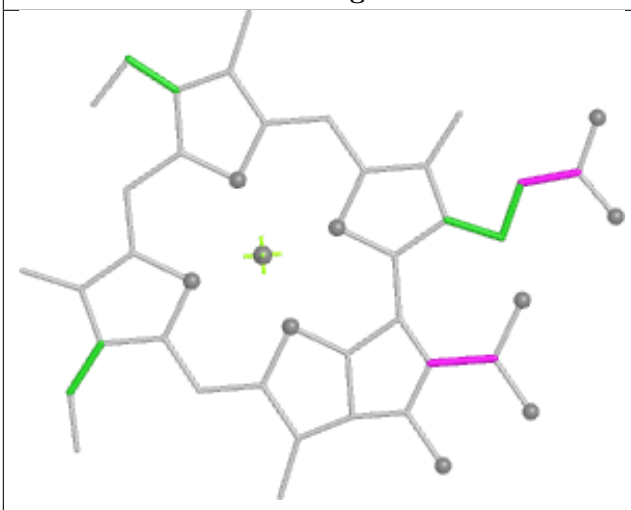
Ligand CLA A 801



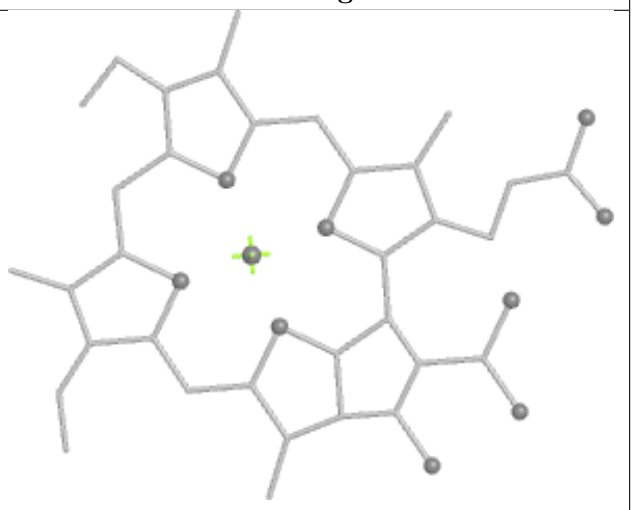
Bond lengths



Bond angles

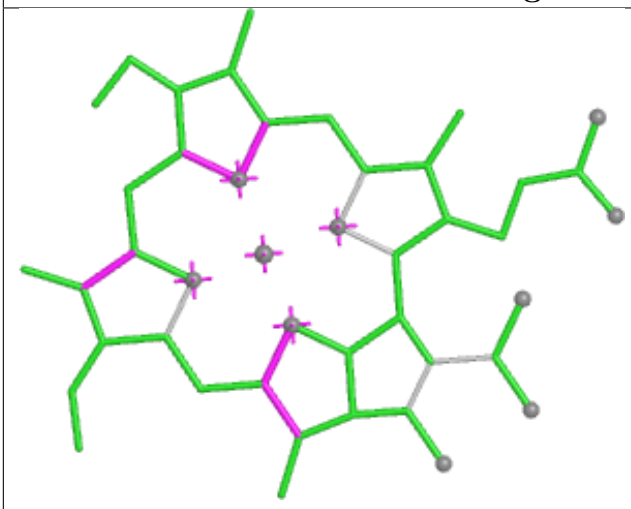


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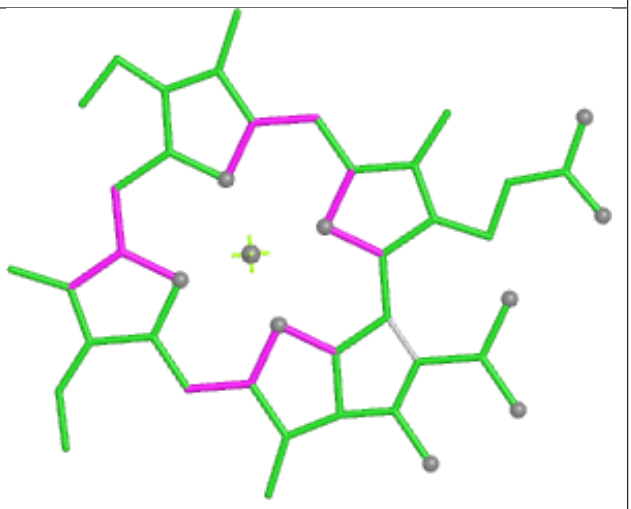


Rings

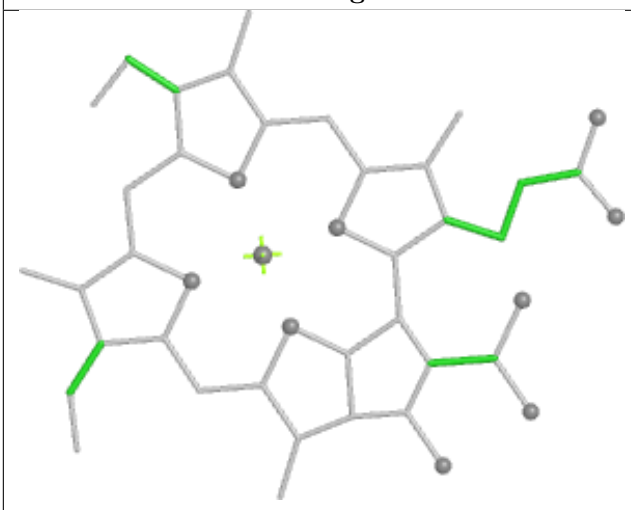
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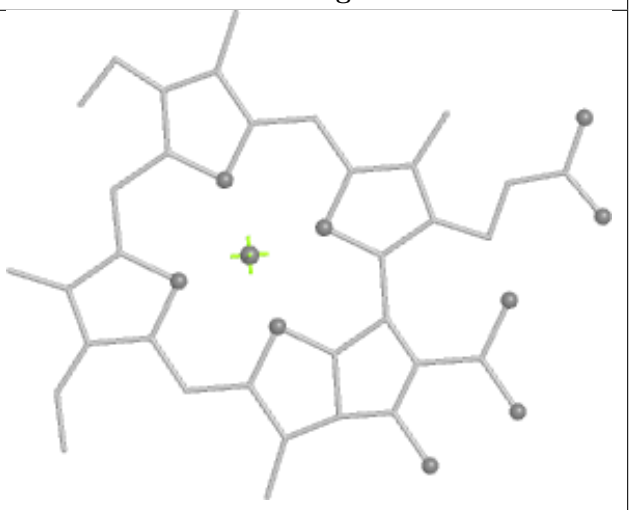
Bond lengths



Bond angles

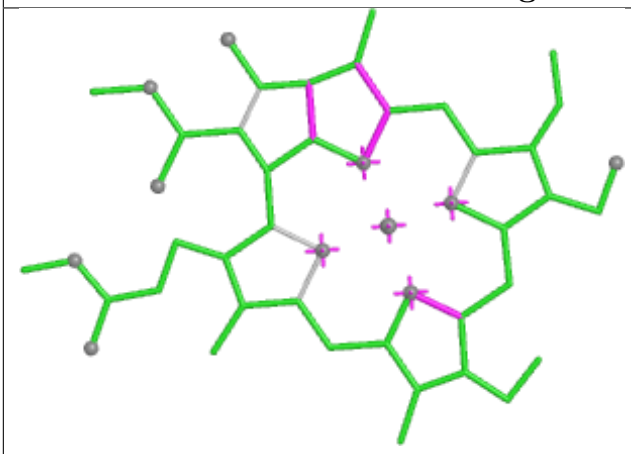


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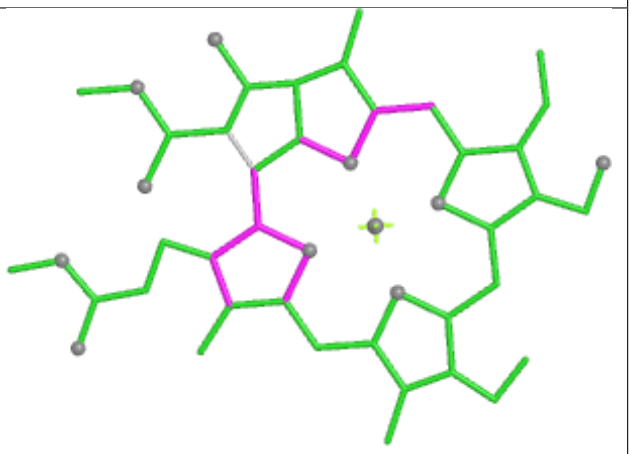


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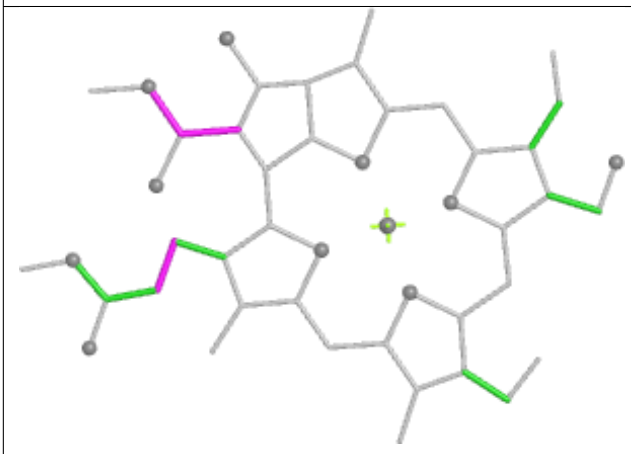
Ligand CHL 7 1012



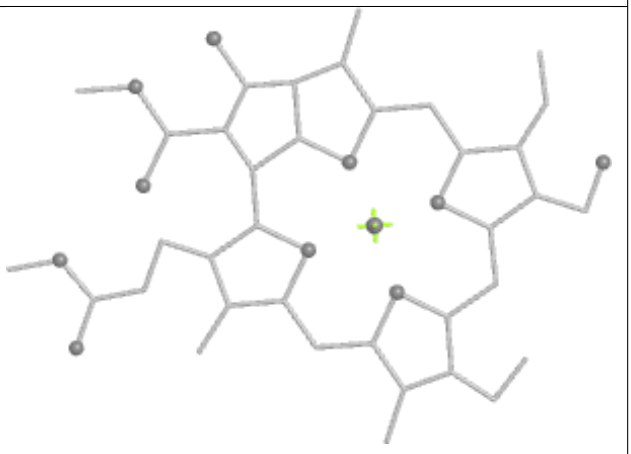
Bond lengths



Bond angles

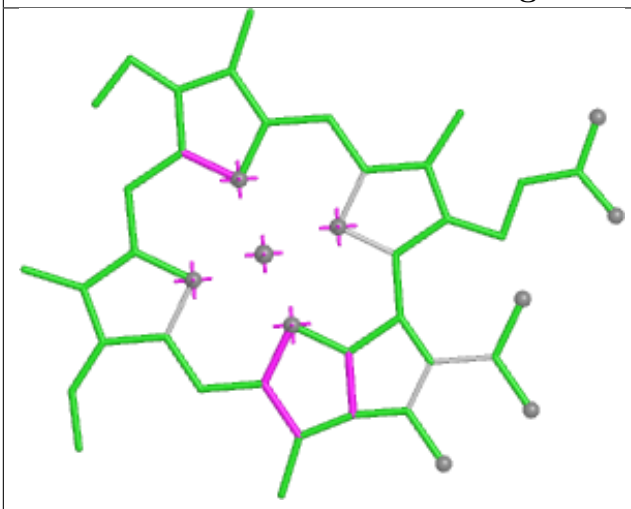


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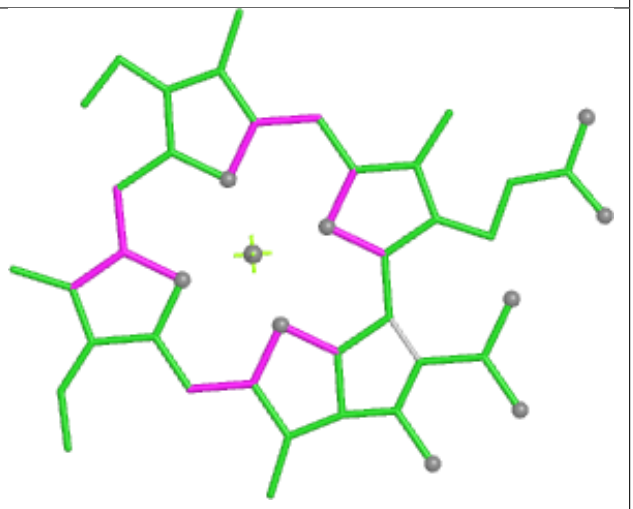


Rings

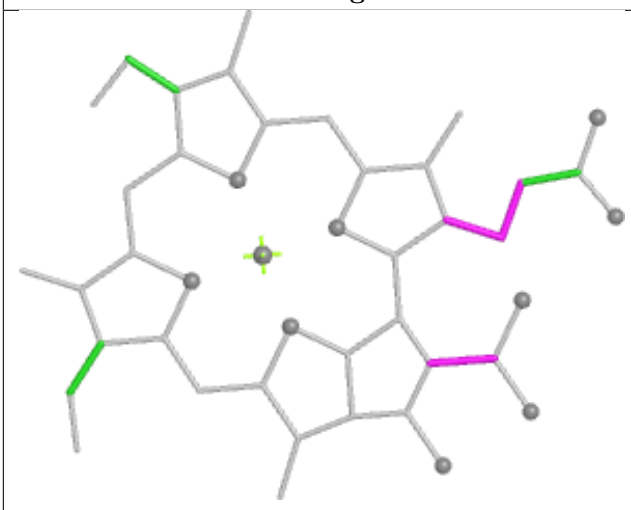
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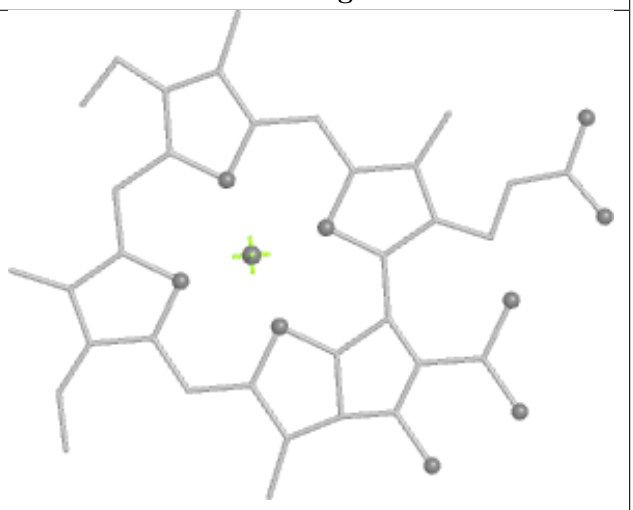
Bond lengths



Bond angles

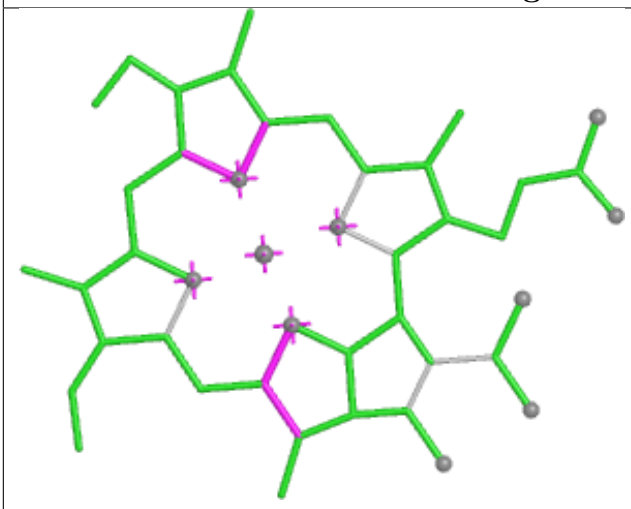


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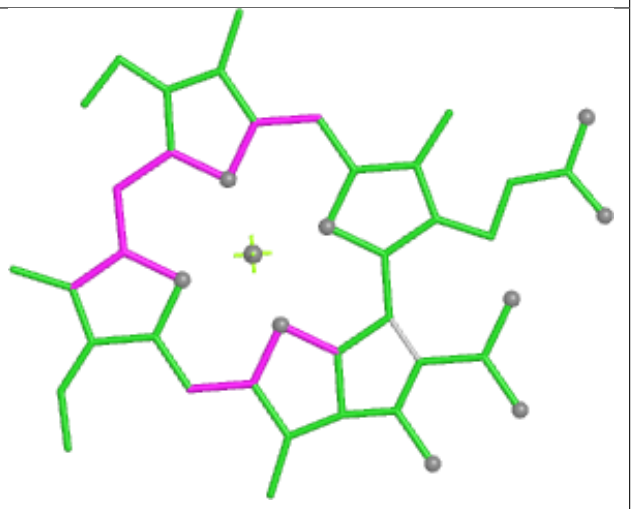


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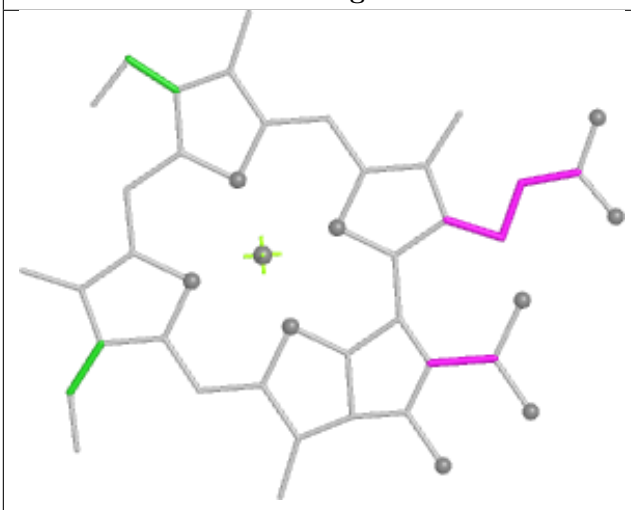
Ligand CLA K 201



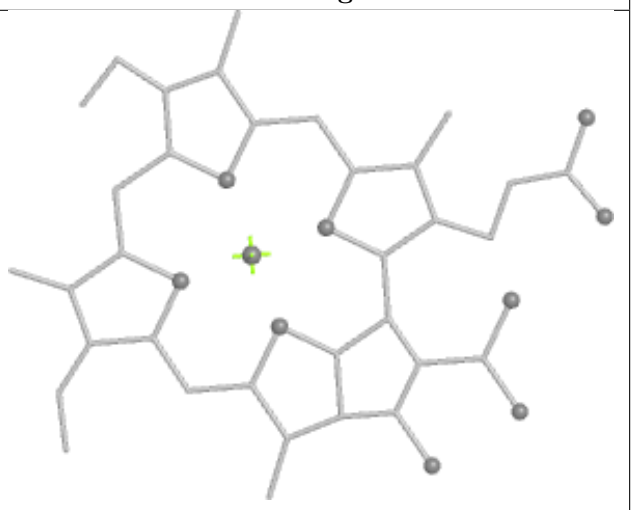
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Bond angles

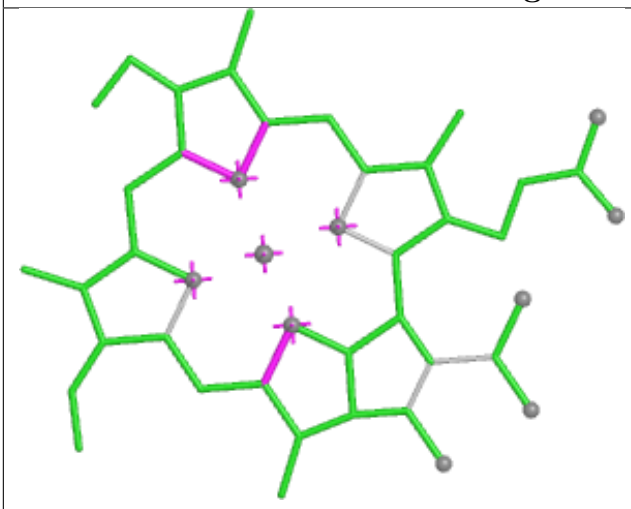


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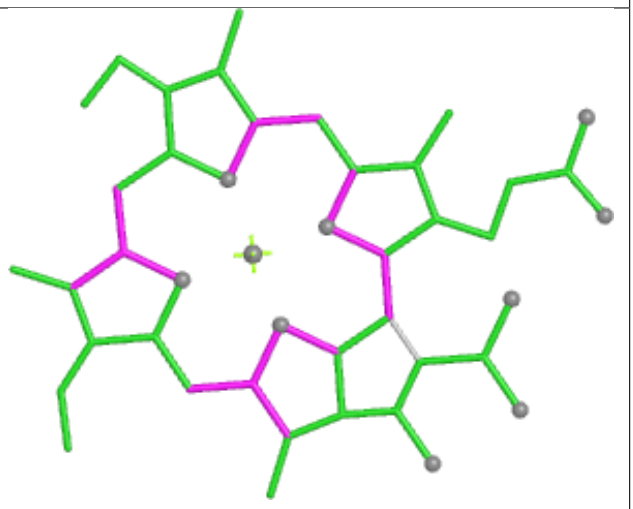


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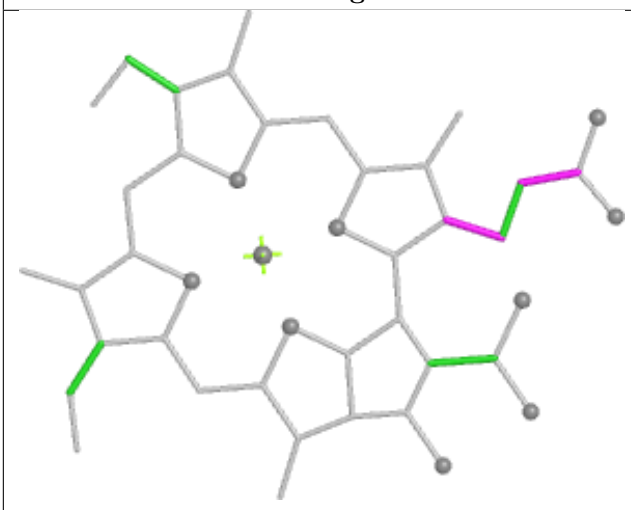
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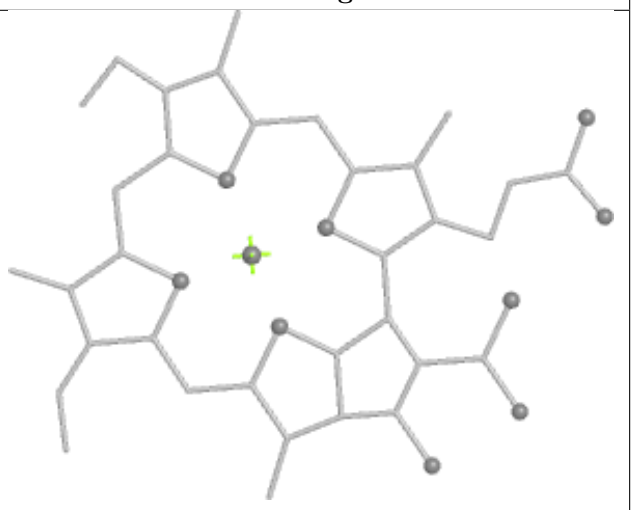
Bond lengths



Bond angles

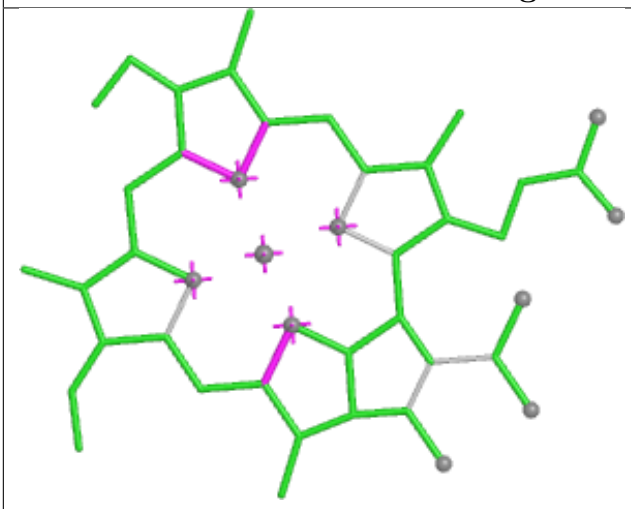


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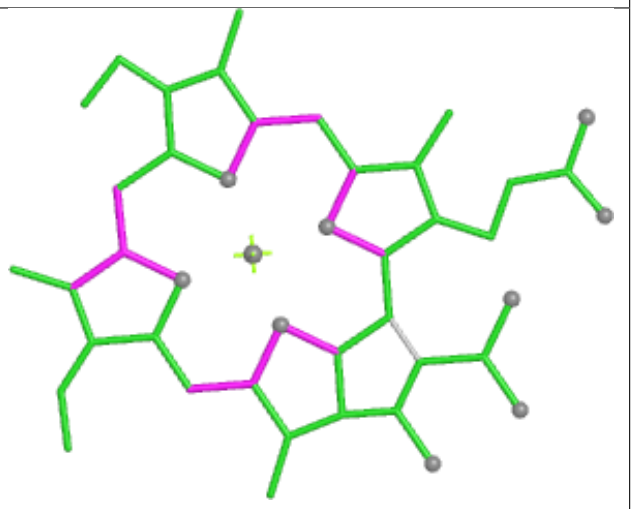


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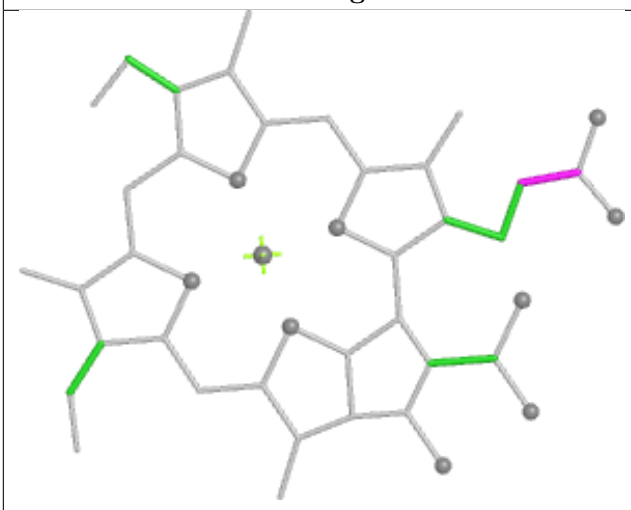
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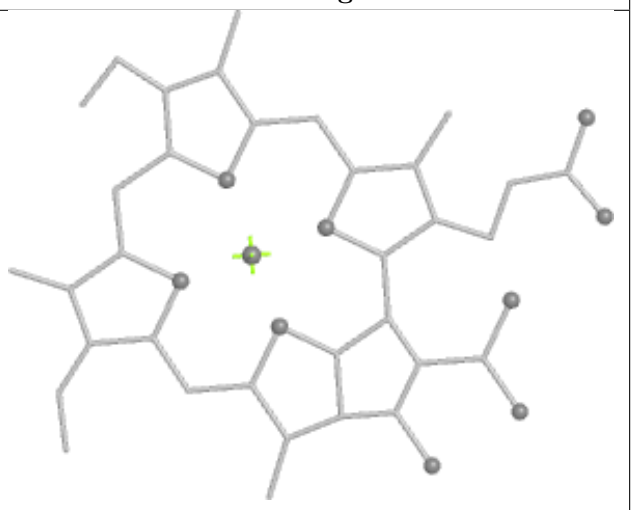
Bond lengths



Bond angles

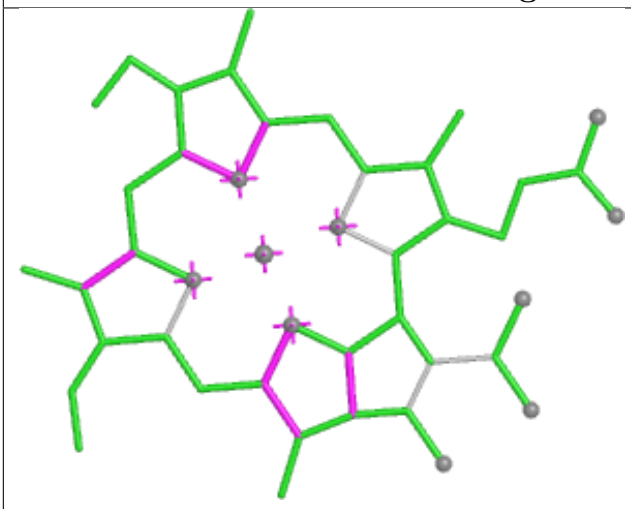


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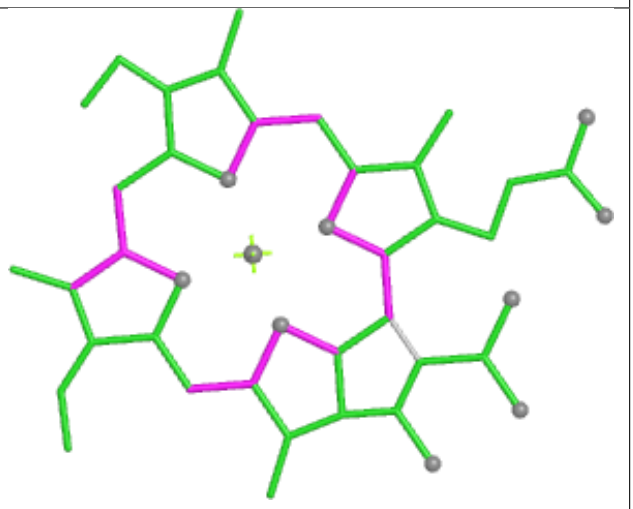


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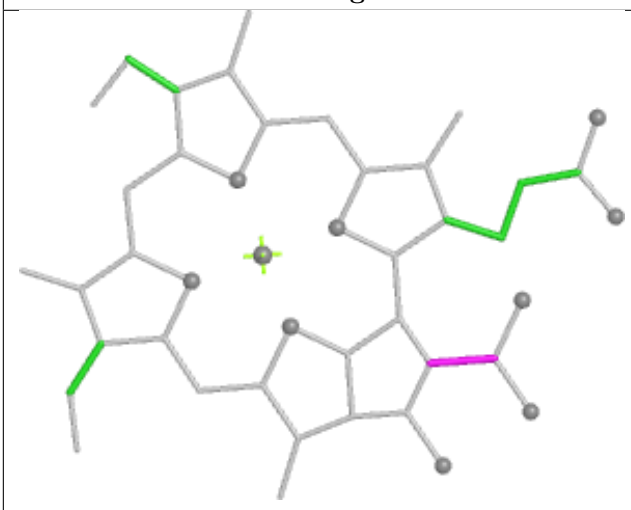
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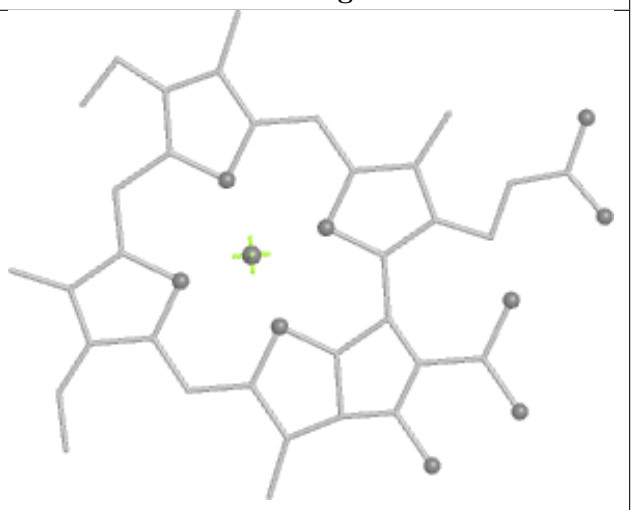
Bond lengths



Bond angles

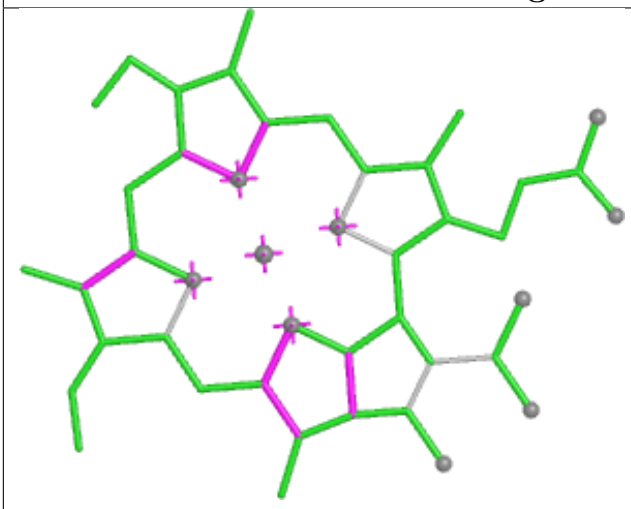


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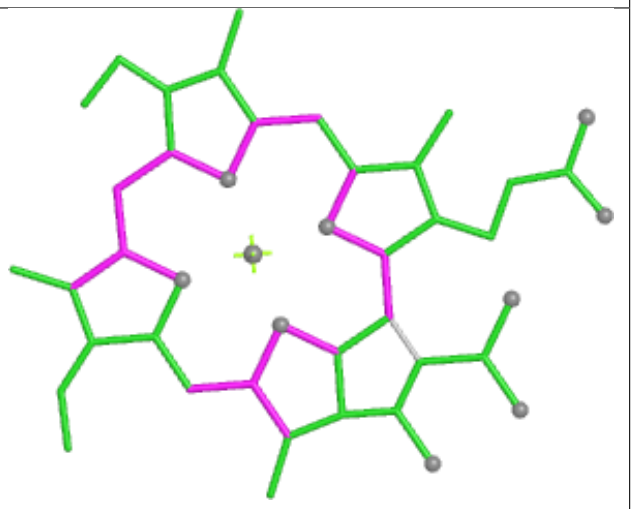


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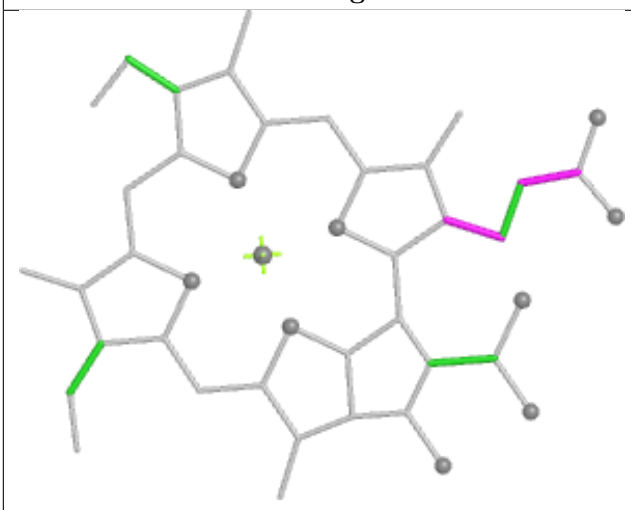
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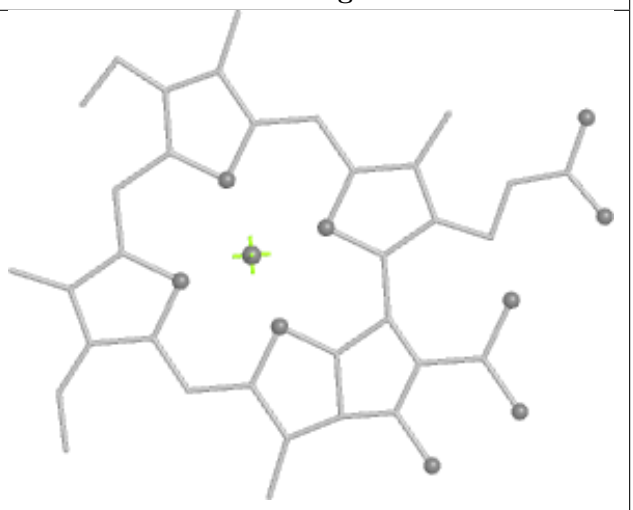
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Bond angles

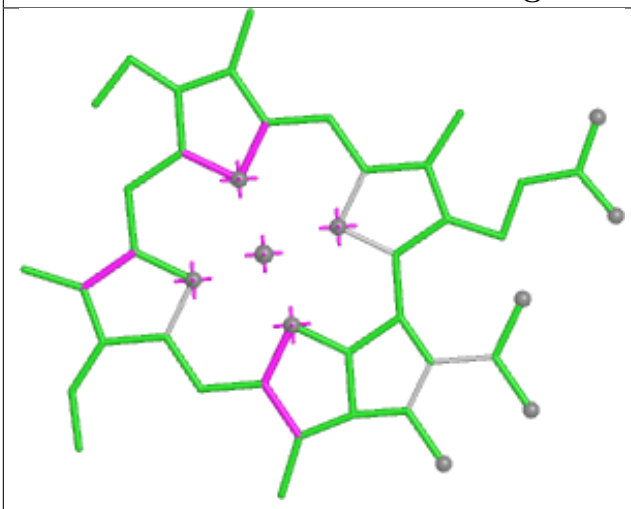


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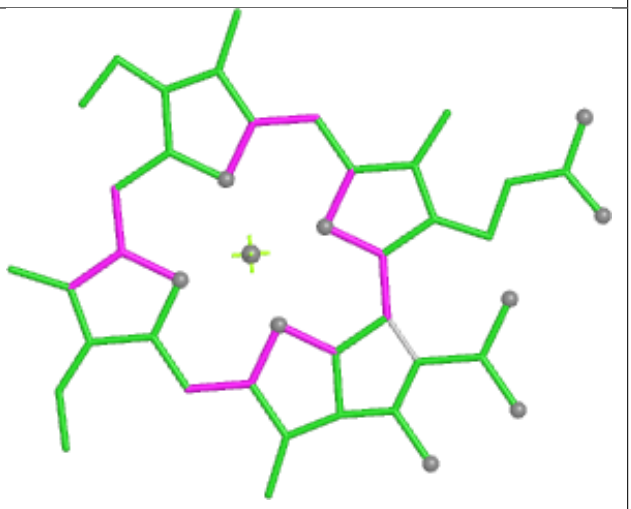


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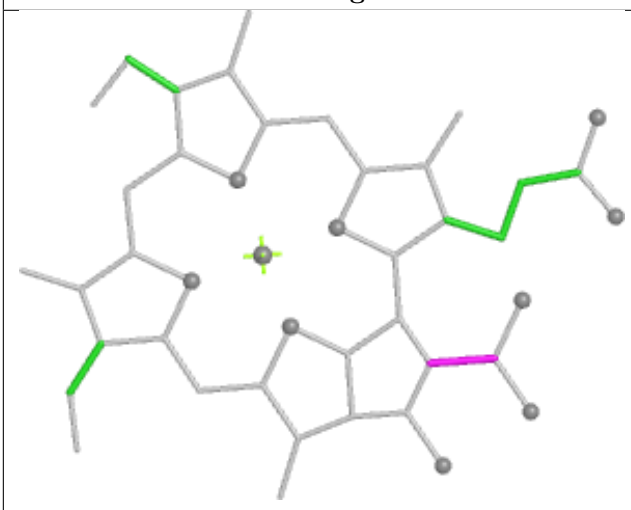
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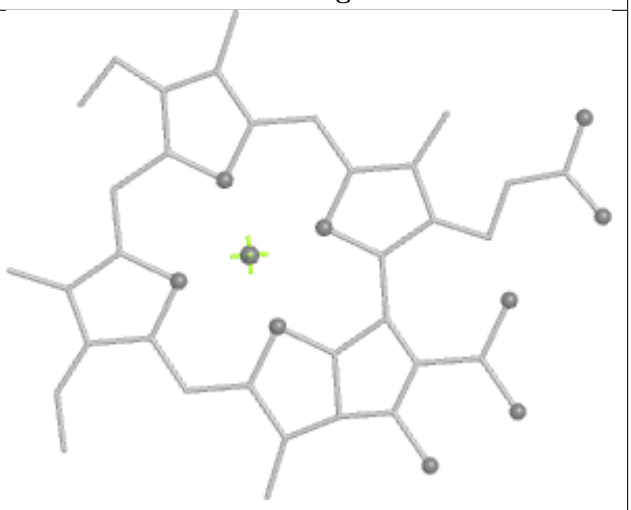
Bond lengths



Bond angles

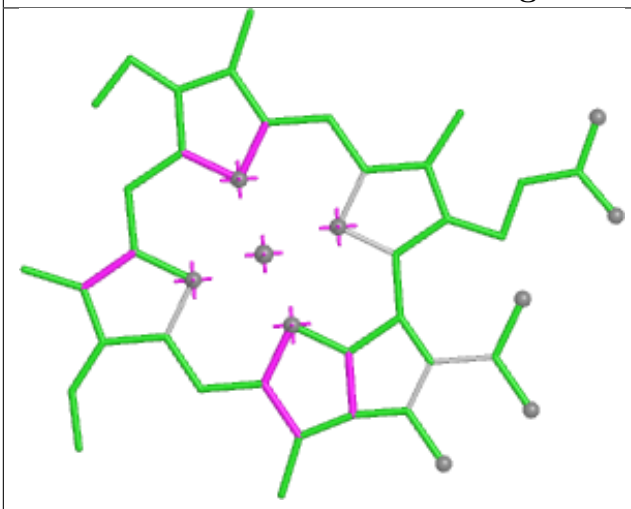


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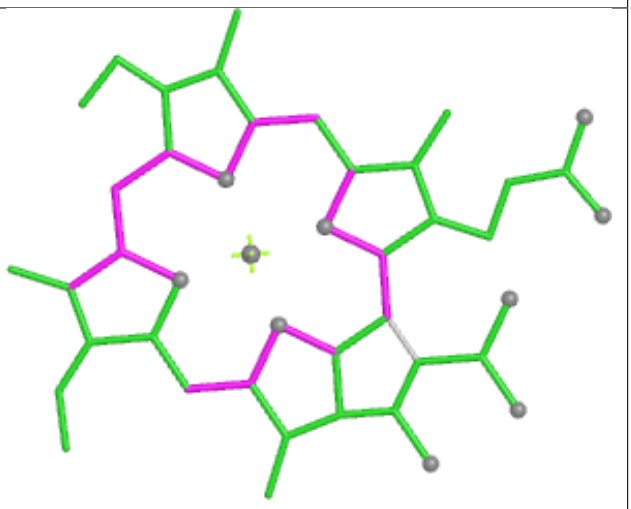


Rings

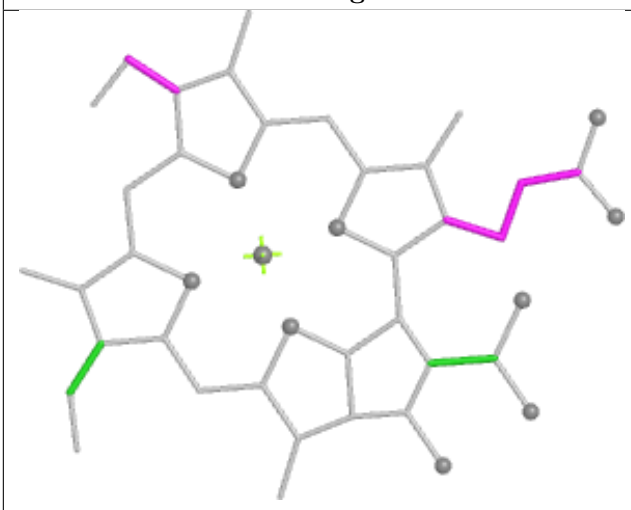
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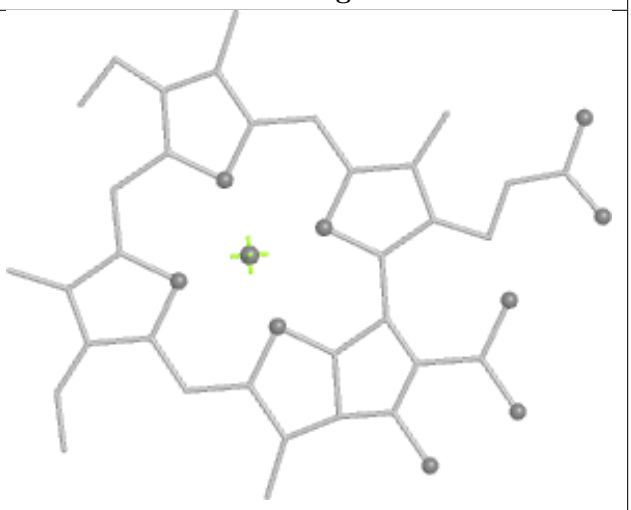
Bond lengths



Bond angles

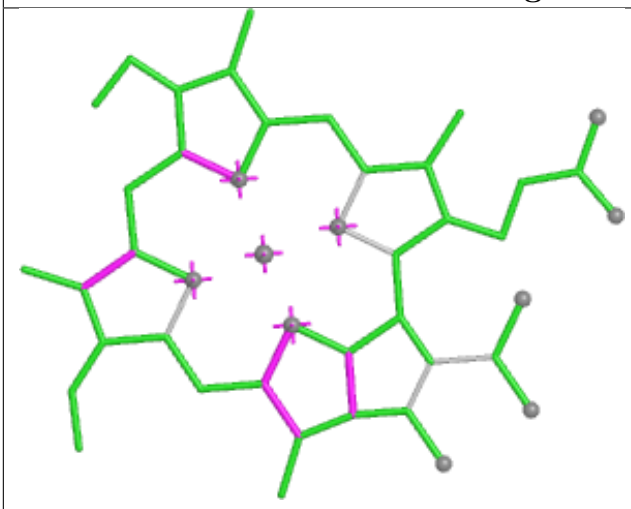


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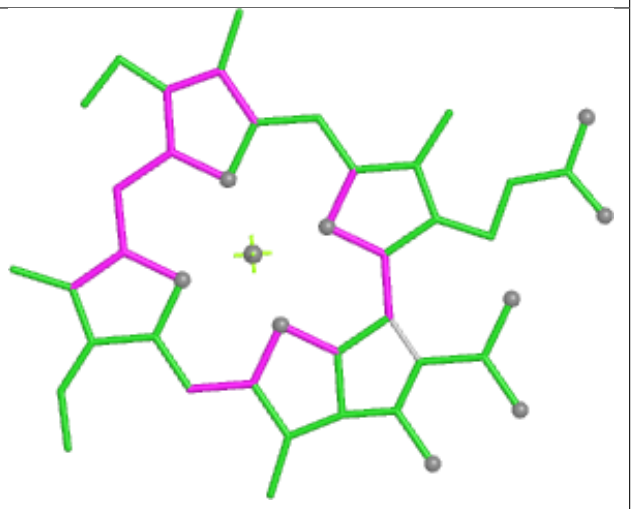


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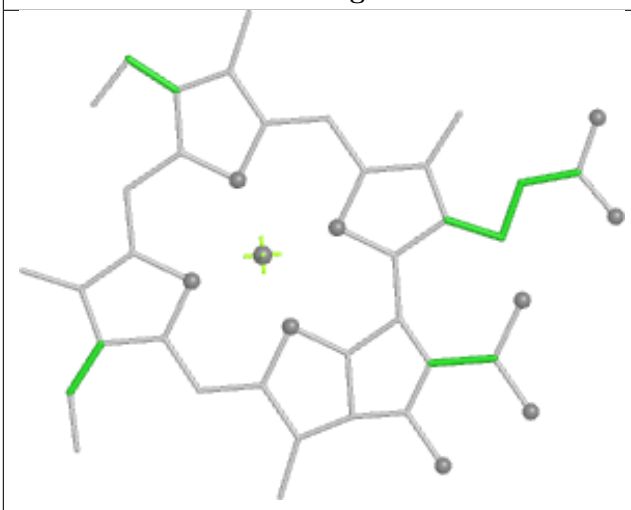
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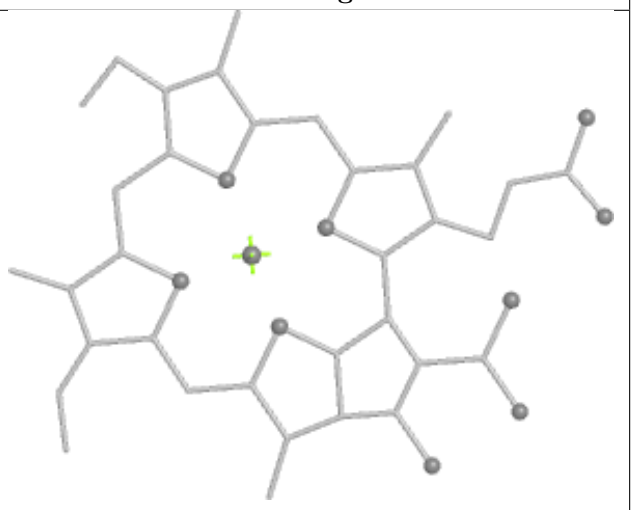
Bond lengths



Bond angles

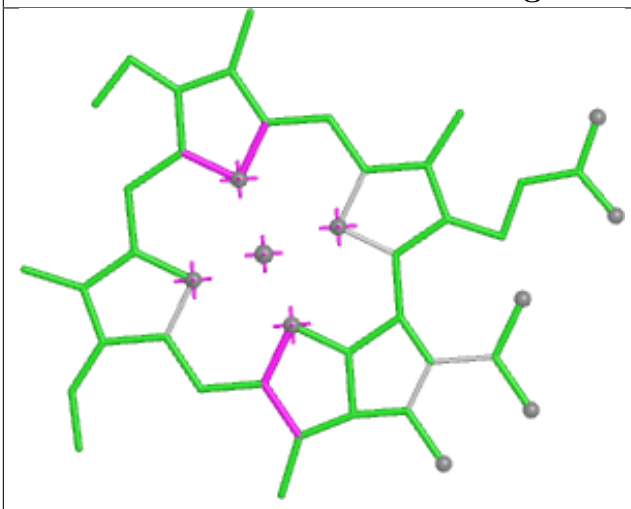


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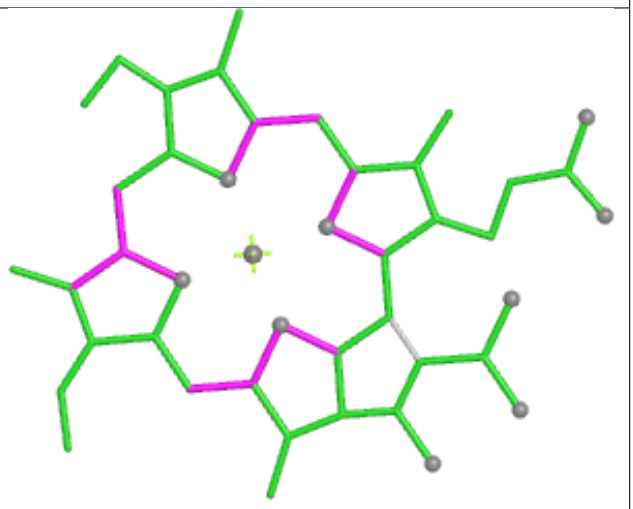


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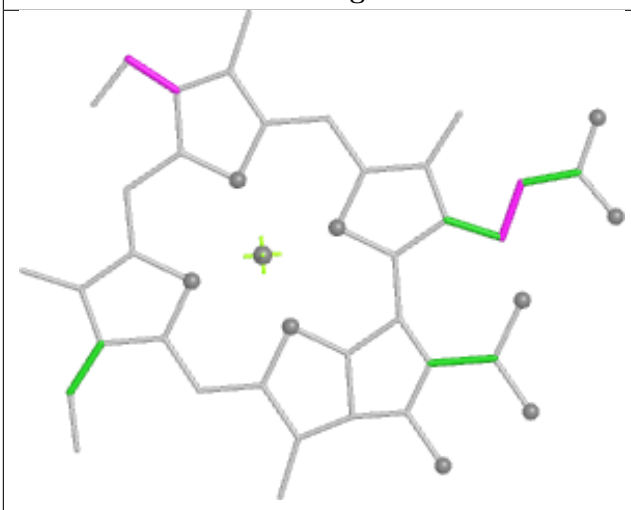
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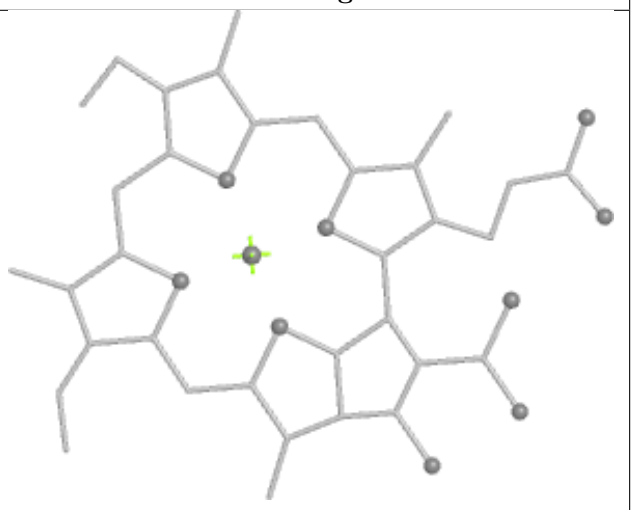
Bond lengths



Bond angles

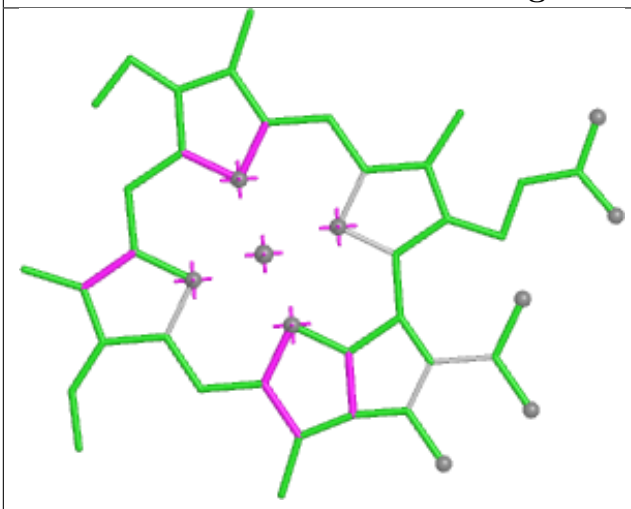


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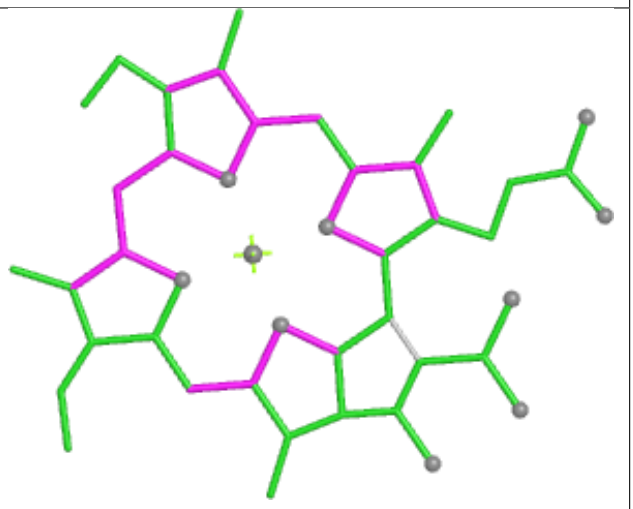


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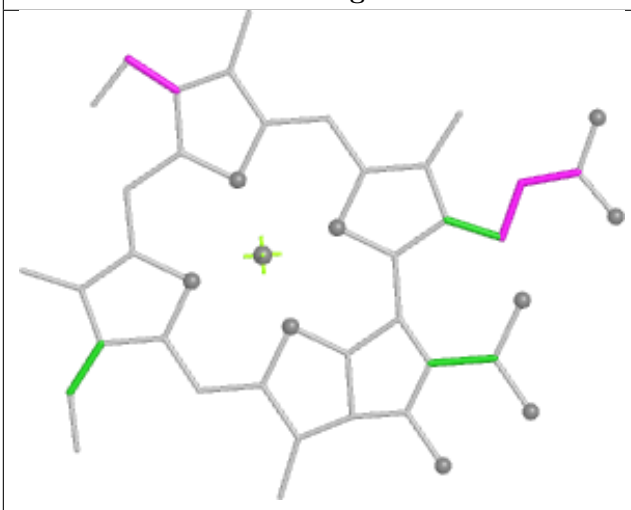
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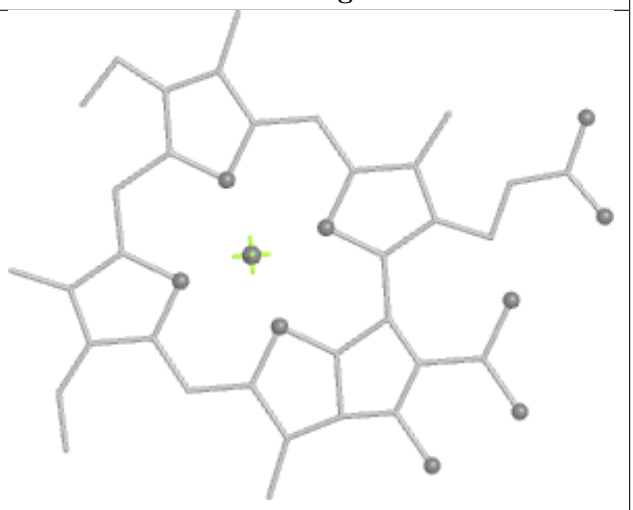
Bond lengths



Bond angles

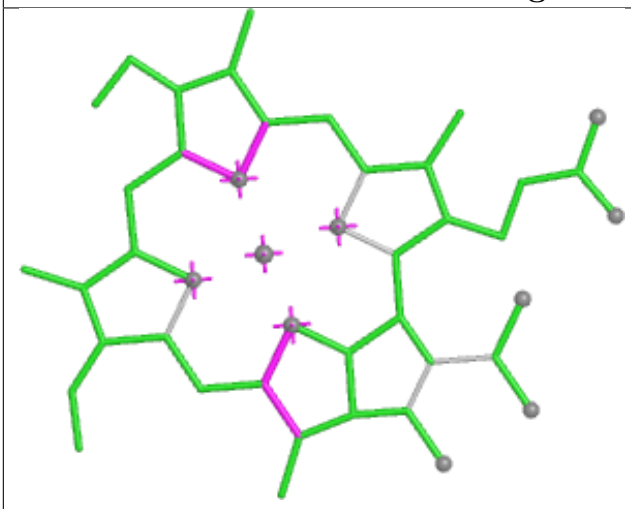


Torsions

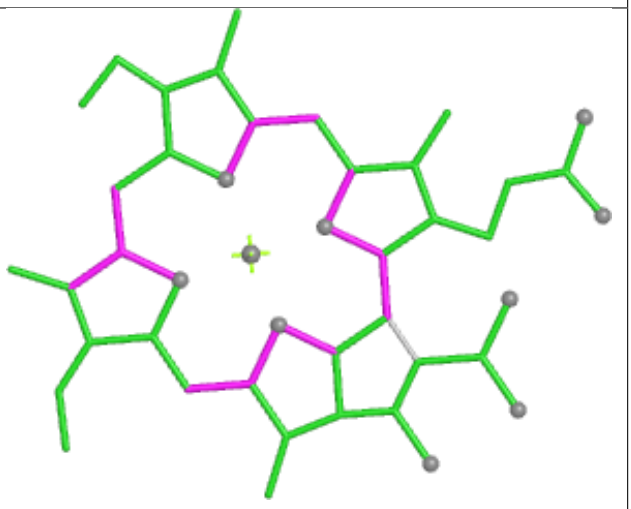


Rings

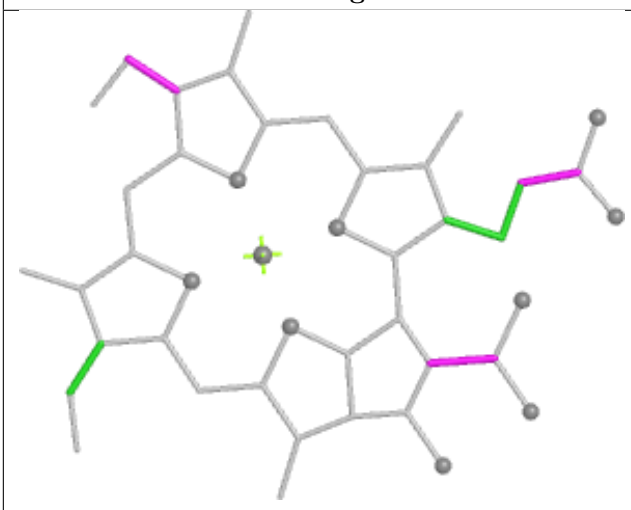
Ligand CLA 5 305



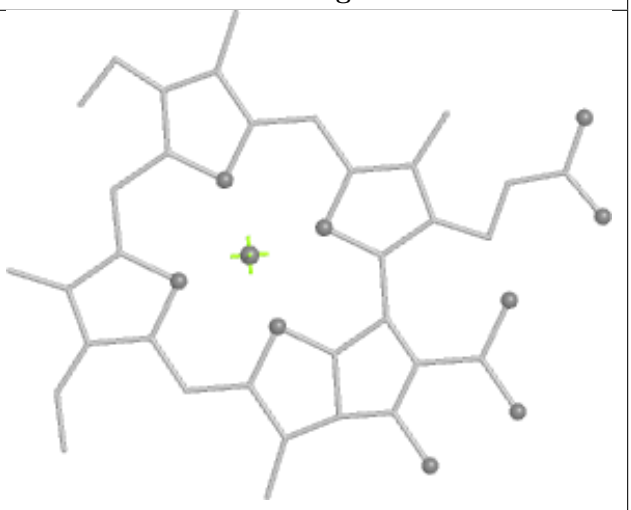
Bond lengths



Bond angles

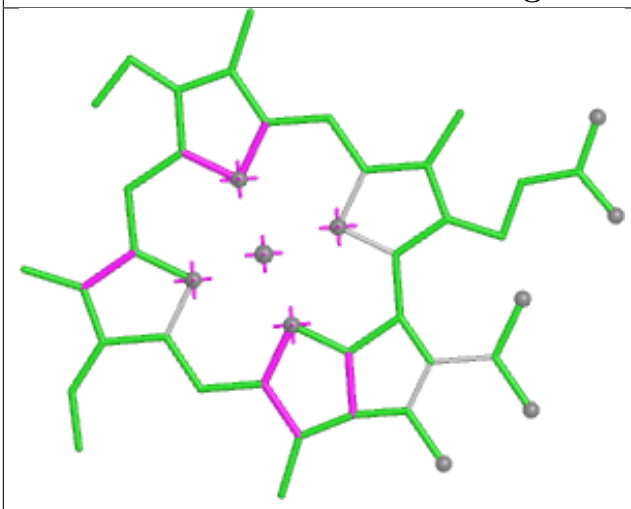


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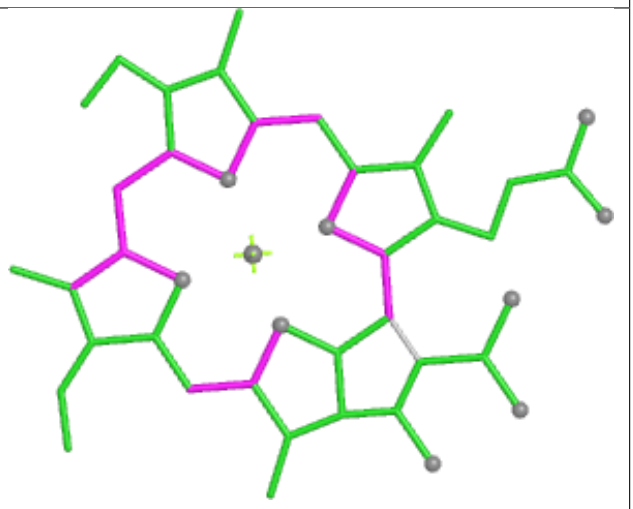


Rings

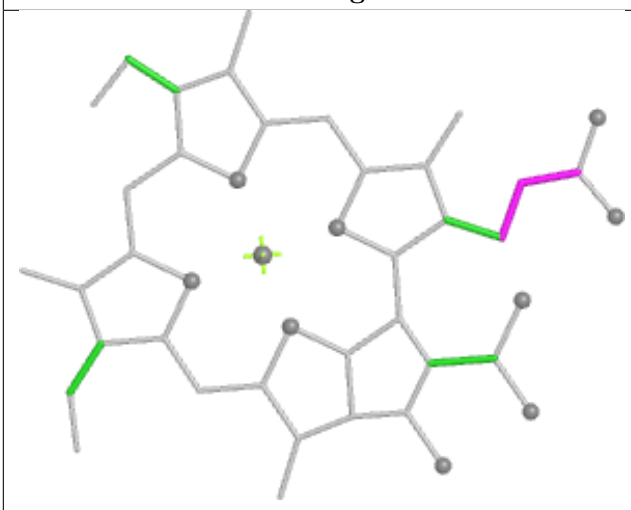
Ligand CLA A 833



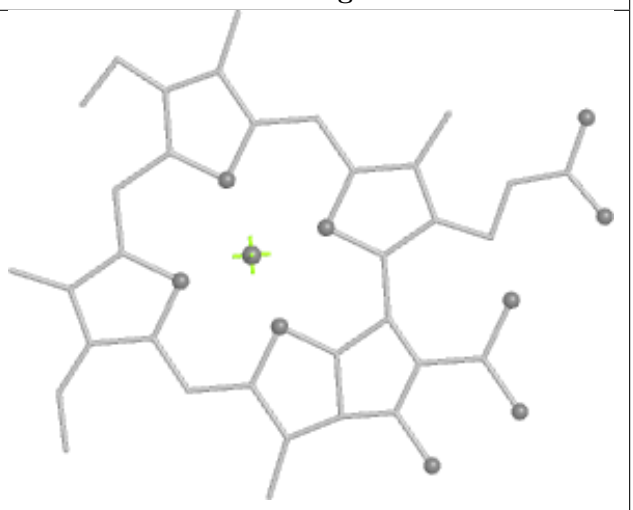
Bond lengths



Bond angles

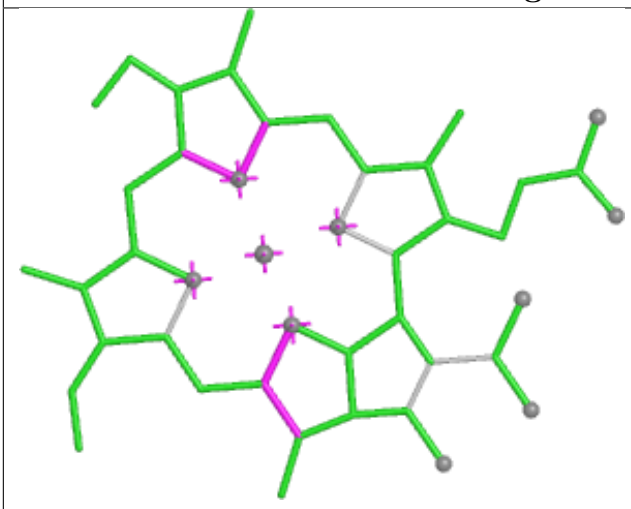


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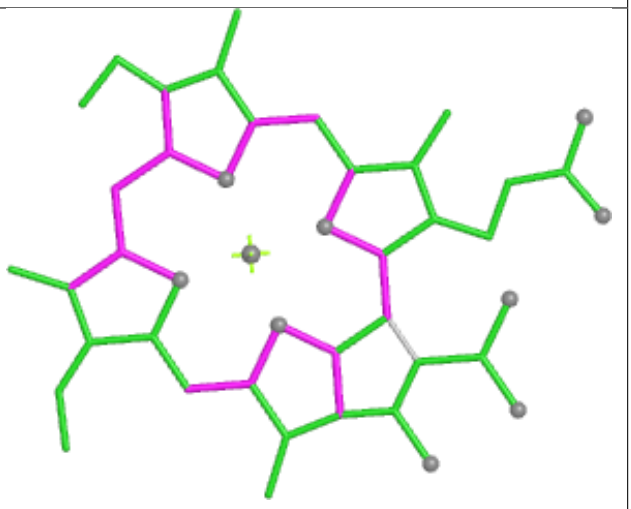


Rings

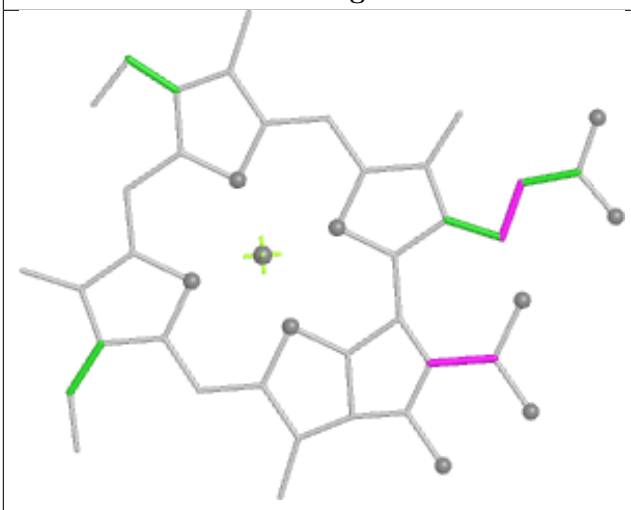
Ligand CLA B 833



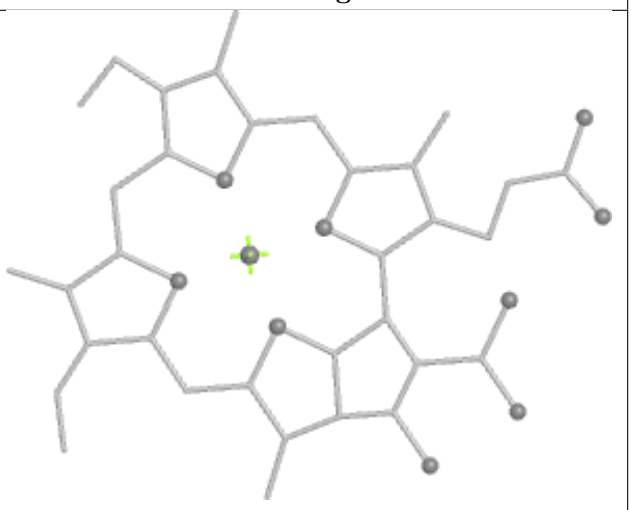
Bond lengths



Bond angles

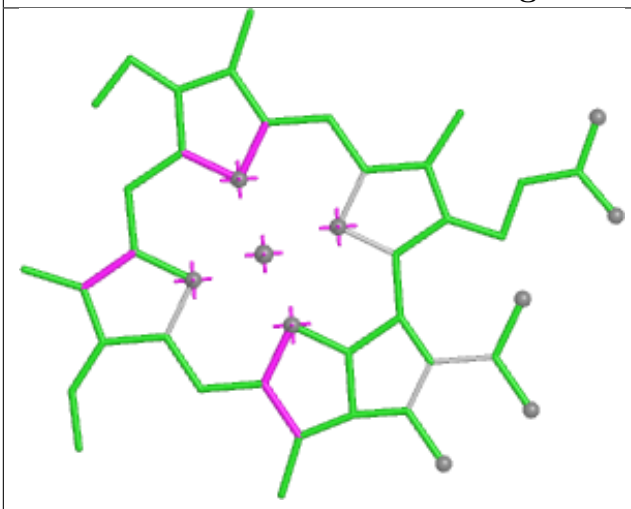


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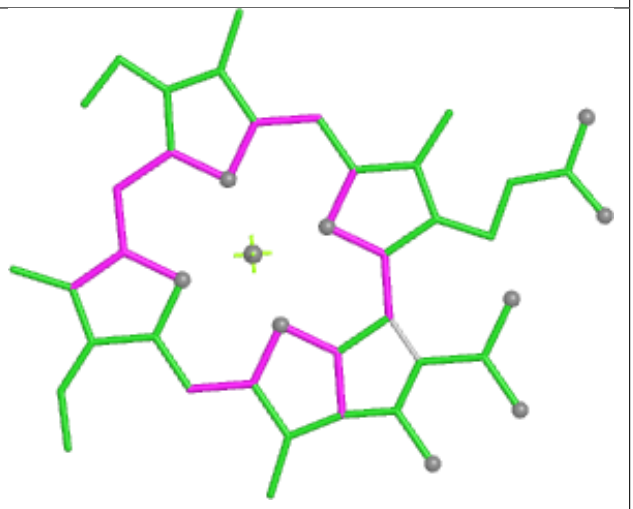


Rings

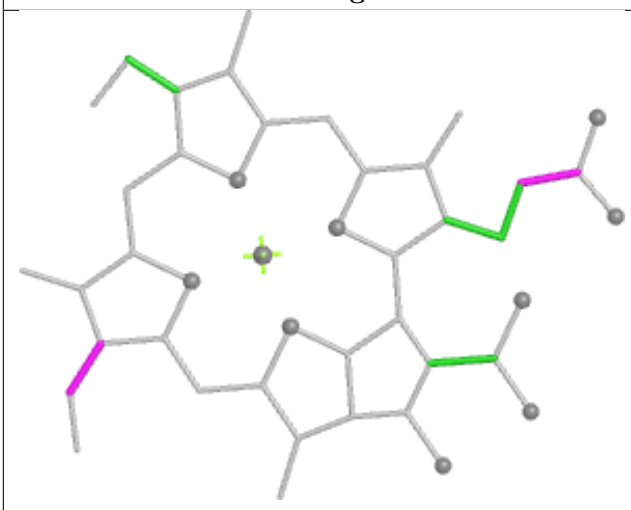
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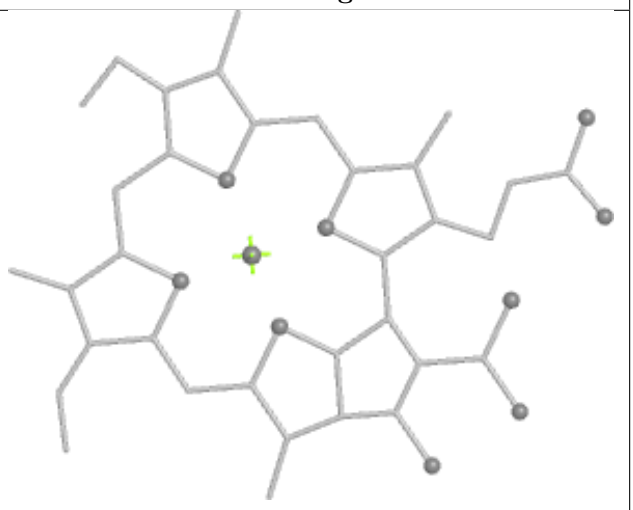
Bond lengths



Bond angles

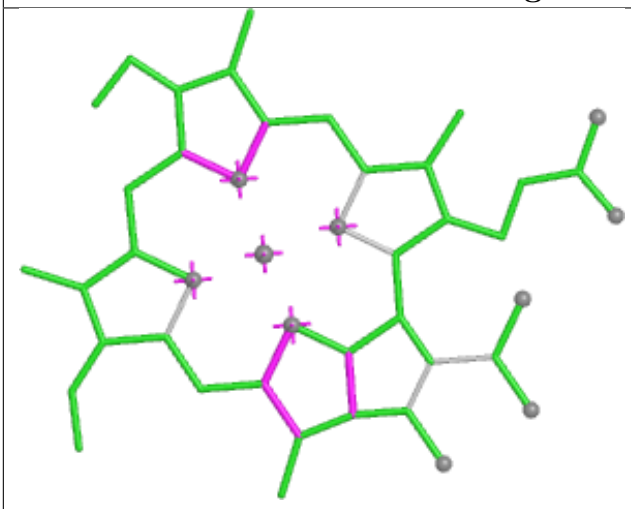


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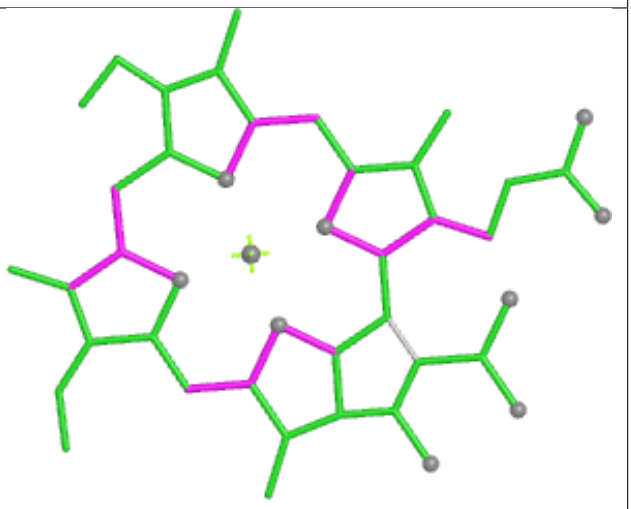


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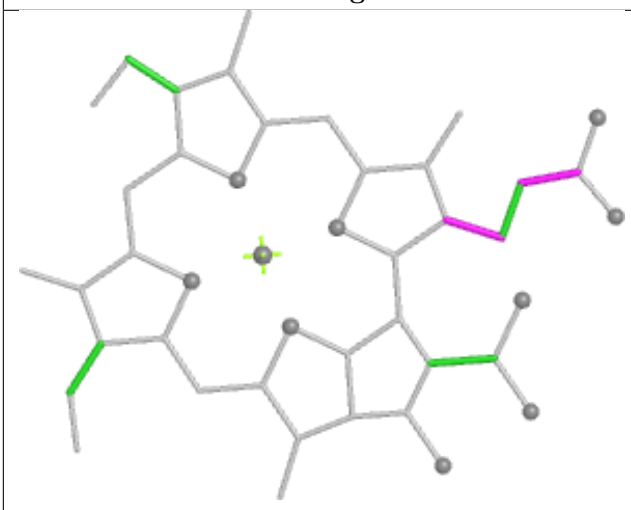
Ligand CLA B 821



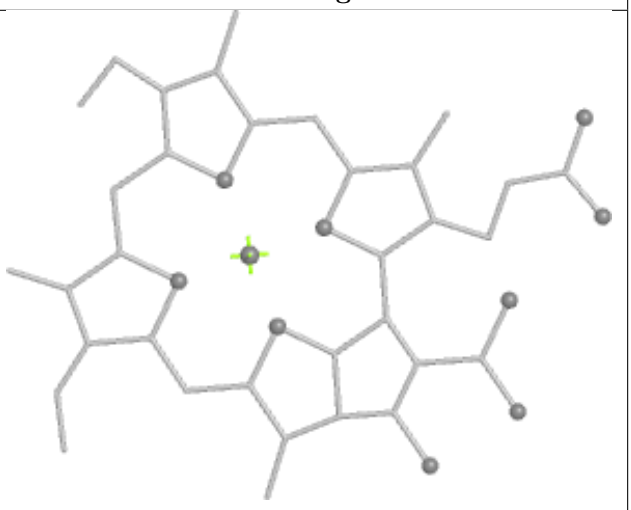
Bond lengths



Bond angles

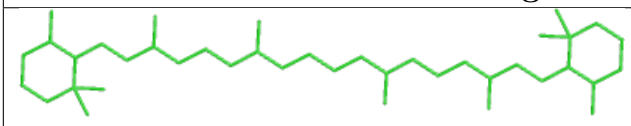


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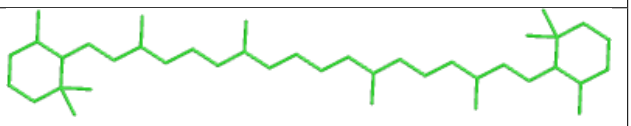


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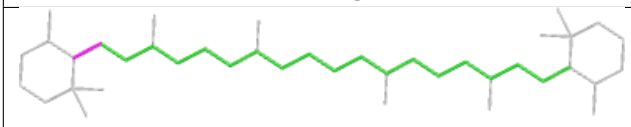
Ligand BCR A 844



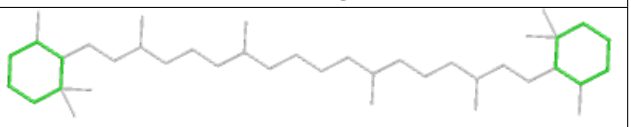
Bond lengths



Bond angles

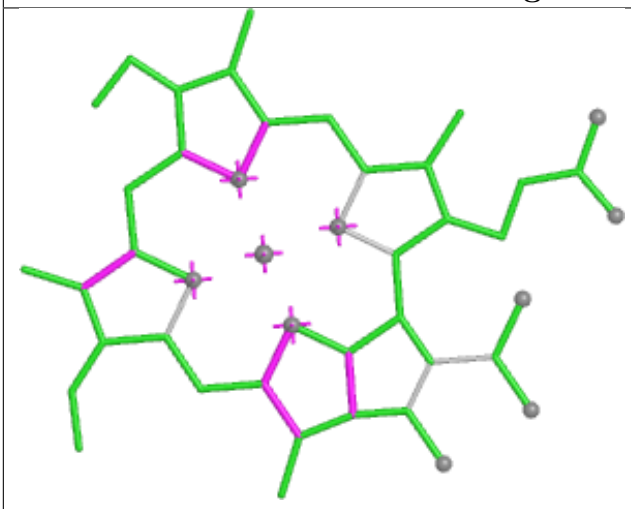


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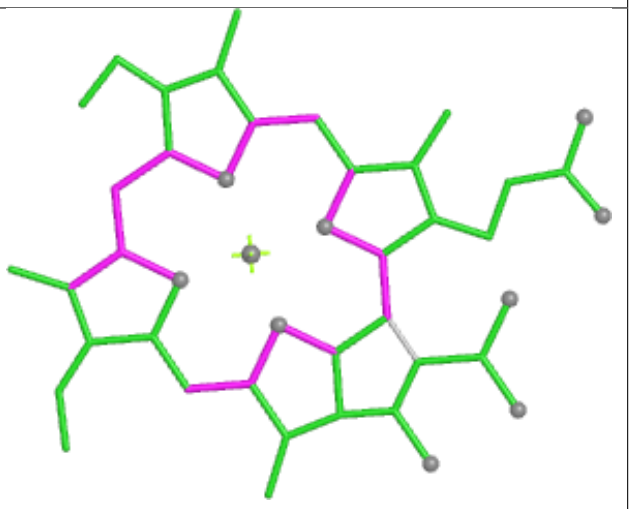


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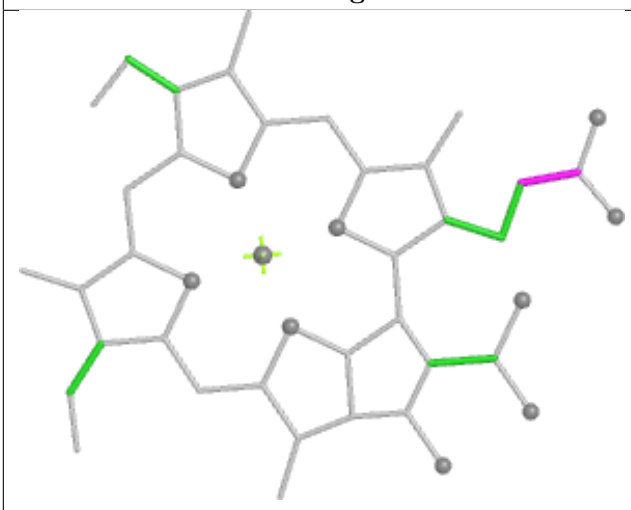
Ligand CLA A 802



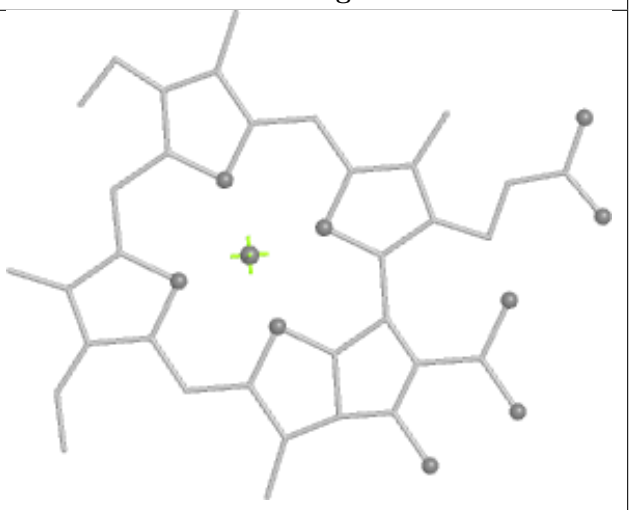
Bond lengths



Bond angles

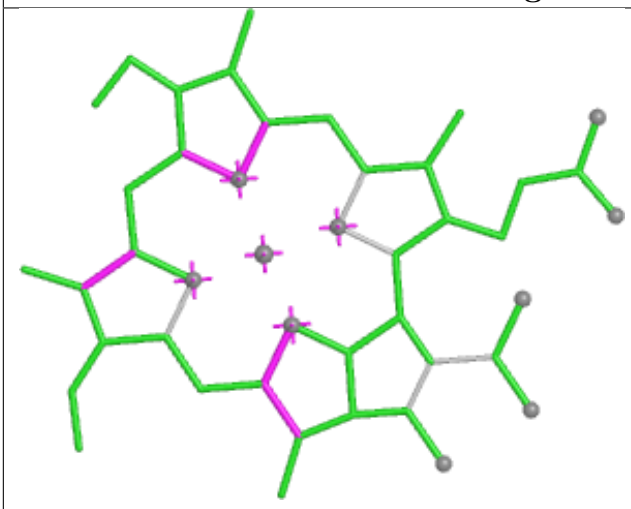


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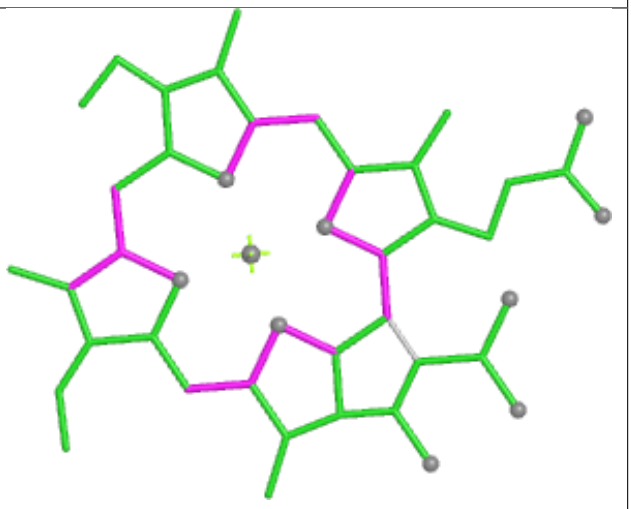


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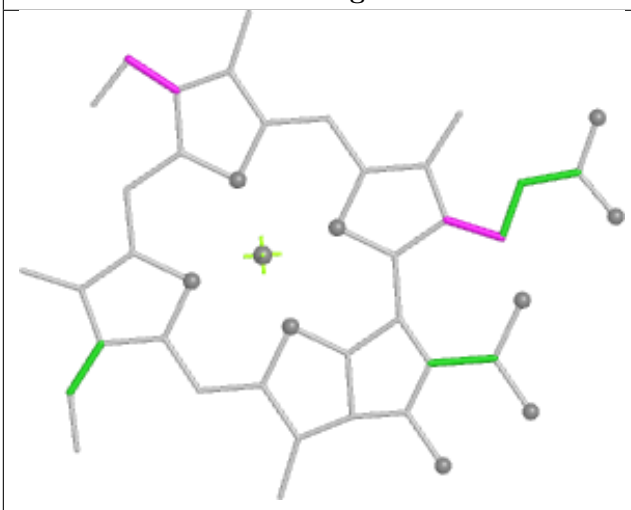
Ligand CLA B 807



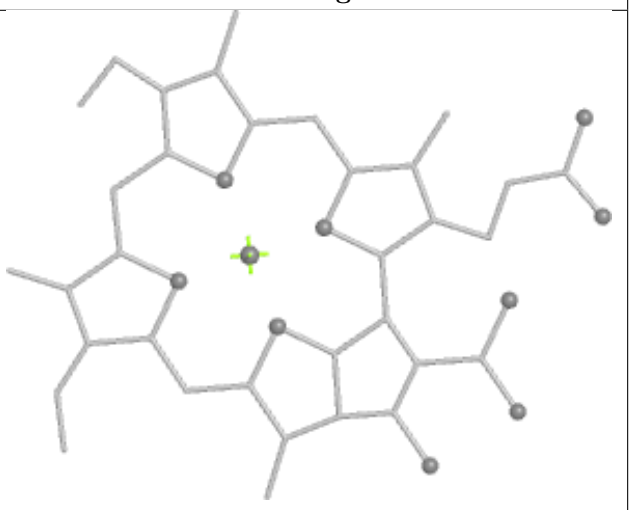
Bond lengths



Bond angles

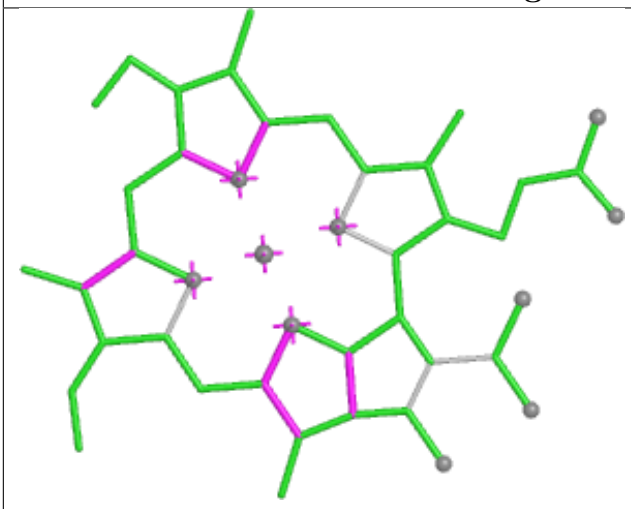


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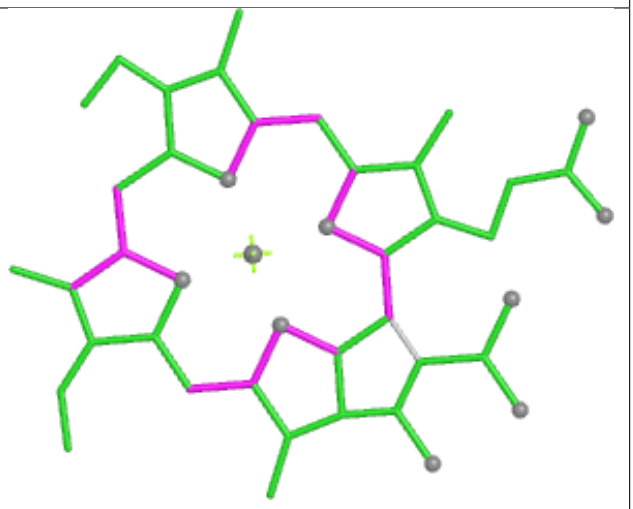


Rings

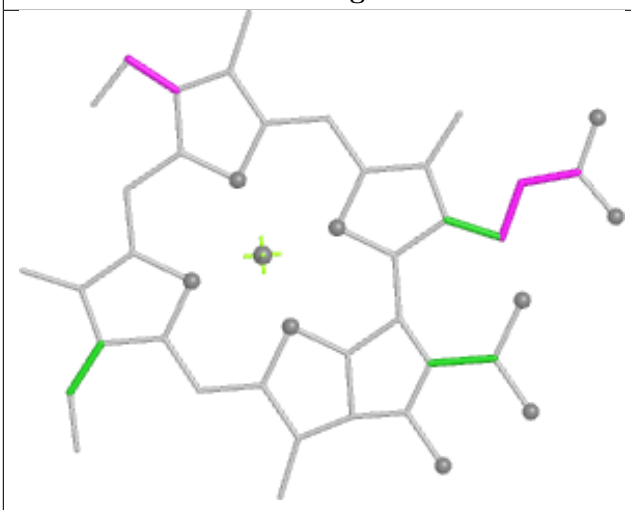
Ligand CLA B 819



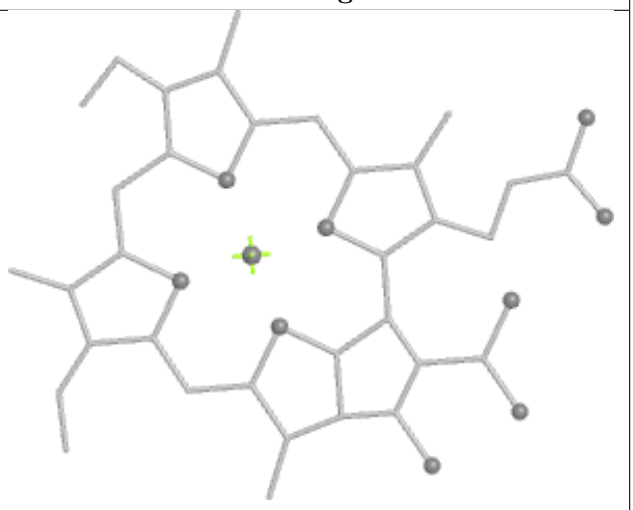
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Bond angles

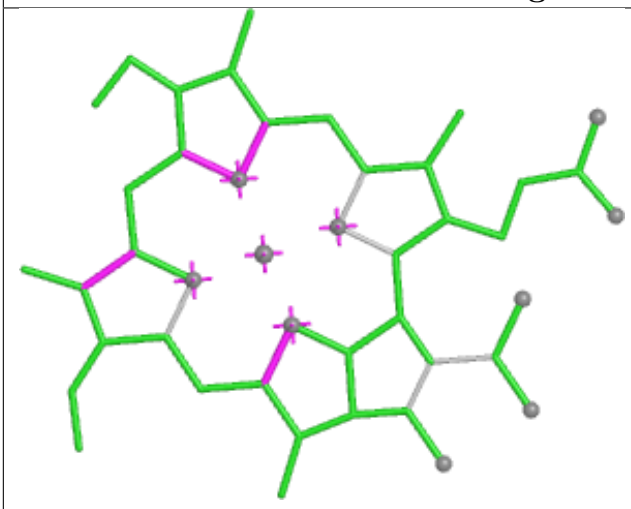


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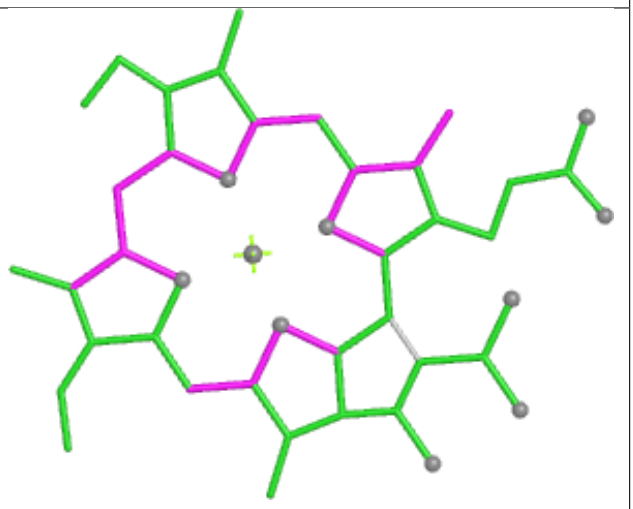


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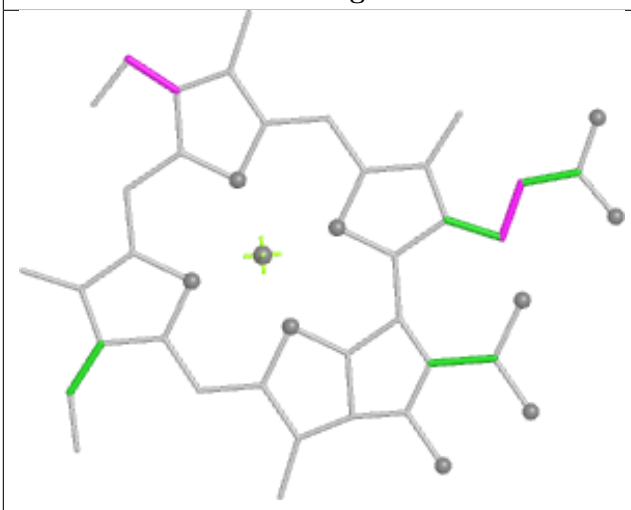
Ligand CLA 6 307



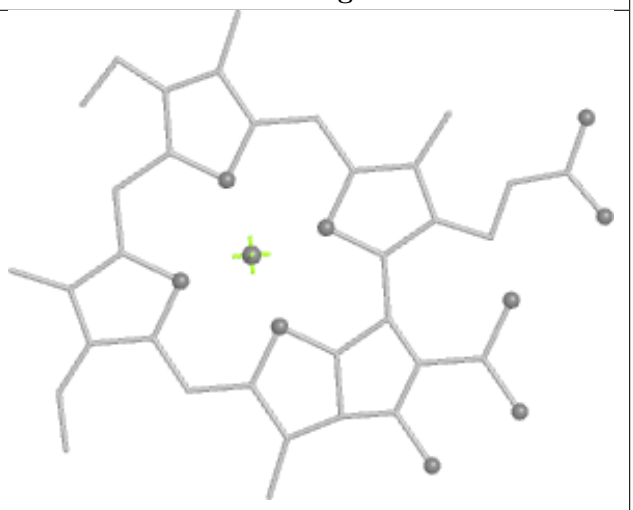
Bond lengths



Bond angles

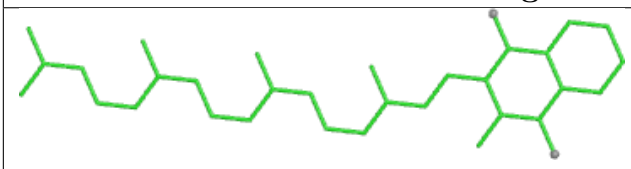


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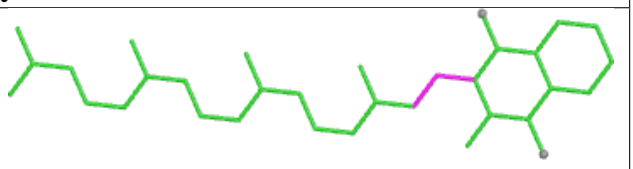


Rings

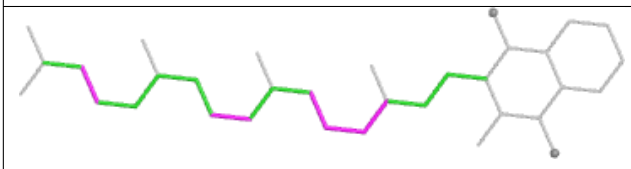
Ligand PQN A 842



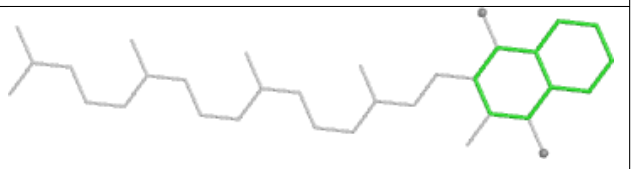
Bond lengths



Bond angles

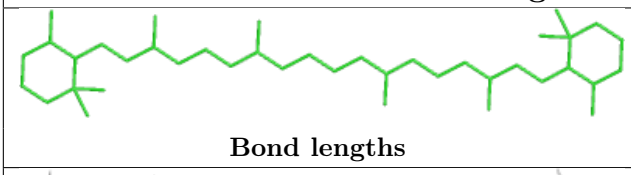


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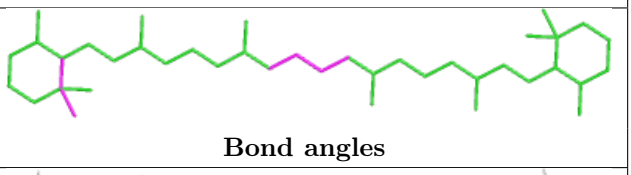


Rings

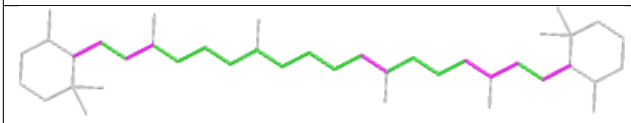
Ligand BCR I 201



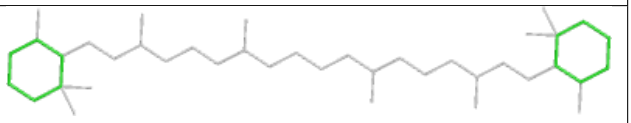
Bond lengths



Bond angles

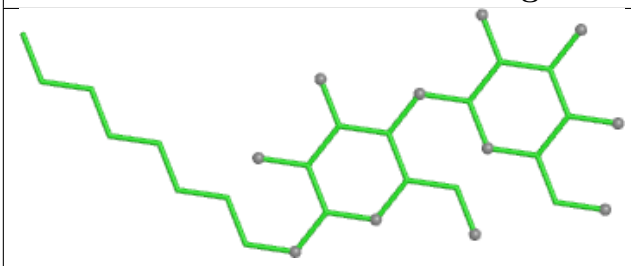


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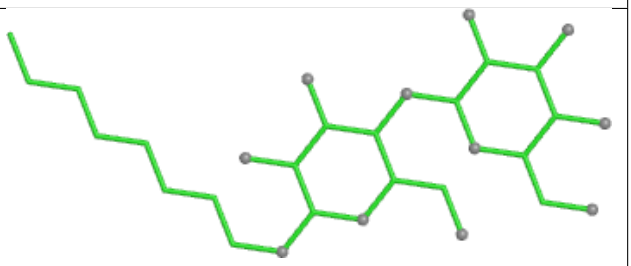


Rings

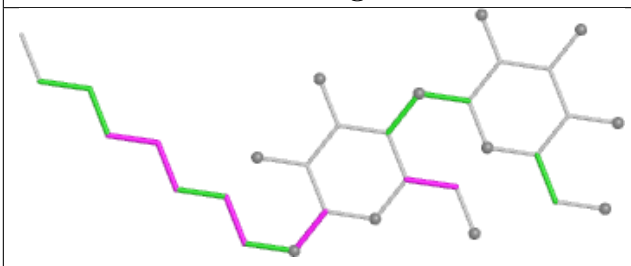
Ligand LMT B 849



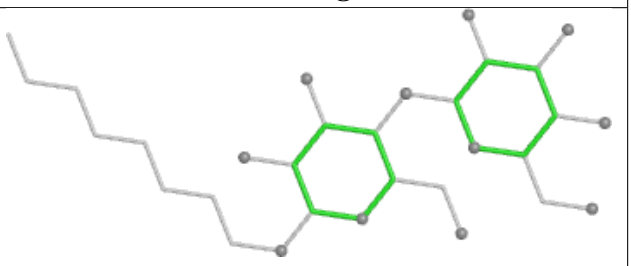
Bond lengths



Bond angles

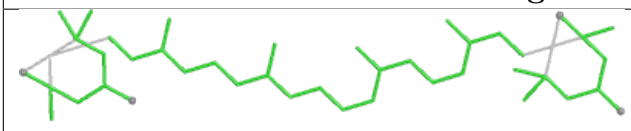


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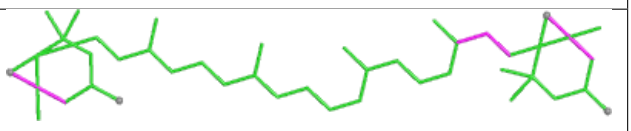


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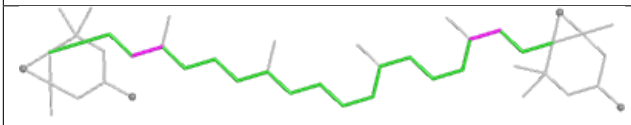
Ligand XAT 5 303



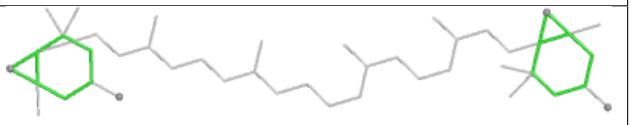
Bond lengths



Bond angles

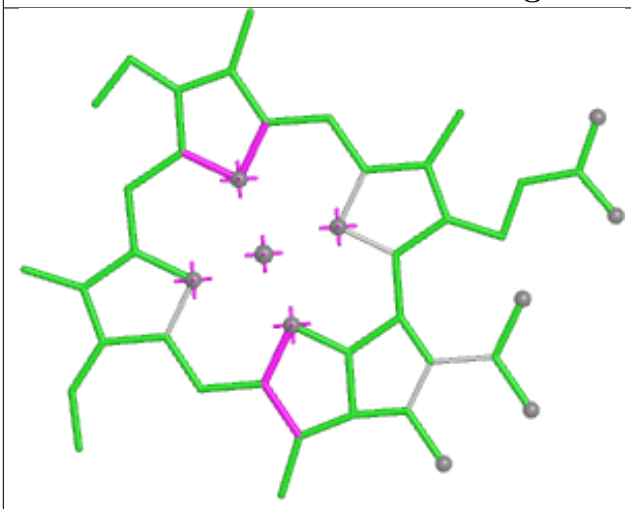


Torsions

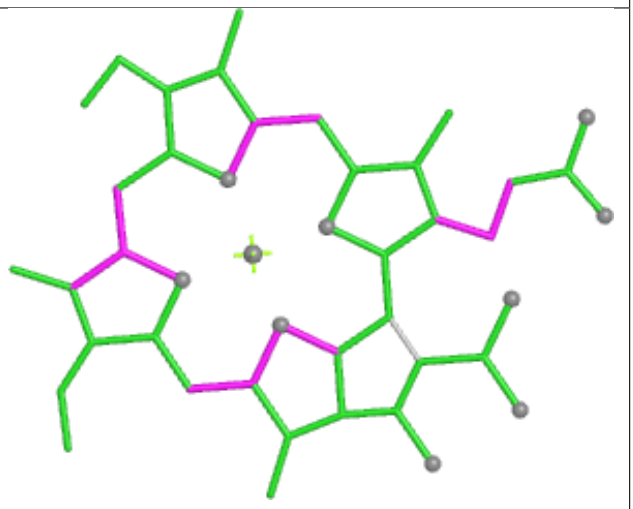


Rings

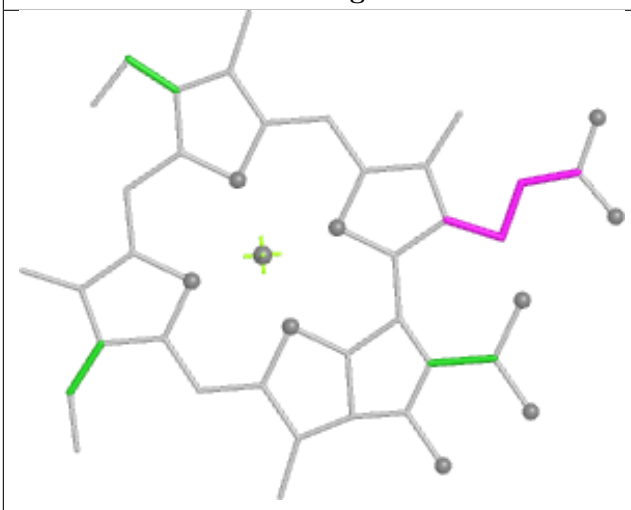
Ligand CLA A 810



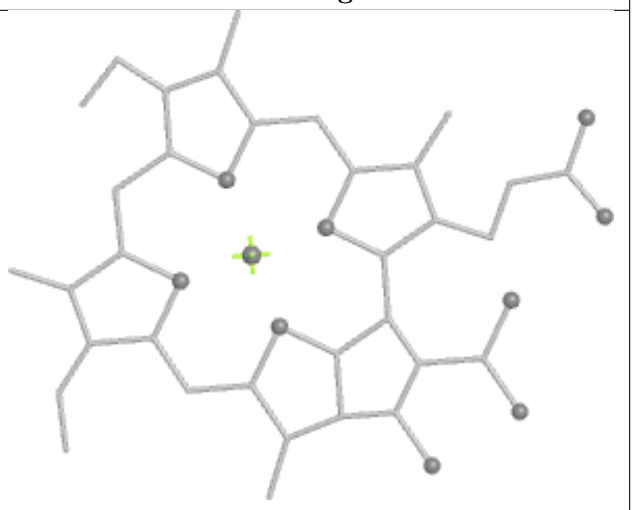
Bond lengths



Bond angles

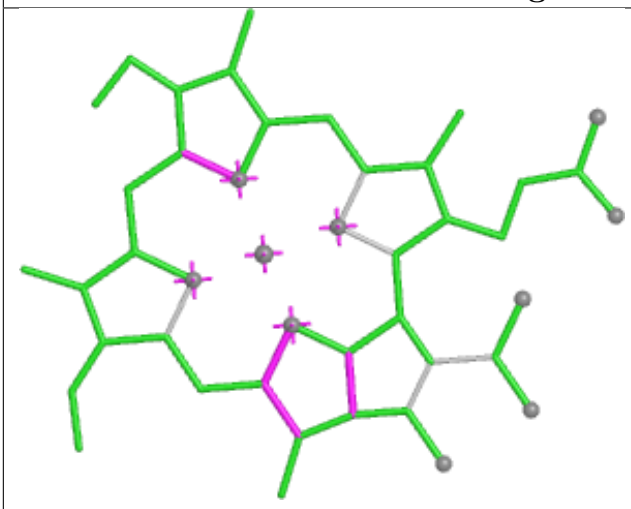


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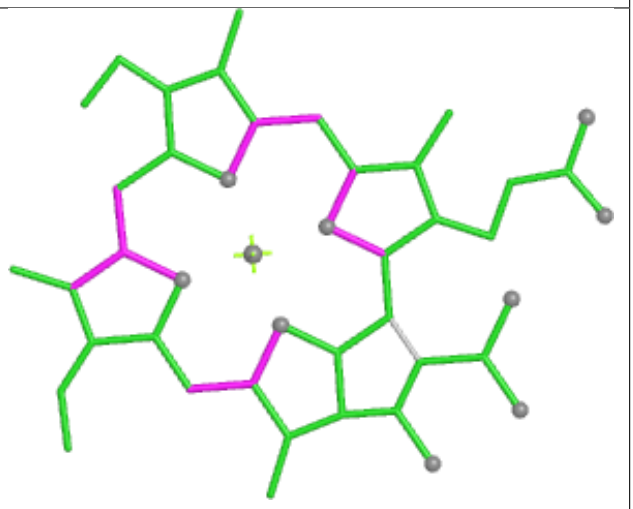


Rings

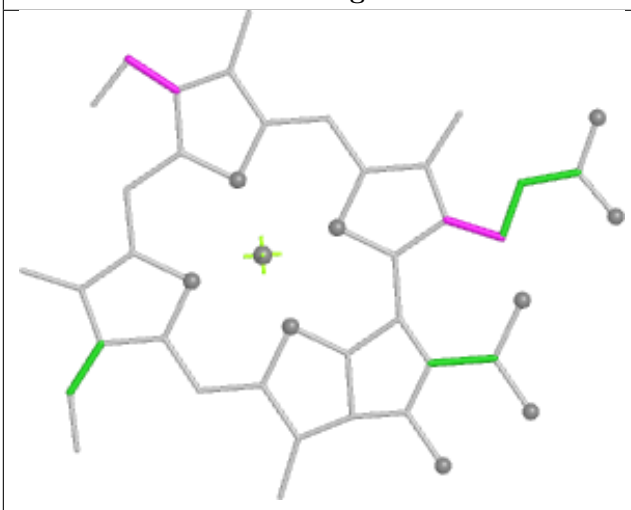
Ligand CLA 8 316



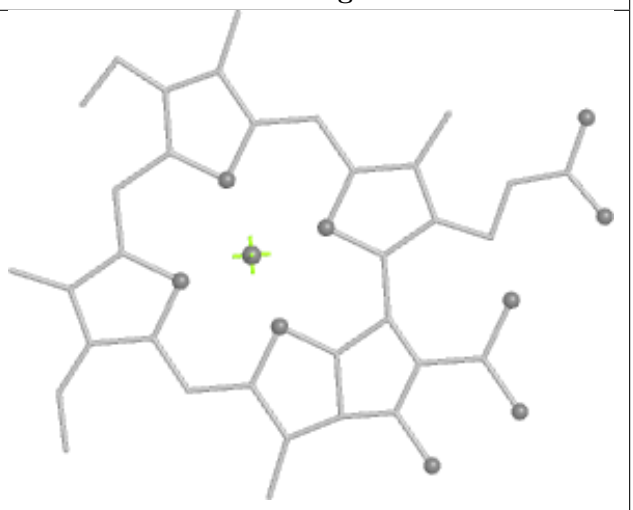
Bond lengths



Bond angles

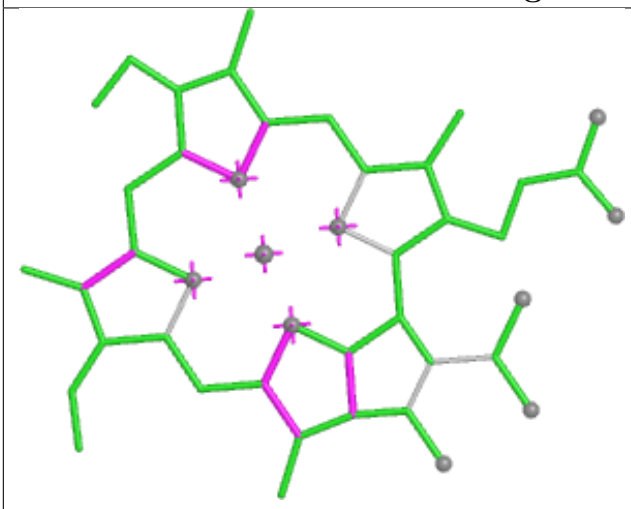


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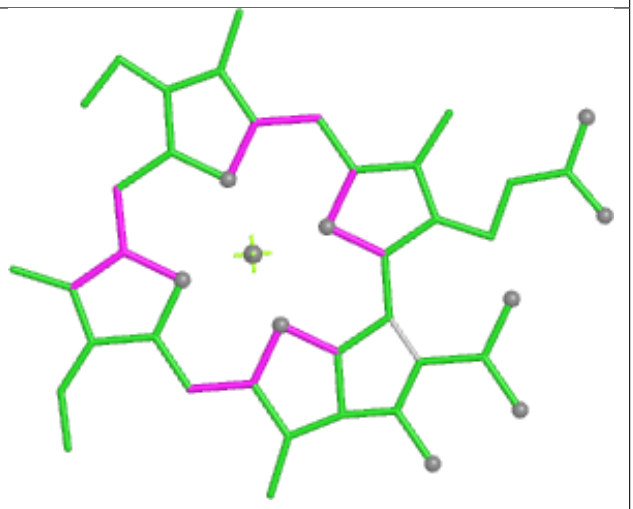


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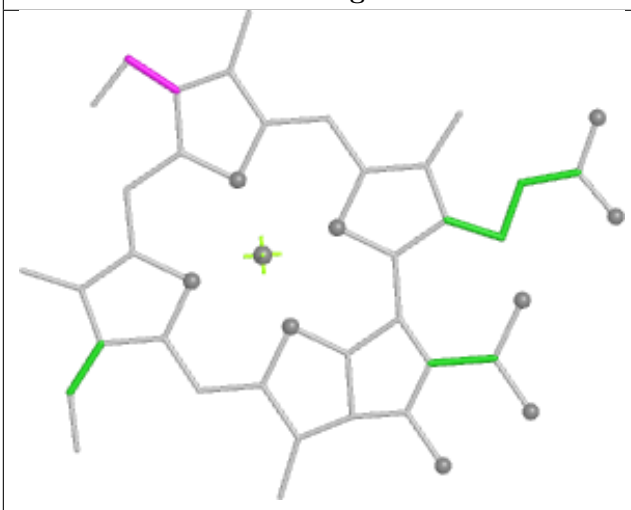
Ligand CLA B 822



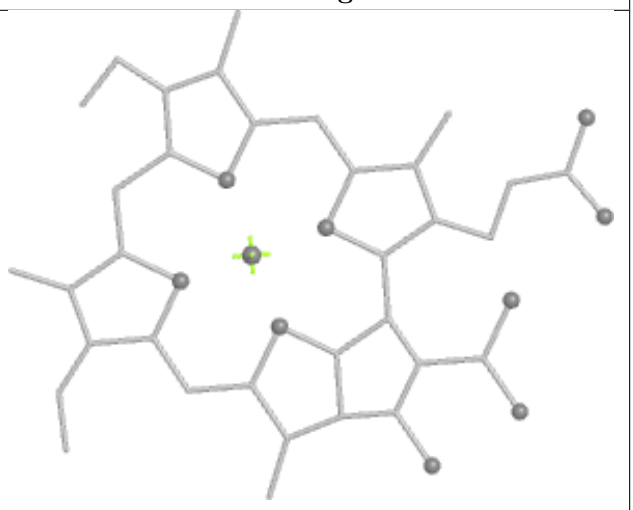
Bond lengths



Bond angles

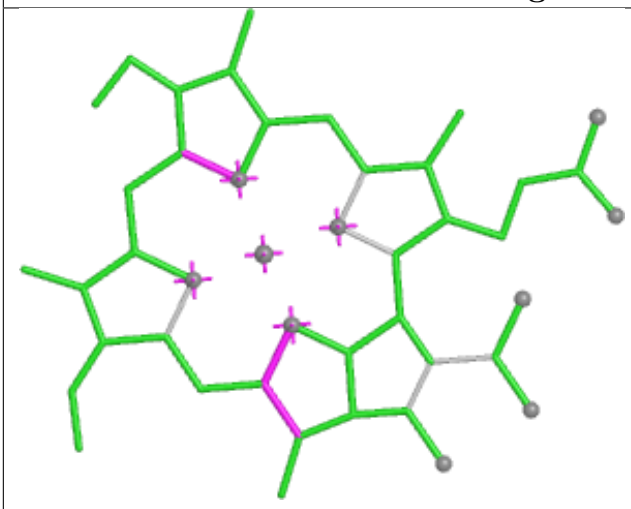


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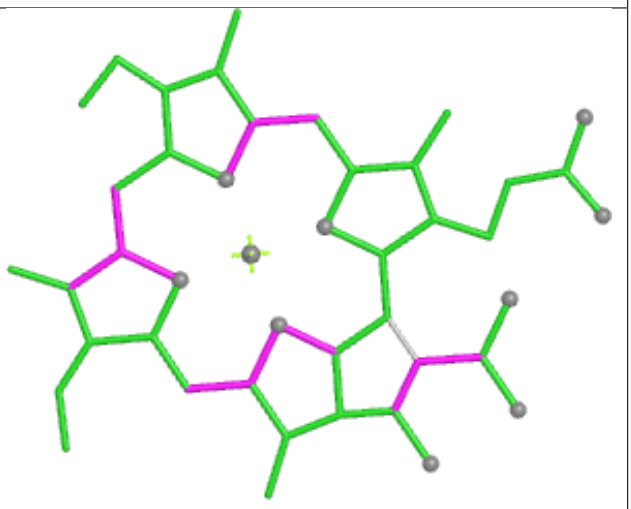


