wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2026 – 12:25 PM EDT

PDB ID	:	3LW5 / pdb_00003lw5
Title	:	Improved model of plant photosystem I
Authors	:	Nelson, N.; Toporik, H.
Deposited on	:	2010-02-23
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

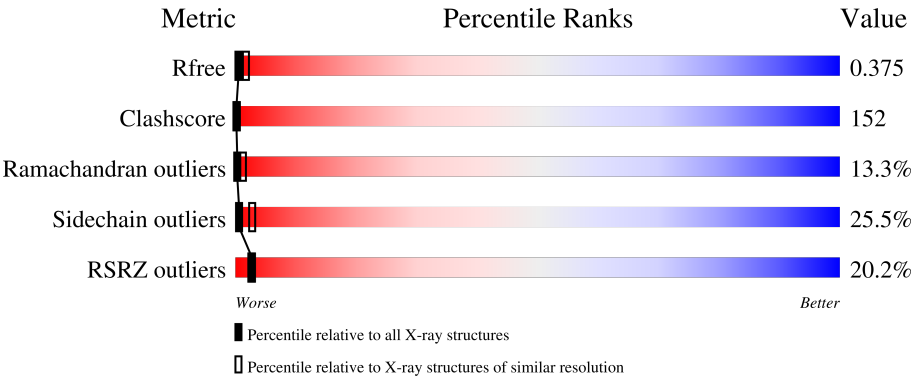
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	738	21% 7% 45% 35% 12%
2	B	733	20% 9% 44% 33% 14%
3	C	81	40% 5% 46% 33% 16%
4	D	138	17% 31% 41% 25%
5	E	64	16% 6% 34% 39% 20%

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Mol	Chain	Length	Quality of chain
6	F	154	17% 8% 36% 42% 13%
7	G	95	7% 5% 35% 36% 24%
8	H	69	7% 6% 33% 30% 30%
9	I	30	17% 67% 30%
10	J	42	14% 14% 50% 21% 14%
11	K	84	7% 11% 32% 31% 26%
12	L	161	16% 8% 36% 45% 11%
13	N	85	6% 7% 24% 35% 34%
14	R	53	28% 42% 30%
15	1	170	35% 8% 29% 35% 25%
16	2	176	23% 7% 24% 41% 27%
17	3	172	11% 9% 25% 37% 19% 9%
18	4	166	32% 6% 39% 36% 20%

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
19	CLA	1	1007	X	-	-	-
19	CLA	1	1008	X	-	-	-
19	CLA	1	1013	X	-	-	-
19	CLA	1	1014	X	-	-	-
19	CLA	1	1303	X	-	-	-
19	CLA	2	2002	X	-	-	-
19	CLA	2	2006	X	-	-	-
19	CLA	2	2007	X	-	-	-
19	CLA	2	2014	X	-	X	-
19	CLA	2	4009	X	-	-	-
19	CLA	3	2009	X	-	X	-
19	CLA	3	3011	X	-	-	-
19	CLA	3	3013	X	-	-	-
19	CLA	3	3016	X	-	-	-
19	CLA	4	1004	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	1304	X	-	X	-
19	CLA	4	1306	X	-	-	-
19	CLA	4	4002	X	-	X	-
19	CLA	4	4003	X	-	-	-
19	CLA	4	4006	X	-	-	-
19	CLA	A	1102	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1104	X	-	-	-
19	CLA	A	1105	-	-	X	-
19	CLA	A	1106	X	-	X	-
19	CLA	A	1107	X	-	X	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1112	-	-	X	-
19	CLA	A	1115	X	-	X	-
19	CLA	A	1117	X	-	X	-
19	CLA	A	1119	X	-	X	-
19	CLA	A	1122	X	-	X	-
19	CLA	A	1123	X	-	X	-
19	CLA	A	1124	X	-	X	-
19	CLA	A	1125	X	-	X	-
19	CLA	A	1126	X	-	X	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	-	-
19	CLA	A	1131	X	-	X	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	-	-	X	-
19	CLA	A	1134	-	-	X	-
19	CLA	A	1135	-	-	X	-
19	CLA	A	1136	X	-	X	-
19	CLA	A	1138	X	-	X	-
19	CLA	A	1139	-	-	X	-
19	CLA	A	1140	X	-	X	-
19	CLA	A	1141	X	-	X	-
19	CLA	A	1149	X	-	-	-
19	CLA	A	1237	X	-	X	-
19	CLA	A	9011	X	-	-	-
19	CLA	A	9012	X	-	X	-
19	CLA	A	9013	X	-	X	-
19	CLA	A	9022	X	-	X	-
19	CLA	A	9023	X	-	X	-
19	CLA	B	1202	X	-	X	-
19	CLA	B	1203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1205	X	-	X	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	X	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-
19	CLA	B	1214	X	-	X	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	-	-	X	-
19	CLA	B	1221	-	-	X	-
19	CLA	B	1222	X	-	X	-
19	CLA	B	1223	X	-	X	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	X	-
19	CLA	B	1226	X	-	X	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	X	-
19	CLA	B	1236	-	-	X	-
19	CLA	B	1238	X	-	-	-
19	CLA	B	1239	X	-	X	-
19	CLA	B	9010	X	-	-	-
19	CLA	F	1305	X	-	-	-
19	CLA	H	1145	X	-	X	-
19	CLA	H	1207	X	-	X	-
19	CLA	H	1241	X	-	-	-
19	CLA	H	1505	X	-	-	-
19	CLA	I	1204	X	-	-	-
19	CLA	J	1308	X	-	X	-
19	CLA	J	1311	X	-	-	-
19	CLA	K	1143	-	-	X	-
19	CLA	K	3009	X	-	-	-
19	CLA	L	1130	X	-	X	-
19	CLA	L	1148	X	-	X	-
19	CLA	L	1502	-	-	X	-
19	CLA	L	1503	X	-	-	-
19	CLA	L	1504	X	-	-	-
19	CLA	R	1144	X	-	-	-
19	CLA	R	1150	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	PQN	A	5001	X	-	-	-
20	PQN	B	5002	X	-	X	-
21	BCR	A	6002	-	-	X	-
21	BCR	A	6007	-	-	X	-
21	BCR	A	6008	-	-	X	-
21	BCR	A	6011	-	-	X	-
21	BCR	B	6010	-	-	X	-
21	BCR	B	6017	-	-	X	-
21	BCR	B	6020	-	-	X	-
21	BCR	F	6014	-	-	X	-
21	BCR	F	6016	-	-	X	-
21	BCR	I	6021	-	-	X	-
21	BCR	J	6012	-	-	X	-
21	BCR	L	6019	-	-	X	-
22	LMU	3	7005	-	-	X	-
22	LMU	4	7034	-	-	X	-
22	LMU	4	7052	-	-	X	-
22	LMU	D	7050	-	-	X	-
23	SF4	A	8001	-	-	X	-
23	SF4	C	8002	-	-	X	-
23	SF4	C	8003	-	-	X	-

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 36370 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	730	Total	C	N	O	S	0	0	0
			5739	3762	974	985	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5844	3841	997	993	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 4 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1097	704	191	199	3			

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	64	Total	C	N	O	0	0	0
			513	327	90	96			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	0	0	0
			738	481	120	137			

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	69	Total	C	N	O	0	0	0
			517	334	80	103			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			334	228	51	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	84	Total	C	N	O	S	0	0	0
			592	377	102	110	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	161	Total	C	N	O	S	0	0	0
			1209	797	192	219	1			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 14 is a protein called CHAIN R.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 15 is a protein called AT3g54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	165	Total	C	N	O	S	0	0	0
			1257	816	208	229	4			

- Molecule 16 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	2	176	Total	C	N	O	S	0	0	0
			1367	895	223	245	4			

- Molecule 17 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	3	156	Total	C	N	O	S	0	0	0
			1197	784	199	209	5			

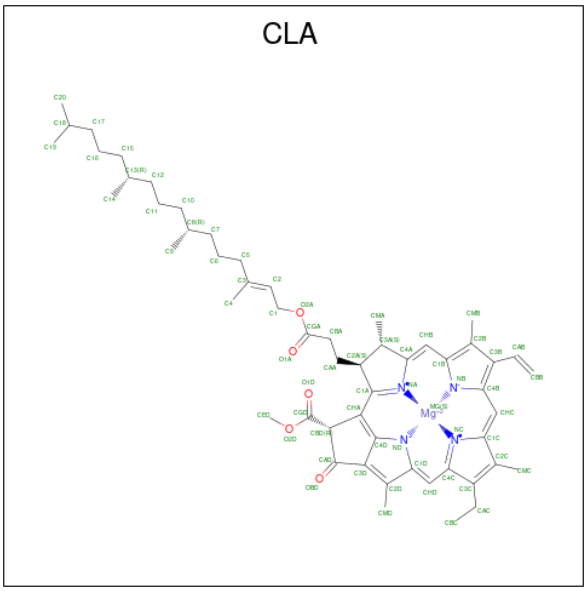
- Molecule 18 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	4	166	Total	C	N	O	S	0	0	0
			1309	856	216	234	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	SEE REMARK 999	UNP Q9SQL2

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	1	1	Total C Mg N O 61 51 1 4 5	0	0
19	1	1	Total C Mg N 25 20 1 4	0	0
19	1	1	Total C Mg N O 51 41 1 4 5	0	0
19	1	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N O 51 41 1 4 5	0	0
19	2	1	Total C Mg N O 56 46 1 4 5	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N O 50 40 1 4 5	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N O 65 55 1 4 5	0	0
19	2	1	Total C Mg N O 65 55 1 4 5	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N 25 20 1 4	0	0
19	2	1	Total C Mg N O 50 40 1 4 5	0	0
19	2	1	Total C Mg N O 50 40 1 4 5	0	0
19	2	1	Total C Mg N O 61 51 1 4 5	0	0
19	2	1	Total C Mg N O 65 55 1 4 5	0	0
19	3	1	Total C Mg N O 36 30 1 4 1	0	0
19	3	1	Total C Mg N O 46 36 1 4 5	0	0

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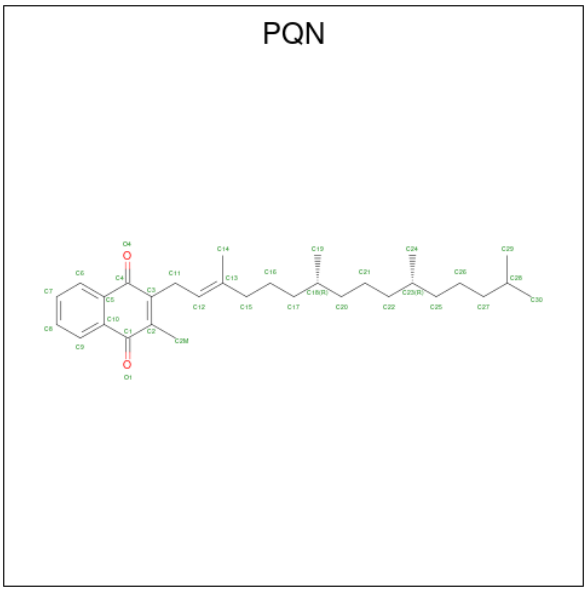
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	3	1	Total C Mg N O 56 46 1 4 5	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N O 36 30 1 4 1	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N O 42 34 1 4 3	0	0
19	3	1	Total C Mg N O 50 40 1 4 5	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N O 65 55 1 4 5	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N O 65 55 1 4 5	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N 25 20 1 4	0	0
19	3	1	Total C Mg N O 65 55 1 4 5	0	0
19	3	1	Total C Mg N O 50 40 1 4 5	0	0
19	4	1	Total C Mg N O 55 45 1 4 5	0	0
19	4	1	Total C Mg N O 36 30 1 4 1	0	0
19	4	1	Total C Mg N O 65 55 1 4 5	0	0
19	4	1	Total C Mg N O 55 45 1 4 5	0	0

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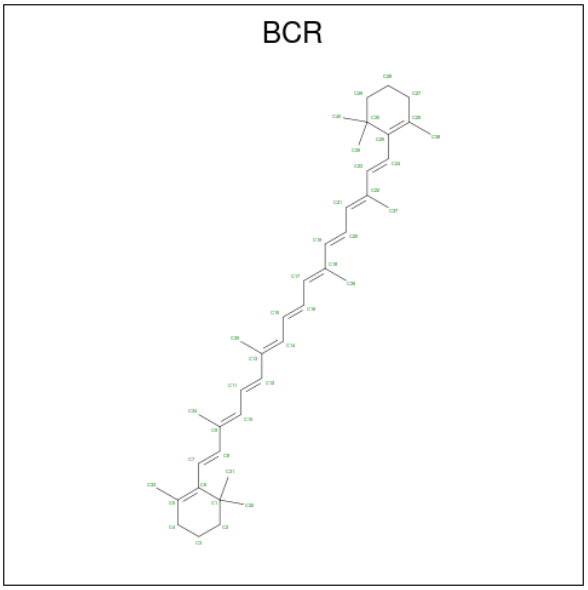
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	4	1	Total C Mg N O 50 40 1 4 5	0	0
19	4	1	Total C Mg N O 52 42 1 4 5	0	0
19	4	1	Total C Mg N O 55 45 1 4 5	0	0
19	4	1	Total C Mg N 25 20 1 4	0	0
19	4	1	Total C Mg N 25 20 1 4	0	0
19	4	1	Total C Mg N O 55 45 1 4 5	0	0
19	4	1	Total C Mg N O 52 42 1 4 5	0	0
19	4	1	Total C Mg N 25 20 1 4	0	0
19	4	1	Total C Mg N 25 20 1 4	0	0
19	4	1	Total C Mg N O 36 30 1 4 1	0	0
19	4	1	Total C Mg N 25 20 1 4	0	0
19	4	1	Total C Mg N O 47 37 1 4 5	0	0
19	4	1	Total C Mg N O 46 36 1 4 5	0	0

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



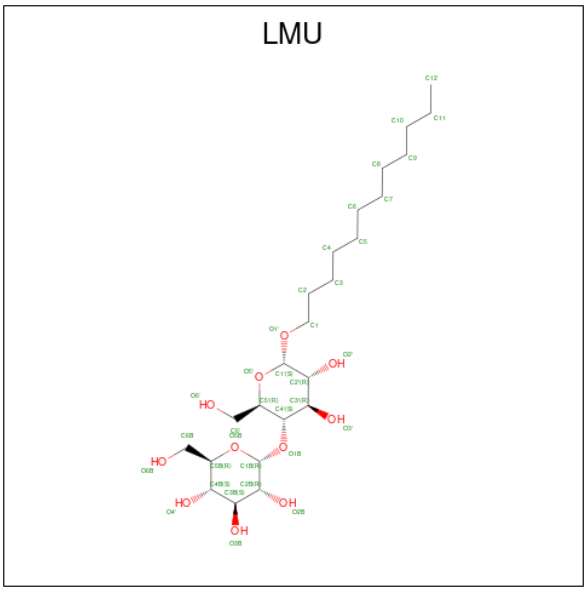
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	1	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0

- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O 35 24 11	0	0
22	A	1	Total C O 35 24 11	0	0
22	A	1	Total C O 35 24 11	0	0
22	A	1	Total C O 35 24 11	0	0
22	A	1	Total C O 35 24 11	0	0
22	A	1	Total C O 35 24 11	0	0
22	B	1	Total C O 25 14 11	0	0
22	B	1	Total C O 35 24 11	0	0
22	B	1	Total C O 35 24 11	0	0
22	C	1	Total C O 35 24 11	0	0
22	D	1	Total C O 35 24 11	0	0
22	E	1	Total C O 35 24 11	0	0
22	E	1	Total C O 35 24 11	0	0
22	F	1	Total C O 34 23 11	0	0

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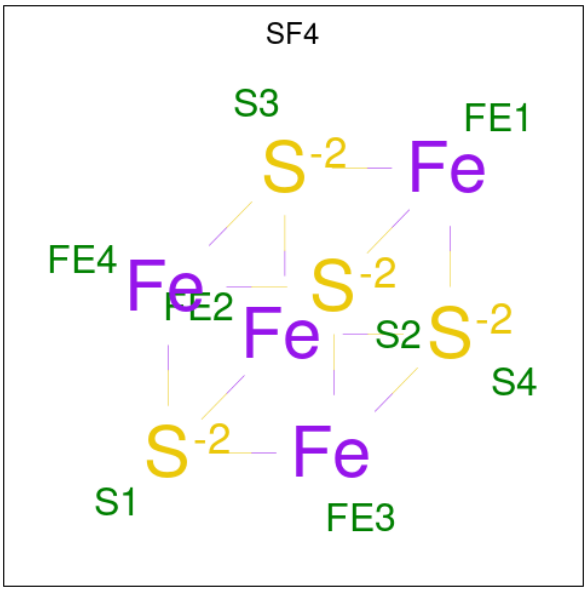
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	G	1	Total C O 35 24 11	0	0
22	G	1	Total C O 35 24 11	0	0
22	G	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	H	1	Total C O 35 24 11	0	0
22	K	1	Total C O 35 24 11	0	0
22	K	1	Total C O 35 24 11	0	0
22	K	1	Total C O 35 24 11	0	0
22	K	1	Total C O 35 24 11	0	0
22	L	1	Total C O 35 24 11	0	0
22	N	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0

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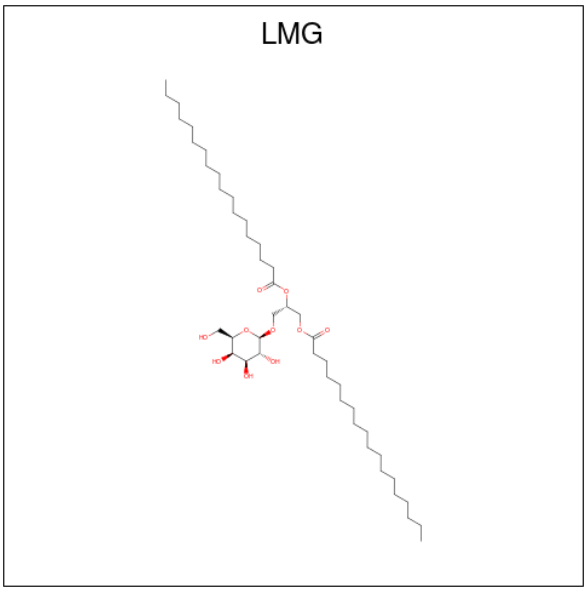
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	R	1	Total C O 35 24 11	0	0
22	R	1	Total C O 35 24 11	0	0
22	1	1	Total C O 35 24 11	0	0
22	1	1	Total C O 35 24 11	0	0
22	2	1	Total C O 35 24 11	0	0
22	2	1	Total C O 35 24 11	0	0
22	2	1	Total C O 35 24 11	0	0
22	2	1	Total C O 35 24 11	0	0
22	3	1	Total C O 35 24 11	0	0
22	3	1	Total C O 35 24 11	0	0
22	4	1	Total C O 35 24 11	0	0
22	4	1	Total C O 34 23 11	0	0
22	4	1	Total C O 35 24 11	0	0
22	4	1	Total C O 35 24 11	0	0
22	4	1	Total C O 35 24 11	0	0
22	4	1	Total C O 35 24 11	0	0
22	4	1	Total C O 35 24 11	0	0

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total 49	C 39	O 10	0	0

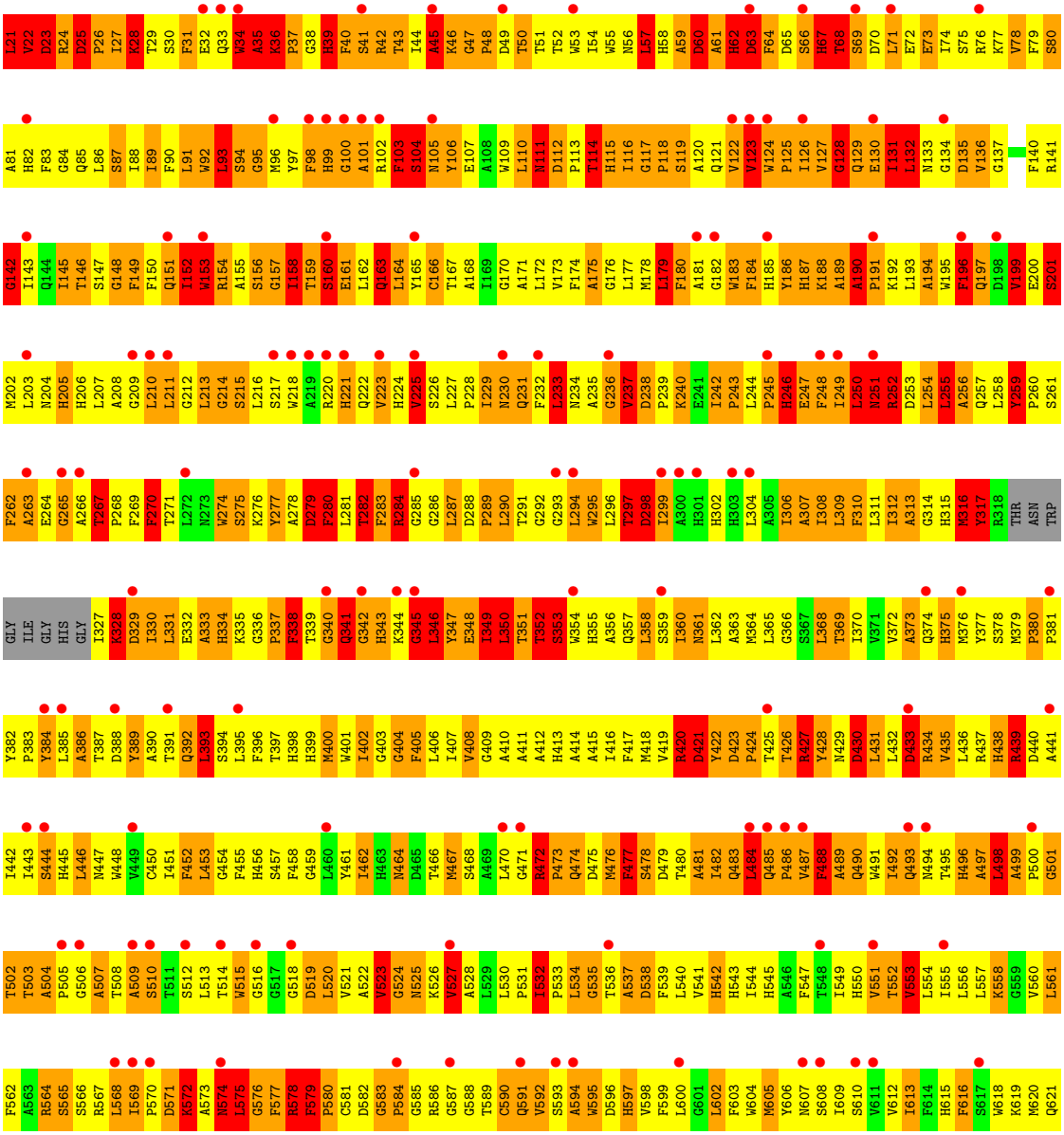
3 Residue-property plots (i)

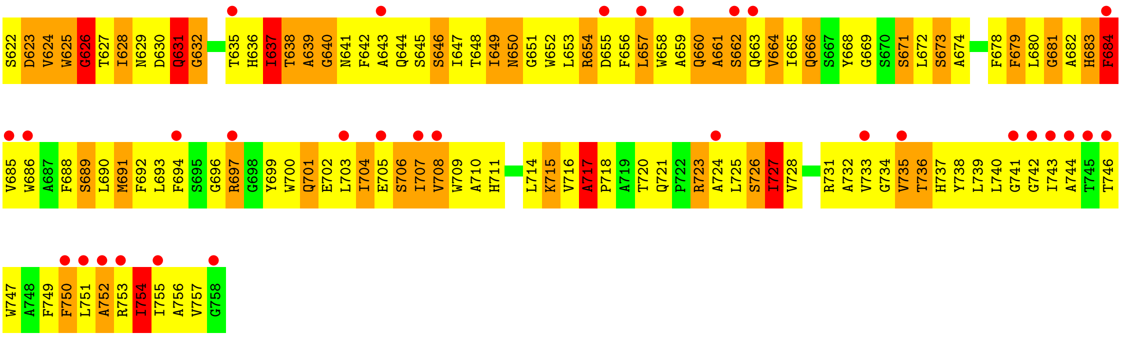
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:



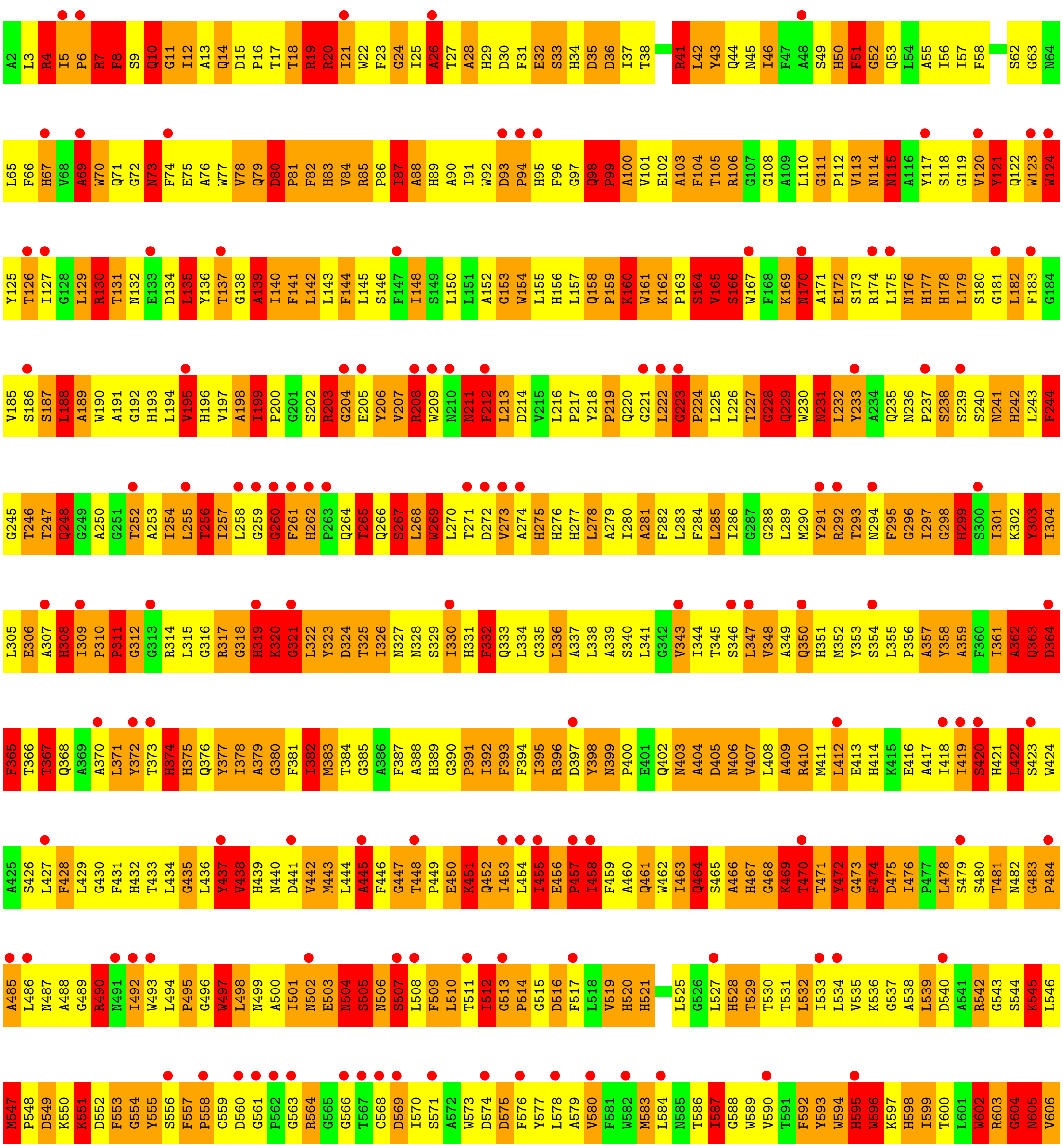


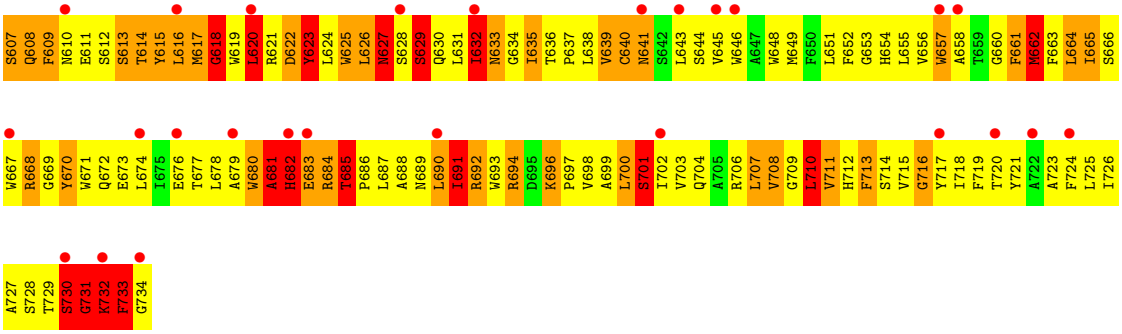


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



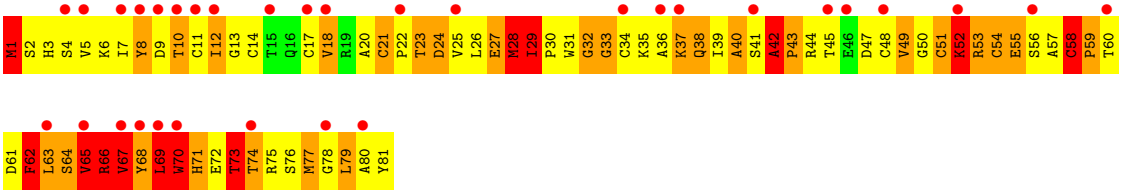




• Molecule 3: Photosystem I iron-sulfur center

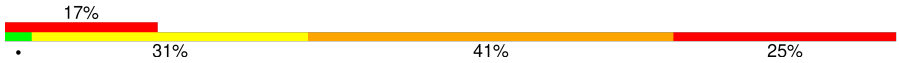
Chain C:

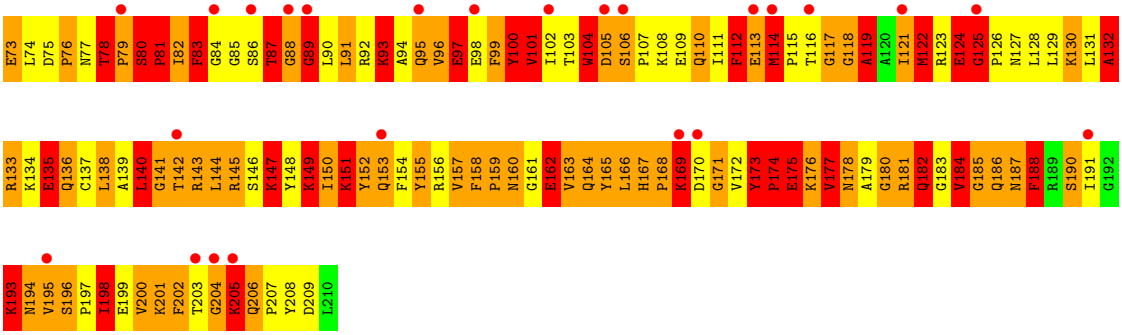




• Molecule 4: Putative uncharacterized protein

Chain D:

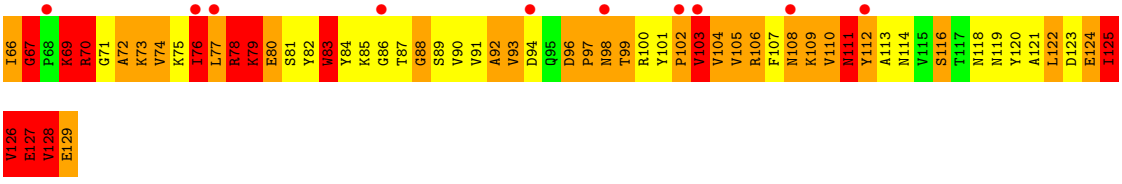




• Molecule 5: Putative uncharacterized protein

Chain E:

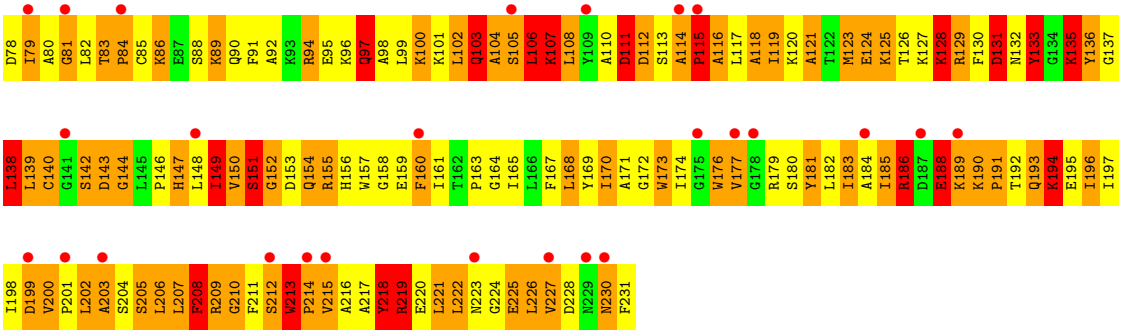




• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

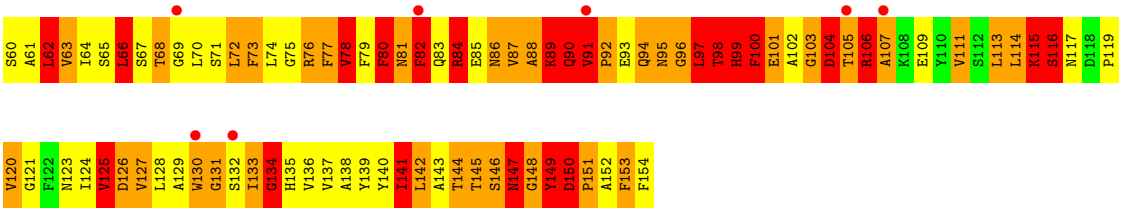
Chain F:





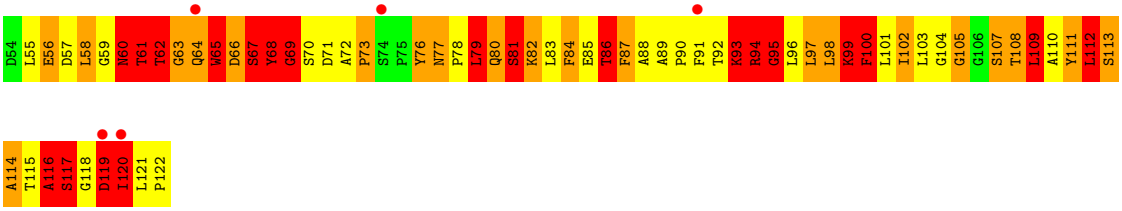
• Molecule 7: Putative uncharacterized protein





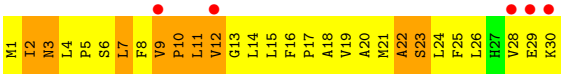
• Molecule 8: Putative uncharacterized protein



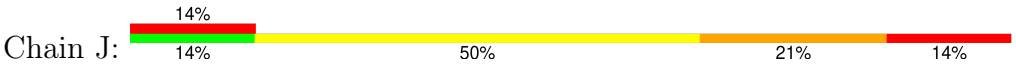


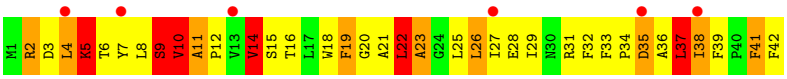
• Molecule 9: Photosystem I reaction center subunit VIII





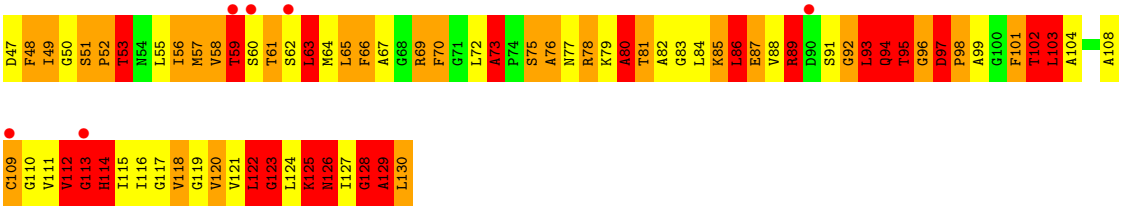
• Molecule 10: Photosystem I reaction center subunit IX





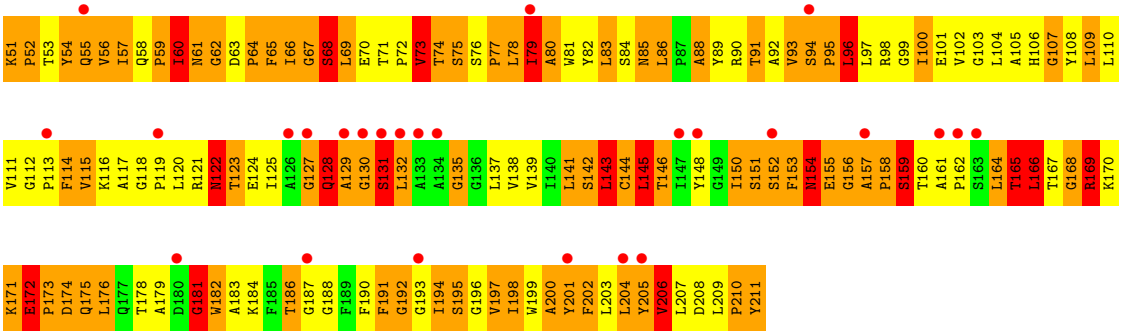
• Molecule 11: Photosystem I reaction center subunit X psaK





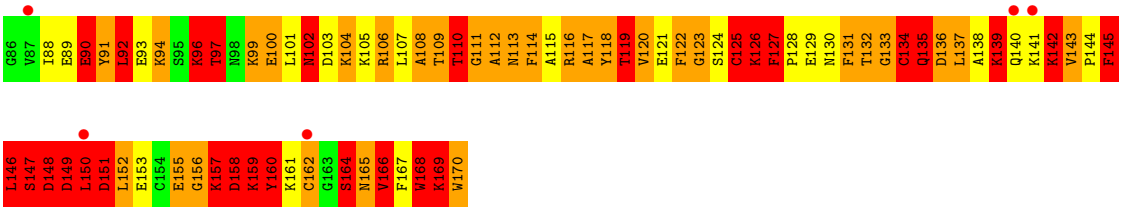
• Molecule 12: Putative uncharacterized protein





• Molecule 13: Photosystem I-N subunit





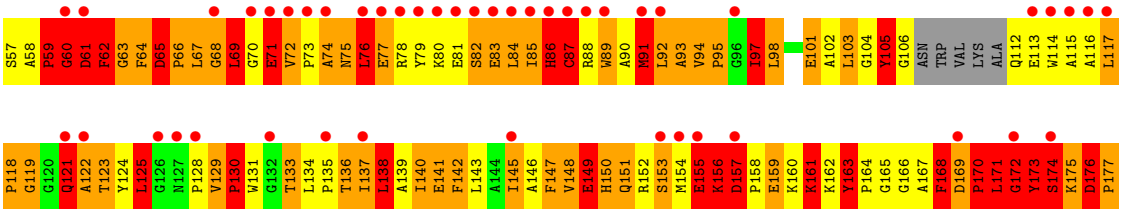
• Molecule 14: CHAIN R

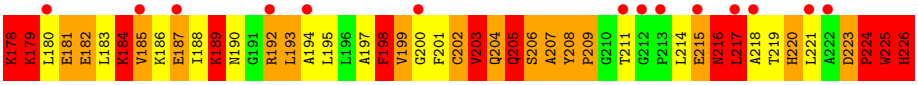




• Molecule 15: AT3g54890

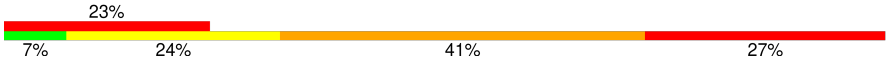




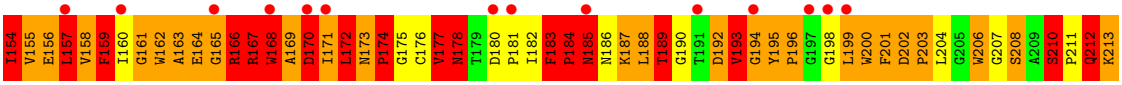


• Molecule 16: Type II chlorophyll a/b binding protein from photosystem I

Chain 2:



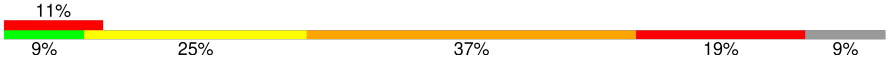


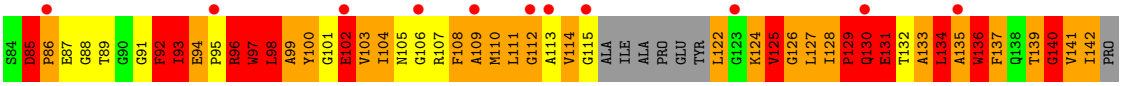




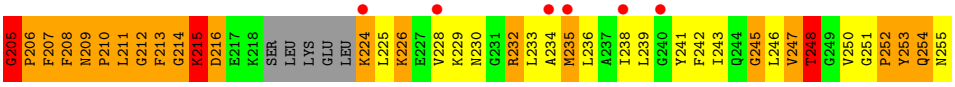
• Molecule 17: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:





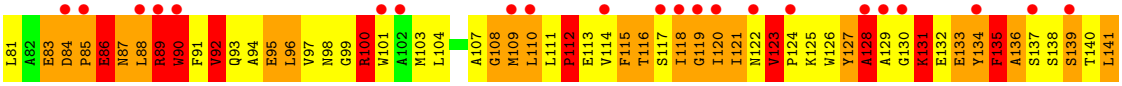


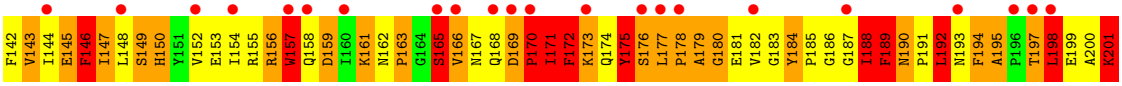


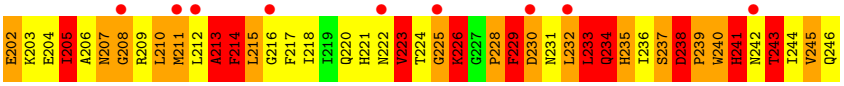
• Molecule 18: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.6 (30.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.349 , 0.383 0.353 , 0.375	Depositor DCC
R_{free} test set	4705 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.12 , 75.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	36370	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 (i)

5.1 Standard geometry (i)

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

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	1.18	19/5932 (0.3%)	1.88	231/8096 (2.9%)
2	B	1.26	25/6054 (0.4%)	1.81	216/8273 (2.6%)
3	C	1.35	2/632 (0.3%)	2.04	24/856 (2.8%)
4	D	1.45	9/1124 (0.8%)	2.27	65/1516 (4.3%)
5	E	1.49	2/523 (0.4%)	2.15	27/710 (3.8%)
6	F	1.29	3/1250 (0.2%)	1.91	53/1687 (3.1%)
7	G	1.34	11/757 (1.5%)	2.20	52/1031 (5.0%)
8	H	1.60	7/530 (1.3%)	2.27	40/722 (5.5%)
9	I	1.05	0/235	1.16	0/320
10	J	1.05	1/344 (0.3%)	1.43	5/469 (1.1%)
11	K	1.60	11/599 (1.8%)	2.38	36/811 (4.4%)
12	L	1.39	5/1244 (0.4%)	2.08	61/1703 (3.6%)
13	N	1.54	8/699 (1.1%)	2.19	42/936 (4.5%)
15	1	1.98	26/1295 (2.0%)	2.35	89/1763 (5.0%)
16	2	1.63	23/1413 (1.6%)	2.44	98/1934 (5.1%)
17	3	1.43	12/1231 (1.0%)	2.27	76/1658 (4.6%)
18	4	1.57	19/1349 (1.4%)	2.29	88/1839 (4.8%)
All	All	1.38	183/25211 (0.7%)	2.04	1203/34324 (3.5%)

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	81
2	B	0	83
3	C	0	14
4	D	0	37
5	E	0	10
6	F	0	27

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	1	24
8	H	2	22
11	K	0	21
12	L	0	23
13	N	0	40
14	R	0	17
15	1	0	37
16	2	0	45
17	3	0	35
18	4	0	28
All	All	3	544

The worst 5 of 183 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	172	GLY	C-O	22.39	1.44	1.23
15	1	225	TRP	C-N	17.72	1.58	1.33
16	2	122	ILE	CA-CB	15.02	1.62	1.54
15	1	119	GLY	N-CA	14.78	1.66	1.45
15	1	63	GLY	C-O	14.09	1.42	1.23

The worst 5 of 1203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	2	258	GLY	N-CA-C	22.18	139.35	112.73
11	K	113	GLY	N-CA-C	-18.74	90.24	112.73
18	4	84	ASP	C-N-CD	-18.22	50.30	125.00
17	3	131	GLU	N-CA-C	-18.13	90.86	111.71
4	D	122	MET	N-CA-C	17.10	130.01	111.03

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	77	PHE	CA
8	H	60	ASN	CA
8	H	68	TYR	CA

5 of 544 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	LEU	Peptide
1	A	22	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	23	ASP	Peptide
1	A	25	ASP	Peptide
1	A	26	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5739	0	5574	1954	6
2	B	5844	0	5648	1960	14
3	C	619	0	605	334	0
4	D	1097	0	1101	440	4
5	E	513	0	514	254	0
6	F	1221	0	1247	385	28
7	G	738	0	709	342	6
8	H	517	0	503	210	2
9	I	229	0	252	55	1
10	J	334	0	344	85	0
11	K	592	0	618	269	5
12	L	1209	0	1220	448	64
13	N	685	0	667	354	0
14	R	265	0	67	79	0
15	1	1257	0	1220	611	37
16	2	1367	0	1312	655	35
17	3	1197	0	1137	532	2
18	4	1309	0	1264	540	45
19	1	665	0	453	118	1
19	2	663	0	494	135	0
19	3	736	0	453	157	0
19	4	729	0	496	151	0
19	A	2676	0	2544	1012	0
19	B	2177	0	2072	648	0
19	F	130	0	85	20	0
19	G	51	0	40	10	0
19	H	240	0	237	62	0
19	I	60	0	58	6	0
19	J	116	0	107	51	0
19	K	210	0	179	39	8

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	322	0	275	110	0
19	R	122	0	123	13	0
20	A	33	0	45	6	0
20	B	33	0	46	22	0
21	1	40	0	54	6	0
21	3	40	0	54	6	0
21	A	200	0	271	161	0
21	B	240	0	323	112	0
21	F	80	0	107	61	0
21	I	80	0	111	46	0
21	J	40	0	52	32	0
21	L	40	0	53	34	0
22	1	70	0	92	10	0
22	2	140	0	184	14	0
22	3	70	0	90	38	0
22	4	278	0	357	69	0
22	A	210	0	275	27	0
22	B	95	0	115	11	0
22	C	35	0	46	0	0
22	D	35	0	45	21	0
22	E	70	0	92	24	0
22	F	34	0	41	12	0
22	G	105	0	138	14	0
22	H	245	0	322	40	0
22	K	140	0	184	37	2
22	L	35	0	46	12	0
22	N	35	0	46	9	0
22	R	245	0	322	34	0
23	A	8	0	0	2	0
23	C	16	0	0	9	0
24	B	49	0	71	19	0
All	All	36370	0	35200	10903	130

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 152.

The worst 5 of 10903 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)
22:4:7034:LMU:C9	22:4:7052:LMU:H1'	1.24	1.64
2:B:459:PHE:CE2	19:B:1235:CLA:C2D	1.76	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1125:CLA:HBB2	19:A:1133:CLA:CMA	1.18	1.60
1:A:244:LEU:CB	1:A:247:GLU:HG3	1.25	1.60
16:2:130:GLY:CA	16:2:131:ILE:HG13	1.29	1.60

The worst 5 of 130 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:173:TYR:OH	16:2:132:LEU:C[2_646]	0.71	1.49
6:F:130:PHE:CG	12:L:170:LYS:NZ[2_556]	0.72	1.48
2:B:205:GLU:OE2	11:K:69:ARG:NH1[1_554]	0.79	1.41
12:L:123:THR:O	18:4:180:GLY:CA[1_455]	0.88	1.32
15:1:171:LEU:N	16:2:132:LEU:N[2_646]	0.98	1.22

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	726/738 (98%)	483 (66%)	139 (19%)	104 (14%)	0 1
2	B	731/733 (100%)	527 (72%)	111 (15%)	93 (13%)	0 1
3	C	79/81 (98%)	42 (53%)	18 (23%)	19 (24%)	0 0
4	D	136/138 (99%)	94 (69%)	24 (18%)	18 (13%)	0 1
5	E	62/64 (97%)	44 (71%)	11 (18%)	7 (11%)	0 2
6	F	152/154 (99%)	105 (69%)	27 (18%)	20 (13%)	0 1
7	G	93/95 (98%)	60 (64%)	22 (24%)	11 (12%)	0 1
8	H	67/69 (97%)	49 (73%)	9 (13%)	9 (13%)	0 1
9	I	28/30 (93%)	11 (39%)	9 (32%)	8 (29%)	0 0
10	J	40/42 (95%)	19 (48%)	11 (28%)	10 (25%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	K	82/84 (98%)	66 (80%)	9 (11%)	7 (8%)	0 4
12	L	159/161 (99%)	110 (69%)	23 (14%)	26 (16%)	0 1
13	N	83/85 (98%)	50 (60%)	19 (23%)	14 (17%)	0 1
15	1	161/170 (95%)	119 (74%)	28 (17%)	14 (9%)	0 4
16	2	174/176 (99%)	129 (74%)	26 (15%)	19 (11%)	0 2
17	3	148/172 (86%)	111 (75%)	20 (14%)	17 (12%)	0 2
18	4	164/166 (99%)	129 (79%)	21 (13%)	14 (8%)	0 4
All	All	3085/3158 (98%)	2148 (70%)	527 (17%)	410 (13%)	0 1

5 of 410 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	41	SER
1	A	98	PHE
1	A	99	HIS
1	A	158	ILE

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	590/599 (98%)	461 (78%)	129 (22%)	1 5
2	B	597/599 (100%)	464 (78%)	133 (22%)	1 5
3	C	70/70 (100%)	60 (86%)	10 (14%)	3 14
4	D	117/117 (100%)	83 (71%)	34 (29%)	0 2
5	E	56/56 (100%)	39 (70%)	17 (30%)	0 1
6	F	127/127 (100%)	91 (72%)	36 (28%)	0 2
7	G	78/79 (99%)	59 (76%)	19 (24%)	1 3
8	H	55/55 (100%)	43 (78%)	12 (22%)	1 5
9	I	26/26 (100%)	23 (88%)	3 (12%)	5 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	35/36 (97%)	23 (66%)	12 (34%)	0 1
11	K	62/62 (100%)	43 (69%)	19 (31%)	0 1
12	L	127/127 (100%)	102 (80%)	25 (20%)	1 6
13	N	74/74 (100%)	53 (72%)	21 (28%)	0 2
15	1	126/134 (94%)	75 (60%)	51 (40%)	0 0
16	2	139/142 (98%)	89 (64%)	50 (36%)	0 1
17	3	113/129 (88%)	73 (65%)	40 (35%)	0 1
18	4	136/140 (97%)	103 (76%)	33 (24%)	1 3
All	All	2528/2572 (98%)	1884 (74%)	644 (26%)	0 3

5 of 644 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	N	150	LEU
17	3	93	ILE
15	1	91	MET
13	N	145	PHE
15	1	226	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	110	GLN
12	L	106	HIS
4	D	182	GLN
8	H	77	ASN
13	N	135	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

252 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	$\#\|Z\| > 2$
19	CLA	A	1237	-	69,73,73	2.12	15 (21%)	82,113,113	2.73	28 (34%)
19	CLA	3	3001	-	24,32,73	2.44	9 (37%)	31,54,113	2.87	20 (64%)
22	LMU	4	7034	-	36,36,36	0.64	0	47,47,47	0.71	0
19	CLA	3	3006	-	24,32,73	2.36	9 (37%)	31,54,113	2.92	17 (54%)
19	CLA	B	1209	2	59,63,73	2.30	16 (27%)	70,101,113	2.70	25 (35%)
22	LMU	A	7044	-	36,36,36	0.87	1 (2%)	47,47,47	1.59	9 (19%)
19	CLA	B	1208	2	58,62,73	2.61	13 (22%)	71,100,113	2.76	28 (39%)
22	LMU	B	7038	-	36,36,36	0.74	0	47,47,47	1.71	11 (23%)
22	LMU	L	7029	-	36,36,36	0.69	1 (2%)	47,47,47	0.74	0
22	LMU	K	7042	-	36,36,36	0.63	0	47,47,47	1.17	5 (10%)
22	LMU	H	7043	-	36,36,36	0.86	2 (5%)	47,47,47	1.66	10 (21%)
19	CLA	2	2011	-	24,32,73	2.36	8 (33%)	31,54,113	2.81	18 (58%)
19	CLA	3	3017	-	54,58,73	2.51	17 (31%)	64,95,113	3.24	29 (45%)
19	CLA	4	4014	-	51,55,73	2.50	15 (29%)	60,91,113	3.30	26 (43%)
19	CLA	4	4002	18	56,60,73	2.70	23 (41%)	65,97,113	3.28	34 (52%)
21	BCR	B	6004	-	41,41,41	1.11	4 (9%)	56,56,56	4.38	30 (53%)
21	BCR	B	6010	-	41,41,41	1.20	2 (4%)	56,56,56	4.37	30 (53%)
19	CLA	1	1014	-	65,69,73	2.32	17 (26%)	77,108,113	2.65	23 (29%)
19	CLA	K	1143	-	54,58,73	2.44	14 (25%)	64,95,113	2.82	27 (42%)
19	CLA	A	1109	19,1	69,73,73	2.14	13 (18%)	82,113,113	2.81	29 (35%)
23	SF4	C	8003	3	0,12,12	-	-	-		
19	CLA	A	1115	-	69,73,73	2.22	17 (24%)	82,113,113	2.65	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	K	3009	2	69,73,73	2.20	13 (18%)	82,113,113	2.55	28 (34%)
19	CLA	2	2001	-	55,59,73	2.43	16 (29%)	64,96,113	2.81	25 (39%)
21	BCR	A	6008	-	41,41,41	1.16	4 (9%)	56,56,56	4.18	28 (50%)
19	CLA	2	2005	-	24,32,73	2.35	8 (33%)	31,54,113	2.92	18 (58%)
19	CLA	A	1137	-	51,55,73	2.51	16 (31%)	60,91,113	2.96	25 (41%)
19	CLA	B	1223	2	69,73,73	2.18	15 (21%)	82,113,113	2.45	25 (30%)
19	CLA	4	4013	18	24,32,73	2.33	8 (33%)	31,54,113	2.66	19 (61%)
19	CLA	3	3014	-	24,32,73	2.43	9 (37%)	31,54,113	3.01	19 (61%)
19	CLA	A	1128	1	69,73,73	2.16	15 (21%)	82,113,113	2.55	26 (31%)
19	CLA	G	1242	-	55,59,73	2.48	14 (25%)	64,96,113	2.92	27 (42%)
19	CLA	R	1144	-	61,65,73	2.33	13 (21%)	72,103,113	2.81	28 (38%)
19	CLA	I	1204	-	64,68,73	2.26	15 (23%)	76,107,113	2.73	22 (28%)
19	CLA	2	2002	-	60,64,73	2.36	14 (23%)	71,102,113	2.87	31 (43%)
22	LMU	B	7012	-	26,26,36	0.79	1 (3%)	37,37,47	1.43	8 (21%)
21	BCR	B	6005	-	41,41,41	1.19	4 (9%)	56,56,56	4.84	32 (57%)
19	CLA	A	1104	-	61,65,73	2.28	14 (22%)	72,103,113	2.88	29 (40%)
22	LMU	H	7017	-	36,36,36	0.74	1 (2%)	47,47,47	1.92	11 (23%)
19	CLA	A	1140	1	69,73,73	2.15	16 (23%)	82,113,113	2.51	26 (31%)
19	CLA	A	1126	-	69,73,73	2.15	15 (21%)	82,113,113	2.59	28 (34%)
19	CLA	1	1303	-	55,59,73	2.71	24 (43%)	64,96,113	3.15	29 (45%)
19	CLA	A	1107	-	59,63,73	2.30	14 (23%)	70,101,113	2.77	31 (44%)
23	SF4	A	8001	2,1	0,12,12	-	-	-		
20	PQN	B	5002	-	34,34,34	1.64	2 (5%)	43,45,45	1.52	6 (13%)
19	CLA	3	3003	-	38,44,73	2.80	12 (31%)	52,78,113	3.07	22 (42%)
19	CLA	B	1219	2	59,63,73	2.47	16 (27%)	70,101,113	2.70	21 (30%)
19	CLA	A	1112	1	49,53,73	2.56	13 (26%)	58,89,113	2.92	26 (44%)
22	LMU	H	7032	-	36,36,36	0.73	1 (2%)	47,47,47	1.45	6 (12%)
19	CLA	2	2007	-	69,73,73	2.15	12 (17%)	82,113,113	2.58	28 (34%)
19	CLA	B	1238	-	69,73,73	2.16	14 (20%)	82,113,113	2.67	29 (35%)
19	CLA	4	4005	-	24,32,73	2.39	9 (37%)	31,54,113	2.92	18 (58%)
19	CLA	1	1015	-	24,32,73	2.41	8 (33%)	31,54,113	2.82	18 (58%)
19	CLA	4	4011	-	24,32,73	2.49	8 (33%)	31,54,113	2.88	19 (61%)
19	CLA	1	1002	15	51,55,73	2.54	14 (27%)	60,91,113	2.82	23 (38%)
19	CLA	A	1127	1	59,63,73	2.30	16 (27%)	70,101,113	2.73	25 (35%)
19	CLA	B	1229	2	69,73,73	2.23	16 (23%)	82,113,113	2.83	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LMU	G	7039	-	36,36,36	0.68	0	47,47,47	1.37	4 (8%)
19	CLA	B	1213	-	50,54,73	2.50	13 (26%)	59,90,113	2.89	26 (44%)
19	CLA	2	1307	-	24,32,73	2.38	8 (33%)	31,54,113	2.87	19 (61%)
19	CLA	3	3008	-	54,58,73	2.47	18 (33%)	64,95,113	3.09	25 (39%)
19	CLA	A	1119	-	69,73,73	2.19	15 (21%)	82,113,113	2.62	24 (29%)
19	CLA	4	4003	-	59,63,73	2.38	16 (27%)	70,101,113	2.66	24 (34%)
22	LMU	2	7046	-	36,36,36	0.71	1 (2%)	47,47,47	0.88	3 (6%)
22	LMU	3	7005	-	36,36,36	0.71	0	47,47,47	2.12	13 (27%)
19	CLA	H	1505	-	59,63,73	2.36	13 (22%)	70,101,113	2.89	27 (38%)
19	CLA	2	2010	-	24,32,73	2.36	7 (29%)	31,54,113	2.74	17 (54%)
19	CLA	A	9011	-	69,73,73	2.15	17 (24%)	82,113,113	2.67	27 (32%)
22	LMU	E	7048	-	36,36,36	0.83	1 (2%)	47,47,47	2.05	10 (21%)
19	CLA	B	1212	2	64,68,73	2.21	12 (18%)	76,107,113	2.53	25 (32%)
19	CLA	B	1214	-	63,67,73	2.30	14 (22%)	74,105,113	2.51	22 (29%)
19	CLA	2	4009	-	69,73,73	2.19	14 (20%)	82,113,113	2.71	26 (31%)
19	CLA	4	1306	-	59,63,73	2.31	13 (22%)	70,101,113	2.83	26 (37%)
19	CLA	B	1227	2	54,58,73	2.56	15 (27%)	64,95,113	2.75	25 (39%)
22	LMU	3	7003	-	36,36,36	0.80	0	47,47,47	1.48	7 (14%)
19	CLA	A	1117	-	69,73,73	2.17	15 (21%)	82,113,113	2.58	27 (32%)
19	CLA	L	1148	-	59,63,73	2.64	24 (40%)	70,101,113	3.37	34 (48%)
19	CLA	3	3011	-	69,73,73	2.15	16 (23%)	82,113,113	2.51	23 (28%)
19	CLA	L	1503	-	54,58,73	2.60	19 (35%)	64,95,113	3.22	24 (37%)
19	CLA	B	1221	-	58,62,73	2.41	19 (32%)	68,99,113	2.77	26 (38%)
19	CLA	A	9022	-	69,73,73	2.16	15 (21%)	82,113,113	2.63	28 (34%)
19	CLA	B	1201	-	49,53,73	2.61	17 (34%)	58,89,113	3.06	21 (36%)
19	CLA	4	4010	-	24,32,73	2.33	8 (33%)	31,54,113	2.86	18 (58%)
19	CLA	B	1228	2	54,58,73	2.36	13 (24%)	64,95,113	2.98	29 (45%)
22	LMU	A	7035	-	36,36,36	0.61	0	47,47,47	1.59	8 (17%)
21	BCR	A	6002	-	41,41,41	1.83	5 (12%)	56,56,56	4.74	35 (62%)
19	CLA	J	1308	-	59,63,73	2.40	19 (32%)	70,101,113	2.96	27 (38%)
19	CLA	3	3005	-	24,32,73	2.35	8 (33%)	31,54,113	2.90	17 (54%)
19	CLA	A	1133	1	54,58,73	2.46	15 (27%)	64,95,113	2.85	25 (39%)
22	LMU	A	7010	-	36,36,36	1.32	2 (5%)	47,47,47	1.21	5 (10%)
19	CLA	A	1135	-	55,59,73	2.45	17 (30%)	64,96,113	2.75	23 (35%)
19	CLA	1	1011	-	38,44,73	3.12	19 (50%)	52,78,113	3.82	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LMU	R	7020	-	36,36,36	0.67	0	47,47,47	1.40	6 (12%)
19	CLA	F	1302	-	45,49,73	2.68	16 (35%)	54,84,113	3.09	24 (44%)
19	CLA	4	1009	-	38,44,73	3.01	14 (36%)	52,78,113	3.46	21 (40%)
19	CLA	4	1304	-	69,73,73	2.26	21 (30%)	82,113,113	3.03	32 (39%)
19	CLA	L	1130	1	69,73,73	2.22	15 (21%)	82,113,113	2.56	26 (31%)
19	CLA	B	1231	2,19	49,53,73	2.62	16 (32%)	58,89,113	2.96	21 (36%)
21	BCR	3	6022	-	41,41,41	1.23	3 (7%)	56,56,56	5.03	26 (46%)
19	CLA	B	1234	2	64,68,73	2.21	15 (23%)	76,107,113	2.89	20 (26%)
19	CLA	B	1220	-	69,73,73	2.47	22 (31%)	82,113,113	2.76	30 (36%)
24	LMG	B	7101	-	49,49,55	1.04	3 (6%)	57,57,63	1.02	3 (5%)
21	BCR	F	6014	-	41,41,41	1.27	4 (9%)	56,56,56	4.95	27 (48%)
19	CLA	1	1012	-	38,44,73	2.79	11 (28%)	52,78,113	3.11	21 (40%)
22	LMU	R	7022	-	36,36,36	0.73	1 (2%)	47,47,47	1.34	7 (14%)
22	LMU	H	7030	-	36,36,36	0.77	2 (5%)	47,47,47	1.20	5 (10%)
19	CLA	K	1142	-	49,53,73	2.56	15 (30%)	58,89,113	2.91	19 (32%)
19	CLA	A	1151	-	54,58,73	2.49	17 (31%)	64,95,113	2.73	23 (35%)
19	CLA	3	3015	-	24,32,73	2.38	7 (29%)	31,54,113	2.77	19 (61%)
19	CLA	A	1122	-	59,63,73	2.38	15 (25%)	70,101,113	2.75	24 (34%)
19	CLA	K	1146	-	54,58,73	2.65	21 (38%)	64,95,113	3.00	27 (42%)
19	CLA	B	1235	2	69,73,73	2.10	14 (20%)	82,113,113	2.48	23 (28%)
19	CLA	B	1206	2	69,73,73	2.13	15 (21%)	82,113,113	2.45	22 (26%)
22	LMU	4	7009	-	35,35,36	1.36	2 (5%)	46,46,47	1.26	4 (8%)
22	LMU	4	7033	-	36,36,36	0.76	1 (2%)	47,47,47	1.61	9 (19%)
19	CLA	4	4001	-	54,58,73	2.51	14 (25%)	64,95,113	2.78	23 (35%)
22	LMU	K	7001	-	36,36,36	0.82	2 (5%)	47,47,47	1.38	7 (14%)
19	CLA	B	1239	-	69,73,73	2.10	15 (21%)	82,113,113	2.69	27 (32%)
19	CLA	B	1210	-	69,73,73	2.20	16 (23%)	82,113,113	2.46	24 (29%)
22	LMU	2	7006	-	36,36,36	0.64	1 (2%)	47,47,47	0.73	0
21	BCR	B	6020	-	41,41,41	1.89	10 (24%)	56,56,56	4.54	27 (48%)
19	CLA	1	1310	-	24,32,73	2.37	7 (29%)	31,54,113	3.08	19 (61%)
19	CLA	3	3002	-	24,32,73	2.44	8 (33%)	31,54,113	2.79	19 (61%)
22	LMU	C	7015	-	36,36,36	0.69	1 (2%)	47,47,47	1.28	6 (12%)
19	CLA	A	1131	1	69,73,73	2.20	16 (23%)	82,113,113	2.60	23 (28%)
22	LMU	N	7049	-	36,36,36	0.58	1 (2%)	47,47,47	1.37	4 (8%)
19	CLA	1	1013	-	55,59,73	2.67	20 (36%)	64,96,113	3.54	26 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A	1132	-	69,73,73	2.20	14 (20%)	82,113,113	2.82	29 (35%)
19	CLA	B	1216	-	65,69,73	2.18	16 (24%)	77,108,113	2.73	25 (32%)
19	CLA	B	1218	-	50,54,73	2.48	15 (30%)	59,90,113	3.11	19 (32%)
19	CLA	4	1004	-	59,63,73	2.45	18 (30%)	70,101,113	2.89	29 (41%)
22	LMU	A	7045	-	36,36,36	0.75	1 (2%)	47,47,47	1.50	9 (19%)
22	LMU	G	7026	-	36,36,36	0.87	2 (5%)	47,47,47	1.52	6 (12%)
22	LMU	1	7004	-	36,36,36	0.68	1 (2%)	47,47,47	0.81	1 (2%)
22	LMU	1	7013	-	36,36,36	0.71	1 (2%)	47,47,47	1.07	1 (2%)
19	CLA	B	1226	2	69,73,73	2.15	16 (23%)	82,113,113	2.72	27 (32%)
19	CLA	1	1007	-	65,69,73	2.25	15 (23%)	77,108,113	2.59	28 (36%)
22	LMU	4	7053	-	35,35,36	0.71	1 (2%)	46,46,47	1.27	6 (13%)
19	CLA	2	2004	-	54,58,73	2.45	14 (25%)	64,95,113	2.69	22 (34%)
19	CLA	2	2006	-	69,73,73	2.17	13 (18%)	82,113,113	2.69	22 (26%)
19	CLA	A	1136	1	69,73,73	2.16	16 (23%)	82,113,113	2.60	25 (30%)
19	CLA	A	1141	-	69,73,73	2.17	14 (20%)	82,113,113	2.63	26 (31%)
19	CLA	B	1230	2	54,58,73	2.50	18 (33%)	64,95,113	2.93	24 (37%)
19	CLA	A	1125	1	69,73,73	2.18	16 (23%)	82,113,113	2.43	23 (28%)
19	CLA	B	9010	2	69,73,73	2.12	16 (23%)	82,113,113	2.62	33 (40%)
19	CLA	1	1006	-	38,44,73	2.92	13 (34%)	52,78,113	3.24	23 (44%)
19	CLA	4	4015	-	50,54,73	2.54	20 (40%)	59,90,113	2.98	25 (42%)
19	CLA	4	4007	-	56,60,73	2.41	14 (25%)	65,97,113	2.70	25 (38%)
21	BCR	A	6003	-	41,41,41	1.42	2 (4%)	56,56,56	4.20	29 (51%)
21	BCR	I	6018	-	41,41,41	1.30	4 (9%)	56,56,56	4.80	32 (57%)
21	BCR	I	6021	-	41,41,41	1.97	8 (19%)	56,56,56	4.87	32 (57%)
21	BCR	J	6012	-	41,41,41	1.31	5 (12%)	56,56,56	5.56	27 (48%)
19	CLA	3	1147	-	50,54,73	2.88	25 (50%)	59,90,113	3.20	34 (57%)
19	CLA	H	1241	-	59,63,73	2.40	12 (20%)	70,101,113	2.65	25 (35%)
19	CLA	3	3012	-	24,32,73	2.37	9 (37%)	31,54,113	2.98	18 (58%)
21	BCR	B	6006	-	41,41,41	1.49	8 (19%)	56,56,56	4.62	26 (46%)
21	BCR	A	6007	-	41,41,41	1.45	4 (9%)	56,56,56	3.89	32 (57%)
22	LMU	H	7002	-	36,36,36	0.61	0	47,47,47	1.54	7 (14%)
19	CLA	B	1205	-	69,73,73	2.18	13 (18%)	82,113,113	2.70	25 (30%)
22	LMU	B	7040	-	36,36,36	0.75	1 (2%)	47,47,47	1.62	10 (21%)
19	CLA	A	1121	1	46,50,73	2.55	13 (28%)	53,85,113	3.25	24 (45%)
22	LMU	2	7027	-	36,36,36	0.81	1 (2%)	47,47,47	1.69	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LMU	D	7050	-	36,36,36	0.62	1 (2%)	47,47,47	0.83	1 (2%)
19	CLA	A	1116	1	56,60,73	2.46	13 (23%)	65,97,113	2.96	26 (40%)
19	CLA	1	1001	-	50,54,73	2.73	20 (40%)	59,90,113	3.56	31 (52%)
22	LMU	H	7028	-	36,36,36	0.59	0	47,47,47	0.99	2 (4%)
19	CLA	3	3013	-	69,73,73	2.29	20 (28%)	82,113,113	2.94	25 (30%)
19	CLA	B	1215	2	64,68,73	2.21	14 (21%)	76,107,113	2.69	29 (38%)
22	LMU	4	7052	-	36,36,36	1.23	4 (11%)	47,47,47	1.81	8 (17%)
19	CLA	A	1113	1	54,58,73	2.51	13 (24%)	64,95,113	2.76	26 (40%)
21	BCR	B	6017	-	41,41,41	1.33	5 (12%)	56,56,56	4.06	25 (44%)
19	CLA	J	1311	-	65,69,73	2.24	15 (23%)	77,108,113	2.72	25 (32%)
19	CLA	4	4006	-	59,63,73	2.36	12 (20%)	70,101,113	2.72	25 (35%)
19	CLA	A	1309	-	24,32,73	2.33	8 (33%)	31,54,113	2.78	18 (58%)
19	CLA	2	2013	-	54,58,73	2.51	12 (22%)	64,95,113	2.97	25 (39%)
19	CLA	B	1217	-	54,58,73	2.38	14 (25%)	64,95,113	2.95	26 (40%)
22	LMU	R	7025	-	36,36,36	0.77	1 (2%)	47,47,47	1.21	4 (8%)
19	CLA	L	1502	12	51,55,73	2.50	13 (25%)	60,91,113	3.18	24 (40%)
19	CLA	B	1202	-	69,73,73	2.17	15 (21%)	82,113,113	2.91	30 (36%)
19	CLA	B	1232	19	49,53,73	2.59	13 (26%)	58,89,113	3.04	22 (37%)
22	LMU	F	7036	-	35,35,36	0.76	1 (2%)	46,46,47	1.44	6 (13%)
23	SF4	C	8002	3	0,12,12	-	-	-		
19	CLA	3	1118	-	38,44,73	2.81	13 (34%)	52,78,113	3.36	23 (44%)
19	CLA	2	2012	16	54,58,73	2.40	14 (25%)	64,95,113	2.89	25 (39%)
19	CLA	A	1129	1	54,58,73	2.46	14 (25%)	64,95,113	2.98	25 (39%)
22	LMU	R	7021	-	36,36,36	0.75	1 (2%)	47,47,47	1.37	6 (12%)
19	CLA	A	9023	-	69,73,73	2.22	14 (20%)	82,113,113	2.57	28 (34%)
19	CLA	F	1240	-	38,44,73	2.79	15 (39%)	52,78,113	3.09	26 (50%)
19	CLA	A	1120	-	55,59,73	2.48	15 (27%)	64,96,113	2.91	24 (37%)
19	CLA	1	1003	-	51,55,73	2.50	12 (23%)	60,91,113	3.17	26 (43%)
19	CLA	B	1211	-	69,73,73	2.18	13 (18%)	82,113,113	2.51	26 (31%)
19	CLA	F	1305	-	57,61,73	2.62	23 (40%)	67,98,113	2.80	27 (40%)
19	CLA	A	1149	-	50,54,73	2.78	16 (32%)	61,90,113	3.76	34 (55%)
19	CLA	3	2009	-	60,64,73	2.44	19 (31%)	71,102,113	2.74	27 (38%)
19	CLA	3	3016	-	69,73,73	2.18	15 (21%)	82,113,113	2.57	24 (29%)
21	BCR	1	6023	-	41,41,41	1.56	3 (7%)	56,56,56	6.49	30 (53%)
19	CLA	A	1123	-	69,73,73	2.10	15 (21%)	82,113,113	2.45	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	A	1108	-	49,53,73	2.64	16 (32%)	58,89,113	3.02	24 (41%)
19	CLA	B	1301	-	38,44,73	2.90	13 (34%)	52,78,113	3.36	29 (55%)
19	CLA	4	4012	-	38,44,73	2.79	12 (31%)	52,78,113	3.45	25 (48%)
22	LMU	A	7016	-	36,36,36	0.68	0	47,47,47	1.44	6 (12%)
19	CLA	A	1110	1	58,62,73	2.37	15 (25%)	68,99,113	2.60	24 (35%)
22	LMU	E	7037	-	36,36,36	0.74	1 (2%)	47,47,47	1.77	11 (23%)
19	CLA	A	1106	-	69,73,73	2.16	16 (23%)	82,113,113	2.62	28 (34%)
19	CLA	A	9013	-	69,73,73	2.28	16 (23%)	82,113,113	2.71	28 (34%)
19	CLA	2	2014	-	65,69,73	2.30	21 (32%)	77,108,113	2.78	27 (35%)
19	CLA	B	1222	-	62,66,73	2.29	15 (24%)	73,104,113	2.74	26 (35%)
22	LMU	K	7047	-	36,36,36	0.80	1 (2%)	47,47,47	1.06	3 (6%)
22	LMU	K	7041	-	36,36,36	0.57	0	47,47,47	1.07	3 (6%)
19	CLA	A	1139	-	55,59,73	2.45	16 (29%)	64,96,113	2.91	25 (39%)
19	CLA	L	1501	12	54,58,73	2.47	15 (27%)	64,95,113	2.83	25 (39%)
19	CLA	A	1105	1	50,54,73	2.49	12 (24%)	59,90,113	2.93	25 (42%)
19	CLA	R	1150	-	69,73,73	2.26	13 (18%)	82,113,113	2.60	28 (34%)
19	CLA	2	2008	-	24,32,73	2.41	8 (33%)	31,54,113	2.95	18 (58%)
21	BCR	L	6019	-	41,41,41	1.50	11 (26%)	56,56,56	4.39	24 (42%)
22	LMU	H	7011	-	36,36,36	0.77	2 (5%)	47,47,47	1.99	10 (21%)
22	LMU	A	7023	-	36,36,36	0.60	0	47,47,47	1.19	4 (8%)
19	CLA	B	1236	-	51,55,73	2.47	15 (29%)	60,91,113	2.94	26 (43%)
19	CLA	3	3007	-	46,50,73	2.50	12 (26%)	53,85,113	3.14	26 (49%)
19	CLA	H	1145	-	69,73,73	2.14	16 (23%)	82,113,113	2.86	26 (31%)
21	BCR	A	6011	-	41,41,41	1.22	4 (9%)	56,56,56	4.29	31 (55%)
19	CLA	A	1134	1	49,53,73	2.54	15 (30%)	58,89,113	3.09	22 (37%)
19	CLA	B	1233	-	55,59,73	2.49	12 (21%)	64,96,113	2.98	26 (40%)
22	LMU	2	7031	-	36,36,36	1.23	2 (5%)	47,47,47	1.35	6 (12%)
22	LMU	R	7014	-	36,36,36	0.91	2 (5%)	47,47,47	2.03	8 (17%)
19	CLA	2	2003	16	24,32,73	2.36	8 (33%)	31,54,113	2.89	19 (61%)
19	CLA	A	1103	1	69,73,73	2.12	14 (20%)	82,113,113	2.67	28 (34%)
19	CLA	A	1124	-	69,73,73	2.14	15 (21%)	82,113,113	2.55	26 (31%)
22	LMU	4	7018	-	36,36,36	0.75	1 (2%)	47,47,47	1.08	3 (6%)
19	CLA	1	1010	-	50,54,73	2.79	22 (44%)	59,90,113	3.38	28 (47%)
19	CLA	A	1101	-	54,58,73	2.39	14 (25%)	64,95,113	3.06	26 (40%)
22	LMU	G	7051	-	36,36,36	0.87	1 (2%)	47,47,47	2.12	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LMU	R	7024	-	36,36,36	0.76	1 (2%)	47,47,47	1.47	8 (17%)
22	LMU	R	7007	-	36,36,36	0.58	1 (2%)	47,47,47	0.81	2 (4%)
22	LMU	4	7008	-	36,36,36	0.58	0	47,47,47	0.88	1 (2%)
19	CLA	B	1224	-	69,73,73	2.27	15 (21%)	82,113,113	2.76	23 (28%)
19	CLA	A	1138	-	69,73,73	2.17	14 (20%)	82,113,113	2.54	25 (30%)
19	CLA	A	9012	-	69,73,73	2.21	17 (24%)	82,113,113	2.58	25 (30%)
19	CLA	B	1225	-	69,73,73	2.11	14 (20%)	82,113,113	2.73	28 (34%)
19	CLA	B	1203	-	69,73,73	2.18	16 (23%)	82,113,113	2.87	32 (39%)
19	CLA	1	1008	-	55,59,73	2.51	14 (25%)	64,96,113	3.36	25 (39%)
19	CLA	3	3004	-	24,32,73	2.33	10 (41%)	31,54,113	3.10	19 (61%)
19	CLA	3	3010	-	24,32,73	2.33	9 (37%)	31,54,113	2.81	18 (58%)
20	PQN	A	5001	-	34,34,34	1.73	2 (5%)	43,45,45	1.44	7 (16%)
19	CLA	4	4004	-	24,32,73	2.39	7 (29%)	31,54,113	2.87	17 (54%)
19	CLA	1	1005	-	50,54,73	2.78	14 (28%)	59,90,113	2.85	22 (37%)
21	BCR	F	6016	-	41,41,41	1.58	9 (21%)	56,56,56	3.72	27 (48%)
22	LMU	4	7019	-	36,36,36	0.82	1 (2%)	47,47,47	1.36	9 (19%)
19	CLA	A	1102	19	59,63,73	2.38	15 (25%)	70,101,113	2.80	27 (38%)
19	CLA	H	1207	-	69,73,73	2.23	15 (21%)	82,113,113	2.79	26 (31%)
19	CLA	L	1504	-	59,63,73	2.38	13 (22%)	70,101,113	2.73	30 (42%)
19	CLA	A	1111	1	58,62,73	2.29	15 (25%)	68,99,113	2.78	26 (38%)

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
19	CLA	A	1237	-	1/1/15/20	15/39/115/115	-
22	LMU	4	7034	-	-	13/21/61/61	0/2/2/2
22	LMU	A	7044	-	-	16/21/61/61	0/2/2/2
19	CLA	B	1209	2	1/1/13/20	10/27/103/115	-
22	LMU	L	7029	-	-	16/21/61/61	0/2/2/2
19	CLA	B	1208	2	1/1/13/20	9/25/101/115	-
22	LMU	B	7038	-	-	13/21/61/61	0/2/2/2
22	LMU	K	7042	-	-	18/21/61/61	0/2/2/2
22	LMU	H	7043	-	-	11/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	3	3017	-	-	8/21/97/115	-
19	CLA	4	4014	-	-	13/18/94/115	-
21	BCR	B	6004	-	-	16/29/63/63	0/2/2/2
19	CLA	4	4002	18	1/1/12/20	7/24/100/115	-
21	BCR	B	6010	-	-	13/29/63/63	0/2/2/2
19	CLA	1	1014	-	1/1/14/20	15/35/111/115	-
19	CLA	K	1143	-	-	7/21/97/115	-
19	CLA	A	1109	19,1	1/1/15/20	25/39/115/115	-
23	SF4	C	8003	3	-	-	0/6/5/5
19	CLA	A	1115	-	1/1/15/20	15/39/115/115	-
19	CLA	K	3009	2	1/1/15/20	20/39/115/115	-
19	CLA	2	2001	-	-	10/23/99/115	-
21	BCR	A	6008	-	-	15/29/63/63	0/2/2/2
19	CLA	B	1223	2	1/1/15/20	19/39/115/115	-
19	CLA	A	1137	-	-	10/18/94/115	-
19	CLA	A	1111	1	-	13/26/102/115	-
19	CLA	A	1128	1	1/1/15/20	18/39/115/115	-
19	CLA	G	1242	-	-	10/23/99/115	-
19	CLA	R	1144	-	1/1/13/20	14/30/106/115	-
19	CLA	I	1204	-	1/1/14/20	12/33/109/115	-
19	CLA	2	2002	-	1/1/13/20	10/29/105/115	-
22	LMU	B	7012	-	-	5/11/51/61	0/2/2/2
21	BCR	B	6005	-	-	8/29/63/63	0/2/2/2
19	CLA	A	1104	-	1/1/13/20	7/30/106/115	-
22	LMU	H	7017	-	-	13/21/61/61	0/2/2/2
19	CLA	A	1140	1	1/1/15/20	17/39/115/115	-
19	CLA	A	1126	-	1/1/15/20	14/39/115/115	-
19	CLA	1	1303	-	2/2/12/20	11/23/99/115	-
19	CLA	A	1107	-	1/1/13/20	12/27/103/115	-
23	SF4	A	8001	2,1	-	-	0/6/5/5
20	PQN	B	5002	-	1/1/8/9	9/23/43/43	0/2/2/2
19	CLA	B	1219	2	1/1/13/20	10/27/103/115	-
19	CLA	A	1112	1	-	11/15/91/115	-
22	LMU	H	7032	-	-	18/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	2	2007	-	1/1/15/20	18/39/115/115	-
19	CLA	B	1238	-	1/1/15/20	19/39/115/115	-
22	LMU	G	7039	-	-	17/21/61/61	0/2/2/2
19	CLA	1	1002	15	-	11/18/94/115	-
19	CLA	A	1127	1	1/1/13/20	10/27/103/115	-
19	CLA	B	1229	2	1/1/15/20	18/39/115/115	-
19	CLA	B	1213	-	-	12/17/93/115	-
19	CLA	3	3008	-	-	7/21/97/115	-
19	CLA	A	1119	-	1/1/15/20	17/39/115/115	-
19	CLA	4	4003	-	1/1/13/20	14/27/103/115	-
22	LMU	2	7046	-	-	16/21/61/61	0/2/2/2
22	LMU	3	7005	-	-	15/21/61/61	0/2/2/2
19	CLA	H	1505	-	1/1/13/20	12/27/103/115	-
19	CLA	A	9011	-	1/1/15/20	23/39/115/115	-
22	LMU	E	7048	-	-	12/21/61/61	0/2/2/2
19	CLA	B	1212	2	1/1/14/20	12/33/109/115	-
19	CLA	B	1214	-	1/1/13/20	12/32/108/115	-
19	CLA	2	4009	-	1/1/15/20	17/39/115/115	-
19	CLA	4	1306	-	1/1/13/20	14/27/103/115	-
19	CLA	B	1227	2	-	8/21/97/115	-
22	LMU	3	7003	-	-	14/21/61/61	0/2/2/2
19	CLA	A	1117	-	1/1/15/20	19/39/115/115	-
19	CLA	L	1148	-	2/2/13/20	13/27/103/115	-
19	CLA	3	3011	-	1/1/15/20	20/39/115/115	-
19	CLA	L	1503	-	1/1/12/20	10/21/97/115	-
19	CLA	B	1221	-	-	8/26/102/115	-
19	CLA	A	9022	-	1/1/15/20	19/39/115/115	-
19	CLA	B	1201	-	-	6/15/91/115	-
22	LMU	A	7035	-	-	13/21/61/61	0/2/2/2
19	CLA	B	1228	2	-	13/21/97/115	-
21	BCR	A	6002	-	-	16/29/63/63	0/2/2/2
19	CLA	J	1308	-	1/1/13/20	14/27/103/115	-
19	CLA	A	1133	1	-	12/21/97/115	-
22	LMU	A	7010	-	-	18/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1135	-	-	9/23/99/115	-
22	LMU	R	7020	-	-	11/21/61/61	0/2/2/2
19	CLA	F	1302	-	-	7/10/86/115	-
19	CLA	4	1304	-	2/2/15/20	19/39/115/115	-
19	CLA	L	1130	1	1/1/15/20	17/39/115/115	-
19	CLA	B	1231	2,19	-	9/15/91/115	-
21	BCR	3	6022	-	-	19/29/63/63	0/2/2/2
19	CLA	B	1234	2	1/1/14/20	14/33/109/115	-
19	CLA	B	1220	-	-	18/39/115/115	-
24	LMG	B	7101	-	-	24/44/64/70	0/1/1/1
21	BCR	F	6014	-	-	17/29/63/63	0/2/2/2
22	LMU	R	7022	-	-	14/21/61/61	0/2/2/2
22	LMU	H	7030	-	-	14/21/61/61	0/2/2/2
19	CLA	K	1142	-	-	3/15/91/115	-
19	CLA	A	1151	-	-	9/21/97/115	-
19	CLA	A	1122	-	1/1/13/20	10/27/103/115	-
19	CLA	K	1146	-	-	8/21/97/115	-
19	CLA	B	1206	2	1/1/15/20	18/39/115/115	-
22	LMU	4	7009	-	-	13/20/60/61	0/2/2/2
22	LMU	4	7033	-	-	11/21/61/61	0/2/2/2
19	CLA	4	4001	-	-	5/21/97/115	-
22	LMU	K	7001	-	-	13/21/61/61	0/2/2/2
19	CLA	B	1239	-	1/1/15/20	19/39/115/115	-
19	CLA	B	1210	-	1/1/15/20	23/39/115/115	-
22	LMU	2	7006	-	-	14/21/61/61	0/2/2/2
21	BCR	B	6020	-	-	14/29/63/63	0/2/2/2
22	LMU	C	7015	-	-	14/21/61/61	0/2/2/2
19	CLA	A	1131	1	1/1/15/20	19/39/115/115	-
22	LMU	N	7049	-	-	16/21/61/61	0/2/2/2
19	CLA	1	1013	-	1/1/12/20	8/23/99/115	-
19	CLA	A	1132	-	1/1/15/20	23/39/115/115	-
19	CLA	B	1216	-	1/1/14/20	17/35/111/115	-
19	CLA	B	1218	-	-	12/17/93/115	-
19	CLA	4	1004	-	1/1/13/20	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMU	A	7045	-	-	14/21/61/61	0/2/2/2
22	LMU	G	7026	-	-	15/21/61/61	0/2/2/2
22	LMU	1	7004	-	-	16/21/61/61	0/2/2/2
22	LMU	1	7013	-	-	10/21/61/61	0/2/2/2
19	CLA	B	1226	2	1/1/15/20	27/39/115/115	-
19	CLA	1	1007	-	1/1/14/20	21/35/111/115	-
22	LMU	4	7053	-	-	13/20/60/61	0/2/2/2
19	CLA	2	2004	-	-	10/21/97/115	-
19	CLA	2	2006	-	1/1/15/20	18/39/115/115	-
19	CLA	A	1136	1	1/1/15/20	11/39/115/115	-
19	CLA	A	1141	-	1/1/15/20	20/39/115/115	-
19	CLA	B	1230	2	-	10/21/97/115	-
19	CLA	A	1125	1	1/1/15/20	24/39/115/115	-
19	CLA	B	9010	2	1/1/15/20	18/39/115/115	-
19	CLA	4	4015	-	-	12/17/93/115	-
22	LMU	R	7014	-	-	12/21/61/61	0/2/2/2
19	CLA	4	4007	-	-	12/24/100/115	-
21	BCR	A	6003	-	-	14/29/63/63	0/2/2/2
21	BCR	I	6018	-	-	14/29/63/63	0/2/2/2
21	BCR	I	6021	-	-	12/29/63/63	0/2/2/2
21	BCR	J	6012	-	-	13/29/63/63	0/2/2/2
19	CLA	3	1147	-	-	9/17/93/115	-
19	CLA	H	1241	-	1/1/13/20	7/27/103/115	-
22	LMU	H	7002	-	-	14/21/61/61	0/2/2/2
21	BCR	B	6006	-	-	11/29/63/63	0/2/2/2
21	BCR	A	6007	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1205	-	1/1/15/20	12/39/115/115	-
22	LMU	B	7040	-	-	14/21/61/61	0/2/2/2
19	CLA	A	1121	1	-	4/12/88/115	-
22	LMU	2	7027	-	-	11/21/61/61	0/2/2/2
22	LMU	D	7050	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1116	1	-	11/24/100/115	-
19	CLA	1	1001	-	-	10/17/93/115	-
22	LMU	H	7028	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	3	3013	-	1/1/15/20	18/39/115/115	-
19	CLA	B	1215	2	1/1/14/20	13/33/109/115	-
22	LMU	4	7052	-	-	18/21/61/61	0/2/2/2
19	CLA	A	1113	1	-	8/21/97/115	-
21	BCR	B	6017	-	-	14/29/63/63	0/2/2/2
19	CLA	J	1311	-	1/1/14/20	23/35/111/115	-
19	CLA	4	4006	-	1/1/13/20	12/27/103/115	-
19	CLA	2	2013	-	-	8/21/97/115	-
19	CLA	B	1217	-	-	7/21/97/115	-
22	LMU	R	7025	-	-	13/21/61/61	0/2/2/2
19	CLA	L	1502	12	-	9/18/94/115	-
19	CLA	B	1202	-	1/1/15/20	20/39/115/115	-
19	CLA	B	1232	19	-	8/15/91/115	-
22	LMU	F	7036	-	-	11/20/60/61	0/2/2/2
23	SF4	C	8002	3	-	-	0/6/5/5
19	CLA	2	2012	16	-	4/21/97/115	-
19	CLA	A	1129	1	-	4/21/97/115	-
22	LMU	R	7021	-	-	14/21/61/61	0/2/2/2
19	CLA	A	9023	-	1/1/15/20	17/39/115/115	-
19	CLA	A	1120	-	-	10/23/99/115	-
19	CLA	1	1003	-	-	9/18/94/115	-
19	CLA	B	1211	-	1/1/15/20	23/39/115/115	-
19	CLA	F	1305	-	3/3/12/20	12/25/101/115	-
19	CLA	A	1149	-	2/2/11/20	12/16/92/115	-
19	CLA	3	2009	-	1/1/13/20	16/29/105/115	-
19	CLA	3	3016	-	1/1/15/20	23/39/115/115	-
21	BCR	1	6023	-	-	15/29/63/63	0/2/2/2
19	CLA	A	1123	-	1/1/15/20	20/39/115/115	-
19	CLA	A	1108	-	-	6/15/91/115	-
22	LMU	A	7016	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1110	1	-	13/26/102/115	-
22	LMU	E	7037	-	-	16/21/61/61	0/2/2/2
19	CLA	A	1106	-	1/1/15/20	22/39/115/115	-
19	CLA	A	9013	-	1/1/15/20	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	2	2014	-	1/1/14/20	18/35/111/115	-
19	CLA	B	1222	-	1/1/13/20	15/31/107/115	-
22	LMU	K	7047	-	-	9/21/61/61	0/2/2/2
22	LMU	K	7041	-	-	12/21/61/61	0/2/2/2
19	CLA	A	1139	-	-	11/23/99/115	-
19	CLA	L	1501	12	-	8/21/97/115	-
19	CLA	A	1105	1	-	8/17/93/115	-
19	CLA	R	1150	-	1/1/15/20	20/39/115/115	-
21	BCR	L	6019	-	-	13/29/63/63	0/2/2/2
22	LMU	H	7011	-	-	17/21/61/61	0/2/2/2
22	LMU	A	7023	-	-	17/21/61/61	0/2/2/2
19	CLA	B	1236	-	-	10/18/94/115	-
19	CLA	3	3007	-	-	4/12/88/115	-
19	CLA	H	1145	-	2/2/15/20	20/39/115/115	-
21	BCR	A	6011	-	-	11/29/63/63	0/2/2/2
19	CLA	A	1134	1	-	9/15/91/115	-
19	CLA	B	1233	-	-	10/23/99/115	-
22	LMU	2	7031	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1124	-	1/1/15/20	20/39/115/115	-
19	CLA	A	1103	1	1/1/15/20	22/39/115/115	-
22	LMU	4	7018	-	-	13/21/61/61	0/2/2/2
19	CLA	1	1010	-	-	8/17/93/115	-
19	CLA	A	1101	-	-	6/21/97/115	-
22	LMU	G	7051	-	-	13/21/61/61	0/2/2/2
22	LMU	R	7024	-	-	14/21/61/61	0/2/2/2
22	LMU	R	7007	-	-	16/21/61/61	0/2/2/2
22	LMU	4	7008	-	-	12/21/61/61	0/2/2/2
19	CLA	B	1224	-	1/1/15/20	16/39/115/115	-
19	CLA	A	1138	-	1/1/15/20	19/39/115/115	-
19	CLA	A	9012	-	1/1/15/20	20/39/115/115	-
19	CLA	B	1225	-	1/1/15/20	17/39/115/115	-
19	CLA	B	1203	-	1/1/15/20	19/39/115/115	-
19	CLA	1	1008	-	1/1/12/20	10/23/99/115	-
20	PQN	A	5001	-	1/1/8/9	11/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	1005	-	-	7/17/93/115	-
21	BCR	F	6016	-	-	13/29/63/63	0/2/2/2
22	LMU	4	7019	-	-	15/21/61/61	0/2/2/2
19	CLA	A	1102	19	1/1/13/20	12/27/103/115	-
19	CLA	H	1207	-	1/1/15/20	18/39/115/115	-
19	CLA	L	1504	-	1/1/13/20	8/27/103/115	-
19	CLA	B	1235	2	1/1/15/20	13/39/115/115	-

The worst 5 of 2668 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1011	CLA	CAB-C3B	-8.57	1.33	1.50
19	1	1006	CLA	CAB-C3B	-8.56	1.33	1.50
19	1	1005	CLA	OBD-CAD	8.45	1.37	1.22
19	4	1009	CLA	CAB-C3B	-8.22	1.33	1.50
19	B	1208	CLA	CAB-C3B	-7.94	1.34	1.50

The worst 5 of 5208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	6012	BCR	C20-C21-C22	30.62	170.21	127.28
21	A	6002	BCR	C20-C21-C22	25.17	162.58	127.28
21	3	6022	BCR	C20-C21-C22	24.97	162.30	127.28
21	F	6014	BCR	C20-C21-C22	23.10	159.67	127.28
21	B	6005	BCR	C20-C21-C22	22.66	159.05	127.28

5 of 97 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1102	CLA	C8
19	A	1103	CLA	C8
19	A	1104	CLA	C8
19	A	1106	CLA	C8
19	A	1107	CLA	C8

5 of 2930 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1101	CLA	C3A-C2A-CAA-CBA
19	A	1101	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	A	1102	CLA	C3A-C2A-CAA-CBA
19	A	1102	CLA	CBA-CGA-O2A-C1
19	A	1102	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

234 monomers are involved in 3027 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1237	CLA	28	0
22	4	7034	LMU	36	0
19	3	3006	CLA	9	0
19	B	1209	CLA	15	0
22	A	7044	LMU	1	0
19	B	1208	CLA	5	0
22	B	7038	LMU	7	0
22	L	7029	LMU	12	0
22	K	7042	LMU	16	0
22	H	7043	LMU	3	0
19	2	2011	CLA	1	0
19	3	3017	CLA	5	0
19	4	4014	CLA	8	0
19	4	4002	CLA	24	0
21	B	6004	BCR	5	0
21	B	6010	BCR	21	0
19	1	1014	CLA	17	0
19	K	1143	CLA	28	0
19	A	1109	CLA	17	0
23	C	8003	SF4	3	0
19	A	1115	CLA	71	0
19	K	3009	CLA	3	7
19	2	2001	CLA	14	0
21	A	6008	BCR	25	0
19	A	1137	CLA	8	0
19	B	1223	CLA	36	0
19	4	4013	CLA	11	0
19	A	1128	CLA	18	0
19	G	1242	CLA	10	0
19	R	1144	CLA	10	0
19	I	1204	CLA	6	0
19	2	2002	CLA	17	0
22	B	7012	LMU	1	0
21	B	6005	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1104	CLA	13	0
22	H	7017	LMU	2	0
19	A	1140	CLA	44	0
19	A	1126	CLA	40	0
19	1	1303	CLA	7	0
19	A	1107	CLA	38	0
23	A	8001	SF4	2	0
20	B	5002	PQN	22	0
19	3	3003	CLA	8	0
19	B	1219	CLA	13	0
19	A	1112	CLA	31	0
22	H	7032	LMU	11	0
19	2	2007	CLA	15	0
19	B	1238	CLA	18	0
19	1	1015	CLA	3	0
19	4	4011	CLA	2	0
19	1	1002	CLA	9	0
19	A	1127	CLA	18	0
19	B	1229	CLA	20	0
22	G	7039	LMU	4	0
19	B	1213	CLA	20	0
19	3	3008	CLA	14	0
19	A	1119	CLA	44	0
19	4	4003	CLA	3	0
22	2	7046	LMU	1	0
22	3	7005	LMU	38	0
19	H	1505	CLA	3	0
19	A	9011	CLA	13	0
22	E	7048	LMU	17	0
19	B	1212	CLA	14	0
19	B	1214	CLA	21	0
19	2	4009	CLA	6	0
19	4	1306	CLA	18	0
19	B	1227	CLA	10	0
22	3	7003	LMU	20	0
19	A	1117	CLA	27	0
19	L	1148	CLA	21	0
19	3	3011	CLA	13	0
19	L	1503	CLA	8	0
19	B	1221	CLA	23	0
19	A	9022	CLA	38	0
19	B	1201	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	4010	CLA	2	0
19	B	1228	CLA	15	0
21	A	6002	BCR	44	0
19	J	1308	CLA	33	0
19	3	3005	CLA	9	0
19	A	1133	CLA	33	0
22	A	7010	LMU	6	0
19	A	1135	CLA	24	0
19	1	1011	CLA	5	0
22	R	7020	LMU	10	0
19	F	1302	CLA	10	0
19	4	1009	CLA	2	0
19	4	1304	CLA	22	0
19	L	1130	CLA	26	0
19	B	1231	CLA	14	0
21	3	6022	BCR	6	0
19	B	1234	CLA	8	0
19	B	1220	CLA	43	0
24	B	7101	LMG	19	0
21	F	6014	BCR	25	0
19	1	1012	CLA	2	0
22	R	7022	LMU	5	0
22	H	7030	LMU	4	0
19	K	1142	CLA	15	1
19	A	1151	CLA	18	0
19	A	1122	CLA	24	0
19	K	1146	CLA	7	0
19	B	1235	CLA	61	0
19	B	1206	CLA	17	0
22	4	7009	LMU	3	0
22	4	7033	LMU	7	0
19	4	4001	CLA	4	0
22	K	7001	LMU	11	0
19	B	1239	CLA	21	0
19	B	1210	CLA	21	0
22	2	7006	LMU	8	0
21	B	6020	BCR	24	0
19	A	1131	CLA	35	0
22	N	7049	LMU	9	0
19	1	1013	CLA	14	0
19	A	1132	CLA	17	0
19	B	1216	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1218	CLA	15	0
19	4	1004	CLA	32	0
22	A	7045	LMU	2	0
22	G	7026	LMU	9	0
22	1	7004	LMU	6	0
22	1	7013	LMU	4	0
19	B	1226	CLA	21	0
19	1	1007	CLA	19	0
22	4	7053	LMU	13	0
19	2	2004	CLA	16	0
19	2	2006	CLA	8	0
19	A	1136	CLA	24	0
19	A	1141	CLA	31	0
19	B	1230	CLA	20	0
19	A	1125	CLA	66	0
19	B	9010	CLA	15	0
19	1	1006	CLA	15	0
19	4	4015	CLA	4	0
21	A	6003	BCR	14	0
21	I	6018	BCR	15	0
21	I	6021	BCR	32	0
21	J	6012	BCR	32	0
19	3	1147	CLA	14	0
19	H	1241	CLA	11	0
19	3	3012	CLA	11	0
21	B	6006	BCR	12	0
21	A	6007	BCR	32	0
22	H	7002	LMU	3	0
19	B	1205	CLA	25	0
22	B	7040	LMU	3	0
19	A	1121	CLA	8	0
22	2	7027	LMU	3	0
22	D	7050	LMU	21	0
19	A	1116	CLA	8	0
19	1	1001	CLA	11	0
22	H	7028	LMU	2	0
19	3	3013	CLA	18	0
19	B	1215	CLA	11	0
22	4	7052	LMU	36	0
19	A	1113	CLA	11	0
21	B	6017	BCR	43	0
19	J	1311	CLA	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	4006	CLA	11	0
19	2	2013	CLA	6	0
19	B	1217	CLA	10	0
22	R	7025	LMU	1	0
19	L	1502	CLA	26	0
19	B	1202	CLA	28	0
19	B	1232	CLA	18	0
22	F	7036	LMU	12	0
23	C	8002	SF4	6	0
19	2	2012	CLA	17	0
19	A	1129	CLA	6	0
22	R	7021	LMU	9	0
19	A	9023	CLA	50	0
19	A	1120	CLA	8	0
19	1	1003	CLA	4	0
19	B	1211	CLA	18	0
19	F	1305	CLA	12	0
19	A	1149	CLA	7	0
19	3	2009	CLA	36	0
19	3	3016	CLA	13	0
21	1	6023	BCR	6	0
19	A	1123	CLA	30	0
19	A	1108	CLA	6	0
19	B	1301	CLA	7	0
19	4	4012	CLA	6	0
22	A	7016	LMU	12	0
19	A	1110	CLA	1	0
22	E	7037	LMU	7	0
19	A	1106	CLA	27	0
19	A	9013	CLA	31	0
19	2	2014	CLA	34	0
19	B	1222	CLA	42	0
22	K	7047	LMU	5	2
22	K	7041	LMU	6	0
19	A	1139	CLA	30	0
19	L	1501	CLA	16	0
19	A	1105	CLA	25	0
19	R	1150	CLA	3	0
21	L	6019	BCR	34	0
22	H	7011	LMU	15	0
22	A	7023	LMU	6	0
19	B	1236	CLA	25	0

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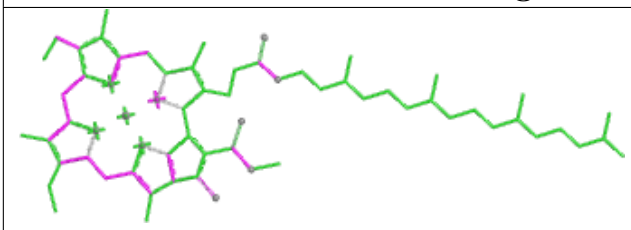
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	3007	CLA	2	0
19	H	1145	CLA	25	0
21	A	6011	BCR	46	0
19	A	1134	CLA	21	0
19	B	1233	CLA	6	0
22	2	7031	LMU	2	0
22	R	7014	LMU	4	0
19	2	2003	CLA	1	0
19	A	1103	CLA	17	0
19	A	1124	CLA	60	0
19	1	1010	CLA	9	0
19	A	1101	CLA	14	0
22	G	7051	LMU	1	0
22	R	7007	LMU	5	0
22	4	7008	LMU	3	0
19	B	1224	CLA	16	0
19	A	1138	CLA	29	0
19	A	9012	CLA	37	0
19	B	1225	CLA	28	0
19	B	1203	CLA	18	0
19	1	1008	CLA	6	1
19	3	3004	CLA	7	0
19	3	3010	CLA	5	0
20	A	5001	PQN	6	0
19	4	4004	CLA	2	0
19	1	1005	CLA	4	0
21	F	6016	BCR	36	0
22	4	7019	LMU	1	0
19	A	1102	CLA	19	0
19	H	1207	CLA	23	0
19	L	1504	CLA	20	0
19	A	1111	CLA	20	0

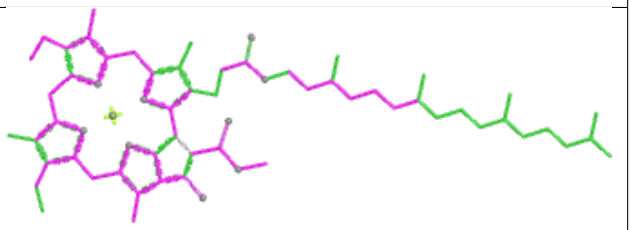
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

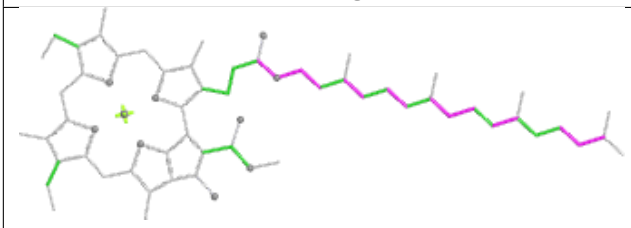
Ligand CLA A 1237



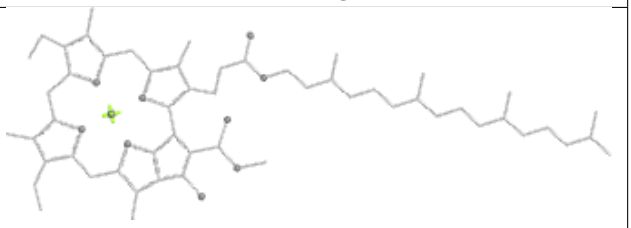
Bond lengths



Bond angles

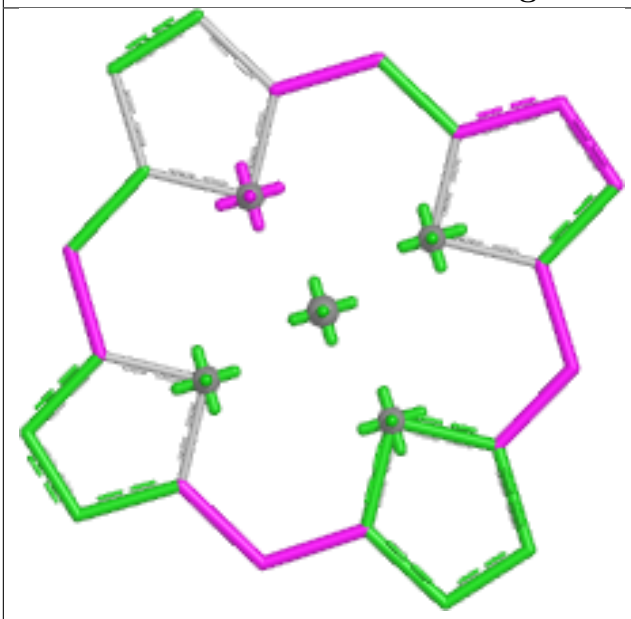


Torsions

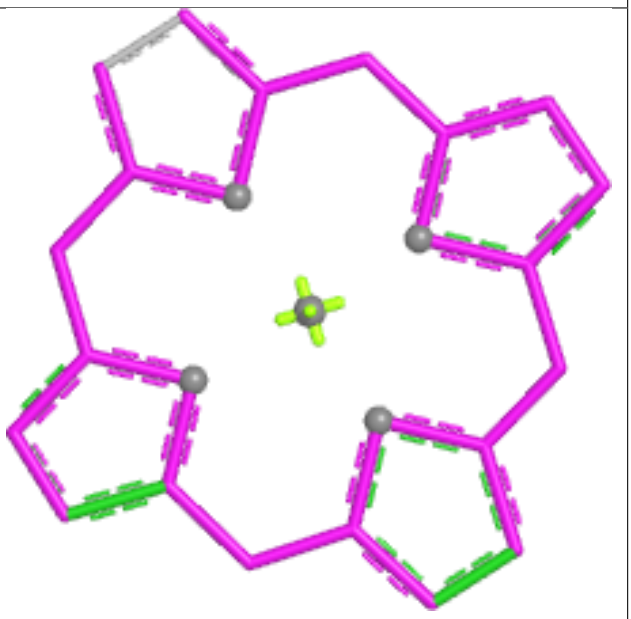


Rings

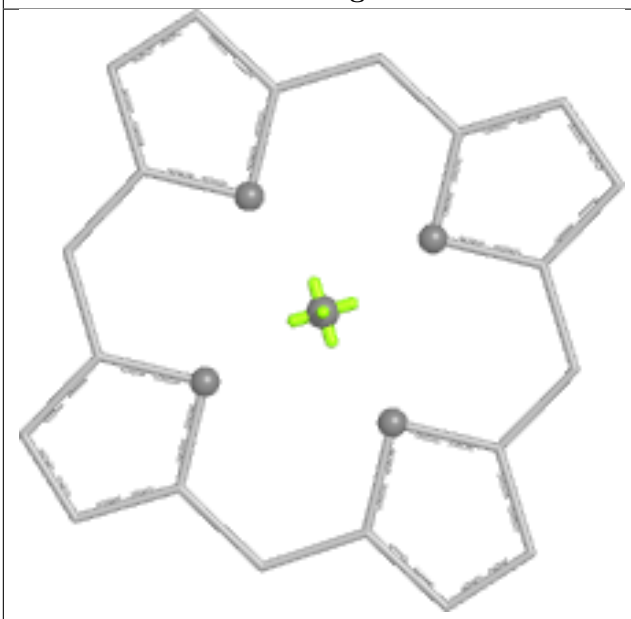
Ligand CLA 3 3001



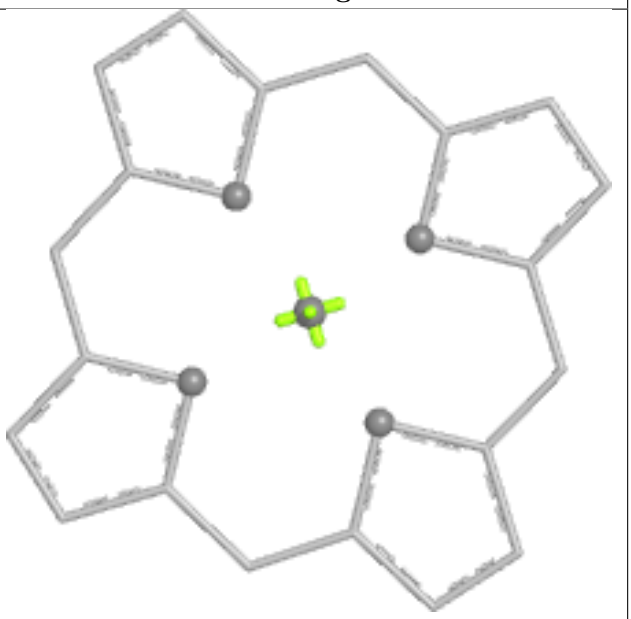
Bond lengths



Bond angles

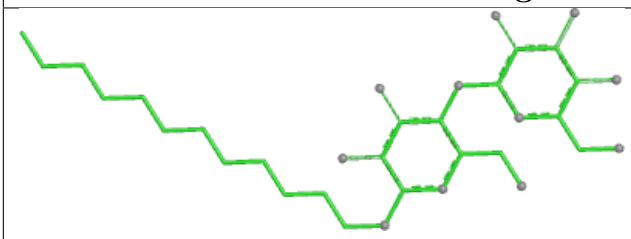


Torsions

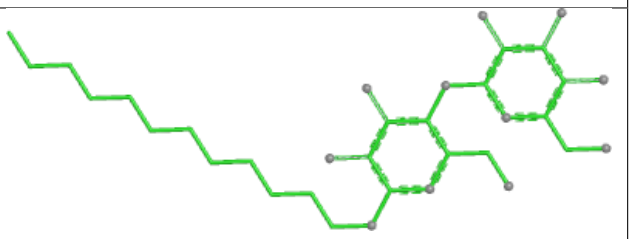


Rings

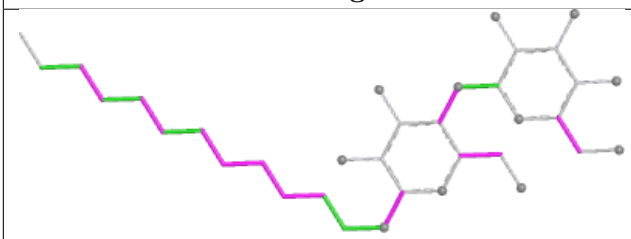
Ligand LMU 4 7034



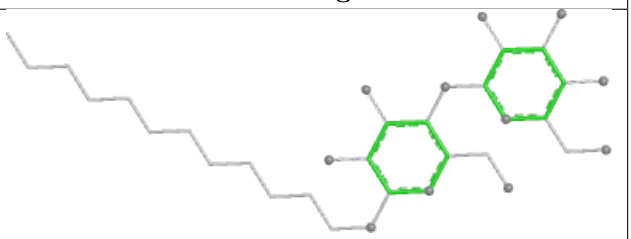
Bond lengths



Bond angles

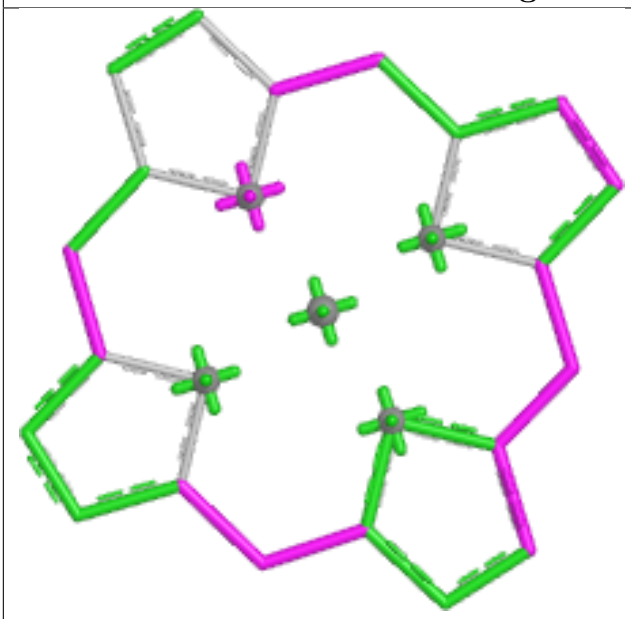


Torsions

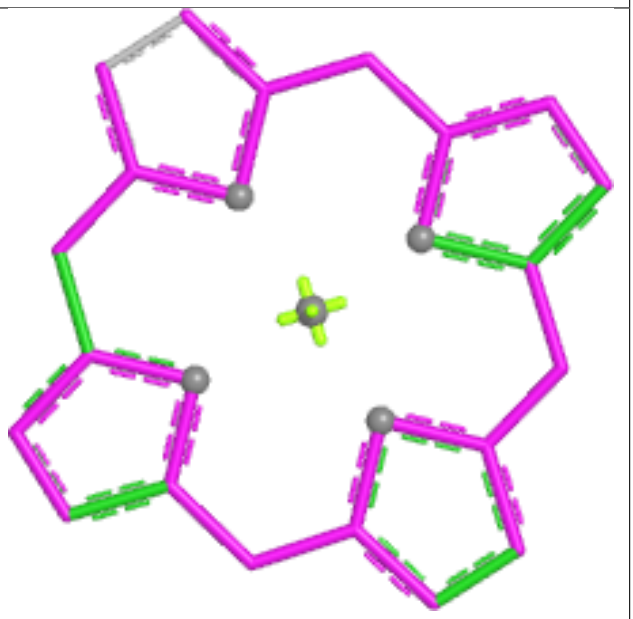


Rings

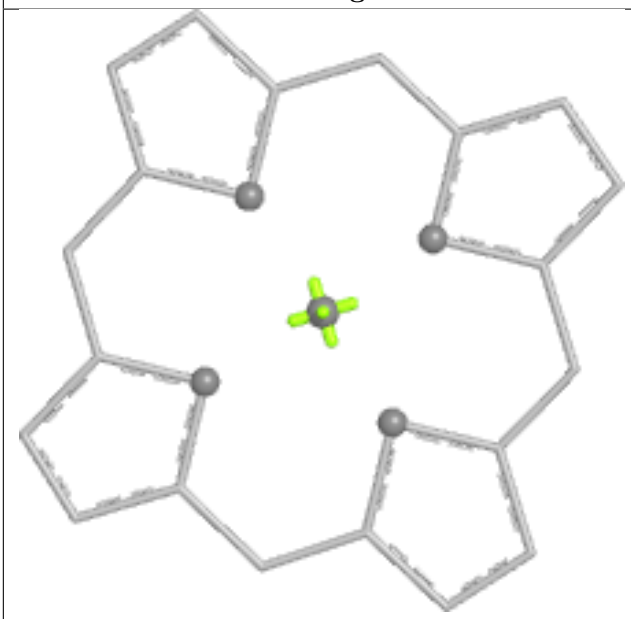
Ligand CLA 3 3006



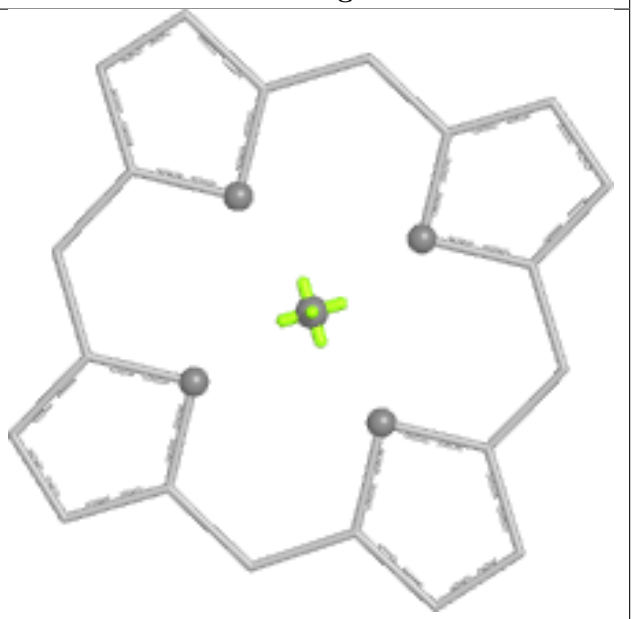
Bond lengths



Bond angles

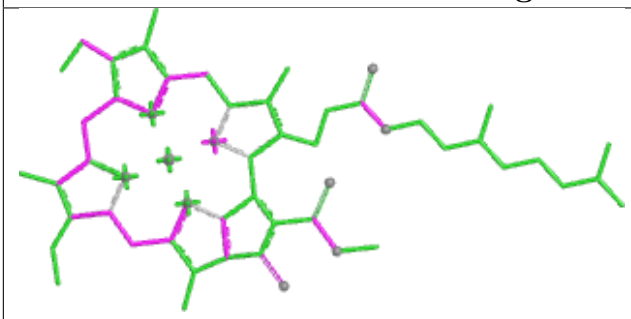


Torsions

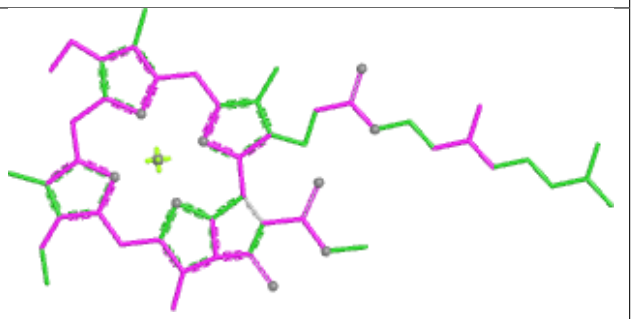


Rings

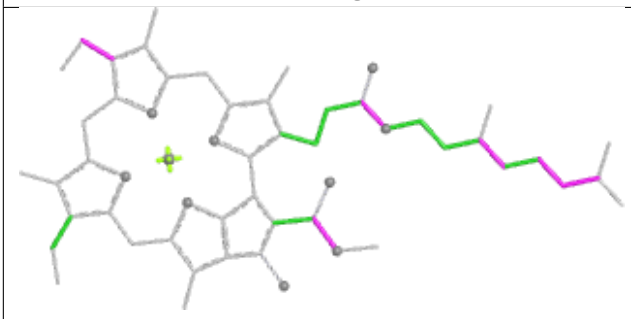
Ligand CLA B 1209



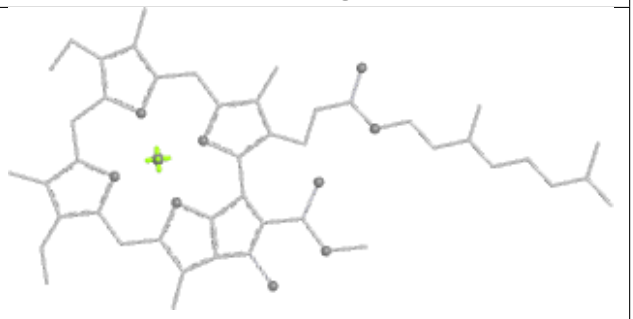
Bond lengths



Bond angles

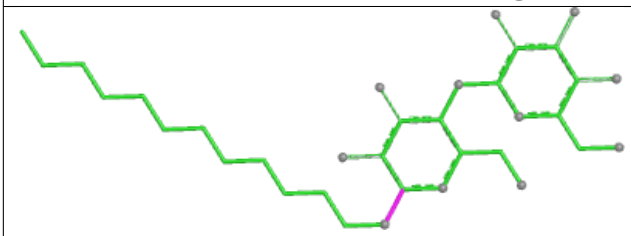


Torsions

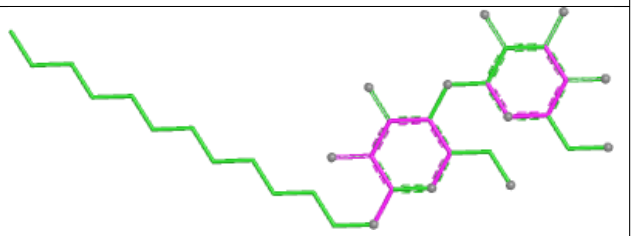


Rings

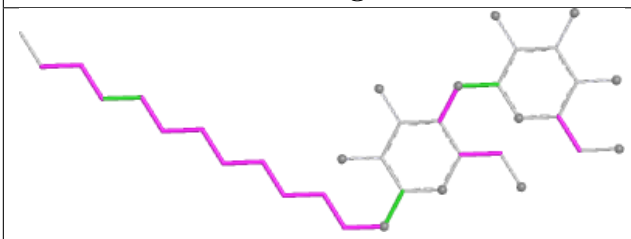
Ligand LMU A 7044



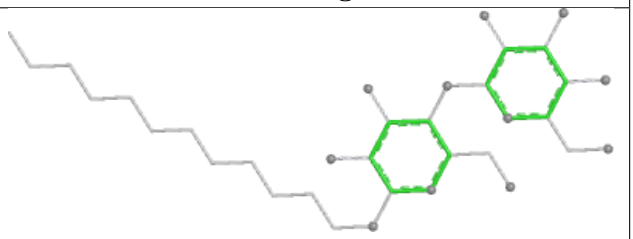
Bond lengths



Bond angles

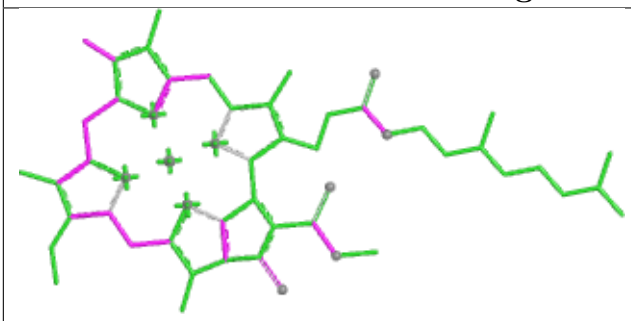


Torsions

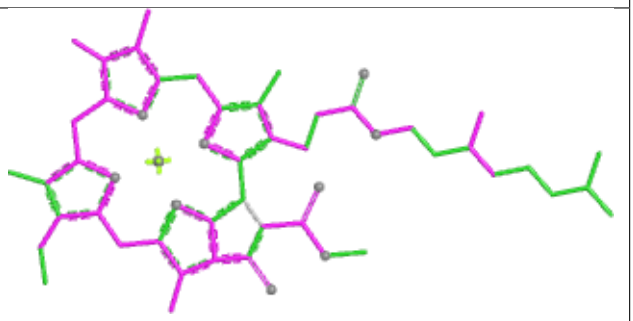


Rings

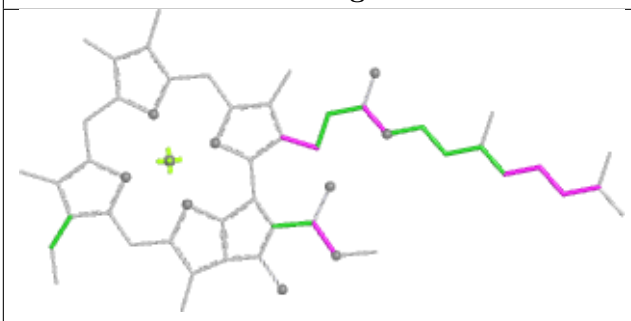
Ligand CLA B 1208



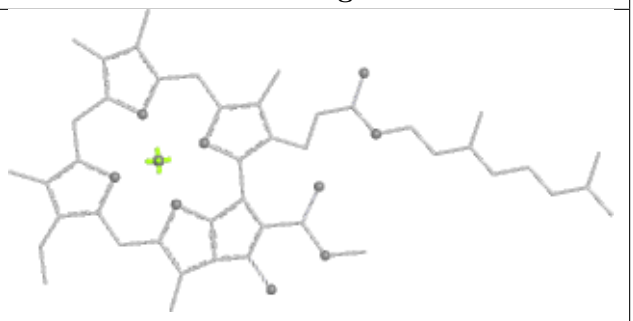
Bond lengths



Bond angles

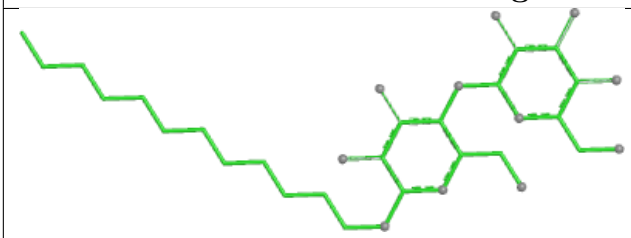


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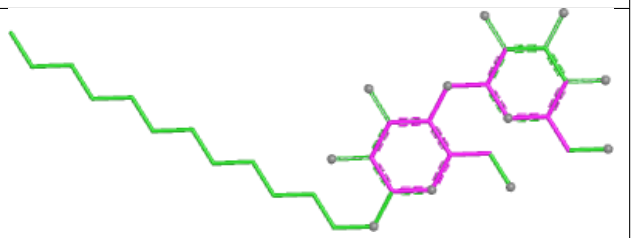


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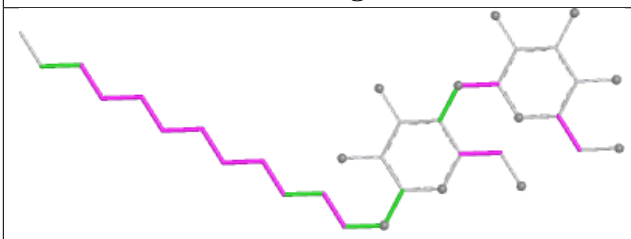
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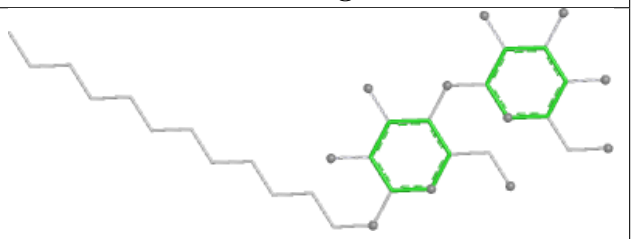
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Bond angles

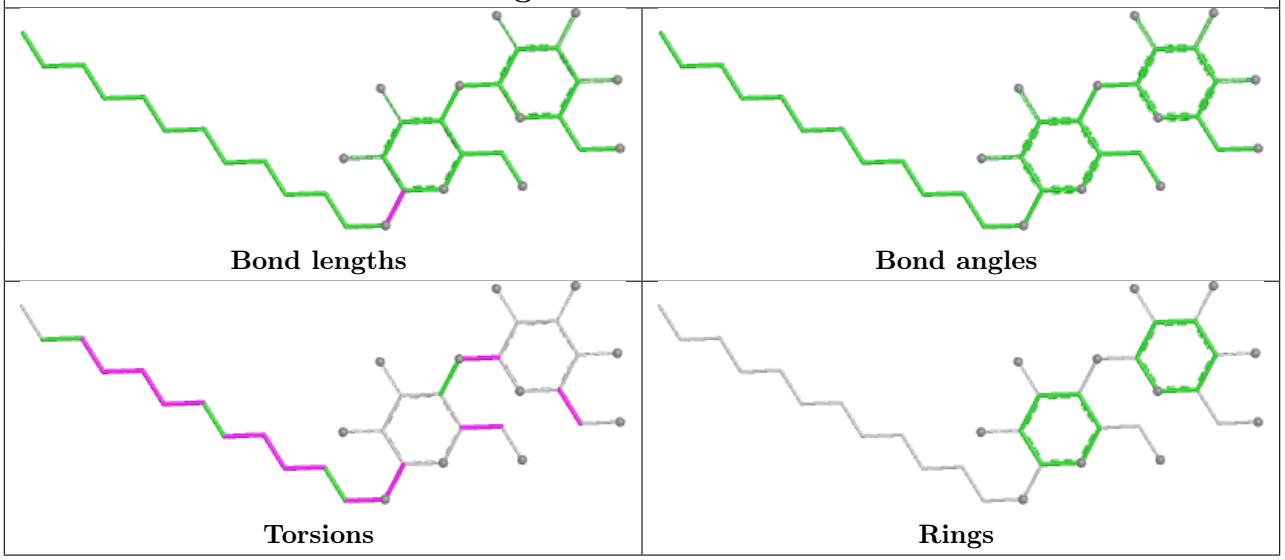


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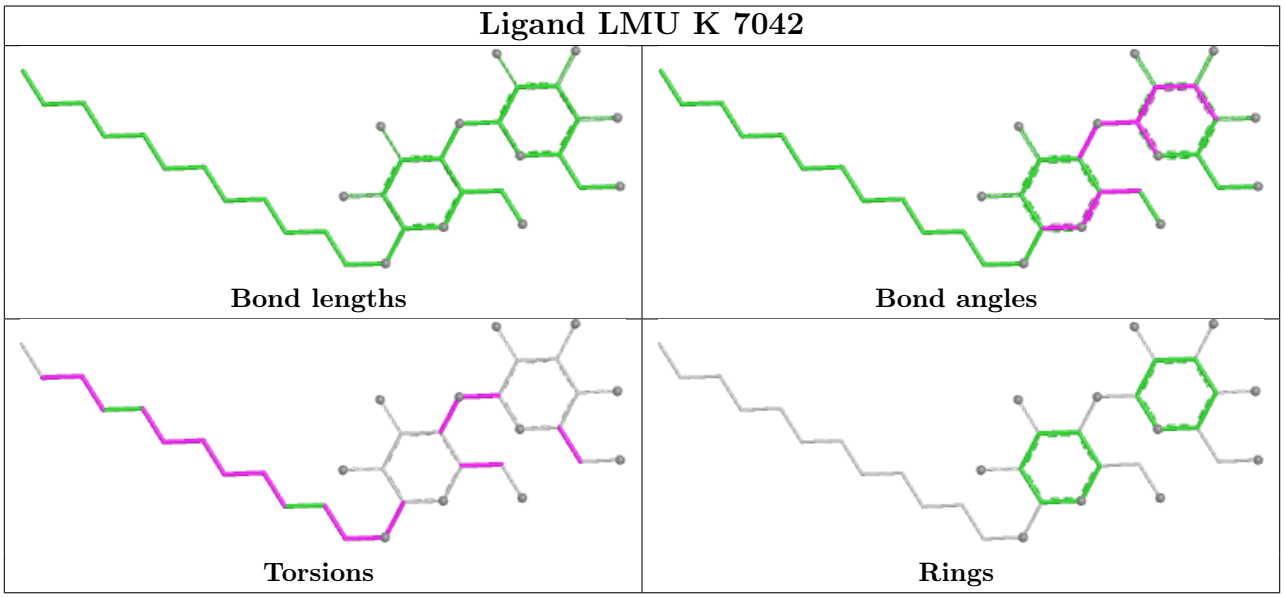


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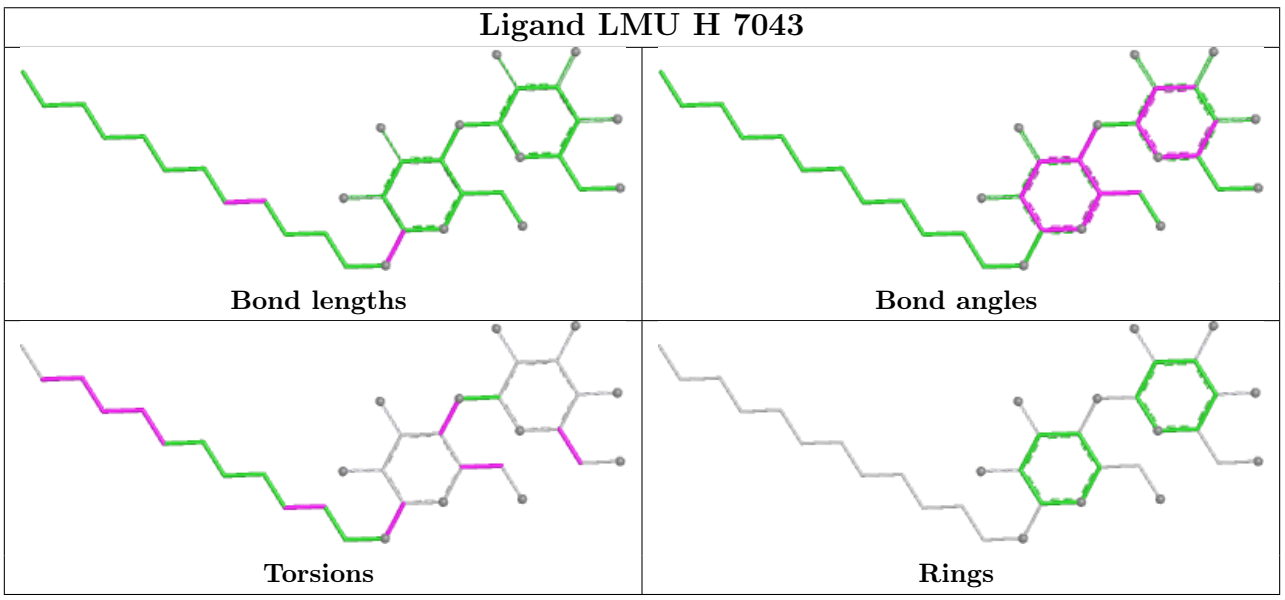
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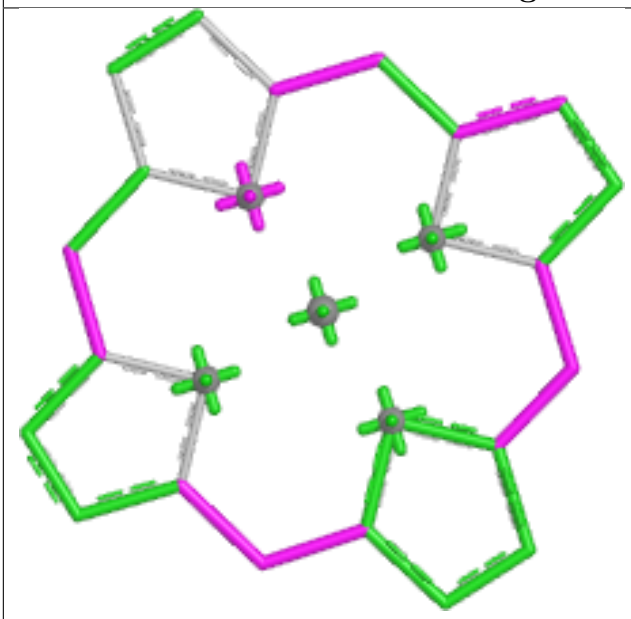
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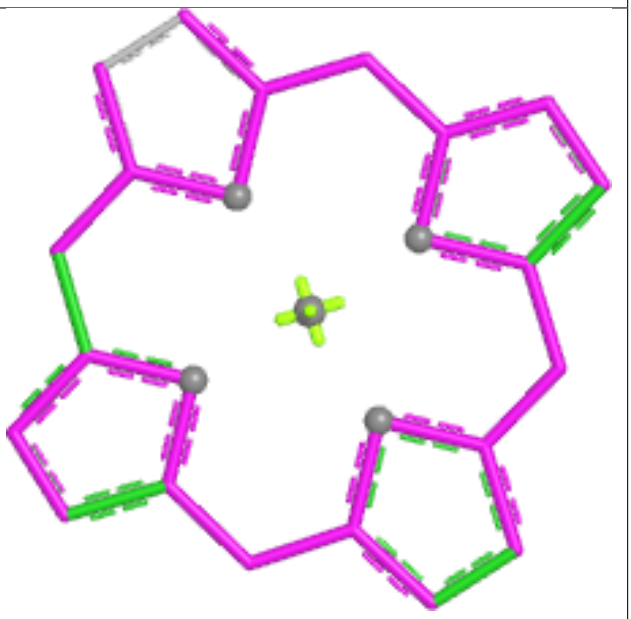
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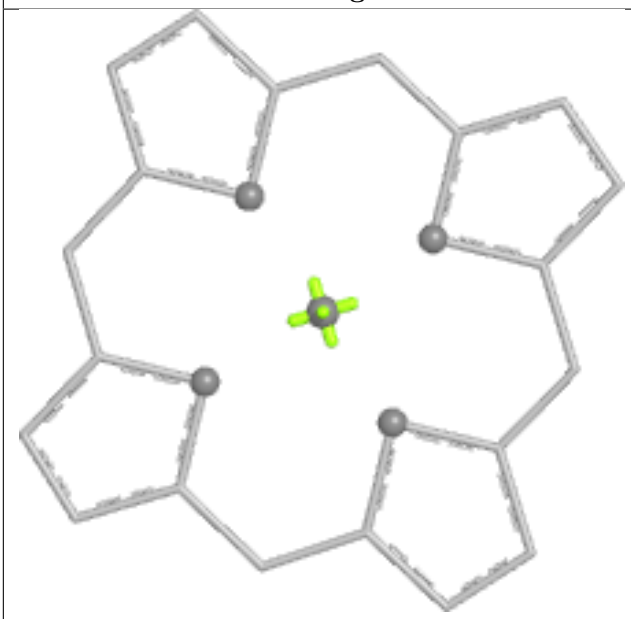
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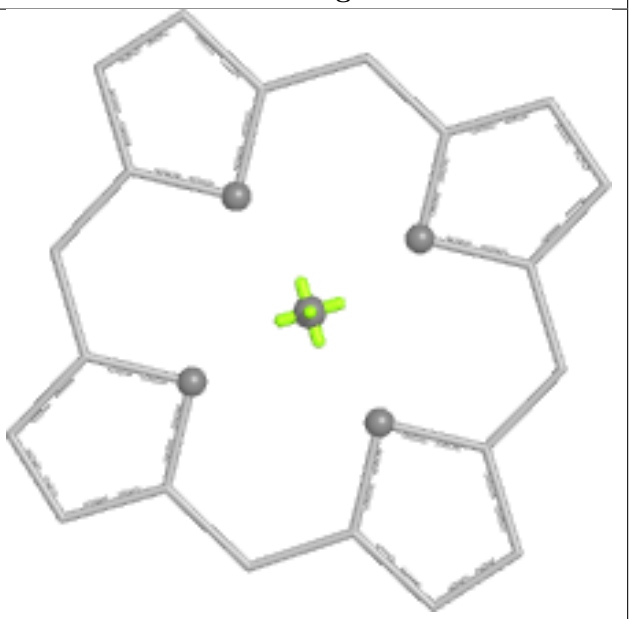
Bond lengths



Bond angles

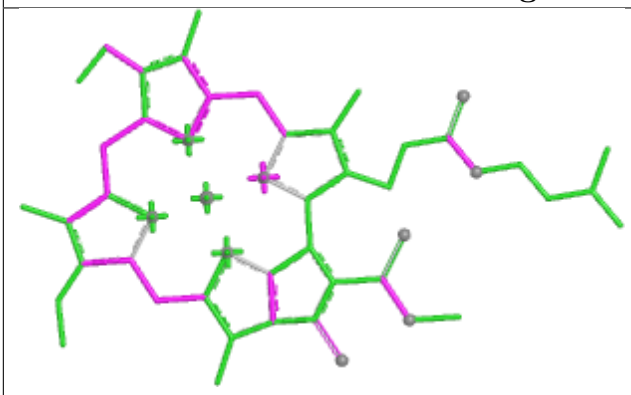


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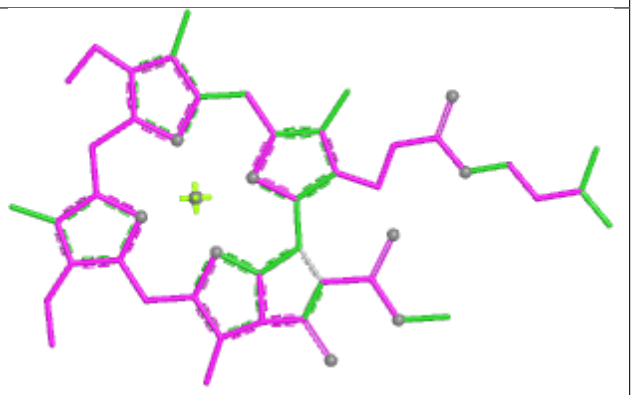


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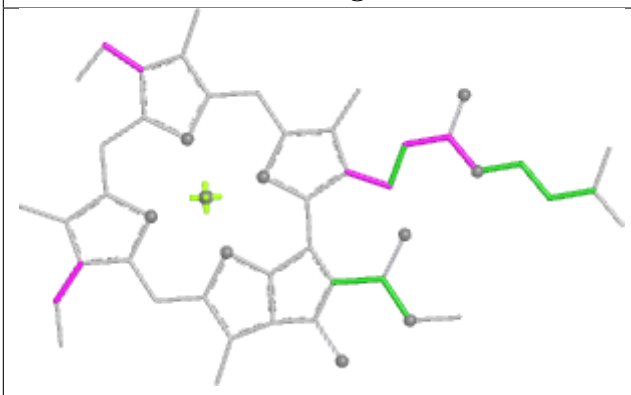
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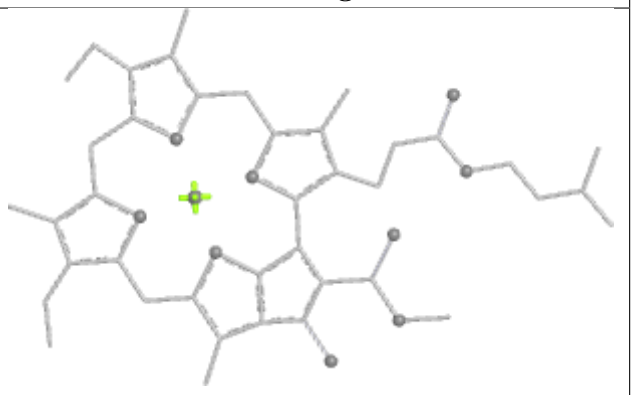
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Bond angles

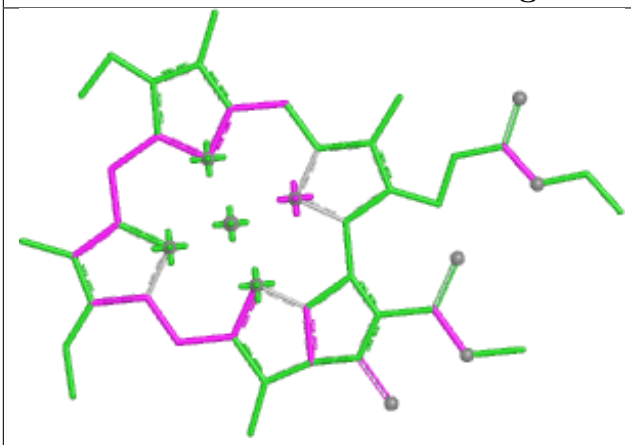


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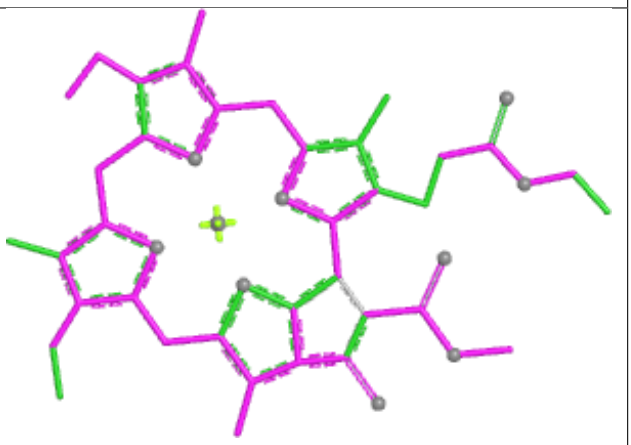


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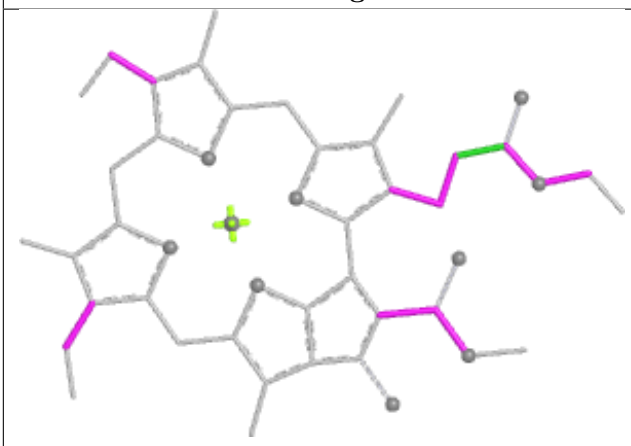
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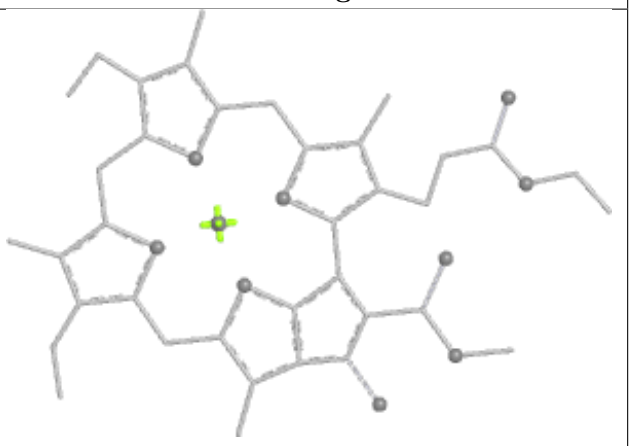
Bond lengths



Bond angles

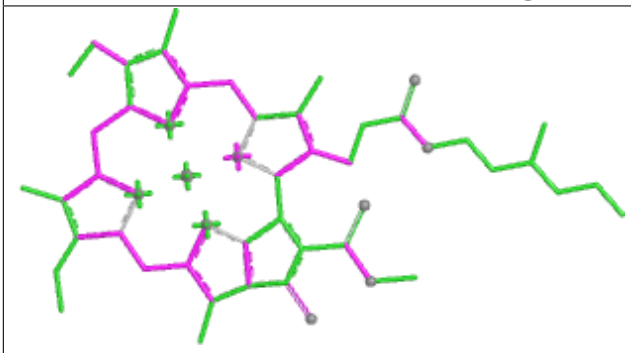


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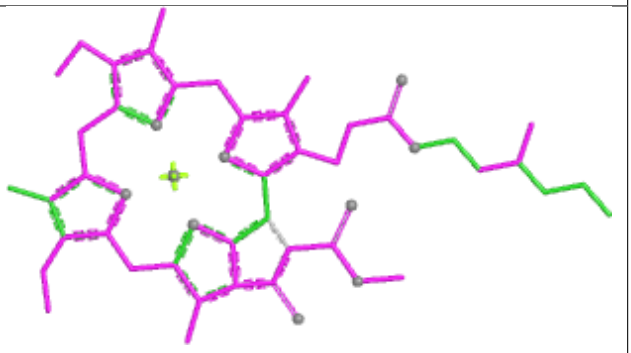


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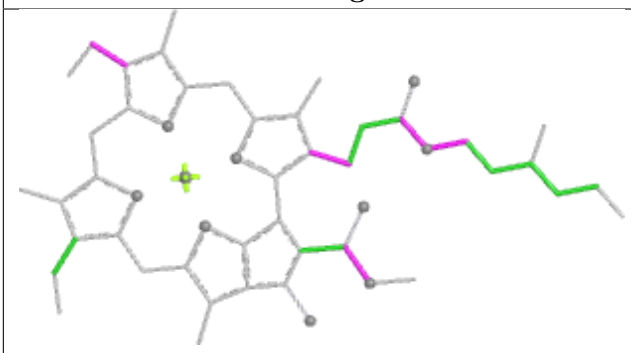
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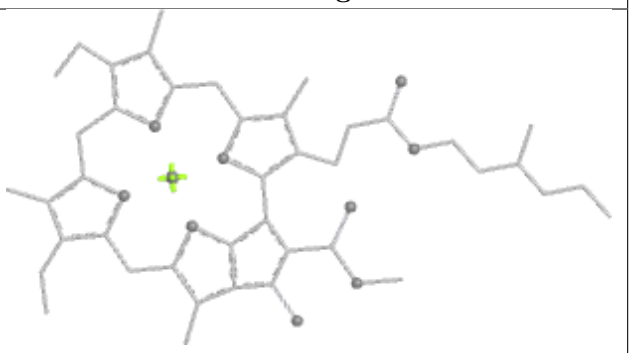
Bond lengths



Bond angles

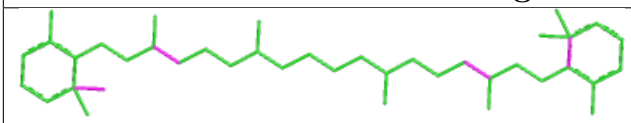


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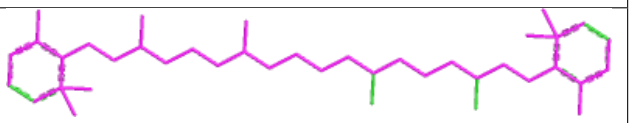


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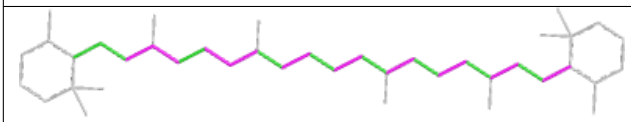
Ligand BCR B 6004



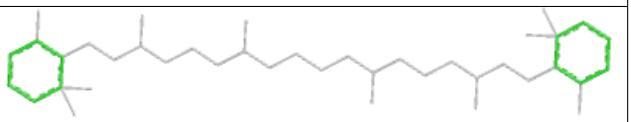
Bond lengths



Bond angles



Torsions



Rings

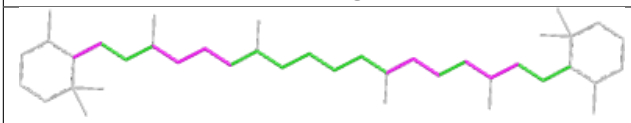
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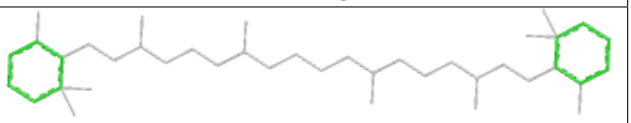
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Bond angles

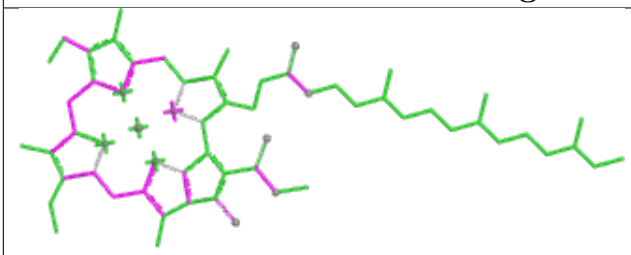


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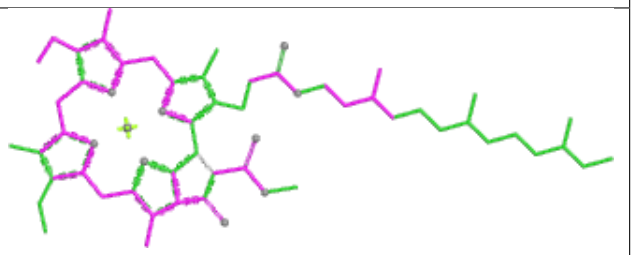


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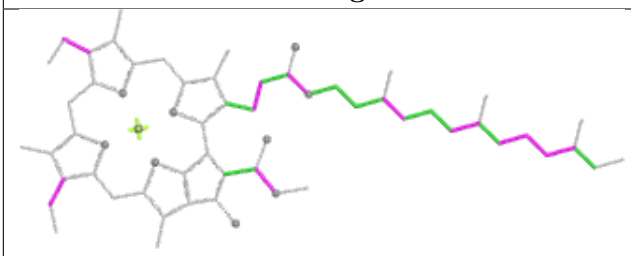
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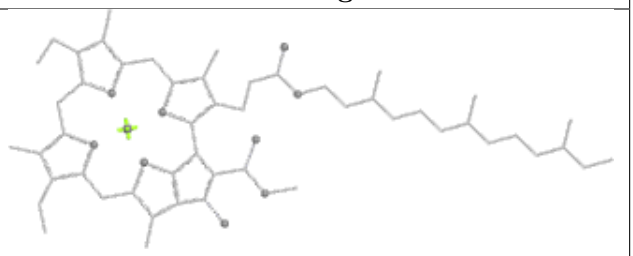
Bond lengths



Bond angles

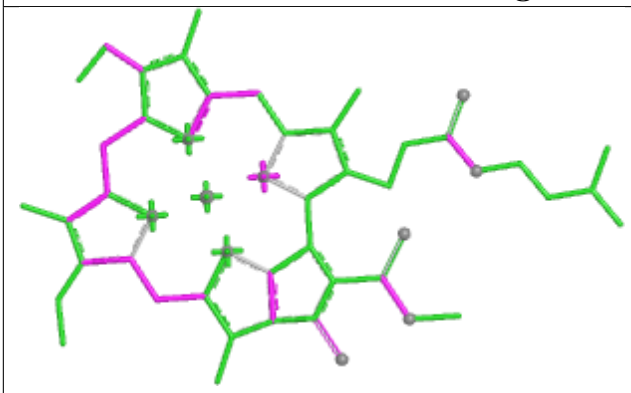


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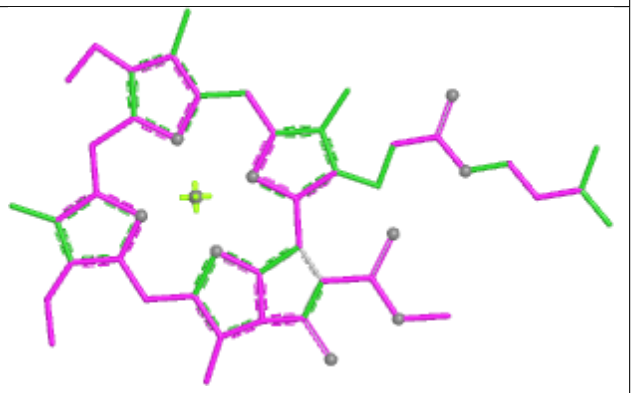


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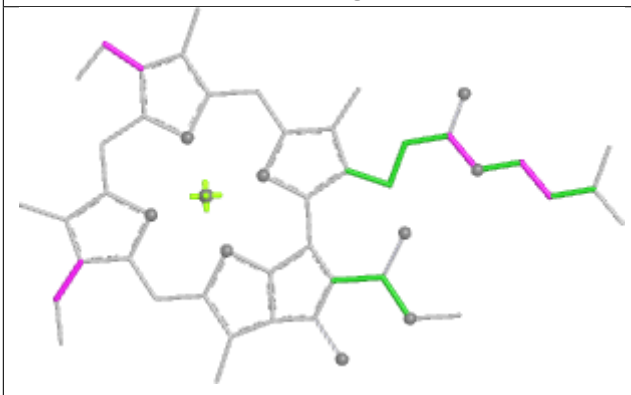
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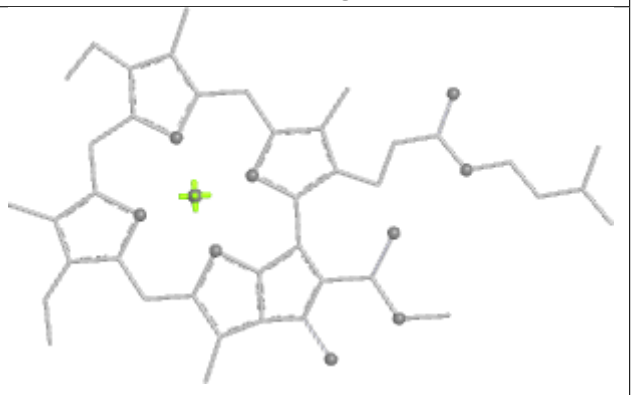
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Bond angles

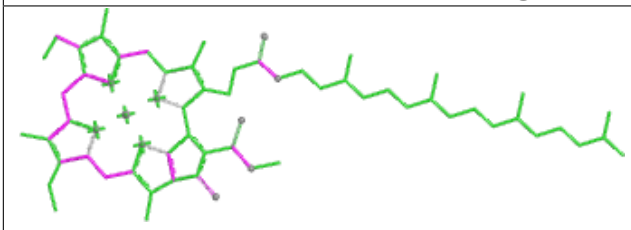


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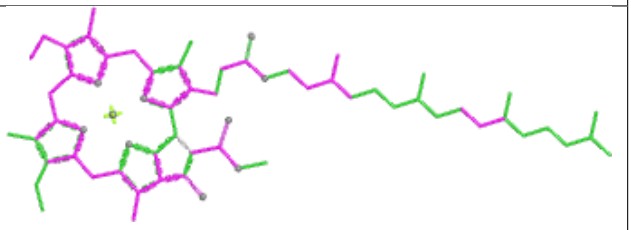


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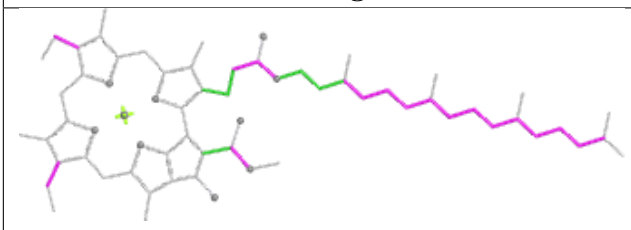
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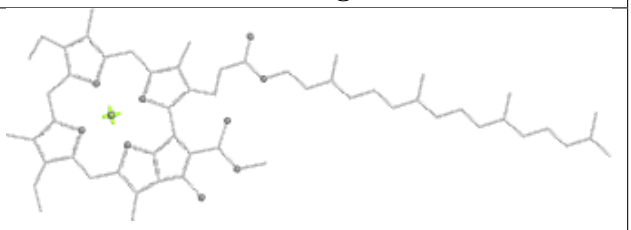
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Bond angles

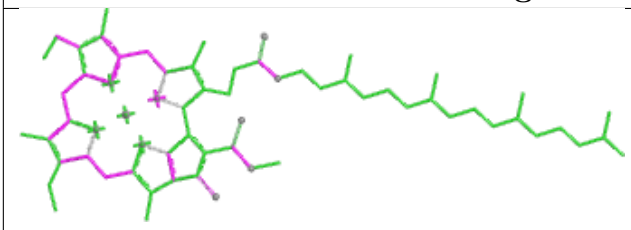


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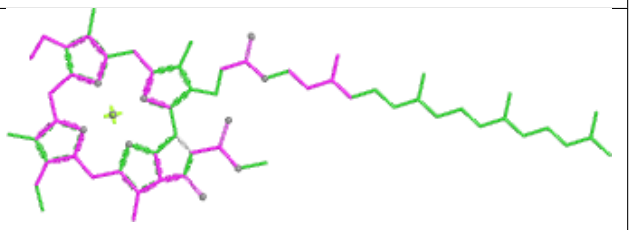


