wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 11:55 PM EDT

PDB ID	:	2WSC
Title	:	Improved Model of Plant Photosystem I
Authors	:	Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on	:	2009-09-04
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:

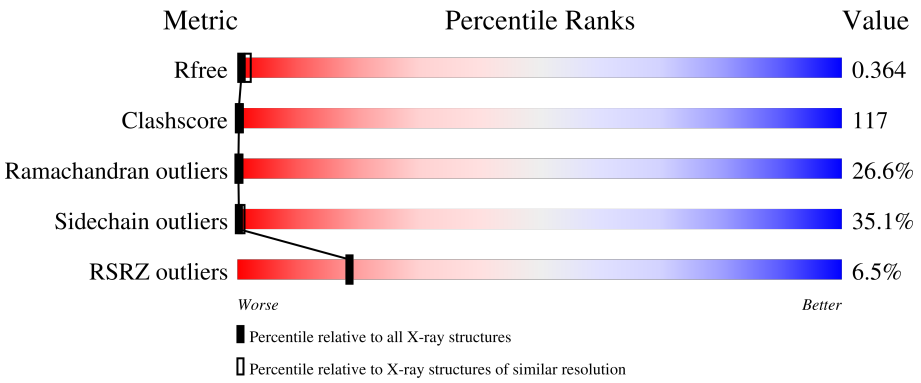
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	1	241	10%; 30%, 25%, 11%, •, 32%
2	2	269	6%; 24%, 30%, 10%, •, 35%
3	3	276	7%; 16%, 21%, 16%, 6%, 41%
4	4	251	9%; 22%, 27%, 14%, •, 34%
5	A	758	4%; 6%, 48%, 34%, 9%, •

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Mol	Chain	Length	Quality of chain
6	B	734	%, 10%, 44%, 35%, 10%
7	C	81	14%, 5%, 43%, 35%, 17%
8	D	212	5%, 6%, 27%, 27%, 5%, 35%
9	E	143	5%, •, 20%, 15%, 7%, 55%
10	F	231	4%, 7%, 30%, 22%, 8%, 33%
11	G	167	5%, •, 22%, 20%, 11%, 43%
12	H	144	2%, •, 17%, 19%, 10%, 52%
13	I	40	•, 45%, 22%, 5%, 25%
14	J	44	2%, 11%, 50%, 27%, 7%, 5%
15	K	131	17%, 27%, 21%, 9%, 7%, 36%
16	L	216	4%, 8%, 35%, 24%, 7%, 25%
17	N	170	2%, •, 9%, 20%, 19%, 50%
18	R	53	28%, 42%, 30%
19	M	2	100%
19	O	2	100%
19	P	2	100%
19	Q	2	100%
19	S	2	50%, 50%
19	T	2	100%
19	U	2	100%
19	V	2	100%
19	W	2	100%
19	X	2	100%
19	Y	2	100%
19	Z	2	100%

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Mol	Chain	Length	Quality of chain
19	a	2	100%

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	GLC	M	1	-	-	X	-
19	FRU	M	2	X	-	X	-
19	FRU	O	2	X	-	X	-
19	FRU	P	2	X	-	-	-
19	GLC	Q	1	-	-	X	-
19	FRU	Q	2	X	-	X	-
19	FRU	S	2	X	-	-	-
19	GLC	T	1	-	-	X	-
19	FRU	T	2	X	-	X	-
19	GLC	U	1	-	-	X	-
19	FRU	U	2	X	-	X	-
19	FRU	V	2	X	-	-	-
19	GLC	W	1	-	-	X	-
19	FRU	W	2	X	-	X	-
19	GLC	X	1	-	-	X	-
19	FRU	X	2	X	-	X	-
19	FRU	Y	2	X	-	-	-
19	GLC	Z	1	-	-	X	-
19	FRU	Z	2	X	-	X	-
19	FRU	a	2	X	-	-	-
20	CLA	1	1187	X	-	-	-
20	CLA	1	1188	X	-	-	-
20	CLA	1	1189	X	-	-	-
20	CLA	1	1190	X	-	-	-
20	CLA	1	1191	X	-	-	-
20	CLA	1	1192	X	-	-	-
20	CLA	1	1193	X	-	-	-
20	CLA	1	1194	X	-	-	-
20	CLA	1	1195	X	-	-	-
20	CLA	1	1196	X	-	-	-
20	CLA	1	1197	X	-	-	X
20	CLA	1	1198	X	-	-	-
20	CLA	1	1199	X	-	-	-
20	CLA	1	1200	X	-	-	-
20	CLA	1	1201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	2	1212	X	-	-	-
20	CLA	2	1213	X	-	-	-
20	CLA	2	1214	X	-	-	X
20	CLA	2	1215	X	-	X	-
20	CLA	2	1216	X	-	-	-
20	CLA	2	1217	X	-	-	-
20	CLA	2	1218	X	-	-	-
20	CLA	2	1219	X	-	-	-
20	CLA	2	1220	X	-	X	-
20	CLA	2	1221	X	-	-	-
20	CLA	2	1222	X	-	-	-
20	CLA	2	1223	X	-	-	-
20	CLA	2	1224	X	-	-	-
20	CLA	2	1227	X	-	-	X
20	CLA	2	2010	X	-	-	-
20	CLA	3	1212	X	-	-	-
20	CLA	3	1213	X	-	-	-
20	CLA	3	1214	X	-	-	-
20	CLA	3	1215	X	-	-	-
20	CLA	3	1216	X	-	-	-
20	CLA	3	1217	X	-	-	-
20	CLA	3	1218	X	-	X	-
20	CLA	3	1219	X	-	-	X
20	CLA	3	3001	X	-	-	-
20	CLA	3	3002	X	-	-	-
20	CLA	3	3007	X	-	-	-
20	CLA	3	3008	X	-	-	-
20	CLA	3	3011	X	-	-	-
20	CLA	3	3014	X	-	-	X
20	CLA	3	3015	X	-	-	-
20	CLA	4	1196	X	-	X	-
20	CLA	4	1197	X	-	-	-
20	CLA	4	1198	X	-	X	-
20	CLA	4	1199	X	-	X	-
20	CLA	4	1200	X	-	-	X
20	CLA	4	1201	X	-	X	-
20	CLA	4	1202	X	-	-	-
20	CLA	4	1203	X	-	-	-
20	CLA	4	1204	X	-	-	-
20	CLA	4	1205	X	-	-	-
20	CLA	4	1206	X	-	-	-
20	CLA	4	1207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	4	1208	X	-	-	-
20	CLA	4	1209	X	-	-	-
20	CLA	4	4003	X	-	-	-
20	CLA	4	4007	X	-	-	-
20	CLA	4	4014	X	-	-	-
20	CLA	A	1759	X	-	-	-
20	CLA	A	1760	X	-	X	-
20	CLA	A	1761	X	-	X	-
20	CLA	A	1762	X	-	-	-
20	CLA	A	1763	X	-	X	-
20	CLA	A	1764	X	-	X	-
20	CLA	A	1765	X	-	X	-
20	CLA	A	1766	X	-	-	-
20	CLA	A	1767	X	-	X	-
20	CLA	A	1768	X	-	-	-
20	CLA	A	1769	X	-	X	-
20	CLA	A	1770	X	-	X	-
20	CLA	A	1771	X	-	-	-
20	CLA	A	1772	X	-	X	-
20	CLA	A	1773	X	-	-	-
20	CLA	A	1774	X	-	X	-
20	CLA	A	1775	X	-	-	-
20	CLA	A	1776	X	-	X	-
20	CLA	A	1777	X	-	-	-
20	CLA	A	1778	X	-	-	-
20	CLA	A	1779	X	-	X	-
20	CLA	A	1780	X	-	-	-
20	CLA	A	1781	X	-	X	-
20	CLA	A	1782	X	-	X	-
20	CLA	A	1783	X	-	X	-
20	CLA	A	1784	X	-	-	-
20	CLA	A	1785	X	-	-	-
20	CLA	A	1786	X	-	-	-
20	CLA	A	1787	X	-	X	-
20	CLA	A	1788	X	-	X	-
20	CLA	A	1789	X	-	-	-
20	CLA	A	1790	X	-	-	-
20	CLA	A	1791	X	-	X	-
20	CLA	A	1792	X	-	X	-
20	CLA	A	1793	X	-	X	-
20	CLA	A	1794	X	-	X	-
20	CLA	A	1795	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	1796	X	-	X	-
20	CLA	A	1797	X	-	X	-
20	CLA	A	1798	X	-	X	-
20	CLA	A	1799	X	-	-	X
20	CLA	A	1800	X	-	X	-
20	CLA	A	1801	X	-	-	X
20	CLA	A	1811	X	-	-	-
20	CLA	A	1812	X	-	X	-
20	CLA	A	1813	X	-	X	-
20	CLA	A	1815	X	-	-	-
20	CLA	A	1816	X	-	X	-
20	CLA	A	1817	X	-	-	-
20	CLA	B	1735	X	-	X	-
20	CLA	B	1736	X	-	-	-
20	CLA	B	1737	X	-	X	-
20	CLA	B	1738	X	-	-	-
20	CLA	B	1739	X	-	X	-
20	CLA	B	1740	X	-	-	-
20	CLA	B	1741	X	-	-	-
20	CLA	B	1742	X	-	-	-
20	CLA	B	1743	X	-	X	-
20	CLA	B	1744	X	-	-	-
20	CLA	B	1745	X	-	-	-
20	CLA	B	1746	X	-	X	-
20	CLA	B	1747	X	-	X	-
20	CLA	B	1748	X	-	-	-
20	CLA	B	1749	X	-	-	-
20	CLA	B	1750	X	-	-	-
20	CLA	B	1751	X	-	-	-
20	CLA	B	1752	X	-	-	-
20	CLA	B	1753	X	-	X	-
20	CLA	B	1754	X	-	X	-
20	CLA	B	1755	X	-	X	X
20	CLA	B	1756	X	-	X	-
20	CLA	B	1757	X	-	X	-
20	CLA	B	1758	X	-	X	-
20	CLA	B	1759	X	-	X	-
20	CLA	B	1760	X	-	-	-
20	CLA	B	1761	X	-	-	-
20	CLA	B	1762	X	-	X	-
20	CLA	B	1763	X	-	-	-
20	CLA	B	1764	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	1765	X	-	-	-
20	CLA	B	1766	X	-	-	-
20	CLA	B	1767	X	-	-	-
20	CLA	B	1768	X	-	X	-
20	CLA	B	1769	X	-	X	-
20	CLA	B	1770	X	-	X	-
20	CLA	B	1771	X	-	X	-
20	CLA	B	1772	X	-	-	-
20	CLA	B	1785	X	-	X	-
20	CLA	B	1786	X	-	X	-
20	CLA	B	1787	X	-	X	-
20	CLA	F	1155	X	-	-	-
20	CLA	F	1156	X	-	-	-
20	CLA	F	1157	X	-	-	-
20	CLA	G	1099	X	-	-	-
20	CLA	H	1079	X	-	-	-
20	CLA	I	1031	X	-	-	-
20	CLA	I	1033	X	-	-	-
20	CLA	J	1043	X	-	X	-
20	CLA	J	1044	X	-	X	-
20	CLA	J	1045	X	-	X	-
20	CLA	J	1046	X	-	-	X
20	CLA	K	1085	X	-	X	-
20	CLA	K	1142	X	-	X	-
20	CLA	K	1146	X	-	-	-
20	CLA	K	3009	X	-	-	-
20	CLA	L	1166	X	-	-	-
20	CLA	L	1167	X	-	-	-
20	CLA	L	1168	X	-	-	-
20	CLA	L	1505	X	-	-	-
20	CLA	R	1054	X	-	-	-
20	CLA	R	1055	X	-	-	-
21	LMU	1	7004	-	-	-	X
21	LMU	A	7016	-	-	X	-
21	LMU	A	7020	-	-	X	-
21	LMU	A	7021	-	-	X	-
21	LMU	A	7023	-	-	X	-
21	LMU	A	7026	-	-	X	-
21	LMU	A	7032	-	-	X	-
21	LMU	A	7037	-	-	X	-
21	LMU	A	7042	-	-	X	-
21	LMU	R	1057	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	BCR	3	1220	-	-	X	-
22	BCR	A	1803	-	-	X	X
22	BCR	A	1804	-	-	X	-
22	BCR	A	1805	-	-	X	-
22	BCR	A	1806	-	-	X	-
22	BCR	A	1807	-	-	X	-
22	BCR	A	1808	-	-	X	-
22	BCR	B	1777	-	-	X	-
22	BCR	B	1778	-	-	X	-
22	BCR	B	1779	-	-	X	-
22	BCR	B	1780	-	-	X	-
22	BCR	I	1032	-	-	X	-
22	BCR	L	1169	-	-	X	X
23	PQN	A	1802	X	-	-	-
23	PQN	B	1773	X	-	X	-
24	LMG	B	1783	-	-	X	-
25	SF4	B	1784	-	-	X	-
25	SF4	C	1082	-	-	X	-
25	SF4	C	1083	-	-	X	-

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 36379 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 AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	165	1264	822	208	230	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	conflict	UNP Q9C5R7
1	-1	ARG	LYS	conflict	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	176	1374	899	226	245	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	insertion	UNP Q41038
2	?	-	GLY	deletion	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	162	1254	826	203	220	5	0	0	0

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	166	1319	861	219	236	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	deletion	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	A	730	5745	3766	974	987	18	0	0	0

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	B	733	5848	3843	997	995	13	0	0	0

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

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

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	D	138	1095	704	189	198	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	conflict	UNP P12353
D	-50	PRO	GLN	conflict	UNP P12353
D	-44	ARG	PRO	conflict	UNP P12353
D	-34	GLU	ASP	conflict	UNP P12353
D	-11	LEU	HIS	conflict	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	conflict	UNP P12353
D	12	THR	PRO	conflict	UNP P12353
D	14	ALA	GLY	conflict	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	E	65	520	332	93	95	0	0	0

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

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

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	G	95	740	481	120	137	2	0	0	0

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	H	69	529	344	82	103	0	0	0

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

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

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	J	42	338	230	51	56	1	0	0	0

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	K	84	593	374	102	113	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	ILE	LEU	conflict	UNP P36886

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	L	161	1203	791	193	214	5	0	0	0

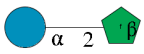
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

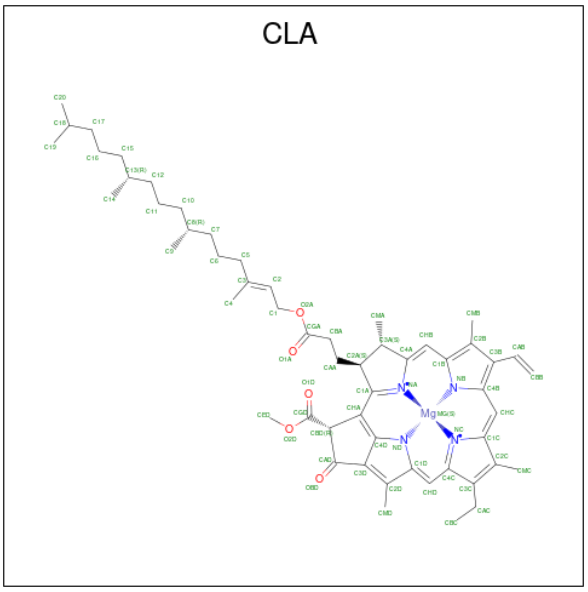
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	53	265	159	53	53	0	0	0

- Molecule 19 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
19	M	2	22	12	10	0	0	0
			Total	C	O			
19	O	2	23	12	11	0	0	0
			Total	C	O			
19	P	2	23	12	11	0	0	0
			Total	C	O			
19	Q	2	23	12	11	0	0	0
			Total	C	O			
19	S	2	23	12	11	0	0	0
			Total	C	O			
19	T	2	23	12	11	0	0	0
			Total	C	O			
19	U	2	23	12	11	0	0	0
			Total	C	O			
19	V	2	23	12	11	0	0	0
			Total	C	O			
19	W	2	23	12	11	0	0	0
			Total	C	O			
19	X	2	23	12	11	0	0	0
			Total	C	O			
19	Y	2	23	12	11	0	0	0
			Total	C	O			
19	Z	2	23	12	11	0	0	0
			Total	C	O			
19	a	2	23	12	11	0	0	0

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	1	1	Total C Mg N O 46 36 1 4 5	0	0
20	1	1	Total C Mg N O 47 37 1 4 5	0	0
20	1	1	Total C Mg N O 47 37 1 4 5	0	0
20	1	1	Total C Mg N O 46 36 1 4 5	0	0
20	1	1	Total C Mg N O 36 30 1 4 1	0	0
20	1	1	Total C Mg N O 61 51 1 4 5	0	0
20	1	1	Total C Mg N O 51 41 1 4 5	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	1	1	Total C Mg N O 36 30 1 4 1	0	0
20	1	1	Total C Mg N O 36 30 1 4 1	0	0
20	1	1	Total C Mg N O 51 41 1 4 5	0	0
20	1	1	Total C Mg N O 61 51 1 4 5	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	1	1	Total C Mg N O 51 41 1 4 5	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 51 41 1 4 5	0	0
20	2	1	Total C Mg N O 56 46 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 50 40 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 65 55 1 4 5	0	0
20	2	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 56 46 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 50 40 1 4 5	0	0
20	2	1	Total C Mg N O 50 40 1 4 5	0	0
20	2	1	Total C Mg N O 65 55 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 36 30 1 4 1	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 65 55 1 4 5	0	0
20	3	1	Total C Mg N O 65 55 1 4 5	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 42 34 1 4 3	0	0
20	3	1	Total C Mg N O 50 40 1 4 5	0	0
20	3	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 55 45 1 4 5	0	0
20	4	1	Total C Mg N O 36 30 1 4 1	0	0
20	4	1	Total C Mg N O 65 55 1 4 5	0	0
20	4	1	Total C Mg N O 55 45 1 4 5	0	0
20	4	1	Total C Mg N O 50 40 1 4 5	0	0
20	4	1	Total C Mg N O 52 42 1 4 5	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 55 45 1 4 5	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 36 30 1 4 1	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 46 36 1 4 5	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 52 42 1 4 5	0	0
20	4	1	Total C Mg N O 47 37 1 4 5	0	0
20	A	1	Total C Mg N O 50 40 1 4 5	0	0
20	A	1	Total C Mg N O 55 45 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
20	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	57	47	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	46	36	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	52	42	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	36	30	1	4	1	0	0
			Total	C	Mg	N	O		
20	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	51	41	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	42	34	1	4	3	0	0
			Total	C	Mg	N	O		
20	A	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	A	1	65	55	1	4	5	0	0

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
20	B	1	46	36	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	58	48	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	51	41	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	47	37	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
20	B	1	36	30	1	4	1	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	F	1	36	30	1	4	1	0	0
			Total	C	Mg	N	O		
20	F	1	41	33	1	4	3	0	0
			Total	C	Mg	N	O		
20	F	1	53	43	1	4	5	0	0
			Total	C	Mg	N	O		
20	G	1	51	41	1	4	5	0	0
			Total	C	Mg	N	O		
20	H	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	I	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
20	I	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
20	J	1	61	51	1	4	5	0	0
			Total	C	Mg	N	O		
20	J	1	61	51	1	4	5	0	0
			Total	C	Mg	N	O		
20	J	1	55	45	1	4	5	0	0
			Total	C	Mg	N			
20	J	1	25	20	1	4		0	0
			Total	C	Mg	N	O		
20	K	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
20	K	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
20	K	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
20	K	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
20	L	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
20	L	1	47	37	1	4	5	0	0

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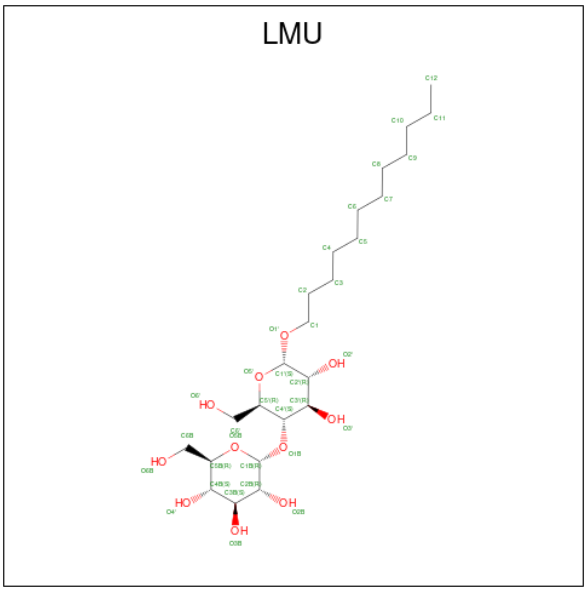
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
20	L	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
20	L	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
20	R	1	57	47	1	4	5	0	0
			Total	C	Mg	N	O		
20	R	1	65	55	1	4	5	0	0

- Molecule 21 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	1	1	35	24	11	0	0
			Total	C	O		
21	1	1	35	24	11	0	0
			Total	C	O		
21	2	1	35	24	11	0	0
			Total	C	O		
21	2	1	35	24	11	0	0
			Total	C	O		
21	2	1	35	24	11	0	0
			Total	C	O		
21	3	1	35	24	11	0	0
			Total	C	O		
21	4	1	35	24	11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 34 23 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0

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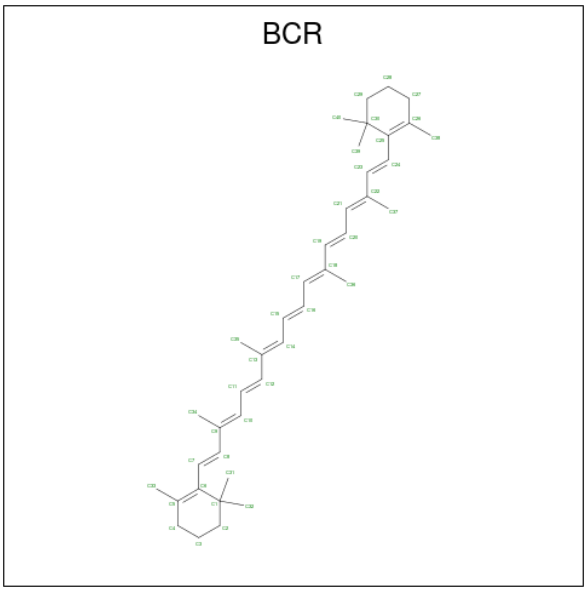
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 34 23 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	B	1	Total C O 25 14 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	L	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
22	3	1	40	40	0	0
22	A	1	40	40	0	0
22	A	1	40	40	0	0
22	A	1	40	40	0	0
22	A	1	40	40	0	0
22	A	1	40	40	0	0
22	A	1	40	40	0	0
22	B	1	40	40	0	0
22	B	1	40	40	0	0
22	B	1	40	40	0	0
22	B	1	40	40	0	0
22	B	1	40	40	0	0
22	B	1	40	40	0	0
22	B	1	40	40	0	0

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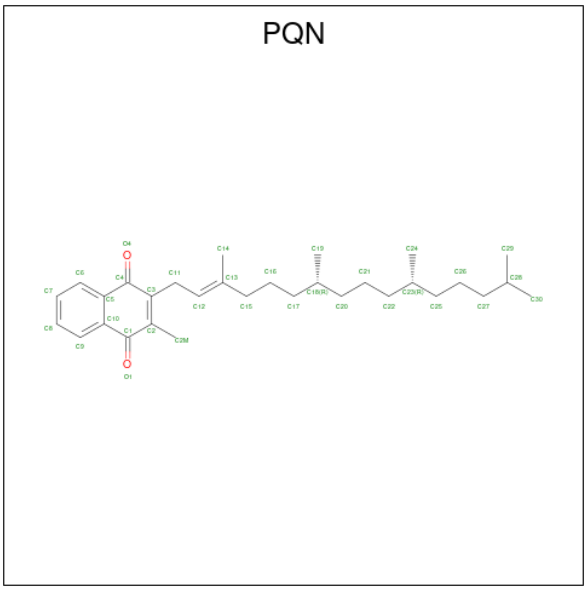
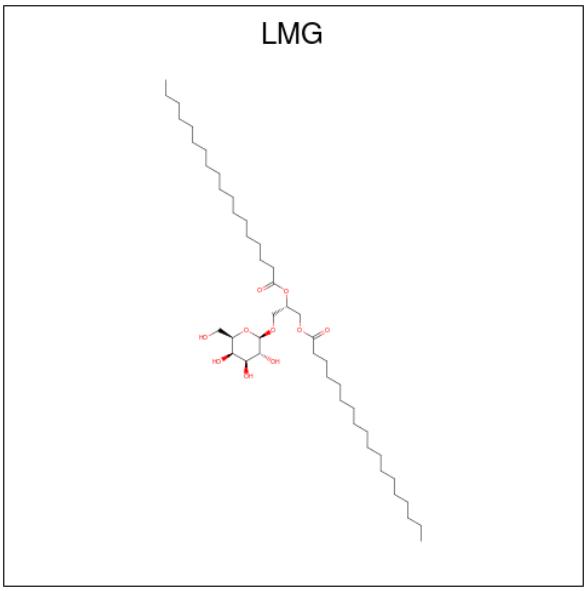
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
22	B	1	40	40	0	0
			Total	C		
22	I	1	40	40	0	0
			Total	C		
22	L	1	40	40	0	0
			Total	C		
22	L	1	40	40	0	0

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



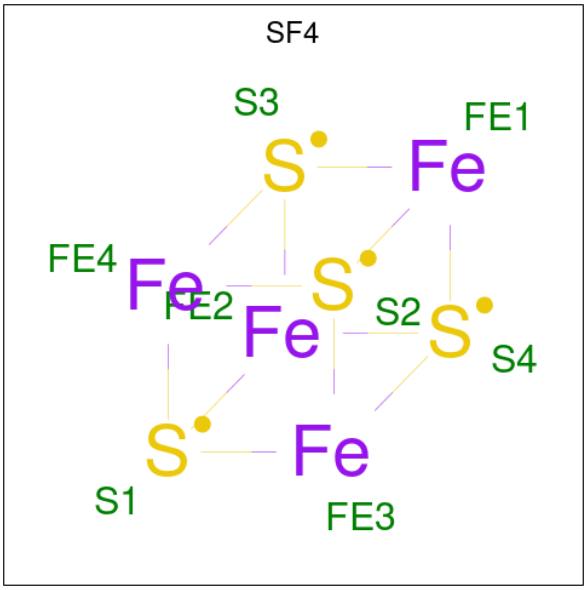
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
23	A	1	33	31	2	0	0
			Total	C	O		
23	B	1	33	31	2	0	0

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



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

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

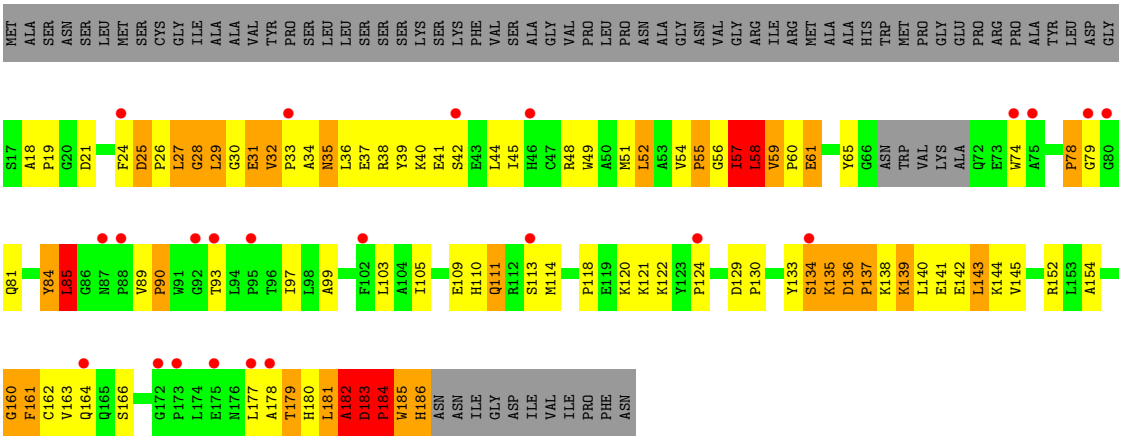
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
26	B	1	23	12	11	0	0

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.

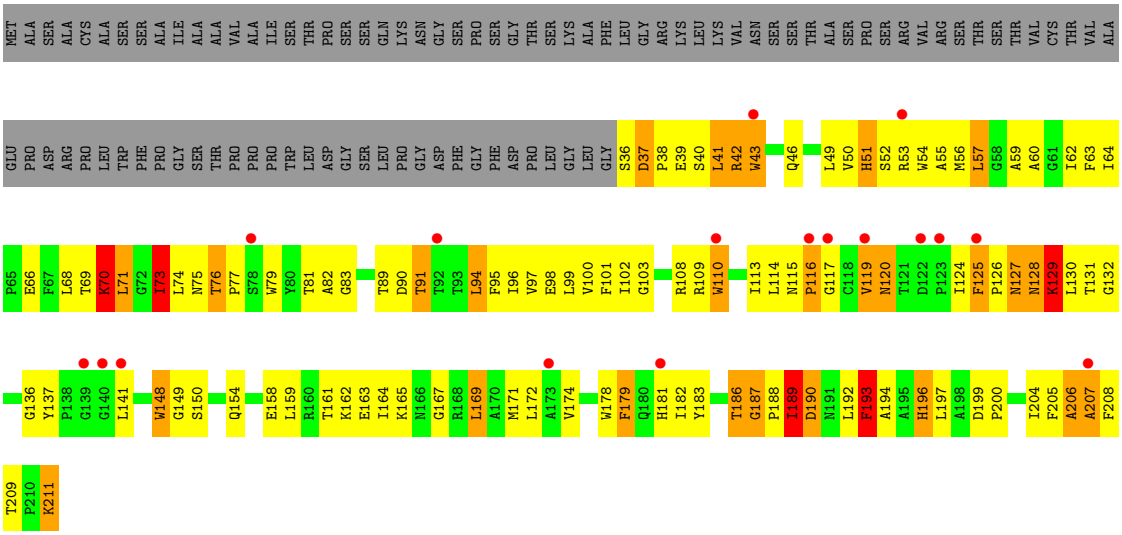
- Molecule 1: AT3G54890

Chain 1:



- Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I

Chain 2:



- Molecule 3: LHCA3

Chain 3: 7% 16% 21% 16% 6% 41%

MET ALA ALA GLN ALA LEU VAL SER SER SER SER LEU THR PHE SER ALA GLU ALA ALA ARG GLN SER LEU GLY PRO ARG SER LEU GLN SER PRO PHE GLY PHE SER ARG LYS ALA SER PHE LEU VAL LYS ALA ALA ALA THR PRO PRO VAL LYS GLN GLY SER ASP ARG PRO LEU TRP PHE

ALA SER LYS GLN SER LEU SER TYR LEU ASP GLY SER LEU PRO GLY ASP TYR GLY PHE ASP PRO LEU GLY LEU S40 D41 P42 T45 G46 G47 F48 I49 E50 P51 K52 W53 L54 A55 Y56 G57 E58 I59 I60 N61 G62 R63 Y64 A65 M66 L67 G68 A69 A72 I73 A74 P75 E76 I77

L78 G79 K80 L83 I84 P85 Q86 E87 T88 A89 L90 P91 W92 F93 R94 T95 G96 F97 I98 PRO PRO ALA GLY THR Y104 N105 Y106 W107 A108 D109 S110 Y111 T112 L113 F114 V115 F116 L120 M121 G122 F123 R127 R128 F129 Q130 D131 W132 A133 K134 P135 G136 S137 K140 Q141 Y142

L146 L150 S153 G154 E155 P156 A157 Y158 P159 G160 G161 P162 F163 F164 N165 P166 L167 G168 F169 G170 K171 D172 E173 K174 SER LEU LYS ASP LEU K180 L181 K182 E183 V184 K185 N186 G187 R188 L189 A190 M191 L192 A193 I194 L195 G196 Y197 F198 V199 Q200 A201 L202 V203 T204 G205 V206 G207 P208

Y209 Q210 N211 LEU LEU ASP HIS LEU THR ASP PRO VAL HIS ASN ASN ILE LEU THR SER LEU LYS PHE HIS

- Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC

Chain 4: 9% 22% 27% 14% • 34%

MET ALA THR VAL THR THR GLN ALA SER ALA ALA ILE PHE GLY PRO CYS GLY LEU LYS SER ARG PHE LEU GLY GLY SER SER GLY LYS LEU ASN ARG GLY VAL ALA PHE ARG PRO VAL GLY CYS SER PRO SER ALA SER PHE LYS VAL GLU ALA LYS LYS GLY GLU TRP LEU PRO GLY LEU

ALA SER PRO GLY TYR LEU THR GLY SER LEU PRO GLY ASP ASN GLY PHE ASP PRO LEU GLY L30 A31 E32 D33 P34 E35 N36 L37 R38 W39 F40 V41 G48 R49 W50 A51 M52 L53 G54 M58 L59 L60 P61 E62 V63 F64 T65 S66 I67 G68 I69 I70 N71 V72 P73 K74 W75 Y76

A77 A78 Y83 F84 A85 S86 S87 S88 T89 L90 F91 E94 F95 S98 V101 E102 I103 R104 R105 W106 Q107 D108 I109 K110 S114 V115 N116 Q117 D118 P119 I120 F121 K122 Q123 Y124 S125 L126 P127 A128 G129 E130 V131 G132 Y133 P134 G135 G136 I137 F138 N139 P140 L141 N142 F143 A144

P145 T146 L147 E148 A149 K150 E151 K152 E153 I154 A155 N156 G157 R158 L159 M160 L161 A162 F163 L164 G165 I168 Q169 H170 N171 V172 T173 G174 K175 G176 P177 F178 I185 S186 D187 P188 W189 H190 N191 T192 I193 V194 Q195 THR LEU GLY GLY ASN

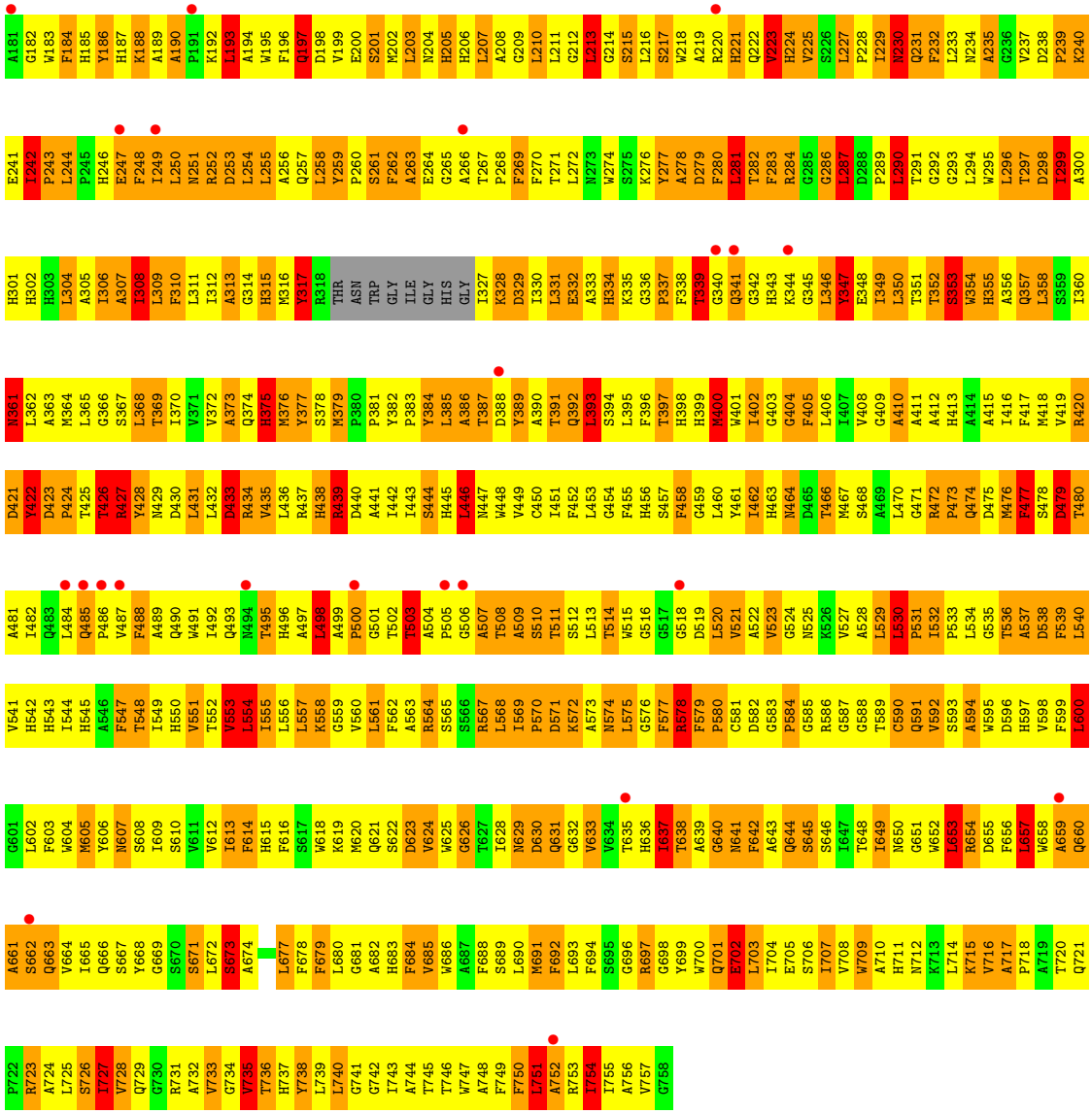
- Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1

Chain A: 4% 6% 48% 34% 9% •

MET ILE ILE ARG SER PRO GLU PRO LYS VAL GLN ILE LEU ALA ASP PRO GLU VAL LYS ILE L21 V22 D23 R24 D25 P26 I27 K28 T29 S30 F31 E32 Q33 W34 A35 K36 P37 G38 H39 F40 S41 R42 T43 I44 A45 K46 G47 P48 D49 T50 T51 T52 W53 I54 W55 N56 L57 H58 A59 D60

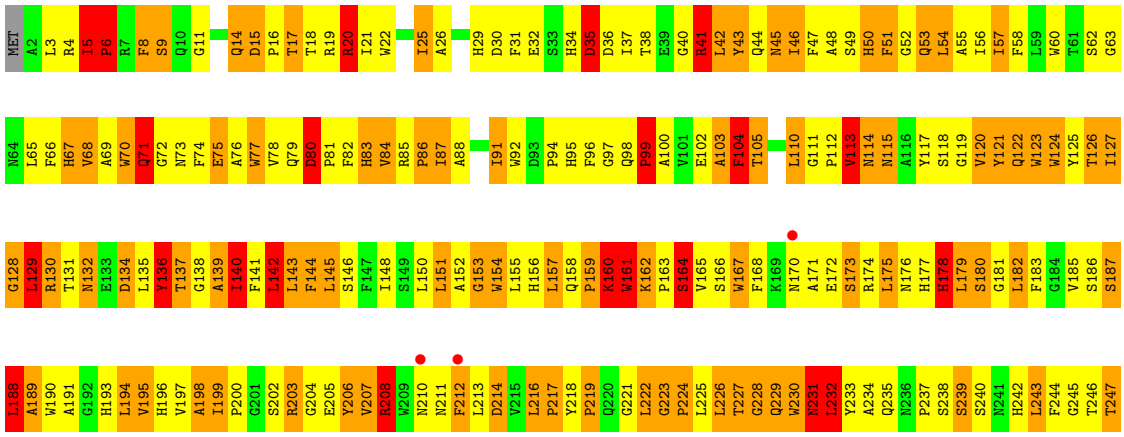
A61 H62 D63 F64 D65 S66 H67 T68 S69 D70 L71 E72 E73 I74 S75 R76 K77 V78 F79 S80 A81 H82 F83 G84 Q85 L86 S87 I88 I89 F90 L91 W92 L93 S94 G95 M96 Y97 F98 H99 G100 A101 R102 F103 S104 N105 Y106 E107 A108 W109 L110 N111 D112 P113 T114 H115 I116 G117 P118 S119 A120

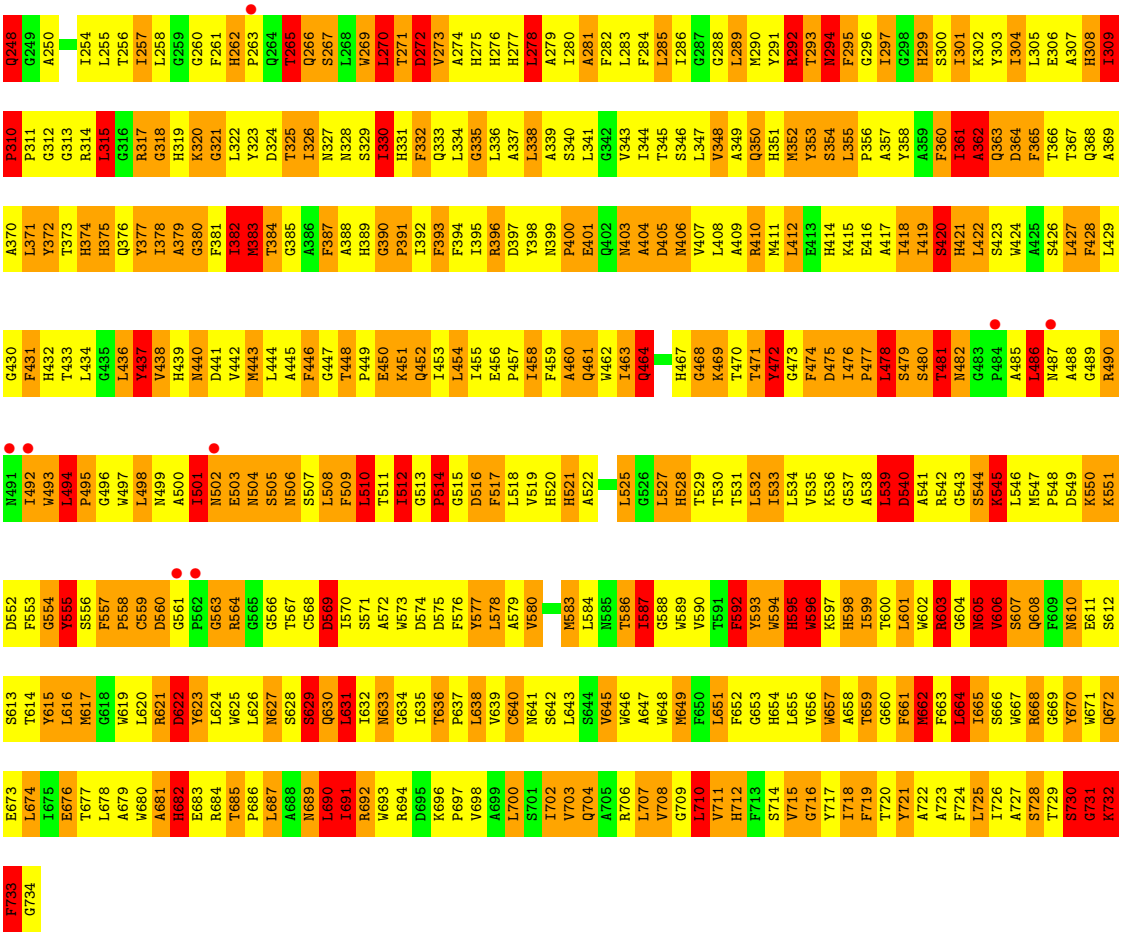
Q121 V122 V123 W124 P125 I126 V127 G128 Q129 E130 I131 L132 N133 G134 D135 V136 G137 G138 G139 F140 R141 G142 I143 Q144 I145 T146 S147 G148 F149 F150 Q151 I152 W153 R154 A155 S156 G157 I158 T159 S160 E161 L162 Q163 L164 Y165 C166 T167 A168 I169 G170 A171 L172 V173 F174 A175 G176 L177 M178 L179 F180



• Molecule 6: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

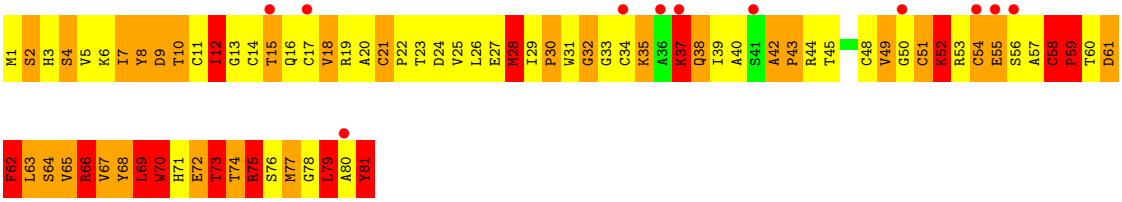
Chain B:





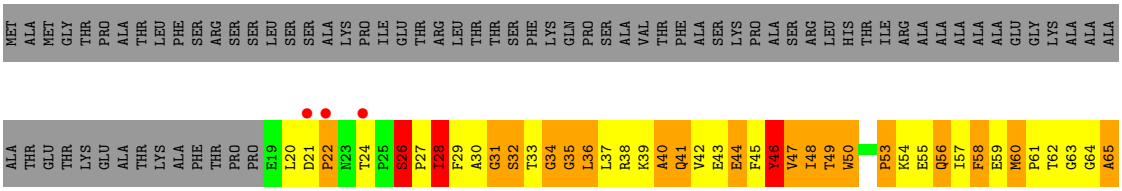
• Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER

Chain C: 14% 5% 43% 35% 17%



• Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC

Chain D: 5% 6% 27% 27% 5% 35%



A66 I67 M68 R69 E70 G71 P72 N73 L74 L75 K76 L77 A78 R79 K80 E81 Q82 C83 L84 A85 L86 G87 T88 R89 L90 R91 S92 K93 Y94 K95 I96 K97 Y98 Q99 F100 Y101 R102 V103 F104 P105 S106 G107 E108 V109 Q110 Y111 L112 H113 P114 K115 D116 G117 V118 Y119 P120 E121 K122 V123 N124 P125

G126 R127 Q128 G129 V130 G131 L132 N133 M134 R135 S136 I137 G138 K139 N140 V141 S142 P143 I144 E145 V146 K147 F148 T149 G150 K151 Q152 P153 Y154 D155 L156

• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC

Chain E: 5% 20% 15% 7% 55%

MET ALA MET THR THR ALA SER THR VAL PHE VAL LEU PRO ALA ASN VAL THR SER VAL ALA GLY ALA SER SER SER ARG SER SER VAL SER PHE LEU PRO MET ARG ASN ALA GLY SER ARG LEU VAL VAL ARG ALA ALA GLU ASP PRO ALA PRO ALA SER SER SER SER LYS ASP SER PRO

ALA ALA ALA ALA ALA PRO ASP GLY ALA THR ALA THR LYS PRO LYS PRO PRO PRO I28 G29 P30 K31 R32 G33 S34 K35 V36 K37 I38 L39 R40 R41 E42 S43 Y44 W45 F46 K47 N48 V49 G50 S51 V52 V53 A54 V55 D56 Q57 D58 P59 K60 T61 R62 Y63 P64 V65 V66 V67 R68 F69

A70 K71 V72 N73 Y74 A75 N76 I77 S78 T79 N80 N81 Y82 A83 L84 D85 E86 V87 E88 E89 V90 A91 A92

• Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC

Chain F: 4% 7% 30% 22% 8% 33%

MET SER PHE THR ILE PRO THR ASN LEU TYR LYS PRO LEU ALA THR LYS PRO LYS HIS LEU SER SER SER SER PHE ALA PRO ARG SER LYS ILE VAL CYS GLN GLN GLU ASN ASP GLN GLN GLN PRO LYS LYS LEU GLU LEU ALA LYS VAL GLY ALA ASN ASN ALA ALA ALA ALA ALA LEU ALA LEU

SER SER VAL LEU LEU SER SER TRP SER VAL ALA PRO ASP ALA ALA MET ALA D1 I2 A3 G4 L5 T6 P7 C8 K9 E10 S11 K12 Q13 F14 A15 K16 R17 E18 K19 Q20 A21 L22 K23 K24 L25 Q26 A27 S28 L29 K30 L31 Y32 A33 D34 D35 S36 A37 P38 A39 L40 A41 I42 K43

A44 T45 M46 E47 K48 T49 K50 K51 R52 F53 D54 N55 Y56 G57 K58 Y59 G60 L61 L62 C63 G64 S65 D66 G67 L68 P69 H70 L71 I72 V73 D76 Q77 R78 H79 W80 G81 E82 F83 I84 T85 P86 G87 I88 L89 F90 L91 Y92 I93 A94 G95 W96 I97 G98 W99 V100 G101 R102 S103 Y104

L105 I106 A107 I108 R109 D110 E111 K112 K113 P114 T115 Q116 K117 E118 I119 I120 I121 D122 V123 P124 L125 A126 S127 S128 L129 L130 F131 R132 G133 F134 S135 W136 P137 V138 A139 A140 Y141 R142 E143 L144 L145 N146 G147 E148 L149 V150 D151 N152 N153 F154

• Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC

Chain G: 5% 22% 20% 11% 43%

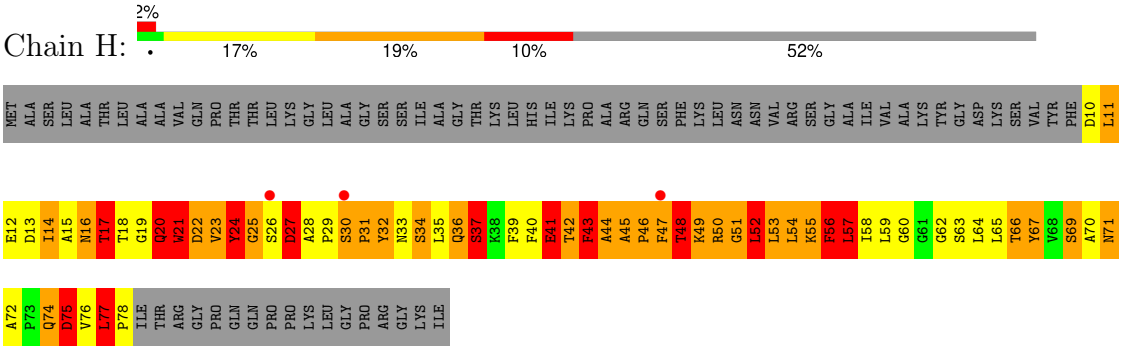
MET ALA ALA ALA THR ALA SER LEU SER SER THR LEU LEU ALA PRO CYS SER SER LYS GLN PRO GLN PRO GLN GLN GLN HIS GLN HIS GLN GLN LEU LYS CYS LYS SER PHE SER GLY LEU ARG PRO LEU LYS LEU ASN ILE SER SER ASN ASN SER SER SER SER LEU SER MET SER SER

ALA ARG ARG SER MET THR CYS ARG ALA GLU LEU SER P4 S5 L6 V7 I8 S9 L10 S11 T12 G13 L14 S15 L16 F17 L18 G19 R20 F21 V22 F23 F24 N25 F26 Q27 R28 E29 N30 R31 A32 K33 Q34 V35 P36 E37 Q38 N39 G40 M41 S42 H43 F44 E45 A46 G47 D48 T49 R50 A51

Y54 V55 S56 L57 L58 K59 S60 N61 D62 P63 V64 G65 F66 N67 I68 V69 D70 V71 L72 A73 W74 G75 S76 I77 G78 H79 I80 V81 A82 Y83 Y84 I85 L86 A87 T88 A89 S90 N91 G92 Y93 D94 P95 S96 F97 F98

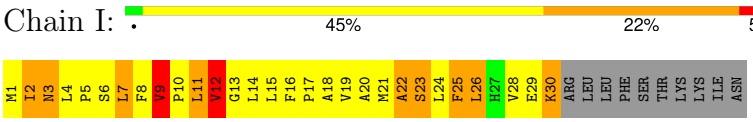
• Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC

Chain H:



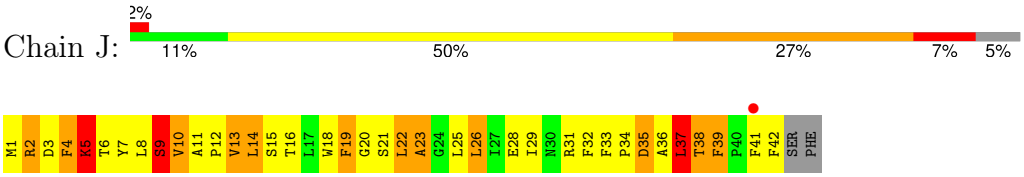
• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII

Chain I:



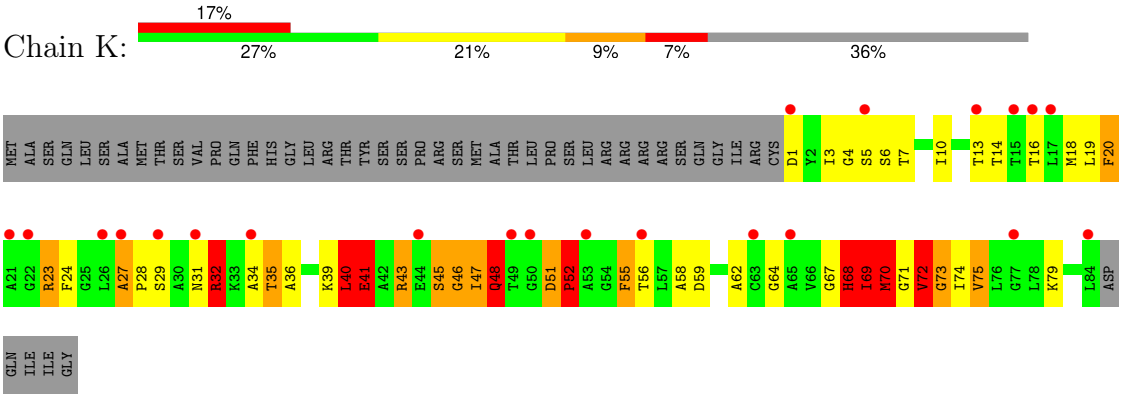
• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

Chain J:



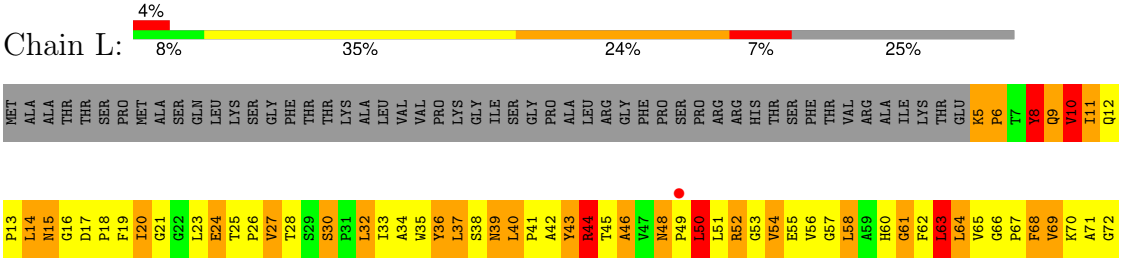
• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

Chain K:



• Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

Chain L:



P73 L74 R75 N76 T77 E78 Y79 A80 G81 A82 A83 G84 S85 L86 A87 A88 A89 G90 L91 V92 V93 I94 L95 S96 M97 C98 L99 T100 M101 Y102 G103 I104 A105 S106 F107 K108 E109 G110 E111 P112 S113 I114 A115 P116 A117 L118 T119 L120 T121 G122 R123 K124 K125 Q126 P127 D128 Q129 L130 Q131 S132

A133 D134 G135 W136 A137 K138 F139 T140 G141 G142 F143 F144 F145 G146 G147 V148 S149 G150 V151 T152 W153 A154 C155 F156 L157 M158 Y159 V160 L161 D162 L163 P164 Y165 TYR PHE LYS

- Molecule 17: PHOTOSYSTEM I-N SUBUNIT

Chain N: 2% 9% 20% 19% 50%

MET SER ALA MET ASN SER THR VAL LEU ALA CYS ASN TYR ALA ARG SER GLY CYS SER ASP LEU ASN ALA LYS LEU THR SER MET PRO SER VAL ALA SER PRO GLN LEU SER ALA LEU LYS LEU PRO LEU ILE LYS ALA HIS GLN ALA LYS VAL THR GLU SER LYS SER ASP GLN GLY ARG

ARG SER ALA LEU VAL TYR LEU ALA ALA THR LEU PHE THR ALA ALA ALA ALA ALA SER ASN SER SER SER ALA ASN ALA G1 V2 I3 E4 E5 Y6 L7 E8 K9 S10 K11 T12 E15 L16 N17 D18 K19 K20 R21 L22 A23 T24 T25 G26 A27 N28 F29 A30 R31 A32 Y33 T34 V35 E36

F37 G38 S39 C40 K41 F42 P43 E44 N45 P46 T47 G48 C49 Q50 D51 L52 A53 K54 Q55 K56 K57 V58 P59 F60 L61 S62 D63 D64 L65 D66 L67 E68 C69 E70 G71 K72 D73 K74 Y75 K76 C77 G78 S79 N80 V81 F82 W83 K84 W85

- Molecule 18: PHOTOSYSTEM I-N SUBUNIT

Chain R: 28% 42% 30%

X1 X2 X3 X4 X5 X6 X7 X8 X9 X10 X11 X24 X25 X26 X27 X28 X29 X30 X31 X32 X33 X34 X35 X36 X37 X38 X39 X40 X41 X42 X43 X44 X45 X46 X47 X48 X49 X50 X51 X52 X53

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M: 100%

GLC1 FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O: 100%

GLC1 FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain P: 100%

GLC1 FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Q: 100%

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain S: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain T: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain U: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain V: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain W: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain X: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Y: 

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Z: 100%

GLC1
FRU2

• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain a: 100%

GLC1
FRU2

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 49.14 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 98.5 (49.14-3.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.363 , 0.366 0.359 , 0.364	Depositor DCC
R_{free} test set	4685 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	78.5	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.15 , 81.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	36379	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: GLC, PQN, LMG, UNL, BCR, LMU, SF4, CLA, FRU

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	1	0.48	0/1303	0.72	3/1774 (0.2%)
2	2	0.45	0/1420	0.71	0/1943
3	3	0.87	6/1292 (0.5%)	0.96	3/1743 (0.2%)
4	4	0.49	0/1359	0.75	2/1851 (0.1%)
5	A	0.95	3/5938 (0.1%)	1.04	11/8104 (0.1%)
6	B	0.95	2/6058 (0.0%)	1.02	14/8278 (0.2%)
7	C	1.43	7/632 (1.1%)	1.33	4/856 (0.5%)
8	D	1.10	0/1122	1.05	0/1514
9	E	1.15	0/530	1.17	2/718 (0.3%)
10	F	1.10	1/1250 (0.1%)	1.07	2/1687 (0.1%)
11	G	1.07	0/760	1.28	9/1031 (0.9%)
12	H	1.16	0/543	1.19	3/741 (0.4%)
13	I	1.00	0/235	0.97	0/320
14	J	1.02	0/349	1.09	1/475 (0.2%)
15	K	0.55	0/599	0.83	1/810 (0.1%)
16	L	1.08	0/1238	1.10	5/1691 (0.3%)
17	N	1.23	1/699 (0.1%)	1.33	7/936 (0.7%)
All	All	0.94	20/25327 (0.1%)	1.02	67/34472 (0.2%)

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	1	0	3
2	2	0	1
3	3	0	19
5	A	0	28
6	B	0	20
7	C	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	6
9	E	0	6
10	F	0	12
11	G	1	16
12	H	0	9
15	K	0	2
16	L	0	3
17	N	0	21
18	R	0	17
All	All	1	166

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	92	TRP	CB-CG	16.88	1.80	1.50
3	3	93	PHE	CE1-CZ	8.69	1.53	1.37
6	B	640	CYS	CB-SG	7.67	1.95	1.82
7	C	72	GLU	CD-OE1	-7.43	1.17	1.25
3	3	93	PHE	CD2-CE2	7.38	1.54	1.39

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	732	LYS	N-CA-C	-8.11	89.10	111.00
5	A	93	LEU	CA-CB-CG	8.06	133.84	115.30
5	A	530	LEU	CA-CB-CG	7.27	132.02	115.30
6	B	486	LEU	CA-CB-CG	7.27	132.01	115.30
6	B	315	LEU	CA-CB-CG	7.21	131.88	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

5 of 166 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	182	ALA	Peptide
1	1	183	ASP	Peptide
1	1	184	PRO	Peptide
2	2	120	ASN	Peptide
3	3	49	ILE	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	1	1264	0	1230	91	1
2	2	1374	0	1329	142	0
3	3	1254	0	1221	333	1
4	4	1319	0	1283	201	13
5	A	5745	0	5595	1661	0
6	B	5848	0	5655	1449	1
7	C	619	0	608	236	0
8	D	1095	0	1112	226	0
9	E	520	0	528	150	0
10	F	1221	0	1246	289	0
11	G	740	0	709	297	7
12	H	529	0	514	117	0
13	I	229	0	252	58	0
14	J	338	0	340	80	0
15	K	593	0	619	65	1
16	L	1203	0	1213	326	13
17	N	685	0	671	448	7
18	R	265	0	67	77	0
19	M	22	0	18	11	0
19	O	23	0	21	14	0
19	P	23	0	21	0	0
19	Q	23	0	21	11	0
19	S	23	0	20	1	0
19	T	23	0	21	8	0
19	U	23	0	21	9	0
19	V	23	0	21	3	0
19	W	23	0	21	17	0
19	X	23	0	21	7	0
19	Y	23	0	21	1	0
19	Z	23	0	20	20	0
19	a	23	0	19	0	0
20	1	644	0	429	113	2
20	2	658	0	480	160	0
20	3	548	0	326	115	0
20	4	699	0	454	157	0
20	A	2777	0	2599	1120	1
20	B	2372	0	2285	808	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	F	130	0	86	27	0
20	G	51	0	40	6	0
20	H	65	0	71	19	0
20	I	115	0	106	26	0
20	J	202	0	169	99	0
20	K	210	0	177	44	2
20	L	202	0	158	40	0
20	R	122	0	123	17	0
21	1	70	0	92	15	0
21	2	105	0	138	15	1
21	3	35	0	46	3	0
21	4	35	0	46	0	0
21	A	1153	0	1505	397	0
21	B	25	0	23	1	0
21	K	35	0	45	6	0
21	L	35	0	46	3	0
21	R	70	0	91	24	0
22	3	40	0	54	21	0
22	A	240	0	323	250	0
22	B	320	0	432	225	0
22	I	40	0	54	47	0
22	L	80	0	105	61	0
23	A	33	0	46	12	0
23	B	33	0	46	33	0
24	B	49	0	71	30	0
25	B	8	0	0	18	0
25	C	16	0	0	9	0
26	B	23	0	0	2	0
All	All	36379	0	35124	8371	25

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 117.

The worst 5 of 8371 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)
4:4:160:MET:SD	20:4:1201:CLA:HBB1	1.28	1.66
20:A:1776:CLA:H92	22:A:1805:BCR:C37	1.17	1.58
6:B:25:ILE:HG21	22:L:1169:BCR:C29	1.11	1.58
5:A:51:THR:HG21	20:A:1795:CLA:CBB	1.24	1.57
21:A:7036:LMU:H82	21:A:7036:LMU:C2	1.34	1.57

The worst 5 of 25 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)
11:G:31:MET:CE	17:N:85:TRP:NE1[2_546]	0.92	1.28
4:4:130:GLU:C	16:L:159:TYR:OH[1_655]	1.18	1.02
11:G:31:MET:CE	17:N:85:TRP:CE2[2_546]	1.19	1.01
20:1:1193:CLA:O2D	20:K:1142:CLA:O2A[1_654]	1.34	0.86
4:4:130:GLU:CA	16:L:159:TYR:OH[1_655]	1.43	0.77

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	1	161/241 (67%)	83 (52%)	43 (27%)	35 (22%)	0	0
2	2	174/269 (65%)	88 (51%)	56 (32%)	30 (17%)	0	1
3	3	156/276 (56%)	78 (50%)	43 (28%)	35 (22%)	0	0
4	4	164/251 (65%)	79 (48%)	47 (29%)	38 (23%)	0	0
5	A	726/758 (96%)	334 (46%)	200 (28%)	192 (26%)	0	0
6	B	731/734 (100%)	361 (49%)	189 (26%)	181 (25%)	0	0
7	C	79/81 (98%)	23 (29%)	29 (37%)	27 (34%)	0	0
8	D	136/212 (64%)	48 (35%)	42 (31%)	46 (34%)	0	0
9	E	63/143 (44%)	29 (46%)	14 (22%)	20 (32%)	0	0
10	F	152/231 (66%)	67 (44%)	44 (29%)	41 (27%)	0	0
11	G	93/167 (56%)	35 (38%)	28 (30%)	30 (32%)	0	0
12	H	67/144 (46%)	28 (42%)	15 (22%)	24 (36%)	0	0
13	I	28/40 (70%)	10 (36%)	11 (39%)	7 (25%)	0	0
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	0
15	K	82/131 (63%)	49 (60%)	15 (18%)	18 (22%)	0	0
16	L	159/216 (74%)	66 (42%)	47 (30%)	46 (29%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	N	83/170 (49%)	22 (26%)	19 (23%)	42 (51%)	0 0
All	All	3094/4108 (75%)	1419 (46%)	853 (28%)	822 (27%)	0 0

5 of 822 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	29	LEU
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU

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	1	127/190 (67%)	102 (80%)	25 (20%)	1 5
2	2	140/216 (65%)	107 (76%)	33 (24%)	1 3
3	3	120/215 (56%)	82 (68%)	38 (32%)	0 1
4	4	138/201 (69%)	103 (75%)	35 (25%)	0 2
5	A	592/618 (96%)	392 (66%)	200 (34%)	0 1
6	B	598/600 (100%)	367 (61%)	231 (39%)	0 0
7	C	70/70 (100%)	40 (57%)	30 (43%)	0 0
8	D	118/173 (68%)	75 (64%)	43 (36%)	0 0
9	E	56/114 (49%)	37 (66%)	19 (34%)	0 1
10	F	127/190 (67%)	73 (58%)	54 (42%)	0 0
11	G	79/144 (55%)	46 (58%)	33 (42%)	0 0
12	H	57/115 (50%)	26 (46%)	31 (54%)	0 0
13	I	26/36 (72%)	18 (69%)	8 (31%)	0 1
14	J	36/39 (92%)	25 (69%)	11 (31%)	0 1
15	K	61/102 (60%)	43 (70%)	18 (30%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	L	124/169 (73%)	81 (65%)	43 (35%)	0 1
17	N	74/139 (53%)	33 (45%)	41 (55%)	0 0
All	All	2543/3331 (76%)	1650 (65%)	893 (35%)	0 1

5 of 893 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	440	ASN
17	N	73	ASP
7	C	37	LYS
17	N	62	SER
15	K	41	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	277	HIS
17	N	55	GLN
6	B	595	HIS
17	N	45	ASN
12	H	33	ASN

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)

26 monosaccharides 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	GLC	M	1	19	10,10,12	1.47	3 (30%)	14,14,17	2.99	9 (64%)
19	FRU	M	2	19	11,12,12	1.03	1 (9%)	10,18,18	2.30	3 (30%)
19	GLC	O	1	19	11,11,12	0.90	0	15,15,17	3.29	8 (53%)
19	FRU	O	2	19	11,12,12	1.10	1 (9%)	10,18,18	1.70	2 (20%)
19	GLC	P	1	19	11,11,12	0.98	0	15,15,17	2.39	3 (20%)
19	FRU	P	2	19	11,12,12	1.04	1 (9%)	10,18,18	0.98	0
19	GLC	Q	1	19	11,11,12	1.16	1 (9%)	15,15,17	2.07	4 (26%)
19	FRU	Q	2	19	11,12,12	0.99	1 (9%)	10,18,18	1.76	4 (40%)
19	GLC	S	1	19	11,11,12	0.42	0	15,15,17	0.98	1 (6%)
19	FRU	S	2	21,19	11,12,12	0.65	0	10,18,18	1.11	0
19	GLC	T	1	19	11,11,12	1.05	1 (9%)	15,15,17	1.46	2 (13%)
19	FRU	T	2	19	11,12,12	1.94	4 (36%)	10,18,18	2.78	4 (40%)
19	GLC	U	1	19	11,11,12	1.02	1 (9%)	15,15,17	2.43	5 (33%)
19	FRU	U	2	19	11,12,12	0.95	0	10,18,18	1.53	2 (20%)
19	GLC	V	1	19	11,11,12	1.51	2 (18%)	15,15,17	1.79	4 (26%)
19	FRU	V	2	19	11,12,12	0.90	0	10,18,18	1.97	5 (50%)
19	GLC	W	1	19	11,11,12	1.27	2 (18%)	15,15,17	2.73	8 (53%)
19	FRU	W	2	19	11,12,12	1.18	2 (18%)	10,18,18	2.04	2 (20%)
19	GLC	X	1	19	11,11,12	1.17	1 (9%)	15,15,17	1.64	4 (26%)
19	FRU	X	2	19	11,12,12	1.54	2 (18%)	10,18,18	2.34	4 (40%)
19	GLC	Y	1	19	11,11,12	1.08	0	15,15,17	3.33	7 (46%)
19	FRU	Y	2	19	11,12,12	1.14	0	10,18,18	2.25	4 (40%)
19	GLC	Z	1	19	11,11,12	1.70	2 (18%)	15,15,17	4.23	8 (53%)
19	FRU	Z	2	21,19	11,12,12	1.05	1 (9%)	10,18,18	2.32	3 (30%)
19	GLC	a	1	19	11,11,12	1.02	0	15,15,17	1.34	3 (20%)
19	FRU	a	2	19,12	11,12,12	1.07	0	10,18,18	2.13	3 (30%)

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	GLC	M	1	19	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FRU	M	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	O	1	19	-	1/2/19/22	0/1/1/1
19	FRU	O	2	19	1/1/4/4	4/5/24/24	0/1/1/1
19	GLC	P	1	19	-	2/2/19/22	0/1/1/1
19	FRU	P	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	Q	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Q	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	S	1	19	-	1/2/19/22	0/1/1/1
19	FRU	S	2	21,19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	T	1	19	-	2/2/19/22	0/1/1/1
19	FRU	T	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	U	1	19	-	2/2/19/22	0/1/1/1
19	FRU	U	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	V	1	19	-	0/2/19/22	0/1/1/1
19	FRU	V	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	W	1	19	-	1/2/19/22	0/1/1/1
19	FRU	W	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	X	1	19	-	2/2/19/22	0/1/1/1
19	FRU	X	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	Y	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Y	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	Z	1	19	-	0/2/19/22	0/1/1/1
19	FRU	Z	2	21,19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	a	1	19	-	2/2/19/22	0/1/1/1
19	FRU	a	2	19,12	1/1/4/4	2/5/24/24	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	1	GLC	O5-C1	-3.89	1.37	1.43
19	T	2	FRU	O5-C2	-3.79	1.37	1.43
19	V	1	GLC	O5-C5	-2.74	1.38	1.43
19	M	1	GLC	O5-C5	-2.71	1.38	1.43
19	V	1	GLC	O5-C1	-2.68	1.39	1.43

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	1	GLC	C1-O5-C5	-11.58	96.66	112.19
19	P	1	GLC	C1-O5-C5	7.80	122.64	112.19
19	Y	1	GLC	C1-O5-C5	7.58	122.35	112.19
19	T	2	FRU	O1-C1-C2	-6.73	96.79	111.67
19	M	1	GLC	C1-C2-C3	6.70	119.40	109.64

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	M	2	FRU	C2
19	O	2	FRU	C2
19	P	2	FRU	C2
19	Q	2	FRU	C2
19	S	2	FRU	C2

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	O	2	FRU	O1-C1-C2-C3
19	O	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-O5

There are no ring outliers.

21 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	M	2	FRU	7	0
19	O	2	FRU	14	0
19	T	2	FRU	8	0
19	X	1	GLC	7	0
19	Y	1	GLC	1	0
19	S	1	GLC	1	0
19	X	2	FRU	7	0
19	W	1	GLC	13	0
19	O	1	GLC	5	0
19	Q	1	GLC	10	0
19	M	1	GLC	10	0
19	V	1	GLC	3	0
19	Z	1	GLC	7	0
19	V	2	FRU	3	0
19	Q	2	FRU	9	0

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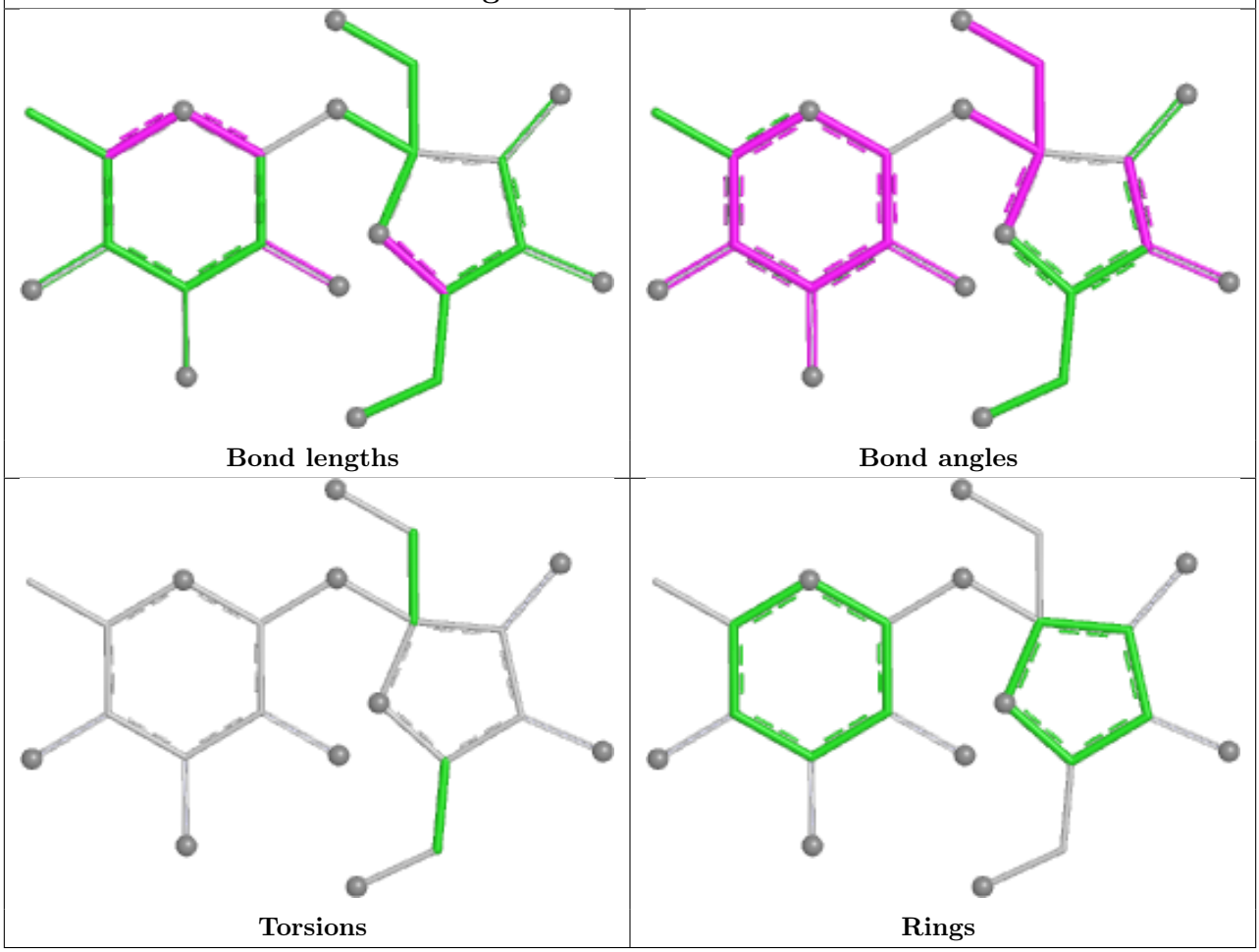
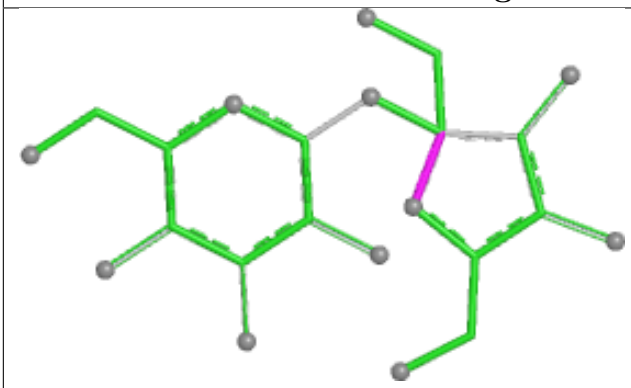
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Z	2	FRU	18	0
19	U	2	FRU	9	0
19	Y	2	FRU	1	0
19	T	1	GLC	7	0
19	U	1	GLC	6	0
19	W	2	FRU	15	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

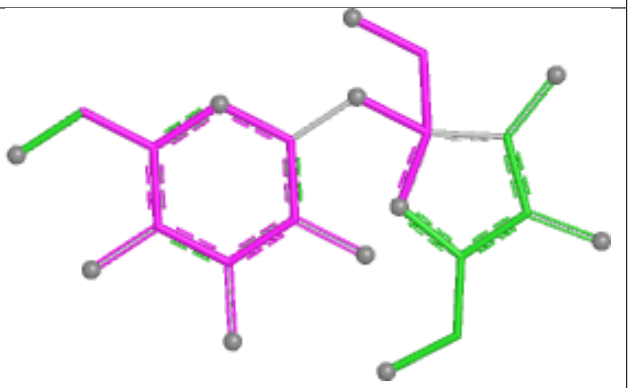
Oligosaccharide Chain M



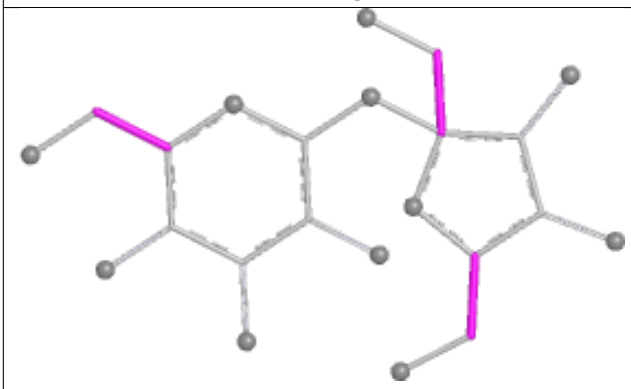
Oligosaccharide Chain O



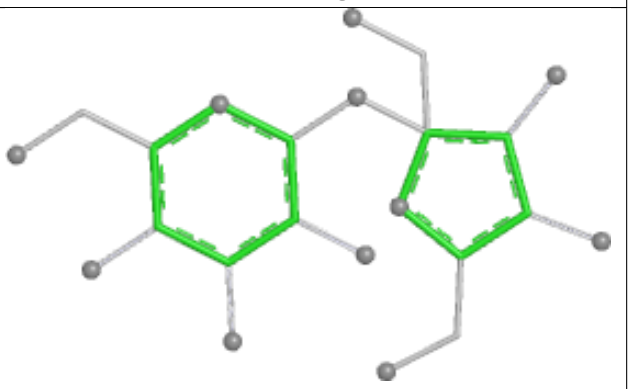
Bond lengths



Bond angles

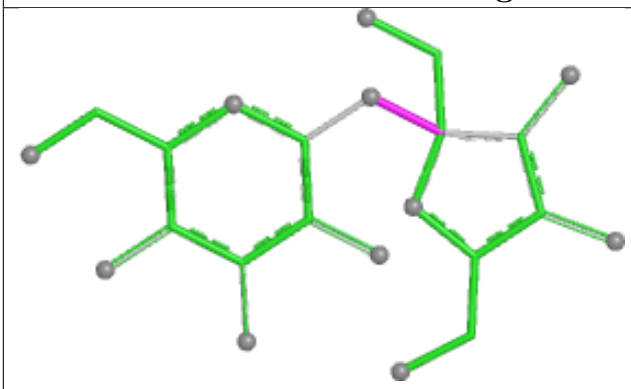


Torsions

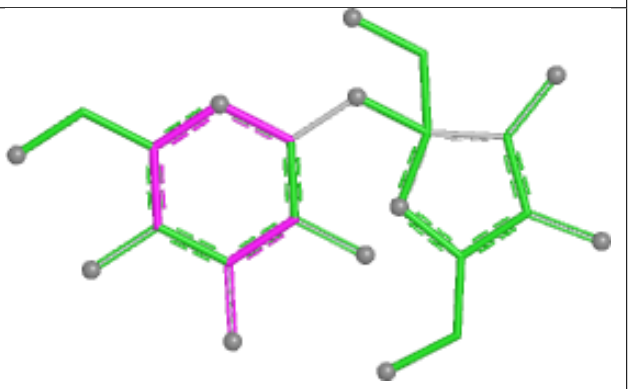


Rings

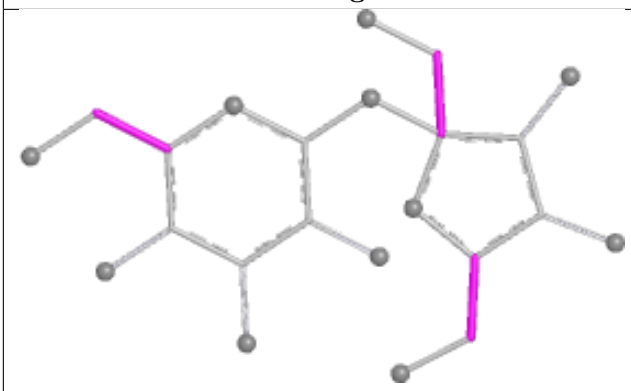
Oligosaccharide Chain P



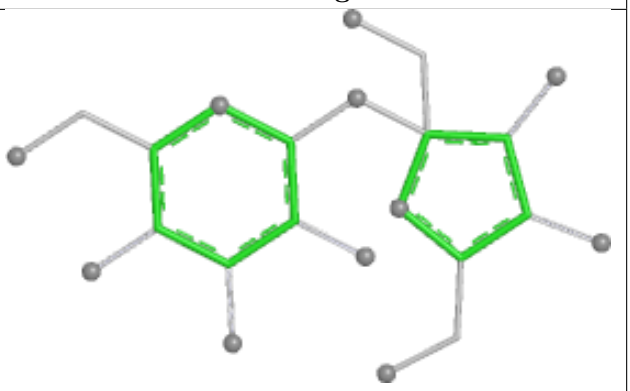
Bond lengths



Bond angles

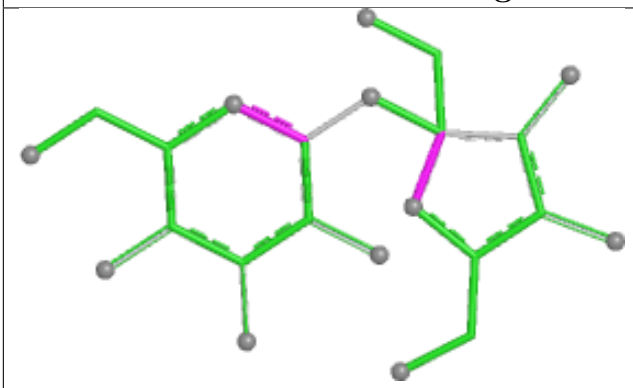


Torsions

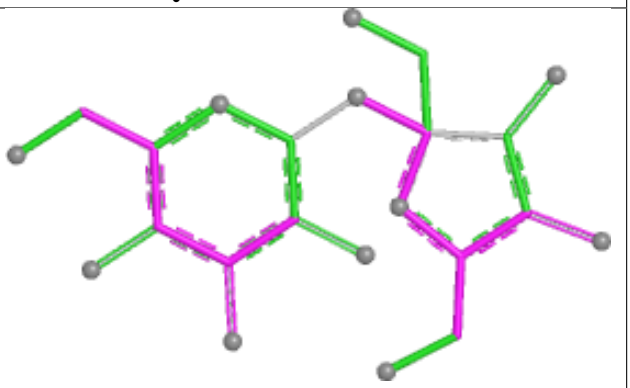


Rings

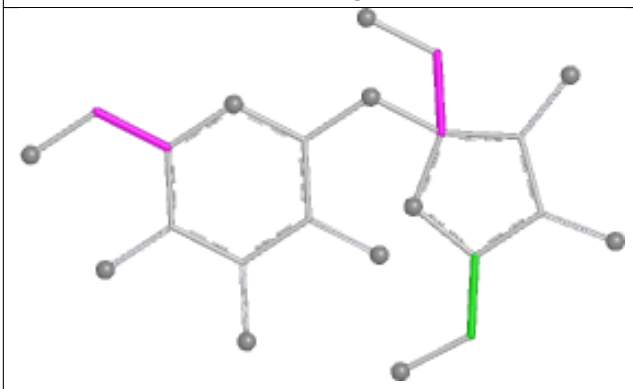
Oligosaccharide Chain Q



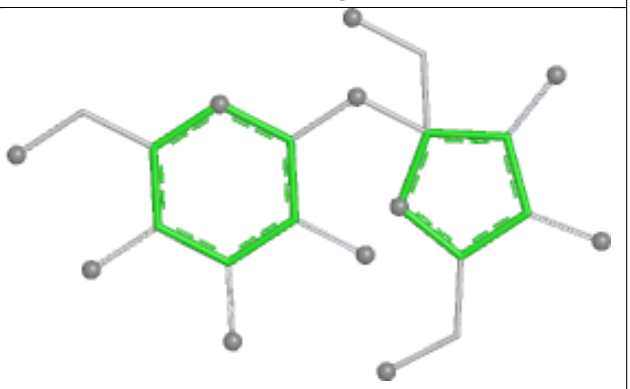
Bond lengths



Bond angles

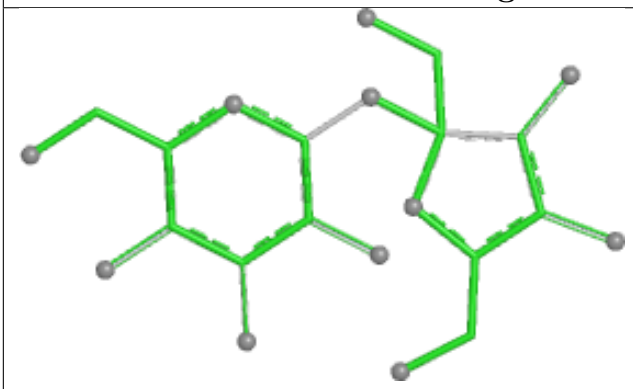


Torsions

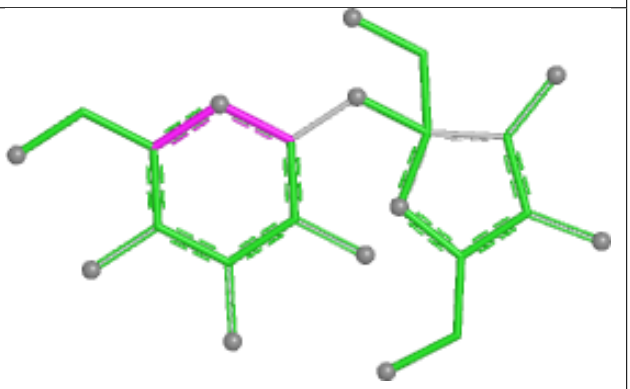


Rings

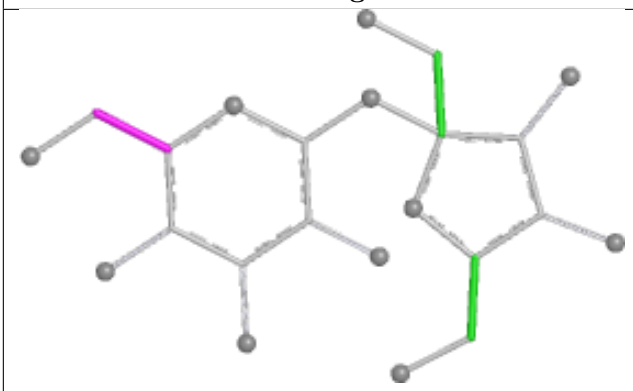
Oligosaccharide Chain S



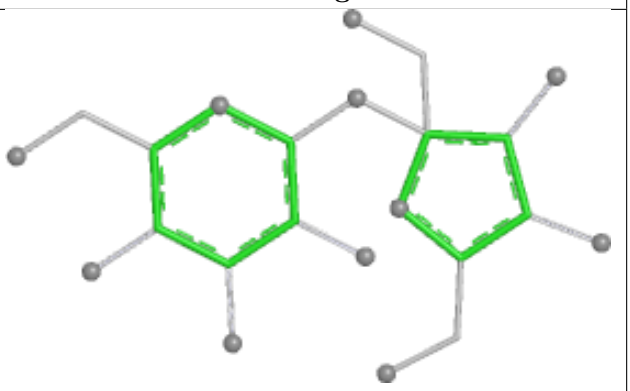
Bond lengths



Bond angles

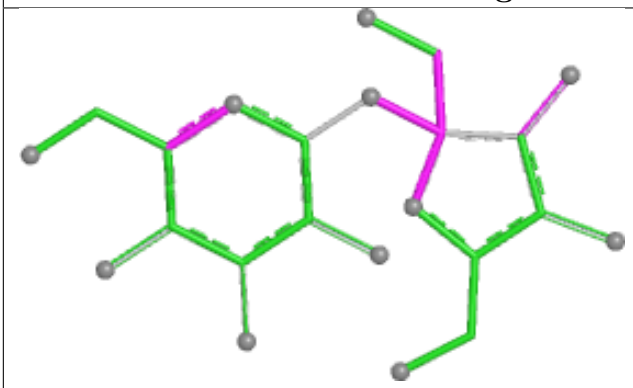


Torsions

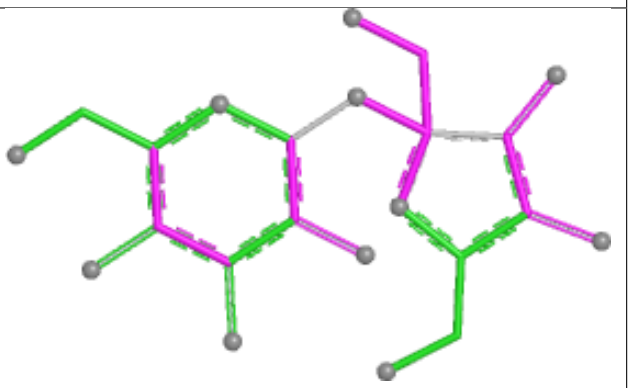


Rings

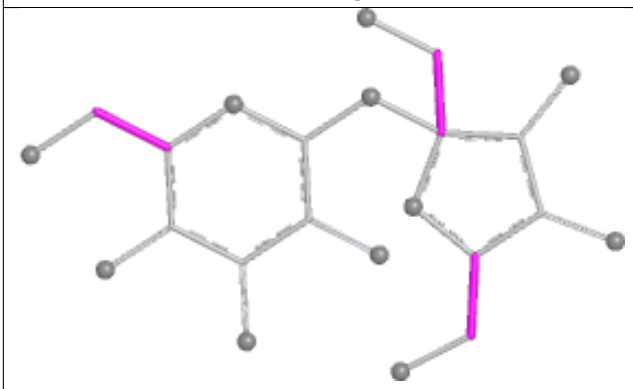
Oligosaccharide Chain T



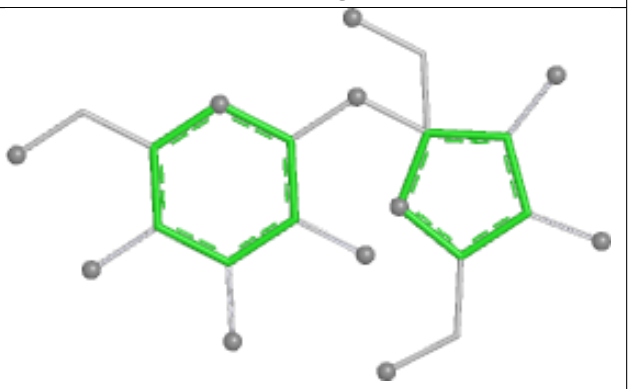
Bond lengths



Bond angles

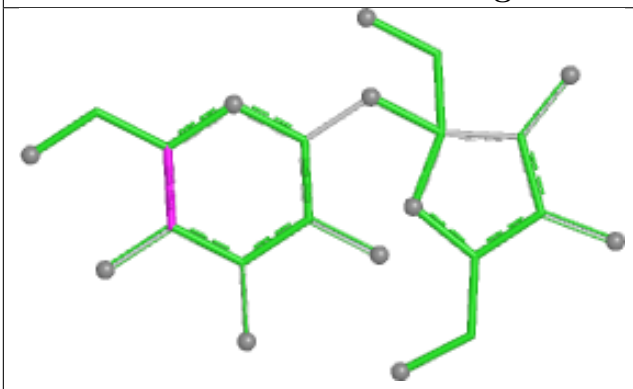


Torsions

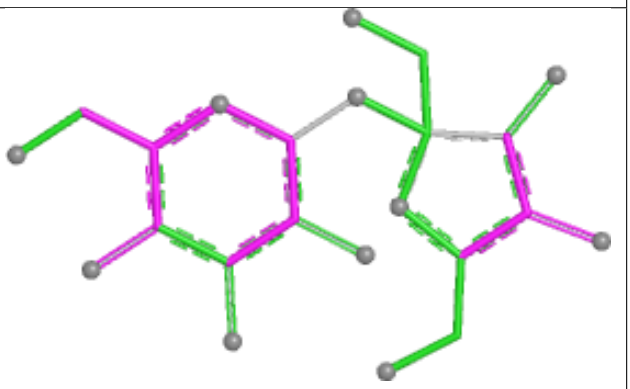


Rings

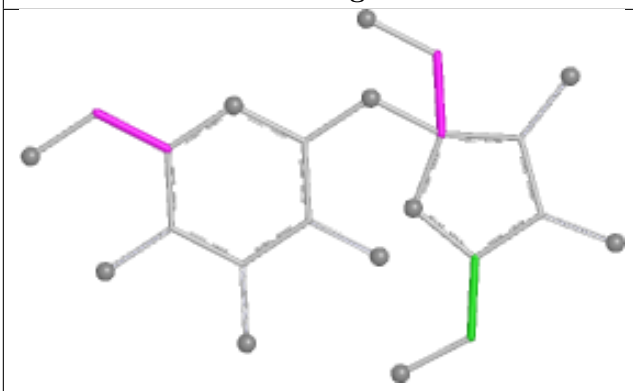
Oligosaccharide Chain U



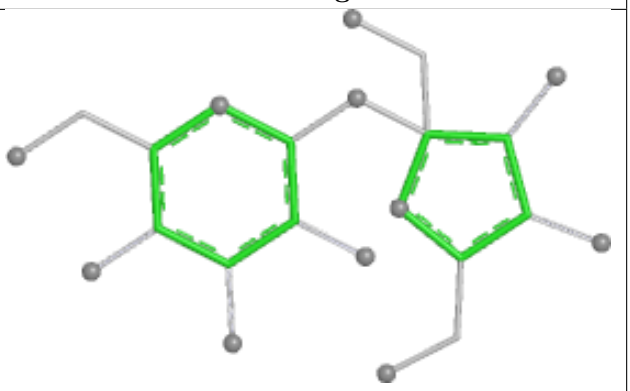
Bond lengths



Bond angles

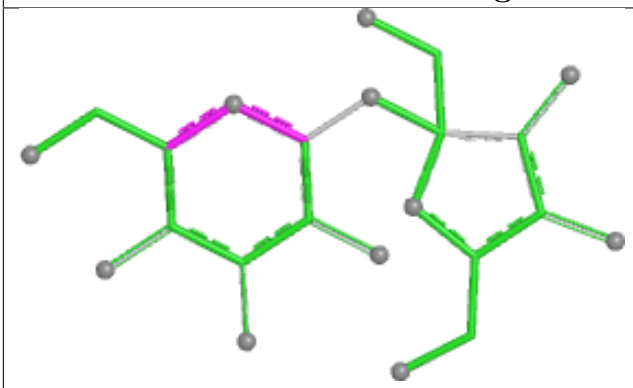


Torsions

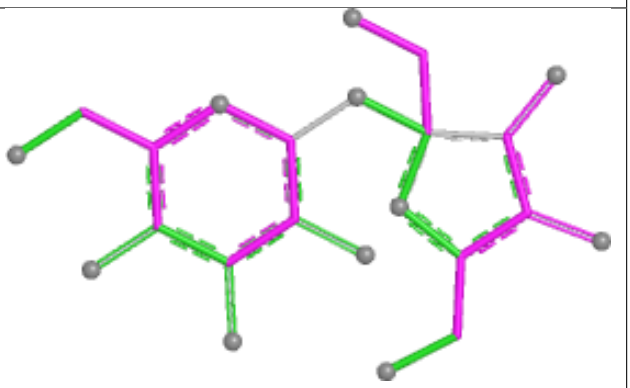


Rings

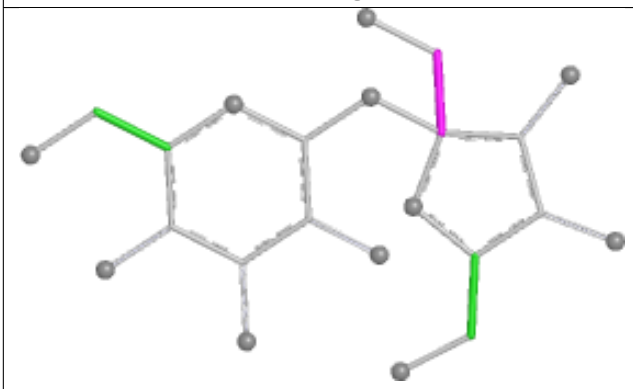
Oligosaccharide Chain V



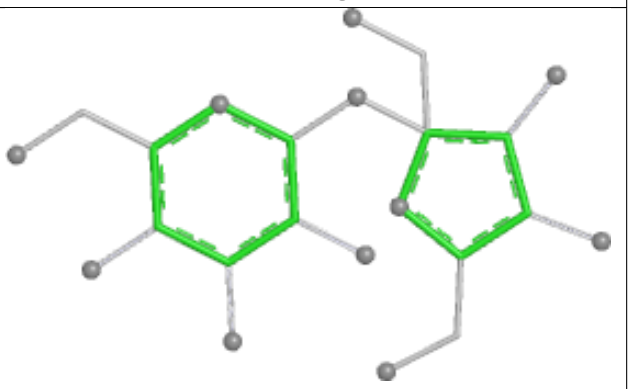
Bond lengths



Bond angles

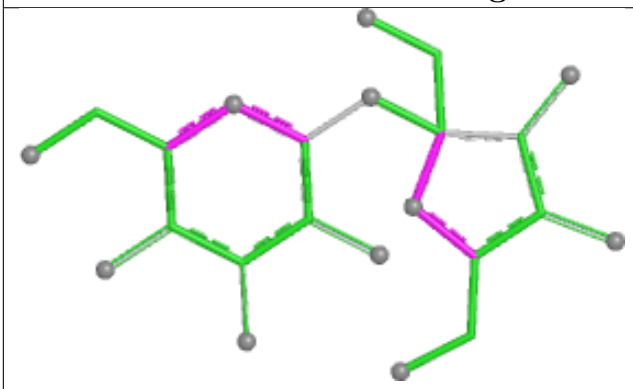


Torsions

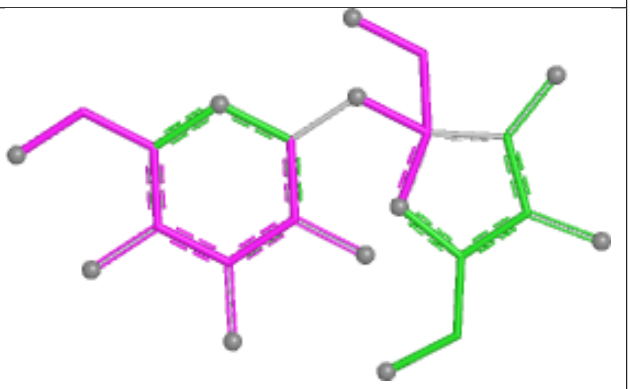


Rings

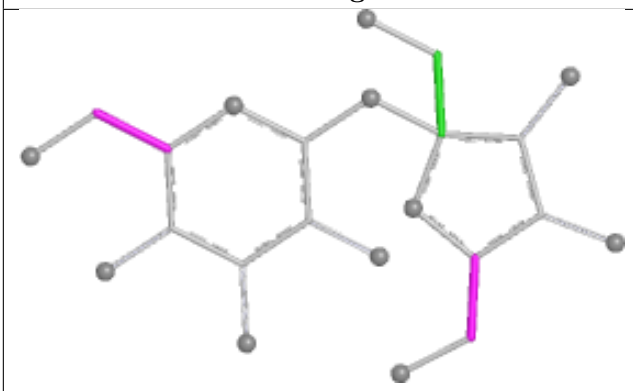
Oligosaccharide Chain W



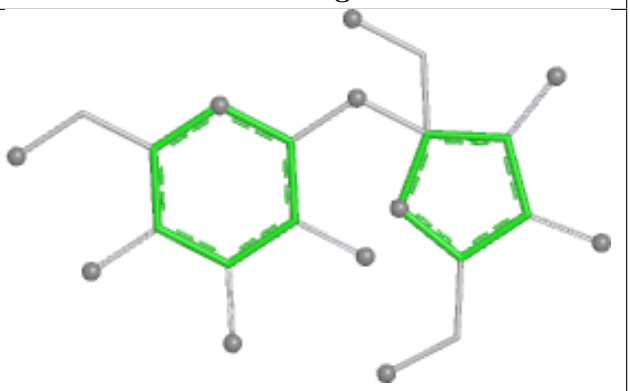
Bond lengths



Bond angles

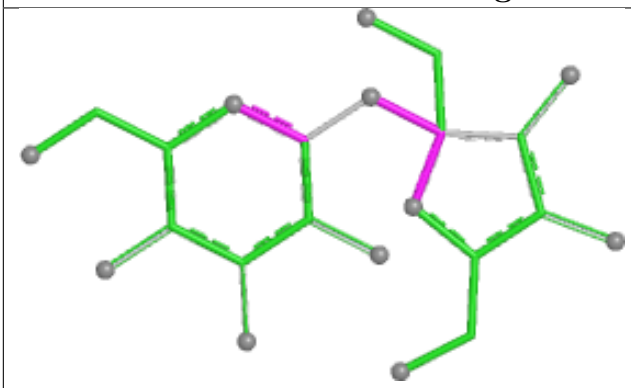


Torsions

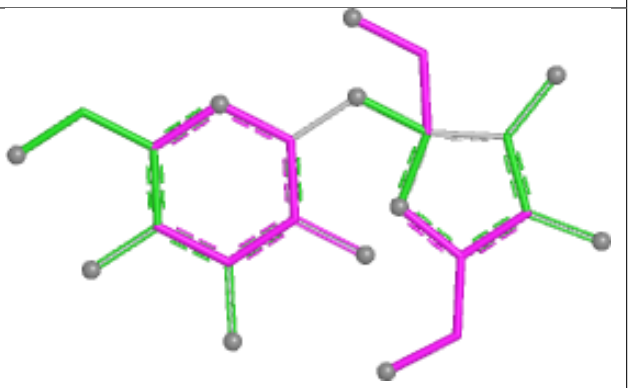


Rings

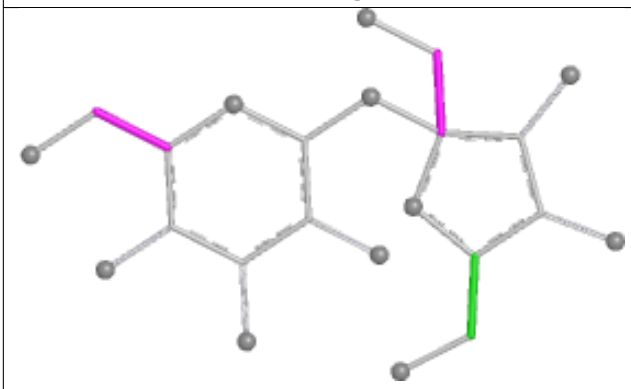
Oligosaccharide Chain X



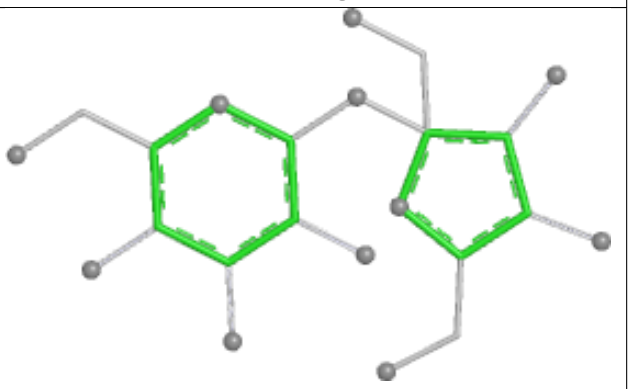
Bond lengths



Bond angles

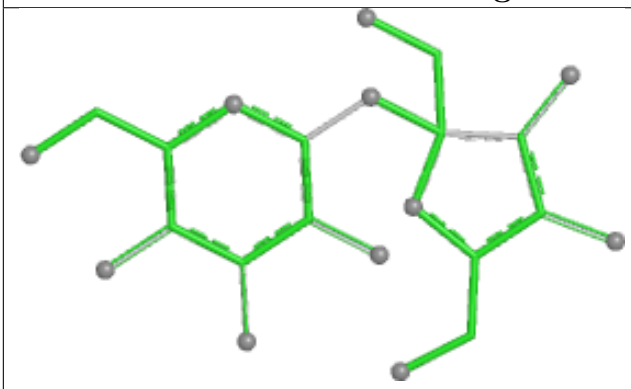


Torsions

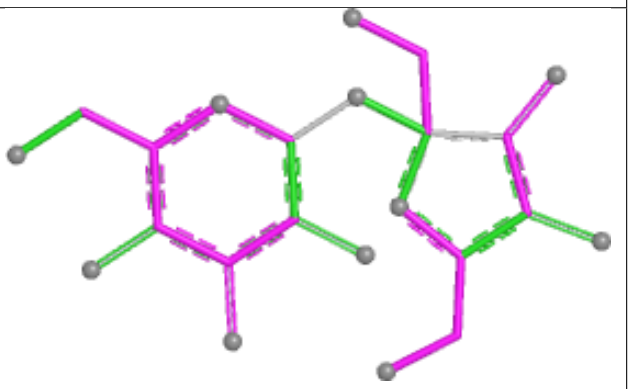


Rings

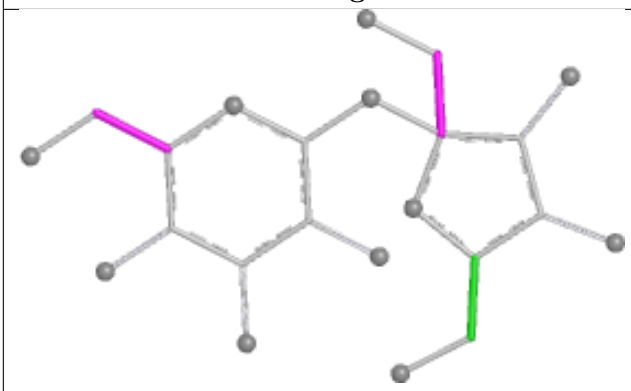
Oligosaccharide Chain Y



Bond lengths



Bond angles



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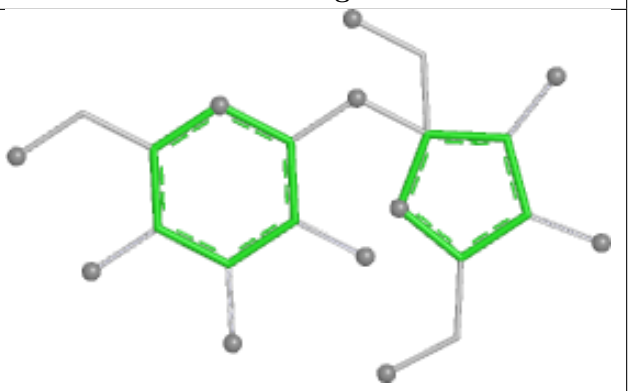
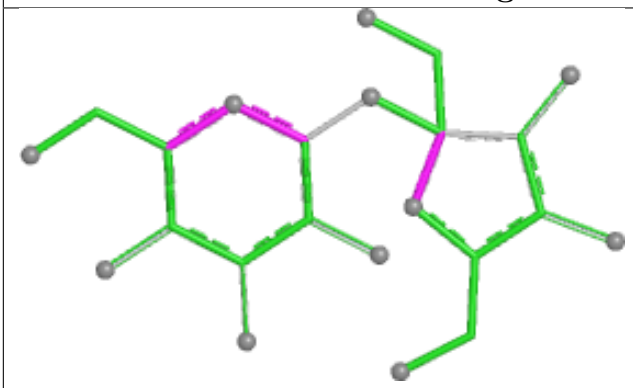
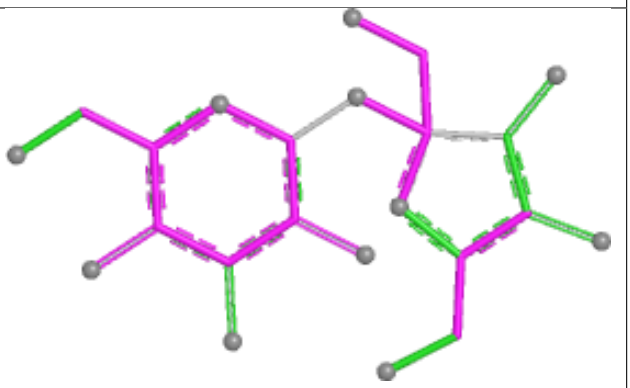


Rings

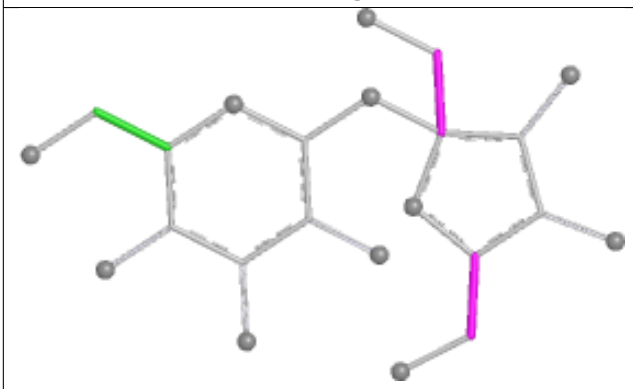
Oligosaccharide Chain Z



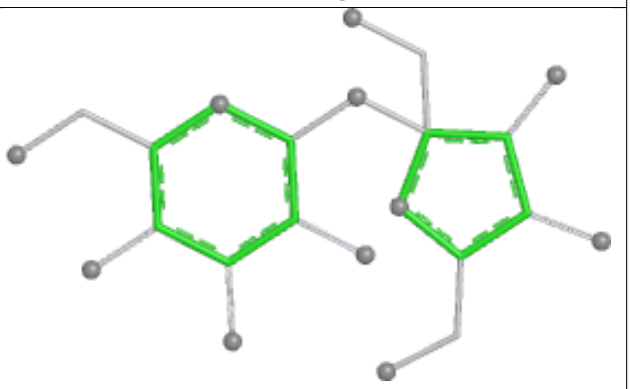
Bond lengths



Bond angles

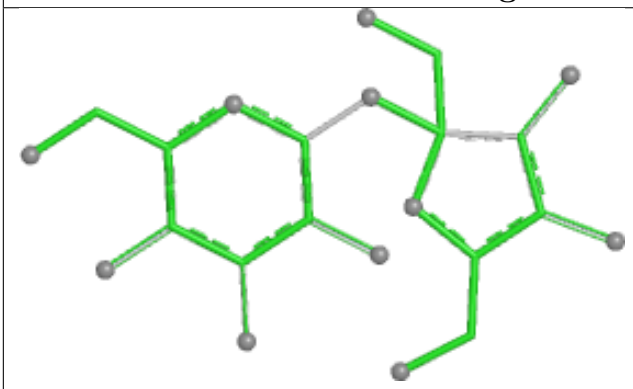


Torsions

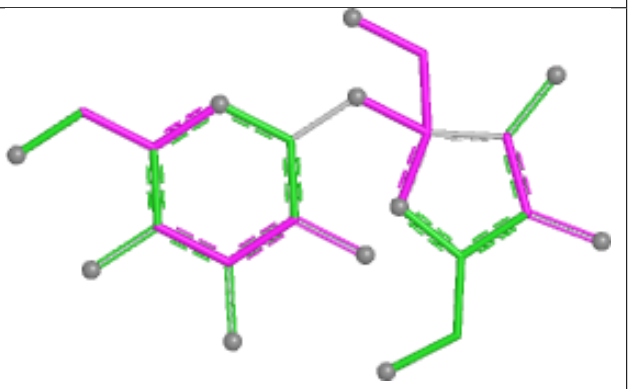


Rings

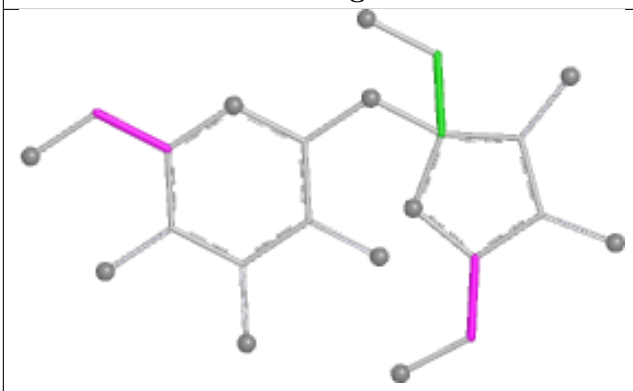
Oligosaccharide Chain a



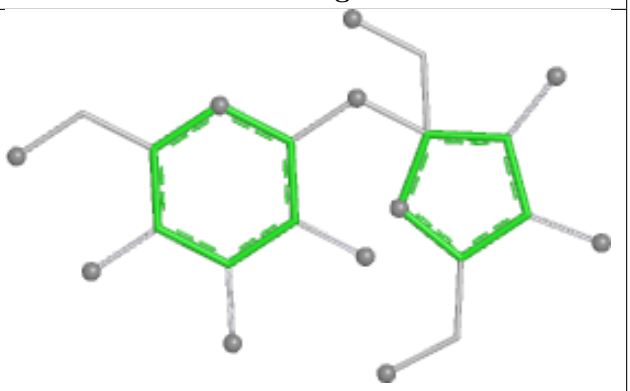
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 243 ligands modelled in this entry, 1 is unknown - leaving 242 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	B	1749	-	59,69,73	2.12	13 (22%)	69,108,113	2.54	22 (31%)
20	CLA	R	1054	-	55,65,73	2.34	11 (20%)	64,103,113	2.69	22 (34%)
21	LMU	3	7005	-	36,36,36	0.41	0	47,47,47	0.69	1 (2%)
20	CLA	B	1760	-	48,58,73	2.56	11 (22%)	56,95,113	2.40	23 (41%)
21	LMU	A	7039	-	36,36,36	0.98	2 (5%)	47,47,47	2.60	13 (27%)
21	LMU	1	1202	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
20	CLA	B	1750	-	48,58,73	2.34	11 (22%)	56,95,113	2.77	20 (35%)
20	CLA	2	1212	-	49,59,73	2.33	12 (24%)	56,96,113	2.66	18 (32%)
20	CLA	J	1044	20	59,69,73	2.27	20 (33%)	69,108,113	2.73	28 (40%)
20	CLA	A	1760	-	53,63,73	2.35	13 (24%)	62,101,113	2.34	20 (32%)
20	CLA	A	1773	-	50,60,73	2.39	11 (22%)	57,97,113	2.76	20 (35%)
20	CLA	A	1797	-	63,73,73	2.05	12 (19%)	74,113,113	2.35	18 (24%)
20	CLA	A	1764	5	63,73,73	2.11	12 (19%)	74,113,113	2.63	25 (33%)
20	CLA	A	1817	-	45,54,73	2.88	14 (31%)	55,90,113	4.23	29 (52%)
20	CLA	4	4007	-	50,60,73	2.41	12 (24%)	57,97,113	2.70	20 (35%)
20	CLA	B	1751	-	44,54,73	2.48	9 (20%)	51,90,113	3.06	17 (33%)
21	LMU	A	7036	-	35,35,36	1.20	4 (11%)	46,46,47	2.36	15 (32%)
22	BCR	A	1804	-	41,41,41	1.67	3 (7%)	56,56,56	6.06	17 (30%)
20	CLA	B	1746	-	44,54,73	2.49	11 (25%)	51,90,113	2.77	18 (35%)
20	CLA	B	1755	-	56,66,73	2.18	12 (21%)	65,104,113	2.50	20 (30%)
23	PQN	B	1773	-	34,34,34	1.69	2 (5%)	43,45,45	1.59	6 (13%)
20	CLA	K	3009	-	63,73,73	2.15	10 (15%)	74,113,113	2.23	22 (29%)
20	CLA	B	1786	-	63,73,73	2.06	12 (19%)	74,113,113	2.54	24 (32%)
20	CLA	4	1208	4	25,32,73	2.04	8 (32%)	27,54,113	2.68	15 (55%)
20	CLA	3	3014	-	25,32,73	2.27	9 (36%)	27,54,113	3.32	17 (62%)
20	CLA	1	1195	-	33,44,73	3.48	17 (51%)	46,78,113	4.47	21 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	J	1046	-	25,32,73	2.08	9 (36%)	27,54,113	2.88	15 (55%)
20	CLA	K	1085	21	48,58,73	2.36	12 (25%)	56,95,113	2.66	18 (32%)
20	CLA	1	1188	-	45,55,73	2.43	9 (20%)	52,91,113	2.76	19 (36%)
20	CLA	B	1748	-	58,68,73	2.15	13 (22%)	68,107,113	2.38	21 (30%)
20	CLA	3	3015	-	25,32,73	2.09	7 (28%)	27,54,113	2.92	17 (62%)
20	CLA	L	1505	-	53,63,73	2.34	10 (18%)	62,101,113	2.66	18 (29%)
21	LMU	4	1210	-	36,36,36	0.86	1 (2%)	47,47,47	1.19	3 (6%)
20	CLA	4	1198	-	63,73,73	2.26	21 (33%)	74,113,113	3.45	32 (43%)
20	CLA	1	1192	-	59,69,73	2.22	14 (23%)	69,108,113	2.41	23 (33%)
20	CLA	4	1197	-	33,44,73	3.14	12 (36%)	46,78,113	4.00	22 (47%)
20	CLA	B	1757	-	63,73,73	2.25	12 (19%)	74,113,113	2.66	22 (29%)
20	CLA	F	1155	-	33,44,73	2.92	10 (30%)	46,78,113	3.25	23 (50%)
22	BCR	I	1032	-	41,41,41	2.45	8 (19%)	56,56,56	6.68	29 (51%)
20	CLA	A	1784	-	53,63,73	2.23	12 (22%)	62,101,113	2.46	20 (32%)
20	CLA	B	1758	-	63,73,73	2.12	15 (23%)	74,113,113	2.63	22 (29%)
22	BCR	B	1780	-	41,41,41	1.67	5 (12%)	56,56,56	6.07	17 (30%)
20	CLA	1	1189	-	45,55,73	2.52	11 (24%)	52,91,113	3.07	18 (34%)
21	LMU	A	7027	-	36,36,36	1.12	1 (2%)	47,47,47	1.94	14 (29%)
22	BCR	B	1777	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	19 (33%)
20	CLA	3	3001	-	25,32,73	2.21	9 (36%)	27,54,113	3.10	17 (62%)
20	CLA	B	1744	-	63,73,73	2.15	10 (15%)	74,113,113	2.20	21 (28%)
20	CLA	1	1193	-	49,59,73	2.50	14 (28%)	56,96,113	3.31	26 (46%)
20	CLA	B	1735	-	63,73,73	2.05	12 (19%)	74,113,113	2.35	18 (24%)
20	CLA	J	1045	20	53,63,73	2.32	15 (28%)	62,101,113	2.75	22 (35%)
21	LMU	A	7015	-	36,36,36	0.94	1 (2%)	47,47,47	1.36	7 (14%)
20	CLA	B	1742	-	53,63,73	2.25	14 (26%)	62,101,113	2.55	21 (33%)
22	BCR	3	1220	-	41,41,41	1.79	5 (12%)	56,56,56	6.05	22 (39%)
20	CLA	B	1764	20	43,53,73	2.63	13 (30%)	50,89,113	2.86	16 (32%)
20	CLA	A	1796	-	63,73,73	2.05	12 (19%)	74,113,113	2.35	18 (24%)
21	LMU	2	7006	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
20	CLA	3	3011	-	63,73,73	2.02	9 (14%)	74,113,113	2.16	19 (25%)
20	CLA	3	1212	-	33,44,73	2.90	10 (30%)	46,78,113	3.28	18 (39%)
20	CLA	A	1772	-	63,73,73	2.09	14 (22%)	74,113,113	2.51	25 (33%)
23	PQN	A	1802	-	34,34,34	1.80	3 (8%)	43,45,45	1.49	9 (20%)
20	CLA	B	1745	-	58,68,73	2.18	10 (17%)	68,107,113	2.20	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	A	1779	-	53,63,73	2.31	11 (20%)	62,101,113	2.55	19 (30%)
25	SF4	C	1082	7	0,12,12	-	-	-		
20	CLA	B	1754	-	52,62,73	2.30	14 (26%)	60,99,113	2.51	23 (38%)
20	CLA	A	1789	-	63,73,73	2.15	11 (17%)	74,113,113	2.62	25 (33%)
20	CLA	2	1213	-	54,64,73	2.32	11 (20%)	63,102,113	2.73	26 (41%)
20	CLA	B	1761	-	48,58,73	2.31	10 (20%)	56,95,113	2.70	22 (39%)
21	LMU	R	1056	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
22	BCR	A	1808	-	41,41,41	1.67	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	2	1219	-	25,32,73	2.09	7 (28%)	27,54,113	3.09	17 (62%)
20	CLA	A	1791	5	43,53,73	2.48	12 (27%)	50,89,113	2.71	15 (30%)
21	LMU	A	1810	-	36,36,36	0.95	1 (2%)	47,47,47	1.66	11 (23%)
20	CLA	L	1166	16	48,58,73	2.43	10 (20%)	56,95,113	2.56	19 (33%)
20	CLA	A	1759	-	48,58,73	2.29	11 (22%)	56,95,113	2.93	22 (39%)
21	LMU	A	7038	-	36,36,36	0.64	0	47,47,47	2.42	15 (31%)
20	CLA	3	3007	-	40,50,73	2.52	10 (25%)	45,85,113	2.85	20 (44%)
20	CLA	A	1767	-	63,73,73	2.13	11 (17%)	74,113,113	2.56	24 (32%)
20	CLA	A	1776	-	63,73,73	2.12	12 (19%)	74,113,113	2.42	23 (31%)
20	CLA	2	1221	-	25,32,73	2.09	7 (28%)	27,54,113	3.06	17 (62%)
20	CLA	A	1763	-	44,54,73	2.47	10 (22%)	51,90,113	2.59	20 (39%)
20	CLA	1	1191	-	33,44,73	3.10	10 (30%)	46,78,113	3.49	20 (43%)
20	CLA	B	1767	-	58,68,73	2.15	12 (20%)	68,107,113	2.80	15 (22%)
20	CLA	B	1771	-	63,73,73	2.00	11 (17%)	74,113,113	2.25	22 (29%)
25	SF4	C	1083	7	0,12,12	-	-	-		
20	CLA	1	1194	-	25,32,73	2.04	7 (28%)	27,54,113	3.01	18 (66%)
20	CLA	A	1786	-	48,58,73	2.43	10 (20%)	56,95,113	2.80	22 (39%)
20	CLA	4	1199	-	53,63,73	2.24	10 (18%)	62,101,113	2.61	20 (32%)
21	LMU	A	7019	-	36,36,36	1.03	1 (2%)	47,47,47	1.42	8 (17%)
21	LMU	A	7023	-	36,36,36	0.67	1 (2%)	47,47,47	1.96	17 (36%)
22	BCR	A	1807	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	A	1762	-	55,65,73	2.25	12 (21%)	64,103,113	2.56	21 (32%)
20	CLA	B	1743	-	63,73,73	2.07	12 (19%)	74,113,113	2.32	21 (28%)
20	CLA	2	1215	-	48,58,73	2.44	11 (22%)	56,95,113	2.43	20 (35%)
20	CLA	1	1190	-	44,54,73	2.58	12 (27%)	51,90,113	2.54	19 (37%)
20	CLA	4	1204	-	53,63,73	2.40	12 (22%)	62,101,113	2.61	22 (35%)
20	CLA	B	1737	-	63,73,73	2.13	12 (19%)	74,113,113	2.74	27 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	LMU	2	1225	-	36,36,36	0.90	1 (2%)	47,47,47	0.94	2 (4%)
21	LMU	A	7017	-	36,36,36	0.70	2 (5%)	47,47,47	2.44	15 (31%)
20	CLA	B	1787	-	63,73,73	2.16	13 (20%)	74,113,113	2.45	24 (32%)
20	CLA	A	1788	-	63,73,73	2.15	13 (20%)	74,113,113	2.35	19 (25%)
20	CLA	F	1157	20	51,61,73	2.52	17 (33%)	59,98,113	2.64	22 (37%)
20	CLA	3	1218	-	63,73,73	2.33	19 (30%)	74,113,113	3.00	23 (31%)
20	CLA	G	1099	-	49,59,73	2.49	11 (22%)	56,96,113	2.67	24 (42%)
20	CLA	A	1780	-	63,73,73	2.00	8 (12%)	74,113,113	2.20	21 (28%)
21	LMU	A	7024	-	36,36,36	0.98	2 (5%)	47,47,47	1.64	11 (23%)
20	CLA	I	1033	-	53,63,73	2.36	10 (18%)	62,101,113	2.60	20 (32%)
21	LMU	2	7003	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
20	CLA	2	1217	-	63,73,73	2.11	11 (17%)	74,113,113	2.49	18 (24%)
20	CLA	A	1798	-	53,63,73	2.29	11 (20%)	62,101,113	2.58	19 (30%)
25	SF4	B	1784	6,5	0,12,12	-	-	-		
20	CLA	A	1770	-	43,53,73	2.60	11 (25%)	50,89,113	2.46	16 (32%)
20	CLA	A	1790	20	48,58,73	2.36	10 (20%)	56,95,113	2.58	19 (33%)
20	CLA	B	1747	-	57,67,73	2.22	11 (19%)	66,105,113	2.19	21 (31%)
20	CLA	1	1201	-	25,32,73	2.30	8 (32%)	27,54,113	3.65	16 (59%)
21	LMU	A	7010	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
24	LMG	B	1783	-	49,49,55	0.96	2 (4%)	57,57,63	1.02	3 (5%)
21	LMU	A	7020	-	36,36,36	0.40	0	47,47,47	1.75	12 (25%)
21	LMU	A	7035	-	36,36,36	0.83	1 (2%)	47,47,47	1.62	8 (17%)
20	CLA	A	1815	-	53,63,73	2.40	12 (22%)	62,101,113	2.76	23 (37%)
21	LMU	A	7021	-	36,36,36	0.75	0	47,47,47	2.09	14 (29%)
21	LMU	A	7025	-	36,36,36	0.96	1 (2%)	47,47,47	1.59	10 (21%)
21	LMU	B	1782	-	26,26,36	1.04	1 (3%)	37,37,47	1.44	6 (16%)
21	LMU	A	7034	20	36,36,36	0.85	1 (2%)	47,47,47	1.25	4 (8%)
20	CLA	B	1785	-	63,73,73	2.09	14 (22%)	74,113,113	2.46	28 (37%)
20	CLA	A	1792	-	49,59,73	2.33	12 (24%)	56,96,113	2.67	18 (32%)
21	LMU	A	7033	-	36,36,36	1.02	3 (8%)	47,47,47	2.30	13 (27%)
22	BCR	A	1806	-	41,41,41	1.68	5 (12%)	56,56,56	6.07	17 (30%)
22	BCR	B	1781	-	41,41,41	2.38	16 (39%)	56,56,56	5.48	31 (55%)
20	CLA	A	1771	-	48,58,73	2.51	11 (22%)	56,95,113	2.49	23 (41%)
20	CLA	4	1202	-	25,32,73	2.17	8 (32%)	27,54,113	3.13	17 (62%)
20	CLA	A	1778	5	40,50,73	2.63	12 (30%)	45,85,113	3.05	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	1	1197	-	49,59,73	2.69	20 (40%)	56,96,113	4.05	27 (48%)
20	CLA	2	2010	-	25,32,73	2.16	8 (32%)	27,54,113	2.78	15 (55%)
20	CLA	1	1187	1	44,54,73	2.65	17 (38%)	51,90,113	3.92	28 (54%)
20	CLA	4	1203	-	25,32,73	2.14	8 (32%)	27,54,113	3.12	16 (59%)
21	LMU	A	7043	19	36,36,36	0.76	0	47,47,47	2.27	16 (34%)
20	CLA	L	1168	-	48,58,73	2.56	15 (31%)	56,95,113	3.04	20 (35%)
21	LMU	A	7031	-	36,36,36	1.09	1 (2%)	47,47,47	1.31	6 (12%)
20	CLA	3	1216	-	25,32,73	2.15	9 (36%)	27,54,113	2.90	15 (55%)
20	CLA	A	1766	-	43,53,73	2.69	11 (25%)	50,89,113	2.89	18 (36%)
20	CLA	B	1763	-	48,58,73	2.49	15 (31%)	56,95,113	2.94	22 (39%)
20	CLA	4	1200	-	48,58,73	2.55	11 (22%)	56,95,113	2.63	17 (30%)
20	CLA	B	1739	-	63,73,73	2.12	12 (19%)	74,113,113	2.49	22 (29%)
20	CLA	A	1801	-	53,63,73	2.41	11 (20%)	62,101,113	2.57	22 (35%)
20	CLA	B	1765	20	43,53,73	2.57	11 (25%)	50,89,113	2.82	19 (38%)
20	CLA	B	1756	-	63,73,73	2.06	12 (19%)	74,113,113	2.35	18 (24%)
22	BCR	L	1170	20	41,41,41	2.74	18 (43%)	56,56,56	6.57	27 (48%)
20	CLA	B	1762	-	63,73,73	2.16	14 (22%)	74,113,113	2.67	23 (31%)
20	CLA	2	1214	-	25,32,73	2.10	9 (36%)	27,54,113	3.07	16 (59%)
20	CLA	4	4014	21	45,55,73	2.44	12 (26%)	52,91,113	2.66	16 (30%)
20	CLA	A	1811	-	63,73,73	2.12	13 (20%)	74,113,113	2.35	20 (27%)
20	CLA	2	1227	-	25,32,73	2.31	12 (48%)	27,54,113	3.27	18 (66%)
21	LMU	A	1809	-	36,36,36	0.94	0	47,47,47	1.40	6 (12%)
20	CLA	A	1794	-	45,55,73	2.42	12 (26%)	52,91,113	2.67	16 (30%)
20	CLA	A	1783	-	63,73,73	2.04	11 (17%)	74,113,113	2.51	26 (35%)
20	CLA	4	1209	-	44,54,73	2.60	18 (40%)	51,90,113	2.77	20 (39%)
20	CLA	A	1768	-	52,62,73	2.34	12 (23%)	60,99,113	2.37	16 (26%)
20	CLA	A	1761	-	63,73,73	2.08	12 (19%)	74,113,113	2.40	22 (29%)
20	CLA	1	1199	-	25,32,73	2.18	8 (32%)	27,54,113	3.12	17 (62%)
21	LMU	A	7030	-	36,36,36	0.89	1 (2%)	47,47,47	2.30	16 (34%)
20	CLA	B	1770	-	63,73,73	2.09	11 (17%)	74,113,113	2.51	24 (32%)
20	CLA	2	1222	2	48,58,73	2.34	10 (20%)	56,95,113	2.79	18 (32%)
20	CLA	2	1224	-	63,73,73	2.13	12 (19%)	74,113,113	2.58	21 (28%)
20	CLA	A	1799	-	48,58,73	2.45	9 (18%)	56,95,113	2.49	17 (30%)
21	LMU	K	1086	20	36,36,36	0.75	0	47,47,47	2.28	12 (25%)
20	CLA	B	1753	-	63,73,73	2.64	24 (38%)	74,113,113	2.65	20 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	4	1196	-	53,63,73	2.25	12 (22%)	62,101,113	2.54	19 (30%)
20	CLA	B	1741	-	53,62,73	2.67	12 (22%)	65,100,113	2.96	24 (36%)
20	CLA	3	1215	-	25,32,73	2.12	9 (36%)	27,54,113	3.14	16 (59%)
20	CLA	3	1213	-	25,32,73	2.37	11 (44%)	27,54,113	3.56	17 (62%)
20	CLA	3	1217	-	25,32,73	2.24	7 (28%)	27,54,113	3.38	16 (59%)
20	CLA	A	1816	-	53,63,73	2.61	19 (35%)	62,101,113	3.61	27 (43%)
20	CLA	3	1214	-	25,32,73	2.14	9 (36%)	27,54,113	3.12	16 (59%)
20	CLA	3	1219	-	63,73,73	2.05	12 (19%)	74,113,113	2.35	18 (24%)
20	CLA	A	1785	-	63,73,73	2.13	13 (20%)	74,113,113	2.53	26 (35%)
20	CLA	B	1752	-	53,63,73	2.38	12 (22%)	62,101,113	2.45	17 (27%)
21	LMU	A	7013	-	36,36,36	0.45	0	47,47,47	1.65	9 (19%)
20	CLA	3	3008	-	48,58,73	2.38	14 (29%)	56,95,113	2.95	23 (41%)
20	CLA	4	4003	-	25,32,73	2.09	7 (28%)	27,54,113	2.75	15 (55%)
22	BCR	B	1775	-	41,41,41	1.69	5 (12%)	56,56,56	6.05	19 (33%)
22	BCR	B	1774	-	41,41,41	1.69	5 (12%)	56,56,56	6.05	19 (33%)
21	LMU	A	7037	-	36,36,36	0.89	2 (5%)	47,47,47	3.11	22 (46%)
20	CLA	1	1200	-	49,59,73	2.65	19 (38%)	56,96,113	3.35	29 (51%)
20	CLA	4	1207	-	33,44,73	2.84	10 (30%)	46,78,113	3.77	20 (43%)
21	LMU	A	7047	-	36,36,36	1.12	1 (2%)	47,47,47	1.37	4 (8%)
20	CLA	1	1196	1	33,44,73	2.96	11 (33%)	46,78,113	3.44	18 (39%)
20	CLA	A	1765	-	53,63,73	2.27	11 (20%)	62,101,113	2.70	24 (38%)
20	CLA	2	1218	20	63,73,73	2.12	11 (17%)	74,113,113	2.40	22 (29%)
20	CLA	A	1813	-	63,73,73	2.21	13 (20%)	74,113,113	2.53	20 (27%)
20	CLA	B	1766	-	49,59,73	2.46	10 (20%)	56,96,113	2.72	19 (33%)
20	CLA	L	1167	22	45,55,73	2.39	10 (22%)	52,91,113	3.10	24 (46%)
20	CLA	A	1795	-	49,59,73	2.33	12 (24%)	56,96,113	2.66	18 (32%)
22	BCR	B	1779	-	41,41,41	2.48	12 (29%)	56,56,56	6.23	32 (57%)
20	CLA	A	1800	-	63,73,73	2.08	13 (20%)	74,113,113	2.49	23 (31%)
21	LMU	A	7022	-	36,36,36	0.69	0	47,47,47	2.19	17 (36%)
20	CLA	B	1769	-	45,55,73	2.47	14 (31%)	52,91,113	2.63	17 (32%)
22	BCR	A	1805	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	18 (32%)
21	LMU	A	7032	-	36,36,36	0.98	3 (8%)	47,47,47	2.76	20 (42%)
21	LMU	A	7040	-	36,36,36	0.96	3 (8%)	47,47,47	2.48	13 (27%)
20	CLA	3	3002	-	25,32,73	2.16	8 (32%)	27,54,113	2.96	16 (59%)
20	CLA	B	1759	-	63,73,73	2.16	14 (22%)	74,113,113	2.64	20 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	BCR	B	1778	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	B	1736	-	43,53,73	2.57	11 (25%)	50,89,113	2.93	17 (34%)
20	CLA	A	1787	-	63,73,73	2.13	10 (15%)	74,113,113	2.29	22 (29%)
21	LMU	R	1057	-	36,36,36	1.15	2 (5%)	47,47,47	2.46	15 (31%)
20	CLA	4	1201	-	50,60,73	2.92	24 (48%)	57,97,113	3.81	34 (59%)
21	LMU	L	1171	-	36,36,36	0.99	3 (8%)	47,47,47	1.49	9 (19%)
20	CLA	A	1812	-	63,73,73	2.11	13 (20%)	74,113,113	2.28	19 (25%)
20	CLA	K	1142	-	43,53,73	2.47	12 (27%)	50,89,113	2.70	15 (30%)
21	LMU	A	7009	-	35,35,36	0.41	0	46,46,47	0.71	1 (2%)
20	CLA	2	1223	-	48,58,73	2.49	11 (22%)	56,95,113	2.84	18 (32%)
20	CLA	A	1777	-	49,59,73	2.43	12 (24%)	56,96,113	2.67	20 (35%)
20	CLA	B	1768	-	63,73,73	2.01	11 (17%)	74,113,113	2.37	18 (24%)
20	CLA	4	1205	-	25,32,73	2.11	8 (32%)	27,54,113	3.11	17 (62%)
20	CLA	B	1772	-	33,44,73	2.98	11 (33%)	46,78,113	3.71	23 (50%)
20	CLA	R	1055	-	63,73,73	2.21	12 (19%)	74,113,113	2.36	25 (33%)
22	BCR	A	1803	-	41,41,41	1.68	4 (9%)	56,56,56	6.06	18 (32%)
20	CLA	2	1216	-	25,32,73	2.18	10 (40%)	27,54,113	3.24	17 (62%)
20	CLA	K	1146	-	48,58,73	2.68	18 (37%)	56,95,113	3.05	24 (42%)
20	CLA	A	1775	-	33,44,73	2.96	11 (33%)	46,78,113	3.61	18 (39%)
20	CLA	A	1774	-	63,73,73	2.10	12 (19%)	74,113,113	2.27	23 (31%)
20	CLA	F	1156	20	39,49,73	2.57	12 (30%)	46,84,113	2.83	15 (32%)
21	LMU	A	7041	-	36,36,36	0.61	0	47,47,47	1.91	14 (29%)
20	CLA	A	1782	20	63,73,73	2.05	12 (19%)	74,113,113	2.35	18 (24%)
20	CLA	I	1031	-	58,68,73	2.20	11 (18%)	68,107,113	2.52	19 (27%)
20	CLA	2	1220	20	54,64,73	2.31	15 (27%)	63,102,113	2.69	23 (36%)
20	CLA	B	1740	6	63,73,73	1.99	10 (15%)	74,113,113	2.47	21 (28%)
21	LMU	A	7016	-	36,36,36	0.62	1 (2%)	47,47,47	1.89	11 (23%)
21	LMU	A	7042	-	36,36,36	0.47	0	47,47,47	2.08	16 (34%)
22	BCR	B	1776	-	41,41,41	1.70	5 (12%)	56,56,56	5.15	23 (41%)
22	BCR	L	1169	-	41,41,41	2.17	10 (24%)	56,56,56	5.87	20 (35%)
21	LMU	1	7004	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
20	CLA	4	1206	-	25,32,73	2.24	6 (24%)	27,54,113	3.16	18 (66%)
20	CLA	A	1781	-	63,73,73	2.05	12 (19%)	74,113,113	2.36	19 (25%)
20	CLA	H	1079	-	63,73,73	2.20	11 (17%)	74,113,113	2.44	19 (25%)
21	LMU	A	7026	19	36,36,36	1.21	3 (8%)	47,47,47	3.10	22 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	A	1769	-	52,62,73	2.20	11 (21%)	60,99,113	2.58	23 (38%)
20	CLA	B	1738	-	63,73,73	2.08	14 (22%)	74,113,113	2.71	28 (37%)
21	LMU	A	7028	-	36,36,36	0.73	2 (5%)	47,47,47	1.91	17 (36%)
20	CLA	1	1198	-	59,69,73	2.19	17 (28%)	69,108,113	2.59	23 (33%)
20	CLA	J	1043	-	59,69,73	2.12	12 (20%)	69,108,113	2.42	18 (26%)
20	CLA	A	1793	-	63,73,73	2.05	12 (19%)	74,113,113	2.36	18 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1749	-	2/2/14/20	17/33/111/115	-
20	CLA	R	1054	-	2/2/13/20	13/28/106/115	-
21	LMU	3	7005	-	-	17/21/61/61	0/2/2/2
20	CLA	B	1760	-	1/1/12/20	6/19/97/115	-
21	LMU	A	7039	-	-	14/21/61/61	0/2/2/2
21	LMU	1	1202	-	-	13/21/61/61	0/2/2/2
20	CLA	B	1750	-	1/1/12/20	6/19/97/115	-
20	CLA	2	1212	-	1/1/12/20	11/21/99/115	-
20	CLA	J	1044	20	2/2/14/20	19/33/111/115	-
20	CLA	A	1760	-	2/2/13/20	11/25/103/115	-
20	CLA	A	1773	-	1/1/12/20	10/22/100/115	-
20	CLA	A	1797	-	2/2/15/20	16/37/115/115	-
20	CLA	A	1764	5	2/2/15/20	19/37/115/115	-
20	CLA	A	1817	-	3/3/11/20	12/16/92/115	-
20	CLA	4	4007	-	1/1/12/20	8/22/100/115	-
20	CLA	B	1751	-	1/1/11/20	13/15/93/115	-
21	LMU	A	7036	-	-	14/20/60/61	0/2/2/2
22	BCR	A	1804	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1746	-	1/1/11/20	9/15/93/115	-
20	CLA	B	1755	-	2/2/13/20	15/29/107/115	-
23	PQN	B	1773	-	1/1/8/9	10/23/43/43	0/2/2/2
20	CLA	K	3009	-	2/2/15/20	19/37/115/115	-
20	CLA	B	1786	-	2/2/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	1208	4	1/1/4/20	-	-
20	CLA	3	3014	-	1/1/4/20	-	-
20	CLA	1	1195	-	1/1/9/20	-	-
20	CLA	J	1046	-	1/1/4/20	-	-
20	CLA	K	1085	21	1/1/12/20	5/19/97/115	-
20	CLA	1	1188	-	1/1/11/20	9/16/94/115	-
20	CLA	B	1748	-	2/2/14/20	13/31/109/115	-
20	CLA	3	3015	-	1/1/4/20	-	-
20	CLA	L	1505	-	2/2/13/20	13/25/103/115	-
21	LMU	4	1210	-	-	13/21/61/61	0/2/2/2
20	CLA	4	1198	-	3/3/15/20	18/37/115/115	-
20	CLA	1	1192	-	2/2/14/20	20/33/111/115	-
20	CLA	4	1197	-	1/1/9/20	-	-
20	CLA	B	1757	-	2/2/15/20	16/37/115/115	-
20	CLA	F	1155	-	1/1/9/20	-	-
22	BCR	I	1032	-	-	13/29/63/63	0/2/2/2
20	CLA	A	1784	-	2/2/13/20	9/25/103/115	-
20	CLA	B	1758	-	2/2/15/20	14/37/115/115	-
22	BCR	B	1780	-	-	14/29/63/63	0/2/2/2
20	CLA	1	1189	-	1/1/11/20	7/16/94/115	-
21	LMU	A	7027	-	-	13/21/61/61	0/2/2/2
22	BCR	B	1777	-	-	13/29/63/63	0/2/2/2
20	CLA	3	3001	-	1/1/4/20	-	-
20	CLA	B	1744	-	2/2/15/20	23/37/115/115	-
20	CLA	1	1193	-	2/2/12/20	8/21/99/115	-
20	CLA	B	1735	-	2/2/15/20	20/37/115/115	-
20	CLA	J	1045	20	2/2/13/20	13/25/103/115	-
21	LMU	A	7015	-	-	14/21/61/61	0/2/2/2
20	CLA	B	1742	-	2/2/13/20	11/25/103/115	-
22	BCR	3	1220	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1764	20	1/1/11/20	9/13/91/115	-
20	CLA	A	1796	-	2/2/15/20	15/37/115/115	-
21	LMU	2	7006	-	-	14/21/61/61	0/2/2/2
20	CLA	3	3011	-	2/2/15/20	19/37/115/115	-
20	CLA	3	1212	-	1/1/9/20	-	-
20	CLA	A	1772	-	2/2/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PQN	A	1802	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	B	1745	-	2/2/14/20	9/31/109/115	-
20	CLA	A	1779	-	2/2/13/20	9/25/103/115	-
25	SF4	C	1082	7	-	-	0/6/5/5
20	CLA	B	1754	-	1/1/12/20	6/24/102/115	-
20	CLA	A	1789	-	2/2/15/20	22/37/115/115	-
20	CLA	2	1213	-	2/2/13/20	11/27/105/115	-
20	CLA	B	1761	-	1/1/12/20	12/19/97/115	-
21	LMU	R	1056	-	-	16/21/61/61	0/2/2/2
22	BCR	A	1808	-	-	12/29/63/63	0/2/2/2
20	CLA	2	1219	-	1/1/4/20	-	-
20	CLA	A	1791	5	1/1/11/20	7/13/91/115	-
21	LMU	A	1810	-	-	13/21/61/61	0/2/2/2
20	CLA	L	1166	16	1/1/12/20	8/19/97/115	-
20	CLA	A	1759	-	1/1/12/20	4/19/97/115	-
21	LMU	A	7038	-	-	16/21/61/61	0/2/2/2
20	CLA	3	3007	-	1/1/10/20	4/10/88/115	-
20	CLA	A	1767	-	2/2/15/20	24/37/115/115	-
20	CLA	A	1776	-	2/2/15/20	13/37/115/115	-
20	CLA	2	1221	-	1/1/4/20	-	-
20	CLA	A	1763	-	1/1/11/20	7/15/93/115	-
20	CLA	1	1191	-	1/1/9/20	-	-
20	CLA	B	1767	-	2/2/14/20	16/31/109/115	-
20	CLA	B	1771	-	2/2/15/20	16/37/115/115	-
25	SF4	C	1083	7	-	-	0/6/5/5
20	CLA	1	1194	-	1/1/4/20	-	-
20	CLA	A	1786	-	1/1/12/20	3/19/97/115	-
20	CLA	4	1199	-	2/2/13/20	12/25/103/115	-
21	LMU	A	7019	-	-	15/21/61/61	0/2/2/2
21	LMU	A	7023	-	-	14/21/61/61	0/2/2/2
22	BCR	A	1807	-	-	10/29/63/63	0/2/2/2
20	CLA	A	1762	-	2/2/13/20	7/28/106/115	-
20	CLA	B	1743	-	2/2/15/20	19/37/115/115	-
20	CLA	2	1215	-	1/1/12/20	9/19/97/115	-
20	CLA	1	1190	-	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	1204	-	2/2/13/20	13/25/103/115	-
20	CLA	B	1737	-	2/2/15/20	18/37/115/115	-
21	LMU	2	1225	-	-	16/21/61/61	0/2/2/2
21	LMU	A	7017	-	-	15/21/61/61	0/2/2/2
20	CLA	B	1787	-	2/2/15/20	17/37/115/115	-
20	CLA	A	1788	-	2/2/15/20	19/37/115/115	-
20	CLA	F	1157	20	4/4/12/20	10/23/101/115	-
20	CLA	3	1218	-	2/2/15/20	19/37/115/115	-
20	CLA	G	1099	-	1/1/12/20	10/21/99/115	-
20	CLA	A	1780	-	2/2/15/20	19/37/115/115	-
21	LMU	A	7024	-	-	15/21/61/61	0/2/2/2
20	CLA	I	1033	-	2/2/13/20	9/25/103/115	-
21	LMU	2	7003	-	-	11/21/61/61	0/2/2/2
20	CLA	2	1217	-	2/2/15/20	16/37/115/115	-
20	CLA	A	1798	-	2/2/13/20	6/25/103/115	-
25	SF4	B	1784	6,5	-	-	0/6/5/5
20	CLA	A	1770	-	1/1/11/20	11/13/91/115	-
20	CLA	A	1790	20	1/1/12/20	12/19/97/115	-
20	CLA	B	1747	-	2/2/13/20	12/30/108/115	-
20	CLA	1	1201	-	1/1/4/20	-	-
21	LMU	A	7010	-	-	19/21/61/61	0/2/2/2
24	LMG	B	1783	-	-	23/44/64/70	0/1/1/1
21	LMU	A	7020	-	-	11/21/61/61	0/2/2/2
21	LMU	A	7035	-	-	14/21/61/61	0/2/2/2
20	CLA	A	1815	-	3/3/13/20	12/25/103/115	-
21	LMU	A	7021	-	-	13/21/61/61	0/2/2/2
21	LMU	A	7025	-	-	13/21/61/61	0/2/2/2
21	LMU	B	1782	-	-	4/11/51/61	0/2/2/2
21	LMU	A	7034	20	-	14/21/61/61	0/2/2/2
20	CLA	B	1785	-	2/2/15/20	16/37/115/115	-
20	CLA	A	1792	-	1/1/12/20	10/21/99/115	-
21	LMU	A	7033	-	-	13/21/61/61	0/2/2/2
22	BCR	A	1806	-	-	15/29/63/63	0/2/2/2
22	BCR	B	1781	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1771	-	1/1/12/20	9/19/97/115	-
20	CLA	4	1202	-	1/1/4/20	-	-
20	CLA	A	1778	5	1/1/10/20	2/10/88/115	-
20	CLA	1	1197	-	2/2/12/20	8/21/99/115	-
20	CLA	2	2010	-	1/1/4/20	-	-
20	CLA	1	1187	1	1/1/11/20	10/15/93/115	-
20	CLA	4	1203	-	1/1/4/20	-	-
21	LMU	A	7043	19	-	11/21/61/61	0/2/2/2
20	CLA	L	1168	-	2/2/12/20	9/19/97/115	-
21	LMU	A	7031	-	-	13/21/61/61	0/2/2/2
20	CLA	3	1216	-	1/1/4/20	-	-
20	CLA	A	1766	-	1/1/11/20	4/13/91/115	-
20	CLA	B	1763	-	1/1/12/20	8/19/97/115	-
20	CLA	4	1200	-	1/1/12/20	6/19/97/115	-
20	CLA	B	1739	-	2/2/15/20	10/37/115/115	-
20	CLA	A	1801	-	2/2/13/20	7/25/103/115	-
20	CLA	B	1765	20	1/1/11/20	7/13/91/115	-
20	CLA	B	1756	-	2/2/15/20	20/37/115/115	-
22	BCR	L	1170	20	-	12/29/63/63	0/2/2/2
20	CLA	B	1762	-	2/2/15/20	20/37/115/115	-
20	CLA	2	1214	-	1/1/4/20	-	-
20	CLA	4	4014	21	1/1/11/20	9/16/94/115	-
20	CLA	A	1811	-	2/2/15/20	21/37/115/115	-
20	CLA	2	1227	-	1/1/4/20	-	-
21	LMU	A	1809	-	-	16/21/61/61	0/2/2/2
20	CLA	A	1794	-	1/1/11/20	8/16/94/115	-
20	CLA	A	1783	-	2/2/15/20	17/37/115/115	-
20	CLA	4	1209	-	1/1/11/20	9/15/93/115	-
20	CLA	A	1768	-	1/1/12/20	12/24/102/115	-
20	CLA	A	1761	-	2/2/15/20	21/37/115/115	-
20	CLA	1	1199	-	1/1/4/20	-	-
21	LMU	A	7030	-	-	17/21/61/61	0/2/2/2
20	CLA	B	1770	-	2/2/15/20	17/37/115/115	-
20	CLA	2	1222	2	1/1/12/20	5/19/97/115	-
20	CLA	2	1224	-	2/2/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1799	-	1/1/12/20	9/19/97/115	-
21	LMU	K	1086	20	-	12/21/61/61	0/2/2/2
20	CLA	B	1753	-	1/1/15/20	16/37/115/115	-
20	CLA	4	1196	-	2/2/13/20	14/25/103/115	-
20	CLA	B	1741	-	2/2/13/20	11/25/101/115	-
20	CLA	3	1215	-	1/1/4/20	-	-
20	CLA	3	1213	-	1/1/4/20	-	-
20	CLA	3	1217	-	1/1/4/20	-	-
20	CLA	A	1816	-	3/3/13/20	12/25/103/115	-
20	CLA	3	1214	-	1/1/4/20	-	-
20	CLA	3	1219	-	2/2/15/20	21/37/115/115	-
20	CLA	A	1785	-	2/2/15/20	17/37/115/115	-
20	CLA	B	1752	-	2/2/13/20	8/25/103/115	-
21	LMU	A	7013	-	-	10/21/61/61	0/2/2/2
20	CLA	3	3008	-	1/1/12/20	5/19/97/115	-
20	CLA	4	4003	-	1/1/4/20	-	-
22	BCR	B	1775	-	-	8/29/63/63	0/2/2/2
22	BCR	B	1774	-	-	10/29/63/63	0/2/2/2
21	LMU	A	7037	-	-	14/21/61/61	0/2/2/2
20	CLA	1	1200	-	3/3/12/20	12/21/99/115	-
20	CLA	4	1207	-	1/1/9/20	-	-
21	LMU	A	7047	-	-	8/21/61/61	0/2/2/2
20	CLA	1	1196	1	1/1/9/20	-	-
20	CLA	A	1765	-	2/2/13/20	11/25/103/115	-
20	CLA	2	1218	20	2/2/15/20	14/37/115/115	-
20	CLA	A	1813	-	2/2/15/20	22/37/115/115	-
20	CLA	B	1766	-	1/1/12/20	8/21/99/115	-
20	CLA	L	1167	22	1/1/11/20	10/16/94/115	-
20	CLA	A	1795	-	1/1/12/20	11/21/99/115	-
22	BCR	B	1779	-	-	12/29/63/63	0/2/2/2
20	CLA	A	1800	-	2/2/15/20	13/37/115/115	-
21	LMU	A	7022	-	-	17/21/61/61	0/2/2/2
20	CLA	B	1769	-	1/1/11/20	6/16/94/115	-
22	BCR	A	1805	-	-	17/29/63/63	0/2/2/2
21	LMU	A	7032	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	A	7040	-	-	11/21/61/61	0/2/2/2
20	CLA	3	3002	-	1/1/4/20	-	-
20	CLA	B	1759	-	2/2/15/20	25/37/115/115	-
22	BCR	B	1778	-	-	12/29/63/63	0/2/2/2
20	CLA	B	1736	-	1/1/11/20	5/13/91/115	-
20	CLA	A	1787	-	2/2/15/20	13/37/115/115	-
21	LMU	R	1057	-	1/1/10/10	11/21/61/61	0/2/2/2
20	CLA	4	1201	-	2/2/12/20	6/22/100/115	-
21	LMU	L	1171	-	-	14/21/61/61	0/2/2/2
20	CLA	A	1812	-	2/2/15/20	15/37/115/115	-
20	CLA	K	1142	-	1/1/11/20	4/13/91/115	-
21	LMU	A	7009	-	-	15/20/60/61	0/2/2/2
20	CLA	2	1223	-	1/1/12/20	8/19/97/115	-
20	CLA	A	1777	-	1/1/12/20	9/21/99/115	-
20	CLA	B	1768	-	2/2/15/20	12/37/115/115	-
20	CLA	4	1205	-	1/1/4/20	-	-
20	CLA	B	1772	-	1/1/9/20	-	-
20	CLA	R	1055	-	2/2/15/20	20/37/115/115	-
22	BCR	A	1803	-	-	12/29/63/63	0/2/2/2
20	CLA	2	1216	-	1/1/4/20	-	-
20	CLA	K	1146	-	1/1/12/20	8/19/97/115	-
20	CLA	A	1775	-	1/1/9/20	-	-
20	CLA	A	1774	-	2/2/15/20	19/37/115/115	-
20	CLA	F	1156	20	1/1/10/20	4/8/86/115	-
21	LMU	A	7041	-	-	12/21/61/61	0/2/2/2
20	CLA	A	1782	20	2/2/15/20	21/37/115/115	-
20	CLA	I	1031	-	2/2/14/20	11/31/109/115	-
20	CLA	2	1220	20	2/2/13/20	13/27/105/115	-
20	CLA	B	1740	6	2/2/15/20	19/37/115/115	-
21	LMU	A	7016	-	-	11/21/61/61	0/2/2/2
21	LMU	A	7042	-	-	18/21/61/61	0/2/2/2
22	BCR	B	1776	-	-	11/29/63/63	0/2/2/2
22	BCR	L	1169	-	-	12/29/63/63	0/2/2/2
21	LMU	1	7004	-	-	13/21/61/61	0/2/2/2
20	CLA	4	1206	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1781	-	2/2/15/20	17/37/115/115	-
20	CLA	H	1079	-	2/2/15/20	17/37/115/115	-
21	LMU	A	7026	19	-	14/21/61/61	0/2/2/2
20	CLA	A	1769	-	1/1/12/20	9/24/102/115	-
20	CLA	B	1738	-	2/2/15/20	18/37/115/115	-
21	LMU	A	7028	-	-	14/21/61/61	0/2/2/2
20	CLA	1	1198	-	2/2/14/20	15/33/111/115	-
20	CLA	J	1043	-	2/2/14/20	24/33/111/115	-
20	CLA	A	1793	-	2/2/15/20	14/37/115/115	-

The worst 5 of 2221 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	1195	CLA	CAB-C3B	-10.64	1.30	1.51
22	L	1170	BCR	C20-C21	-9.80	1.12	1.43
20	1	1191	CLA	CAB-C3B	-9.19	1.33	1.51
20	4	1197	CLA	CAB-C3B	-8.86	1.33	1.51
22	L	1169	BCR	C20-C21	-8.72	1.16	1.43

The worst 5 of 4371 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	1780	BCR	C20-C21-C22	37.59	179.99	127.28
22	A	1808	BCR	C20-C21-C22	37.57	179.97	127.28
22	A	1805	BCR	C20-C21-C22	37.56	179.95	127.28
22	A	1806	BCR	C20-C21-C22	37.56	179.95	127.28
22	A	1804	BCR	C20-C21-C22	37.54	179.93	127.28

5 of 271 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	1187	CLA	ND
20	1	1188	CLA	ND
20	1	1189	CLA	ND
20	1	1190	CLA	ND
20	1	1191	CLA	ND

5 of 2600 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	1	1187	CLA	C1A-C2A-CAA-CBA
20	1	1187	CLA	C3A-C2A-CAA-CBA
20	1	1187	CLA	CBA-CGA-O2A-C1
20	1	1187	CLA	CHA-CBD-CGD-O1D
20	1	1187	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

222 monomers are involved in 3478 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1749	CLA	18	0
20	R	1054	CLA	11	0
21	3	7005	LMU	3	0
20	B	1760	CLA	10	0
21	A	7039	LMU	19	0
21	1	1202	LMU	5	0
20	B	1750	CLA	9	0
20	2	1212	CLA	18	0
20	J	1044	CLA	41	0
20	A	1760	CLA	29	0
20	A	1773	CLA	11	0
20	A	1797	CLA	35	0
20	A	1764	CLA	26	0
20	A	1817	CLA	9	0
20	B	1751	CLA	16	0
21	A	7036	LMU	19	0
22	A	1804	BCR	22	0
20	B	1746	CLA	23	0
20	B	1755	CLA	62	0
23	B	1773	PQN	33	0
20	K	3009	CLA	3	0
20	B	1786	CLA	43	0
20	4	1208	CLA	8	0
20	1	1195	CLA	4	0
20	K	1085	CLA	26	0
20	1	1188	CLA	7	0
20	B	1748	CLA	14	0
20	L	1505	CLA	3	0
20	4	1198	CLA	25	0
20	1	1192	CLA	9	0
20	4	1197	CLA	2	0
20	B	1757	CLA	21	0
20	F	1155	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	I	1032	BCR	47	0
20	A	1784	CLA	18	0
20	B	1758	CLA	34	0
22	B	1780	BCR	53	0
20	1	1189	CLA	11	0
21	A	7027	LMU	6	0
22	B	1777	BCR	31	0
20	B	1744	CLA	20	0
20	1	1193	CLA	6	2
20	B	1735	CLA	33	0
20	J	1045	CLA	45	0
20	B	1742	CLA	9	0
22	3	1220	BCR	21	0
20	B	1764	CLA	21	0
20	A	1796	CLA	63	0
21	2	7006	LMU	11	0
20	3	3011	CLA	17	0
20	3	1212	CLA	9	0
20	A	1772	CLA	35	0
23	A	1802	PQN	12	0
20	B	1745	CLA	12	0
20	A	1779	CLA	35	0
25	C	1082	SF4	5	0
20	B	1754	CLA	23	0
20	A	1789	CLA	20	0
20	2	1213	CLA	13	0
20	B	1761	CLA	12	0
21	R	1056	LMU	19	0
22	A	1808	BCR	43	0
20	A	1791	CLA	24	1
21	A	1810	LMU	4	0
20	L	1166	CLA	7	0
20	A	1759	CLA	20	0
21	A	7038	LMU	13	0
20	3	3007	CLA	2	0
20	A	1767	CLA	23	0
20	A	1776	CLA	47	0
20	A	1763	CLA	31	0
20	1	1191	CLA	10	0
20	B	1767	CLA	15	0
20	B	1771	CLA	24	0
25	C	1083	SF4	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	1194	CLA	5	0
20	A	1786	CLA	9	0
20	4	1199	CLA	22	0
21	A	7019	LMU	2	0
21	A	7023	LMU	26	0
22	A	1807	BCR	62	0
20	A	1762	CLA	18	0
20	B	1743	CLA	29	0
20	2	1215	CLA	24	0
20	1	1190	CLA	5	0
20	4	1204	CLA	8	0
20	B	1737	CLA	24	0
21	2	1225	LMU	1	1
21	A	7017	LMU	3	0
20	B	1787	CLA	50	0
20	A	1788	CLA	40	0
20	F	1157	CLA	13	0
20	3	1218	CLA	25	0
20	G	1099	CLA	6	0
20	A	1780	CLA	17	0
20	I	1033	CLA	15	0
21	2	7003	LMU	3	0
20	2	1217	CLA	9	0
20	A	1798	CLA	29	0
25	B	1784	SF4	18	0
20	A	1770	CLA	27	0
20	A	1790	CLA	16	0
20	B	1747	CLA	23	0
21	A	7010	LMU	8	0
24	B	1783	LMG	30	0
21	A	7020	LMU	21	0
20	A	1815	CLA	19	0
21	A	7021	LMU	24	0
21	A	7025	LMU	1	0
21	B	1782	LMU	1	0
21	A	7034	LMU	1	0
20	B	1785	CLA	22	0
20	A	1792	CLA	22	0
21	A	7033	LMU	19	0
22	A	1806	BCR	36	0
22	B	1781	BCR	17	0
20	A	1771	CLA	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	1202	CLA	4	0
20	A	1778	CLA	11	0
20	1	1197	CLA	20	0
20	1	1187	CLA	11	0
21	A	7043	LMU	16	0
20	L	1168	CLA	12	0
21	A	7031	LMU	4	0
20	3	1216	CLA	7	0
20	A	1766	CLA	5	0
20	B	1763	CLA	13	0
20	4	1200	CLA	3	0
20	B	1739	CLA	22	0
20	A	1801	CLA	15	0
20	B	1765	CLA	20	0
20	B	1756	CLA	46	0
22	L	1170	BCR	13	0
20	B	1762	CLA	28	0
20	2	1214	CLA	7	0
20	4	4014	CLA	11	0
20	A	1811	CLA	20	0
21	A	1809	LMU	4	0
20	A	1794	CLA	21	0
20	A	1783	CLA	61	0
20	4	1209	CLA	5	0
20	A	1768	CLA	4	0
20	A	1761	CLA	32	0
20	1	1199	CLA	2	0
21	A	7030	LMU	12	0
20	B	1770	CLA	24	0
20	2	1222	CLA	14	0
20	2	1224	CLA	7	0
20	A	1799	CLA	7	0
21	K	1086	LMU	6	0
20	B	1753	CLA	40	0
20	4	1196	CLA	34	0
20	B	1741	CLA	6	0
20	3	1215	CLA	17	0
20	3	1213	CLA	1	0
20	3	1217	CLA	8	0
20	A	1816	CLA	35	0
20	3	1214	CLA	3	0
20	3	1219	CLA	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1785	CLA	17	0
20	B	1752	CLA	14	0
21	A	7013	LMU	9	0
20	3	3008	CLA	17	0
22	B	1775	BCR	20	0
22	B	1774	BCR	8	0
21	A	7037	LMU	24	0
20	1	1200	CLA	11	0
20	4	1207	CLA	5	0
20	1	1196	CLA	6	0
20	A	1765	CLA	25	0
20	2	1218	CLA	7	0
20	A	1813	CLA	33	0
20	B	1766	CLA	3	0
20	L	1167	CLA	18	0
20	A	1795	CLA	40	0
22	B	1779	BCR	46	0
20	A	1800	CLA	31	0
21	A	7022	LMU	11	0
20	B	1769	CLA	25	0
22	A	1805	BCR	48	0
21	A	7032	LMU	28	0
21	A	7040	LMU	4	0
20	B	1759	CLA	34	0
22	B	1778	BCR	30	0
20	B	1736	CLA	9	0
20	A	1787	CLA	26	0
21	R	1057	LMU	5	0
20	4	1201	CLA	25	0
21	L	1171	LMU	3	0
20	A	1812	CLA	35	0
20	K	1142	CLA	20	2
21	A	7009	LMU	9	0
20	2	1223	CLA	4	0
20	A	1777	CLA	13	0
20	B	1768	CLA	48	0
20	4	1205	CLA	3	0
20	B	1772	CLA	2	0
20	R	1055	CLA	6	0
22	A	1803	BCR	41	0
20	K	1146	CLA	11	0
20	A	1774	CLA	31	0

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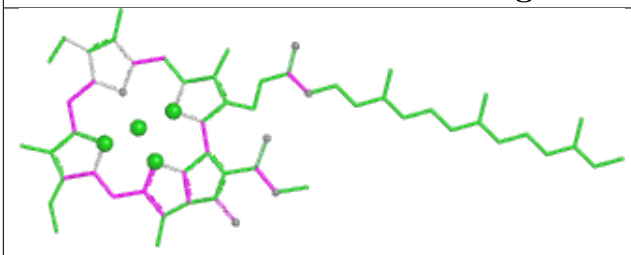
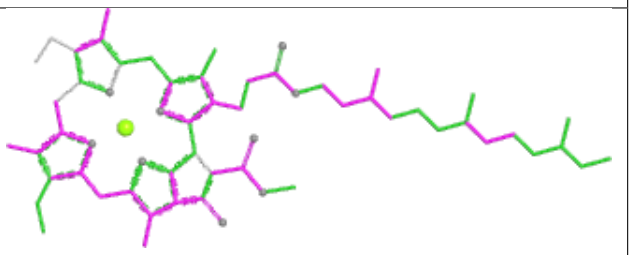
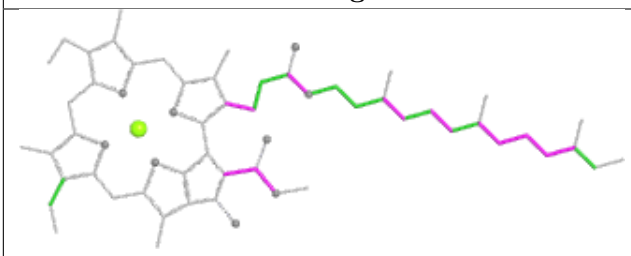
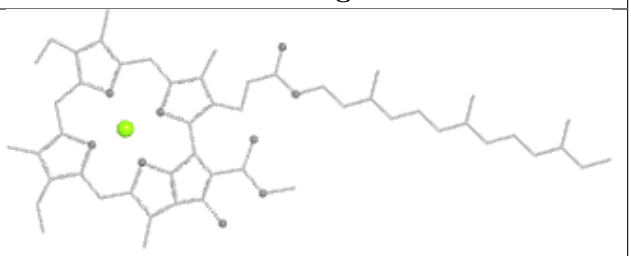
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	F	1156	CLA	13	0
21	A	7041	LMU	9	0
20	A	1782	CLA	81	0
20	I	1031	CLA	11	0
20	2	1220	CLA	74	0
20	B	1740	CLA	20	0
21	A	7016	LMU	42	0
21	A	7042	LMU	35	0
22	B	1776	BCR	20	0
22	L	1169	BCR	48	0
21	1	7004	LMU	10	0
20	4	1206	CLA	2	0
20	A	1781	CLA	85	0
20	H	1079	CLA	19	0
21	A	7026	LMU	21	0
20	A	1769	CLA	22	0
20	B	1738	CLA	19	0
21	A	7028	LMU	4	0
20	1	1198	CLA	20	0
20	J	1043	CLA	29	0
20	A	1793	CLA	35	0