Rings

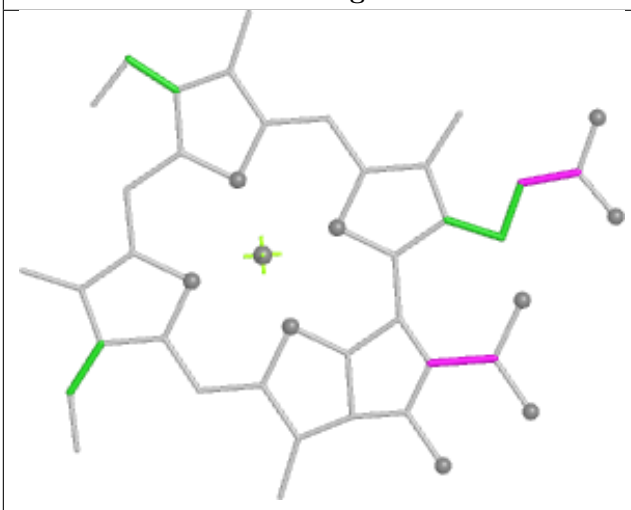
Ligand CLA 8 305



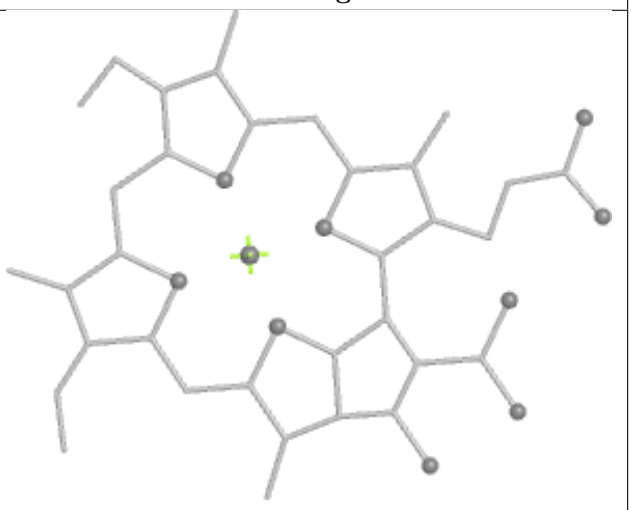
Bond lengths



Bond angles

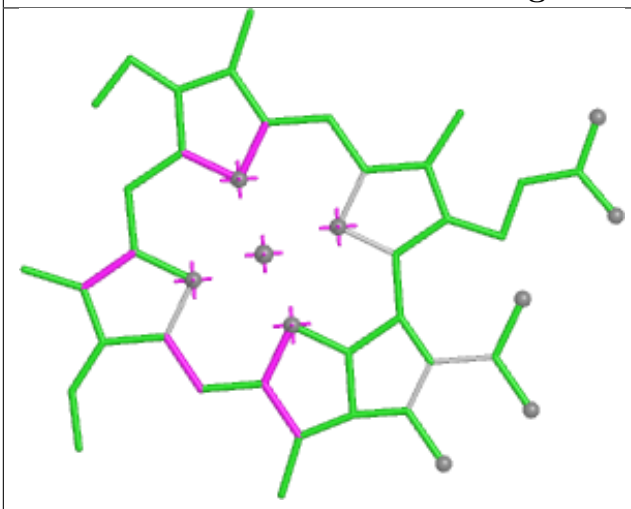


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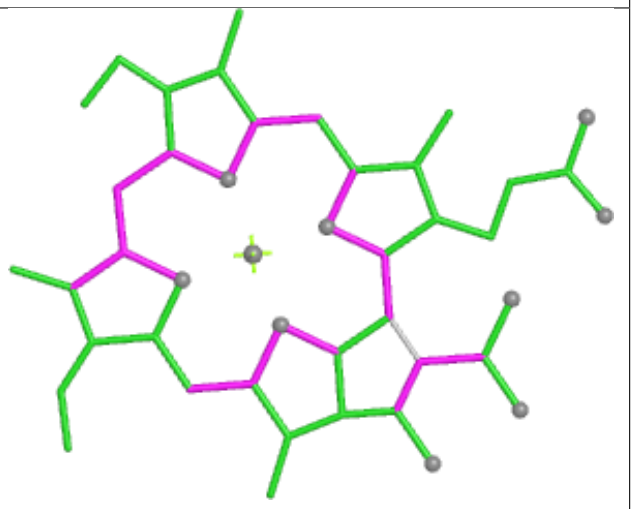


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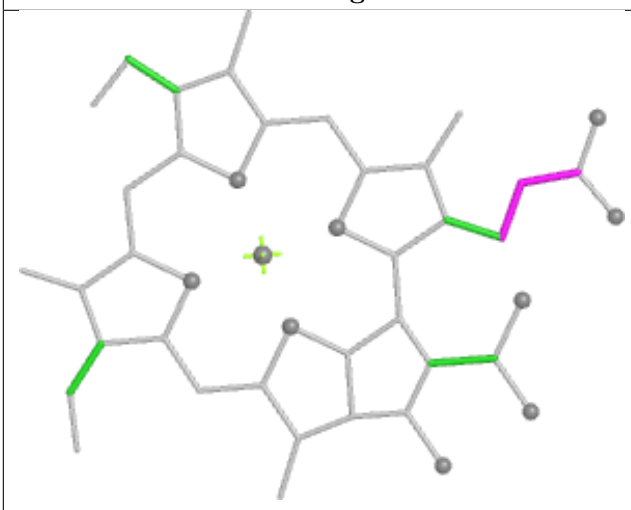
Ligand CLA 0 307



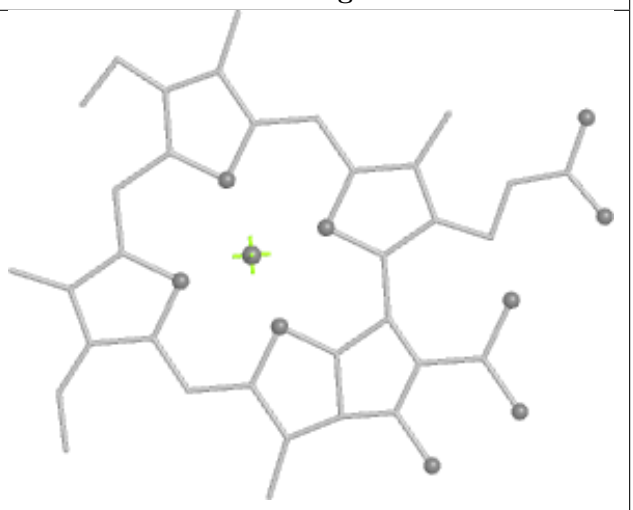
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Bond angles

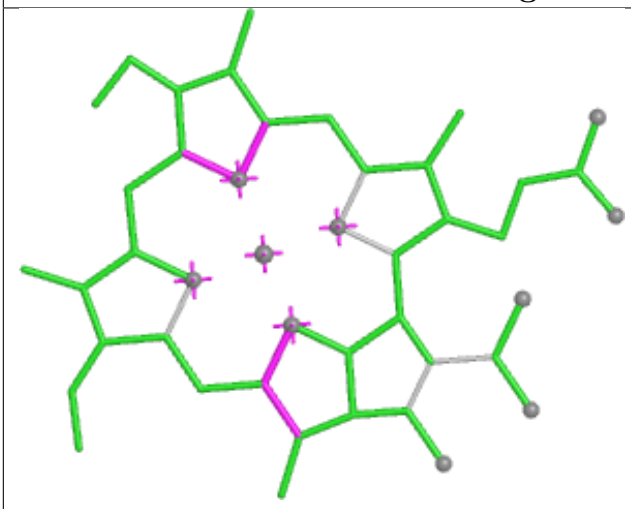


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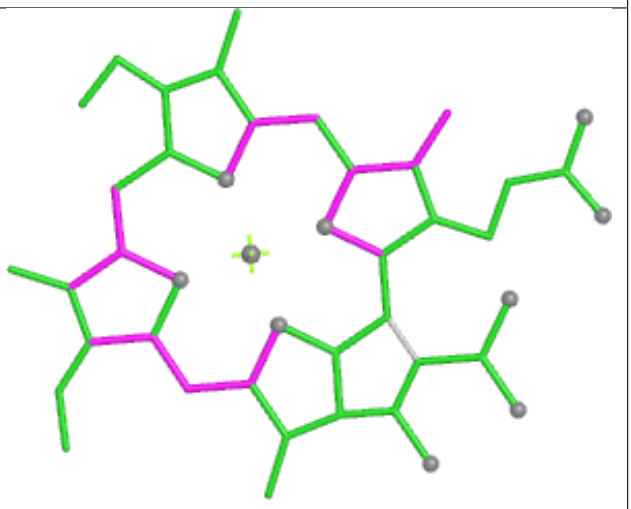


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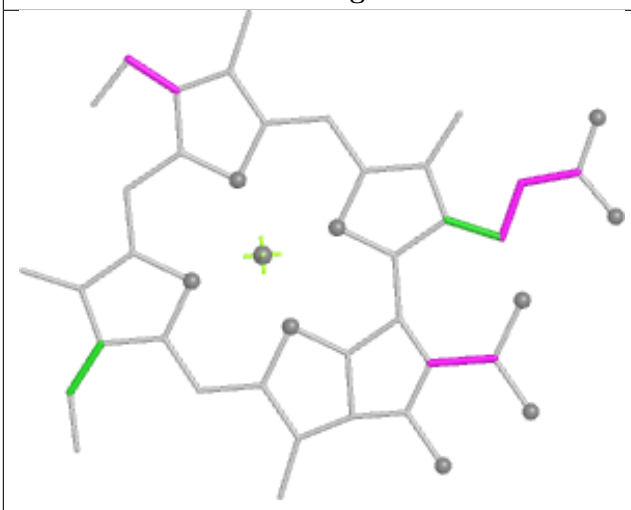
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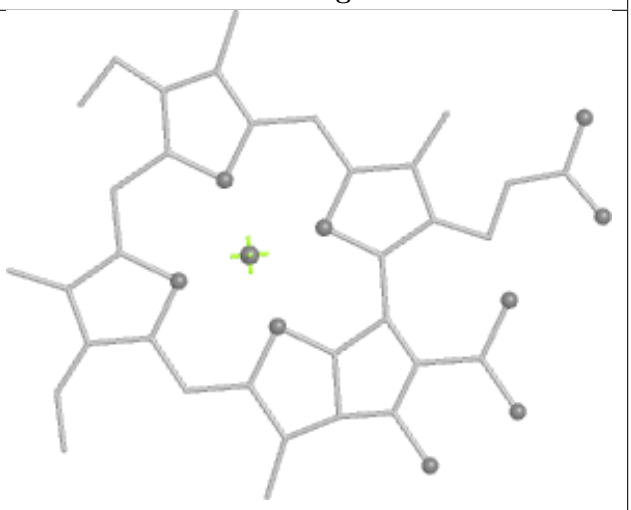
Bond lengths



Bond angles

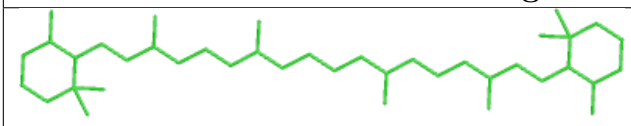


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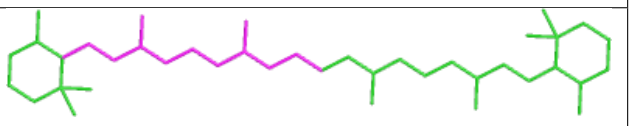


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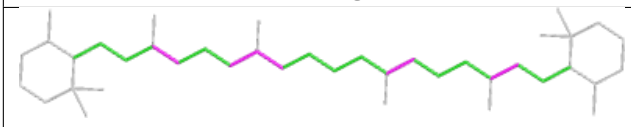
Ligand BCR A 845



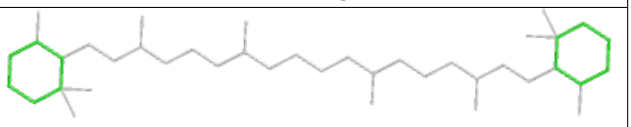
Bond lengths



Bond angles

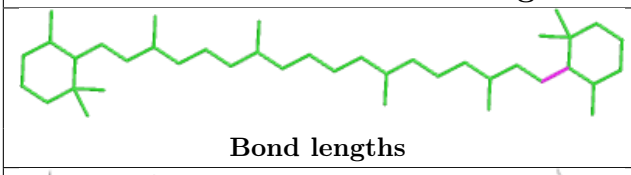


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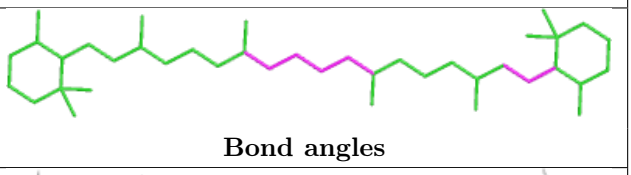


Rings

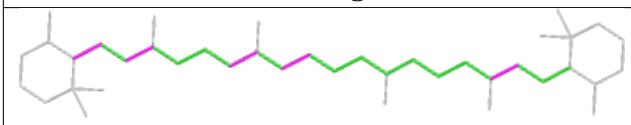
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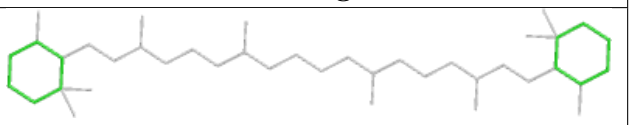
Bond lengths



Bond angles

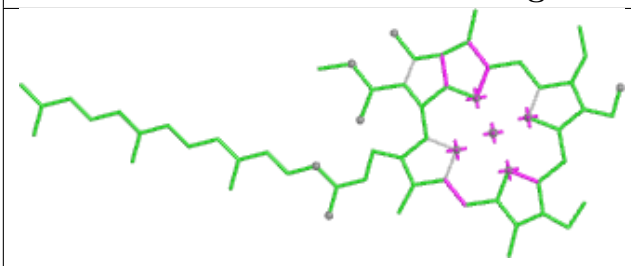


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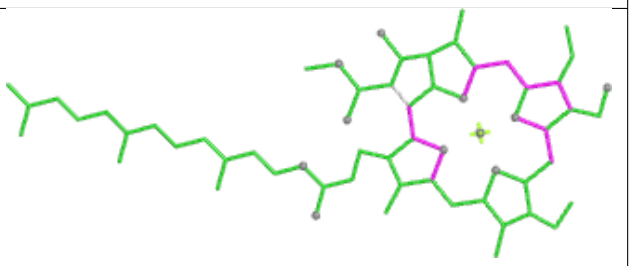


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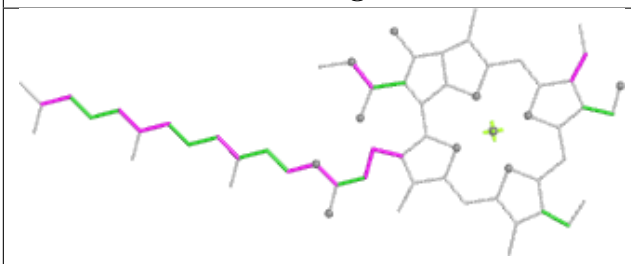
Ligand CHL 4 315



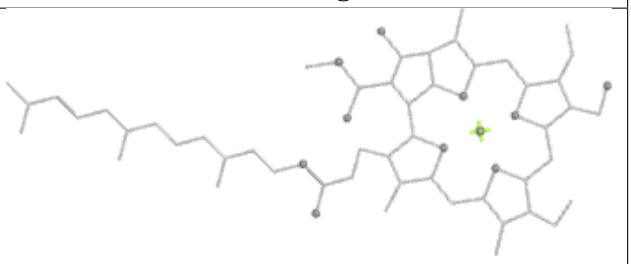
Bond lengths



Bond angles

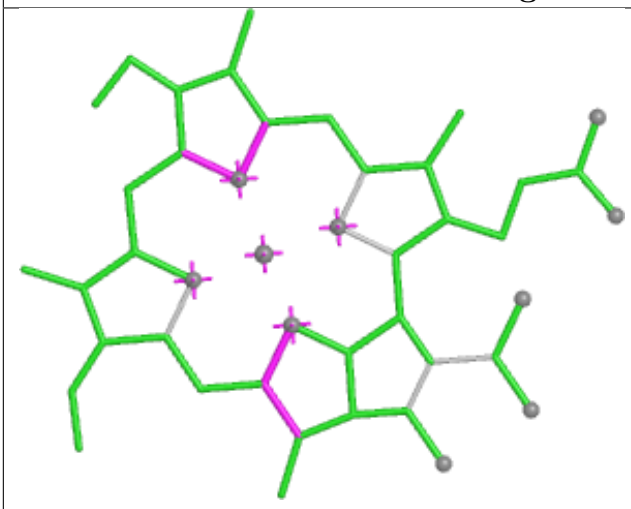


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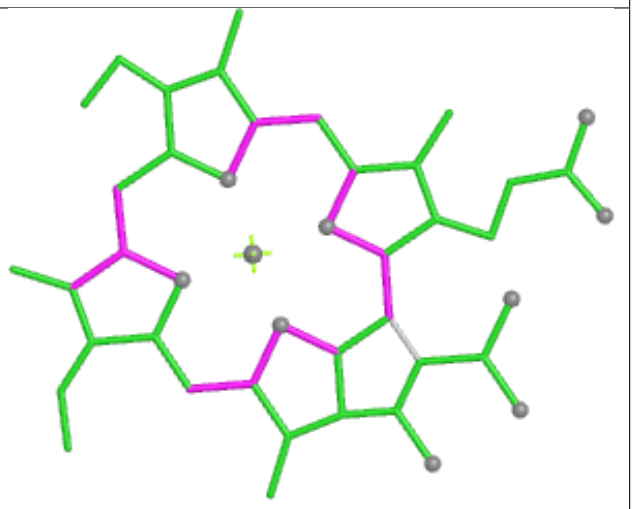


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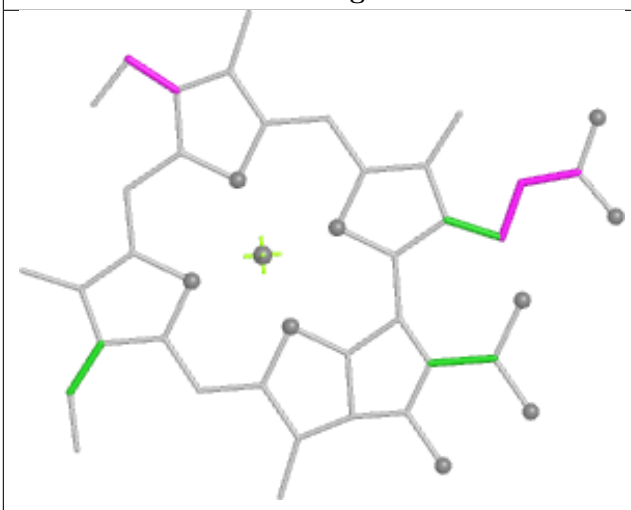
Ligand CLA 3 1010



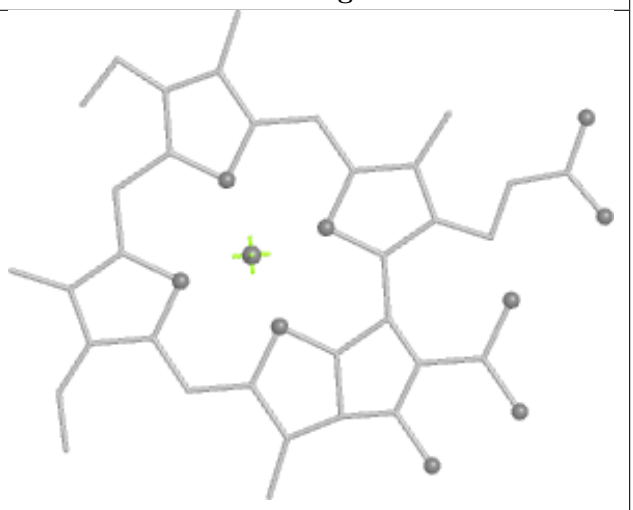
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Bond angles

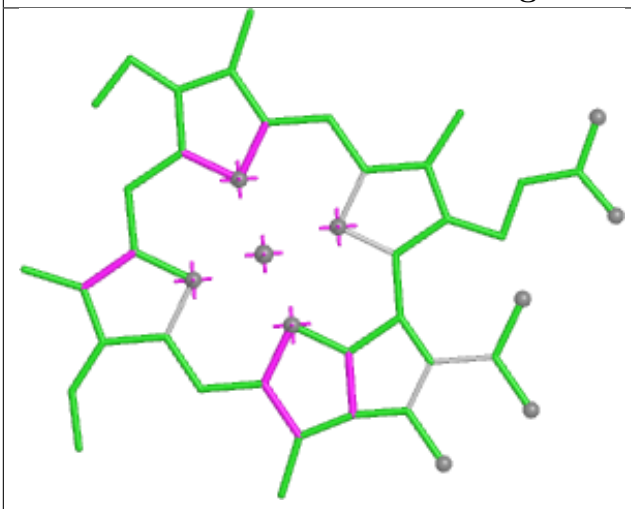


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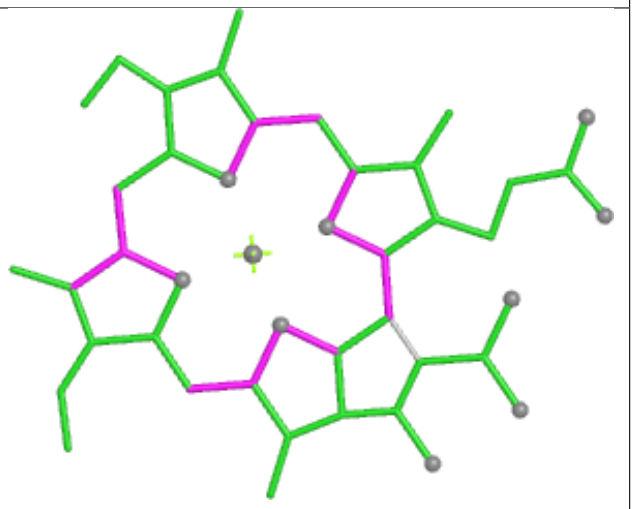


Rings

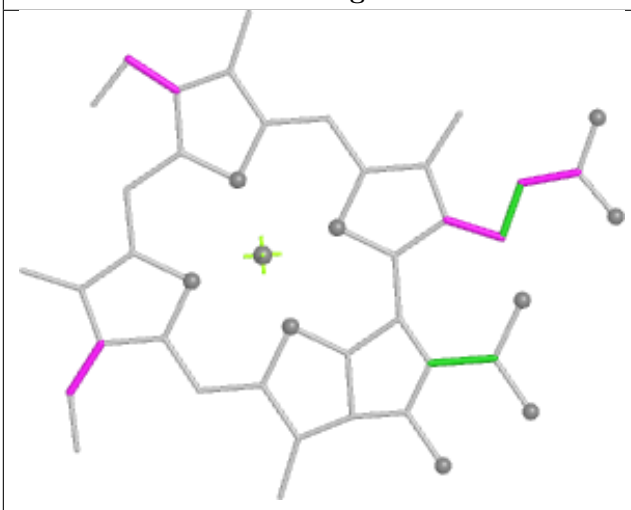
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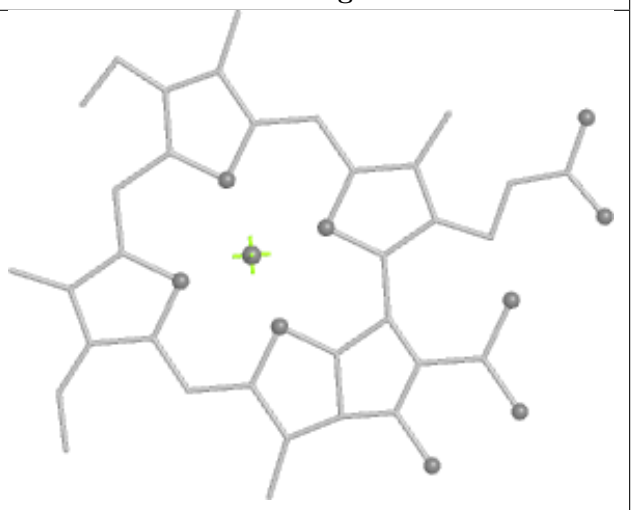
Bond lengths



Bond angles

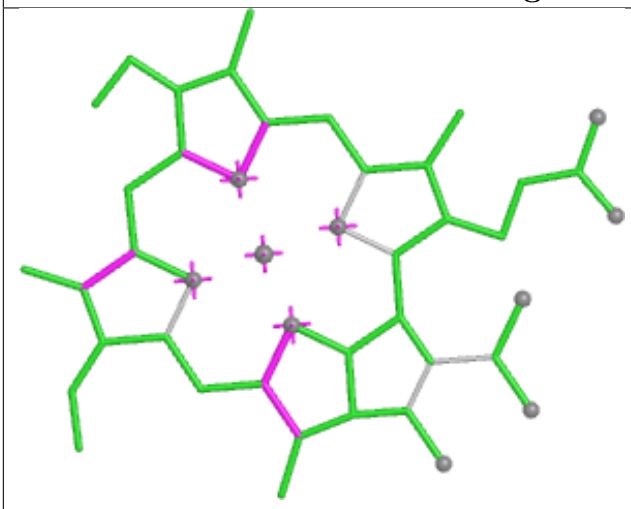


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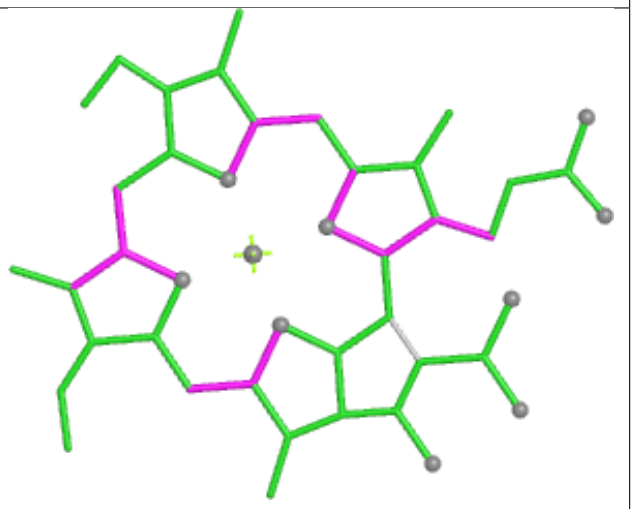


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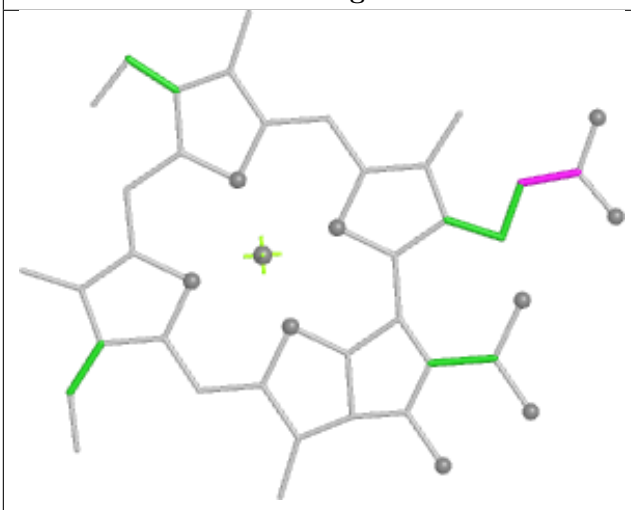
Ligand CLA A 851



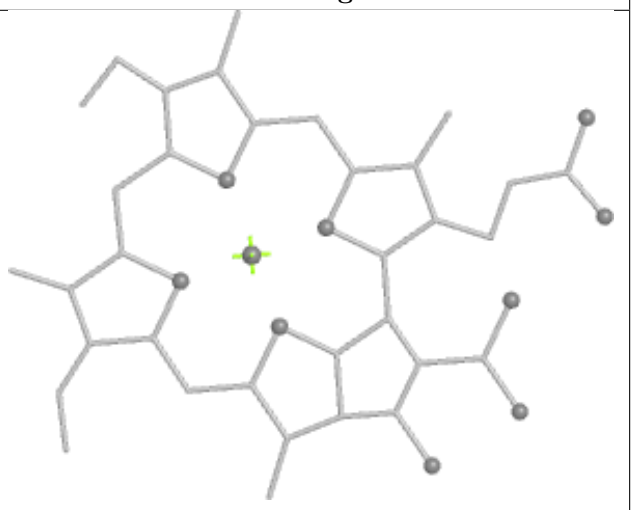
Bond lengths



Bond angles

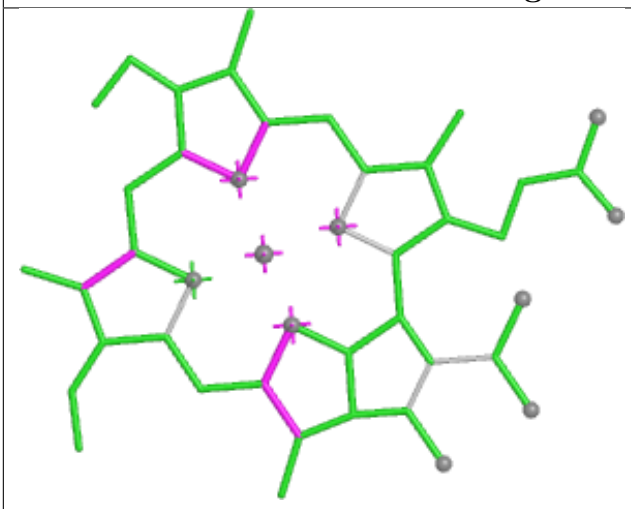


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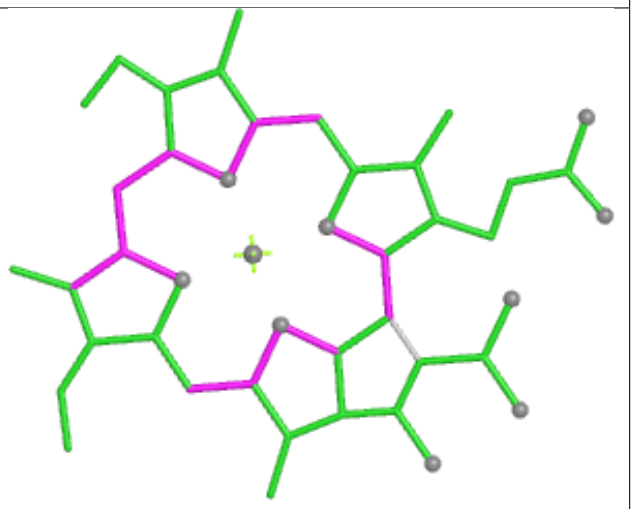


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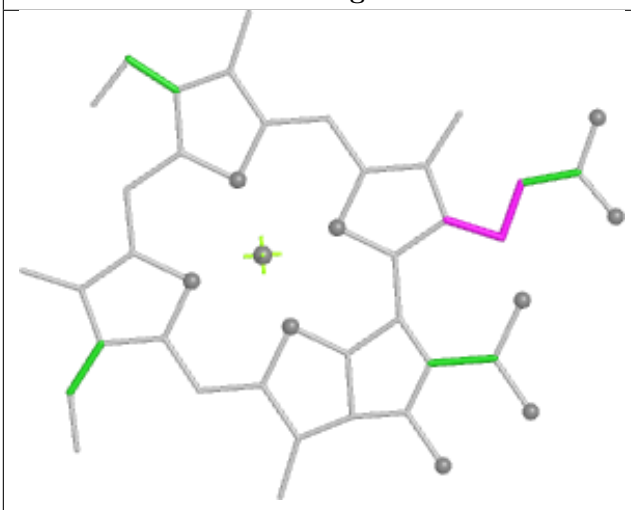
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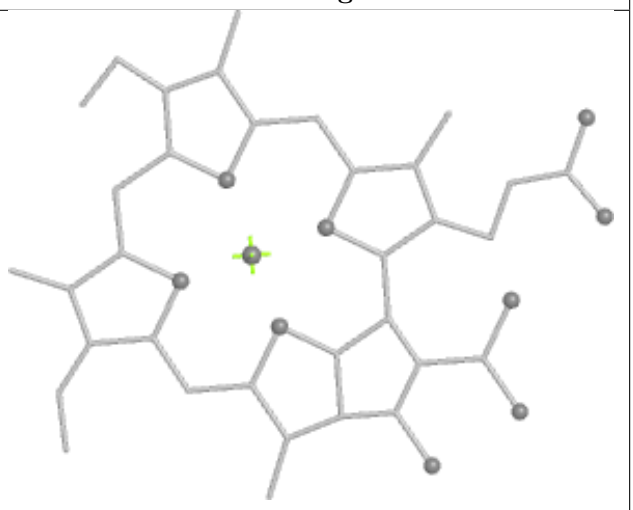
Bond lengths



Bond angles

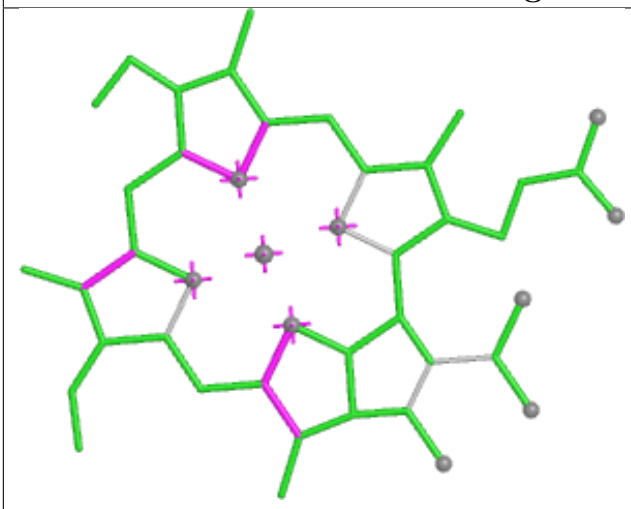


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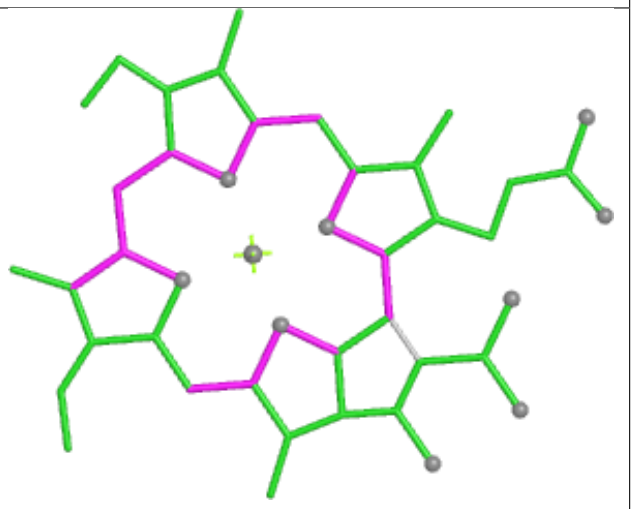


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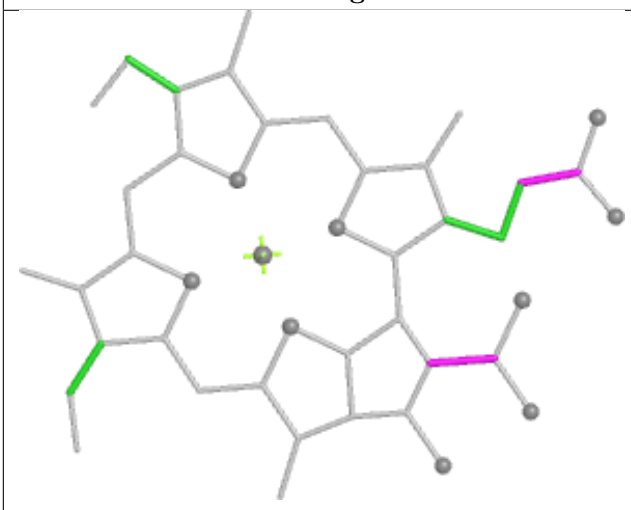
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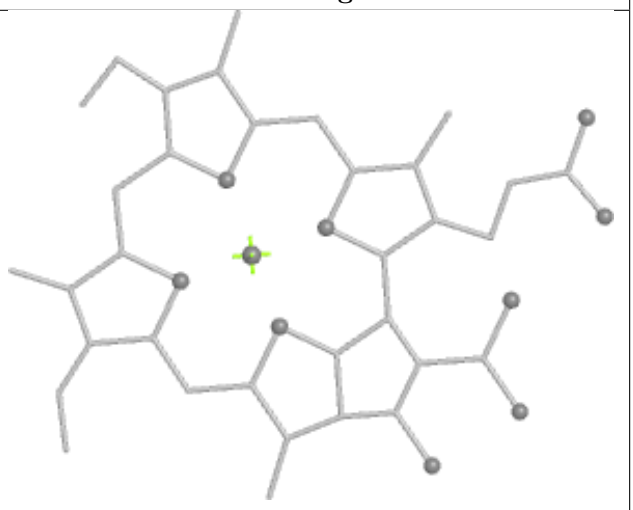
Bond lengths



Bond angles

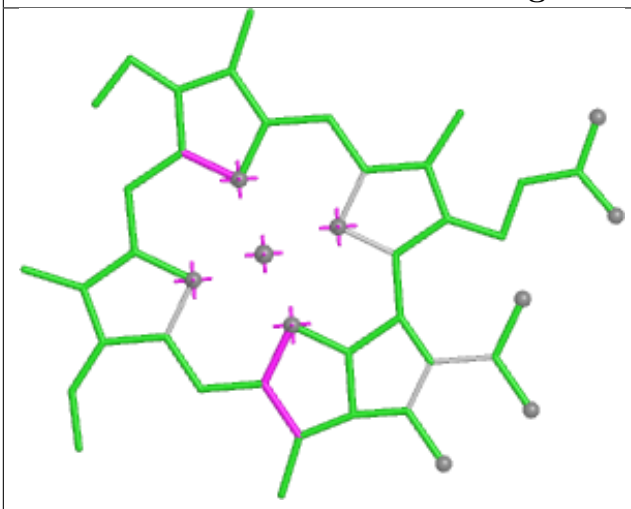


Torsions

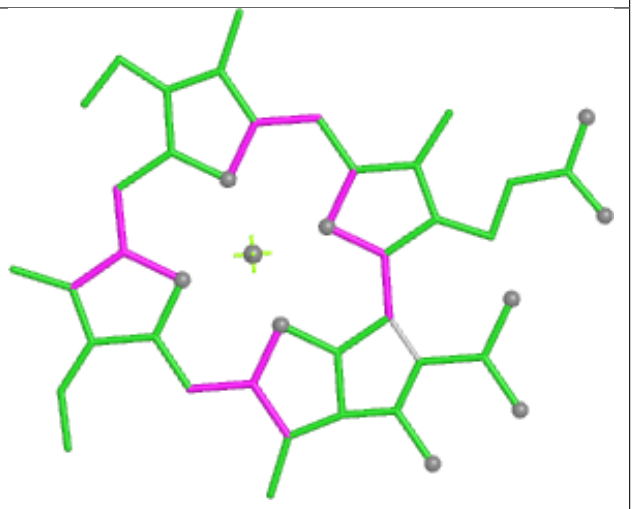


Rings

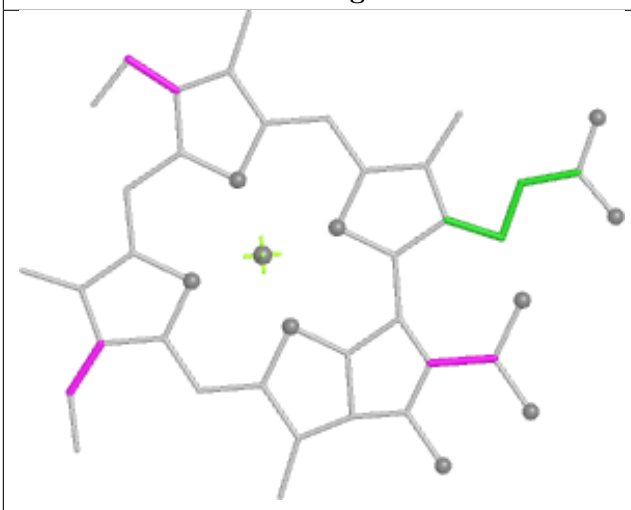
Ligand CLA 4 314



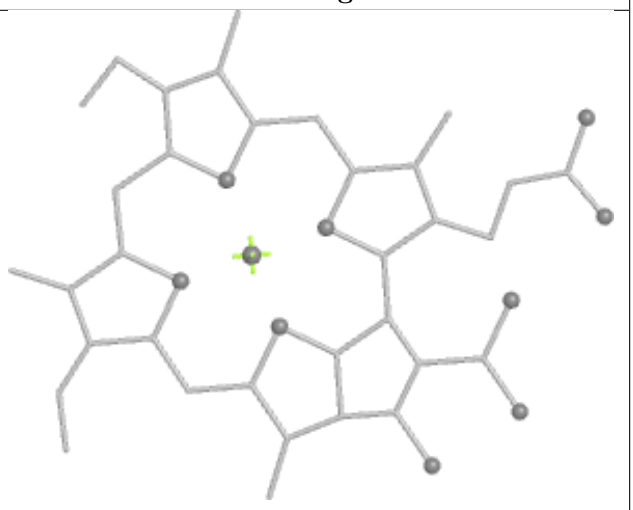
Bond lengths



Bond angles

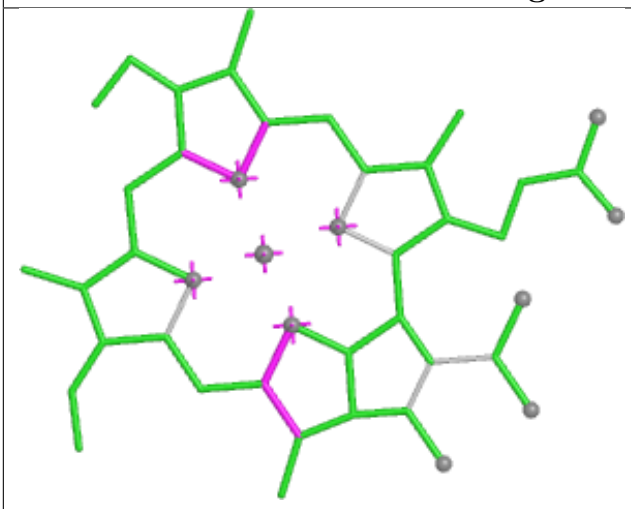


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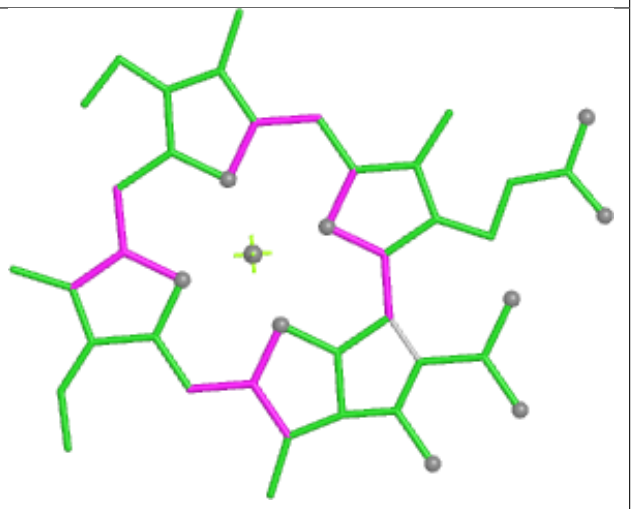


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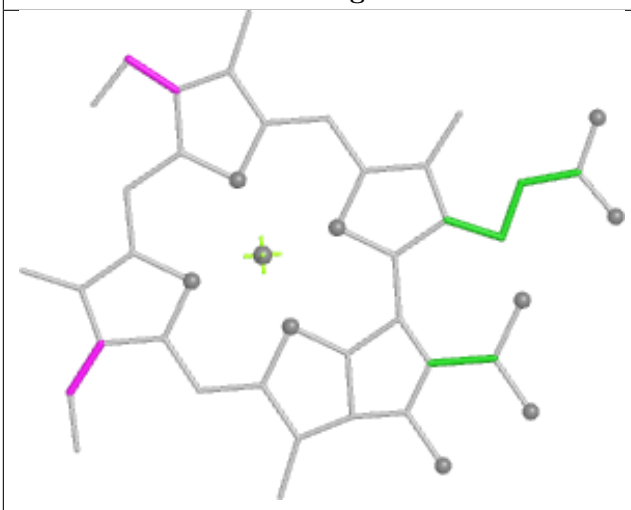
Ligand CLA 0 316



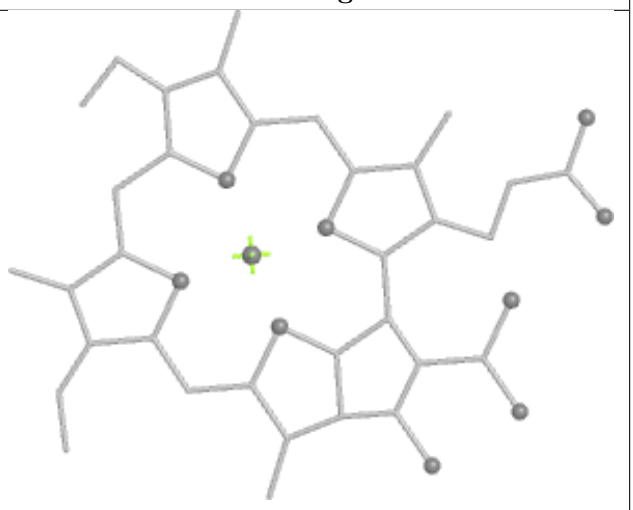
Bond lengths



Bond angles

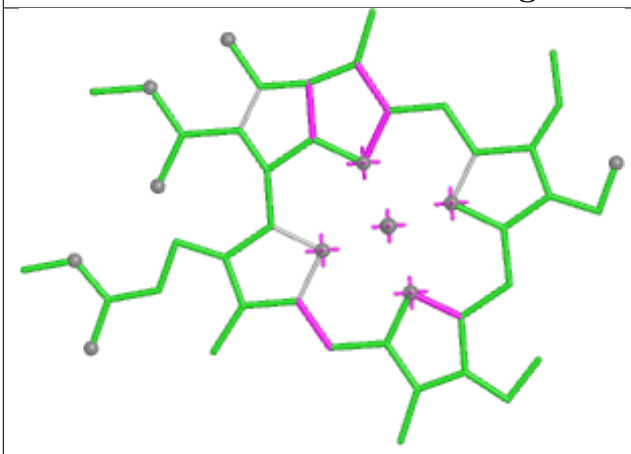


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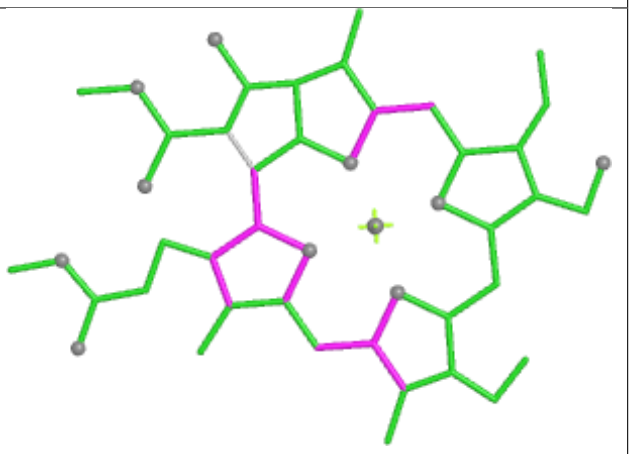


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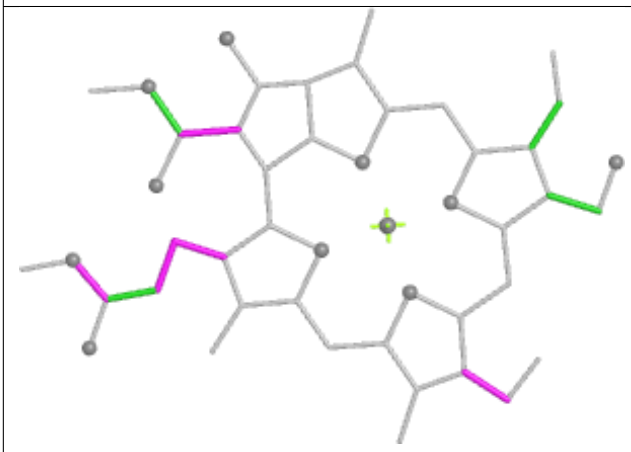
Ligand CHL 3 1014



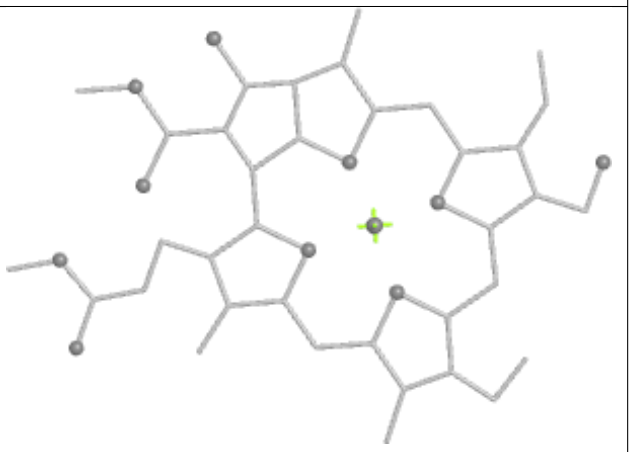
Bond lengths



Bond angles

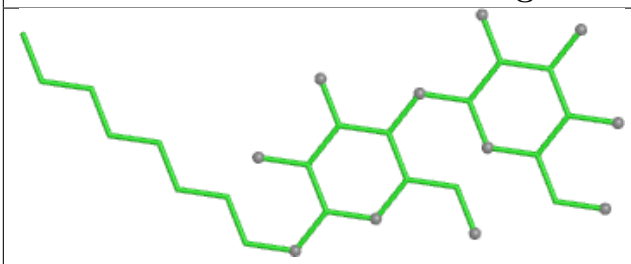


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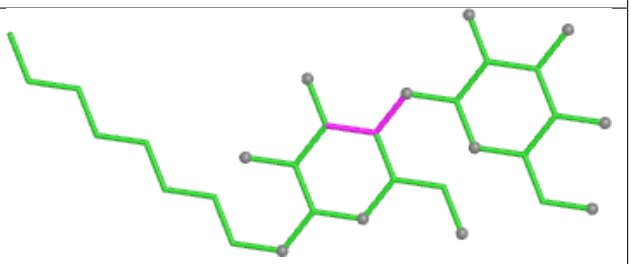


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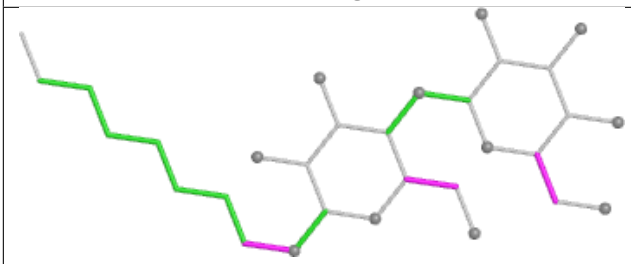
Ligand LMT 3 1018



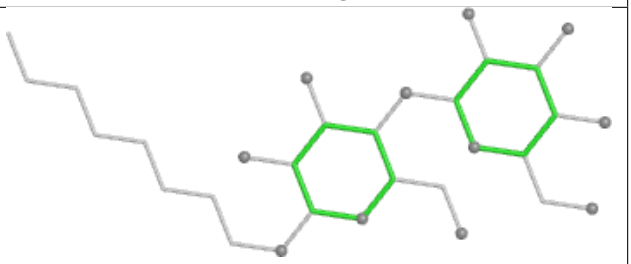
Bond lengths



Bond angles

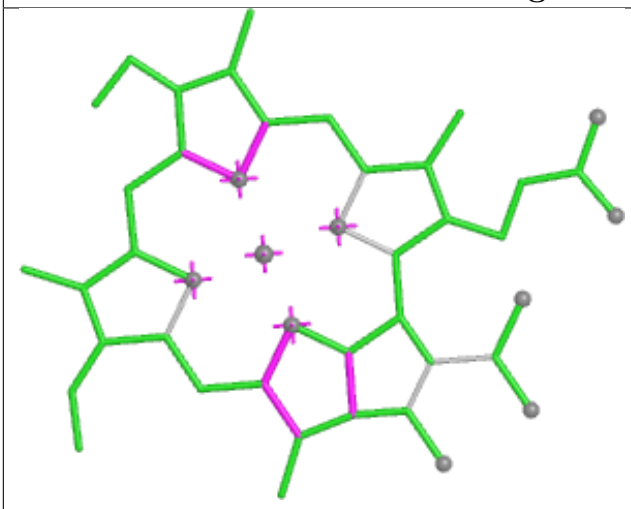


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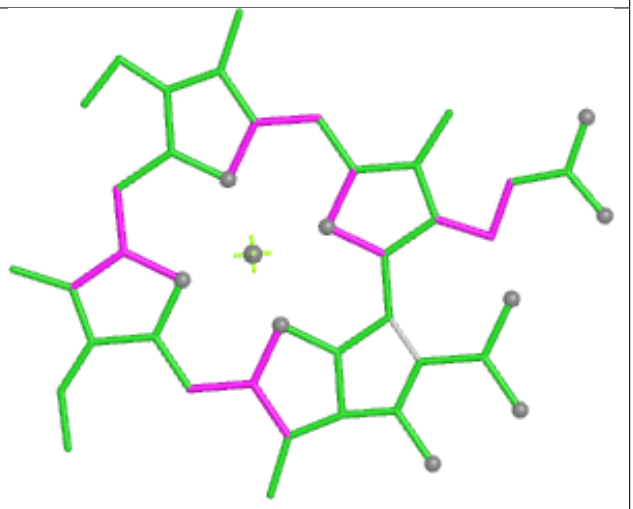


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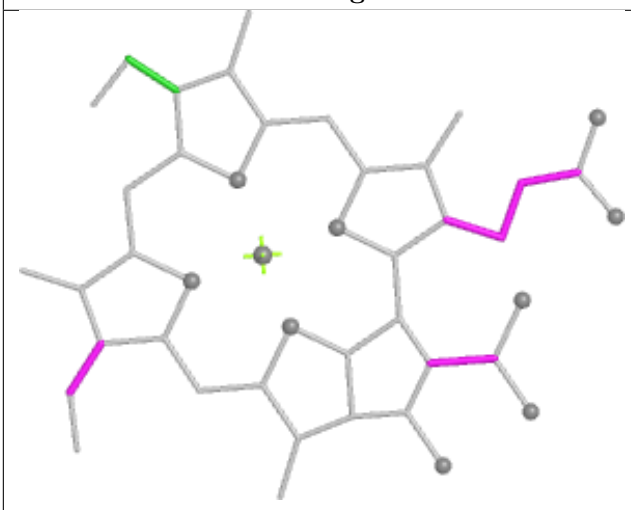
Ligand CLA 4 309



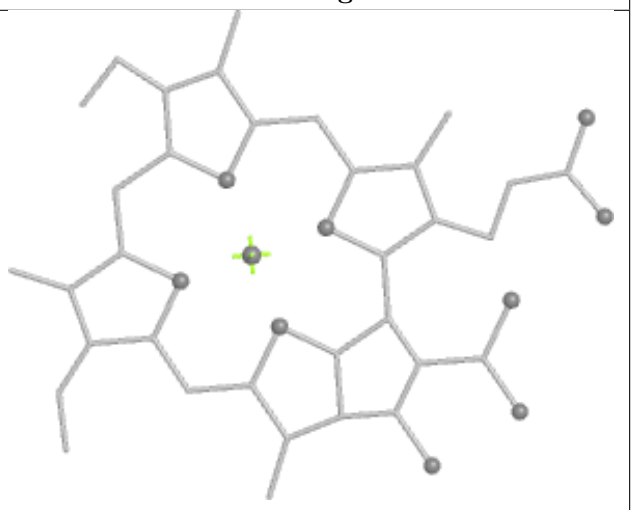
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Bond angles

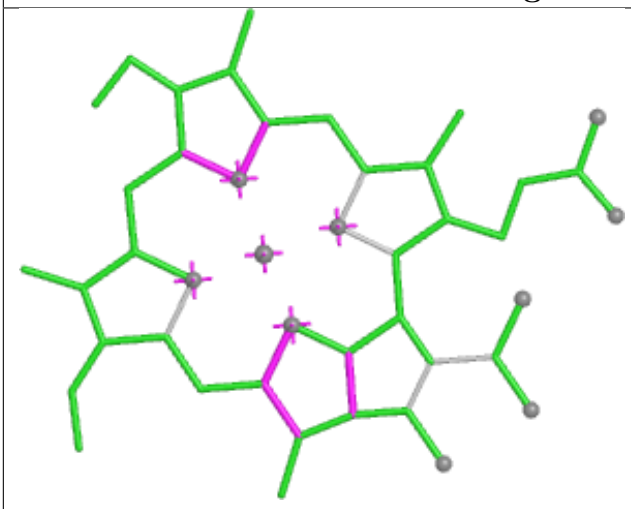


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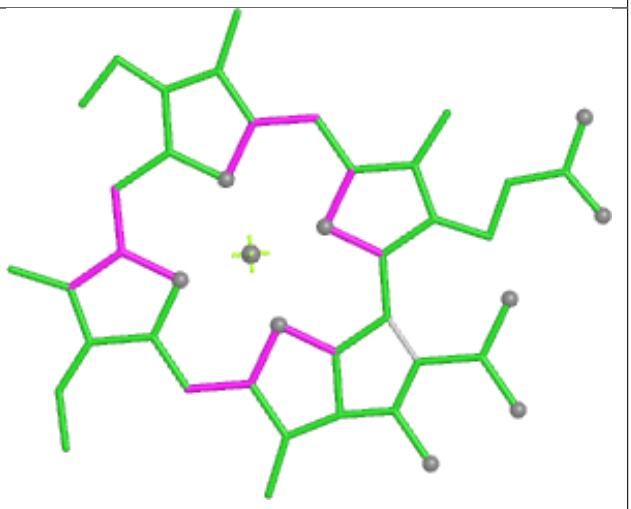


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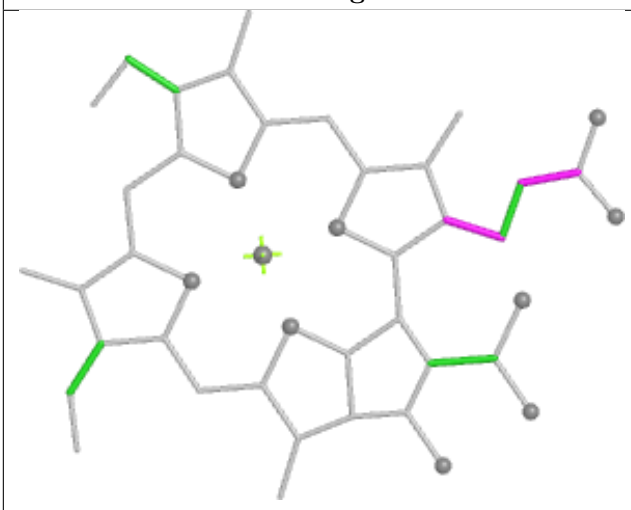
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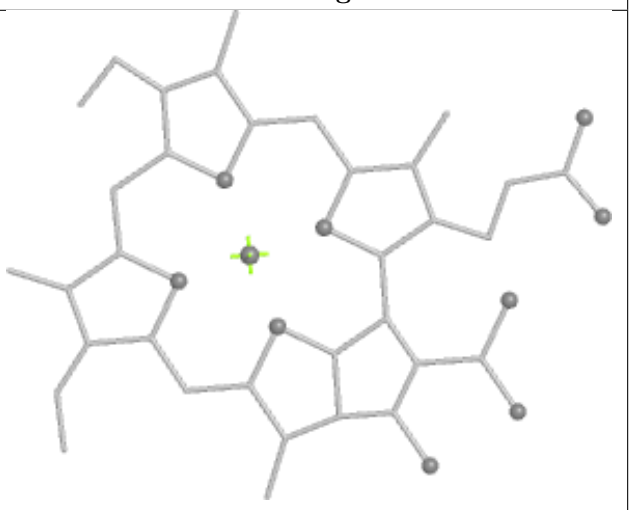
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Bond angles

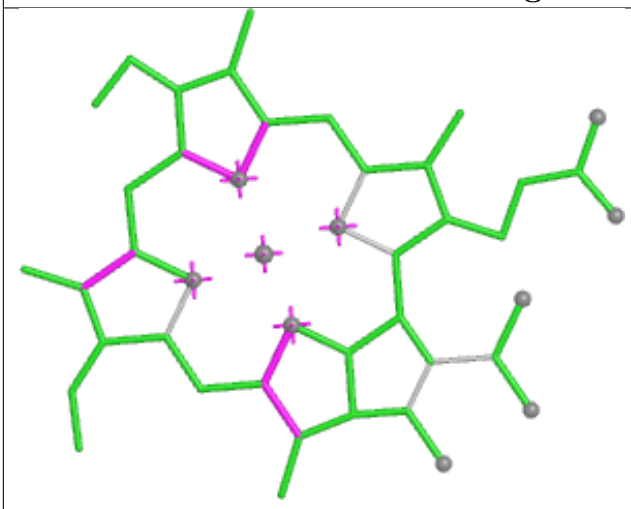


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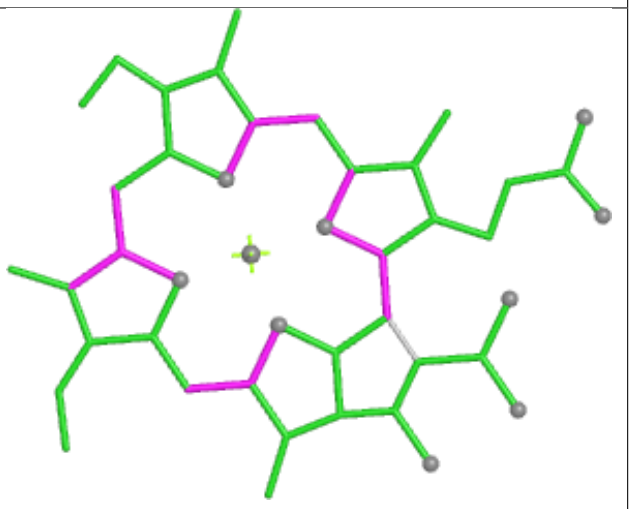


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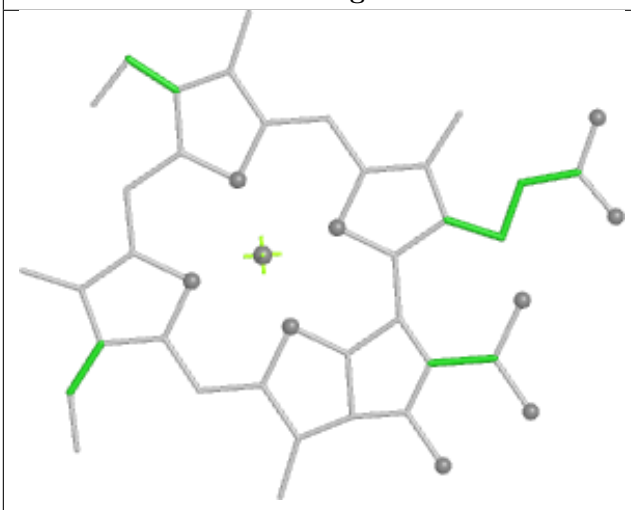
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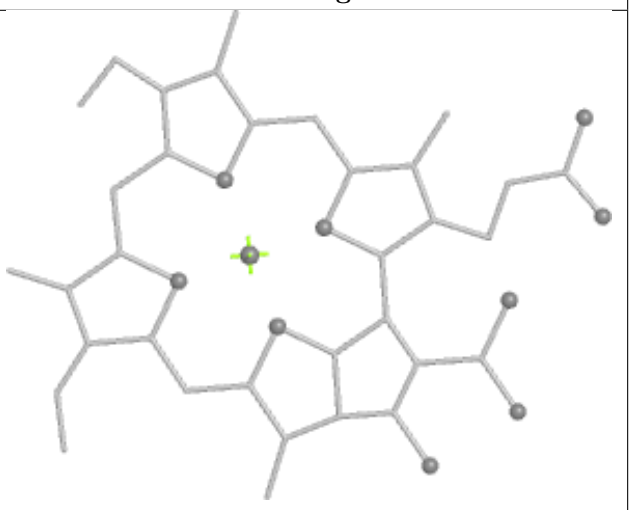
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Bond angles

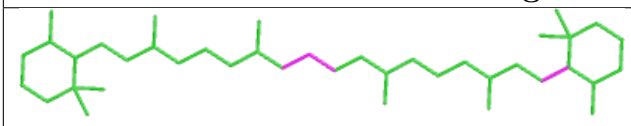


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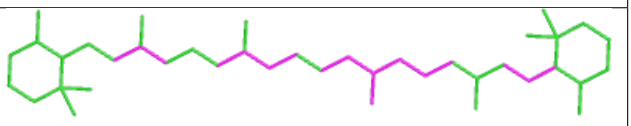


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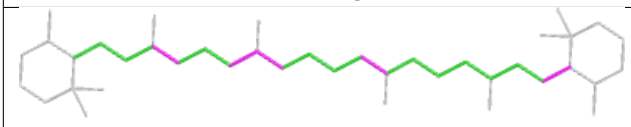
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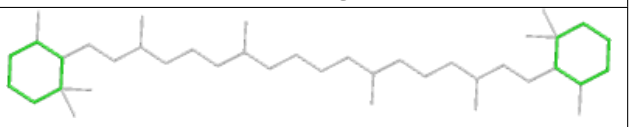
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Bond angles

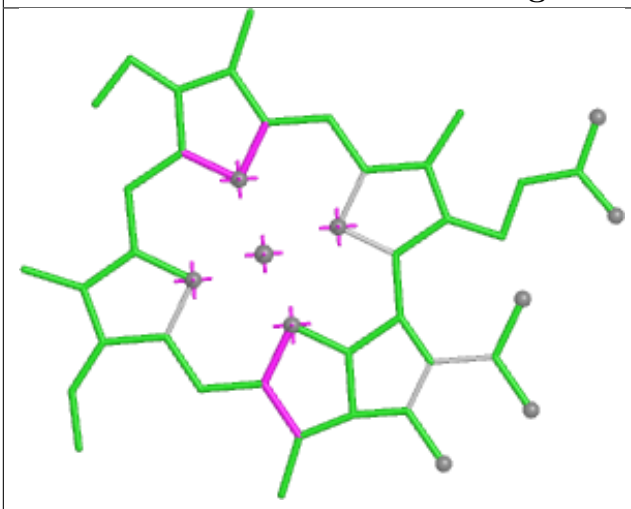


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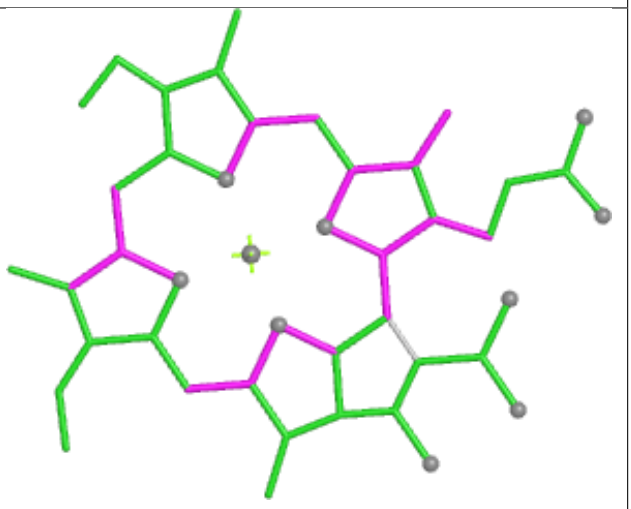


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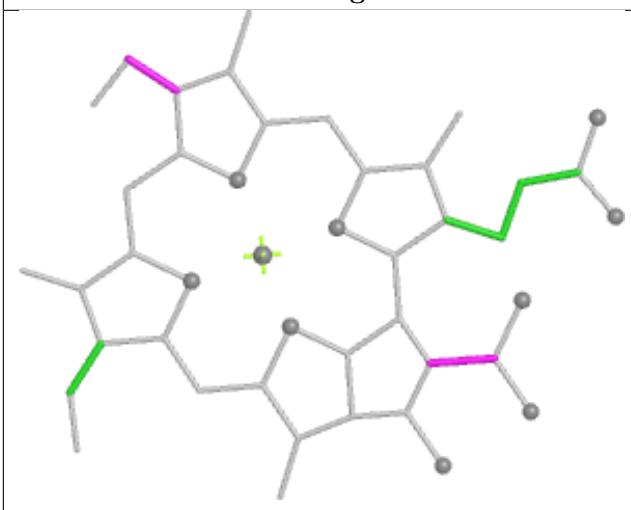
Ligand CLA 0 313



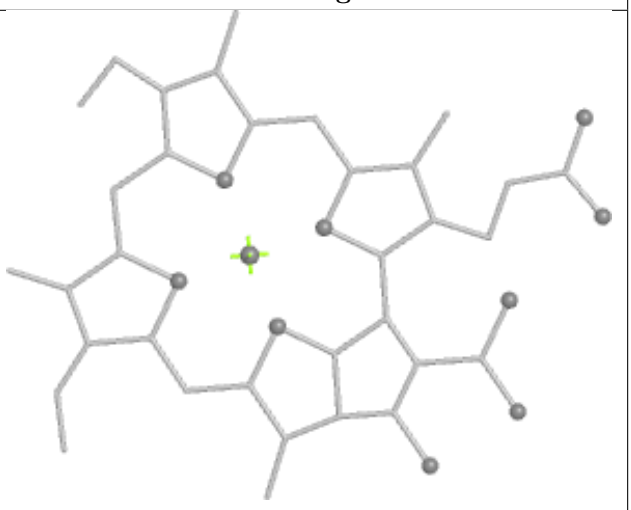
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Bond angles

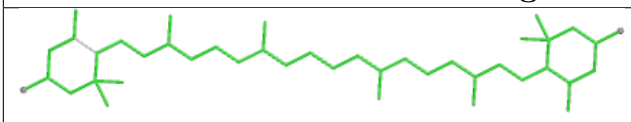


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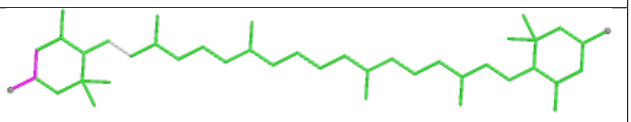


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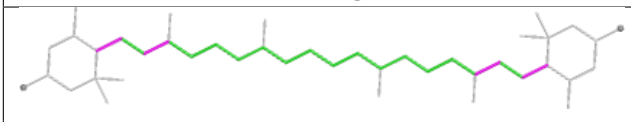
Ligand LUT 3 1002



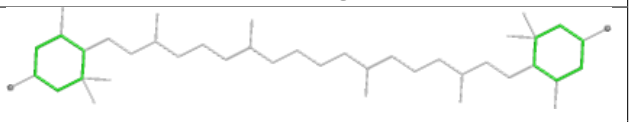
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Bond angles

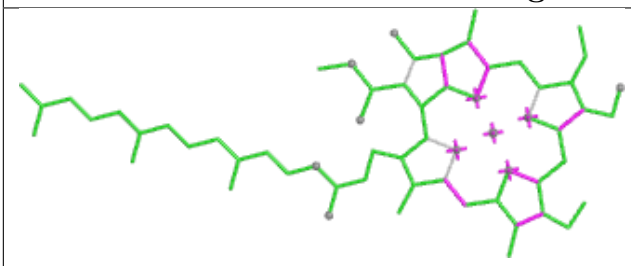


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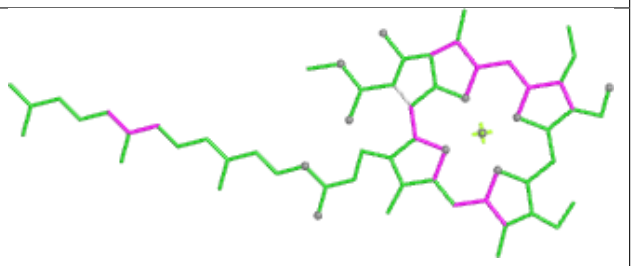


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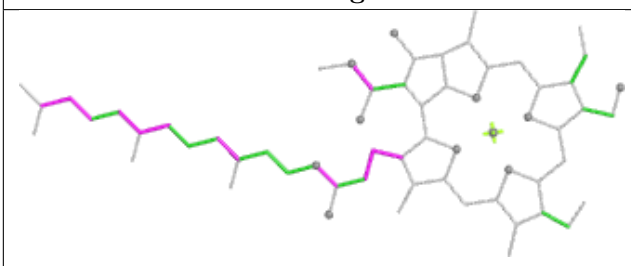
Ligand CHL 5 316



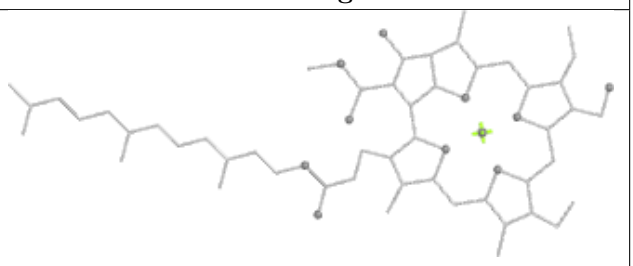
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Bond angles

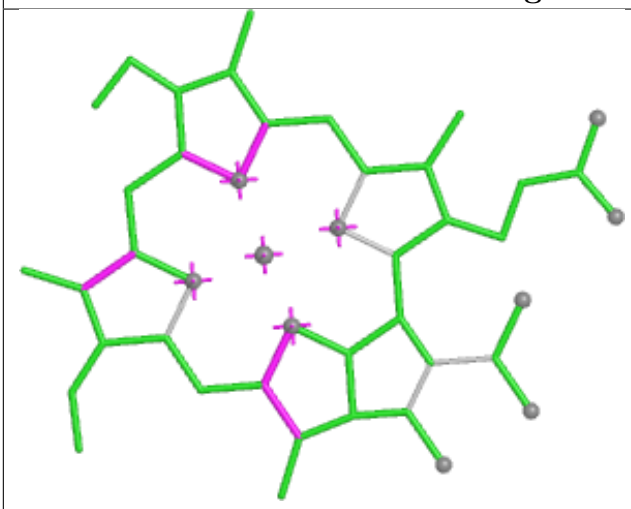


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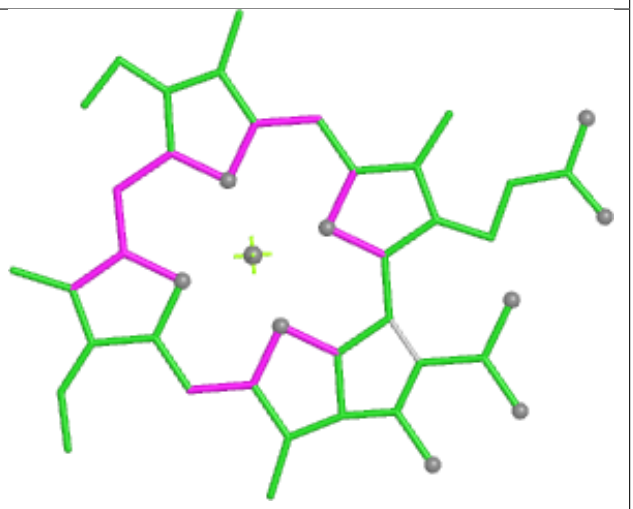


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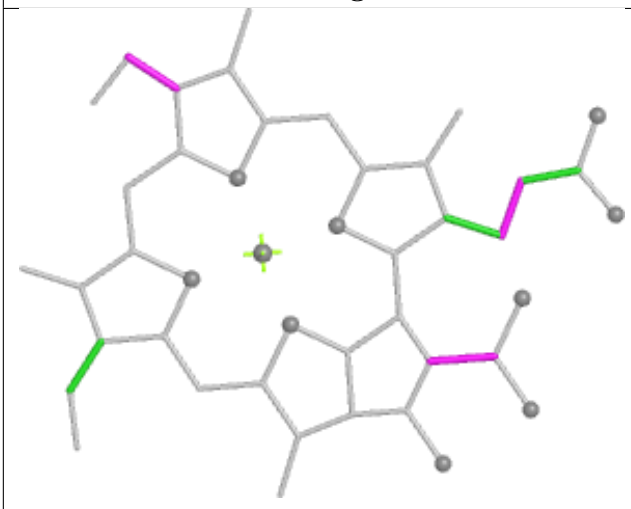
Ligand CLA B 823



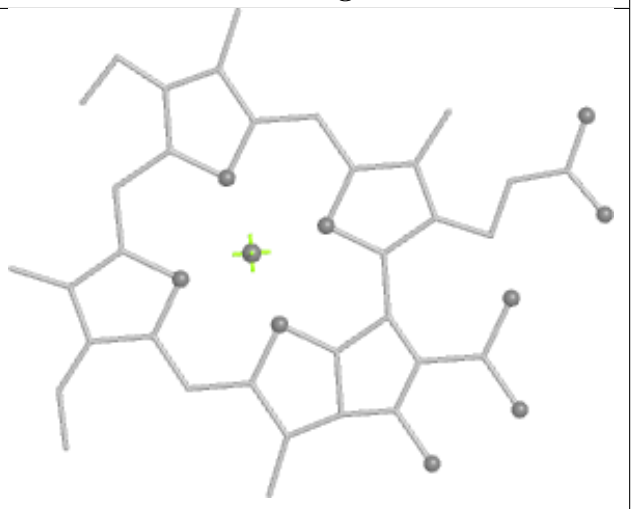
Bond lengths



Bond angles

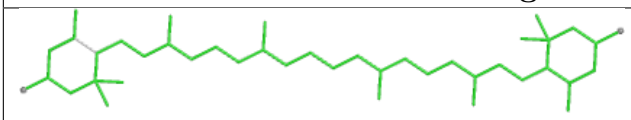


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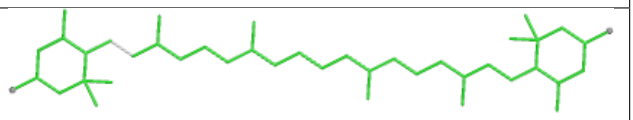


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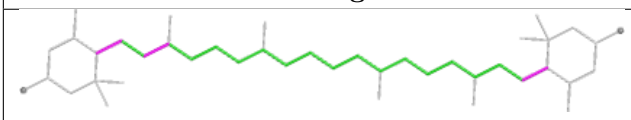
Ligand LUT 1 1002



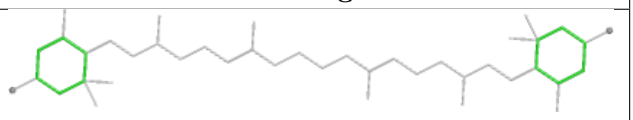
Bond lengths



Bond angles

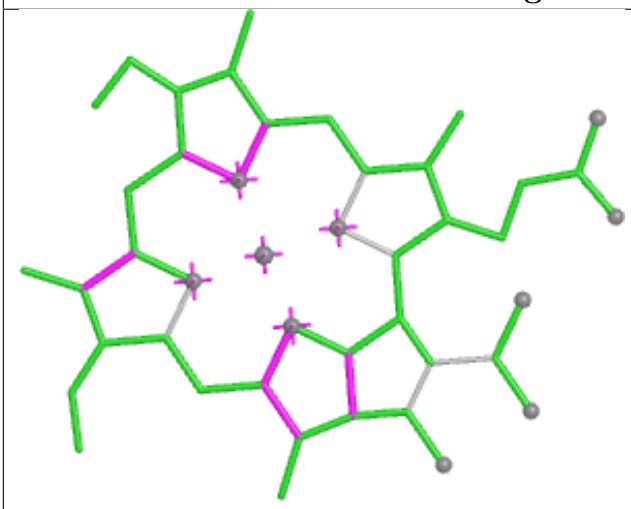


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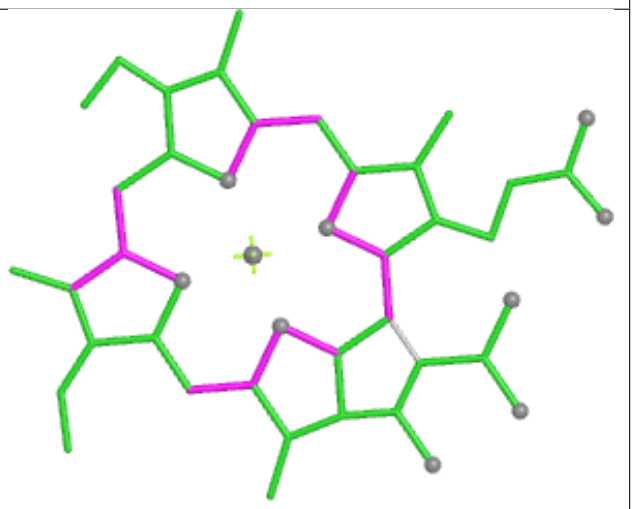


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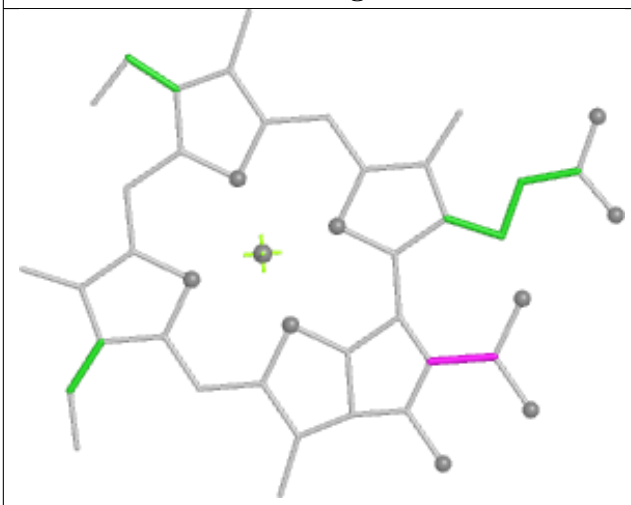
Ligand CLA B 832



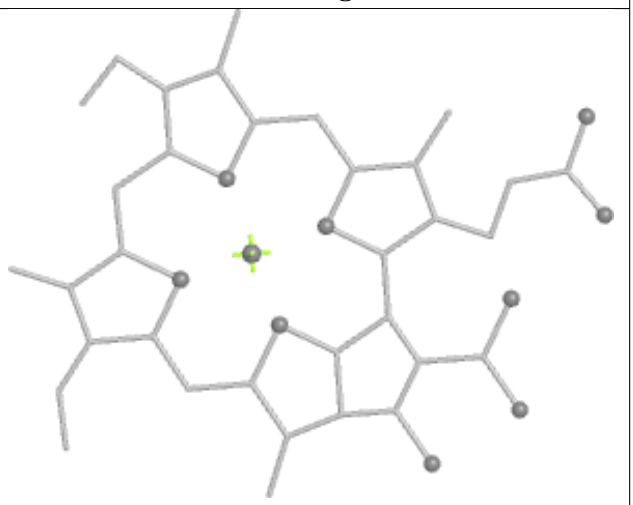
Bond lengths



Bond angles

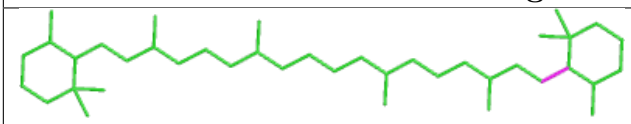


Torsions

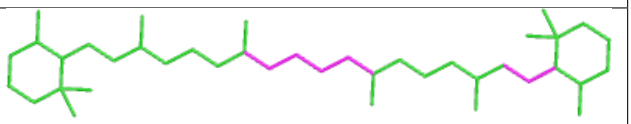


Rings

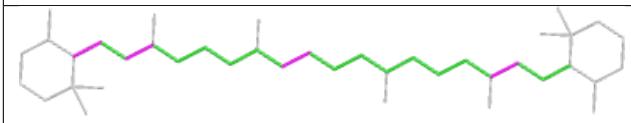
Ligand BCR 4 302



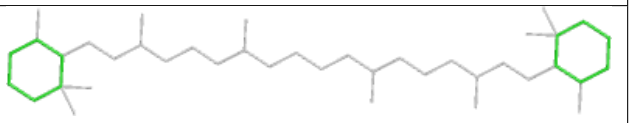
Bond lengths



Bond angles

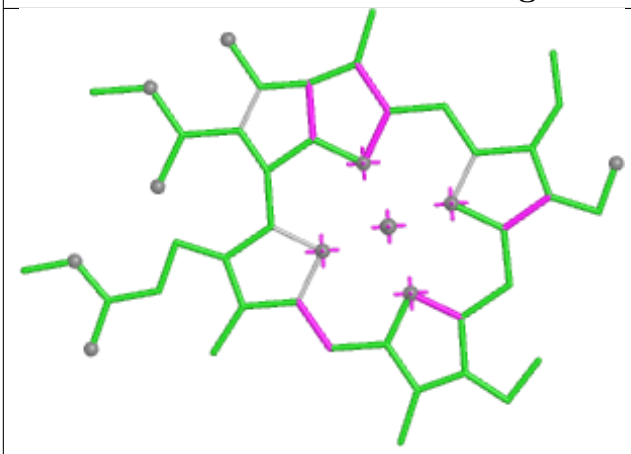


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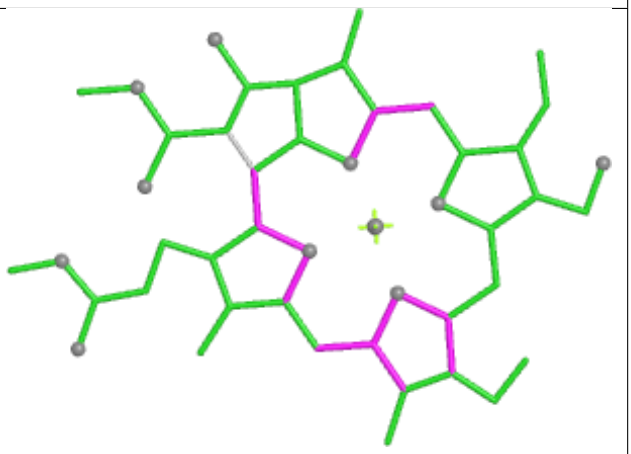


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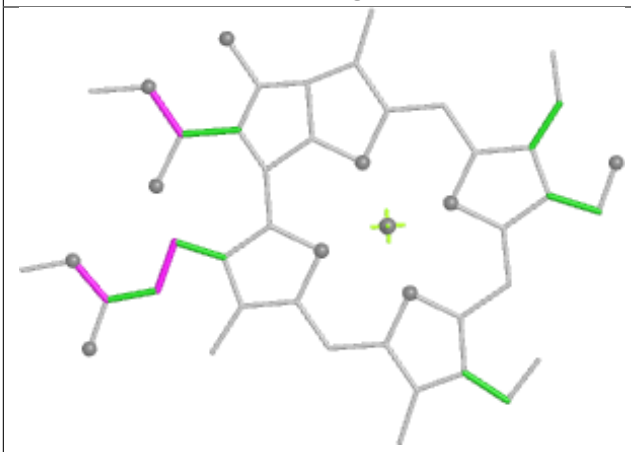
Ligand CHL 1 1012



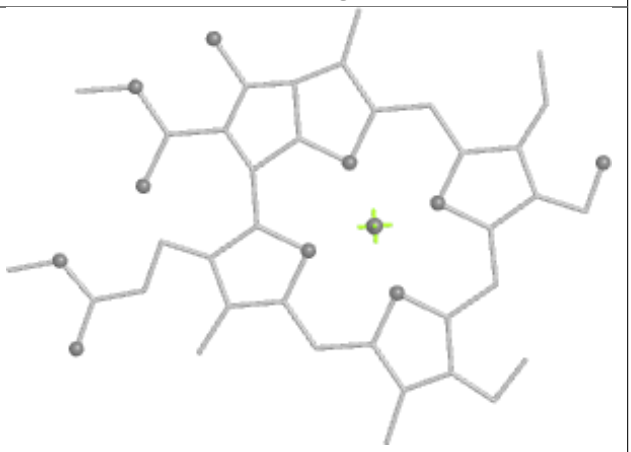
Bond lengths



Bond angles

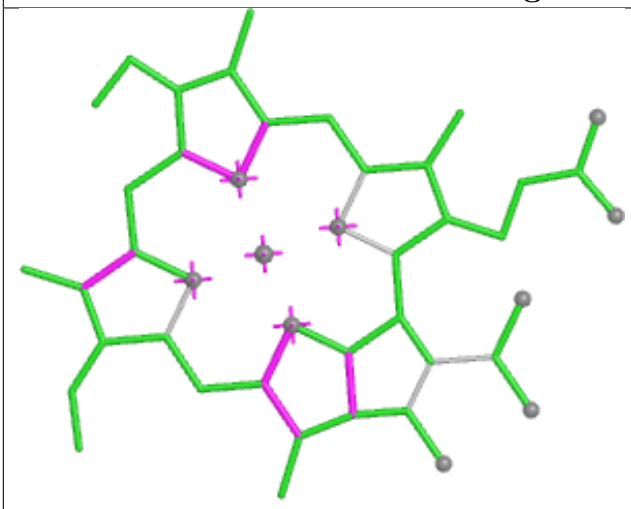


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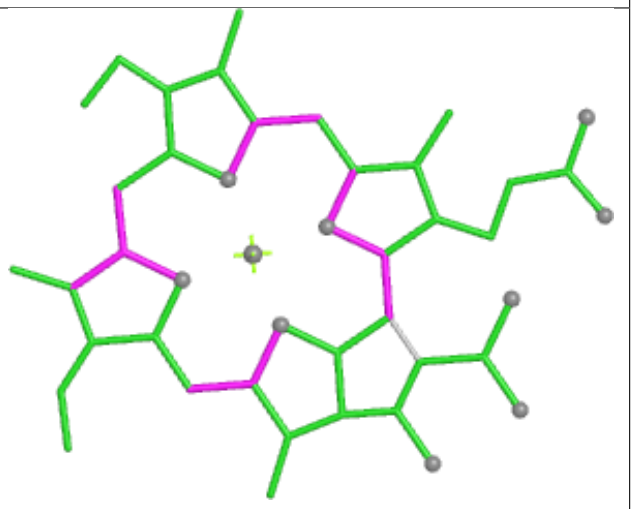


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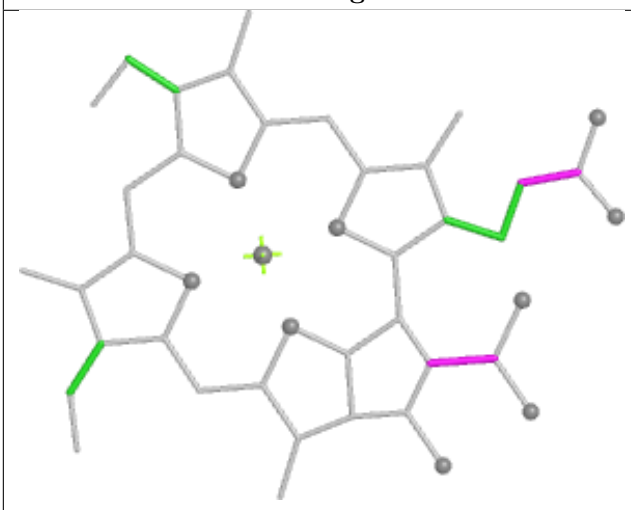
Ligand CLA A 837



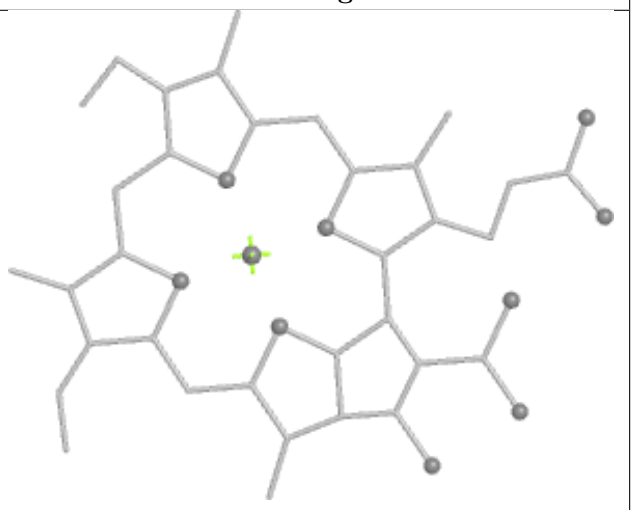
Bond lengths



Bond angles

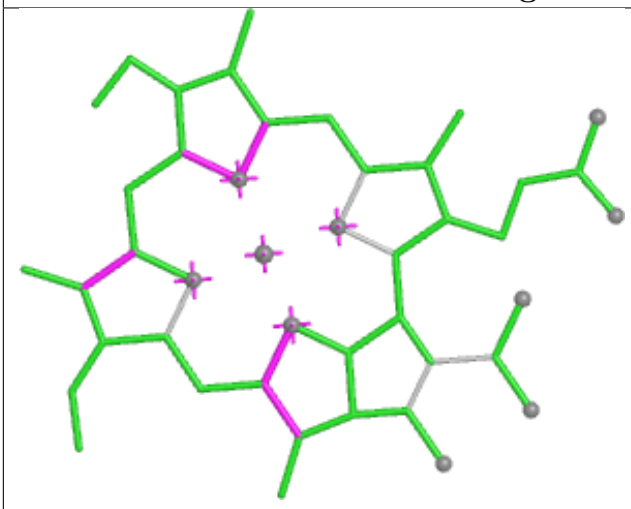


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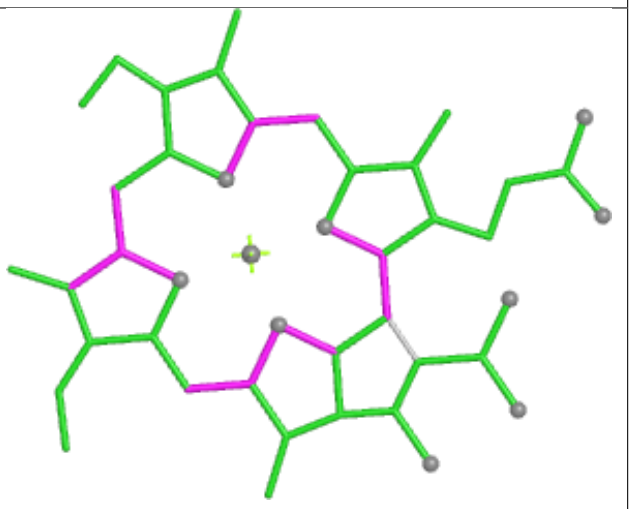


Rings

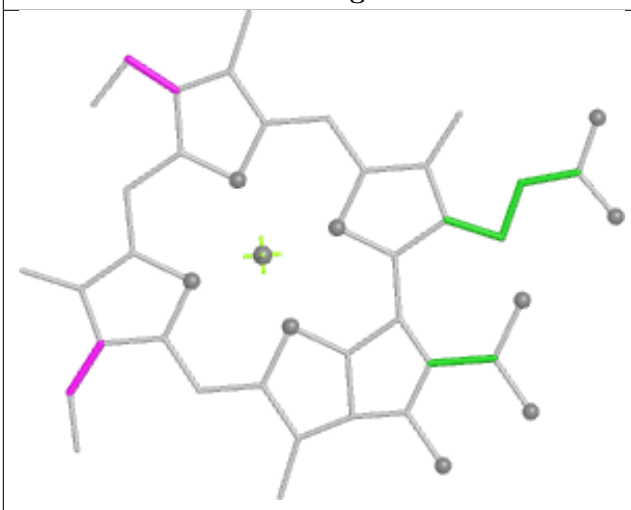
Ligand CLA 1 1009



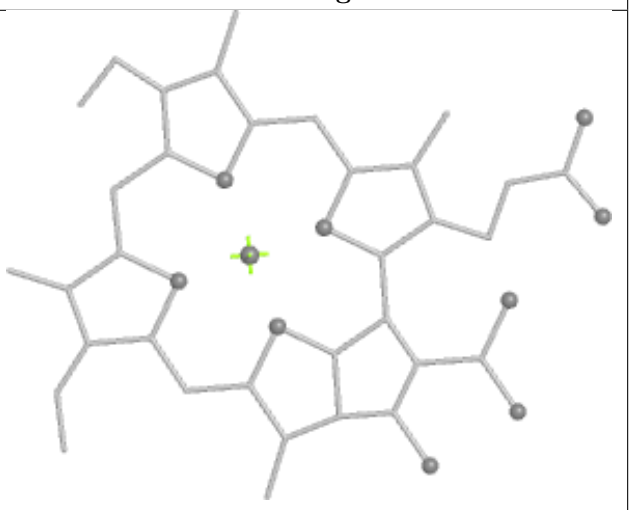
Bond lengths



Bond angles

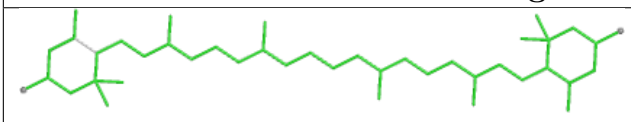


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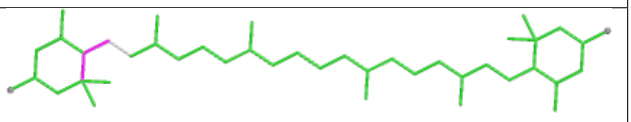


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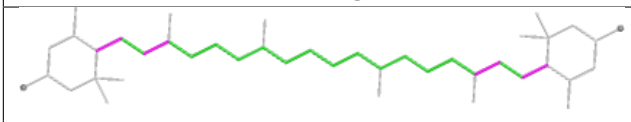
Ligand LUT 0 304



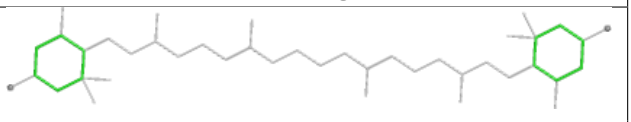
Bond lengths



Bond angles

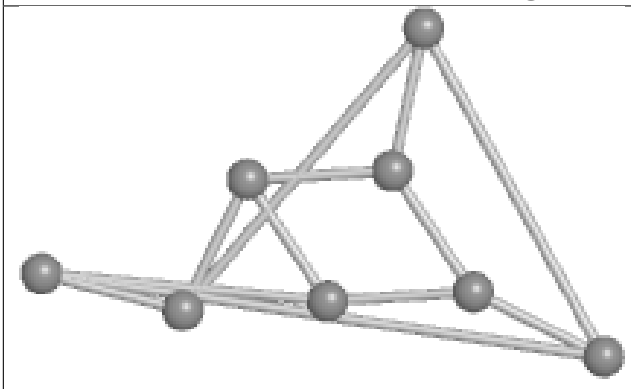


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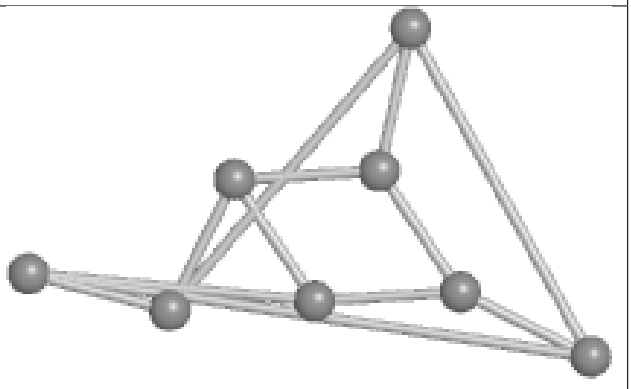


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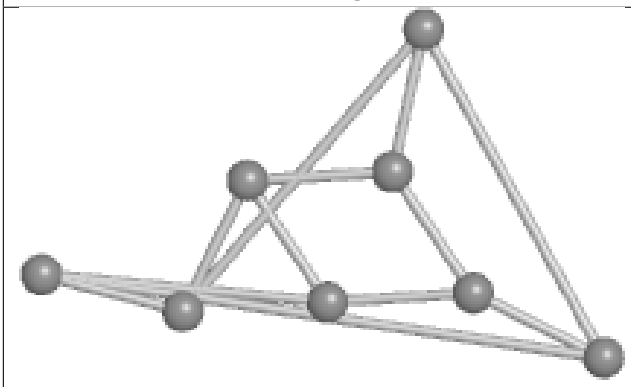
Ligand SF4 C 1002



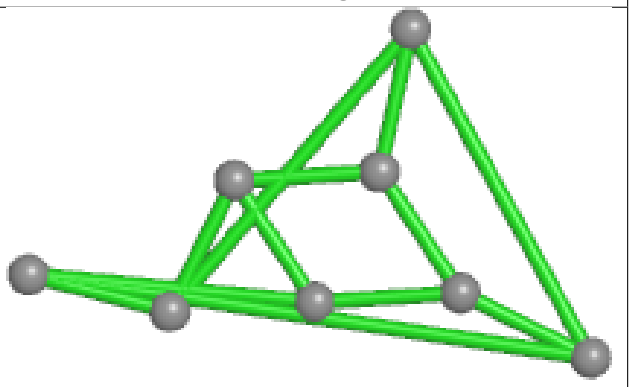
Bond lengths



Bond angles

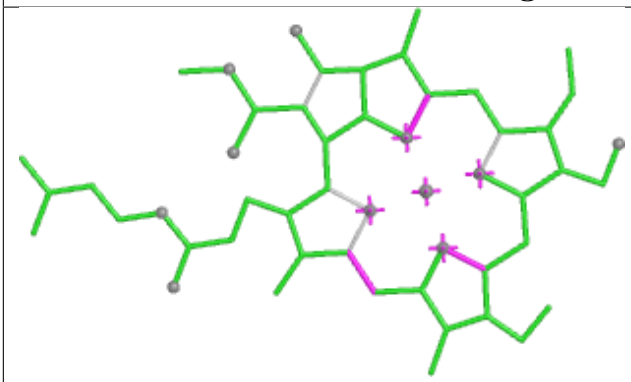


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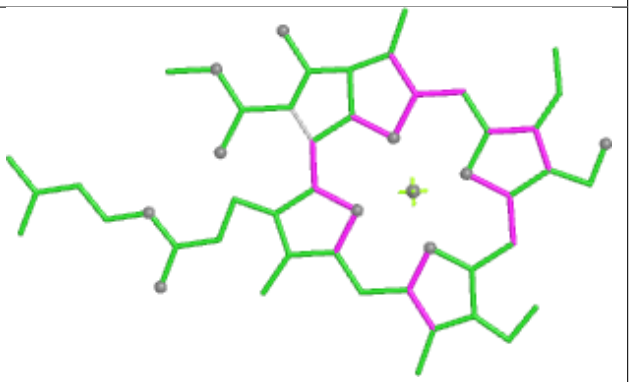


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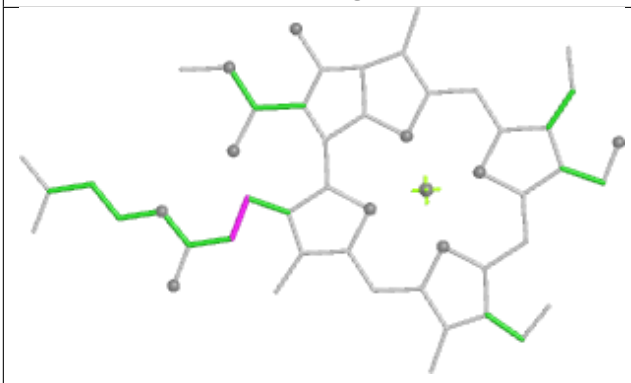
Ligand CHL 1 1013



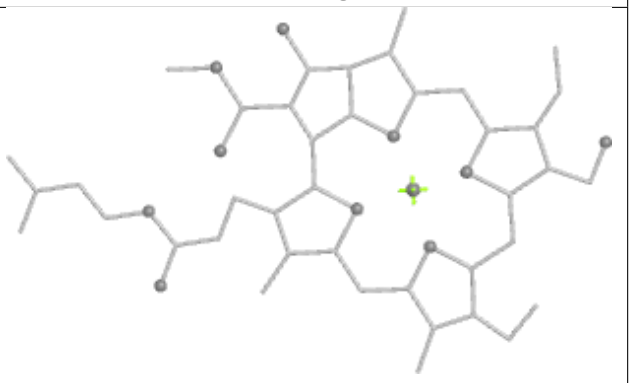
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Bond angles

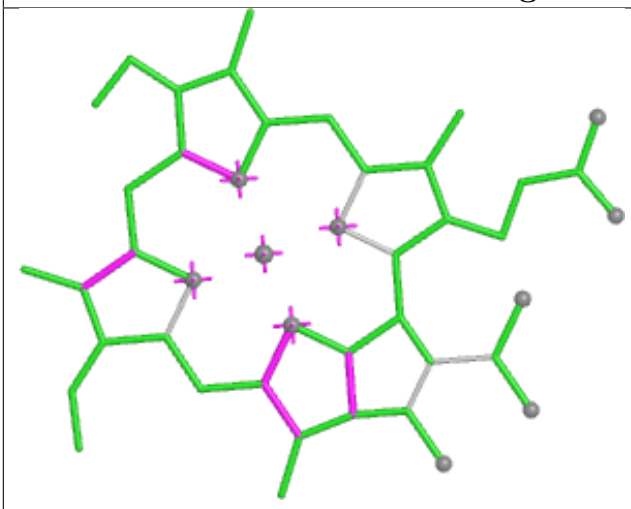


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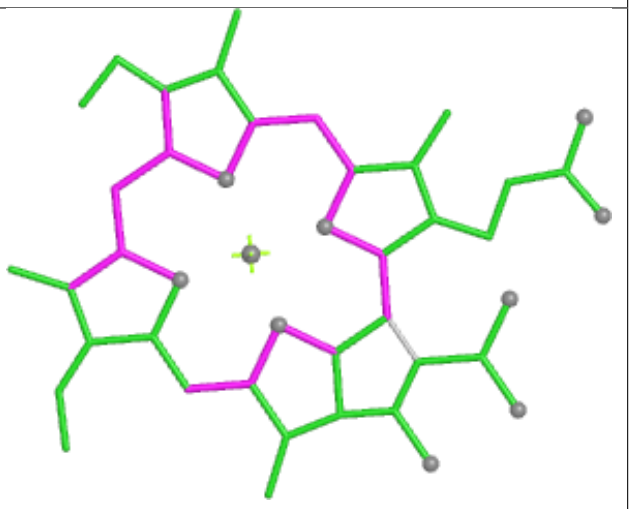


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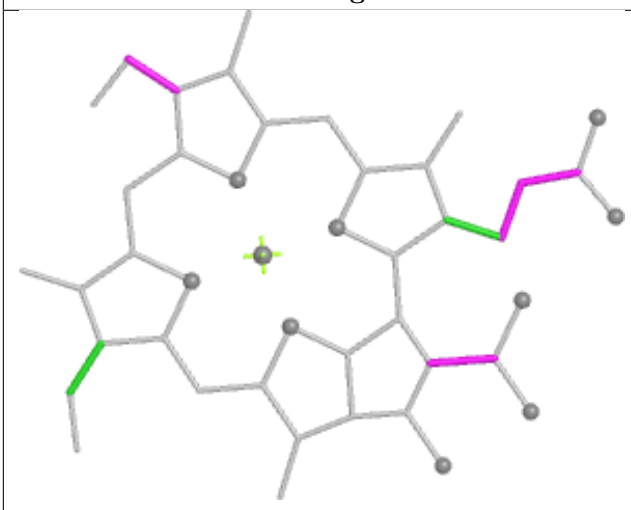
Ligand CLA 7 1011



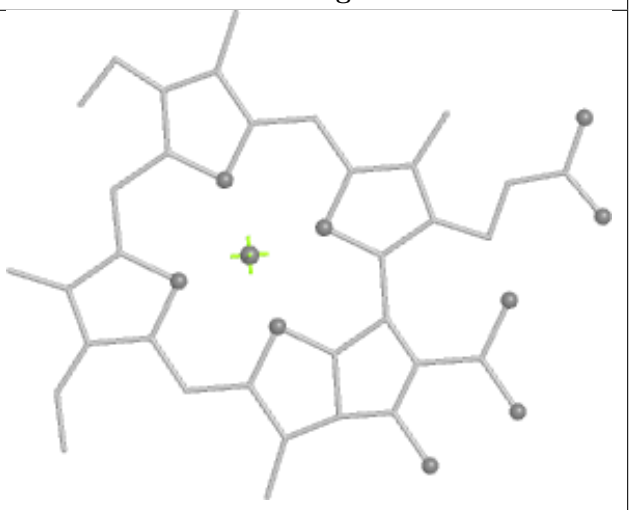
Bond lengths



Bond angles

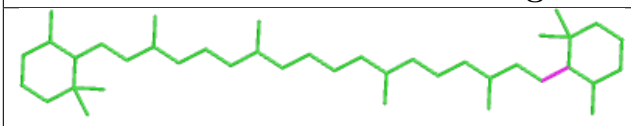


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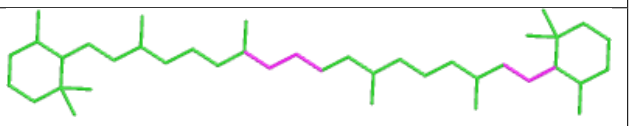


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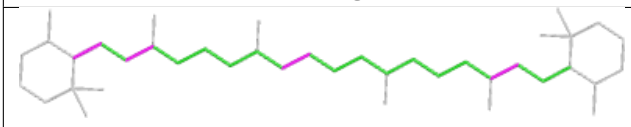
Ligand BCR 6 302



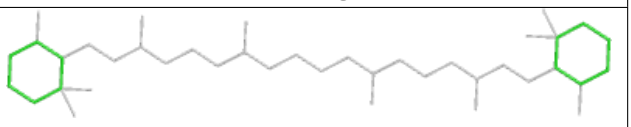
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Bond angles

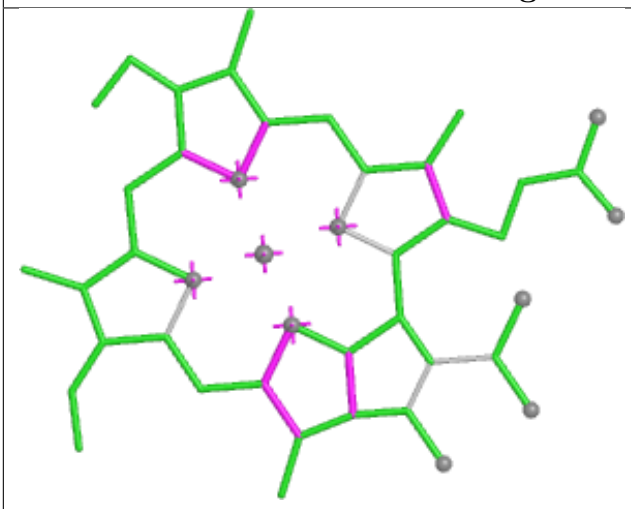


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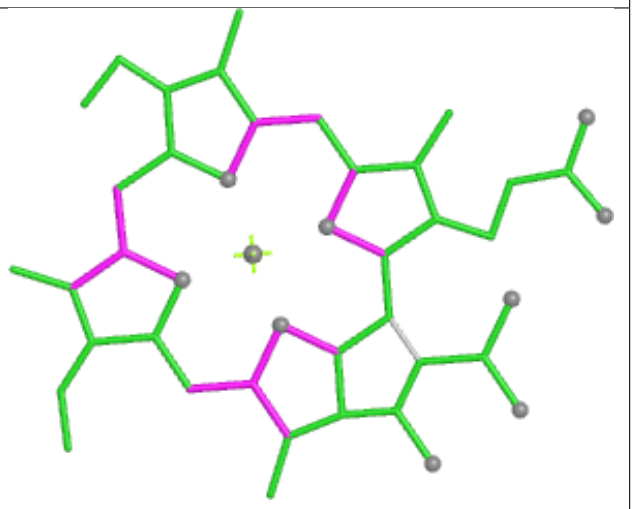


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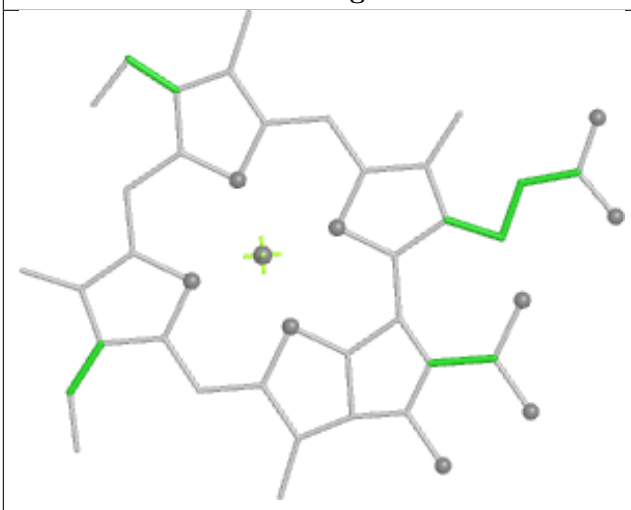
Ligand CLA 7 1014



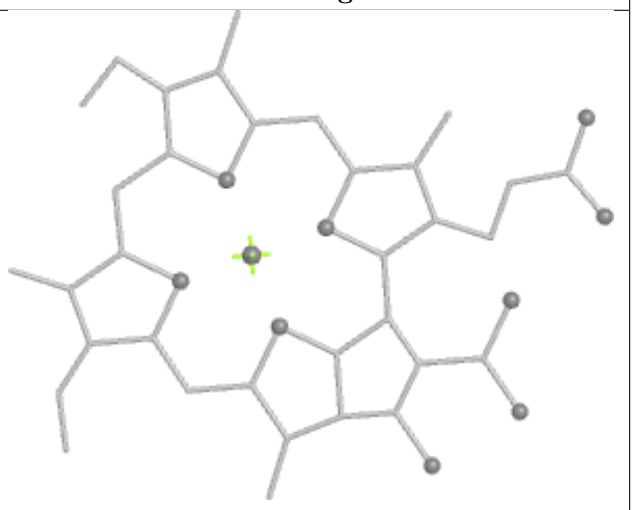
Bond lengths



Bond angles

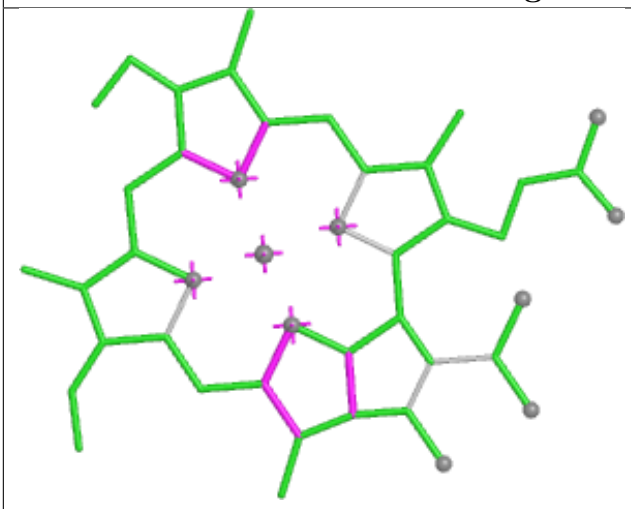


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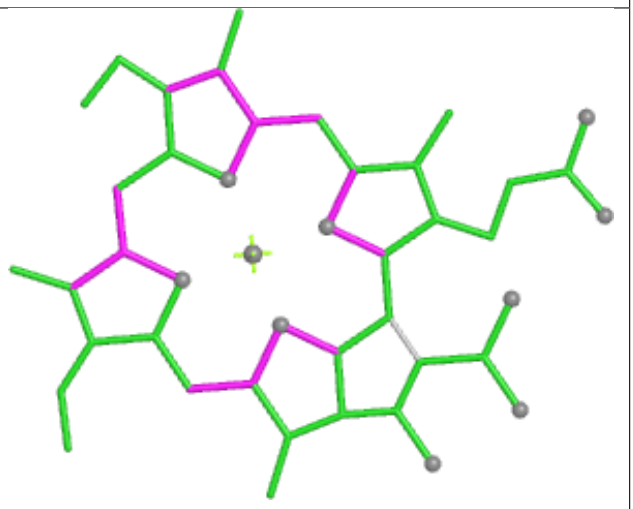


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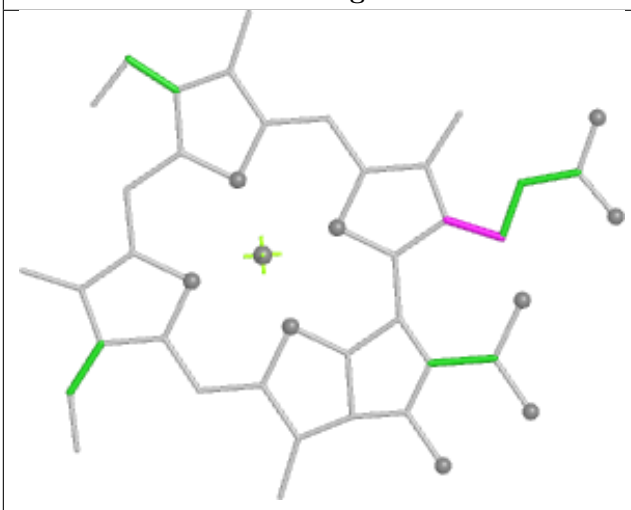
Ligand CLA B 831



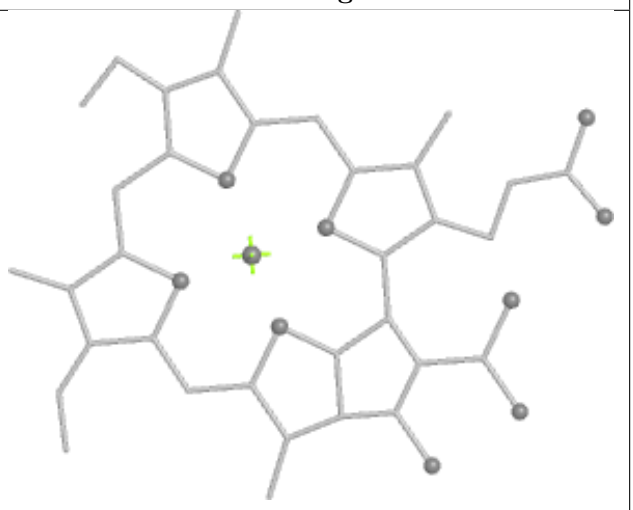
Bond lengths



Bond angles

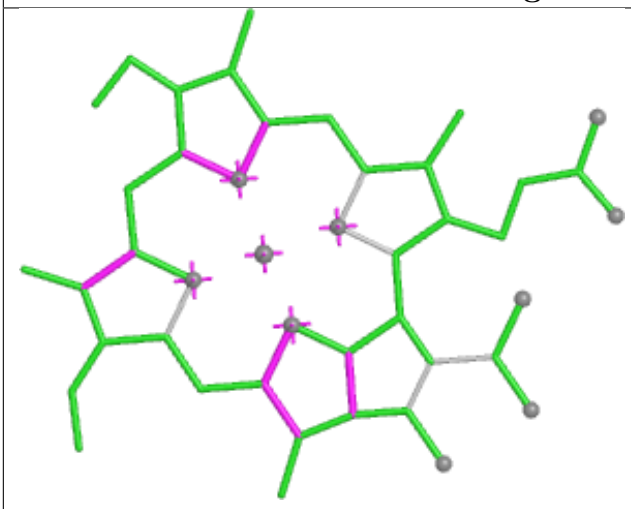


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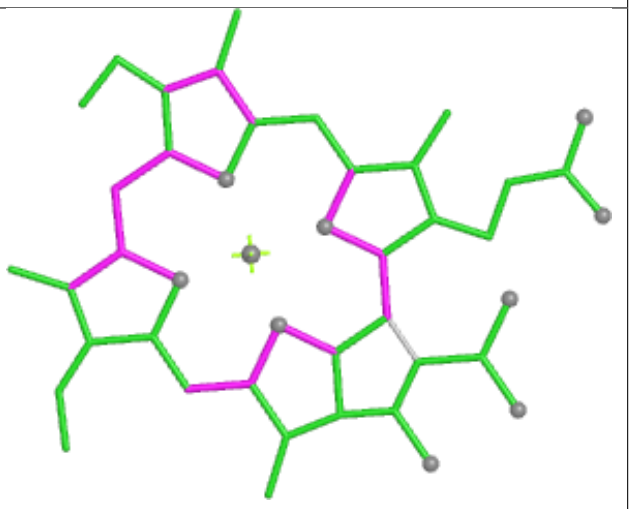


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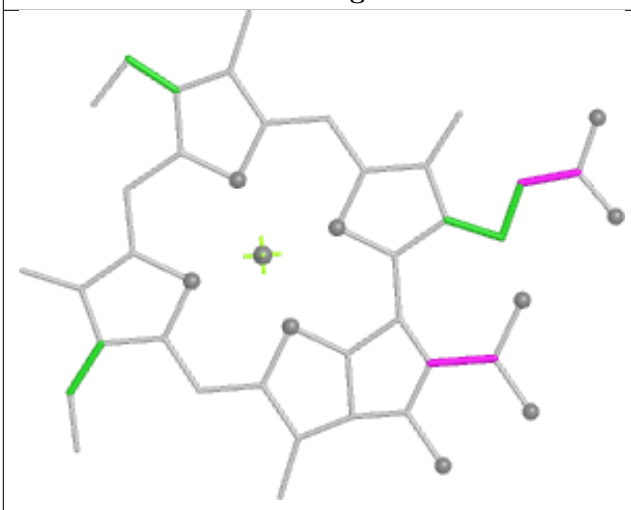
Ligand CLA A 829



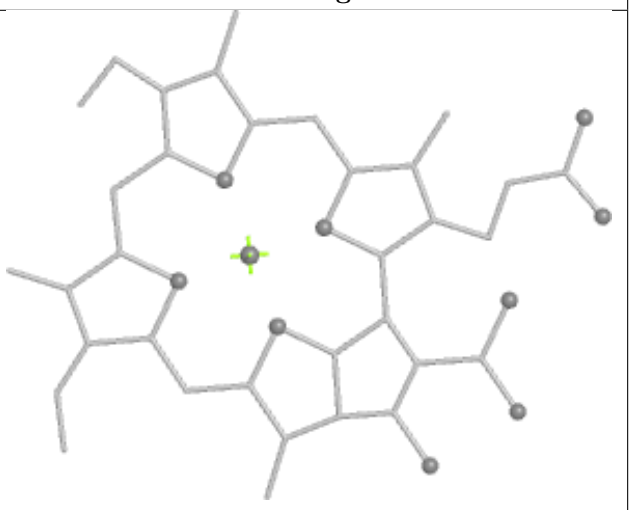
Bond lengths



Bond angles

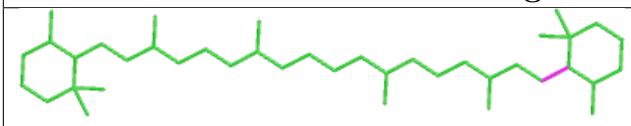


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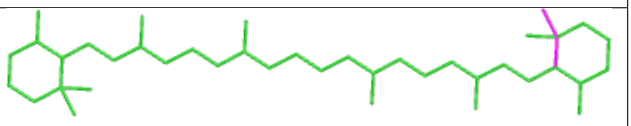