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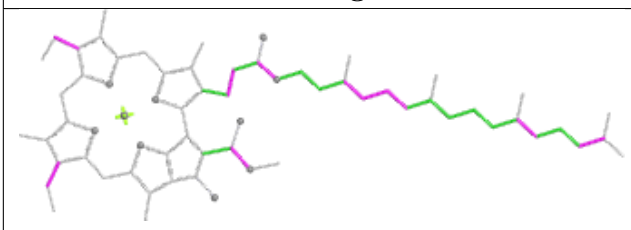
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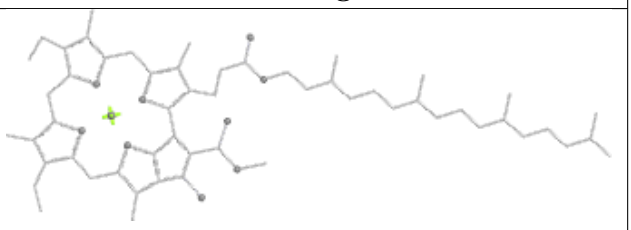
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Bond angles

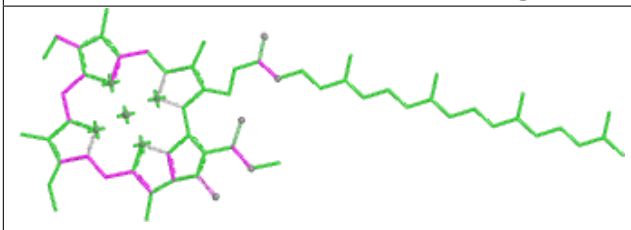


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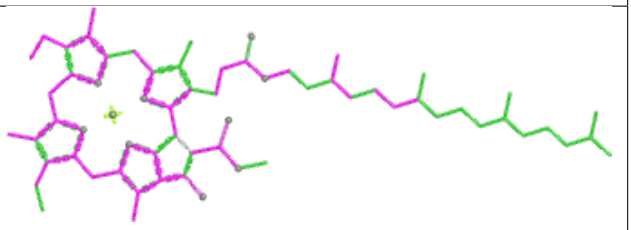


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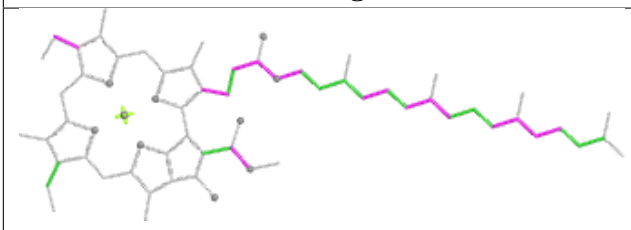
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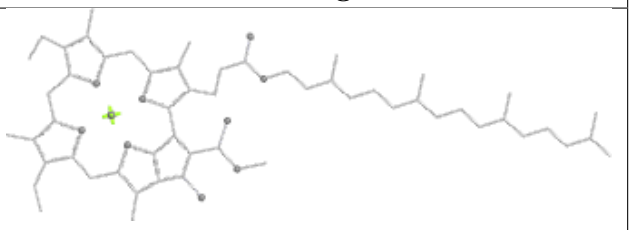
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Bond angles

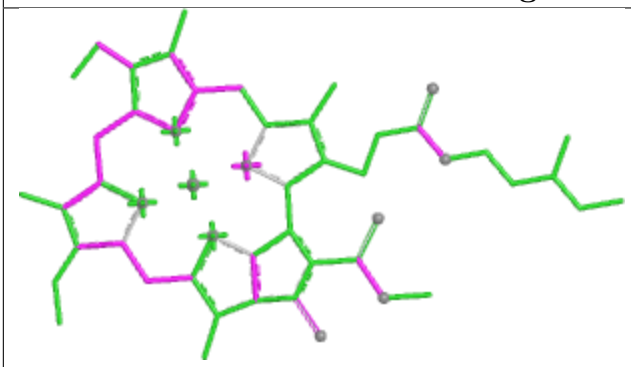


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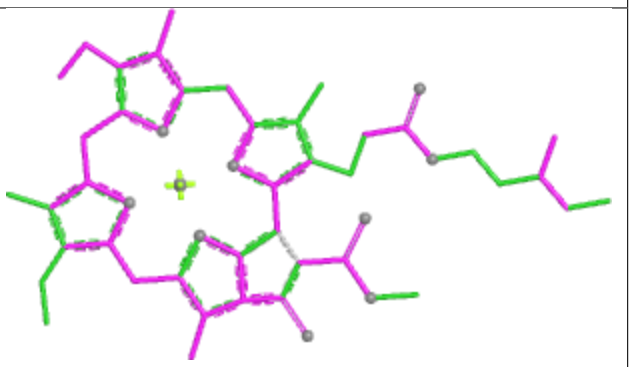


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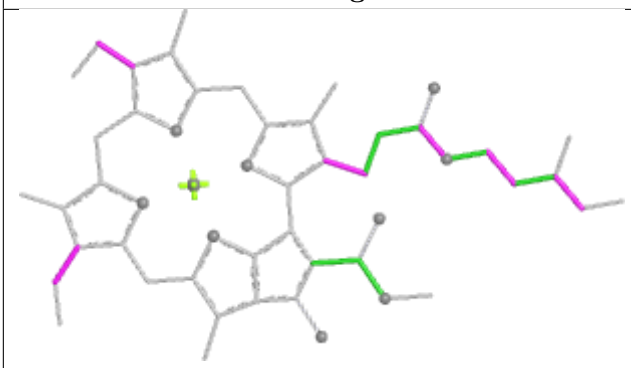
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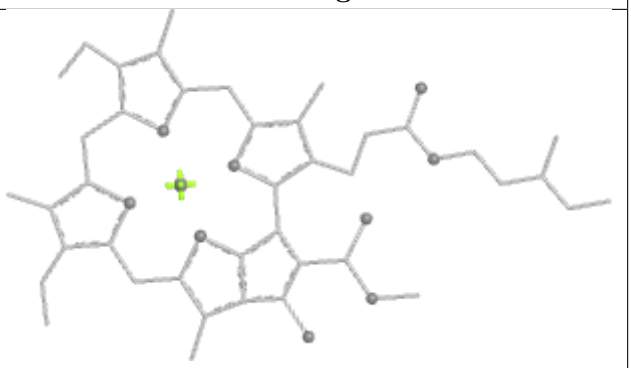
Bond lengths



Bond angles

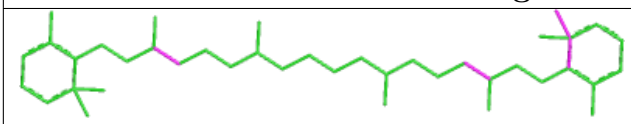


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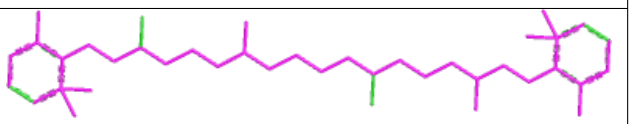


Rings

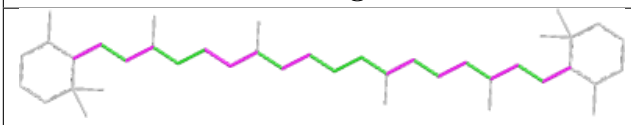
Ligand BCR A 6008



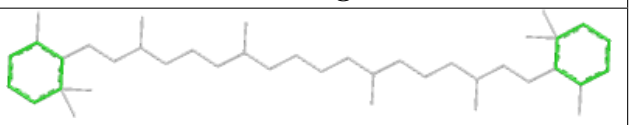
Bond lengths



Bond angles

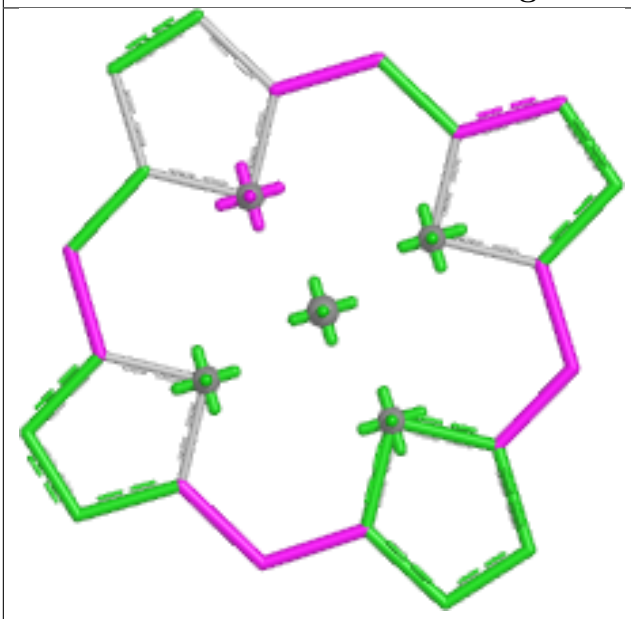


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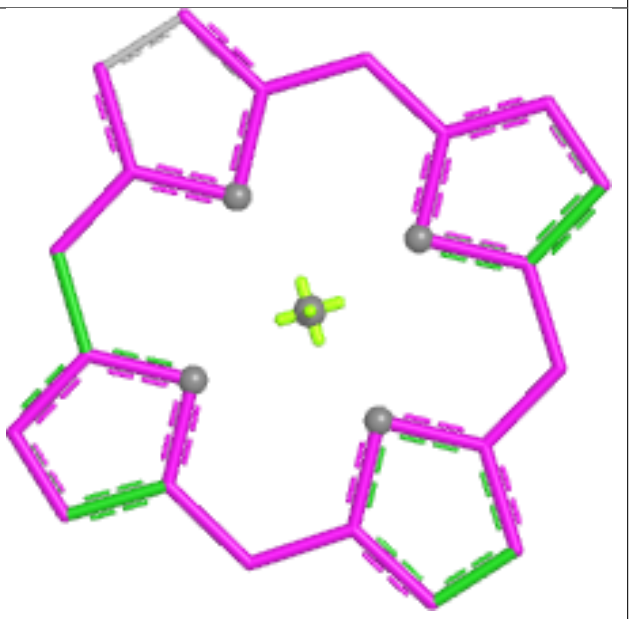


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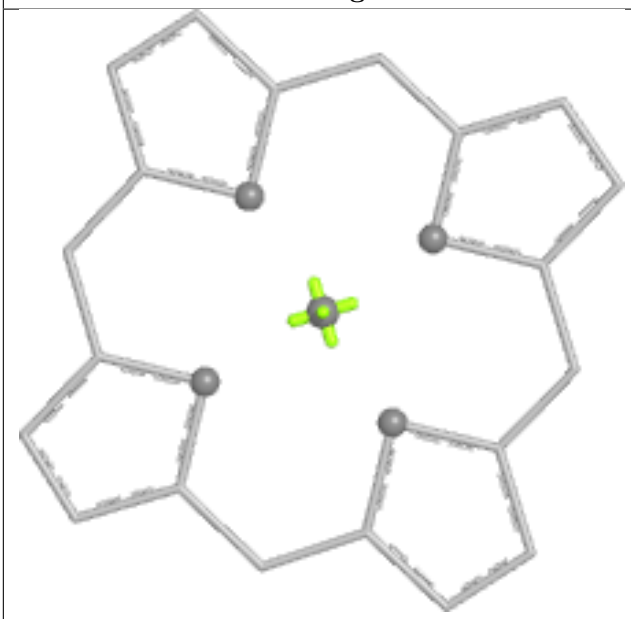
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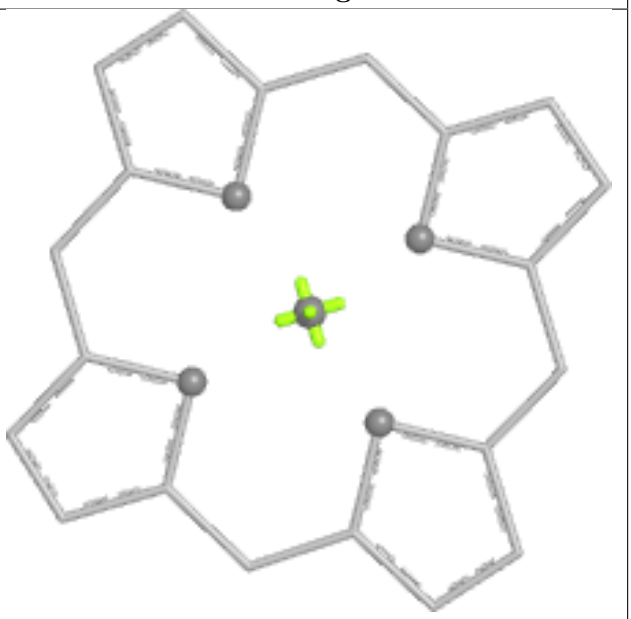
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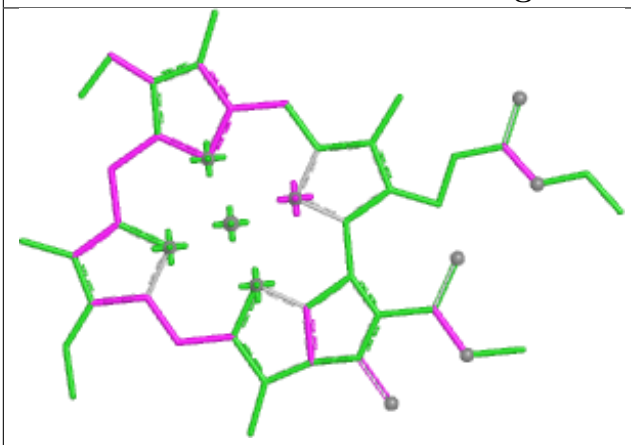


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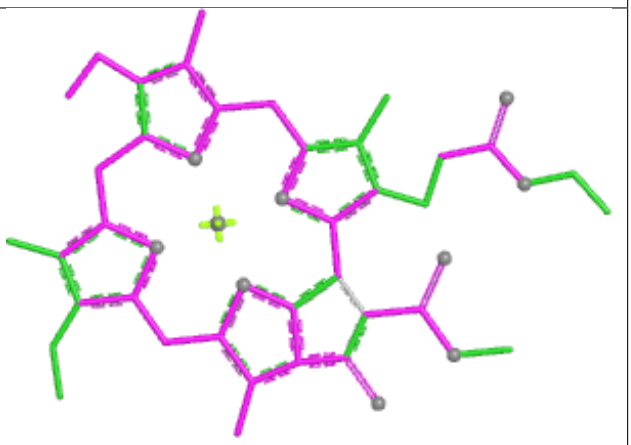


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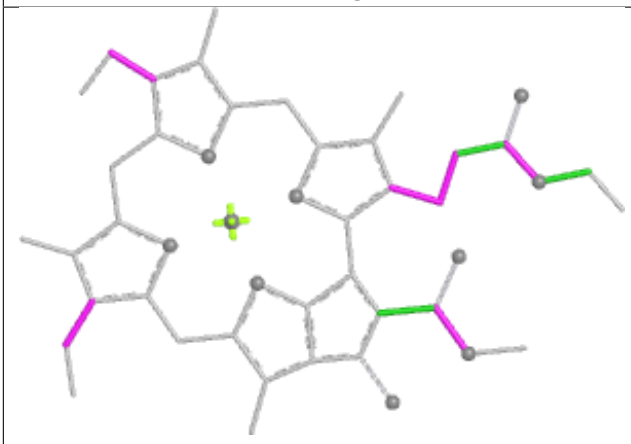
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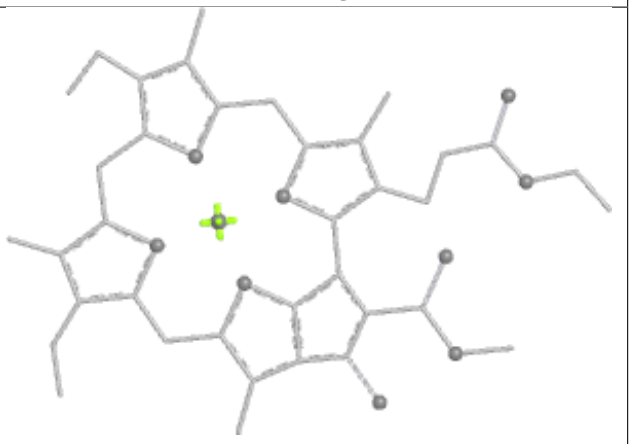
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Bond angles

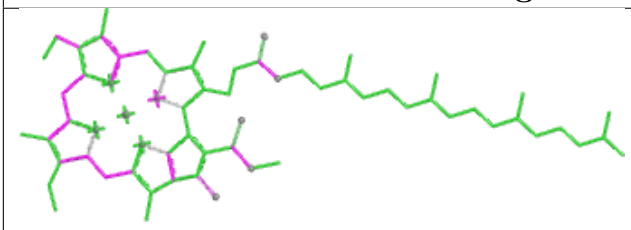


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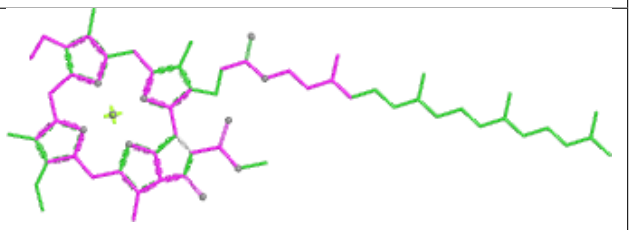


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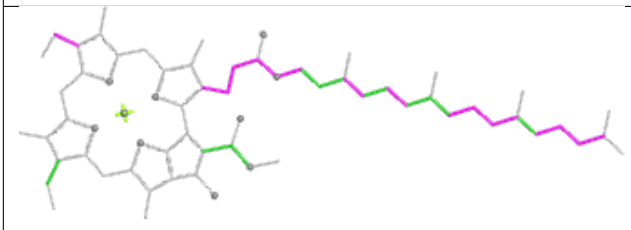
Ligand CLA B 1223



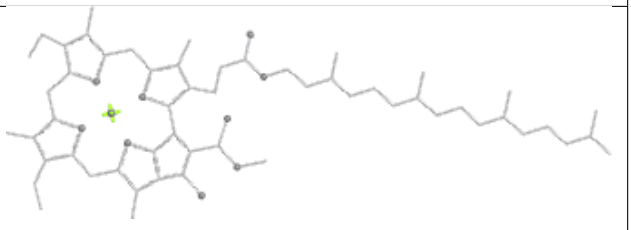
Bond lengths



Bond angles

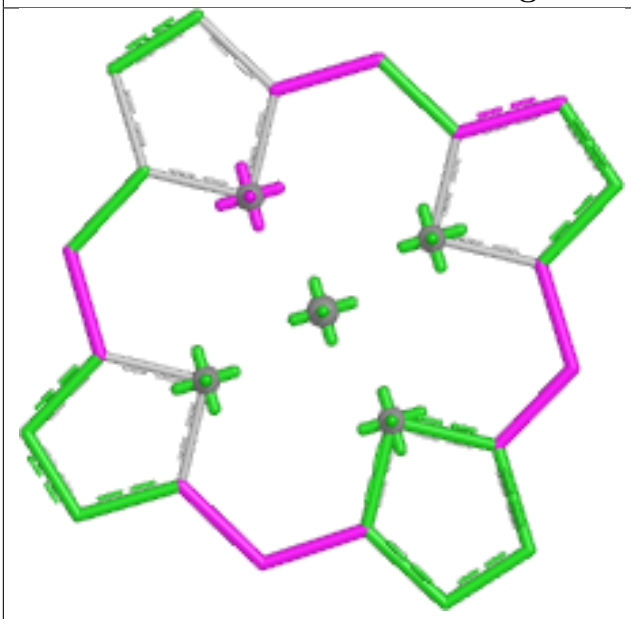


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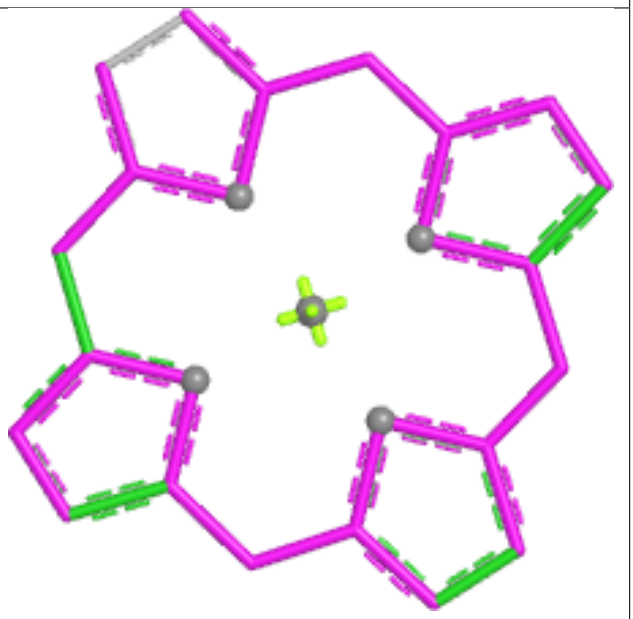


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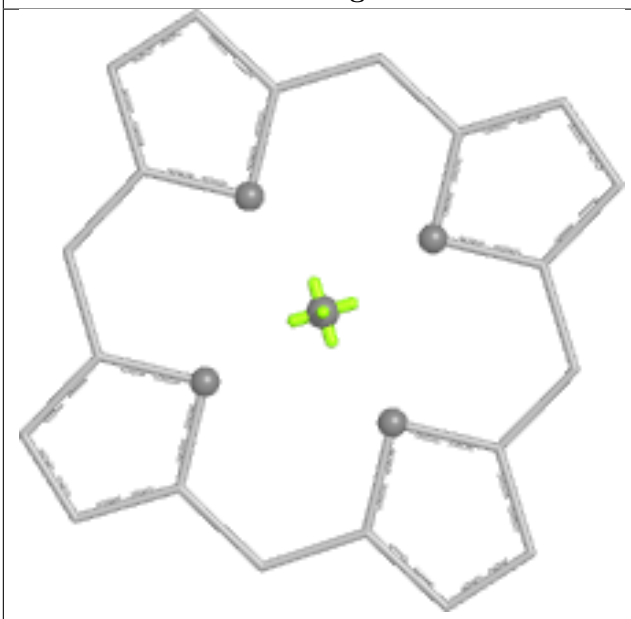
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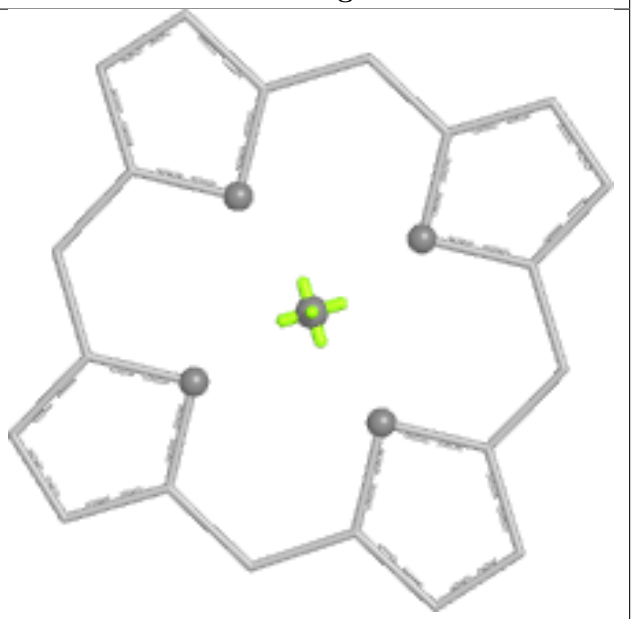
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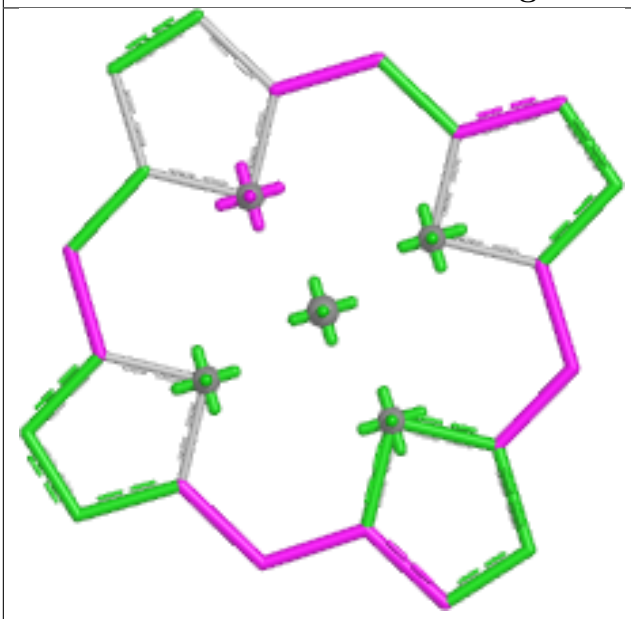


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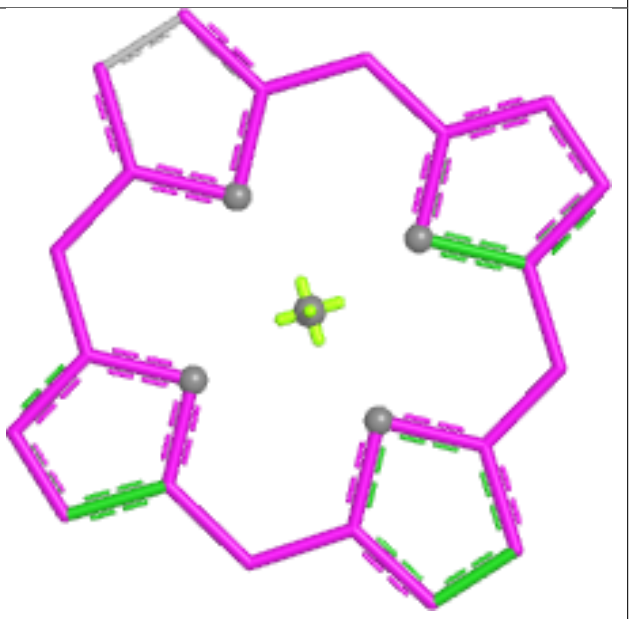


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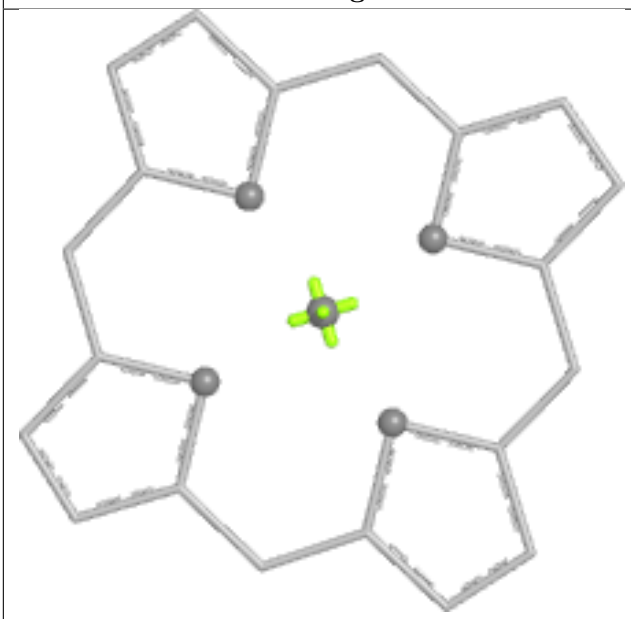
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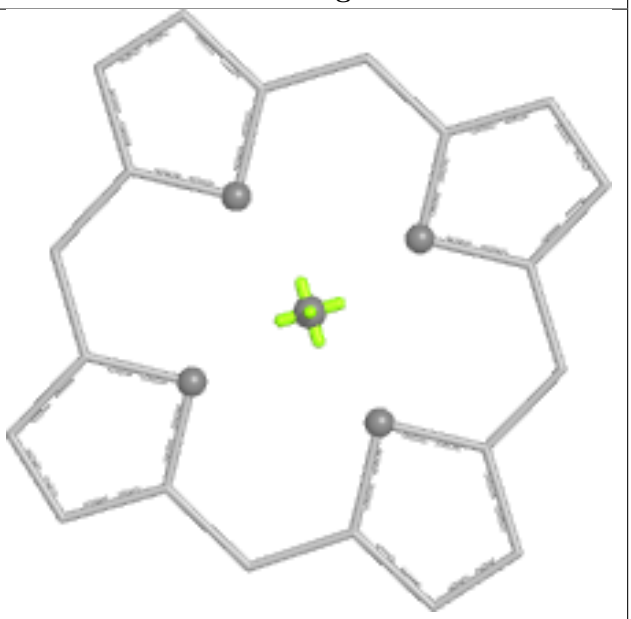
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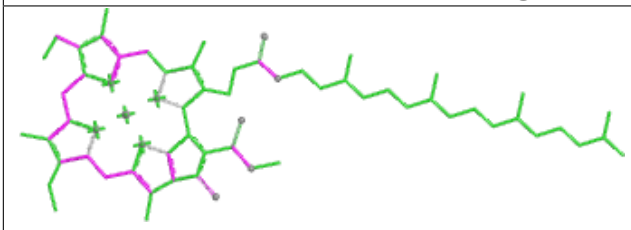


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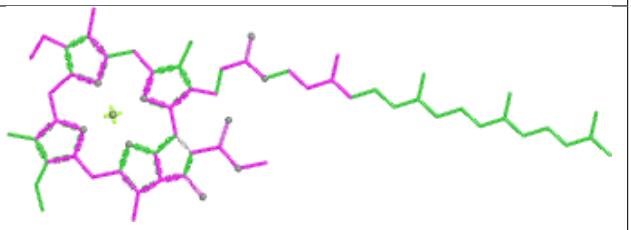


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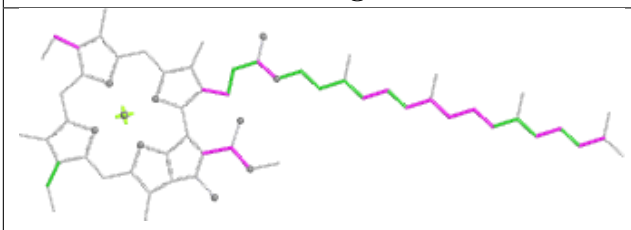
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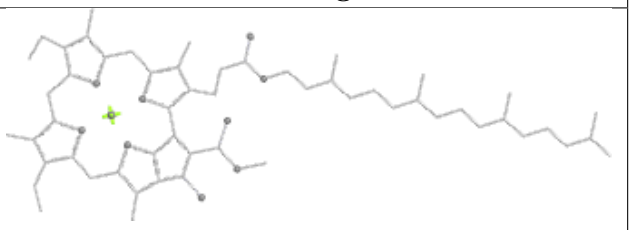
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Bond angles

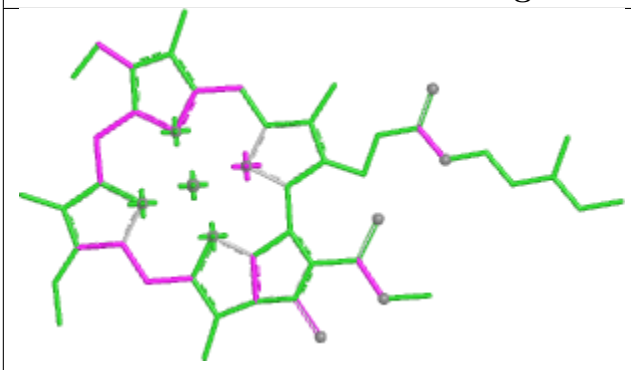


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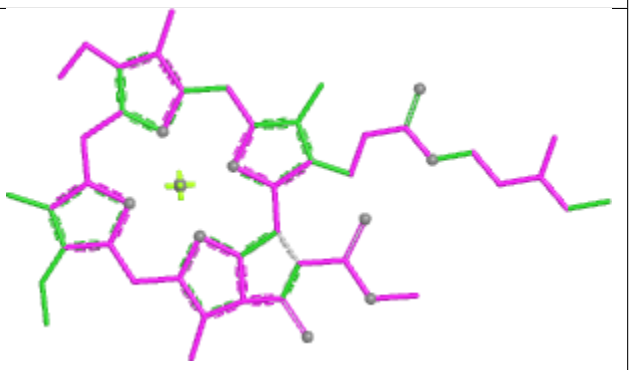


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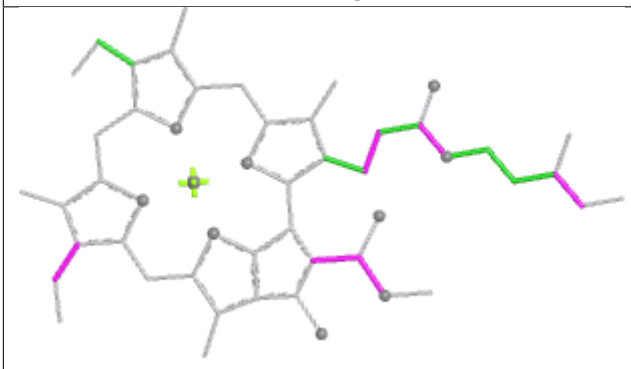
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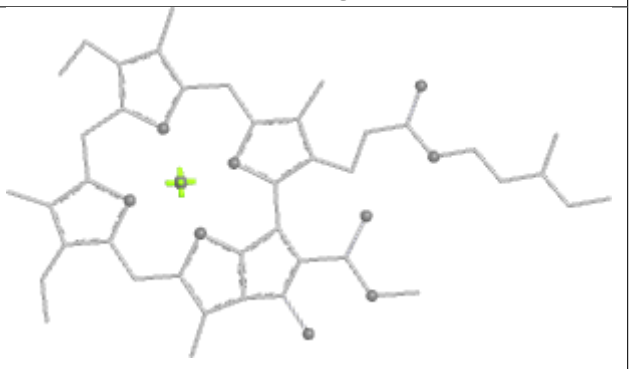
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Bond angles

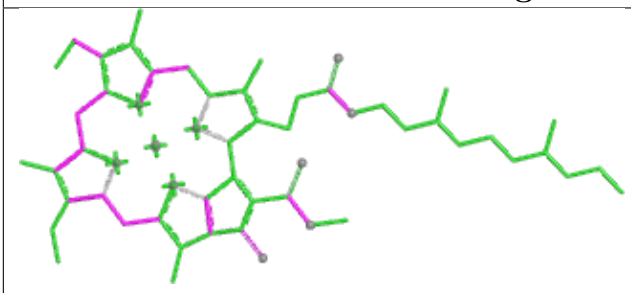


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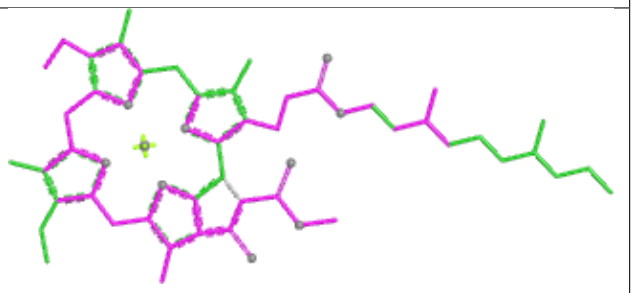


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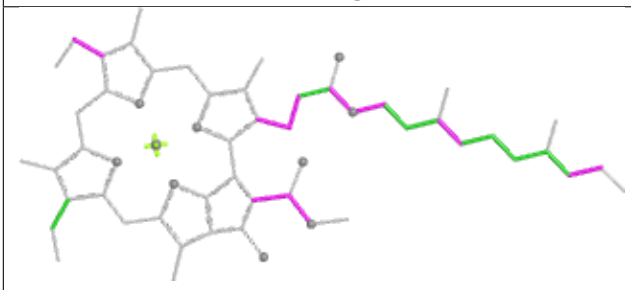
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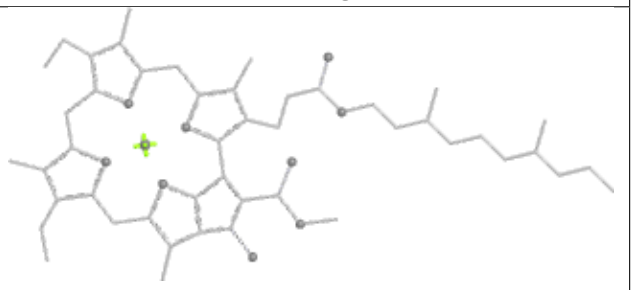
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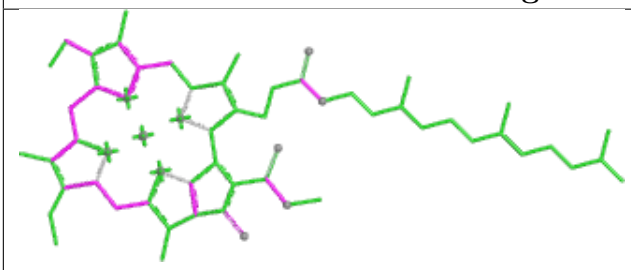


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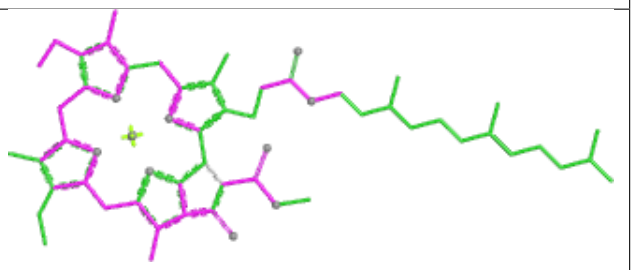


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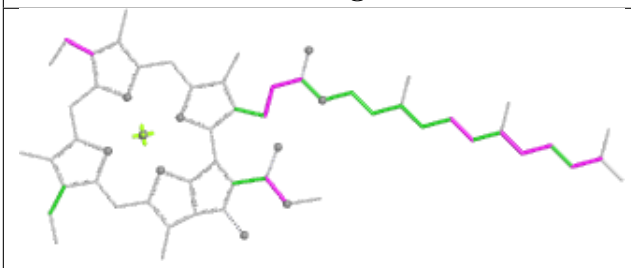
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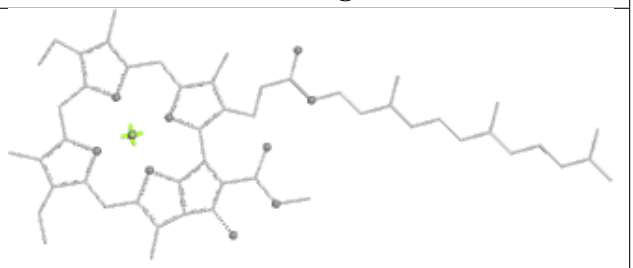
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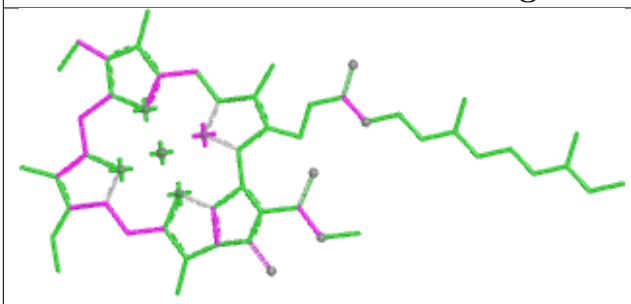


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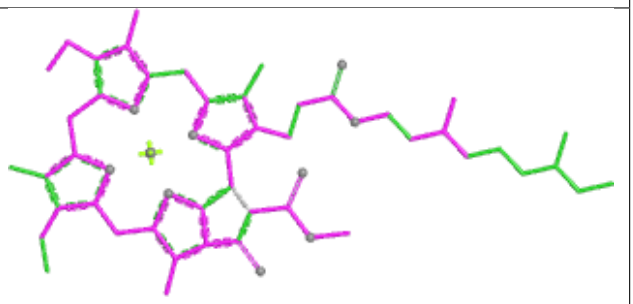


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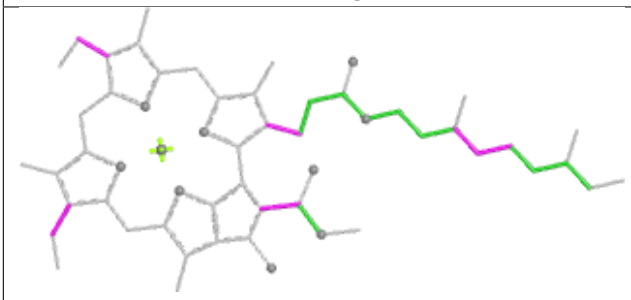
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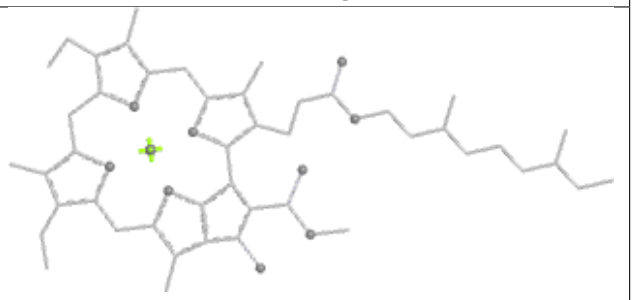
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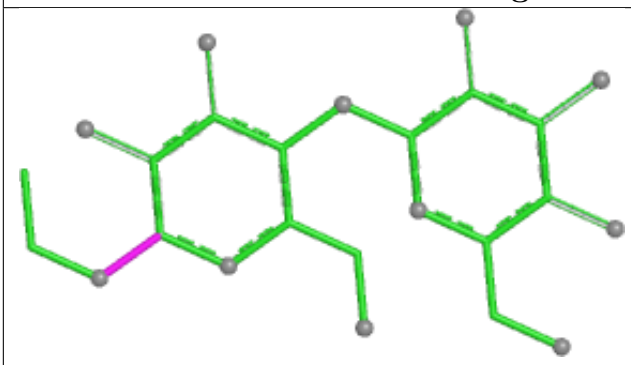


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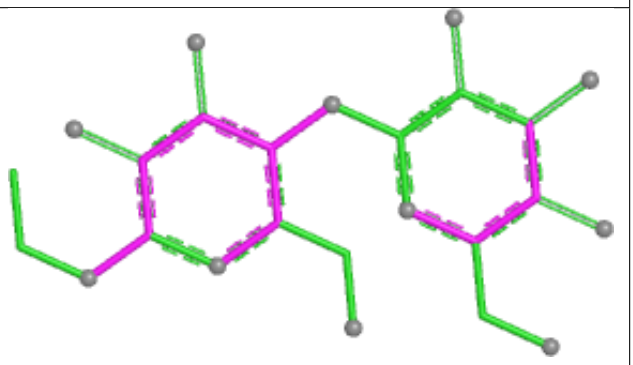


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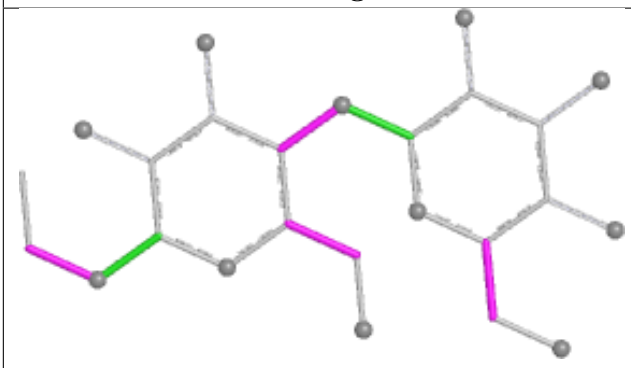
Ligand LMU B 7012



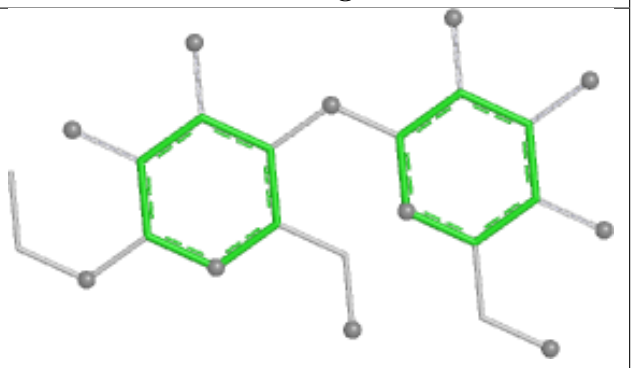
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Bond angles

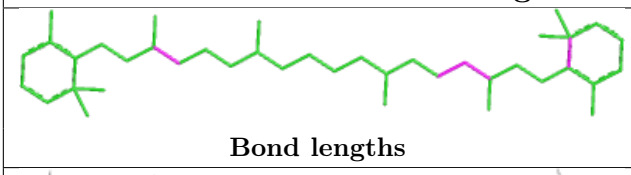


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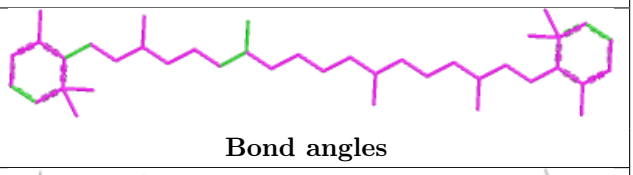


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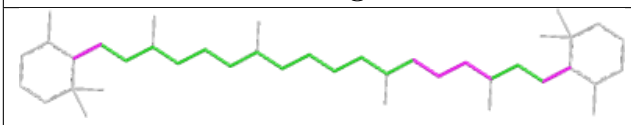
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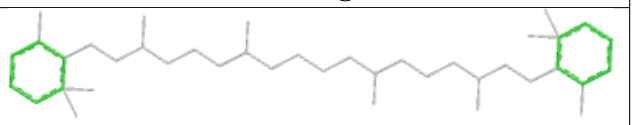
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Bond angles

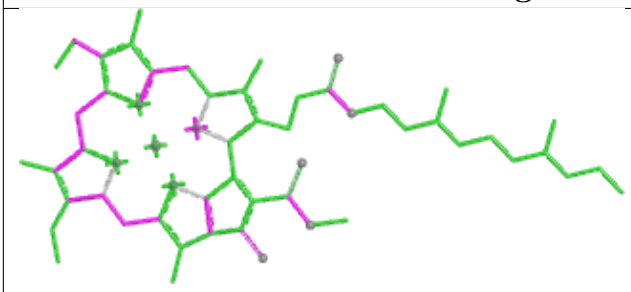


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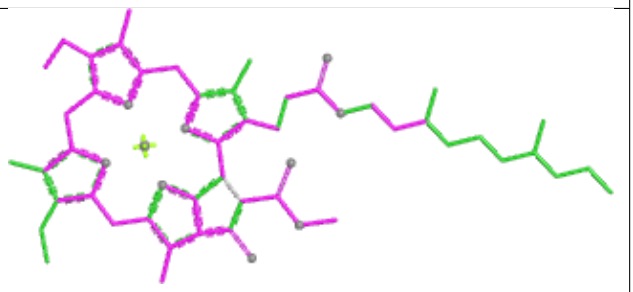


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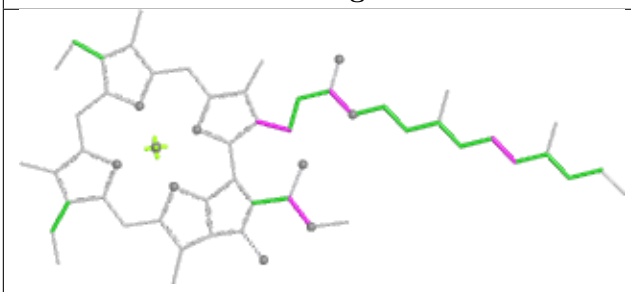
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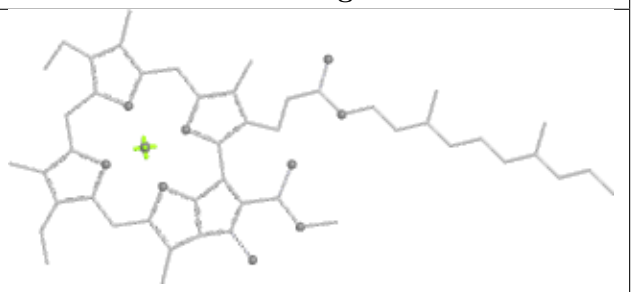
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Bond angles

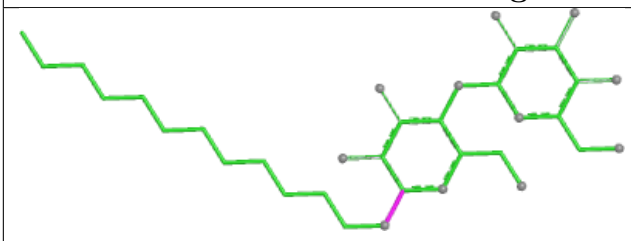


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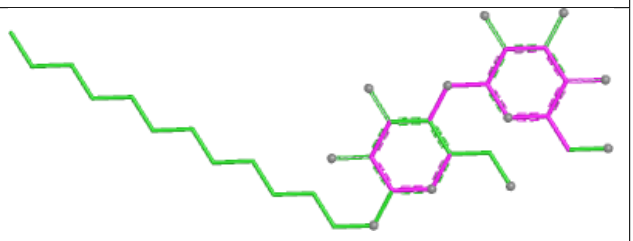


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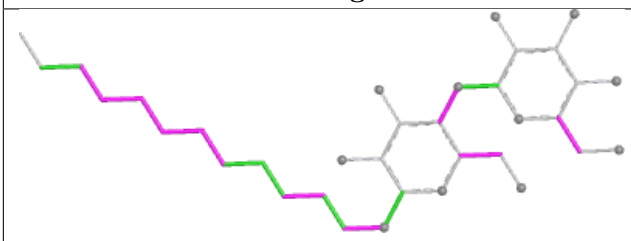
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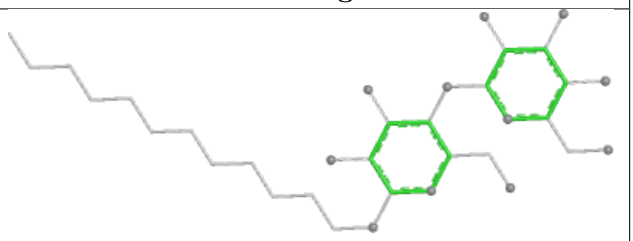
Bond lengths



Bond angles

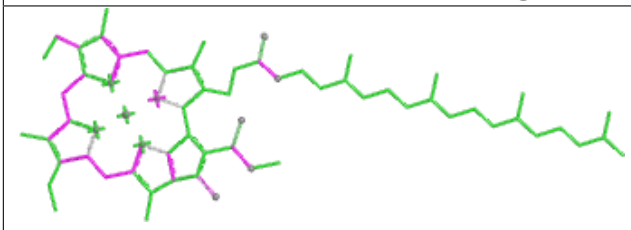


Torsions

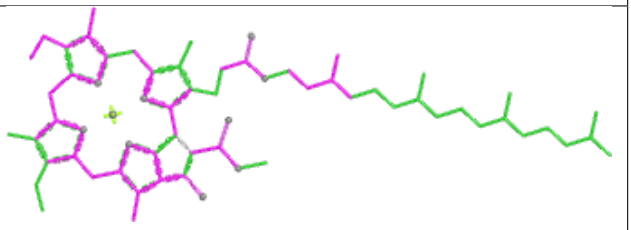


Rings

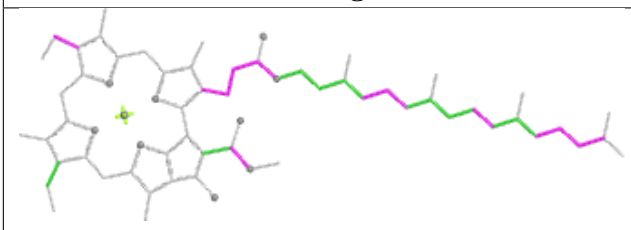
Ligand CLA A 1140



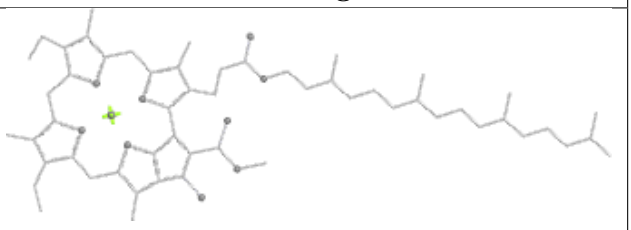
Bond lengths



Bond angles

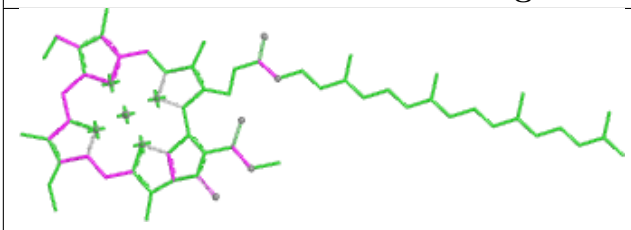


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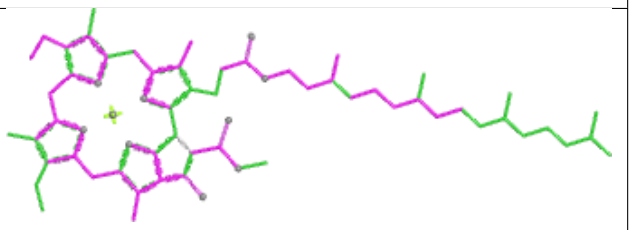


Rings

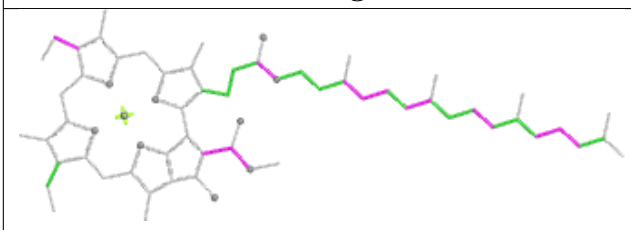
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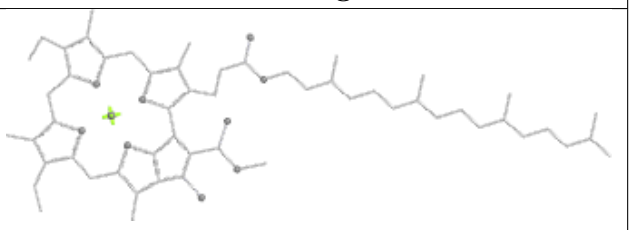
Bond lengths



Bond angles

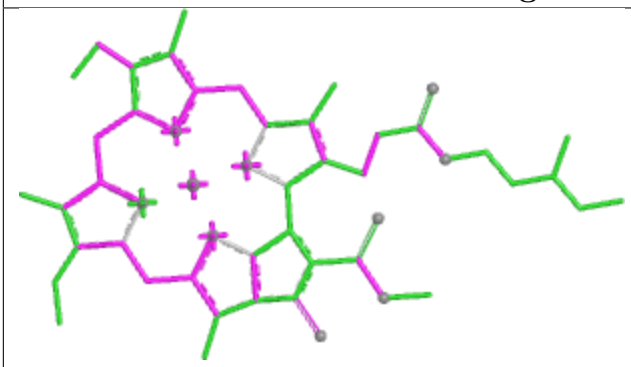


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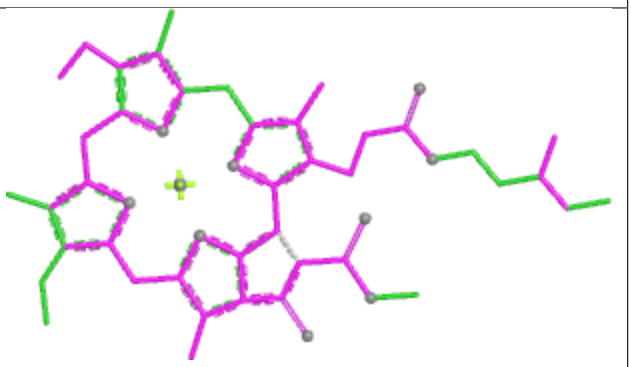


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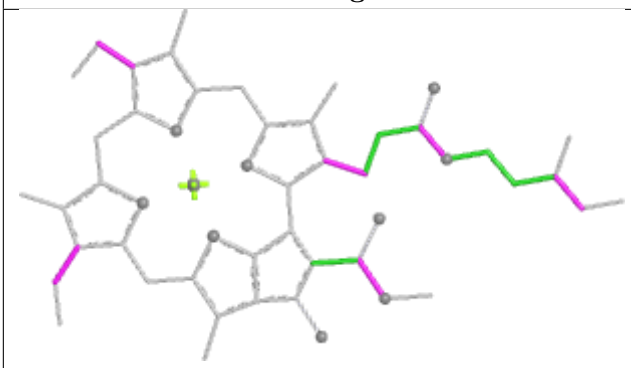
Ligand CLA 1 1303



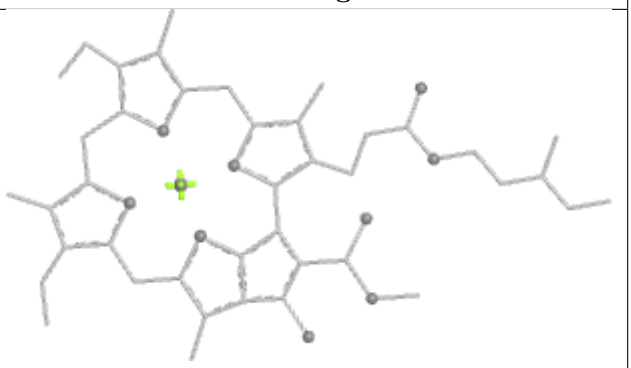
Bond lengths



Bond angles

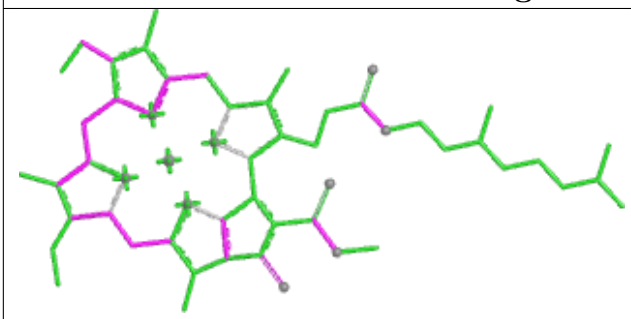


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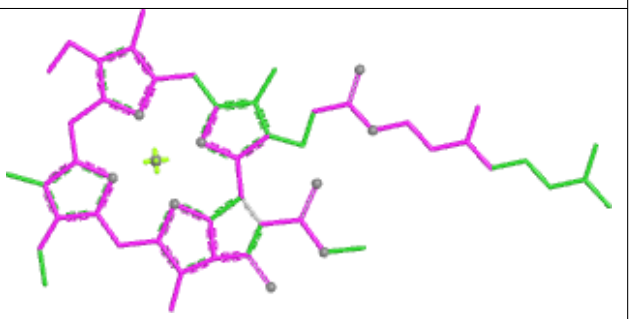


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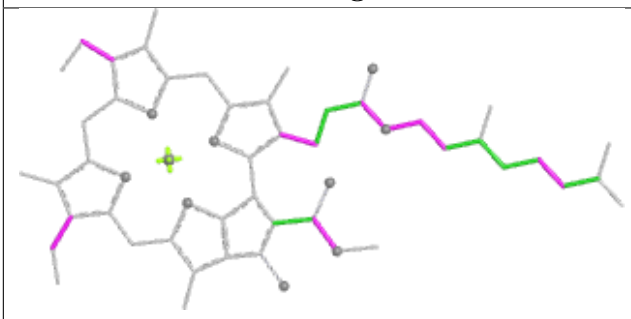
Ligand CLA A 1107



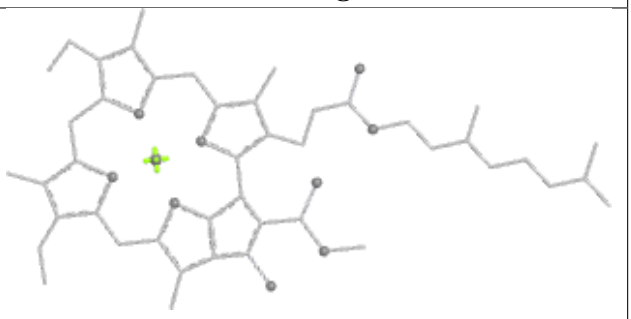
Bond lengths



Bond angles

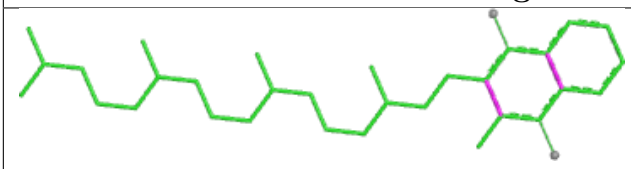


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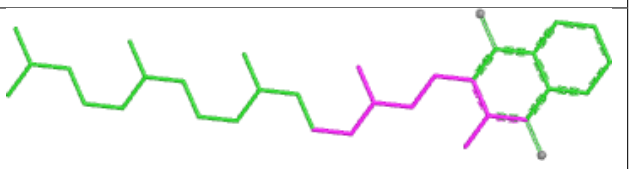


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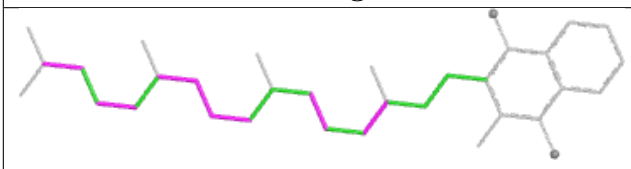
Ligand PQN B 5002



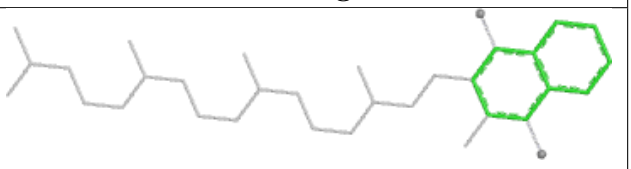
Bond lengths



Bond angles

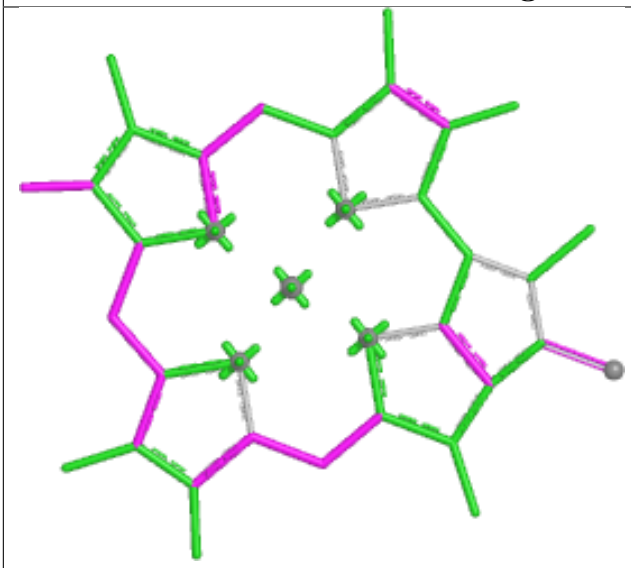


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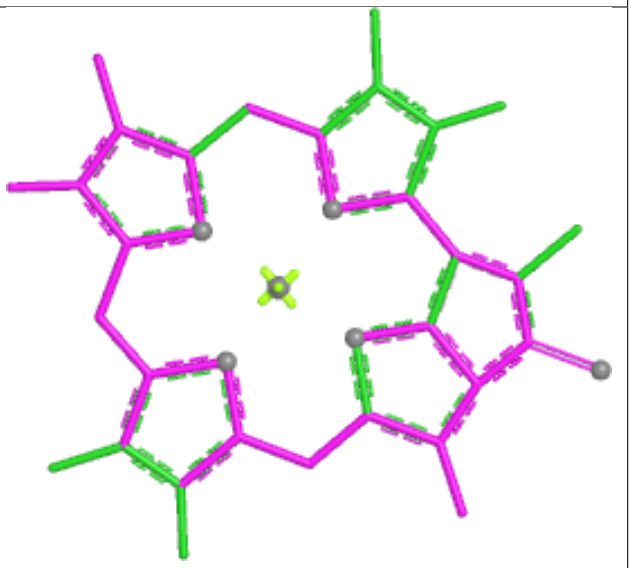


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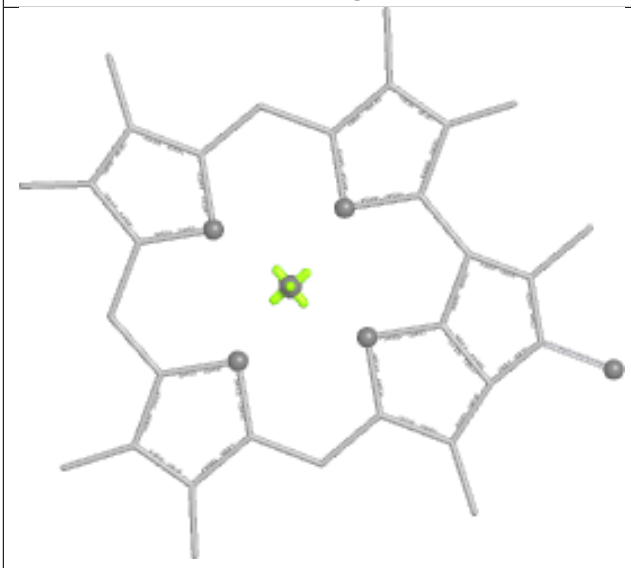
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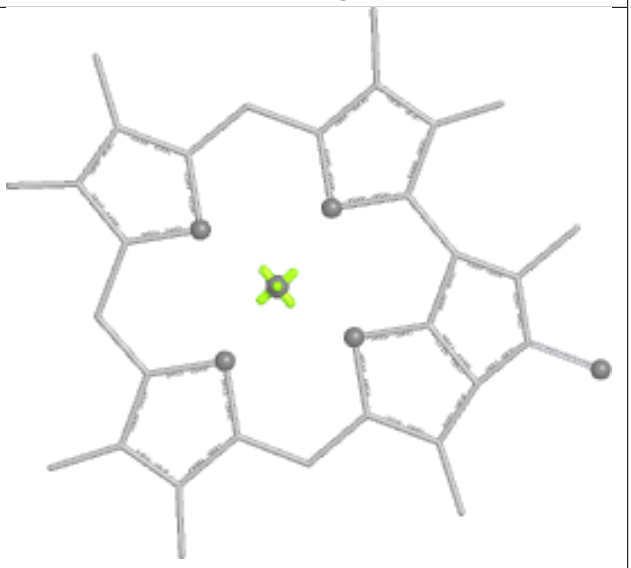
Bond lengths



Bond angles

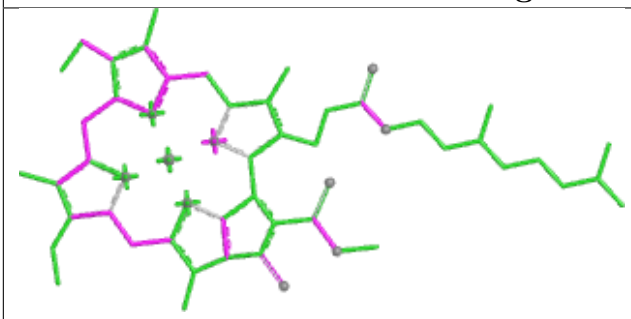


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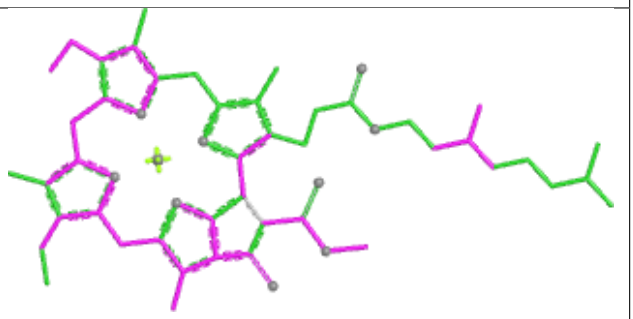


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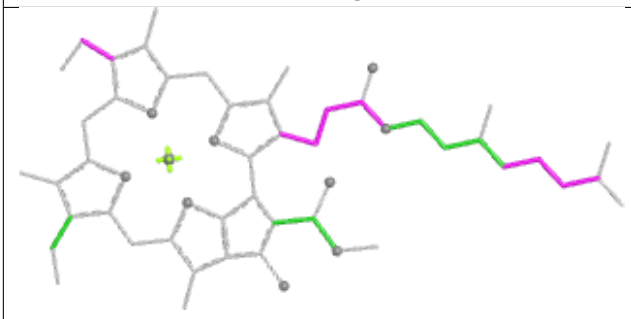
Ligand CLA B 1219



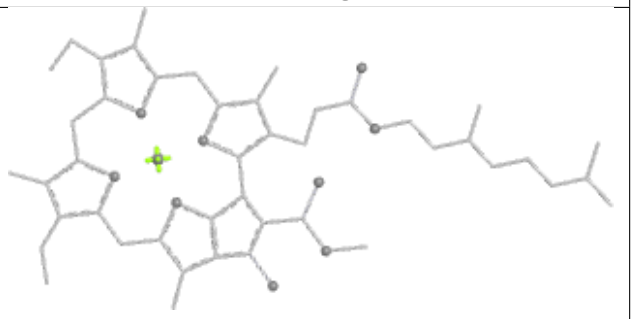
Bond lengths



Bond angles

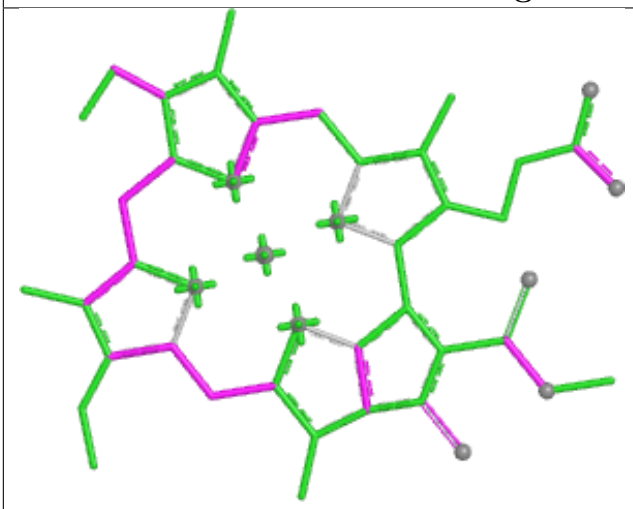


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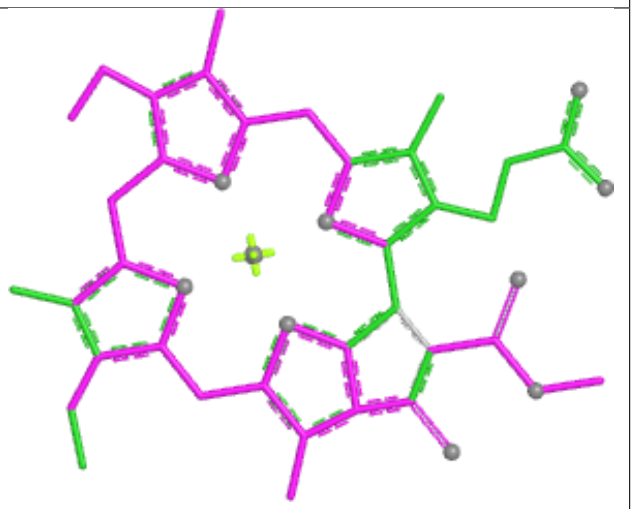


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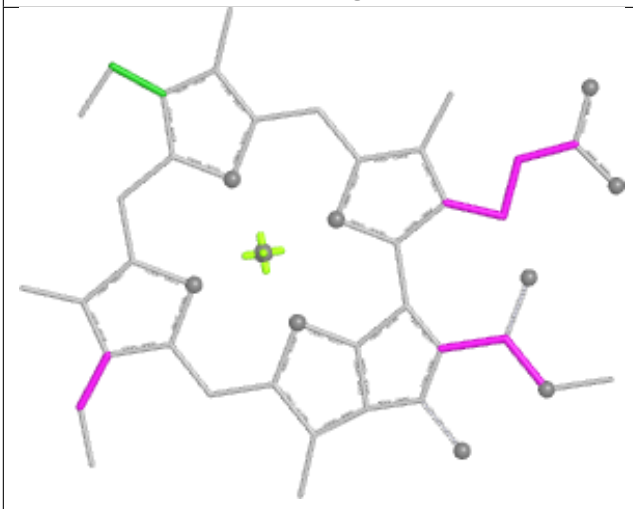
Ligand CLA A 1112



Bond lengths



Bond angles

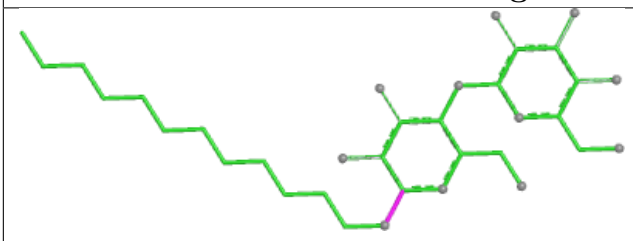


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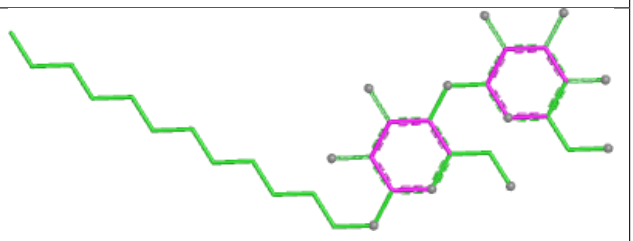


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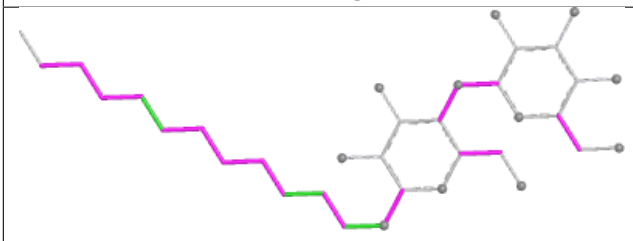
Ligand LMU H 7032



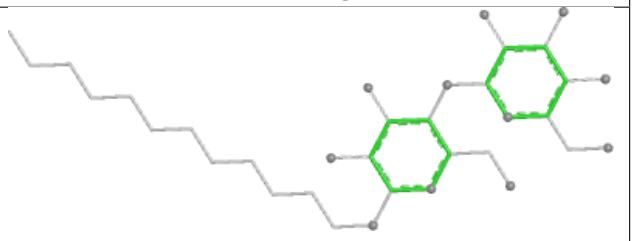
Bond lengths



Bond angles

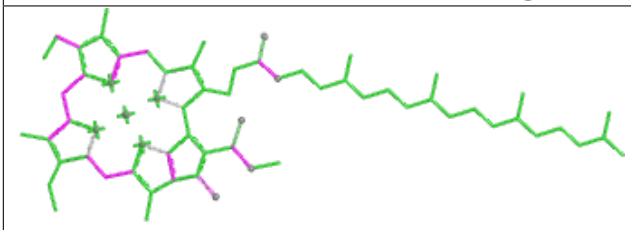


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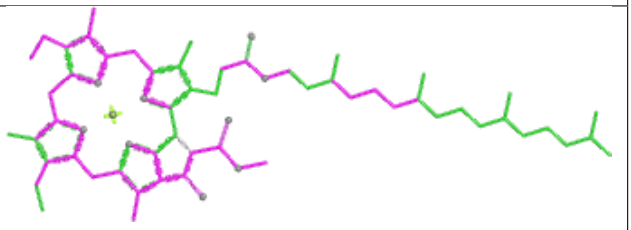


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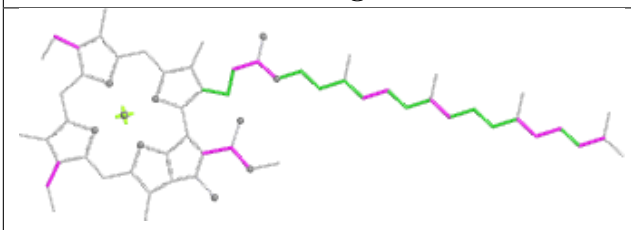
Ligand CLA 2 2007



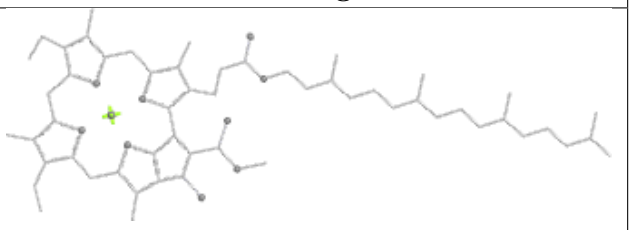
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Bond angles

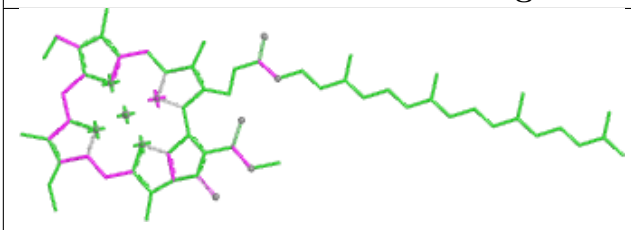


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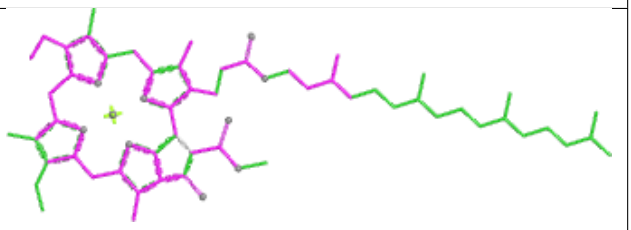


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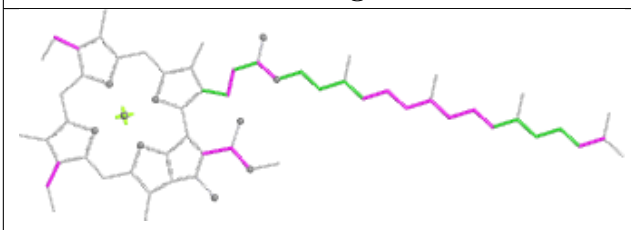
Ligand CLA B 1238



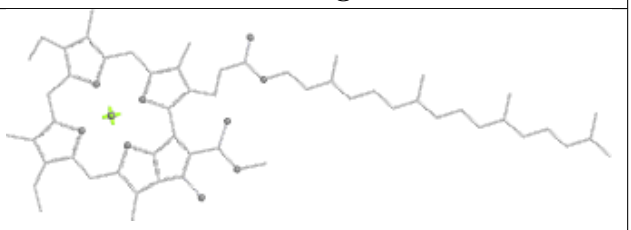
Bond lengths



Bond angles

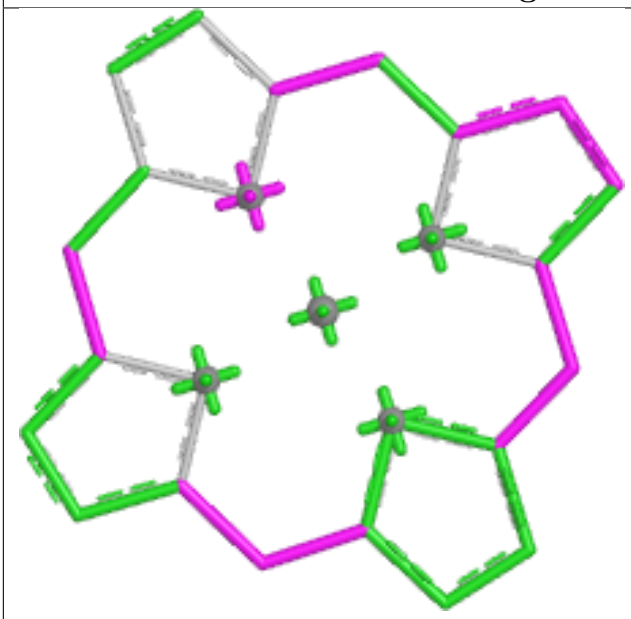


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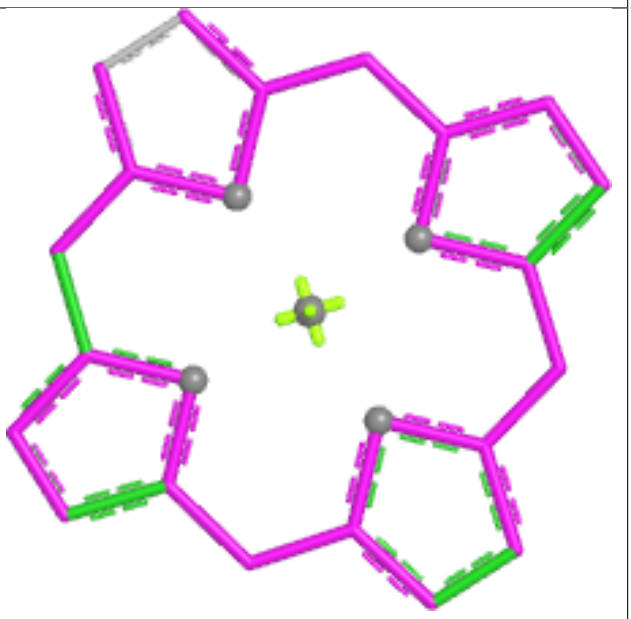


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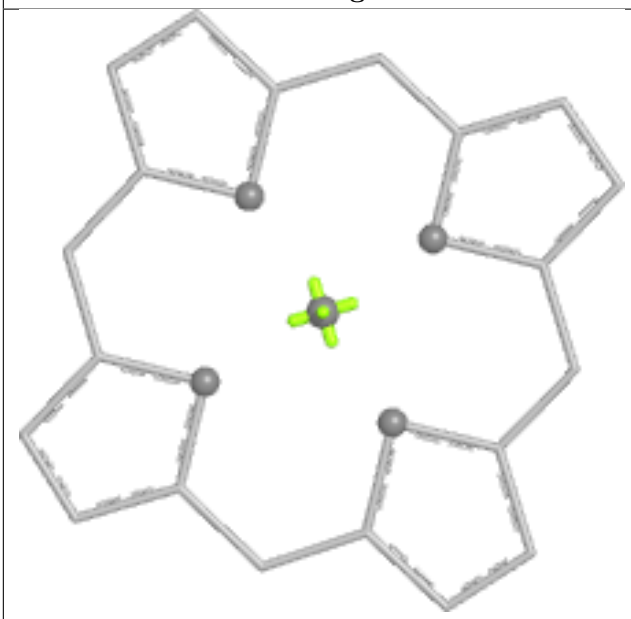
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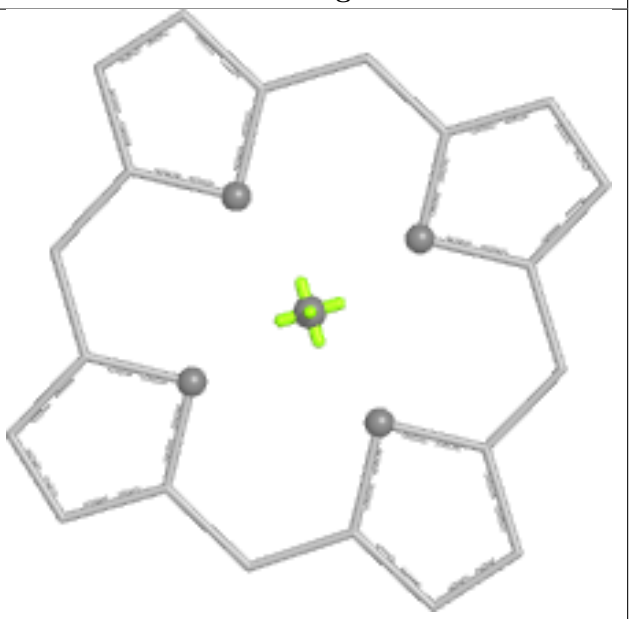
Bond lengths



Bond angles

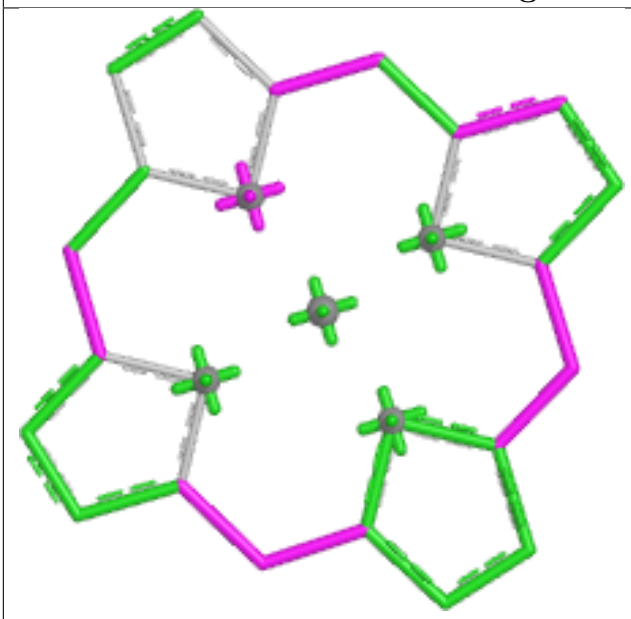


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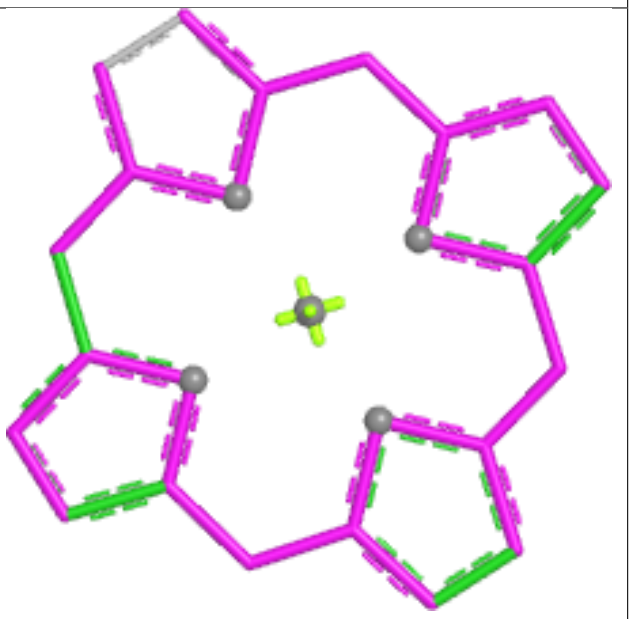


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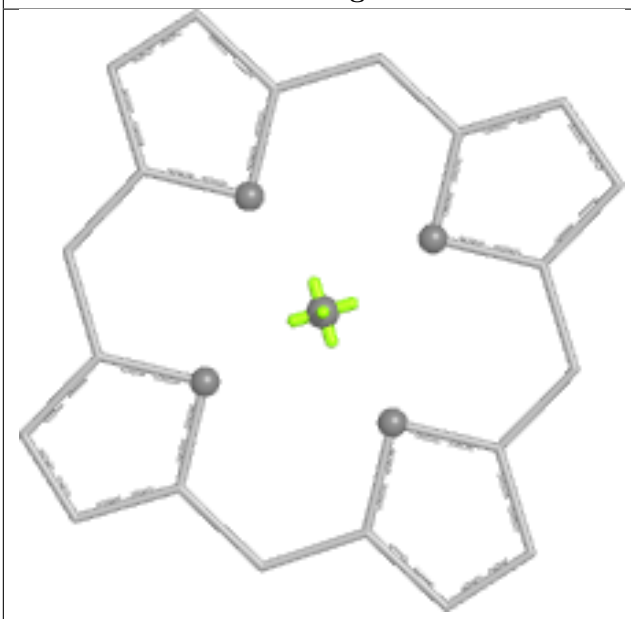
Ligand CLA 1 1015



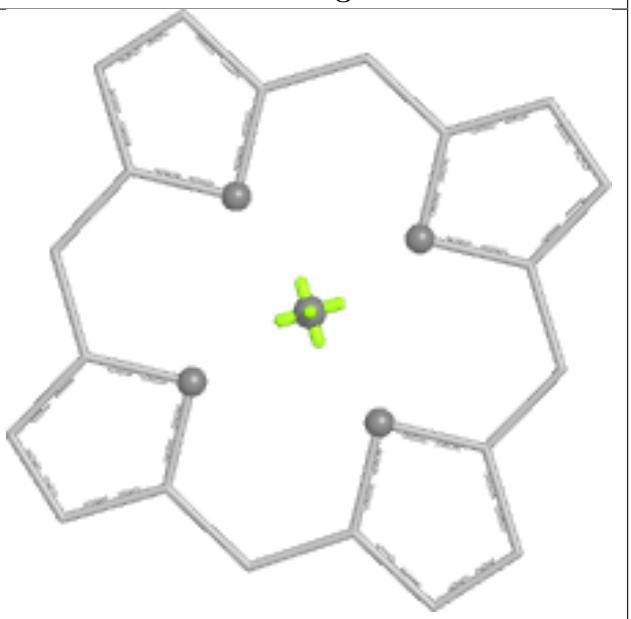
Bond lengths



Bond angles

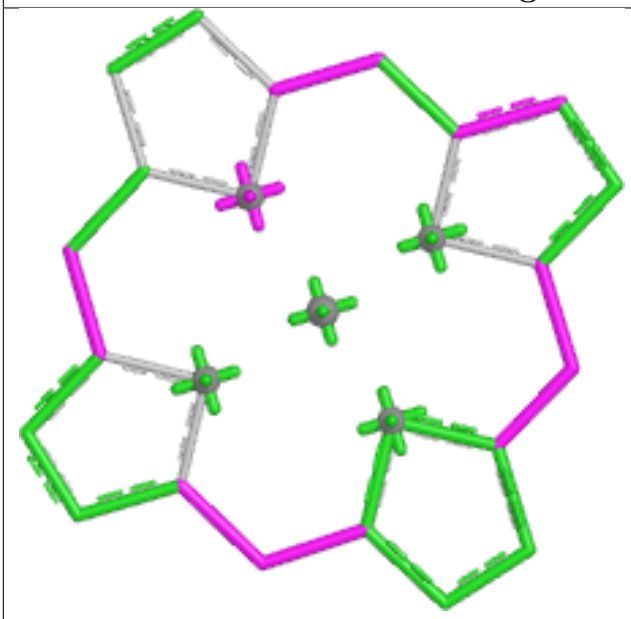


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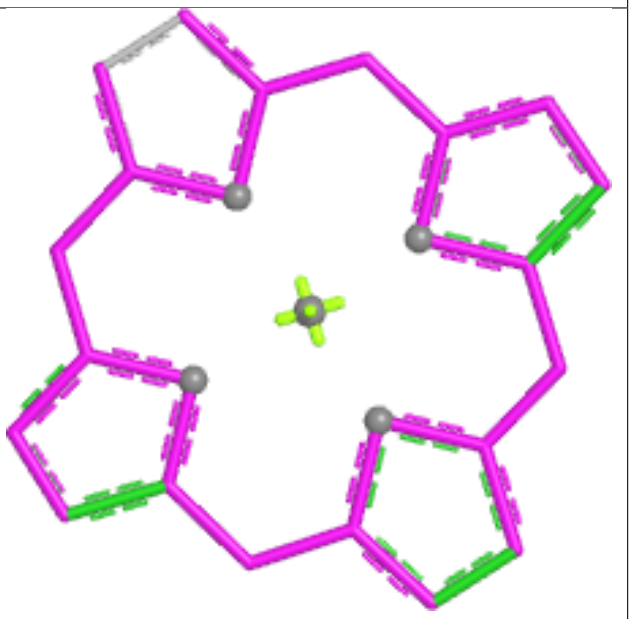


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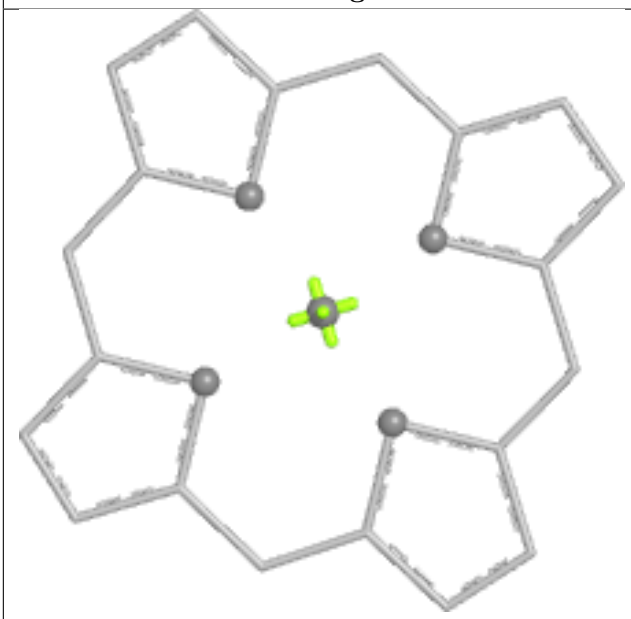
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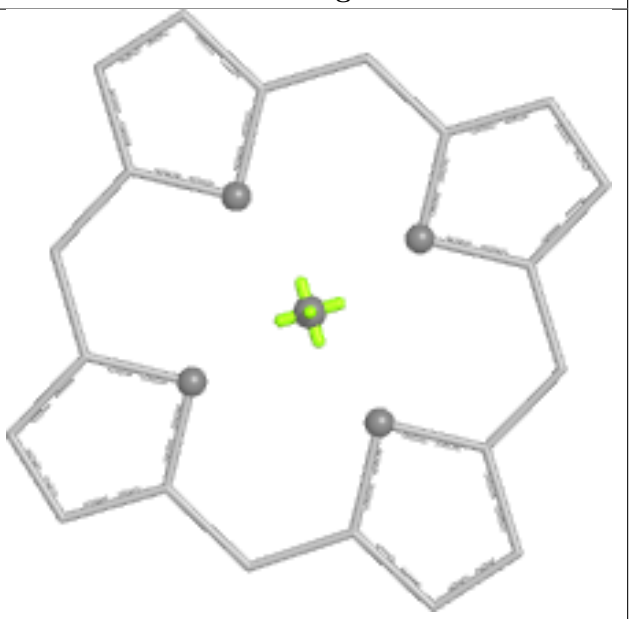
Bond lengths



Bond angles

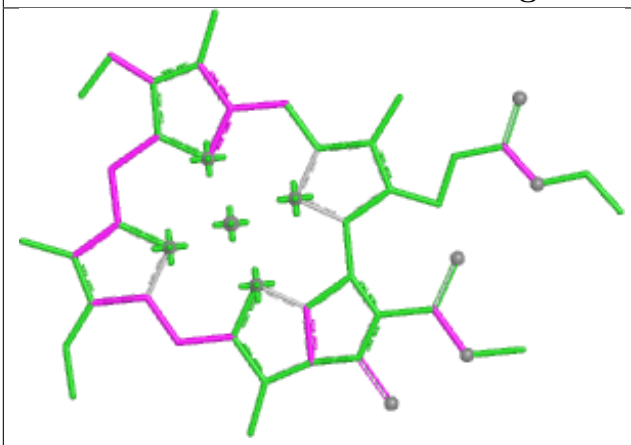


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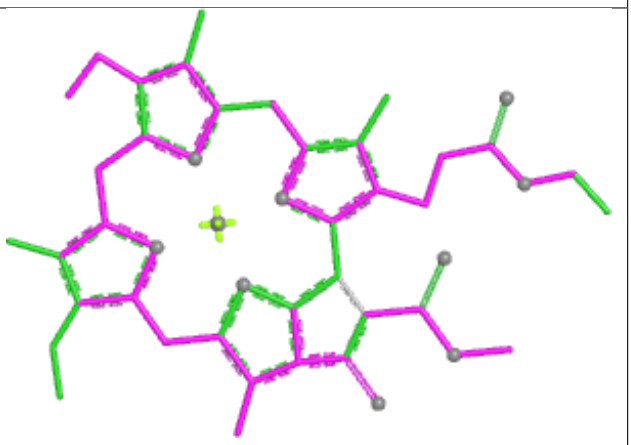


Rings

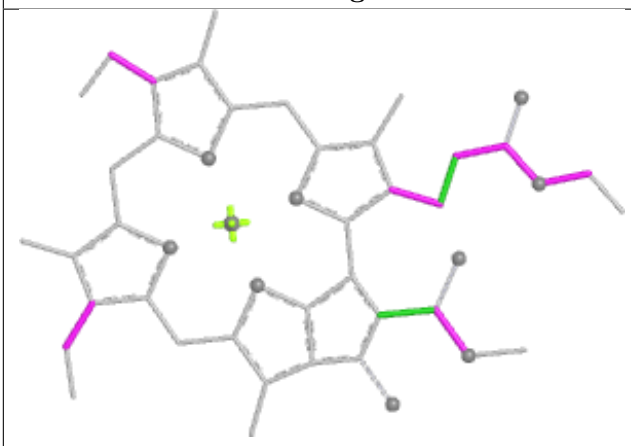
Ligand CLA 1 1002



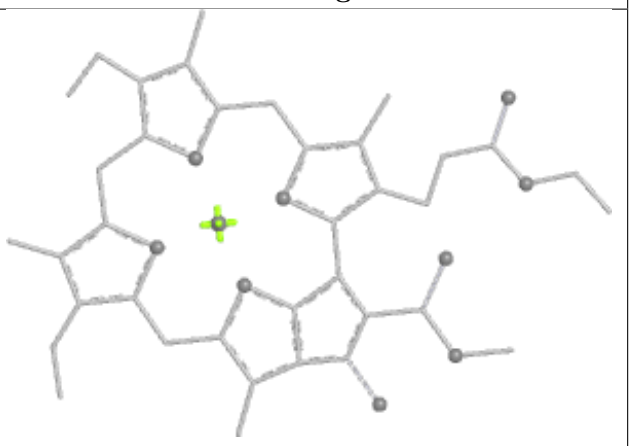
Bond lengths



Bond angles

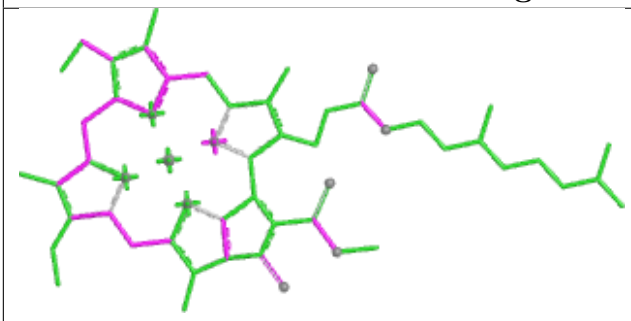


Torsions

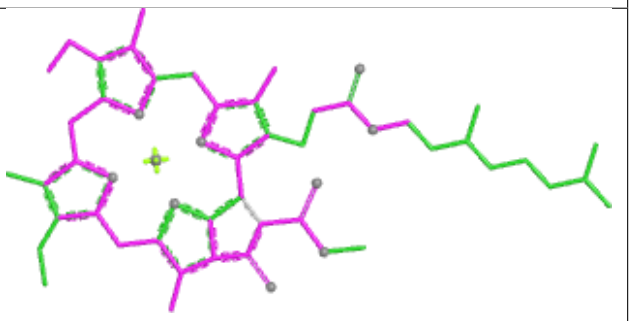


Rings

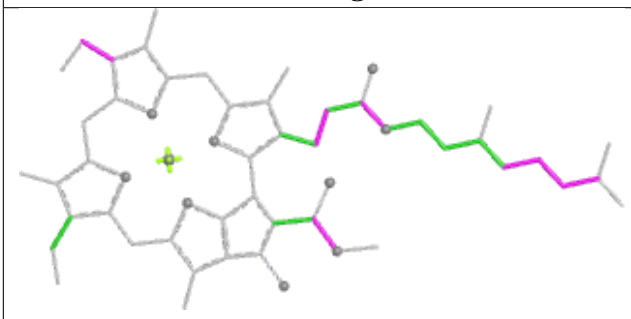
Ligand CLA A 1127



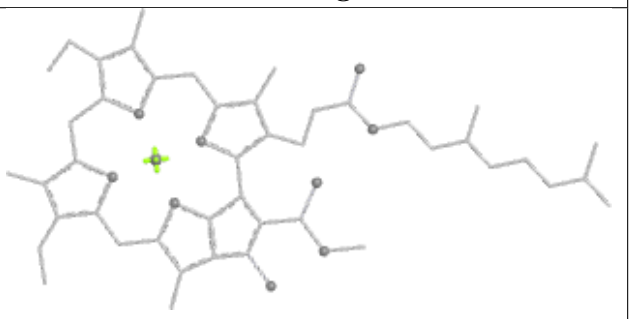
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Bond angles

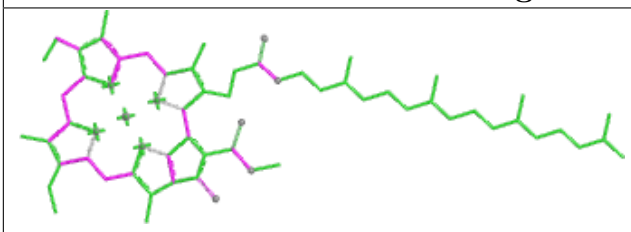


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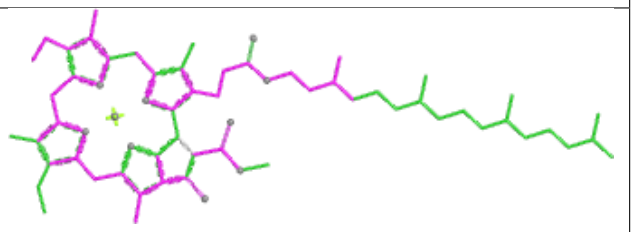


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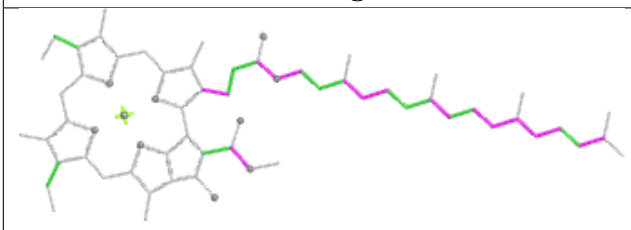
Ligand CLA B 1229



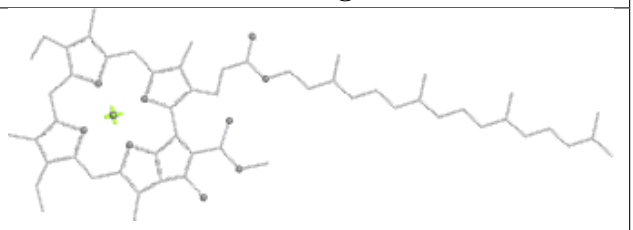
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Bond angles

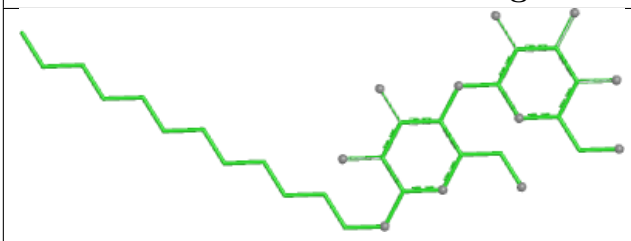


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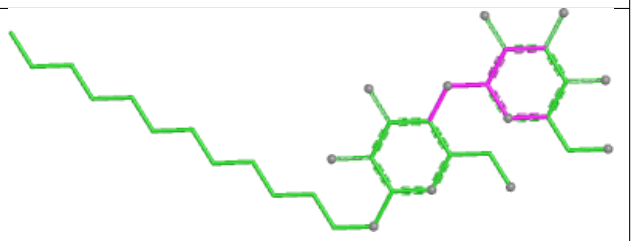


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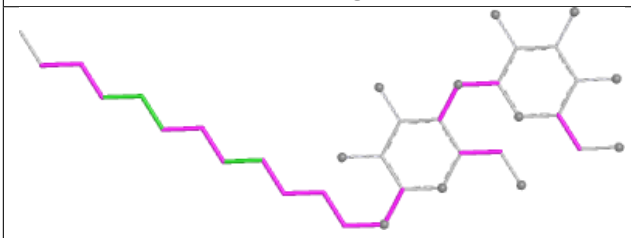
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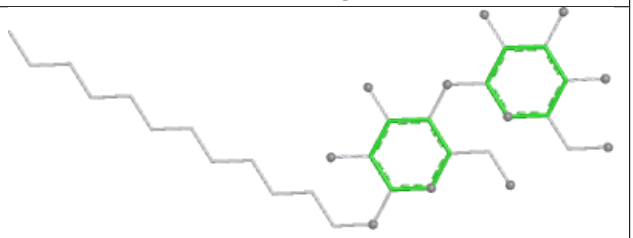
Bond lengths



Bond angles

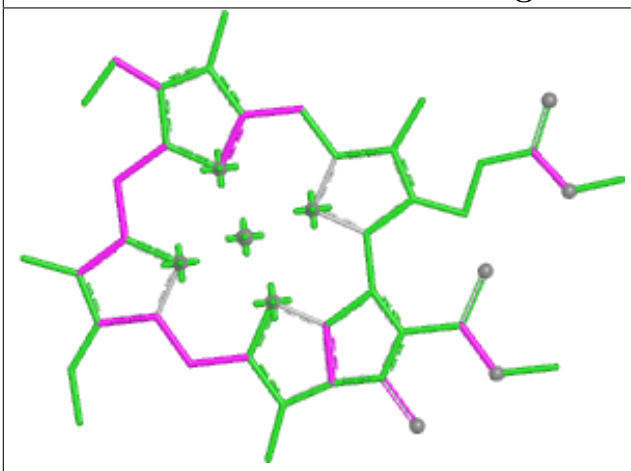


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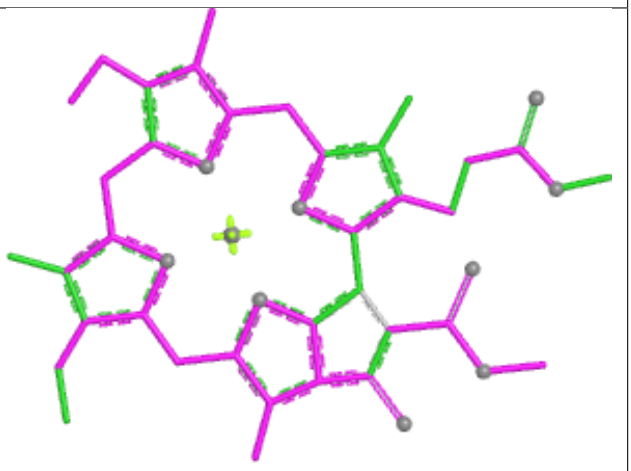


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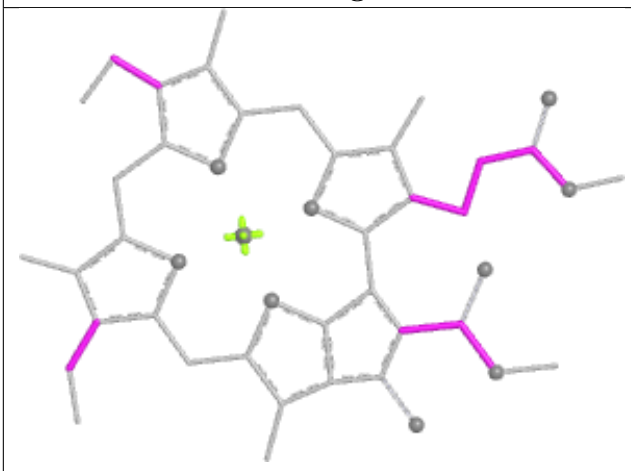
Ligand CLA B 1213



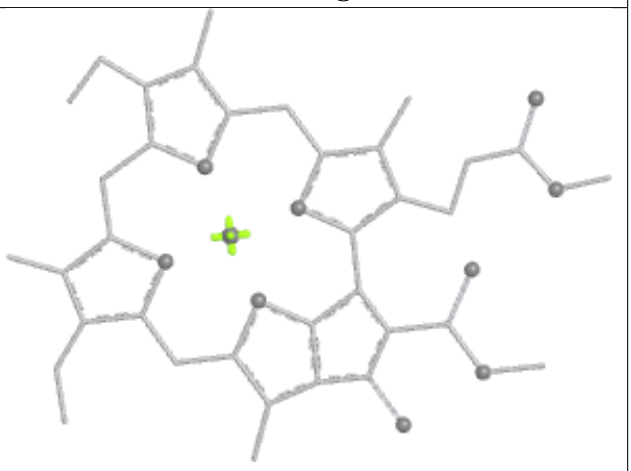
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Bond angles

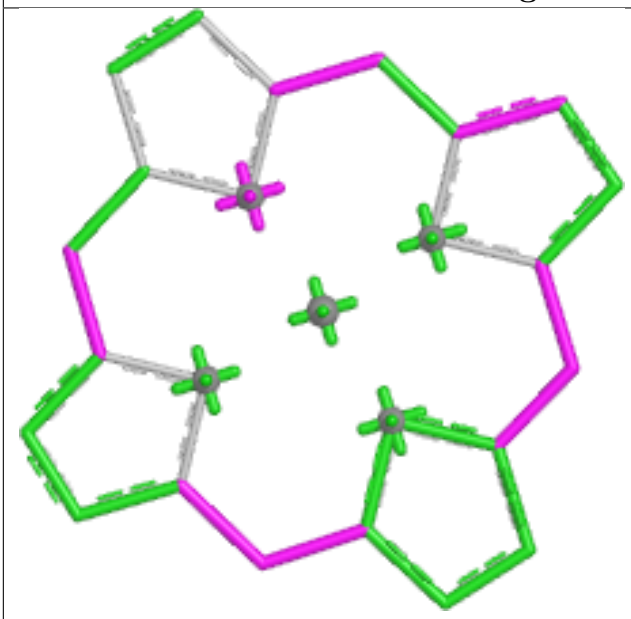


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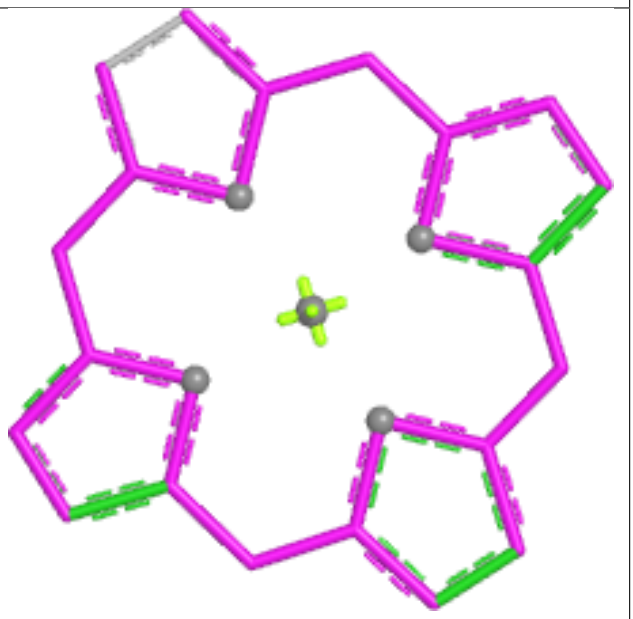


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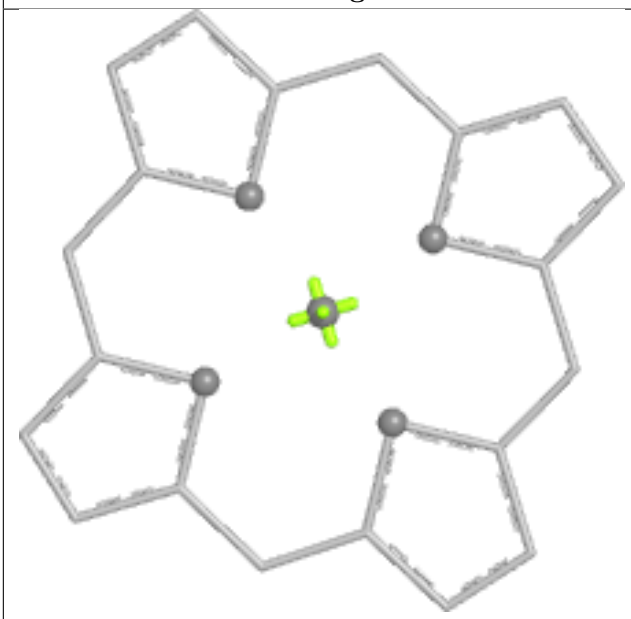
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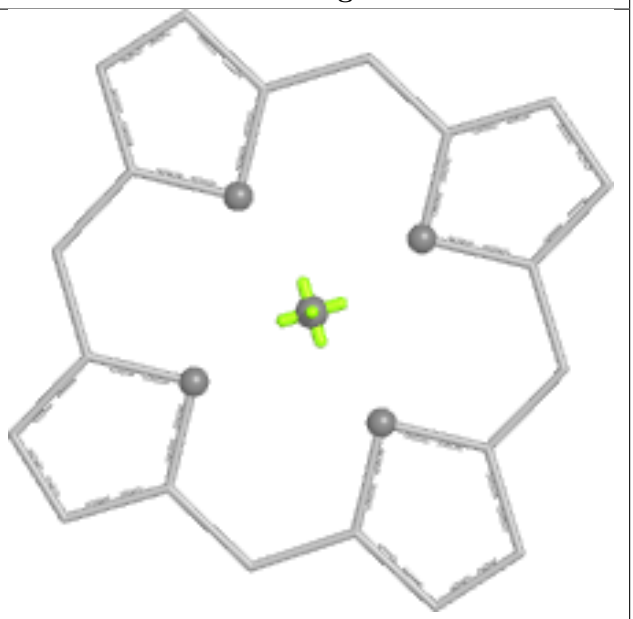
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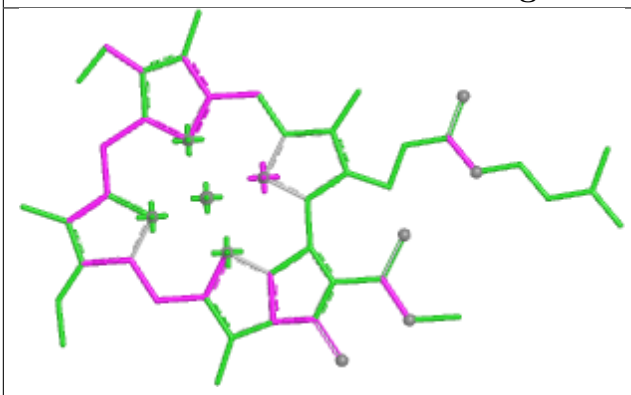


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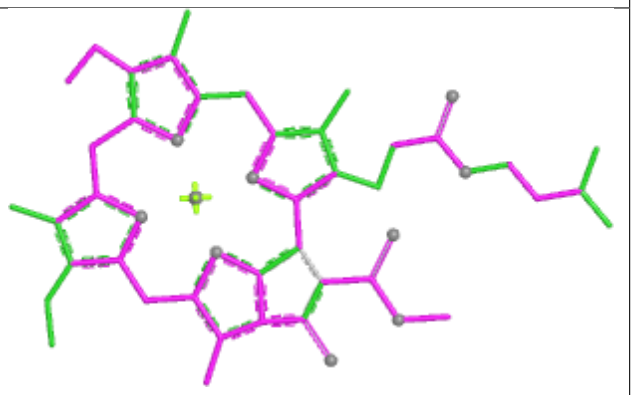


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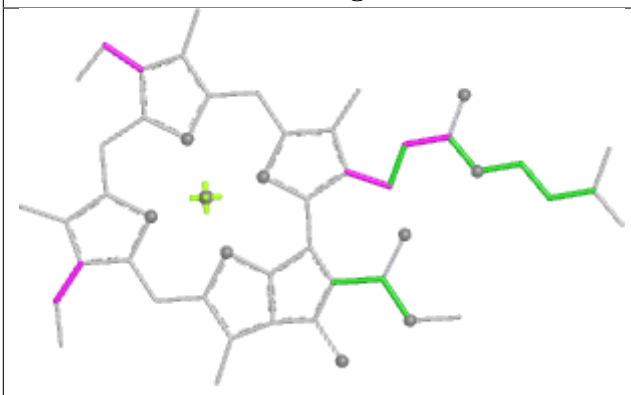
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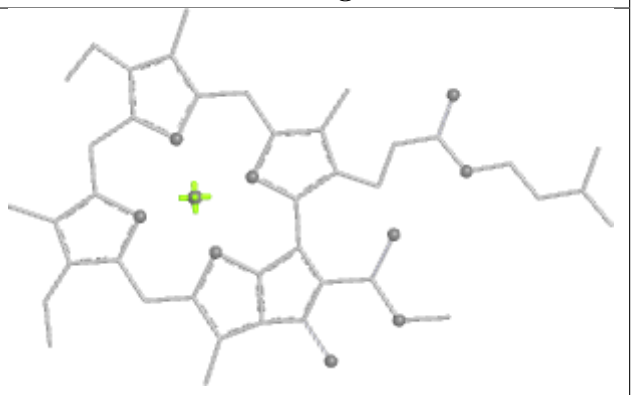
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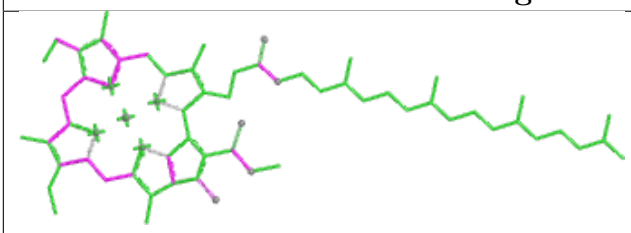


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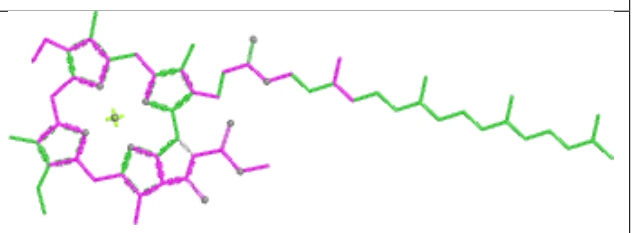


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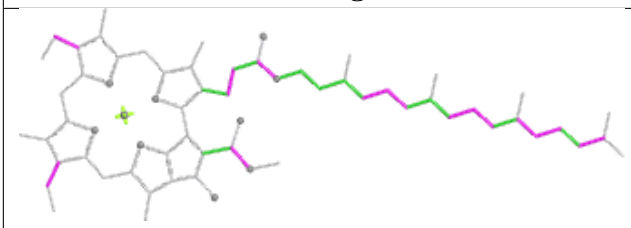
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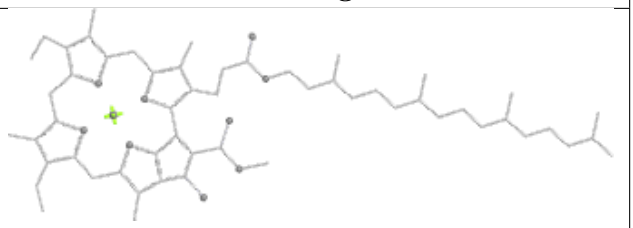
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Bond angles

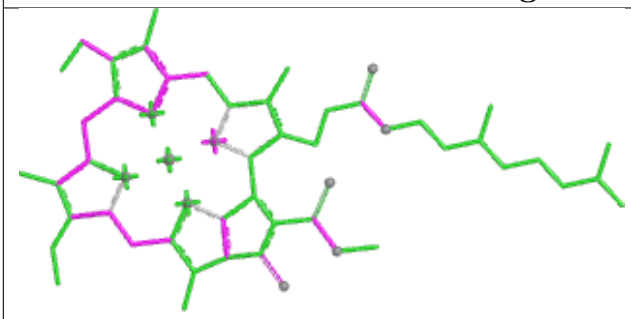


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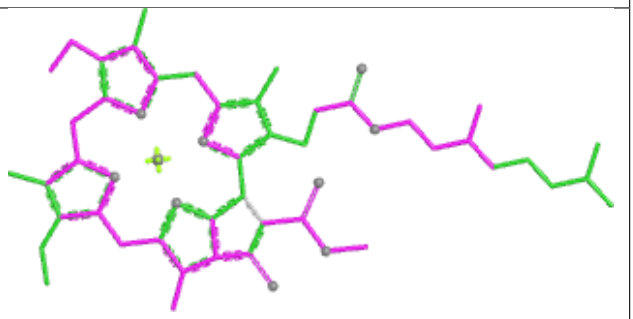


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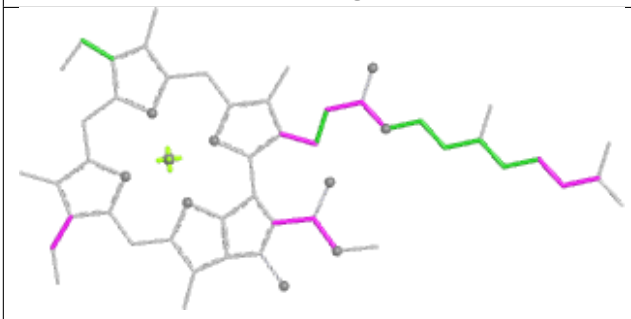
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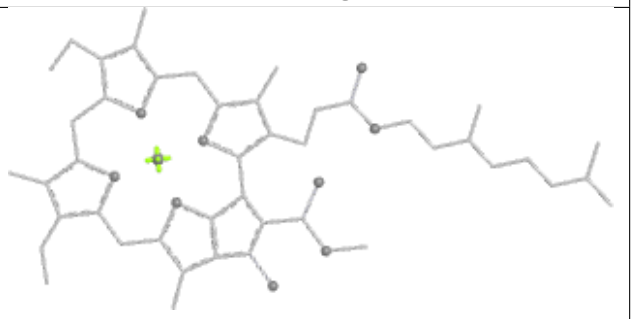
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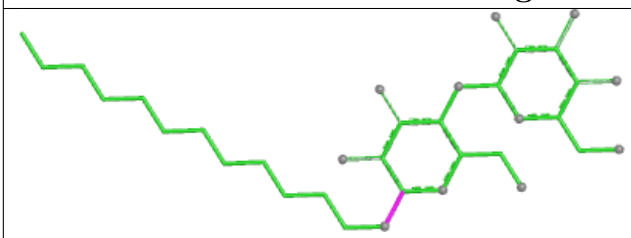


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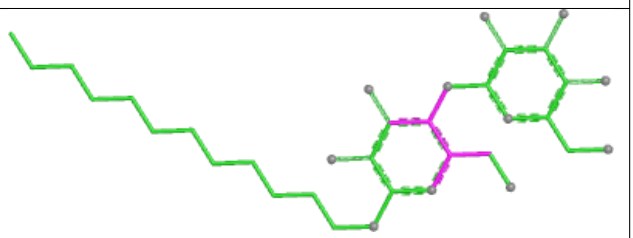


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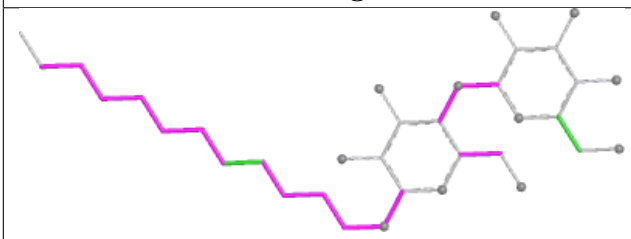
Ligand LMU 2 7046



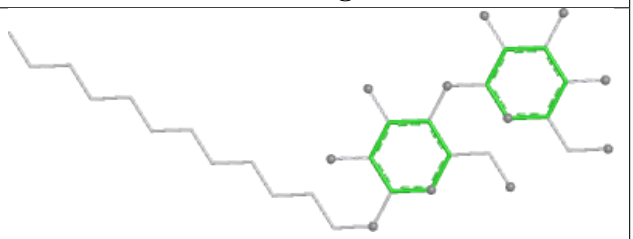
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Bond angles

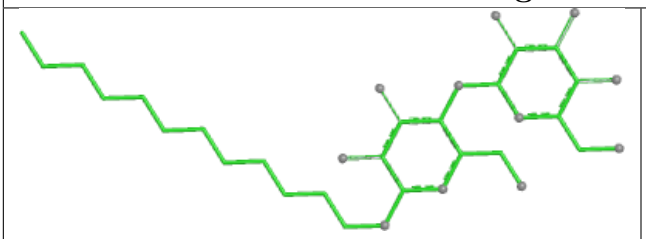


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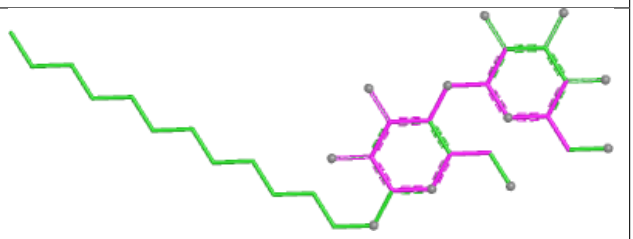


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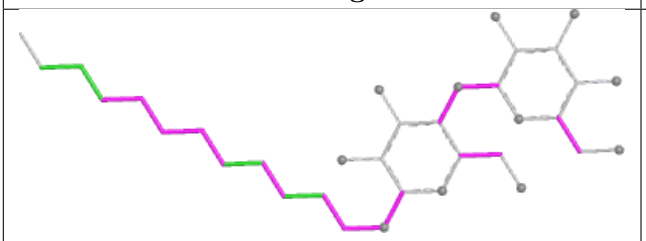
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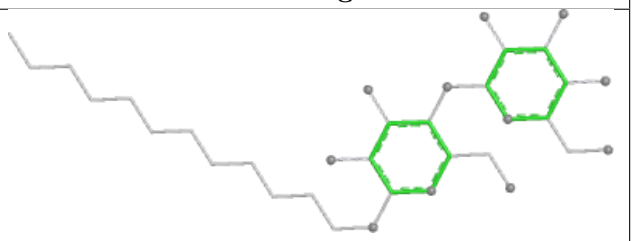
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Bond angles

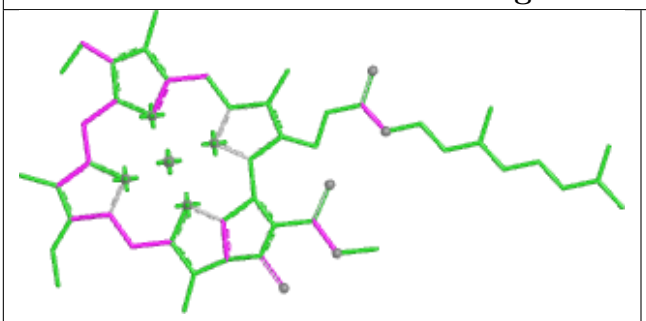


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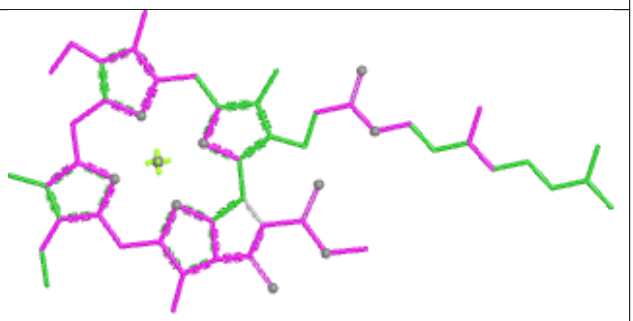


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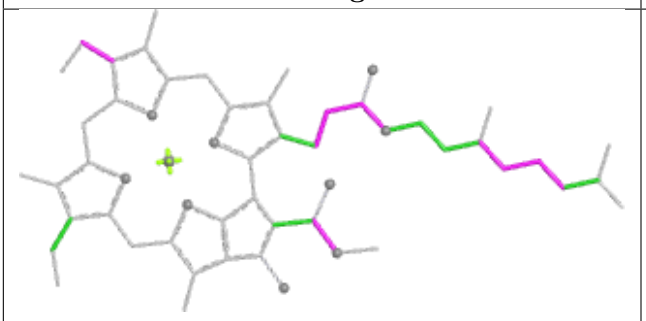
Ligand CLA H 1505



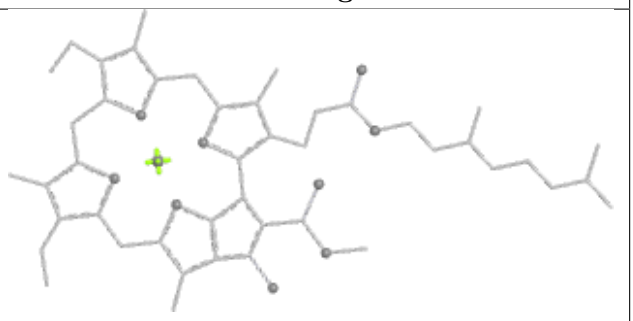
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Bond angles

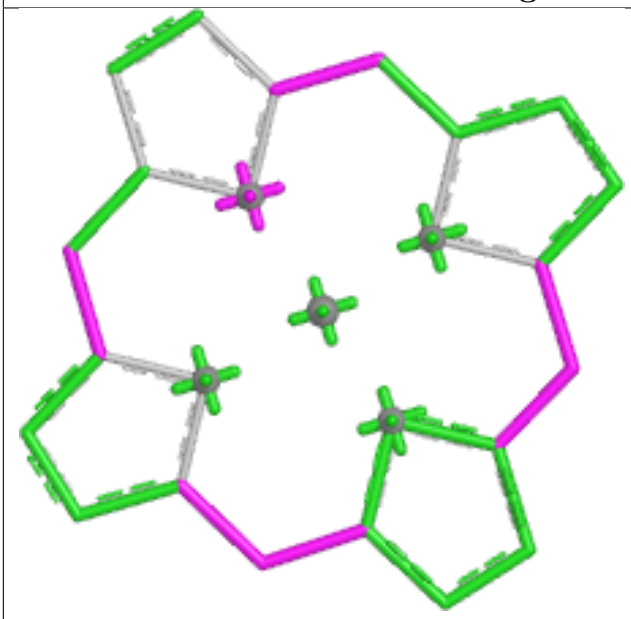


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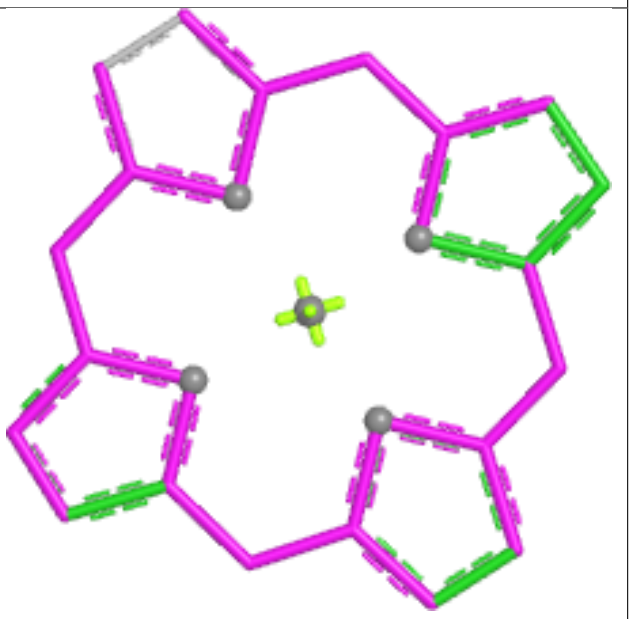


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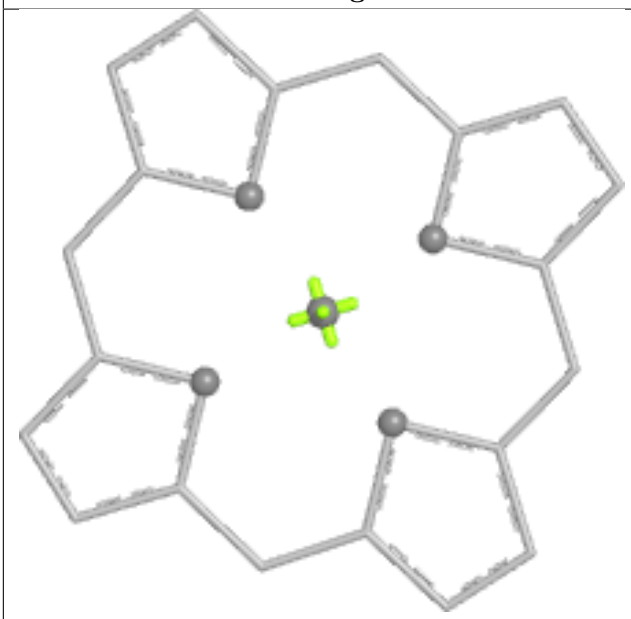
Ligand CLA 2 2010



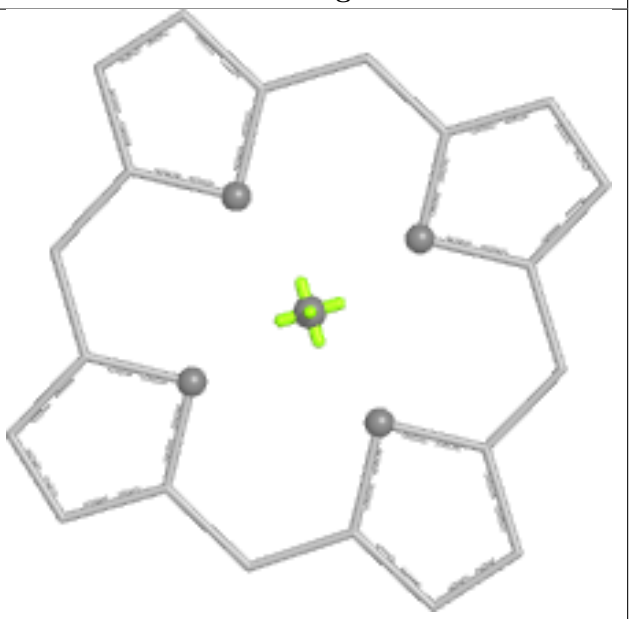
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Bond angles

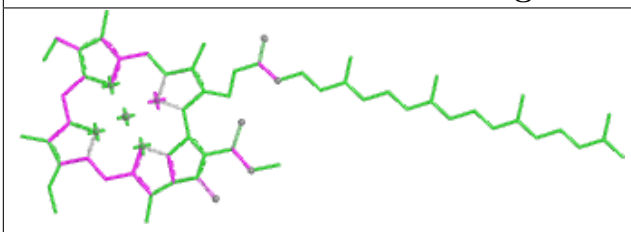


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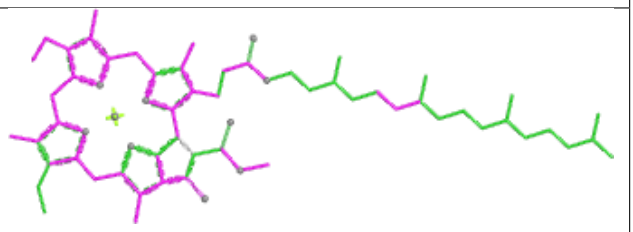


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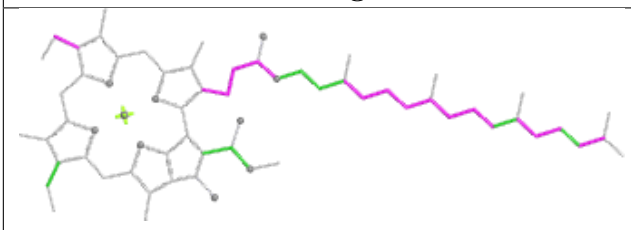
Ligand CLA A 9011



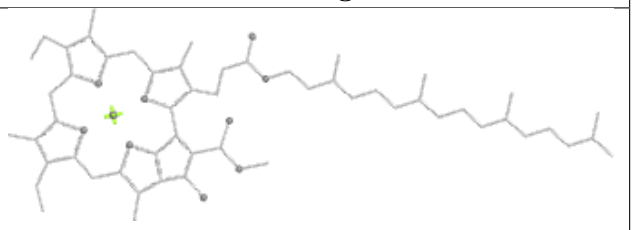
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Bond angles

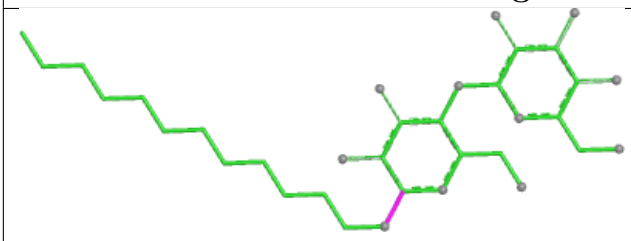


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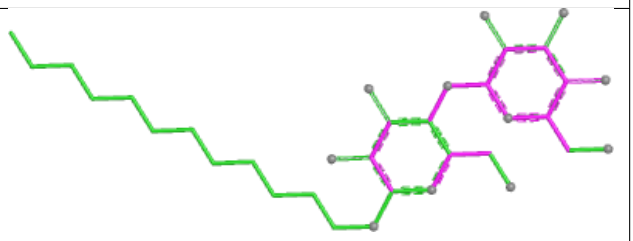


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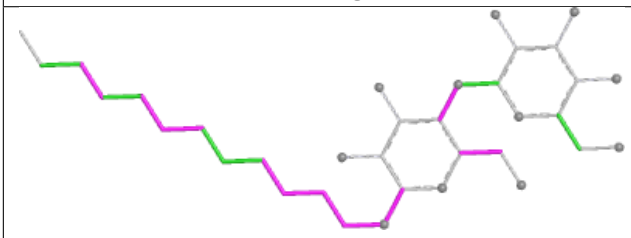
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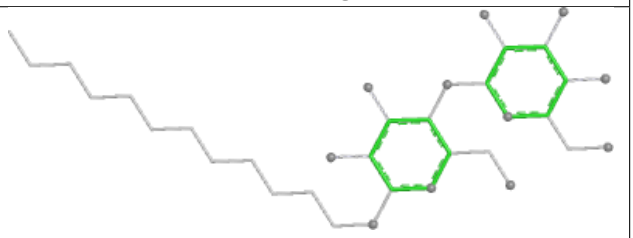
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Bond angles

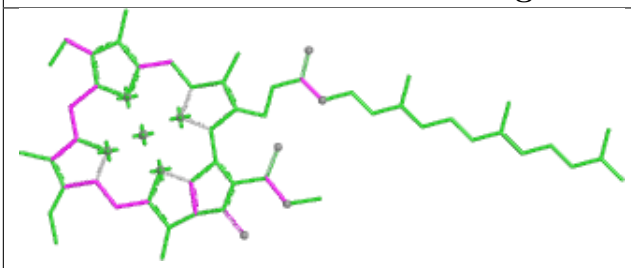


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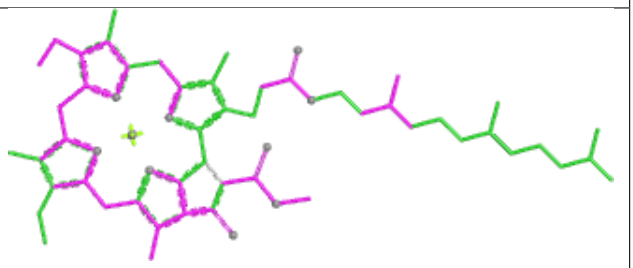


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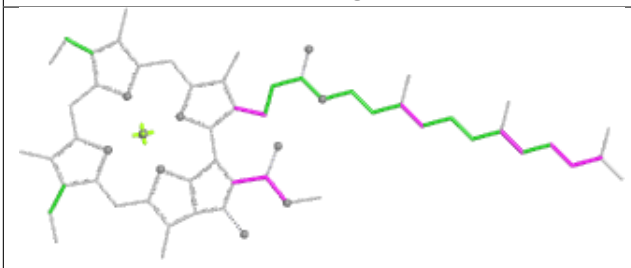
Ligand CLA B 1212



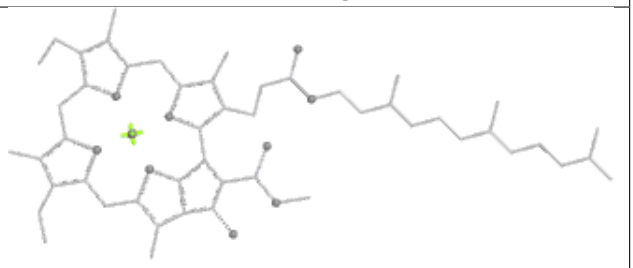
Bond lengths



Bond angles

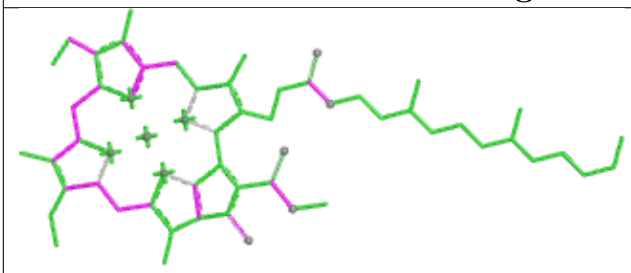


Torsions

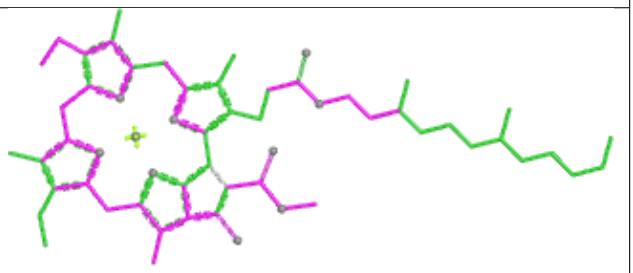


Rings

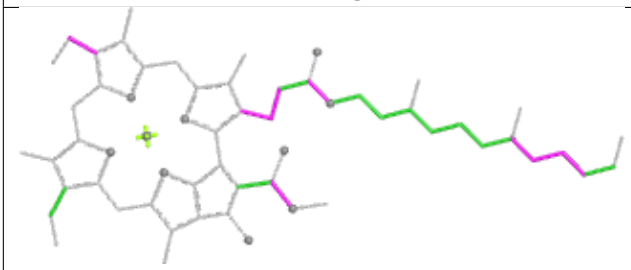
Ligand CLA B 1214



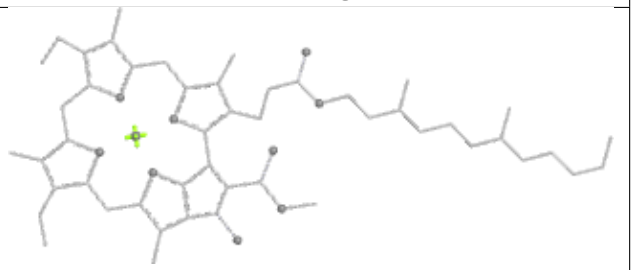
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Bond angles

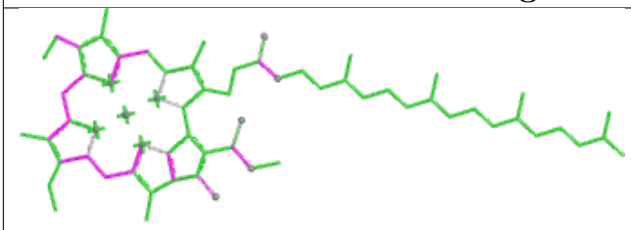


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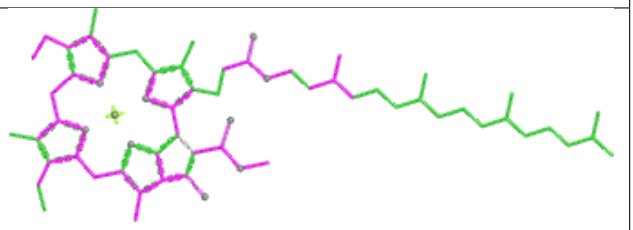


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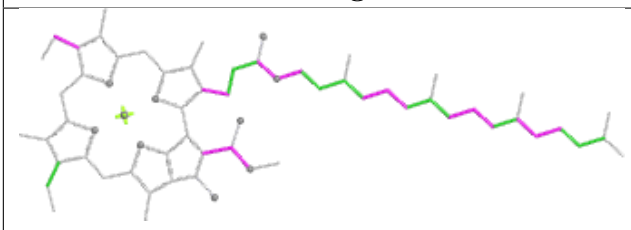
Ligand CLA 2 4009



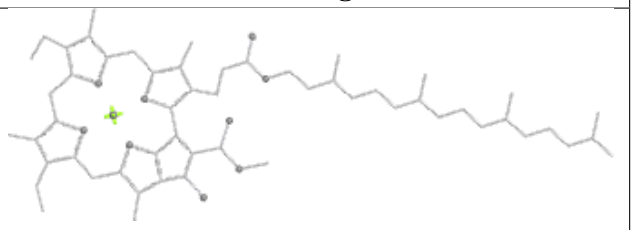
Bond lengths



Bond angles

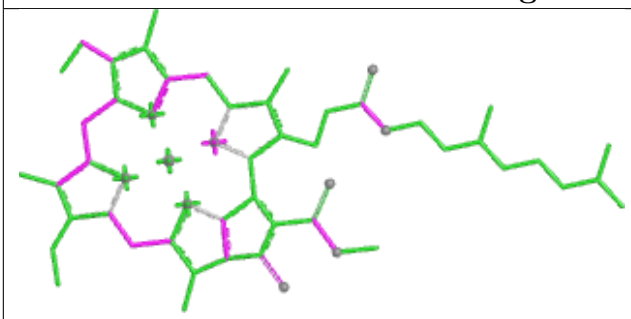


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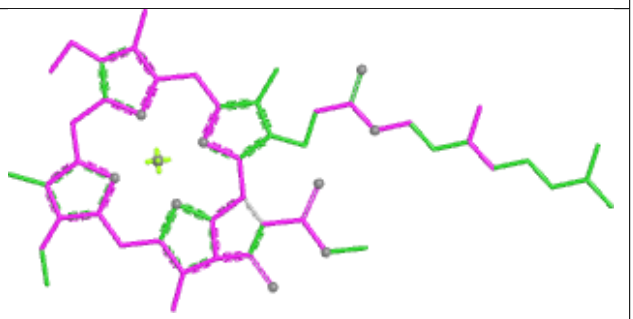


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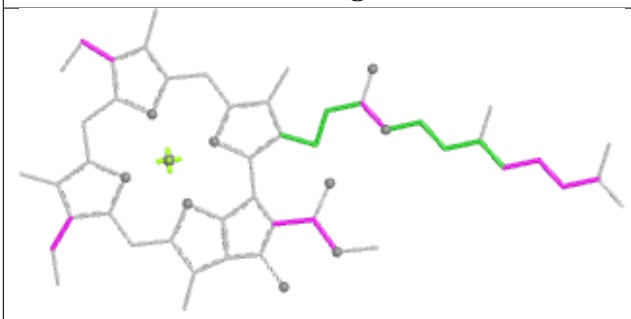
Ligand CLA 4 1306



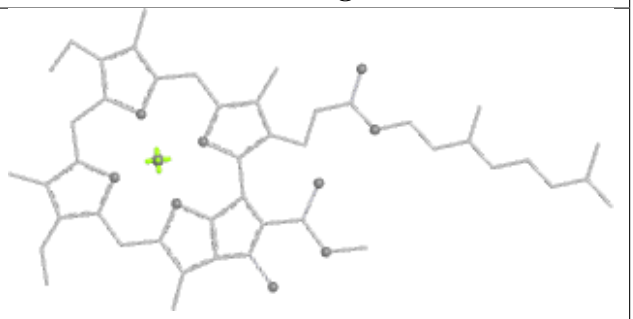
Bond lengths



Bond angles

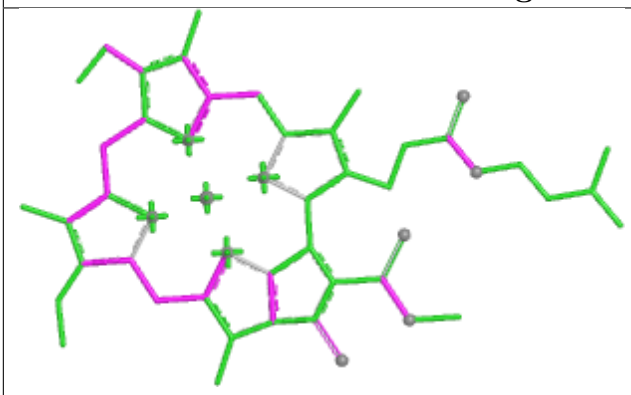


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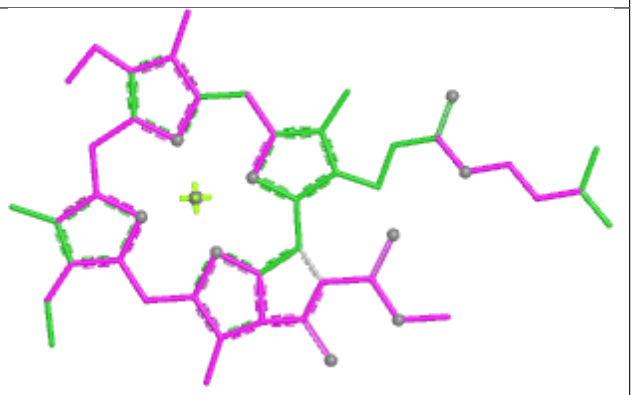


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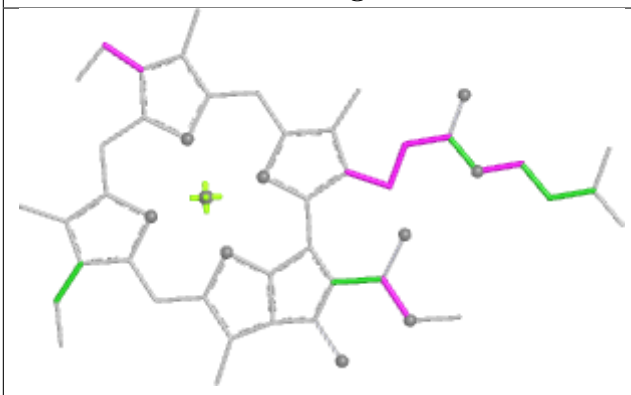
Ligand CLA B 1227



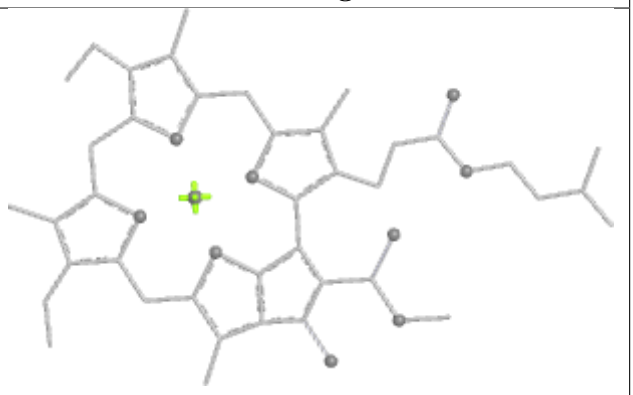
Bond lengths



Bond angles

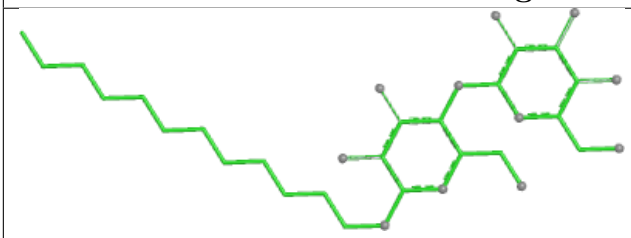


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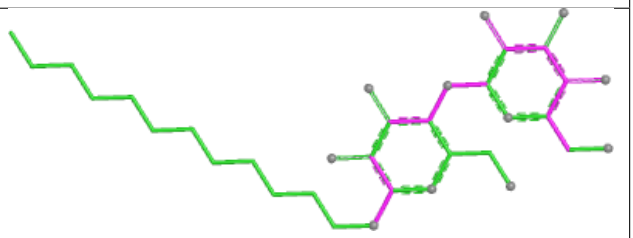


Rings

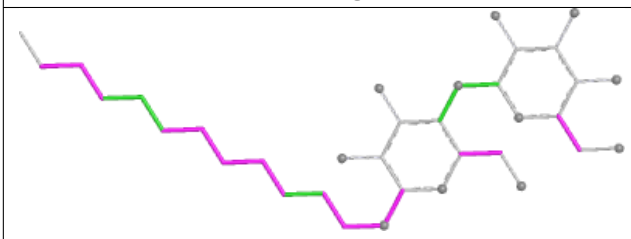
Ligand LMU 3 7003



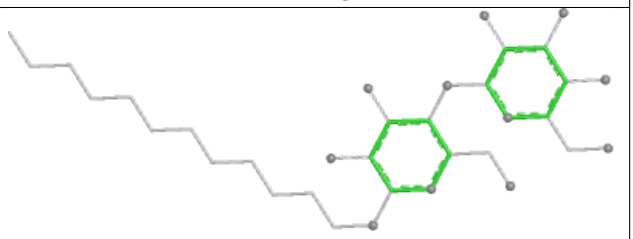
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Bond angles

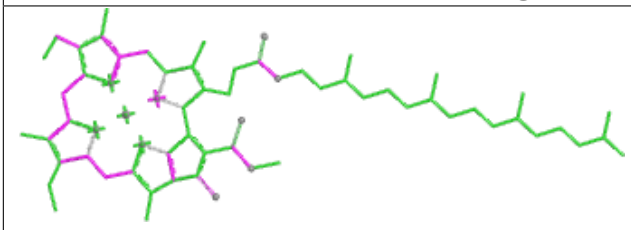


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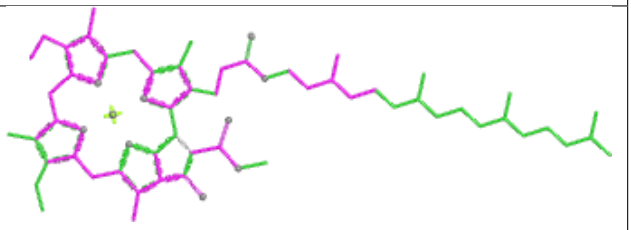


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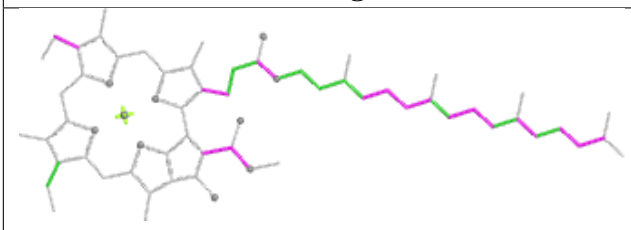
Ligand CLA A 1117



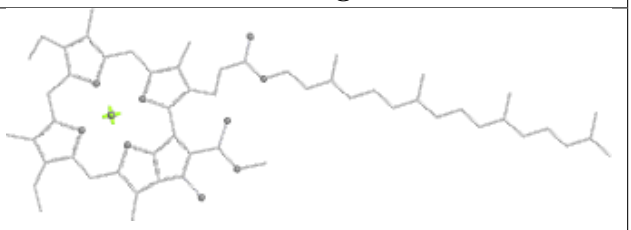
Bond lengths



Bond angles

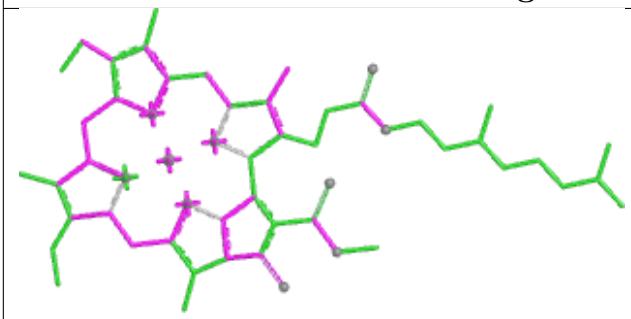


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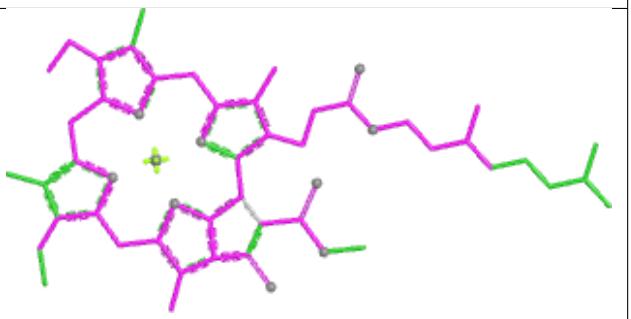


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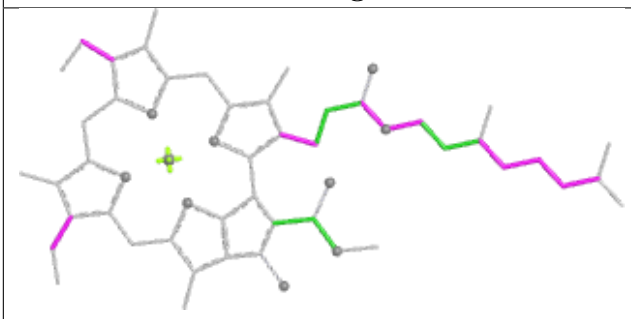
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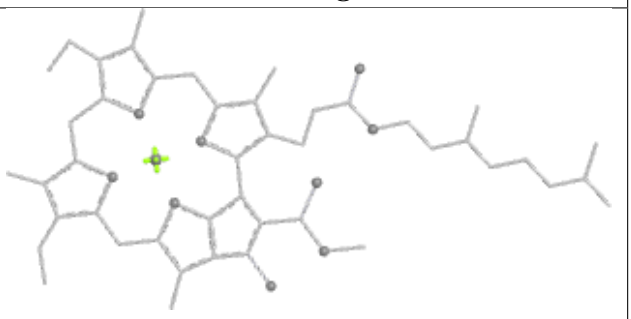
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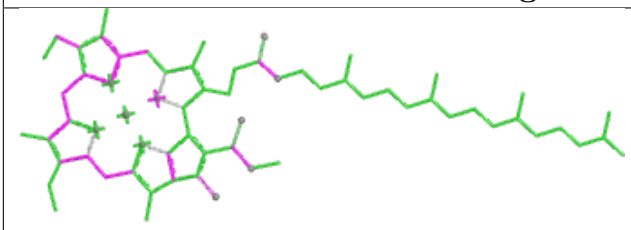


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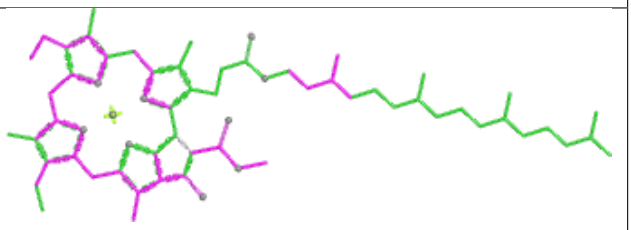


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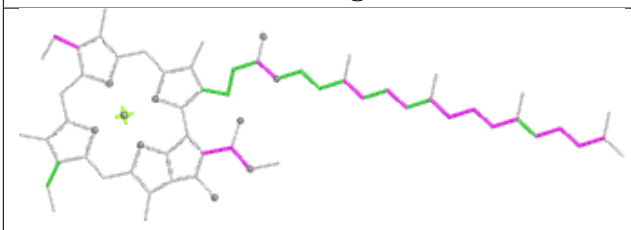
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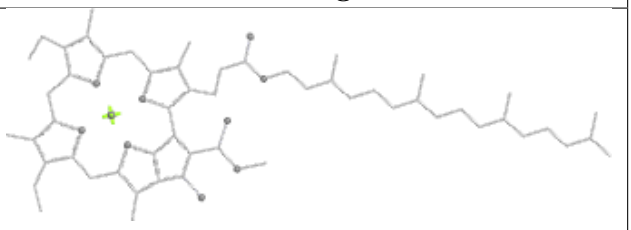
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Bond angles

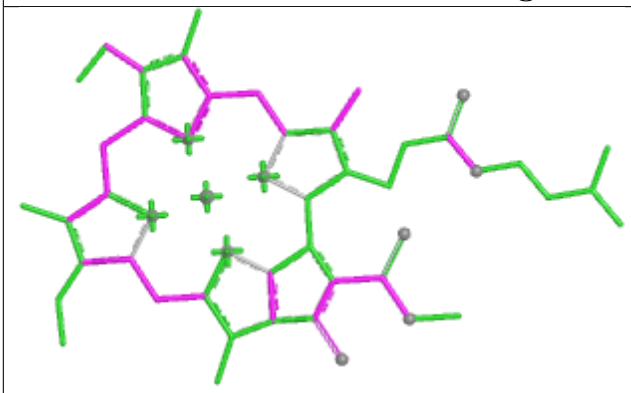


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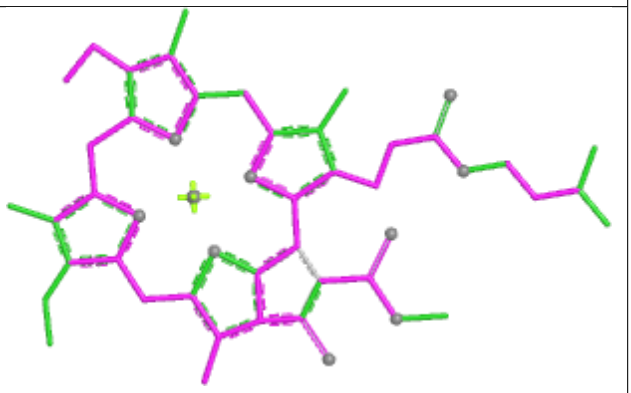