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

Ligand CLA B 1749	
 Bond lengths	 Bond angles
 Torsions	 Rings

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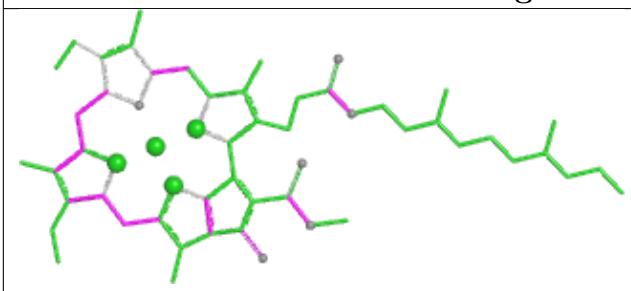
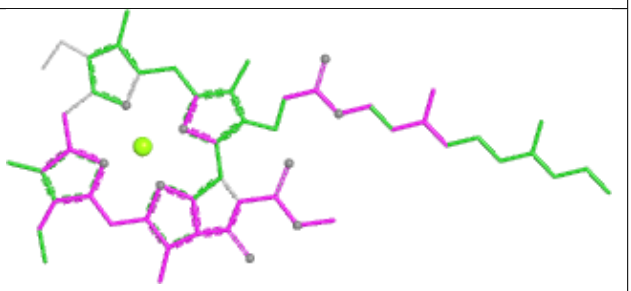
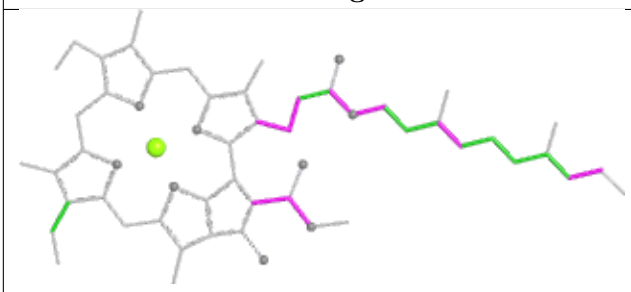
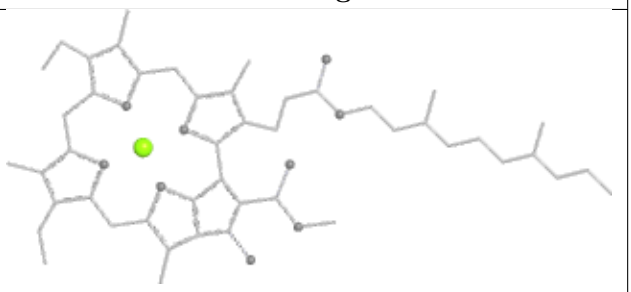
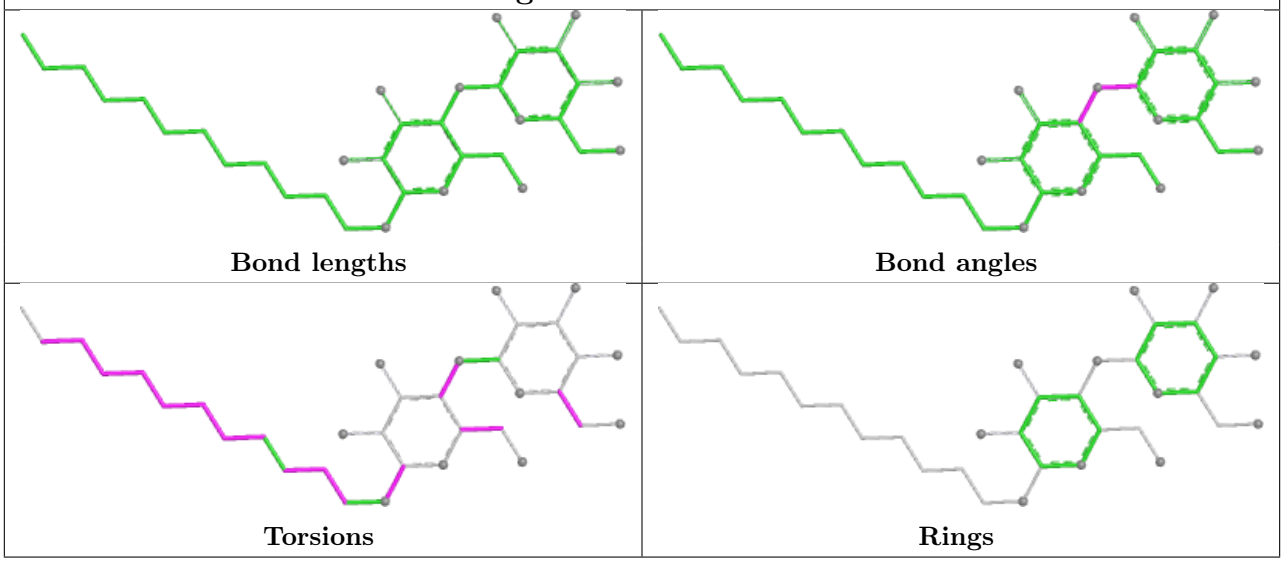
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMU 3 7005



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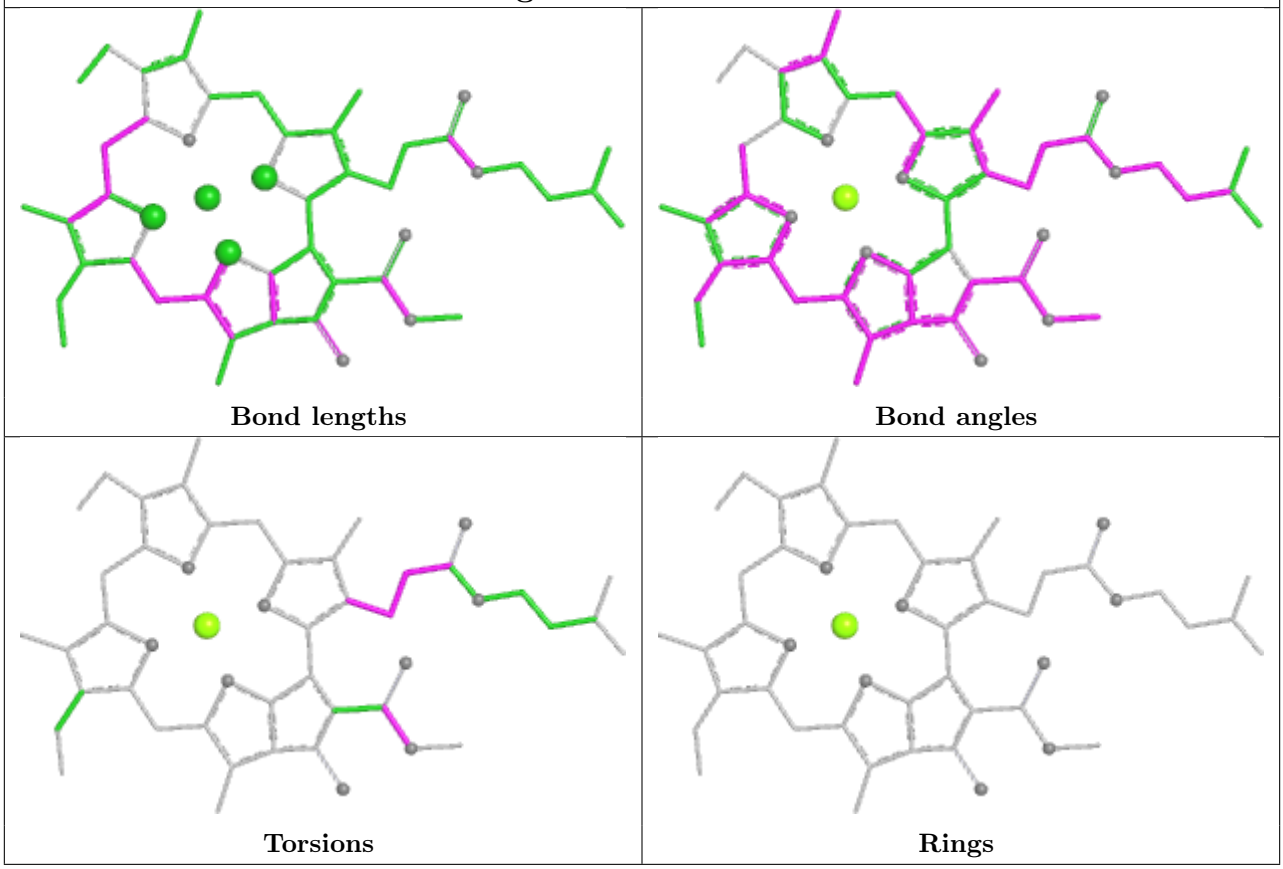

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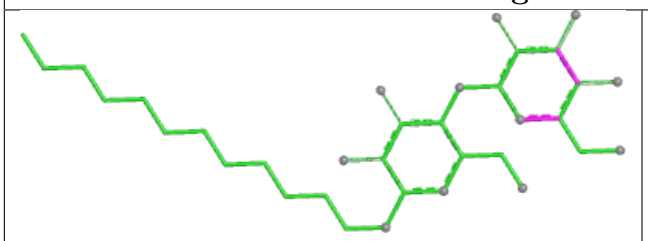
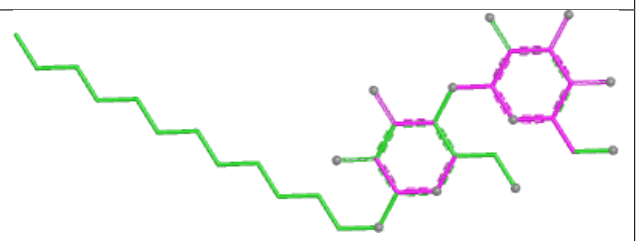
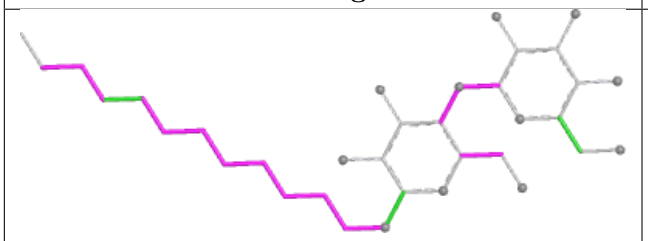


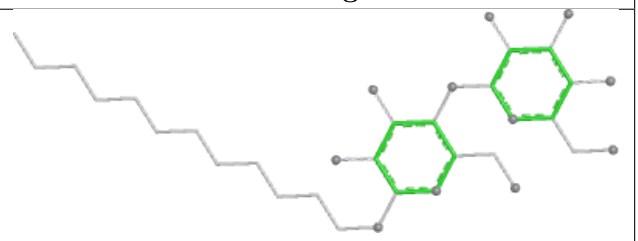
Bond lengths



Bond angles

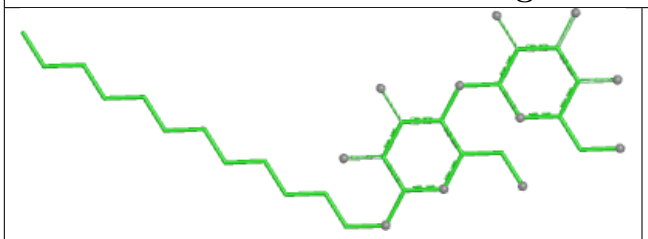


Torsions

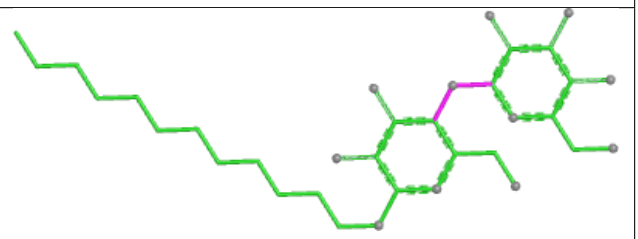


Rings

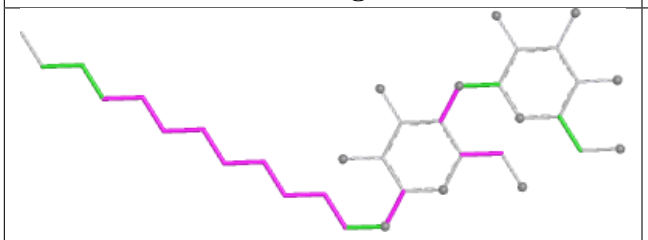
Ligand LMU 1 1202



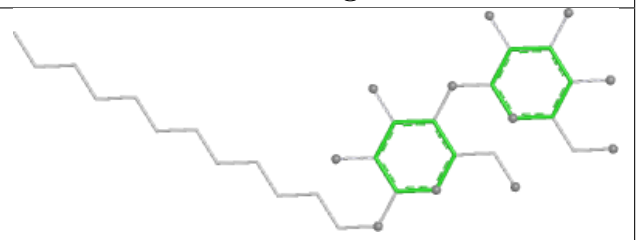
Bond lengths



Bond angles

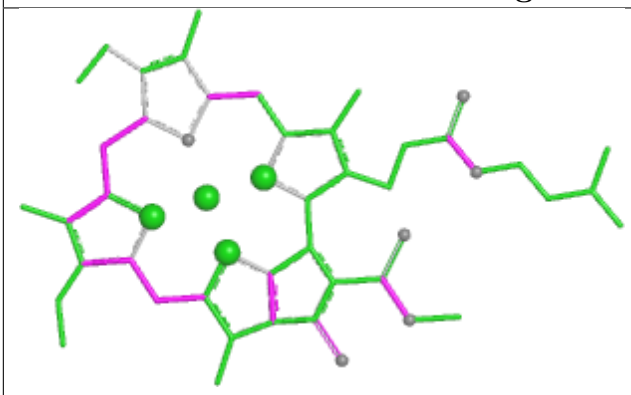


Torsions

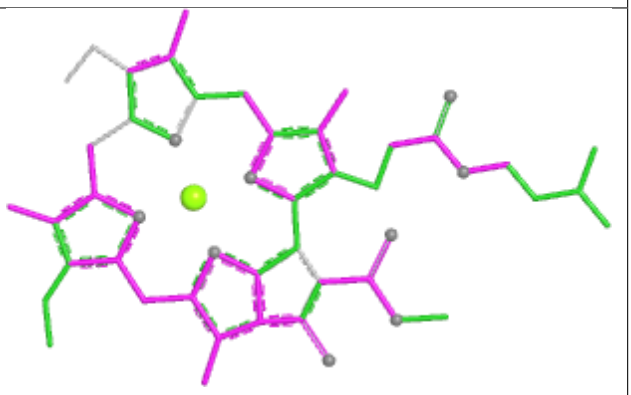


Rings

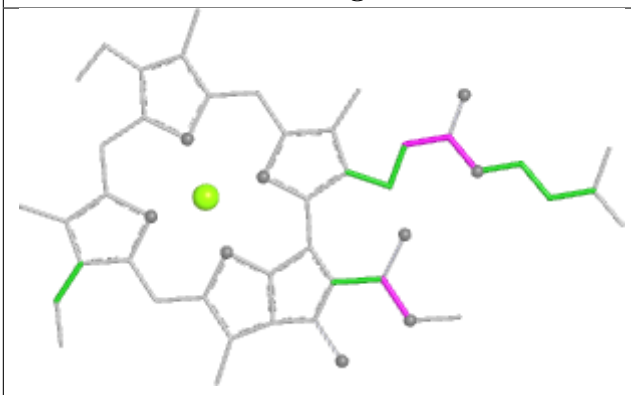
Ligand CLA B 1750



Bond lengths



Bond angles



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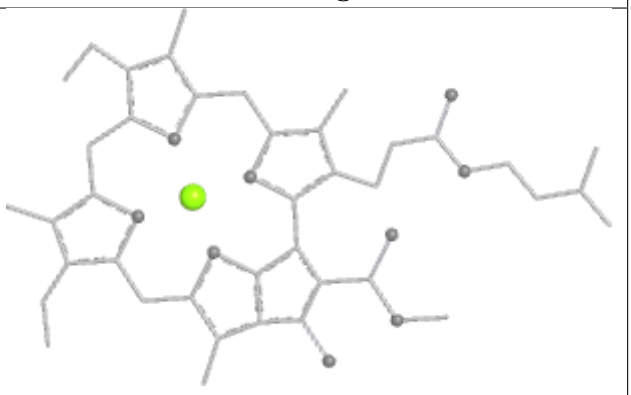
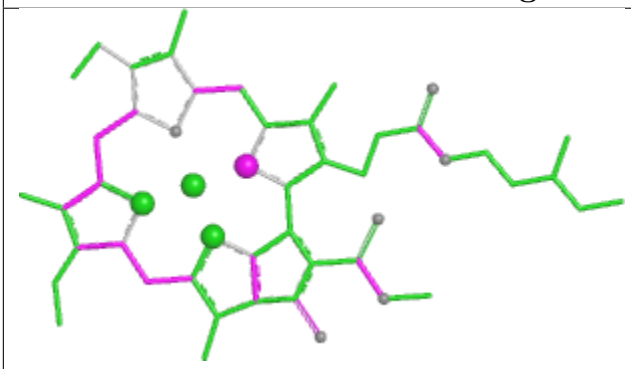
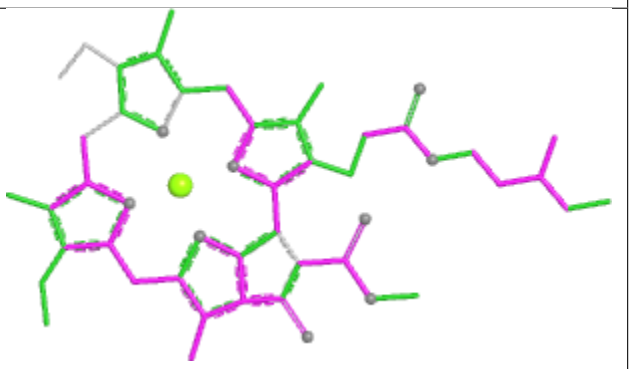


Rings

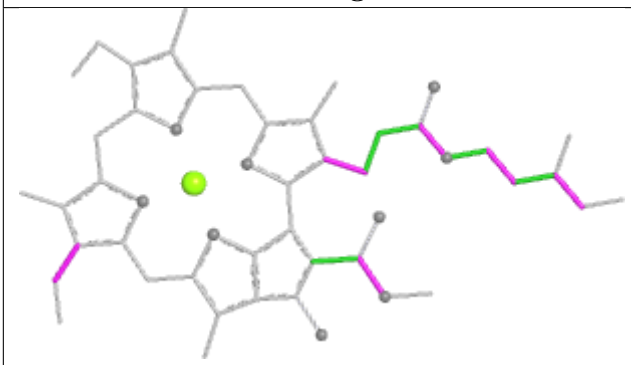
Ligand CLA 2 1212



Bond lengths



Bond angles



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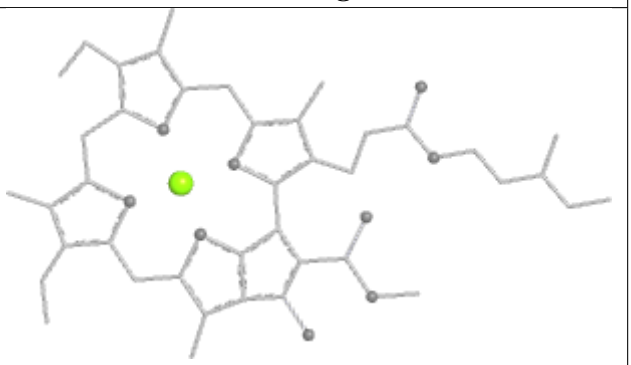
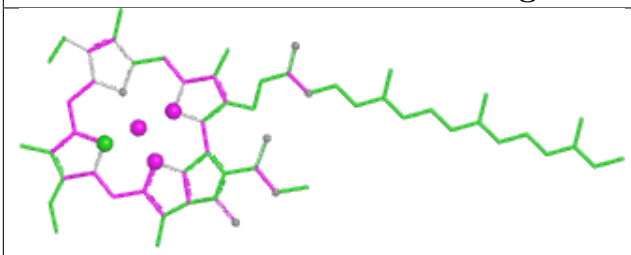
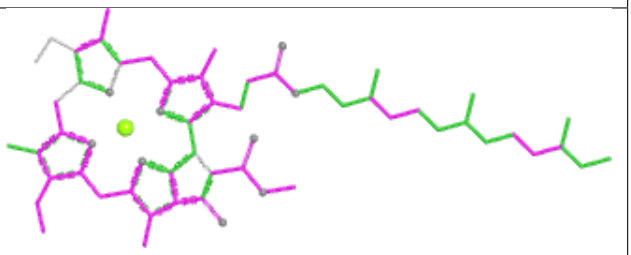
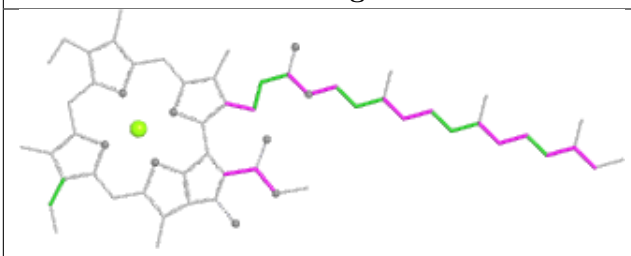
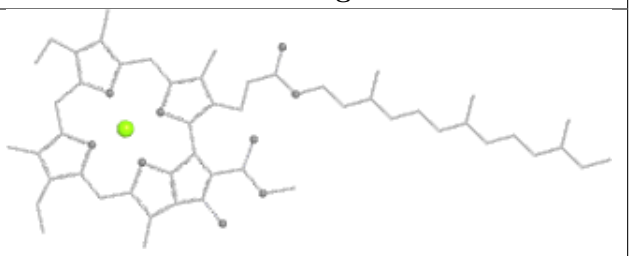
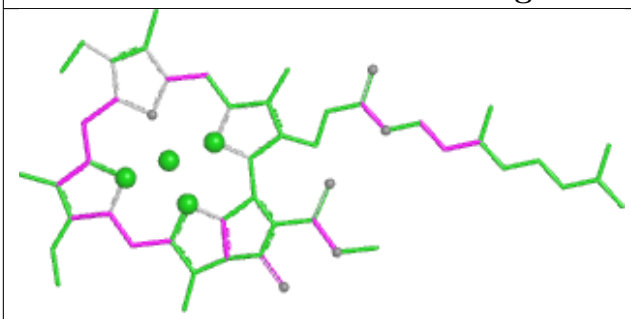
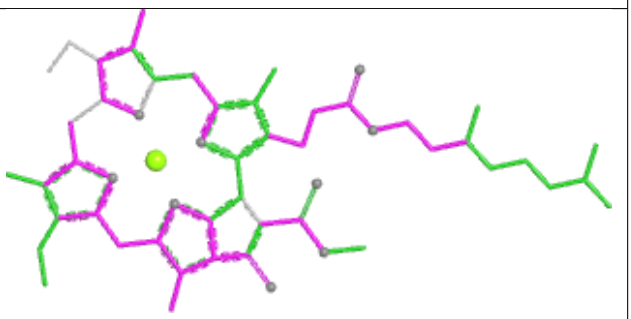
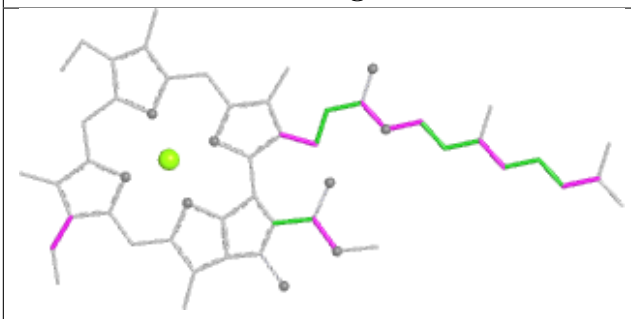
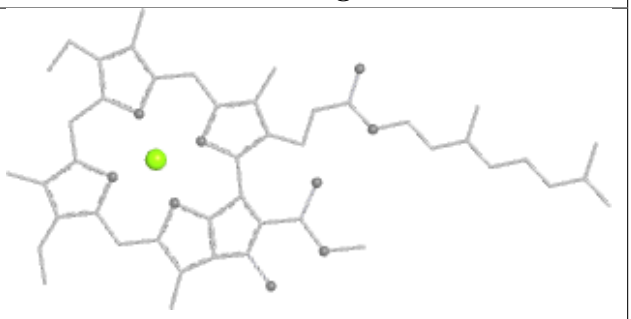


Rings

Ligand CLA J 1044	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1760	
 Bond lengths	 Bond angles
 Torsions	 Rings

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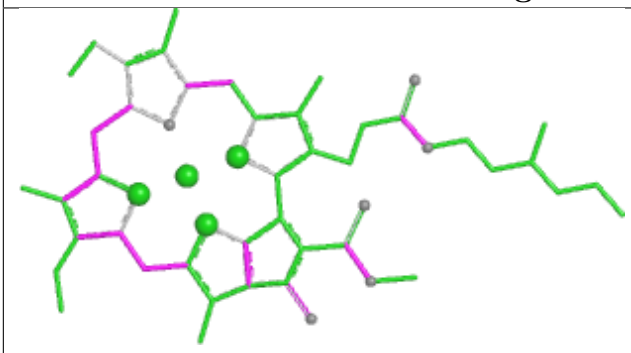
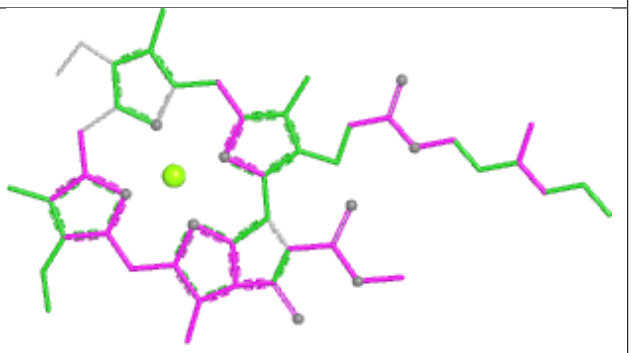
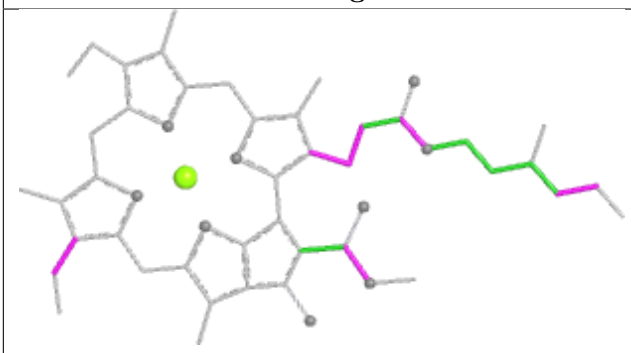
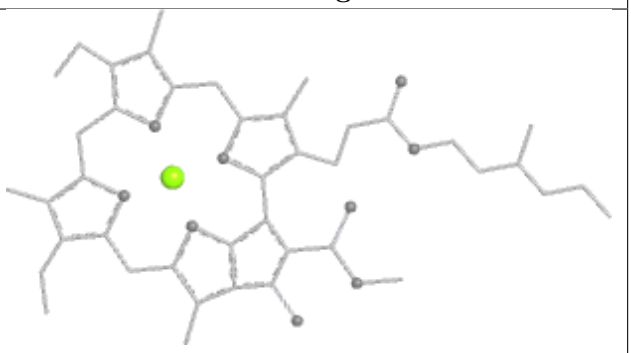
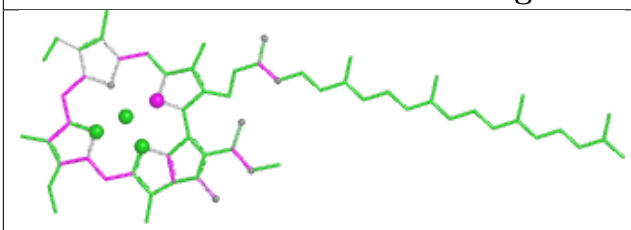
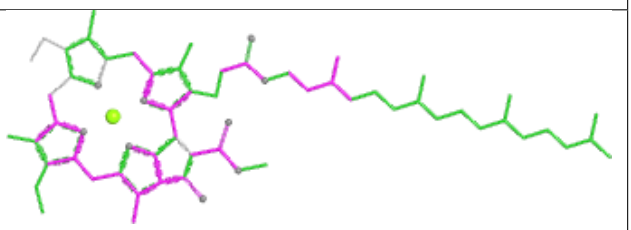
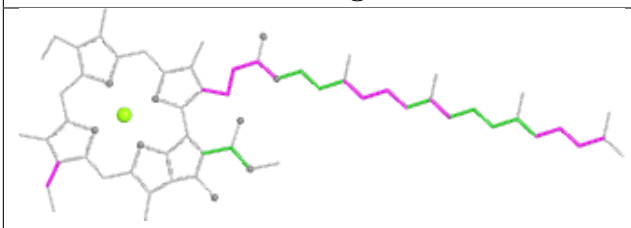
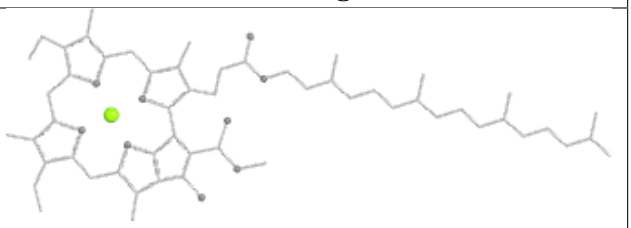
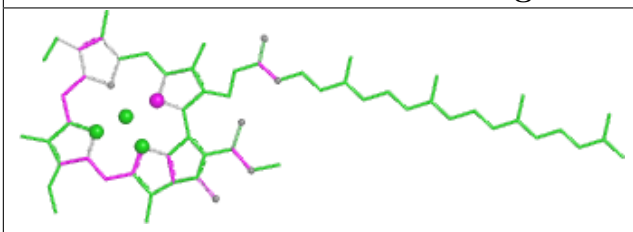
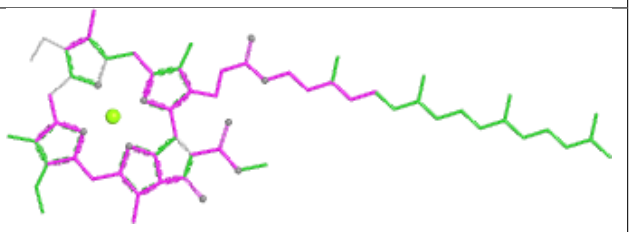
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1797	
 Bond lengths	 Bond angles
 Torsions	 Rings

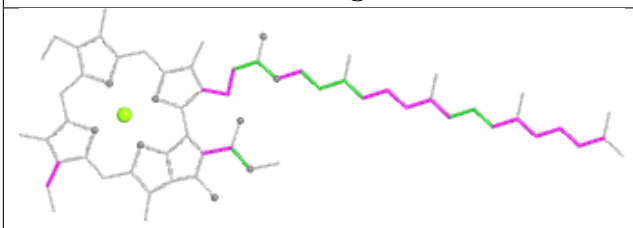
Ligand CLA A 1764



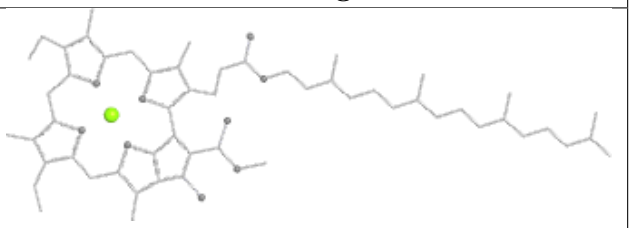
Bond lengths



Bond angles

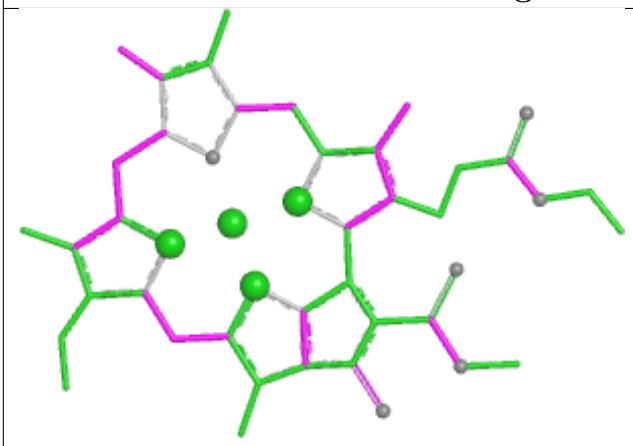


Torsions



Rings

Ligand CLA A 1817



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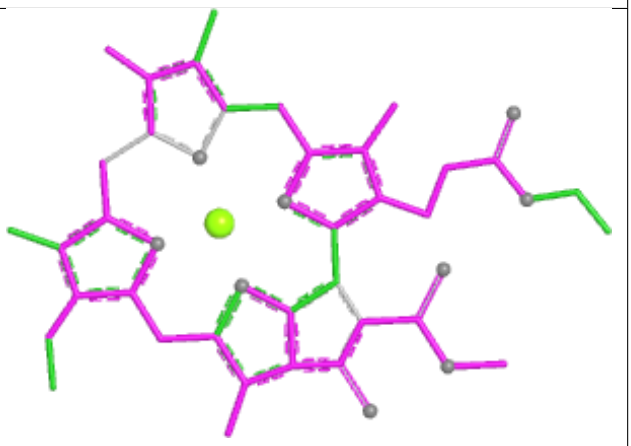
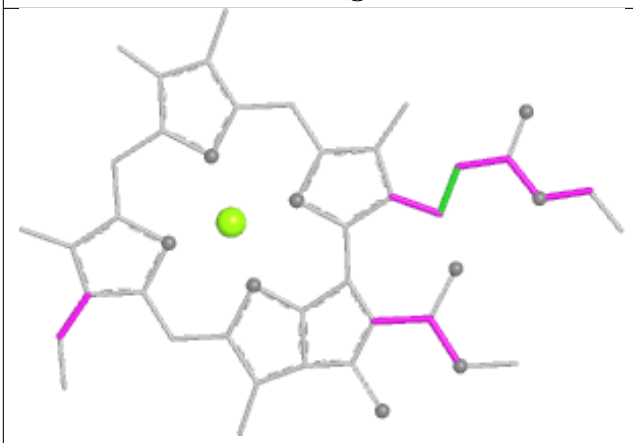


Bond angles



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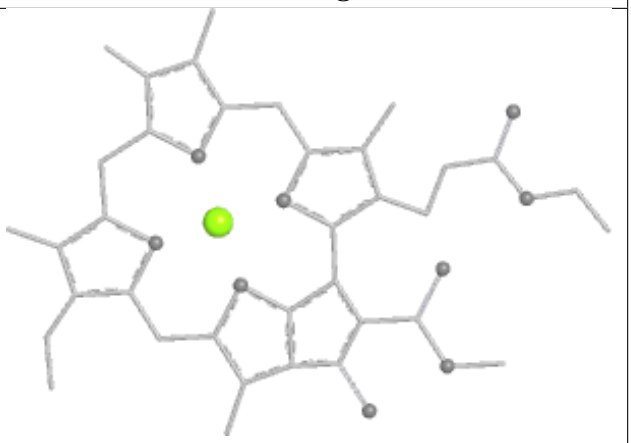
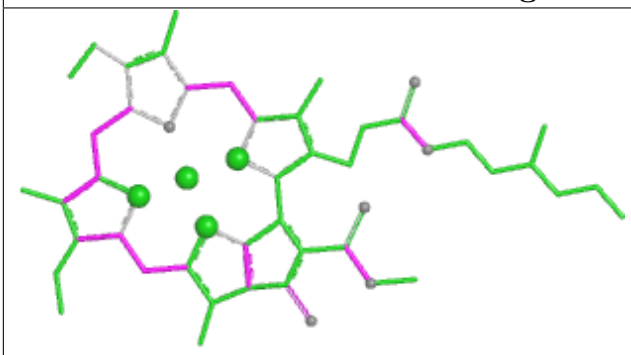
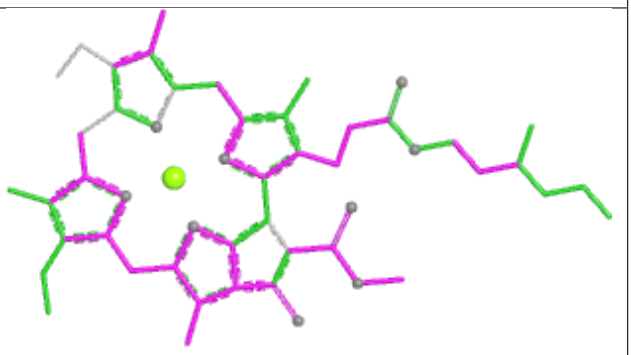
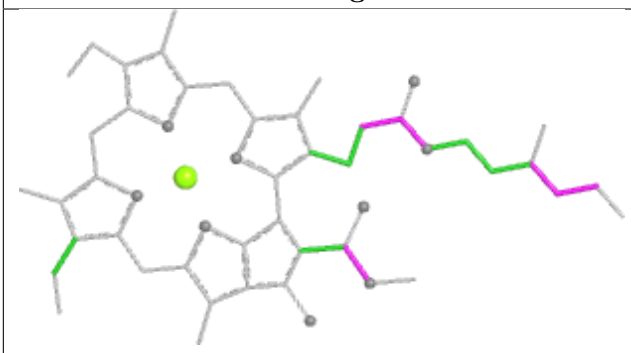
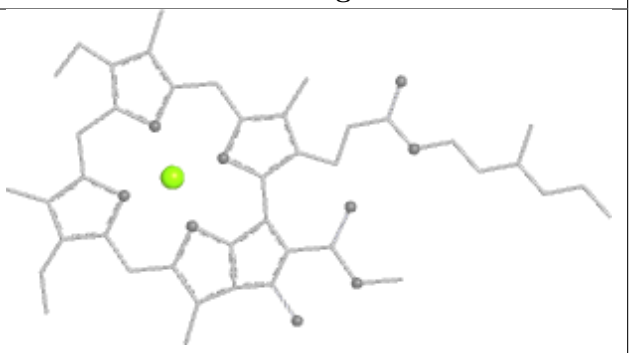
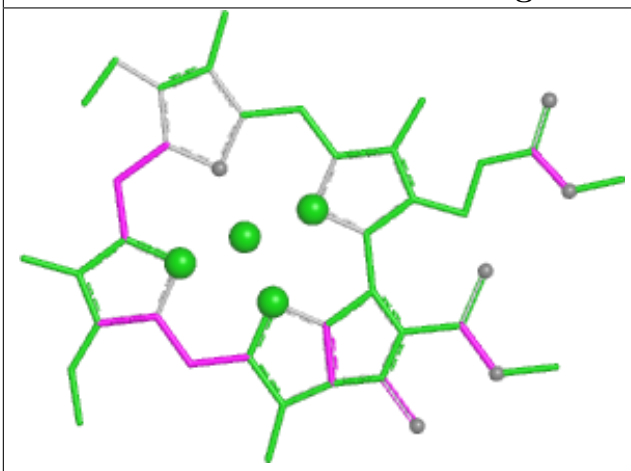


Rings

Ligand CLA 4 4007	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1751



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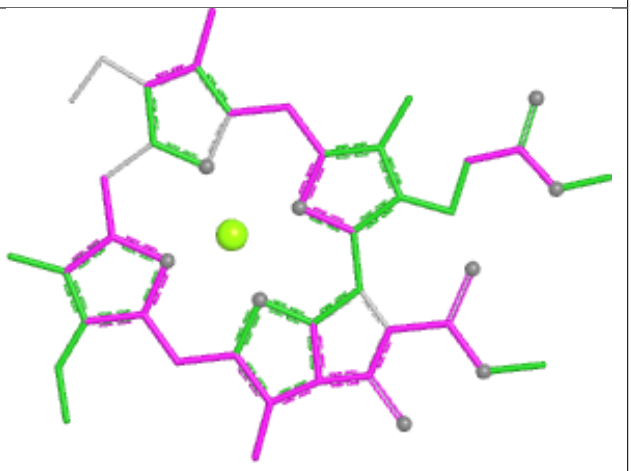
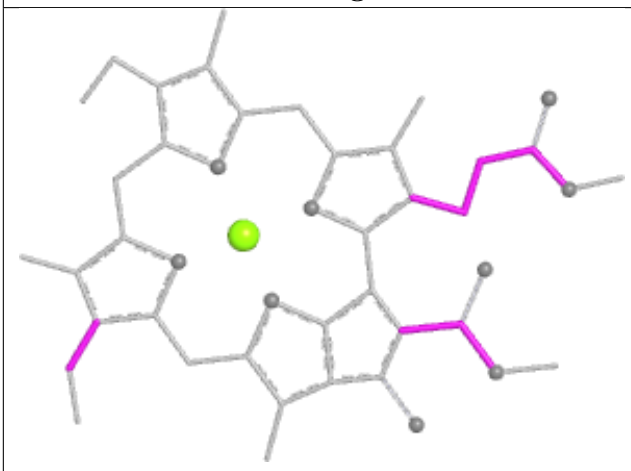


Bond angles



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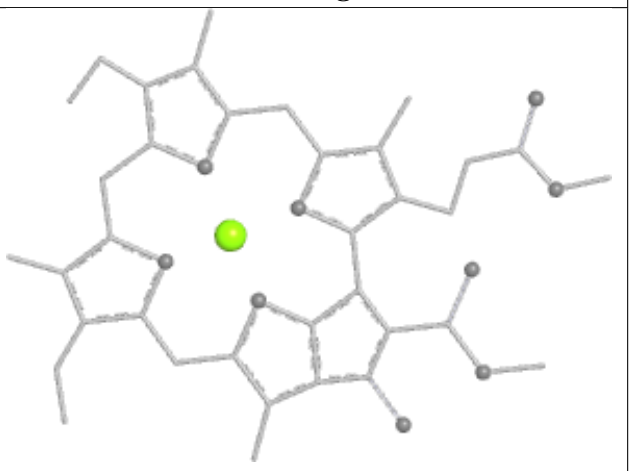
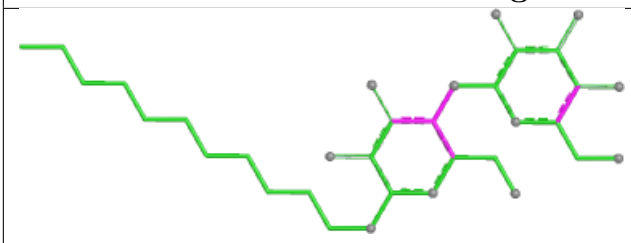


Rings

Ligand LMU A 7036



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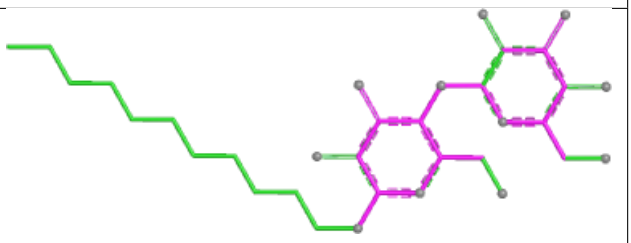
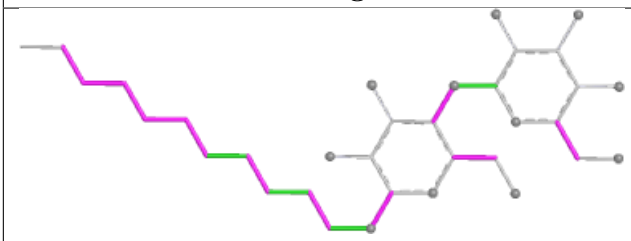


Bond angles



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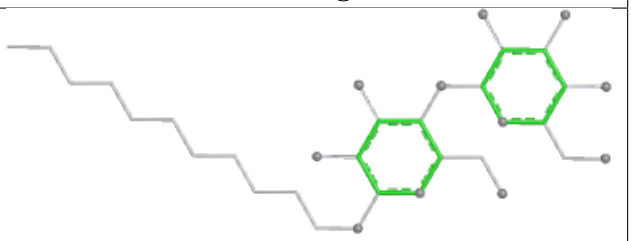
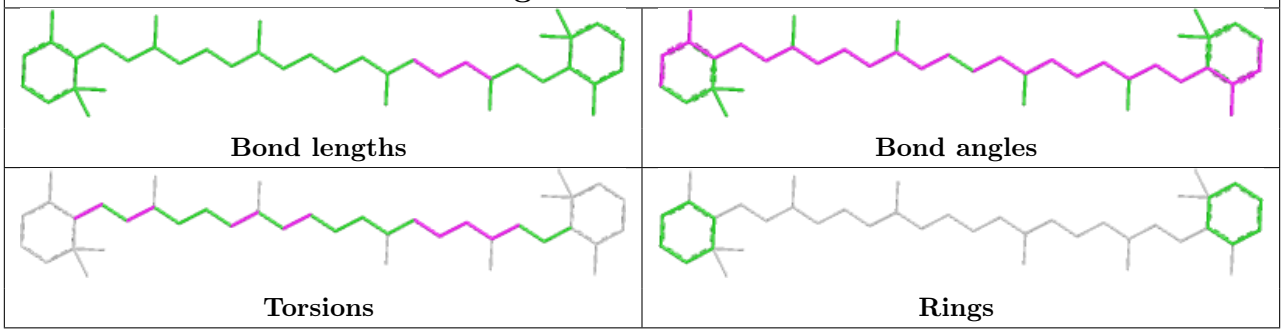
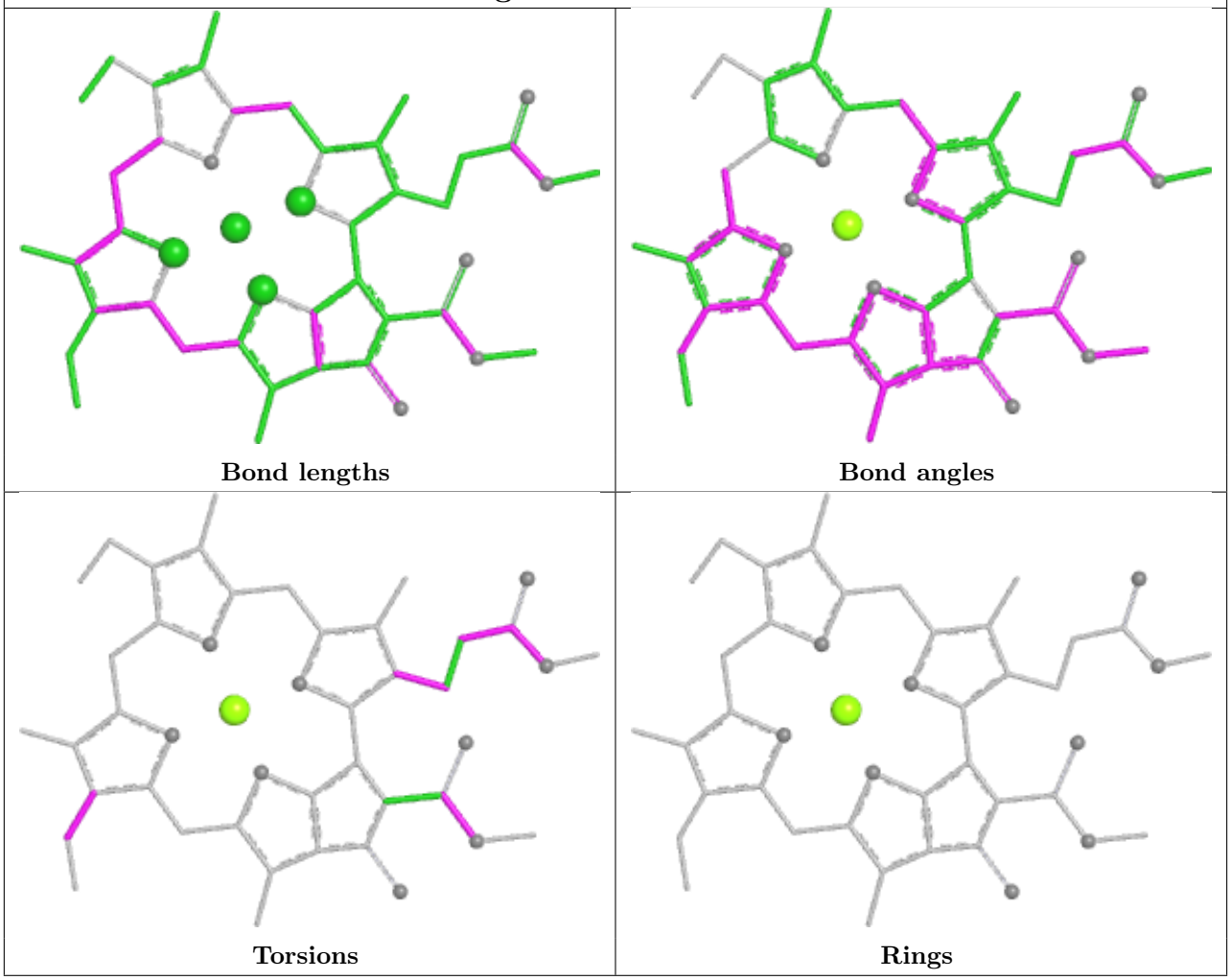


Rings

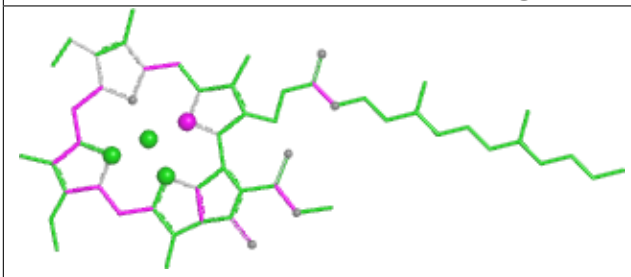
Ligand BCR A 1804



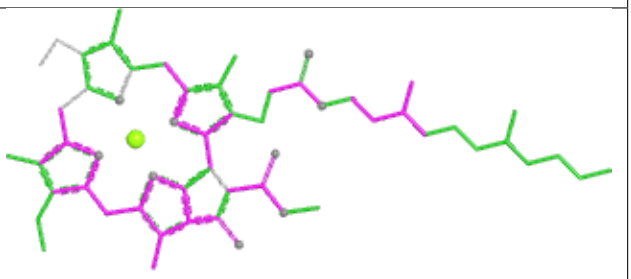
Ligand CLA B 1746



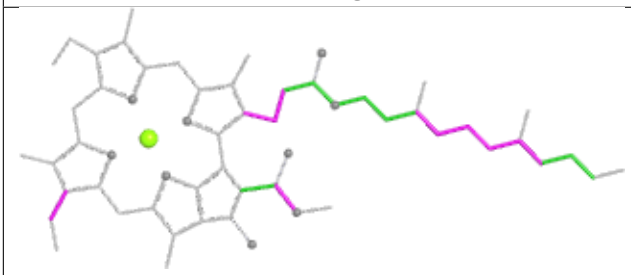
Ligand CLA B 1755



Bond lengths



Bond angles



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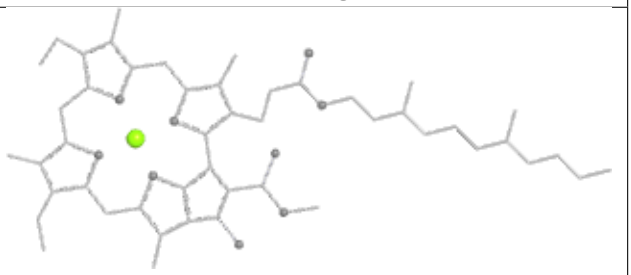
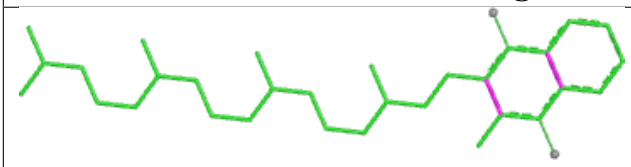


Rings

Ligand PQN B 1773



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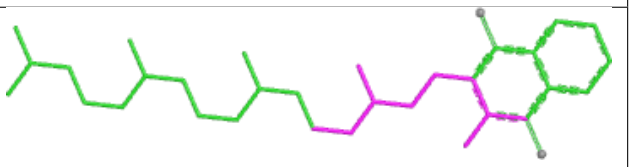
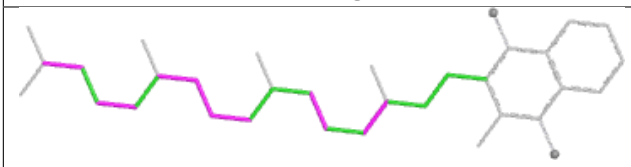


Bond angles



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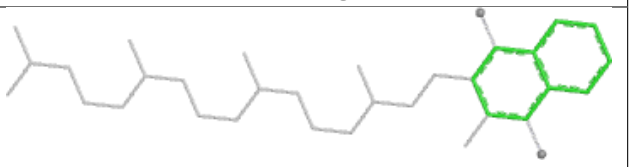
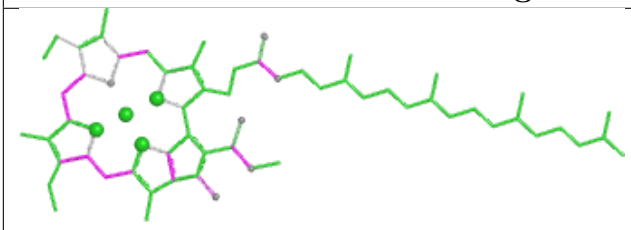
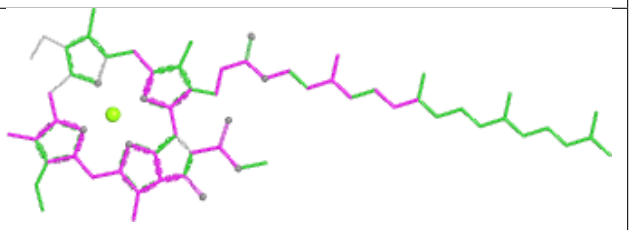


Rings

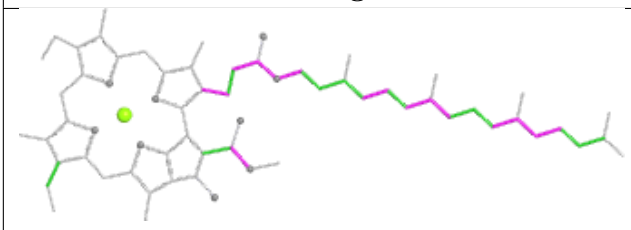
Ligand CLA K 3009



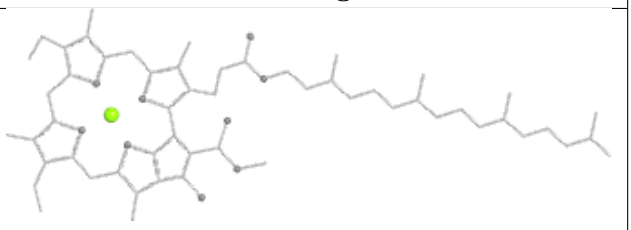
Bond lengths



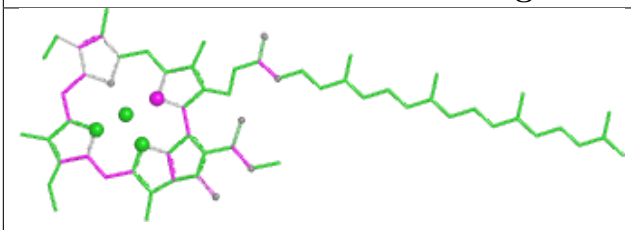
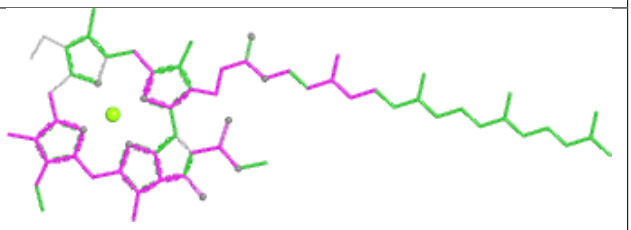
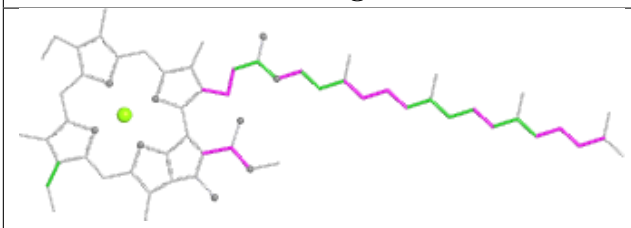
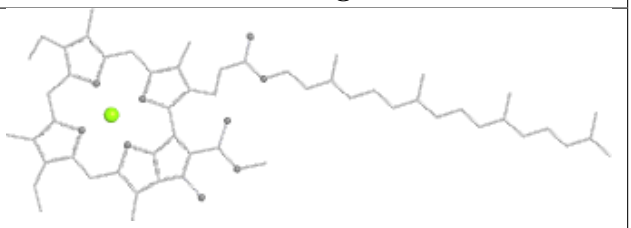
Bond angles



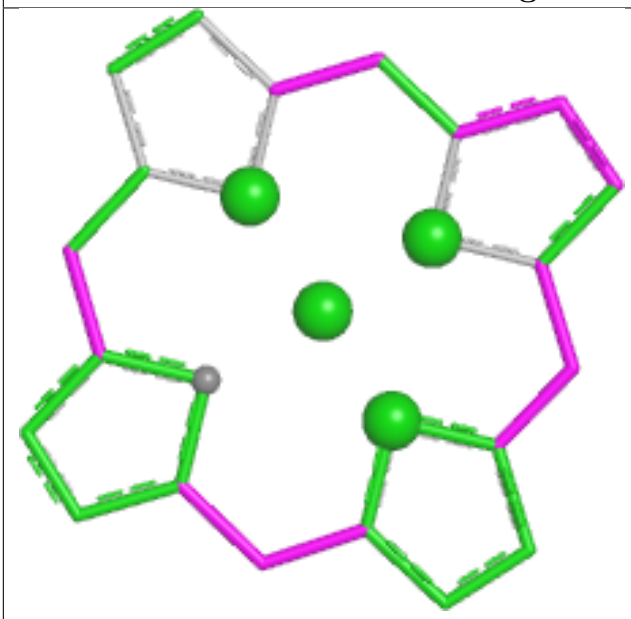
Torsions



Rings

Ligand CLA B 1786	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 1208



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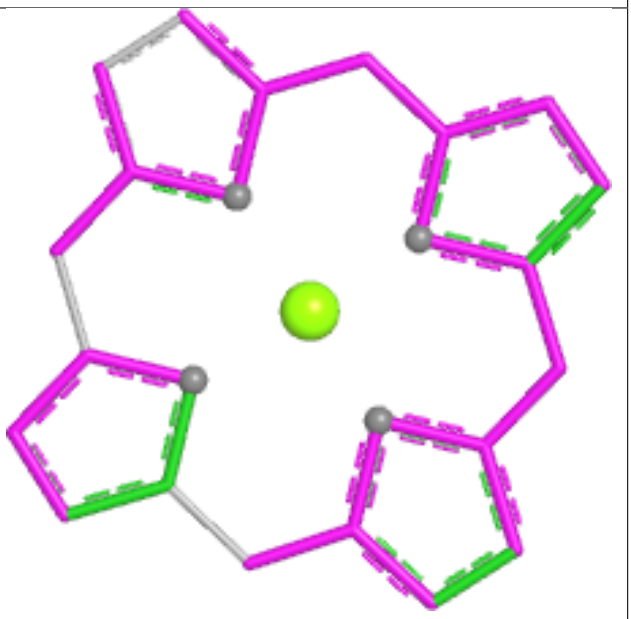
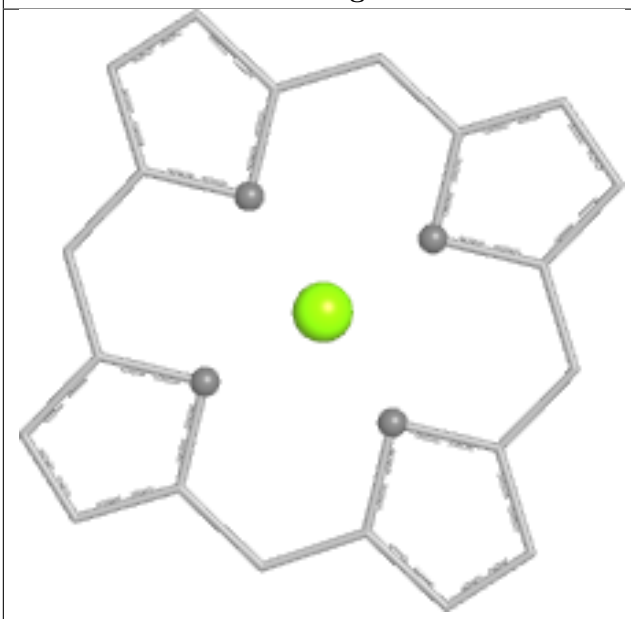
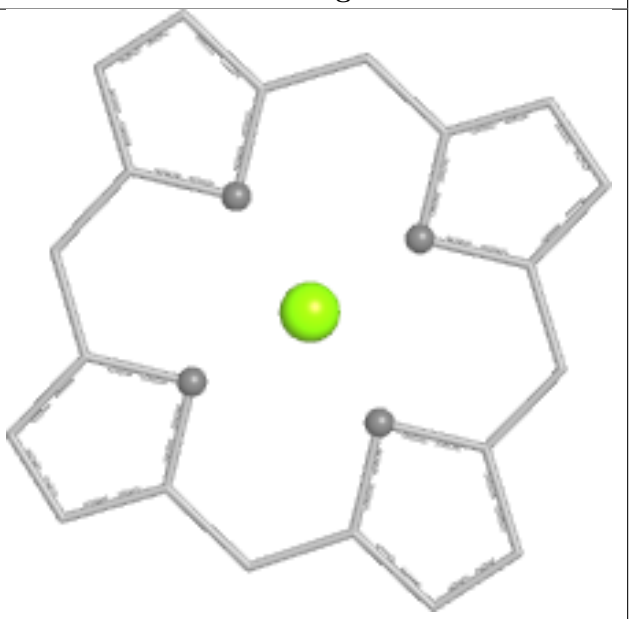


Bond angles

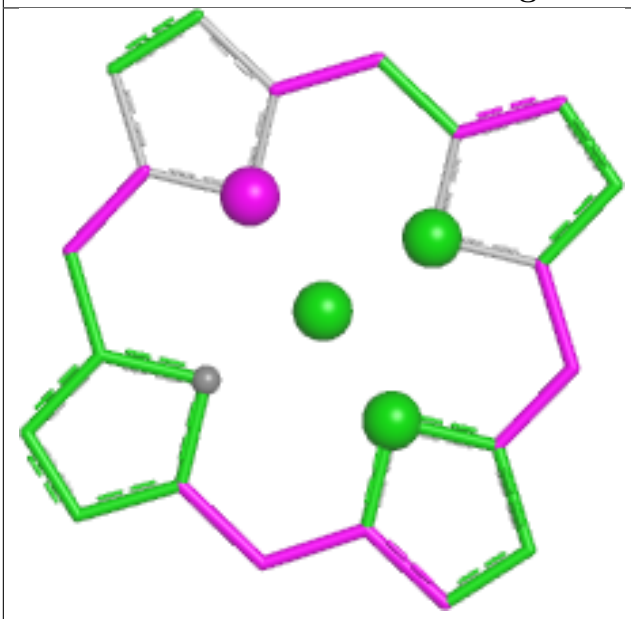


Torsions

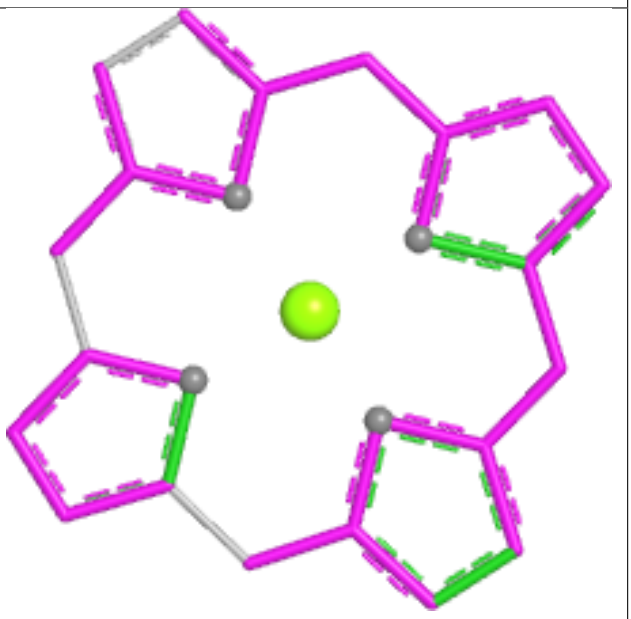


Rings

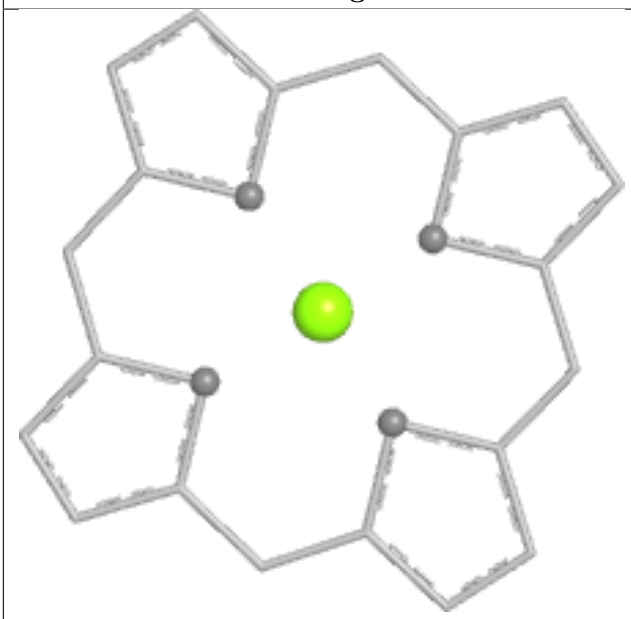
Ligand CLA 3 3014



Bond lengths



Bond angles



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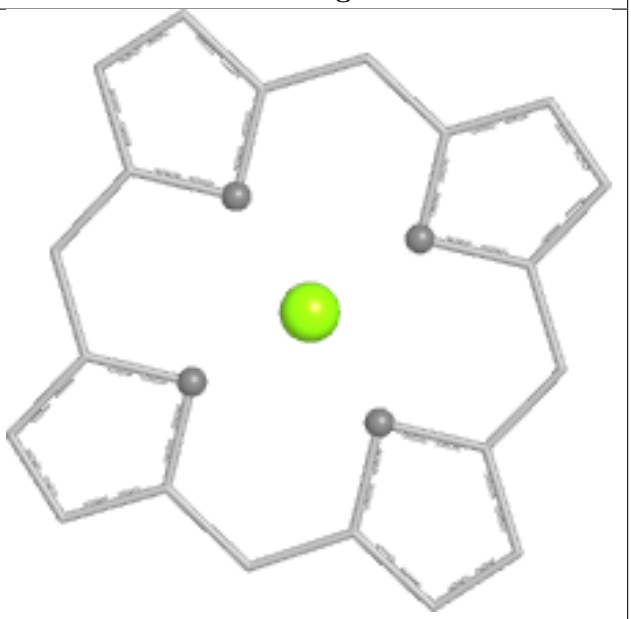
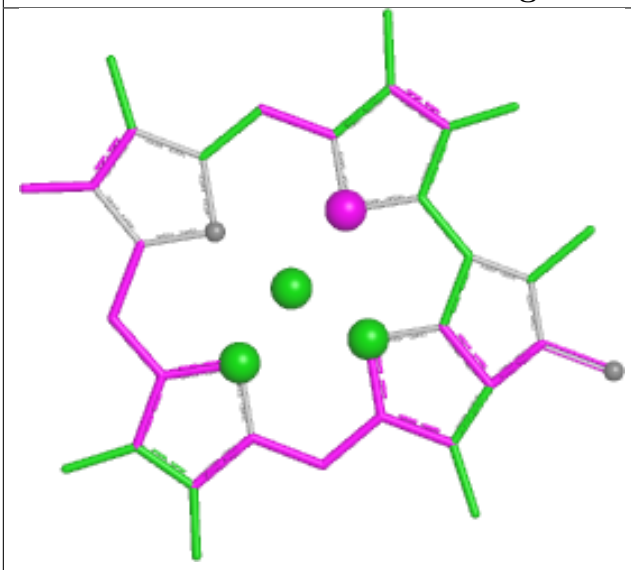


Rings

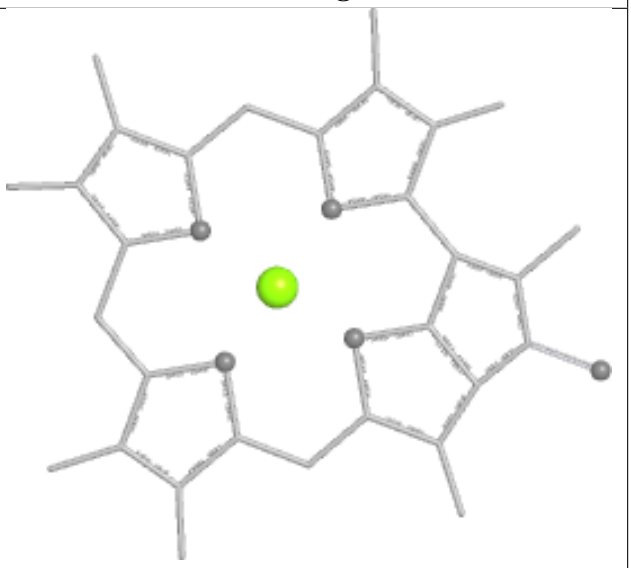
Ligand CLA 1 1195



Bond lengths

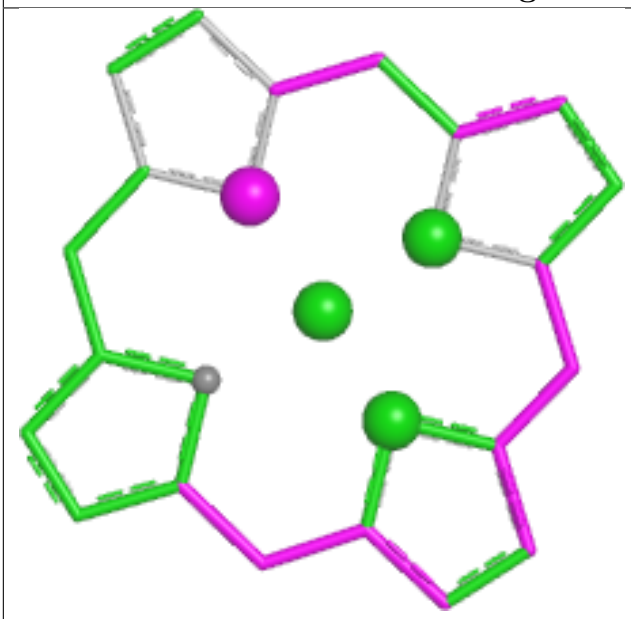
Bond angles

Torsions

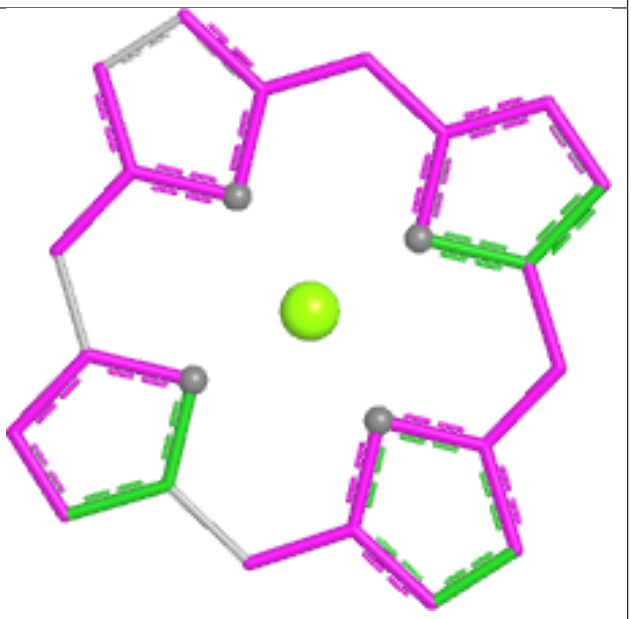


Rings

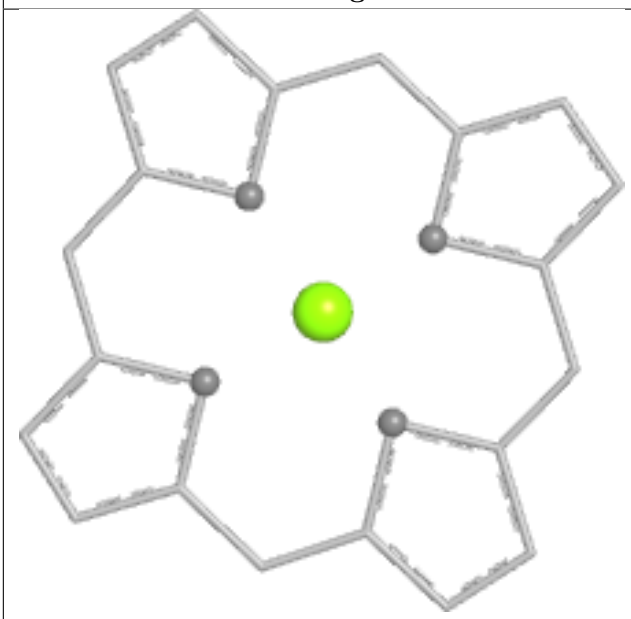
Ligand CLA J 1046



Bond lengths



Bond angles



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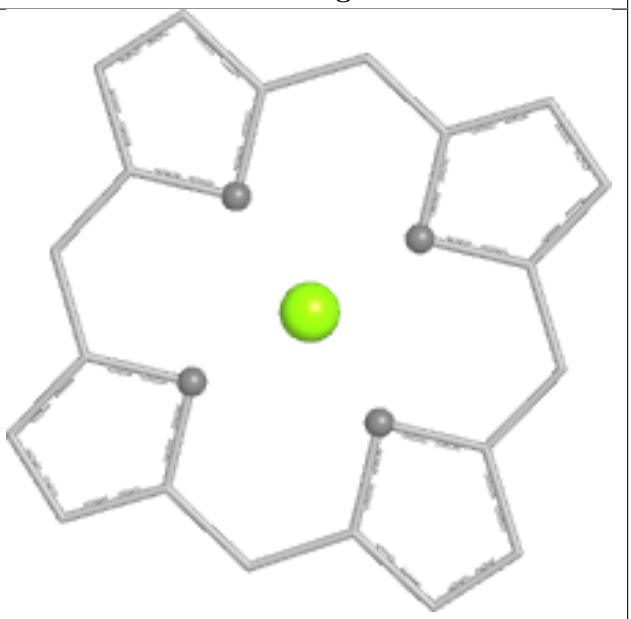
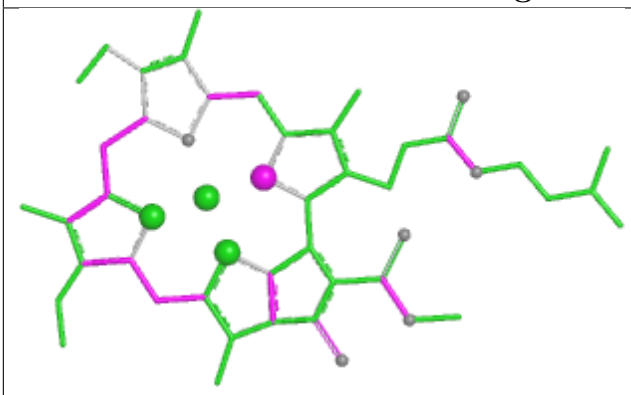
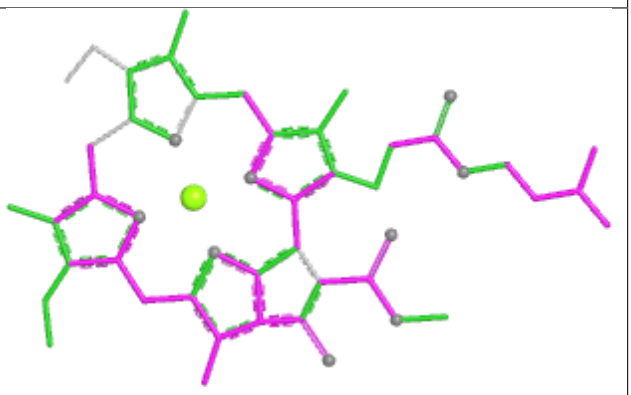
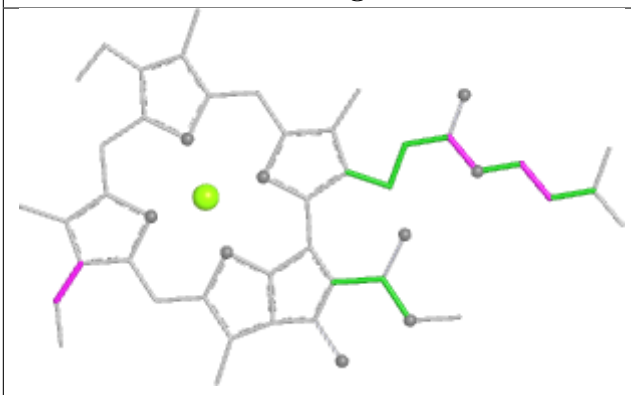
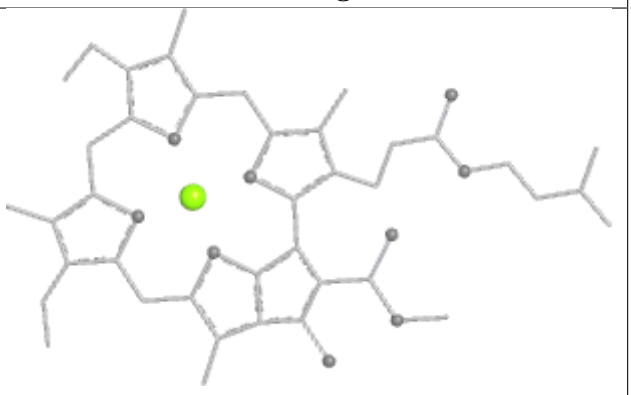
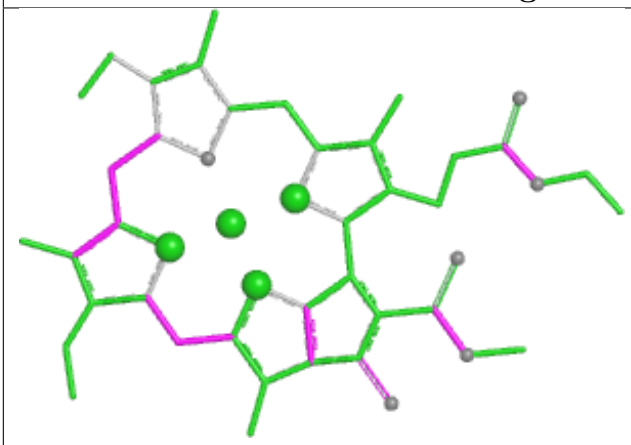


Rings

Ligand CLA K 1085	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1188



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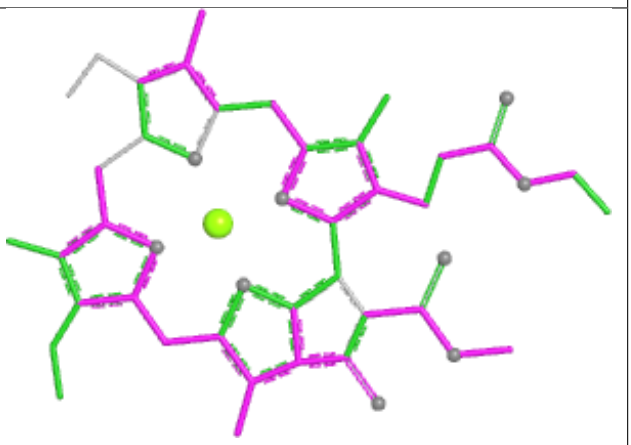
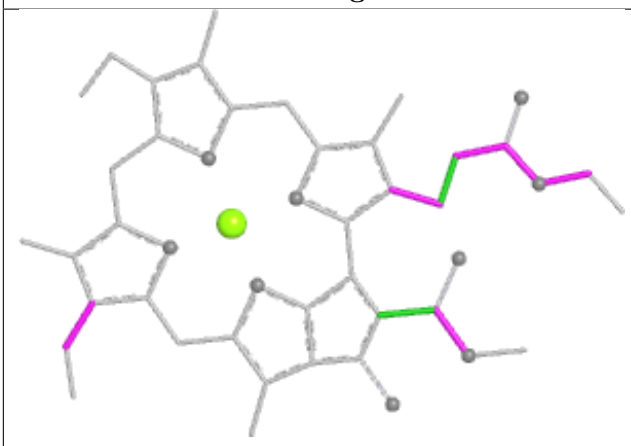


Bond angles



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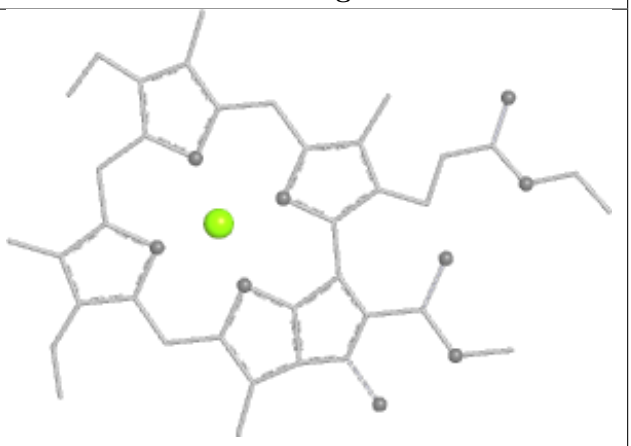
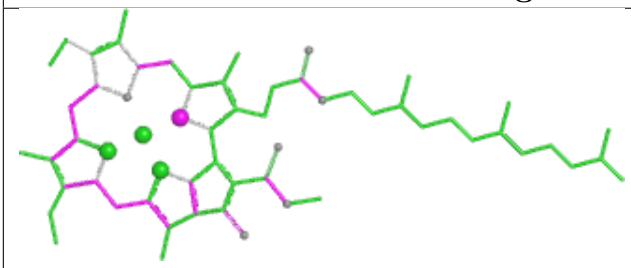


Rings

Ligand CLA B 1748



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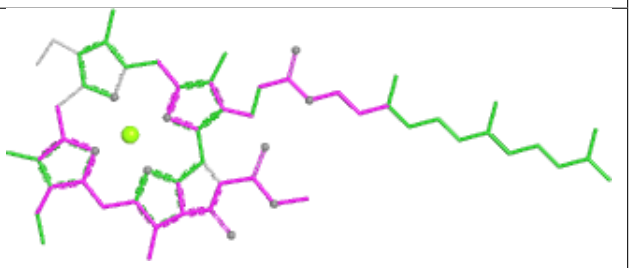

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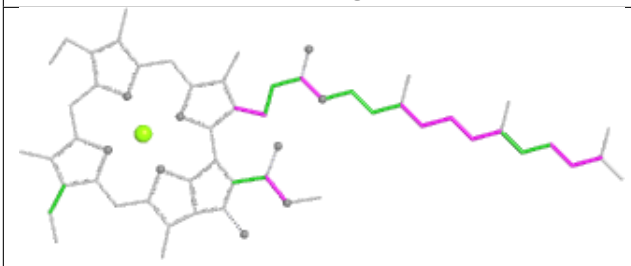

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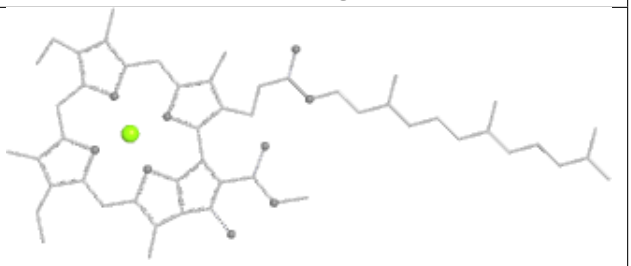
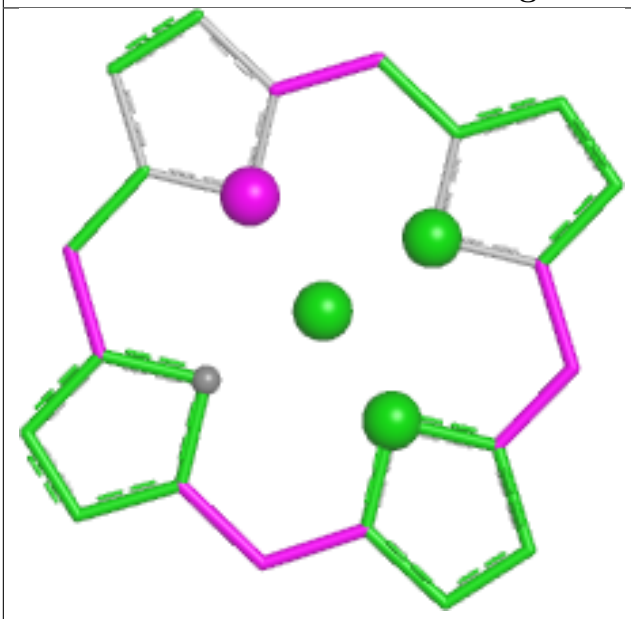


Rings

Ligand CLA 3 3015



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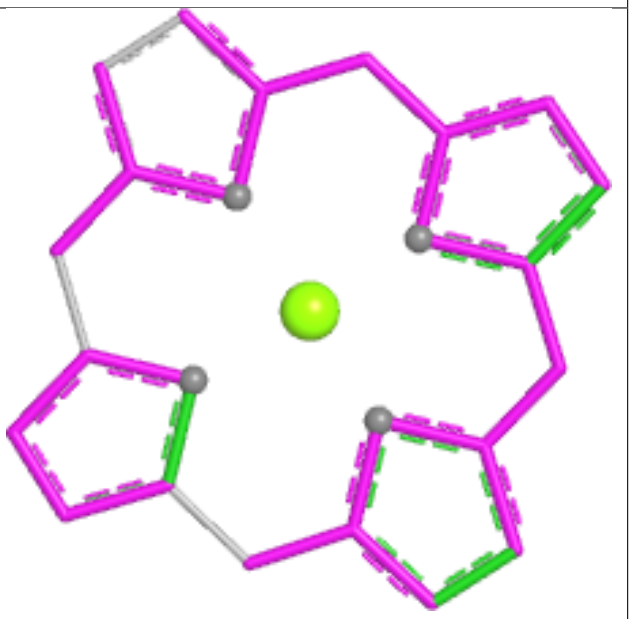

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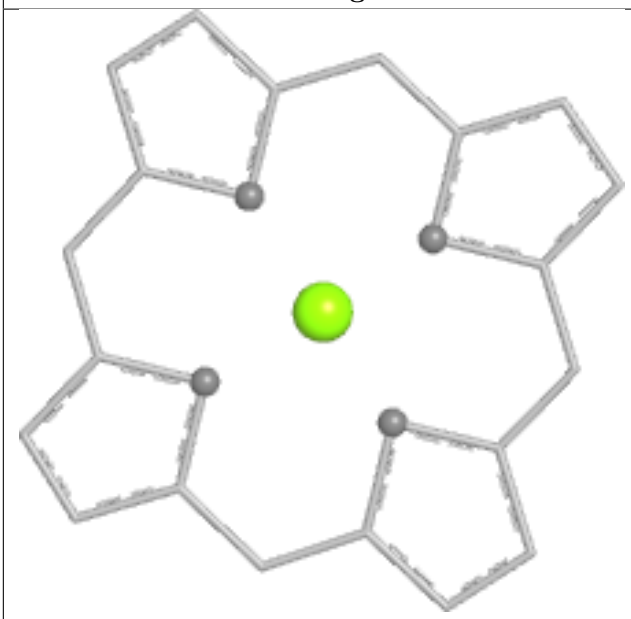

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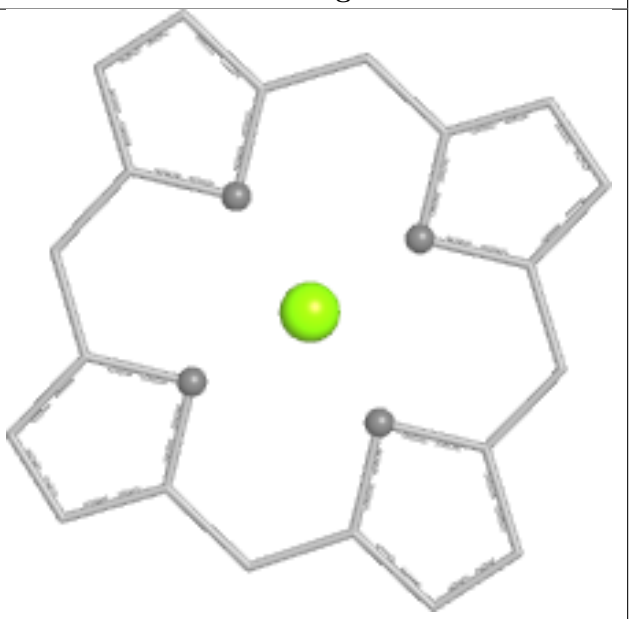
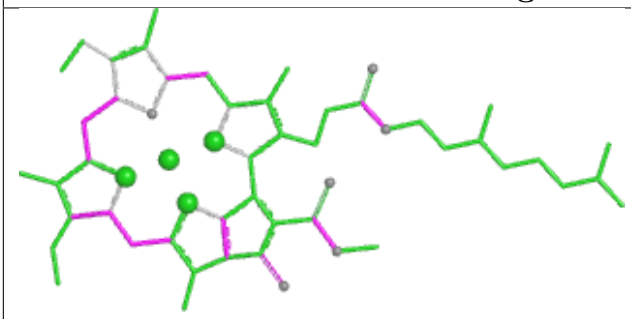


Rings

Ligand CLA L 1505



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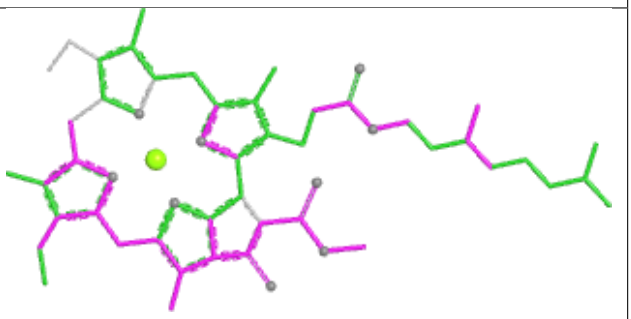
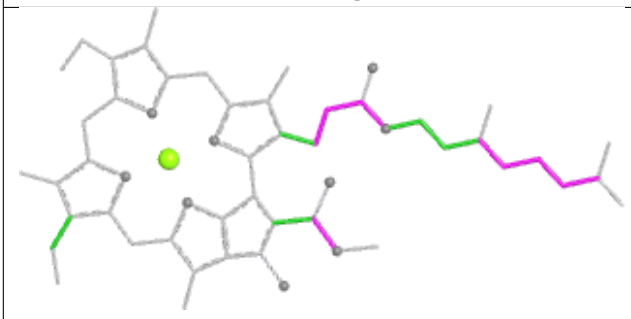


Bond angles



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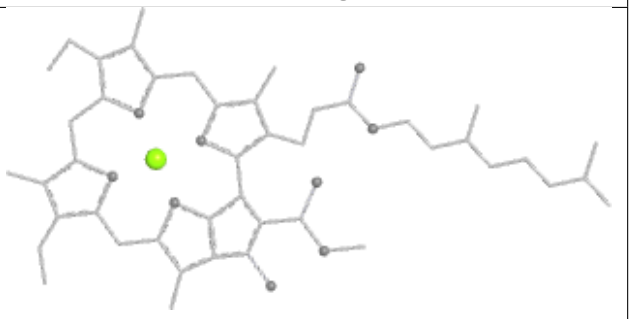
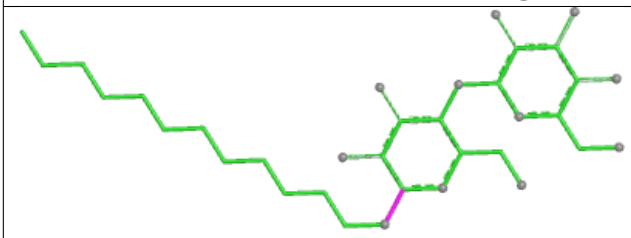


Rings

Ligand LMU 4 1210



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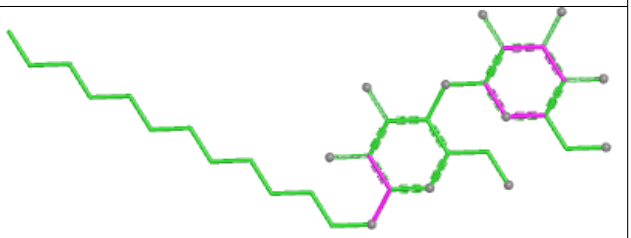

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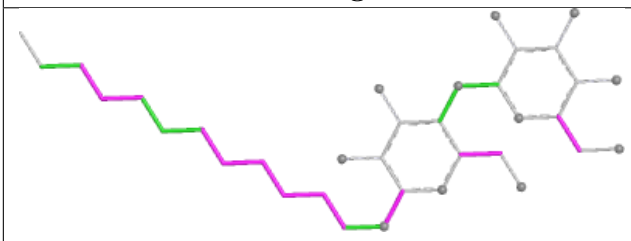

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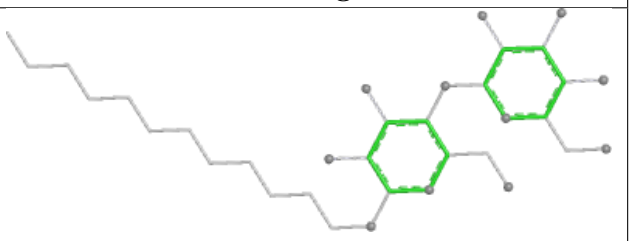
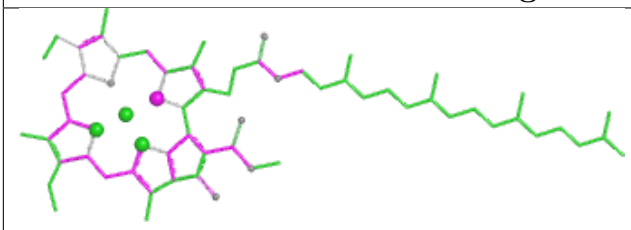
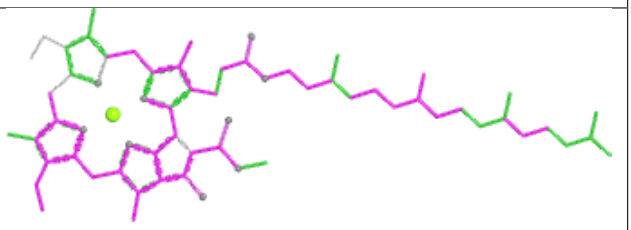
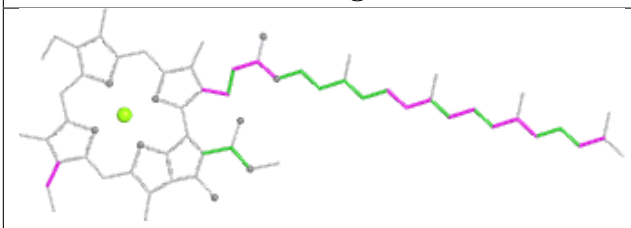
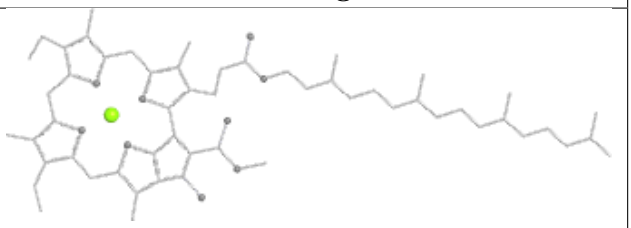
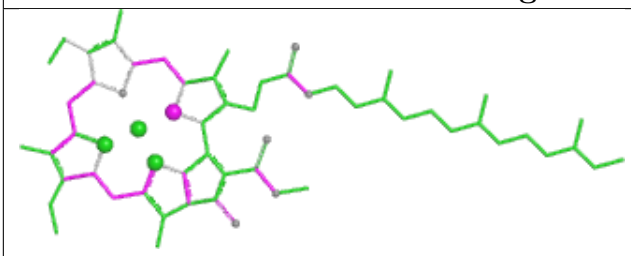
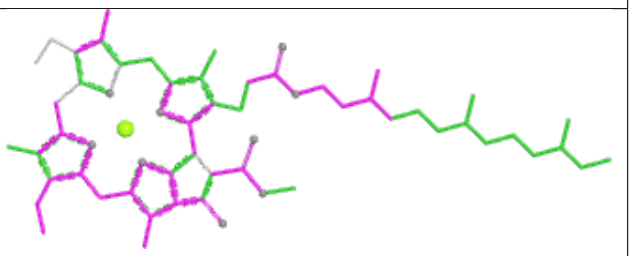
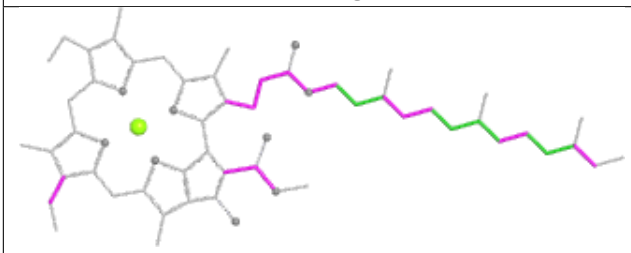
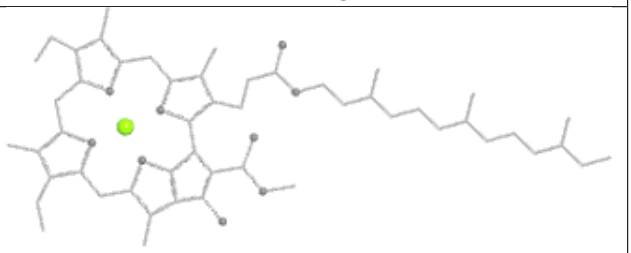
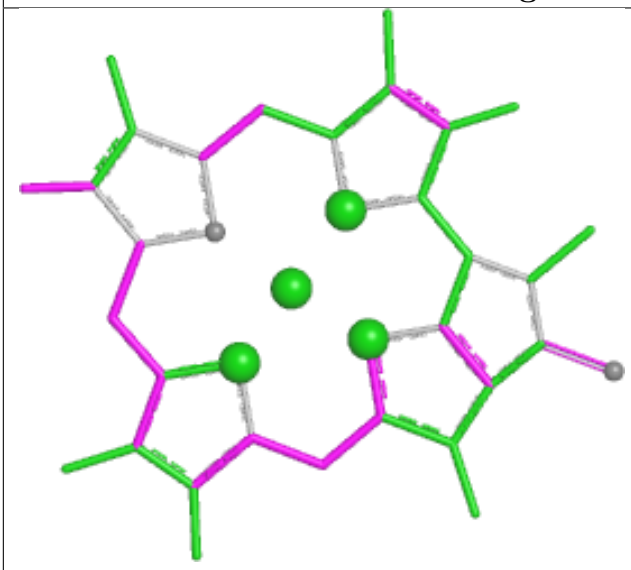


Rings

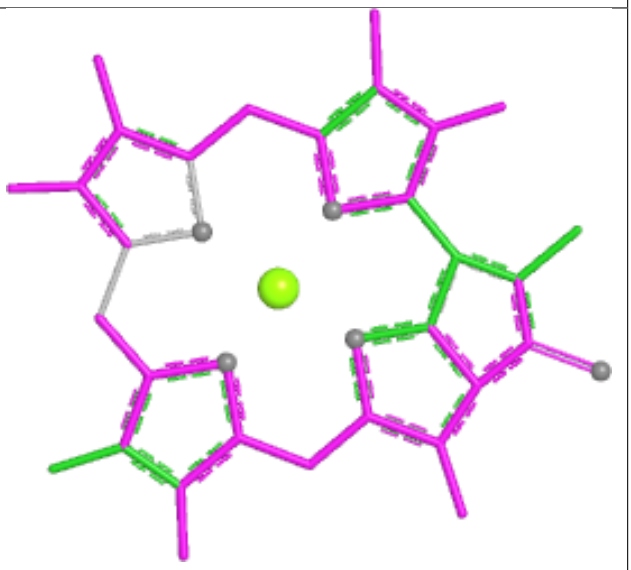
Ligand CLA 4 1198	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1192	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 1197

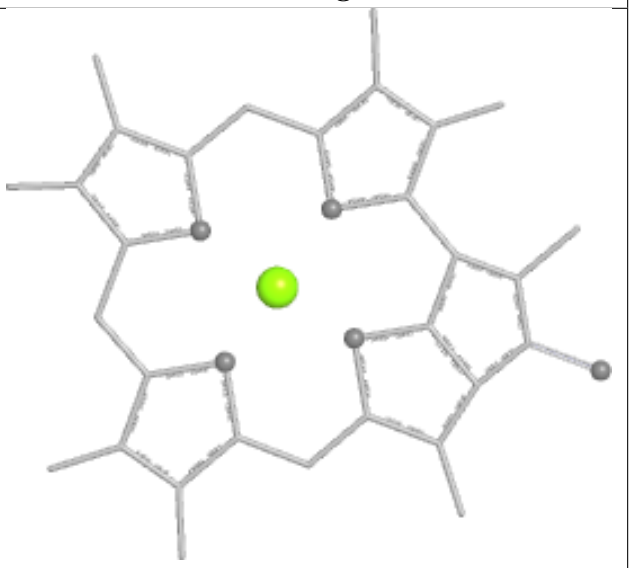


Bond lengths

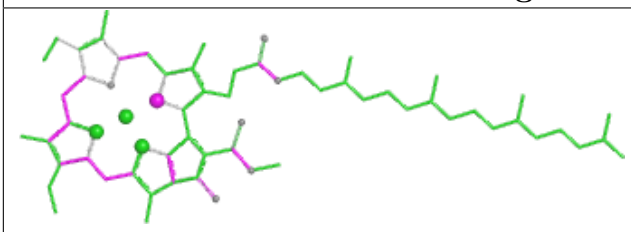
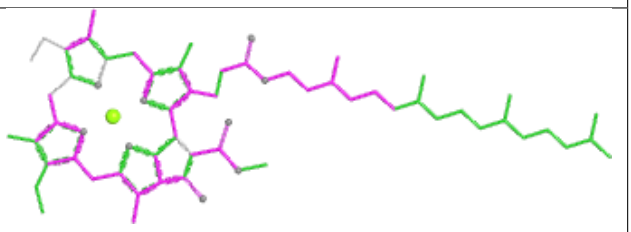
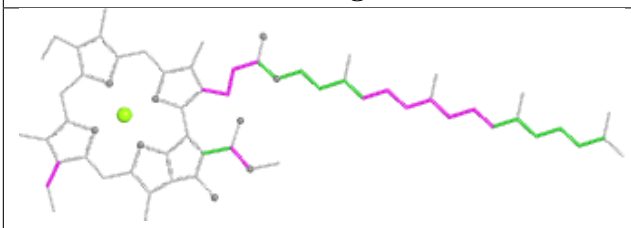
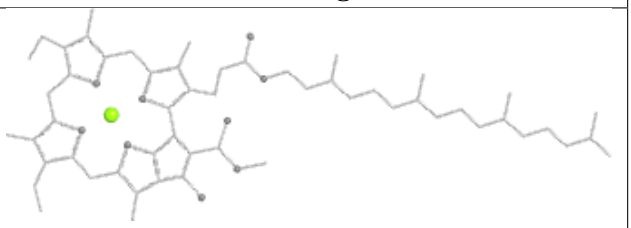


Bond angles

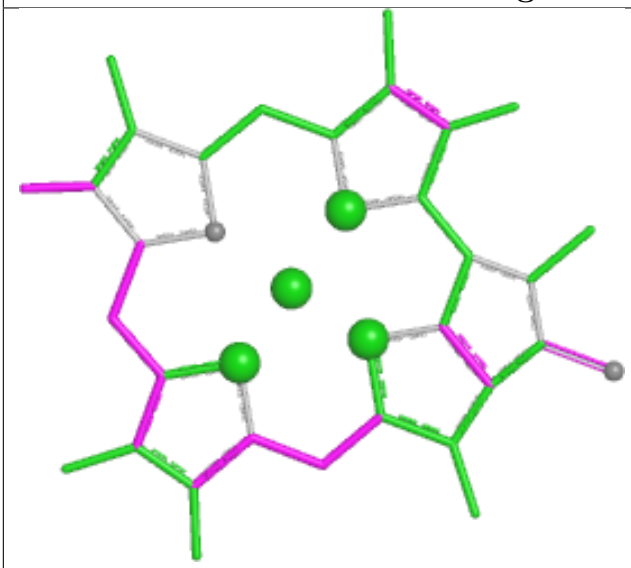
Torsions



Rings

Ligand CLA B 1757	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 1155



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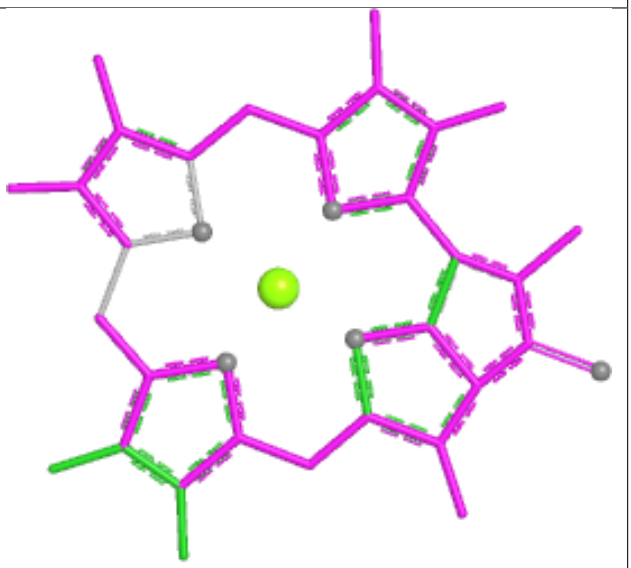
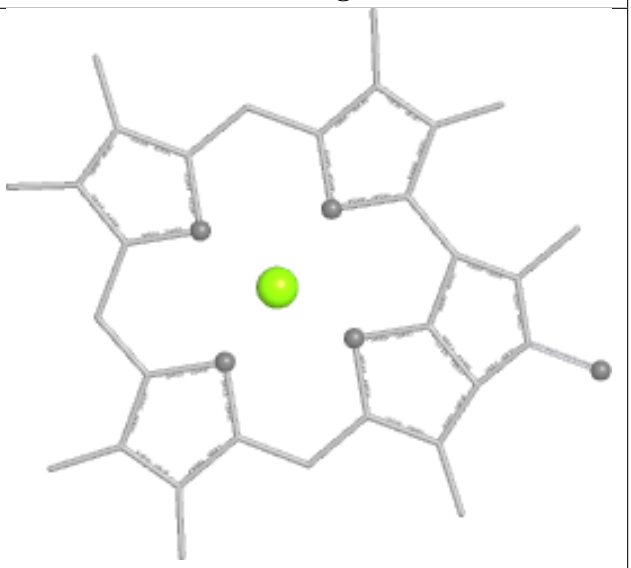


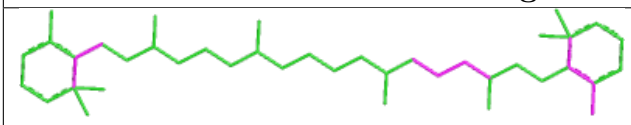
Bond angles

Torsions



Rings

Ligand BCR I 1032



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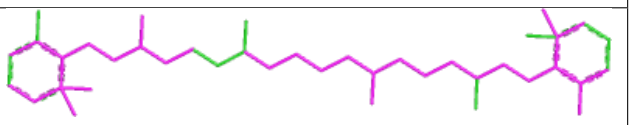
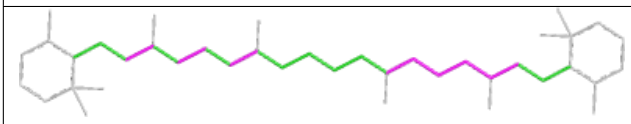
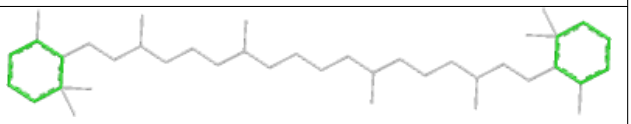


Bond angles

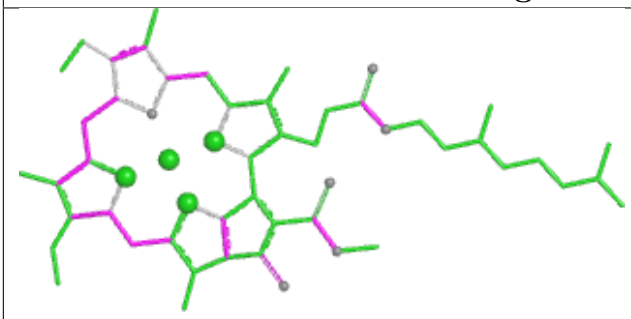


Torsions



Rings

Ligand CLA A 1784



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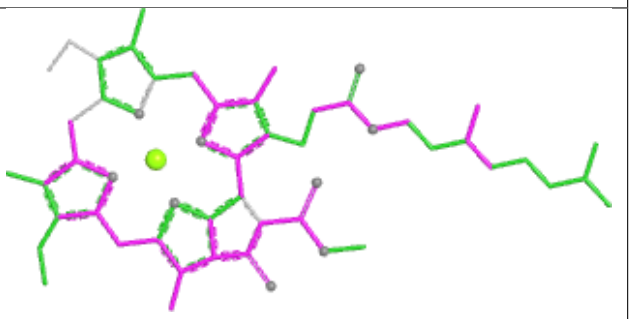
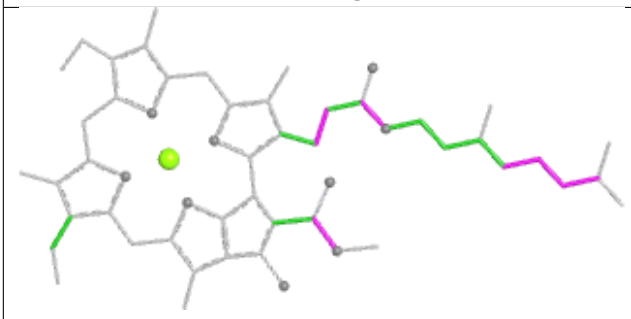


Bond angles



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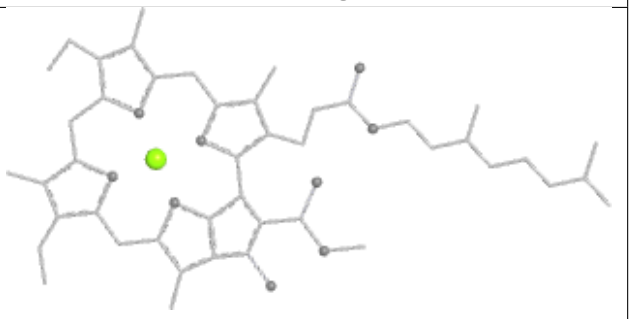
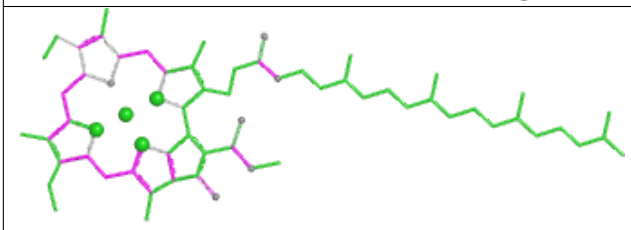


Rings

Ligand CLA B 1758



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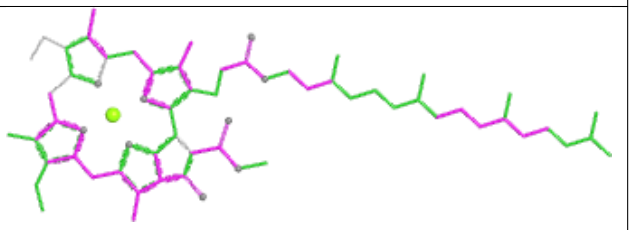
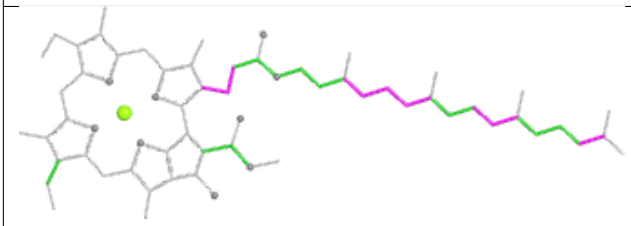


Bond angles



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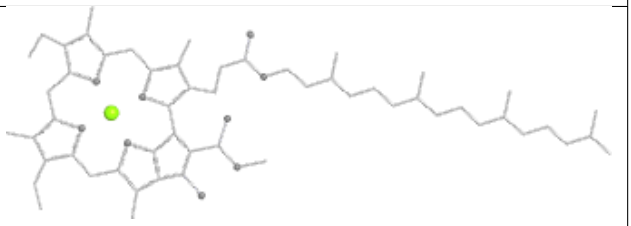
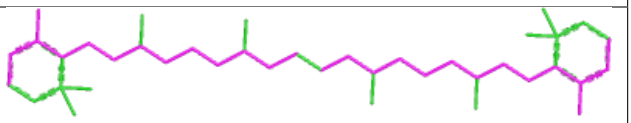


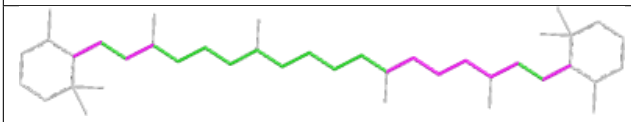
Rings

Ligand BCR B 1780

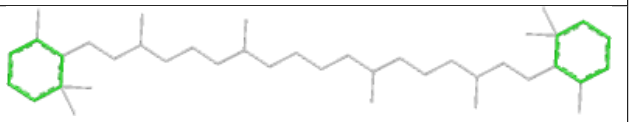
Bond lengths



Bond angles

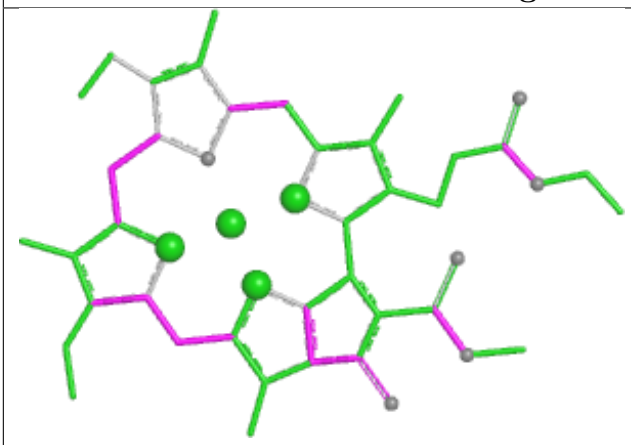


Torsions

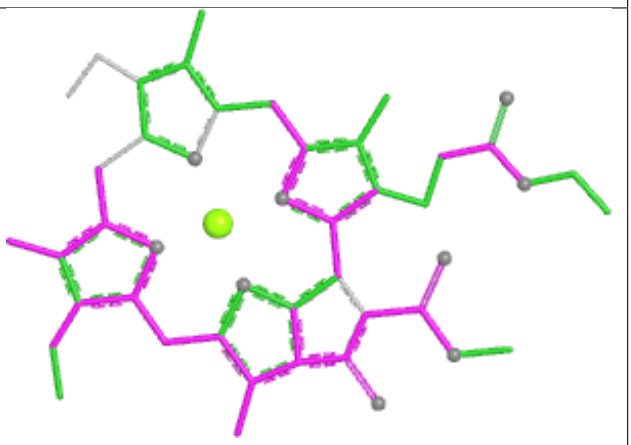


Rings

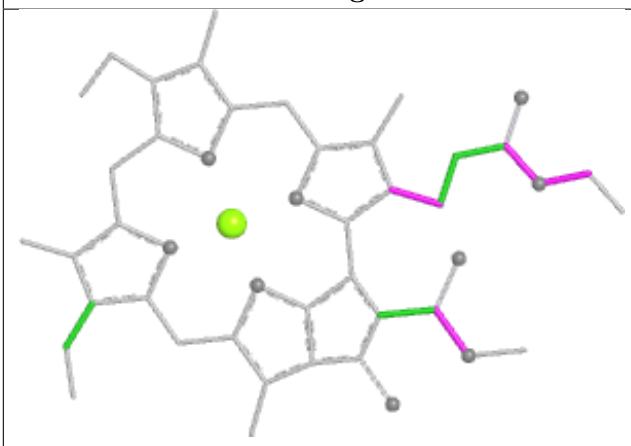
Ligand CLA 1 1189



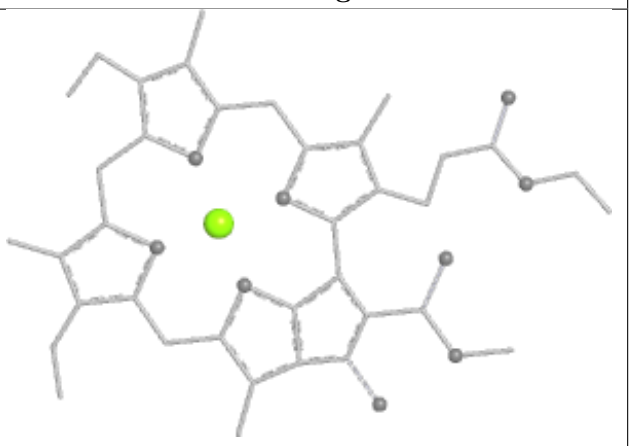
Bond lengths



Bond angles

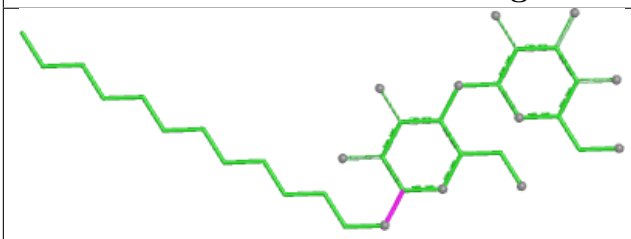


Torsions

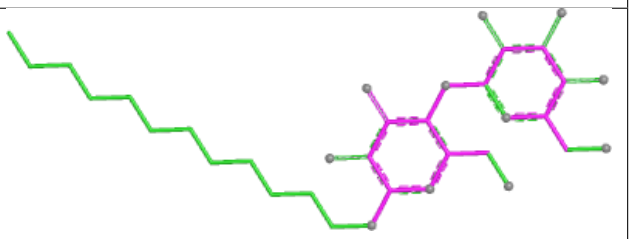


Rings

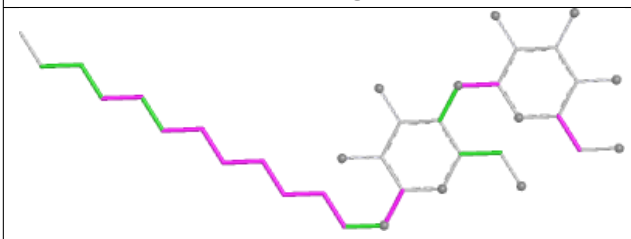
Ligand LMU A 7027



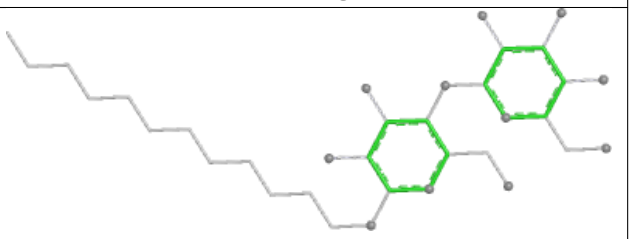
Bond lengths



Bond angles

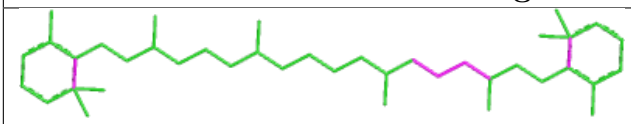


Torsions

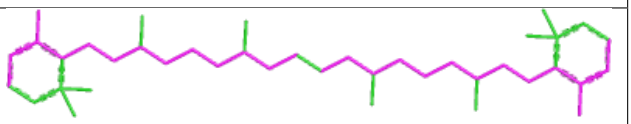


Rings

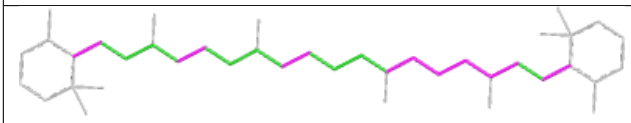
Ligand BCR B 1777



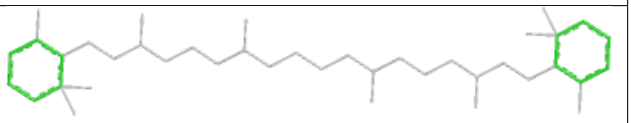
Bond lengths



Bond angles

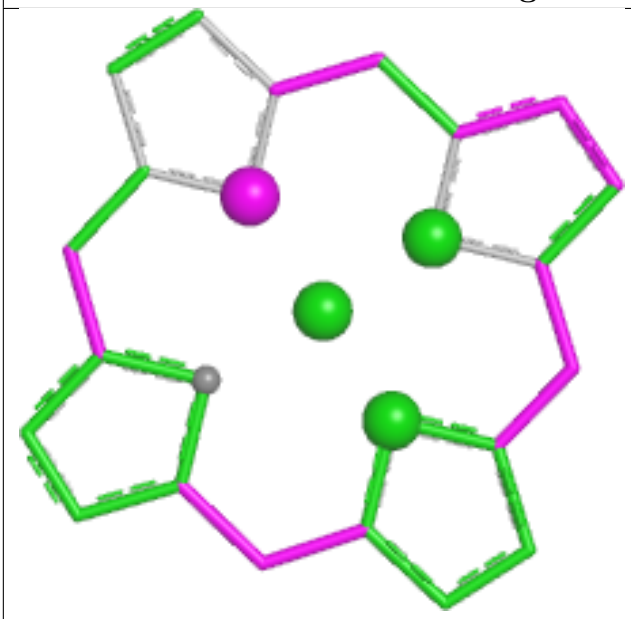


Torsions

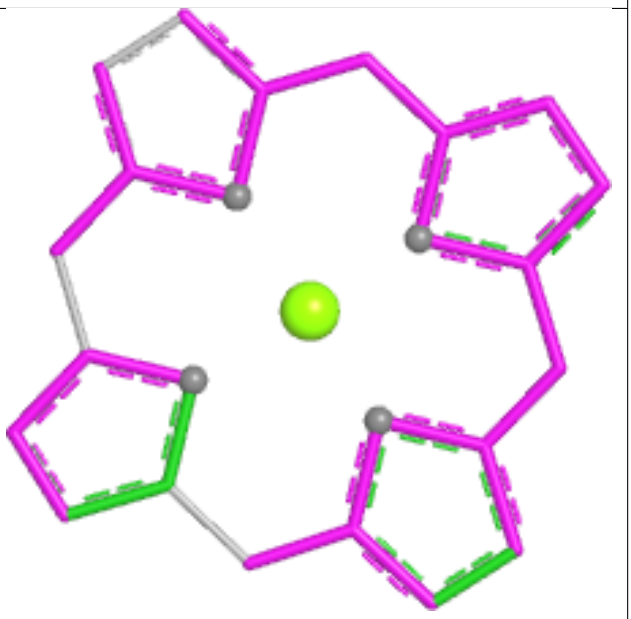


Rings

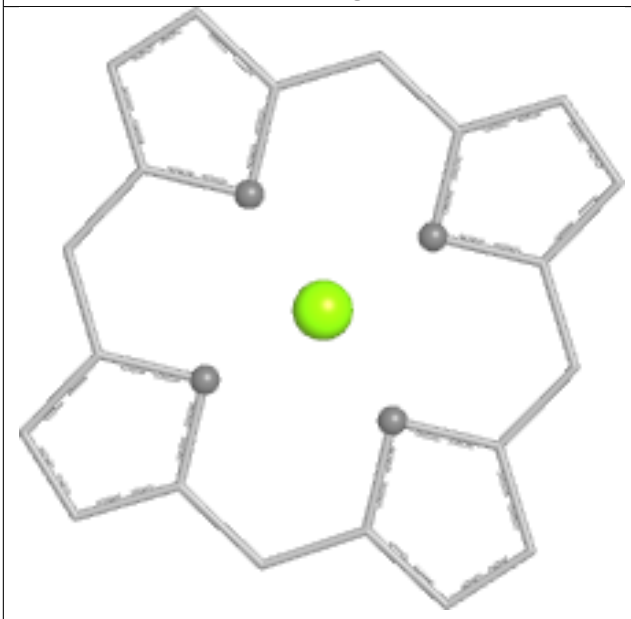
Ligand CLA 3 3001



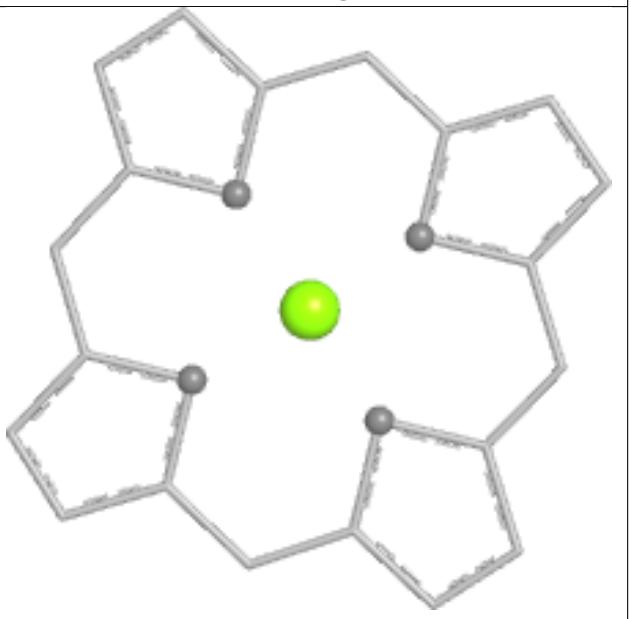
Bond lengths



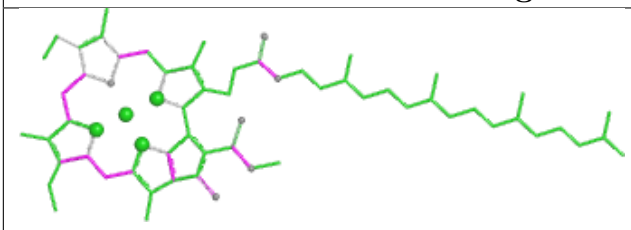
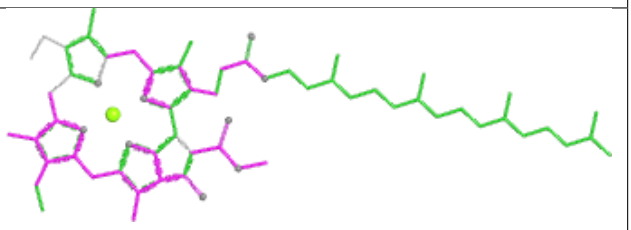
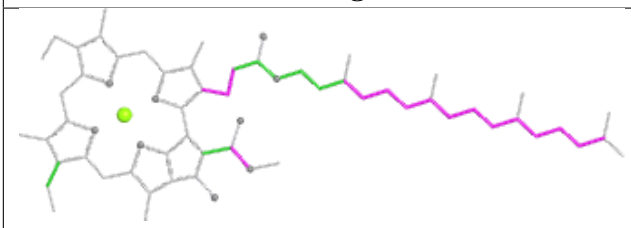
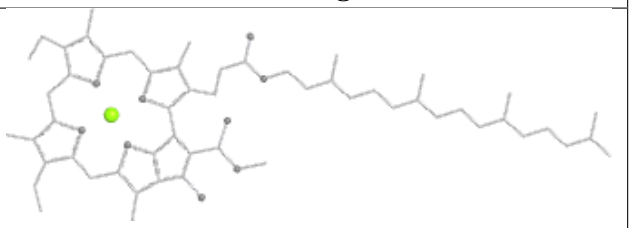
Bond angles

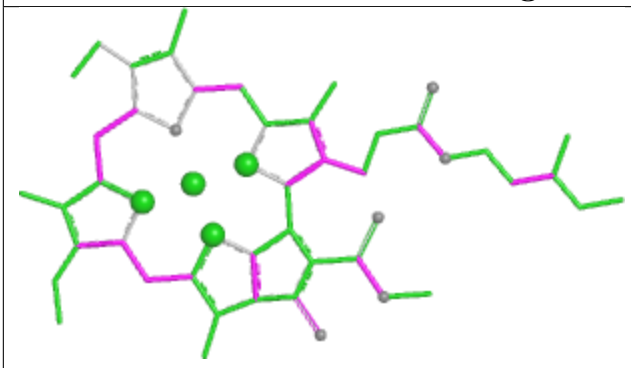
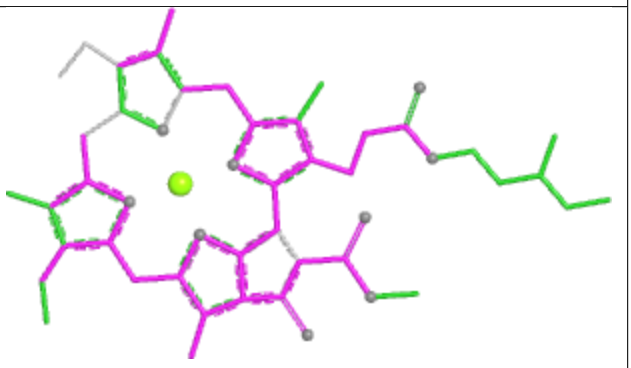
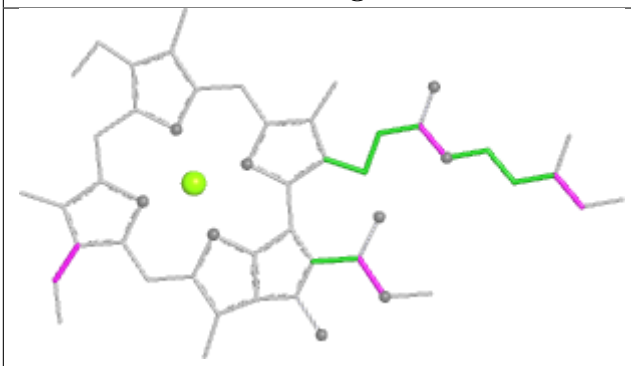
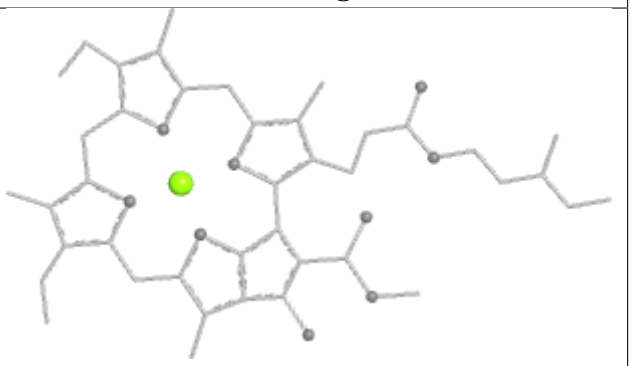


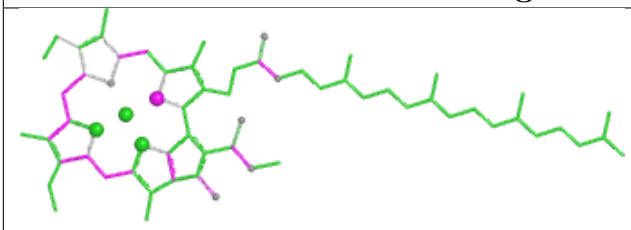
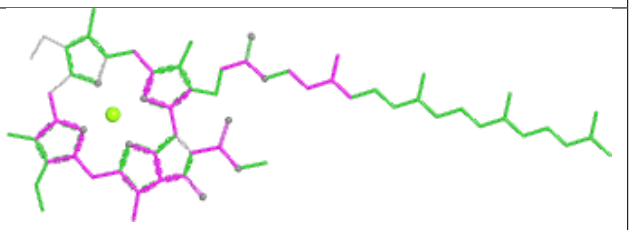
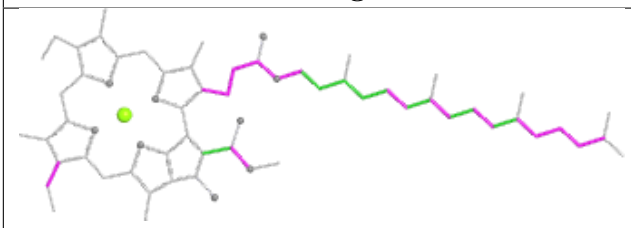
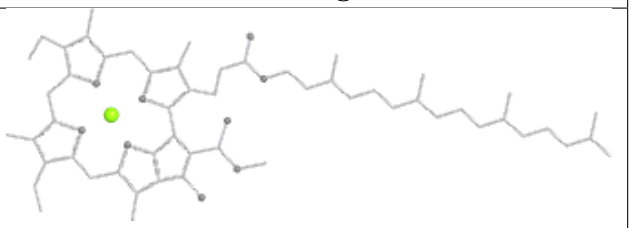
Torsions

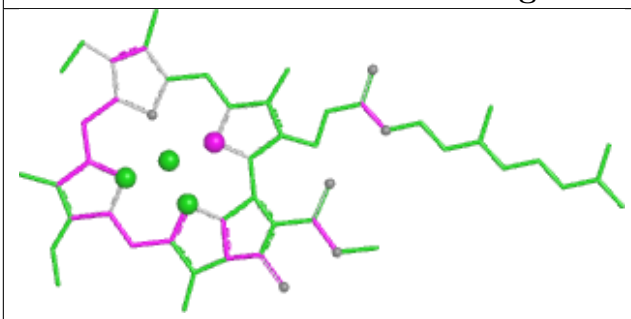
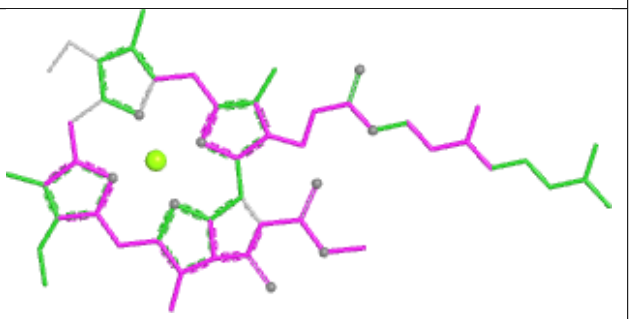
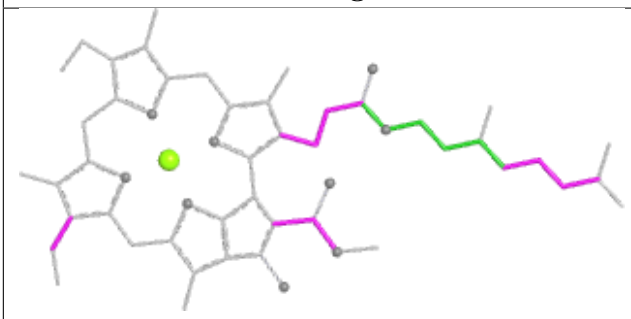
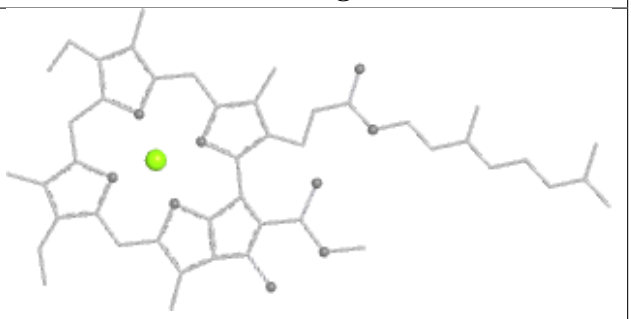


Rings

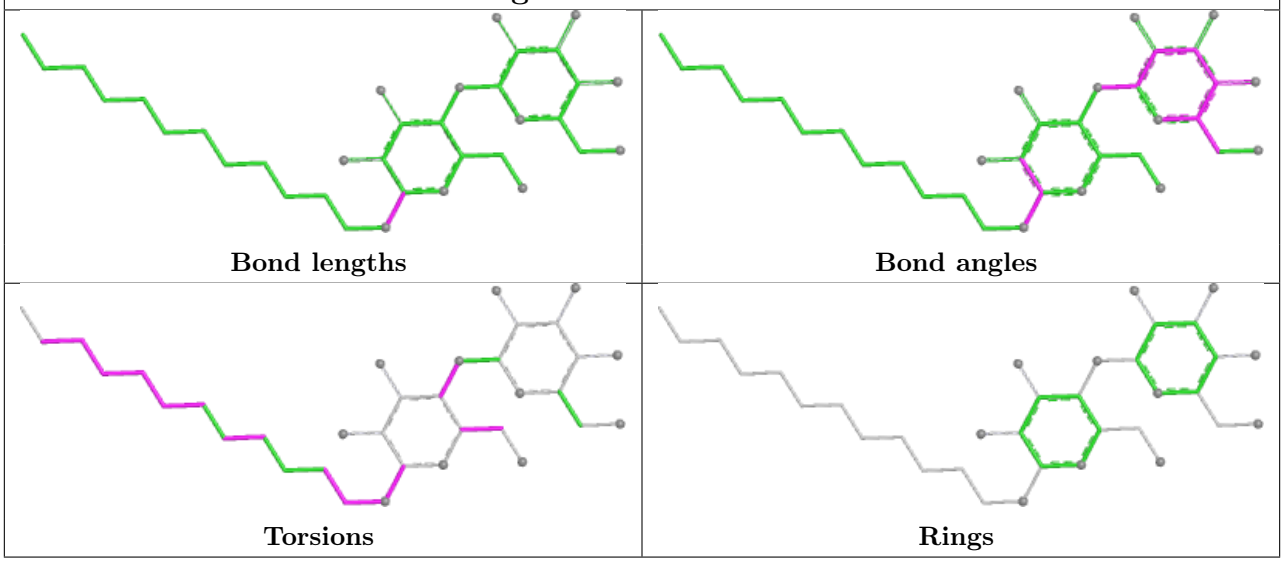
Ligand CLA B 1744	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1193	
 Bond lengths	 Bond angles
 Torsions	 Rings

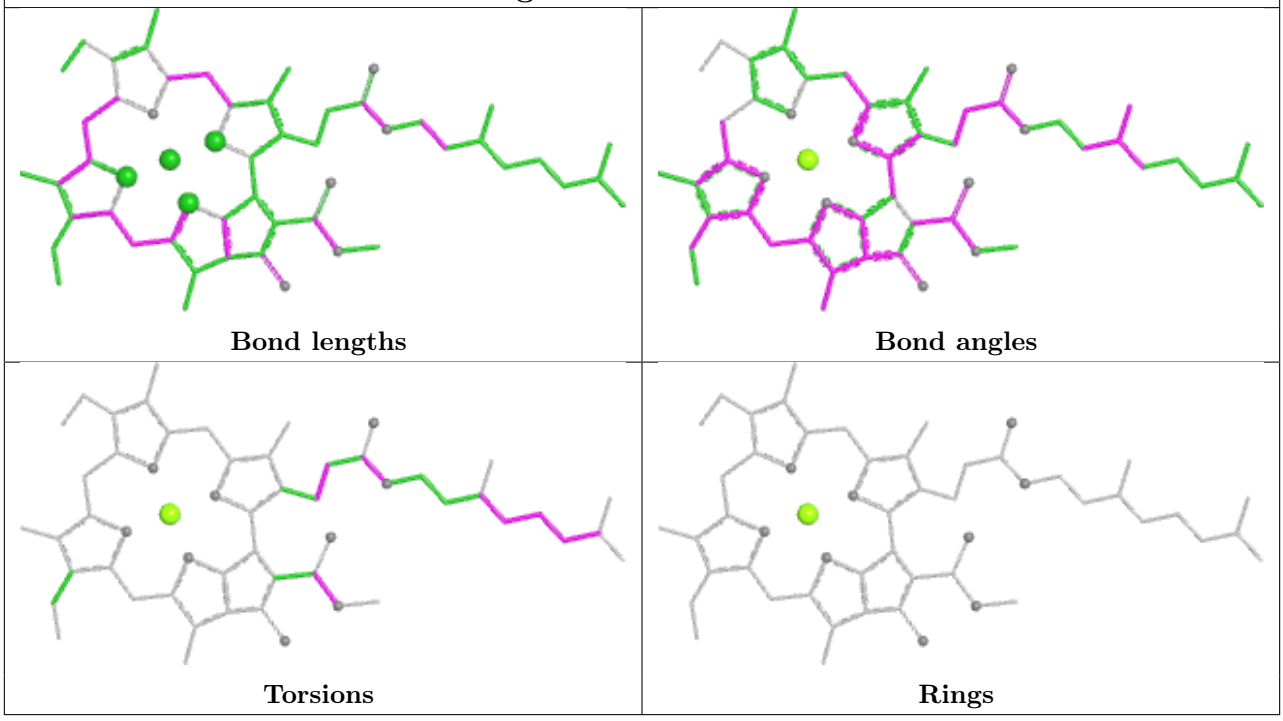
Ligand CLA B 1735	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA J 1045	
 Bond lengths	 Bond angles
 Torsions	 Rings

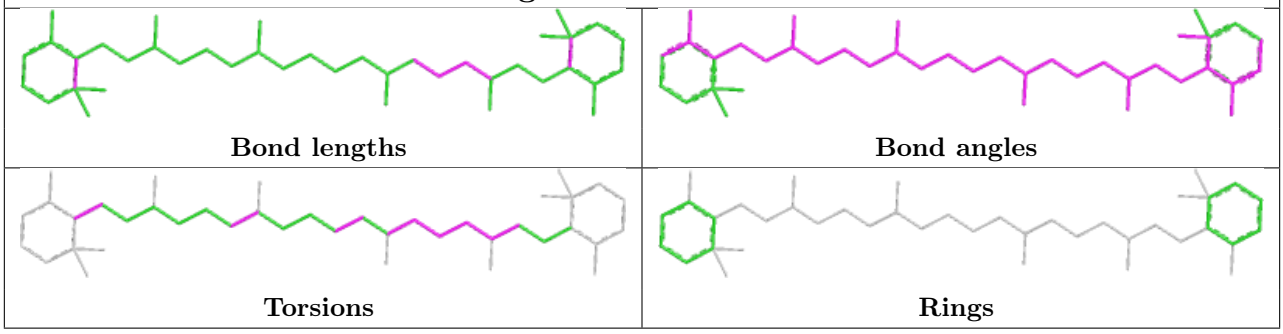
Ligand LMU A 7015



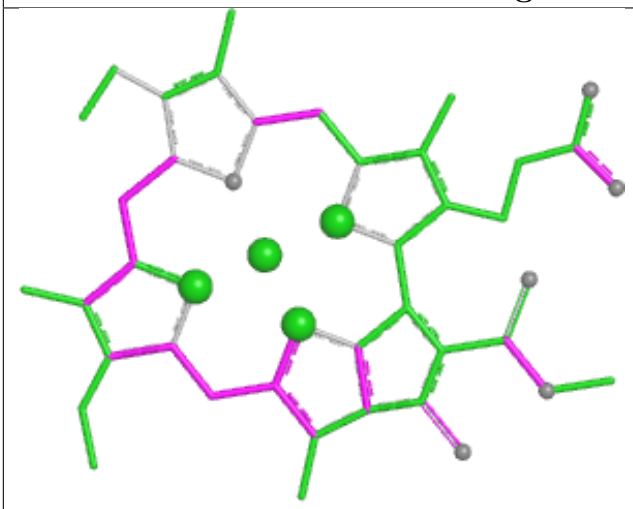
Ligand CLA B 1742



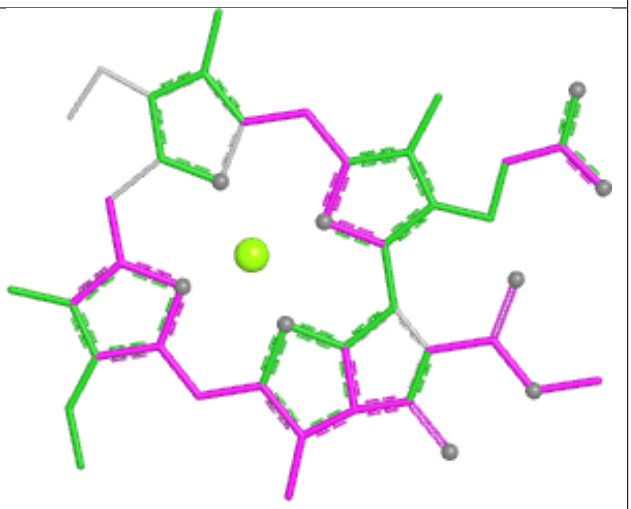
Ligand BCR 3 1220



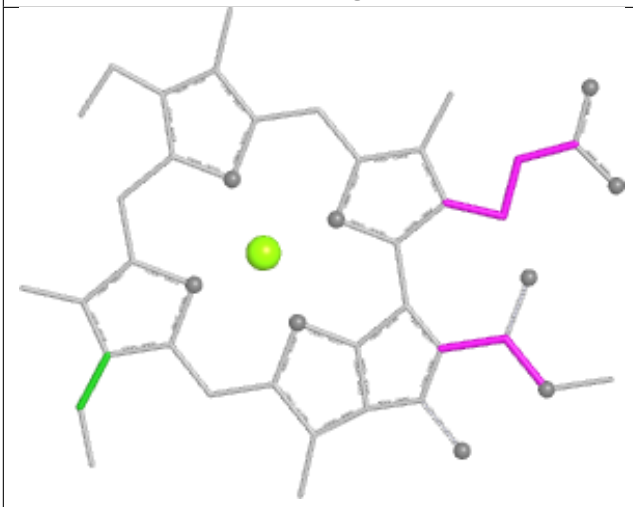
Ligand CLA B 1764



Bond lengths



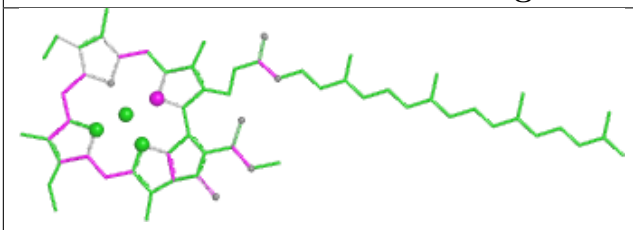
Bond angles



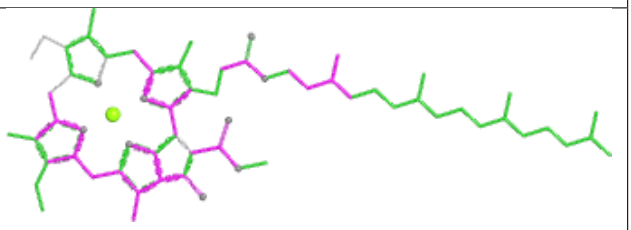
Torsions

Rings

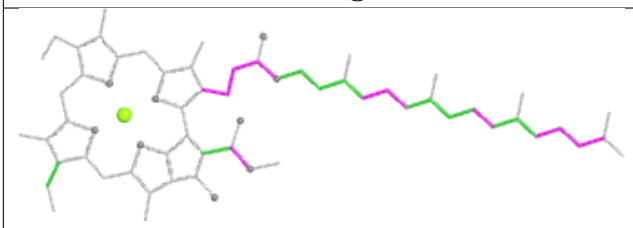
Ligand CLA A 1796



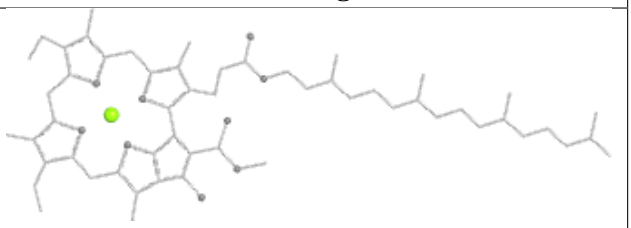
Bond lengths



Bond angles

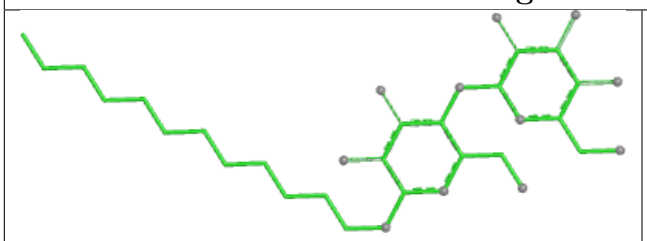


Torsions

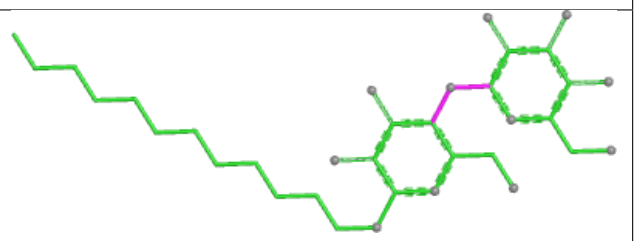


Rings

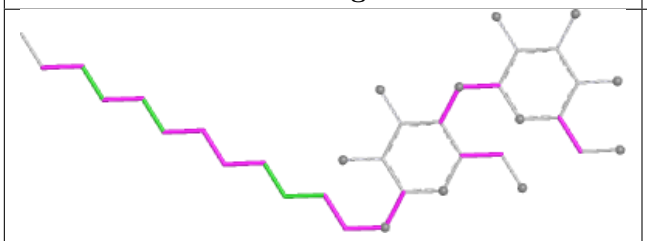
Ligand LMU 2 7006



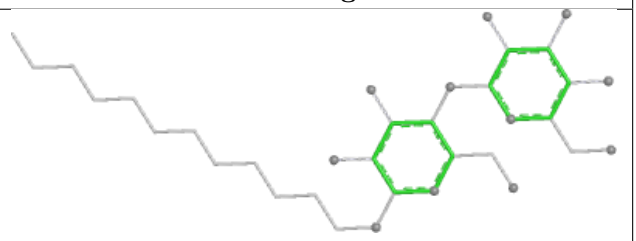
Bond lengths



Bond angles

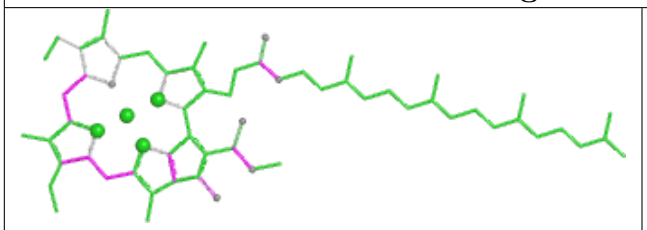


Torsions

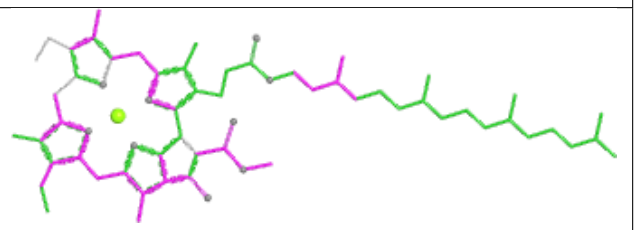


Rings

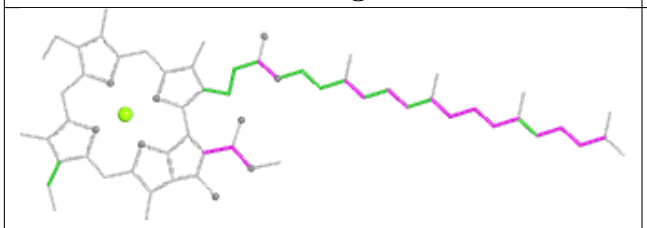
Ligand CLA 3 3011



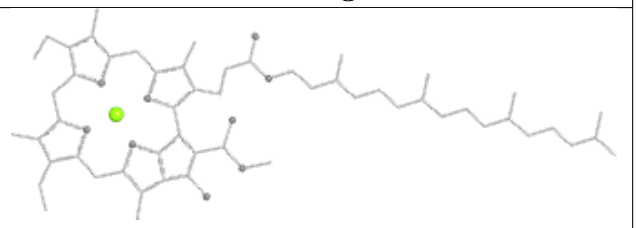
Bond lengths



Bond angles

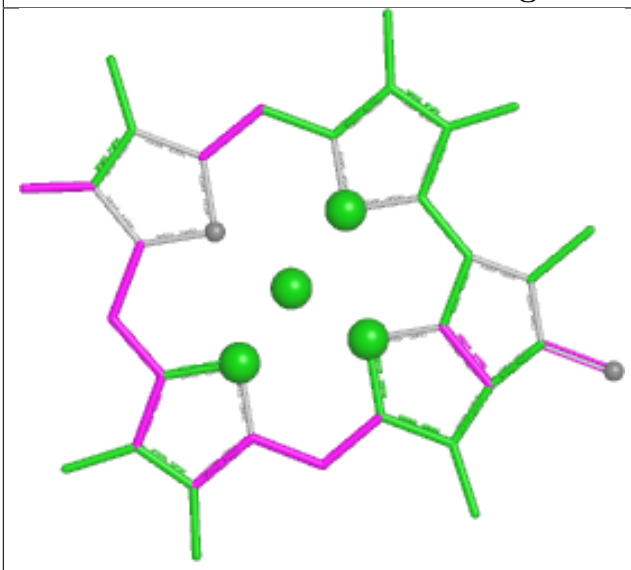


Torsions



Rings

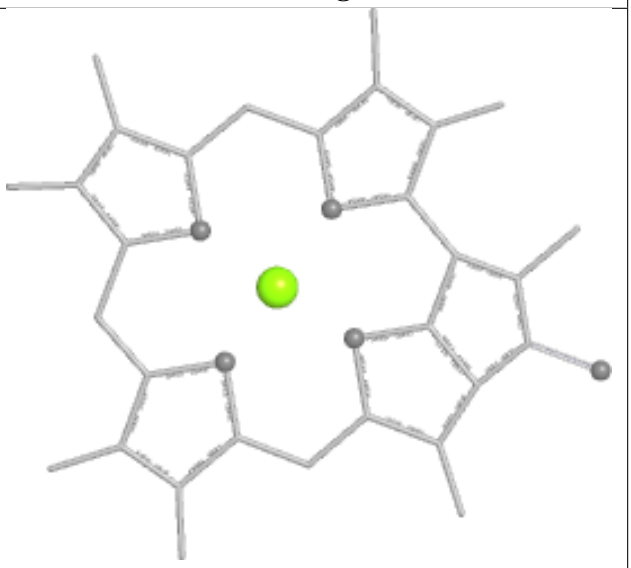
Ligand CLA 3 1212



Bond lengths

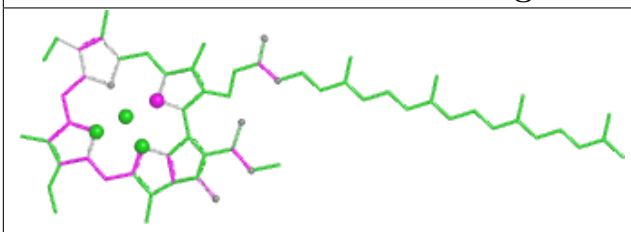
Bond angles

Torsions

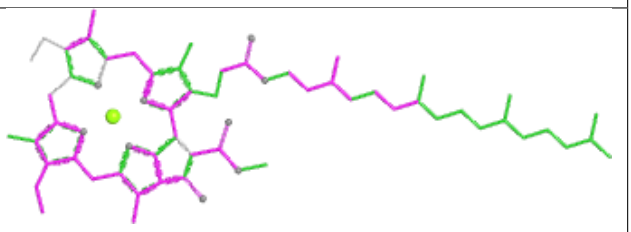


Rings

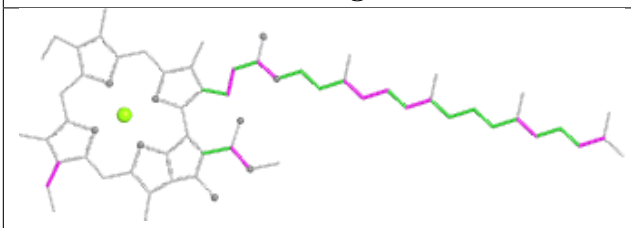
Ligand CLA A 1772



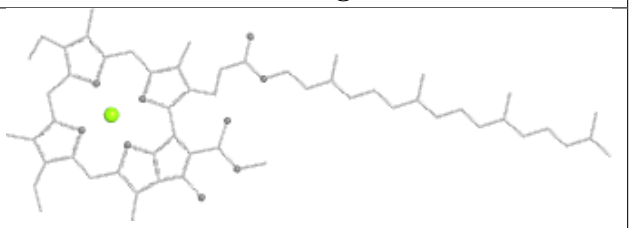
Bond lengths



Bond angles

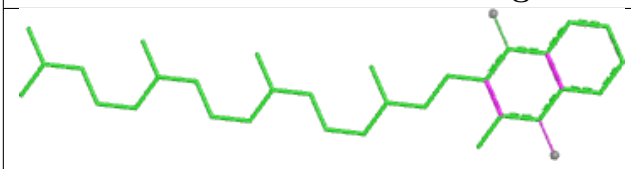


Torsions

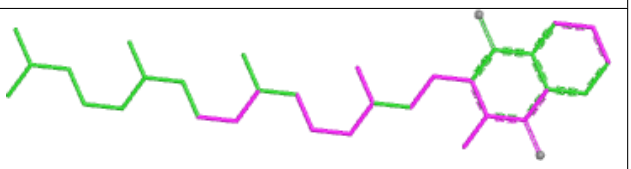


Rings

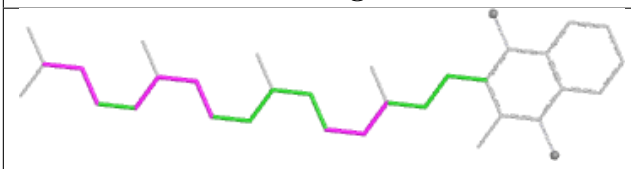
Ligand PQN A 1802



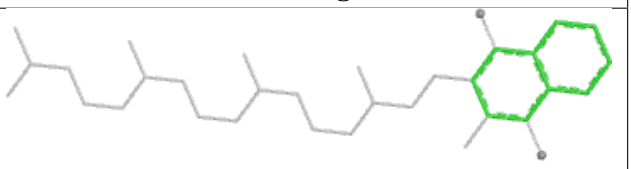
Bond lengths



Bond angles

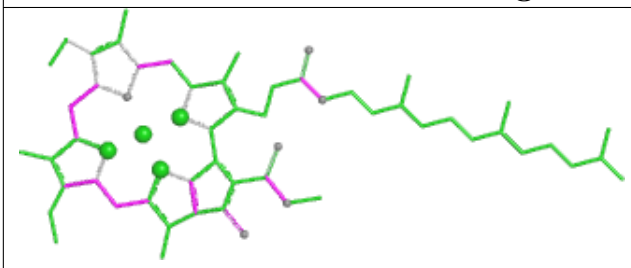


Torsions

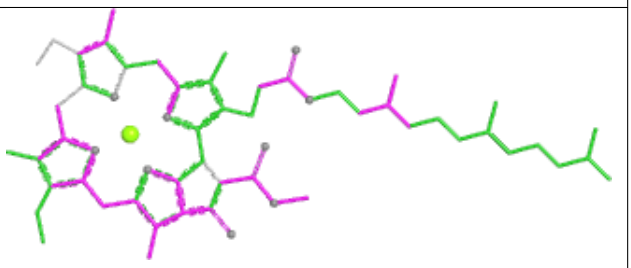


Rings

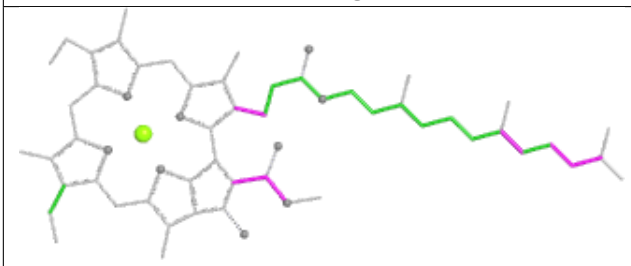
Ligand CLA B 1745



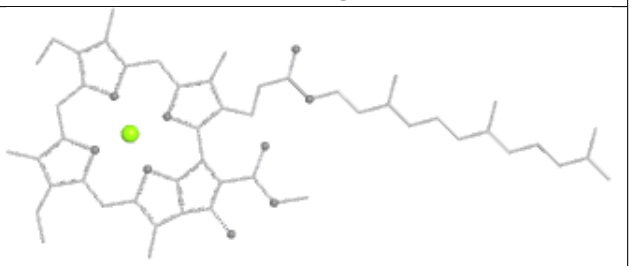
Bond lengths



Bond angles

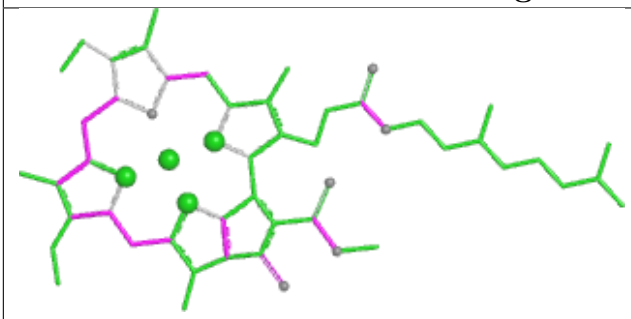


Torsions

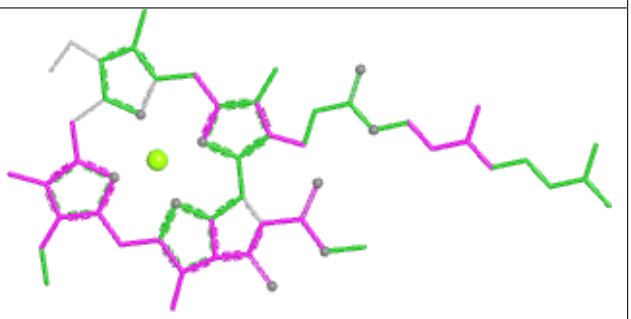


Rings

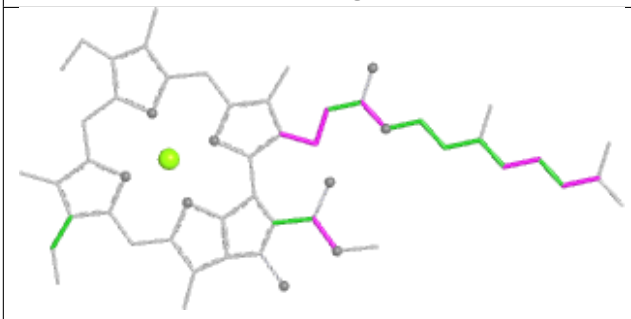
Ligand CLA A 1779



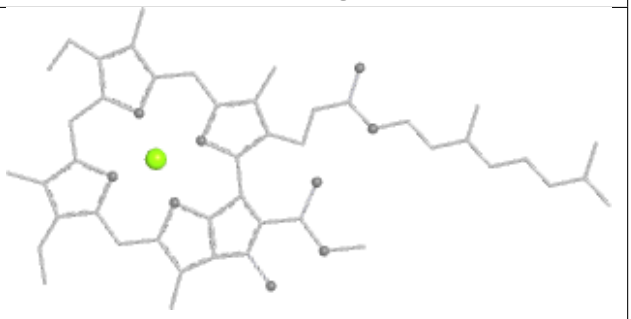
Bond lengths



Bond angles

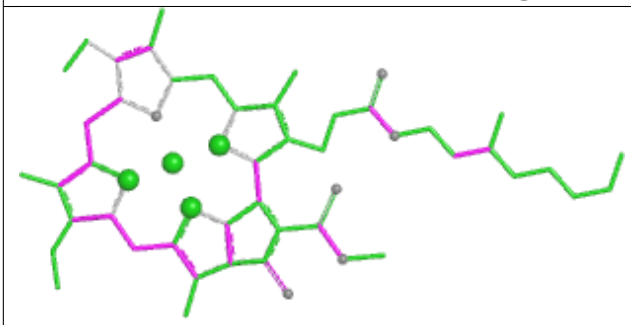


Torsions



Rings

Ligand CLA B 1754



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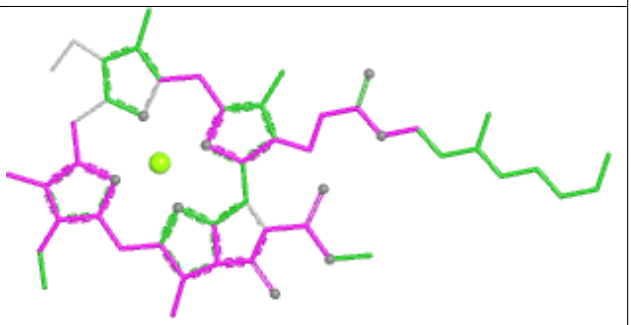
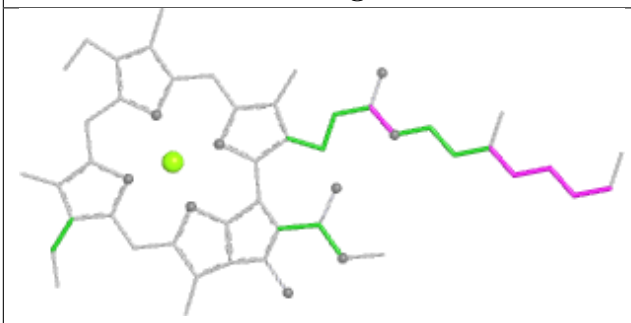
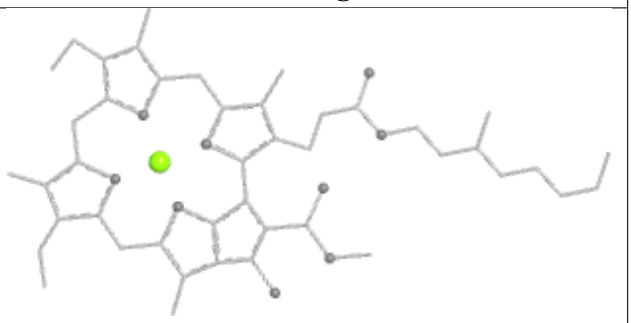


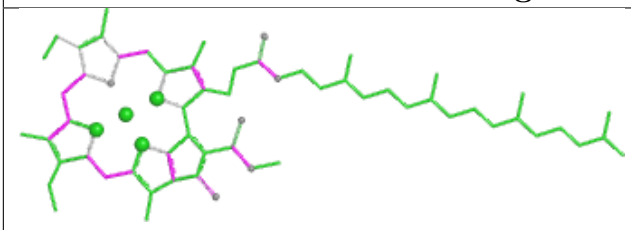
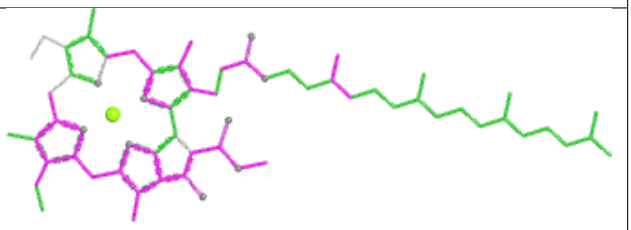
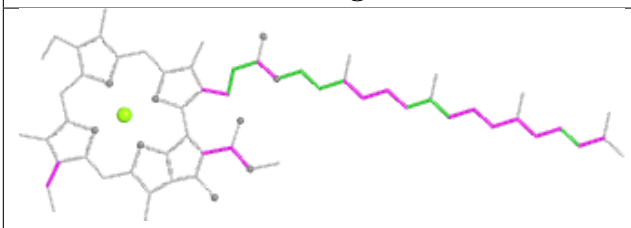
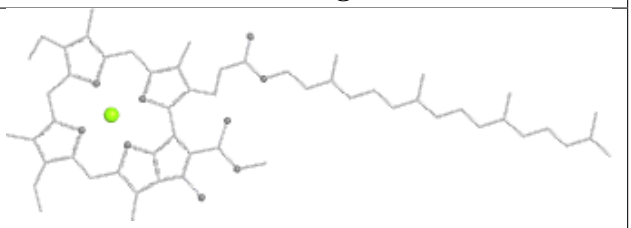
Bond angles