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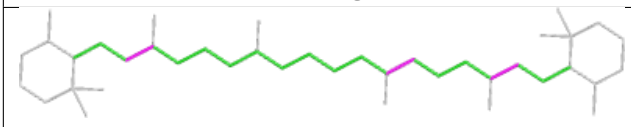
Ligand BCR F 301



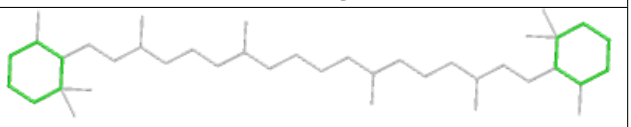
Bond lengths



Bond angles

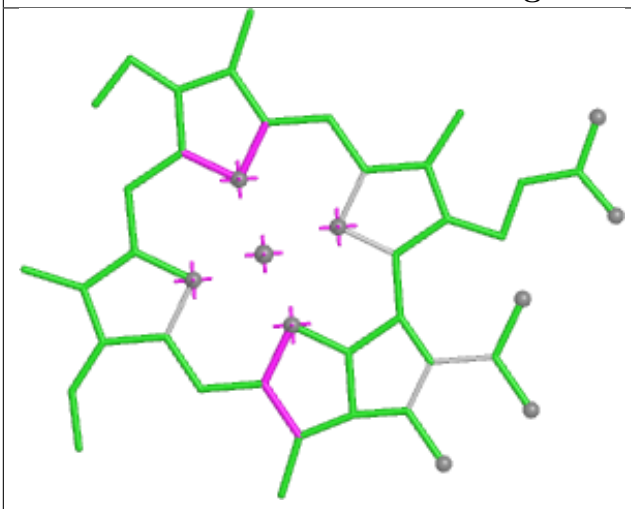


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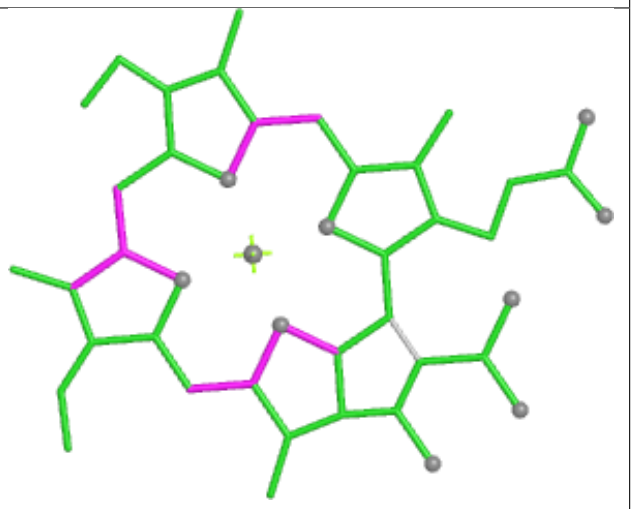


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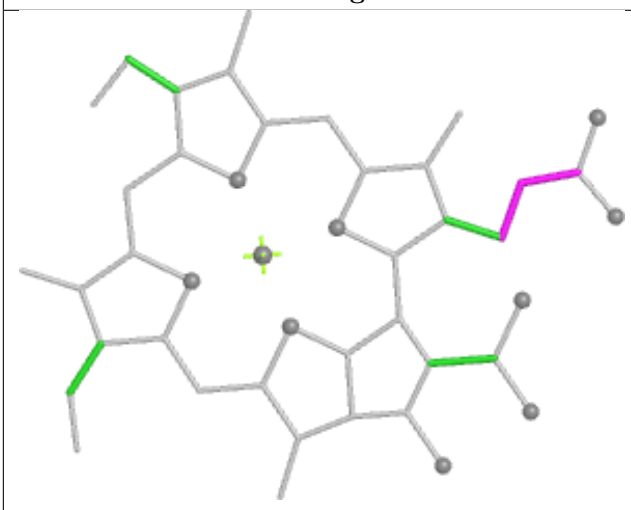
Ligand CLA A 840



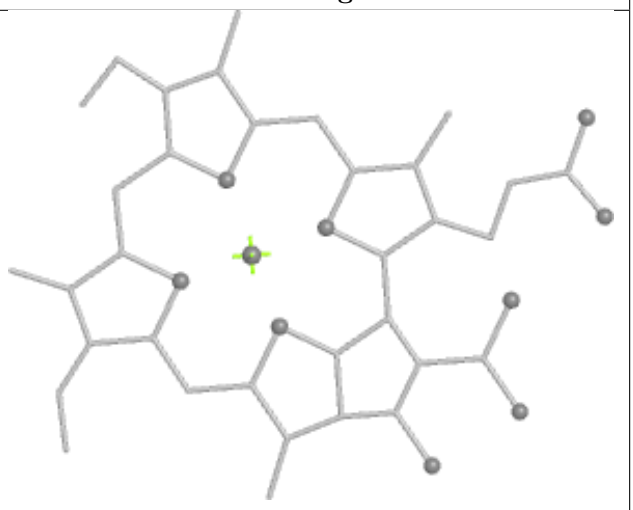
Bond lengths



Bond angles

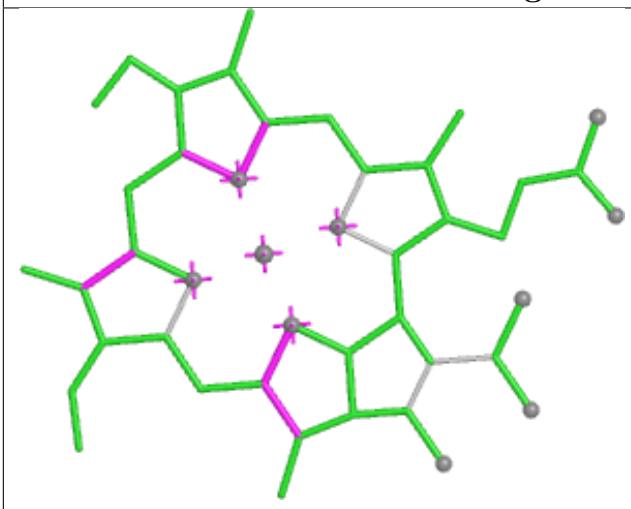


Torsions

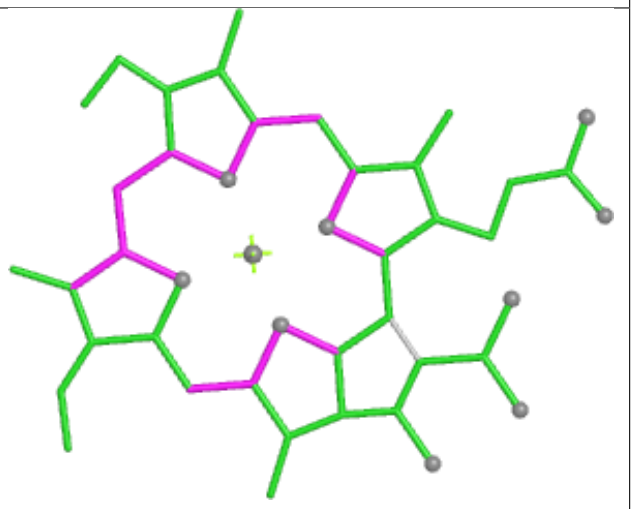


Rings

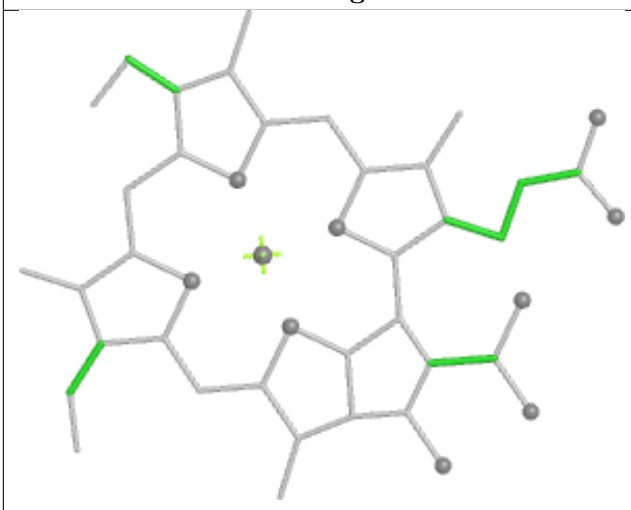
Ligand CLA B 811



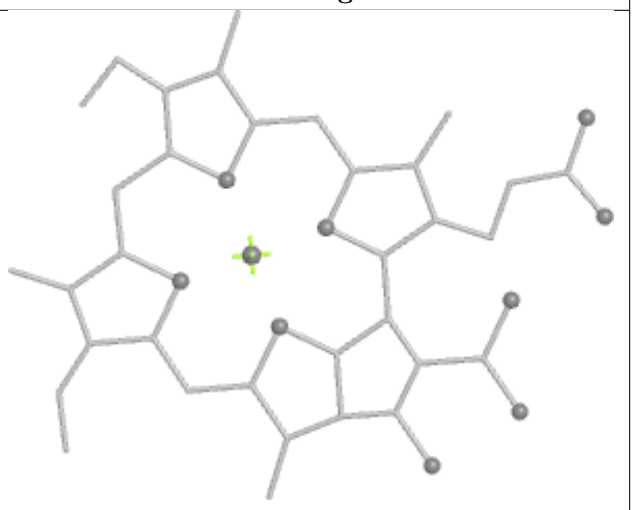
Bond lengths



Bond angles

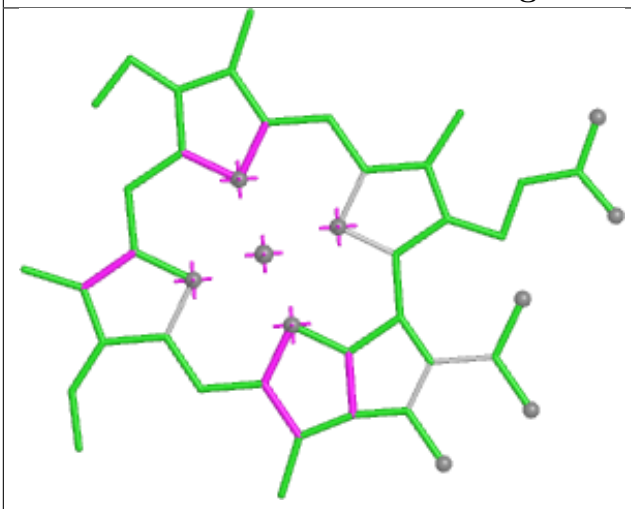


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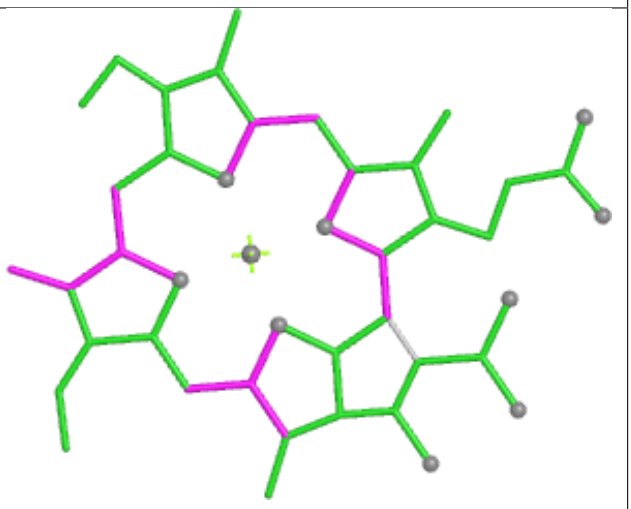


Rings

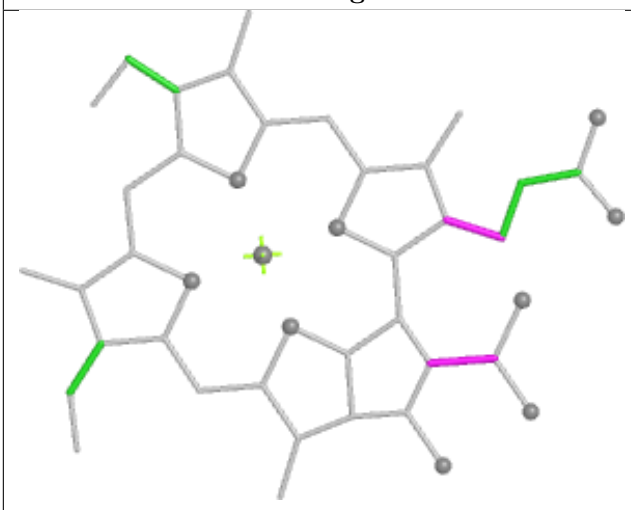
Ligand CLA 7 1007



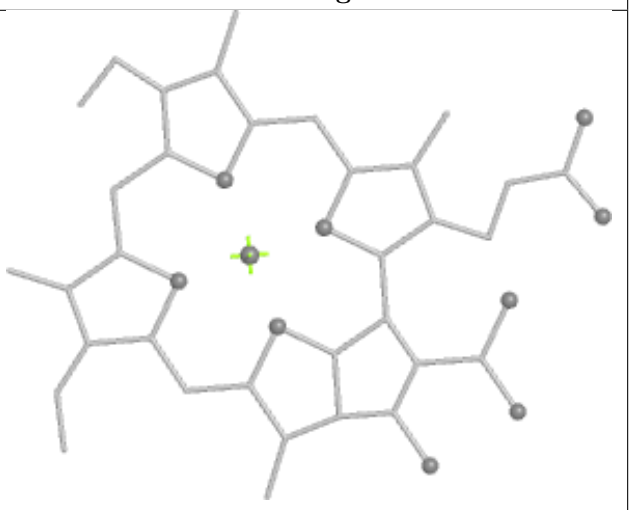
Bond lengths



Bond angles

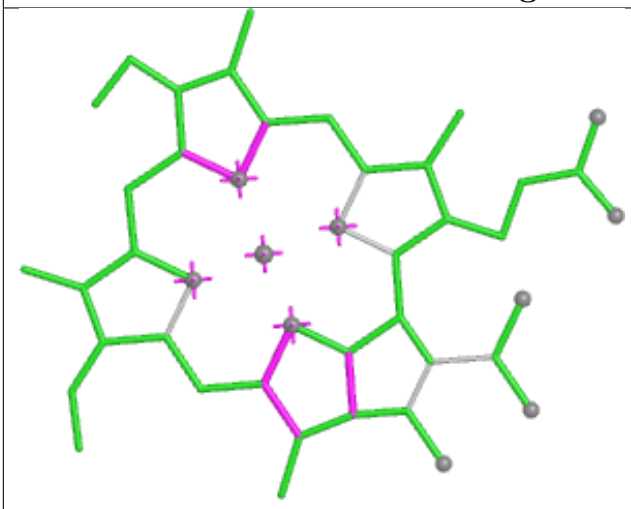


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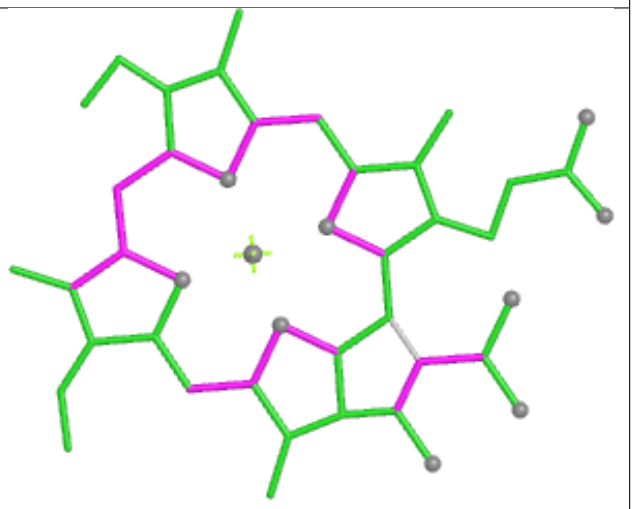


Rings

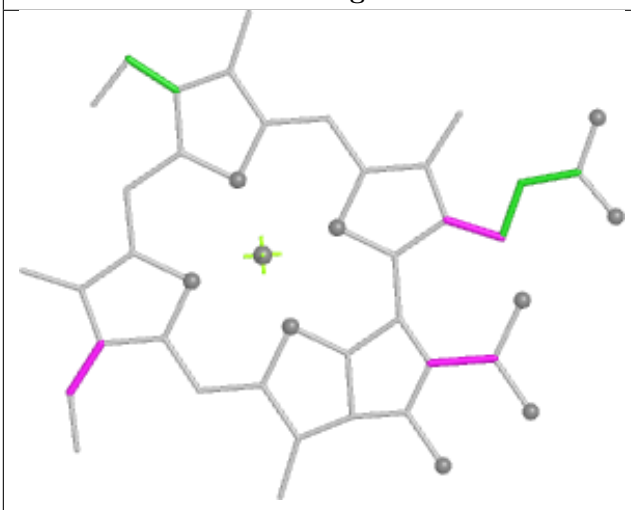
Ligand CLA 1 1007



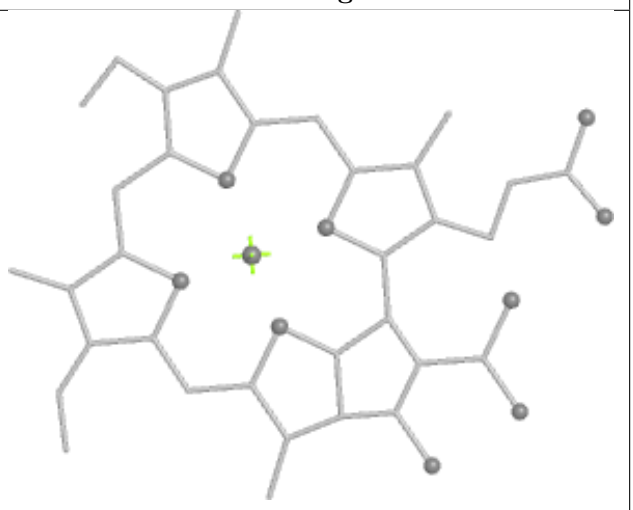
Bond lengths



Bond angles

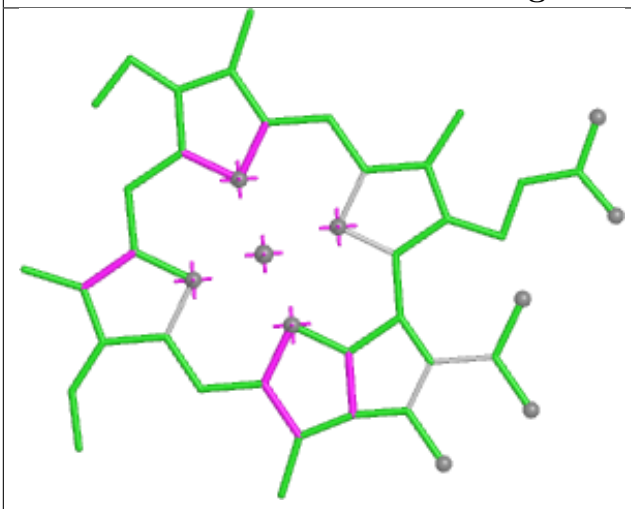


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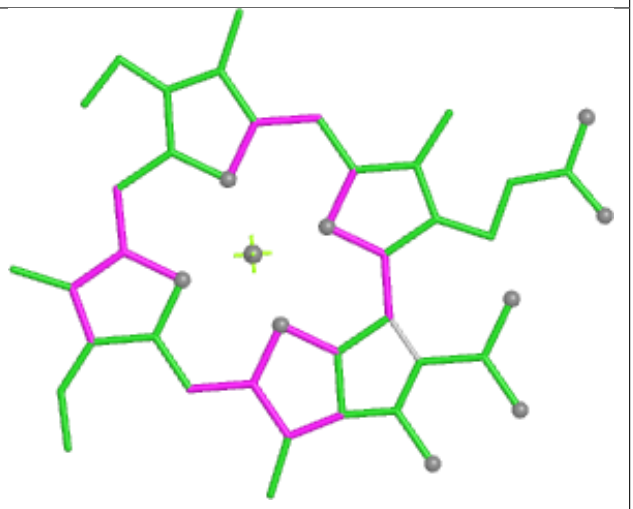


Rings

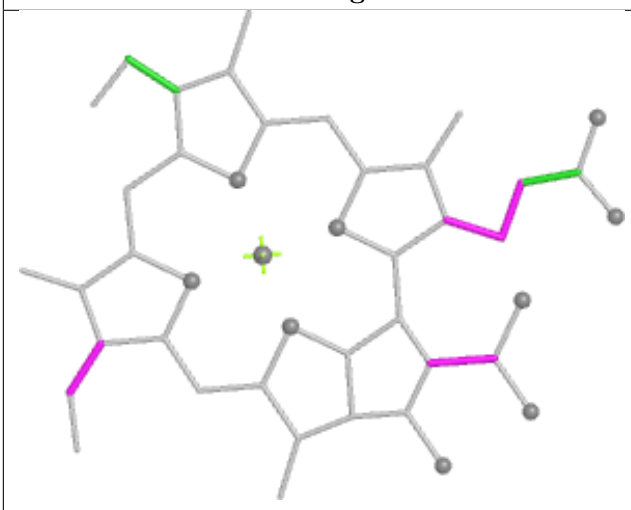
Ligand CLA 8 309



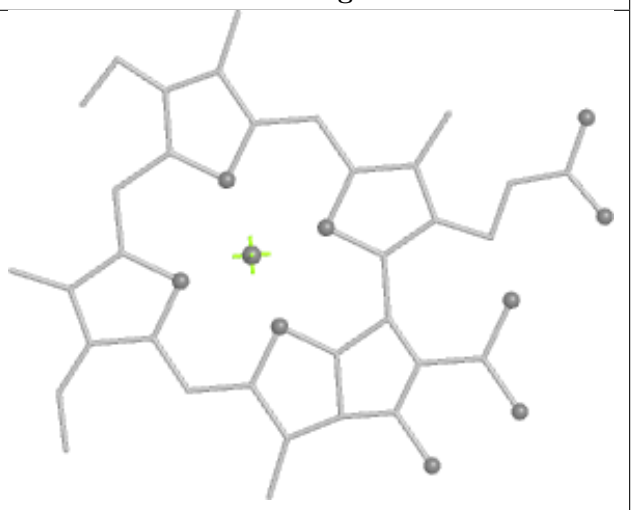
Bond lengths



Bond angles

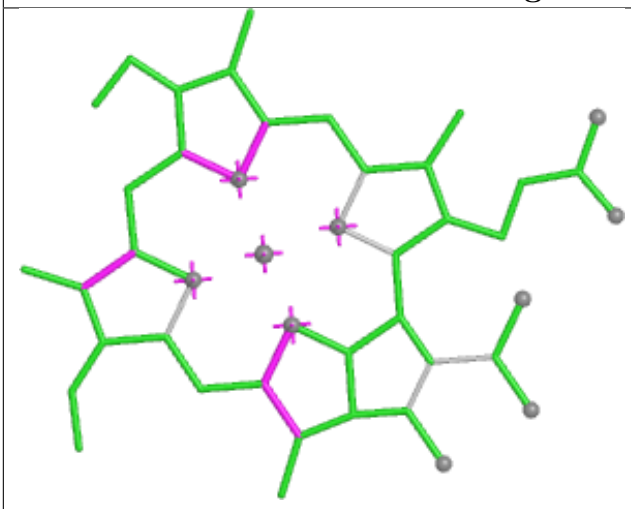


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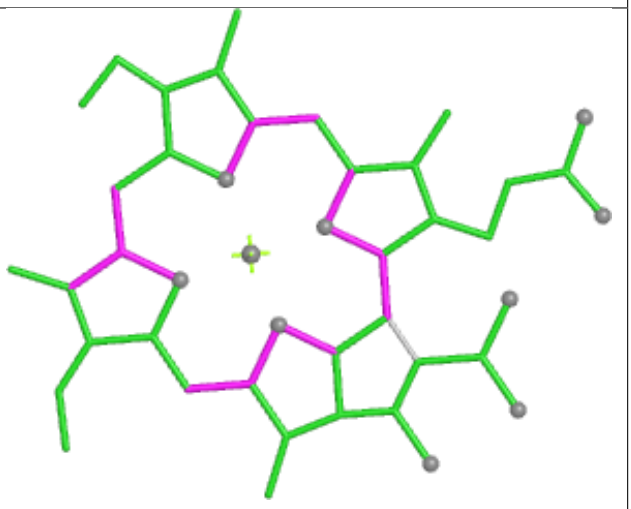


Rings

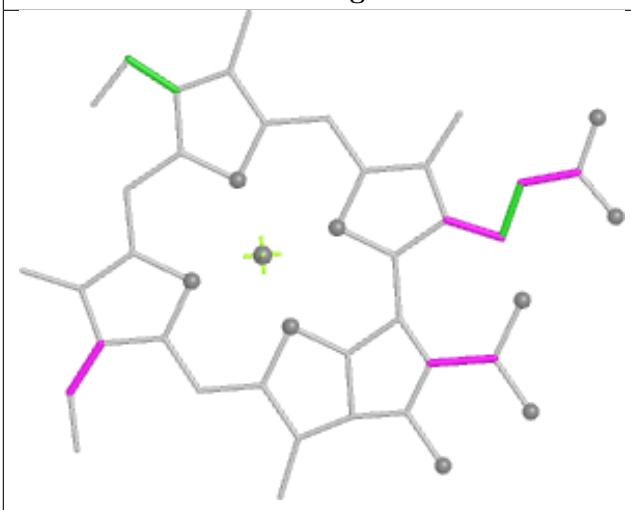
Ligand CLA B 816



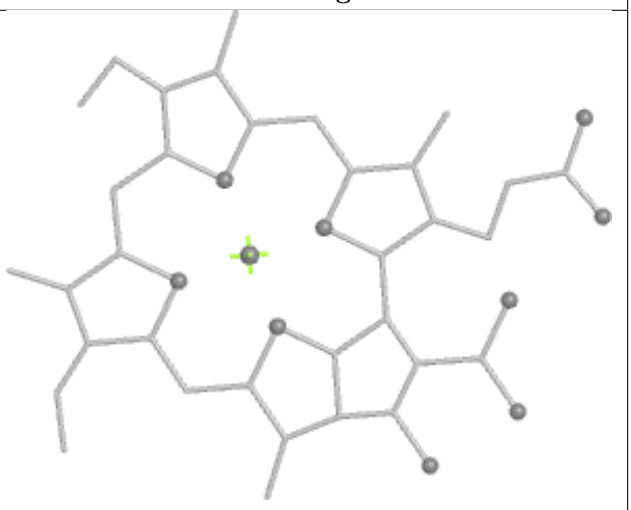
Bond lengths



Bond angles

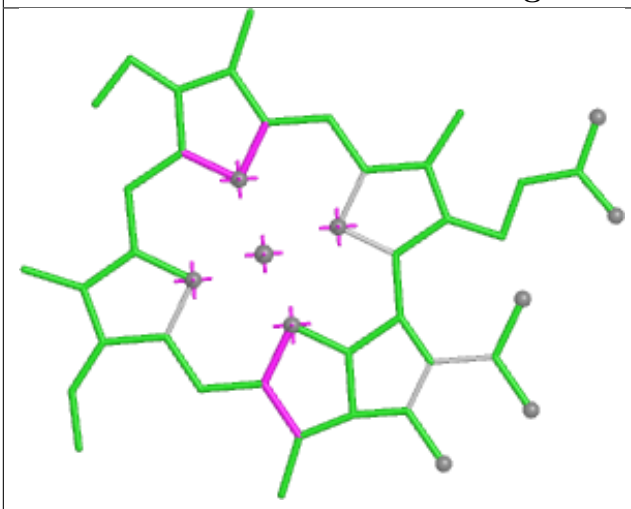


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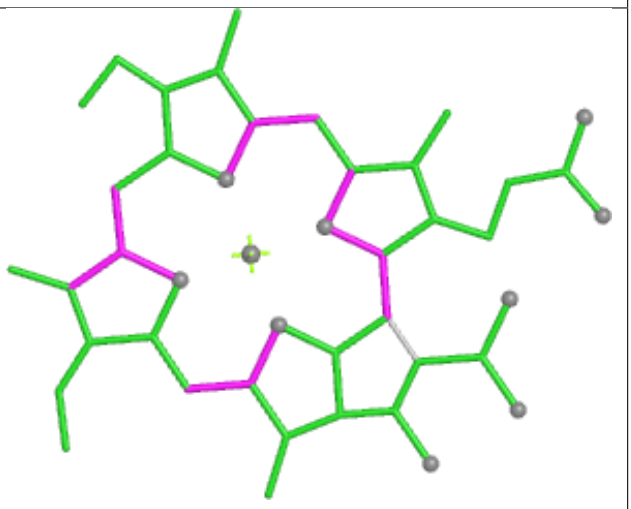


Rings

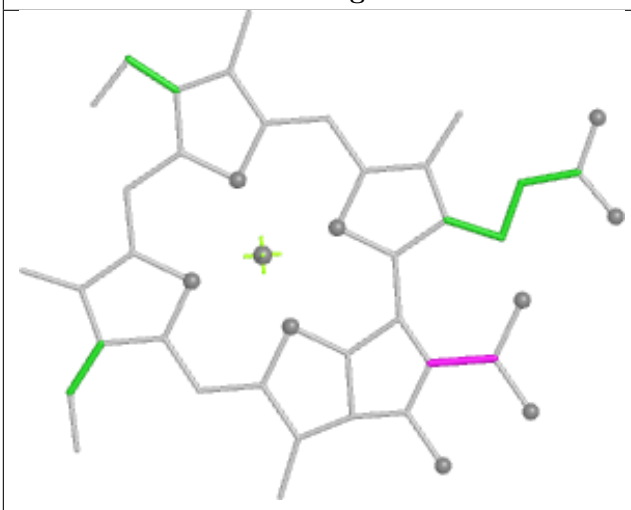
Ligand CLA A 838



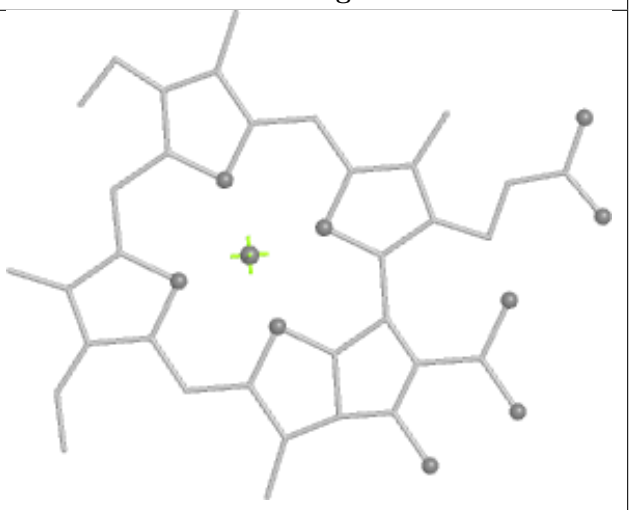
Bond lengths



Bond angles

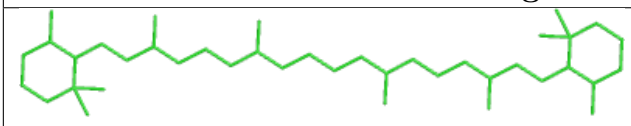


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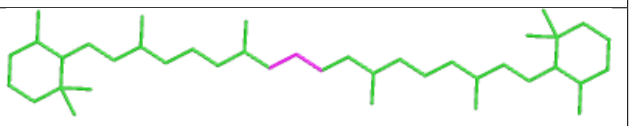


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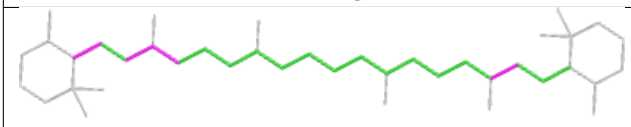
Ligand BCR A 850



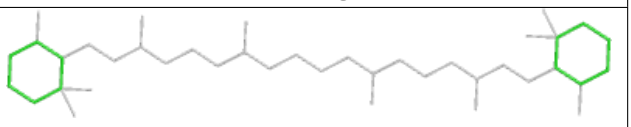
Bond lengths



Bond angles

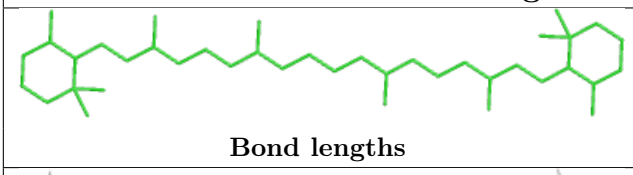


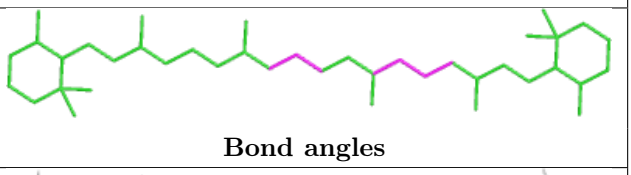
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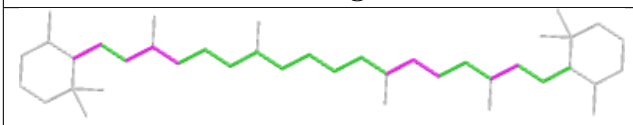


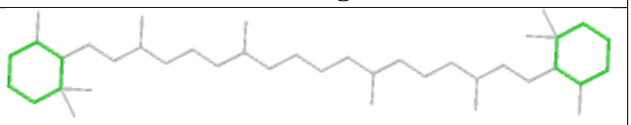
Rings

Ligand BCR B 845


Bond lengths


Bond angles

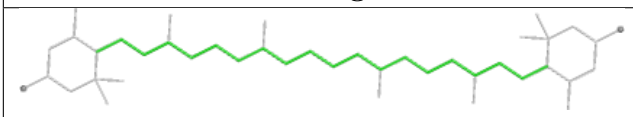

Torsions

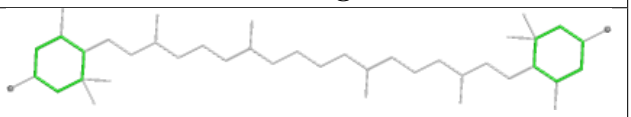

Rings

Ligand LUT 4 317

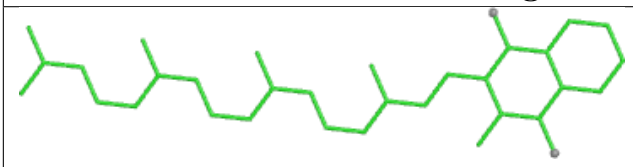

Bond lengths

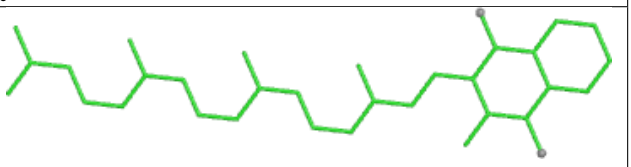

Bond angles

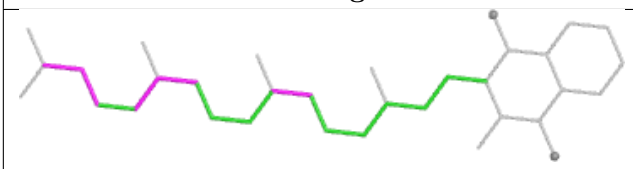

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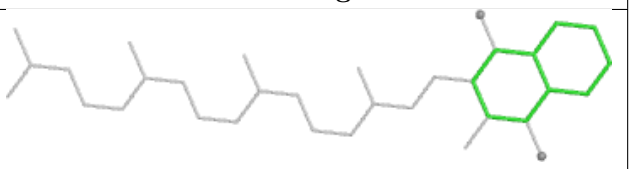

Rings

Ligand PQN B 842

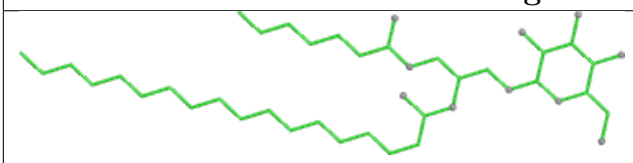

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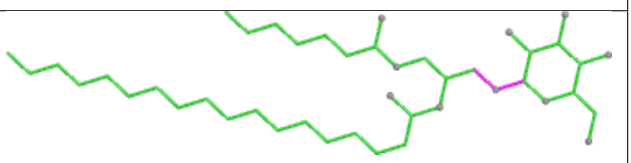

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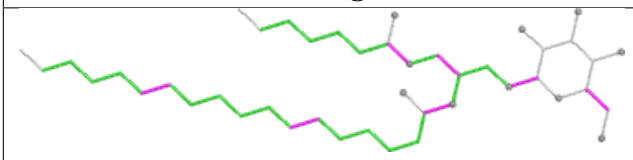

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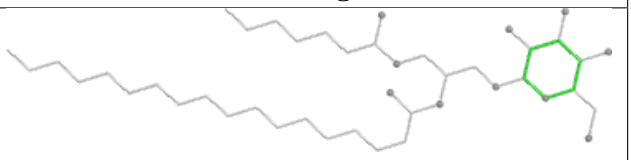

Rings

Ligand LMG 8 319

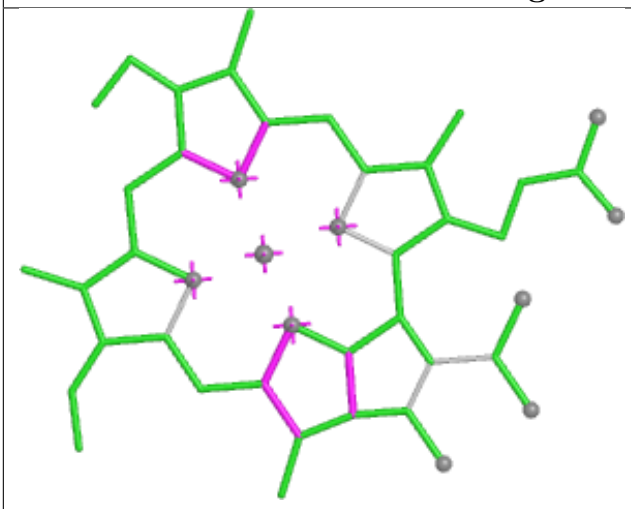

Bond lengths


Bond angles

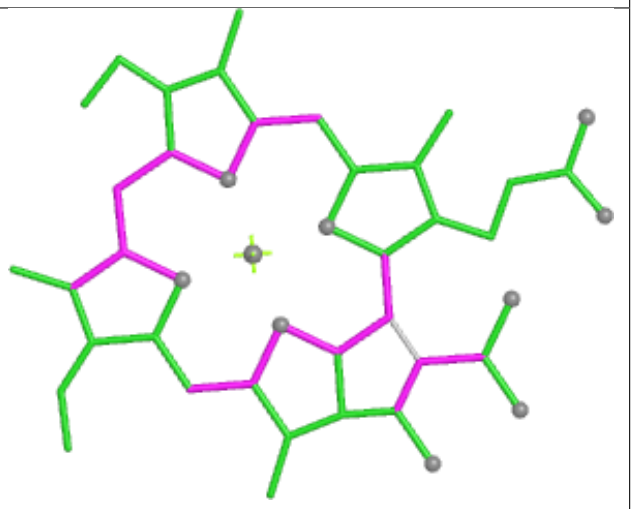

Torsions


Rings

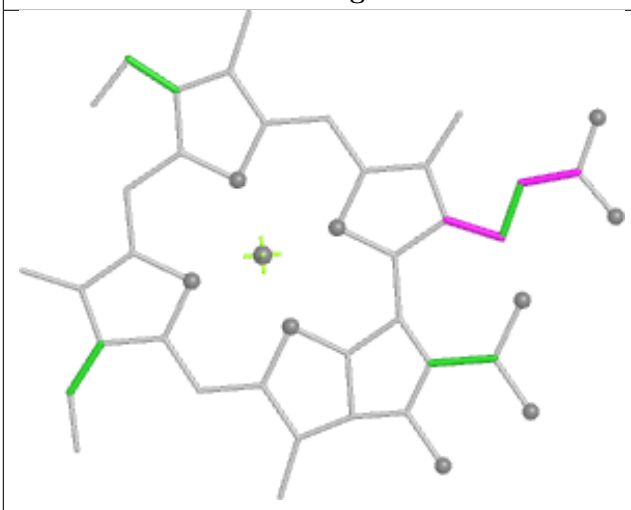
Ligand CLA 4 304



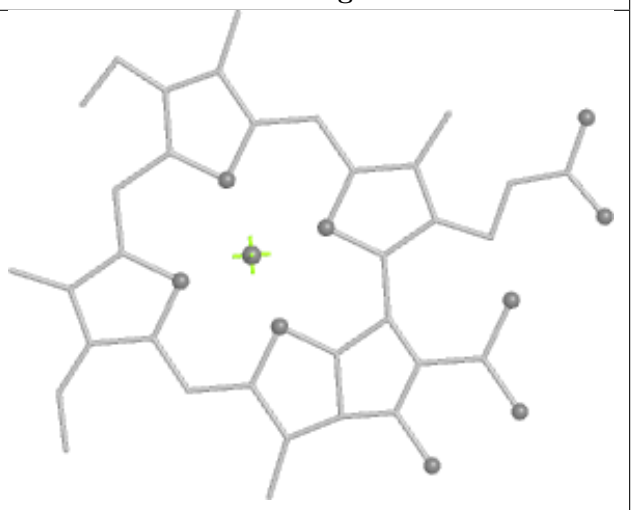
Bond lengths



Bond angles

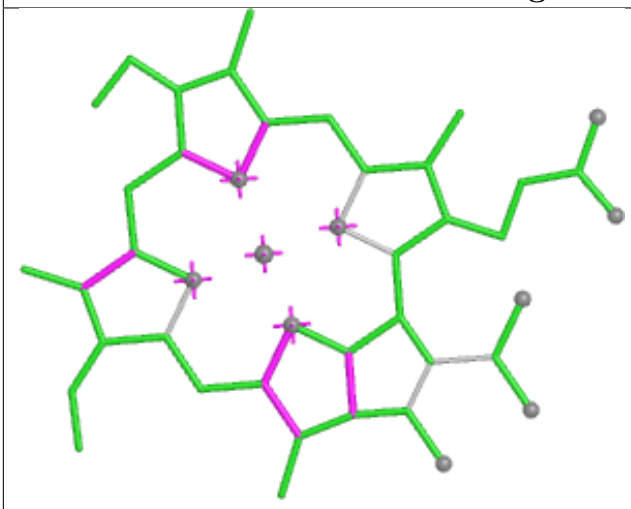


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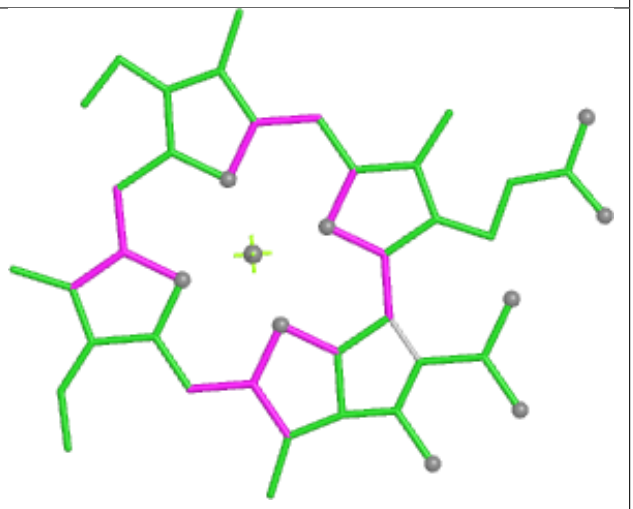


Rings

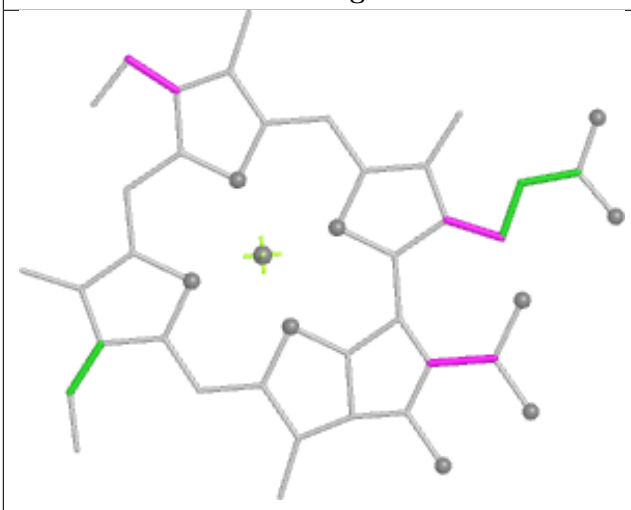
Ligand CLA 6 318



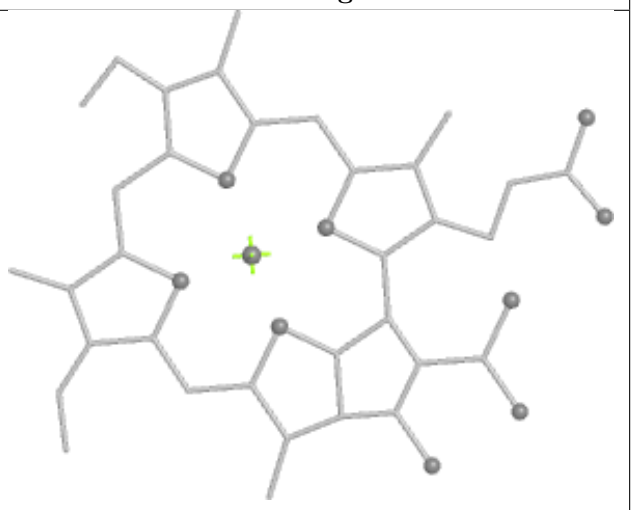
Bond lengths



Bond angles

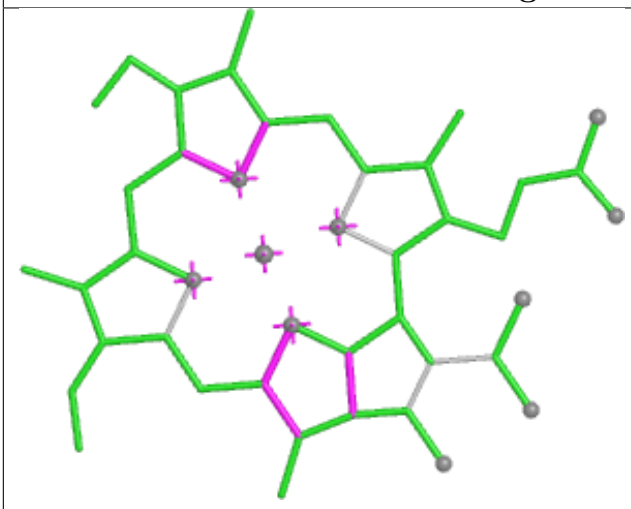


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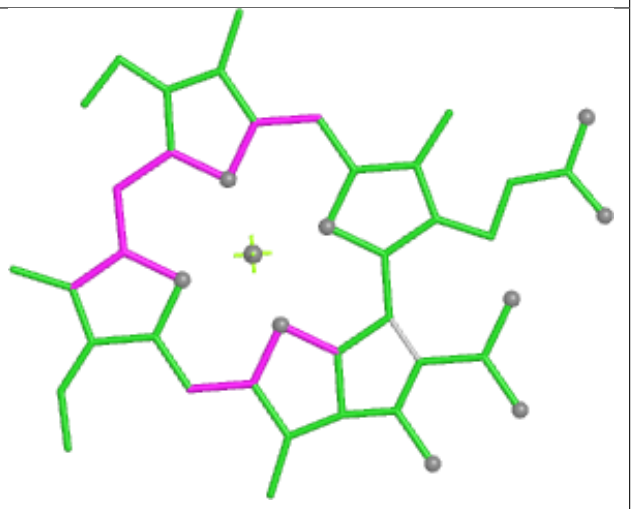


Rings

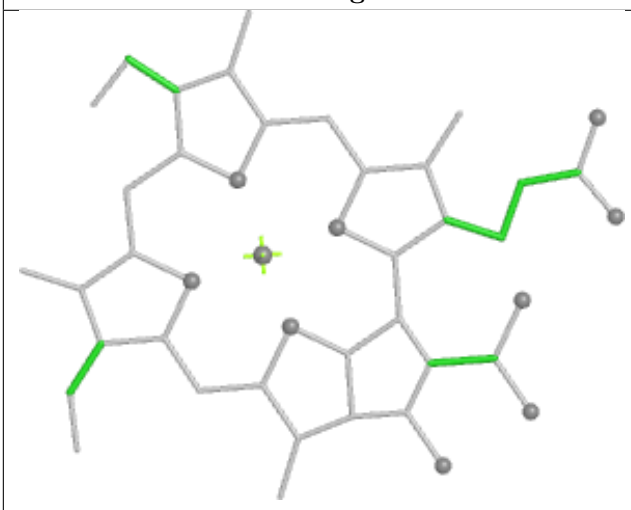
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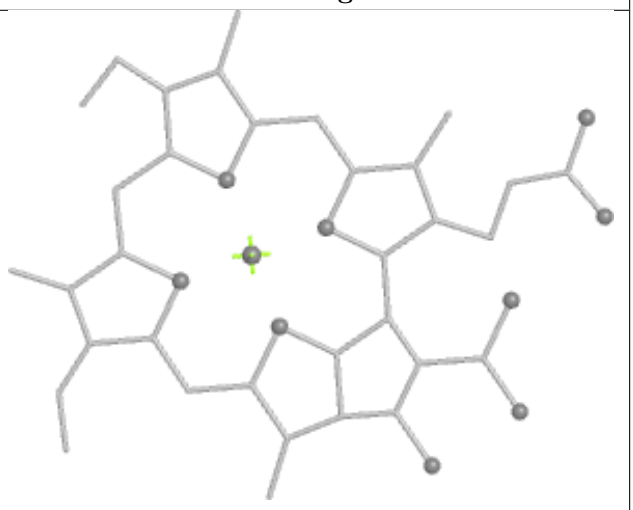
Bond lengths



Bond angles

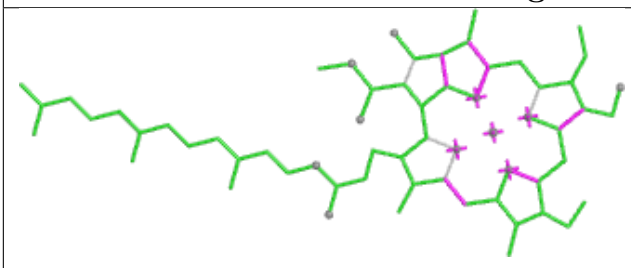


Torsions

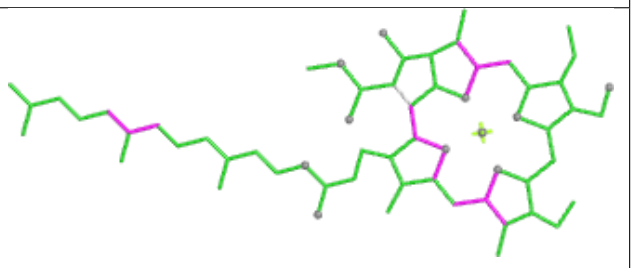


Rings

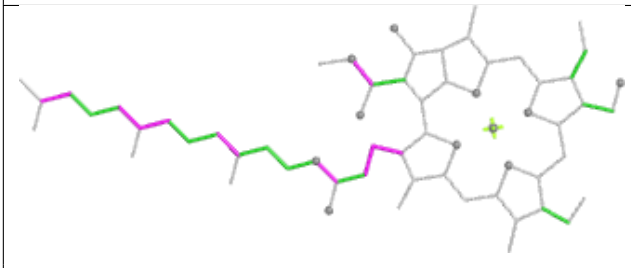
Ligand CHL 0 317



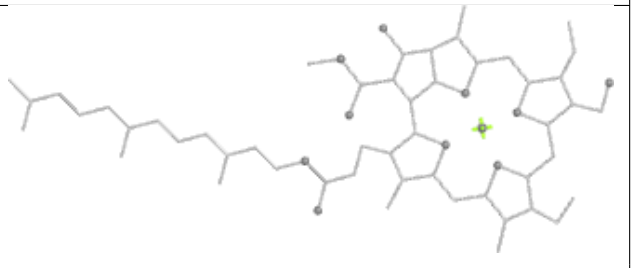
Bond lengths



Bond angles

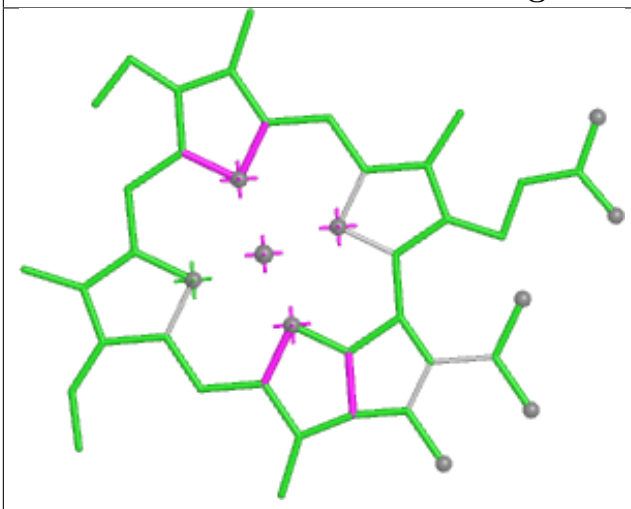


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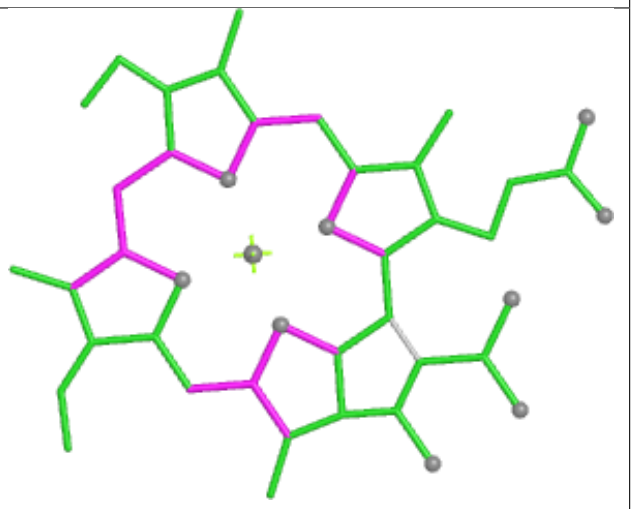


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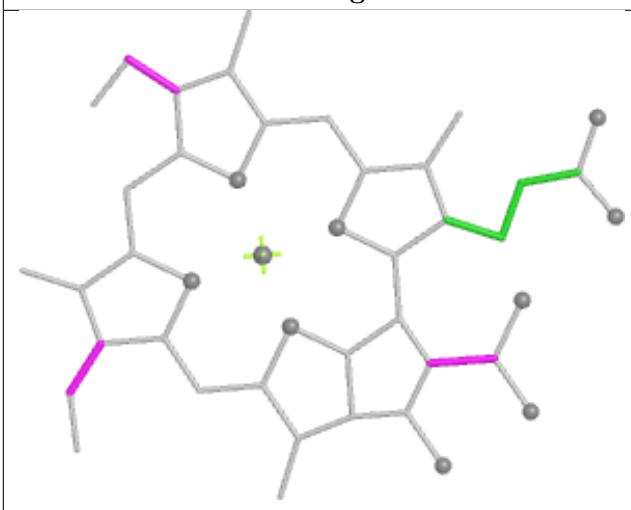
Ligand CLA 8 311



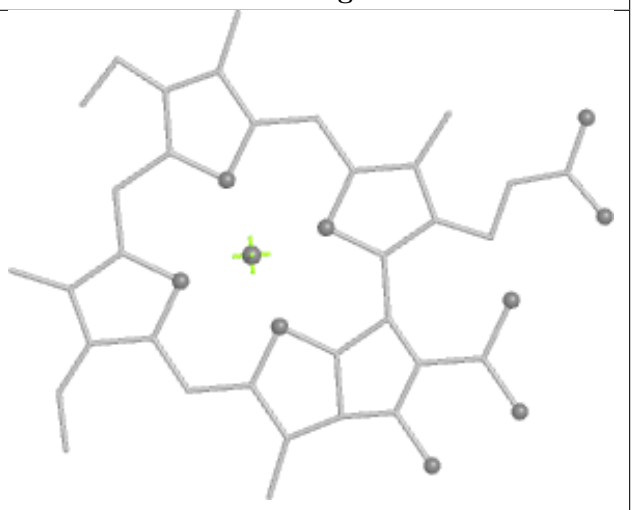
Bond lengths



Bond angles

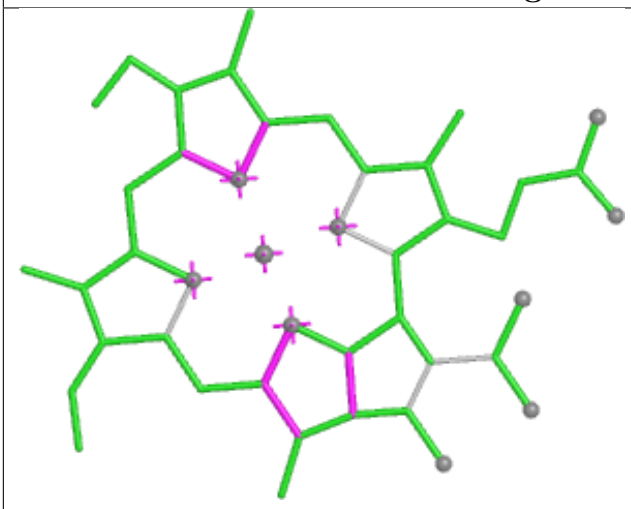


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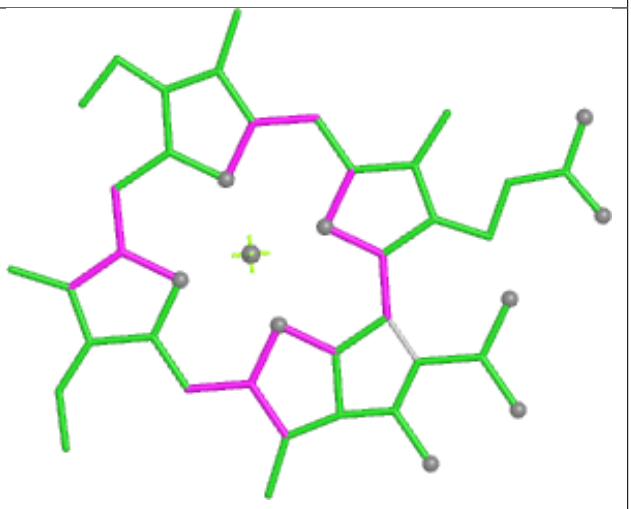


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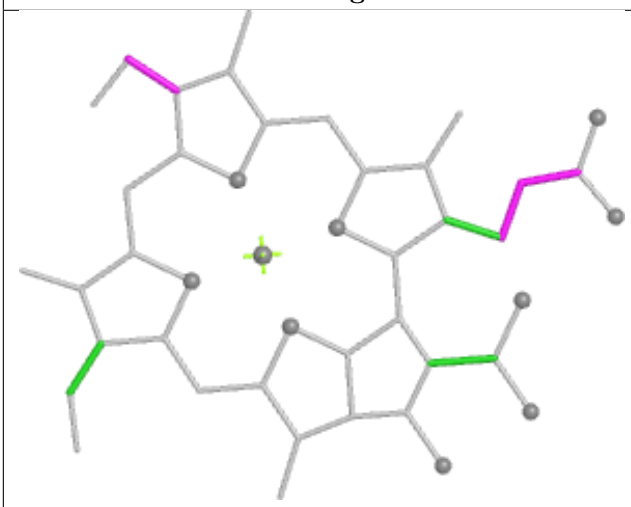
Ligand CLA B 803



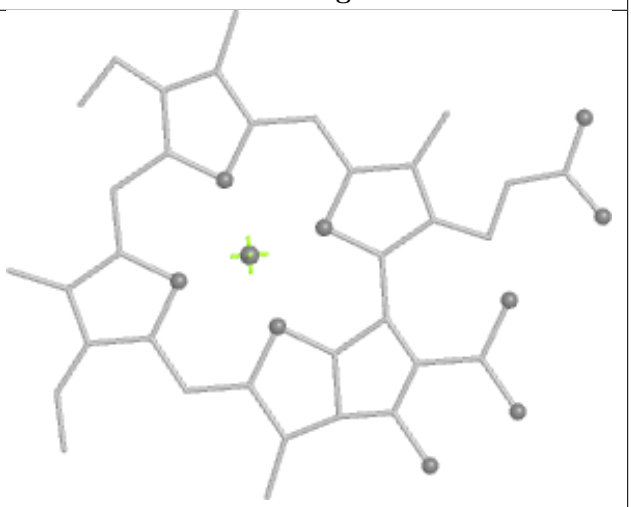
Bond lengths



Bond angles

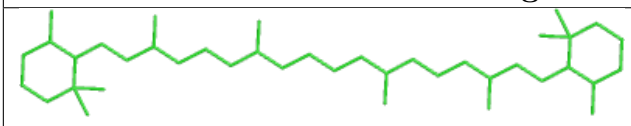


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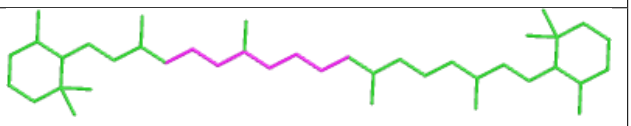


Rings

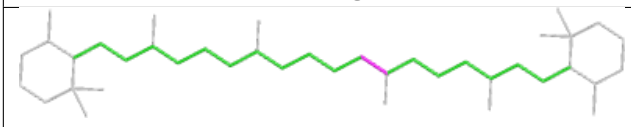
Ligand BCR G 204



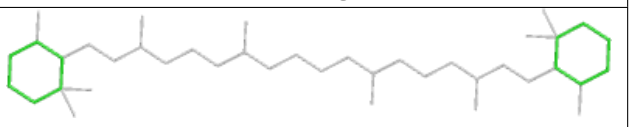
Bond lengths



Bond angles

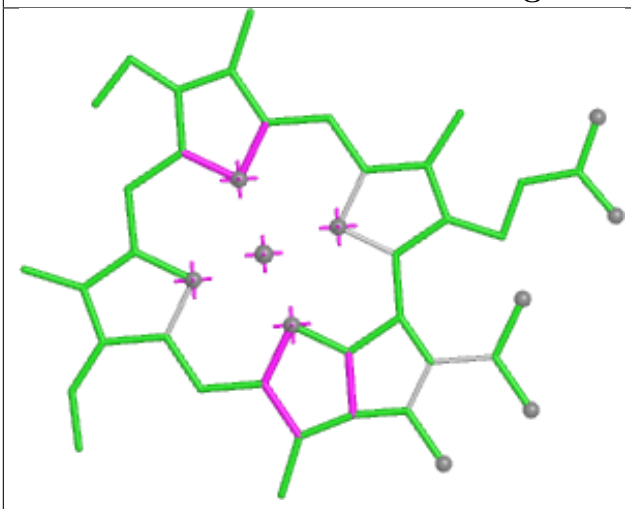


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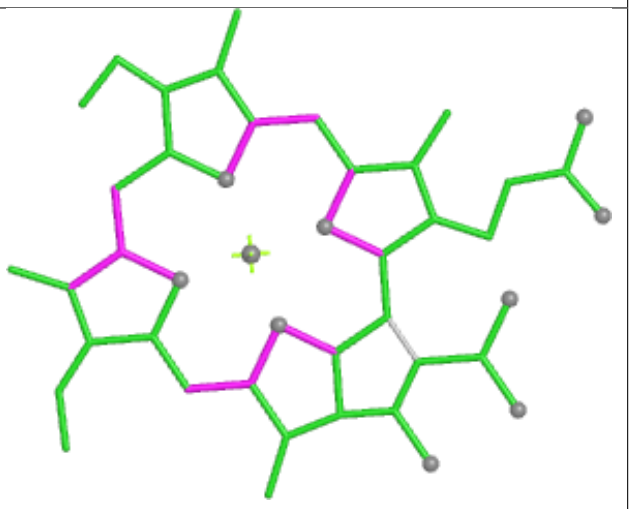


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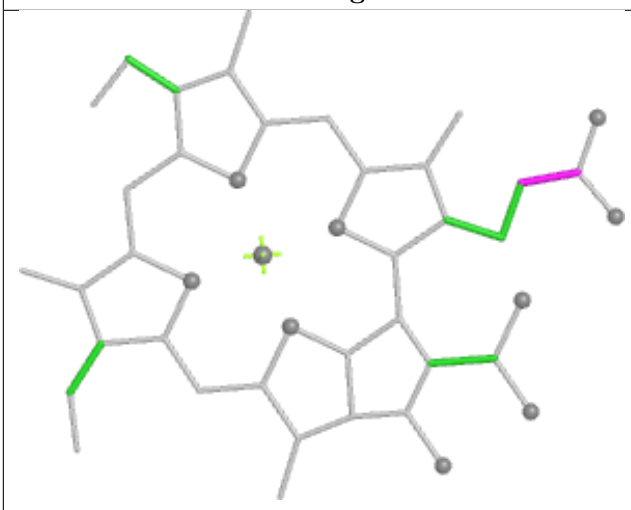
Ligand CLA A 835



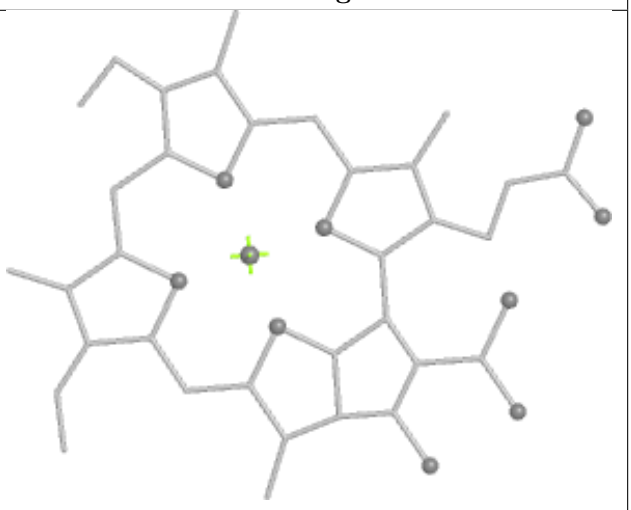
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Bond angles

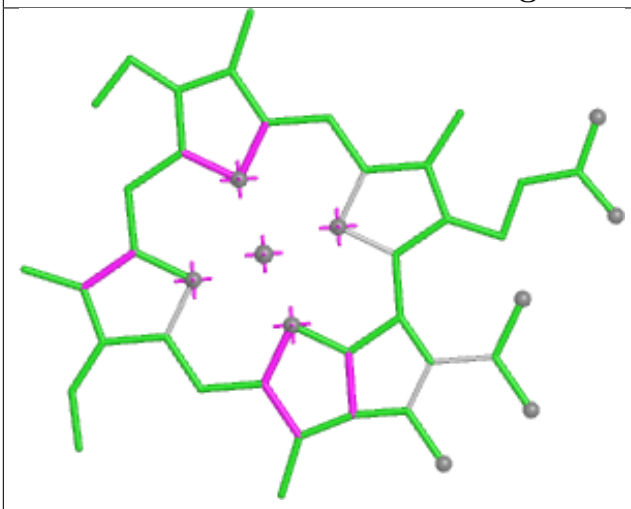


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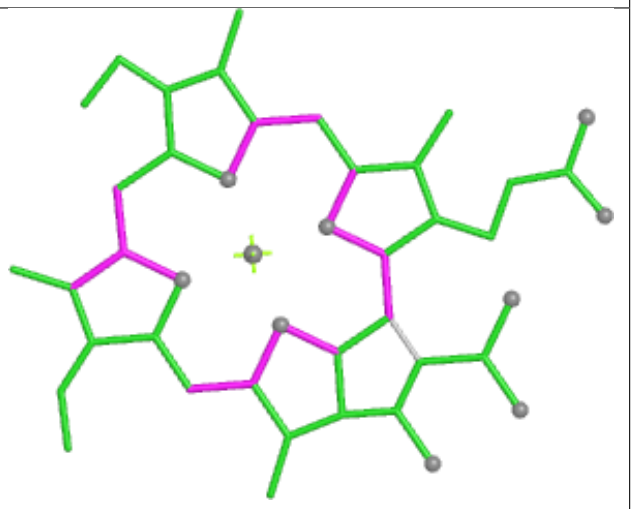


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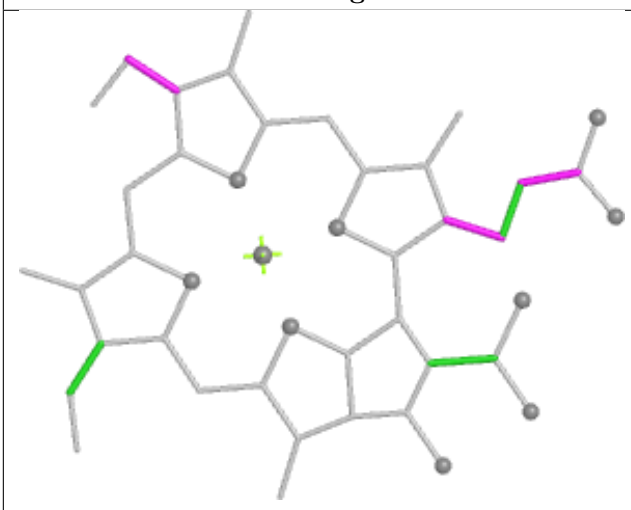
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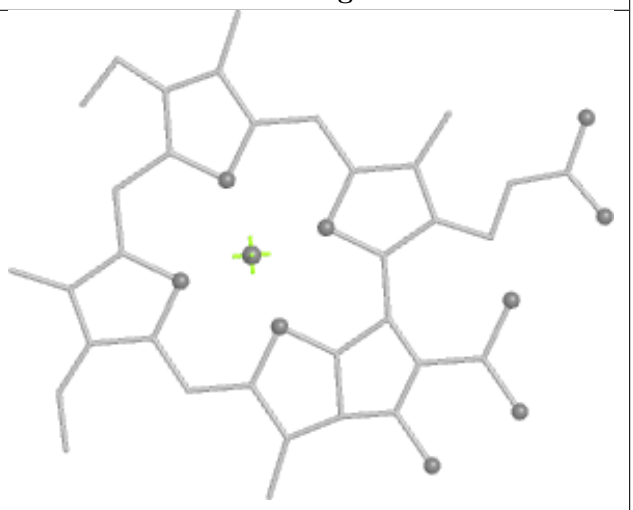
Bond lengths



Bond angles

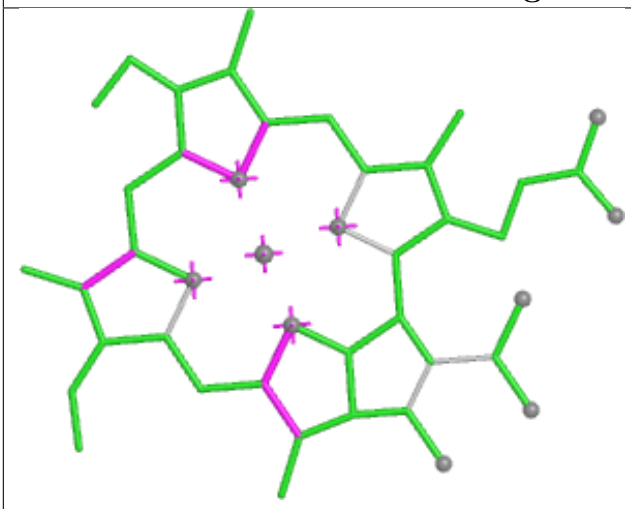


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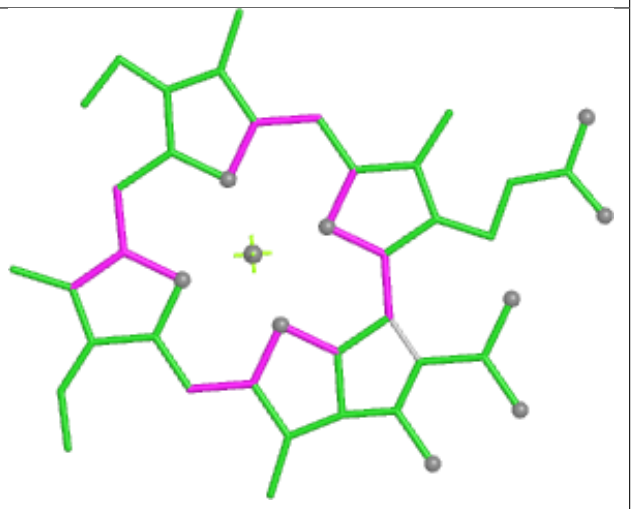


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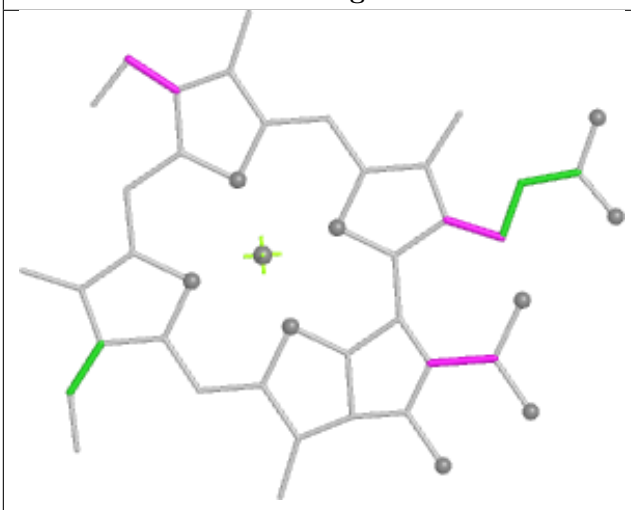
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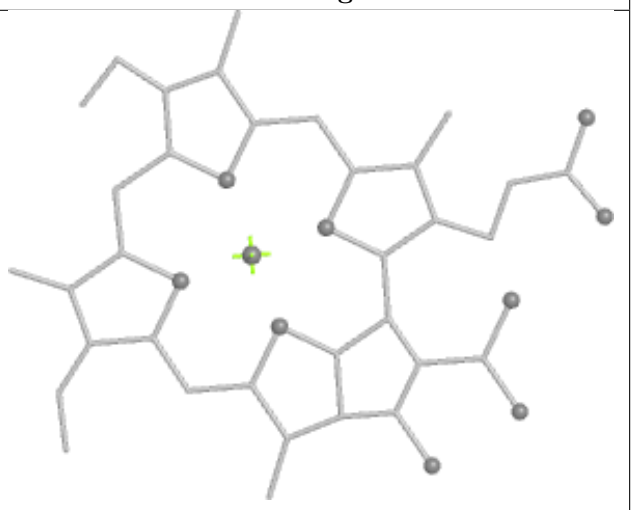
Bond lengths



Bond angles

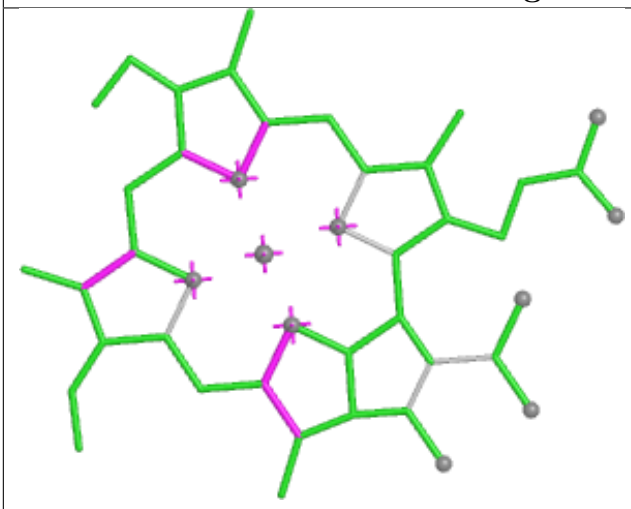


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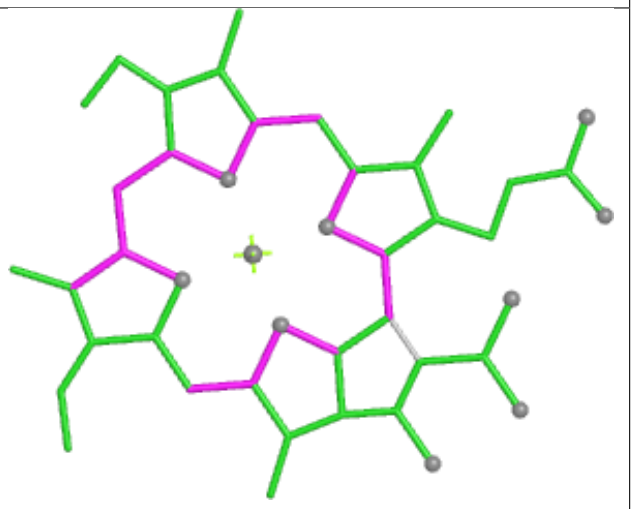


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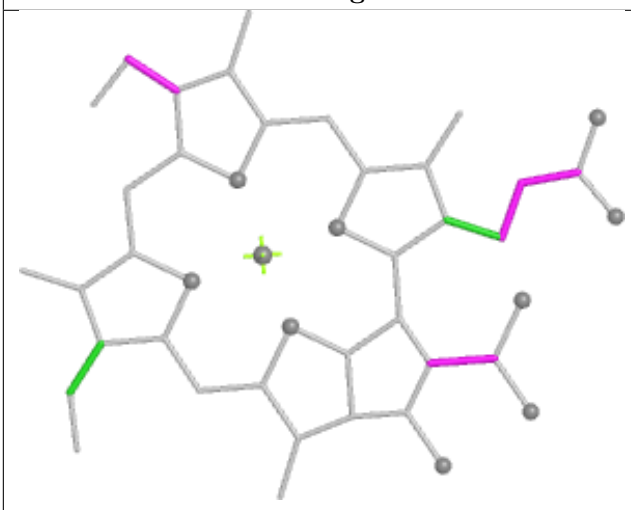
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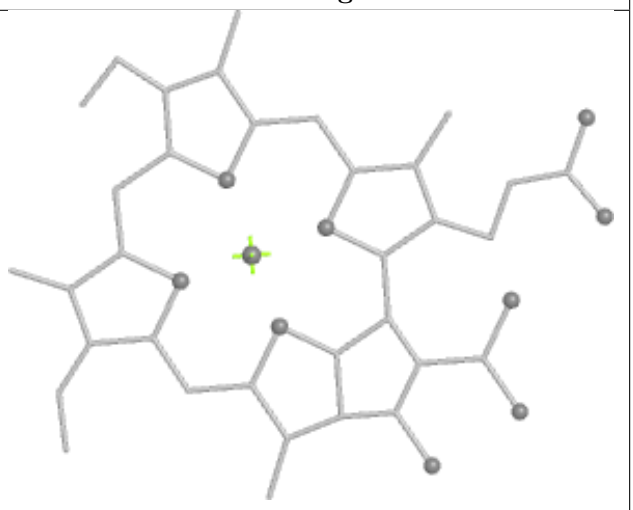
Bond lengths



Bond angles

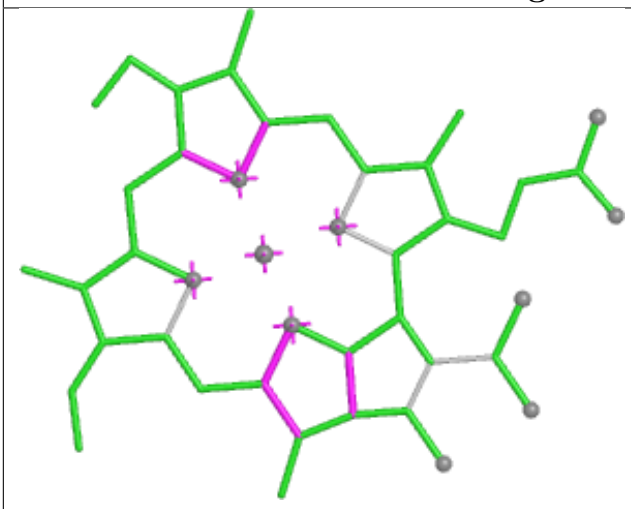


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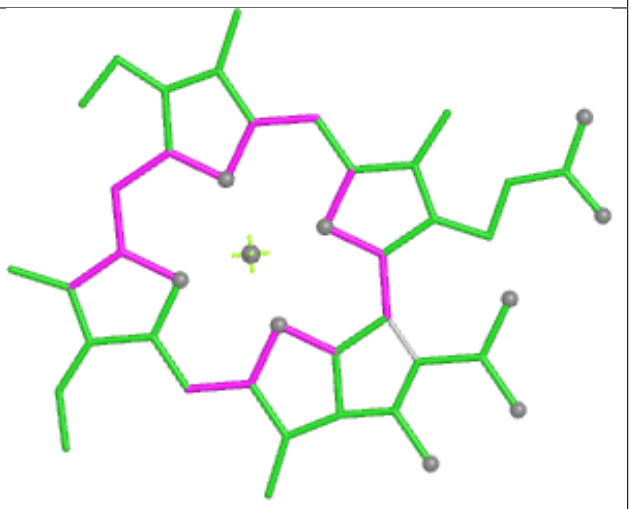


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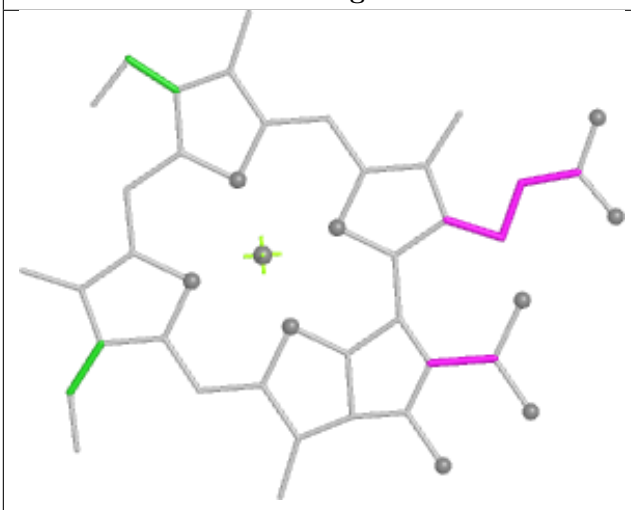
Ligand CLA 6 309



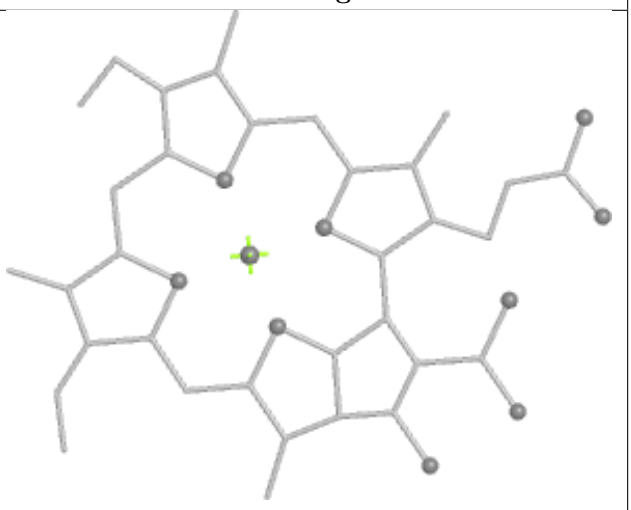
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Bond angles

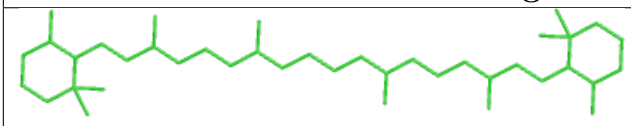


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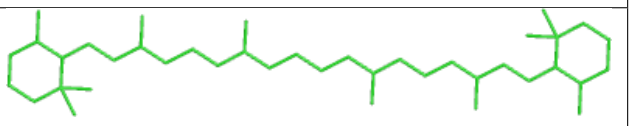


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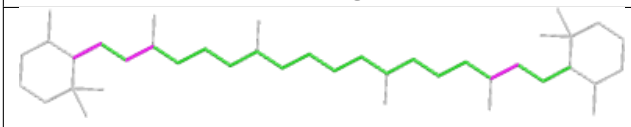
Ligand BCR B 847



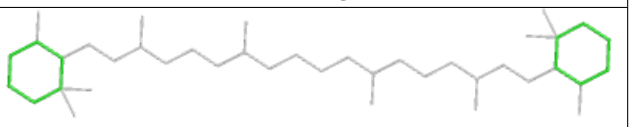
Bond lengths



Bond angles

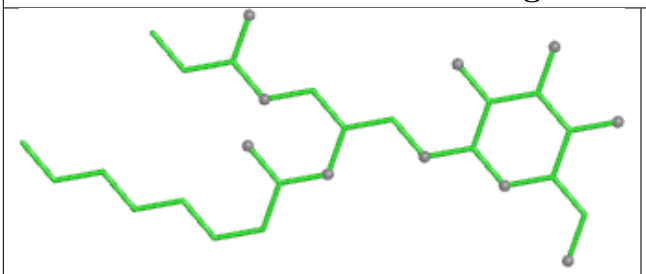


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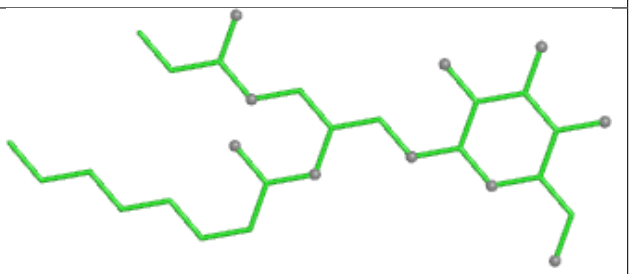


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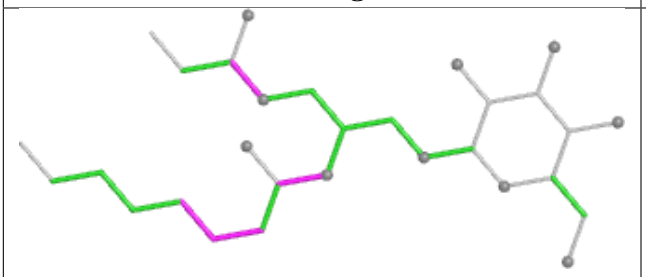
Ligand LMG J 101



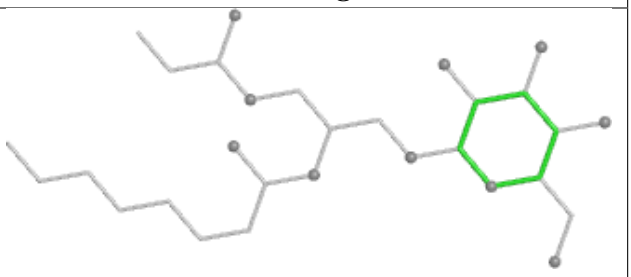
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Bond angles

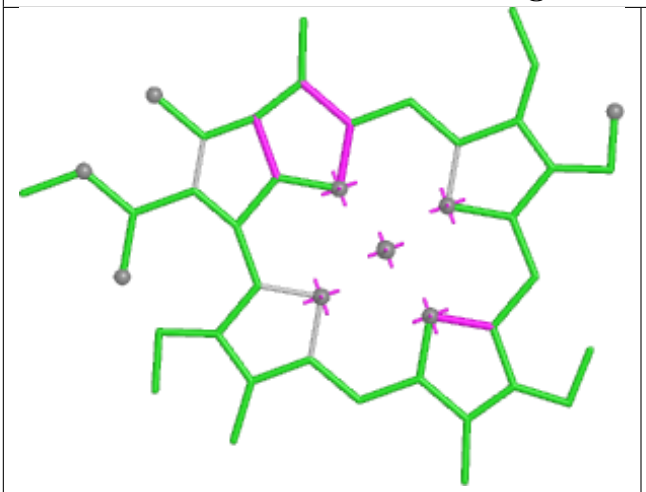


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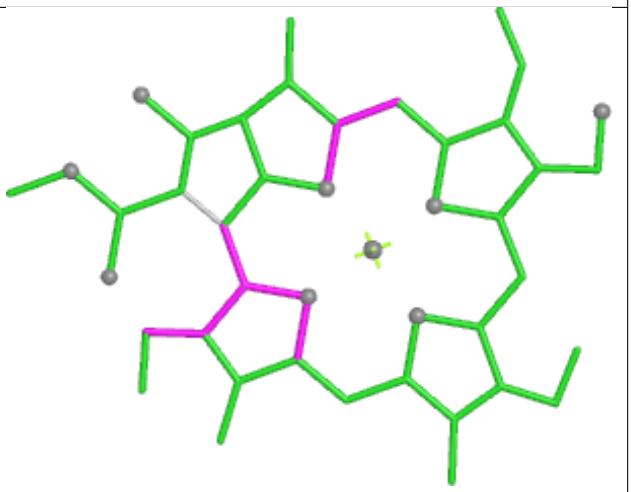


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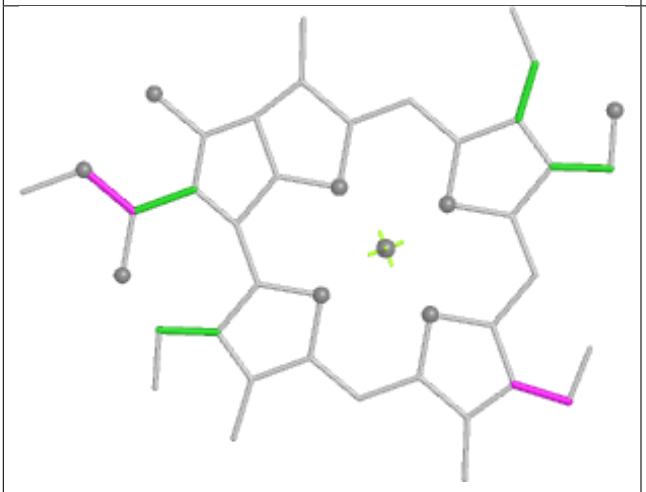
Ligand CHL 5 317



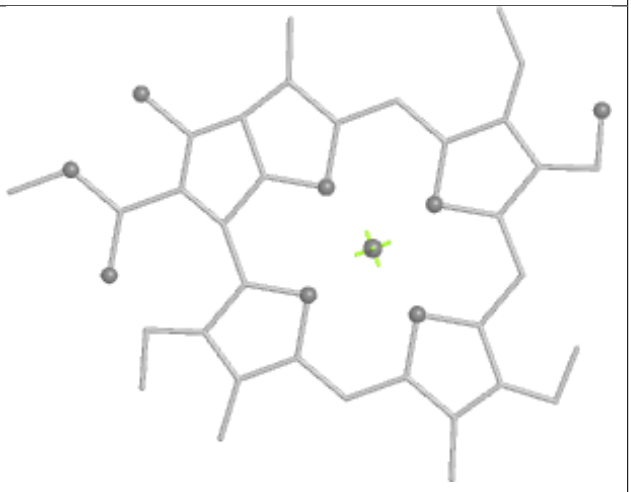
Bond lengths



Bond angles

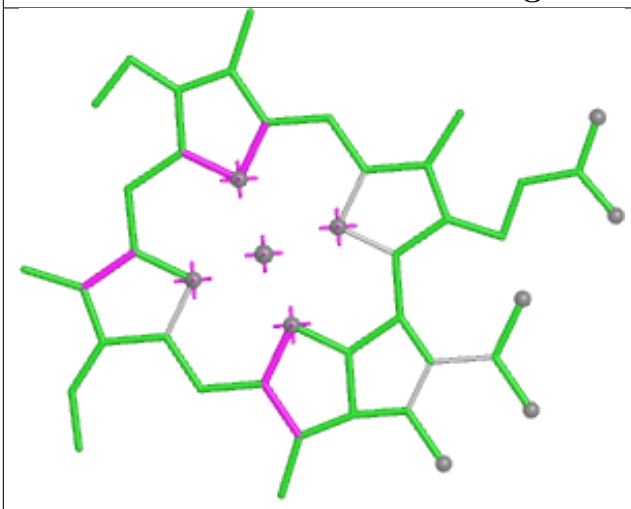


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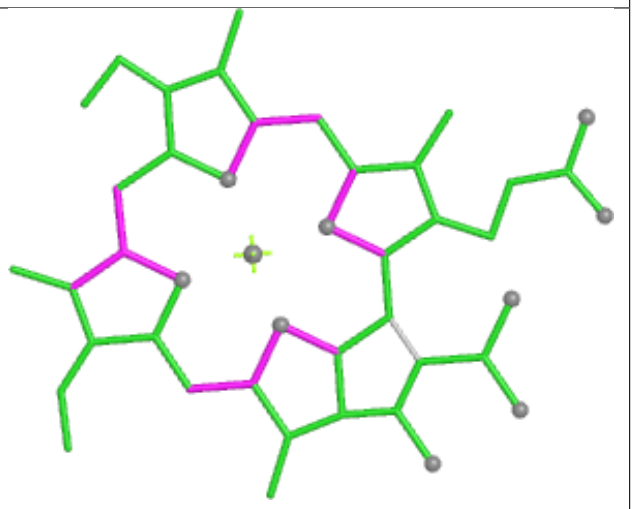


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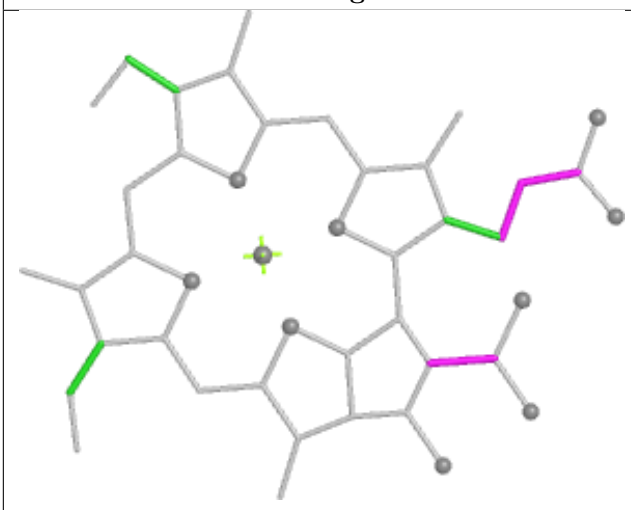
Ligand CLA A 820



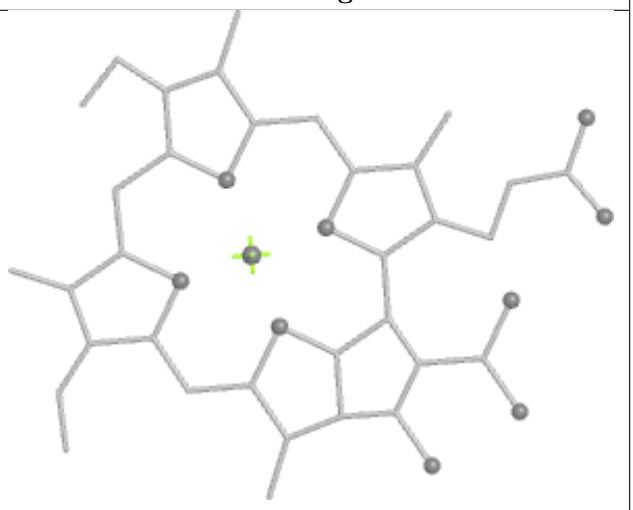
Bond lengths



Bond angles

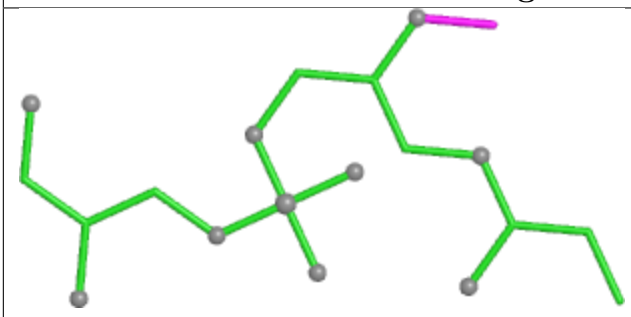


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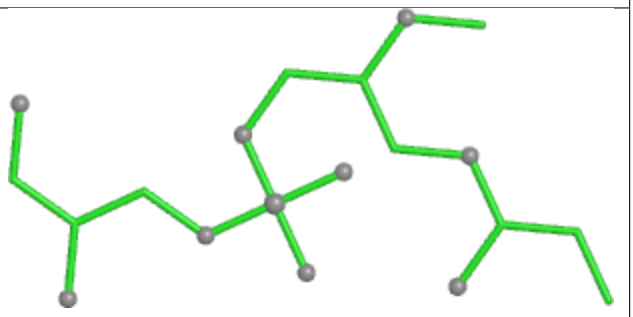


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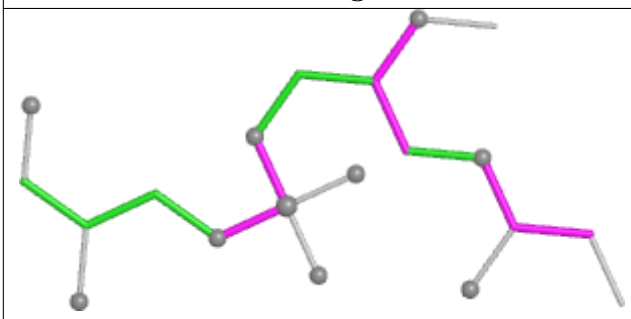
Ligand LHG 3 1019



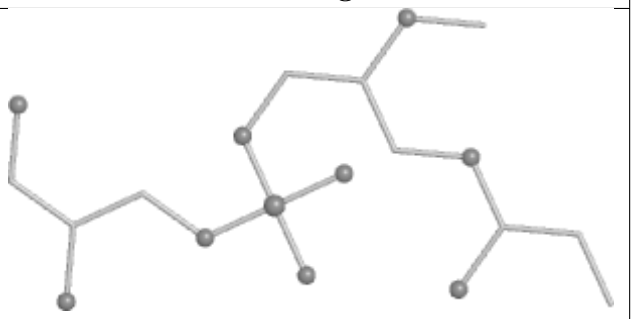
Bond lengths



Bond angles

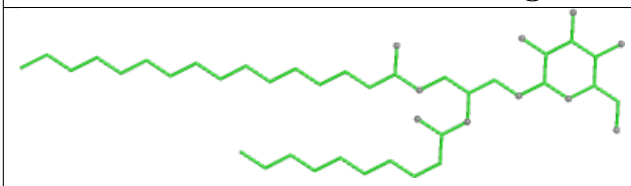


Torsions

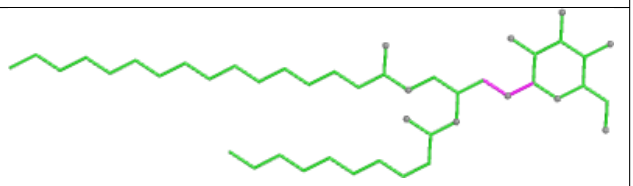


Rings

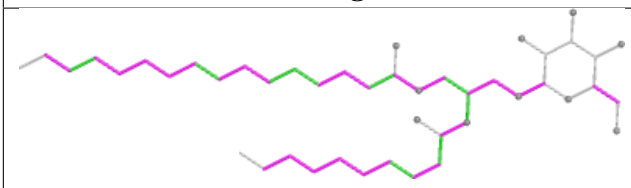
Ligand LMG 5 324



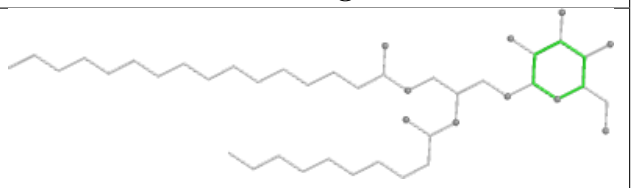
Bond lengths



Bond angles

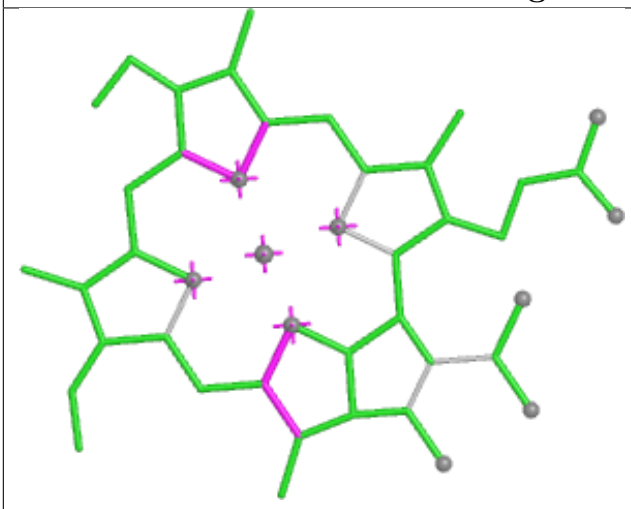


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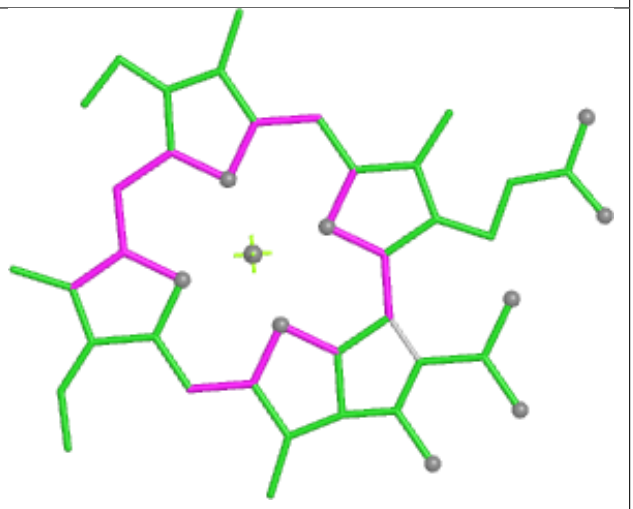


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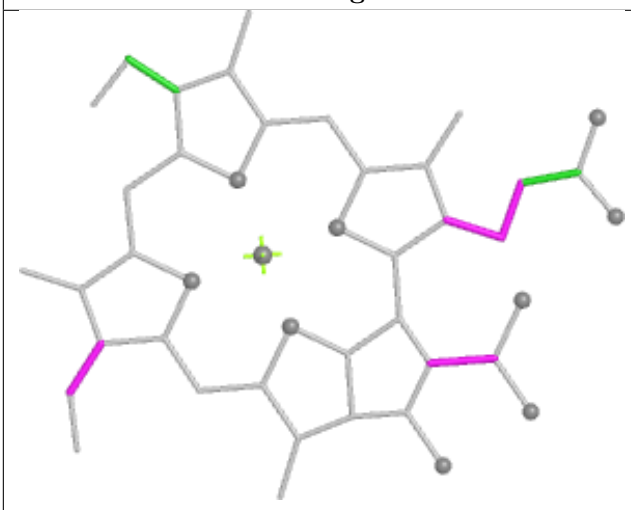
Ligand CLA 4 308



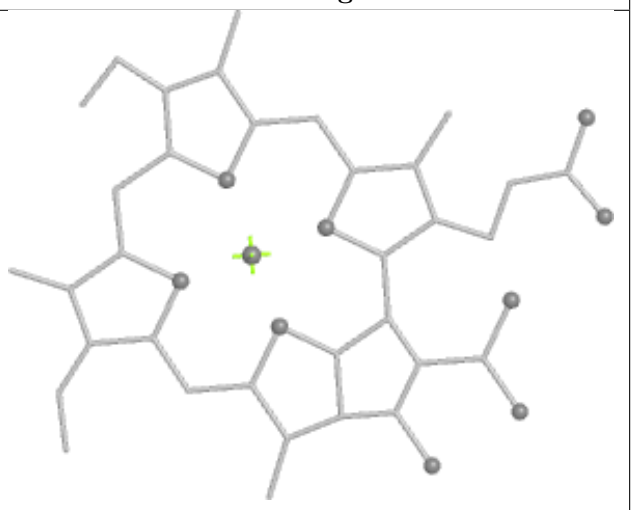
Bond lengths



Bond angles

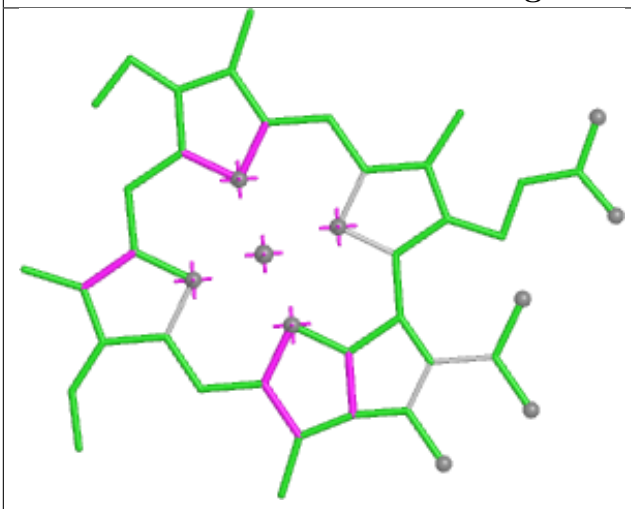


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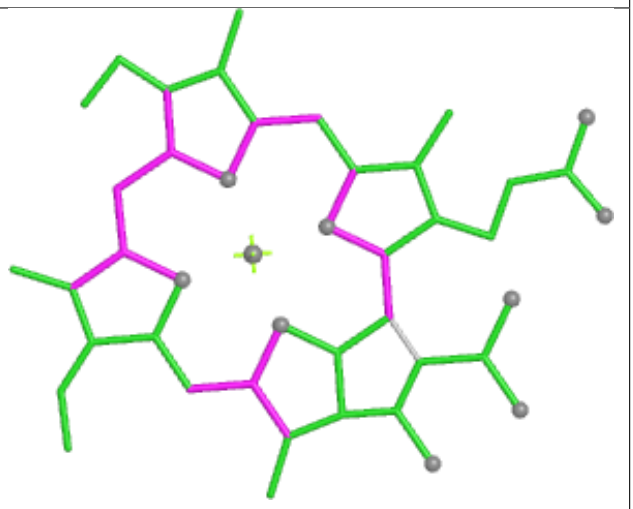


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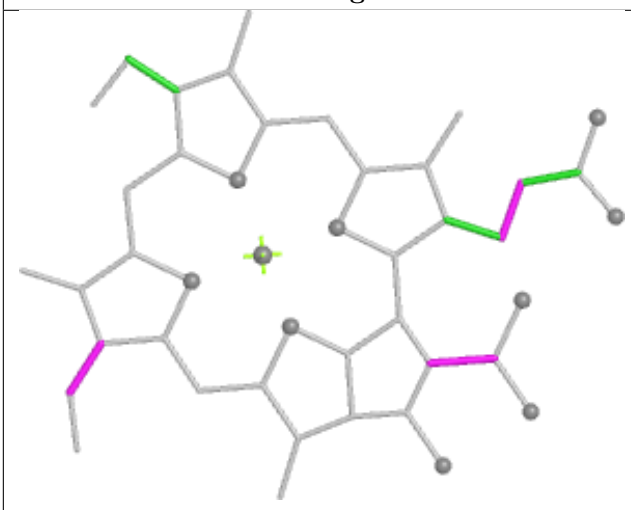
Ligand CLA B 802



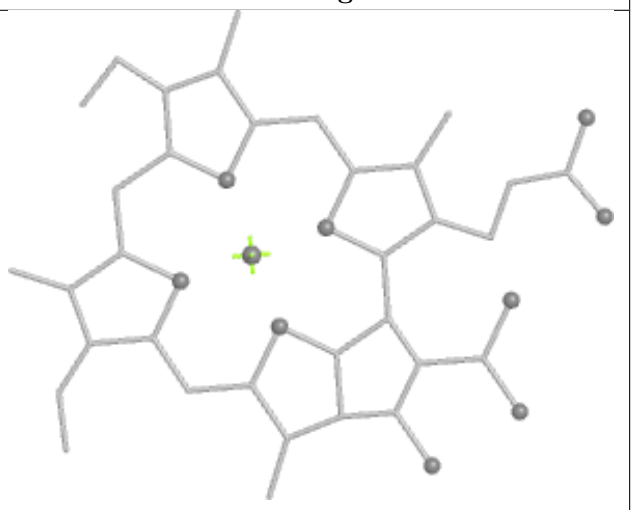
Bond lengths



Bond angles

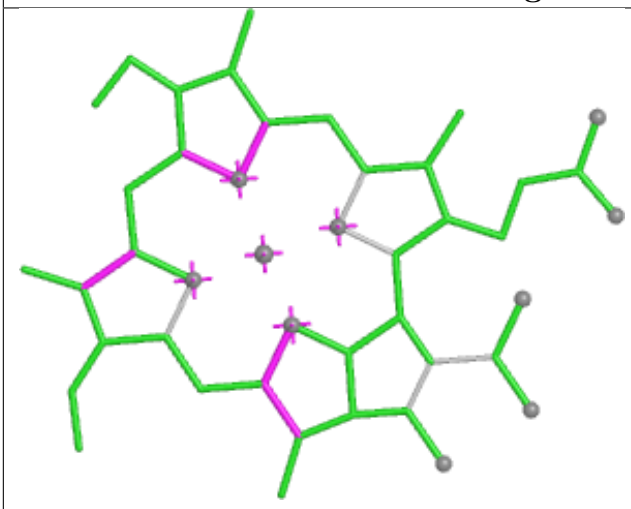


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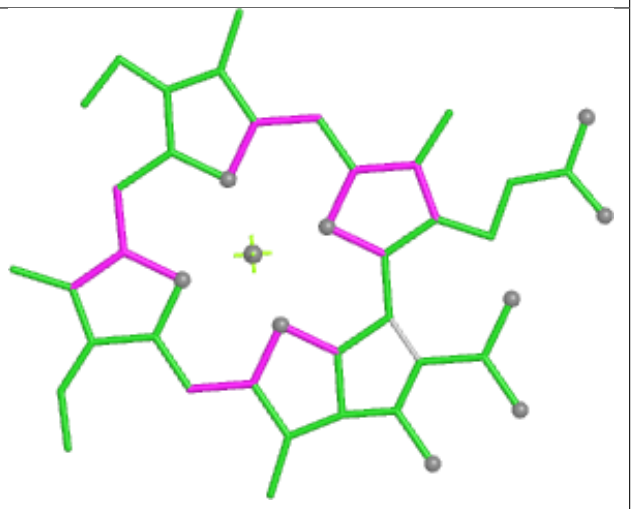


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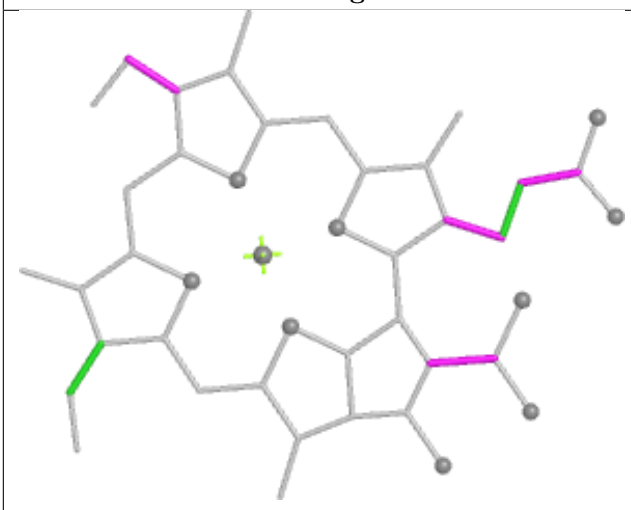
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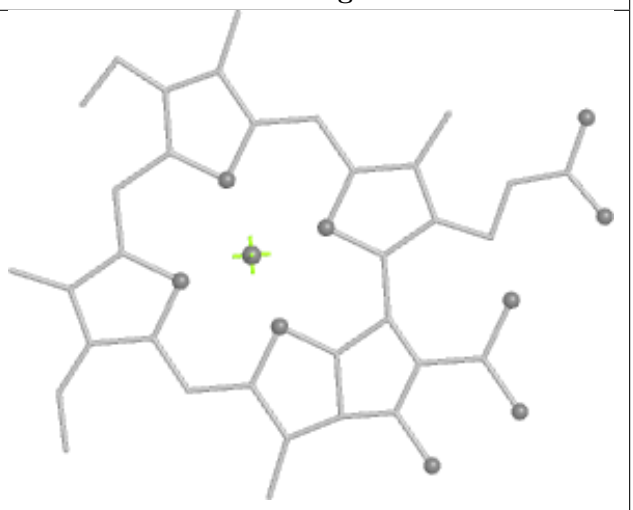
Bond lengths



Bond angles

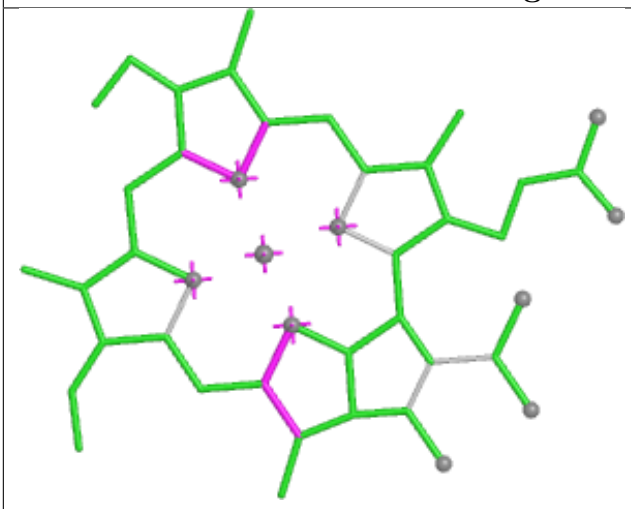


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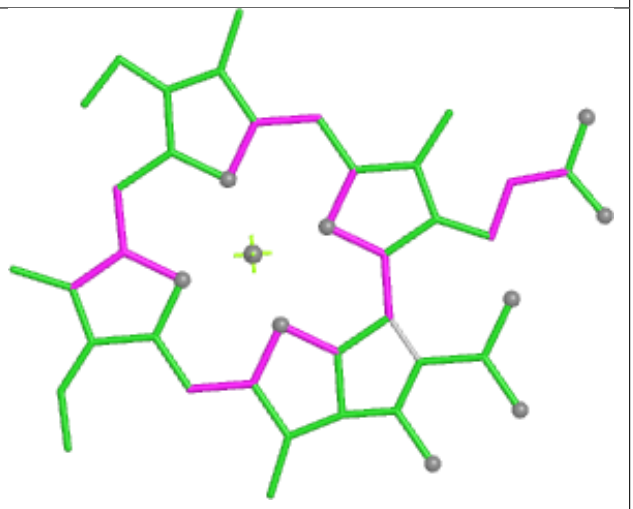


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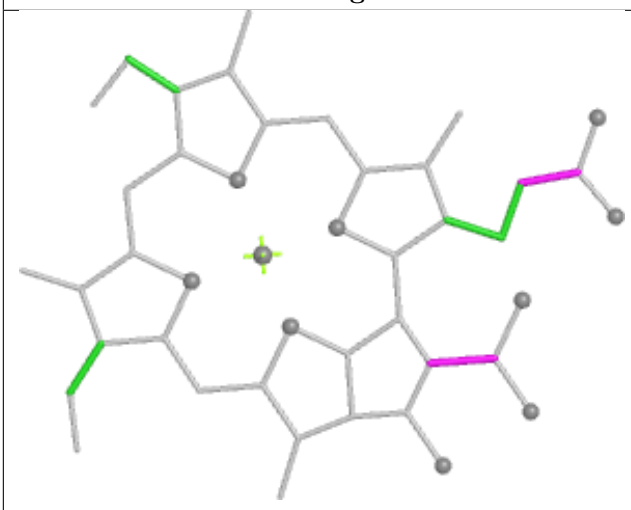
Ligand CLA A 813



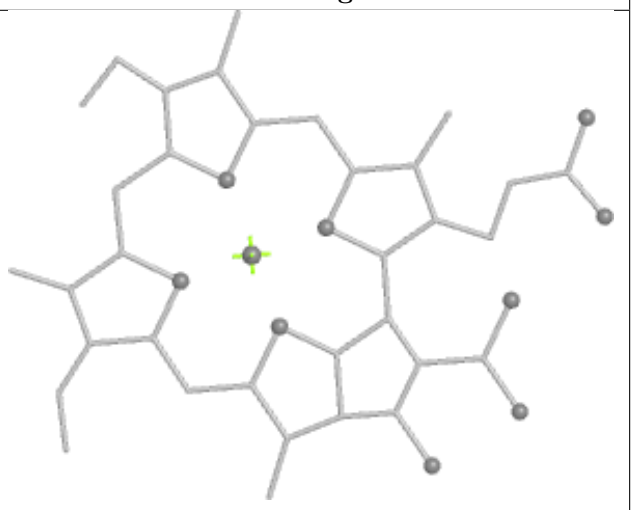
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Bond angles

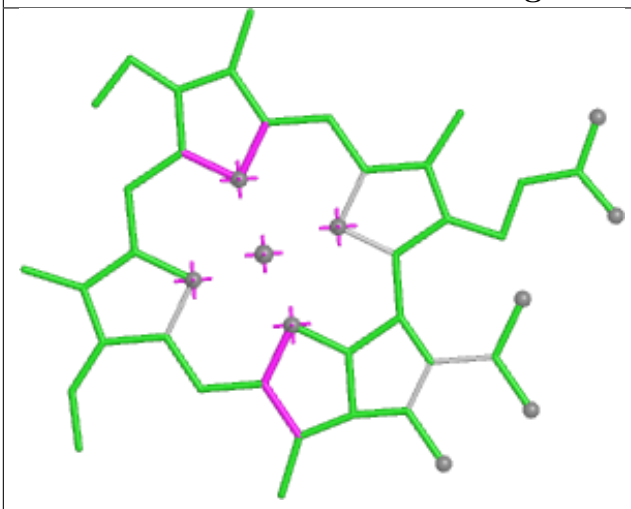


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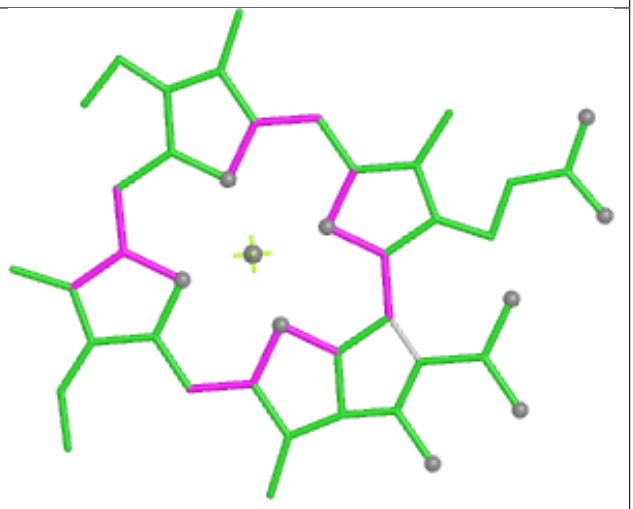