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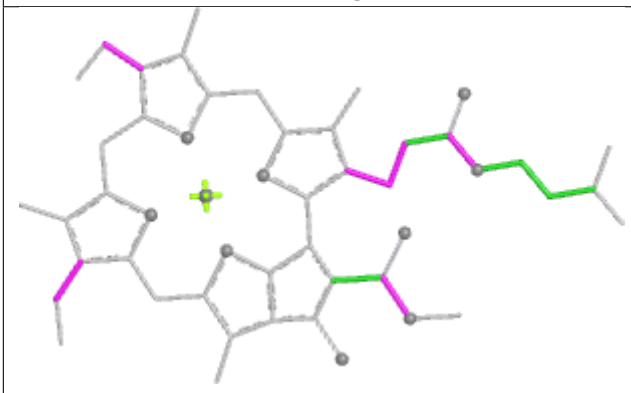
Ligand CLA L 1503



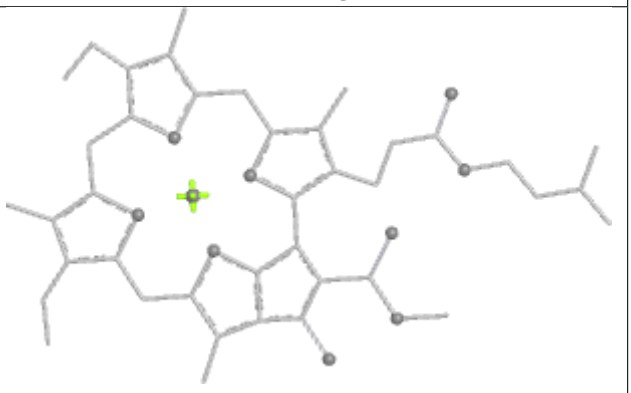
Bond lengths



Bond angles

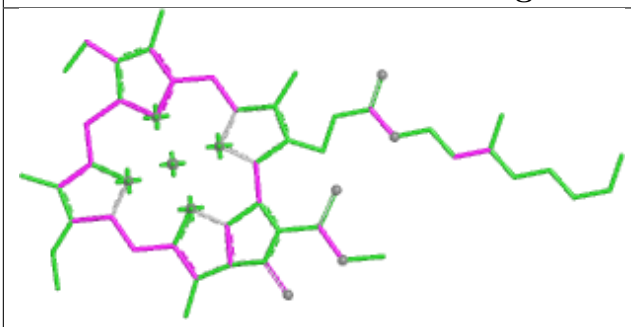


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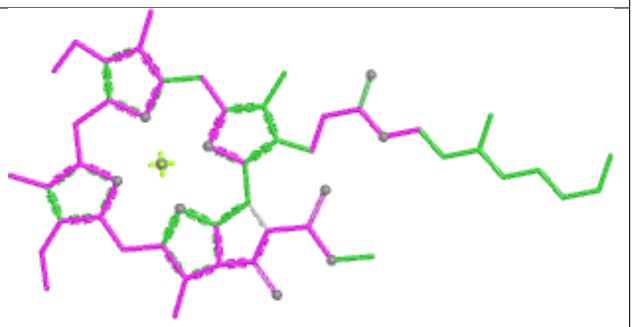


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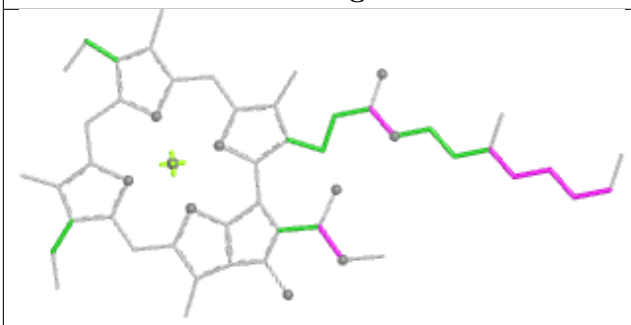
Ligand CLA B 1221



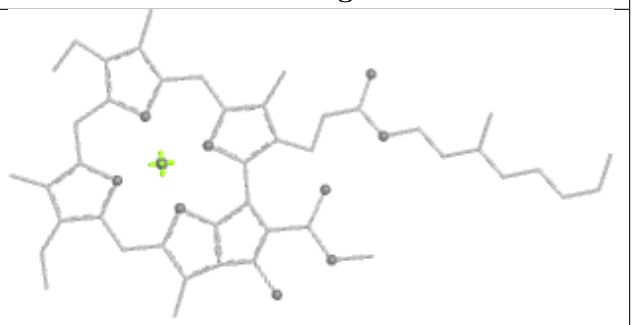
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Bond angles

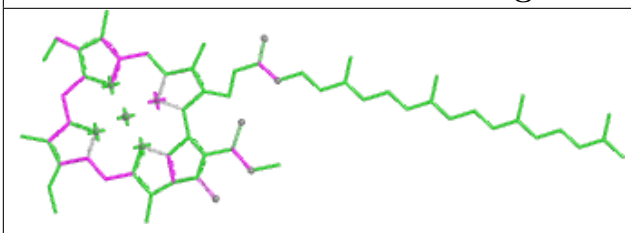


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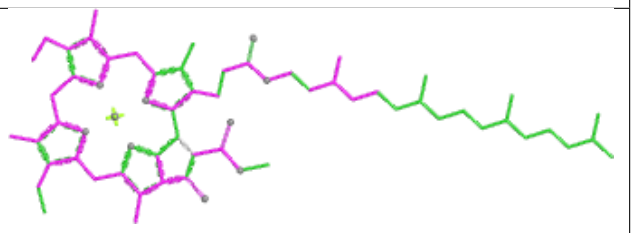


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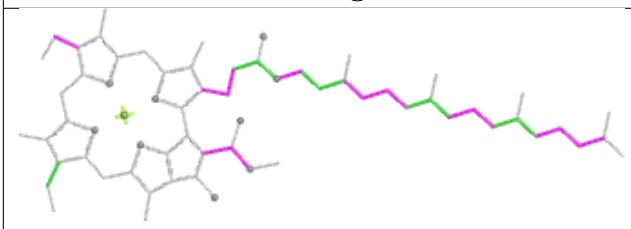
Ligand CLA A 9022



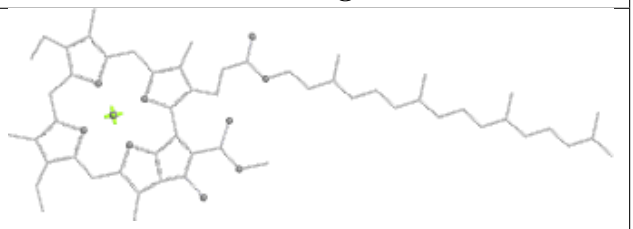
Bond lengths



Bond angles

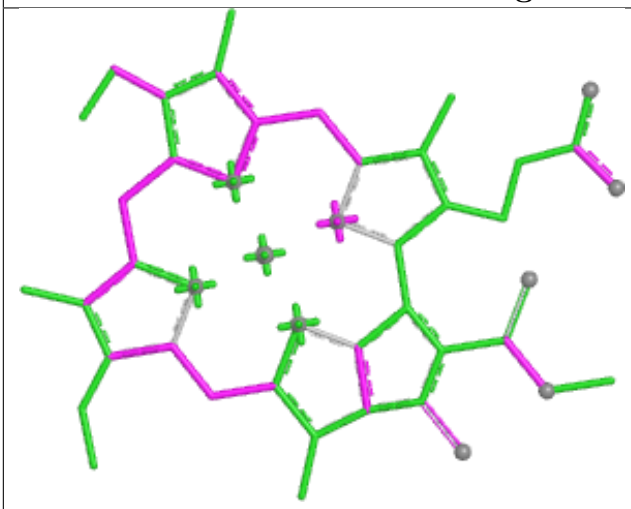


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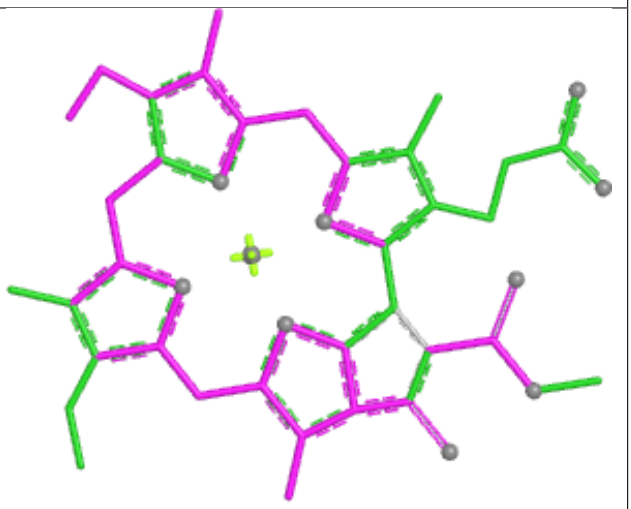


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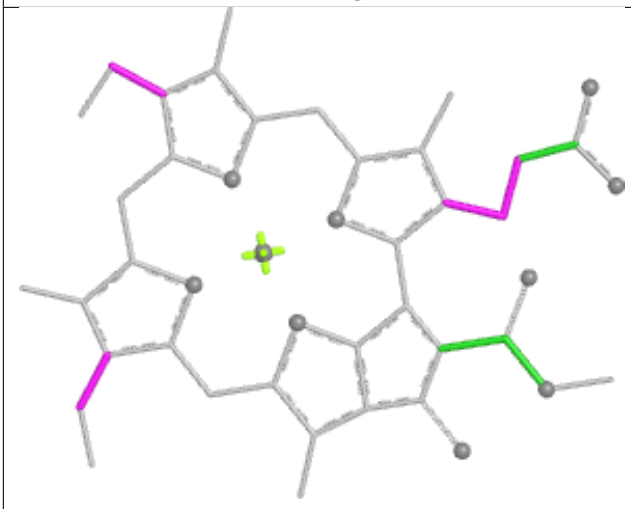
Ligand CLA B 1201



Bond lengths



Bond angles

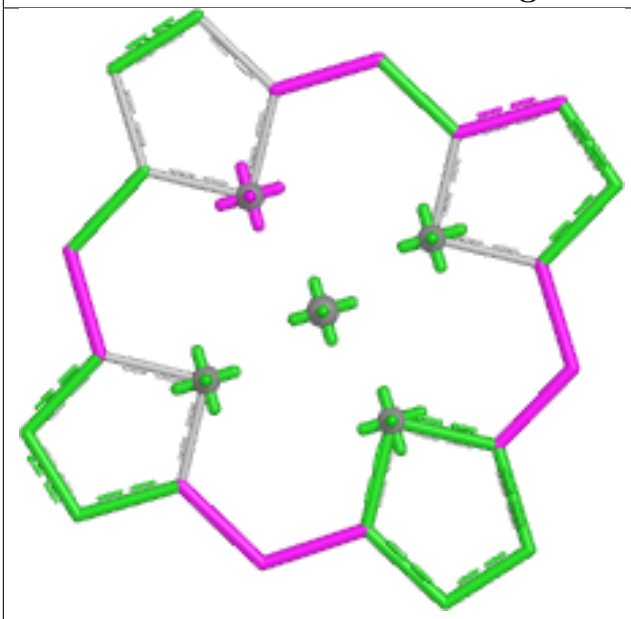


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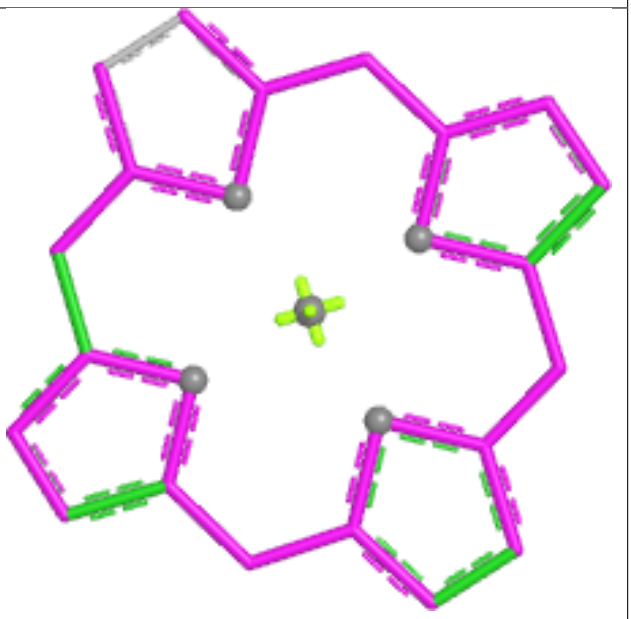


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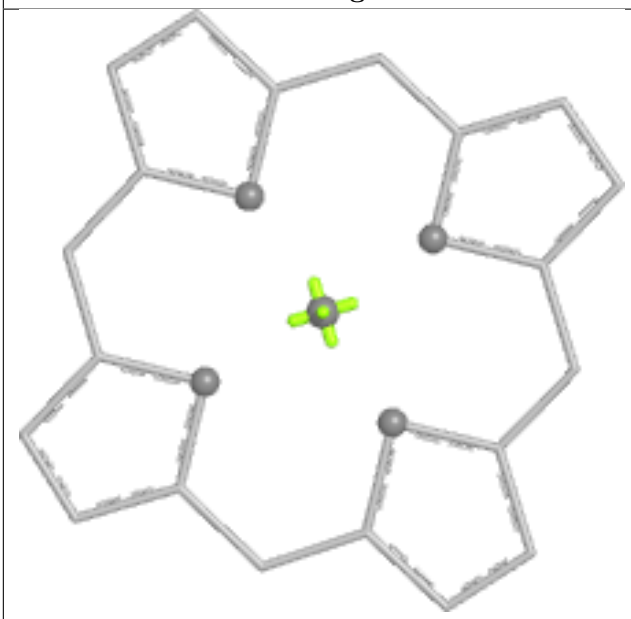
Ligand CLA 4 4010



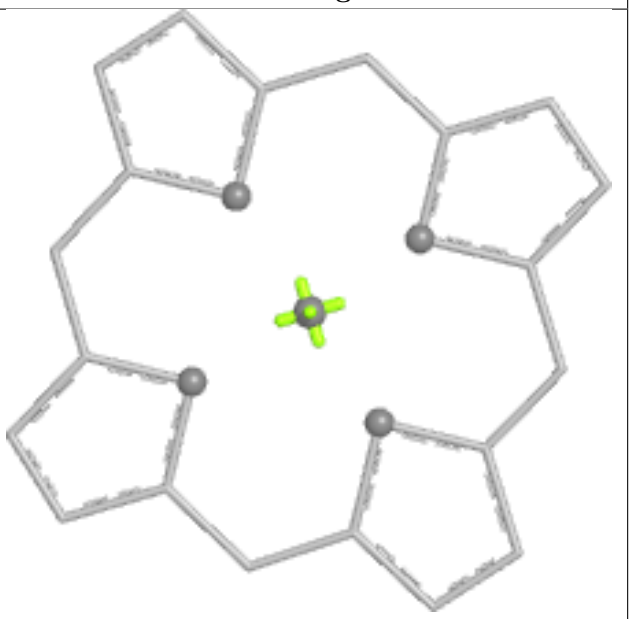
Bond lengths



Bond angles

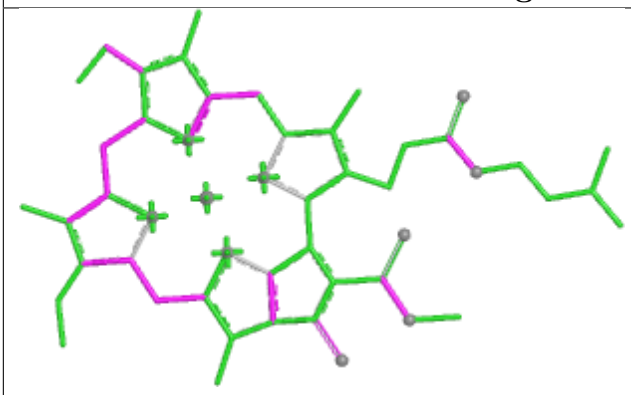


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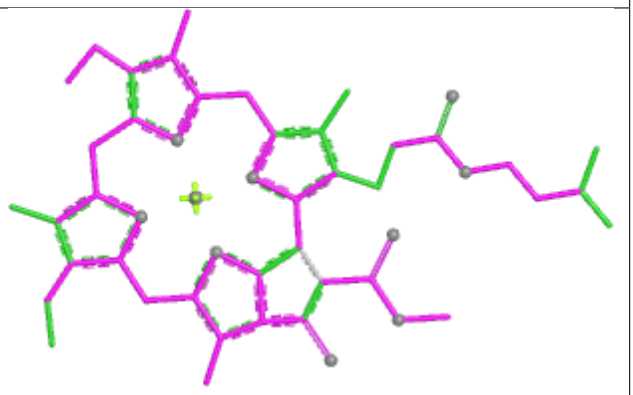


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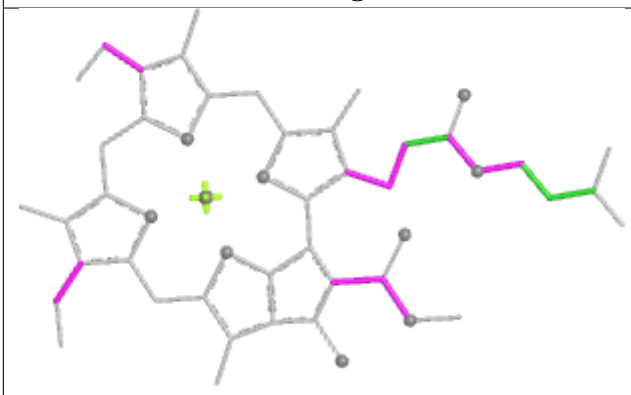
Ligand CLA B 1228



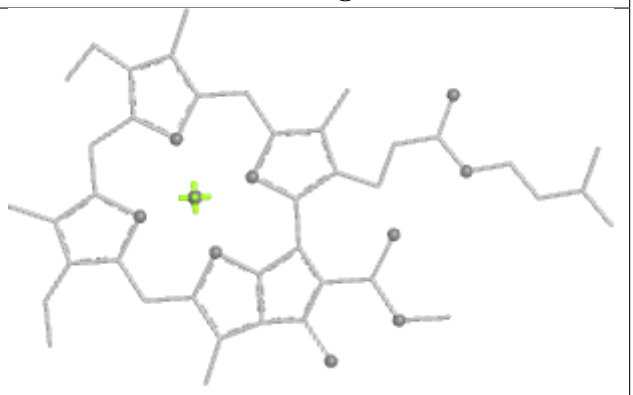
Bond lengths



Bond angles

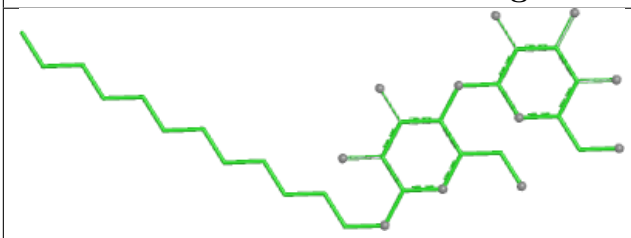


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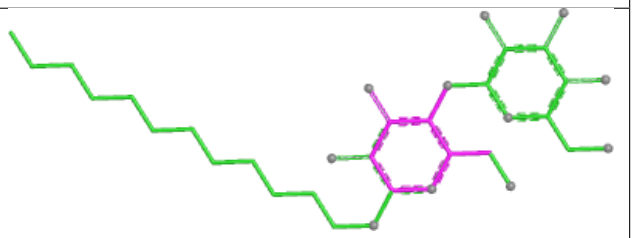


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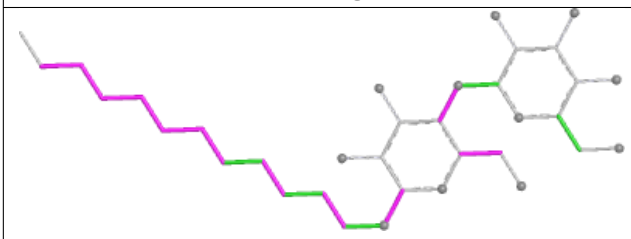
Ligand LMU A 7035



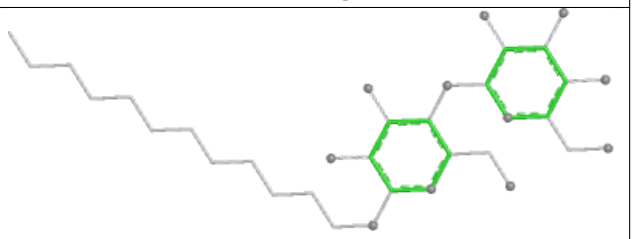
Bond lengths



Bond angles

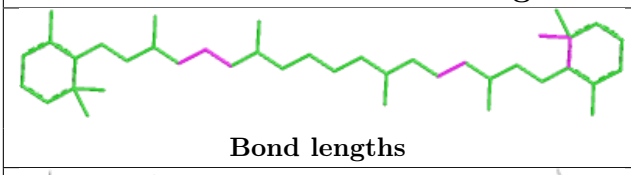


Torsions

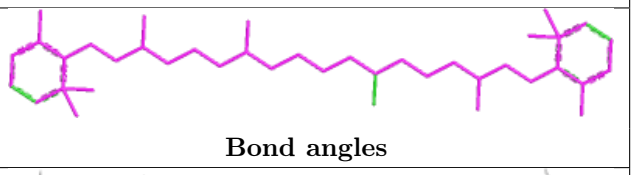


Rings

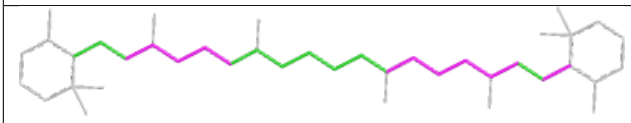
Ligand BCR A 6002



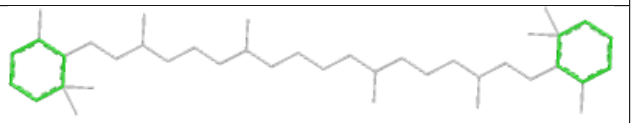
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Bond angles

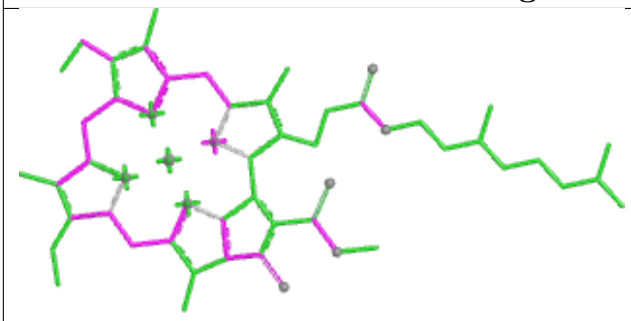


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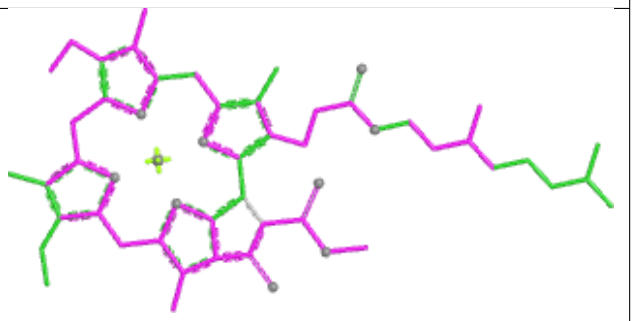


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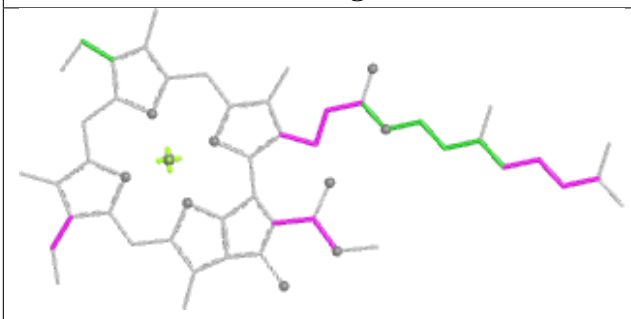
Ligand CLA J 1308



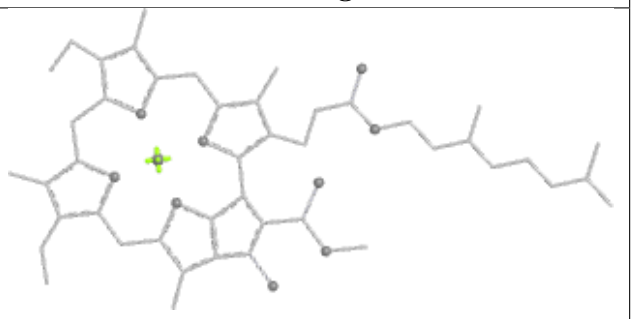
Bond lengths



Bond angles

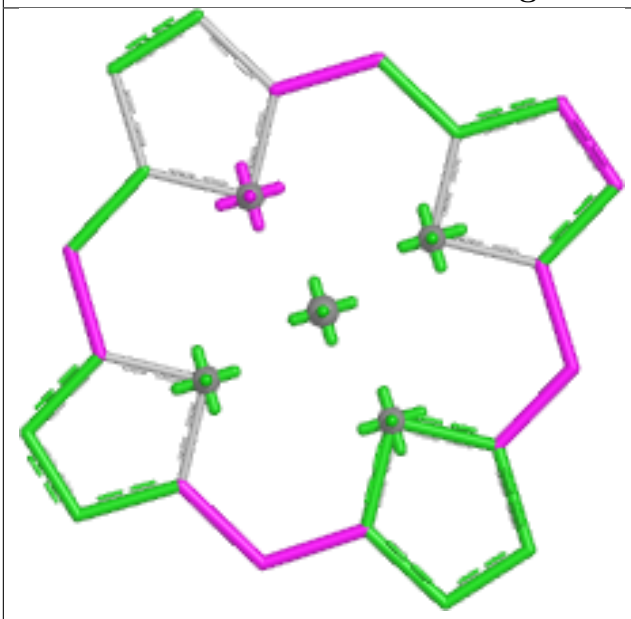


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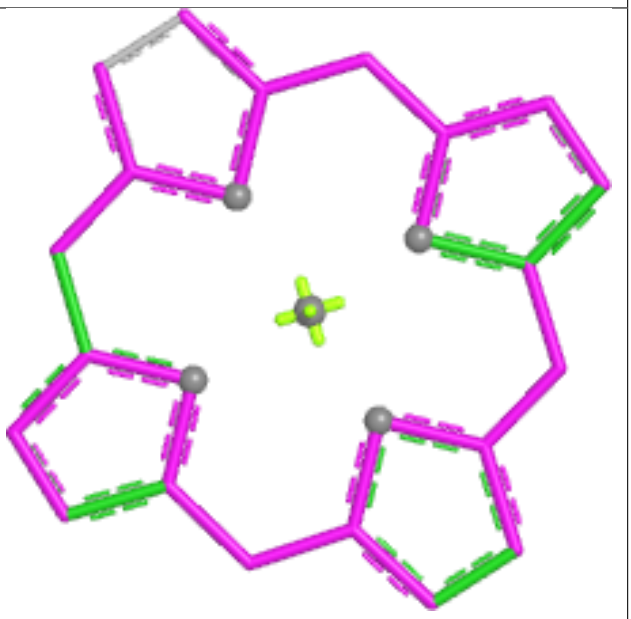


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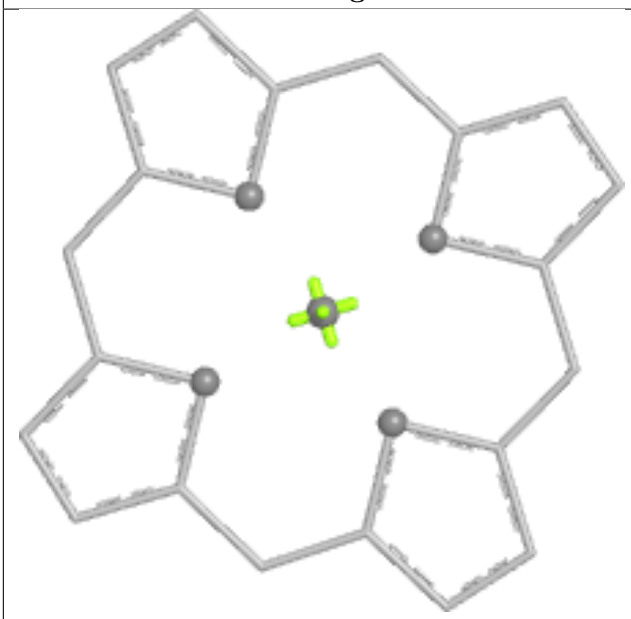
Ligand CLA 3 3005



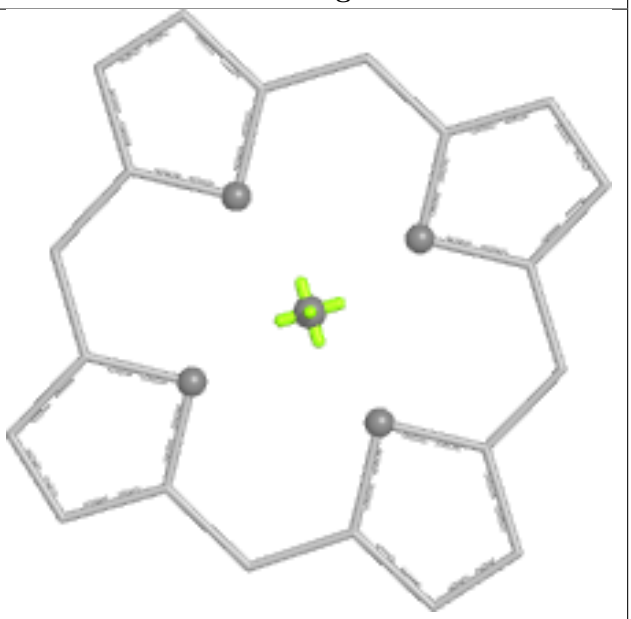
Bond lengths



Bond angles

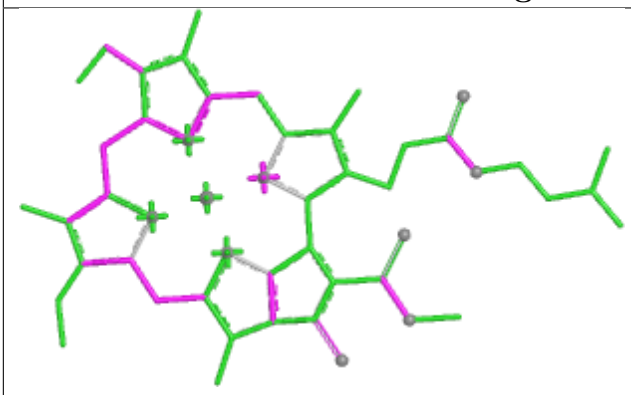


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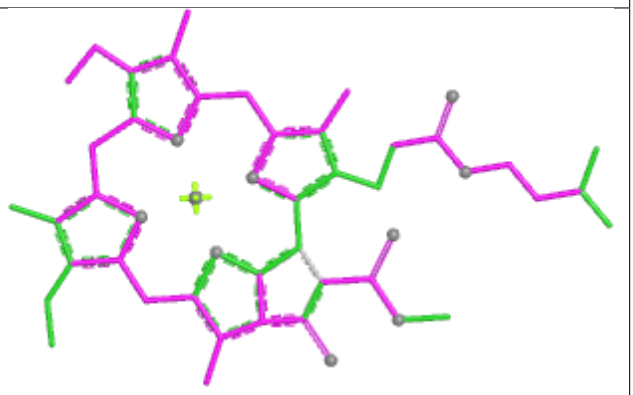


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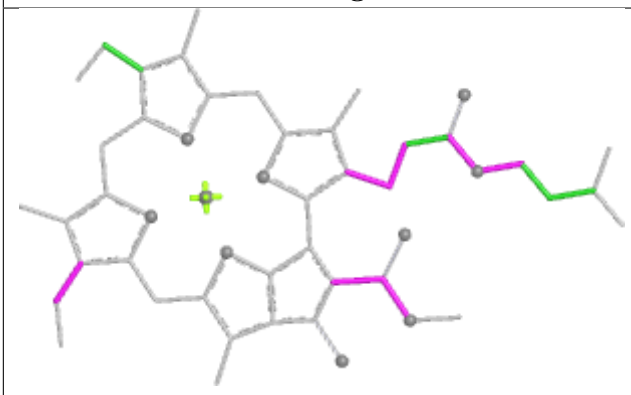
Ligand CLA A 1133



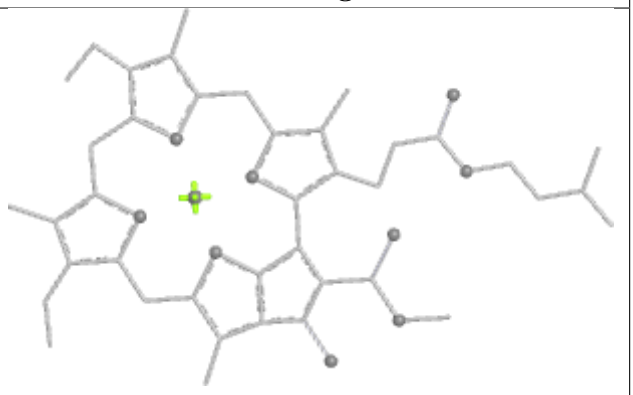
Bond lengths



Bond angles

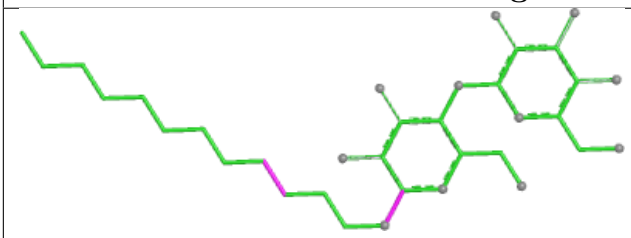


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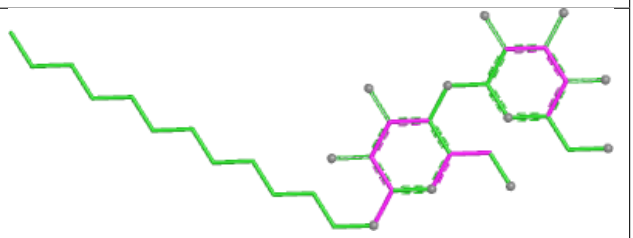


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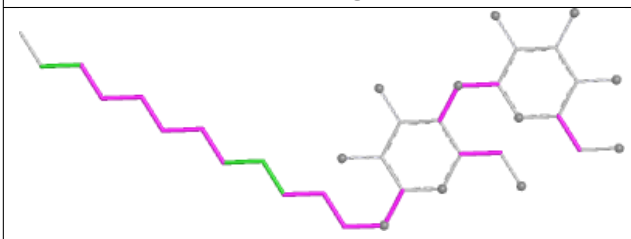
Ligand LMU A 7010



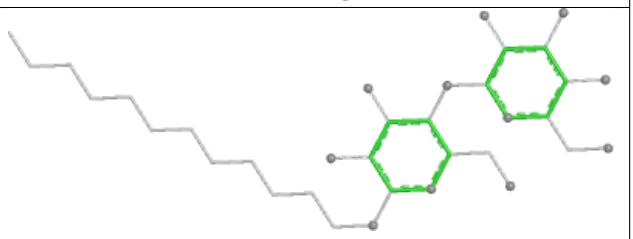
Bond lengths



Bond angles

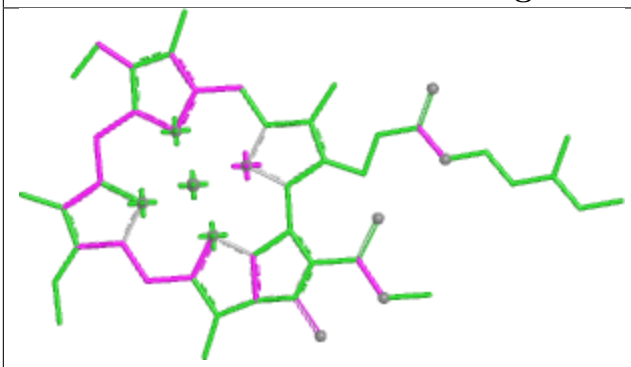


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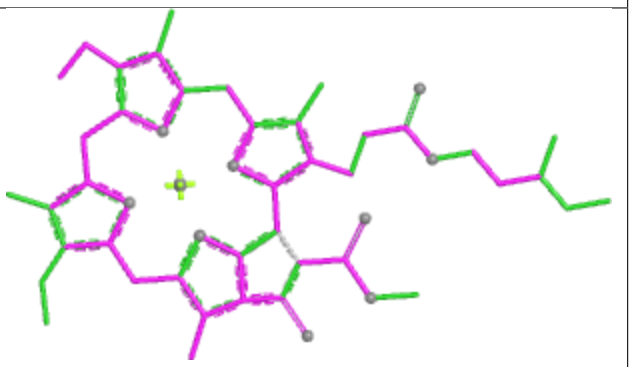


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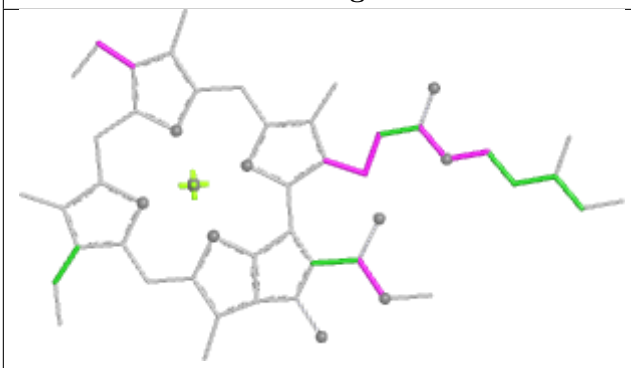
Ligand CLA A 1135



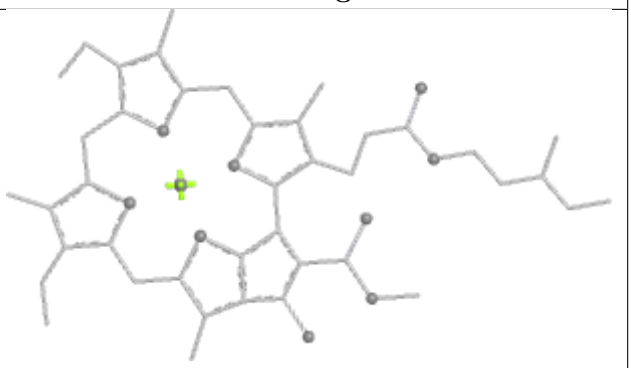
Bond lengths



Bond angles

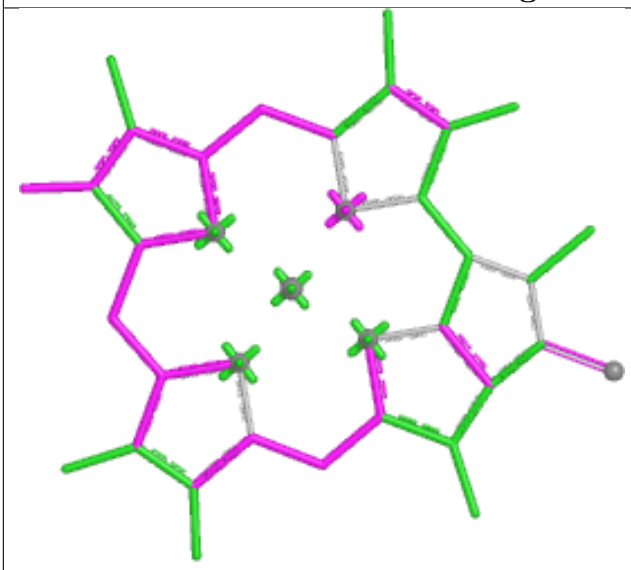


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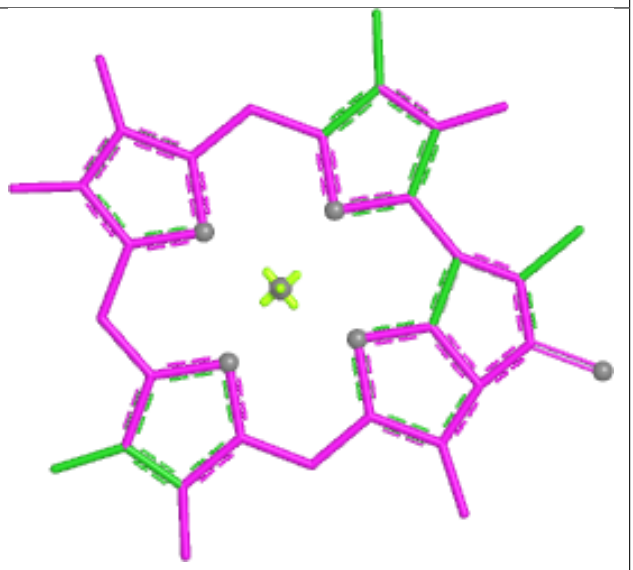


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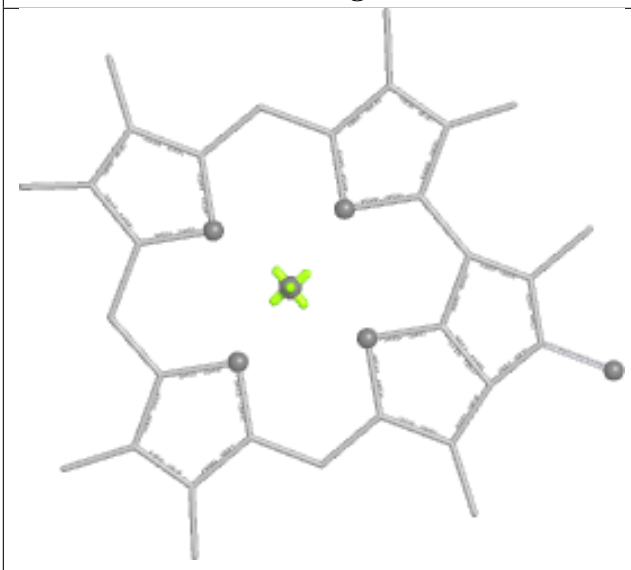
Ligand CLA 1 1011



Bond lengths



Bond angles

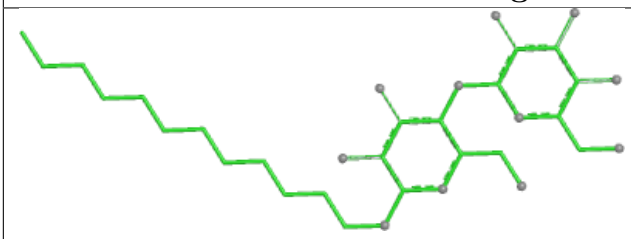


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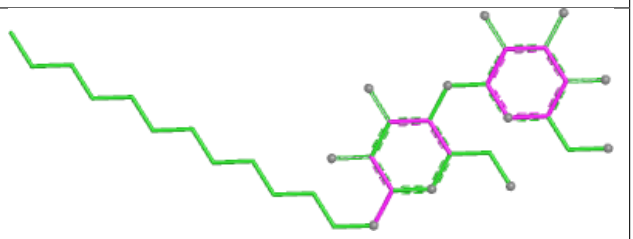


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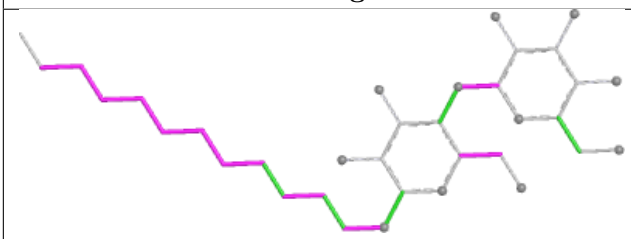
Ligand LMU R 7020



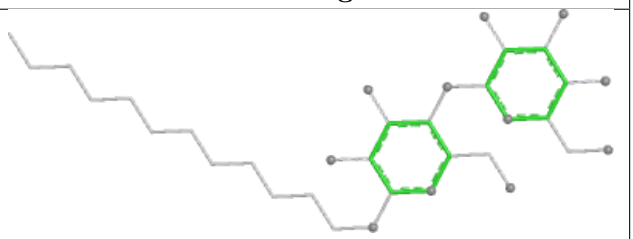
Bond lengths



Bond angles

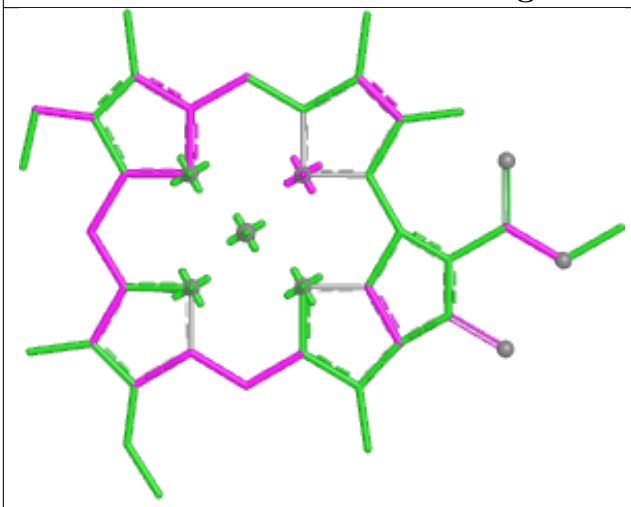


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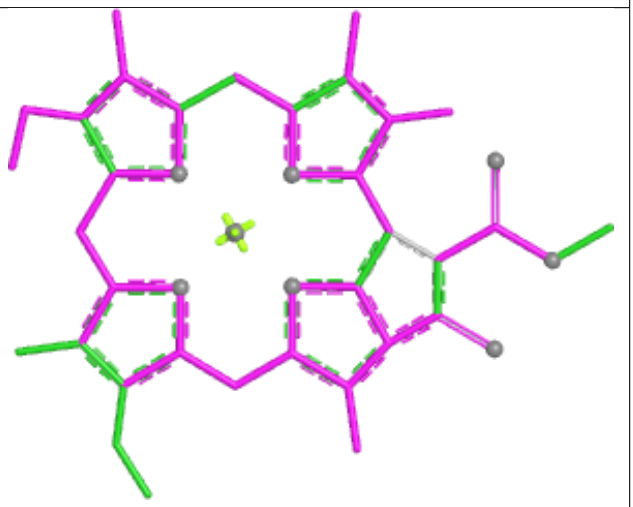


Rings

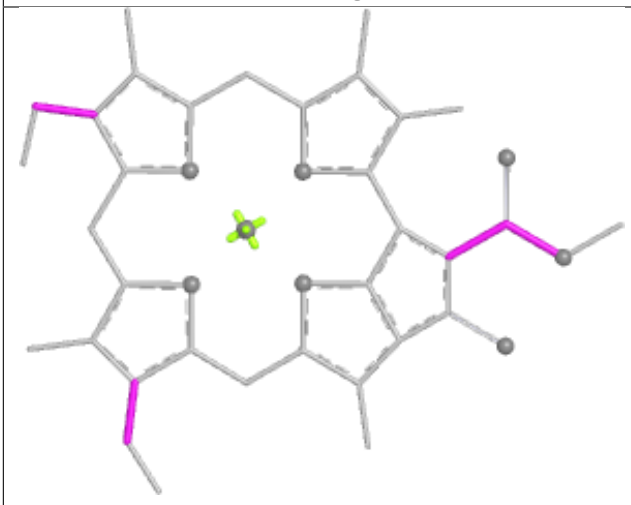
Ligand CLA F 1302



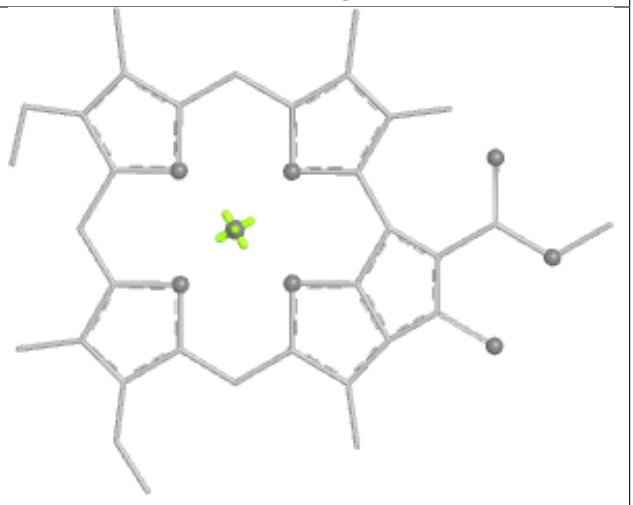
Bond lengths



Bond angles

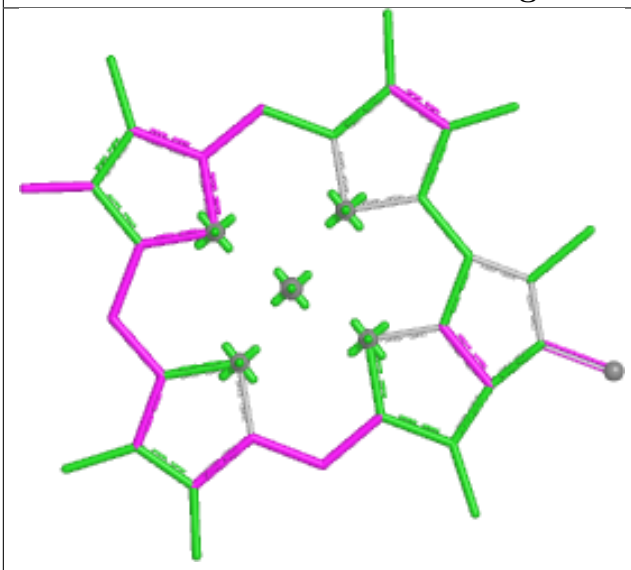


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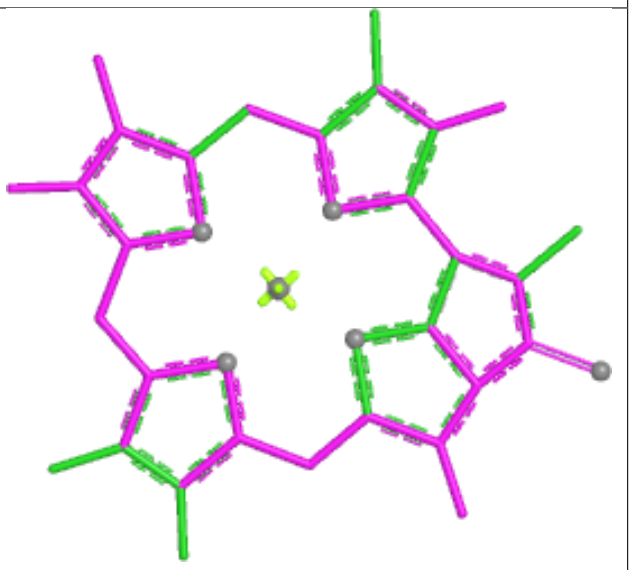


Rings

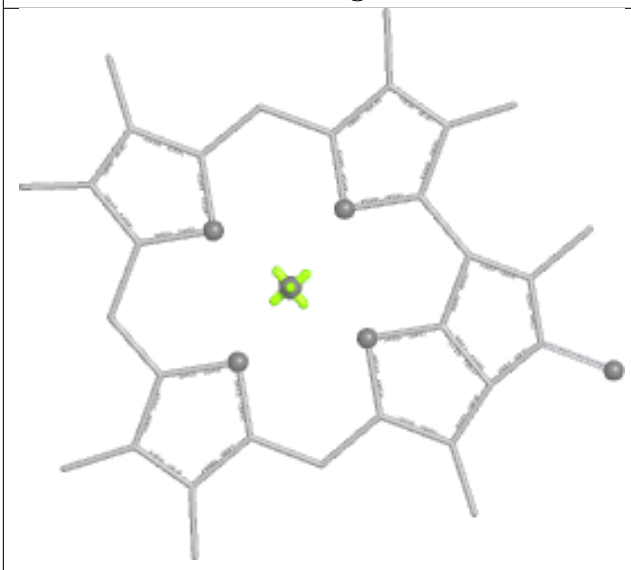
Ligand CLA 4 1009



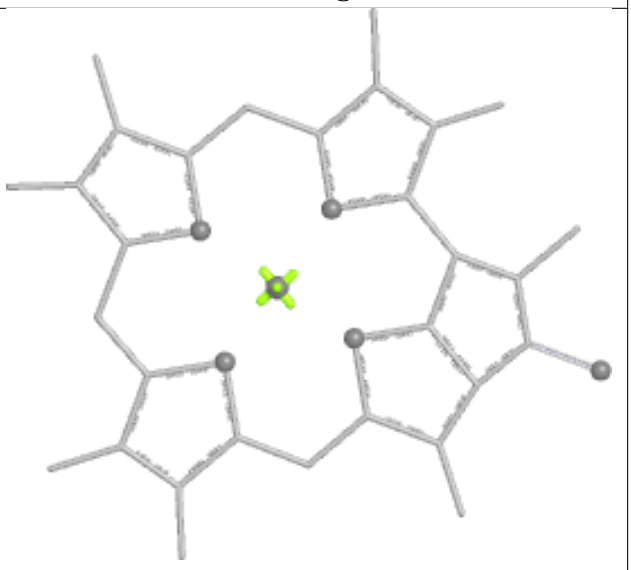
Bond lengths



Bond angles

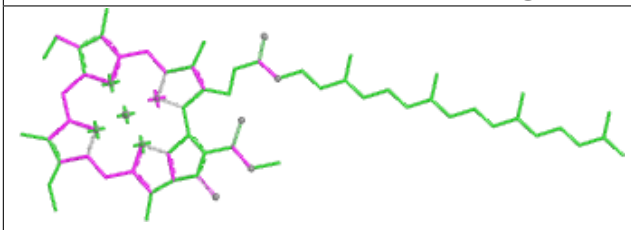


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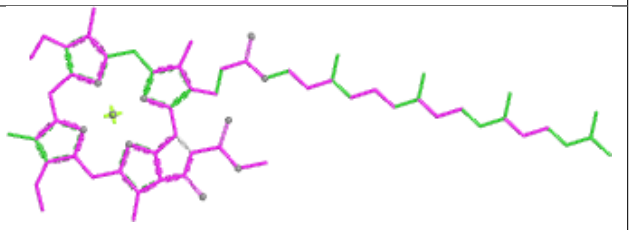


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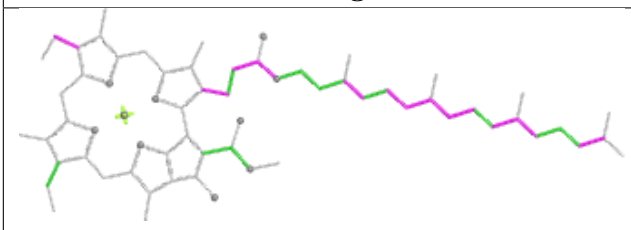
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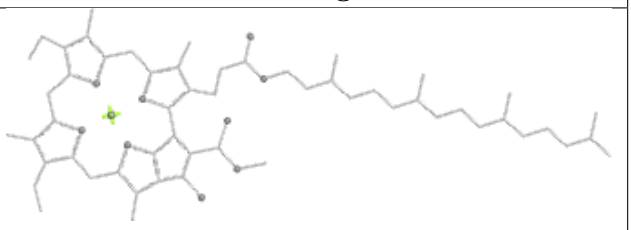
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Bond angles

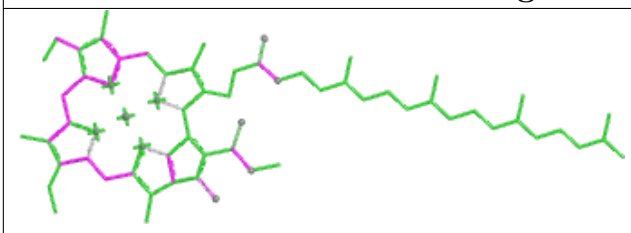


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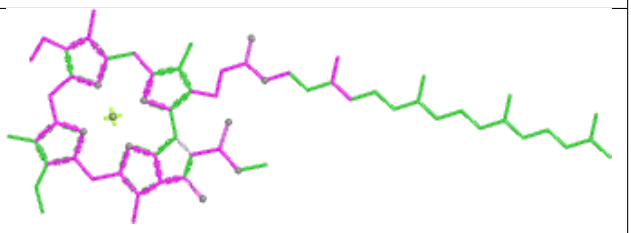


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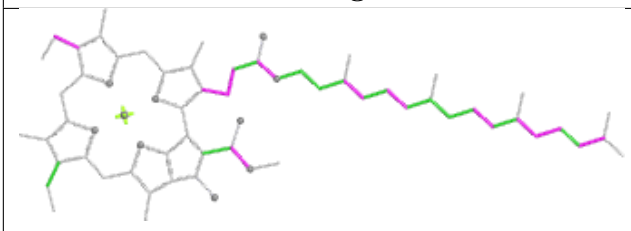
Ligand CLA L 1130



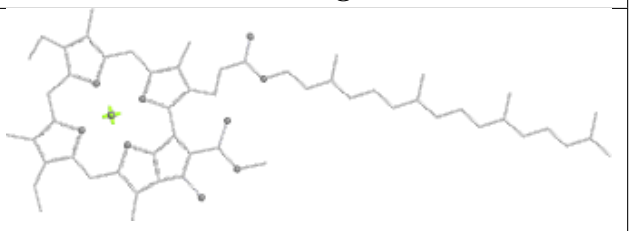
Bond lengths



Bond angles

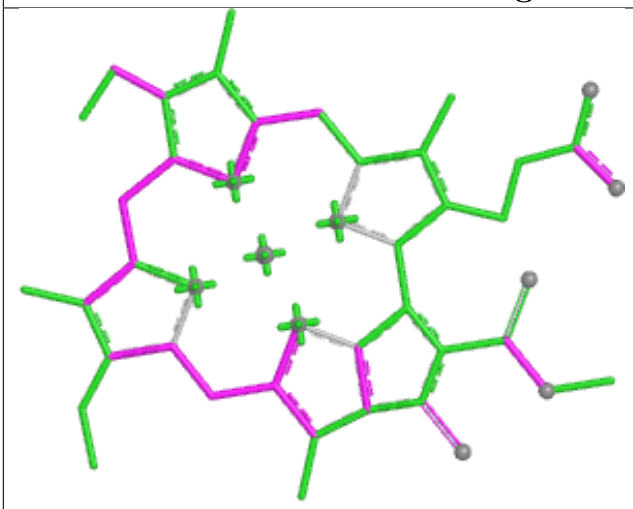


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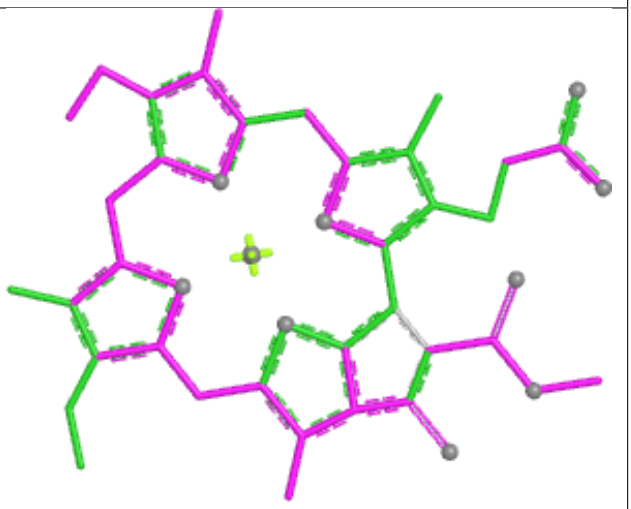


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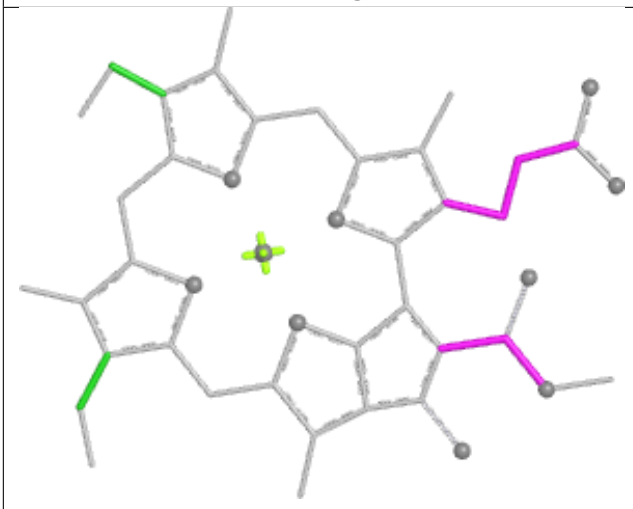
Ligand CLA B 1231



Bond lengths



Bond angles

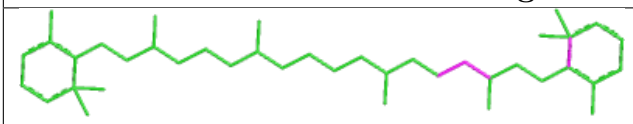


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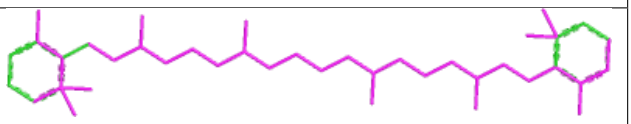


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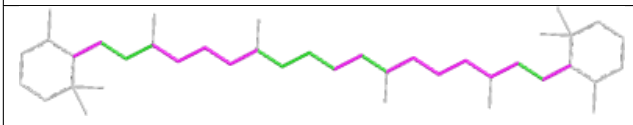
Ligand BCR 3 6022



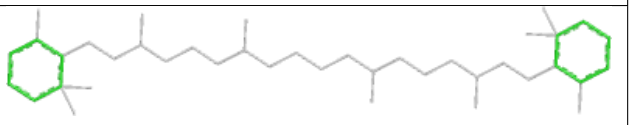
Bond lengths



Bond angles

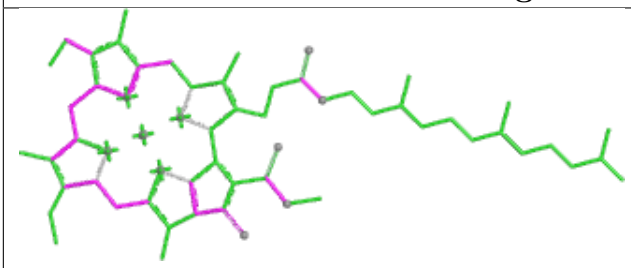


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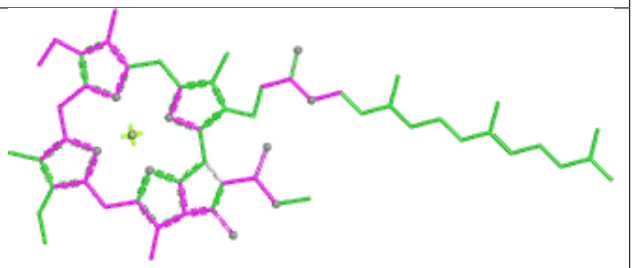


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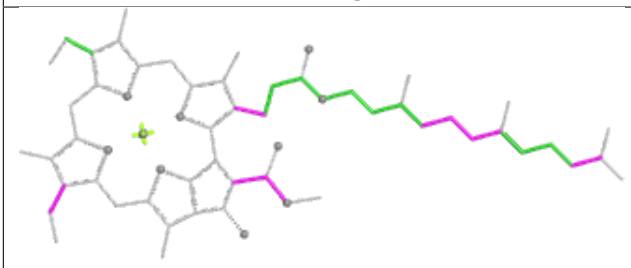
Ligand CLA B 1234



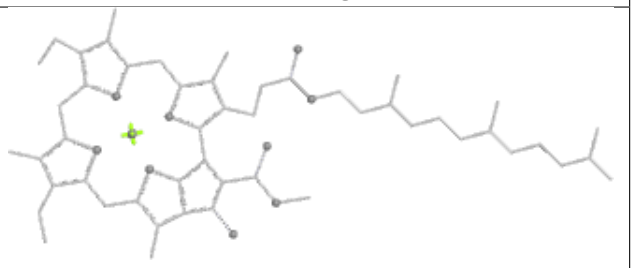
Bond lengths



Bond angles

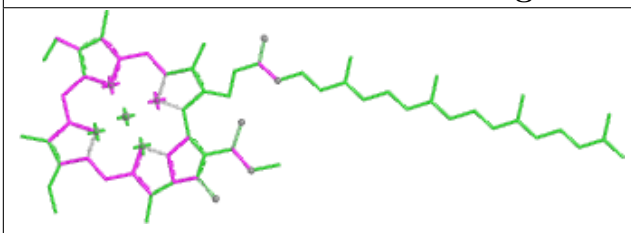


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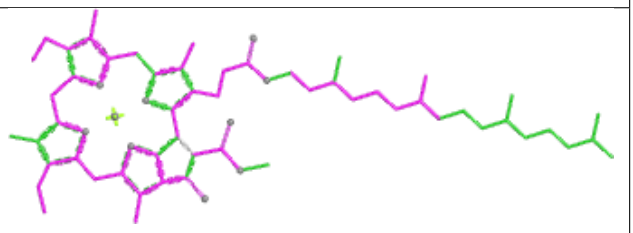


Rings

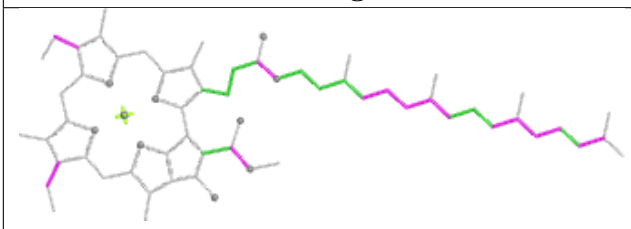
Ligand CLA B 1220



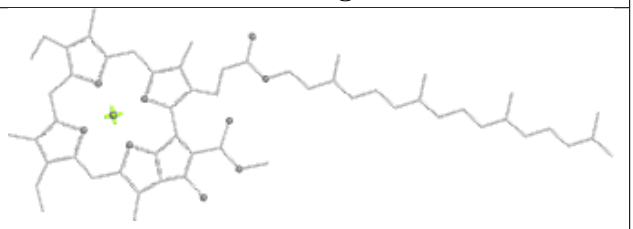
Bond lengths



Bond angles

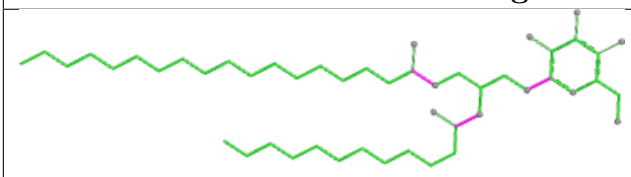


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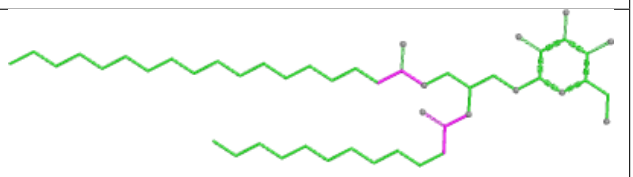


Rings

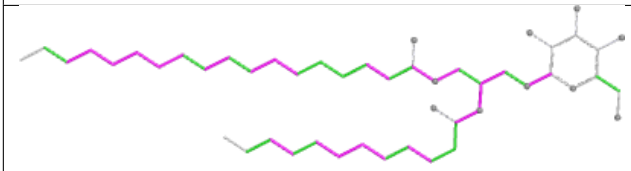
Ligand LMG B 7101



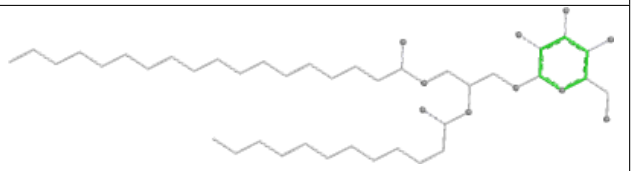
Bond lengths



Bond angles

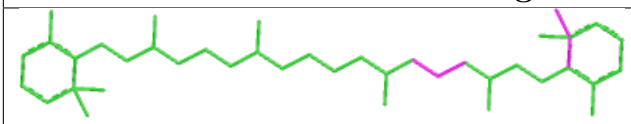


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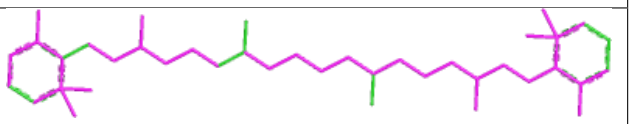


Rings

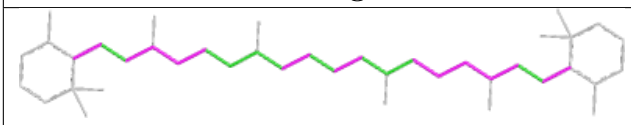
Ligand BCR F 6014



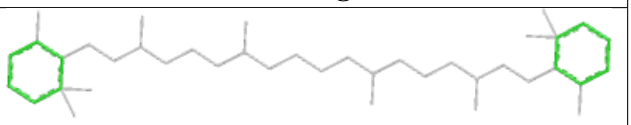
Bond lengths



Bond angles

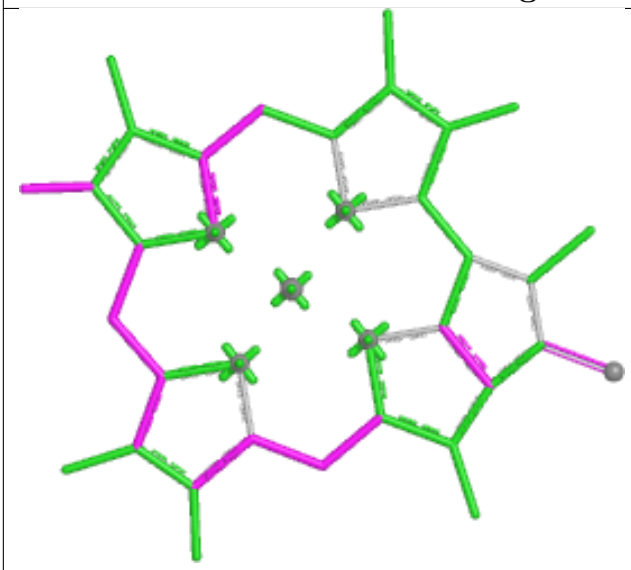


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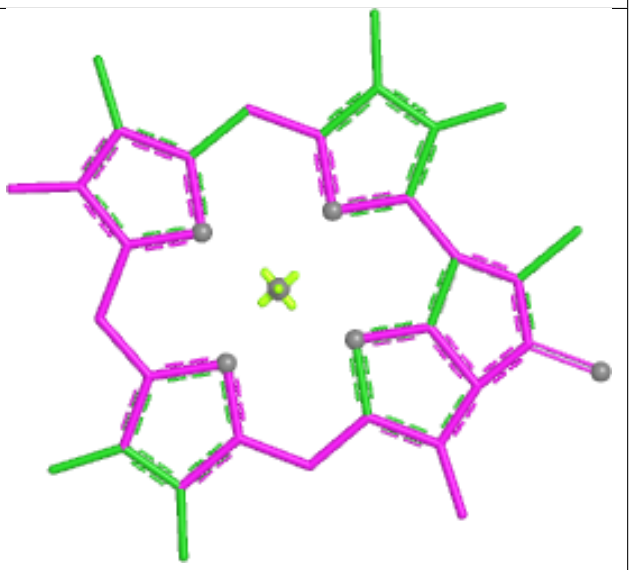


Rings

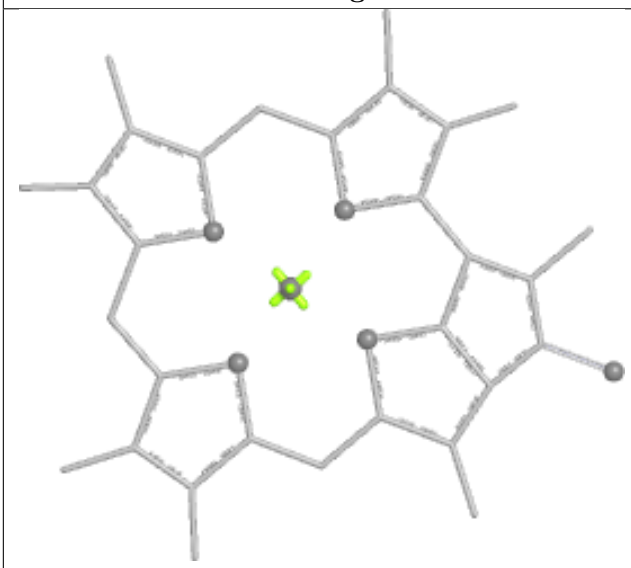
Ligand CLA 1 1012



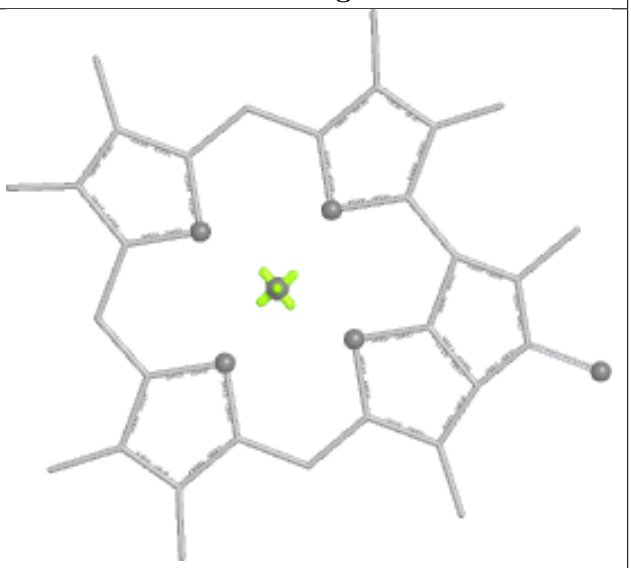
Bond lengths



Bond angles

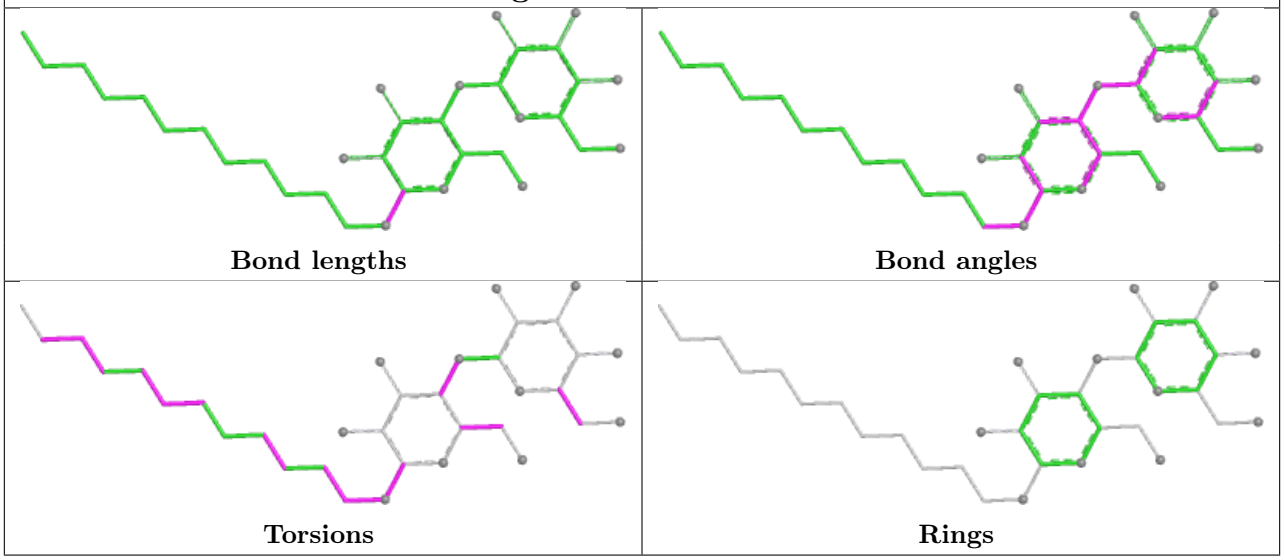


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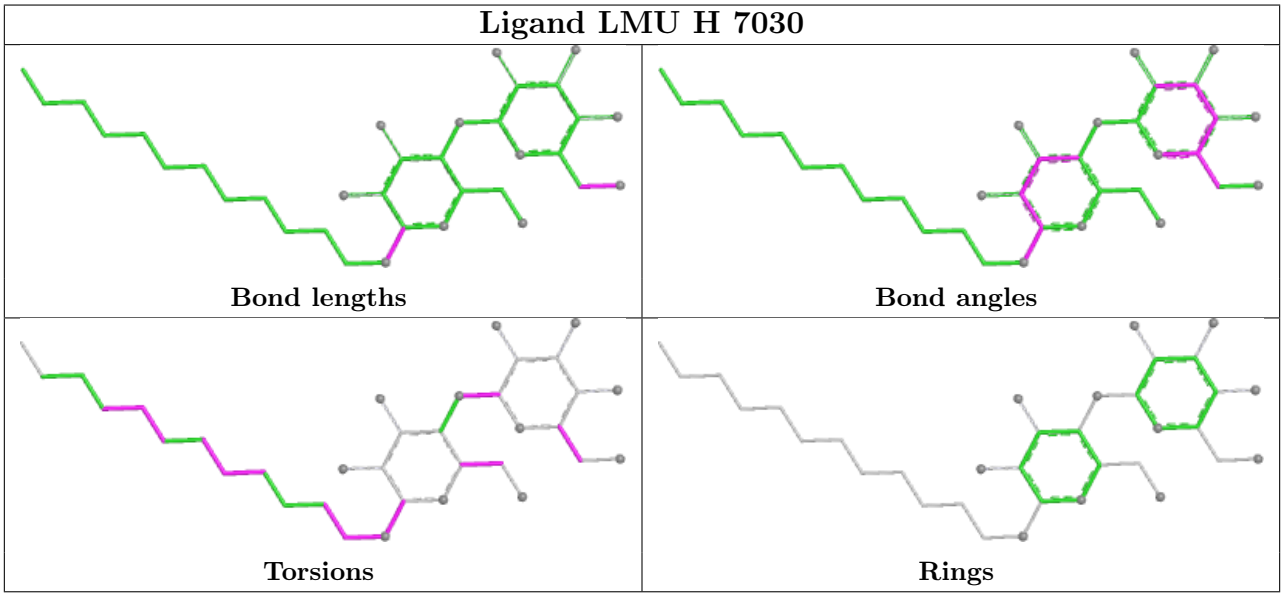


Rings

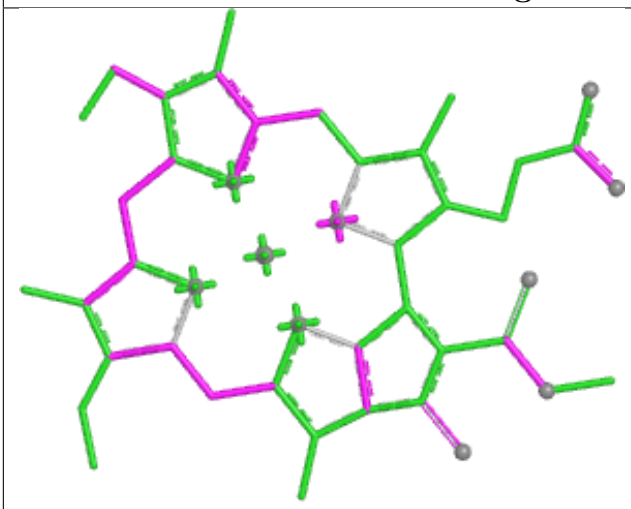
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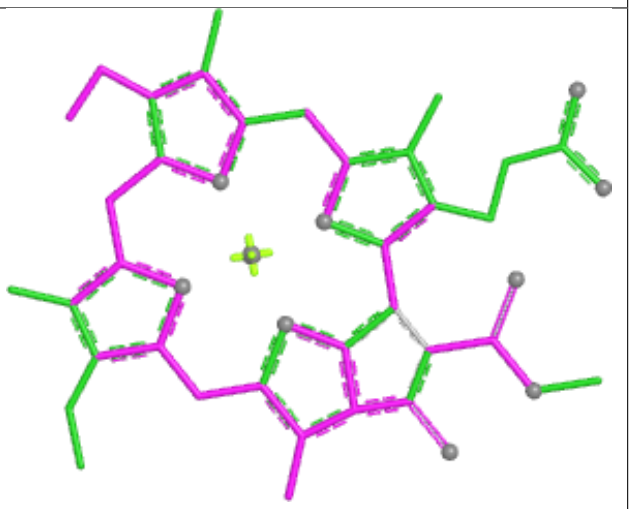
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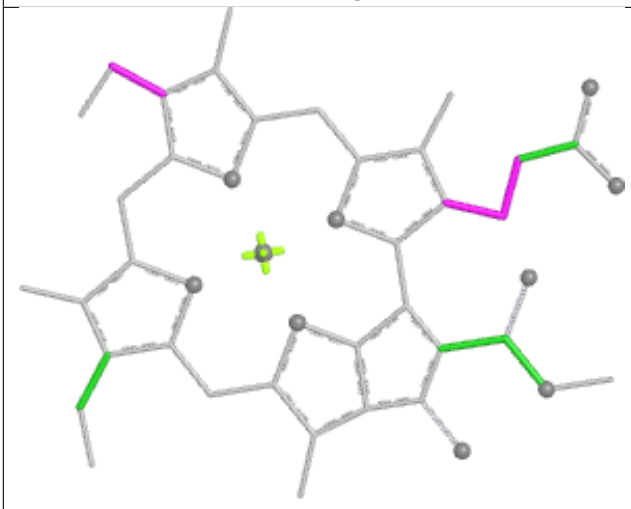
Ligand CLA K 1142



Bond lengths



Bond angles

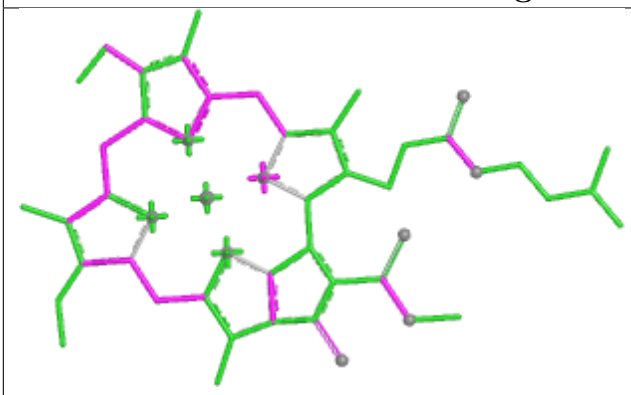


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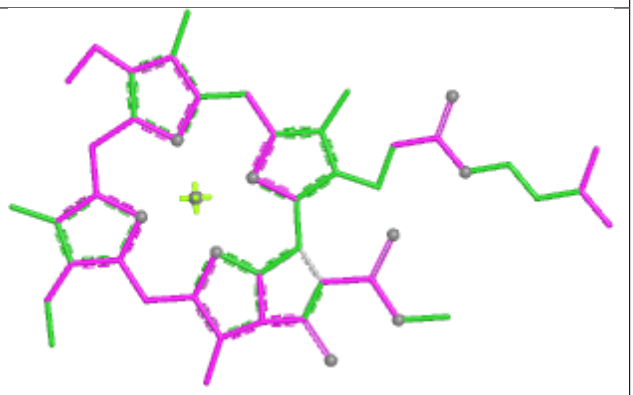


Rings

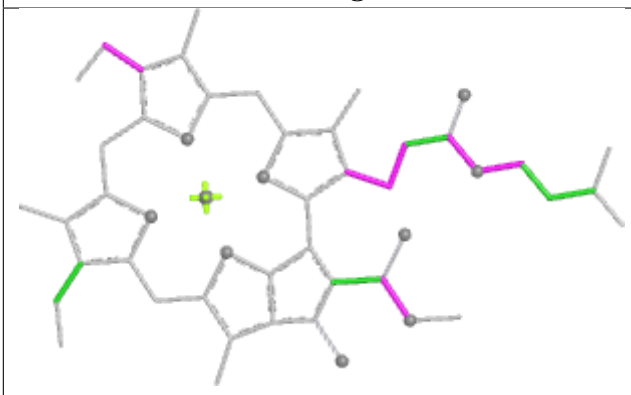
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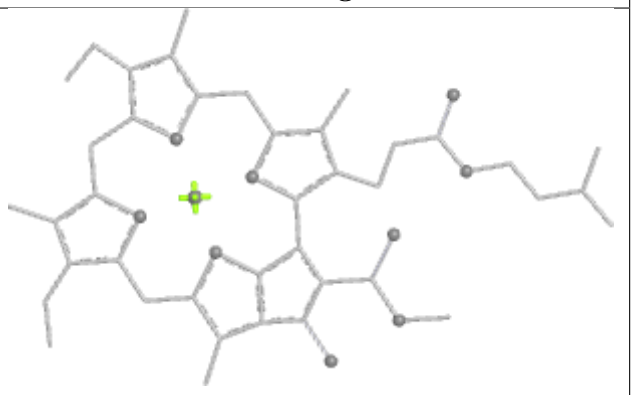
Bond lengths



Bond angles

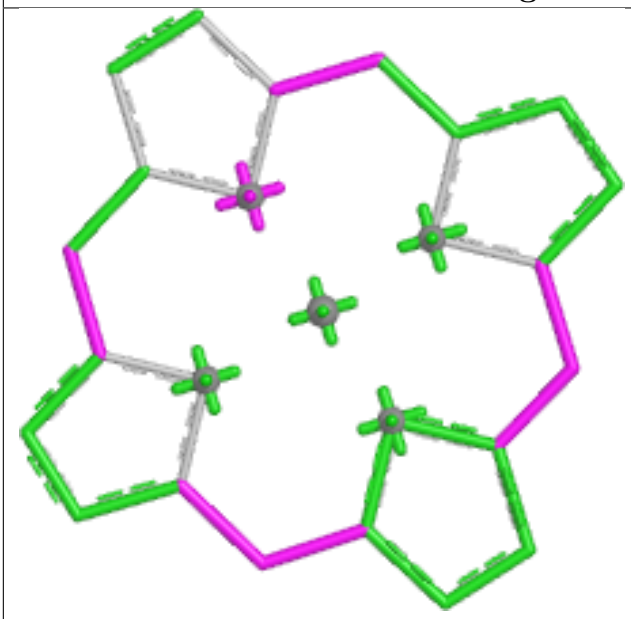


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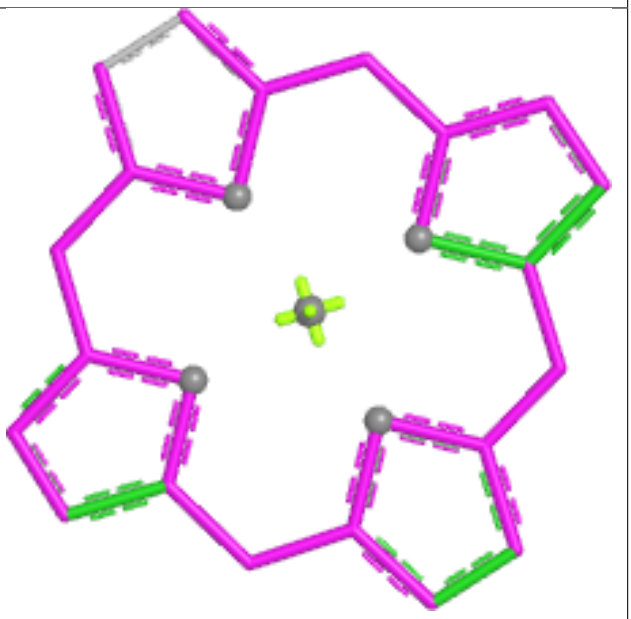


Rings

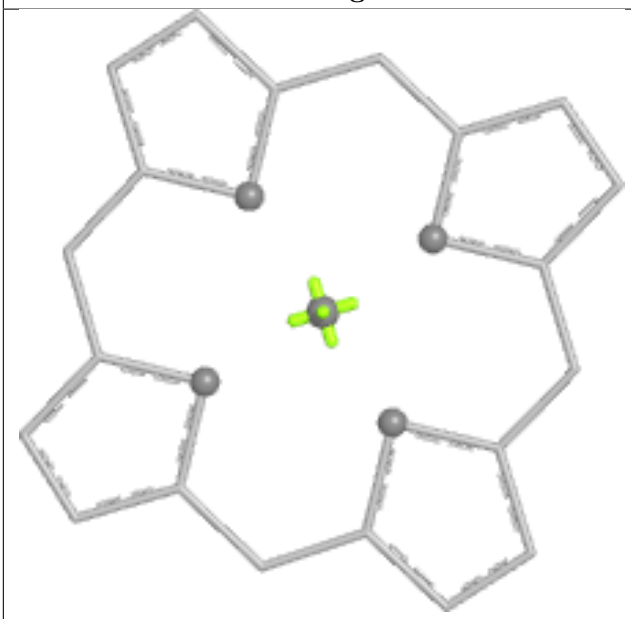
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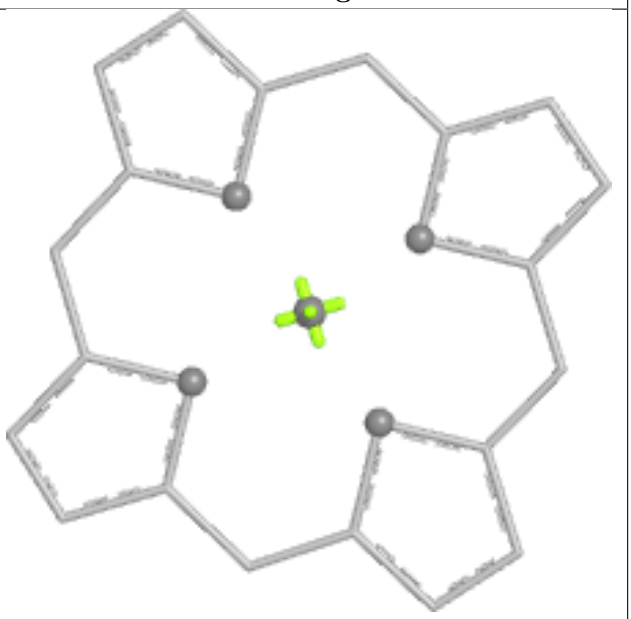
Bond lengths



Bond angles

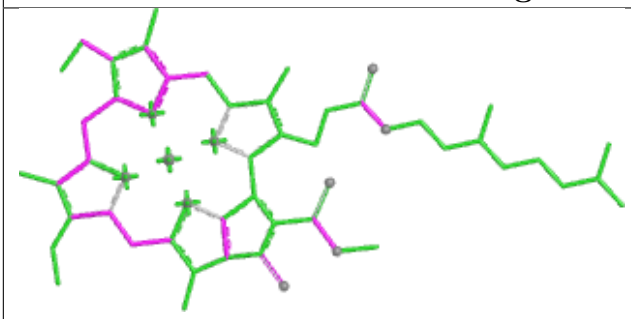


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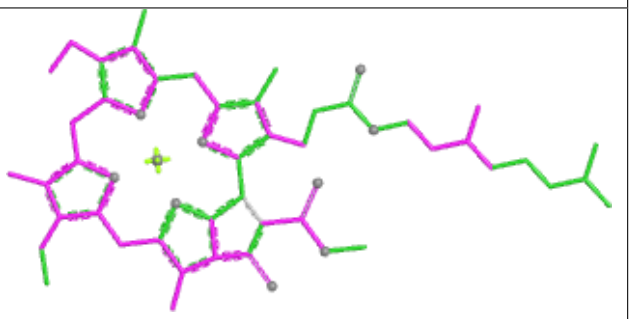


Rings

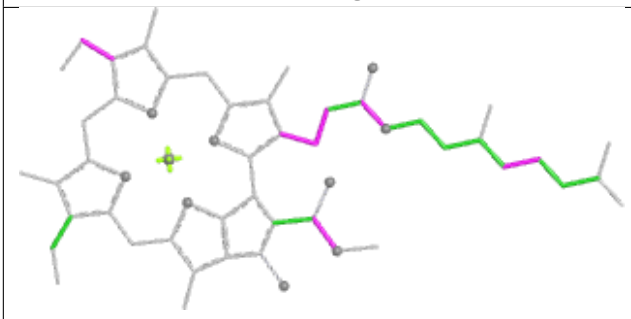
Ligand CLA A 1122



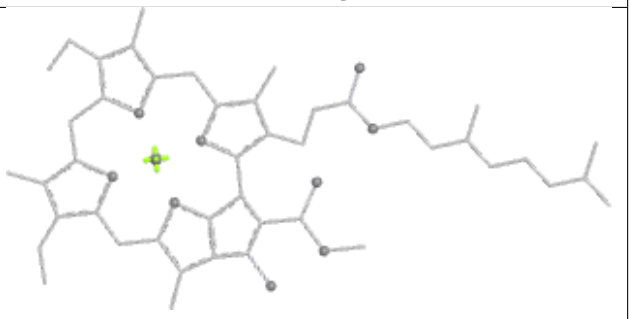
Bond lengths



Bond angles

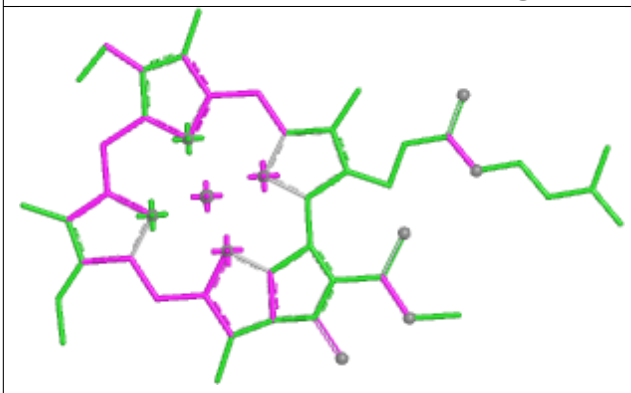


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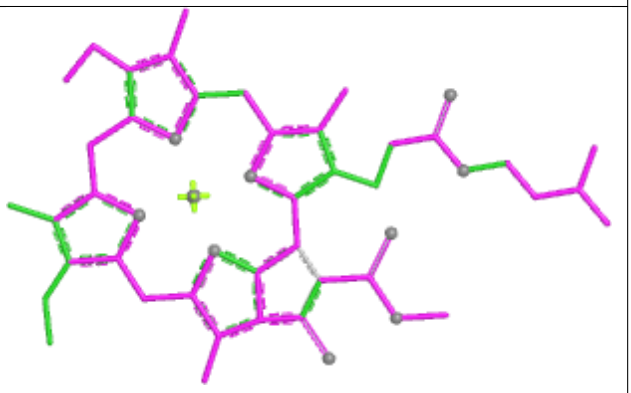


Rings

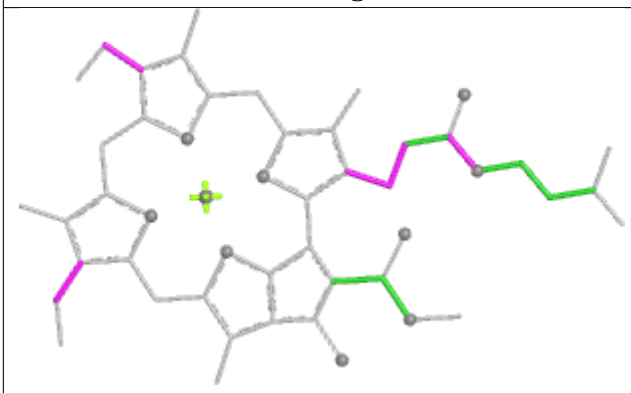
Ligand CLA K 1146



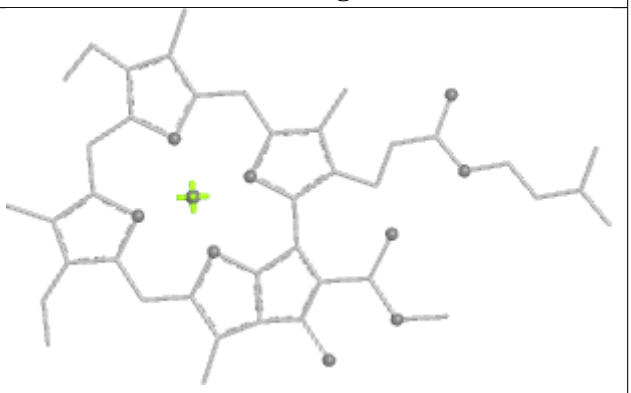
Bond lengths



Bond angles

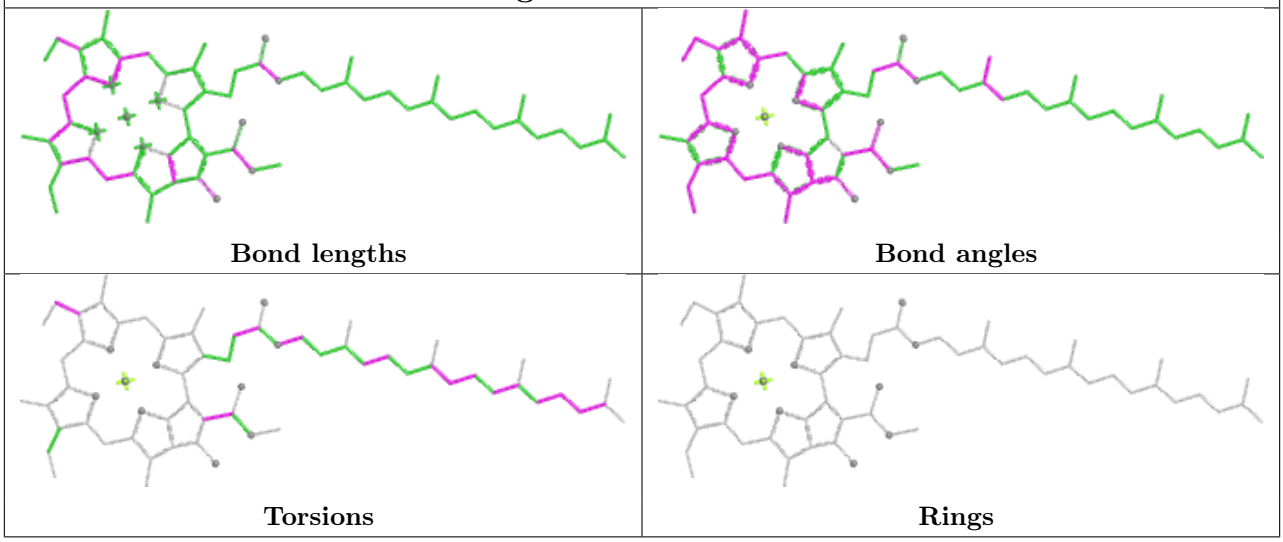


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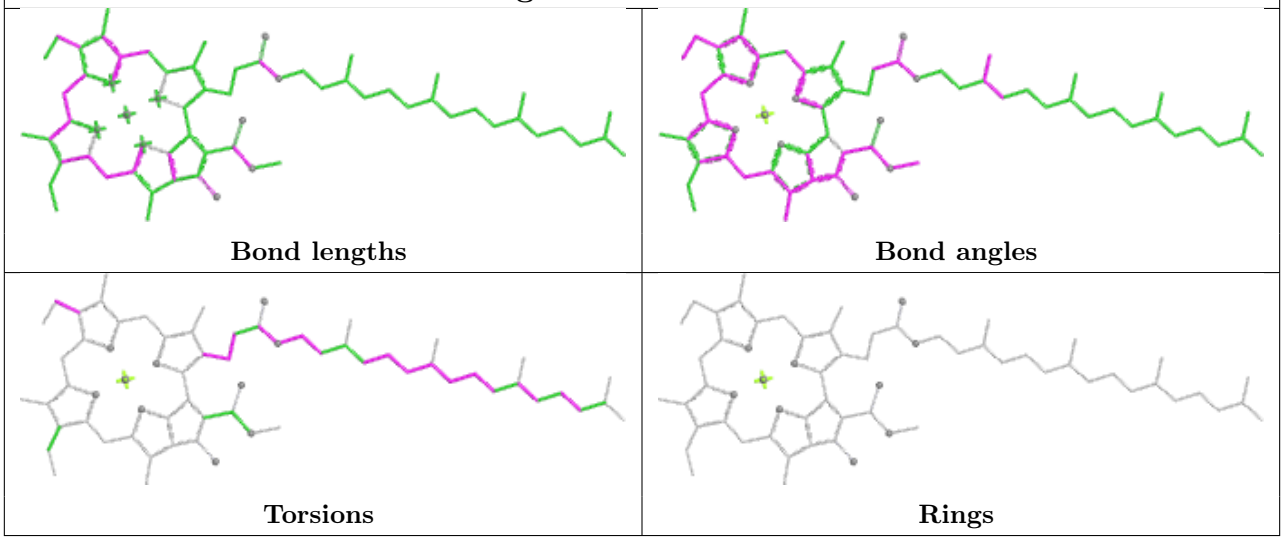


Rings

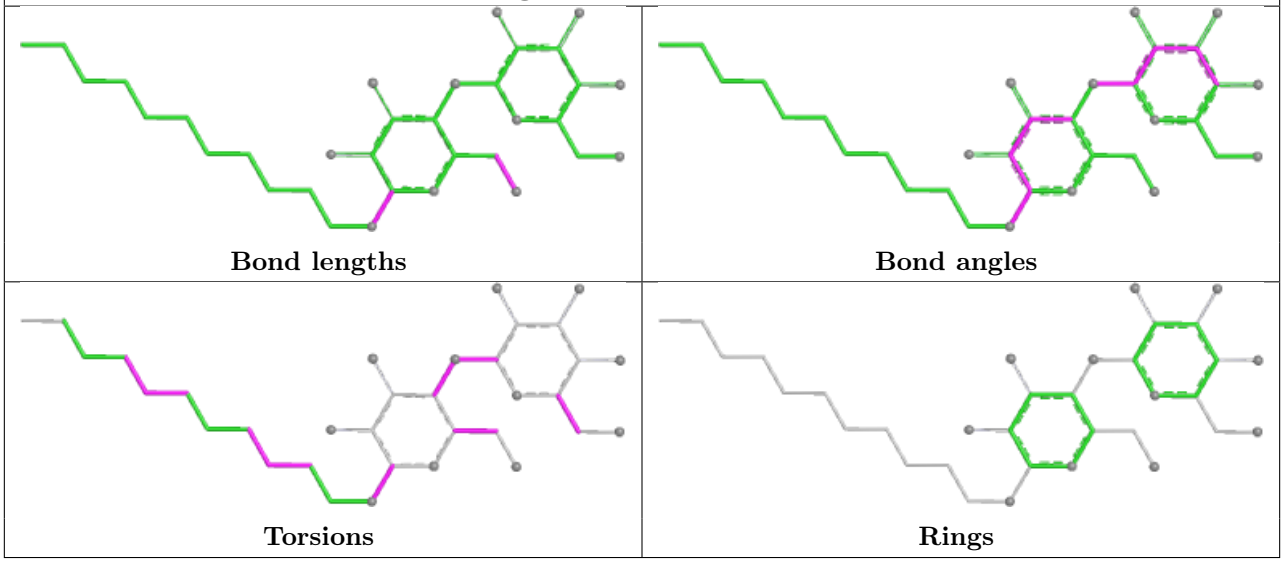
Ligand CLA B 1235



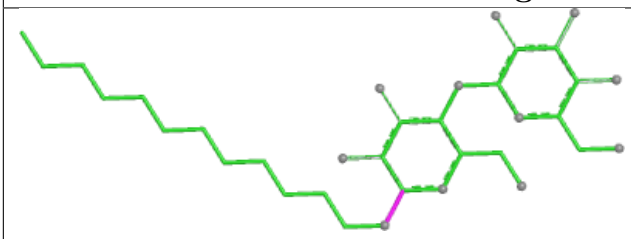
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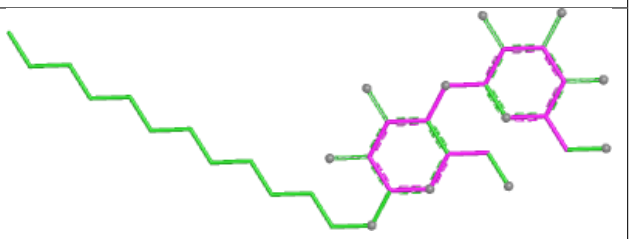
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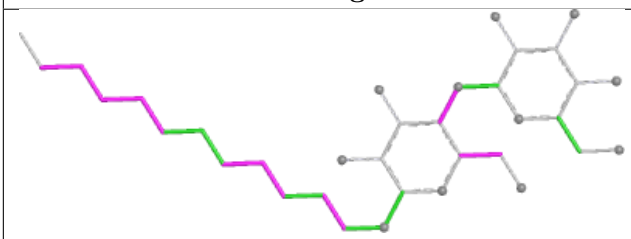
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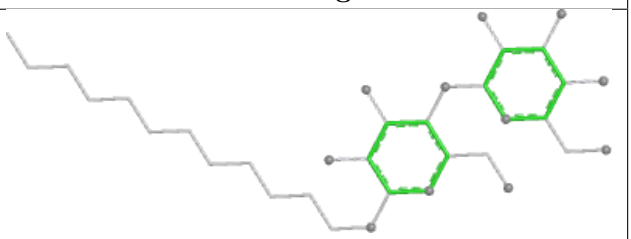
Bond lengths



Bond angles

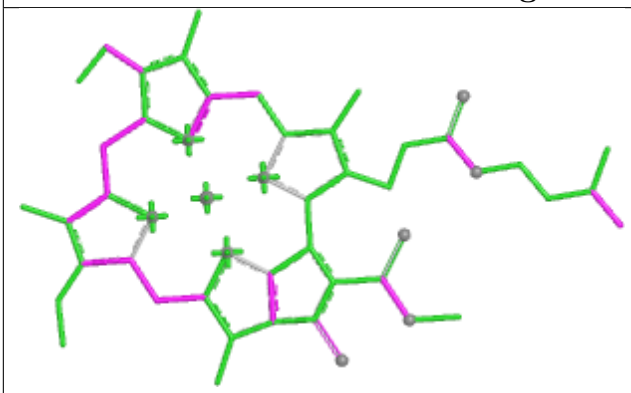


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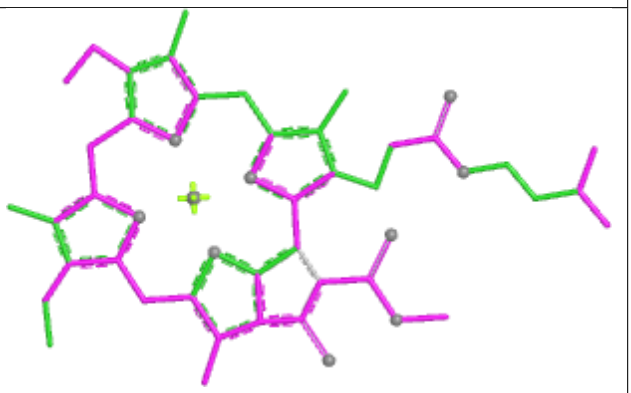


Rings

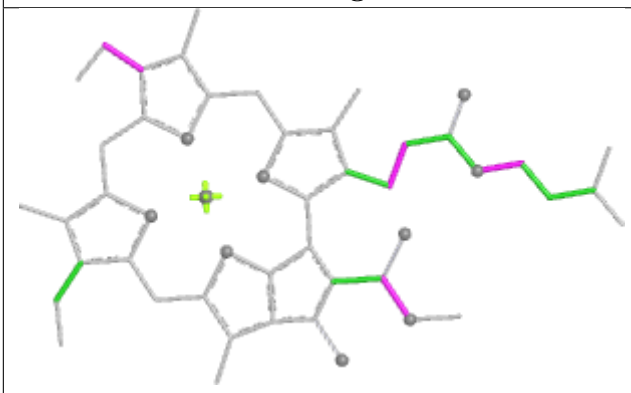
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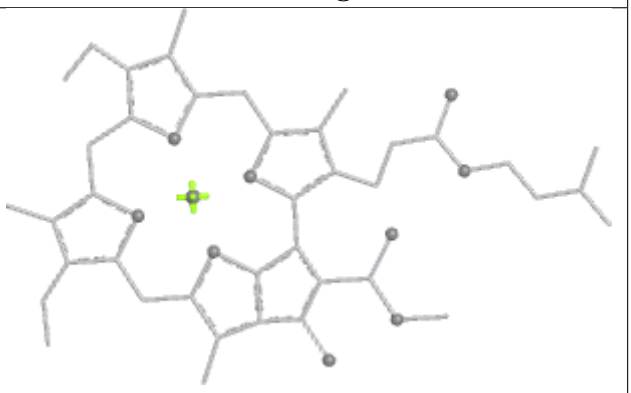
Bond lengths



Bond angles

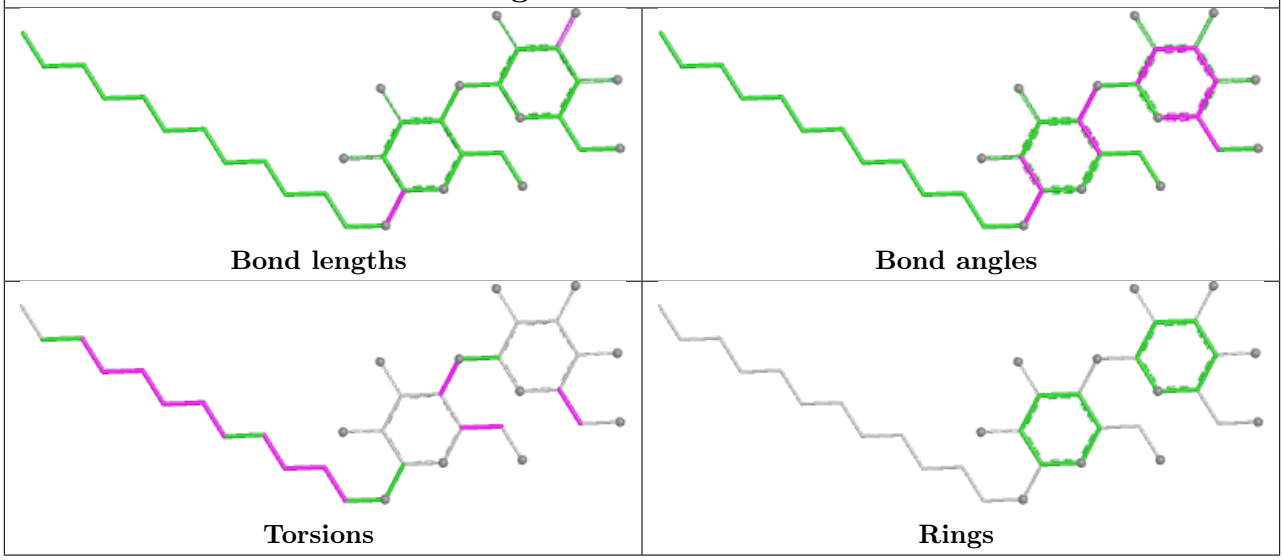


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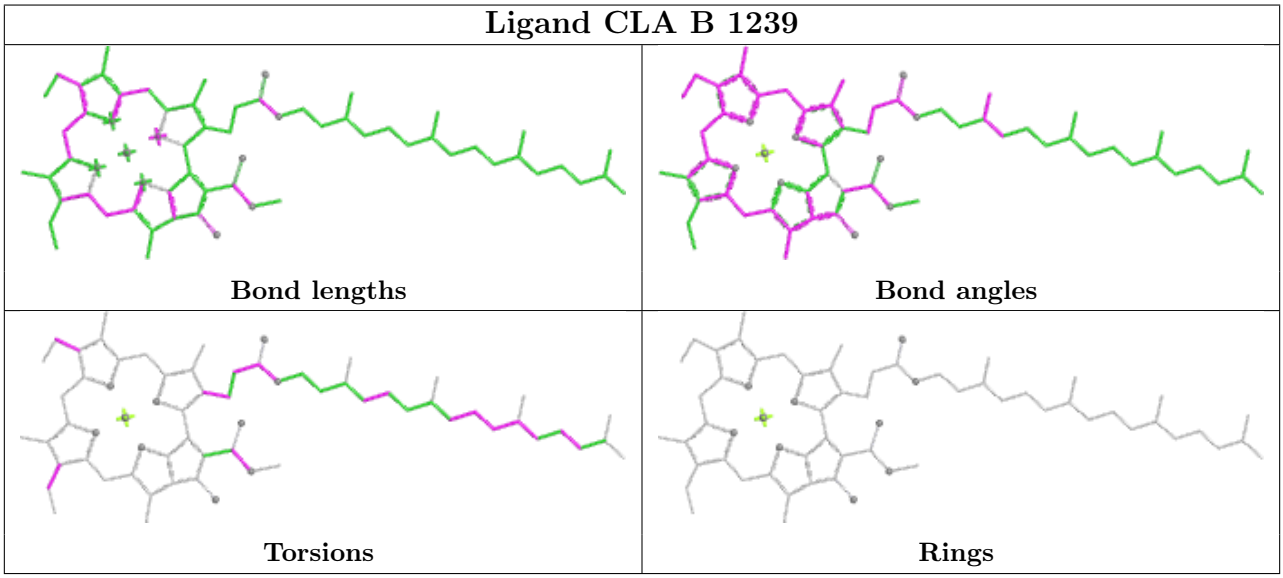


Rings

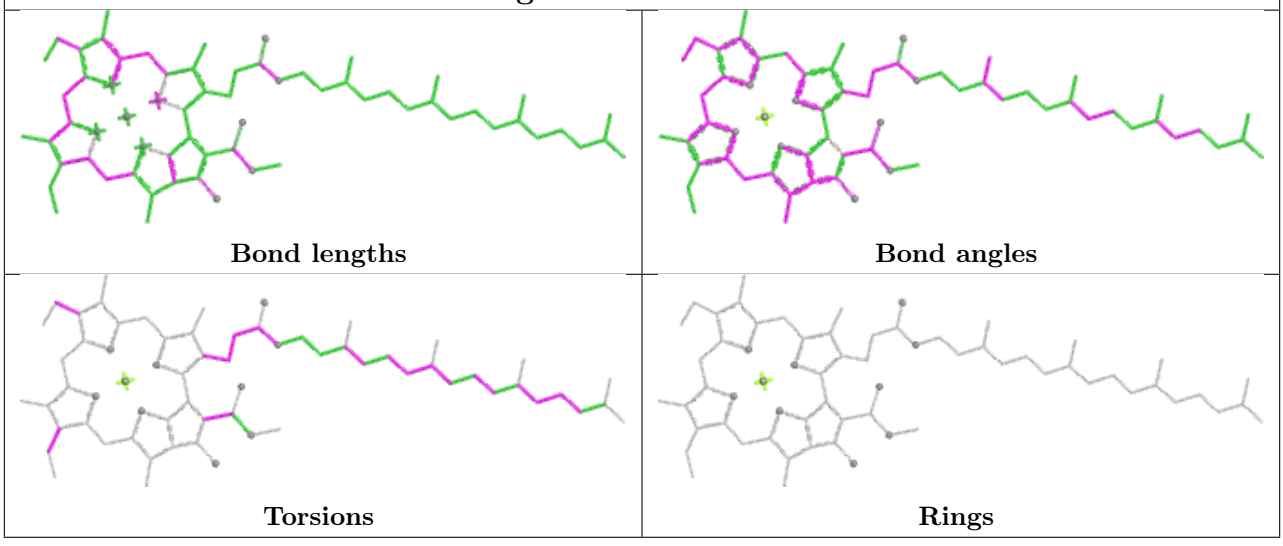
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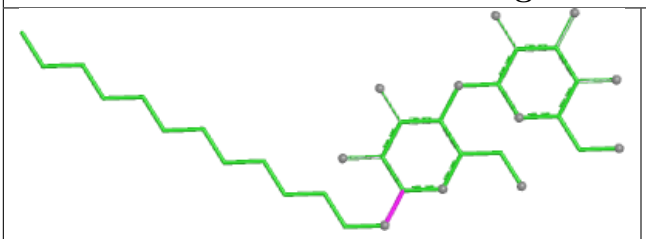
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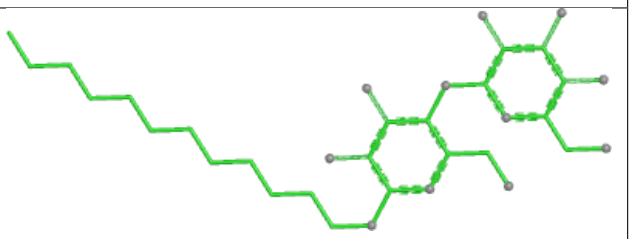
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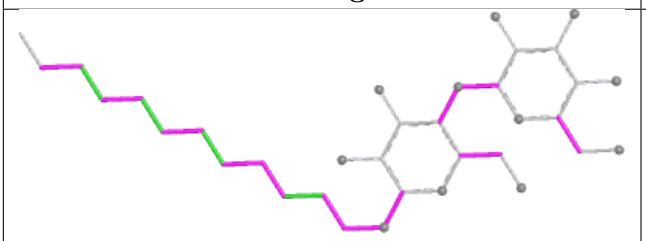
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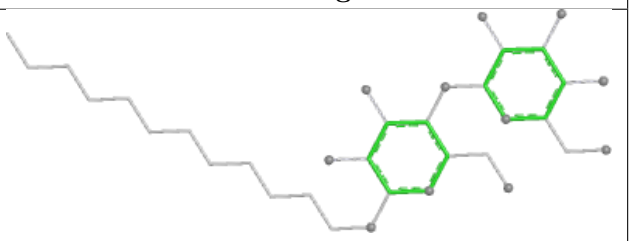
Bond lengths



Bond angles

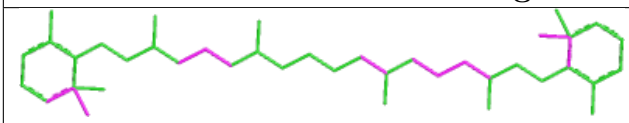


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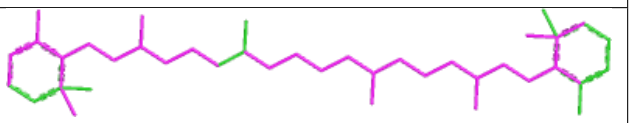


Rings

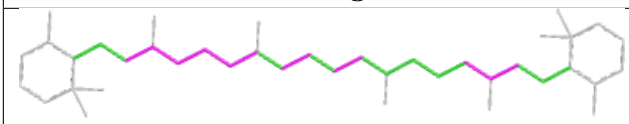
Ligand BCR B 6020



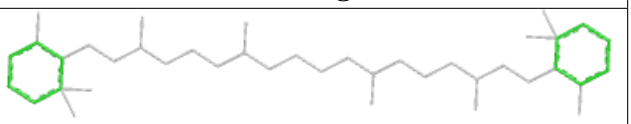
Bond lengths



Bond angles

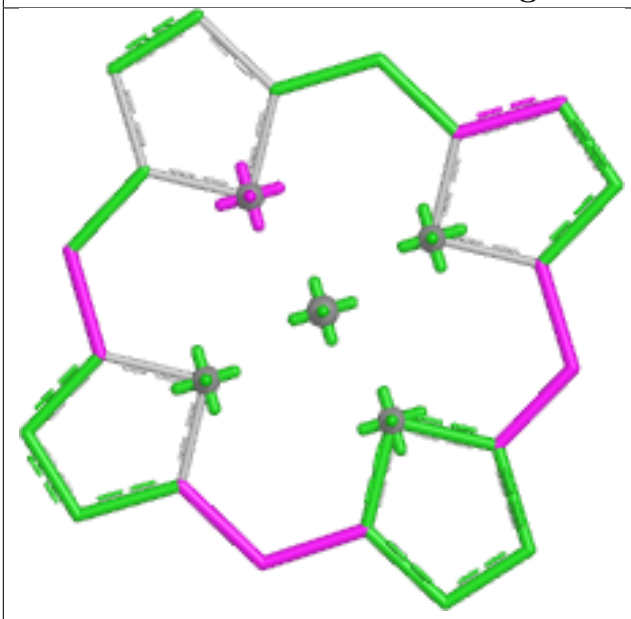


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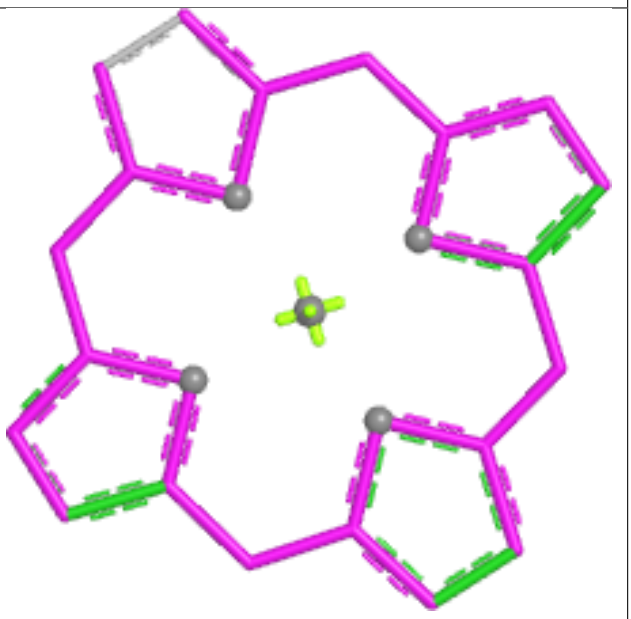


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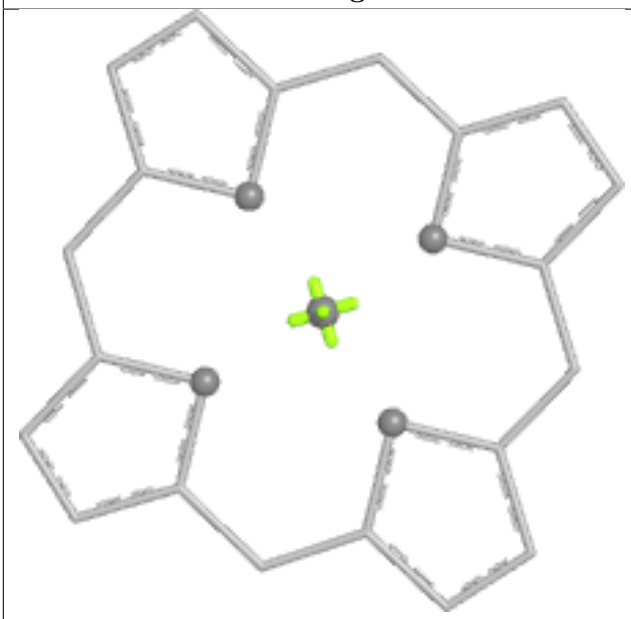
Ligand CLA 1 1310



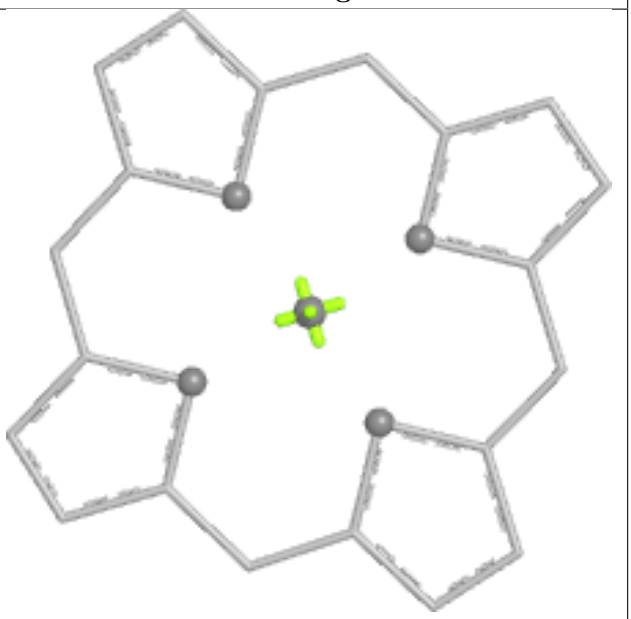
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Bond angles

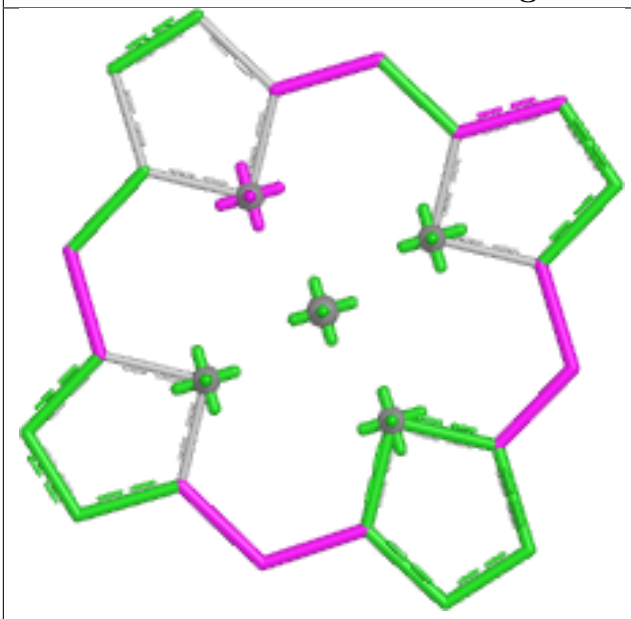


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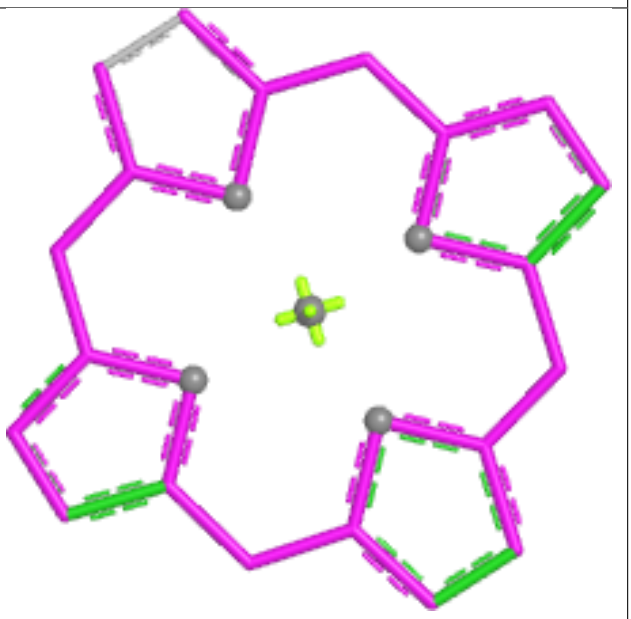


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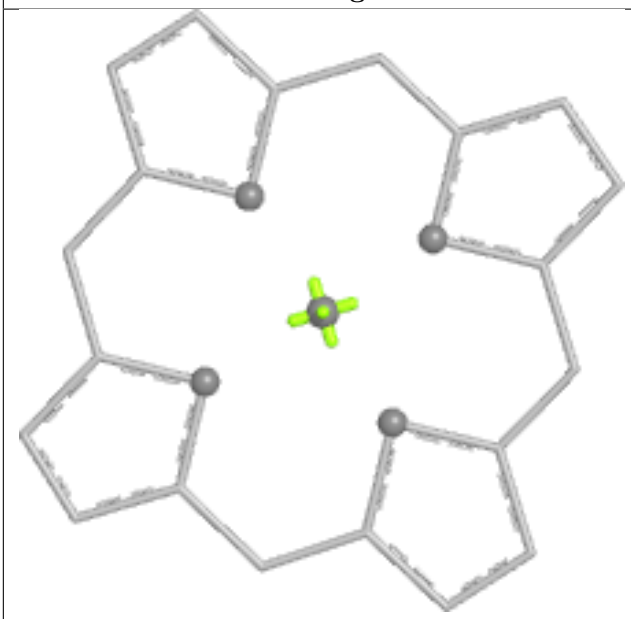
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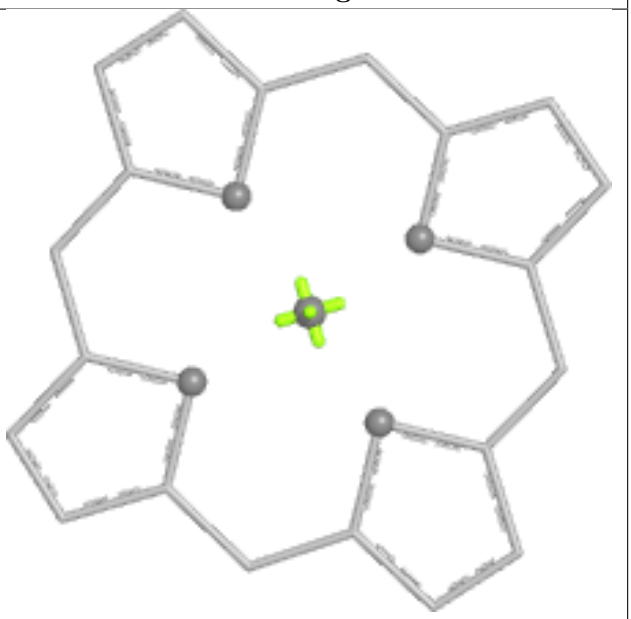
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Bond angles

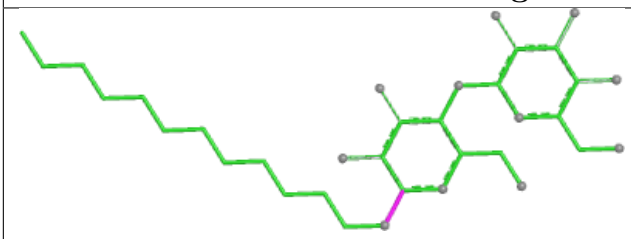


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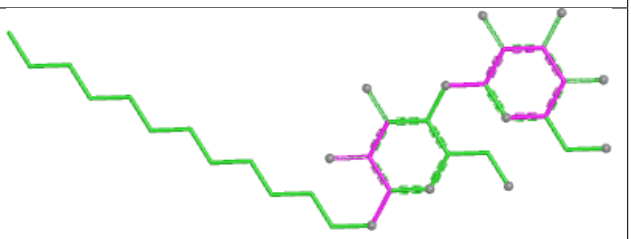


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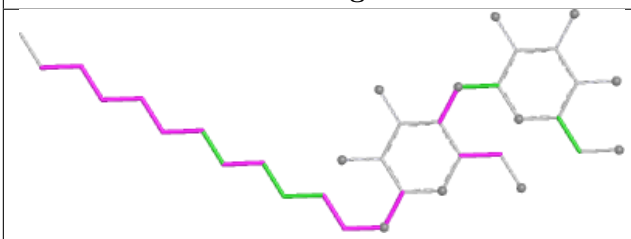
Ligand LMU C 7015



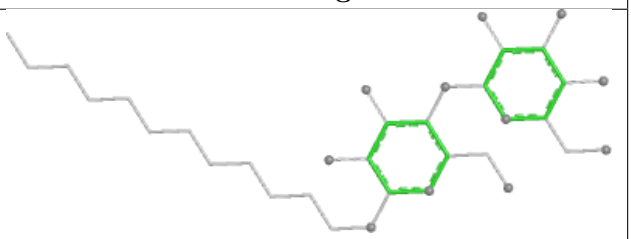
Bond lengths



Bond angles

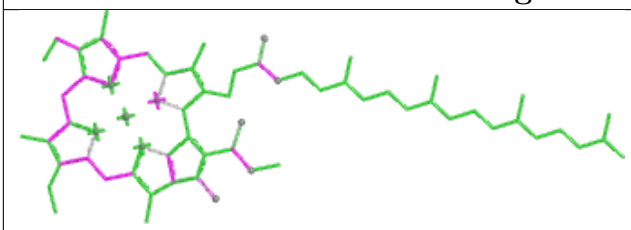


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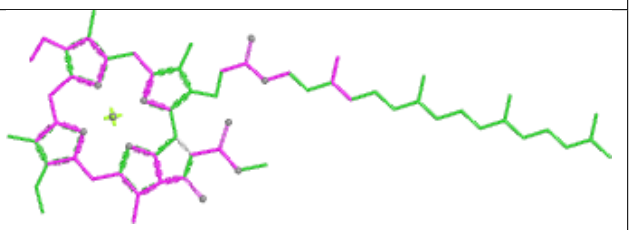


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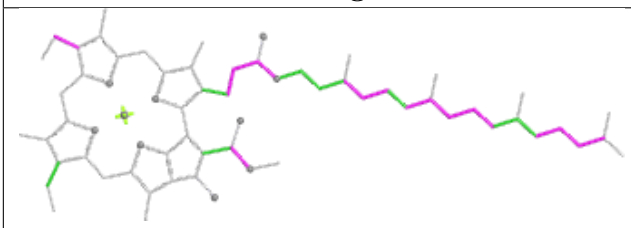
Ligand CLA A 1131



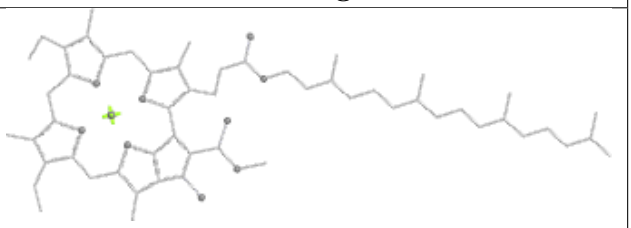
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Bond angles

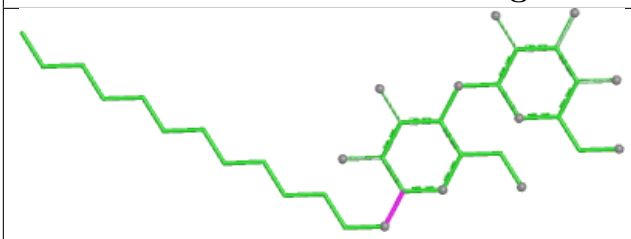


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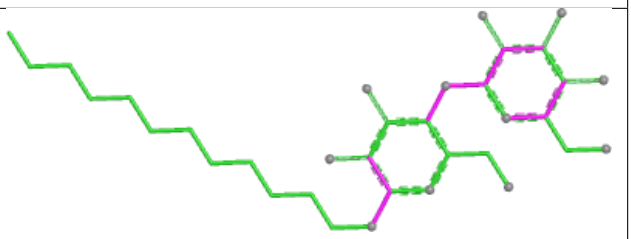


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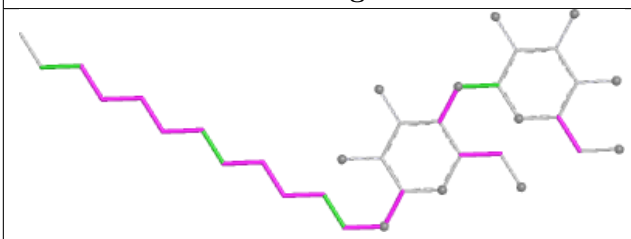
Ligand LMU N 7049



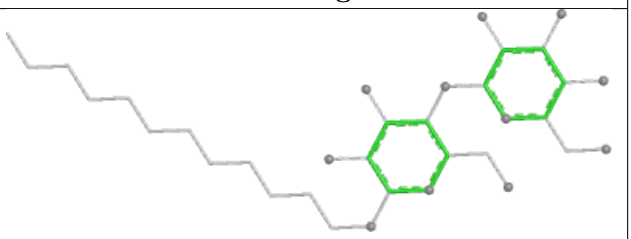
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Bond angles

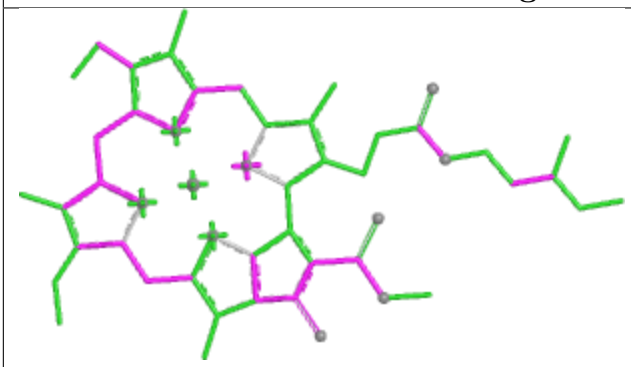


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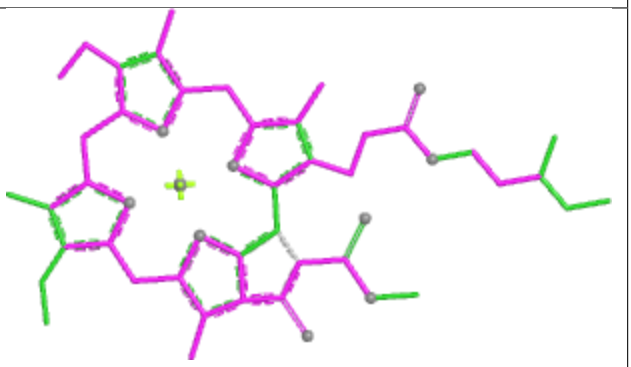


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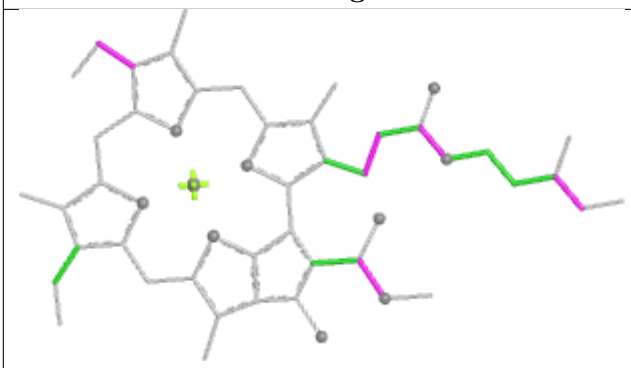
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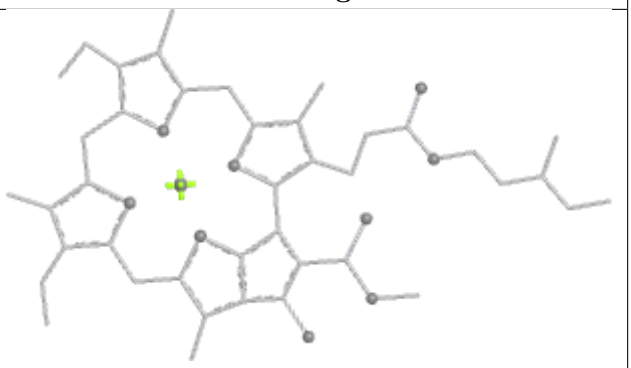
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Bond angles

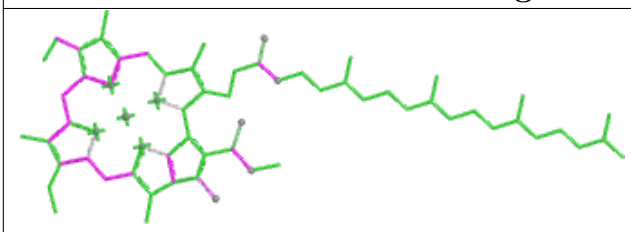


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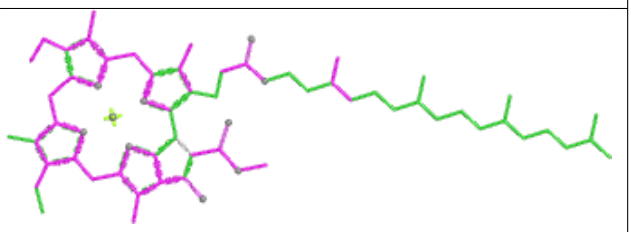


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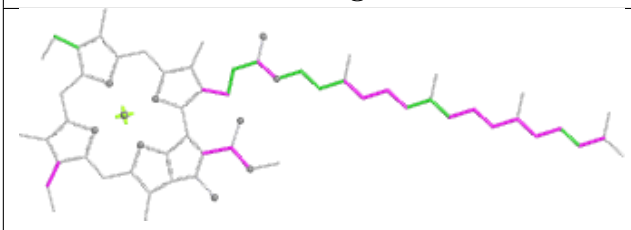
Ligand CLA A 1132



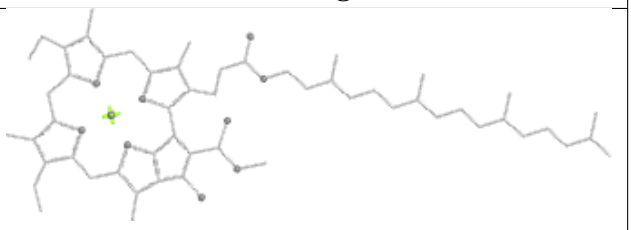
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Bond angles

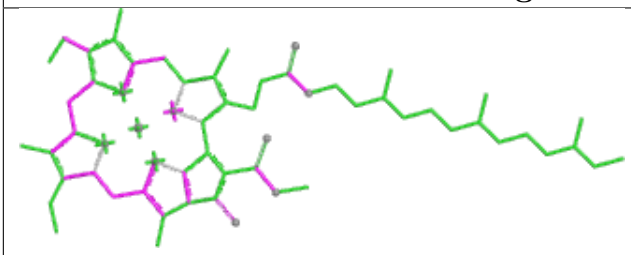


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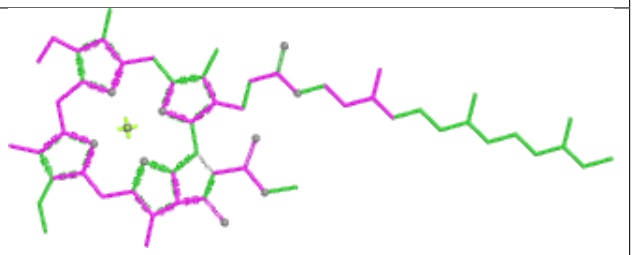


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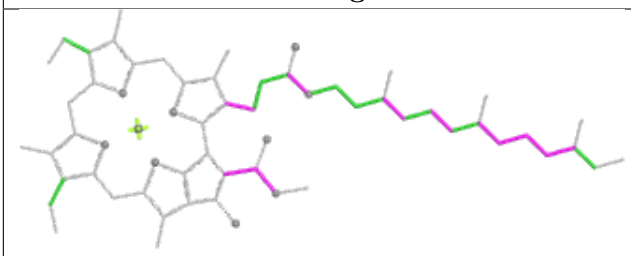
Ligand CLA B 1216



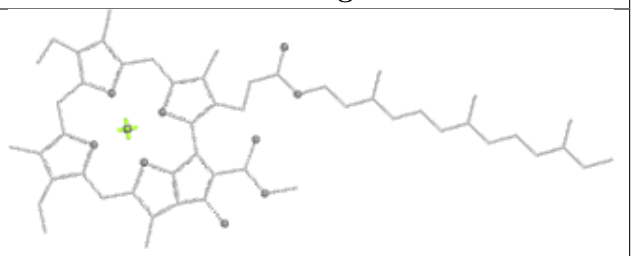
Bond lengths



Bond angles

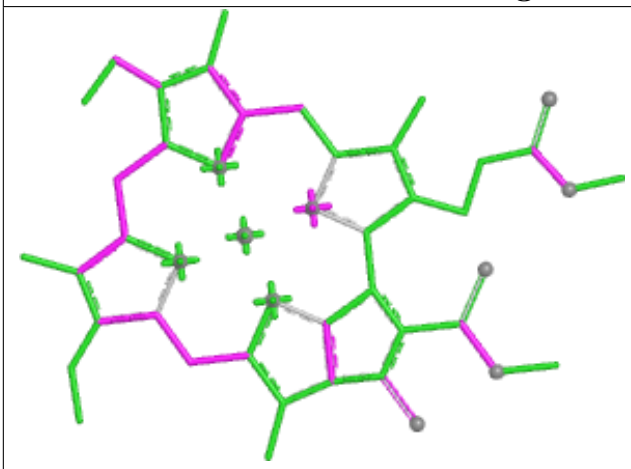


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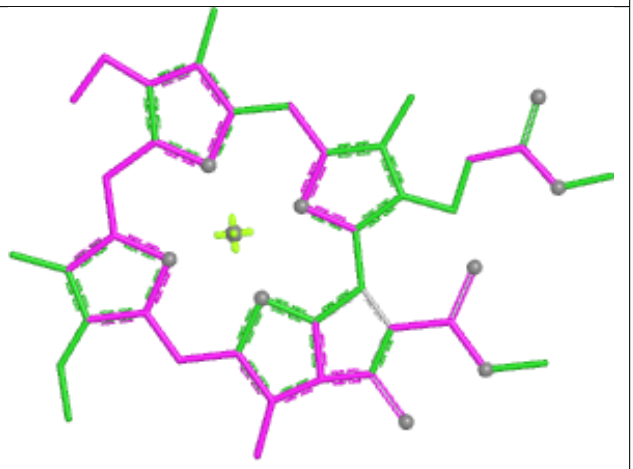


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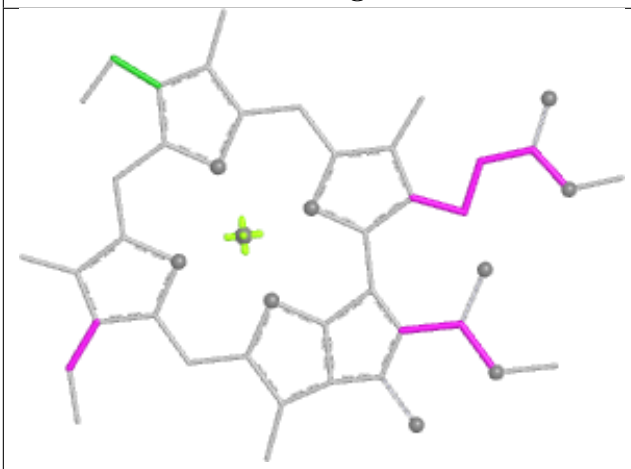
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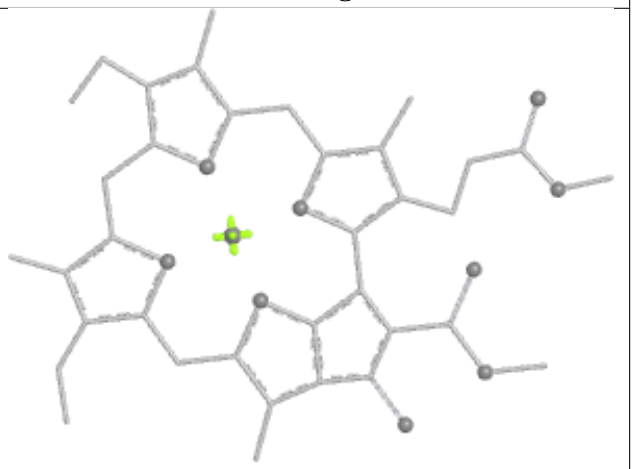
Bond lengths



Bond angles

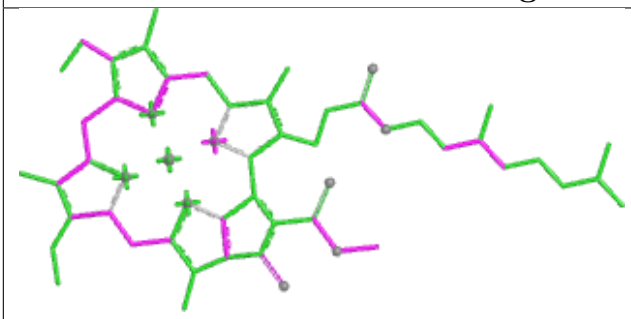


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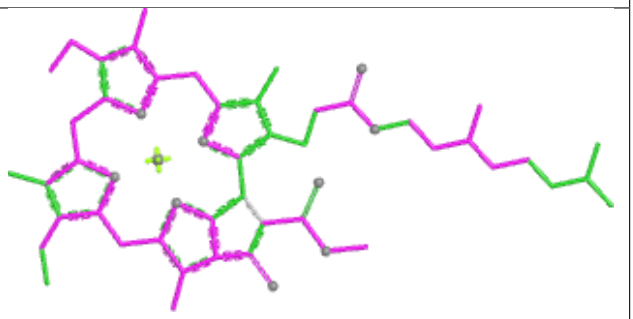


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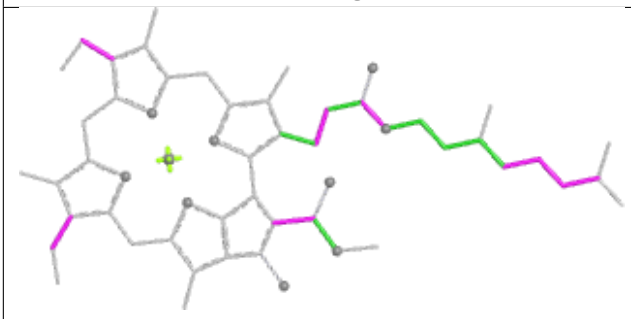
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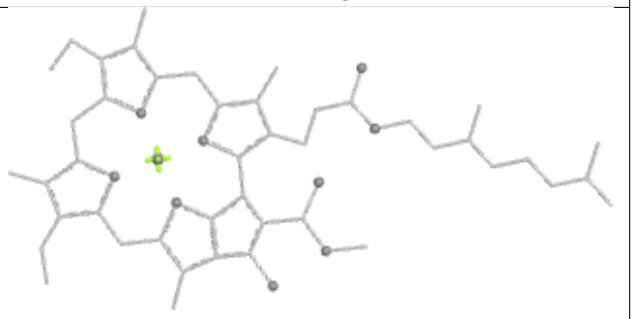
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Bond angles

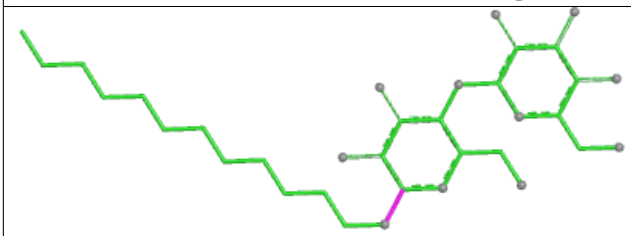


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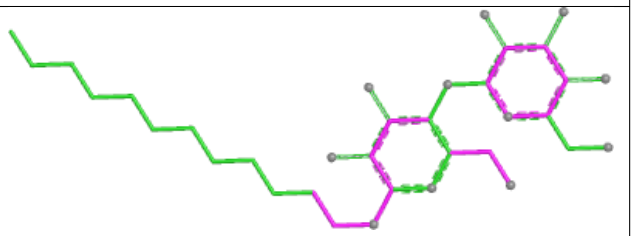


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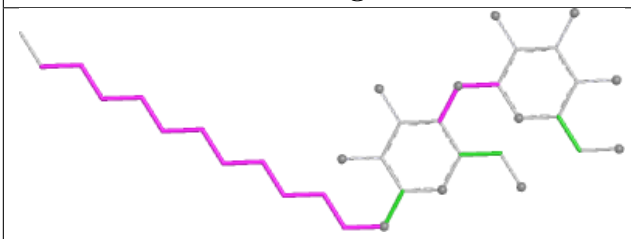
Ligand LMU A 7045



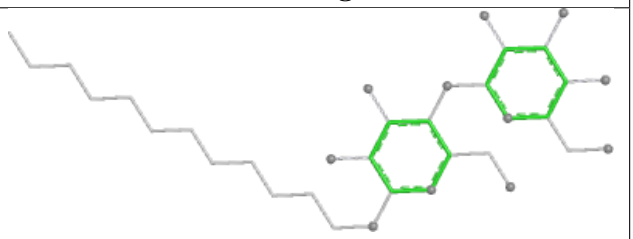
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Bond angles

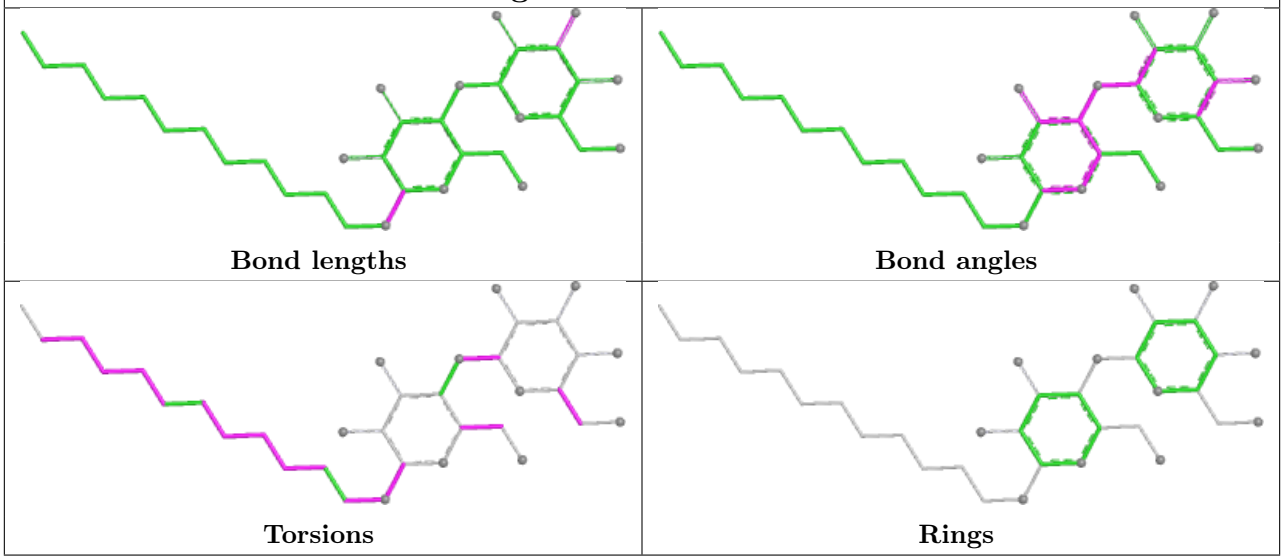


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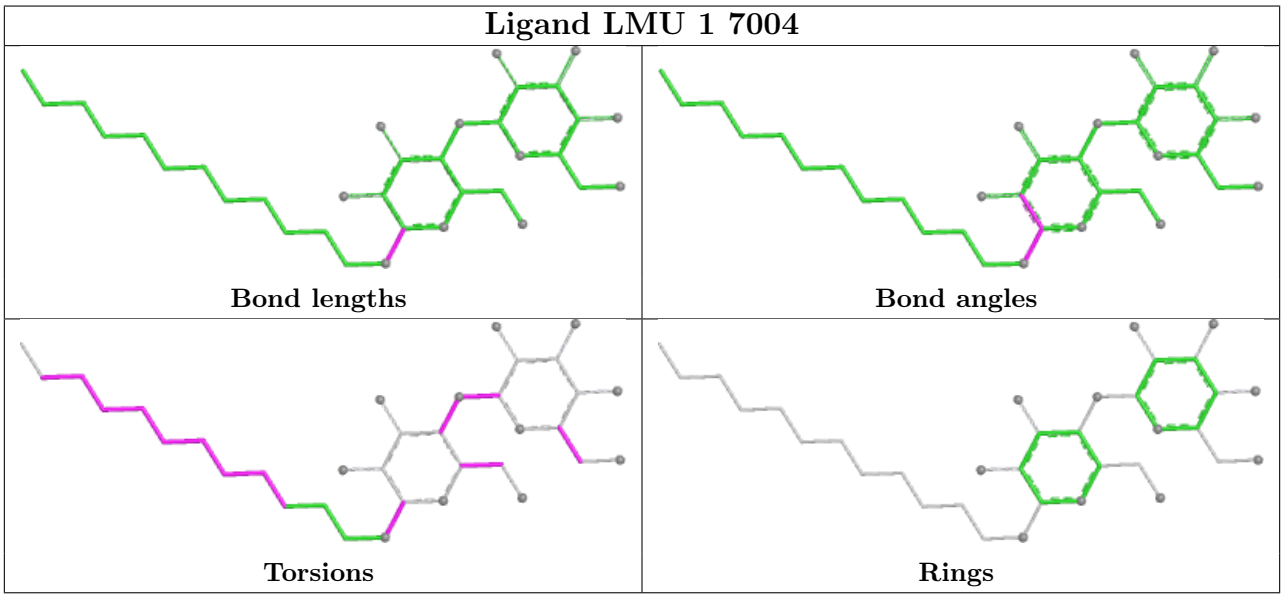


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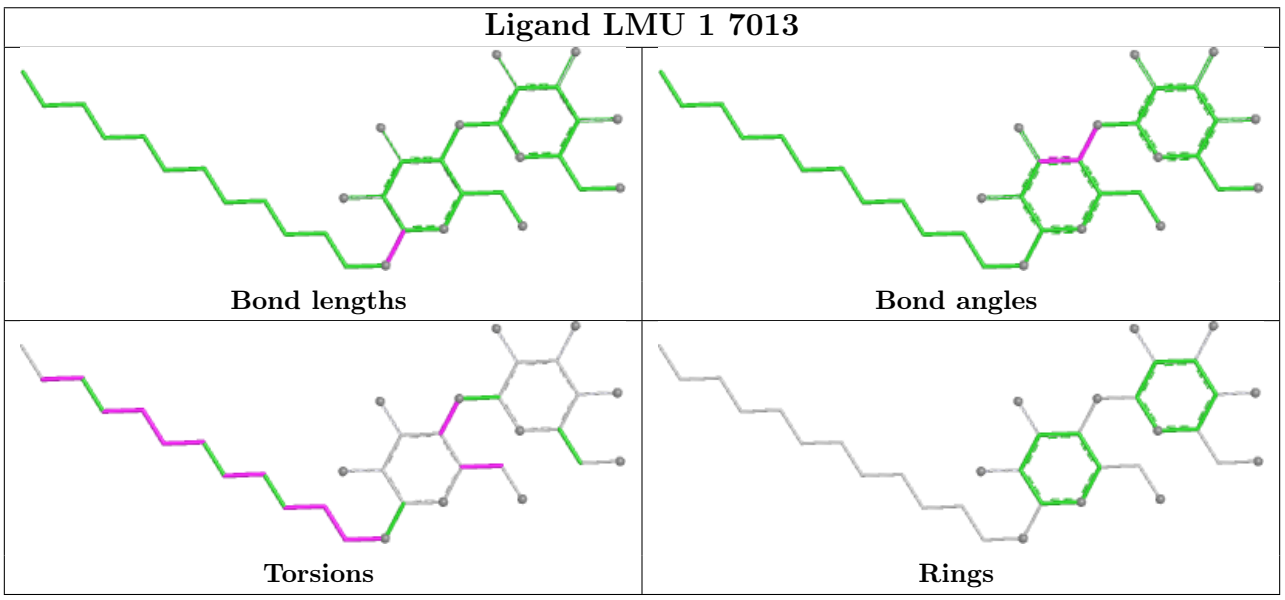
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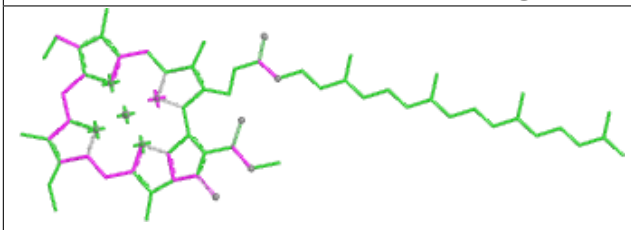
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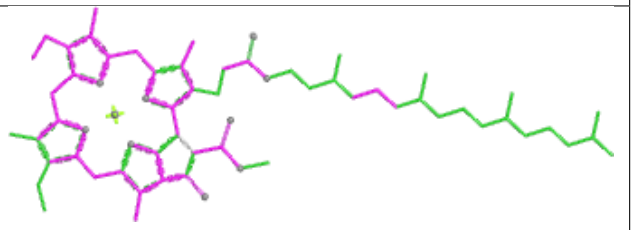
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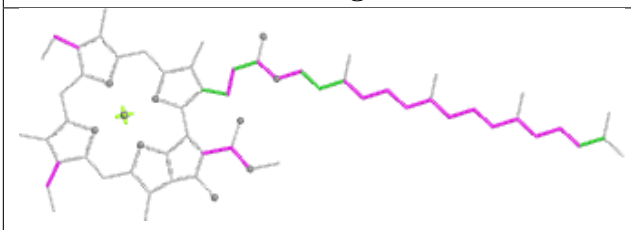
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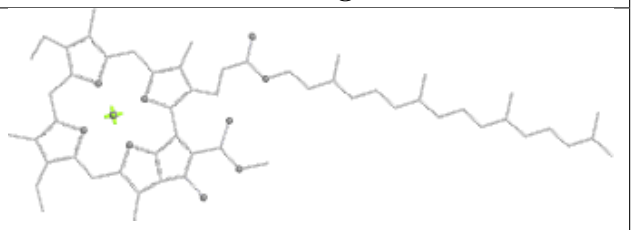
Bond lengths



Bond angles

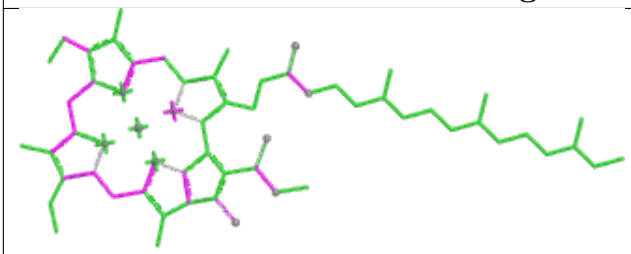


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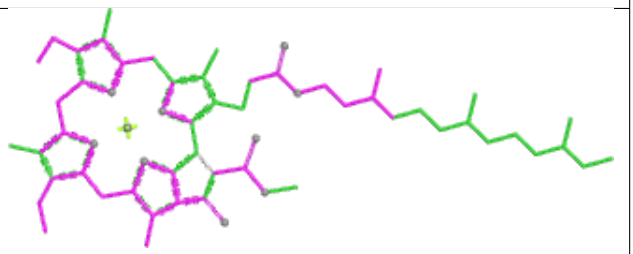