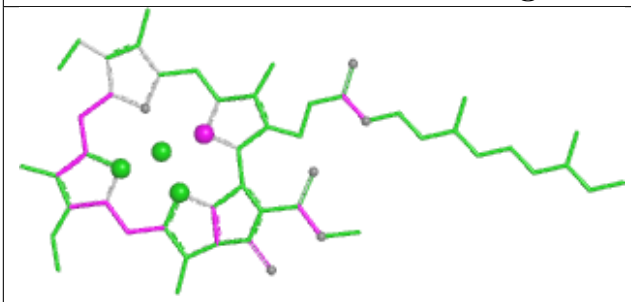
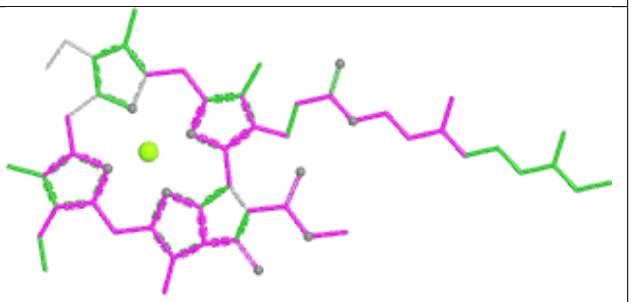
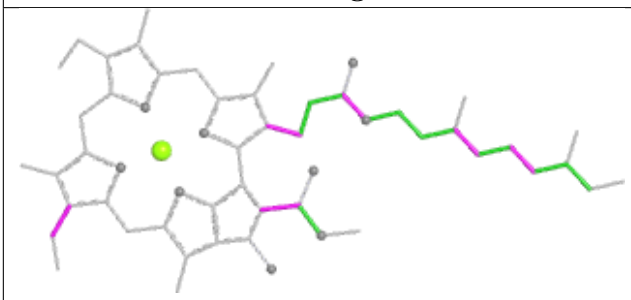
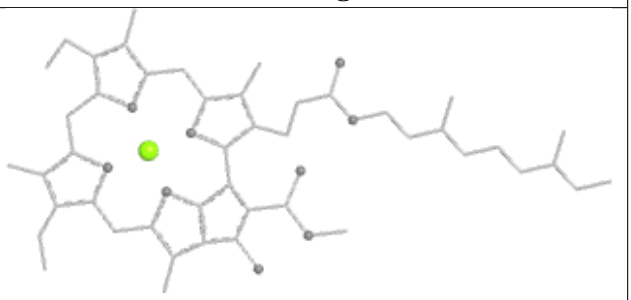


Torsions

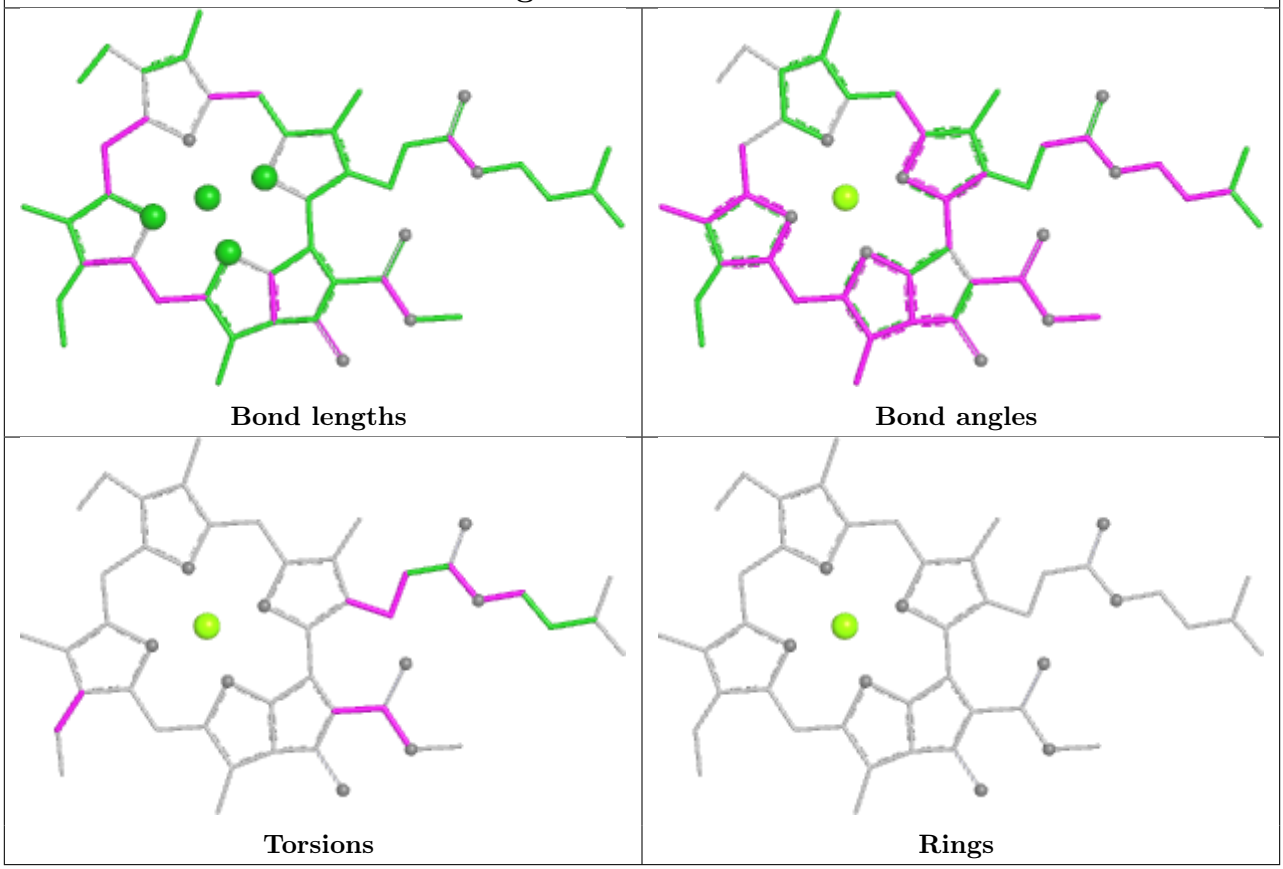


Rings

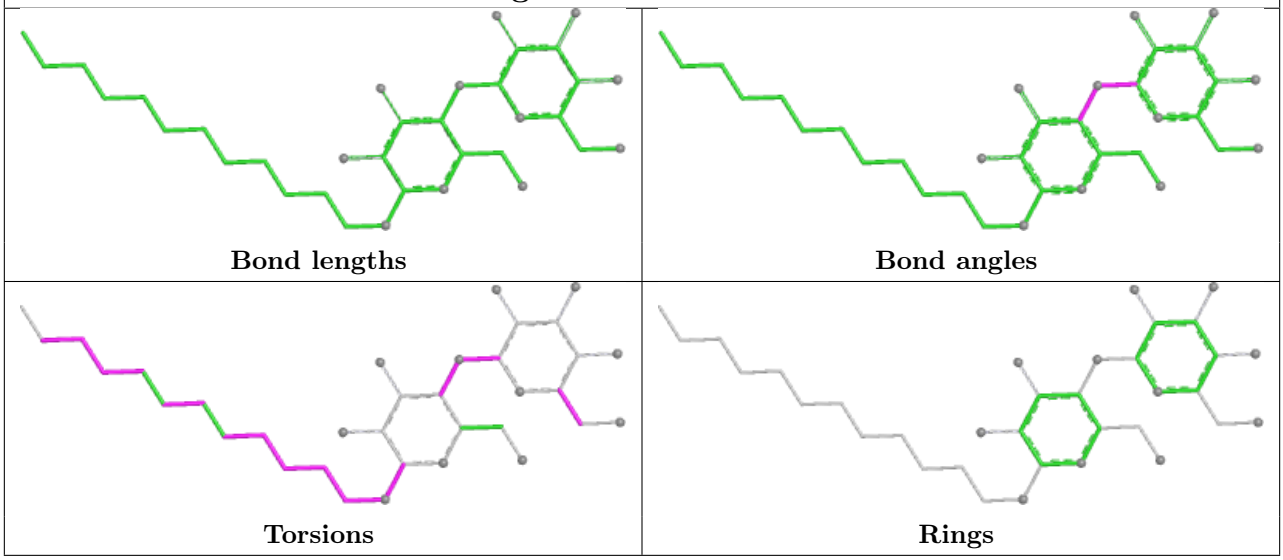
Ligand CLA A 1789	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 1213	
 Bond lengths	 Bond angles
 Torsions	 Rings

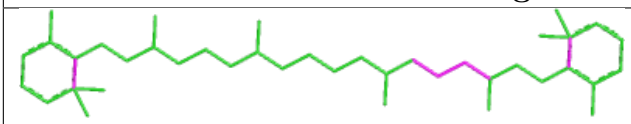
Ligand CLA B 1761



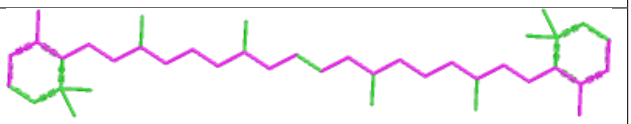
Ligand LMU R 1056



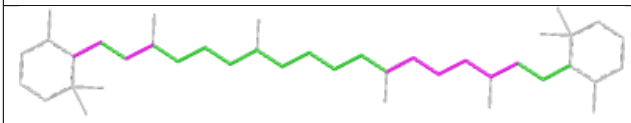
Ligand BCR A 1808



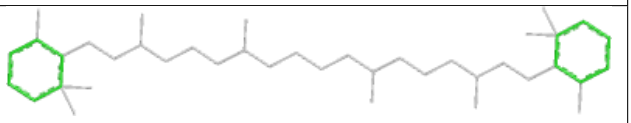
Bond lengths



Bond angles

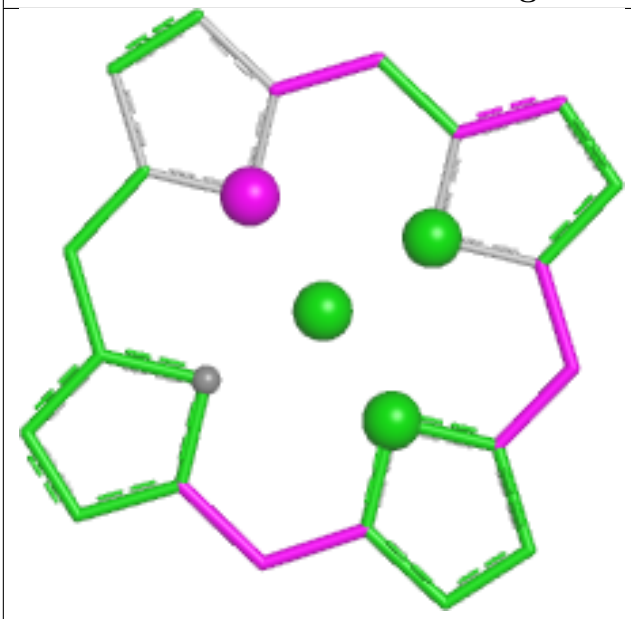


Torsions

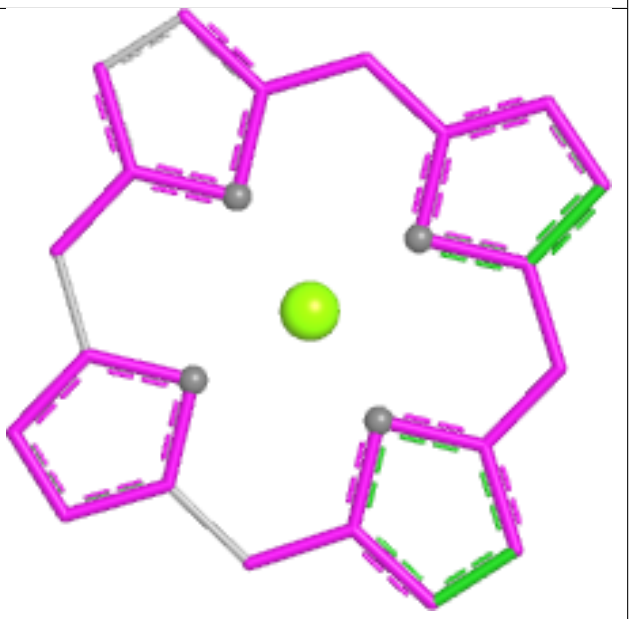


Rings

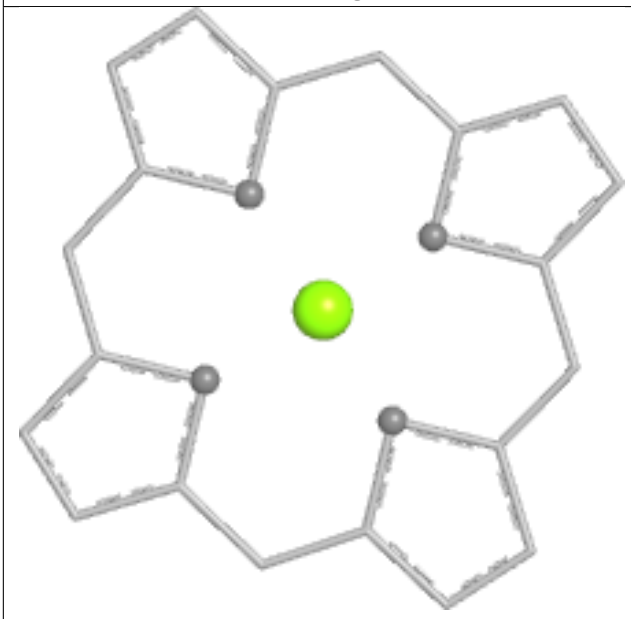
Ligand CLA 2 1219



Bond lengths



Bond angles



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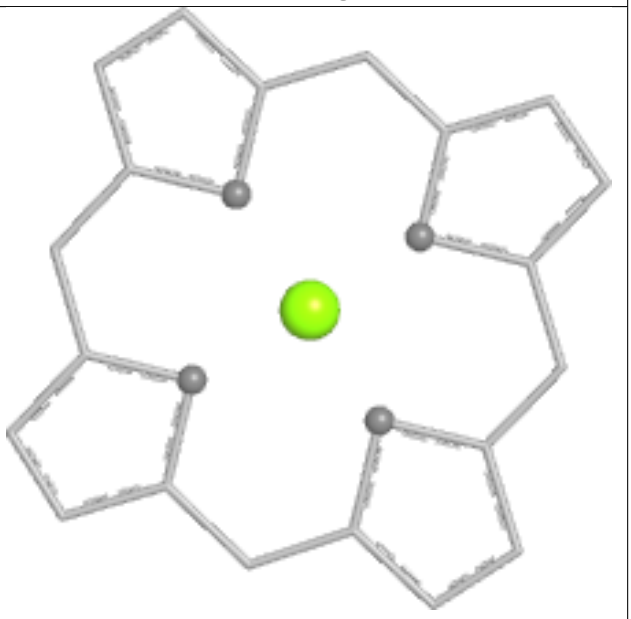
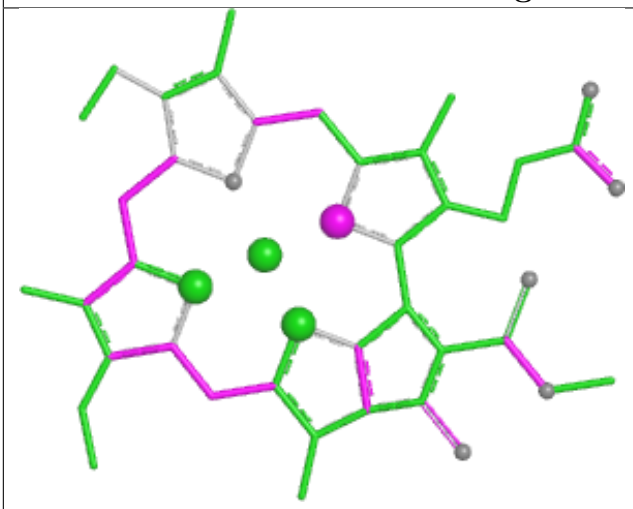
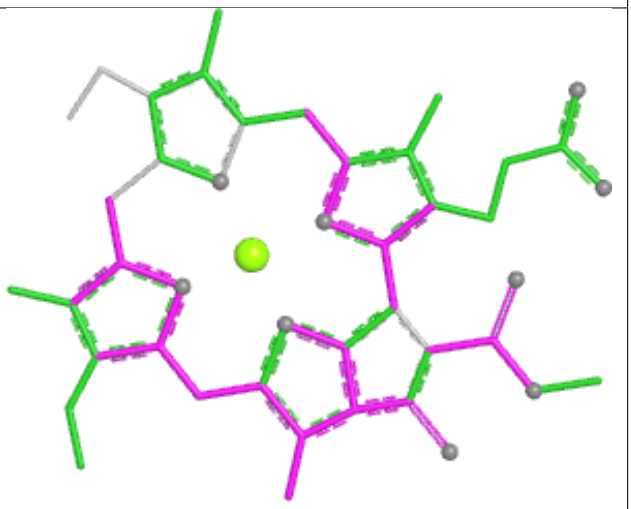


Rings

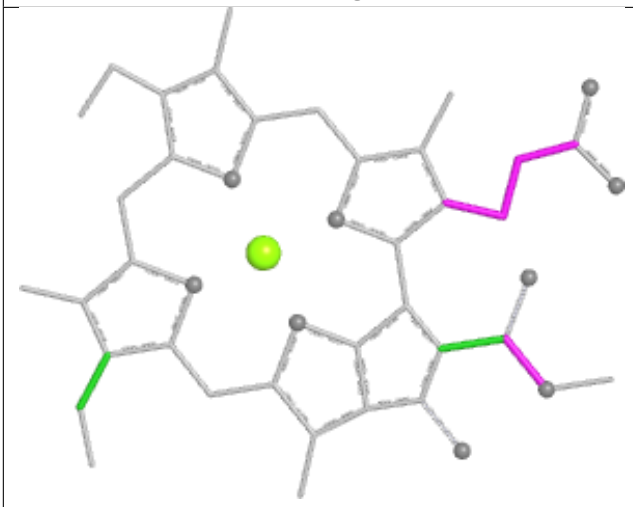
Ligand CLA A 1791



Bond lengths



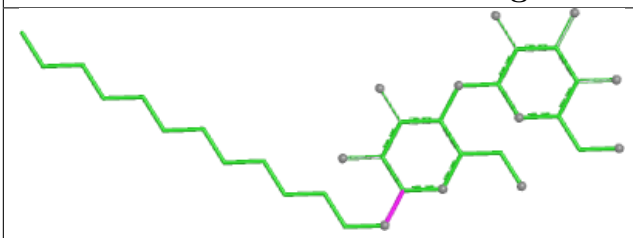
Bond angles



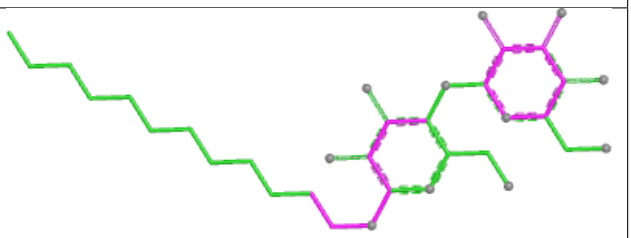
Torsions

Rings

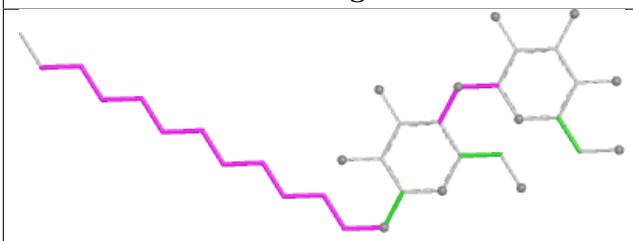
Ligand LMU A 1810



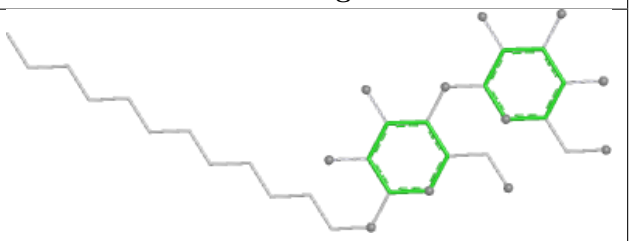
Bond lengths



Bond angles

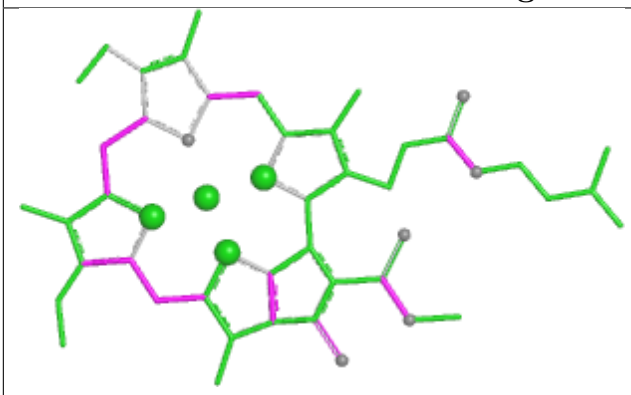


Torsions



Rings

Ligand CLA L 1166



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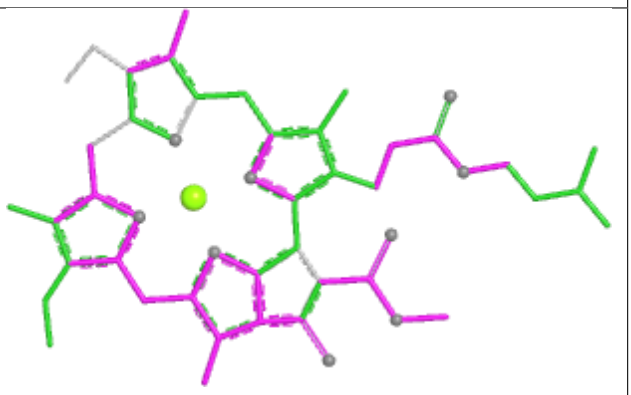
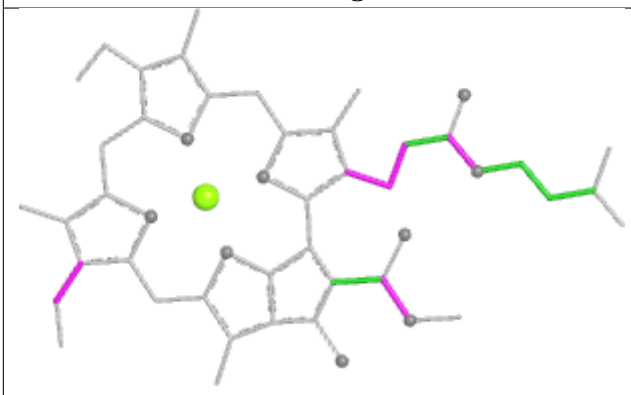
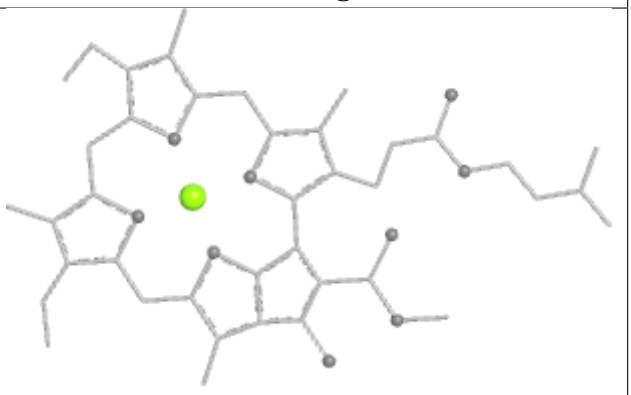


Bond angles

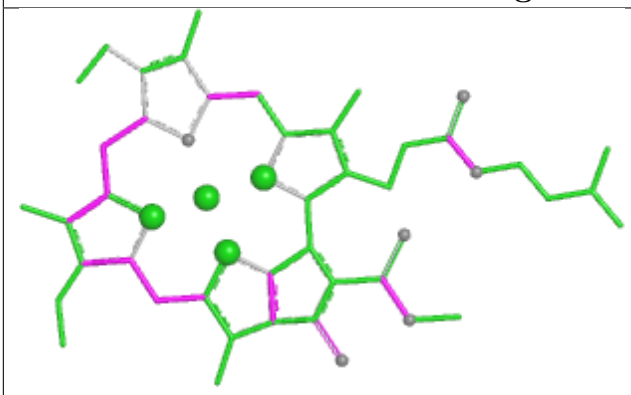


Torsions

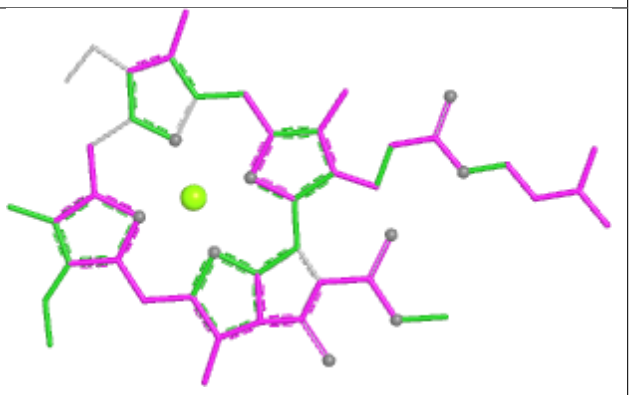


Rings

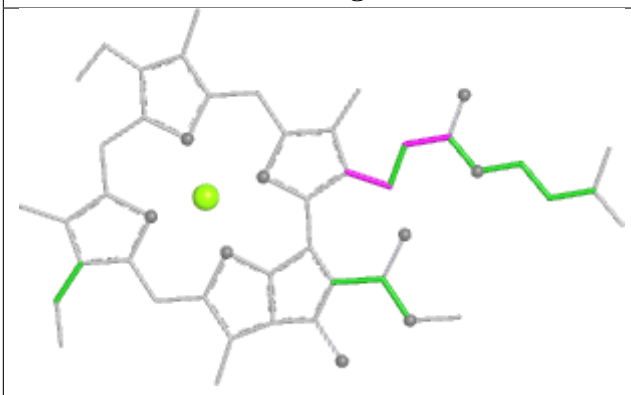
Ligand CLA A 1759



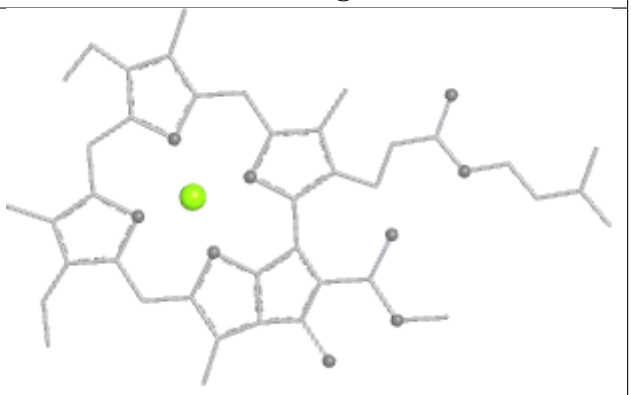
Bond lengths



Bond angles

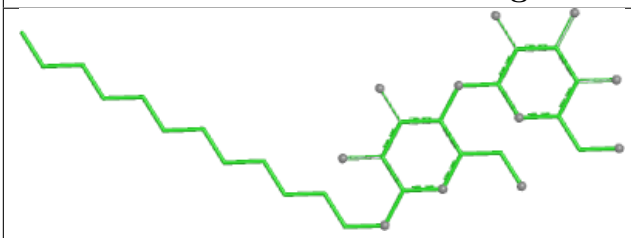


Torsions



Rings

Ligand LMU A 7038



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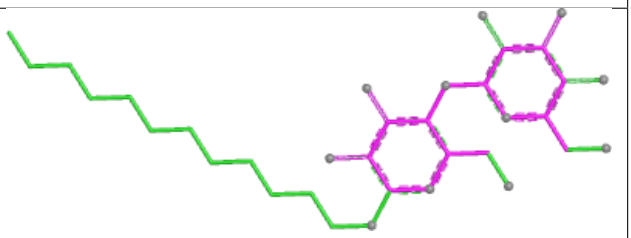
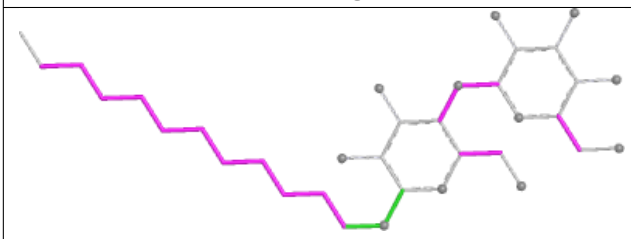


Bond angles



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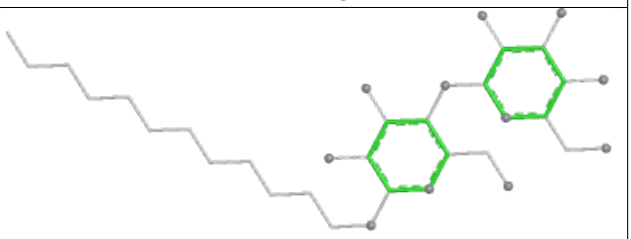
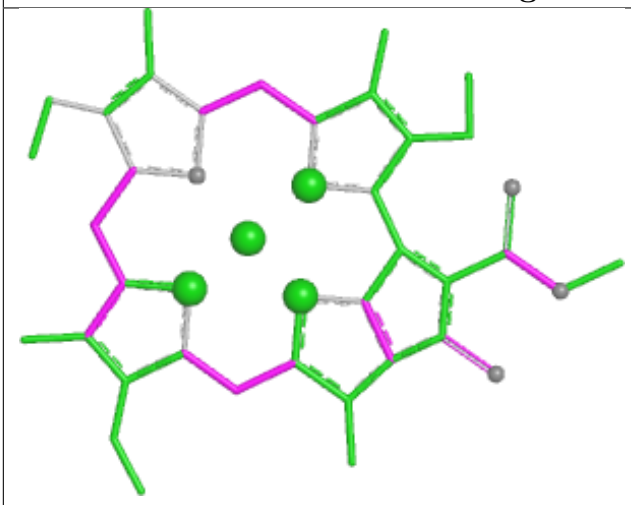
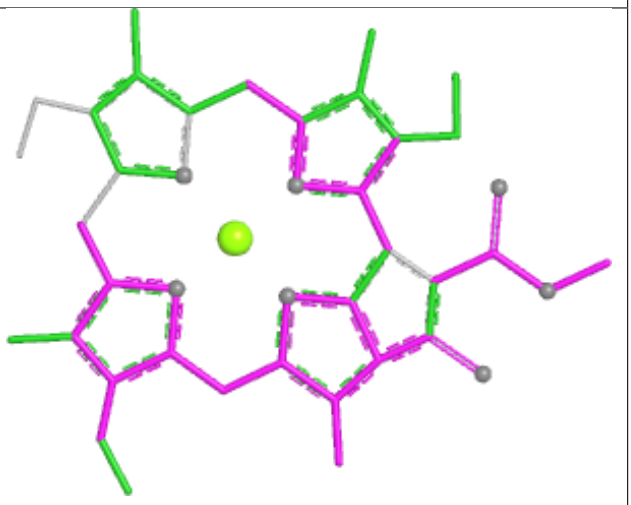


Rings

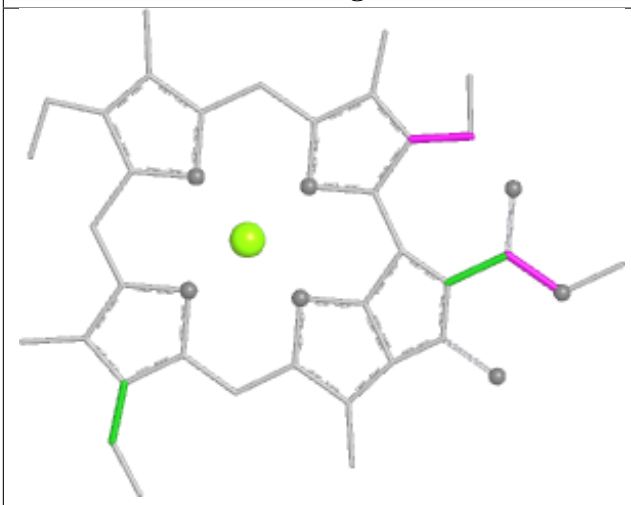
Ligand CLA 3 3007



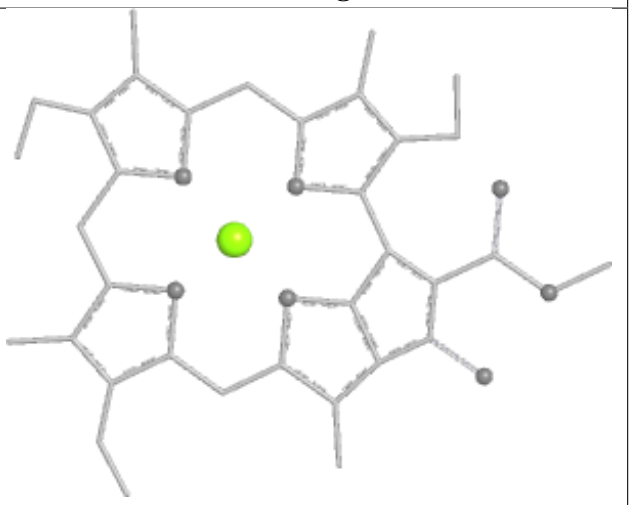
Bond lengths



Bond angles

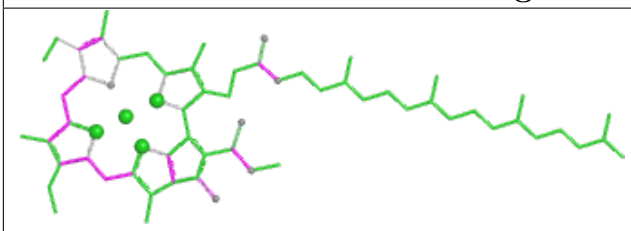


Torsions

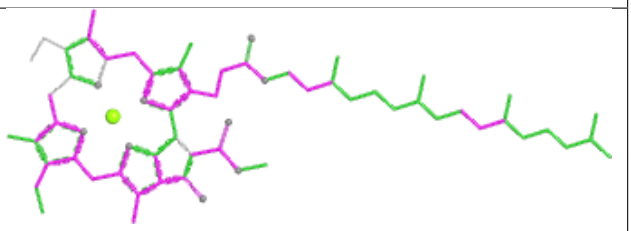


Rings

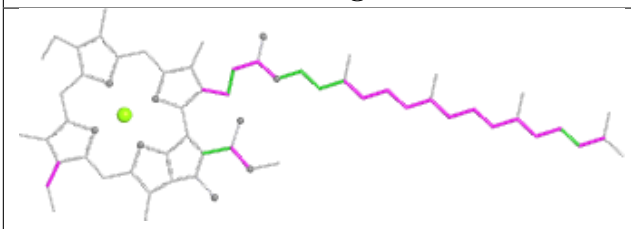
Ligand CLA A 1767



Bond lengths



Bond angles



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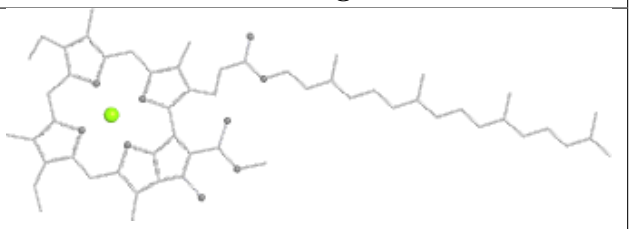
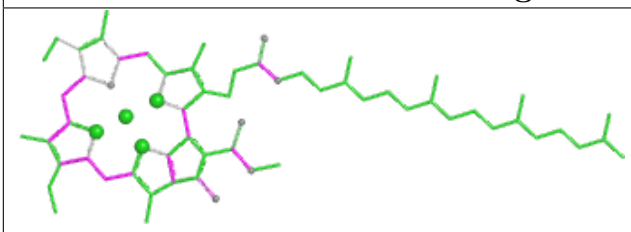
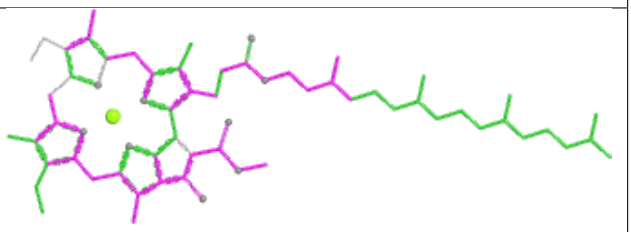
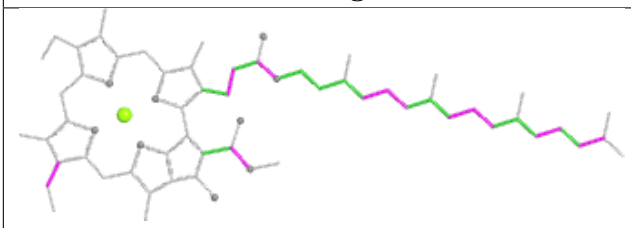
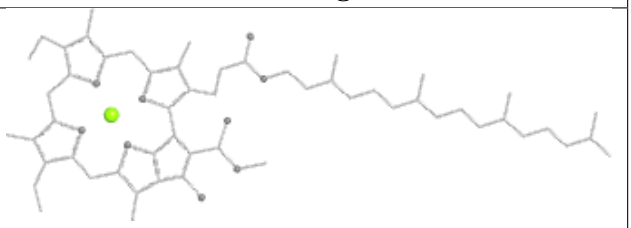
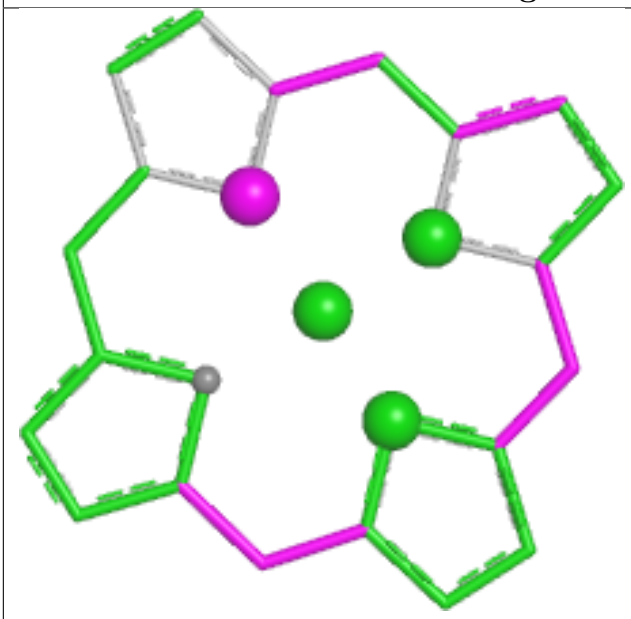


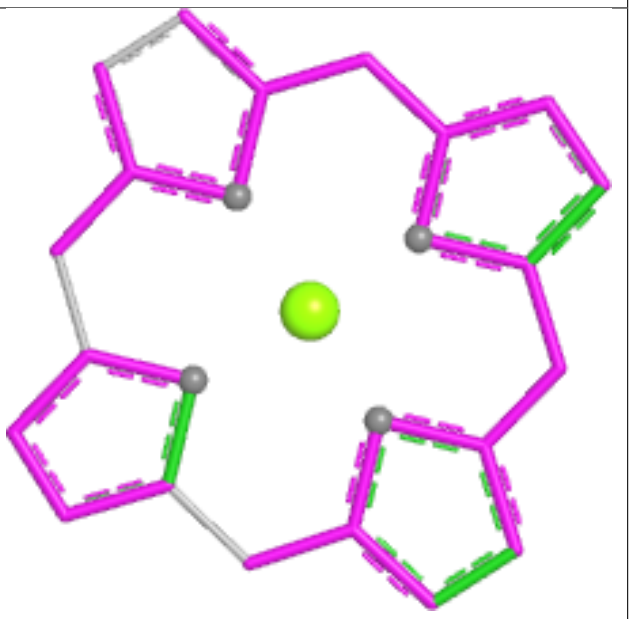
Rings

Ligand CLA A 1776	
 Bond lengths	 Bond angles
 Torsions	 Rings

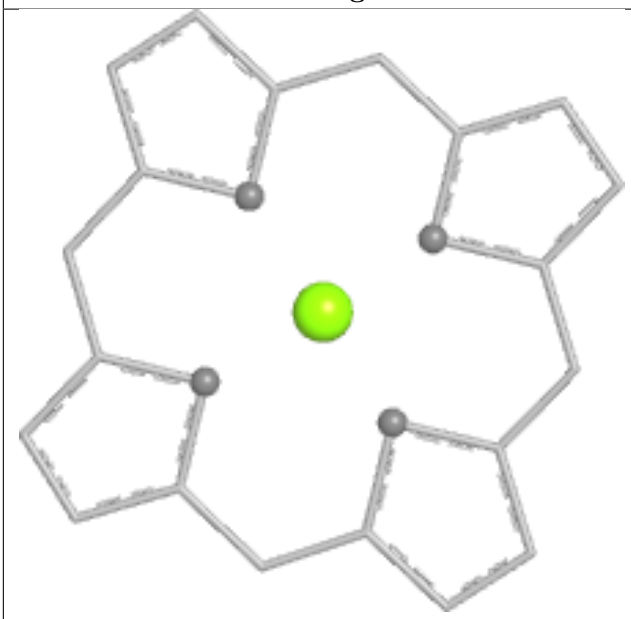
Ligand CLA 2 1221



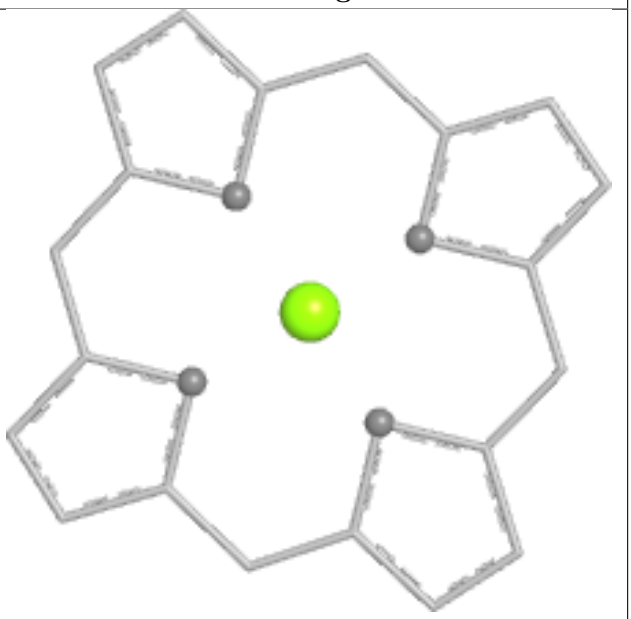
Bond lengths



Bond angles

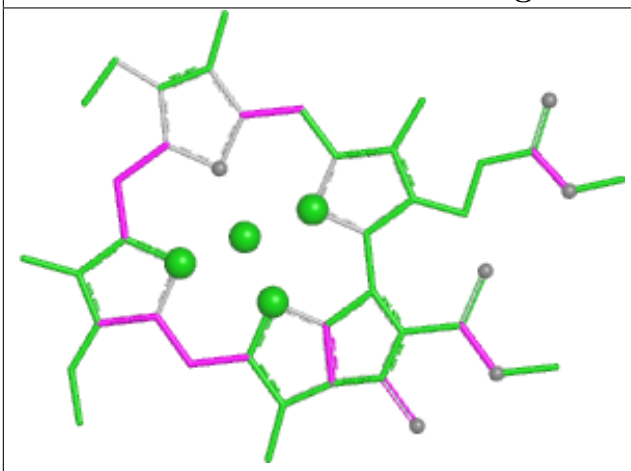


Torsions

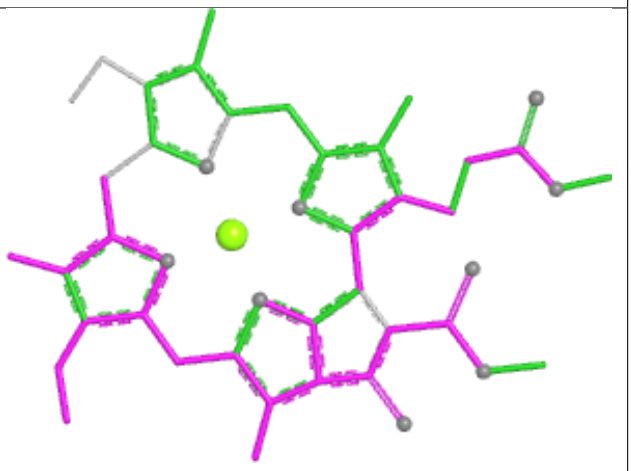


Rings

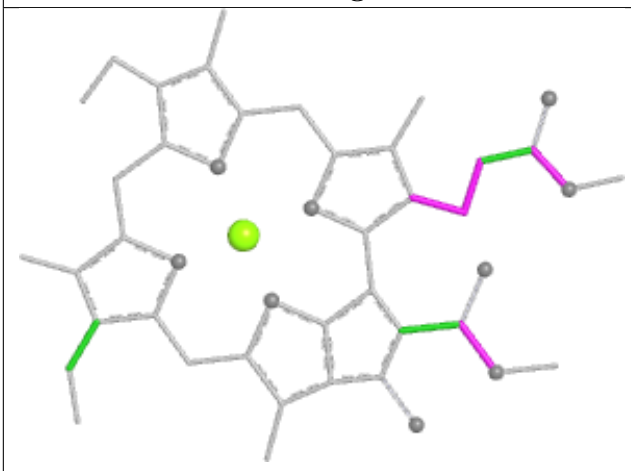
Ligand CLA A 1763



Bond lengths



Bond angles



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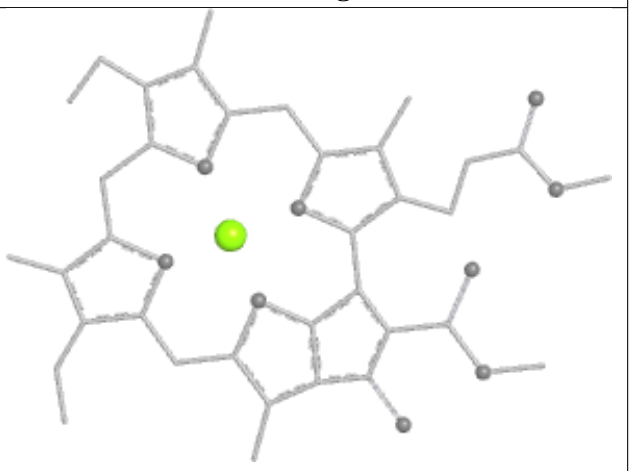
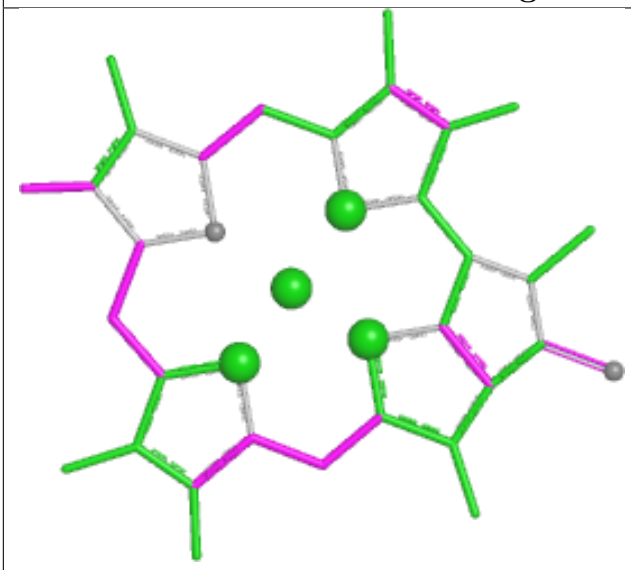


Rings

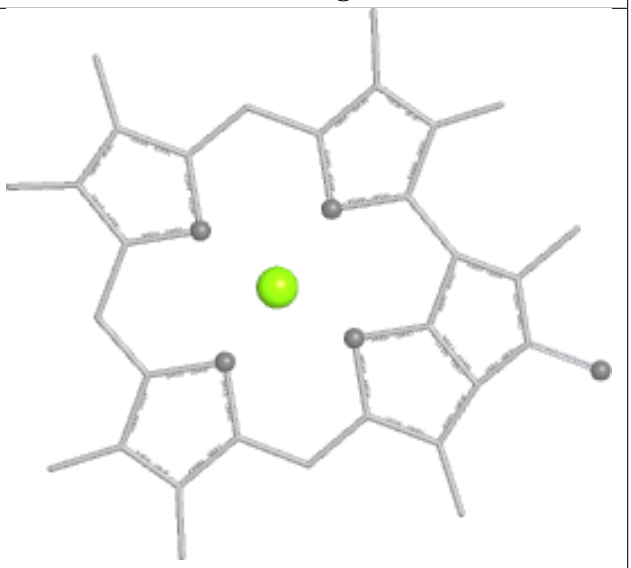
Ligand CLA 1 1191



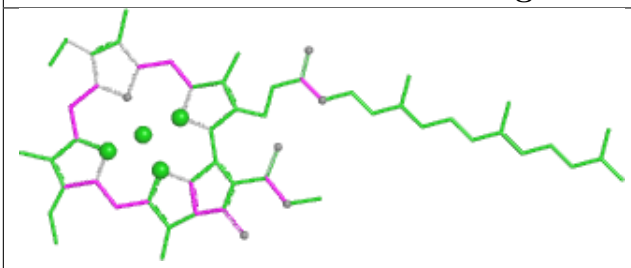
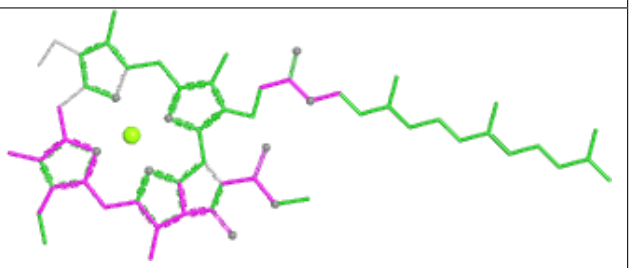
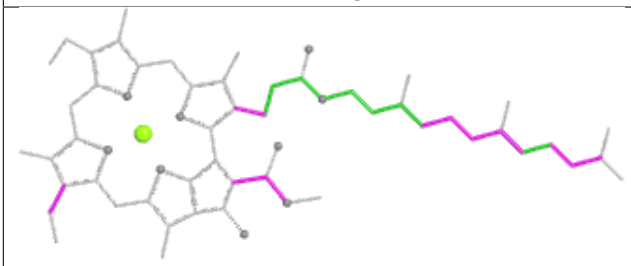
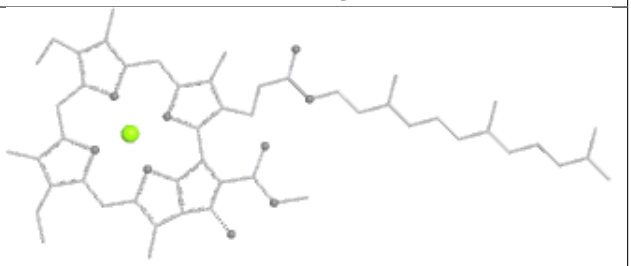
Bond lengths

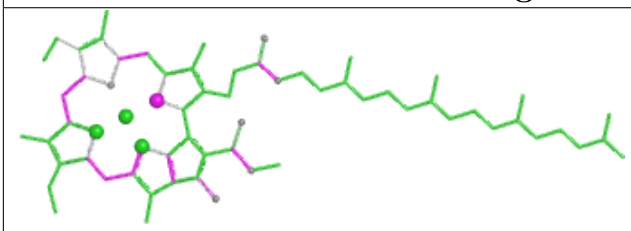
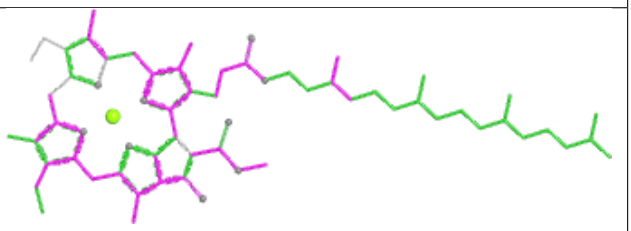
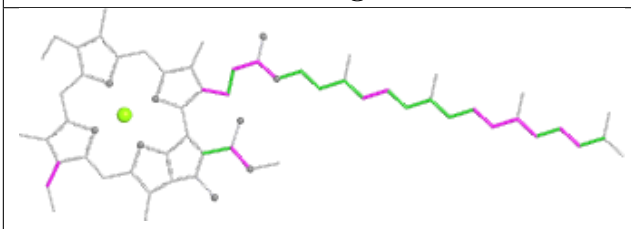
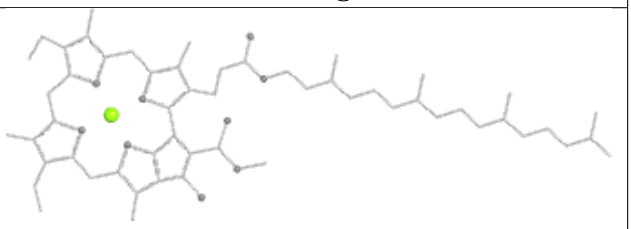
Bond angles

Torsions

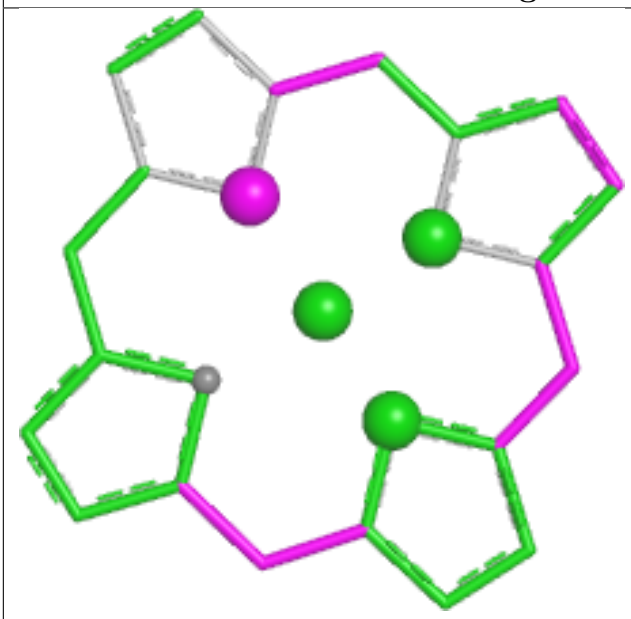


Rings

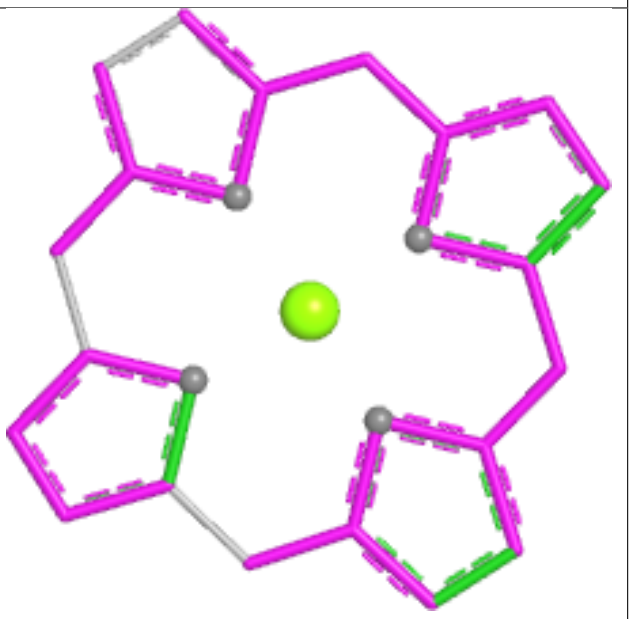
Ligand CLA B 1767	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1771	
 Bond lengths	 Bond angles
 Torsions	 Rings

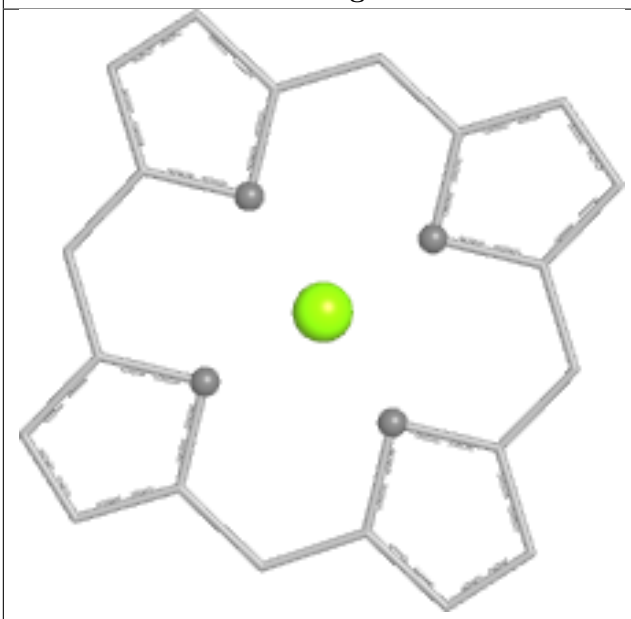
Ligand CLA 1 1194



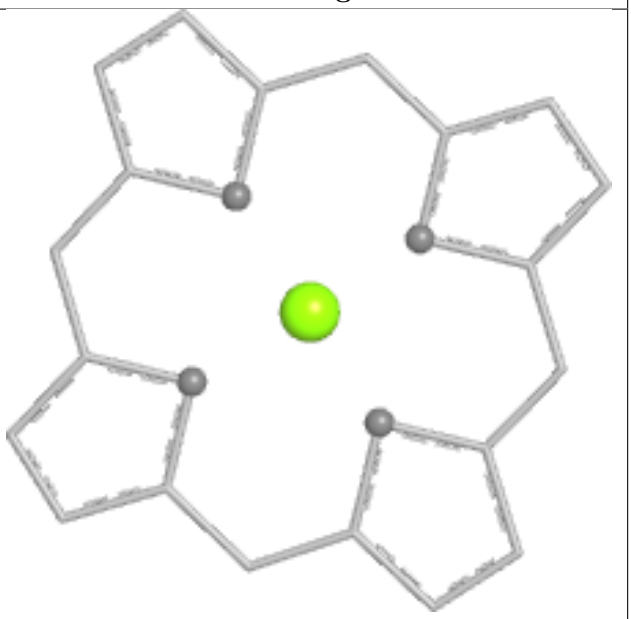
Bond lengths



Bond angles

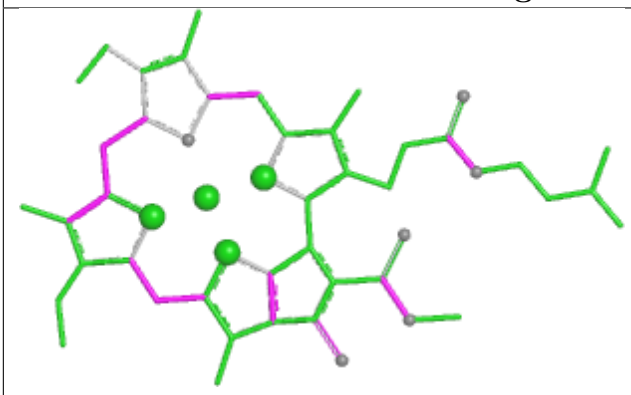


Torsions

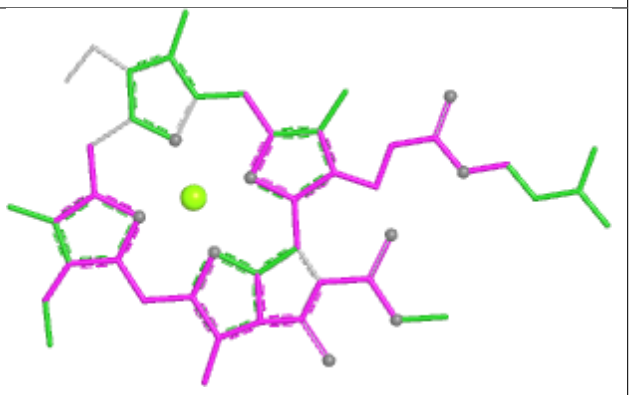


Rings

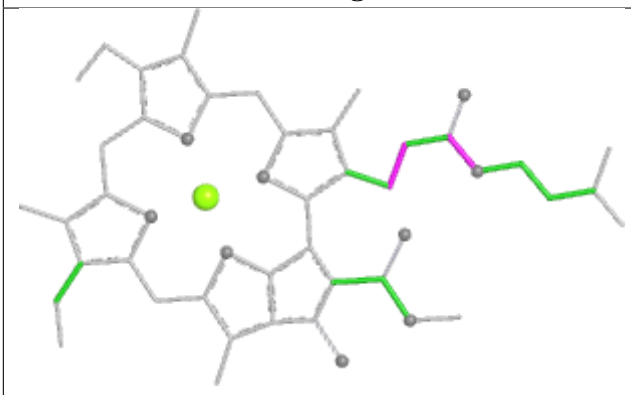
Ligand CLA A 1786



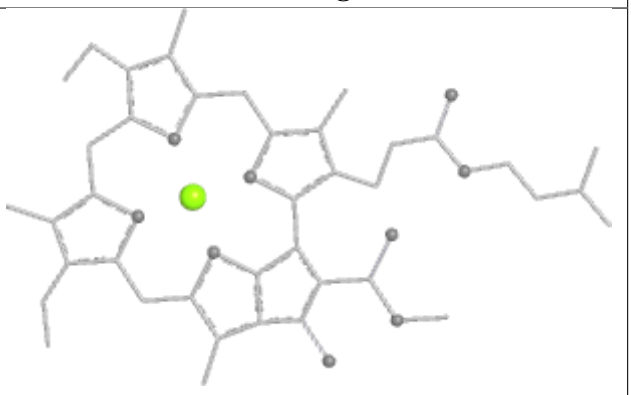
Bond lengths



Bond angles

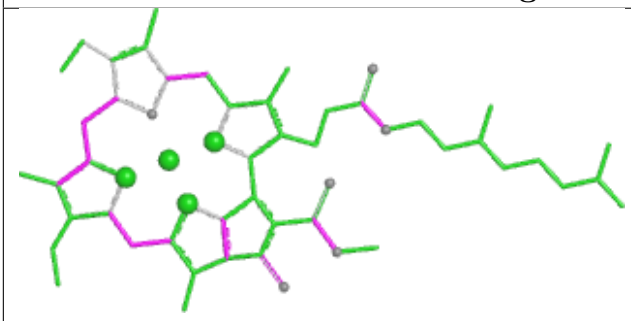


Torsions

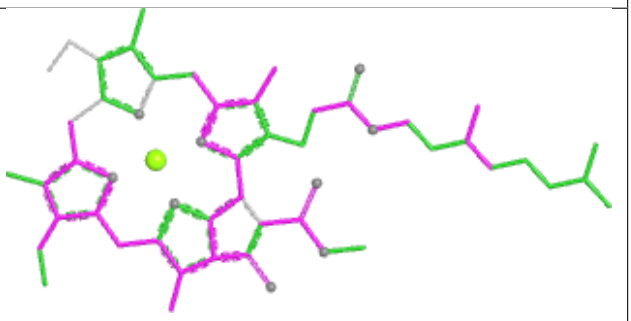


Rings

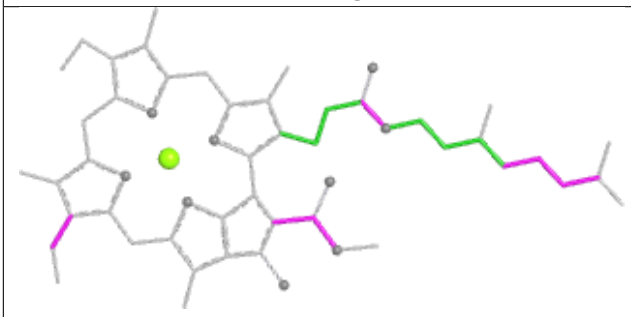
Ligand CLA 4 1199



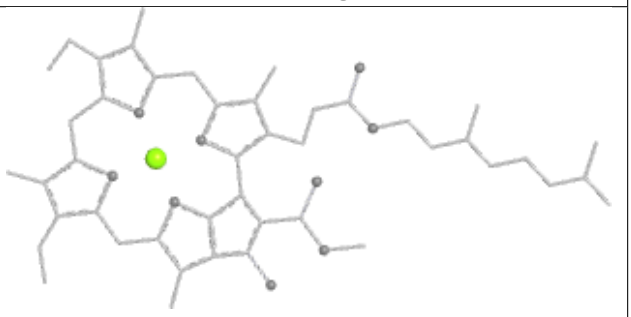
Bond lengths



Bond angles

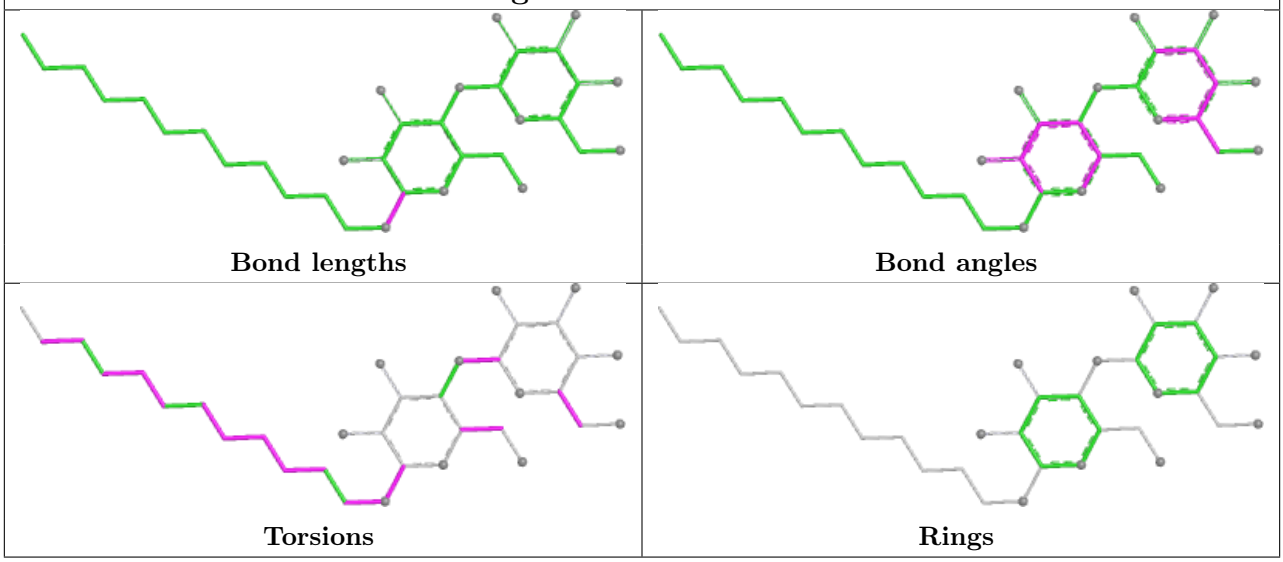


Torsions

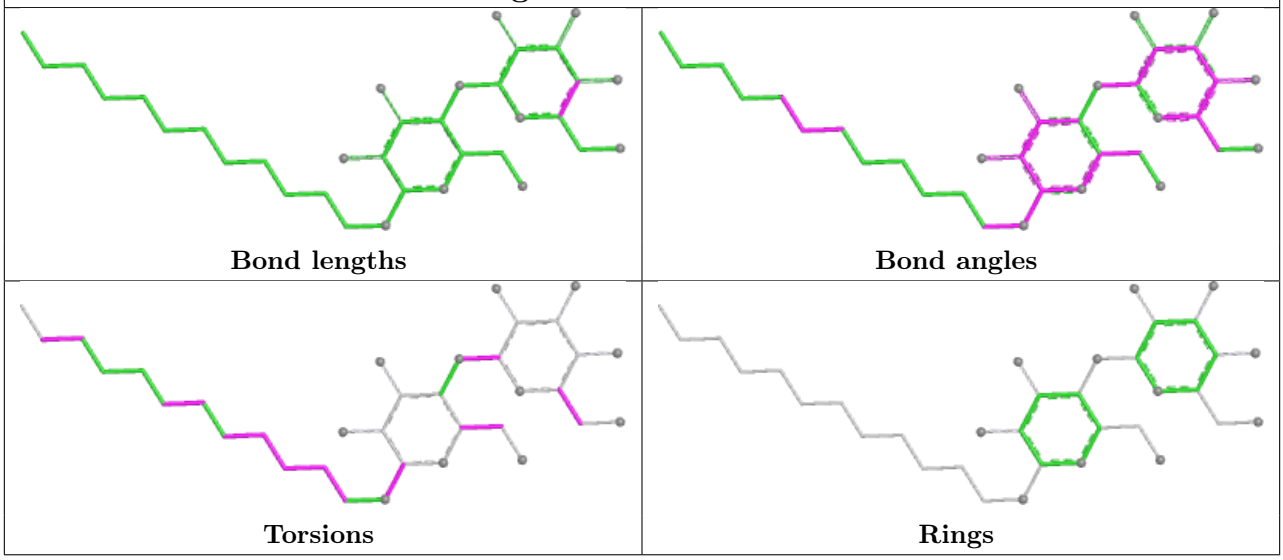


Rings

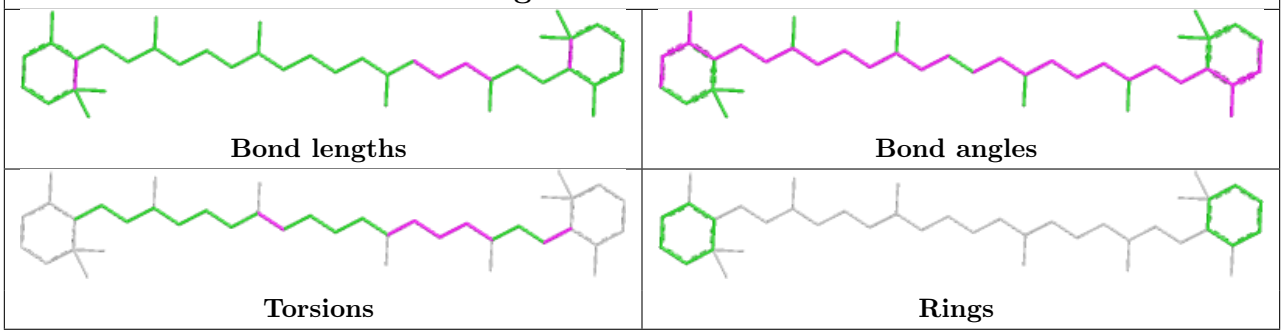
Ligand LMU A 7019

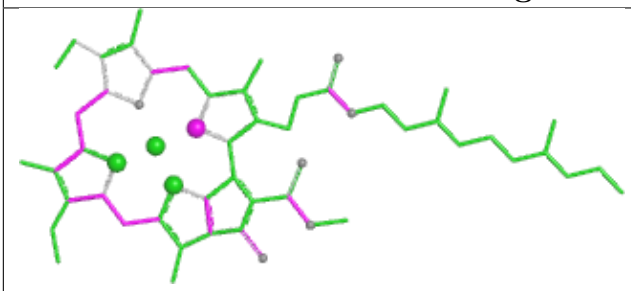
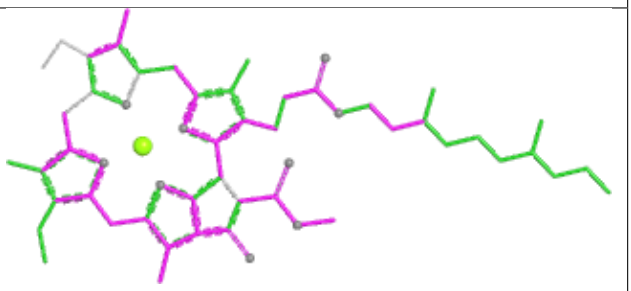
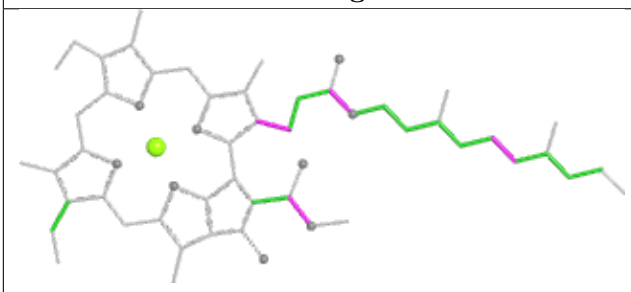
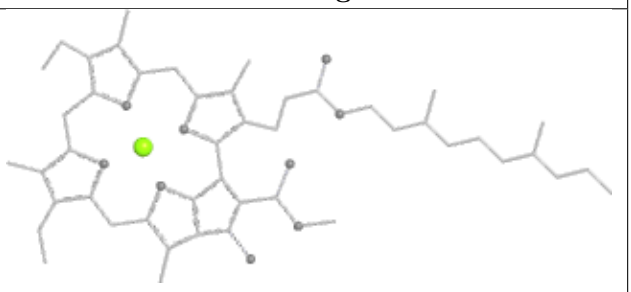


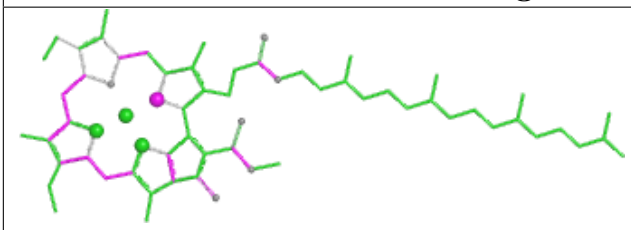
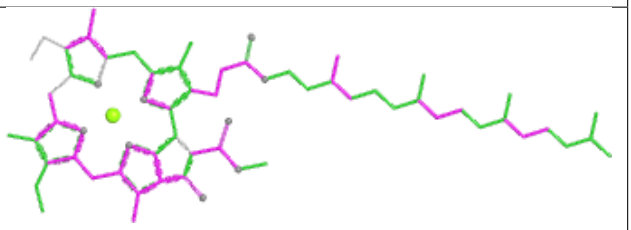
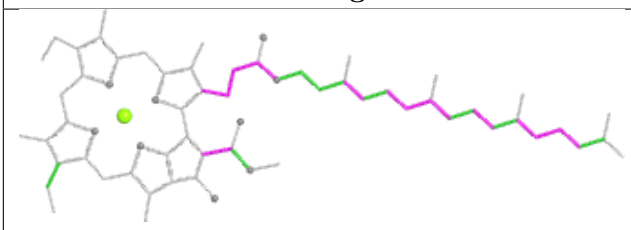
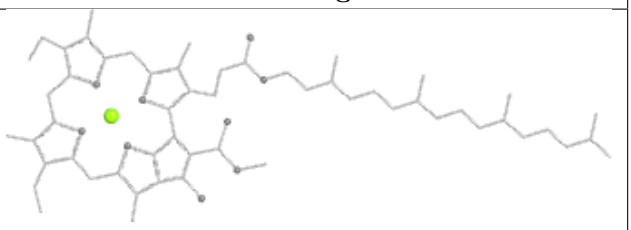
Ligand LMU A 7023



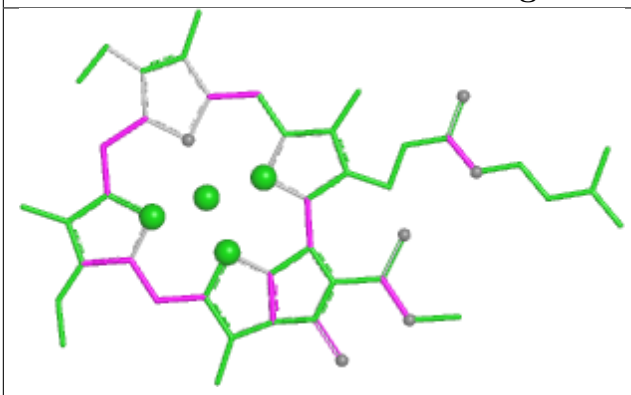
Ligand BCR A 1807



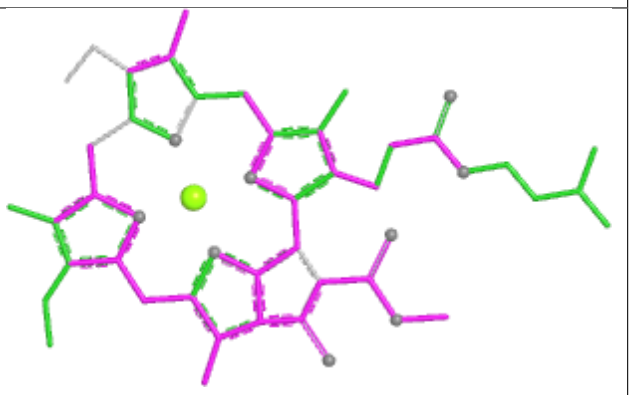
Ligand CLA A 1762	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1743	
 Bond lengths	 Bond angles
 Torsions	 Rings

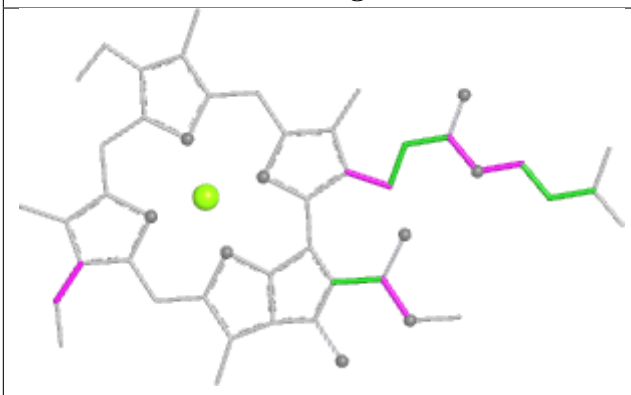
Ligand CLA 2 1215



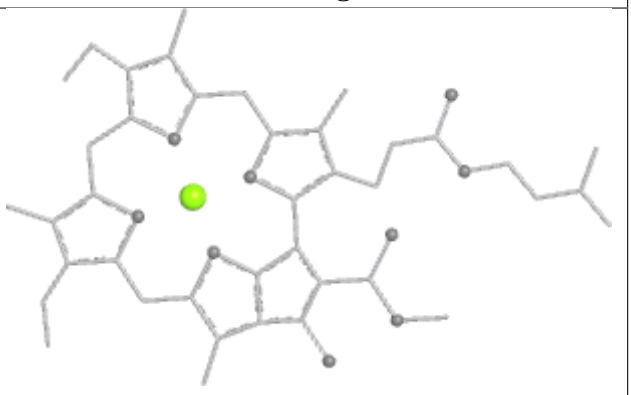
Bond lengths



Bond angles

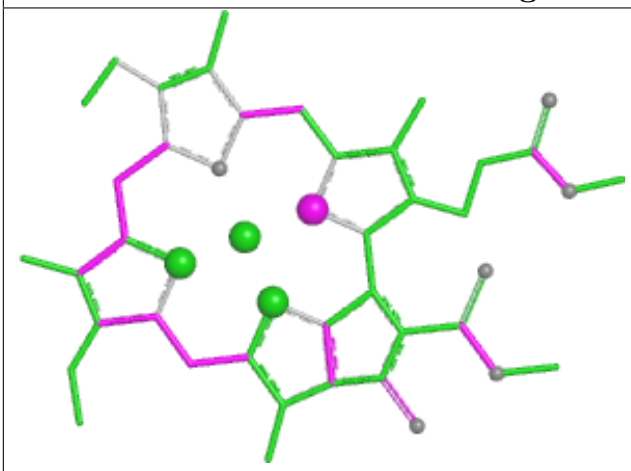


Torsions

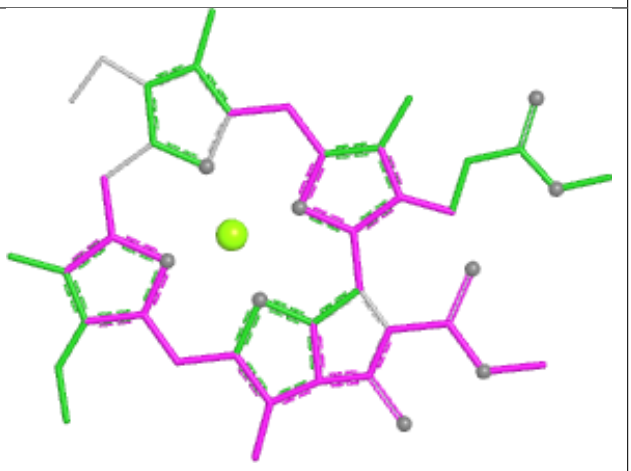


Rings

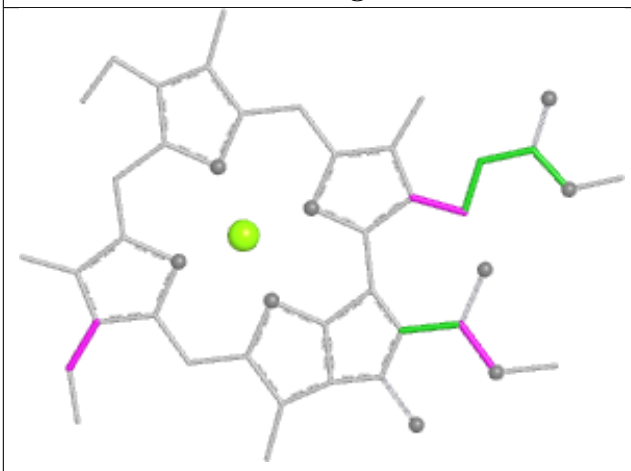
Ligand CLA 1 1190



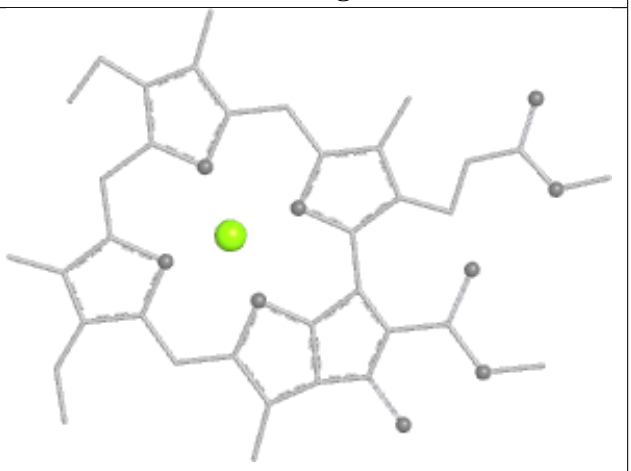
Bond lengths



Bond angles

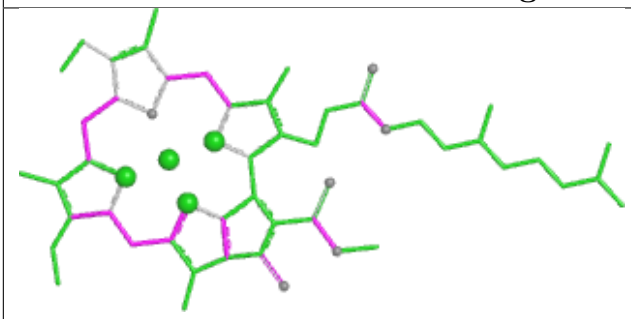


Torsions

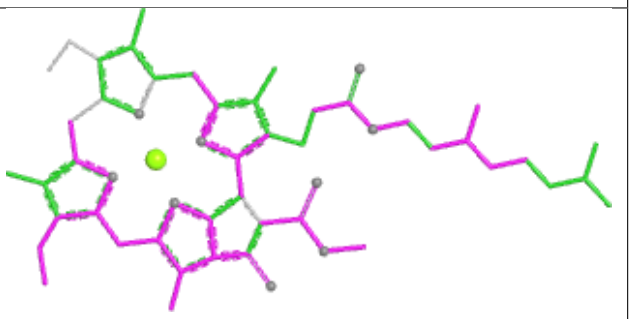


Rings

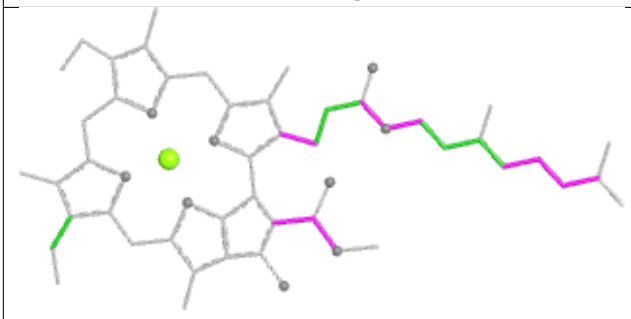
Ligand CLA 4 1204



Bond lengths



Bond angles



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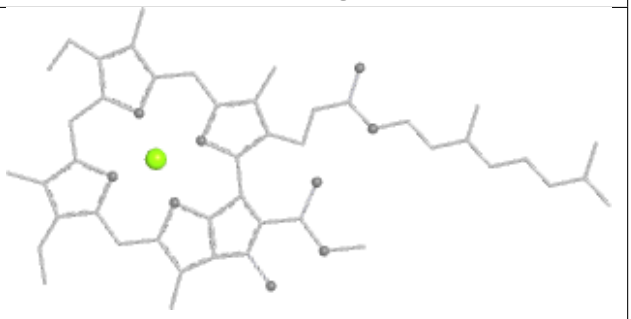
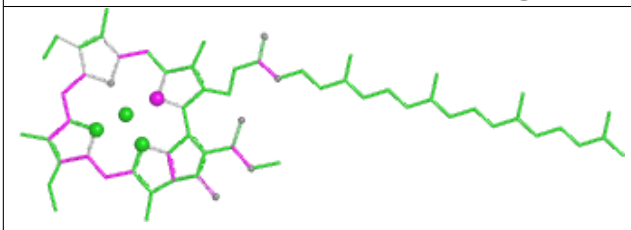
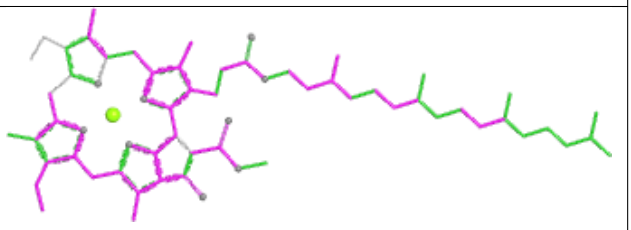


Rings

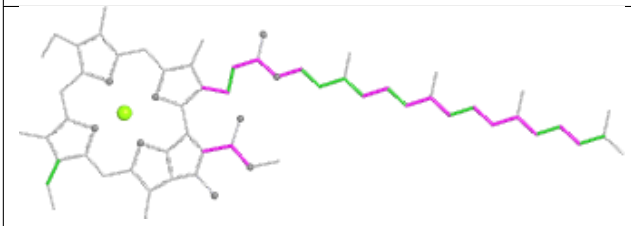
Ligand CLA B 1737



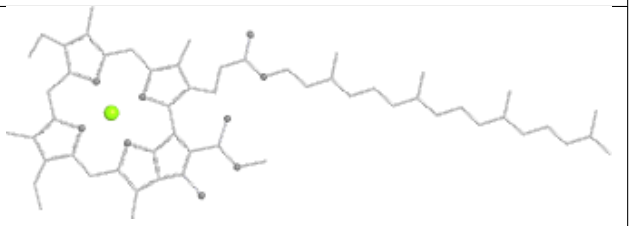
Bond lengths



Bond angles

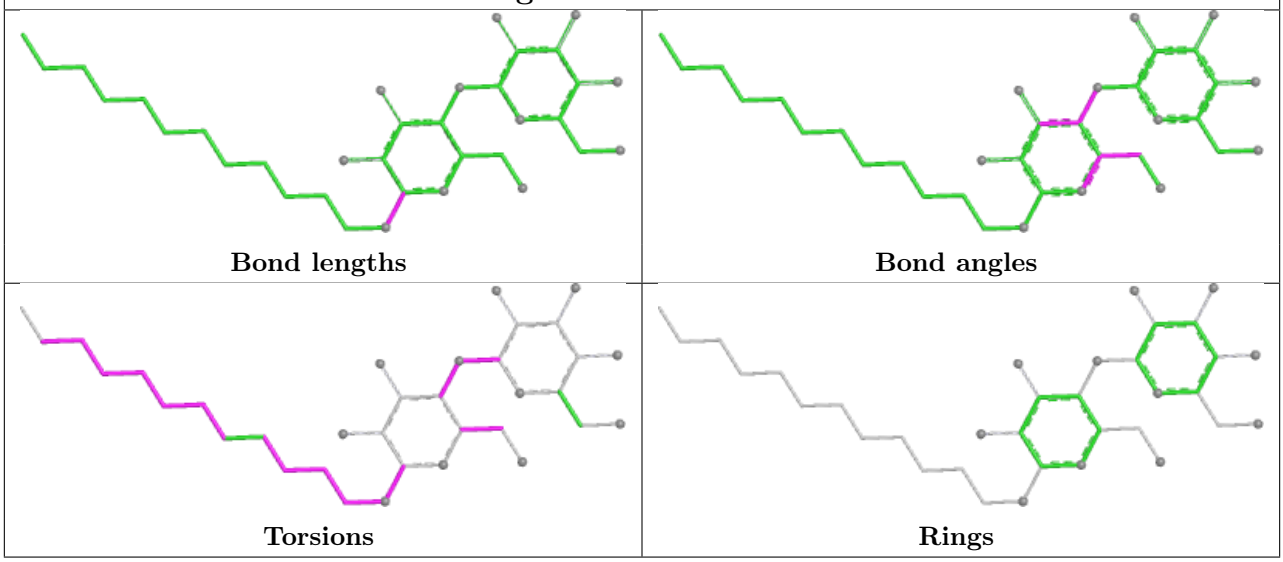


Torsions

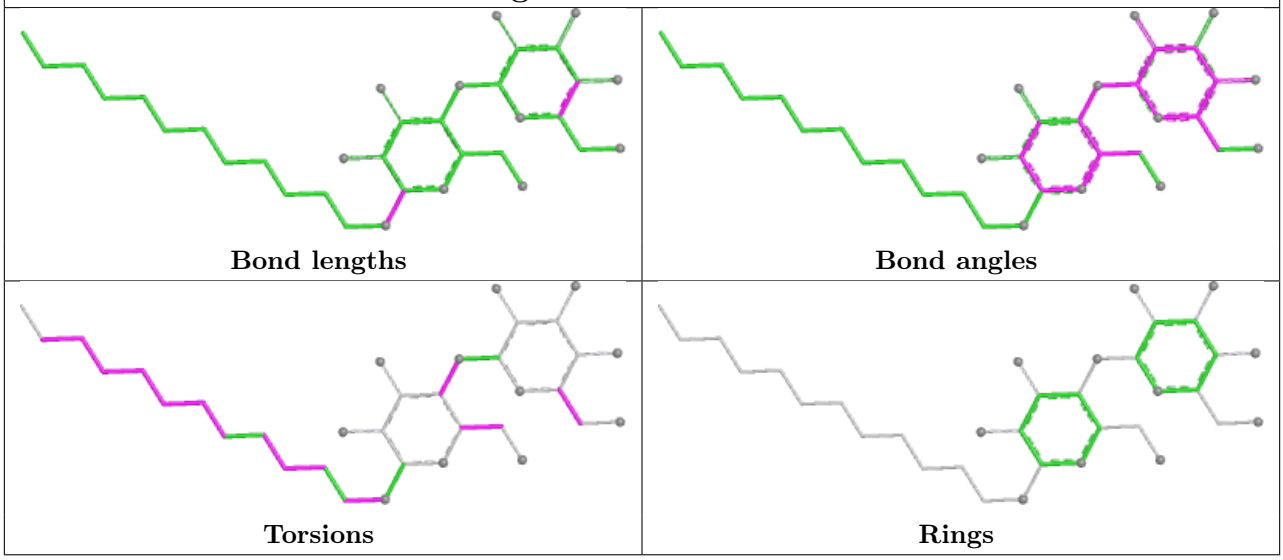


Rings

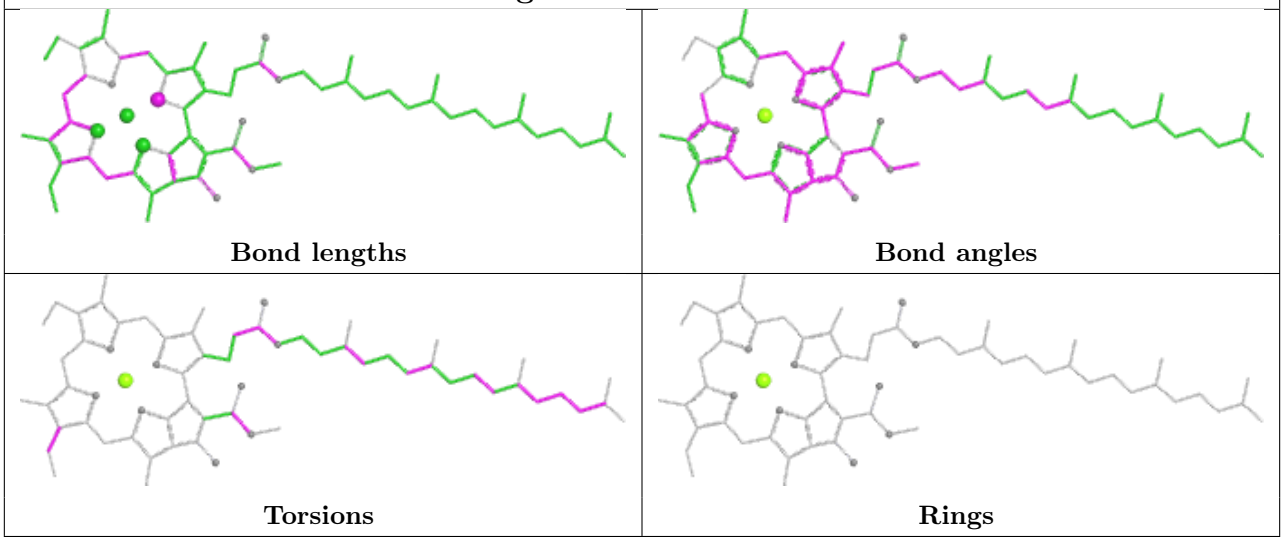
Ligand LMU 2 1225



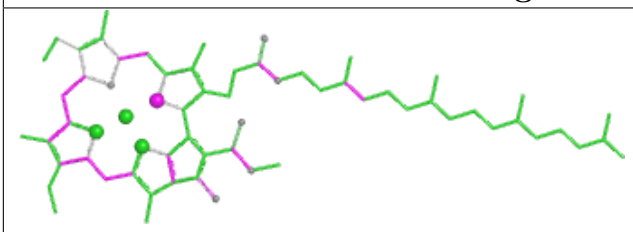
Ligand LMU A 7017



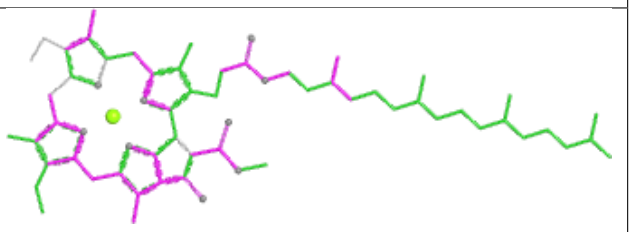
Ligand CLA B 1787



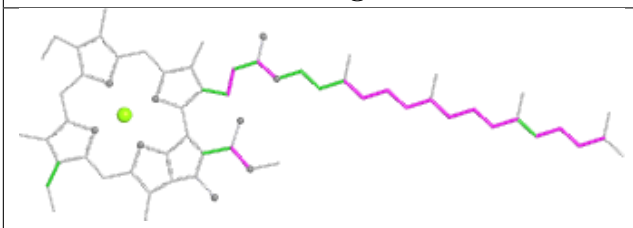
Ligand CLA A 1788



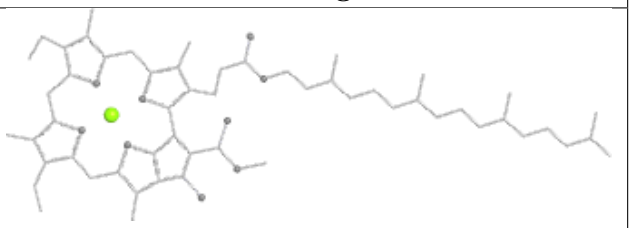
Bond lengths



Bond angles

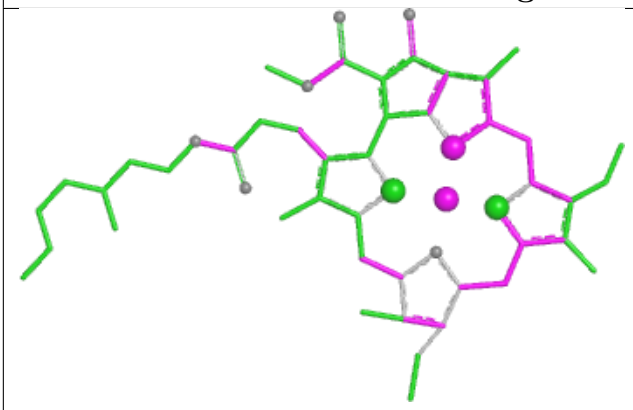


Torsions



Rings

Ligand CLA F 1157



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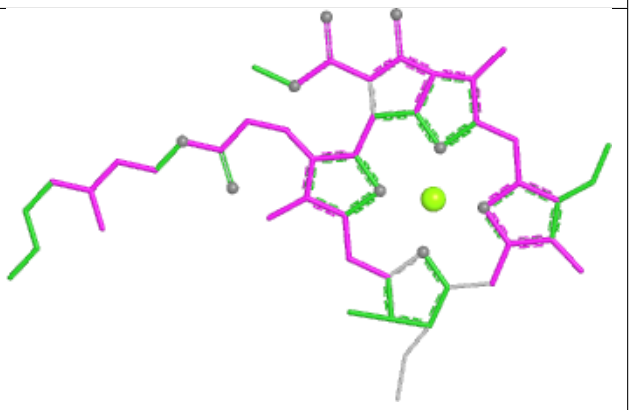
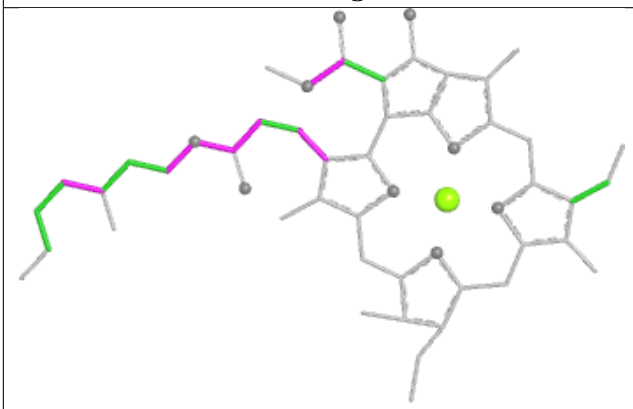


Bond angles



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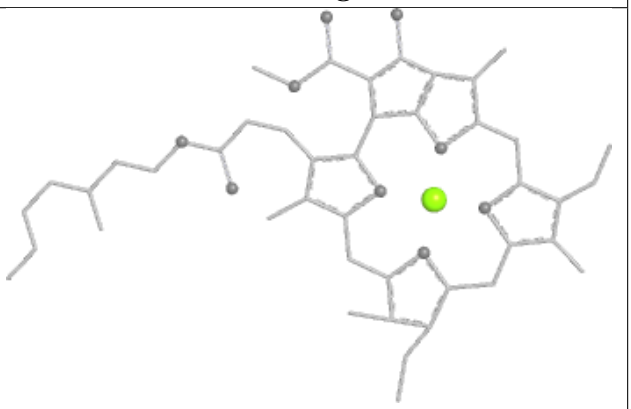
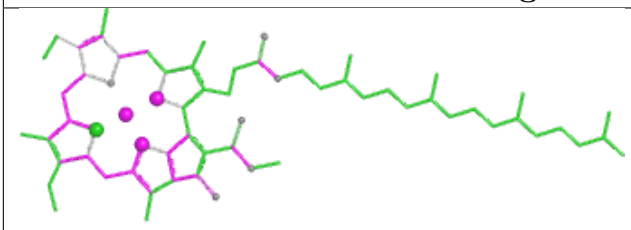
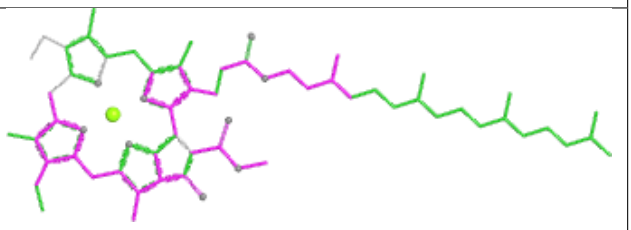
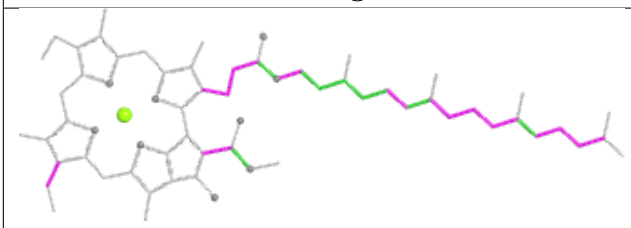
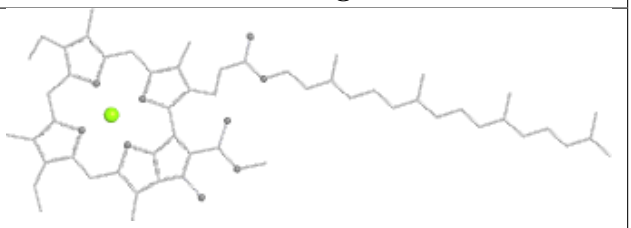
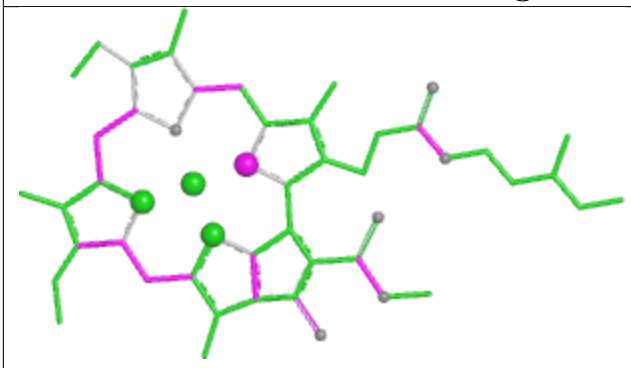
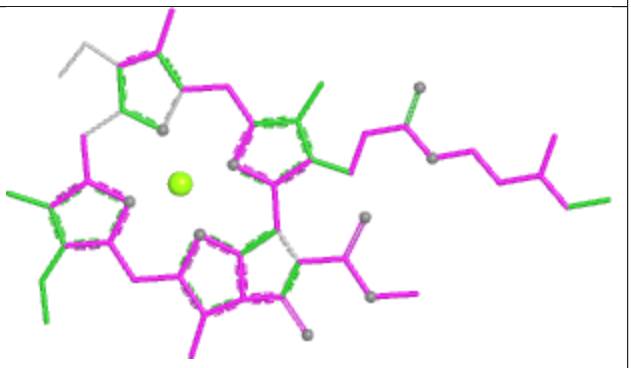
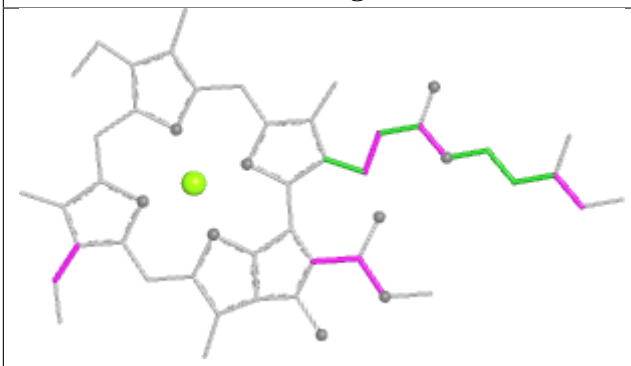
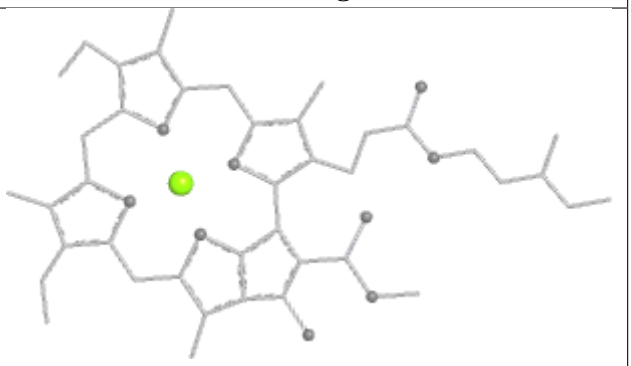
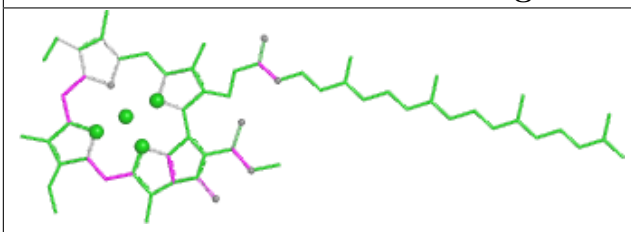


Rings

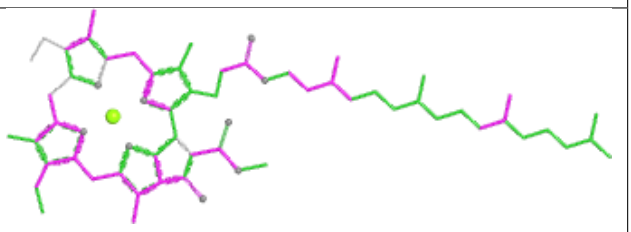
Ligand CLA 3 1218	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1099	
 Bond lengths	 Bond angles
 Torsions	 Rings

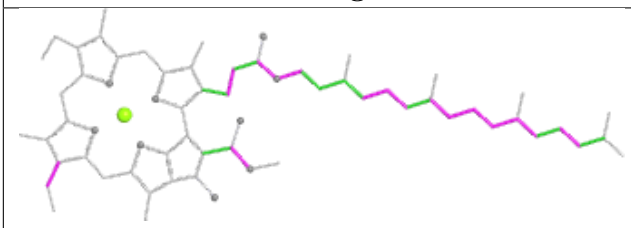
Ligand CLA A 1780



Bond lengths



Bond angles



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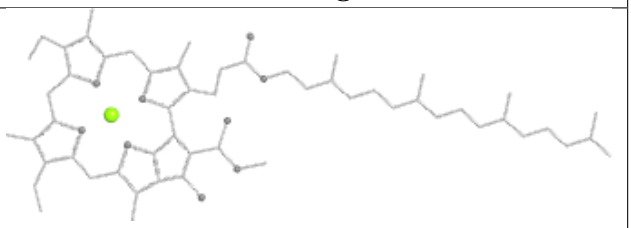
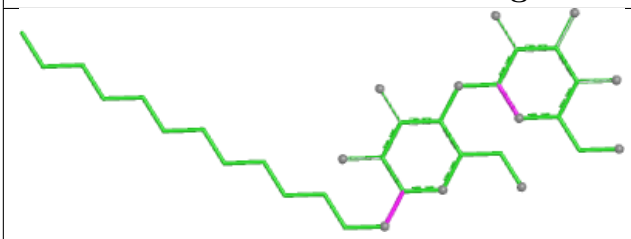


Rings

Ligand LMU A 7024



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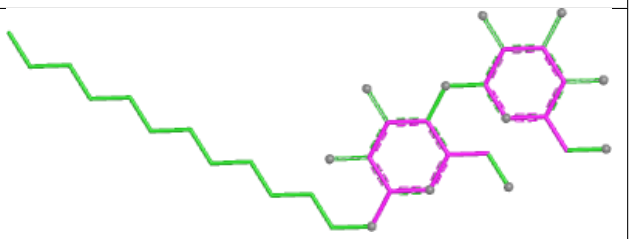
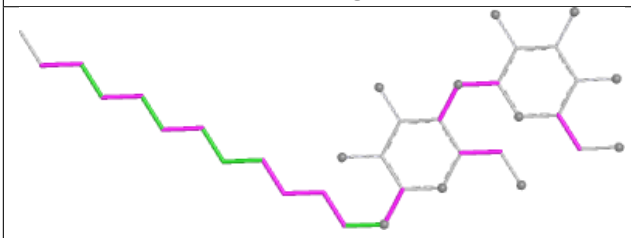


Bond angles



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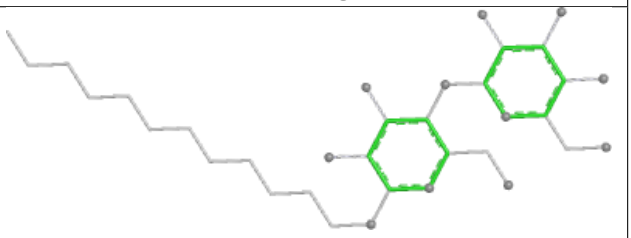
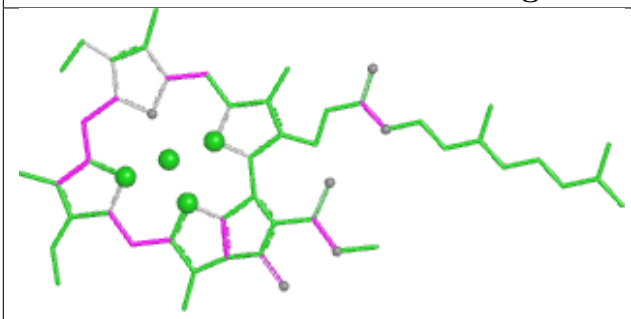
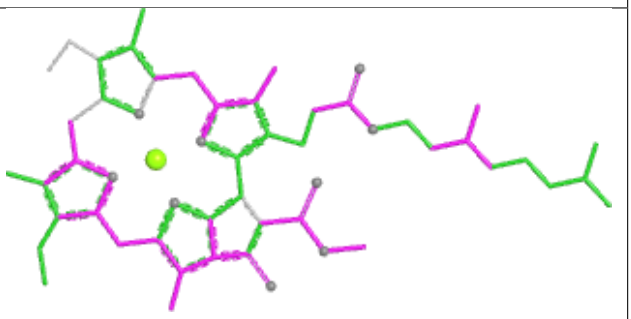


Rings

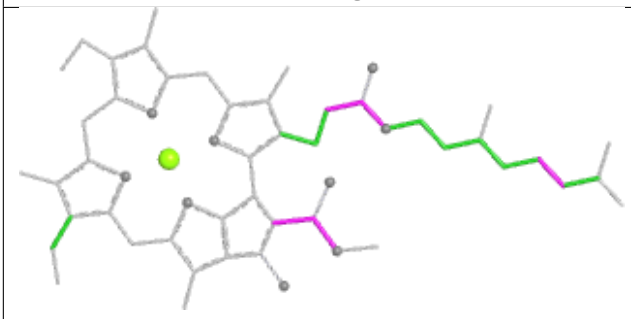
Ligand CLA I 1033



Bond lengths



Bond angles



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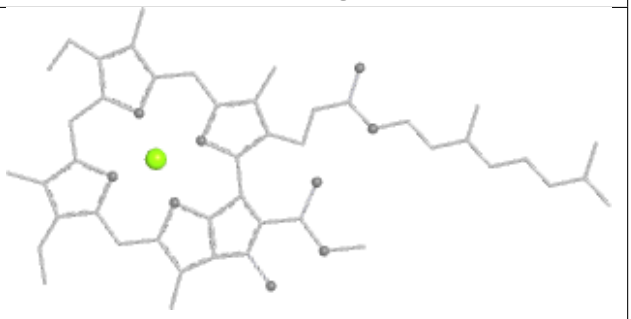
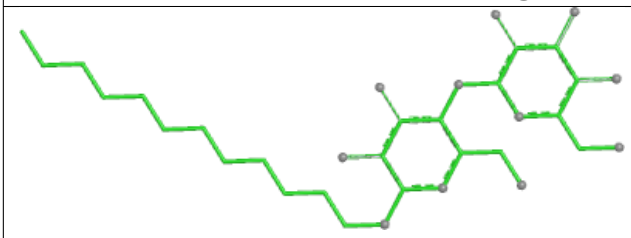
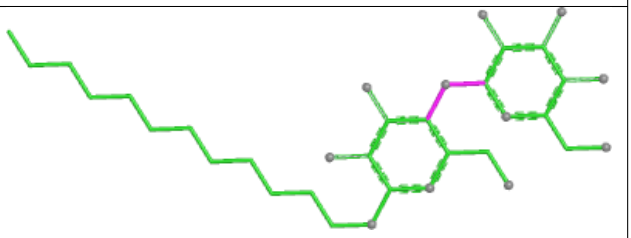


Rings

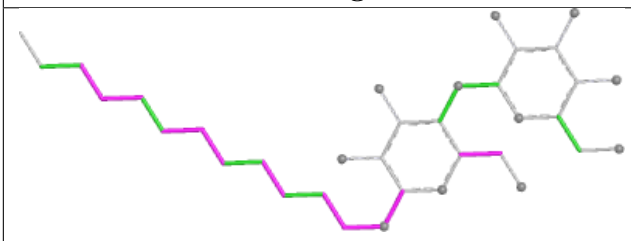
Ligand LMU 2 7003



Bond lengths



Bond angles



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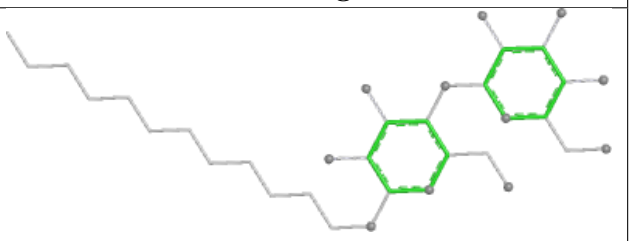
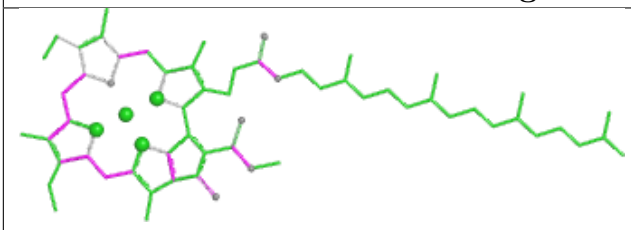
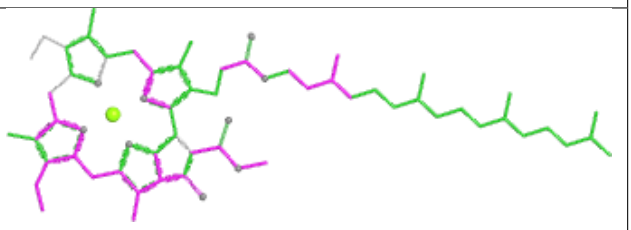
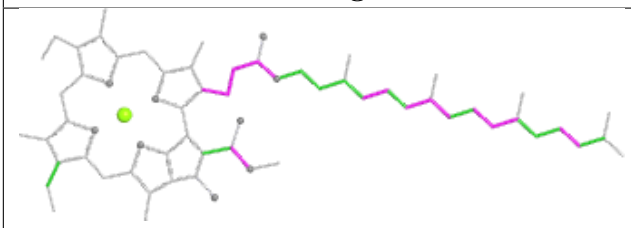
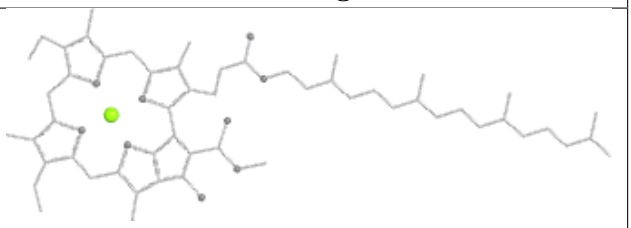
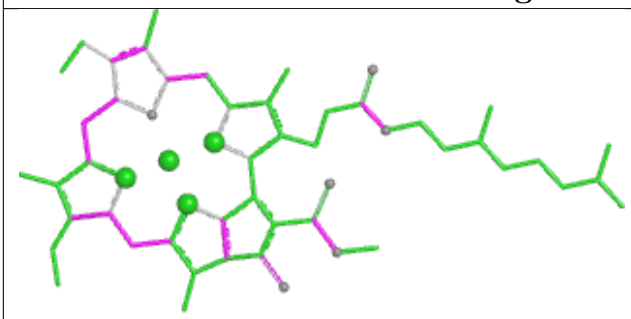
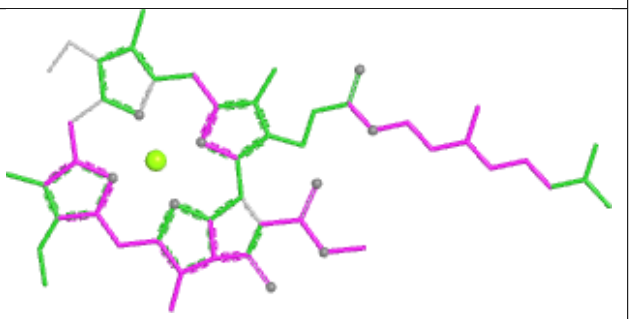
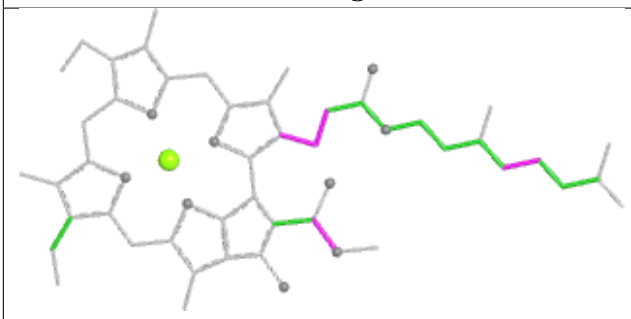
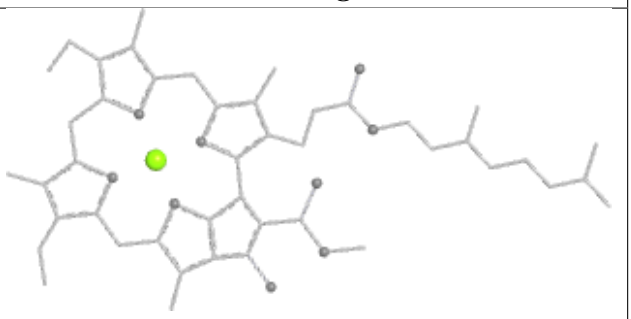
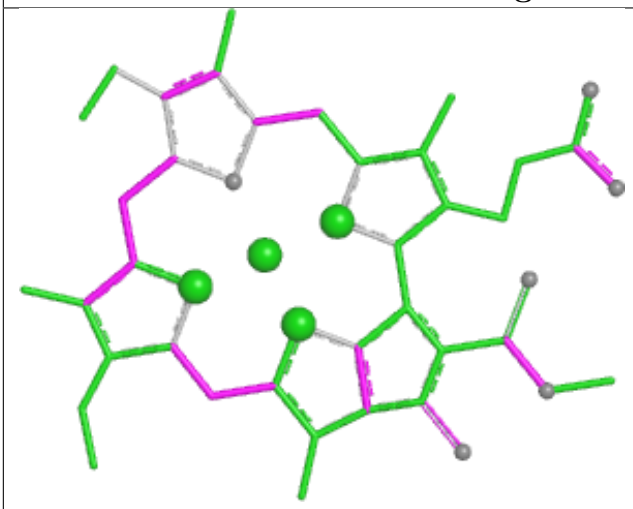


Rings

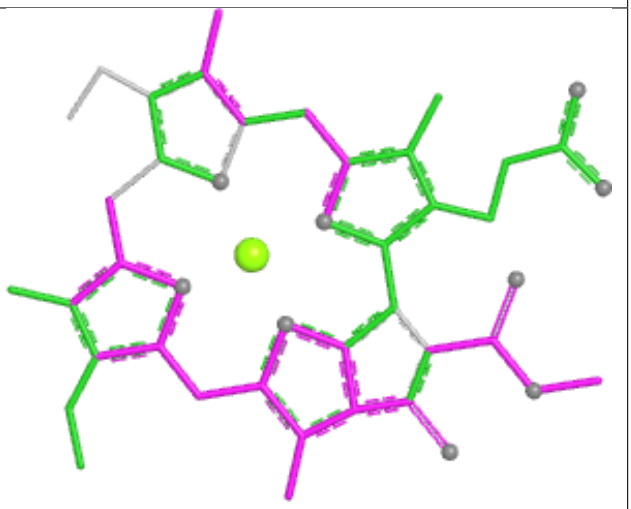
Ligand CLA 2 1217	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1798	
 Bond lengths	 Bond angles
 Torsions	 Rings

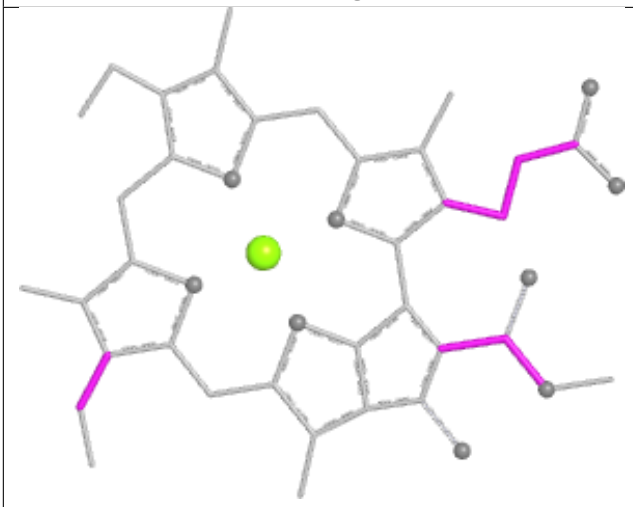
Ligand CLA A 1770



Bond lengths



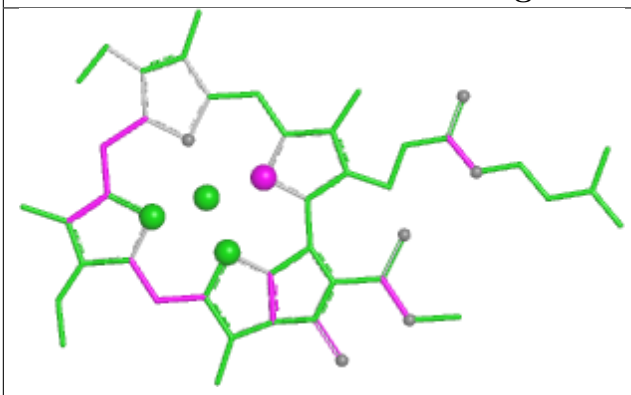
Bond angles



Torsions

Rings

Ligand CLA A 1790



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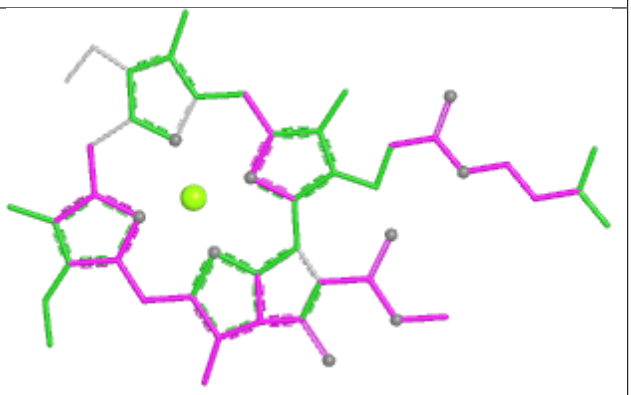
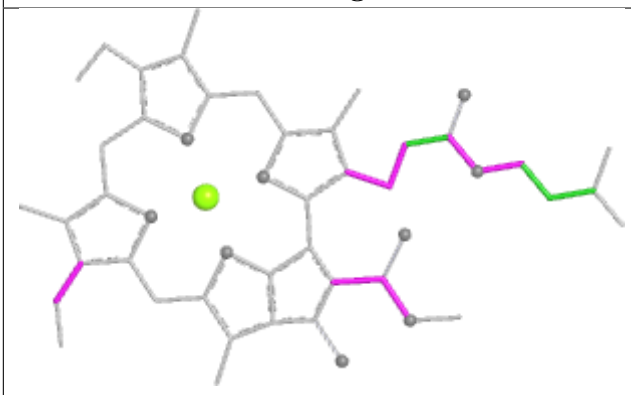
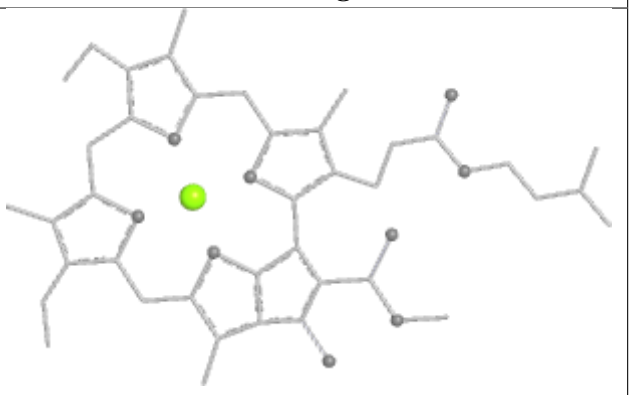


Bond angles

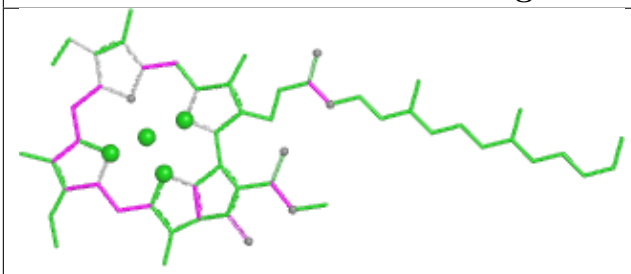


Torsions

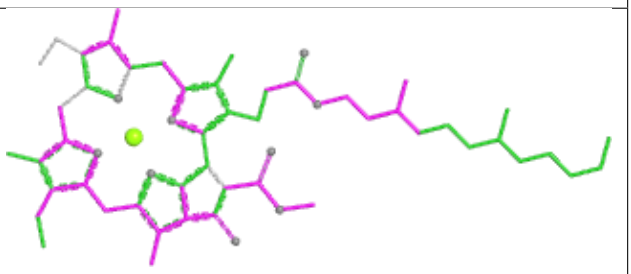


Rings

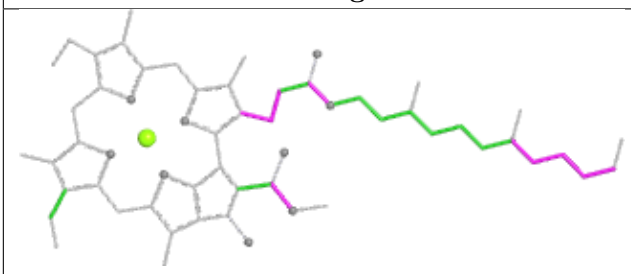
Ligand CLA B 1747



Bond lengths



Bond angles



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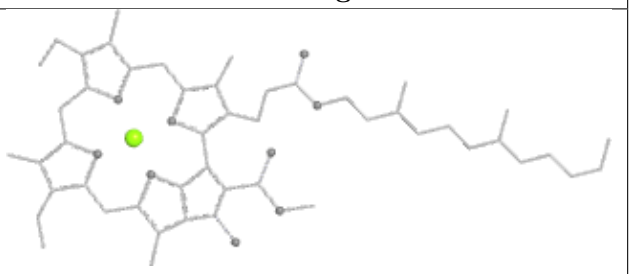
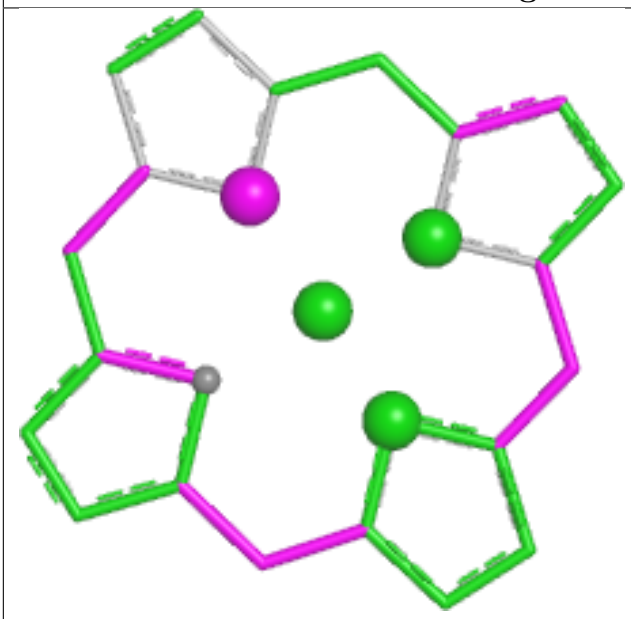
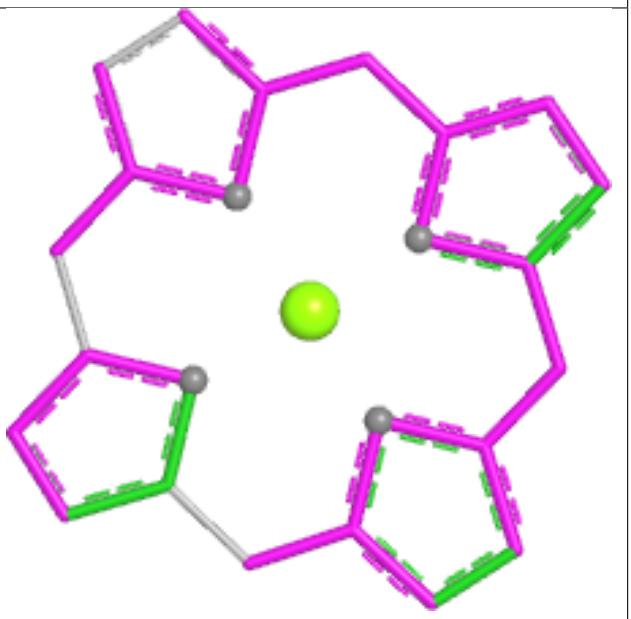


Rings

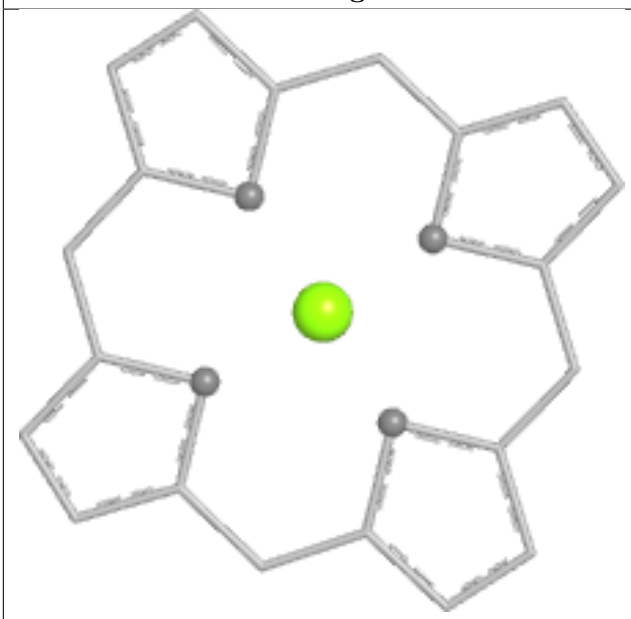
Ligand CLA 1 1201



Bond lengths



Bond angles



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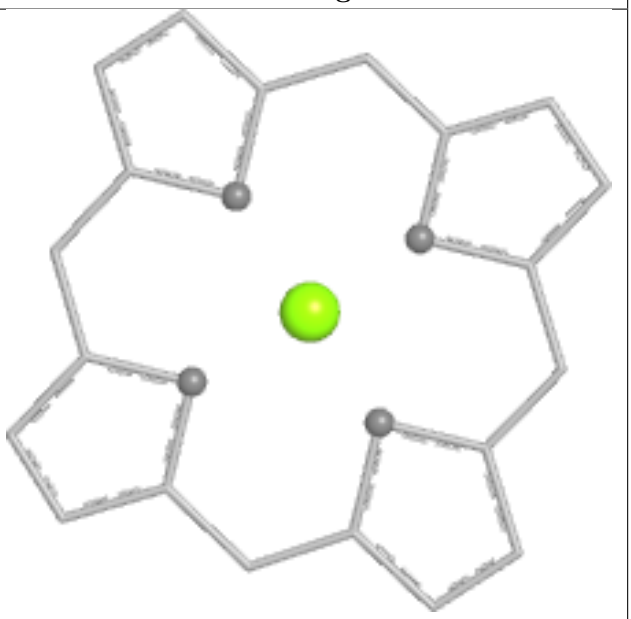
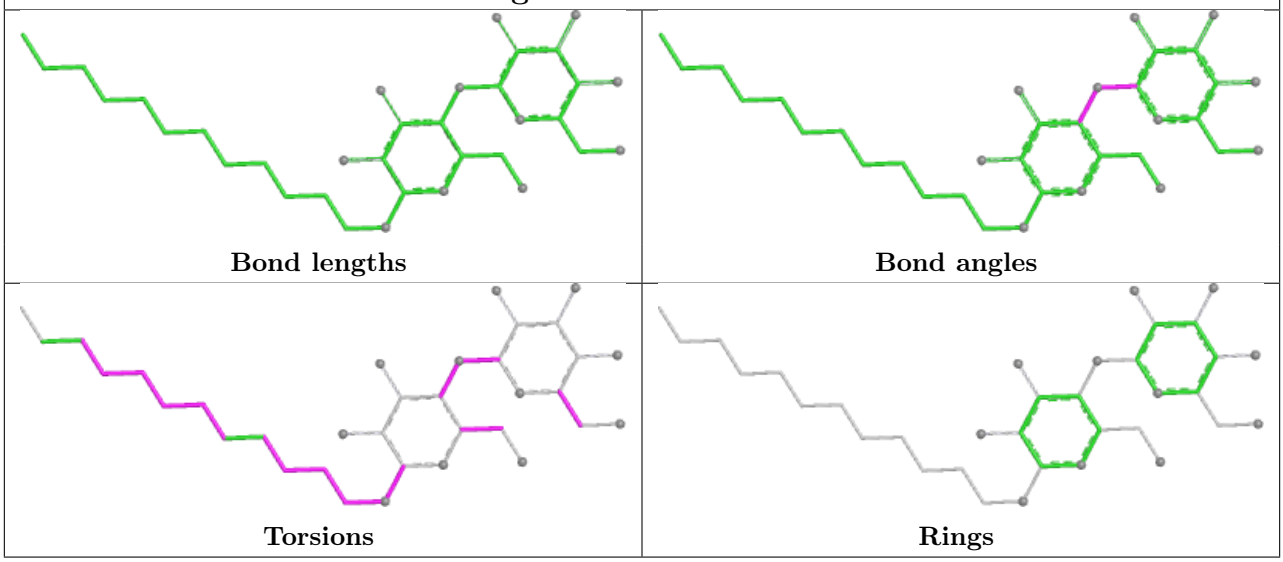
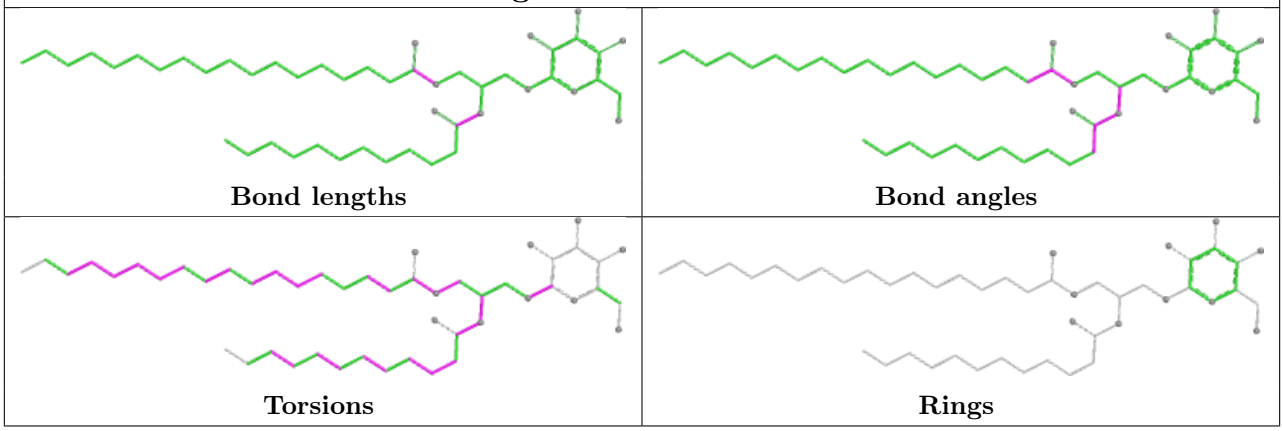


Rings

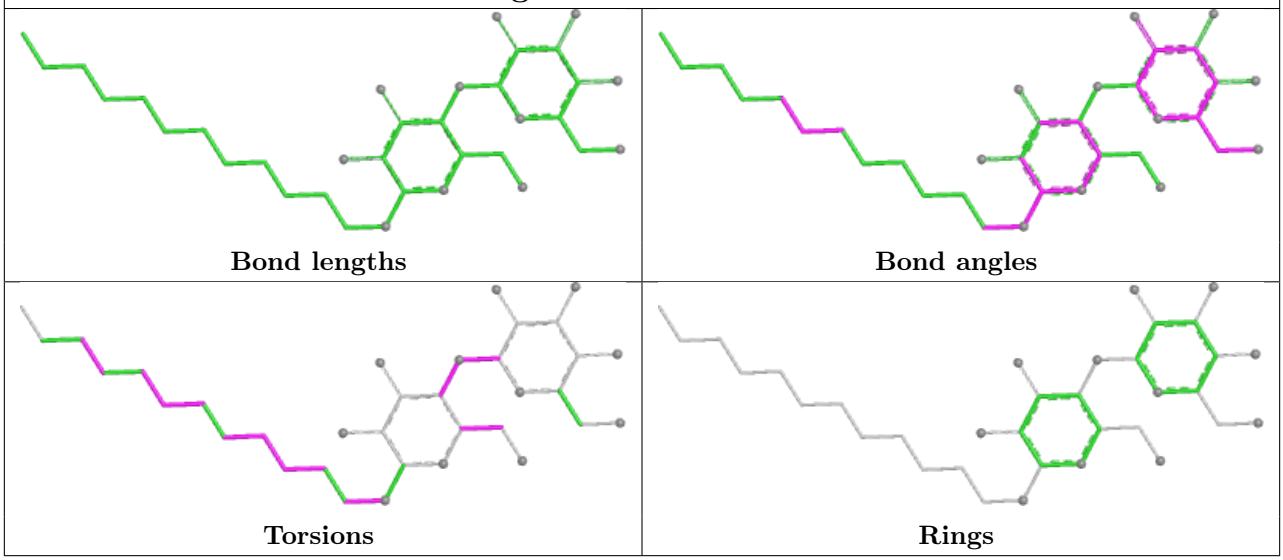
Ligand LMU A 7010



Ligand LMG B 1783



Ligand LMU A 7020



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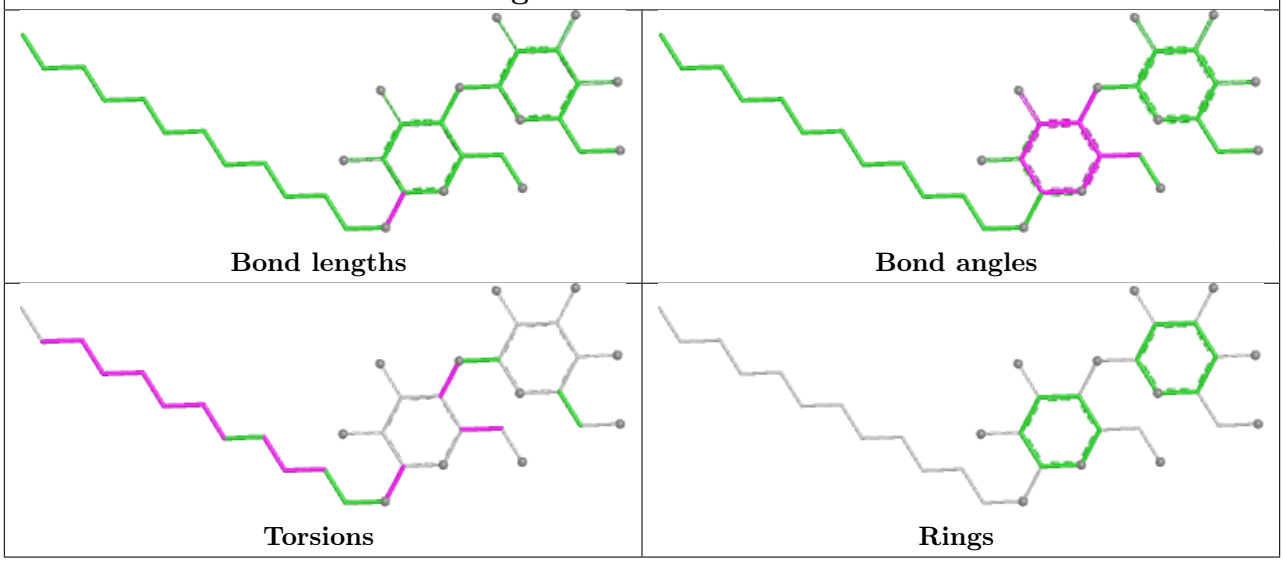
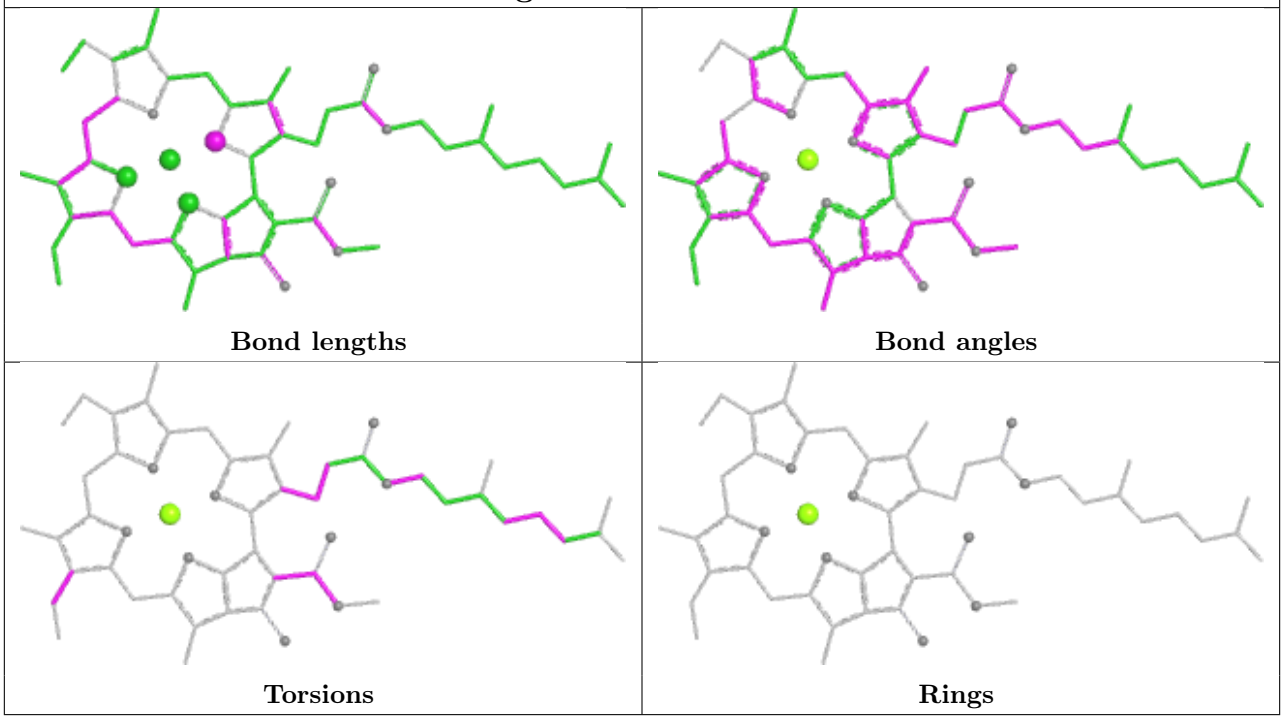
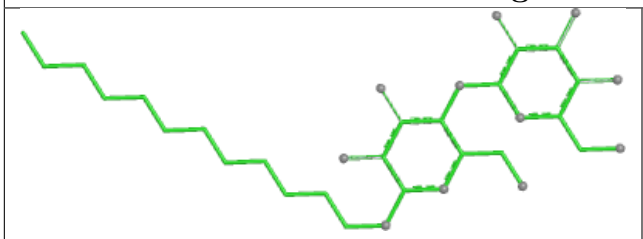
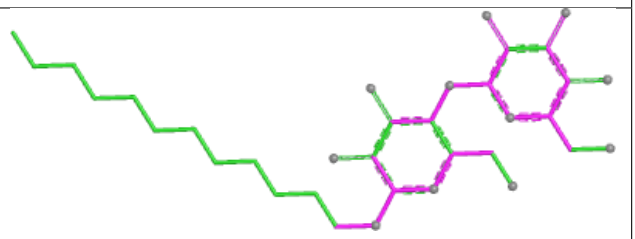
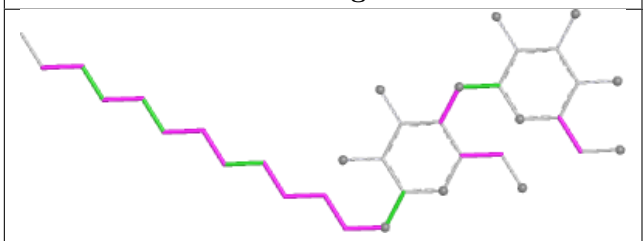
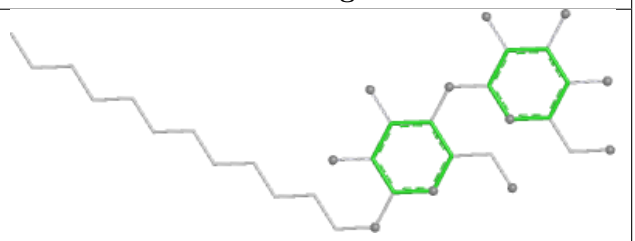
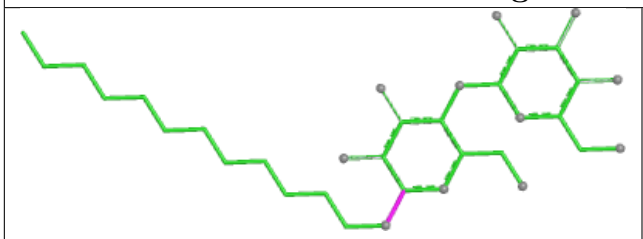
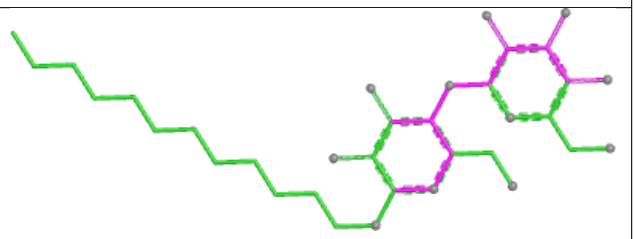
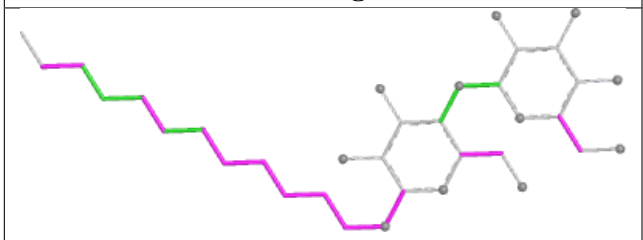
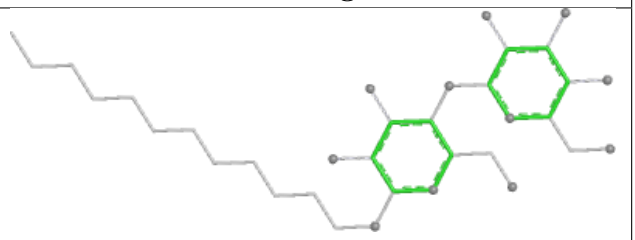


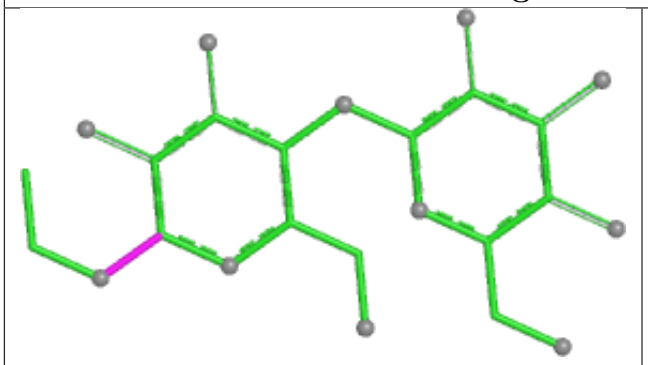
Ligand CLA A 1815



Ligand LMU A 7021	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMU A 7025	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMU B 1782



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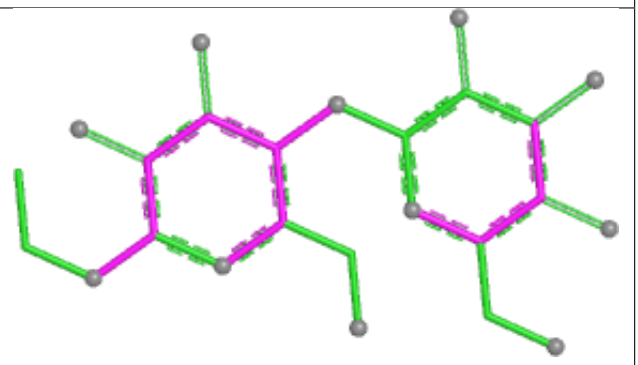
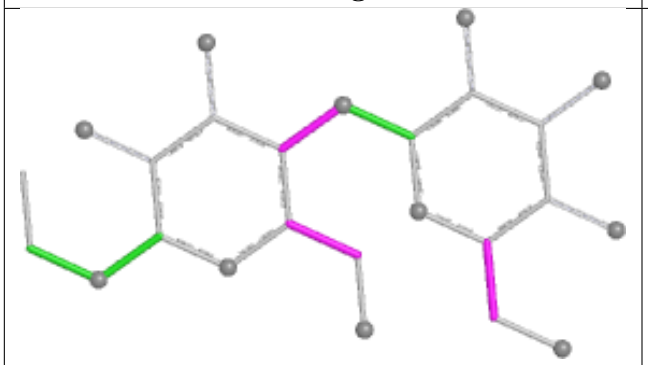


Bond angles



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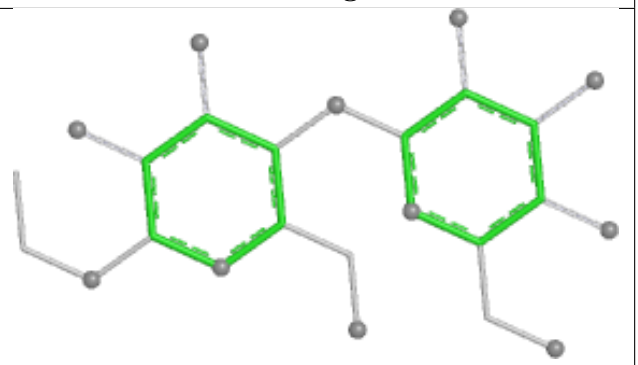
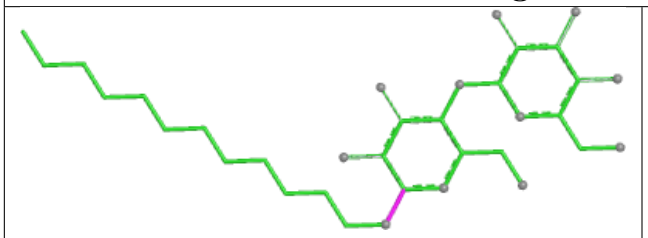
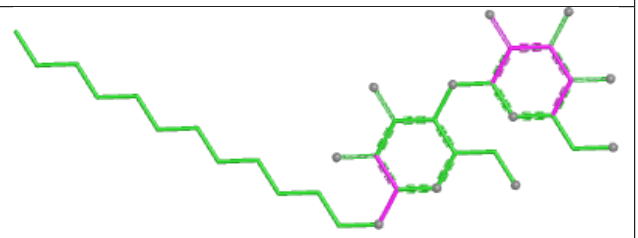


Rings

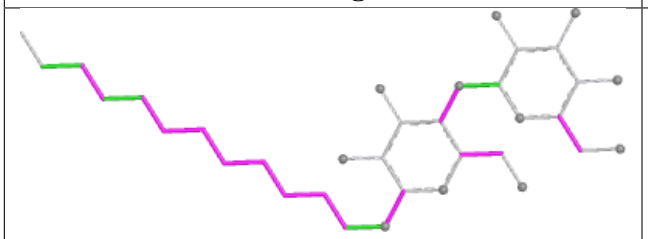
Ligand LMU A 7034



Bond lengths



Bond angles



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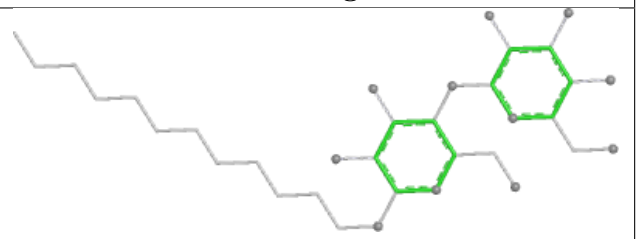
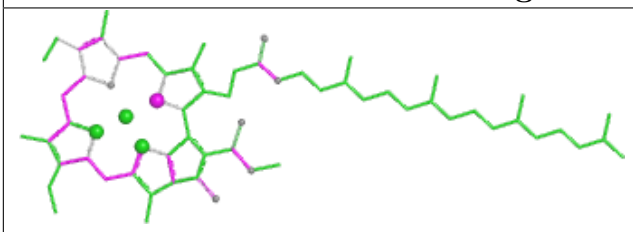


Rings

Ligand CLA B 1785



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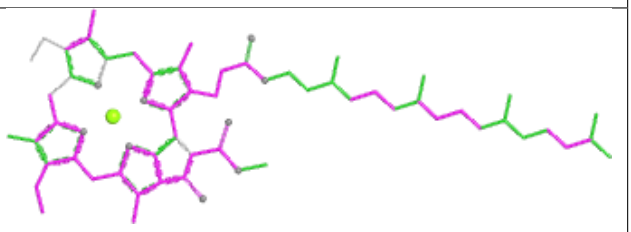
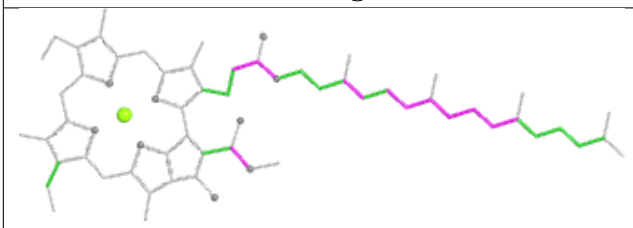


Bond angles



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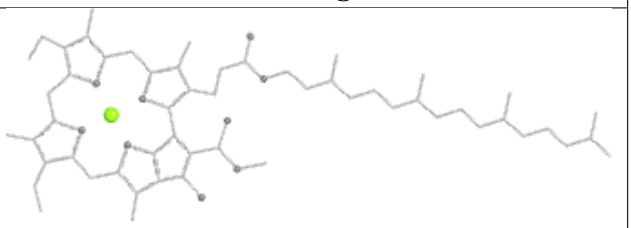
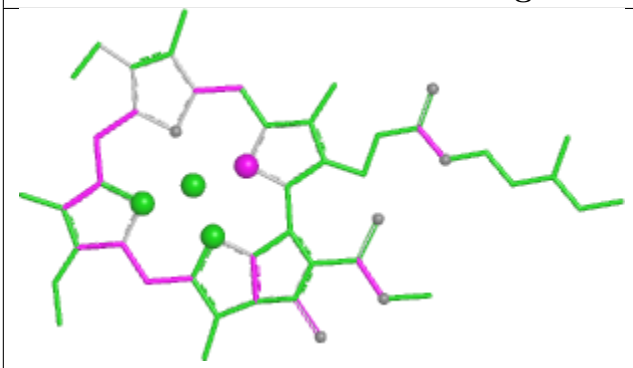


Rings

Ligand CLA A 1792



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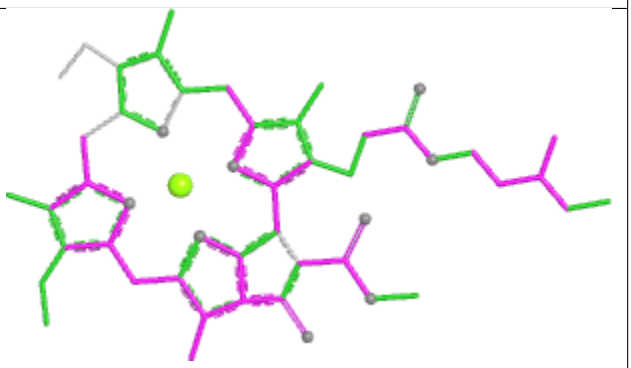
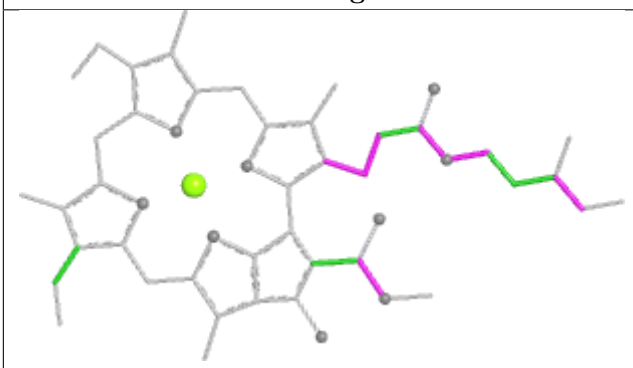


Bond angles



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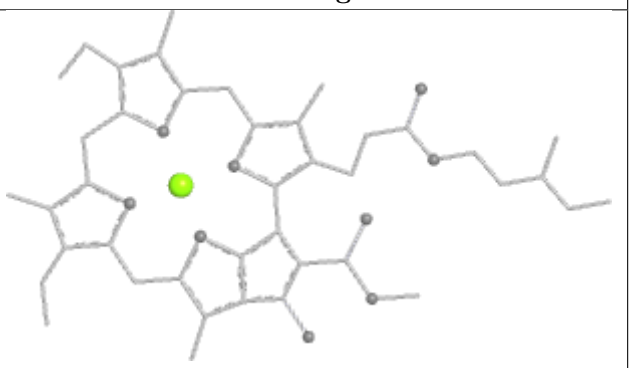
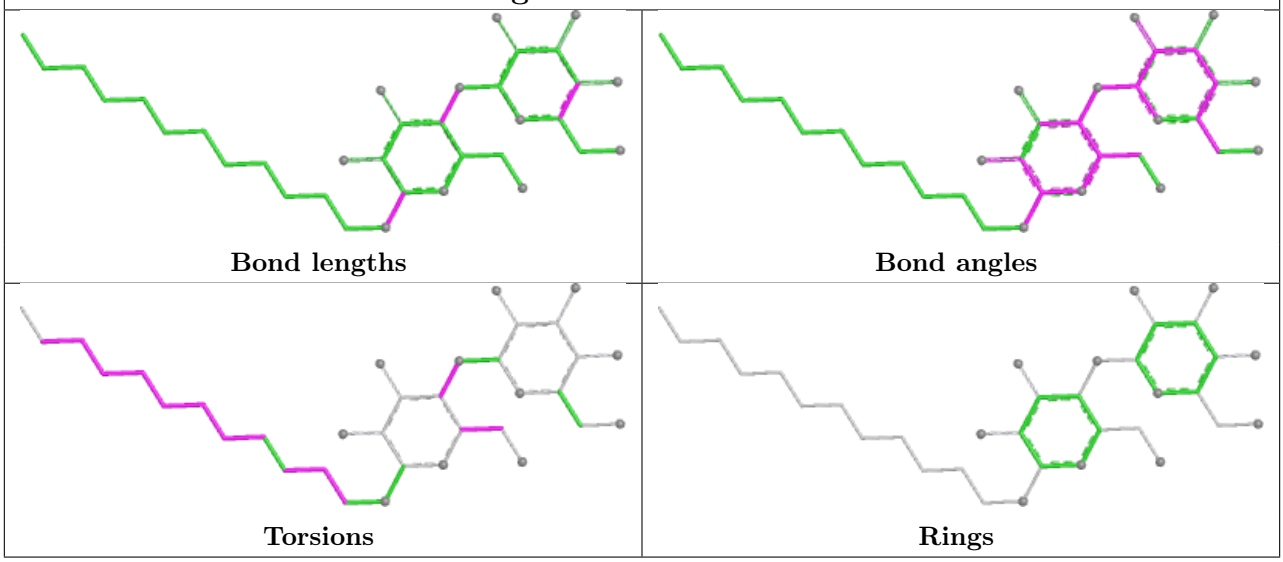
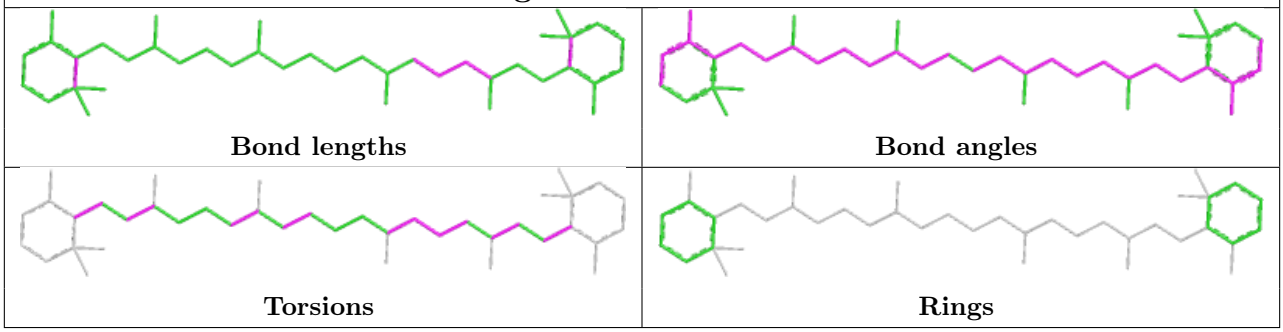


Rings

Ligand LMU A 7033



Ligand BCR A 1806



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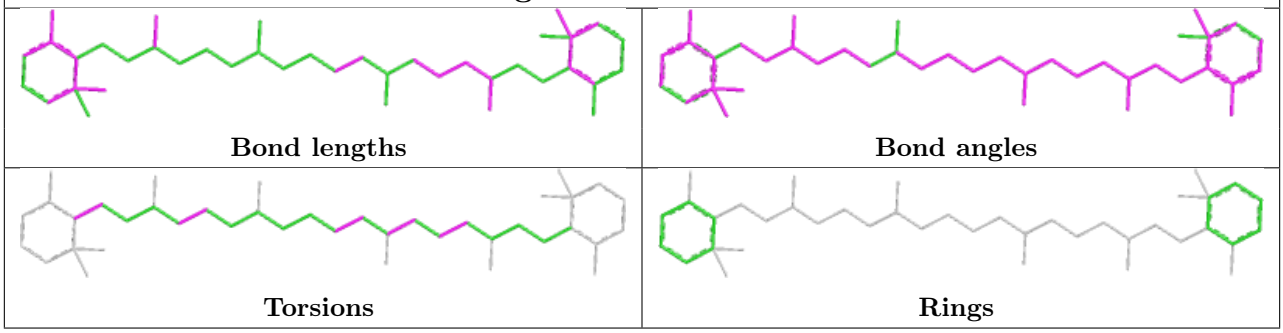
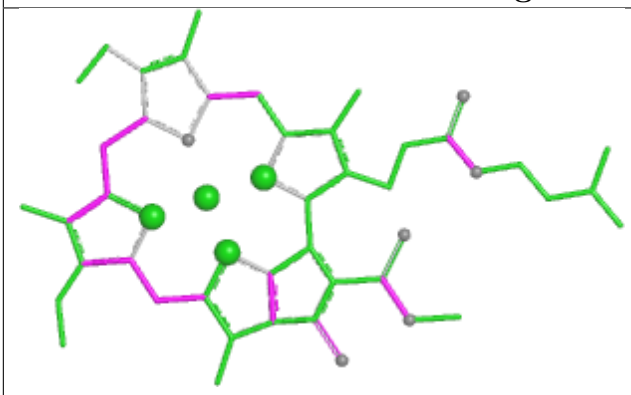
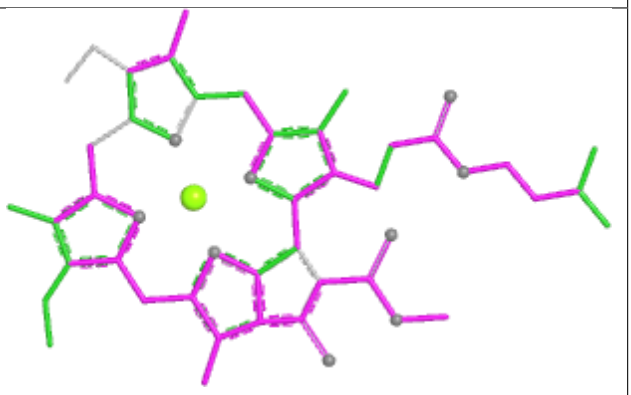
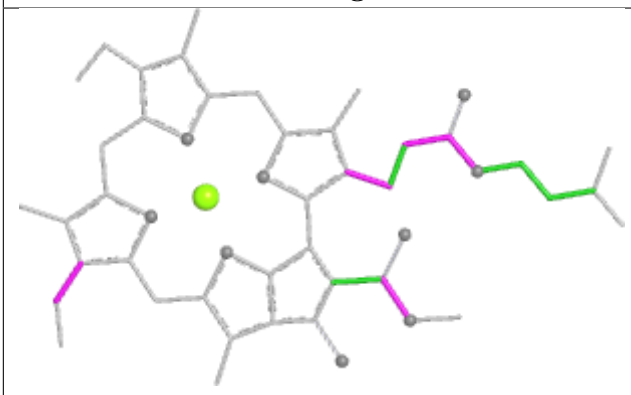
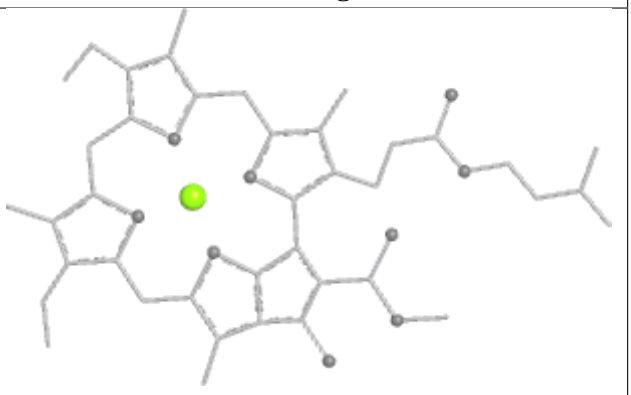
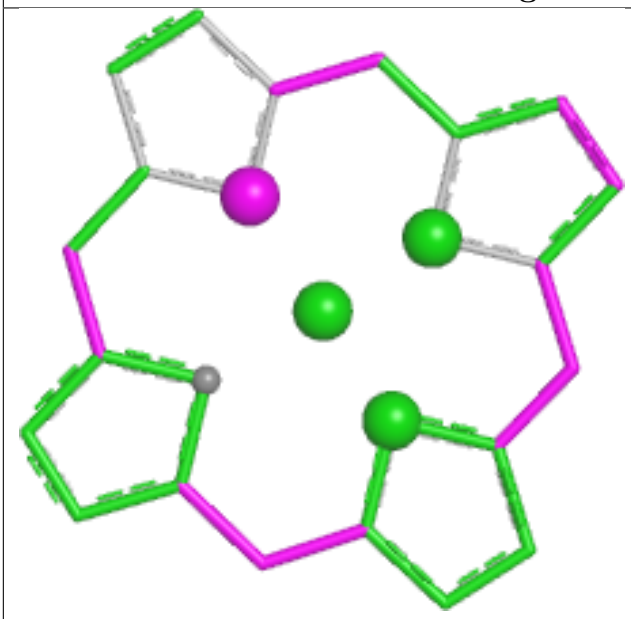
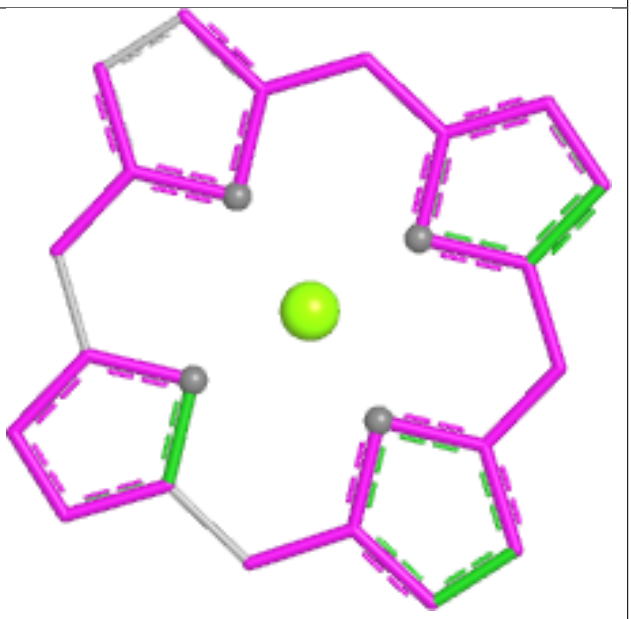