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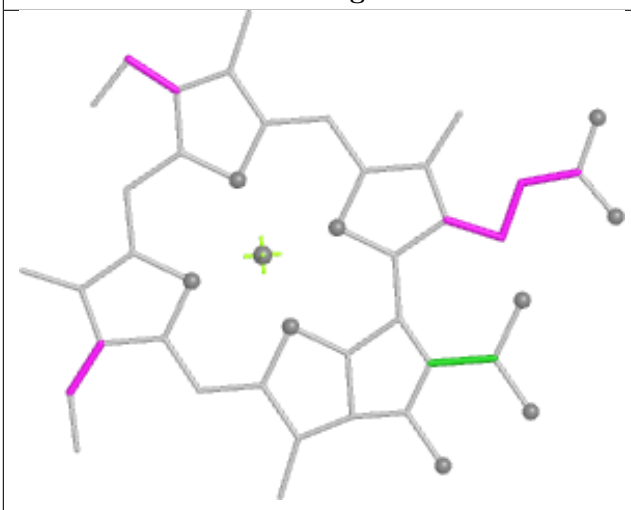
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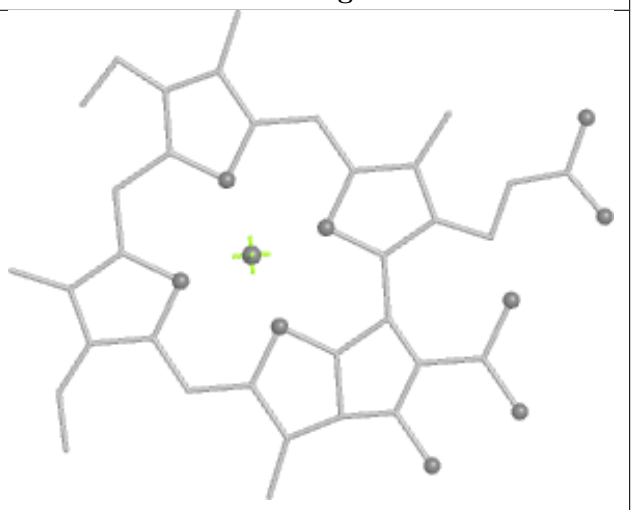
Bond lengths



Bond angles

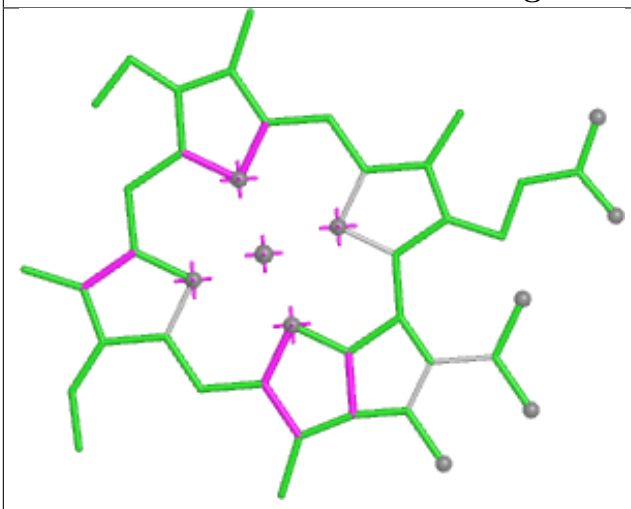


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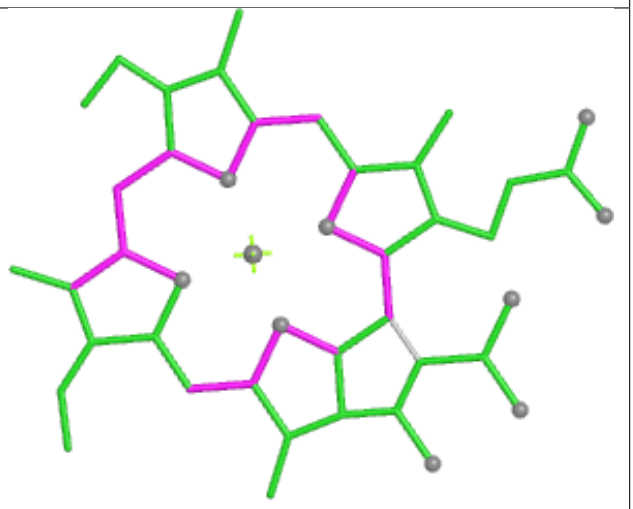


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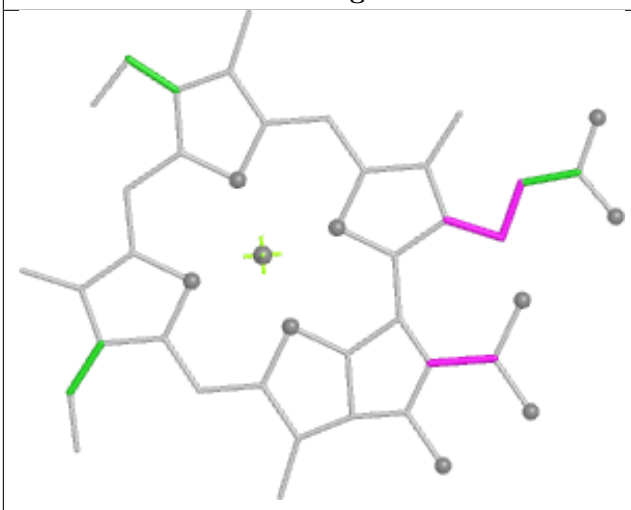
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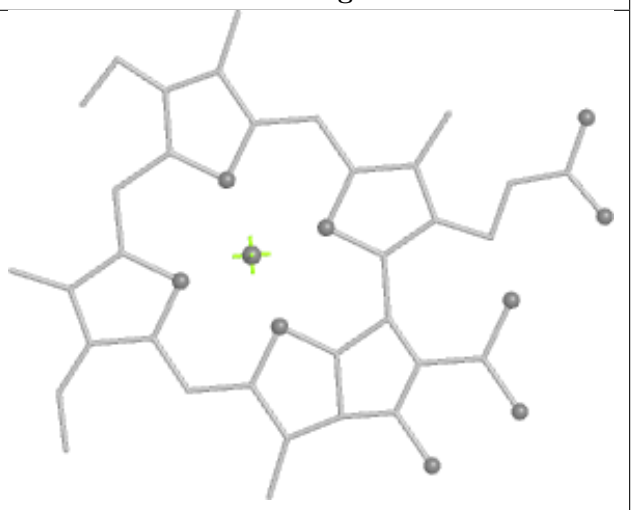
Bond lengths



Bond angles

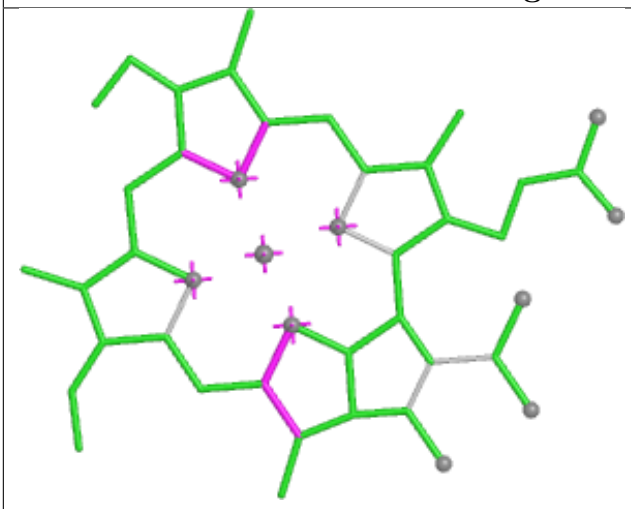


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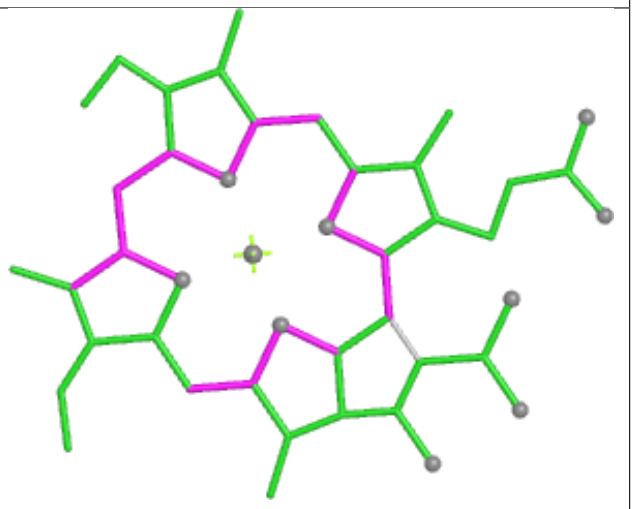


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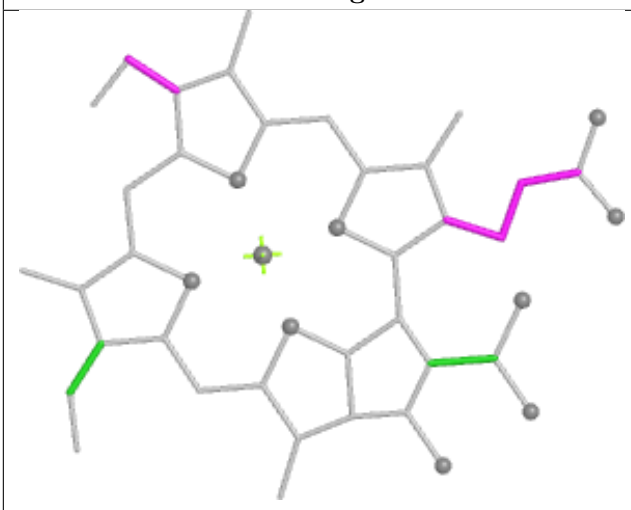
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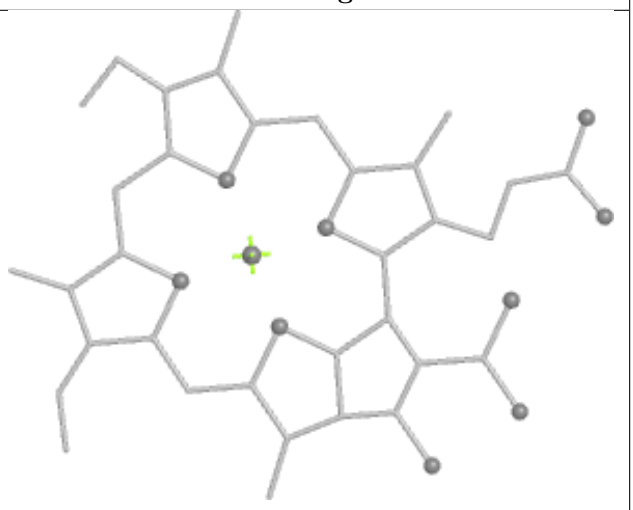
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Bond angles

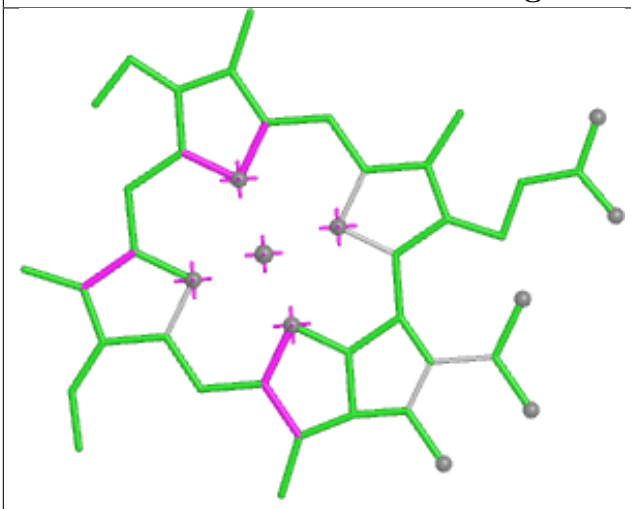


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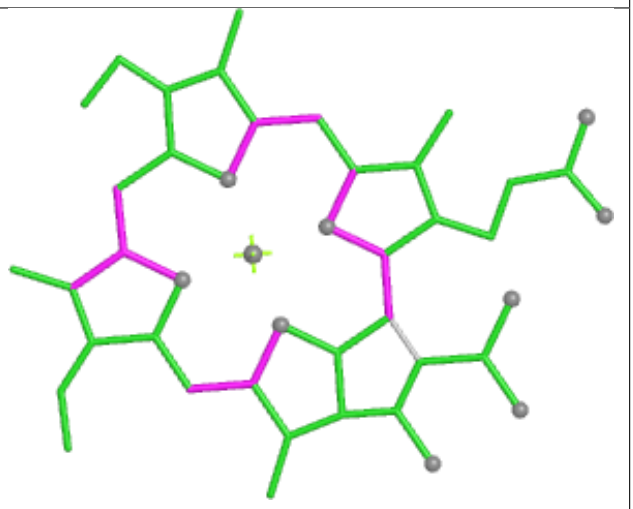


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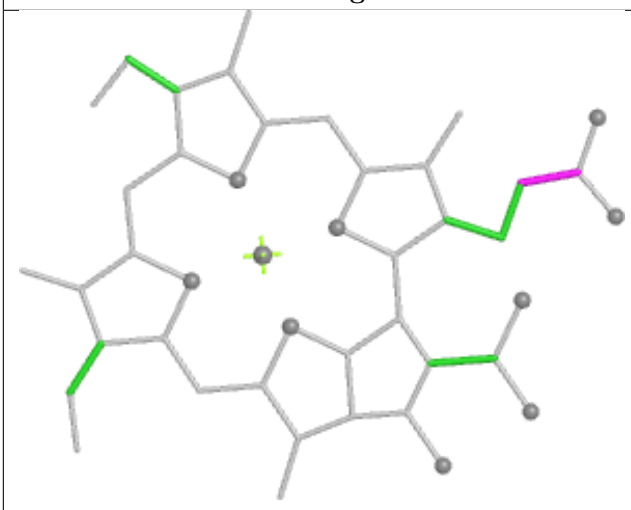
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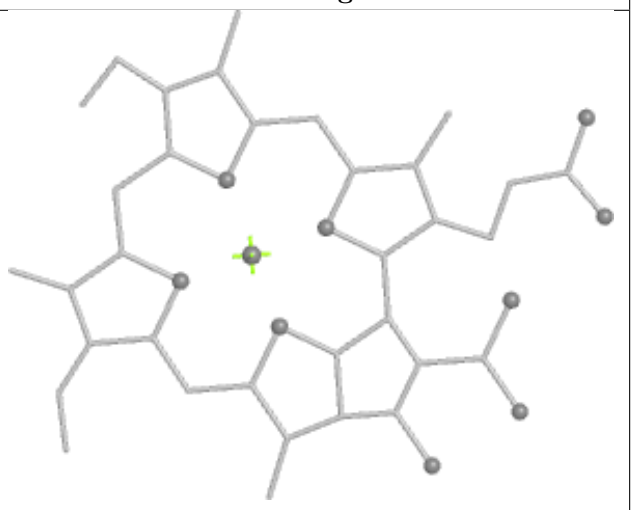
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Bond angles

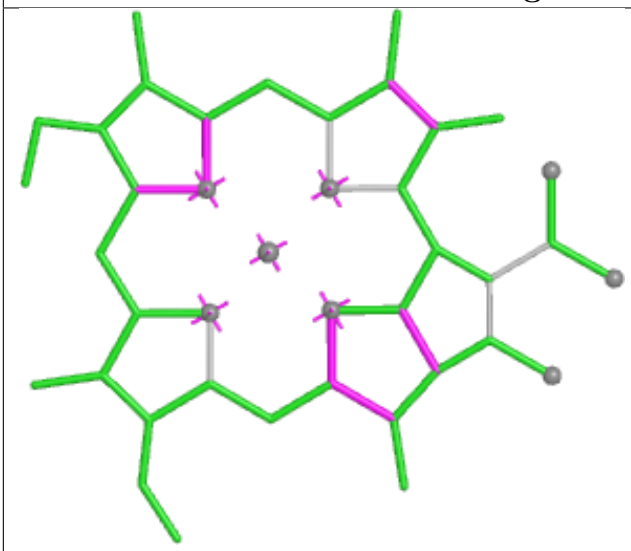


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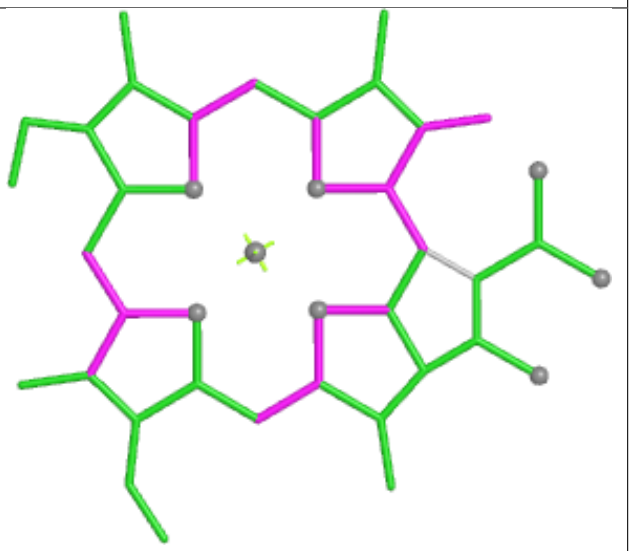


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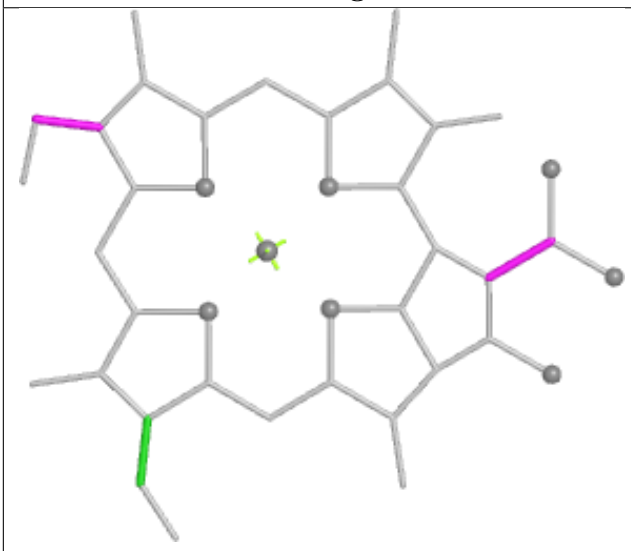
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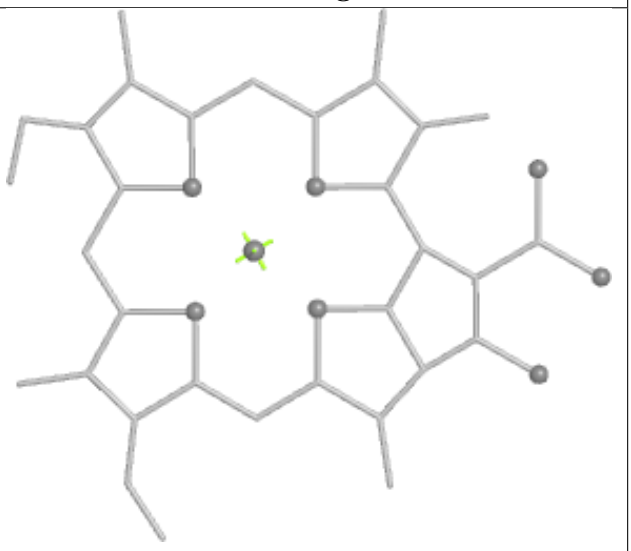
Bond lengths



Bond angles

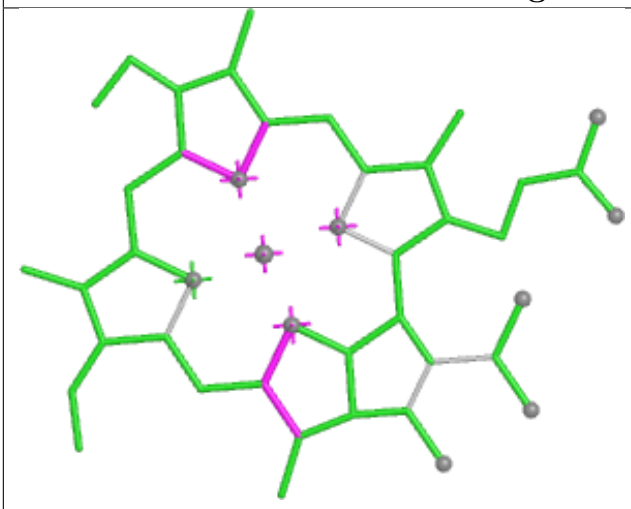


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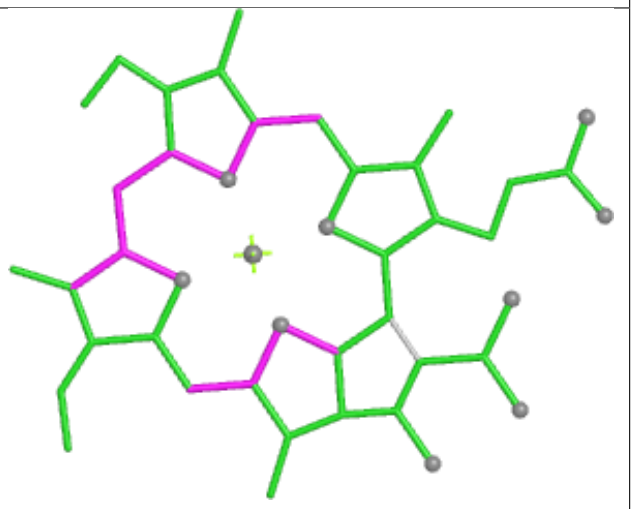


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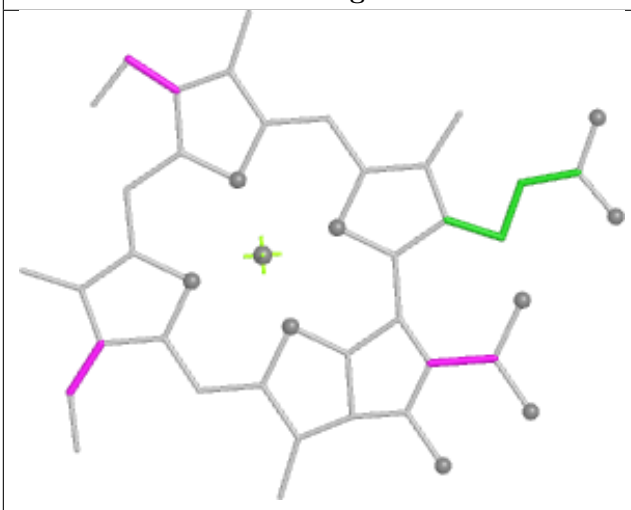
Ligand CLA 4 310



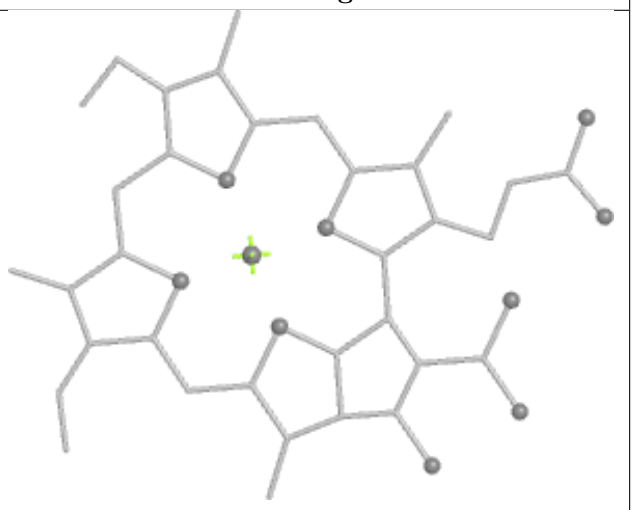
Bond lengths



Bond angles

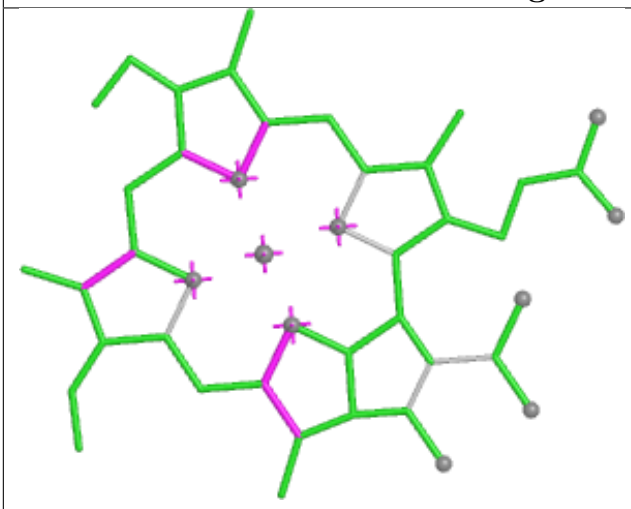


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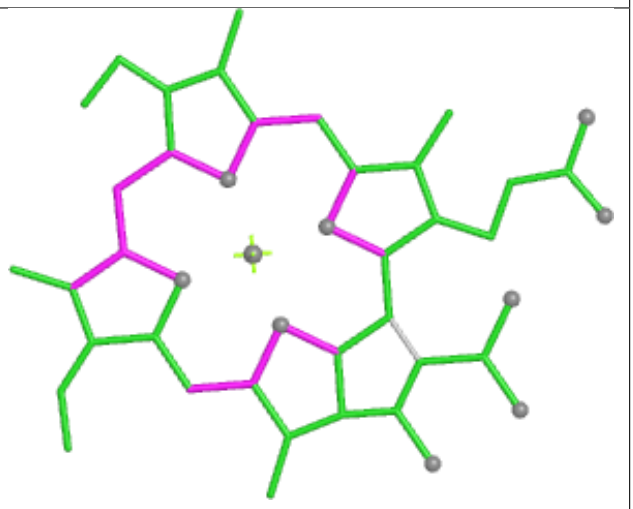


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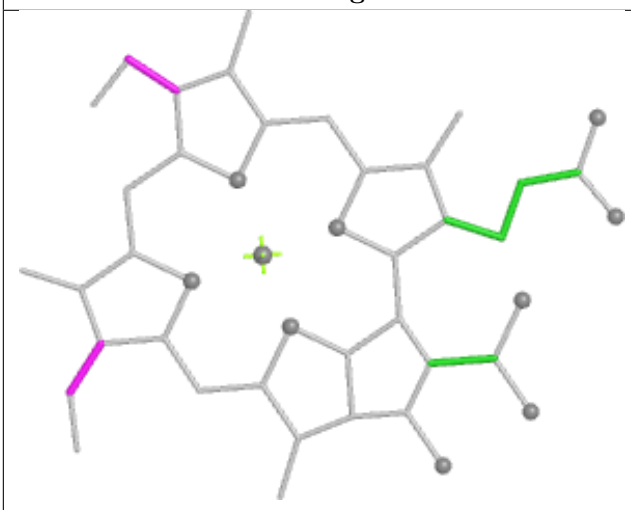
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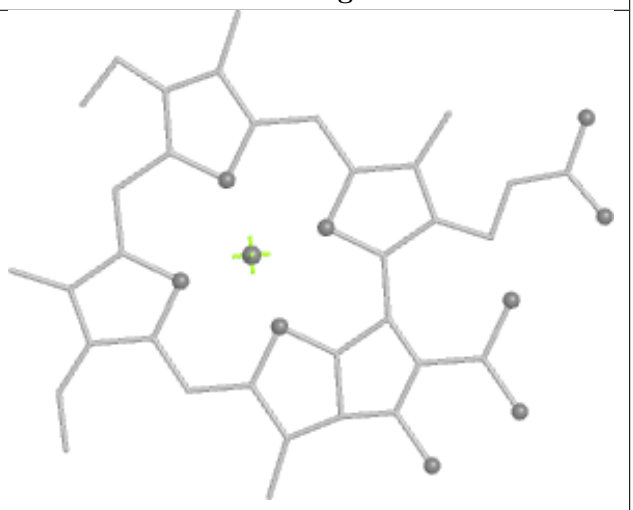
Bond lengths



Bond angles

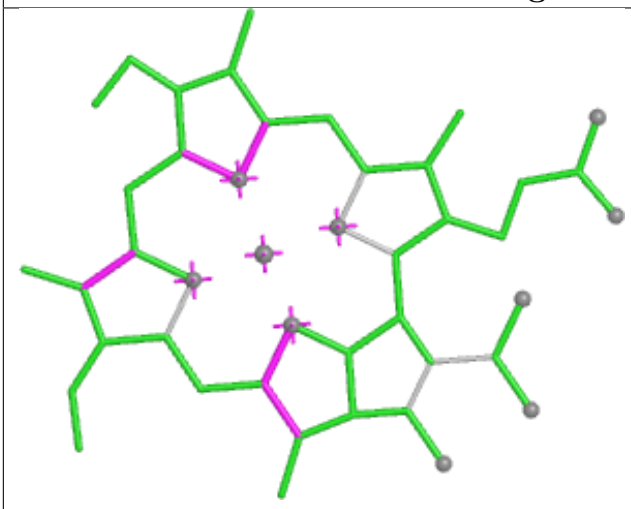


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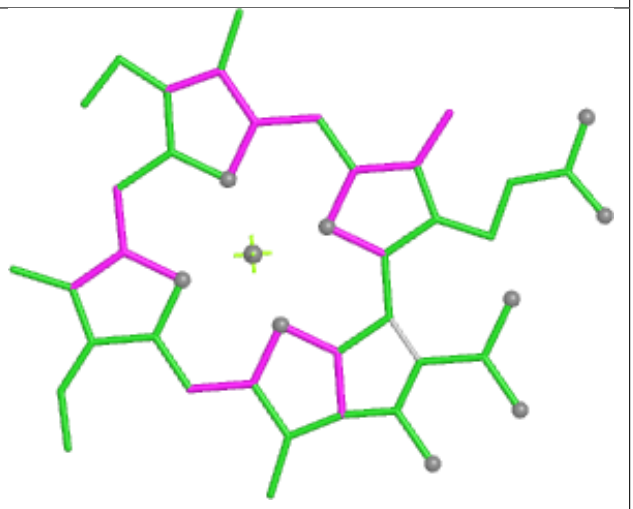


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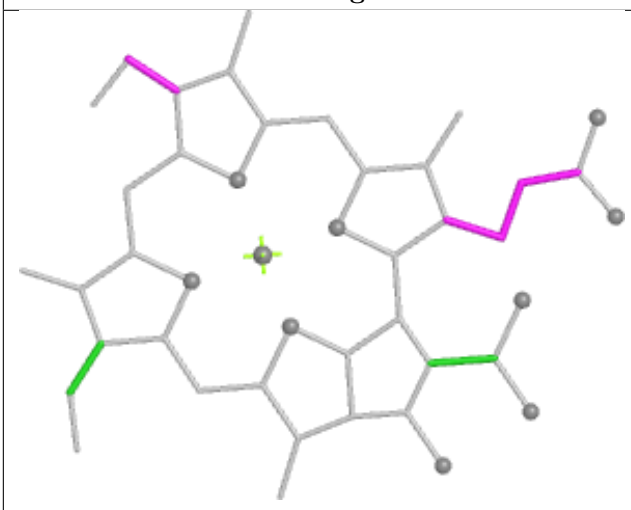
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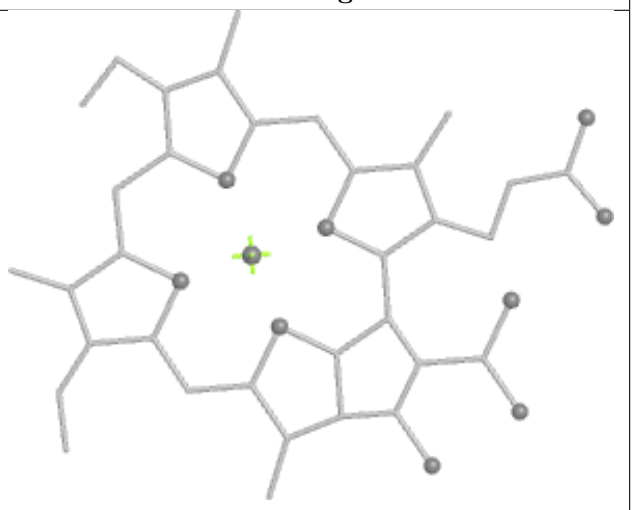
Bond lengths



Bond angles

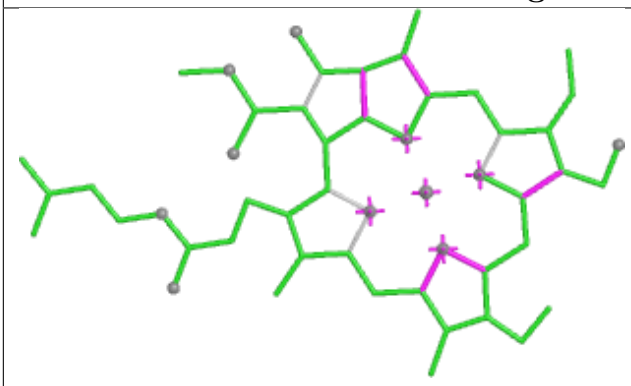


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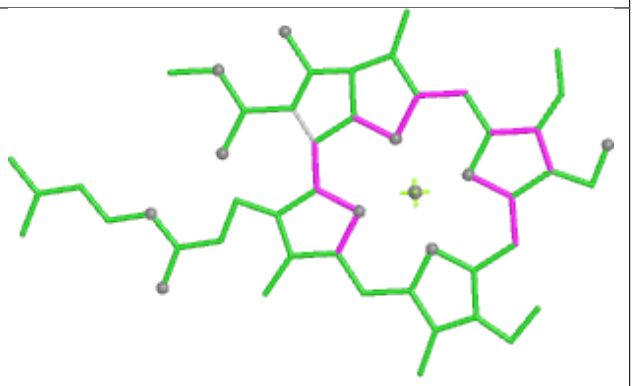


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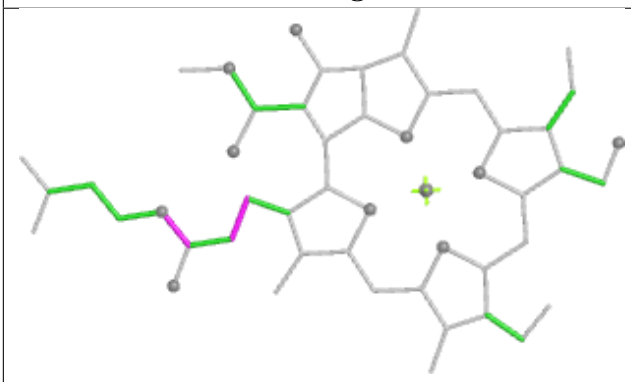
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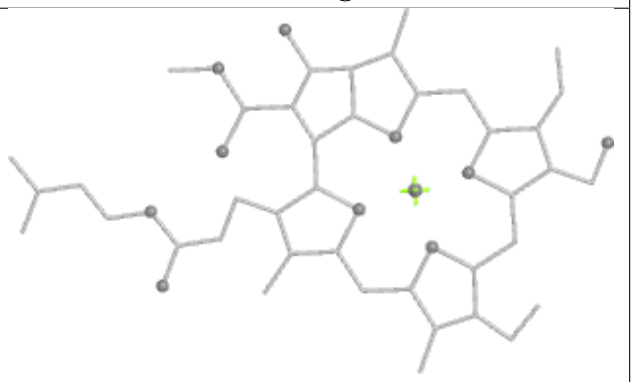
Bond lengths



Bond angles

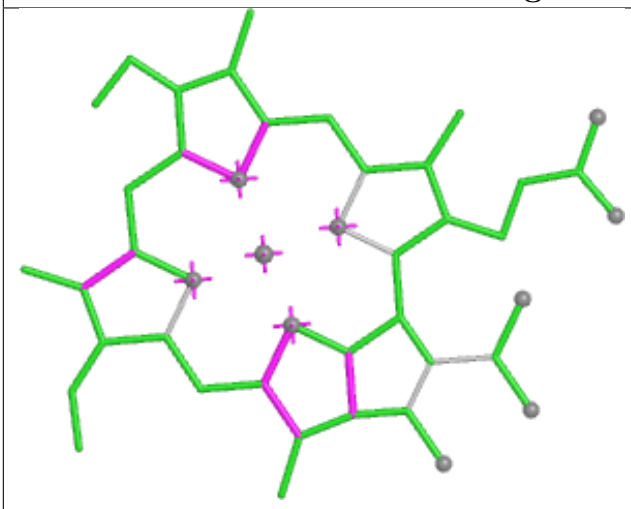


Torsions

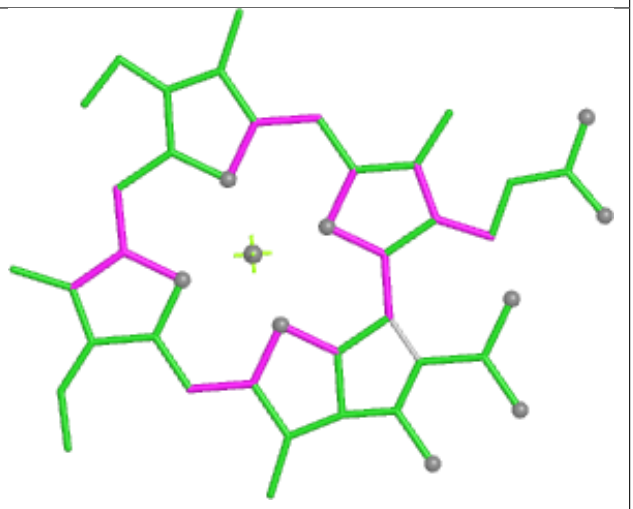


Rings

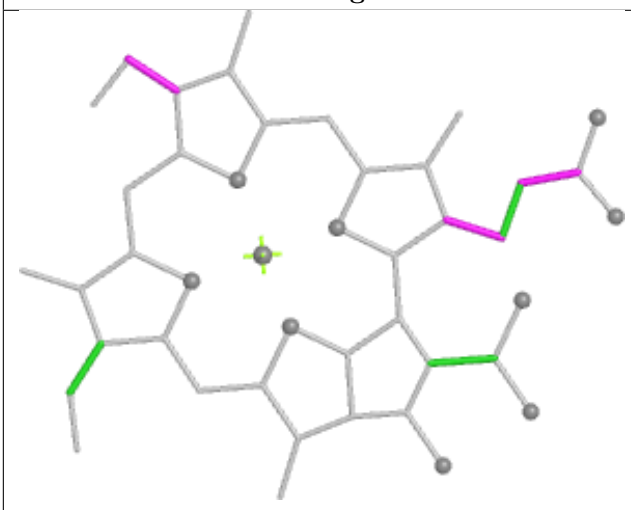
Ligand CLA B 825



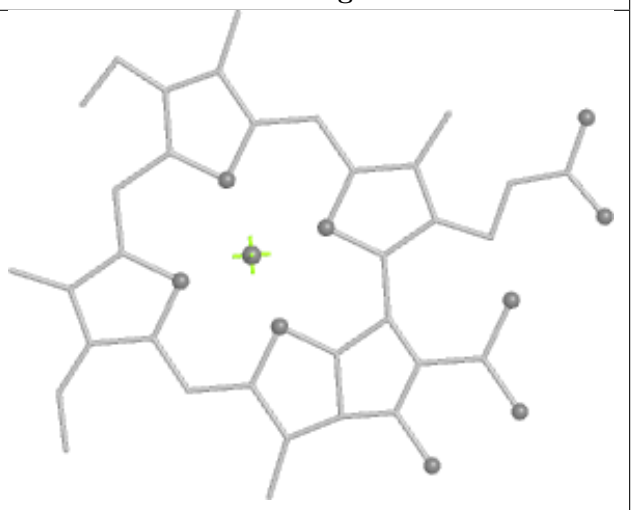
Bond lengths



Bond angles

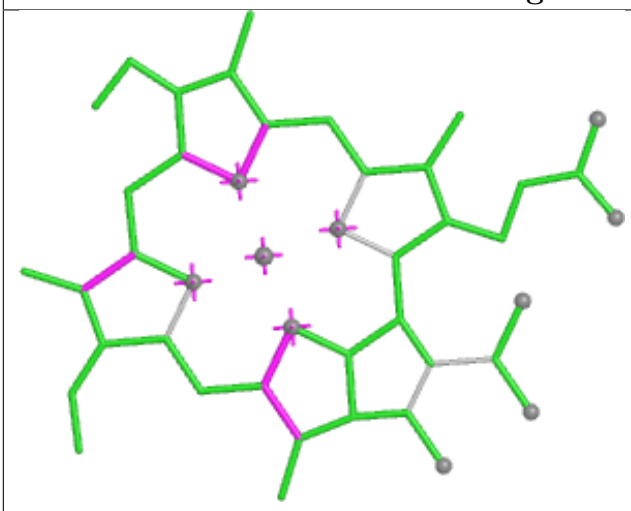


Torsions

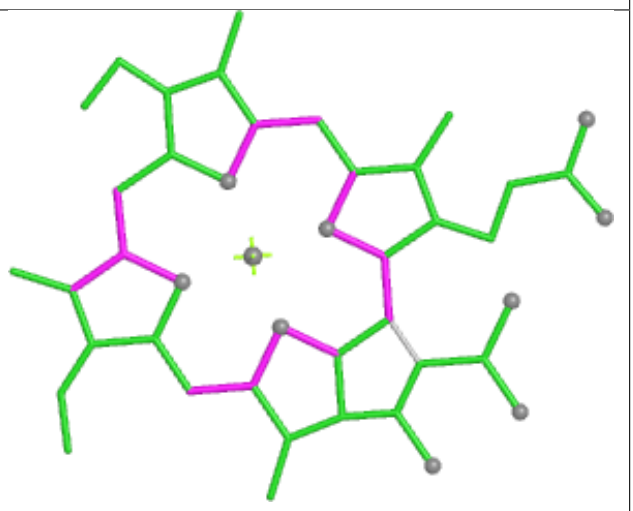


Rings

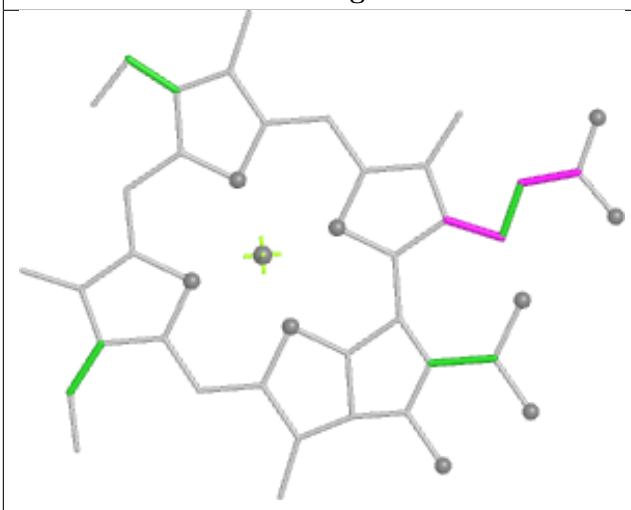
Ligand CLA L 203



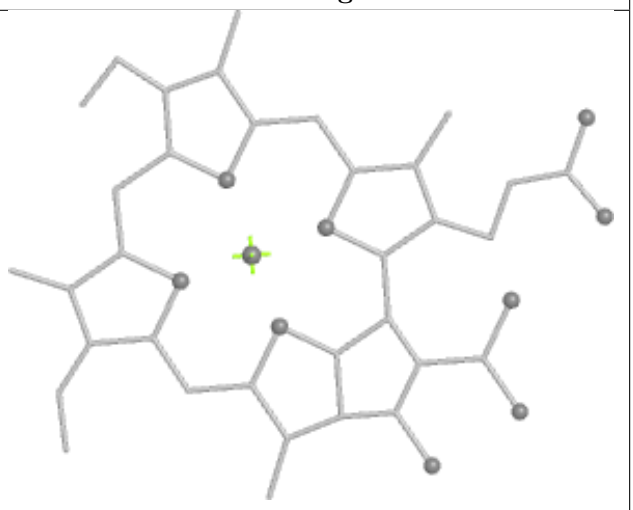
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	738/751 (98%)	0.39	31 (4%) 40 29	91, 155, 210, 250	0
2	B	728/735 (99%)	0.46	26 (3%) 46 33	106, 177, 229, 279	0
3	C	80/81 (98%)	0.58	7 (8%) 15 14	136, 172, 199, 219	0
4	D	141/196 (71%)	0.27	3 (2%) 63 48	132, 182, 217, 255	0
5	E	61/97 (62%)	0.36	0 100 100	111, 159, 184, 195	0
6	F	150/227 (66%)	0.17	6 (4%) 42 30	89, 138, 175, 204	0
7	G	85/126 (67%)	0.48	6 (7%) 22 18	175, 261, 344, 421	0
8	H	90/130 (69%)	0.55	3 (3%) 49 36	197, 283, 367, 430	0
9	I	29/106 (27%)	0.86	2 (6%) 23 18	204, 305, 350, 396	0
10	J	39/41 (95%)	0.12	1 (2%) 57 42	107, 131, 165, 179	0
11	K	44/113 (38%)	0.72	6 (13%) 7 8	195, 342, 432, 470	0
12	L	150/196 (76%)	0.74	7 (4%) 36 27	185, 331, 501, 579	0
13	0	182/228 (79%)	0.63	13 (7%) 22 18	101, 152, 203, 245	0
13	1	182/228 (79%)	0.48	13 (7%) 22 18	80, 119, 167, 195	0
14	8	193/243 (79%)	0.36	9 (4%) 36 27	61, 100, 129, 158	0
15	7	209/241 (86%)	0.48	11 (5%) 32 24	55, 89, 126, 164	0
16	3	201/298 (67%)	0.17	4 (1%) 65 49	73, 122, 160, 195	0
17	4	202/264 (76%)	0.31	7 (3%) 47 34	70, 106, 141, 170	0
18	6	184/257 (71%)	0.14	5 (2%) 56 42	43, 90, 128, 185	0
19	5	193/257 (75%)	0.33	8 (4%) 41 29	56, 95, 137, 166	0
All	All	3881/4815 (80%)	0.41	168 (4%) 40 29	43, 147, 298, 579	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	VAL	5.1
13	1	124	PRO	4.5
7	G	115	LEU	4.4
2	B	65	ASN	4.3
15	7	139	PHE	4.1
1	A	391	PHE	4.0
13	0	223	ILE	4.0
13	0	74	PHE	3.8
14	8	158	ALA	3.7
2	B	109	GLY	3.7
1	A	24	THR	3.6
1	A	427	LEU	3.6
4	D	77	LYS	3.5
1	A	540	ALA	3.5
6	F	137	PRO	3.5
14	8	43	PRO	3.5
1	A	105	LEU	3.4
1	A	220	VAL	3.4
13	1	92	SER	3.3
1	A	513	ASP	3.3
3	C	12	ILE	3.3
1	A	373	ALA	3.3
3	C	28	MET	3.3
1	A	515	VAL	3.3
14	8	233	TYR	3.2
1	A	180	HIS	3.2
1	A	239	LEU	3.2
12	L	60	THR	3.2
7	G	111	GLY	3.1
13	0	55	GLY	3.1
14	8	116	PHE	3.1
4	D	147	VAL	3.0
14	8	240	LEU	3.0
2	B	648	ALA	3.0
11	K	37	ILE	3.0
15	7	210	ALA	2.9
2	B	491	GLN	2.9
13	1	193	ALA	2.9
16	3	197	PHE	2.9
17	4	87	GLY	2.9
16	3	215	LEU	2.9
1	A	224	VAL	2.9
19	5	121	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	235	ALA	2.8
14	8	82	ALA	2.8
2	B	201	PRO	2.8
15	7	115	ILE	2.8
19	5	103	ALA	2.8
13	1	196	ALA	2.7
17	4	130	ALA	2.7
3	C	38	GLN	2.7
1	A	711	PRO	2.7
19	5	71	ARG	2.7
1	A	182	HIS	2.7
18	6	103	GLU	2.7
2	B	360	ALA	2.7
1	A	670	LEU	2.7
12	L	54	MET	2.7
8	H	78	SER	2.7
9	I	90	ILE	2.6
3	C	81	TYR	2.6
1	A	387	GLN	2.6
13	0	56	ASN	2.6
8	H	108	LEU	2.6
15	7	232	ALA	2.6
2	B	558	PHE	2.6
2	B	621	LEU	2.6
6	F	156	PHE	2.5
15	7	204	PHE	2.5
3	C	24	ASP	2.5
2	B	363	ALA	2.5
2	B	392	ALA	2.5
13	1	125	PHE	2.5
1	A	468	PRO	2.5
17	4	124	GLY	2.5
1	A	366	ILE	2.5
3	C	26	LEU	2.5
14	8	84	VAL	2.5
15	7	205	ALA	2.5
13	1	173	LEU	2.5
1	A	588	ALA	2.4
1	A	507	SER	2.4
17	4	149	LEU	2.4
13	0	57	TYR	2.4
2	B	298	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	394	PHE	2.4
12	L	109	VAL	2.4
11	K	103	ILE	2.4
15	7	164	TYR	2.4
18	6	174	VAL	2.4
13	1	175	LEU	2.4
1	A	337	GLY	2.3
2	B	485	ALA	2.3
14	8	161	LYS	2.3
19	5	117	ASN	2.3
13	0	194	GLN	2.3
15	7	95	VAL	2.3
17	4	95	TRP	2.3
3	C	40	ALA	2.3
8	H	111	THR	2.3
12	L	124	LEU	2.3
2	B	651	PHE	2.3
6	F	99	ALA	2.3
13	0	49	LEU	2.3
17	4	122	ASN	2.3
13	0	51	ASP	2.3
11	K	87	VAL	2.3
13	0	225	VAL	2.3
13	1	129	ALA	2.3
11	K	107	LEU	2.3
13	0	48	TRP	2.2
12	L	112	THR	2.2
19	5	114	THR	2.2
1	A	709	VAL	2.2
4	D	95	ILE	2.2
6	F	147	GLY	2.2
19	5	184	THR	2.2
1	A	434	ARG	2.2
17	4	160	VAL	2.2
1	A	158	GLN	2.2
7	G	86	ILE	2.2
13	1	177	GLU	2.2
6	F	135	ALA	2.2
13	0	58	GLY	2.2
2	B	668	TRP	2.2
9	I	94	THR	2.2
2	B	625	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
12	L	55	LEU	2.2
13	0	40	LEU	2.2
1	A	308	ALA	2.2
2	B	205	GLY	2.2
16	3	129	GLY	2.2
14	8	185	TRP	2.2
13	0	87	LEU	2.2
18	6	198	GLY	2.2
1	A	510	TRP	2.2
12	L	167	TRP	2.2
7	G	112	PHE	2.1
18	6	138	VAL	2.1
2	B	50	SER	2.1
13	1	215	GLY	2.1
15	7	82	GLY	2.1
2	B	395	PHE	2.1
15	7	67	TRP	2.1
11	K	86	ILE	2.1
2	B	362	GLN	2.1
2	B	261	GLY	2.1
7	G	34	PRO	2.1
2	B	213	PHE	2.1
16	3	138	ASN	2.1
2	B	47	ILE	2.1
13	1	127	LEU	2.1
7	G	85	THR	2.1
13	1	164	ALA	2.1
1	A	523	MET	2.1
6	F	143	TYR	2.1
11	K	90	LEU	2.0
1	A	462	MET	2.0
1	A	55	ASP	2.0
13	1	220	THR	2.0
18	6	30	PRO	2.0
19	5	110	PRO	2.0
2	B	409	LEU	2.0
2	B	688	LEU	2.0
10	J	37	LEU	2.0
19	5	231	ILE	2.0
15	7	162	ASN	2.0
1	A	431	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	L	204	44/65	0.09	0.18	210,255,268,270	0
20	CLA	K	201	44/65	0.15	0.15	212,242,252,254	0
20	CLA	K	202	27/65	0.24	0.13	214,233,244,248	0
20	CLA	G	203	44/65	0.45	0.15	155,244,268,275	0
20	CLA	G	201	44/65	0.47	0.15	201,273,294,301	0
26	LMT	B	849	31/35	0.48	0.12	164,183,224,228	0
20	CLA	L	202	44/65	0.50	0.13	240,279,308,311	0
20	CLA	L	203	44/65	0.55	0.17	225,282,298,301	0
20	CLA	G	202	44/65	0.58	0.12	177,217,238,249	0
20	CLA	B	813	44/65	0.61	0.12	195,214,224,228	0
24	BCR	H	201	40/40	0.63	0.16	189,232,262,263	0
23	LHG	3	1019	20/49	0.64	0.15	202,256,264,269	0
20	CLA	B	815	44/65	0.65	0.13	128,158,232,249	0
20	CLA	A	840	44/65	0.66	0.14	173,213,233,245	0
24	BCR	I	201	40/40	0.68	0.17	194,224,242,243	0
24	BCR	A	850	40/40	0.68	0.20	177,223,310,313	0
27	LMG	5	324	45/55	0.68	0.16	46,97,156,183	0
24	BCR	G	204	40/40	0.69	0.14	206,227,250,259	0
24	BCR	G	205	40/40	0.69	0.18	119,205,273,275	0
27	LMG	8	319	44/55	0.70	0.21	151,179,216,229	0
29	CHL	0	317	61/66	0.70	0.17	186,220,246,264	0
29	CHL	1	1015	61/66	0.71	0.21	139,177,205,216	0
27	LMG	0	303	50/55	0.72	0.15	196,217,237,261	0
26	LMT	3	1018	31/35	0.73	0.19	111,185,218,227	0
20	CLA	A	822	44/65	0.74	0.15	170,196,205,216	0
24	BCR	1	1001	40/40	0.75	0.18	91,137,239,246	0
20	CLA	B	836	44/65	0.75	0.13	142,175,192,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	5	312	44/65	0.77	0.18	106,124,150,154	0
24	BCR	B	845	40/40	0.77	0.17	142,194,236,238	0
24	BCR	B	847	40/40	0.77	0.17	137,156,174,181	0
24	BCR	B	844	40/40	0.78	0.16	164,196,213,216	0
20	CLA	B	812	44/65	0.78	0.15	140,165,186,188	0
20	CLA	F	303	44/65	0.78	0.17	118,132,162,189	0
24	BCR	A	846	40/40	0.78	0.14	134,183,205,209	0
20	CLA	3	1011	40/65	0.78	0.13	180,202,216,218	0
27	LMG	8	318	28/55	0.79	0.22	72,118,150,161	0
29	CHL	0	314	47/66	0.79	0.19	164,201,252,295	0
20	CLA	3	1012	44/65	0.79	0.12	139,174,214,234	0
27	LMG	4	318	34/55	0.79	0.21	126,166,215,225	0
29	CHL	4	312	47/66	0.79	0.15	97,120,136,169	0
24	BCR	A	844	40/40	0.80	0.20	123,155,197,200	0
23	LHG	8	301	49/49	0.80	0.21	111,140,220,230	0
25	DGD	B	848	61/66	0.80	0.16	120,168,217,250	0
29	CHL	8	317	61/66	0.80	0.17	96,109,139,149	0
25	DGD	5	319	51/66	0.80	0.19	96,147,186,192	0
20	CLA	5	323	44/65	0.80	0.14	75,122,154,168	0
20	CLA	A	821	44/65	0.81	0.12	159,185,199,231	0
20	CLA	5	322	44/65	0.81	0.11	95,115,135,153	0
20	CLA	B	823	44/65	0.81	0.13	153,173,203,206	0
22	PQN	B	842	33/33	0.81	0.17	121,166,191,200	0
24	BCR	8	302	40/40	0.81	0.19	91,102,155,160	0
20	CLA	B	850	43/65	0.82	0.12	183,226,244,260	0
27	LMG	J	101	30/55	0.82	0.15	135,158,176,180	0
27	LMG	6	319	44/55	0.82	0.25	95,120,158,169	0
22	PQN	A	842	33/33	0.83	0.27	106,115,157,162	0
20	CLA	A	831	44/65	0.83	0.11	132,146,202,227	0
23	LHG	0	302	21/49	0.83	0.11	136,159,173,187	0
29	CHL	5	313	47/66	0.83	0.14	65,87,107,125	0
28	LUT	0	318	42/42	0.84	0.18	122,137,164,167	0
24	BCR	F	304	40/40	0.84	0.19	104,116,140,143	0
29	CHL	0	315	51/66	0.84	0.17	154,226,245,260	0
20	CLA	B	826	44/65	0.84	0.12	161,182,190,192	0
24	BCR	B	804	40/40	0.84	0.13	122,142,155,163	0
29	CHL	1	1012	47/66	0.84	0.11	102,132,156,174	0
20	CLA	B	803	44/65	0.84	0.14	170,200,215,220	0
24	BCR	A	845	40/40	0.84	0.18	102,120,156,172	0
20	CLA	B	824	44/65	0.84	0.16	148,171,185,200	0
20	CLA	0	306	44/65	0.85	0.10	123,146,154,163	0
20	CLA	0	311	44/65	0.85	0.12	113,128,159,183	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	0	313	44/65	0.85	0.14	90,114,149,162	0
20	CLA	A	819	44/65	0.85	0.13	147,180,190,194	0
20	CLA	B	816	44/65	0.85	0.12	174,190,199,205	0
20	CLA	5	311	44/65	0.85	0.12	88,107,161,222	0
20	CLA	A	820	44/65	0.85	0.11	135,178,186,193	0
20	CLA	A	815	44/65	0.85	0.15	120,138,154,165	0
28	LUT	0	304	42/42	0.85	0.23	128,147,202,207	0
20	CLA	1	1009	44/65	0.86	0.10	83,108,131,160	0
20	CLA	1	1017	44/65	0.86	0.14	92,114,125,136	0
20	CLA	B	840	44/65	0.86	0.12	158,197,210,214	0
24	BCR	J	103	40/40	0.86	0.15	113,134,148,157	0
20	CLA	J	102	44/65	0.86	0.10	121,142,156,168	0
24	BCR	A	847	40/40	0.86	0.11	120,138,183,185	0
24	BCR	4	302	40/40	0.86	0.18	99,130,160,164	0
20	CLA	0	307	44/65	0.86	0.12	90,104,125,144	0
20	CLA	A	812	44/65	0.86	0.12	95,111,124,135	0
29	CHL	8	314	47/66	0.86	0.15	102,134,169,185	0
20	CLA	B	801	44/65	0.86	0.13	118,166,178,191	0
20	CLA	A	833	44/65	0.86	0.12	181,193,207,213	0
23	LHG	A	849	49/49	0.86	0.18	121,149,179,196	0
20	CLA	B	810	44/65	0.86	0.12	160,186,210,222	0
20	CLA	1	1004	44/65	0.86	0.13	91,123,152,161	0
30	XAT	7	1002	44/44	0.86	0.19	69,83,91,97	0
28	LUT	1	1002	42/42	0.87	0.24	99,133,171,176	0
24	BCR	B	843	40/40	0.87	0.12	175,201,216,221	0
20	CLA	B	822	44/65	0.87	0.09	130,151,188,201	0
20	CLA	B	832	44/65	0.87	0.11	143,153,171,179	0
24	BCR	B	846	40/40	0.87	0.14	143,161,184,187	0
24	BCR	7	1003	40/40	0.87	0.25	92,124,149,156	0
20	CLA	B	835	44/65	0.87	0.14	127,158,171,189	0
29	CHL	1	1013	51/66	0.87	0.19	111,140,153,172	0
24	BCR	F	301	40/40	0.87	0.18	104,125,152,163	0
20	CLA	A	832	44/65	0.87	0.12	155,176,191,202	0
29	CHL	4	315	61/66	0.87	0.19	113,149,173,192	0
20	CLA	B	814	44/65	0.87	0.12	149,201,229,238	0
23	LHG	4	301	49/49	0.87	0.19	110,136,193,195	0
20	CLA	B	820	44/65	0.88	0.14	149,174,193,209	0
20	CLA	1	1014	44/65	0.88	0.12	86,113,129,136	0
20	CLA	A	823	44/65	0.88	0.13	155,173,187,192	0
20	CLA	4	310	44/65	0.88	0.11	85,107,115,129	0
20	CLA	6	310	44/65	0.88	0.13	84,99,108,121	0
20	CLA	A	830	44/65	0.88	0.14	161,200,217,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	A	848	40/40	0.88	0.15	102,125,154,157	0
28	LUT	1	1016	42/42	0.88	0.18	105,124,136,145	0
24	BCR	3	1004	40/40	0.88	0.15	111,134,161,169	0
20	CLA	0	310	44/65	0.88	0.12	98,110,151,172	0
20	CLA	B	841	44/65	0.88	0.10	84,105,159,184	0
24	BCR	6	302	40/40	0.88	0.18	98,133,141,150	0
24	BCR	5	320	40/40	0.88	0.17	81,107,129,134	0
20	CLA	A	809	44/65	0.88	0.15	98,121,134,143	0
20	CLA	0	316	44/65	0.88	0.13	145,186,199,209	0
20	CLA	L	201	44/65	0.88	0.12	149,200,218,235	0
23	LHG	A	843	40/49	0.88	0.13	166,193,211,225	0
20	CLA	A	852	44/65	0.88	0.10	141,151,167,187	0
29	CHL	6	316	61/66	0.88	0.15	95,112,152,159	0
20	CLA	B	819	44/65	0.88	0.14	171,196,246,285	0
20	CLA	1	1007	44/65	0.88	0.12	110,118,130,141	0
20	CLA	A	825	44/65	0.89	0.13	117,135,157,167	0
20	CLA	B	833	44/65	0.89	0.13	94,117,146,175	0
20	CLA	B	808	44/65	0.89	0.11	134,145,169,180	0
20	CLA	8	311	44/65	0.89	0.14	72,109,143,161	0
20	CLA	6	311	44/65	0.89	0.11	89,99,113,132	0
20	CLA	8	313	44/65	0.89	0.13	71,101,113,120	0
20	CLA	3	1007	44/65	0.89	0.11	118,139,154,166	0
20	CLA	A	826	44/65	0.89	0.10	104,122,141,146	0
20	CLA	B	811	44/65	0.89	0.09	130,155,170,179	0
20	CLA	A	816	44/65	0.89	0.12	131,154,200,217	0
20	CLA	1	1005	44/65	0.89	0.11	84,120,130,145	0
20	CLA	0	309	44/65	0.89	0.14	143,171,200,215	0
28	LUT	J	104	42/42	0.89	0.15	79,115,162,172	0
20	CLA	B	830	44/65	0.89	0.14	132,144,168,179	0
29	CHL	5	317	43/66	0.89	0.12	80,97,120,132	0
30	XAT	8	304	44/44	0.89	0.17	50,85,95,109	0
20	CLA	1	1010	44/65	0.89	0.14	95,135,156,184	0
20	CLA	8	316	44/65	0.90	0.14	77,101,116,126	0
20	CLA	3	1006	44/65	0.90	0.10	104,132,140,148	0
20	CLA	B	807	44/65	0.90	0.09	119,158,173,175	0
20	CLA	6	308	44/65	0.90	0.11	32,39,48,71	0
20	CLA	B	829	44/65	0.90	0.12	155,179,193,196	0
20	CLA	B	817	44/65	0.90	0.10	148,178,197,209	0
29	CHL	7	1012	47/66	0.90	0.13	98,115,161,176	0
29	CHL	7	1017	66/66	0.90	0.16	100,117,150,172	0
20	CLA	6	318	44/65	0.90	0.10	79,94,106,123	0
20	CLA	6	320	44/65	0.90	0.11	68,87,93,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	5	305	44/65	0.90	0.10	66,81,103,125	0
20	CLA	5	309	44/65	0.90	0.11	84,103,114,120	0
20	CLA	5	310	44/65	0.90	0.11	91,112,129,150	0
29	CHL	4	316	43/66	0.90	0.12	93,105,118,145	0
29	CHL	6	313	47/66	0.90	0.14	83,98,121,171	0
20	CLA	0	312	44/65	0.90	0.12	101,128,147,160	0
20	CLA	B	831	44/65	0.90	0.12	141,164,178,198	0
20	CLA	0	305	44/65	0.90	0.12	115,150,185,194	0
20	CLA	B	818	44/65	0.90	0.11	214,236,252,260	0
20	CLA	A	811	44/65	0.90	0.12	110,148,160,171	0
28	LUT	3	1001	42/42	0.91	0.15	89,116,145,156	0
20	CLA	A	803	44/65	0.91	0.11	80,90,114,117	0
20	CLA	6	312	44/65	0.91	0.14	59,98,130,141	0
28	LUT	4	317	42/42	0.91	0.14	75,98,117,123	0
28	LUT	6	303	42/42	0.91	0.15	64,81,96,113	0
28	LUT	5	302	42/42	0.91	0.15	68,88,99,105	0
20	CLA	A	835	44/65	0.91	0.11	138,164,192,219	0
20	CLA	3	1013	44/65	0.91	0.11	89,133,159,173	0
20	CLA	1	1003	44/65	0.91	0.12	68,85,114,138	0
20	CLA	5	308	44/65	0.91	0.12	81,90,105,119	0
20	CLA	A	836	44/65	0.91	0.12	143,180,192,207	0
20	CLA	F	302	44/65	0.91	0.11	91,99,108,109	0
20	CLA	A	810	44/65	0.91	0.12	101,123,131,139	0
20	CLA	1	1008	44/65	0.91	0.13	96,118,156,180	0
20	CLA	F	305	44/65	0.91	0.11	102,130,154,167	0
20	CLA	A	817	44/65	0.91	0.09	107,120,144,168	0
20	CLA	1	1011	44/65	0.91	0.13	99,108,125,138	0
29	CHL	4	313	51/66	0.91	0.15	86,105,120,132	0
20	CLA	A	814	40/65	0.91	0.12	147,160,199,217	0
20	CLA	7	1006	44/65	0.91	0.11	62,81,91,104	0
20	CLA	4	305	44/65	0.91	0.10	76,87,106,122	0
20	CLA	4	307	44/65	0.91	0.11	63,79,93,99	0
20	CLA	A	824	44/65	0.91	0.12	102,147,173,183	0
20	CLA	B	806	44/65	0.91	0.13	166,188,198,201	0
20	CLA	3	1010	44/65	0.91	0.12	99,114,127,142	0
28	LUT	7	1001	42/42	0.91	0.14	56,73,85,91	0
30	XAT	4	303	44/44	0.91	0.17	66,91,98,101	0
30	XAT	6	304	44/44	0.91	0.17	39,78,87,91	0
20	CLA	3	1009	44/65	0.92	0.10	87,120,129,132	0
20	CLA	4	308	44/65	0.92	0.10	65,82,94,100	0
20	CLA	4	309	44/65	0.92	0.09	69,79,107,136	0
24	BCR	3	1003	40/40	0.92	0.15	63,111,123,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	A	827	44/65	0.92	0.13	110,133,141,161	0
20	CLA	4	311	44/65	0.92	0.11	63,96,112,119	0
20	CLA	6	307	44/65	0.92	0.12	65,82,89,92	0
20	CLA	A	839	44/65	0.92	0.08	70,83,98,111	0
20	CLA	6	309	44/65	0.92	0.12	64,88,100,134	0
20	CLA	B	838	44/65	0.92	0.13	114,136,149,158	0
29	CHL	7	1015	46/66	0.92	0.12	70,81,108,131	0
20	CLA	A	801	44/65	0.92	0.12	93,116,157,224	0
20	CLA	3	1017	44/65	0.92	0.10	91,110,140,160	0
20	CLA	A	851	44/65	0.92	0.11	115,135,143,146	0
20	CLA	B	809	44/65	0.92	0.10	150,162,177,184	0
20	CLA	5	304	44/65	0.92	0.13	69,97,114,125	0
20	CLA	8	309	44/65	0.92	0.10	75,95,102,114	0
20	CLA	5	307	44/65	0.92	0.11	52,64,76,83	0
20	CLA	A	834	44/65	0.92	0.13	144,167,186,190	0
20	CLA	A	818	44/65	0.92	0.10	113,142,151,156	0
20	CLA	B	802	44/65	0.92	0.12	99,123,145,168	0
20	CLA	B	821	44/65	0.92	0.09	133,160,183,185	0
20	CLA	7	1007	44/65	0.92	0.12	52,60,67,75	0
20	CLA	5	321	44/65	0.92	0.09	60,71,80,82	0
20	CLA	7	1009	44/65	0.92	0.11	62,80,95,104	0
20	CLA	B	834	44/65	0.92	0.10	98,111,121,136	0
20	CLA	0	308	44/65	0.92	0.12	93,113,124,125	0
20	CLA	8	308	44/65	0.93	0.12	53,76,86,92	0
20	CLA	B	837	44/65	0.93	0.10	100,117,128,141	0
20	CLA	4	314	44/65	0.93	0.12	77,98,118,140	0
20	CLA	6	301	44/65	0.93	0.14	93,111,124,154	0
20	CLA	3	1015	44/65	0.93	0.11	99,108,120,132	0
29	CHL	7	1013	48/66	0.93	0.14	73,86,106,112	0
20	CLA	8	310	44/65	0.93	0.10	51,72,106,148	0
20	CLA	A	806	44/65	0.93	0.09	92,115,135,141	0
20	CLA	A	837	44/65	0.93	0.10	91,107,122,126	0
20	CLA	A	838	44/65	0.93	0.11	98,111,134,136	0
20	CLA	7	1005	44/65	0.93	0.08	64,79,92,106	0
20	CLA	A	829	44/65	0.93	0.10	90,109,125,128	0
20	CLA	A	813	44/65	0.93	0.12	112,132,149,155	0
28	LUT	8	303	42/42	0.93	0.12	60,74,91,96	0
20	CLA	7	1008	44/65	0.93	0.10	73,91,104,129	0
20	CLA	B	825	44/65	0.93	0.10	150,176,188,201	0
29	CHL	6	314	51/66	0.93	0.14	73,98,112,134	0
28	LUT	3	1002	42/42	0.93	0.16	97,117,129,142	0
20	CLA	7	1010	44/65	0.93	0.12	85,104,121,130	0

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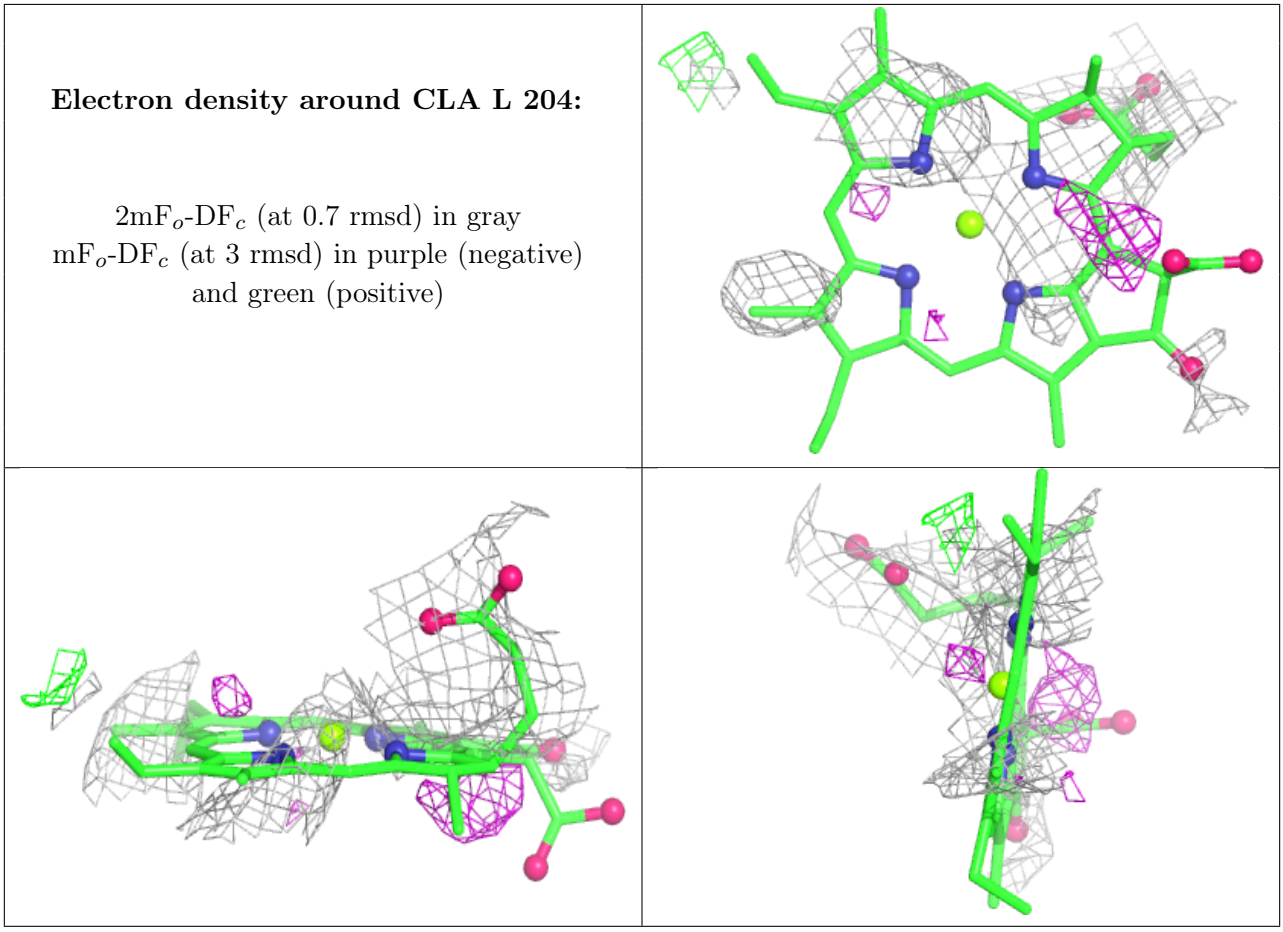
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	A	802	44/65	0.93	0.11	68,90,128,167	0
20	CLA	B	828	44/65	0.93	0.11	134,151,160,167	0
20	CLA	0	301	44/65	0.93	0.13	133,166,178,188	0
20	CLA	8	305	44/65	0.93	0.10	75,87,99,115	0
20	CLA	8	306	44/65	0.93	0.08	59,71,95,103	0
30	XAT	5	303	44/44	0.93	0.13	49,77,104,108	0
20	CLA	7	1011	44/65	0.94	0.11	73,87,129,156	0
20	CLA	8	312	44/65	0.94	0.10	78,90,106,124	0
20	CLA	A	804	44/65	0.94	0.12	124,142,150,157	0
20	CLA	1	1006	44/65	0.94	0.10	56,75,91,94	0
20	CLA	5	301	44/65	0.94	0.10	71,78,106,120	0
20	CLA	B	839	44/65	0.94	0.10	118,134,148,154	0
20	CLA	B	827	44/65	0.94	0.10	98,109,123,130	0
20	CLA	5	306	44/65	0.94	0.11	91,110,117,118	0
20	CLA	8	307	44/65	0.94	0.10	57,65,89,126	0
20	CLA	A	807	44/65	0.94	0.11	117,131,148,155	0
20	CLA	6	306	44/65	0.94	0.08	68,87,93,118	0
29	CHL	6	317	43/66	0.94	0.10	85,96,129,160	0
20	CLA	A	828	44/65	0.94	0.12	112,134,146,155	0
29	CHL	5	316	61/66	0.94	0.12	54,73,167,176	0
20	CLA	A	808	44/65	0.94	0.11	102,112,122,129	0
29	CHL	8	315	51/66	0.94	0.12	56,101,126,149	0
20	CLA	A	805	44/65	0.94	0.10	102,121,133,140	0
20	CLA	5	315	44/65	0.94	0.12	65,89,99,104	0
20	CLA	5	318	44/65	0.94	0.10	55,72,92,103	0
20	CLA	4	304	44/65	0.94	0.10	74,83,90,101	0
29	CHL	3	1014	47/66	0.95	0.12	83,110,124,131	0
23	LHG	7	1016	35/49	0.95	0.15	88,105,127,130	0
20	CLA	6	315	44/65	0.95	0.11	59,82,87,100	0
20	CLA	7	1014	44/65	0.95	0.09	73,91,97,111	0
20	CLA	3	1008	44/65	0.95	0.09	111,129,174,202	0
20	CLA	3	1005	44/65	0.95	0.10	78,106,124,128	0
20	CLA	7	1004	44/65	0.95	0.10	40,58,84,93	0
20	CLA	4	306	44/65	0.95	0.08	71,80,88,96	0
20	CLA	3	1016	44/65	0.95	0.10	66,74,123,169	0
20	CLA	6	305	44/65	0.95	0.08	44,58,76,90	0
29	CHL	5	314	51/66	0.96	0.10	64,82,117,121	0
20	CLA	B	805	44/65	0.96	0.08	87,109,132,149	0
21	SF4	A	841	8/8	0.98	0.03	110,119,124,131	0
21	SF4	C	1001	8/8	0.98	0.03	136,146,148,158	0
21	SF4	C	1002	8/8	0.99	0.03	143,149,158,161	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

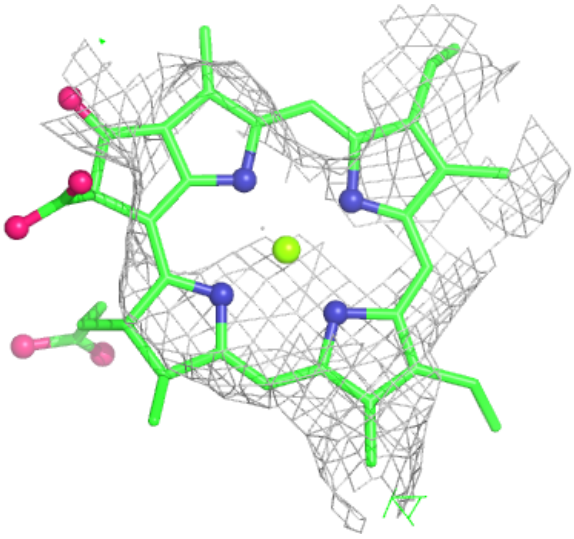
Electron density around CLA L 204:

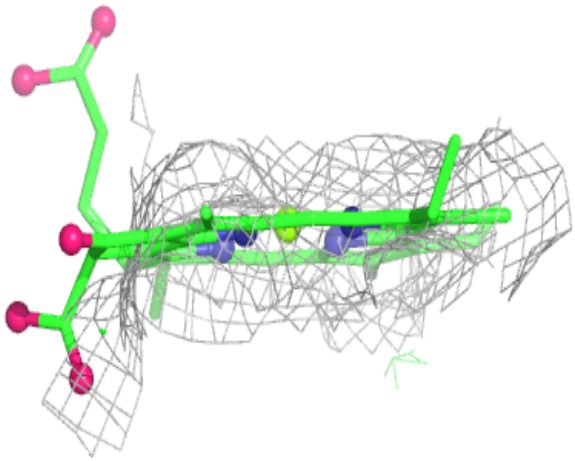
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

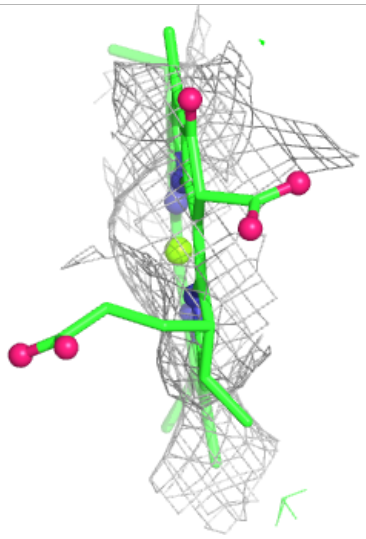


Electron density around CLA K 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

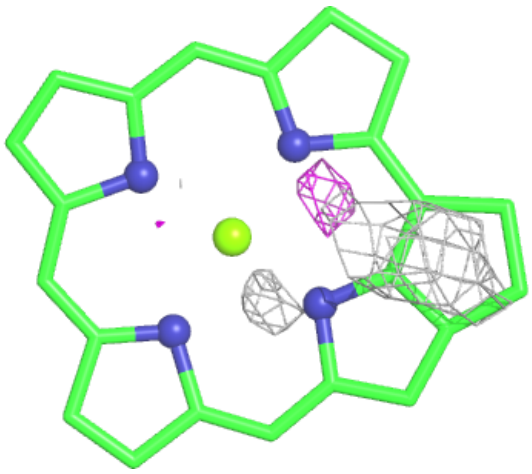


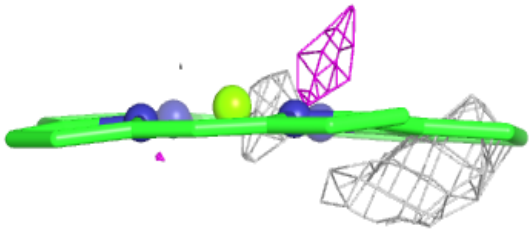


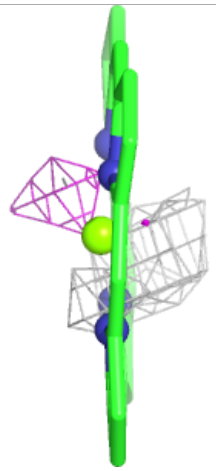


Electron density around CLA K 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

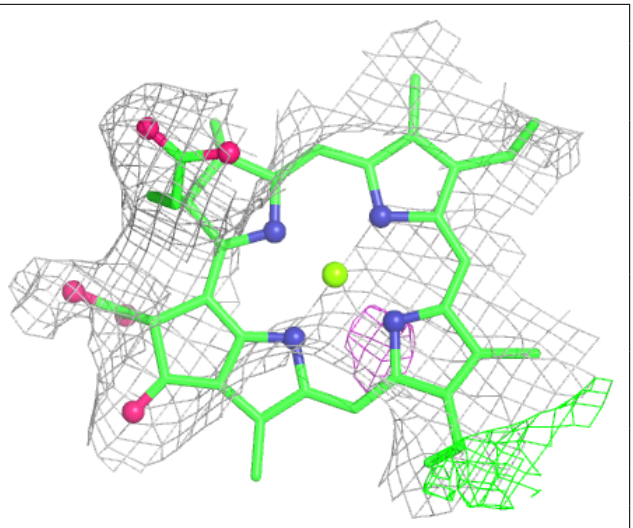


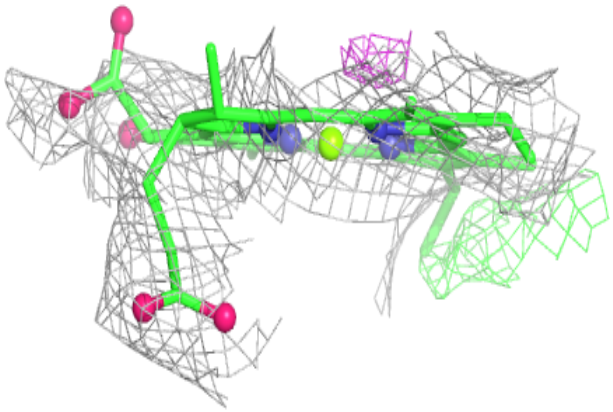


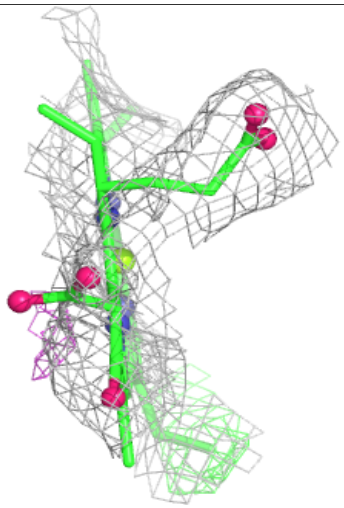


Electron density around CLA G 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

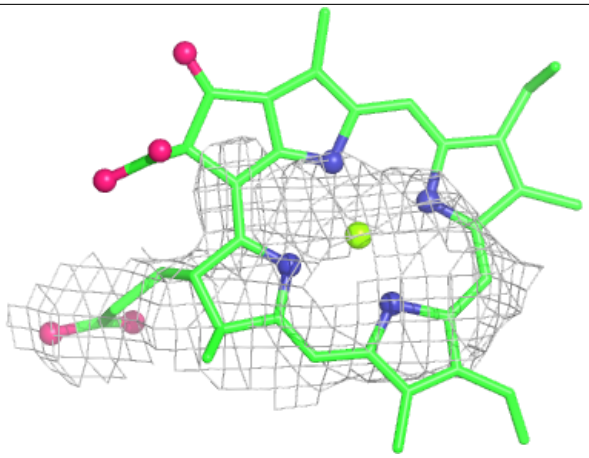


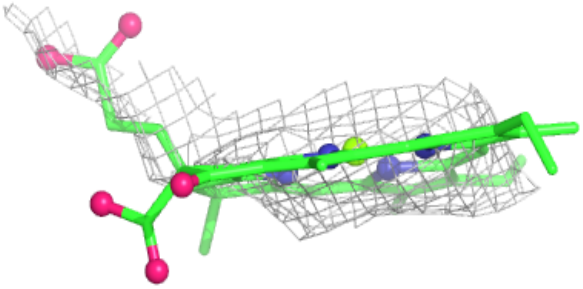


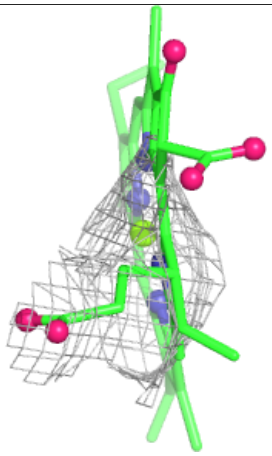


Electron density around CLA G 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

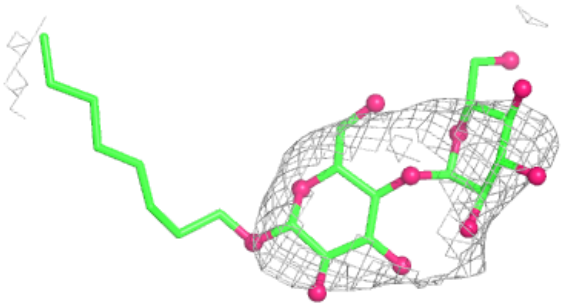


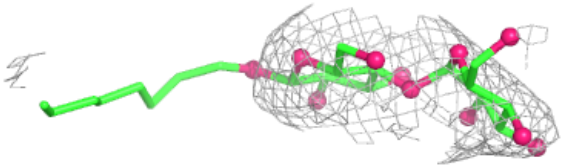


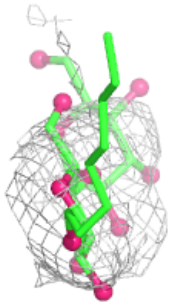


Electron density around LMT B 849:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

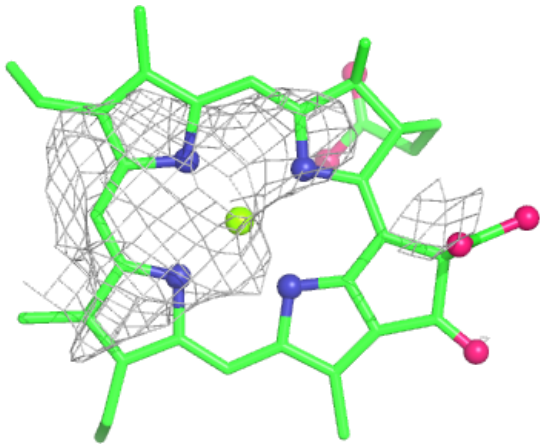


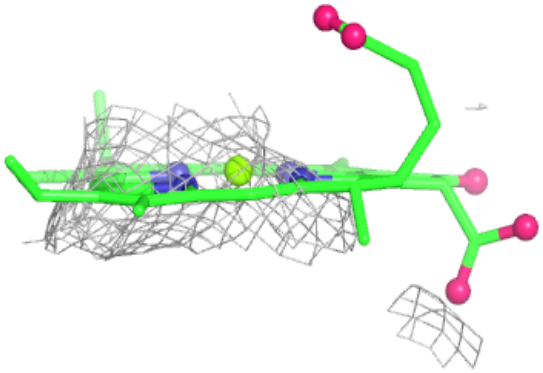


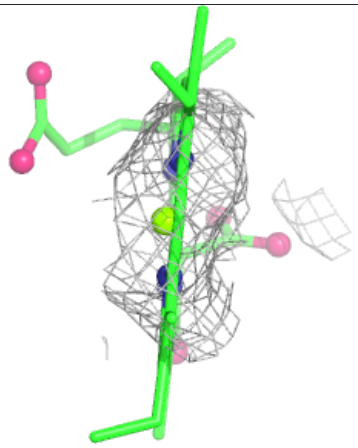


Electron density around CLA L 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

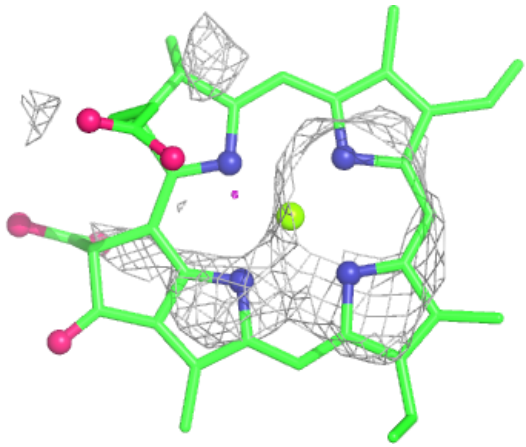


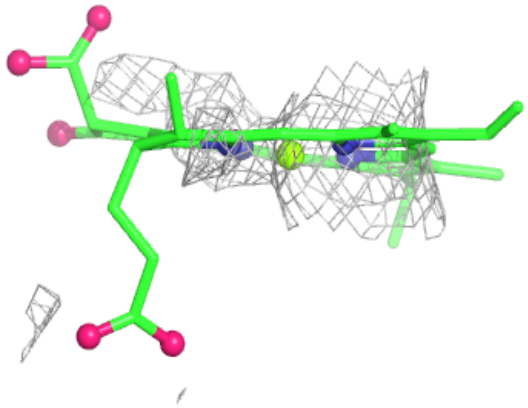


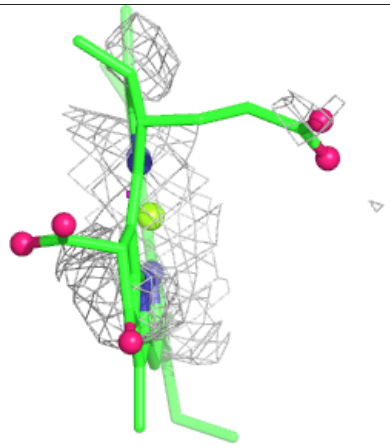


Electron density around CLA L 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

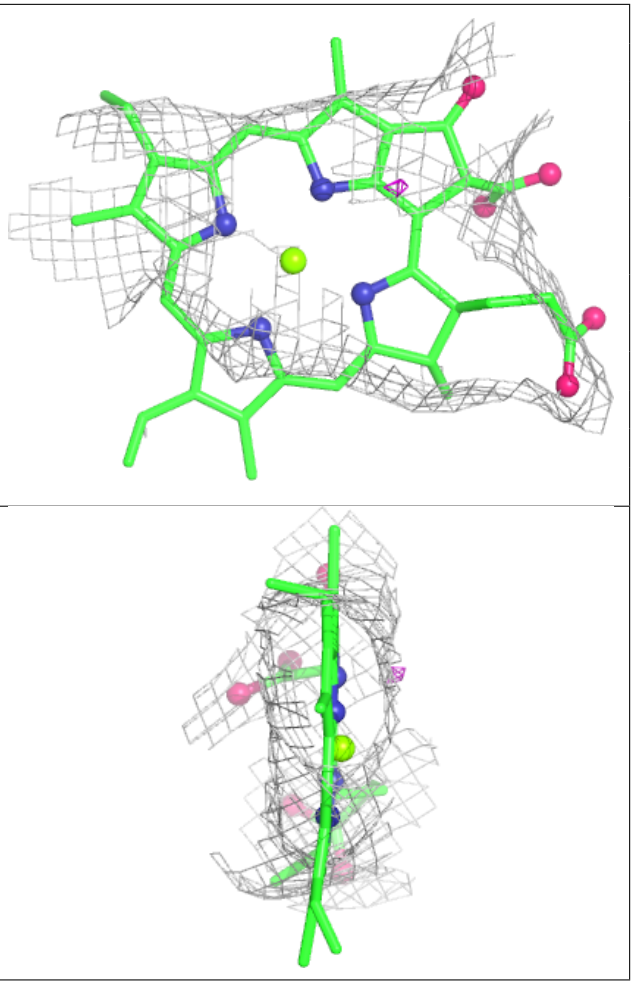






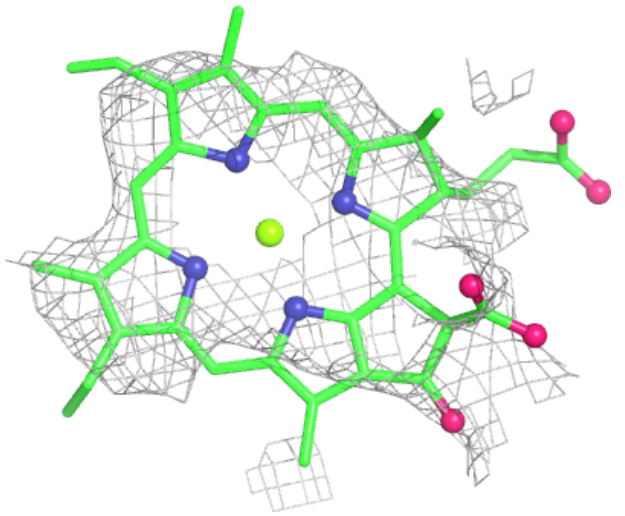
Electron density around CLA G 202:

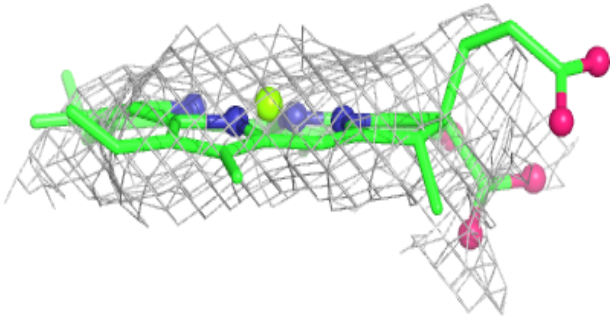
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

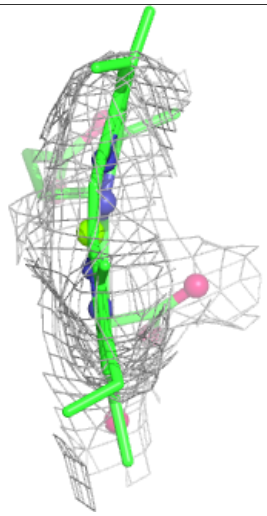


Electron density around CLA B 813:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

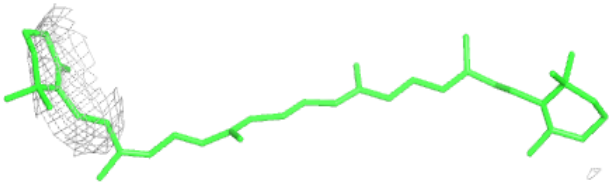


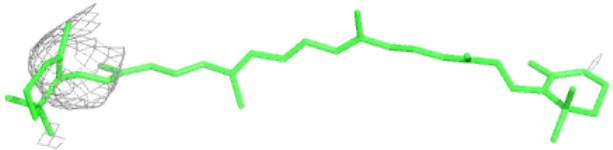


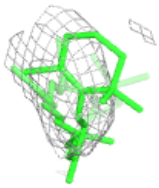


Electron density around BCR H 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

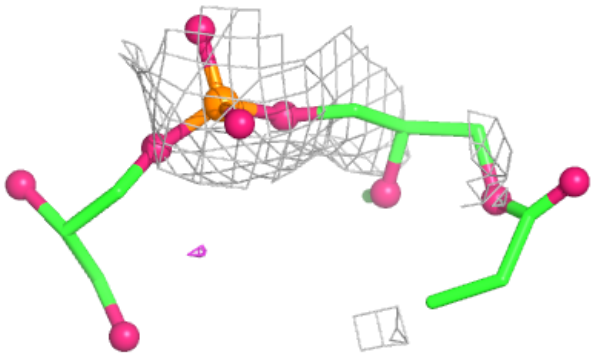


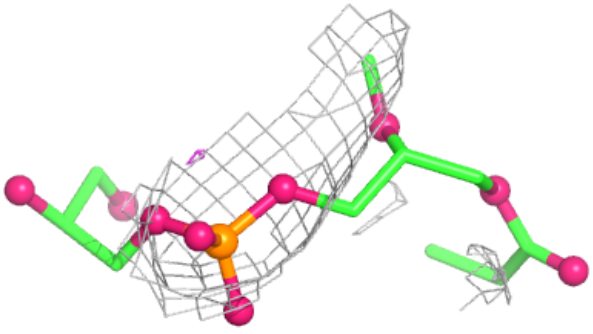


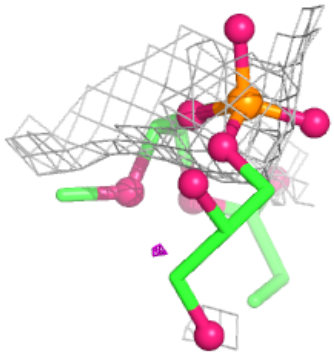


Electron density around LHG 3 1019:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

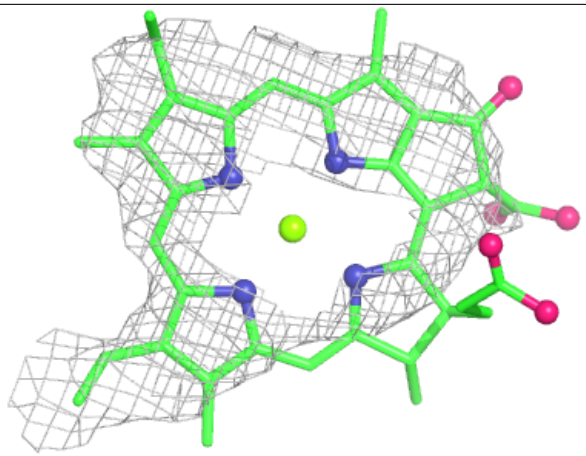


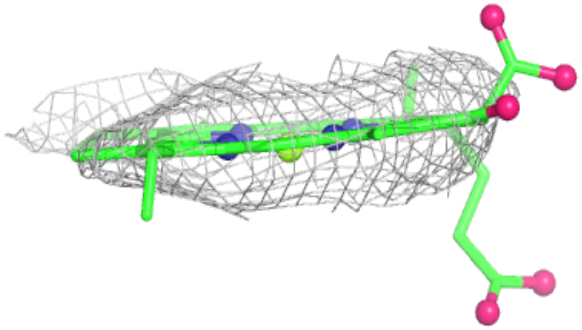


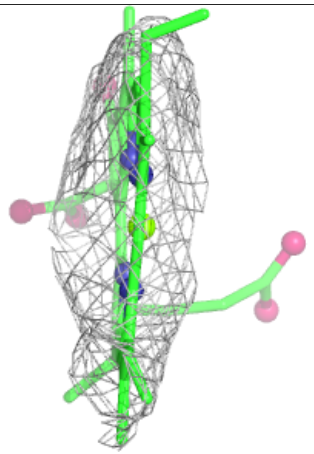


Electron density around CLA B 815:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

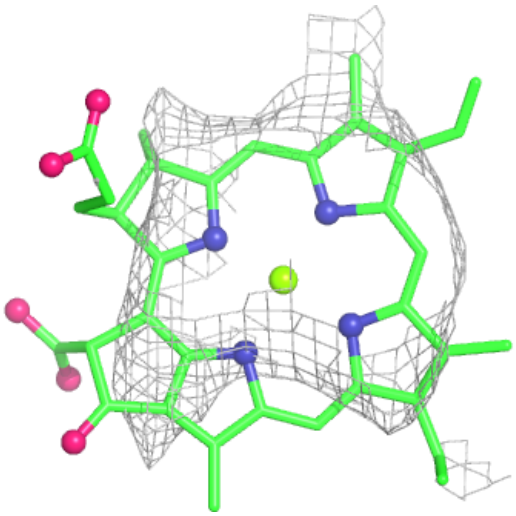


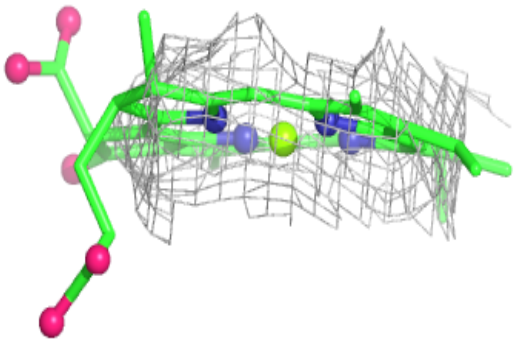


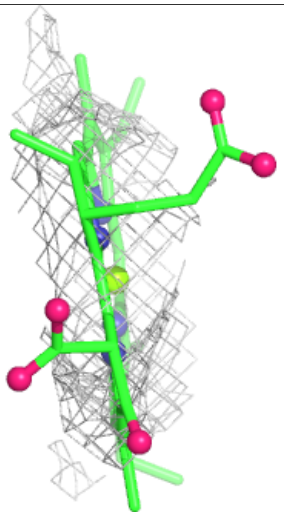


Electron density around CLA A 840:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

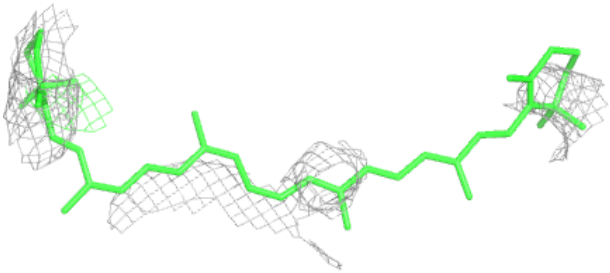


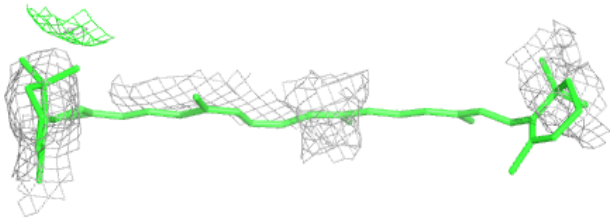




Electron density around BCR I 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

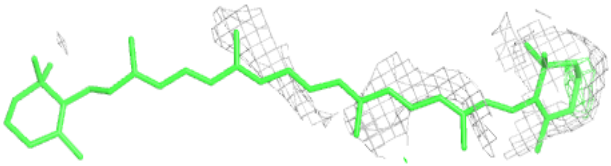


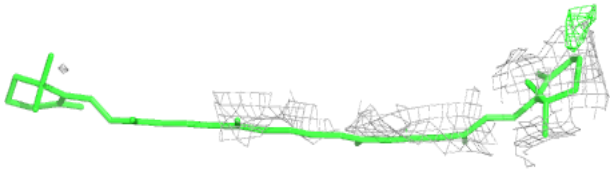


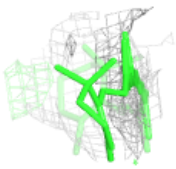


Electron density around BCR A 850:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

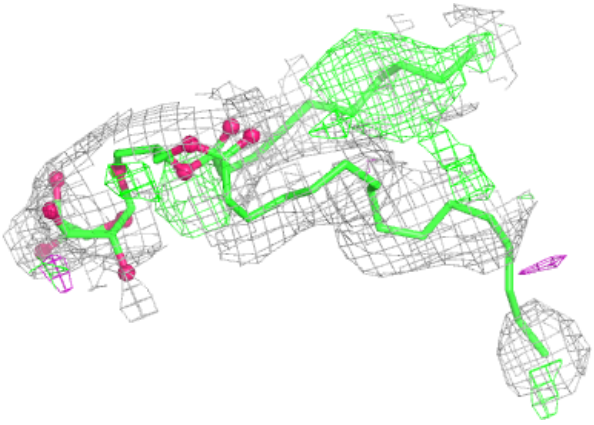


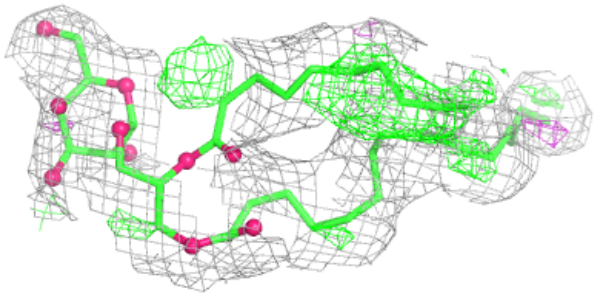


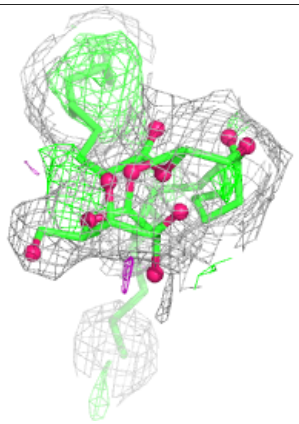


Electron density around LMG 5 324:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

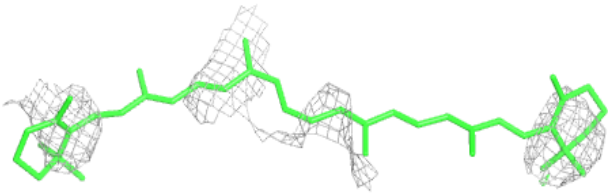


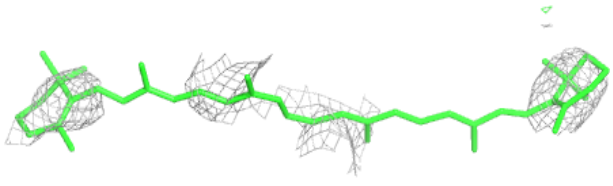


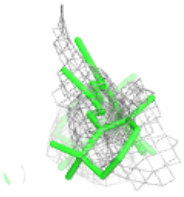


Electron density around BCR G 204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

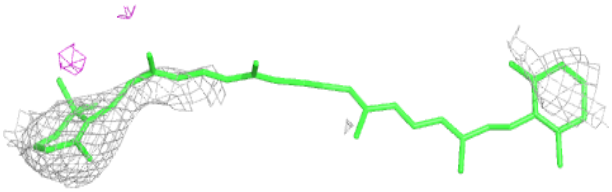


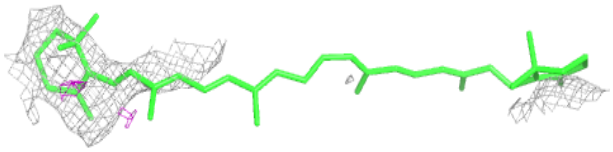


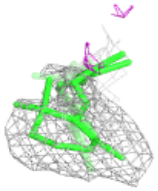


Electron density around BCR G 205:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



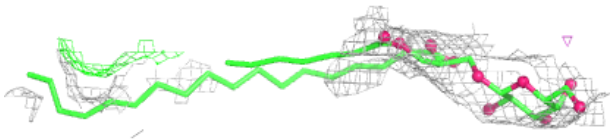


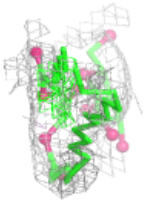


Electron density around LMG 8 319:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

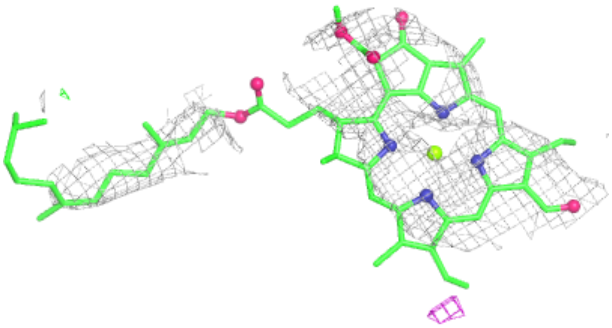


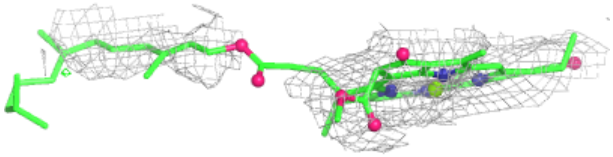


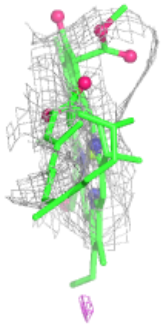


Electron density around CHL 0 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

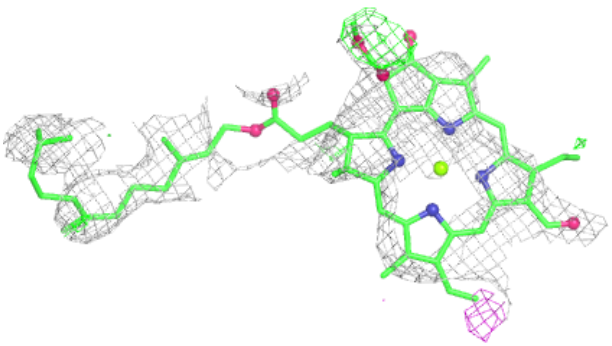


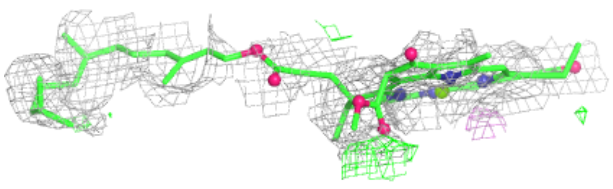


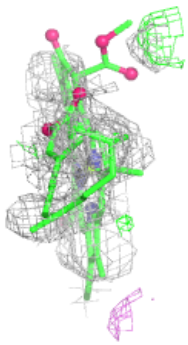


Electron density around CHL 1 1015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

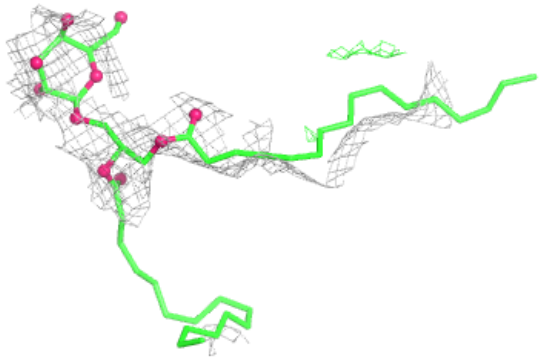


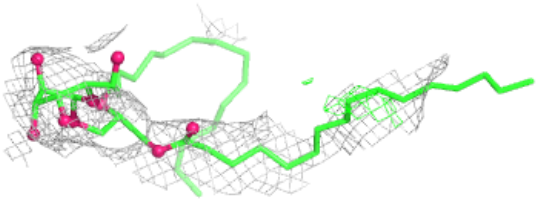




Electron density around LMG 0 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

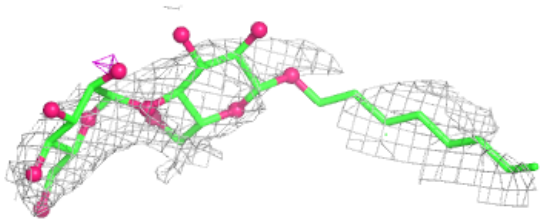


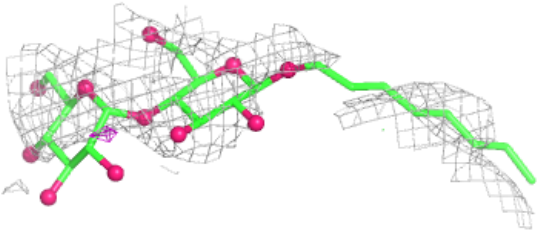


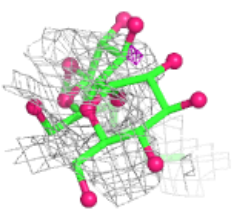


Electron density around LMT 3 1018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

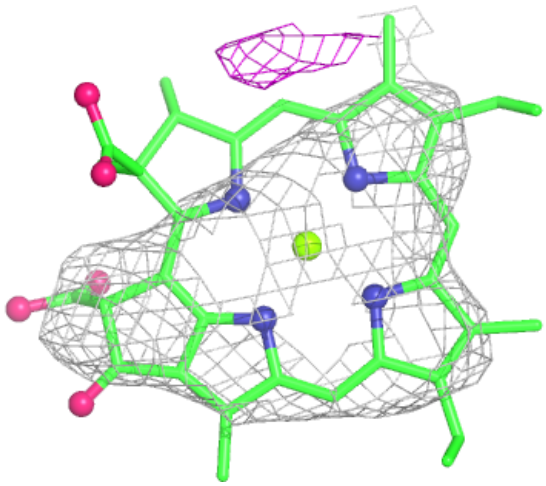


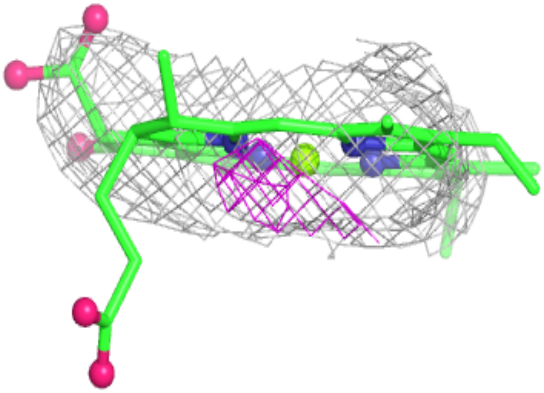


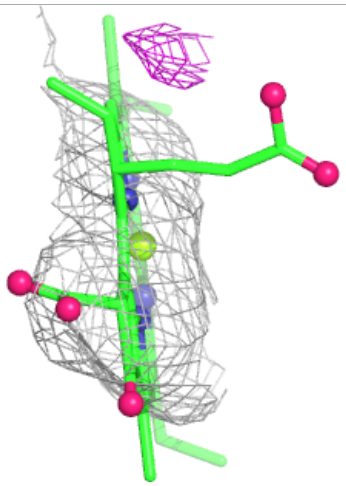


Electron density around CLA A 822:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

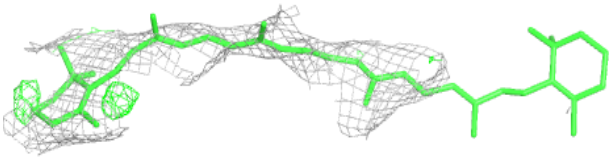


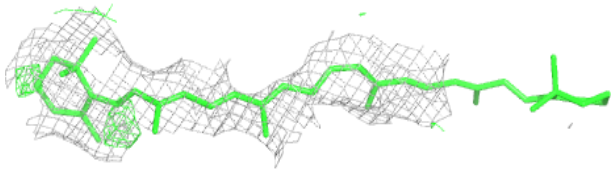


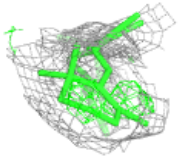


Electron density around BCR 1 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

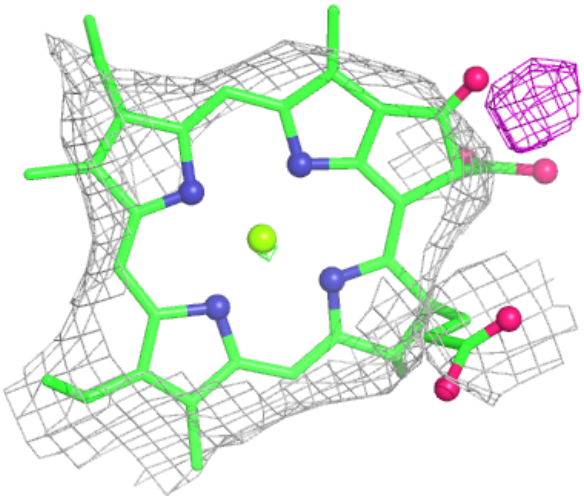


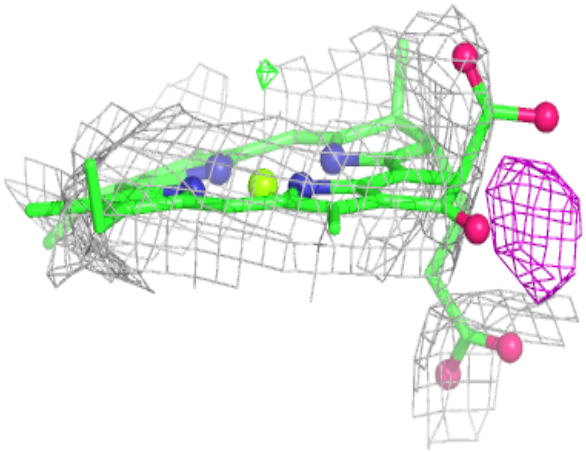


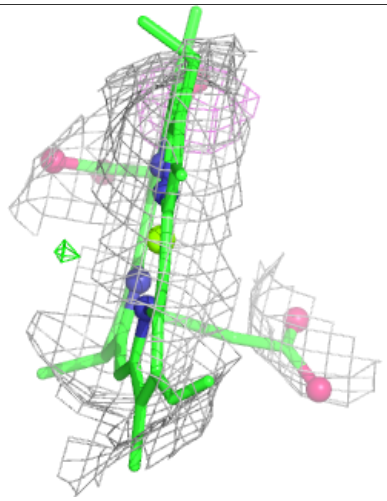


Electron density around CLA B 836:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

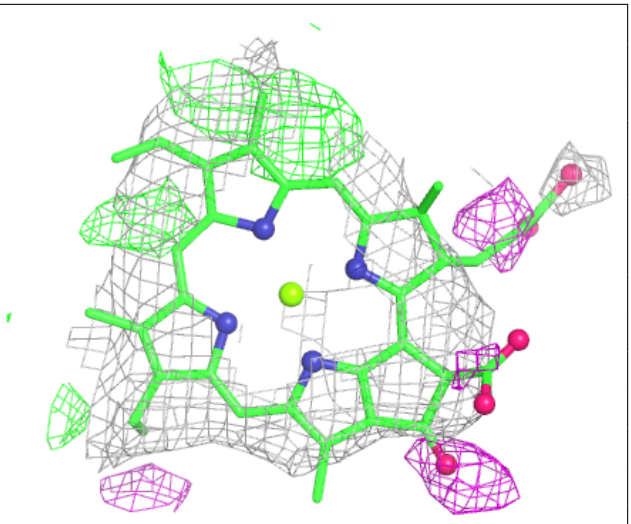


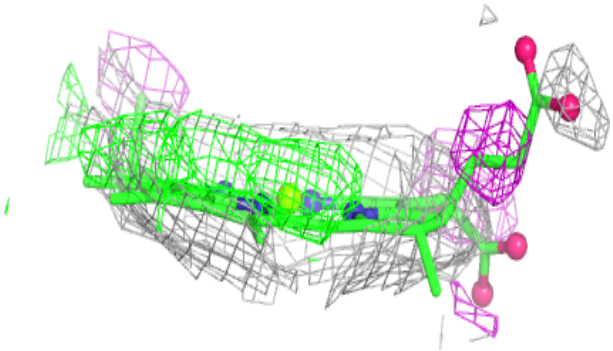


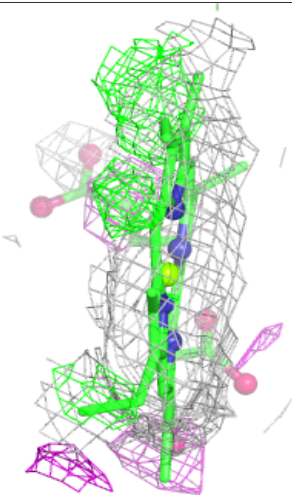


Electron density around CLA 5 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

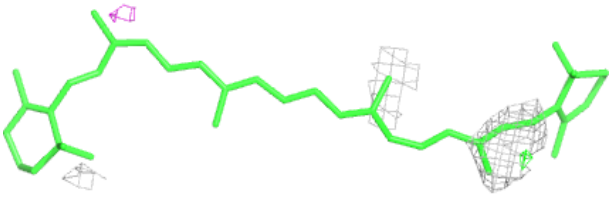


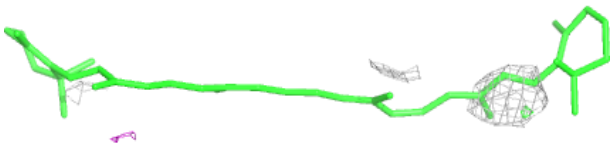


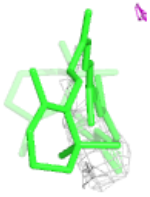


Electron density around BCR B 845:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

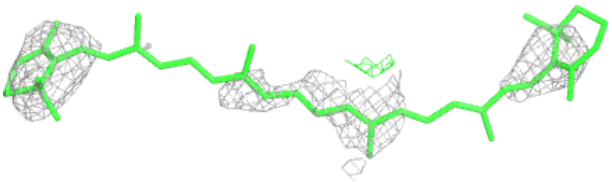


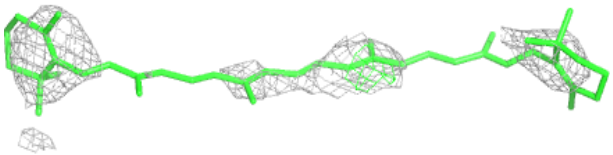


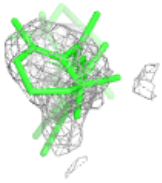


Electron density around BCR B 847:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