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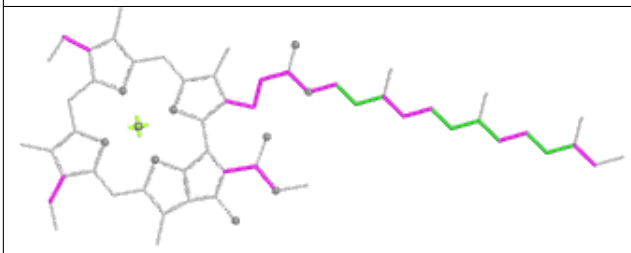
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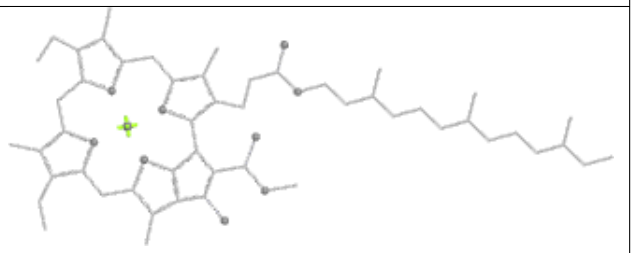
Bond lengths



Bond angles

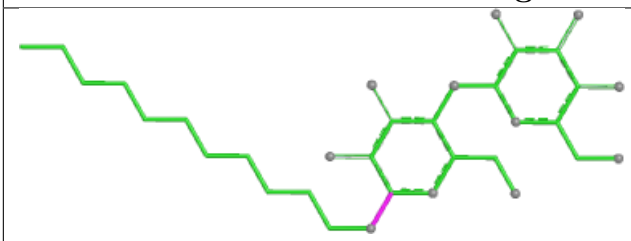


Torsions

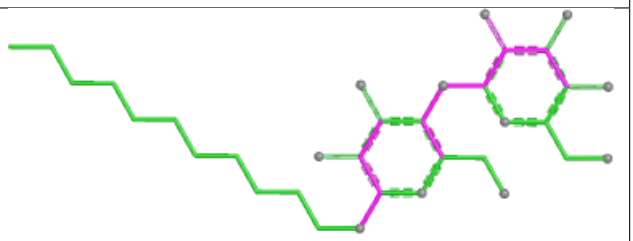


Rings

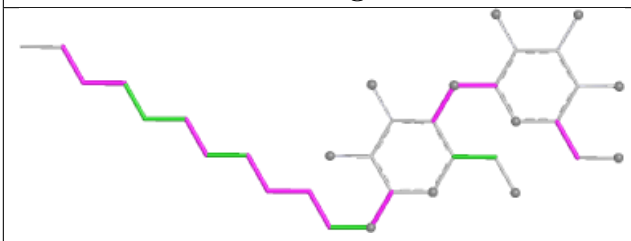
Ligand LMU 4 7053



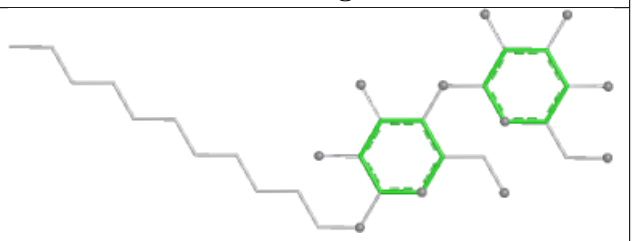
Bond lengths



Bond angles

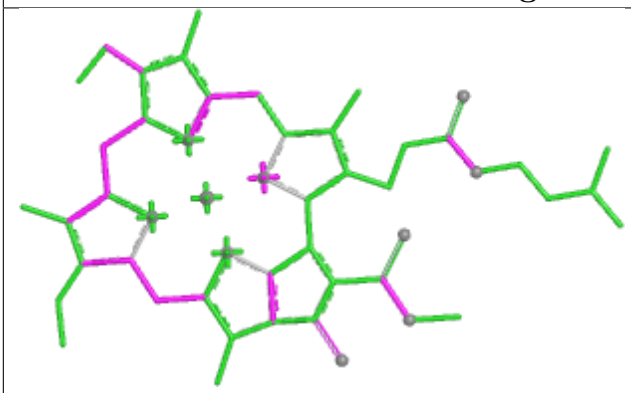


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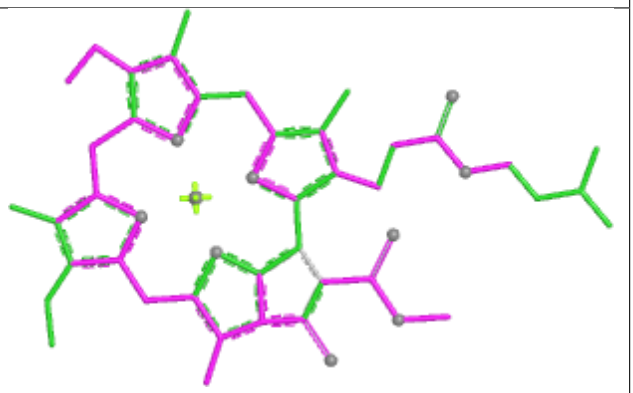


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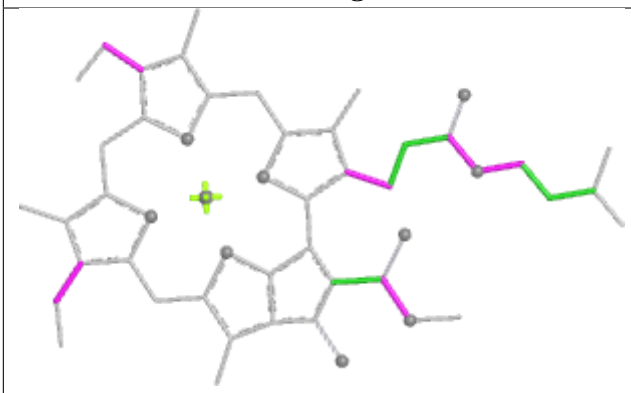
Ligand CLA 2 2004



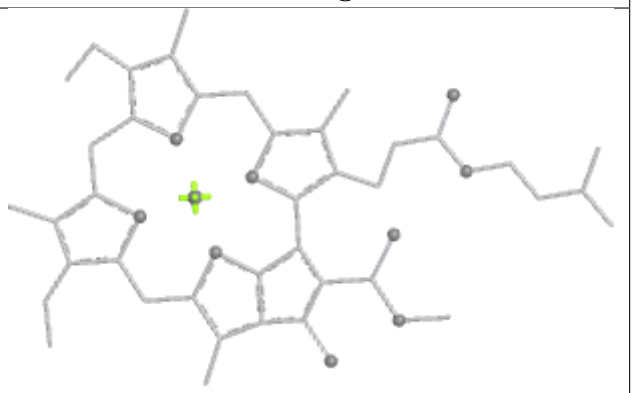
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Bond angles

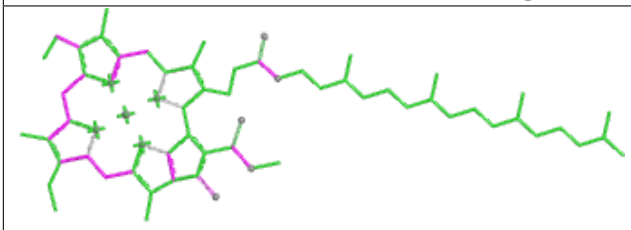


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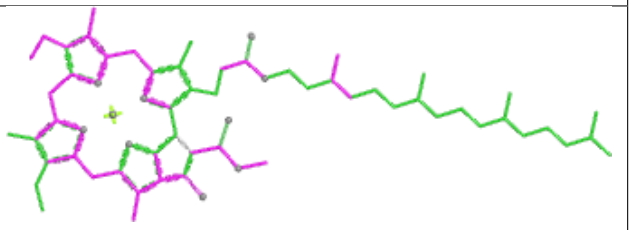


Rings

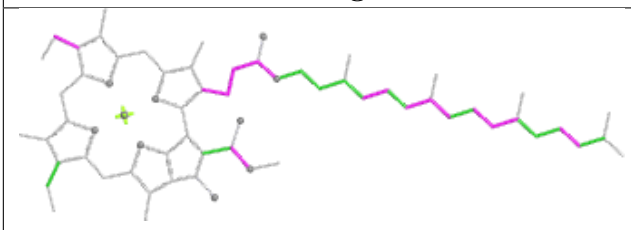
Ligand CLA 2 2006



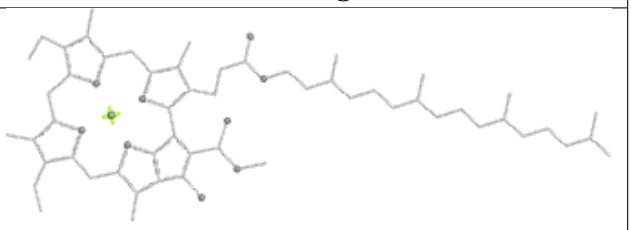
Bond lengths



Bond angles

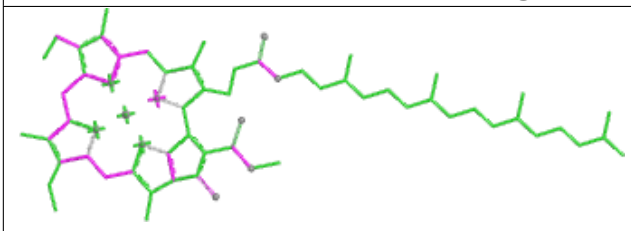


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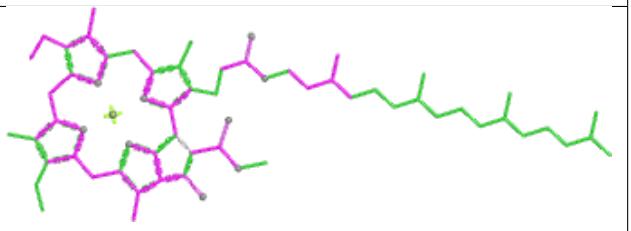


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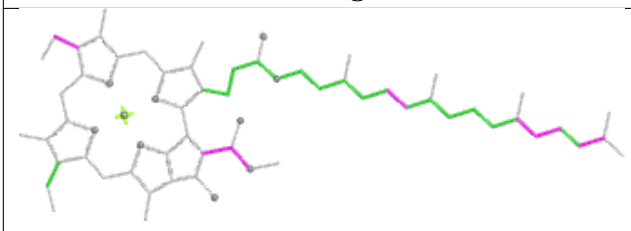
Ligand CLA A 1136



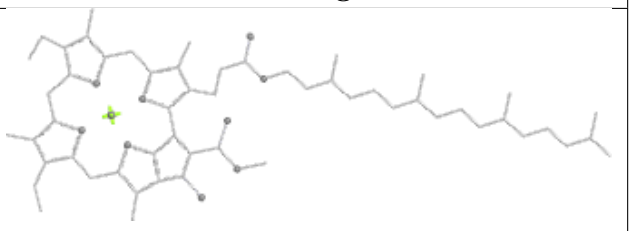
Bond lengths



Bond angles

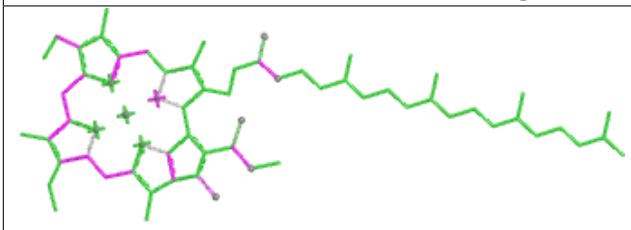


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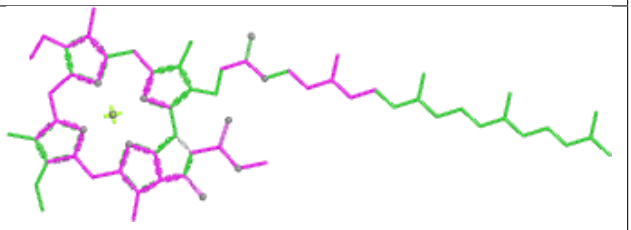


Rings

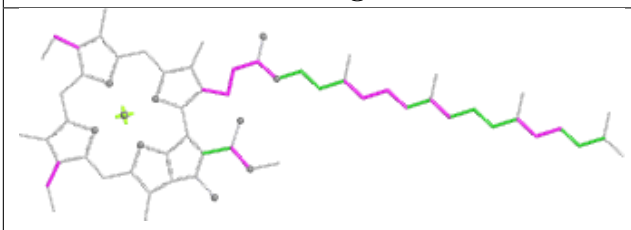
Ligand CLA A 1141



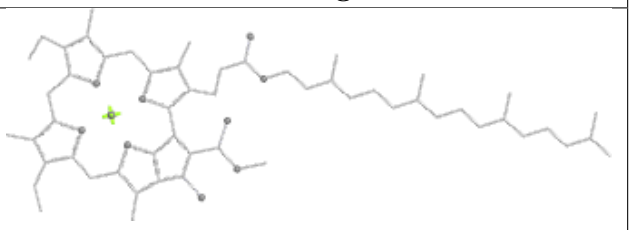
Bond lengths



Bond angles

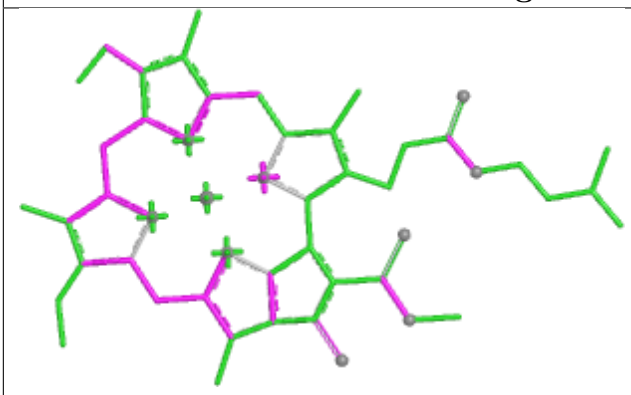


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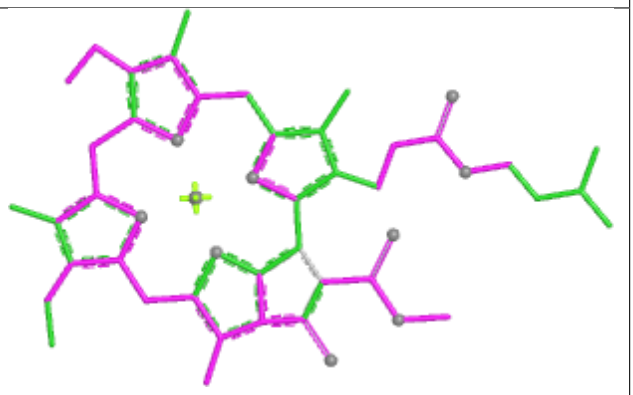


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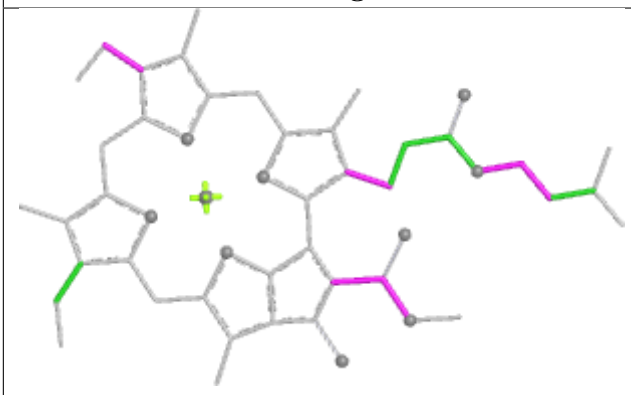
Ligand CLA B 1230



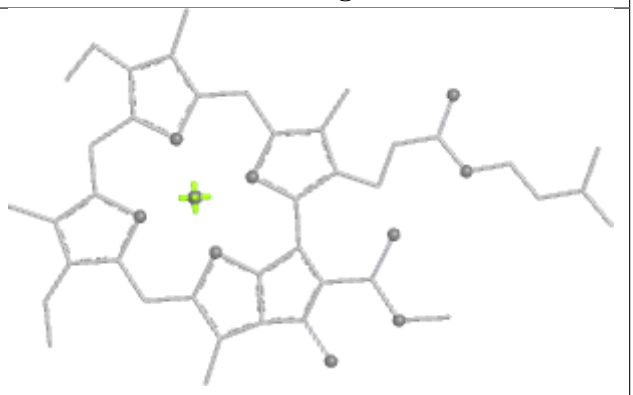
Bond lengths



Bond angles

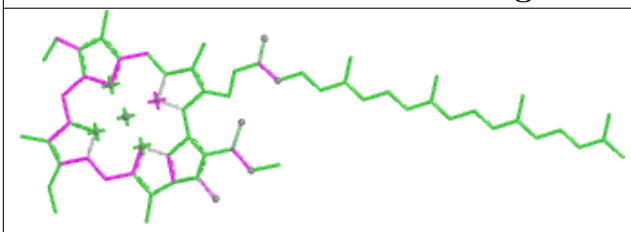


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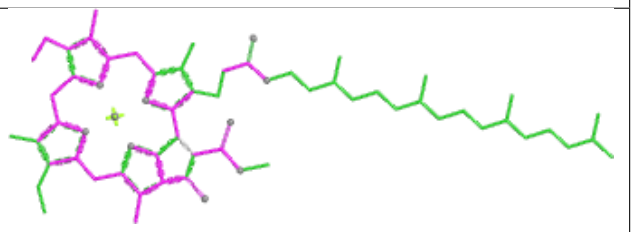


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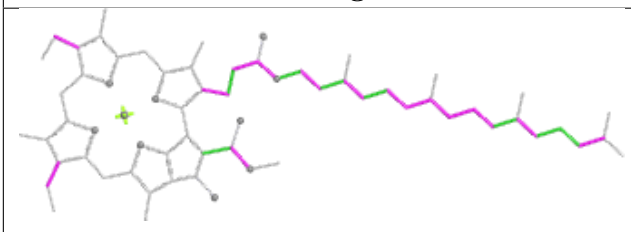
Ligand CLA A 1125



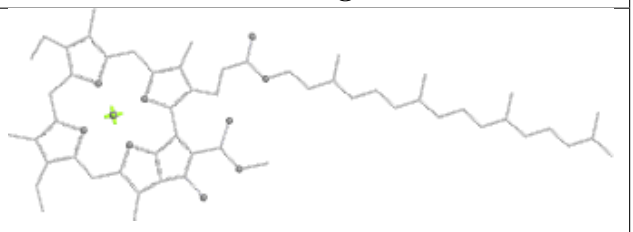
Bond lengths



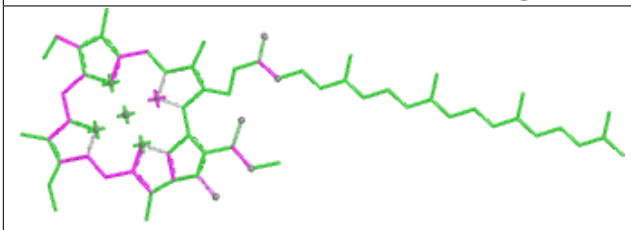
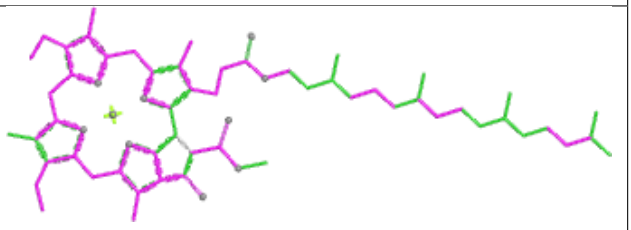
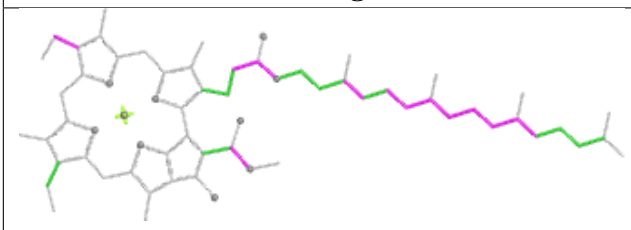
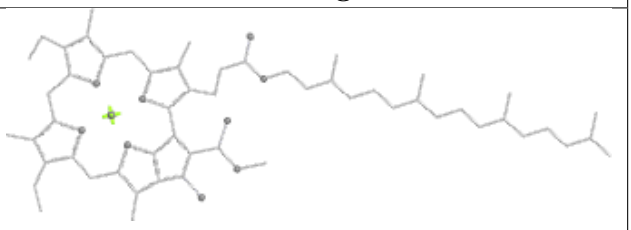
Bond angles



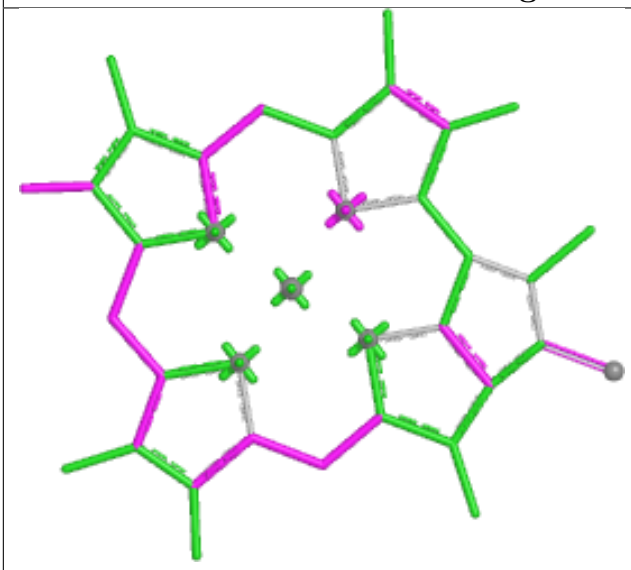
Torsions



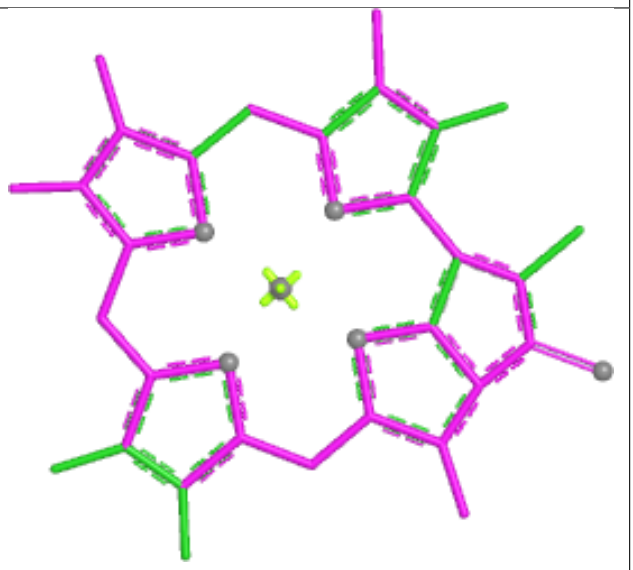
Rings

Ligand CLA B 9010	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

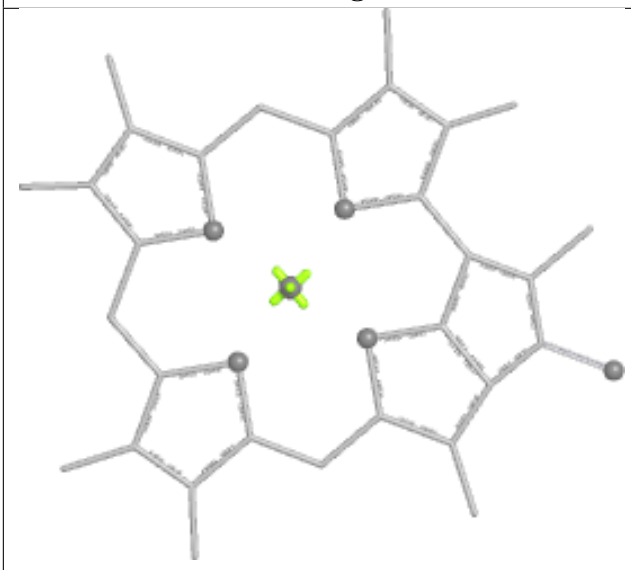
Ligand CLA 1 1006



Bond lengths



Bond angles

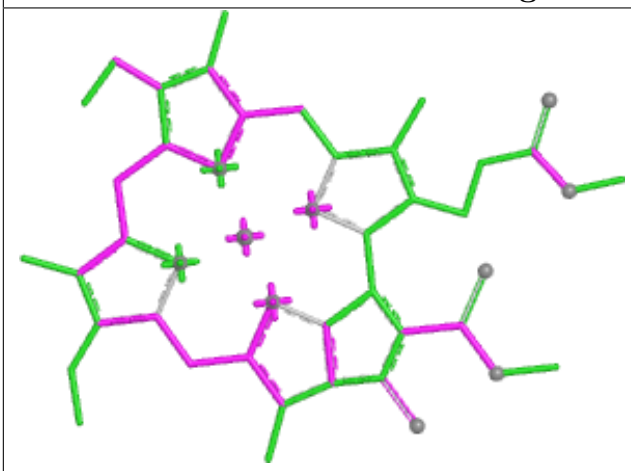


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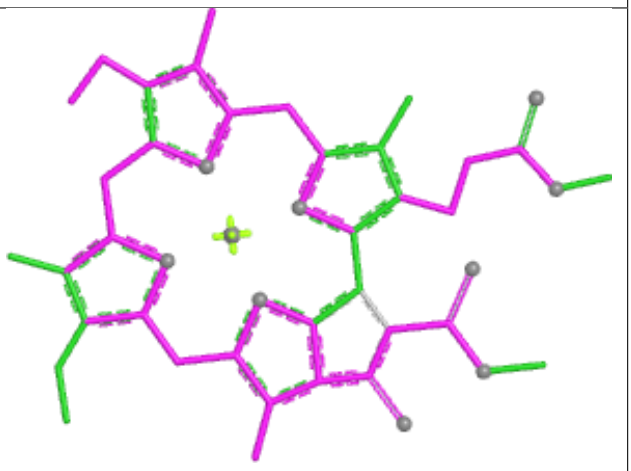


Rings

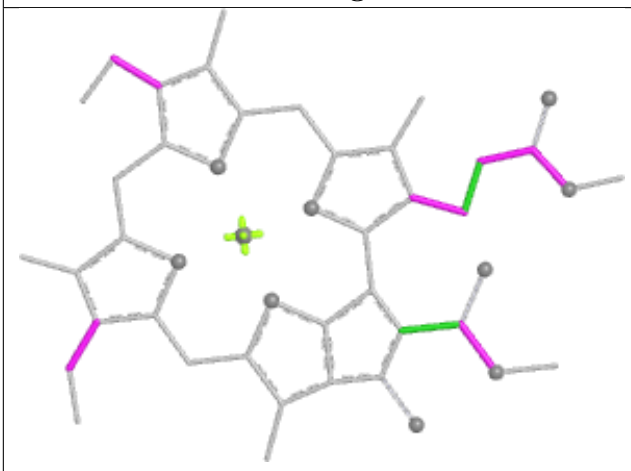
Ligand CLA 4 4015



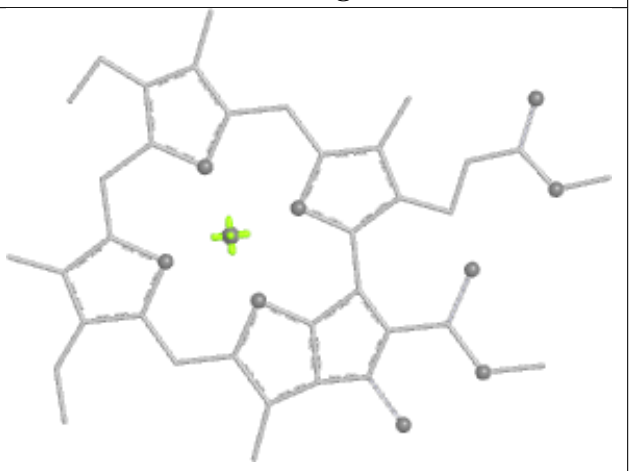
Bond lengths



Bond angles

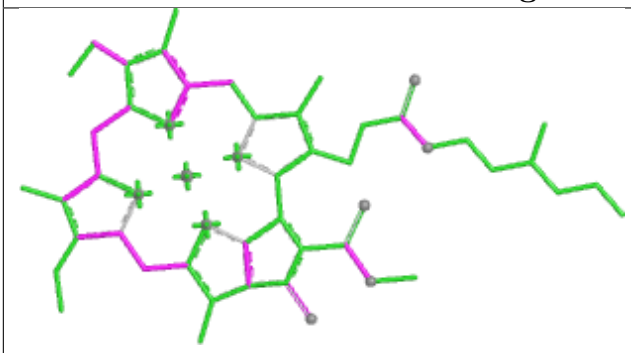


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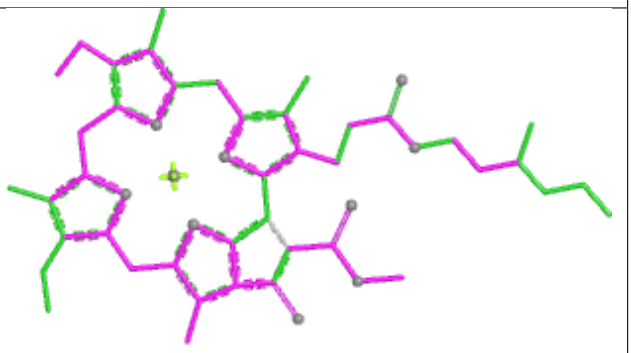


Rings

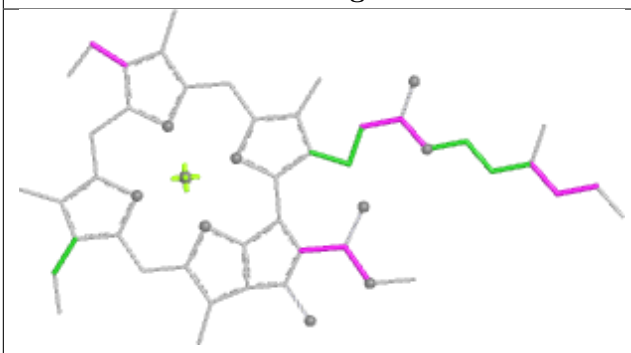
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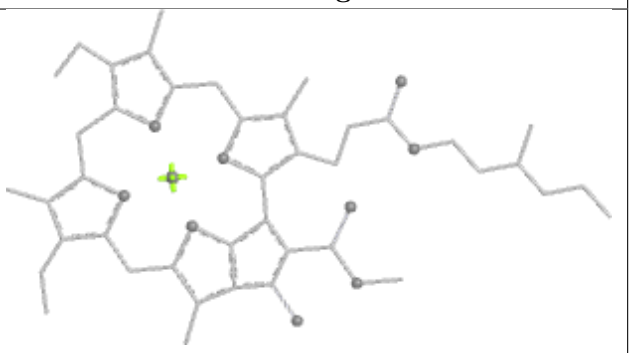
Bond lengths



Bond angles

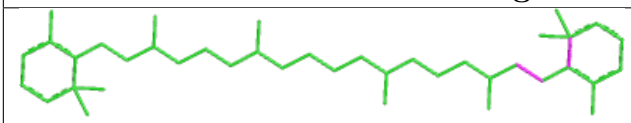


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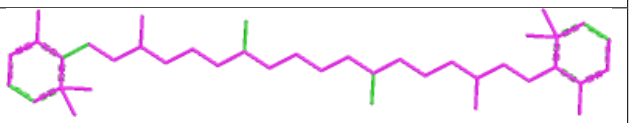


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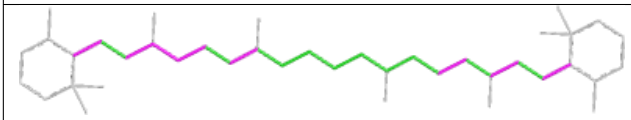
Ligand BCR A 6003



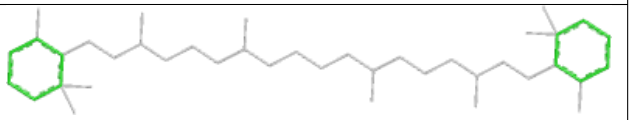
Bond lengths



Bond angles



Torsions

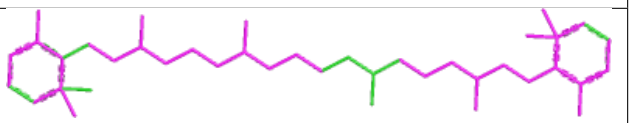


Rings

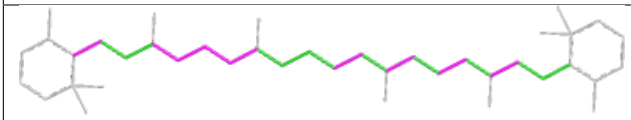
Ligand BCR I 6018



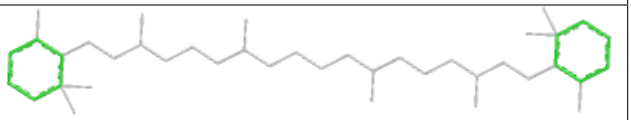
Bond lengths



Bond angles

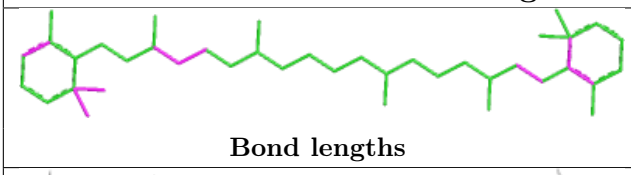


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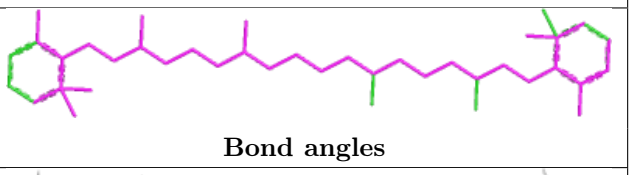


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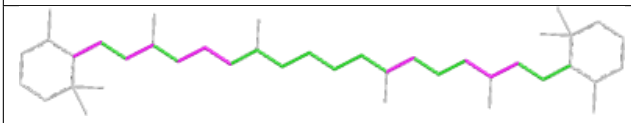
Ligand BCR I 6021



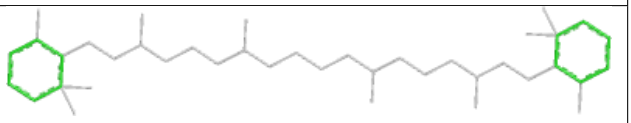
Bond lengths



Bond angles



Torsions



Rings

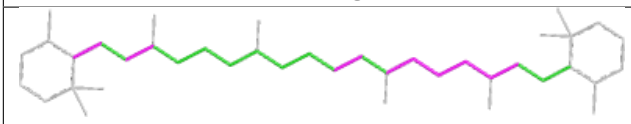
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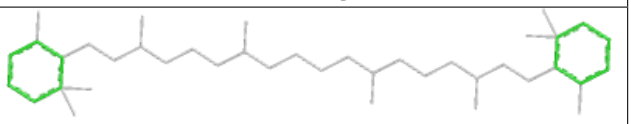
Bond lengths



Bond angles

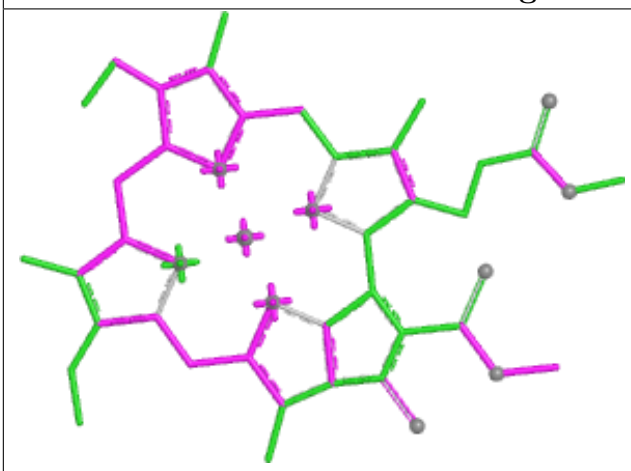


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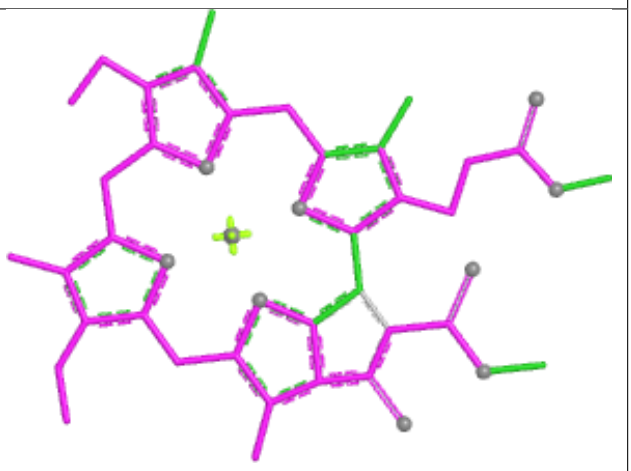


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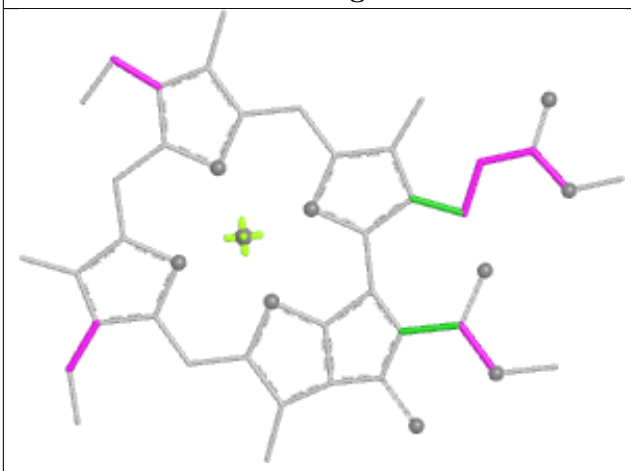
Ligand CLA 3 1147



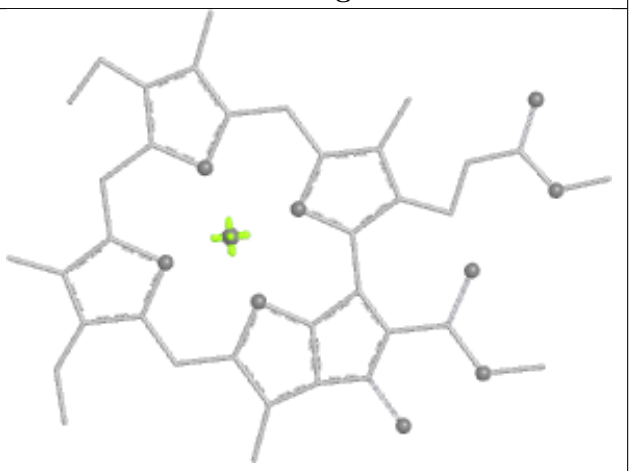
Bond lengths



Bond angles

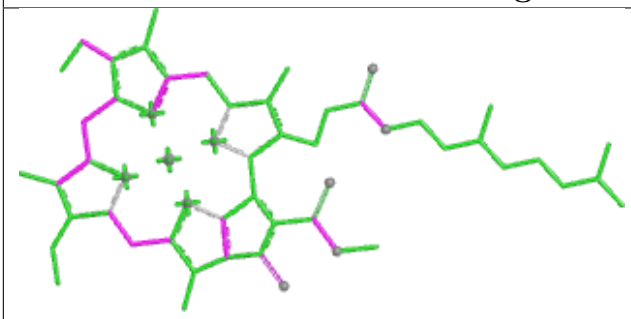


Torsions

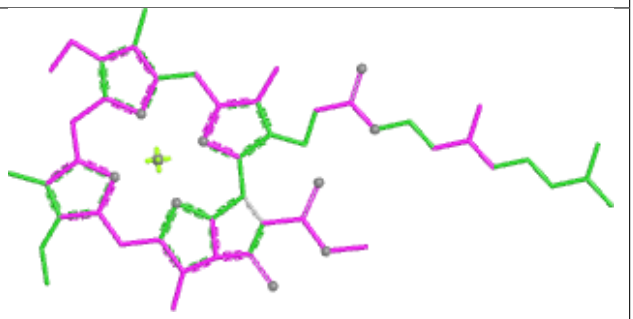


Rings

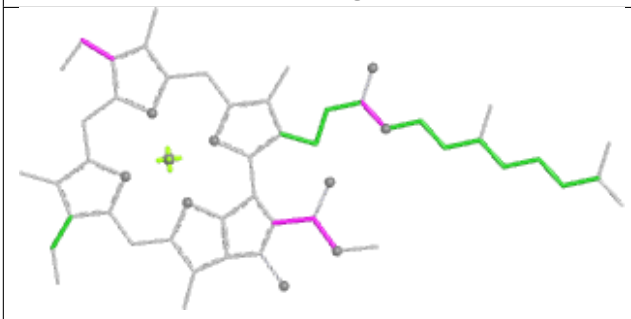
Ligand CLA H 1241



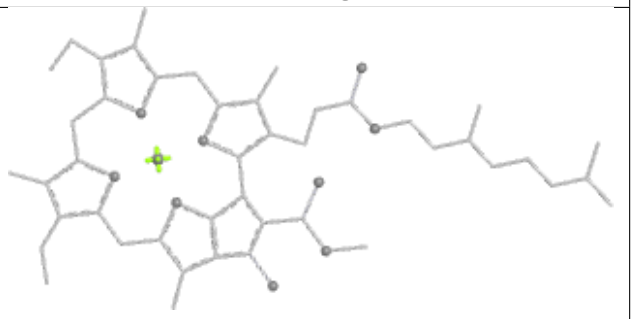
Bond lengths



Bond angles

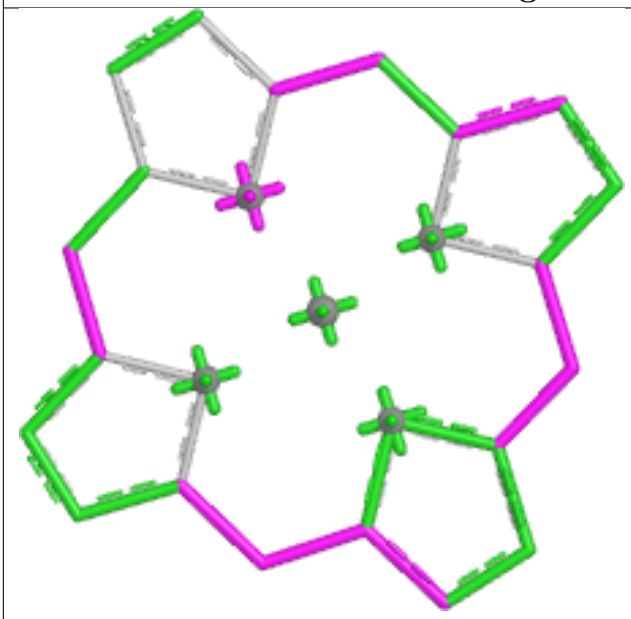


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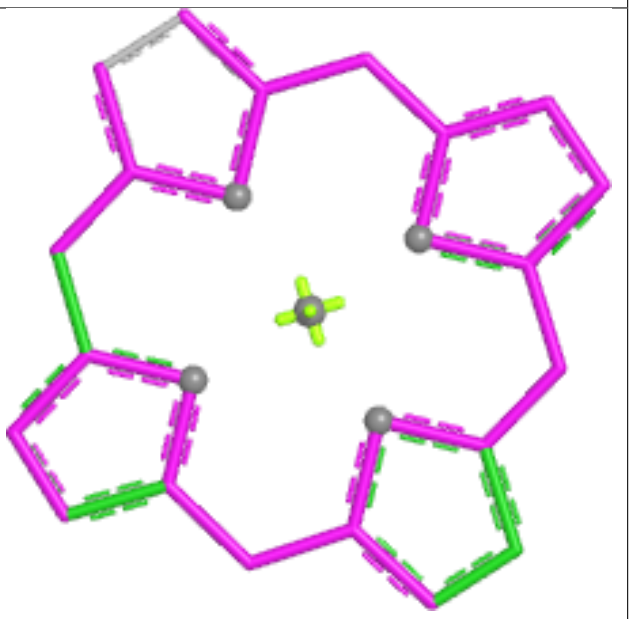


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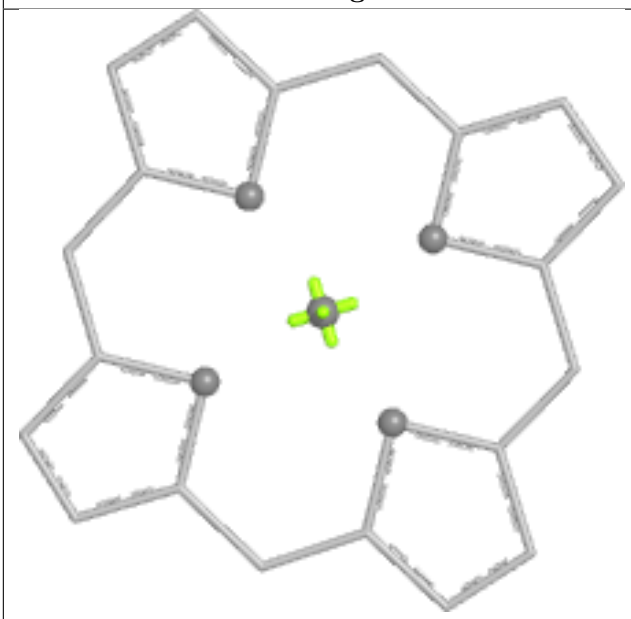
Ligand CLA 3 3012



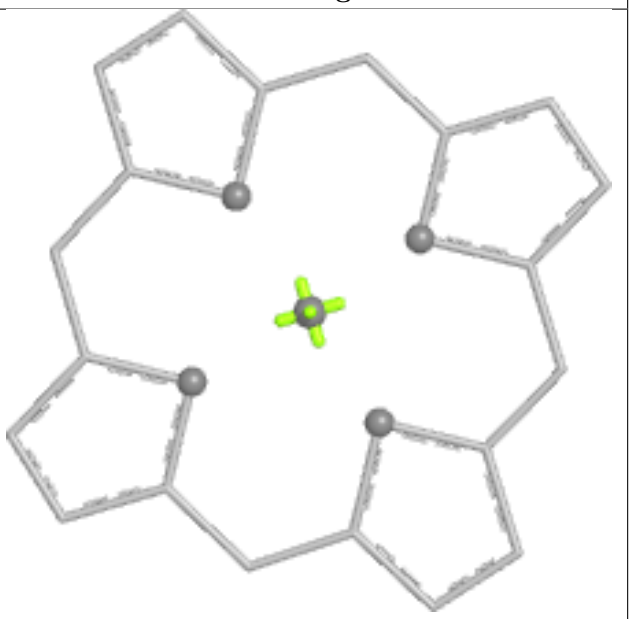
Bond lengths



Bond angles

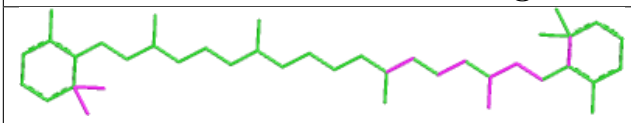


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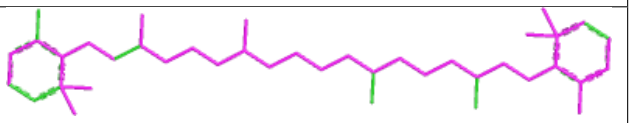


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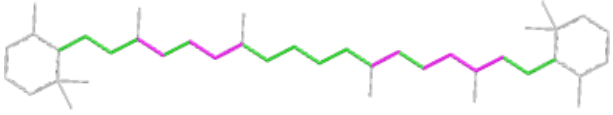
Ligand BCR B 6006



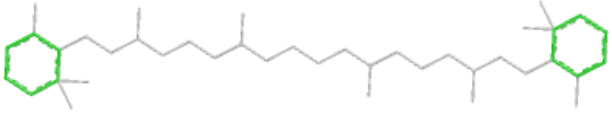
Bond lengths



Bond angles

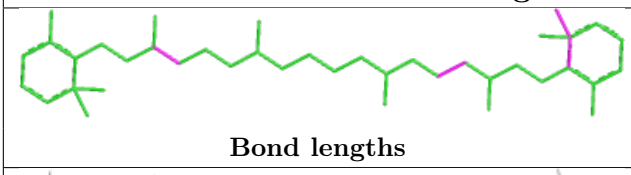


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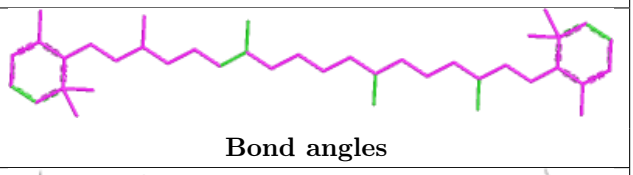


Rings

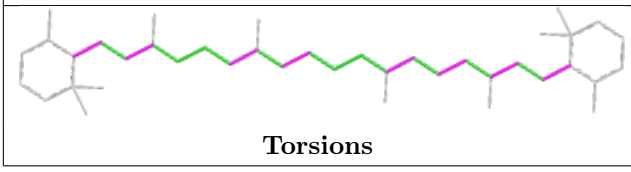
Ligand BCR A 6007



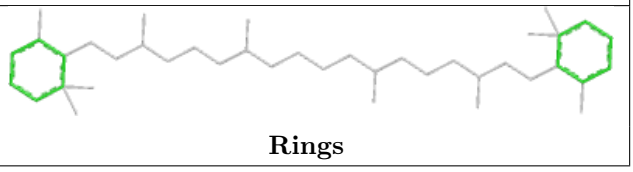
Bond lengths



Bond angles

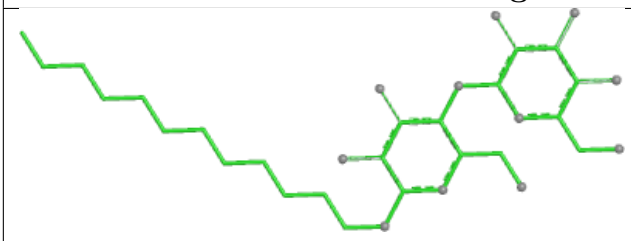


Torsions



Rings

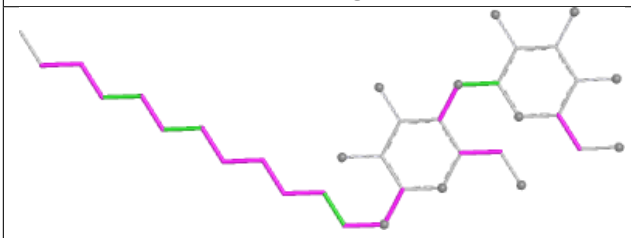
Ligand LMU H 7002



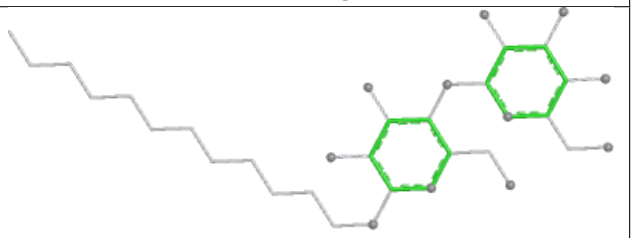
Bond lengths



Bond angles

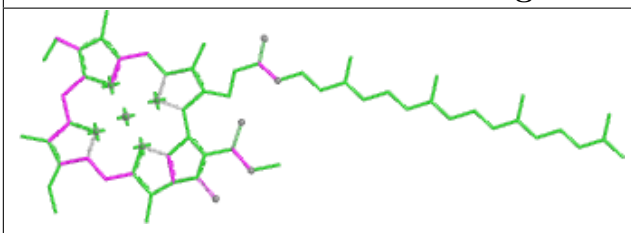


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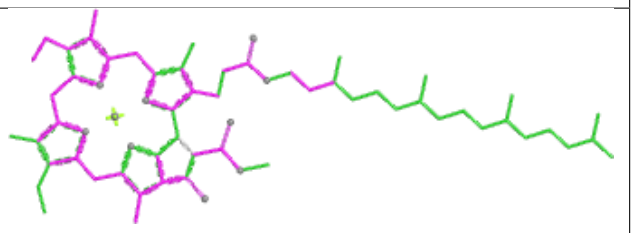


Rings

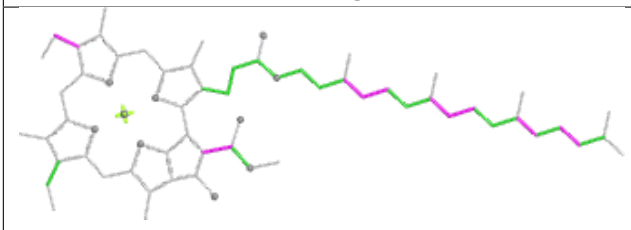
Ligand CLA B 1205



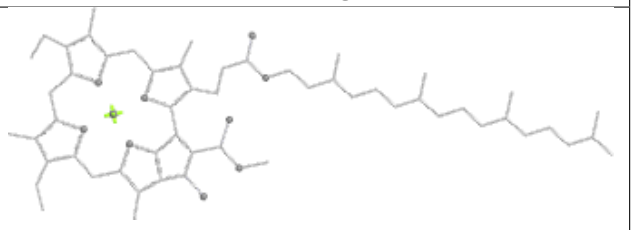
Bond lengths



Bond angles

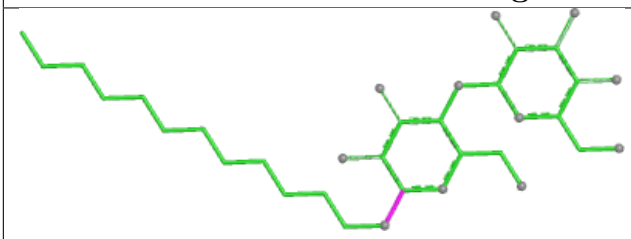


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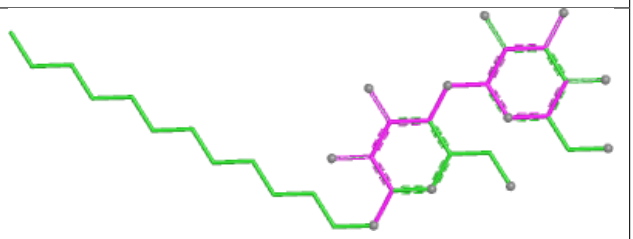


Rings

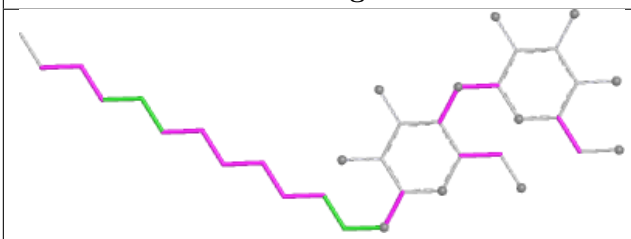
Ligand LMU B 7040



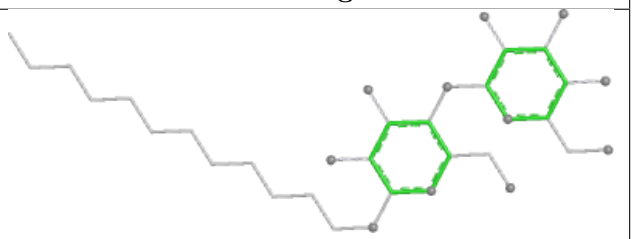
Bond lengths



Bond angles

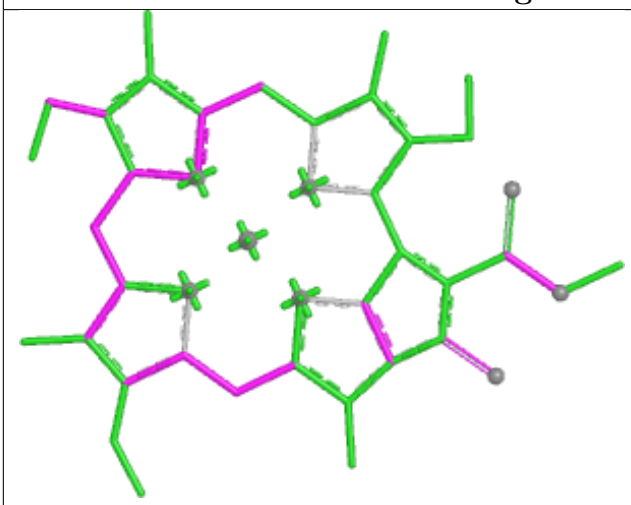


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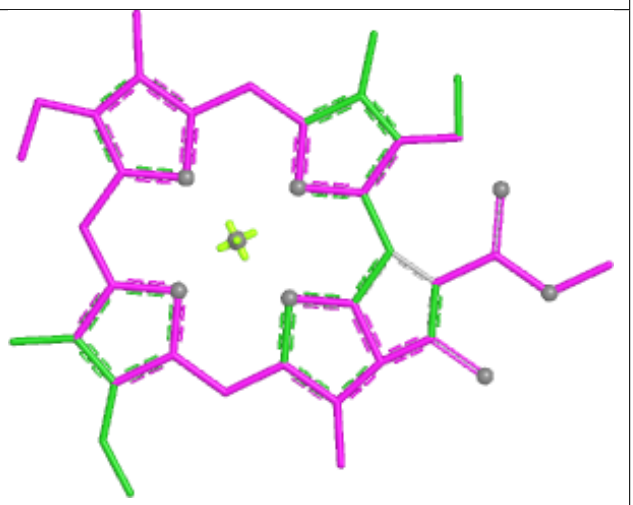


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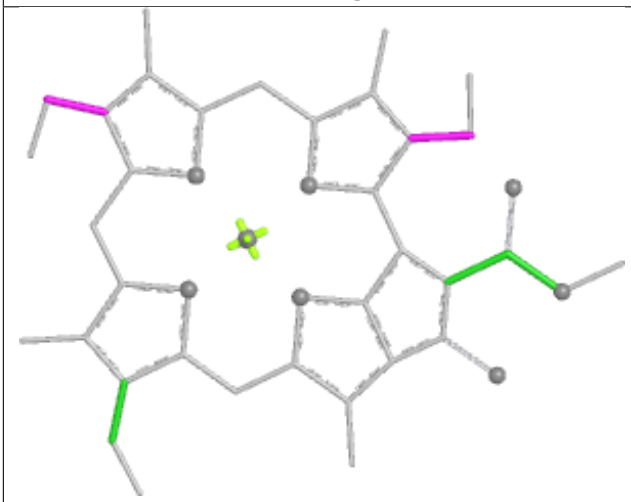
Ligand CLA A 1121



Bond lengths



Bond angles

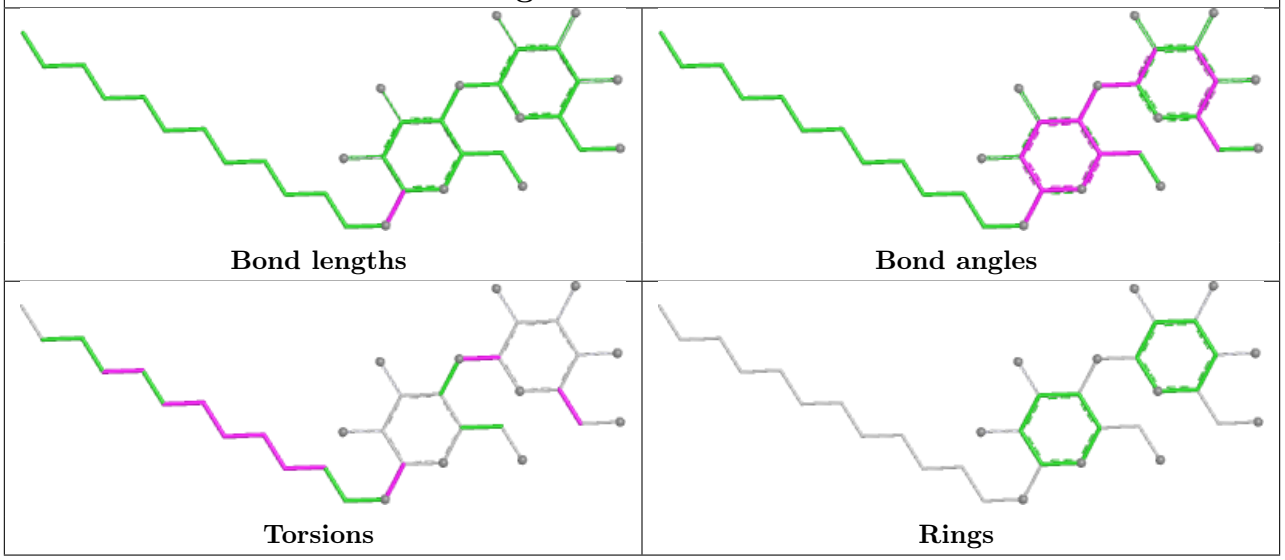


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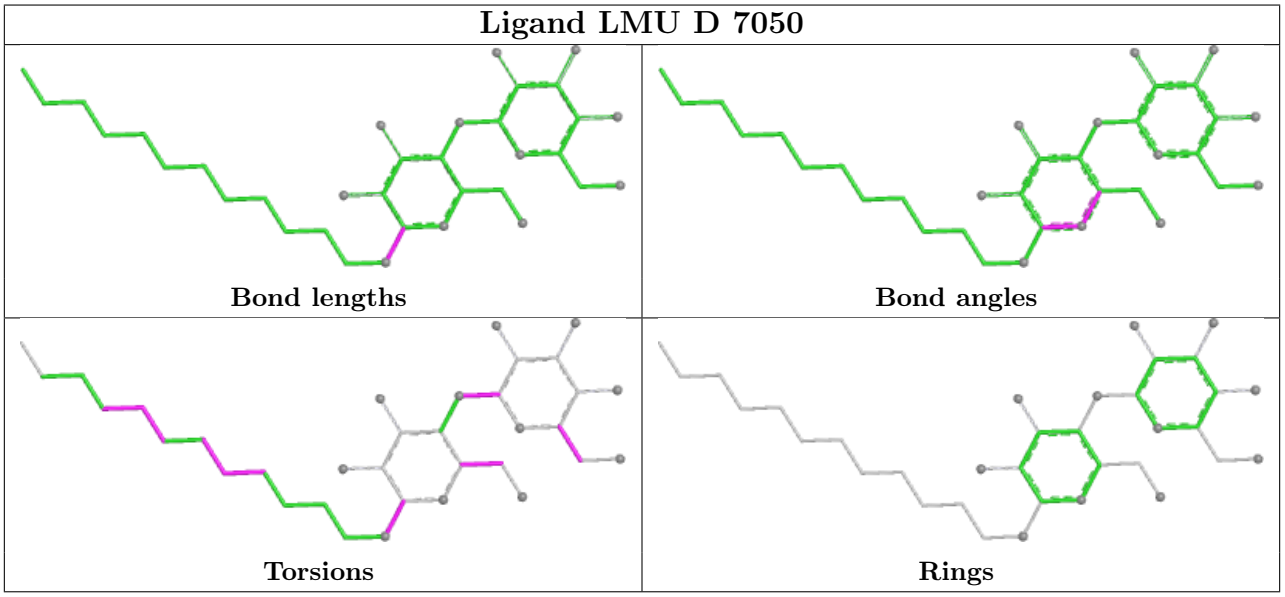


Rings

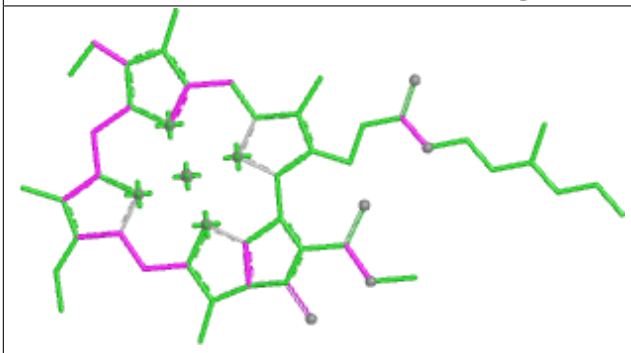
Ligand LMU 2 7027



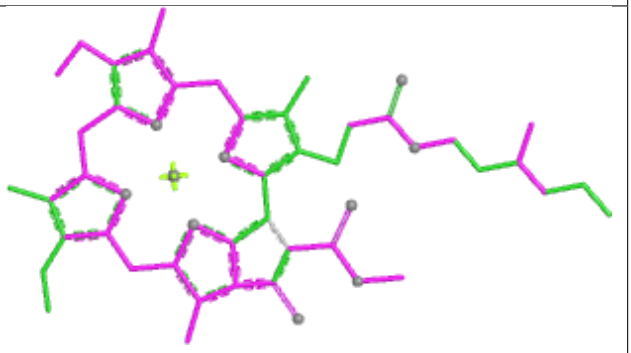
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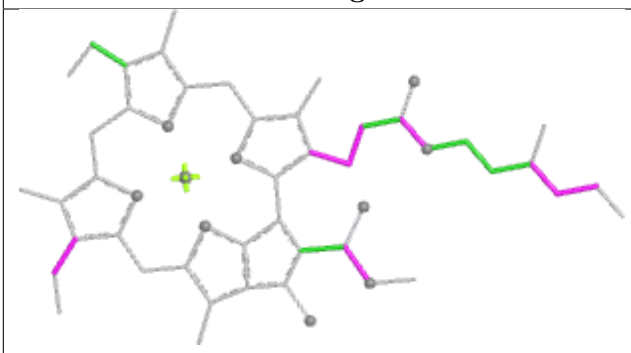
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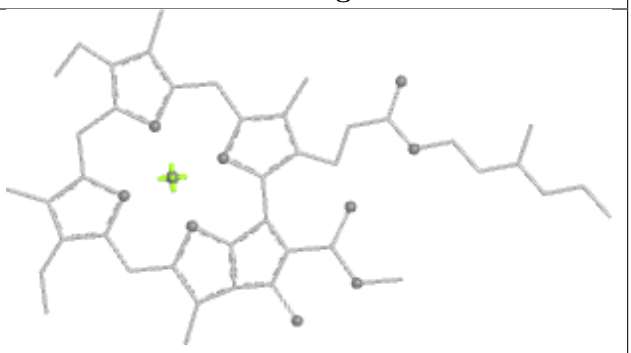
Bond lengths



Bond angles

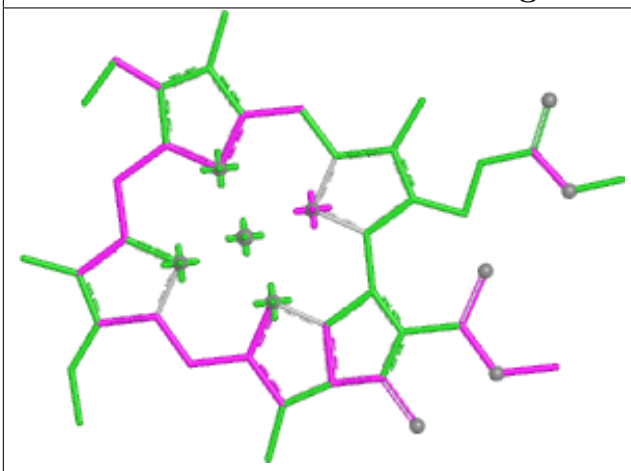


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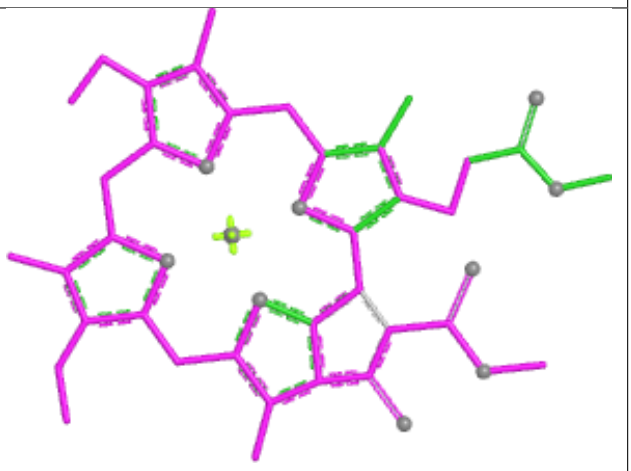


Rings

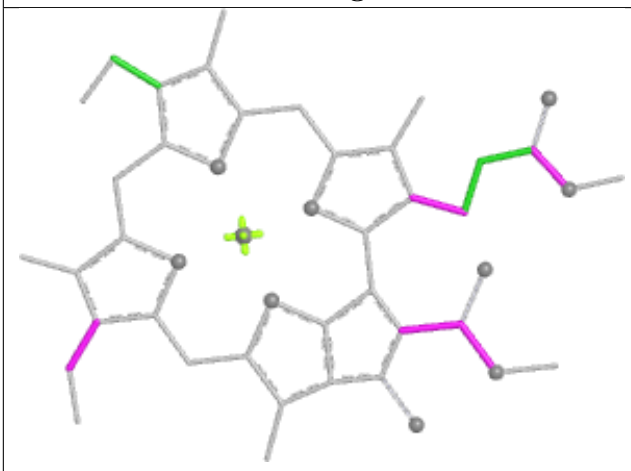
Ligand CLA 1 1001



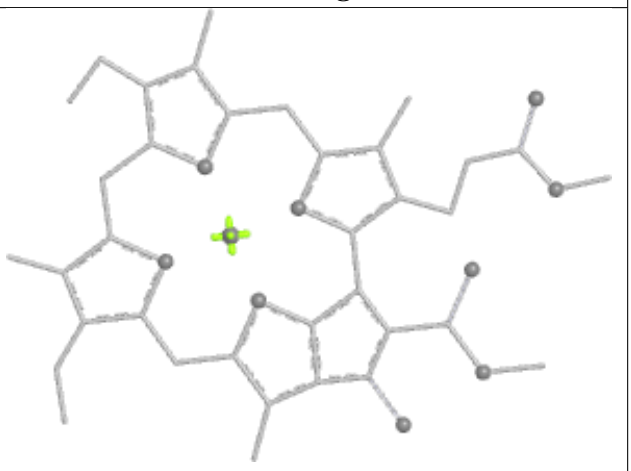
Bond lengths



Bond angles

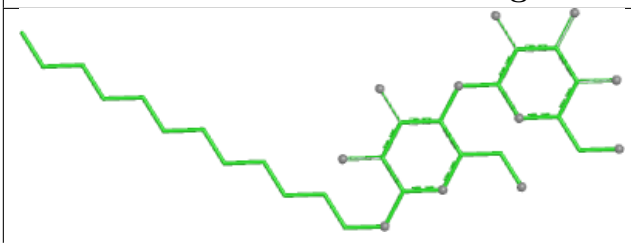


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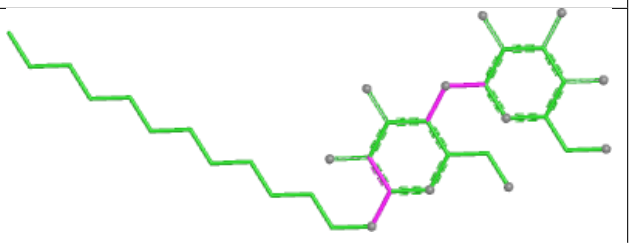


Rings

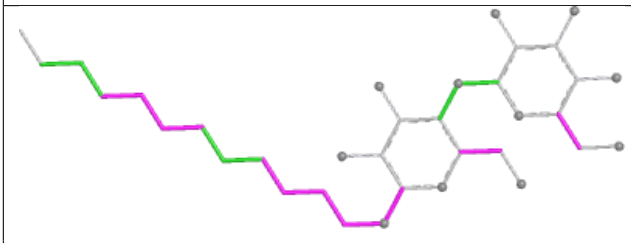
Ligand LMU H 7028



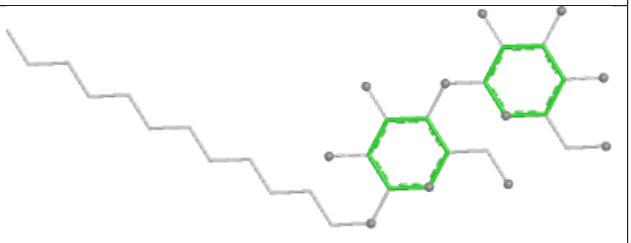
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Bond angles

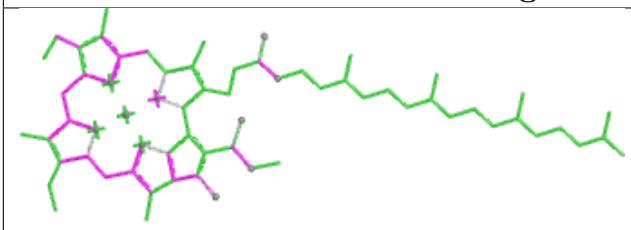


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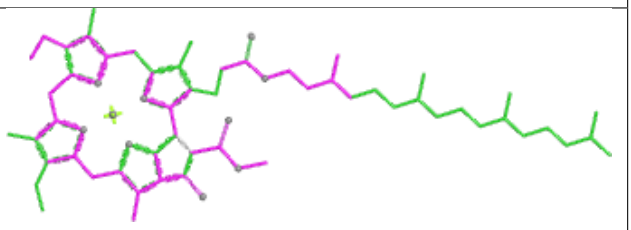


Rings

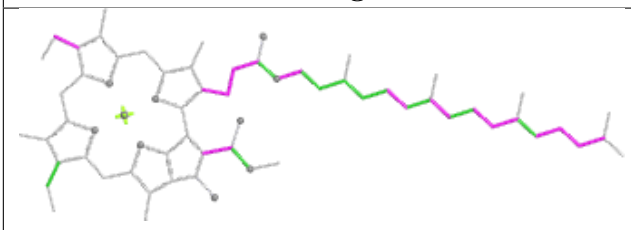
Ligand CLA 3 3013



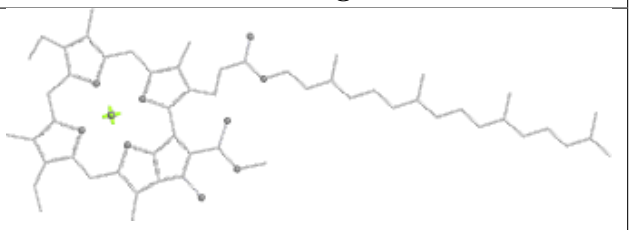
Bond lengths



Bond angles

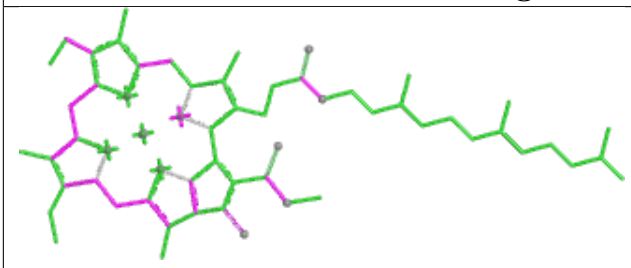


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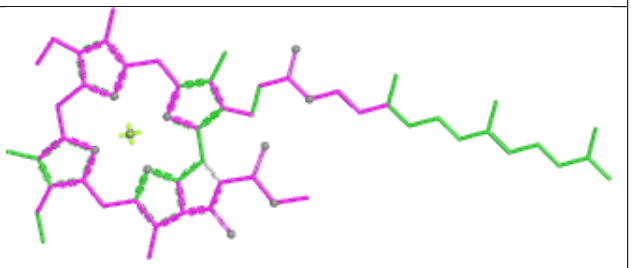


Rings

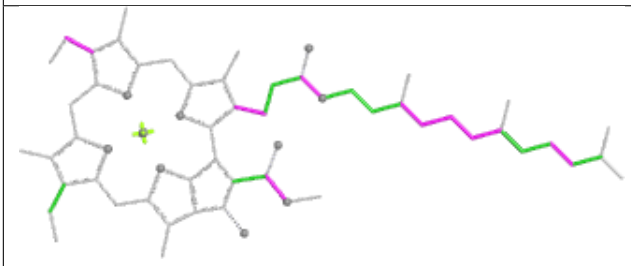
Ligand CLA B 1215



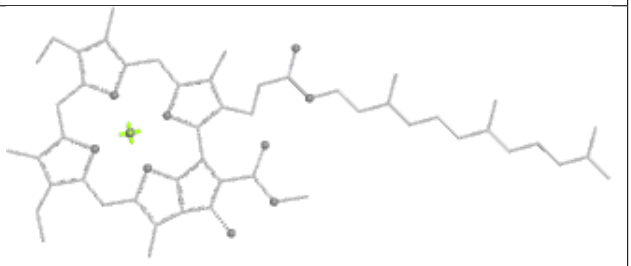
Bond lengths



Bond angles

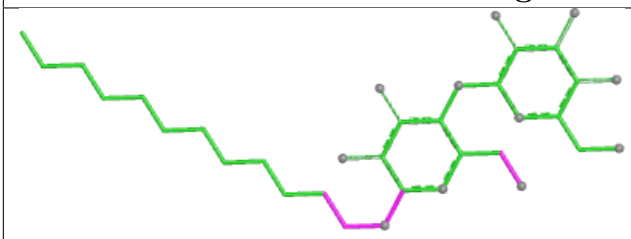


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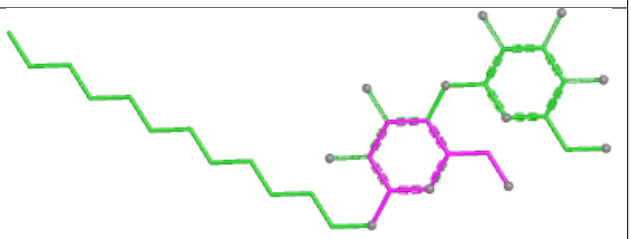


Rings

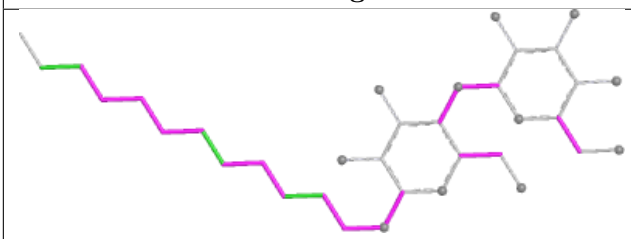
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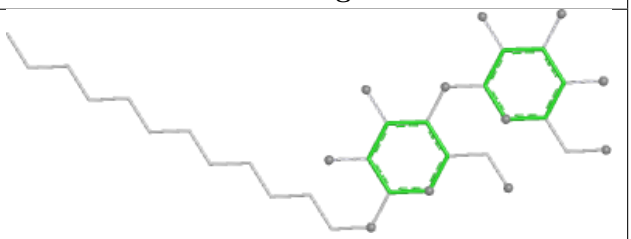
Bond lengths



Bond angles

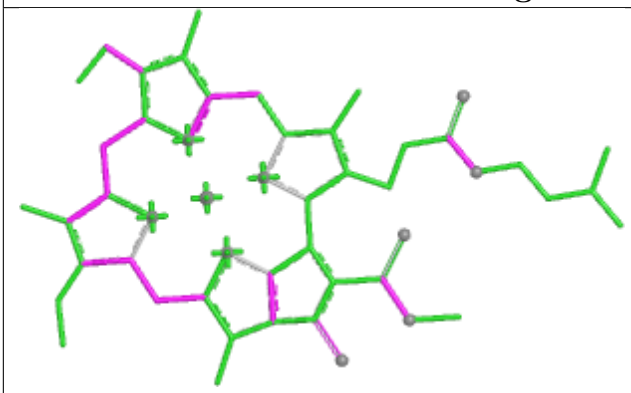


Torsions

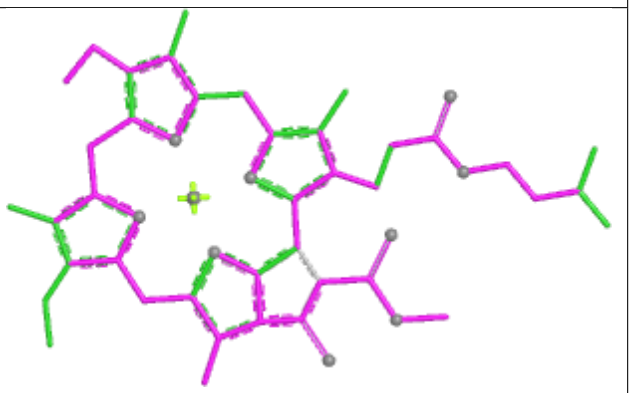


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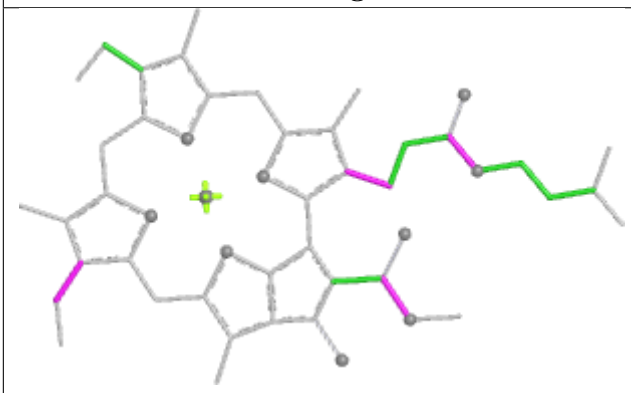
Ligand CLA A 1113



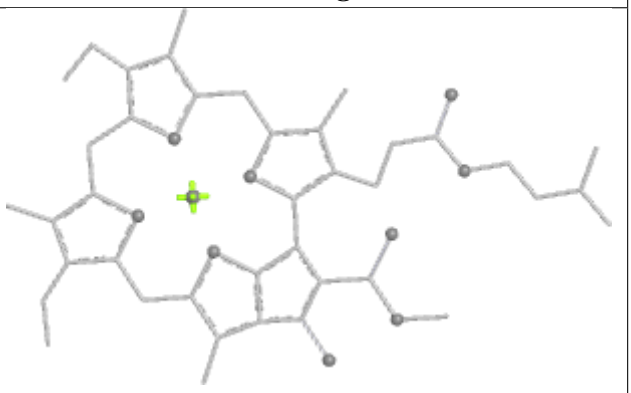
Bond lengths



Bond angles

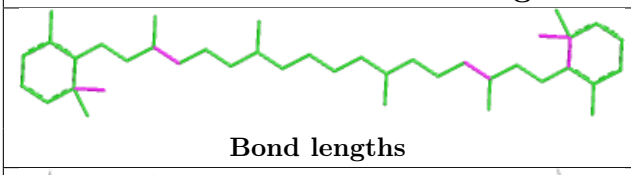


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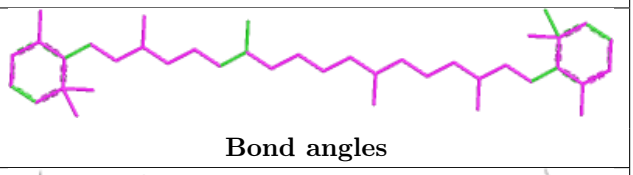


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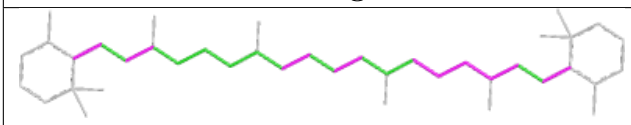
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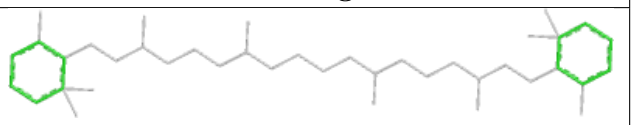
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Bond angles

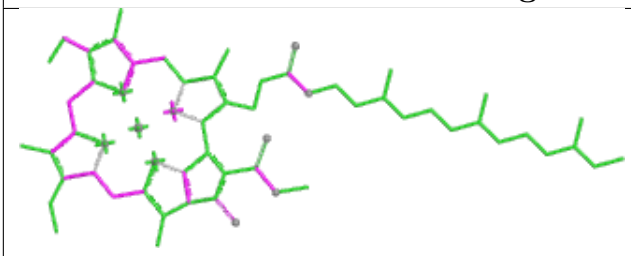


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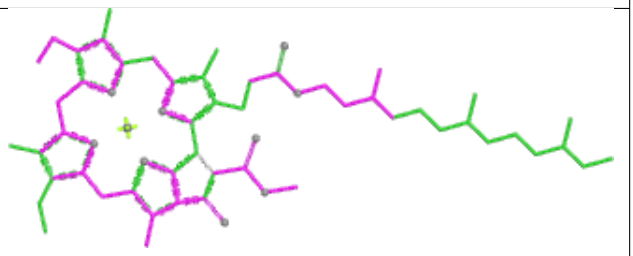


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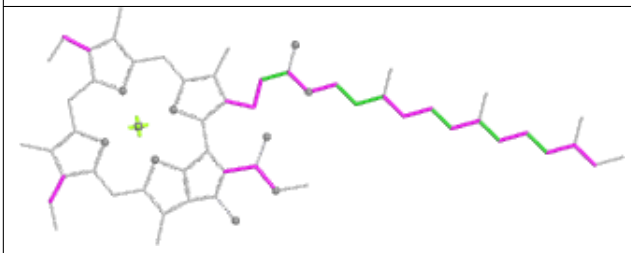
Ligand CLA J 1311



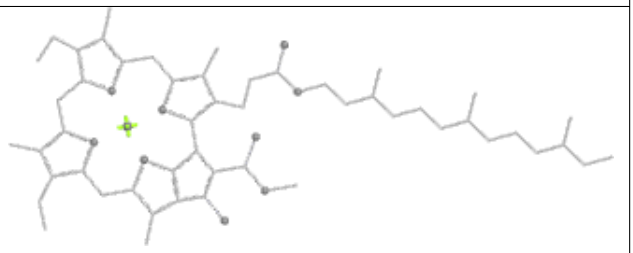
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Bond angles

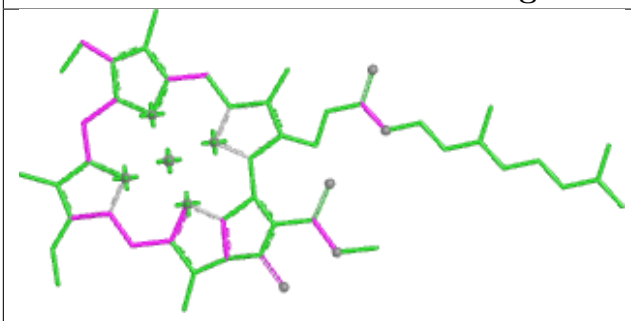


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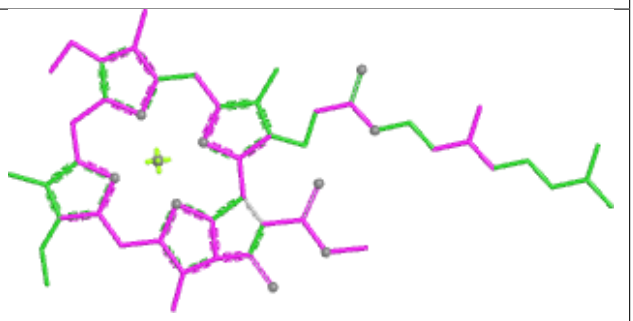


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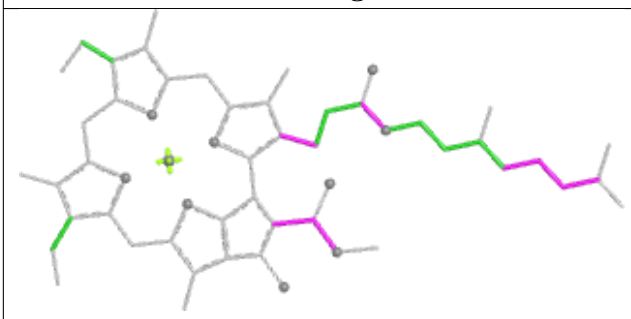
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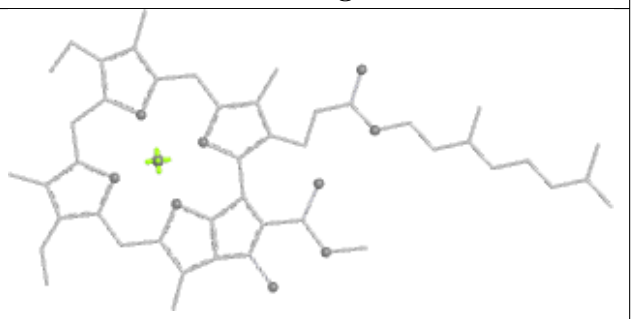
Bond lengths



Bond angles

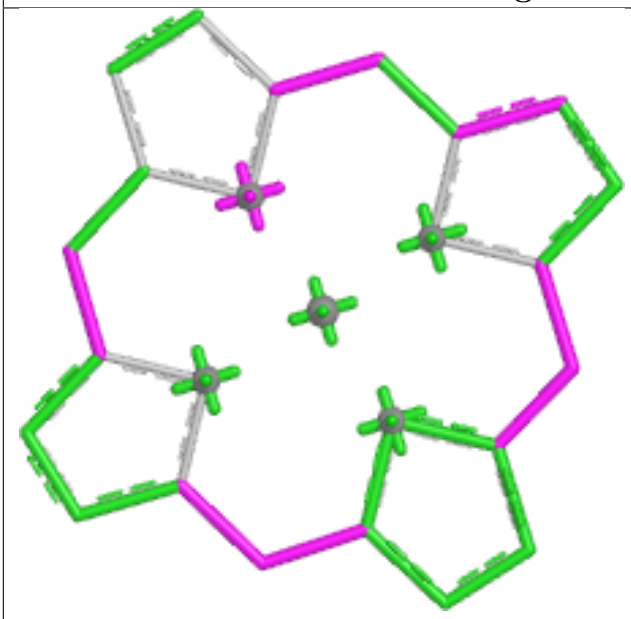


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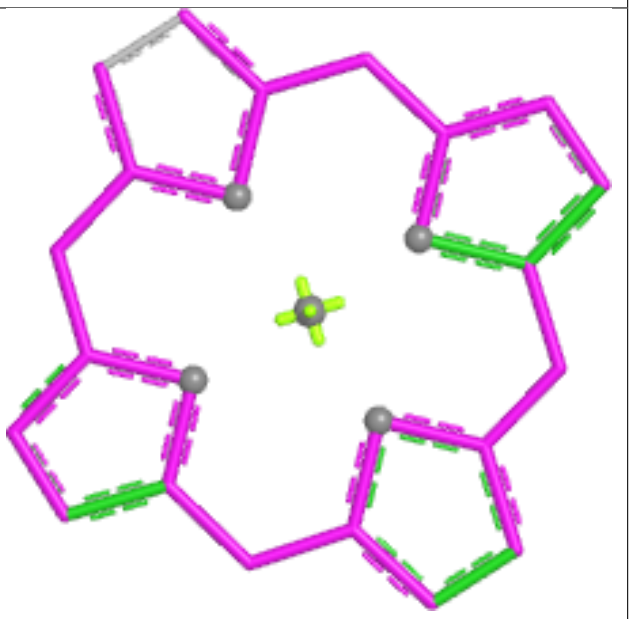


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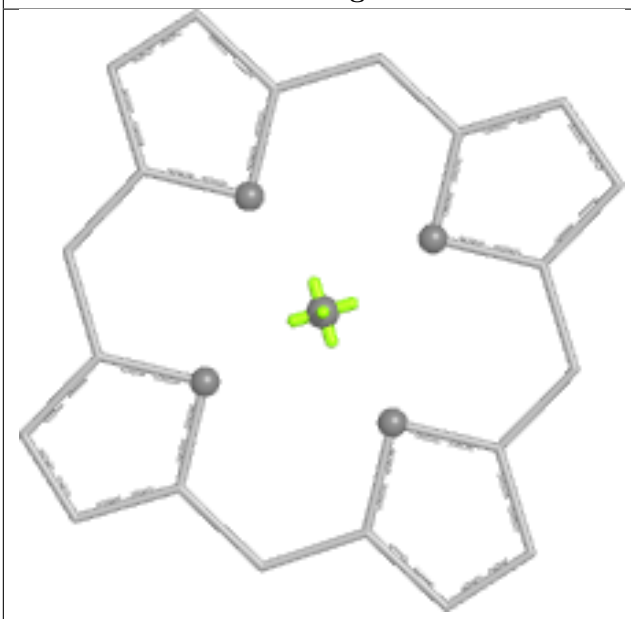
Ligand CLA A 1309



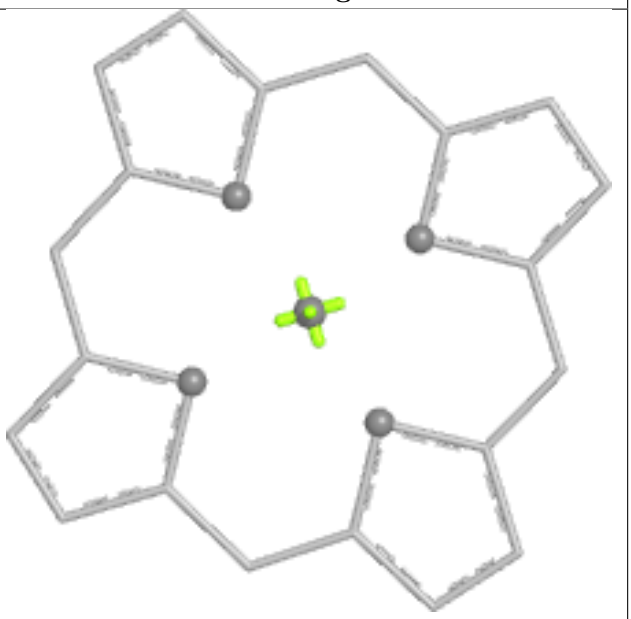
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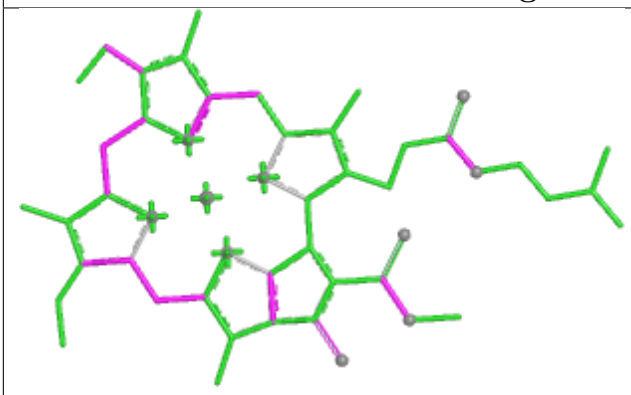


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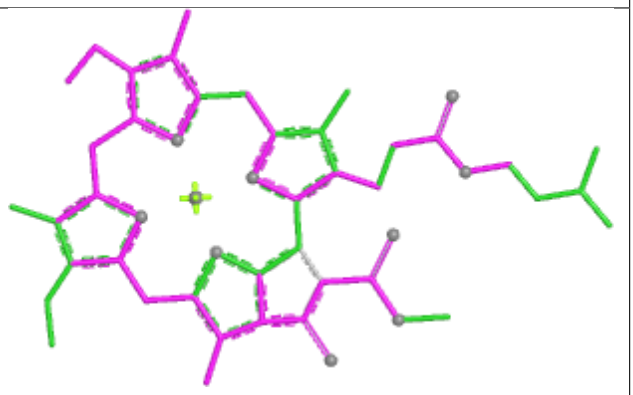


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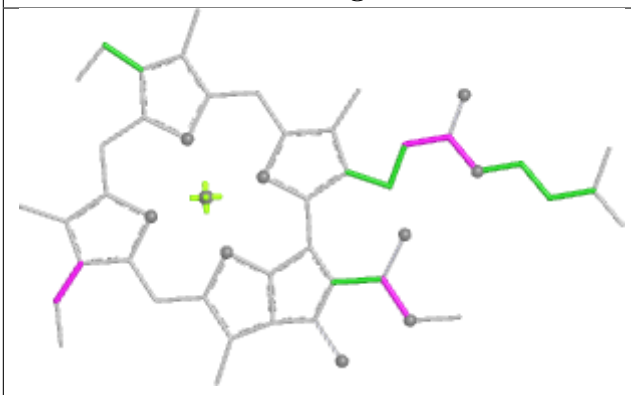
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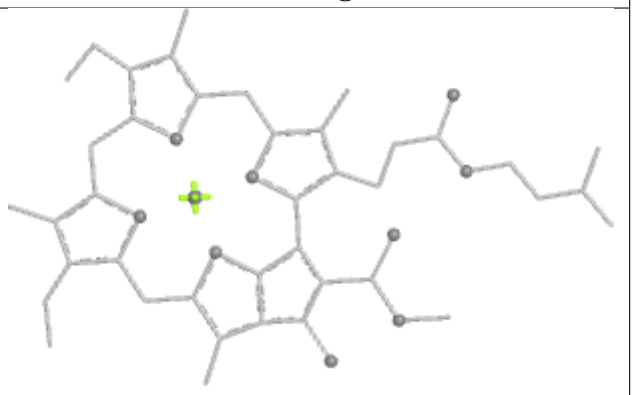
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Bond angles

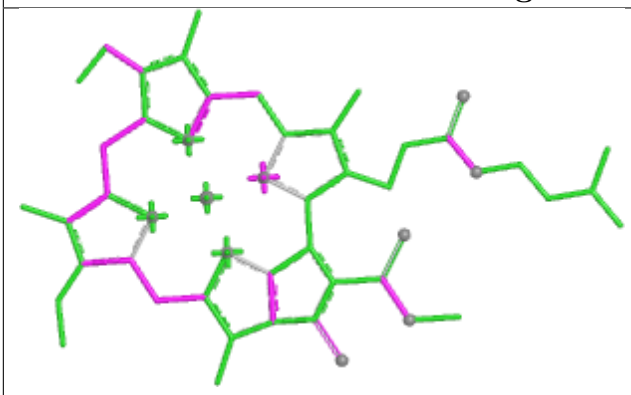


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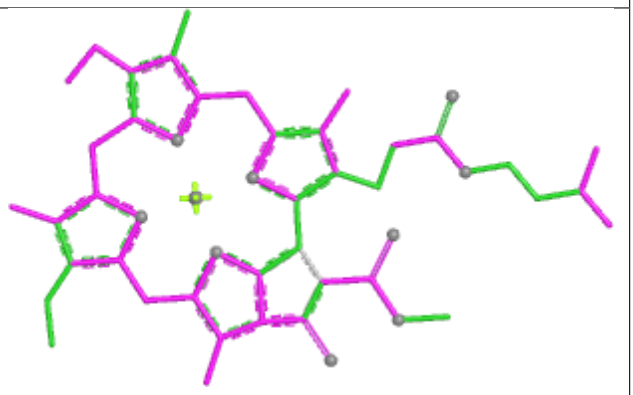


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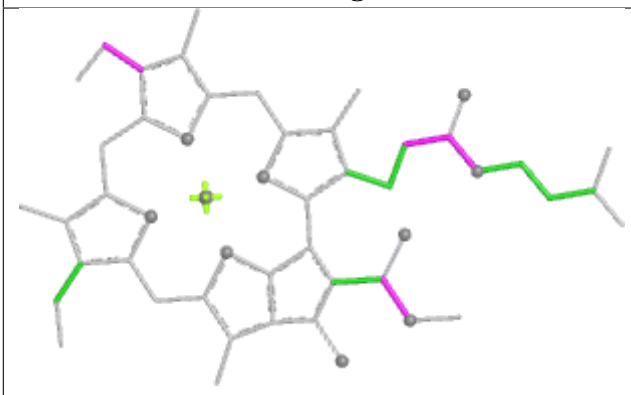
Ligand CLA B 1217



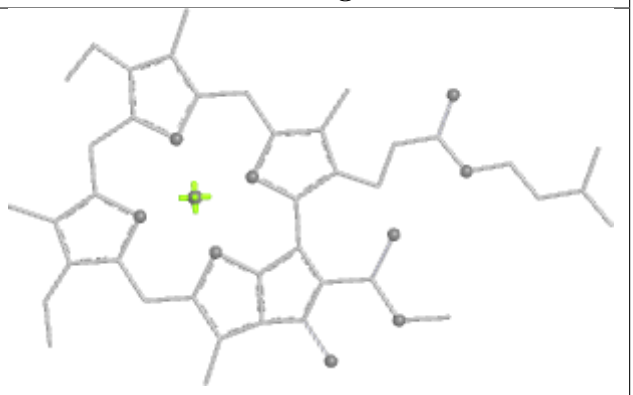
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Bond angles

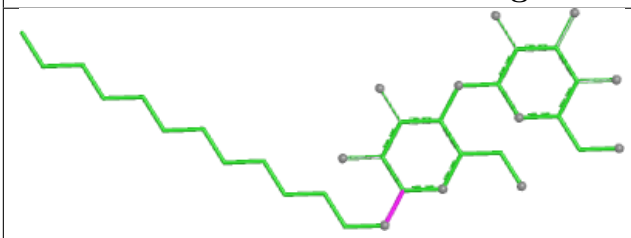


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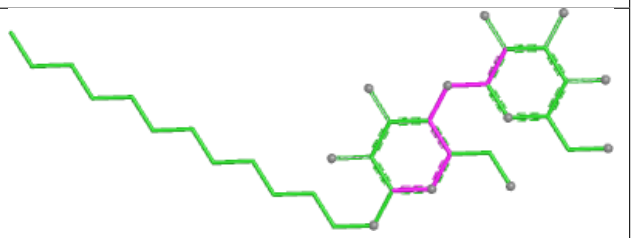


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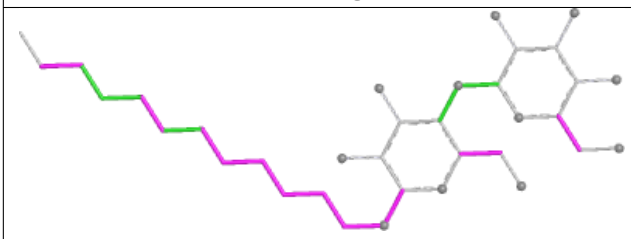
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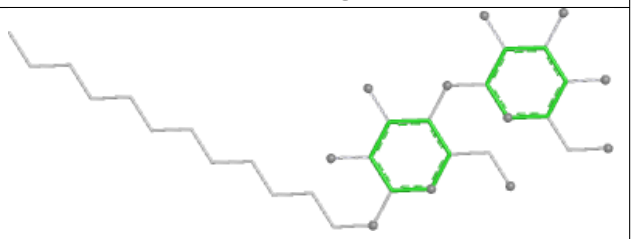
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Bond angles

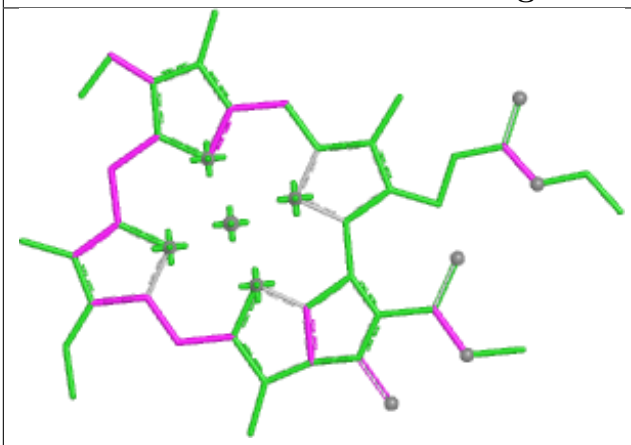


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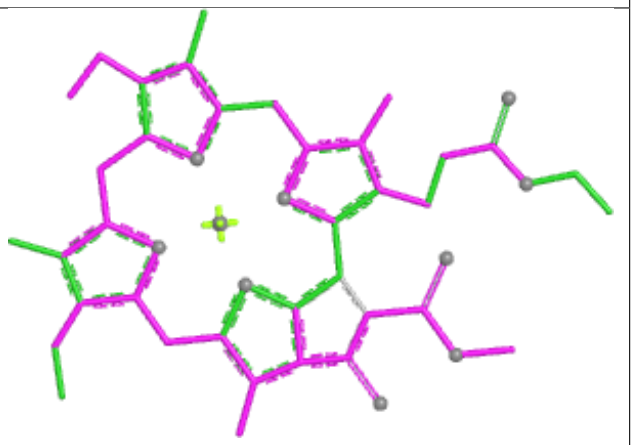


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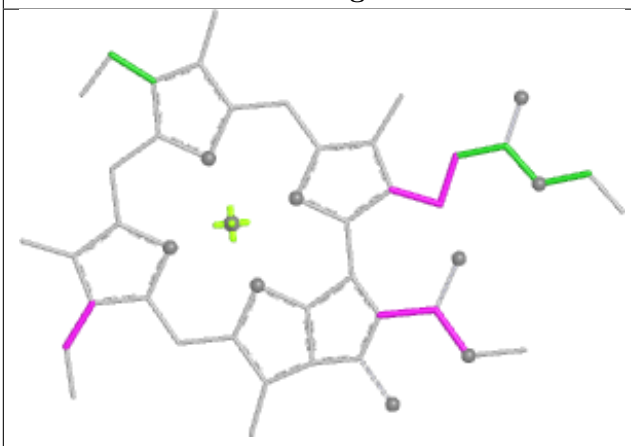
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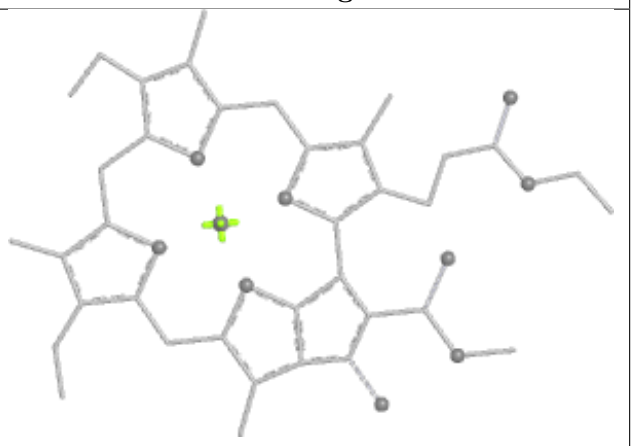
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Bond angles

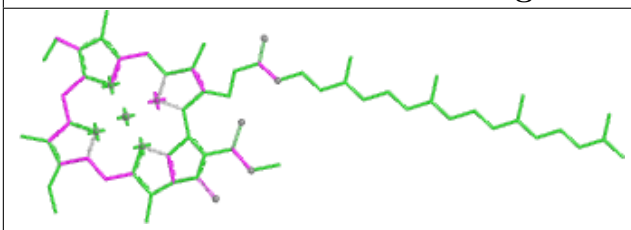


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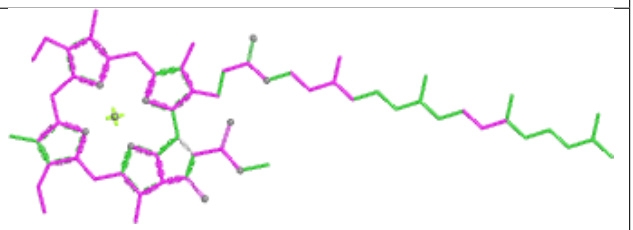


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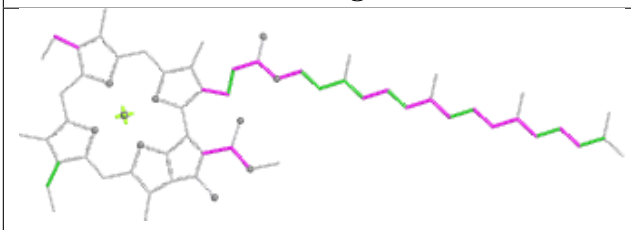
Ligand CLA B 1202



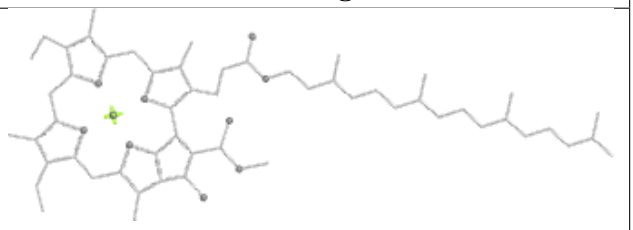
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Bond angles

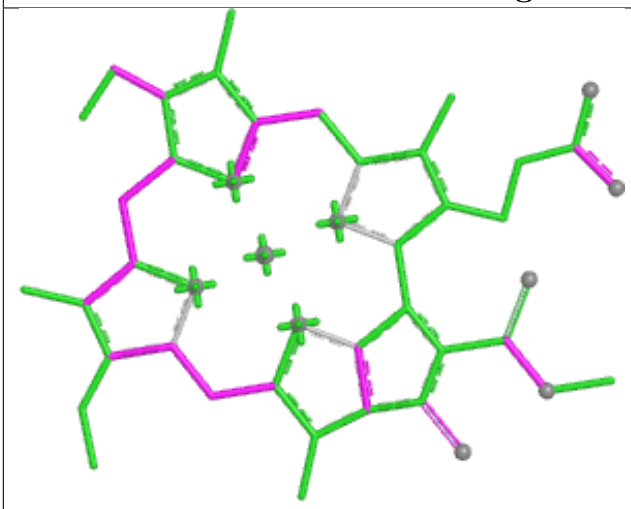


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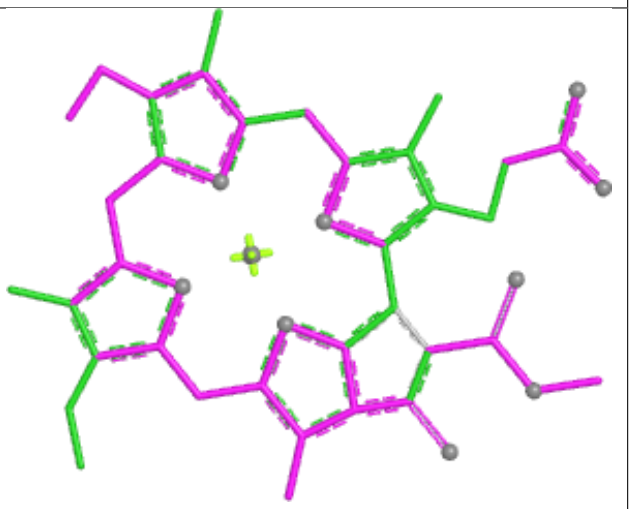


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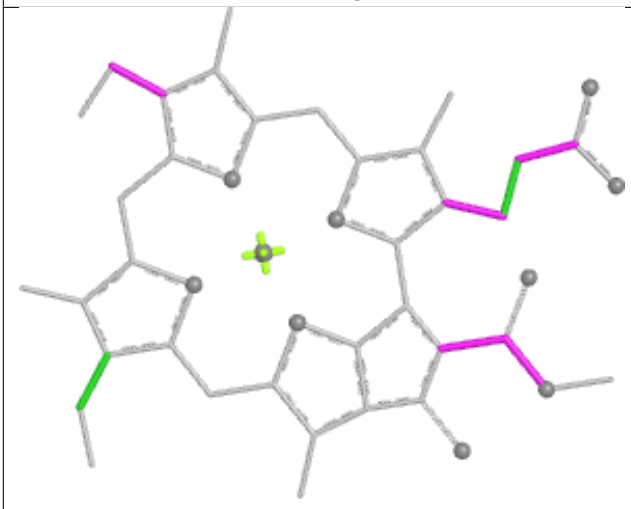
Ligand CLA B 1232



Bond lengths



Bond angles

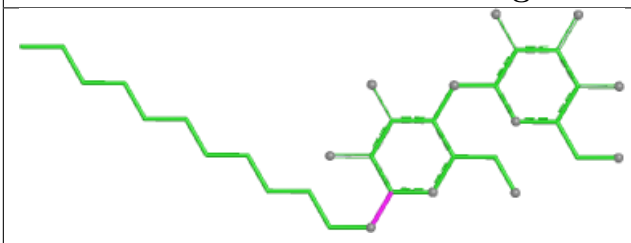


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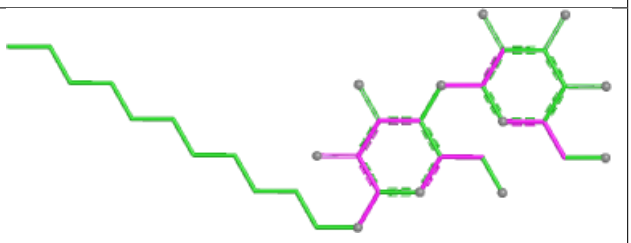


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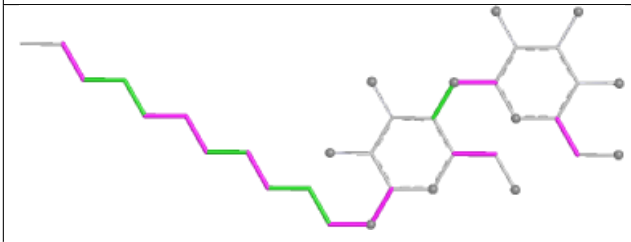
Ligand LMU F 7036



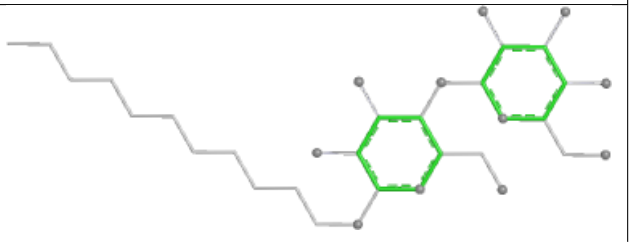
Bond lengths



Bond angles

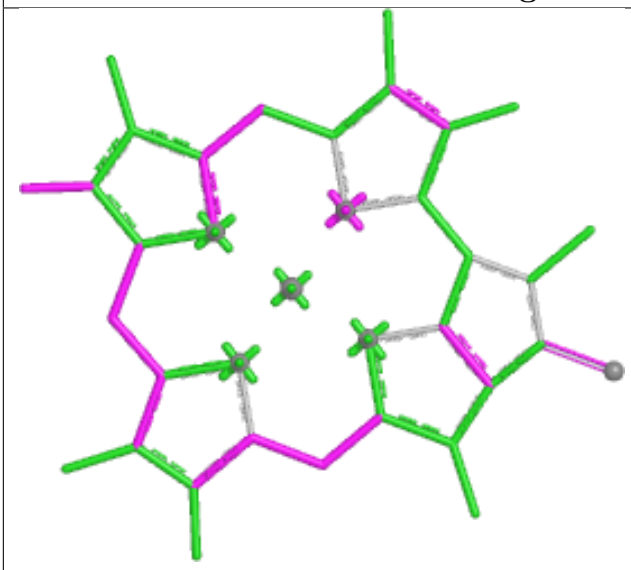


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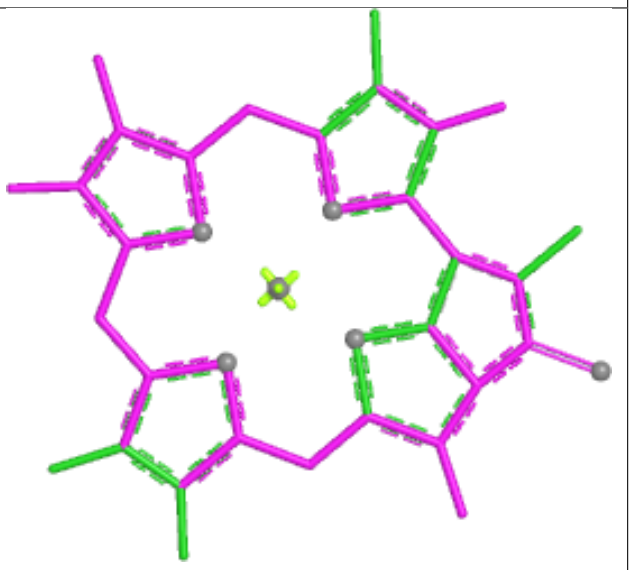


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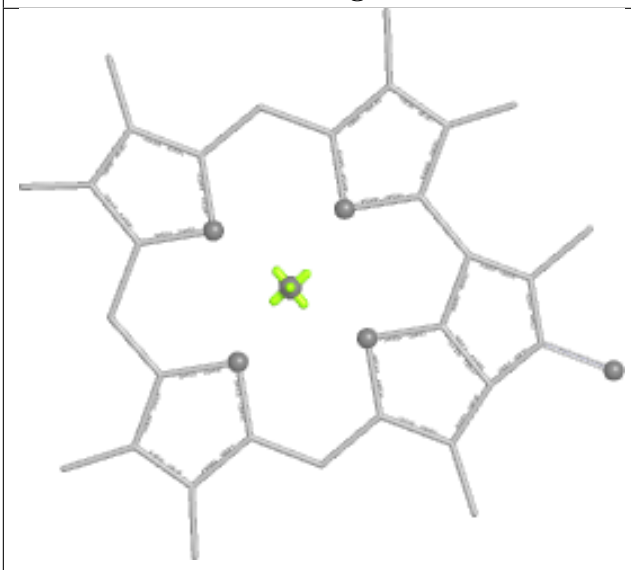
Ligand CLA 3 1118



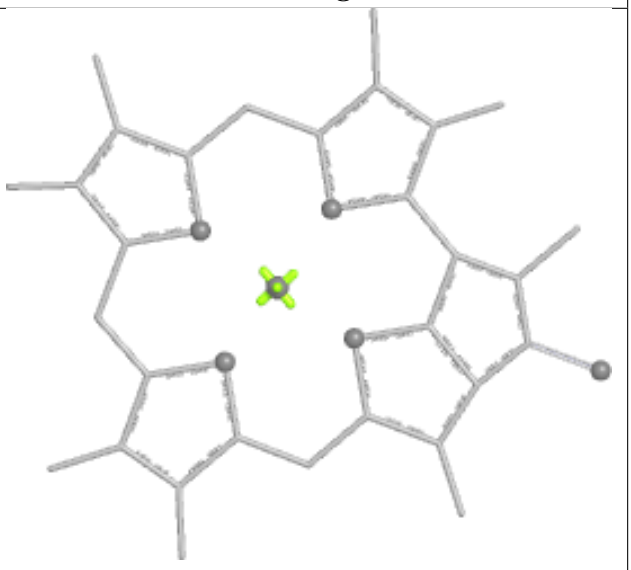
Bond lengths



Bond angles

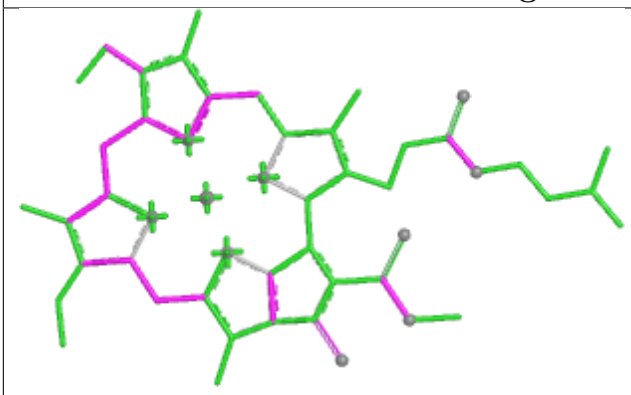


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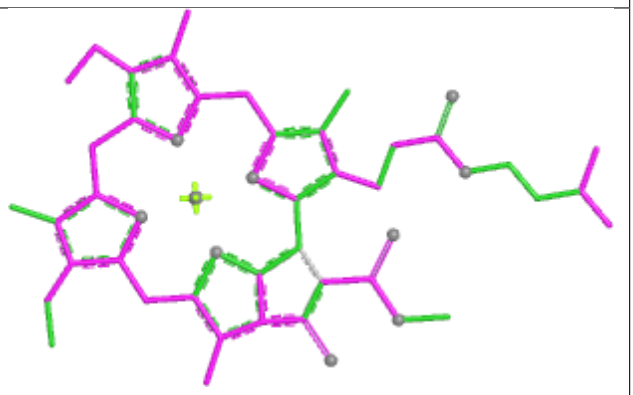


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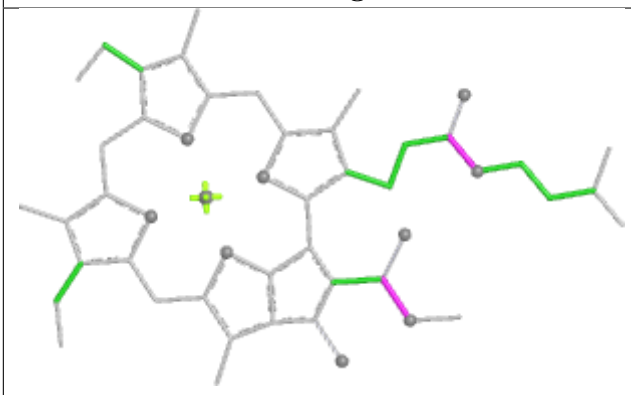
Ligand CLA 2 2012



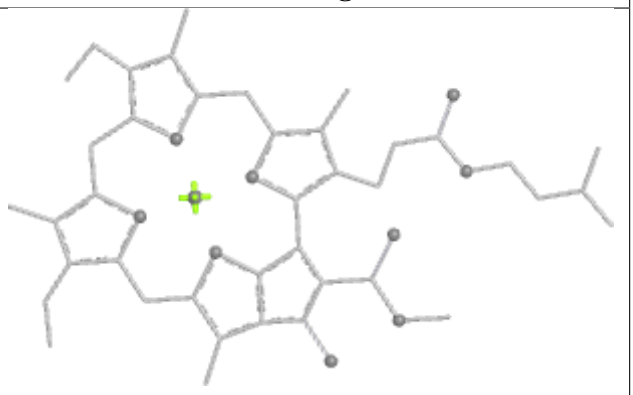
Bond lengths



Bond angles

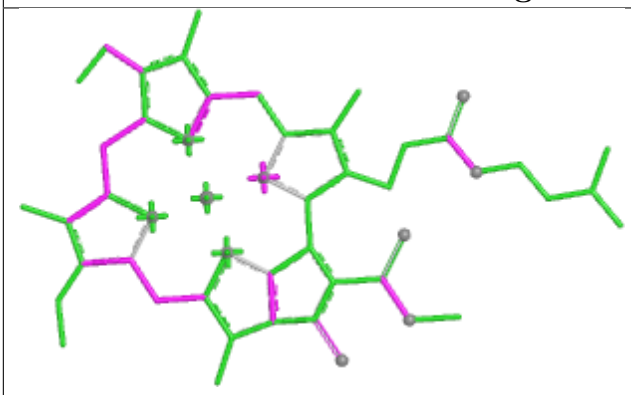


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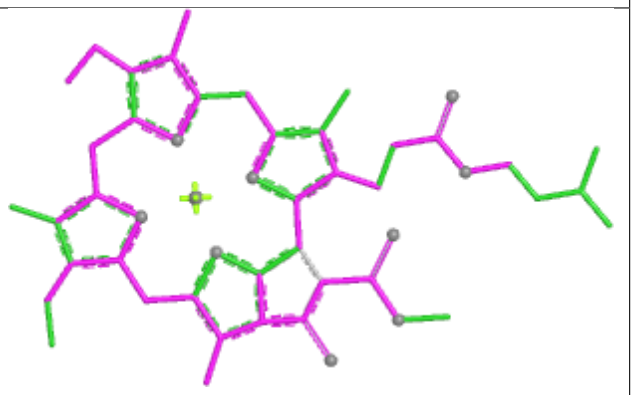


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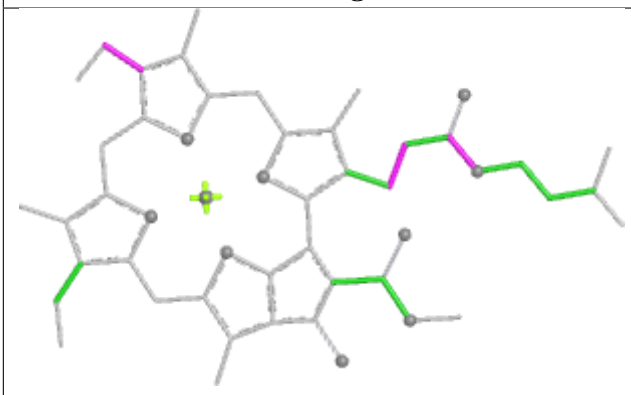
Ligand CLA A 1129



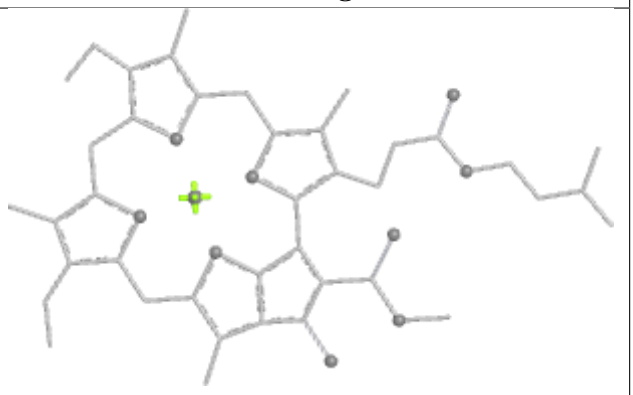
Bond lengths



Bond angles

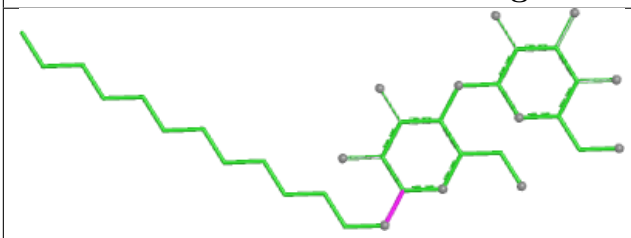


Torsions

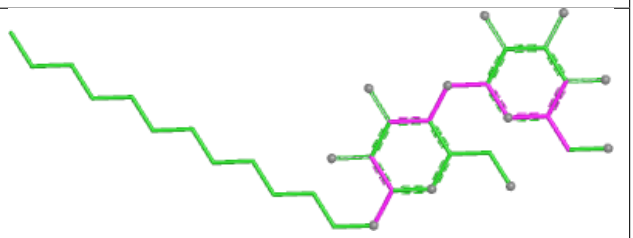


Rings

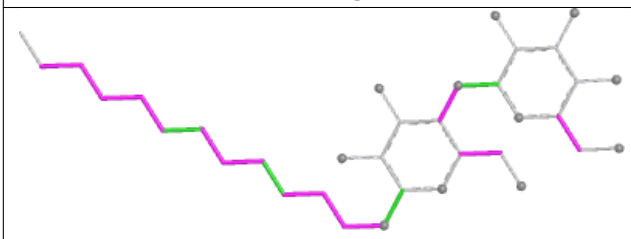
Ligand LMU R 7021



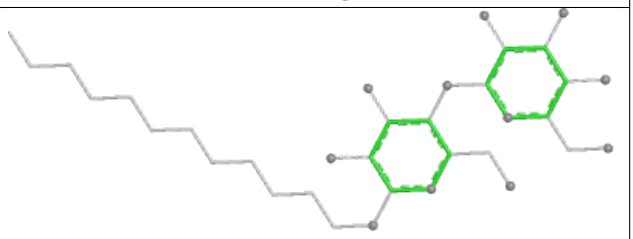
Bond lengths



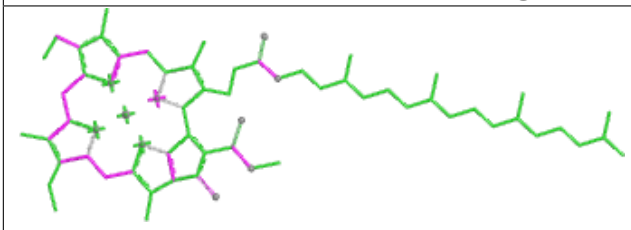
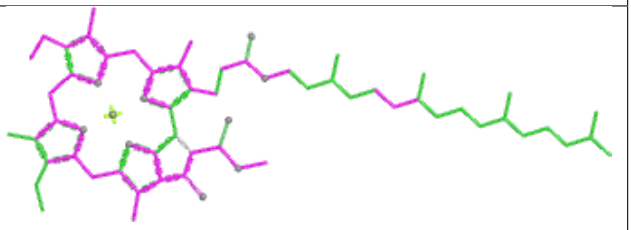
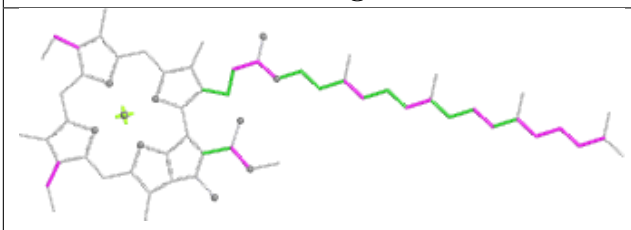
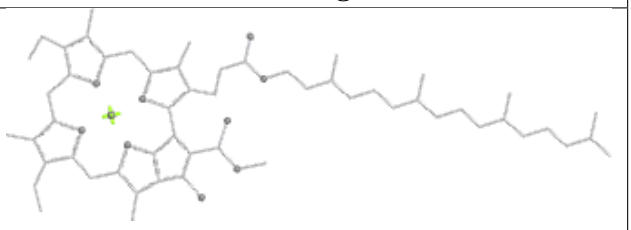
Bond angles



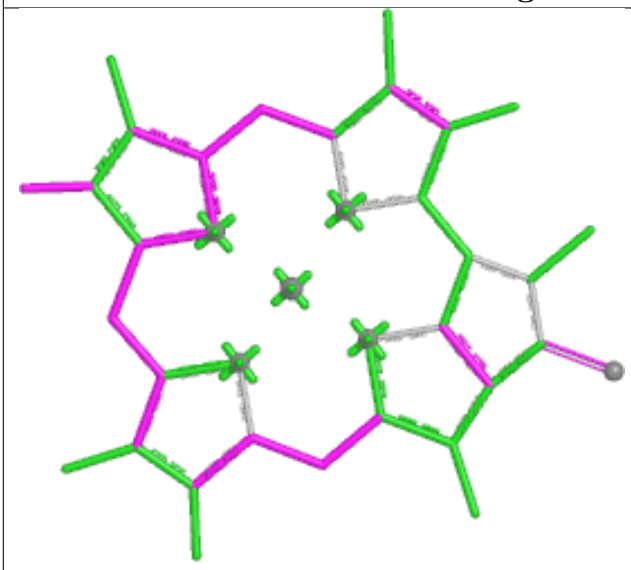
Torsions



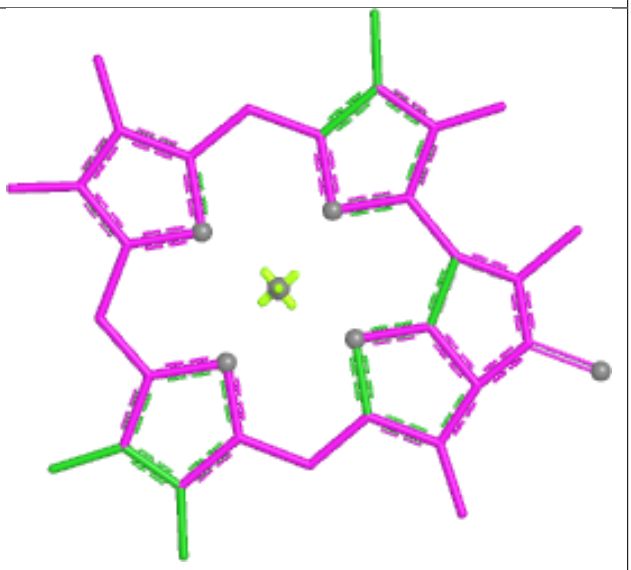
Rings

Ligand CLA A 9023	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

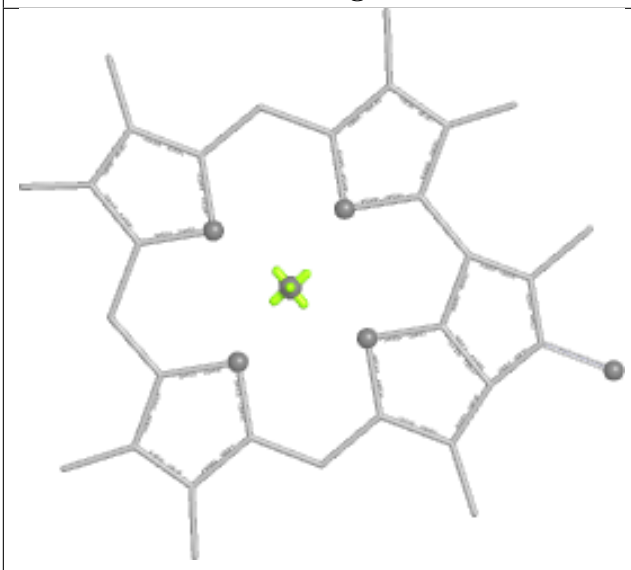
Ligand CLA F 1240



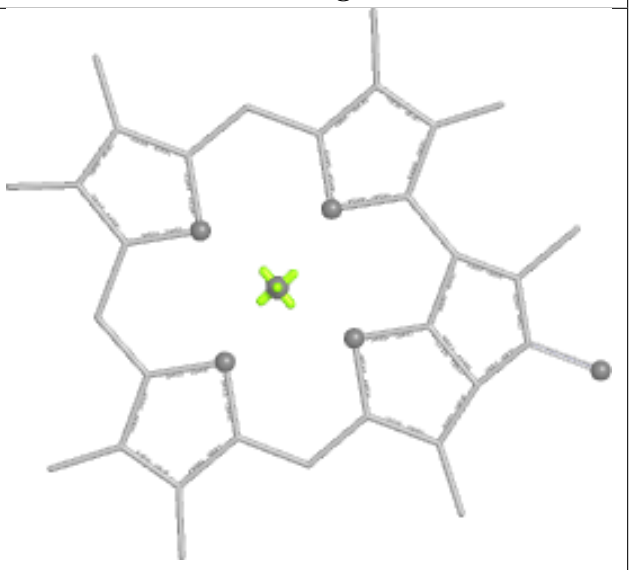
Bond lengths



Bond angles

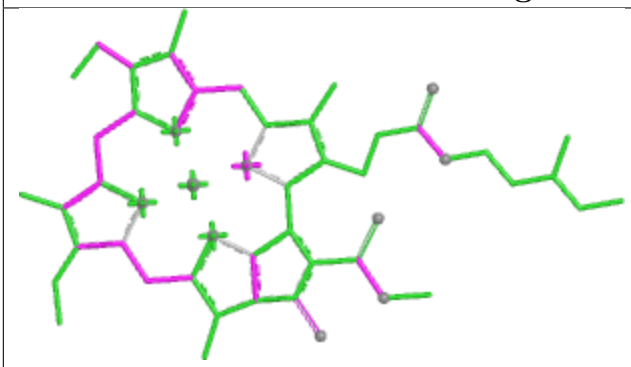


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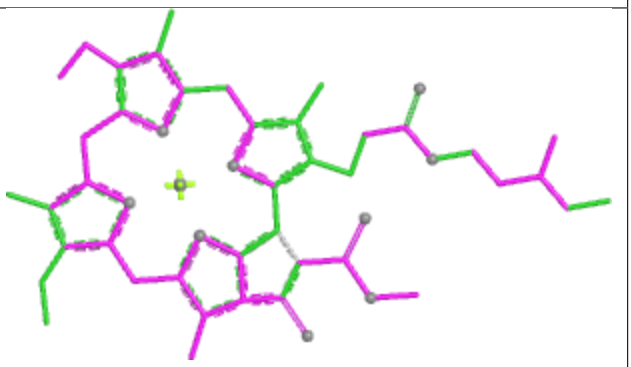


Rings

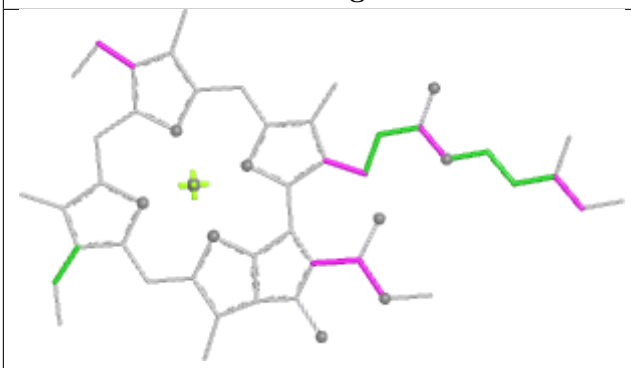
Ligand CLA A 1120



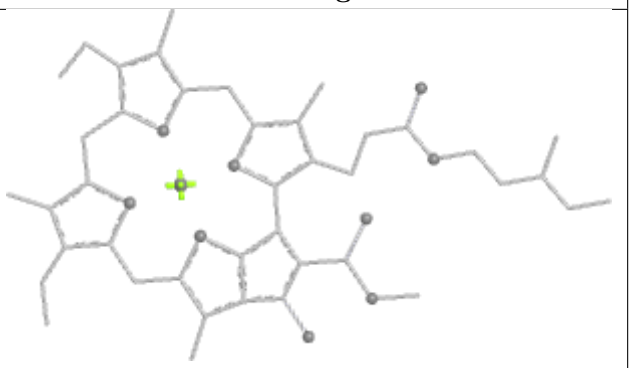
Bond lengths



Bond angles

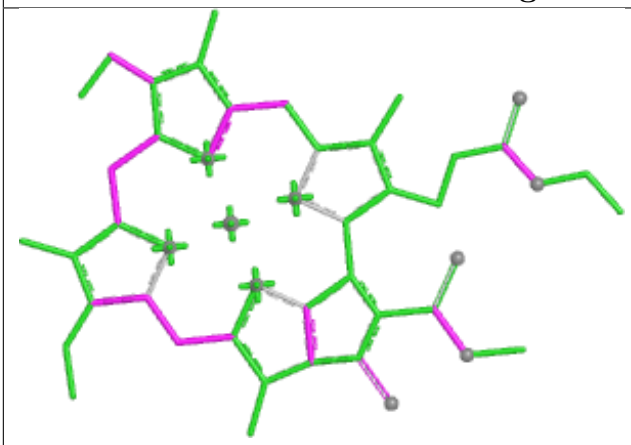


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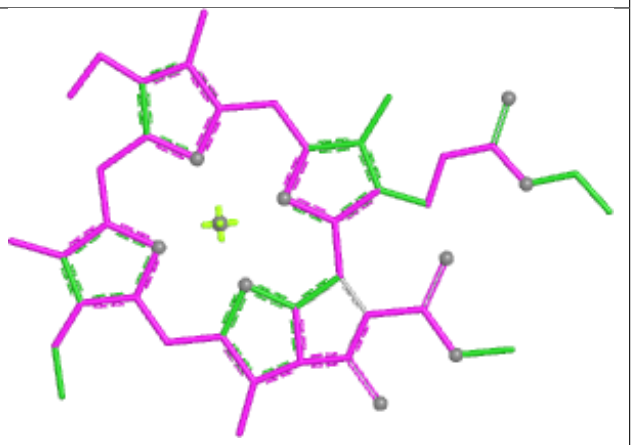


Rings

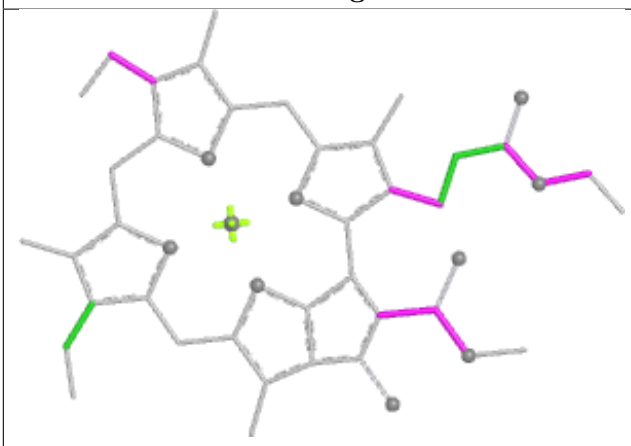
Ligand CLA 1 1003



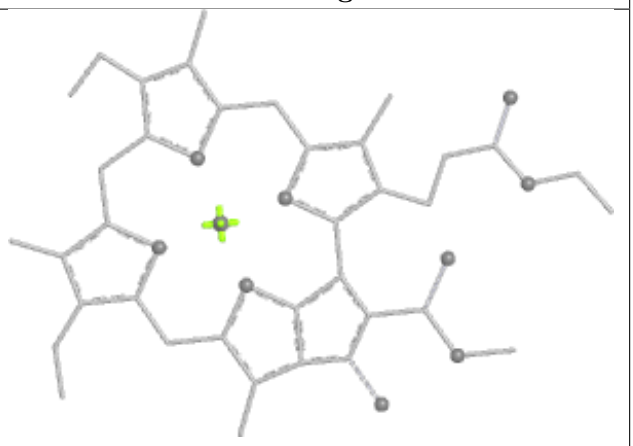
Bond lengths



Bond angles

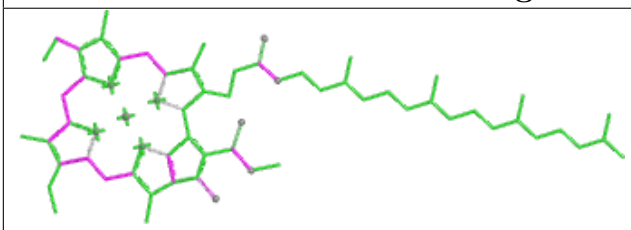


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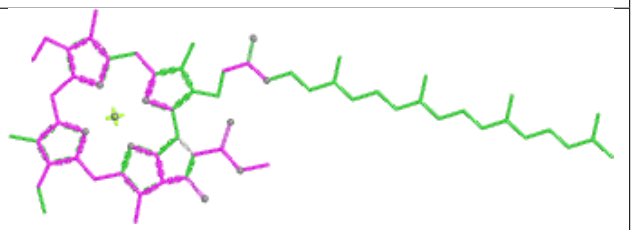


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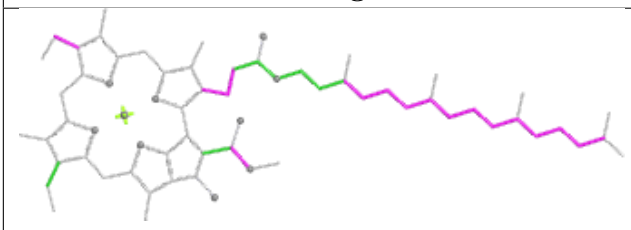
Ligand CLA B 1211



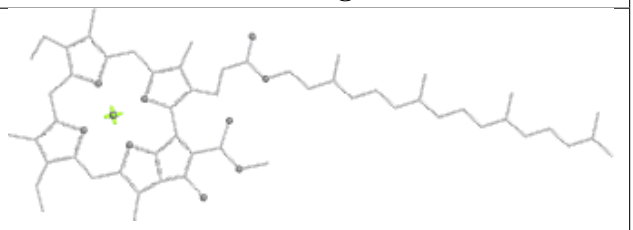
Bond lengths



Bond angles

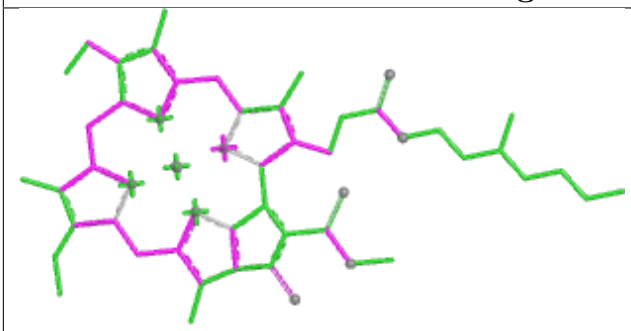


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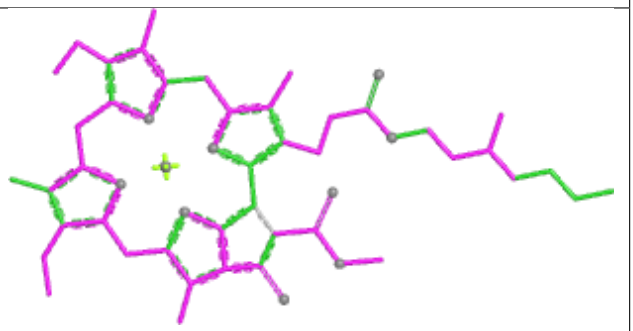


Rings

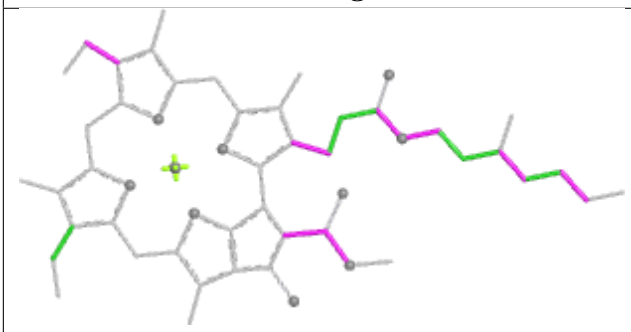
Ligand CLA F 1305



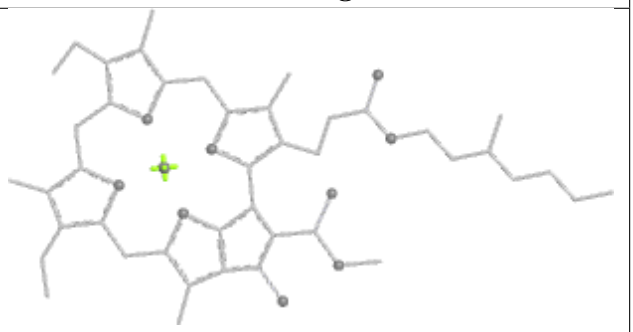
Bond lengths



Bond angles

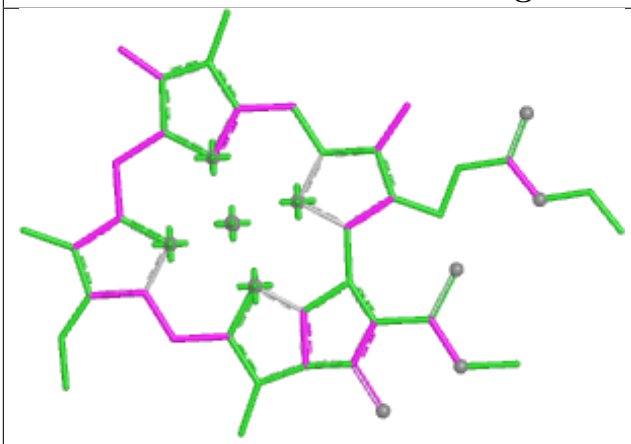


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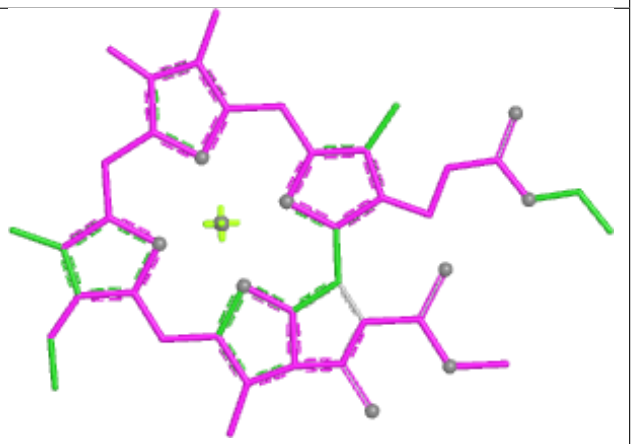


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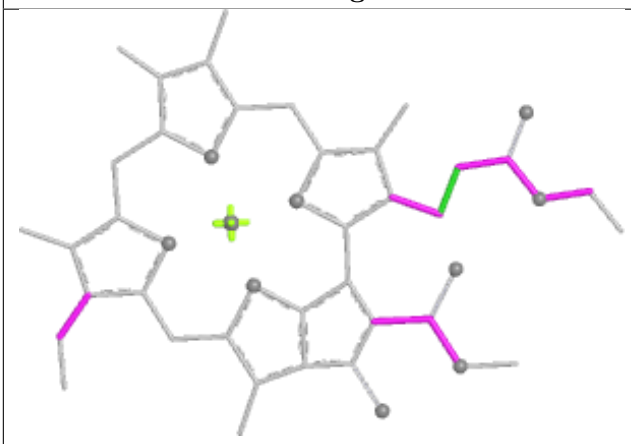
Ligand CLA A 1149



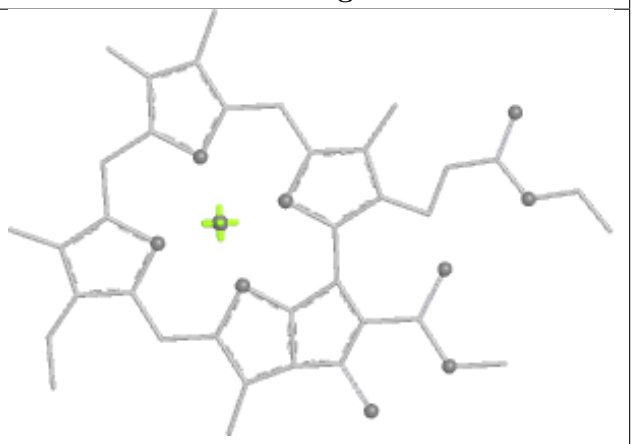
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Bond angles

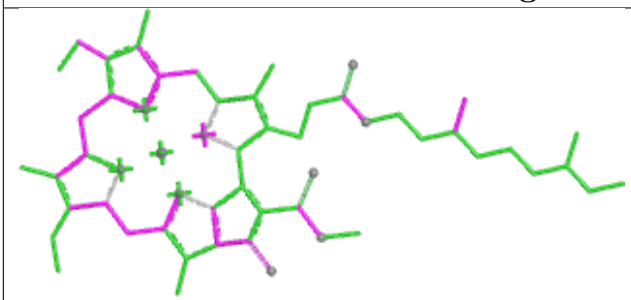


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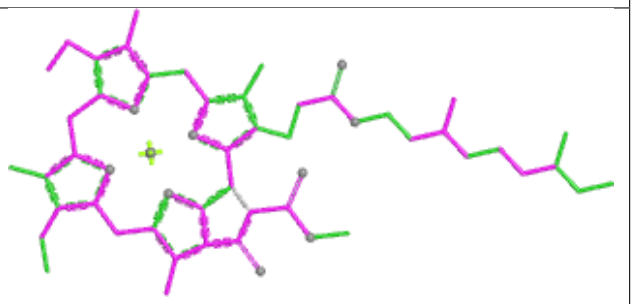


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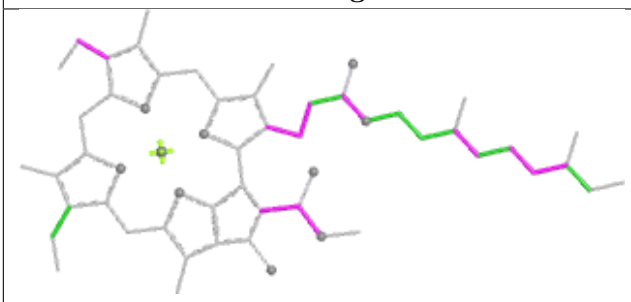
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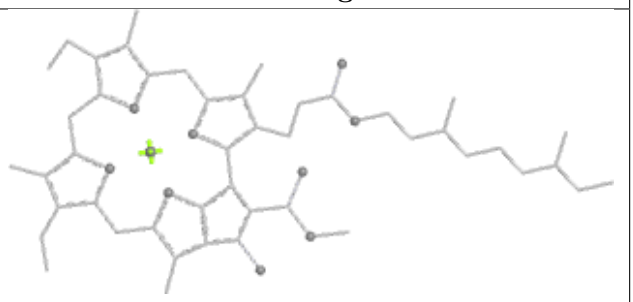
Bond lengths



Bond angles

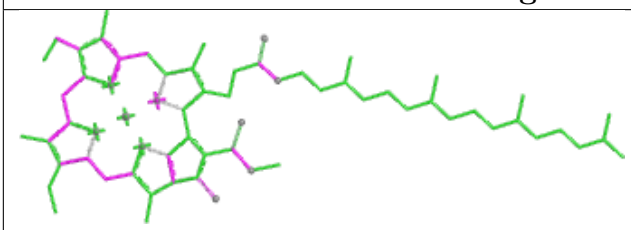


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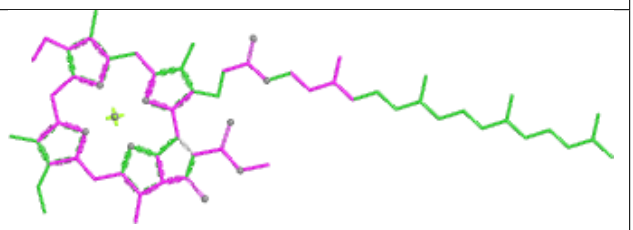


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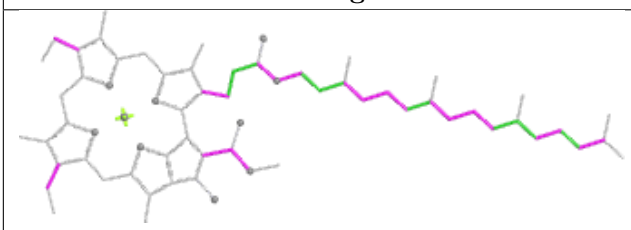
Ligand CLA 3 3016



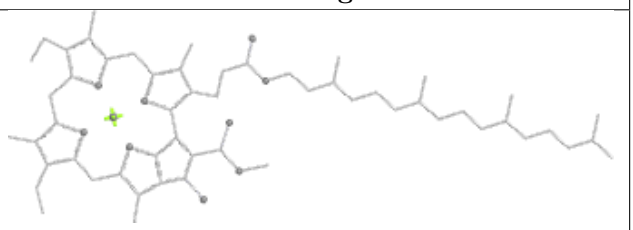
Bond lengths



Bond angles



Torsions

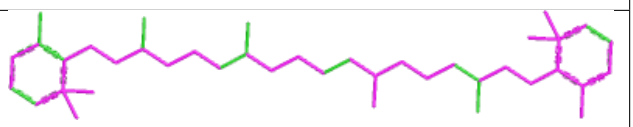


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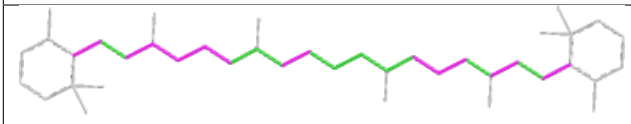
Ligand BCR 1 6023



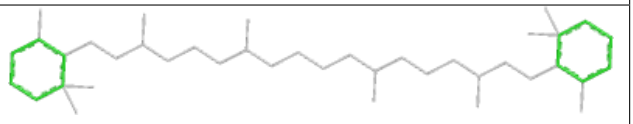
Bond lengths



Bond angles

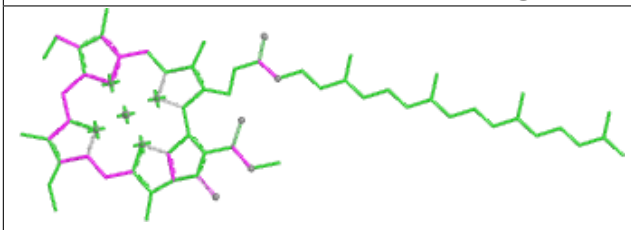


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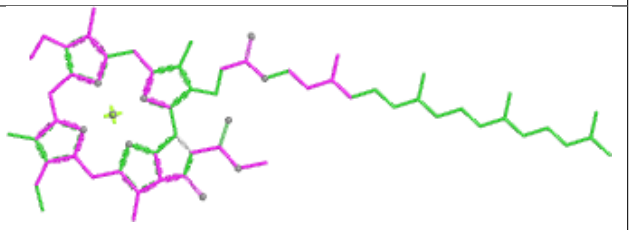


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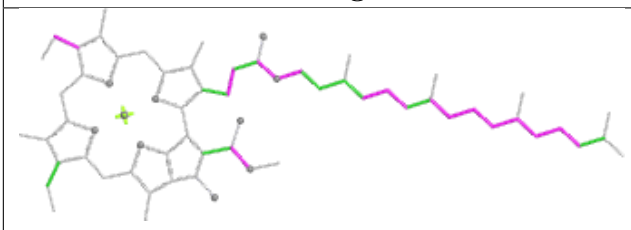
Ligand CLA A 1123



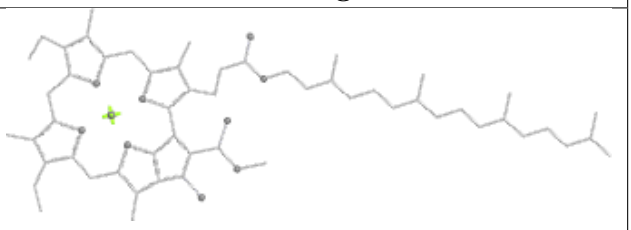
Bond lengths



Bond angles

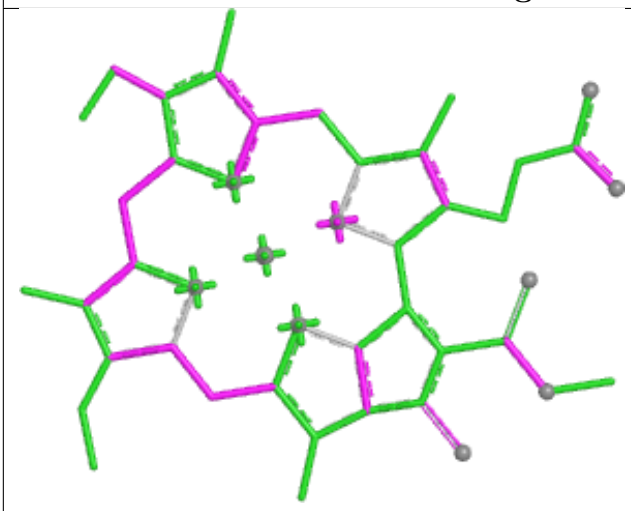


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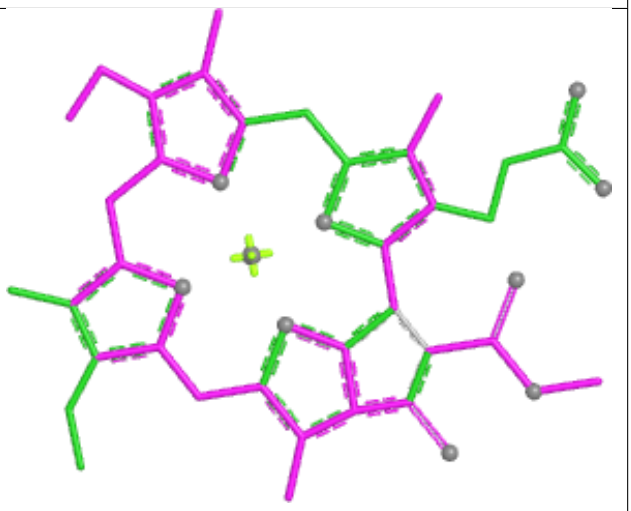


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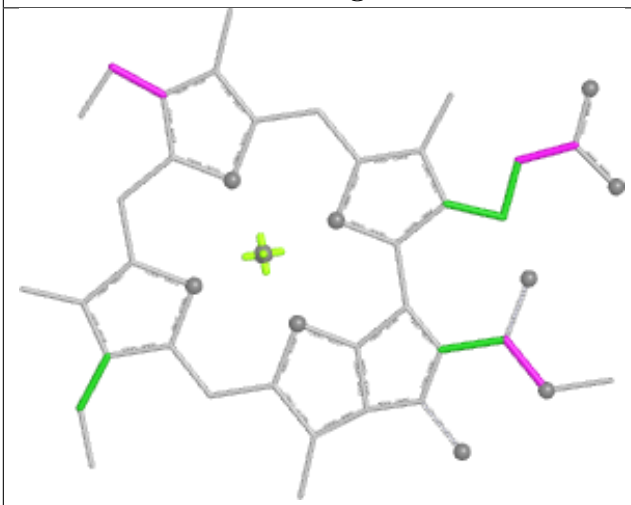
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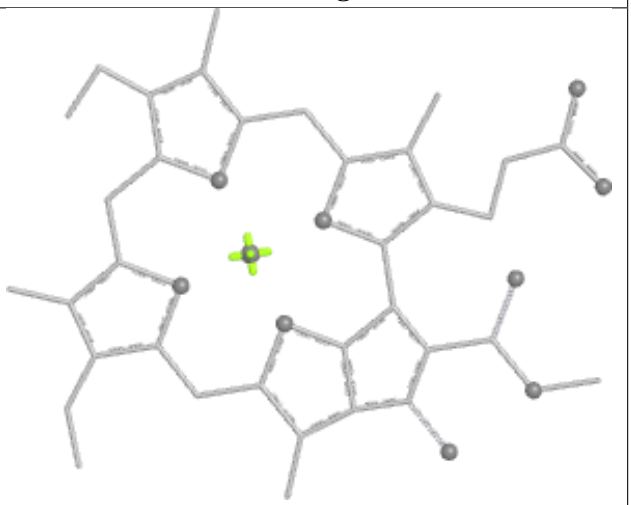
Bond lengths