Ligand CLA A 1771	
 Bond lengths	 Bond angles
 Torsions	 Rings

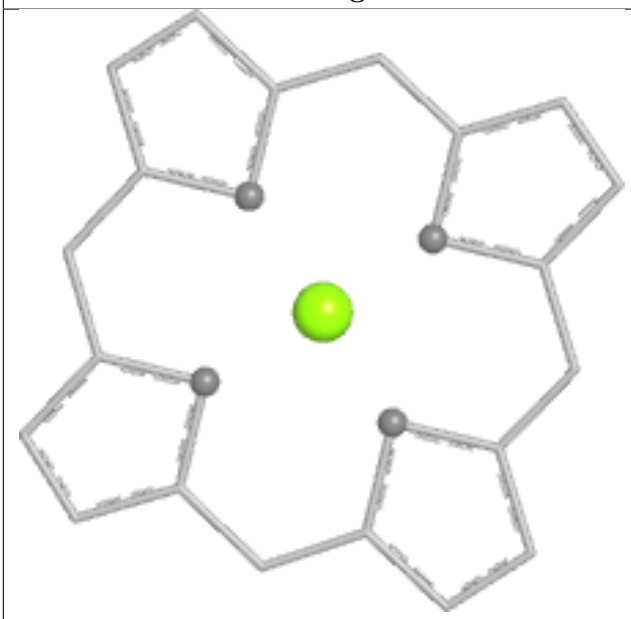
Ligand CLA 4 1202



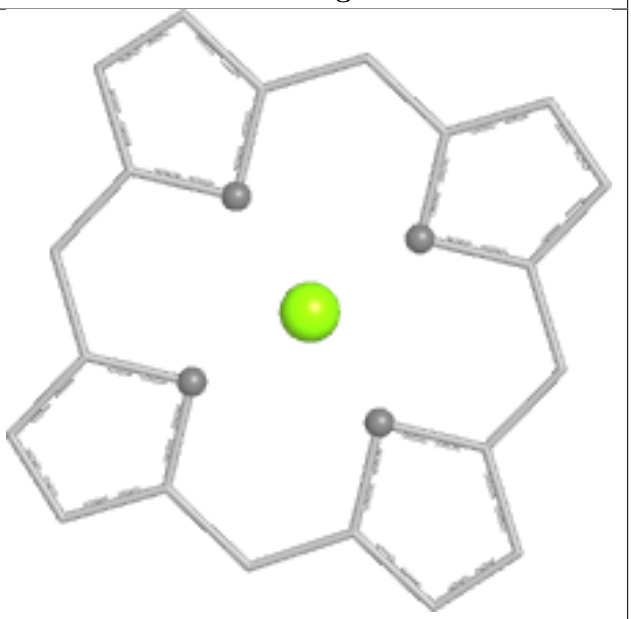
Bond lengths



Bond angles

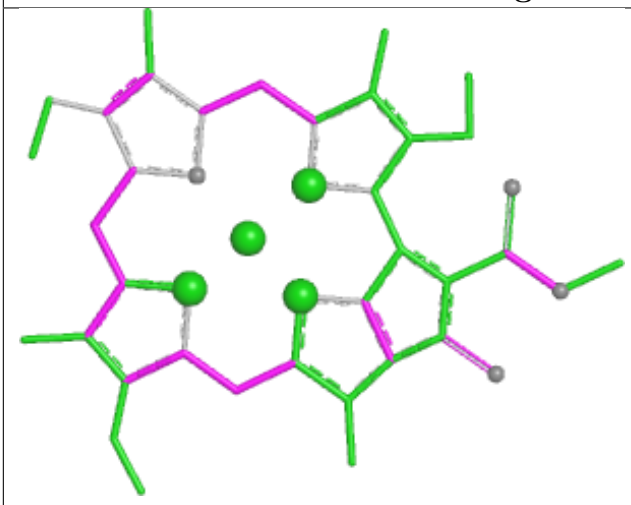


Torsions

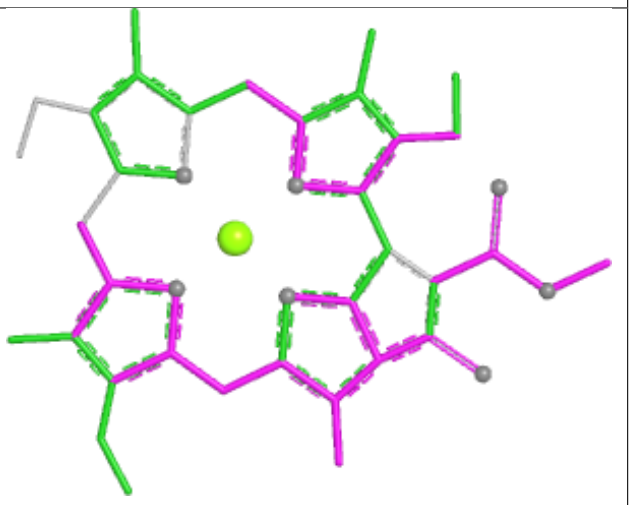


Rings

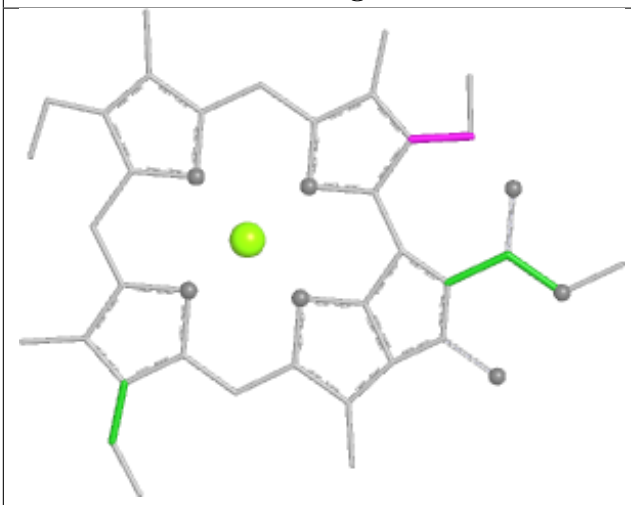
Ligand CLA A 1778



Bond lengths



Bond angles



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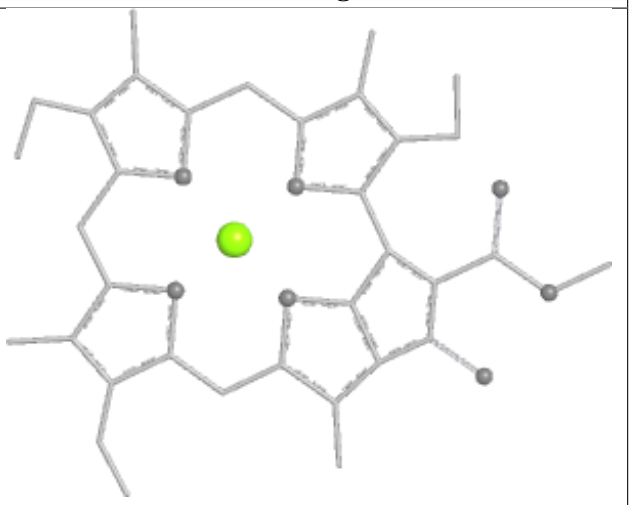
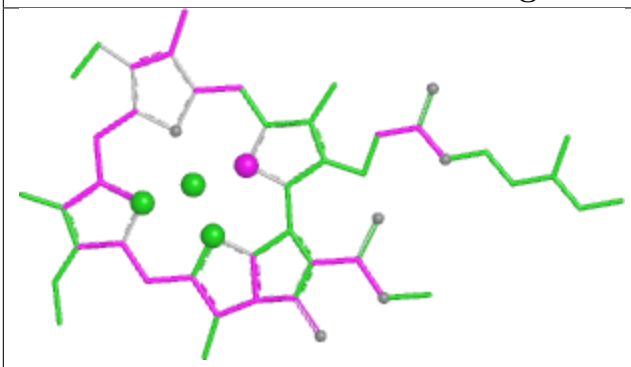
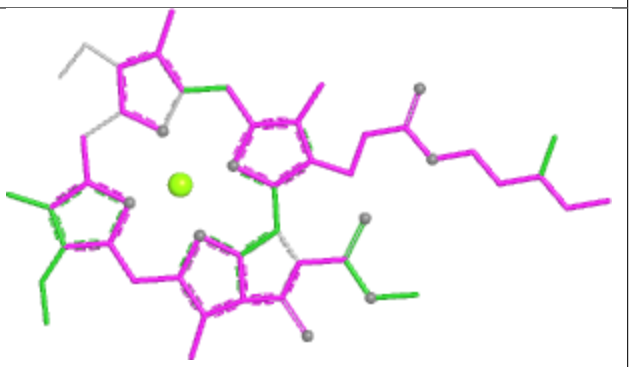
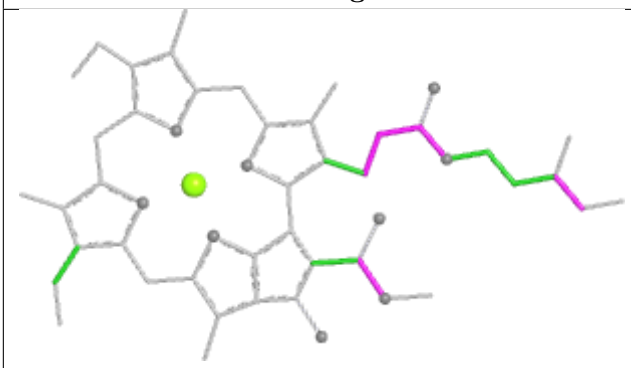
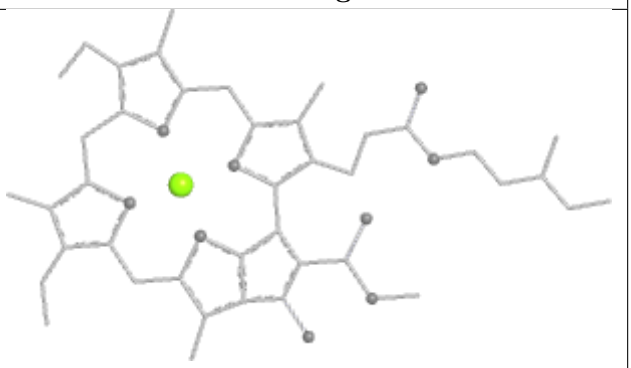
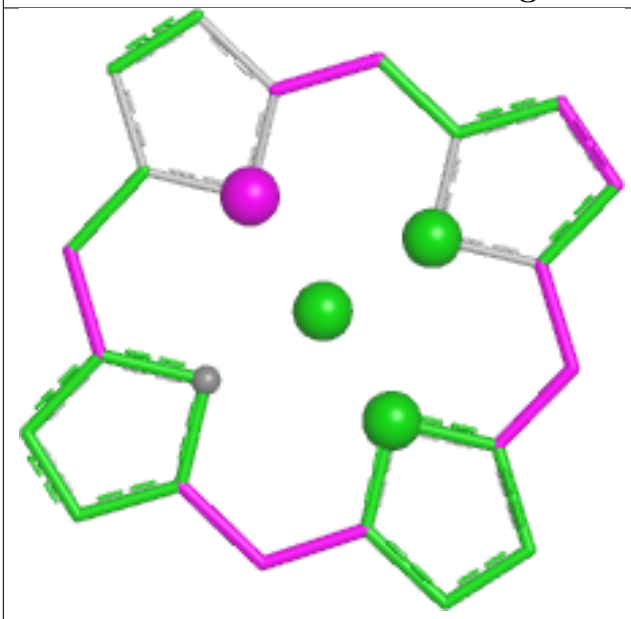


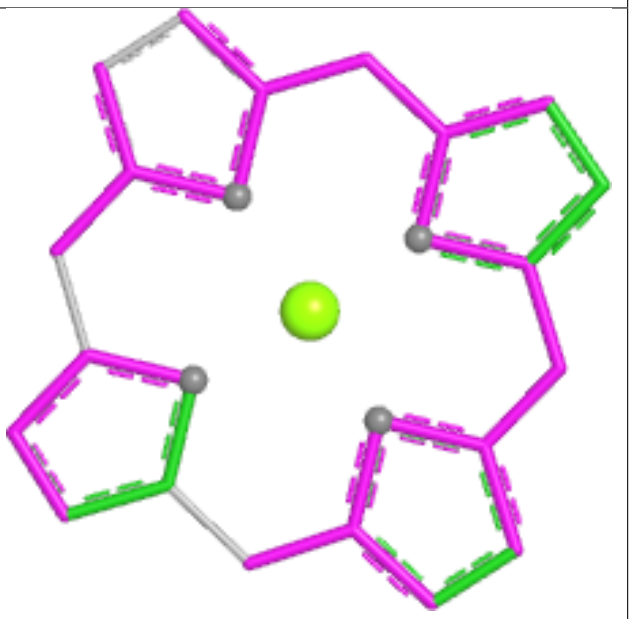
Rings

Ligand CLA 1 1197	
 Bond lengths	 Bond angles
 Torsions	 Rings

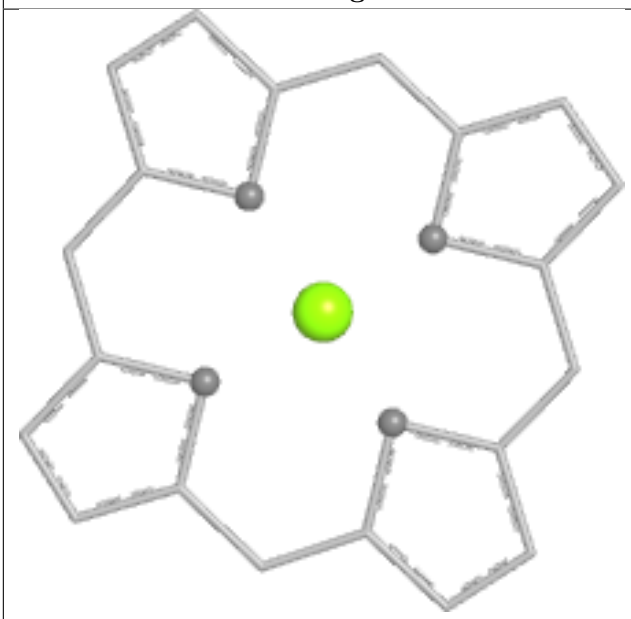
Ligand CLA 2 2010



Bond lengths



Bond angles



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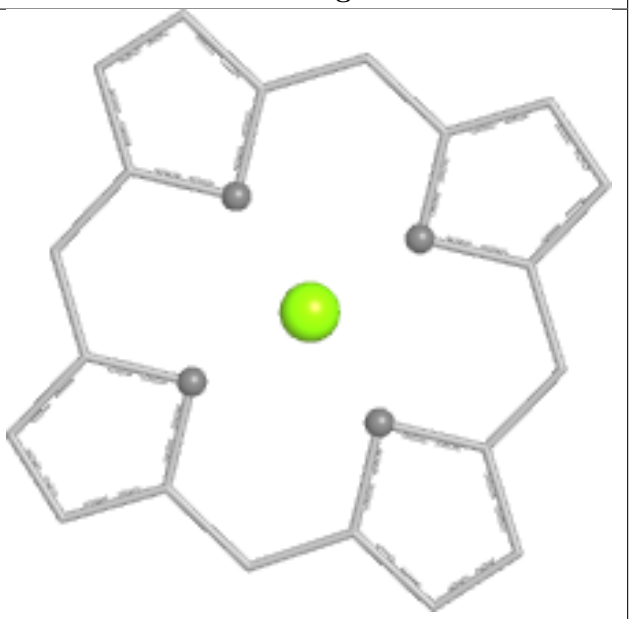
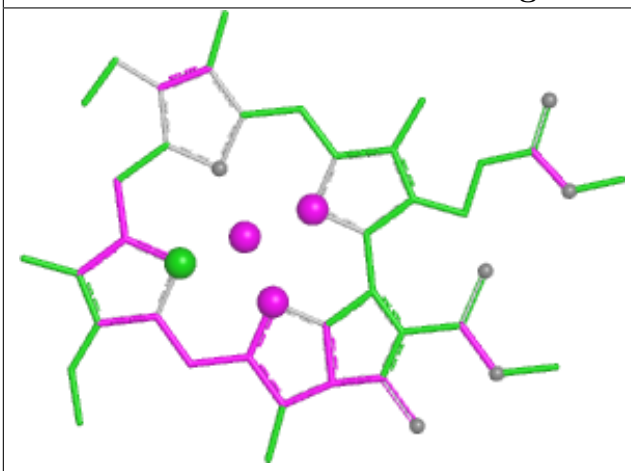
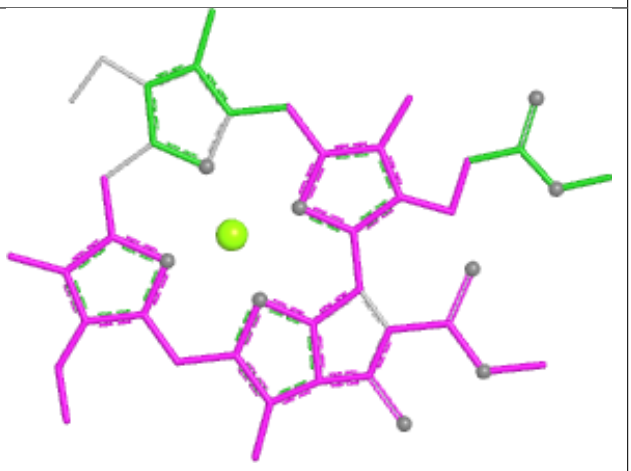


Rings

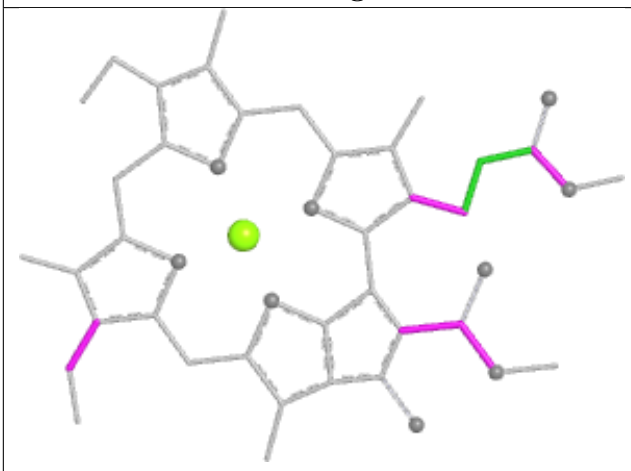
Ligand CLA 1 1187



Bond lengths



Bond angles



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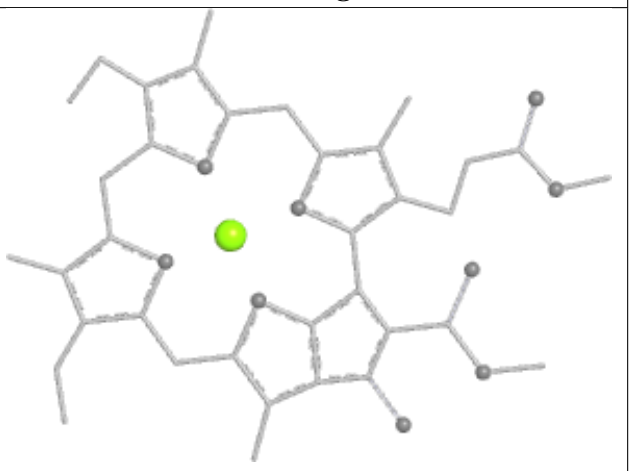
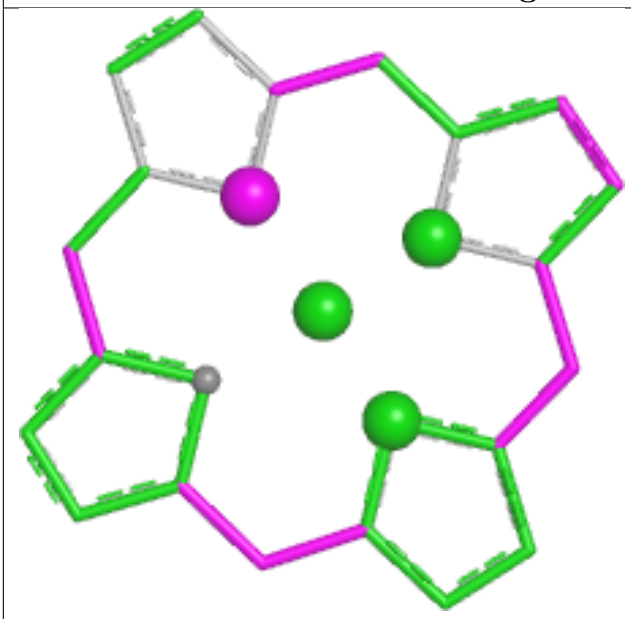


Rings

Ligand CLA 4 1203



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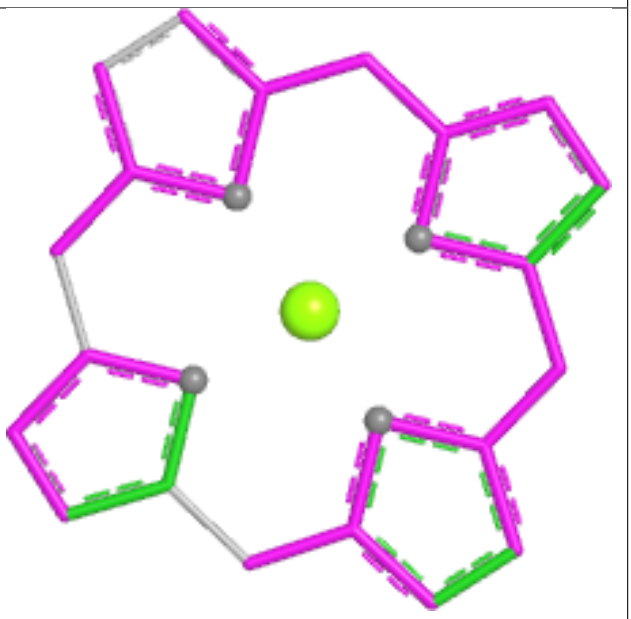
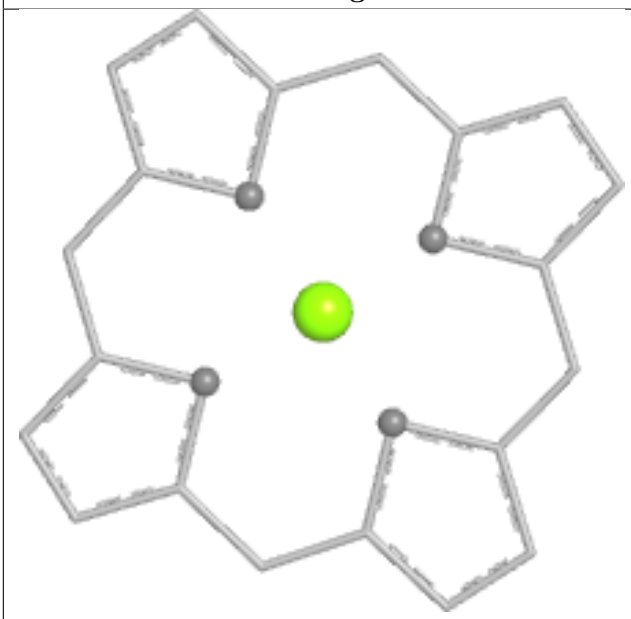


Bond angles



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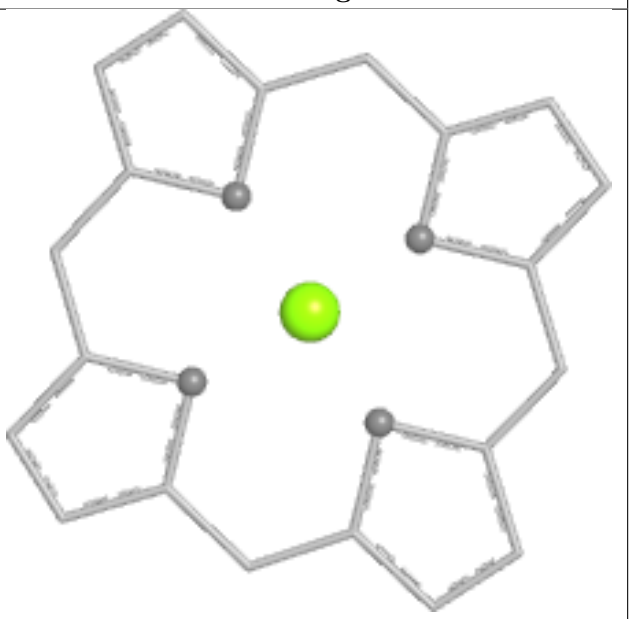
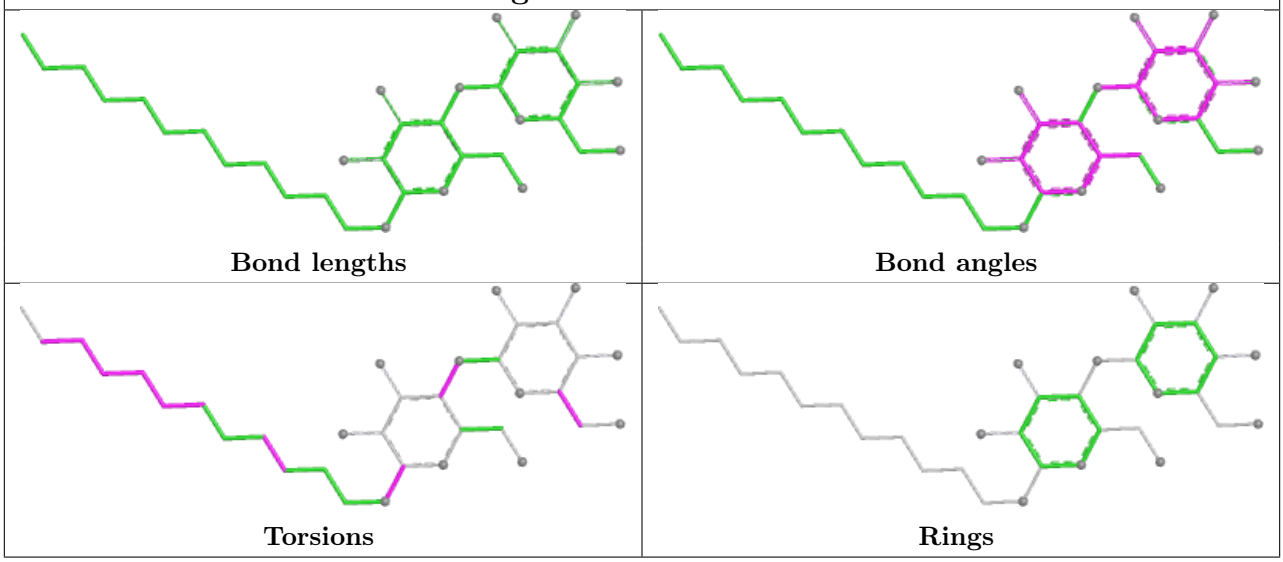
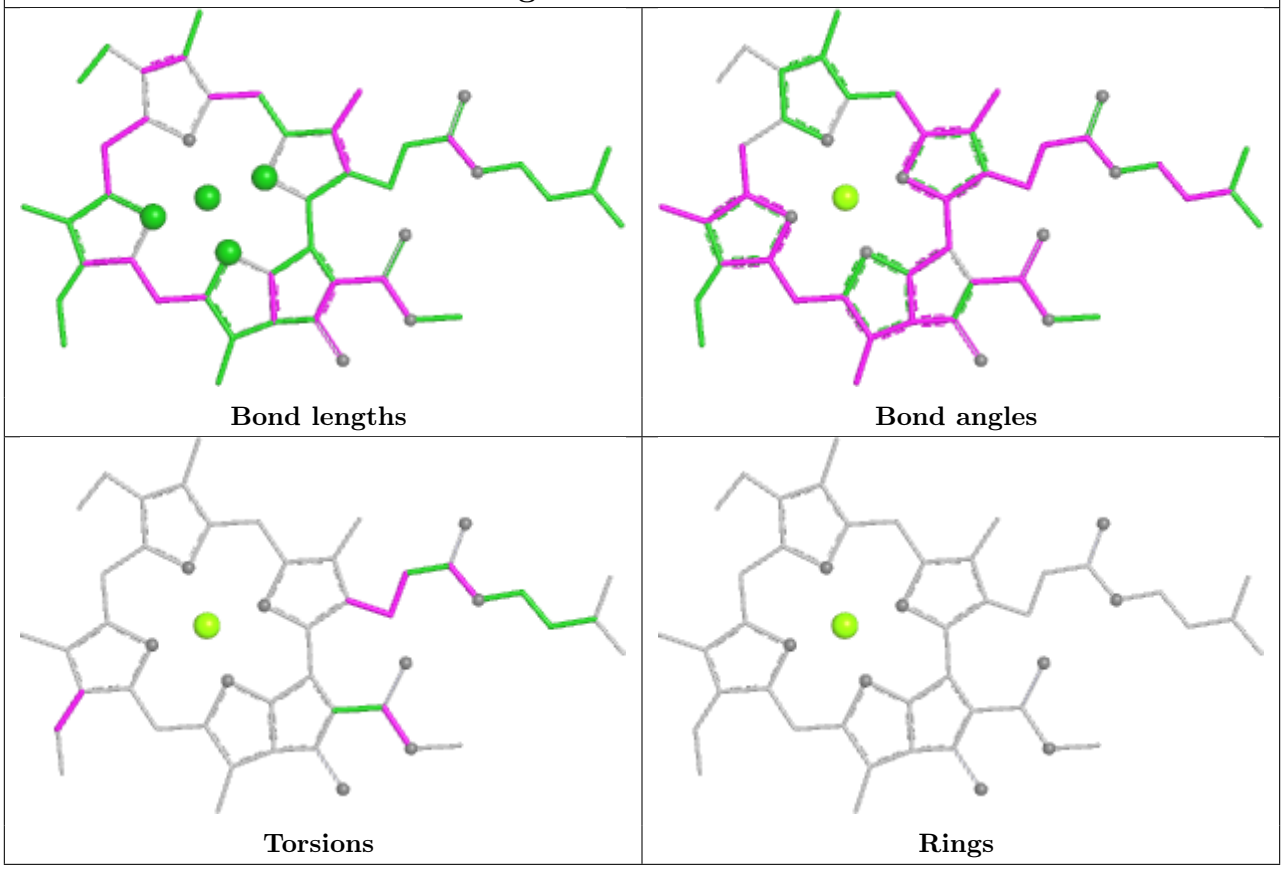


Rings

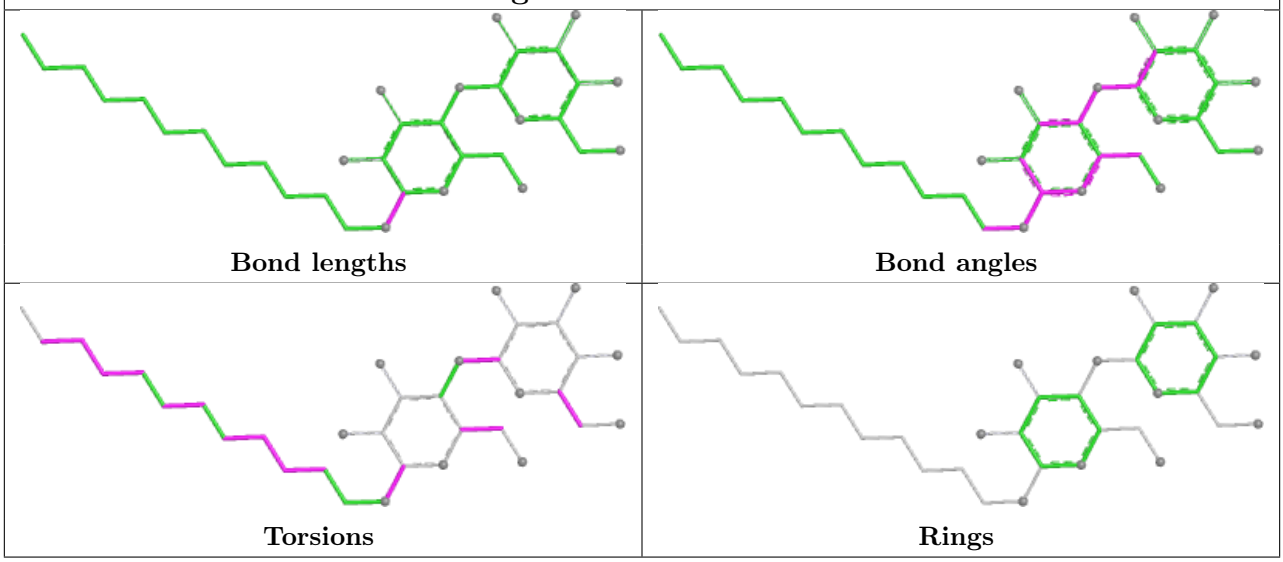
Ligand LMU A 7043



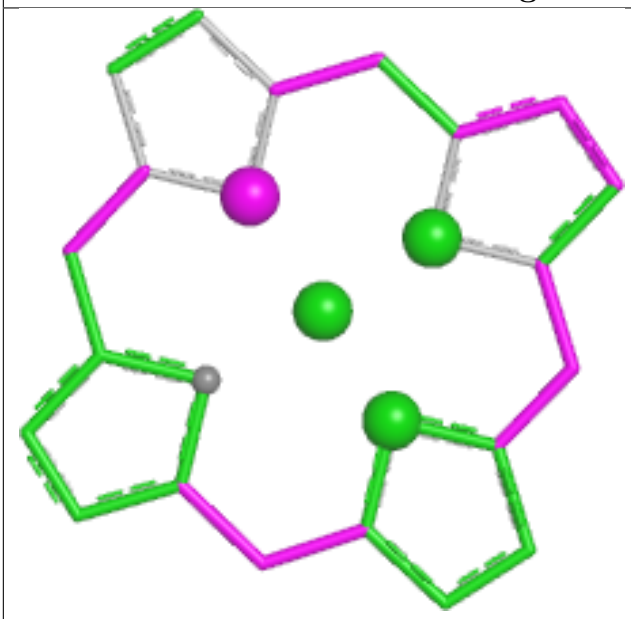
Ligand CLA L 1168



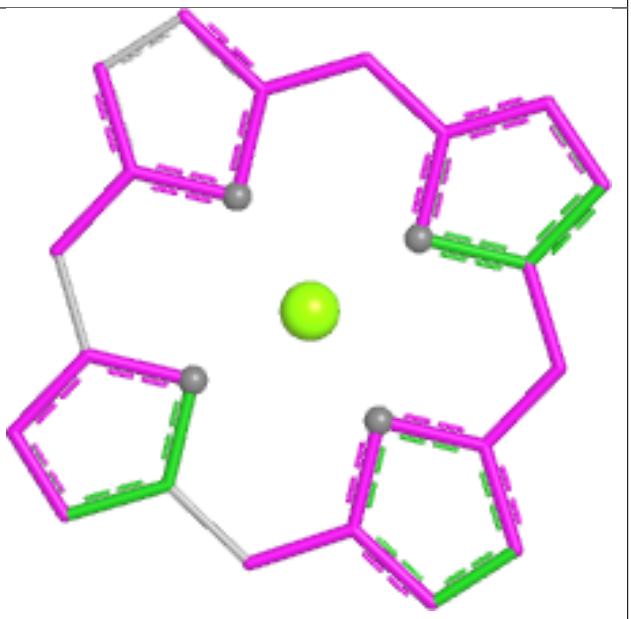
Ligand LMU A 7031



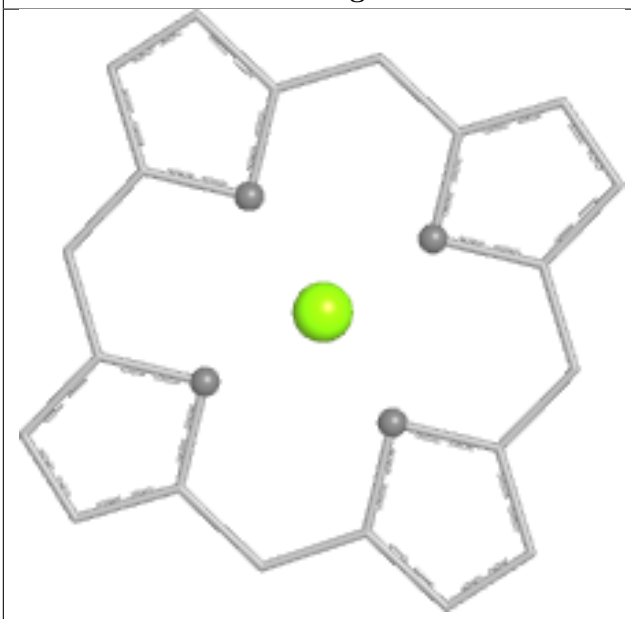
Ligand CLA 3 1216



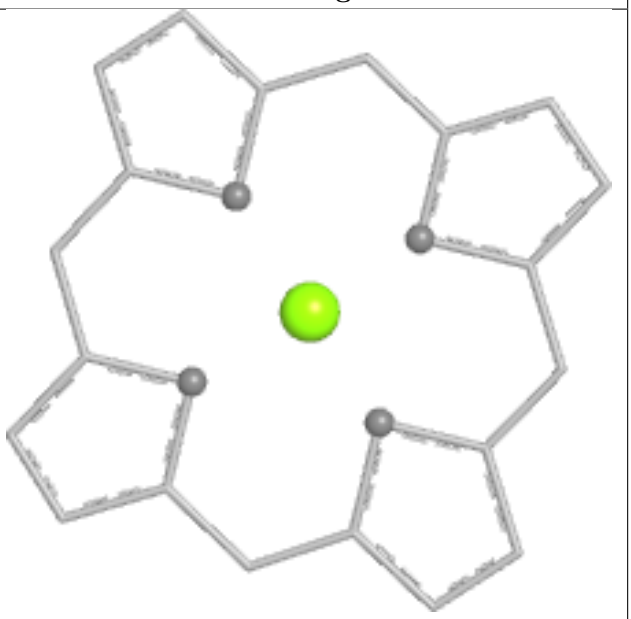
Bond lengths



Bond angles

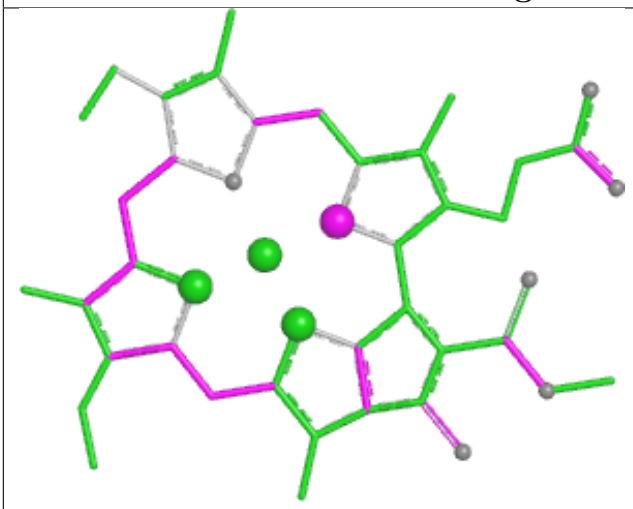


Torsions



Rings

Ligand CLA A 1766



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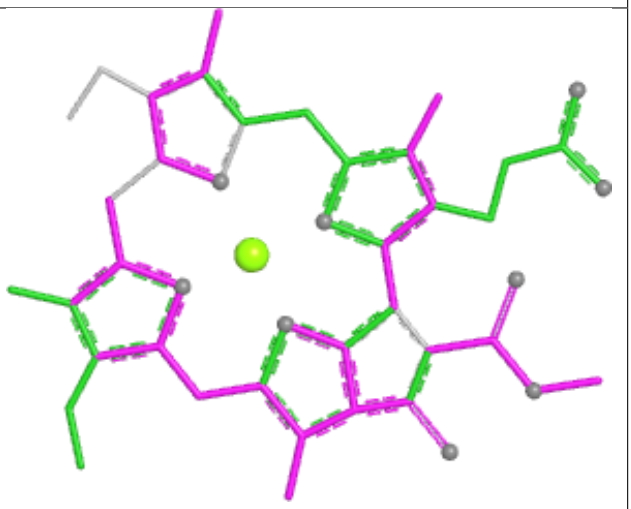
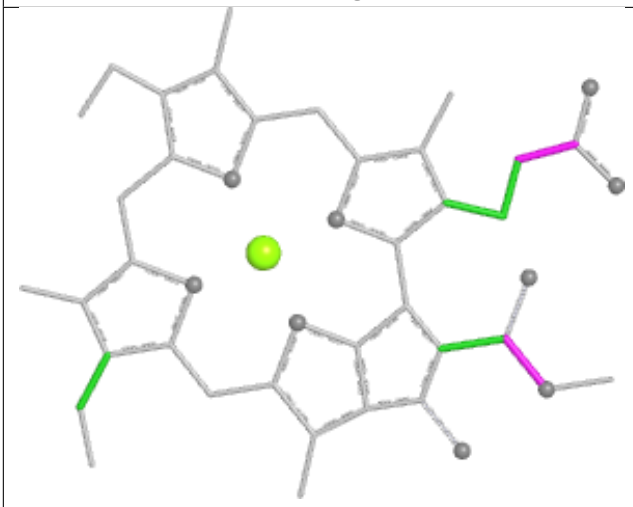
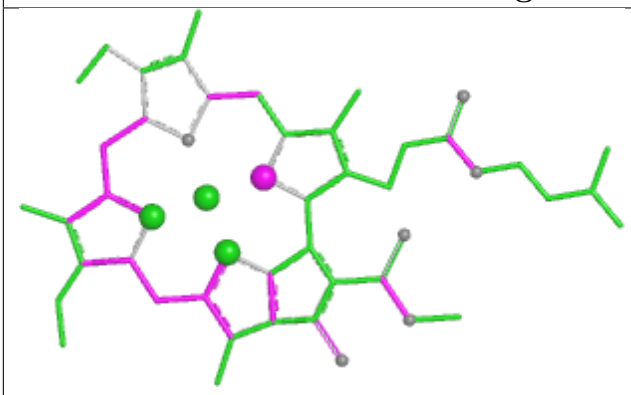
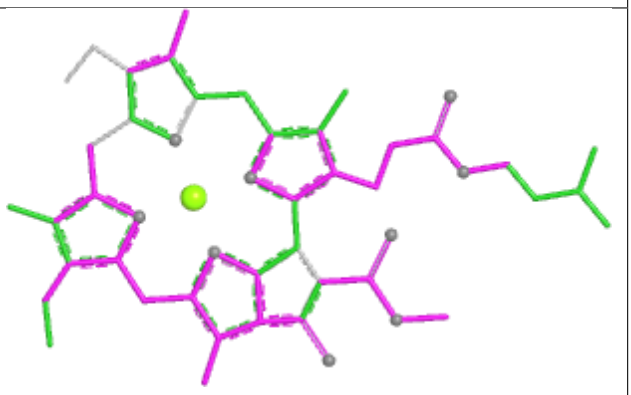
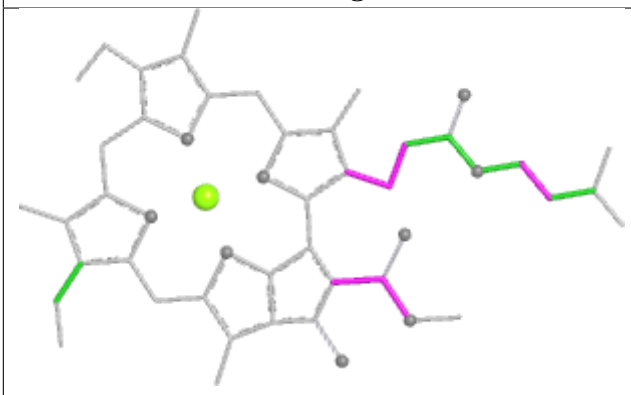
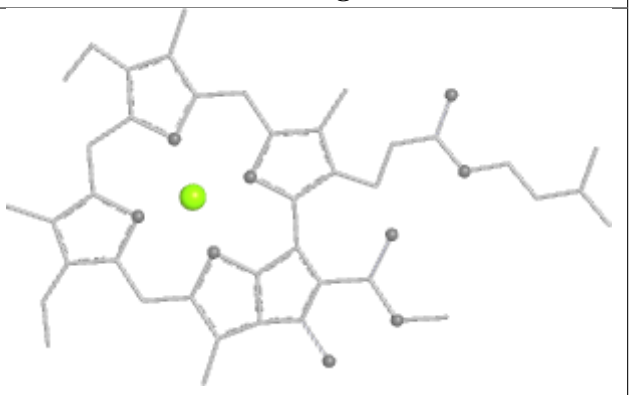


Bond angles

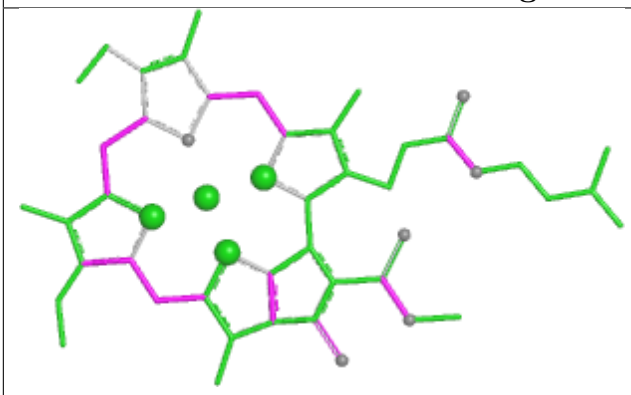


Torsions

Rings

Ligand CLA B 1763	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 1200



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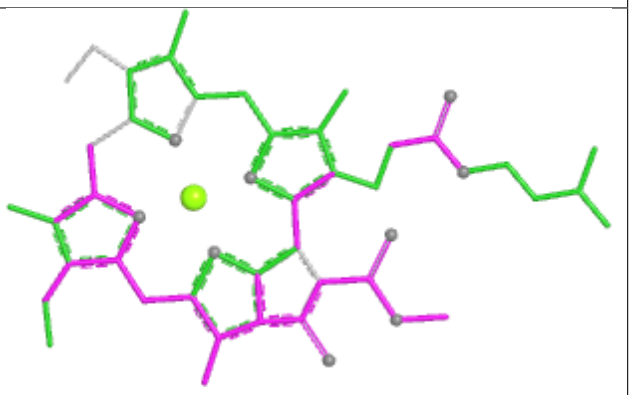
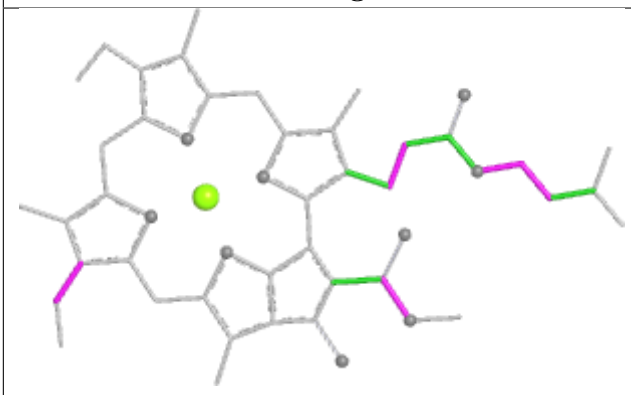
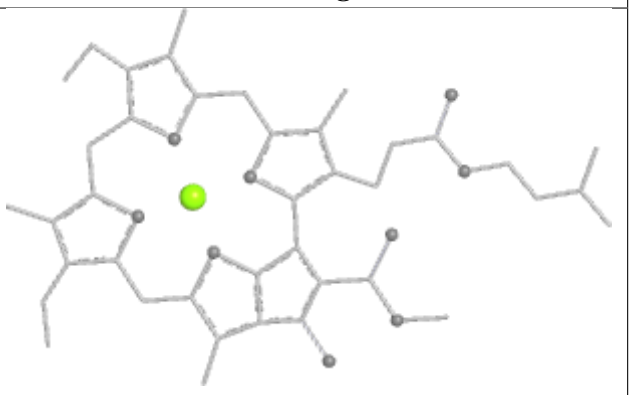


Bond angles

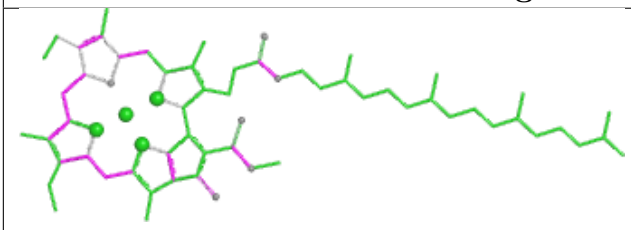


Torsions

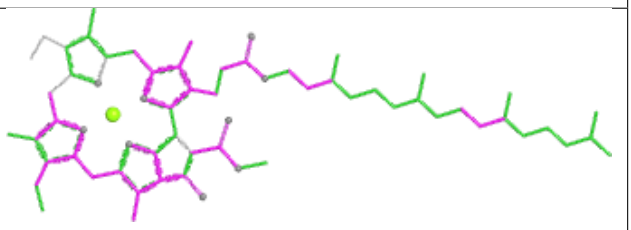


Rings

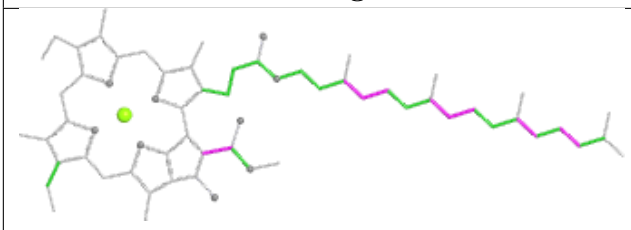
Ligand CLA B 1739



Bond lengths



Bond angles



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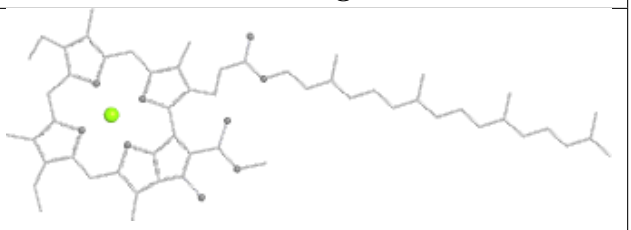
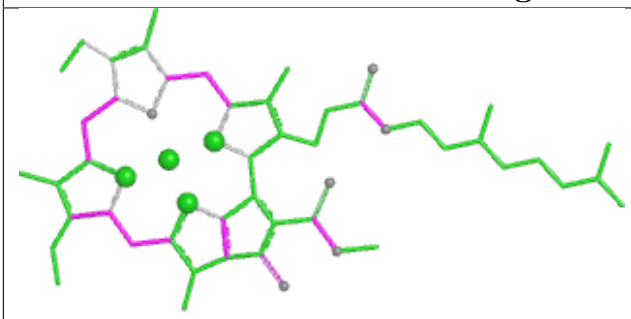
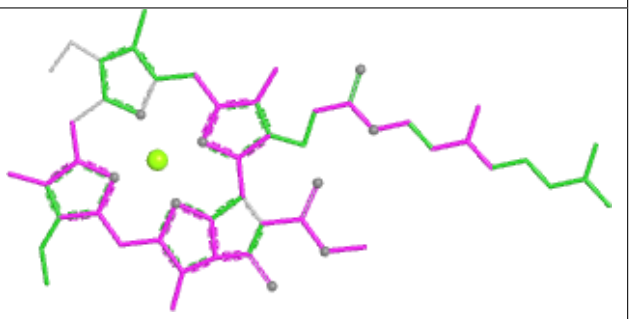
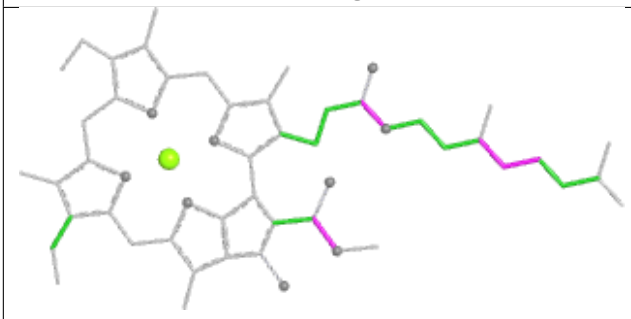
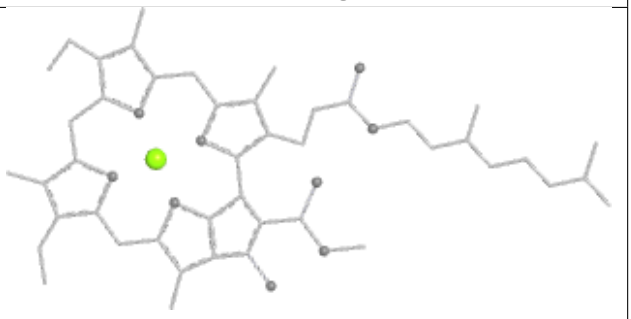
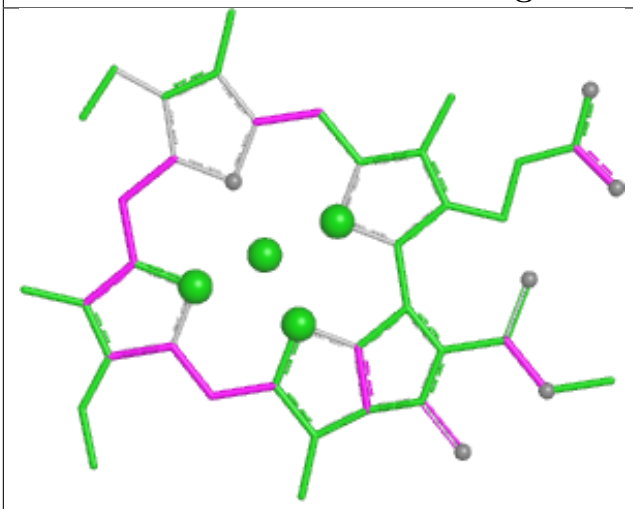


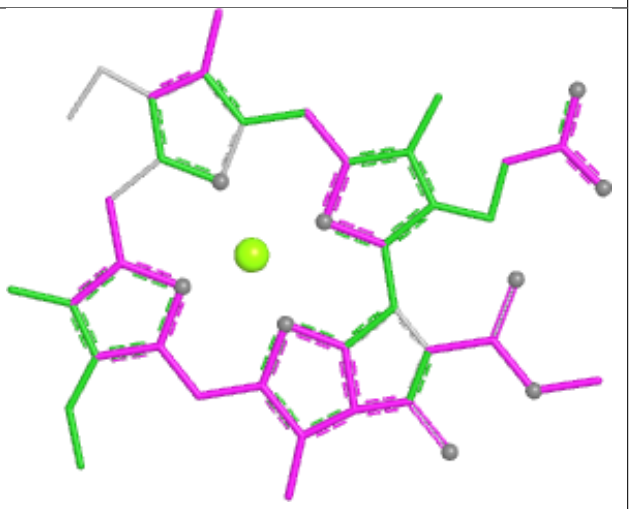
Rings

Ligand CLA A 1801	
 Bond lengths	 Bond angles
 Torsions	 Rings

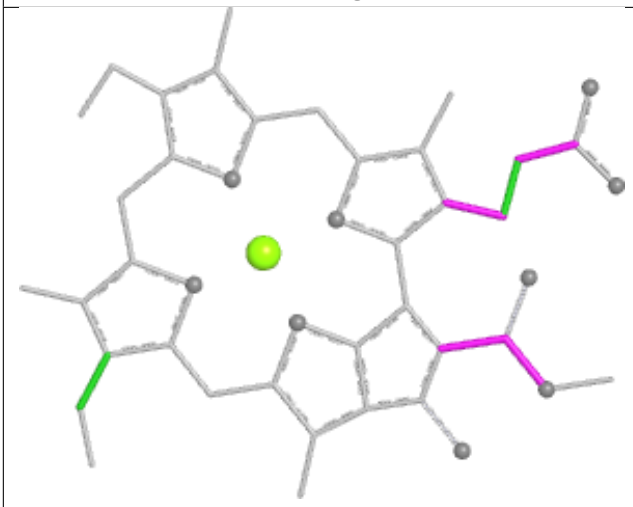
Ligand CLA B 1765



Bond lengths



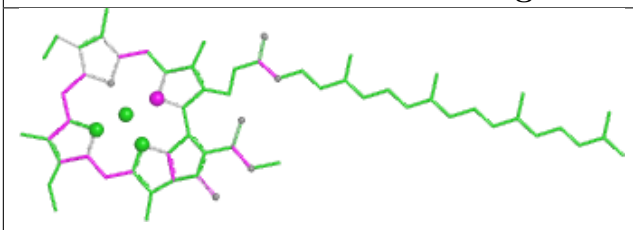
Bond angles



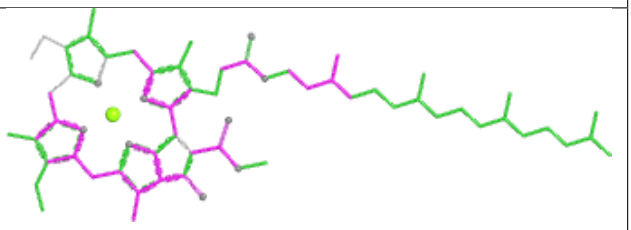
Torsions

Rings

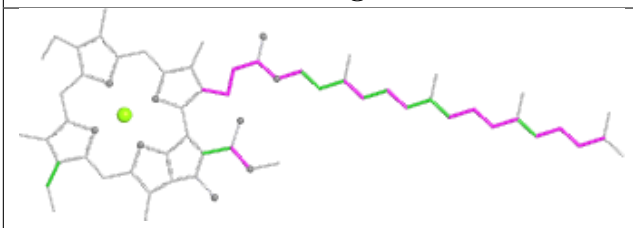
Ligand CLA B 1756



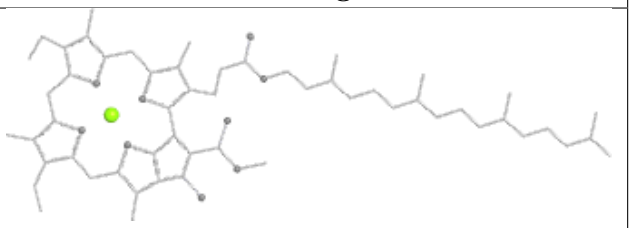
Bond lengths



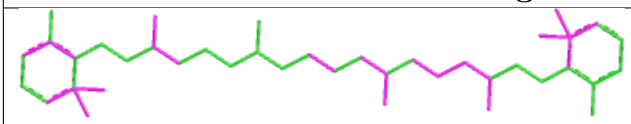
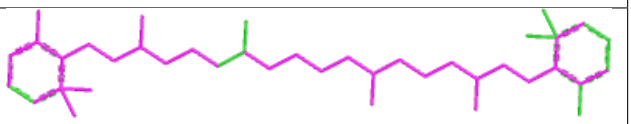
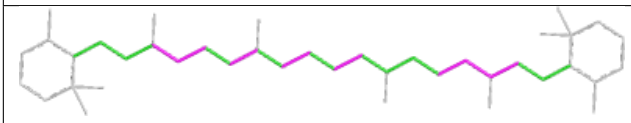
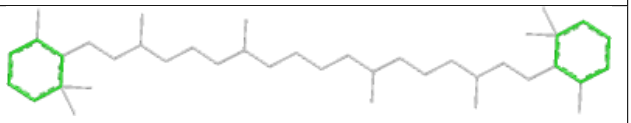
Bond angles

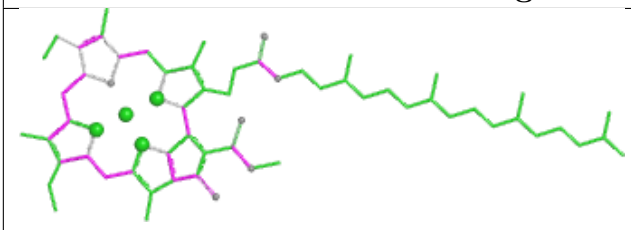
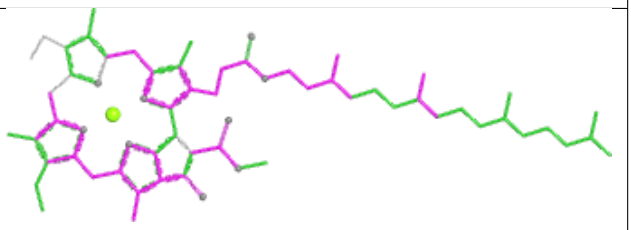
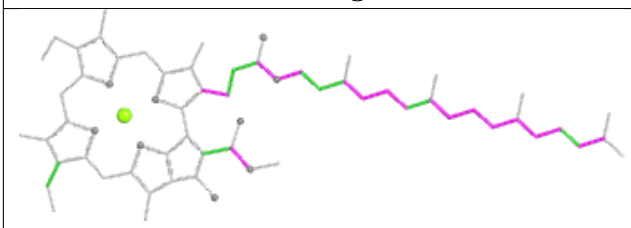
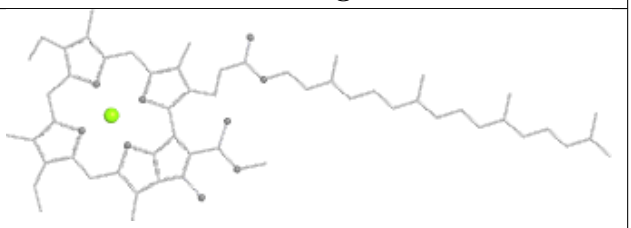


Torsions

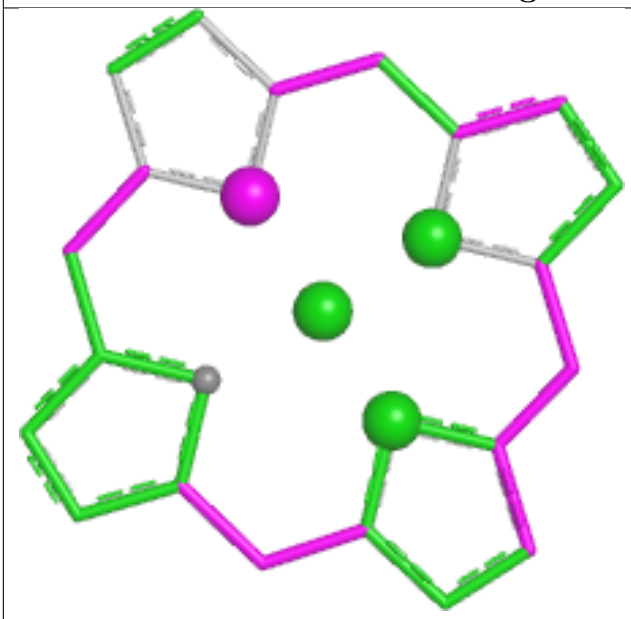


Rings

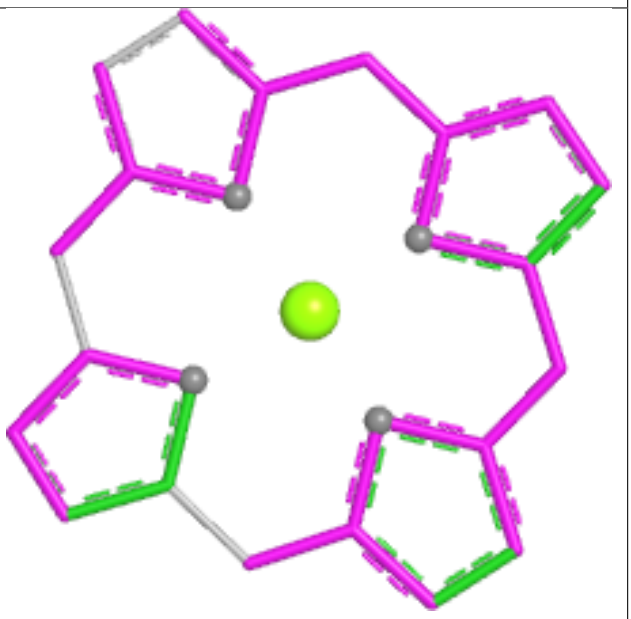
Ligand BCR L 1170	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1762	
 Bond lengths	 Bond angles
 Torsions	 Rings

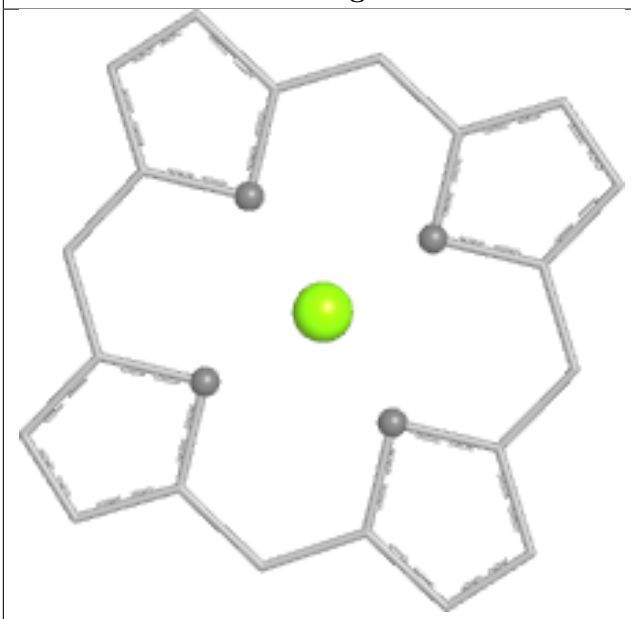
Ligand CLA 2 1214



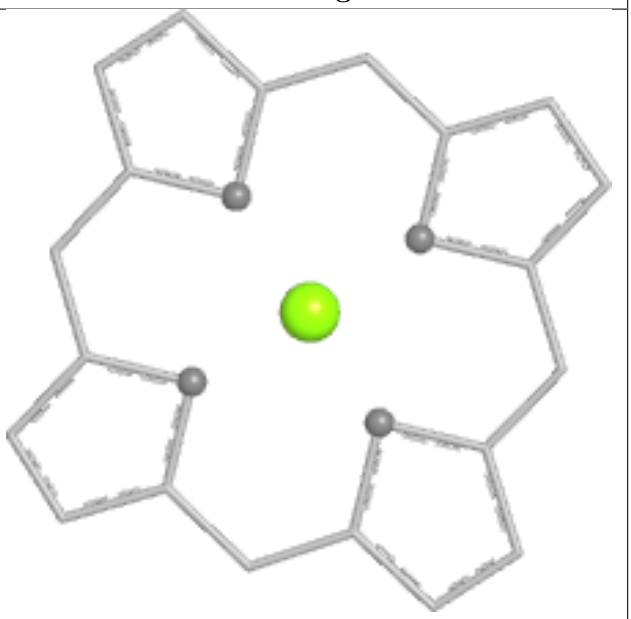
Bond lengths



Bond angles

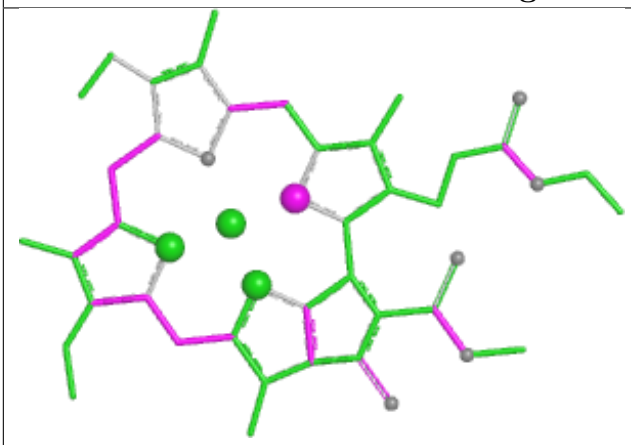


Torsions

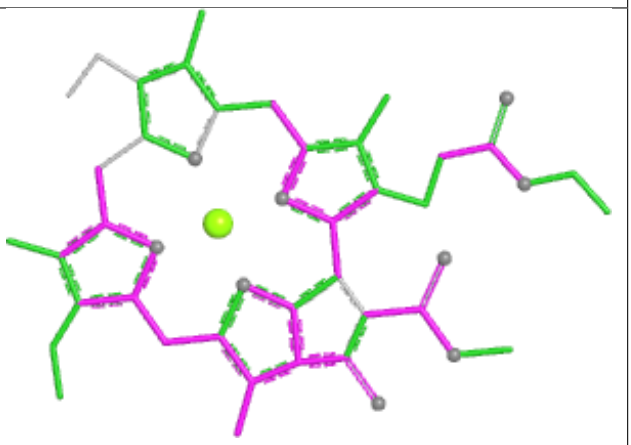


Rings

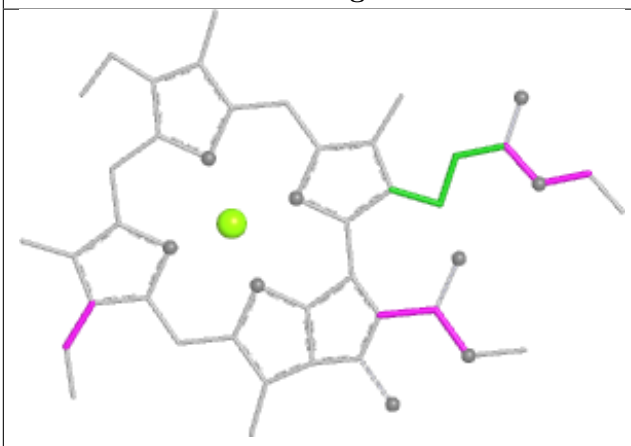
Ligand CLA 4 4014



Bond lengths



Bond angles



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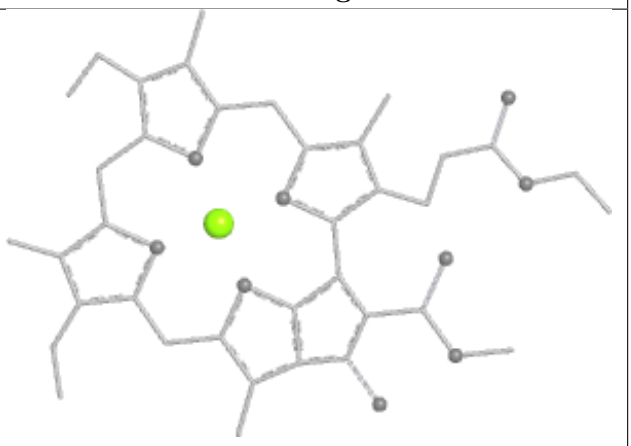
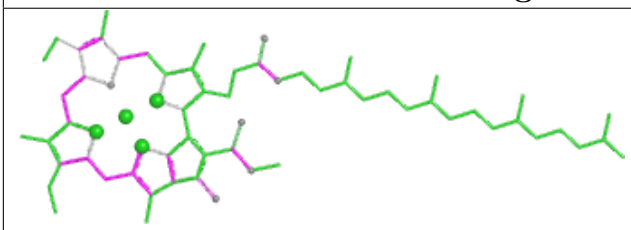
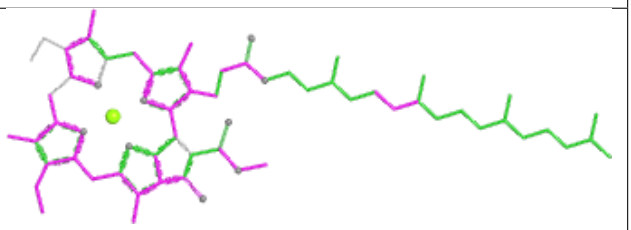


Rings

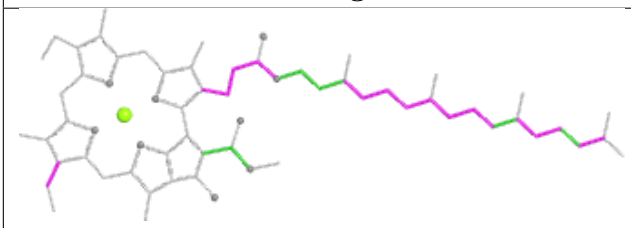
Ligand CLA A 1811



Bond lengths



Bond angles



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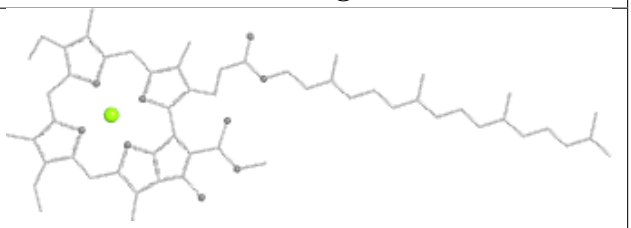
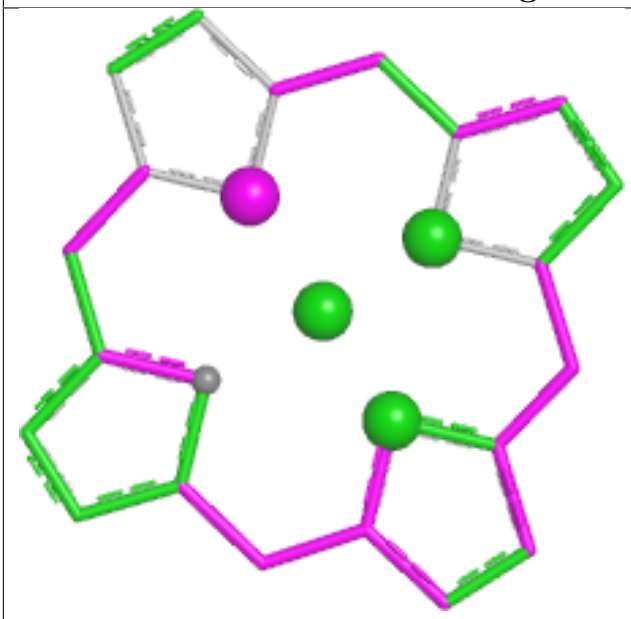
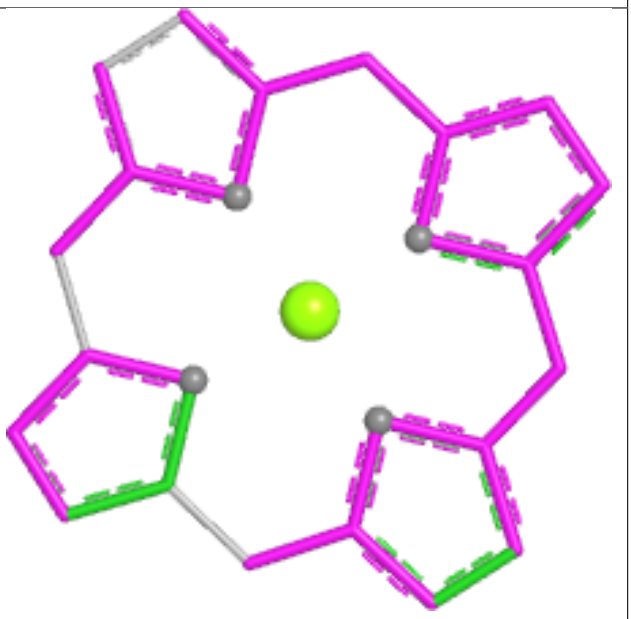


Rings

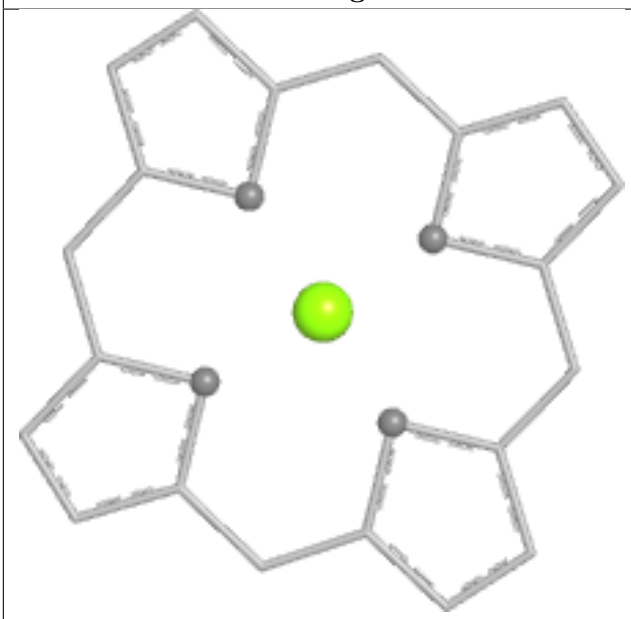
Ligand CLA 2 1227



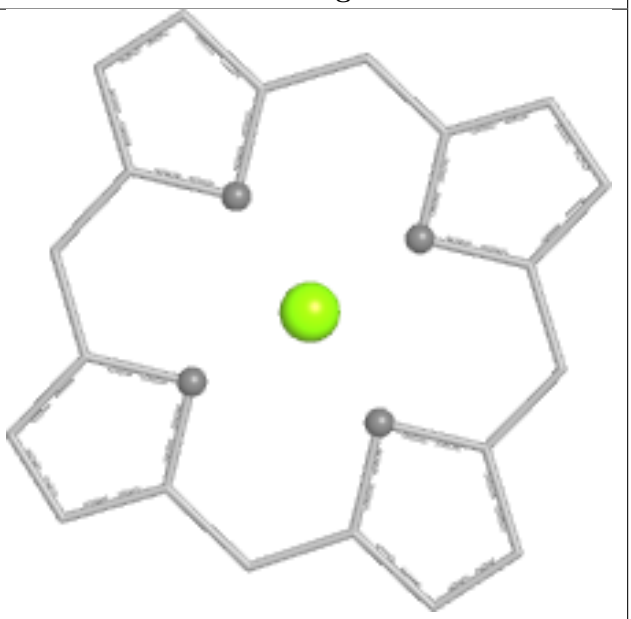
Bond lengths



Bond angles

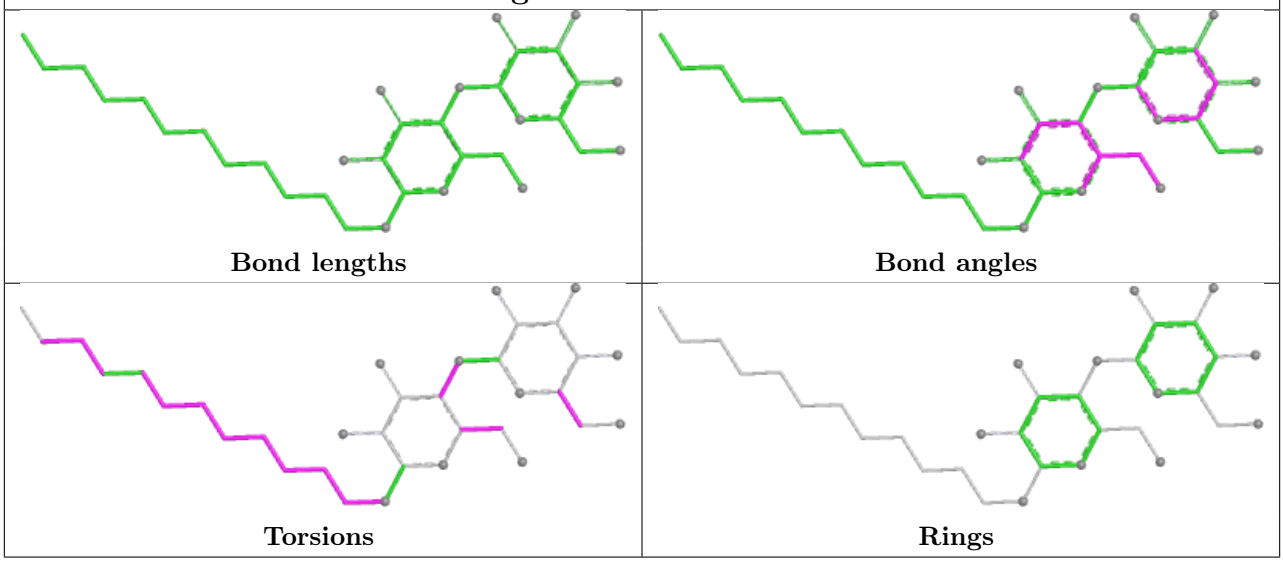


Torsions

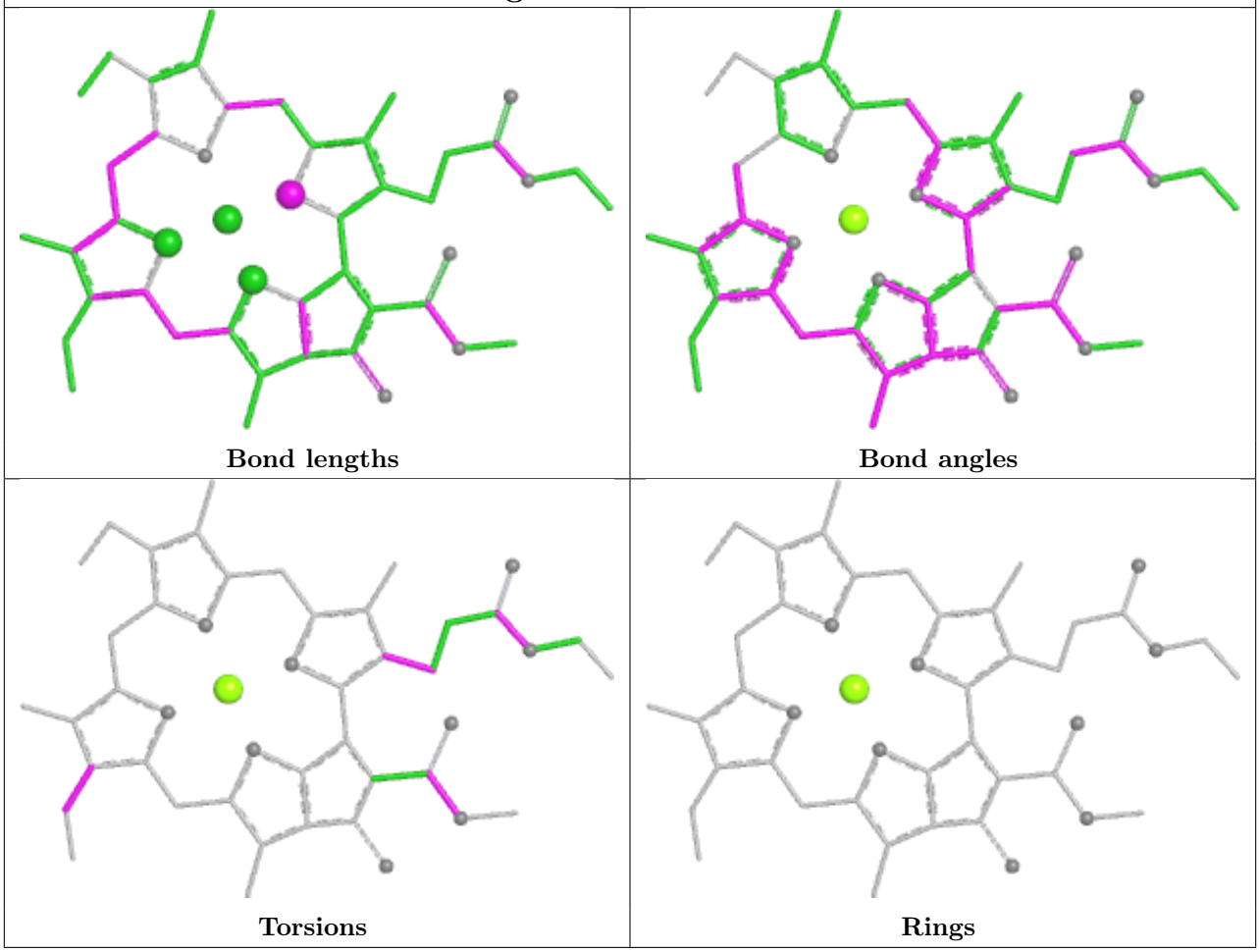


Rings

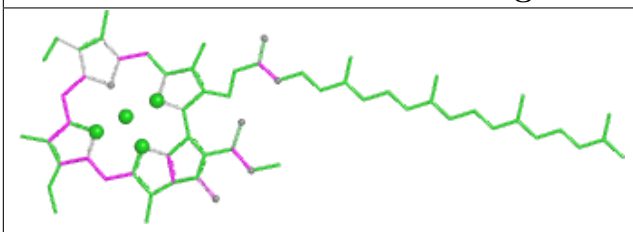
Ligand LMU A 1809



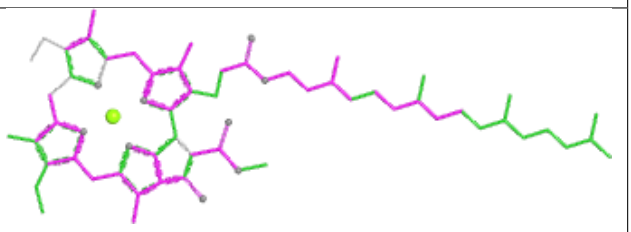
Ligand CLA A 1794



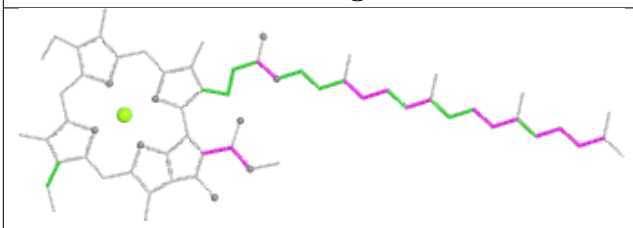
Ligand CLA A 1783



Bond lengths



Bond angles



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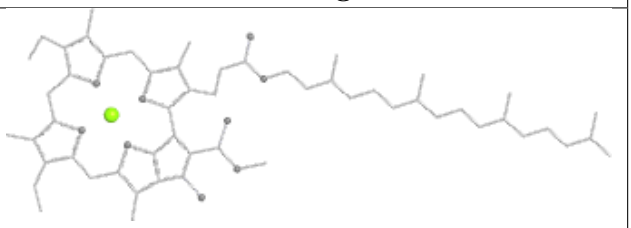
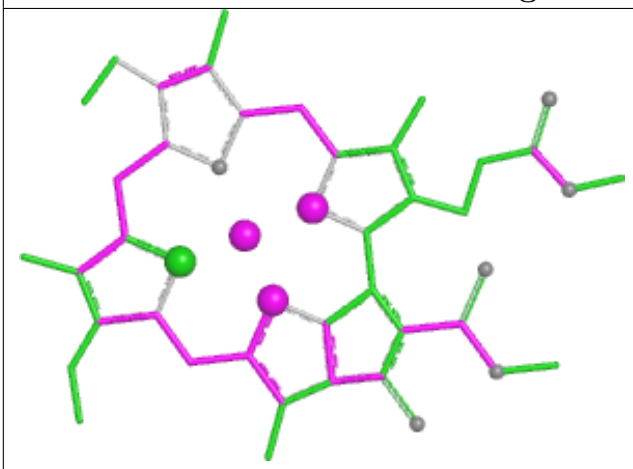
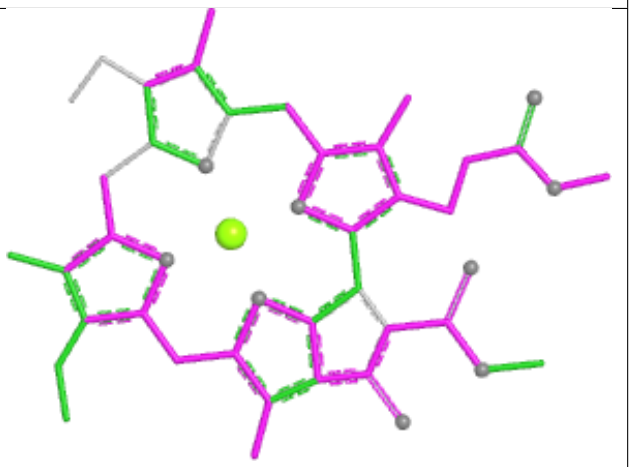


Rings

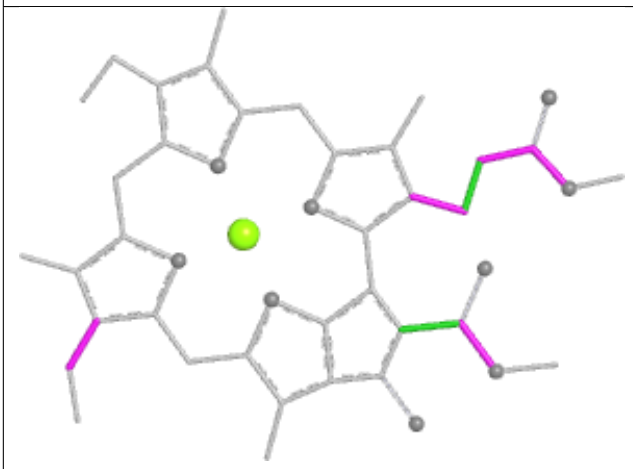
Ligand CLA 4 1209



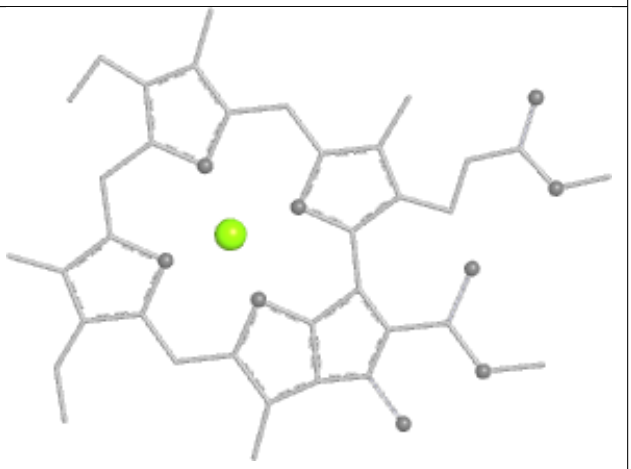
Bond lengths



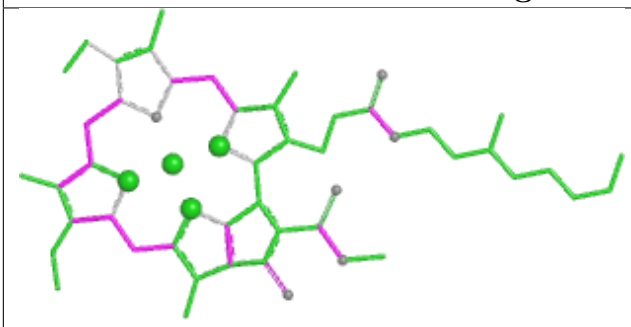
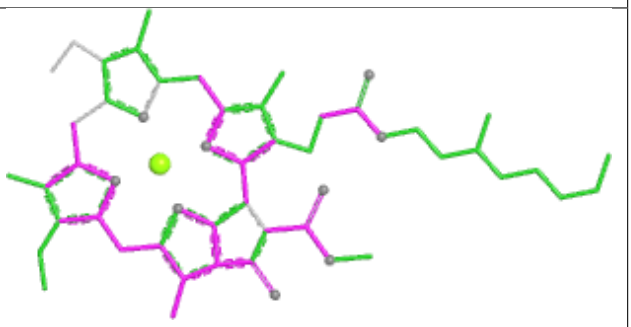
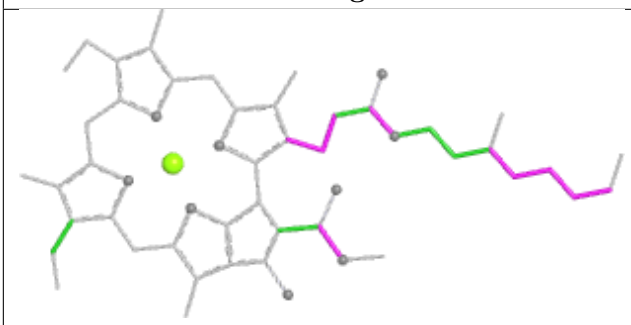
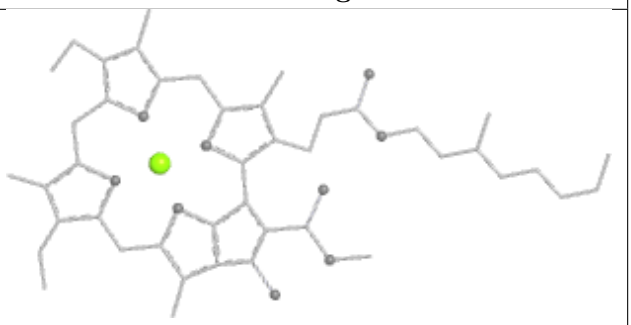
Bond angles

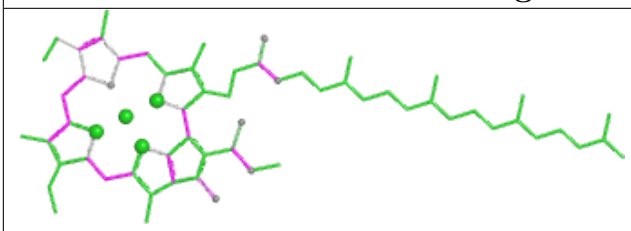
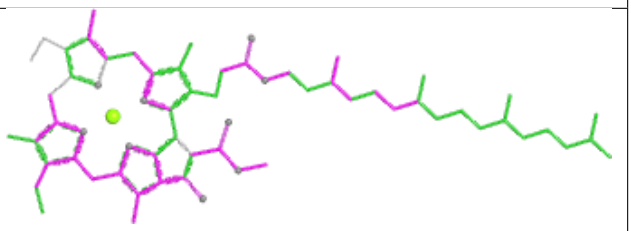
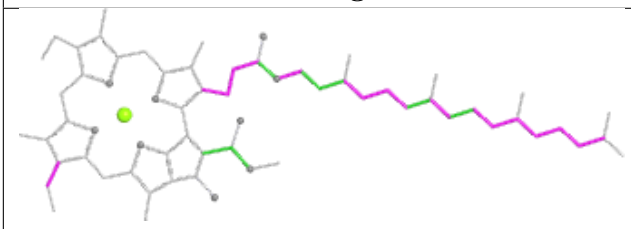
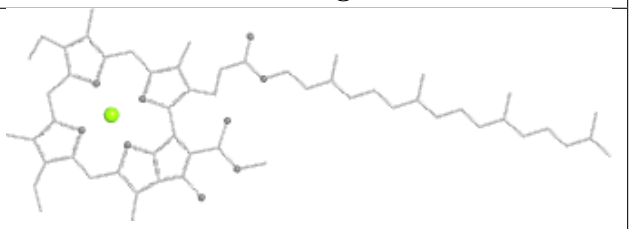


Torsions

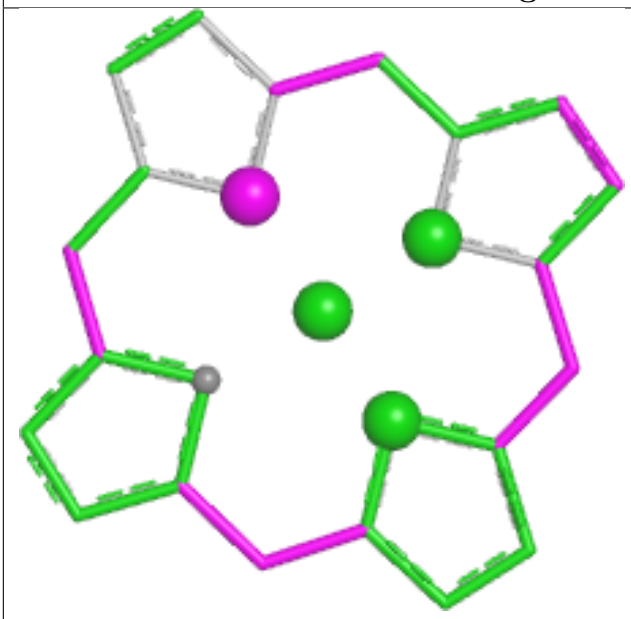


Rings

Ligand CLA A 1768	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1761	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 1199



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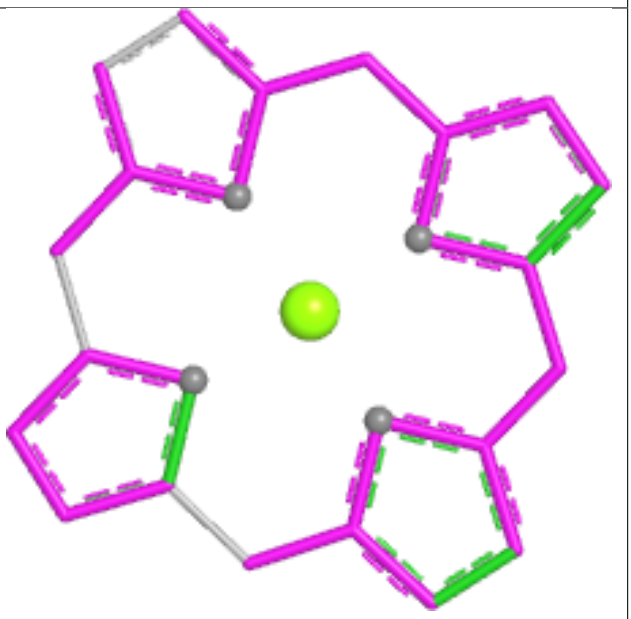
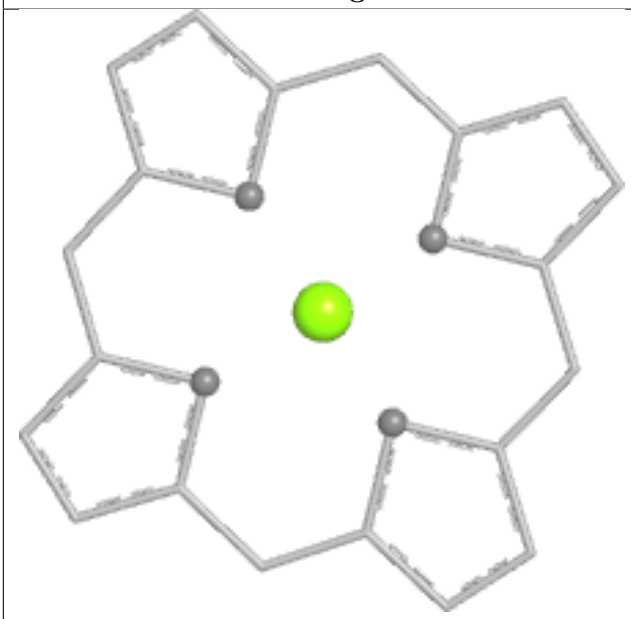


Bond angles



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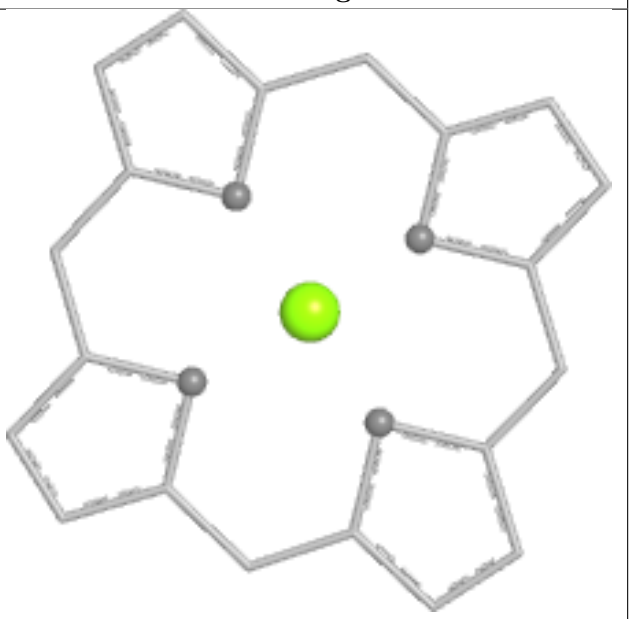
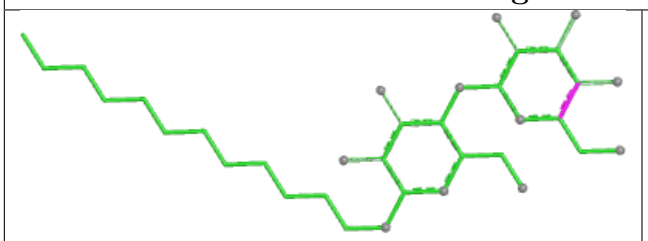


Rings

Ligand LMU A 7030



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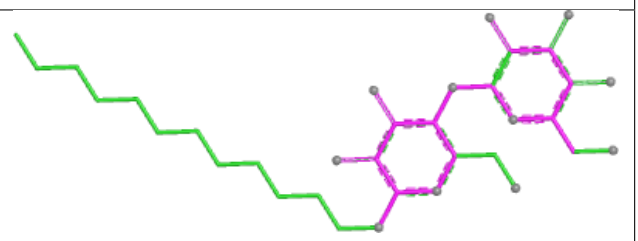
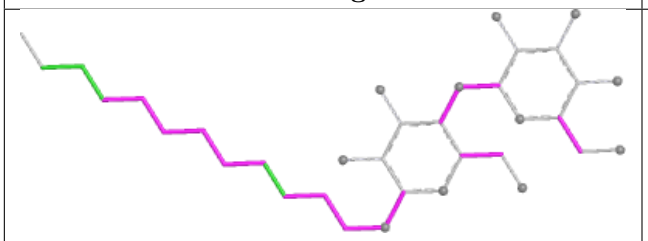


Bond angles



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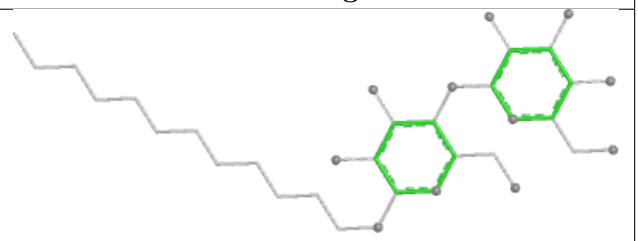
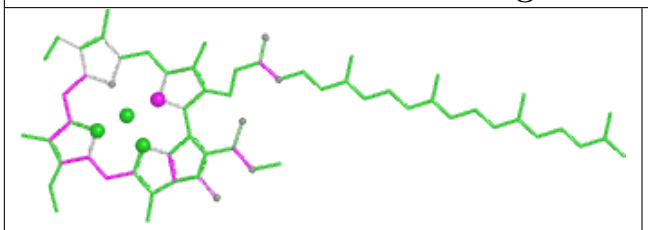


Rings

Ligand CLA B 1770



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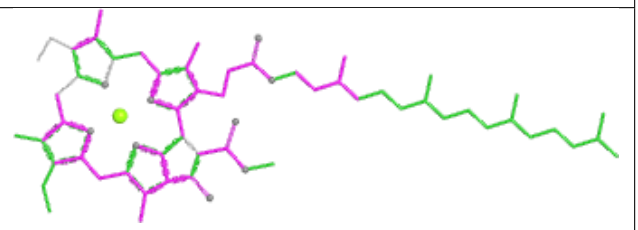
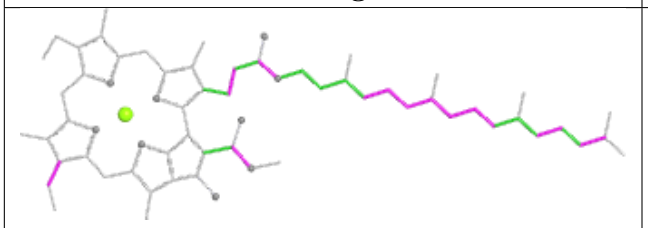


Bond angles



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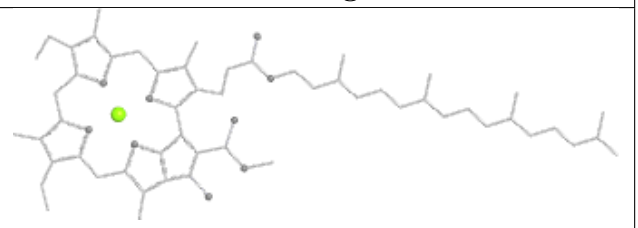
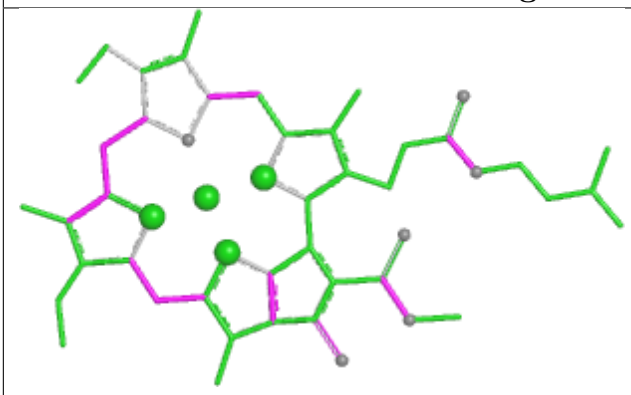


Rings

Ligand CLA 2 1222



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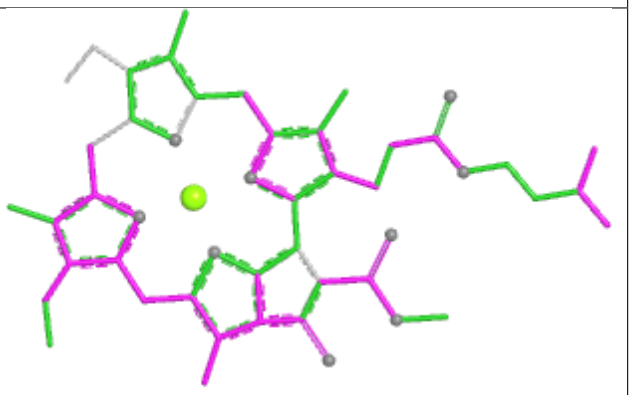
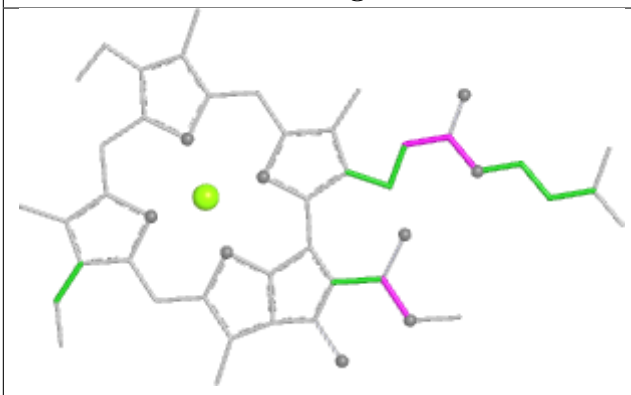


Bond angles



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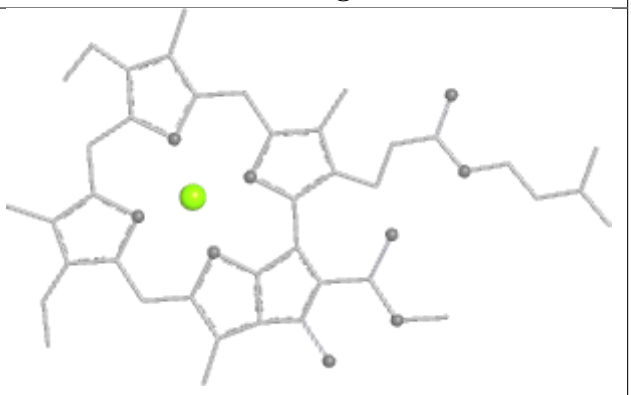
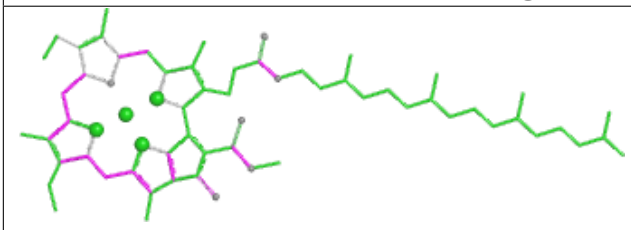


Rings

Ligand CLA 2 1224



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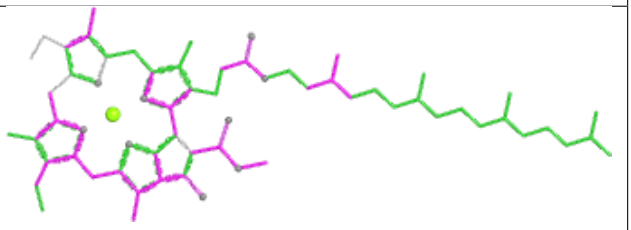
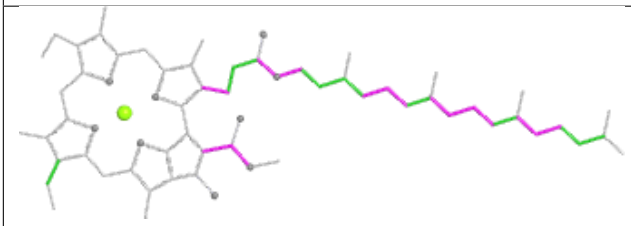


Bond angles



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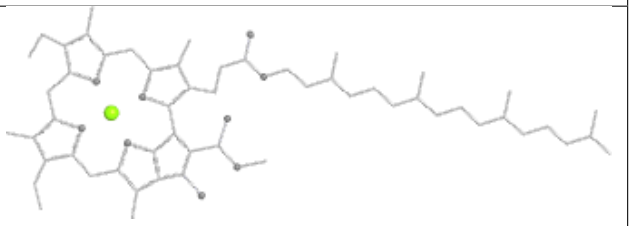
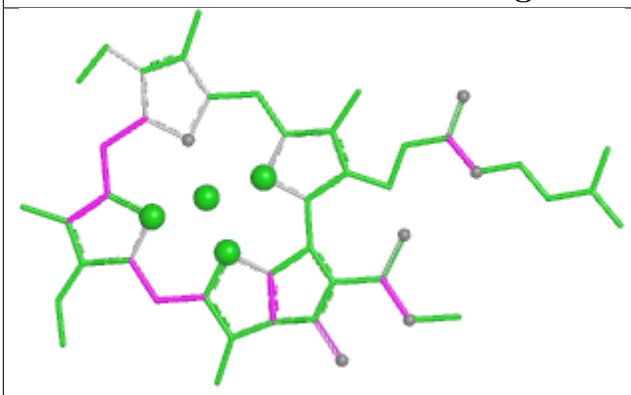


Rings

Ligand CLA A 1799



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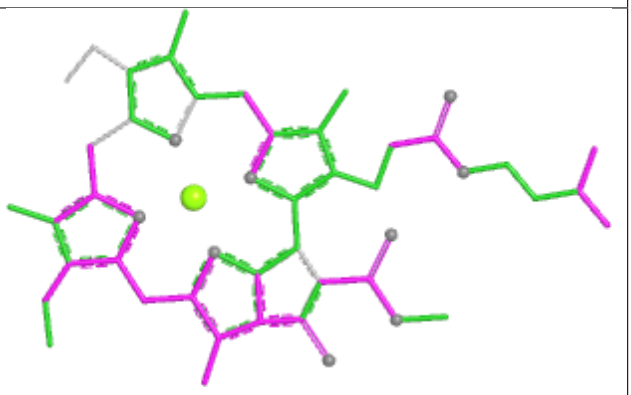
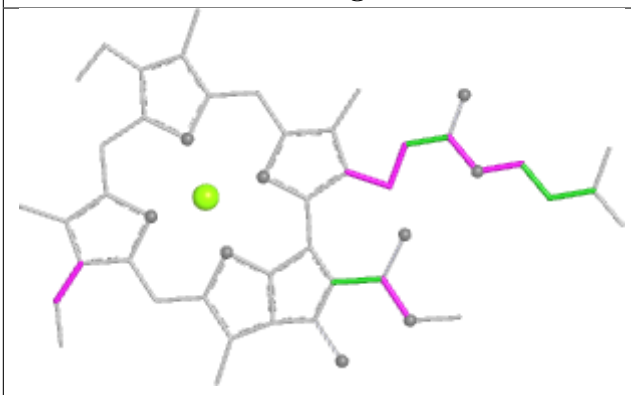
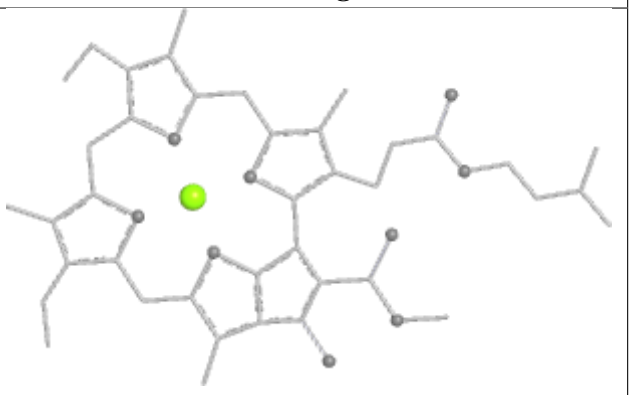


Bond angles

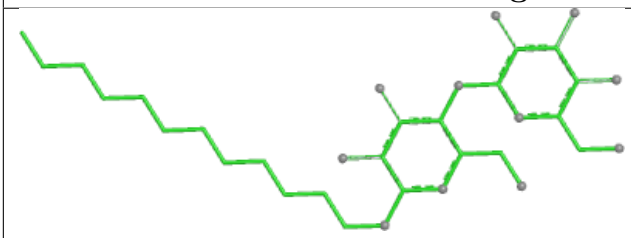


Torsions

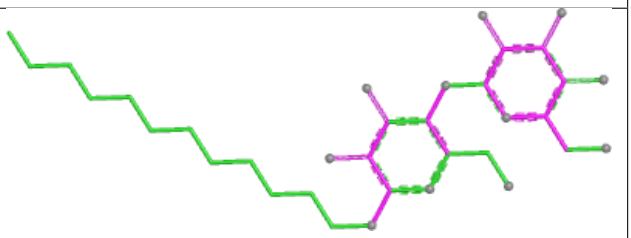


Rings

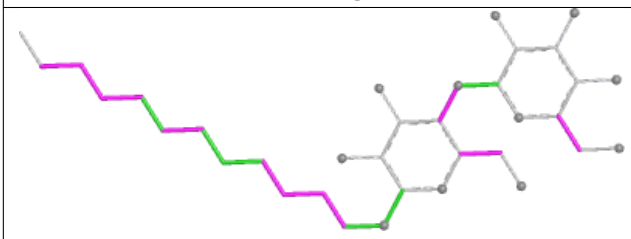
Ligand LMU K 1086



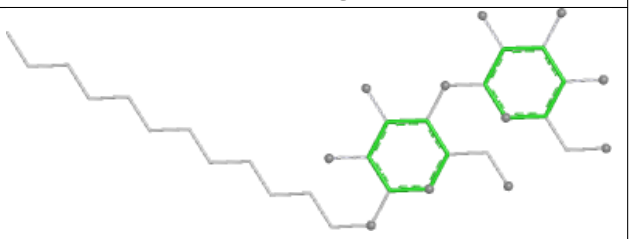
Bond lengths



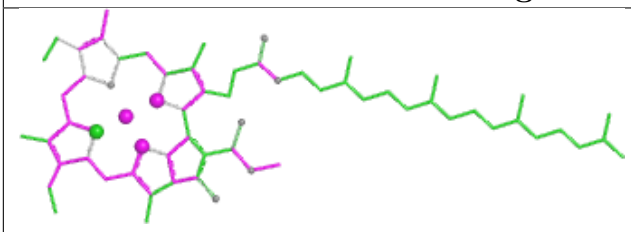
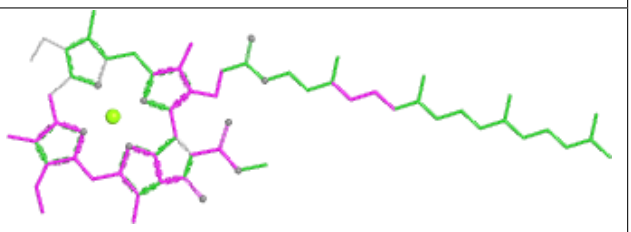
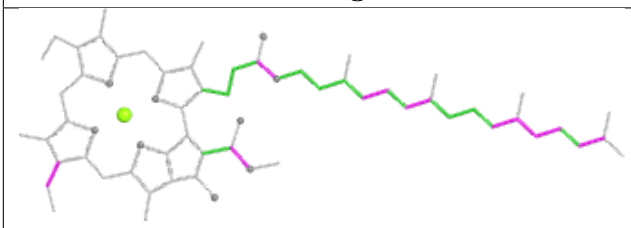
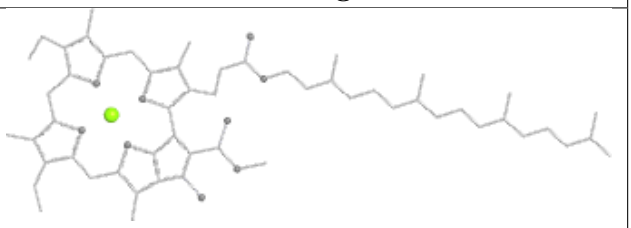
Bond angles

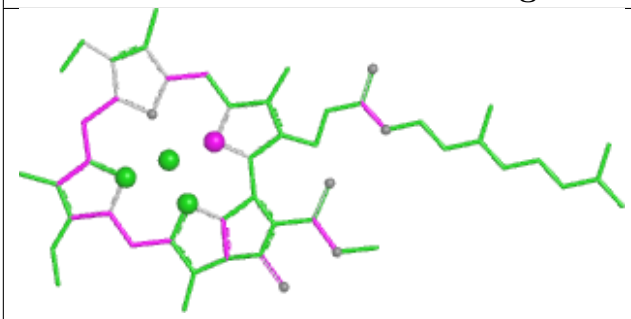
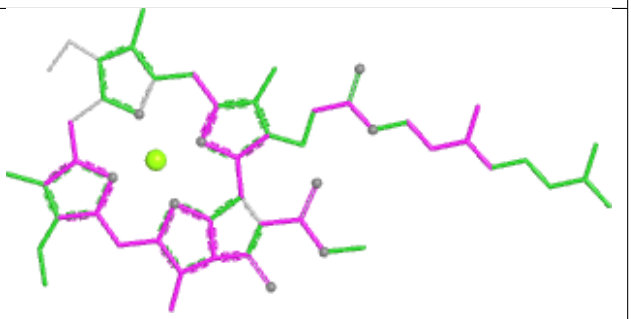
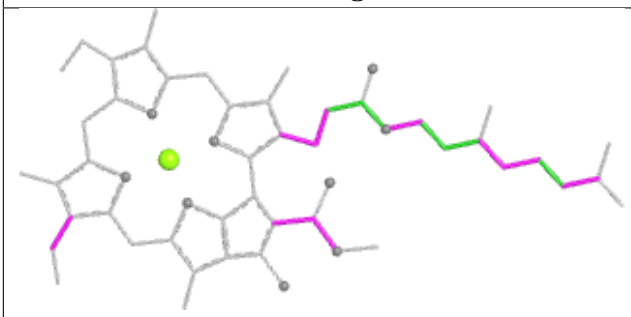
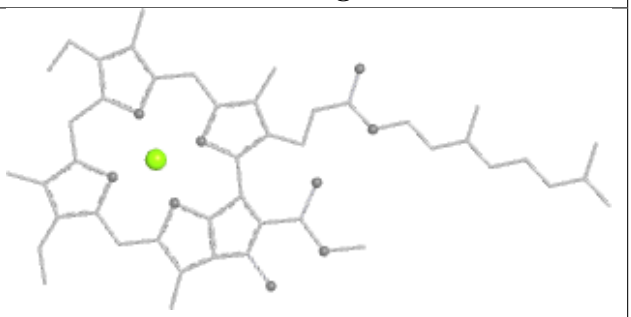


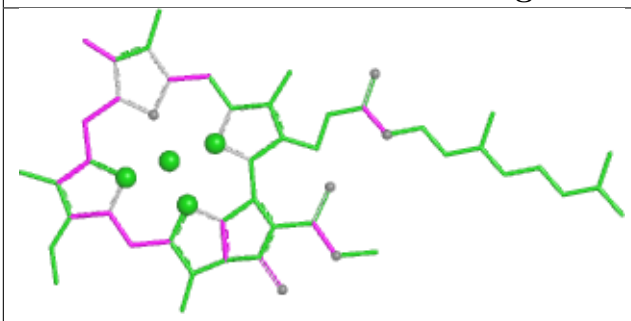
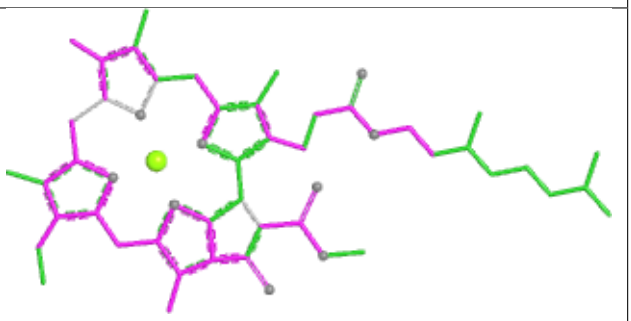
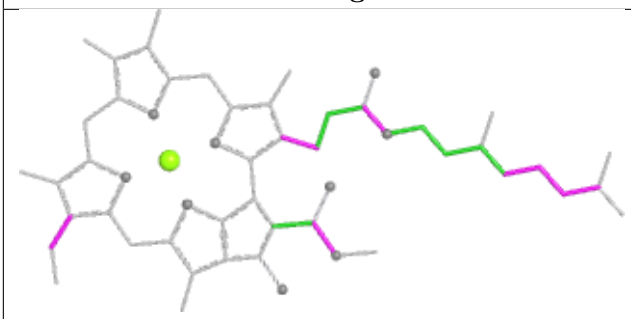
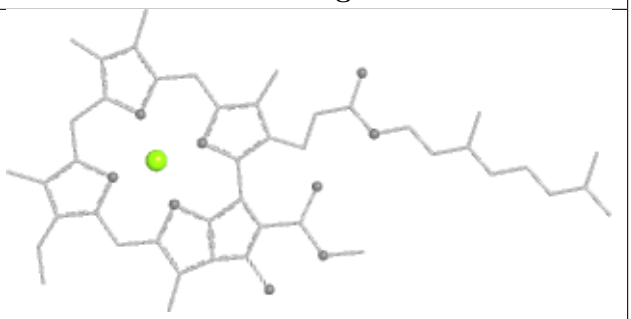
Torsions



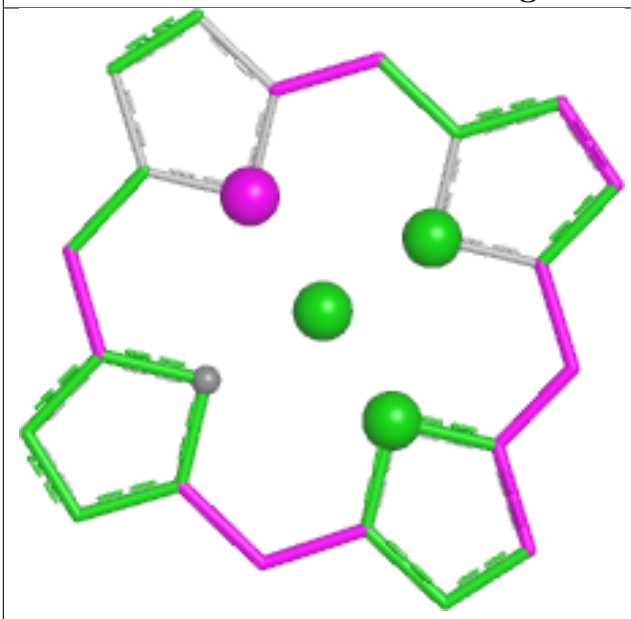
Rings

Ligand CLA B 1753	
 Bond lengths	 Bond angles
 Torsions	 Rings

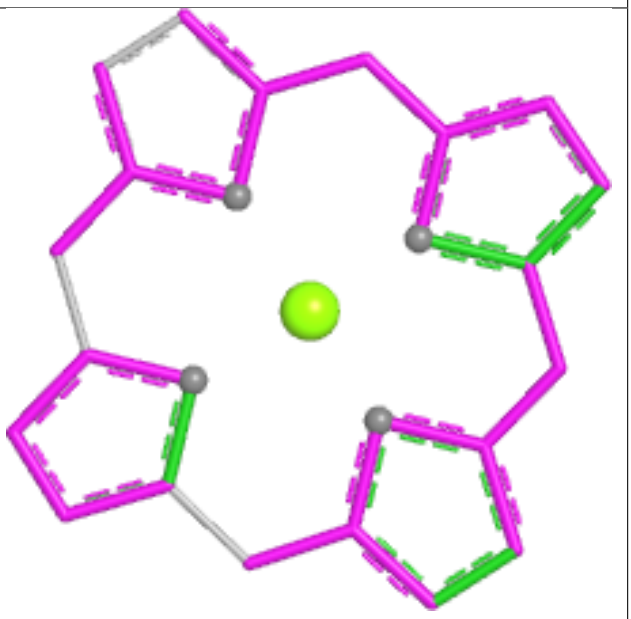
Ligand CLA 4 1196	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1741	
 Bond lengths	 Bond angles
 Torsions	 Rings

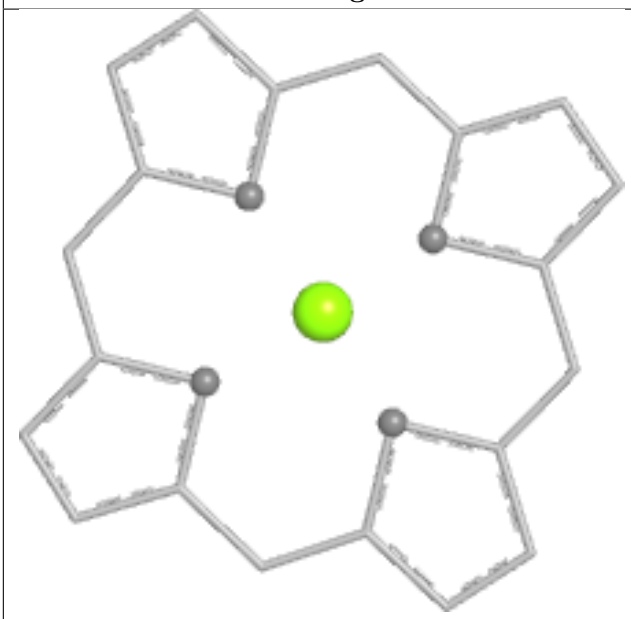
Ligand CLA 3 1215



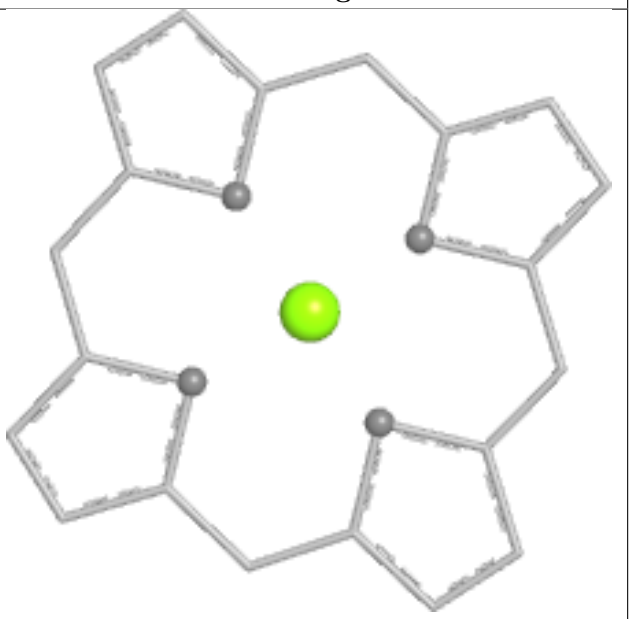
Bond lengths



Bond angles

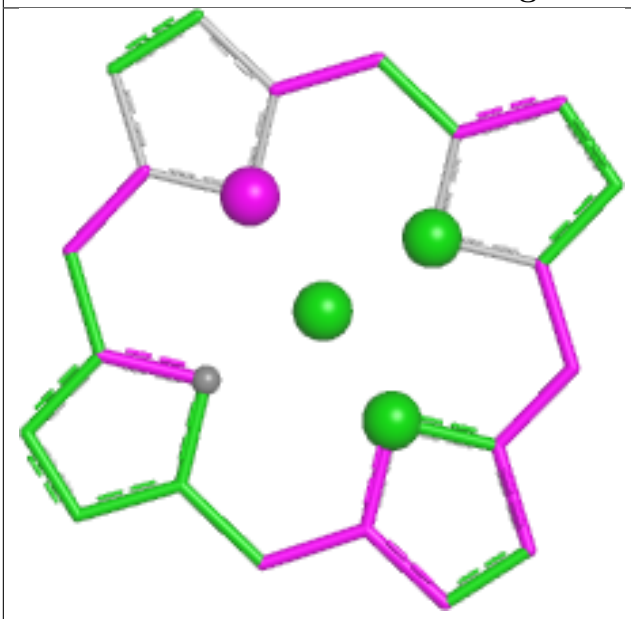


Torsions

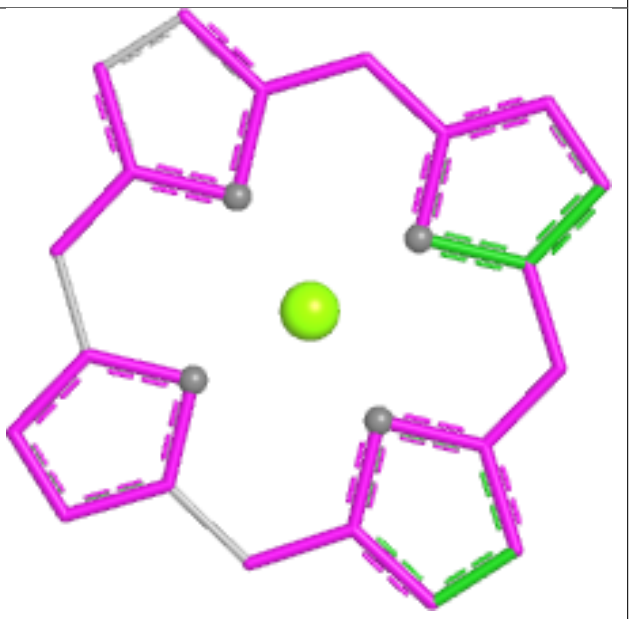


Rings

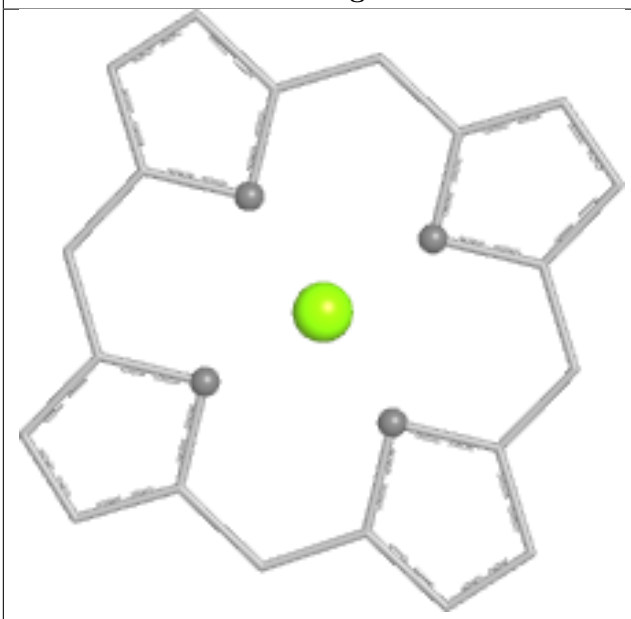
Ligand CLA 3 1213



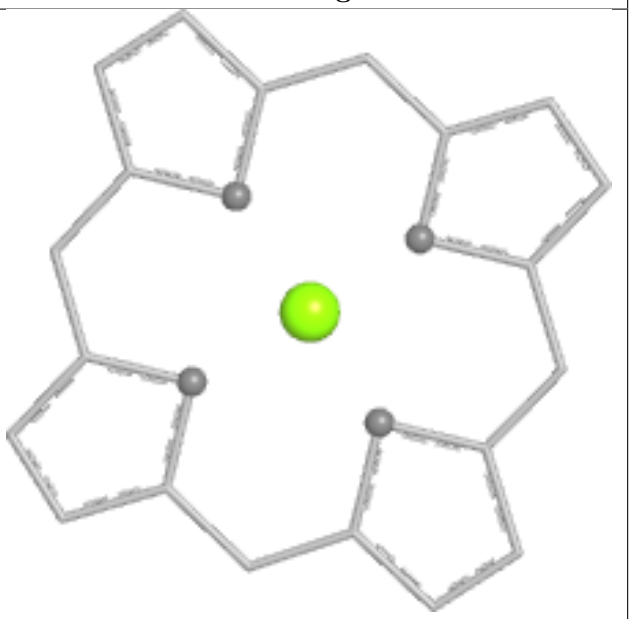
Bond lengths



Bond angles

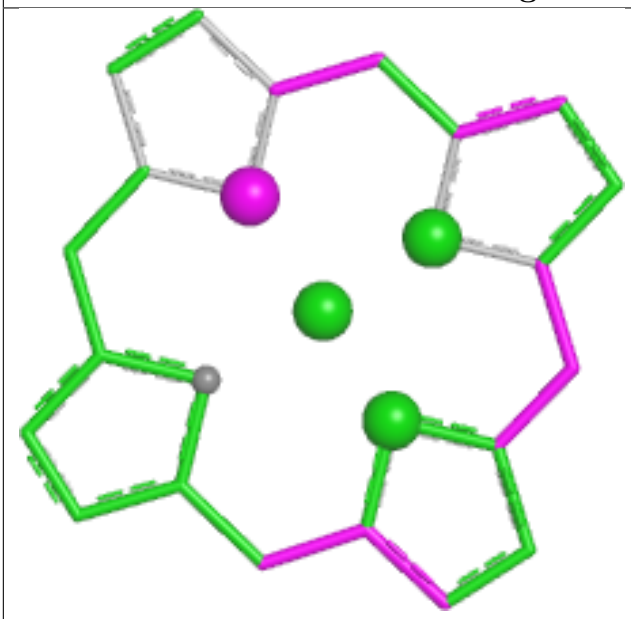


Torsions

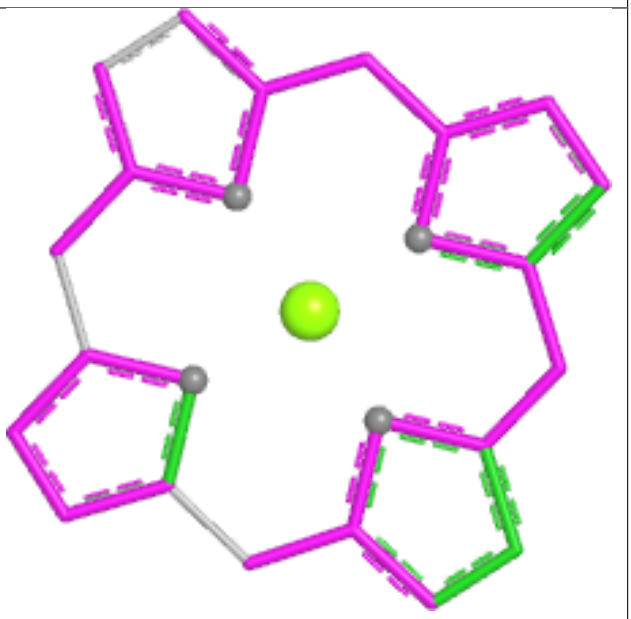


Rings

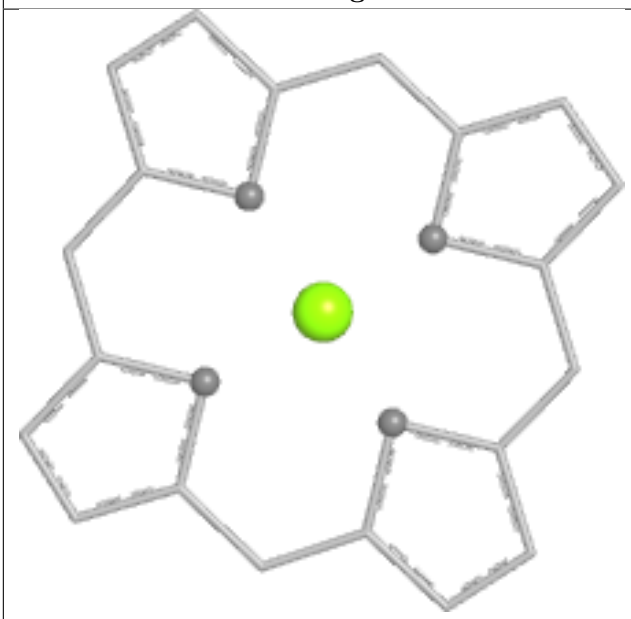
Ligand CLA 3 1217



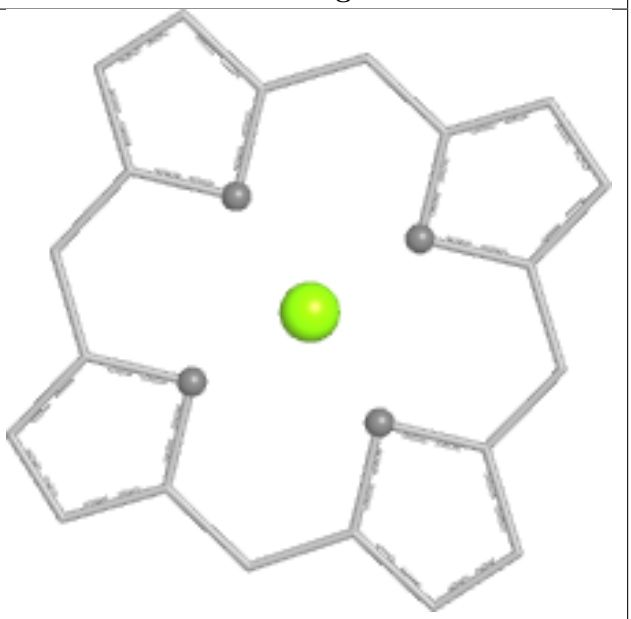
Bond lengths



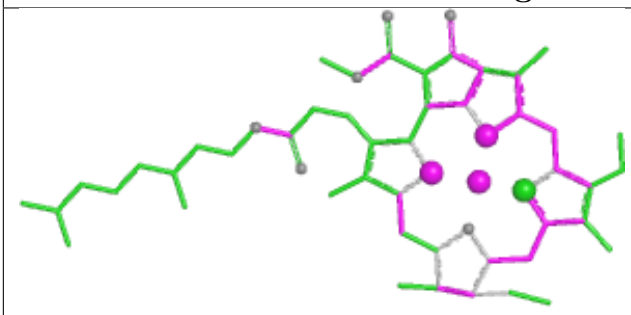
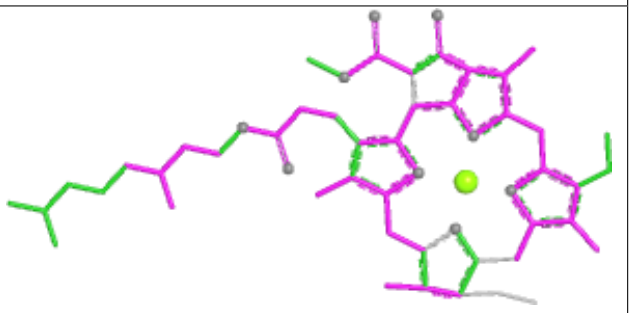
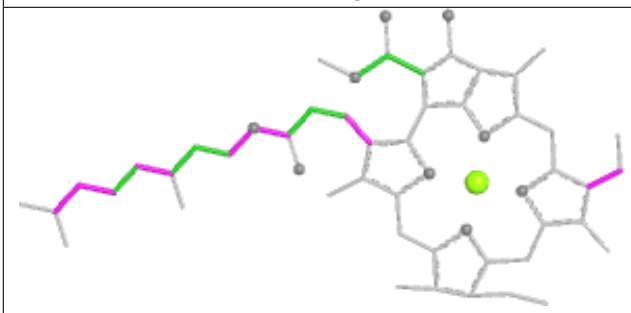
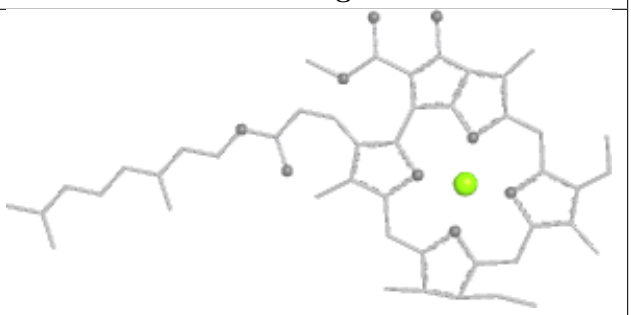
Bond angles



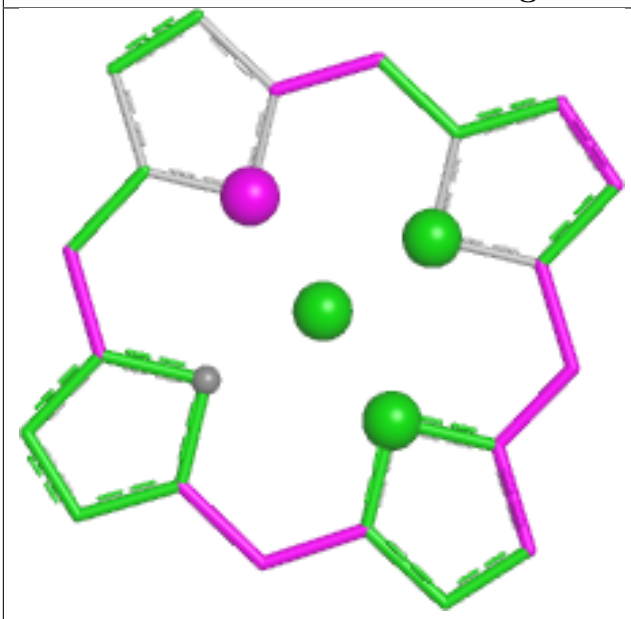
Torsions



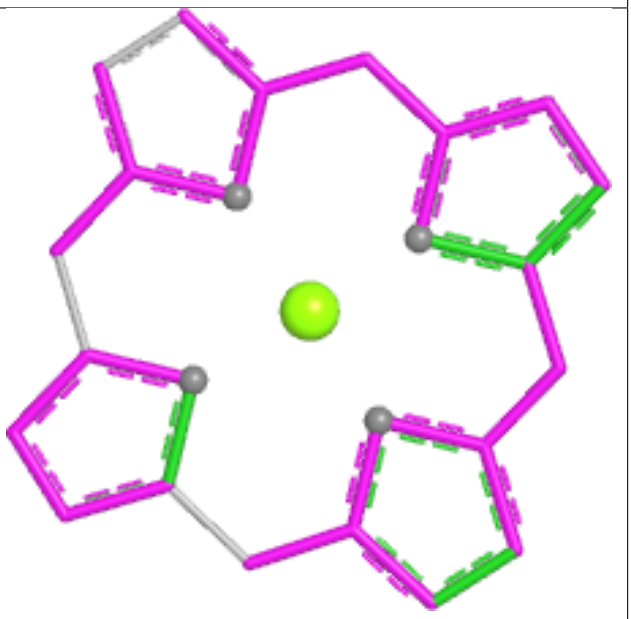
Rings

Ligand CLA A 1816	
 Bond lengths	 Bond angles
 Torsions	 Rings

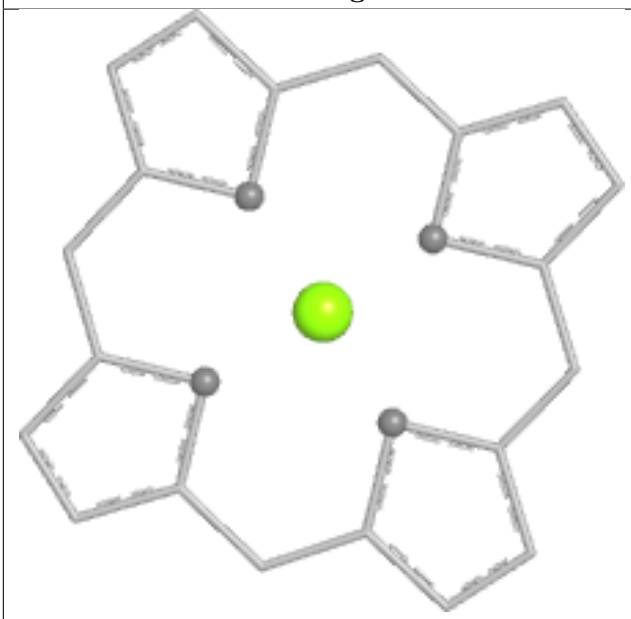
Ligand CLA 3 1214



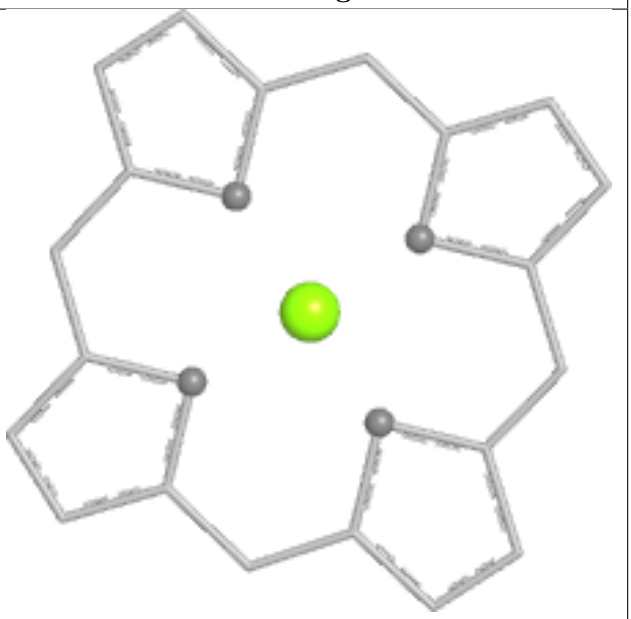
Bond lengths



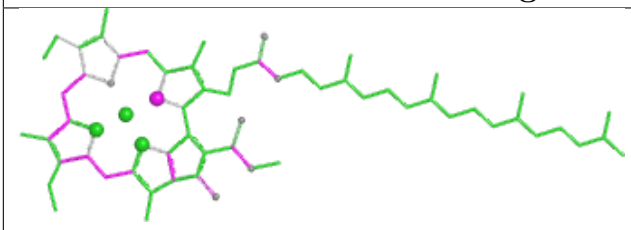
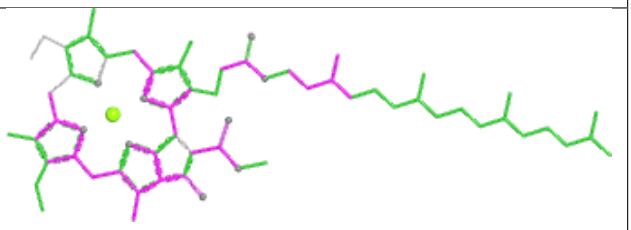
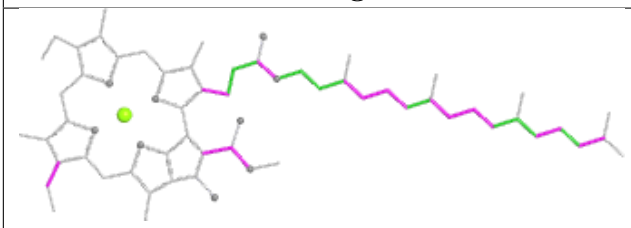
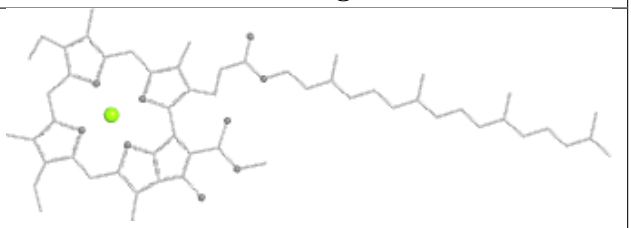
Bond angles

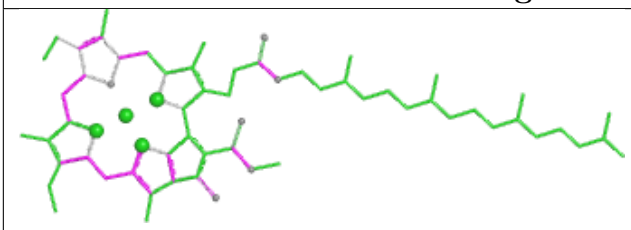
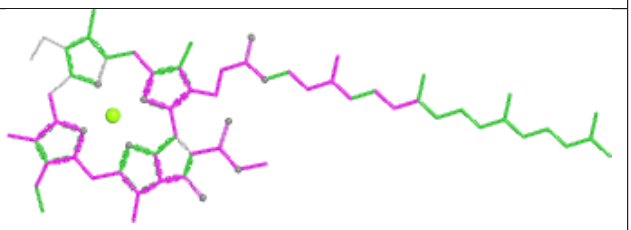
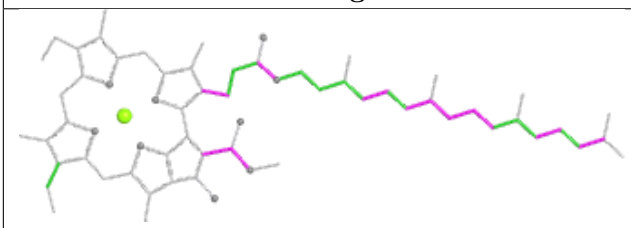
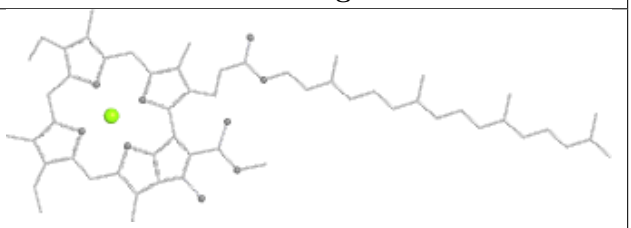


Torsions

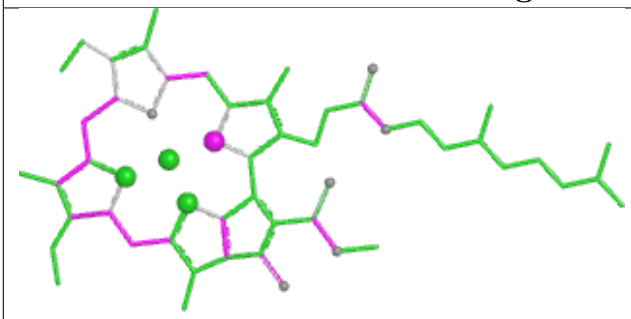


Rings

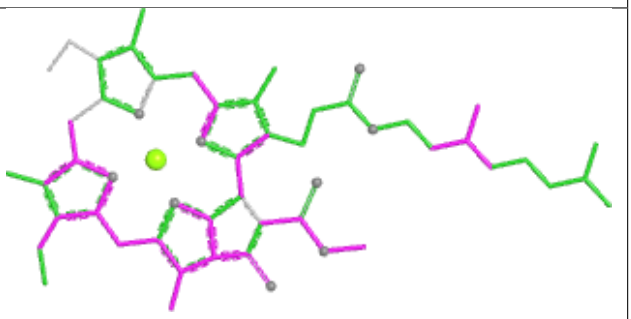
Ligand CLA 3 1219	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1785	
 Bond lengths	 Bond angles
 Torsions	 Rings

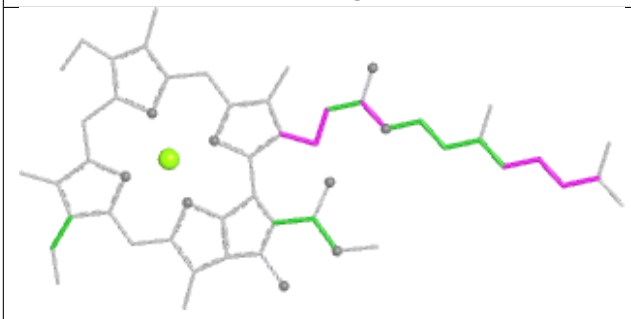
Ligand CLA B 1752



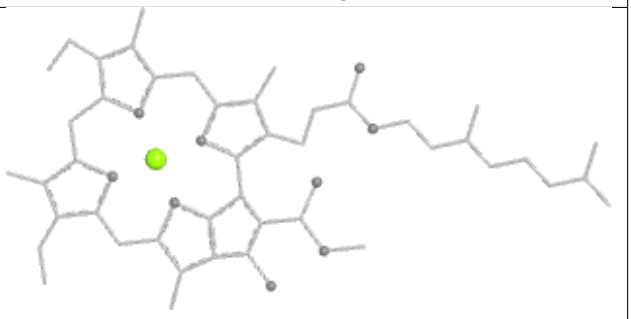
Bond lengths



Bond angles

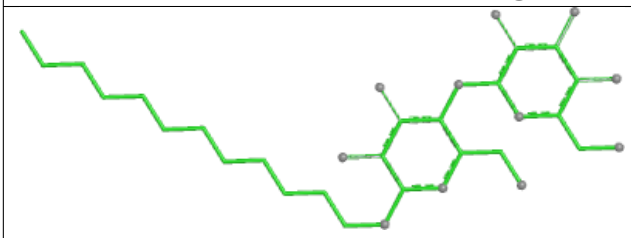


Torsions

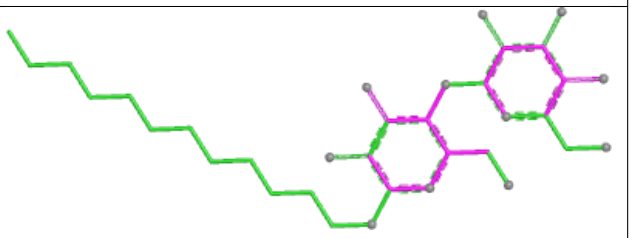


Rings

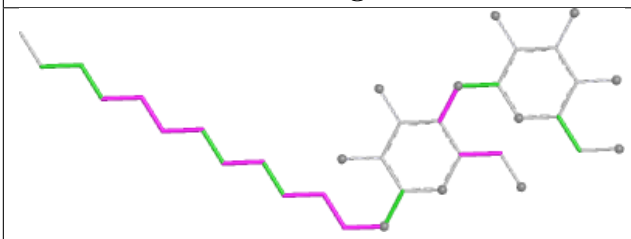
Ligand LMU A 7013



Bond lengths



Bond angles



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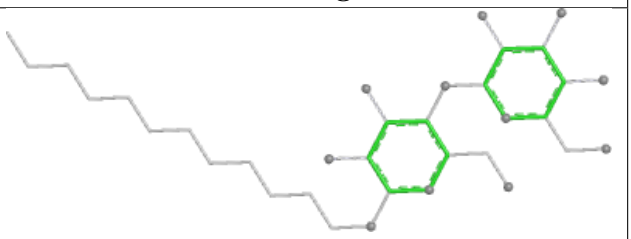
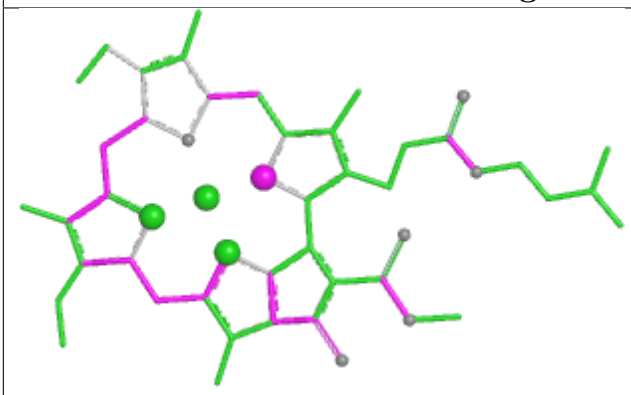
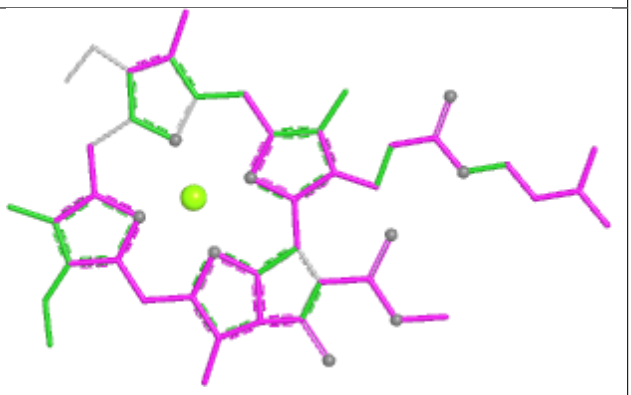
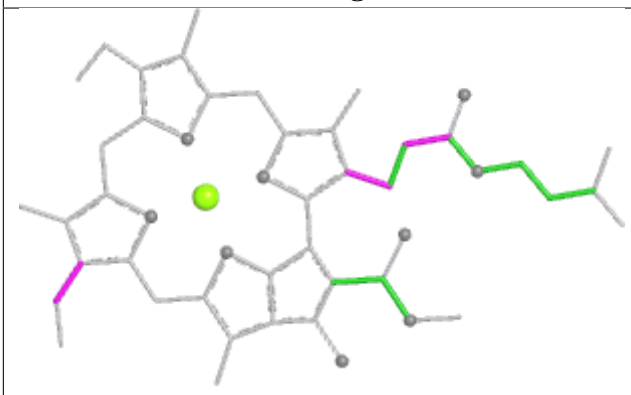
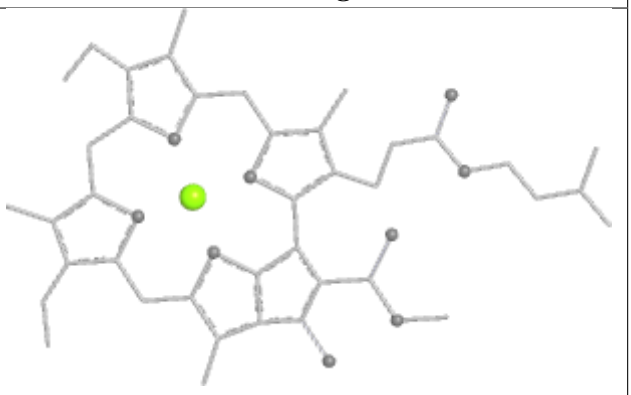
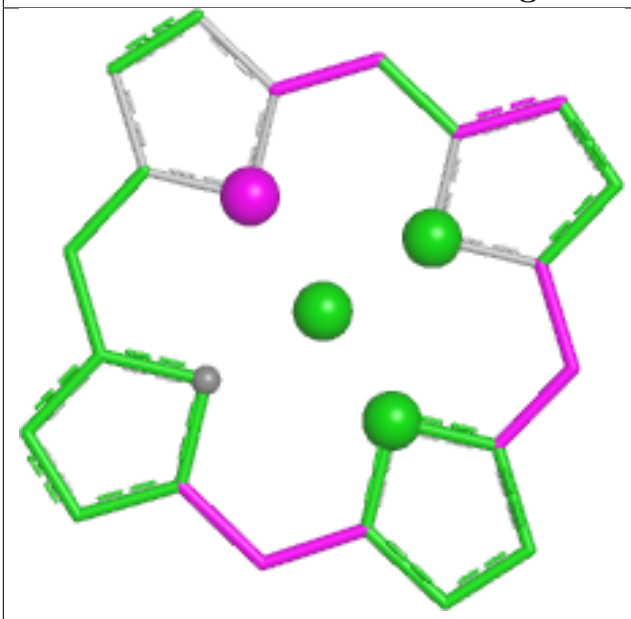


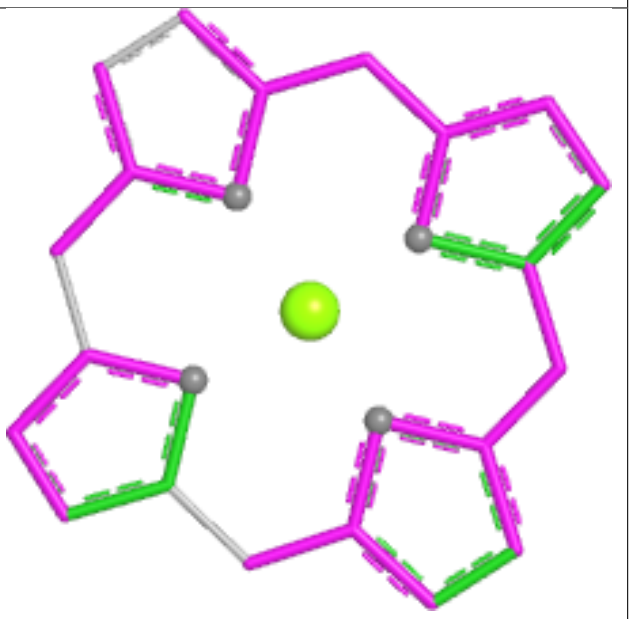
Rings

Ligand CLA 3 3008	
 Bond lengths	 Bond angles
 Torsions	 Rings

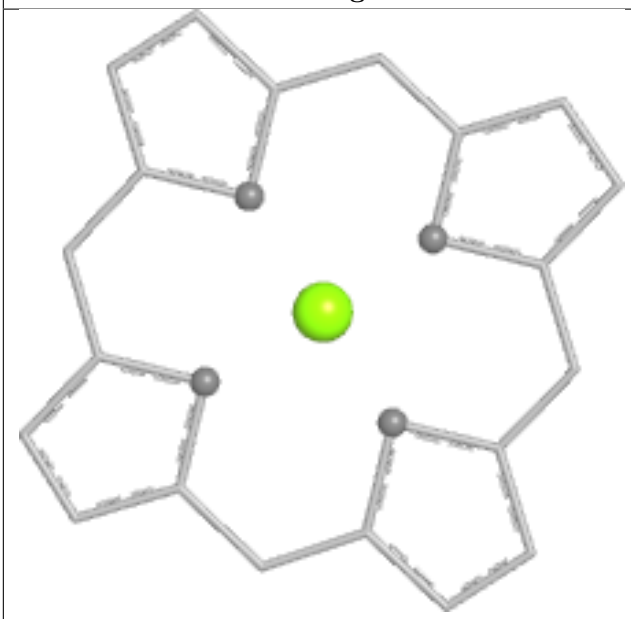
Ligand CLA 4 4003



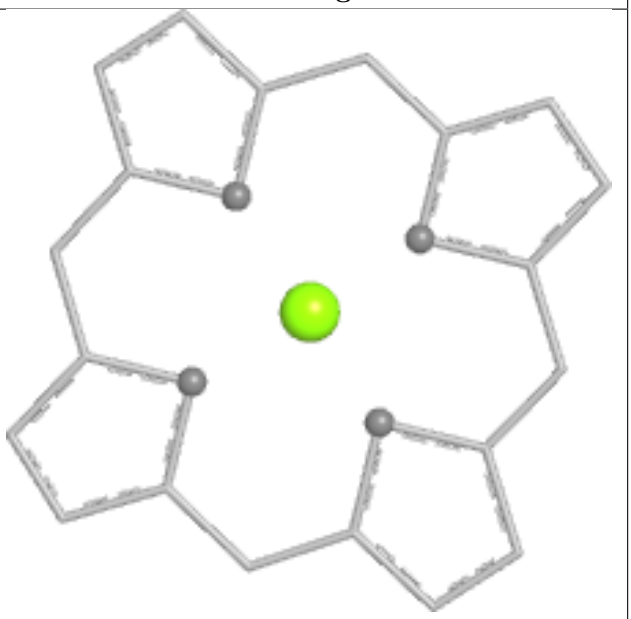
Bond lengths



Bond angles

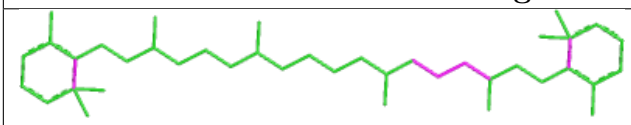


Torsions

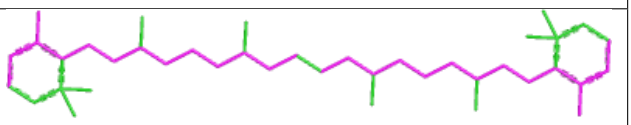


Rings

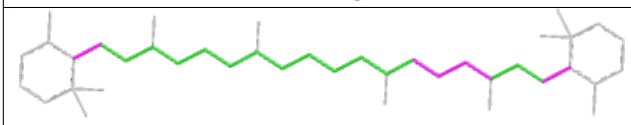
Ligand BCR B 1775



Bond lengths



Bond angles



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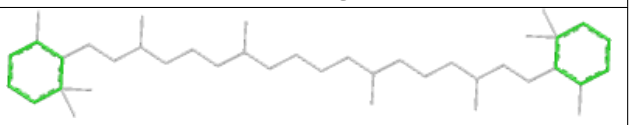
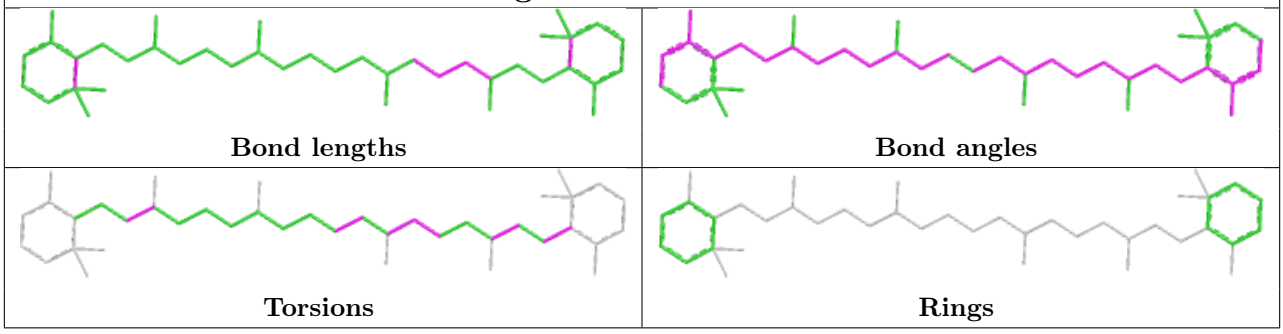
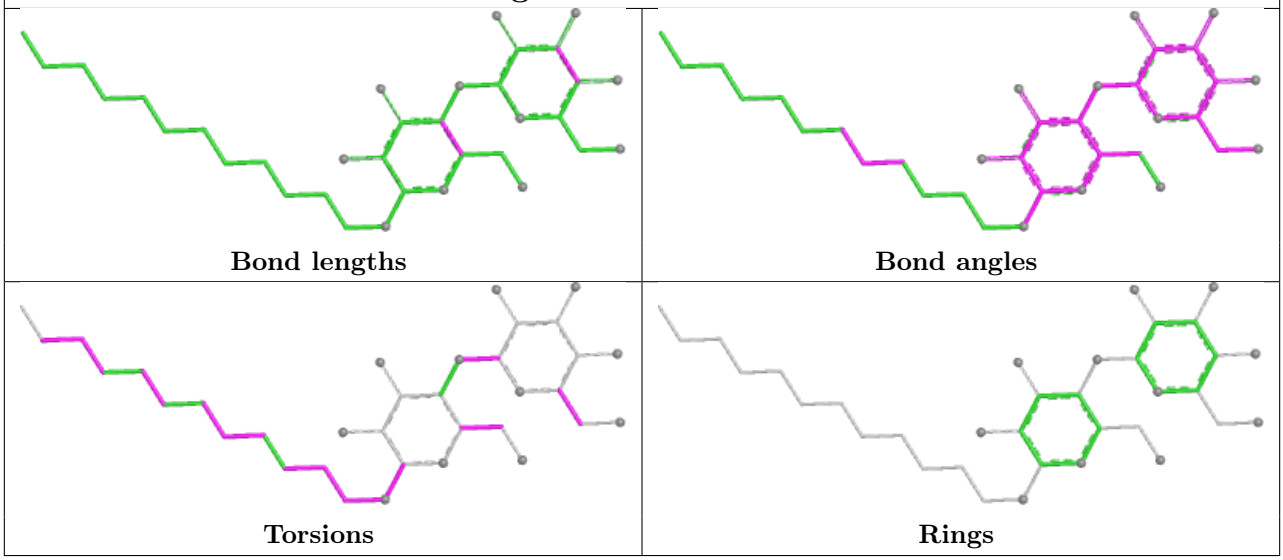