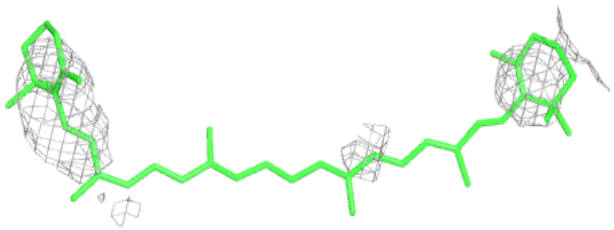


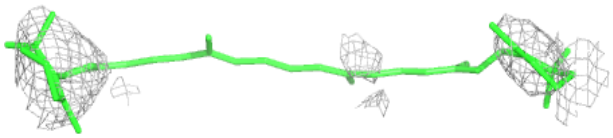


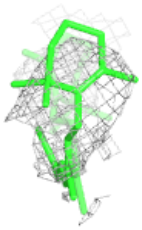


Electron density around BCR B 844:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

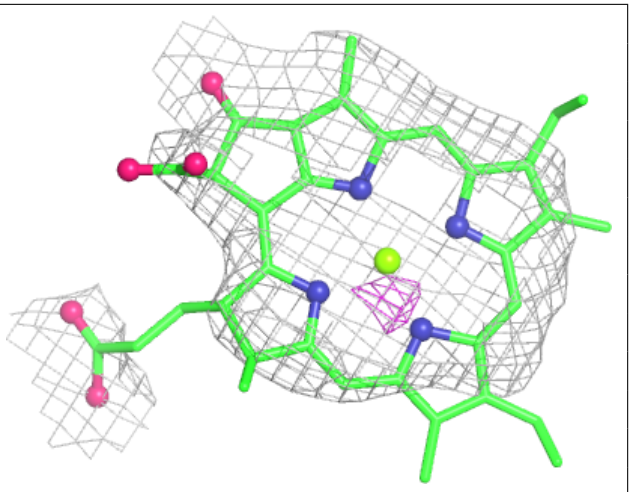


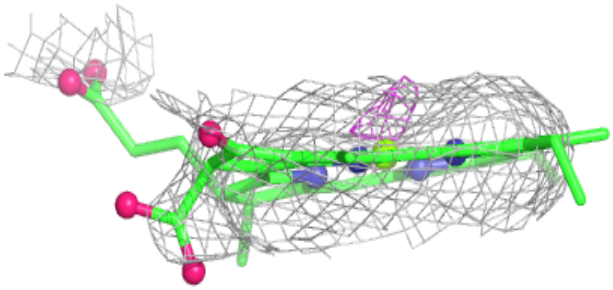


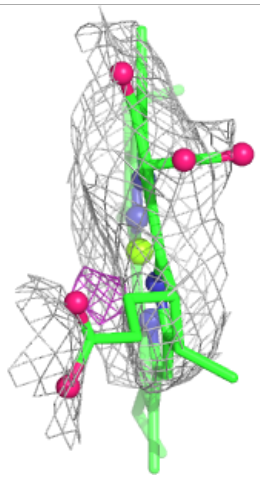


Electron density around CLA B 812:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

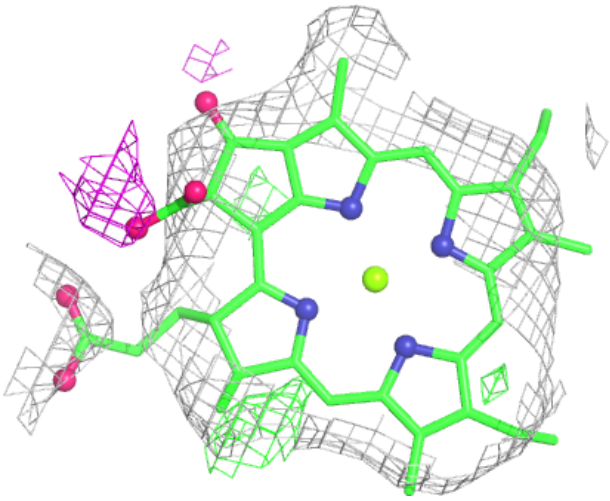


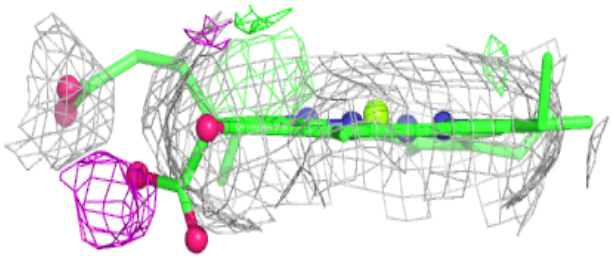


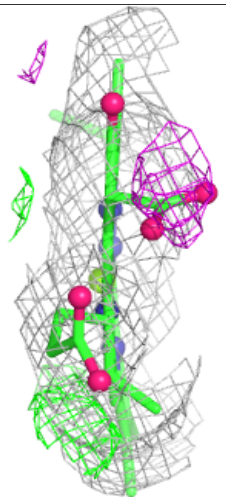


Electron density around CLA F 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

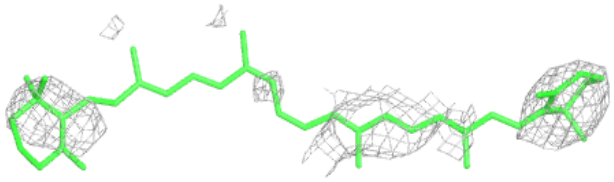


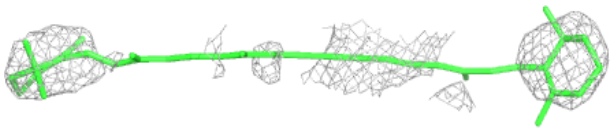


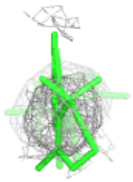


Electron density around BCR A 846:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

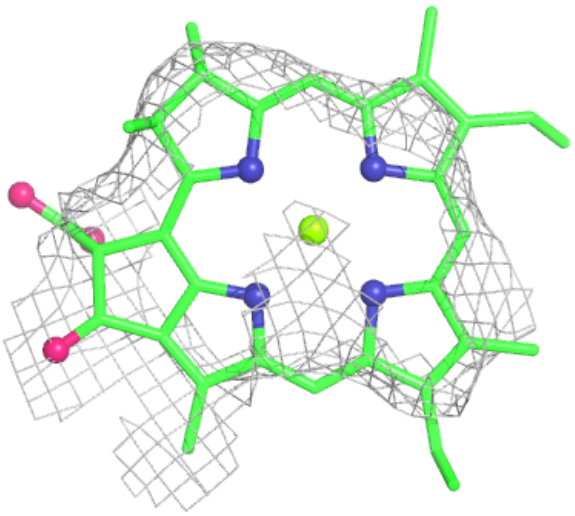


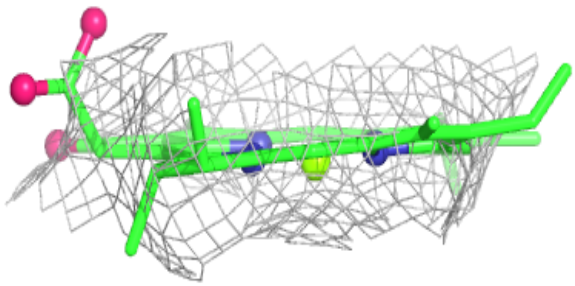


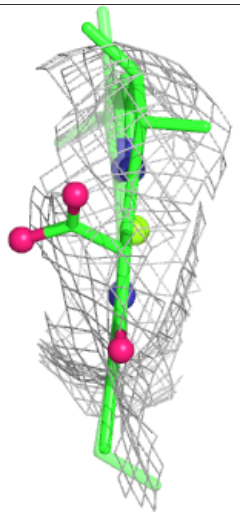


Electron density around CLA 3 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

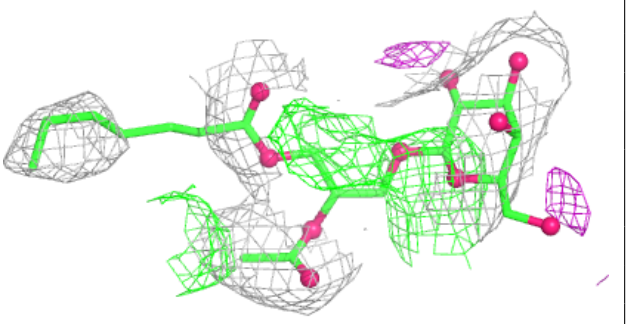


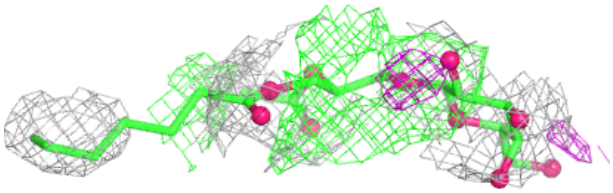


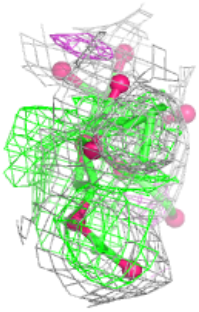


Electron density around LMG 8 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

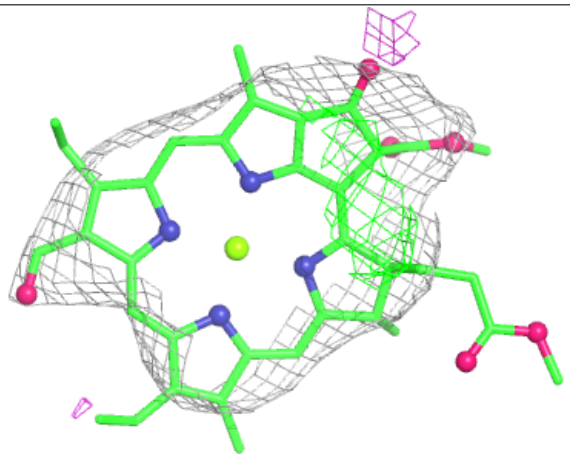


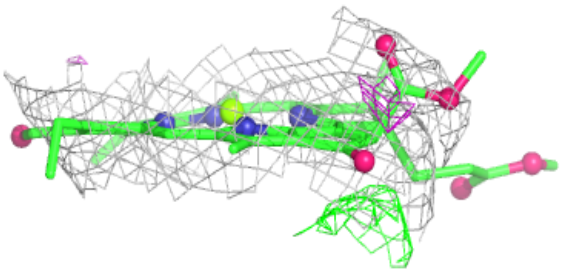


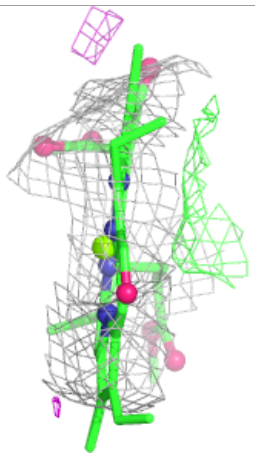


Electron density around CHL 0 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

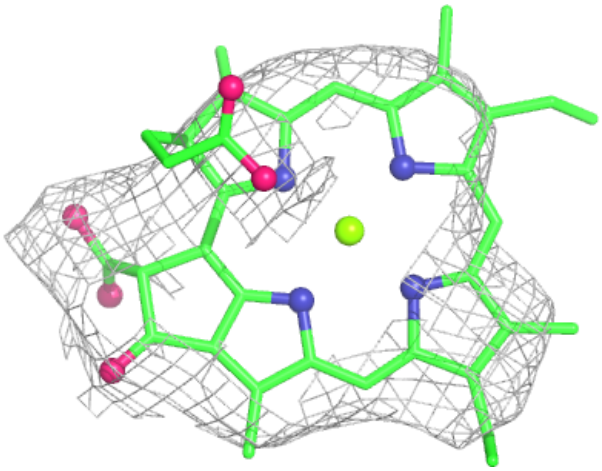


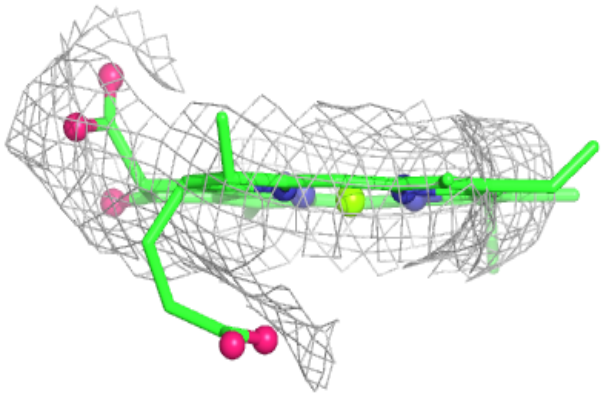


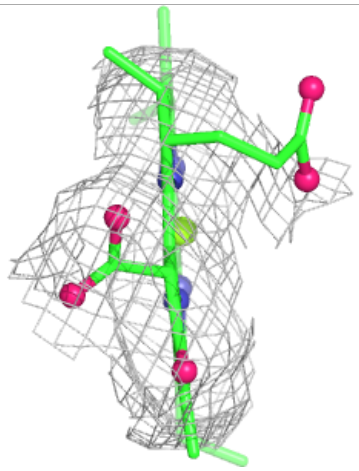


Electron density around CLA 3 1012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

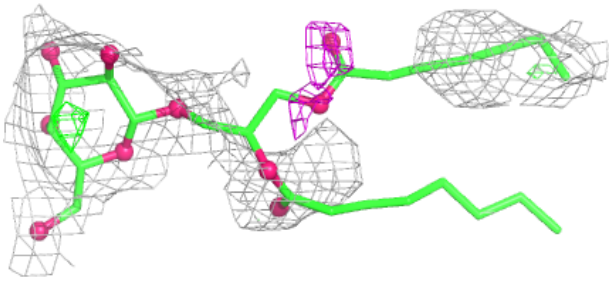


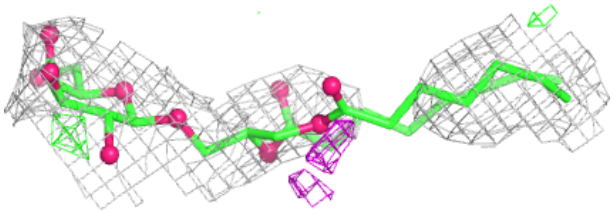


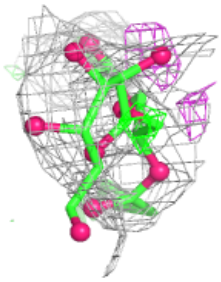


Electron density around LMG 4 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

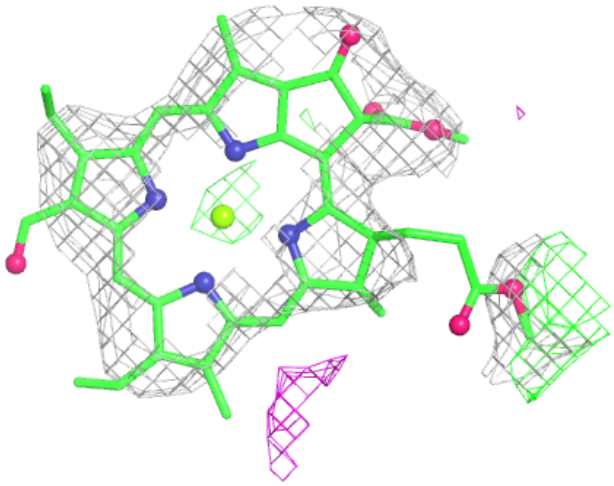


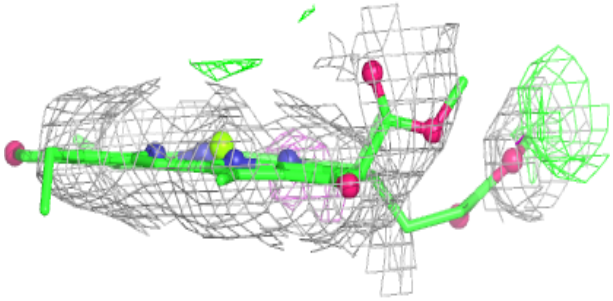


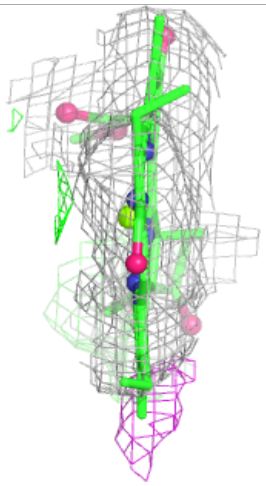


Electron density around CHL 4 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

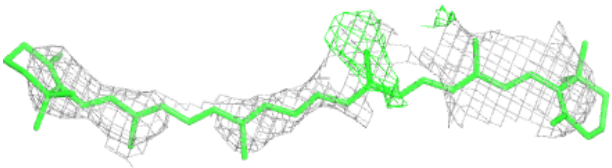


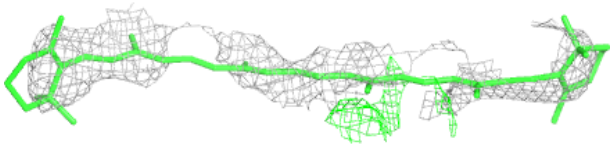


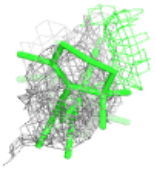


Electron density around BCR A 844:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

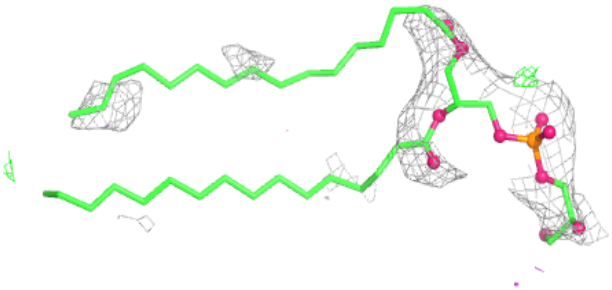


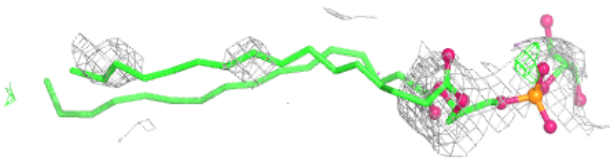




Electron density around LHG 8 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

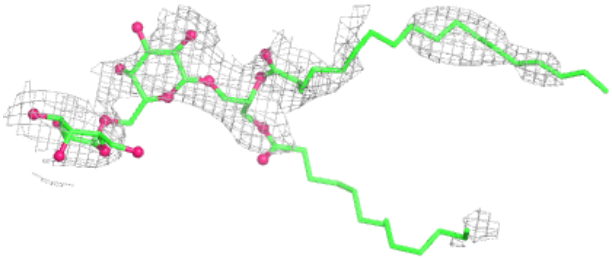






Electron density around DGD B 848:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

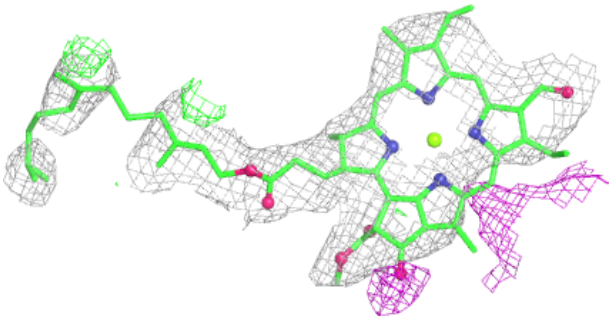


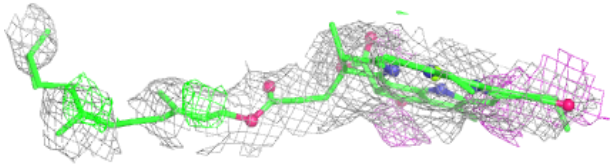




Electron density around CHL 8 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

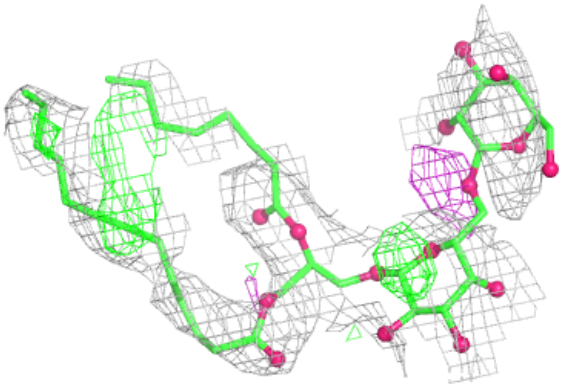


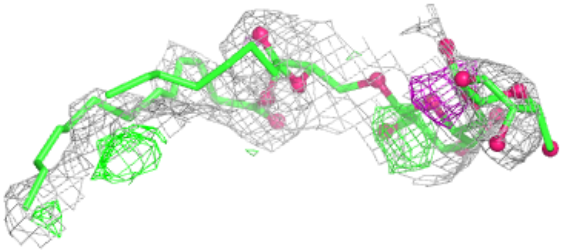




Electron density around DGD 5 319:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

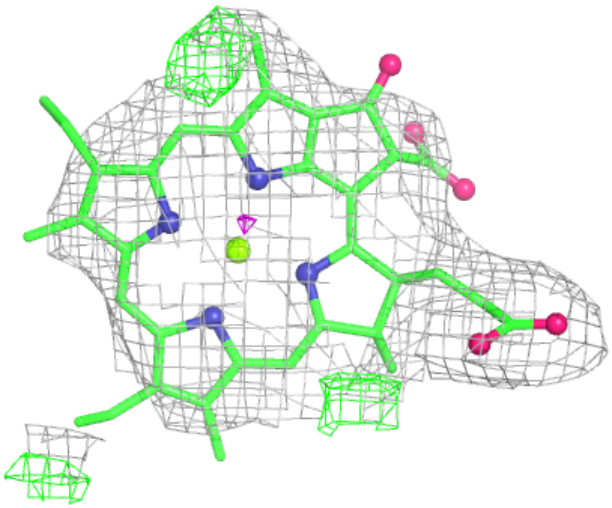


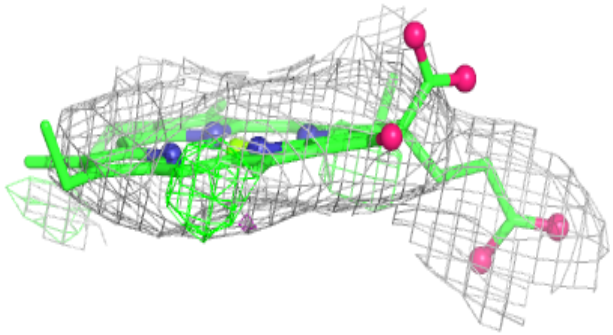


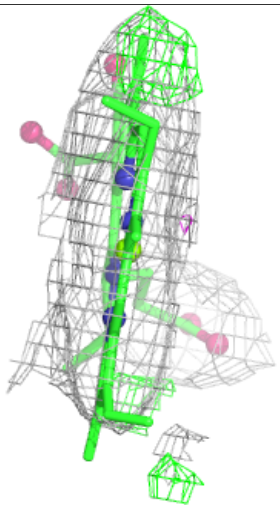


Electron density around CLA 5 323:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

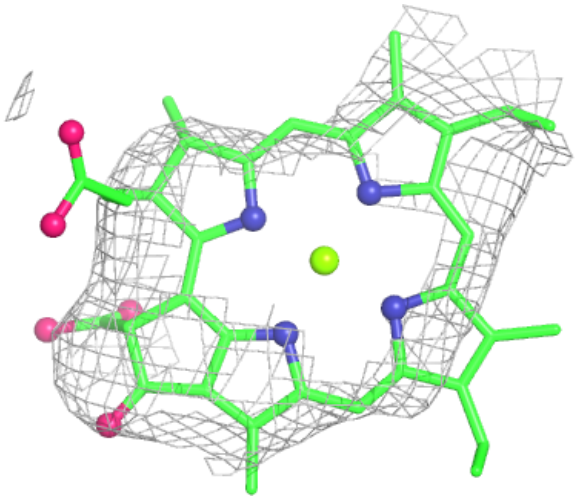


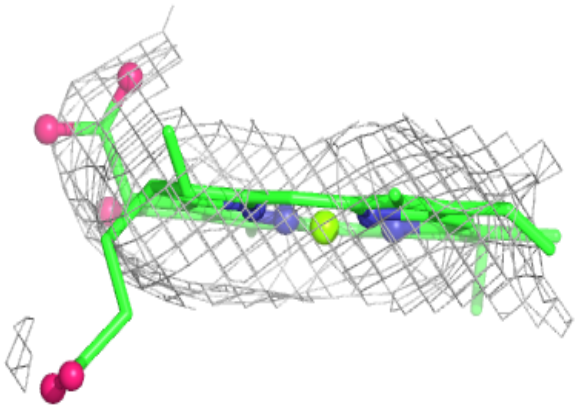


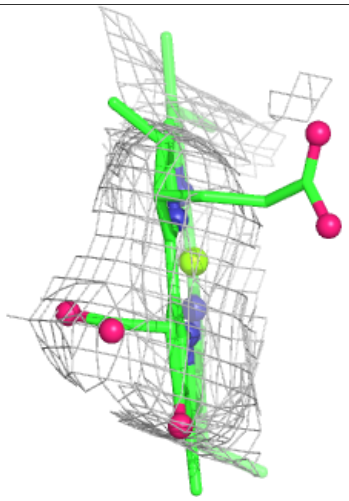


Electron density around CLA A 821:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

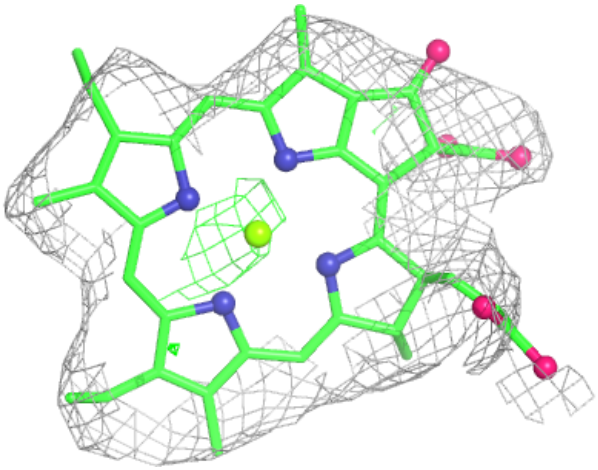


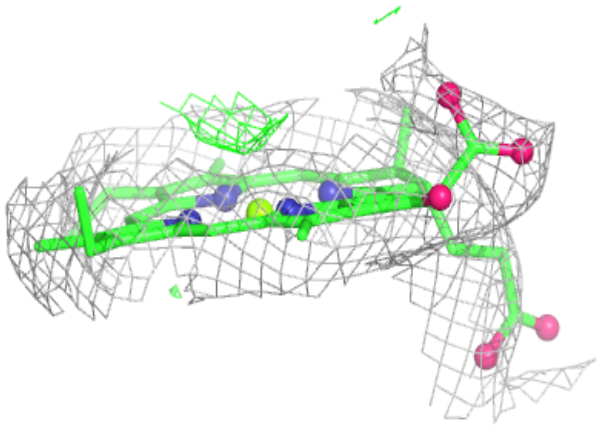




Electron density around CLA 5 322:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

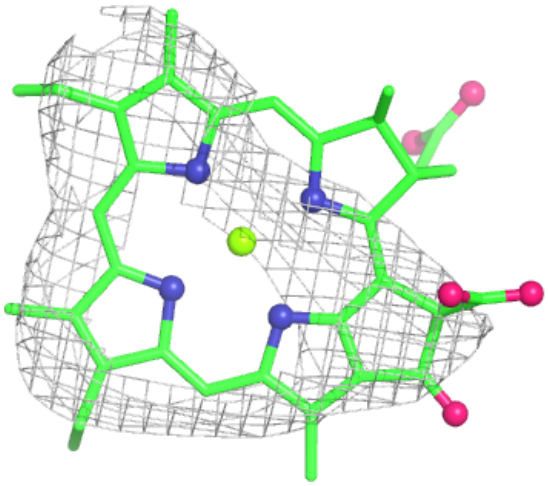


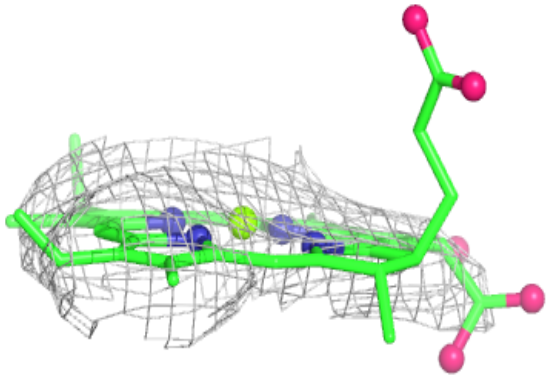


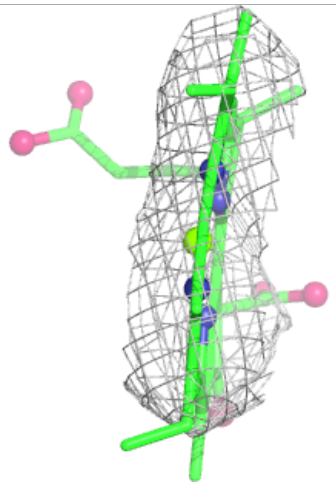


Electron density around CLA B 823:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

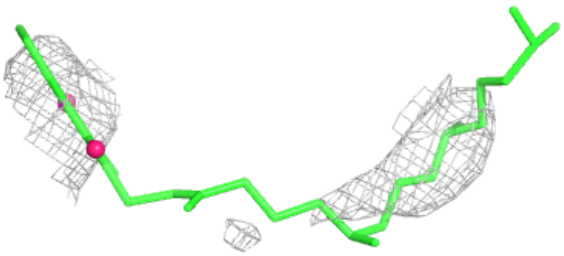


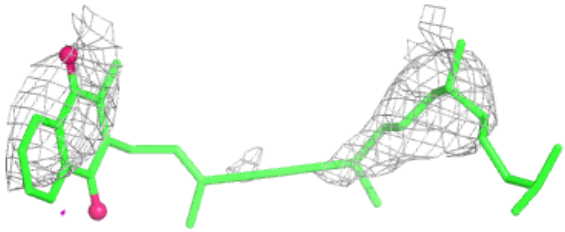


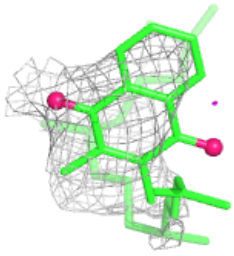


Electron density around PQN B 842:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



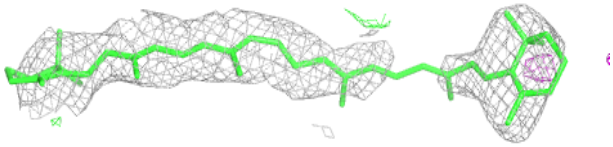


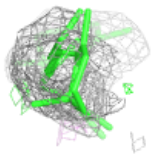


Electron density around BCR 8 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

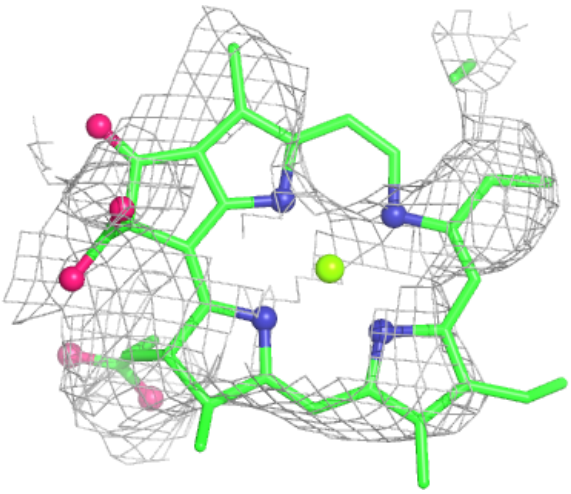


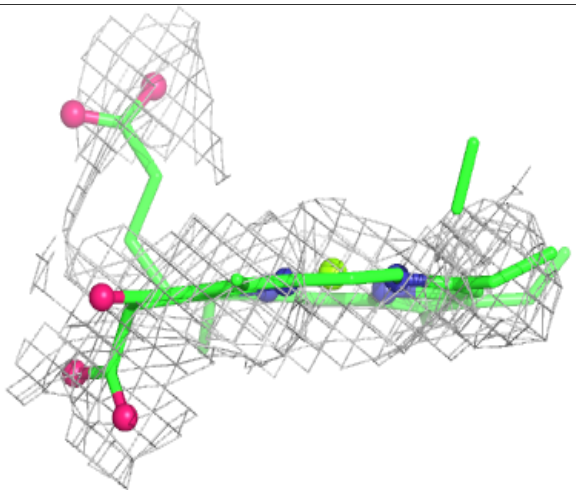




Electron density around CLA B 850:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

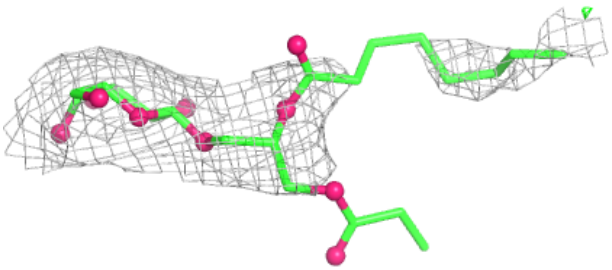


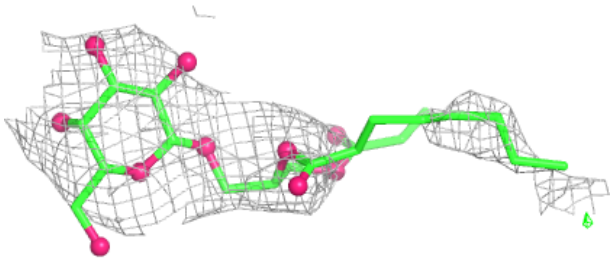


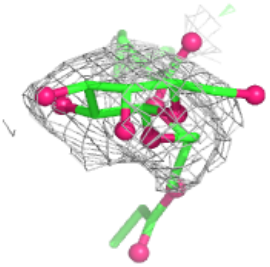


Electron density around LMG J 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

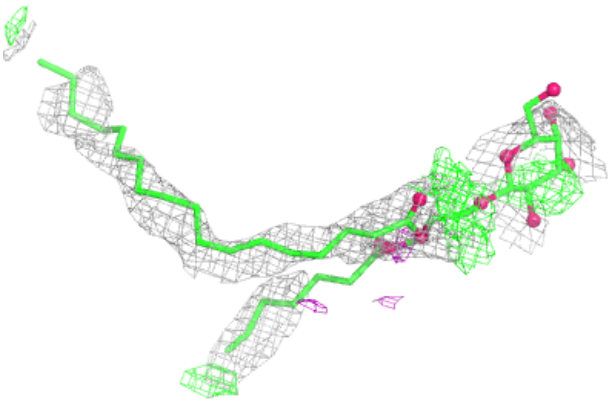


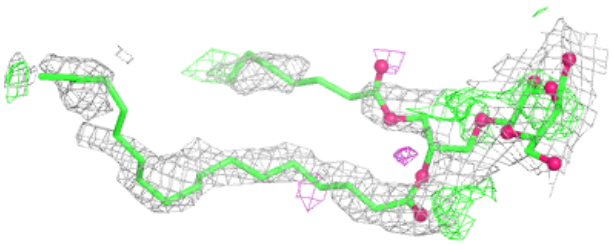




Electron density around LMG 6 319:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

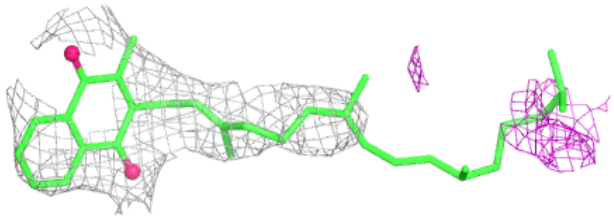


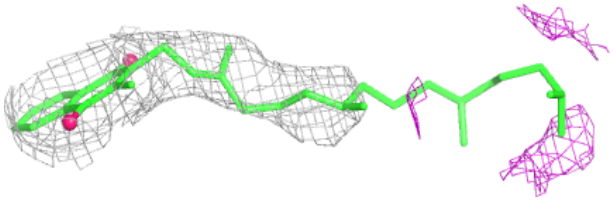


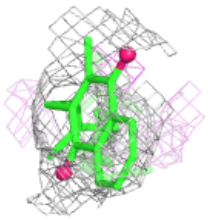


Electron density around PQN A 842:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

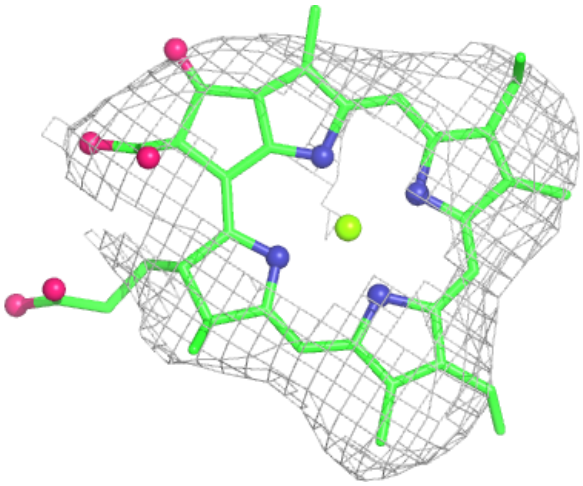


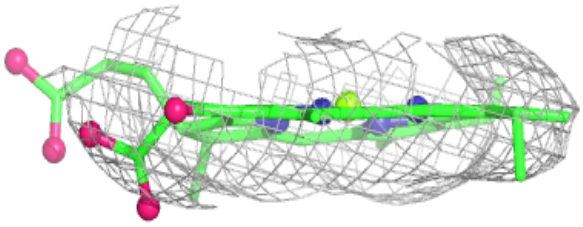


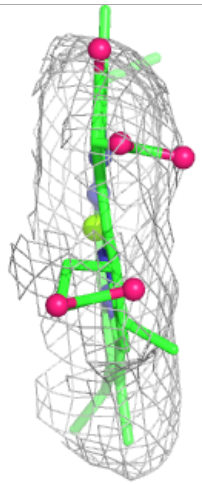


Electron density around CLA A 831:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

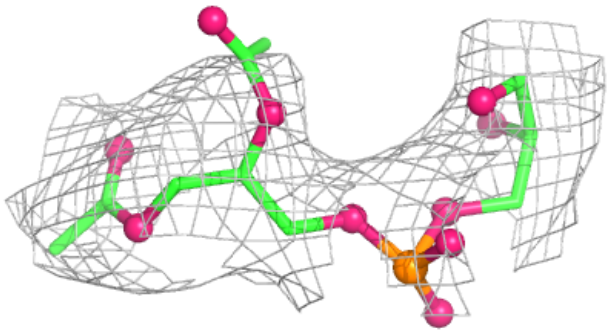


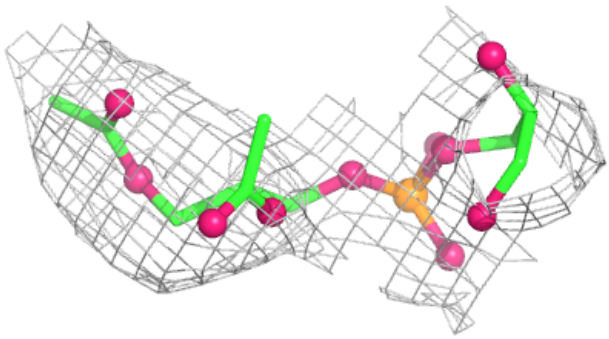


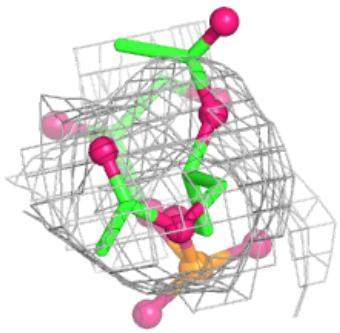


Electron density around LHG 0 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

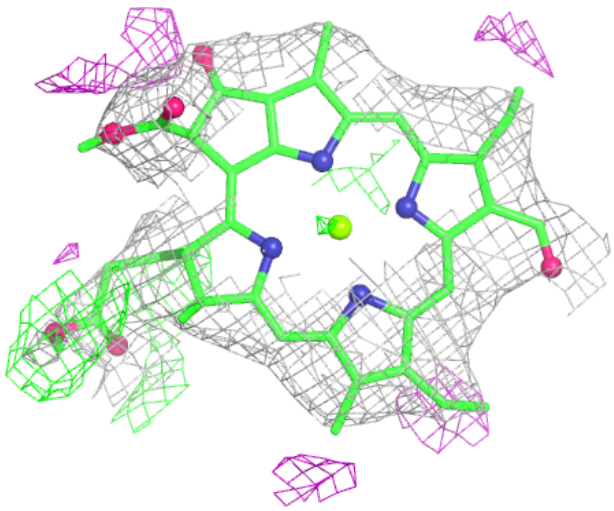


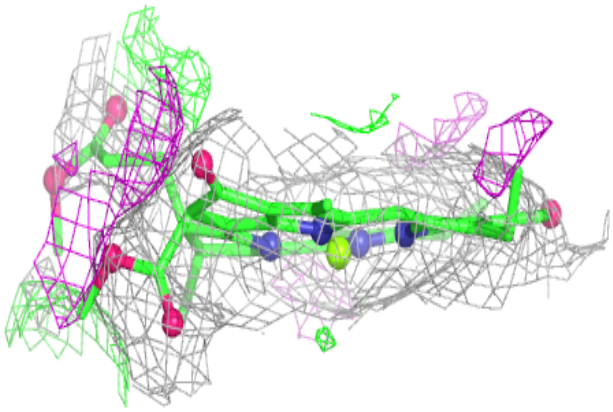


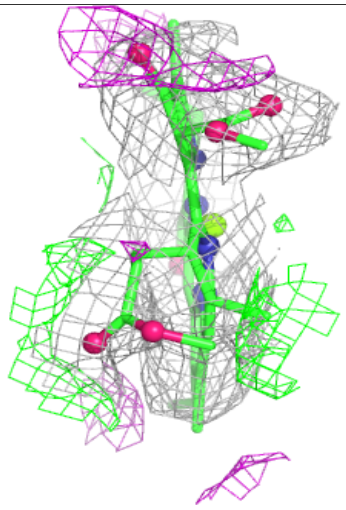


Electron density around CHL 5 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

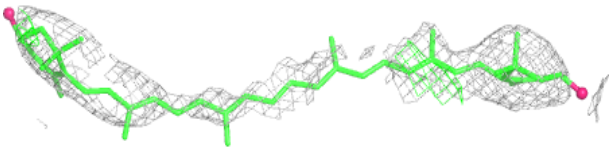


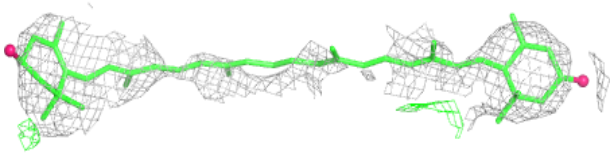


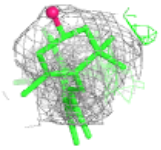


Electron density around LUT 0 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

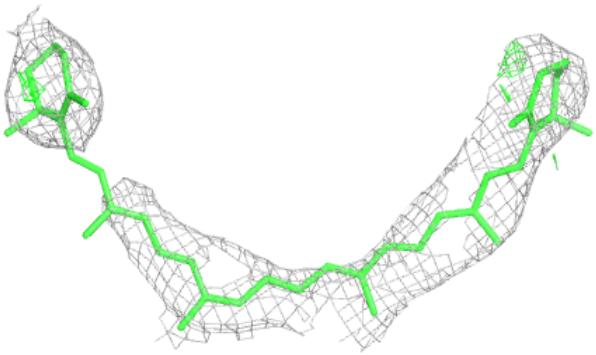


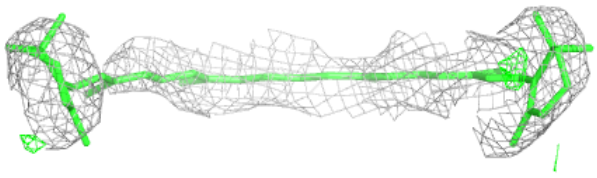


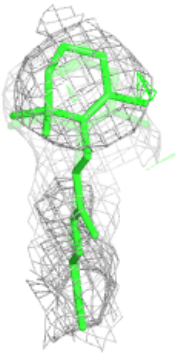


Electron density around BCR F 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

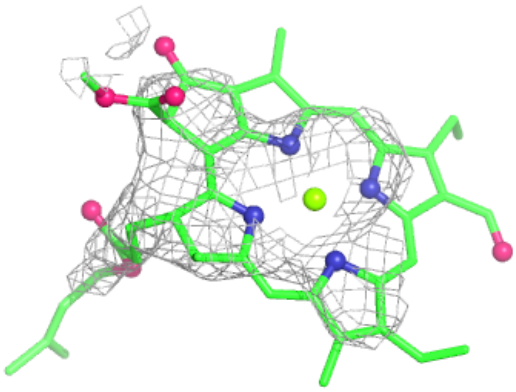


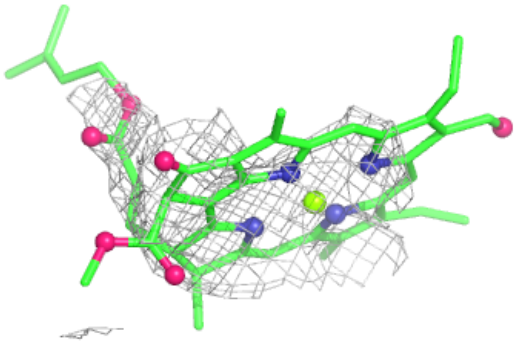


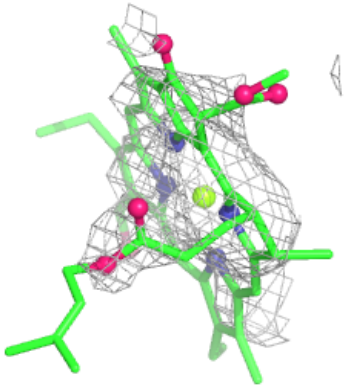


Electron density around CHL 0 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

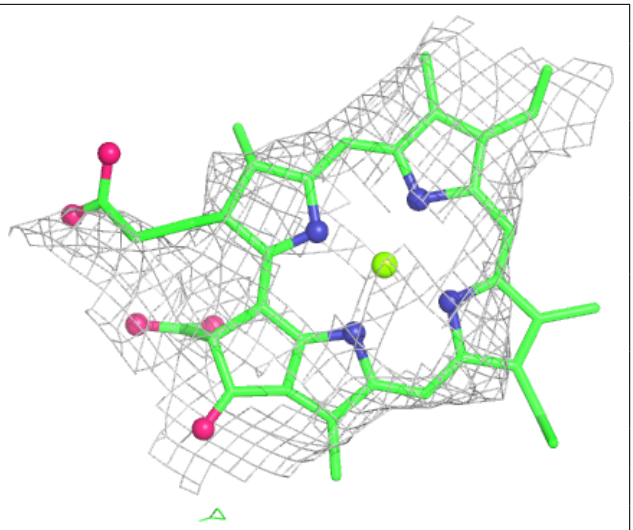


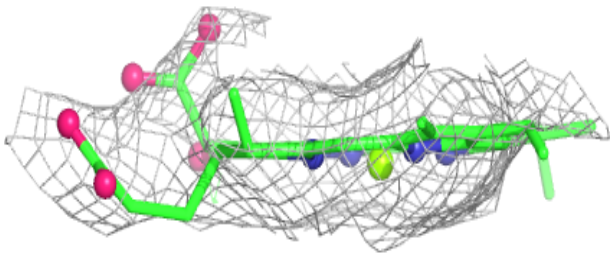


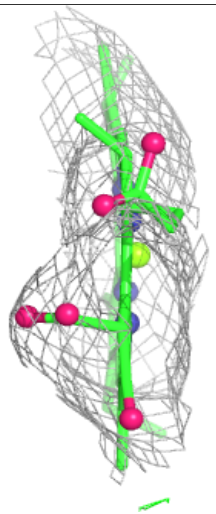


Electron density around CLA B 826:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

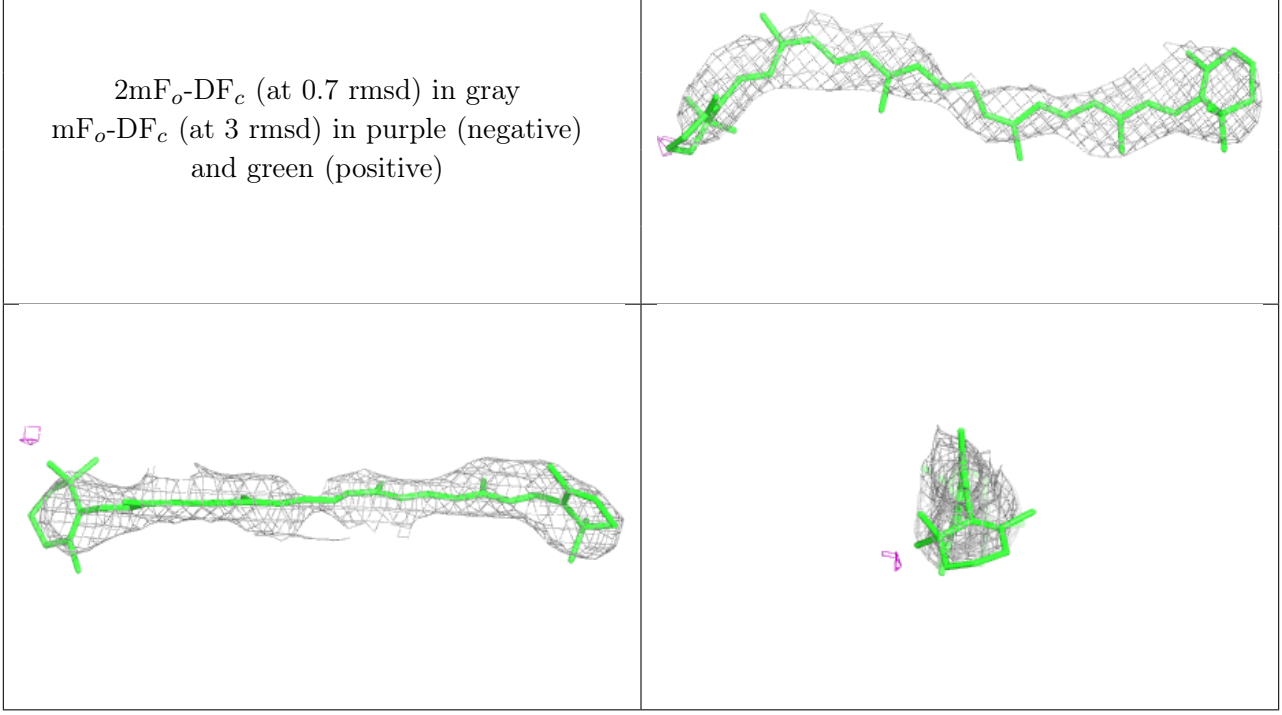






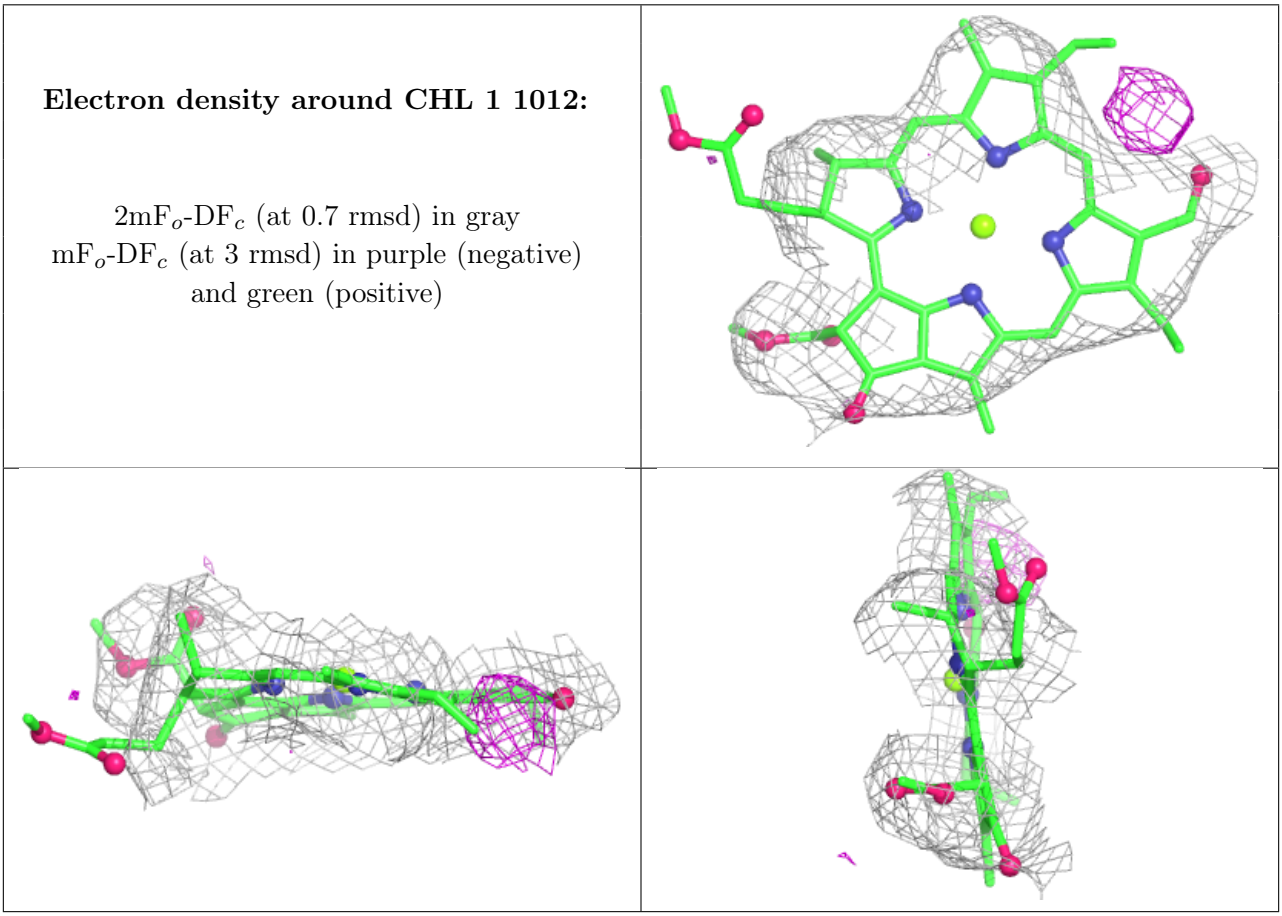
Electron density around BCR B 804:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



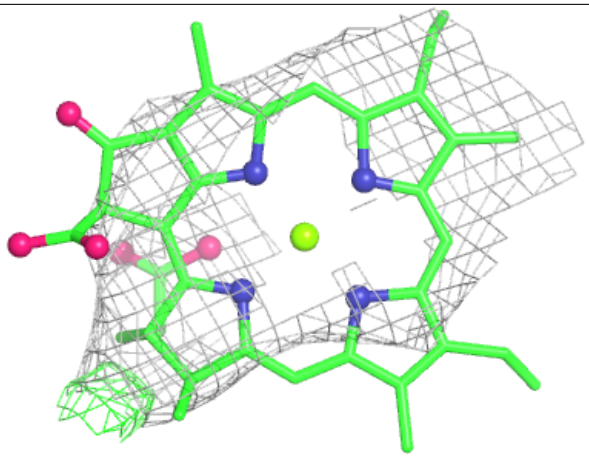
Electron density around CHL 1 1012:

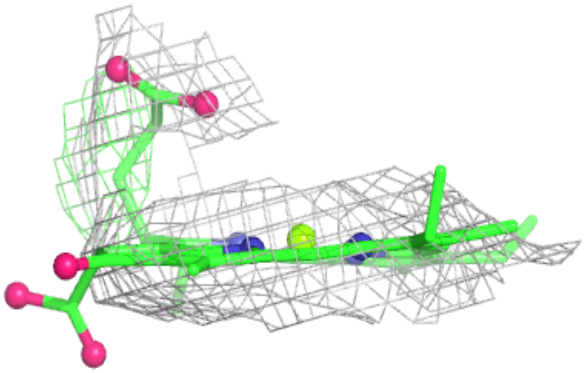
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

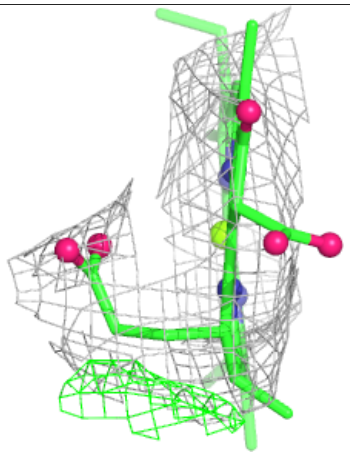


Electron density around CLA B 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

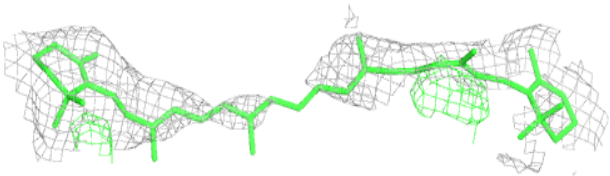


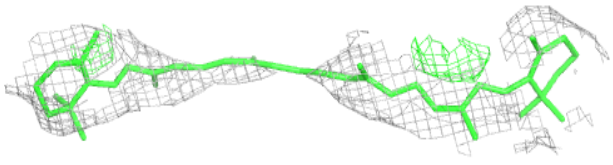


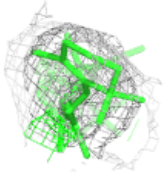


Electron density around BCR A 845:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

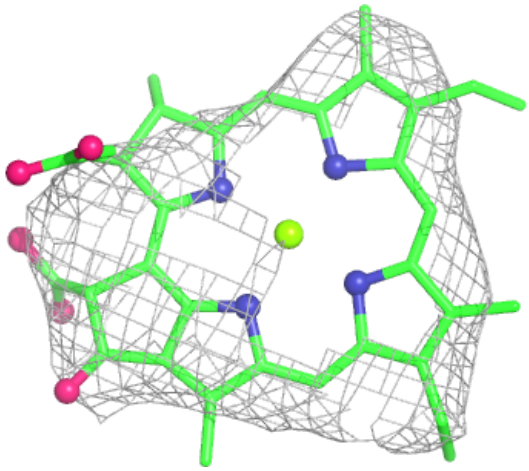


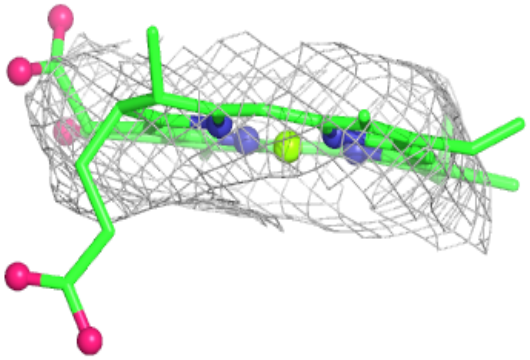


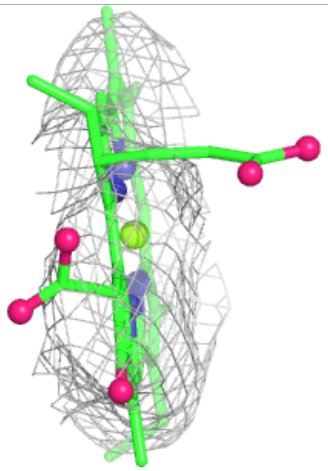


Electron density around CLA B 824:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

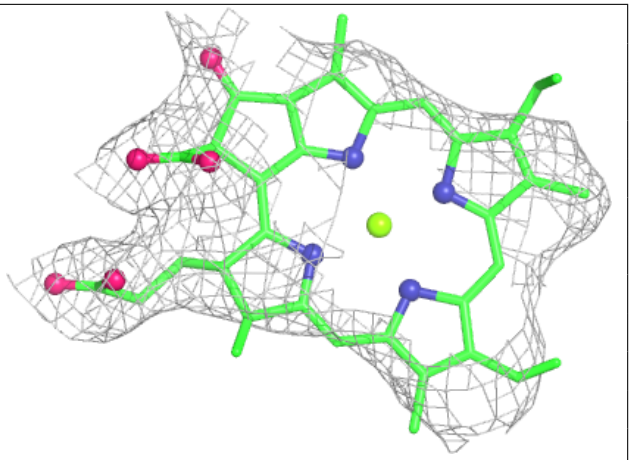


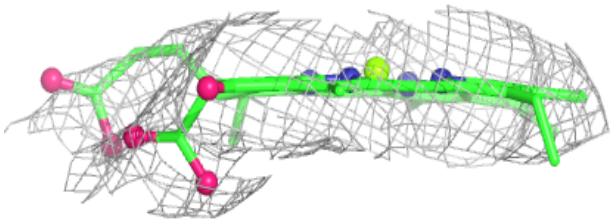


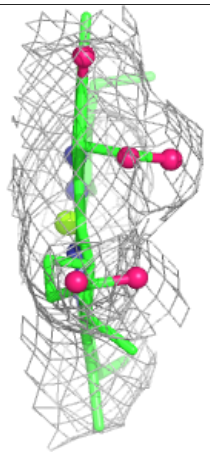


Electron density around CLA 0 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

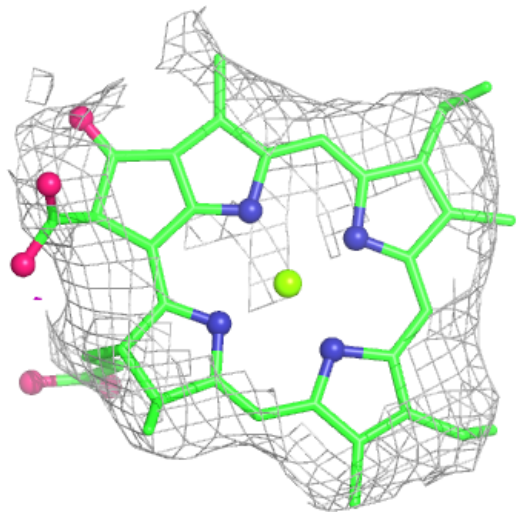


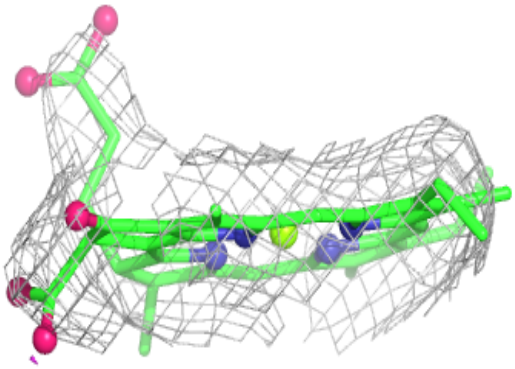


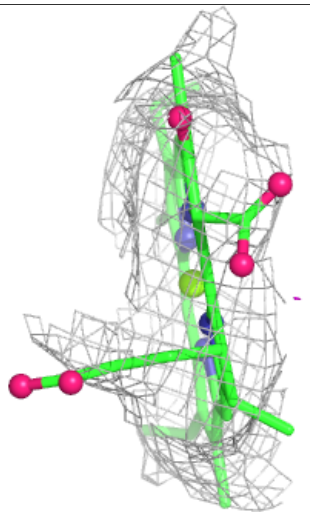


Electron density around CLA 0 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

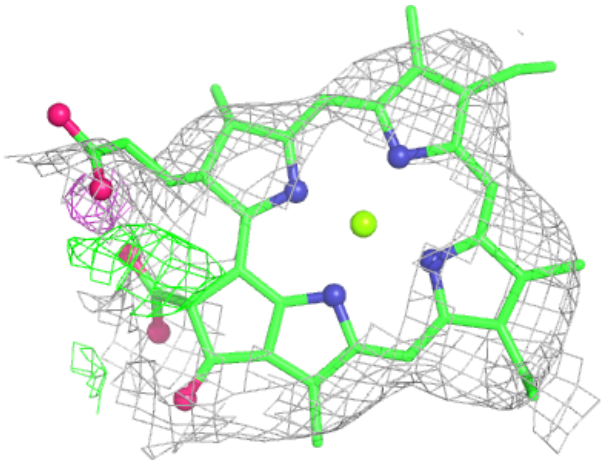


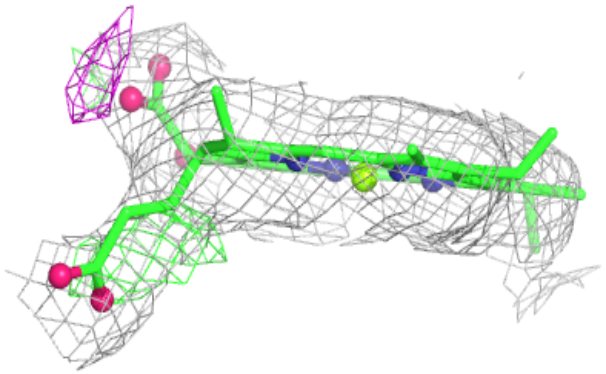


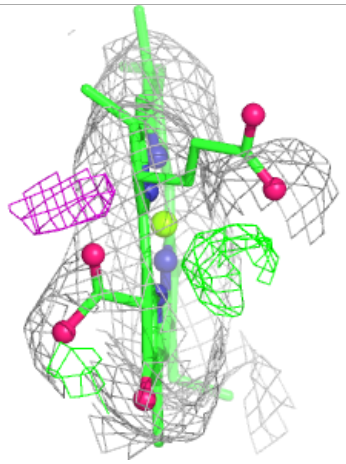


Electron density around CLA 0 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

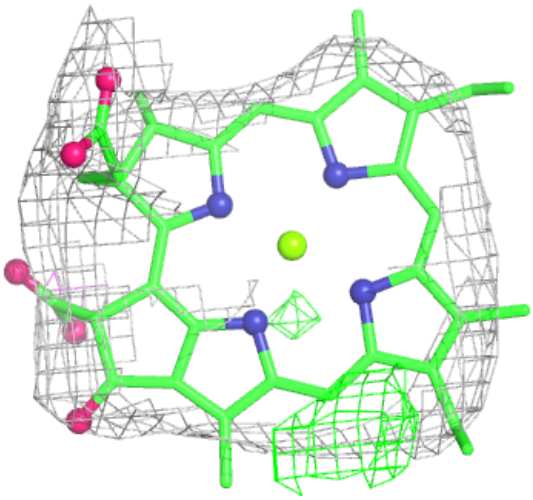


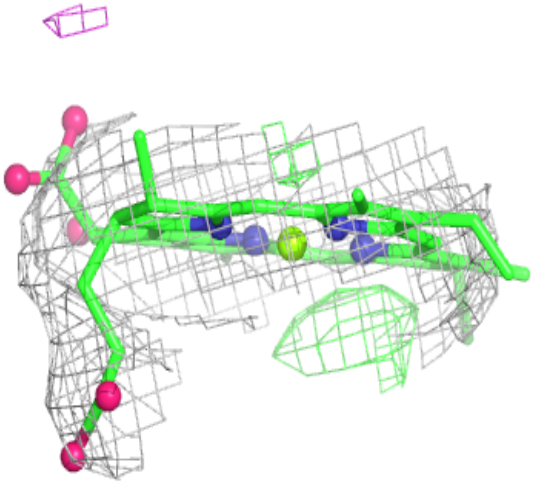


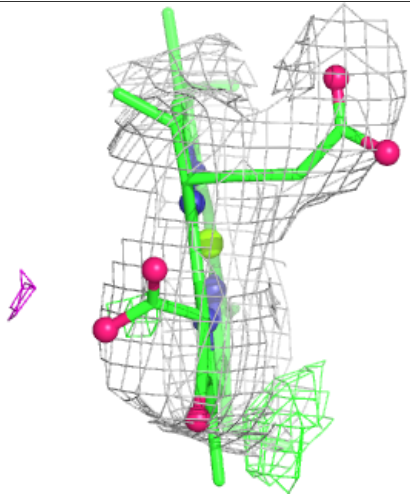


Electron density around CLA A 819:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

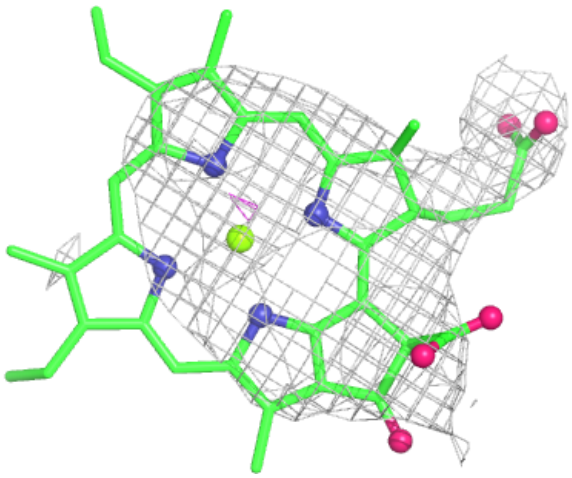


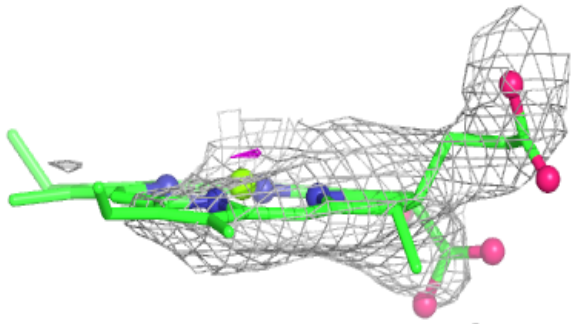


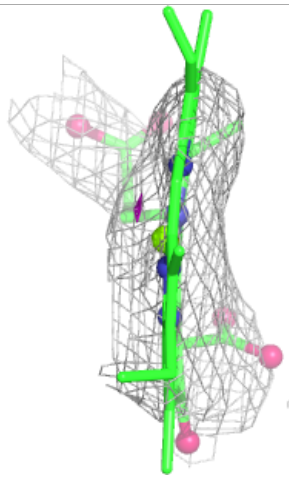


Electron density around CLA B 816:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

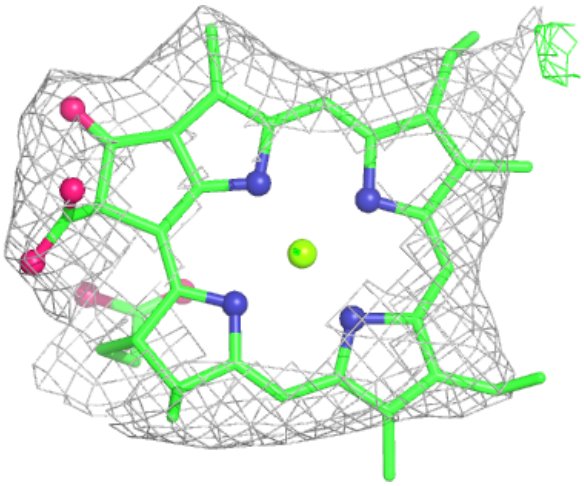


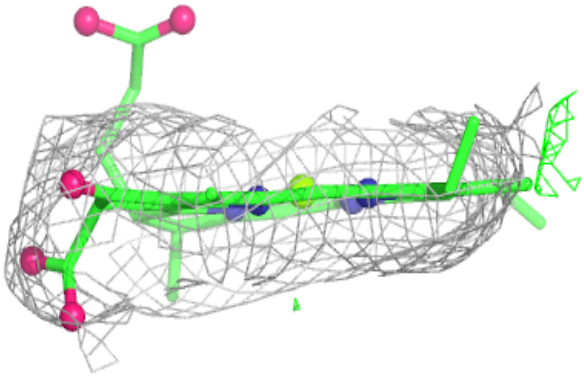


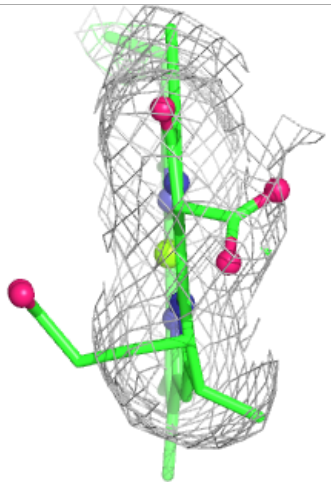


Electron density around CLA 5 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

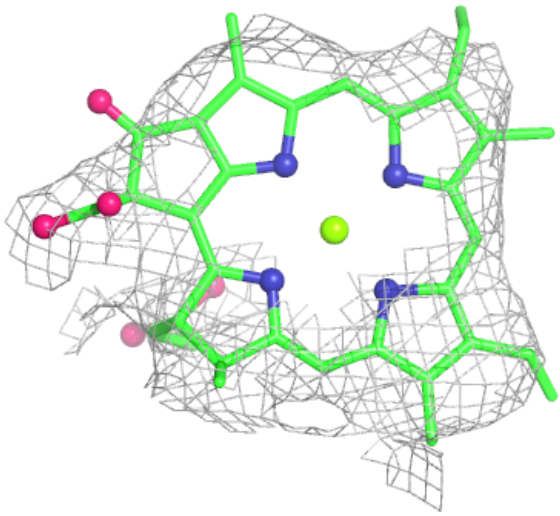


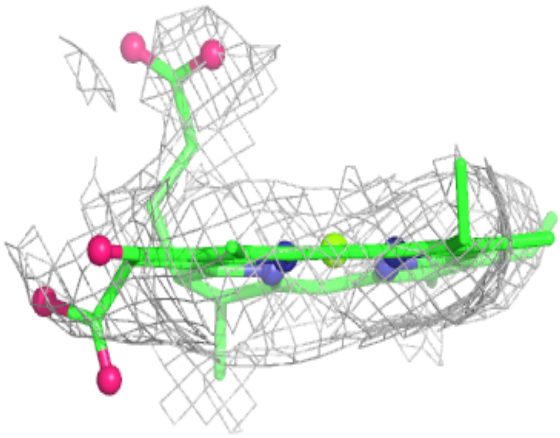


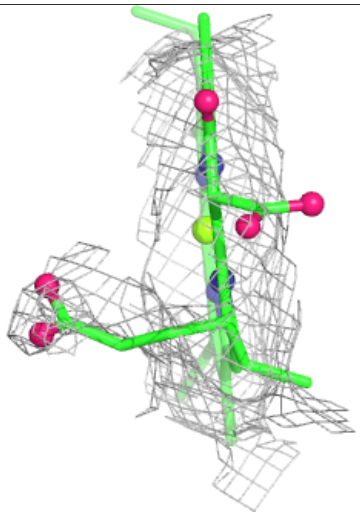


Electron density around CLA A 820:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

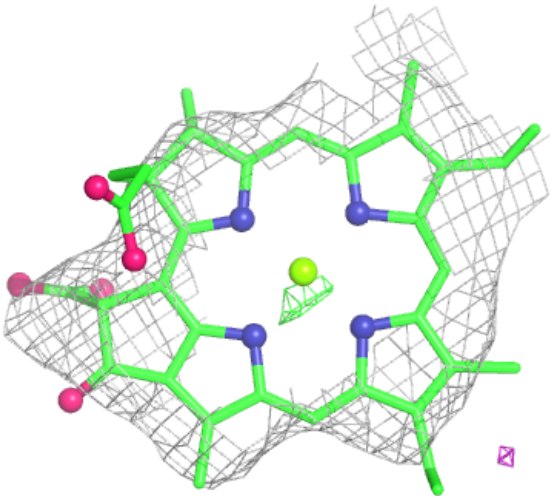


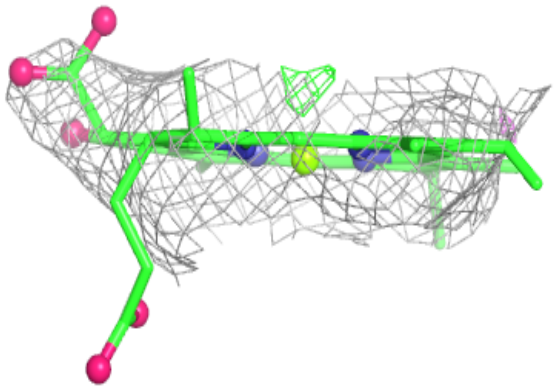


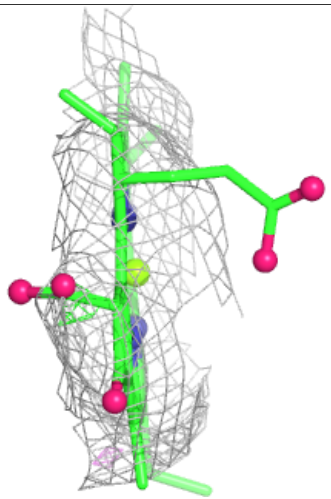


Electron density around CLA A 815:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

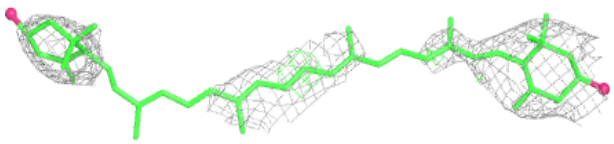


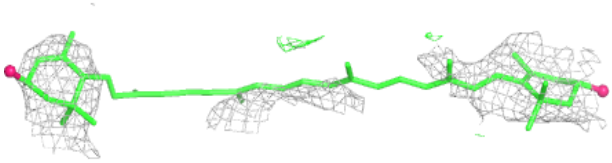


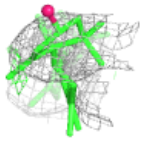


Electron density around LUT 0 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

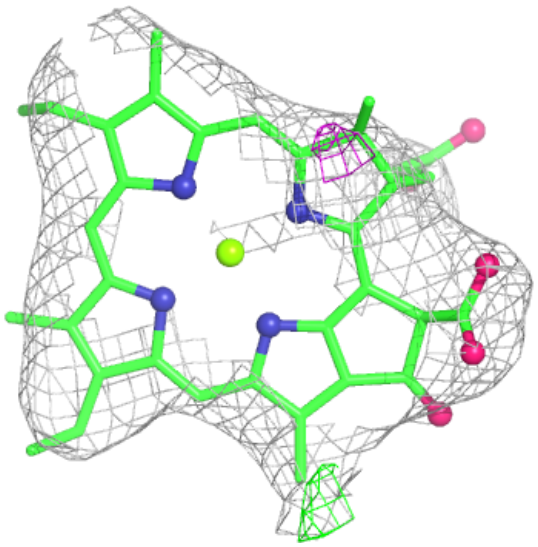


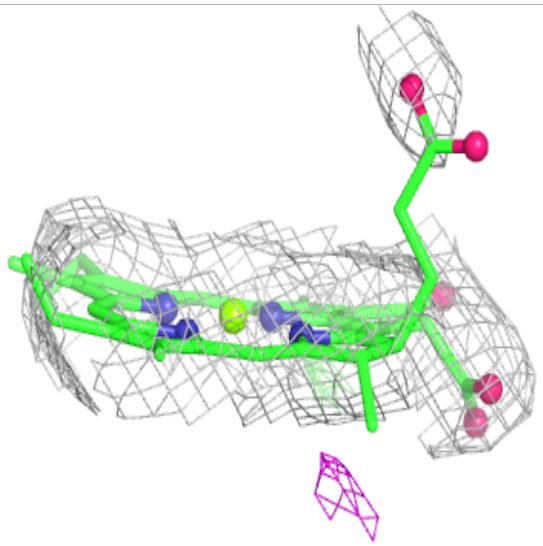




Electron density around CLA 1 1009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

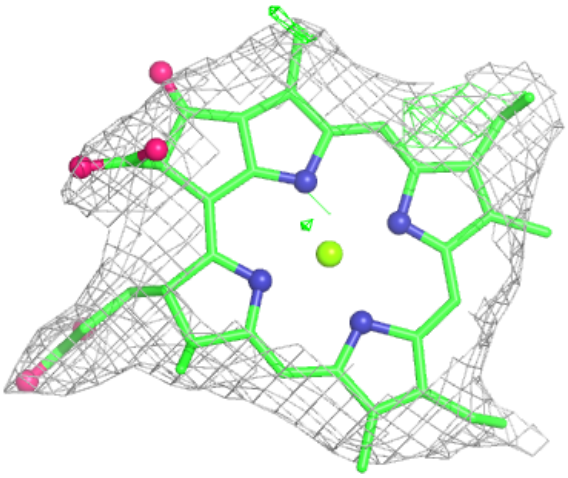


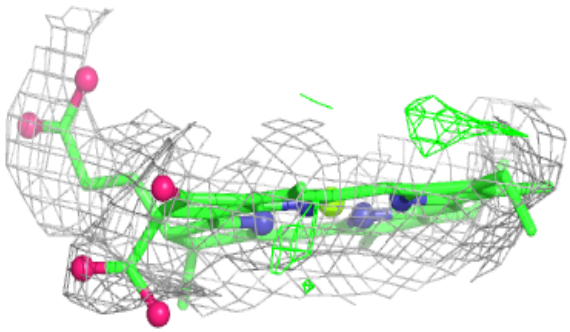


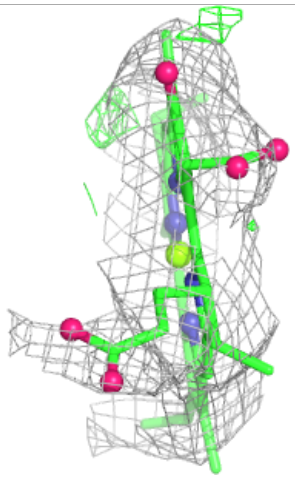


Electron density around CLA 1 1017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

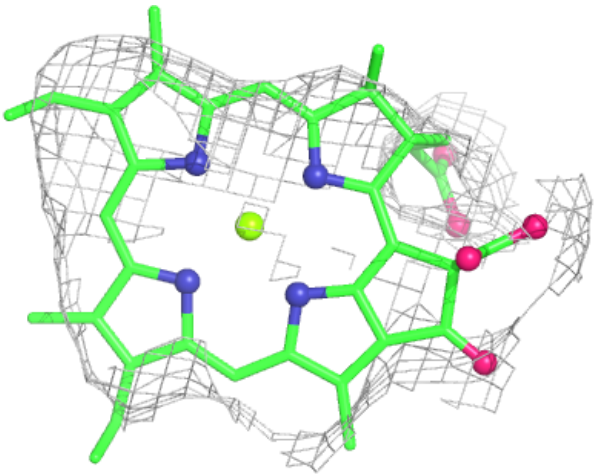


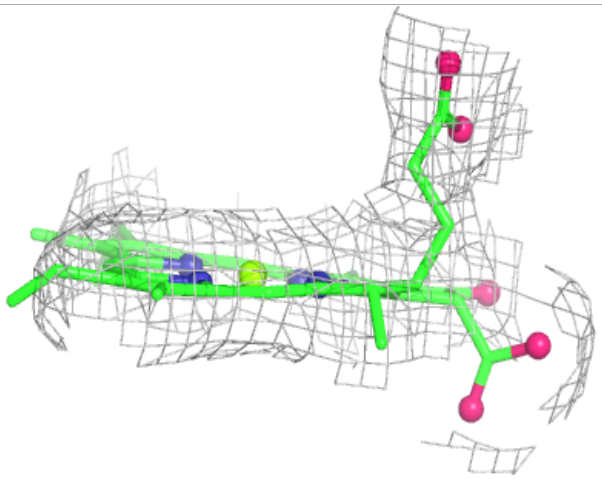


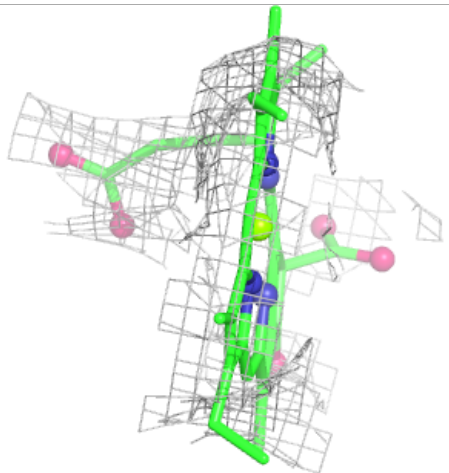


Electron density around CLA B 840:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

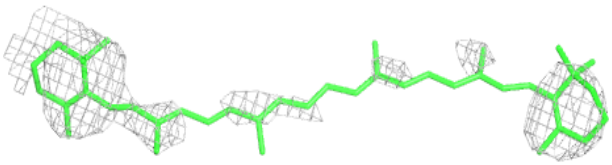


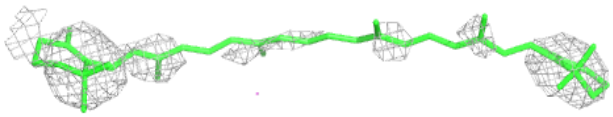


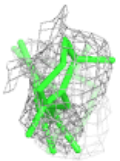


Electron density around BCR J 103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

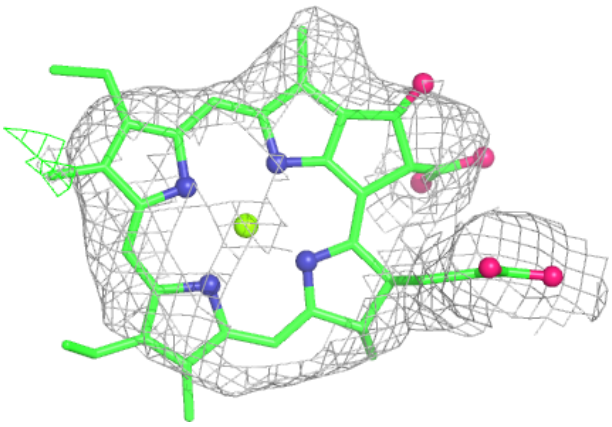


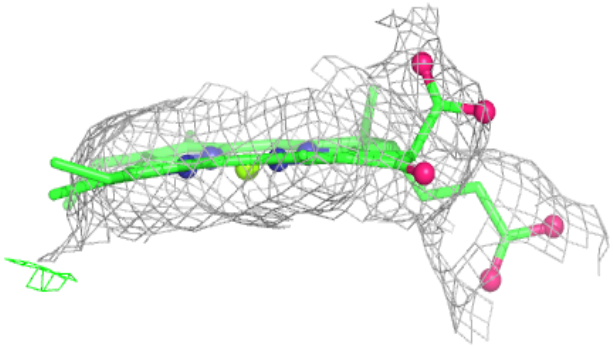


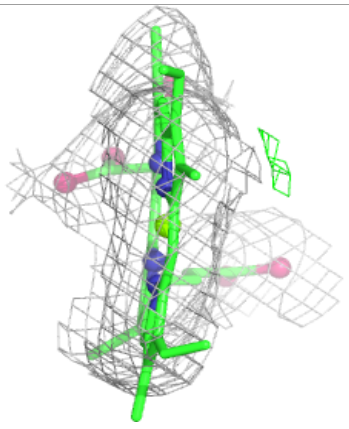


Electron density around CLA J 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

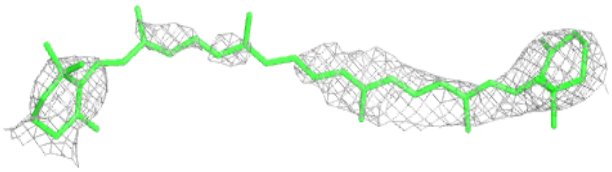


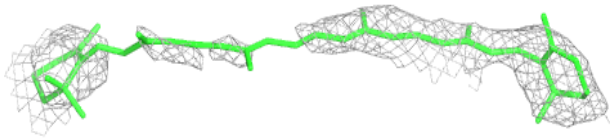


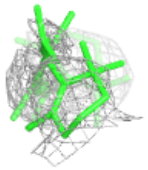


Electron density around BCR A 847:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

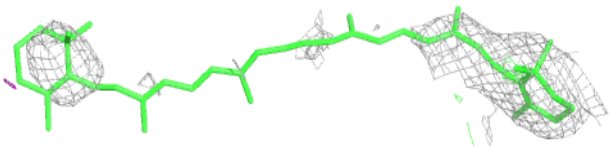


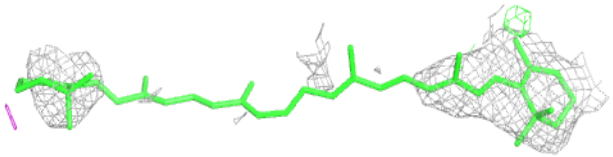


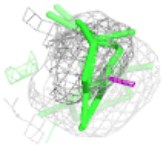


Electron density around BCR 4 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

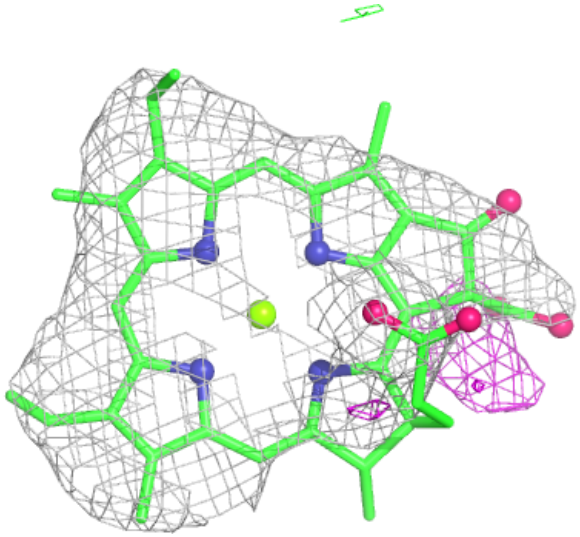


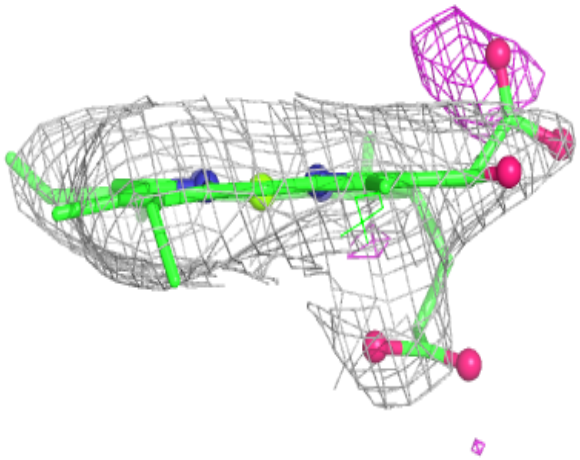


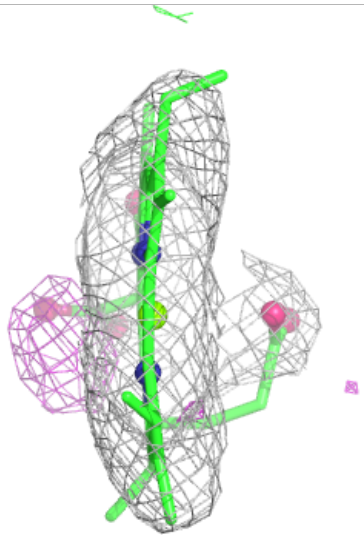


Electron density around CLA 0 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

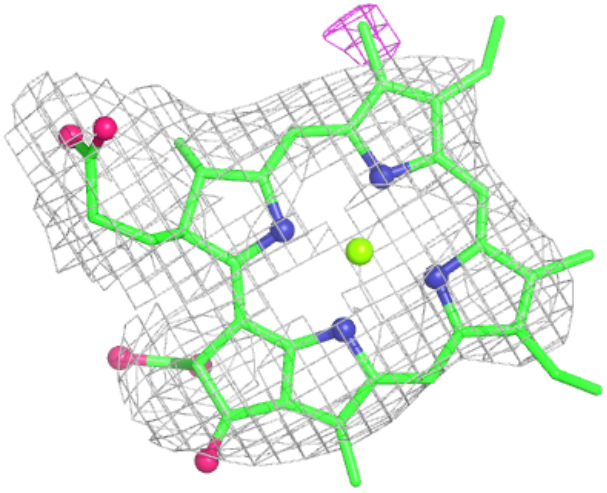


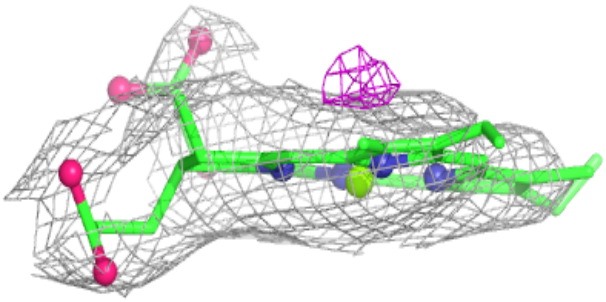


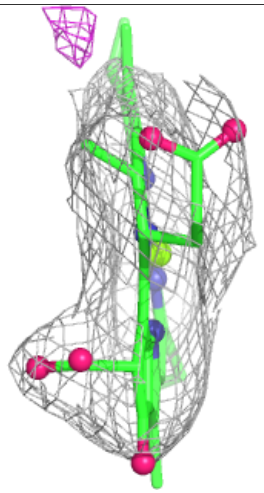


Electron density around CLA A 812:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

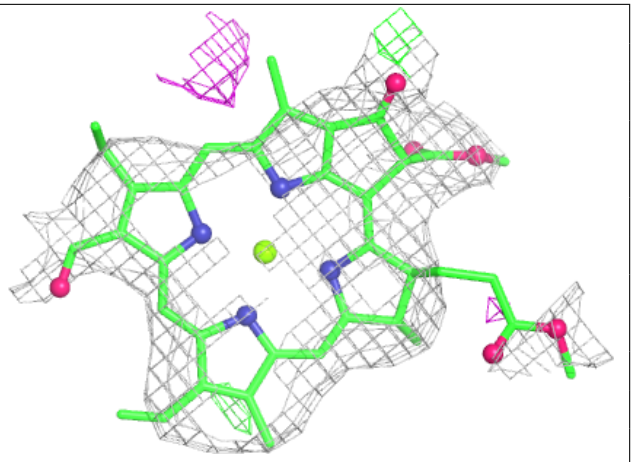


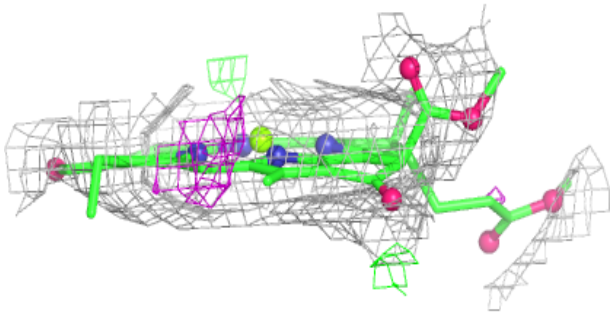


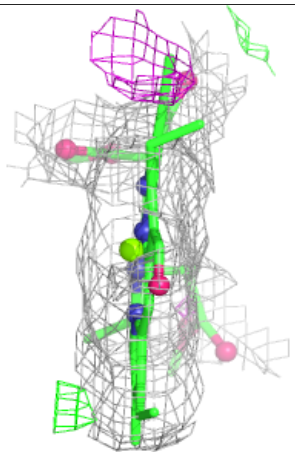


Electron density around CHL 8 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

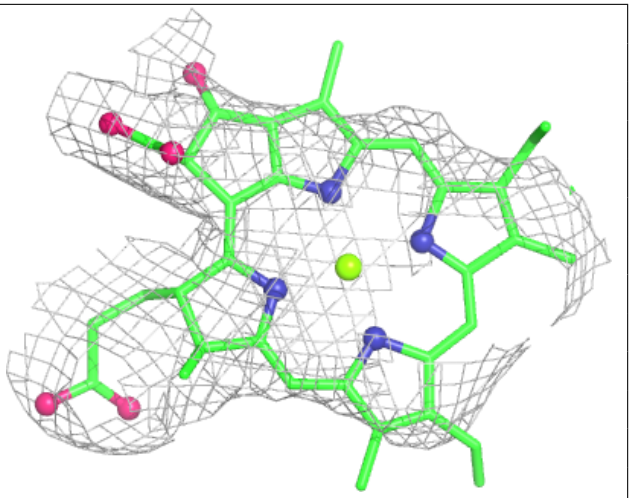


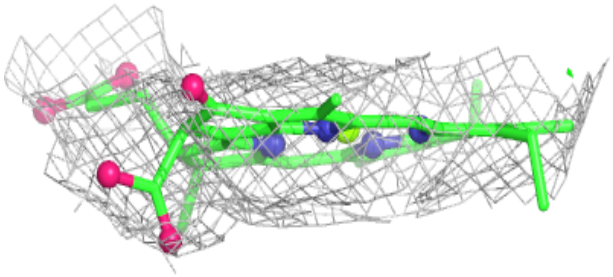


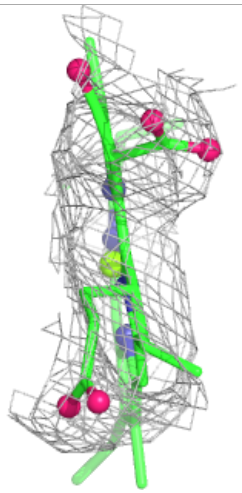


Electron density around CLA B 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

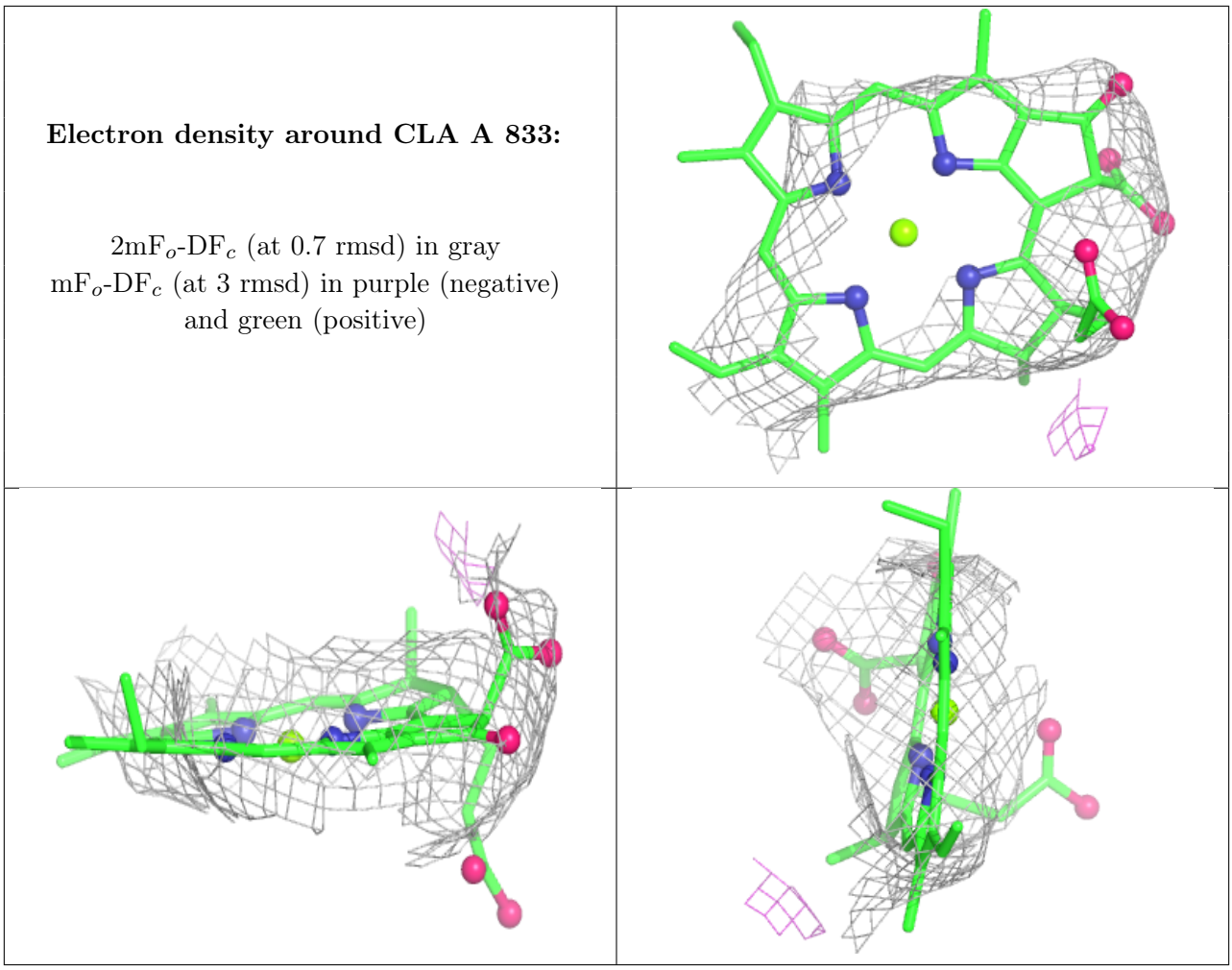






Electron density around CLA A 833:

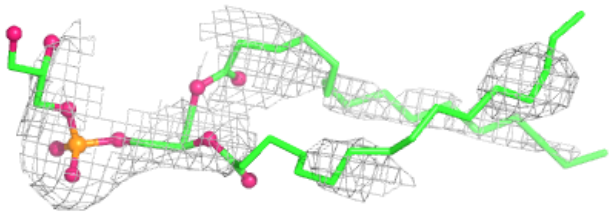
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

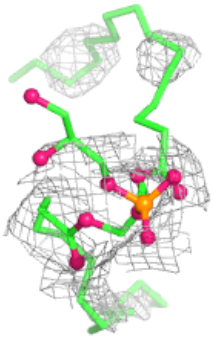


Electron density around LHG A 849:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

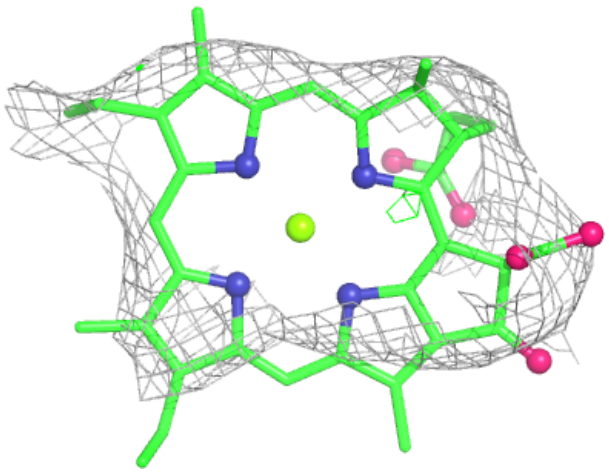


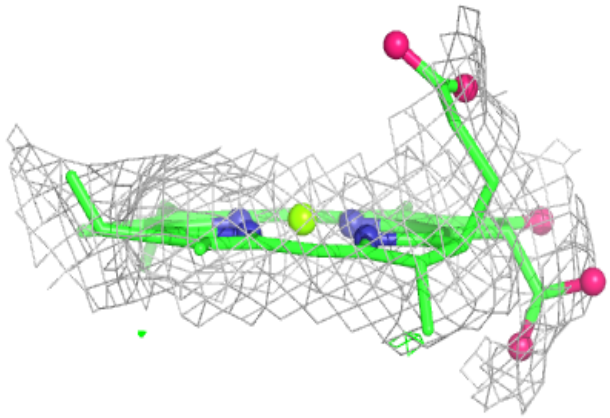


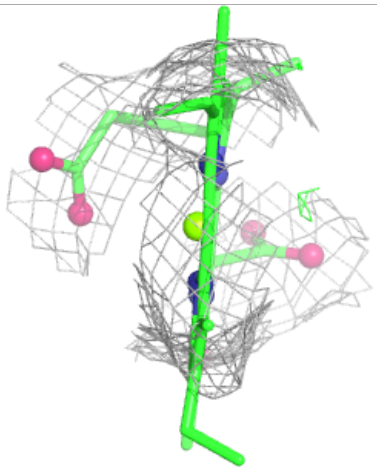


Electron density around CLA B 810:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

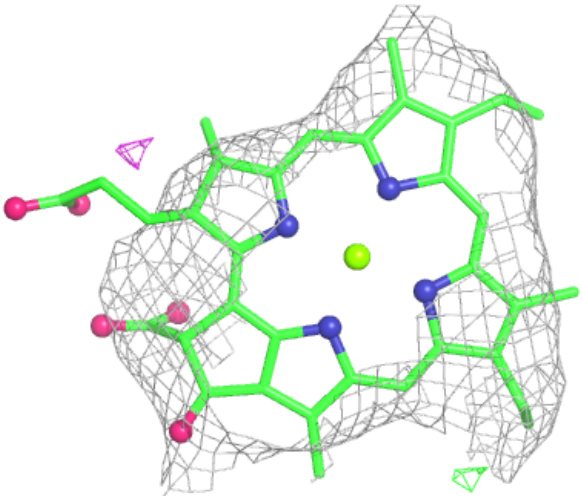


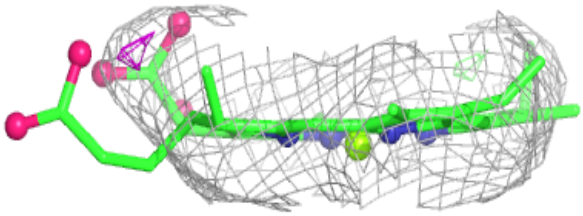


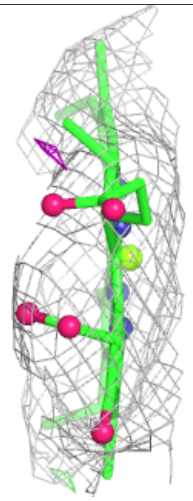


Electron density around CLA 1 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

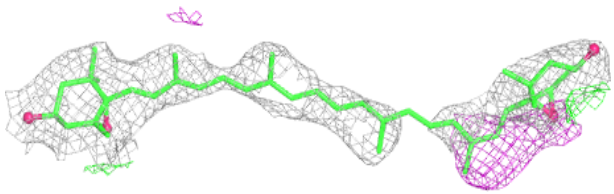


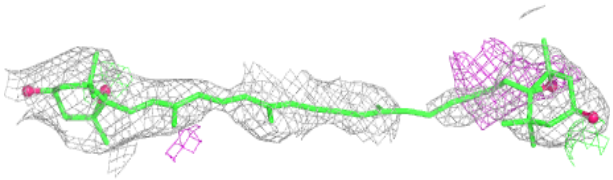


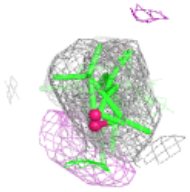


Electron density around XAT 7 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

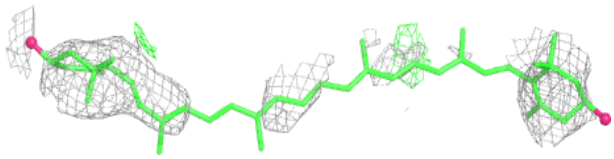


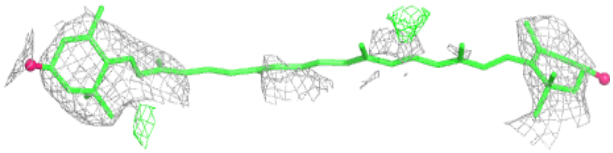


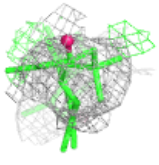


Electron density around LUT 1 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

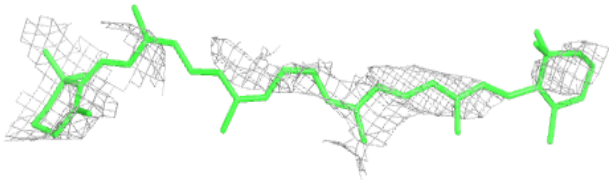


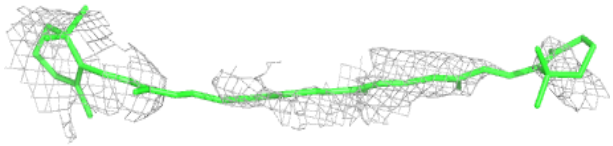


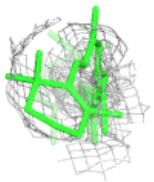


Electron density around BCR B 843:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

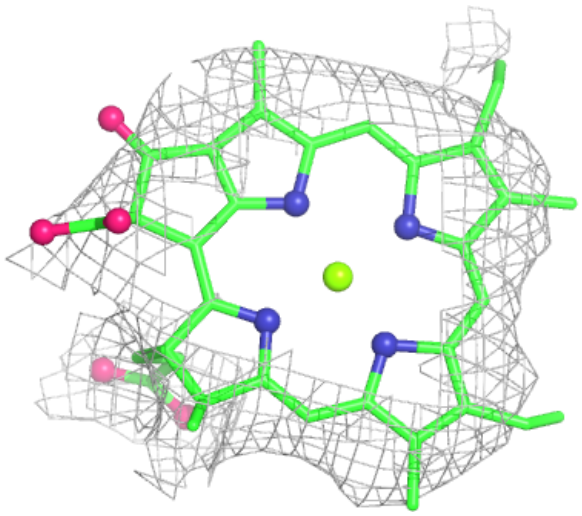


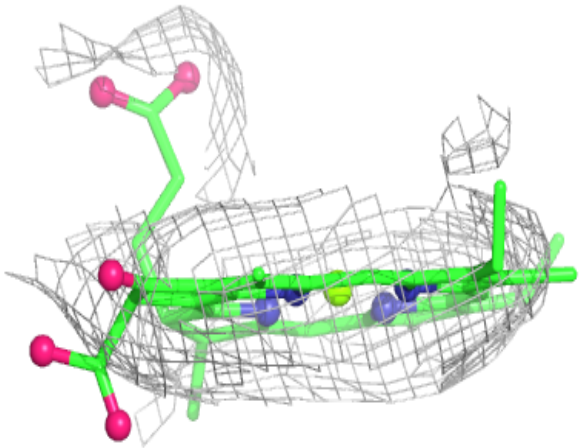


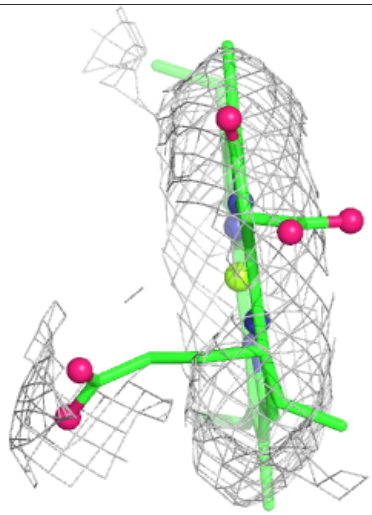


Electron density around CLA B 822:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

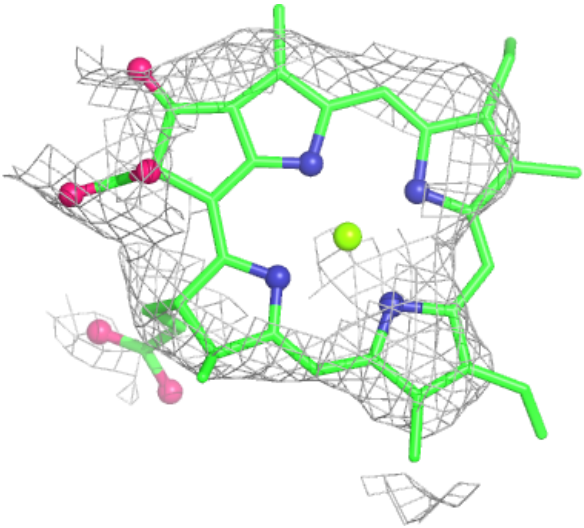


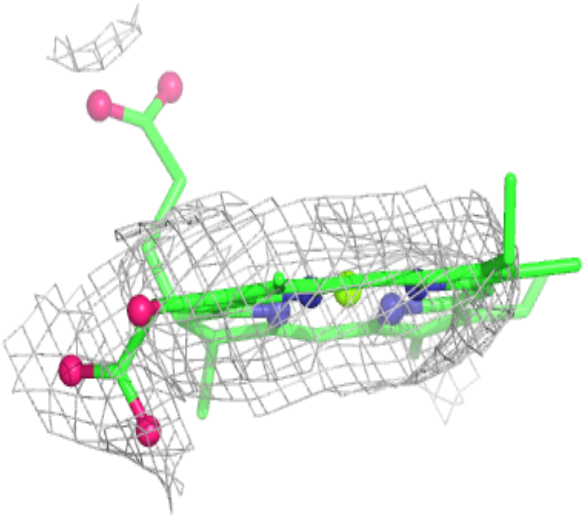


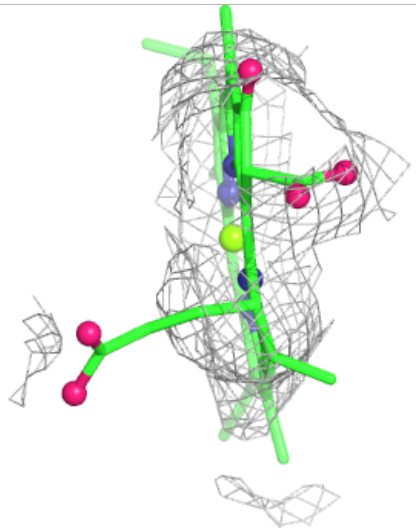


Electron density around CLA B 832:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

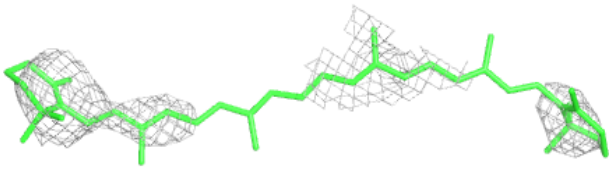


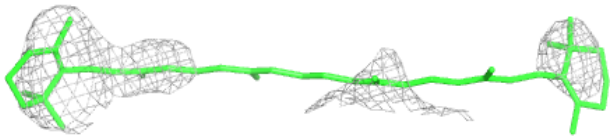


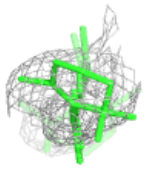


Electron density around BCR B 846:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

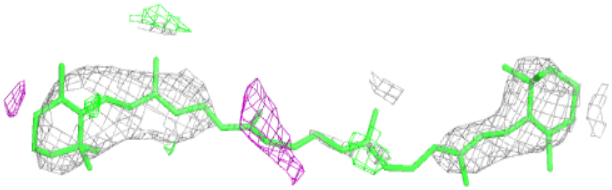


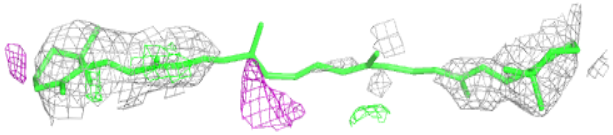


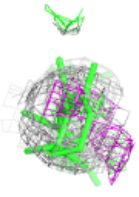


Electron density around BCR 7 1003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

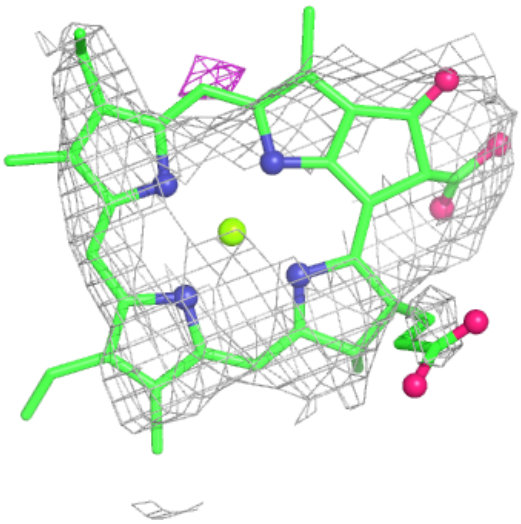


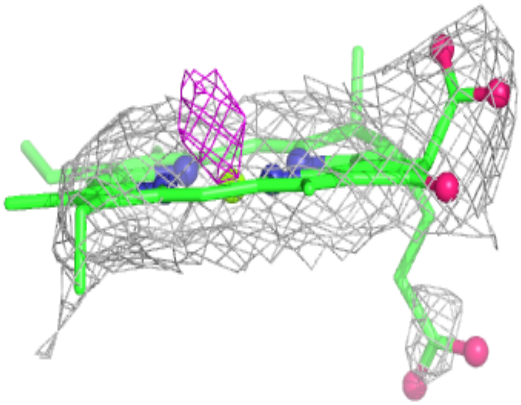


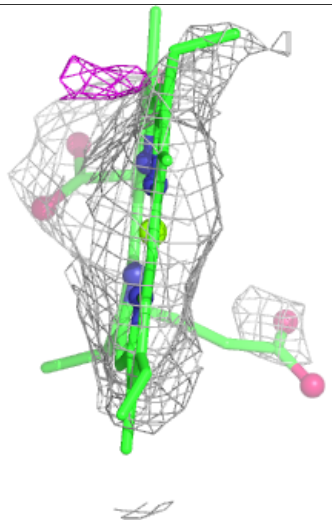


Electron density around CLA B 835:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

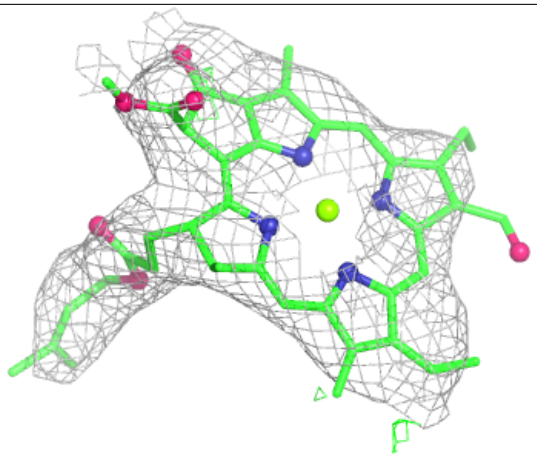


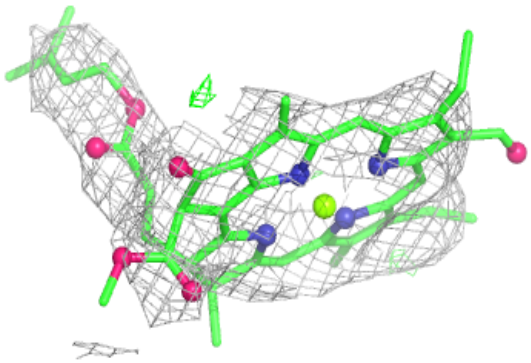


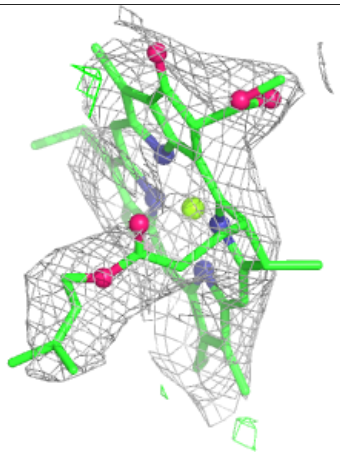


Electron density around CHL 1 1013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

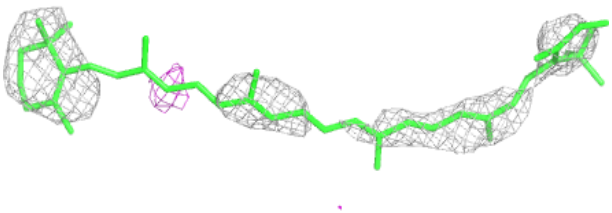


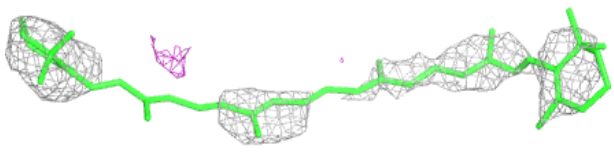


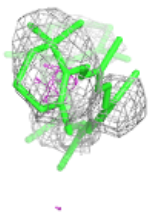


Electron density around BCR F 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