Bond angles

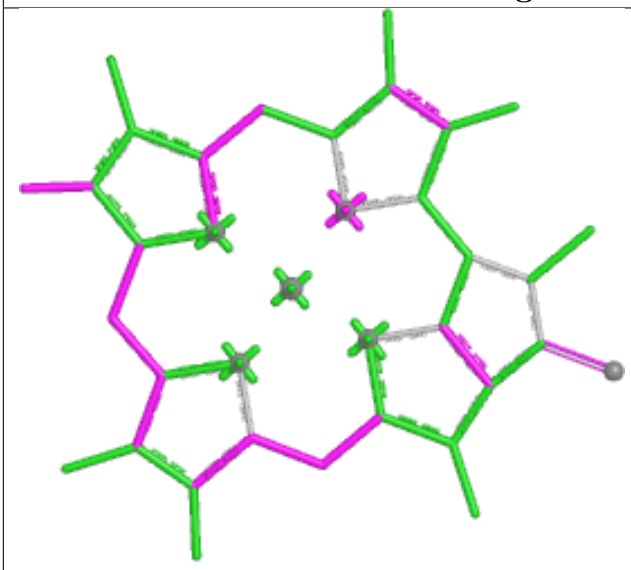


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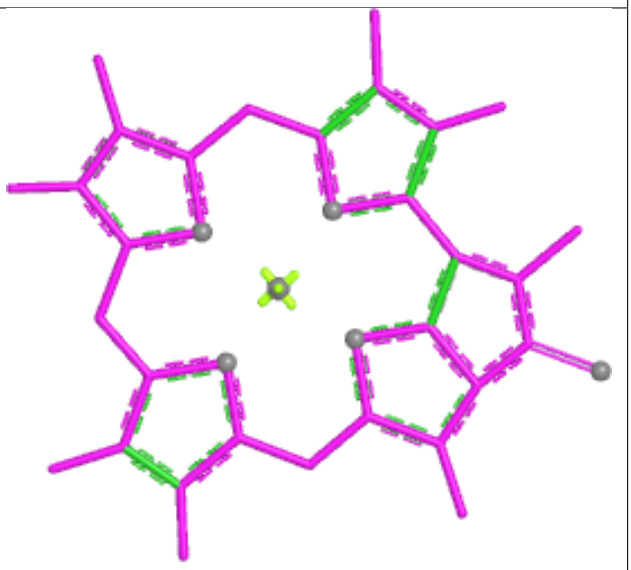


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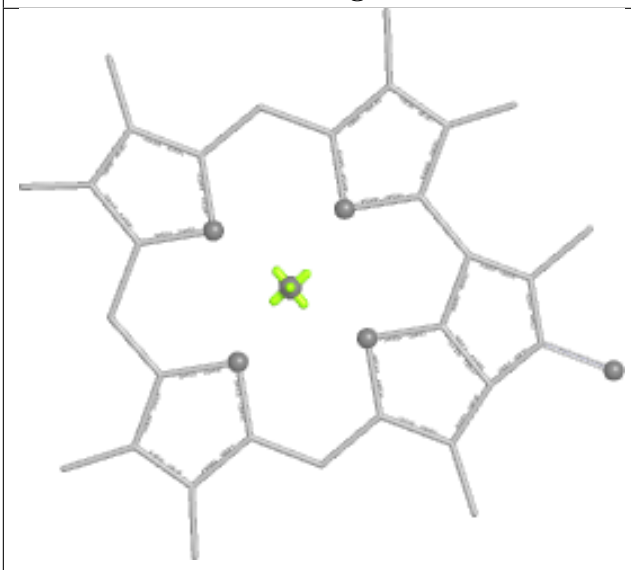
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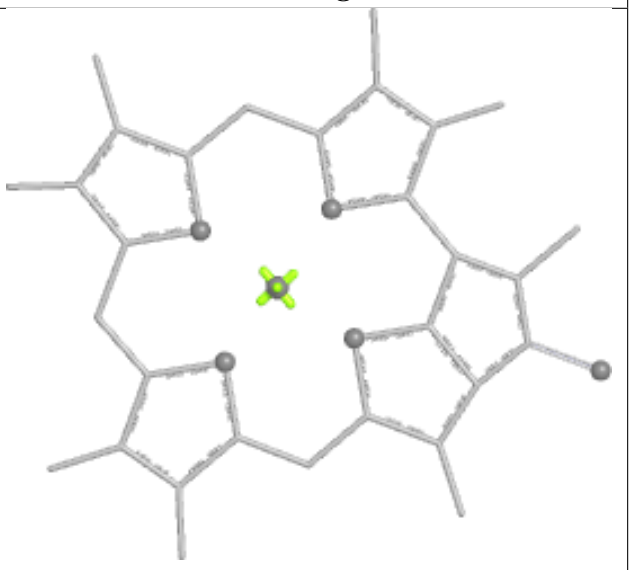
Bond lengths



Bond angles

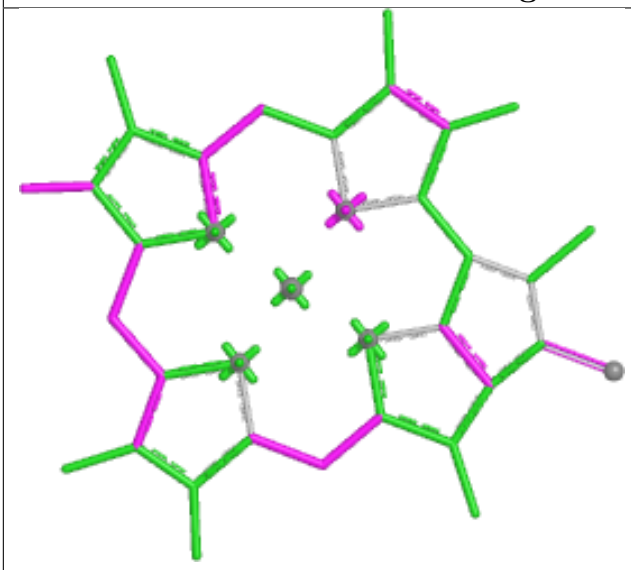


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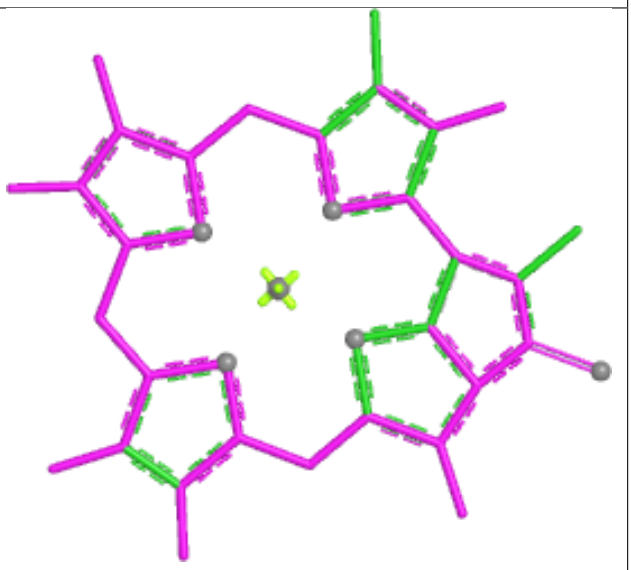


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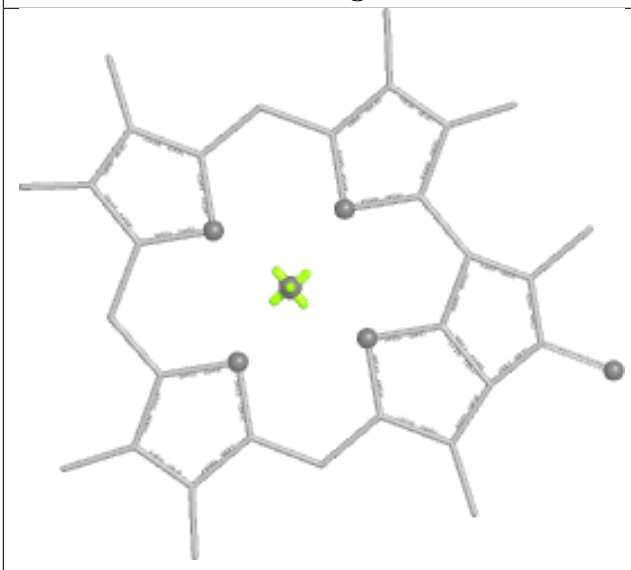
Ligand CLA 4 4012



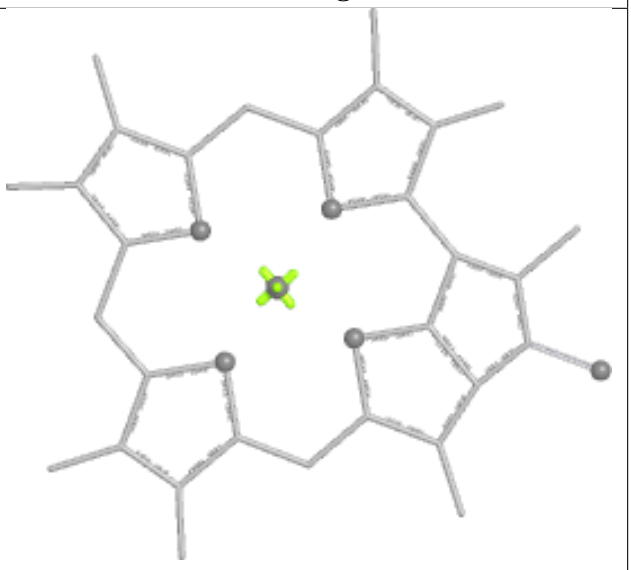
Bond lengths



Bond angles

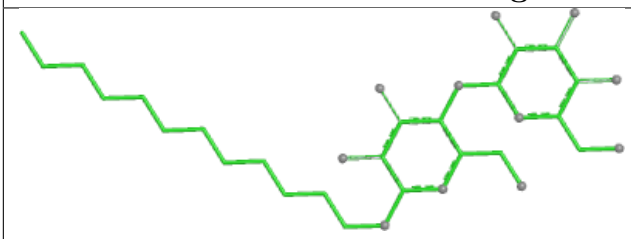


Torsions

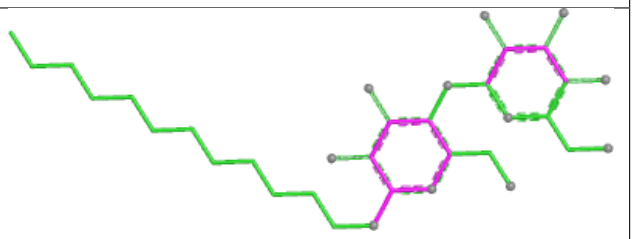


Rings

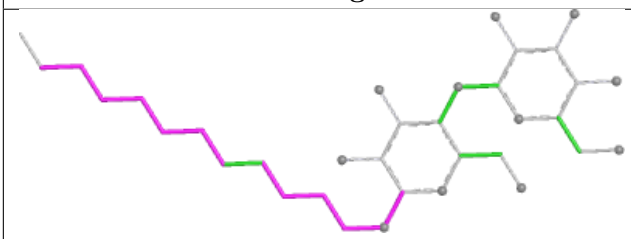
Ligand LMU A 7016



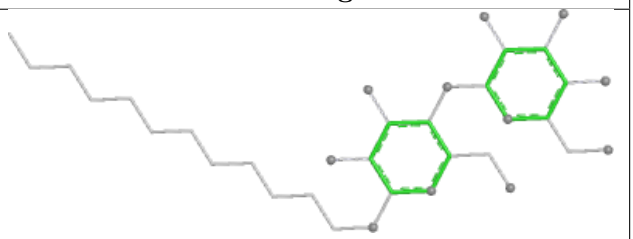
Bond lengths



Bond angles

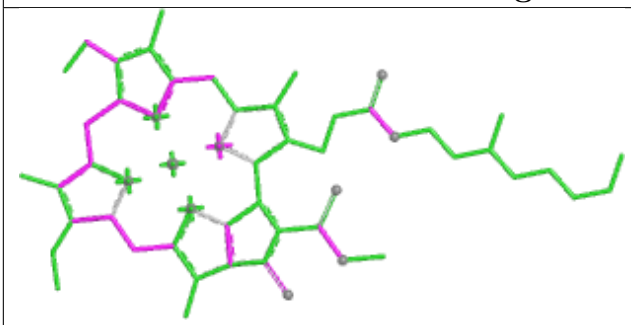


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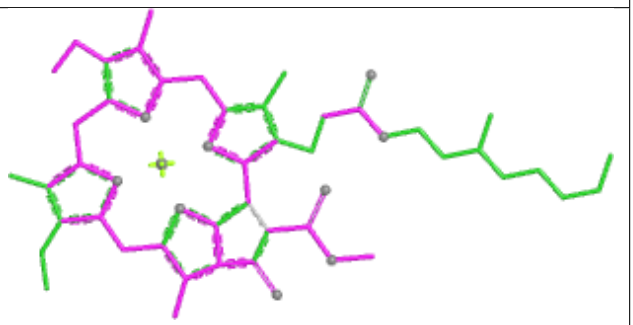


Rings

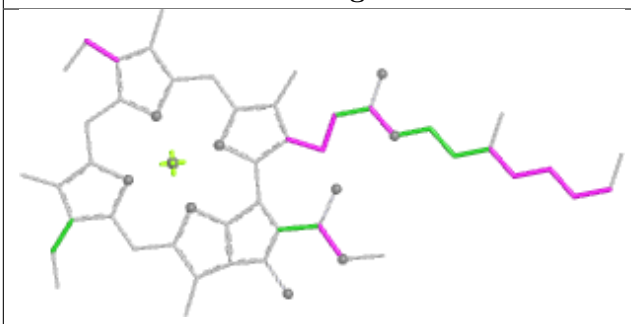
Ligand CLA A 1110



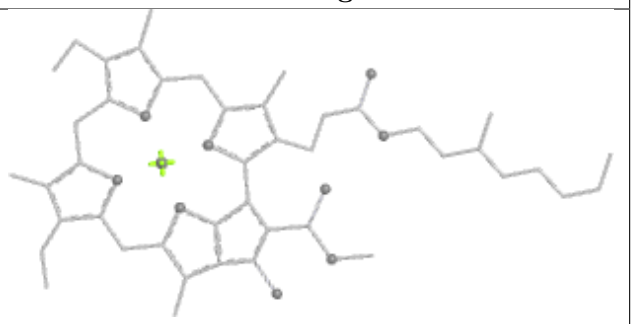
Bond lengths



Bond angles

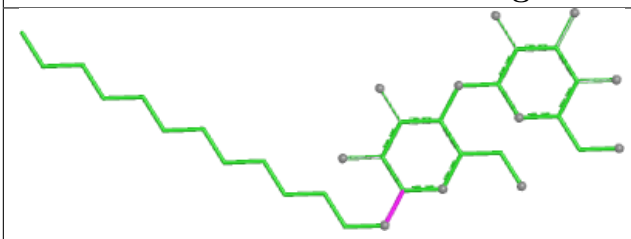


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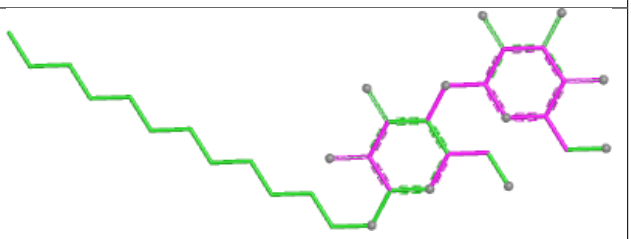


Rings

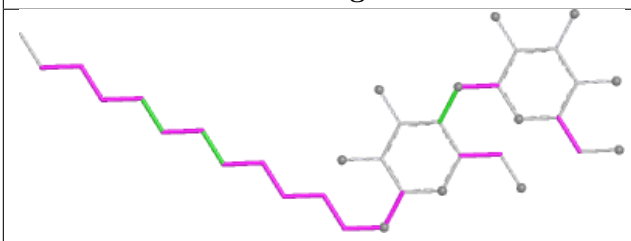
Ligand LMU E 7037



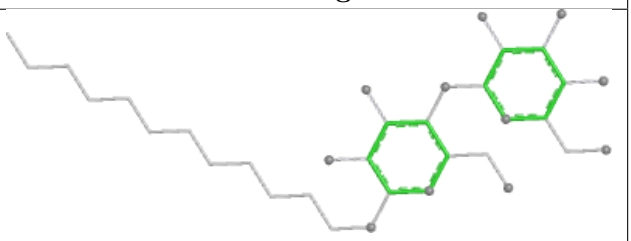
Bond lengths



Bond angles

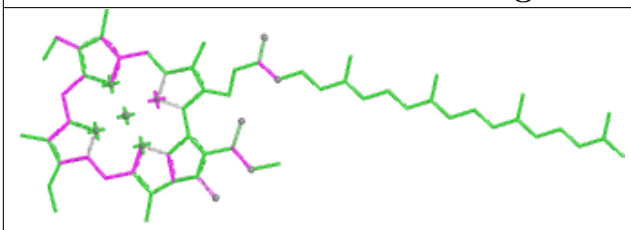


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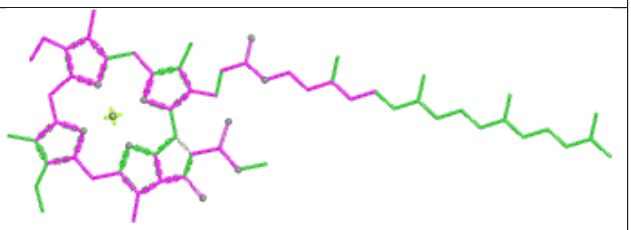


Rings

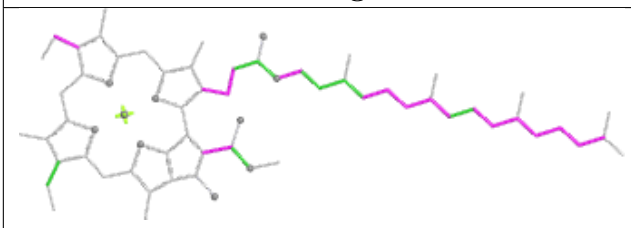
Ligand CLA A 1106



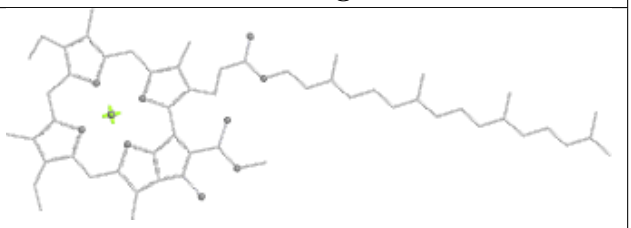
Bond lengths



Bond angles

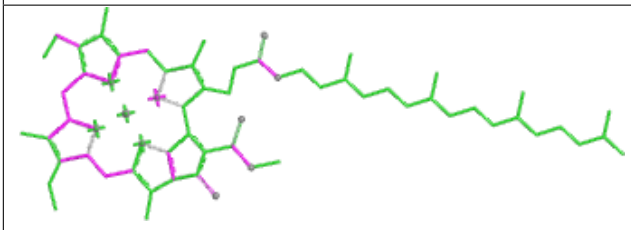


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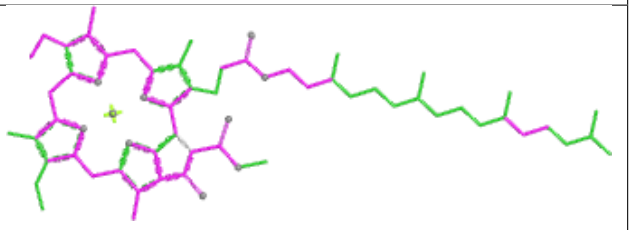


Rings

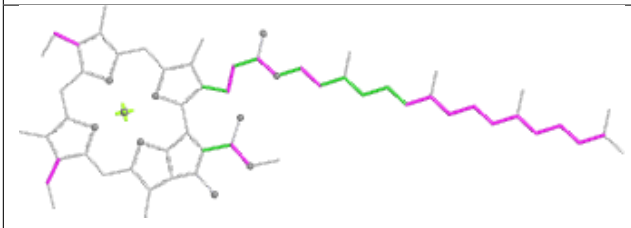
Ligand CLA A 9013



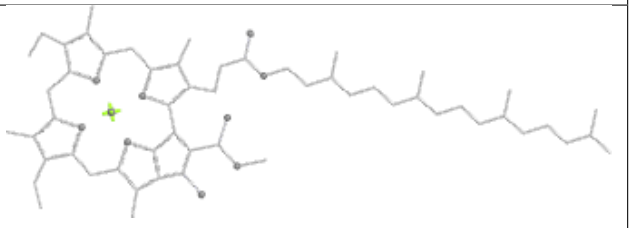
Bond lengths



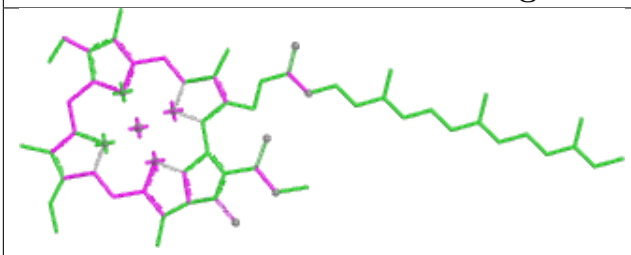
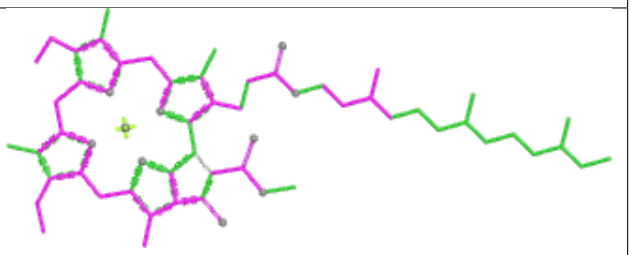
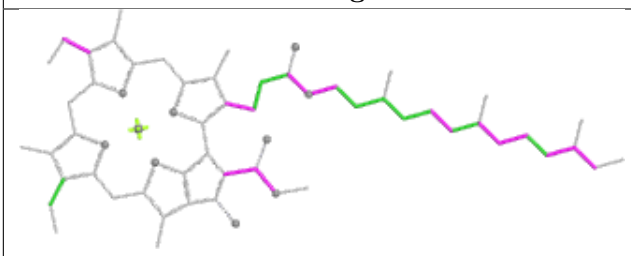
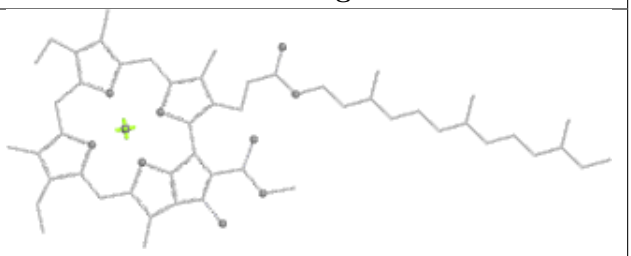
Bond angles

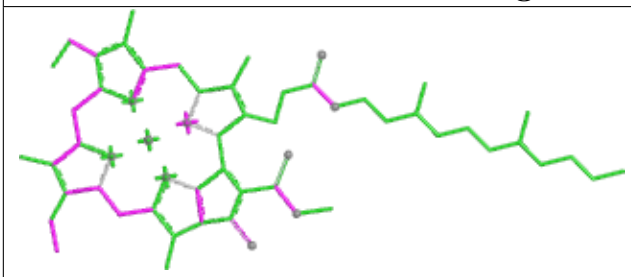
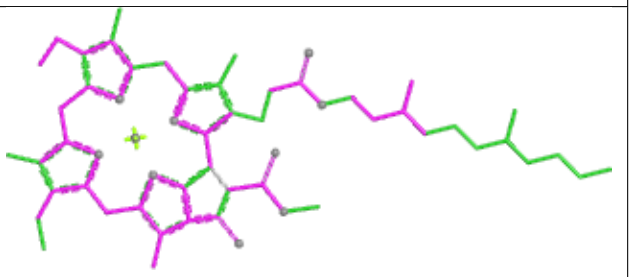
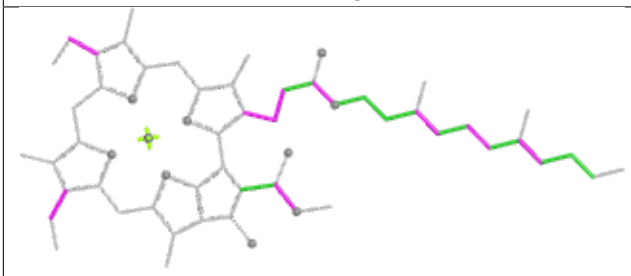
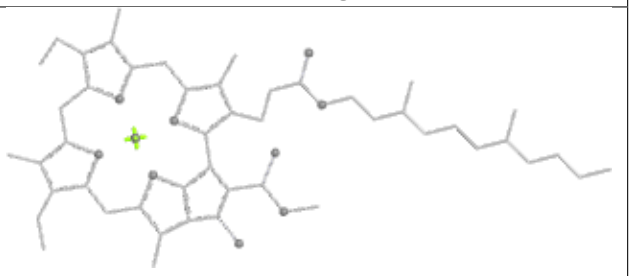


Torsions

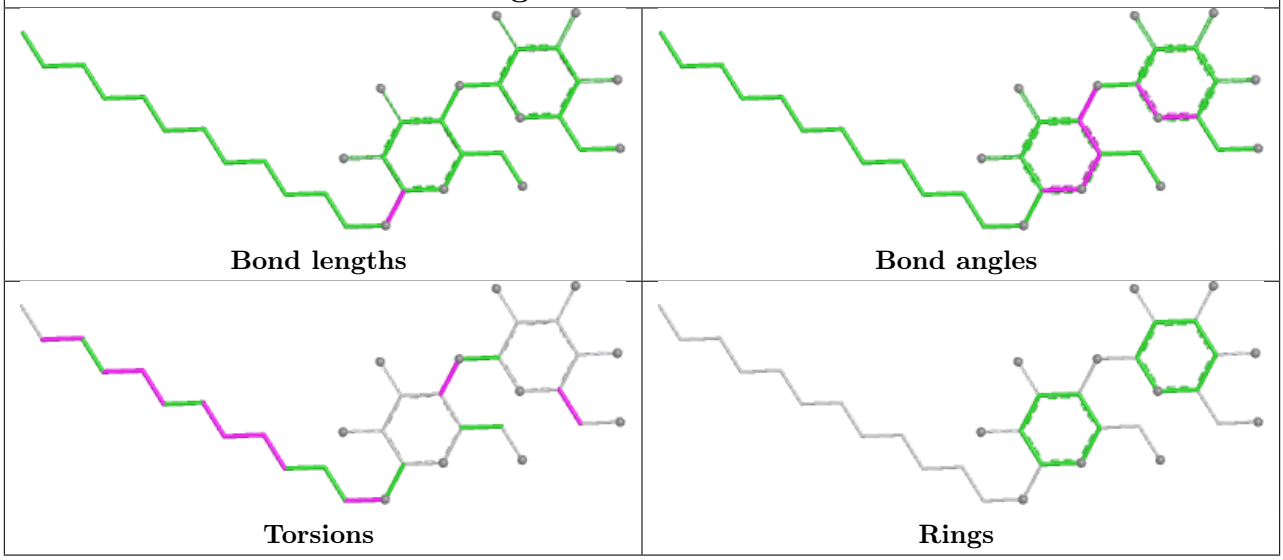


Rings

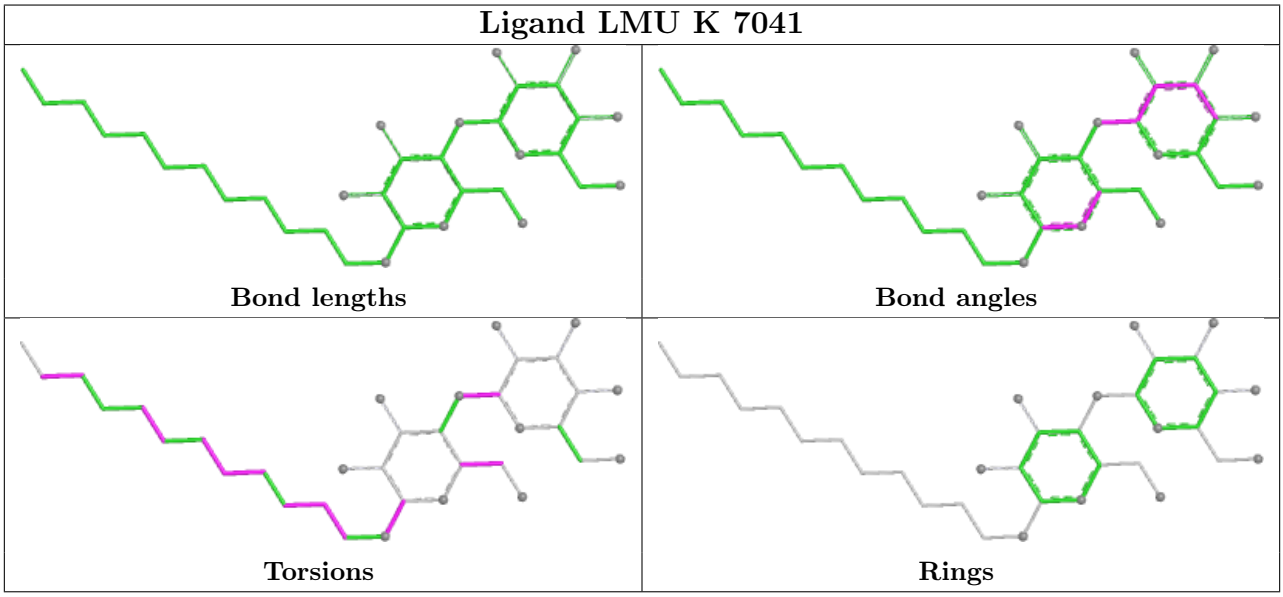
Ligand CLA 2 2014	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1222	
 Bond lengths	 Bond angles
 Torsions	 Rings

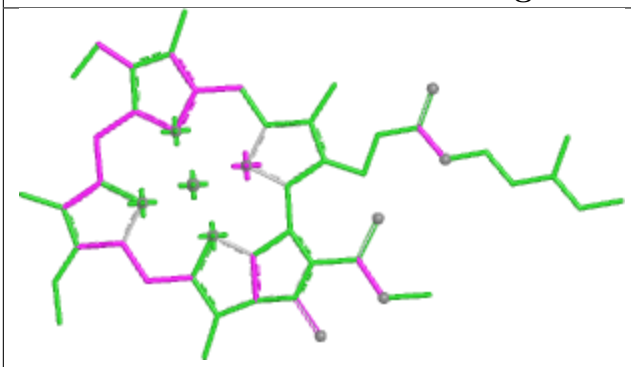
Ligand LMU K 7047



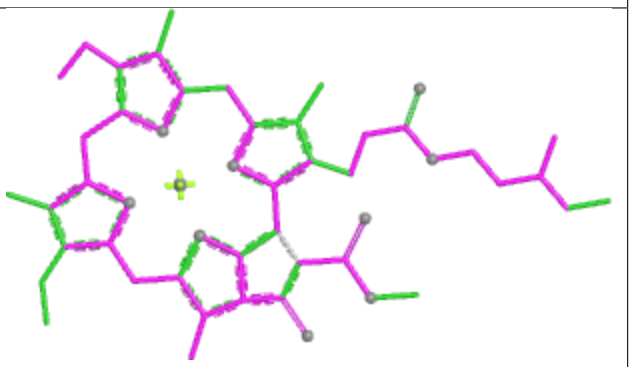
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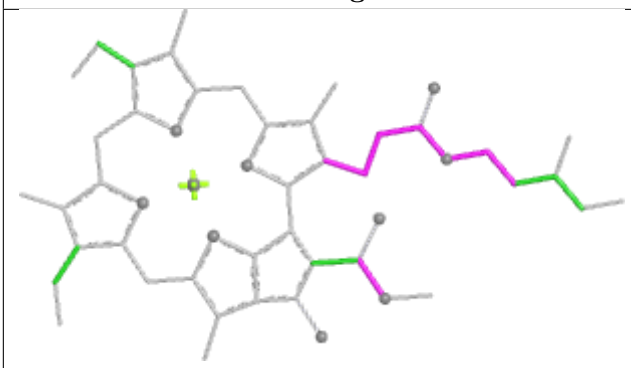
Ligand CLA A 1139



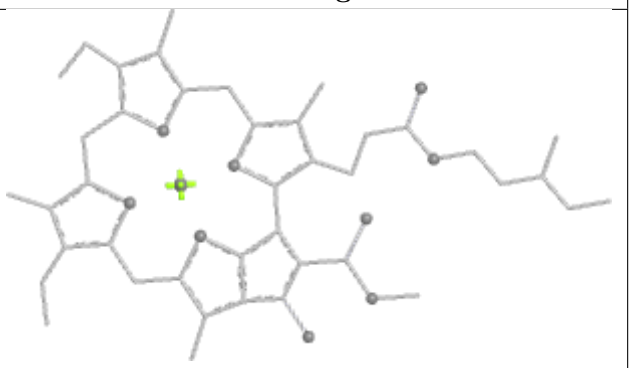
Bond lengths



Bond angles

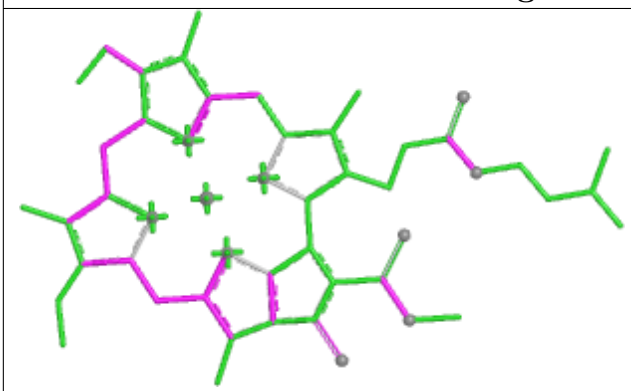


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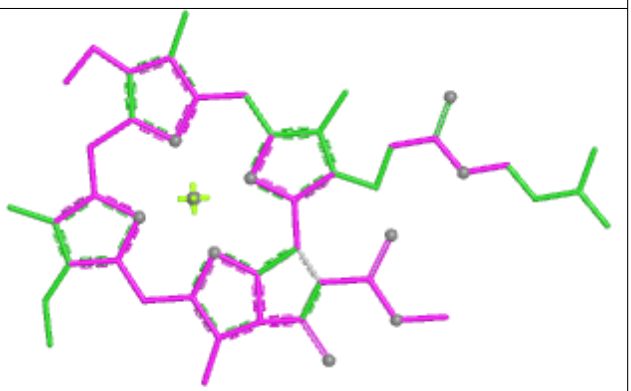


Rings

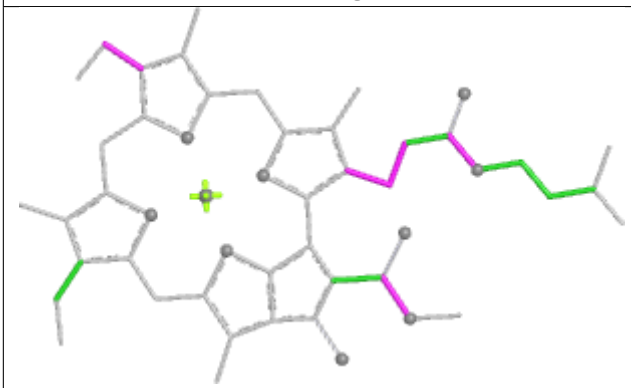
Ligand CLA L 1501



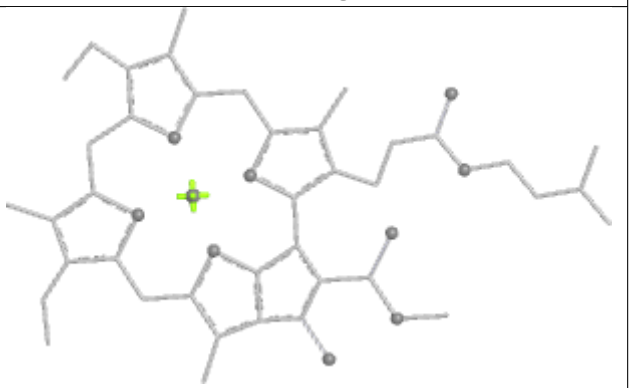
Bond lengths



Bond angles

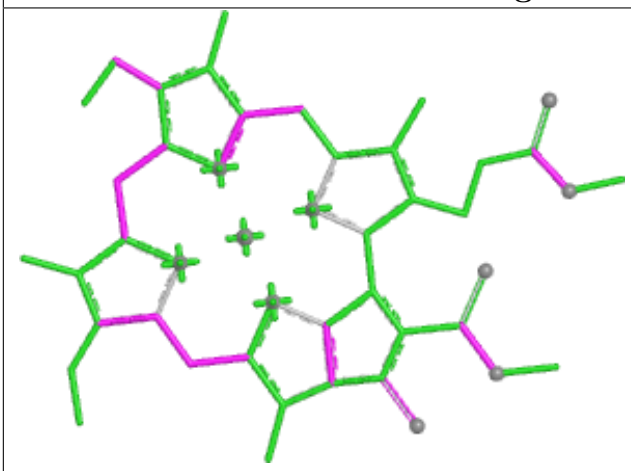


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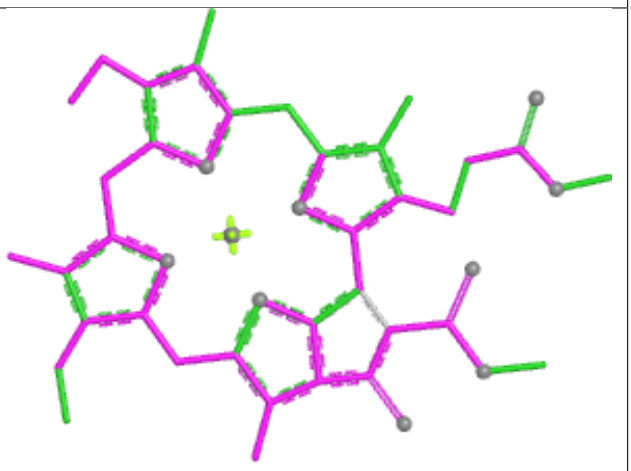


Rings

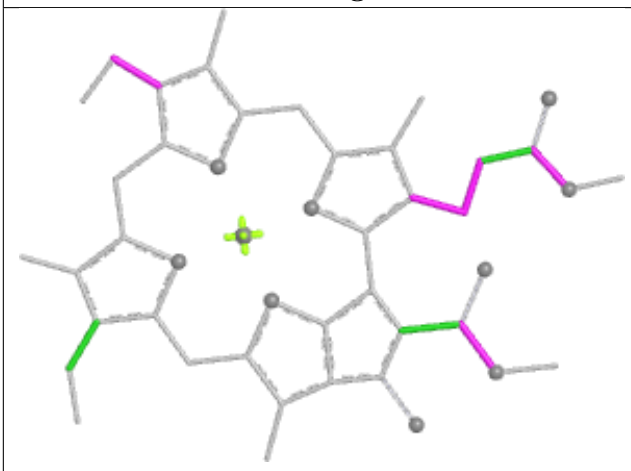
Ligand CLA A 1105



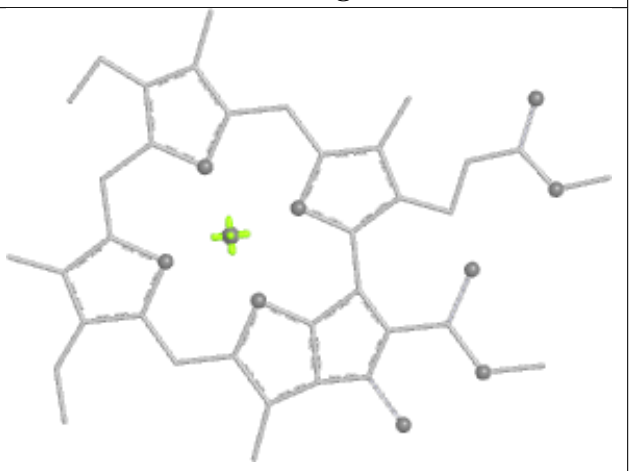
Bond lengths



Bond angles

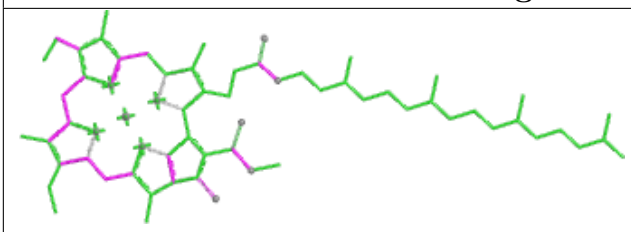


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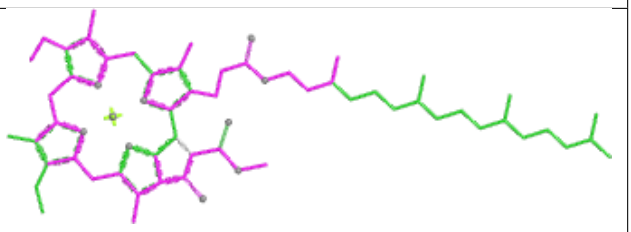


Rings

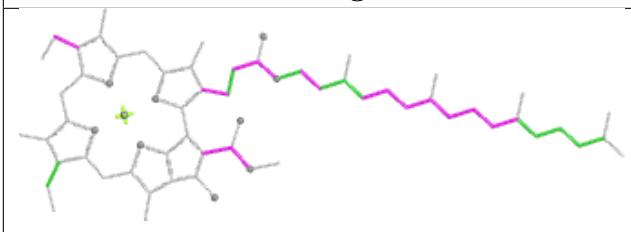
Ligand CLA R 1150



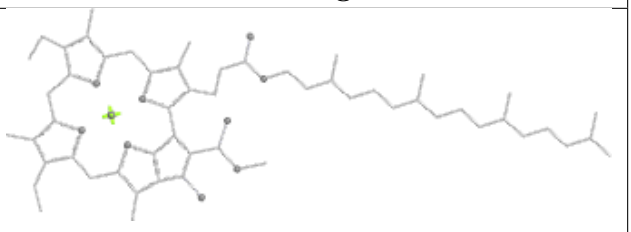
Bond lengths



Bond angles

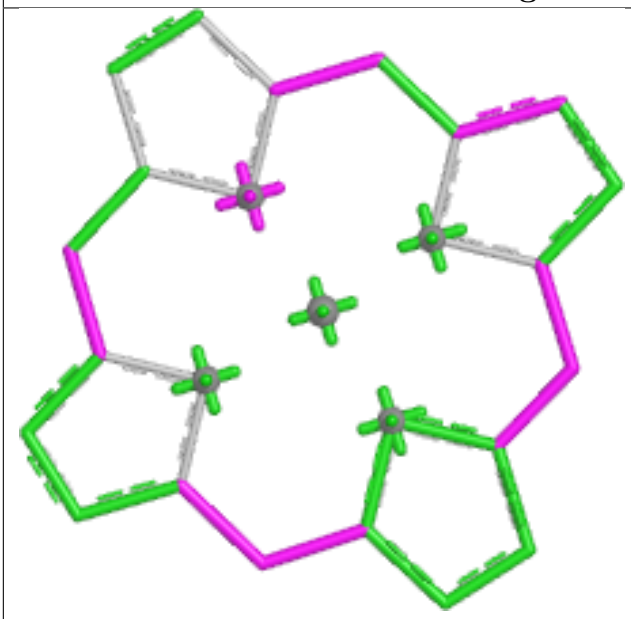


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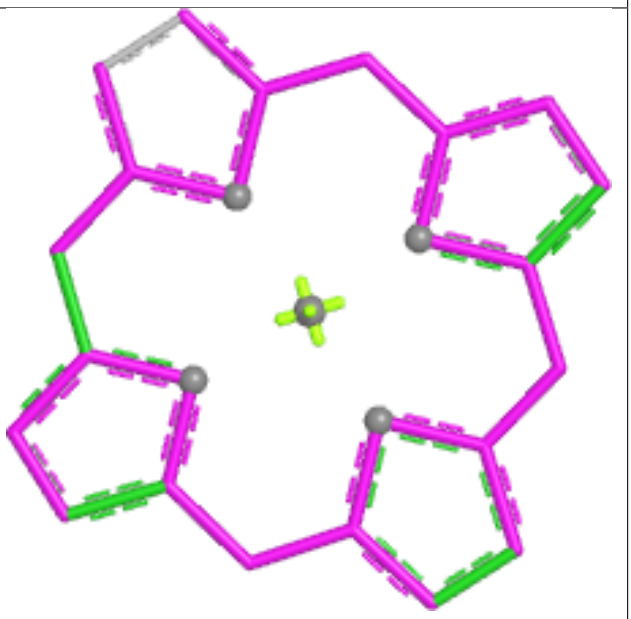


Rings

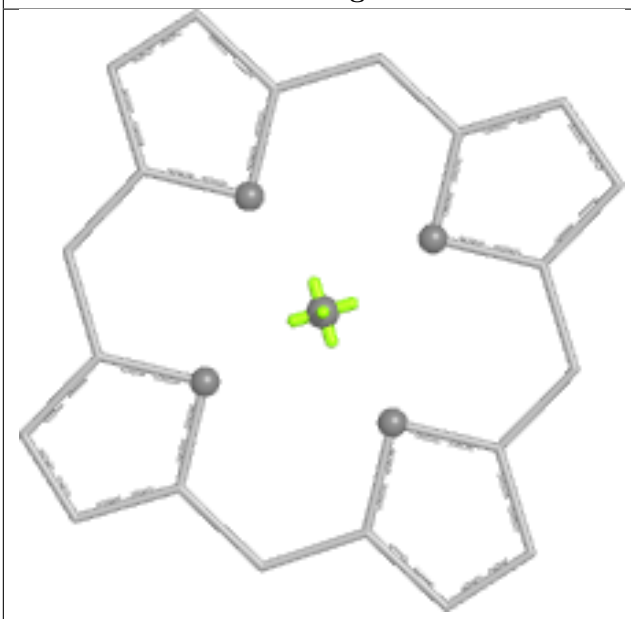
Ligand CLA 2 2008



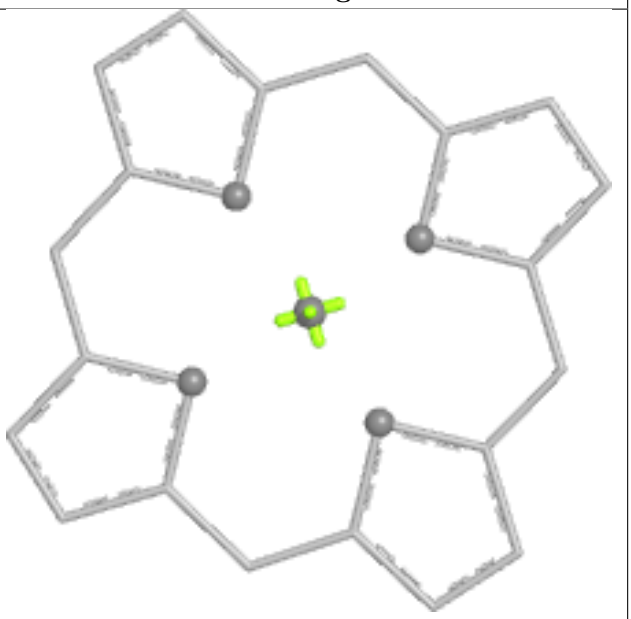
Bond lengths



Bond angles

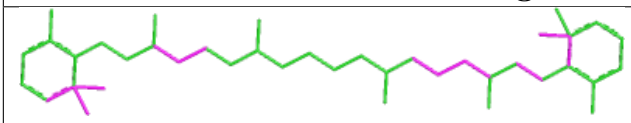


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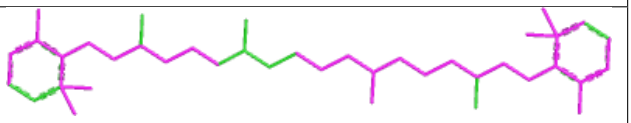


Rings

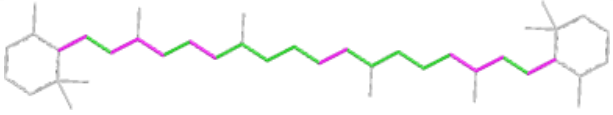
Ligand BCR L 6019



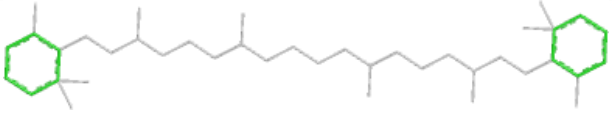
Bond lengths



Bond angles

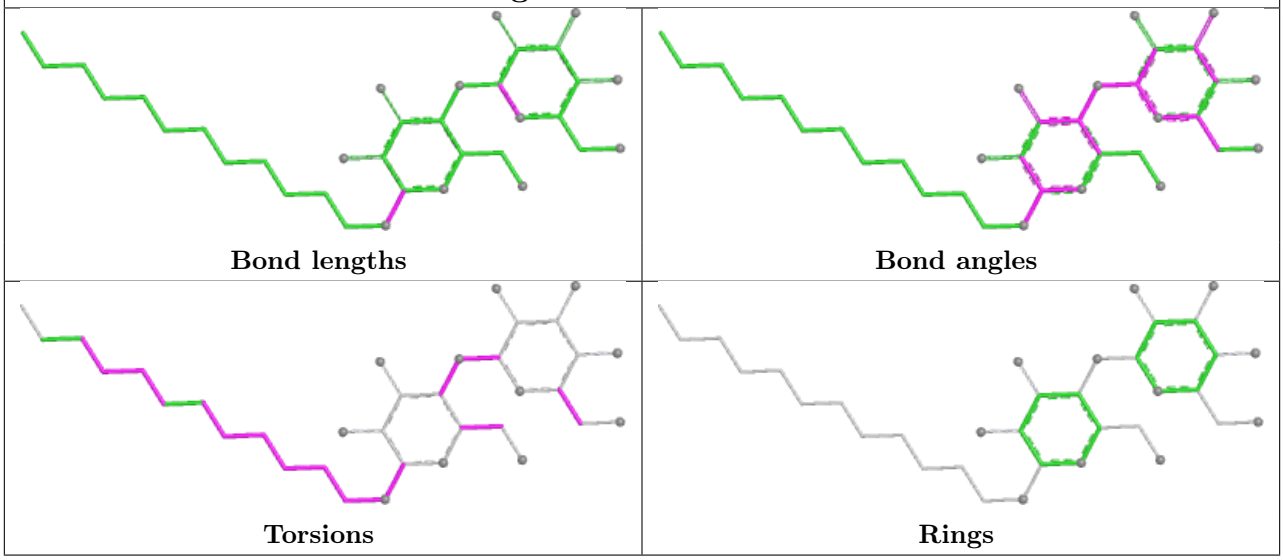


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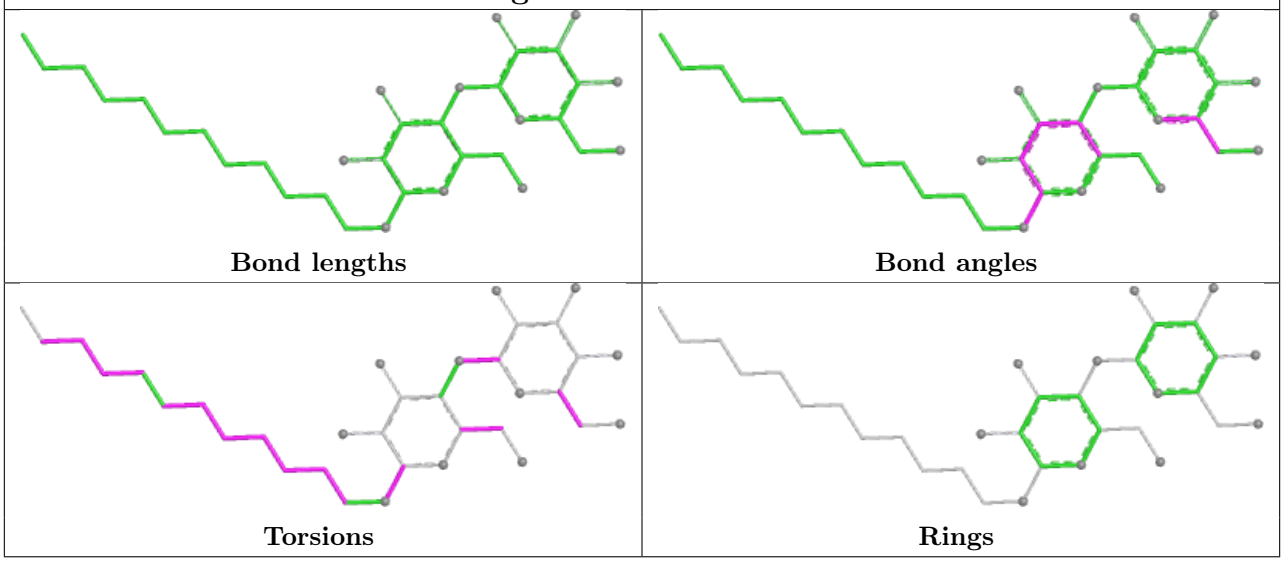


Rings

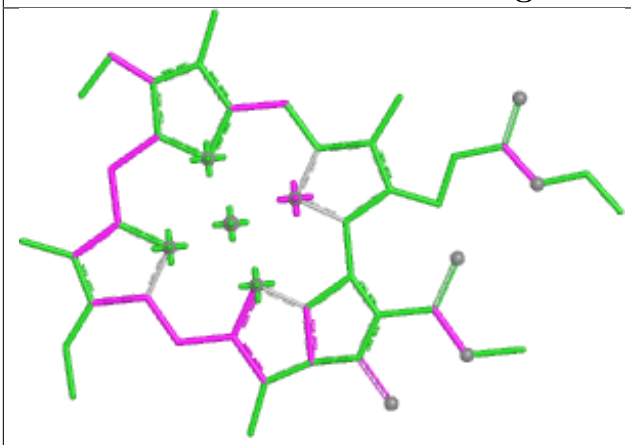
Ligand LMU H 7011



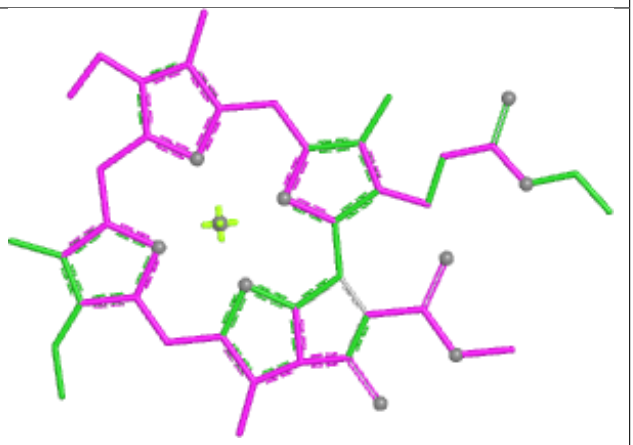
Ligand LMU A 7023



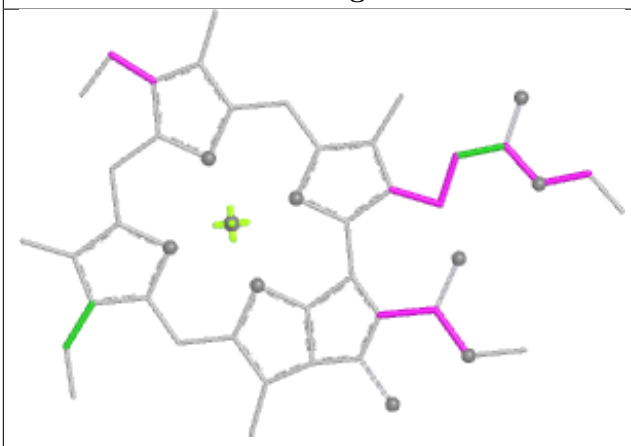
Ligand CLA B 1236



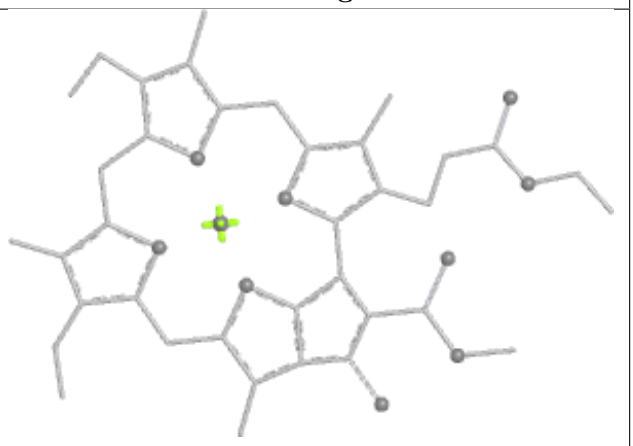
Bond lengths



Bond angles

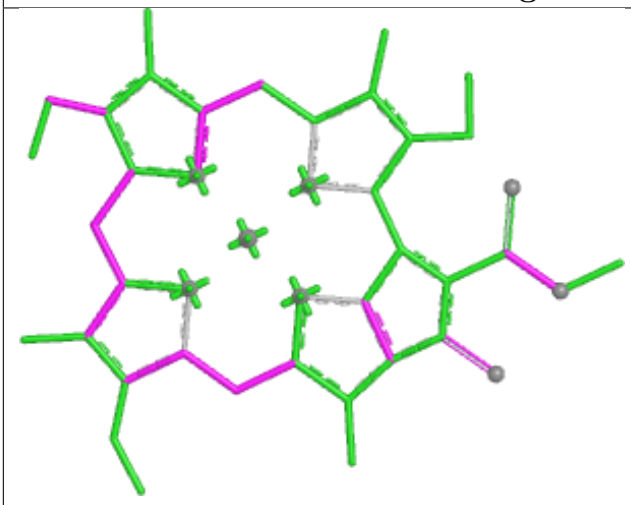


Torsions

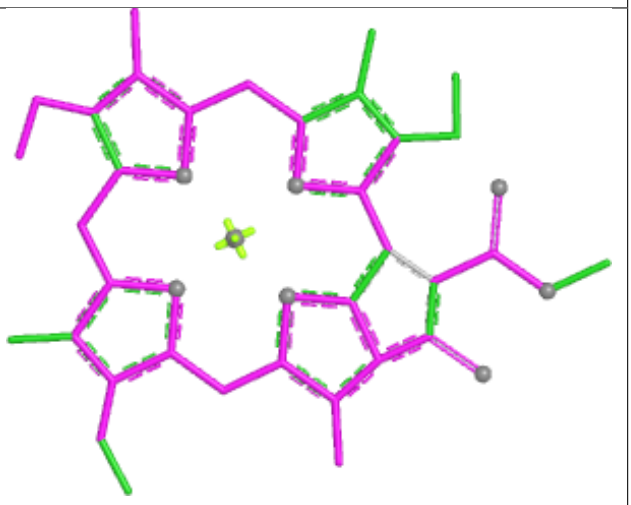


Rings

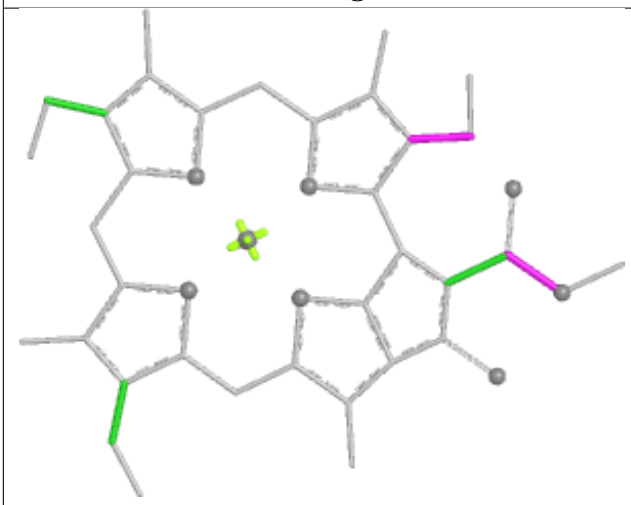
Ligand CLA 3 3007



Bond lengths



Bond angles

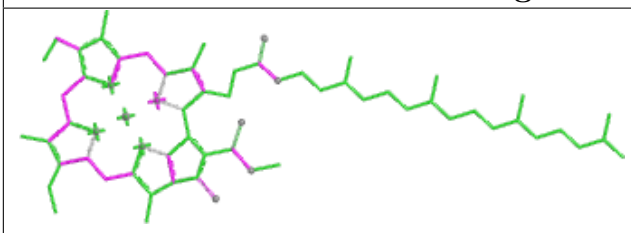


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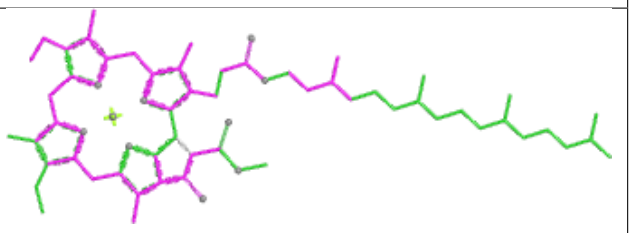


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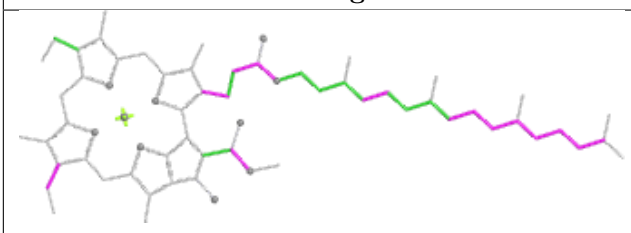
Ligand CLA H 1145



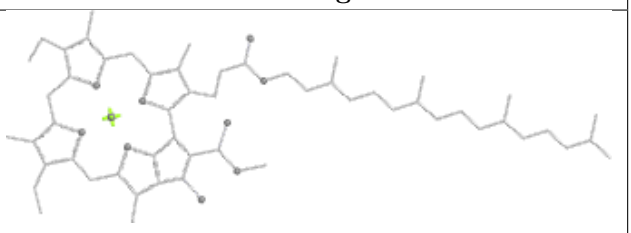
Bond lengths



Bond angles

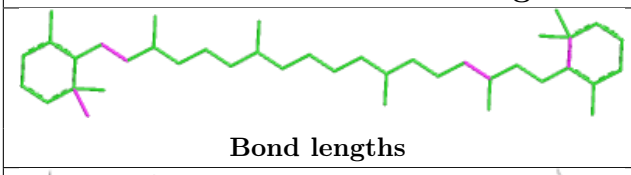


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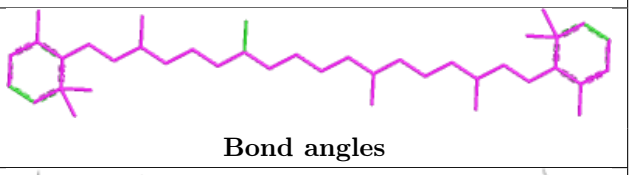


Rings

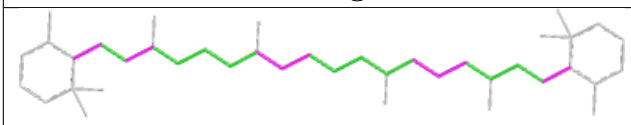
Ligand BCR A 6011



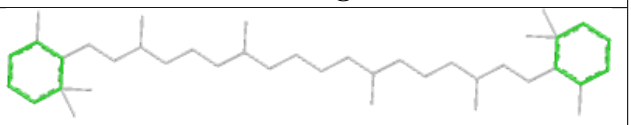
Bond lengths



Bond angles

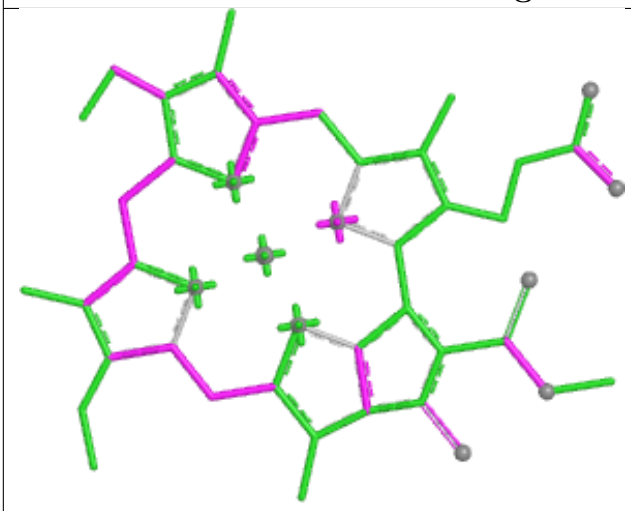


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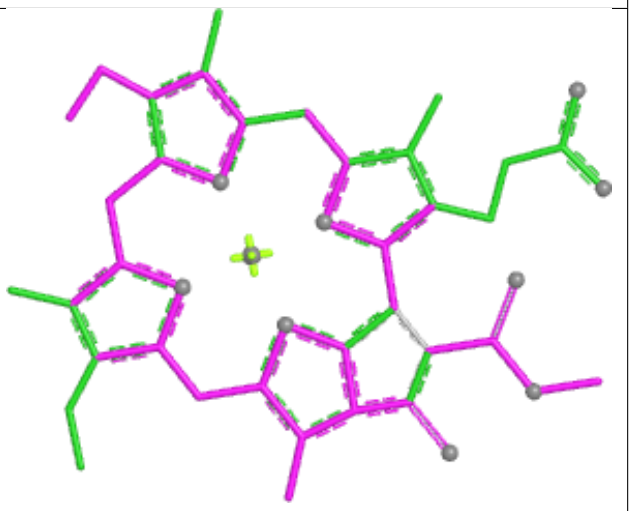


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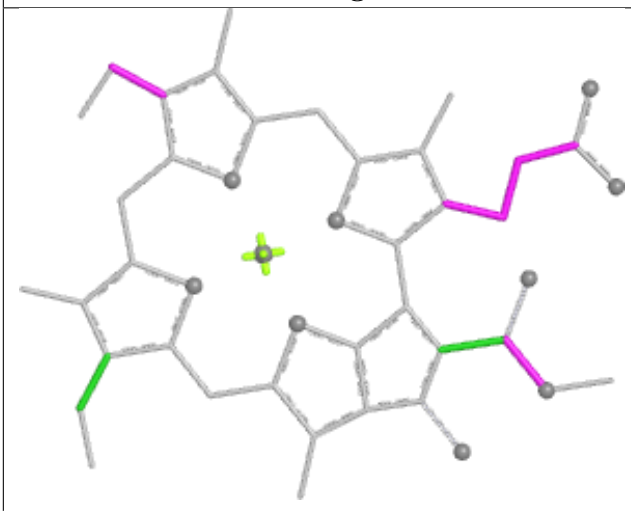
Ligand CLA A 1134



Bond lengths



Bond angles

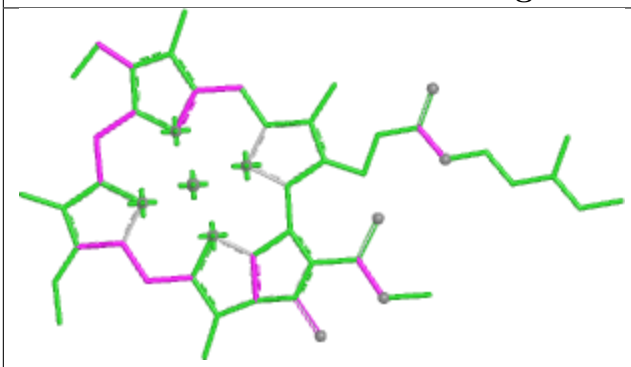


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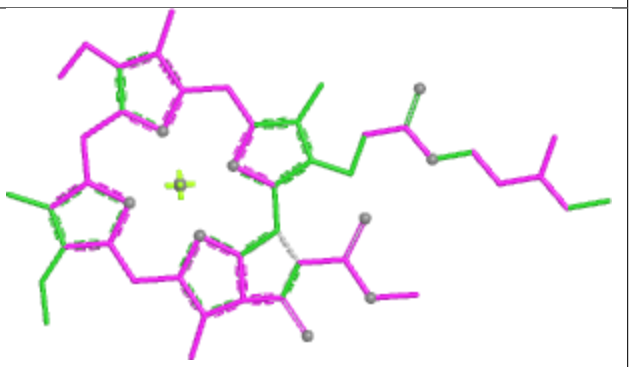


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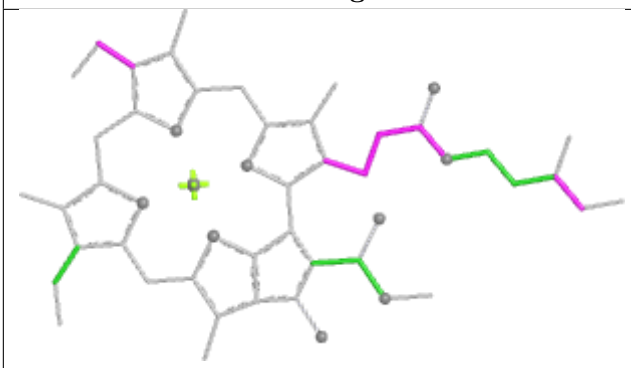
Ligand CLA B 1233



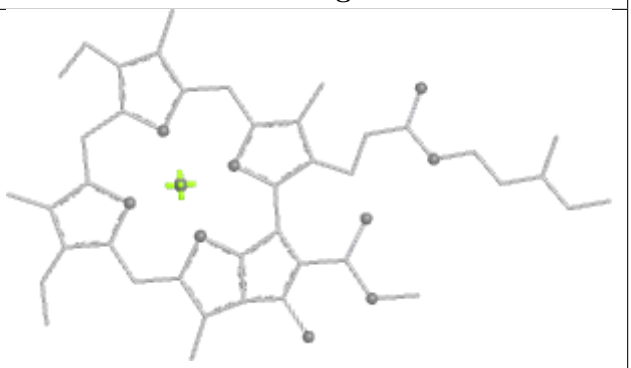
Bond lengths



Bond angles

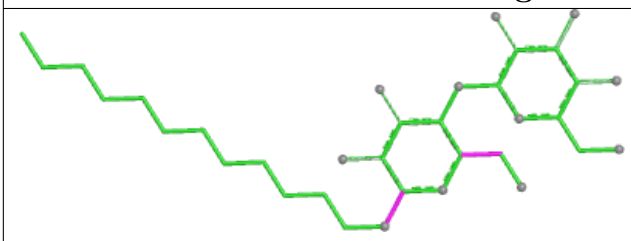


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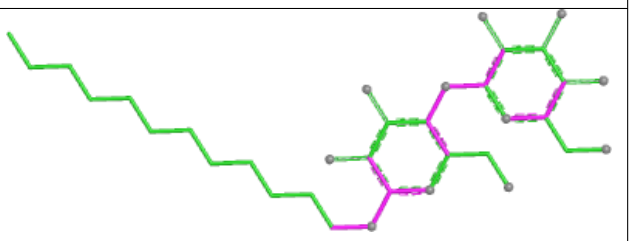


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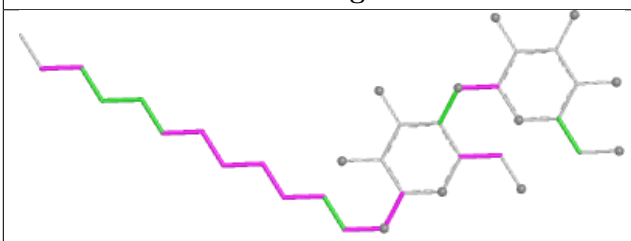
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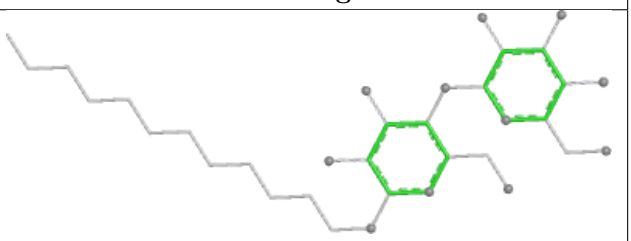
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Bond angles

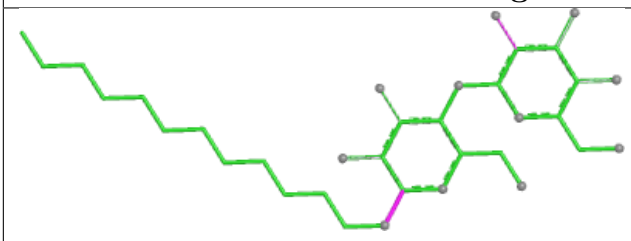


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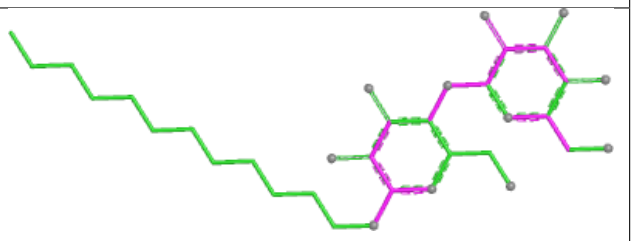


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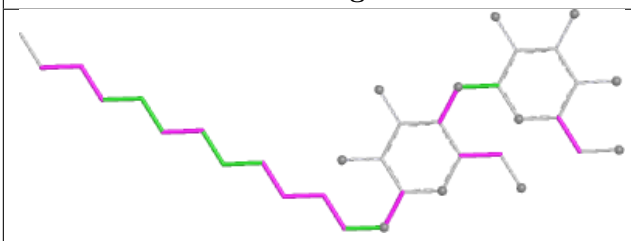
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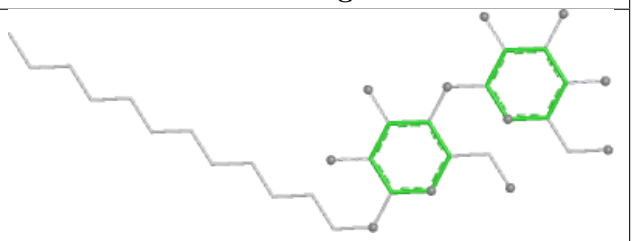
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Bond angles

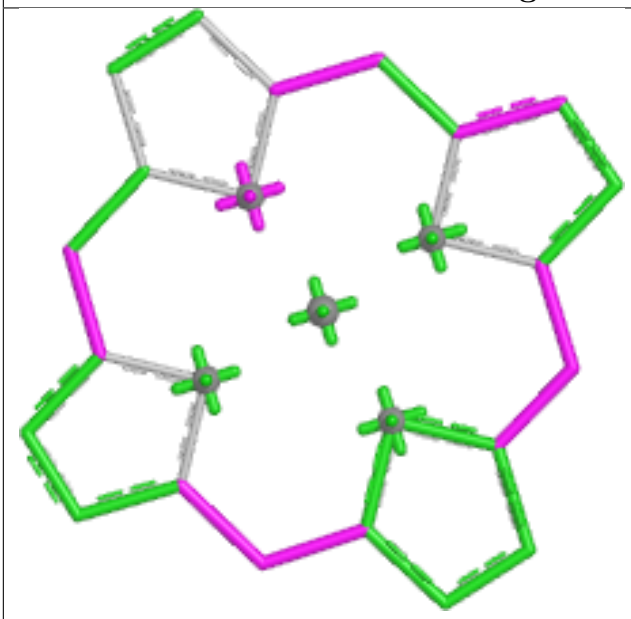


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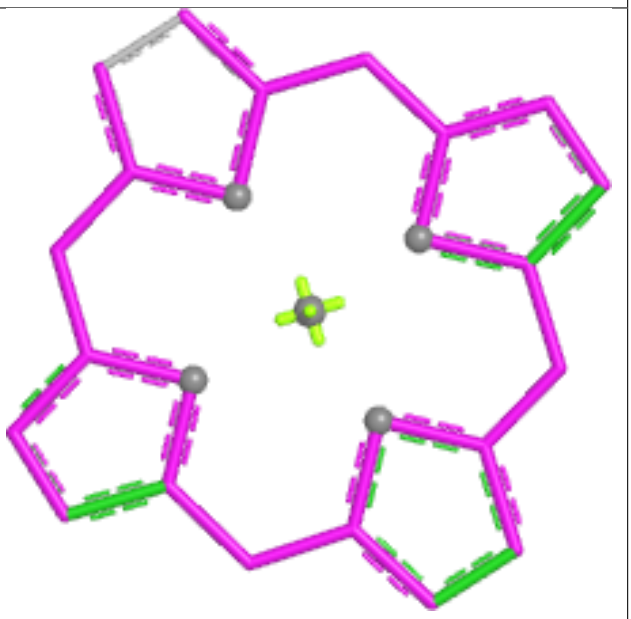


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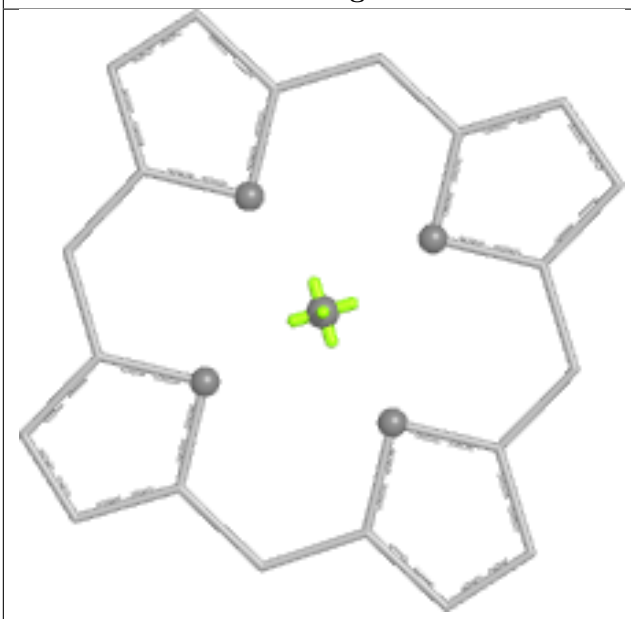
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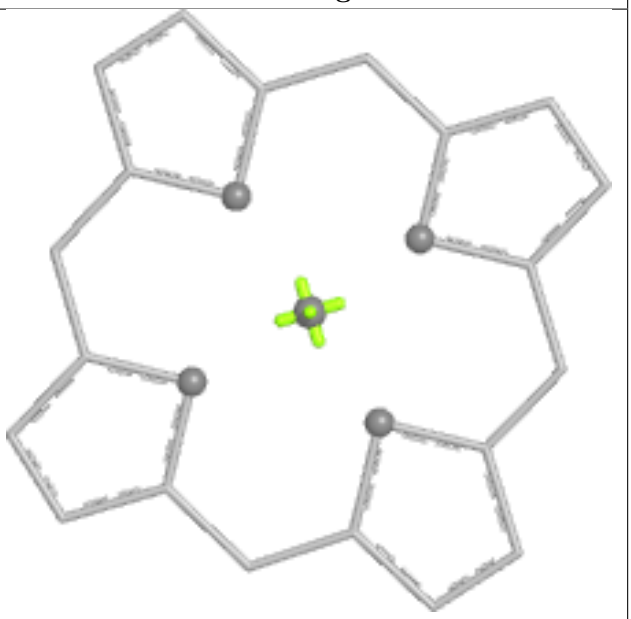
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Bond angles

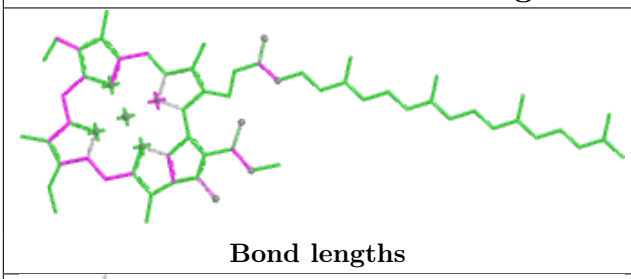


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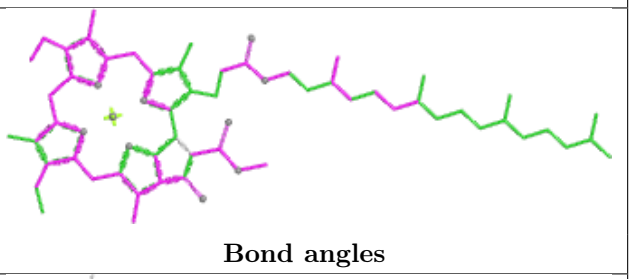


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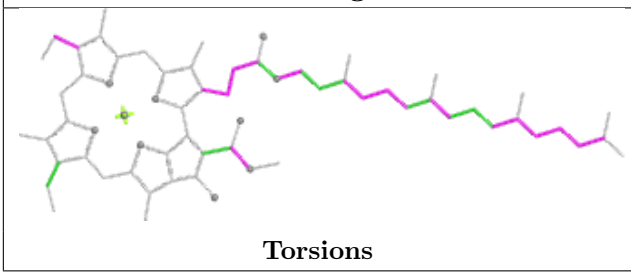
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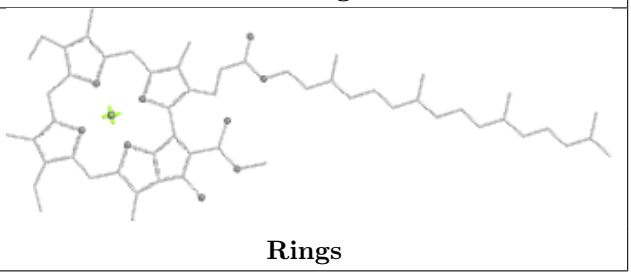
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Bond angles

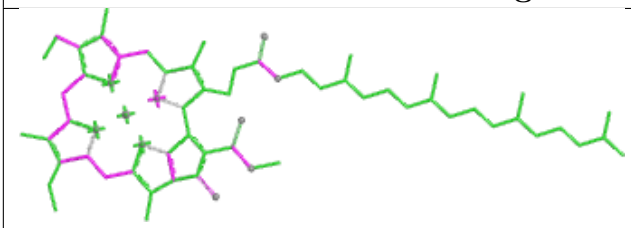


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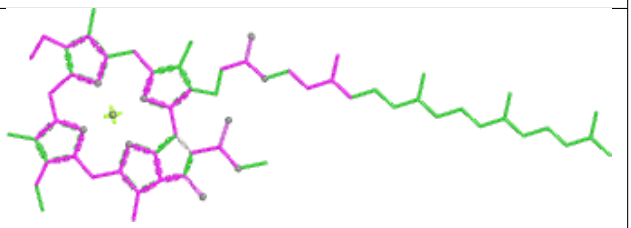


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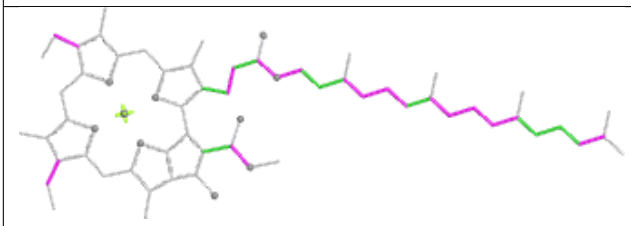
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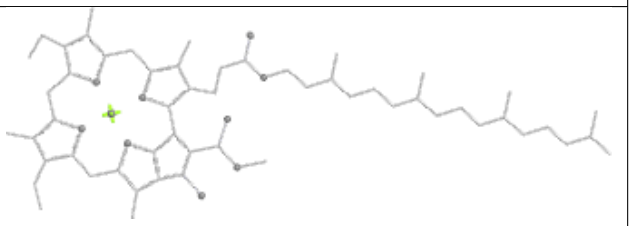
Bond lengths



Bond angles

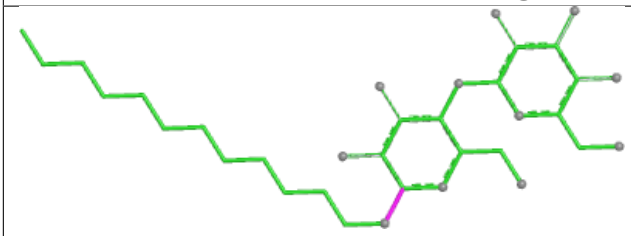


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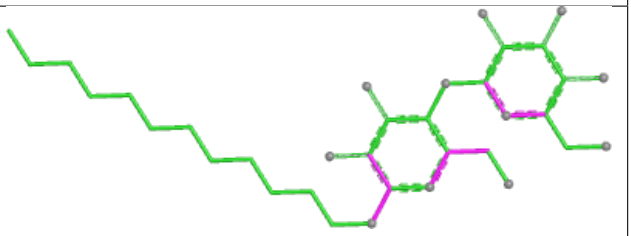


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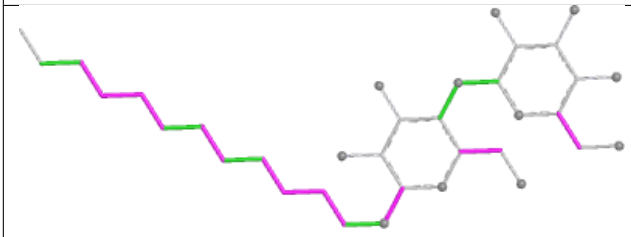
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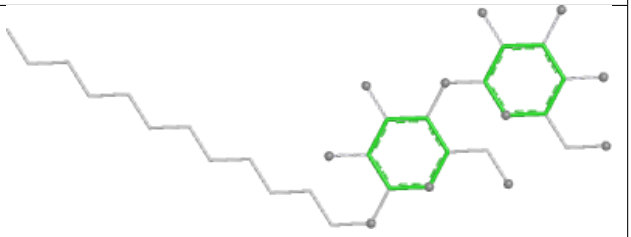
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Bond angles

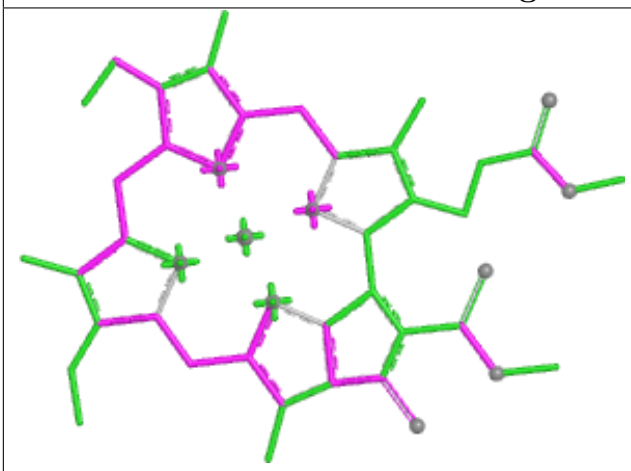


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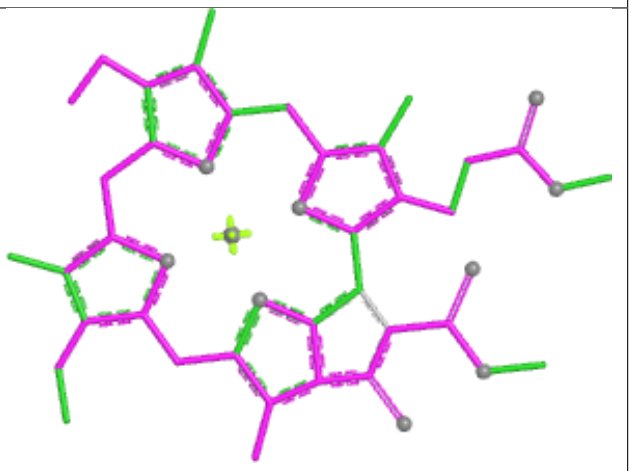


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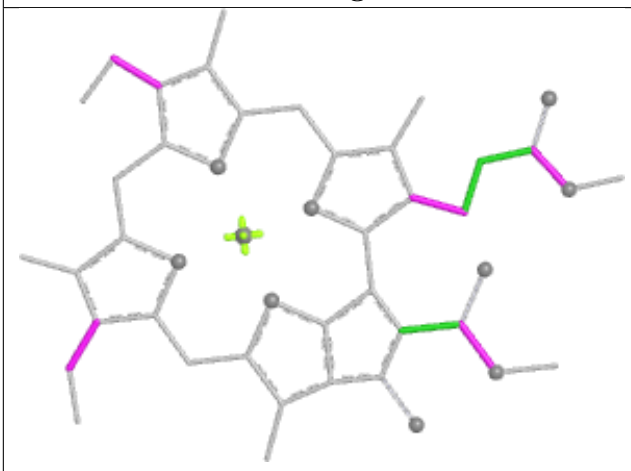
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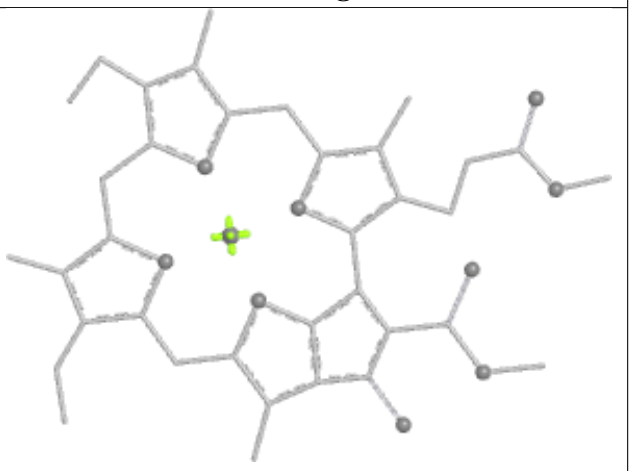
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Bond angles

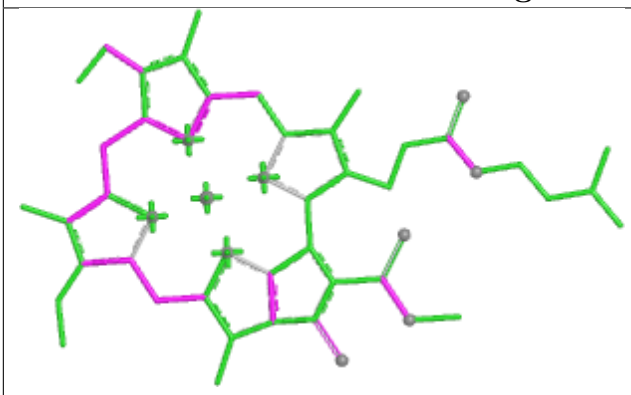


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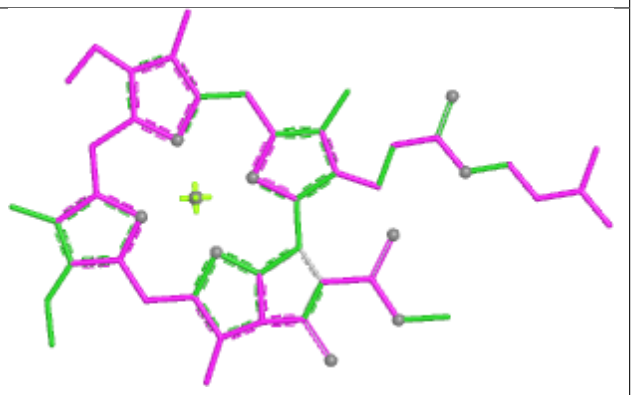


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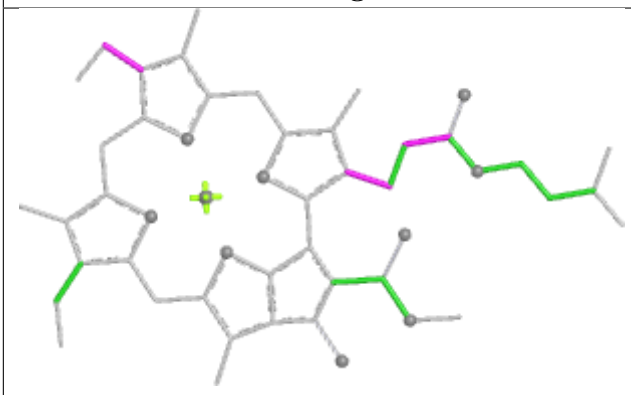
Ligand CLA A 1101



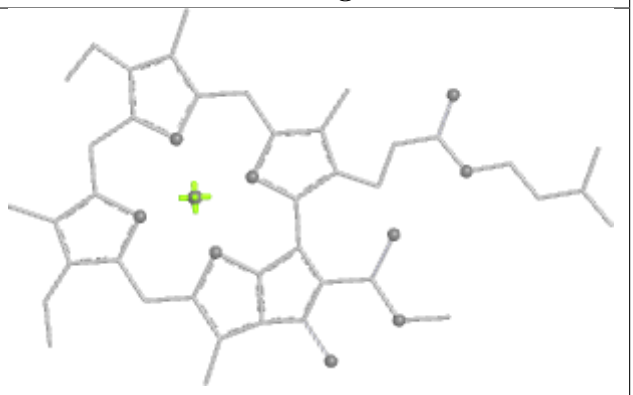
Bond lengths



Bond angles

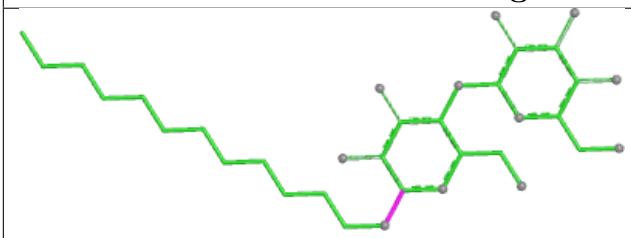


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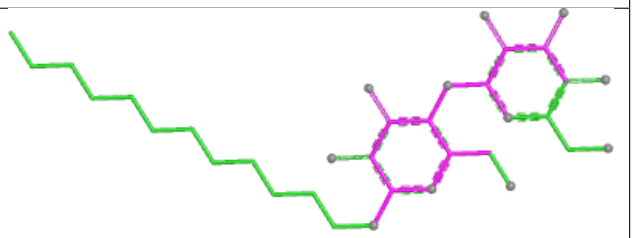


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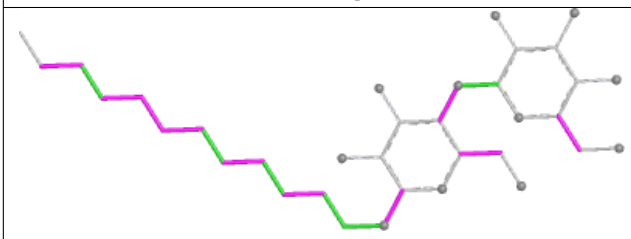
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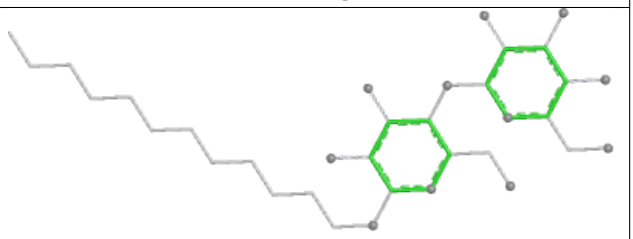
Bond lengths



Bond angles

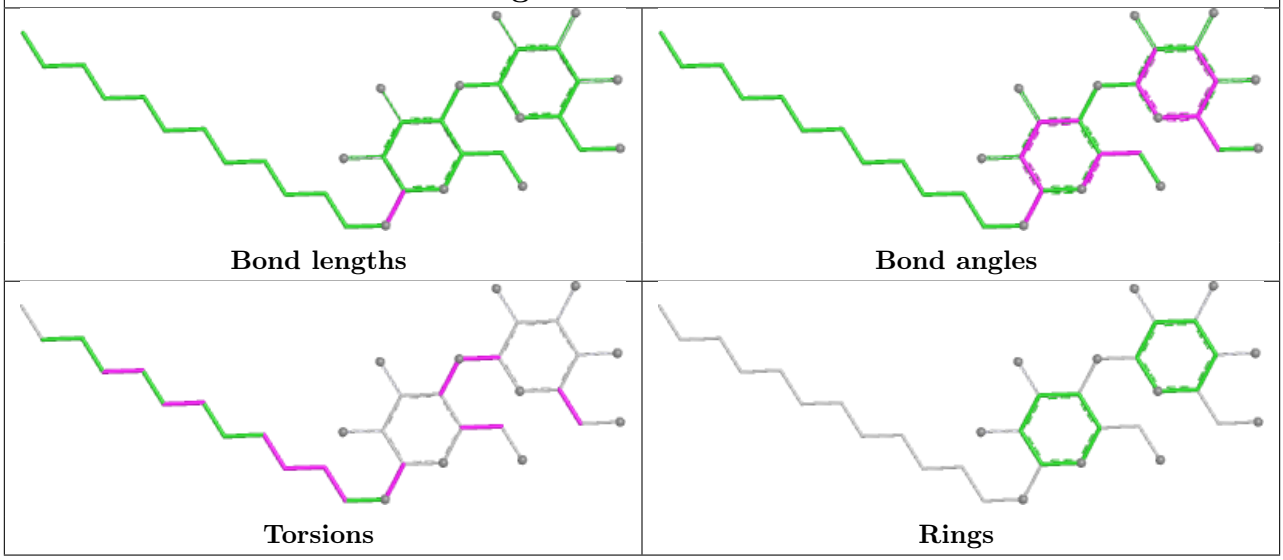


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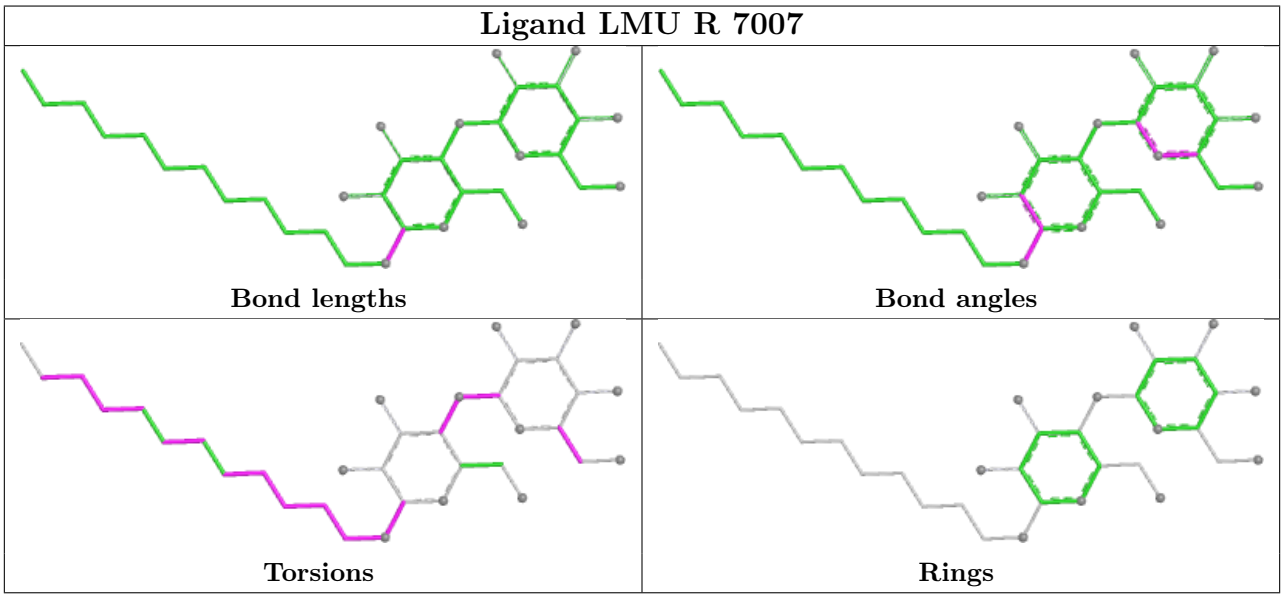


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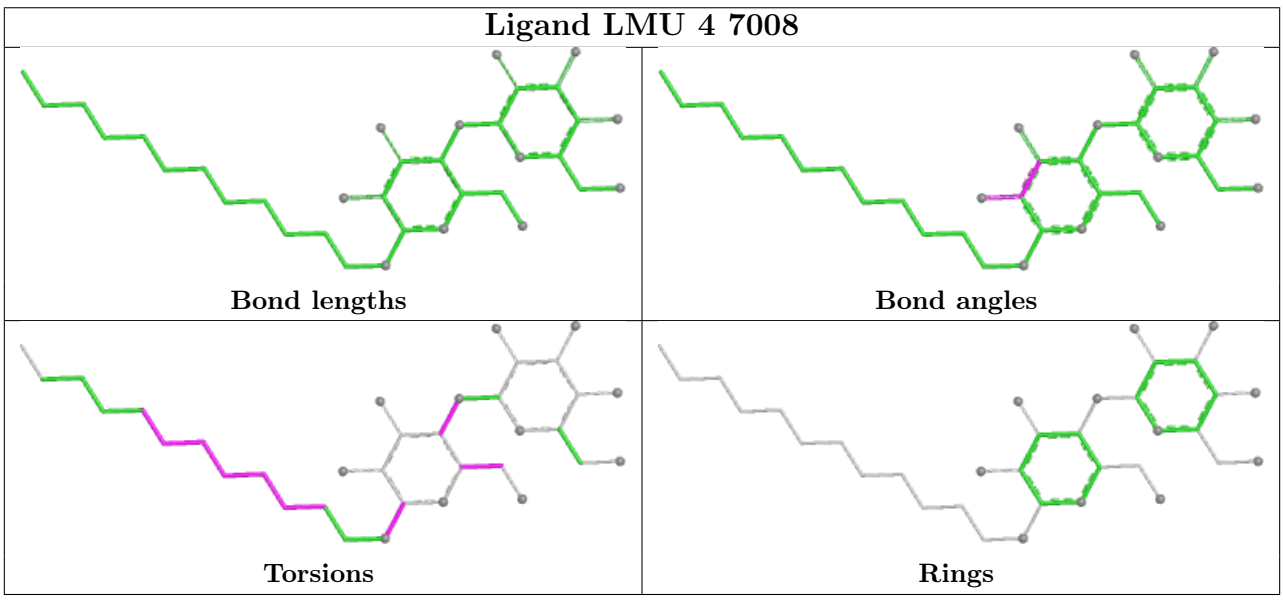
Ligand LMU R 7024



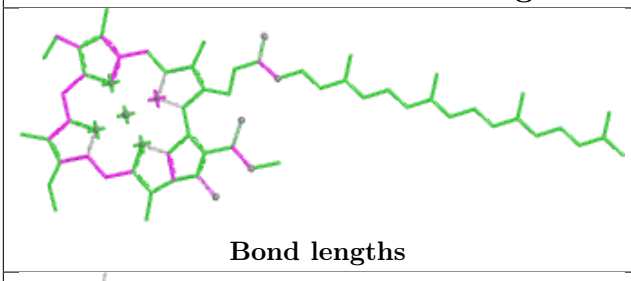
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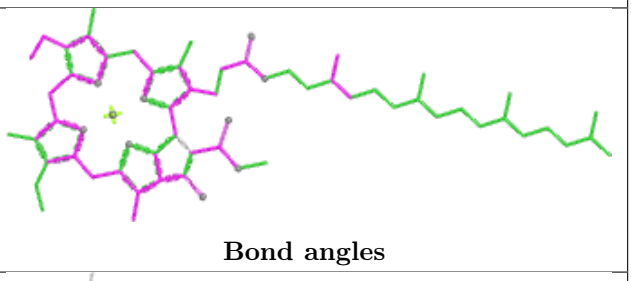
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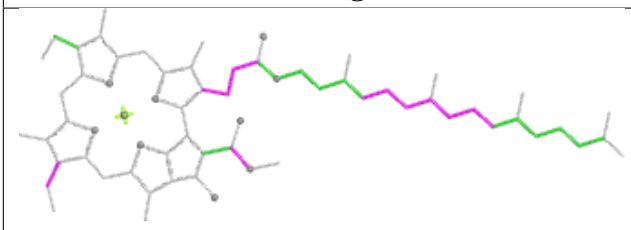
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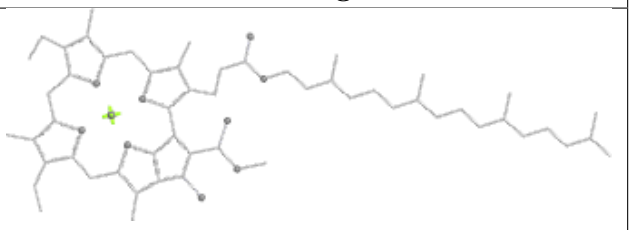
Bond lengths



Bond angles

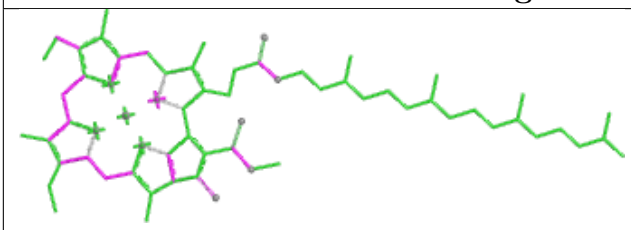


Torsions

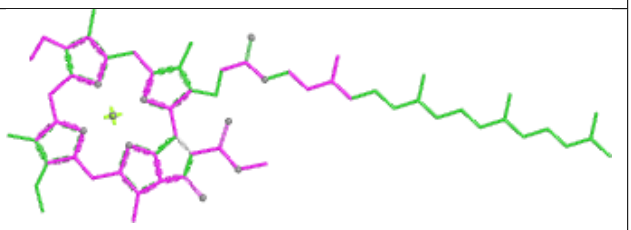


Rings

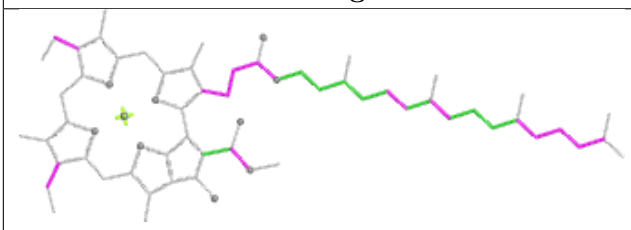
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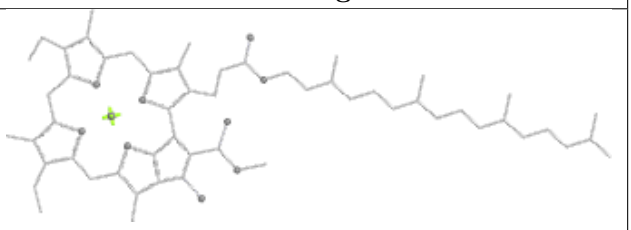
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Bond angles

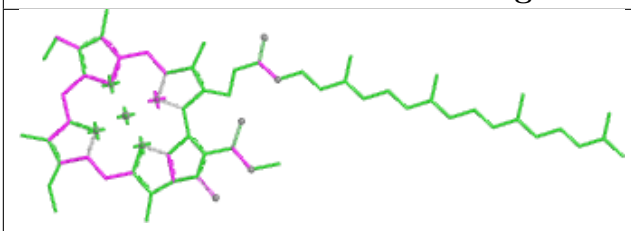


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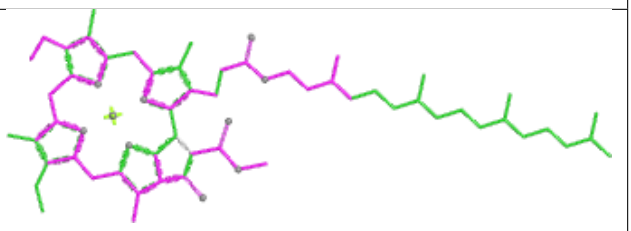


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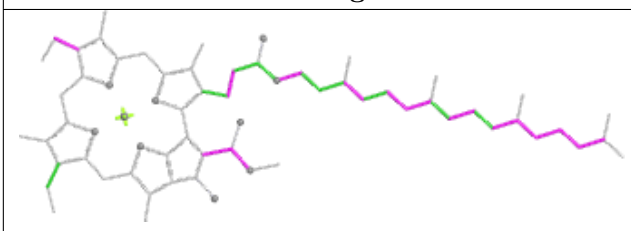
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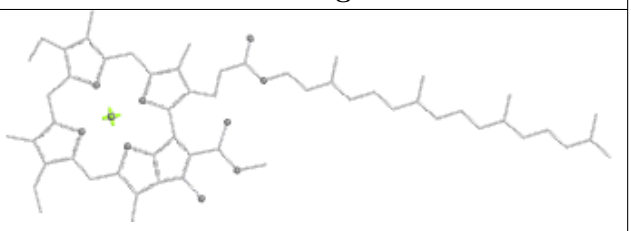
Bond lengths



Bond angles

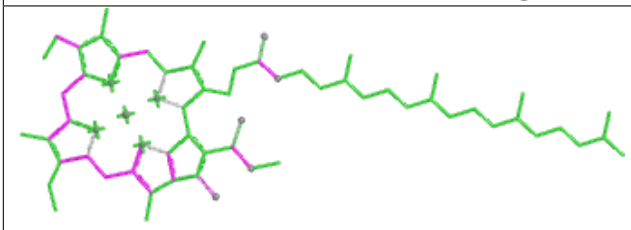


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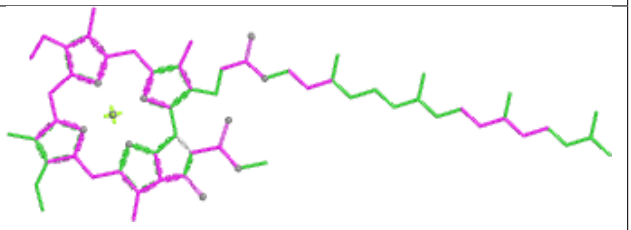


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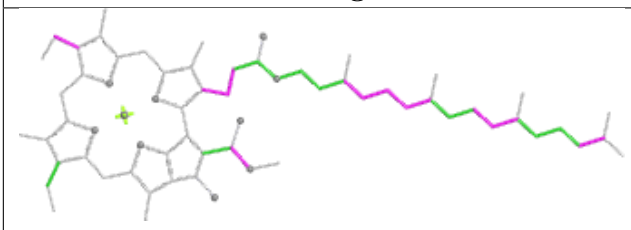
Ligand CLA B 1225



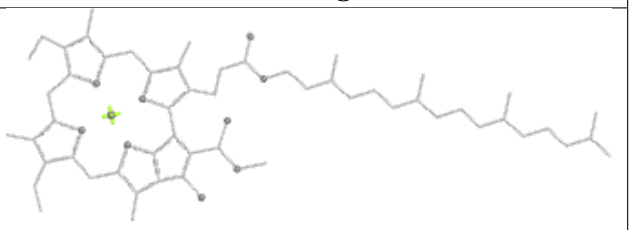
Bond lengths



Bond angles

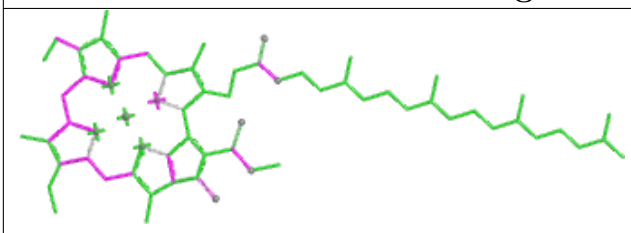


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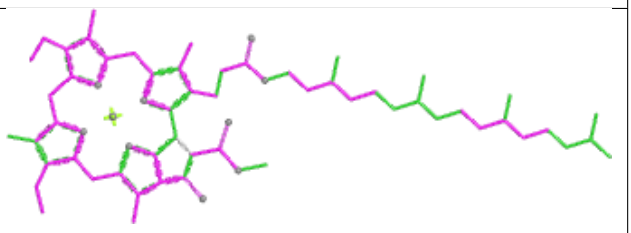


Rings

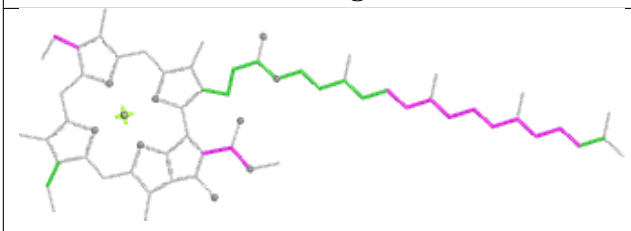
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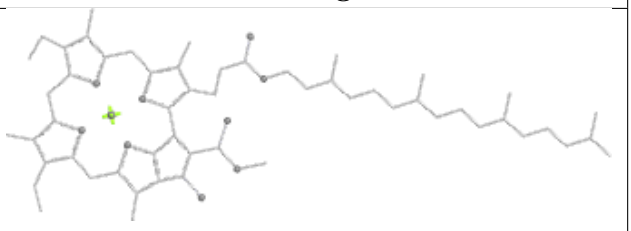
Bond lengths



Bond angles

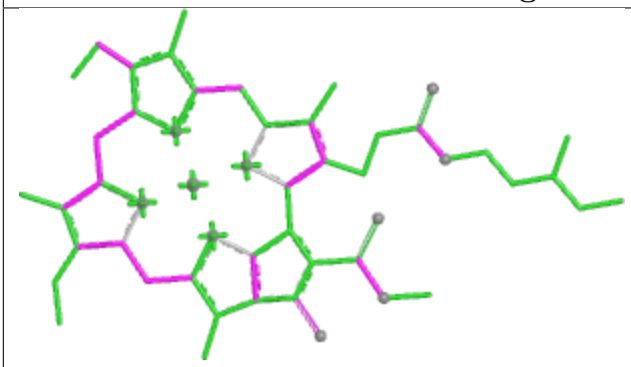


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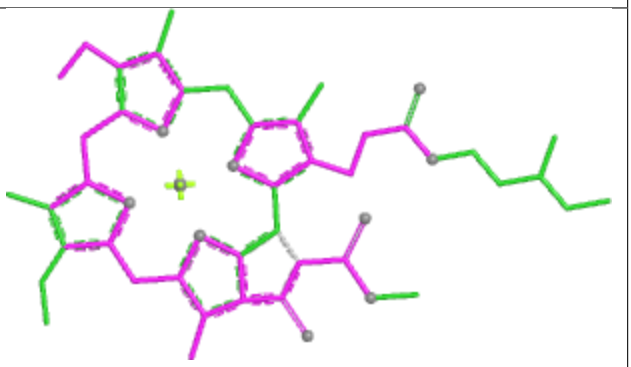


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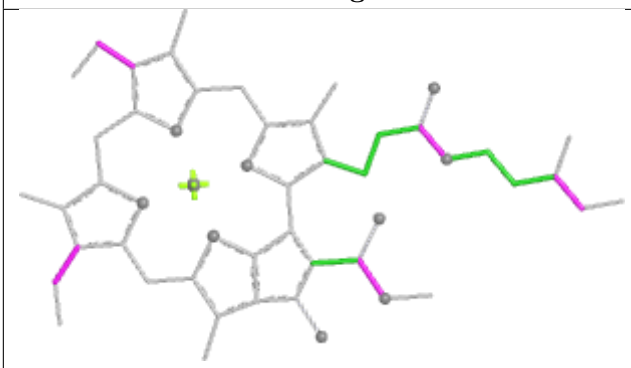
Ligand CLA 1 1008



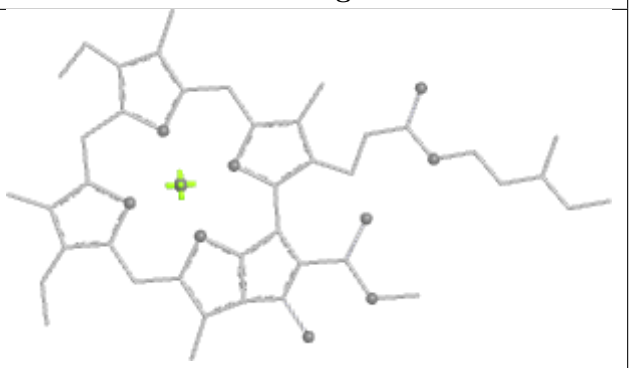
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Bond angles

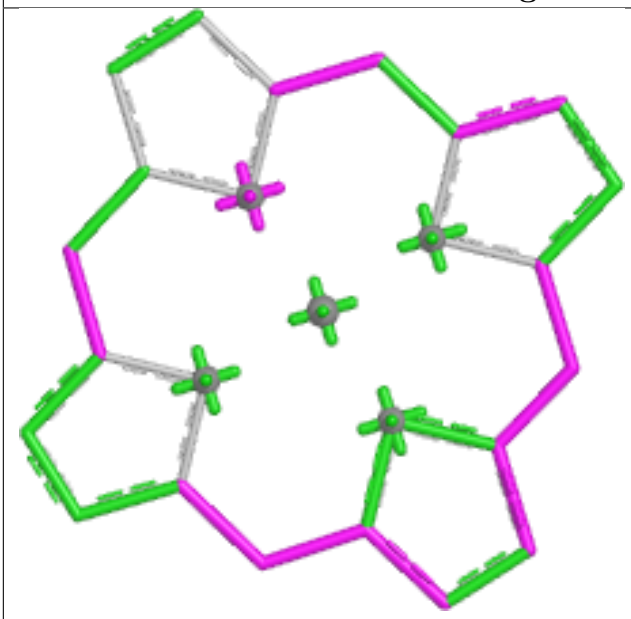


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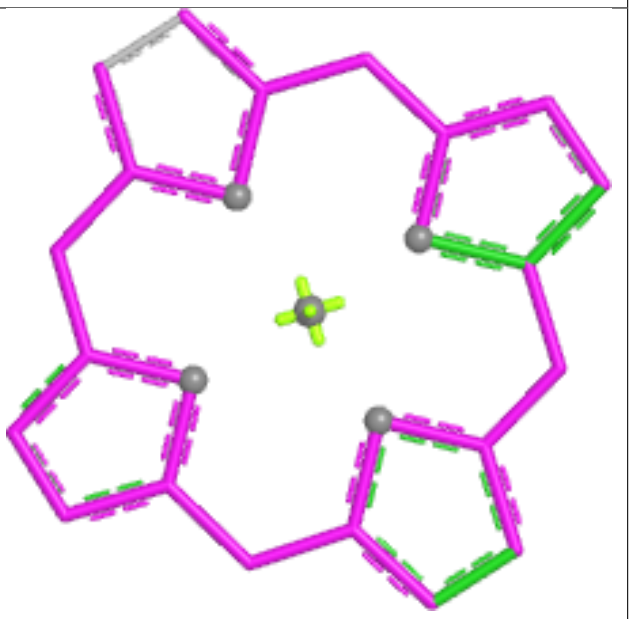


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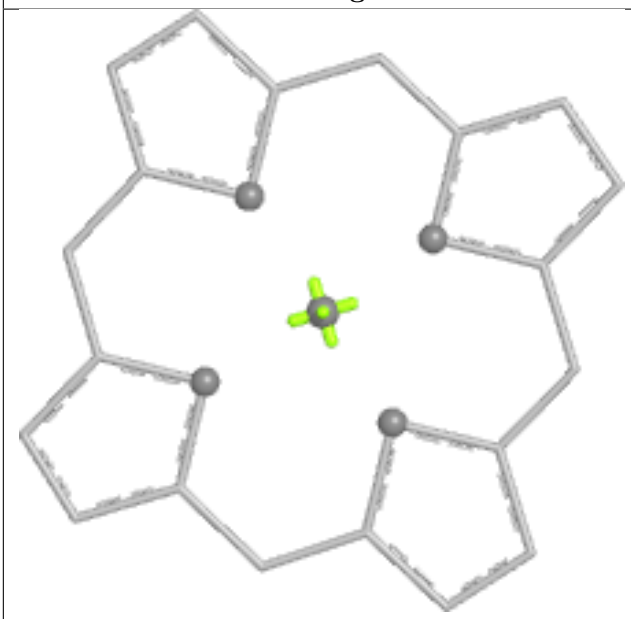
Ligand CLA 3 3004



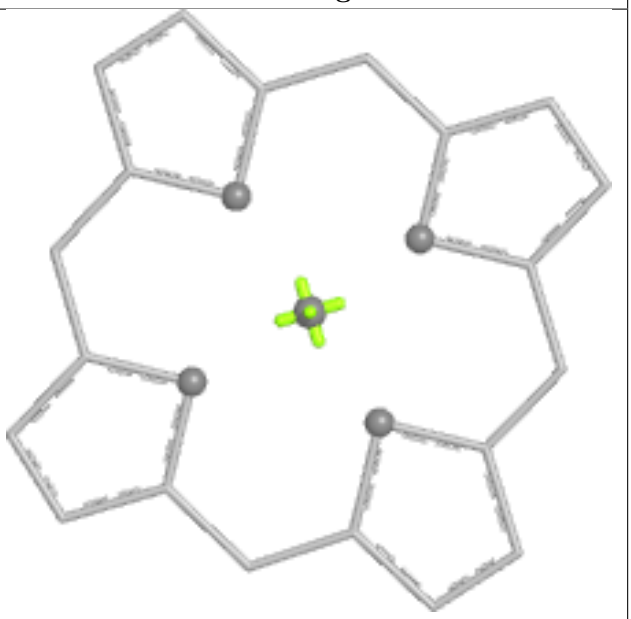
Bond lengths



Bond angles

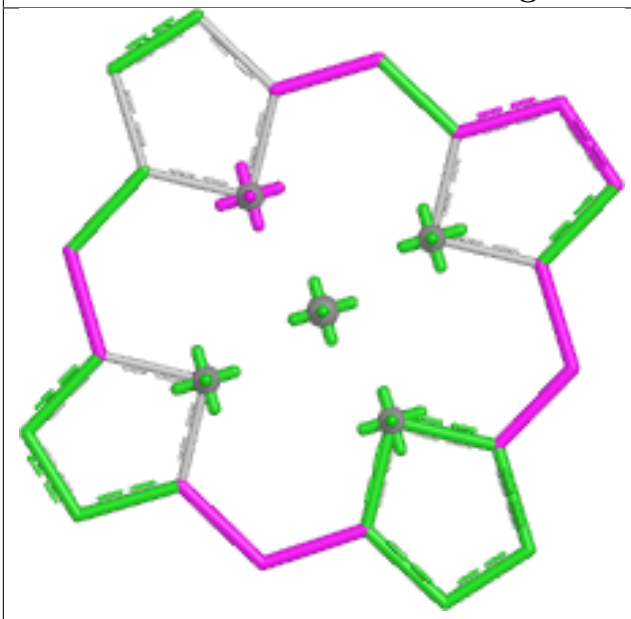


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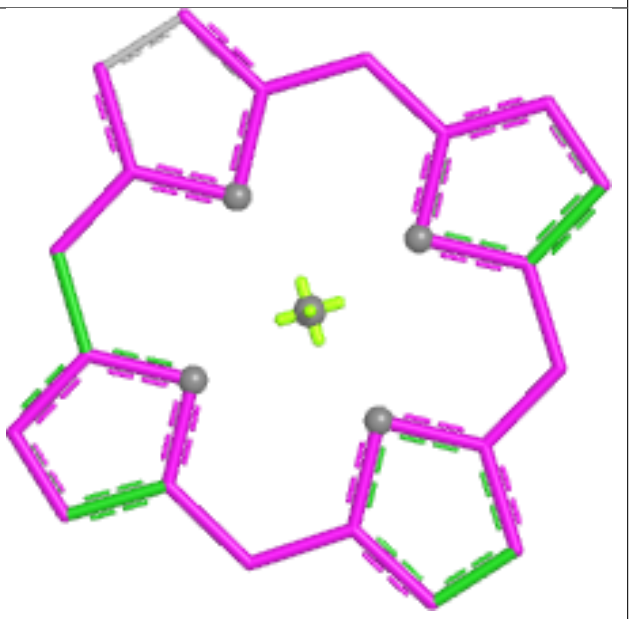


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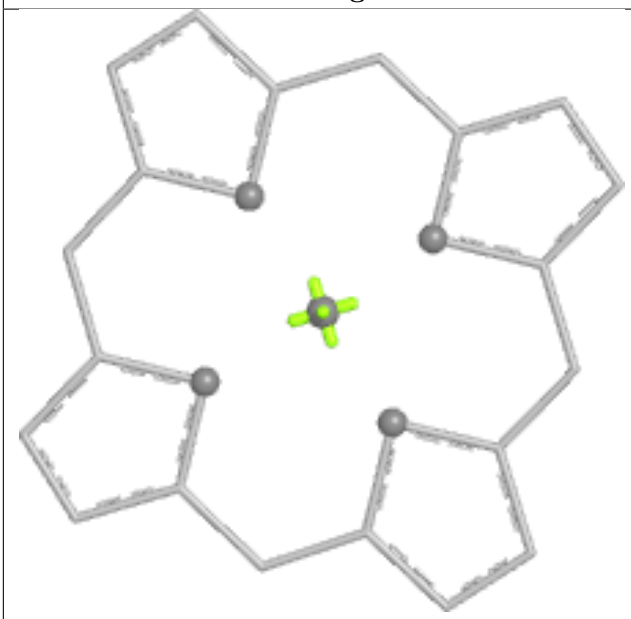
Ligand CLA 3 3010



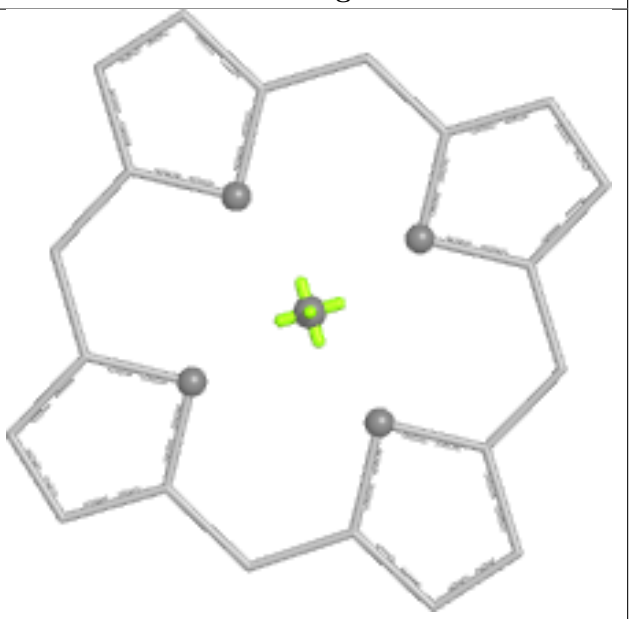
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Bond angles

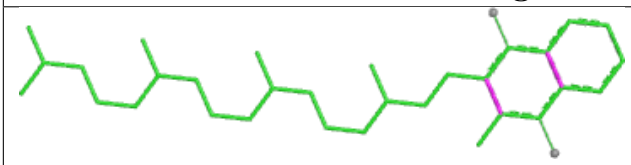


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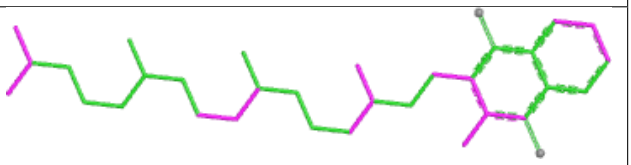


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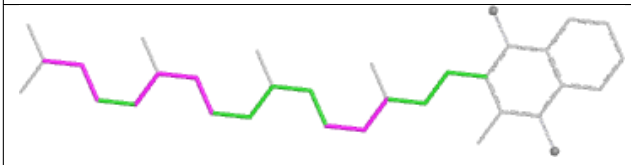
Ligand PQN A 5001



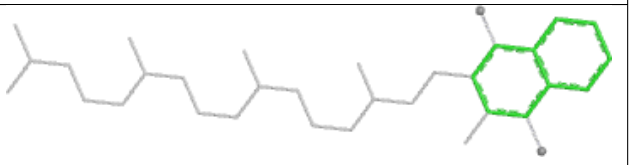
Bond lengths



Bond angles

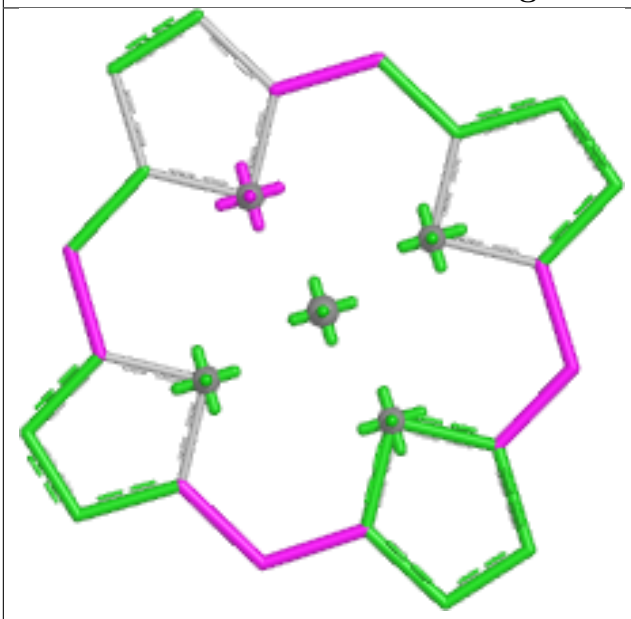


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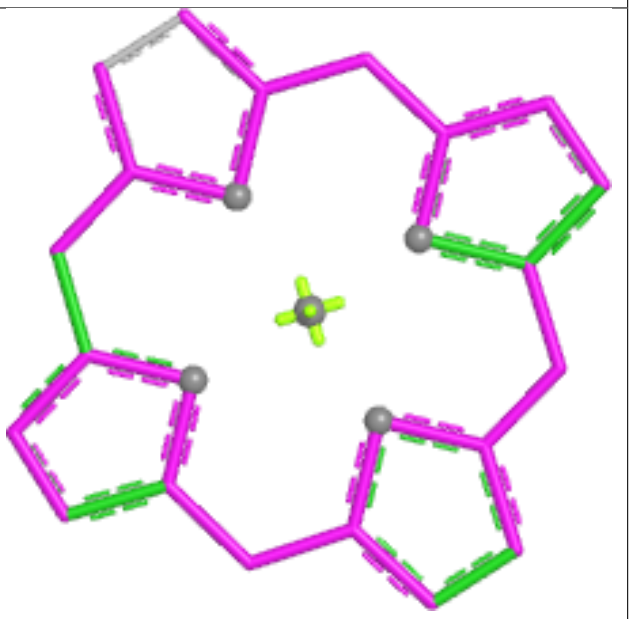


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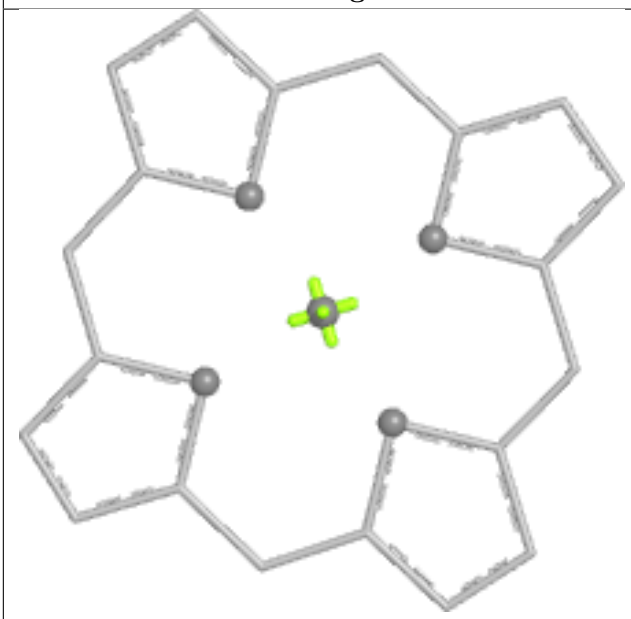
Ligand CLA 4 4004



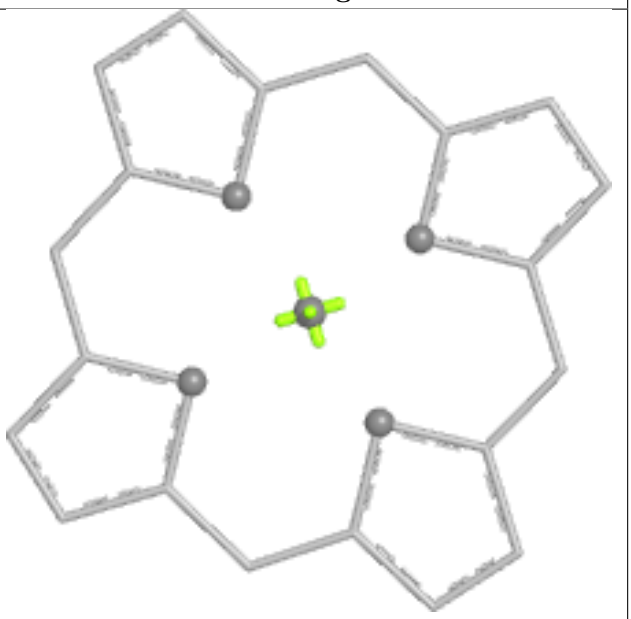
Bond lengths



Bond angles

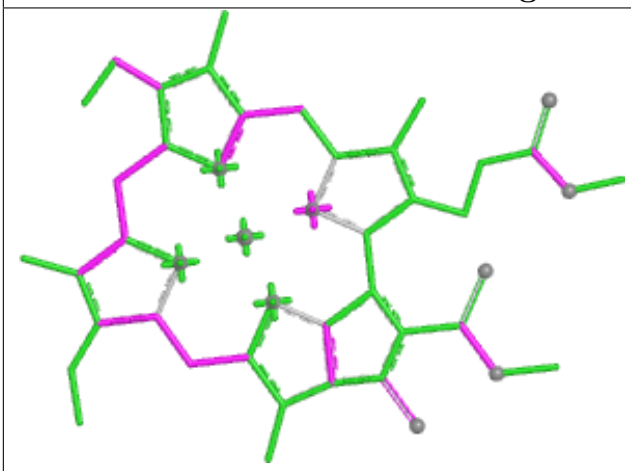


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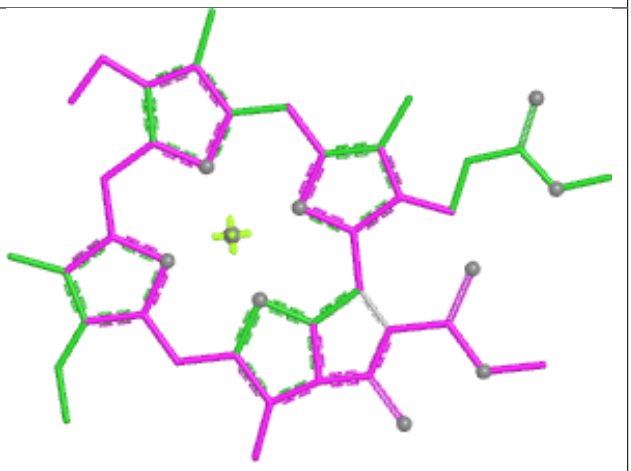


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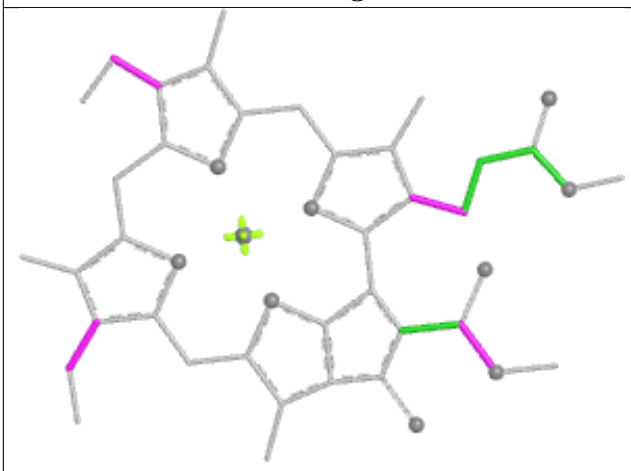
Ligand CLA 1 1005



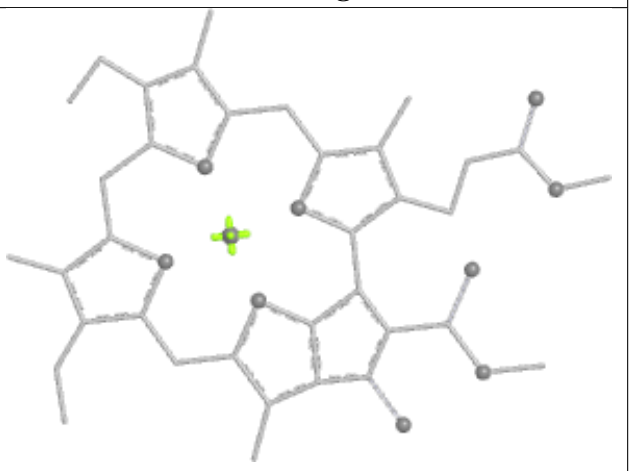
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Bond angles



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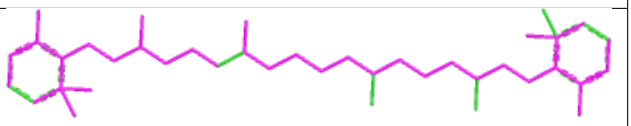


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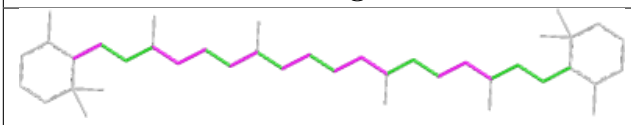
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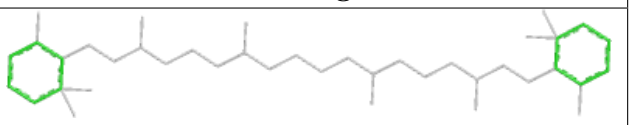
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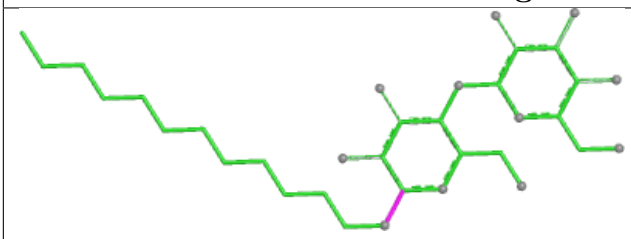


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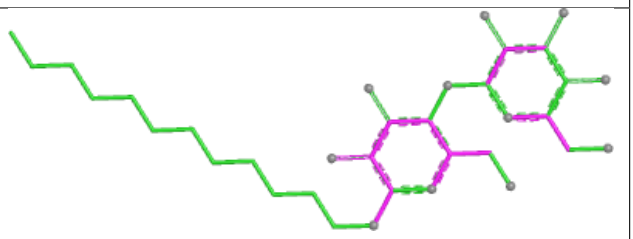


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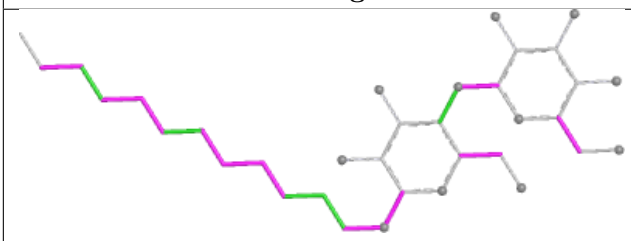
Ligand LMU 4 7019



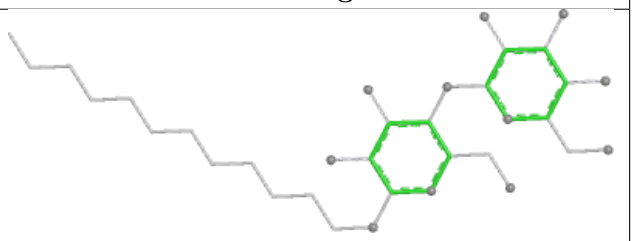
Bond lengths



Bond angles

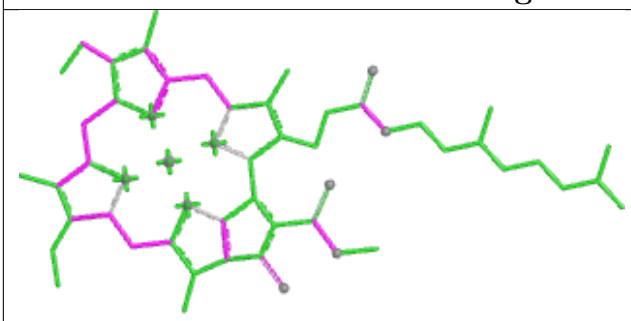


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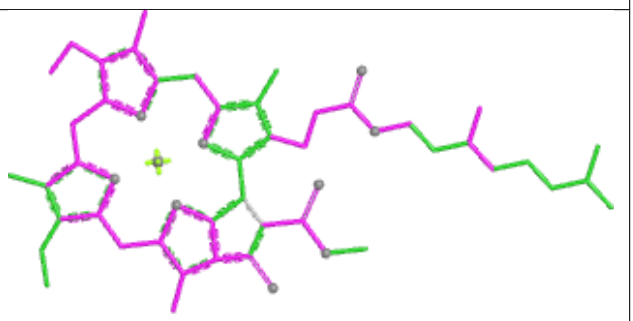


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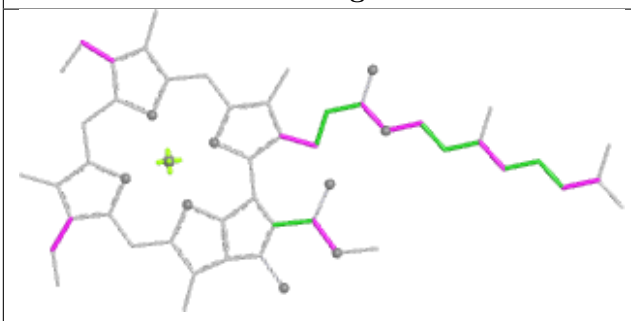
Ligand CLA A 1102



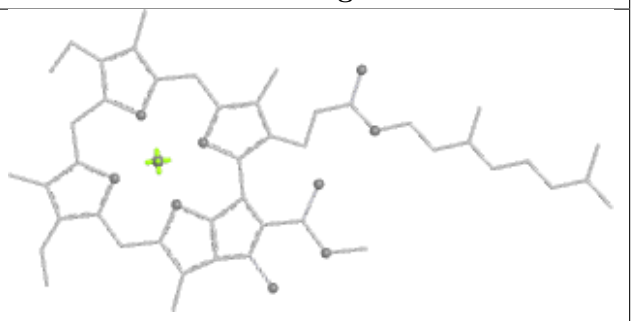
Bond lengths



Bond angles

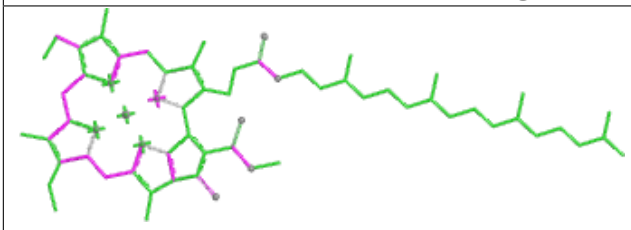


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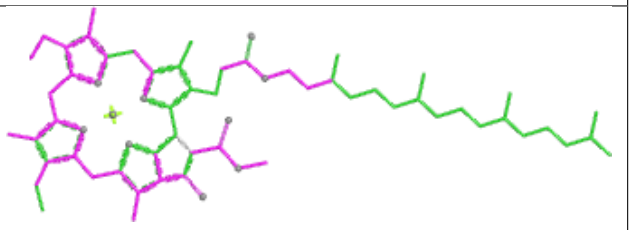


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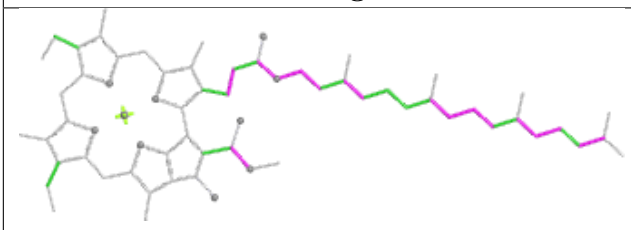
Ligand CLA H 1207



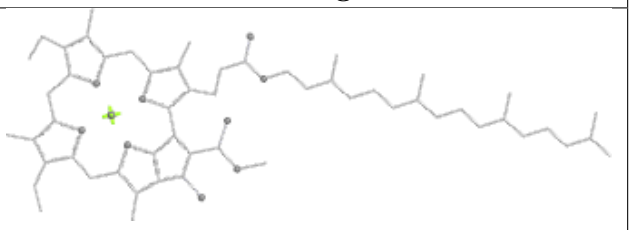
Bond lengths



Bond angles

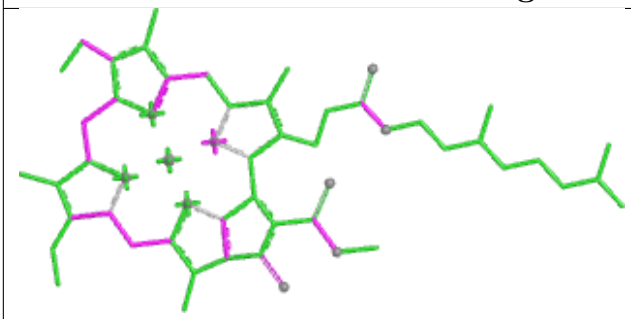


Torsions

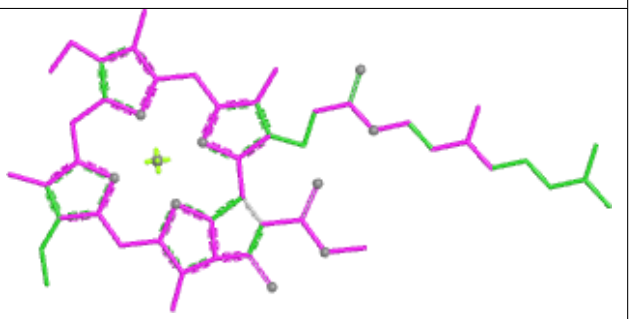


Rings

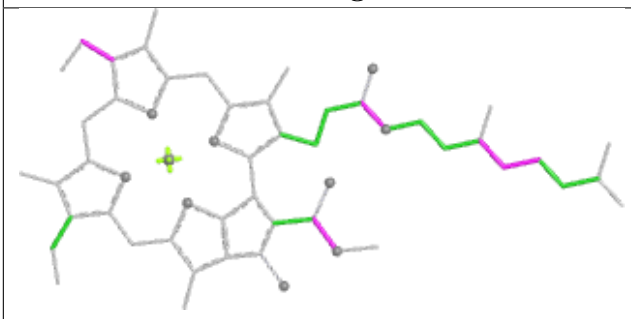
Ligand CLA L 1504



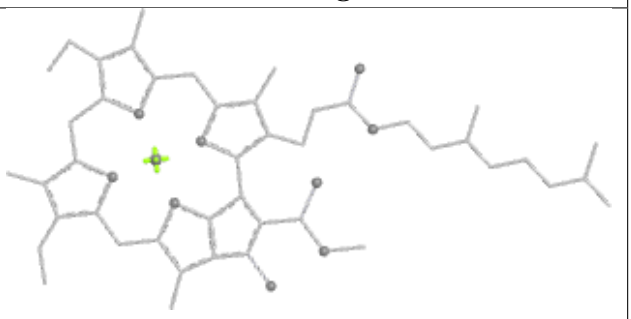
Bond lengths



Bond angles

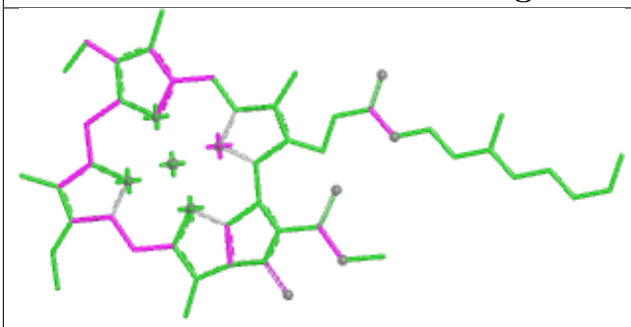


Torsions

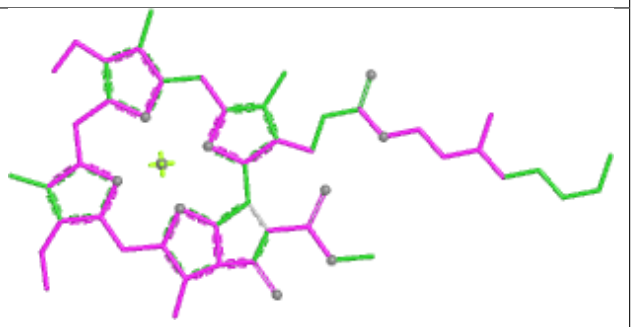


Rings

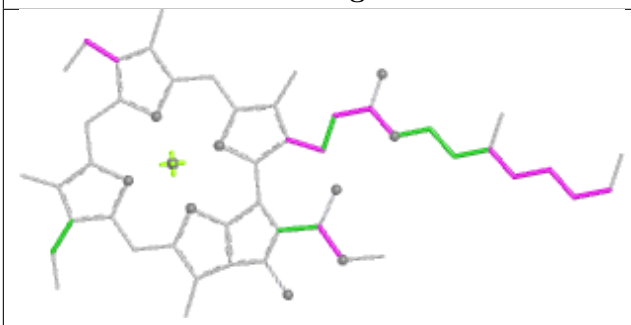
Ligand CLA A 1111



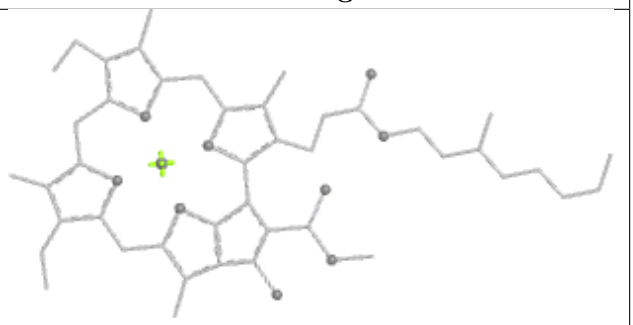
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 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	730/738 (98%)	1.34	157 (21%) 2 2	12, 19, 25, 27	0
2	B	733/733 (100%)	1.39	150 (20%) 2 2	8, 18, 26, 28	0
3	C	81/81 (100%)	1.81	32 (39%) 1 1	17, 21, 23, 24	0
4	D	138/138 (100%)	1.20	24 (17%) 4 4	18, 22, 25, 27	0
5	E	64/64 (100%)	1.08	10 (15%) 5 4	17, 21, 24, 25	0
6	F	154/154 (100%)	1.13	26 (16%) 4 4	17, 22, 25, 26	0
7	G	95/95 (100%)	1.06	7 (7%) 20 15	20, 25, 28, 29	0
8	H	69/69 (100%)	0.95	5 (7%) 21 15	22, 24, 29, 30	0
9	I	30/30 (100%)	0.87	5 (16%) 4 4	17, 19, 22, 22	0
10	J	42/42 (100%)	1.23	6 (14%) 6 5	17, 20, 25, 26	0
11	K	84/84 (100%)	0.89	6 (7%) 22 15	24, 27, 29, 30	0
12	L	161/161 (100%)	1.09	26 (16%) 4 4	16, 20, 26, 27	0
13	N	85/85 (100%)	0.49	5 (5%) 28 19	22, 25, 28, 29	0
14	R	0/53	-	-	-	-
15	1	165/170 (97%)	1.92	60 (36%) 1 1	32, 59, 69, 70	0
16	2	176/176 (100%)	1.50	41 (23%) 2 2	32, 52, 63, 66	0
17	3	156/172 (90%)	0.96	19 (12%) 8 7	25, 28, 32, 33	0
18	4	166/166 (100%)	1.63	53 (31%) 1 1	20, 44, 56, 57	0
All	All	3129/3211 (97%)	1.31	632 (20%) 3 2	8, 22, 57, 70	0

The worst 5 of 632 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	1	132	GLY	11.5
16	2	181	PRO	11.2
2	B	491	ASN	9.6

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Mol	Chain	Res	Type	RSRZ
11	K	62	SER	7.7
15	1	153	SER	7.4

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
19	CLA	A	1309	25/65	0.49	0.16	25,46,54,54	0
19	CLA	3	3012	25/65	0.51	0.21	30,31,31,31	0
21	BCR	1	6023	40/40	0.54	0.17	21,28,29,30	0
21	BCR	A	6002	40/40	0.55	0.22	23,27,32,33	0
19	CLA	4	4003	55/65	0.55	0.18	15,34,47,50	0
19	CLA	1	1015	25/65	0.56	0.22	27,28,28,28	0
22	LMU	1	7004	35/35	0.56	0.15	17,44,50,52	0
19	CLA	L	1504	55/65	0.57	0.21	18,25,27,27	0
19	CLA	3	3016	65/65	0.57	0.18	23,26,29,31	0
19	CLA	3	3005	25/65	0.57	0.21	31,31,31,31	0
19	CLA	B	1233	51/65	0.58	0.18	24,27,27,28	0
19	CLA	2	2007	65/65	0.58	0.18	17,25,26,26	0
19	CLA	1	1006	36/65	0.58	0.16	29,30,30,31	0
22	LMU	1	7013	35/35	0.58	0.15	15,34,47,48	0
19	CLA	A	1141	65/65	0.59	0.16	28,30,31,32	0
22	LMU	A	7010	35/35	0.59	0.16	16,38,45,48	0
19	CLA	H	1505	55/65	0.59	0.17	18,27,28,29	0
19	CLA	3	3014	25/65	0.59	0.18	31,31,32,32	0
22	LMU	4	7053	34/35	0.59	0.16	21,41,47,48	0
19	CLA	3	3007	42/65	0.60	0.17	27,30,30,30	0
19	CLA	4	4014	47/65	0.60	0.17	21,35,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	2	2014	61/65	0.61	0.17	24,26,28,28	0
19	CLA	G	1242	51/65	0.61	0.16	26,28,29,29	0
21	BCR	3	6022	40/40	0.62	0.17	21,22,23,23	0
19	CLA	H	1241	55/65	0.62	0.16	23,25,26,26	0
22	LMU	L	7029	35/35	0.62	0.16	30,44,53,55	0
19	CLA	1	1001	46/65	0.63	0.16	28,29,30,30	0
19	CLA	2	2001	51/65	0.63	0.18	27,28,29,29	0
19	CLA	L	1148	55/65	0.63	0.15	21,25,26,27	0
22	LMU	G	7051	35/35	0.63	0.16	20,32,43,44	0
22	LMU	N	7049	35/35	0.64	0.14	15,28,40,41	0
19	CLA	4	4007	52/65	0.64	0.15	22,26,27,28	0
22	LMU	K	7041	35/35	0.64	0.15	15,31,45,45	0
22	LMU	4	7009	34/35	0.64	0.17	22,44,50,50	0
19	CLA	A	1151	50/65	0.64	0.15	24,27,29,29	0
19	CLA	K	1142	45/65	0.65	0.15	27,29,30,31	0
19	CLA	3	1118	36/65	0.65	0.17	28,29,30,30	0
19	CLA	1	1013	51/65	0.65	0.16	26,27,29,29	0
19	CLA	B	1212	60/65	0.65	0.18	20,23,25,26	0
19	CLA	A	1112	45/65	0.65	0.21	23,26,26,27	0
19	CLA	2	2005	25/65	0.65	0.18	30,31,32,32	0
19	CLA	B	1301	36/65	0.65	0.16	27,28,29,29	0
22	LMU	E	7048	35/35	0.65	0.15	19,30,44,46	0
19	CLA	B	1213	46/65	0.66	0.21	19,21,24,25	0
19	CLA	4	4001	50/65	0.66	0.19	21,23,25,25	0
21	BCR	J	6012	40/40	0.66	0.21	19,24,26,26	0
19	CLA	3	2009	56/65	0.67	0.16	13,35,50,50	0
19	CLA	B	1232	45/65	0.67	0.15	23,26,27,27	0
19	CLA	2	2004	50/65	0.67	0.17	23,25,25,25	0
22	LMU	H	7043	35/35	0.67	0.14	12,31,46,47	0
22	LMU	2	7046	35/35	0.67	0.15	4,27,42,42	0
22	LMU	K	7001	35/35	0.67	0.14	17,34,48,50	0
19	CLA	4	1306	55/65	0.67	0.16	20,26,27,27	0
19	CLA	K	3009	65/65	0.68	0.16	22,25,27,28	0
22	LMU	E	7037	35/35	0.68	0.17	8,21,40,40	0
19	CLA	1	1010	46/65	0.68	0.16	24,25,26,27	0
19	CLA	4	1304	65/65	0.68	0.17	21,23,25,25	0
22	LMU	H	7017	35/35	0.68	0.14	8,23,39,41	0
19	CLA	4	1004	55/65	0.69	0.17	22,25,26,27	0
19	CLA	4	4015	46/65	0.69	0.15	24,25,26,27	0
19	CLA	3	3006	25/65	0.69	0.16	26,27,28,28	0
19	CLA	1	1310	25/65	0.69	0.15	27,28,28,28	0
19	CLA	2	2013	50/65	0.69	0.22	20,22,24,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	3	3003	36/65	0.69	0.15	29,30,31,31	0
19	CLA	F	1305	53/65	0.69	0.15	22,23,25,25	0
19	CLA	3	3013	65/65	0.70	0.16	20,21,24,25	0
19	CLA	H	1145	65/65	0.70	0.14	12,24,33,39	0
19	CLA	K	1143	50/65	0.70	0.15	24,27,28,28	0
19	CLA	J	1311	61/65	0.70	0.14	19,26,27,28	0
19	CLA	3	3008	50/65	0.70	0.14	20,26,27,27	0
22	LMU	4	7052	35/35	0.70	0.14	18,30,48,75	0
19	CLA	2	2002	56/65	0.70	0.17	21,22,25,25	0
19	CLA	2	1307	25/65	0.71	0.14	29,30,31,31	0
19	CLA	3	3015	25/65	0.71	0.15	28,28,29,29	0
19	CLA	3	1147	46/65	0.71	0.15	25,27,28,28	0
19	CLA	3	3017	50/65	0.71	0.12	26,37,49,52	0
19	CLA	F	1302	41/65	0.71	0.17	24,26,26,26	0
19	CLA	3	3010	25/65	0.71	0.17	32,32,33,33	0
22	LMU	4	7034	35/35	0.71	0.16	14,30,42,47	0
19	CLA	A	1108	45/65	0.71	0.15	19,22,23,24	0
19	CLA	A	1134	45/65	0.71	0.17	22,26,27,28	0
22	LMU	H	7030	35/35	0.72	0.12	16,29,46,50	0
21	BCR	A	6007	40/40	0.72	0.22	19,23,28,28	0
19	CLA	2	2006	65/65	0.72	0.15	18,23,24,25	0
19	CLA	L	1503	50/65	0.72	0.20	19,21,23,24	0
22	LMU	K	7047	35/35	0.72	0.15	14,33,46,49	0
19	CLA	4	4004	25/65	0.72	0.18	29,30,30,30	0
19	CLA	4	4006	55/65	0.72	0.17	16,23,24,24	0
22	LMU	A	7045	35/35	0.72	0.14	11,23,41,43	0
19	CLA	1	1303	51/65	0.72	0.15	23,28,28,29	0
19	CLA	3	3004	25/65	0.72	0.15	27,28,28,28	0
19	CLA	A	1105	46/65	0.72	0.19	22,23,24,24	0
22	LMU	H	7011	35/35	0.72	0.14	17,32,38,43	0
19	CLA	A	1121	42/65	0.72	0.15	26,28,28,28	0
22	LMU	H	7028	35/35	0.72	0.14	7,21,40,40	0
22	LMU	C	7015	35/35	0.73	0.13	9,22,37,39	0
22	LMU	K	7042	35/35	0.73	0.15	13,23,42,43	0
22	LMU	D	7050	35/35	0.73	0.12	14,31,46,46	0
19	CLA	3	3011	65/65	0.73	0.15	23,25,26,26	0
19	CLA	1	1002	47/65	0.73	0.17	22,23,24,24	0
19	CLA	K	1146	50/65	0.73	0.14	25,28,30,30	0
19	CLA	1	1007	61/65	0.73	0.15	14,20,21,22	0
22	LMU	2	7031	35/35	0.73	0.12	17,37,45,48	0
19	CLA	R	1144	57/65	0.73	0.14	24,27,28,28	0
19	CLA	R	1150	65/65	0.73	0.14	22,24,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	1	1014	61/65	0.73	0.14	3,31,46,46	0
19	CLA	B	1218	46/65	0.73	0.19	20,20,22,23	0
22	LMU	B	7038	35/35	0.73	0.12	13,35,48,48	0
22	LMU	F	7036	34/35	0.74	0.12	19,32,42,45	0
19	CLA	A	1149	46/65	0.74	0.14	22,25,25,25	0
22	LMU	4	7008	35/35	0.74	0.13	11,29,41,42	0
19	CLA	H	1207	65/65	0.74	0.19	15,17,19,20	0
22	LMU	R	7021	35/35	0.74	0.12	17,28,45,46	0
19	CLA	A	1113	50/65	0.74	0.16	19,22,23,24	0
19	CLA	3	3002	25/65	0.74	0.15	28,28,28,28	0
22	LMU	R	7020	35/35	0.75	0.13	7,26,40,44	0
19	CLA	A	1115	65/65	0.75	0.16	10,28,41,42	0
22	LMU	B	7040	35/35	0.75	0.14	12,26,40,43	0
21	BCR	A	6008	40/40	0.75	0.19	21,24,27,27	0
19	CLA	A	1116	52/65	0.75	0.19	24,25,26,26	0
19	CLA	1	1008	51/65	0.75	0.13	24,26,27,27	0
19	CLA	A	1111	54/65	0.75	0.20	20,24,24,24	0
19	CLA	2	2008	25/65	0.75	0.15	24,24,25,25	0
22	LMU	4	7019	35/35	0.75	0.14	11,25,40,43	0
22	LMU	G	7026	35/35	0.75	0.11	12,35,46,51	0
22	LMU	A	7044	35/35	0.75	0.13	8,20,39,40	0
19	CLA	2	2003	25/65	0.75	0.14	23,24,25,25	0
22	LMU	2	7006	35/35	0.76	0.13	22,25,26,27	0
21	BCR	B	6006	40/40	0.76	0.18	15,19,20,21	0
21	BCR	I	6021	40/40	0.76	0.16	16,20,22,22	0
22	LMU	3	7003	35/35	0.76	0.13	8,25,41,41	0
22	LMU	3	7005	35/35	0.76	0.12	20,32,42,43	0
19	CLA	A	1119	65/65	0.76	0.18	13,18,19,20	0
19	CLA	2	4009	65/65	0.76	0.15	18,23,24,24	0
19	CLA	1	1003	47/65	0.76	0.15	17,19,19,20	0
19	CLA	1	1011	36/65	0.76	0.14	27,27,28,28	0
19	CLA	4	4010	25/65	0.76	0.19	26,27,27,27	0
21	BCR	B	6004	40/40	0.76	0.23	18,20,22,22	0
24	LMG	B	7101	49/55	0.76	0.22	14,18,26,27	0
19	CLA	4	4013	25/65	0.77	0.14	20,21,21,21	0
19	CLA	3	3001	25/65	0.77	0.12	24,25,25,25	0
19	CLA	L	1130	65/65	0.77	0.18	13,18,19,20	0
19	CLA	2	2011	25/65	0.77	0.16	24,25,25,25	0
22	LMU	H	7002	35/35	0.77	0.11	16,29,41,43	0
21	BCR	A	6003	40/40	0.77	0.19	21,24,26,26	0
19	CLA	B	1222	58/65	0.77	0.20	18,21,23,24	0
19	CLA	A	1109	65/65	0.77	0.18	13,20,22,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	BCR	B	6017	40/40	0.78	0.24	15,18,20,20	0
22	LMU	R	7025	35/35	0.78	0.13	5,22,39,42	0
19	CLA	B	1211	65/65	0.78	0.18	17,20,21,21	0
22	LMU	4	7018	35/35	0.78	0.11	9,23,41,42	0
22	LMU	A	7023	35/35	0.78	0.11	6,20,39,41	0
19	CLA	B	1223	65/65	0.78	0.19	13,18,19,20	0
21	BCR	L	6019	40/40	0.78	0.17	15,17,19,19	0
22	LMU	B	7012	25/35	0.78	0.11	22,32,44,49	0
19	CLA	B	1231	45/65	0.78	0.16	19,20,21,21	0
19	CLA	4	4005	25/65	0.79	0.15	20,21,22,22	0
19	CLA	1	1005	46/65	0.79	0.14	19,21,22,22	0
19	CLA	2	2012	50/65	0.79	0.16	20,22,23,23	0
19	CLA	A	1110	54/65	0.79	0.14	19,22,23,23	0
19	CLA	J	1308	55/65	0.79	0.12	12,30,44,45	0
22	LMU	2	7027	35/35	0.79	0.12	6,17,40,40	0
19	CLA	B	1209	55/65	0.79	0.17	18,19,20,21	0
19	CLA	A	1123	65/65	0.79	0.21	12,18,19,20	0
21	BCR	I	6018	40/40	0.79	0.18	14,15,18,18	0
22	LMU	R	7024	35/35	0.80	0.13	6,19,32,40	0
19	CLA	I	1204	60/65	0.80	0.16	13,17,18,18	0
19	CLA	4	1009	36/65	0.80	0.17	20,22,22,23	0
19	CLA	A	1102	55/65	0.80	0.18	13,19,20,20	0
22	LMU	A	7016	35/35	0.80	0.10	10,30,46,46	0
22	LMU	H	7032	35/35	0.80	0.12	8,25,36,45	0
22	LMU	R	7014	35/35	0.80	0.11	9,26,40,44	0
19	CLA	A	1117	65/65	0.80	0.20	10,20,21,22	0
19	CLA	B	1208	54/65	0.80	0.17	18,18,21,22	0
19	CLA	A	1124	65/65	0.81	0.18	18,21,23,24	0
19	CLA	L	1501	50/65	0.81	0.14	20,20,21,21	0
19	CLA	4	4002	52/65	0.81	0.13	21,22,24,25	0
22	LMU	4	7033	35/35	0.81	0.12	12,26,40,41	0
19	CLA	A	1120	51/65	0.81	0.13	22,24,24,26	0
19	CLA	1	1012	36/65	0.81	0.14	23,24,25,25	0
19	CLA	B	1201	45/65	0.81	0.19	19,21,22,22	0
21	BCR	B	6010	40/40	0.81	0.20	13,15,16,16	0
19	CLA	2	2010	25/65	0.82	0.14	23,23,24,24	0
19	CLA	A	1125	65/65	0.82	0.16	15,17,19,20	0
19	CLA	L	1502	47/65	0.82	0.16	17,19,20,20	0
19	CLA	F	1240	36/65	0.82	0.17	15,16,17,17	0
21	BCR	F	6014	40/40	0.82	0.20	9,11,15,15	0
19	CLA	B	1228	50/65	0.82	0.16	12,14,14,15	0
22	LMU	R	7022	35/35	0.82	0.12	5,21,33,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	B	1229	65/65	0.82	0.18	8,12,14,15	0
19	CLA	B	1230	50/65	0.82	0.19	17,18,19,20	0
19	CLA	B	1216	61/65	0.82	0.17	12,18,19,20	0
19	CLA	A	1103	65/65	0.82	0.20	13,14,21,22	0
19	CLA	A	1135	51/65	0.82	0.18	16,19,19,21	0
19	CLA	B	1234	60/65	0.82	0.19	13,14,21,21	0
22	LMU	R	7007	35/35	0.83	0.11	8,21,40,41	0
19	CLA	A	1101	50/65	0.83	0.16	17,18,18,19	0
21	BCR	F	6016	40/40	0.83	0.16	13,16,17,17	0
19	CLA	B	1206	65/65	0.83	0.17	10,12,17,18	0
21	BCR	A	6011	40/40	0.84	0.17	10,15,16,16	0
19	CLA	4	4011	25/65	0.84	0.15	10,11,12,12	0
21	BCR	B	6005	40/40	0.84	0.18	14,16,17,17	0
19	CLA	4	4012	36/65	0.84	0.15	14,15,16,16	0
19	CLA	B	1202	65/65	0.84	0.18	7,16,16,18	0
19	CLA	B	1214	59/65	0.84	0.16	18,20,22,23	0
19	CLA	A	1133	50/65	0.84	0.14	17,19,19,20	0
19	CLA	A	1107	55/65	0.84	0.18	15,16,24,24	0
19	CLA	A	1132	65/65	0.84	0.19	13,17,18,19	0
19	CLA	A	1138	65/65	0.84	0.20	15,18,19,20	0
19	CLA	A	1140	65/65	0.84	0.17	15,18,19,21	0
19	CLA	A	9013	65/65	0.85	0.17	2,10,29,32	0
19	CLA	A	1126	65/65	0.85	0.17	12,14,15,15	0
19	CLA	B	1210	65/65	0.85	0.17	16,20,21,22	0
19	CLA	B	1217	50/65	0.85	0.16	19,21,22,23	0
19	CLA	A	1237	65/65	0.85	0.18	8,17,18,18	0
19	CLA	B	1219	55/65	0.85	0.13	18,18,21,21	0
19	CLA	B	1220	65/65	0.85	0.14	13,15,20,21	0
19	CLA	A	1129	50/65	0.85	0.14	17,19,20,20	0
19	CLA	B	1225	65/65	0.86	0.20	9,12,13,14	0
22	LMU	G	7039	35/35	0.86	0.10	15,30,47,47	0
19	CLA	B	1226	65/65	0.86	0.18	11,12,19,19	0
19	CLA	A	1104	57/65	0.86	0.14	13,15,18,18	0
22	LMU	A	7035	35/35	0.86	0.11	6,18,32,40	0
19	CLA	B	1235	65/65	0.86	0.18	14,15,16,17	0
19	CLA	B	1236	47/65	0.86	0.18	14,15,17,17	0
19	CLA	B	1239	65/65	0.86	0.17	8,11,13,14	0
19	CLA	A	1128	65/65	0.87	0.16	14,16,17,18	0
19	CLA	A	1106	65/65	0.87	0.18	10,12,13,14	0
19	CLA	A	1131	65/65	0.87	0.14	12,14,16,16	0
19	CLA	A	1136	65/65	0.87	0.16	14,15,16,17	0
19	CLA	B	1224	65/65	0.87	0.16	9,13,14,15	0