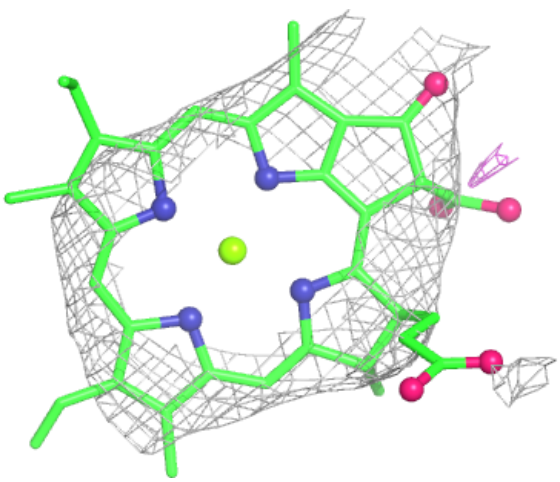


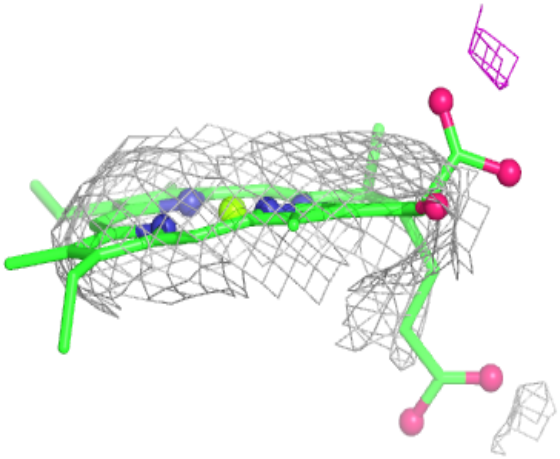


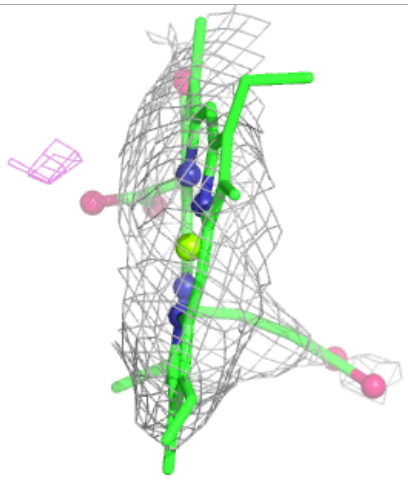


Electron density around CLA A 832:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

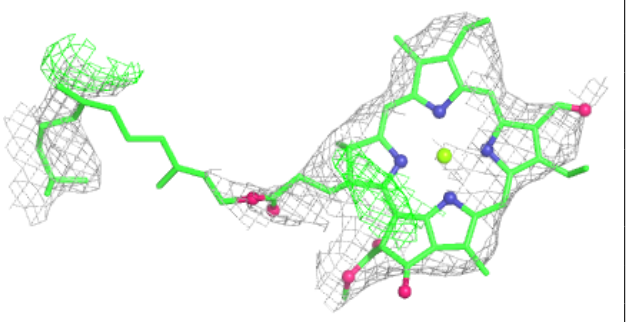


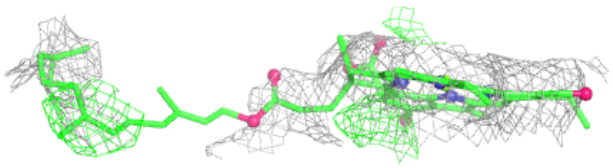




Electron density around CHL 4 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

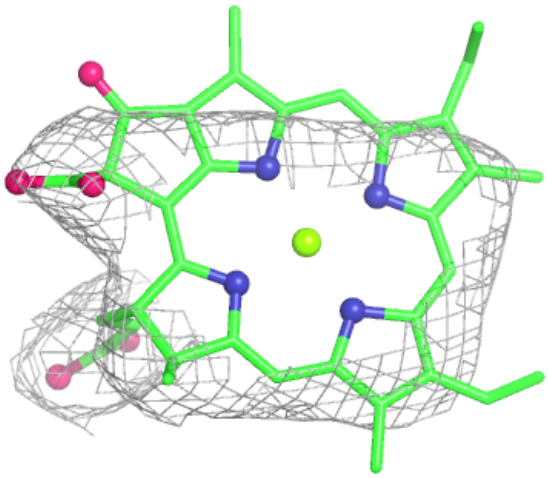


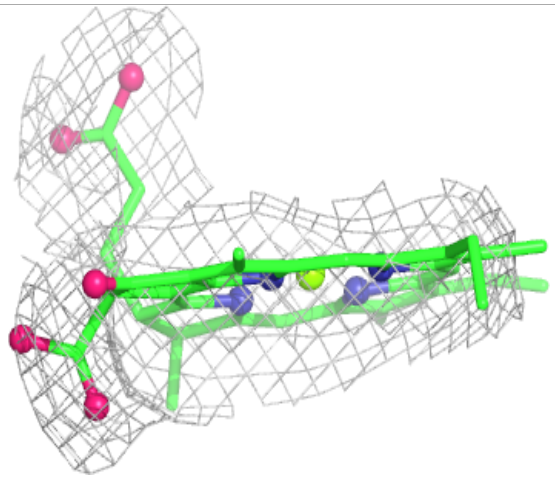


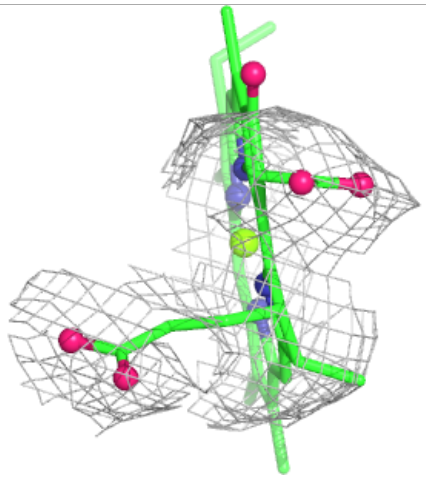


Electron density around CLA B 814:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

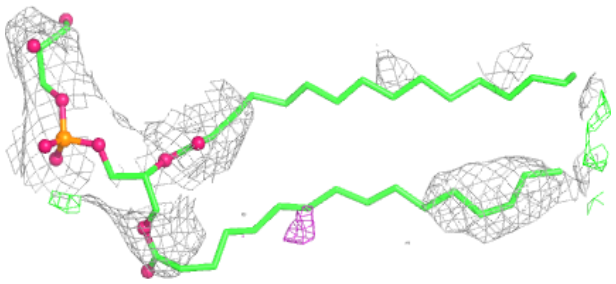


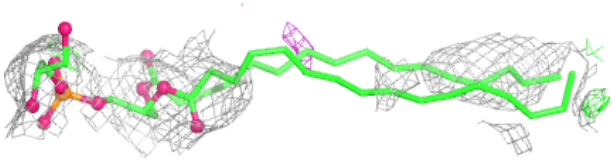




Electron density around LHG 4 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

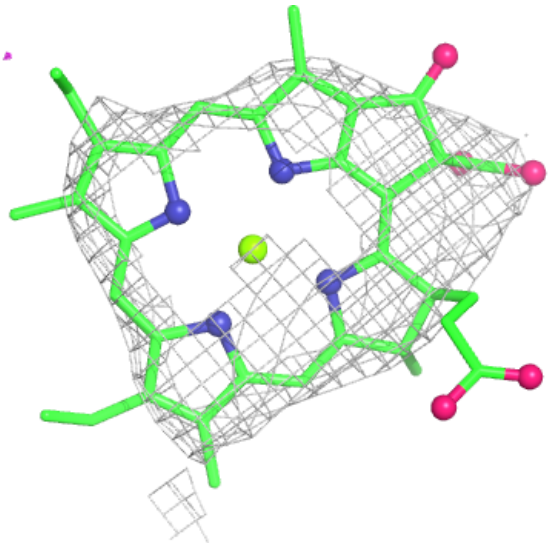


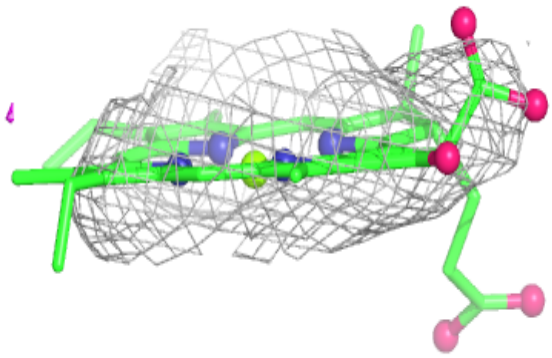


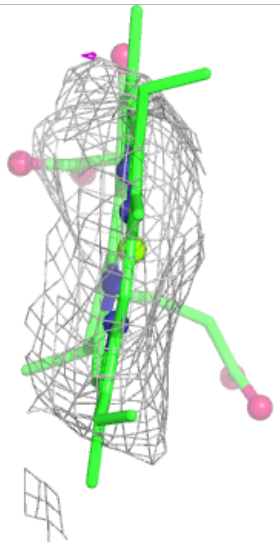


Electron density around CLA B 820:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

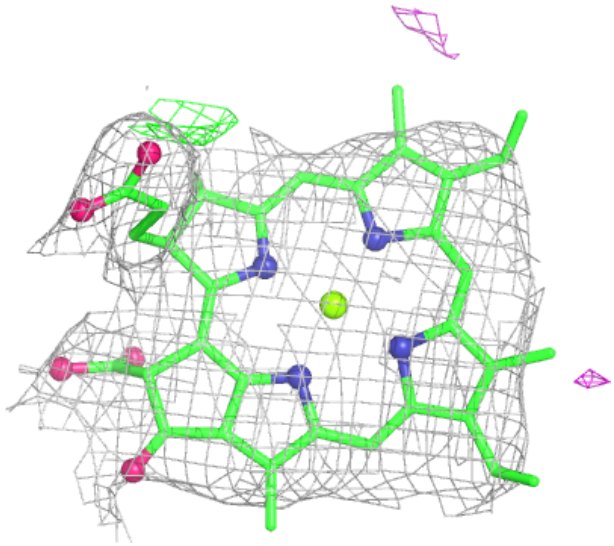


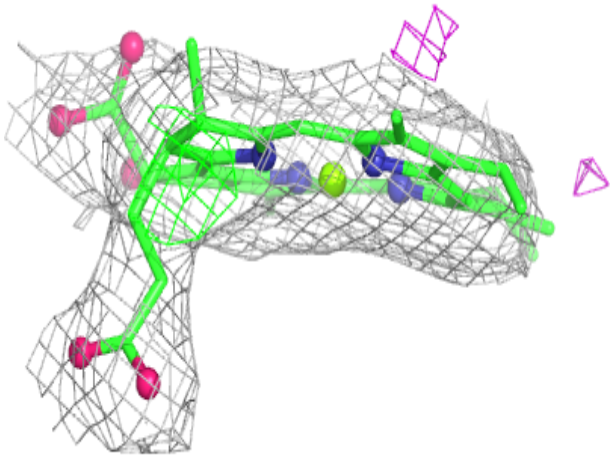


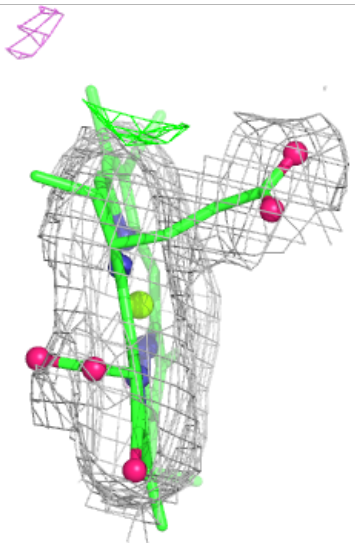


Electron density around CLA 1 1014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

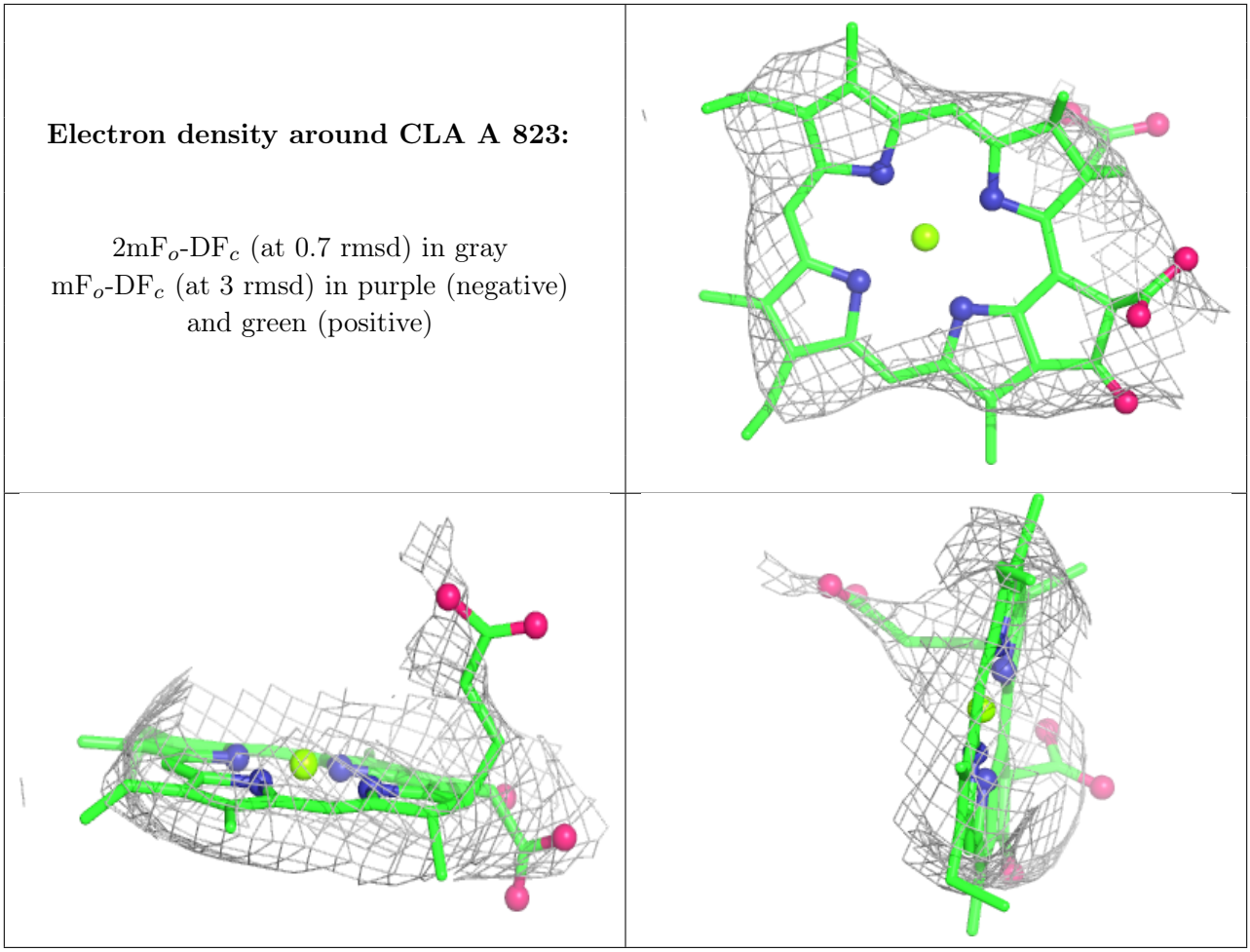






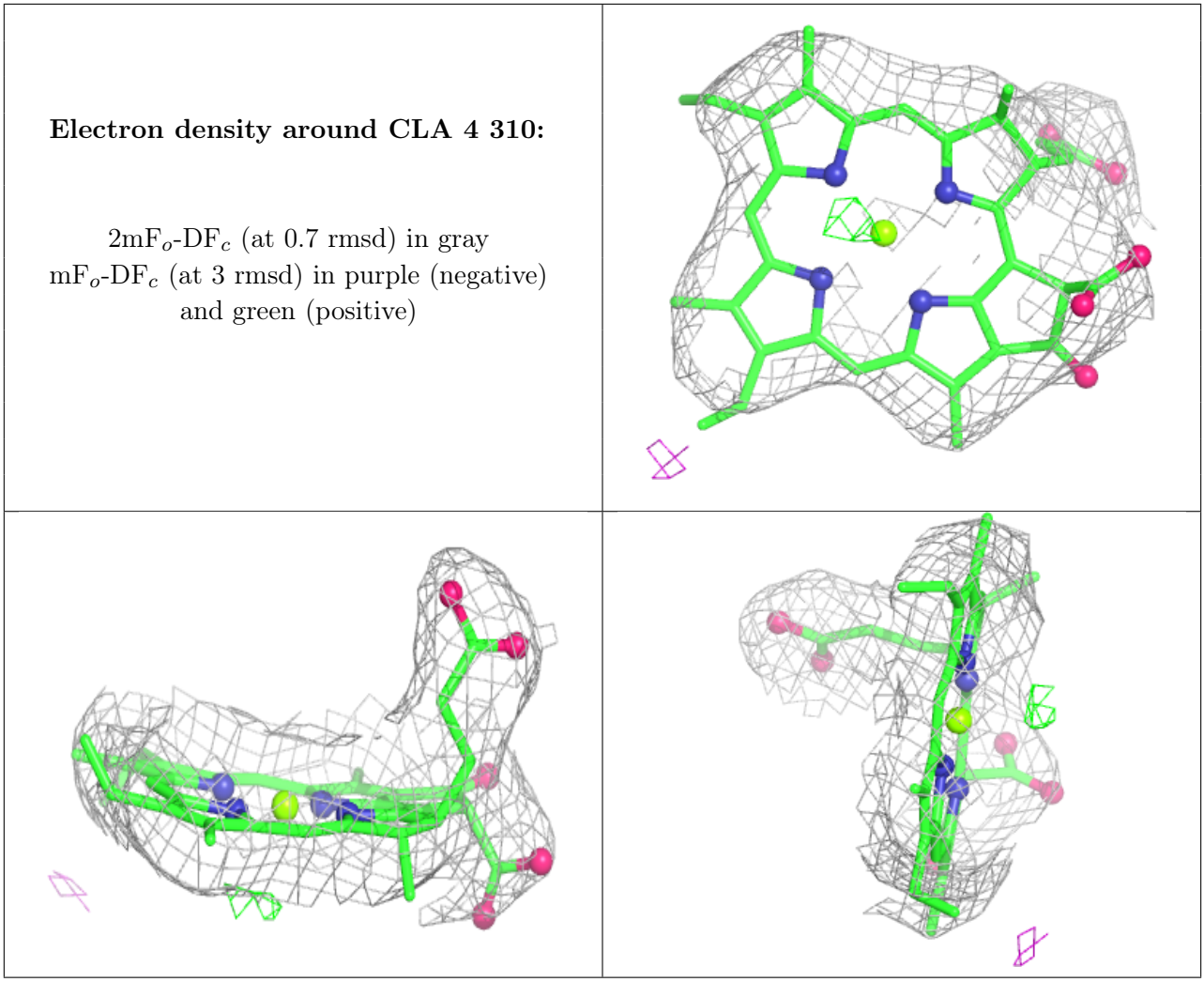
Electron density around CLA A 823:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



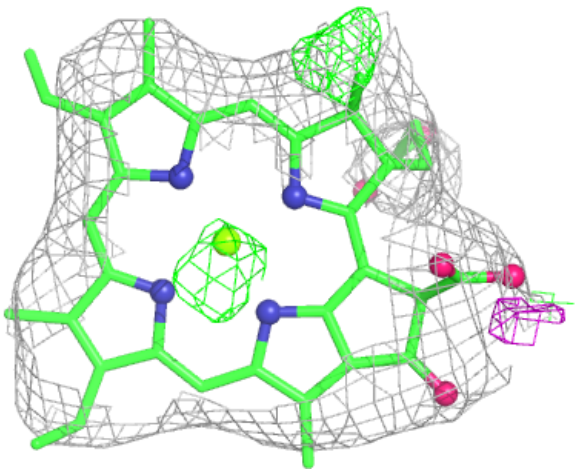
Electron density around CLA 4 310:

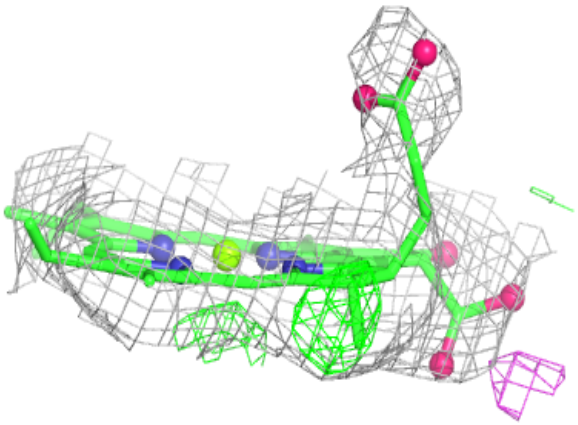
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 6 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

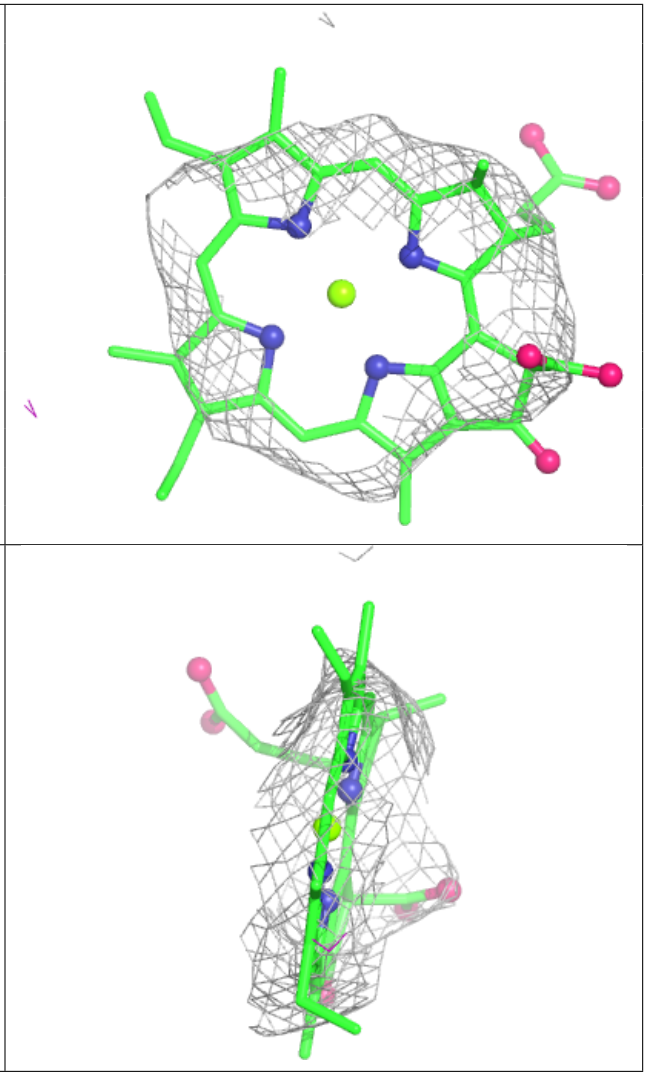






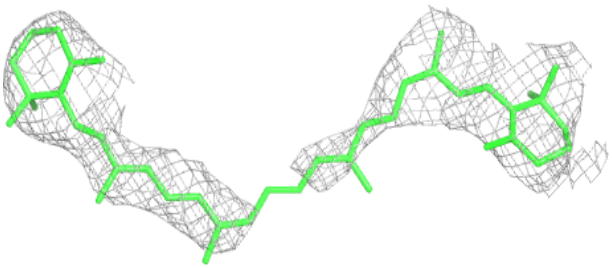
Electron density around CLA A 830:

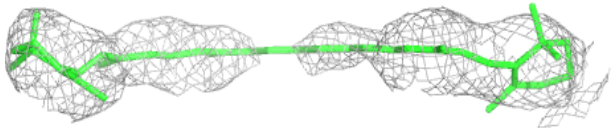
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

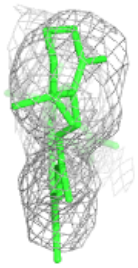


Electron density around BCR A 848:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

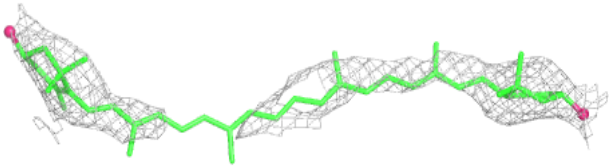


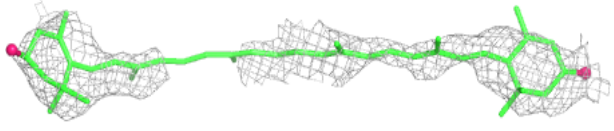


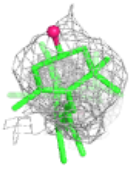


Electron density around LUT 1 1016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

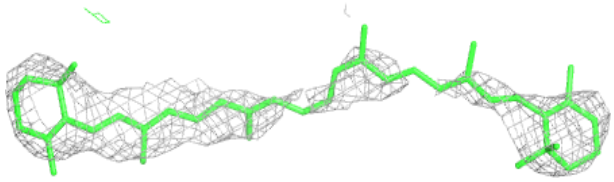


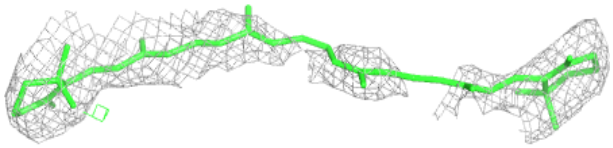


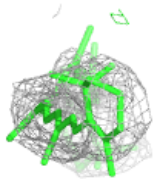


Electron density around BCR 3 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

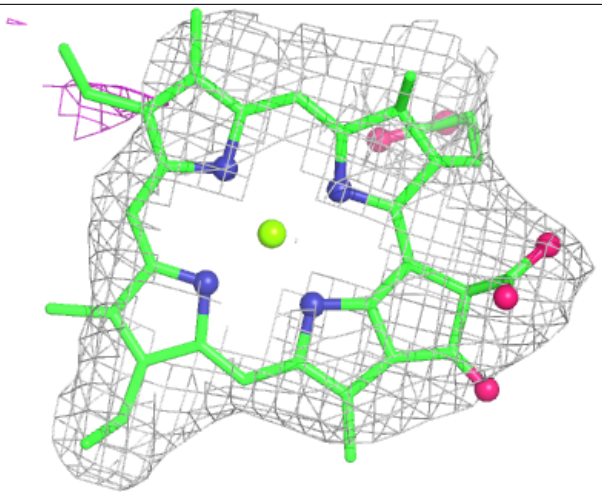


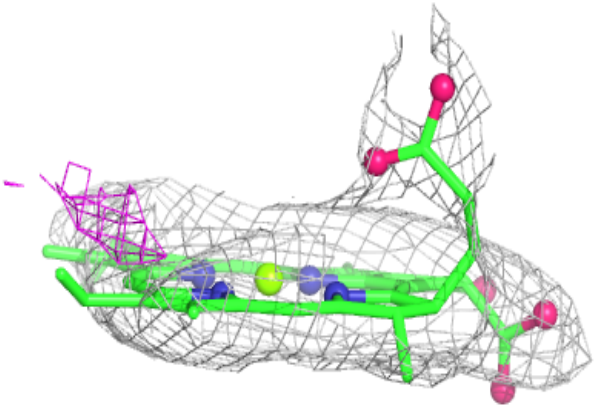


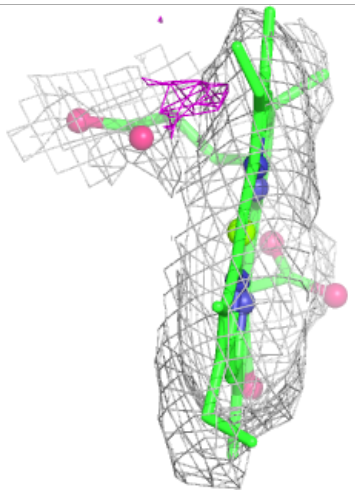


Electron density around CLA 0 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

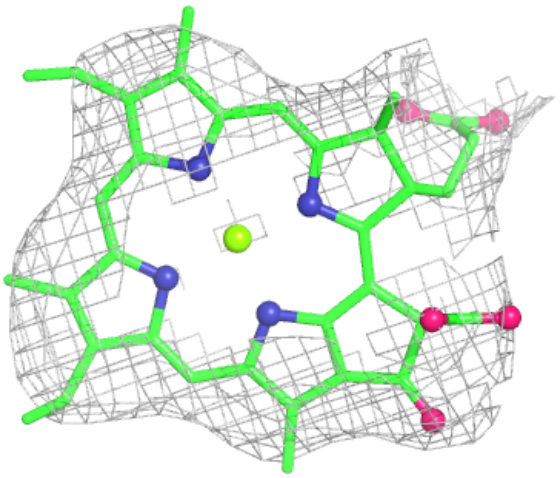


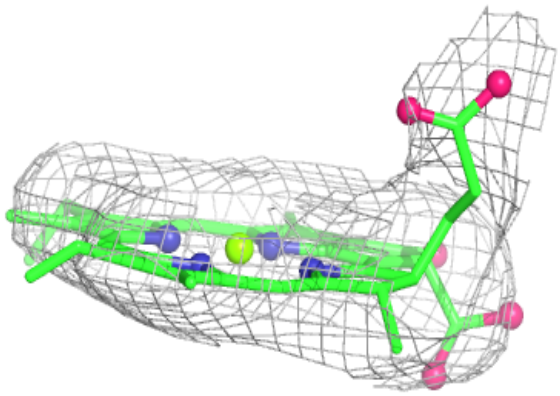


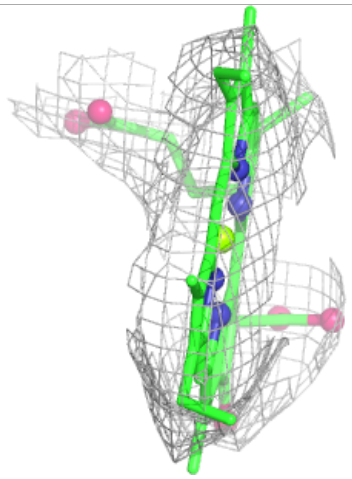


Electron density around CLA B 841:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

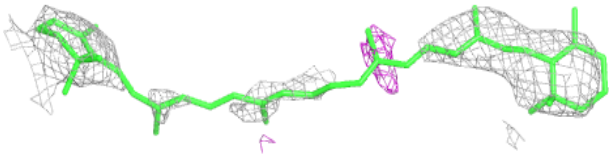


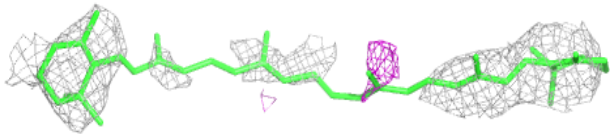


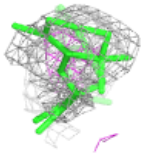


Electron density around BCR 6 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

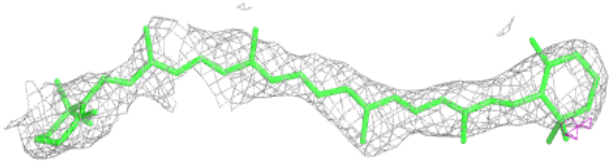




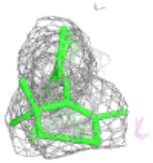


Electron density around BCR 5 320:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

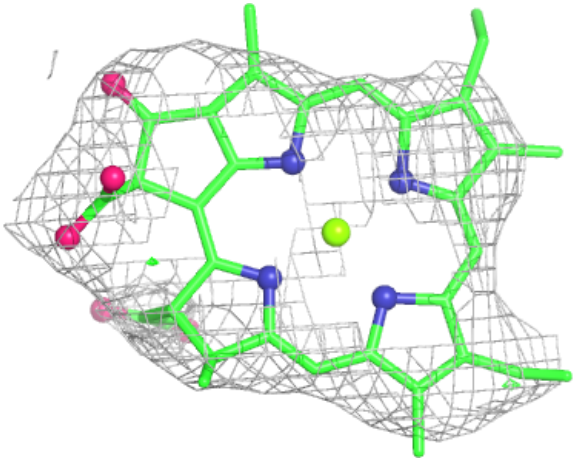


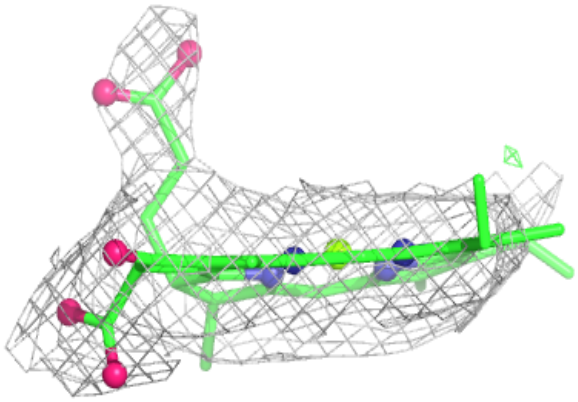




Electron density around CLA A 809:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

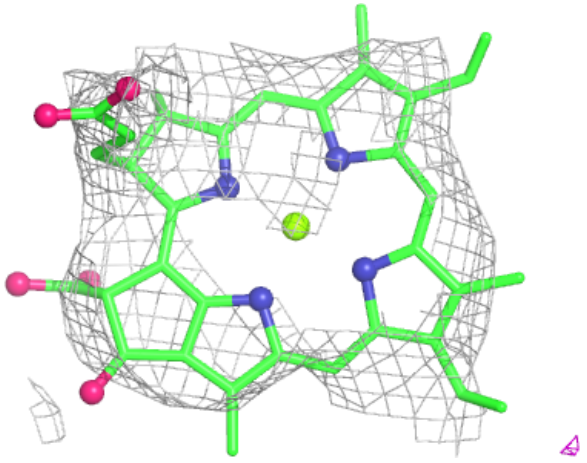


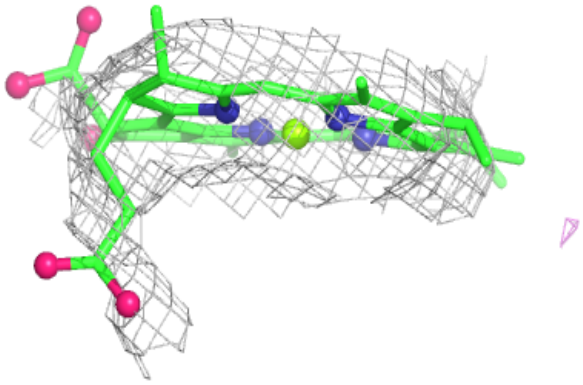


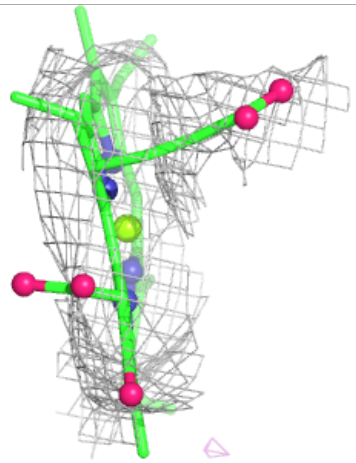


Electron density around CLA 0 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

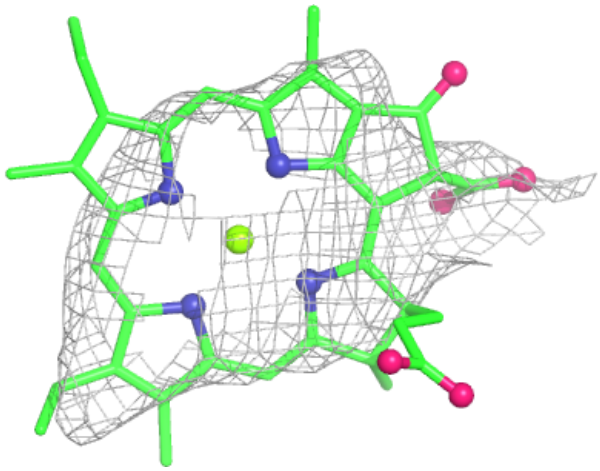


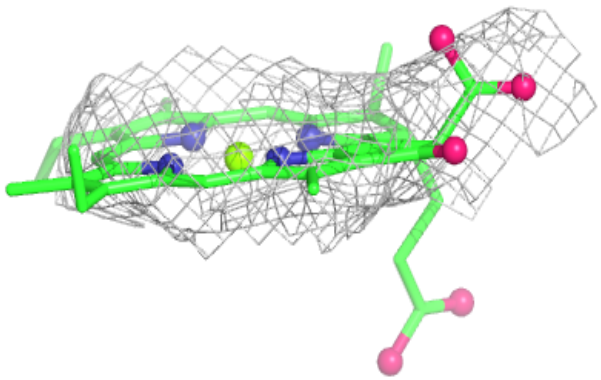


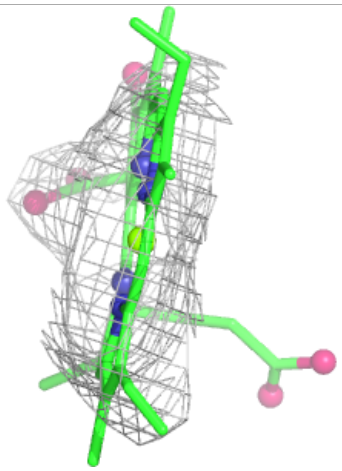


Electron density around CLA L 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



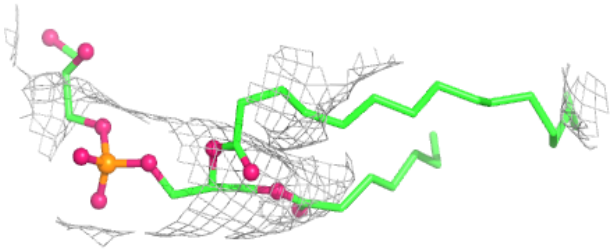


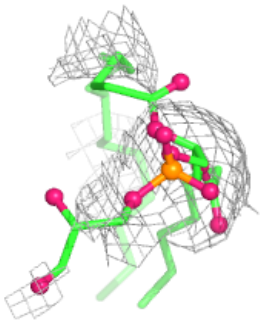


Electron density around LHG A 843:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

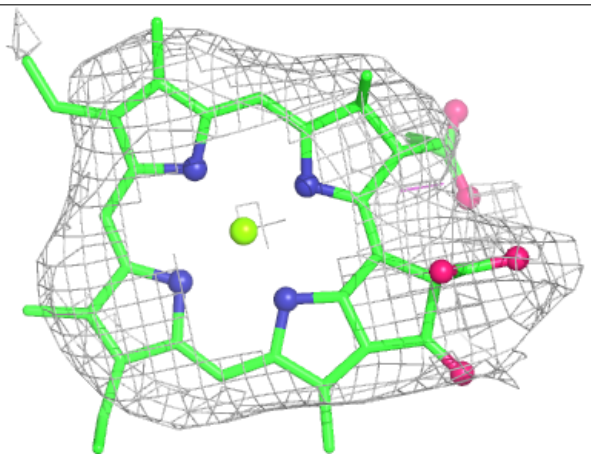


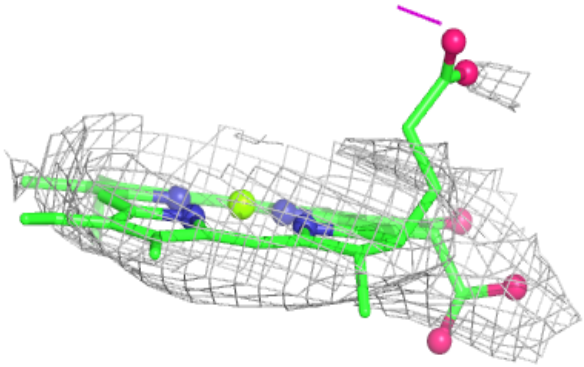


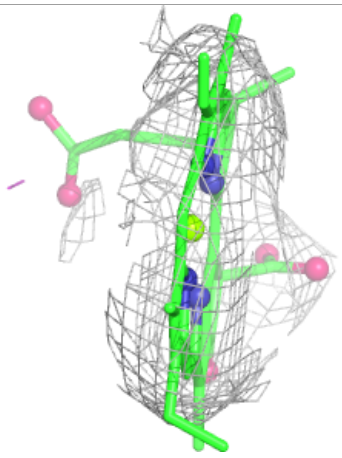


Electron density around CLA A 852:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

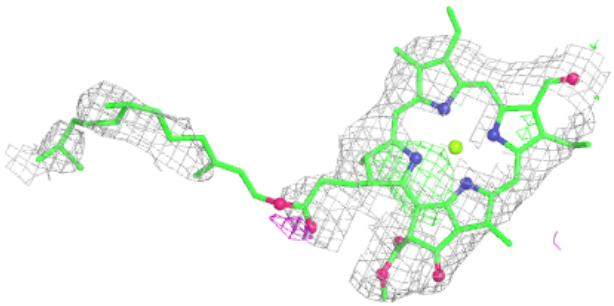


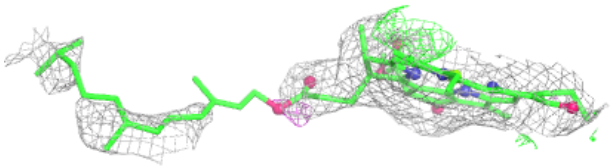




Electron density around CHL 6 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

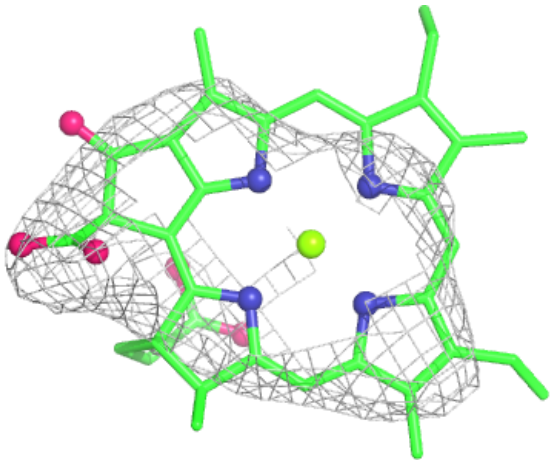


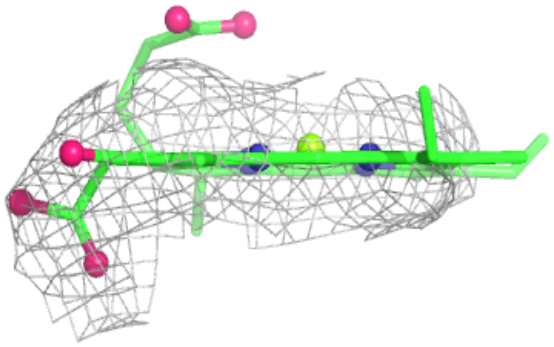


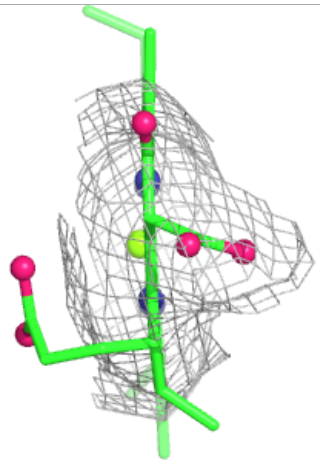


Electron density around CLA B 819:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

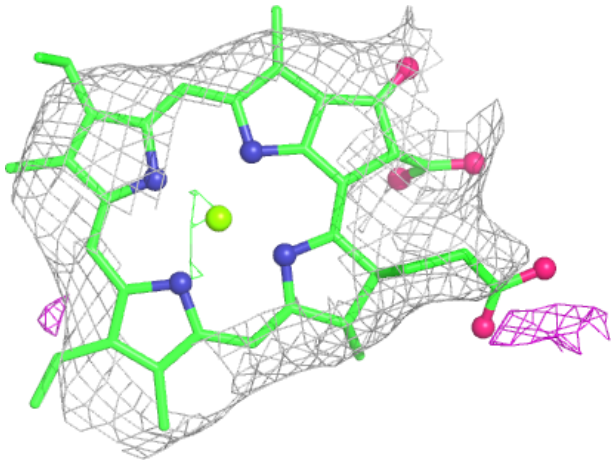


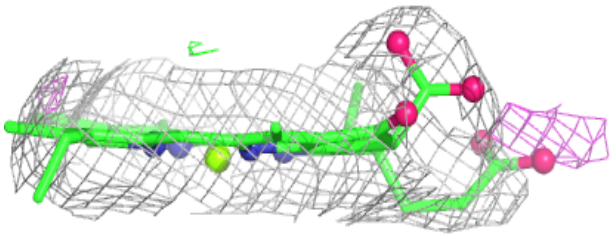


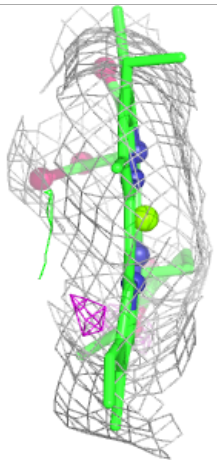


Electron density around CLA 1 1007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

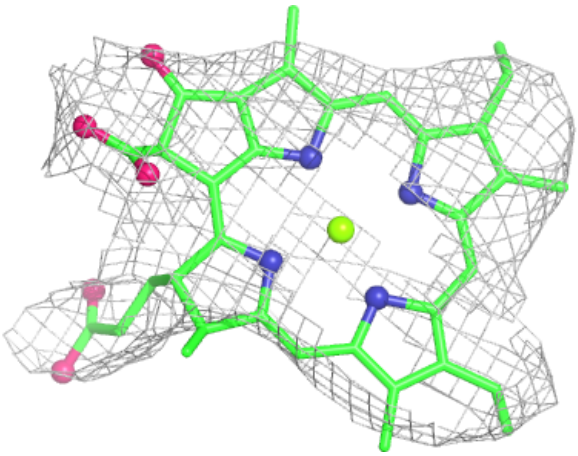


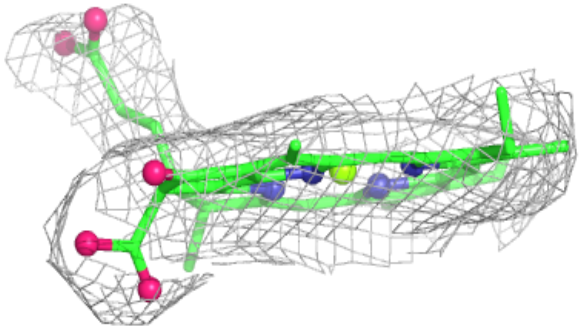


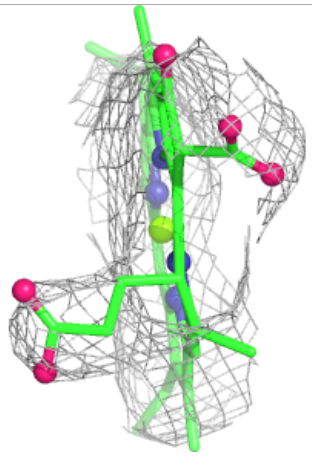


Electron density around CLA A 825:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

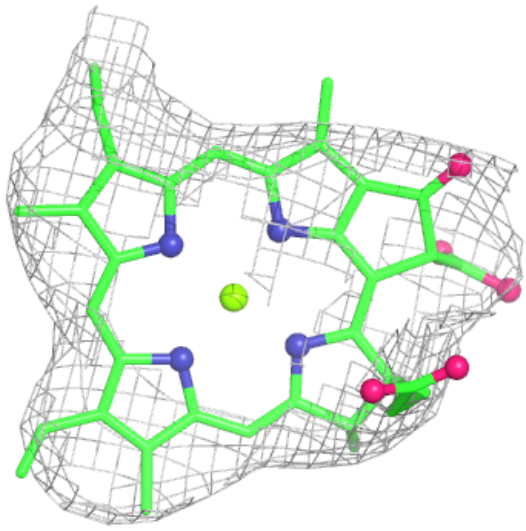


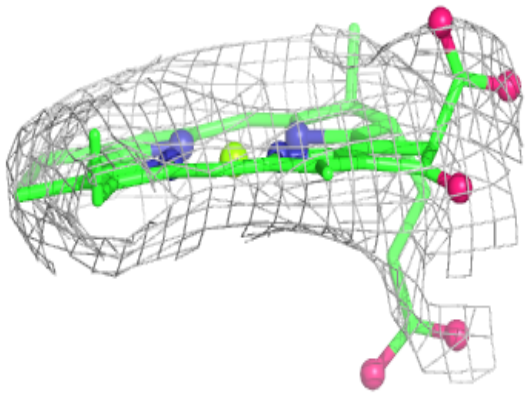


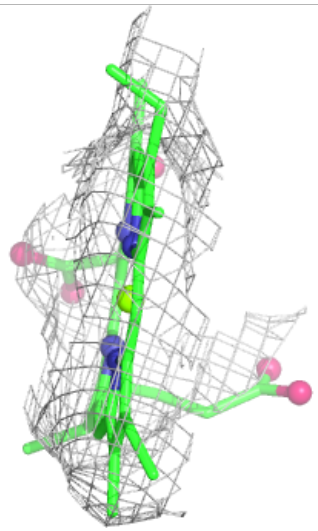


Electron density around CLA B 833:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

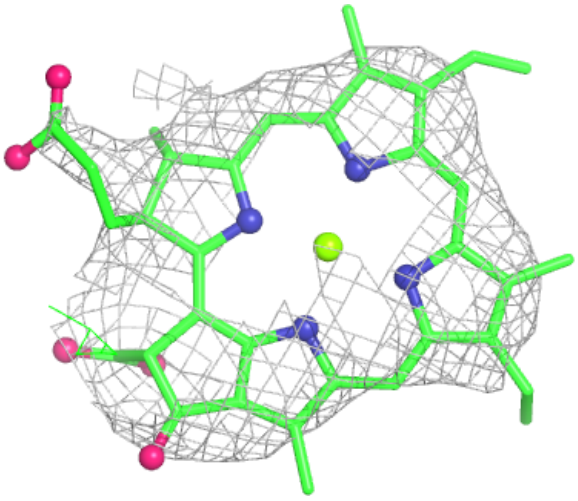


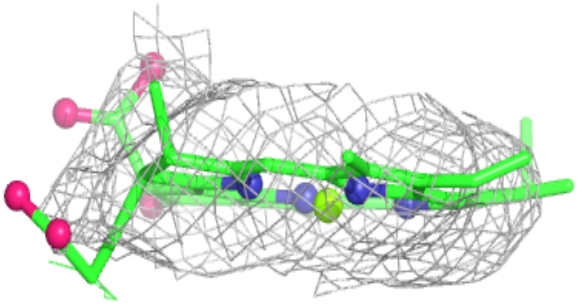


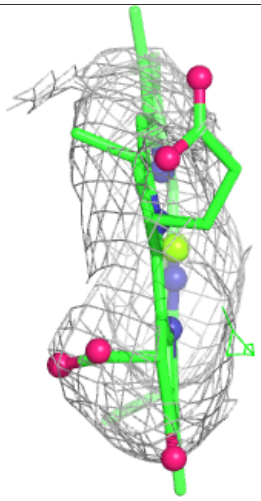


Electron density around CLA B 808:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

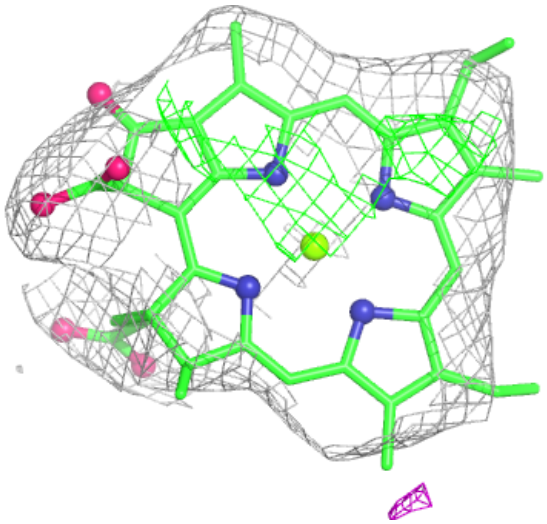


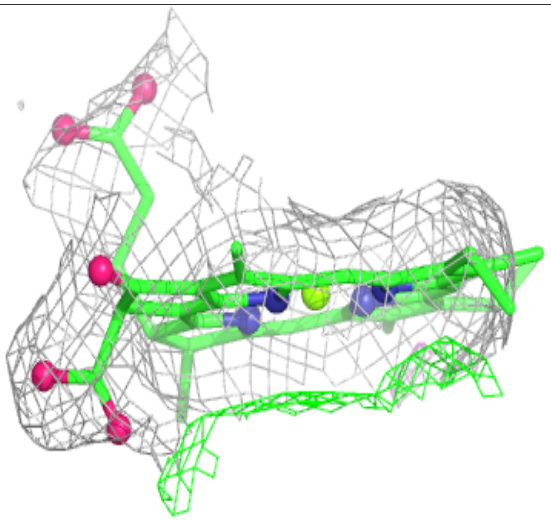


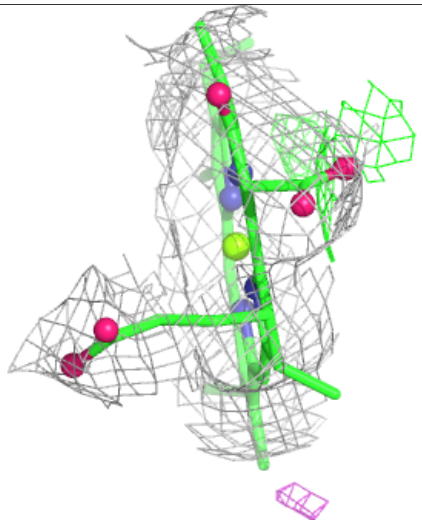


Electron density around CLA 8 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

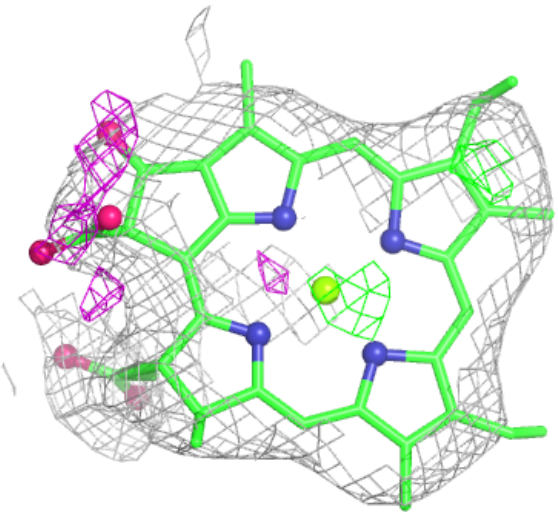


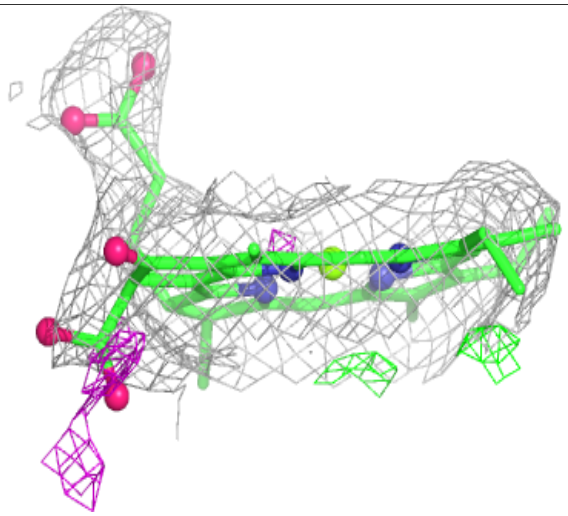


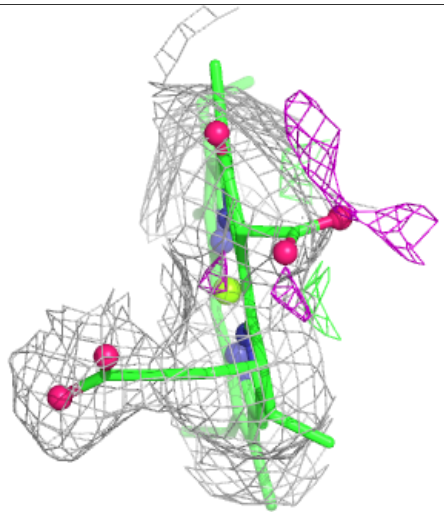


Electron density around CLA 6 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

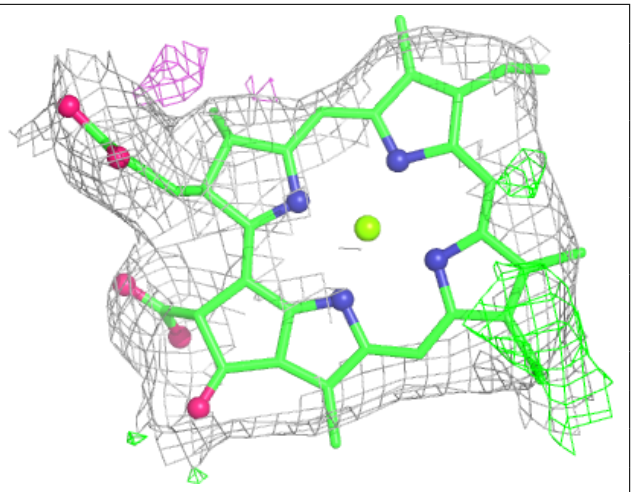


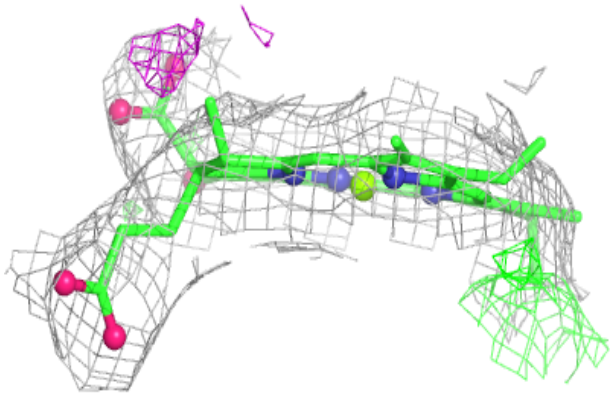




Electron density around CLA 8 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

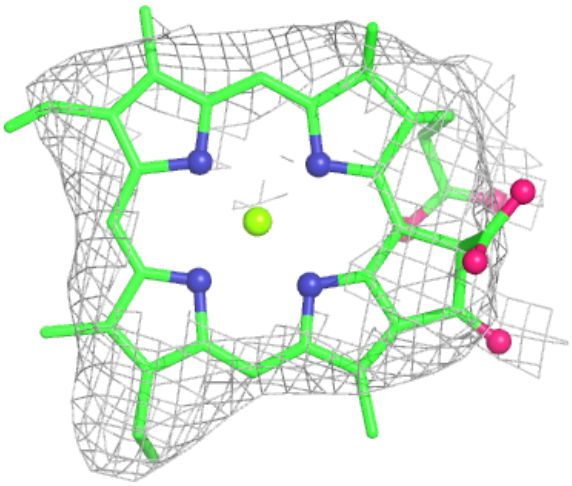


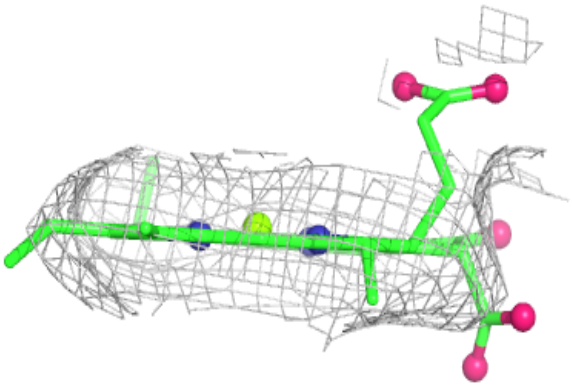


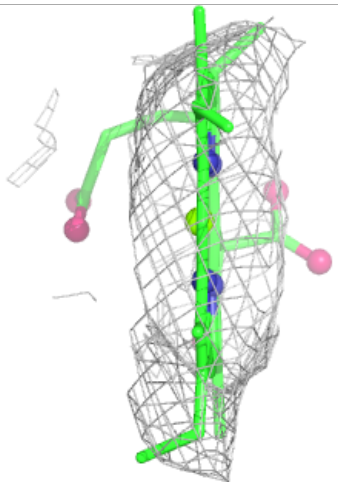


Electron density around CLA 3 1007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

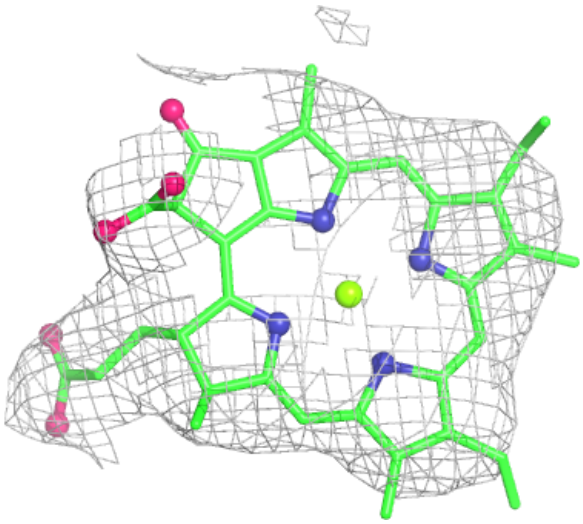


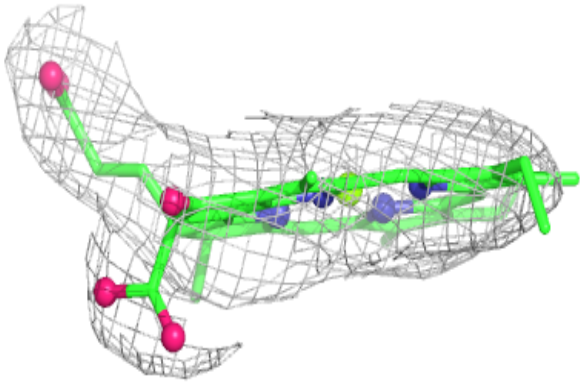


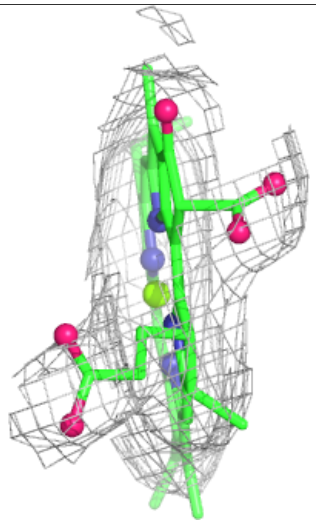


Electron density around CLA A 826:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

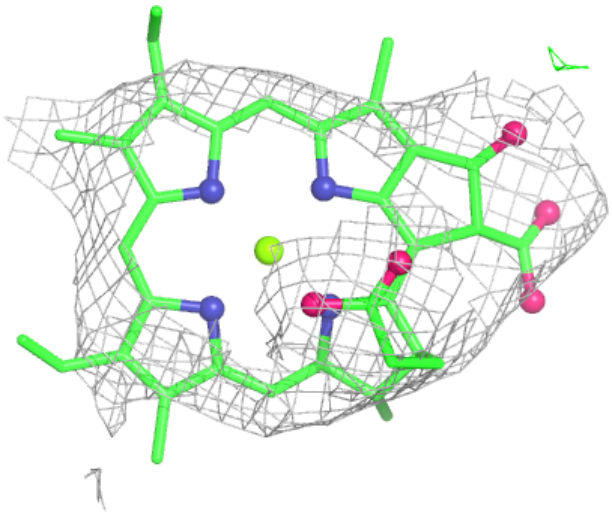


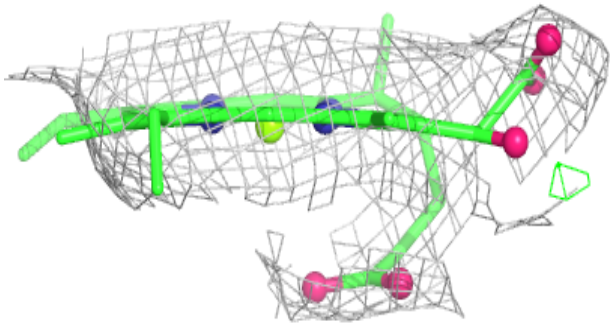


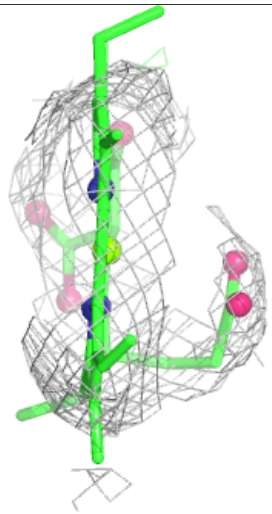


Electron density around CLA B 811:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

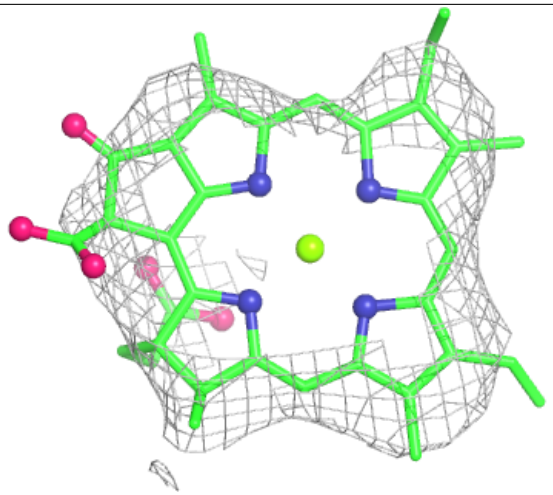


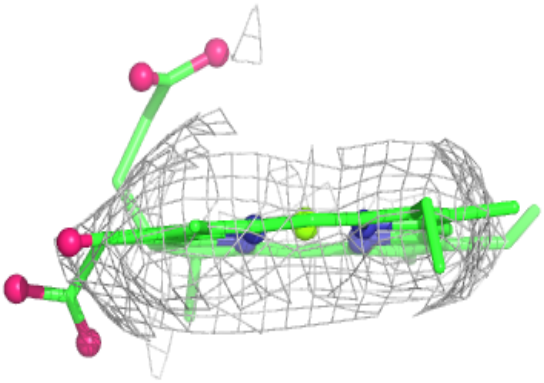


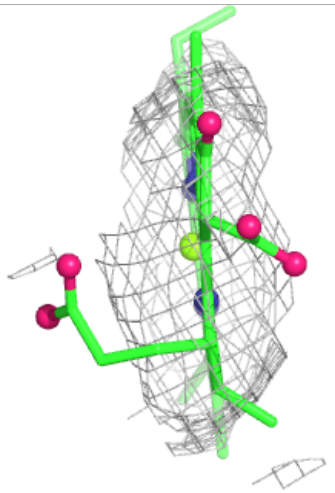


Electron density around CLA A 816:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

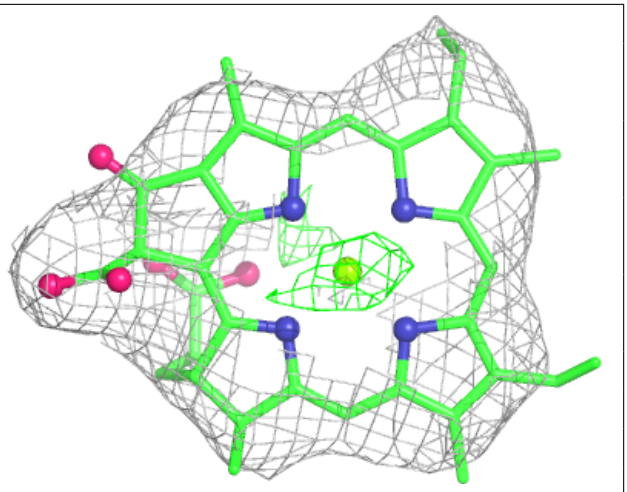


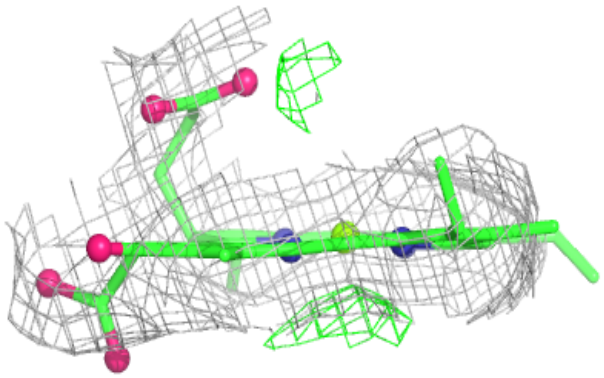


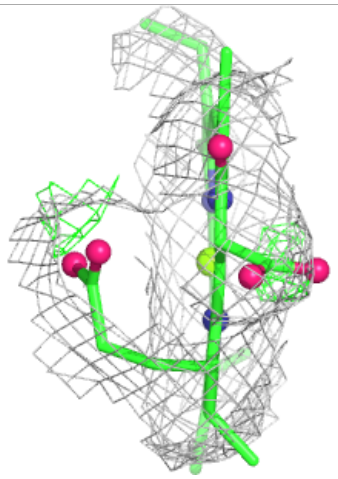


Electron density around CLA 1 1005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

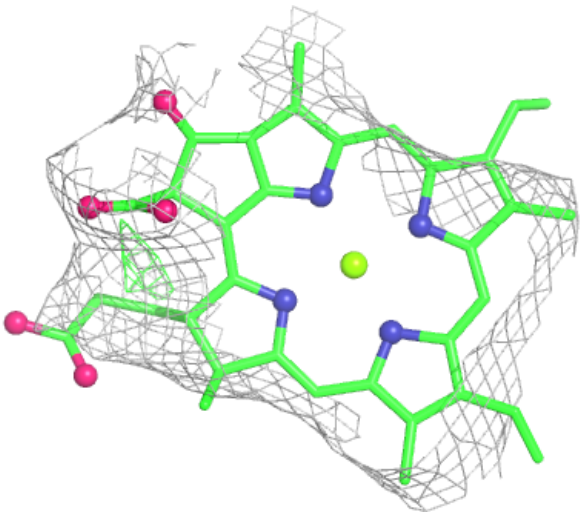


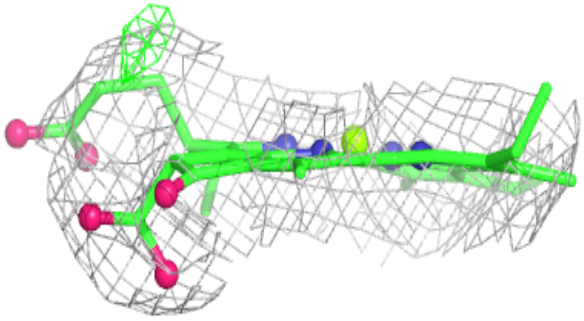


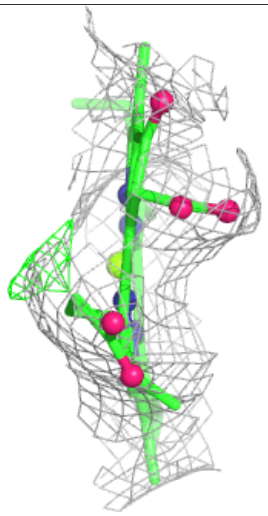


Electron density around CLA 0 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

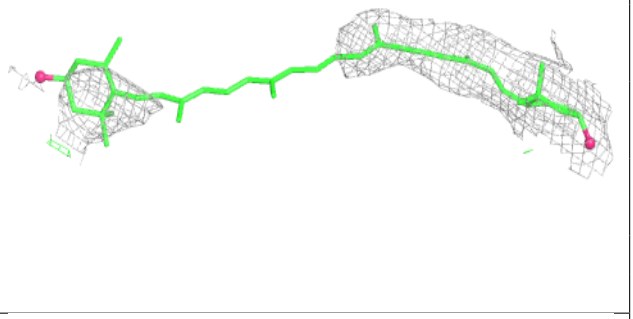


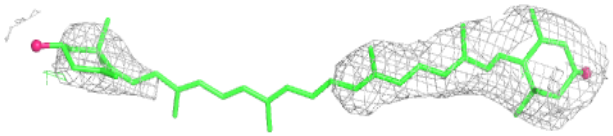


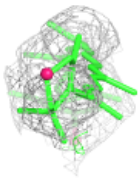


Electron density around LUT J 104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

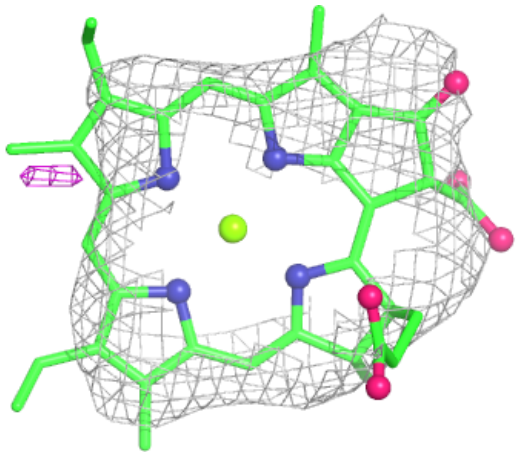


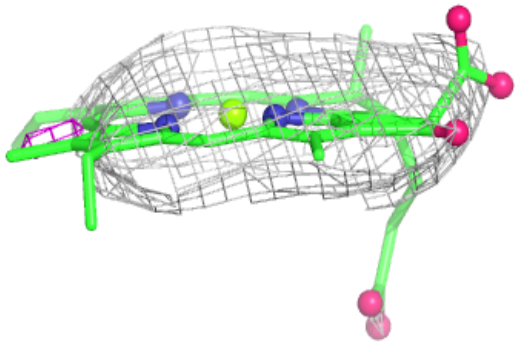


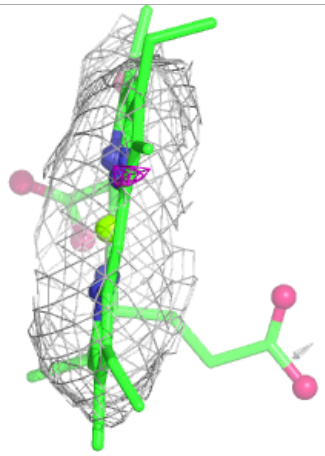


Electron density around CLA B 830:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

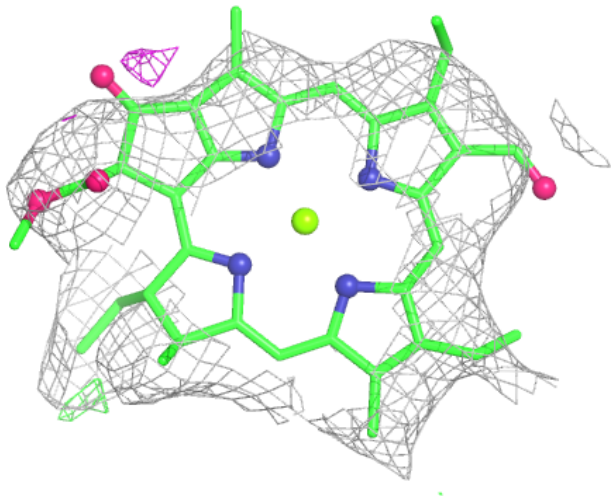


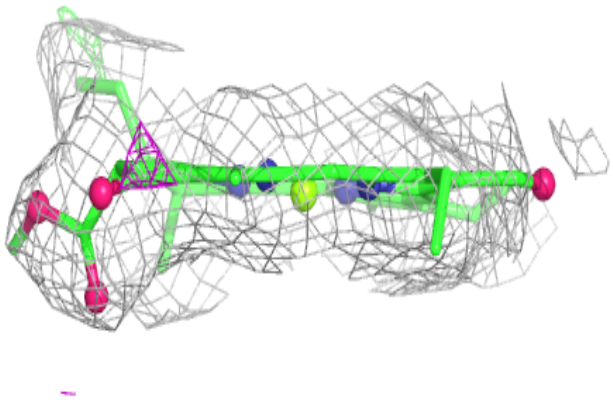


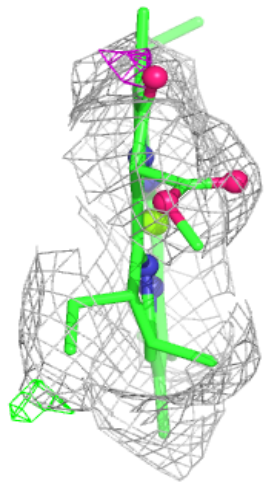


Electron density around CHL 5 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

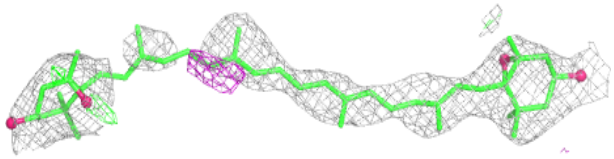


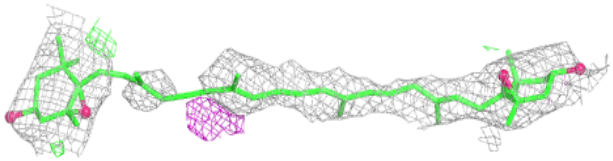


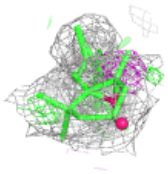


Electron density around XAT 8 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

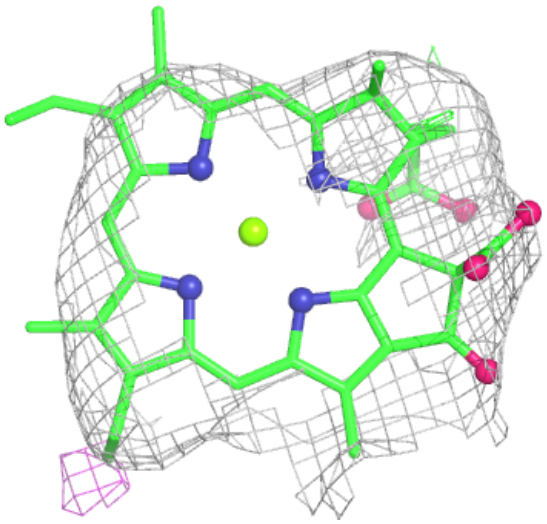


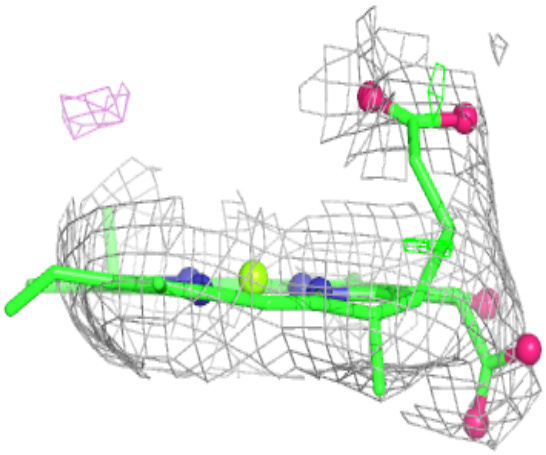


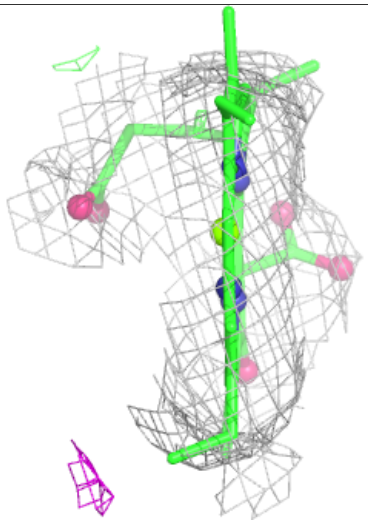


Electron density around CLA 1 1010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

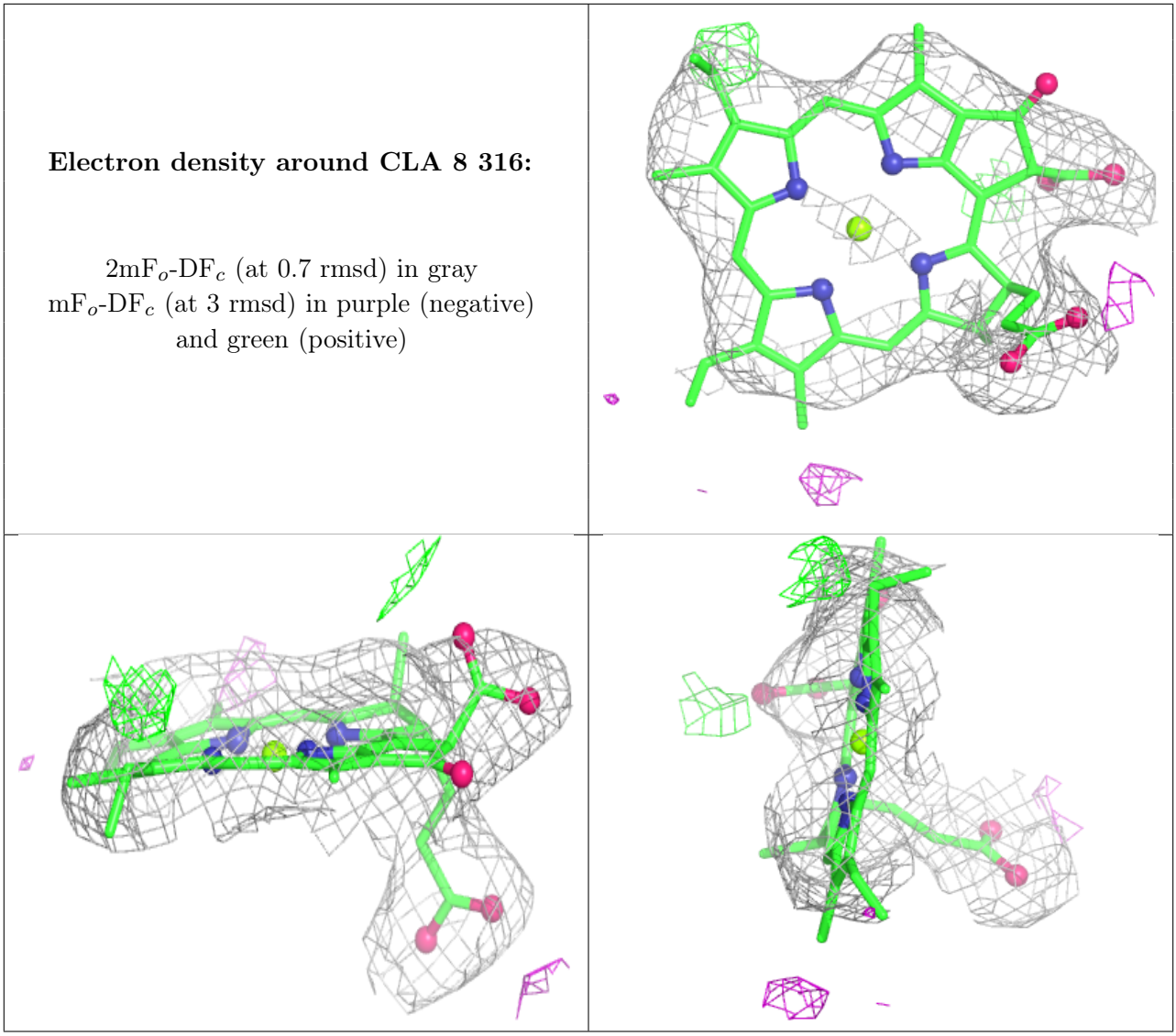






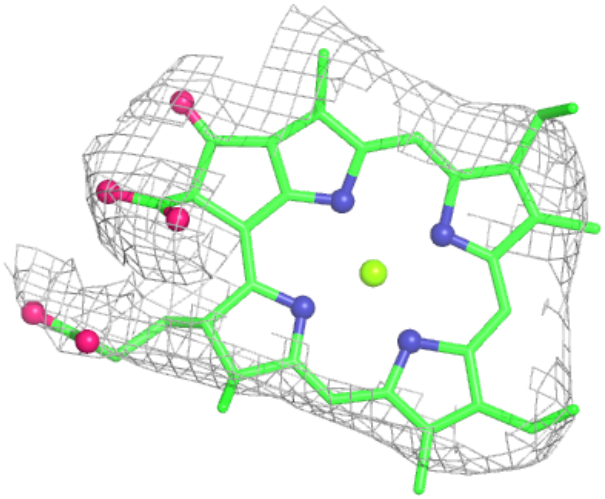
Electron density around CLA 8 316:

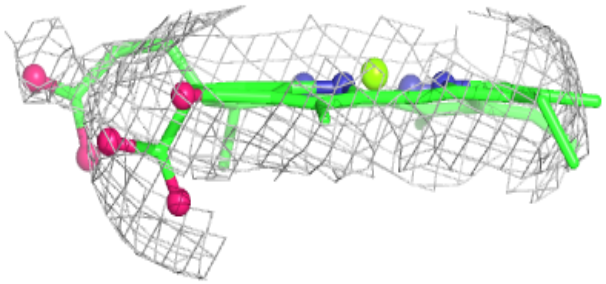
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

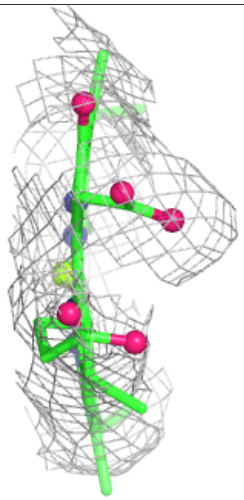


Electron density around CLA 3 1006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

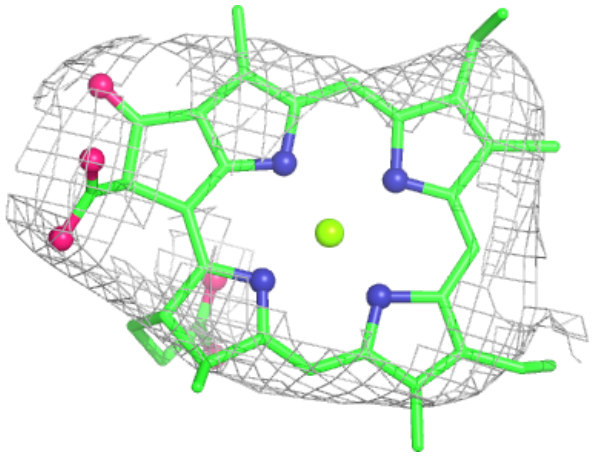


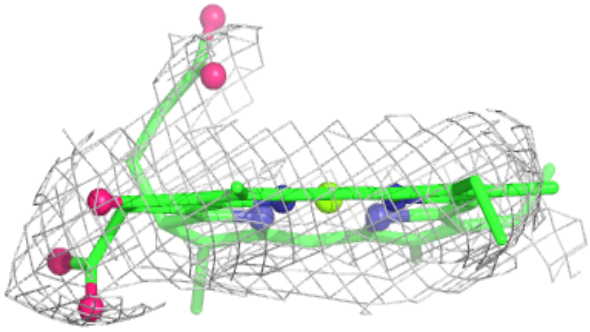


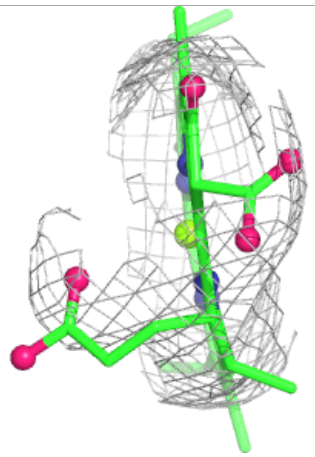


Electron density around CLA B 807:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

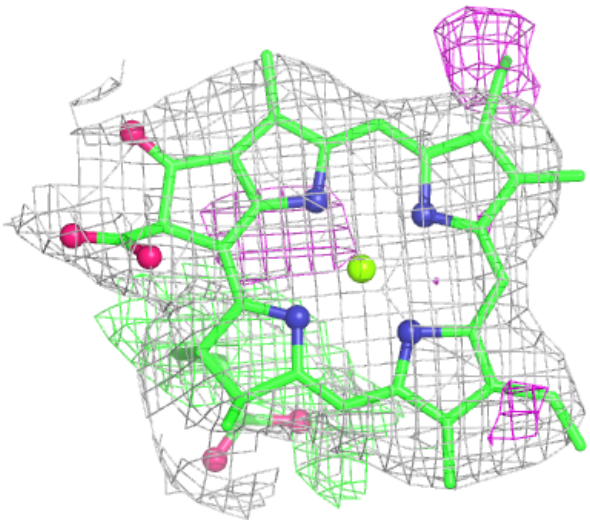


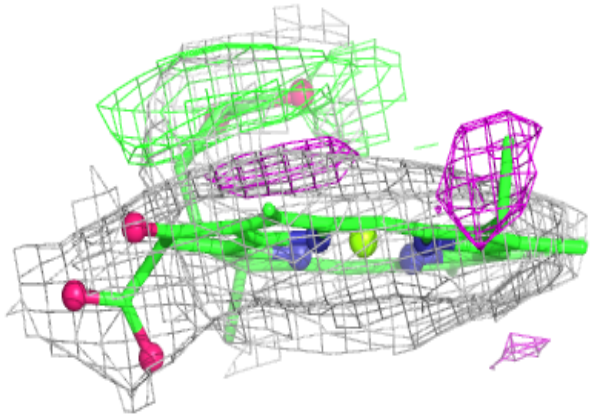


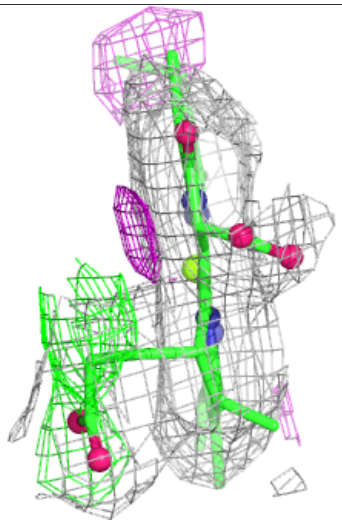


Electron density around CLA 6 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

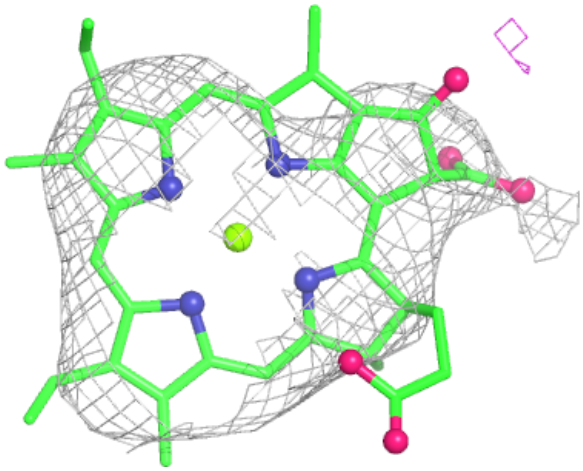


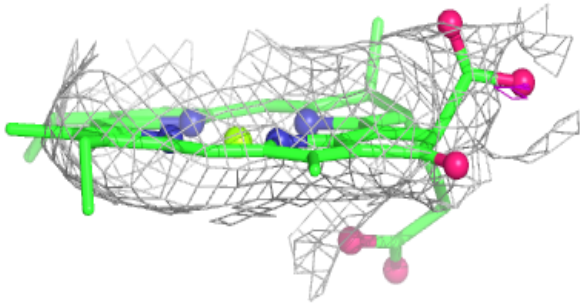


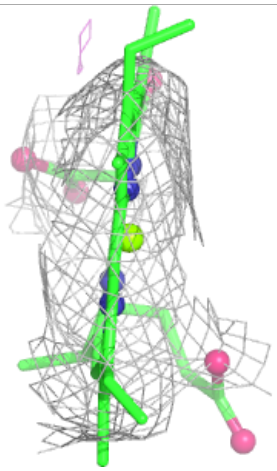


Electron density around CLA B 829:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

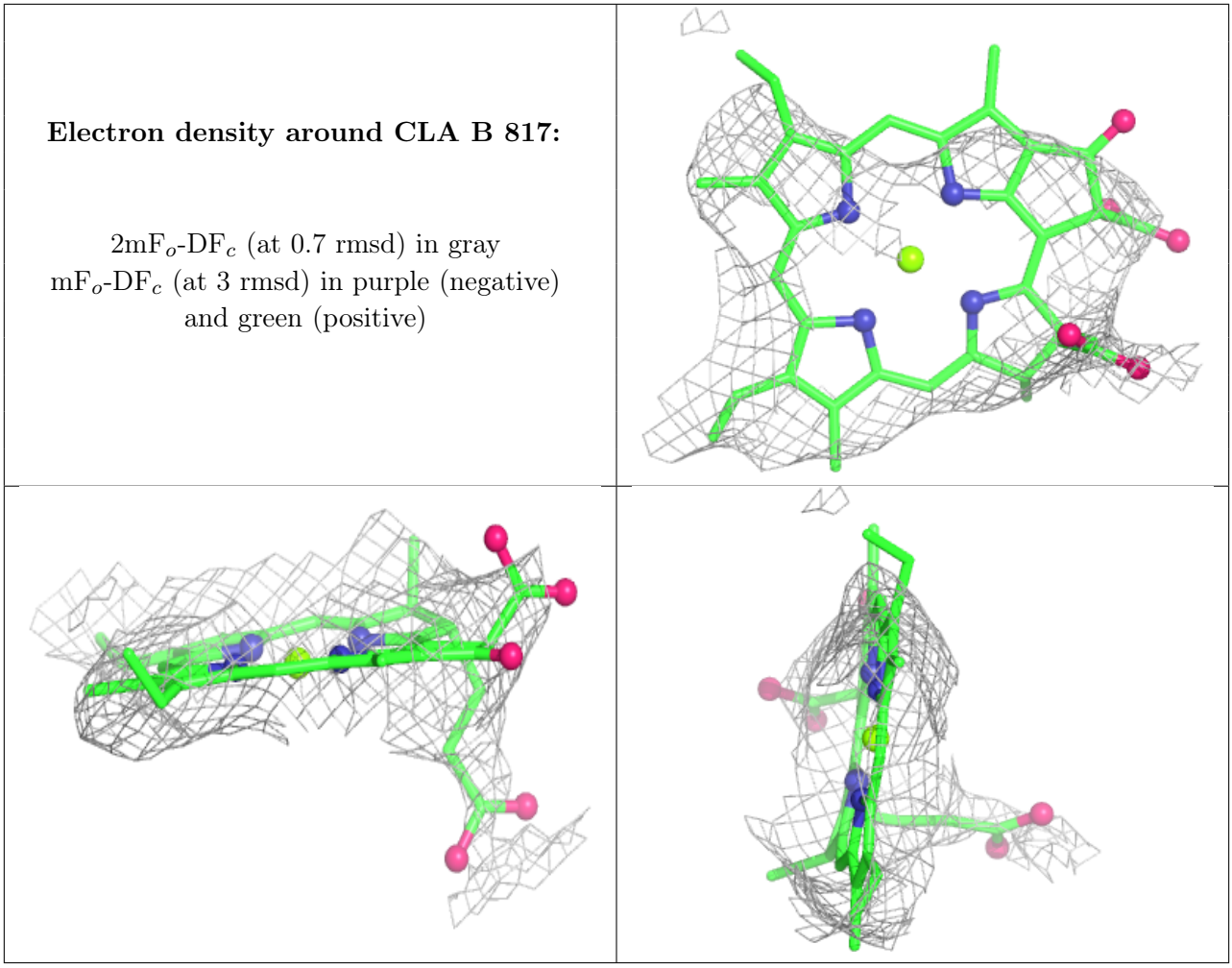






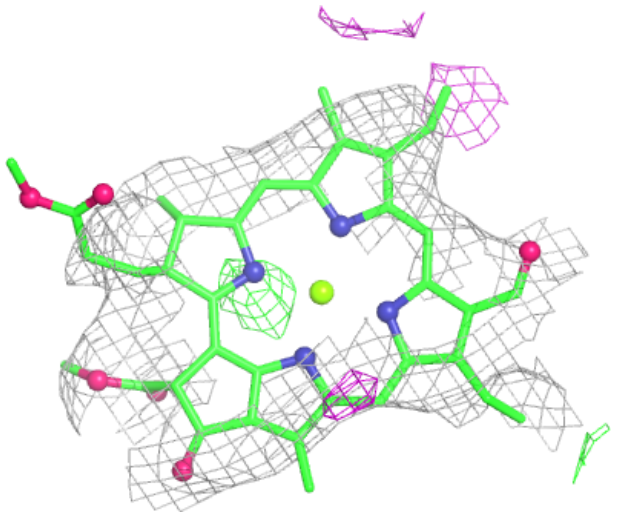
Electron density around CLA B 817:

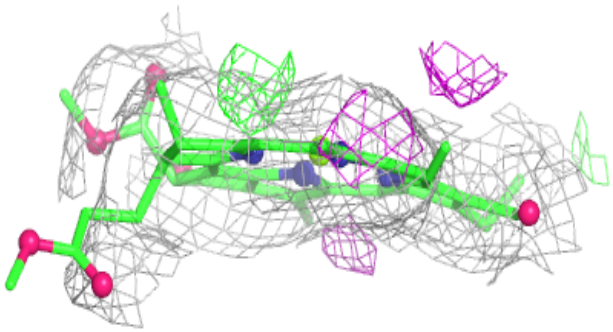
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

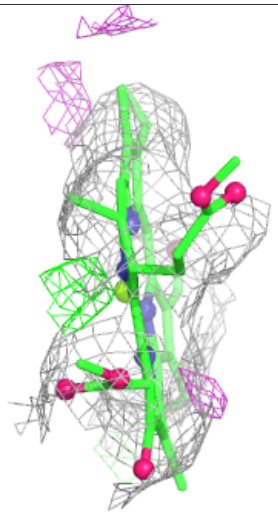


Electron density around CHL 7 1012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

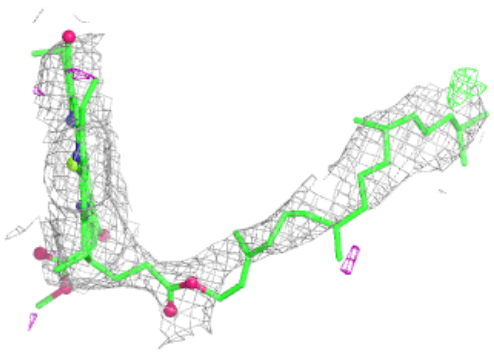


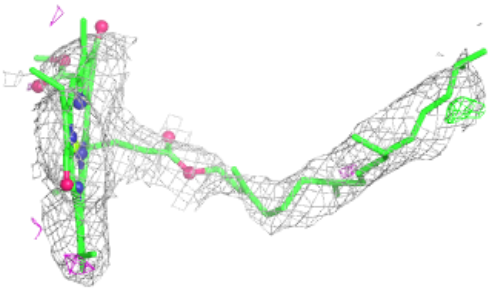


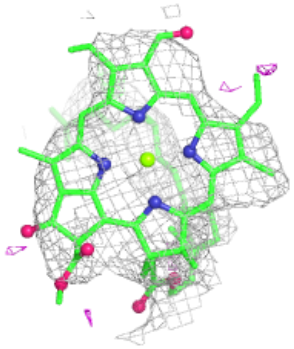


Electron density around CHL 7 1017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

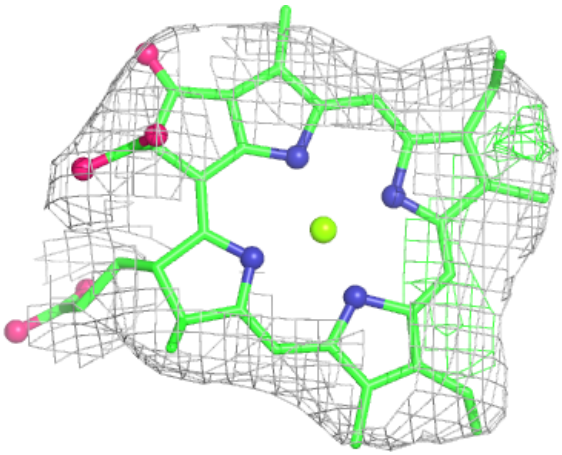


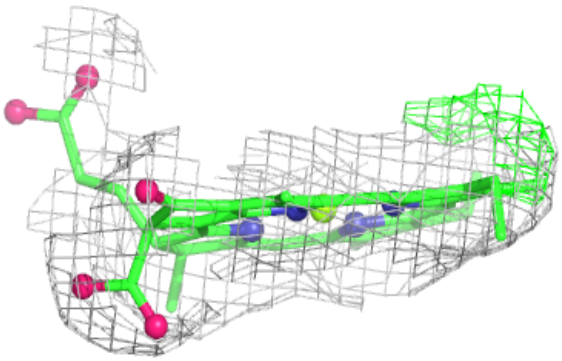




Electron density around CLA 6 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

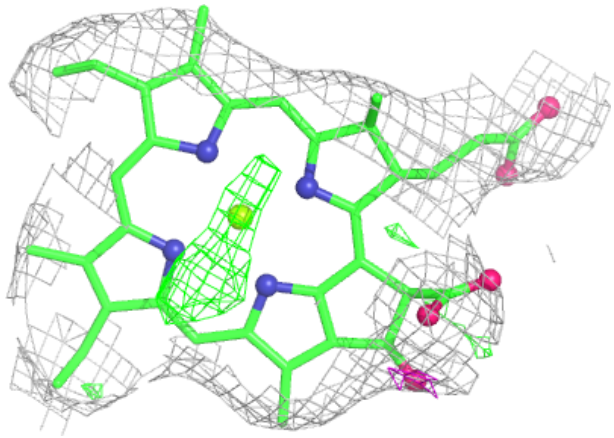


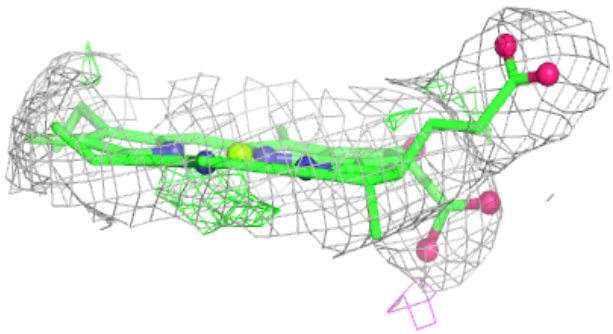




Electron density around CLA 6 320:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

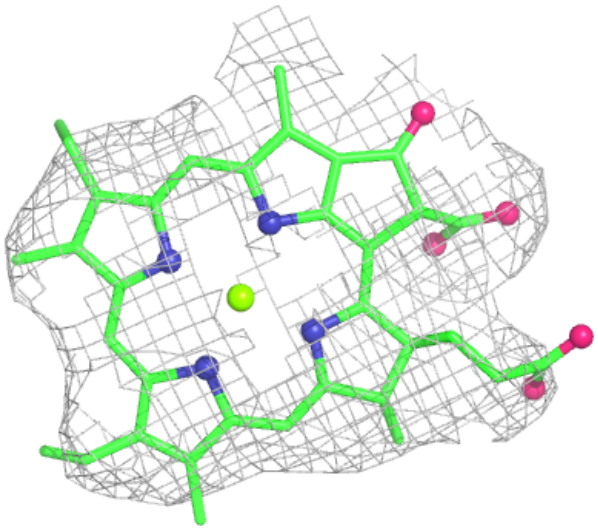


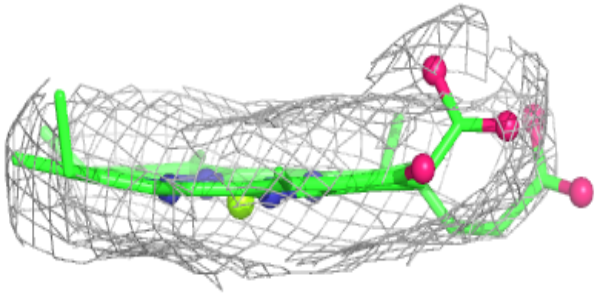


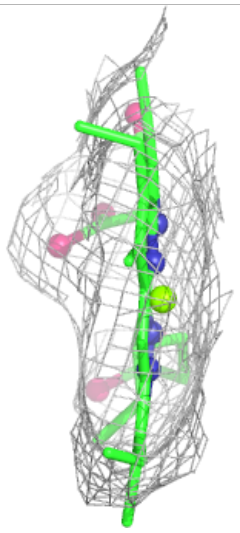


Electron density around CLA 5 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

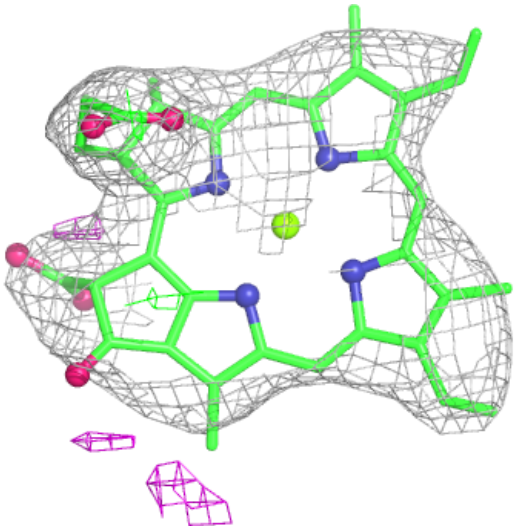


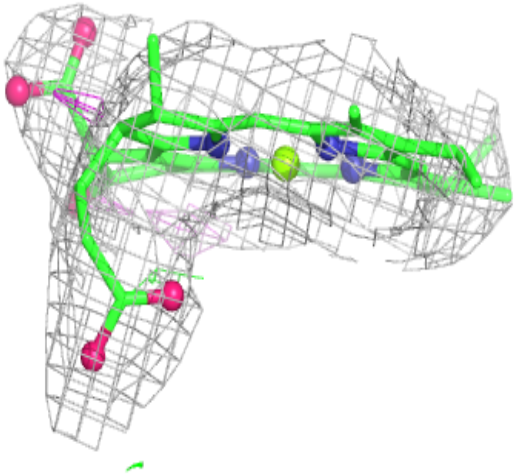


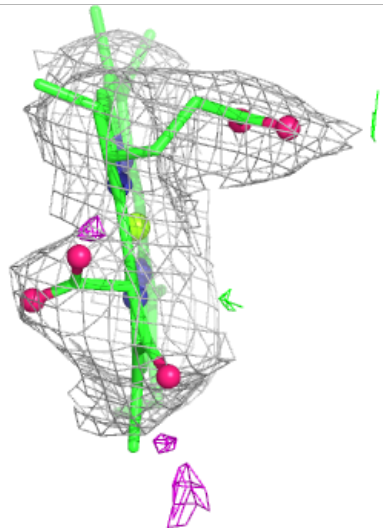


Electron density around CLA 5 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

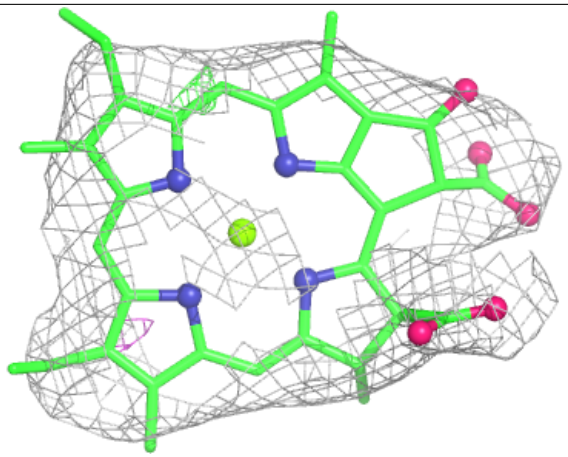


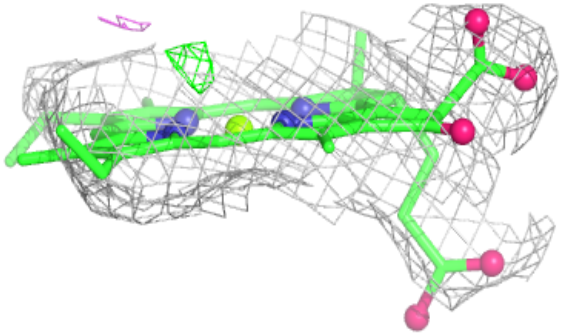


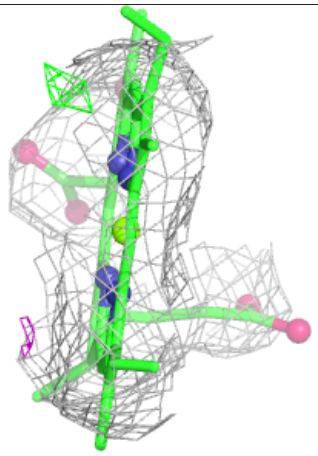


Electron density around CLA 5 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

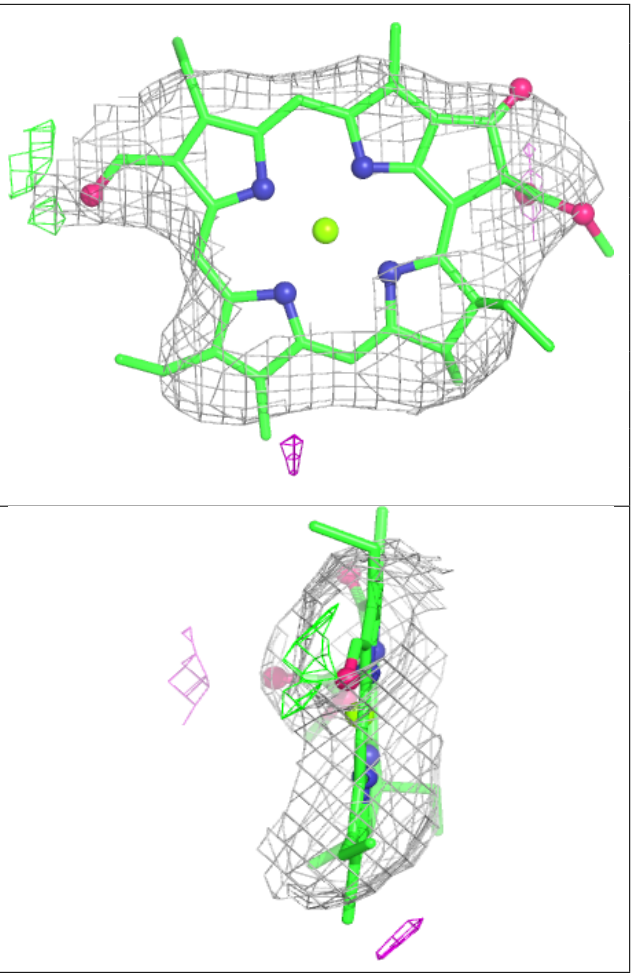






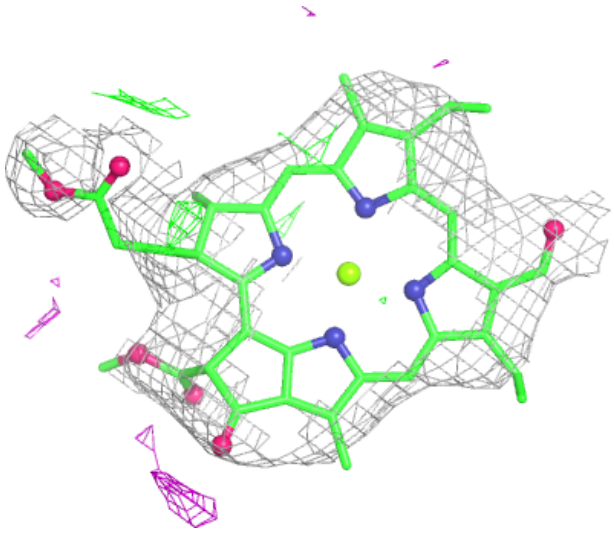
Electron density around CHL 4 316:

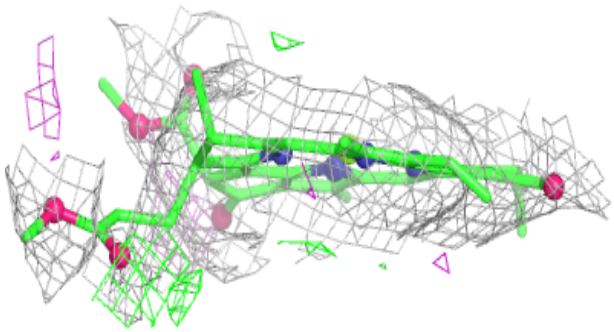
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CHL 6 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

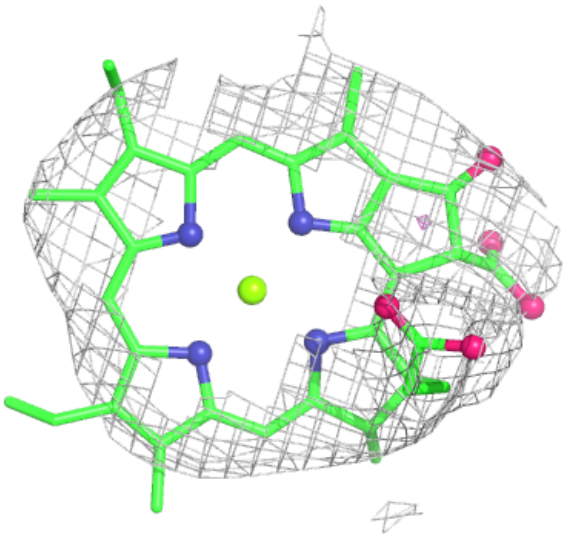


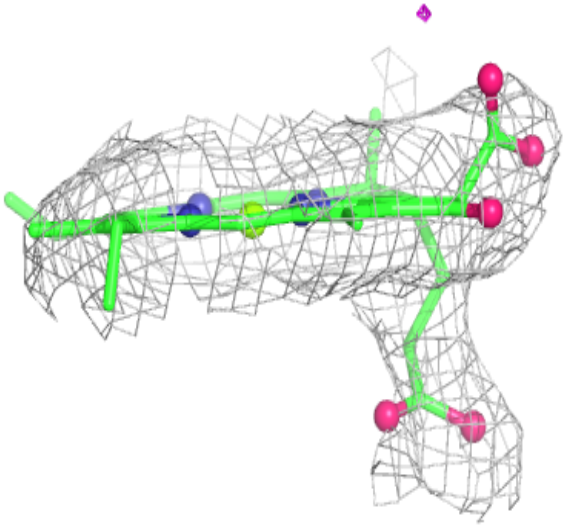


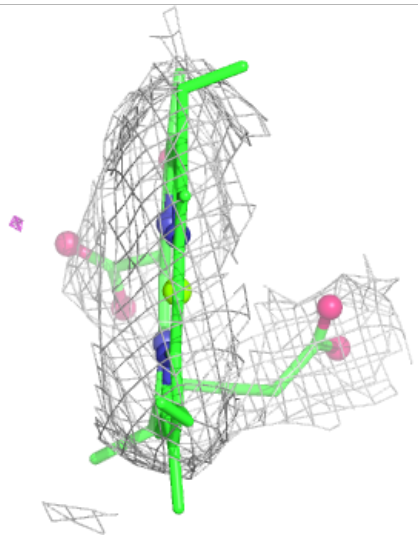


Electron density around CLA 0 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

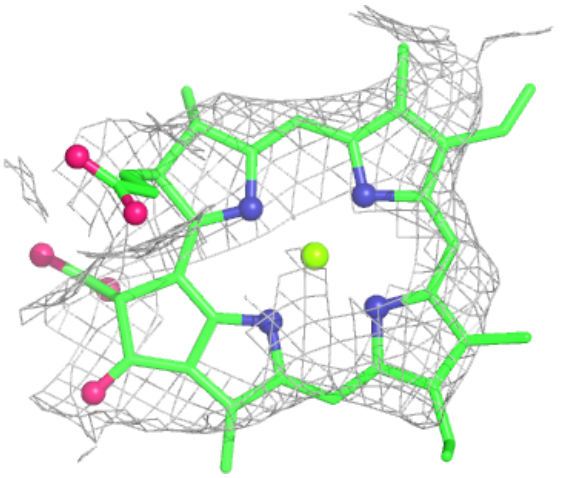


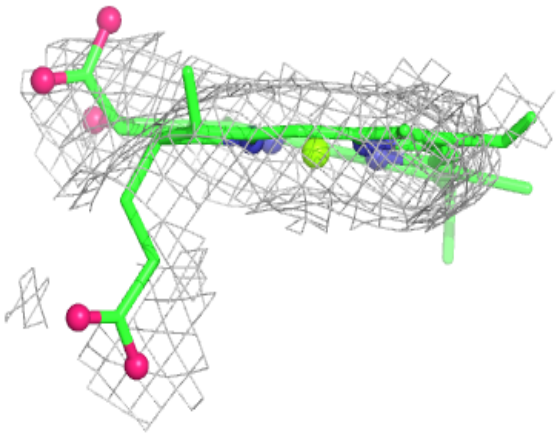


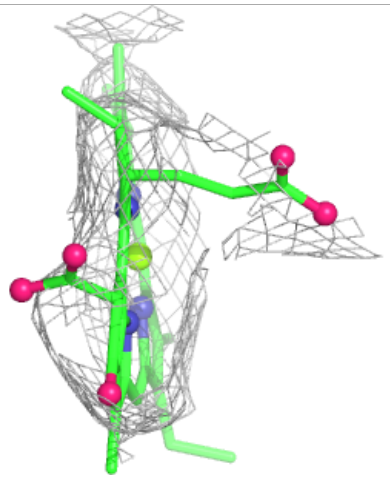


Electron density around CLA B 831:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

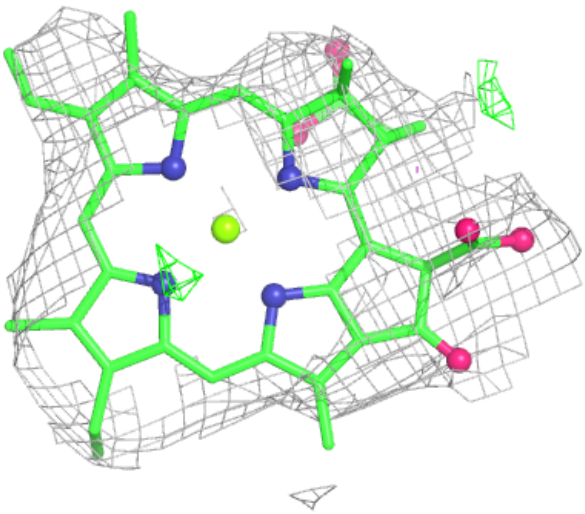


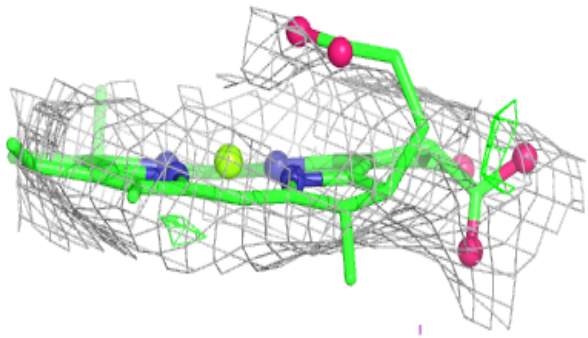


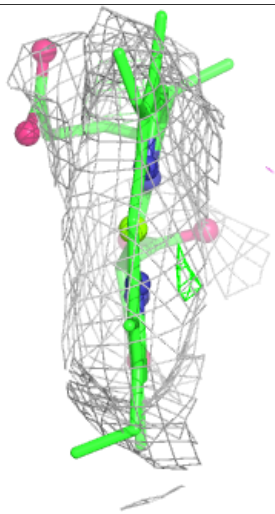


Electron density around CLA 0 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

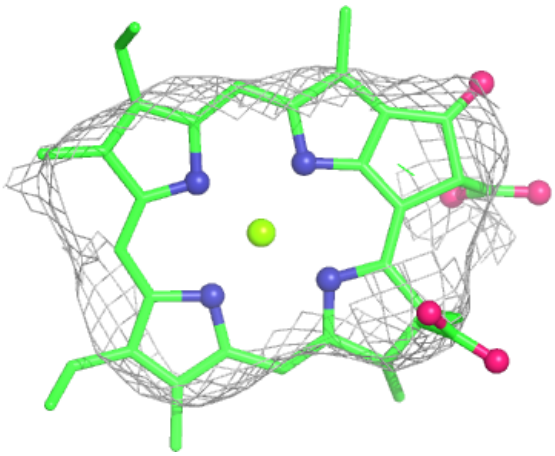


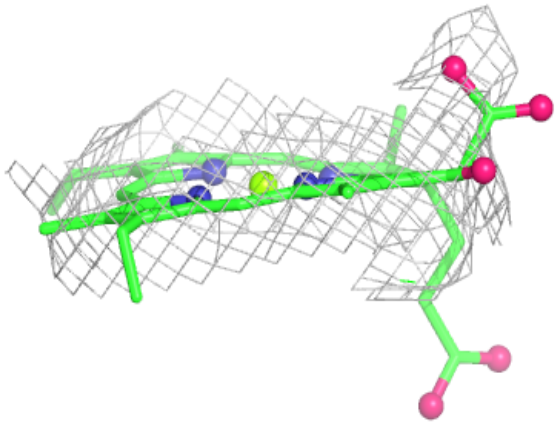


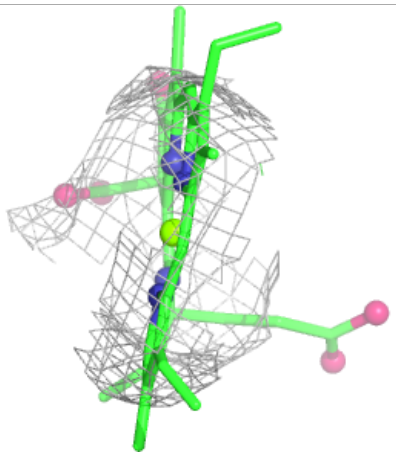


Electron density around CLA B 818:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

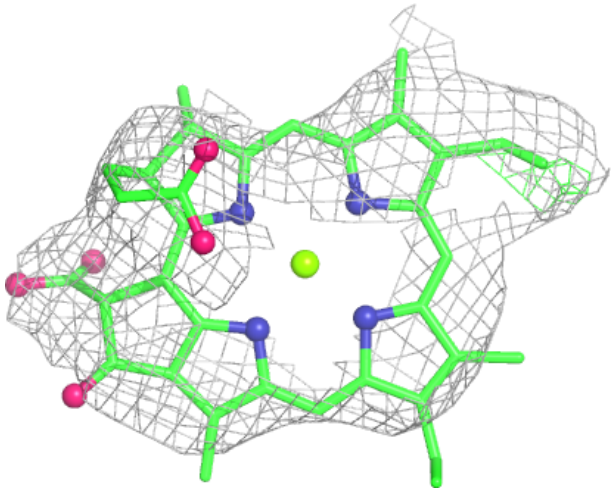


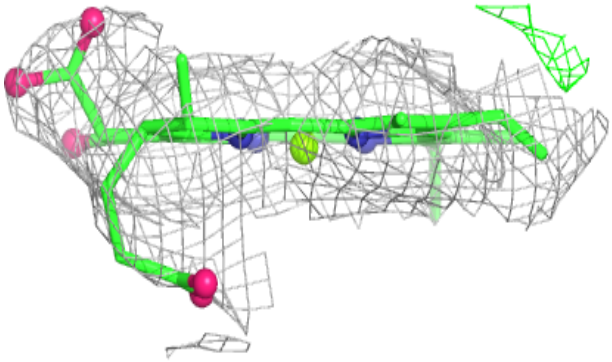


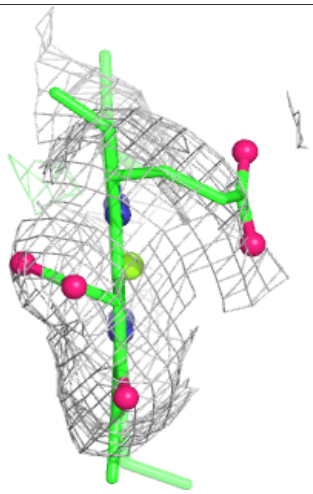


Electron density around CLA A 811:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

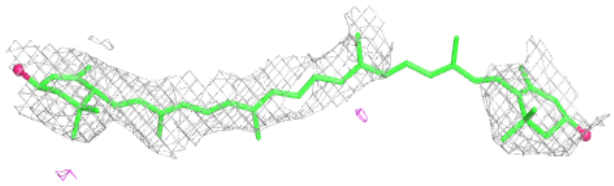


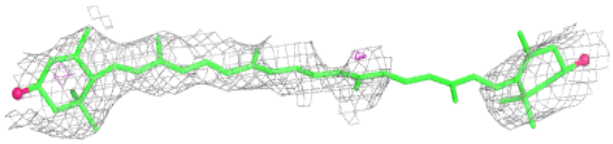


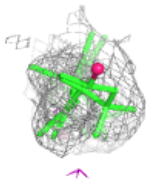


Electron density around LUT 3 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

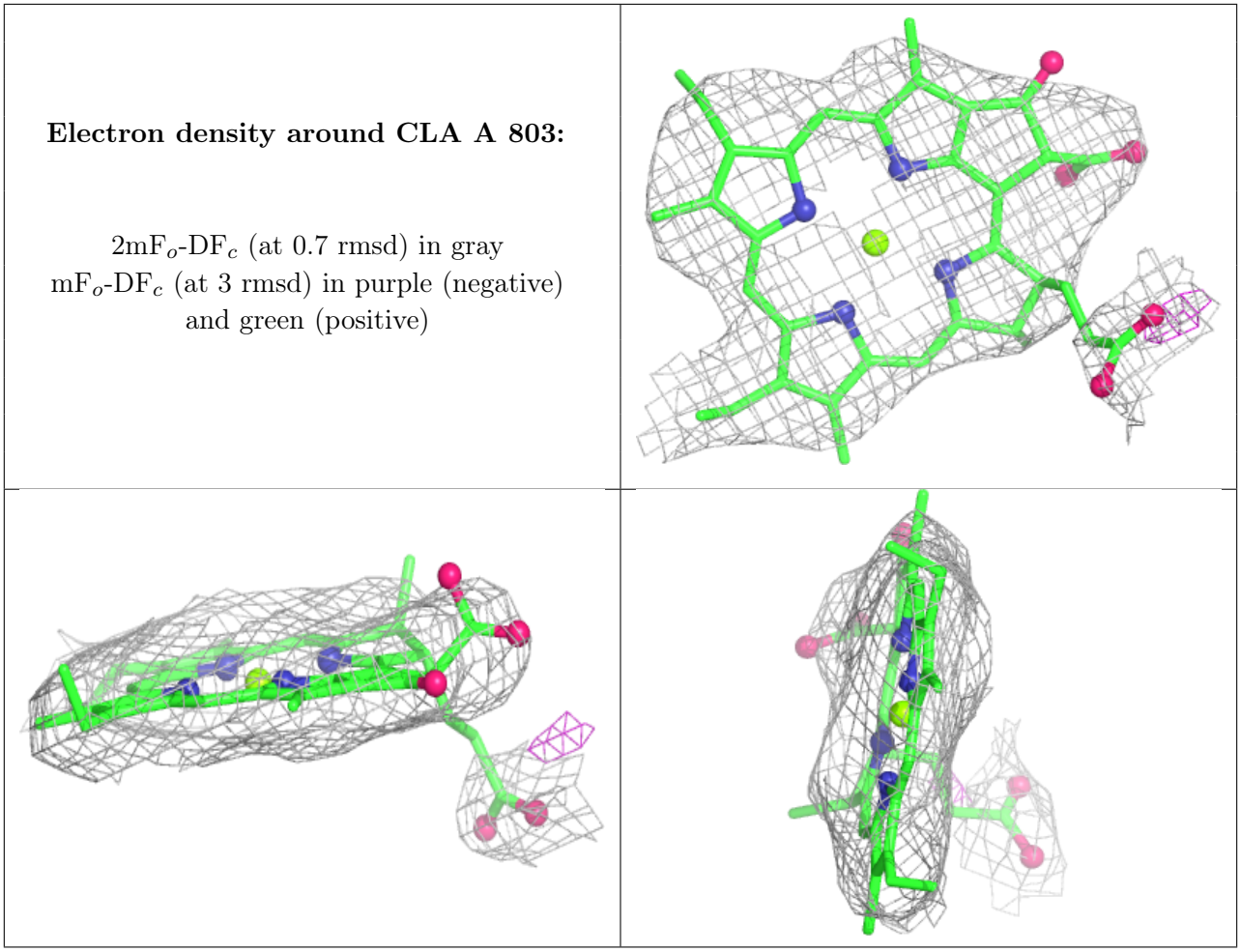






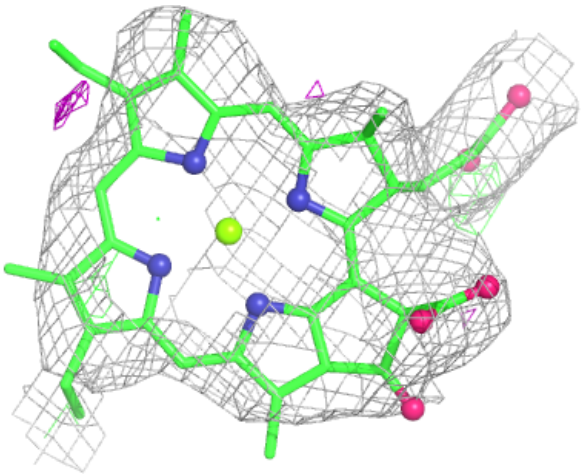
Electron density around CLA A 803:

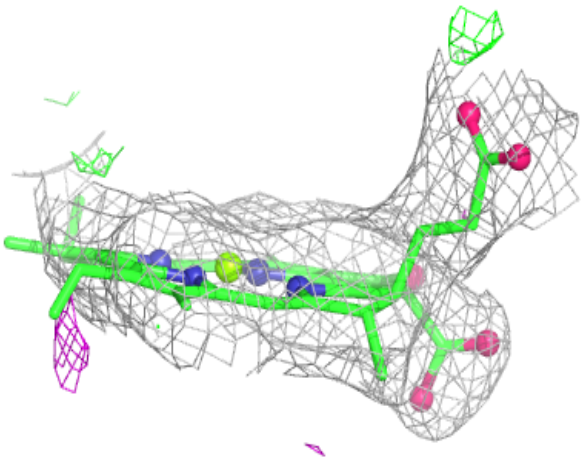
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

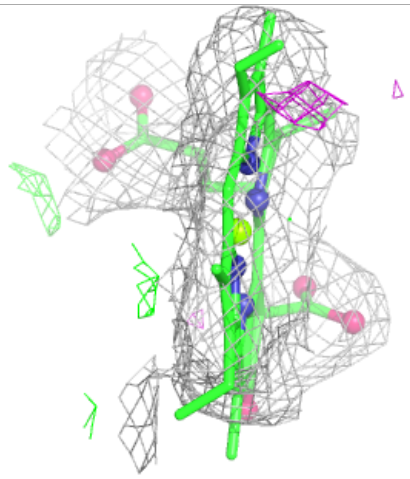


Electron density around CLA 6 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

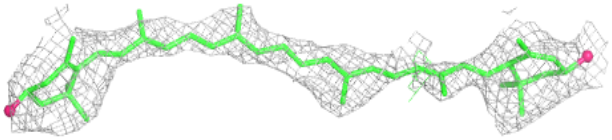


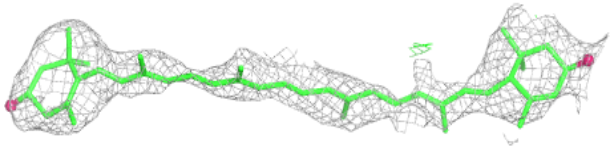


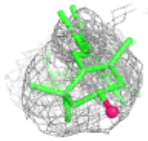


Electron density around LUT 4 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

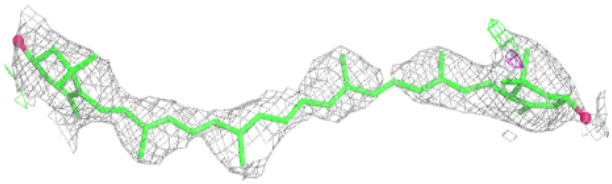


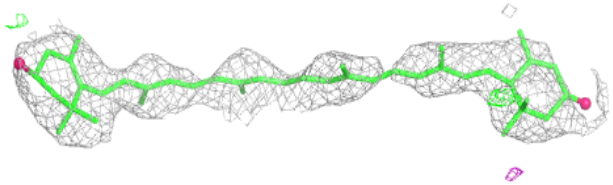


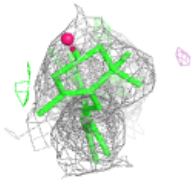


Electron density around LUT 6 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

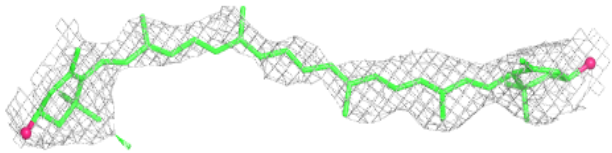


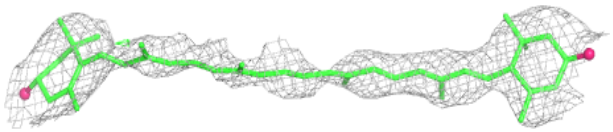


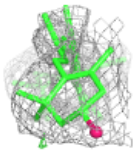


Electron density around LUT 5 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

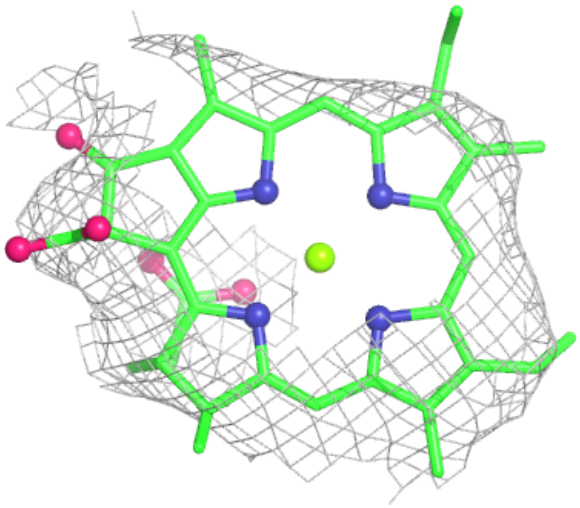


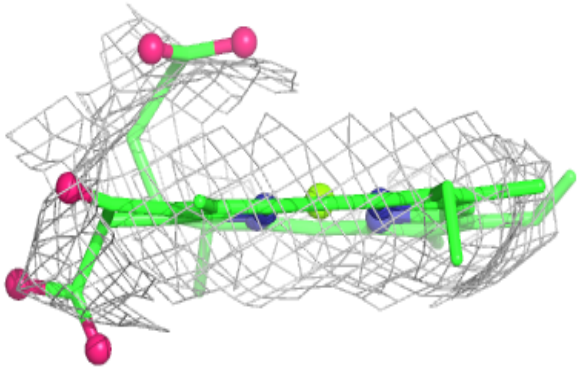


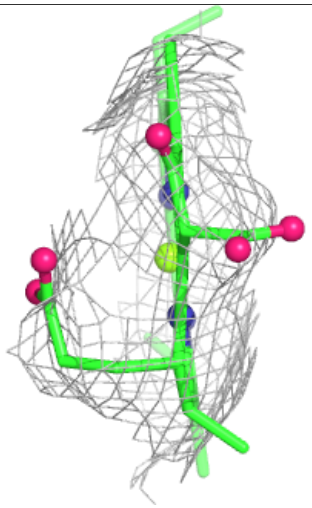


Electron density around CLA A 835:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

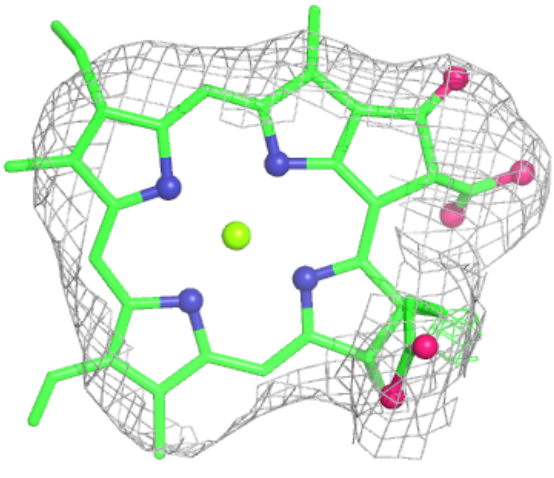


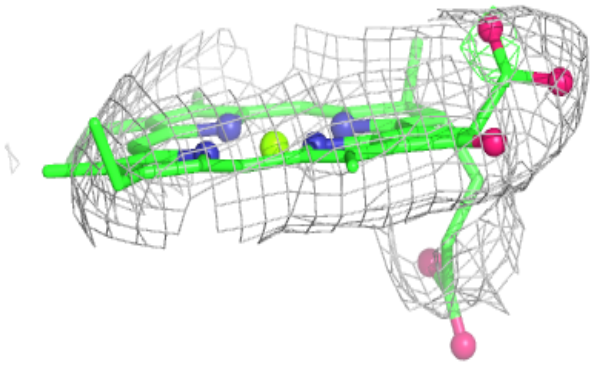




Electron density around CLA 3 1013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

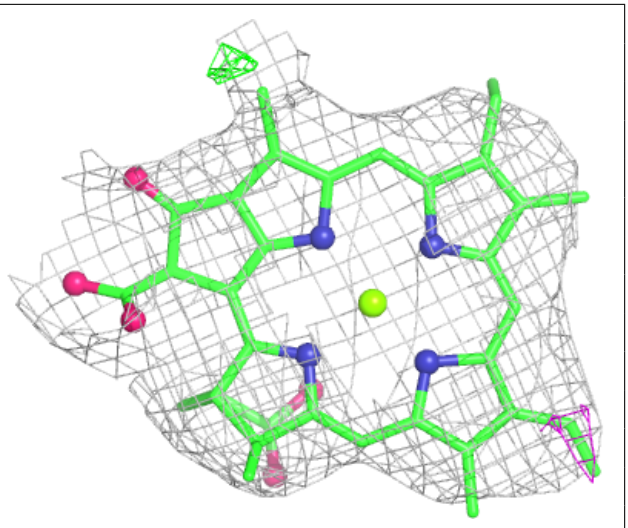


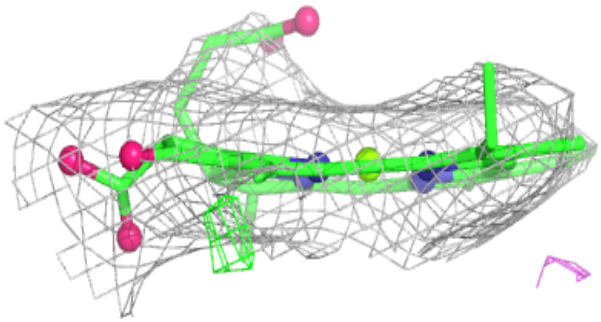


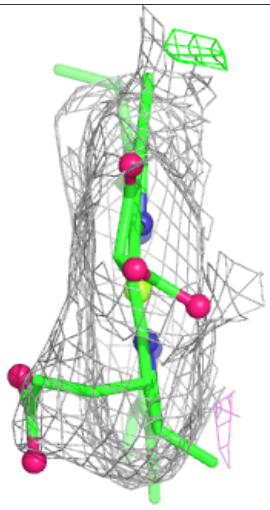


Electron density around CLA 1 1003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

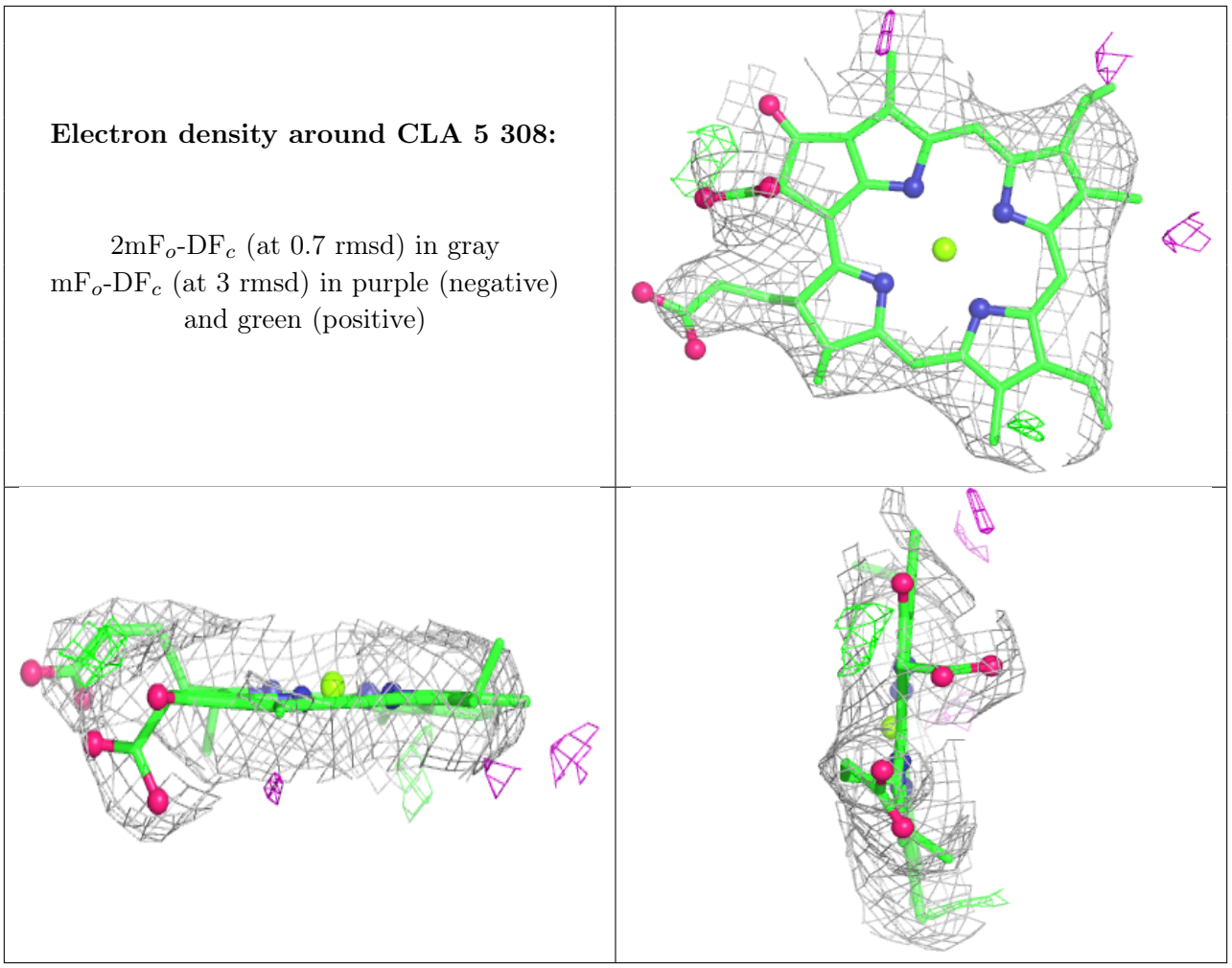






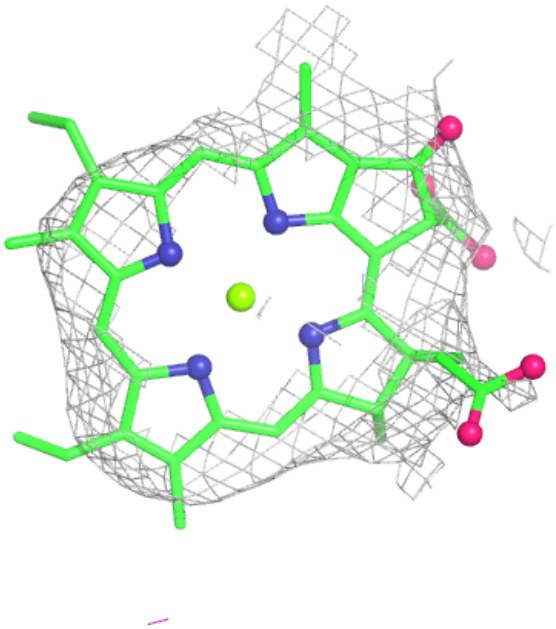
Electron density around CLA 5 308:

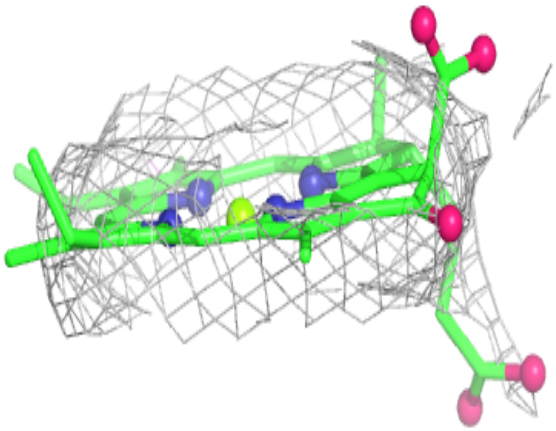
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

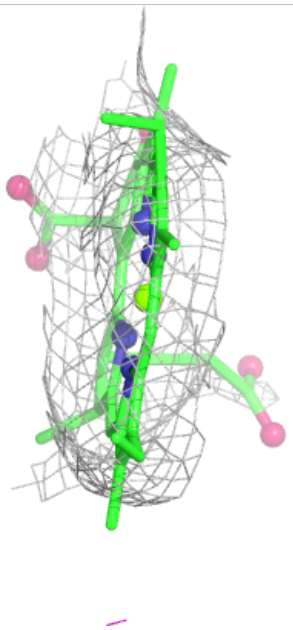


Electron density around CLA A 836:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

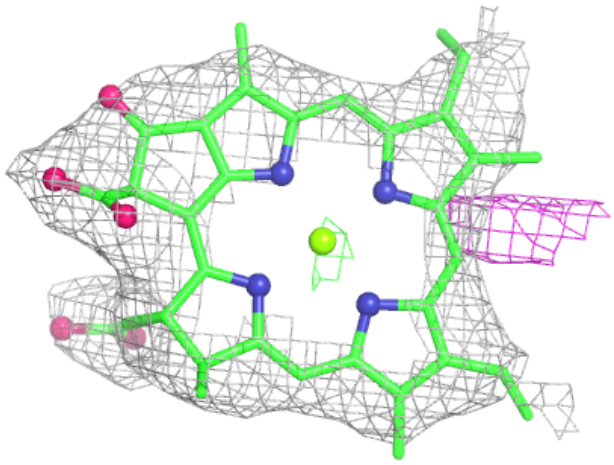


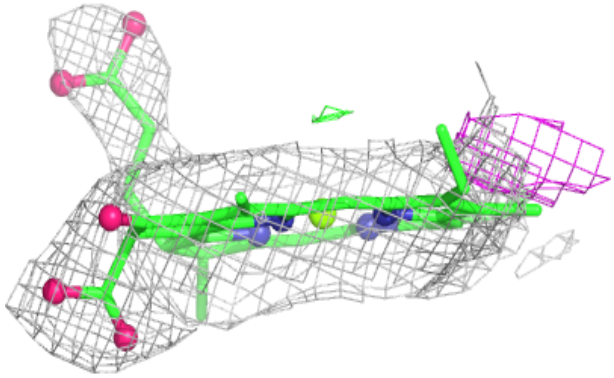




Electron density around CLA F 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

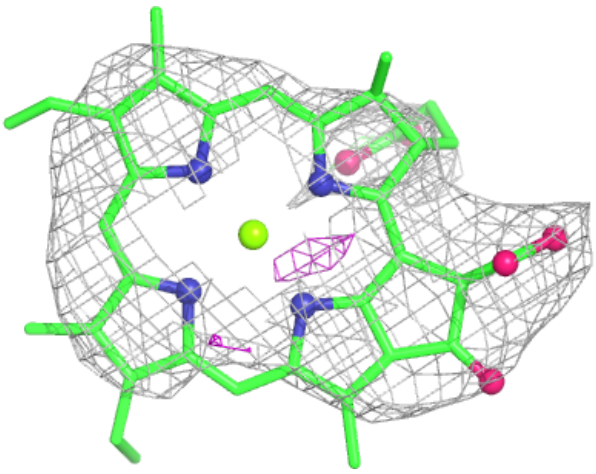


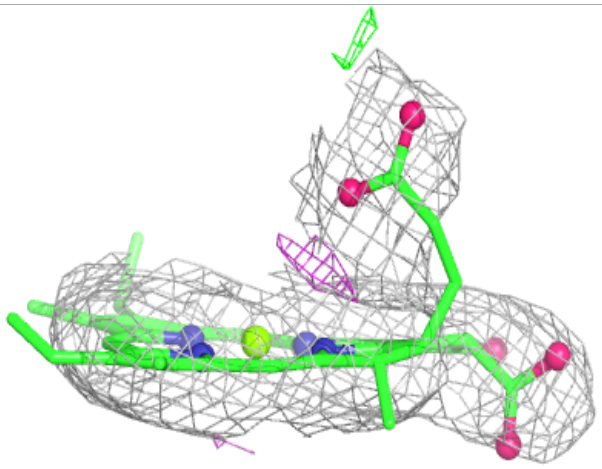


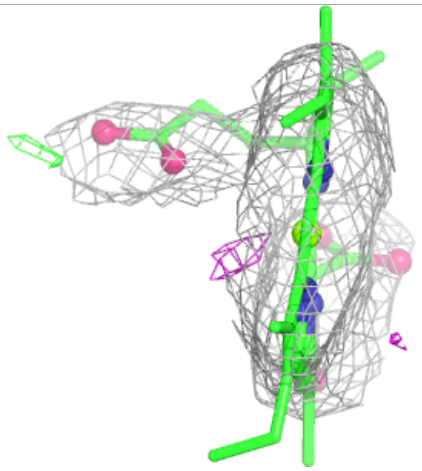


Electron density around CLA A 810:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

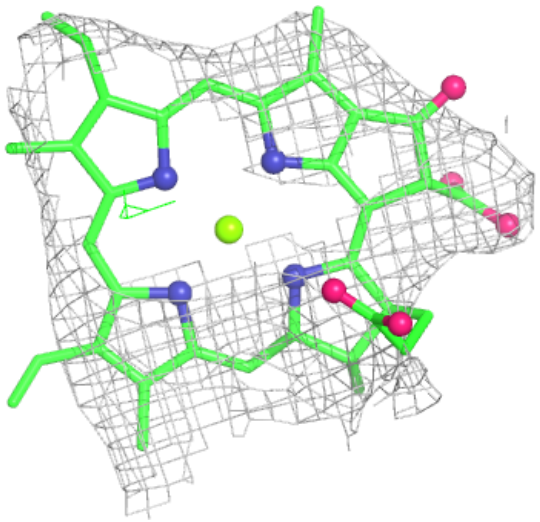


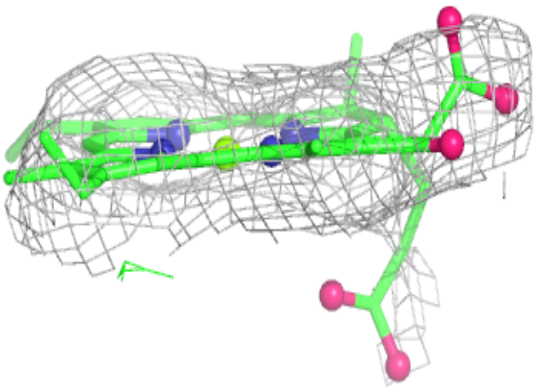


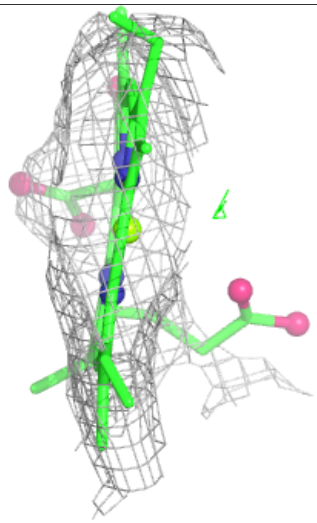


Electron density around CLA 1 1008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

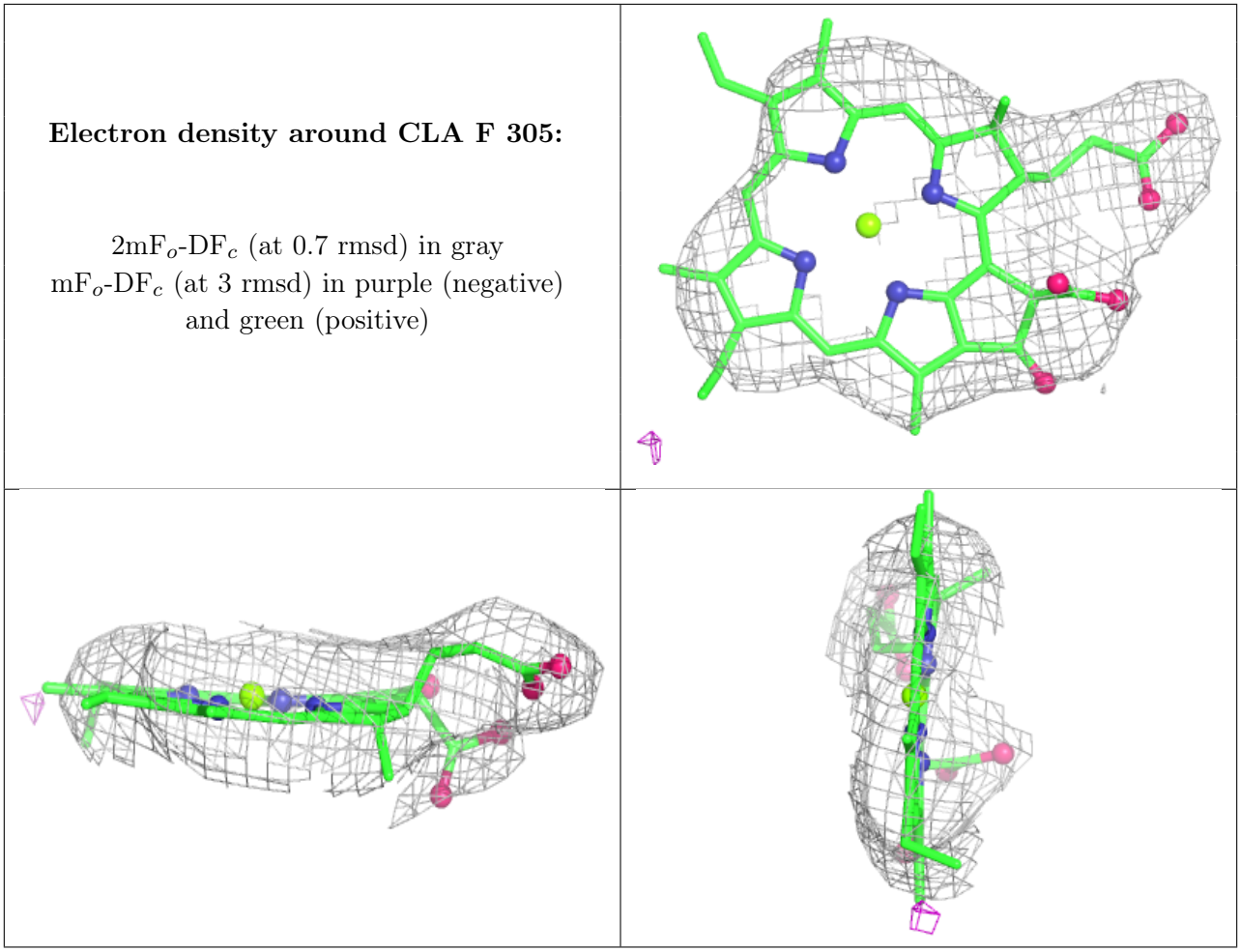






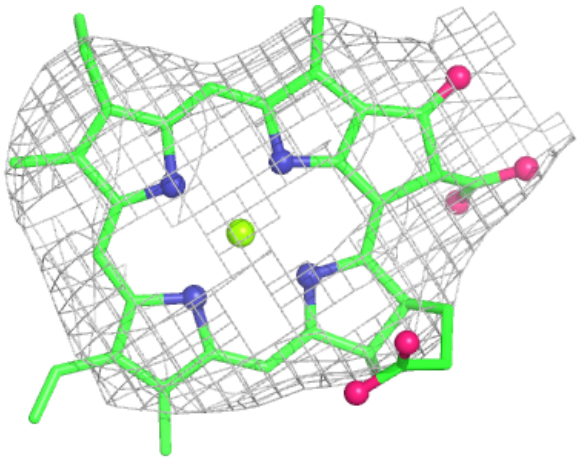
Electron density around CLA F 305:

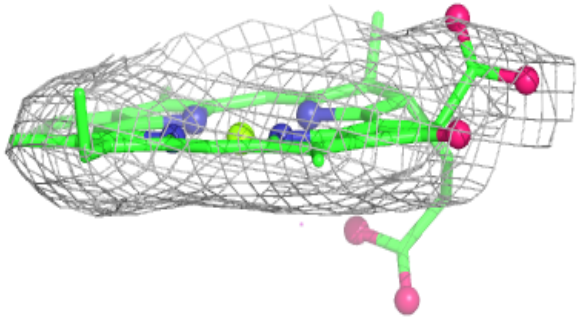
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

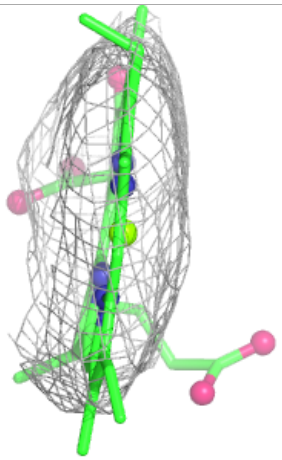


Electron density around CLA A 817:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

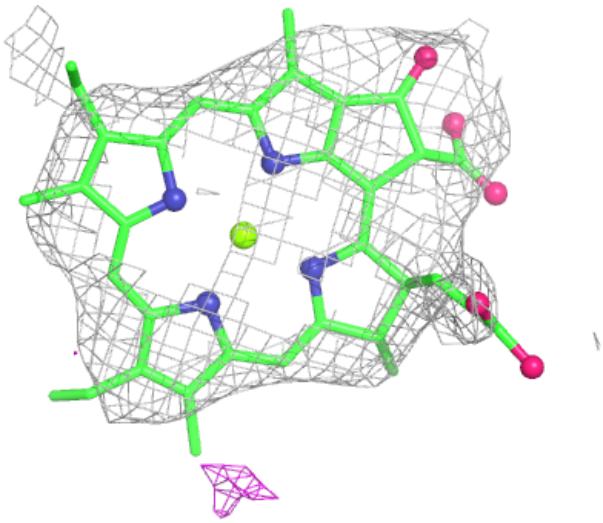


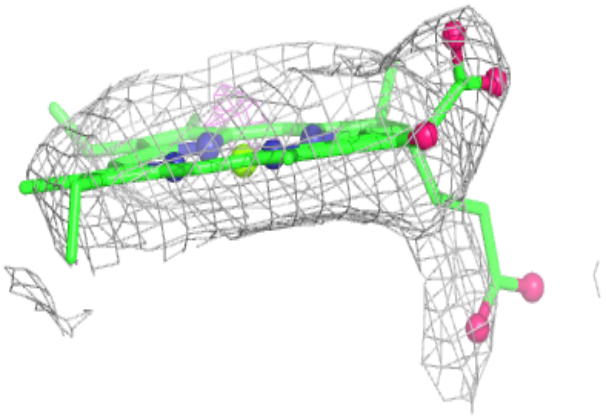


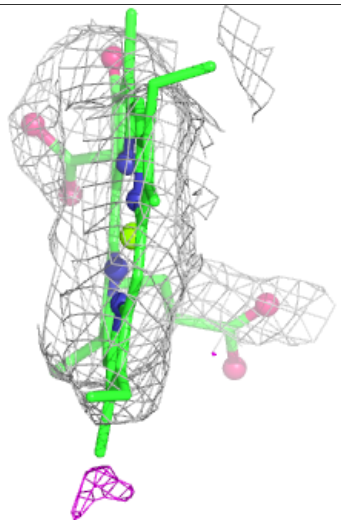


Electron density around CLA 1 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

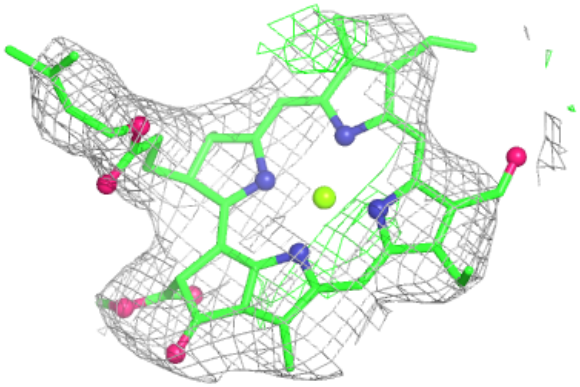


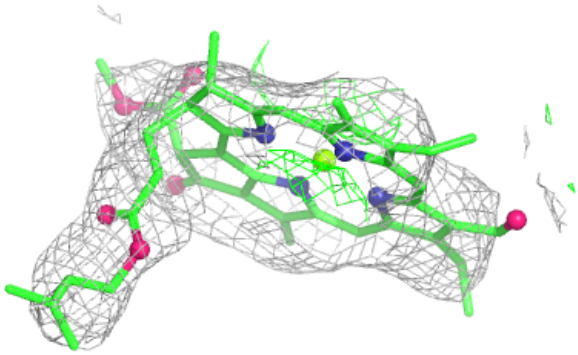


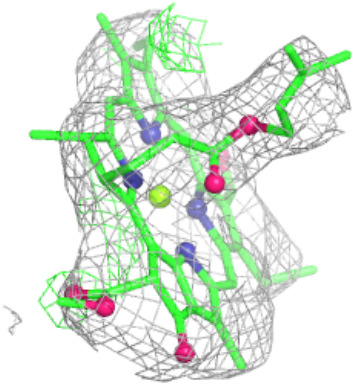


Electron density around CHL 4 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

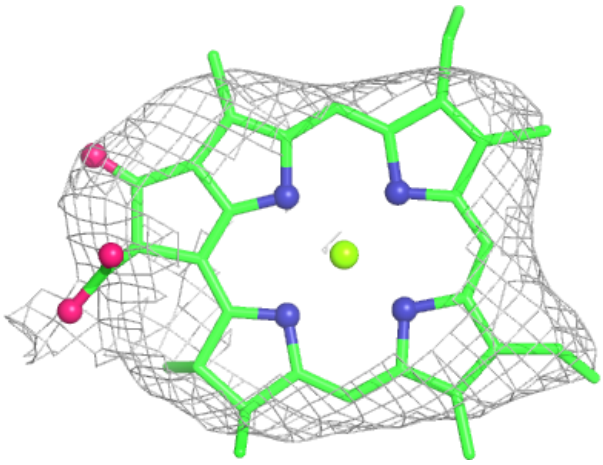


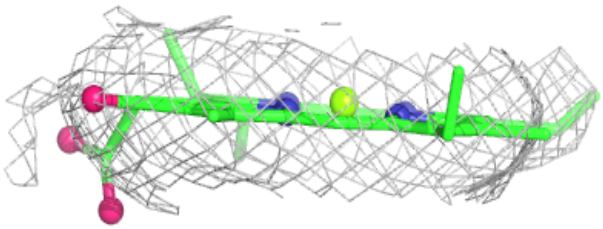


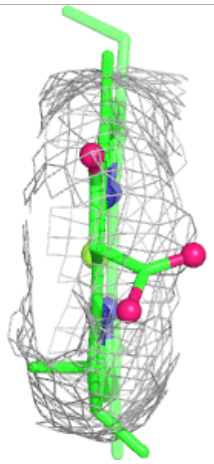


Electron density around CLA A 814:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

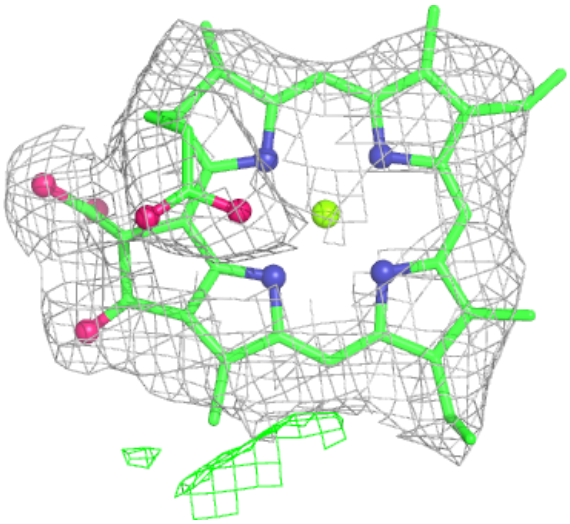


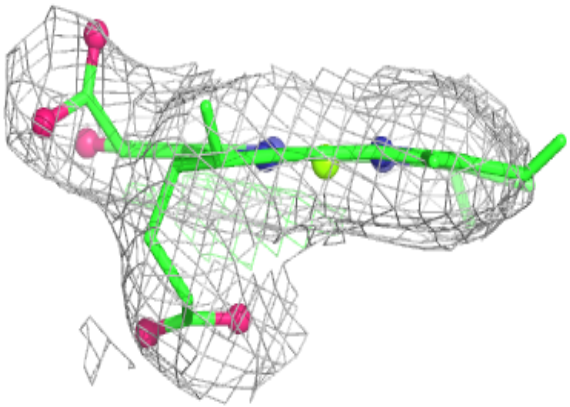


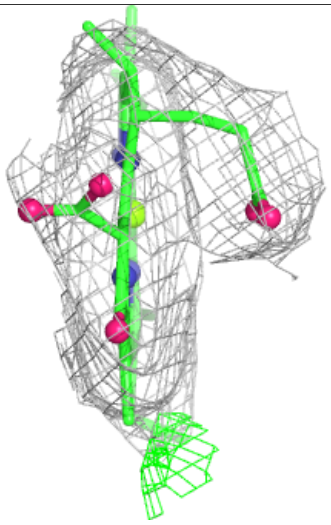


Electron density around CLA 7 1006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

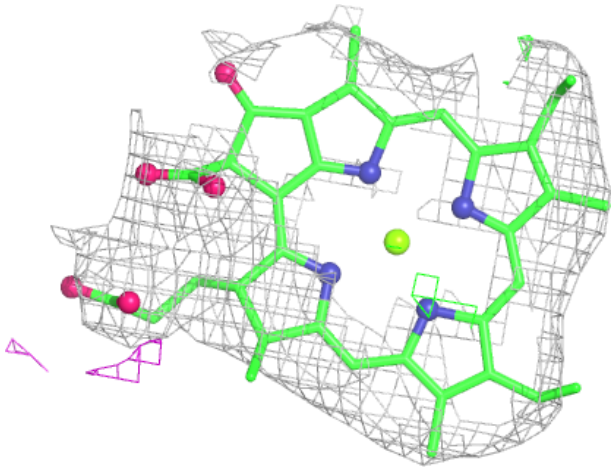


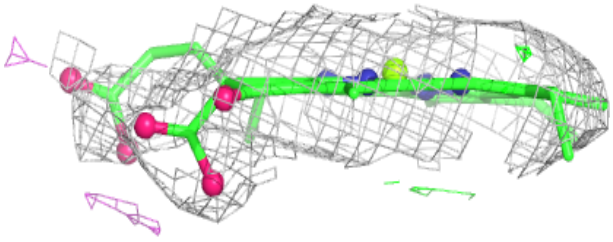


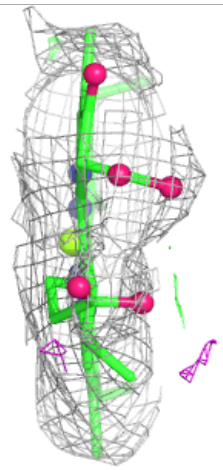


Electron density around CLA 4 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

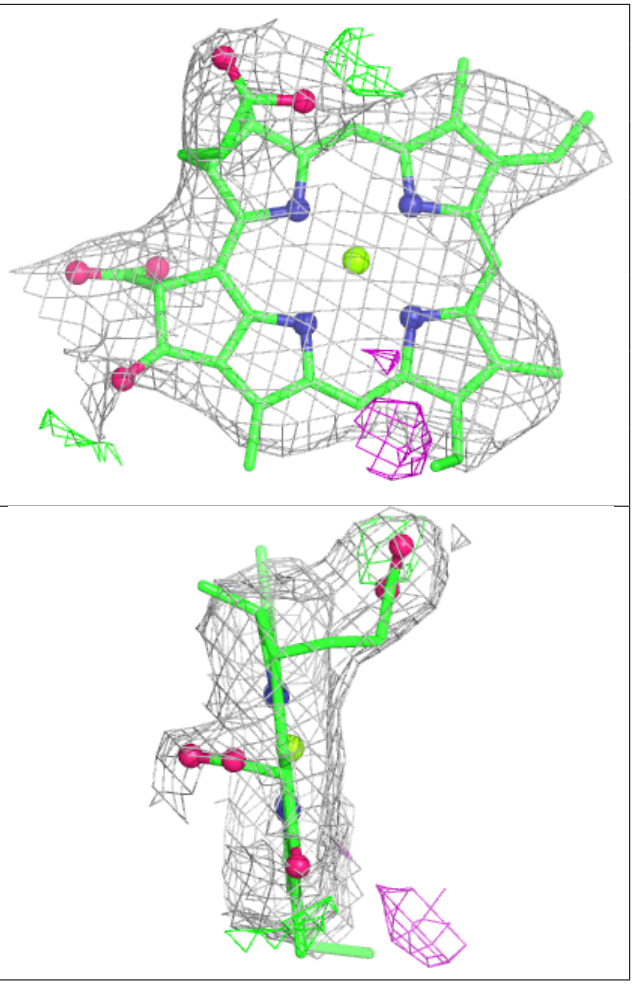


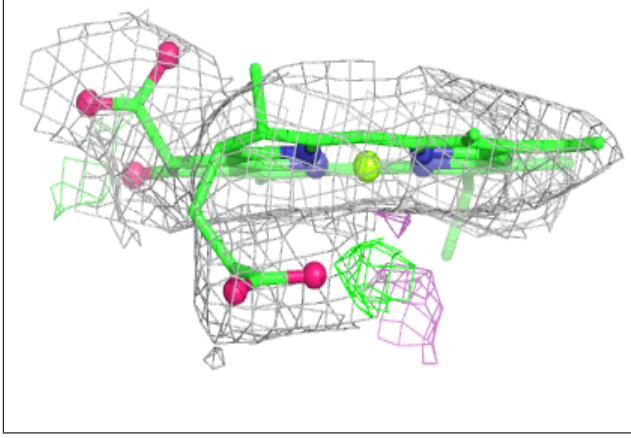




Electron density around CLA 4 307:

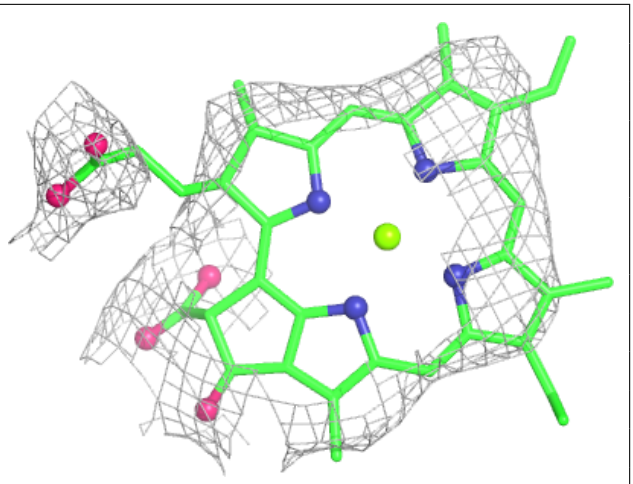
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

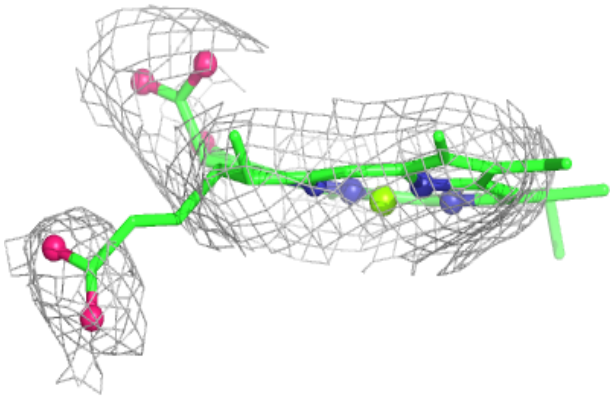


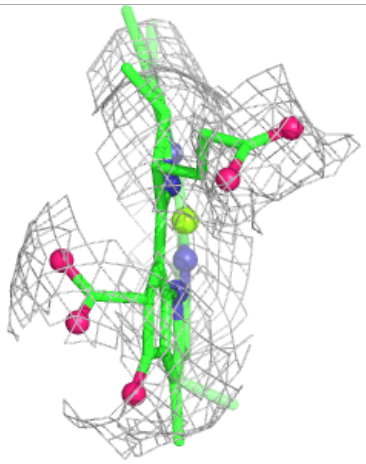


Electron density around CLA A 824:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

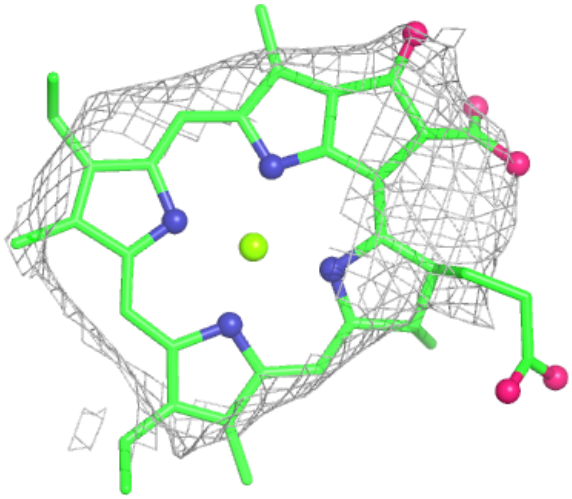


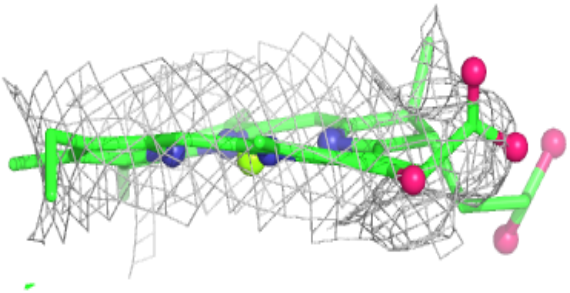


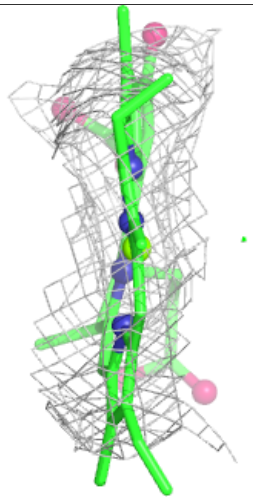


Electron density around CLA B 806:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

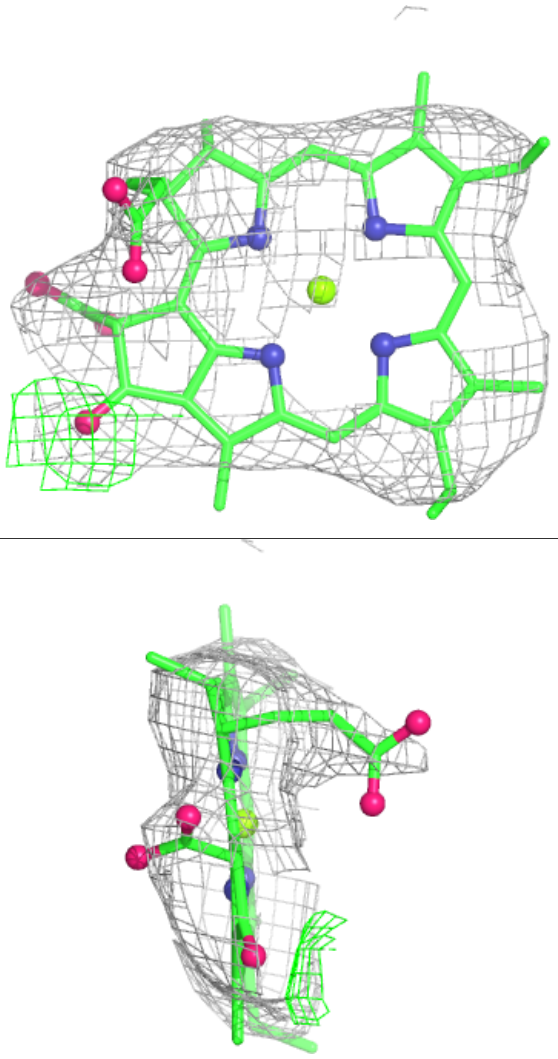


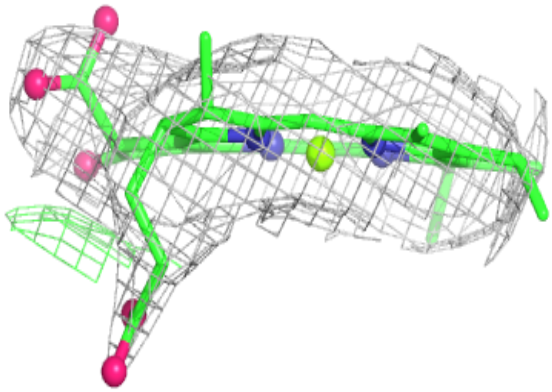




Electron density around CLA 3 1010:

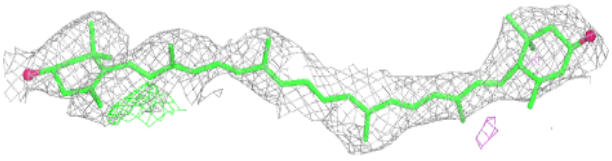
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

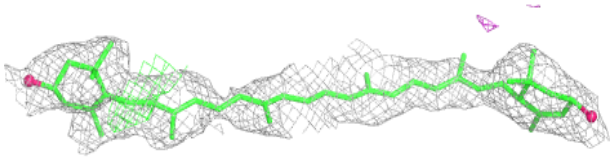


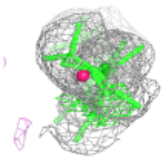


Electron density around LUT 7 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

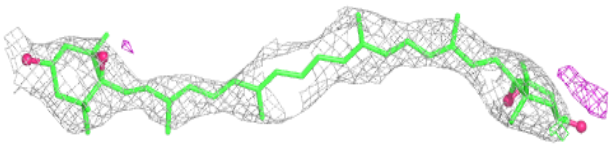


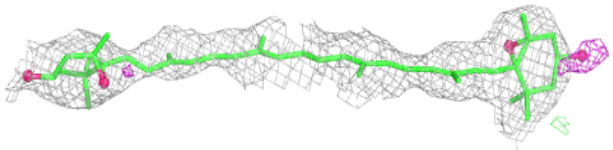


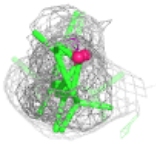


Electron density around XAT 4 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

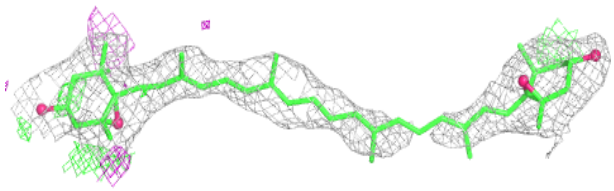


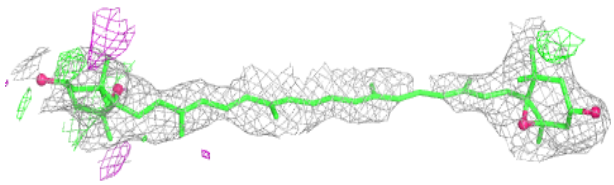


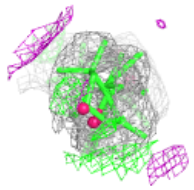


Electron density around XAT 6 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

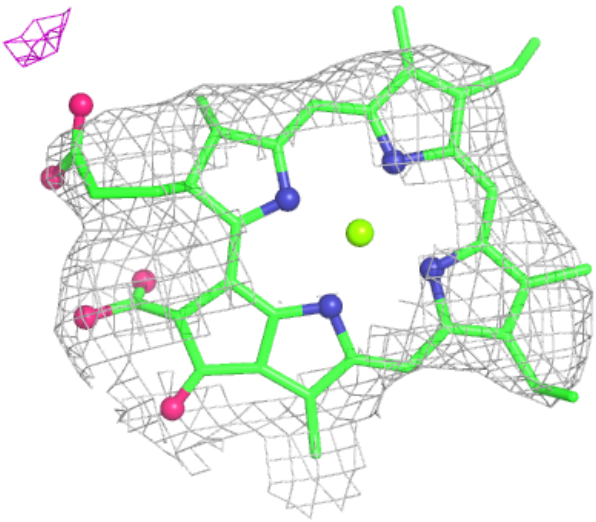


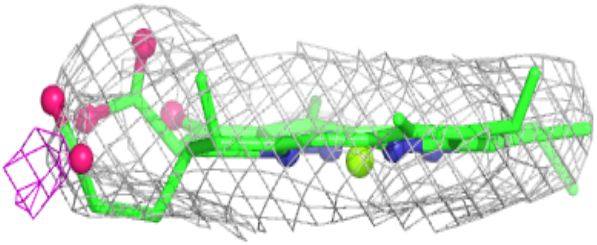


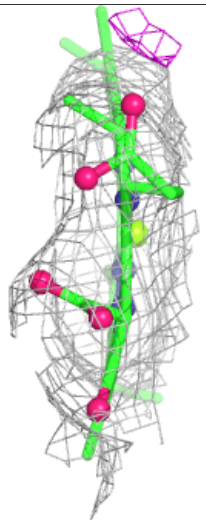


Electron density around CLA 3 1009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

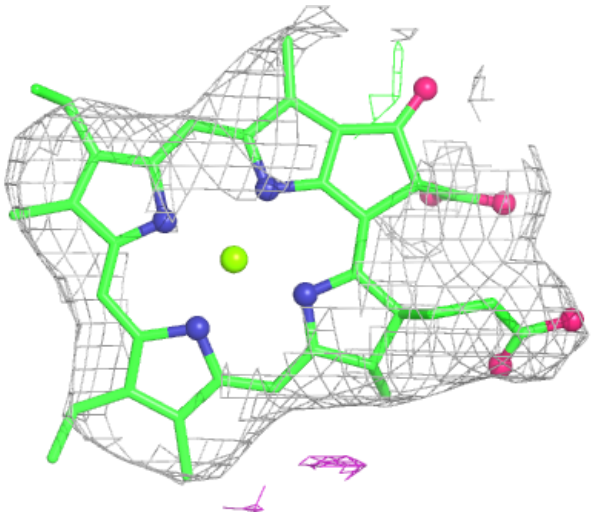


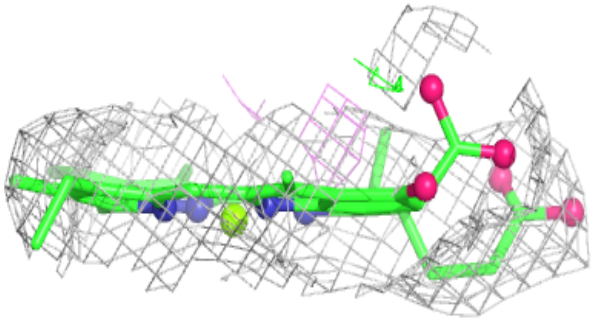




Electron density around CLA 4 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

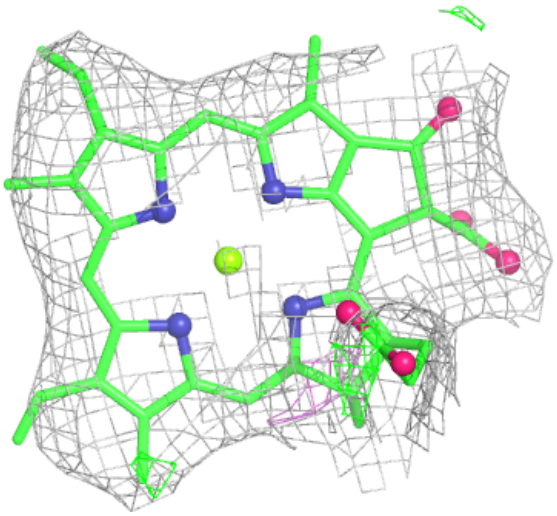


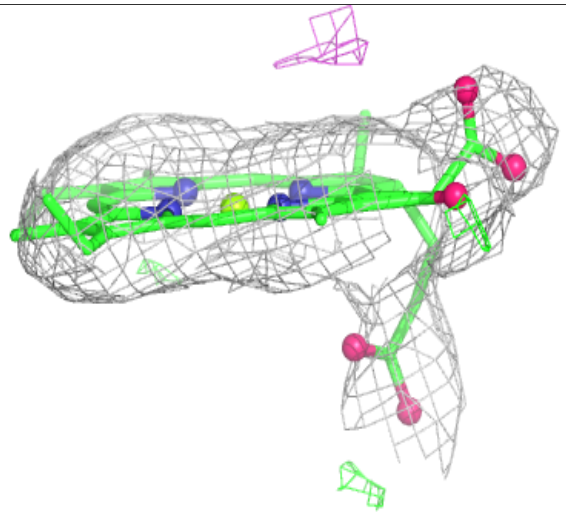


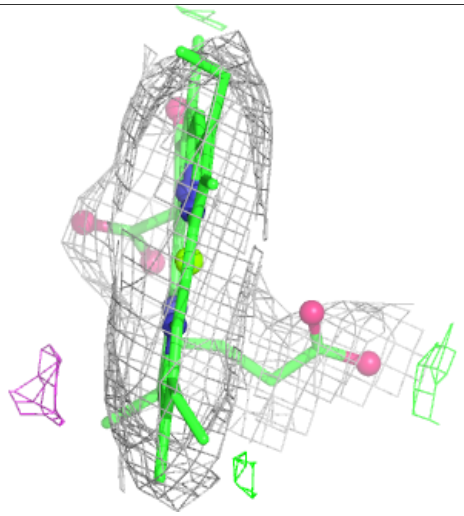


Electron density around CLA 4 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

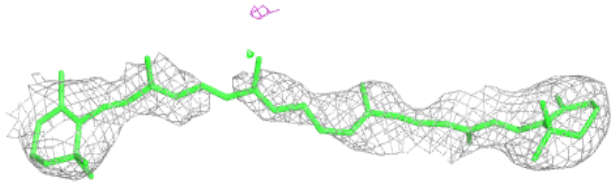


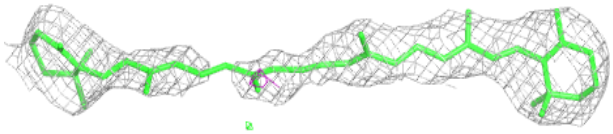


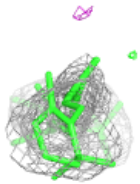


Electron density around BCR 3 1003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

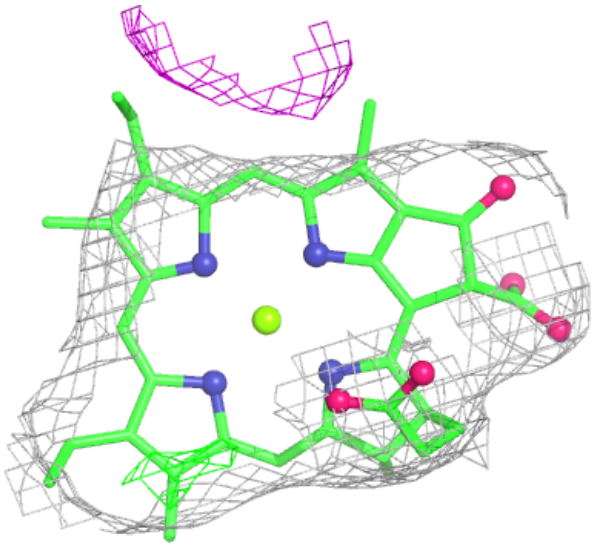


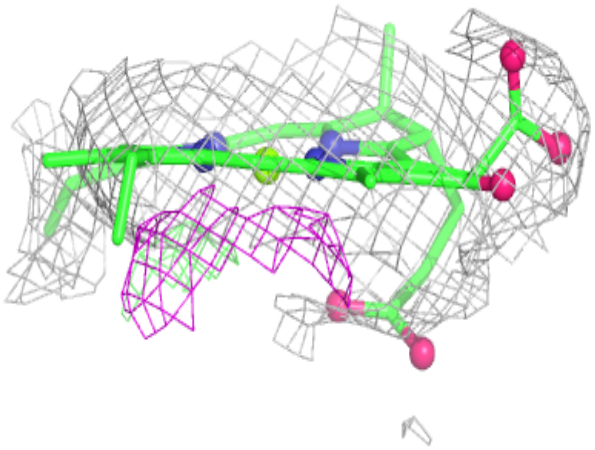


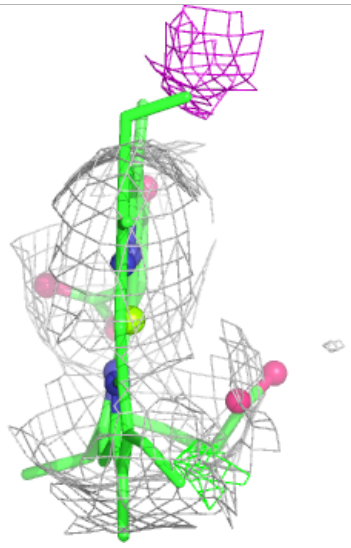


Electron density around CLA A 827:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

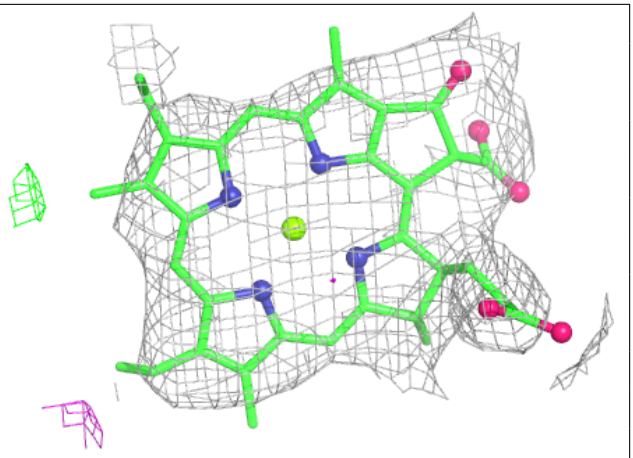


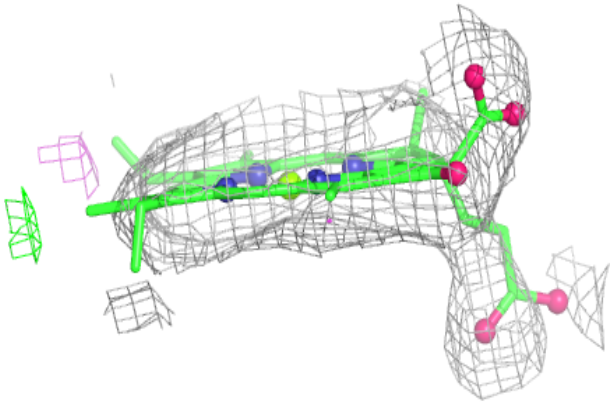


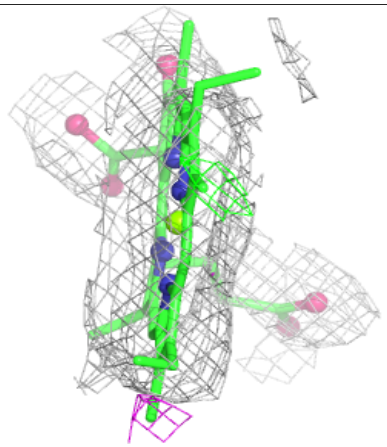


Electron density around CLA 4 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

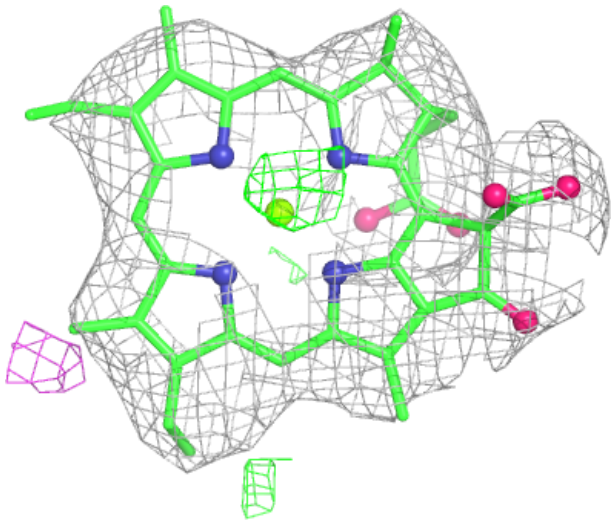


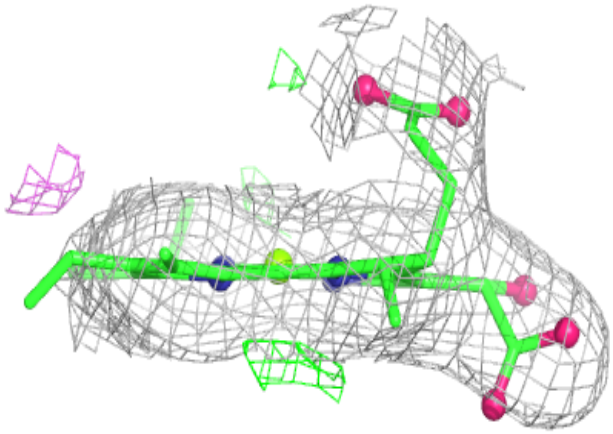


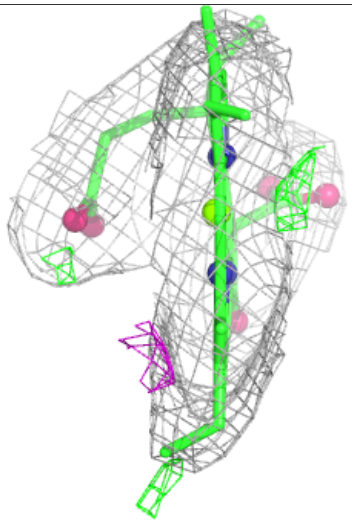


Electron density around CLA 6 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

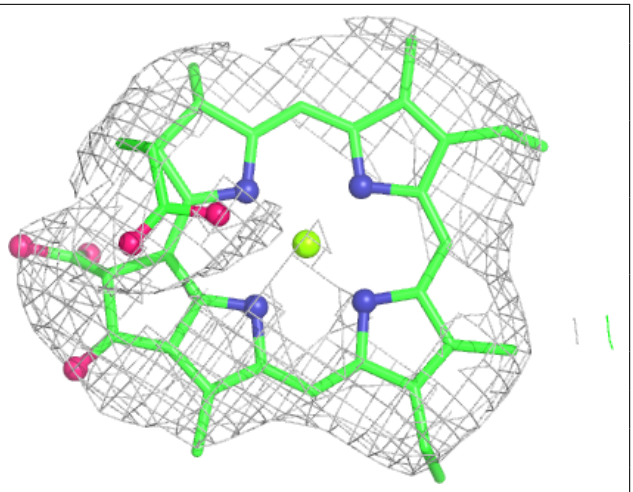


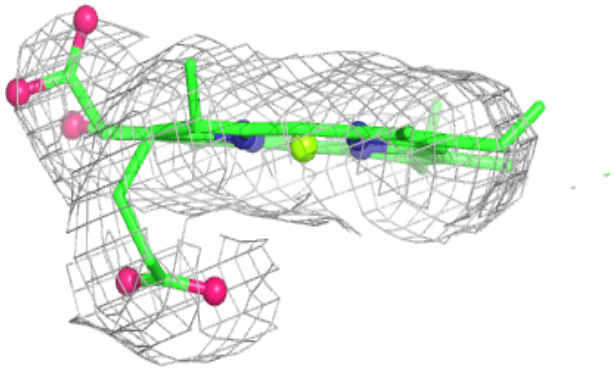


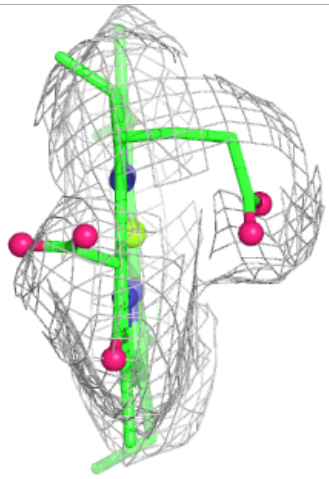


Electron density around CLA A 839:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

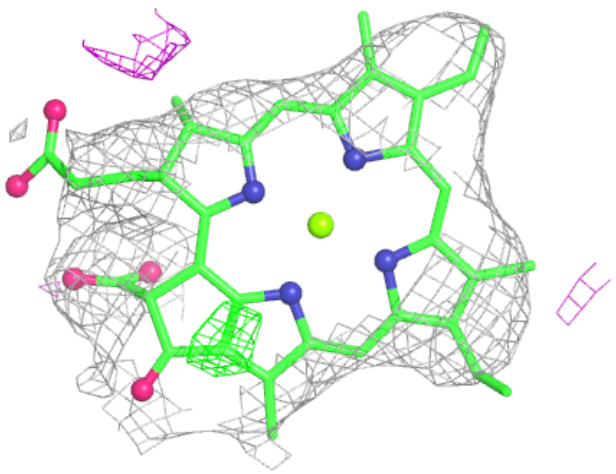


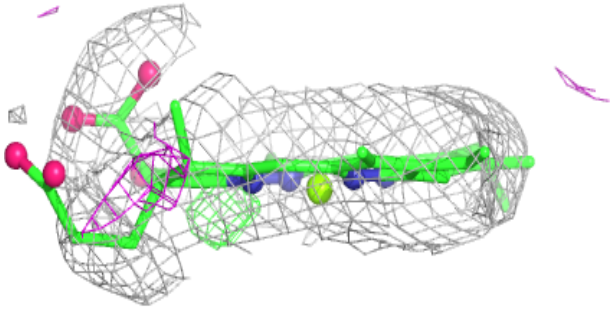


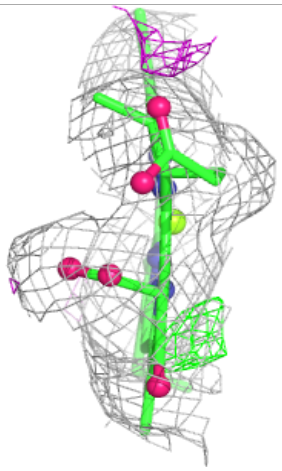


Electron density around CLA 6 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

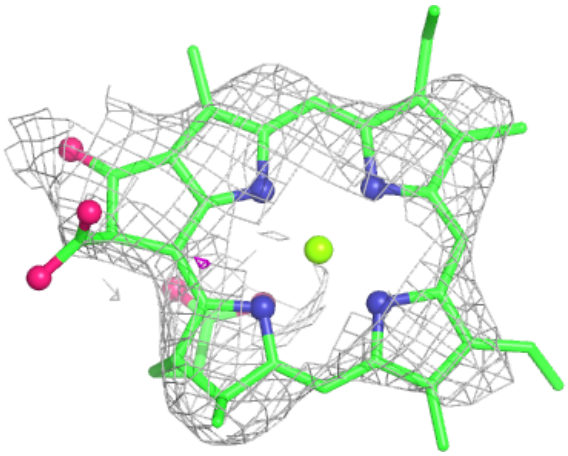


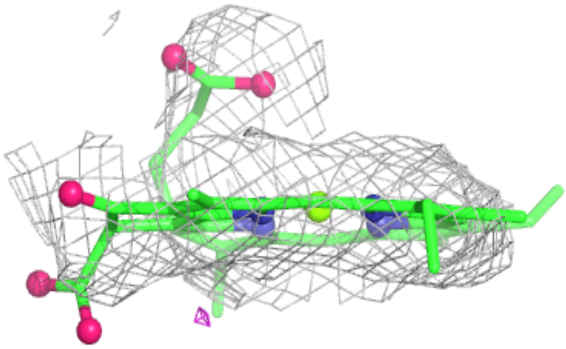


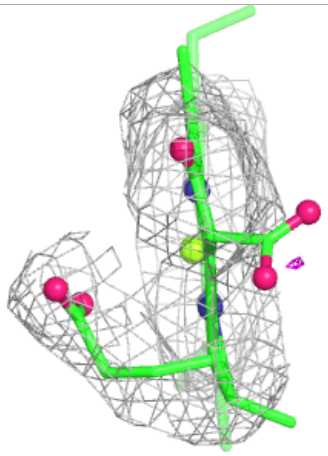


Electron density around CLA B 838:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

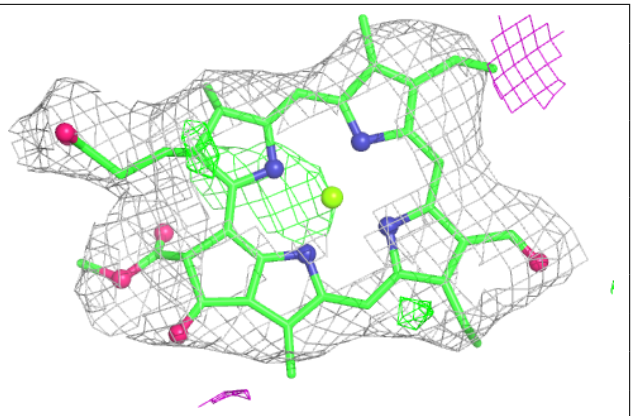


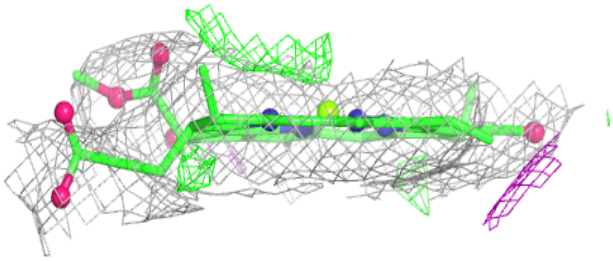


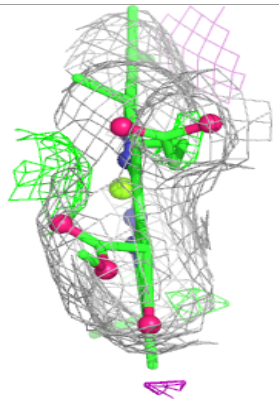


Electron density around CHL 7 1015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

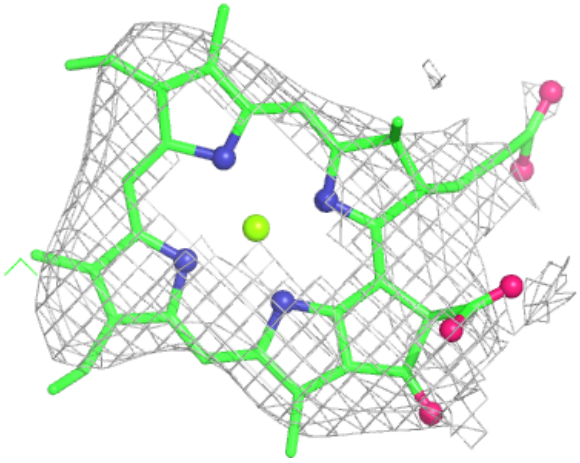


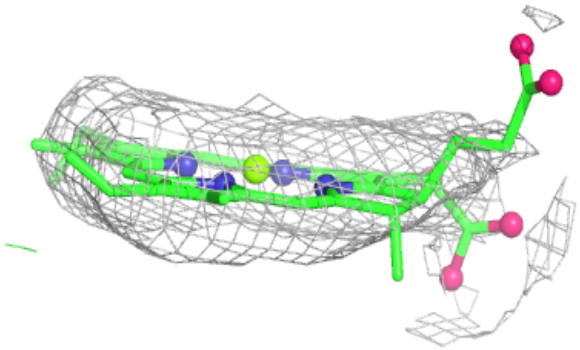


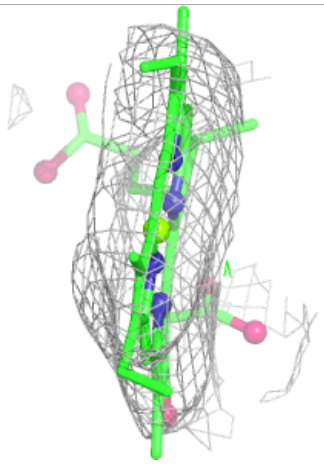


Electron density around CLA A 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

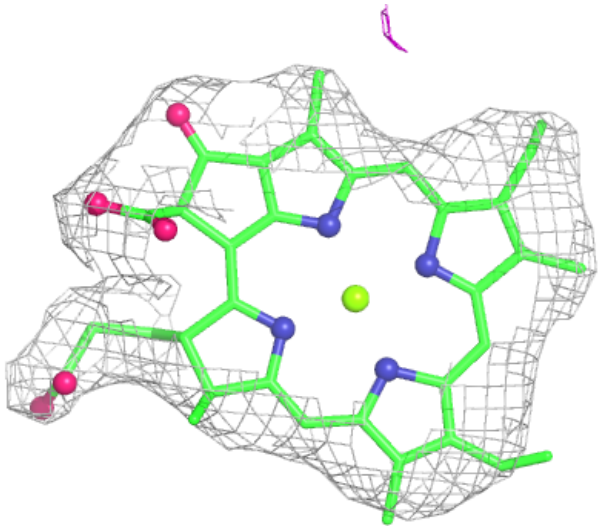


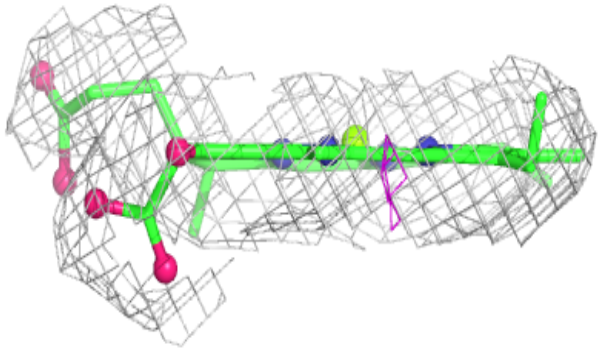


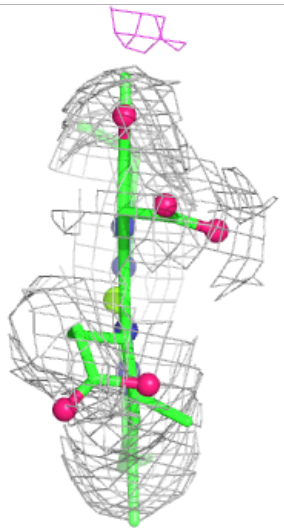


Electron density around CLA 3 1017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

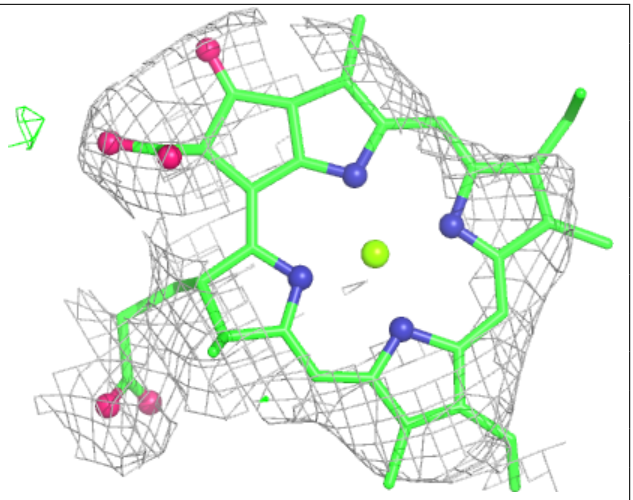


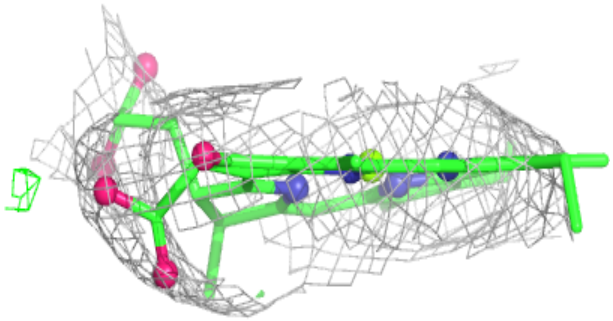


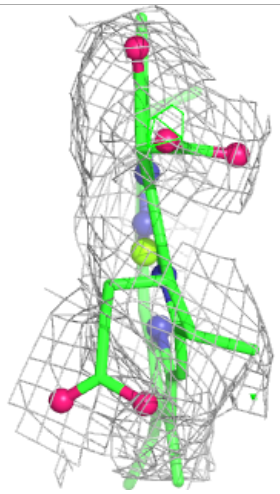


Electron density around CLA A 851:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

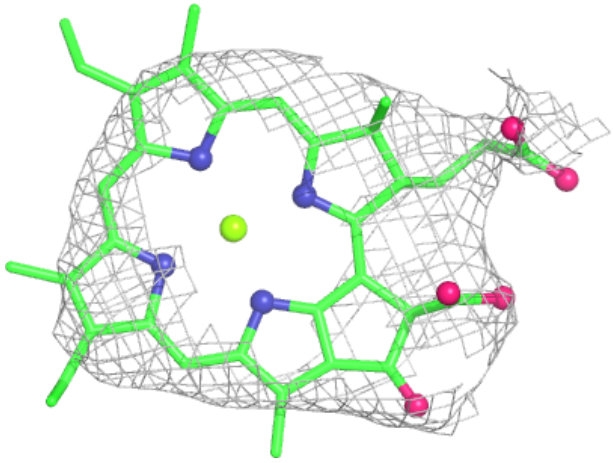


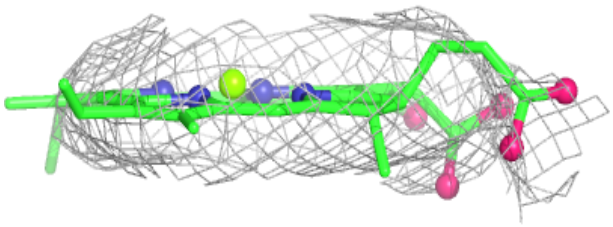


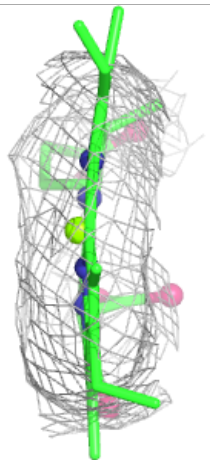


Electron density around CLA B 809:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

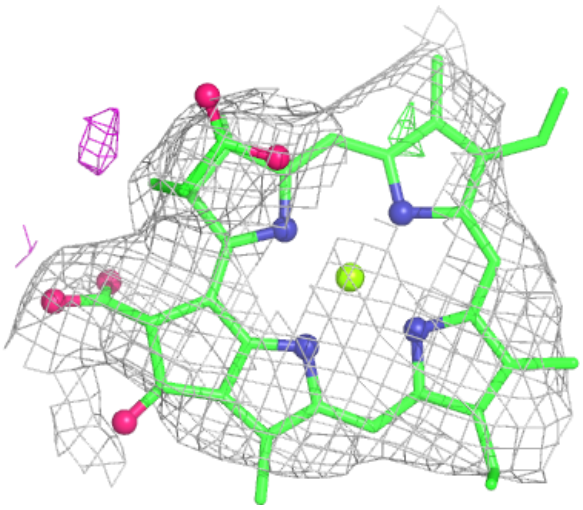


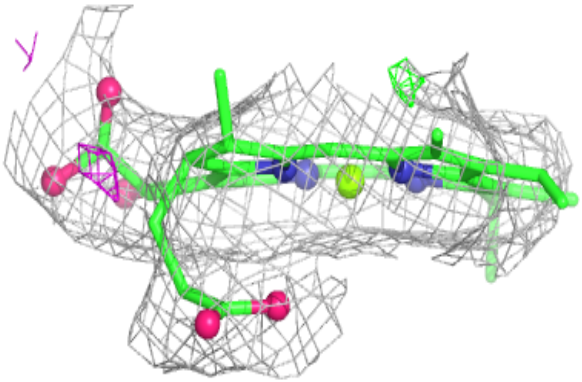


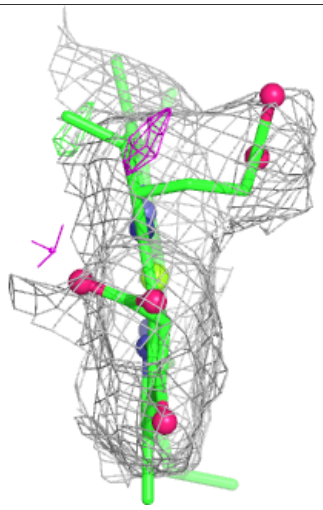


Electron density around CLA 5 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

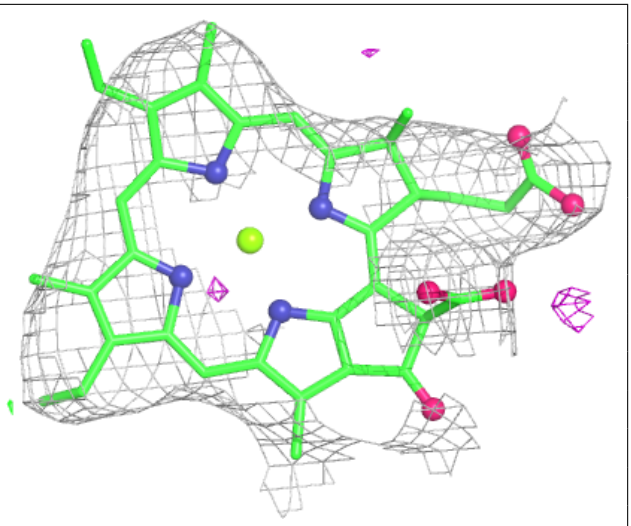


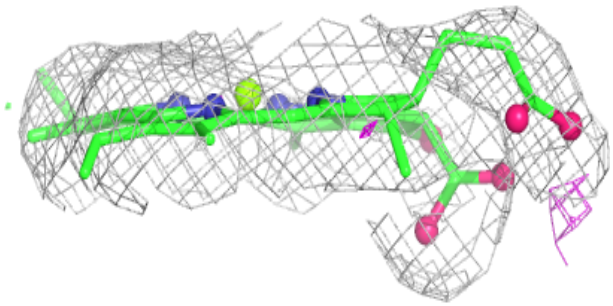


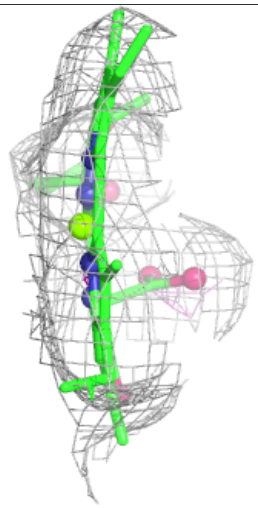


Electron density around CLA 8 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

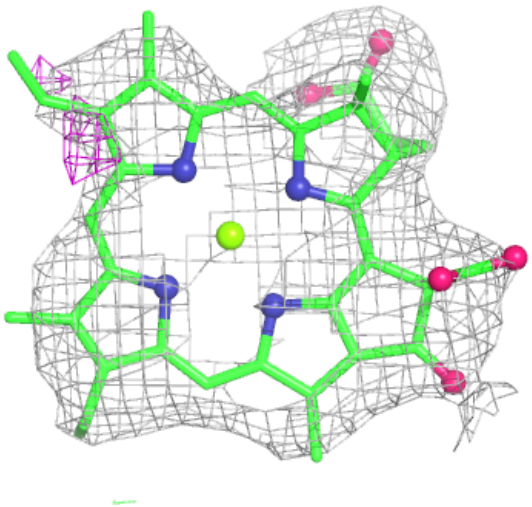


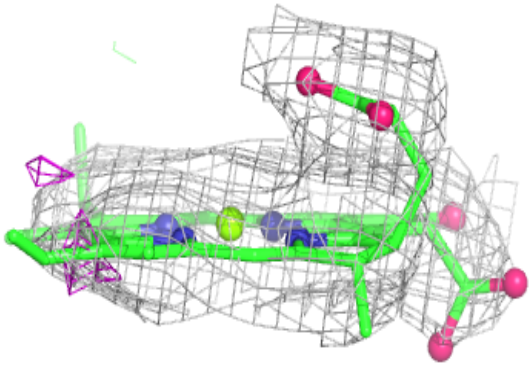


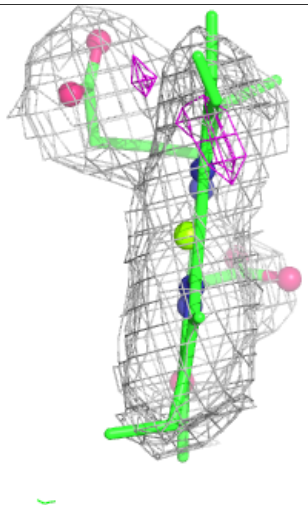


Electron density around CLA 5 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

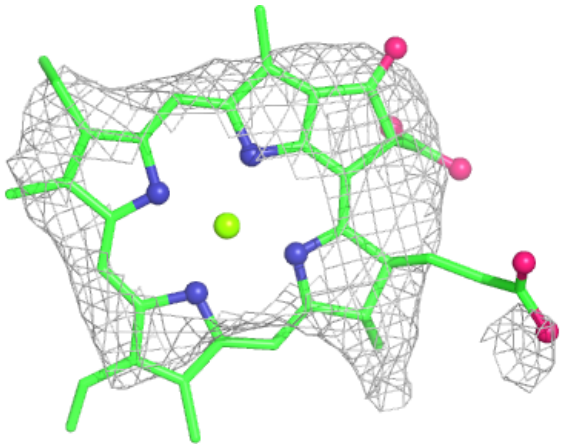


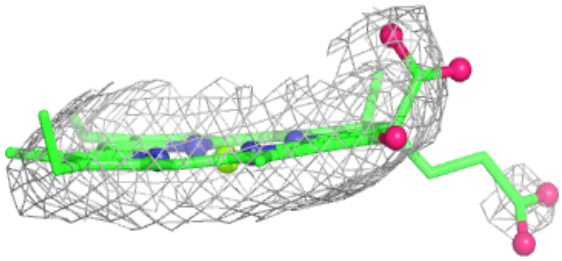


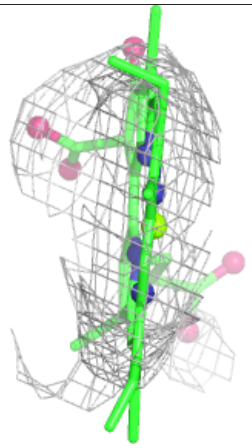


Electron density around CLA A 834:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

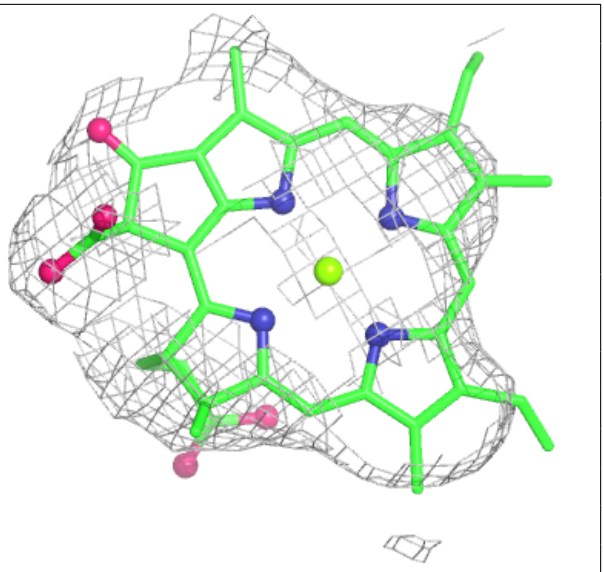


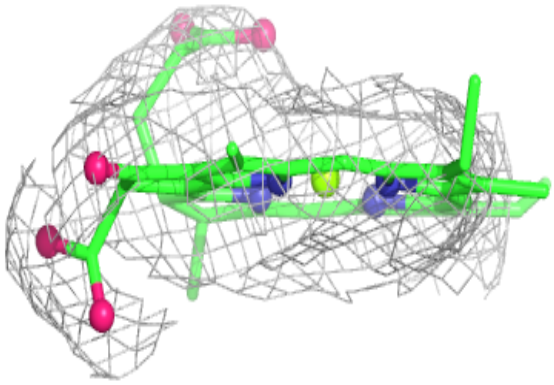


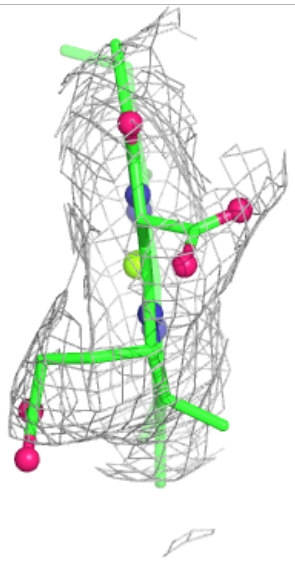


Electron density around CLA A 818:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

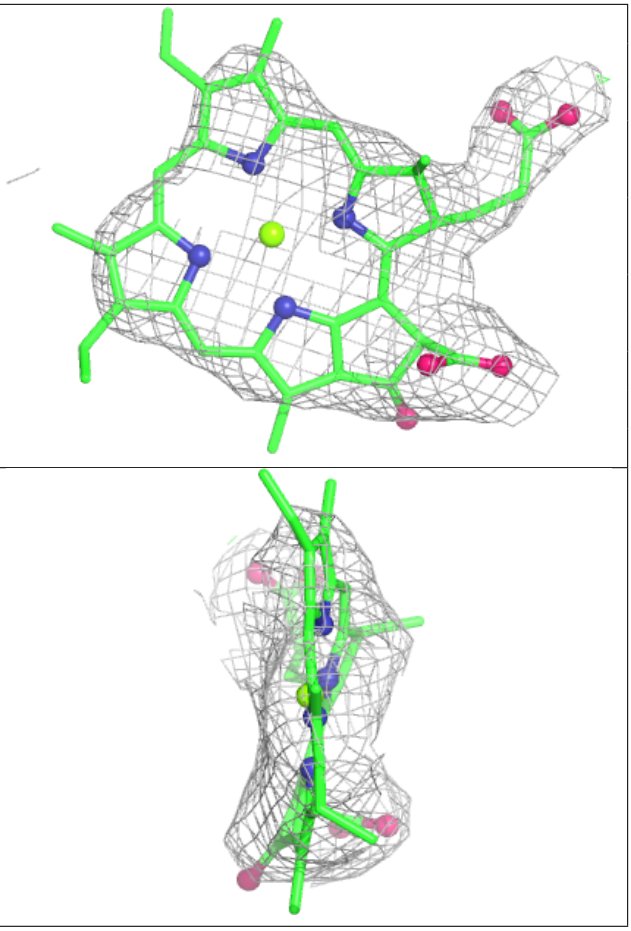


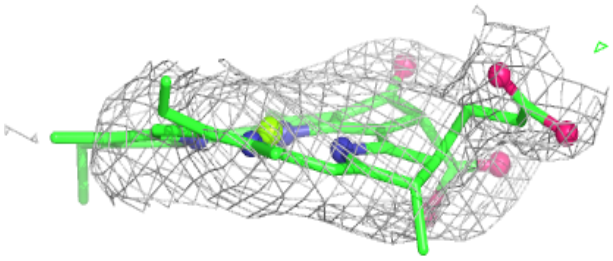




Electron density around CLA B 802:

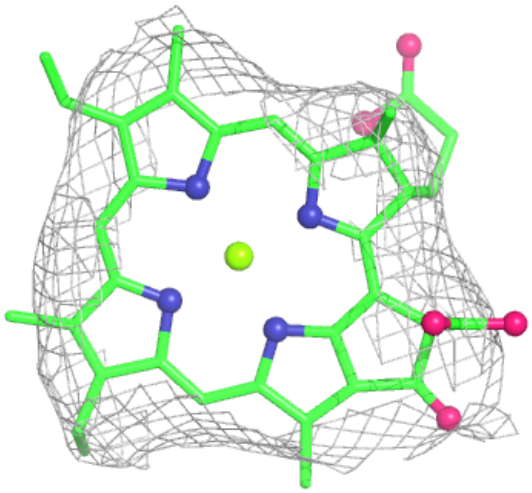
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

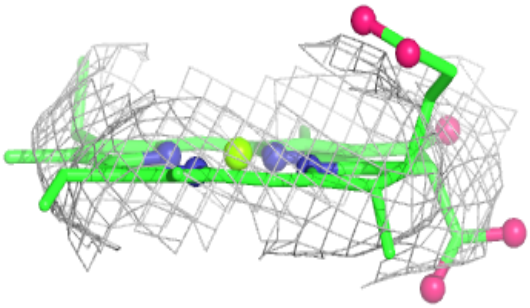


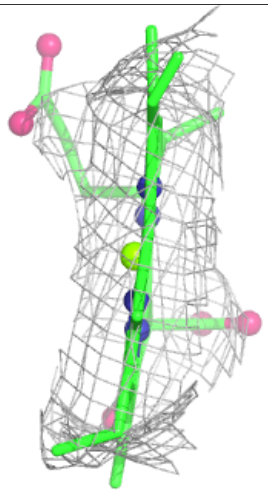


Electron density around CLA B 821:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

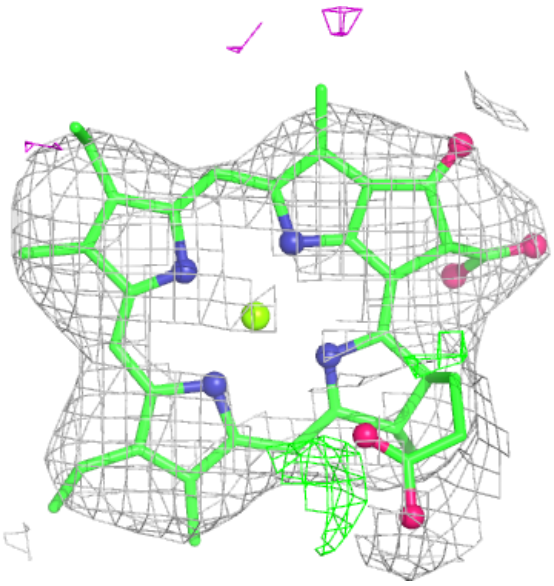


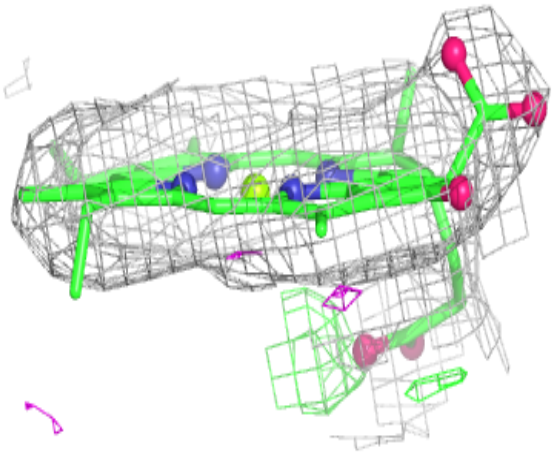




Electron density around CLA 7 1007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

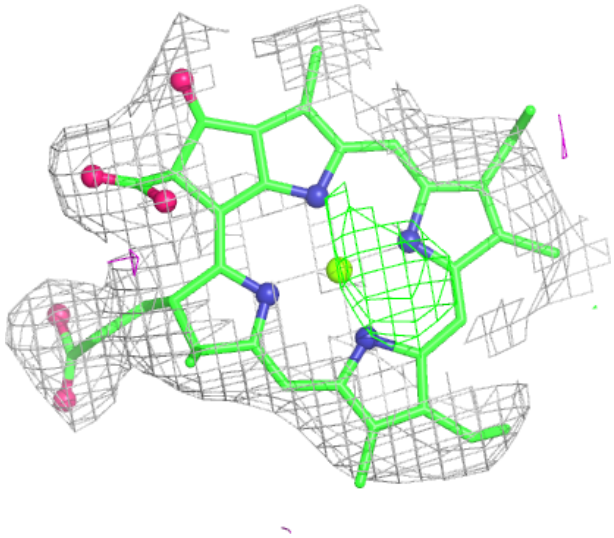


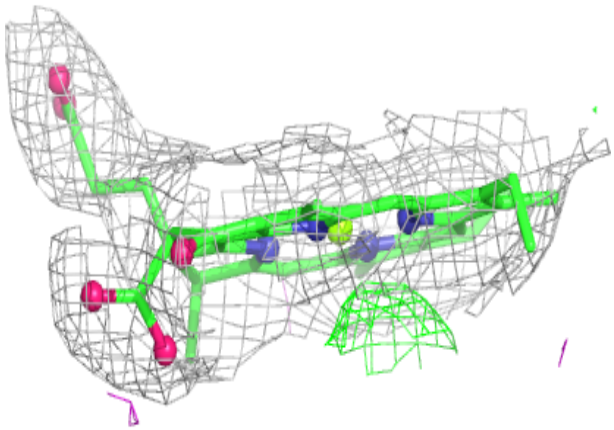


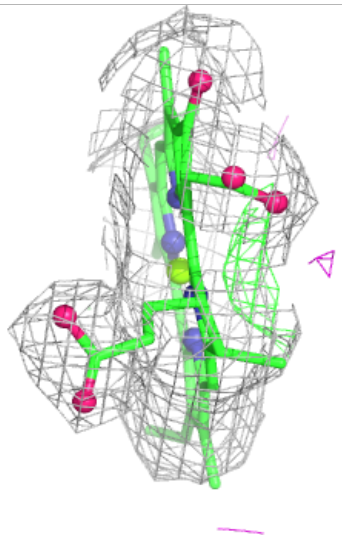


Electron density around CLA 5 321:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

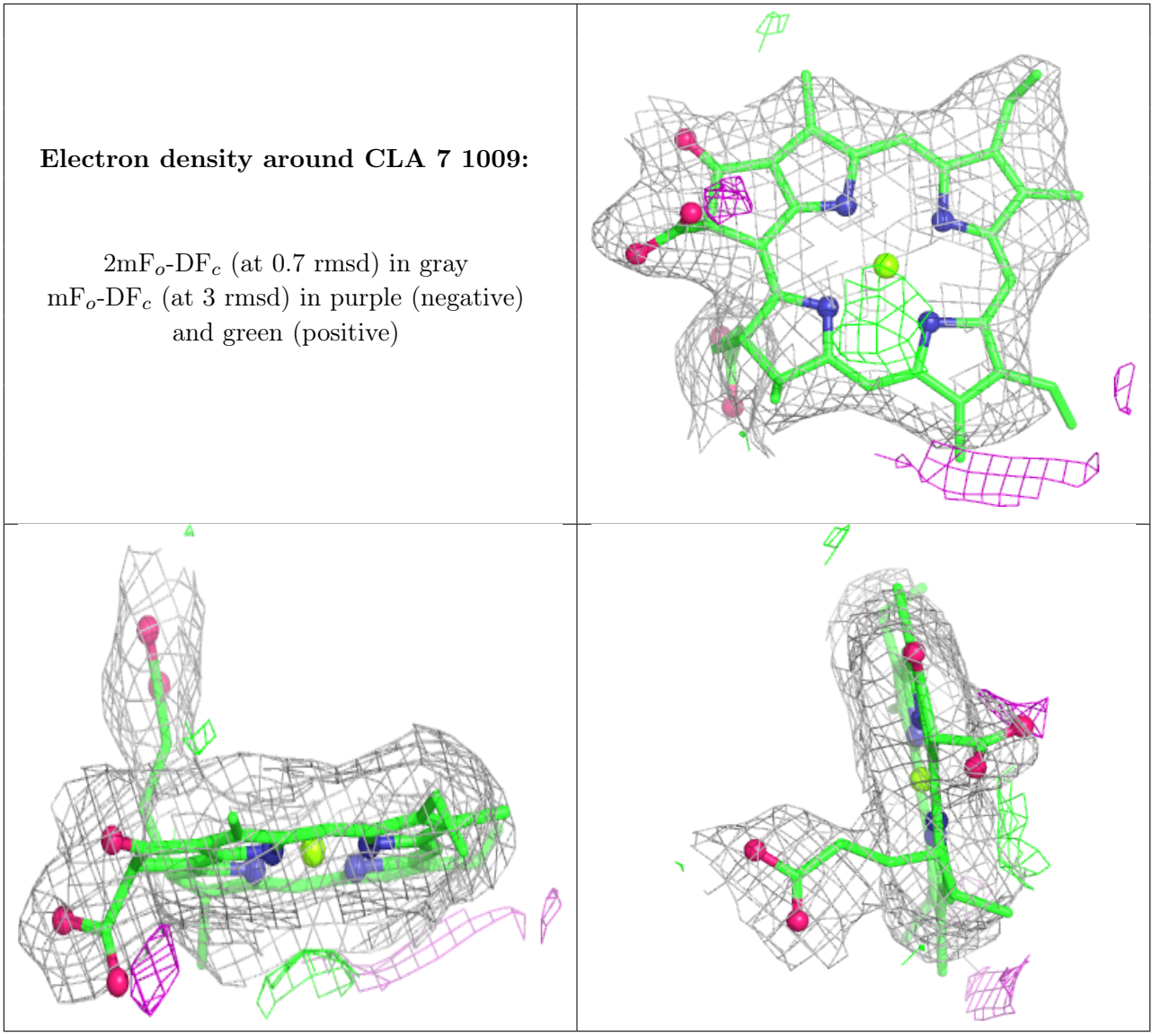






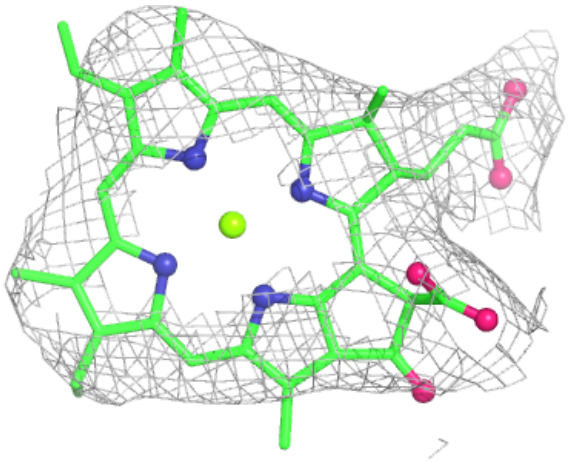
Electron density around CLA 7 1009:

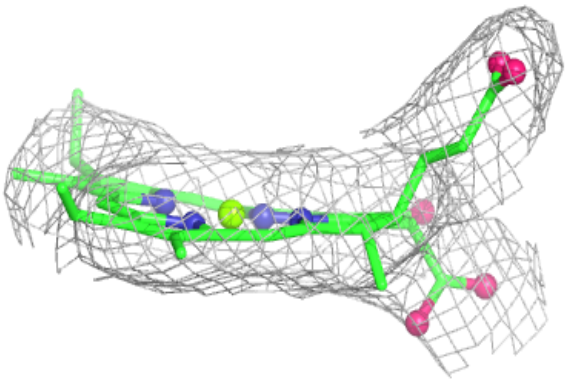
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 834:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

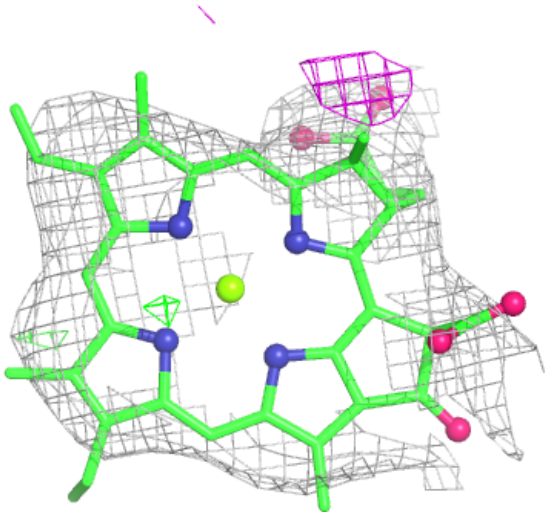


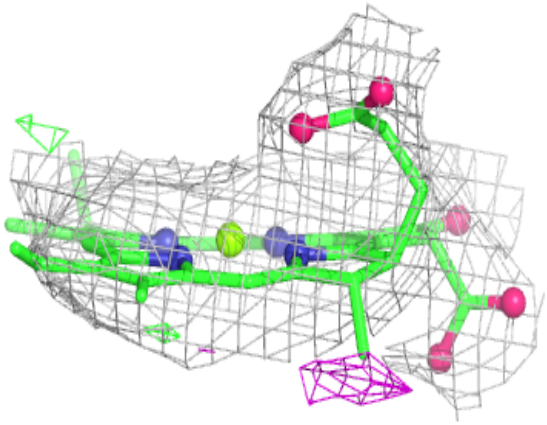




Electron density around CLA 0 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

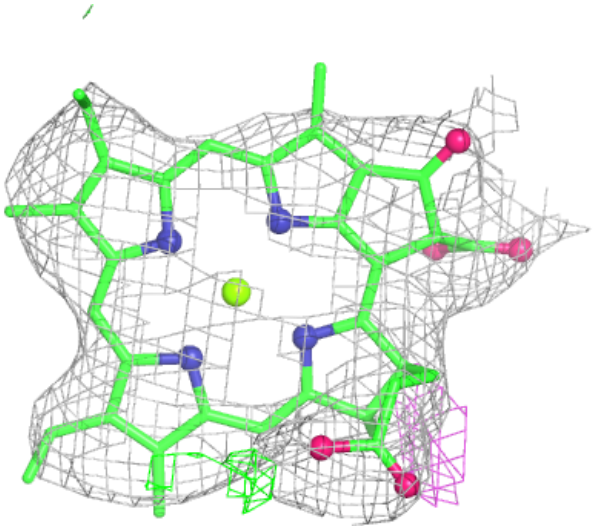


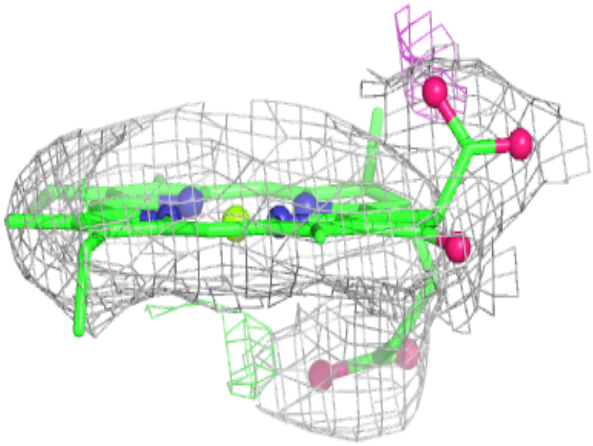




Electron density around CLA 8 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

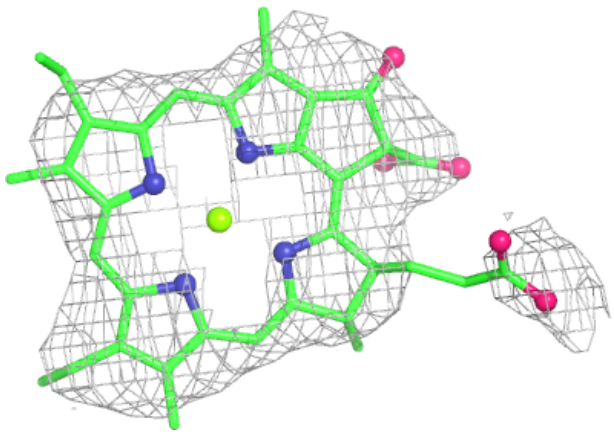


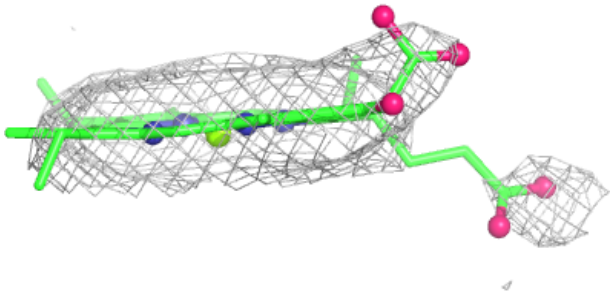


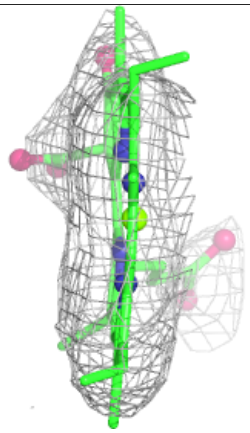


Electron density around CLA B 837:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