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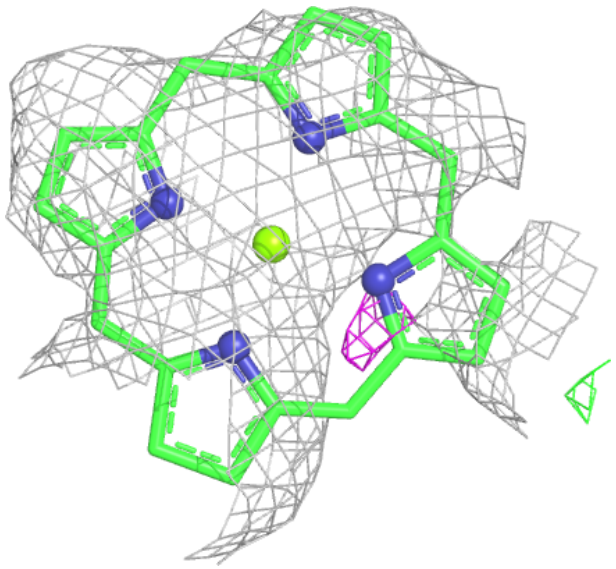
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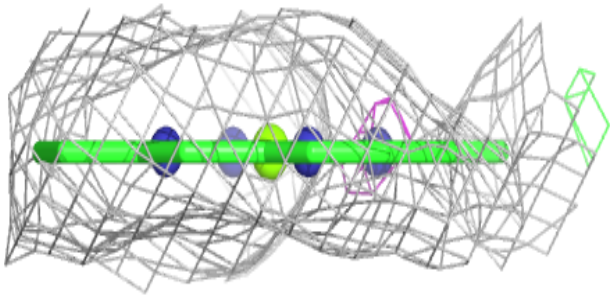
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CLA	B	1215	60/65	0.87	0.17	11,13,15,16	0
19	CLA	A	1122	55/65	0.87	0.15	13,14,18,18	0
19	CLA	B	1238	65/65	0.87	0.16	10,14,15,16	0
19	CLA	A	1139	51/65	0.87	0.17	16,16,17,18	0
21	BCR	B	6020	40/40	0.87	0.18	8,11,12,13	0
20	PQN	A	5001	33/33	0.87	0.19	12,13,14,15	0
19	CLA	A	9012	65/65	0.87	0.16	2,14,28,36	0
19	CLA	A	1127	55/65	0.88	0.15	13,16,17,18	0
19	CLA	B	1205	65/65	0.88	0.18	9,13,14,14	0
19	CLA	A	9022	65/65	0.89	0.15	2,12,26,31	0
19	CLA	B	1221	54/65	0.89	0.17	13,13,16,16	0
19	CLA	B	1203	65/65	0.89	0.14	10,13,14,15	0
19	CLA	A	9023	65/65	0.89	0.17	2,14,29,38	0
20	PQN	B	5002	33/33	0.89	0.16	7,8,14,14	0
19	CLA	A	1137	47/65	0.89	0.14	13,14,15,17	0
19	CLA	B	1227	50/65	0.90	0.13	13,15,16,17	0
19	CLA	B	9010	65/65	0.90	0.16	2,12,34,40	0
19	CLA	A	9011	65/65	0.91	0.19	2,11,30,40	0
23	SF4	C	8002	8/8	0.98	0.07	14,16,24,28	0
23	SF4	C	8003	8/8	0.99	0.05	14,19,21,22	0
23	SF4	A	8001	8/8	0.99	0.07	12,17,19,21	0

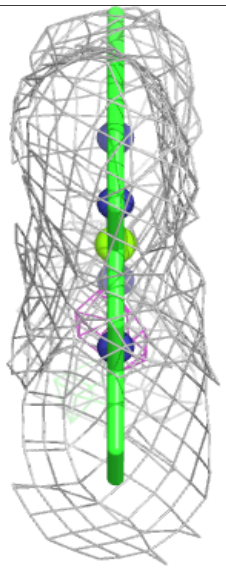
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA A 1309:

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

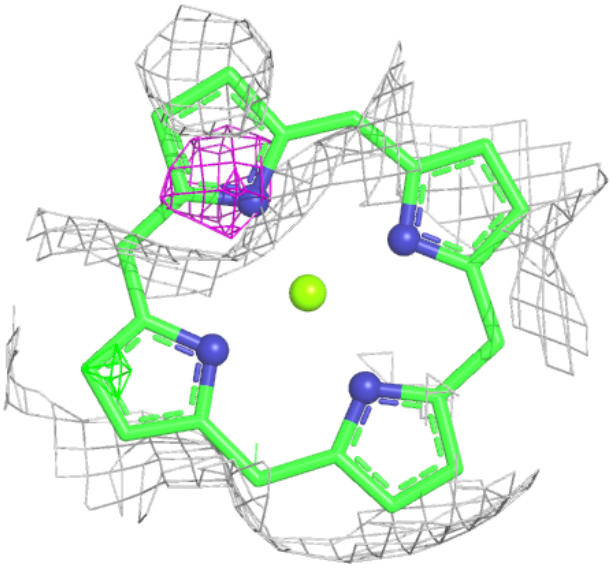


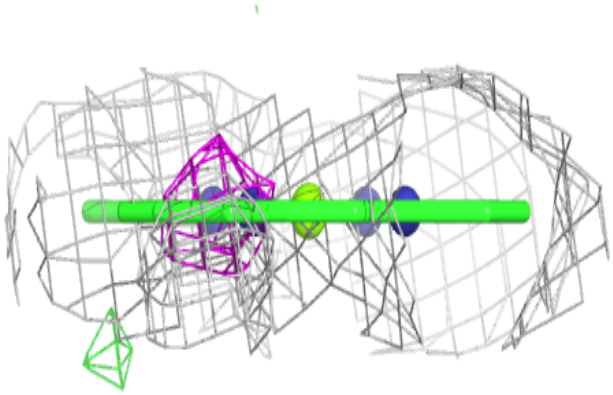


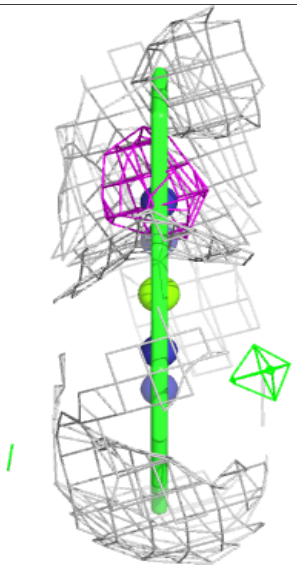


Electron density around CLA 3 3012:

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

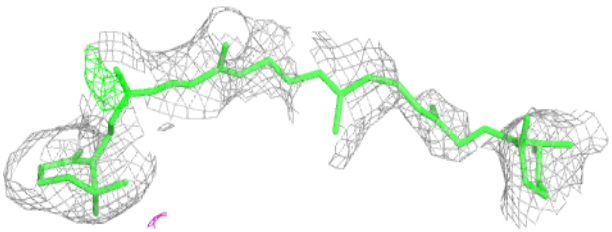


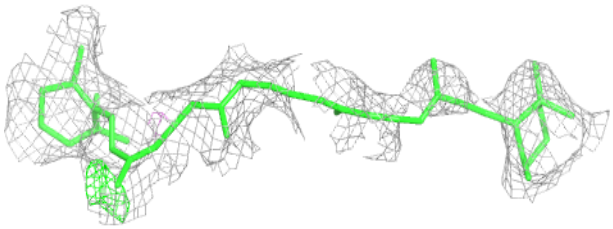


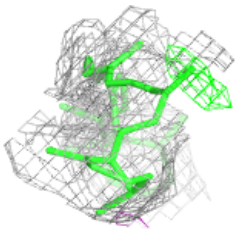


Electron density around BCR 1 6023:

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

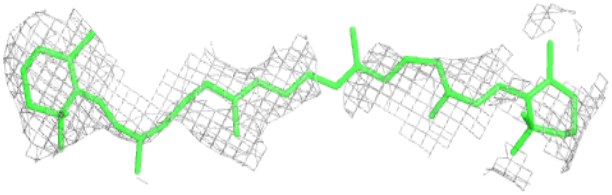


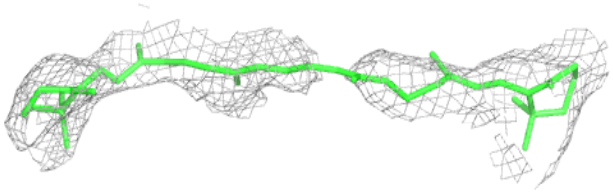


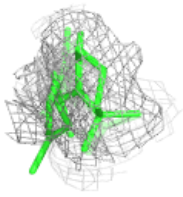


Electron density around BCR A 6002:

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

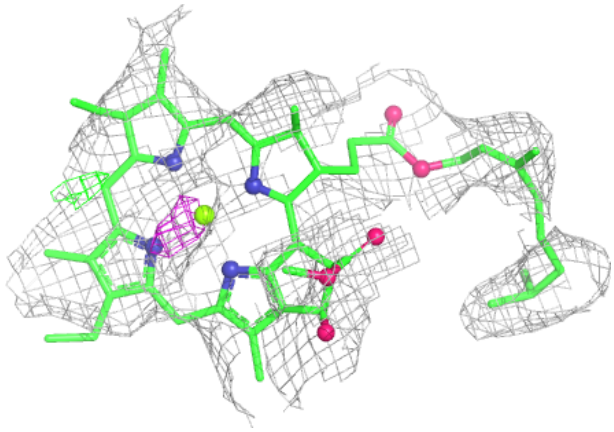


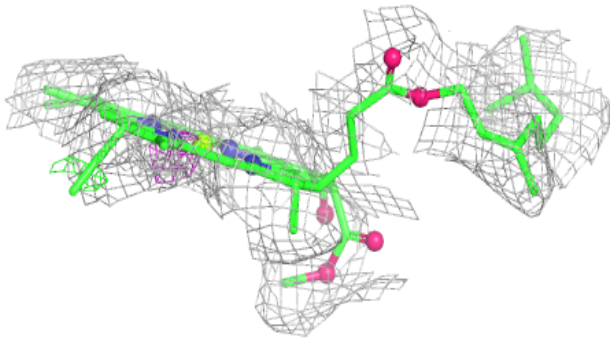


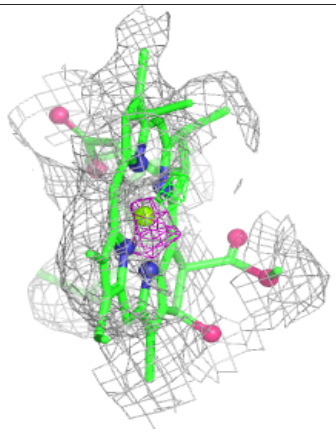


Electron density around CLA 4 4003:

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

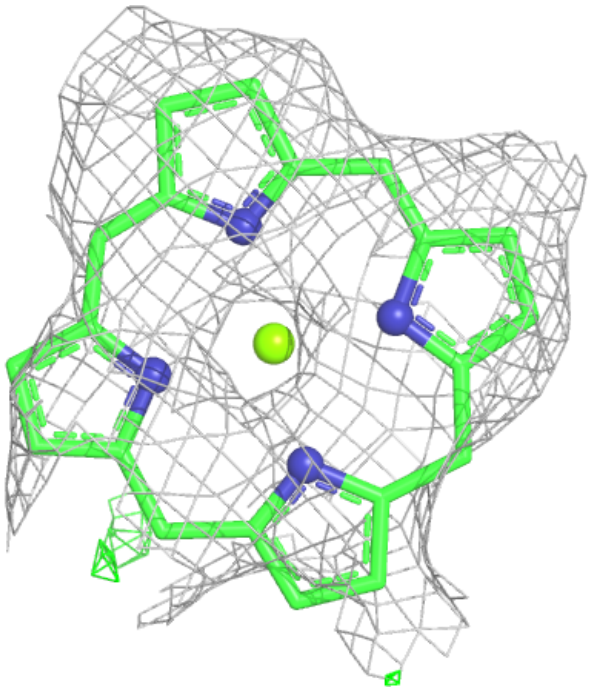


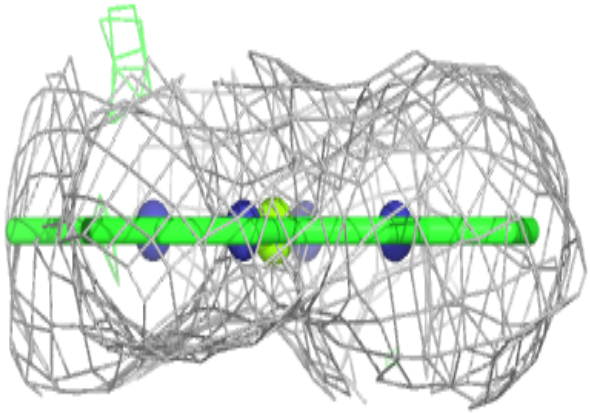


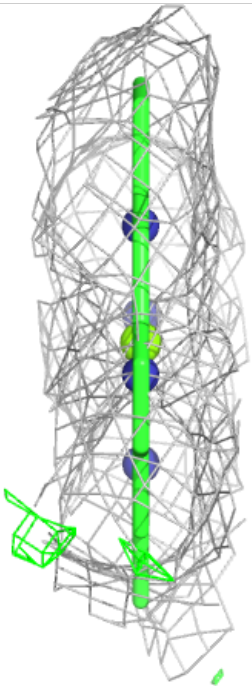


Electron density around CLA 1 1015:

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

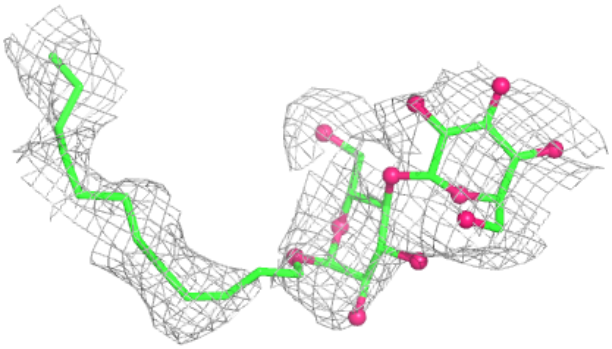


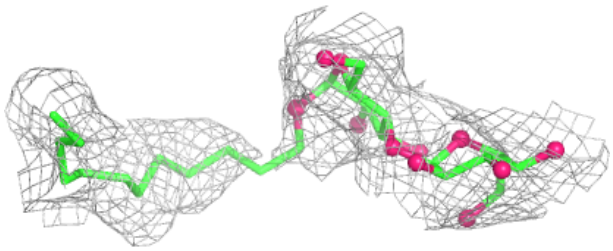


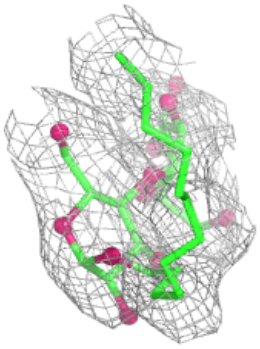


Electron density around LMU 1 7004:

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

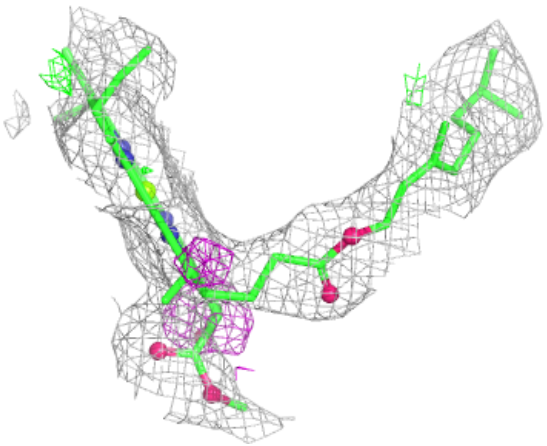


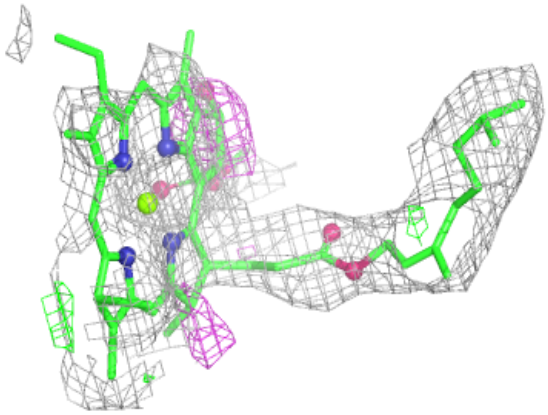


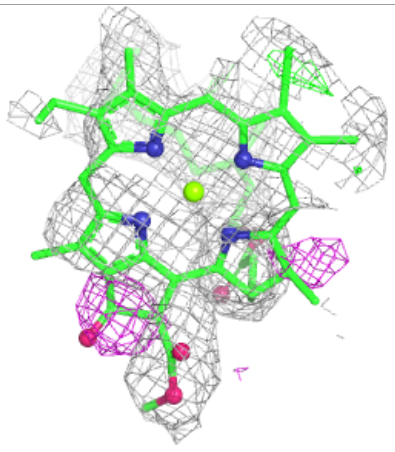


Electron density around CLA L 1504:

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

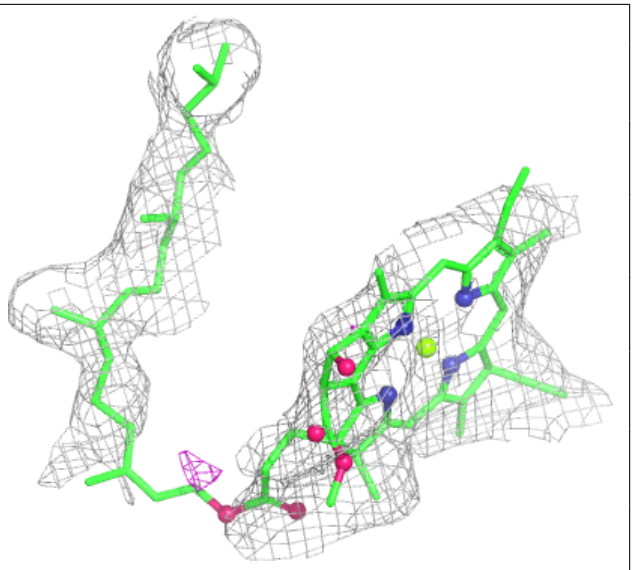


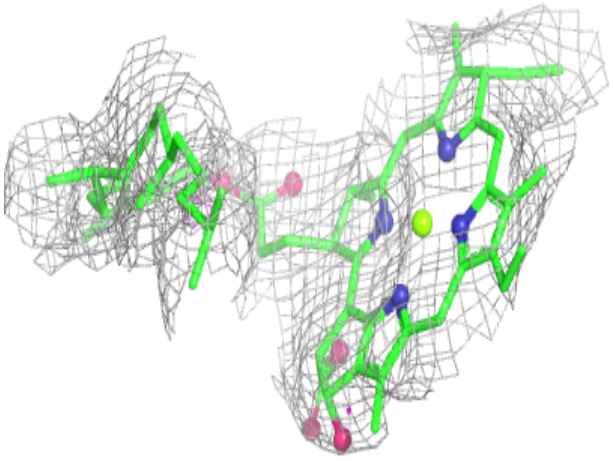


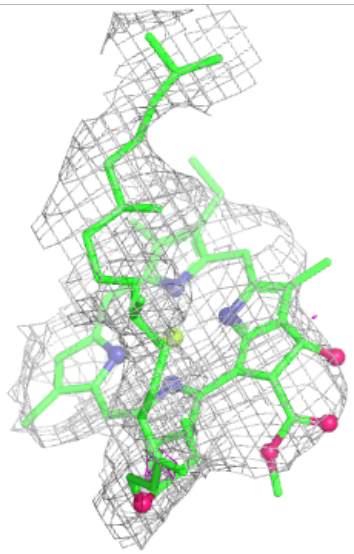


Electron density around CLA 3 3016:

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

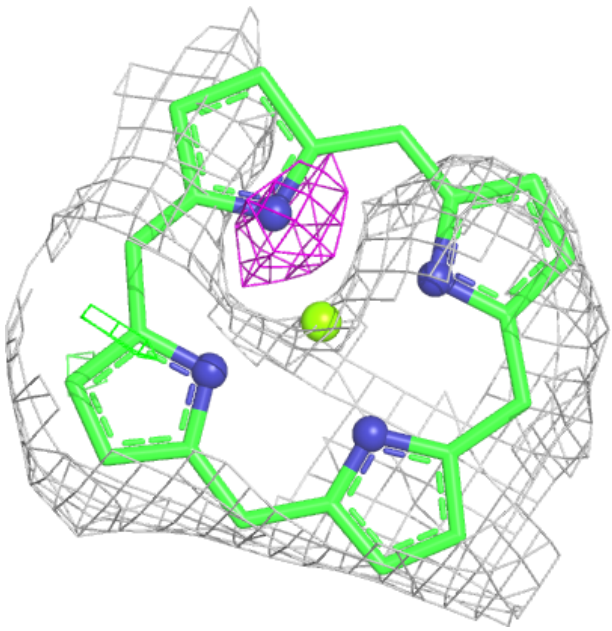


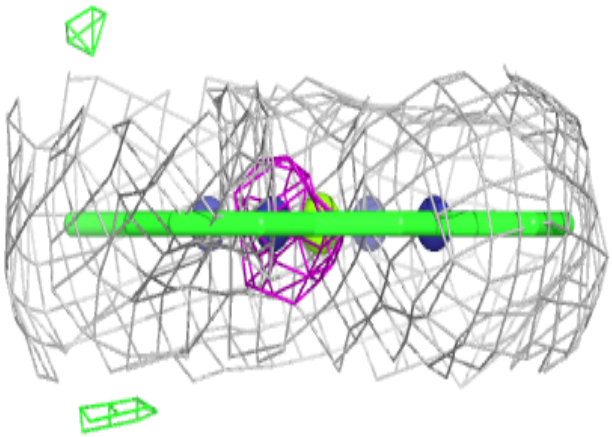


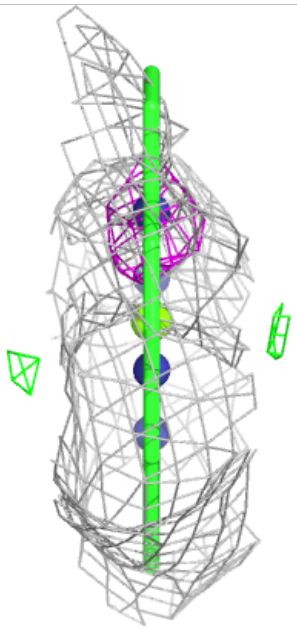


Electron density around CLA 3 3005:

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

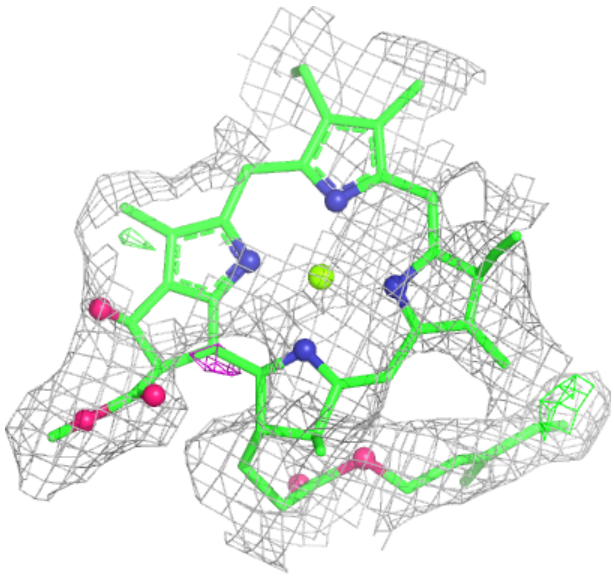


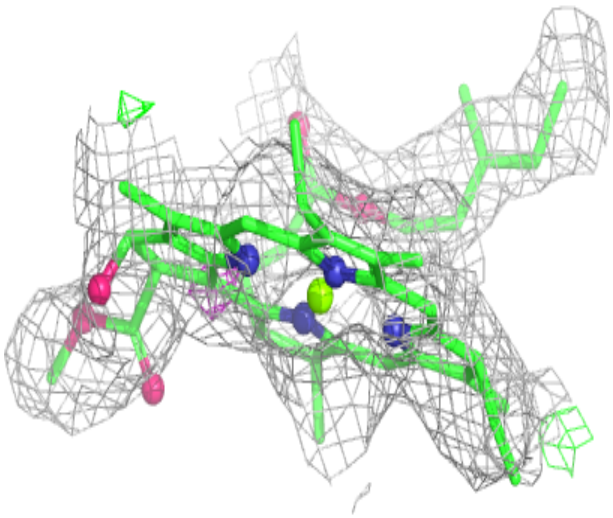


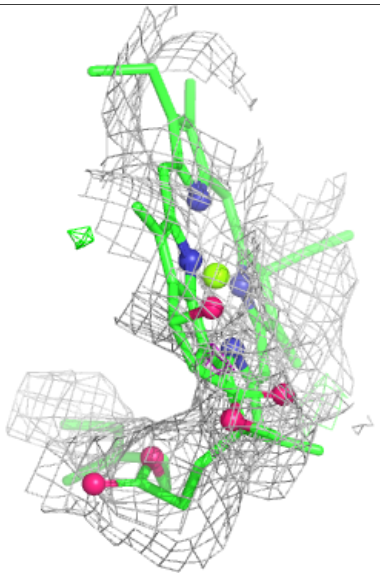


Electron density around CLA B 1233:

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

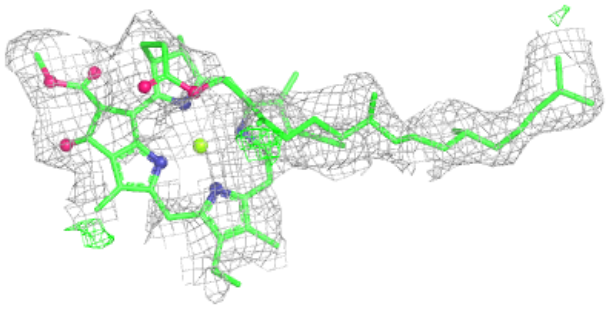


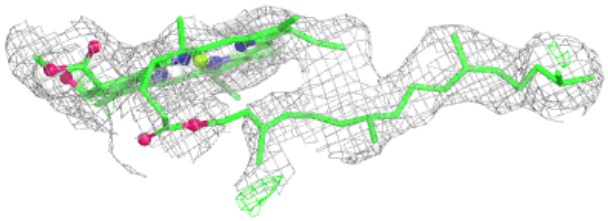


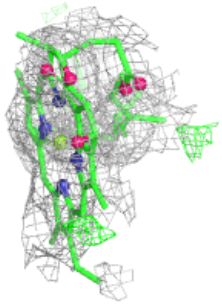


Electron density around CLA 2 2007:

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

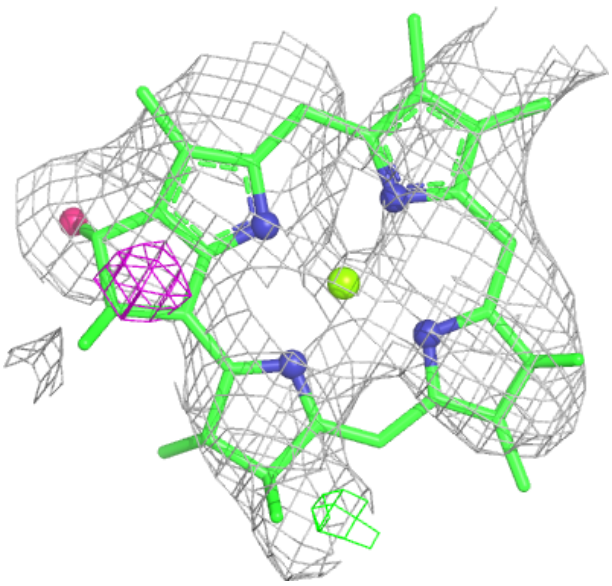


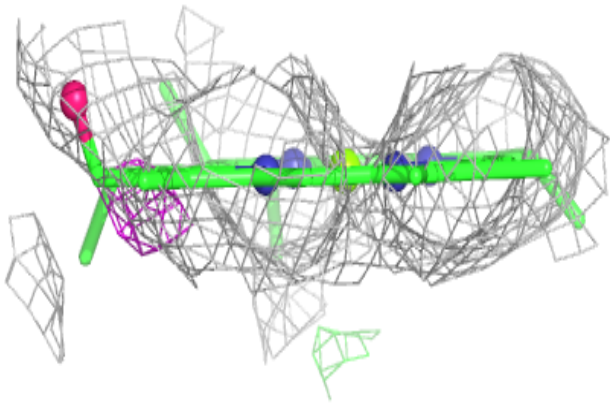




Electron density around CLA 1 1006:

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

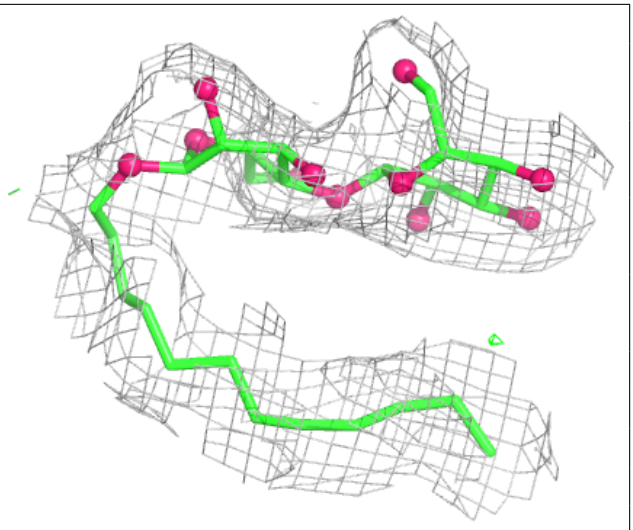


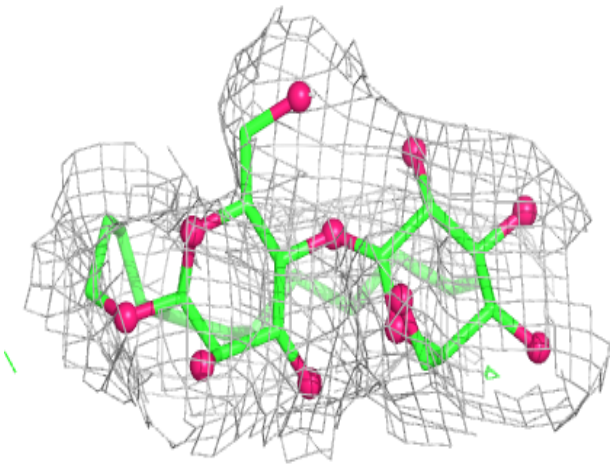


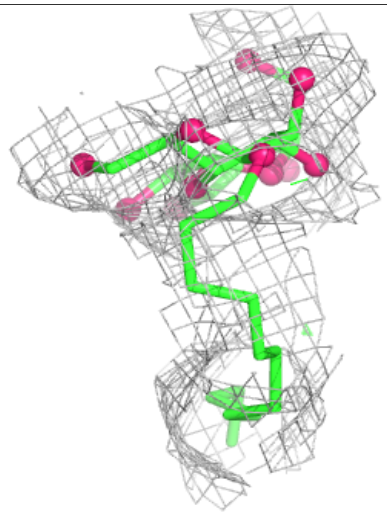


Electron density around LMU 1 7013:

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

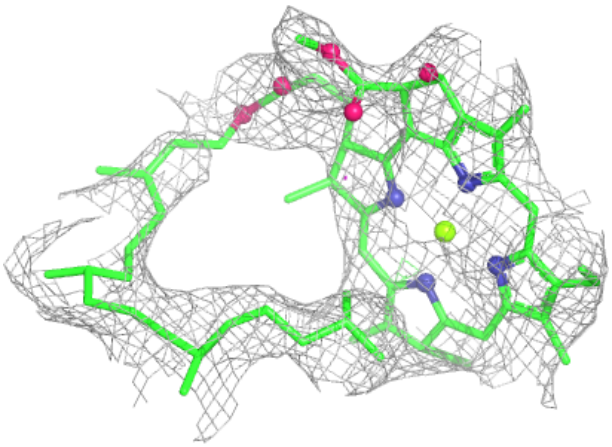


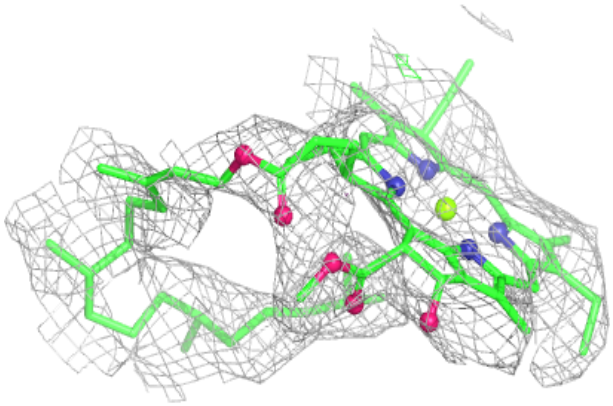




Electron density around CLA A 1141:

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

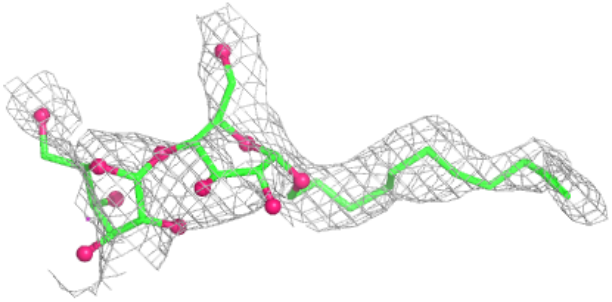


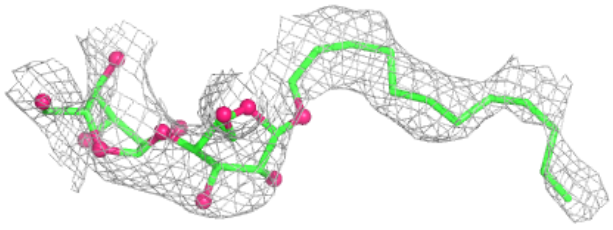


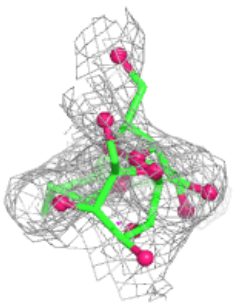


Electron density around LMU A 7010:

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

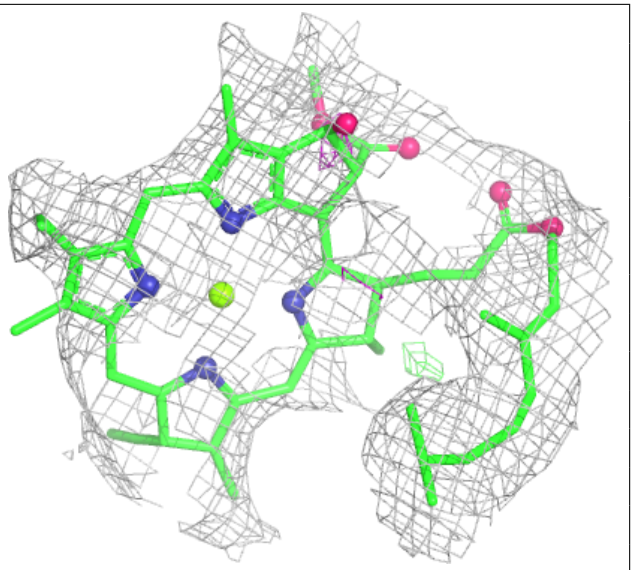


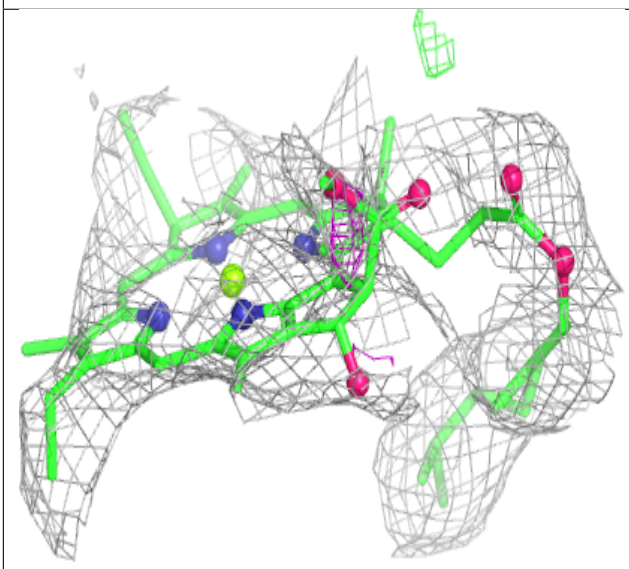


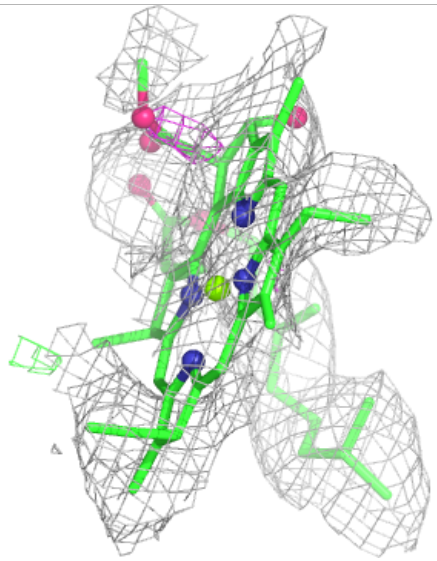


Electron density around CLA H 1505:

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

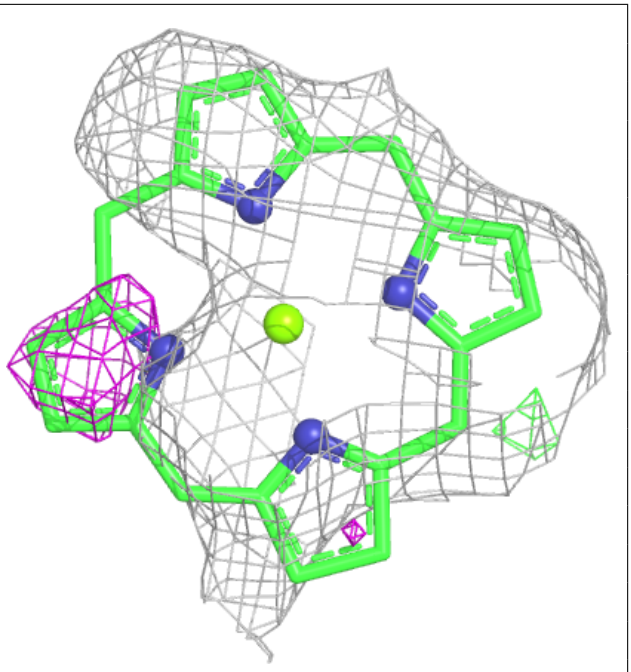


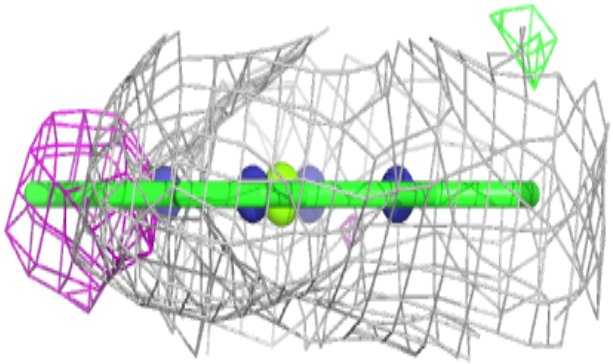


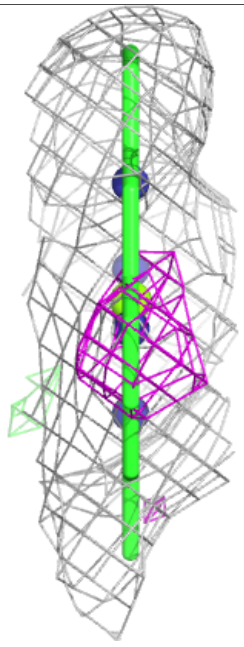


Electron density around CLA 3 3014:

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

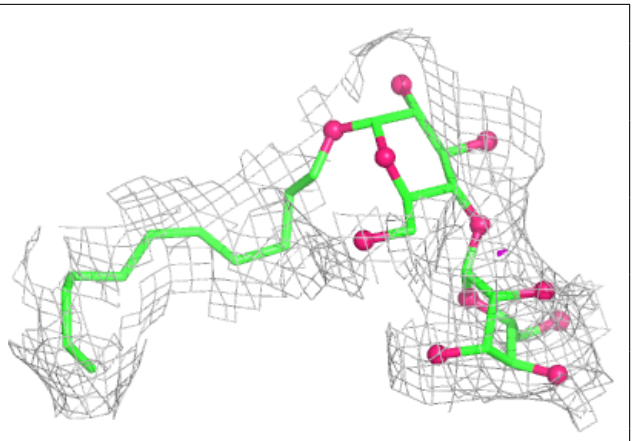


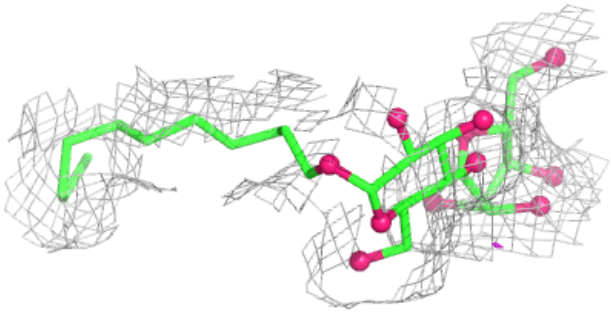


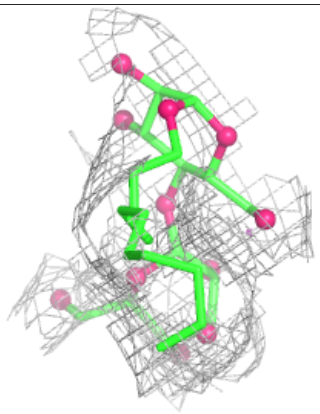


Electron density around LMU 4 7053:

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

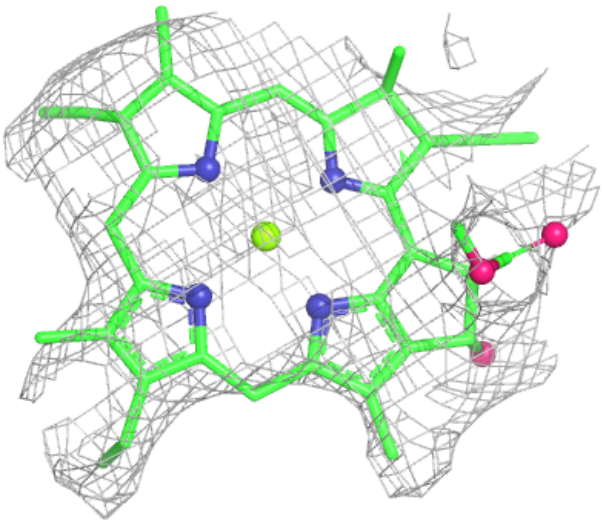


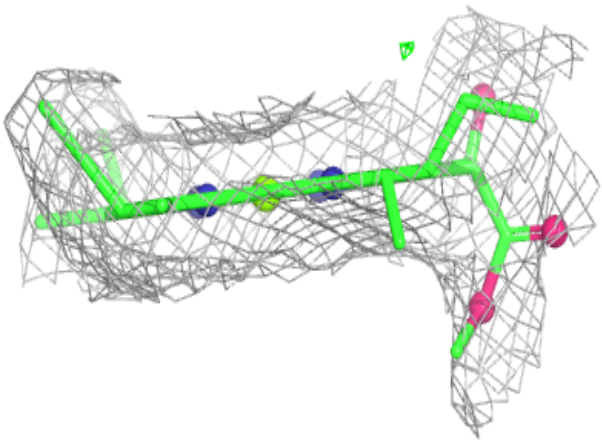


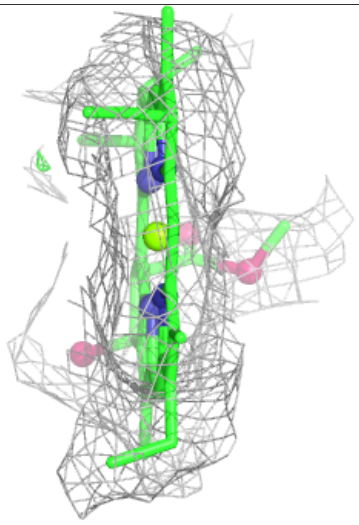


Electron density around CLA 3 3007:

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

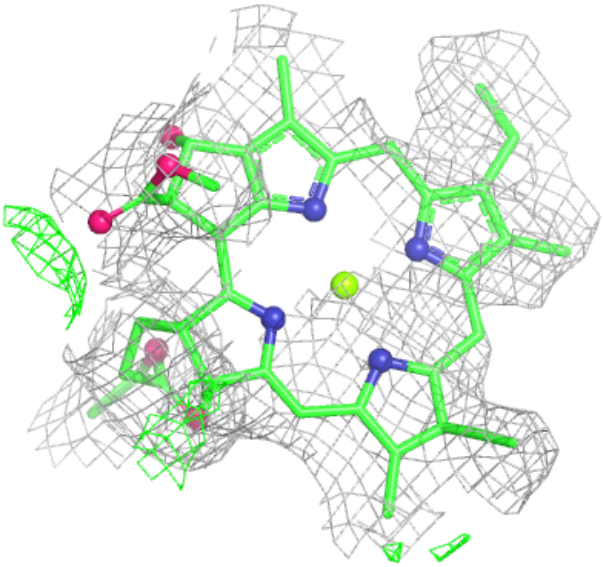


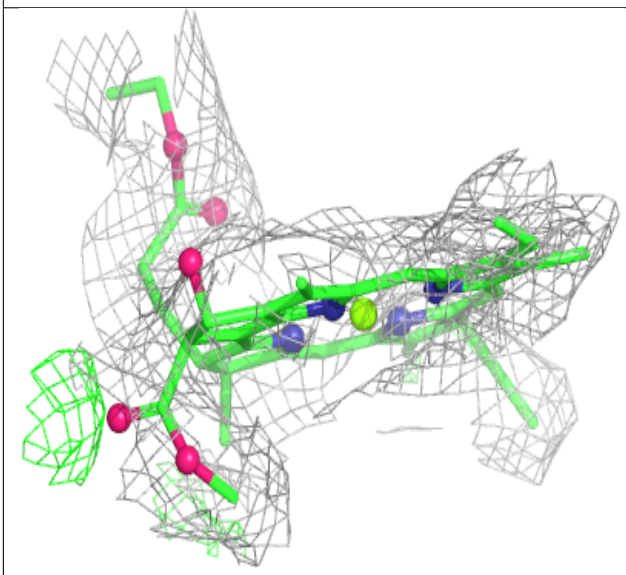


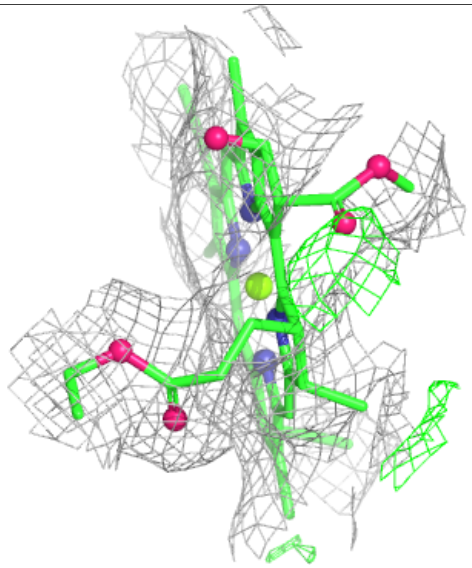


Electron density around CLA 4 4014:

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

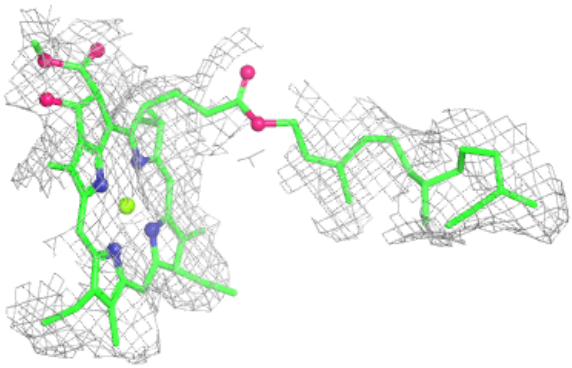


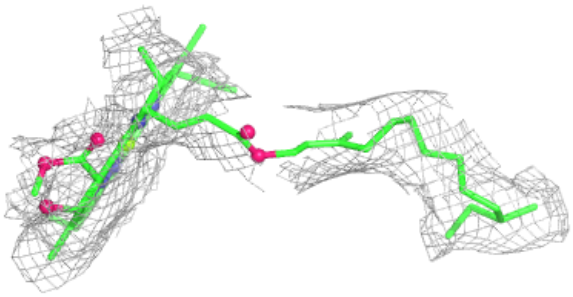


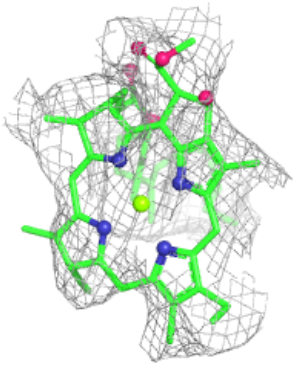


Electron density around CLA 2 2014:

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

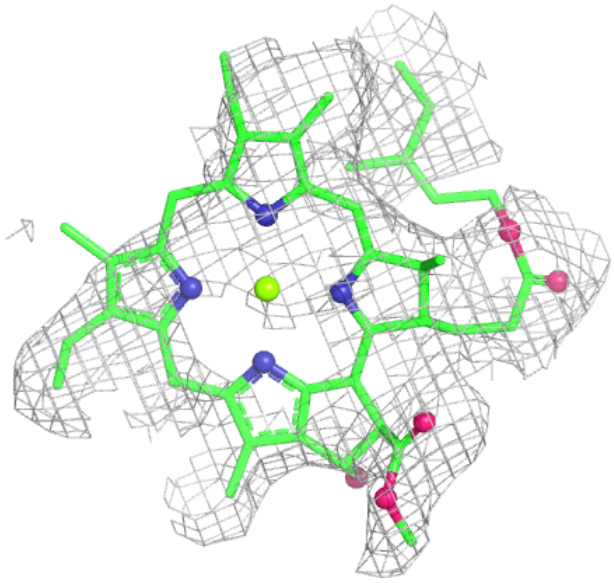


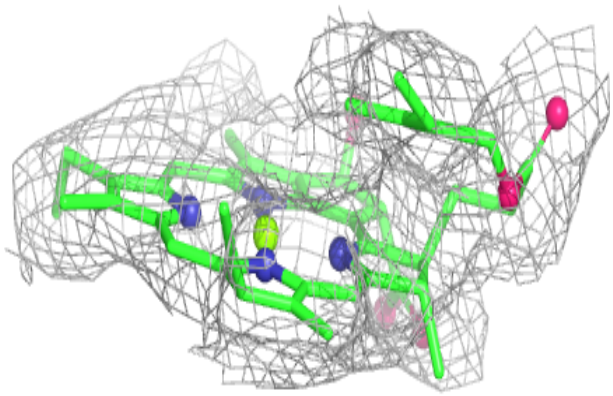


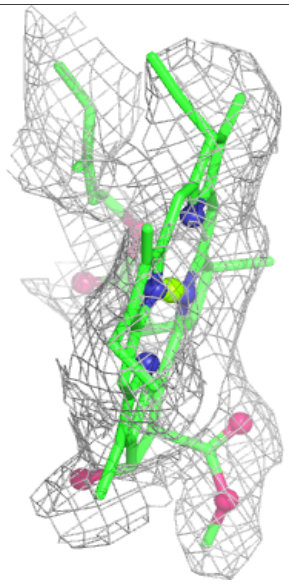


Electron density around CLA G 1242:

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

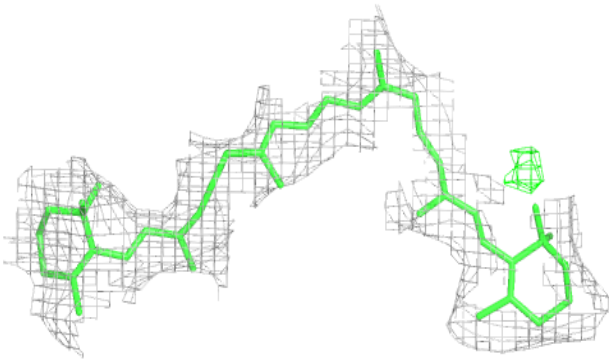


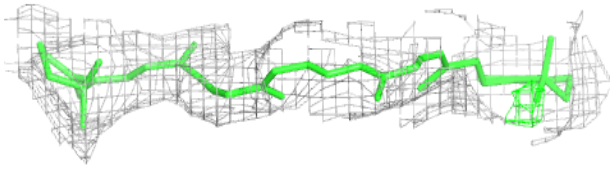




Electron density around BCR 3 6022:

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

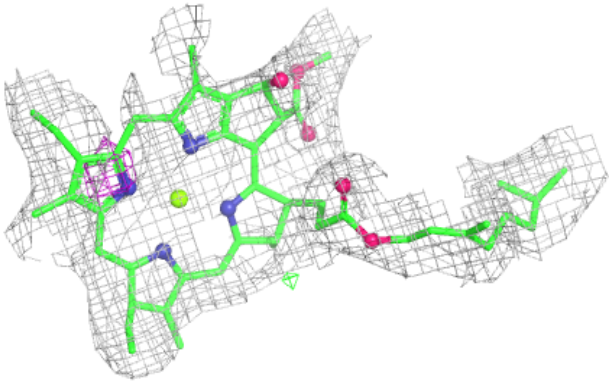


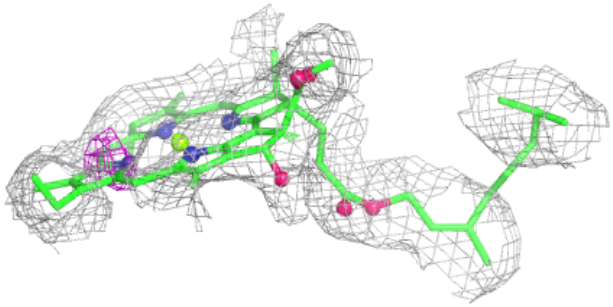


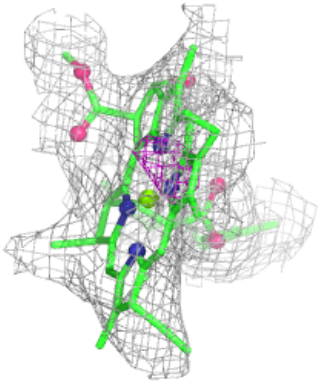


Electron density around CLA H 1241:

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

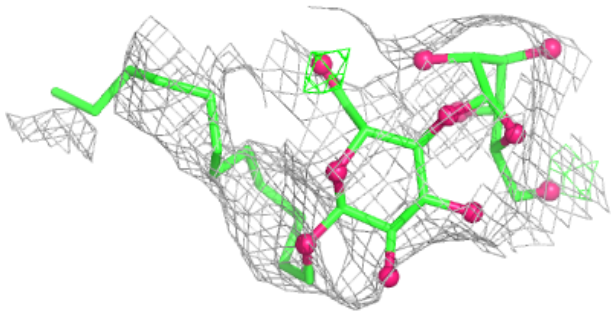


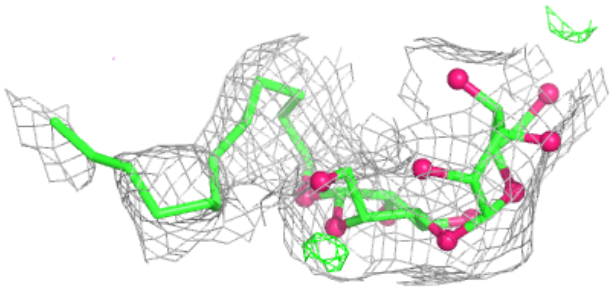


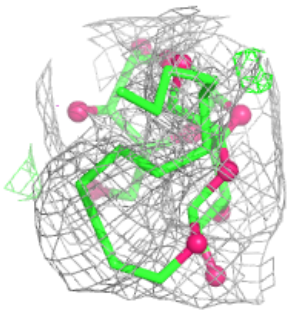


Electron density around LMU L 7029:

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

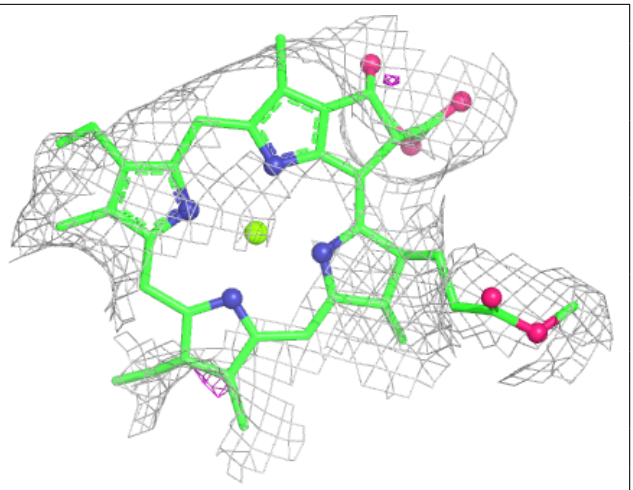


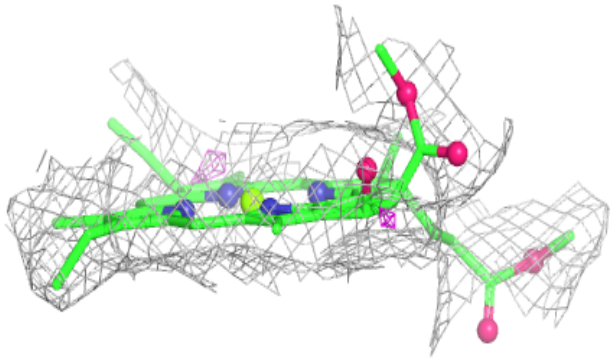


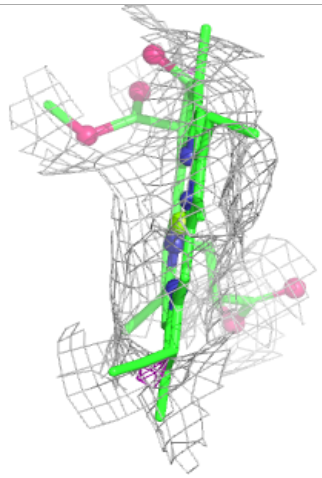


Electron density around CLA 1 1001:

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

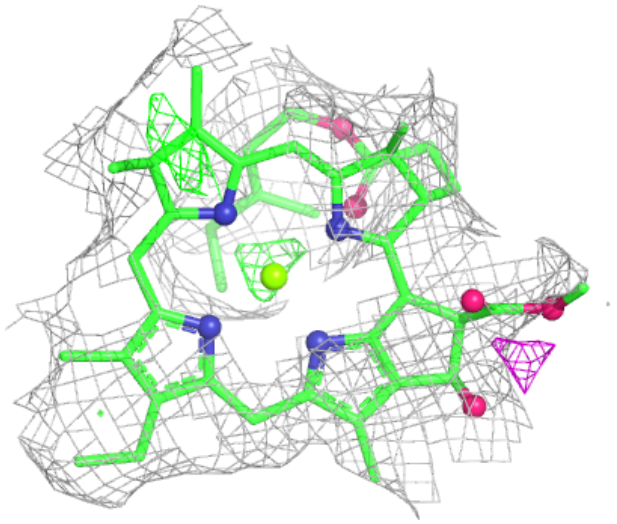


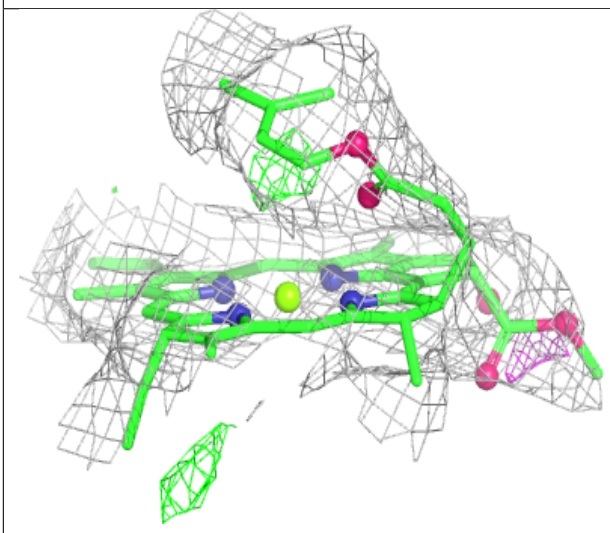


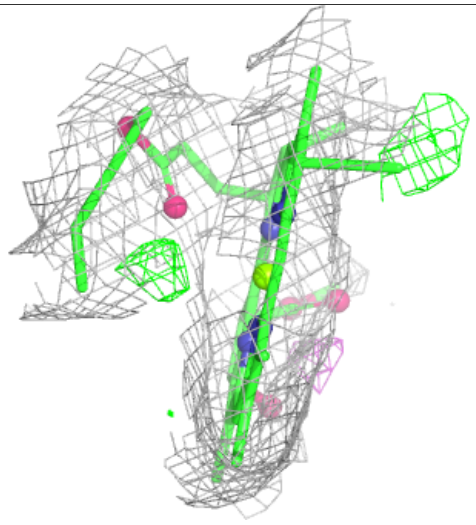


Electron density around CLA 2 2001:

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

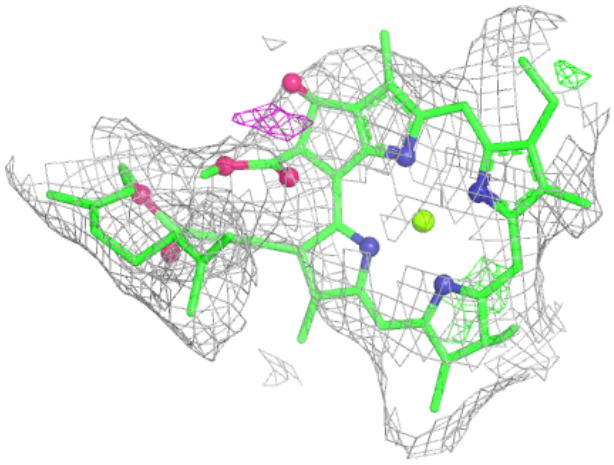


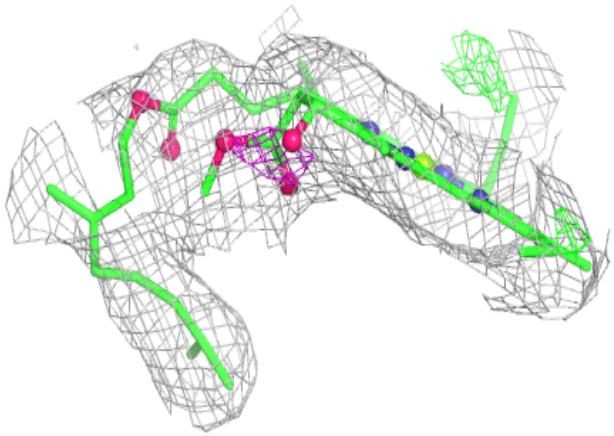


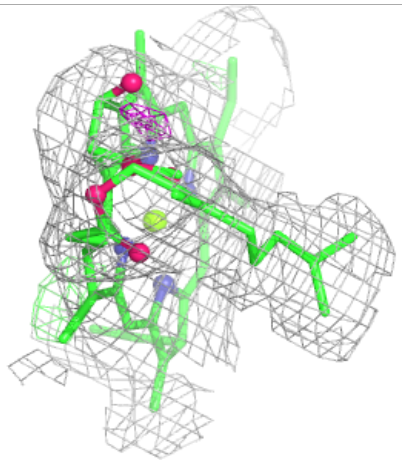


Electron density around CLA L 1148:

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

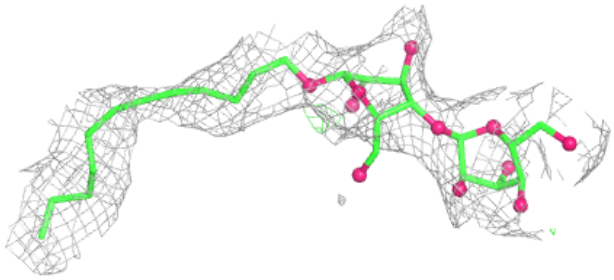


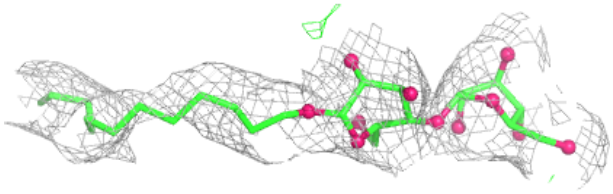


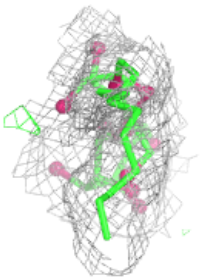


Electron density around LMU G 7051:

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

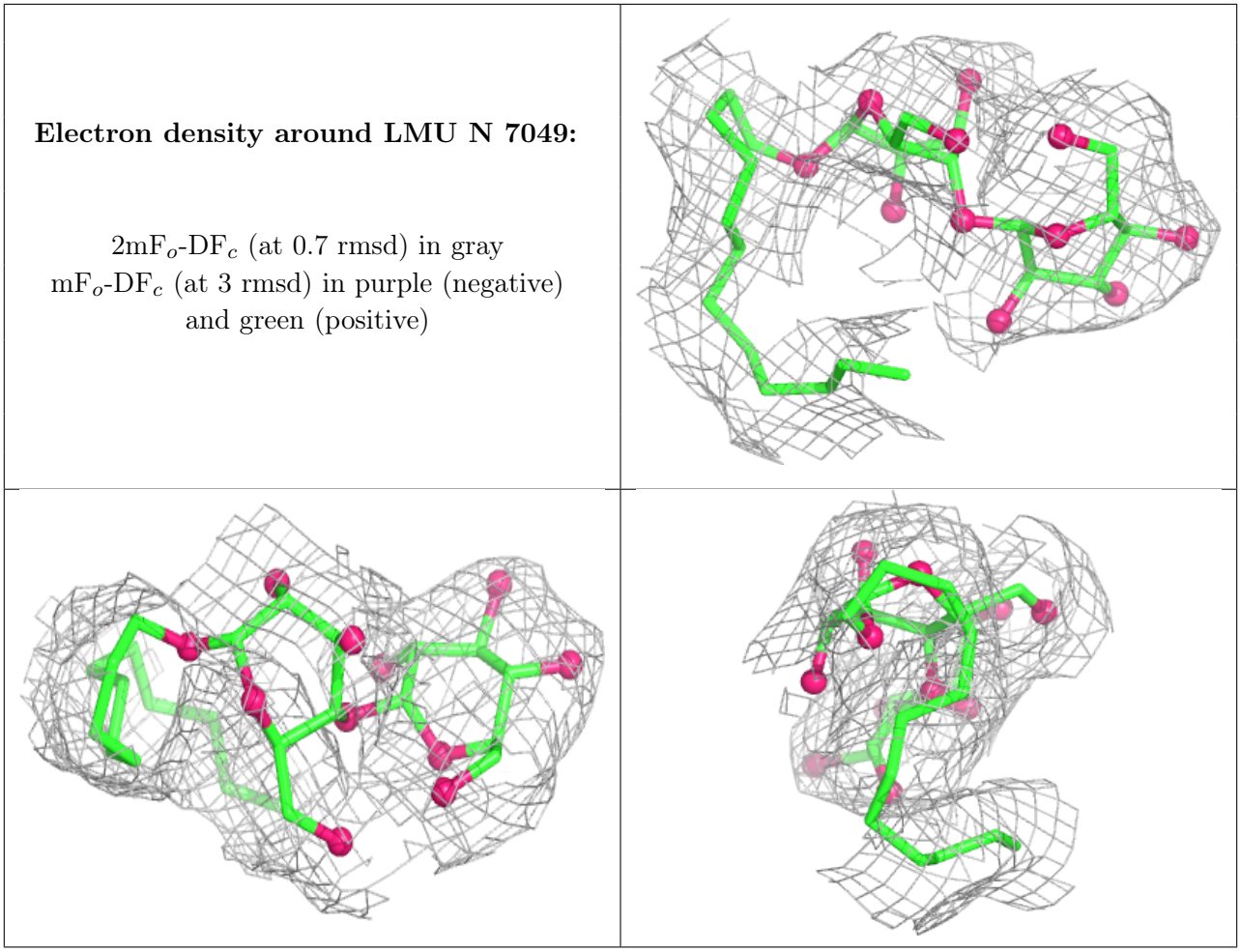






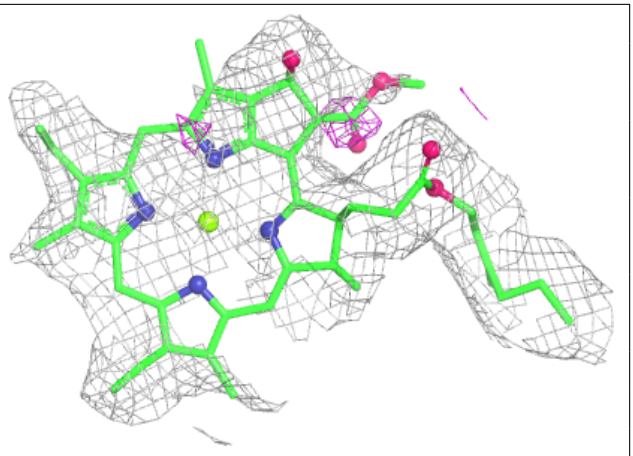
Electron density around LMU N 7049:

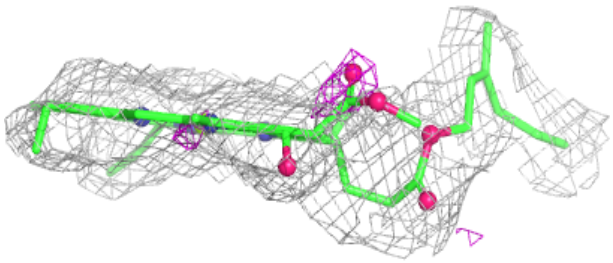
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

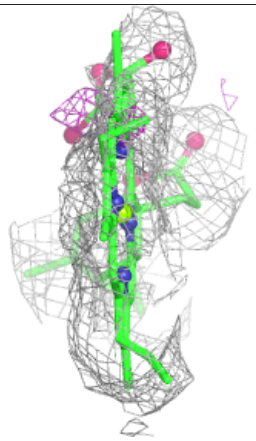


Electron density around CLA 4 4007:

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

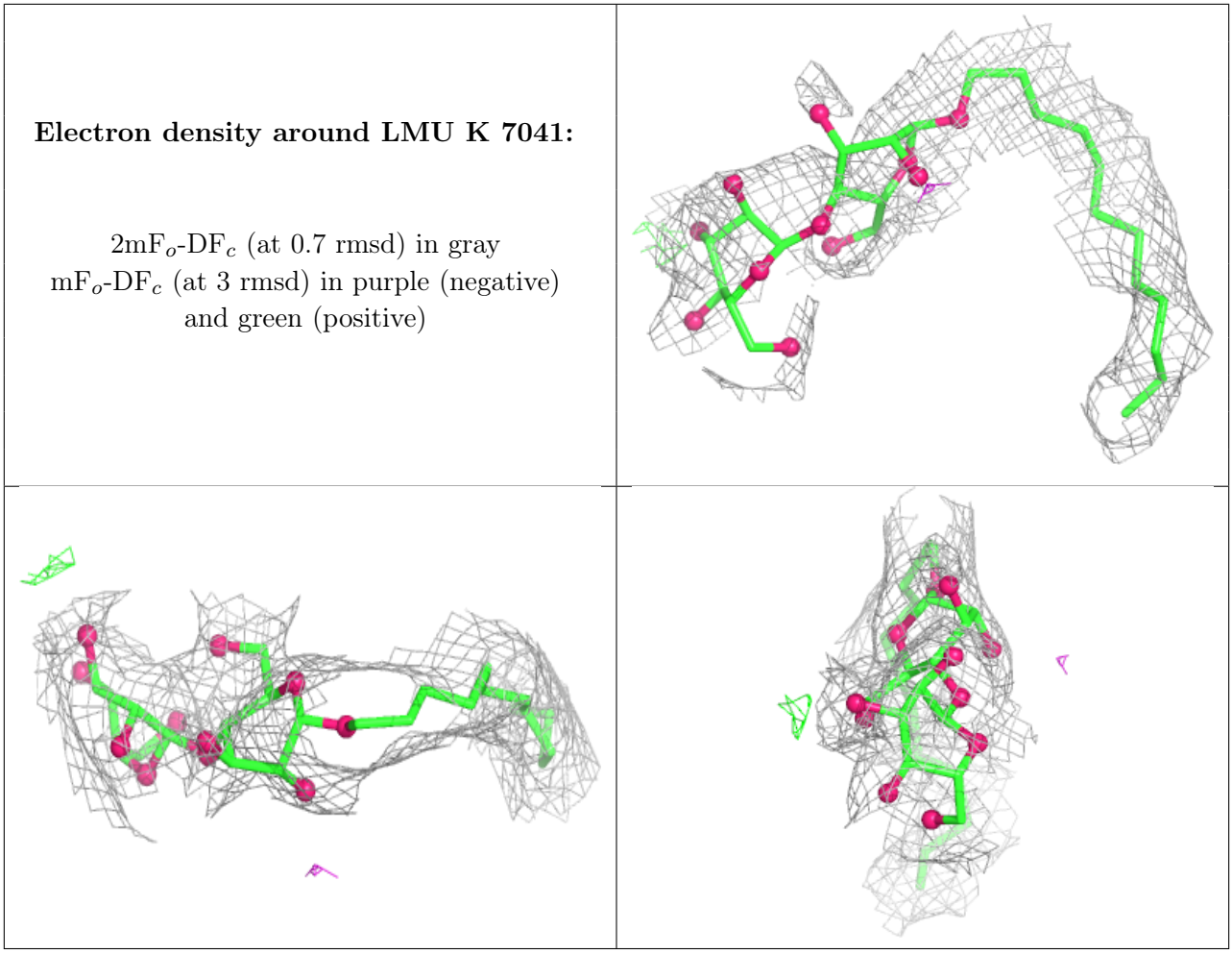






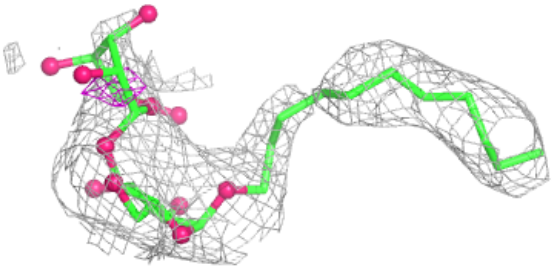
Electron density around LMU K 7041:

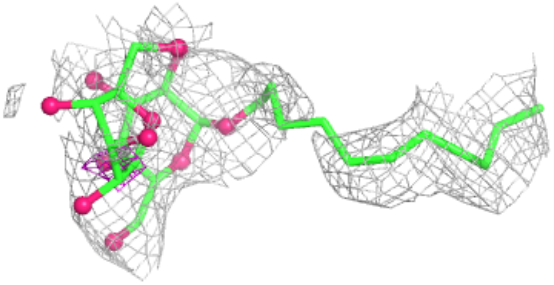
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

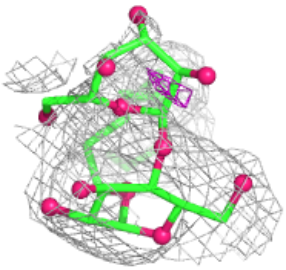


Electron density around LMU 4 7009:

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

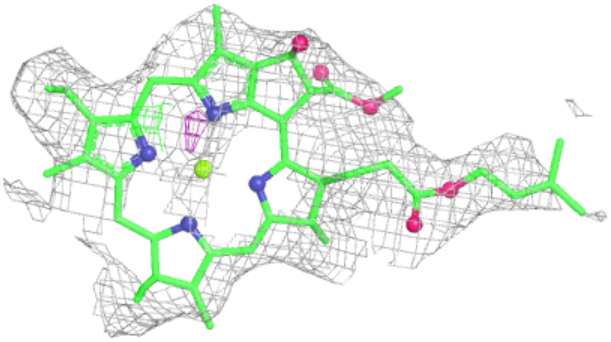


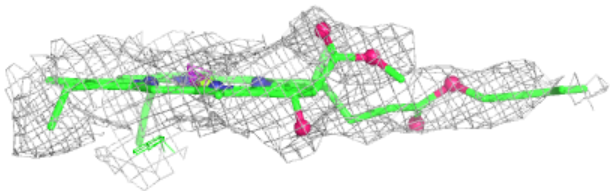




Electron density around CLA A 1151:

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

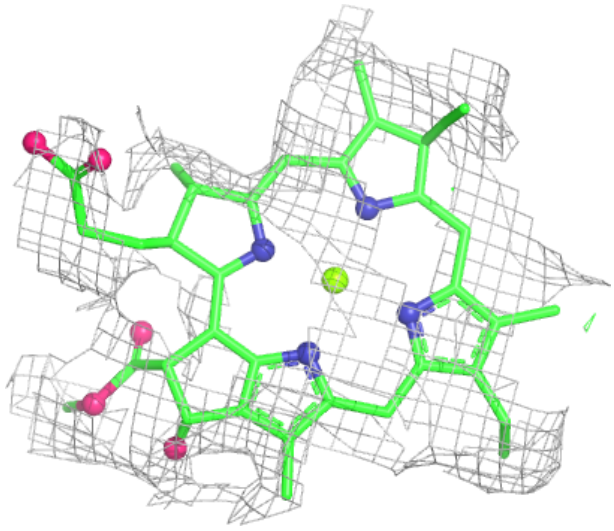


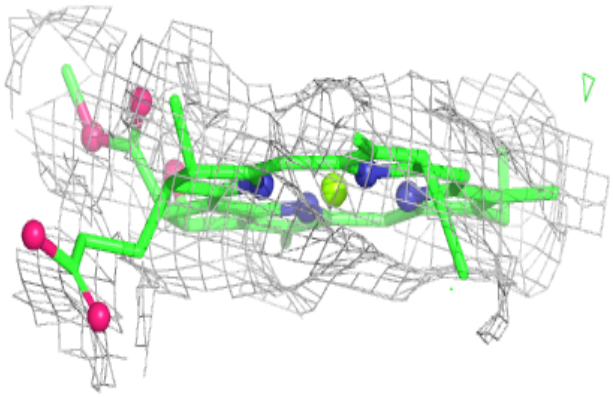


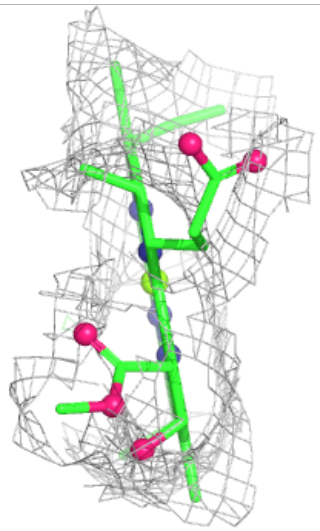


Electron density around CLA K 1142:

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

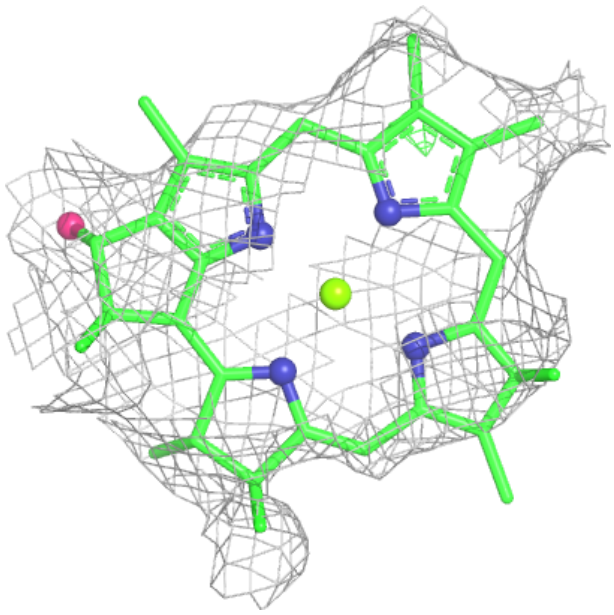


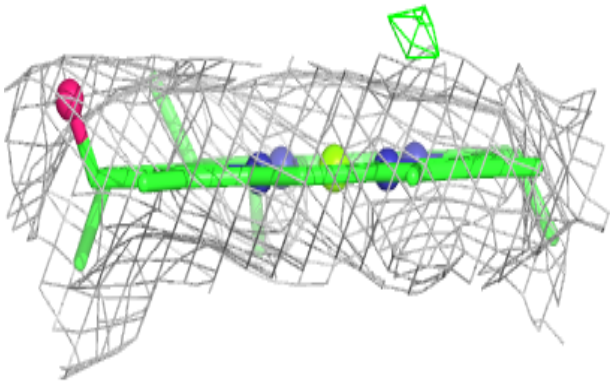


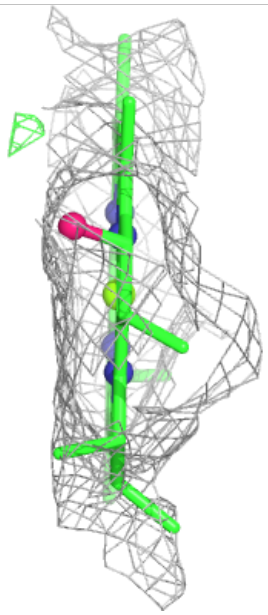


Electron density around CLA 3 1118:

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

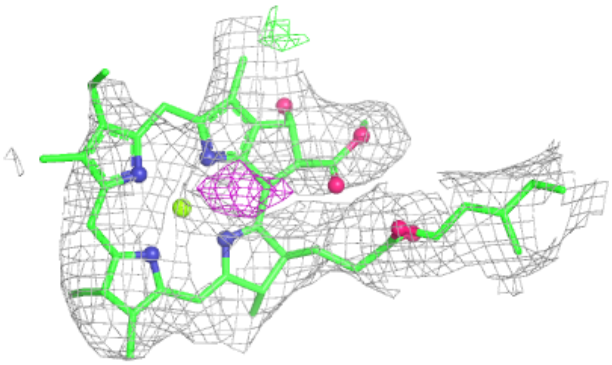


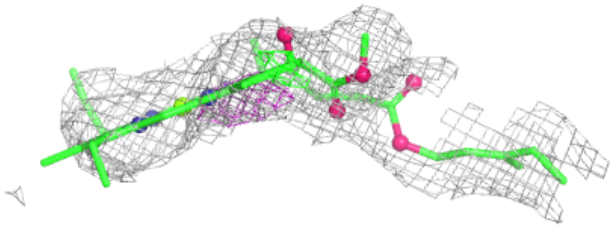


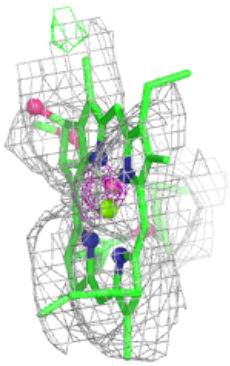


Electron density around CLA 1 1013:

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

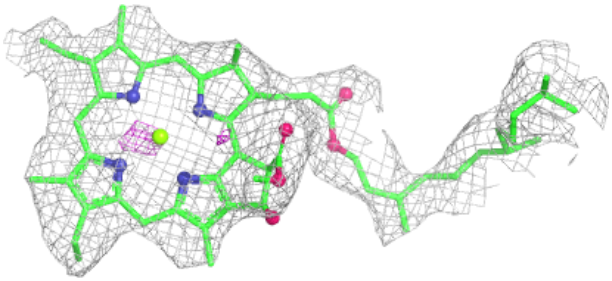


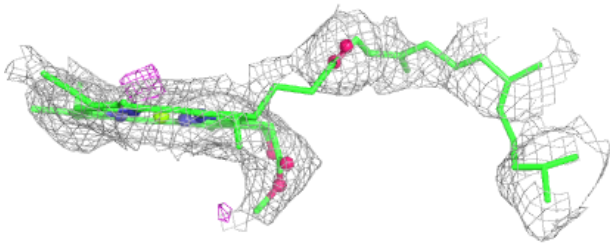


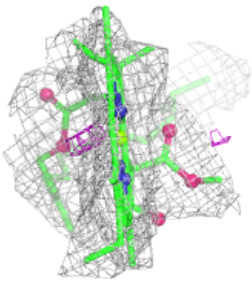


Electron density around CLA B 1212:

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

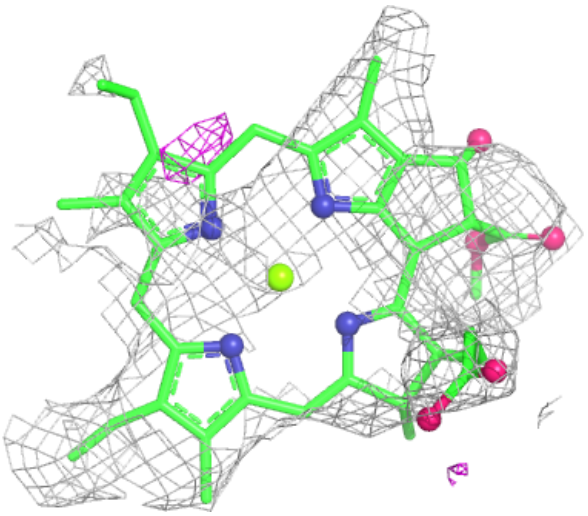


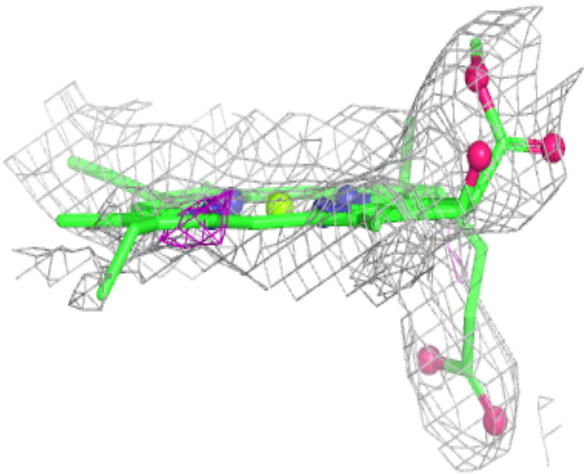




Electron density around CLA A 1112:

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

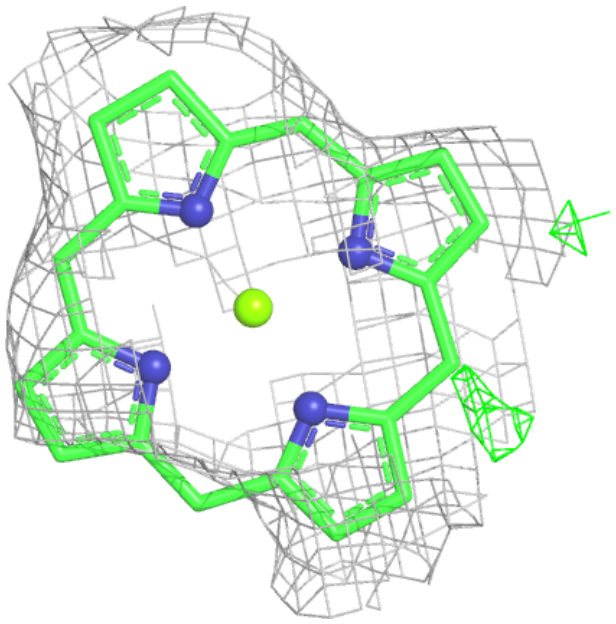


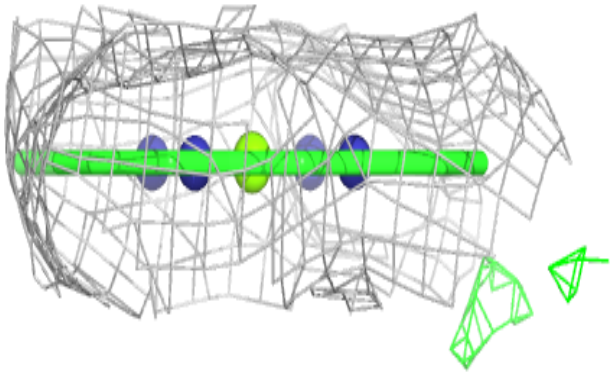


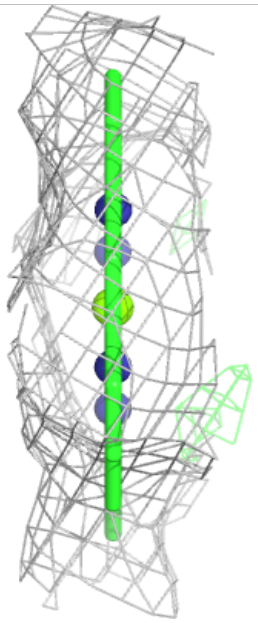


Electron density around CLA 2 2005:

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

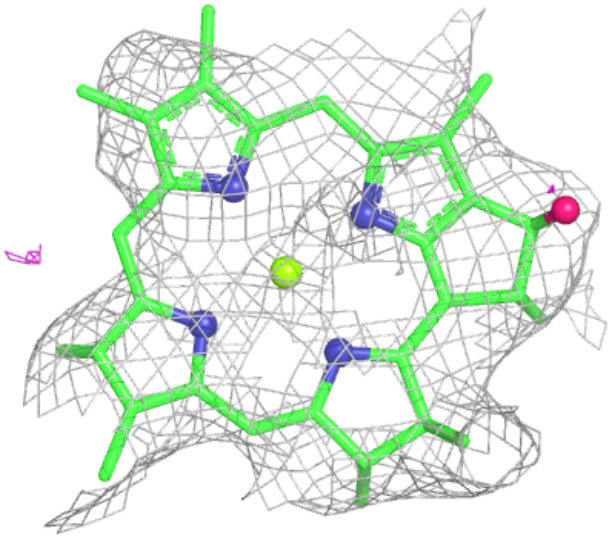


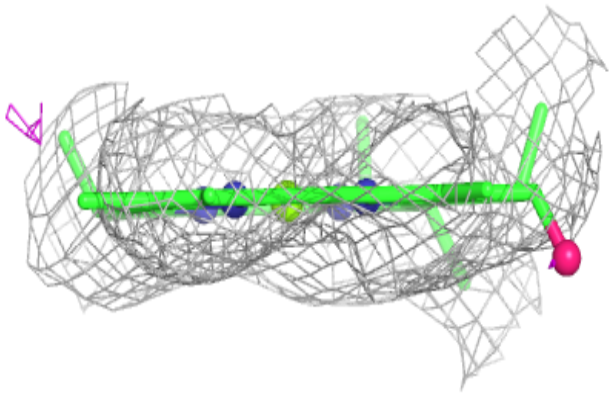


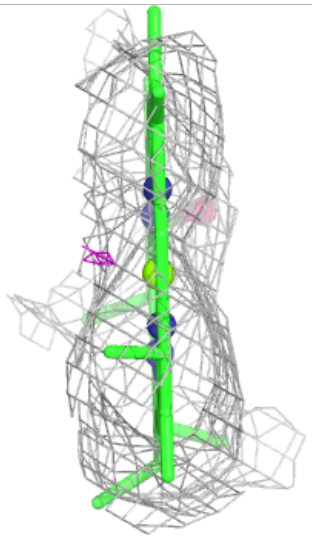


Electron density around CLA B 1301:

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

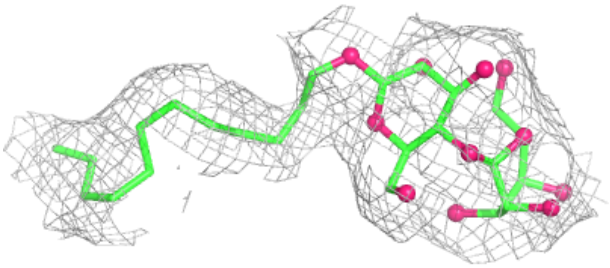


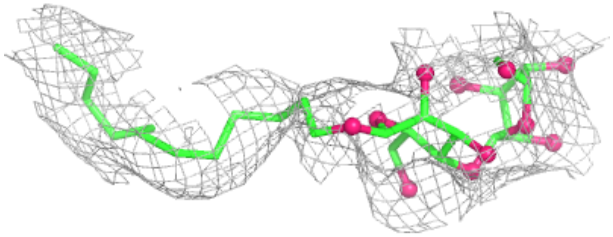


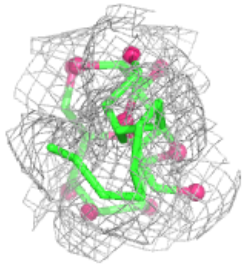


Electron density around LMU E 7048:

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

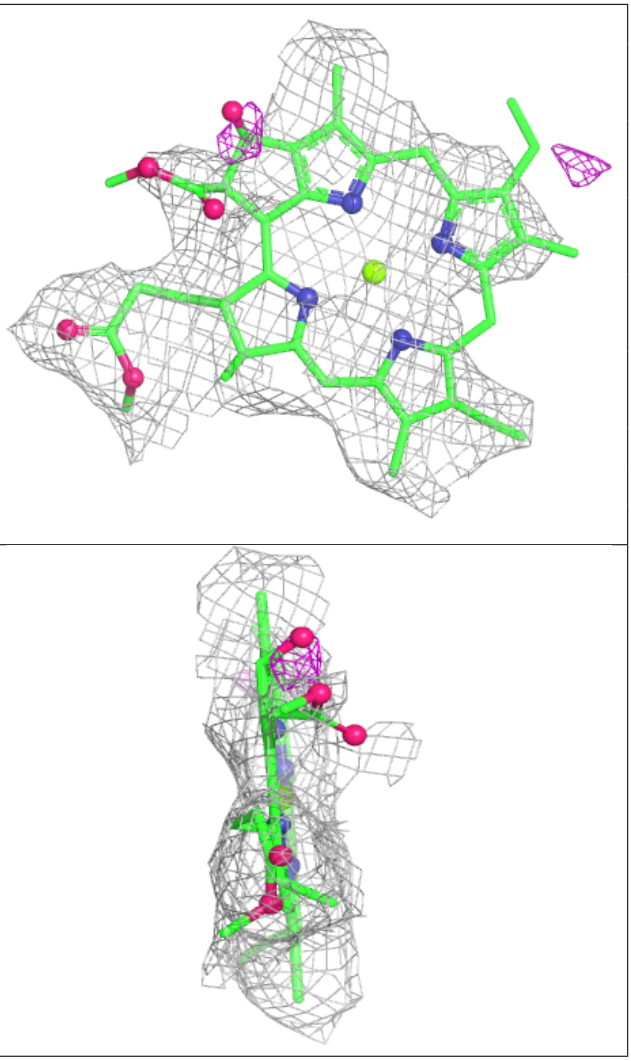






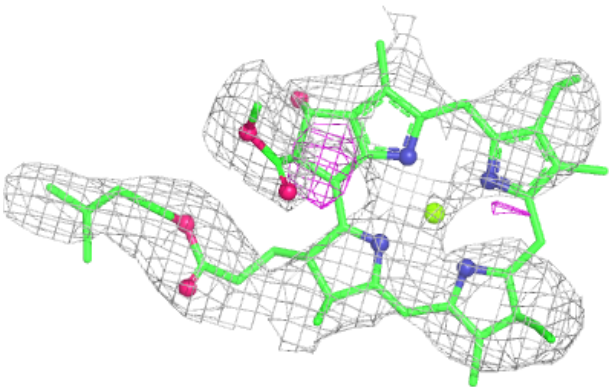
Electron density around CLA B 1213:

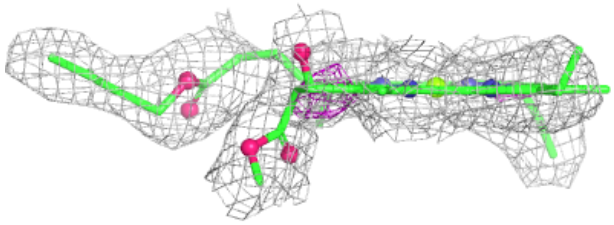
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 4 4001:

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

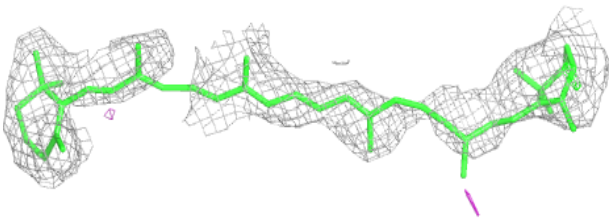


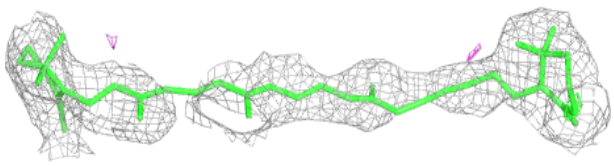


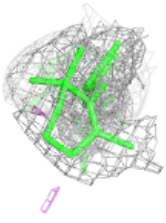


Electron density around BCR J 6012:

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

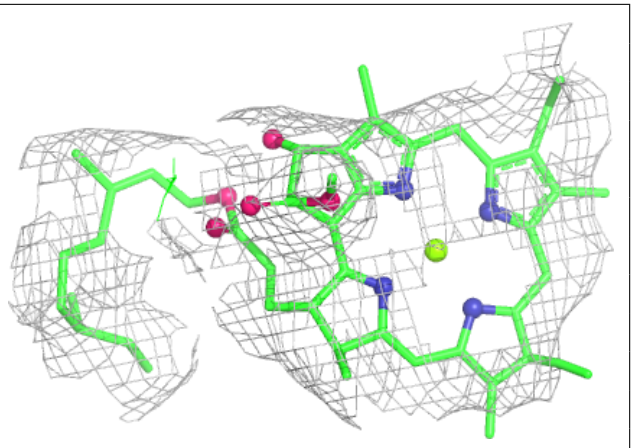


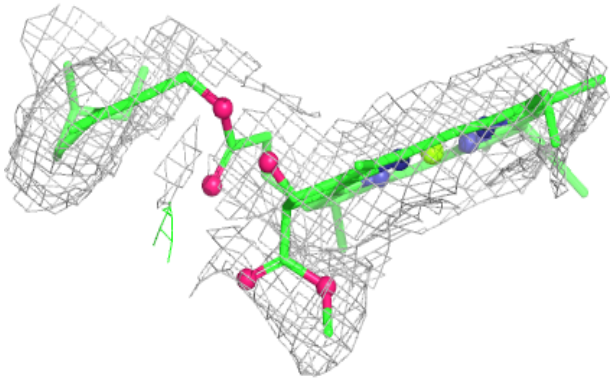


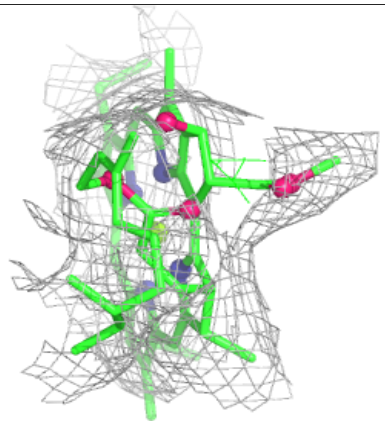


Electron density around CLA 3 2009:

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

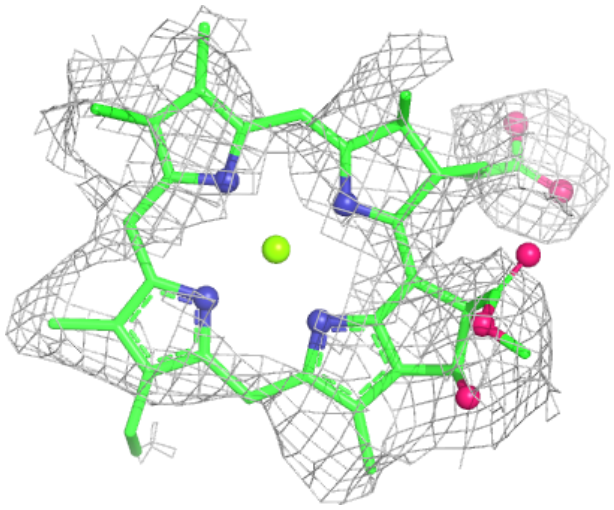


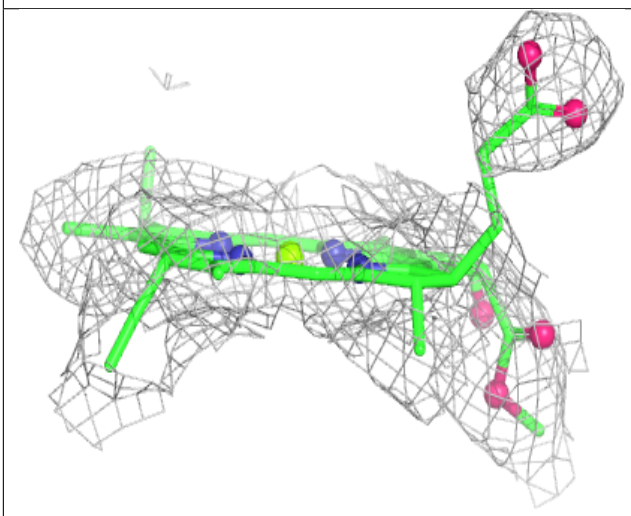


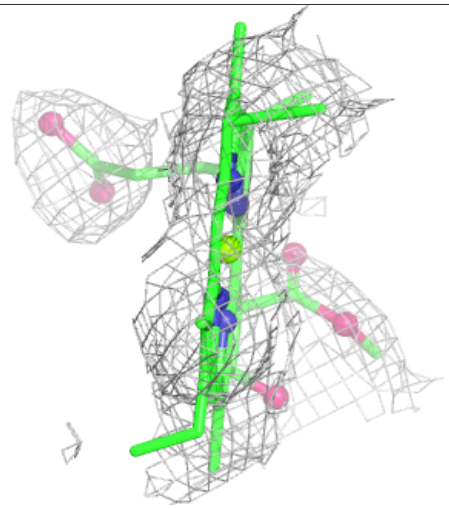


Electron density around CLA B 1232:

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

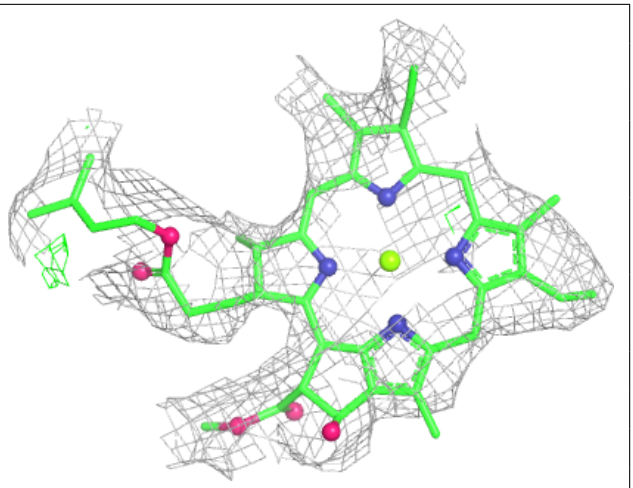


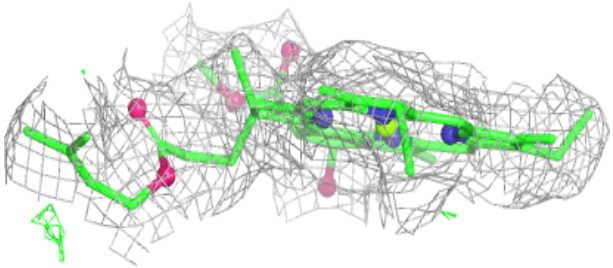


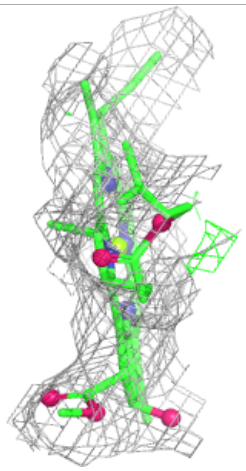


Electron density around CLA 2 2004:

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

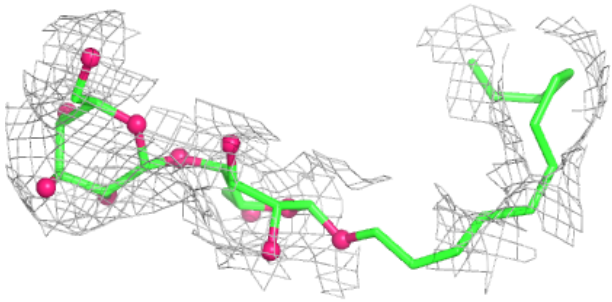


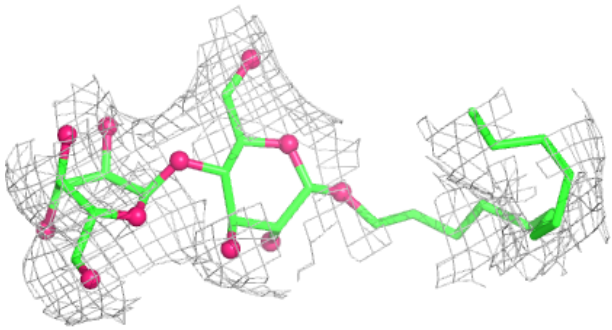


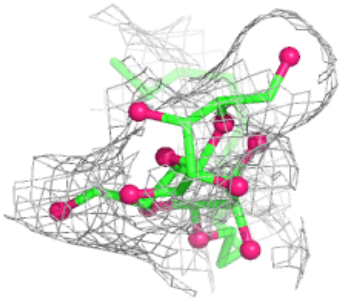


Electron density around LMU H 7043:

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

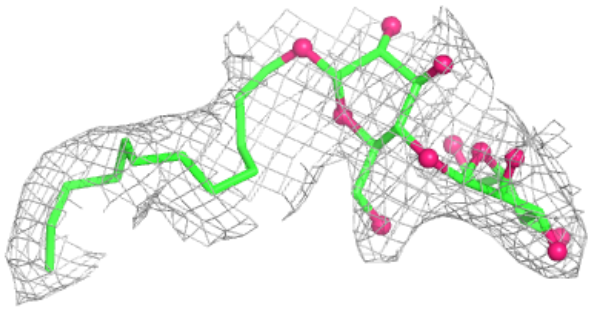


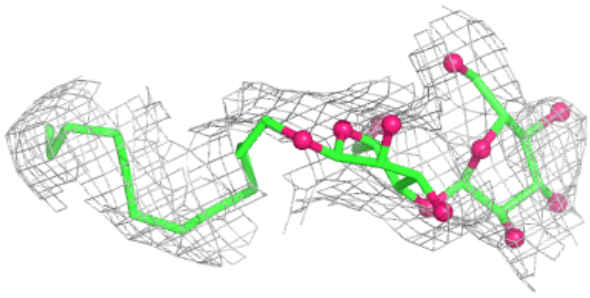


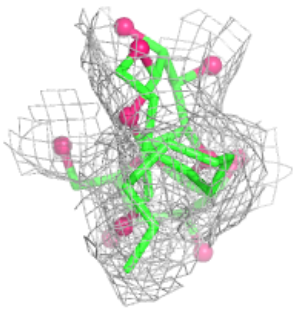


Electron density around LMU 2 7046:

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

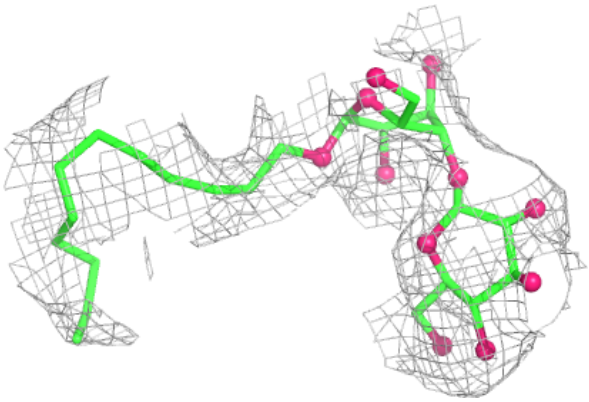


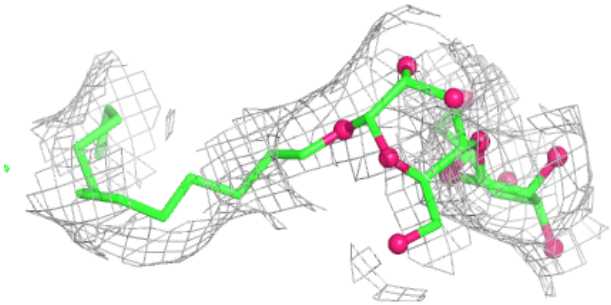


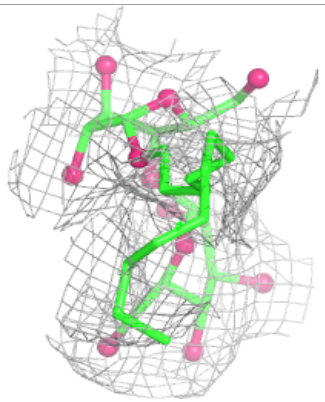


Electron density around LMU K 7001:

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

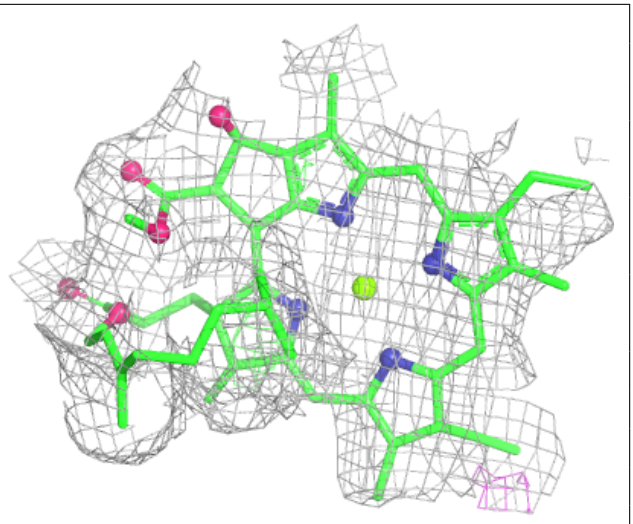


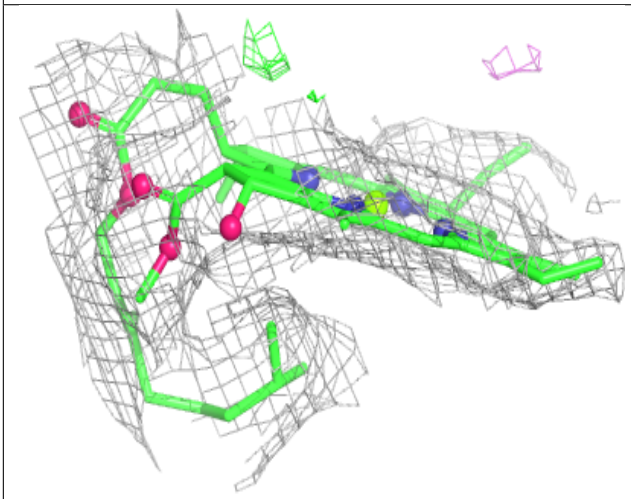




Electron density around CLA 4 1306:

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

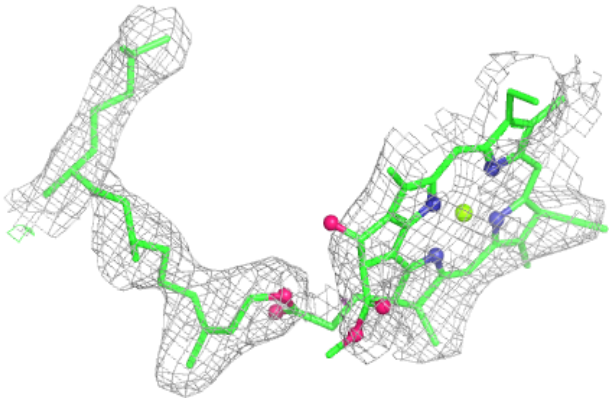


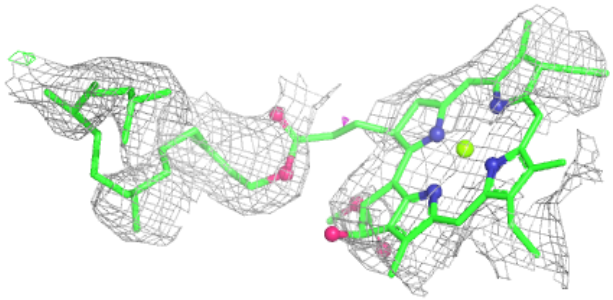


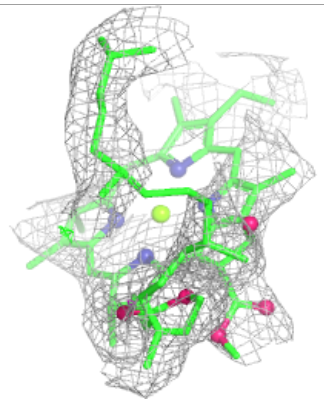


Electron density around CLA K 3009:

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

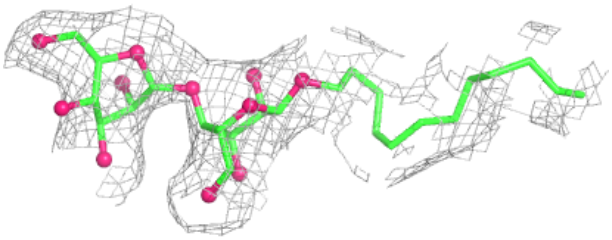


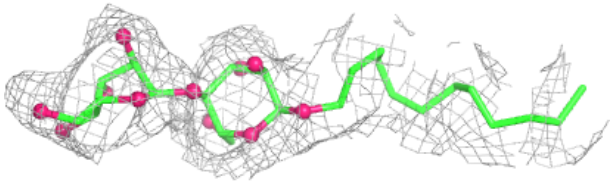


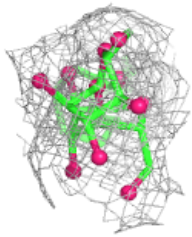


Electron density around LMU E 7037:

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

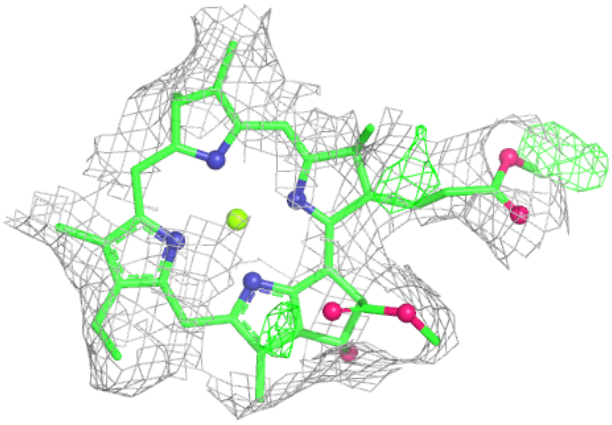


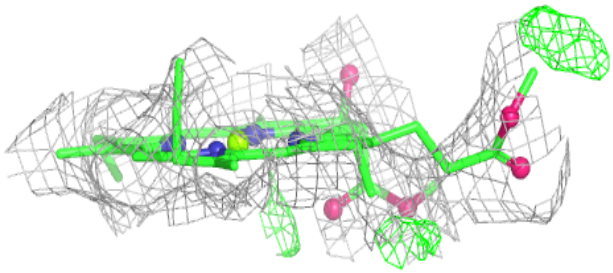


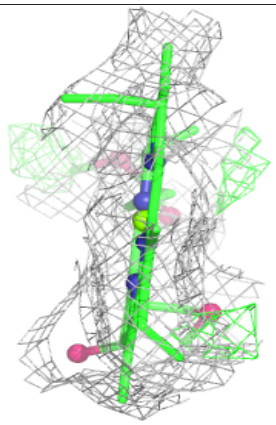


Electron density around CLA 1 1010:

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

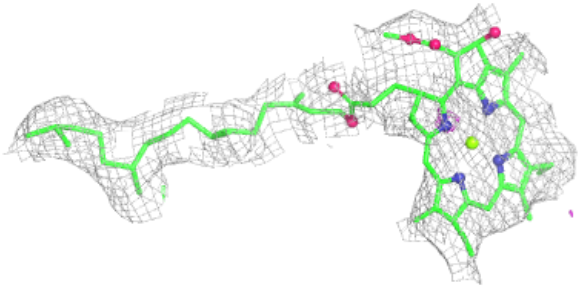


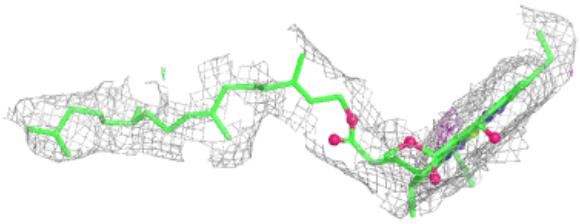


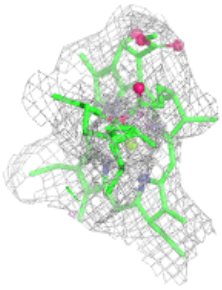


Electron density around CLA 4 1304:

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

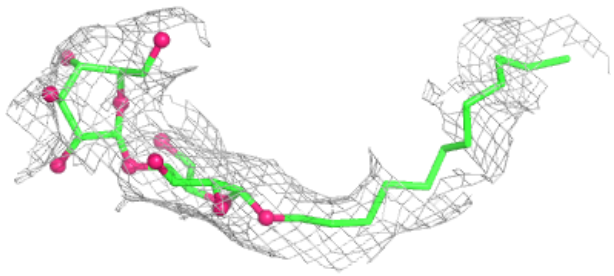


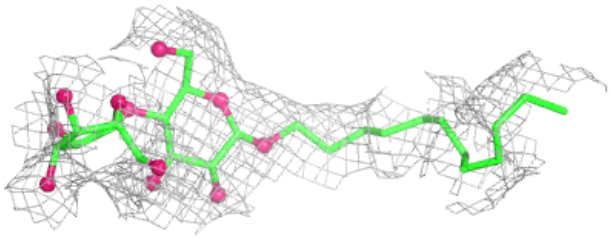


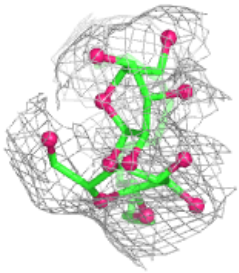


Electron density around LMU H 7017:

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

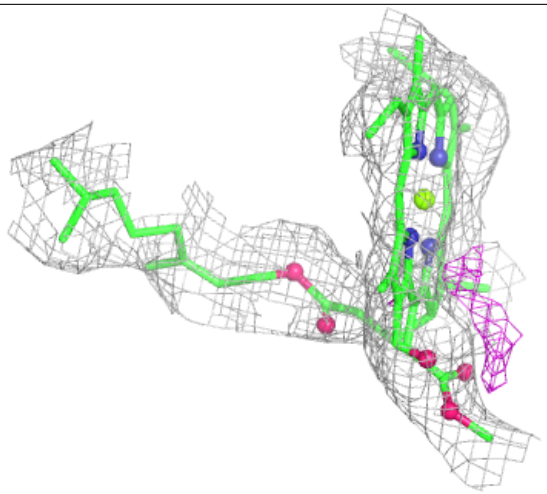


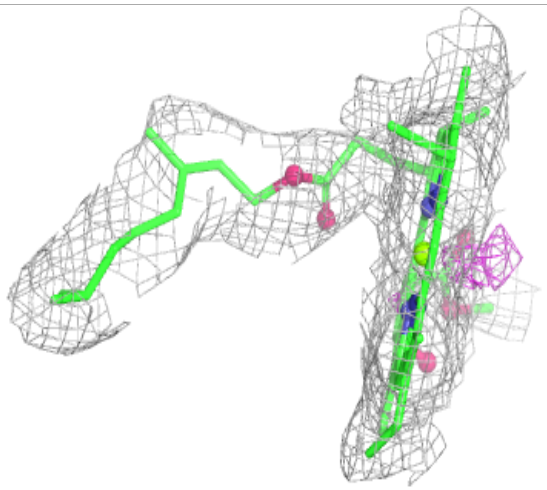


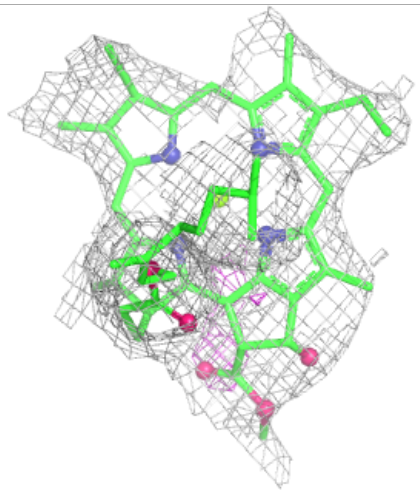


Electron density around CLA 4 1004:

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

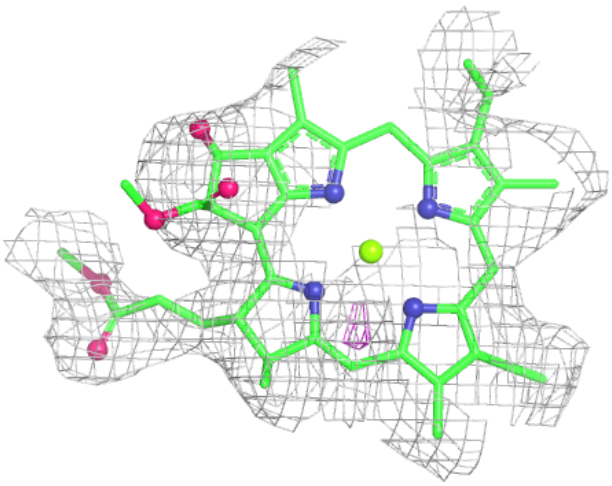


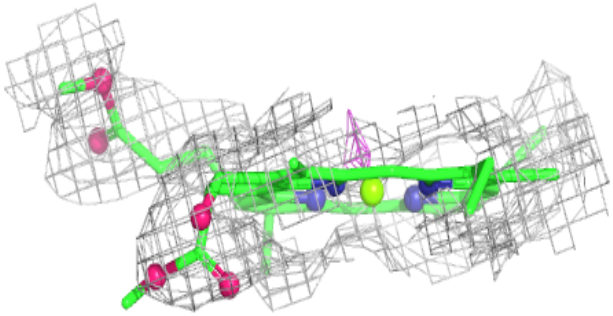


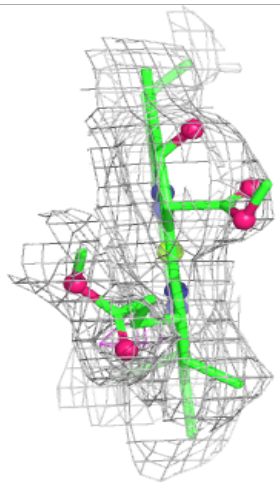


Electron density around CLA 4 4015:

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

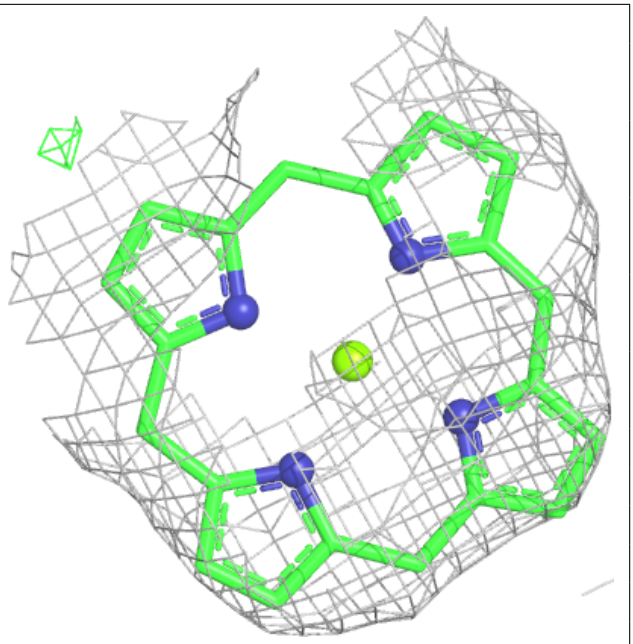


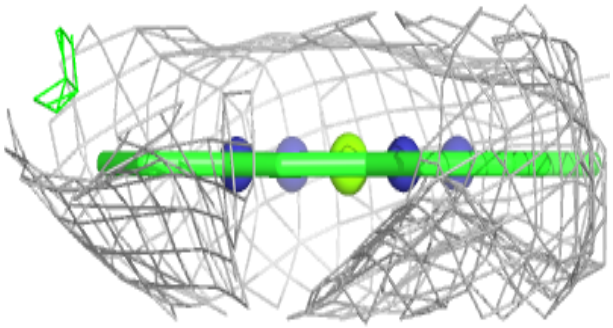


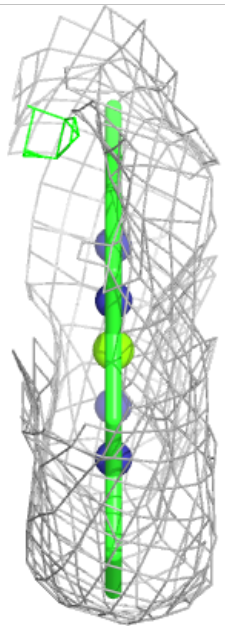


Electron density around CLA 3 3006:

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

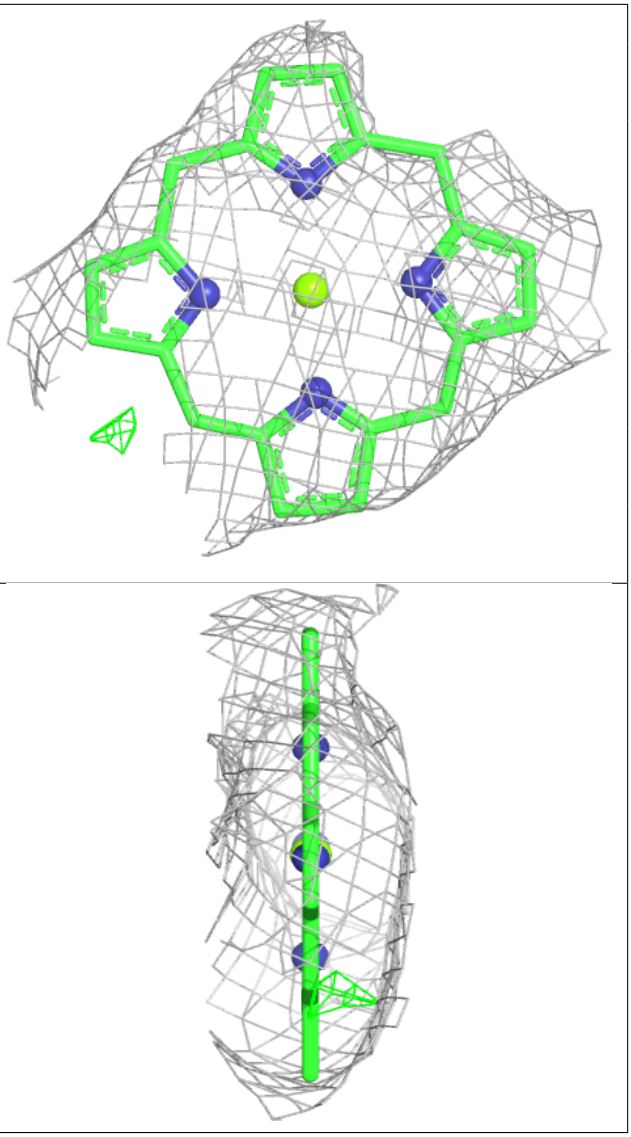


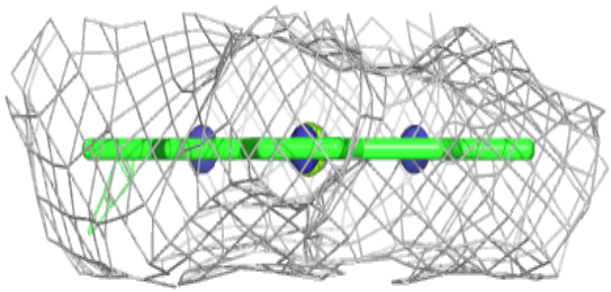




Electron density around CLA 1 1310:

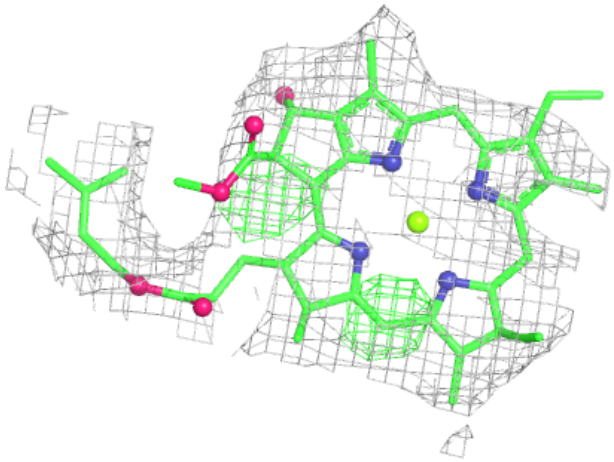
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

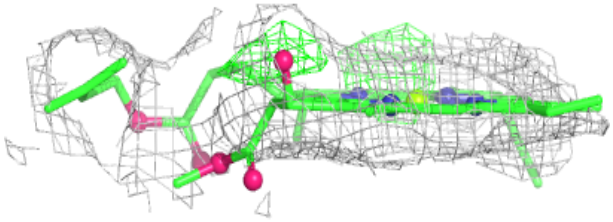


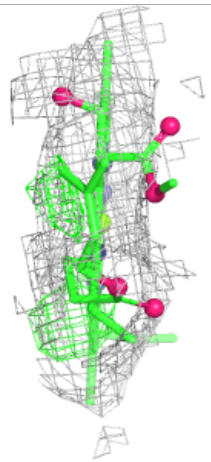


Electron density around CLA 2 2013:

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

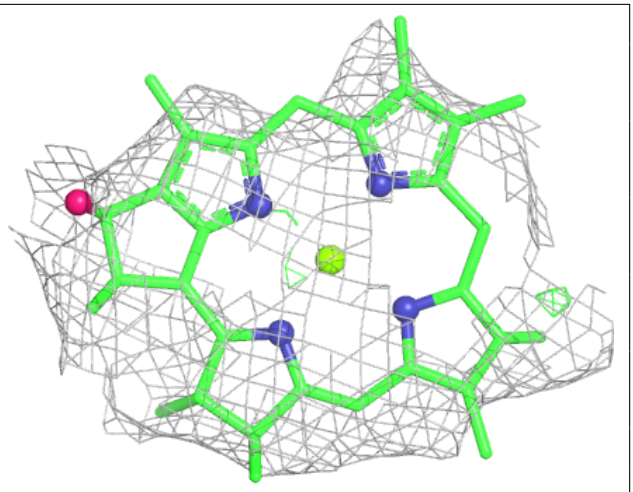


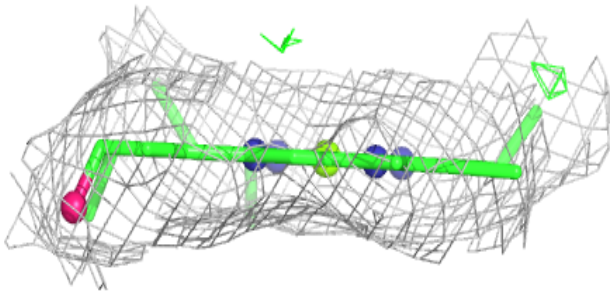


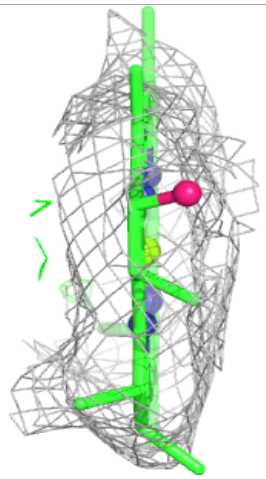


Electron density around CLA 3 3003:

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

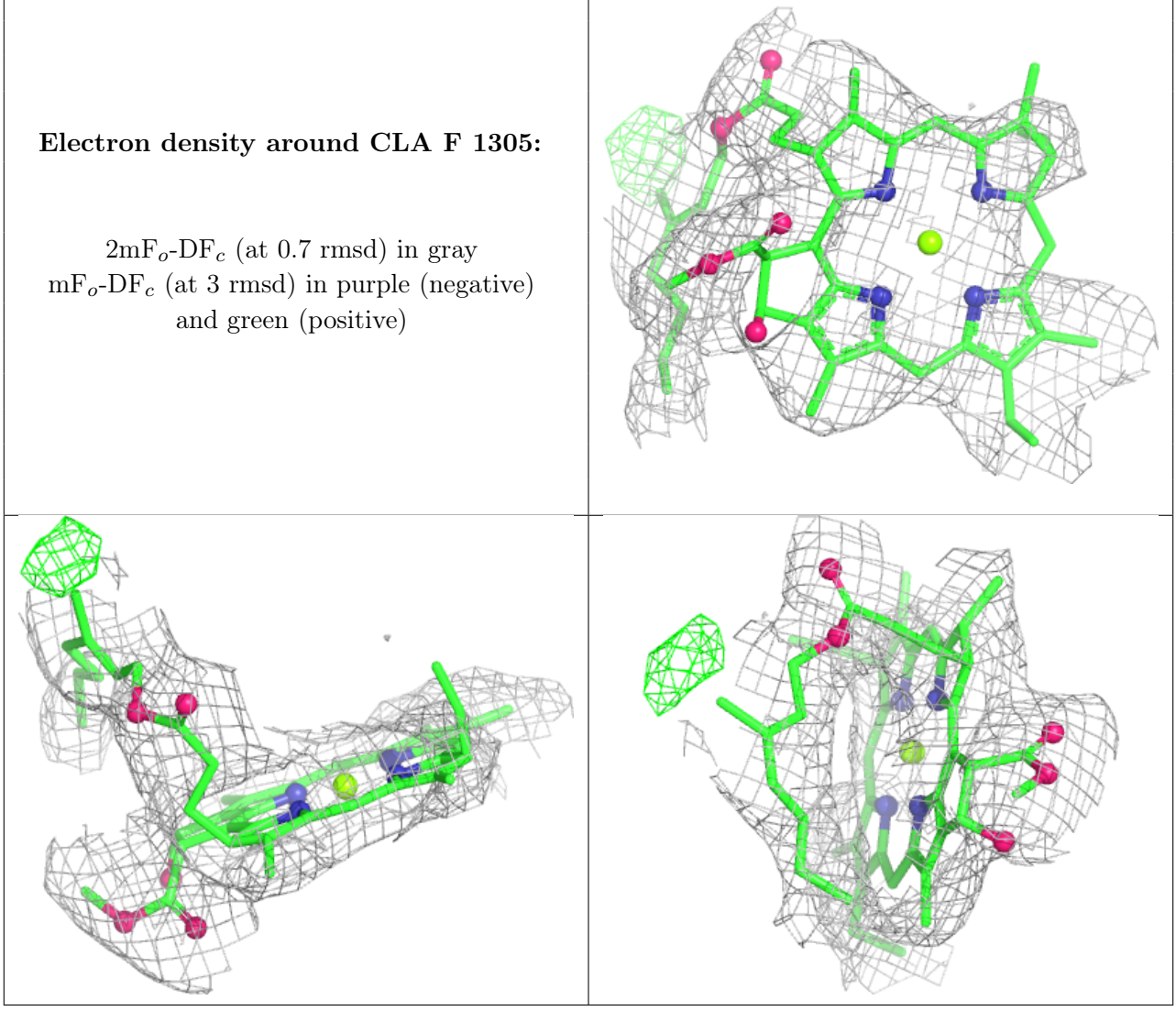






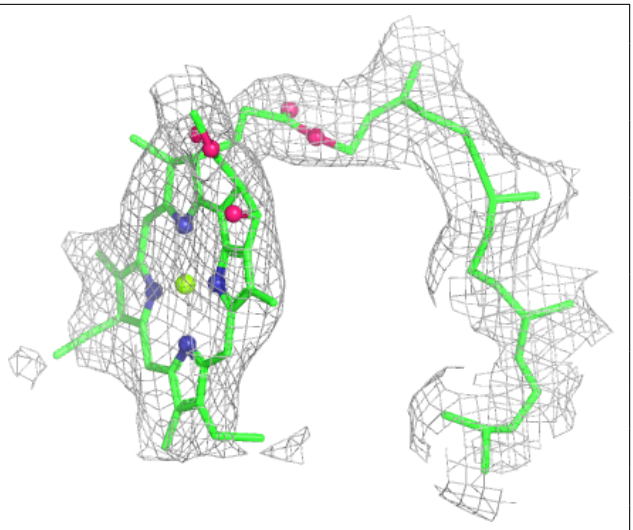
Electron density around CLA F 1305:

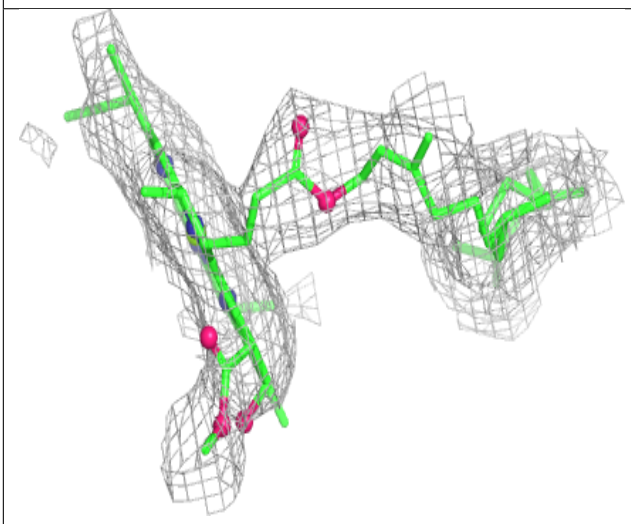
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

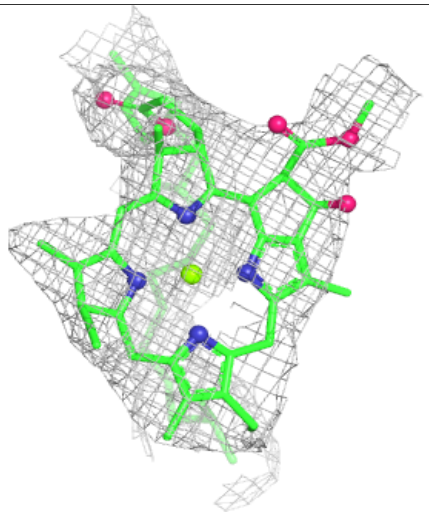


Electron density around CLA 3 3013:

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

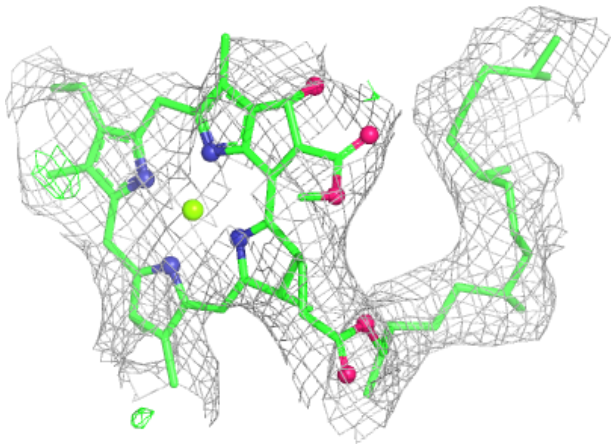


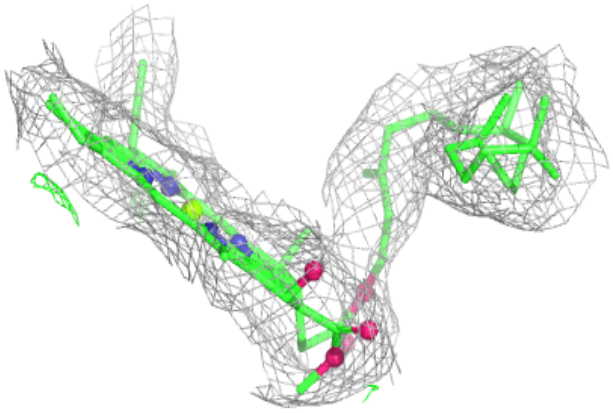


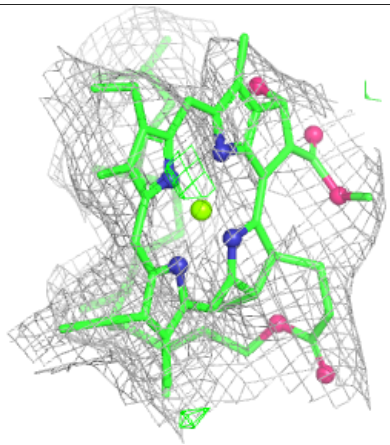


Electron density around CLA H 1145:

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

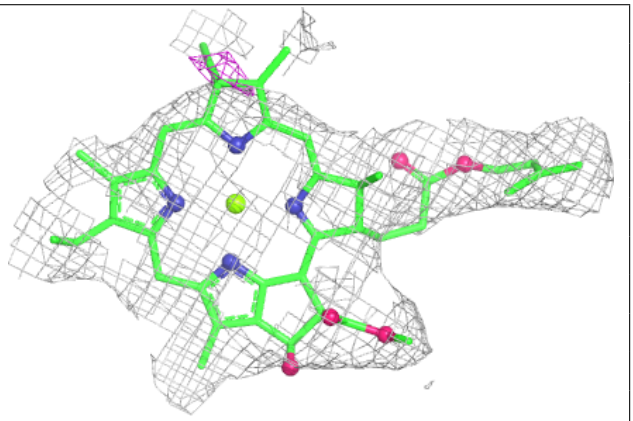


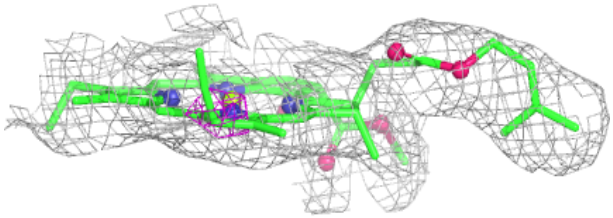


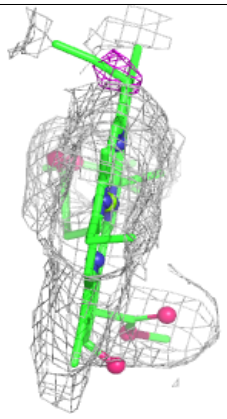


Electron density around CLA K 1143:

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

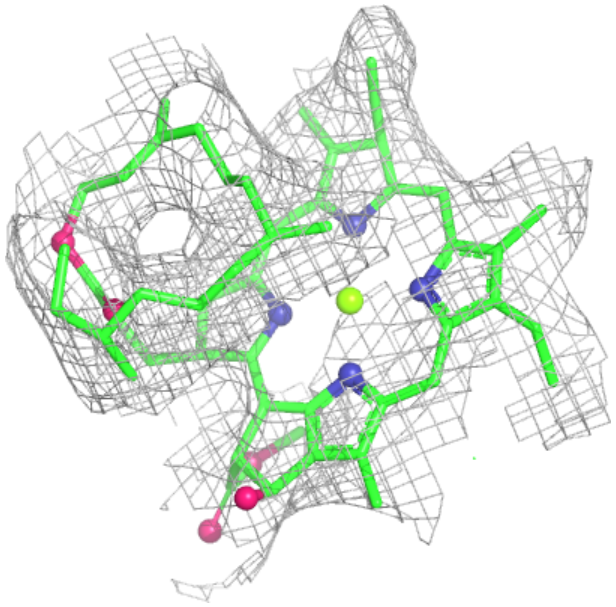


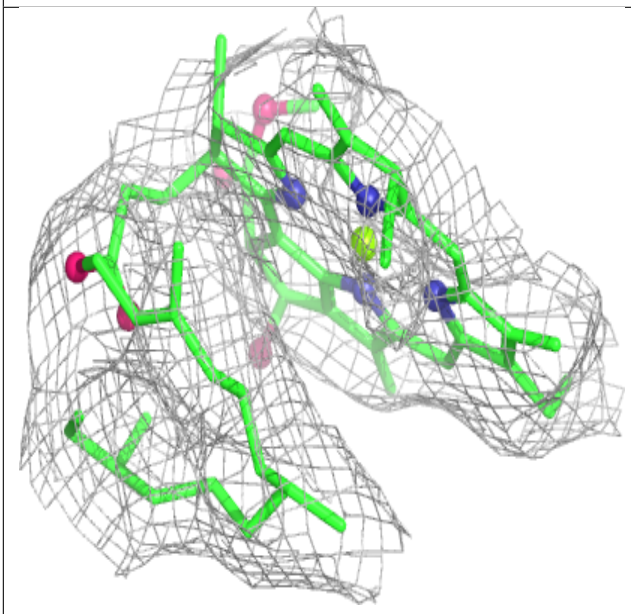


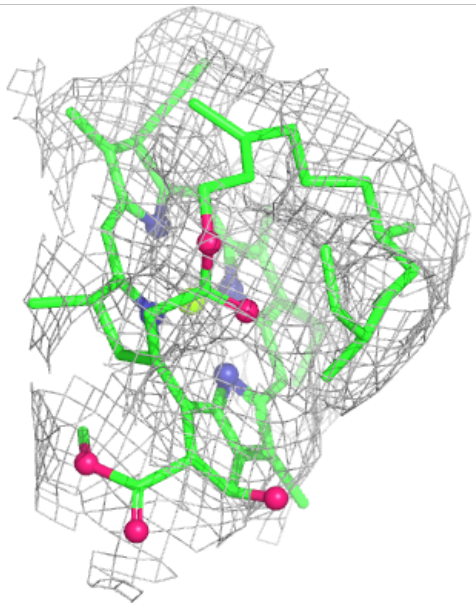


Electron density around CLA J 1311:

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

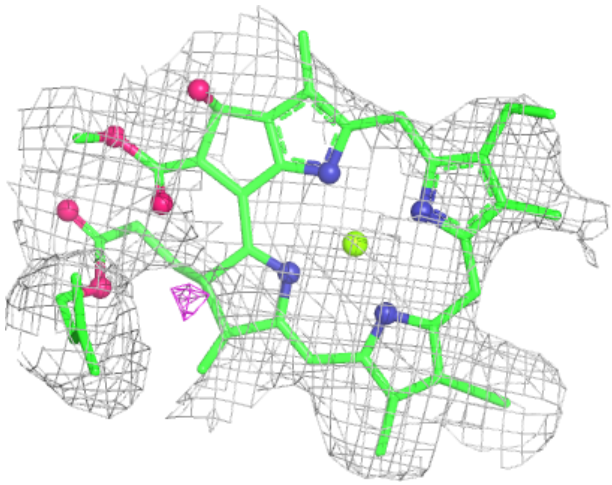


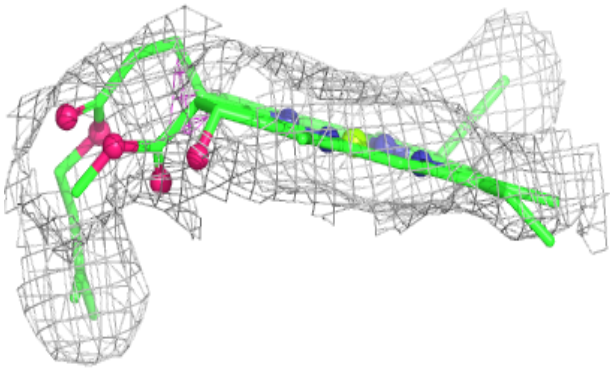


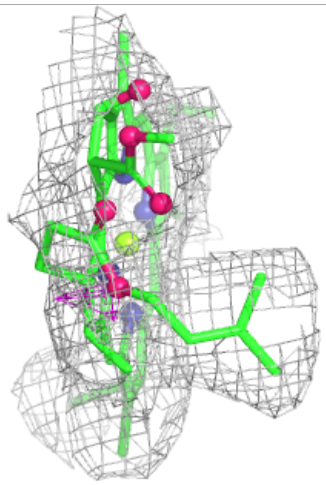


Electron density around CLA 3 3008:

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

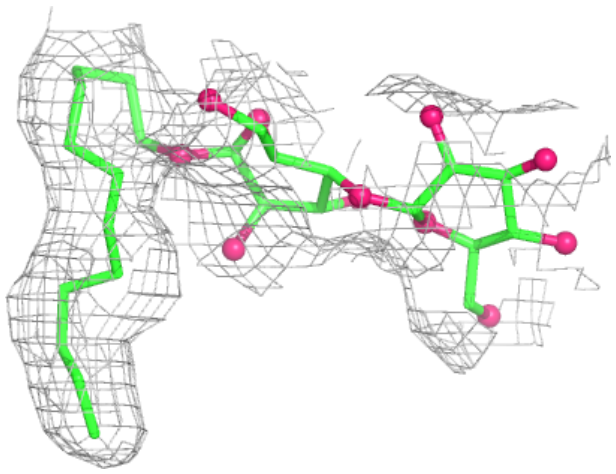


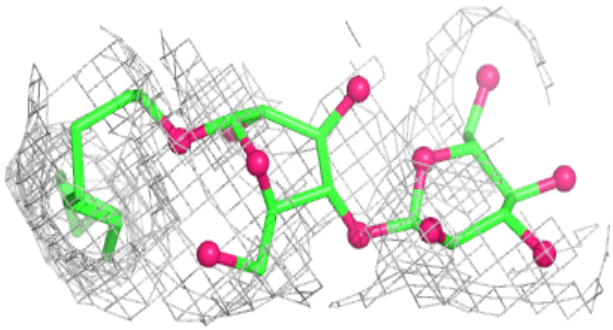


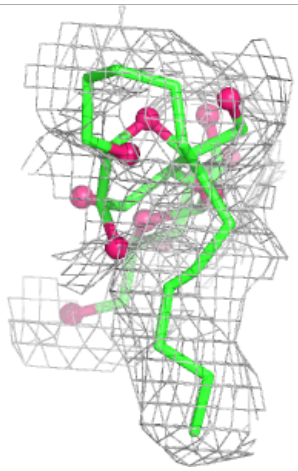


Electron density around LMU 4 7052:

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

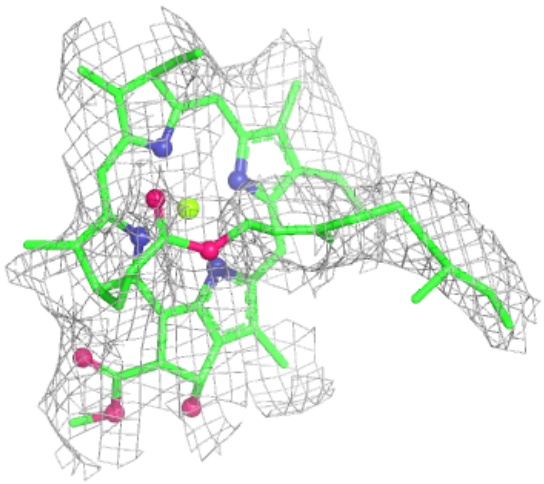


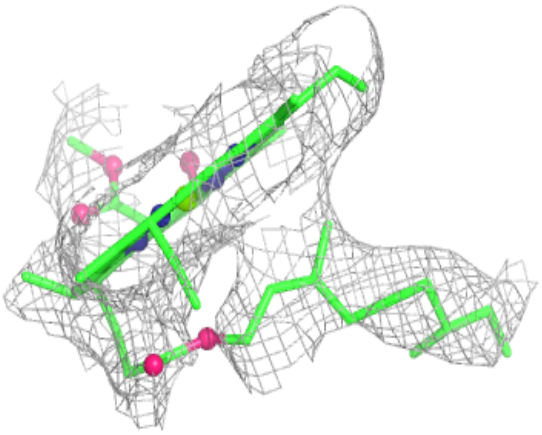


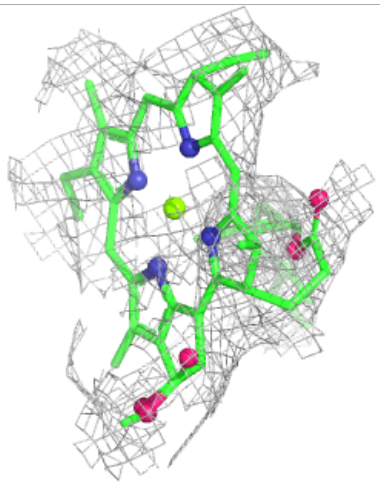


Electron density around CLA 2 2002:

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

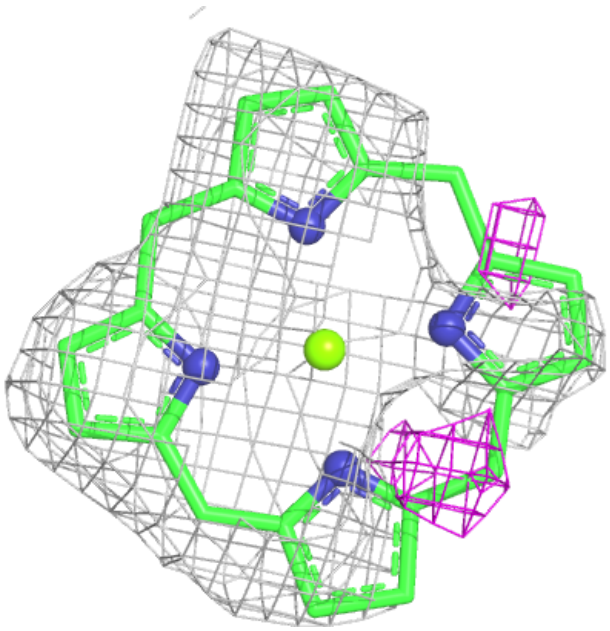


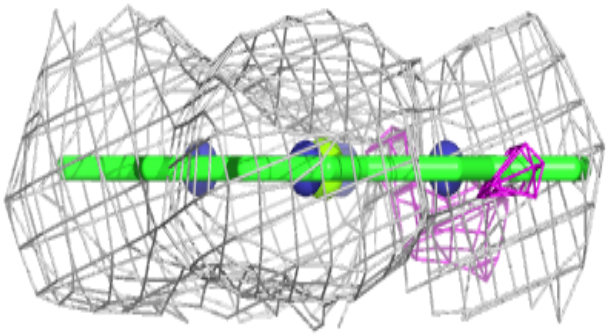


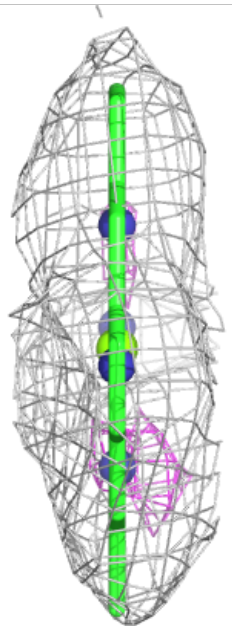


Electron density around CLA 2 1307:

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

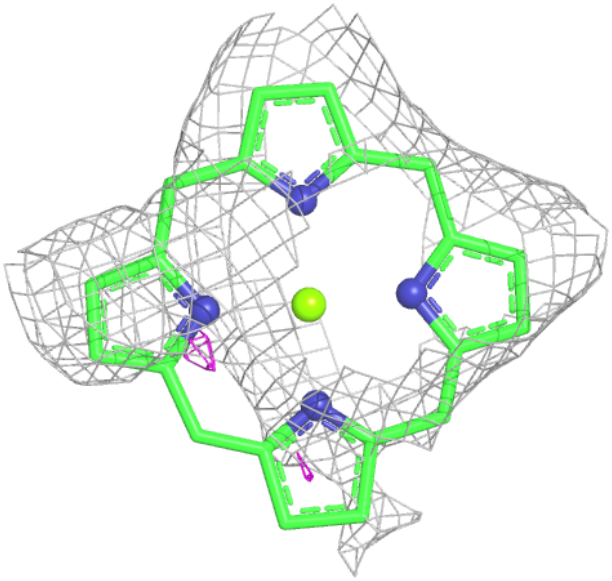


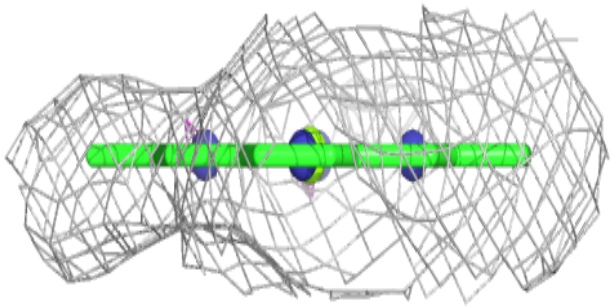


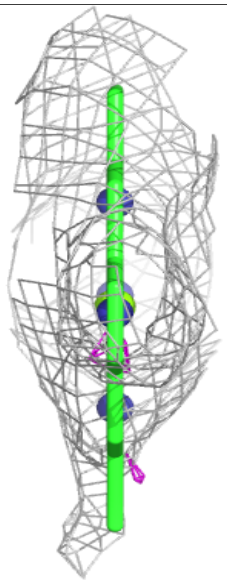


Electron density around CLA 3 3015:

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

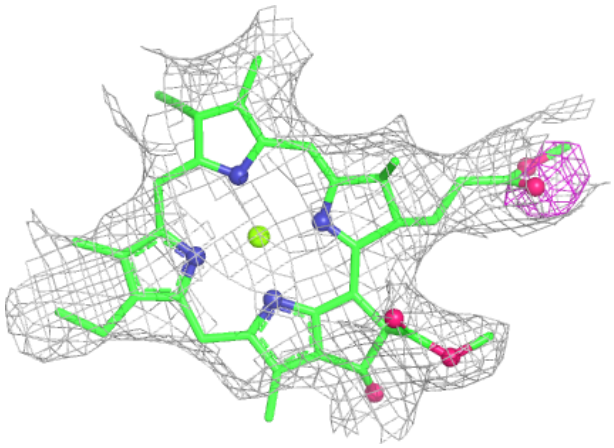


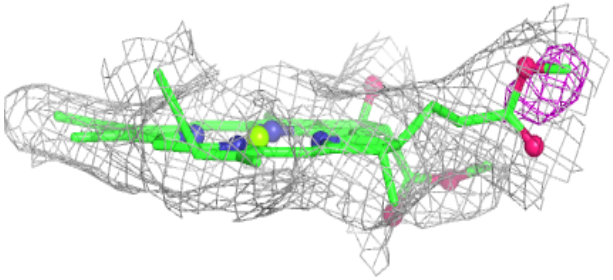


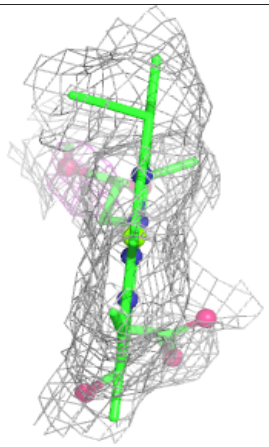


Electron density around CLA 3 1147:

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

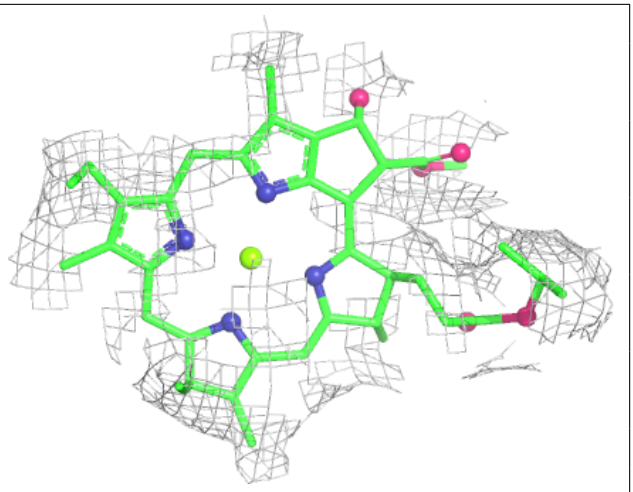


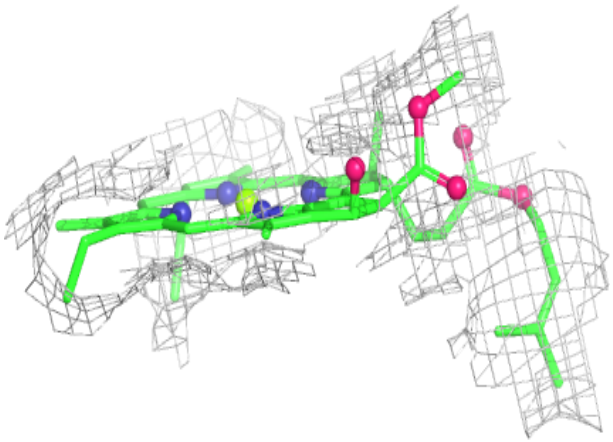


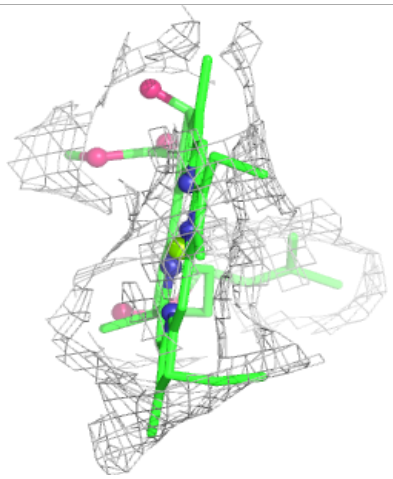


Electron density around CLA 3 3017:

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

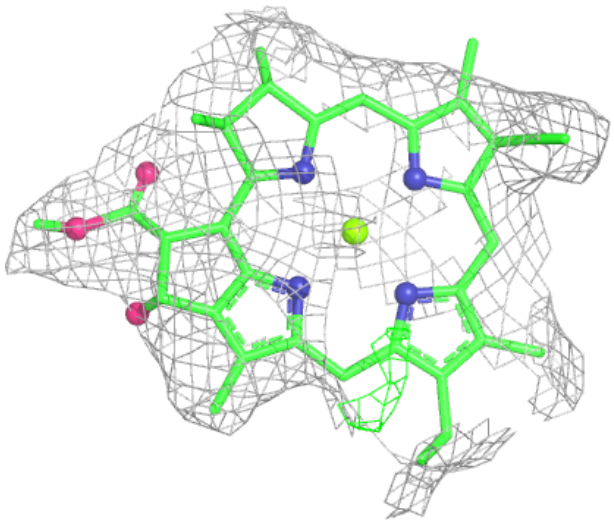


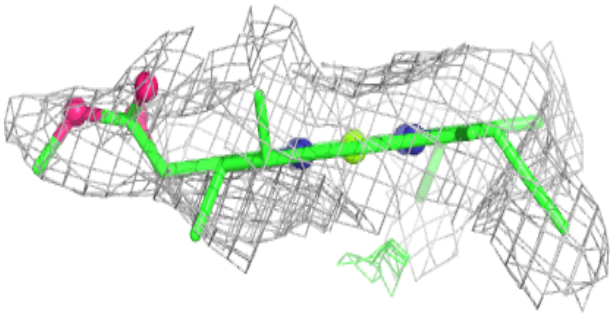


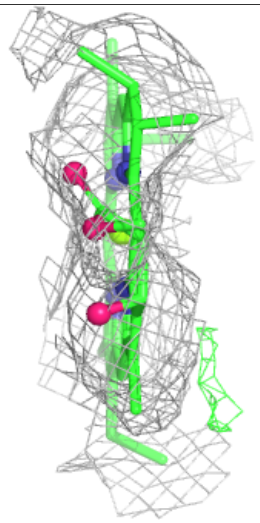


Electron density around CLA F 1302:

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

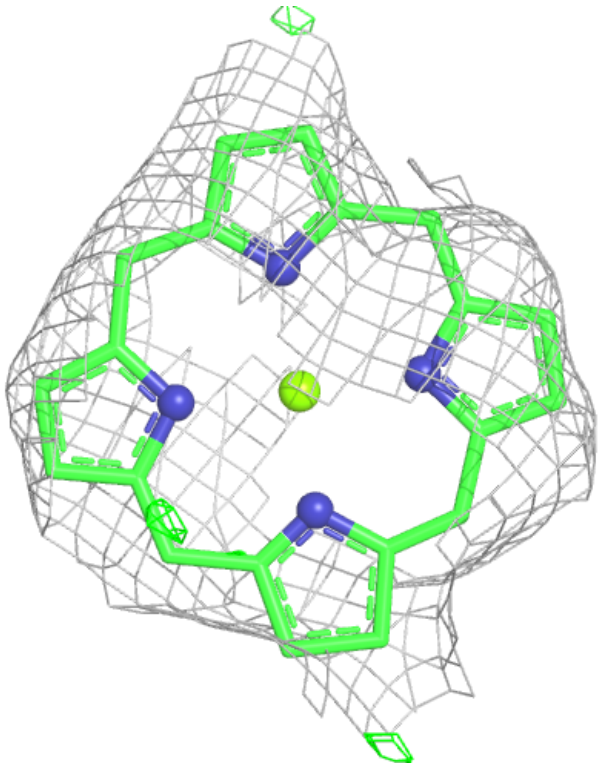


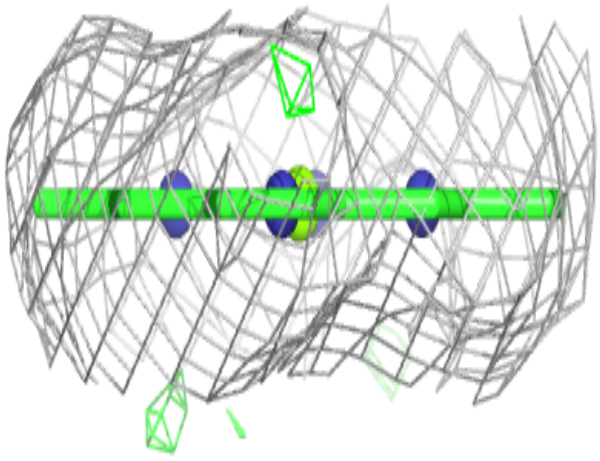


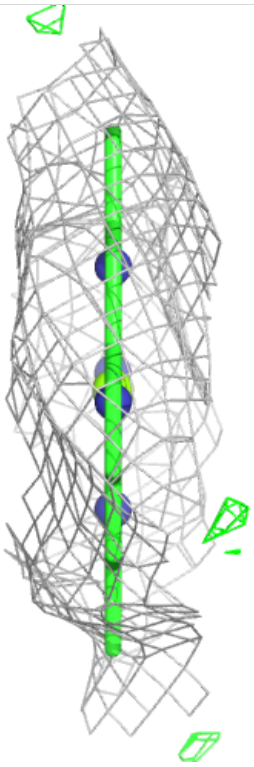


Electron density around CLA 3 3010:

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

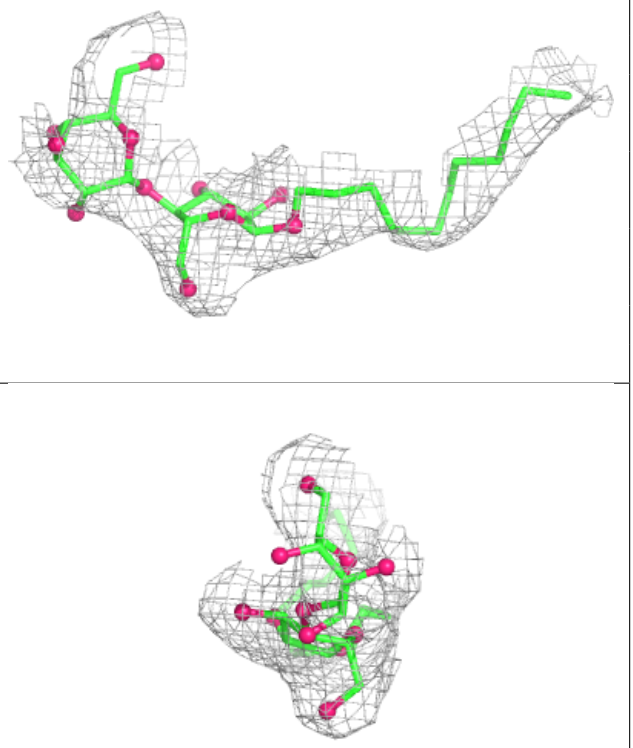


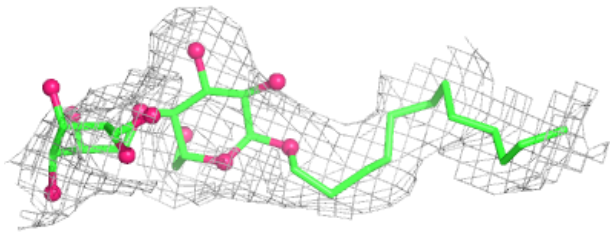




Electron density around LMU 4 7034:

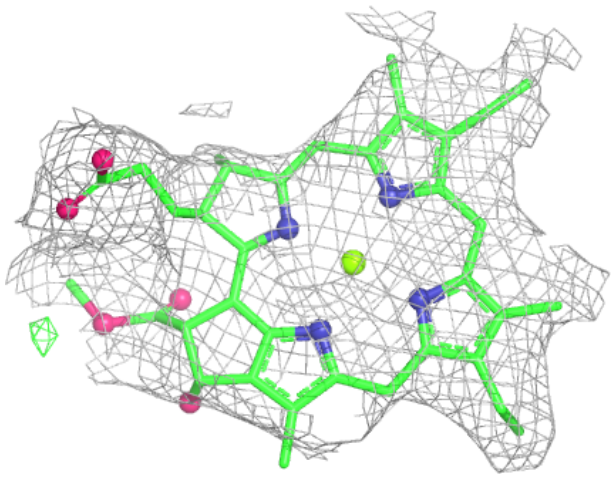
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

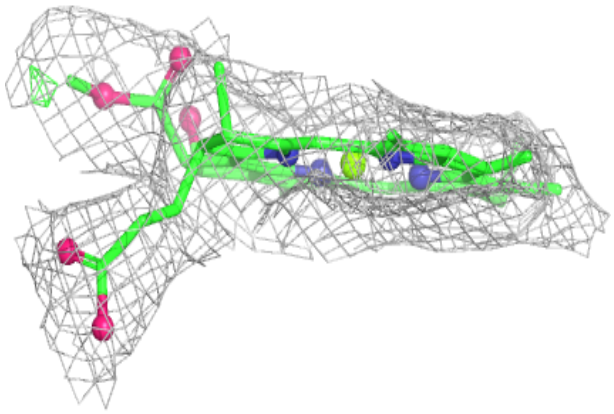


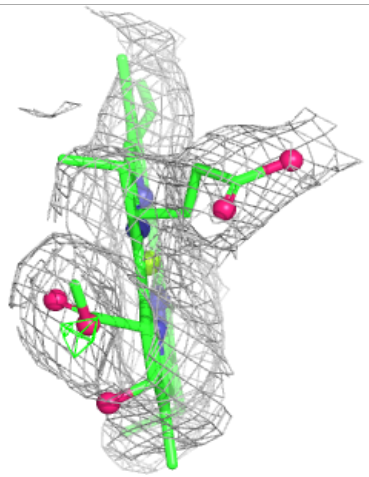


Electron density around CLA A 1108:

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

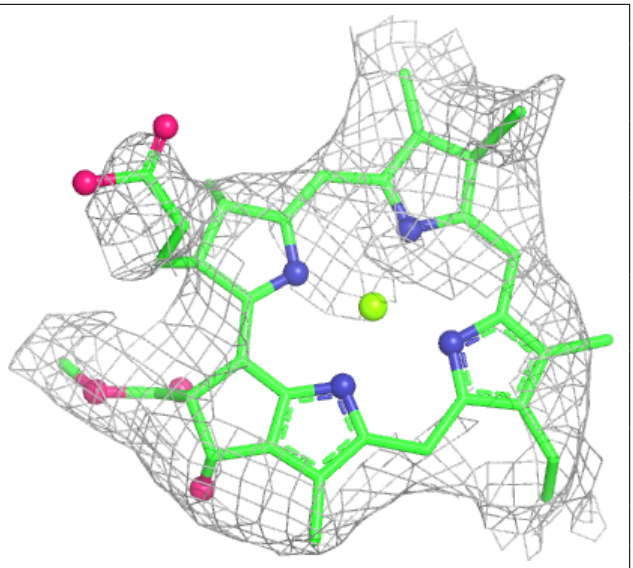


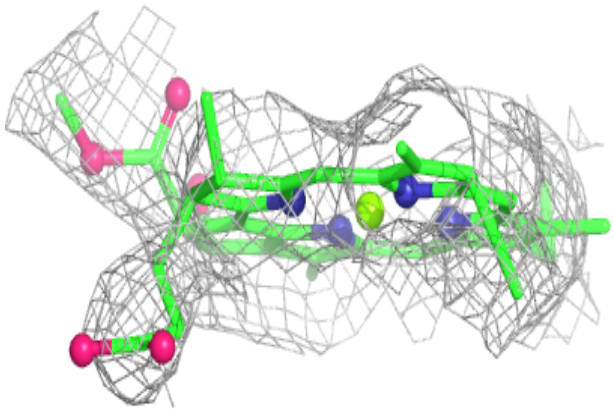


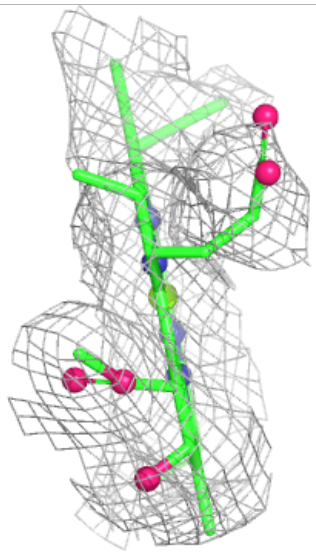


Electron density around CLA A 1134:

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

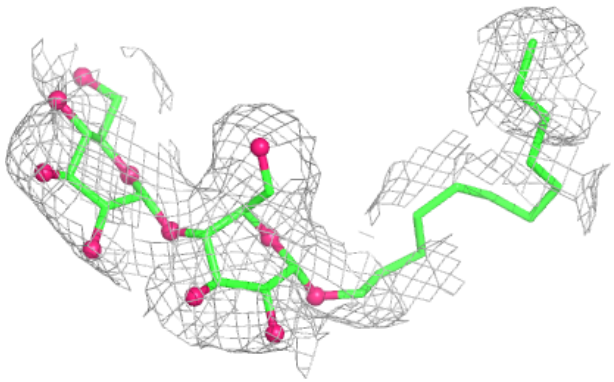


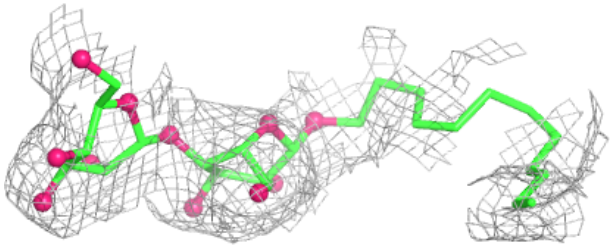




Electron density around LMU H 7030:

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



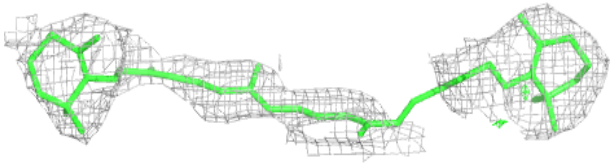


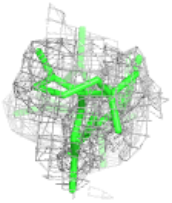


Electron density around BCR A 6007:

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

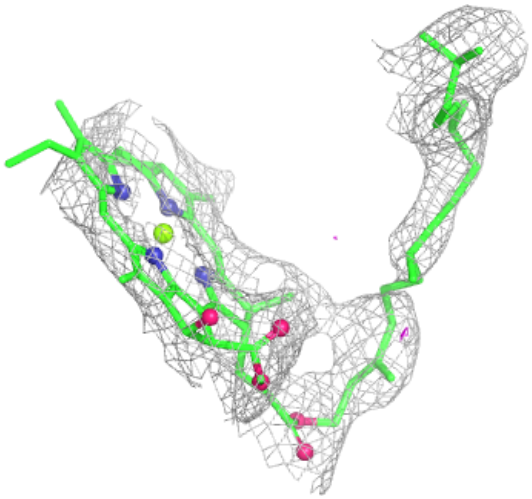


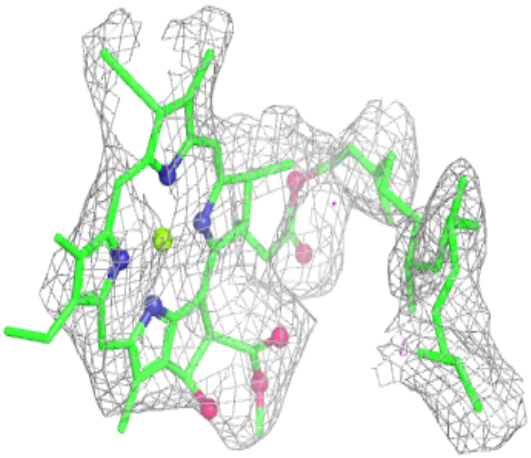


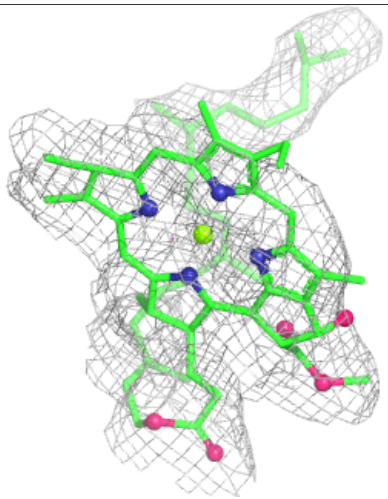


Electron density around CLA 2 2006:

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

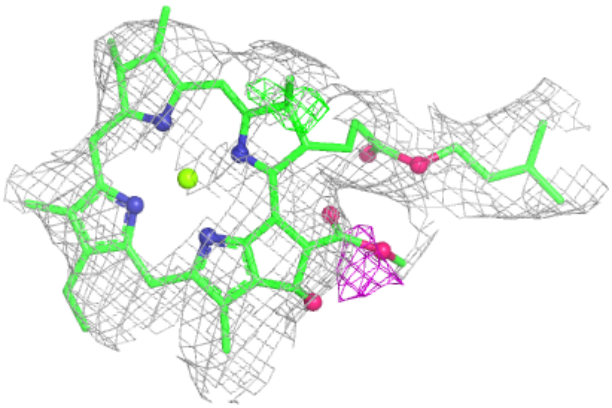


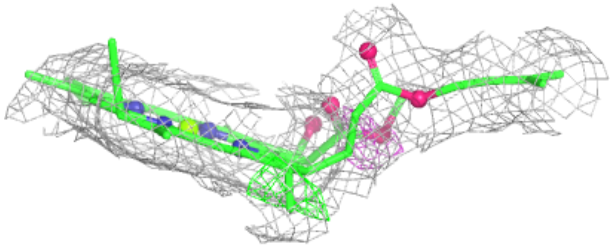


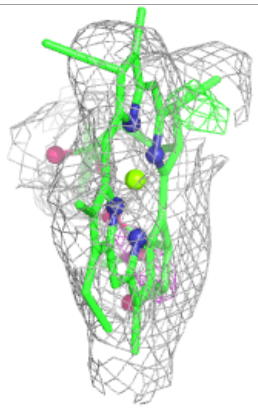


Electron density around CLA L 1503:

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

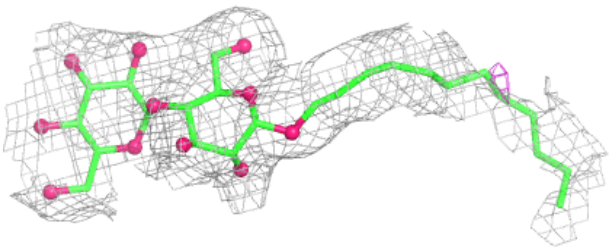


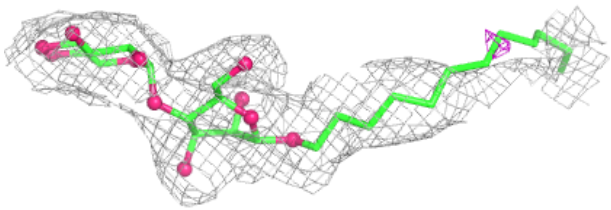


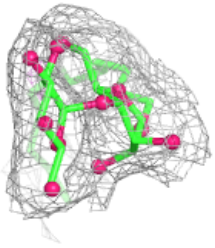


Electron density around LMU K 7047:

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

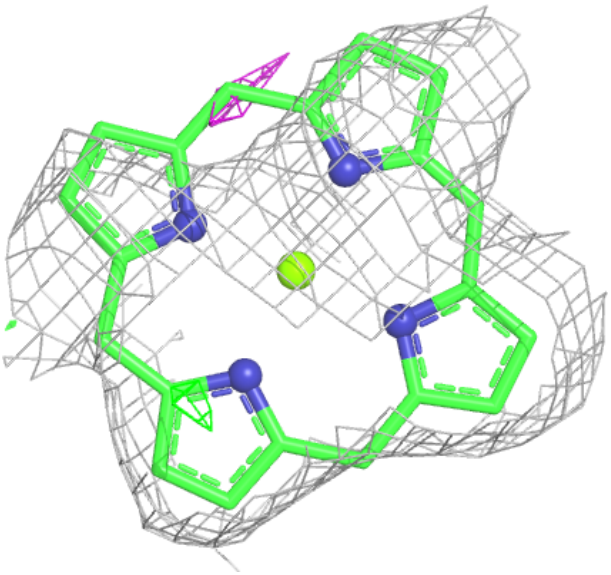


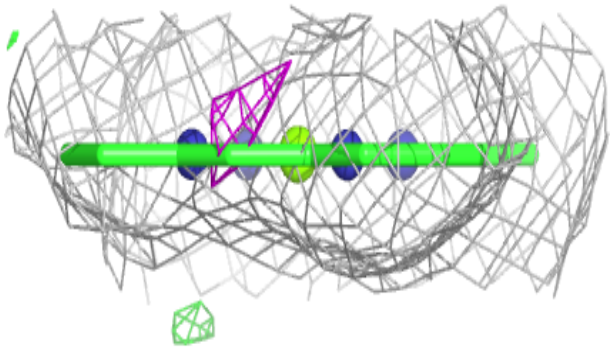


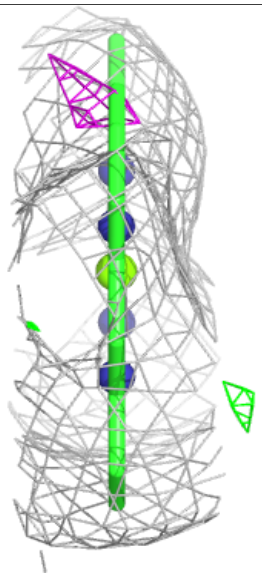


Electron density around CLA 4 4004:

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

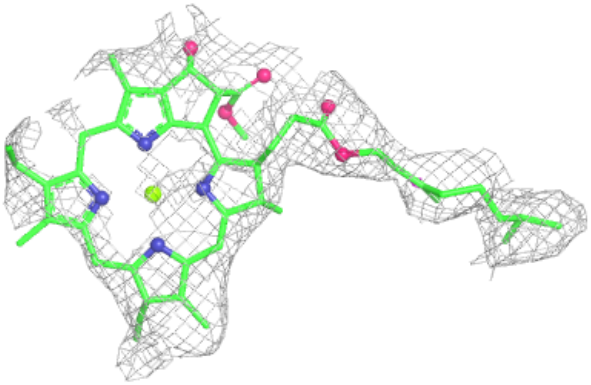


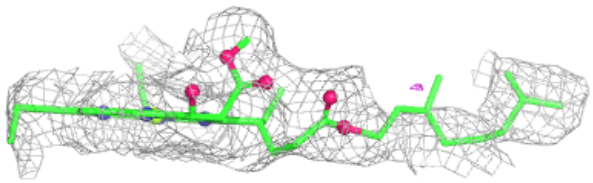


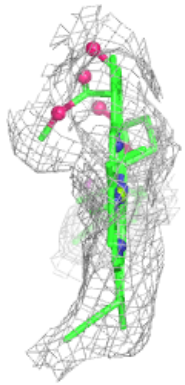


Electron density around CLA 4 4006:

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

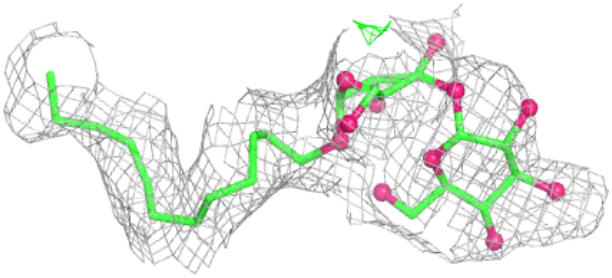


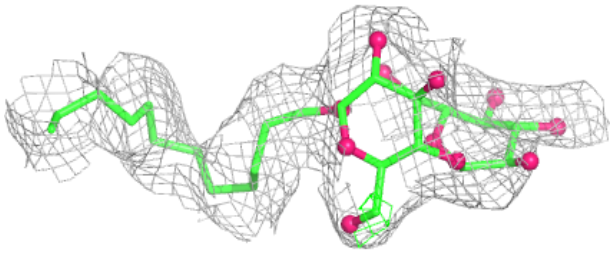


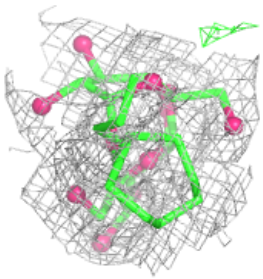


Electron density around LMU A 7045:

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

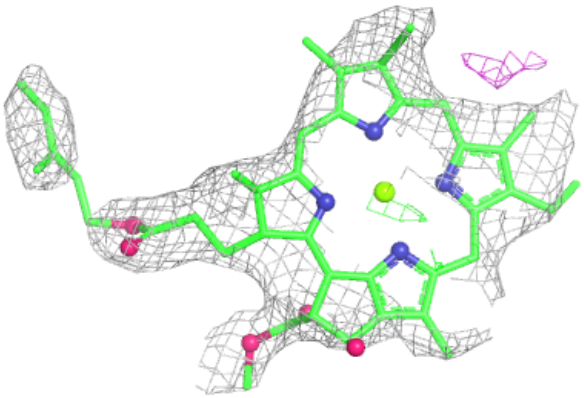


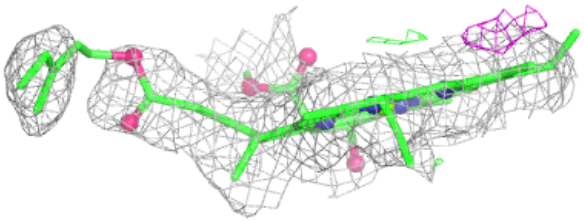


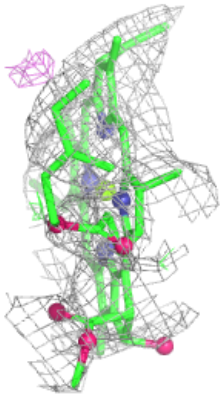


Electron density around CLA 1 1303:

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

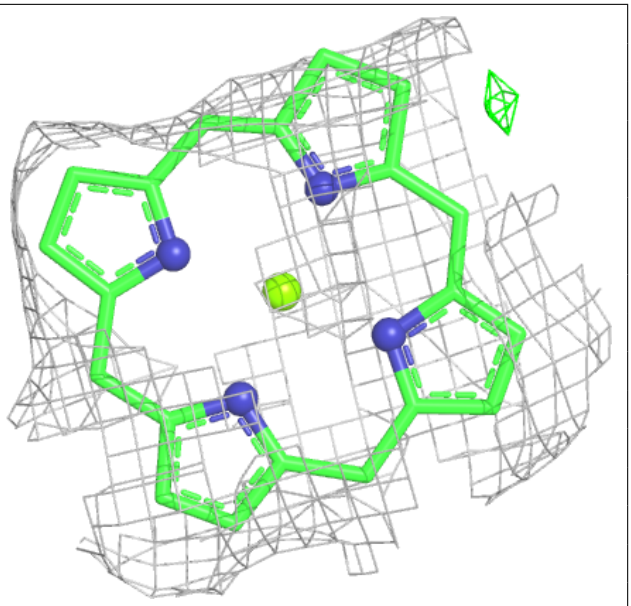


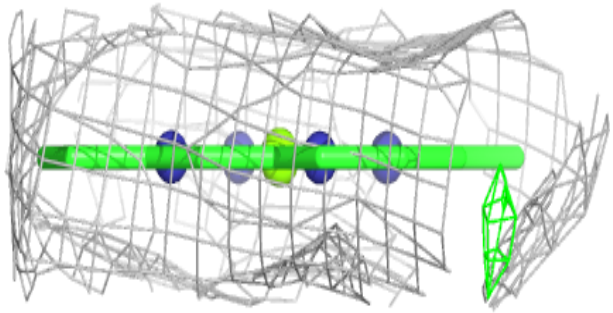


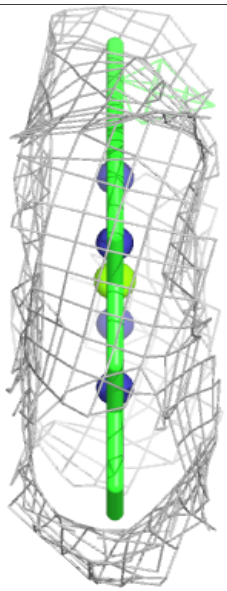


Electron density around CLA 3 3004:

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

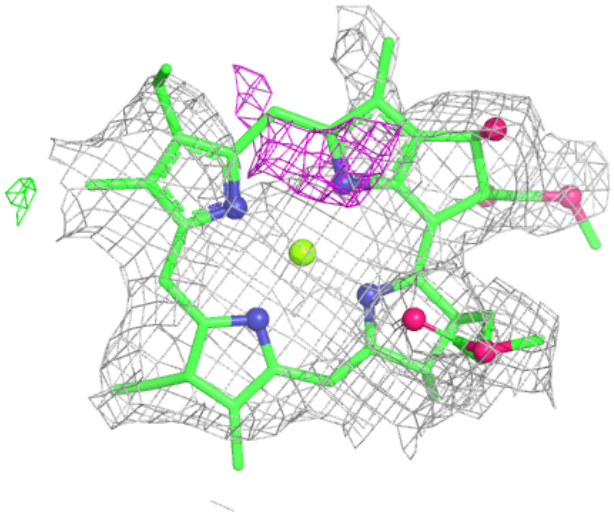


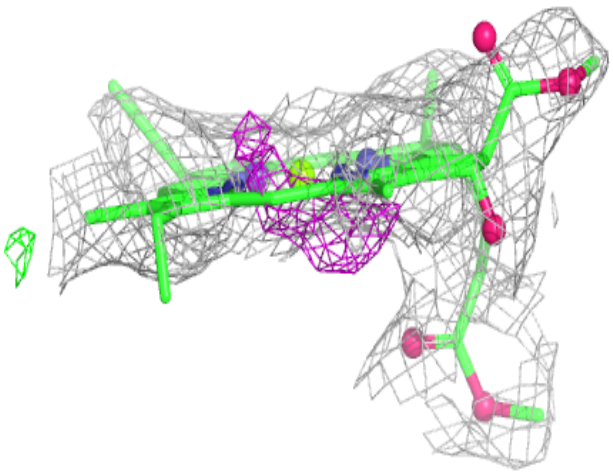


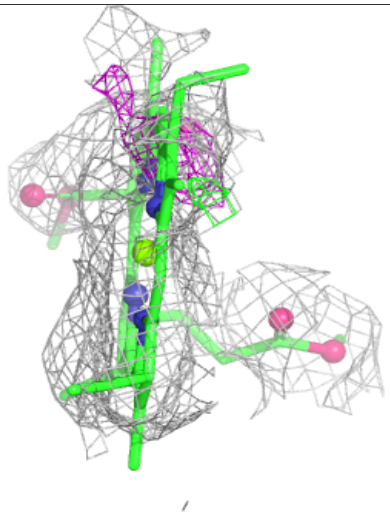


Electron density around CLA A 1105:

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

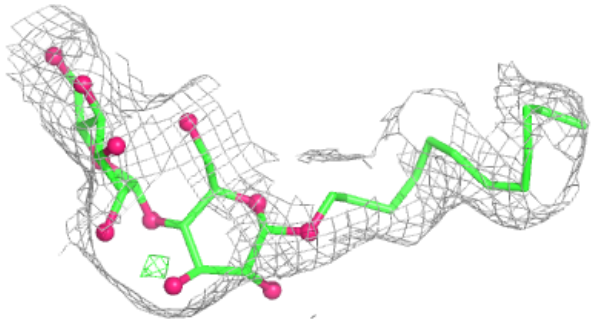


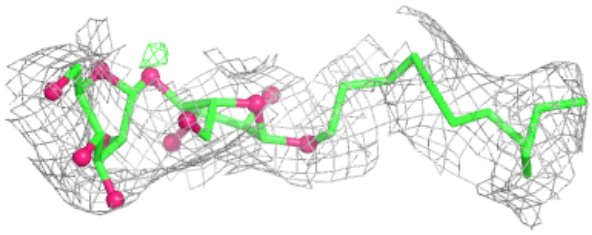


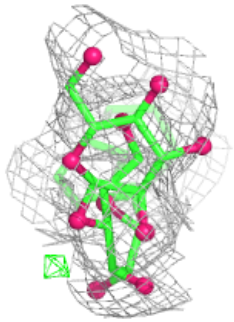


Electron density around LMU H 7011:

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

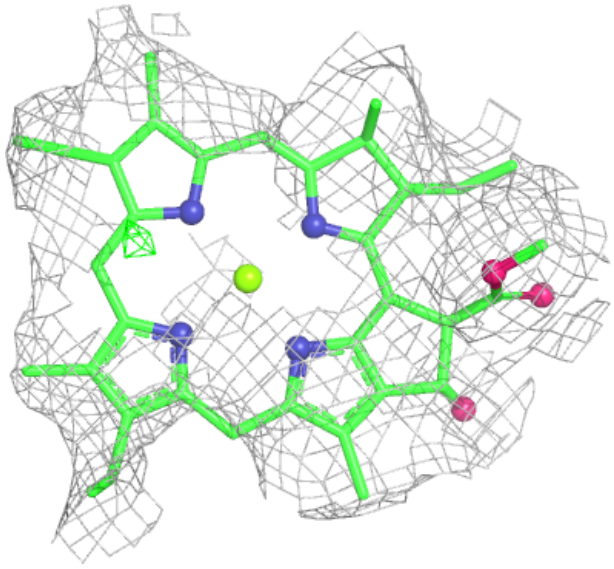


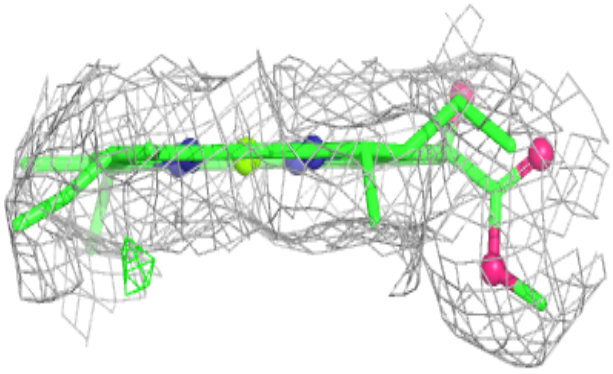




Electron density around CLA A 1121:

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

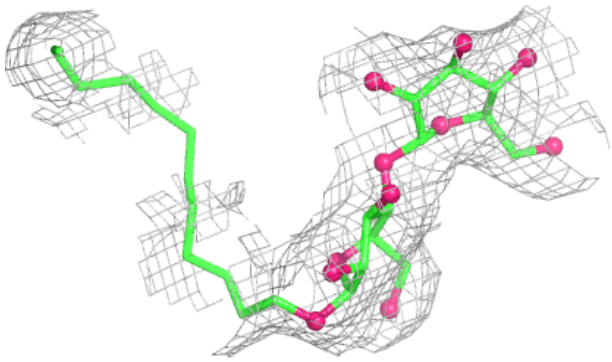


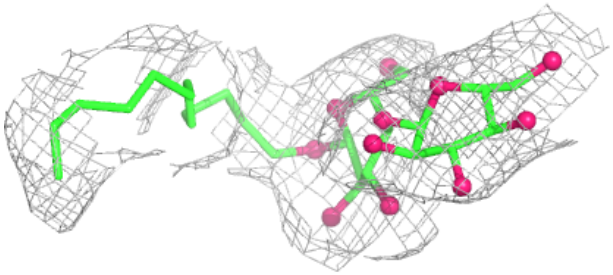


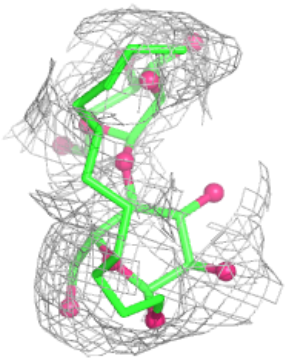


Electron density around LMU H 7028:

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

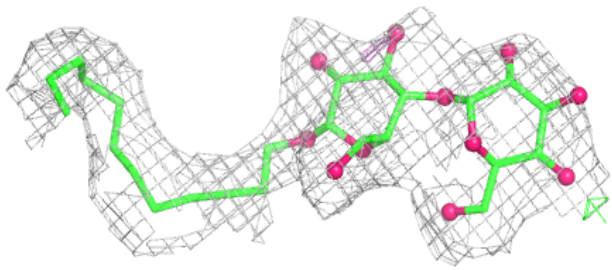


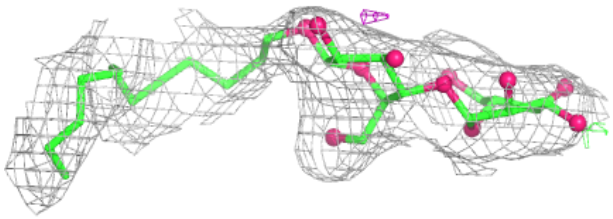


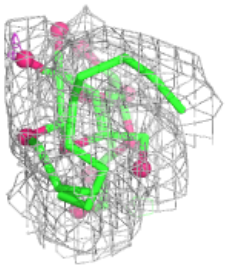


Electron density around LMU C 7015:

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

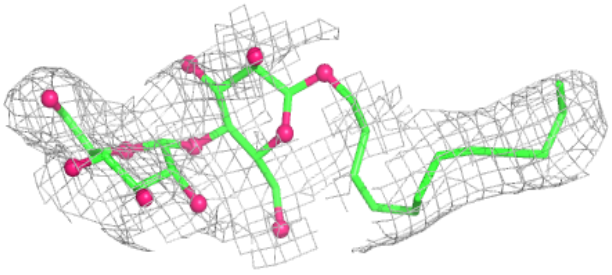


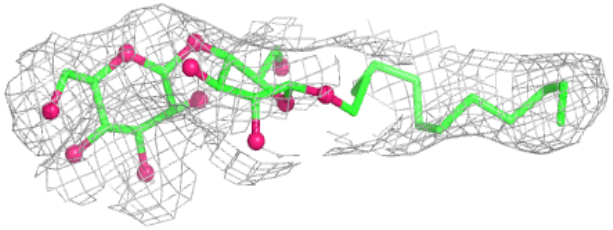


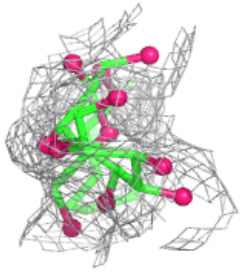


Electron density around LMU K 7042:

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

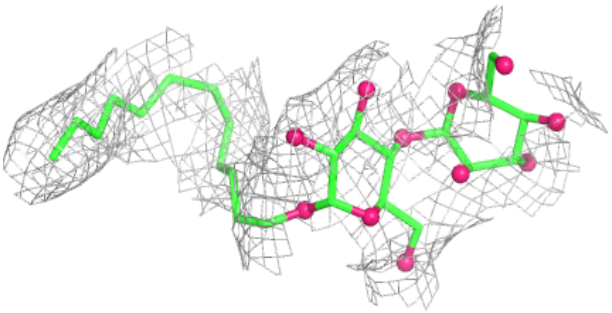


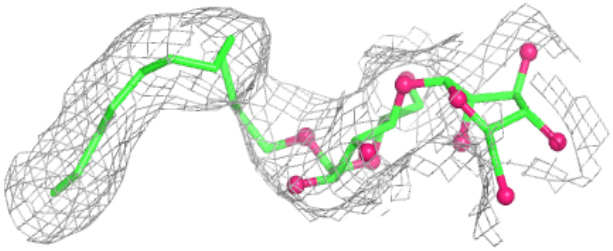


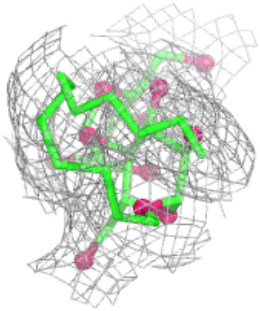


Electron density around LMU D 7050:

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

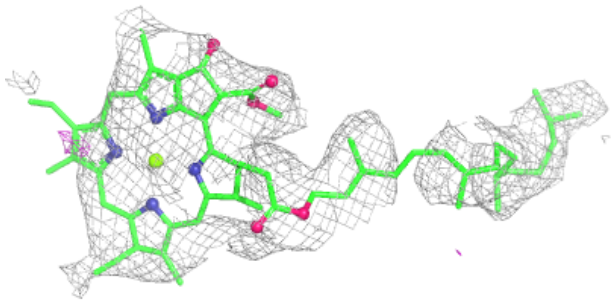


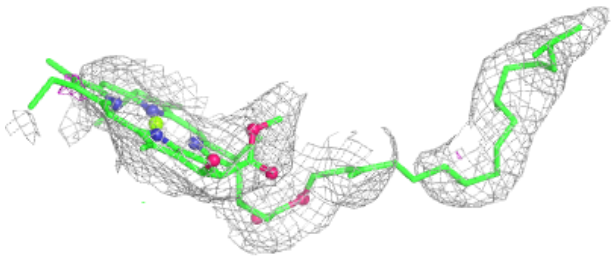


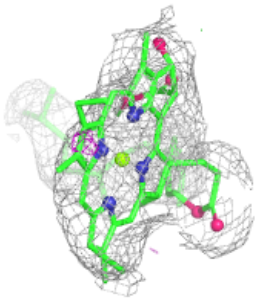


Electron density around CLA 3 3011:

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

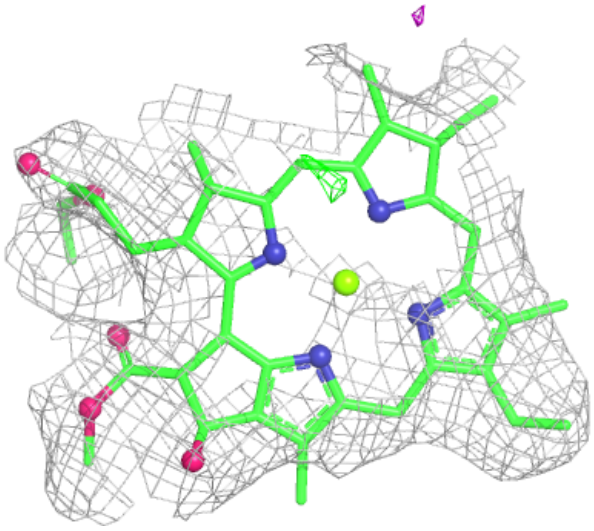


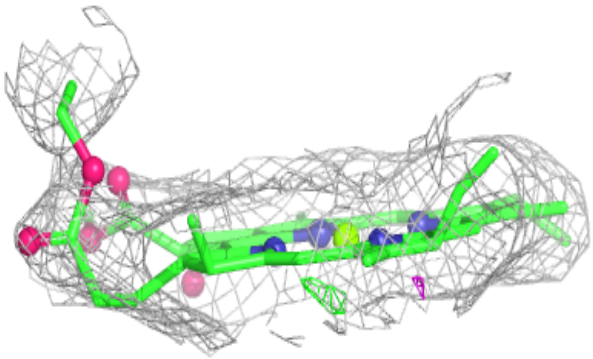


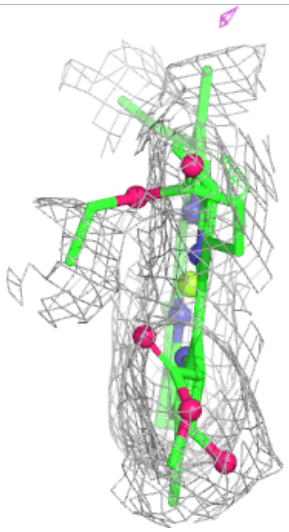


Electron density around CLA 1 1002:

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

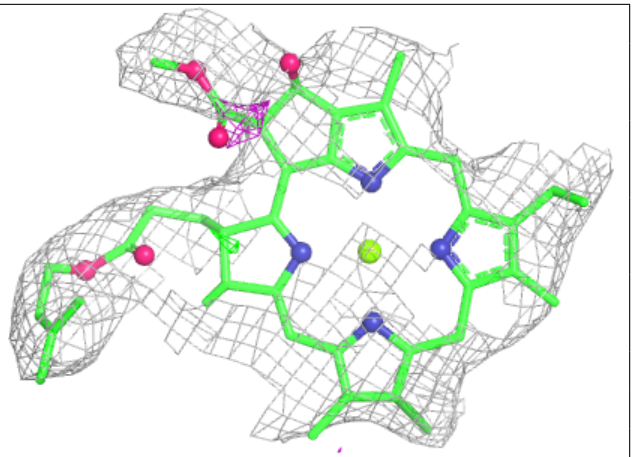


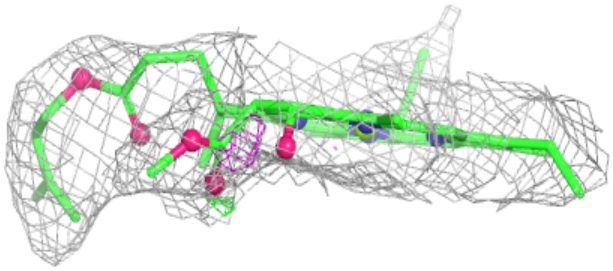


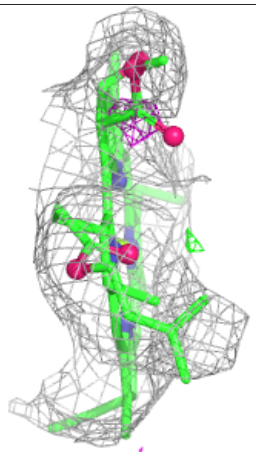


Electron density around CLA K 1146:

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

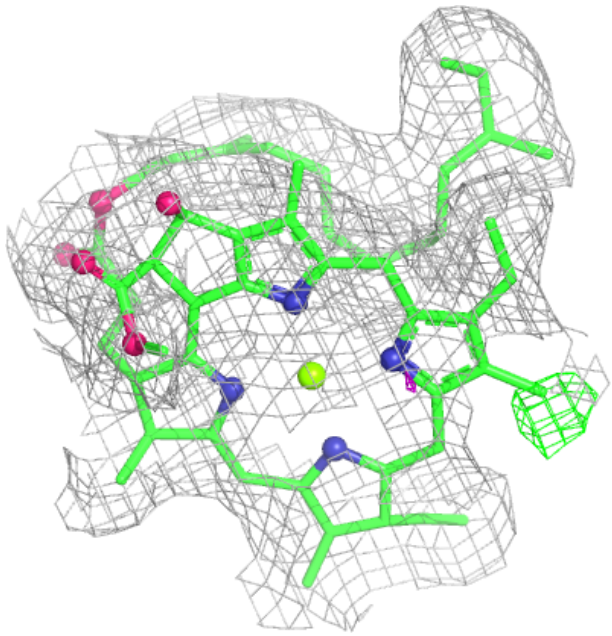


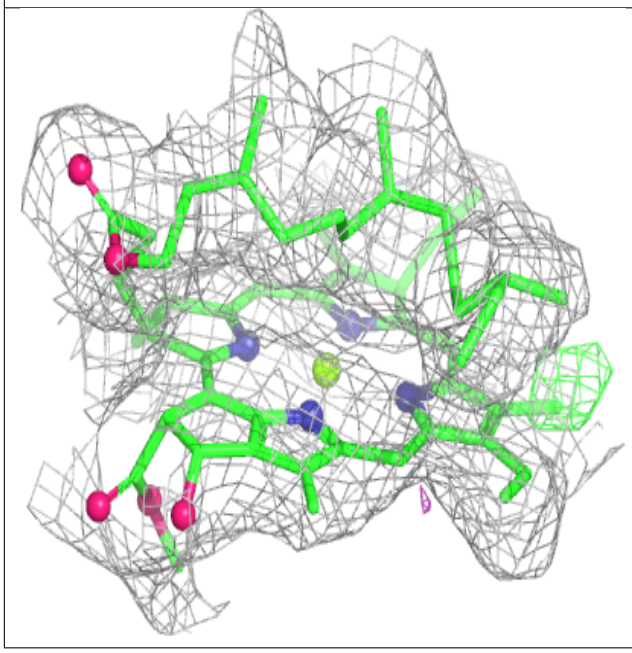


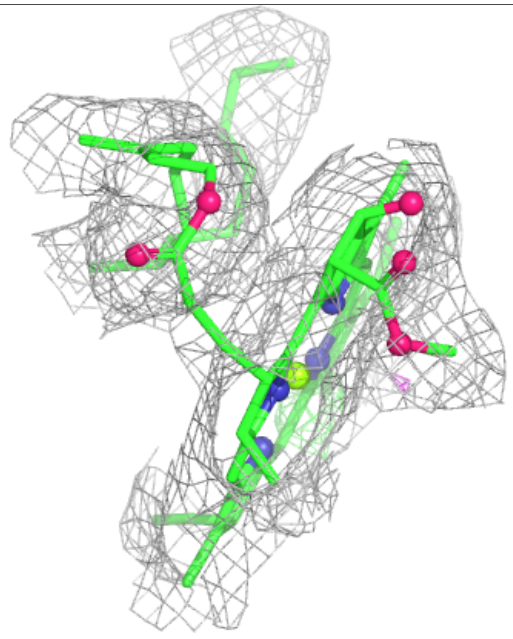


Electron density around CLA 1 1007:

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

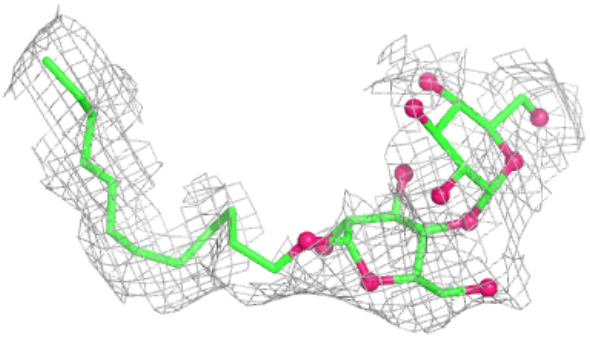


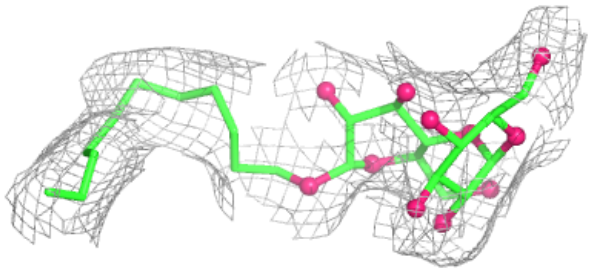




Electron density around LMU 2 7031:

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

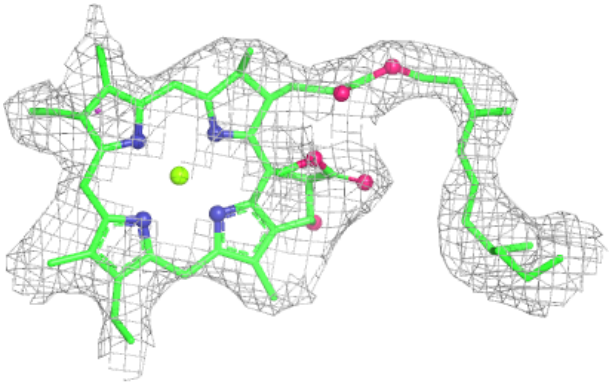


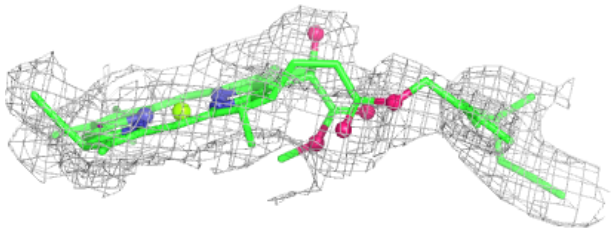


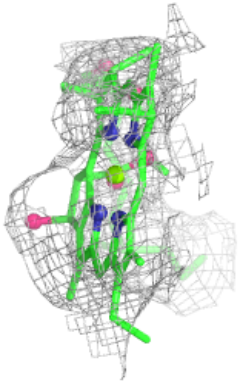


Electron density around CLA R 1144:

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

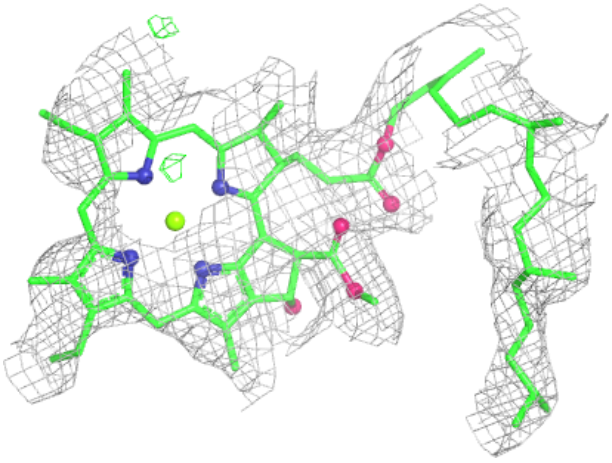


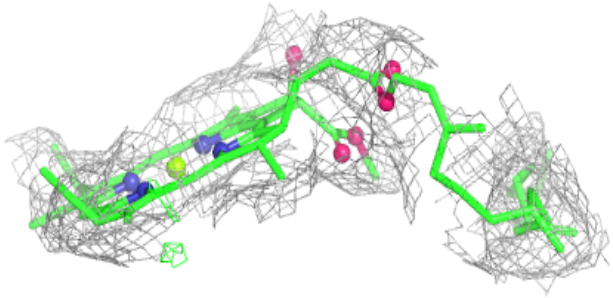


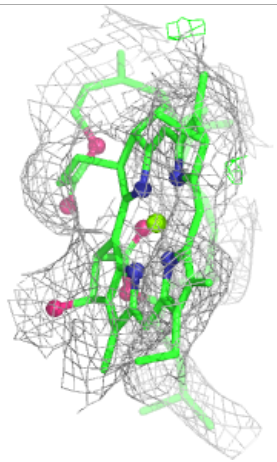


Electron density around CLA R 1150:

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

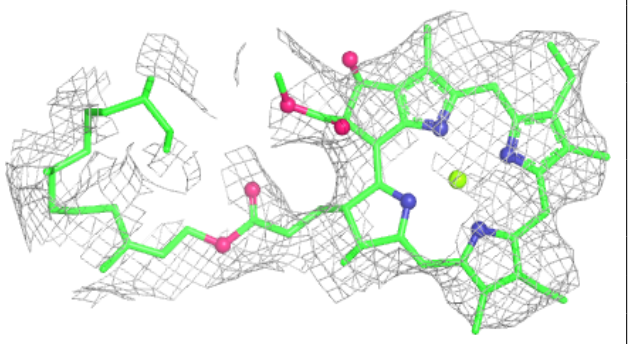


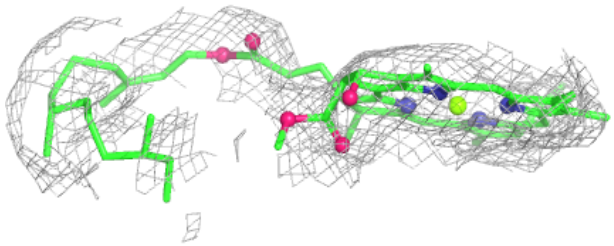


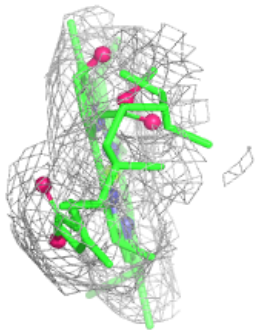


Electron density around CLA 1 1014:

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

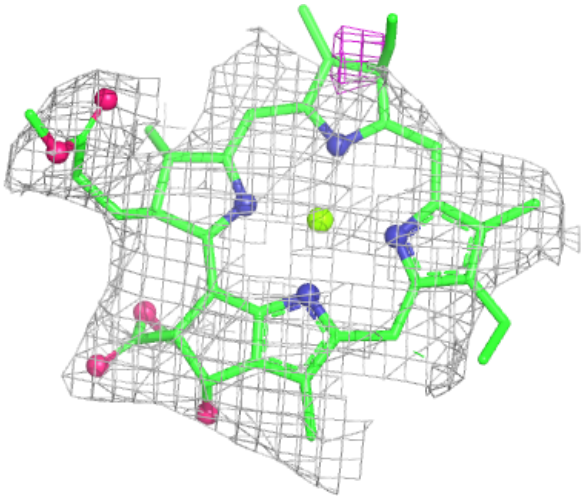


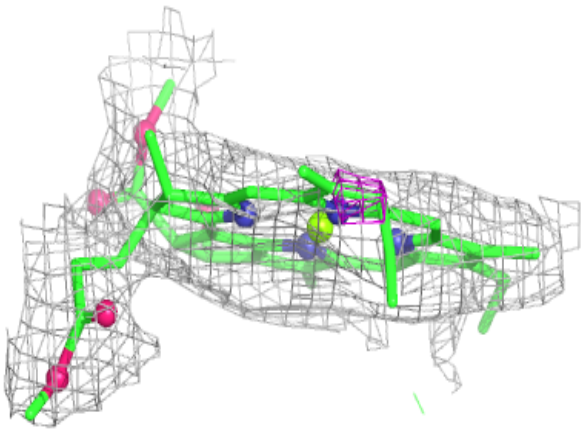


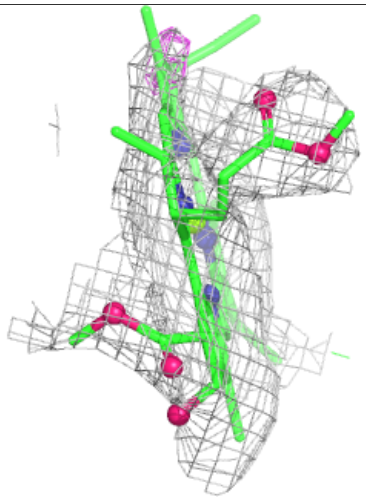


Electron density around CLA B 1218:

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

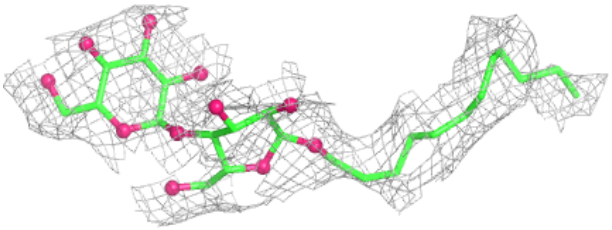


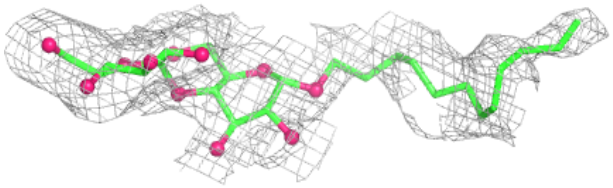


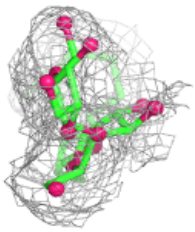


Electron density around LMU B 7038:

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

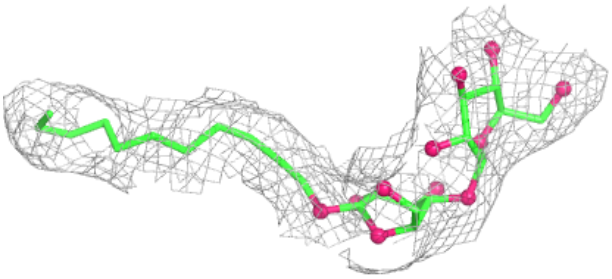


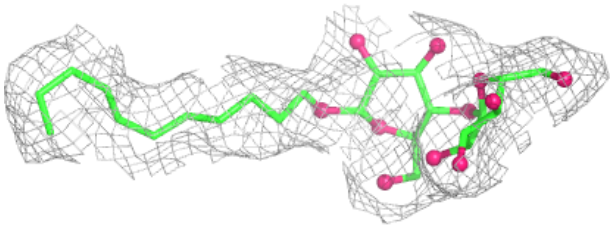


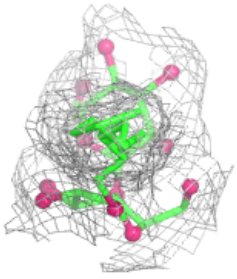


Electron density around LMU F 7036:

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

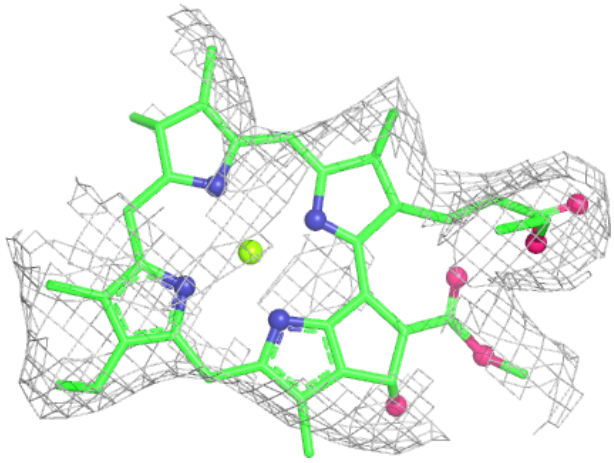


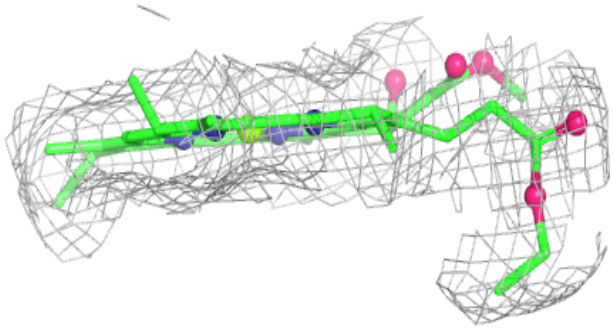


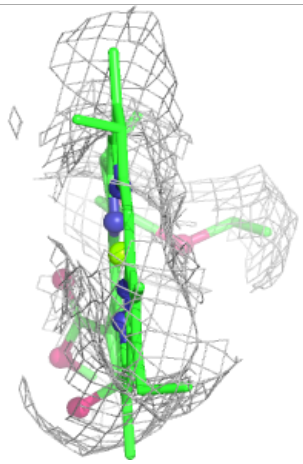


Electron density around CLA A 1149:

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

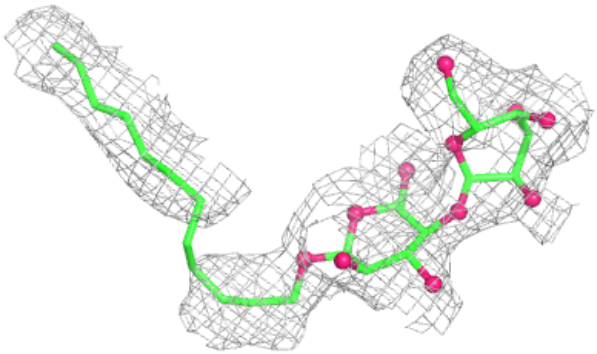


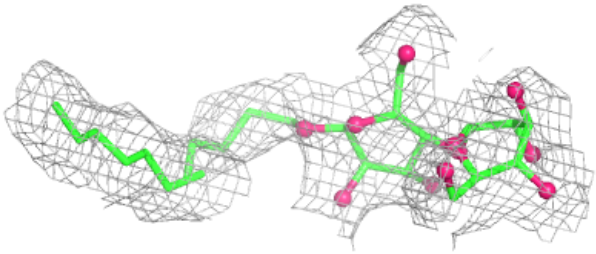


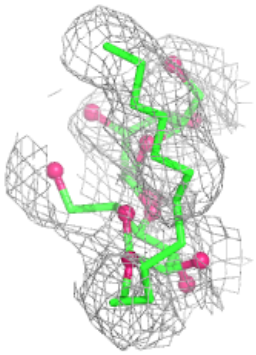


Electron density around LMU 4 7008:

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

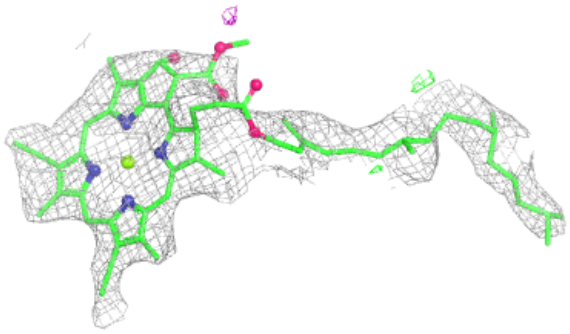


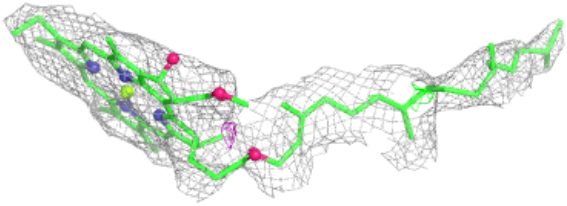


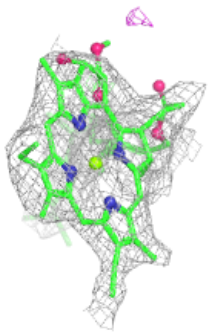


Electron density around CLA H 1207:

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

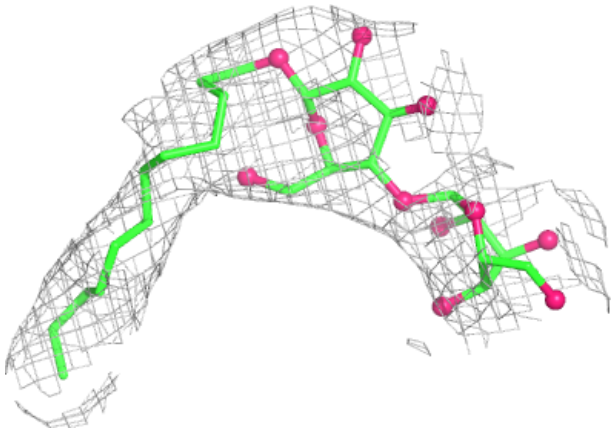


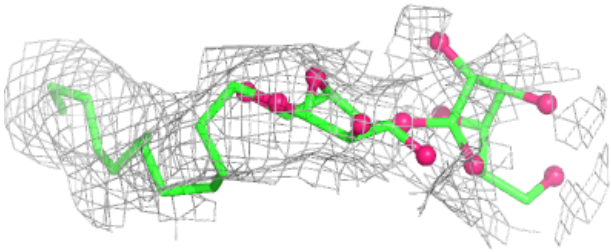




Electron density around LMU R 7021:

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

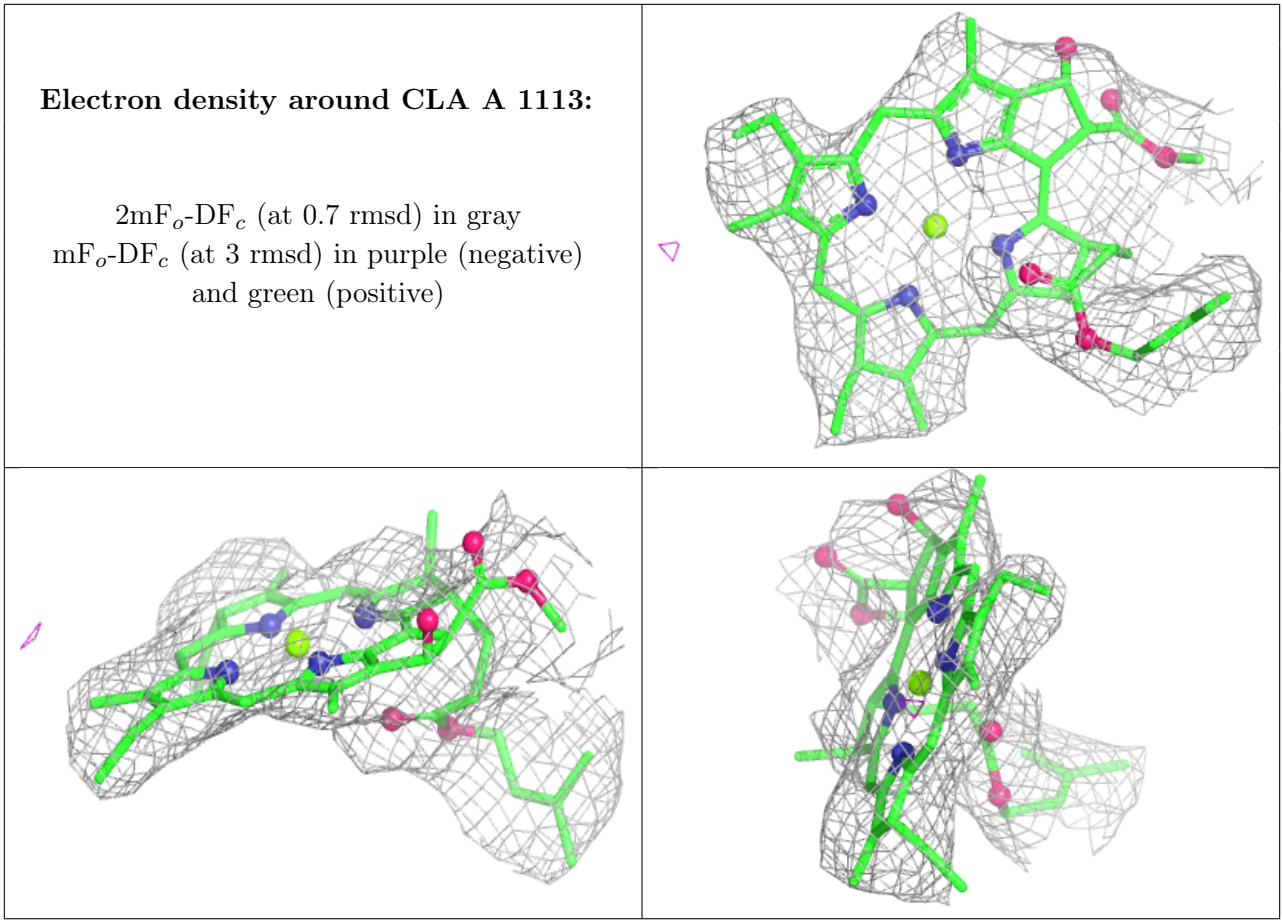






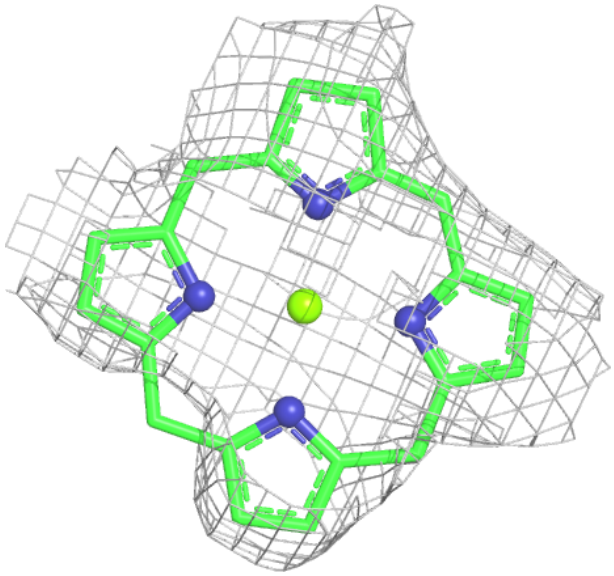
Electron density around CLA A 1113:

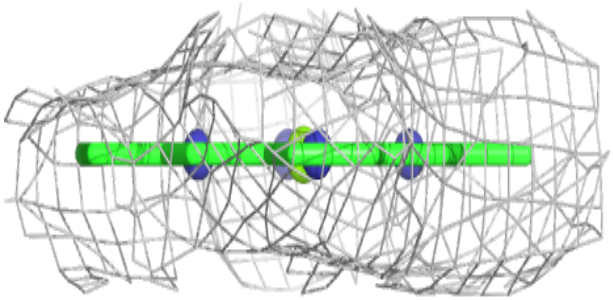
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

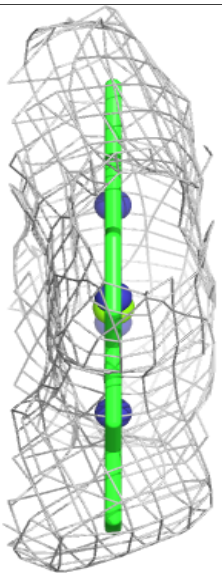


Electron density around CLA 3 3002:

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

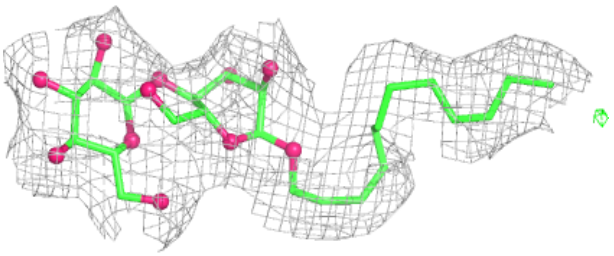


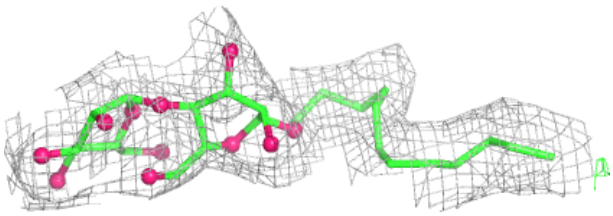


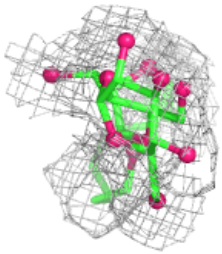


Electron density around LMU R 7020:

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

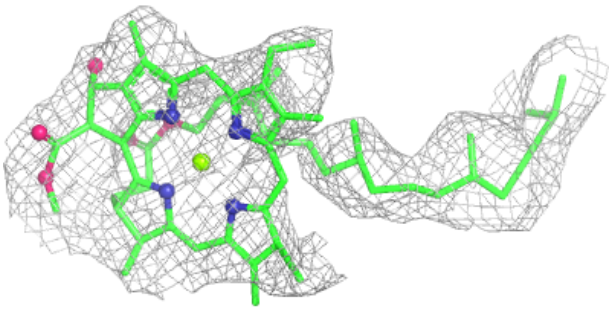


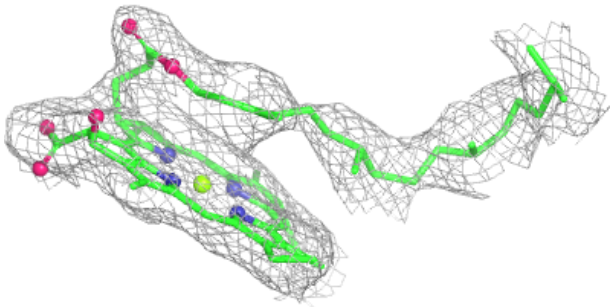


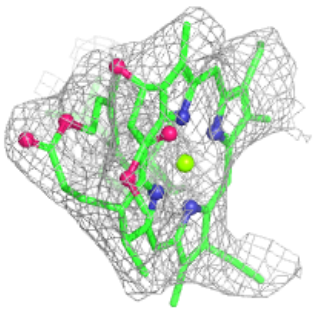


Electron density around CLA A 1115:

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

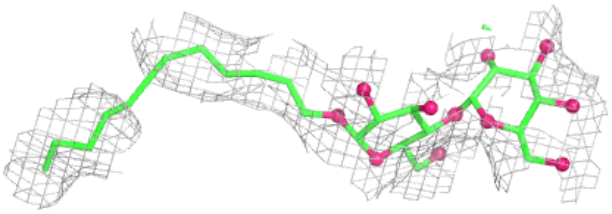


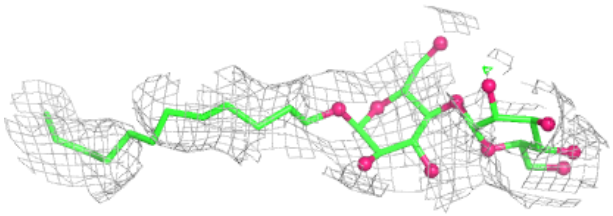


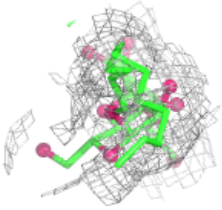


Electron density around LMU B 7040:

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

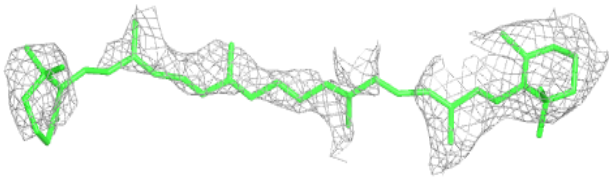


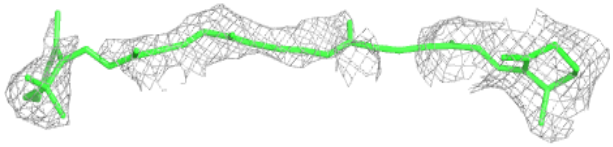


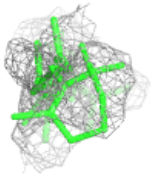


Electron density around BCR A 6008:

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

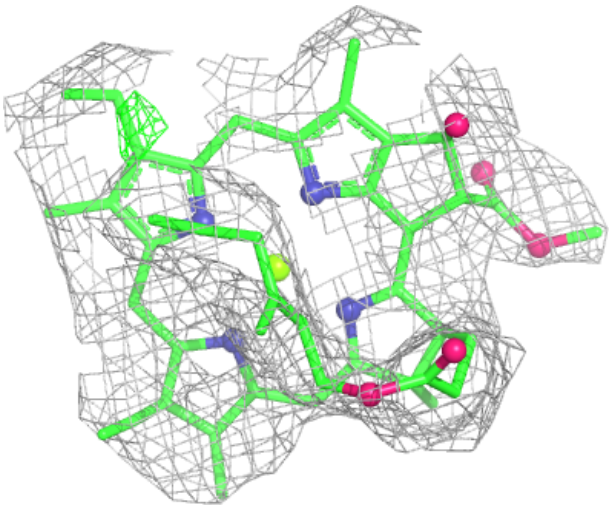


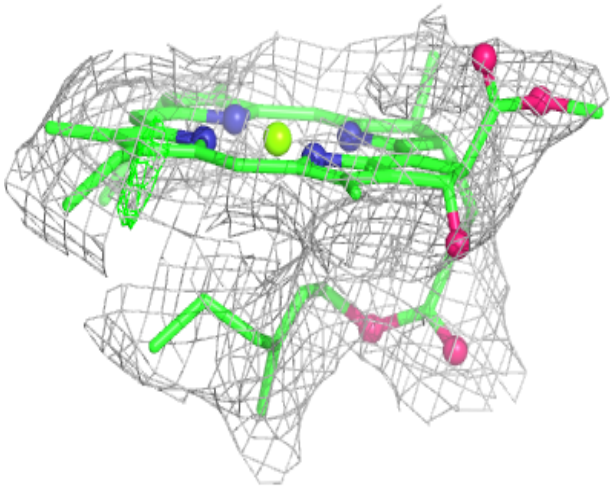




Electron density around CLA A 1116:

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

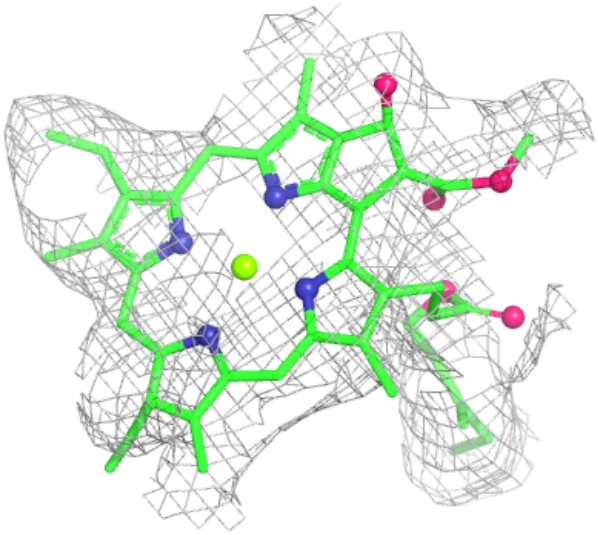


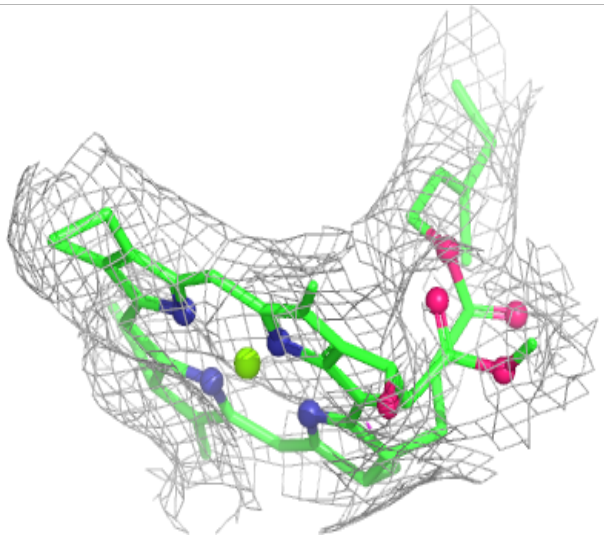


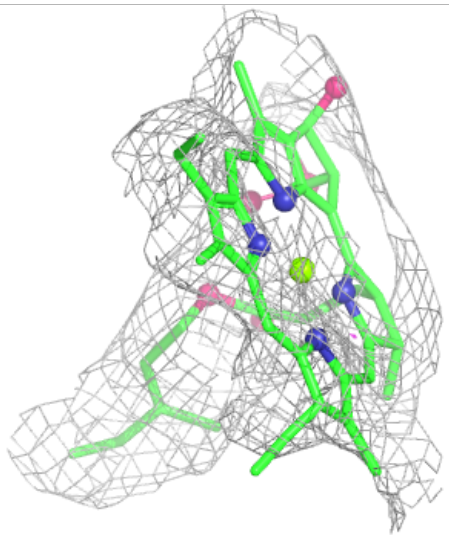


Electron density around CLA 1 1008:

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

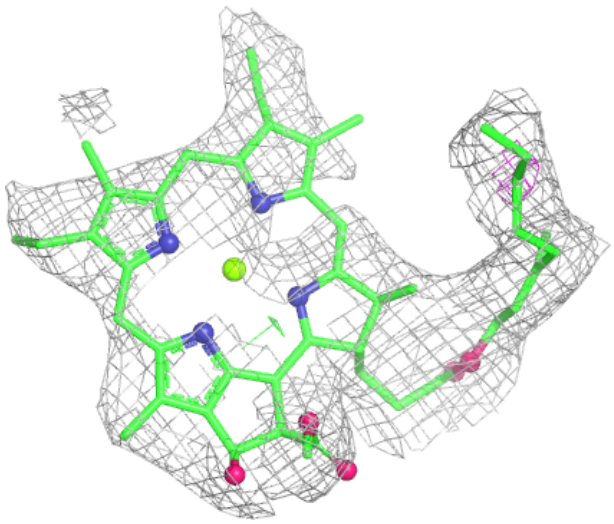


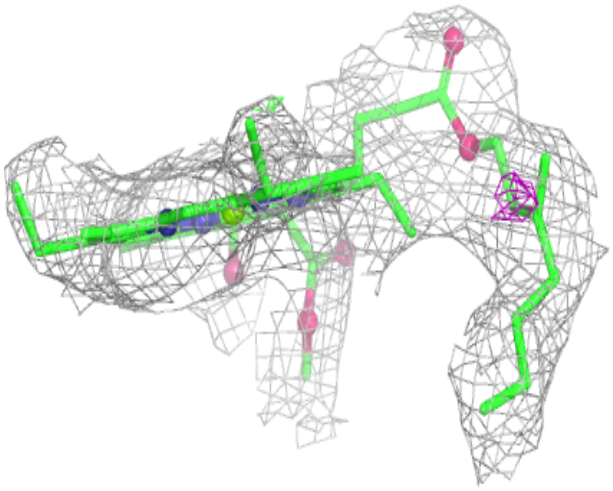




Electron density around CLA A 1111:

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

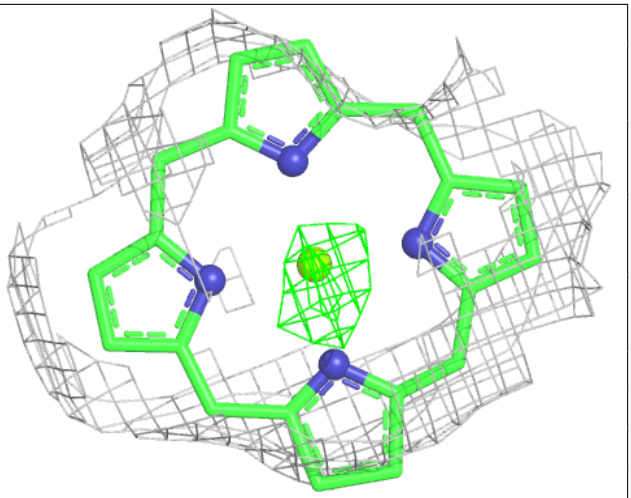


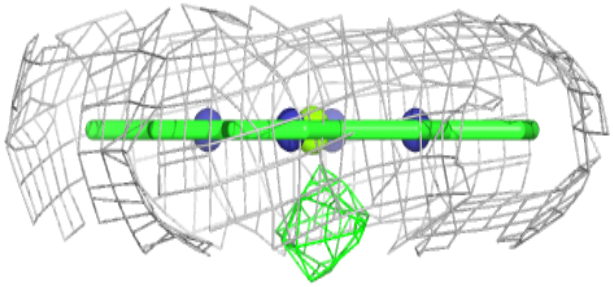


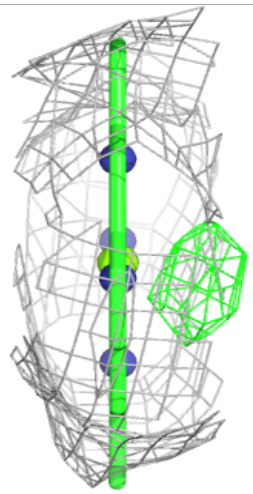


Electron density around CLA 2 2008:

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

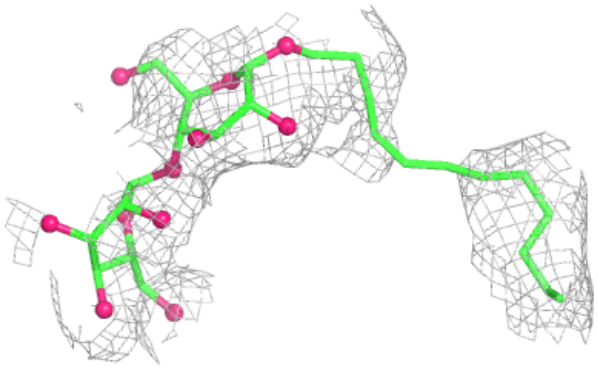


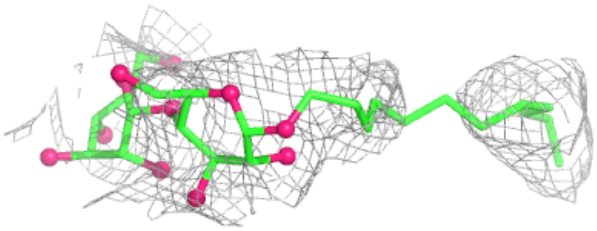


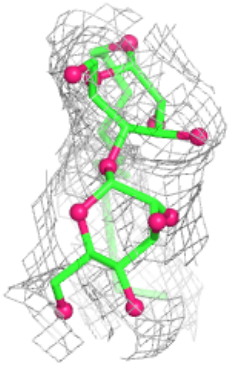


Electron density around LMU 4 7019:

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

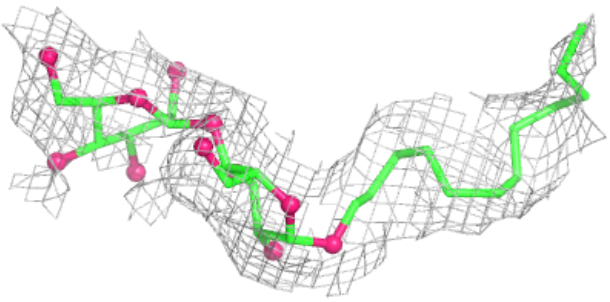


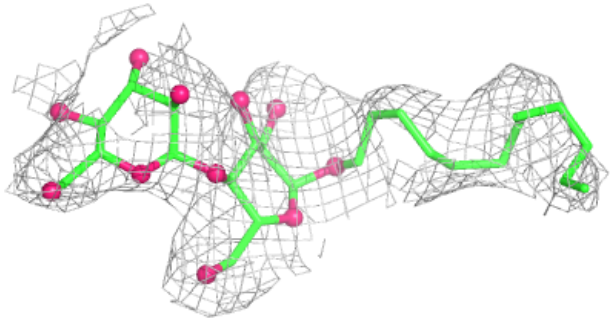


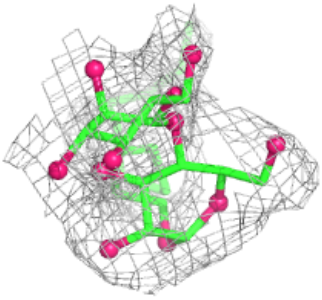


Electron density around LMU G 7026:

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

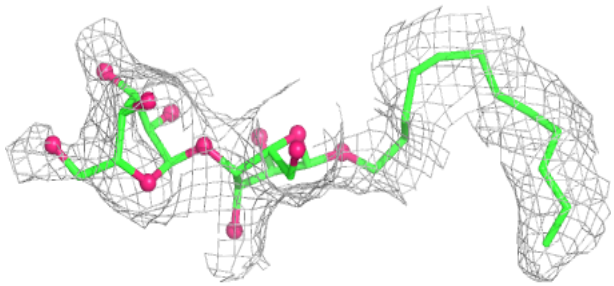


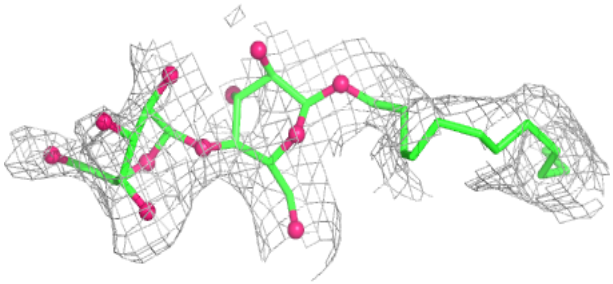


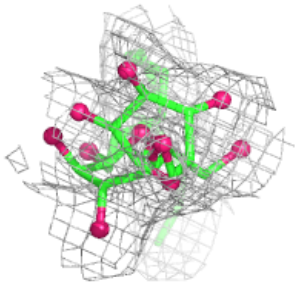


Electron density around LMU A 7044:

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

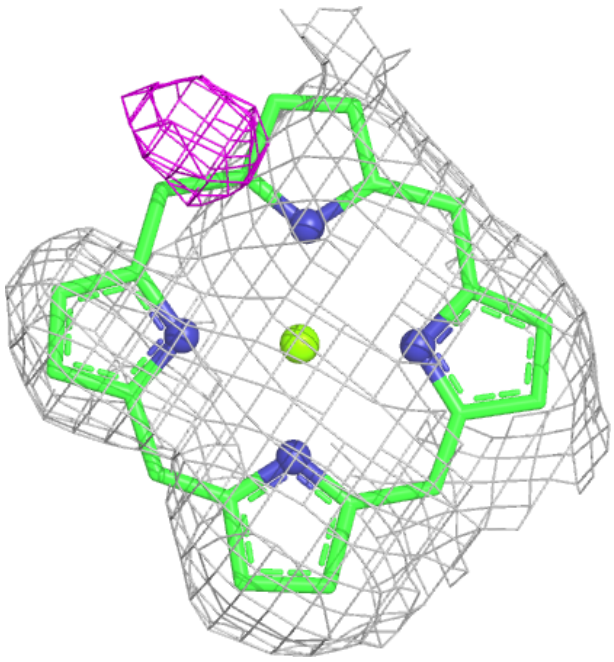


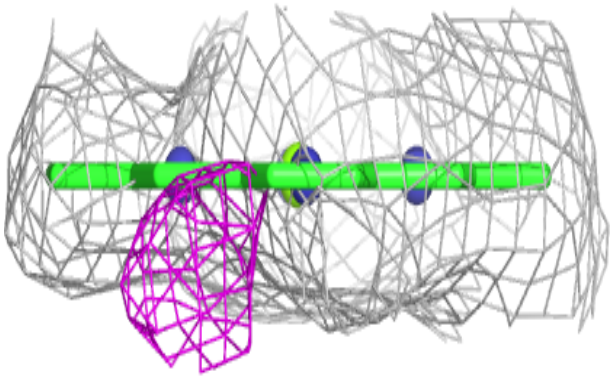


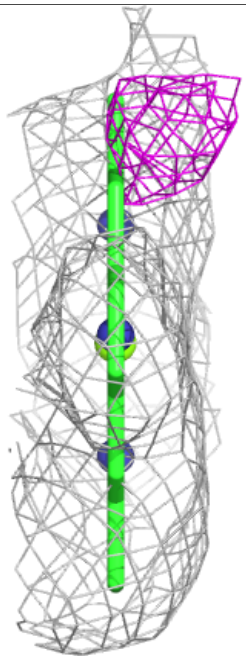


Electron density around CLA 2 2003:

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

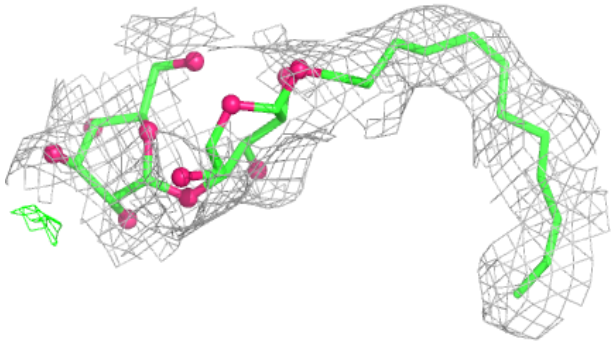


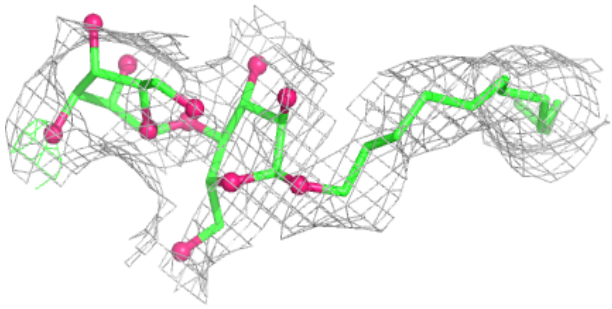


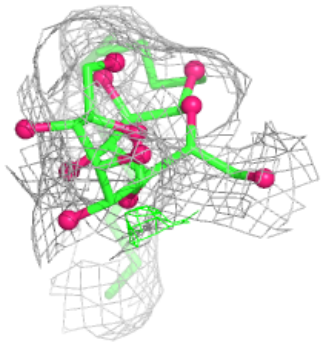


Electron density around LMU 2 7006:

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

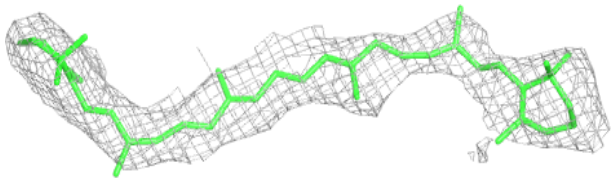


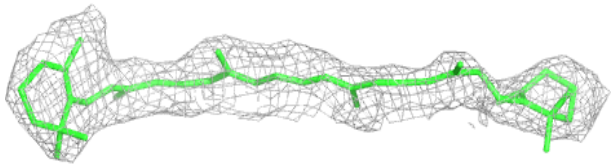


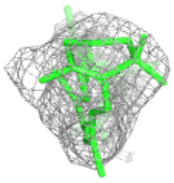


Electron density around BCR B 6006:

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

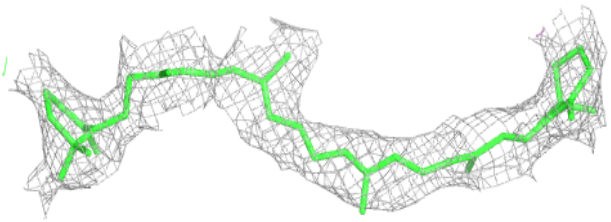


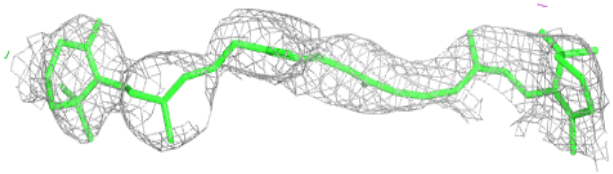


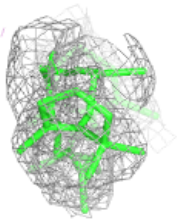


Electron density around BCR I 6021:

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

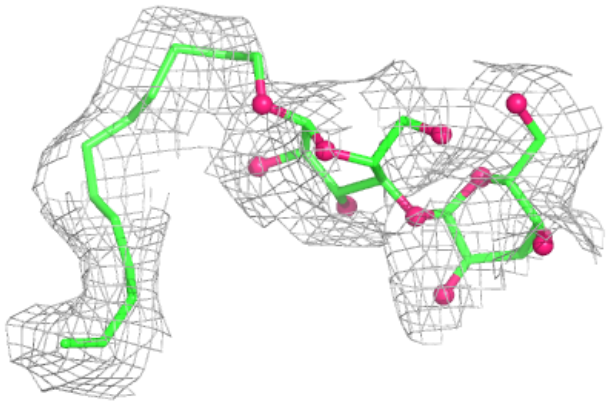


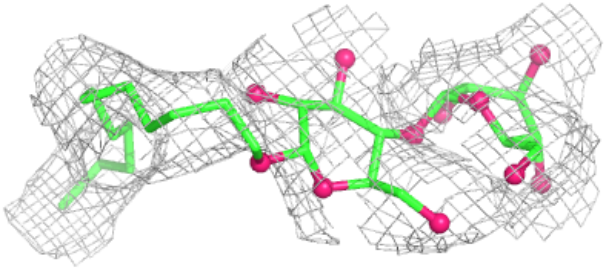


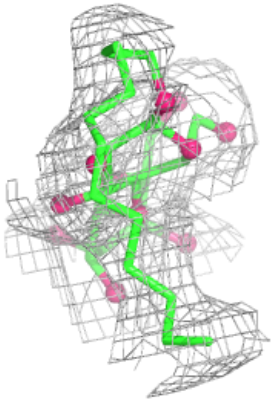


Electron density around LMU 3 7003:

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

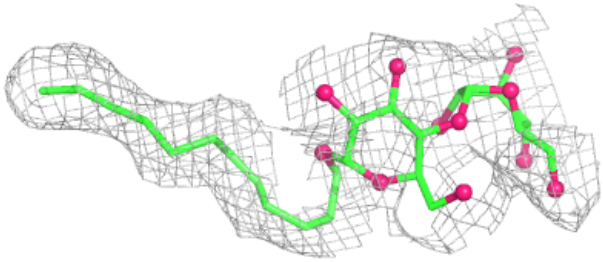


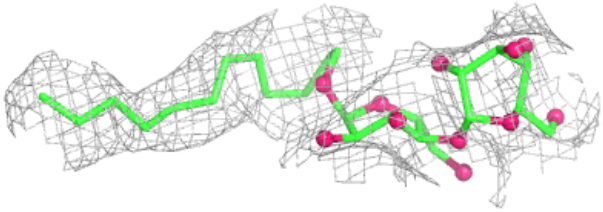


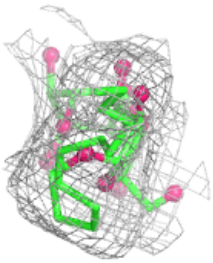


Electron density around LMU 3 7005:

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

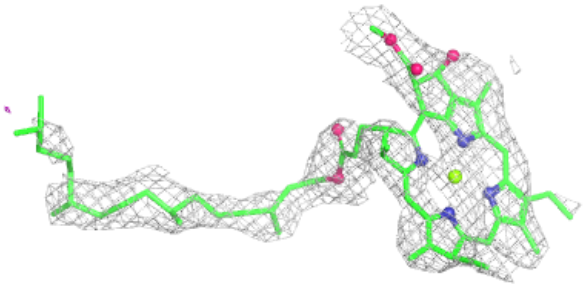


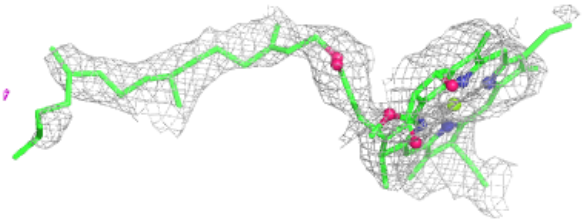




Electron density around CLA A 1119:

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

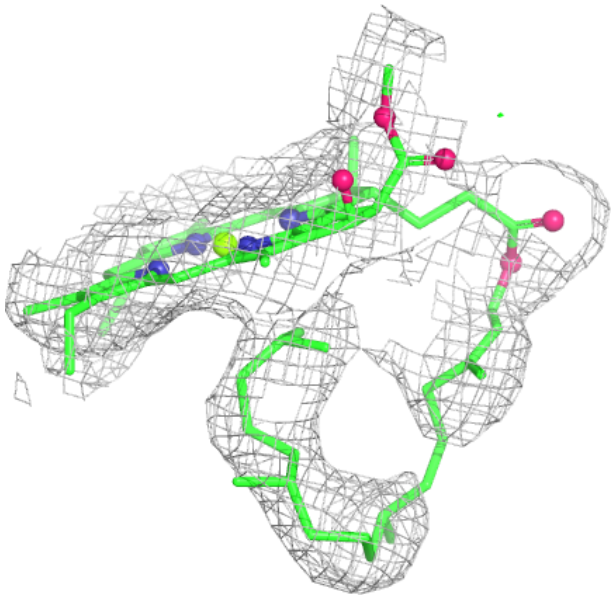


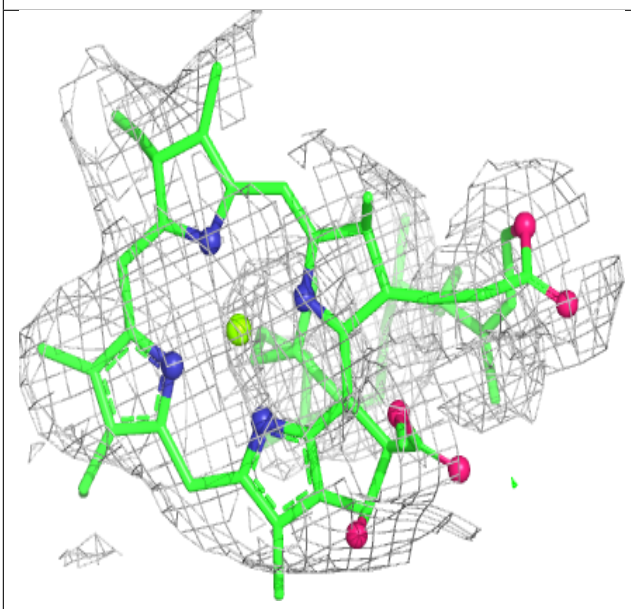


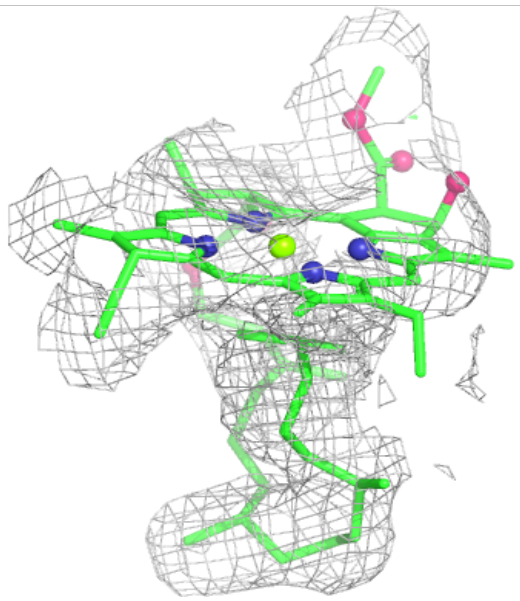


Electron density around CLA 2 4009:

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

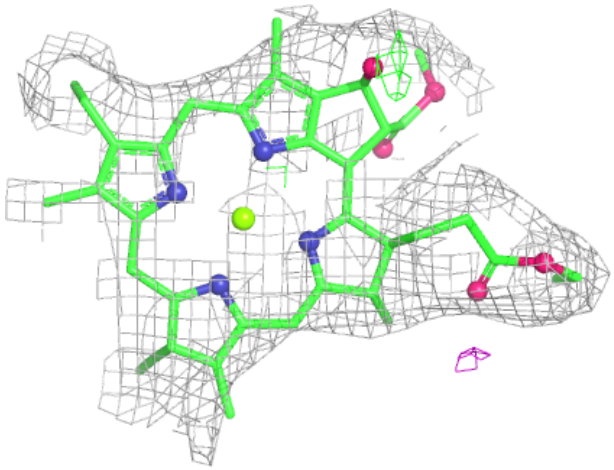


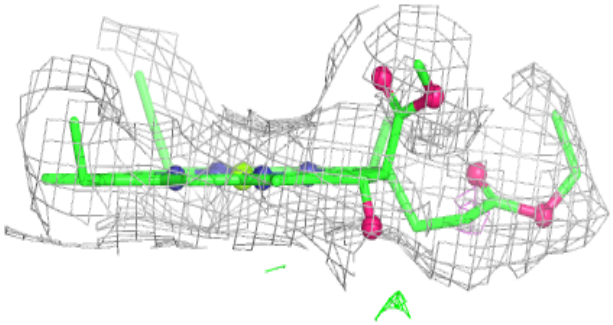


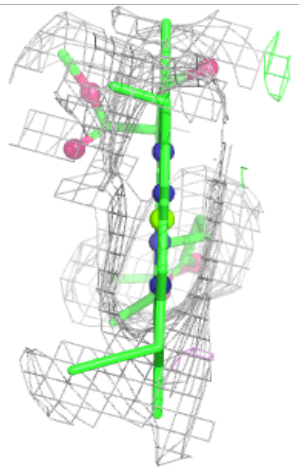


Electron density around CLA 1 1003:

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

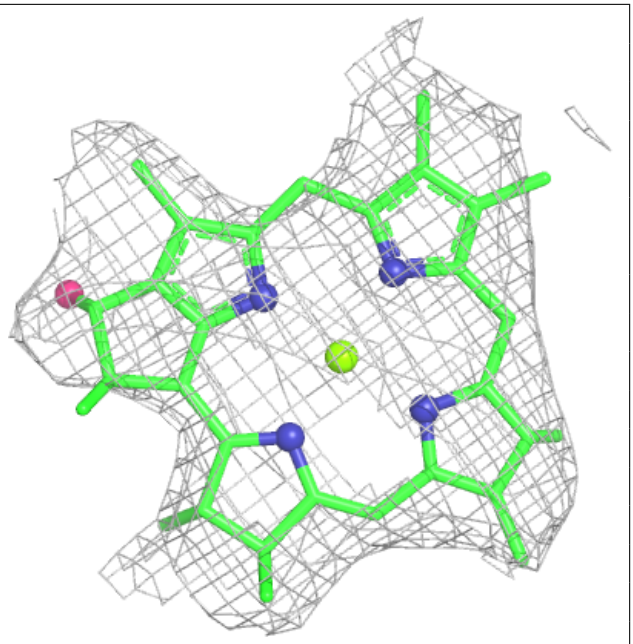


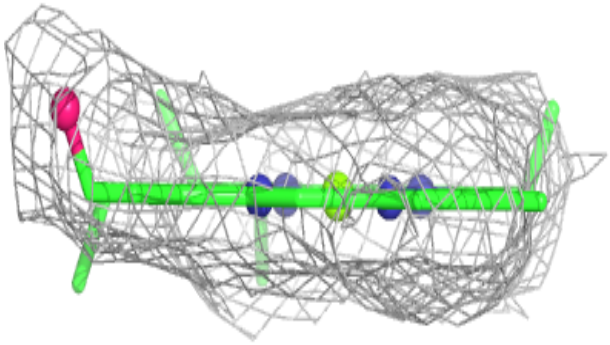


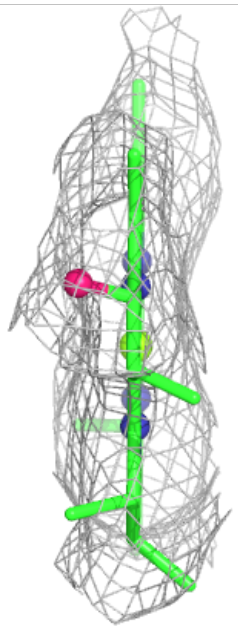


Electron density around CLA 1 1011:

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

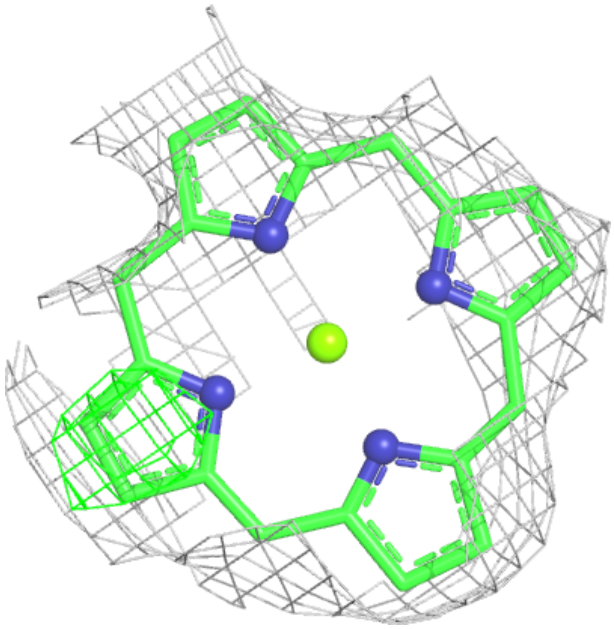


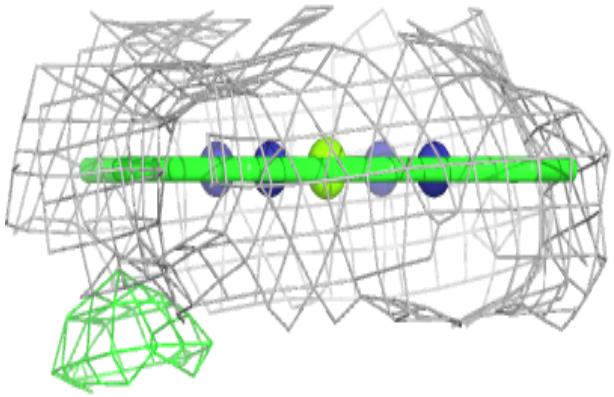


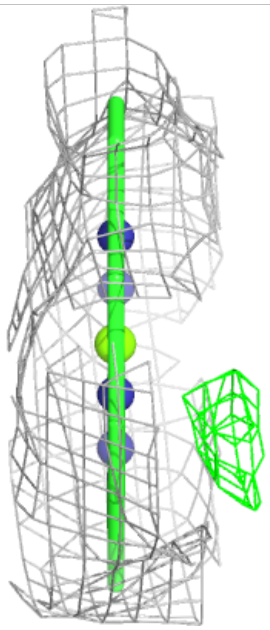


Electron density around CLA 4 4010:

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

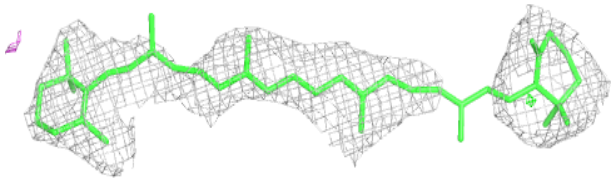


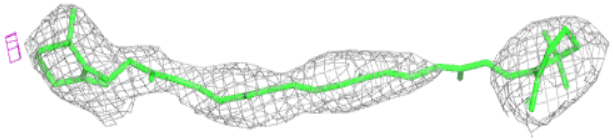


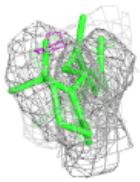


Electron density around BCR B 6004:

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

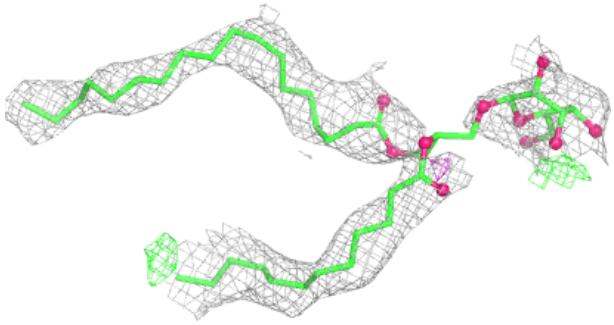


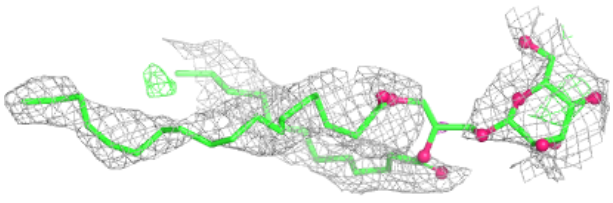


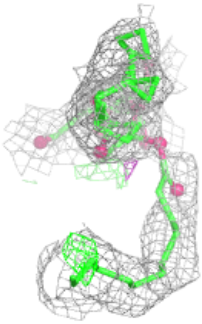


Electron density around LMG B 7101:

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

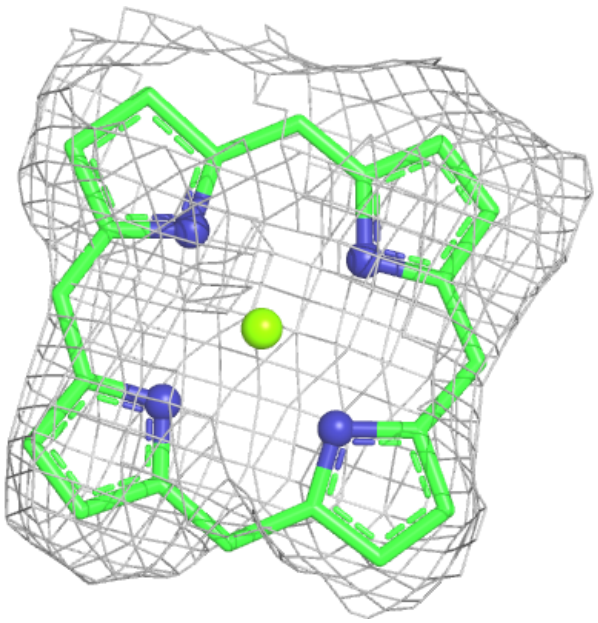


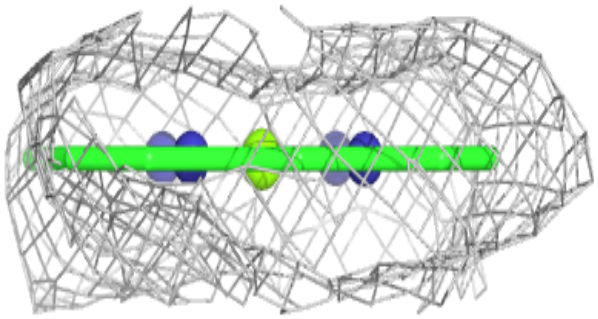


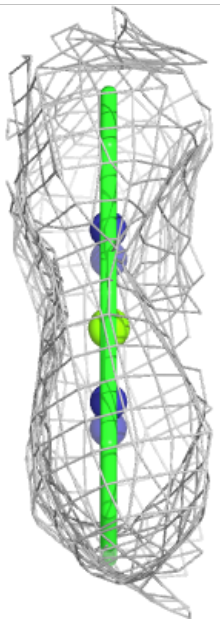


Electron density around CLA 4 4013:

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

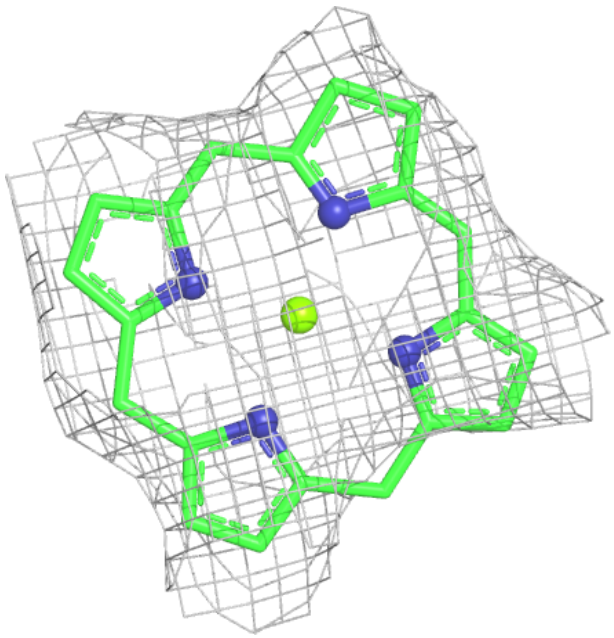


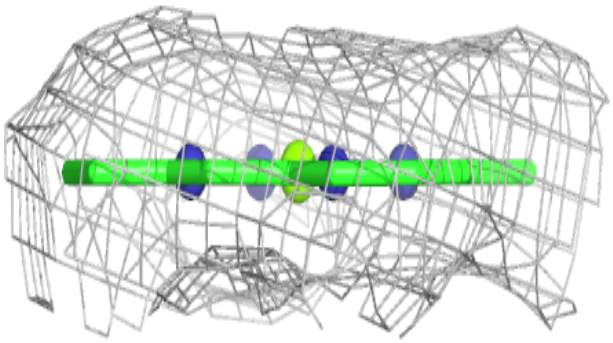


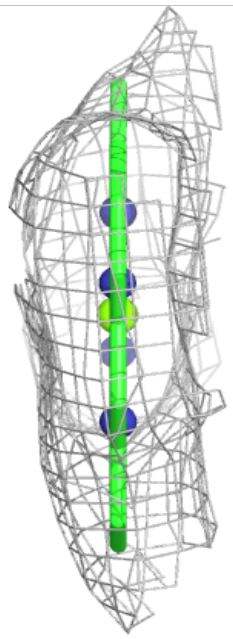


Electron density around CLA 3 3001:

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

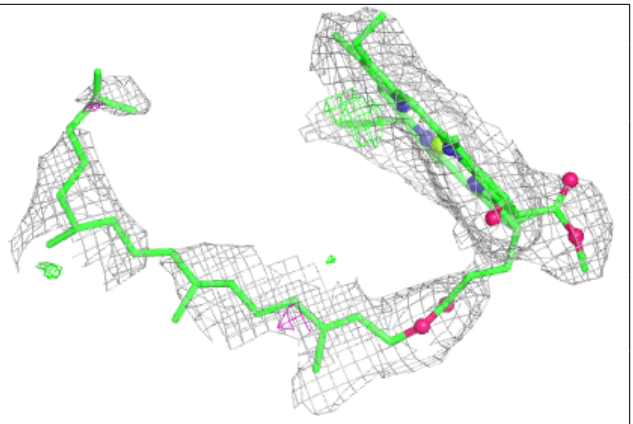


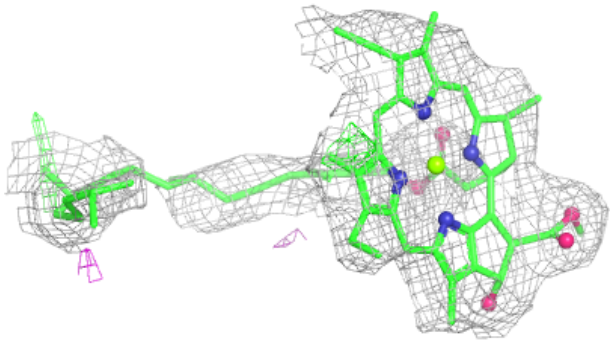


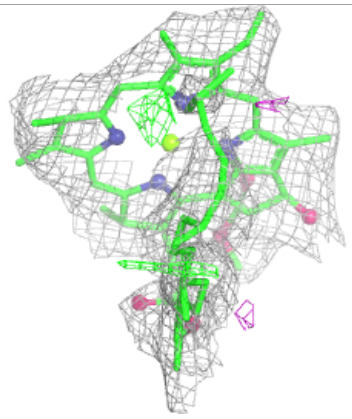


Electron density around CLA L 1130:

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

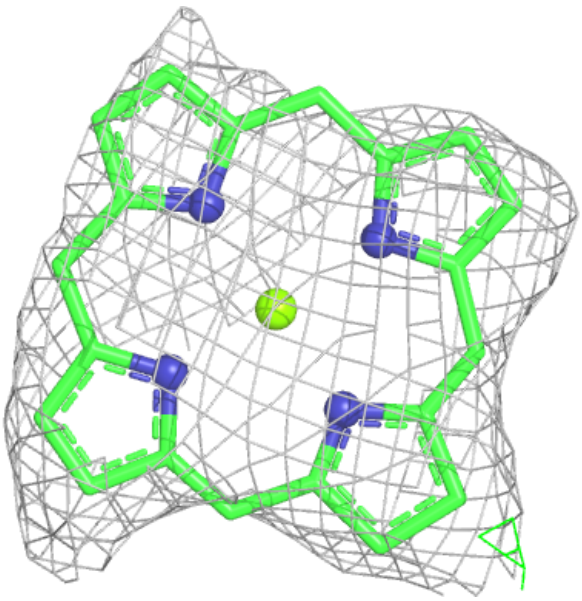


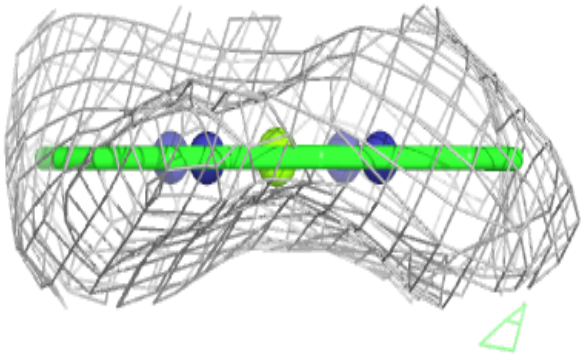


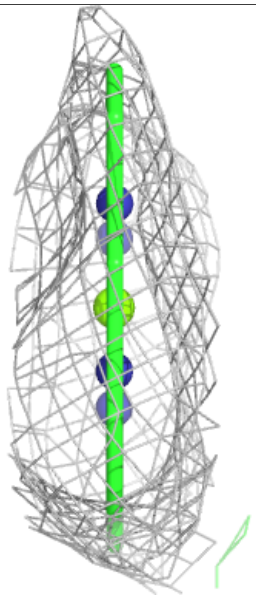


Electron density around CLA 2 2011:

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

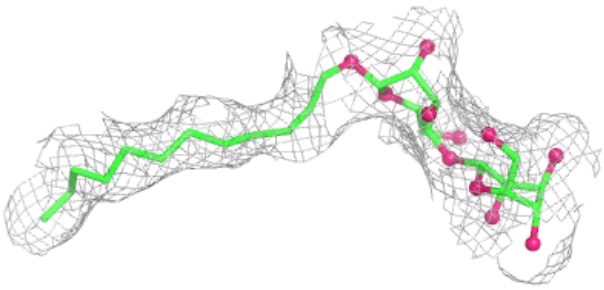


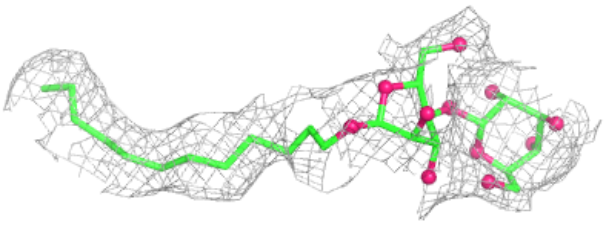


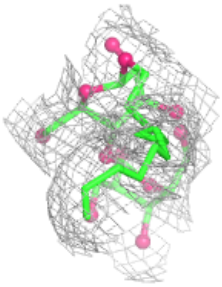


Electron density around LMU H 7002:

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

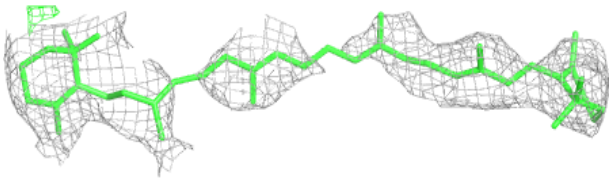


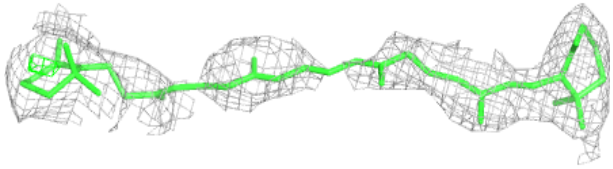


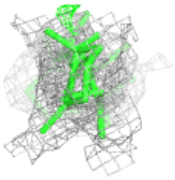


Electron density around BCR A 6003:

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

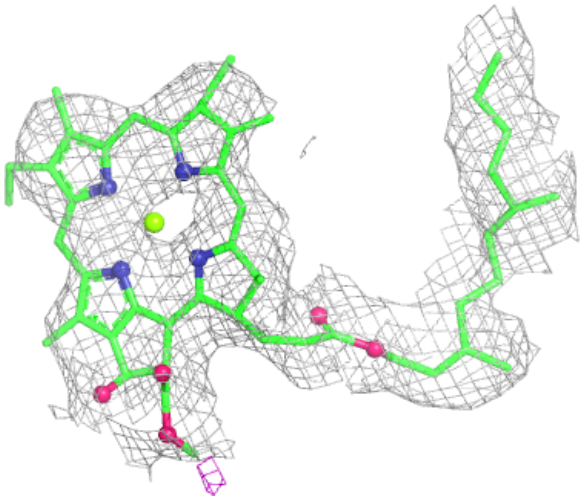


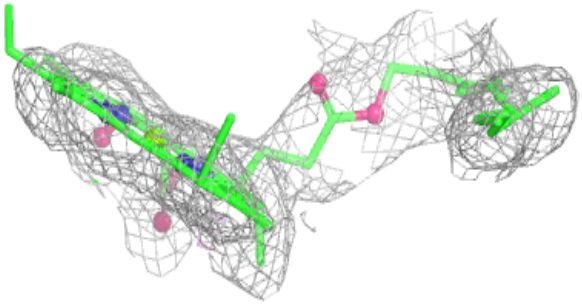


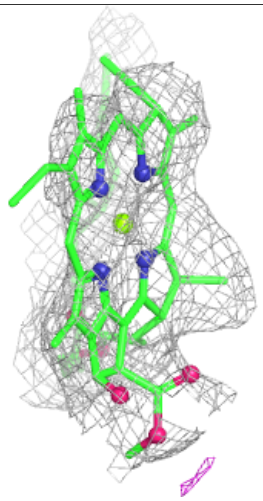


Electron density around CLA B 1222:

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

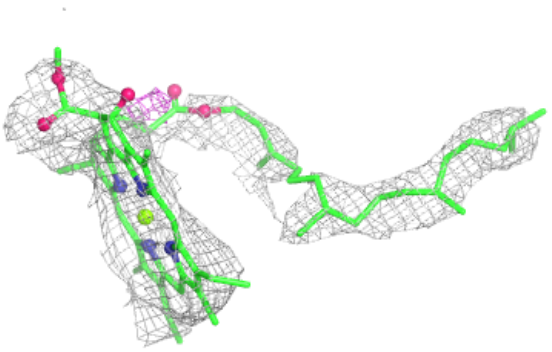


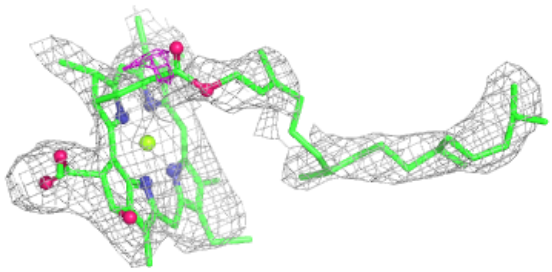


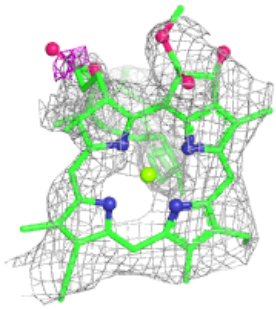


Electron density around CLA A 1109:

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

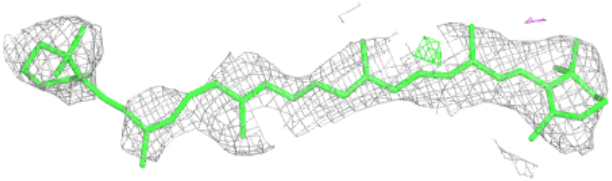


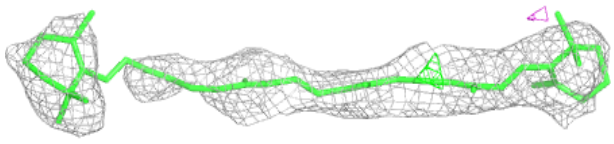


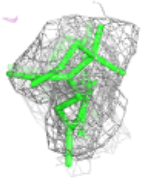


Electron density around BCR B 6017:

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

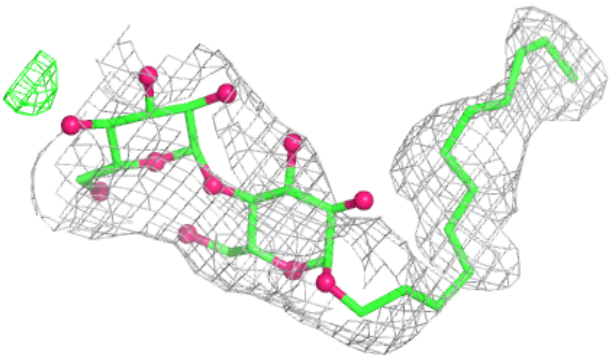


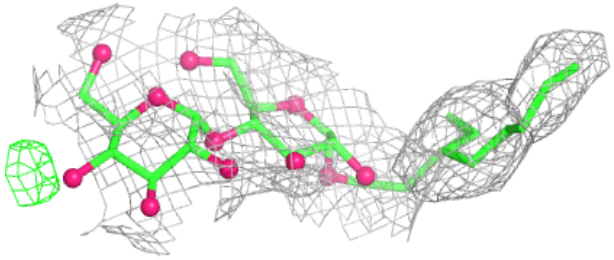


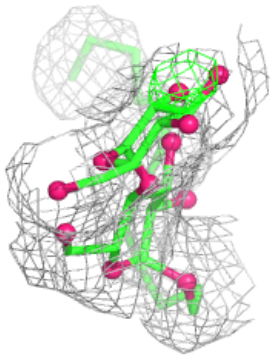


Electron density around LMU R 7025:

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

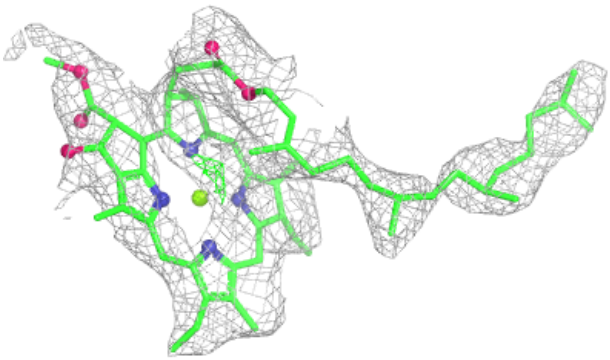


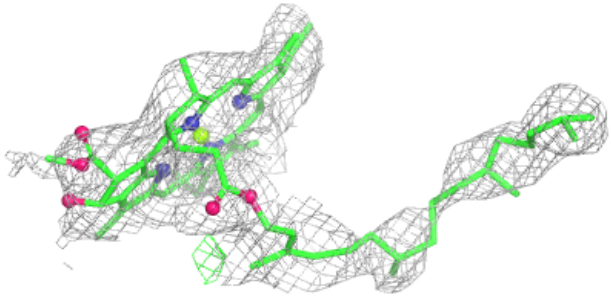


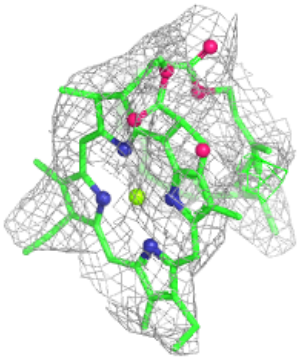


Electron density around CLA B 1211:

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

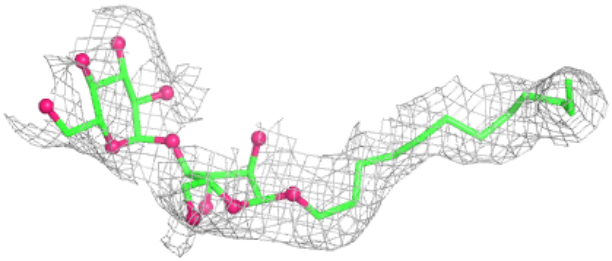




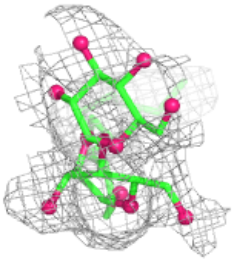


Electron density around LMU 4 7018:

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

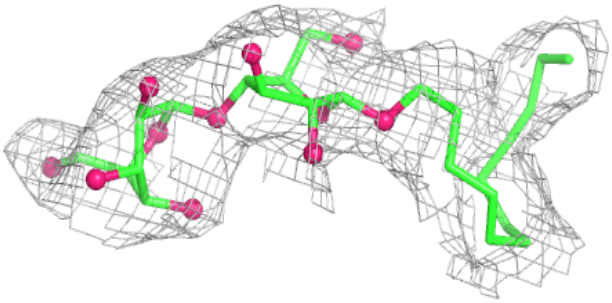


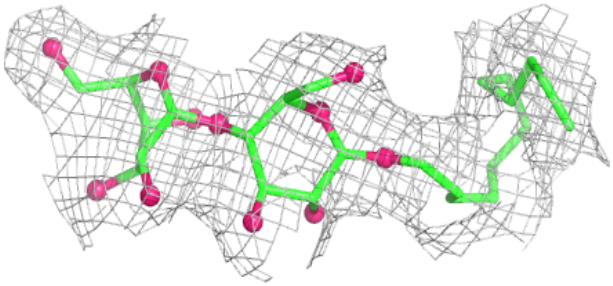


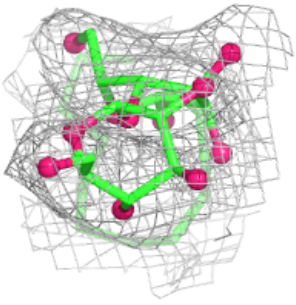


Electron density around LMU A 7023:

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

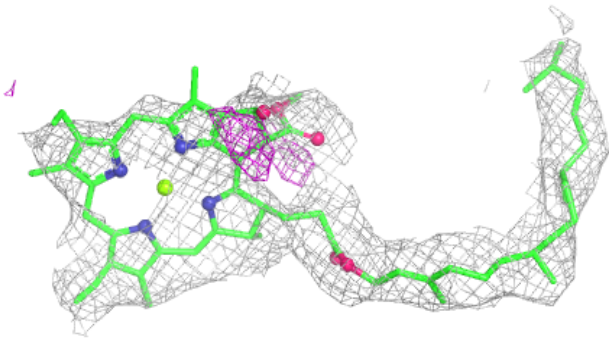


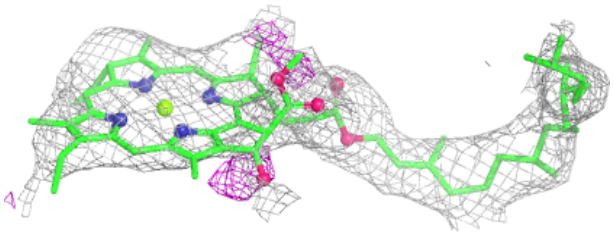


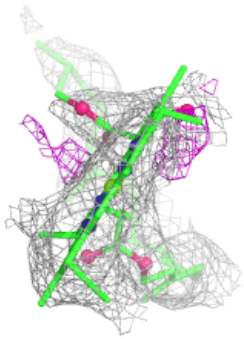


Electron density around CLA B 1223:

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

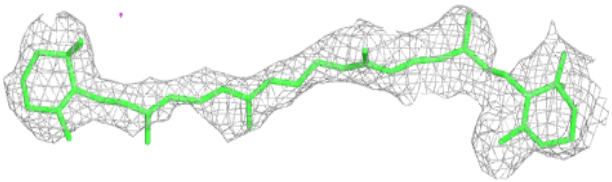


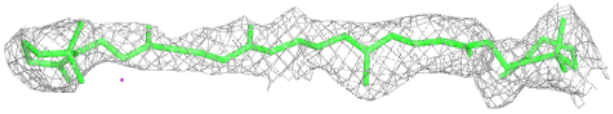


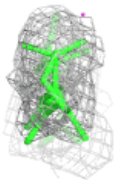


Electron density around BCR L 6019:

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

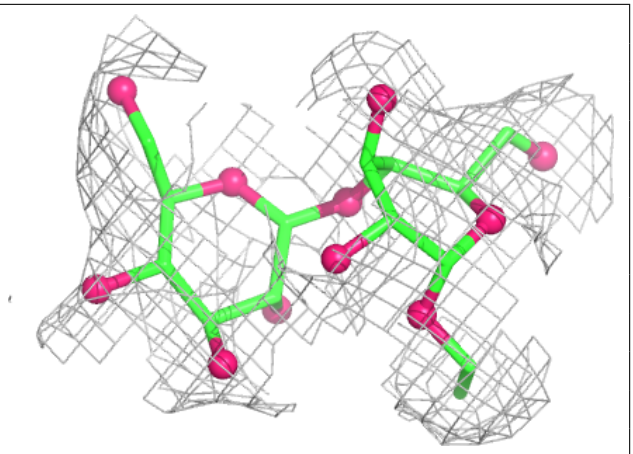


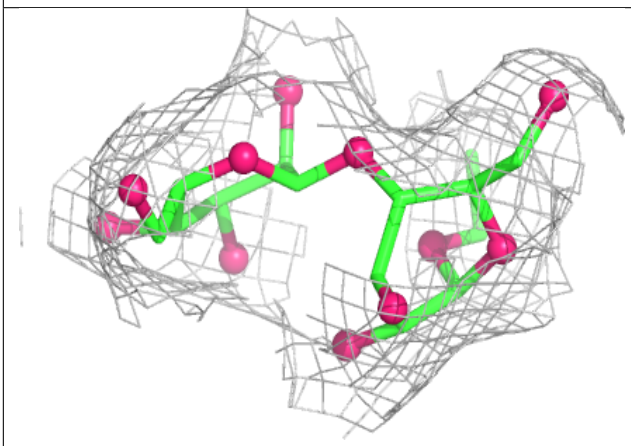


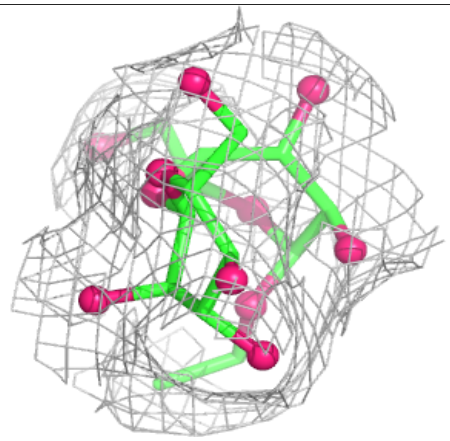


Electron density around LMU B 7012:

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

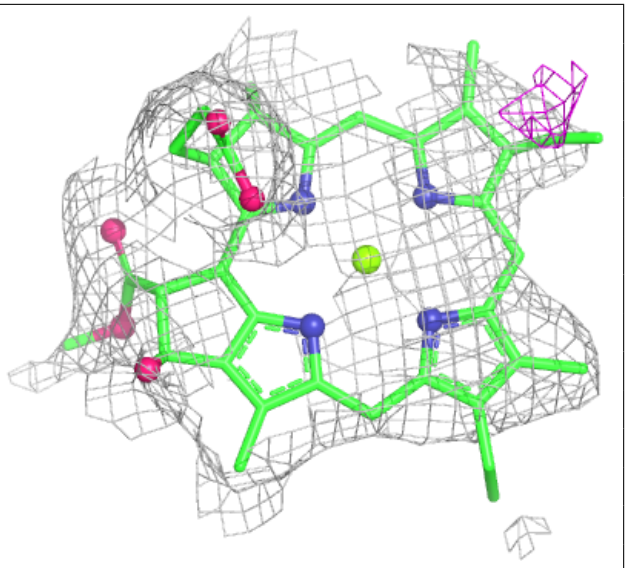


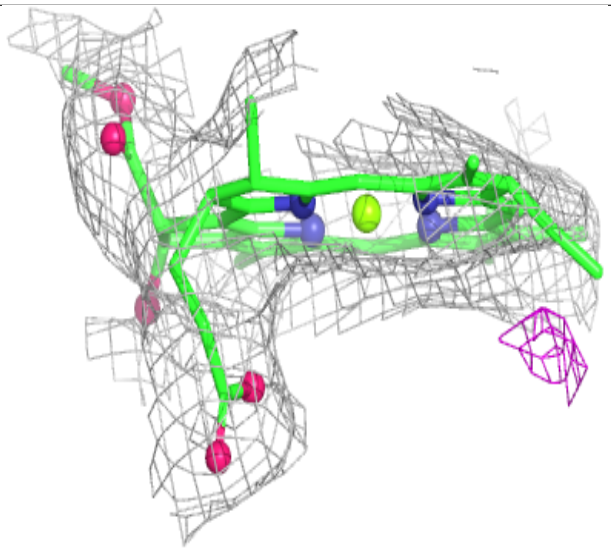


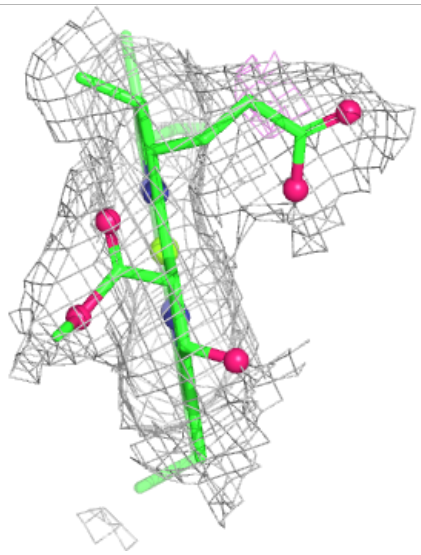


Electron density around CLA B 1231:

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

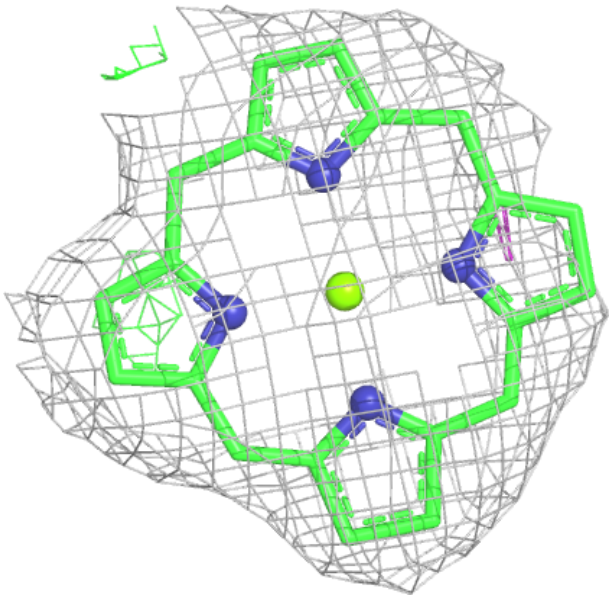


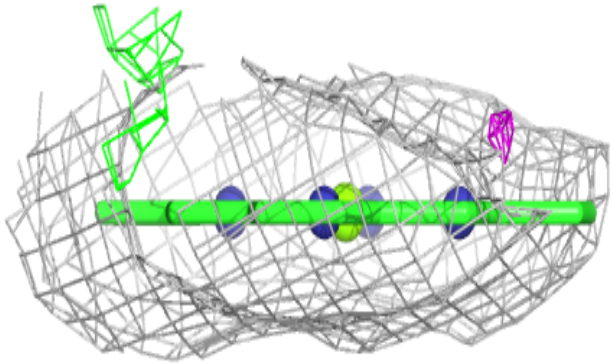


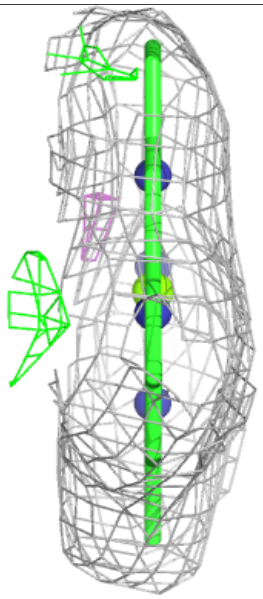


Electron density around CLA 4 4005:

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

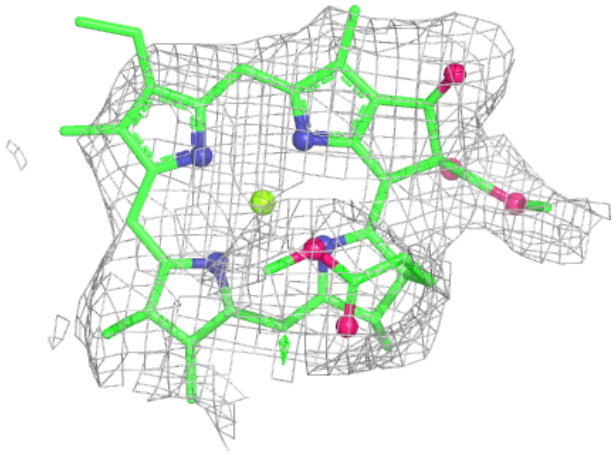


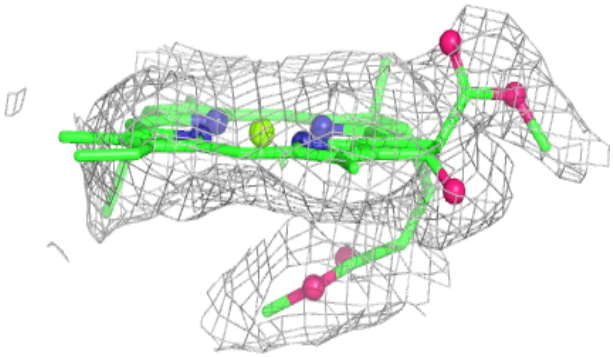


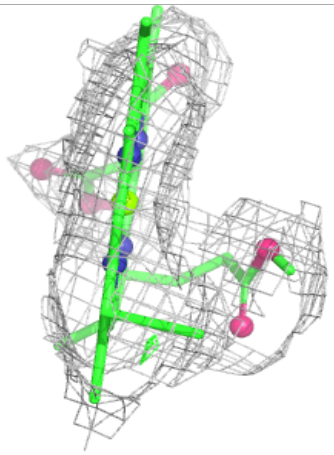


Electron density around CLA 1 1005:

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

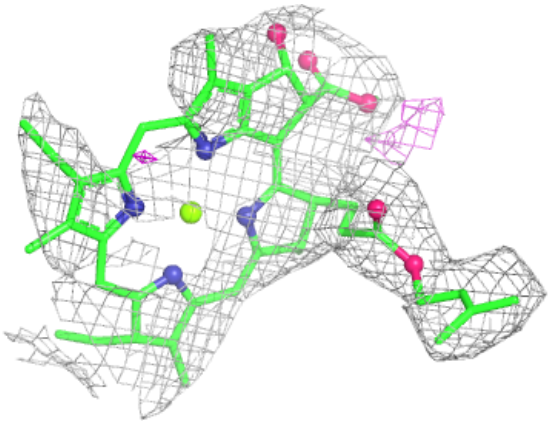


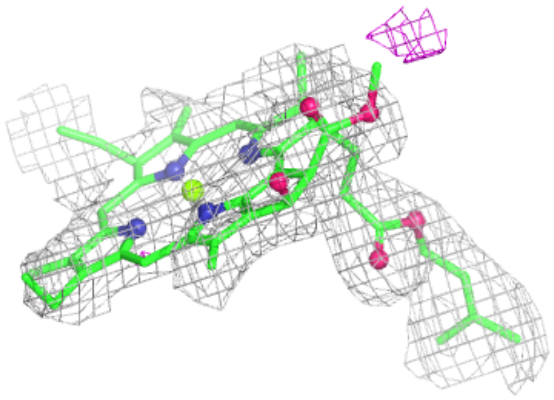


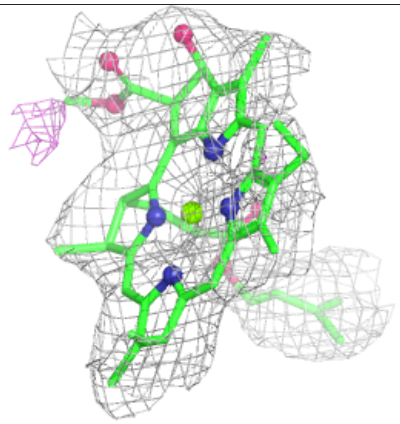


Electron density around CLA 2 2012:

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

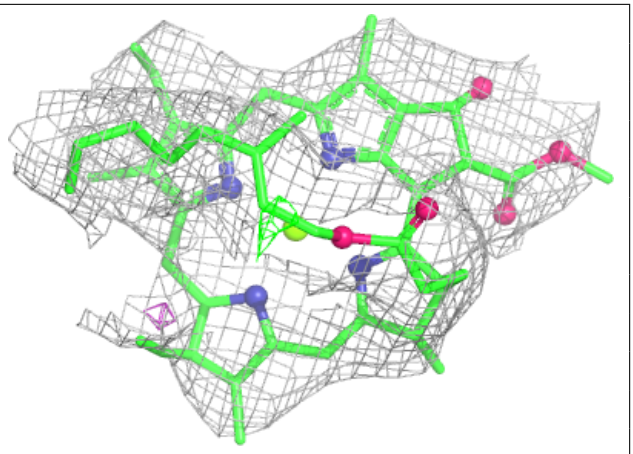


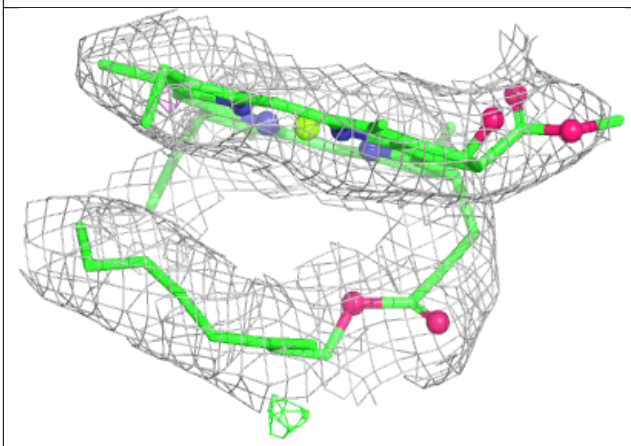




Electron density around CLA A 1110:

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

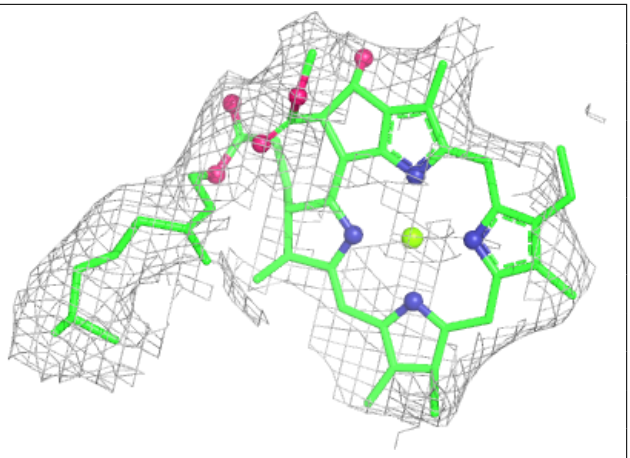


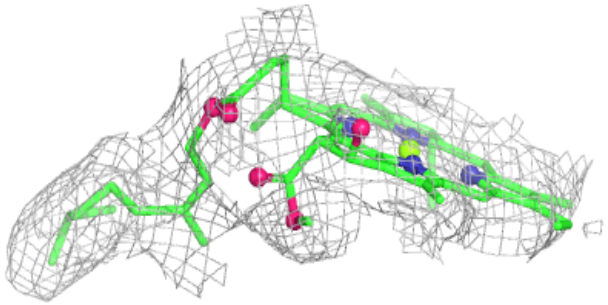




Electron density around CLA J 1308:

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

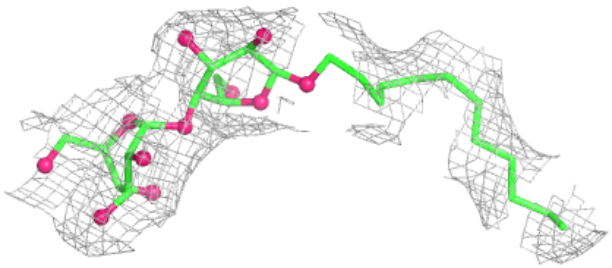


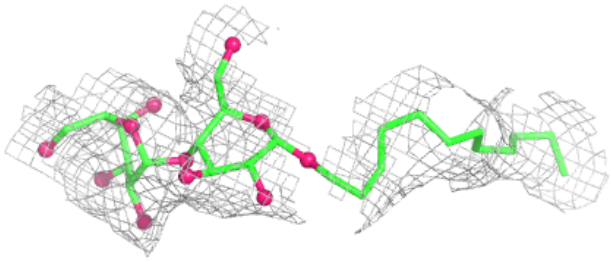


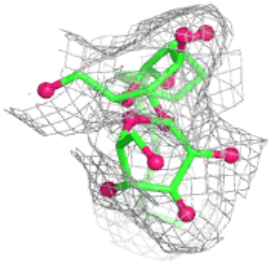


Electron density around LMU 2 7027:

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

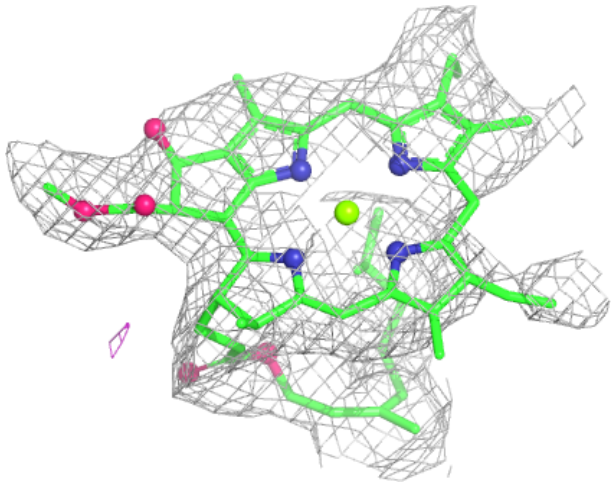


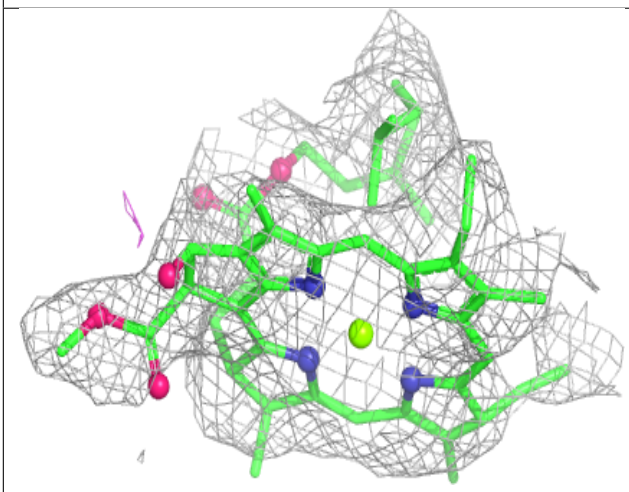


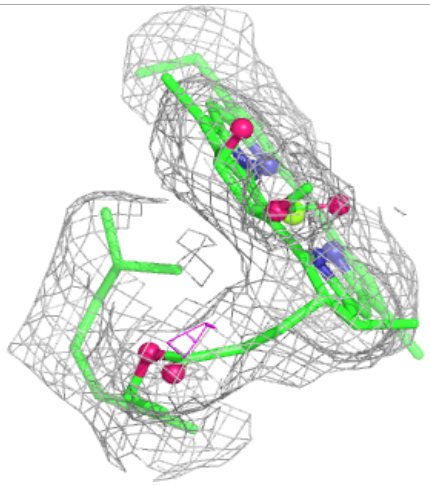


Electron density around CLA B 1209:

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

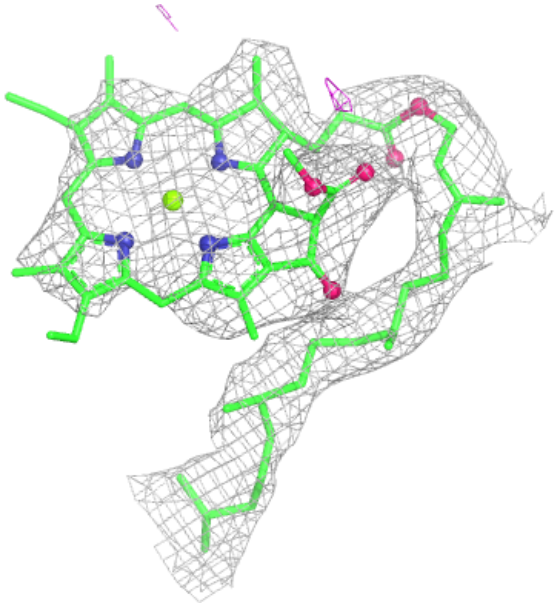


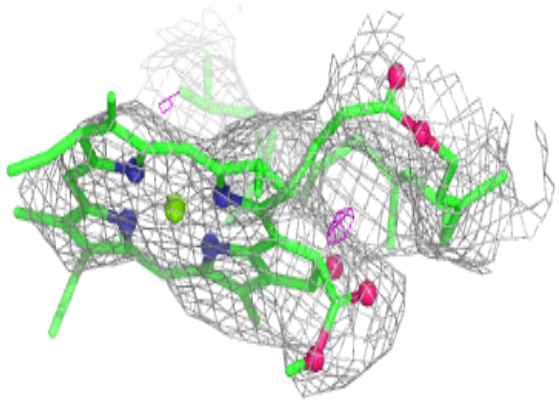


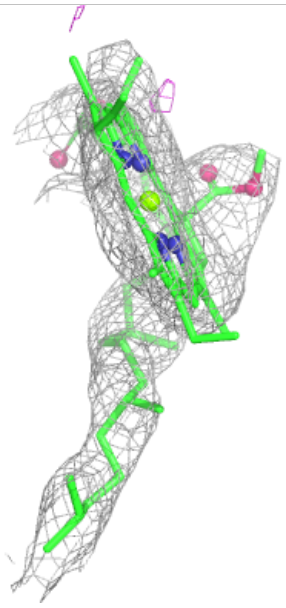


Electron density around CLA A 1123:

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

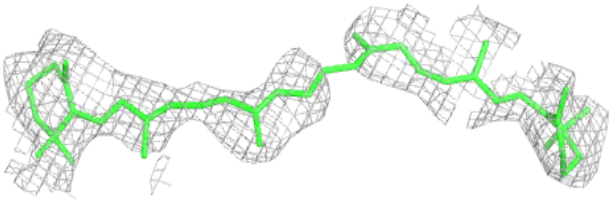


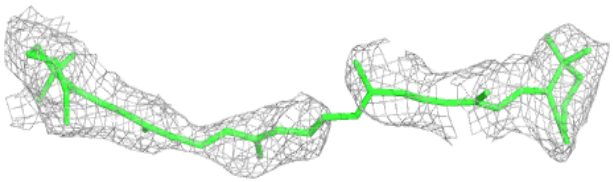


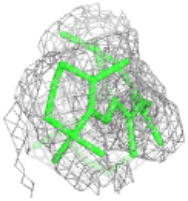


Electron density around BCR I 6018:

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

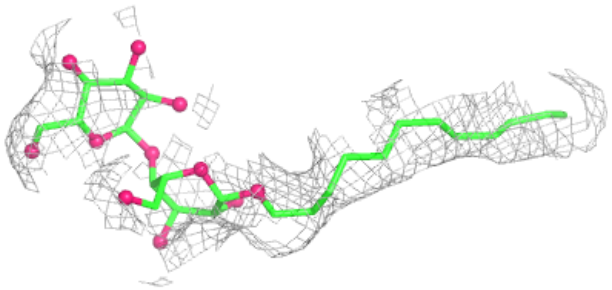


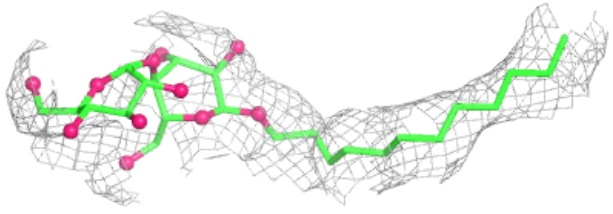


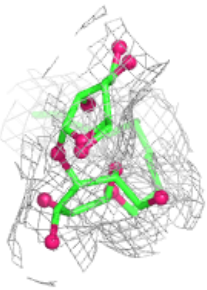


Electron density around LMU R 7024:

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

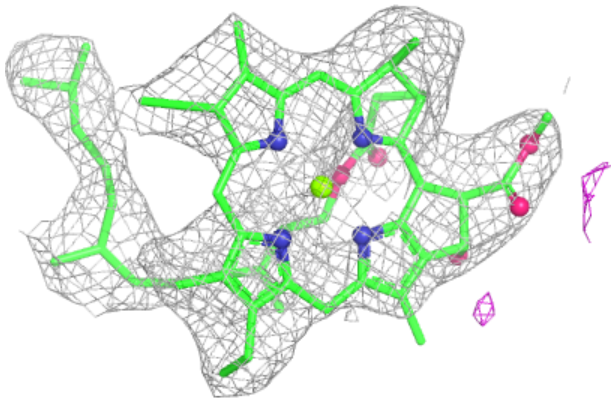


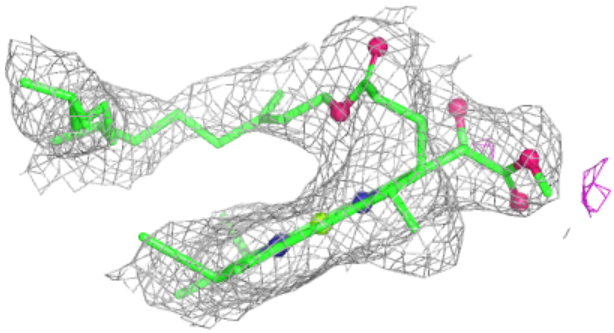




Electron density around CLA I 1204:

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

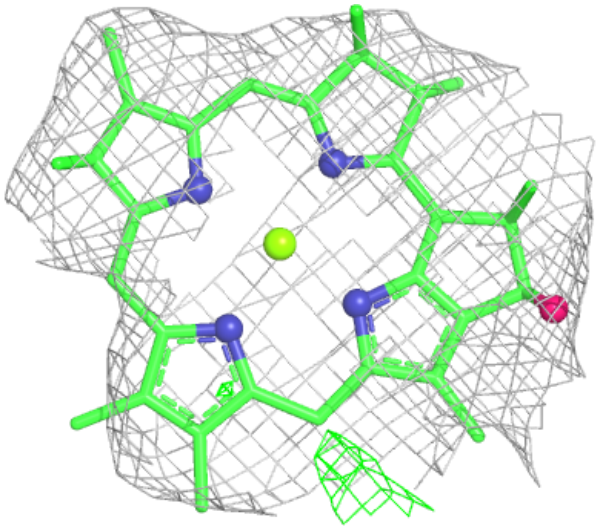


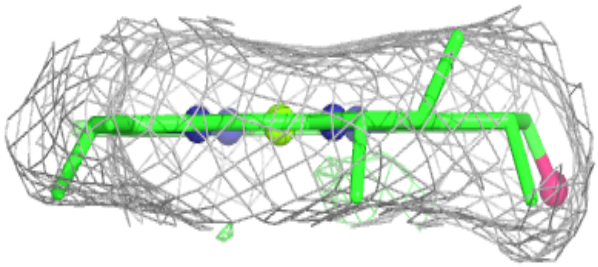


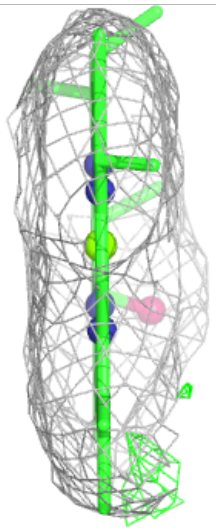


Electron density around CLA 4 1009:

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

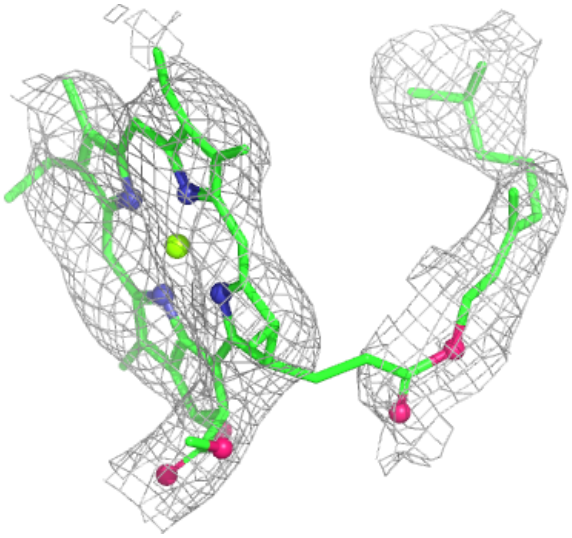


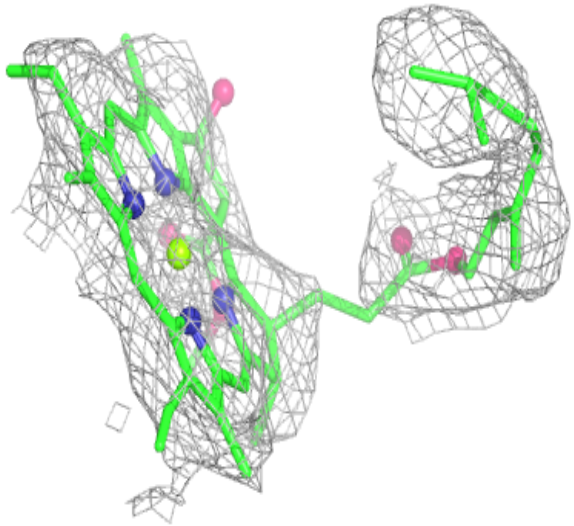


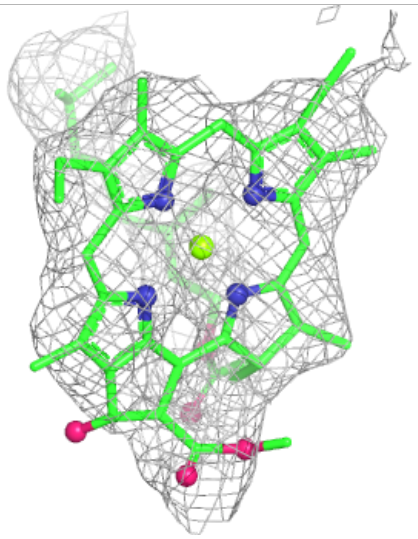


Electron density around CLA A 1102:

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

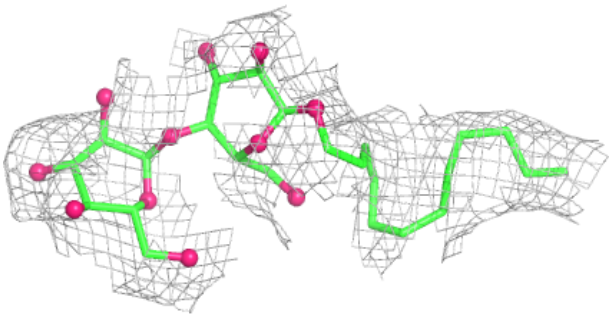


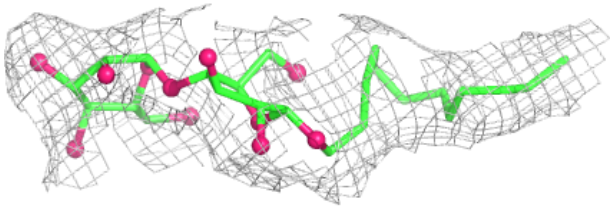


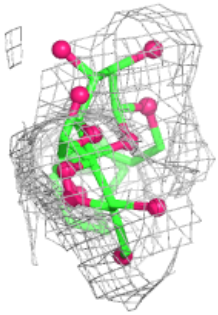


Electron density around LMU A 7016:

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

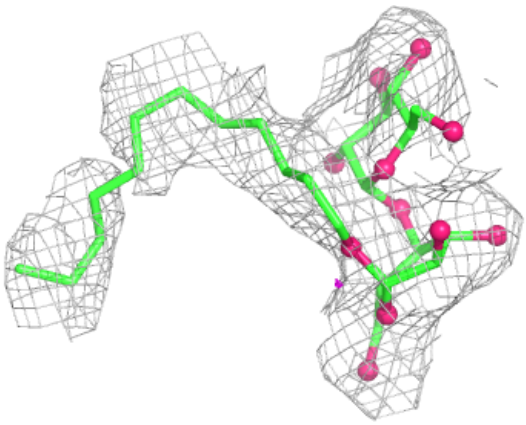


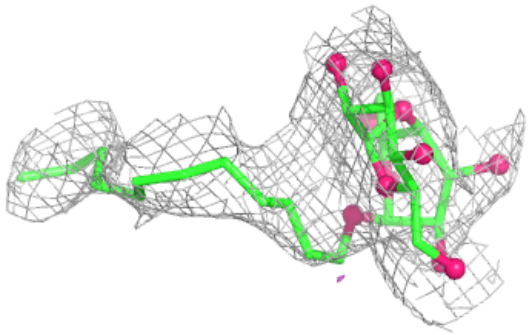




Electron density around LMU H 7032:

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

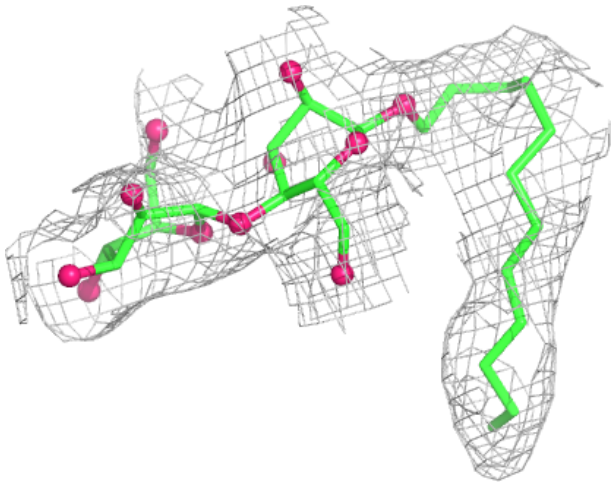


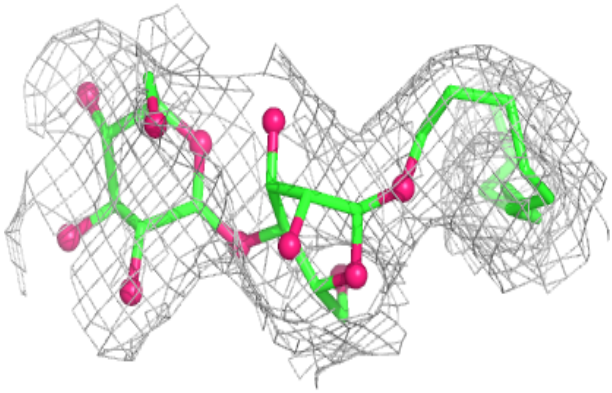




Electron density around LMU R 7014:

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

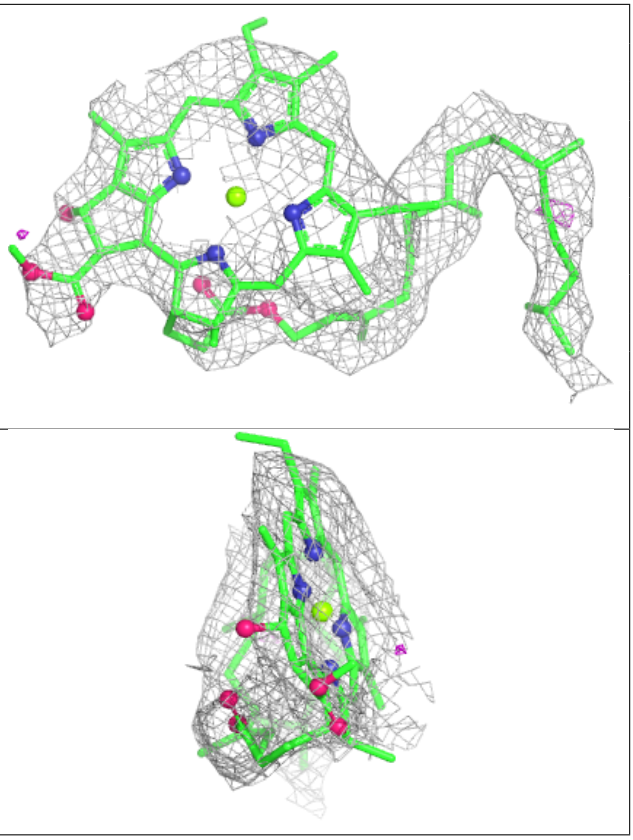


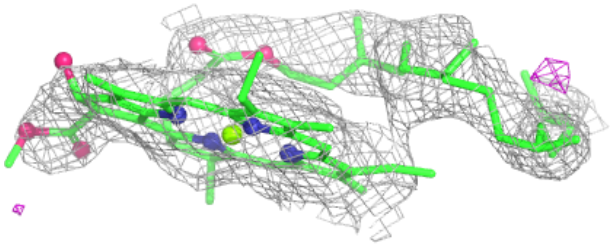




Electron density around CLA A 1117:

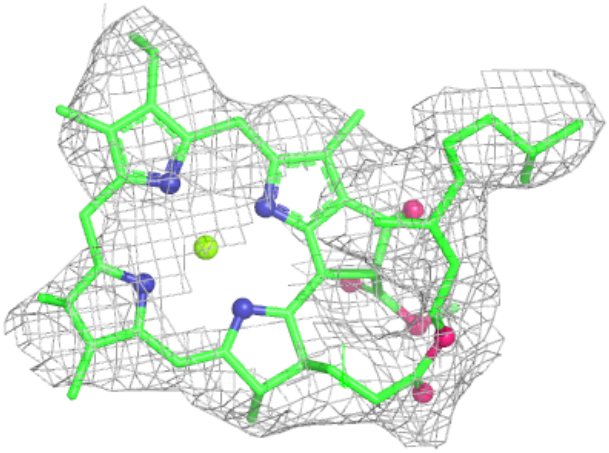
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

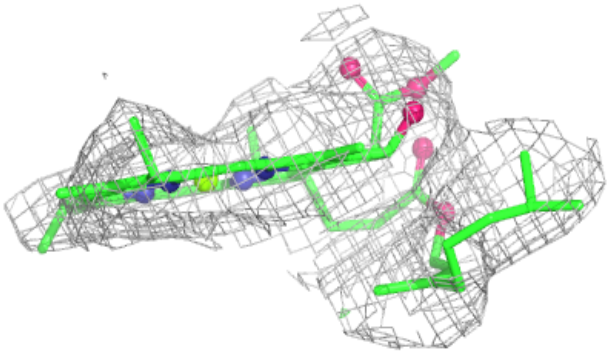


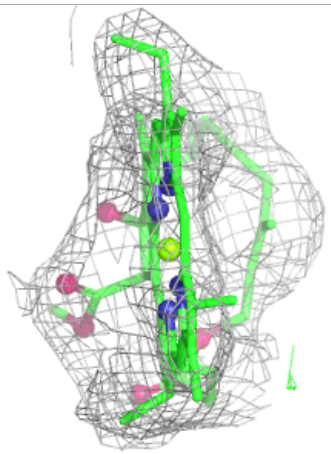


Electron density around CLA B 1208:

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

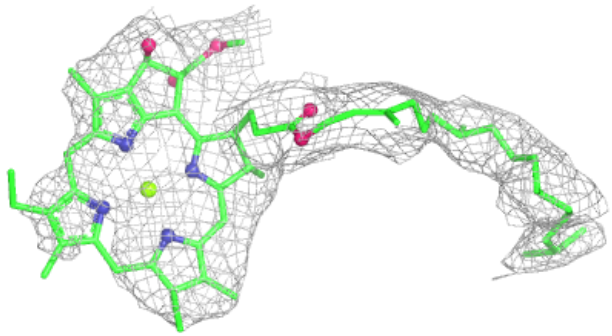


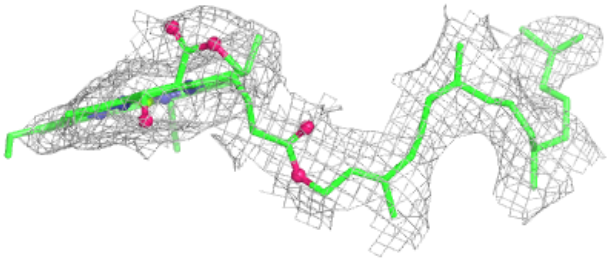




Electron density around CLA A 1124:

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

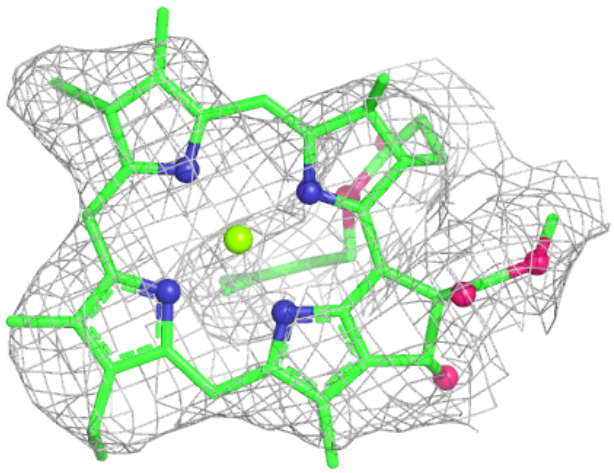


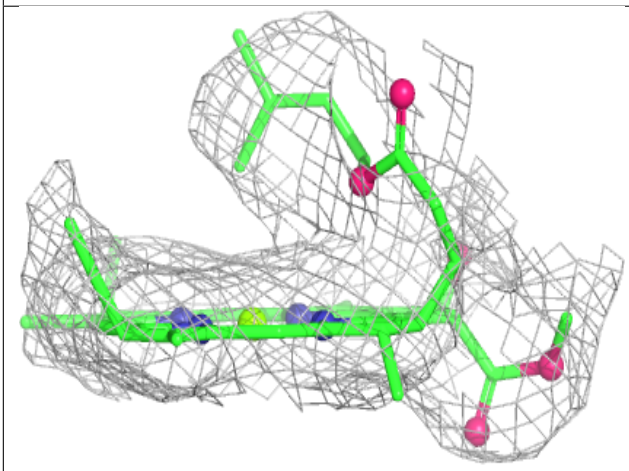


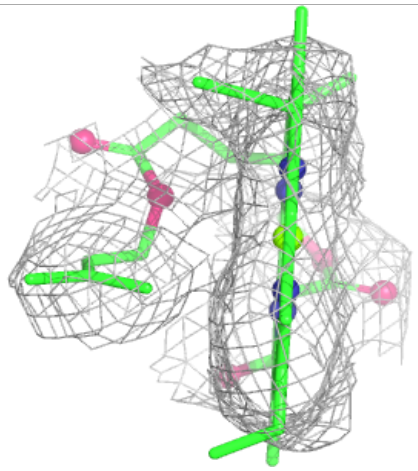


Electron density around CLA L 1501:

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

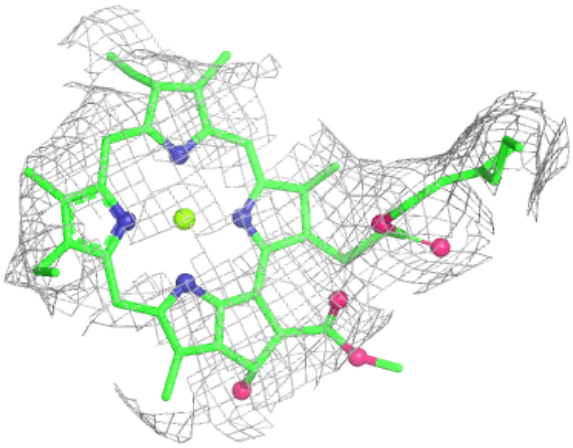


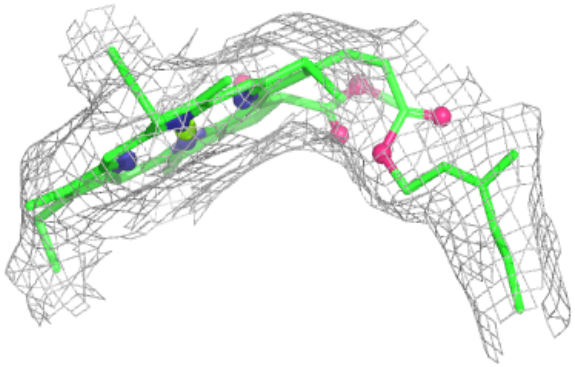


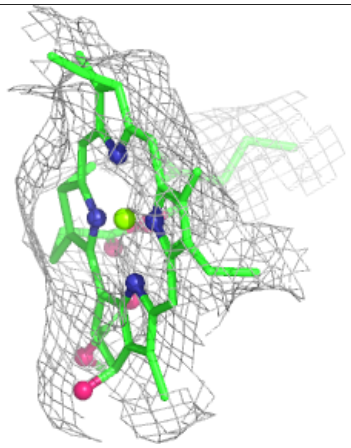


Electron density around CLA 4 4002:

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



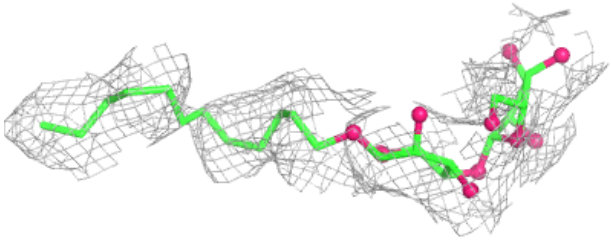


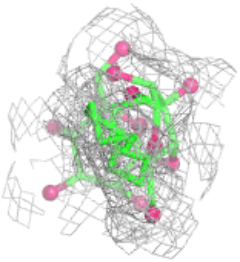


Electron density around LMU 4 7033:

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

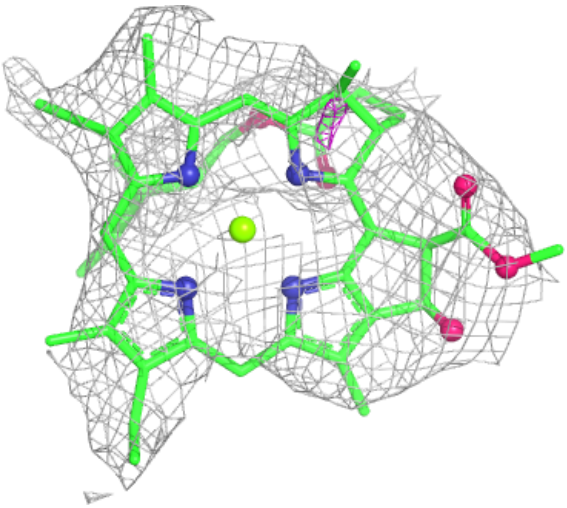


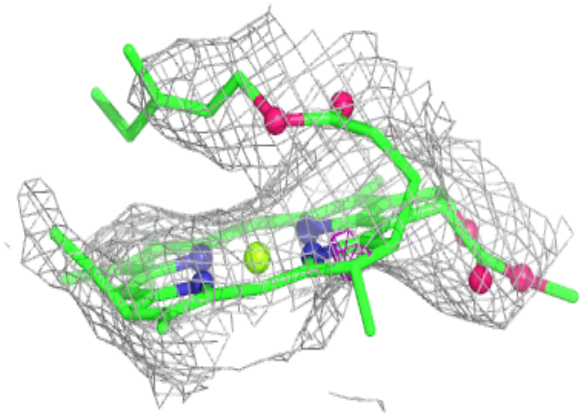


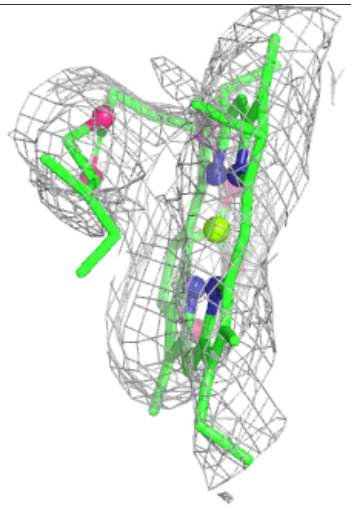


Electron density around CLA A 1120:

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

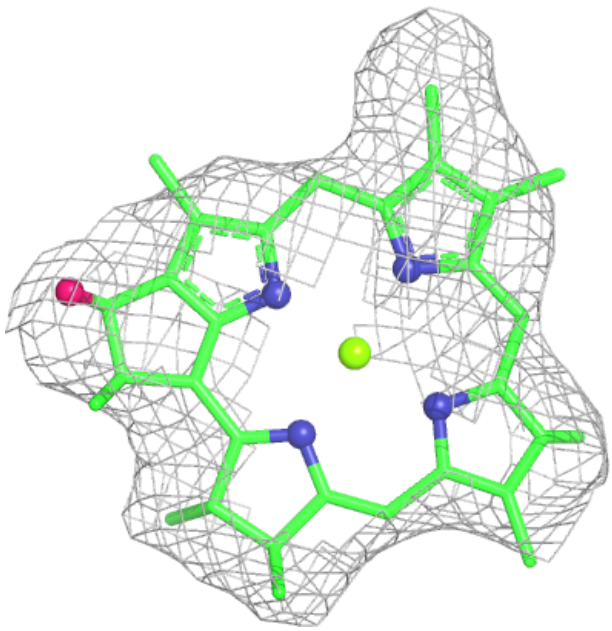


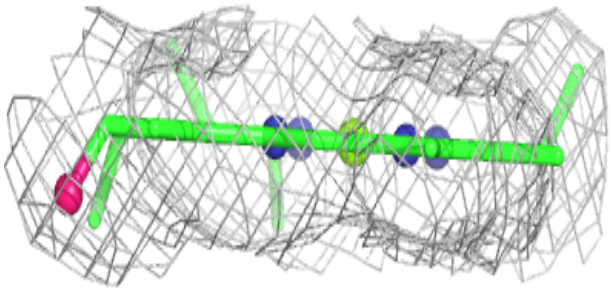


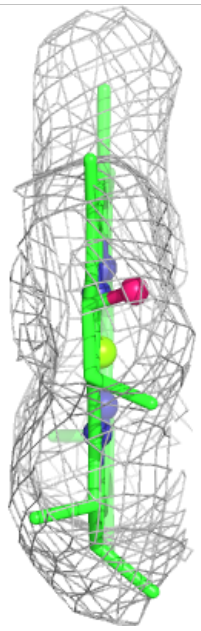


Electron density around CLA 1 1012:

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

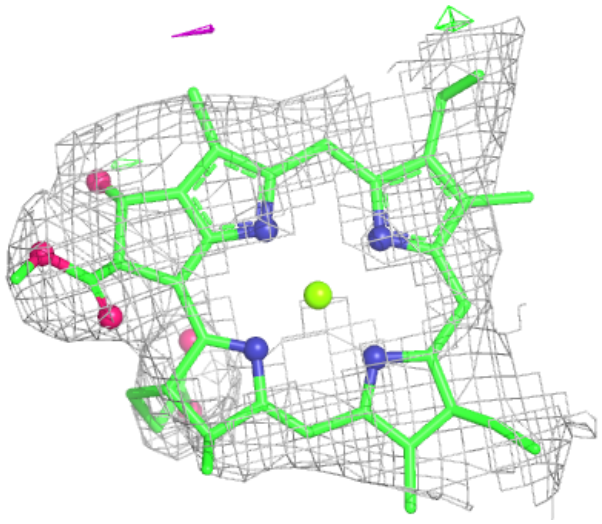


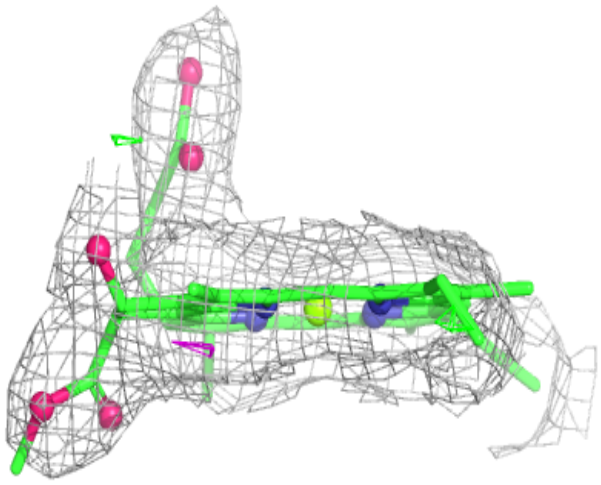




Electron density around CLA B 1201:

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

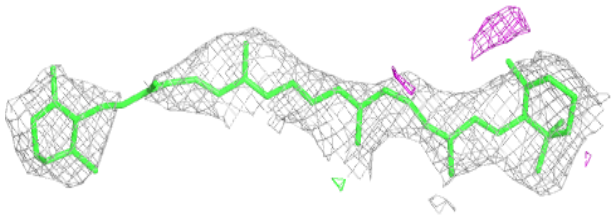


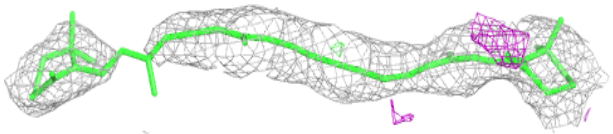


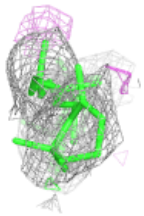


Electron density around BCR B 6010:

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

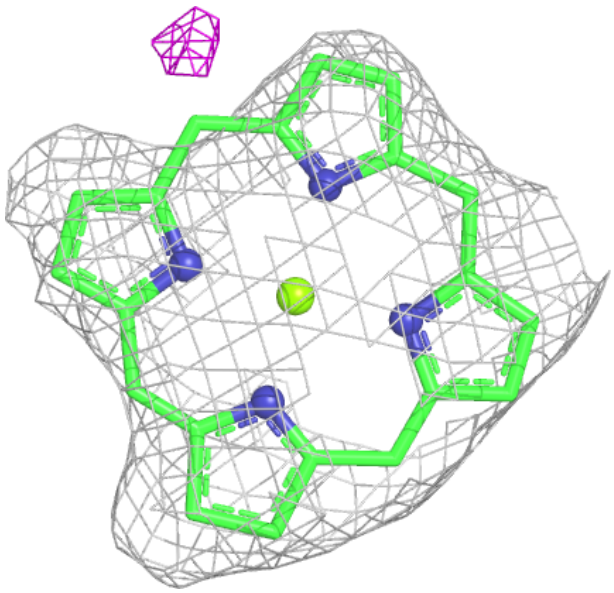


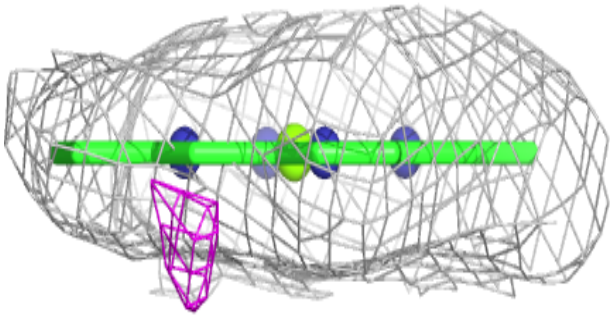


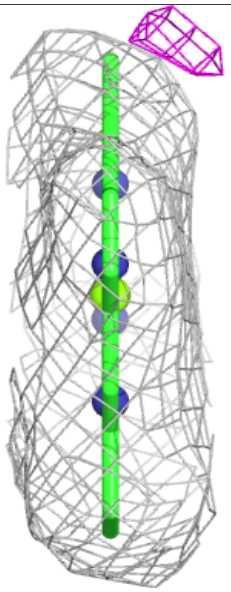


Electron density around CLA 2 2010:

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

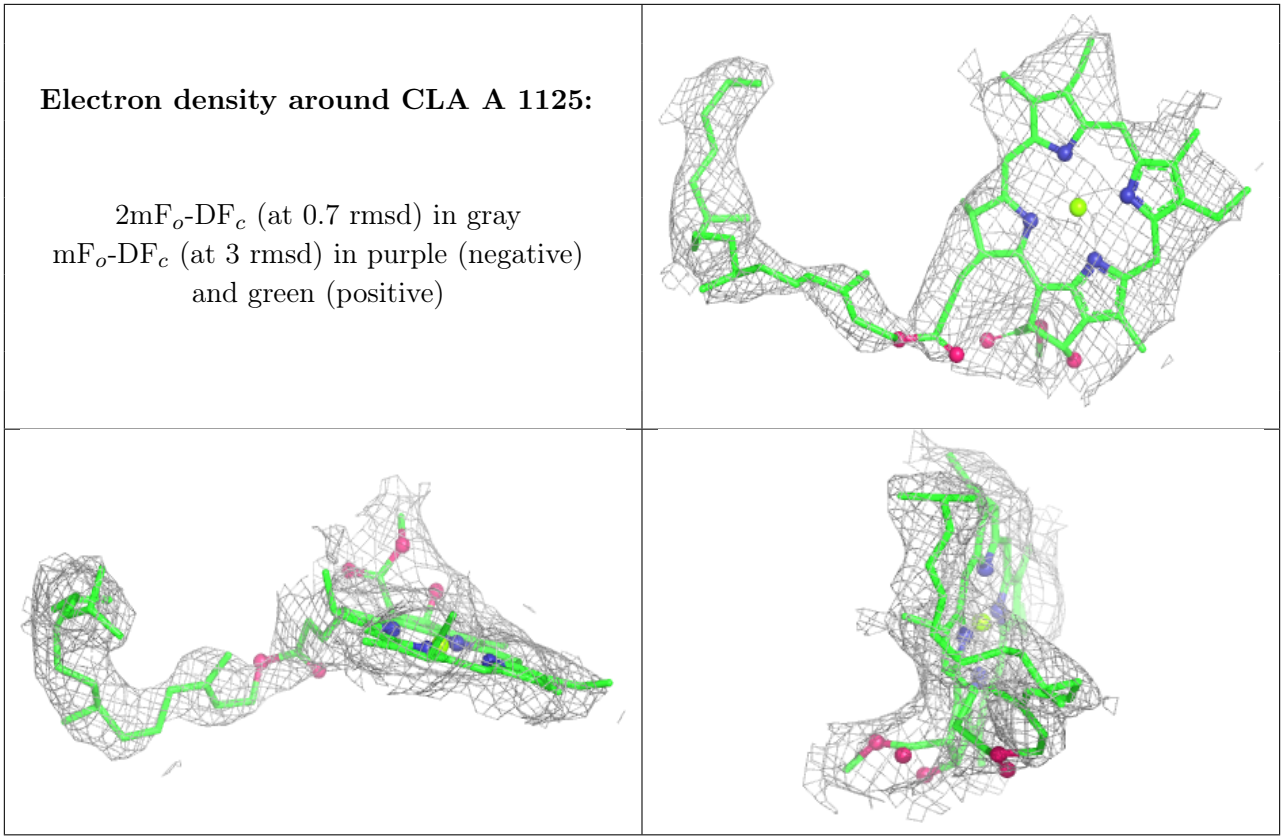






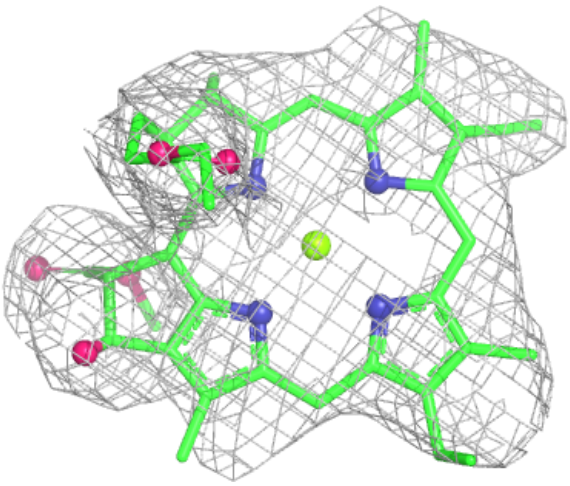
Electron density around CLA A 1125:

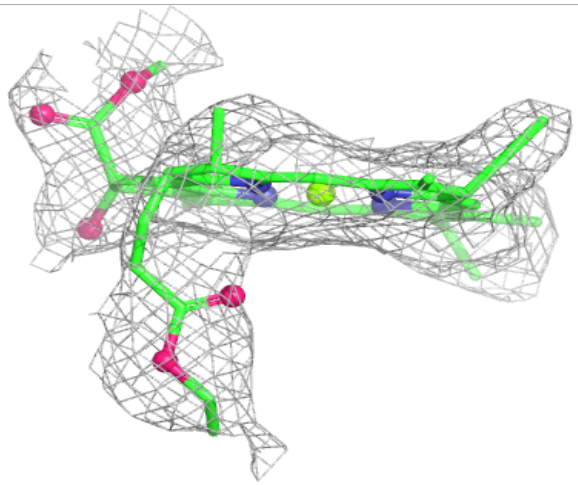
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

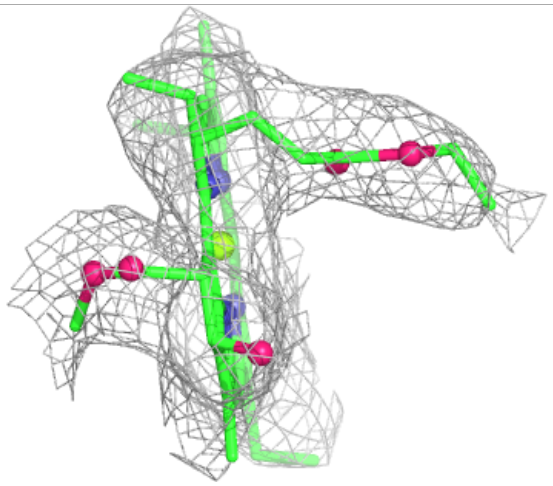


Electron density around CLA L 1502:

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

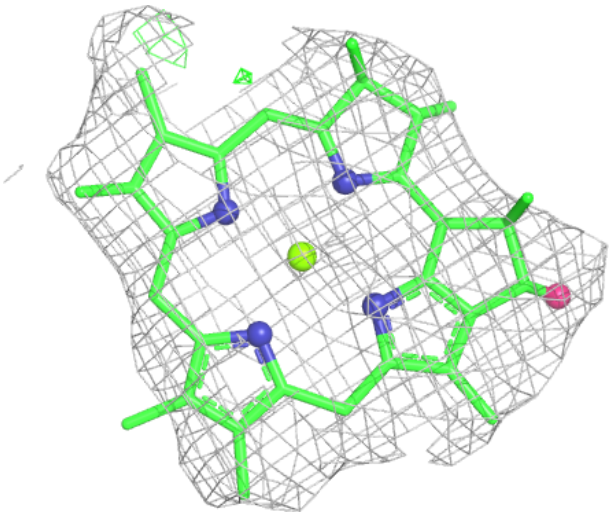


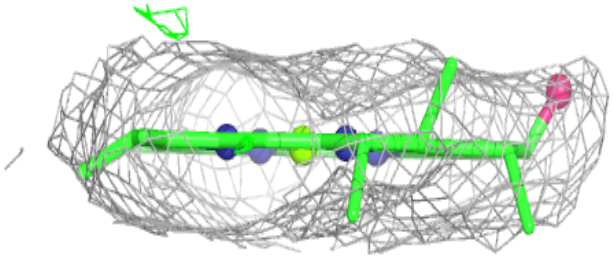


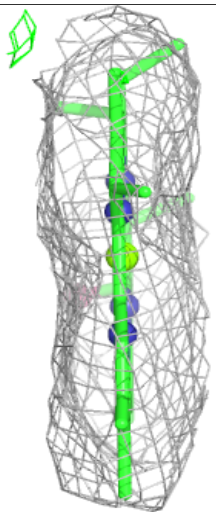


Electron density around CLA F 1240:

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

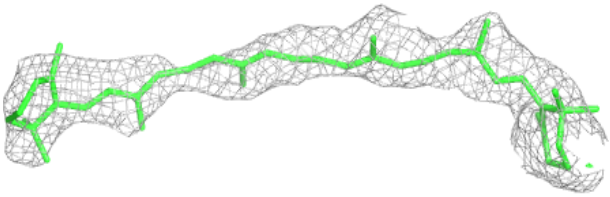


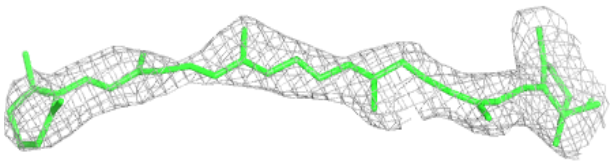


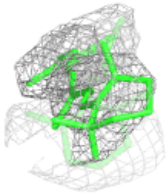


Electron density around BCR F 6014:

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

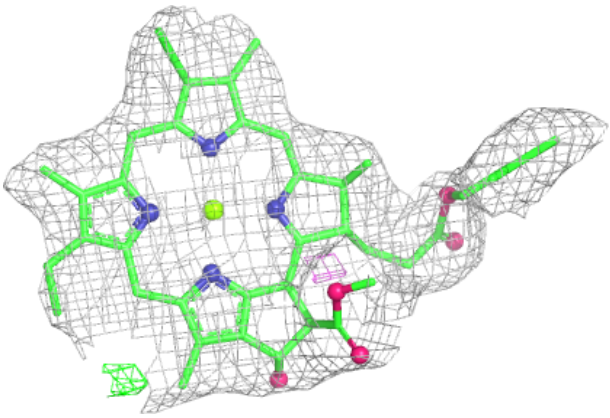


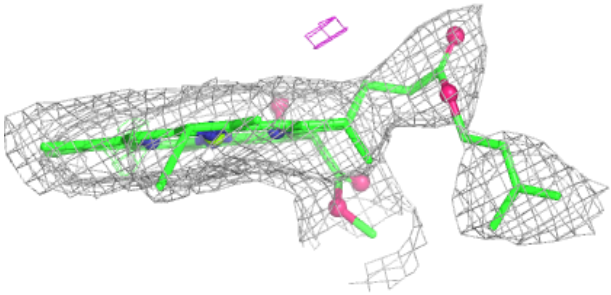




Electron density around CLA B 1228:

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

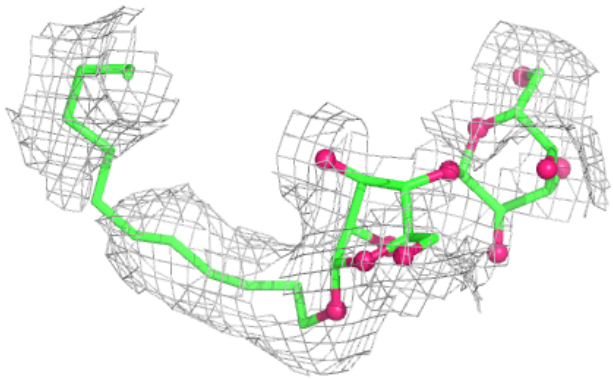


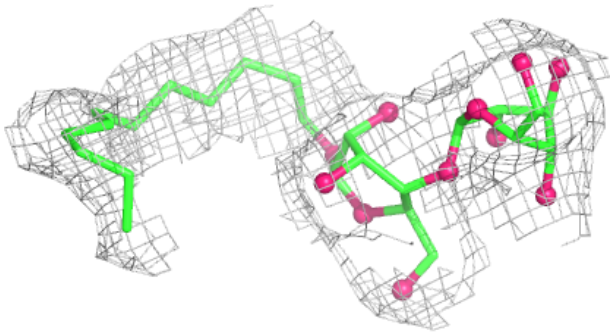


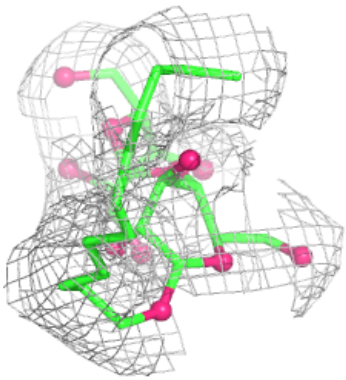


Electron density around LMU R 7022:

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

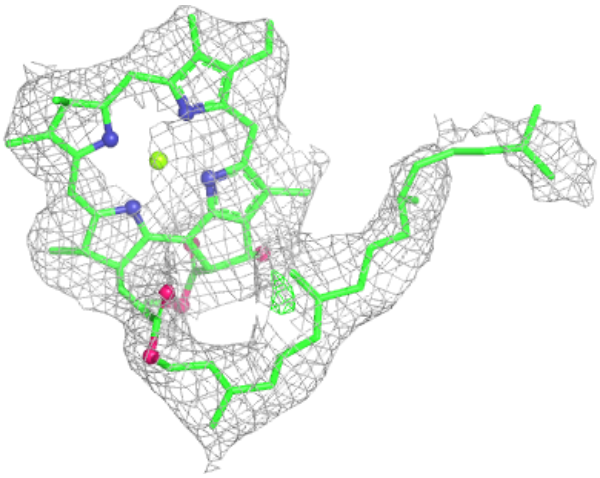


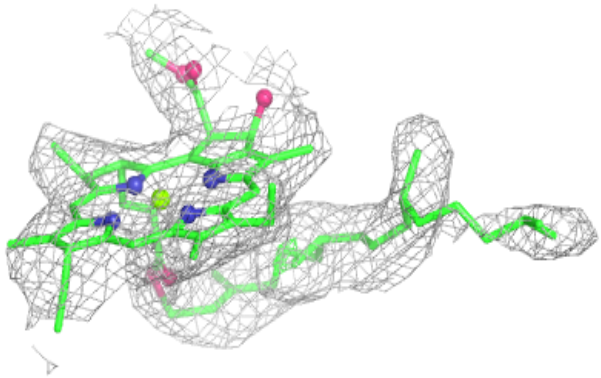


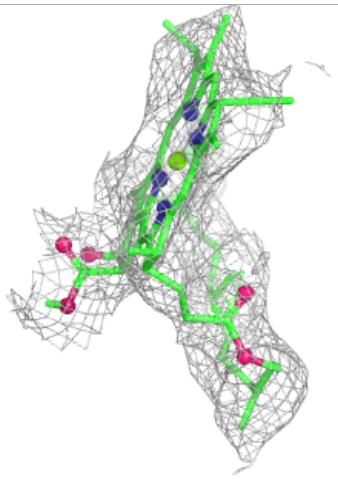


Electron density around CLA B 1229:

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

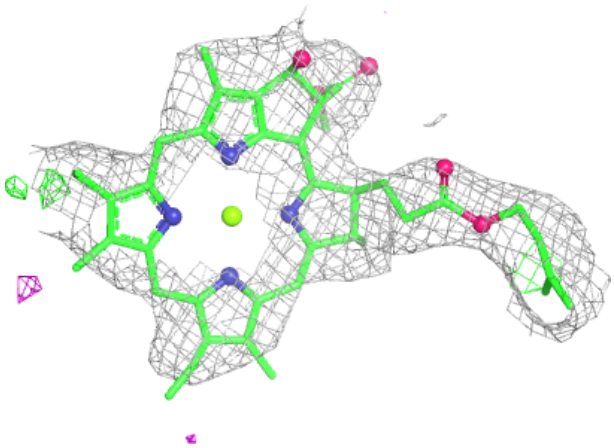


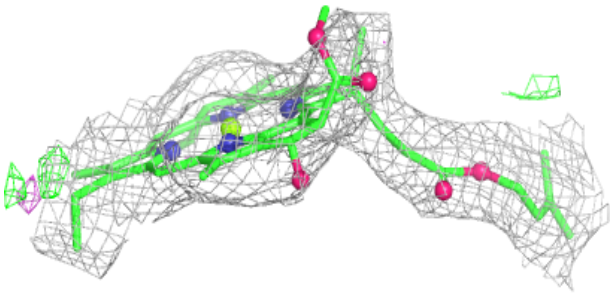


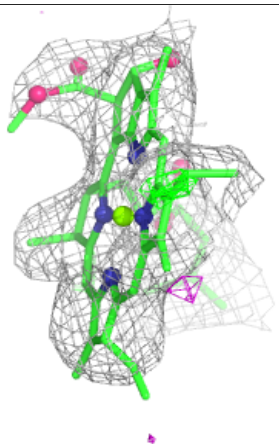


Electron density around CLA B 1230:

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

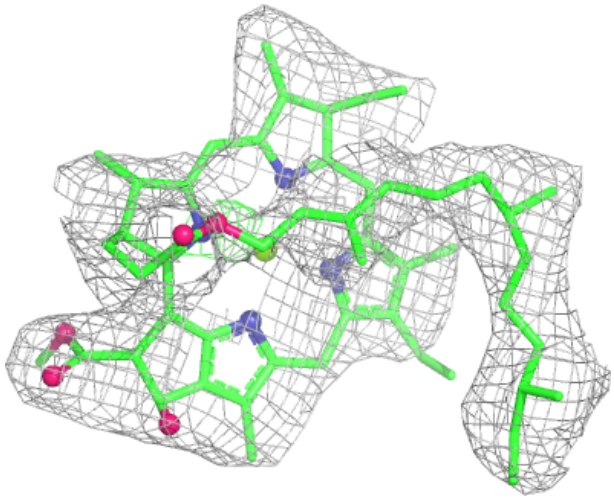


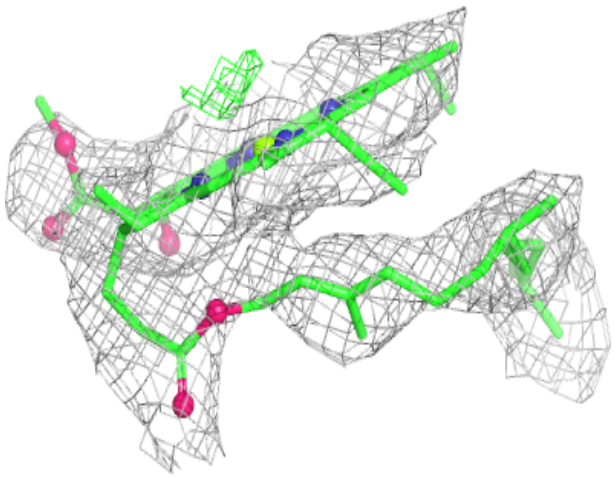


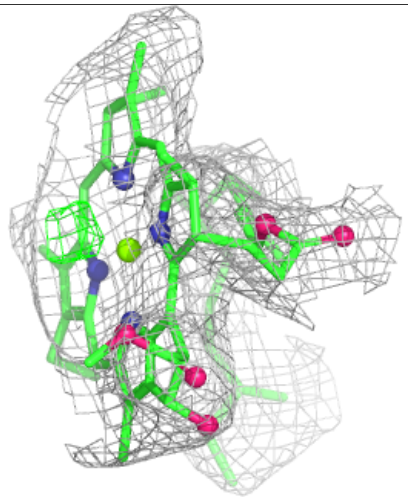


Electron density around CLA B 1216:

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

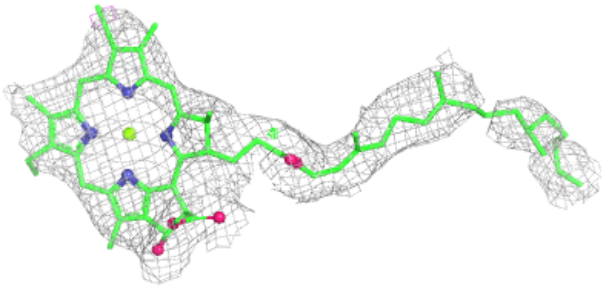


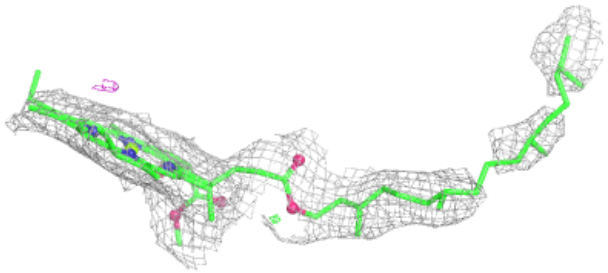


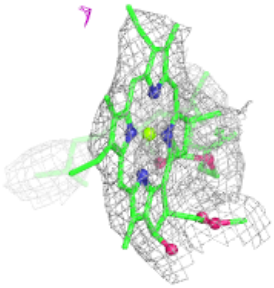


Electron density around CLA A 1103:

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

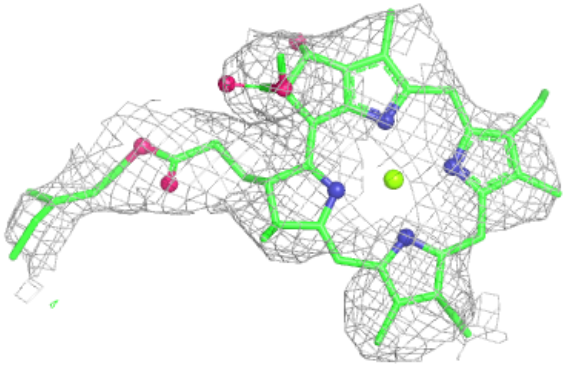


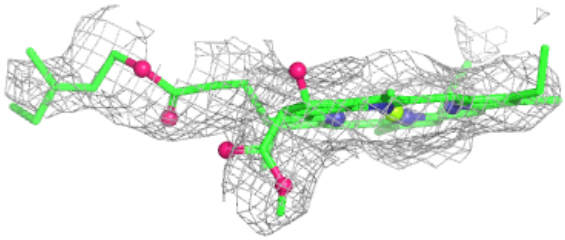


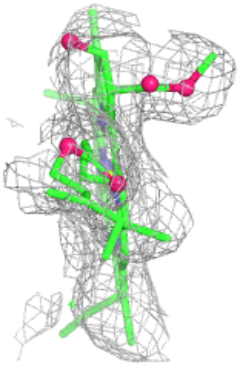


Electron density around CLA A 1135:

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

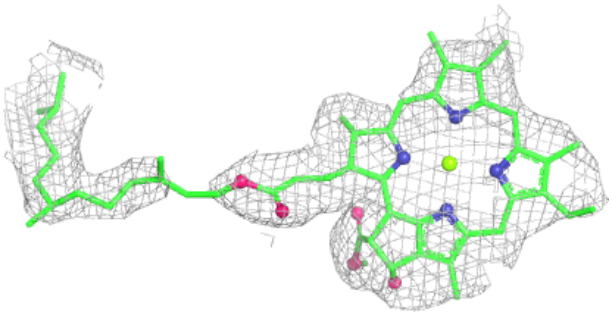


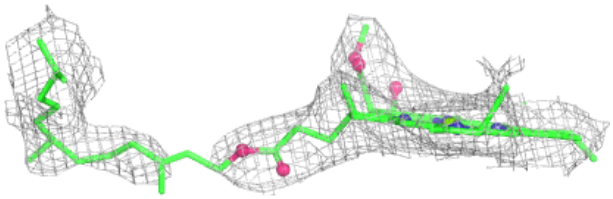




Electron density around CLA B 1234:

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

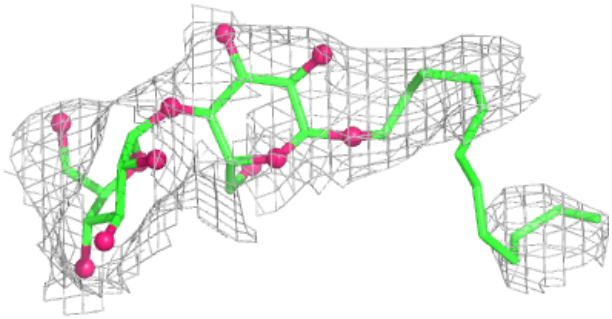


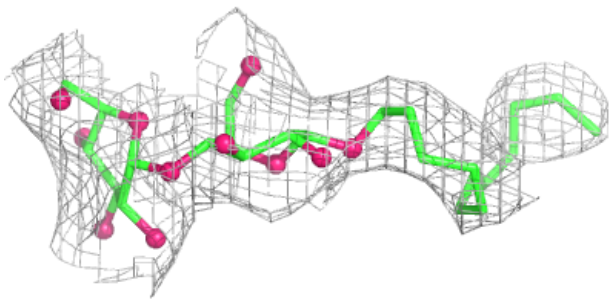


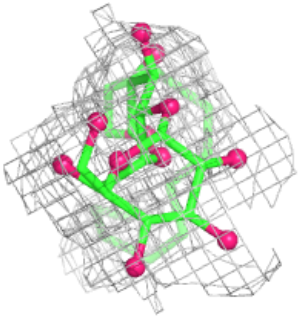


Electron density around LMU R 7007:

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

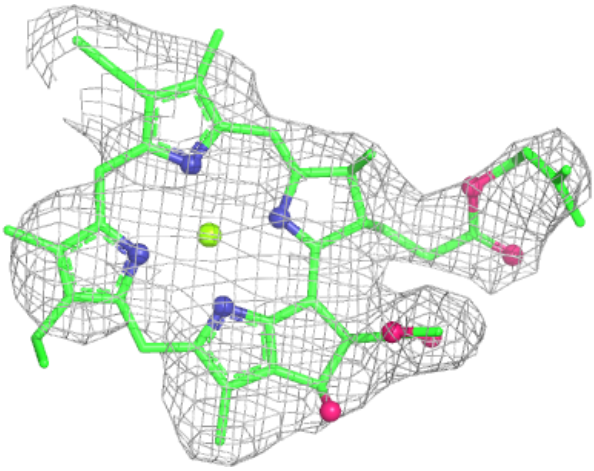


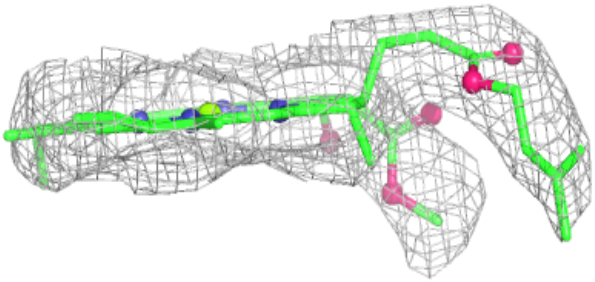


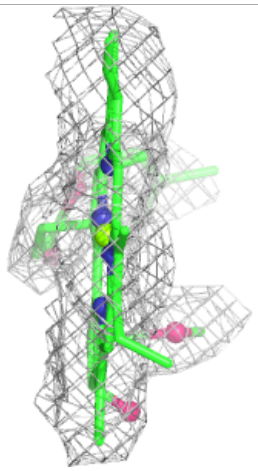


Electron density around CLA A 1101:

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

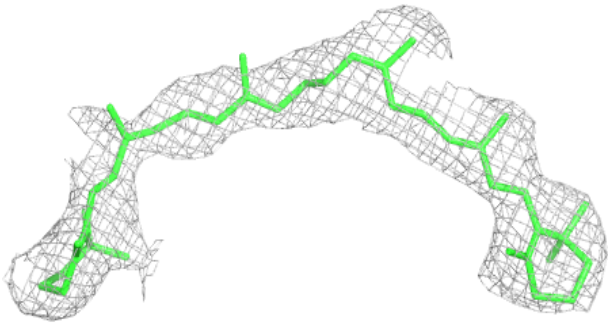


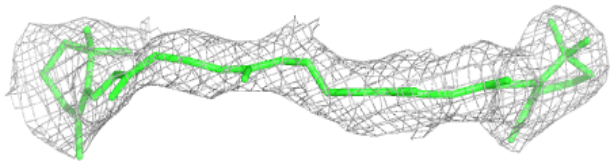


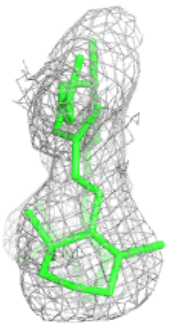


Electron density around BCR F 6016:

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

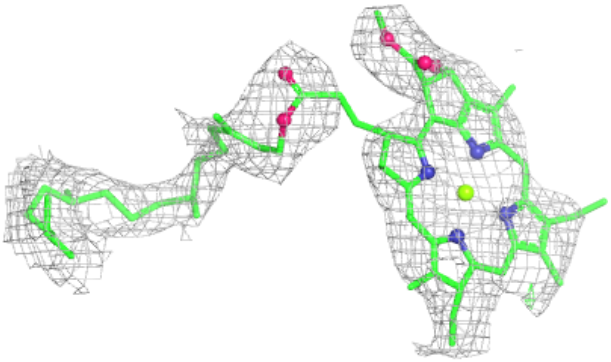


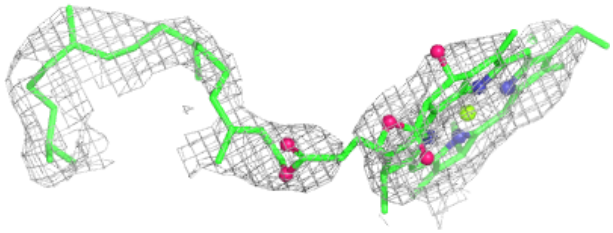


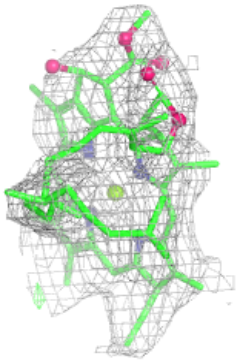


Electron density around CLA B 1206:

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



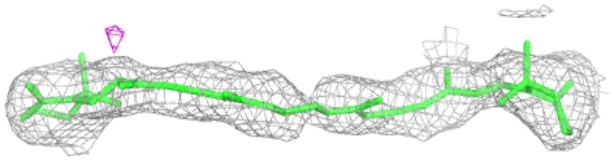


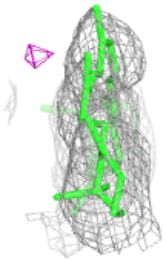


Electron density around BCR A 6011:

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

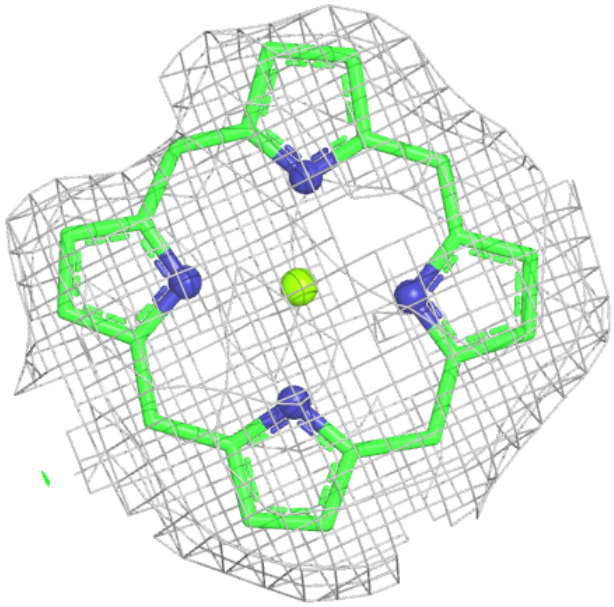


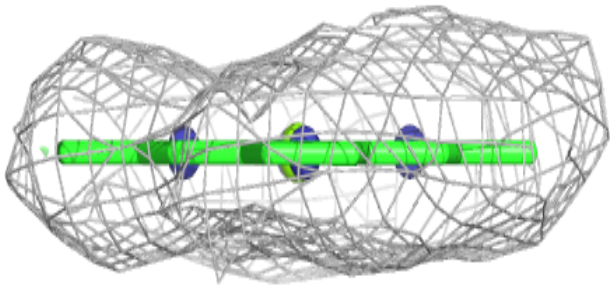


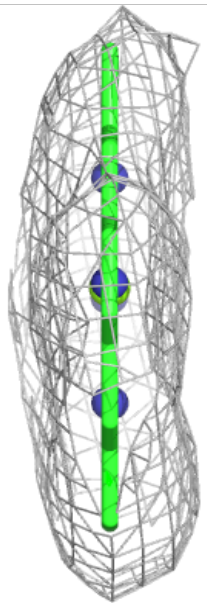


Electron density around CLA 4 4011:

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

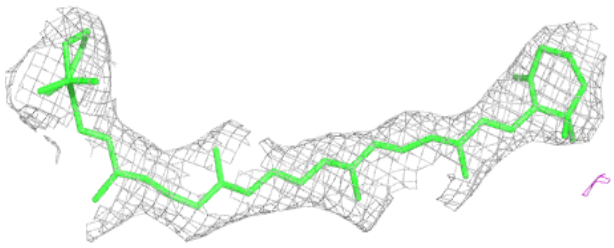


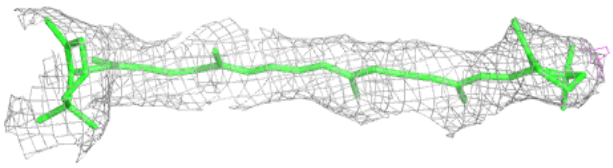




Electron density around BCR B 6005:

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

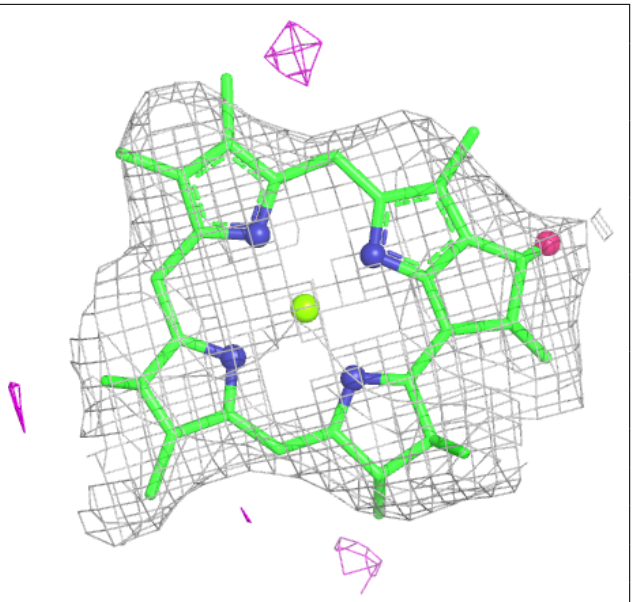


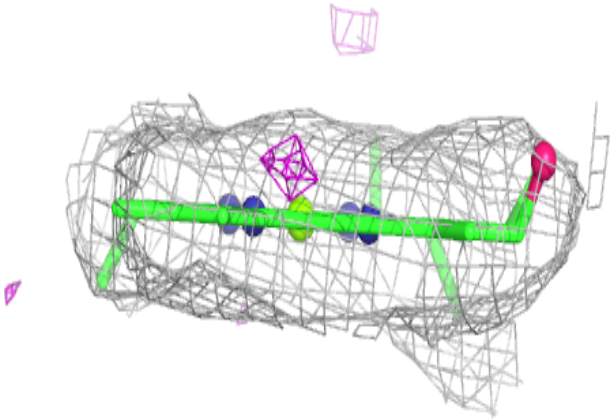


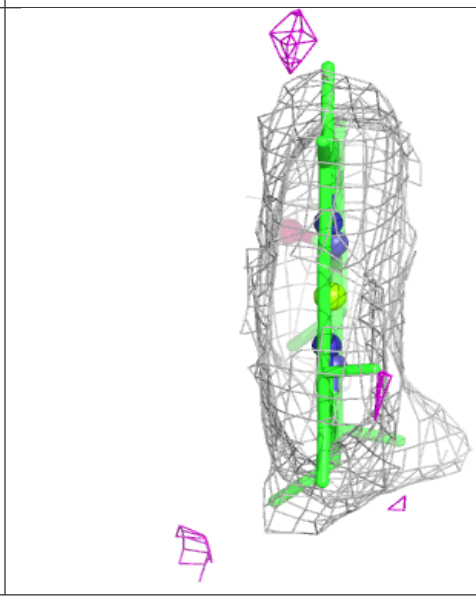


Electron density around CLA 4 4012:

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

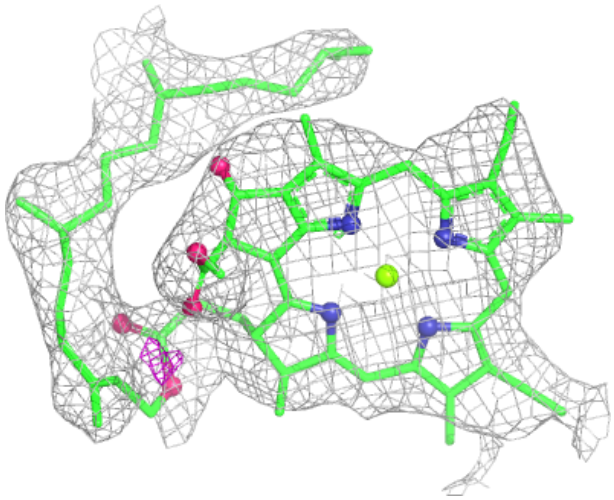


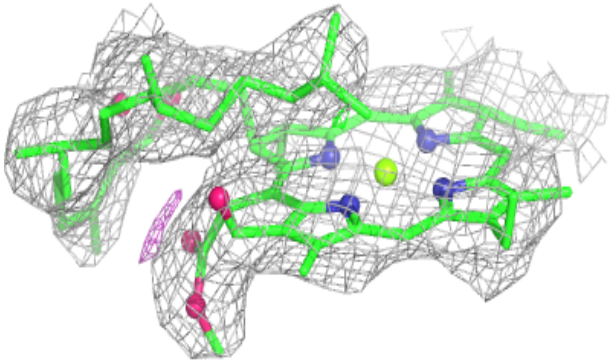


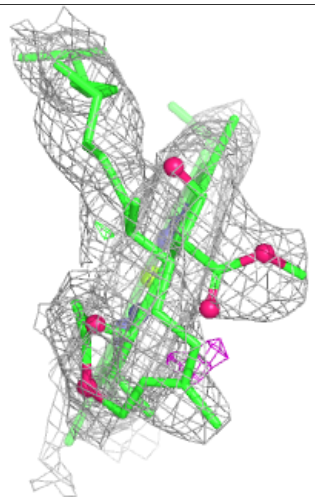


Electron density around CLA B 1202:

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

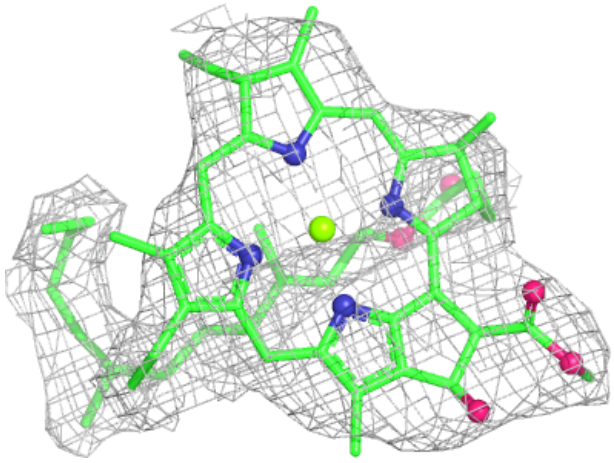


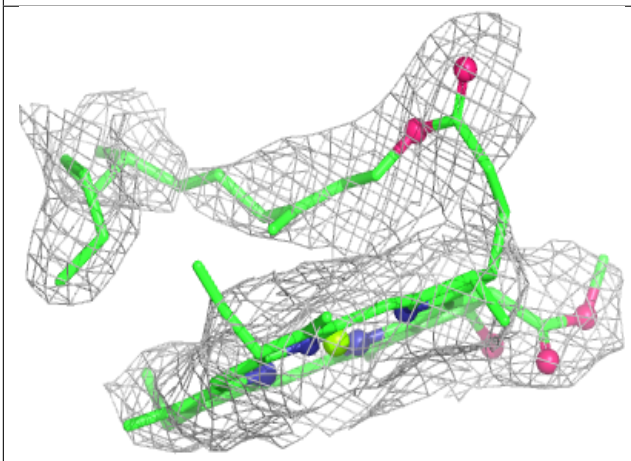


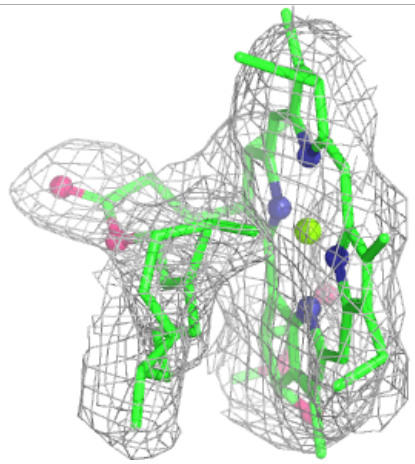


Electron density around CLA B 1214:

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

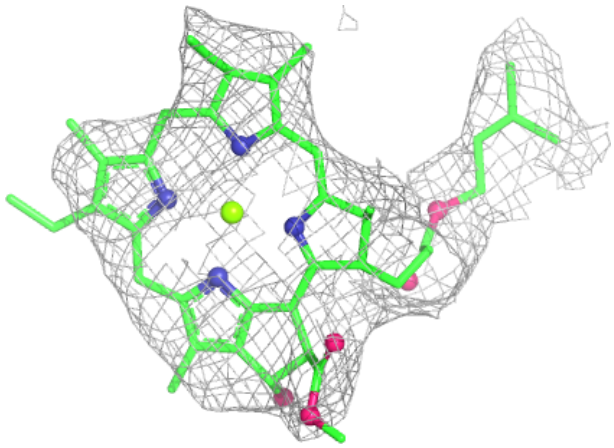


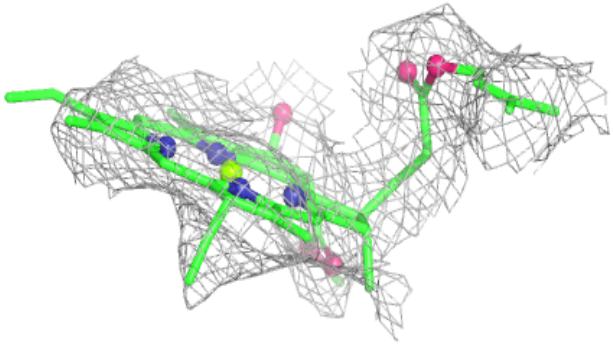


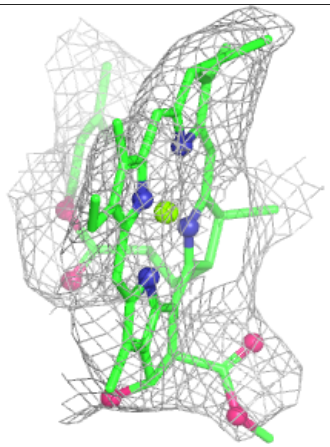


Electron density around CLA A 1133:

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

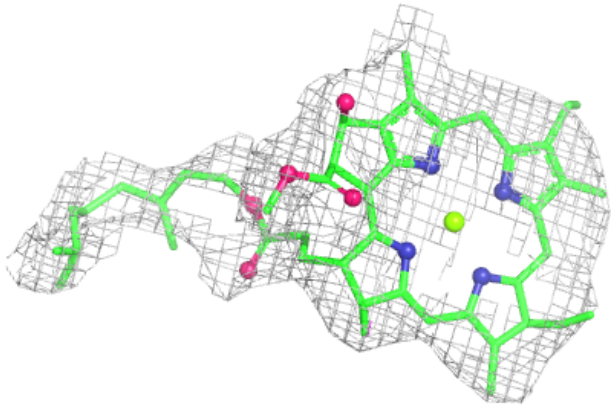


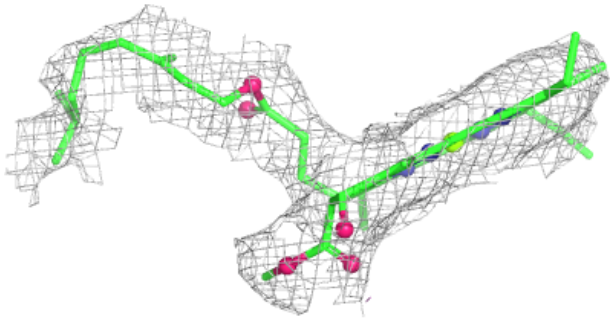




Electron density around CLA A 1107:

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

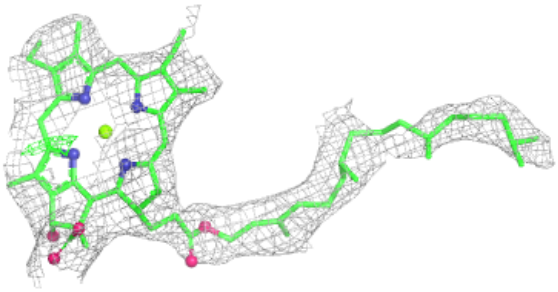


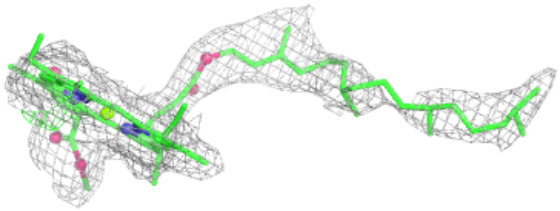


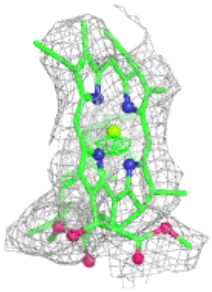


Electron density around CLA A 1132:

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

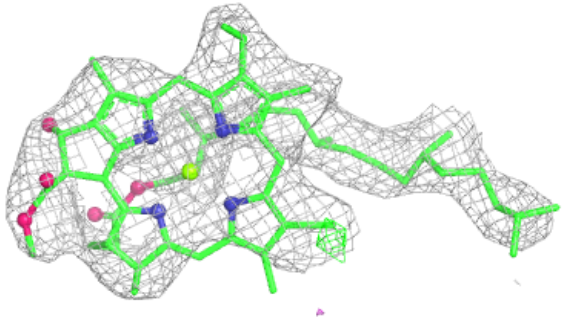


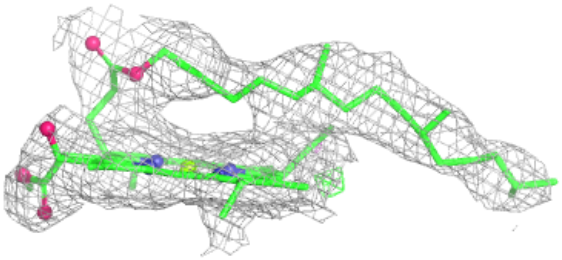


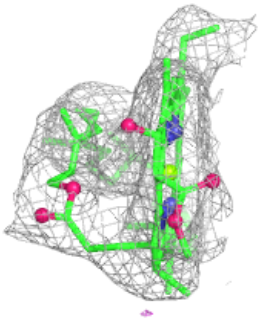


Electron density around CLA A 1138:

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

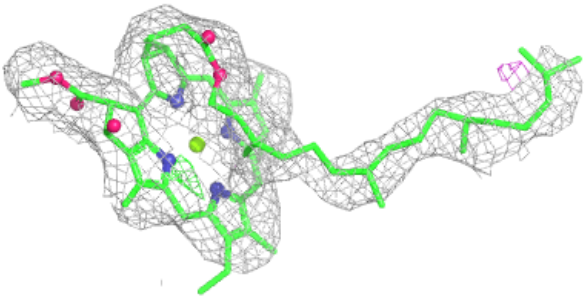


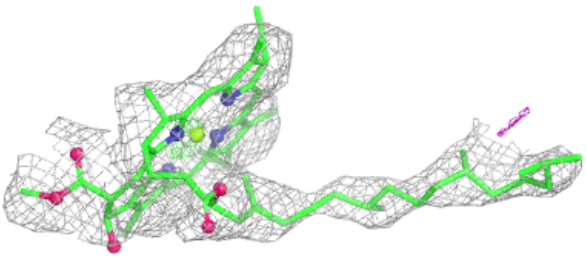


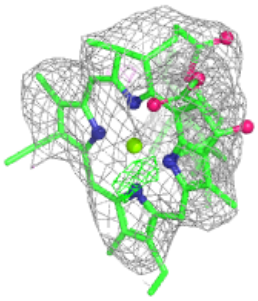


Electron density around CLA A 1140:

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

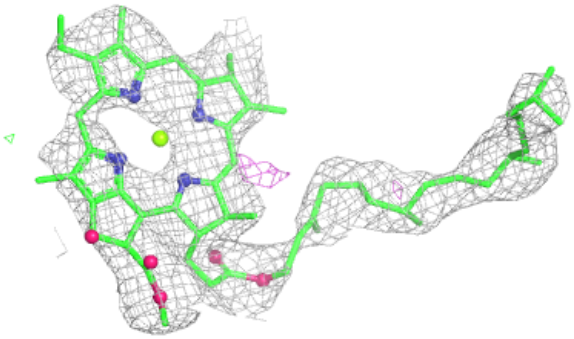


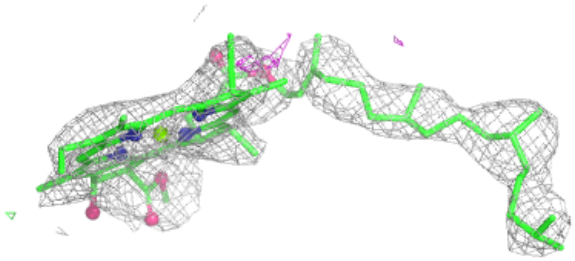


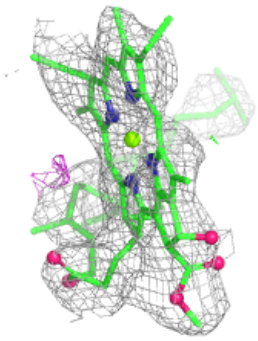


Electron density around CLA A 9013:

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

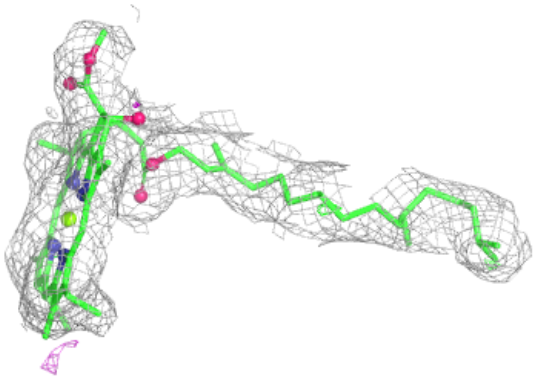


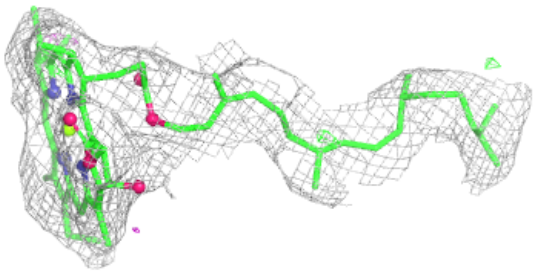


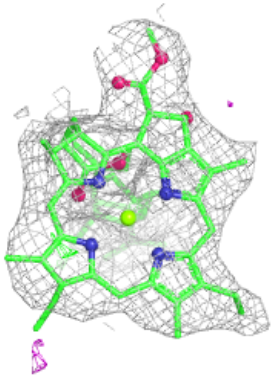


Electron density around CLA A 1126:

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

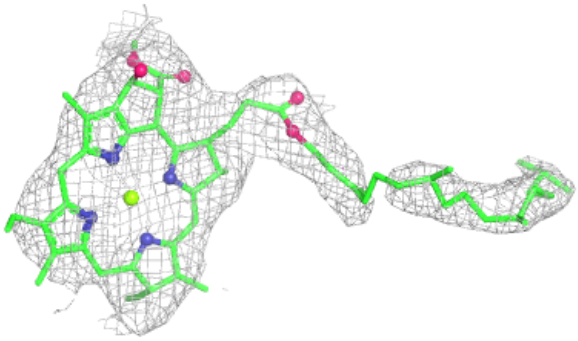


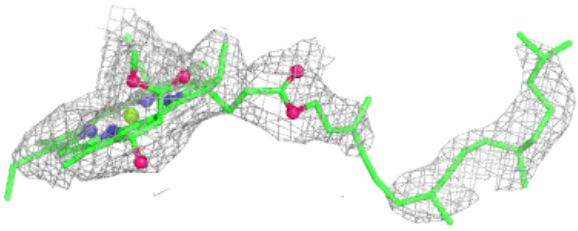


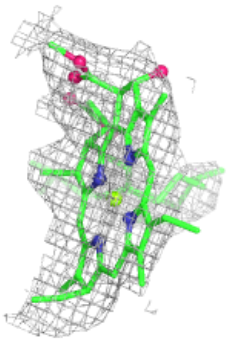


Electron density around CLA B 1210:

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

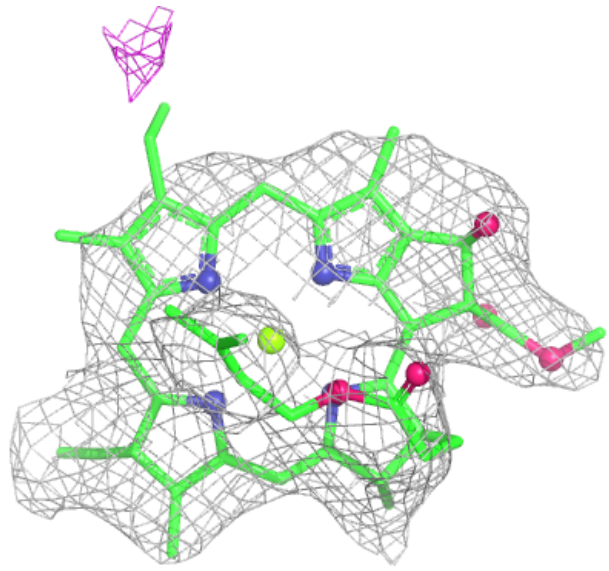


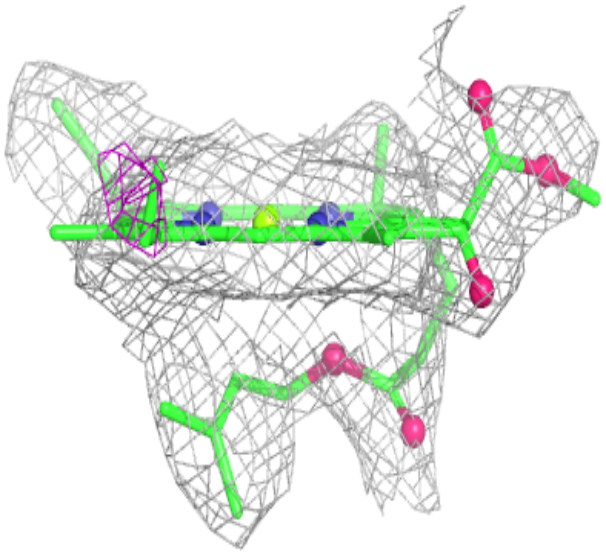


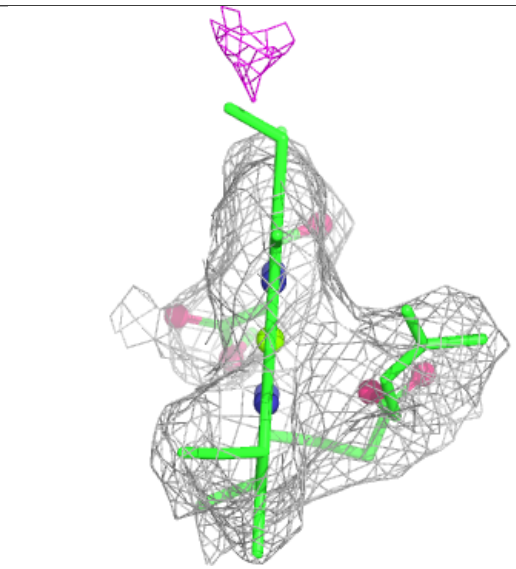


Electron density around CLA B 1217:

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

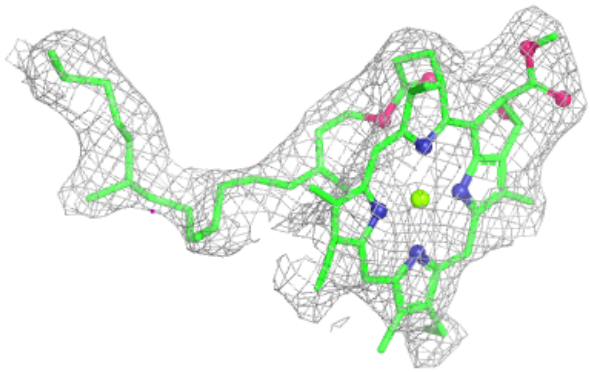


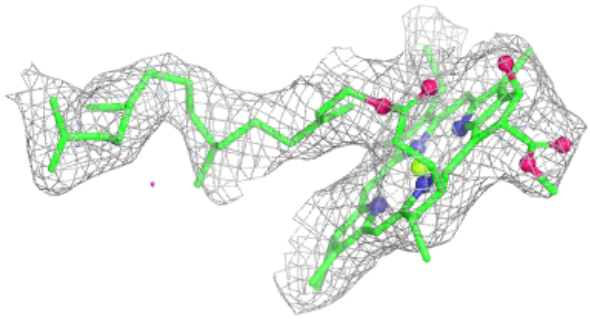




Electron density around CLA A 1237:

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

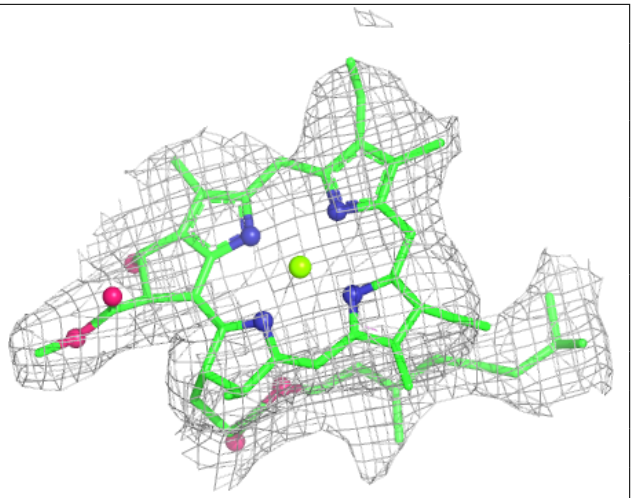


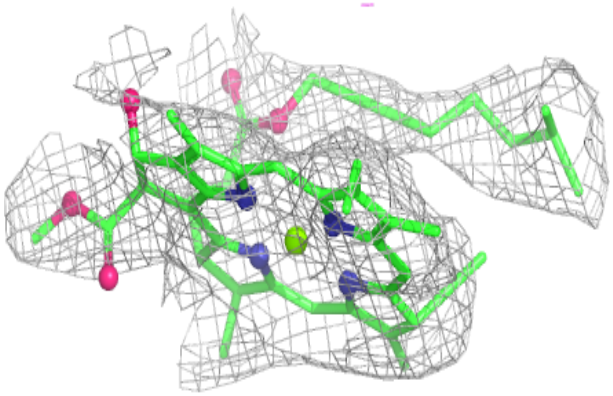


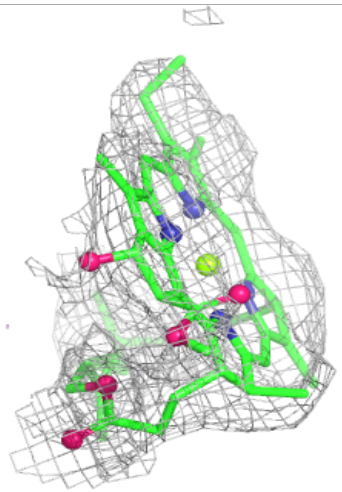


Electron density around CLA B 1219:

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

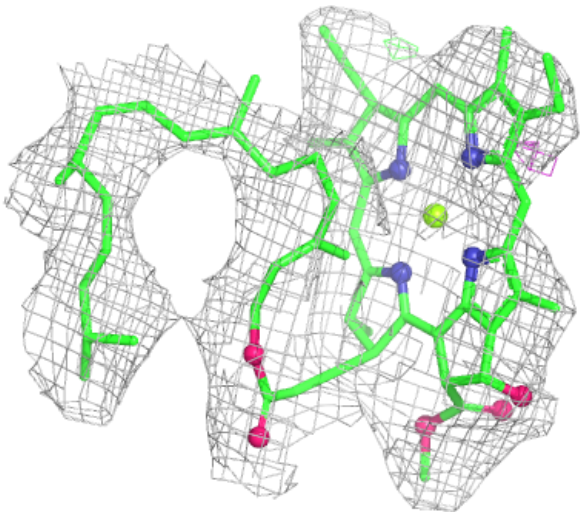


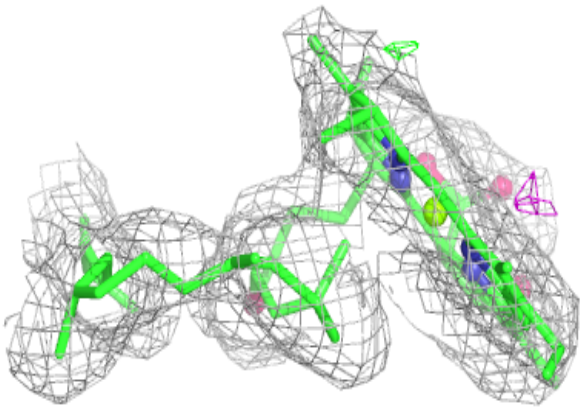




Electron density around CLA B 1220:

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

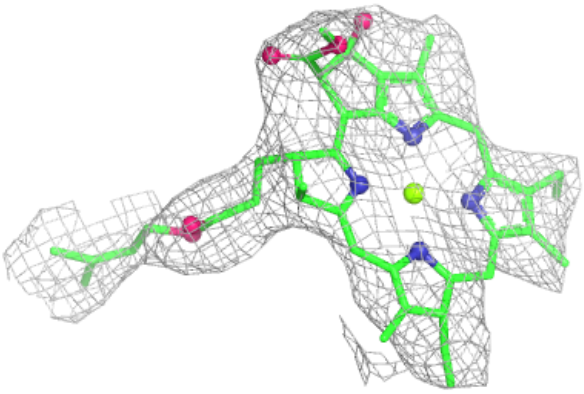


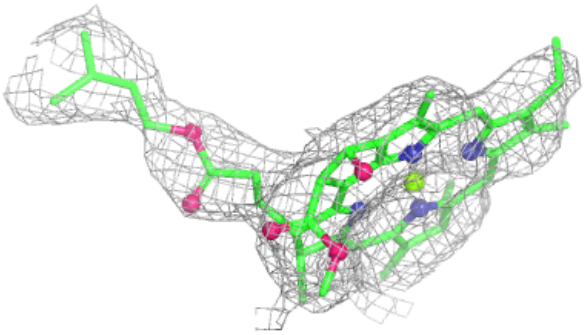


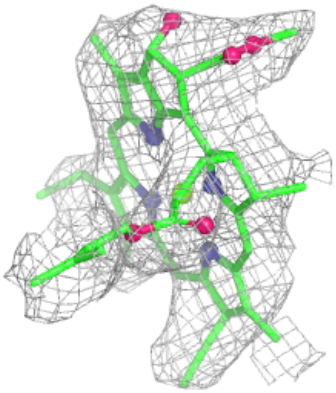


Electron density around CLA A 1129:

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

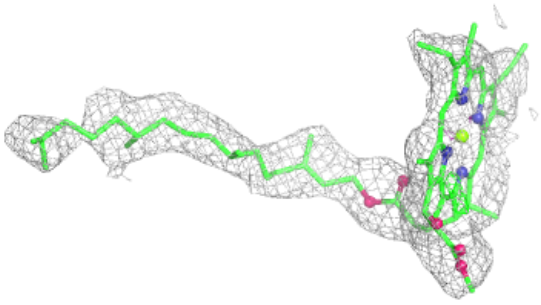


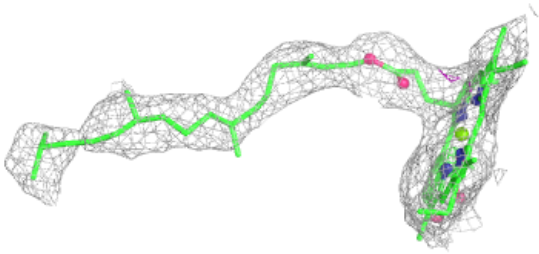


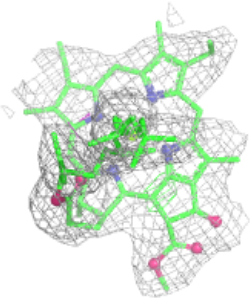


Electron density around CLA B 1225:

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

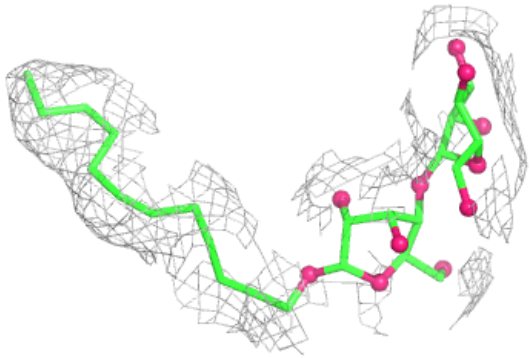


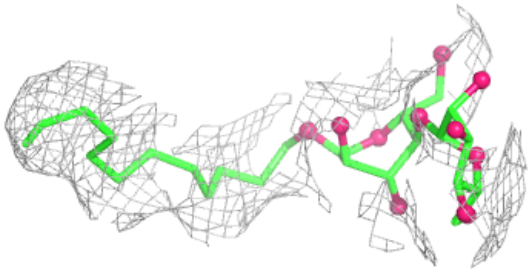


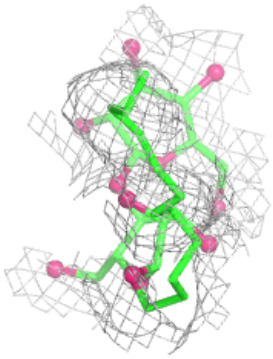


Electron density around LMU G 7039:

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

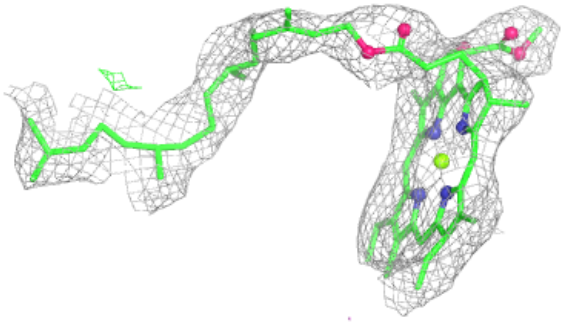


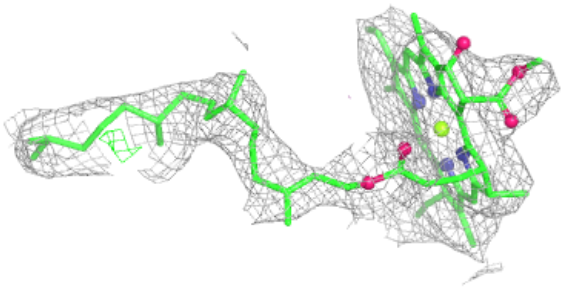


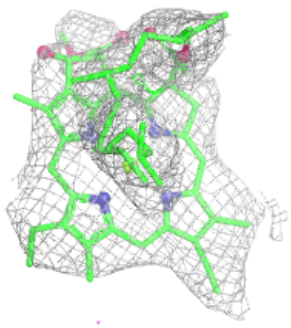


Electron density around CLA B 1226:

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

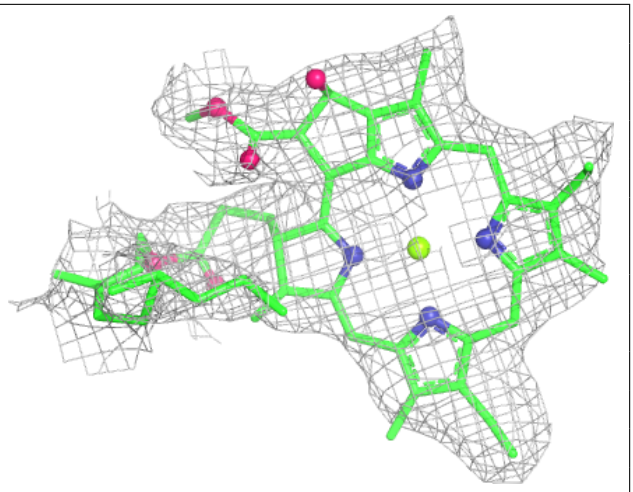


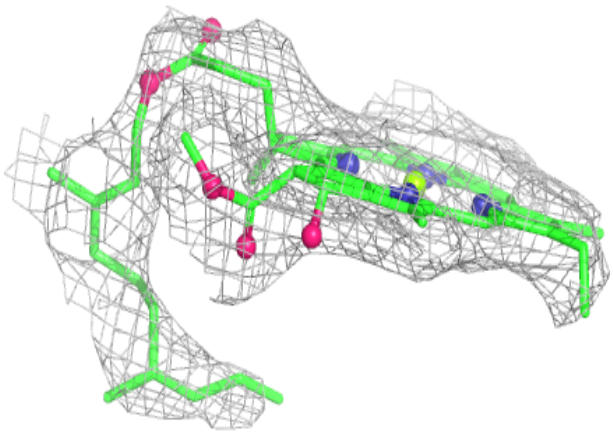


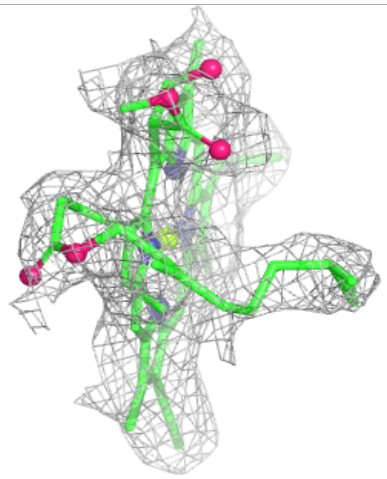


Electron density around CLA A 1104:

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

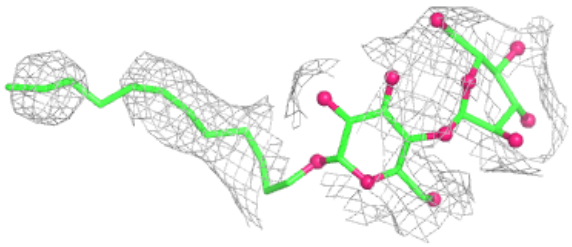


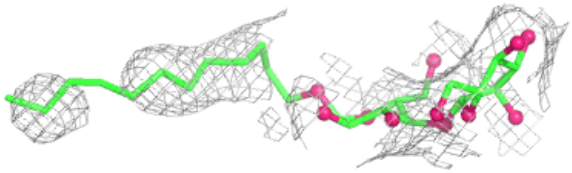




Electron density around LMU A 7035:

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

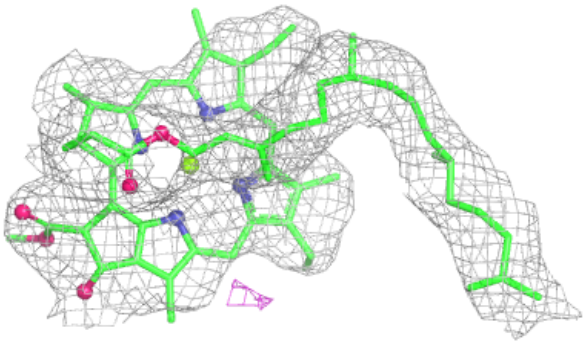


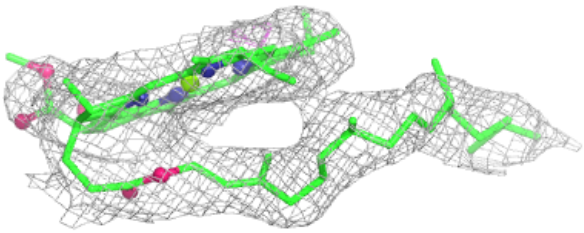


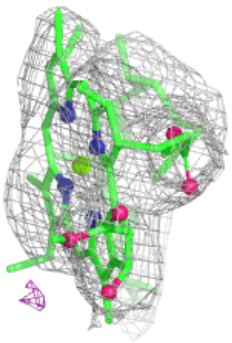


Electron density around CLA B 1235:

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

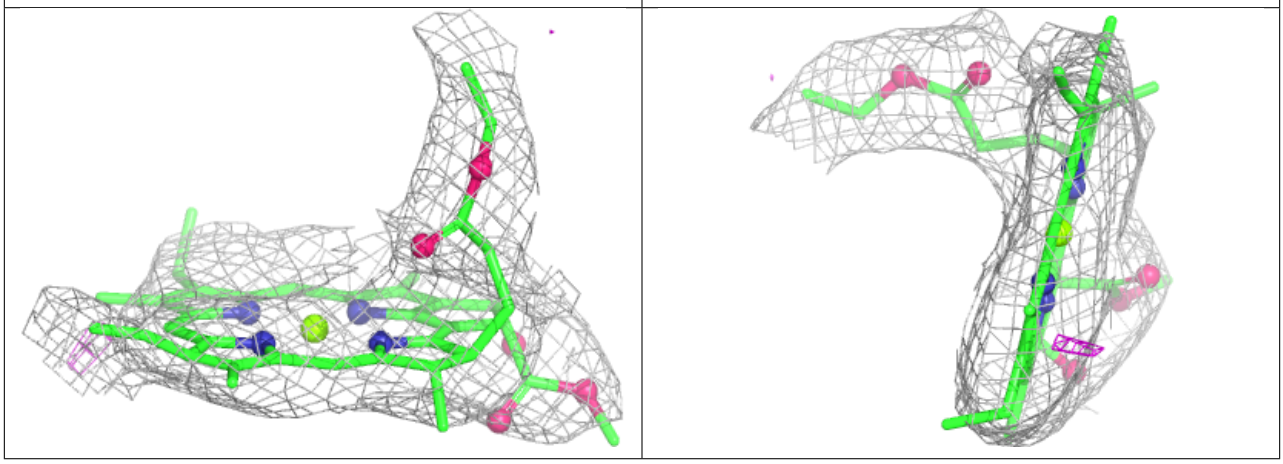






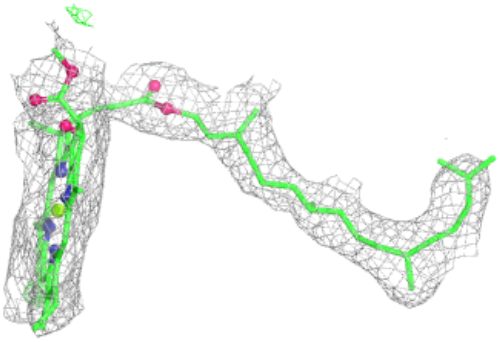
Electron density around CLA B 1236:

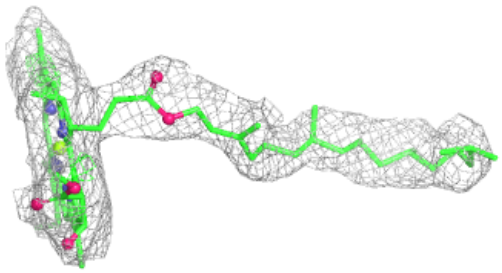
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

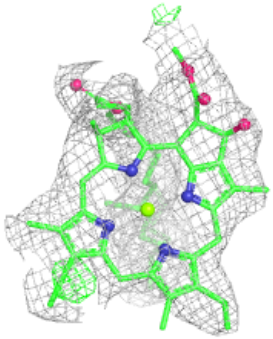


Electron density around CLA B 1239:

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

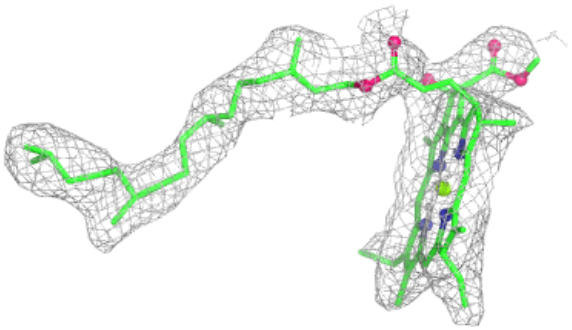


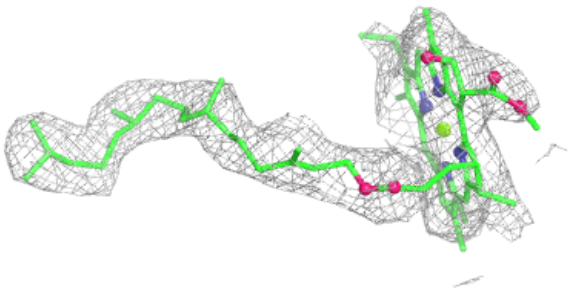


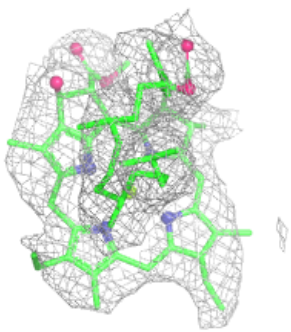


Electron density around CLA A 1128:

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

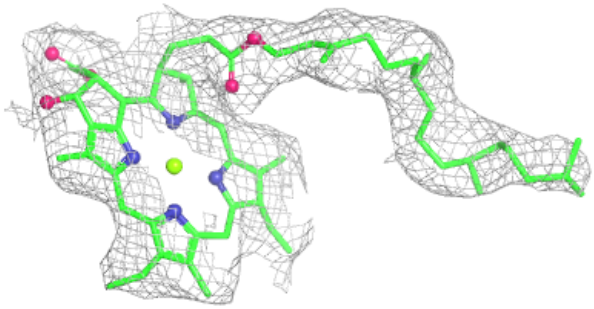


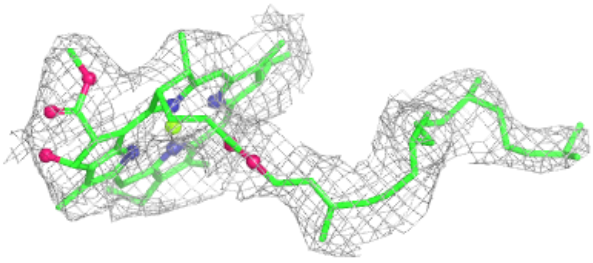


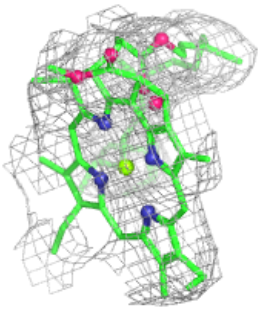


Electron density around CLA A 1106:

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

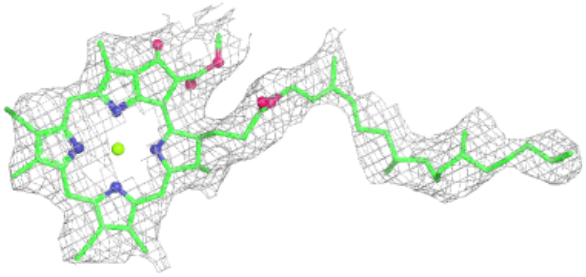


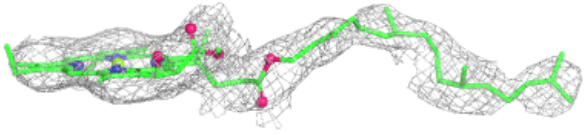


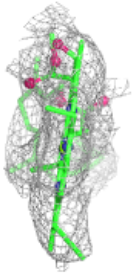


Electron density around CLA A 1131:

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

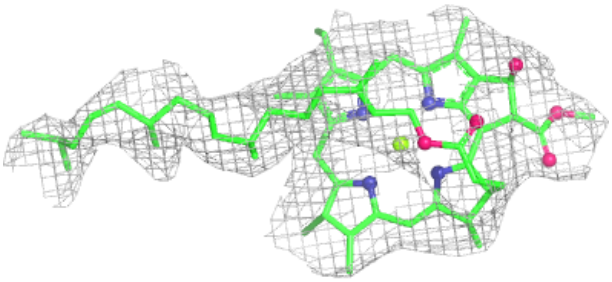


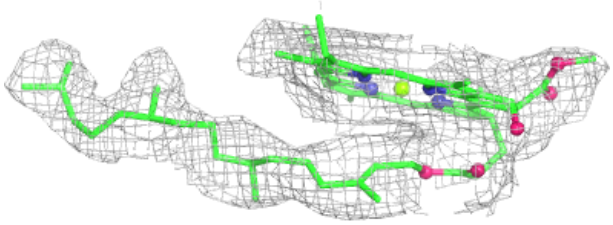


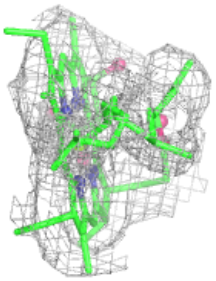


Electron density around CLA A 1136:

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

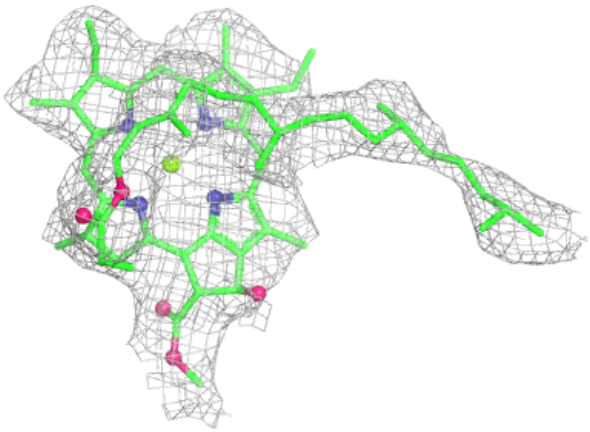


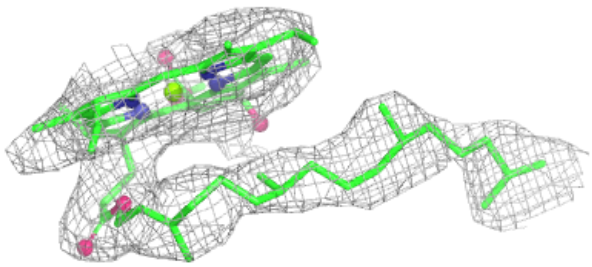


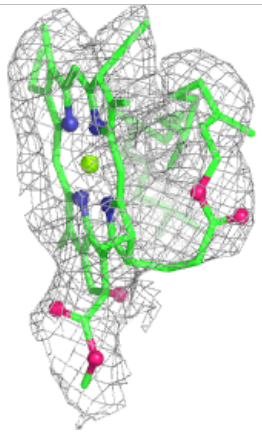


Electron density around CLA B 1224:

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

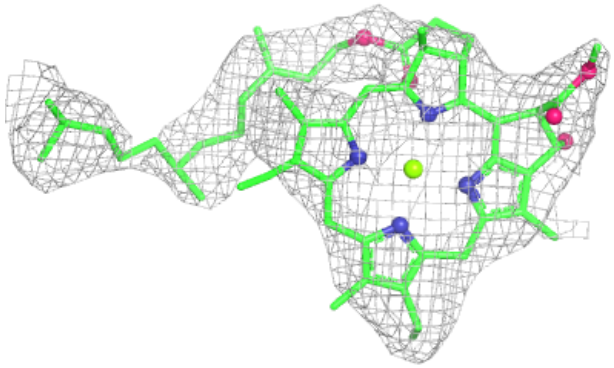


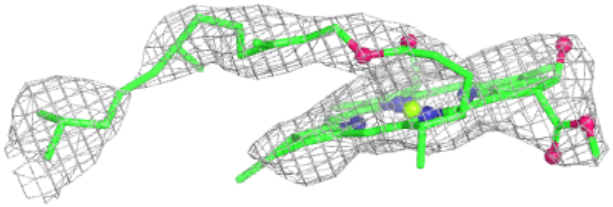


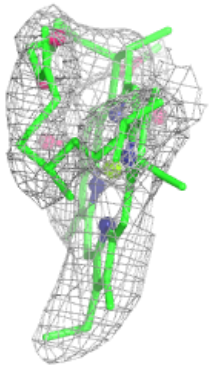


Electron density around CLA B 1215:

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

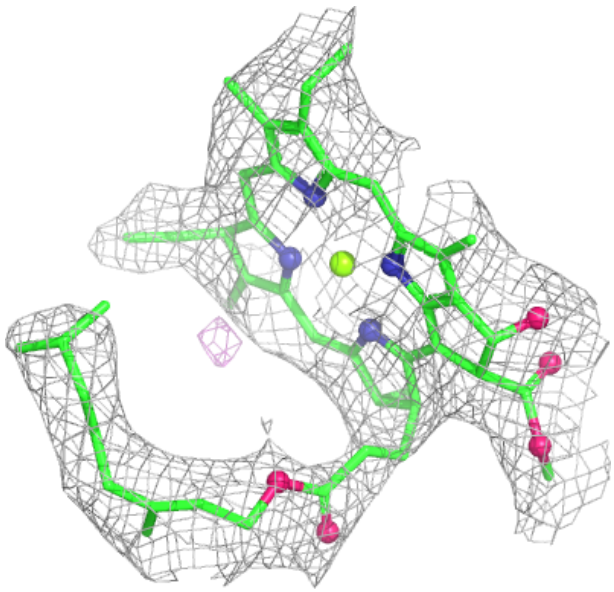


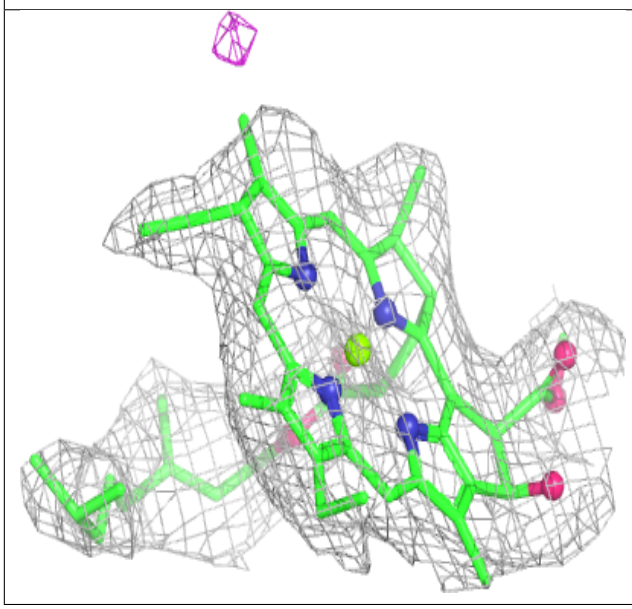


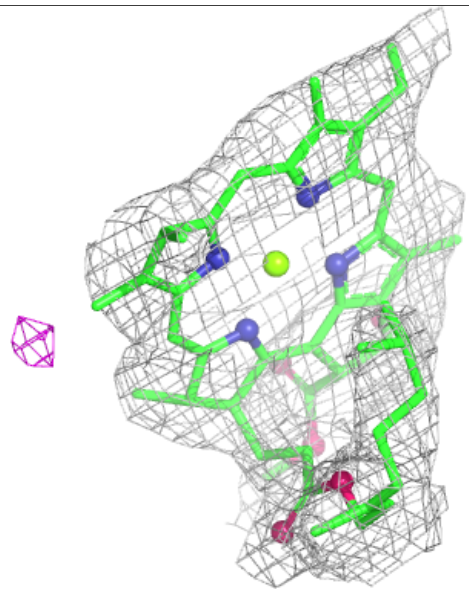


Electron density around CLA A 1122:

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

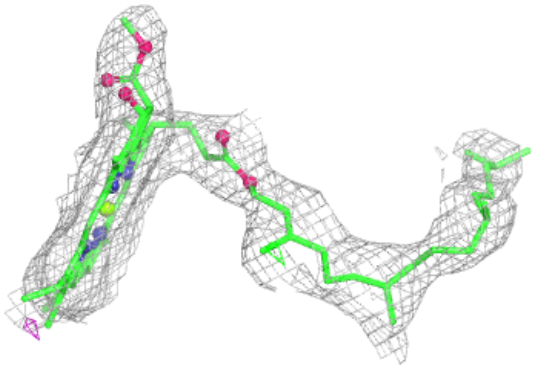


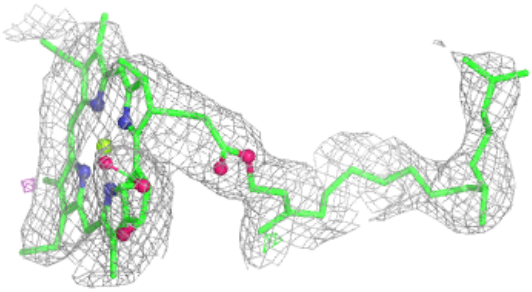


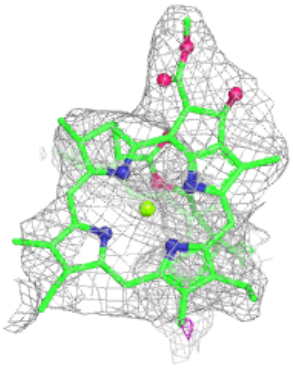


Electron density around CLA B 1238:

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

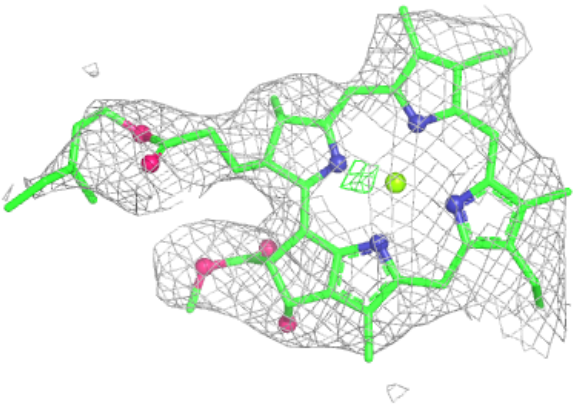


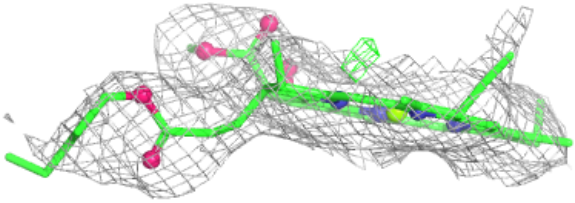


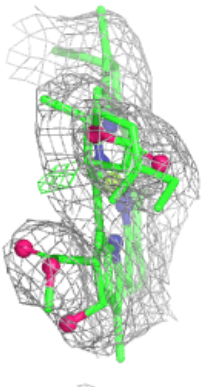


Electron density around CLA A 1139:

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

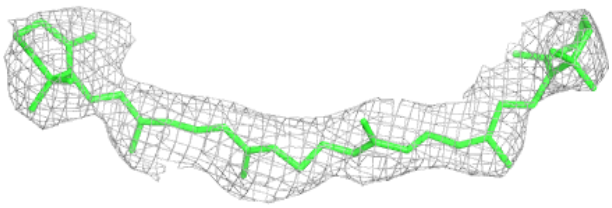


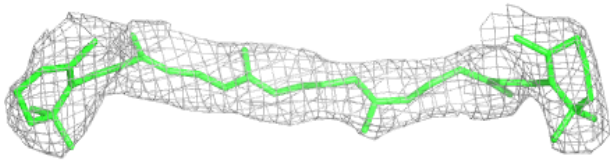


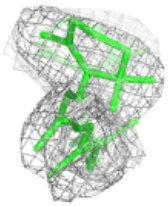


Electron density around BCR B 6020:

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

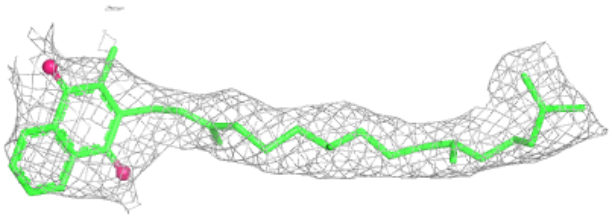


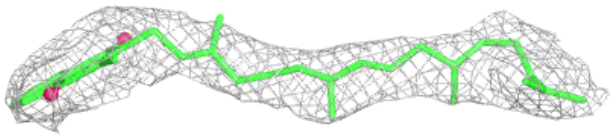


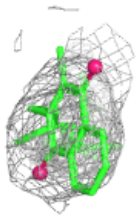


Electron density around PQN A 5001:

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

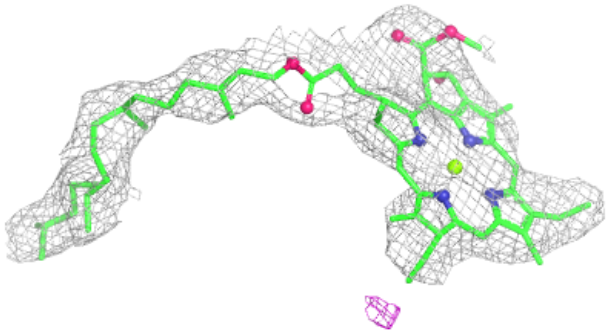


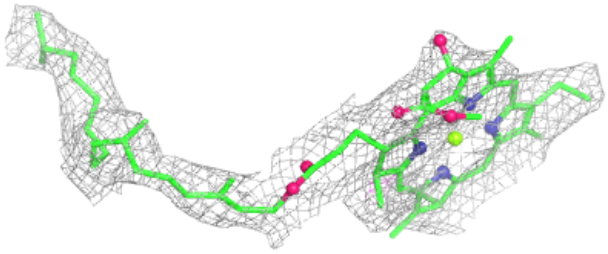


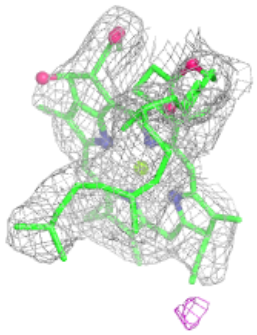


Electron density around CLA A 9012:

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

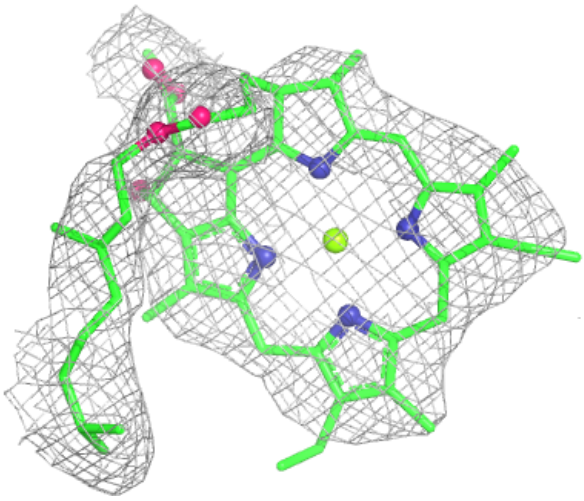


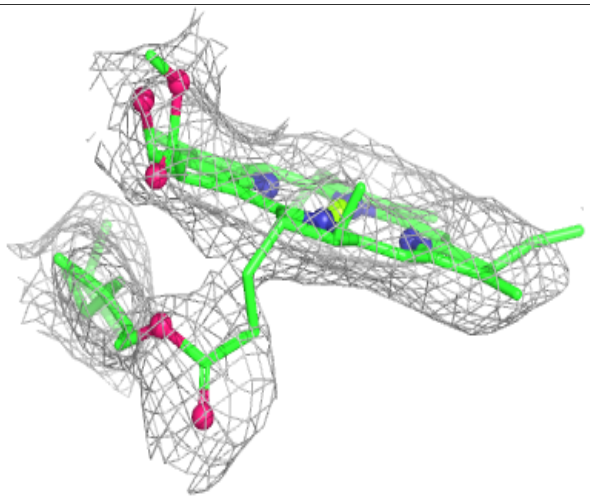


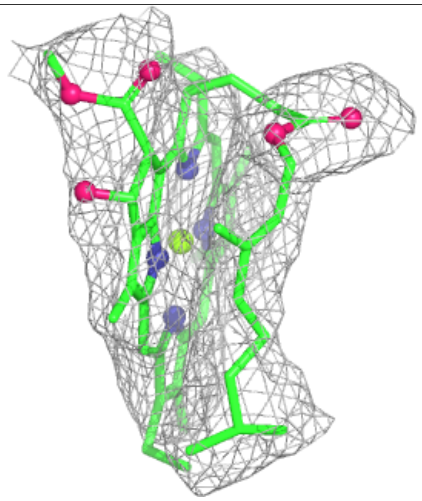


Electron density around CLA A 1127:

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

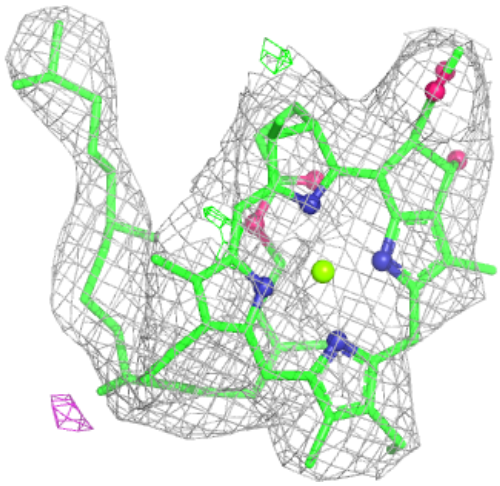


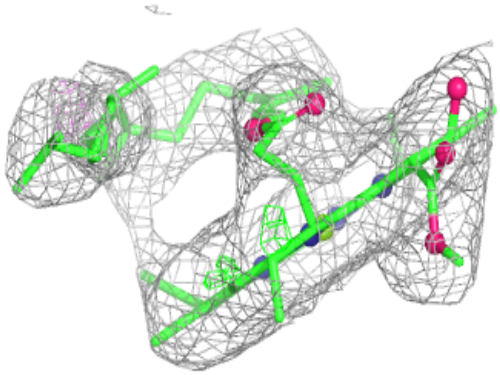


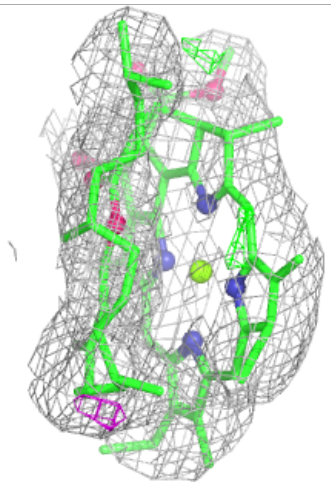


Electron density around CLA B 1205:

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

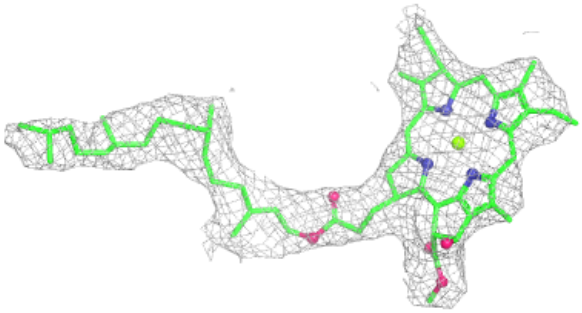


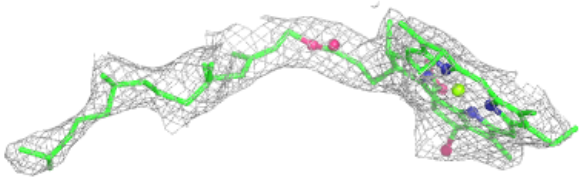


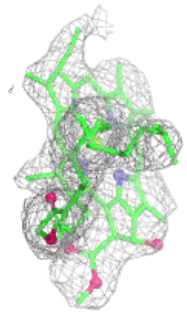


Electron density around CLA A 9022:

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

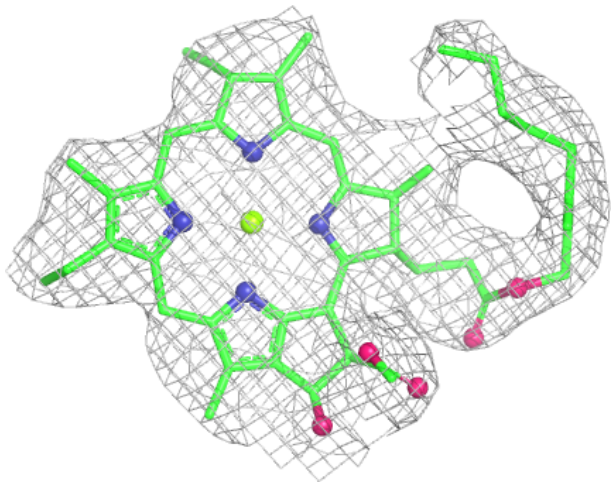


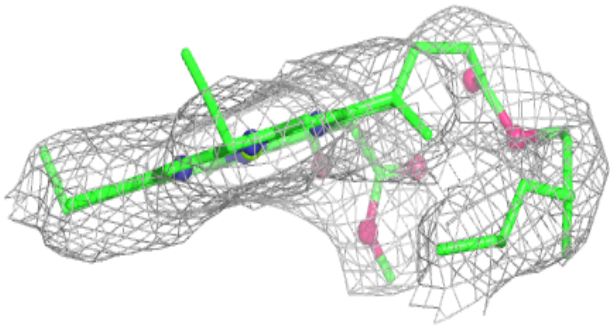


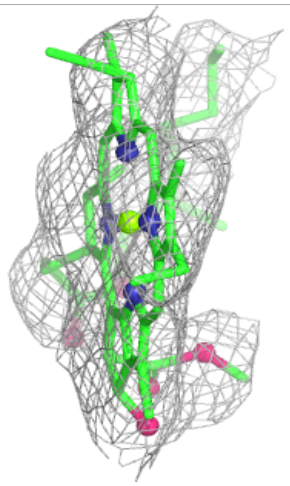


Electron density around CLA B 1221:

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

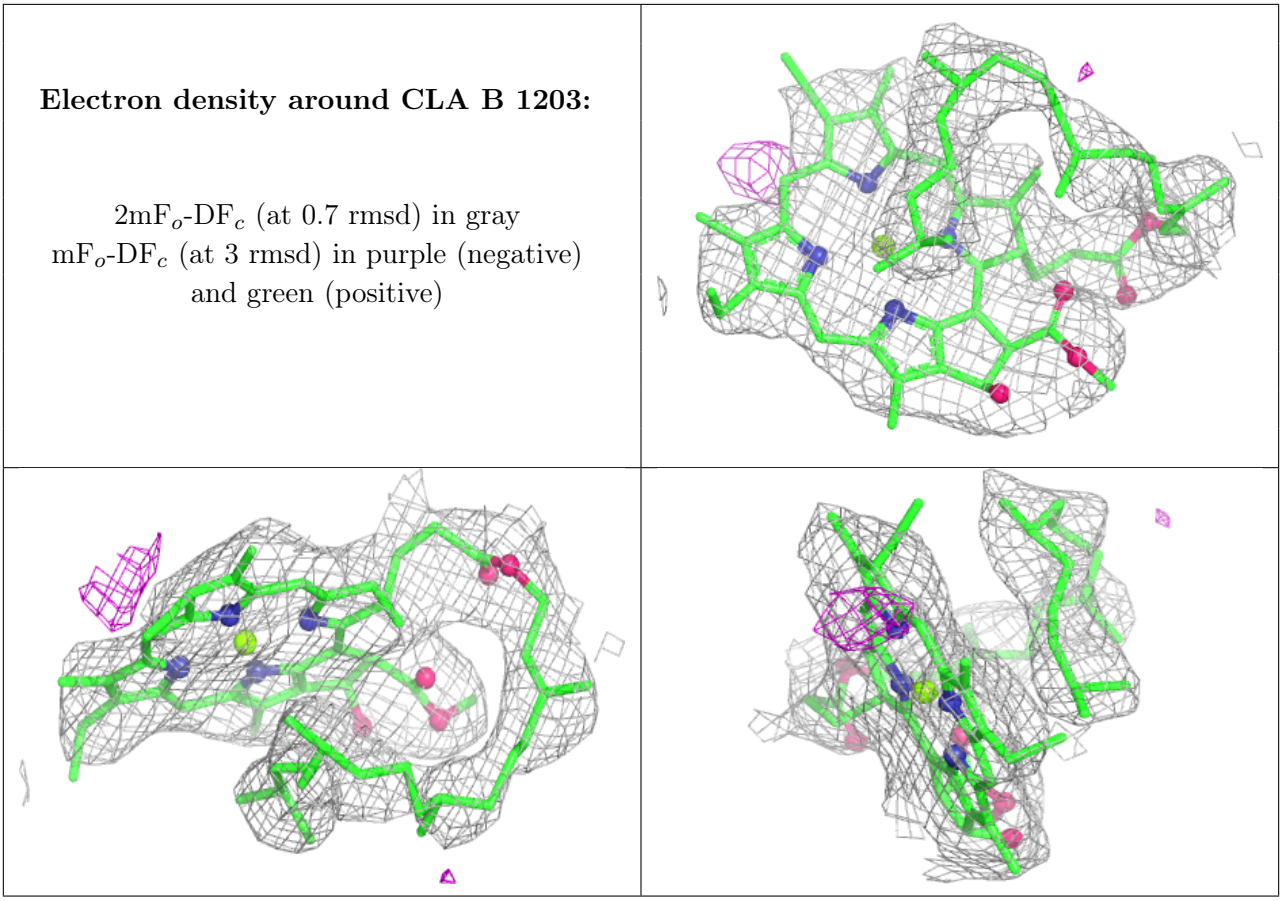






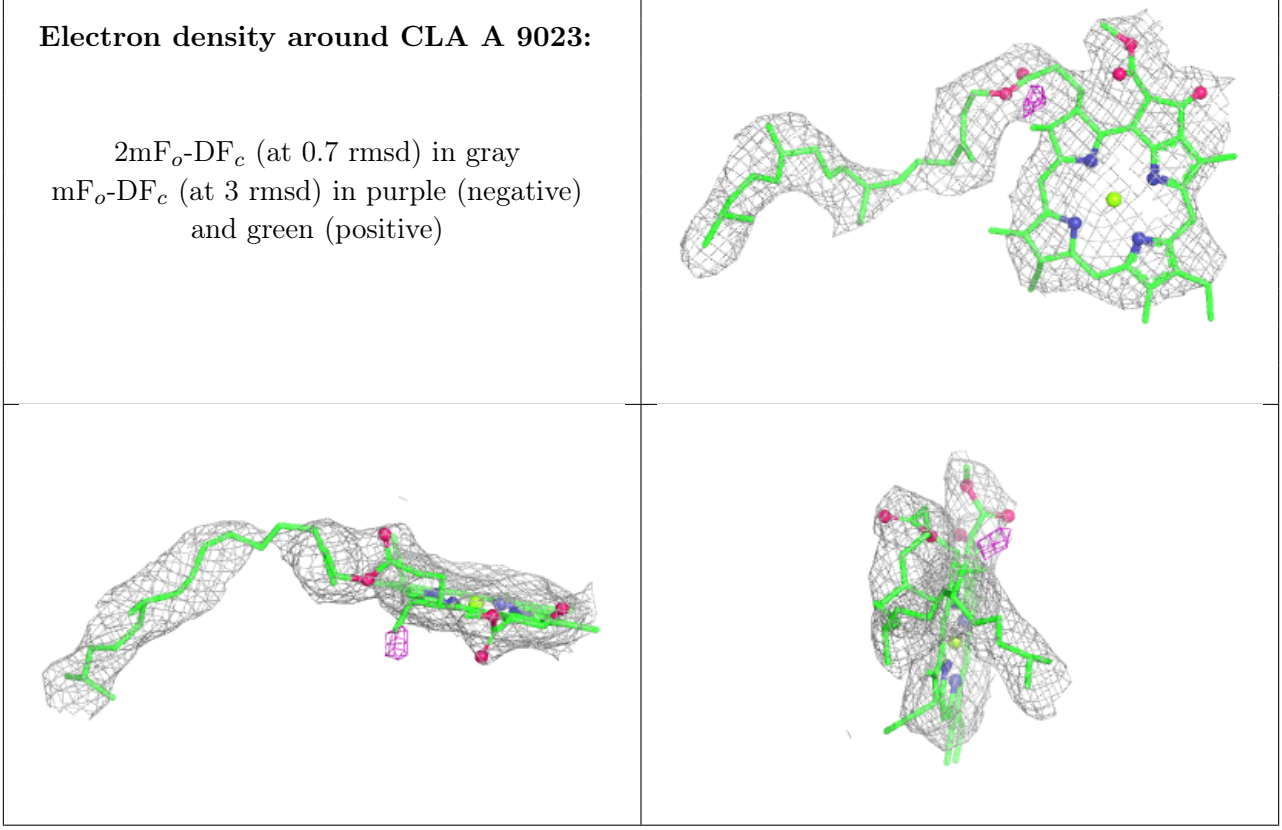
Electron density around CLA B 1203:

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



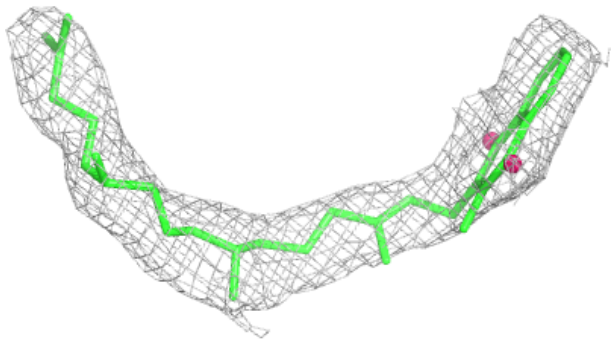
Electron density around CLA A 9023:

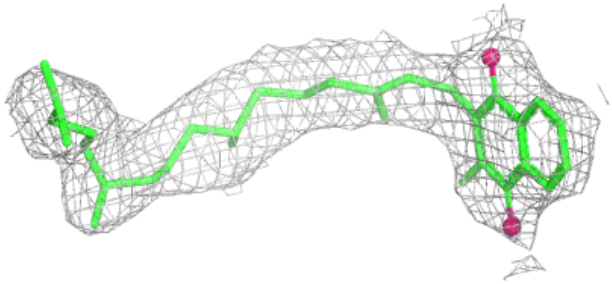
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

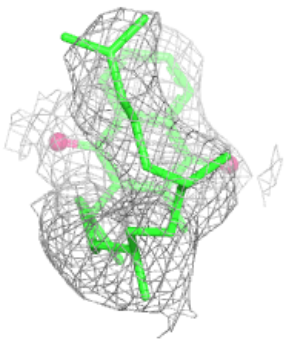


Electron density around PQN B 5002:

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

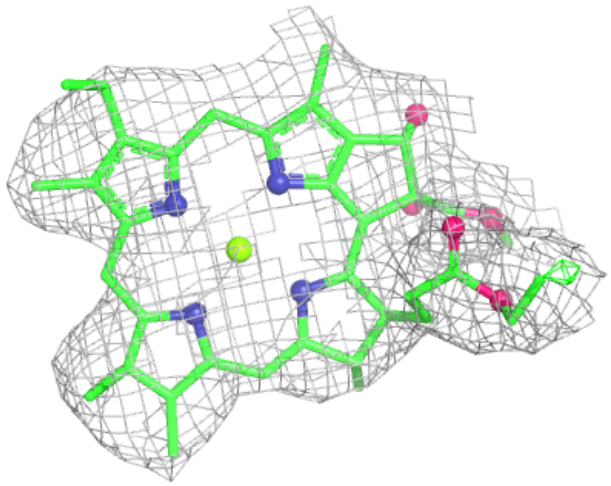


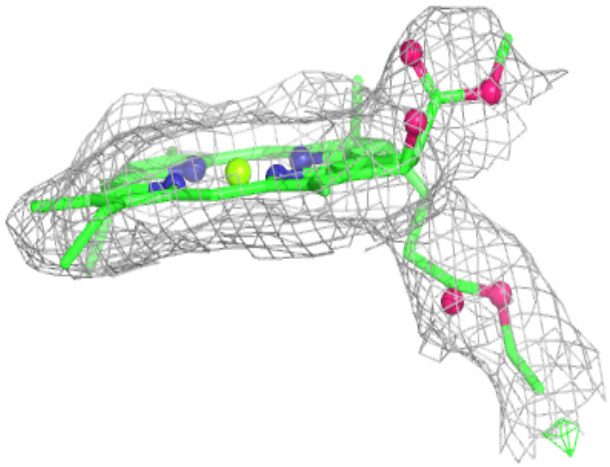


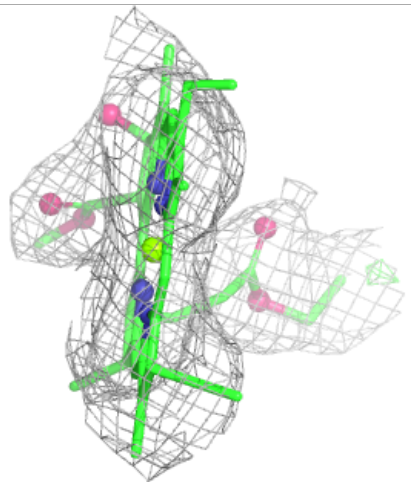


Electron density around CLA A 1137:

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

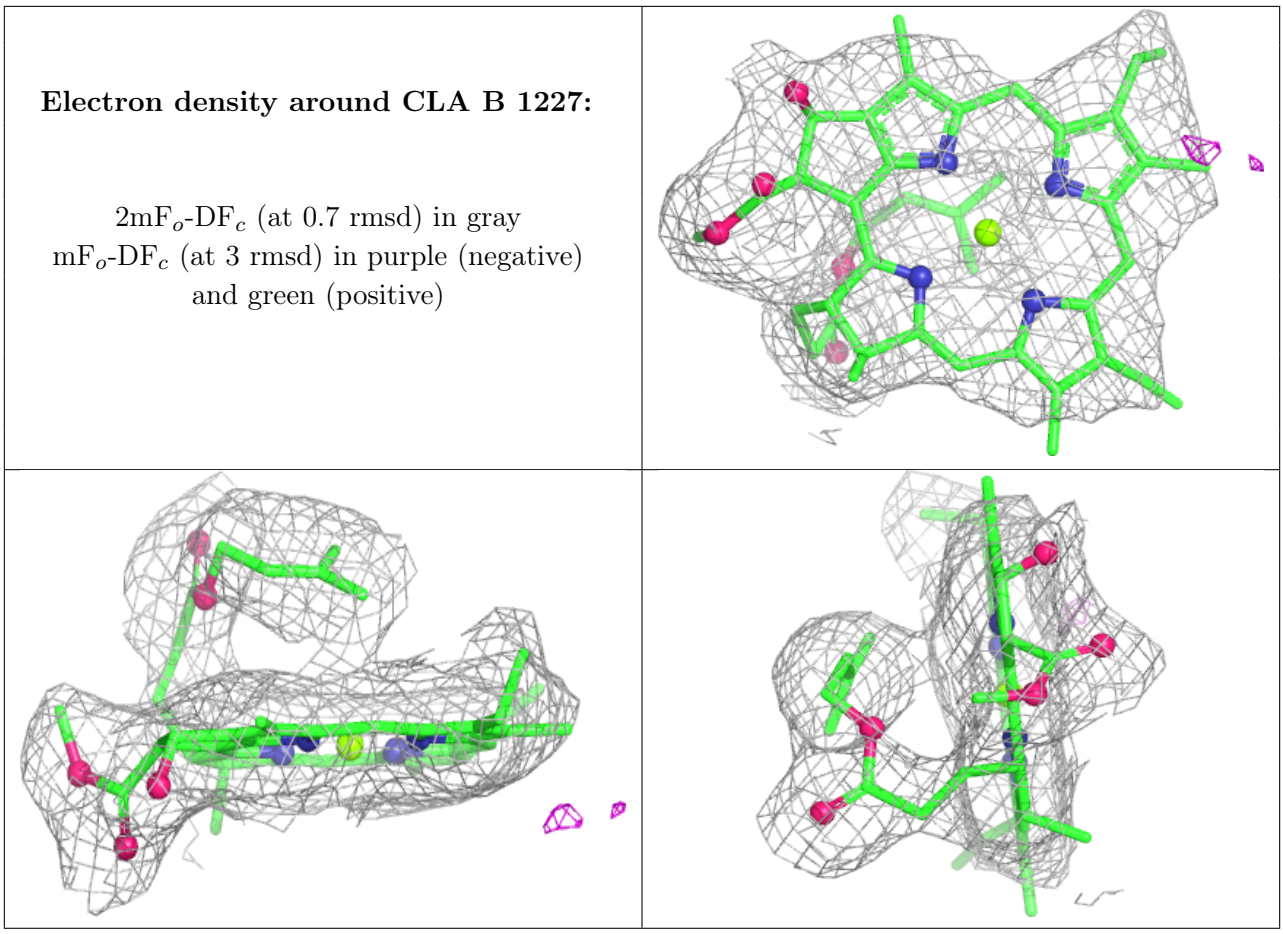






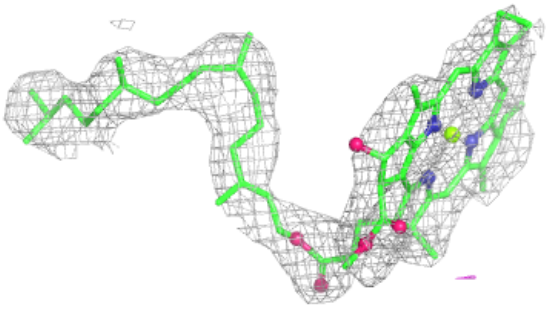
Electron density around CLA B 1227:

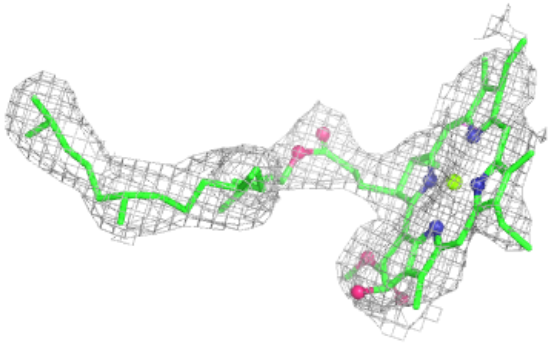
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

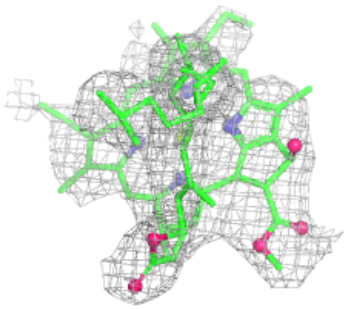


Electron density around CLA B 9010:

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

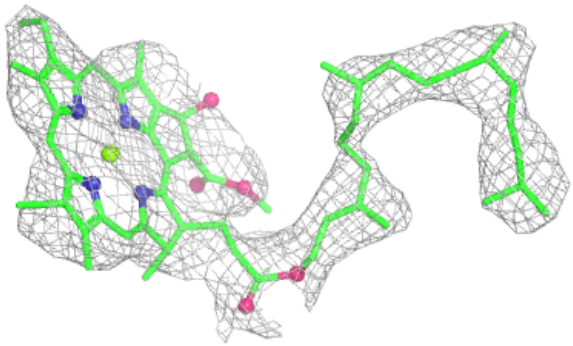


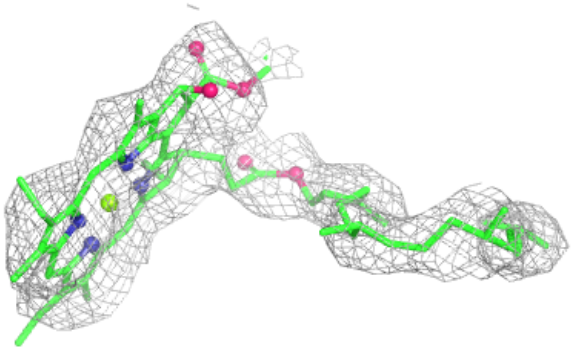


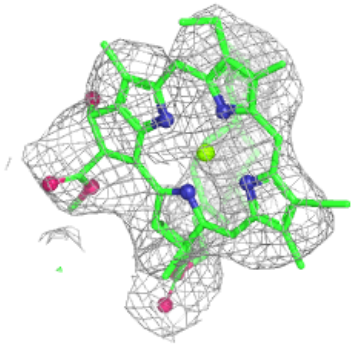


Electron density around CLA A 9011:

$2mF_o$-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 (i)

There are no such residues in this entry.