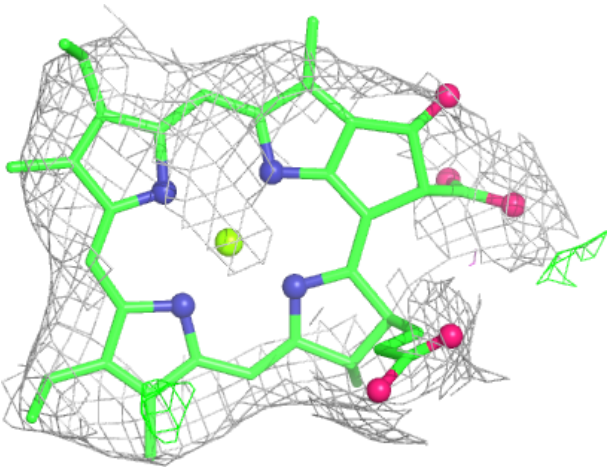


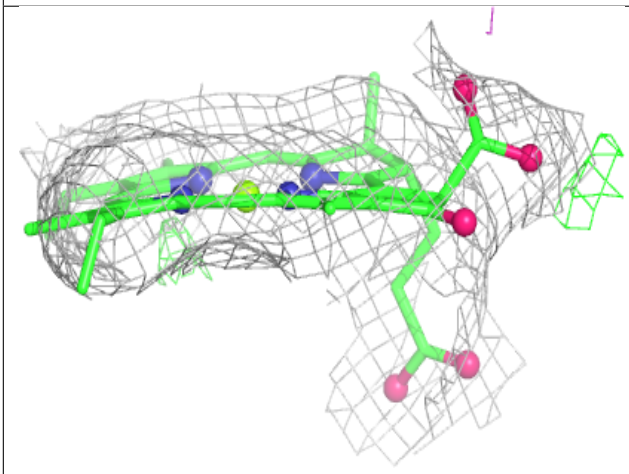




Electron density around CLA 4 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

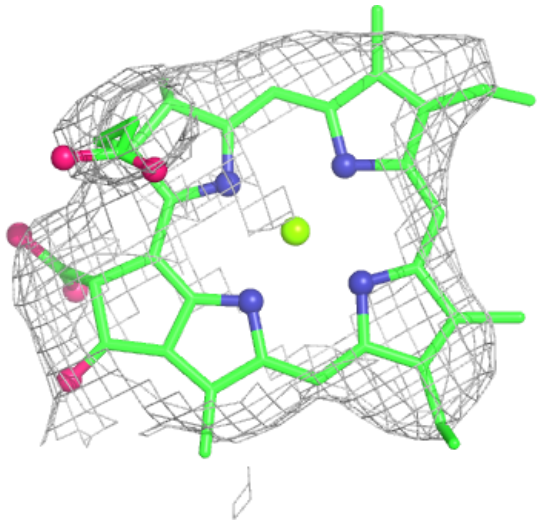


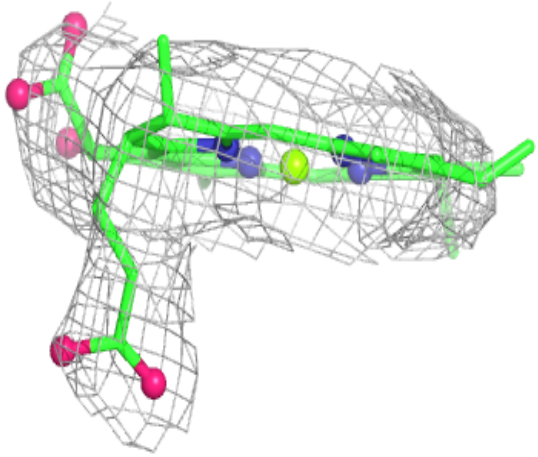


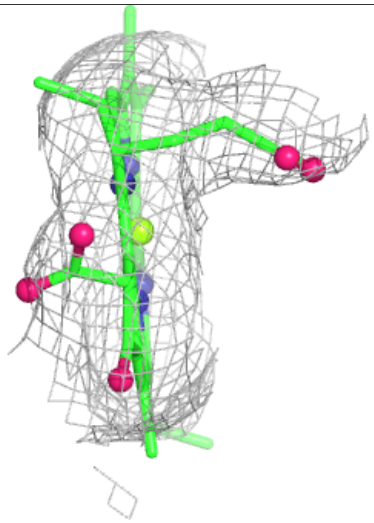


Electron density around CLA 6 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

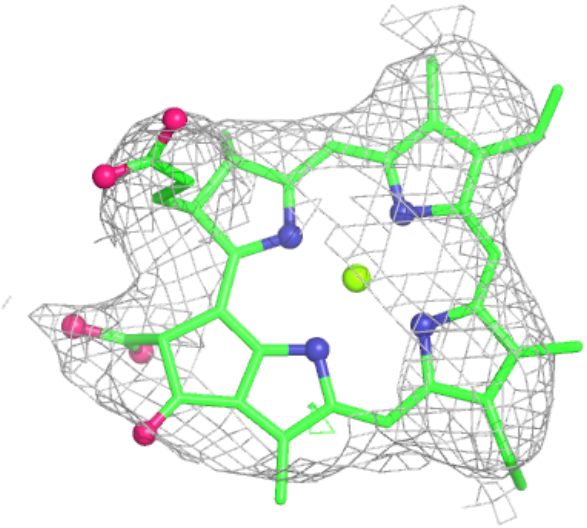


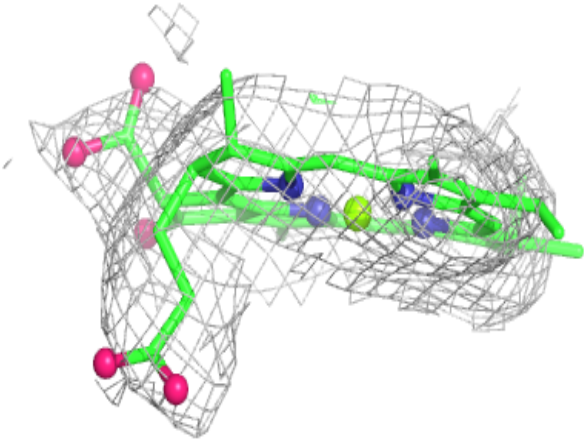


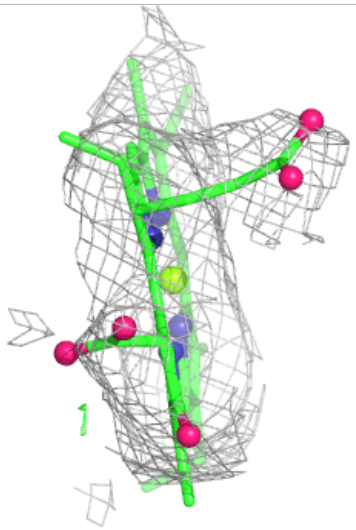


Electron density around CLA 3 1015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

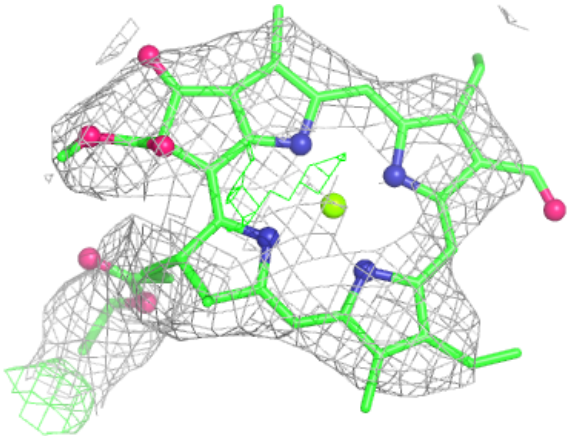


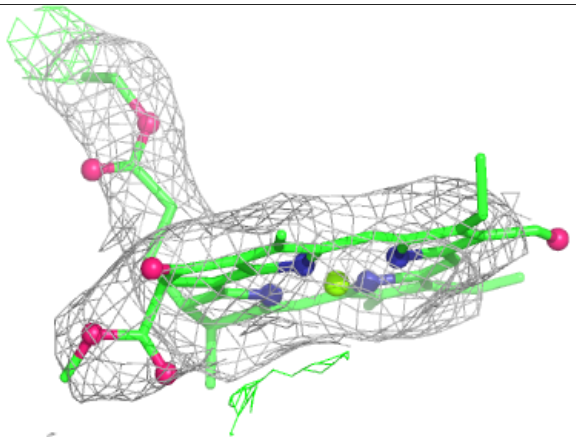


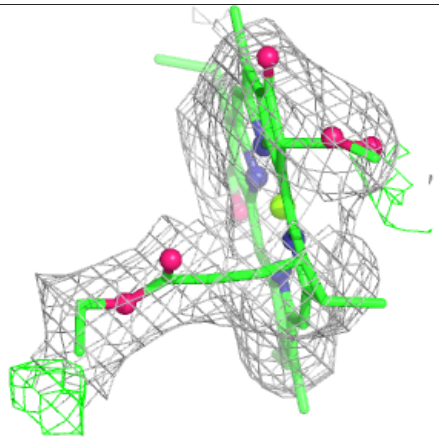


Electron density around CHL 7 1013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

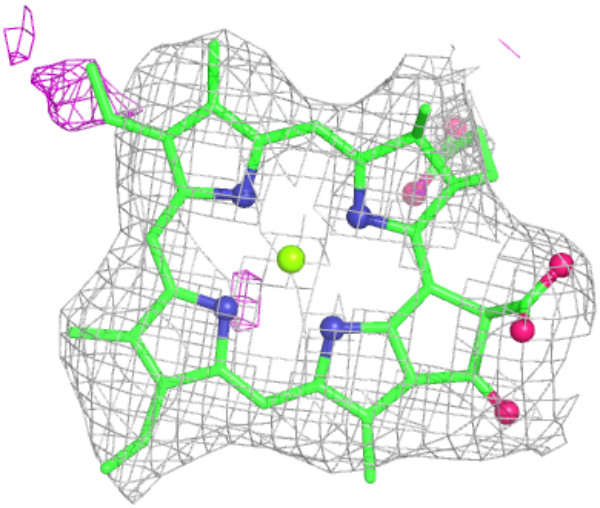


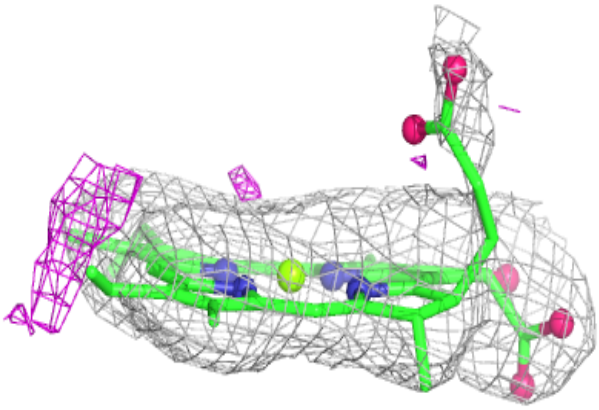




Electron density around CLA 8 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

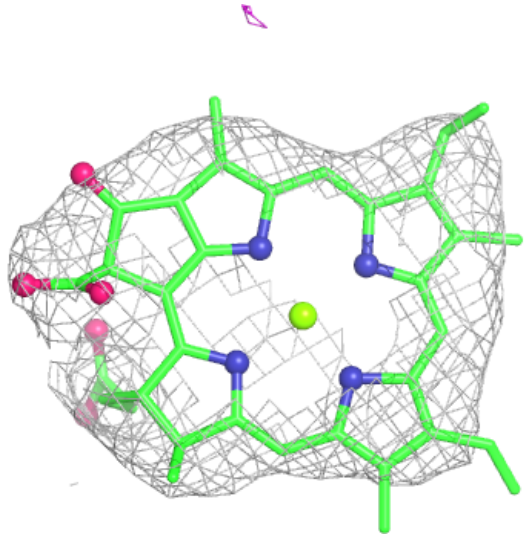


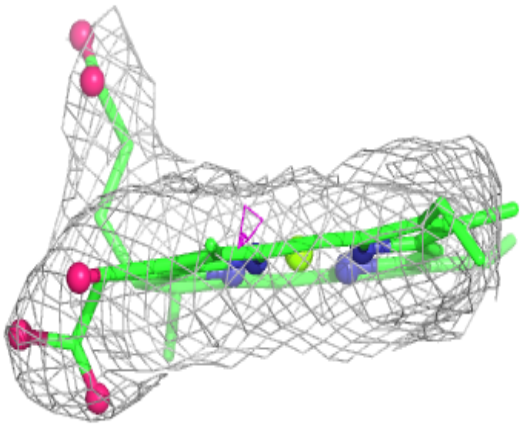


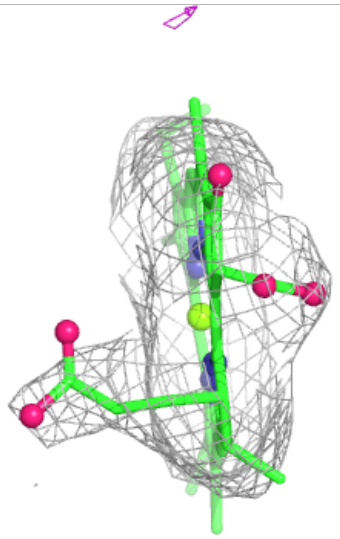


Electron density around CLA A 806:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

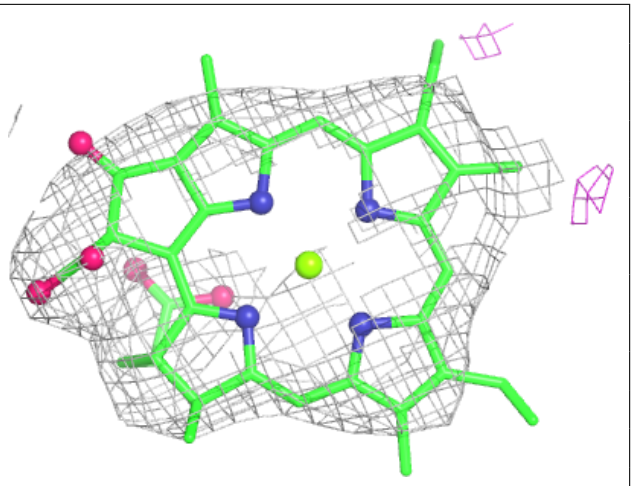


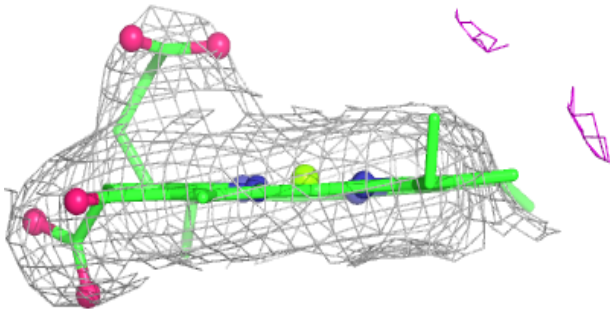


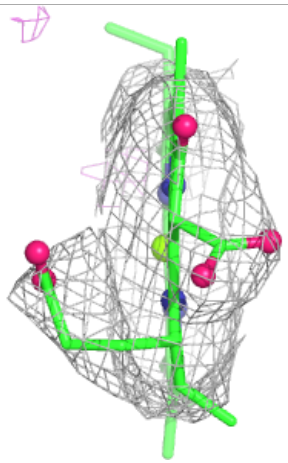


Electron density around CLA A 837:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

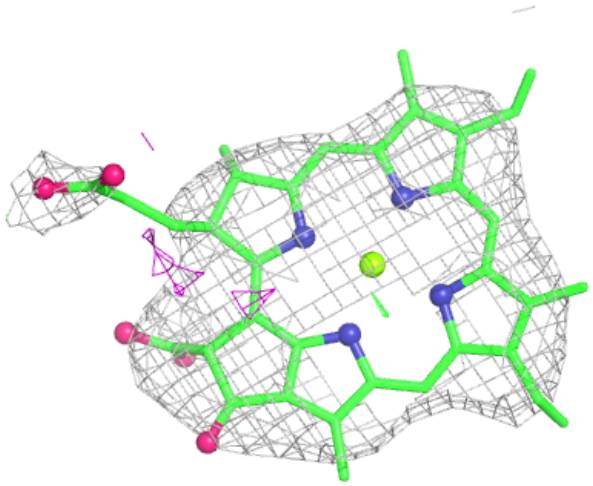


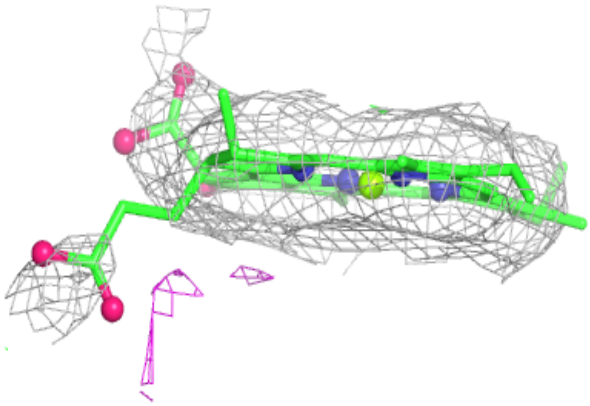


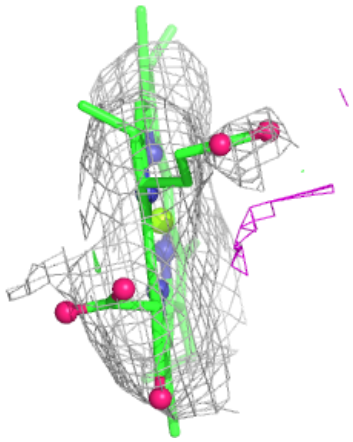


Electron density around CLA A 838:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

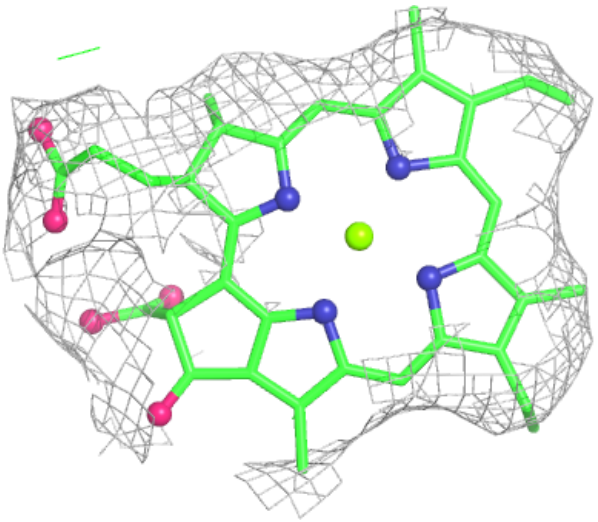


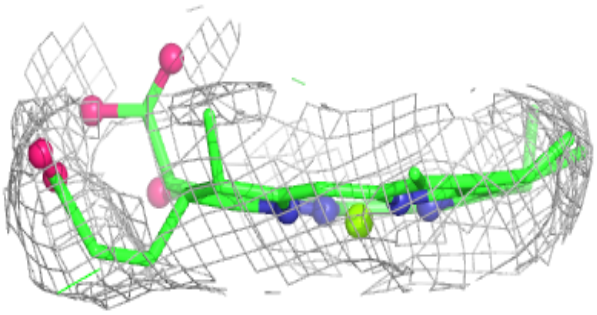


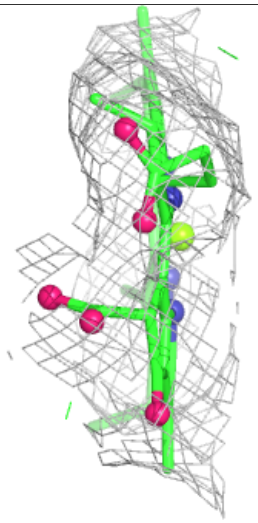


Electron density around CLA 7 1005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

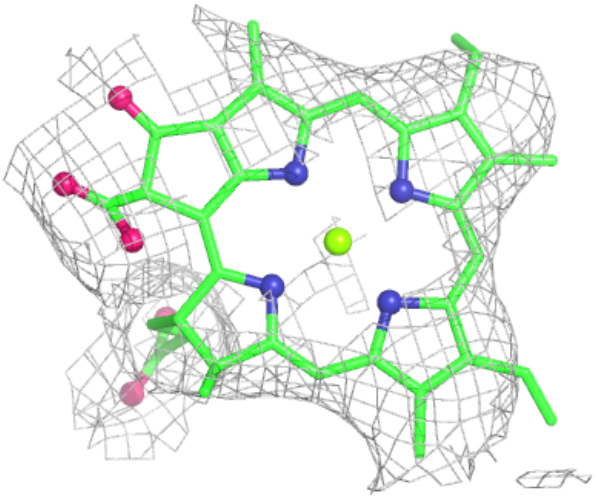


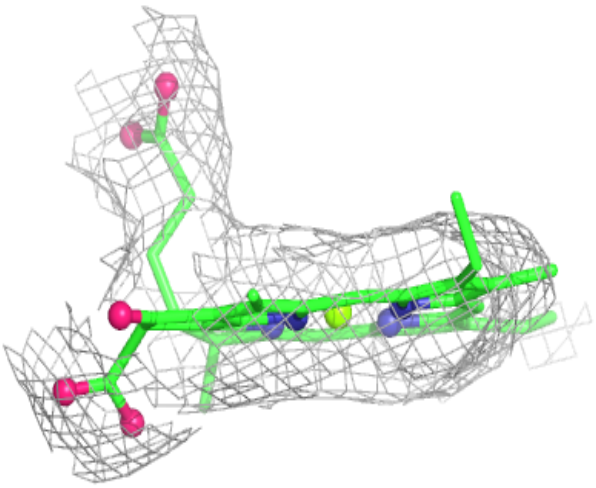


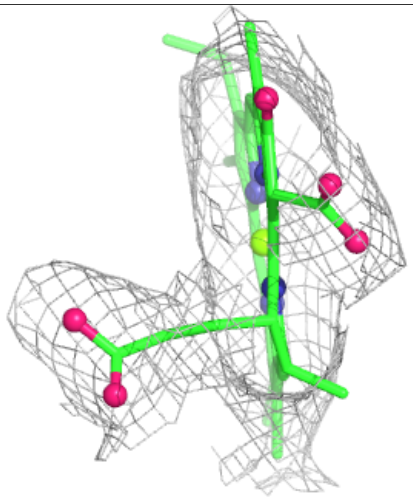


Electron density around CLA A 829:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

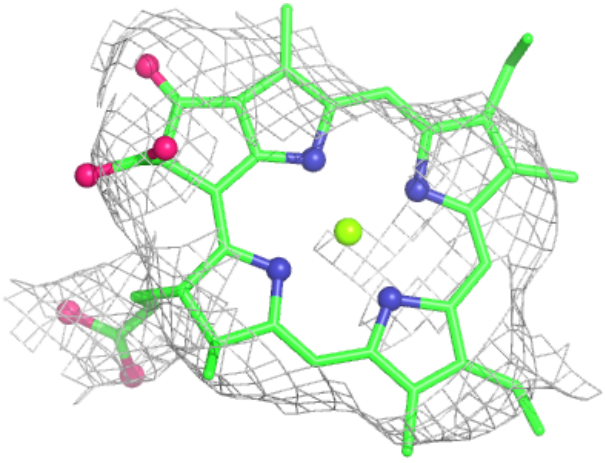


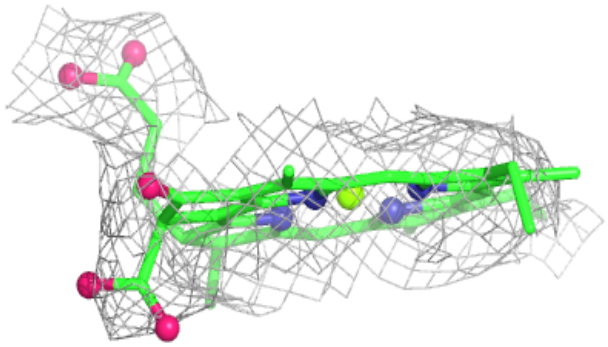


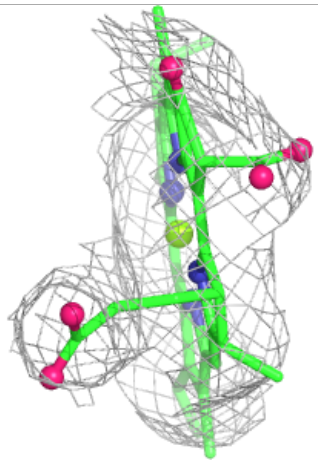


Electron density around CLA A 813:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

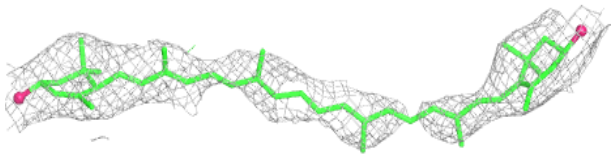


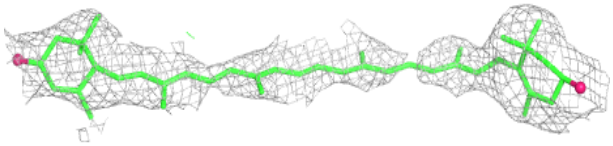


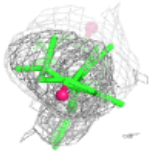


Electron density around LUT 8 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

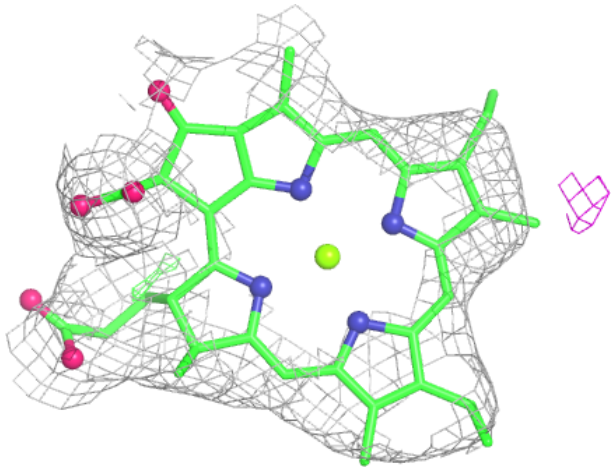


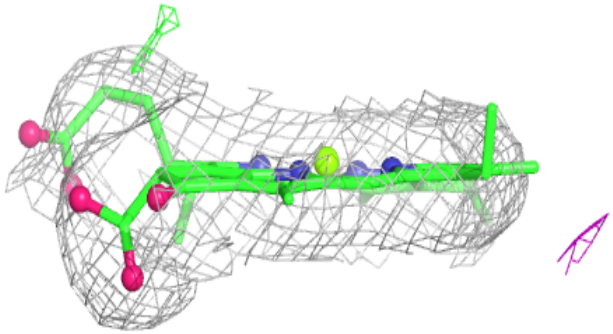


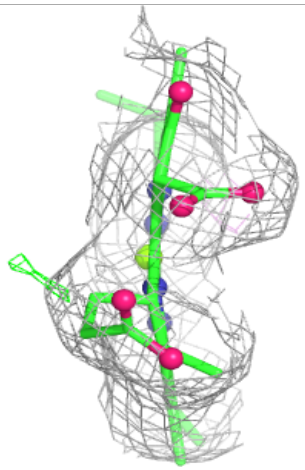


Electron density around CLA 7 1008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

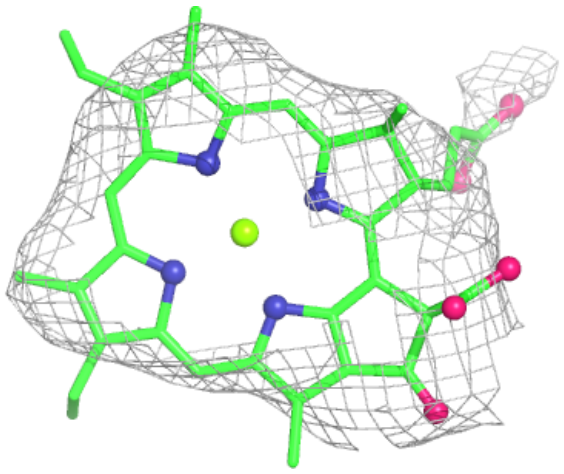


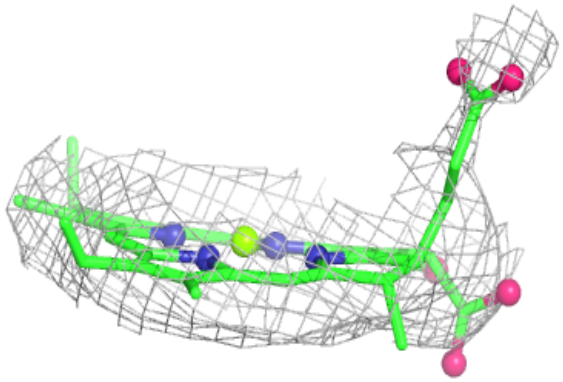


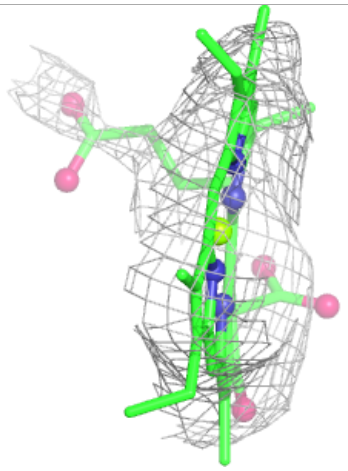


Electron density around CLA B 825:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

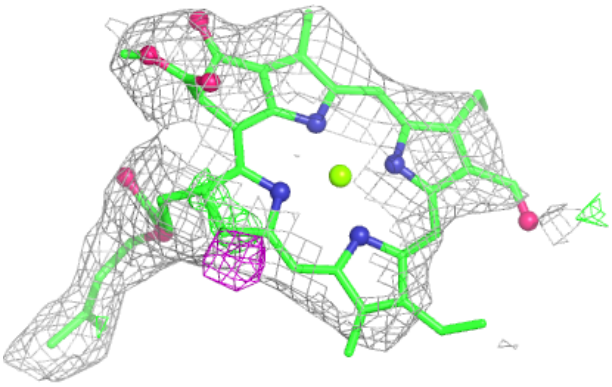


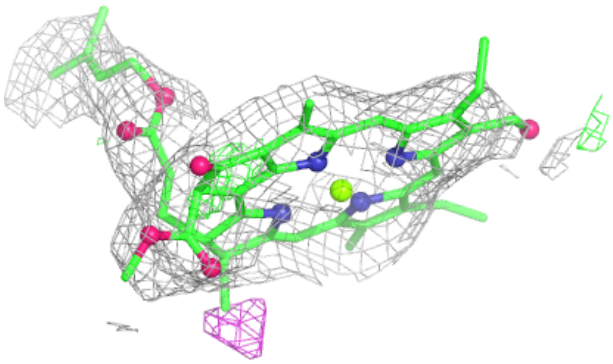


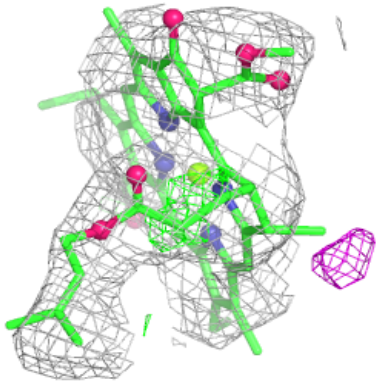


Electron density around CHL 6 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

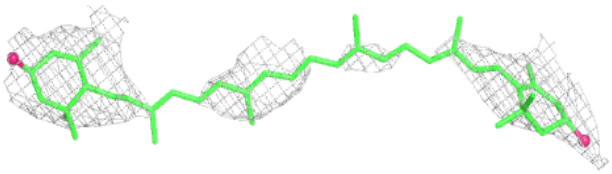


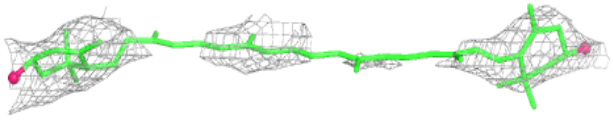


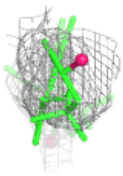


Electron density around LUT 3 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

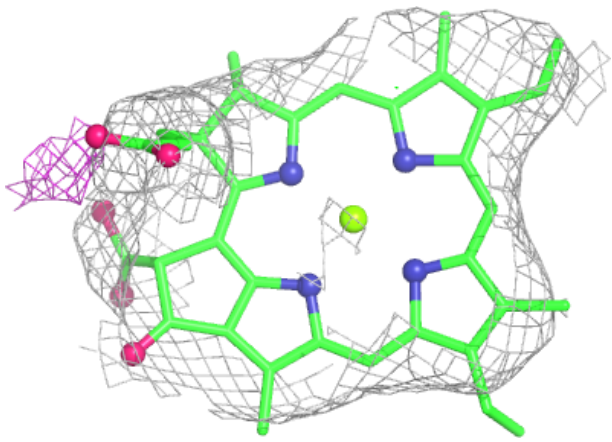


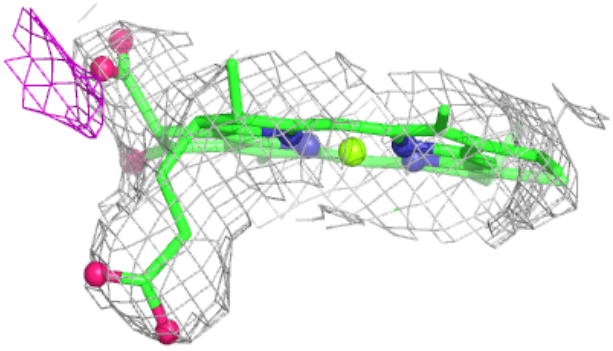


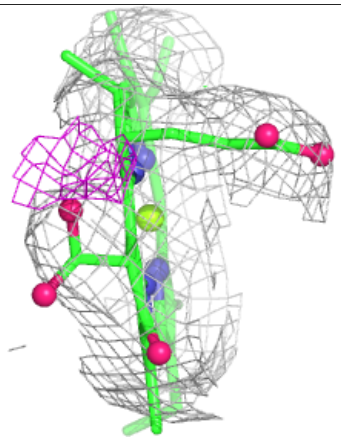


Electron density around CLA 7 1010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

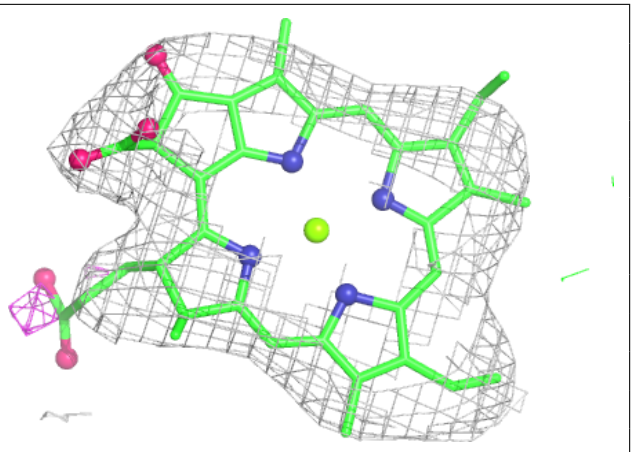


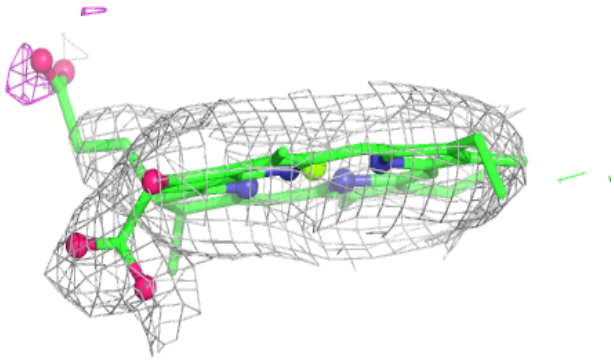


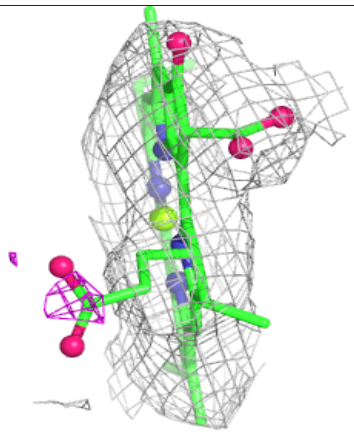


Electron density around CLA A 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

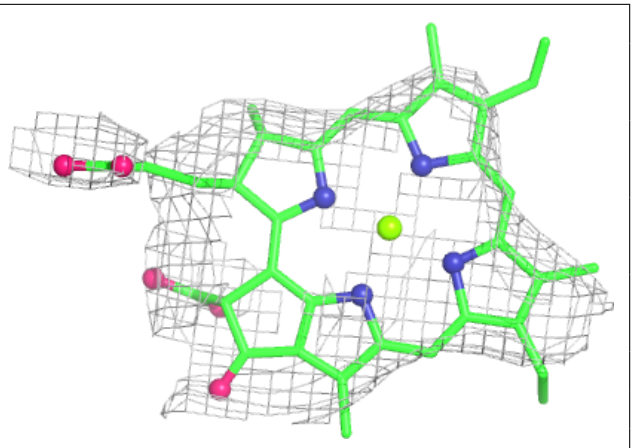


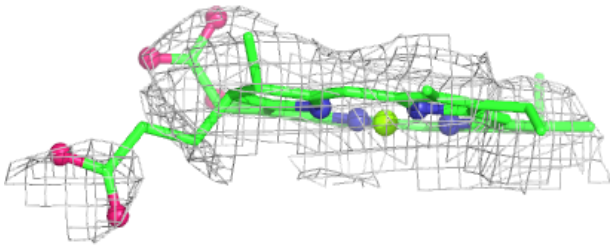


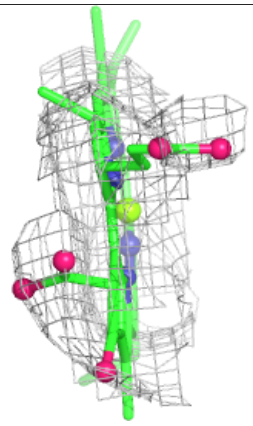


Electron density around CLA B 828:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

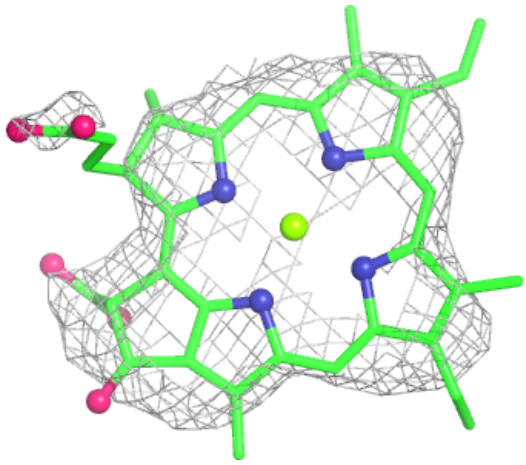


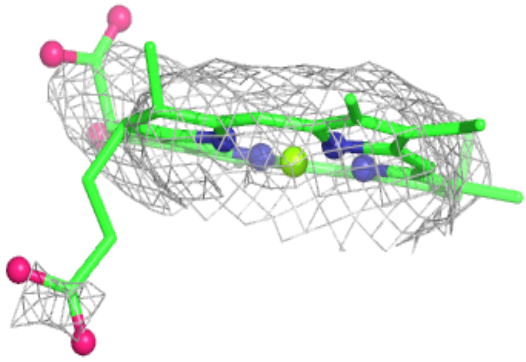


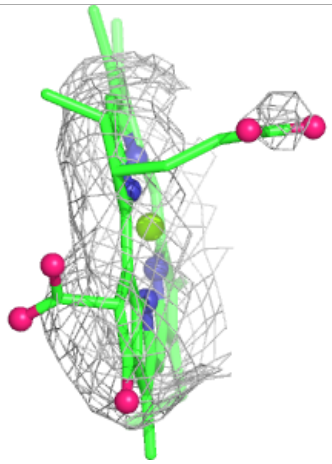


Electron density around CLA 0 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

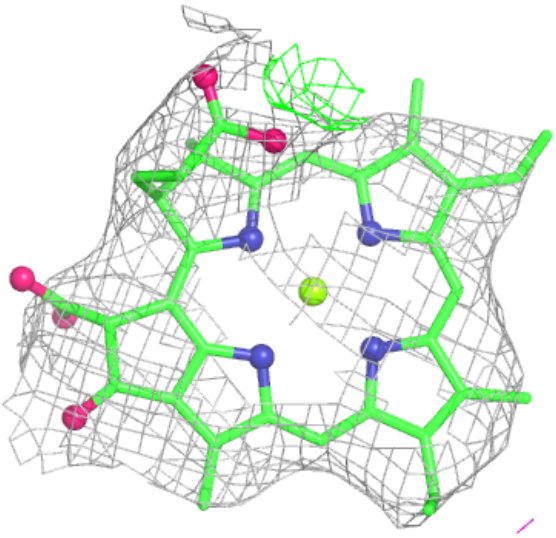


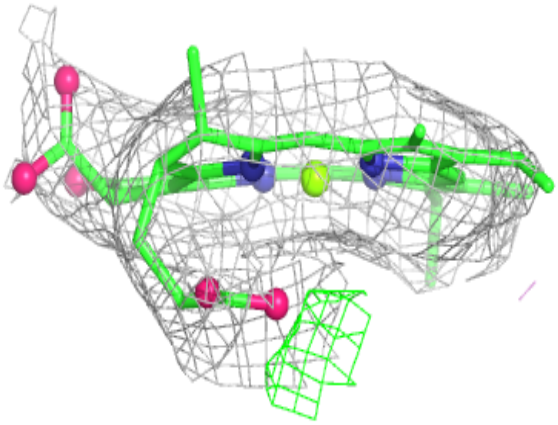


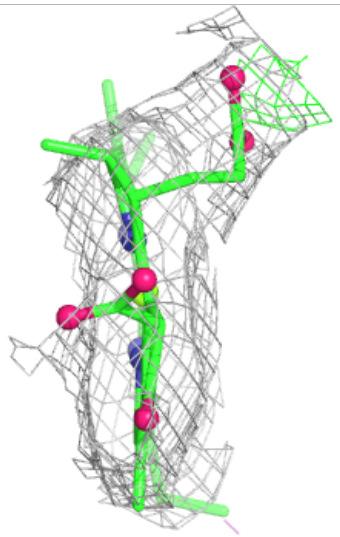


Electron density around CLA 8 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

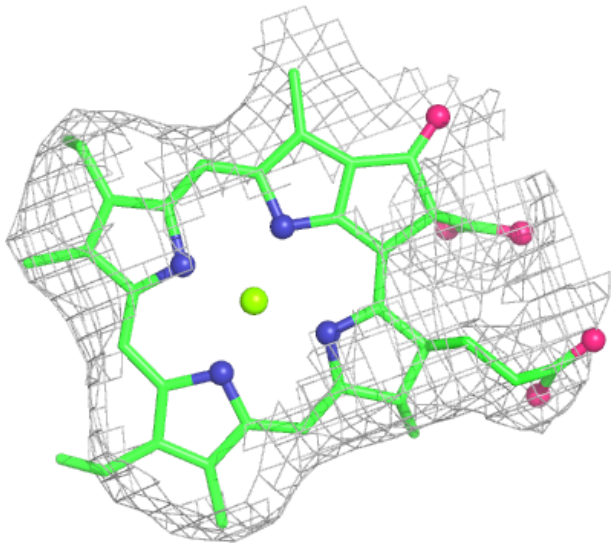


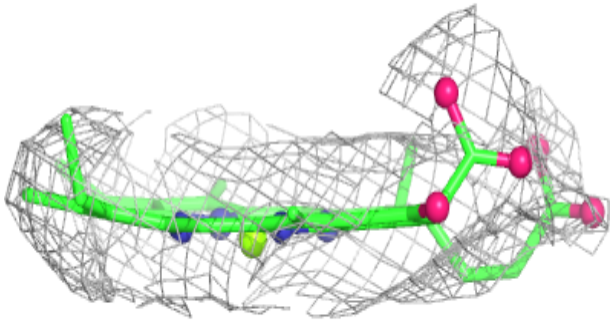




Electron density around CLA 8 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

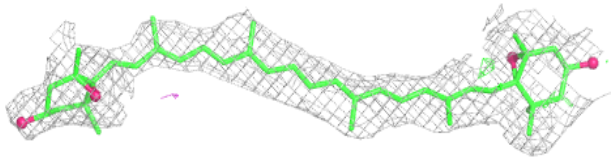


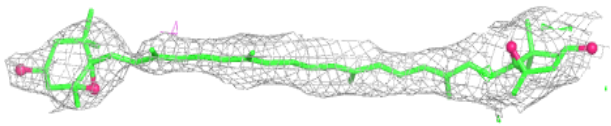


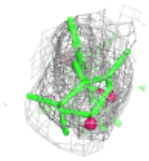


Electron density around XAT 5 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

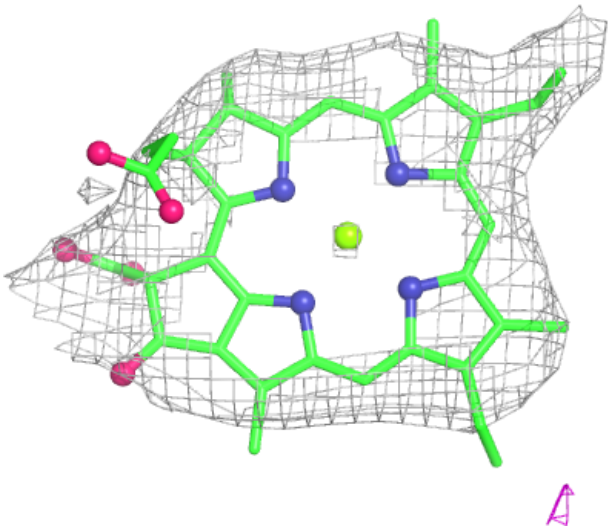


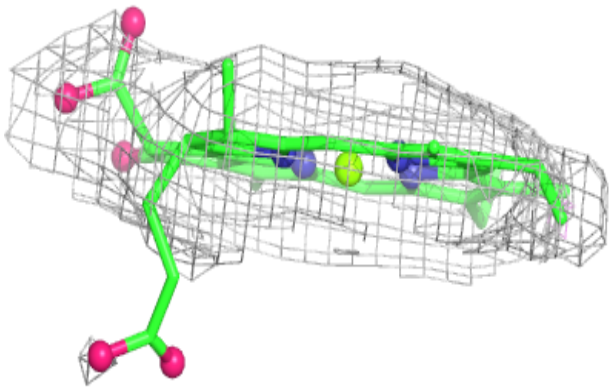


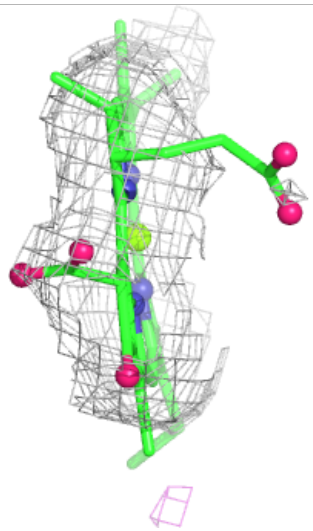


Electron density around CLA 7 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

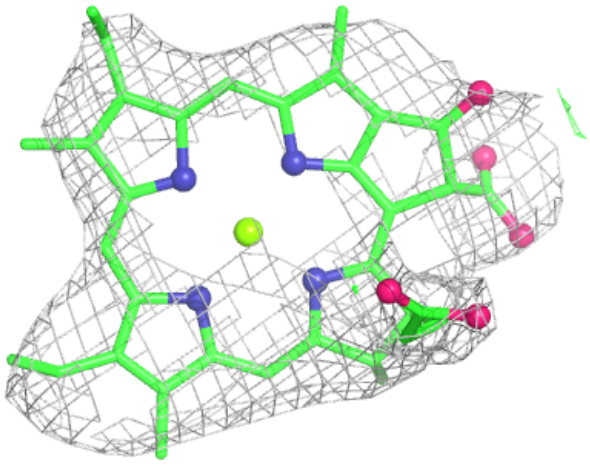


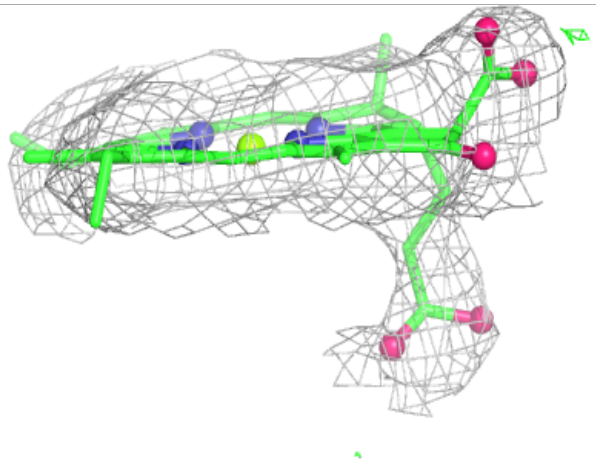


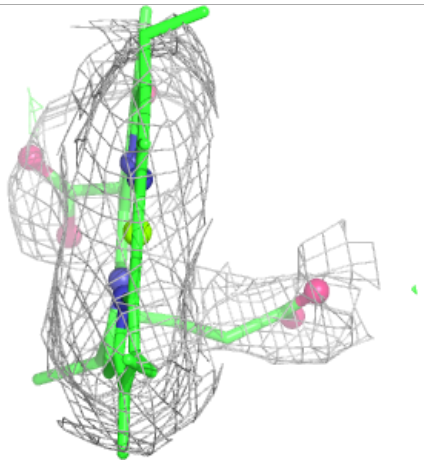


Electron density around CLA 8 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

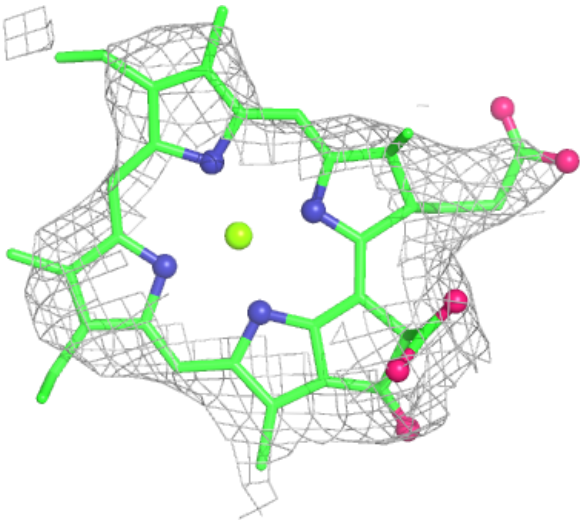


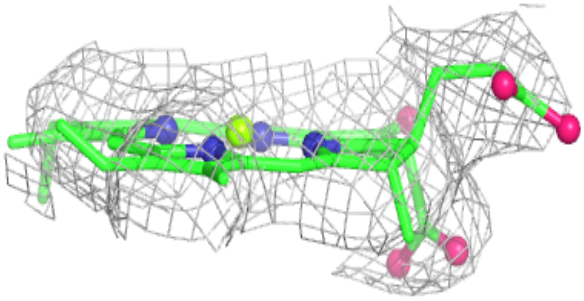


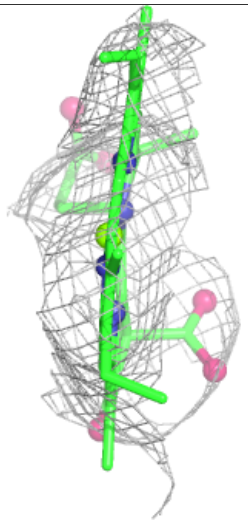


Electron density around CLA A 804:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

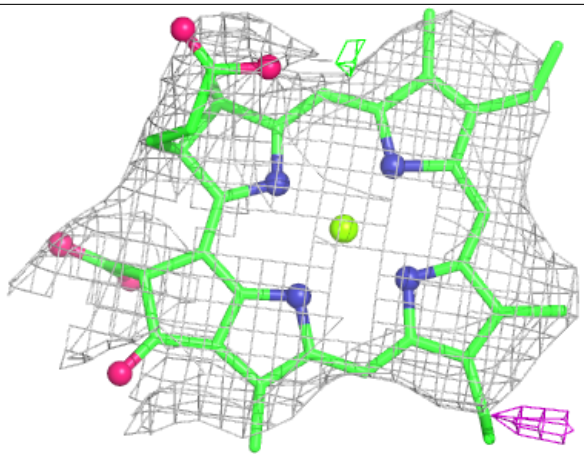


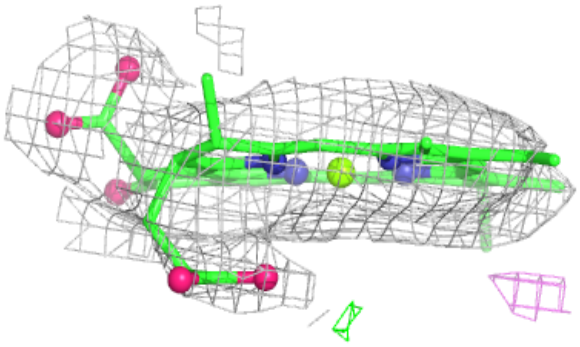


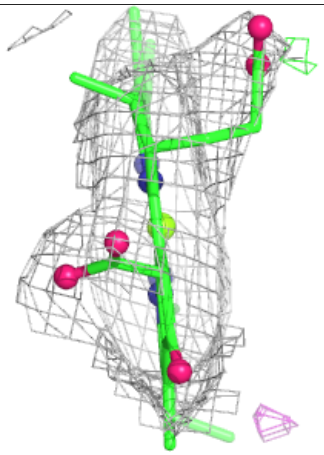


Electron density around CLA 1 1006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

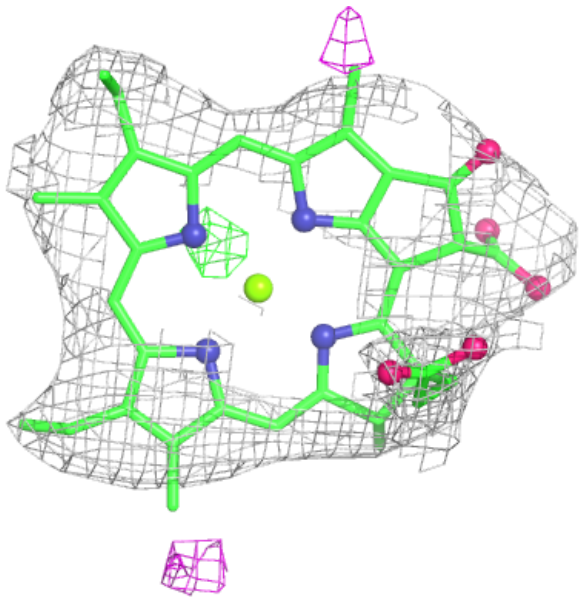




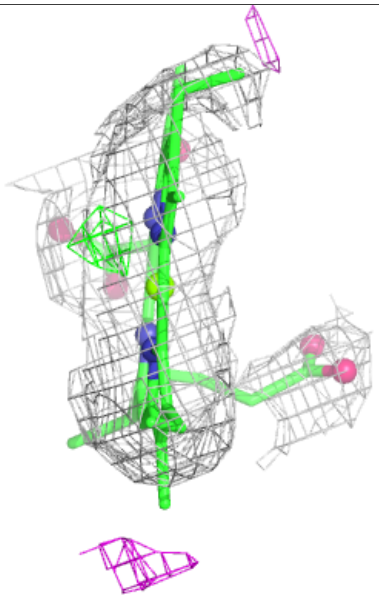


Electron density around CLA 5 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

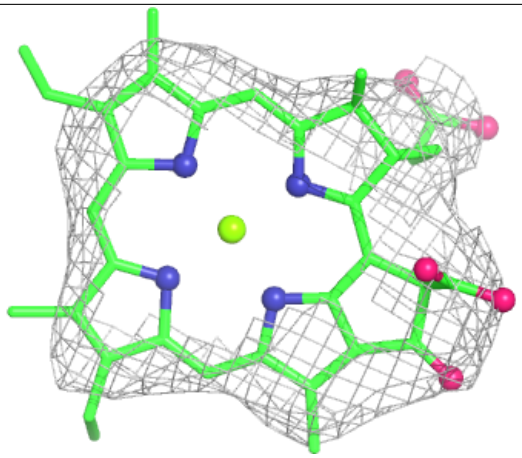


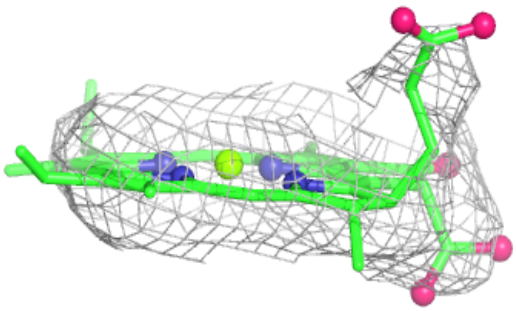


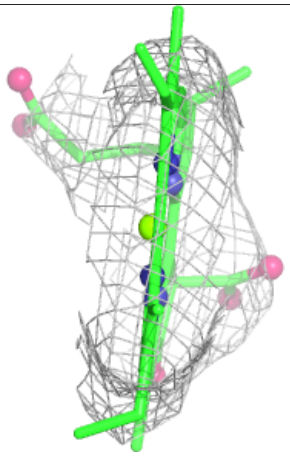


Electron density around CLA B 839:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

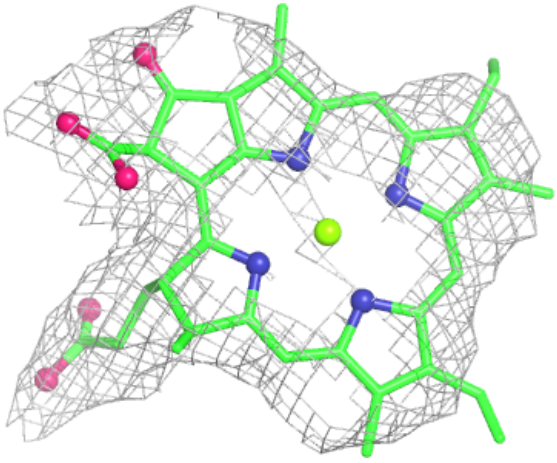


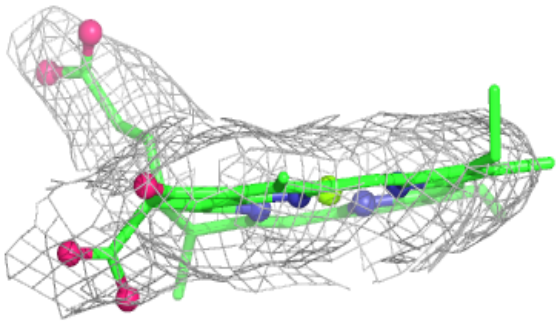


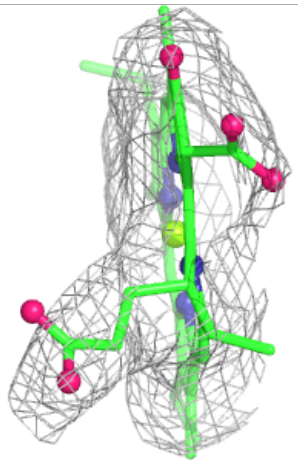


Electron density around CLA B 827:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

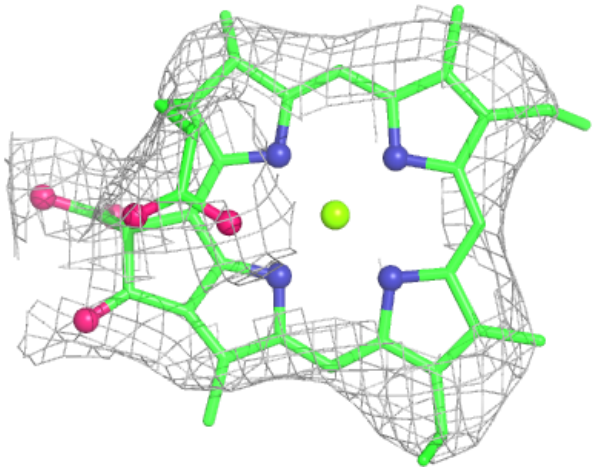


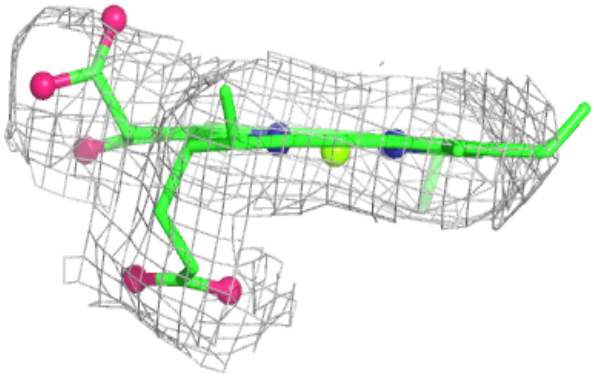


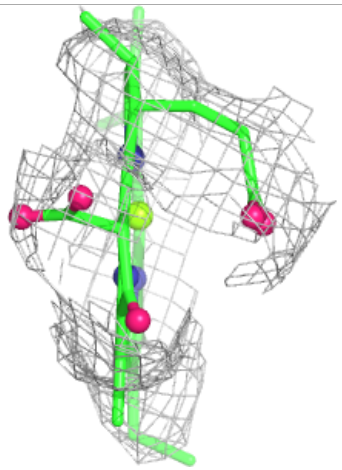


Electron density around CLA 5 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

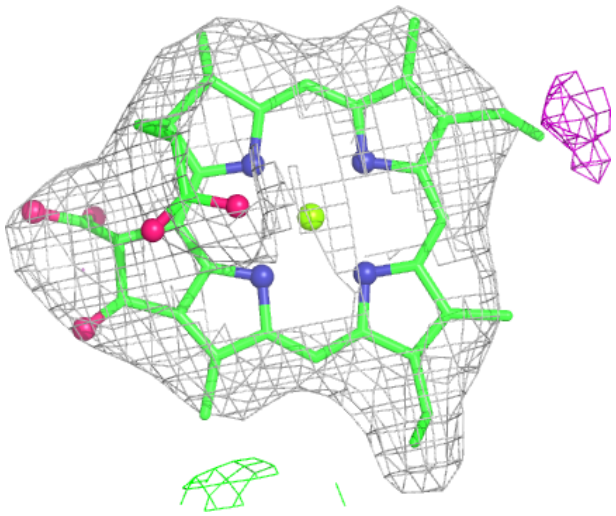


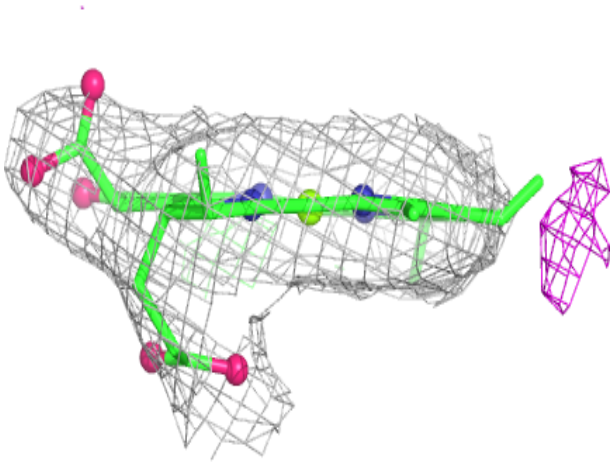


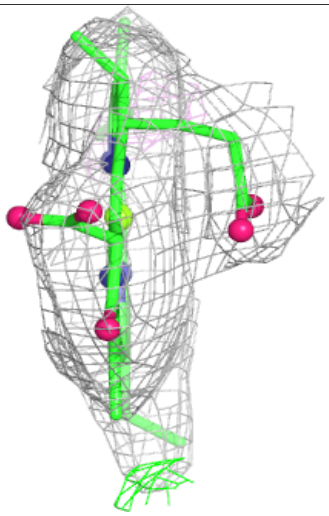


Electron density around CLA 8 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

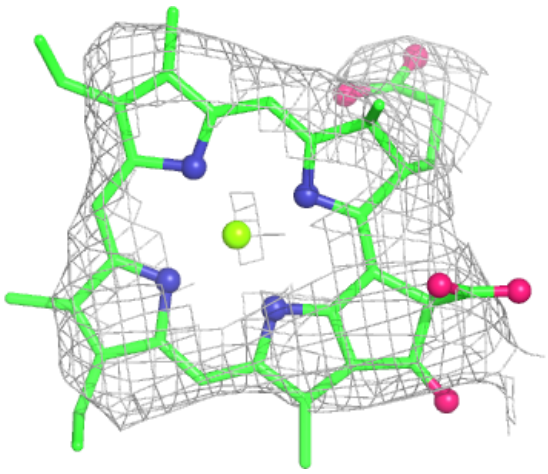


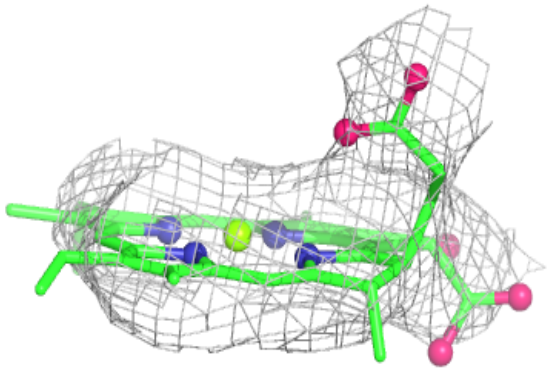


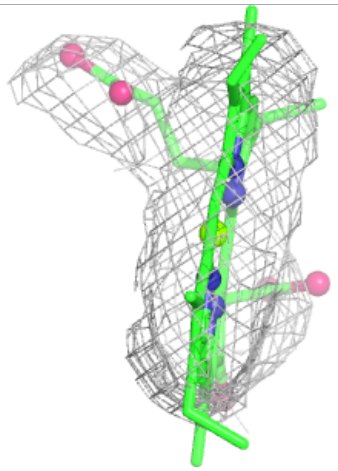


Electron density around CLA A 807:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

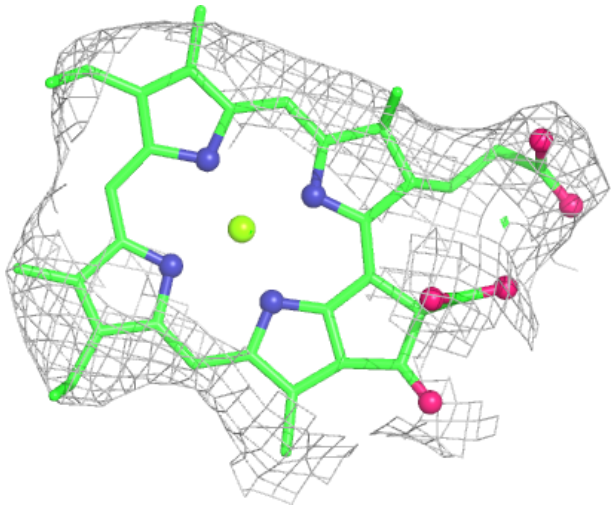


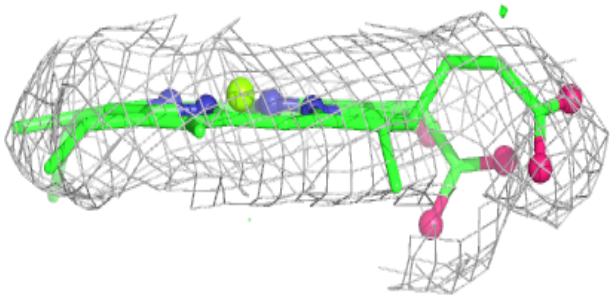




Electron density around CLA 6 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

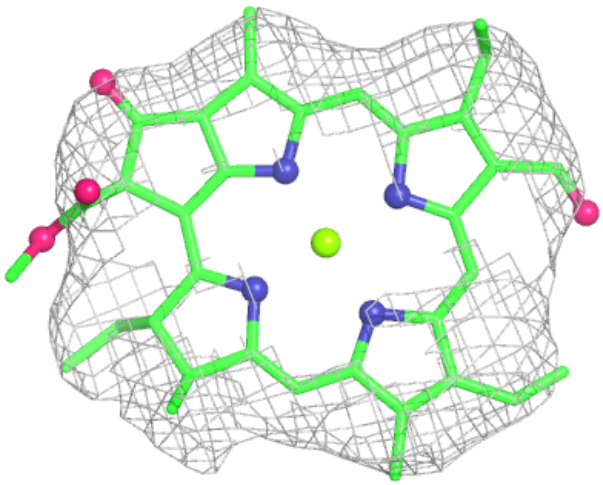


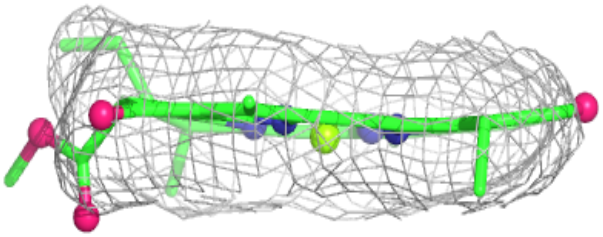


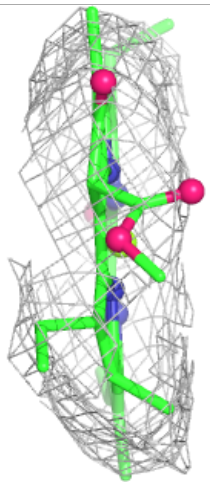


Electron density around CHL 6 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

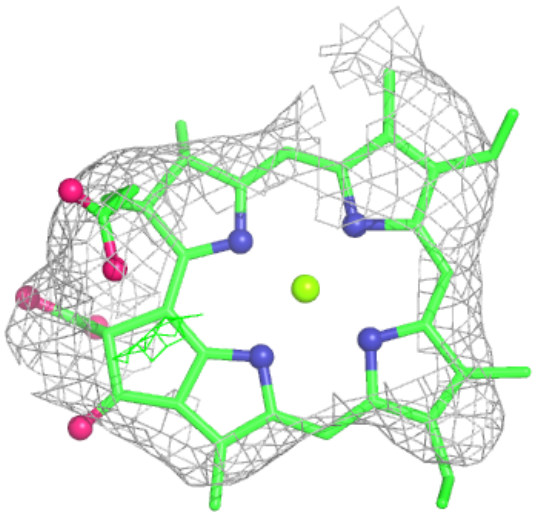


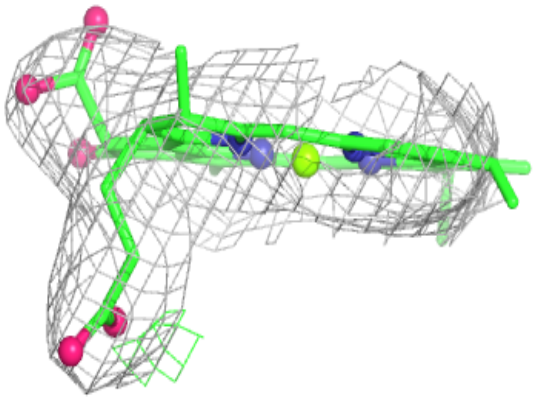


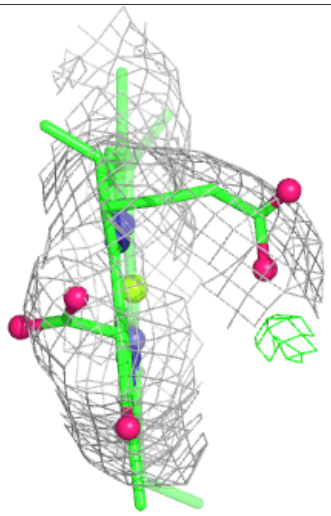


Electron density around CLA A 828:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

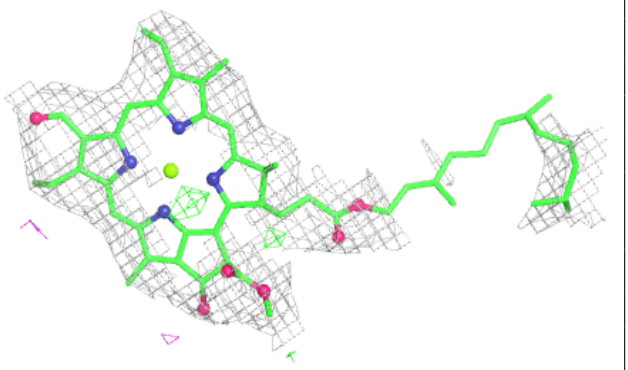


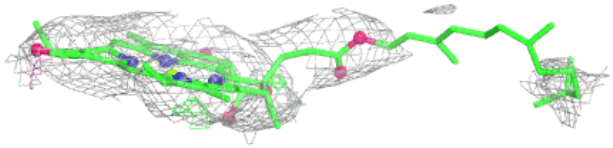


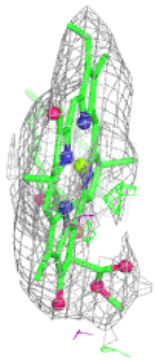


Electron density around CHL 5 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

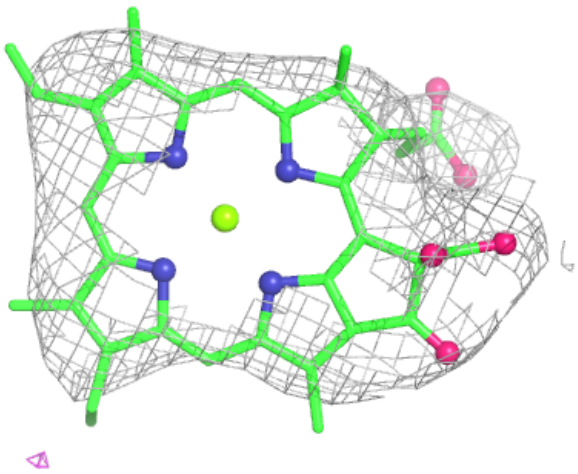


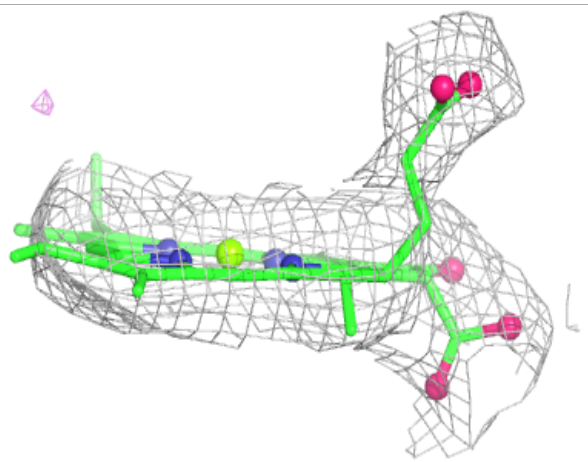


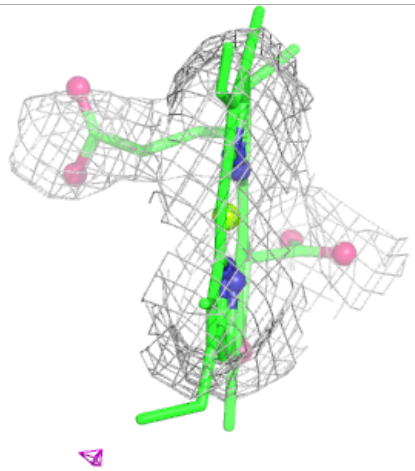


Electron density around CLA A 808:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

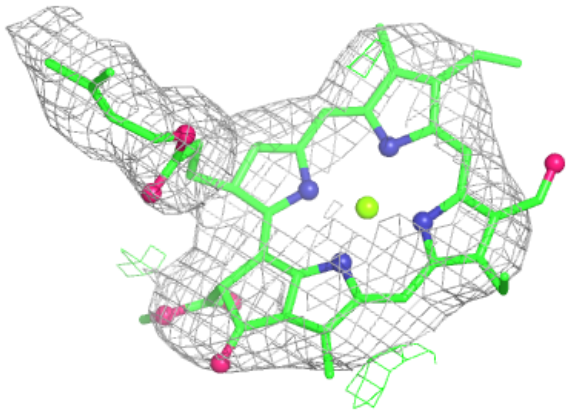


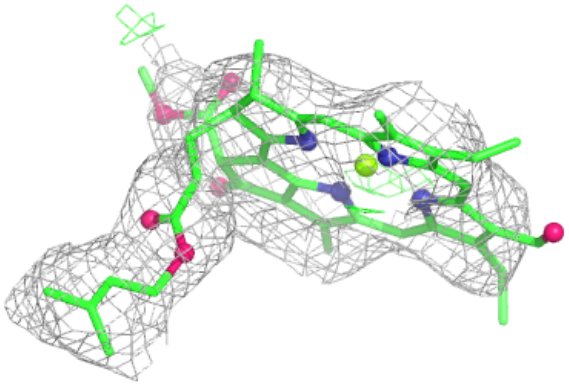


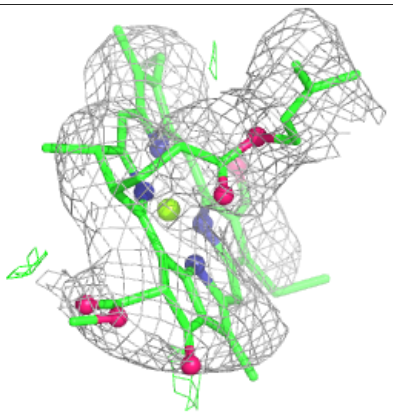


Electron density around CHL 8 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

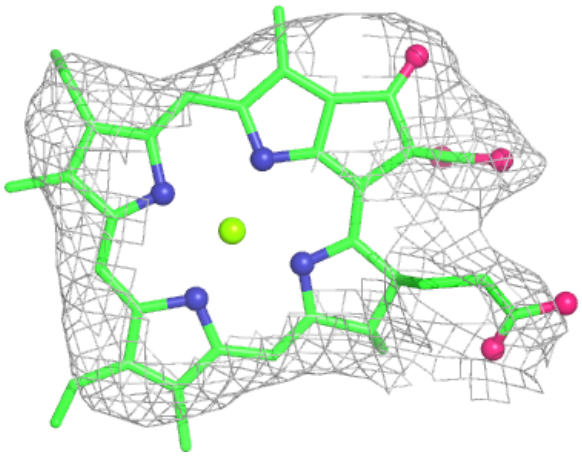


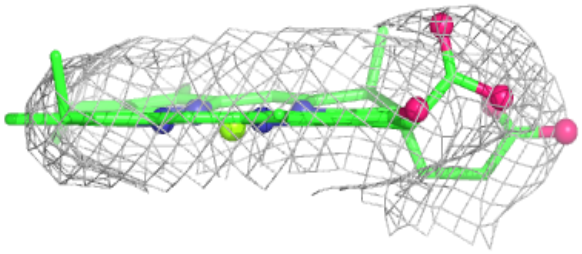


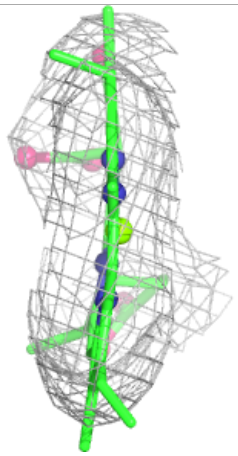


Electron density around CLA A 805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

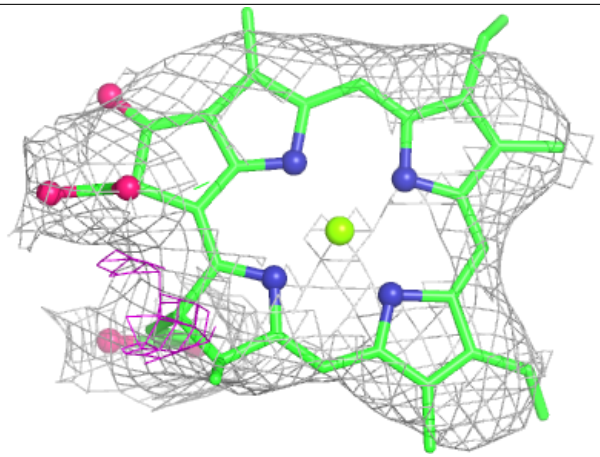


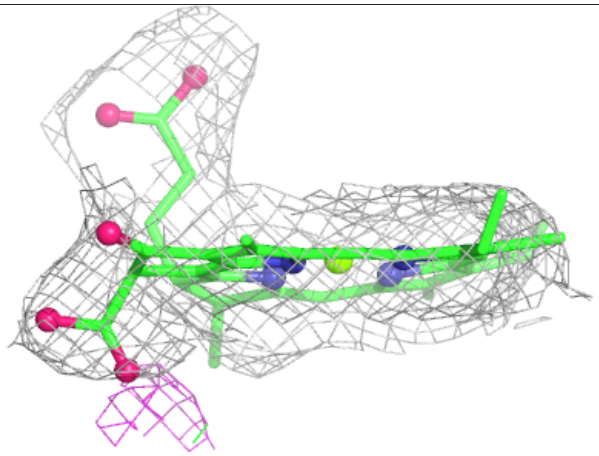


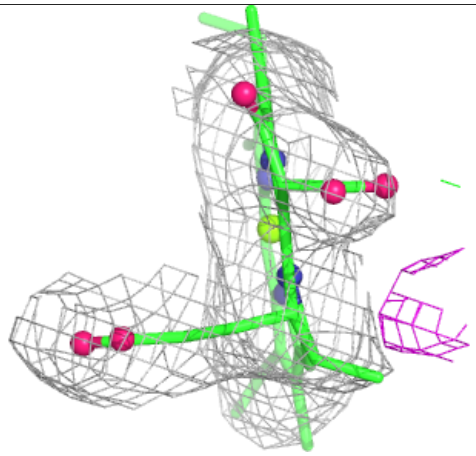


Electron density around CLA 5 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

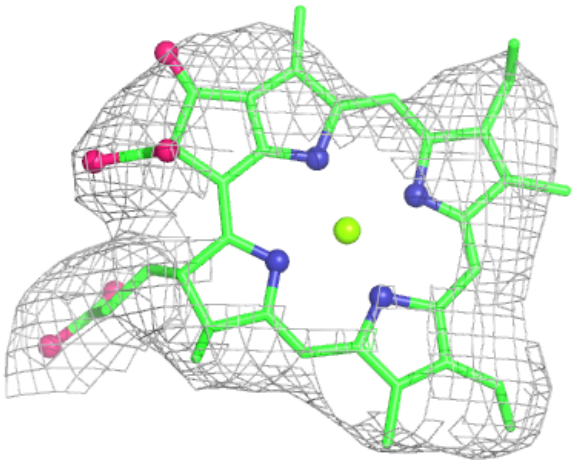


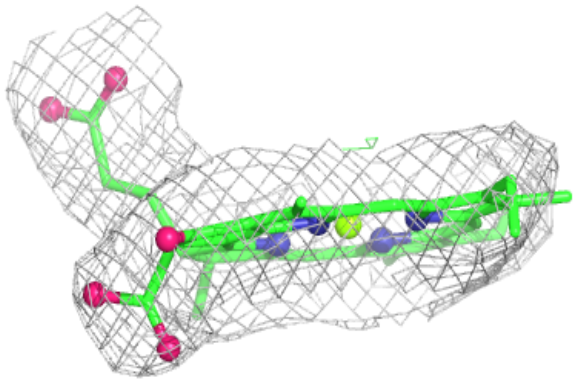


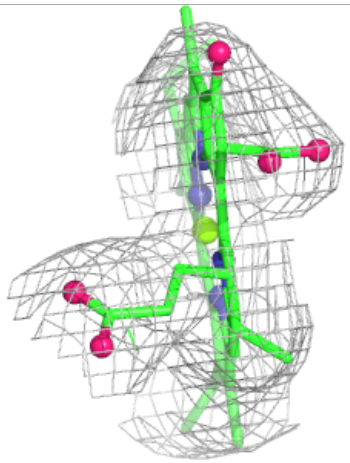


Electron density around CLA 5 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

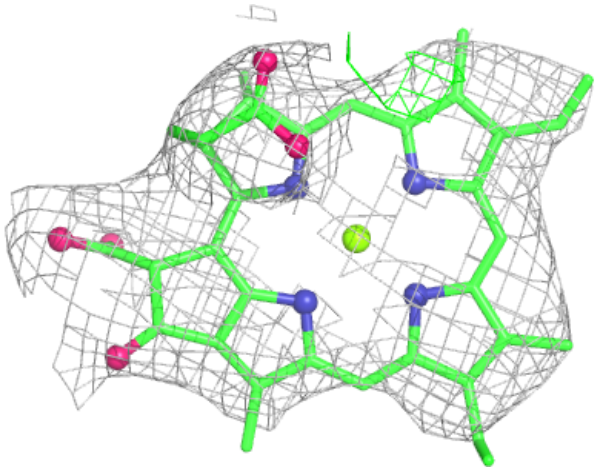


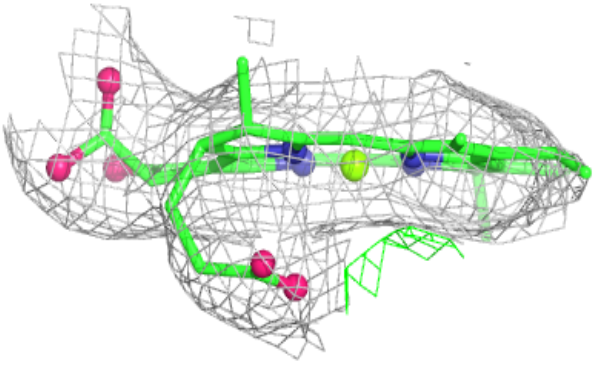


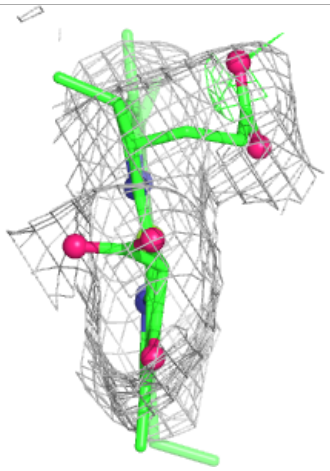


Electron density around CLA 4 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

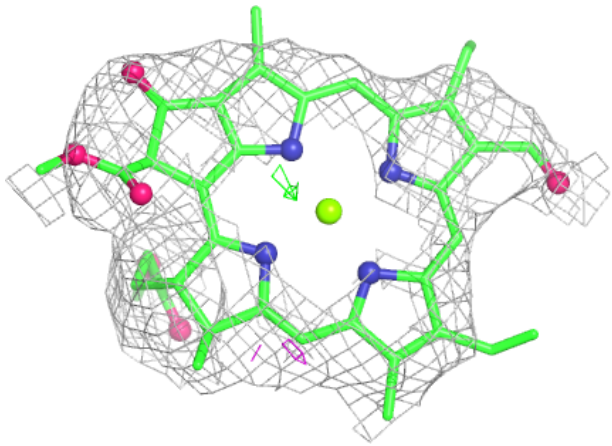


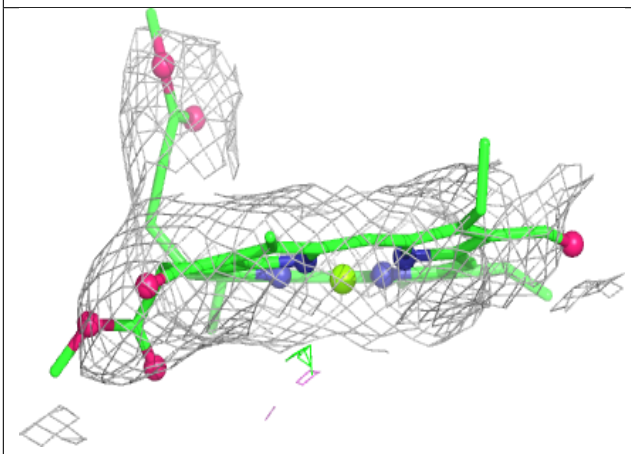


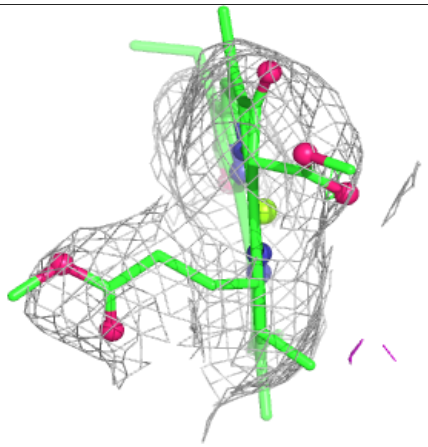


Electron density around CHL 3 1014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

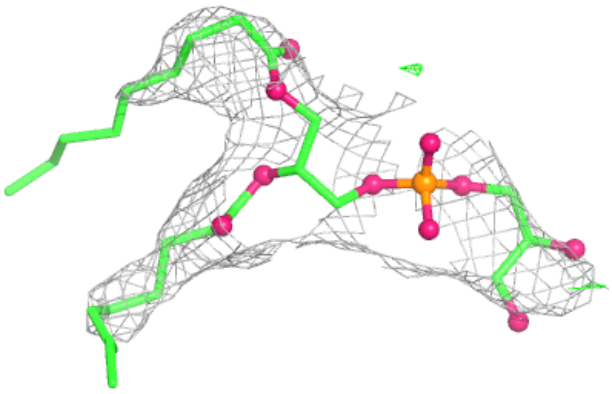


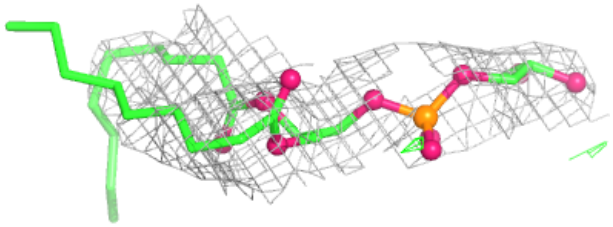


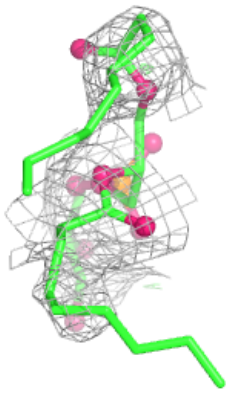


Electron density around LHG 7 1016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

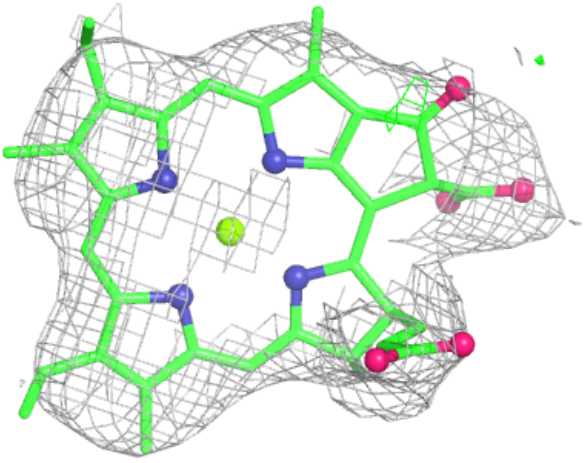


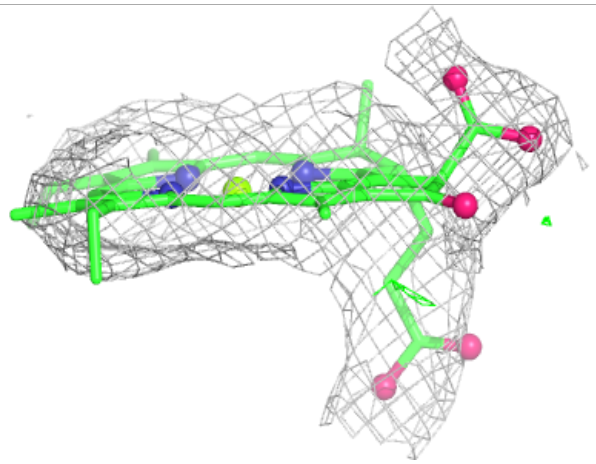


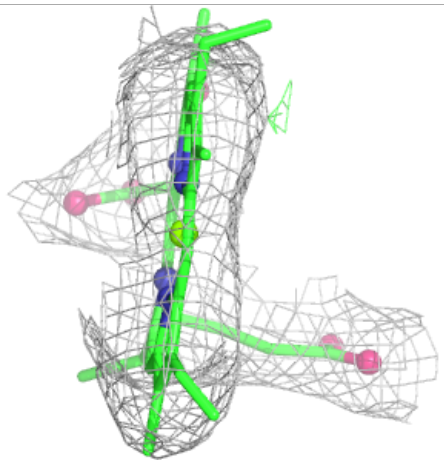


Electron density around CLA 6 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

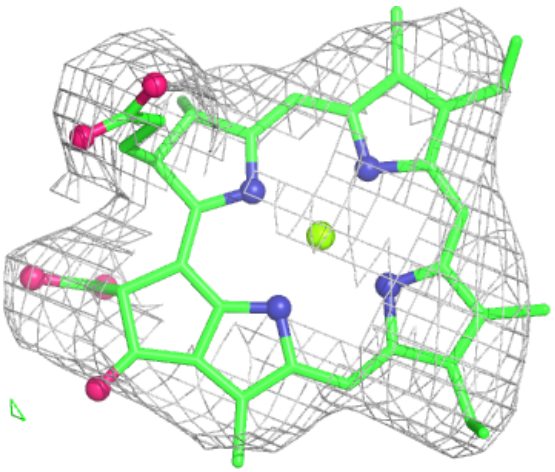


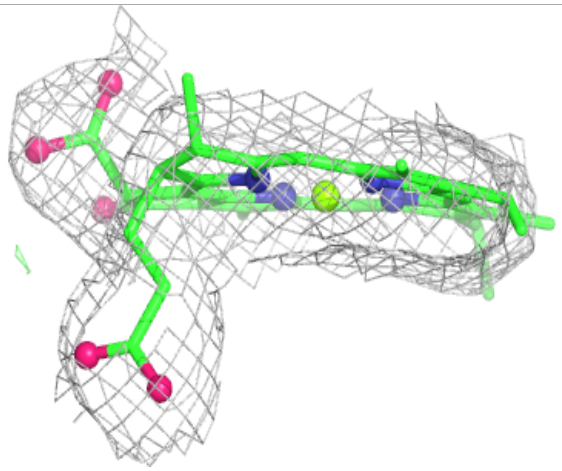




Electron density around CLA 7 1014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

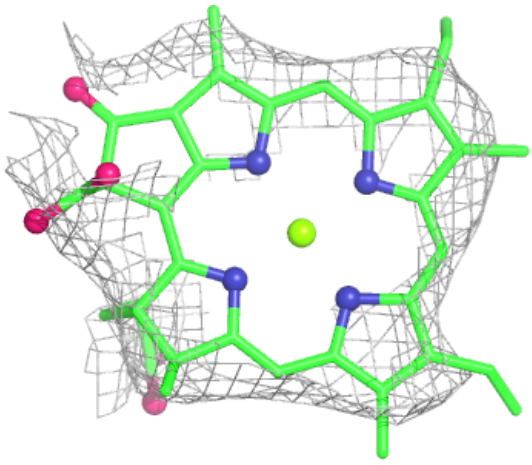


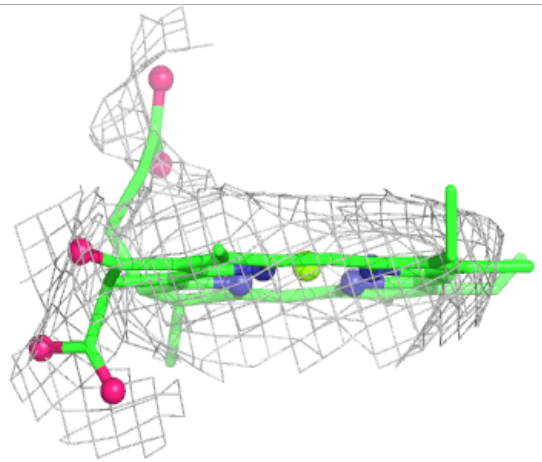


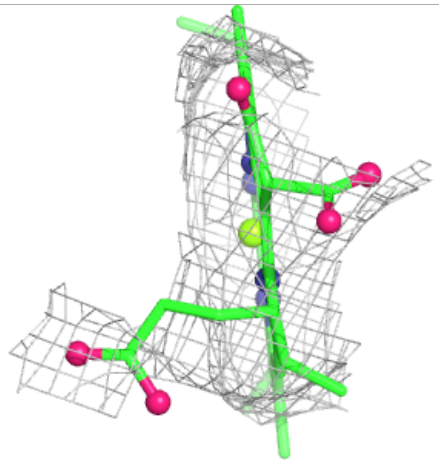


Electron density around CLA 3 1008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

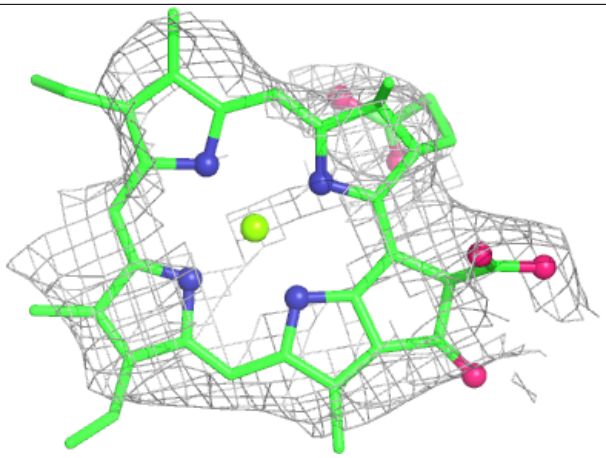


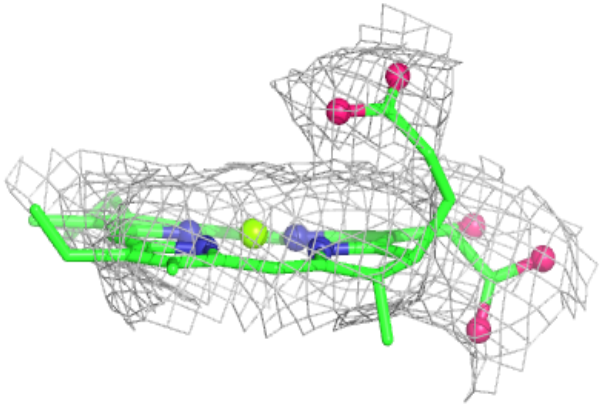




Electron density around CLA 3 1005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

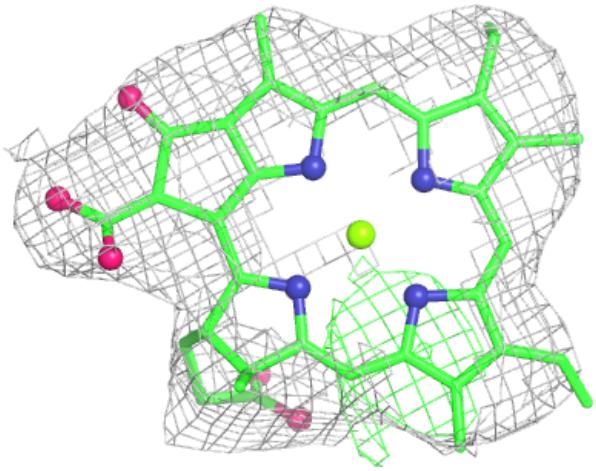


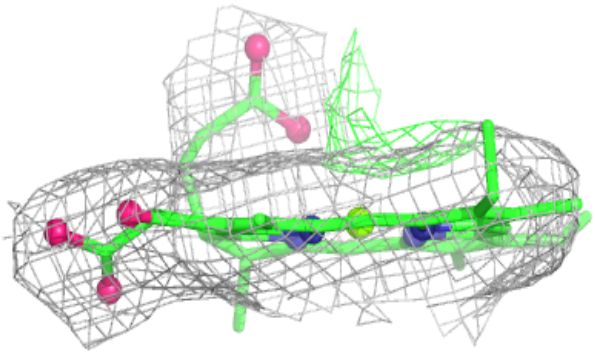


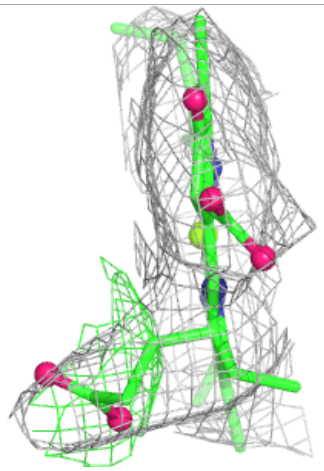


Electron density around CLA 7 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

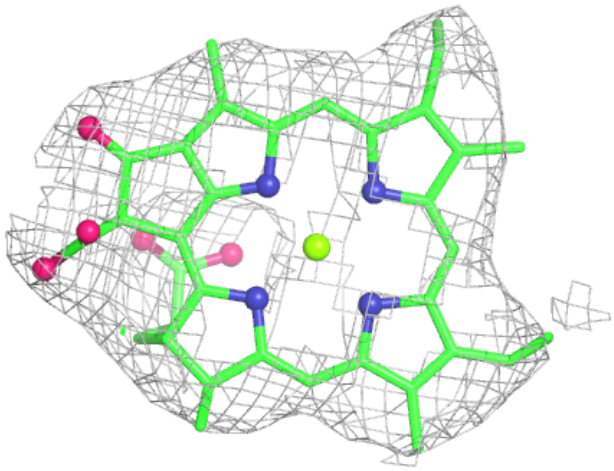


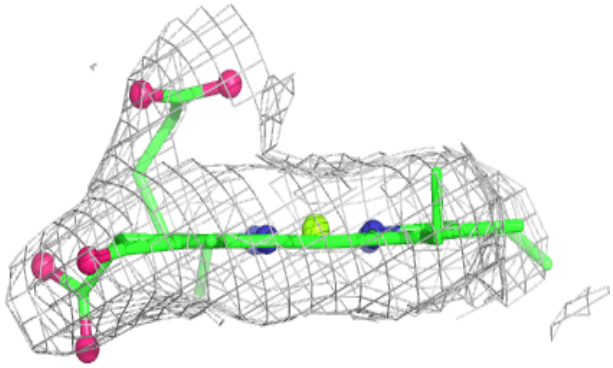


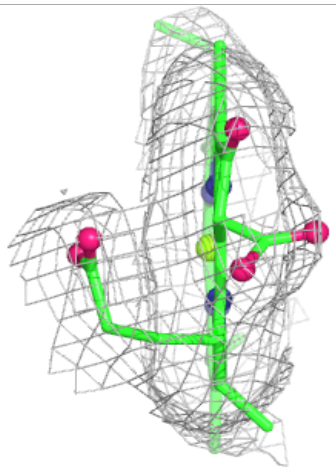


Electron density around CLA 4 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

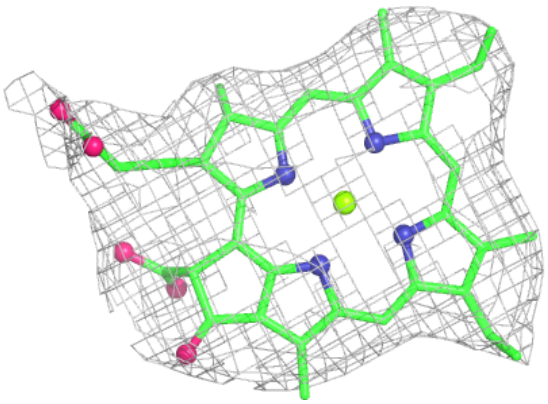


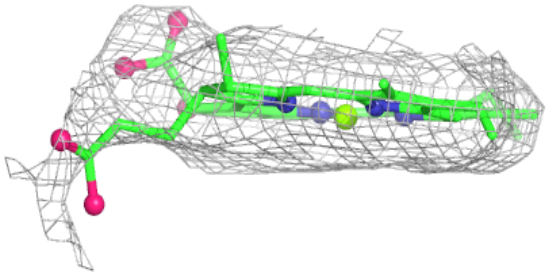


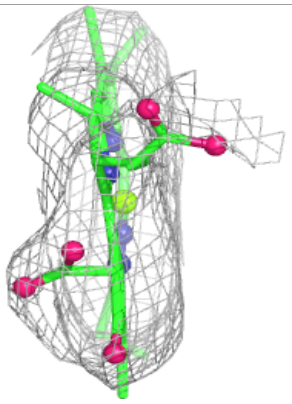


Electron density around CLA 3 1016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

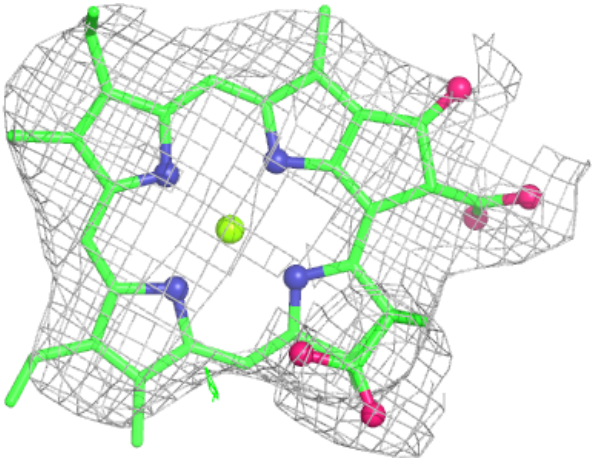


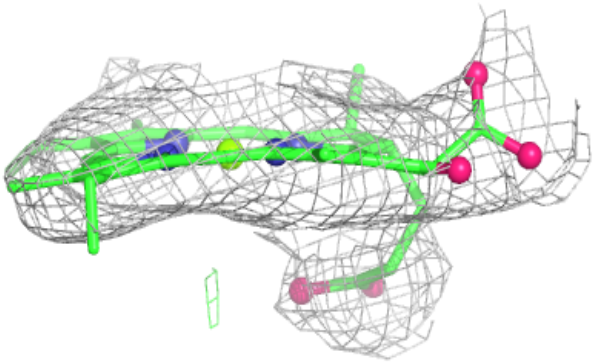




Electron density around CLA 6 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

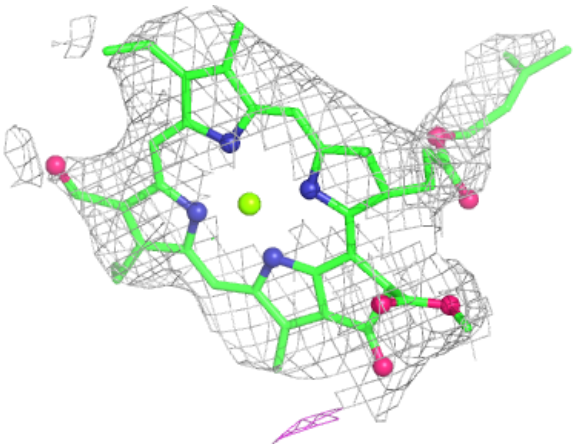


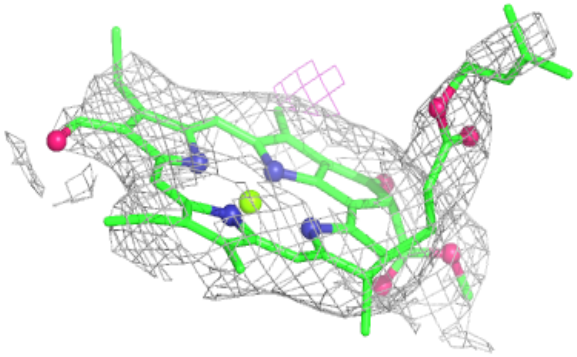


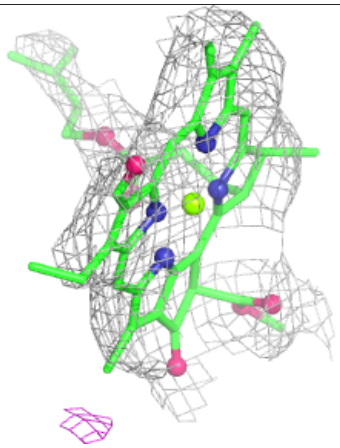


Electron density around CHL 5 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

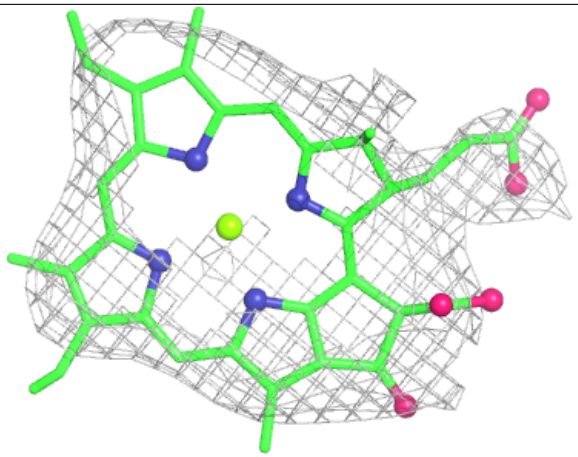


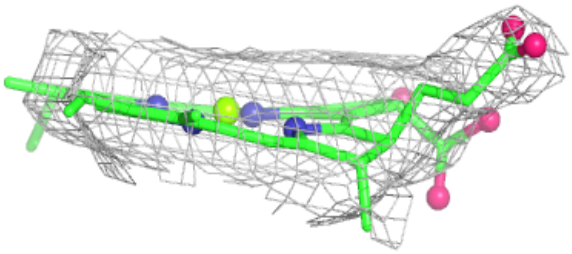


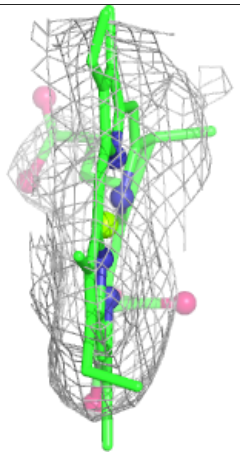


Electron density around CLA B 805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

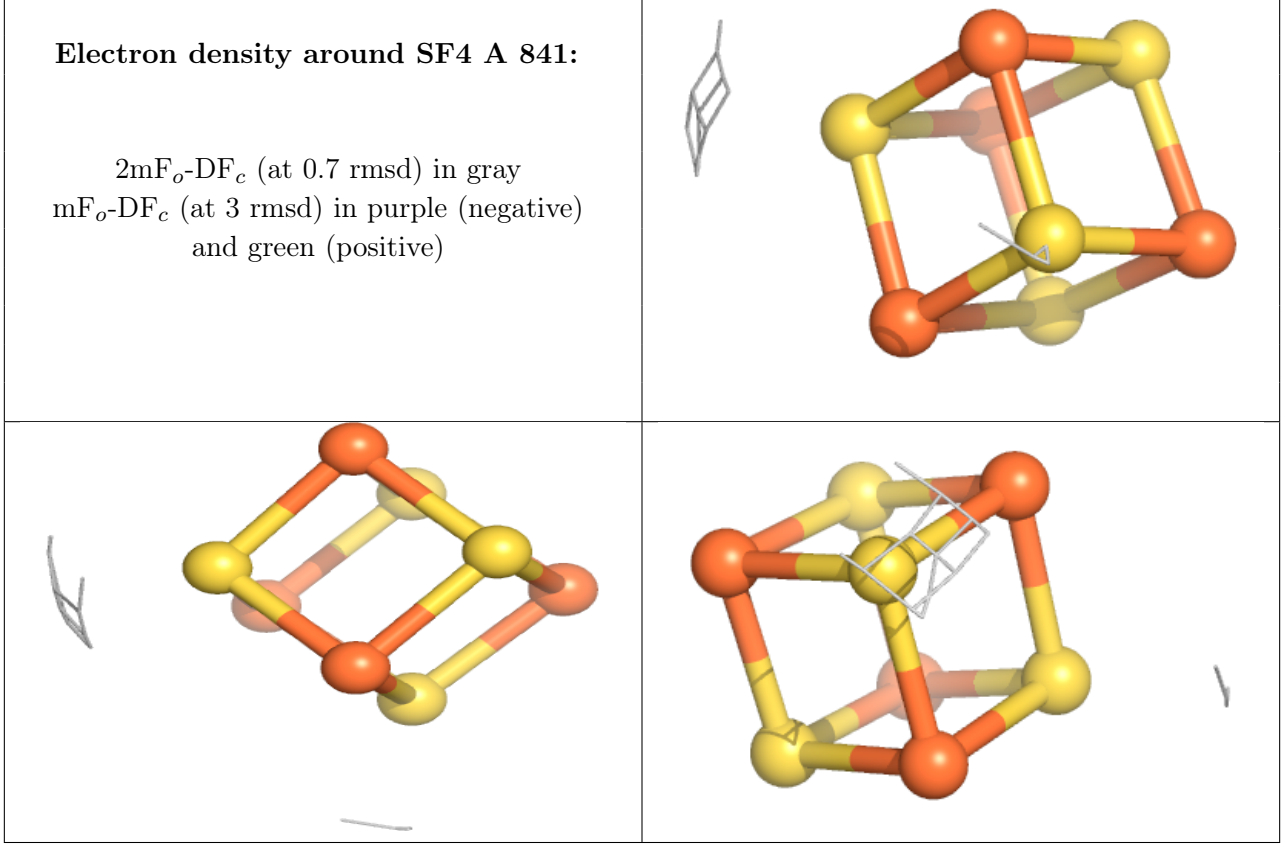






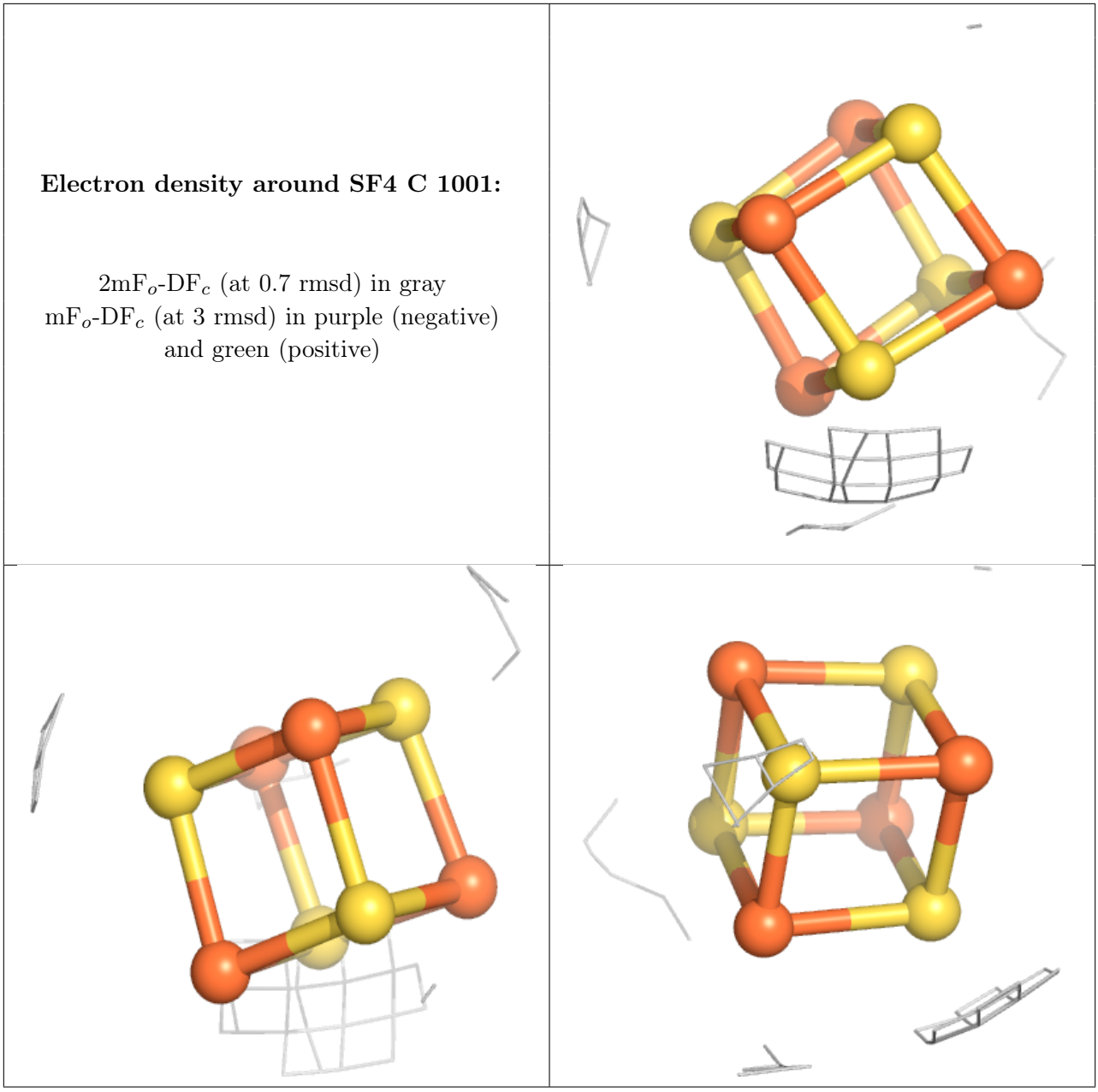
Electron density around SF4 A 841:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



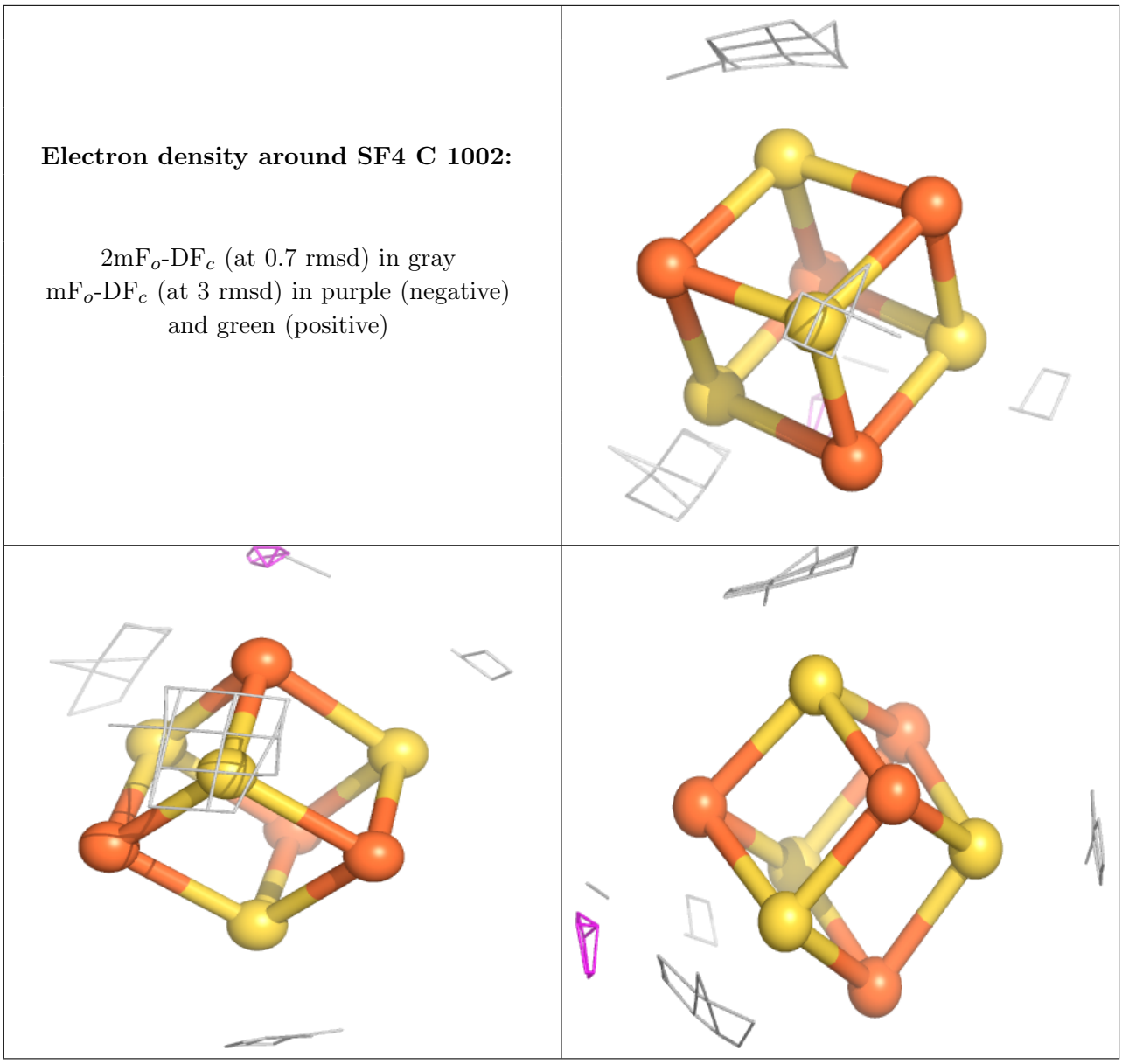
Electron density around SF4 C 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SF4 C 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.