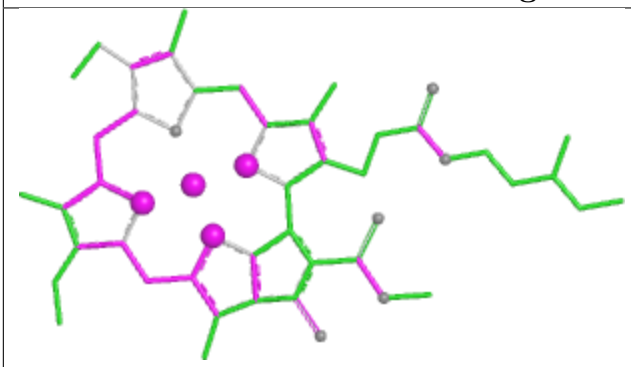
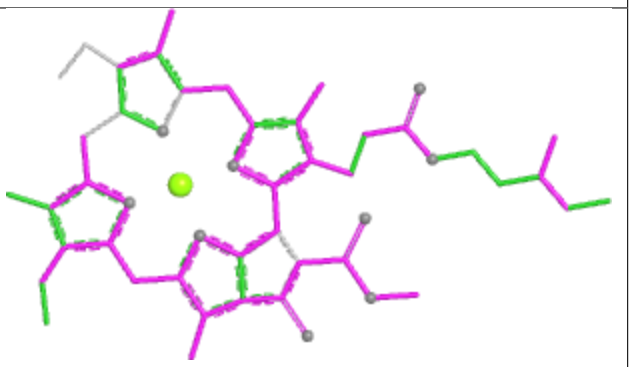
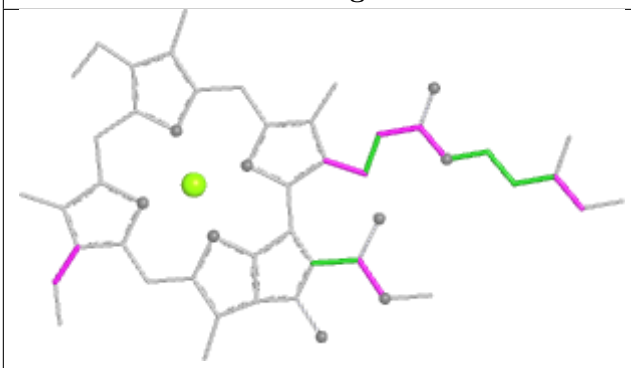
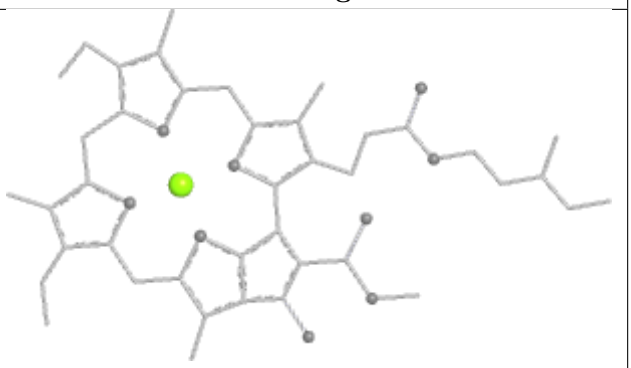
Rings

Ligand BCR B 1774

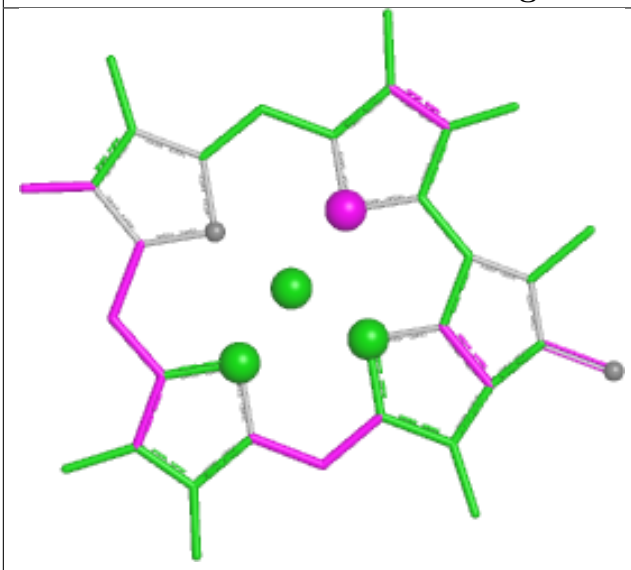


Ligand LMU A 7037



Ligand CLA 1 1200	
 Bond lengths	 Bond angles
 Torsions	 Rings

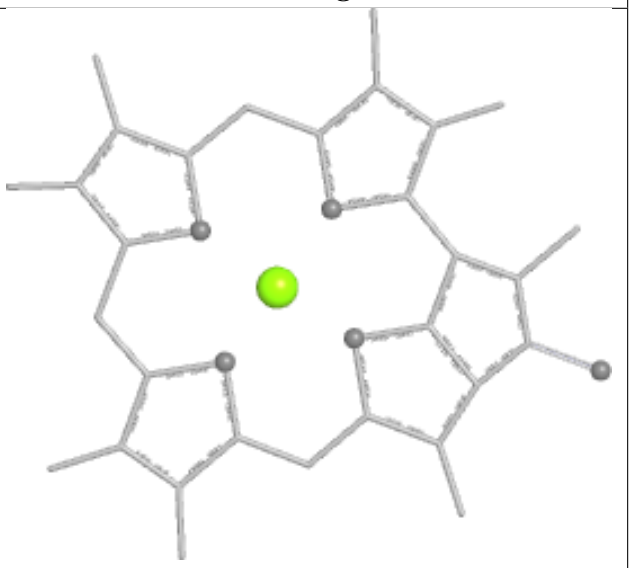
Ligand CLA 4 1207



Bond lengths

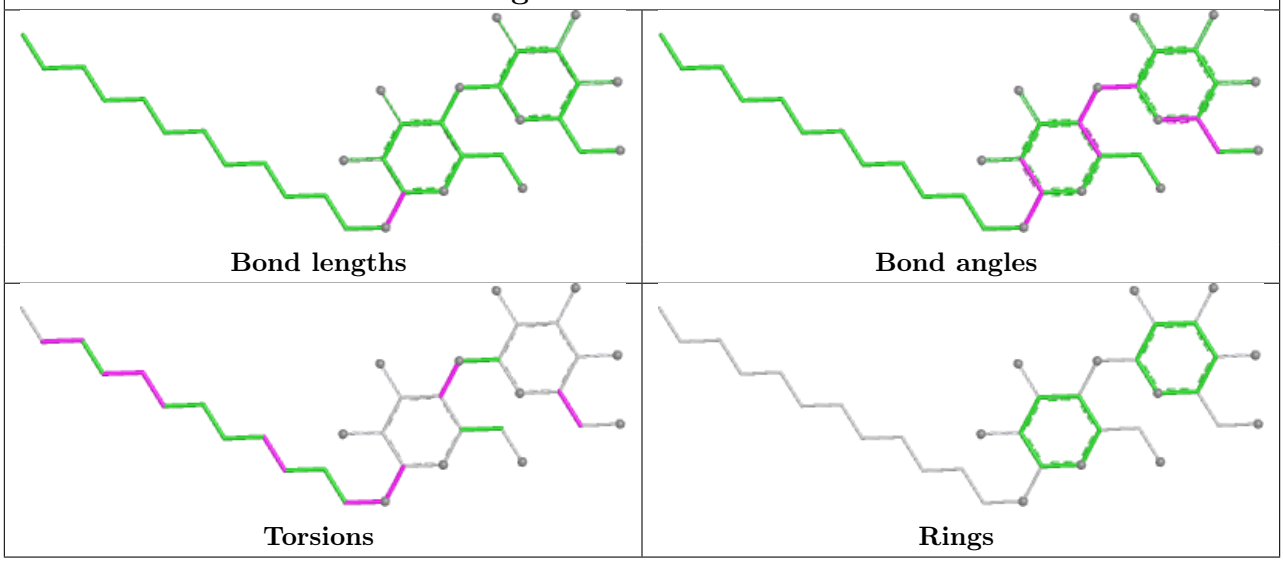
Bond angles

Torsions

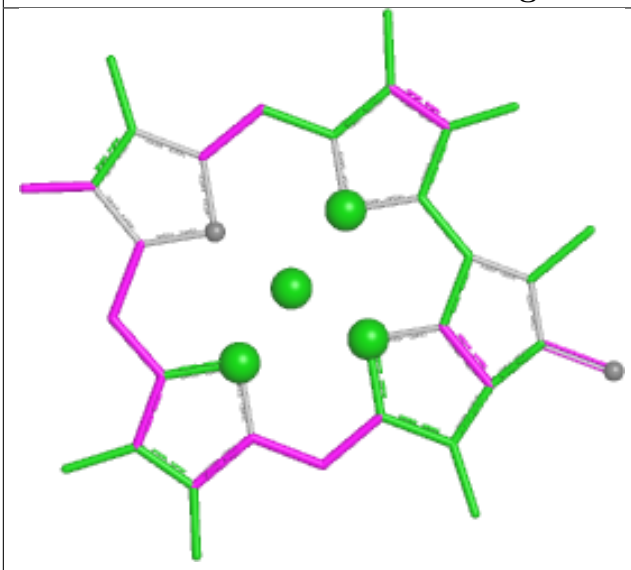


Rings

Ligand LMU A 7047



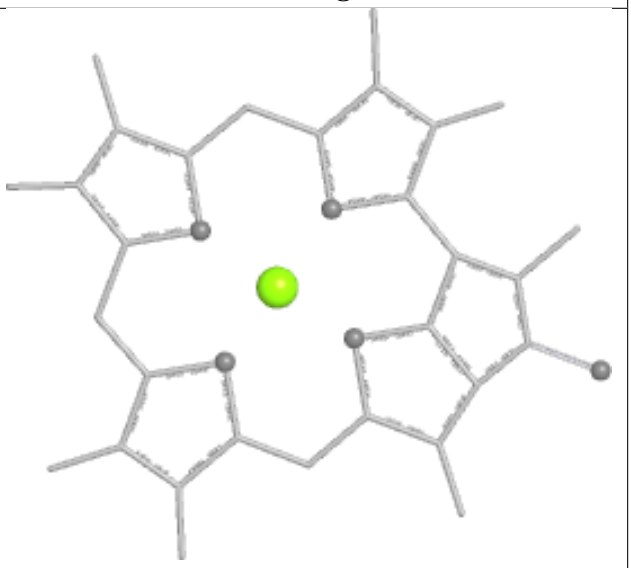
Ligand CLA 1 1196



Bond lengths

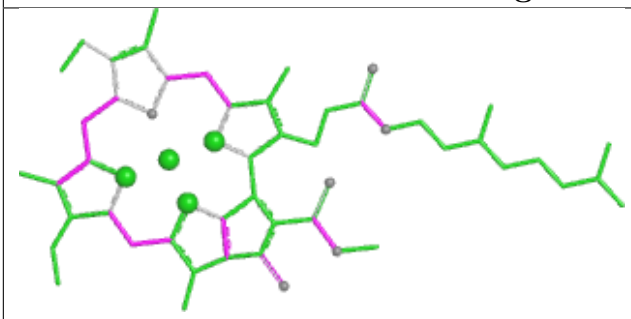
Bond angles

Torsions

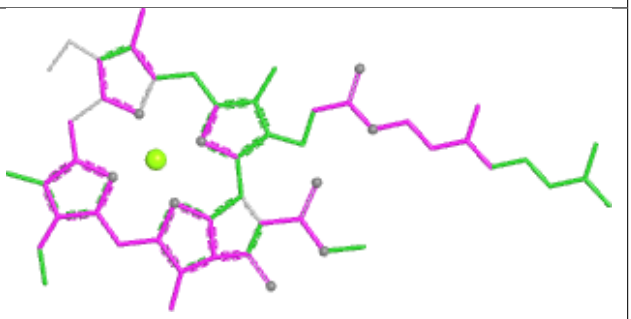


Rings

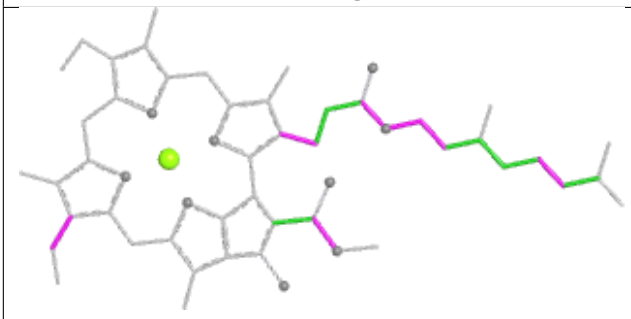
Ligand CLA A 1765



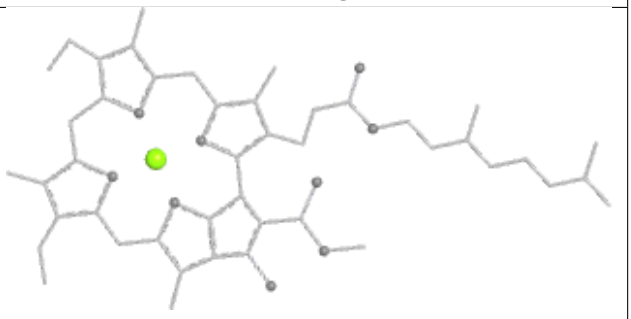
Bond lengths



Bond angles

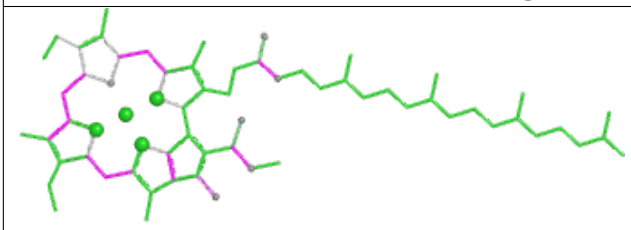


Torsions

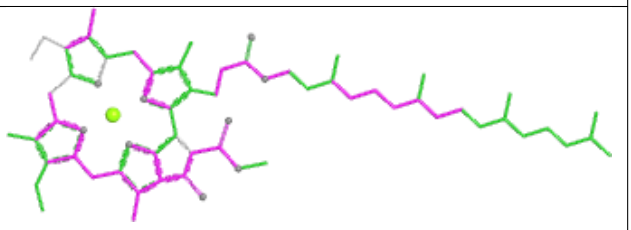


Rings

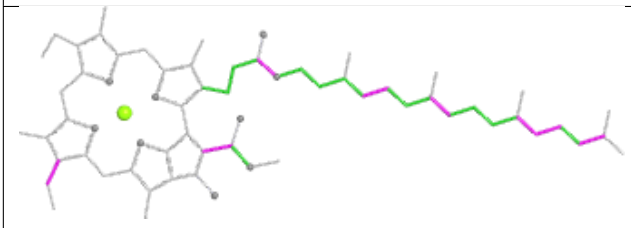
Ligand CLA 2 1218



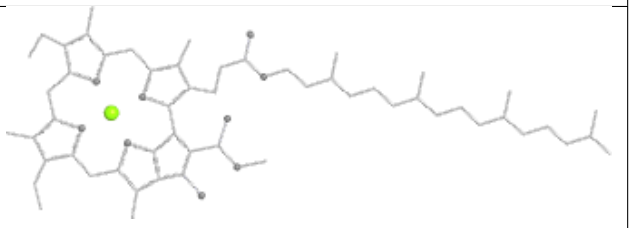
Bond lengths



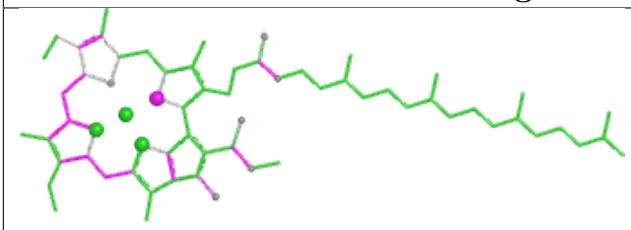
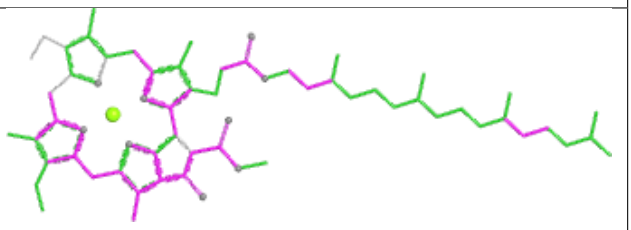
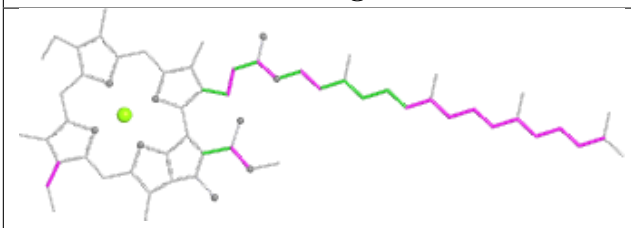
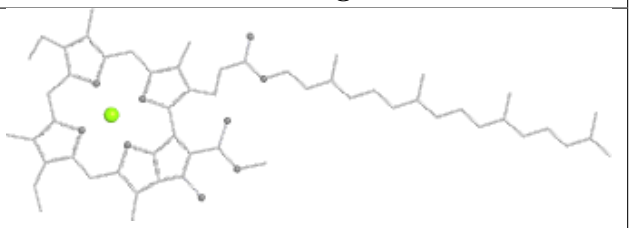
Bond angles

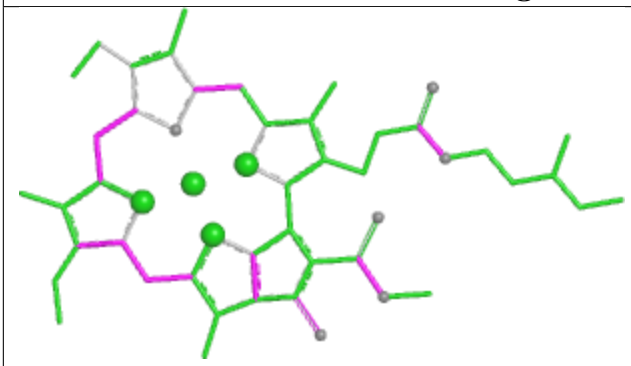
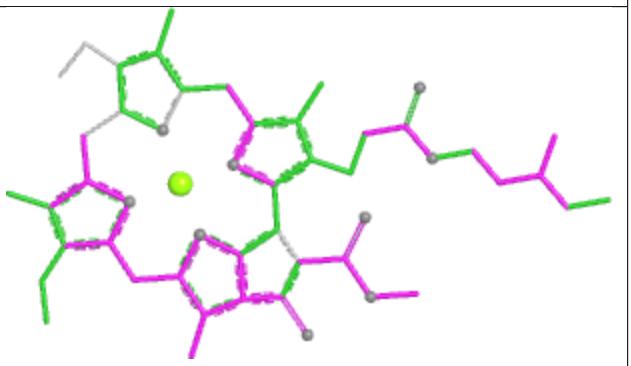
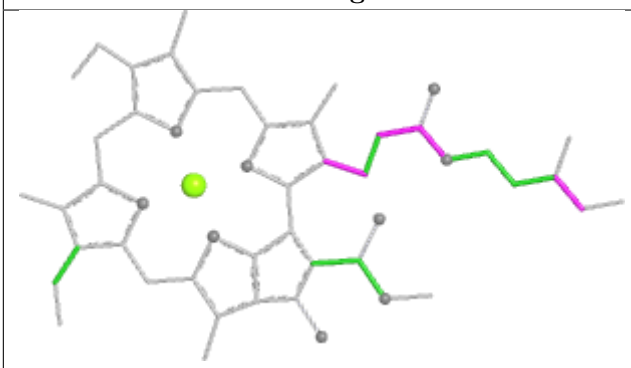
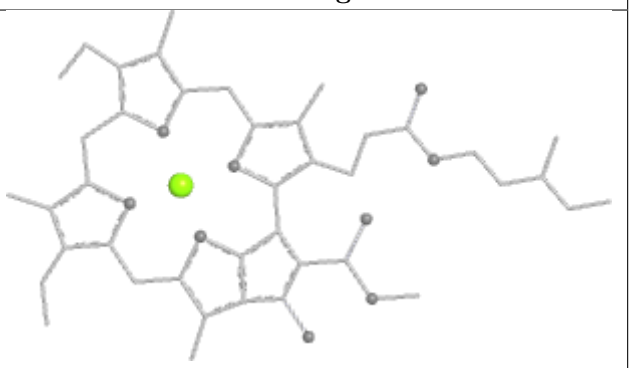


Torsions

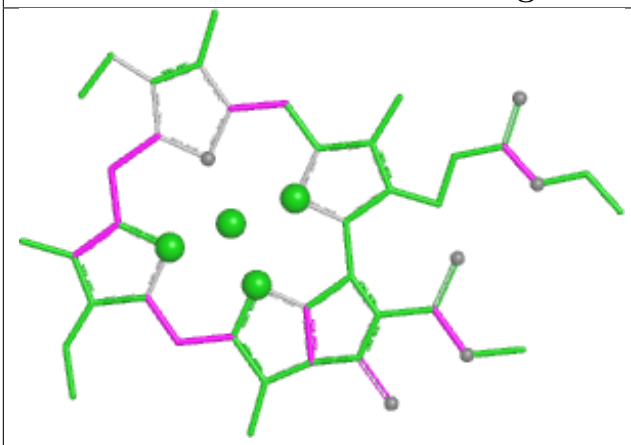


Rings

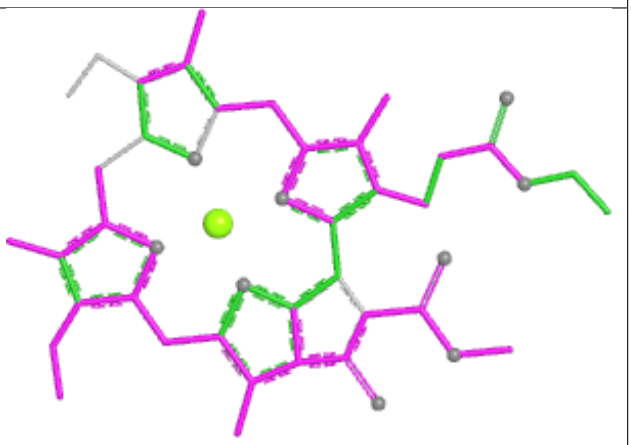
Ligand CLA A 1813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1766	
 Bond lengths	 Bond angles
 Torsions	 Rings

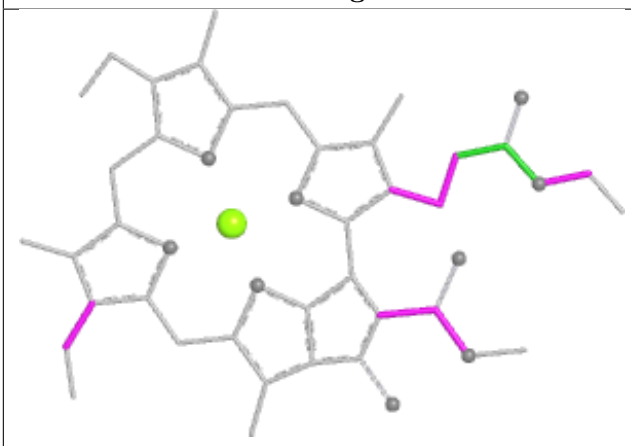
Ligand CLA L 1167



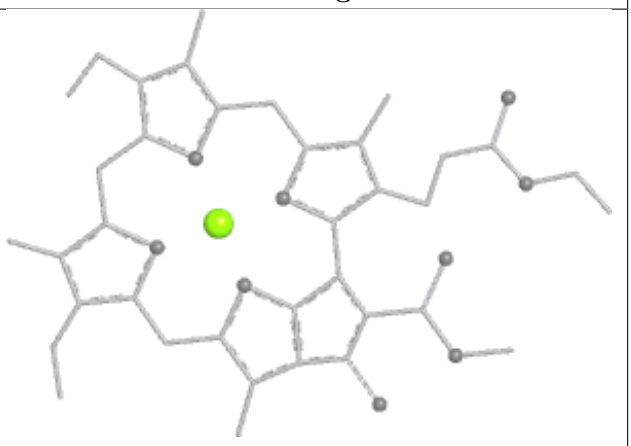
Bond lengths



Bond angles

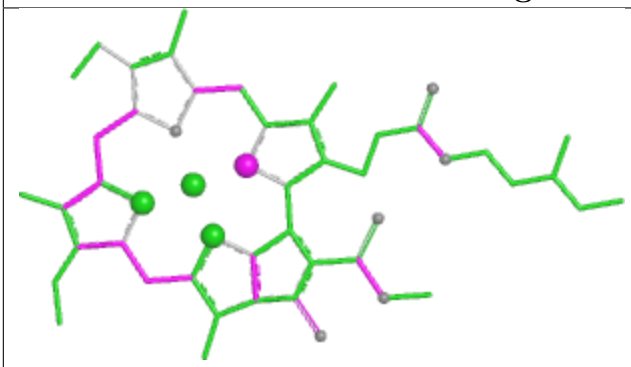


Torsions

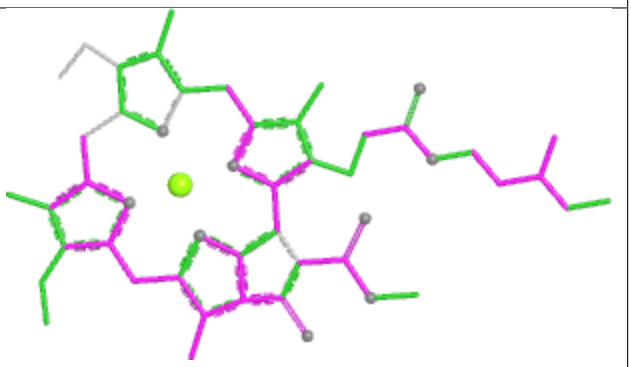


Rings

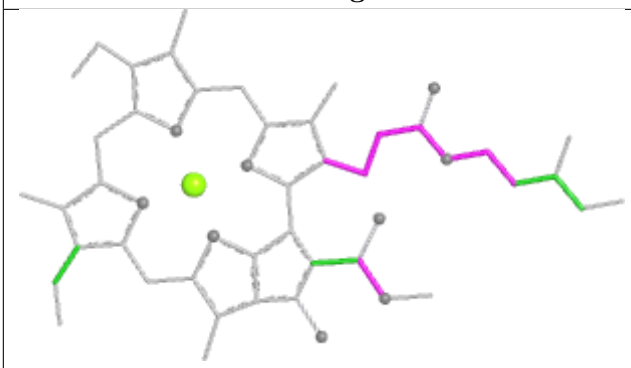
Ligand CLA A 1795



Bond lengths



Bond angles



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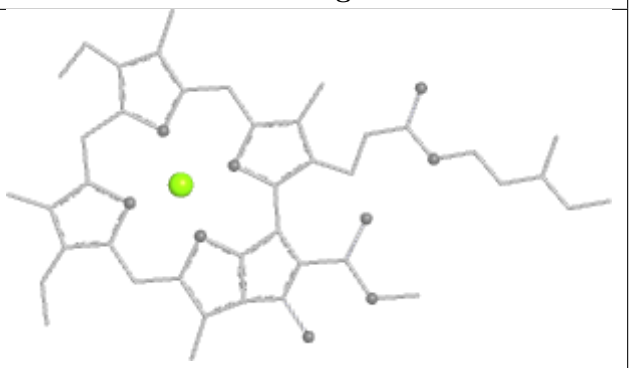
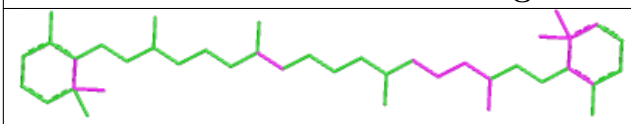
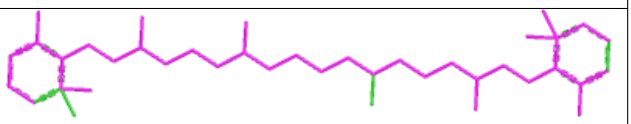


Rings

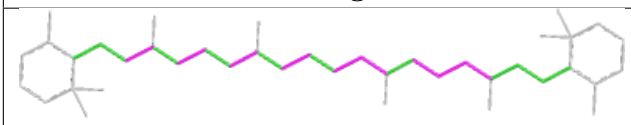
Ligand BCR B 1779



Bond lengths



Bond angles



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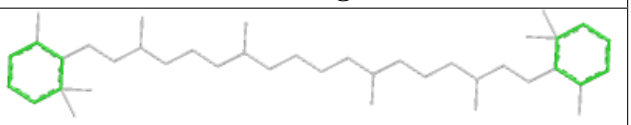
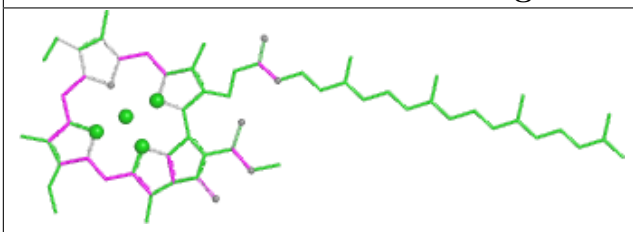


Rings

Ligand CLA A 1800



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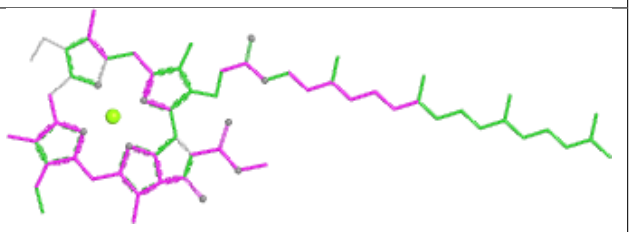
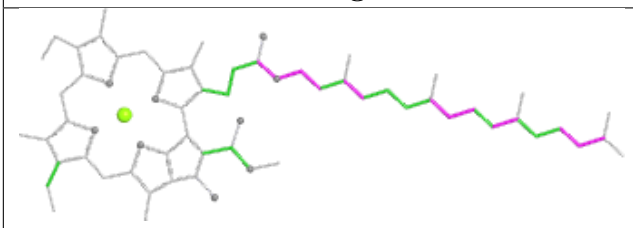


Bond angles



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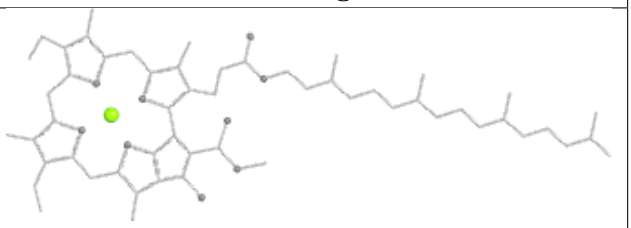
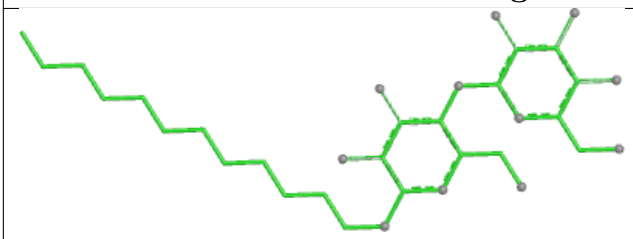
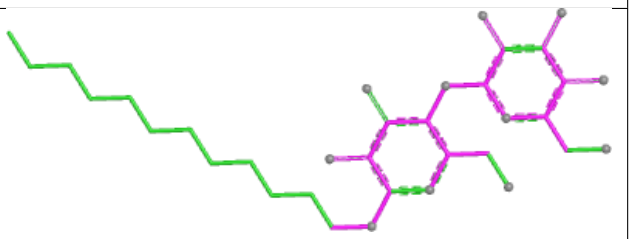


Rings

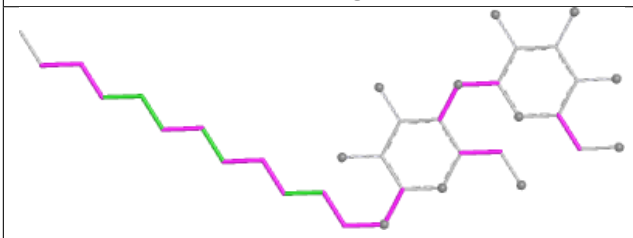
Ligand LMU A 7022



Bond lengths



Bond angles



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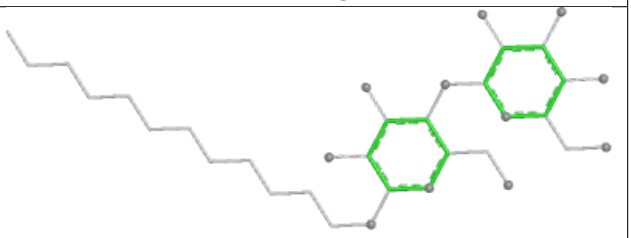
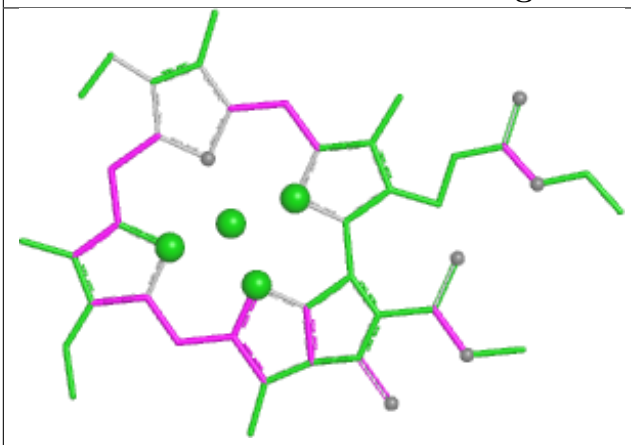
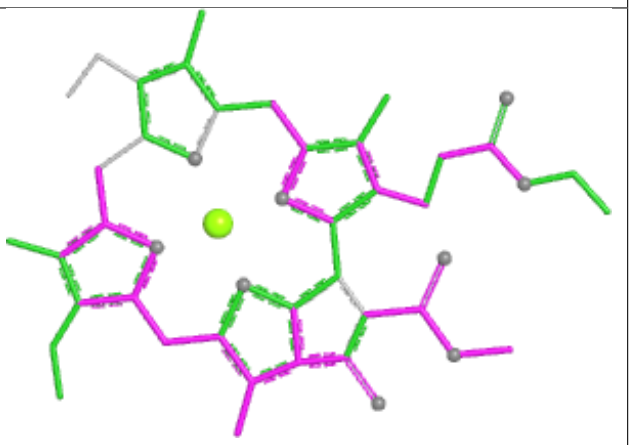


Rings

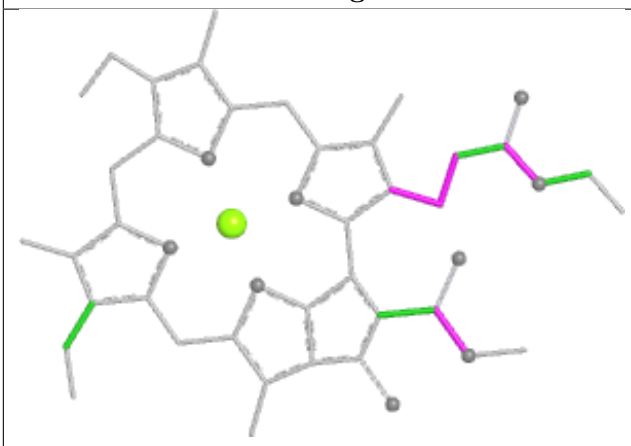
Ligand CLA B 1769



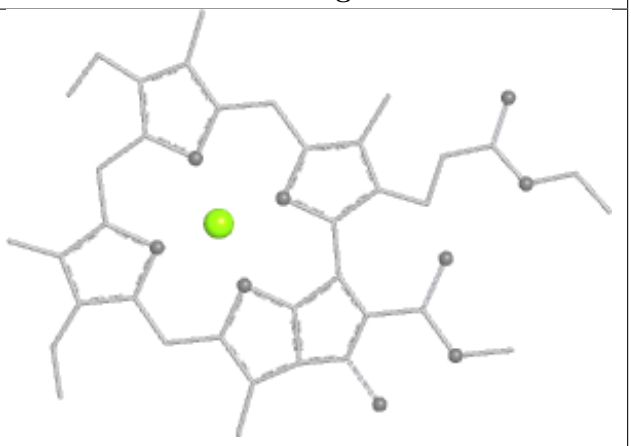
Bond lengths



Bond angles



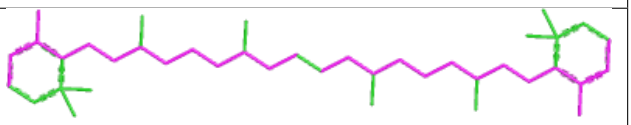
Torsions



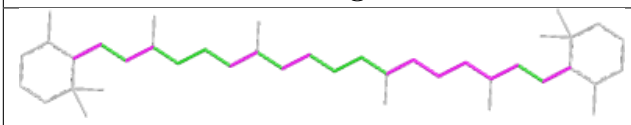
Rings

Ligand BCR A 1805

Bond lengths



Bond angles



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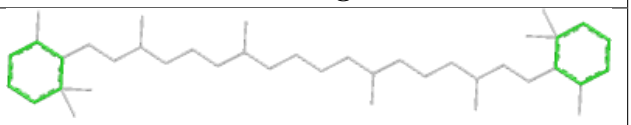
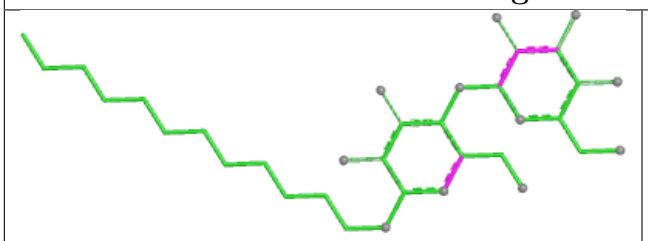
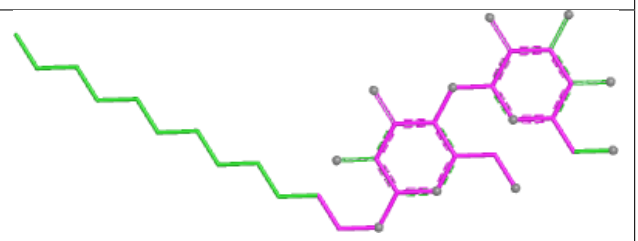


Rings

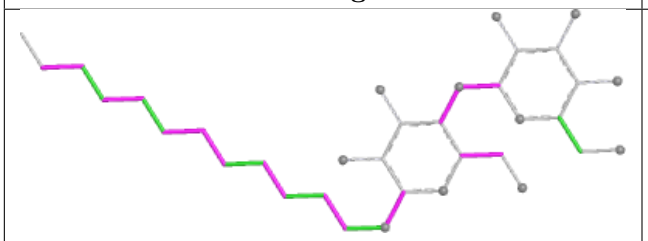
Ligand LMU A 7032



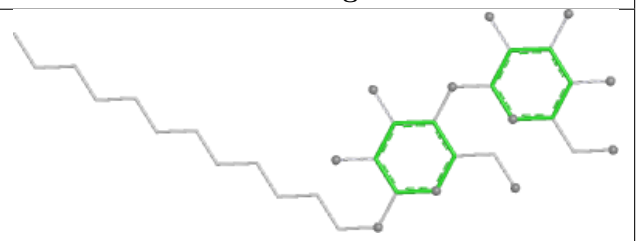
Bond lengths



Bond angles

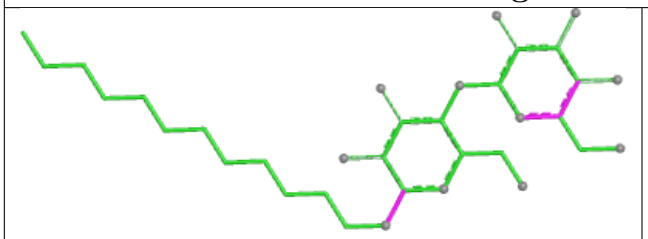


Torsions

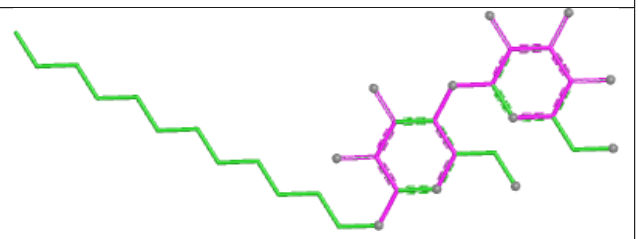


Rings

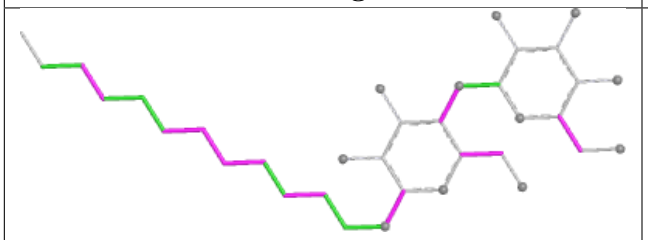
Ligand LMU A 7040



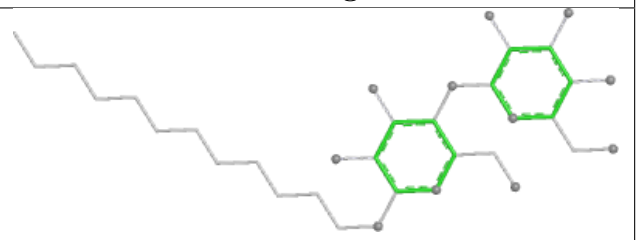
Bond lengths



Bond angles

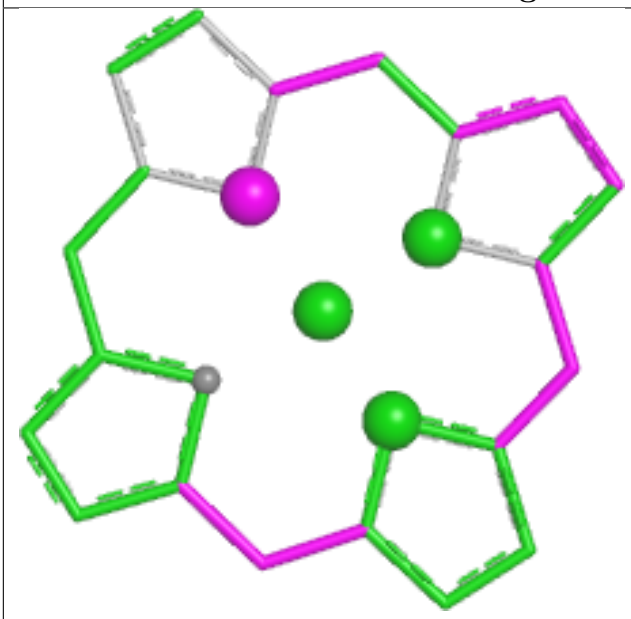


Torsions

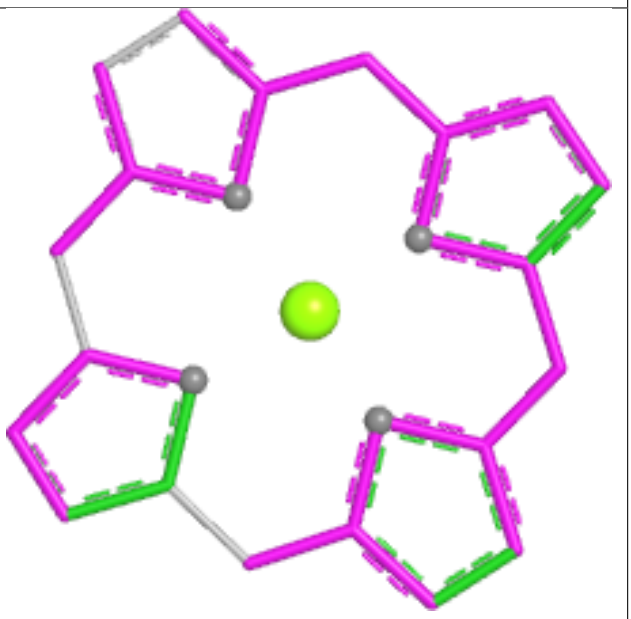


Rings

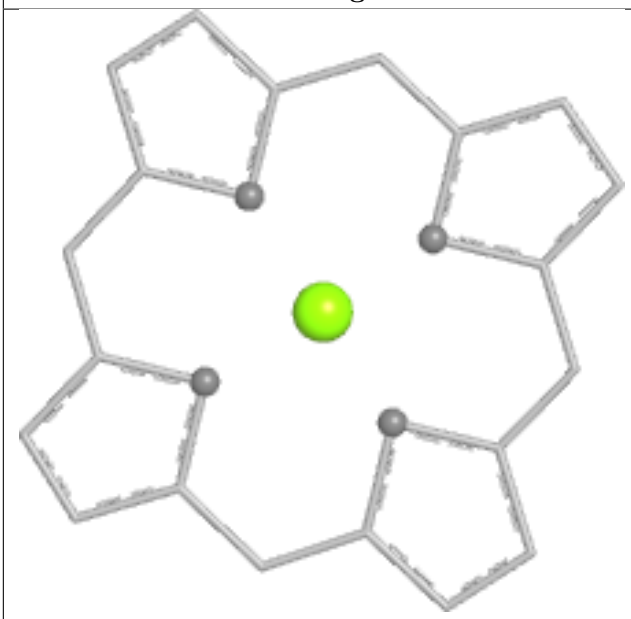
Ligand CLA 3 3002



Bond lengths



Bond angles



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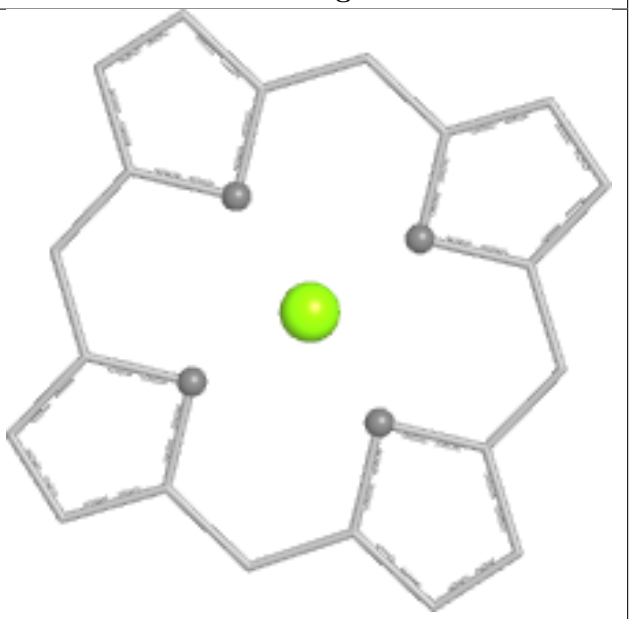
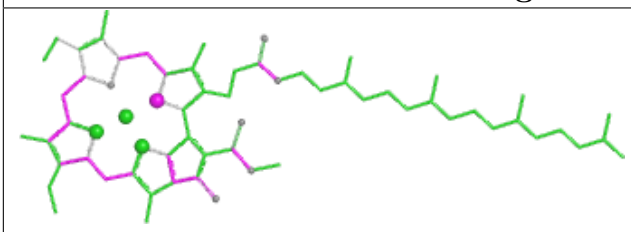
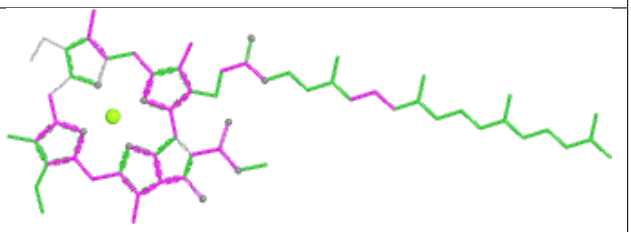
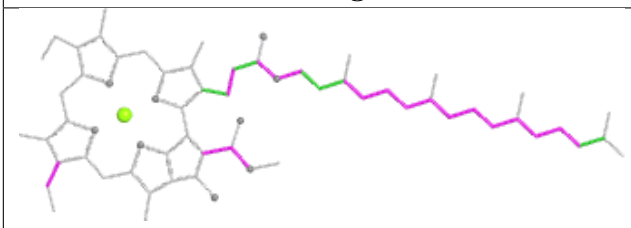
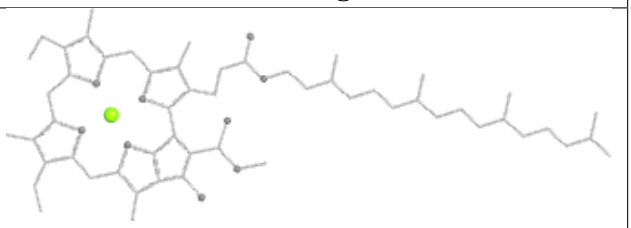
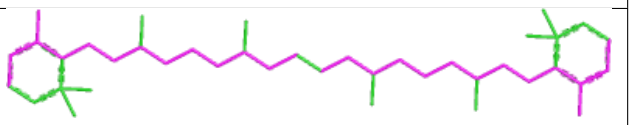
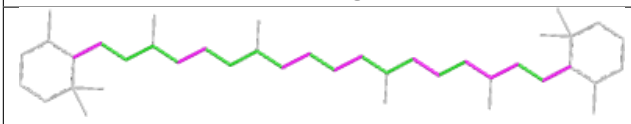
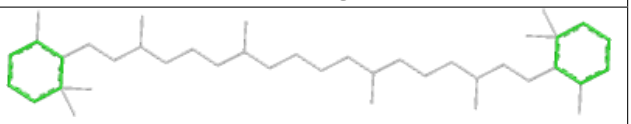
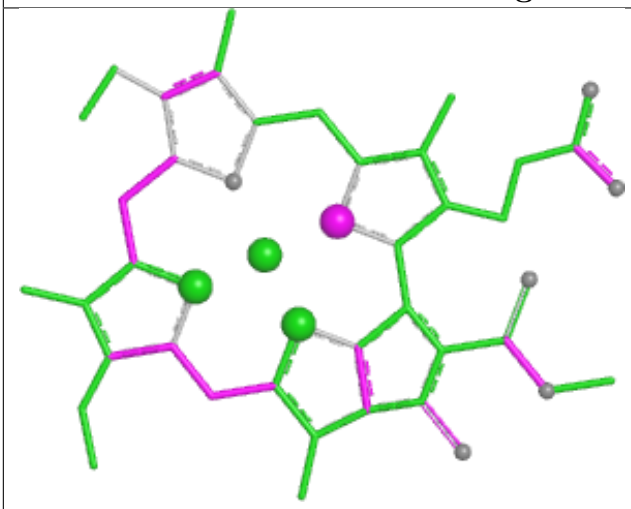


Rings

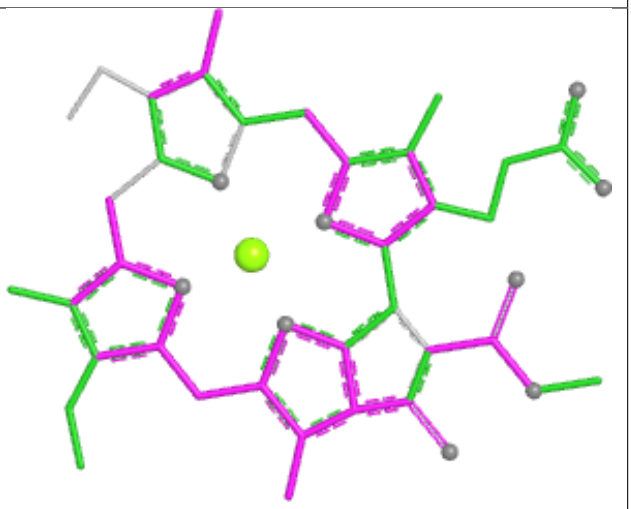
Ligand CLA B 1759	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 1778	
 Bond lengths	 Bond angles
 Torsions	 Rings

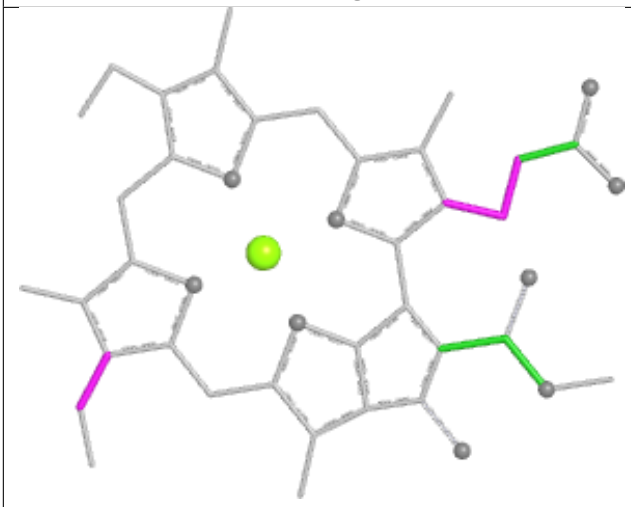
Ligand CLA B 1736



Bond lengths



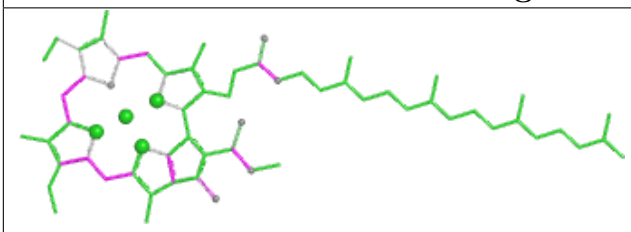
Bond angles



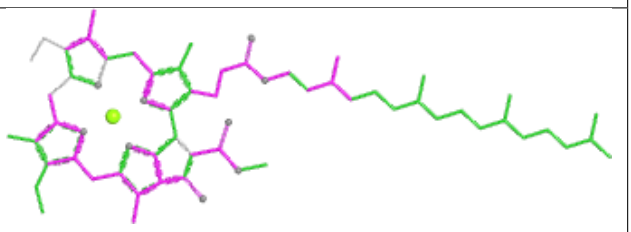
Torsions

Rings

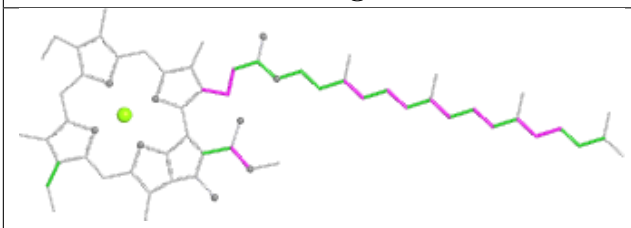
Ligand CLA A 1787



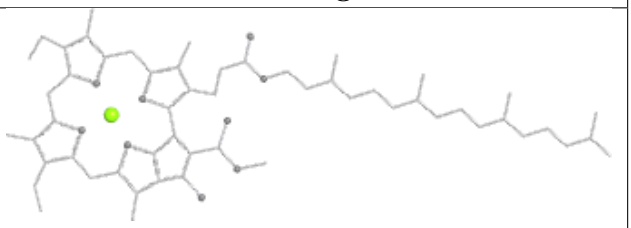
Bond lengths



Bond angles

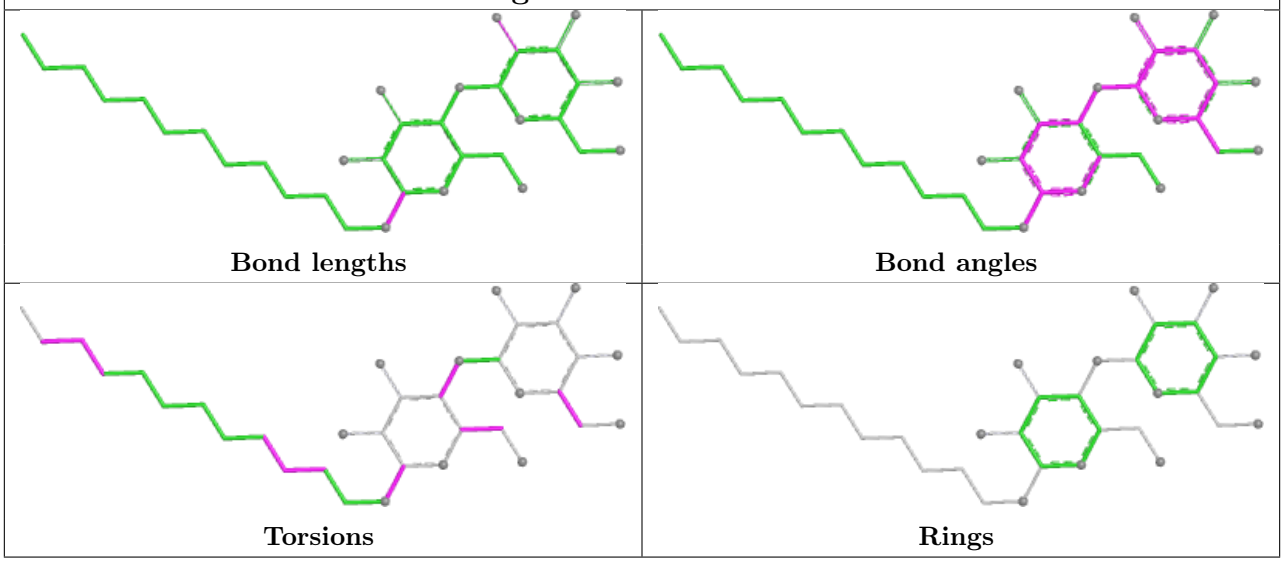


Torsions

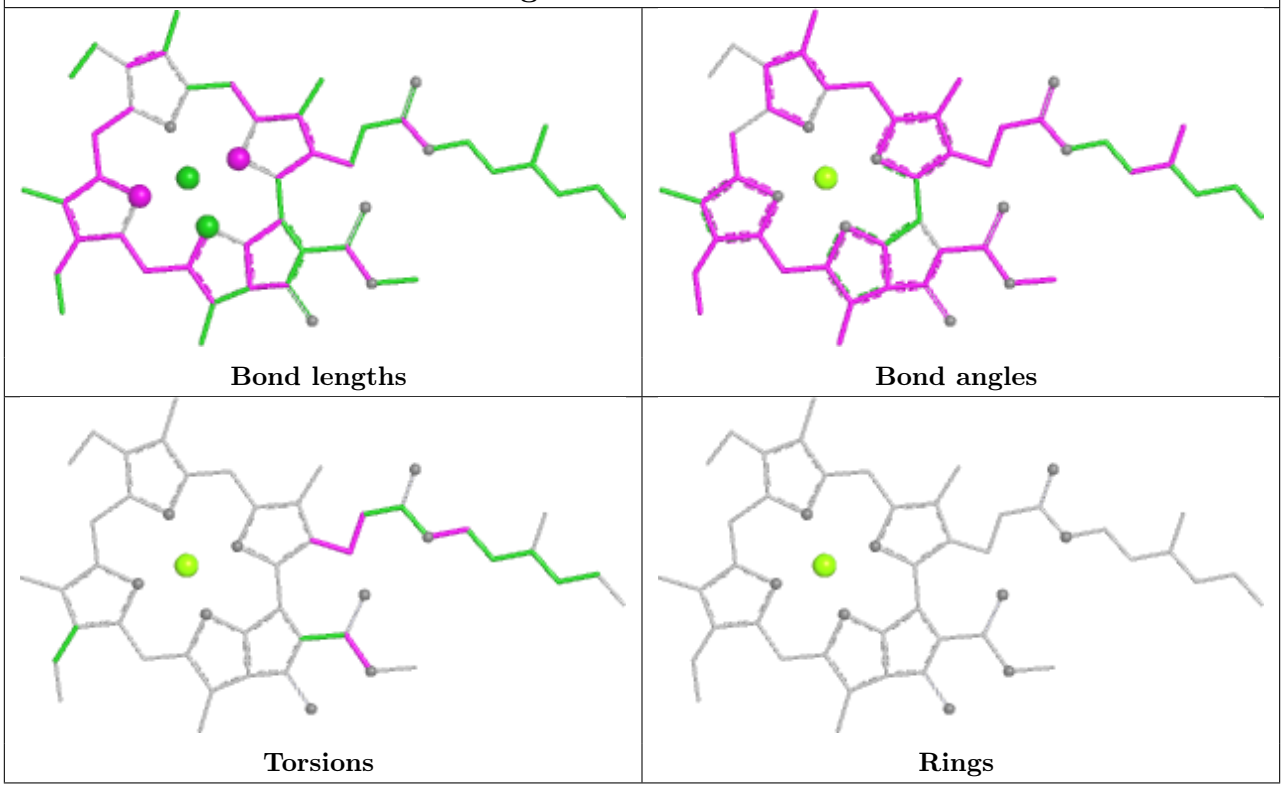


Rings

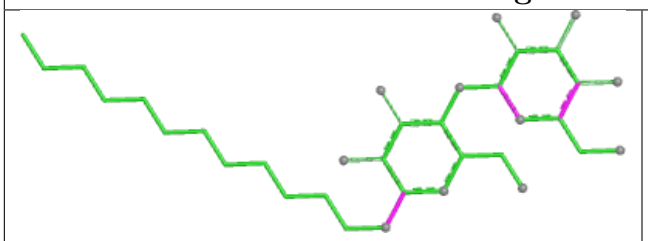
Ligand LMU R 1057



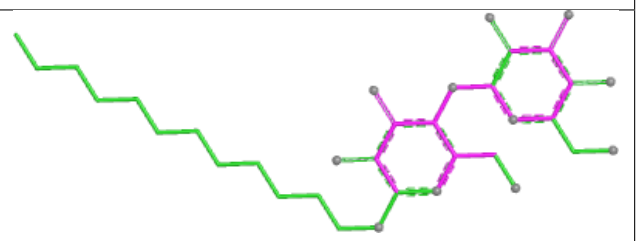
Ligand CLA 4 1201



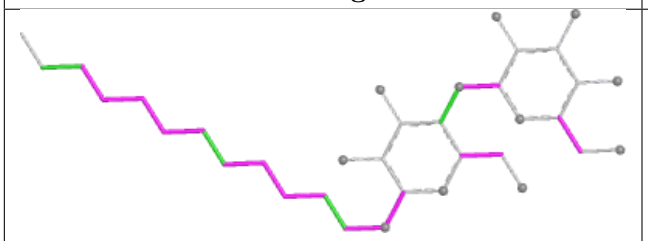
Ligand LMU L 1171



Bond lengths



Bond angles



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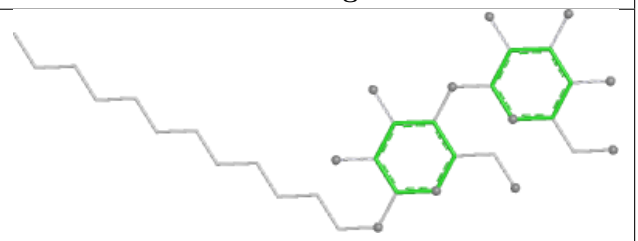
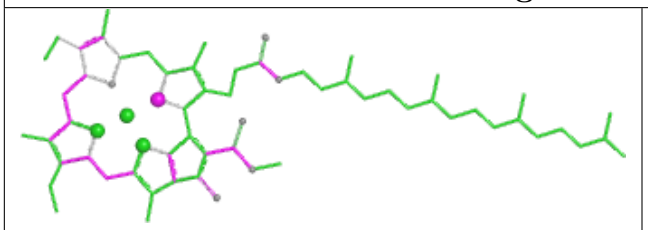


Rings

Ligand CLA A 1812



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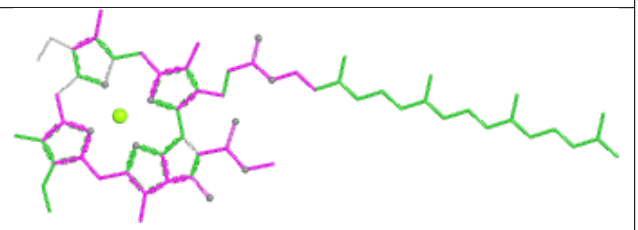
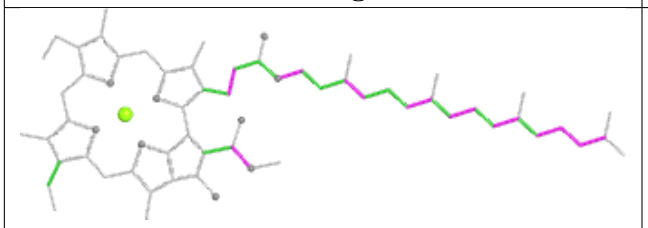


Bond angles



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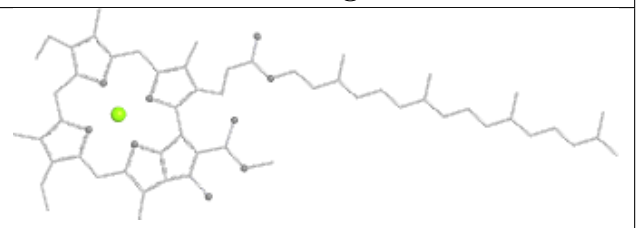
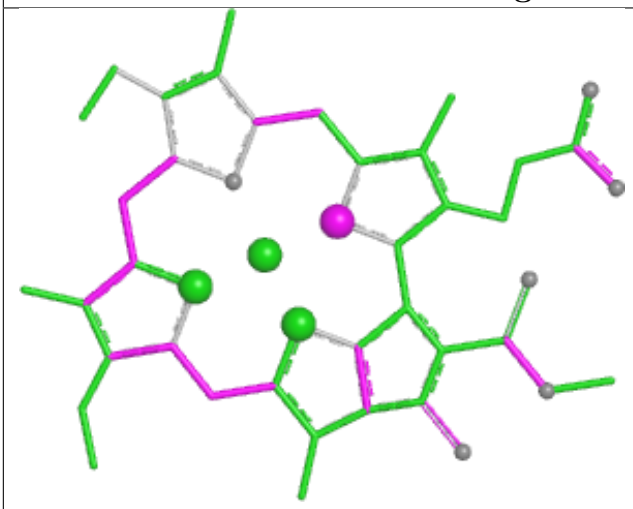


Rings

Ligand CLA K 1142



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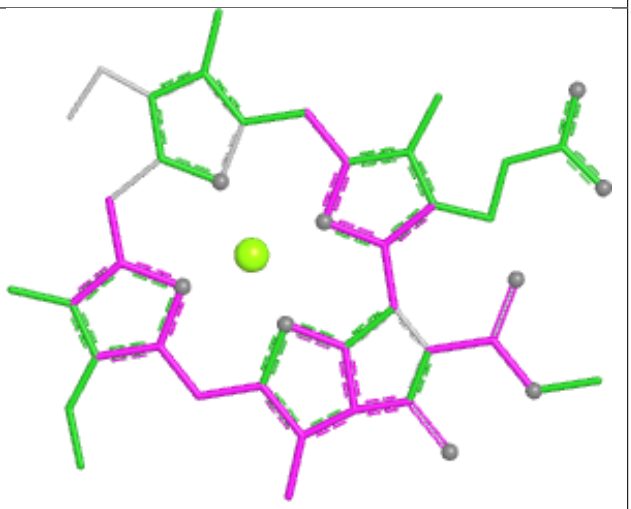
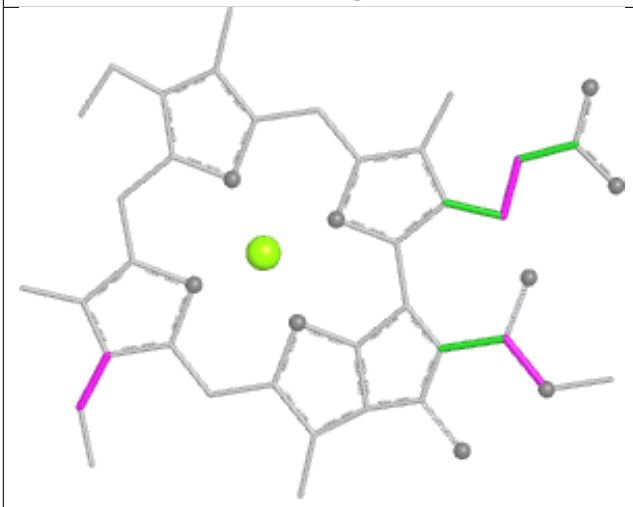


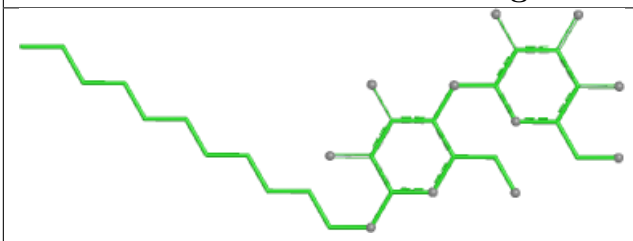
Bond angles



Torsions

Rings

Ligand LMU A 7009



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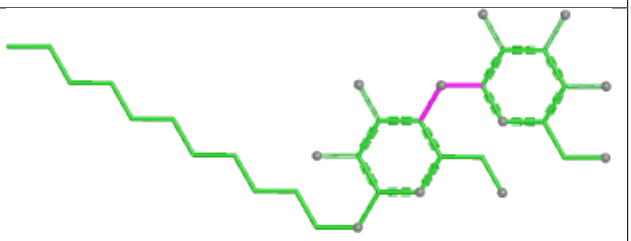
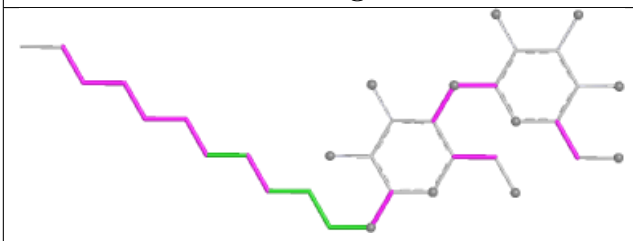


Bond angles



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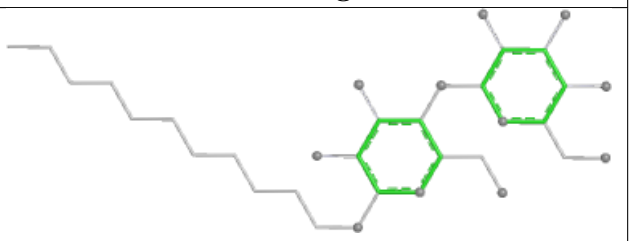
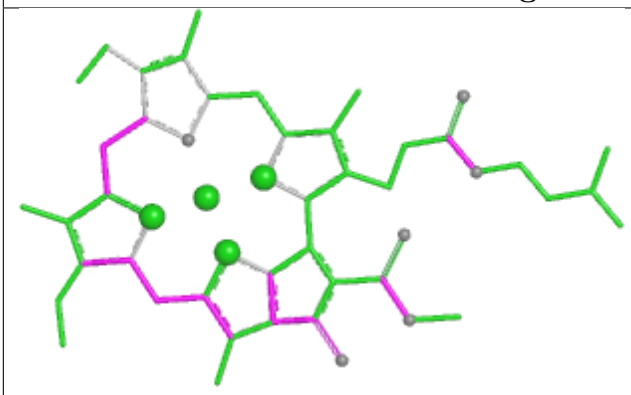


Rings

Ligand CLA 2 1223



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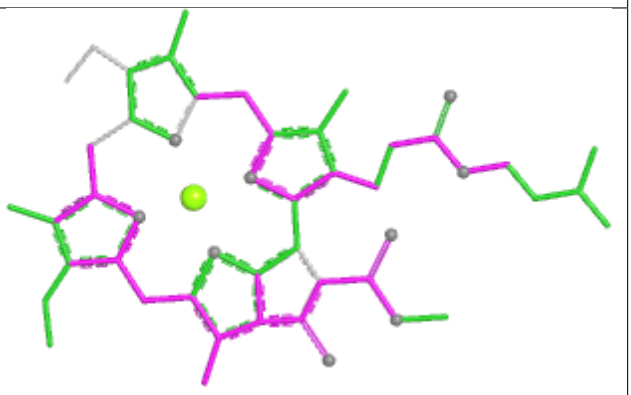
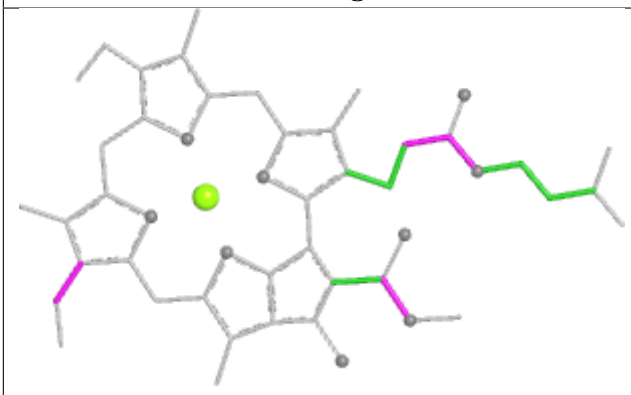


Bond angles



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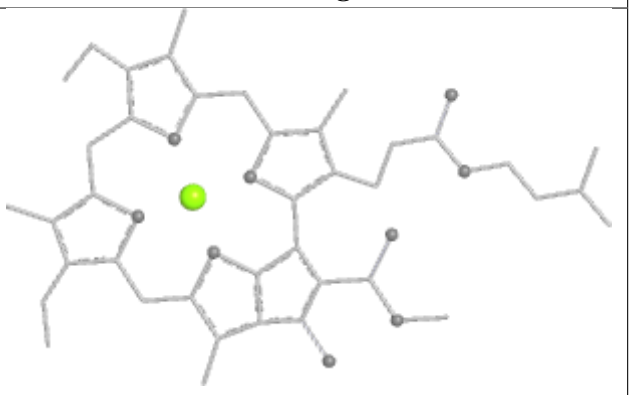
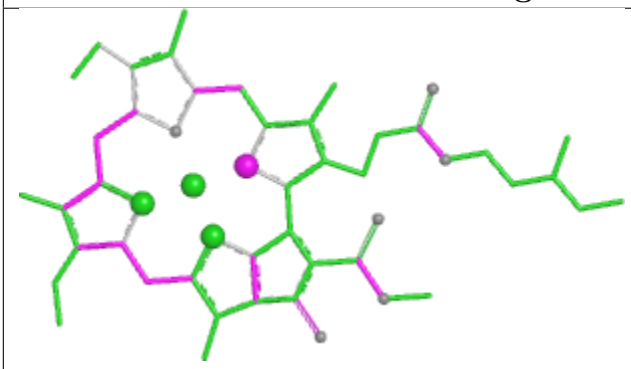


Rings

Ligand CLA A 1777



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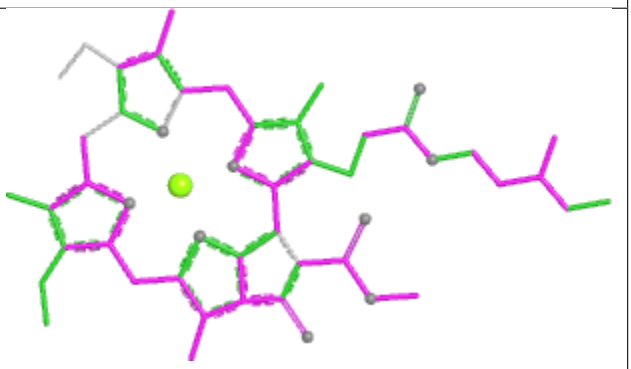
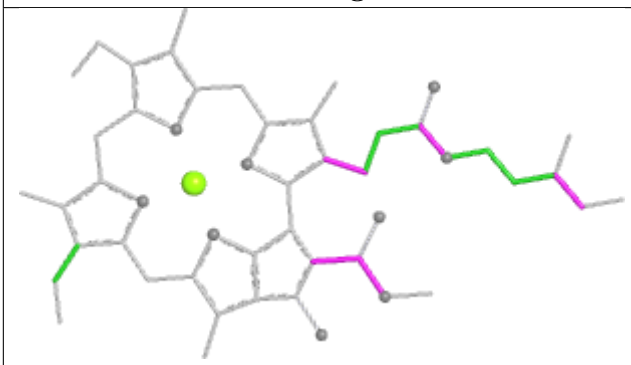


Bond angles



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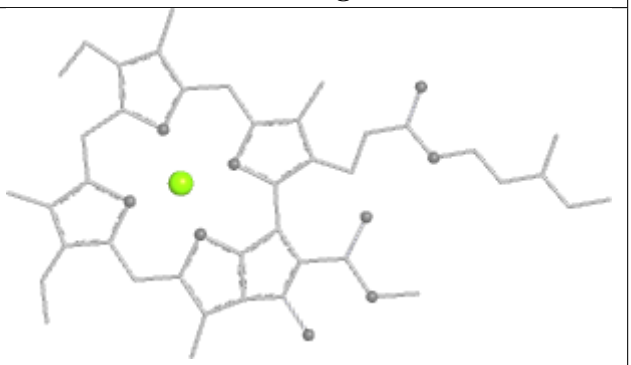
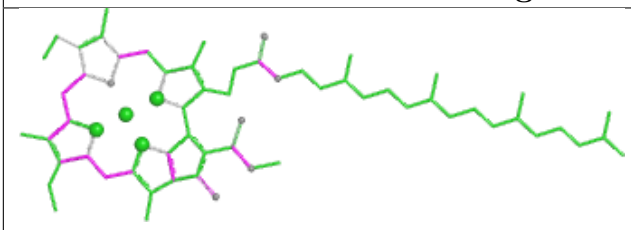
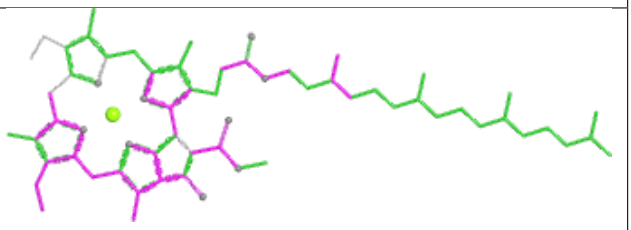
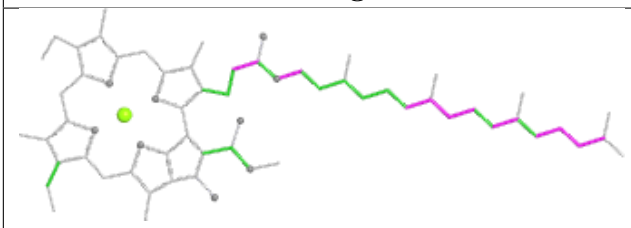
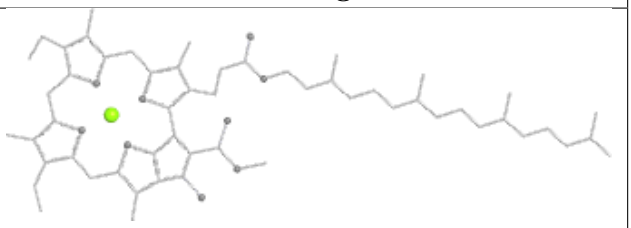
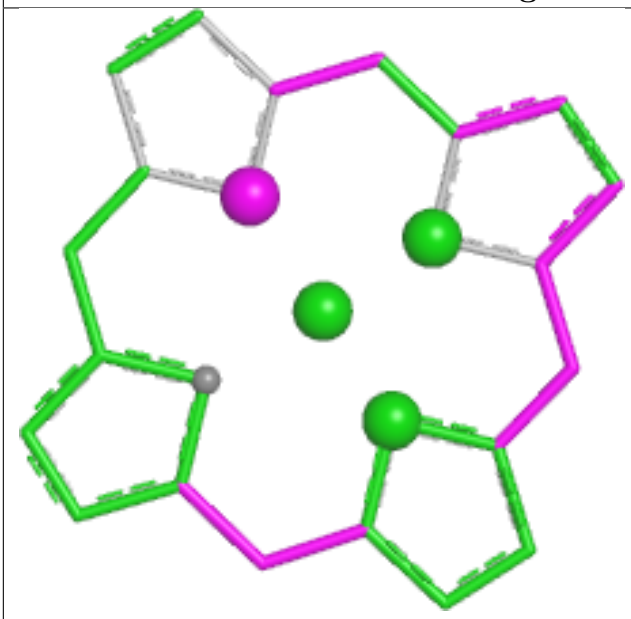


Rings

Ligand CLA B 1768	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 1205



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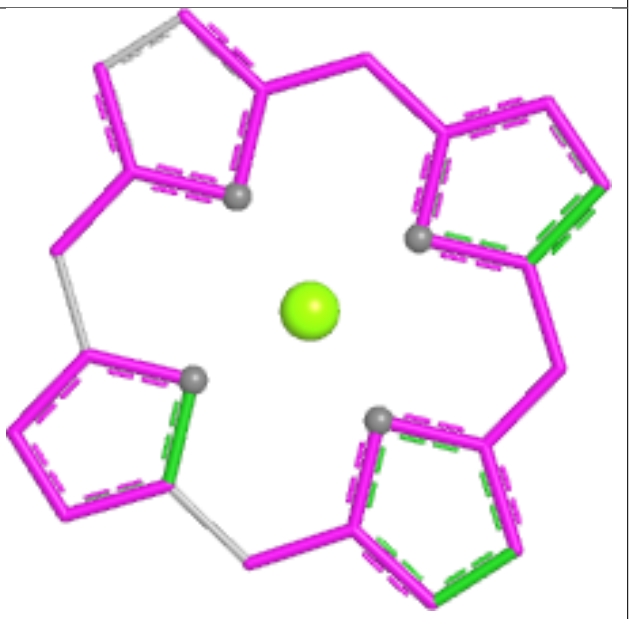
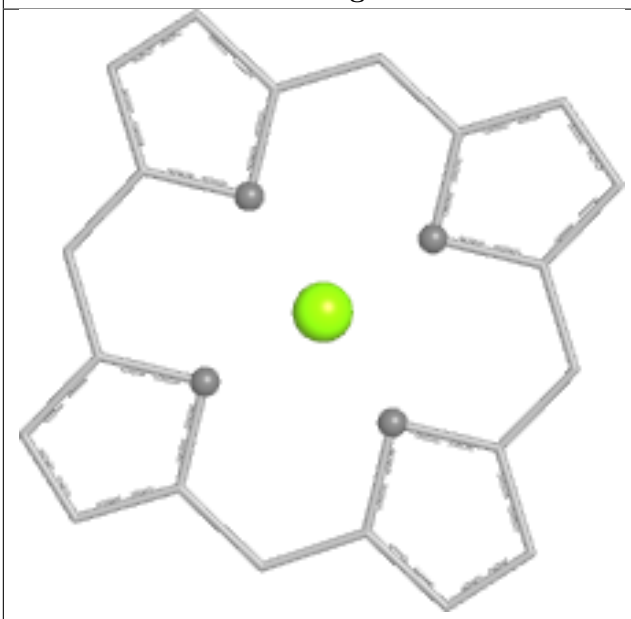


Bond angles



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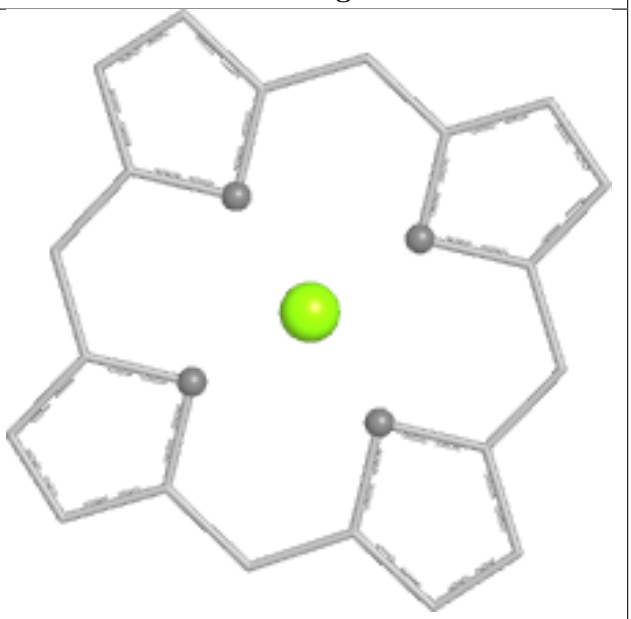
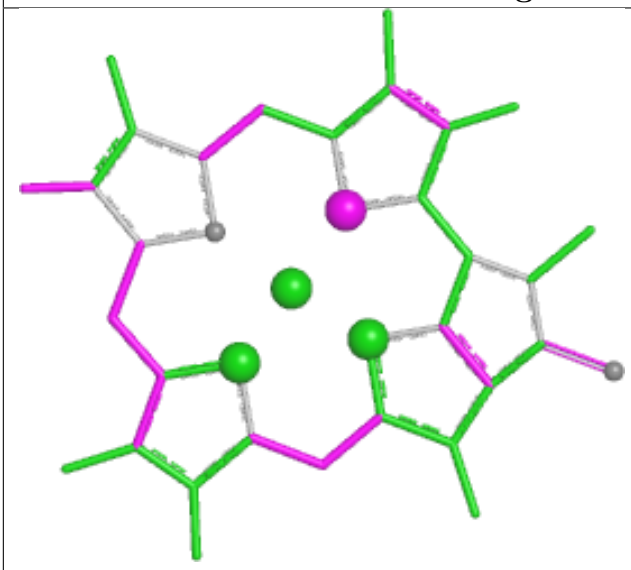


Rings

Ligand CLA B 1772



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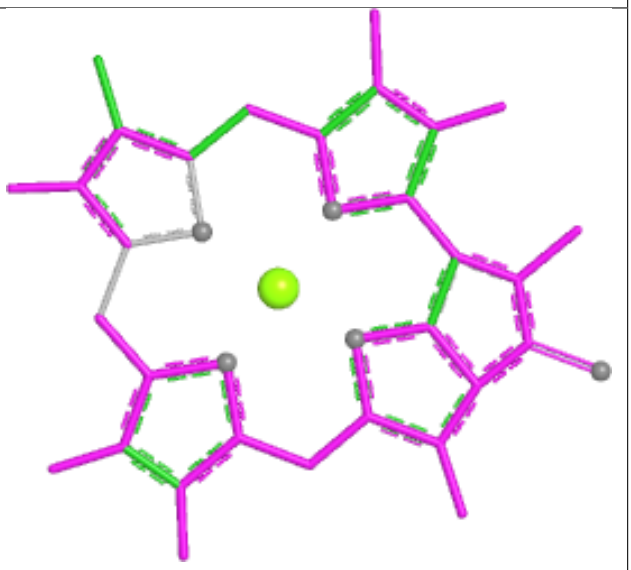
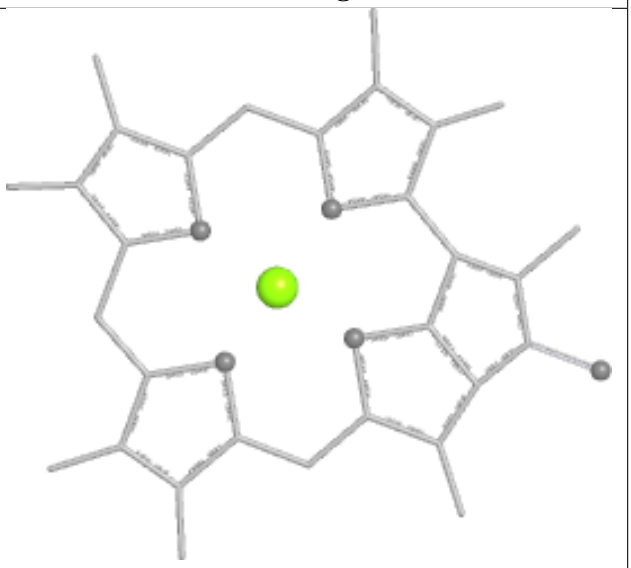


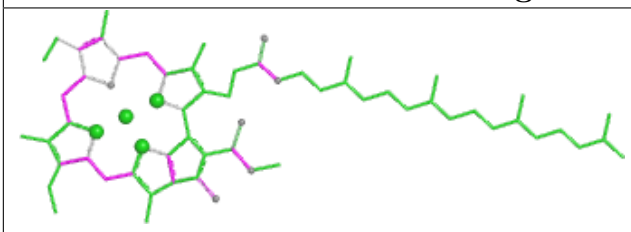
Bond angles

Torsions



Rings

Ligand CLA R 1055



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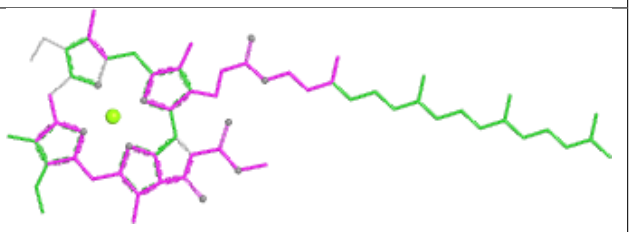
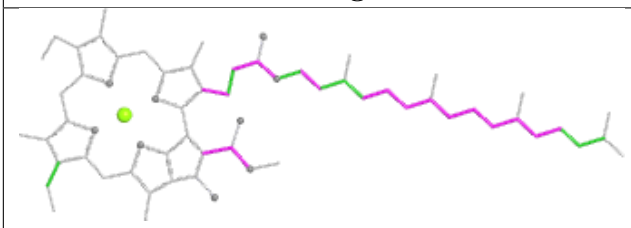


Bond angles



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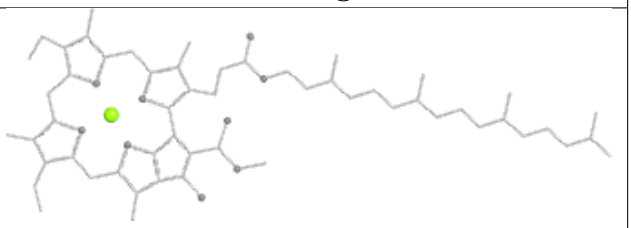
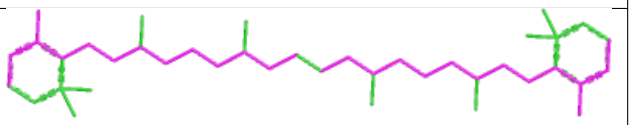


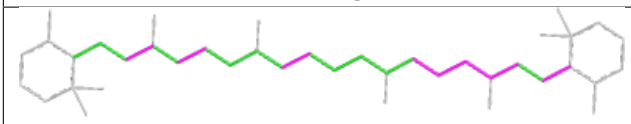
Rings

Ligand BCR A 1803

Bond lengths



Bond angles



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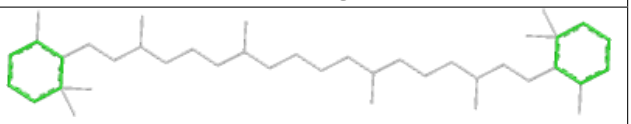
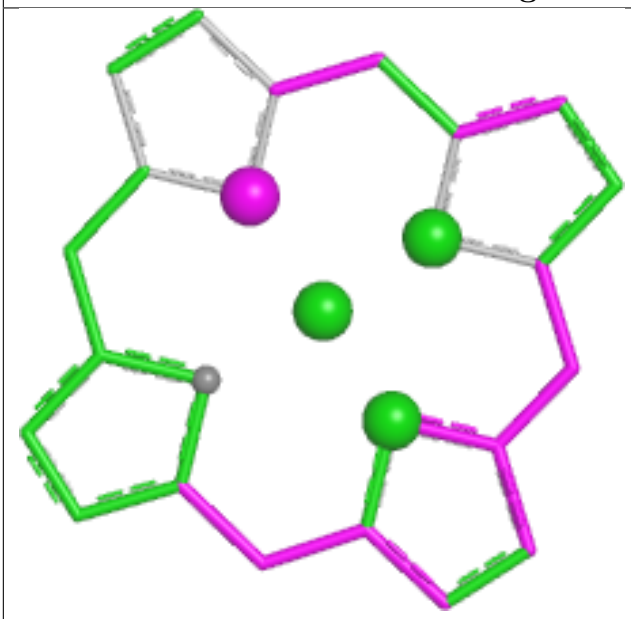


Rings

Ligand CLA 2 1216



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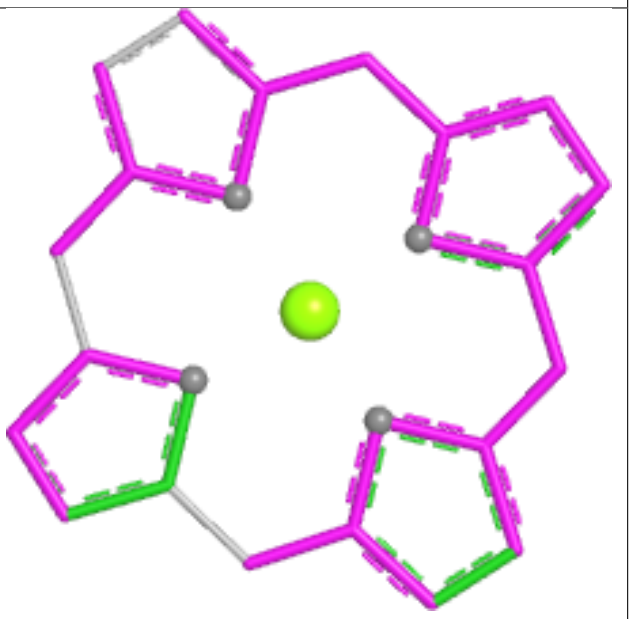
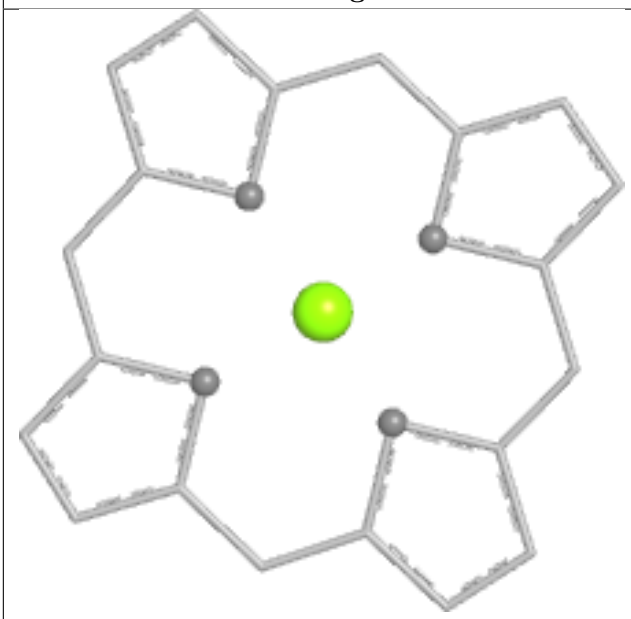


Bond angles



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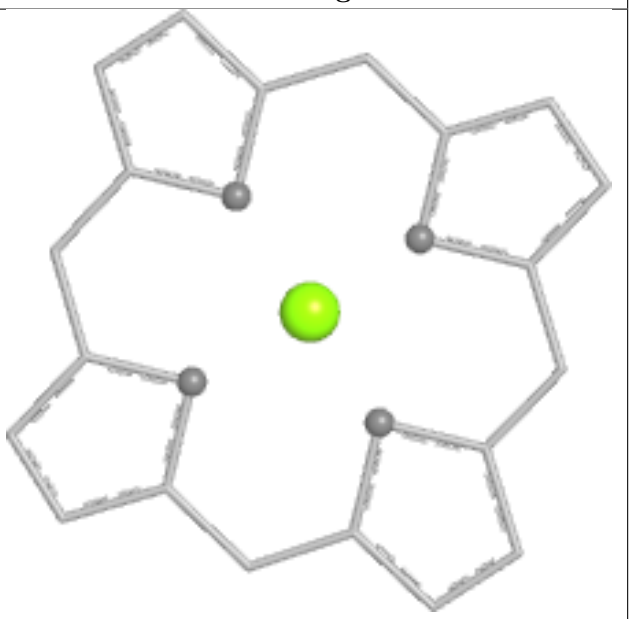
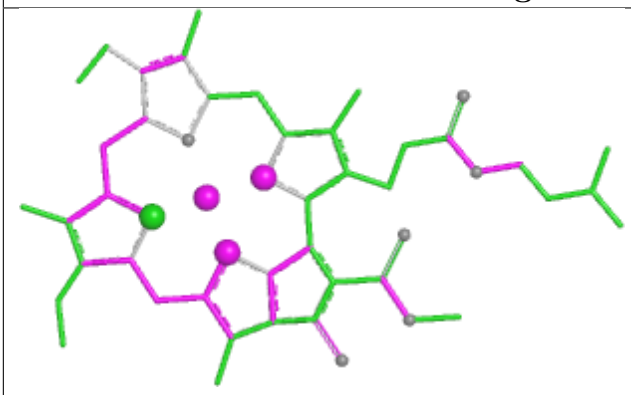
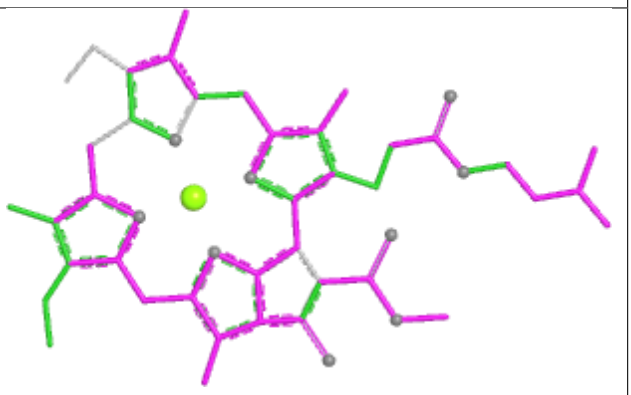
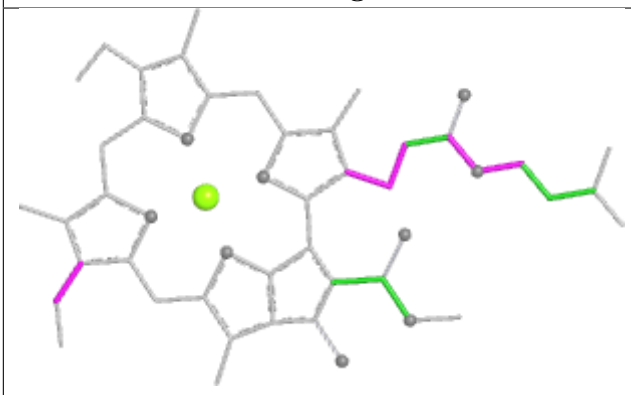
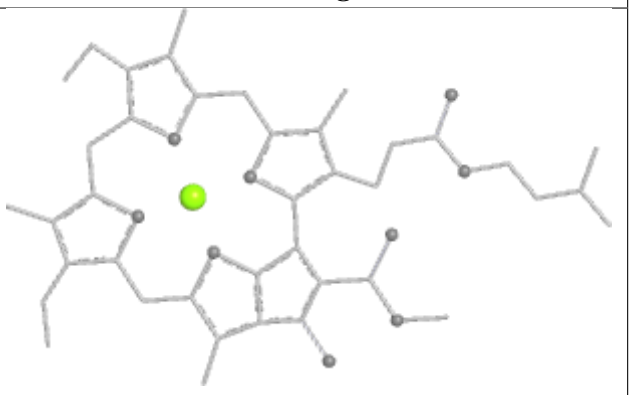
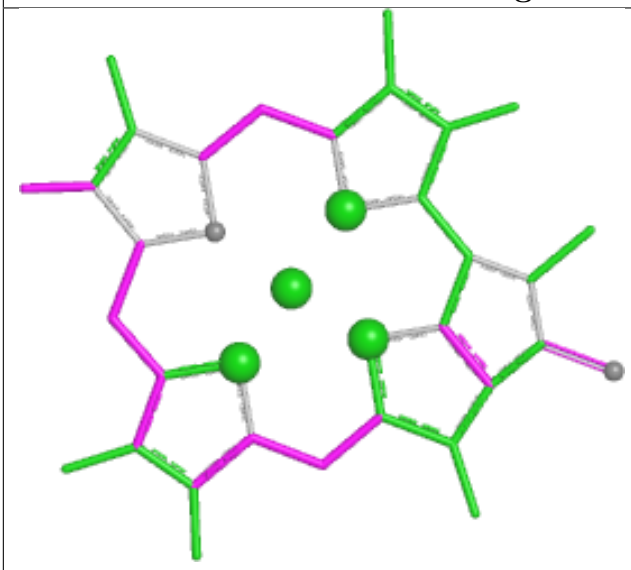


Rings

Ligand CLA K 1146	
 Bond lengths	 Bond angles
 Torsions	 Rings

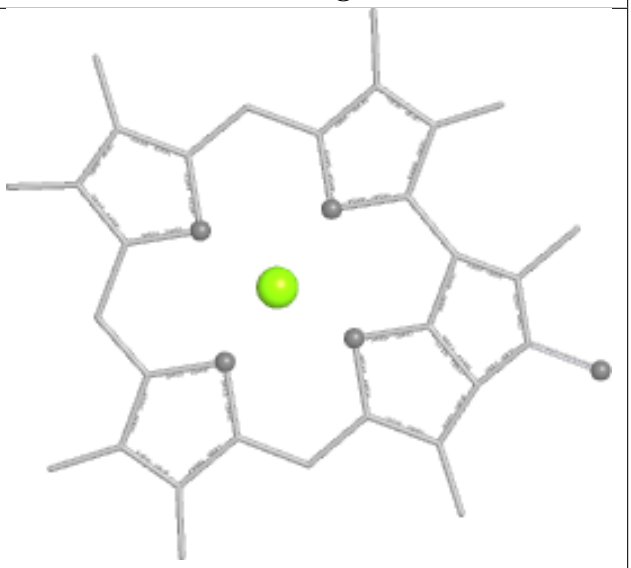
Ligand CLA A 1775



Bond lengths

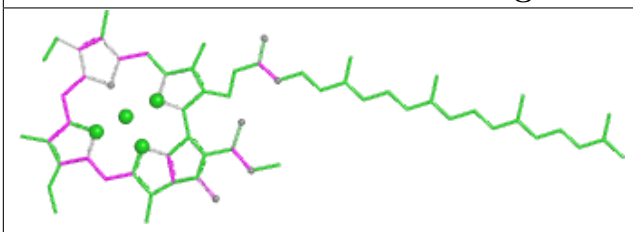
Bond angles

Torsions

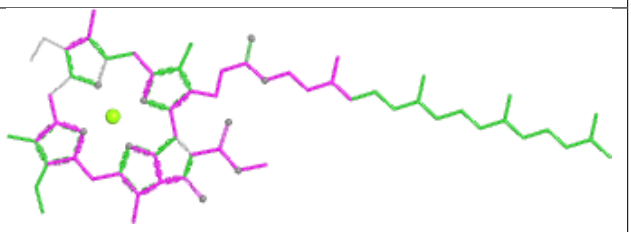


Rings

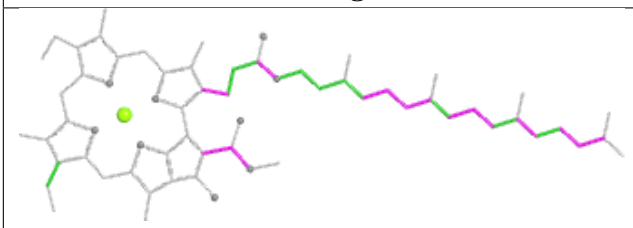
Ligand CLA A 1774



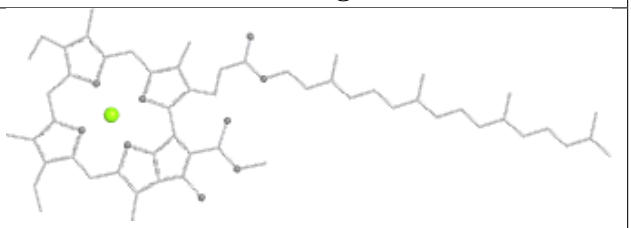
Bond lengths



Bond angles

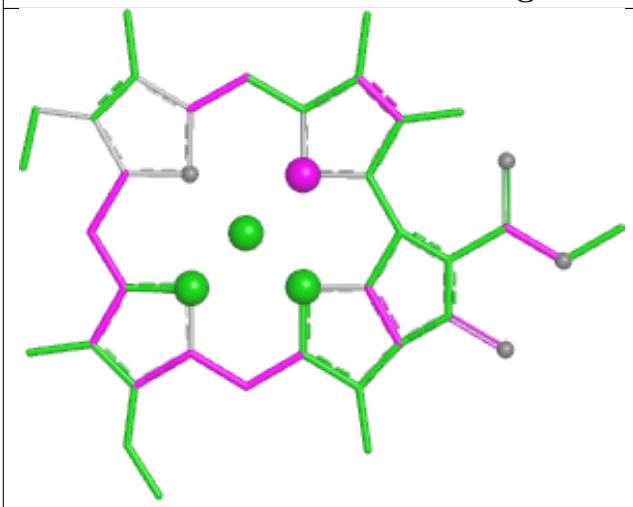


Torsions

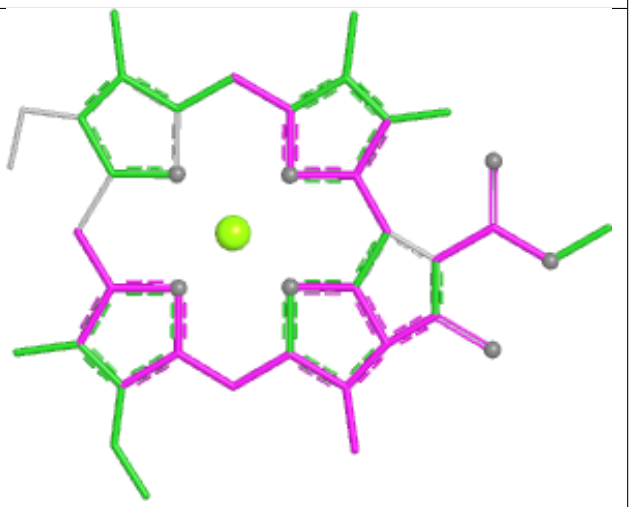


Rings

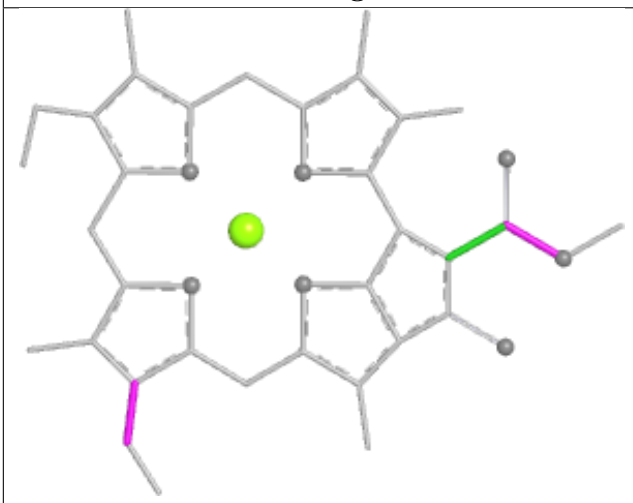
Ligand CLA F 1156



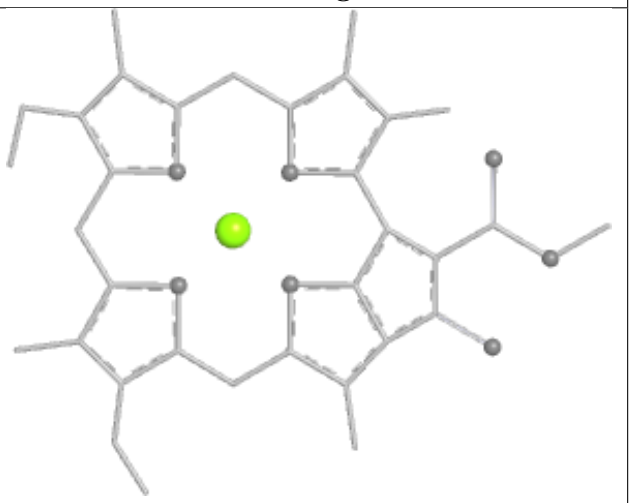
Bond lengths



Bond angles

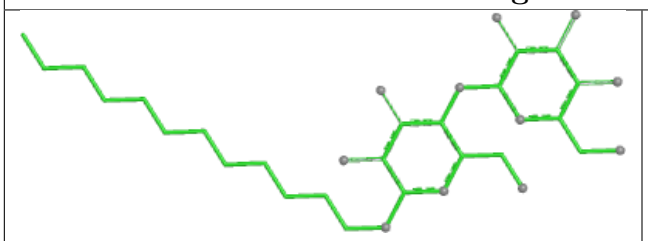


Torsions



Rings

Ligand LMU A 7041



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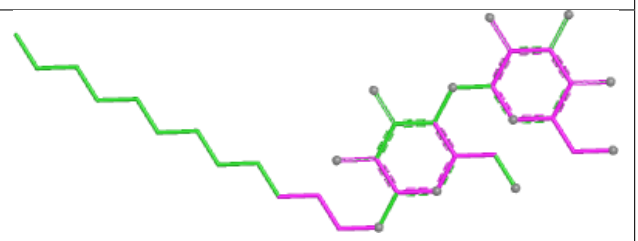
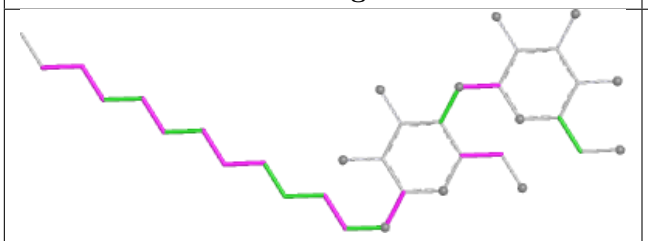


Bond angles



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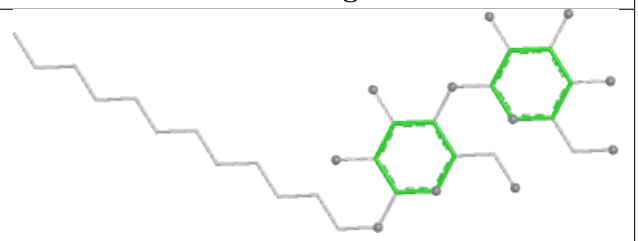
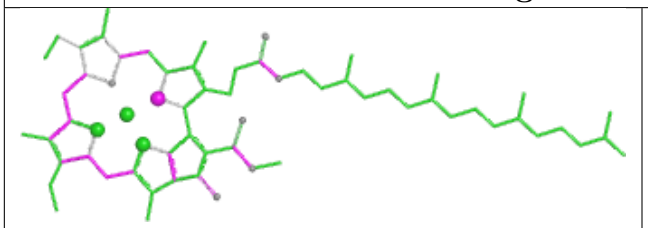
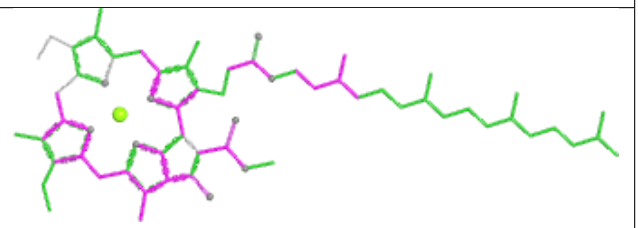


Rings

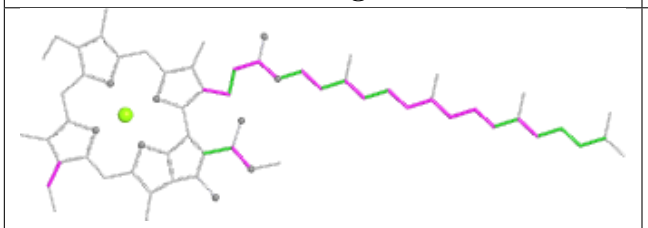
Ligand CLA A 1782



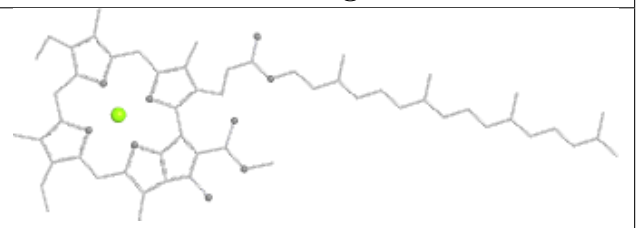
Bond lengths



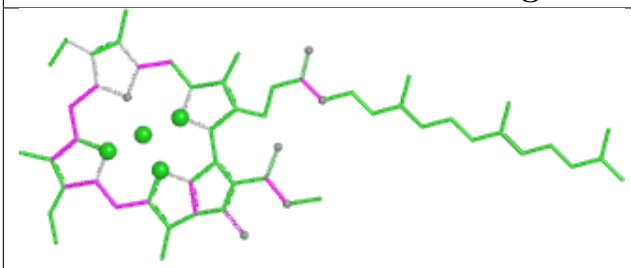
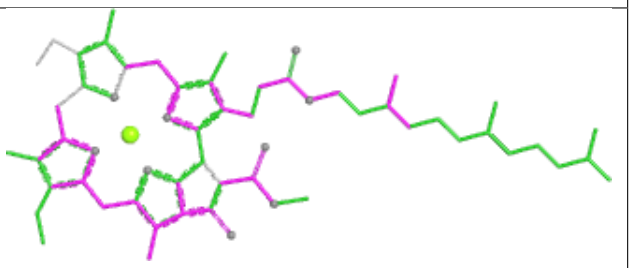
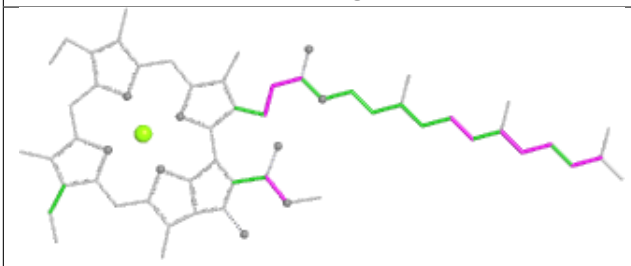
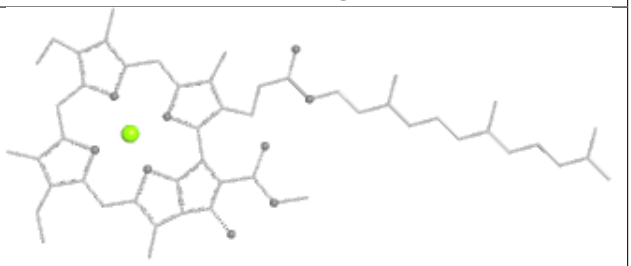
Bond angles

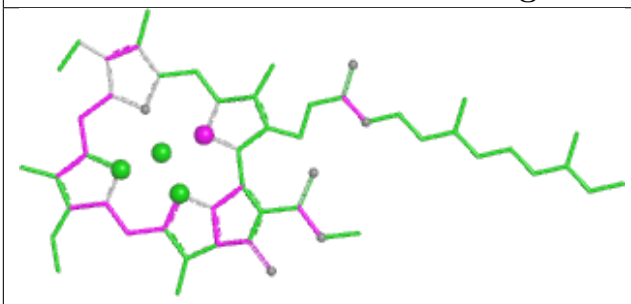
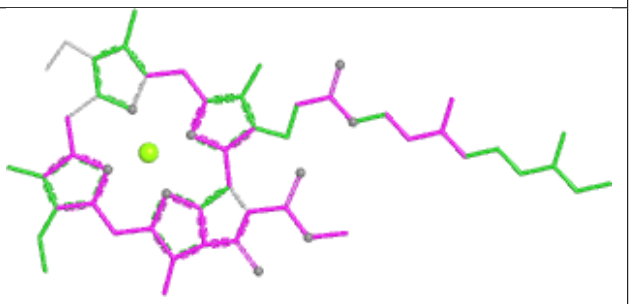
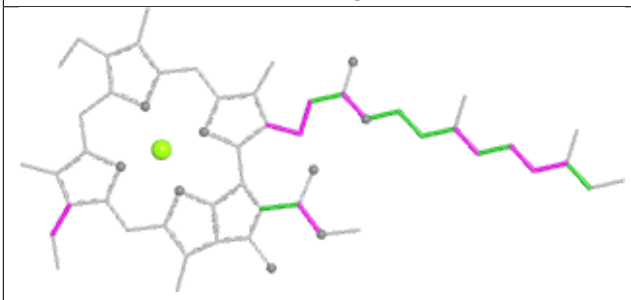
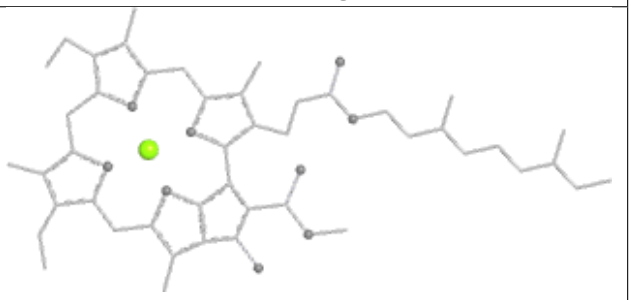


Torsions

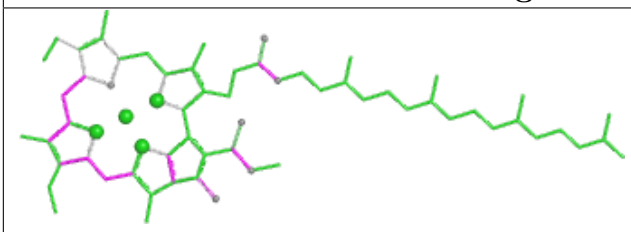


Rings

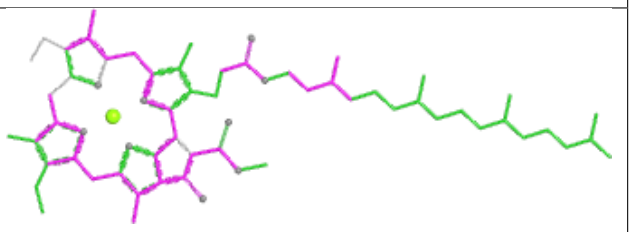
Ligand CLA I 1031	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 1220	
 Bond lengths	 Bond angles
 Torsions	 Rings

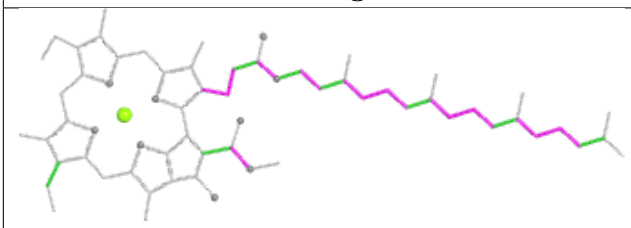
Ligand CLA B 1740



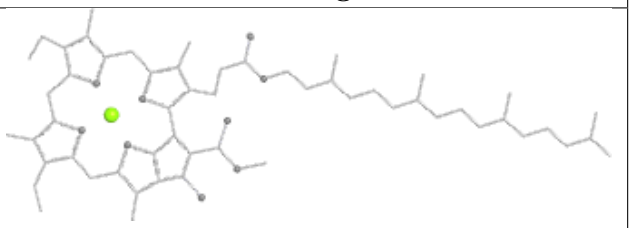
Bond lengths



Bond angles

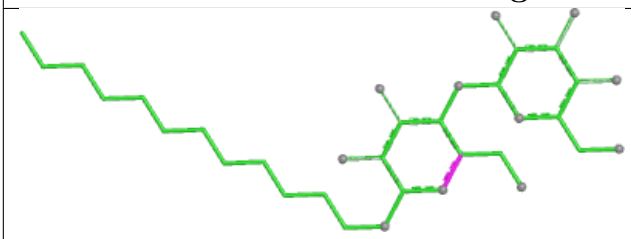


Torsions

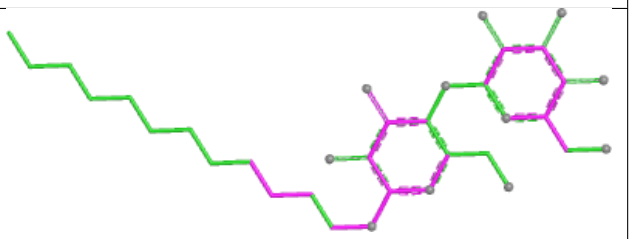


Rings

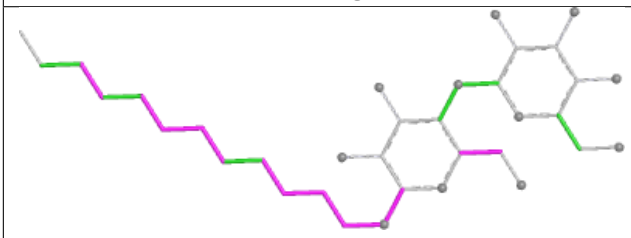
Ligand LMU A 7016



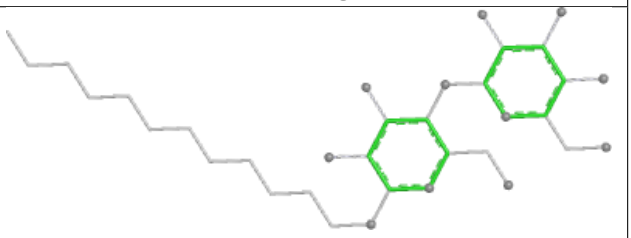
Bond lengths



Bond angles

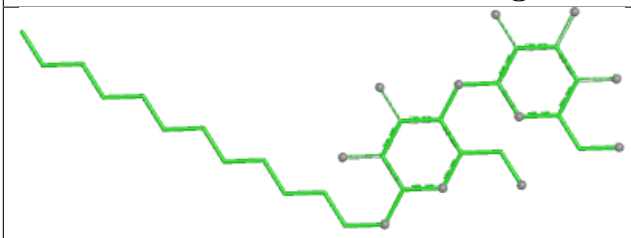


Torsions

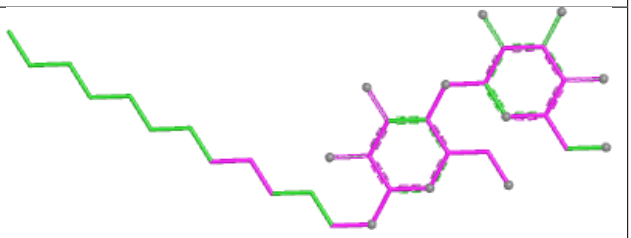


Rings

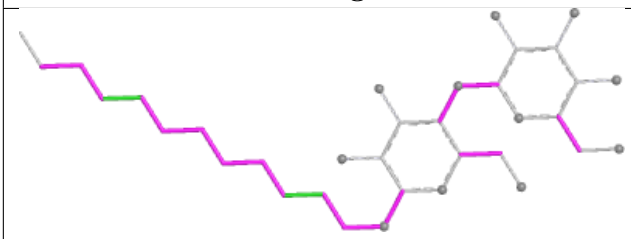
Ligand LMU A 7042



Bond lengths



Bond angles



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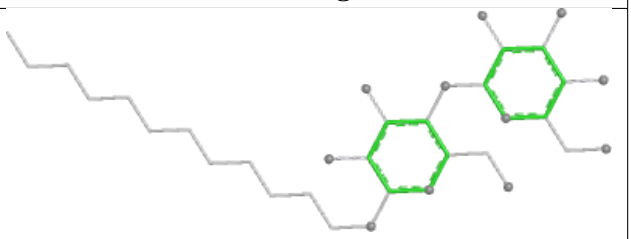
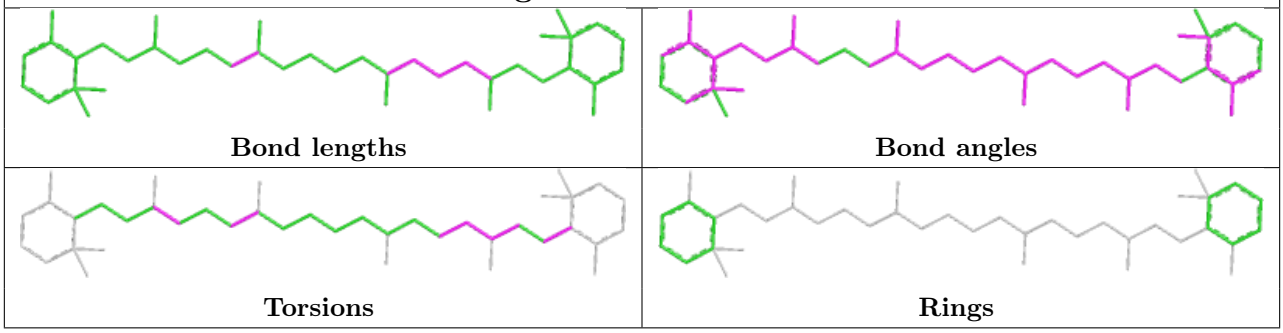
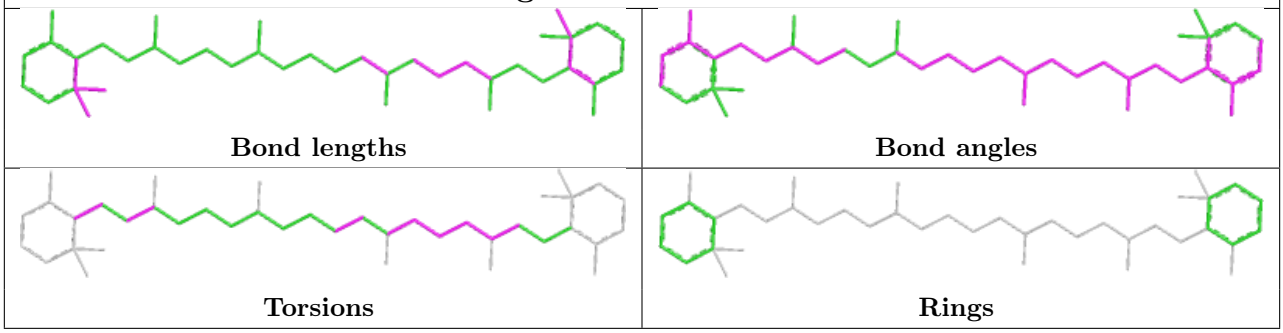


Rings

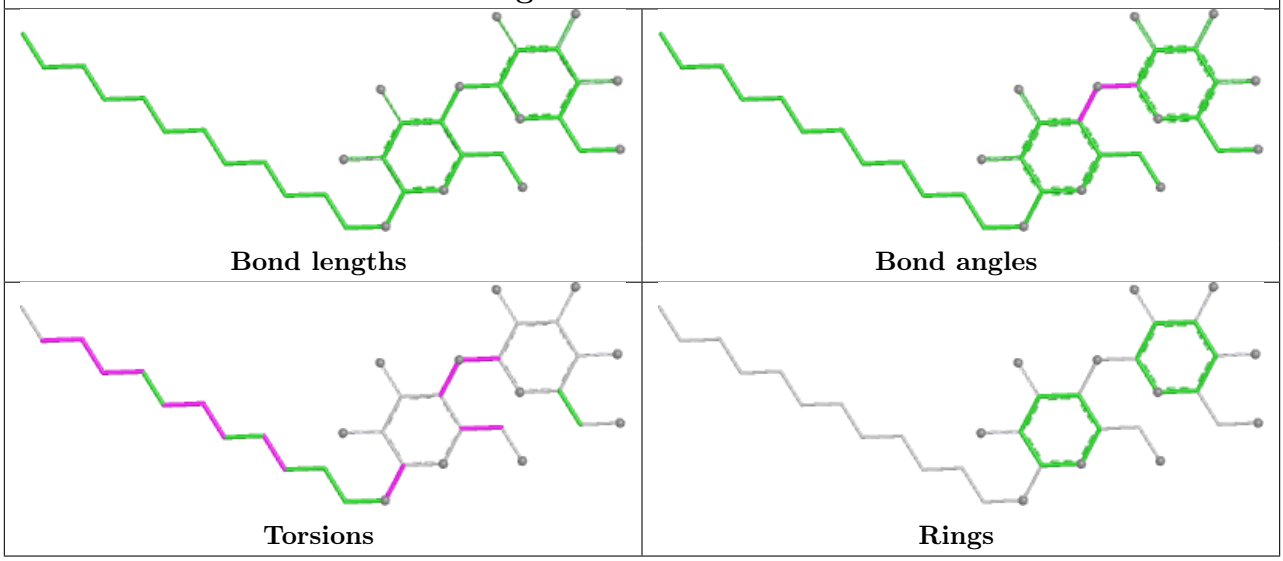
Ligand BCR B 1776



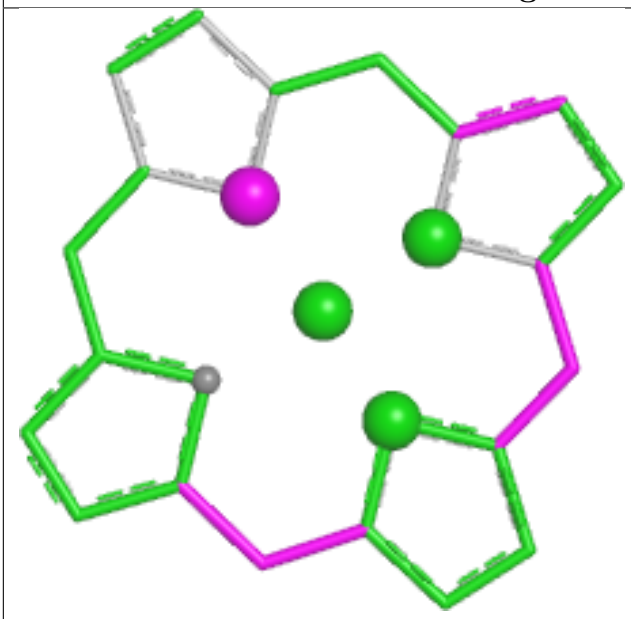
Ligand BCR L 1169



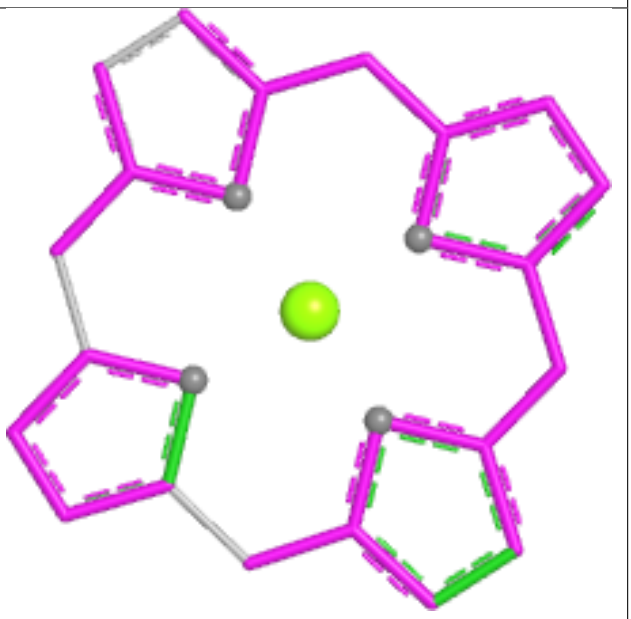
Ligand LMU 1 7004



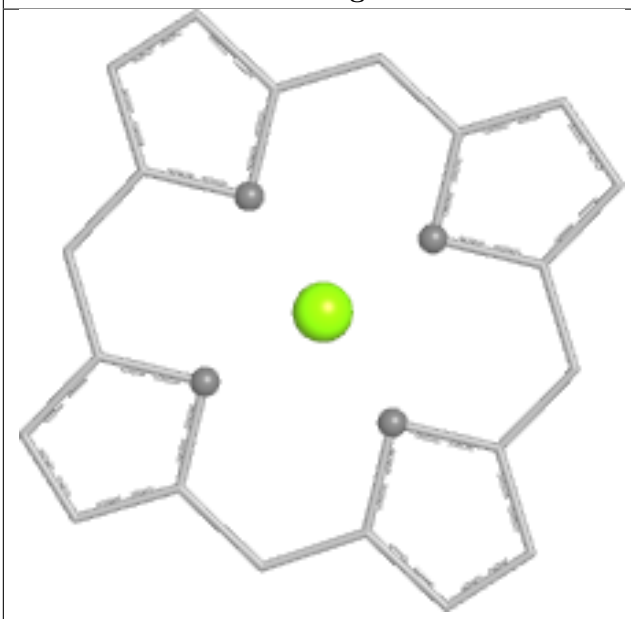
Ligand CLA 4 1206



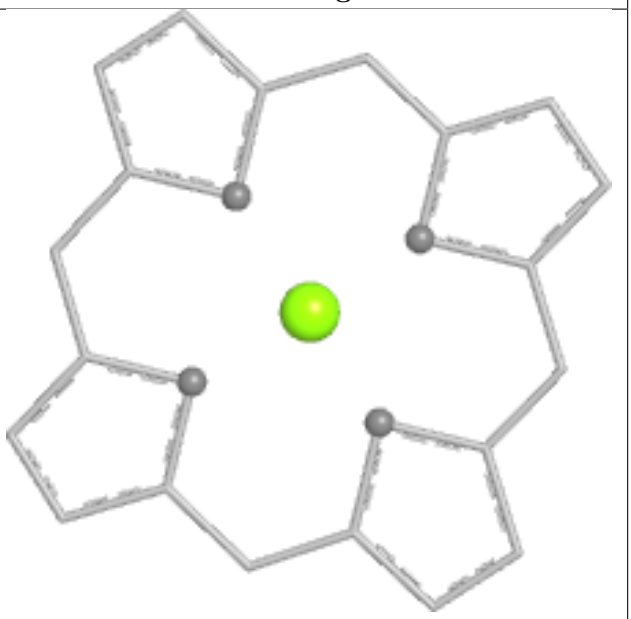
Bond lengths



Bond angles

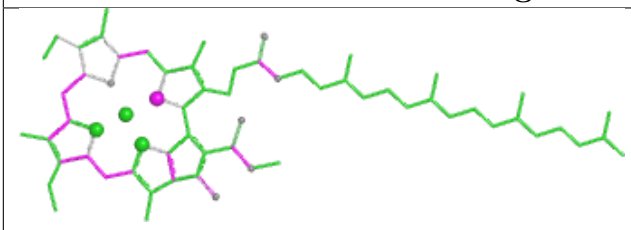


Torsions

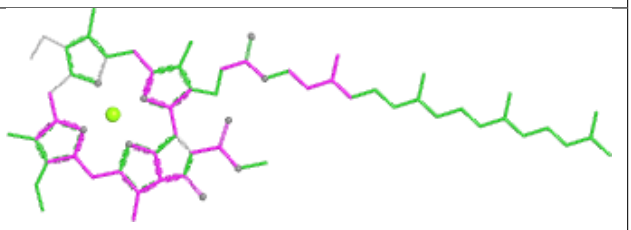


Rings

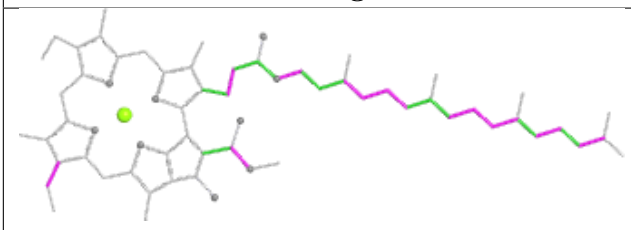
Ligand CLA A 1781



Bond lengths



Bond angles



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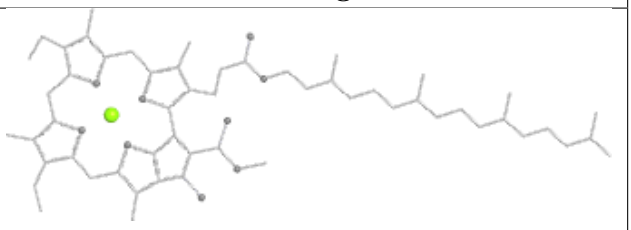
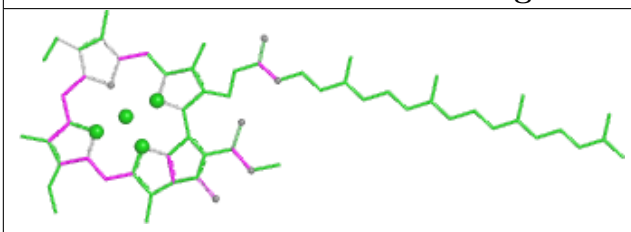
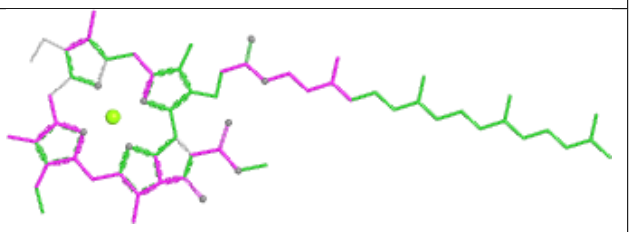


Rings

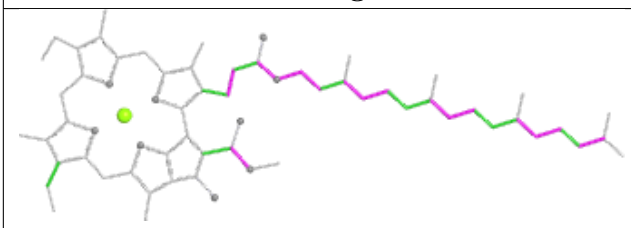
Ligand CLA H 1079



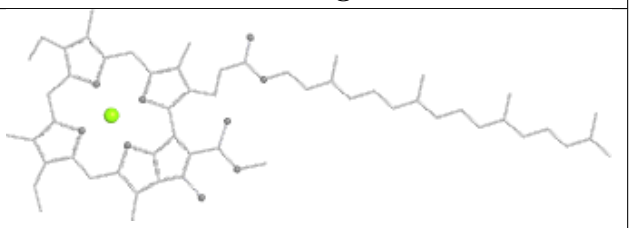
Bond lengths



Bond angles

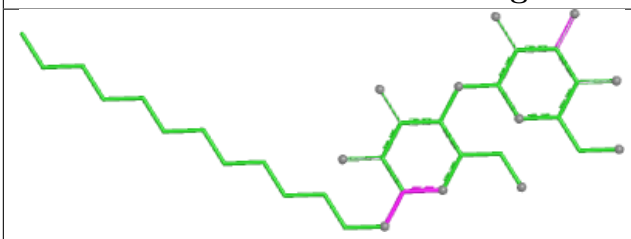


Torsions

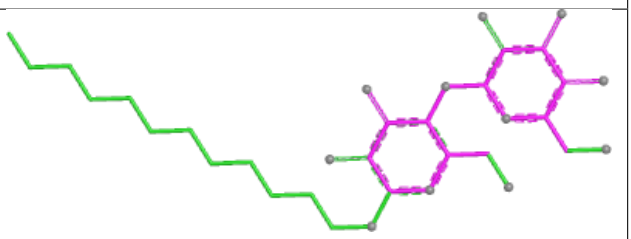


Rings

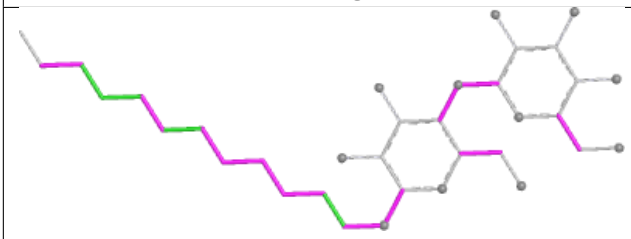
Ligand LMU A 7026



Bond lengths



Bond angles



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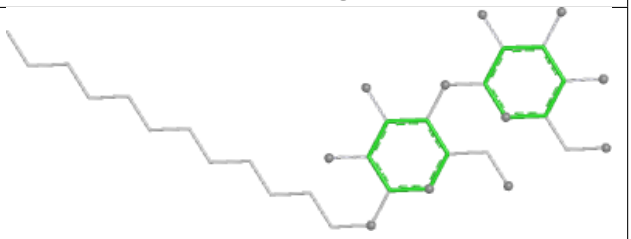
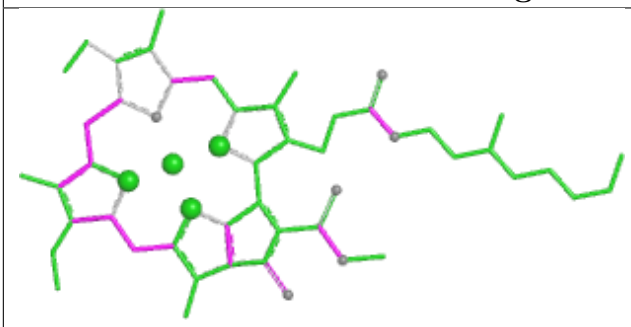
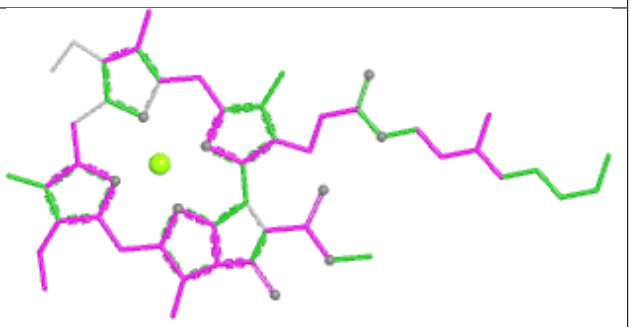
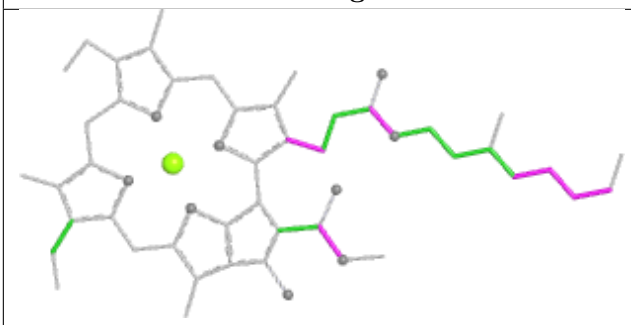
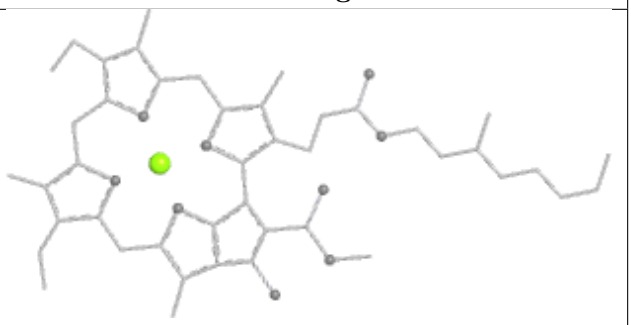
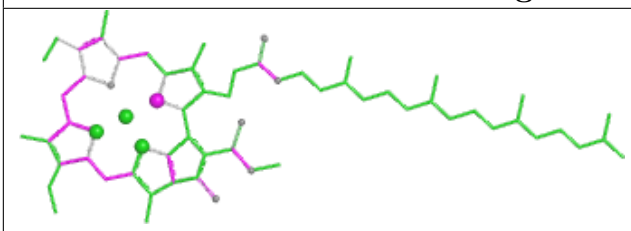
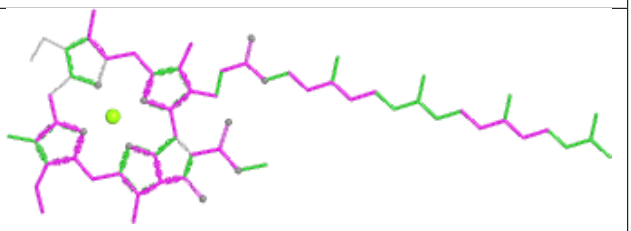
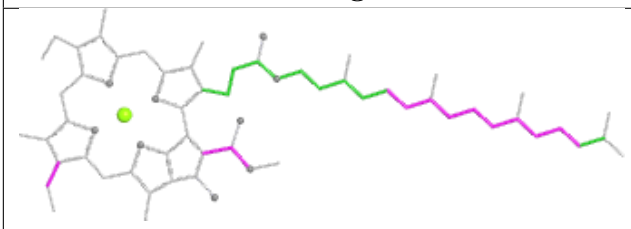
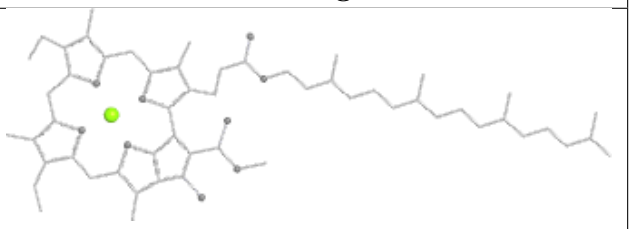
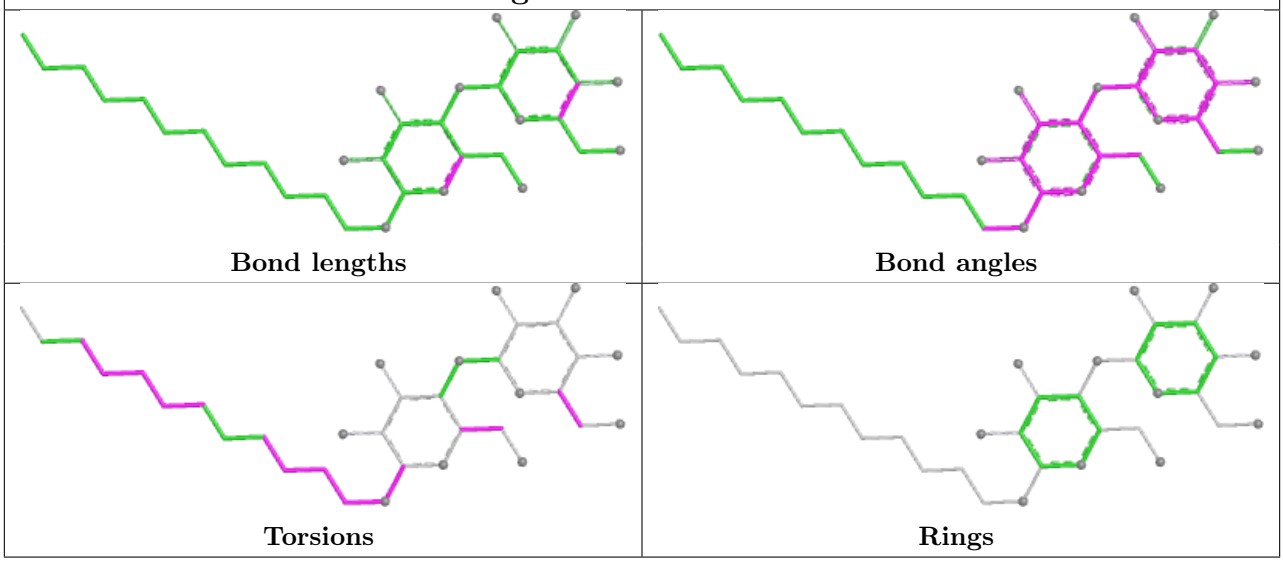


Rings

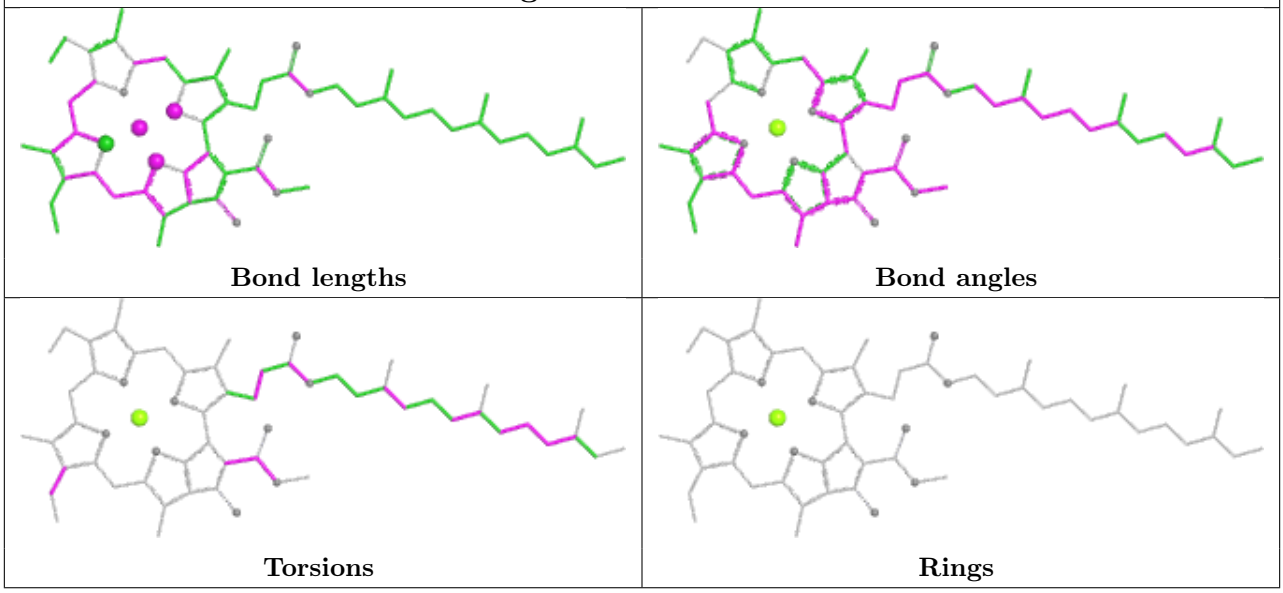
Ligand CLA A 1769	
 Bond lengths	 Bond angles
 Torsions	 Rings

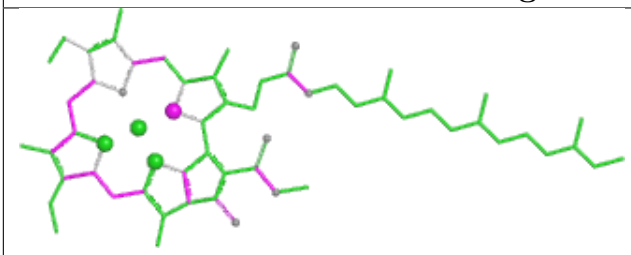
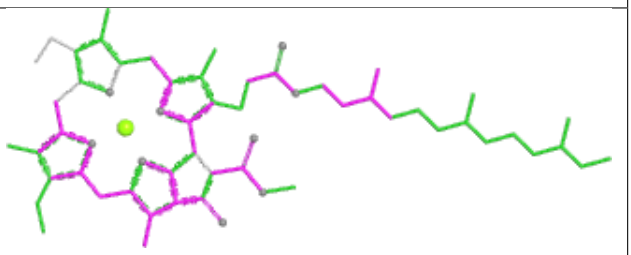
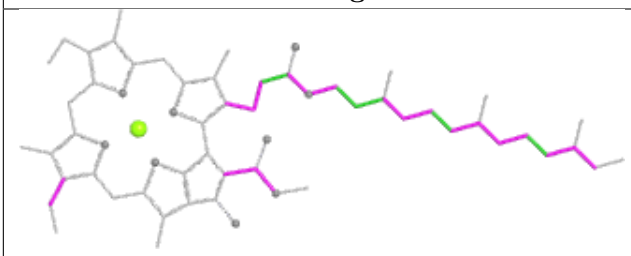
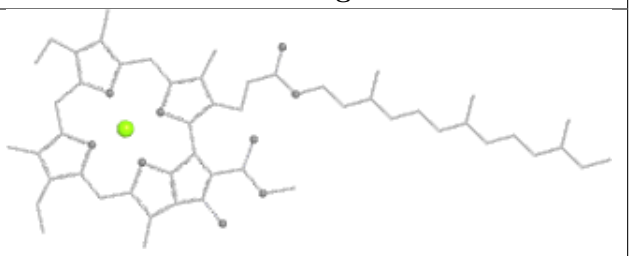
Ligand CLA B 1738	
 Bond lengths	 Bond angles
 Torsions	 Rings

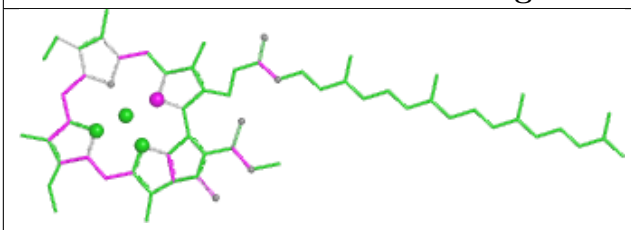
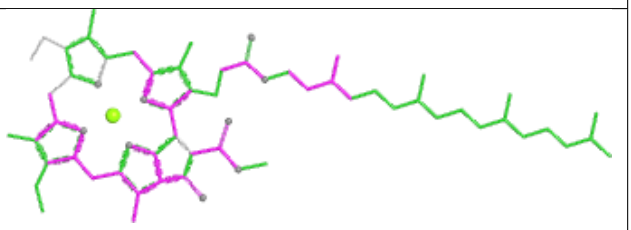
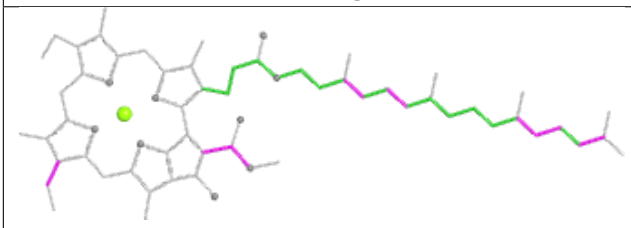
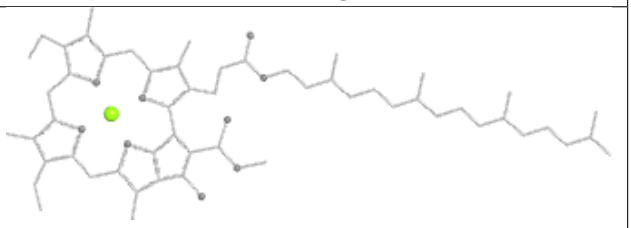
Ligand LMU A 7028



Ligand CLA 1 1198



Ligand CLA J 1043	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1793	
 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	317:TYR	C	318:ARG	N	1.17

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	1	165/241 (68%)	0.82	23 (13%)	2	2	31, 61, 71, 72	0
2	2	176/269 (65%)	0.43	17 (9%)	7	8	33, 52, 64, 68	0
3	3	162/276 (58%)	0.74	20 (12%)	4	3	49, 79, 110, 112	0
4	4	166/251 (66%)	0.60	22 (13%)	3	3	21, 44, 57, 58	0
5	A	730/758 (96%)	0.20	27 (3%)	41	38	20, 20, 20, 20	0
6	B	733/734 (99%)	0.21	11 (1%)	73	72	20, 20, 20, 20	0
7	C	81/81 (100%)	0.72	11 (13%)	3	2	20, 20, 20, 20	0
8	D	138/212 (65%)	0.27	10 (7%)	15	15	20, 20, 20, 20	0
9	E	65/143 (45%)	0.45	7 (10%)	5	5	20, 20, 20, 20	0
10	F	154/231 (66%)	0.17	9 (5%)	23	22	20, 20, 20, 20	0
11	G	95/167 (56%)	0.43	9 (9%)	8	8	20, 20, 20, 20	0
12	H	69/144 (47%)	0.21	3 (4%)	35	34	20, 20, 20, 20	0
13	I	30/40 (75%)	-0.03	0	100	100	20, 20, 20, 20	0
14	J	42/44 (95%)	0.20	1 (2%)	59	56	20, 20, 20, 20	0
15	K	84/131 (64%)	1.36	22 (26%)	0	0	20, 20, 20, 20	0
16	L	161/216 (74%)	0.24	9 (5%)	24	23	20, 20, 20, 20	0
17	N	85/170 (50%)	0.19	3 (3%)	44	42	20, 20, 20, 20	0
18	R	0/53	-	-			-	-
All	All	3136/4161 (75%)	0.35	204 (6%)	18	18	20, 20, 65, 112	0

The worst 5 of 204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	K	16	THR	12.7
6	B	491	ASN	9.6
3	3	42	PRO	8.8

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Mol	Chain	Res	Type	RSRZ
1	1	92	GLY	8.7
2	2	123	PRO	7.6

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)

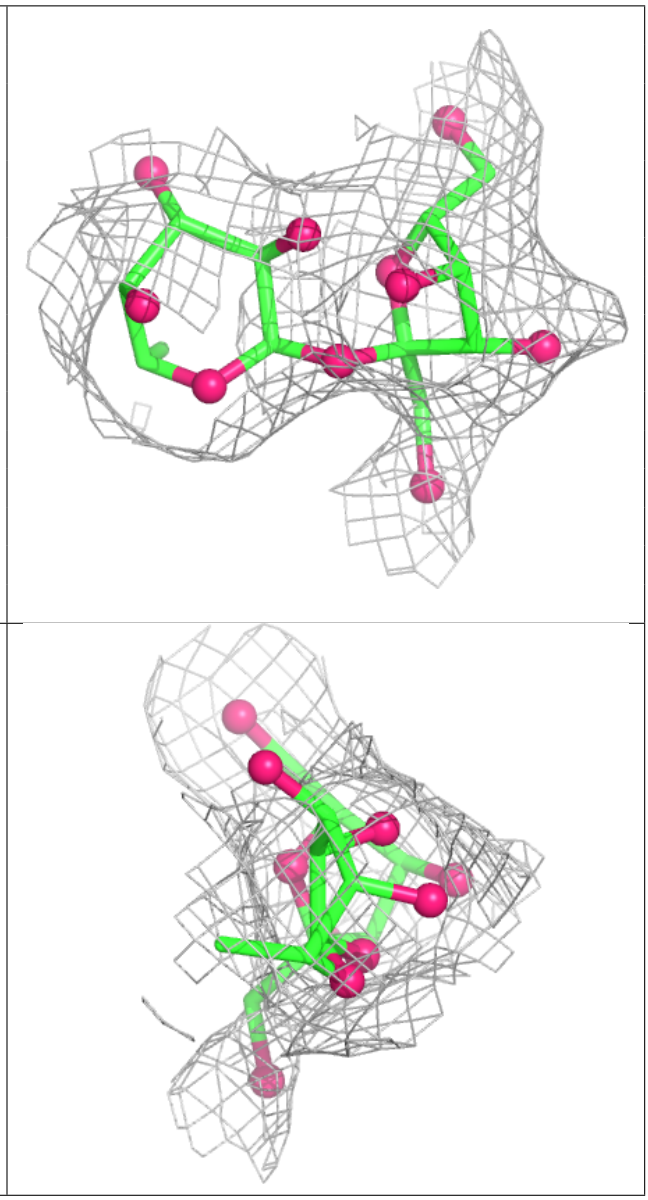
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FRU	S	2	12/12	0.47	0.37	3,43,60,60	0
19	GLC	S	1	11/12	0.67	0.39	4,31,60,60	0
19	FRU	a	2	12/12	0.67	0.31	20,20,20,20	0
19	GLC	Y	1	11/12	0.69	0.38	20,20,20,20	0
19	GLC	P	1	11/12	0.69	0.34	20,20,20,20	0
19	FRU	Q	2	12/12	0.72	0.36	20,20,20,20	0
19	GLC	O	1	11/12	0.73	0.28	20,20,20,20	0
19	GLC	M	1	10/12	0.75	0.22	20,20,20,20	0
19	FRU	Z	2	12/12	0.79	0.30	20,20,20,20	0
19	GLC	V	1	11/12	0.80	0.19	20,20,20,20	0
19	FRU	Y	2	12/12	0.80	0.28	20,20,20,20	0
19	FRU	M	2	12/12	0.81	0.33	20,20,20,20	0
19	GLC	a	1	11/12	0.81	0.29	20,20,20,20	0
19	FRU	P	2	12/12	0.81	0.35	20,20,20,20	0
19	GLC	T	1	11/12	0.82	0.31	20,20,20,20	0
19	FRU	T	2	12/12	0.83	0.18	20,20,20,20	0
19	GLC	Q	1	11/12	0.83	0.55	20,20,20,20	0
19	GLC	Z	1	11/12	0.83	0.30	20,20,20,20	0
19	FRU	W	2	12/12	0.85	0.25	20,20,20,20	0
19	FRU	V	2	12/12	0.86	0.13	20,20,20,20	0
19	FRU	U	2	12/12	0.86	0.26	20,20,20,20	0
19	FRU	X	2	12/12	0.86	0.31	20,20,20,20	0
19	GLC	U	1	11/12	0.88	0.28	20,20,20,20	0
19	GLC	X	1	11/12	0.90	0.23	20,20,20,20	0
19	GLC	W	1	11/12	0.91	0.20	20,20,20,20	0
19	FRU	O	2	12/12	0.92	0.31	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

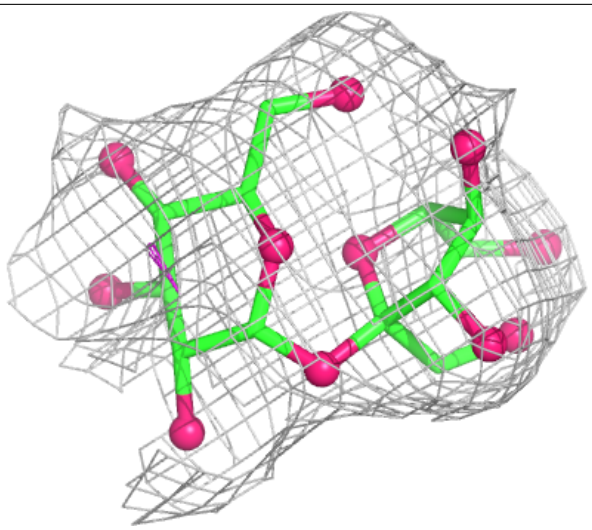
Electron density around Chain M:

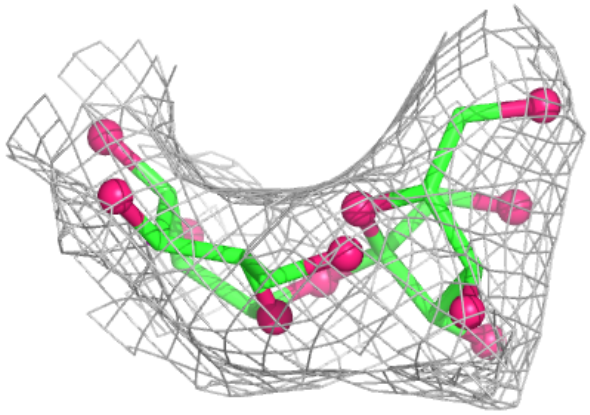
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

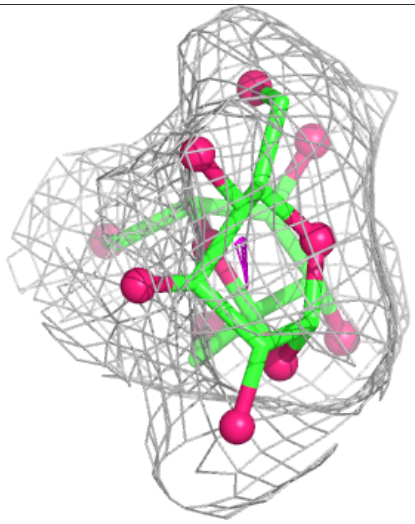


Electron density around Chain O:

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

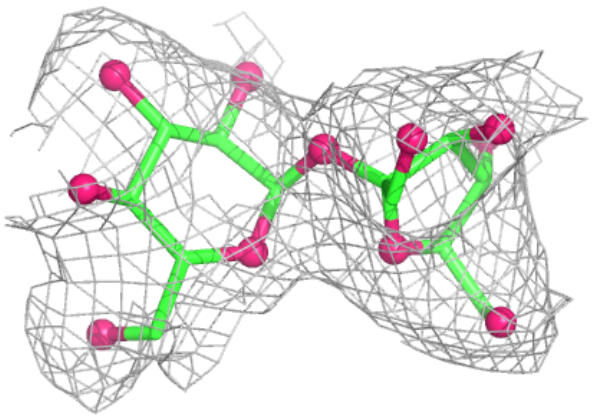


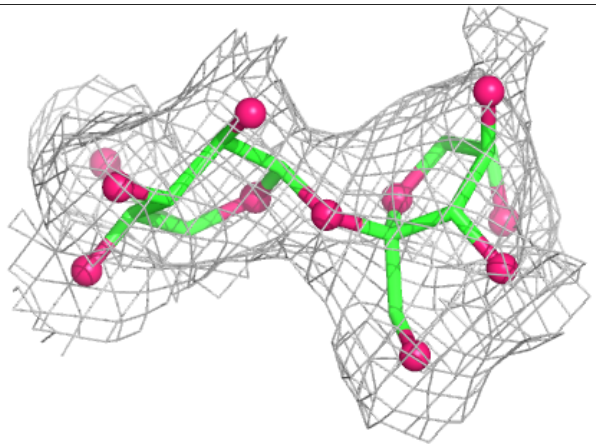


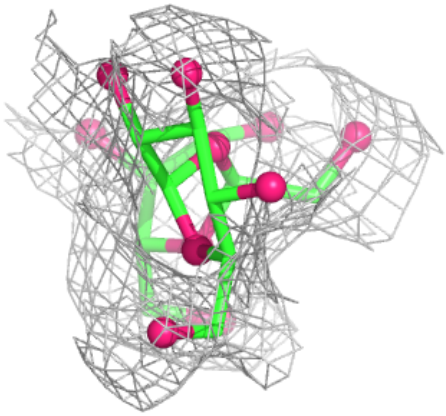


Electron density around Chain P:

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

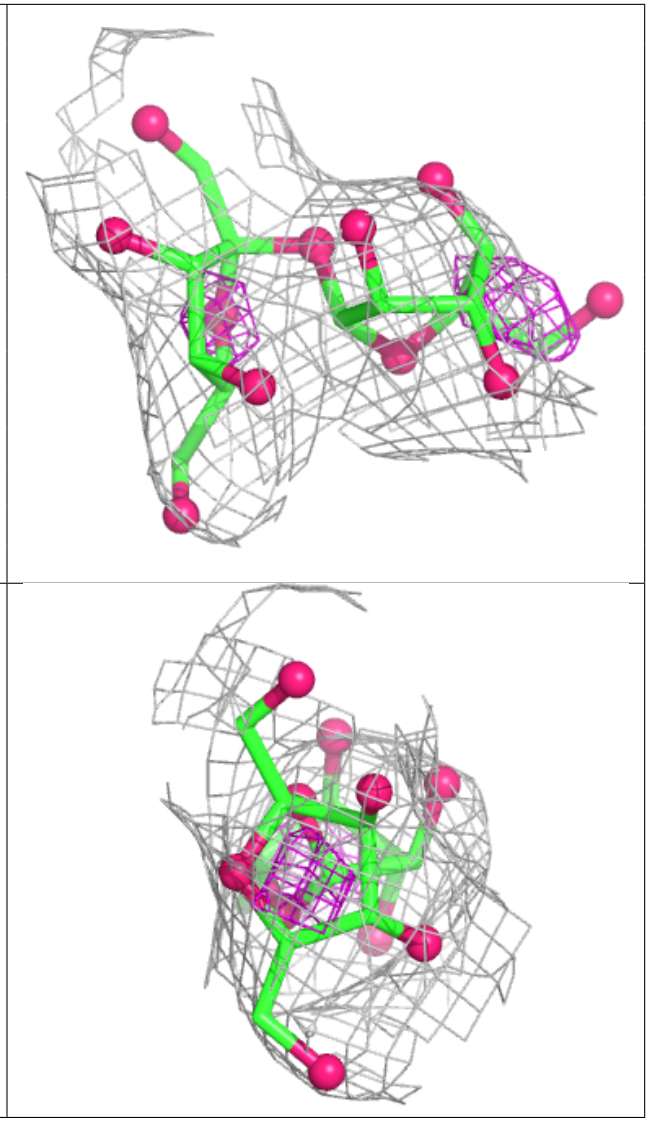






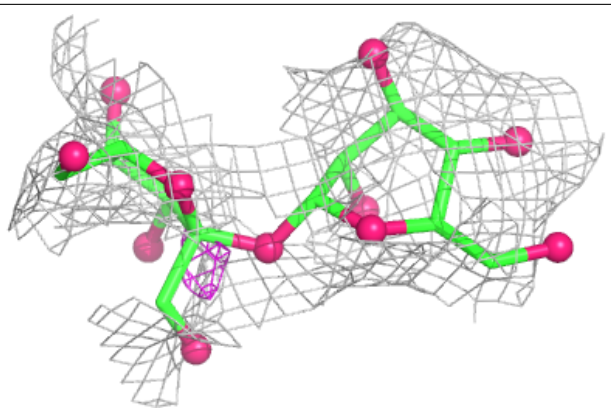
Electron density around Chain Q:

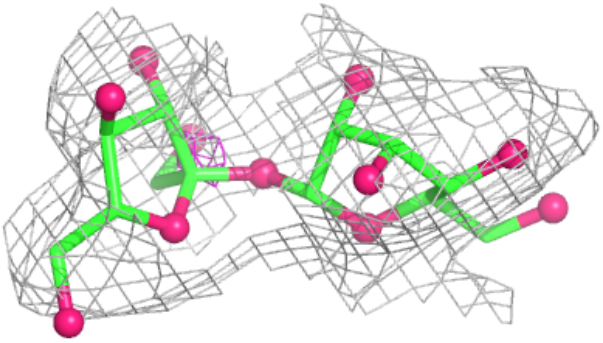
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

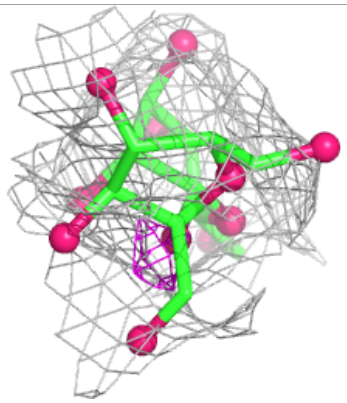


Electron density around Chain S:

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

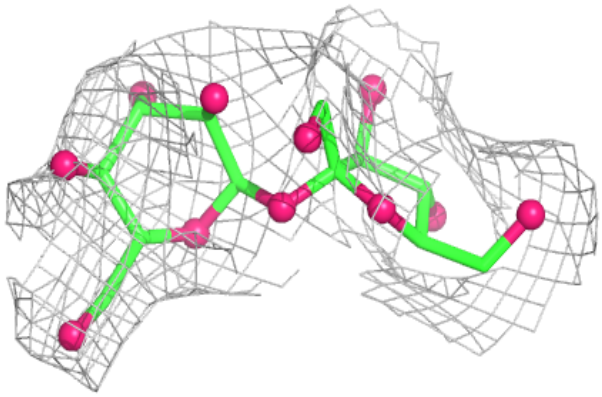


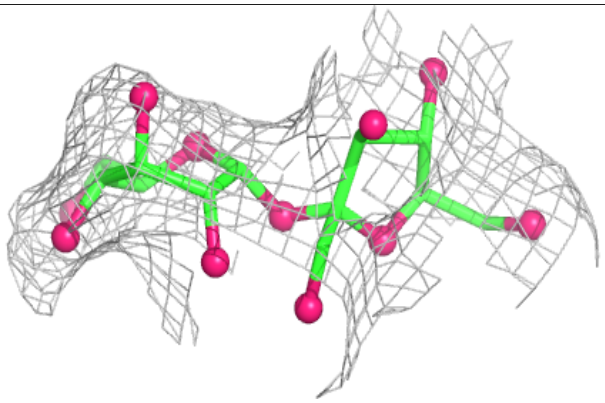


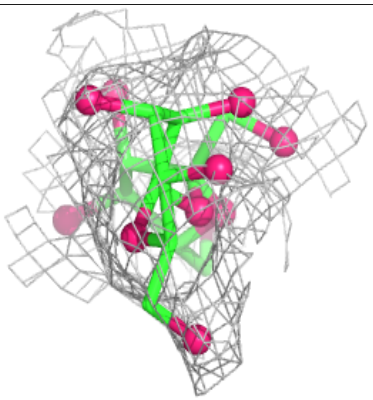


Electron density around Chain T:

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

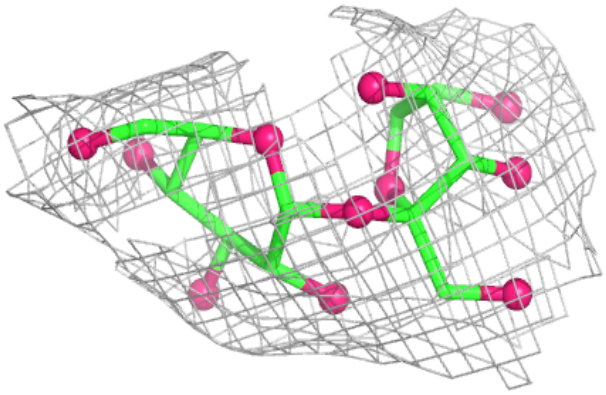


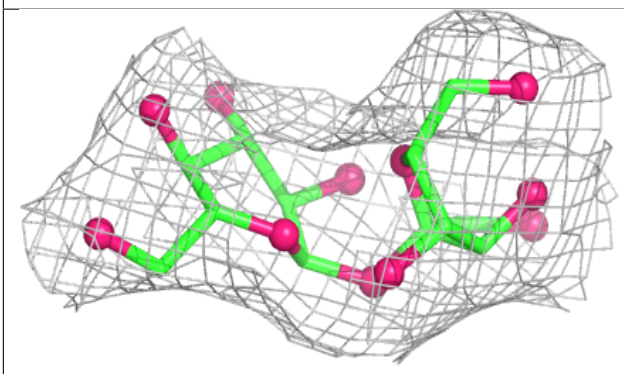


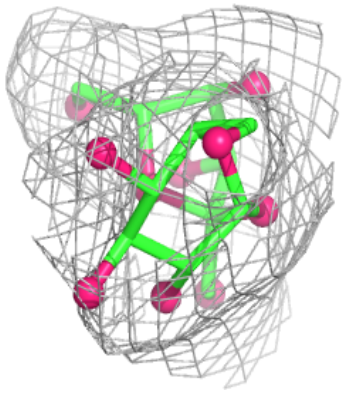


Electron density around Chain U:

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

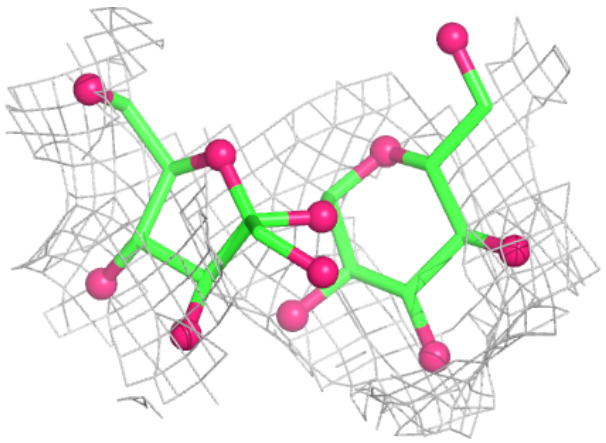


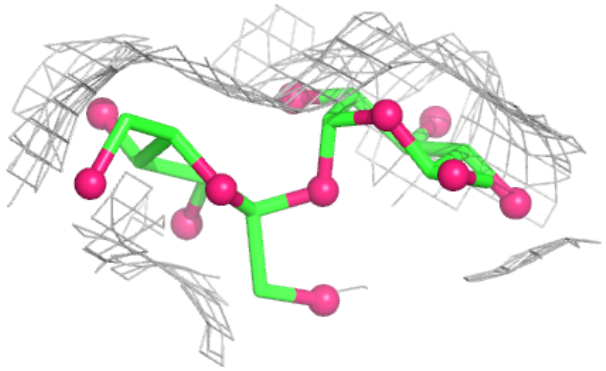


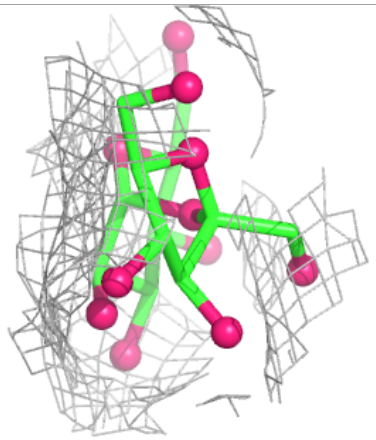


Electron density around Chain V:

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

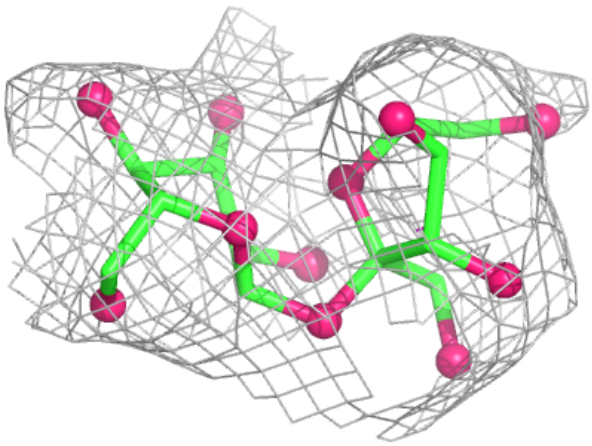


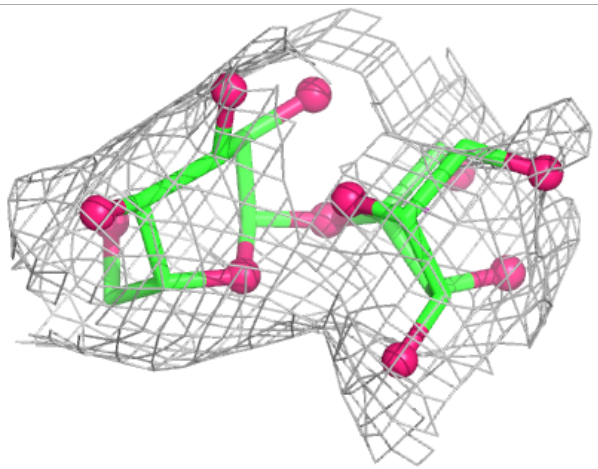


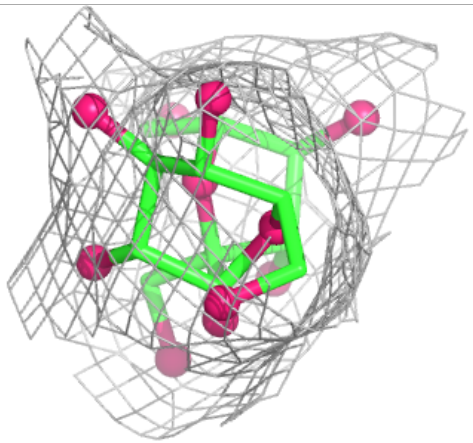


Electron density around Chain W:

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

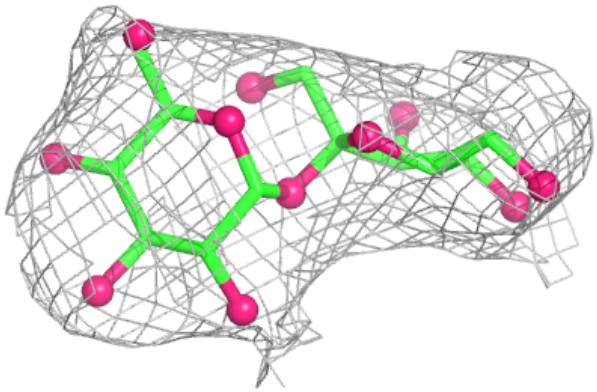


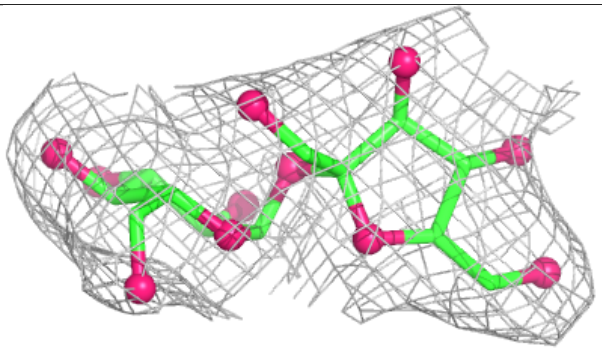


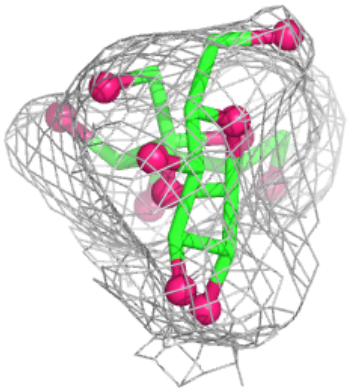


Electron density around Chain X:

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

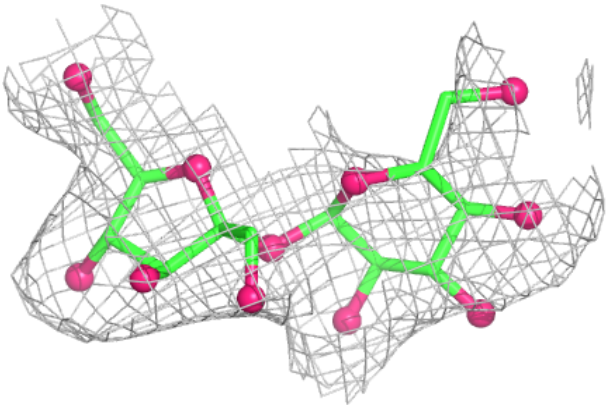


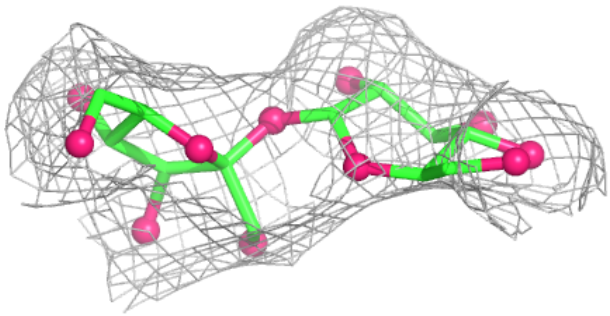


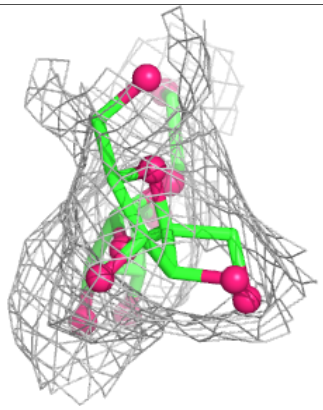


Electron density around Chain Y:

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

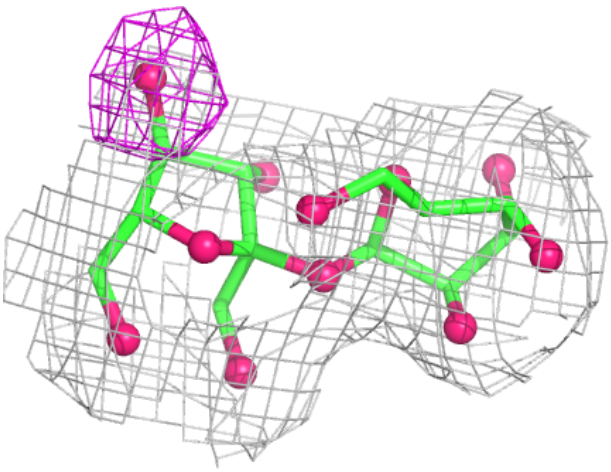


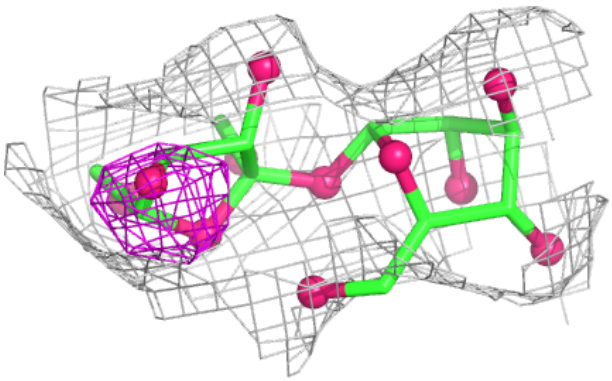


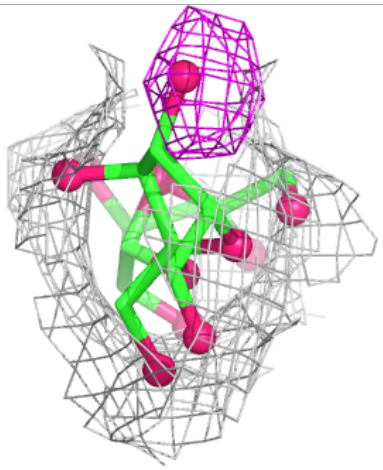


Electron density around Chain Z:

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

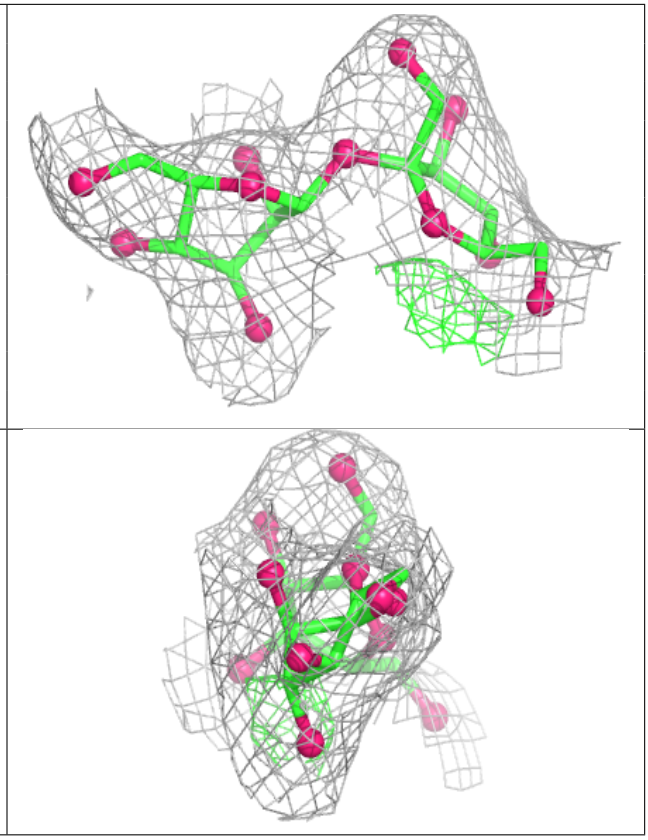






Electron density around Chain a:

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



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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	J	1046	25/65	0.49	0.57	5,42,60,60	0
21	LMU	A	7013	35/35	0.56	0.31	20,20,20,20	0
20	CLA	4	4003	25/65	0.57	0.32	20,20,20,20	0
22	BCR	A	1803	40/40	0.58	0.49	20,20,20,20	0
20	CLA	3	1214	25/65	0.59	0.27	20,20,20,20	0
21	LMU	2	1225	35/35	0.59	0.31	20,20,20,20	0
20	CLA	A	1801	55/65	0.61	0.40	20,20,20,20	0
20	CLA	B	1766	51/65	0.61	0.40	20,20,20,20	0
20	CLA	L	1505	55/65	0.62	0.36	20,20,20,20	0
21	LMU	1	7004	35/35	0.63	0.43	20,20,20,20	0
20	CLA	3	1217	25/65	0.63	0.25	20,20,20,20	0
20	CLA	2	1216	25/65	0.64	0.29	20,20,20,20	0
20	CLA	2	1212	51/65	0.65	0.27	20,20,20,20	0
20	CLA	A	1797	65/65	0.65	0.27	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	3	3014	25/65	0.66	0.50	20,20,20,20	0
20	CLA	J	1044	61/65	0.66	0.33	20,20,20,20	0
20	CLA	3	1219	65/65	0.66	0.46	20,20,20,20	0
21	LMU	A	7015	35/35	0.66	0.40	20,20,20,20	0
21	LMU	A	7038	35/35	0.66	0.37	20,20,20,20	0
21	LMU	A	7041	35/35	0.66	0.23	20,20,20,20	0
20	CLA	B	1746	46/65	0.66	0.40	20,20,20,20	0
21	LMU	A	7037	35/35	0.67	0.24	20,20,20,20	0
20	CLA	B	1765	45/65	0.67	0.40	20,20,20,20	0
20	CLA	B	1755	58/65	0.68	0.41	20,20,20,20	0
20	CLA	2	1227	25/65	0.68	0.57	20,20,20,20	0
20	CLA	K	1142	45/65	0.68	0.27	20,20,20,20	0
21	LMU	R	1057	35/35	0.68	0.38	20,20,20,20	0
20	CLA	A	1799	50/65	0.68	0.41	20,20,20,20	0
20	CLA	2	1220	56/65	0.69	0.27	2,36,60,60	0
20	CLA	4	4007	52/65	0.69	0.36	20,20,20,20	0
20	CLA	4	4014	47/65	0.69	0.32	20,20,20,20	0
20	CLA	4	1200	50/65	0.69	0.44	20,20,20,20	0
20	CLA	4	1202	25/65	0.69	0.34	20,20,20,20	0
20	CLA	I	1033	55/65	0.69	0.28	20,20,20,20	0
21	LMU	A	7009	34/35	0.69	0.33	20,20,20,20	0
22	BCR	A	1808	40/40	0.69	0.38	20,20,20,20	0
21	LMU	A	7025	35/35	0.70	0.24	20,20,20,20	0
21	LMU	A	7030	35/35	0.70	0.35	20,20,20,20	0
20	CLA	A	1775	36/65	0.70	0.29	20,20,20,20	0
20	CLA	2	1218	65/65	0.70	0.28	20,20,20,20	0
21	LMU	3	7005	35/35	0.70	0.32	20,20,20,20	0
20	CLA	1	1198	61/65	0.70	0.28	2,35,60,60	0
20	CLA	1	1200	51/65	0.70	0.37	20,20,20,20	0
20	CLA	G	1099	51/65	0.70	0.35	20,20,20,20	0
20	CLA	1	1197	51/65	0.71	0.53	20,20,20,20	0
21	LMU	A	7031	35/35	0.71	0.27	20,20,20,20	0
20	CLA	A	1815	55/65	0.71	0.27	20,20,20,20	0
20	CLA	A	1770	45/65	0.71	0.39	20,20,20,20	0
20	CLA	3	1218	65/65	0.71	0.29	20,20,20,20	0
21	LMU	A	7043	35/35	0.71	0.19	20,20,20,20	0
20	CLA	1	1187	46/65	0.71	0.27	20,20,20,20	0
22	BCR	3	1220	40/40	0.71	0.25	20,20,20,20	0
20	CLA	K	1146	50/65	0.71	0.31	20,20,20,20	0
20	CLA	1	1194	25/65	0.71	0.25	20,20,20,20	0
21	LMU	A	7021	35/35	0.72	0.26	20,20,20,20	0
20	CLA	2	1215	50/65	0.72	0.27	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	R	1054	57/65	0.72	0.27	20,20,20,20	0
20	CLA	R	1055	65/65	0.72	0.33	20,20,20,20	0
21	LMU	1	1202	35/35	0.72	0.34	20,20,20,20	0
20	CLA	J	1043	61/65	0.72	0.31	20,20,20,20	0
20	CLA	4	1198	65/65	0.72	0.26	20,20,20,20	0
20	CLA	3	1212	36/65	0.72	0.37	20,20,20,20	0
21	LMU	A	7047	35/35	0.72	0.25	20,20,20,20	0
20	CLA	A	1778	42/65	0.72	0.29	20,20,20,20	0
20	CLA	A	1817	46/65	0.72	0.34	20,20,20,20	0
20	CLA	K	3009	65/65	0.72	0.34	20,20,20,20	0
21	LMU	A	7017	35/35	0.72	0.21	20,20,20,20	0
22	BCR	L	1169	40/40	0.72	0.42	20,20,20,20	0
20	CLA	A	1798	55/65	0.73	0.29	20,20,20,20	0
20	CLA	F	1157	53/65	0.73	0.37	20,20,20,20	0
21	LMU	A	7042	35/35	0.73	0.23	20,20,20,20	0
20	CLA	1	1199	25/65	0.73	0.25	20,20,20,20	0
21	LMU	A	7010	35/35	0.73	0.32	20,20,20,20	0
21	LMU	A	7034	35/35	0.74	0.25	20,20,20,20	0
21	LMU	2	7003	35/35	0.74	0.25	20,20,20,20	0
20	CLA	1	1193	51/65	0.74	0.38	20,20,20,20	0
20	CLA	A	1791	45/65	0.74	0.27	20,20,20,20	0
20	CLA	3	3015	25/65	0.74	0.34	20,20,20,20	0
20	CLA	4	1196	55/65	0.74	0.25	20,20,20,20	0
20	CLA	F	1156	41/65	0.74	0.28	20,20,20,20	0
20	CLA	2	1214	25/65	0.74	0.41	20,20,20,20	0
20	CLA	A	1763	46/65	0.74	0.37	20,20,20,20	0
20	CLA	4	1199	55/65	0.74	0.31	20,20,20,20	0
22	BCR	A	1805	40/40	0.74	0.35	20,20,20,20	0
20	CLA	A	1816	55/65	0.74	0.32	20,20,20,20	0
20	CLA	1	1191	36/65	0.74	0.37	20,20,20,20	0
21	LMU	A	7040	35/35	0.75	0.20	20,20,20,20	0
20	CLA	3	1215	25/65	0.75	0.27	20,20,20,20	0
20	CLA	3	3002	25/65	0.75	0.31	20,20,20,20	0
20	CLA	3	3007	42/65	0.75	0.30	20,20,20,20	0
20	CLA	3	1216	25/65	0.75	0.20	20,20,20,20	0
21	LMU	A	7026	35/35	0.75	0.29	20,20,20,20	0
20	CLA	4	1203	25/65	0.75	0.24	20,20,20,20	0
21	LMU	A	1809	35/35	0.75	0.20	20,20,20,20	0
20	CLA	1	1189	47/65	0.75	0.27	20,20,20,20	0
20	CLA	2	1219	25/65	0.75	0.23	20,20,20,20	0
20	CLA	B	1751	46/65	0.75	0.34	20,20,20,20	0
21	LMU	K	1086	35/35	0.76	0.21	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	2	1217	65/65	0.76	0.38	20,20,20,20	0
21	LMU	A	7027	35/35	0.76	0.22	20,20,20,20	0
21	LMU	4	1210	35/35	0.76	0.30	20,20,20,20	0
20	CLA	B	1745	60/65	0.76	0.31	20,20,20,20	0
20	CLA	2	2010	25/65	0.76	0.29	20,20,20,20	0
22	BCR	I	1032	40/40	0.76	0.31	20,20,20,20	0
20	CLA	1	1201	25/65	0.76	0.28	20,20,20,20	0
21	LMU	A	1810	35/35	0.77	0.18	20,20,20,20	0
21	LMU	A	7022	35/35	0.77	0.20	20,20,20,20	0
21	LMU	A	7033	35/35	0.77	0.21	20,20,20,20	0
22	BCR	A	1804	40/40	0.77	0.33	20,20,20,20	0
20	CLA	2	1223	50/65	0.77	0.25	20,20,20,20	0
20	CLA	B	1772	36/65	0.77	0.30	20,20,20,20	0
22	BCR	B	1776	40/40	0.77	0.33	20,20,20,20	0
21	LMU	A	7019	35/35	0.77	0.20	20,20,20,20	0
21	LMU	L	1171	35/35	0.77	0.24	20,20,20,20	0
24	LMG	B	1783	49/55	0.77	0.34	20,20,20,20	0
20	CLA	3	3008	50/65	0.78	0.32	20,20,20,20	0
20	CLA	4	1209	46/65	0.78	0.32	20,20,20,20	0
20	CLA	J	1045	55/65	0.78	0.22	2,33,60,60	0
20	CLA	3	3001	25/65	0.78	0.30	20,20,20,20	0
20	CLA	K	1085	50/65	0.78	0.29	20,20,20,20	0
20	CLA	2	1221	25/65	0.78	0.30	20,20,20,20	0
20	CLA	A	1780	65/65	0.78	0.34	20,20,20,20	0
21	LMU	B	1782	25/35	0.78	0.21	20,20,20,20	0
21	LMU	2	7006	35/35	0.78	0.21	20,20,20,20	0
20	CLA	3	1213	25/65	0.78	0.19	20,20,20,20	0
22	BCR	A	1806	40/40	0.79	0.35	20,20,20,20	0
20	CLA	B	1764	45/65	0.79	0.29	20,20,20,20	0
22	BCR	B	1774	40/40	0.79	0.34	20,20,20,20	0
20	CLA	2	1213	56/65	0.79	0.22	20,20,20,20	0
22	BCR	B	1780	40/40	0.79	0.36	20,20,20,20	0
20	CLA	1	1188	47/65	0.79	0.26	20,20,20,20	0
20	CLA	H	1079	65/65	0.79	0.29	20,20,20,20	0
20	CLA	4	1204	55/65	0.79	0.24	20,20,20,20	0
20	CLA	B	1762	65/65	0.80	0.32	20,20,20,20	0
22	BCR	A	1807	40/40	0.80	0.38	20,20,20,20	0
20	CLA	1	1192	61/65	0.80	0.26	20,20,20,20	0
21	LMU	R	1056	35/35	0.80	0.22	20,20,20,20	0
22	BCR	B	1775	40/40	0.80	0.36	20,20,20,20	0
20	CLA	4	1205	25/65	0.80	0.23	20,20,20,20	0
21	LMU	A	7024	35/35	0.80	0.18	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	A	1771	50/65	0.80	0.29	20,20,20,20	0
21	LMU	A	7036	34/35	0.80	0.28	20,20,20,20	0
20	CLA	A	1781	65/65	0.80	0.30	20,20,20,20	0
26	UNL	B	8057	23/-	0.80	0.17	20,20,20,20	0
21	LMU	A	7035	35/35	0.81	0.26	20,20,20,20	0
20	CLA	A	1766	45/65	0.81	0.26	20,20,20,20	0
20	CLA	4	1208	25/65	0.81	0.18	20,20,20,20	0
20	CLA	1	1190	46/65	0.81	0.23	20,20,20,20	0
21	LMU	A	7039	35/35	0.81	0.19	20,20,20,20	0
20	CLA	1	1196	36/65	0.81	0.25	20,20,20,20	0
20	CLA	L	1166	50/65	0.81	0.27	20,20,20,20	0
20	CLA	L	1168	50/65	0.81	0.23	20,20,20,20	0
20	CLA	4	1197	36/65	0.81	0.25	20,20,20,20	0
20	CLA	3	3011	65/65	0.81	0.26	20,20,20,20	0
21	LMU	A	7028	35/35	0.81	0.18	20,20,20,20	0
20	CLA	2	1224	65/65	0.81	0.22	20,20,20,20	0
20	CLA	A	1787	65/65	0.81	0.28	20,20,20,20	0
20	CLA	B	1736	45/65	0.81	0.27	20,20,20,20	0
21	LMU	A	7016	35/35	0.81	0.24	20,20,20,20	0
21	LMU	A	7020	35/35	0.82	0.22	20,20,20,20	0
20	CLA	A	1777	51/65	0.82	0.40	20,20,20,20	0
20	CLA	A	1774	65/65	0.82	0.32	20,20,20,20	0
21	LMU	A	7032	35/35	0.82	0.33	20,20,20,20	0
21	LMU	A	7023	35/35	0.82	0.24	20,20,20,20	0
20	CLA	B	1756	65/65	0.82	0.32	20,20,20,20	0
20	CLA	B	1742	55/65	0.82	0.26	20,20,20,20	0
20	CLA	A	1773	52/65	0.82	0.25	20,20,20,20	0
20	CLA	A	1776	65/65	0.82	0.31	20,20,20,20	0
20	CLA	B	1744	65/65	0.83	0.30	20,20,20,20	0
20	CLA	A	1772	65/65	0.83	0.23	2,35,60,60	0
20	CLA	1	1195	36/65	0.83	0.28	20,20,20,20	0
20	CLA	B	1750	50/65	0.83	0.26	20,20,20,20	0
20	CLA	A	1768	54/65	0.83	0.23	20,20,20,20	0
20	CLA	A	1785	65/65	0.83	0.31	20,20,20,20	0
20	CLA	A	1769	54/65	0.83	0.27	20,20,20,20	0
20	CLA	A	1760	55/65	0.83	0.29	20,20,20,20	0
22	BCR	B	1779	40/40	0.83	0.32	20,20,20,20	0
20	CLA	B	1763	50/65	0.83	0.28	20,20,20,20	0
20	CLA	B	1735	65/65	0.83	0.30	20,20,20,20	0
20	CLA	A	1792	51/65	0.83	0.28	20,20,20,20	0
20	CLA	B	1741	54/65	0.83	0.30	20,20,20,20	0
20	CLA	4	1201	52/65	0.83	0.21	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	A	1812	65/65	0.84	0.32	20,20,20,20	0
20	CLA	A	1761	65/65	0.84	0.28	20,20,20,20	0
20	CLA	B	1767	60/65	0.84	0.28	20,20,20,20	0
20	CLA	A	1796	65/65	0.84	0.29	20,20,20,20	0
20	CLA	I	1031	60/65	0.84	0.24	20,20,20,20	0
20	CLA	B	1749	61/65	0.85	0.28	20,20,20,20	0
20	CLA	B	1770	65/65	0.85	0.30	20,20,20,20	0
20	CLA	4	1207	36/65	0.85	0.21	20,20,20,20	0
20	CLA	B	1787	65/65	0.85	0.32	20,20,20,20	0
20	CLA	2	1222	50/65	0.85	0.28	20,20,20,20	0
20	CLA	B	1753	65/65	0.85	0.25	20,20,20,20	0
20	CLA	A	1789	65/65	0.85	0.27	20,20,20,20	0
20	CLA	B	1740	65/65	0.85	0.30	20,20,20,20	0
22	BCR	B	1777	40/40	0.85	0.33	20,20,20,20	0
22	BCR	B	1778	40/40	0.85	0.32	20,20,20,20	0
20	CLA	B	1761	50/65	0.85	0.25	20,20,20,20	0
20	CLA	A	1767	65/65	0.85	0.28	20,20,20,20	0
20	CLA	A	1762	57/65	0.85	0.30	20,20,20,20	0
20	CLA	A	1813	65/65	0.85	0.30	20,20,20,20	0
20	CLA	A	1795	51/65	0.85	0.26	20,20,20,20	0
20	CLA	A	1784	55/65	0.85	0.28	20,20,20,20	0
20	CLA	A	1782	65/65	0.86	0.23	20,20,20,20	0
20	CLA	B	1771	65/65	0.86	0.33	20,20,20,20	0
20	CLA	B	1752	55/65	0.86	0.23	20,20,20,20	0
20	CLA	B	1785	65/65	0.86	0.30	20,20,20,20	0
20	CLA	L	1167	47/65	0.86	0.22	20,20,20,20	0
20	CLA	A	1793	65/65	0.86	0.28	20,20,20,20	0
20	CLA	A	1790	50/65	0.86	0.23	20,20,20,20	0
20	CLA	A	1800	65/65	0.86	0.27	20,20,20,20	0
20	CLA	A	1765	55/65	0.86	0.26	20,20,20,20	0
20	CLA	B	1759	65/65	0.87	0.32	20,20,20,20	0
20	CLA	B	1747	59/65	0.87	0.25	20,20,20,20	0
23	PQN	A	1802	33/33	0.87	0.31	20,20,20,20	0
20	CLA	B	1769	47/65	0.87	0.29	20,20,20,20	0
22	BCR	B	1781	40/40	0.87	0.27	20,20,20,20	0
20	CLA	A	1786	50/65	0.88	0.21	20,20,20,20	0
20	CLA	B	1748	60/65	0.88	0.30	20,20,20,20	0
20	CLA	A	1759	50/65	0.88	0.26	20,20,20,20	0
20	CLA	A	1788	65/65	0.88	0.27	20,20,20,20	0
22	BCR	L	1170	40/40	0.88	0.27	20,20,20,20	0
20	CLA	4	1206	25/65	0.88	0.17	20,20,20,20	0
20	CLA	F	1155	36/65	0.88	0.20	20,20,20,20	0

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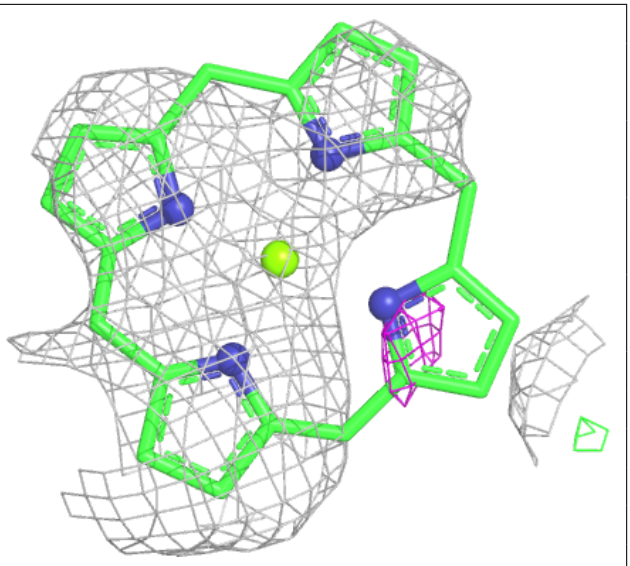
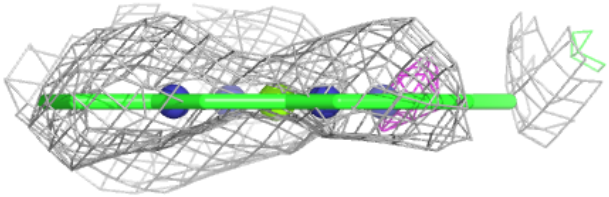
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	A	1794	47/65	0.88	0.27	20,20,20,20	0
20	CLA	B	1737	65/65	0.89	0.25	20,20,20,20	0
20	CLA	A	1764	65/65	0.89	0.33	20,20,20,20	0
20	CLA	B	1757	65/65	0.89	0.29	20,20,20,20	0
20	CLA	B	1758	65/65	0.89	0.30	20,20,20,20	0
20	CLA	A	1811	65/65	0.89	0.30	20,20,20,20	0
20	CLA	B	1768	65/65	0.89	0.26	20,20,20,20	0
20	CLA	B	1760	50/65	0.89	0.24	20,20,20,20	0
20	CLA	A	1779	55/65	0.89	0.23	20,20,20,20	0
20	CLA	B	1743	65/65	0.89	0.23	20,20,20,20	0
20	CLA	B	1738	65/65	0.90	0.27	20,20,20,20	0
23	PQN	B	1773	33/33	0.90	0.29	20,20,20,20	0
20	CLA	B	1786	65/65	0.90	0.27	20,20,20,20	0
20	CLA	B	1739	65/65	0.90	0.28	20,20,20,20	0
20	CLA	B	1754	54/65	0.91	0.23	20,20,20,20	0
20	CLA	A	1783	65/65	0.91	0.30	20,20,20,20	0
25	SF4	C	1082	8/8	0.97	0.09	20,20,20,20	0
25	SF4	C	1083	8/8	0.98	0.06	20,20,20,20	0
25	SF4	B	1784	8/8	0.99	0.06	20,20,20,20	0

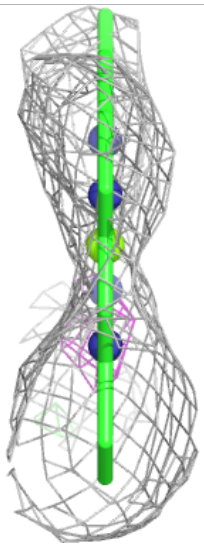
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA J 1046:

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

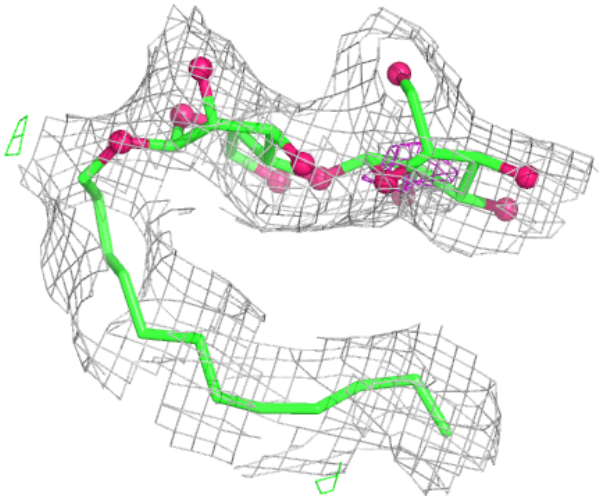


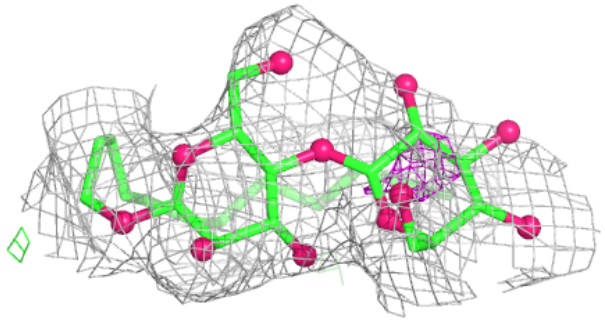


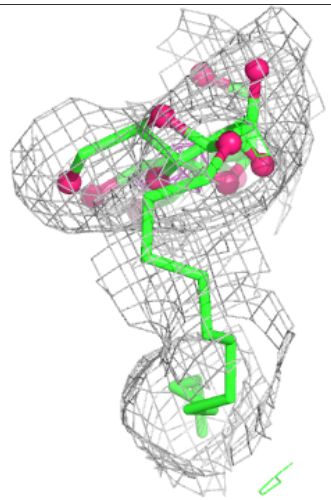


Electron density around LMU A 7013:

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

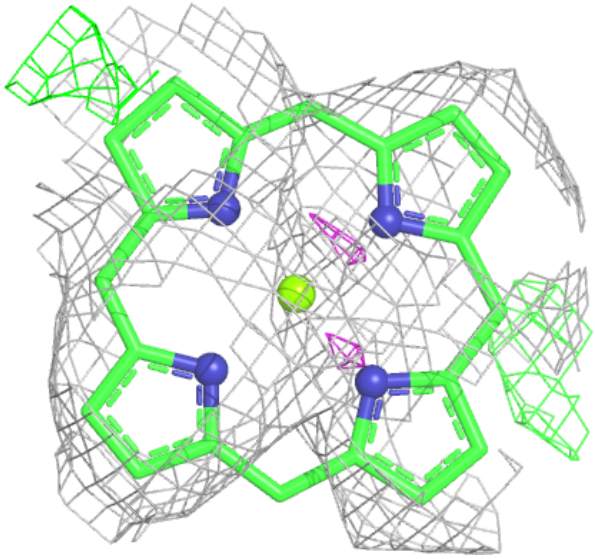


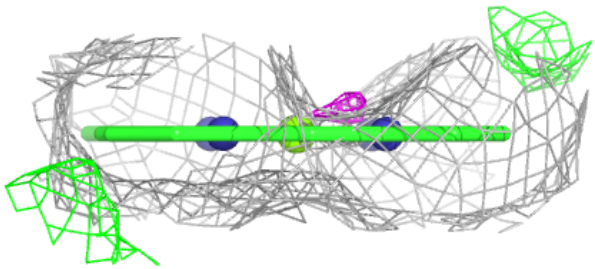


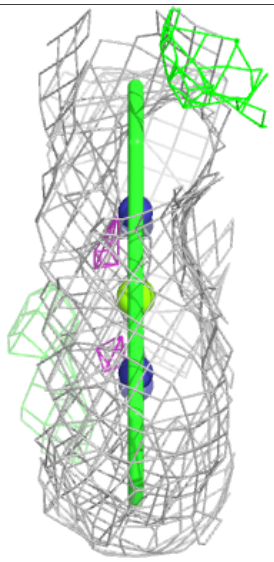


Electron density around CLA 4 4003:

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

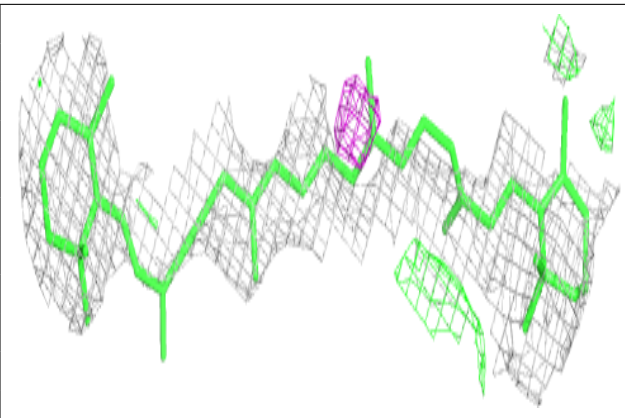


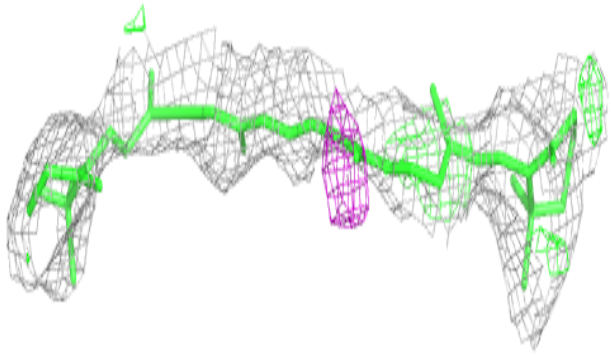


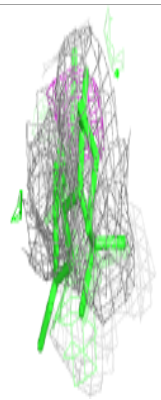


Electron density around BCR A 1803:

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

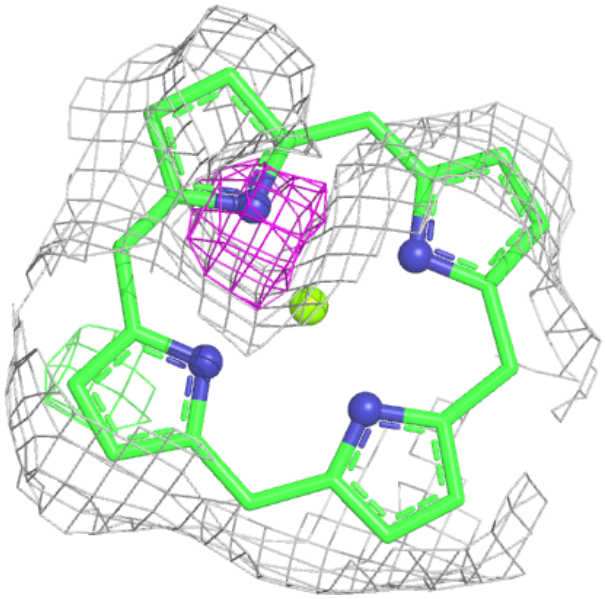


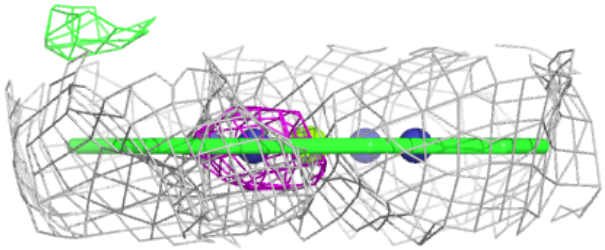


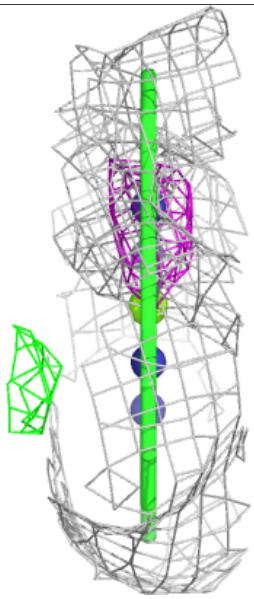


Electron density around CLA 3 1214:

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

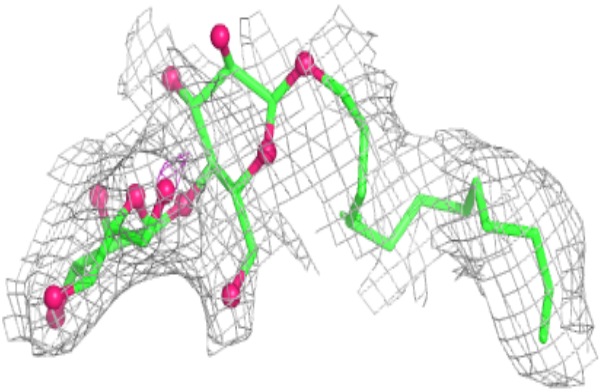


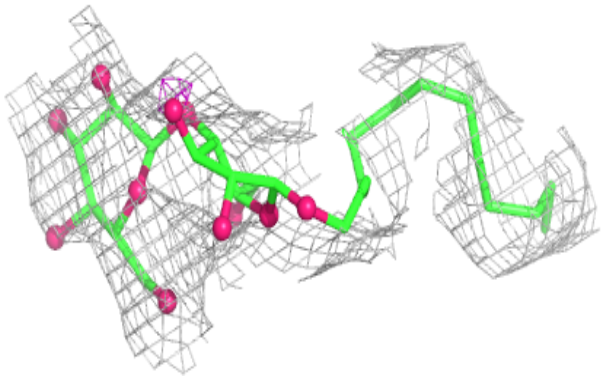


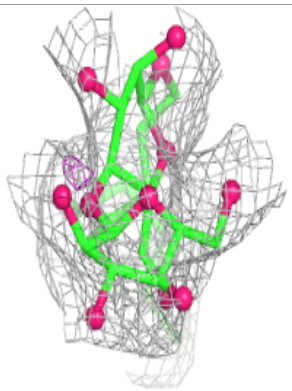


Electron density around LMU 2 1225:

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

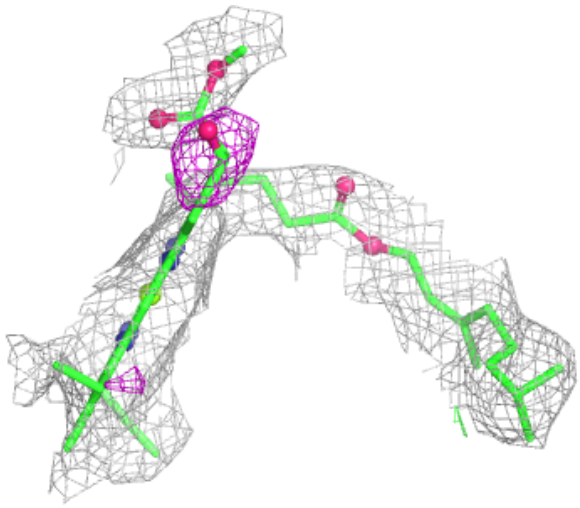


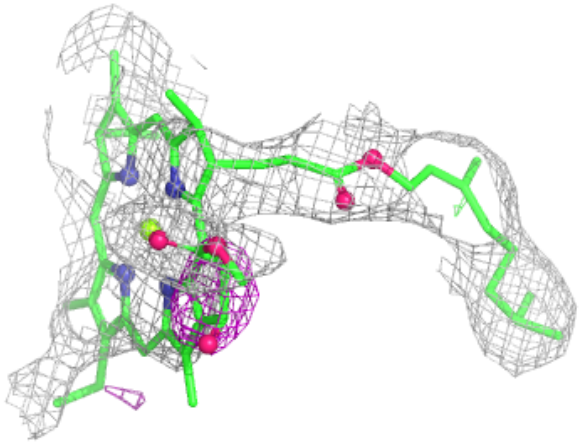


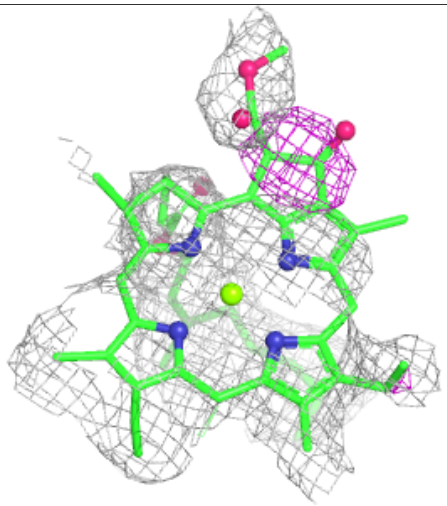


Electron density around CLA A 1801:

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

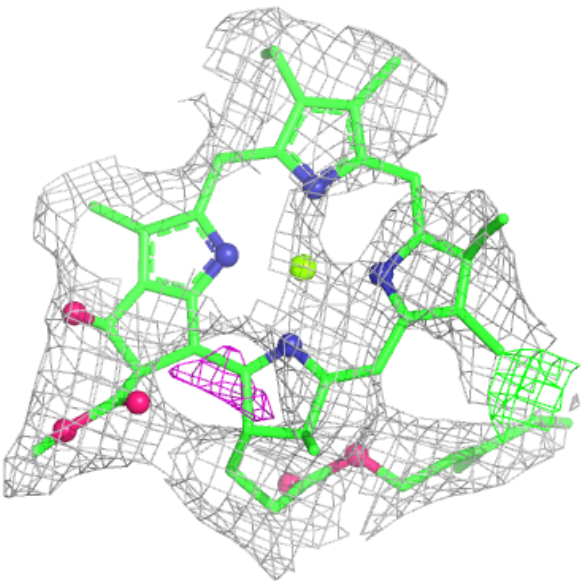


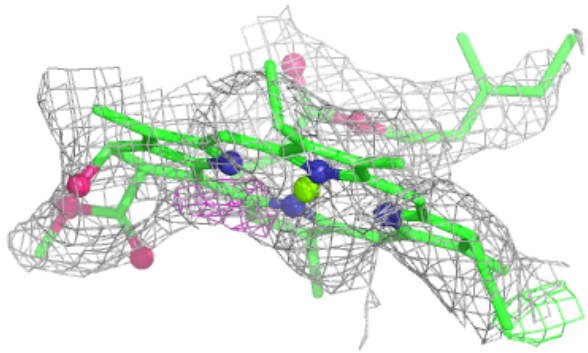


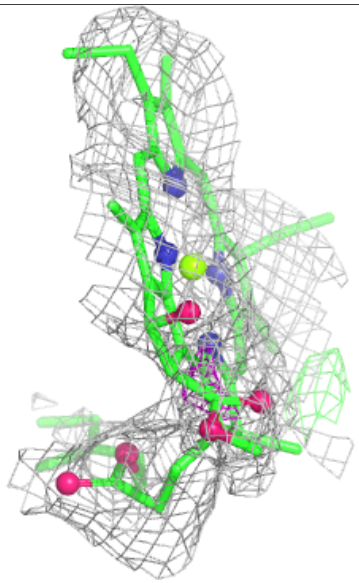


Electron density around CLA B 1766:

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

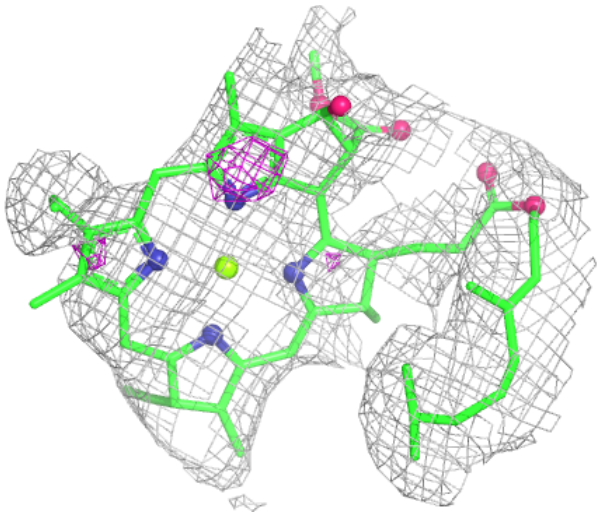


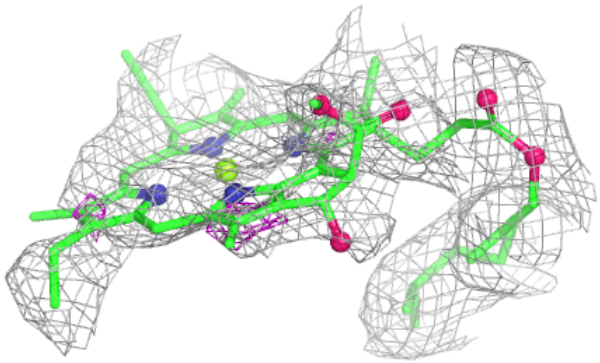


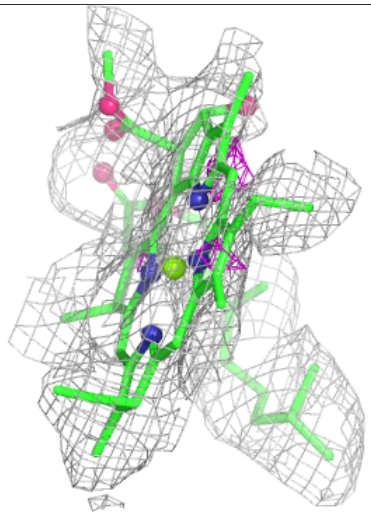


Electron density around CLA L 1505:

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

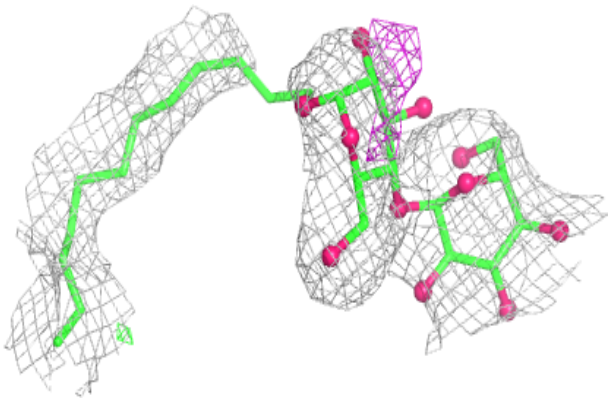


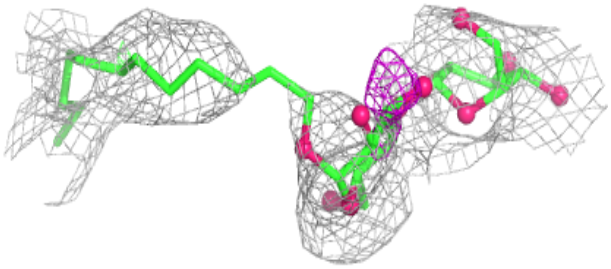


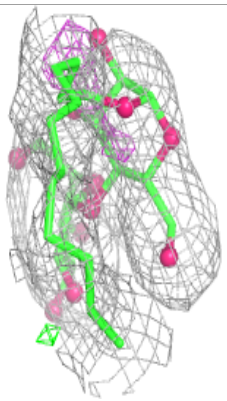


Electron density around LMU 1 7004:

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

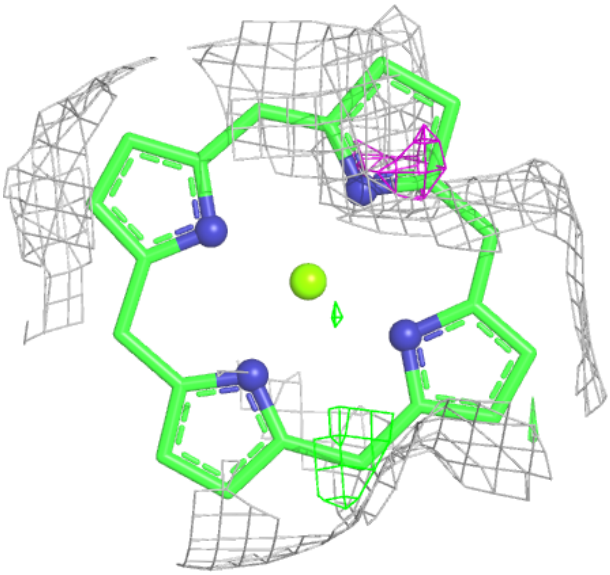


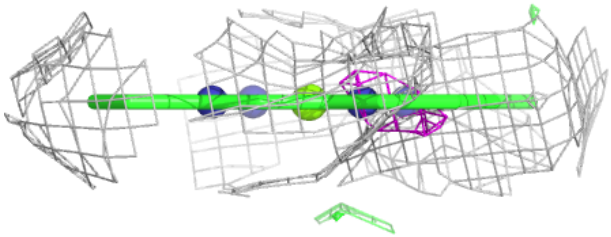


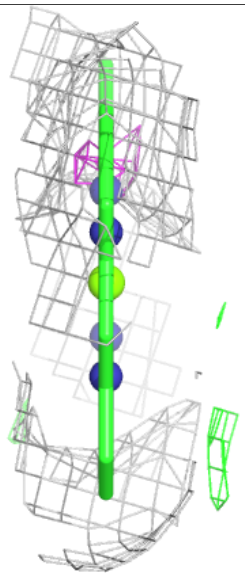


Electron density around CLA 3 1217:

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

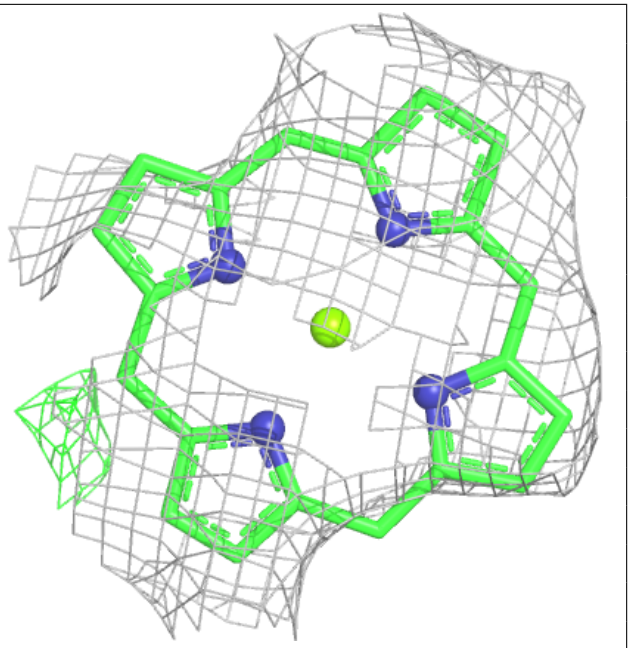


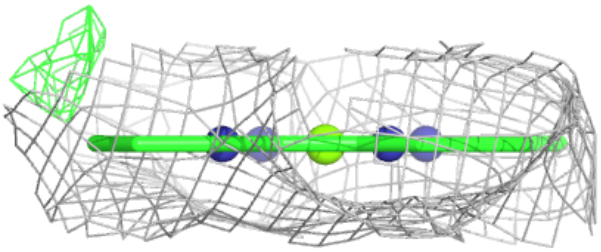


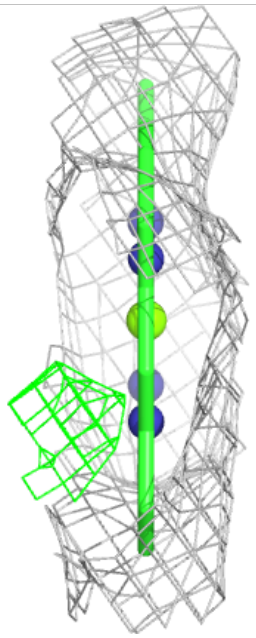


Electron density around CLA 2 1216:

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

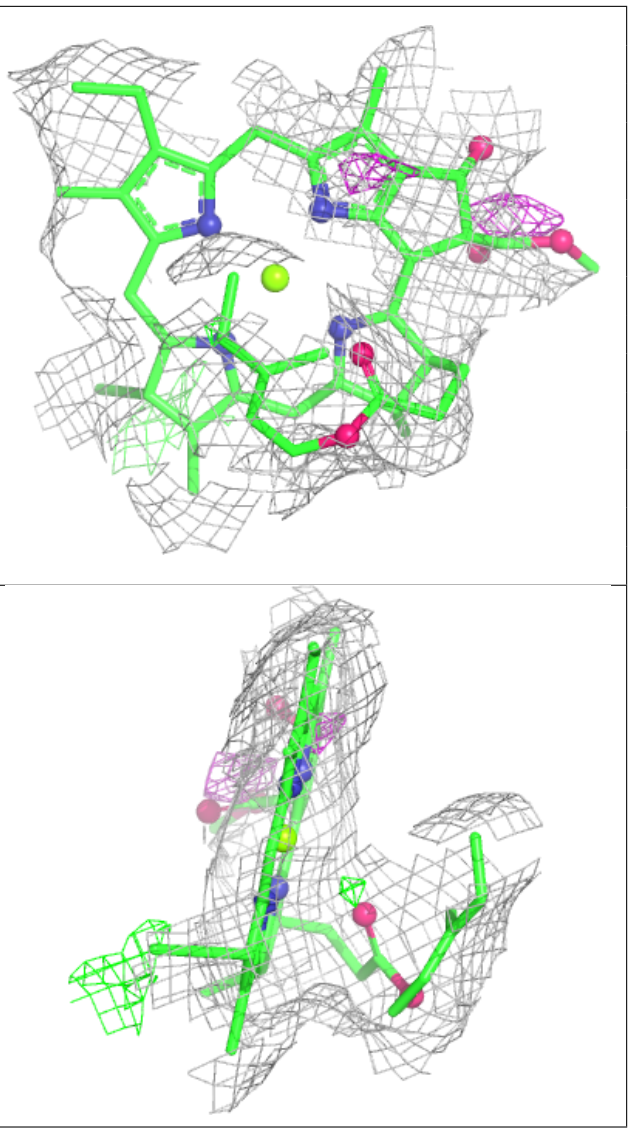






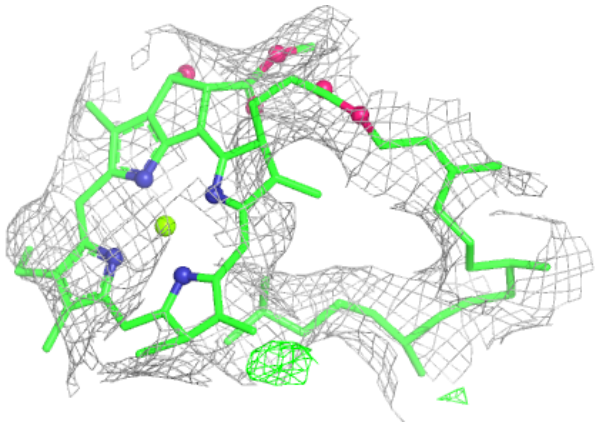
Electron density around CLA 2 1212:

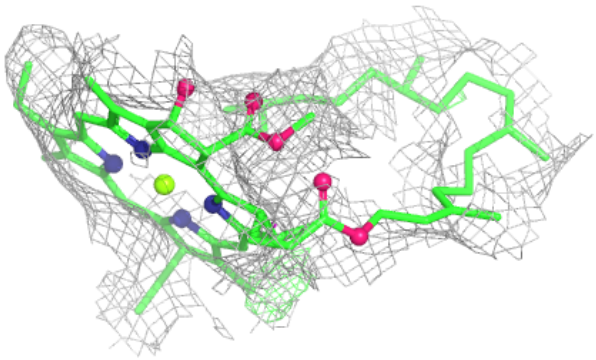
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

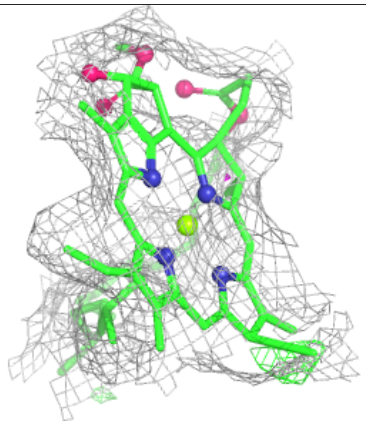


Electron density around CLA A 1797:

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

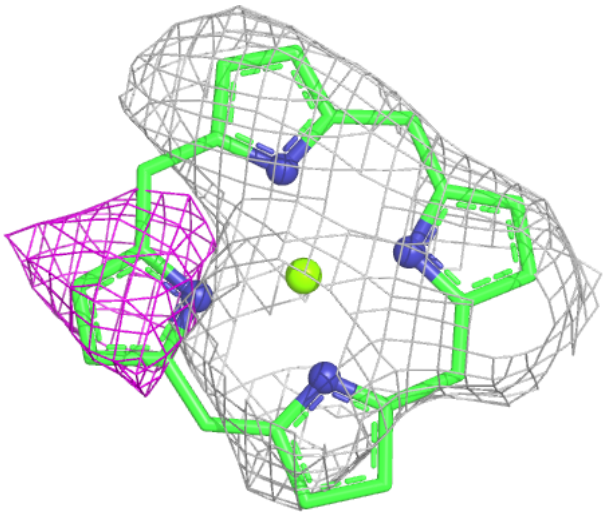


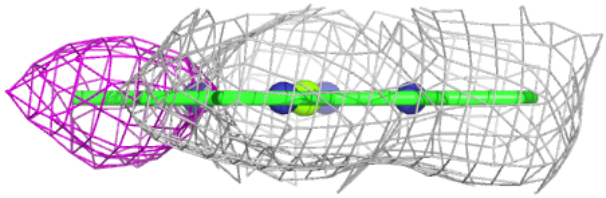


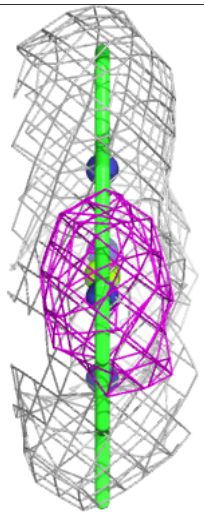


Electron density around CLA 3 3014:

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

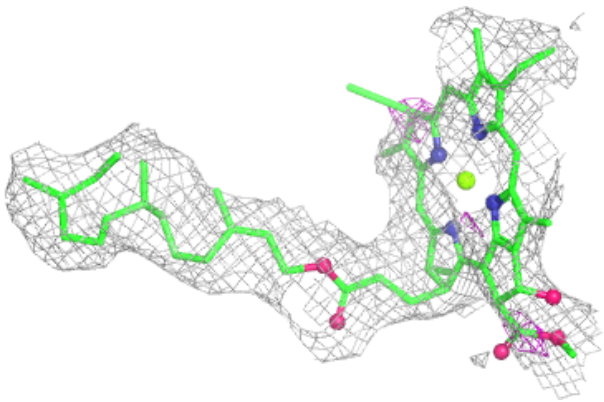


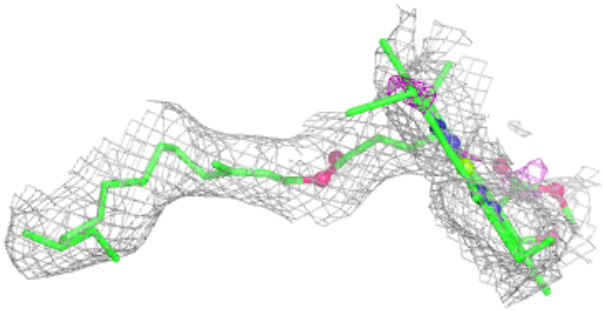


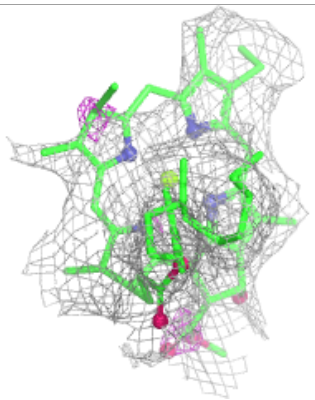


Electron density around CLA J 1044:

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

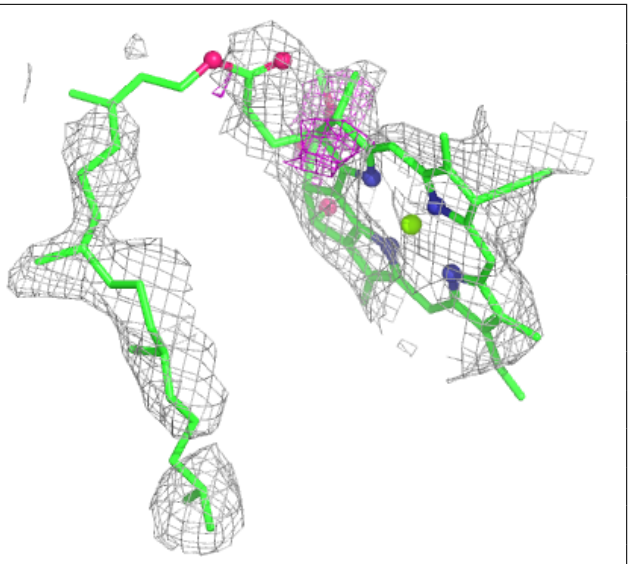


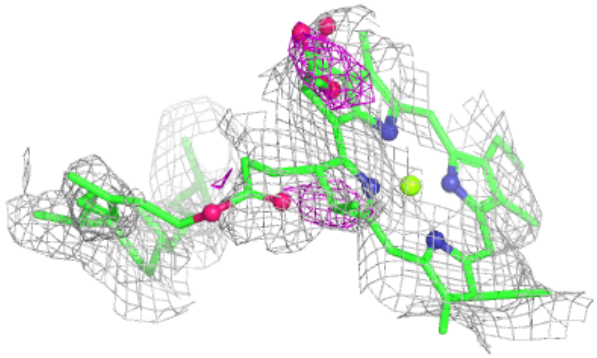


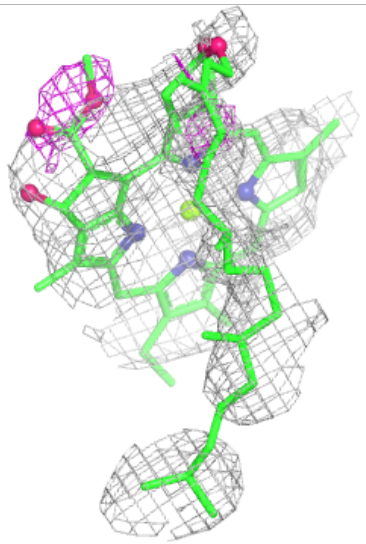


Electron density around CLA 3 1219:

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

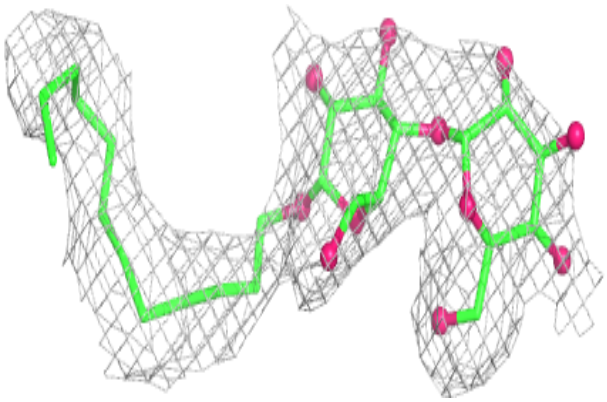


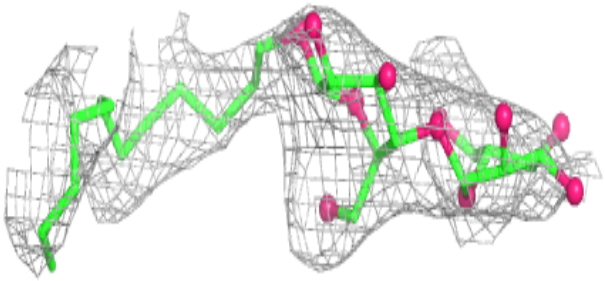


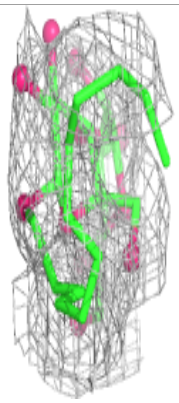


Electron density around LMU A 7015:

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

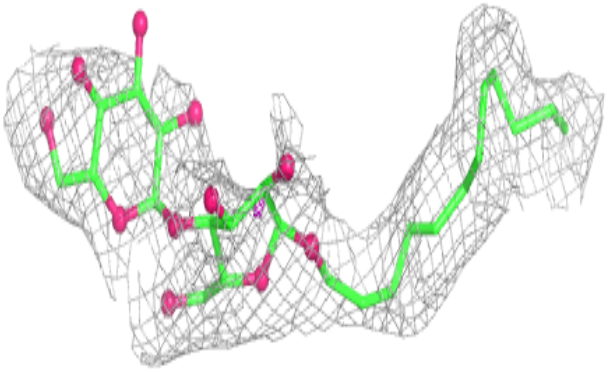


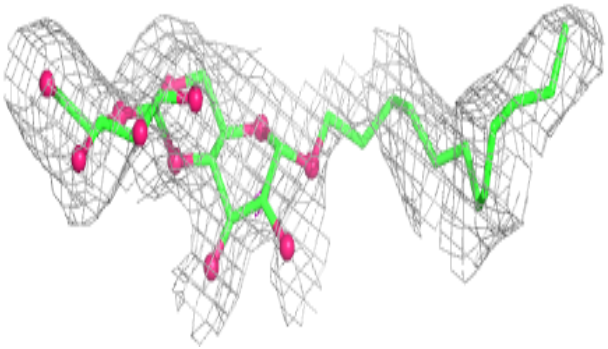


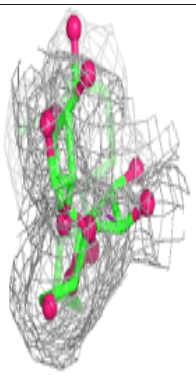


Electron density around LMU A 7038:

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

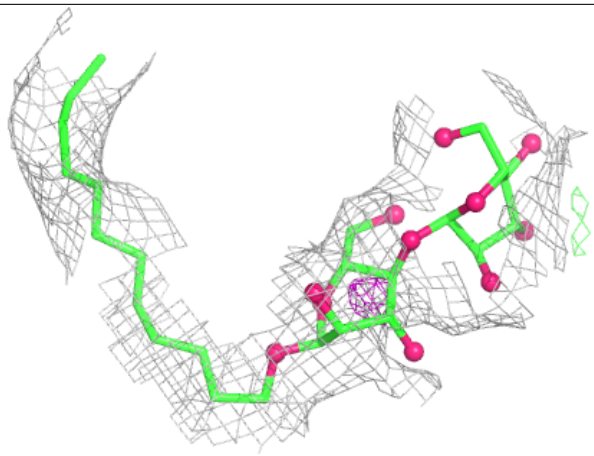


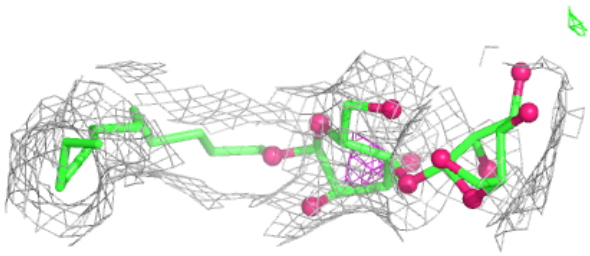


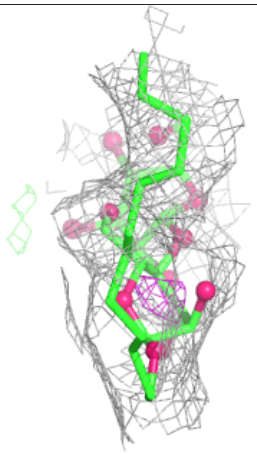


Electron density around LMU A 7041:

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

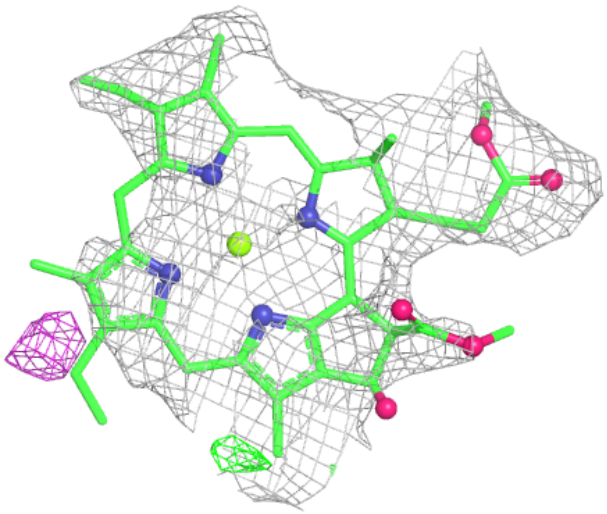


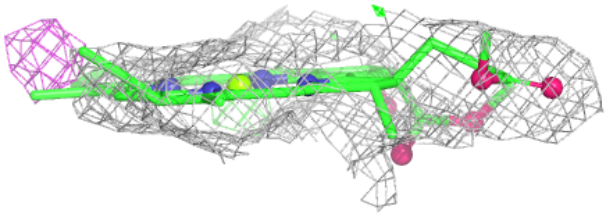


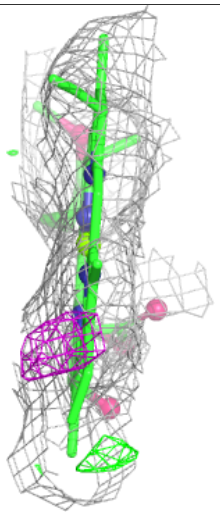


Electron density around CLA B 1746:

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

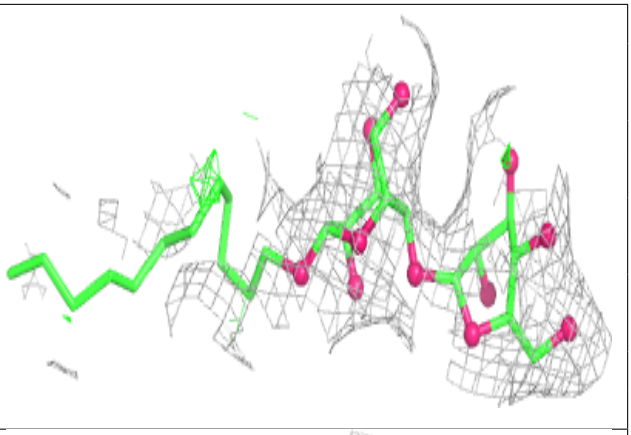


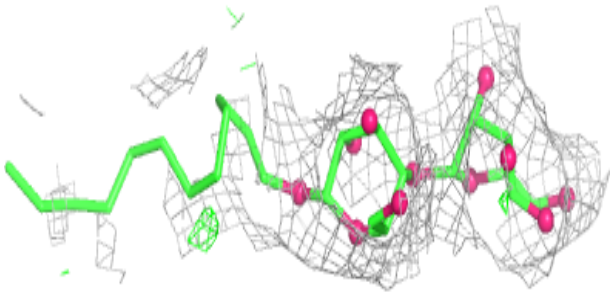


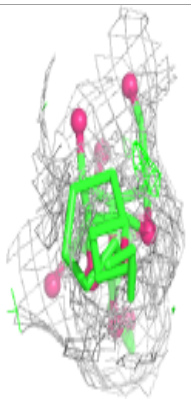


Electron density around LMU A 7037:

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

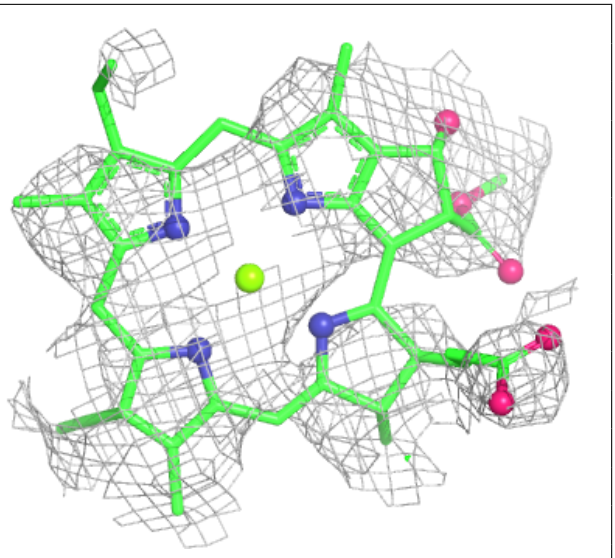


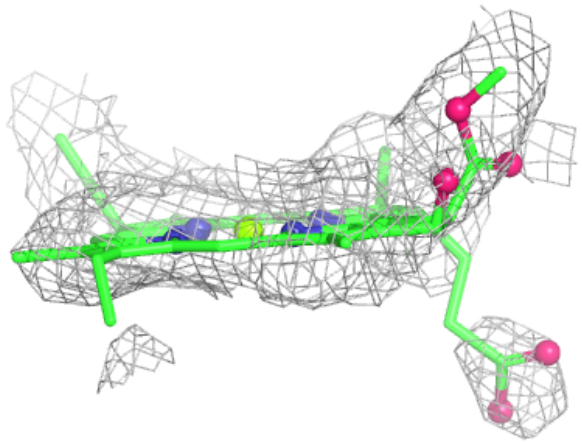


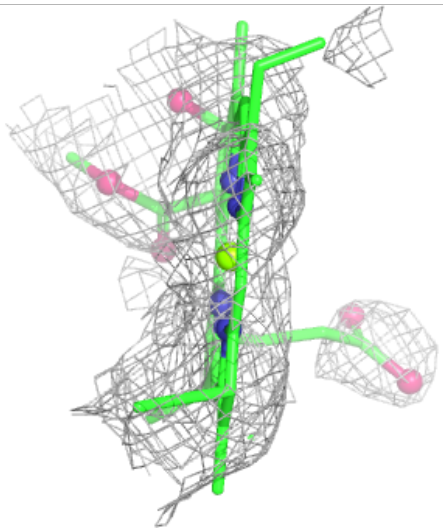


Electron density around CLA B 1765:

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

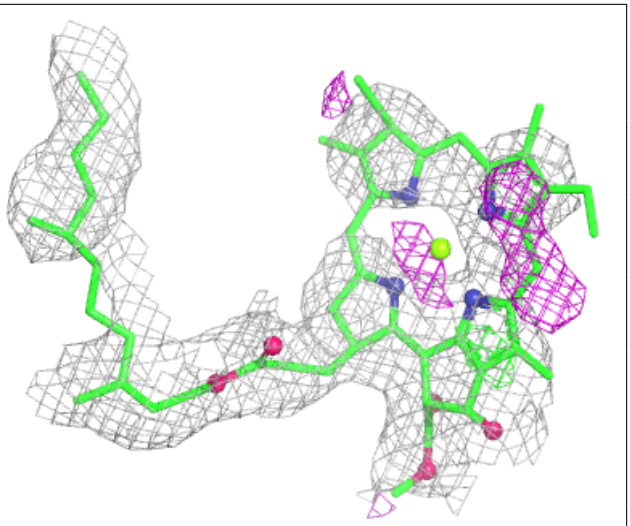


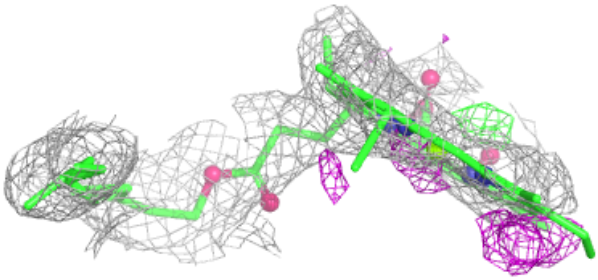


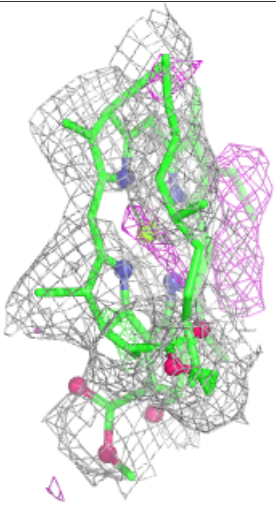


Electron density around CLA B 1755:

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

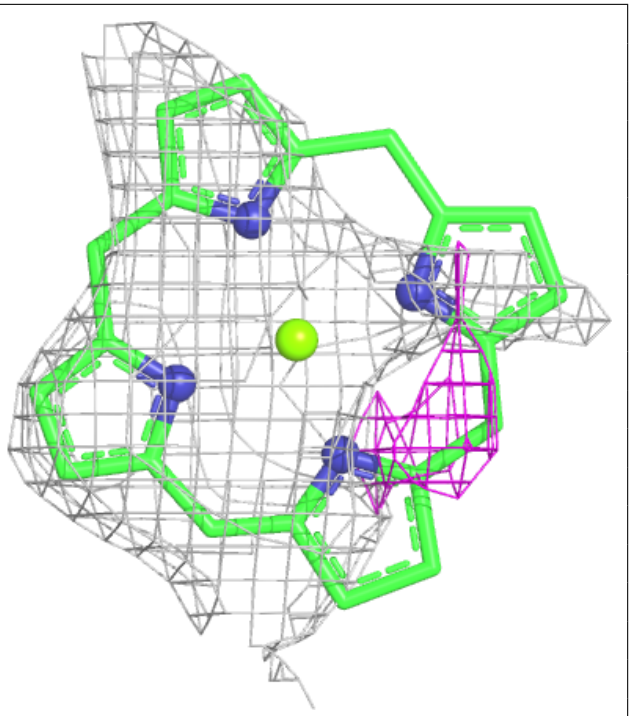


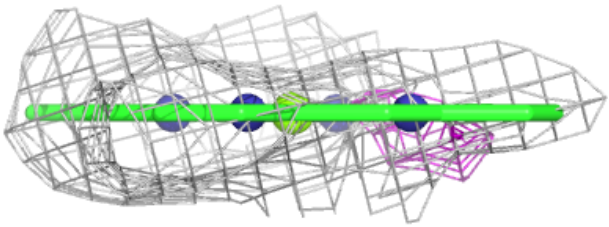


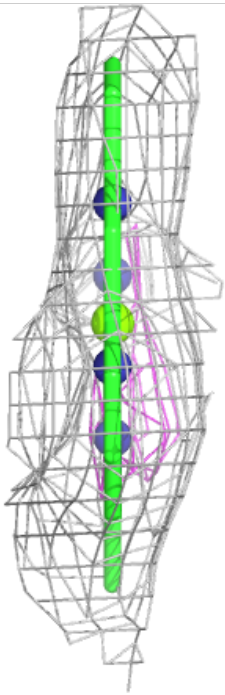


Electron density around CLA 2 1227:

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

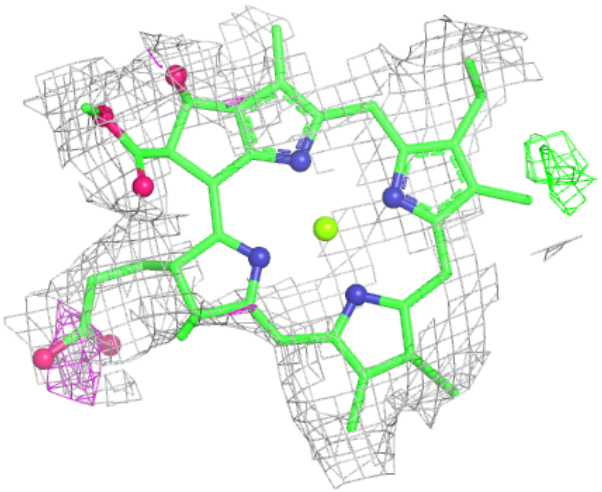


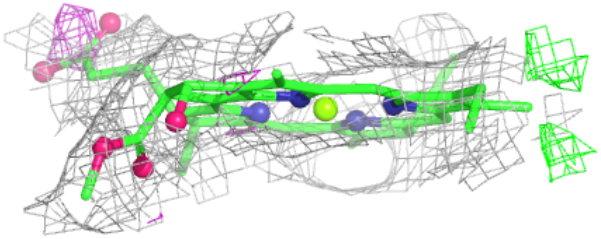


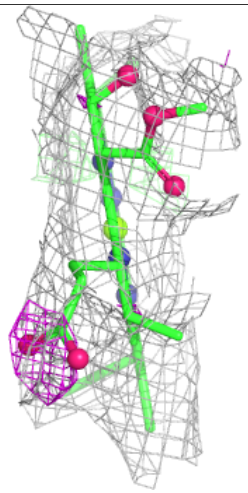


Electron density around CLA K 1142:

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

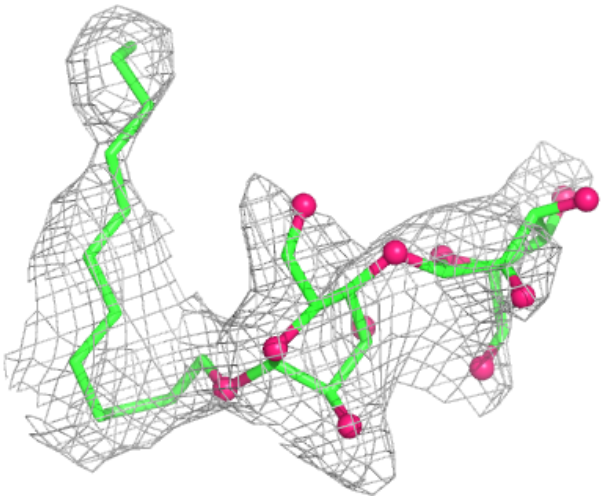


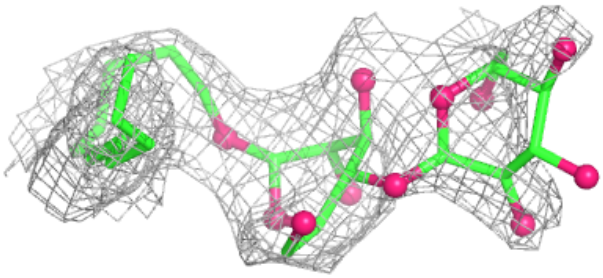


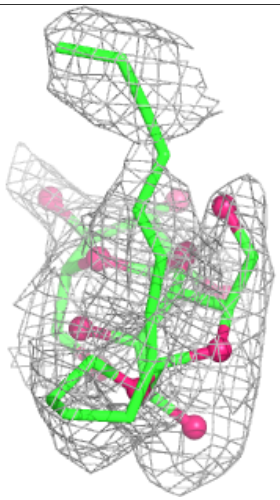


Electron density around LMU R 1057:

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

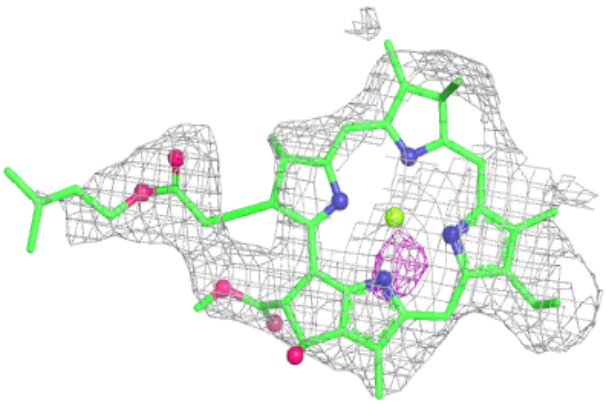


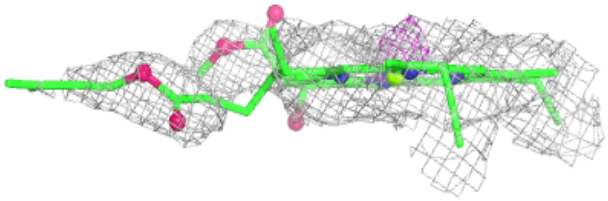


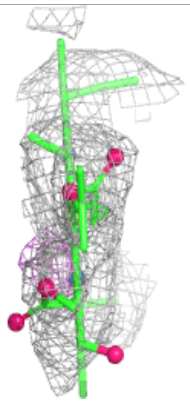


Electron density around CLA A 1799:

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

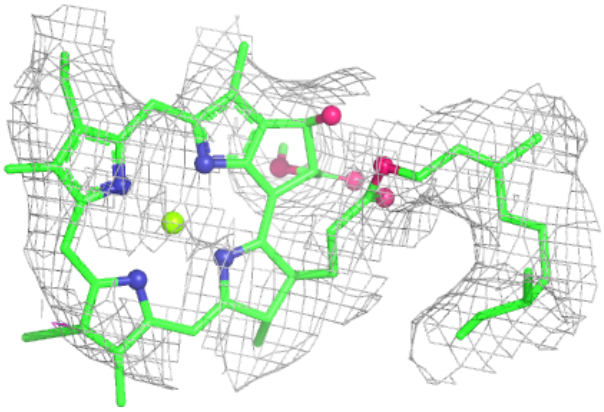


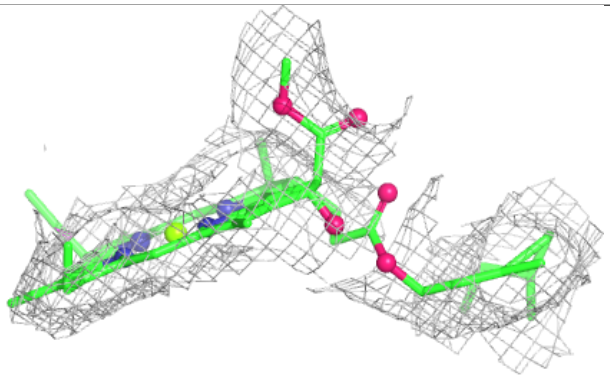




Electron density around CLA 2 1220:

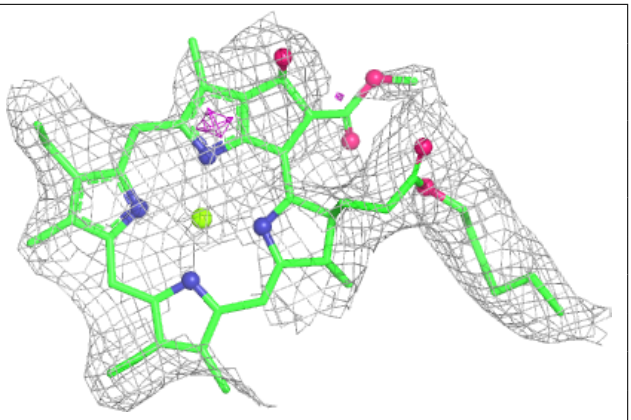
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

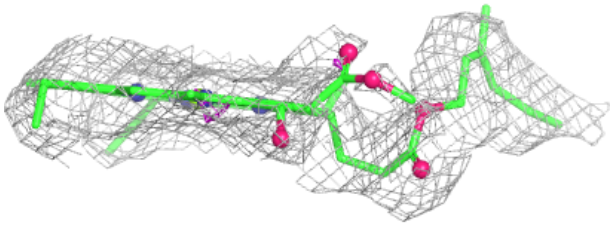


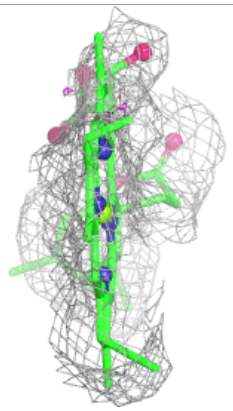


Electron density around CLA 4 4007:

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

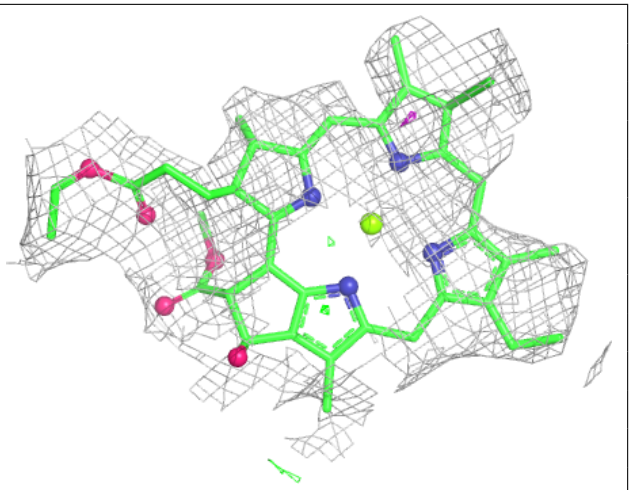


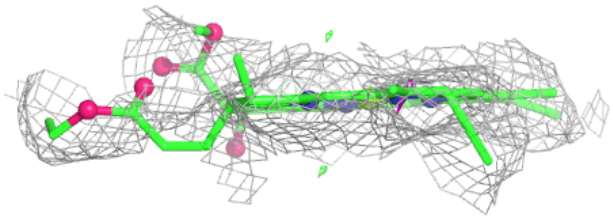


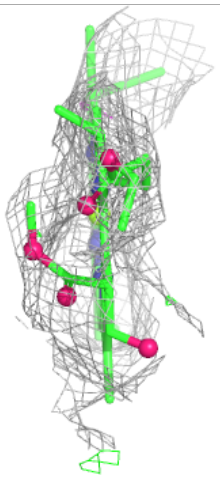


Electron density around CLA 4 4014:

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

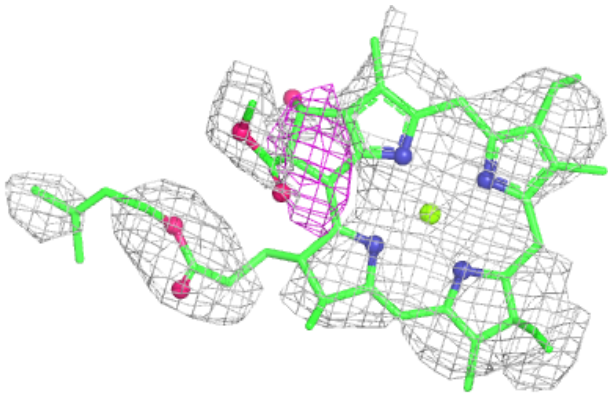


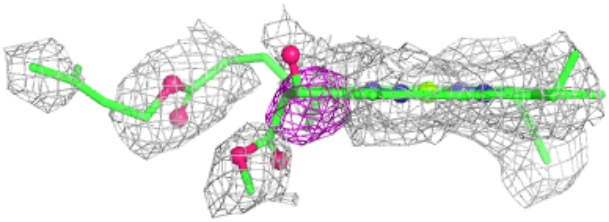


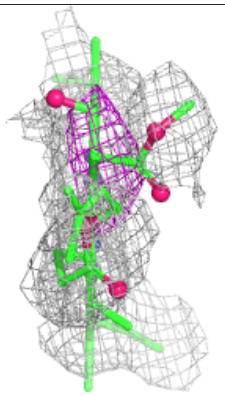


Electron density around CLA 4 1200:

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

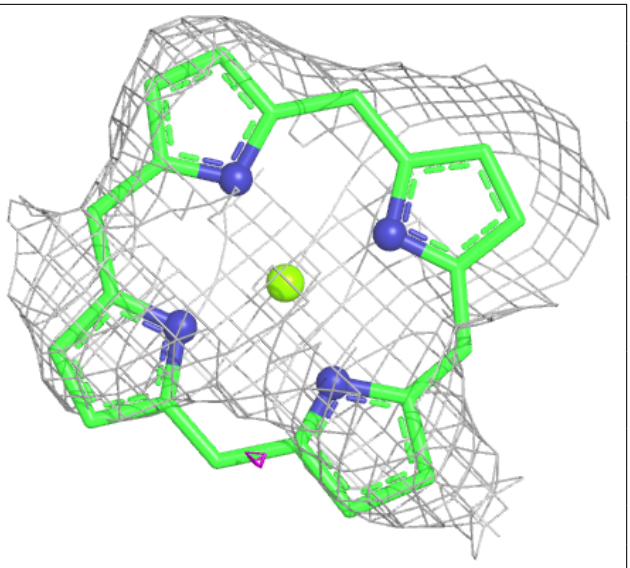


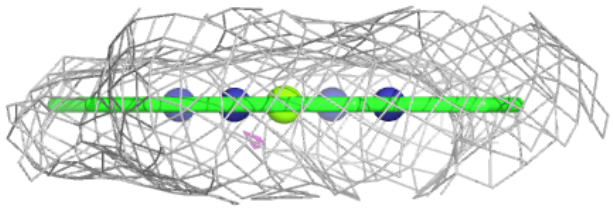


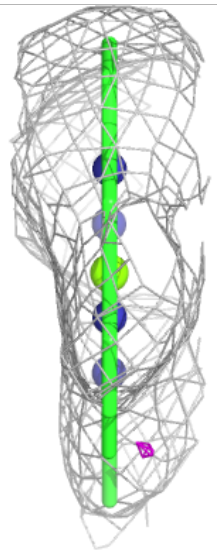


Electron density around CLA 4 1202:

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

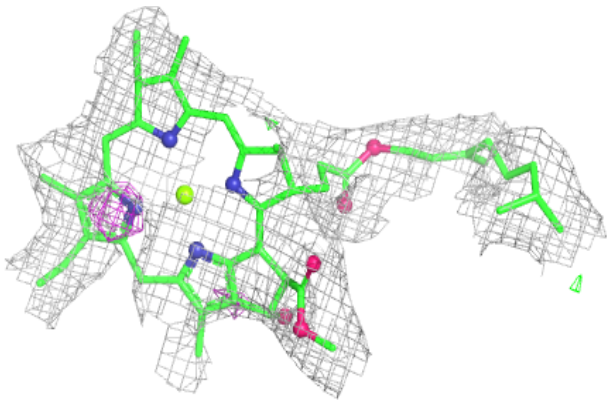


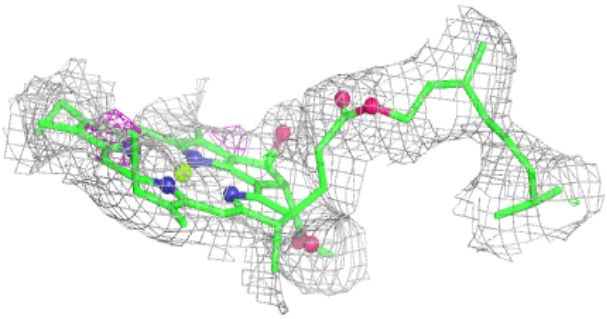




Electron density around CLA I 1033:

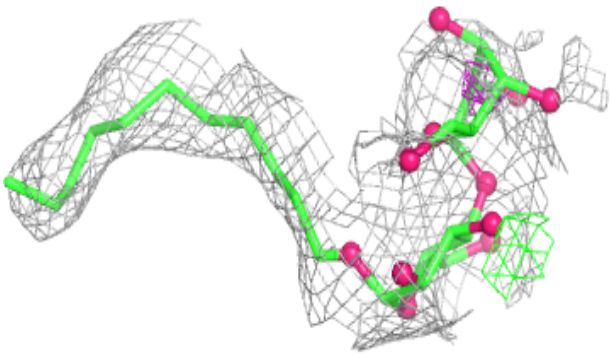
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

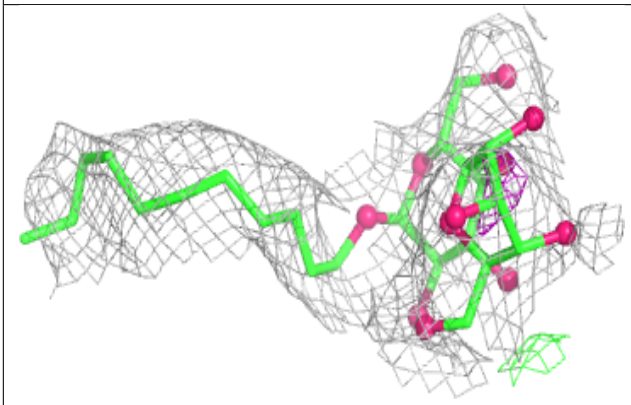


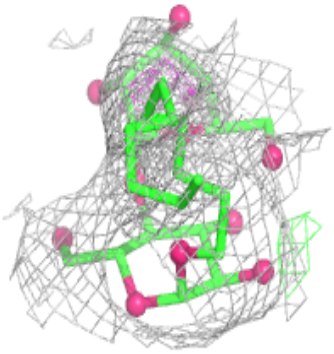


Electron density around LMU A 7009:

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

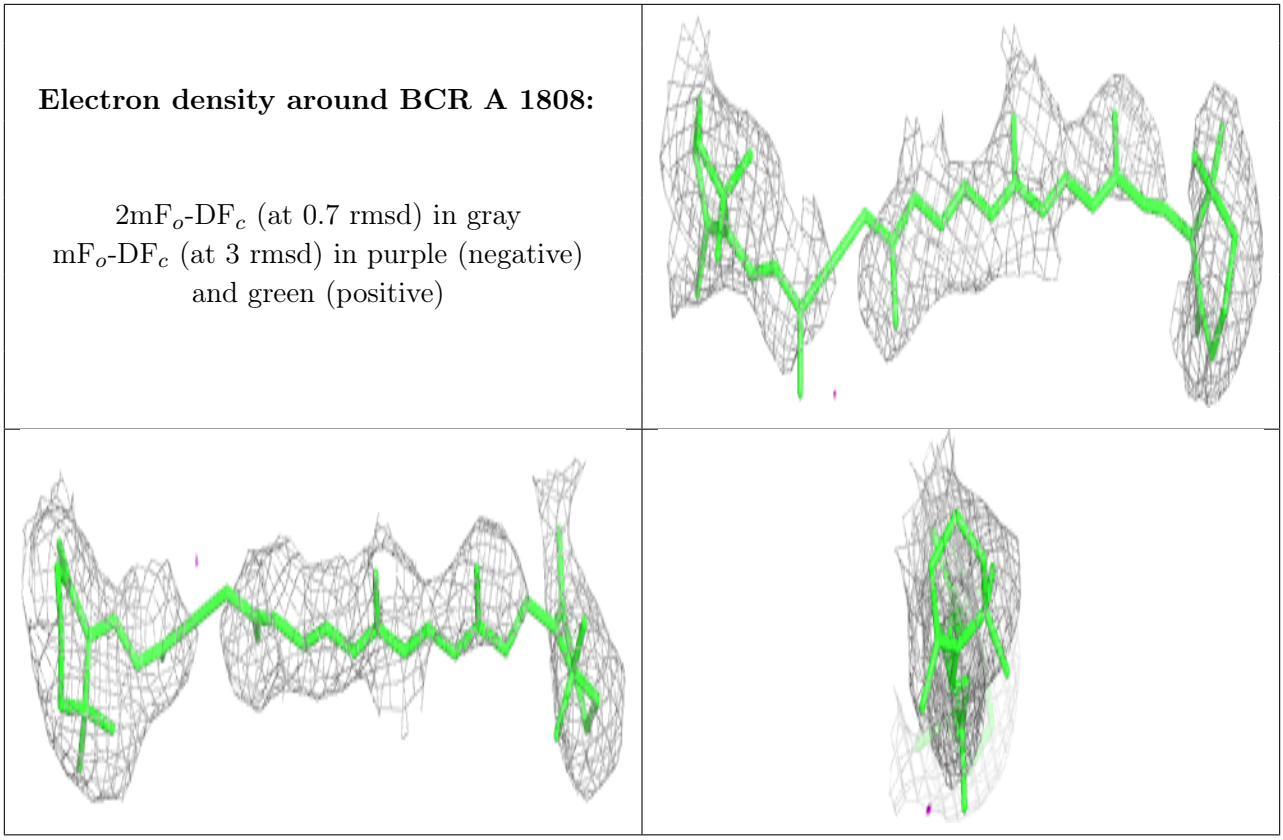






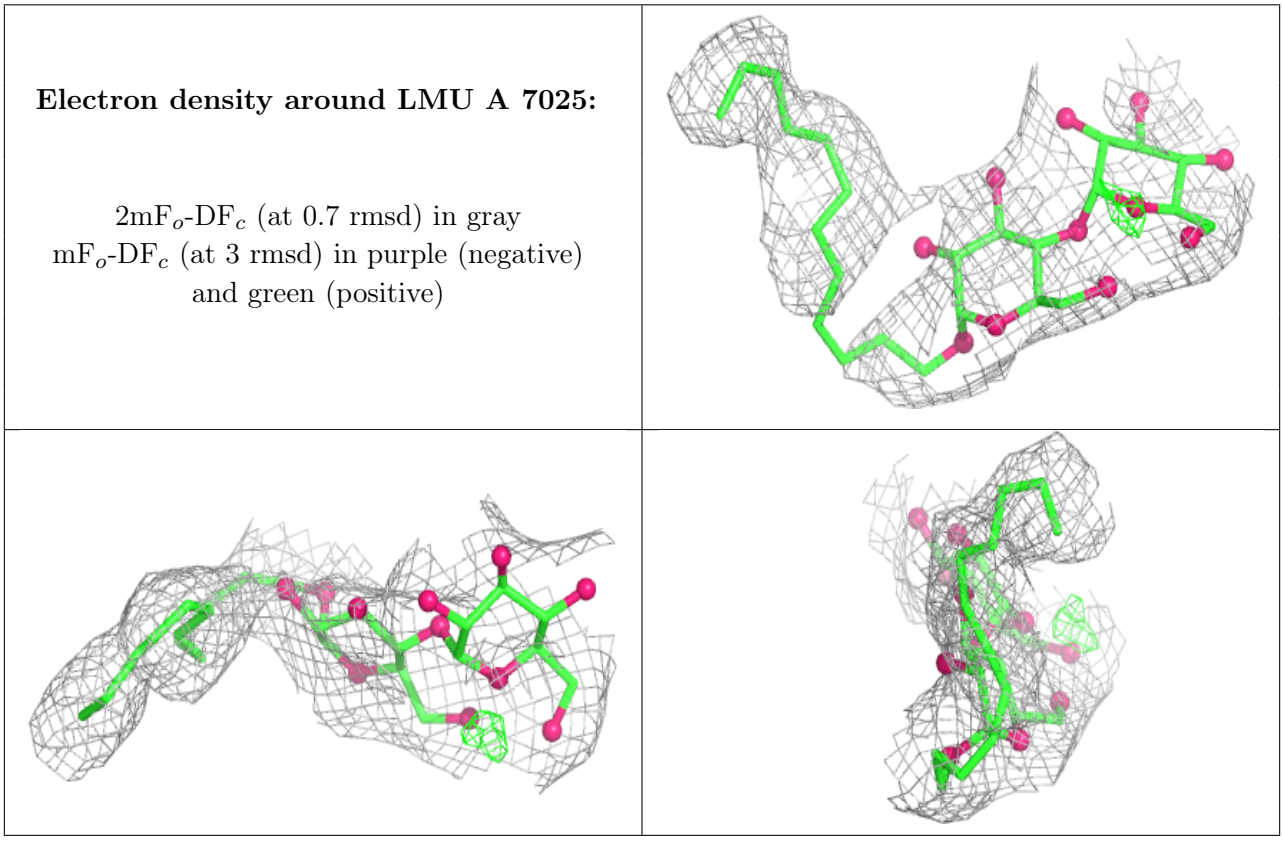
Electron density around BCR A 1808:

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



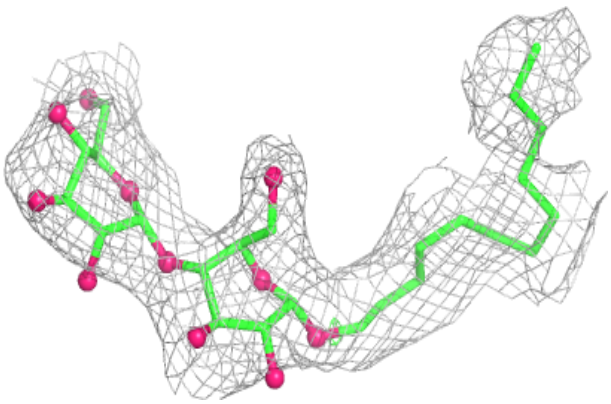
Electron density around LMU A 7025:

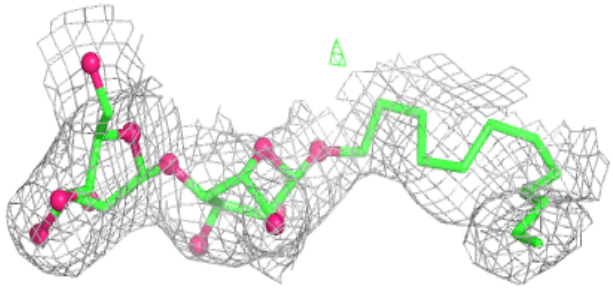
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

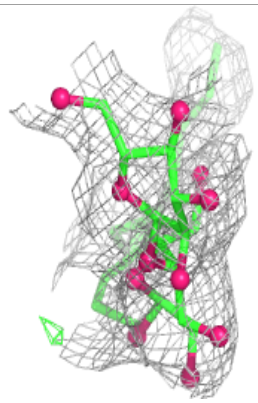


Electron density around LMU A 7030:

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

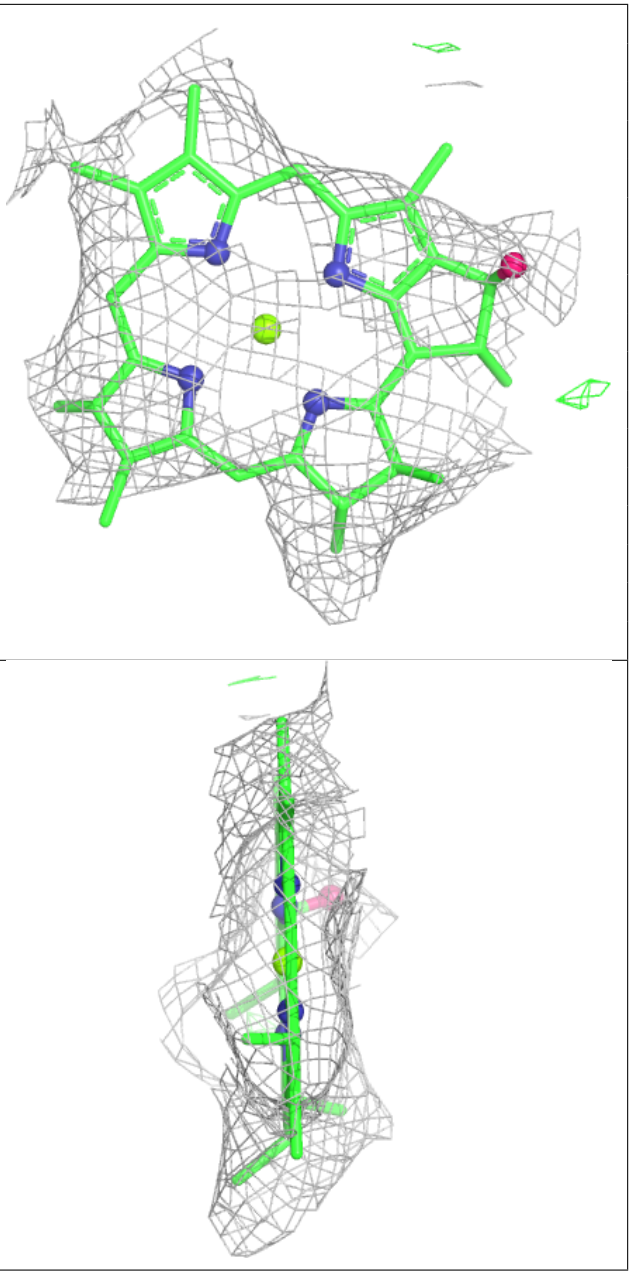






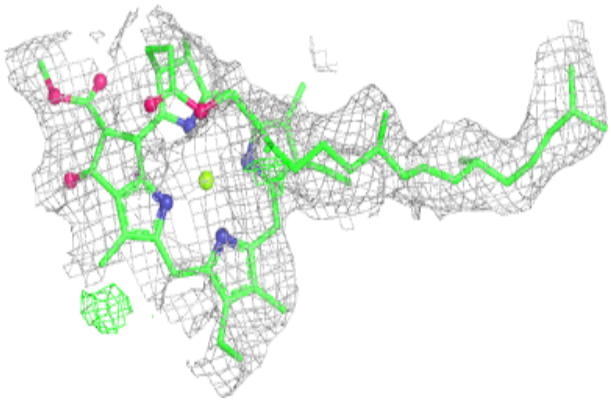
Electron density around CLA A 1775:

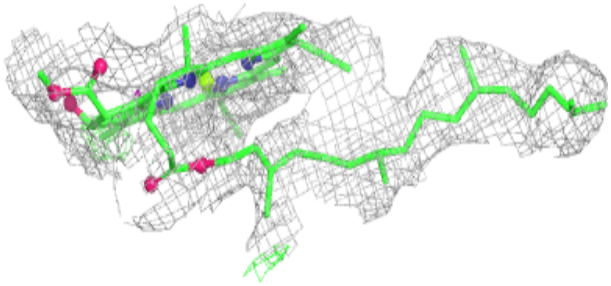
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

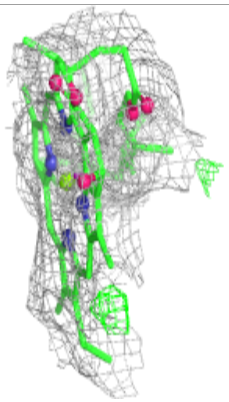


Electron density around CLA 2 1218:

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

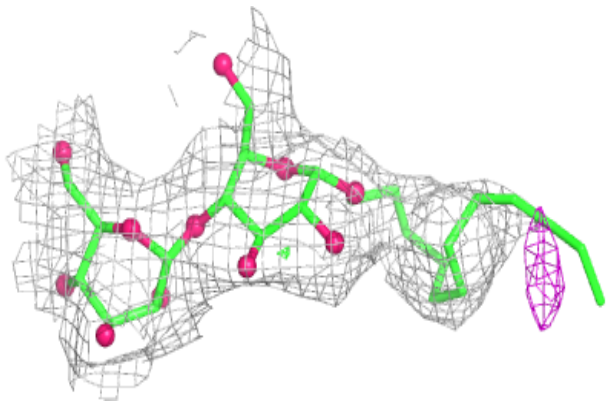


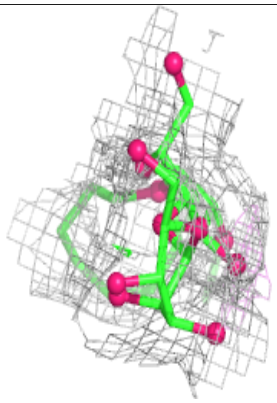




Electron density around LMU 3 7005:

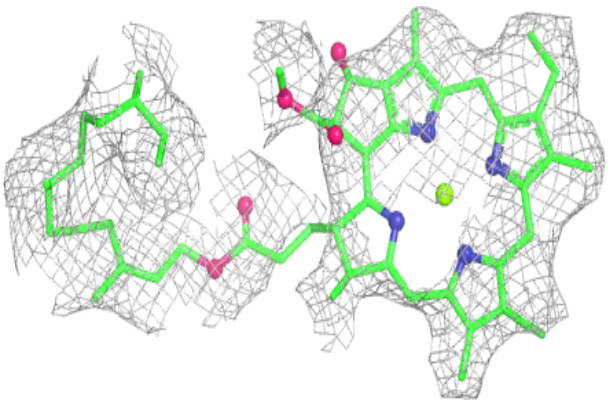
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

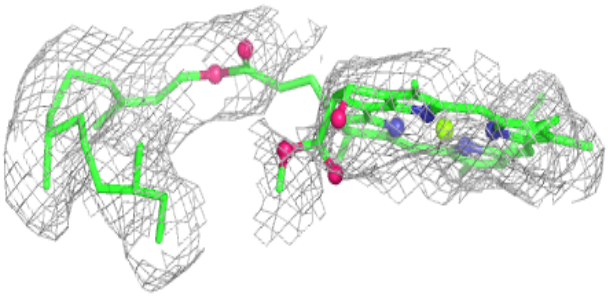


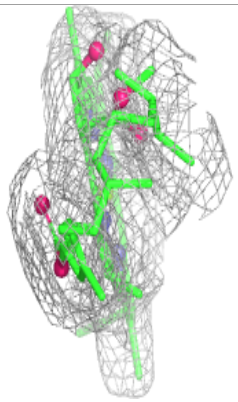


Electron density around CLA 1 1198:

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

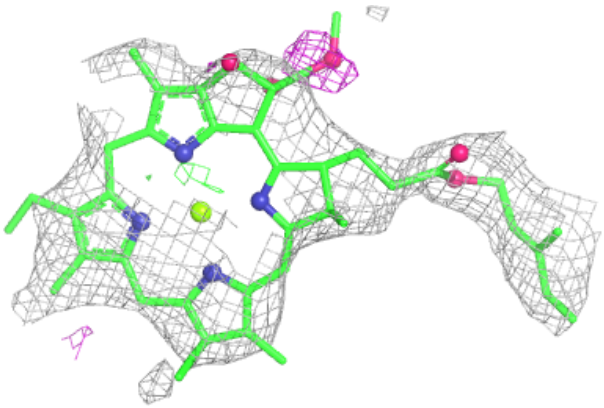


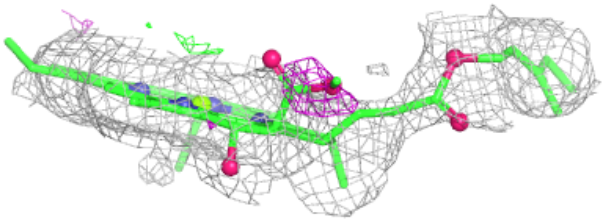


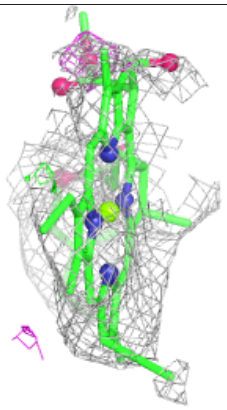


Electron density around CLA 1 1200:

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

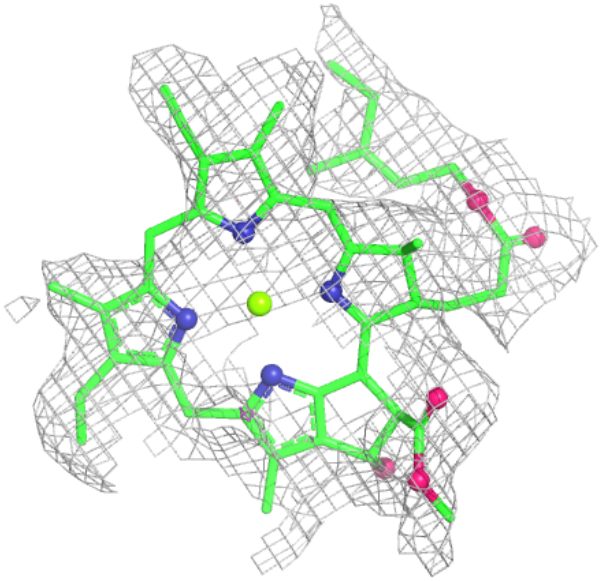


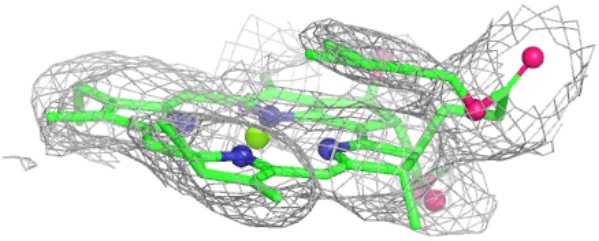


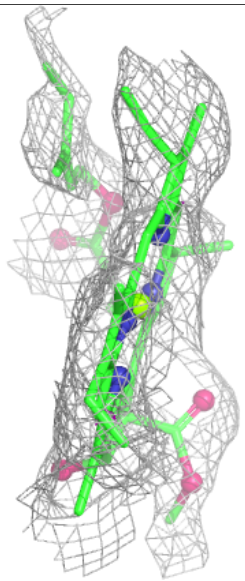


Electron density around CLA G 1099:

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

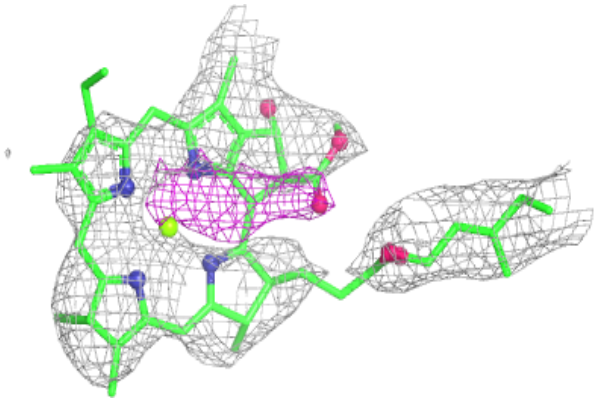


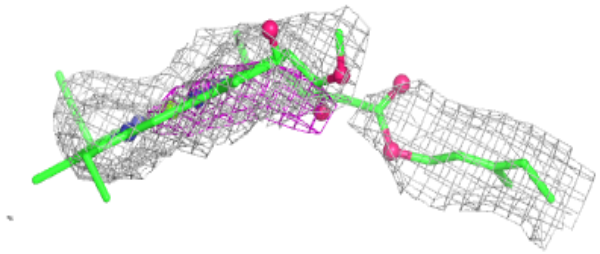


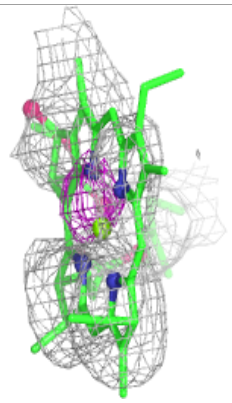


Electron density around CLA 1 1197:

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

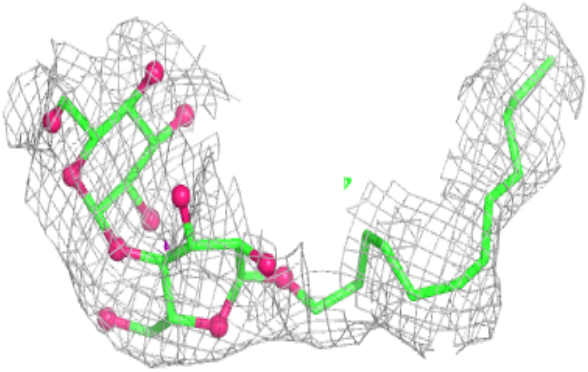


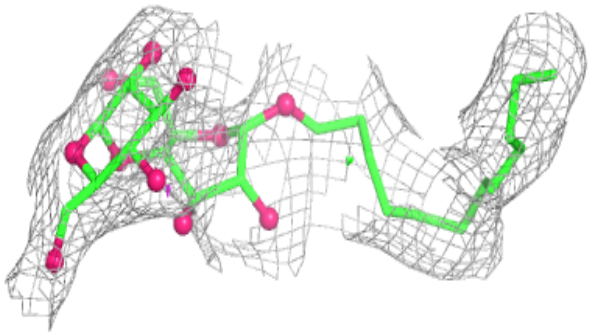


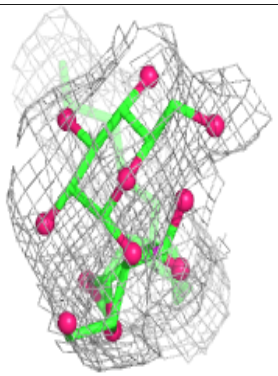


Electron density around LMU A 7031:

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

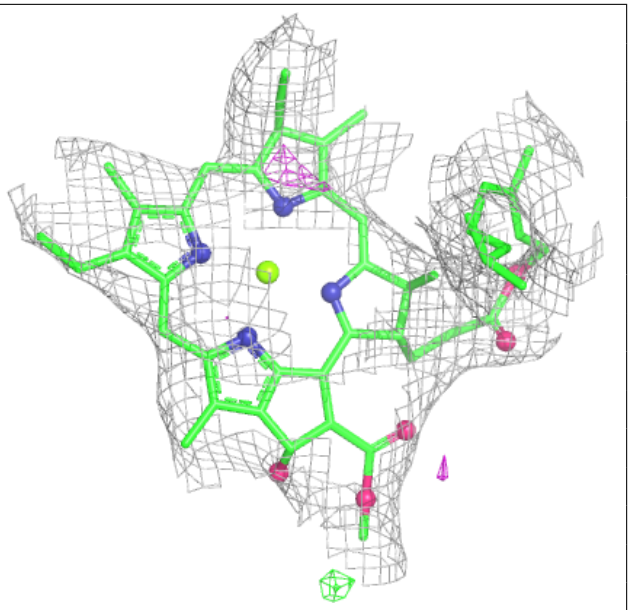


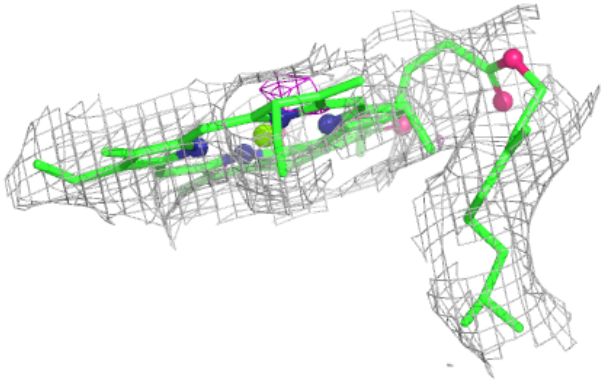


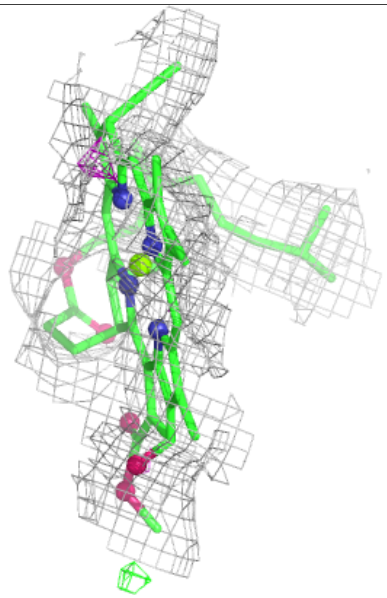


Electron density around CLA A 1815:

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

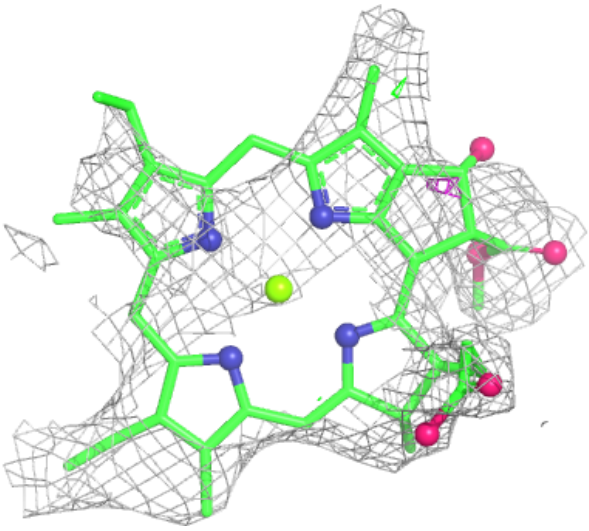


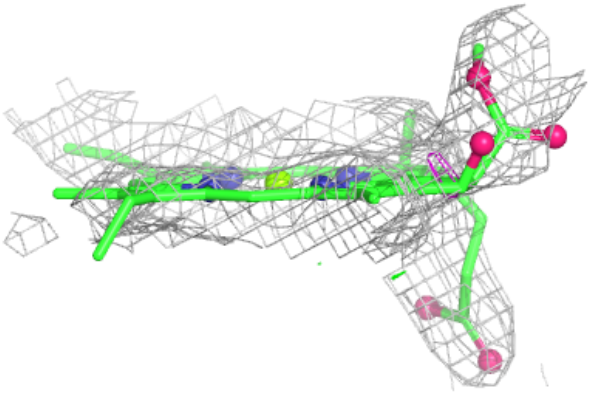


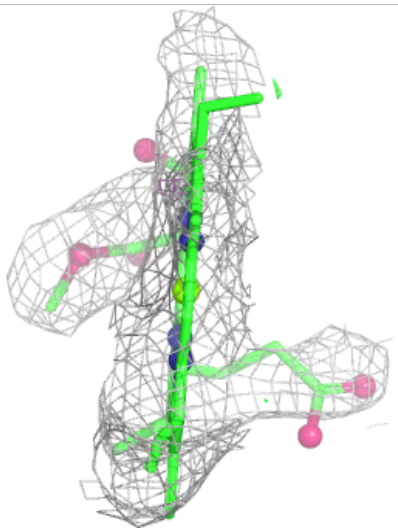


Electron density around CLA A 1770:

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

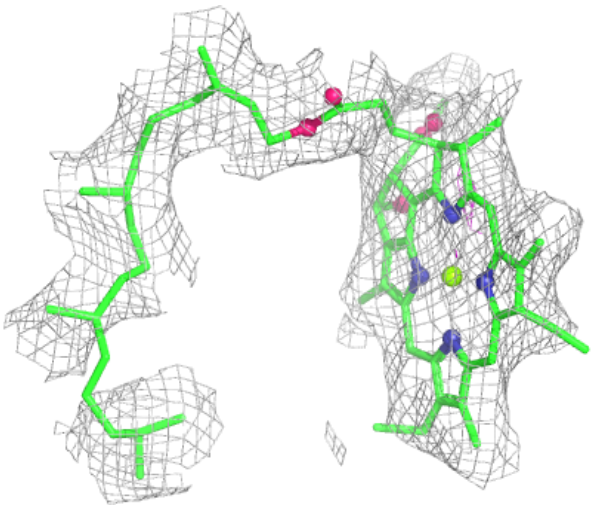


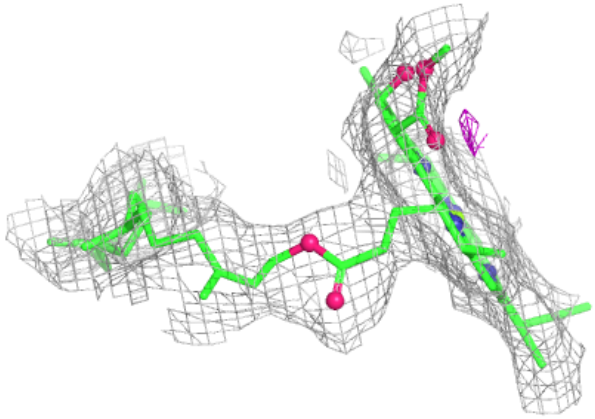


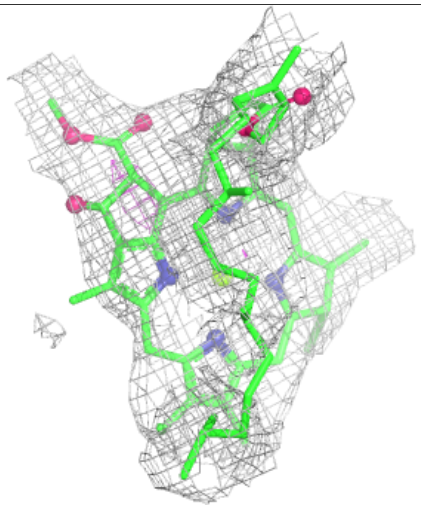


Electron density around CLA 3 1218:

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

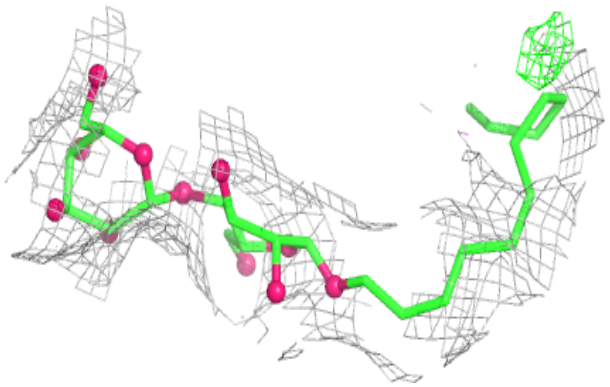


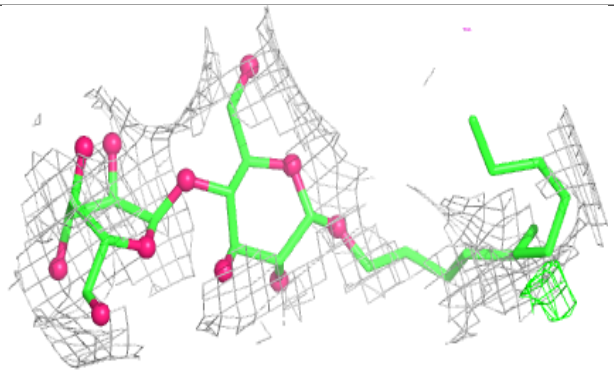


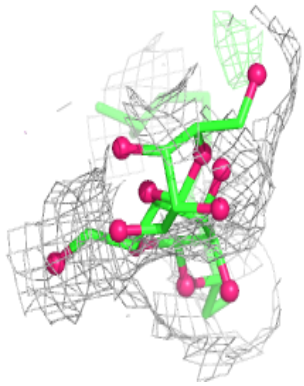


Electron density around LMU A 7043:

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

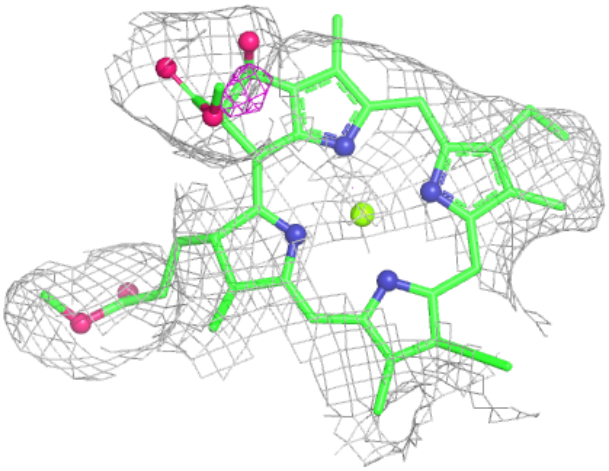


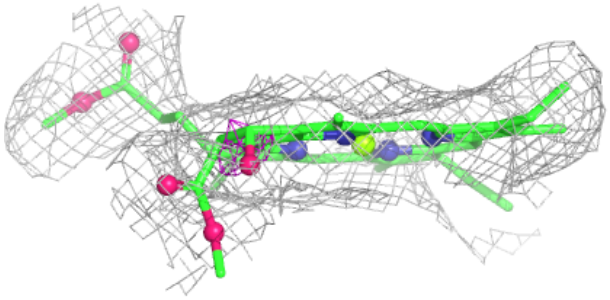


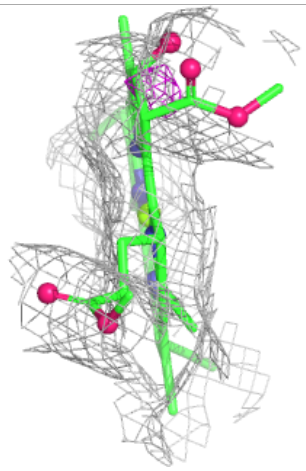


Electron density around CLA 1 1187:

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

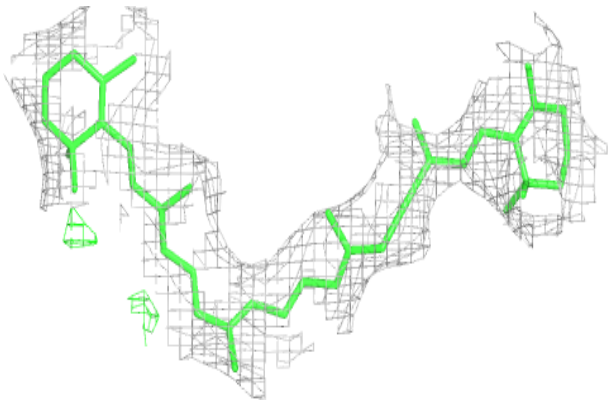


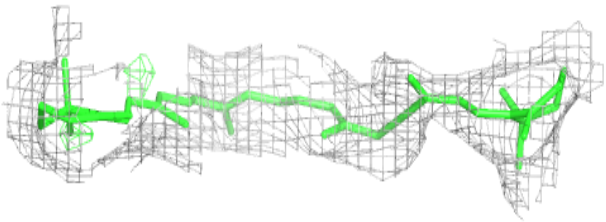




Electron density around BCR 3 1220:

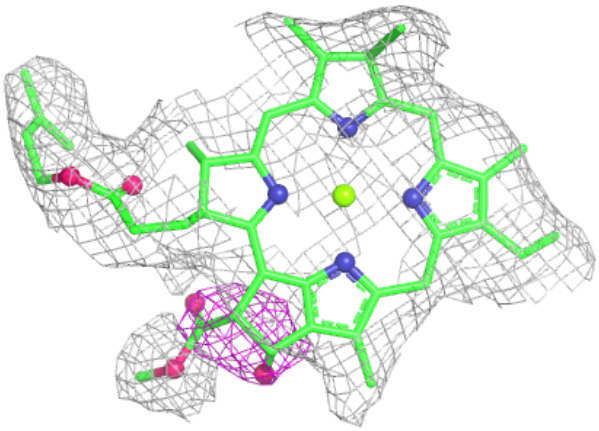
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

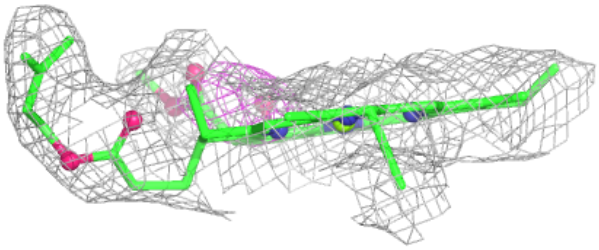


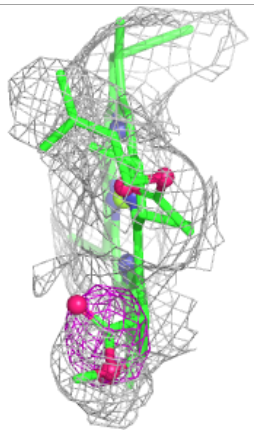


Electron density around CLA K 1146:

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

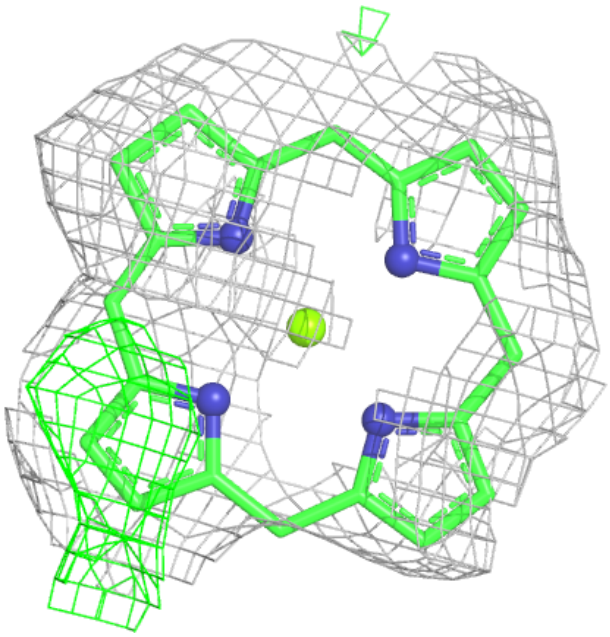


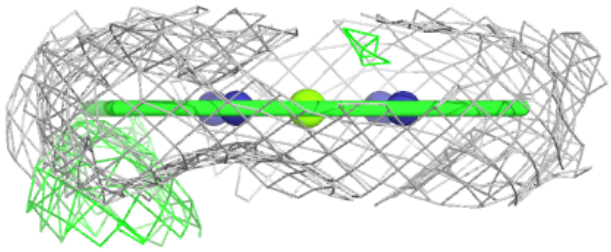


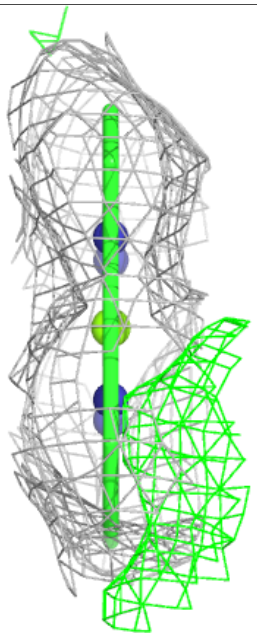


Electron density around CLA 1 1194:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

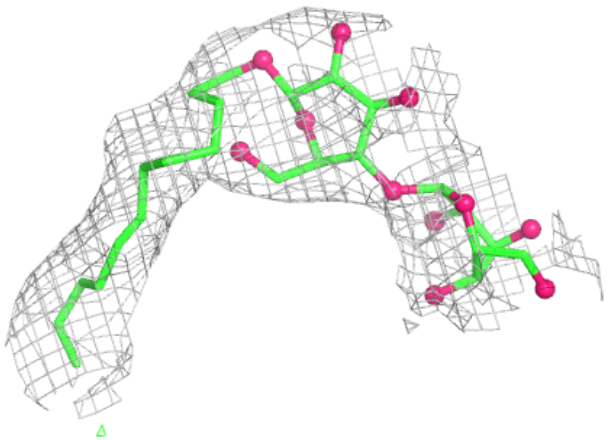


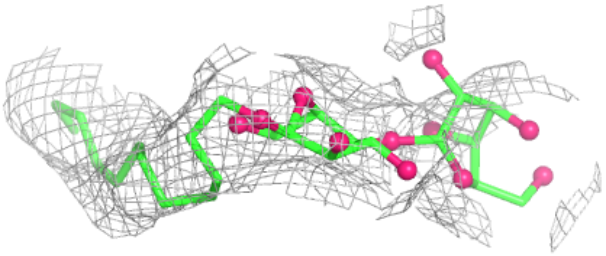


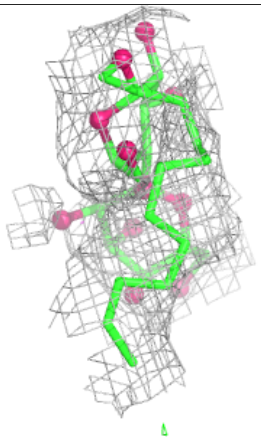


Electron density around LMU A 7021:

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

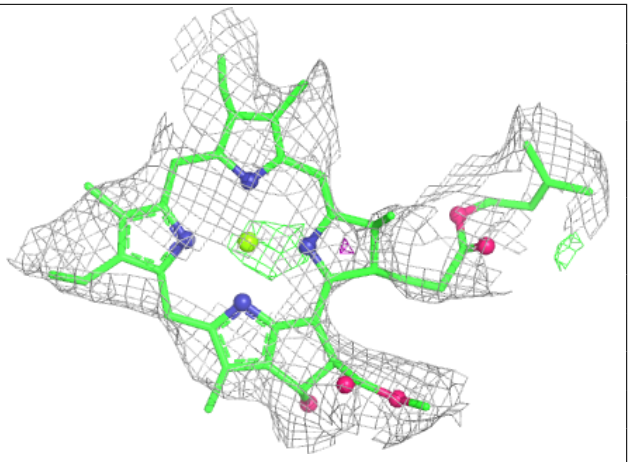


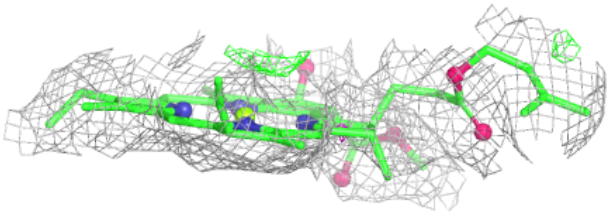


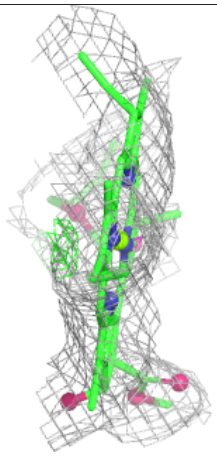


Electron density around CLA 2 1215:

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

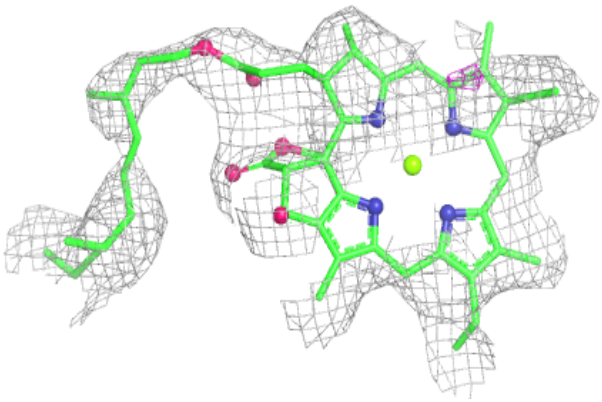


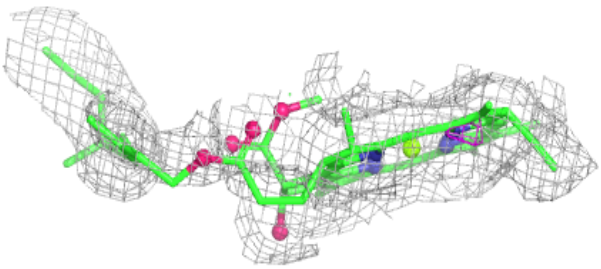




Electron density around CLA R 1054:

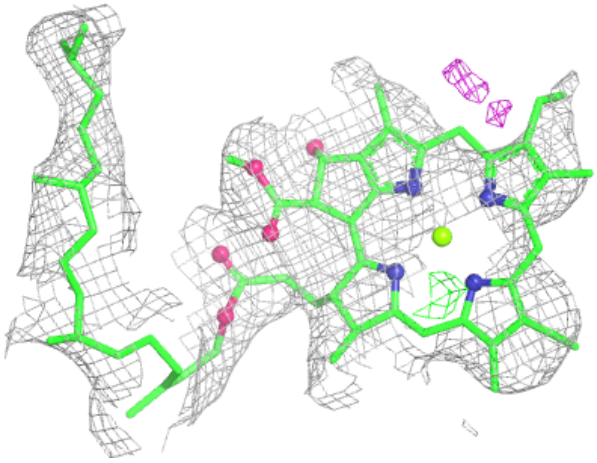
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

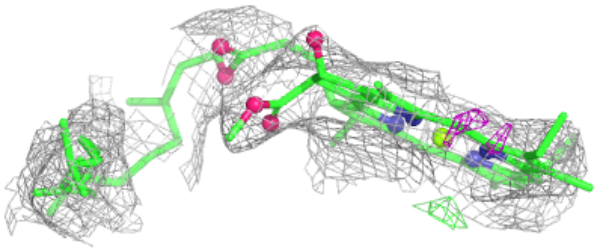


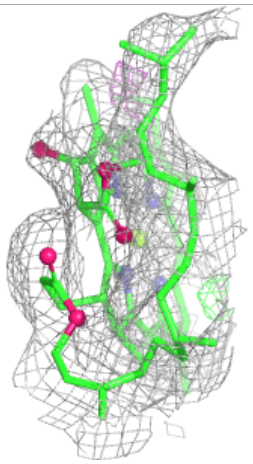


Electron density around CLA R 1055:

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

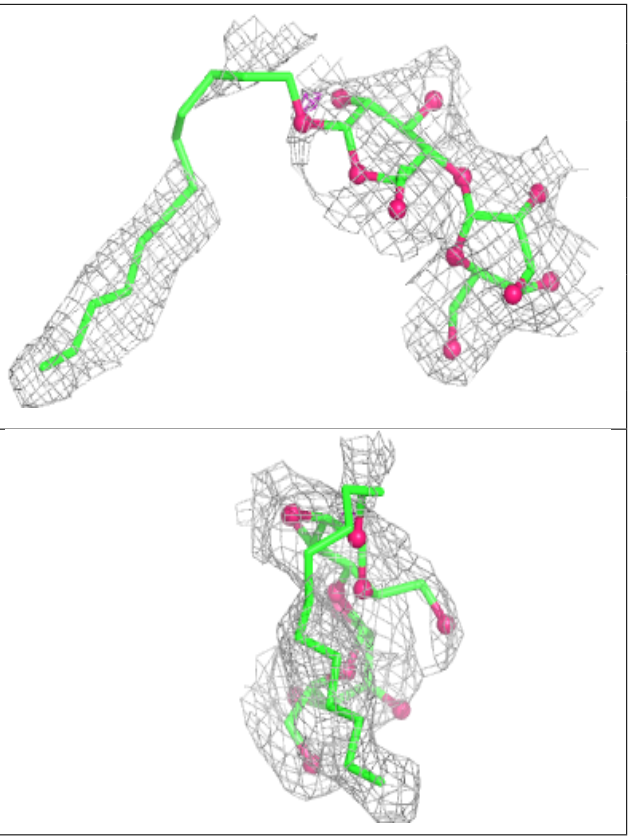






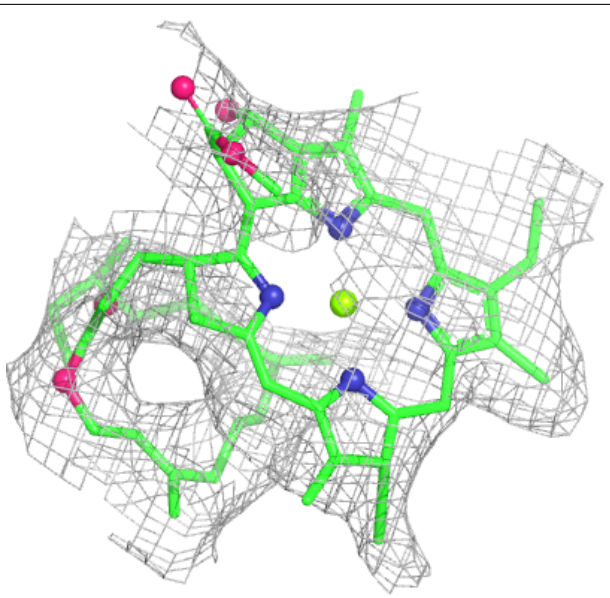
Electron density around LMU 1 1202:

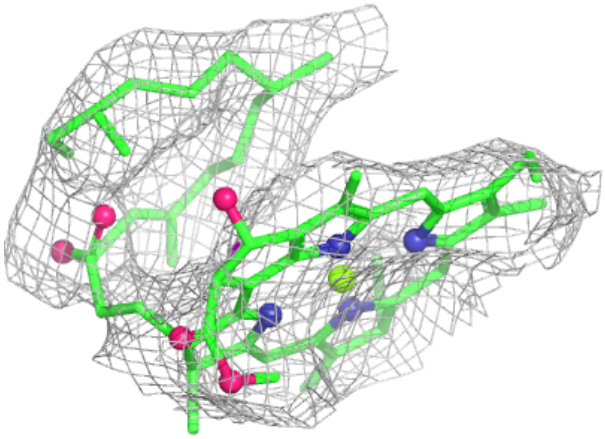
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

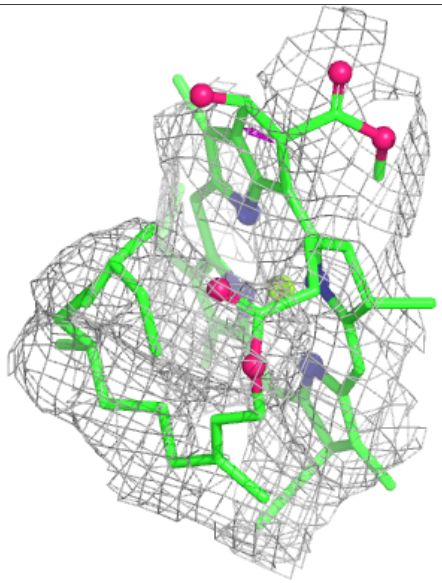


Electron density around CLA J 1043:

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

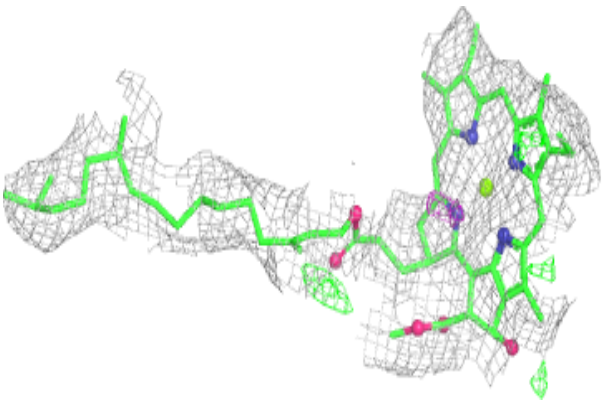


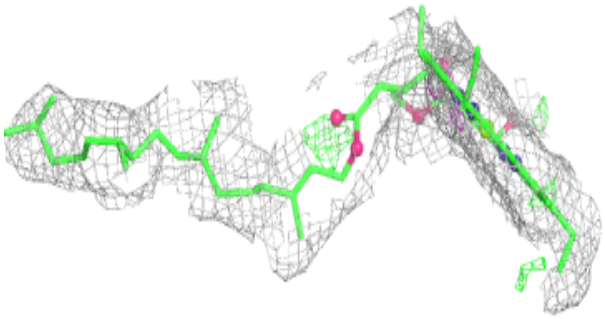




Electron density around CLA 4 1198:

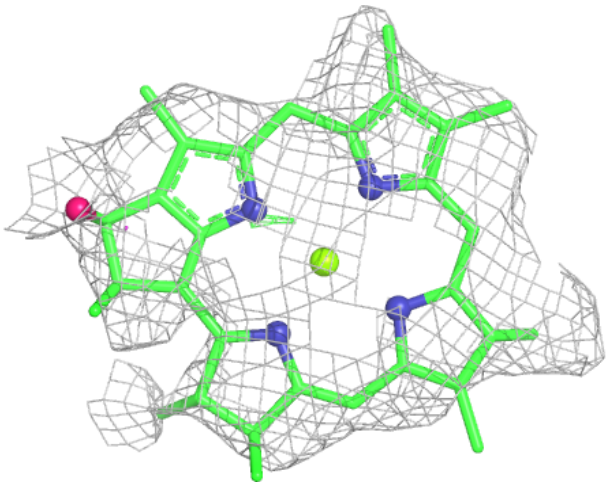
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

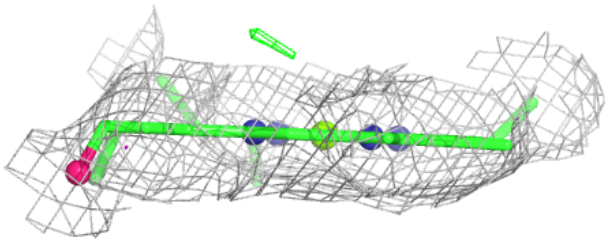


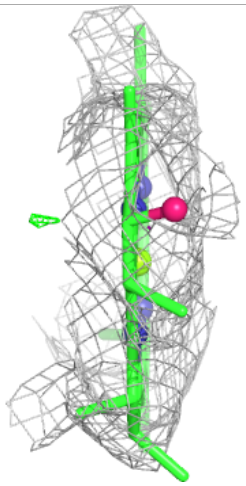


Electron density around CLA 3 1212:

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

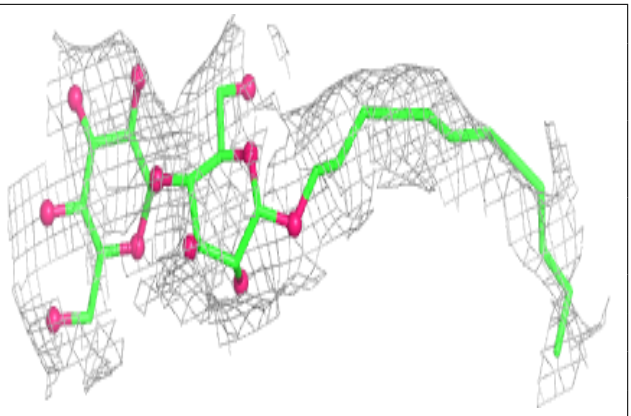


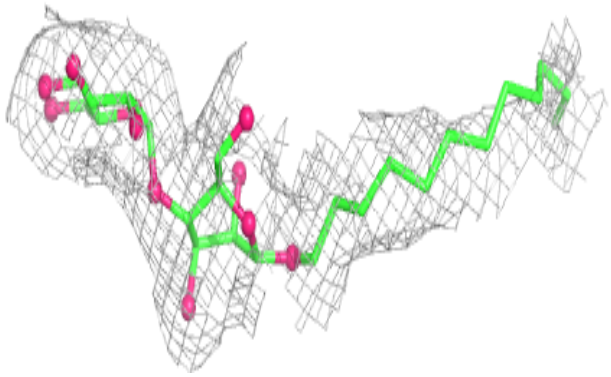


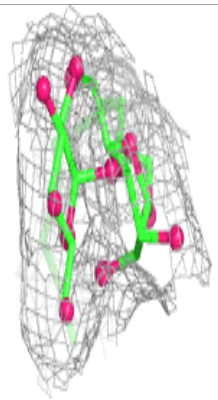


Electron density around LMU A 7047:

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

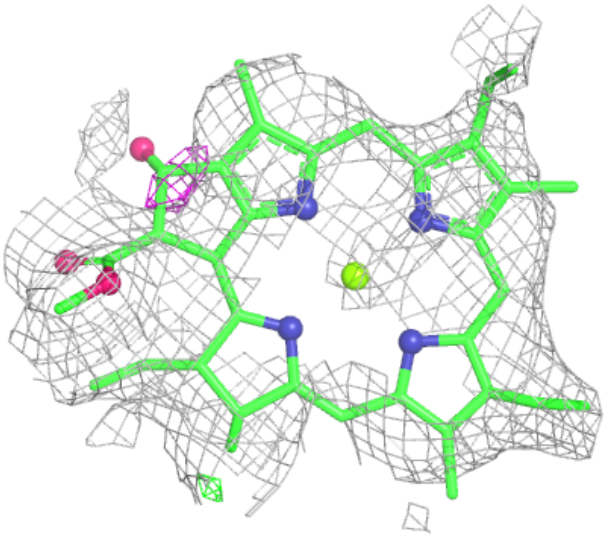


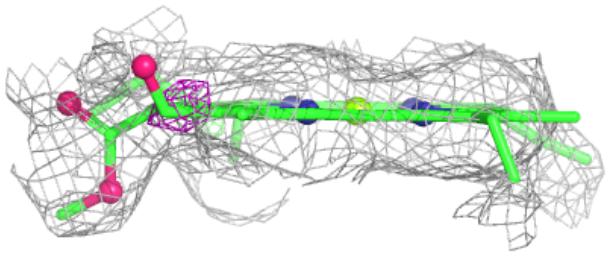


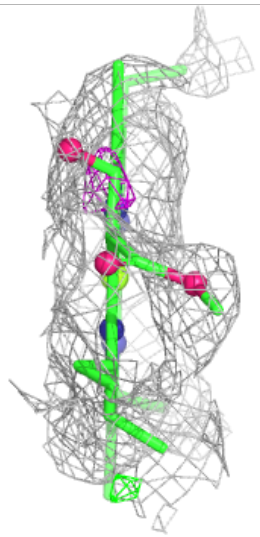


Electron density around CLA A 1778:

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

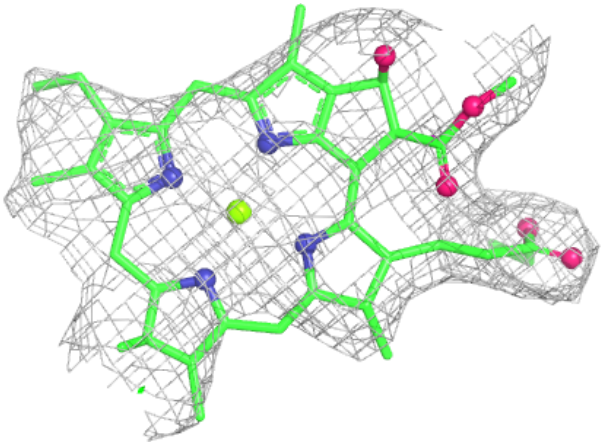


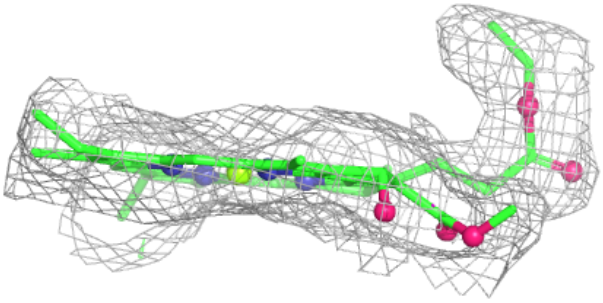


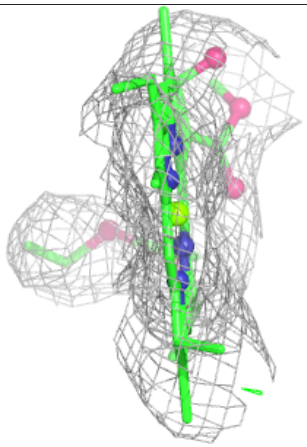


Electron density around CLA A 1817:

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

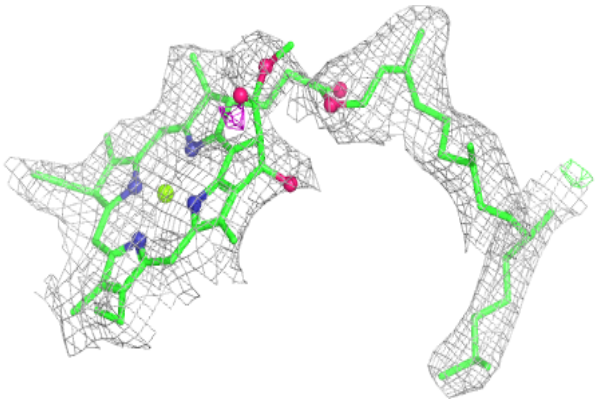


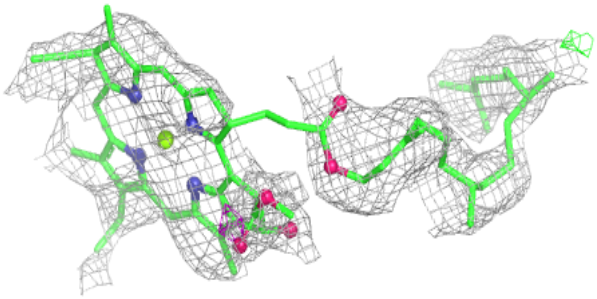


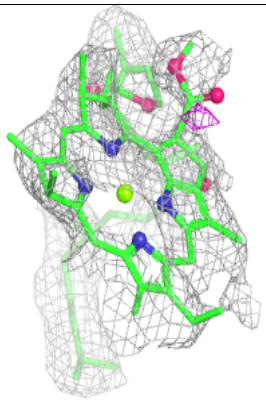


Electron density around CLA K 3009:

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

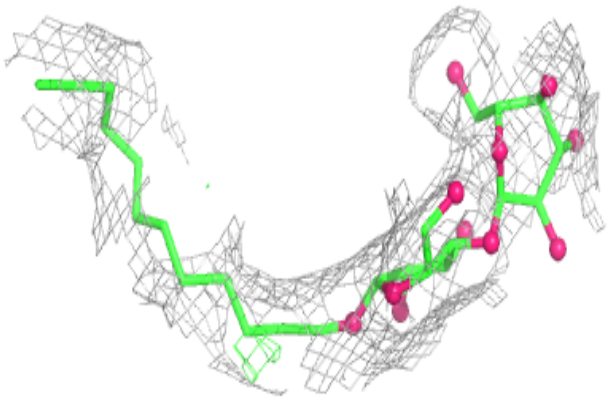


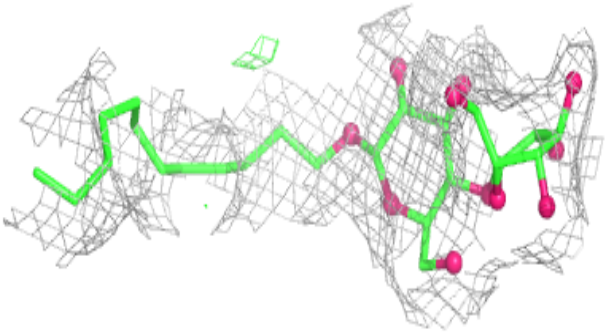




Electron density around LMU A 7017:

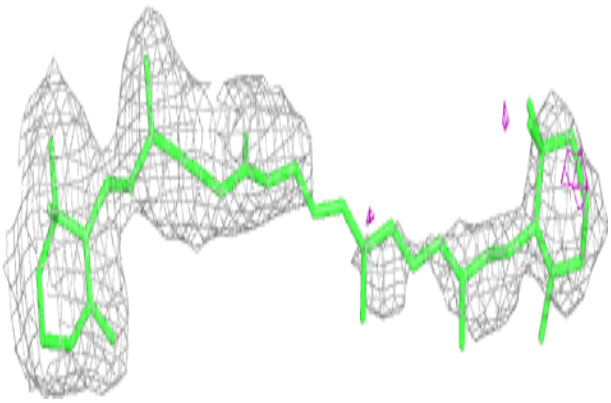
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

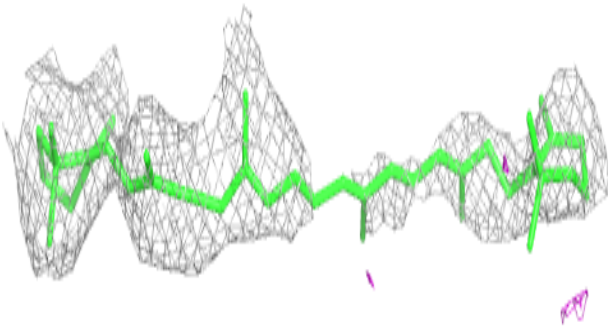


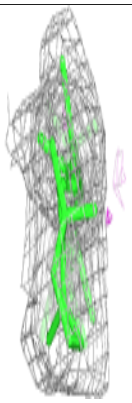


Electron density around BCR L 1169:

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

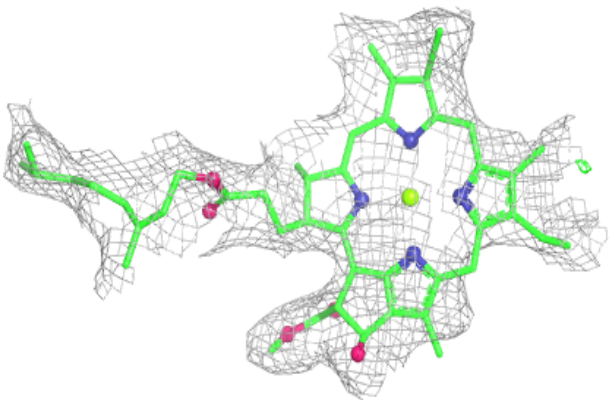


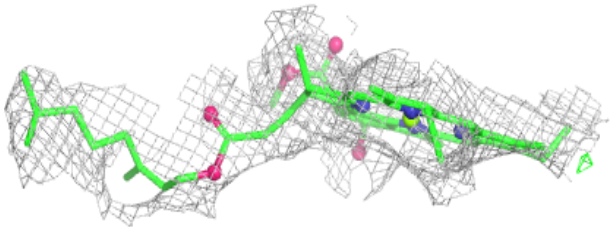


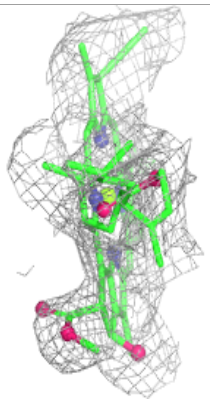


Electron density around CLA A 1798:

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

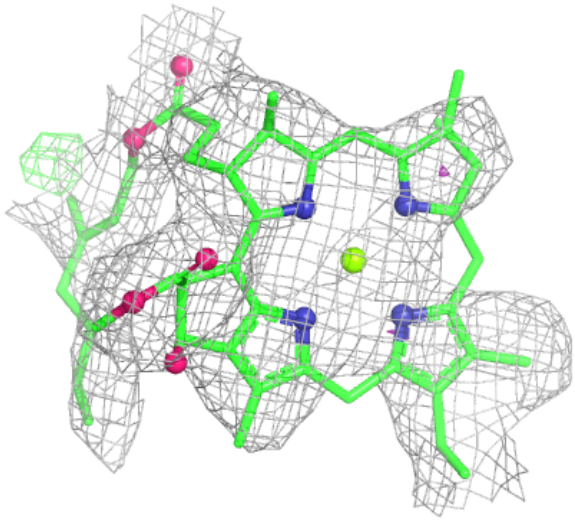


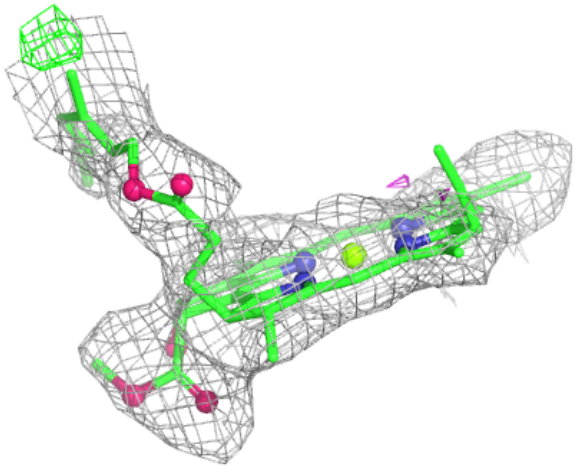


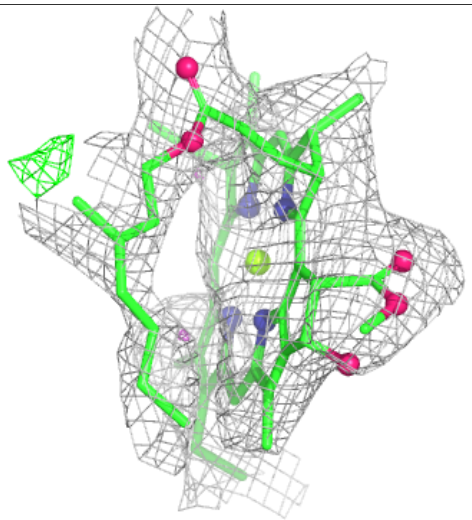


Electron density around CLA F 1157:

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

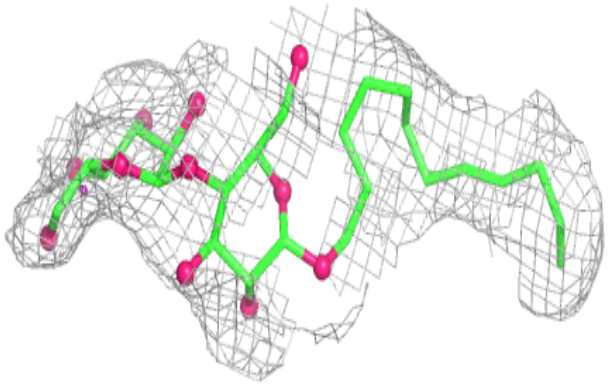


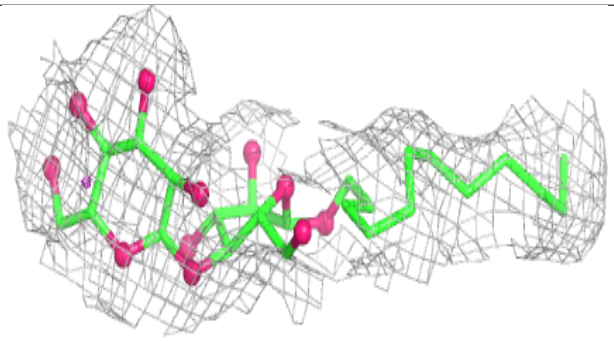




Electron density around LMU A 7042:

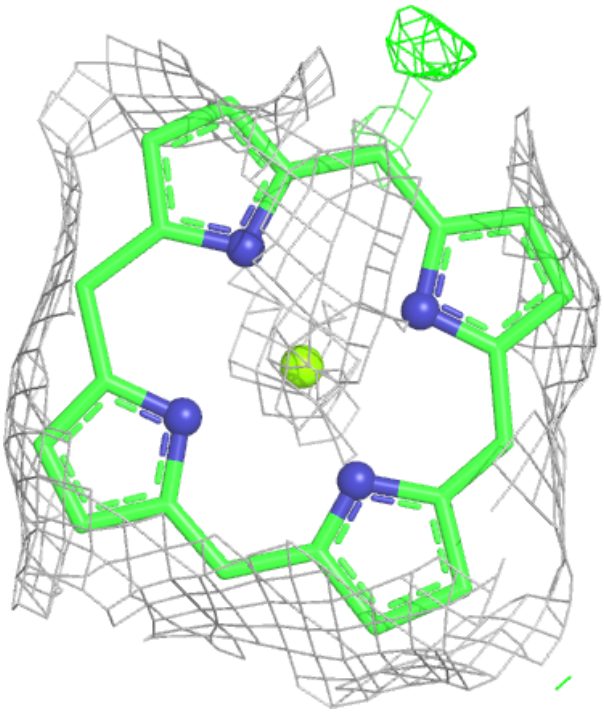
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

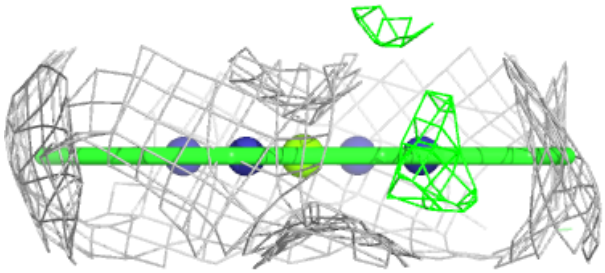


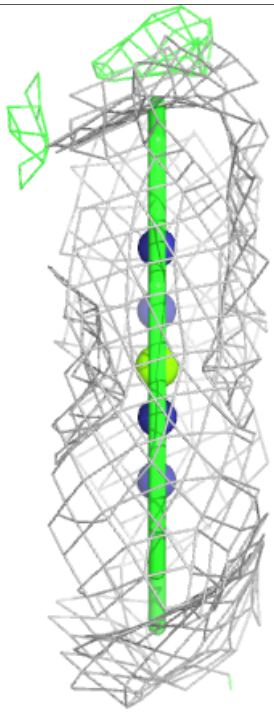


Electron density around CLA 1 1199:

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

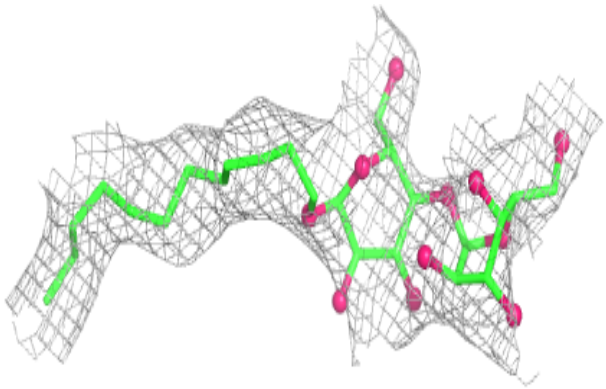


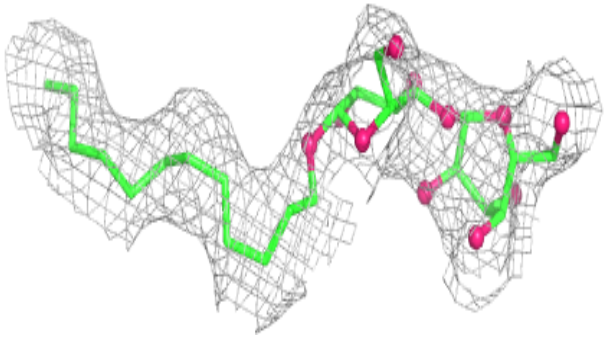


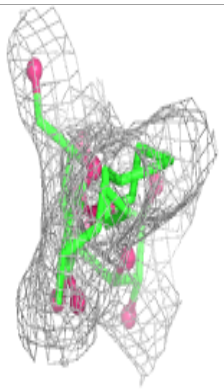


Electron density around LMU A 7010:

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

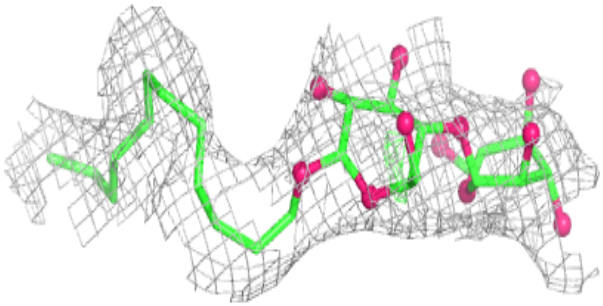


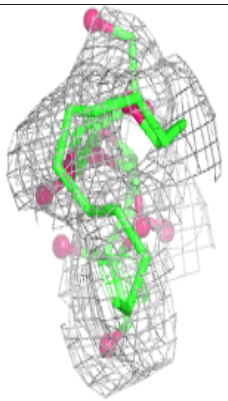




Electron density around LMU A 7034:

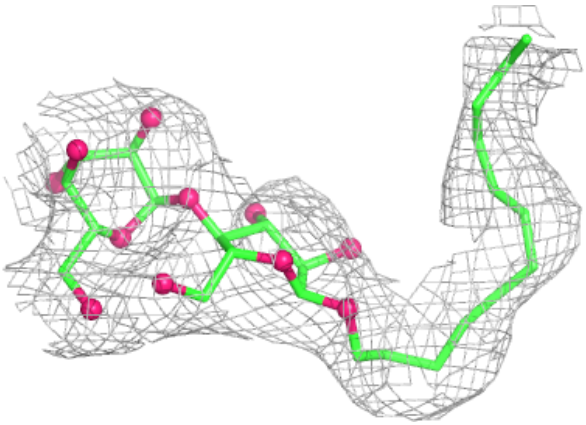
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

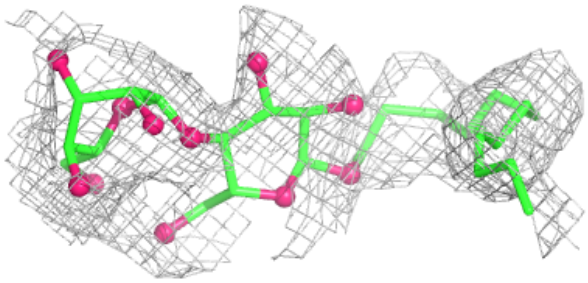


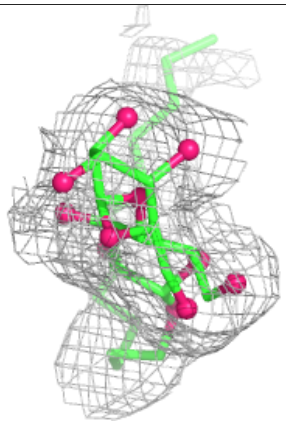


Electron density around LMU 2 7003:

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

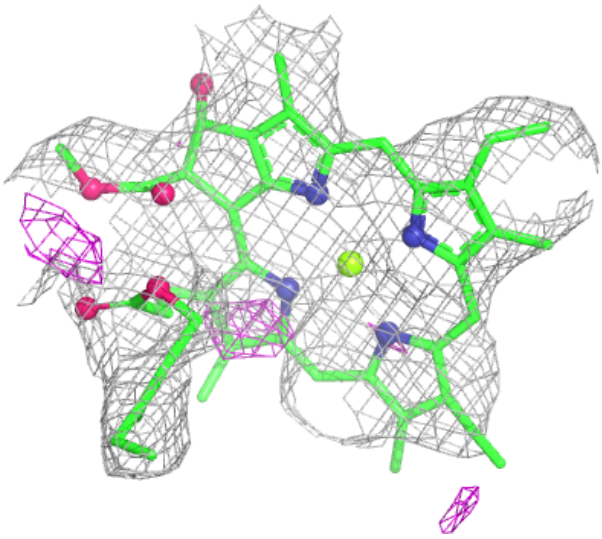


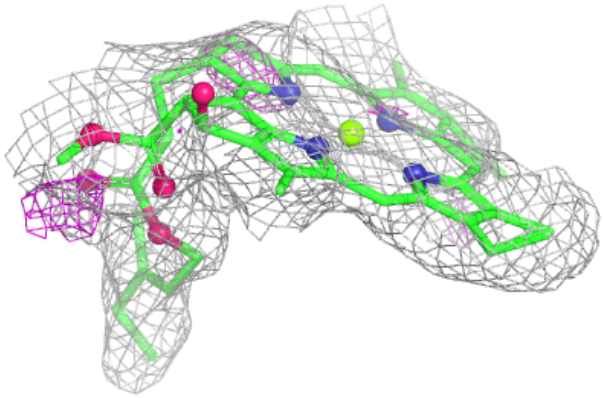


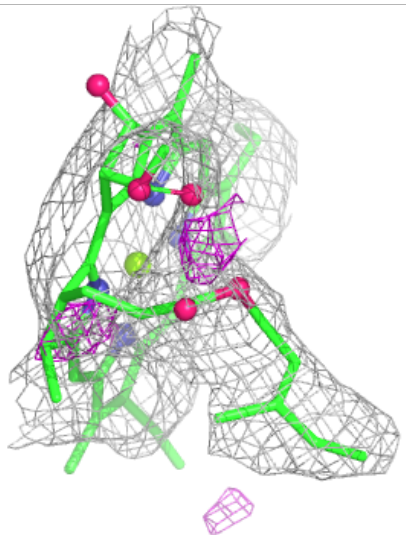


Electron density around CLA 1 1193:

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

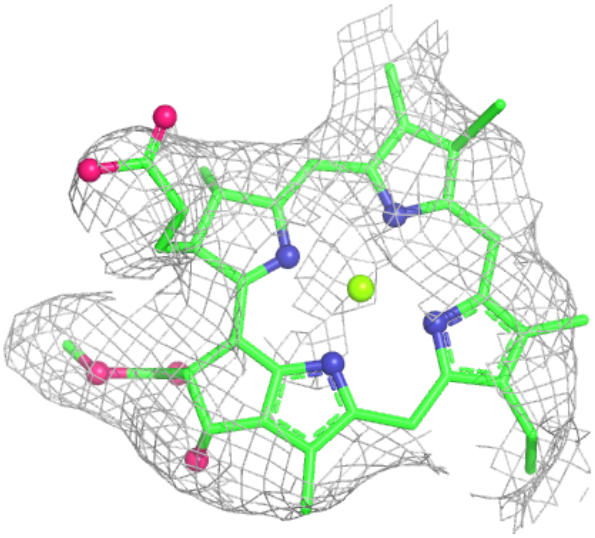


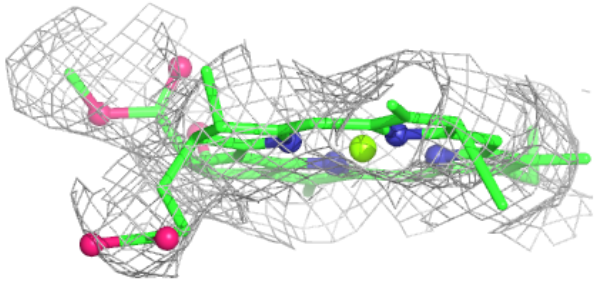


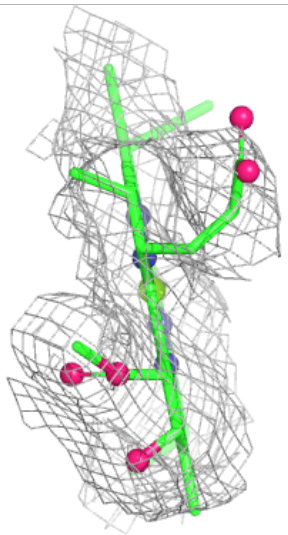


Electron density around CLA A 1791:

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

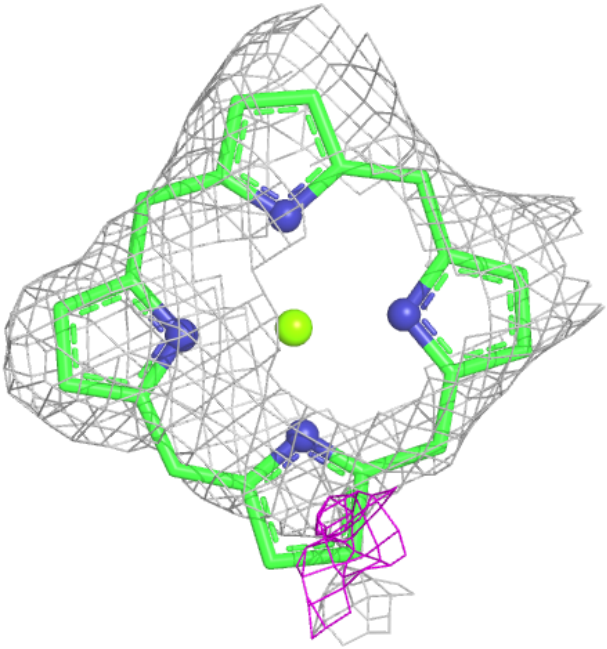


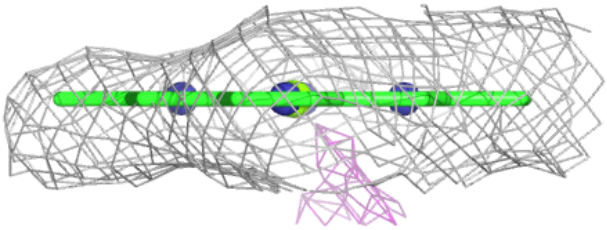


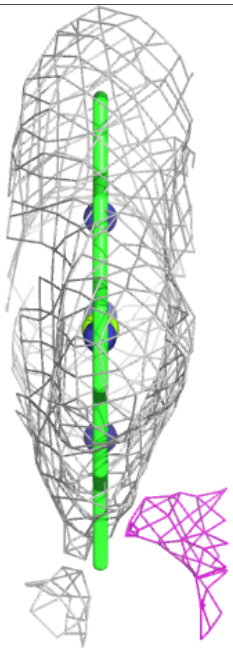


Electron density around CLA 3 3015:

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

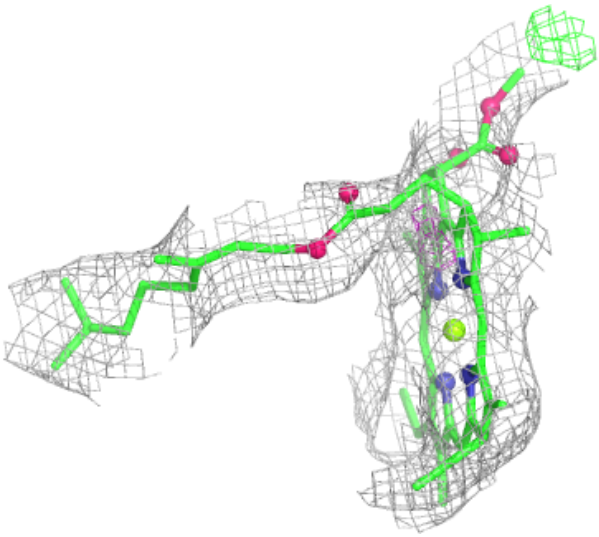


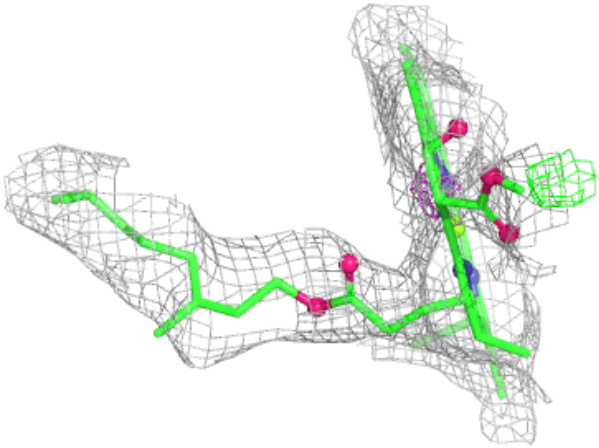


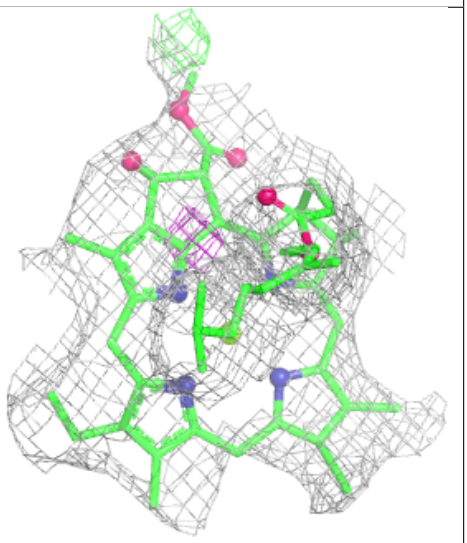


Electron density around CLA 4 1196:

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

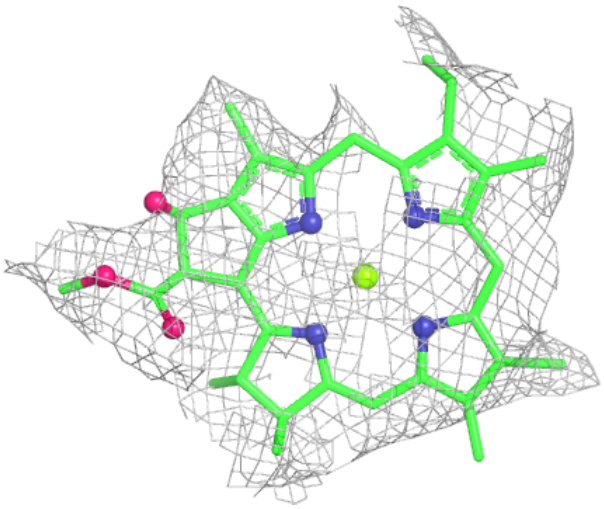


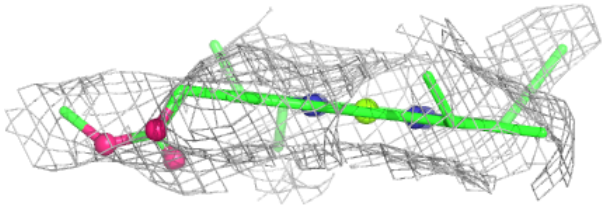


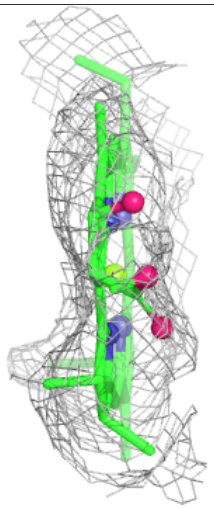


Electron density around CLA F 1156:

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

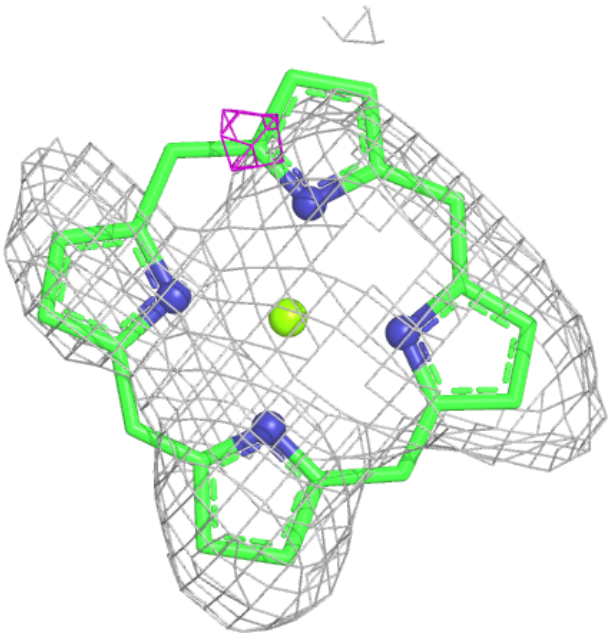


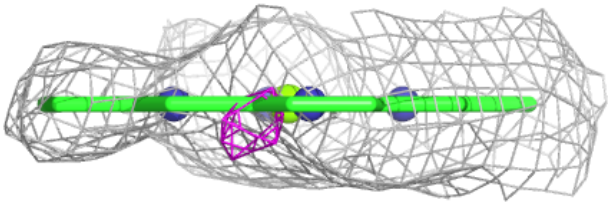


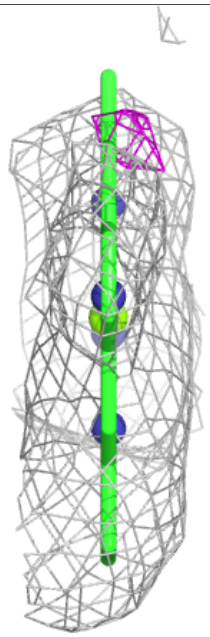


Electron density around CLA 2 1214:

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

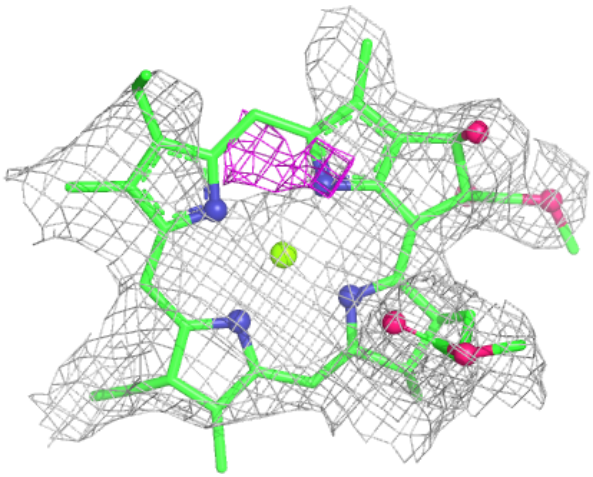


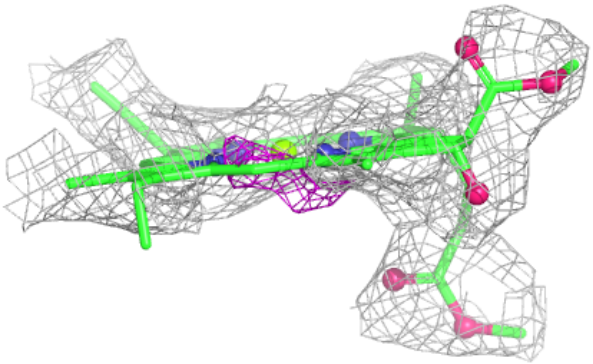


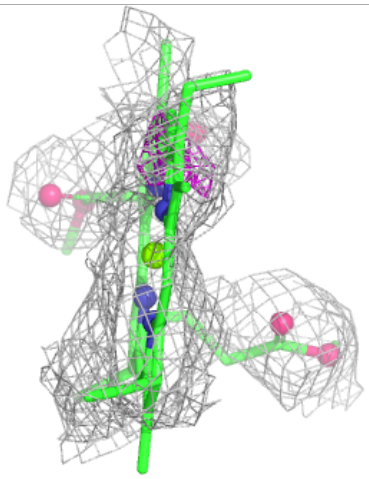


Electron density around CLA A 1763:

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

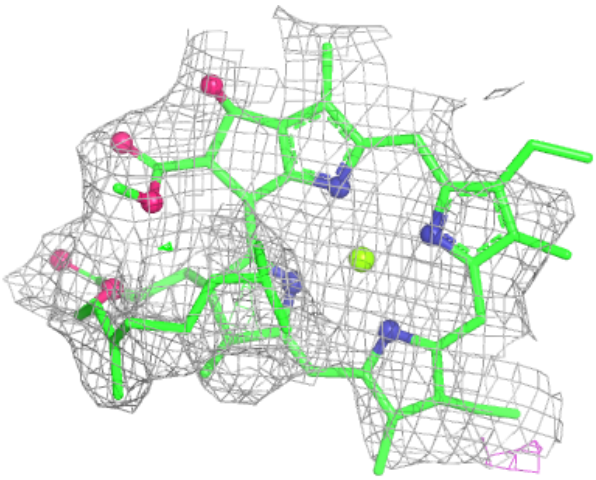


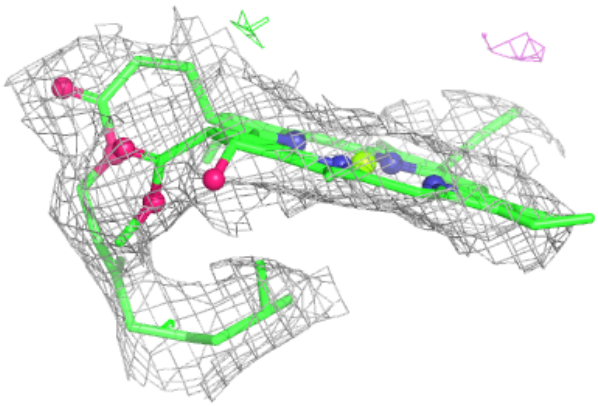




Electron density around CLA 4 1199:

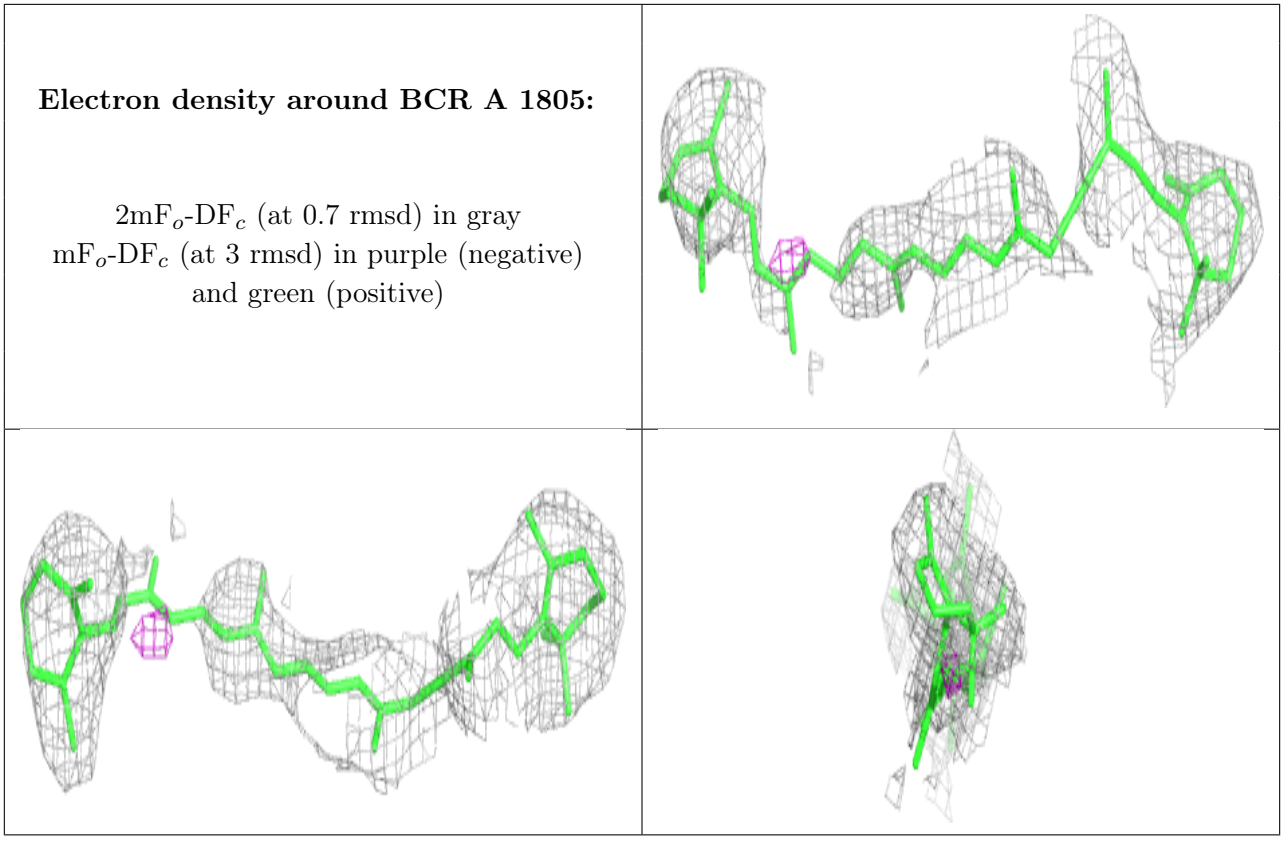
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





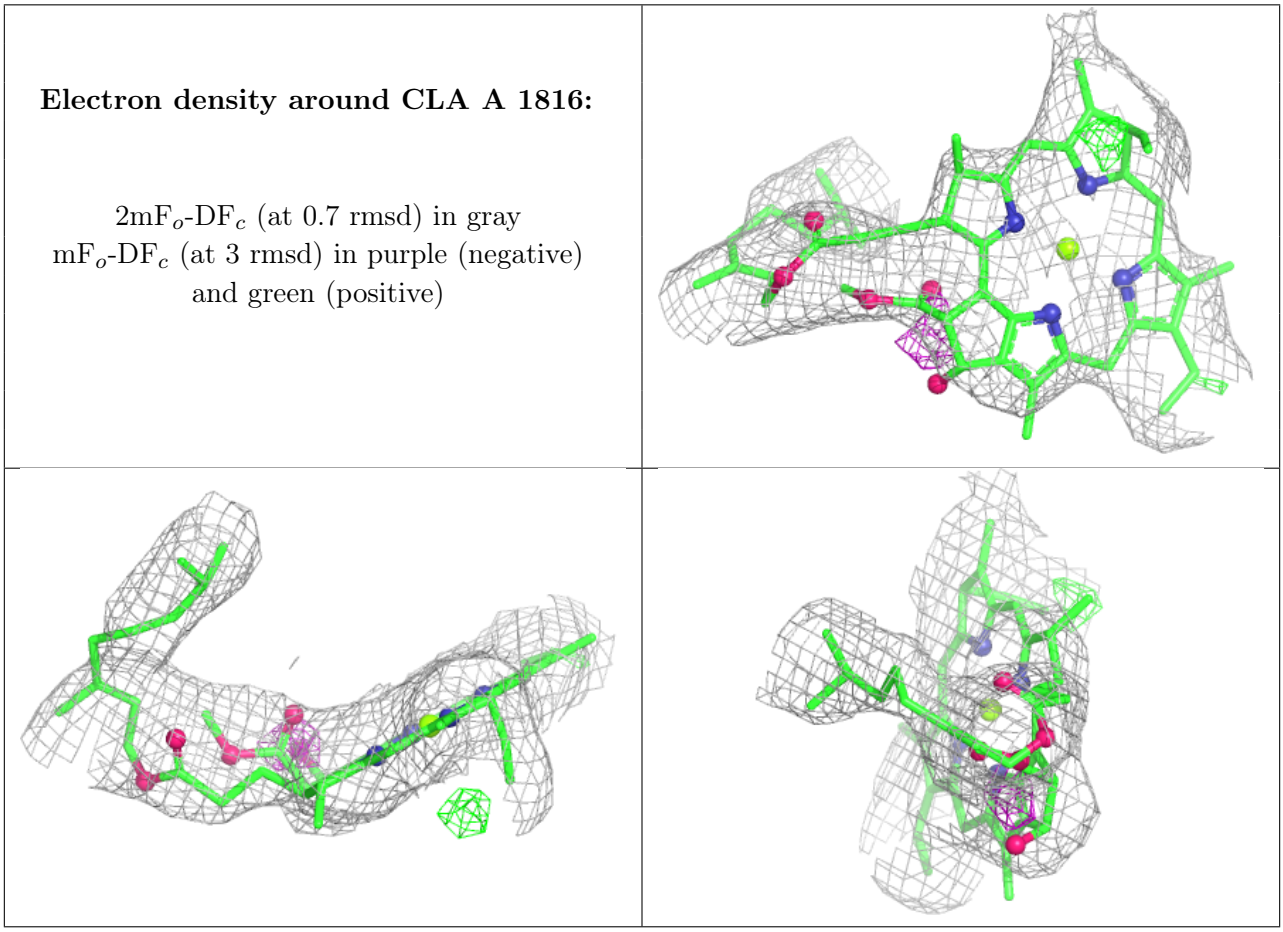
Electron density around BCR A 1805:

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



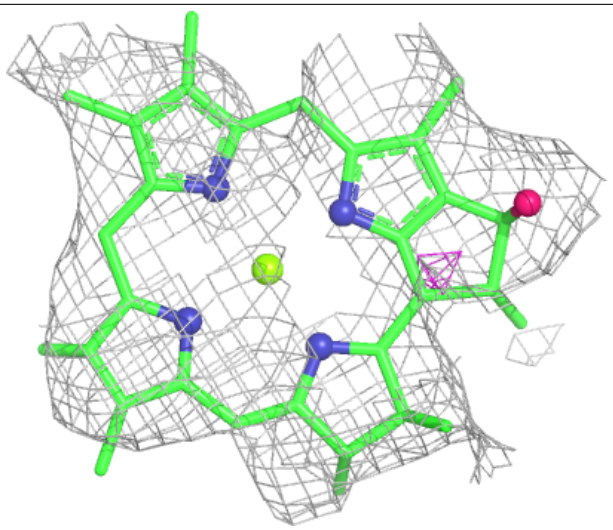
Electron density around CLA A 1816:

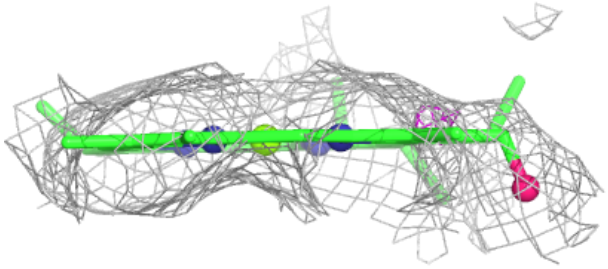
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

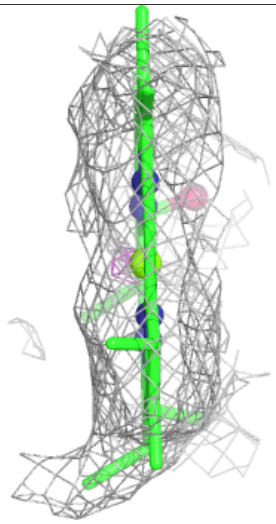


Electron density around CLA 1 1191:

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

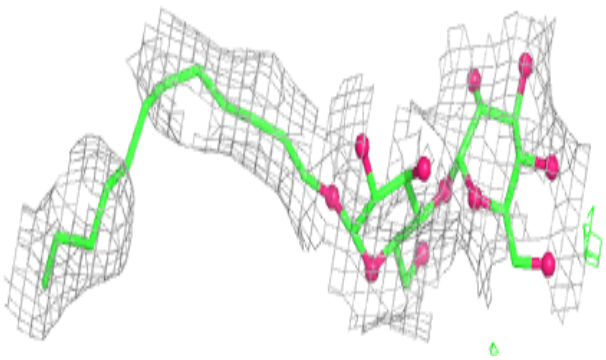


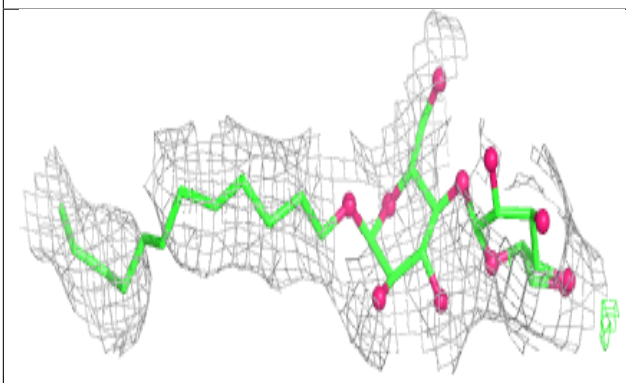




Electron density around LMU A 7040:

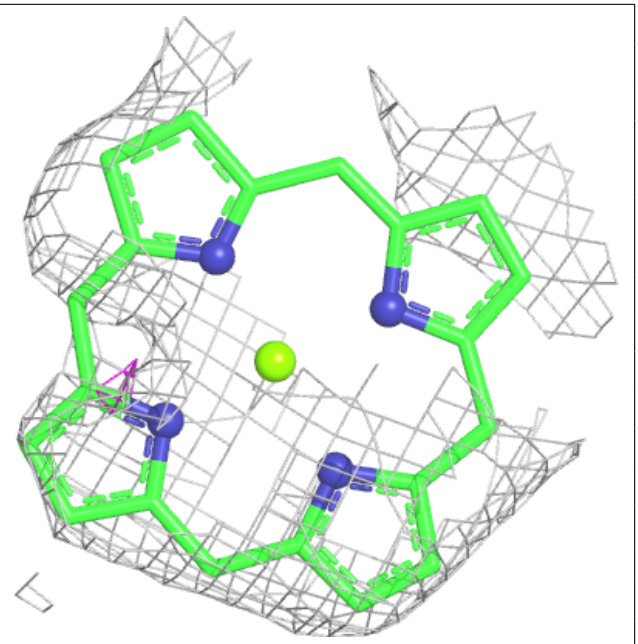
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

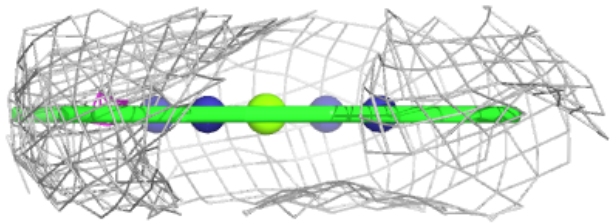


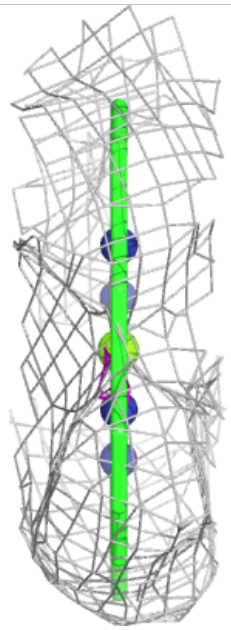


Electron density around CLA 3 1215:

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

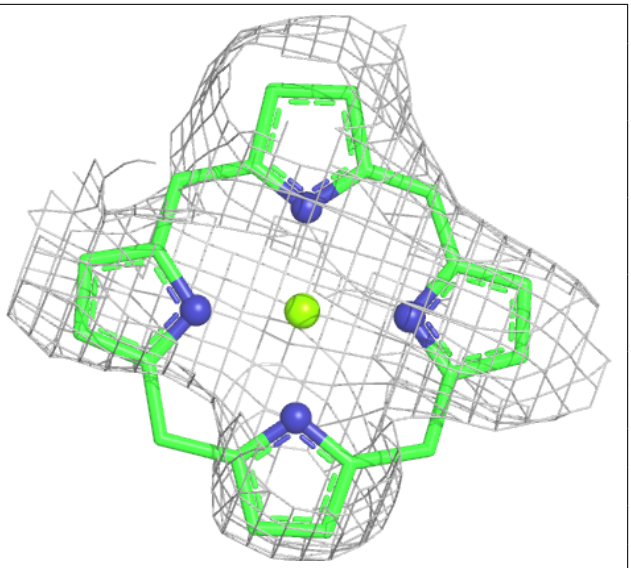


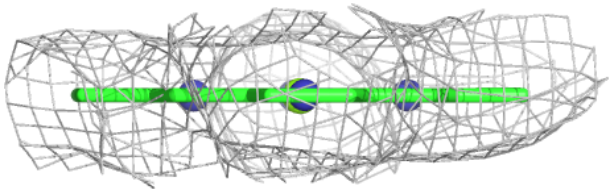


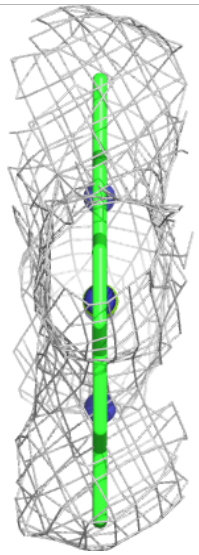


Electron density around CLA 3 3002:

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

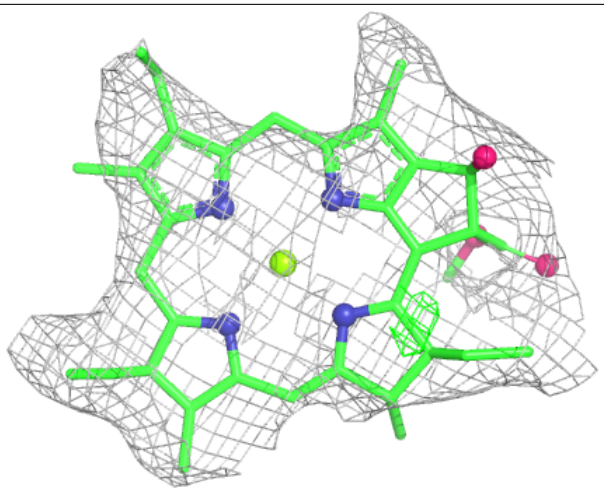


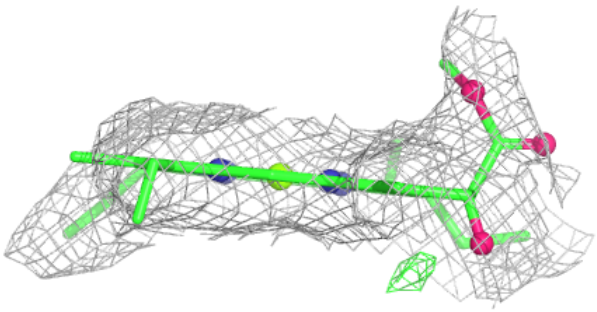


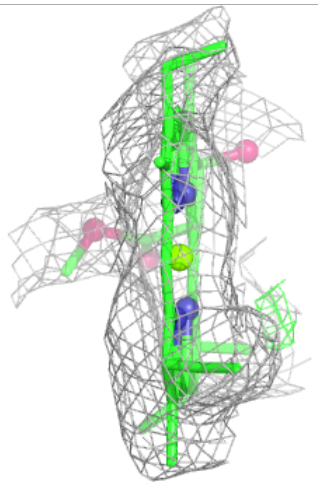


Electron density around CLA 3 3007:

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

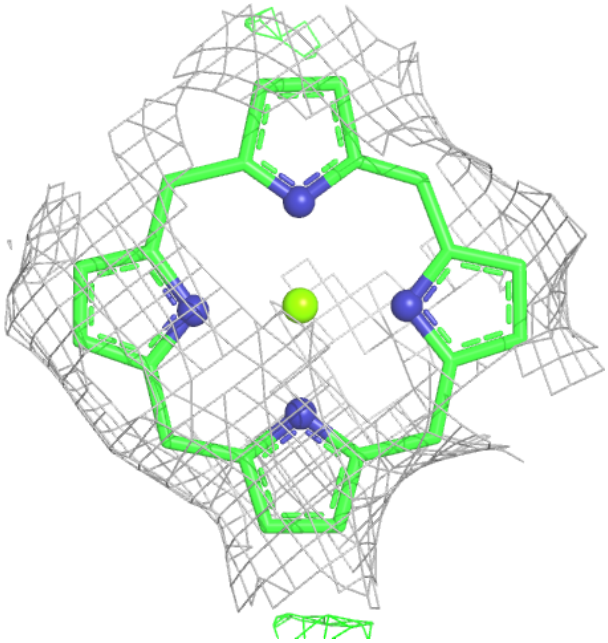


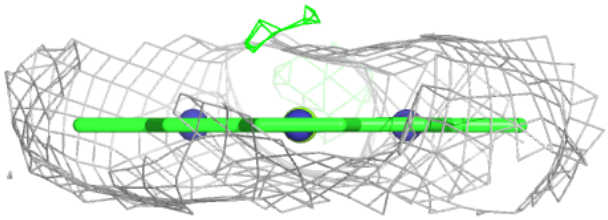


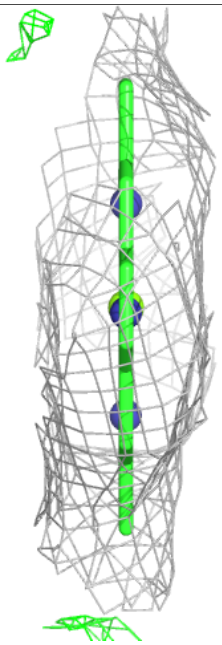


Electron density around CLA 3 1216:

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

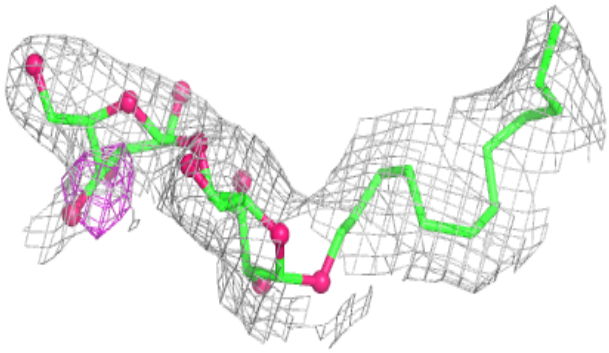


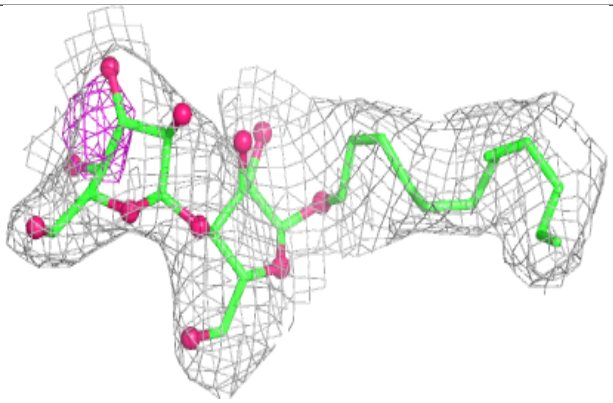


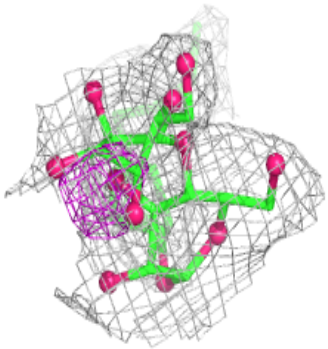


Electron density around LMU A 7026:

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

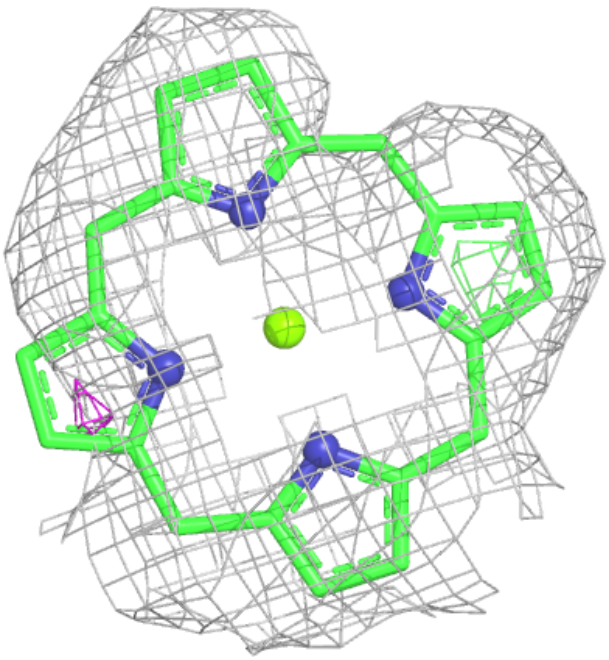


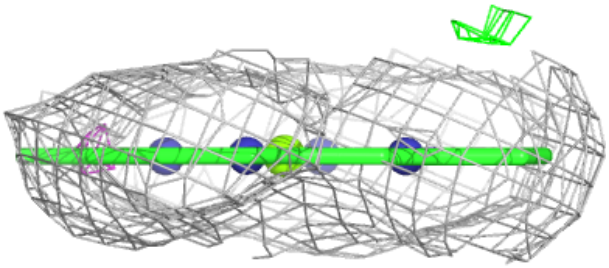


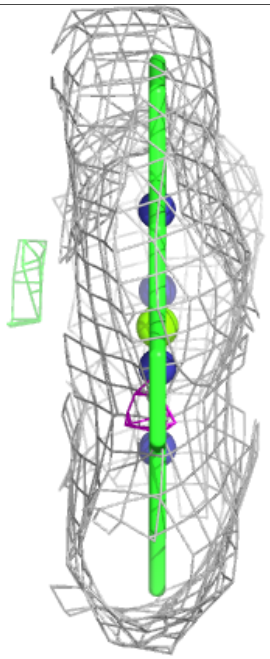


Electron density around CLA 4 1203:

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

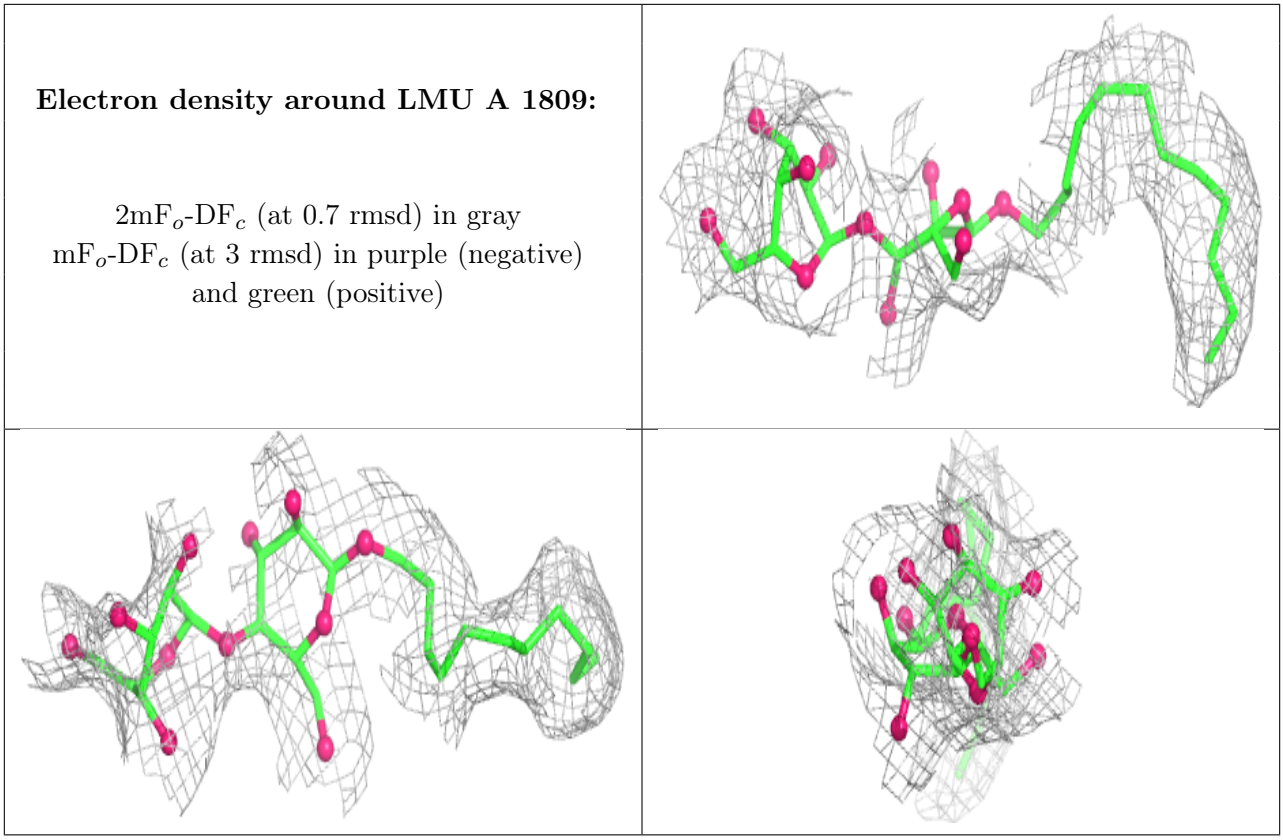






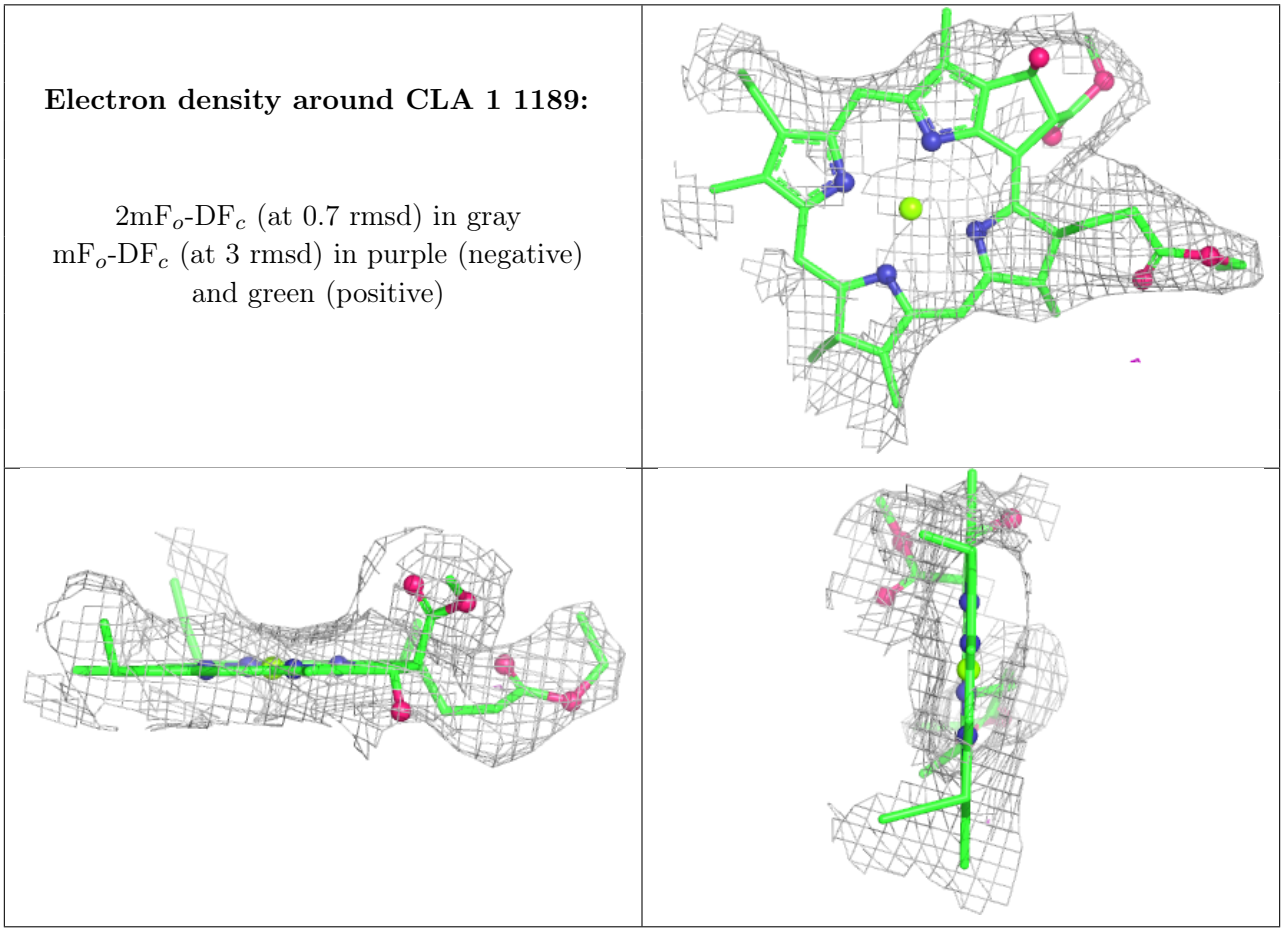
Electron density around LMU A 1809:

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



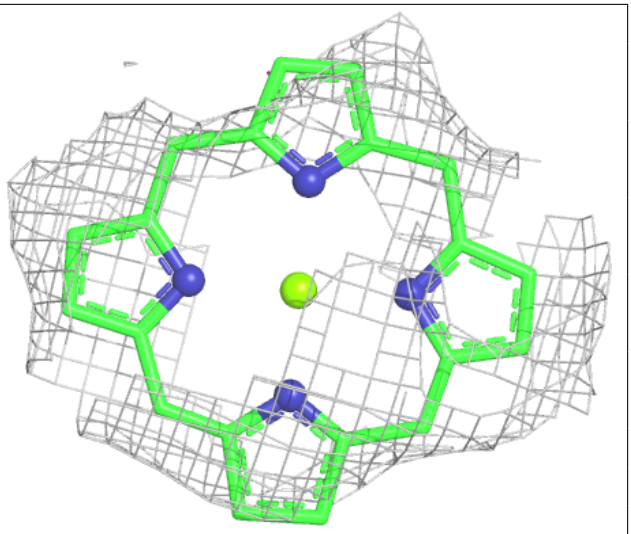
Electron density around CLA 1 1189:

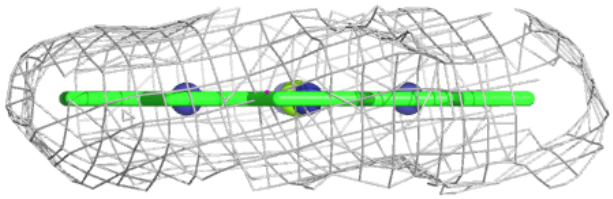
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

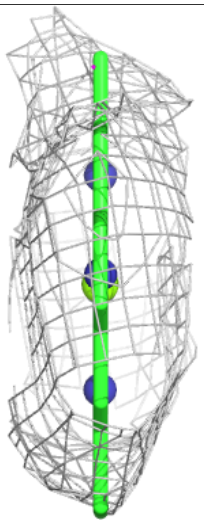


Electron density around CLA 2 1219:

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

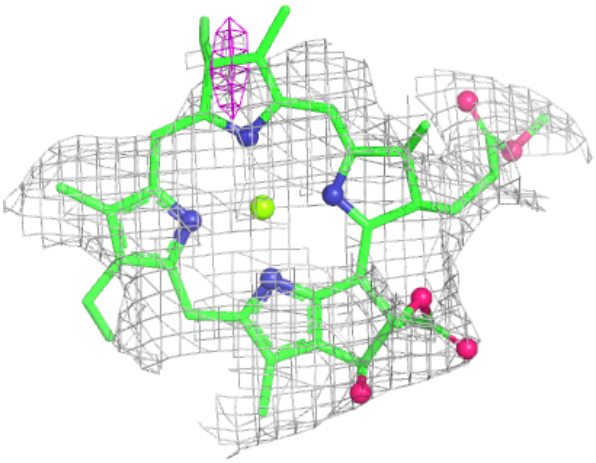


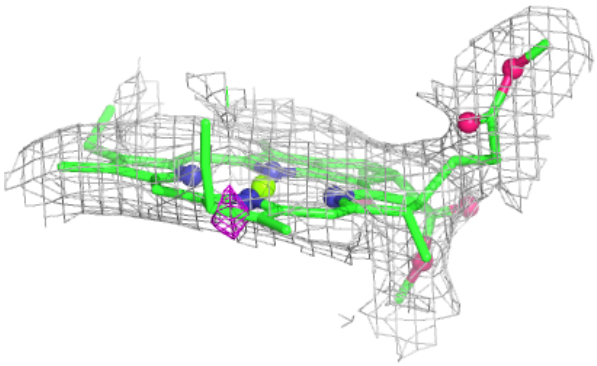


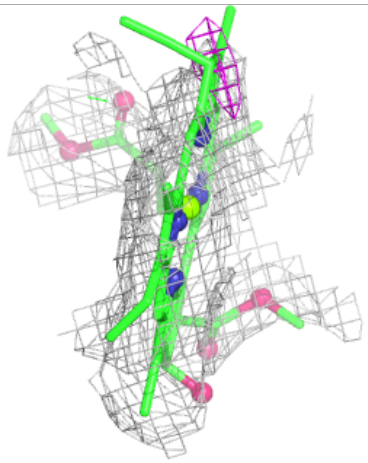


Electron density around CLA B 1751:

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

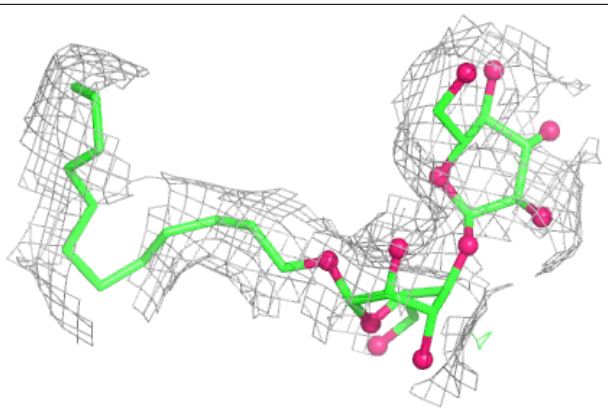


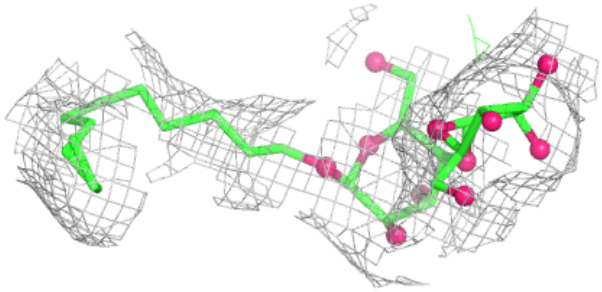


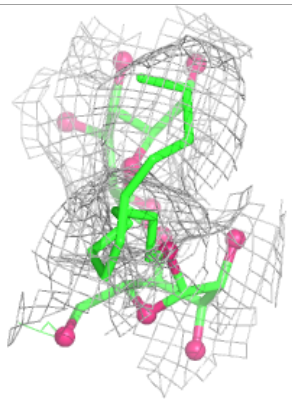


Electron density around LMU K 1086:

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

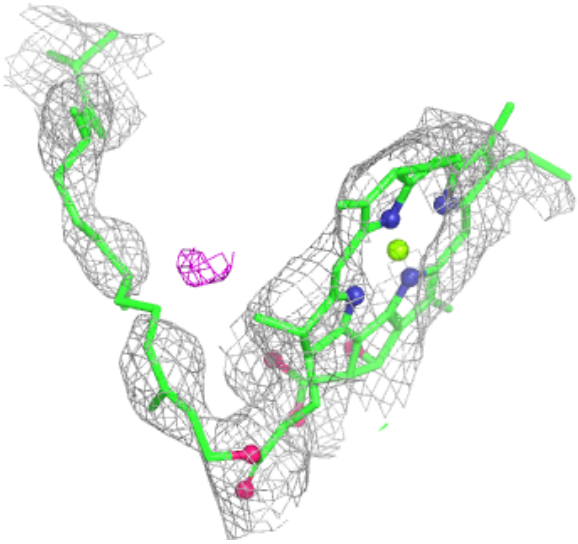


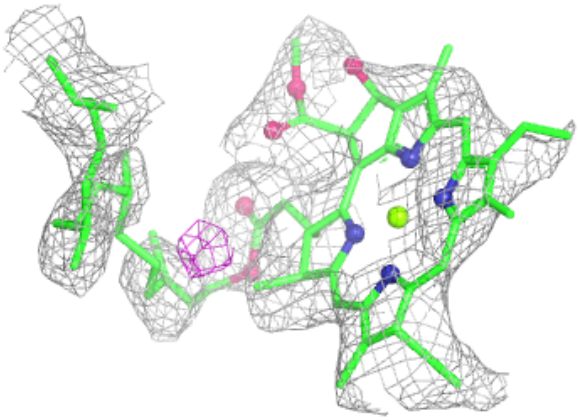


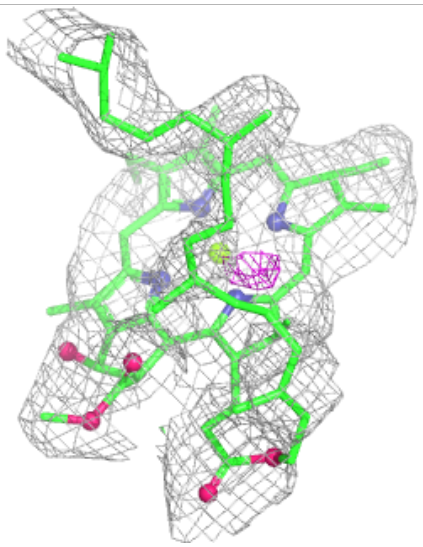


Electron density around CLA 2 1217:

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

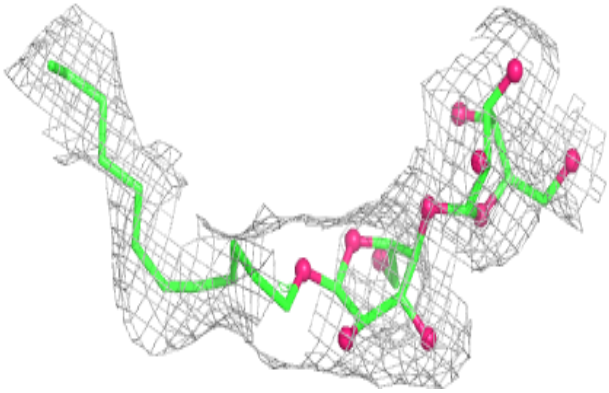


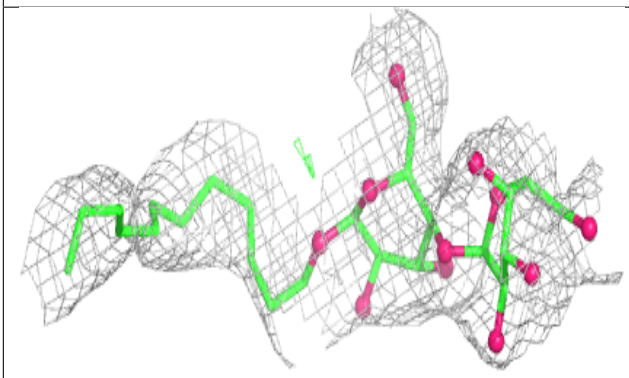


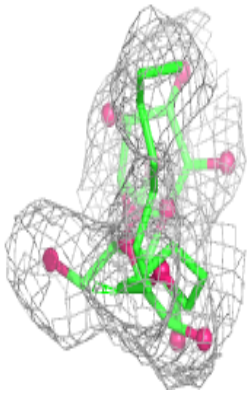


Electron density around LMU A 7027:

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

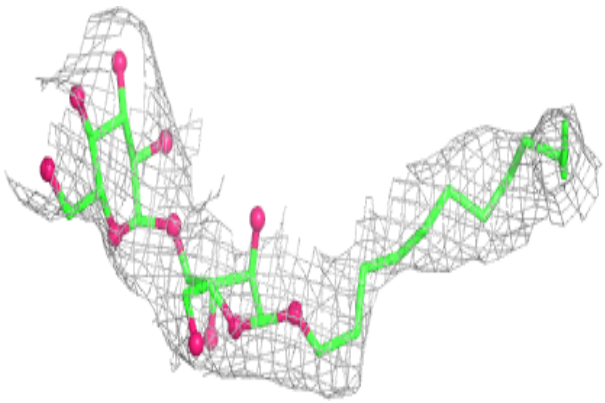


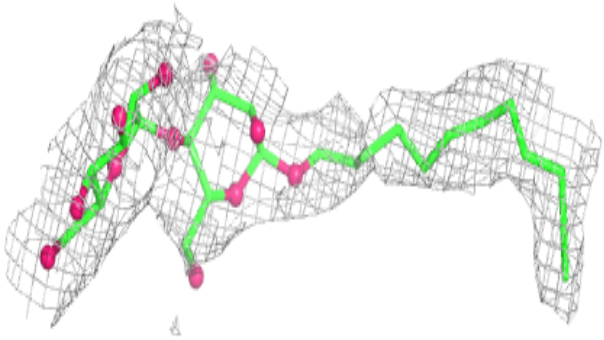


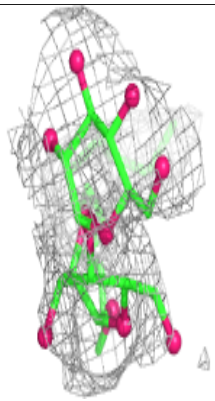


Electron density around LMU 4 1210:

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

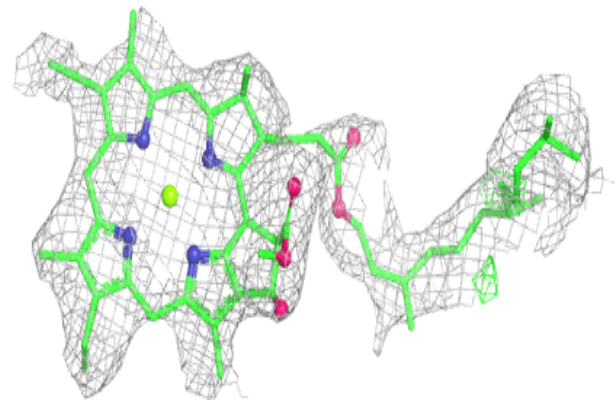


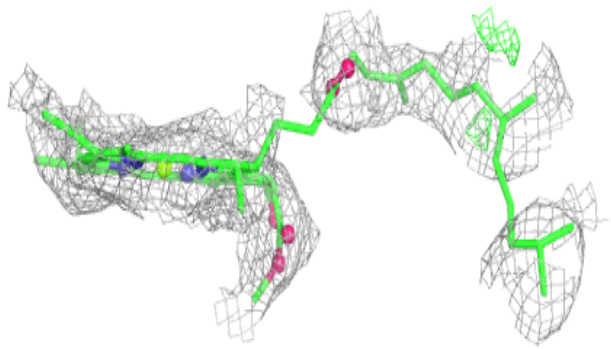


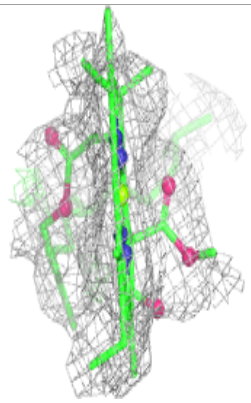


Electron density around CLA B 1745:

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

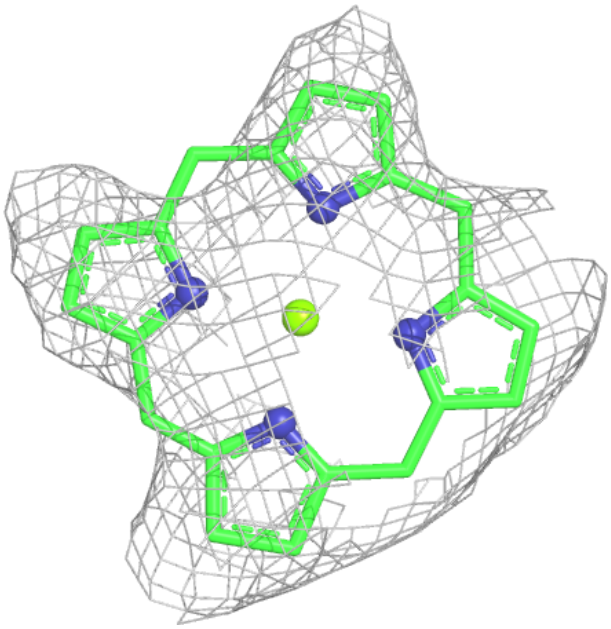


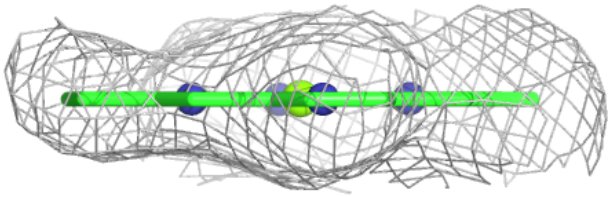


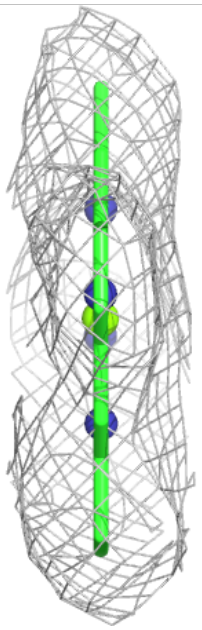


Electron density around CLA 2 2010:

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

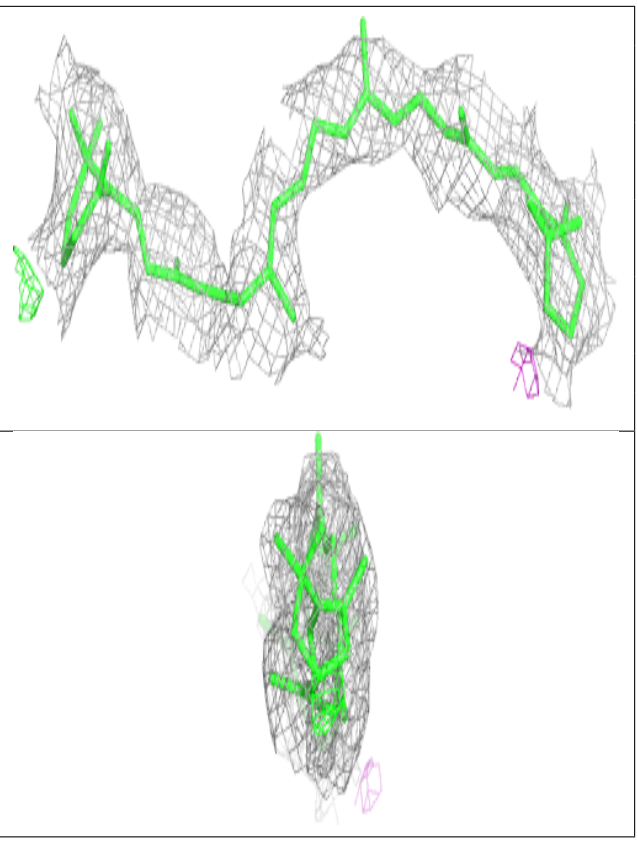






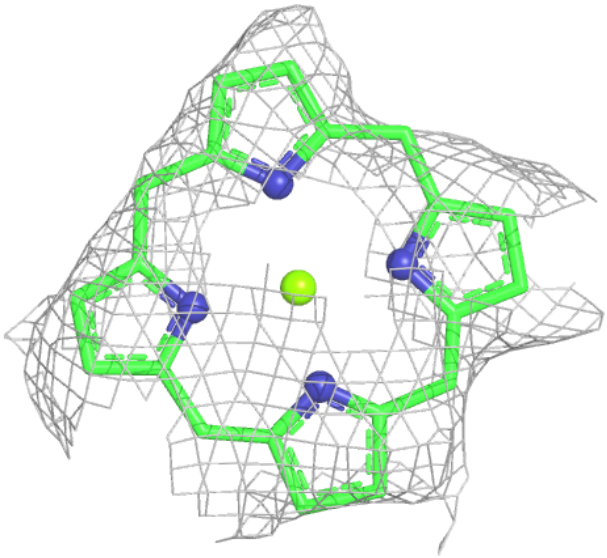
Electron density around BCR I 1032:

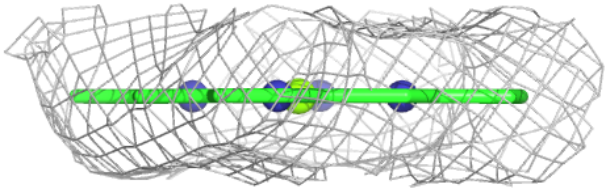
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

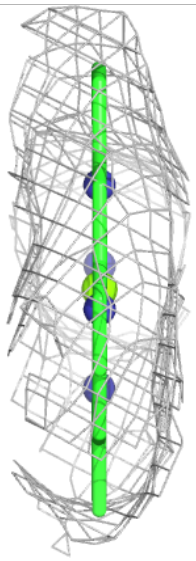


Electron density around CLA 1 1201:

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

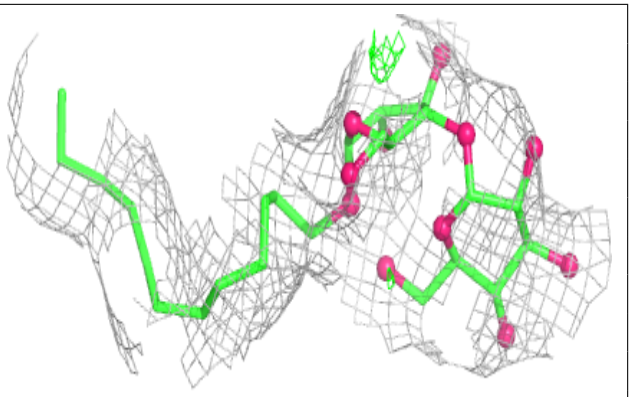


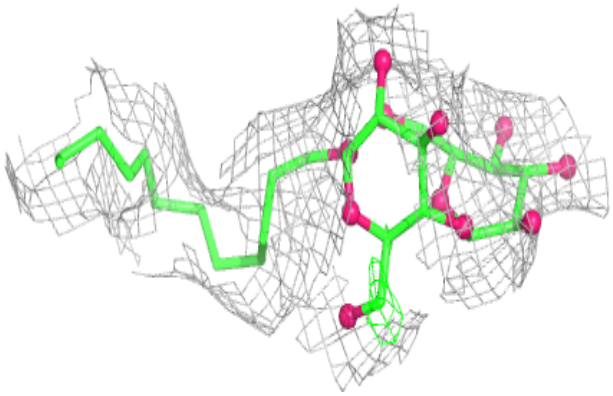


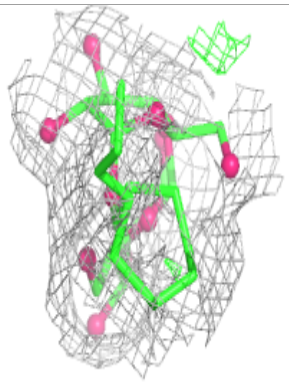


Electron density around LMU A 1810:

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

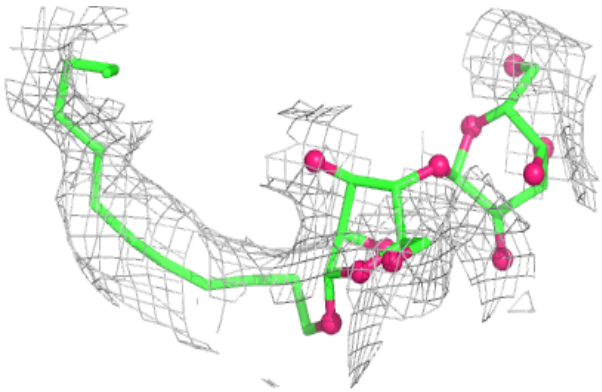


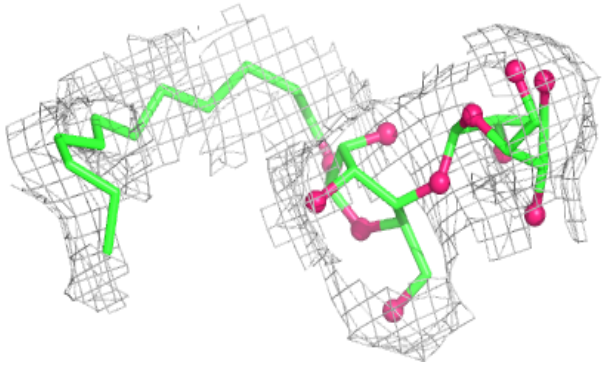




Electron density around LMU A 7022:

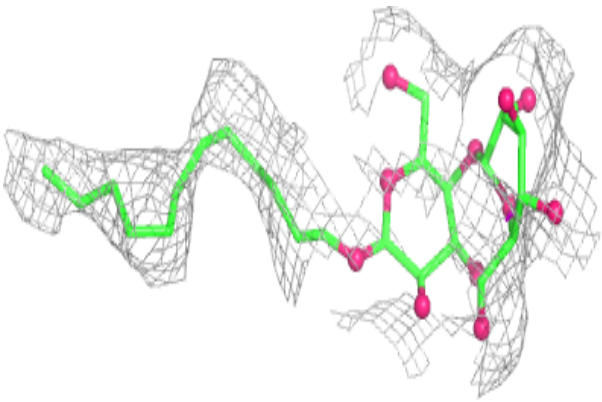
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

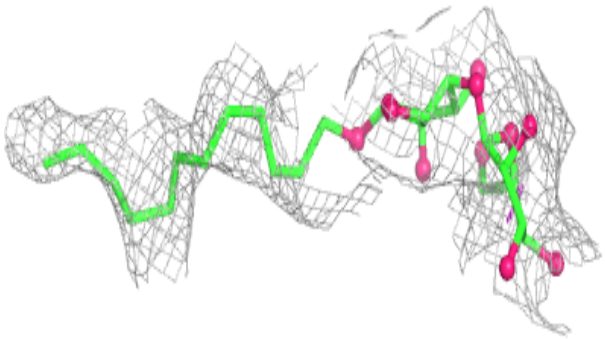


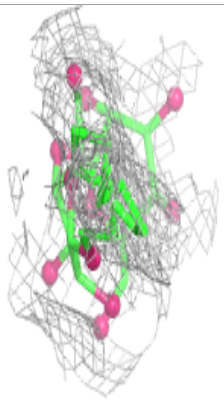


Electron density around LMU A 7033:

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

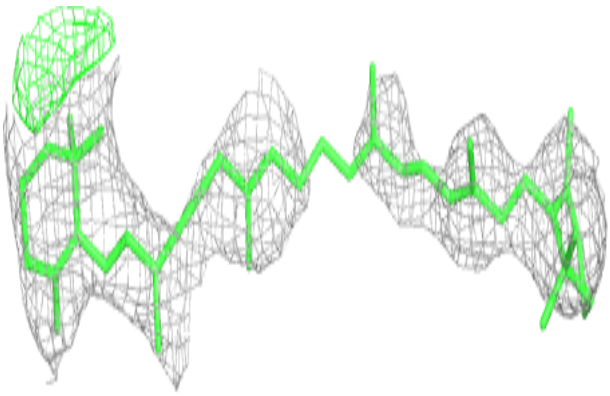


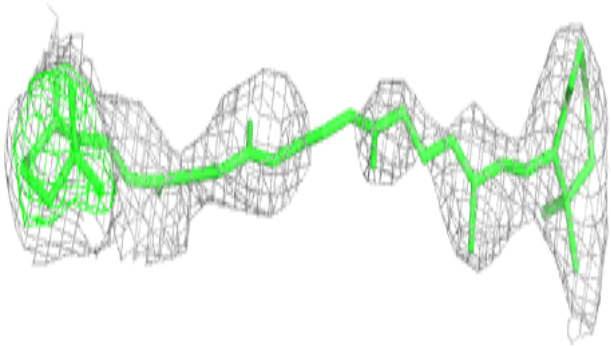


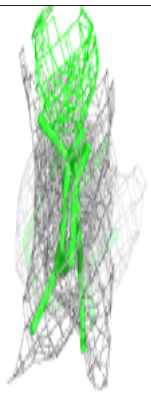


Electron density around BCR A 1804:

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

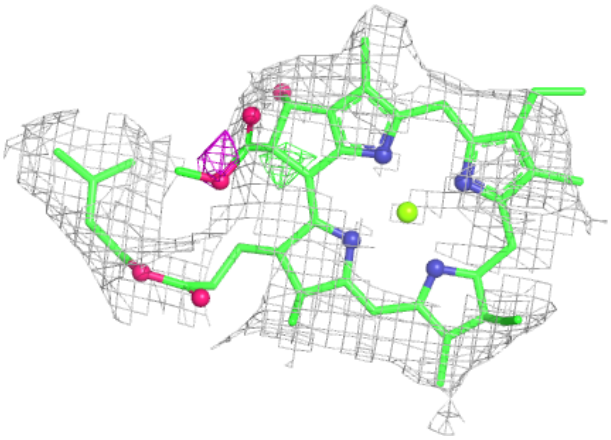


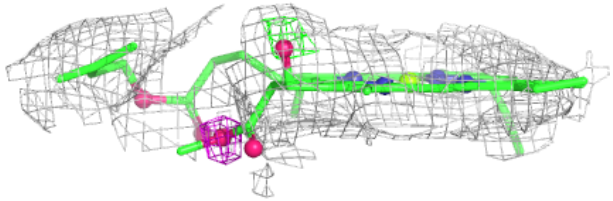




Electron density around CLA 2 1223:

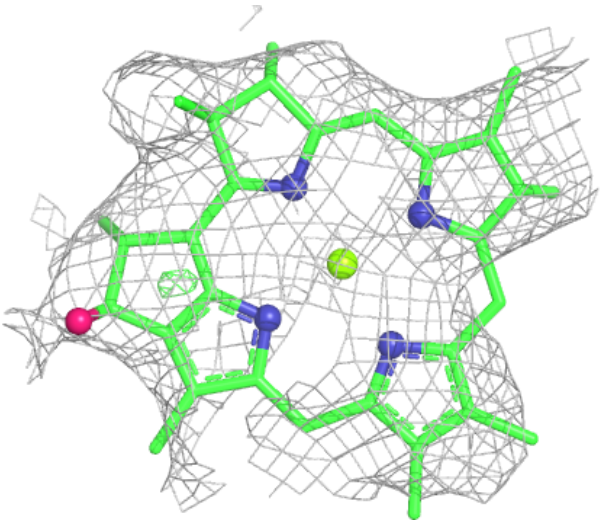
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

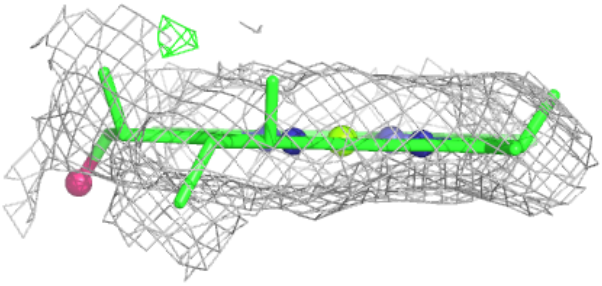


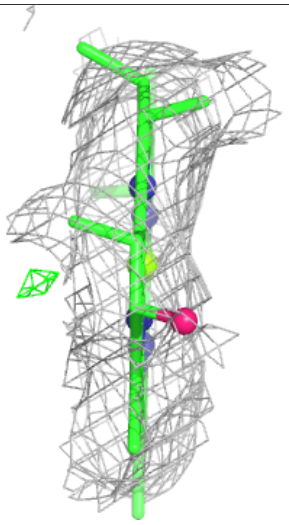


Electron density around CLA B 1772:

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

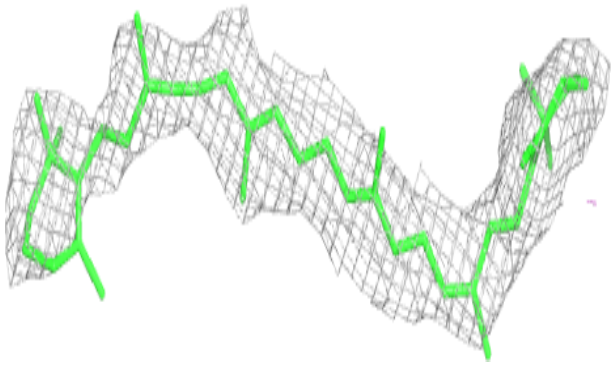


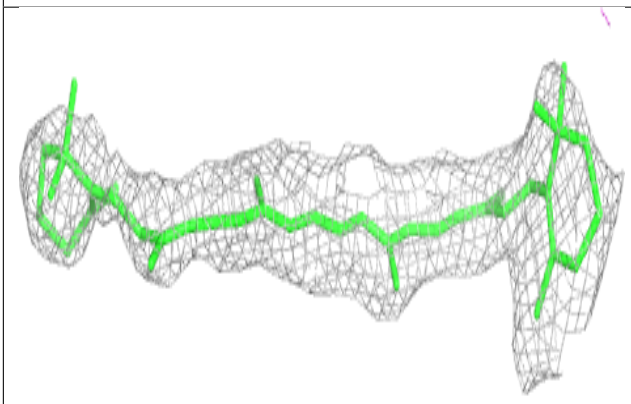


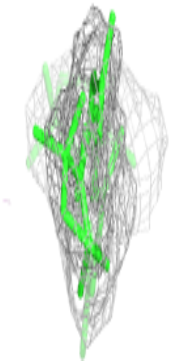


Electron density around BCR B 1776:

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

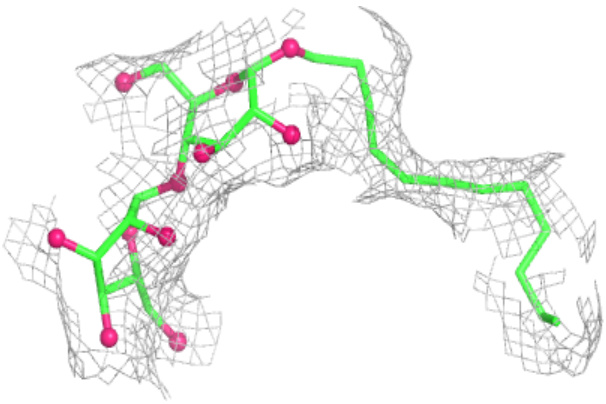


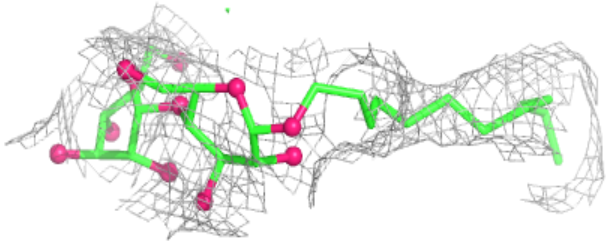


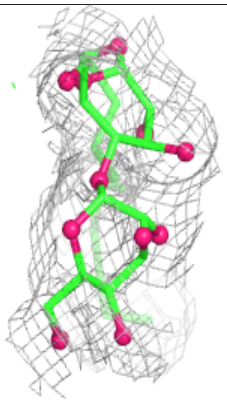


Electron density around LMU A 7019:

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

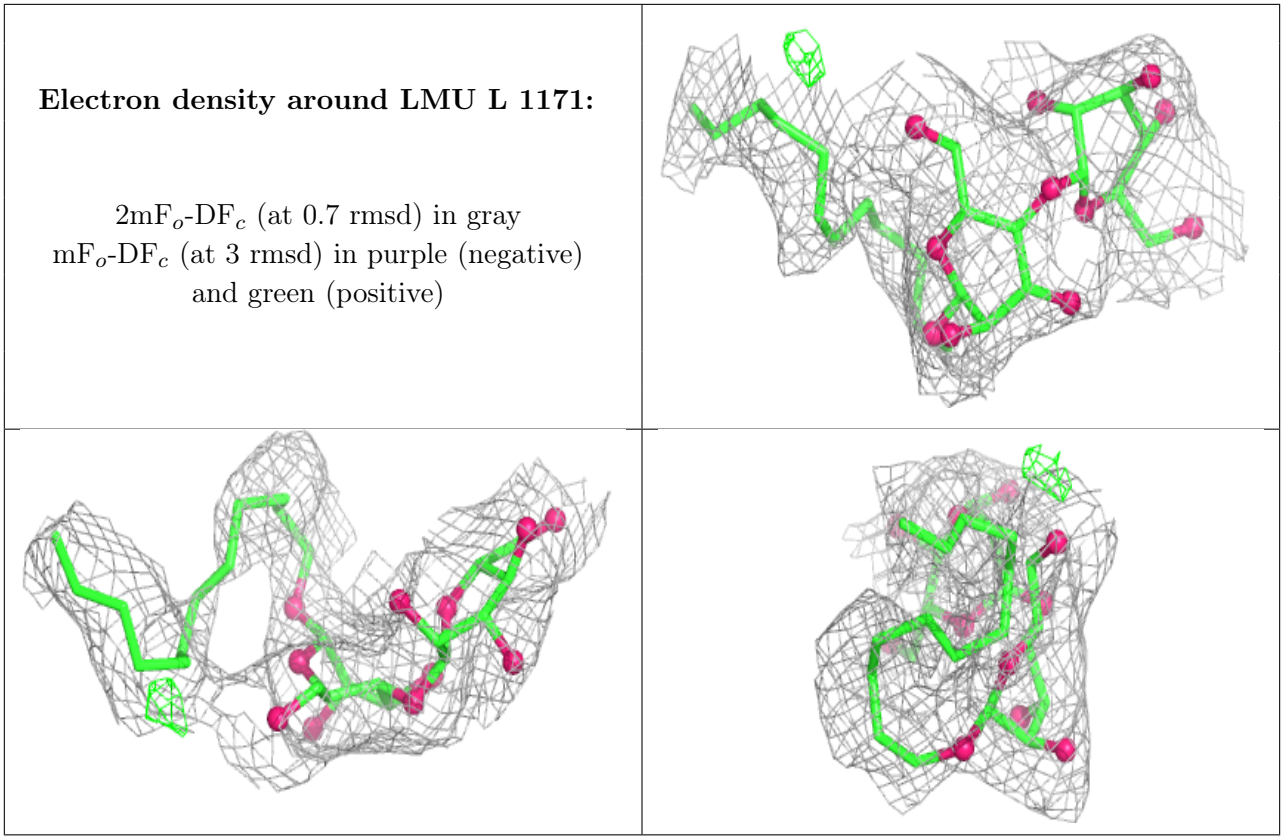






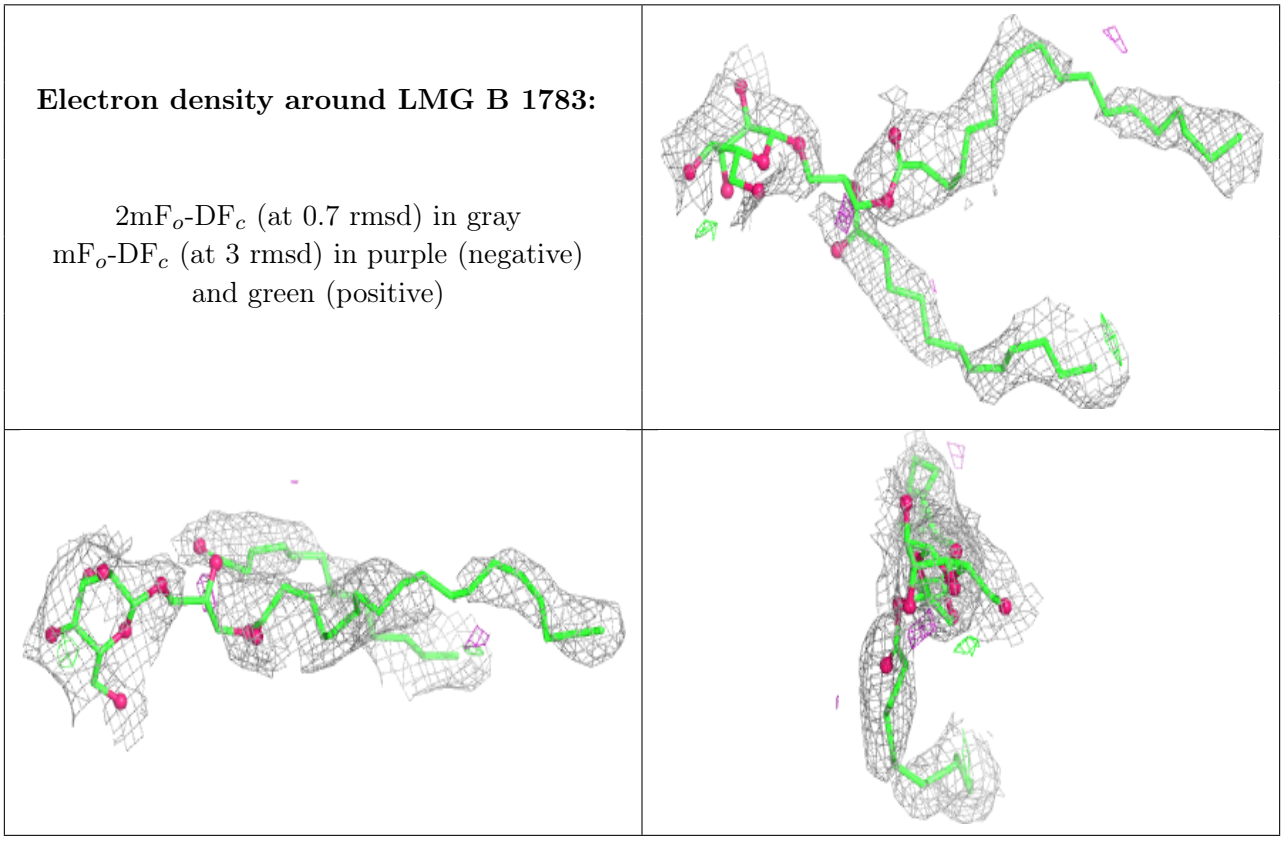
Electron density around LMU L 1171:

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



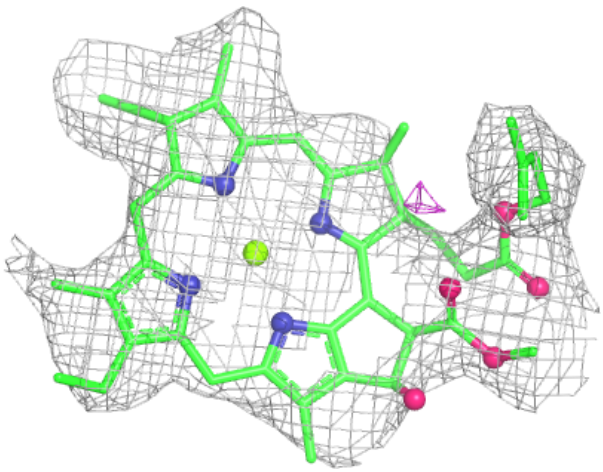
Electron density around LMG B 1783:

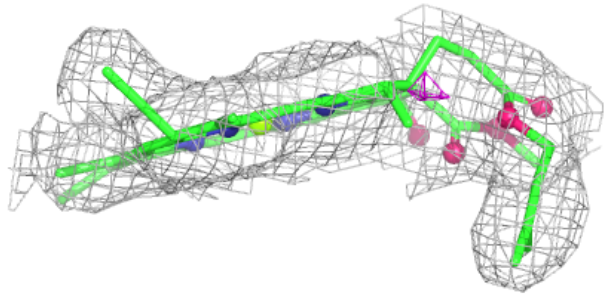
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 3 3008:

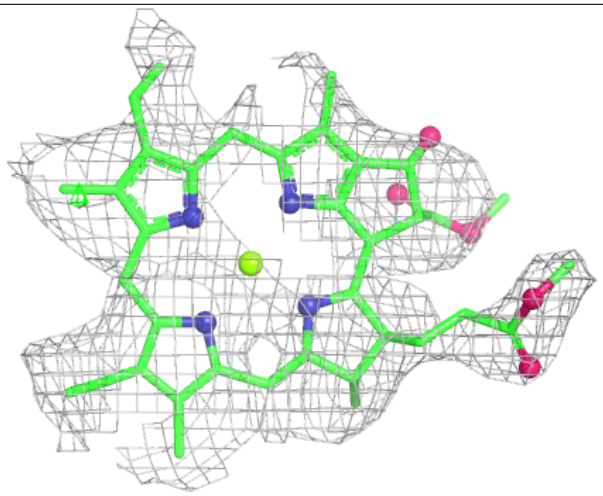
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

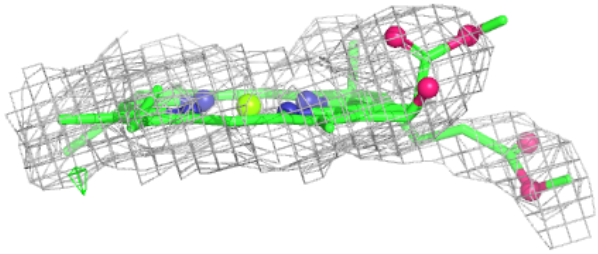




Electron density around CLA 4 1209:

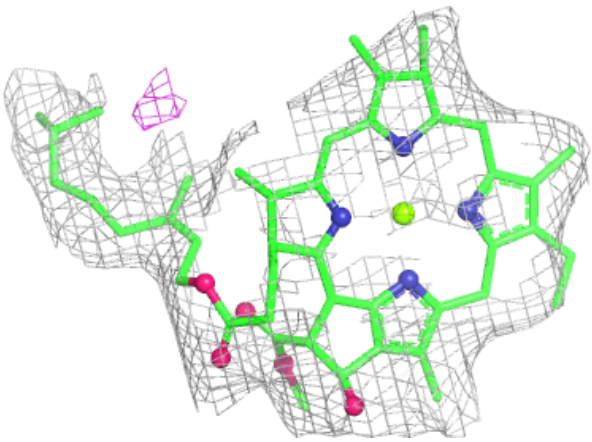
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

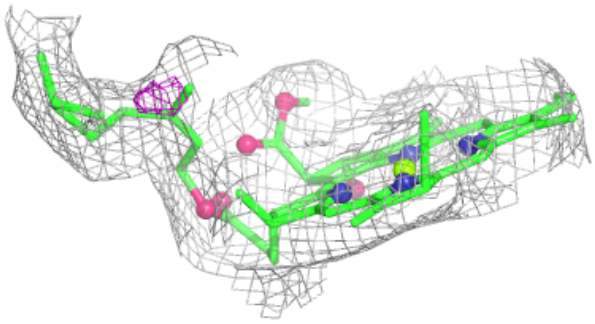




Electron density around CLA J 1045:

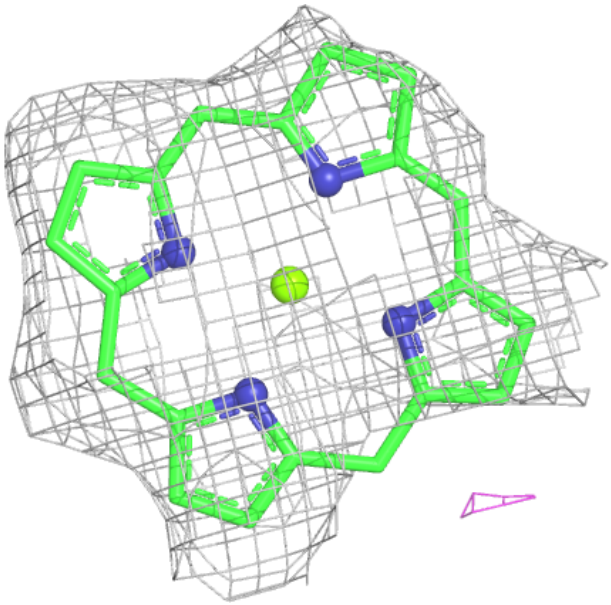
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

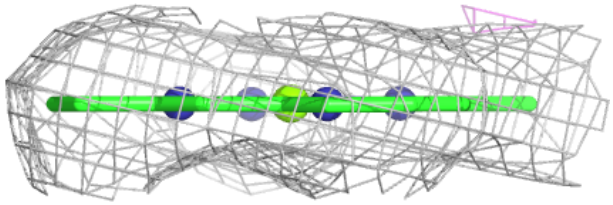


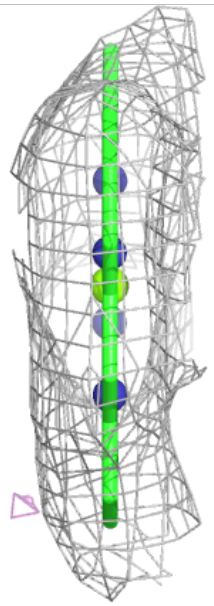


Electron density around CLA 3 3001:

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

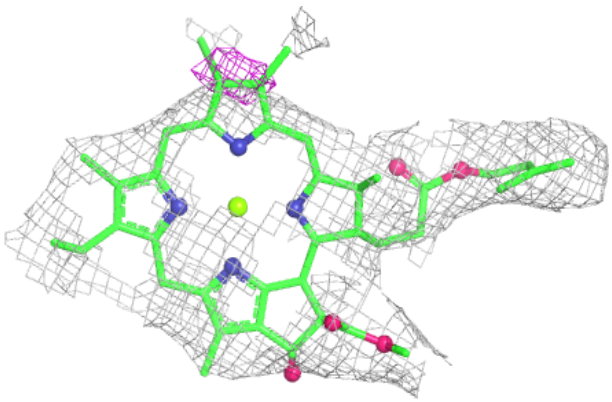


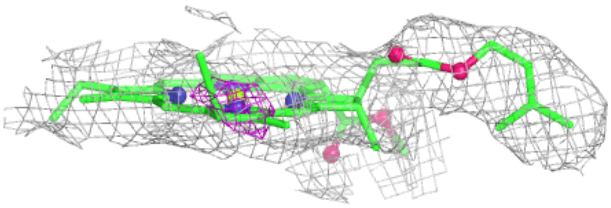


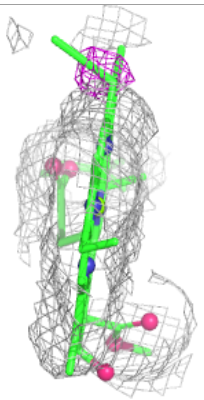


Electron density around CLA K 1085:

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

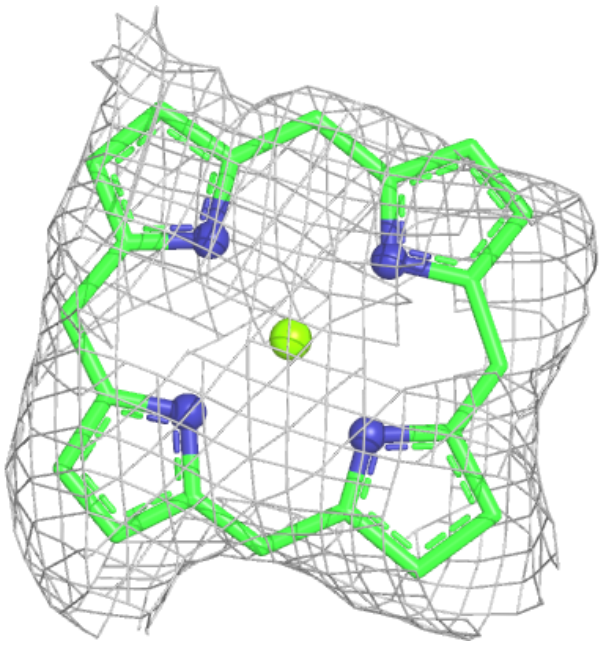


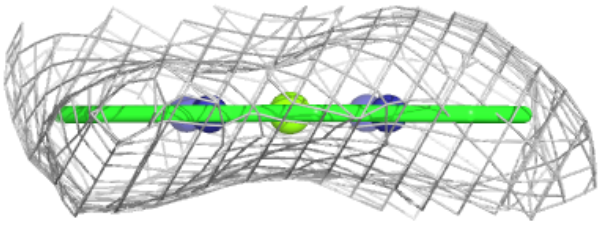


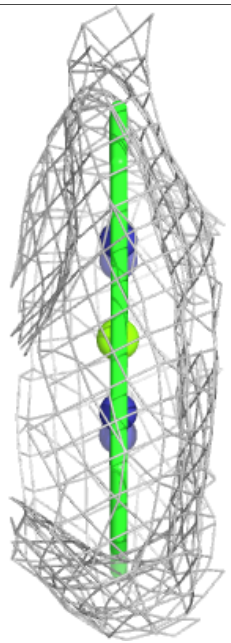


Electron density around CLA 2 1221:

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

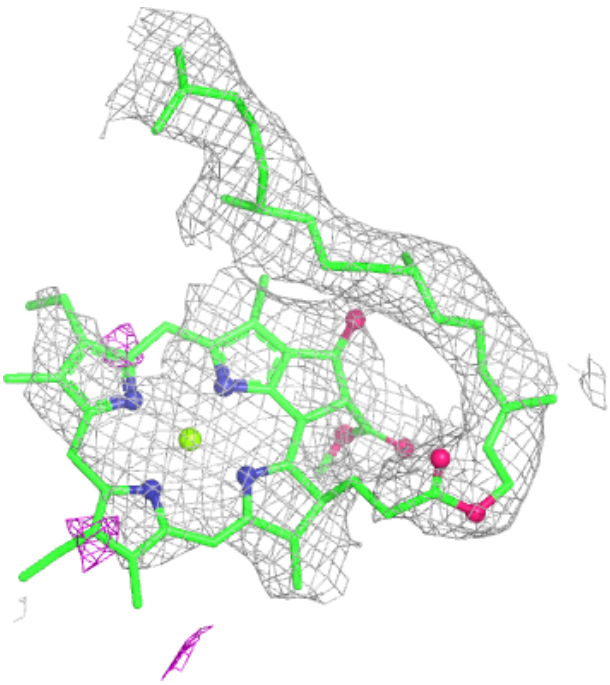


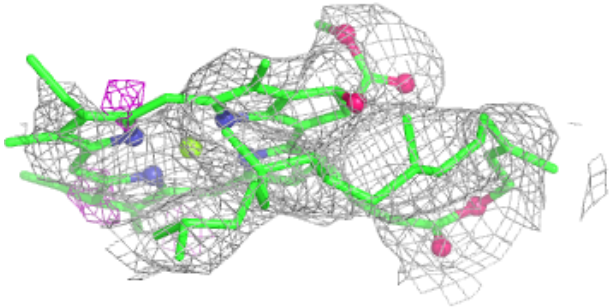


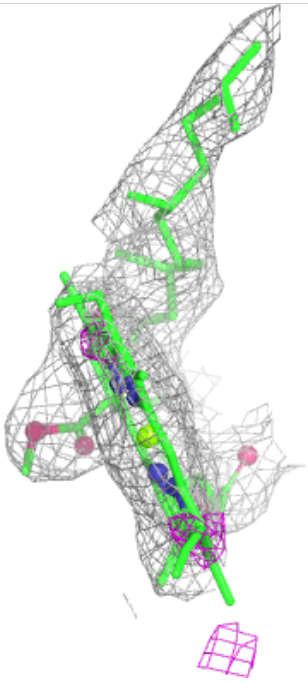


Electron density around CLA A 1780:

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

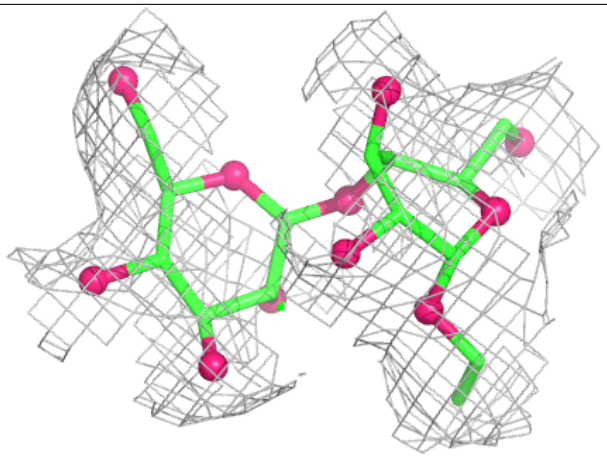


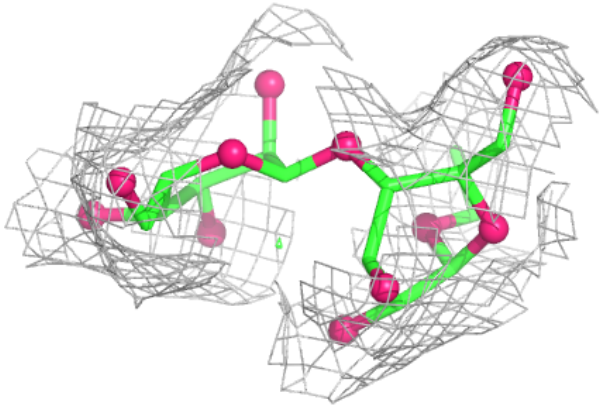


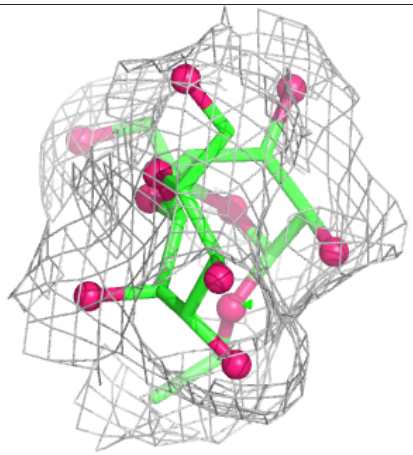


Electron density around LMU B 1782:

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

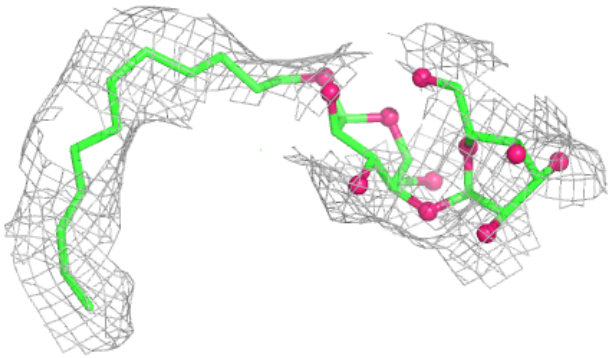


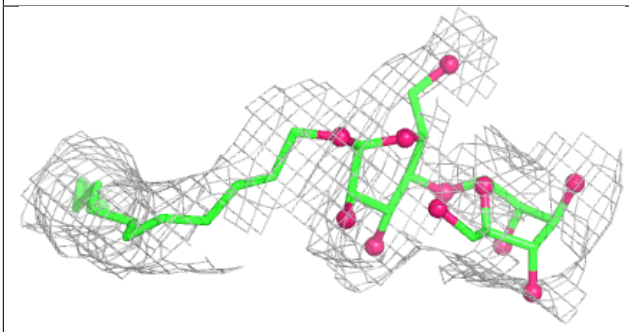


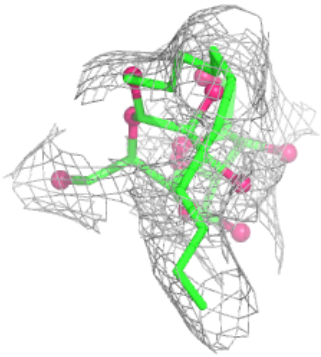


Electron density around LMU 2 7006:

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

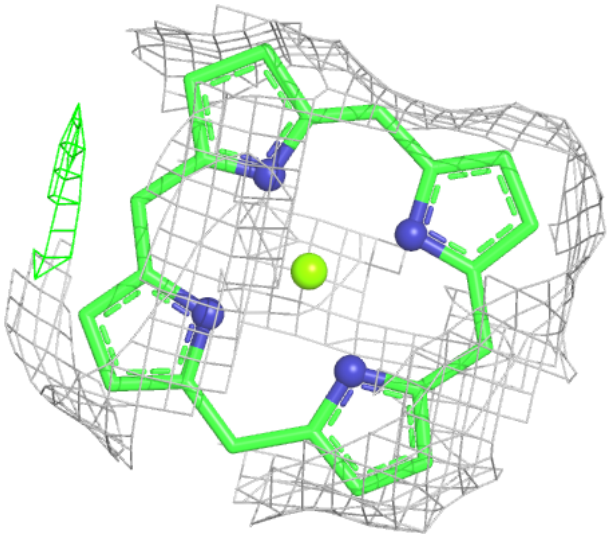


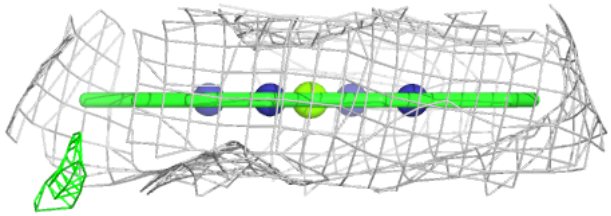


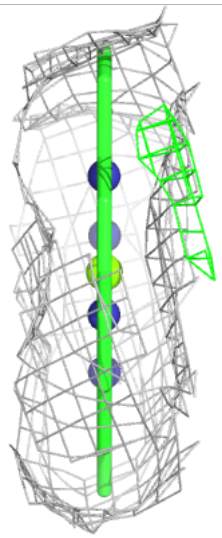


Electron density around CLA 3 1213:

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

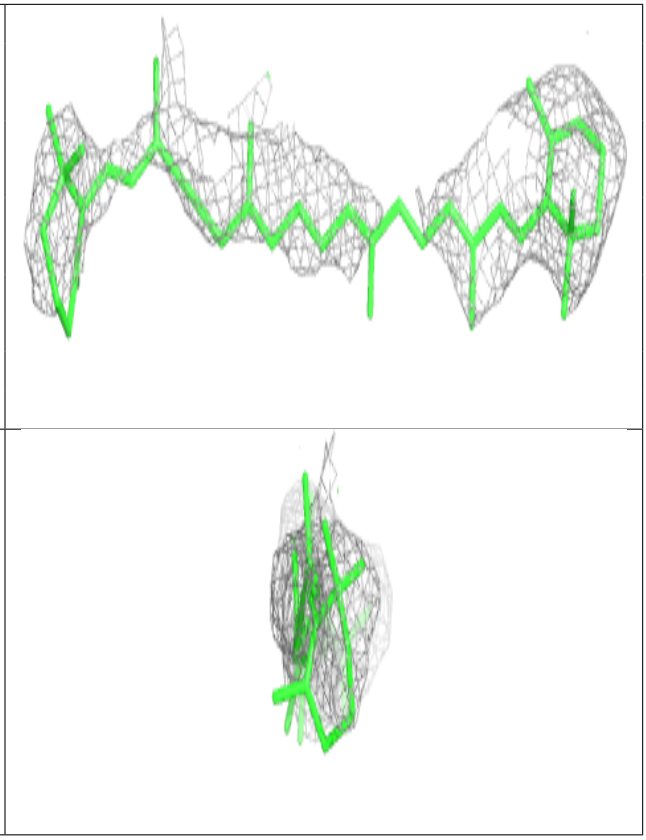






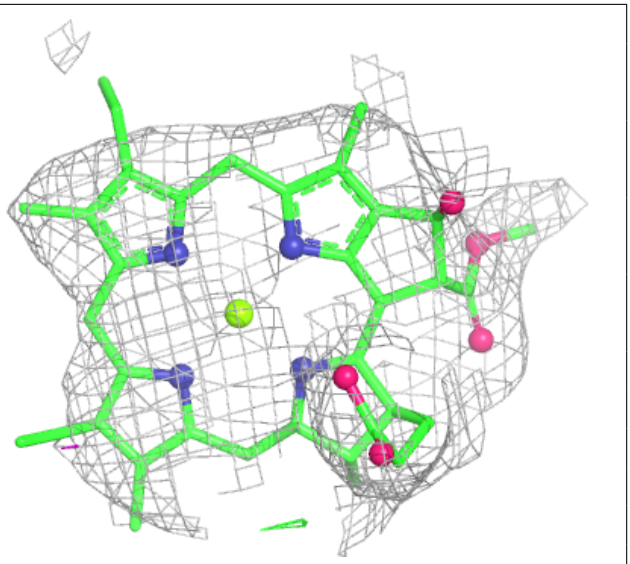
Electron density around BCR A 1806:

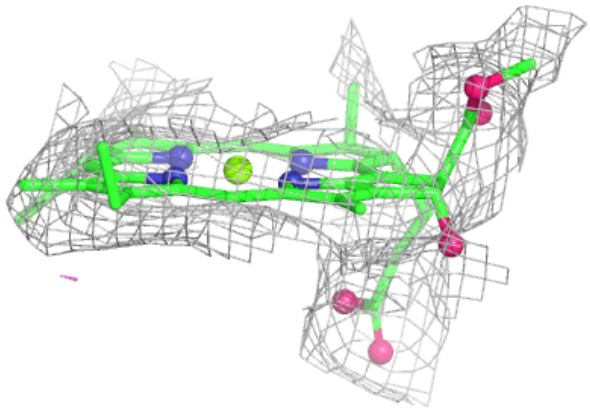
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1764:

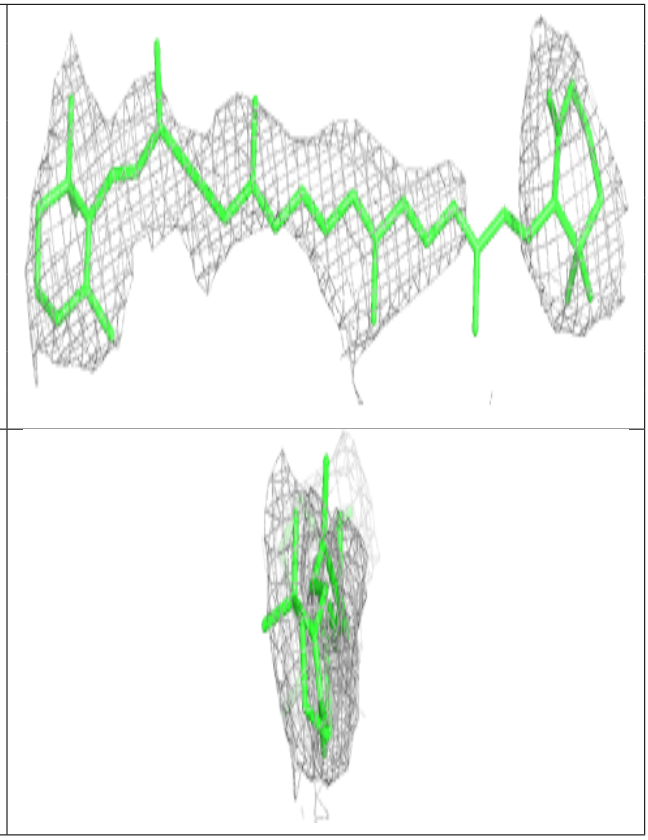
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





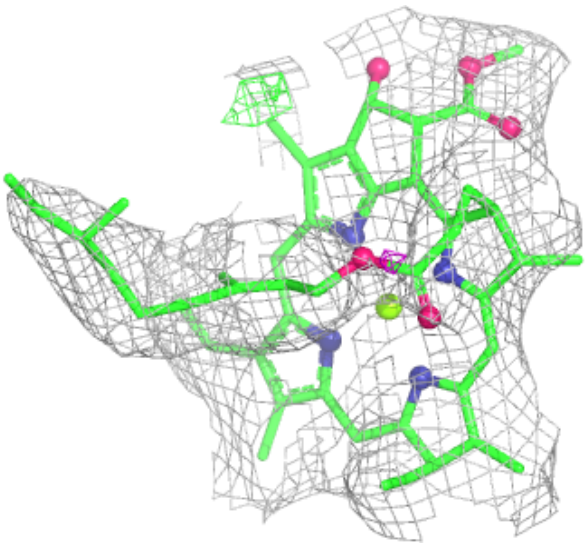
Electron density around BCR B 1774:

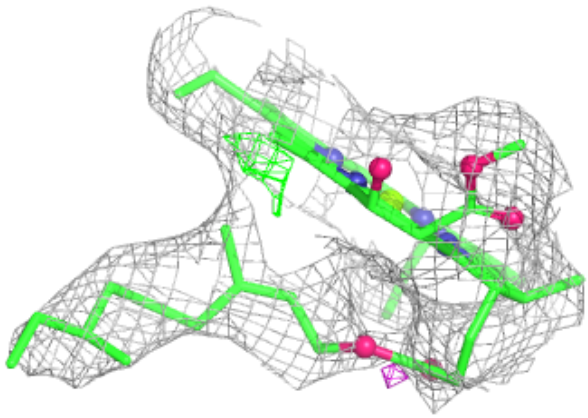
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

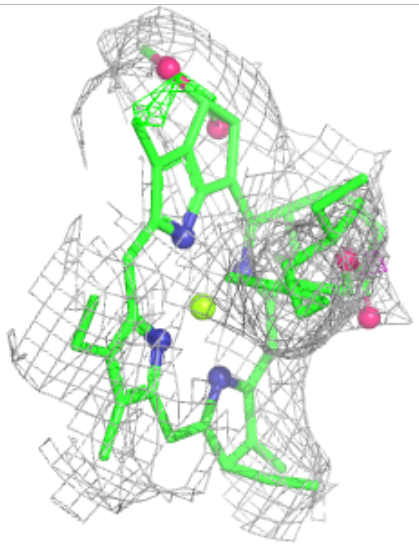


Electron density around CLA 2 1213:

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

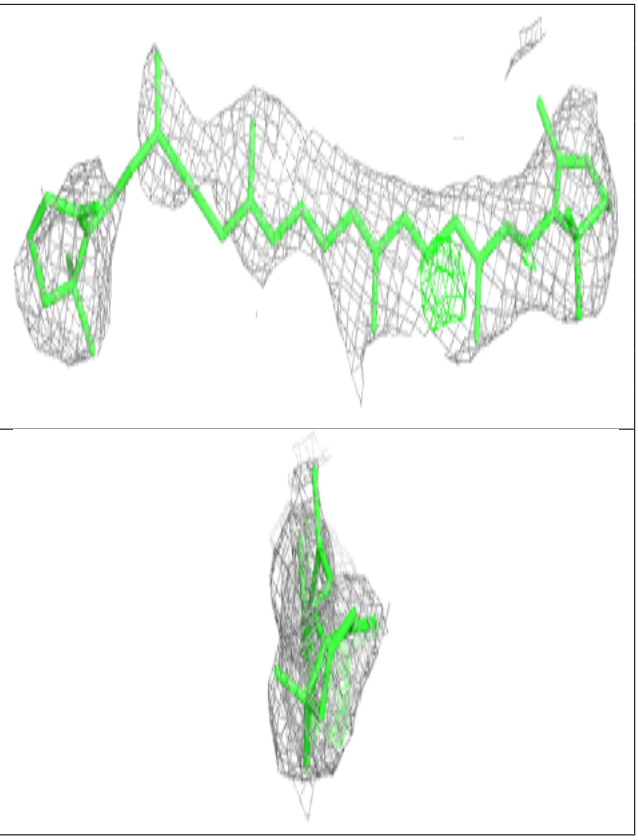






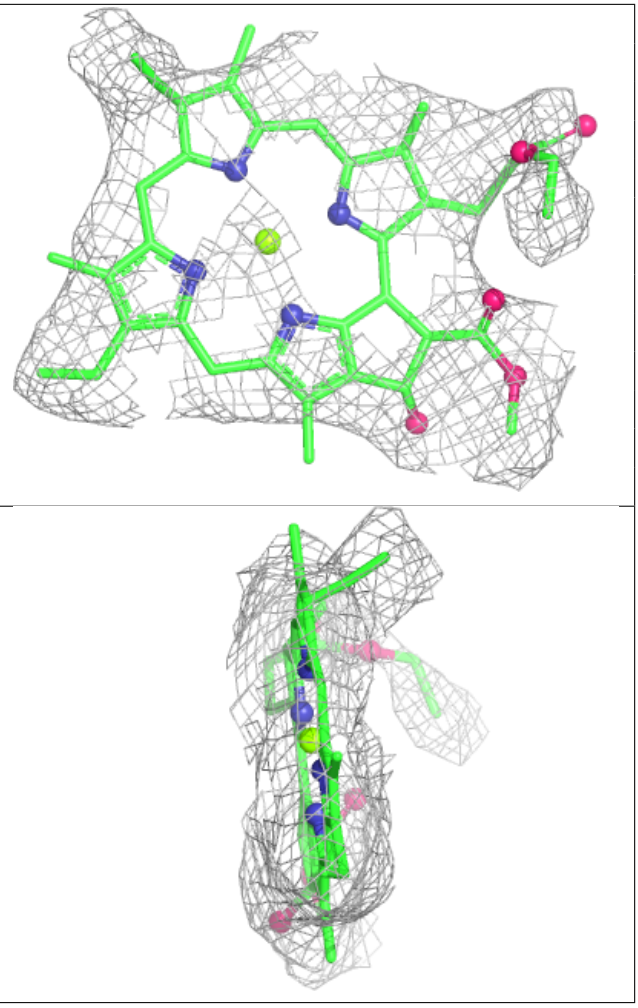
Electron density around BCR B 1780:

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



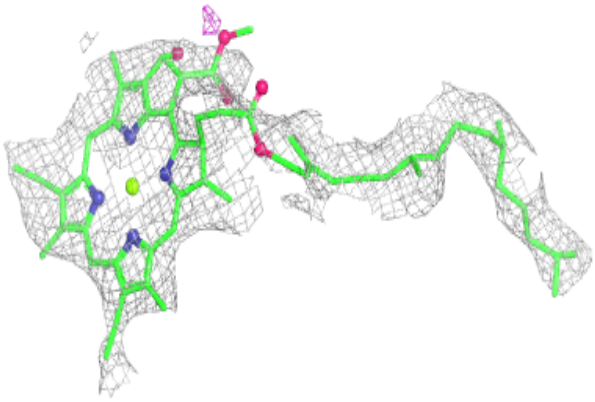
Electron density around CLA 1 1188:

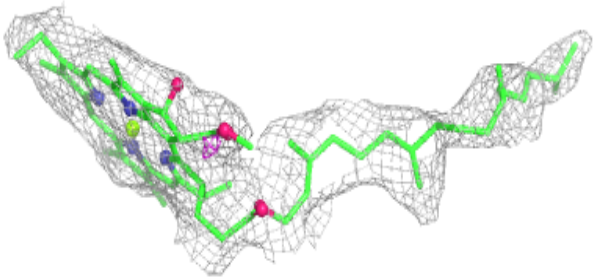
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

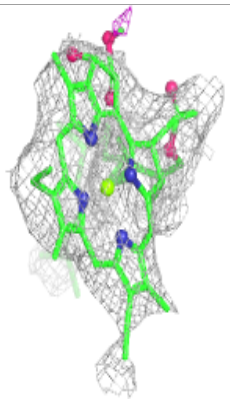


Electron density around CLA H 1079:

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

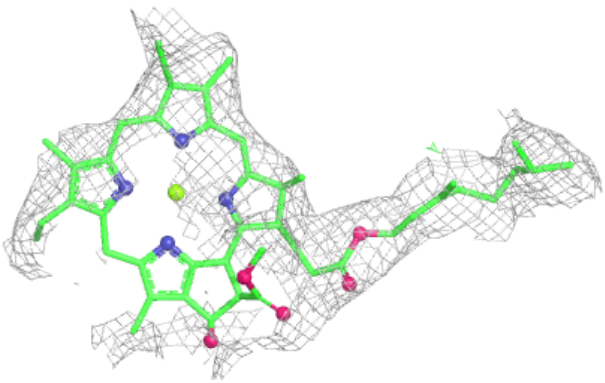


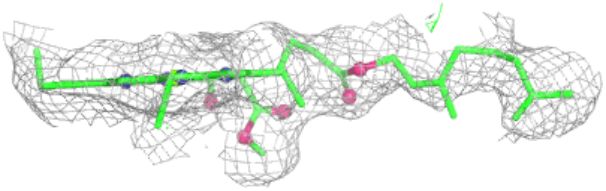


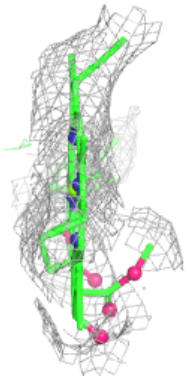


Electron density around CLA 4 1204:

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

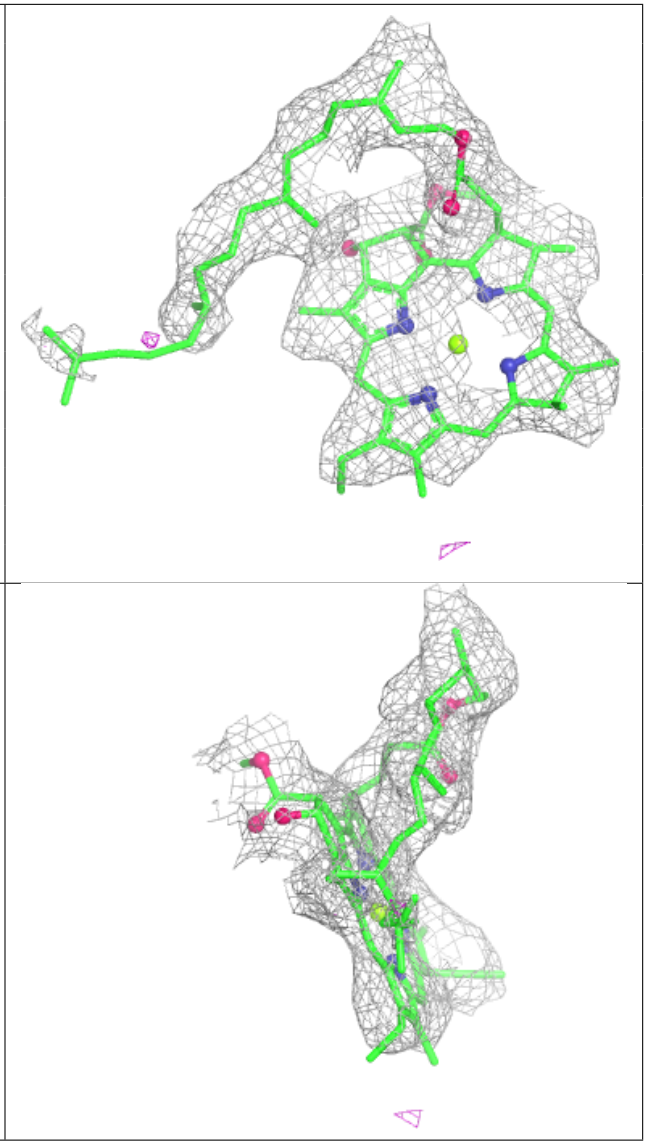






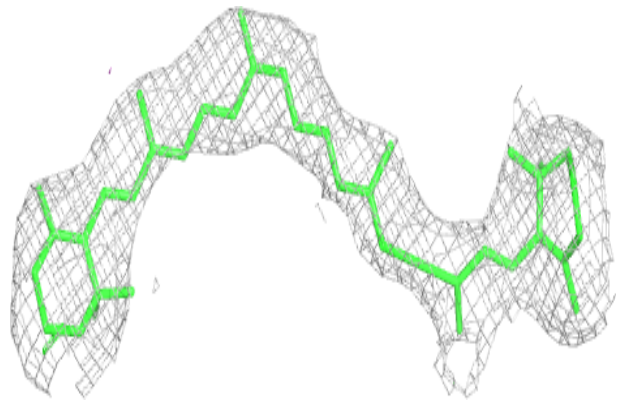
Electron density around CLA B 1762:

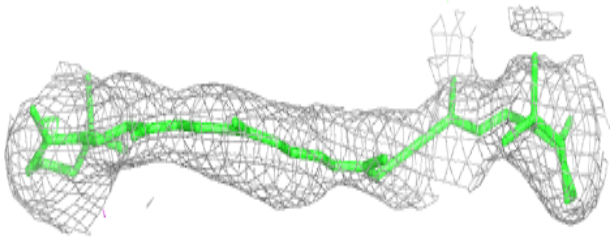
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

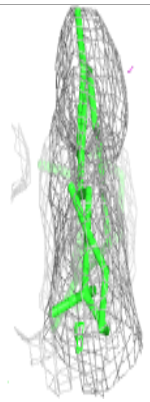


Electron density around BCR A 1807:

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

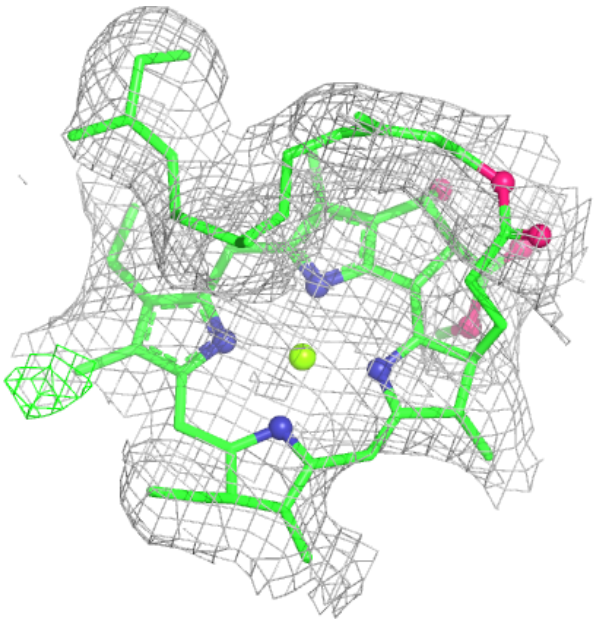


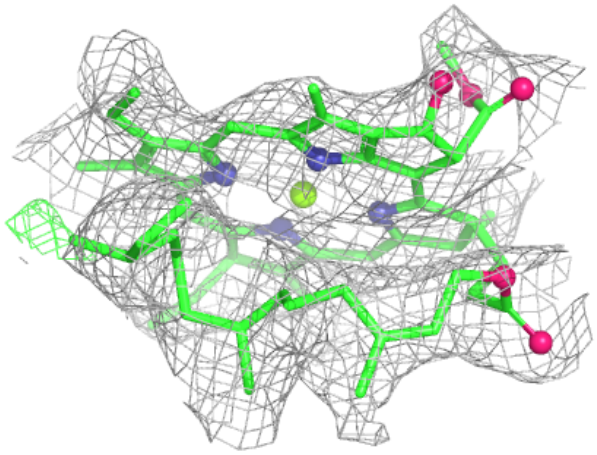


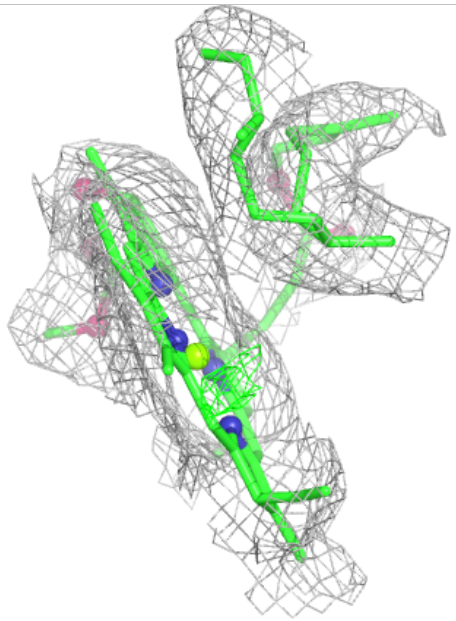


Electron density around CLA 1 1192:

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

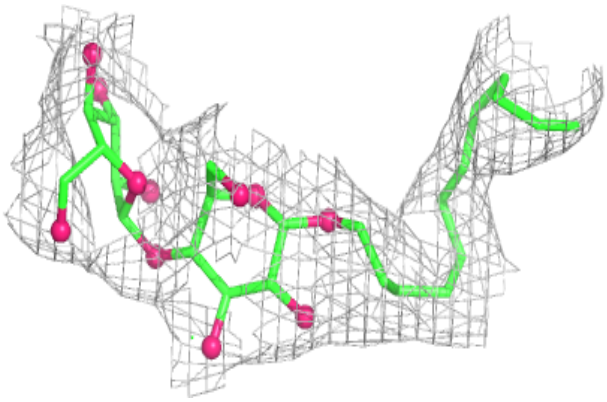


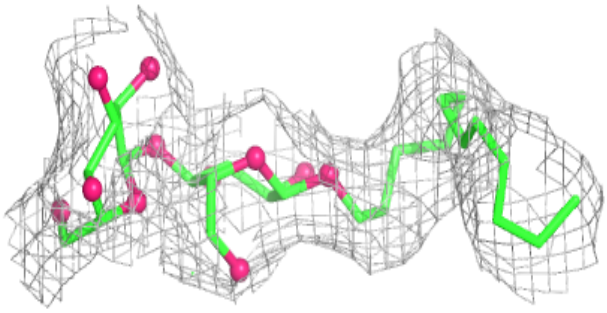


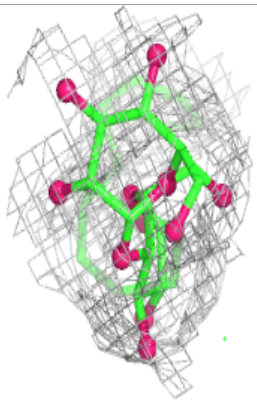


Electron density around LMU R 1056:

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

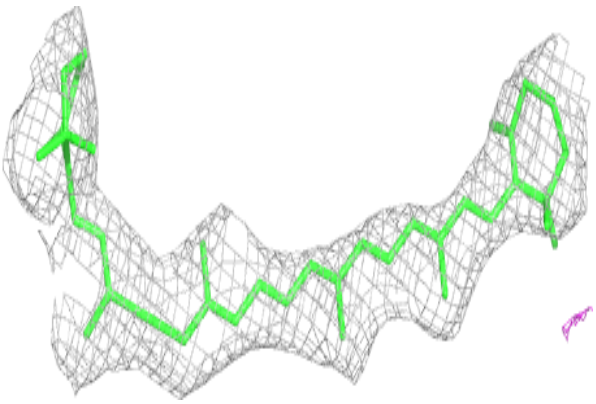


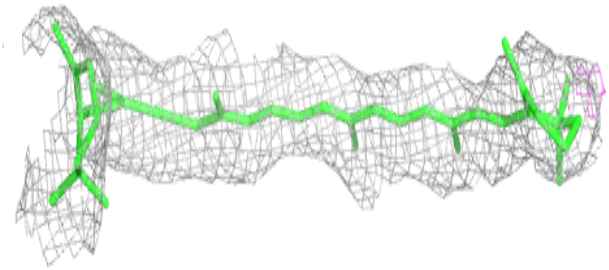


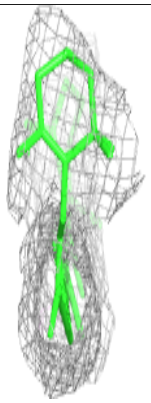


Electron density around BCR B 1775:

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

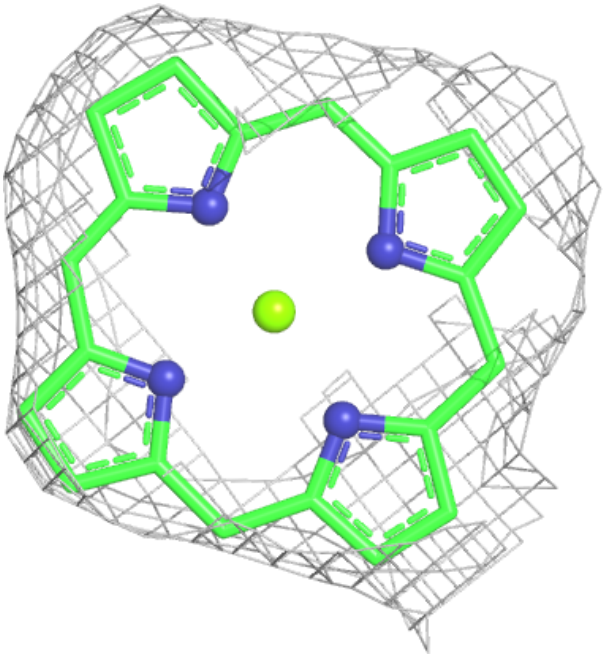


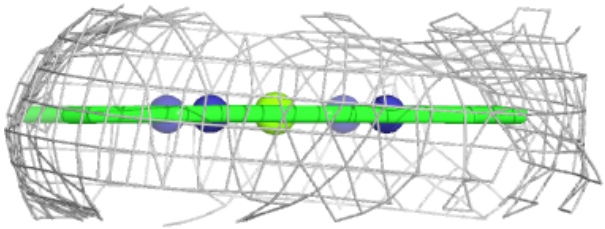


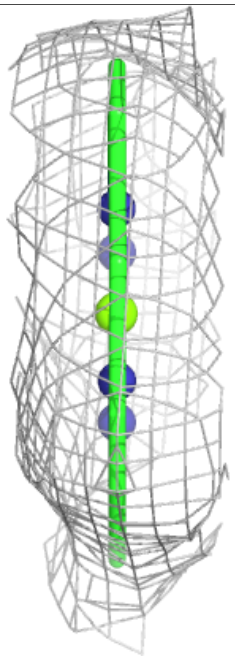


Electron density around CLA 4 1205:

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

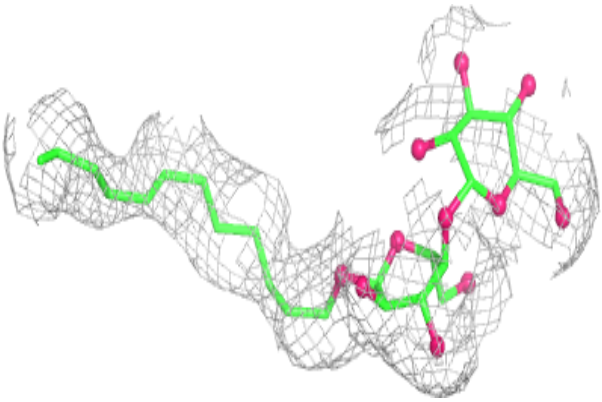


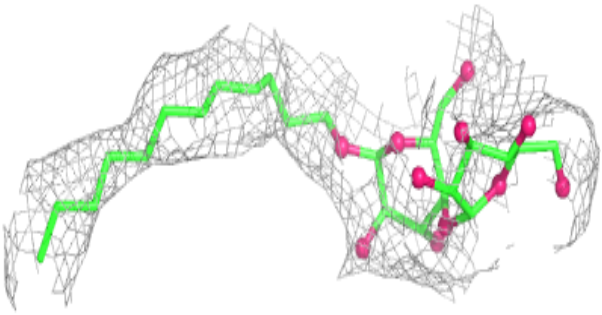


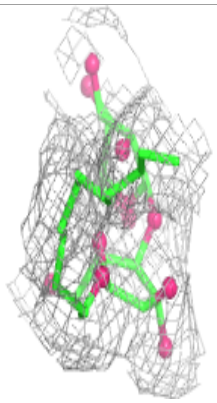


Electron density around LMU A 7024:

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

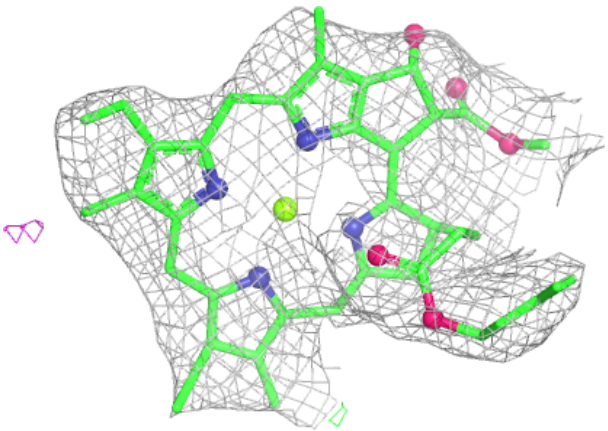


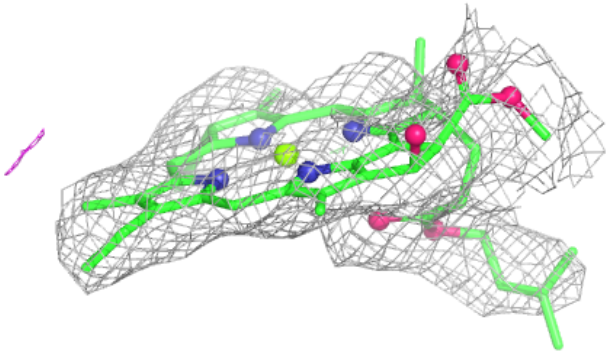


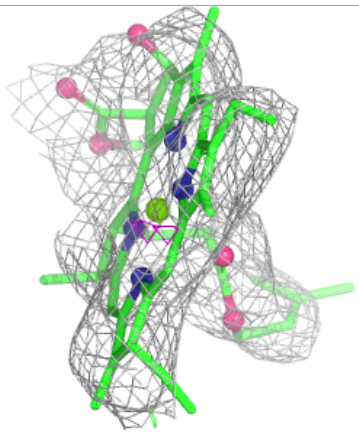


Electron density around CLA A 1771:

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

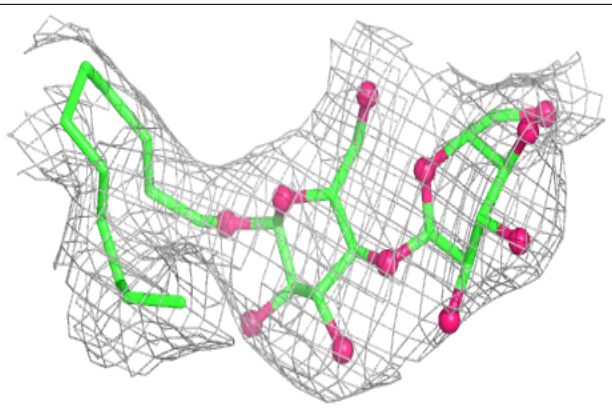


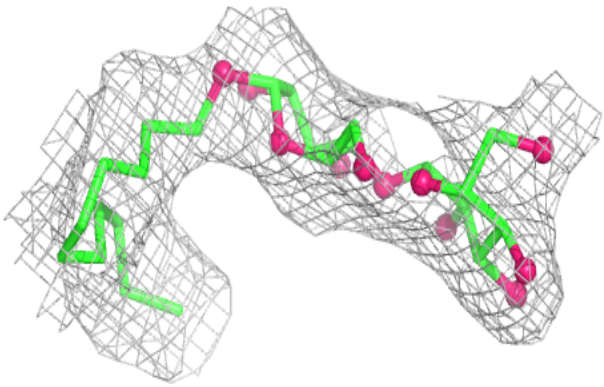


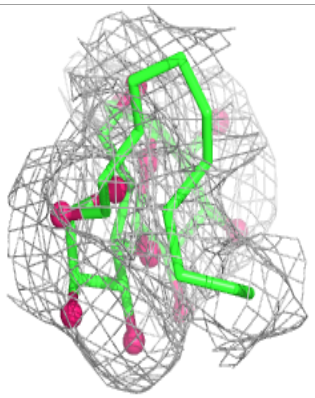


Electron density around LMU A 7036:

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

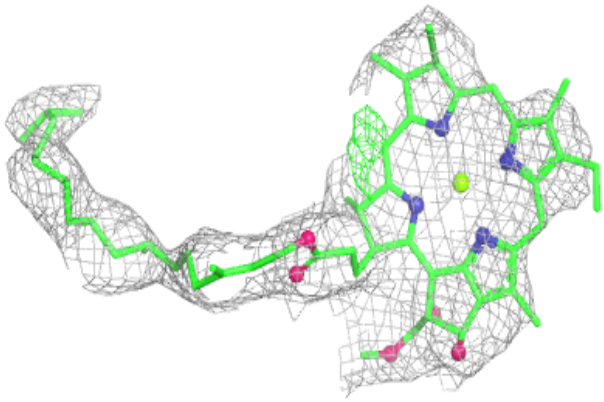


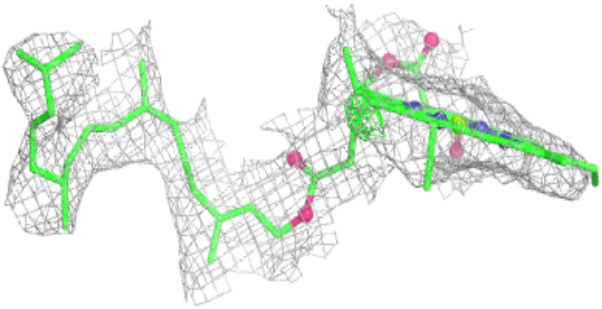


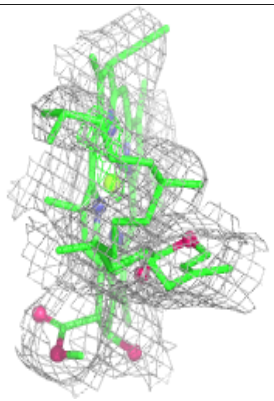


Electron density around CLA A 1781:

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

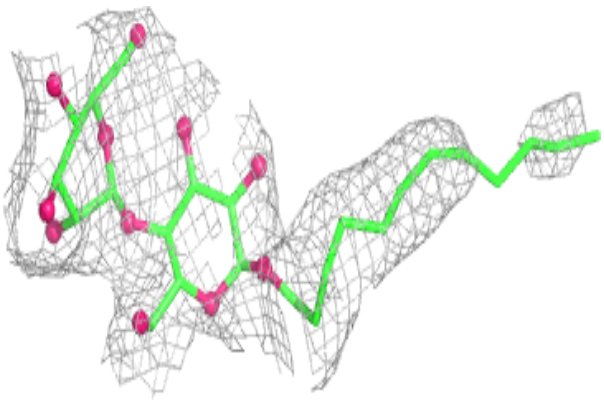


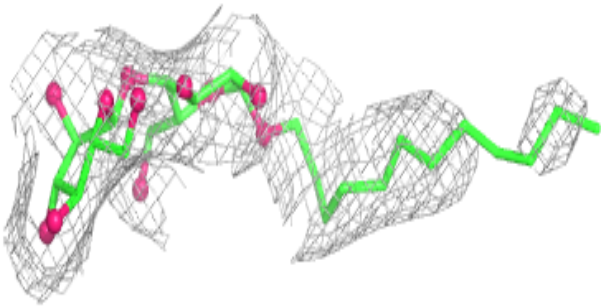


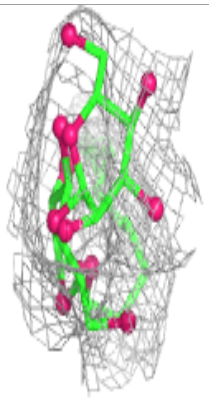


Electron density around LMU A 7035:

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

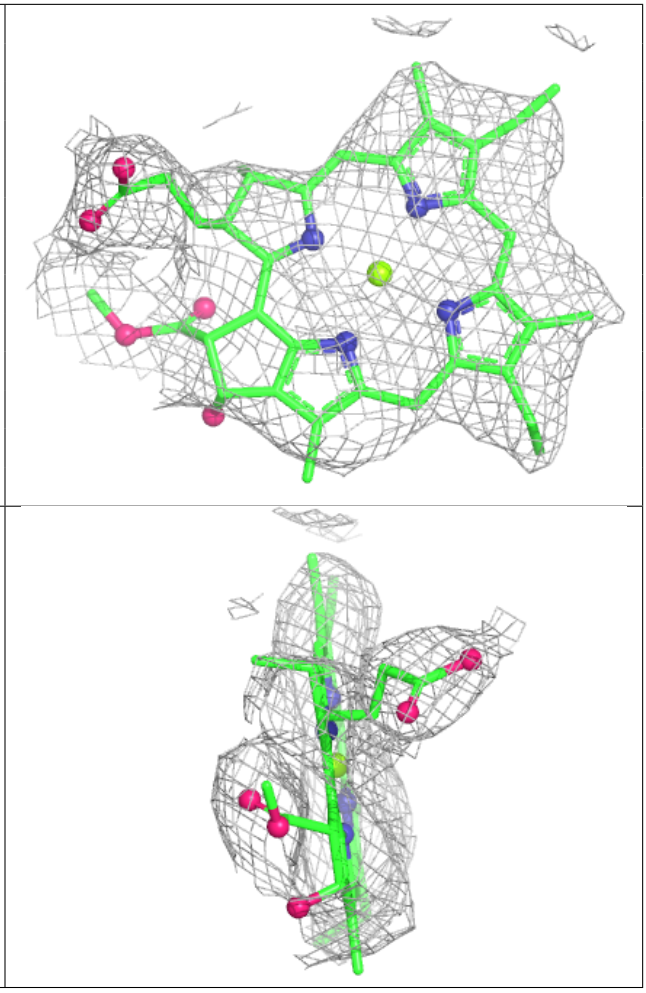






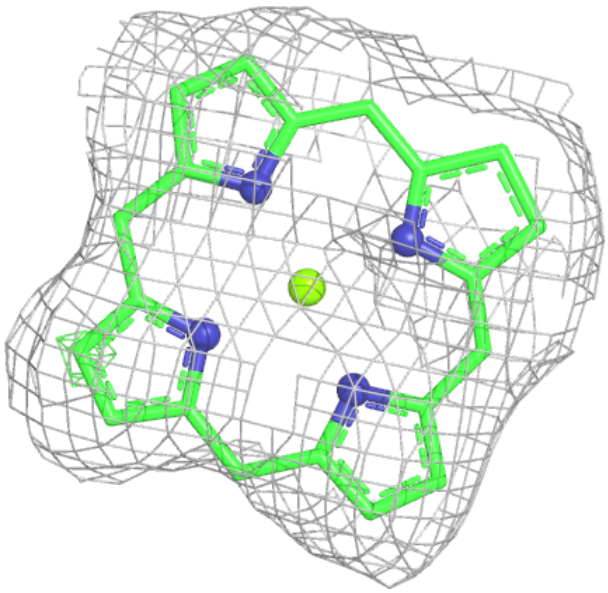
Electron density around CLA A 1766:

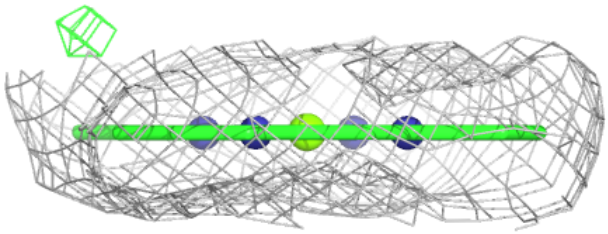
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

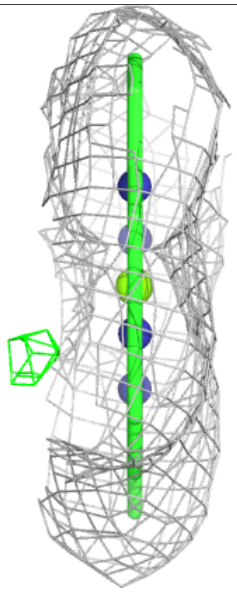


Electron density around CLA 4 1208:

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

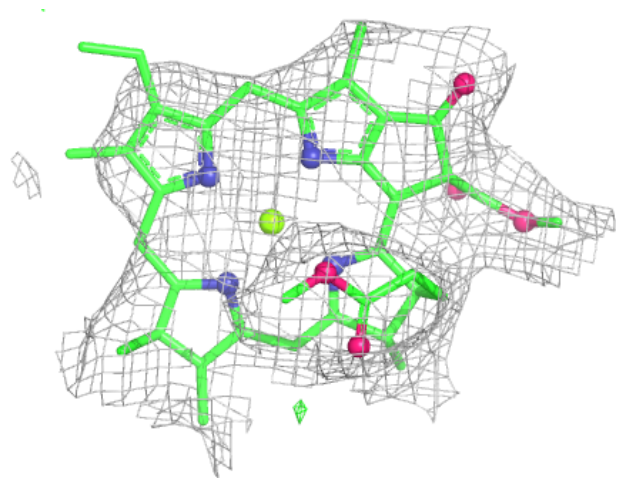


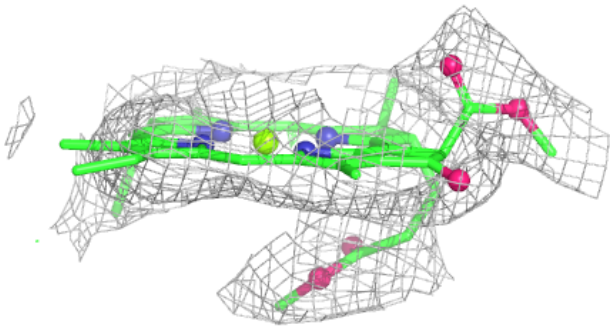


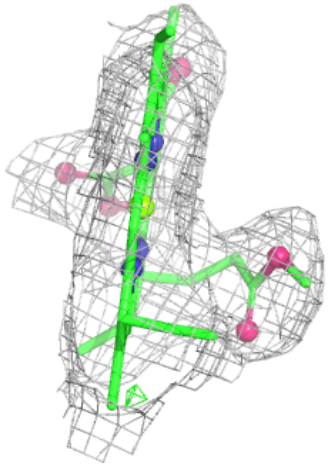


Electron density around CLA 1 1190:

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

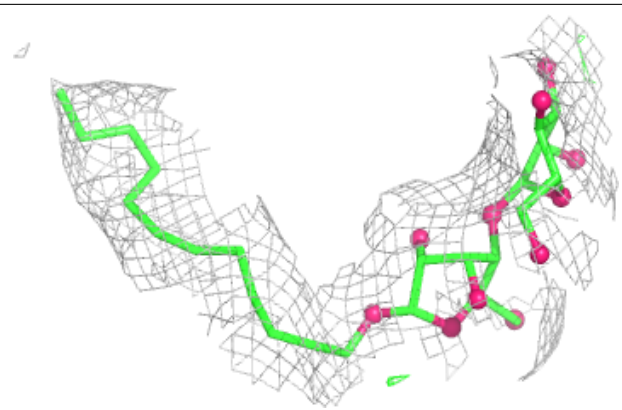


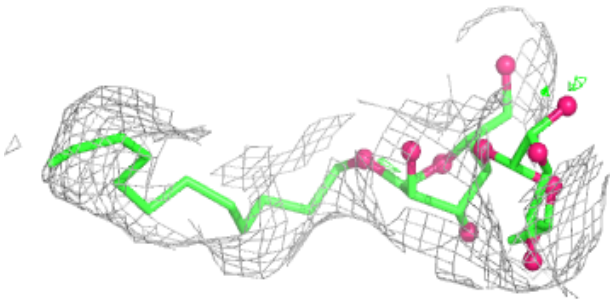




Electron density around LMU A 7039:

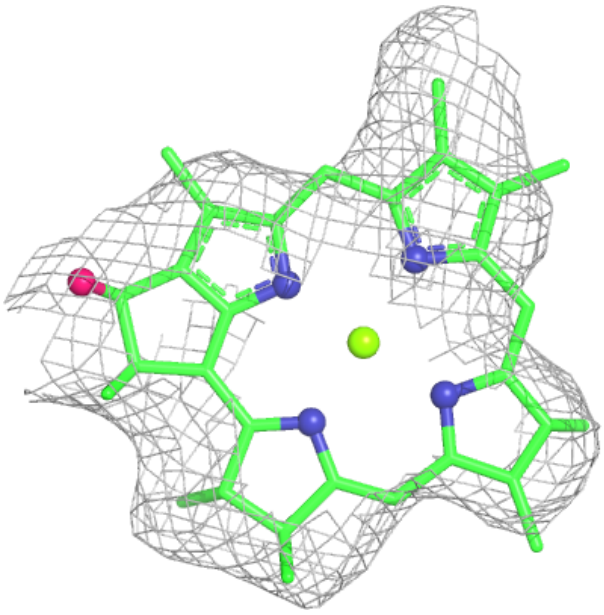
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

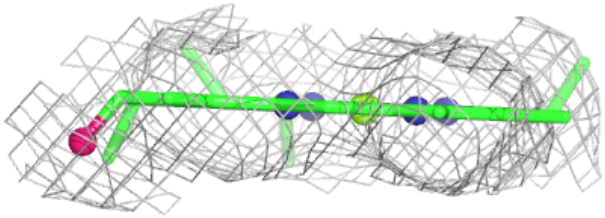


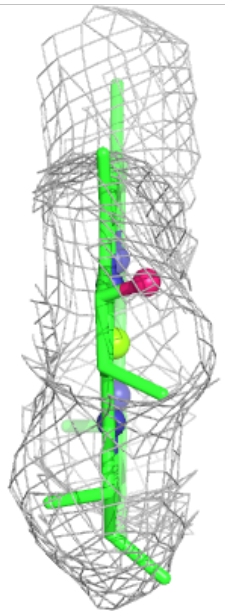


Electron density around CLA 1 1196:

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

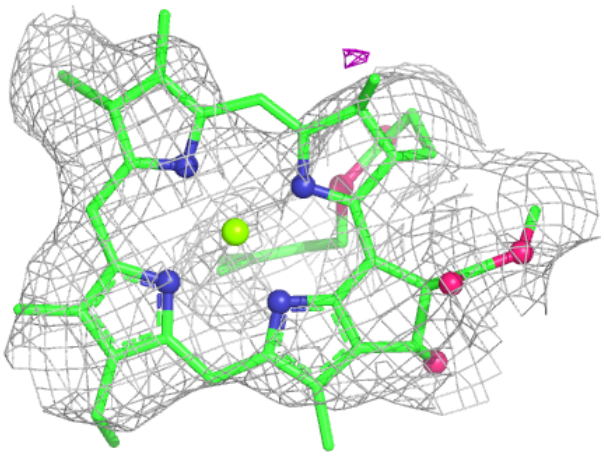


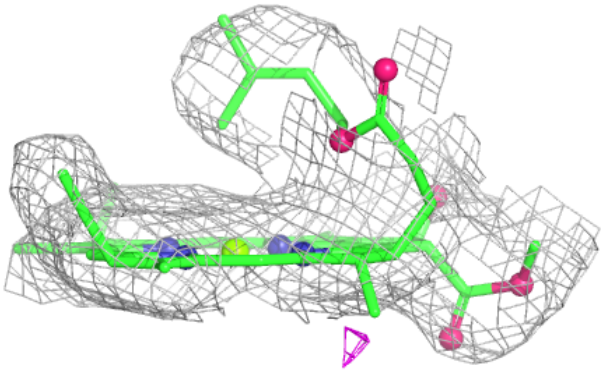


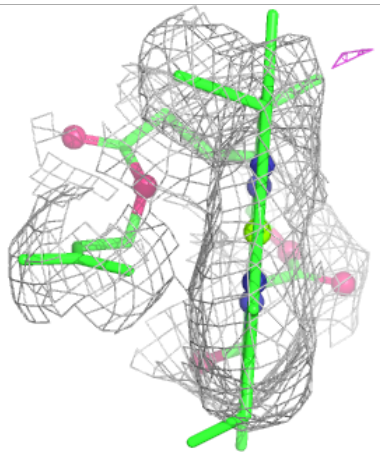


Electron density around CLA L 1166:

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

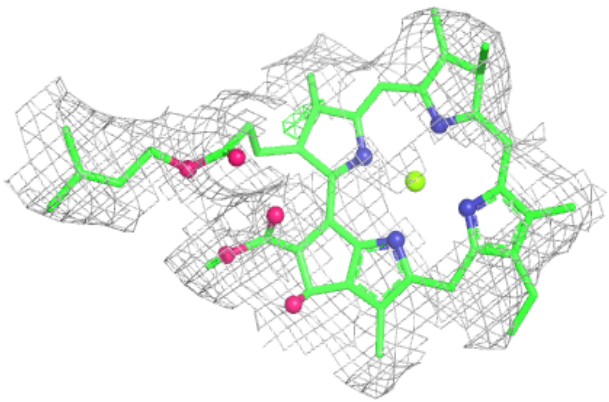


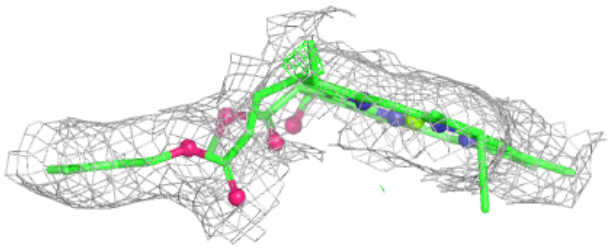


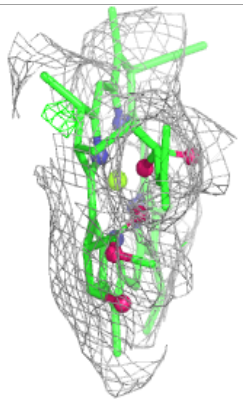


Electron density around CLA L 1168:

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

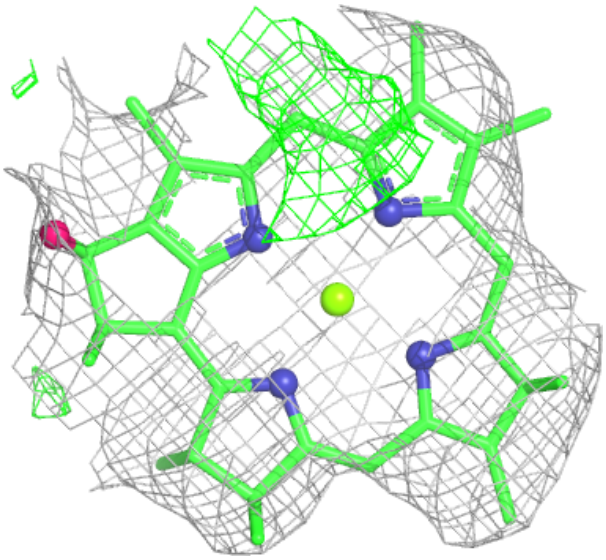


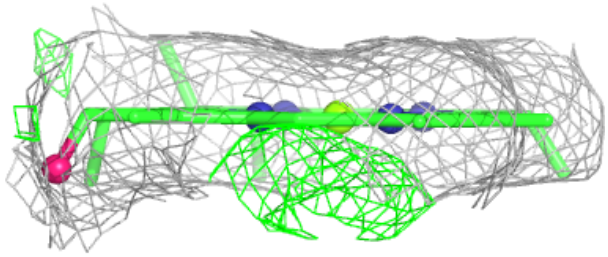


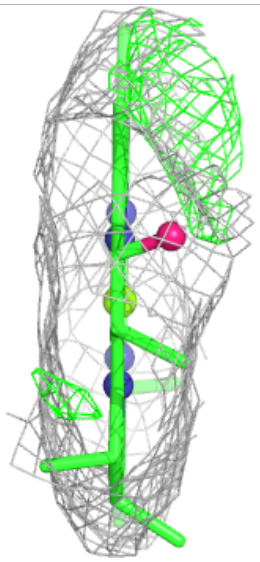


Electron density around CLA 4 1197:

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

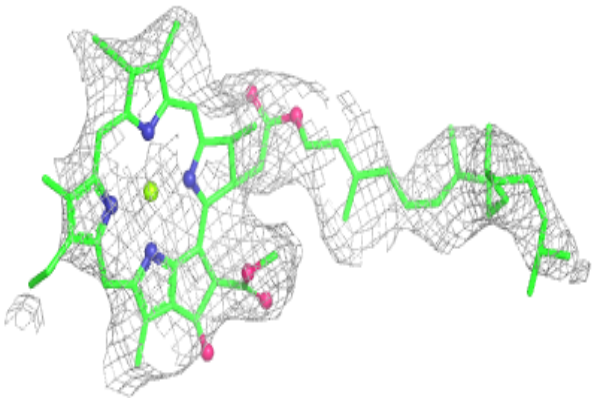


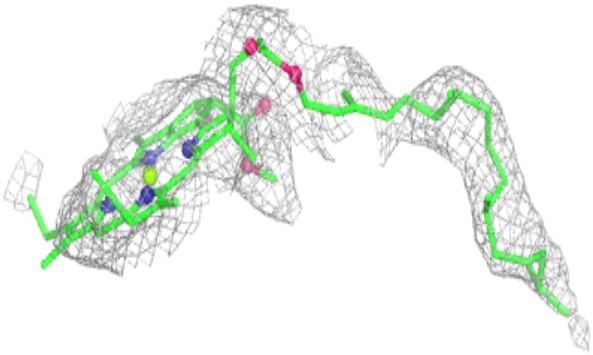


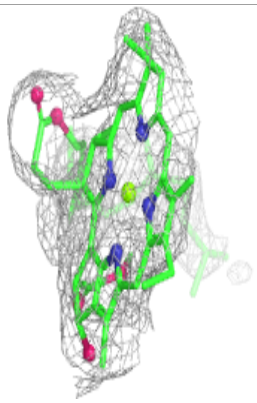


Electron density around CLA 3 3011:

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

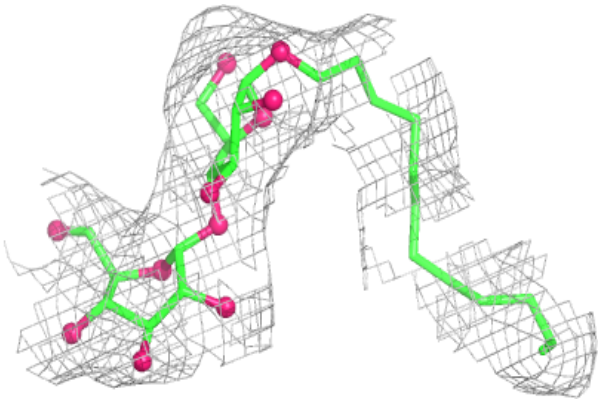


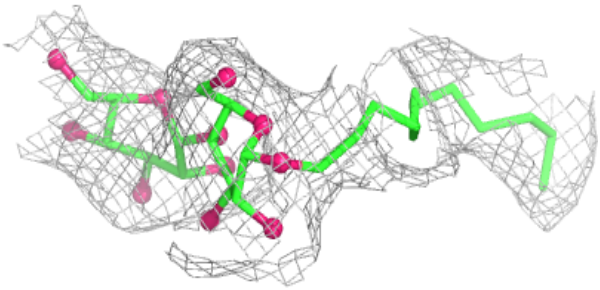


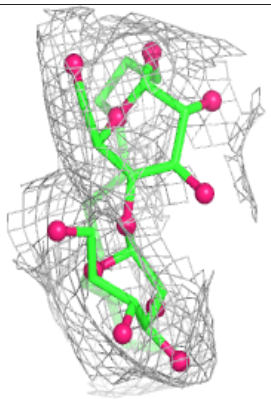


Electron density around LMU A 7028:

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

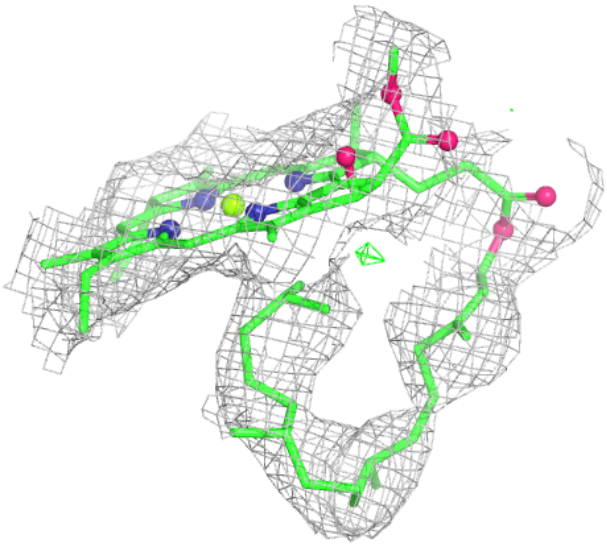


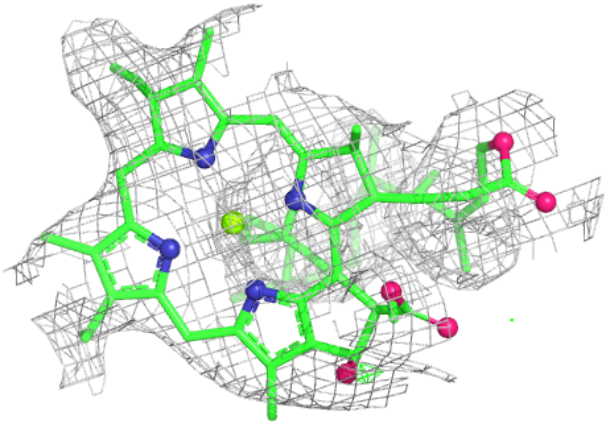


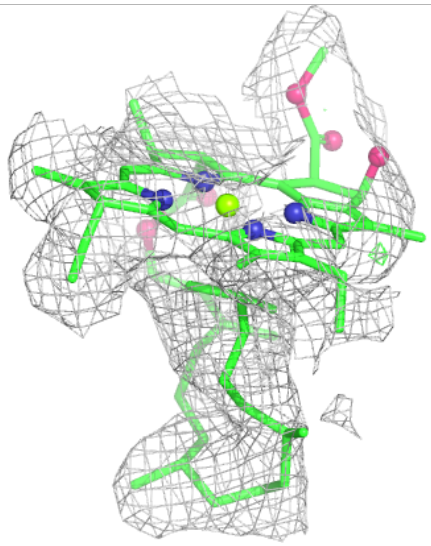


Electron density around CLA 2 1224:

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

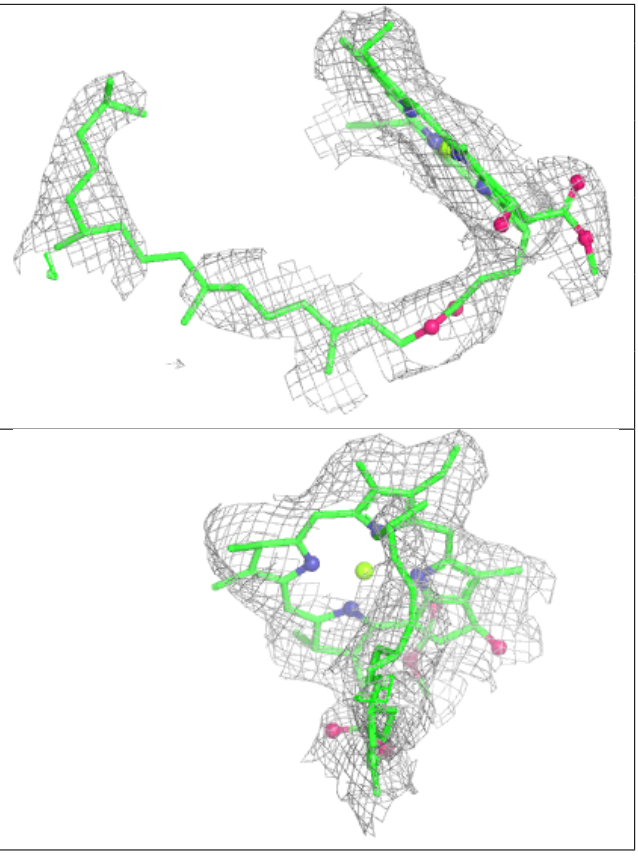






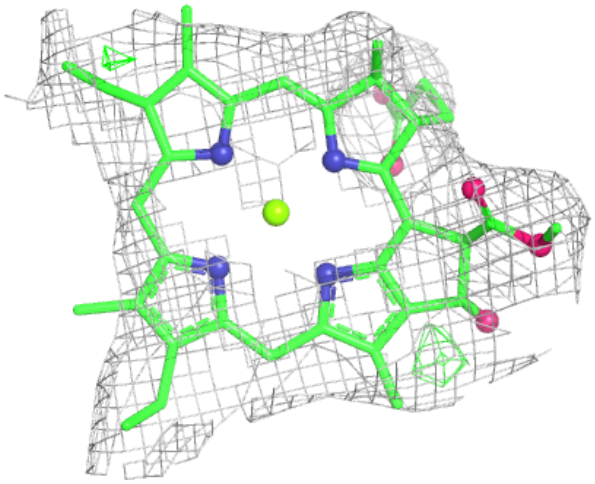
Electron density around CLA A 1787:

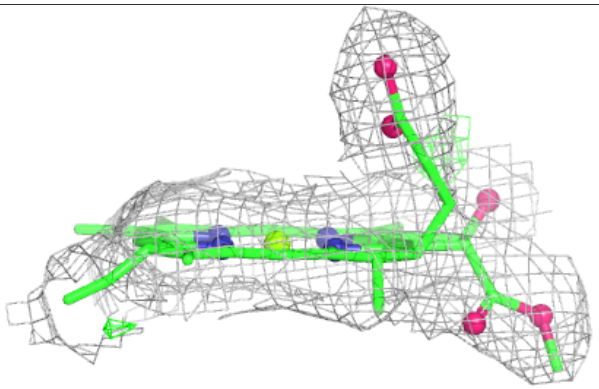
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 1736:

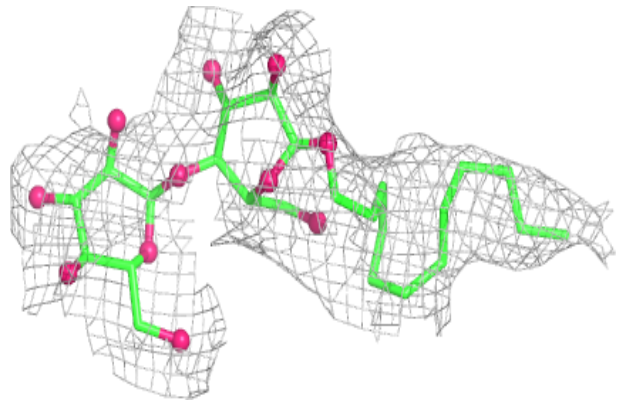
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

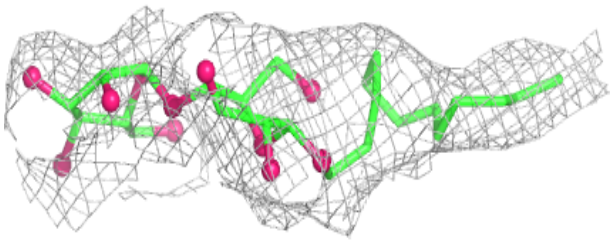


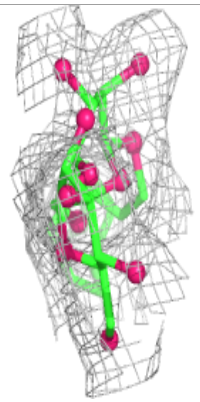


Electron density around LMU A 7016:

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

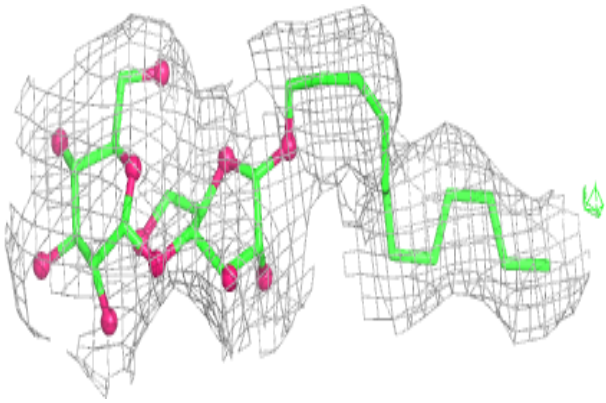


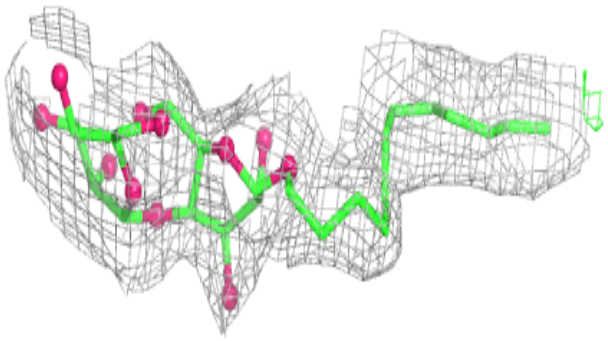


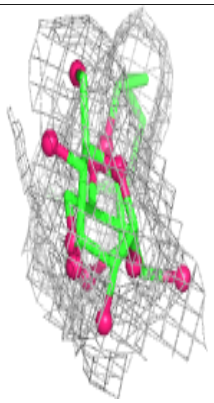


Electron density around LMU A 7020:

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

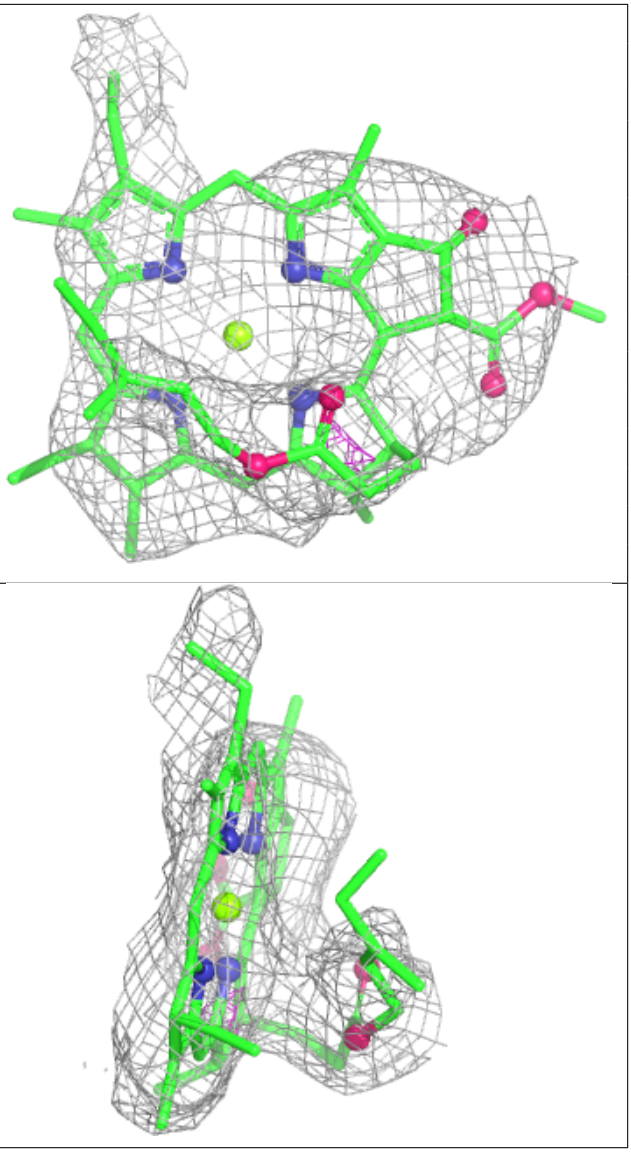






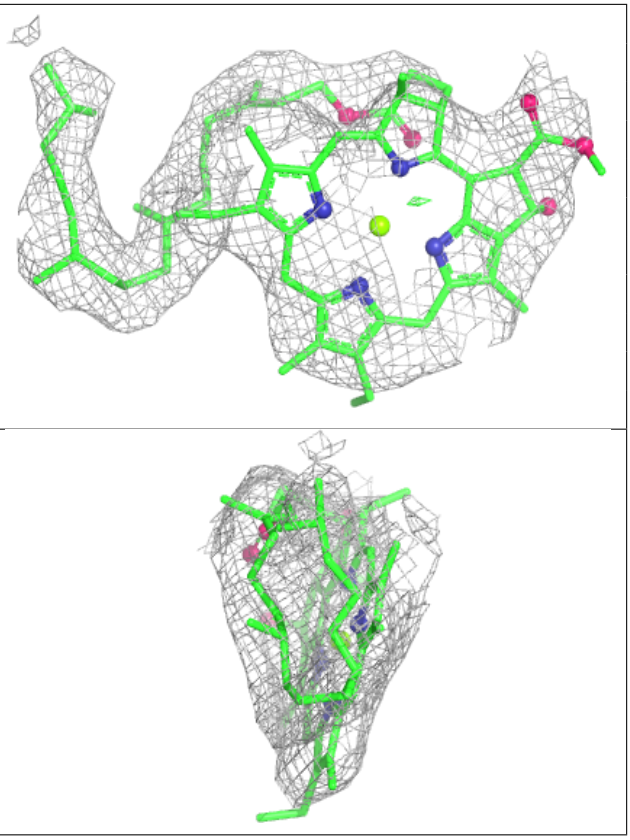
Electron density around CLA A 1777:

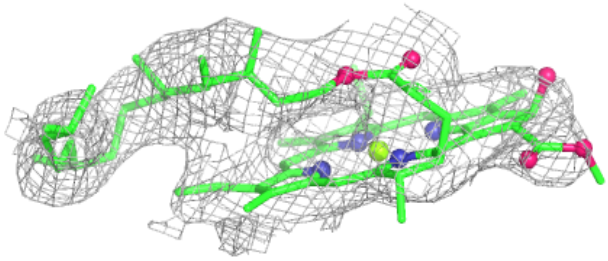
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 1774:

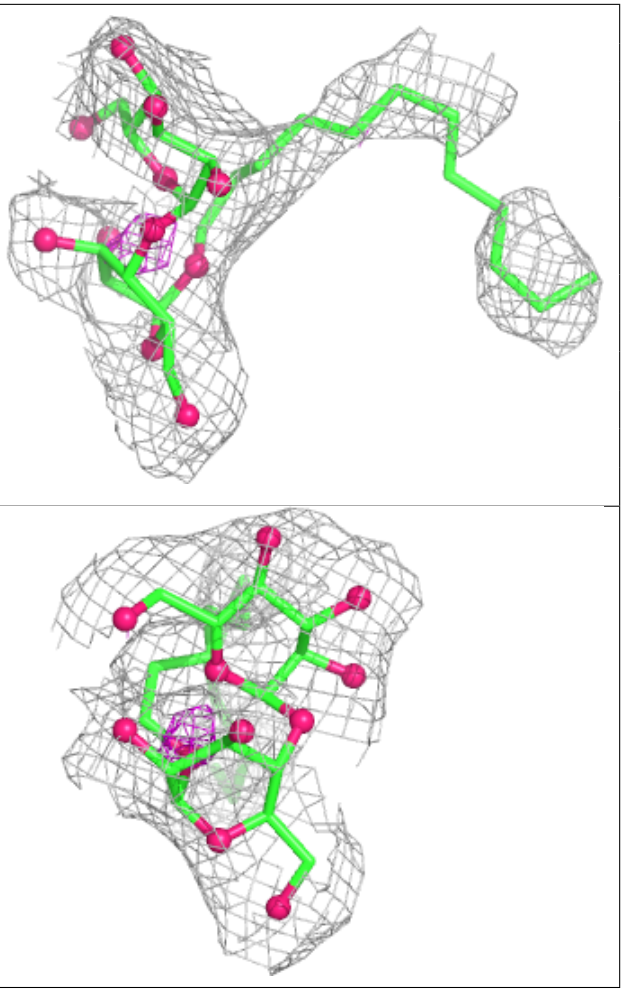
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





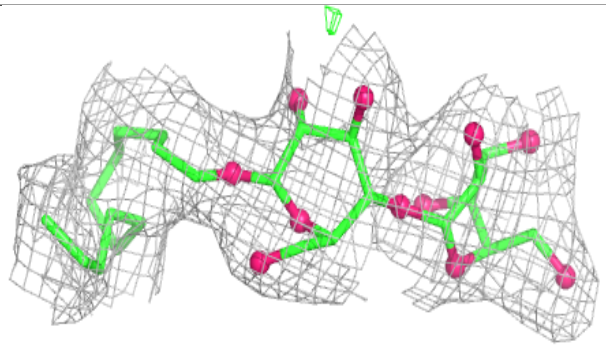
Electron density around LMU A 7032:

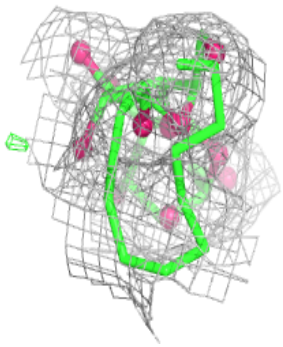
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMU A 7023:

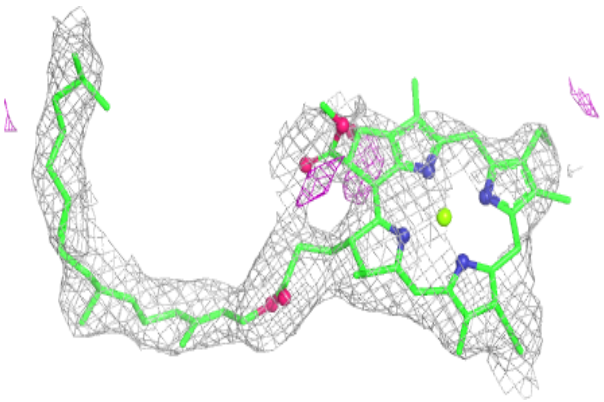
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

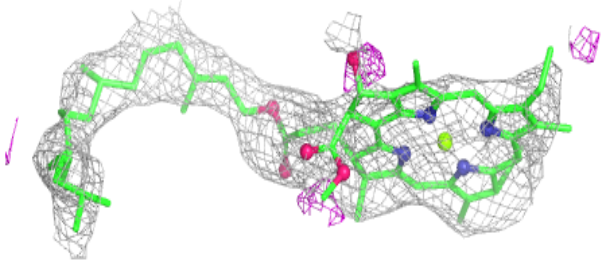




Electron density around CLA B 1756:

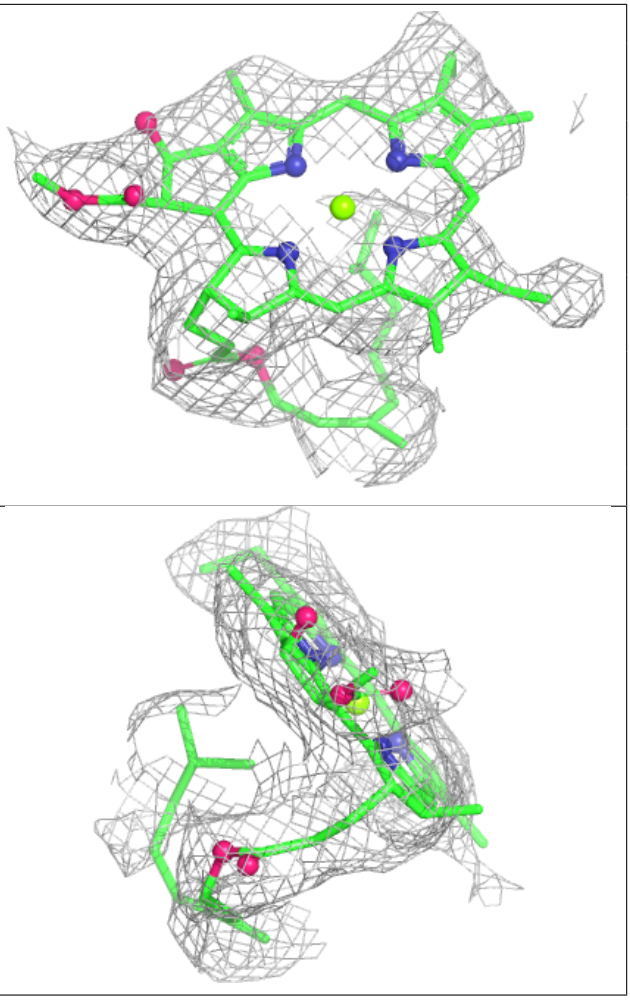
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





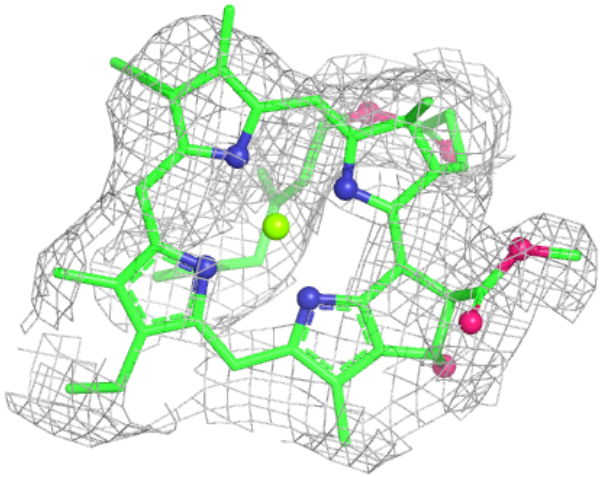
Electron density around CLA B 1742:

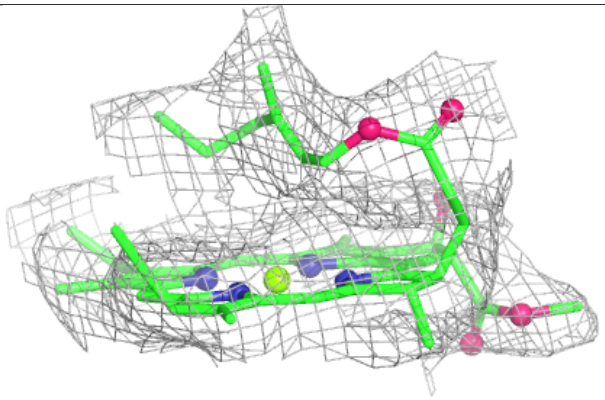
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 1773:

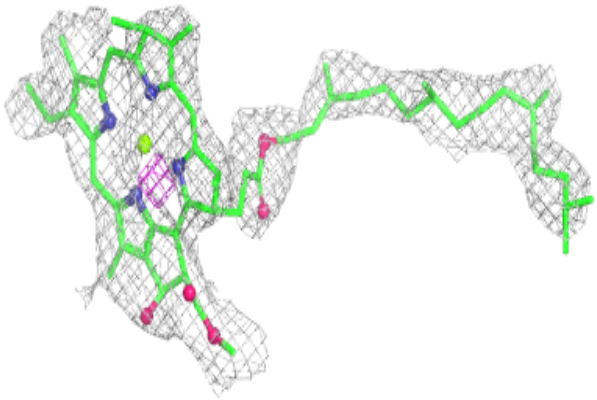
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

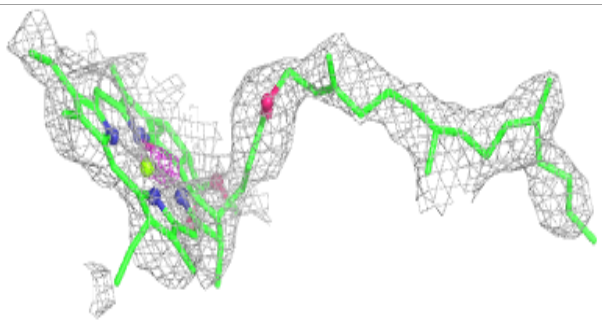


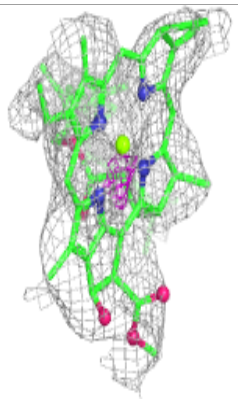


Electron density around CLA A 1776:

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

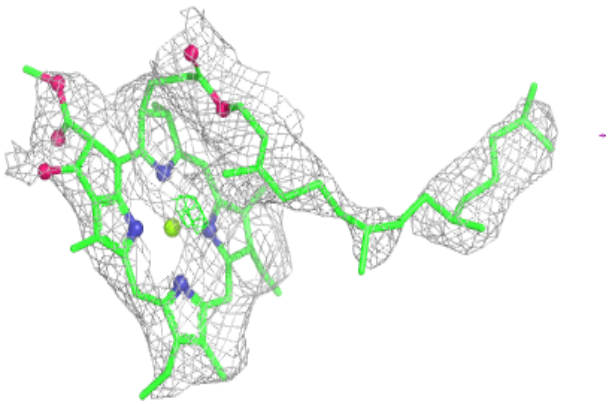


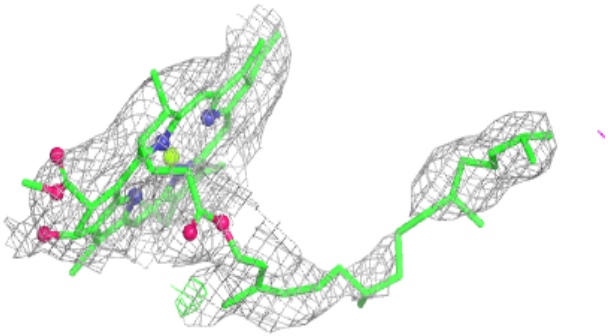


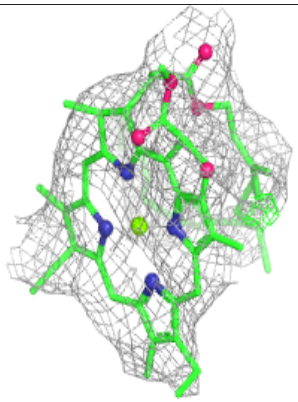


Electron density around CLA B 1744:

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

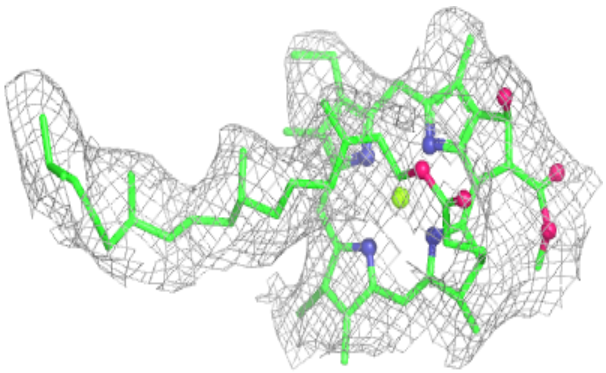


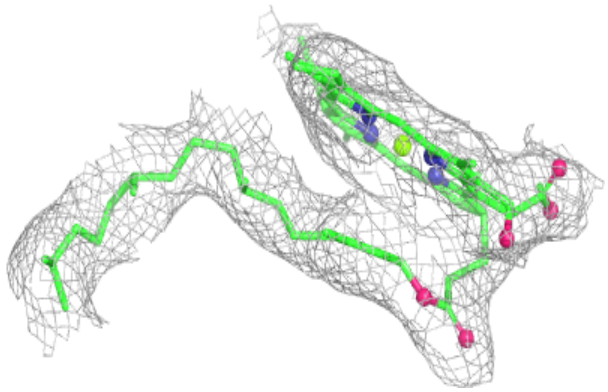


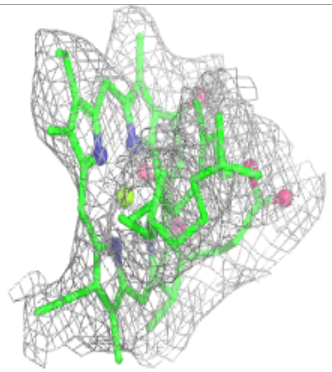


Electron density around CLA A 1772:

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

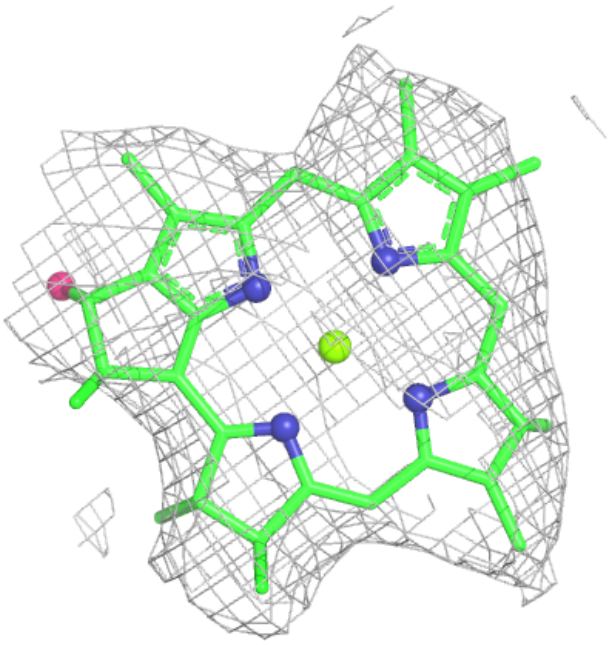


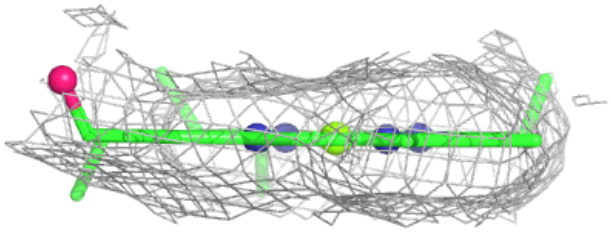


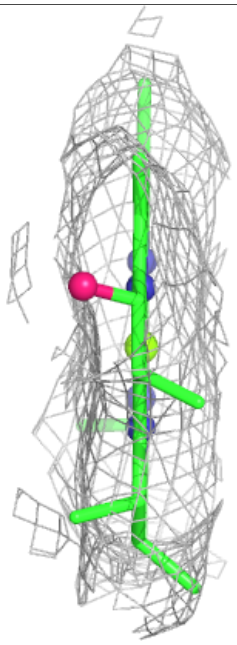


Electron density around CLA 1 1195:

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

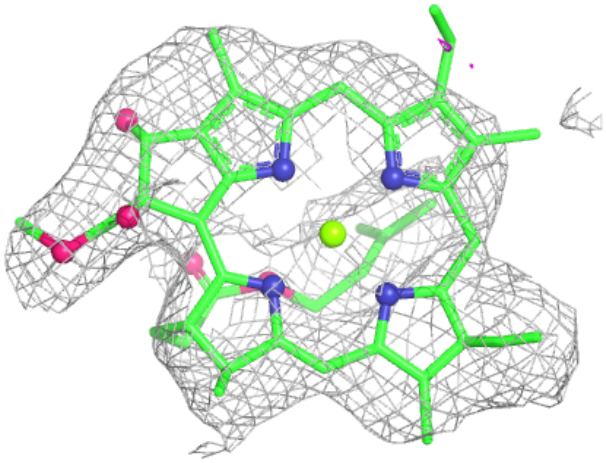


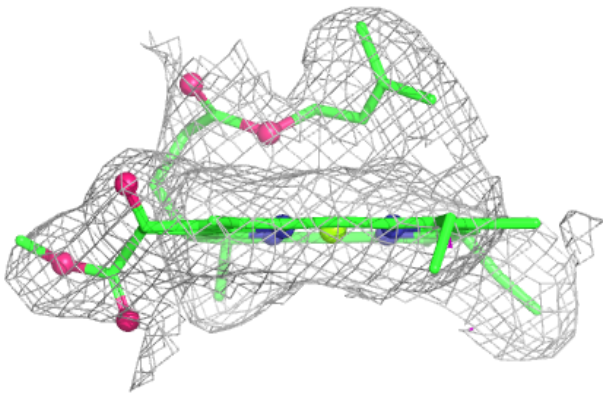


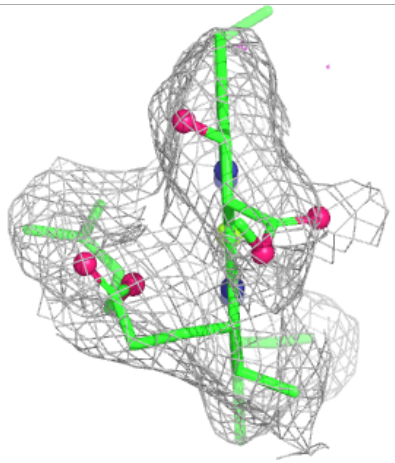


Electron density around CLA B 1750:

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

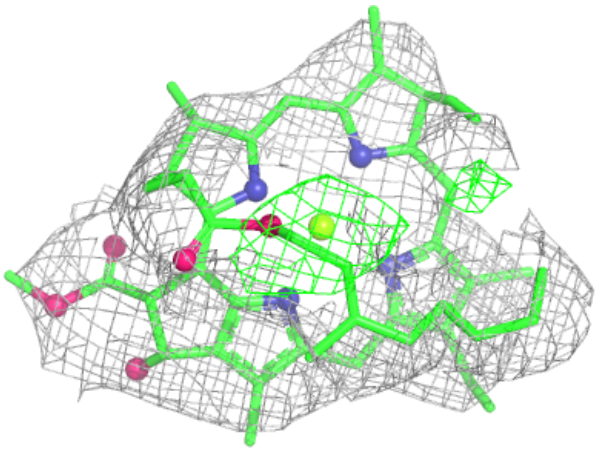


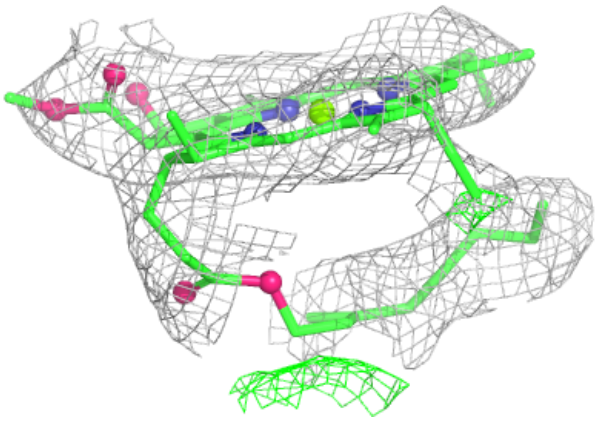


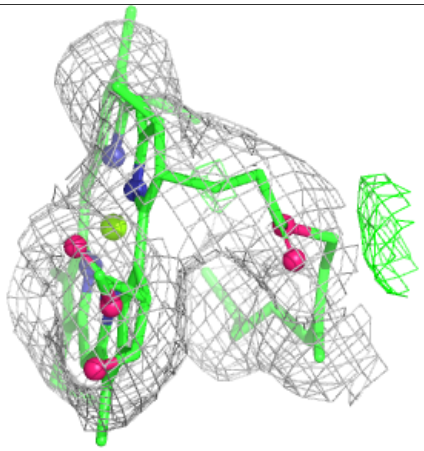


Electron density around CLA A 1768:

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

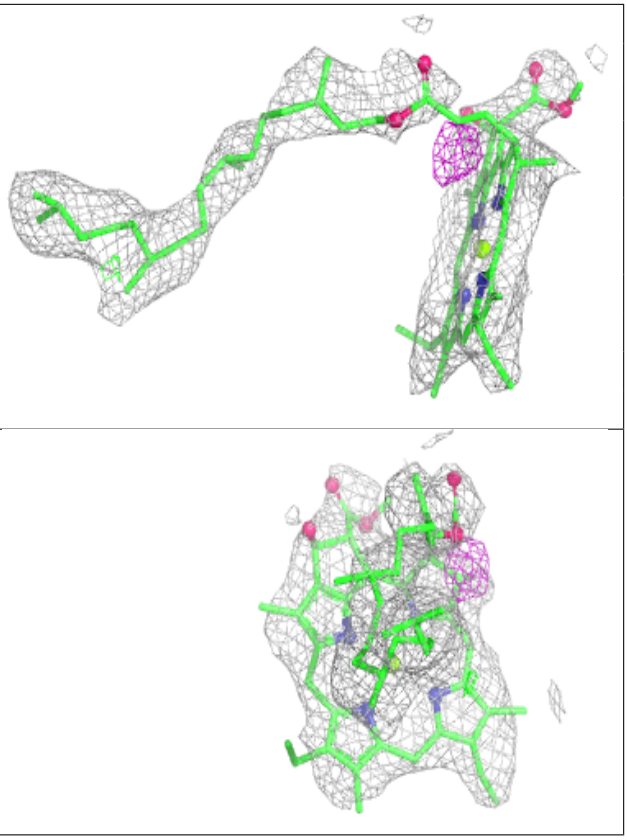






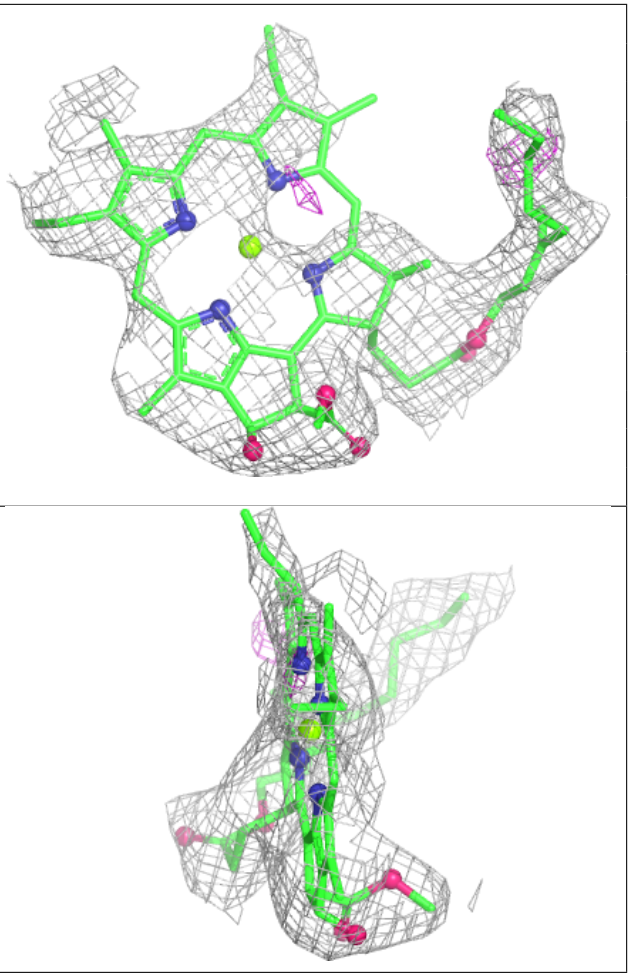
Electron density around CLA A 1785:

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



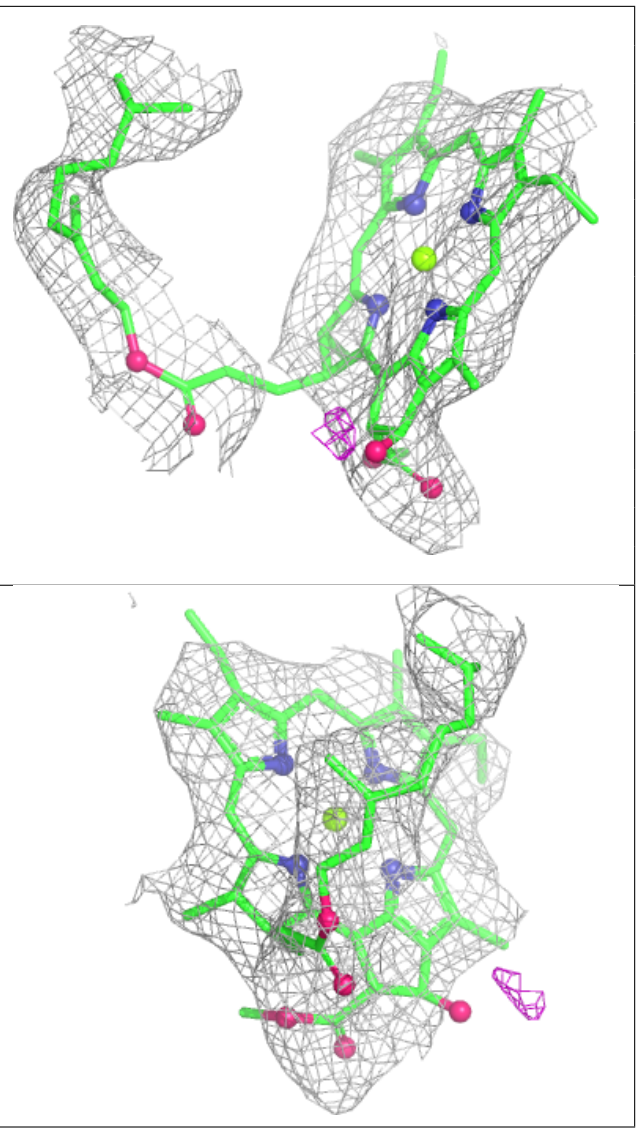
Electron density around CLA A 1769:

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



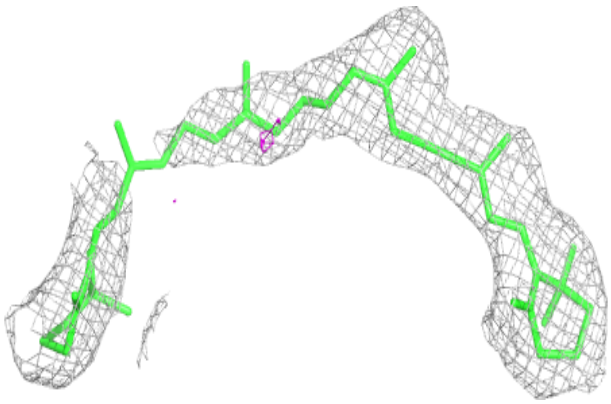
Electron density around CLA A 1760:

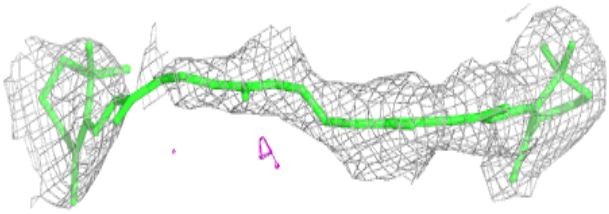
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

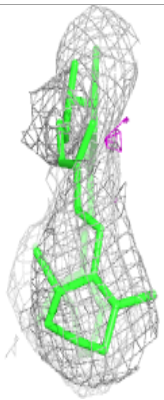


Electron density around BCR B 1779:

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

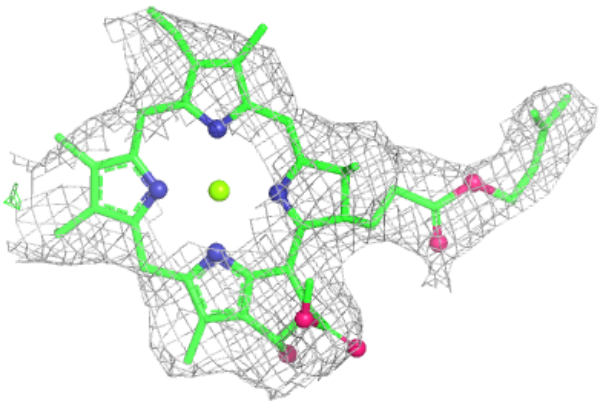


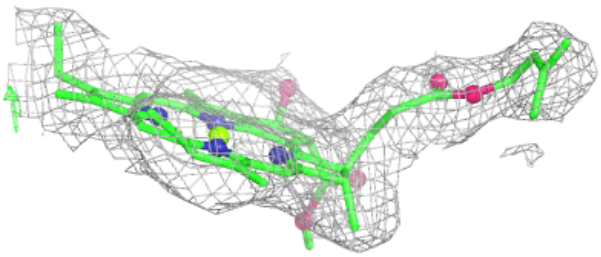


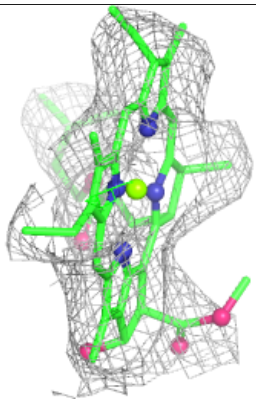


Electron density around CLA B 1763:

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

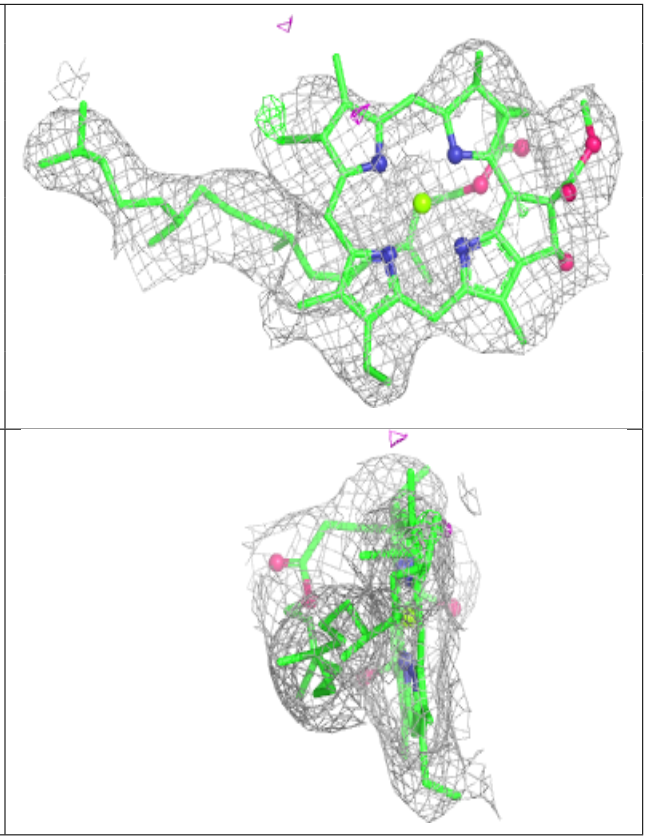






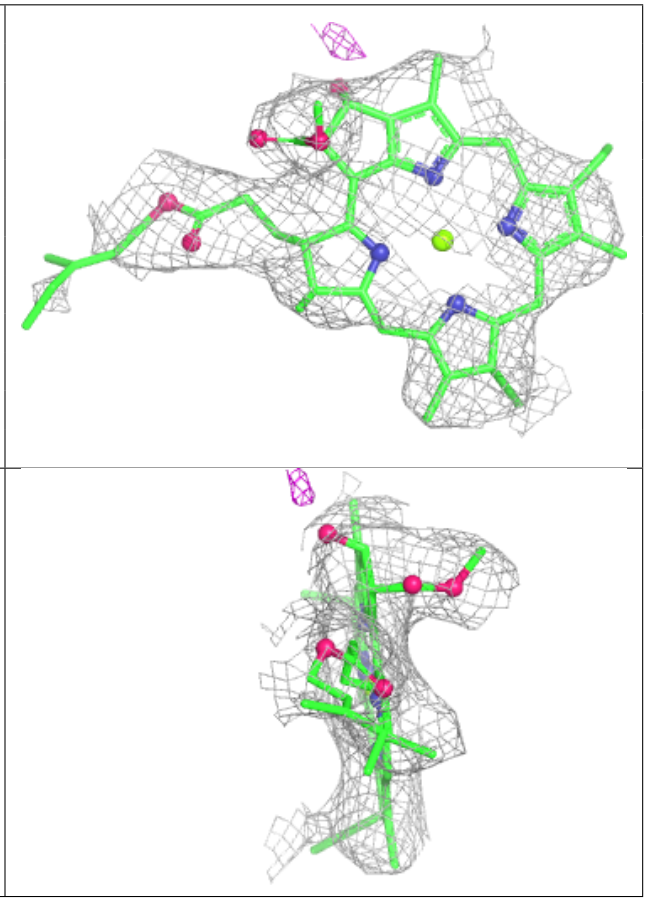
Electron density around CLA B 1735:

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



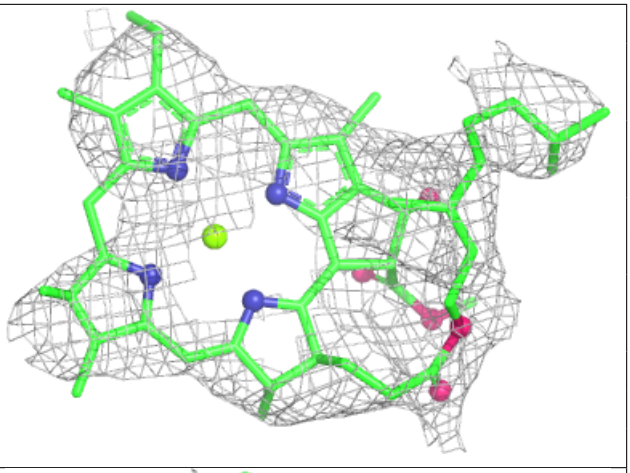
Electron density around CLA A 1792:

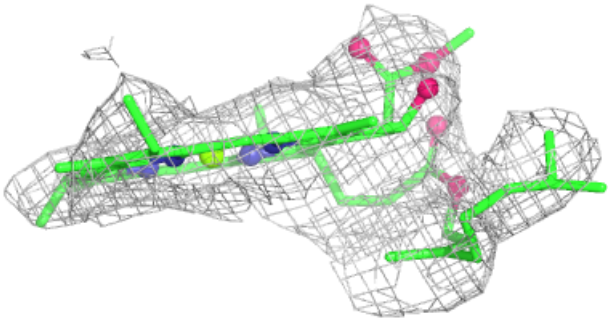
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

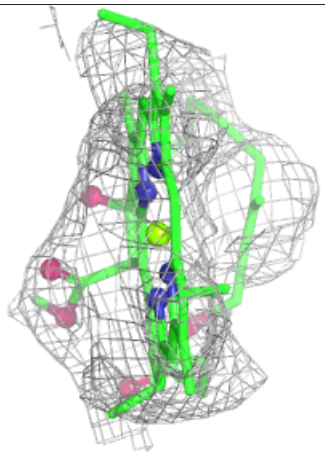


Electron density around CLA B 1741:

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

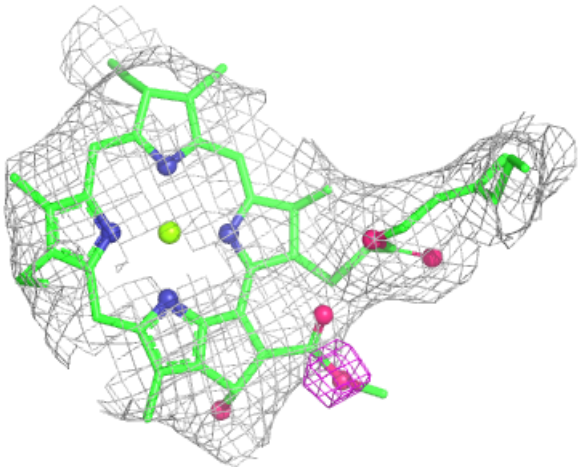


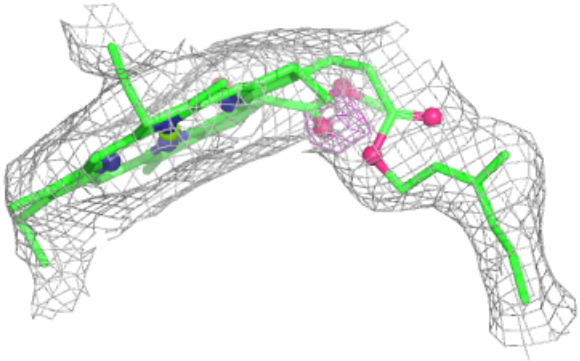


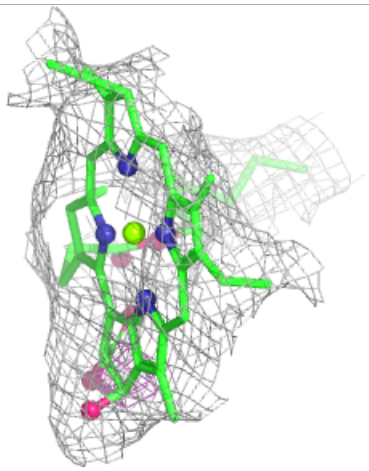


Electron density around CLA 4 1201:

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

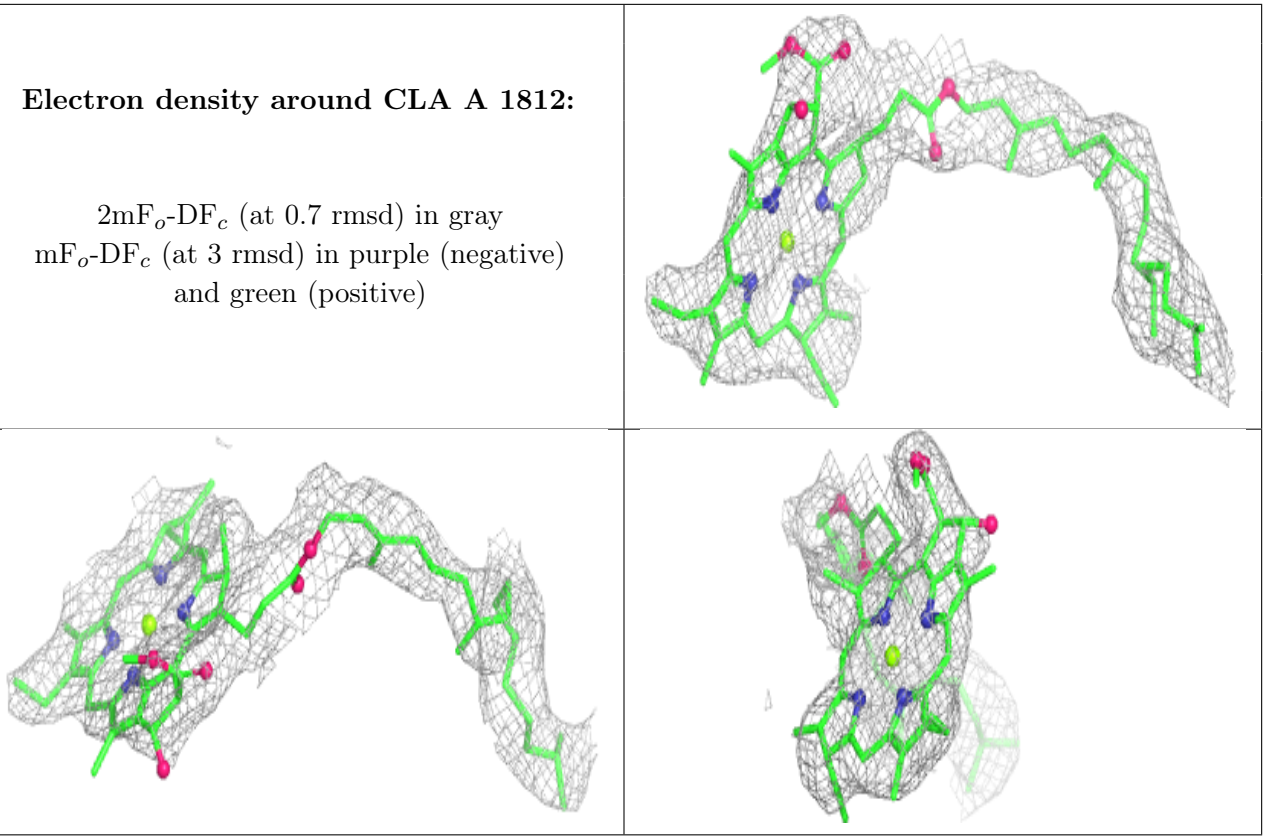






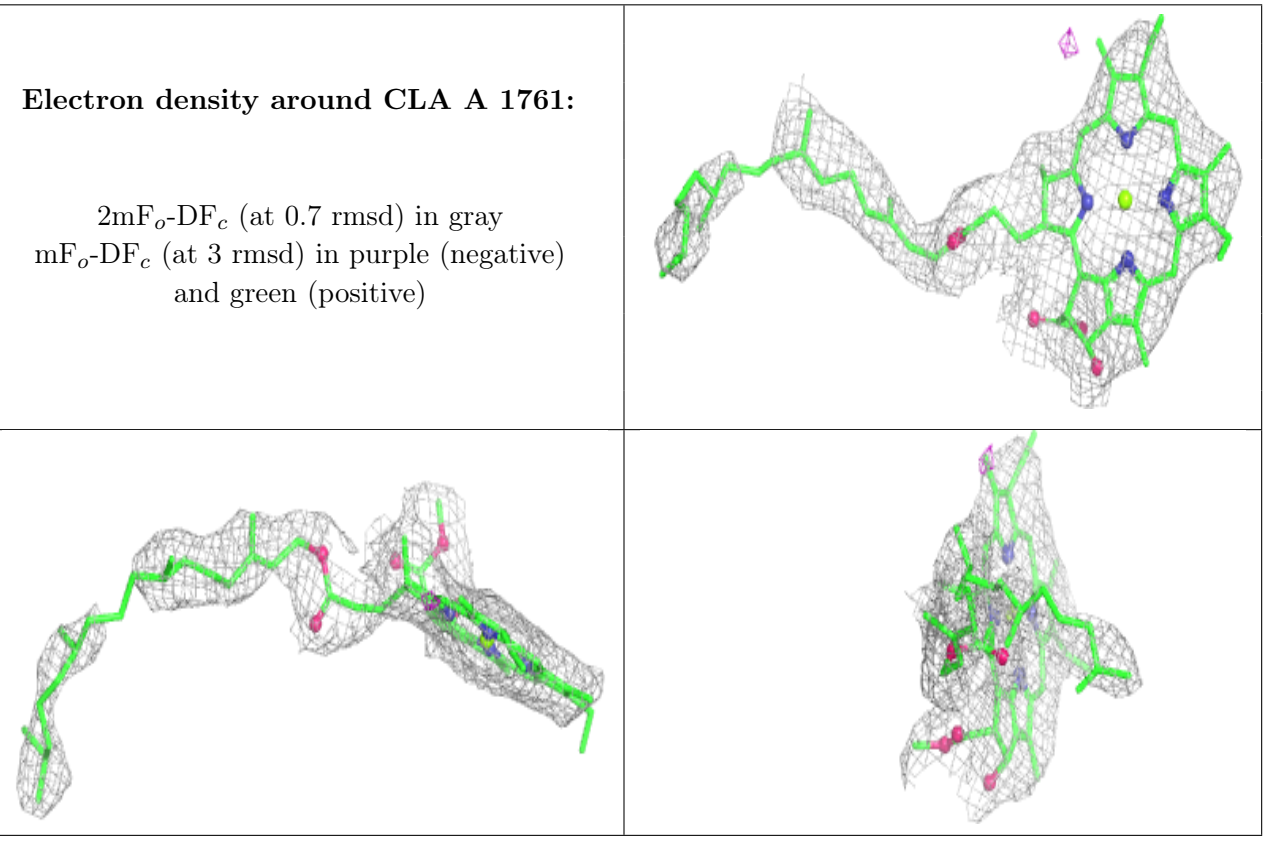
Electron density around CLA A 1812:

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



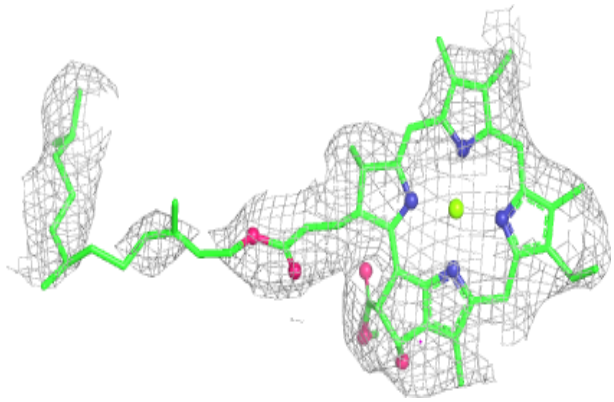
Electron density around CLA A 1761:

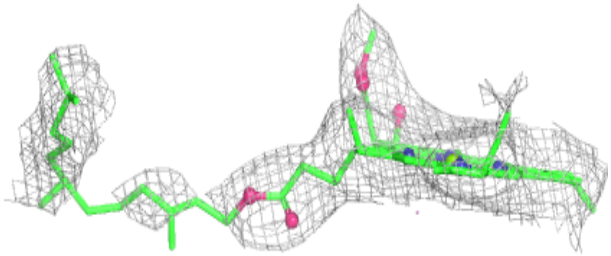
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

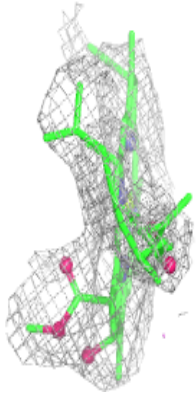


Electron density around CLA B 1767:

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

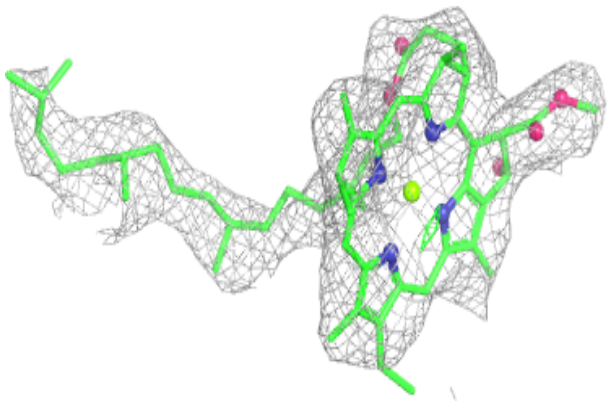


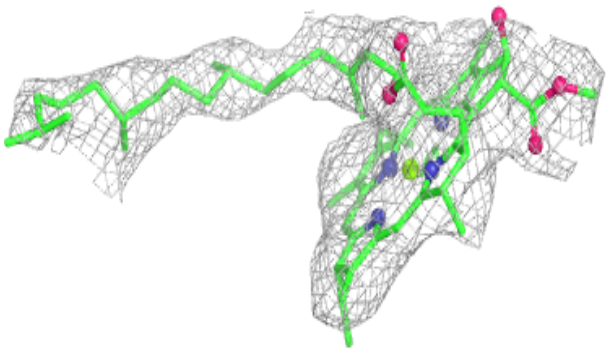


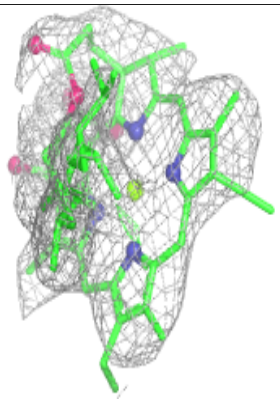


Electron density around CLA A 1796:

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

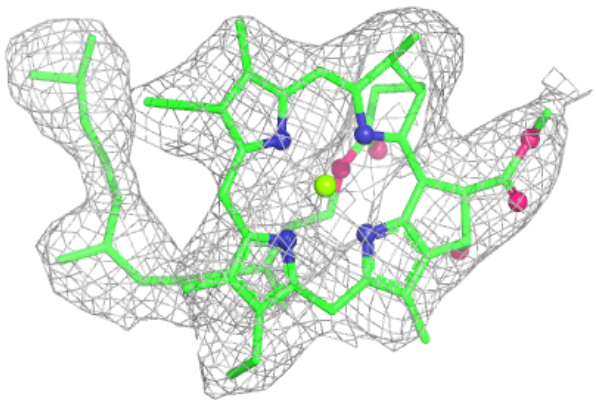


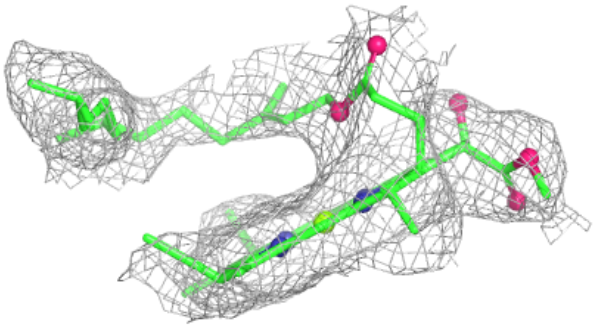


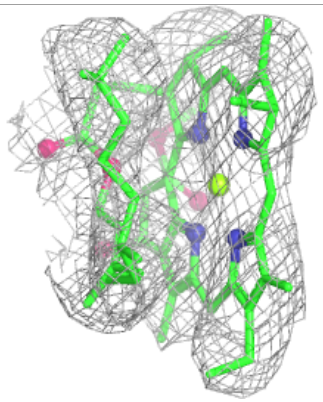


Electron density around CLA I 1031:

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

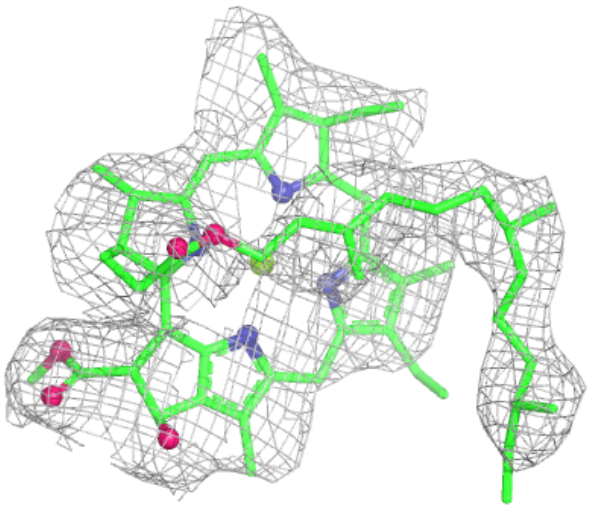


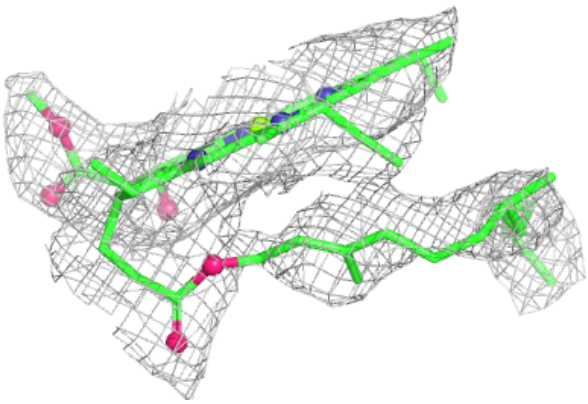


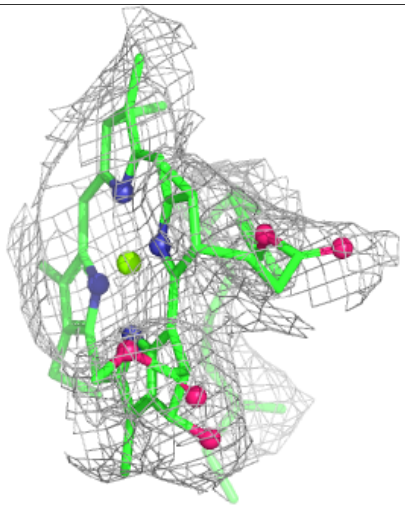


Electron density around CLA B 1749:

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

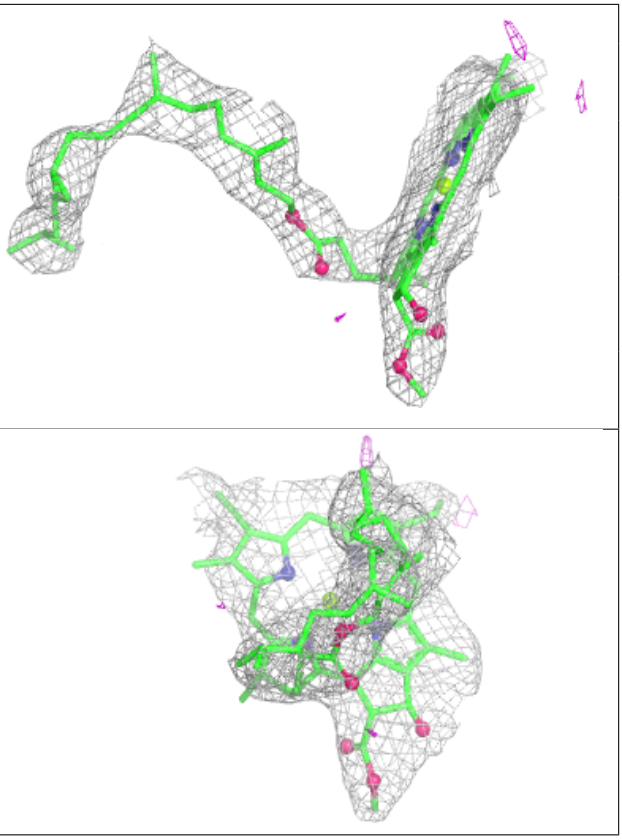






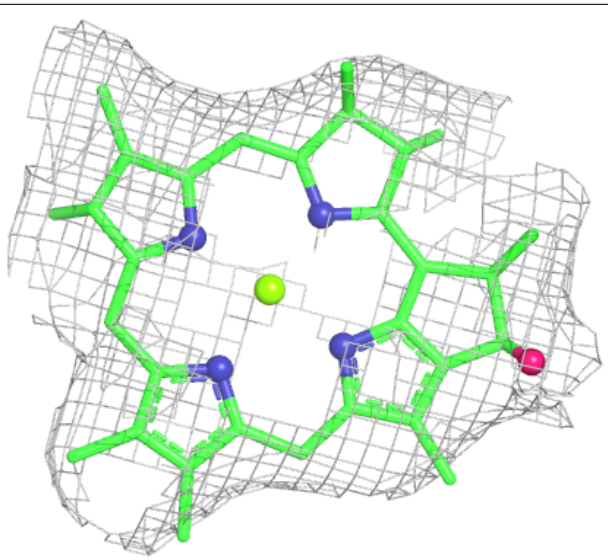
Electron density around CLA B 1770:

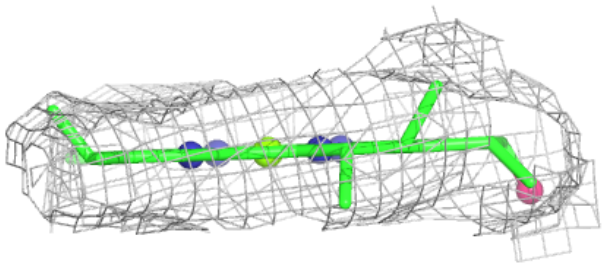
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

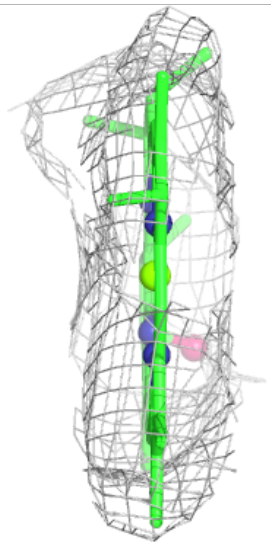


Electron density around CLA 4 1207:

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

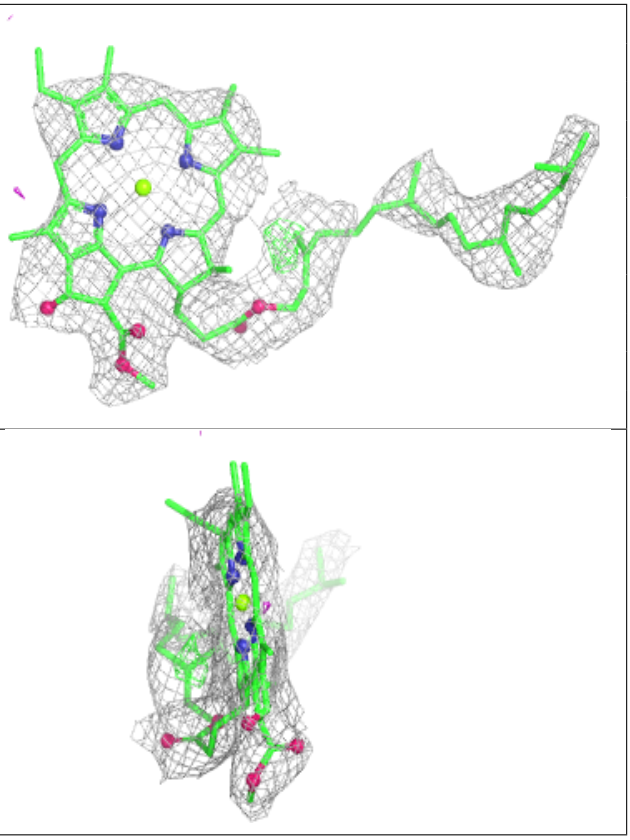






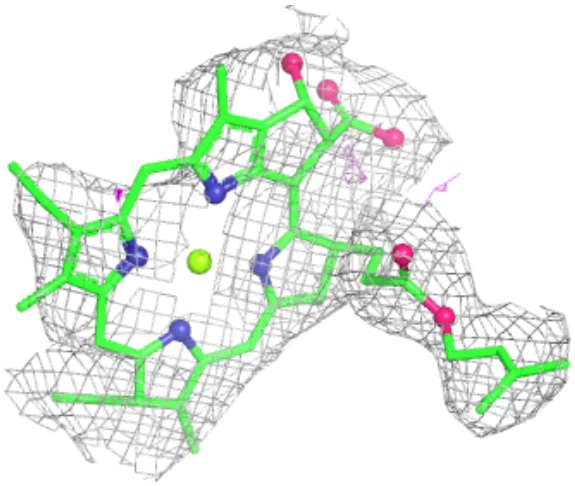
Electron density around CLA B 1787:

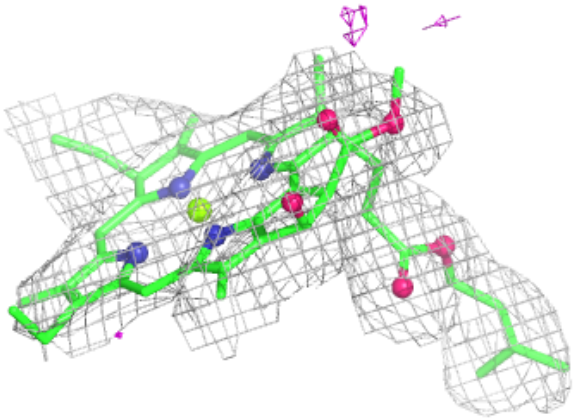
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

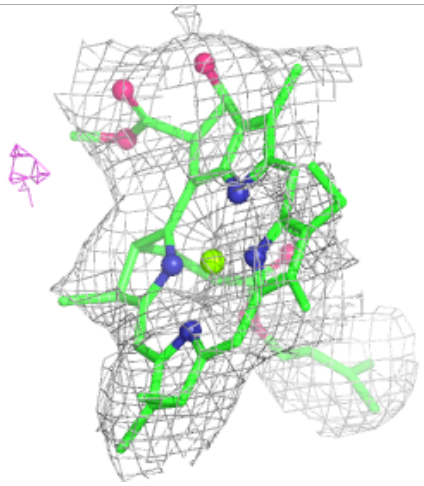


Electron density around CLA 2 1222:

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

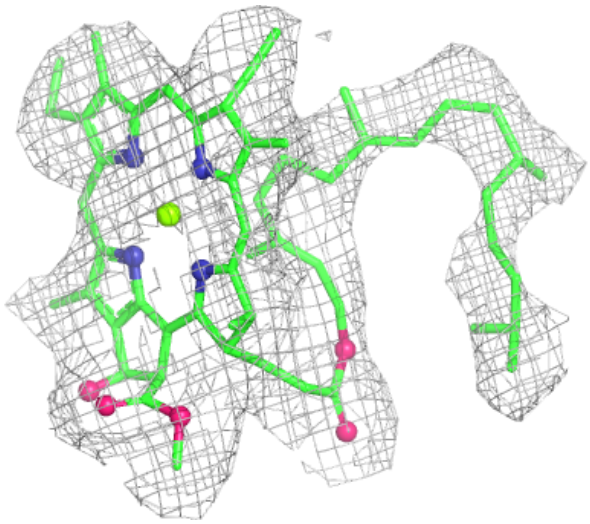


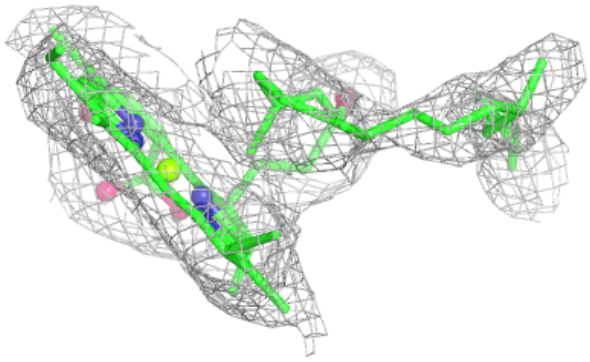


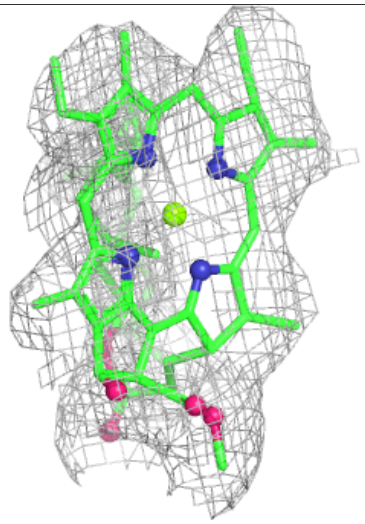


Electron density around CLA B 1753:

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

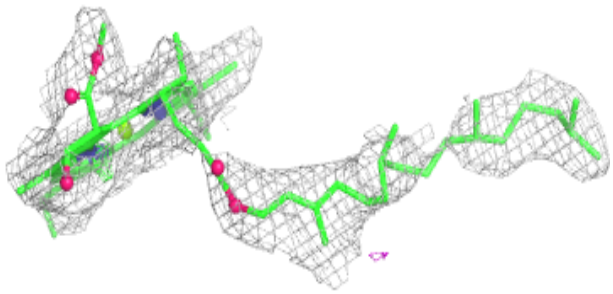


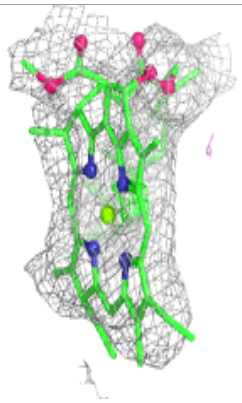




Electron density around CLA A 1789:

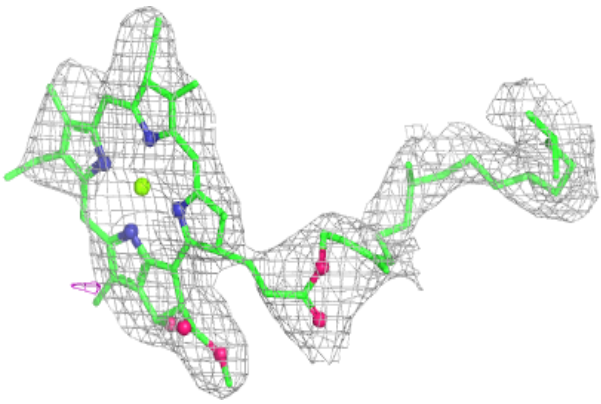
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

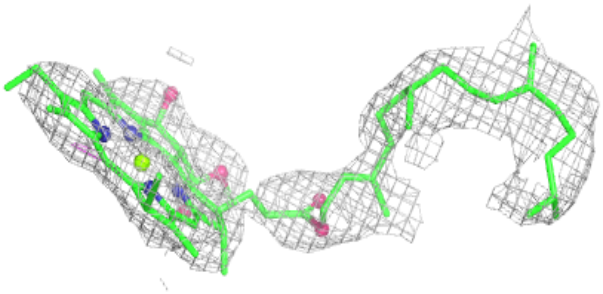


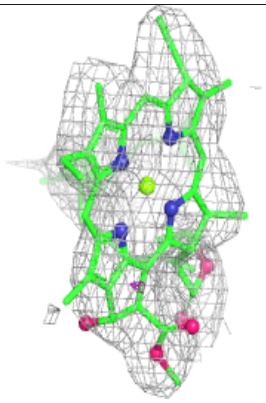


Electron density around CLA B 1740:

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

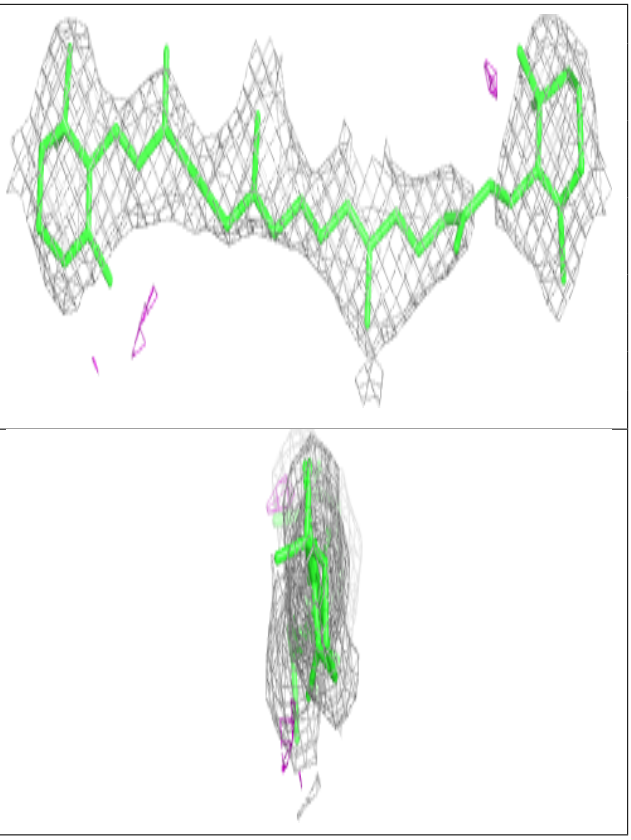






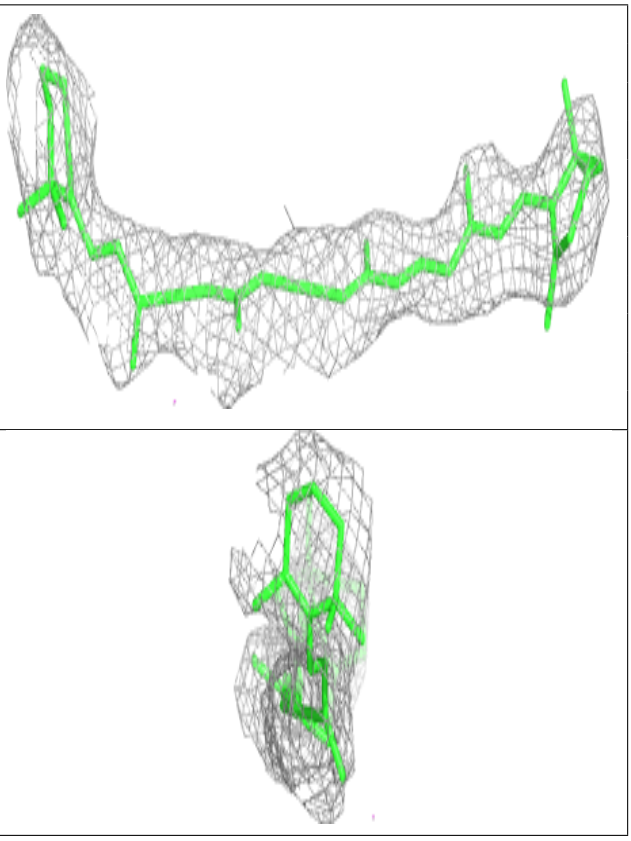
Electron density around BCR B 1777:

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



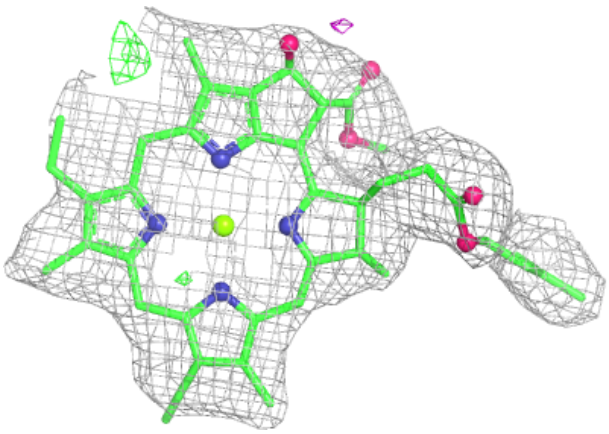
Electron density around BCR B 1778:

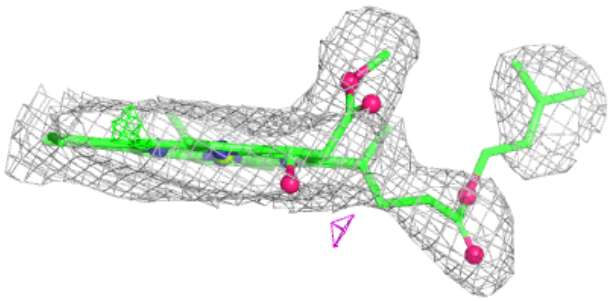
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

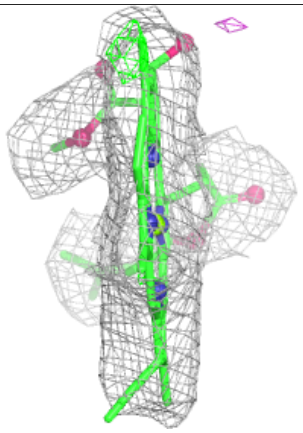


Electron density around CLA B 1761:

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

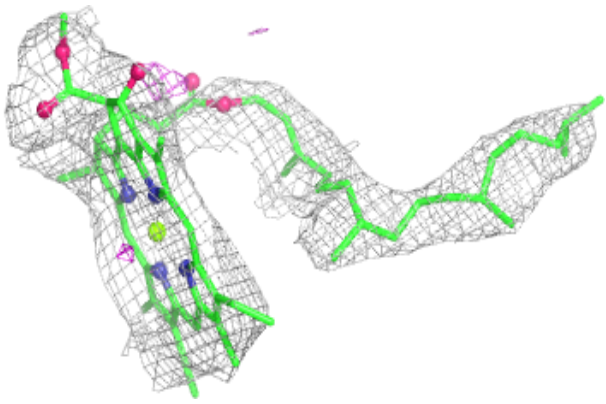


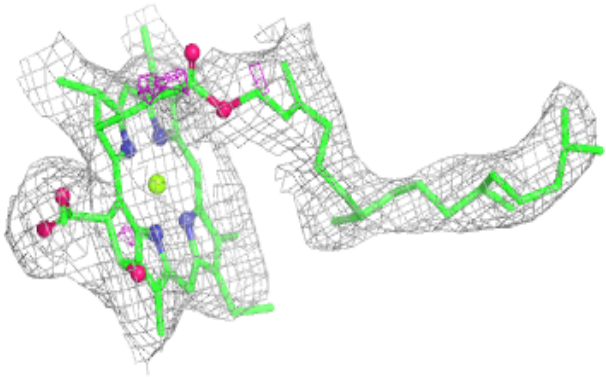


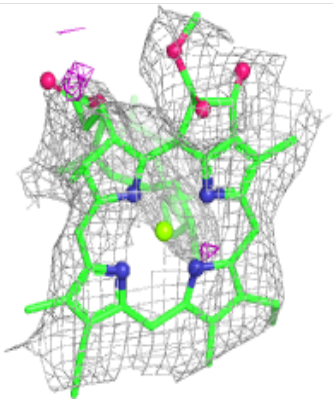


Electron density around CLA A 1767:

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

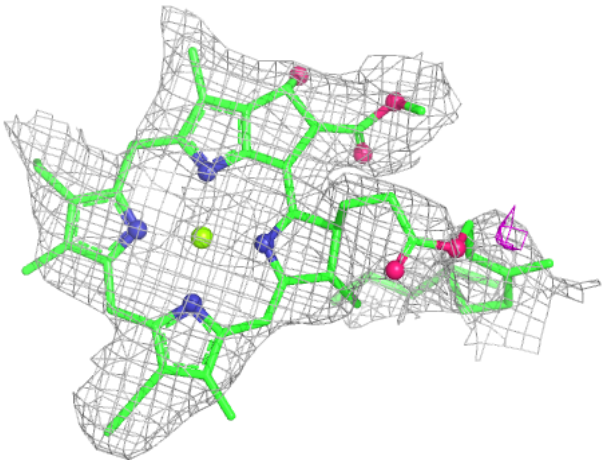


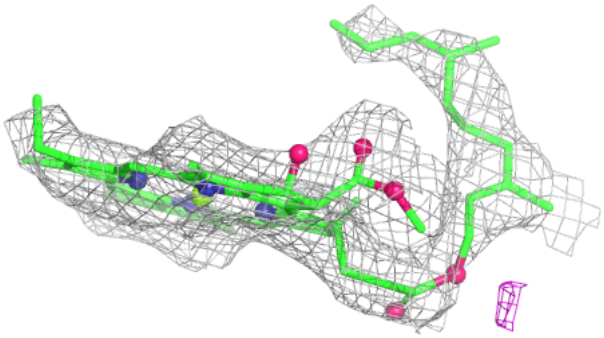


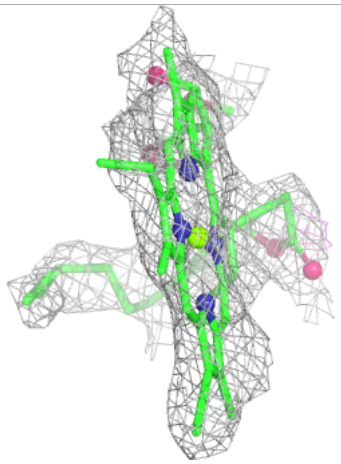


Electron density around CLA A 1762:

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

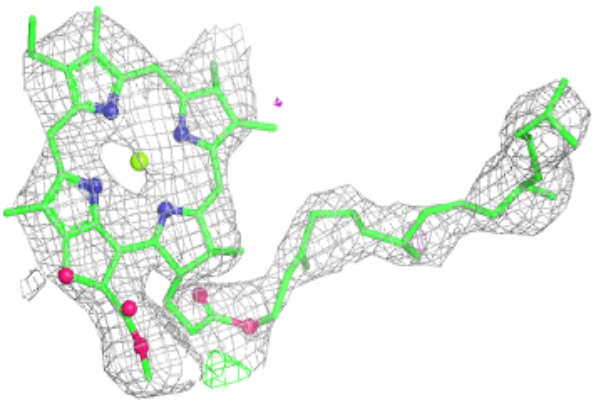


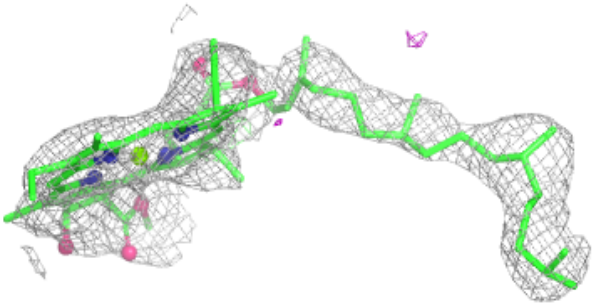




Electron density around CLA A 1813:

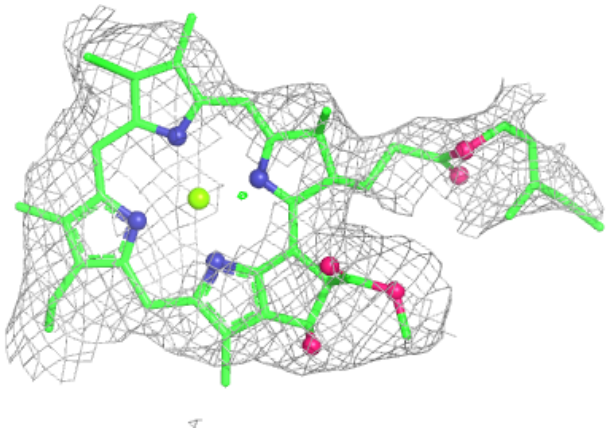
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

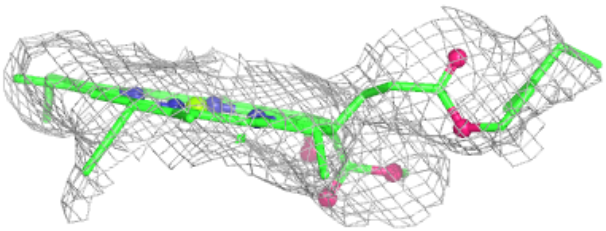


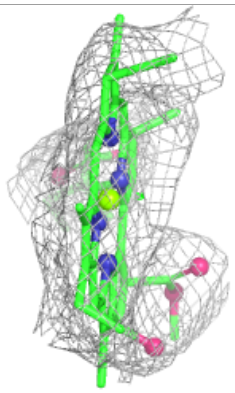


Electron density around CLA A 1795:

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

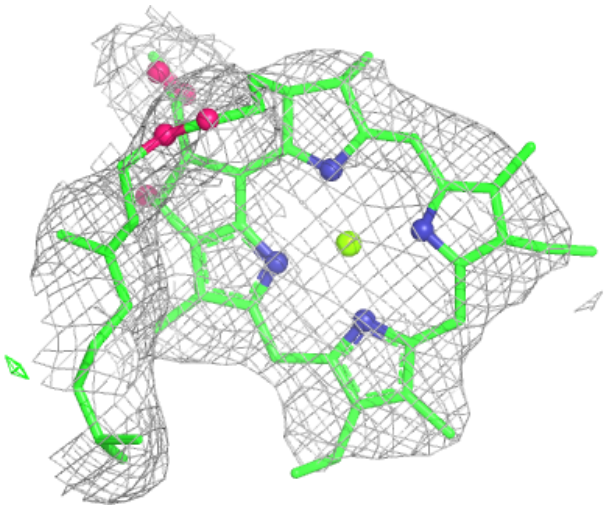


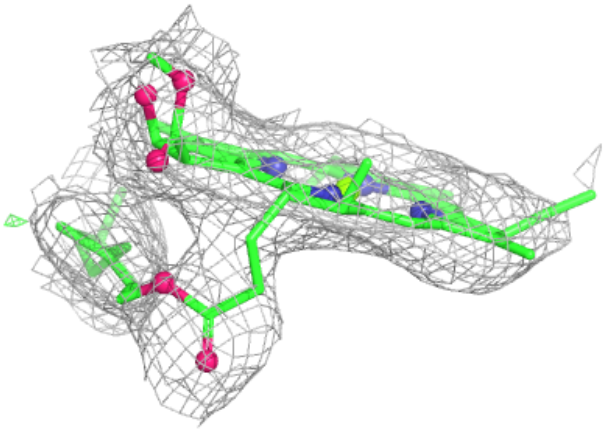


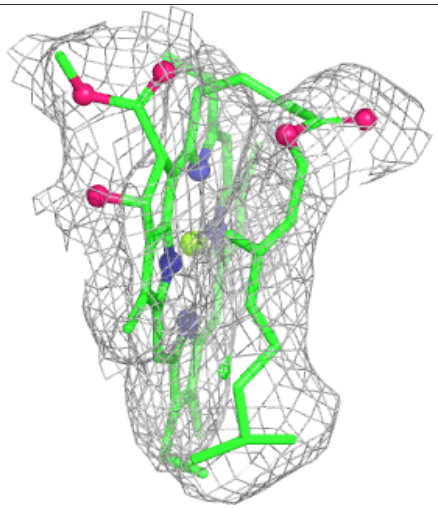


Electron density around CLA A 1784:

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

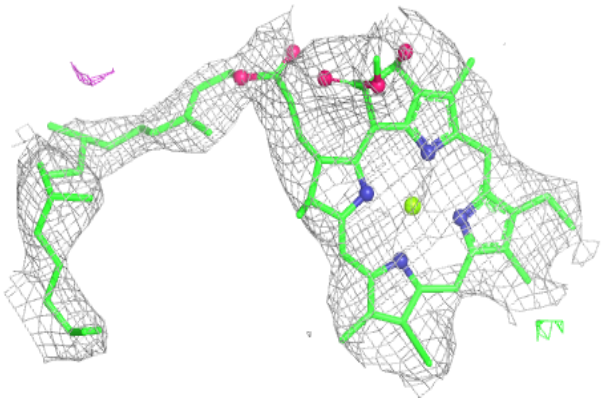


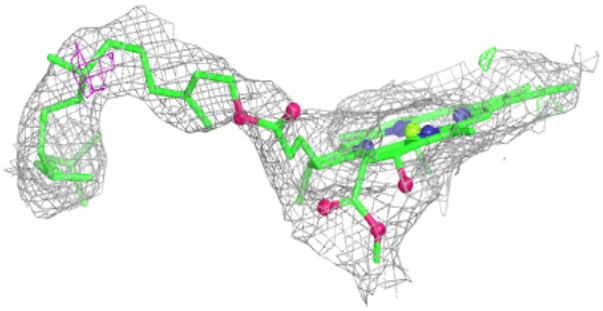


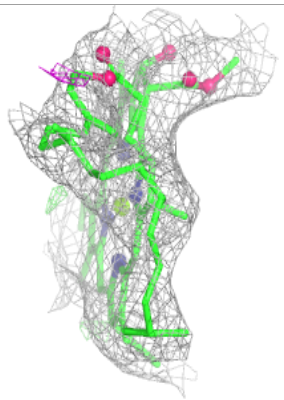


Electron density around CLA A 1782:

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

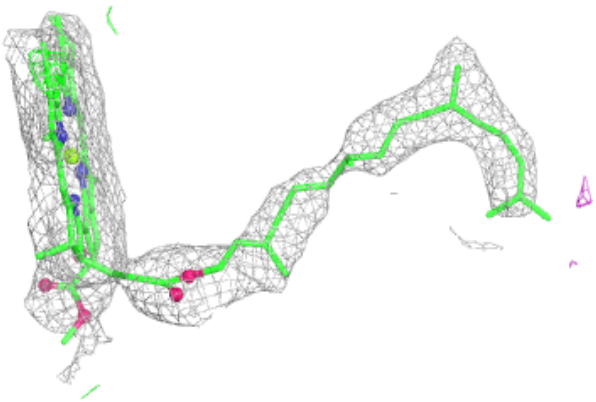


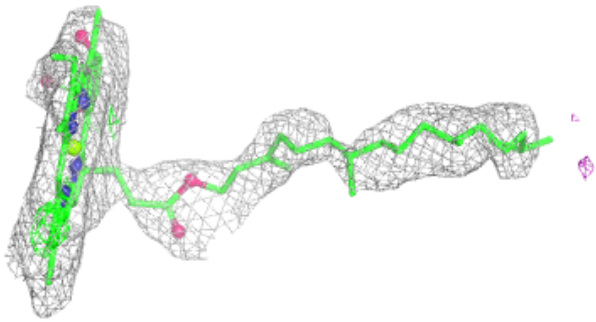


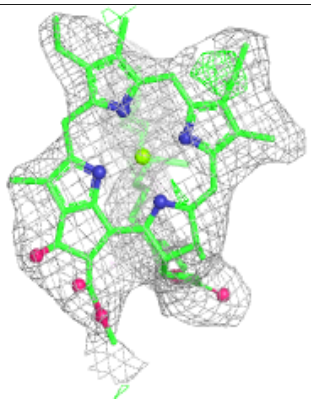


Electron density around CLA B 1771:

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

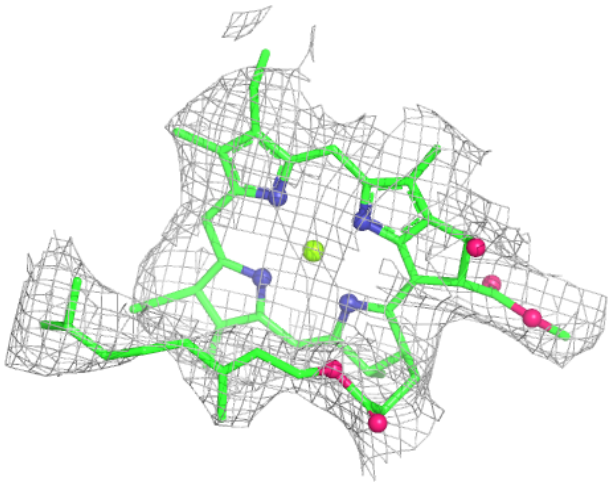


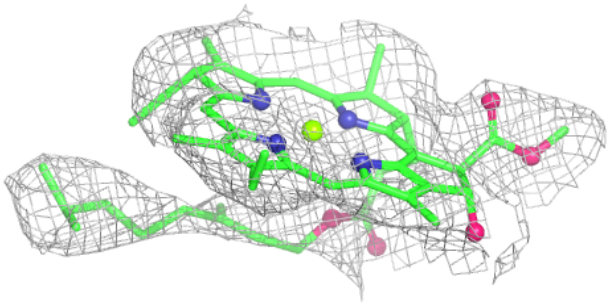




Electron density around CLA B 1752:

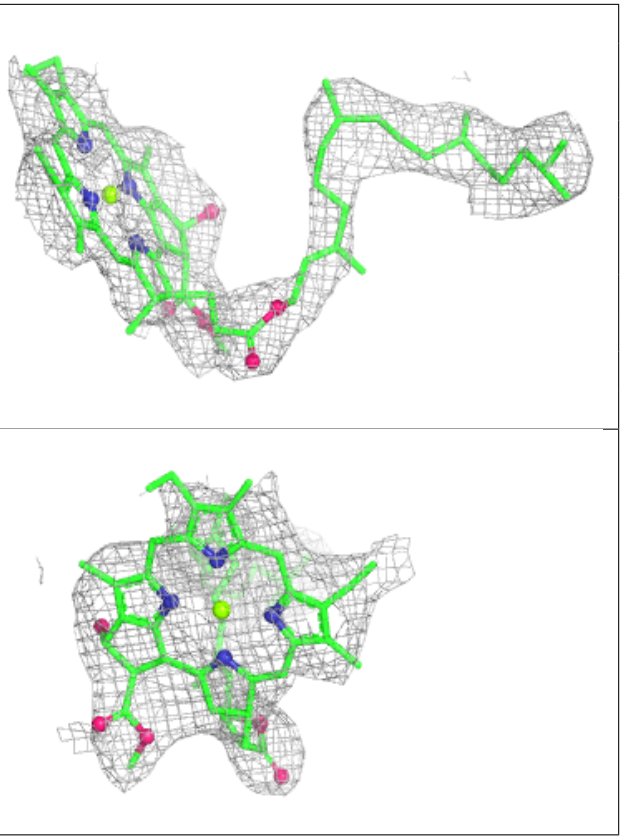
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

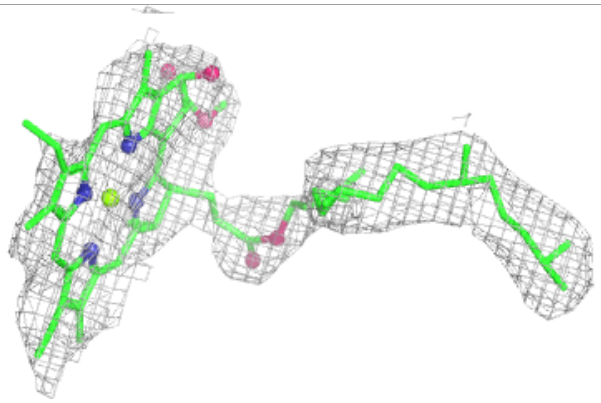




Electron density around CLA B 1785:

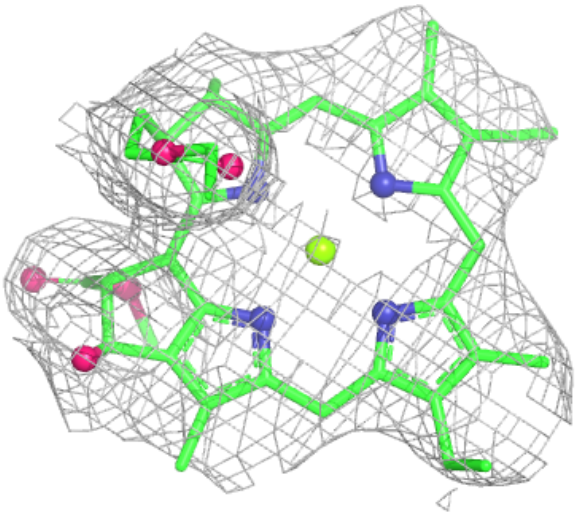
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

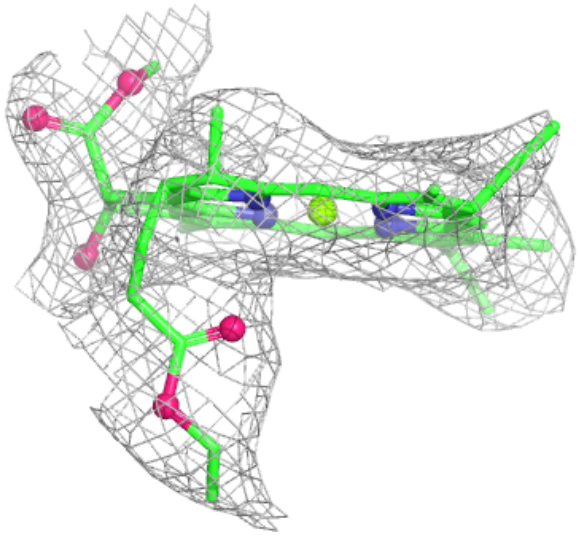


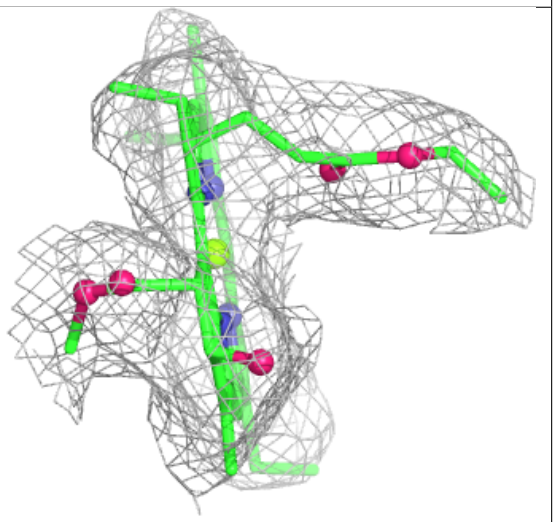


Electron density around CLA L 1167:

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

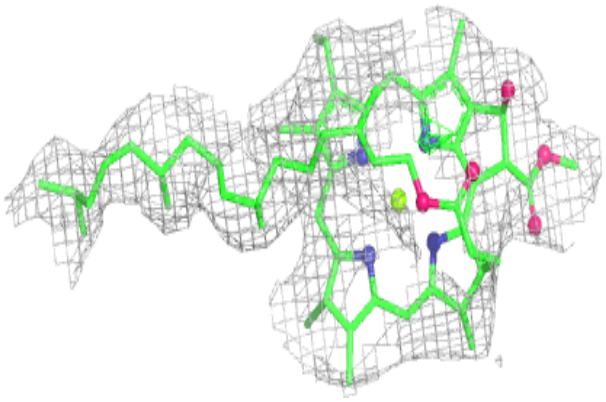


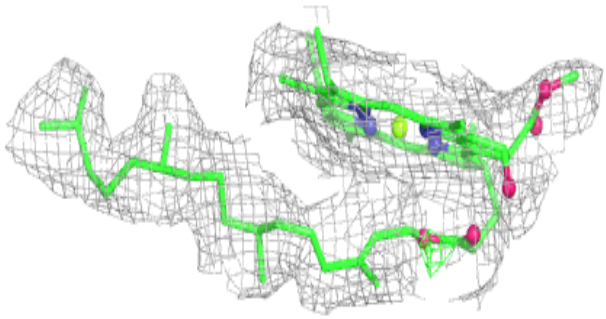


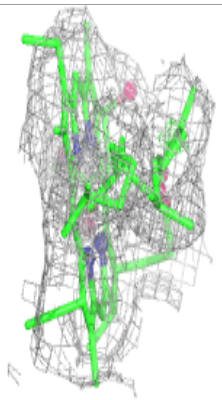


Electron density around CLA A 1793:

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

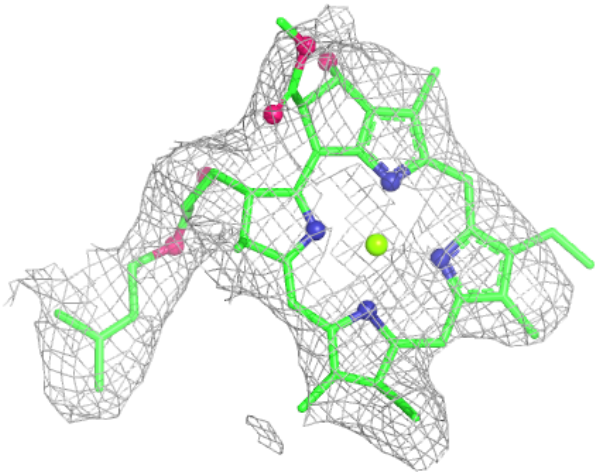


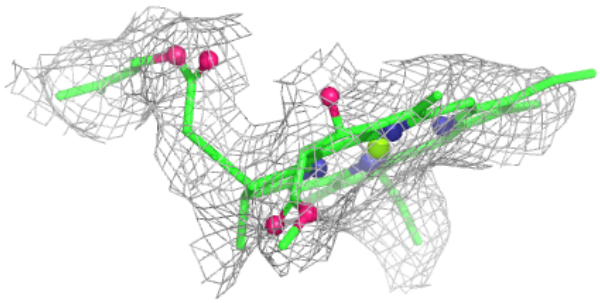




Electron density around CLA A 1790:

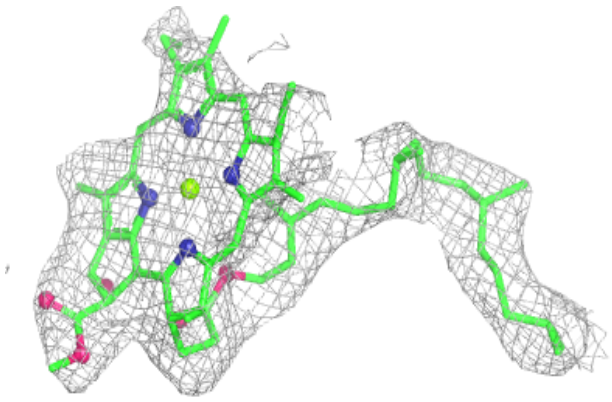
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

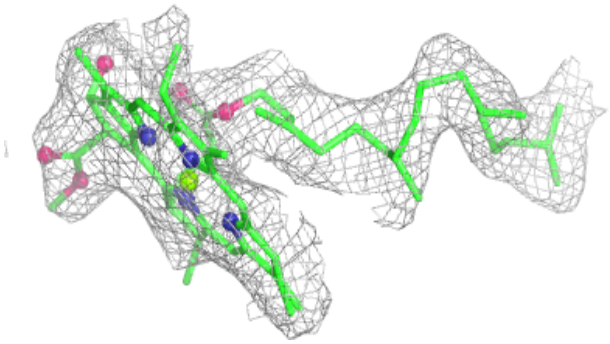


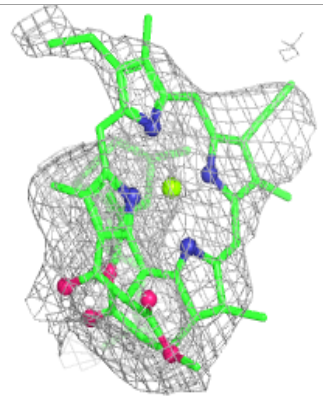


Electron density around CLA A 1800:

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

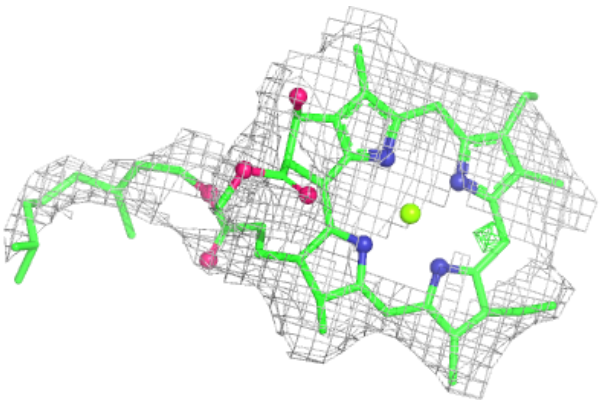


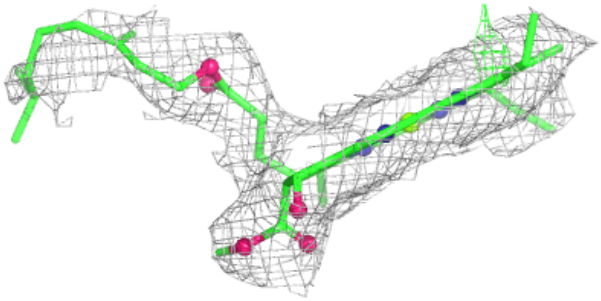


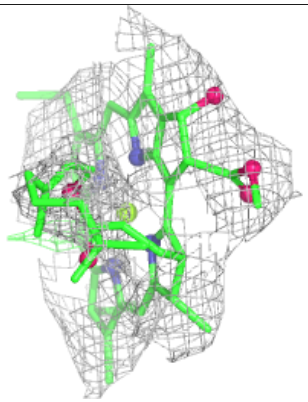


Electron density around CLA A 1765:

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

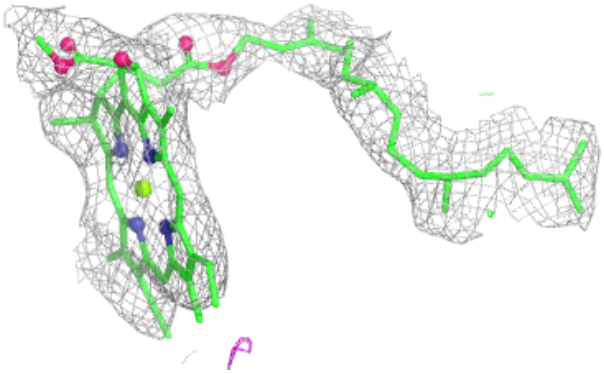


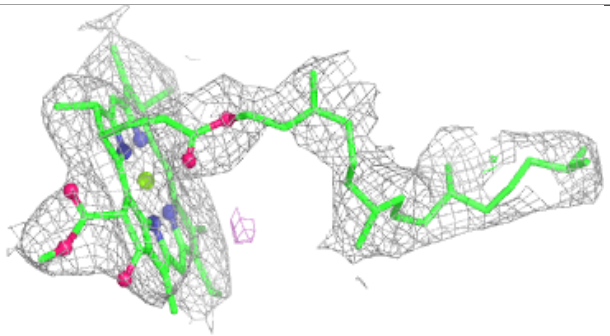


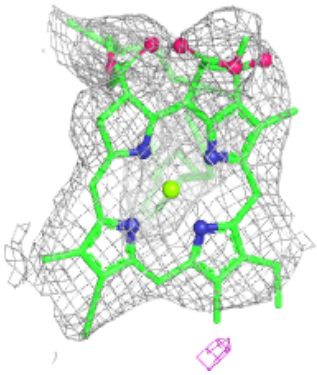


Electron density around CLA B 1759:

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

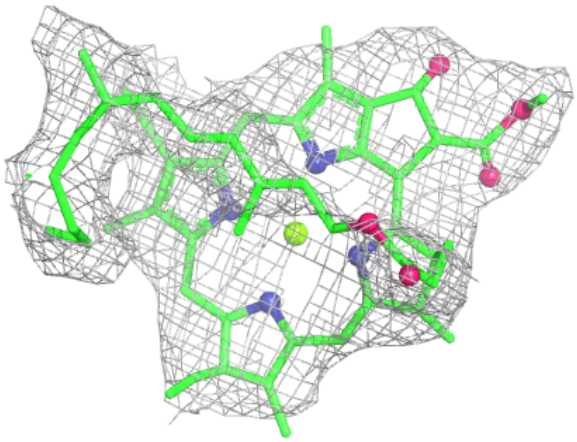


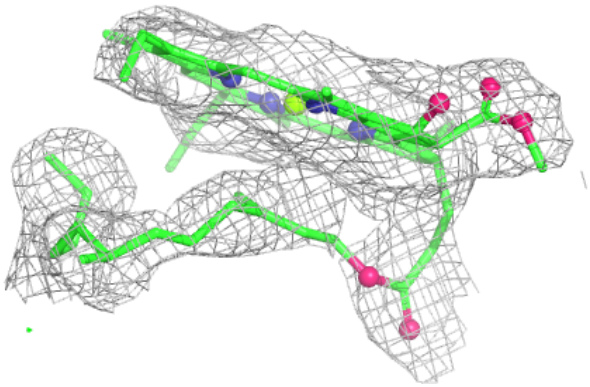


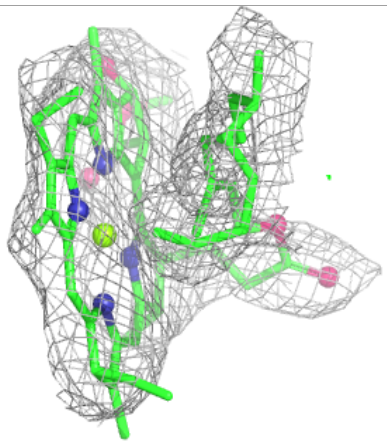


Electron density around CLA B 1747:

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

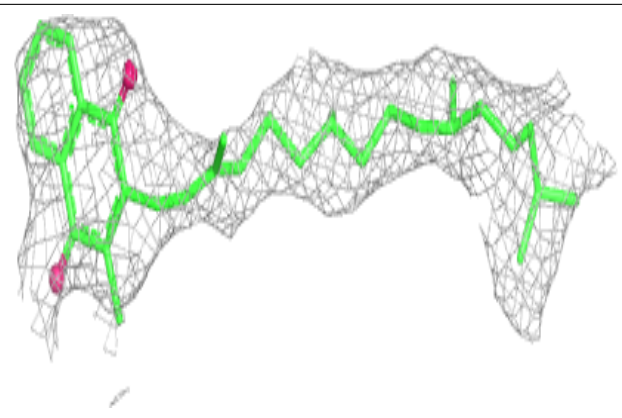


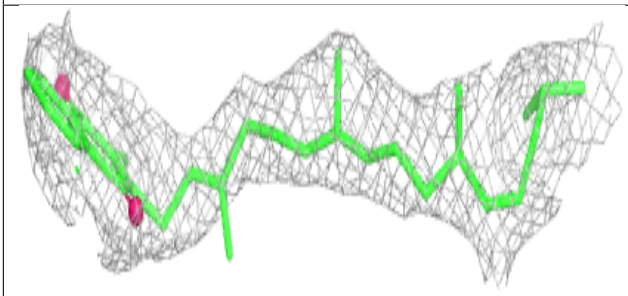




Electron density around PQN A 1802:

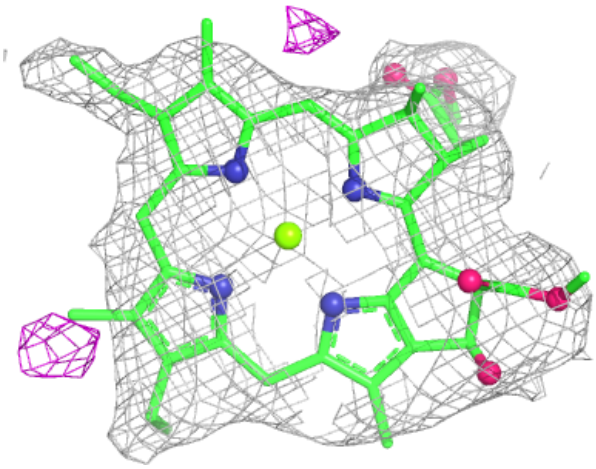
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

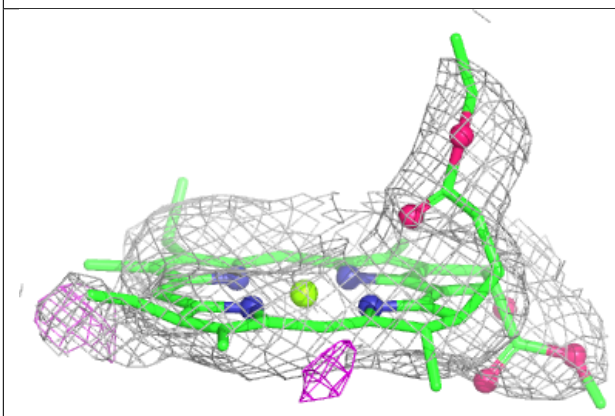


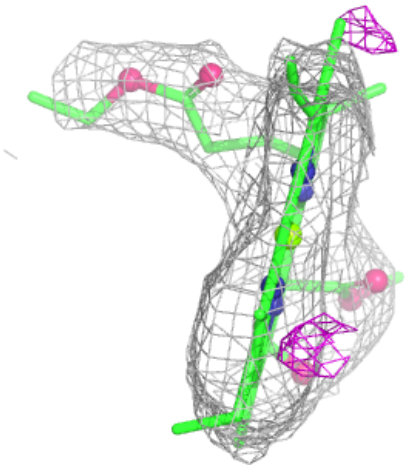


Electron density around CLA B 1769:

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

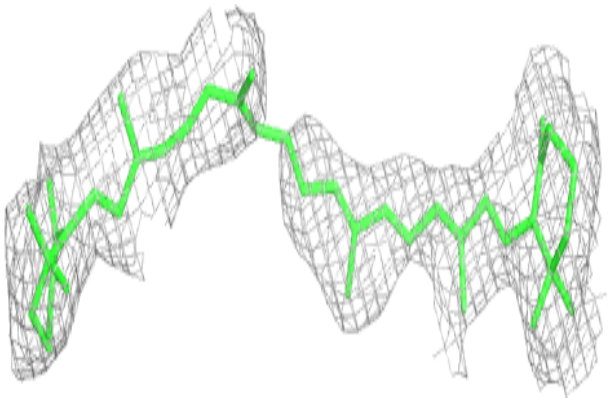


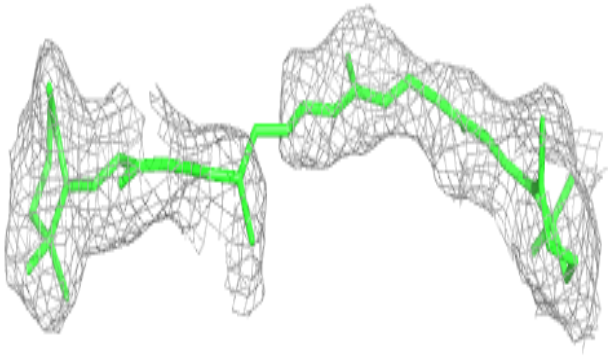


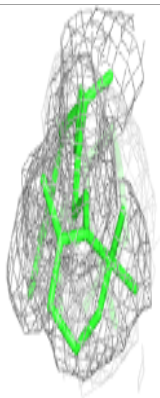


Electron density around BCR B 1781:

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

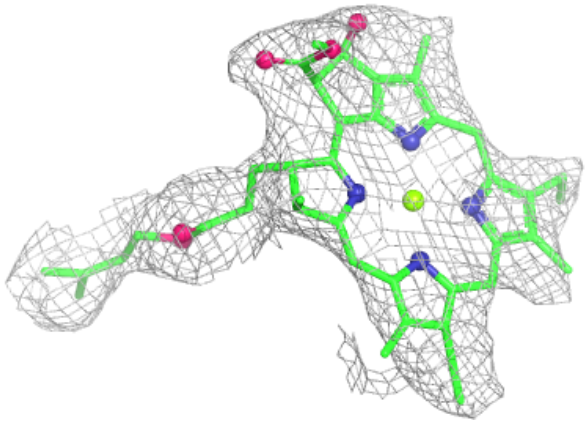


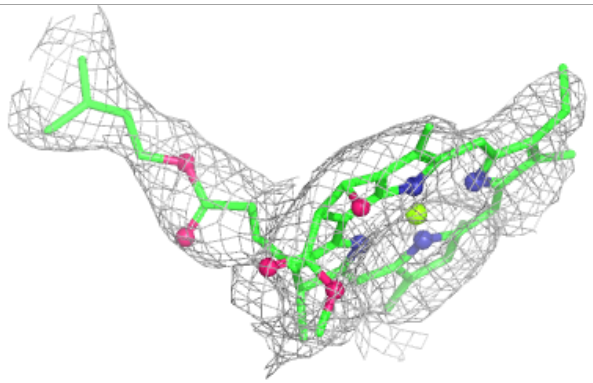




Electron density around CLA A 1786:

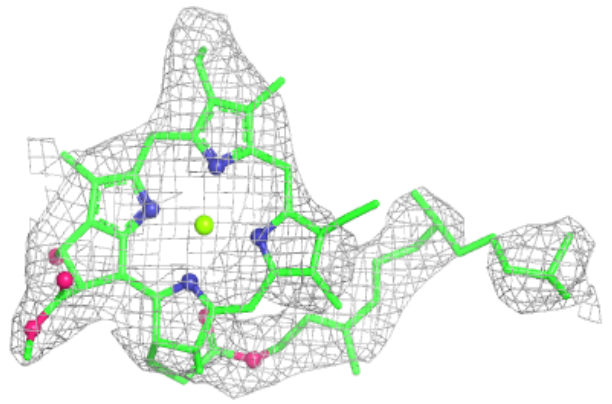
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

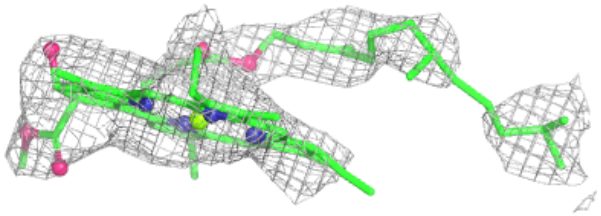


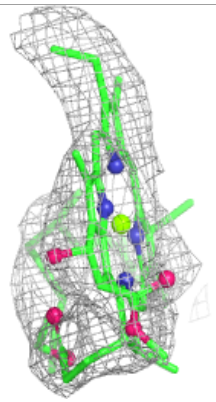


Electron density around CLA B 1748:

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

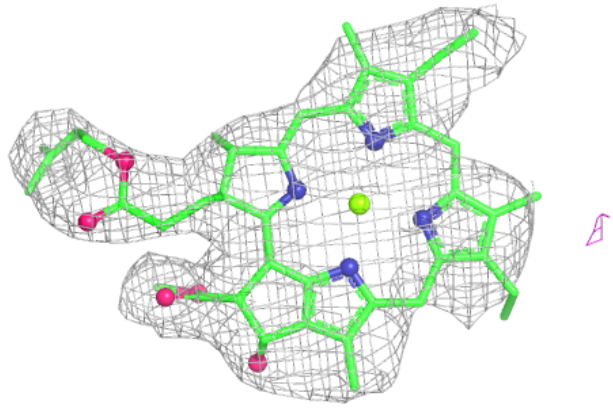


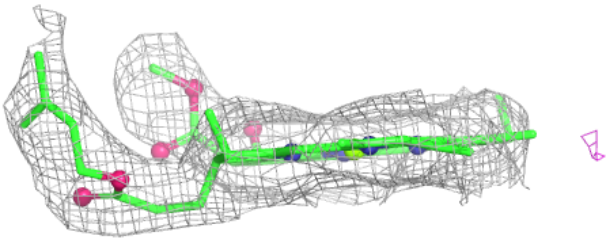


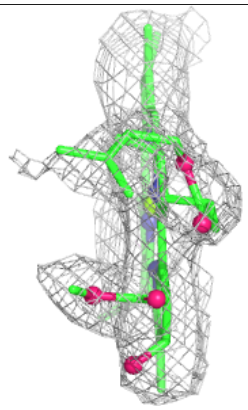


Electron density around CLA A 1759:

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

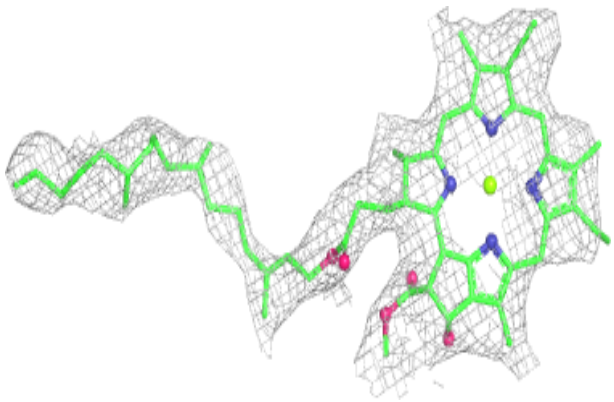


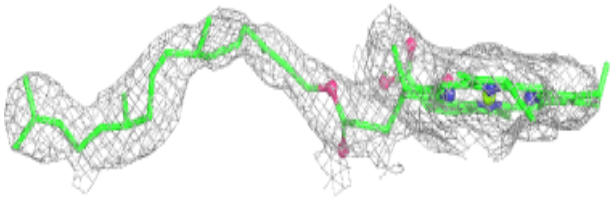


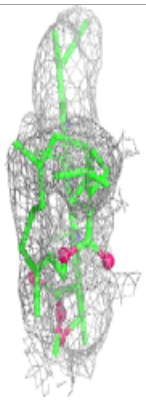


Electron density around CLA A 1788:

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

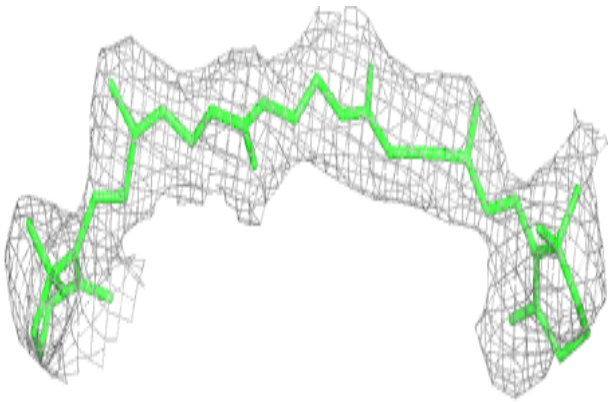


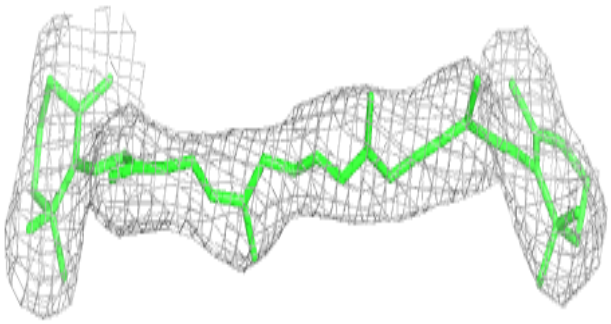


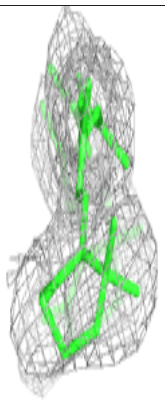


Electron density around BCR L 1170:

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

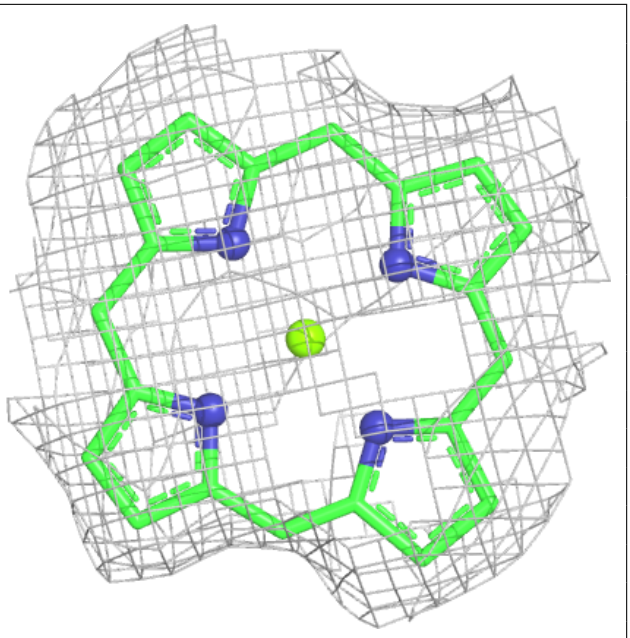


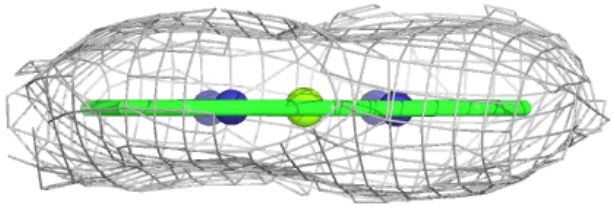


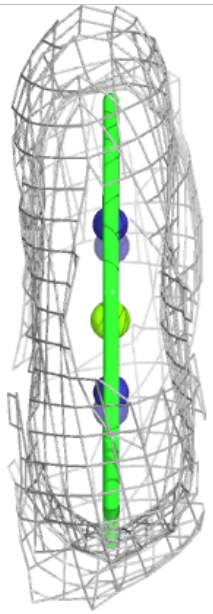


Electron density around CLA 4 1206:

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

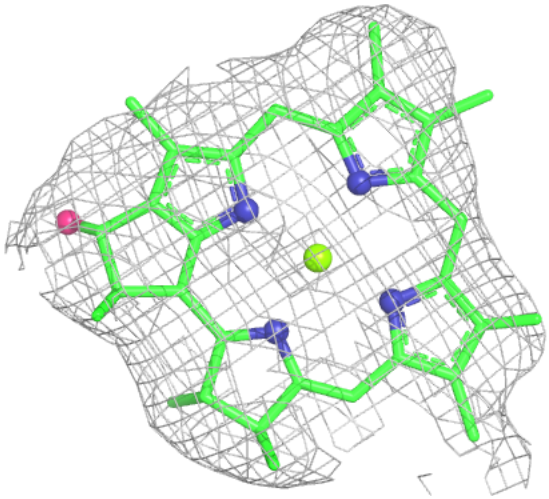


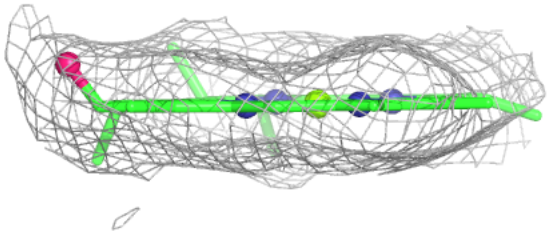


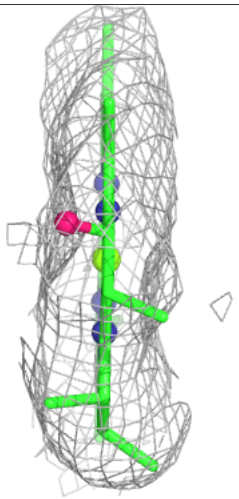


Electron density around CLA F 1155:

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

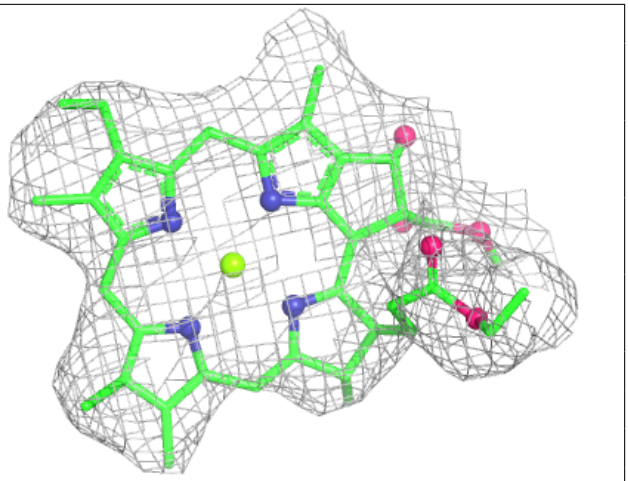


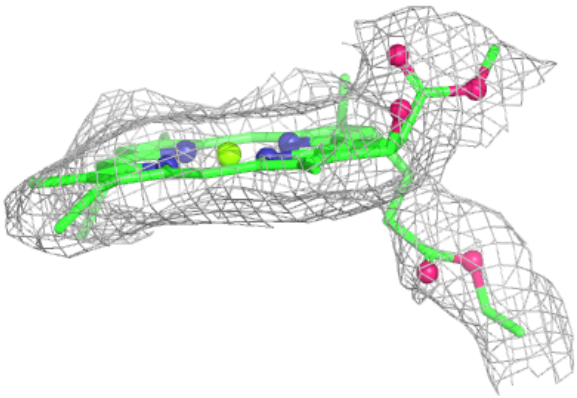


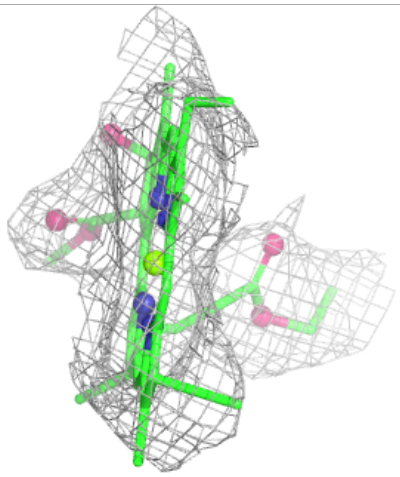


Electron density around CLA A 1794:

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

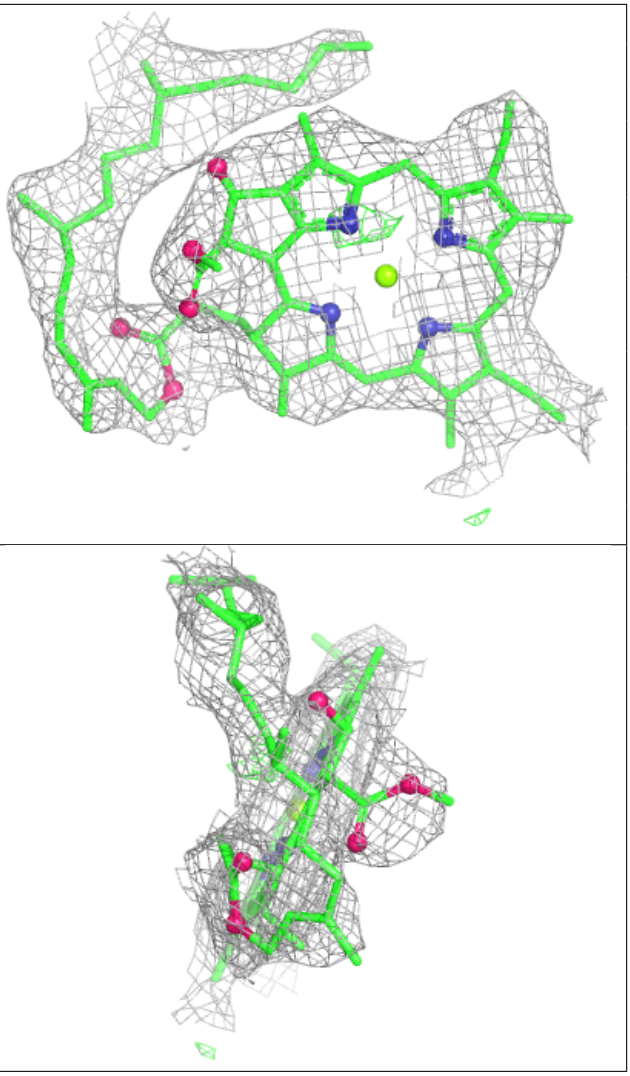






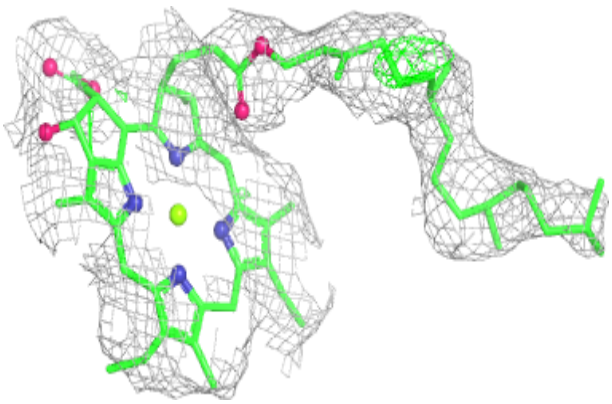
Electron density around CLA B 1737:

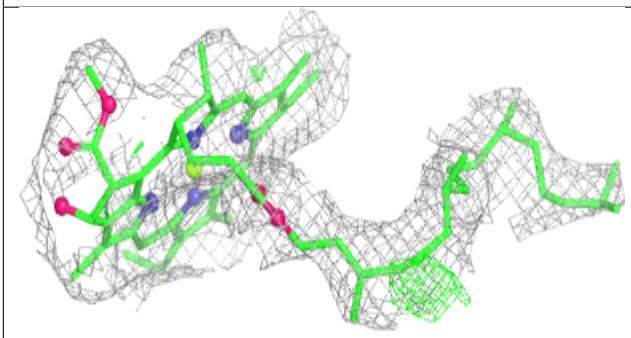
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

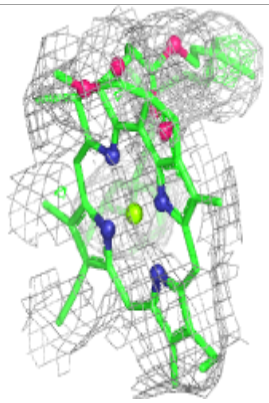


Electron density around CLA A 1764:

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

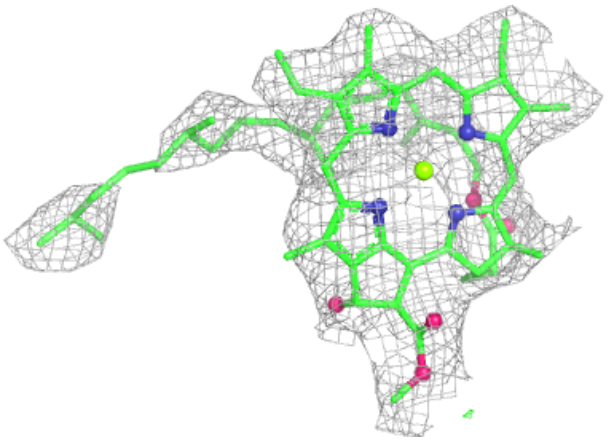


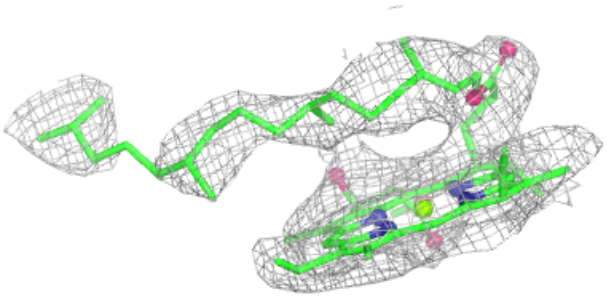


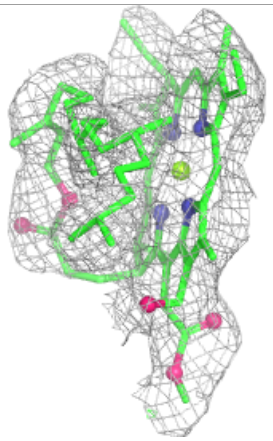


Electron density around CLA B 1757:

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

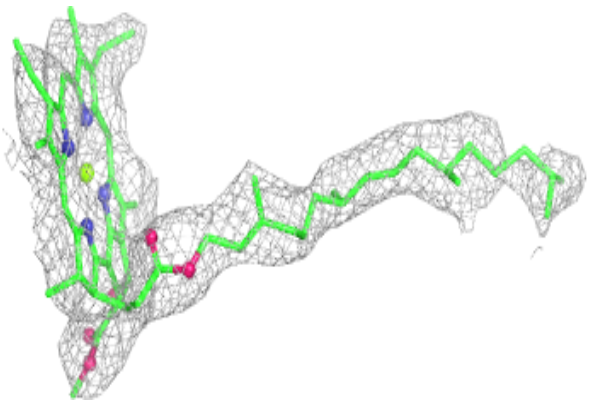


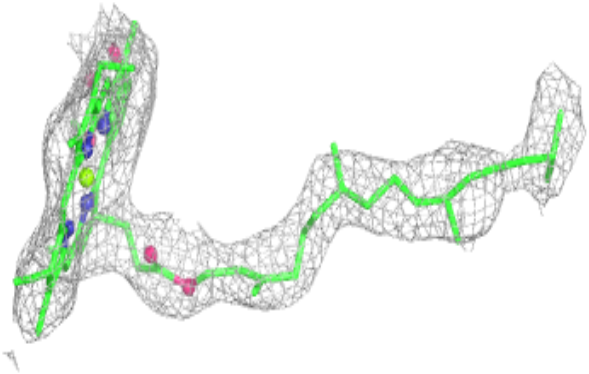


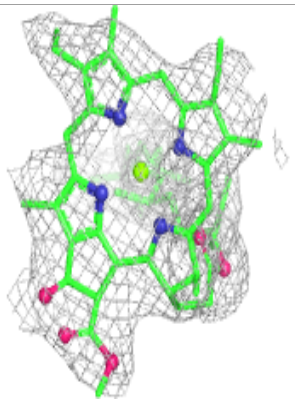


Electron density around CLA B 1758:

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

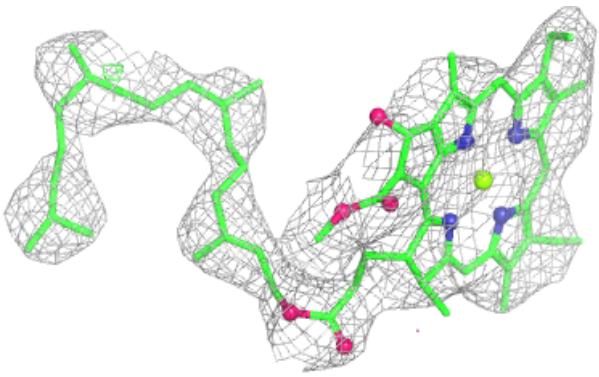


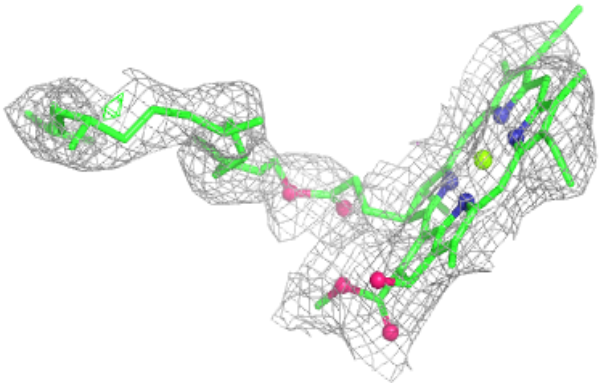


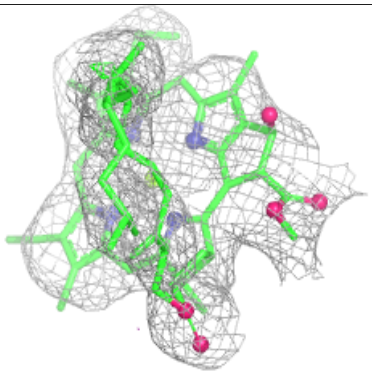


Electron density around CLA A 1811:

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

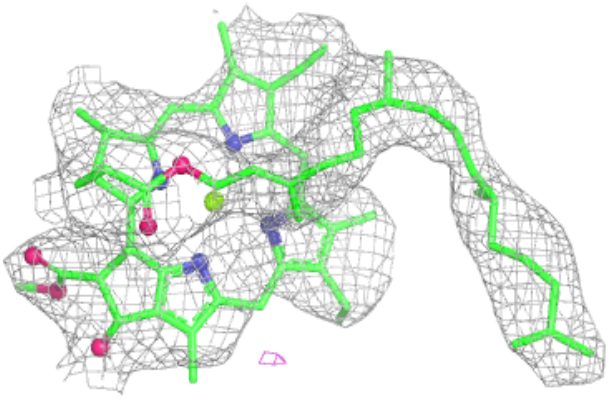


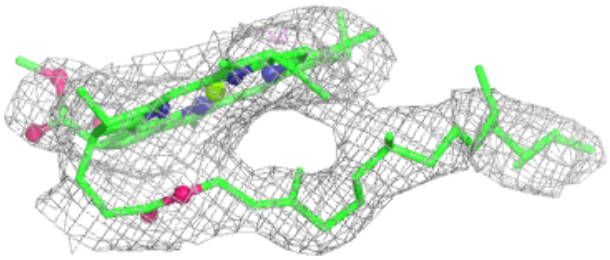


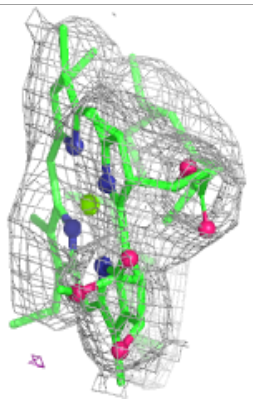


Electron density around CLA B 1768:

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

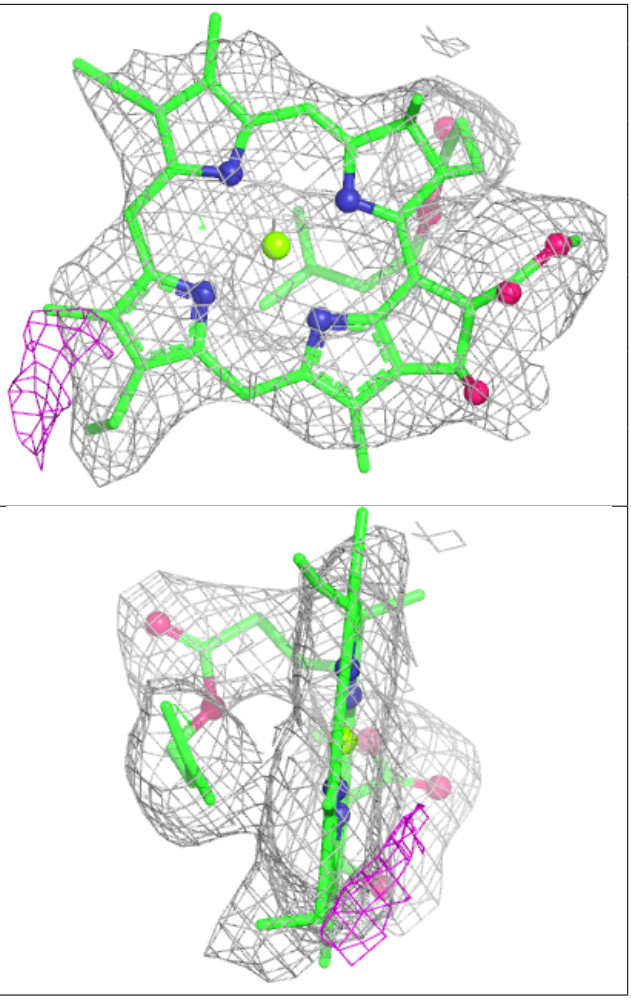






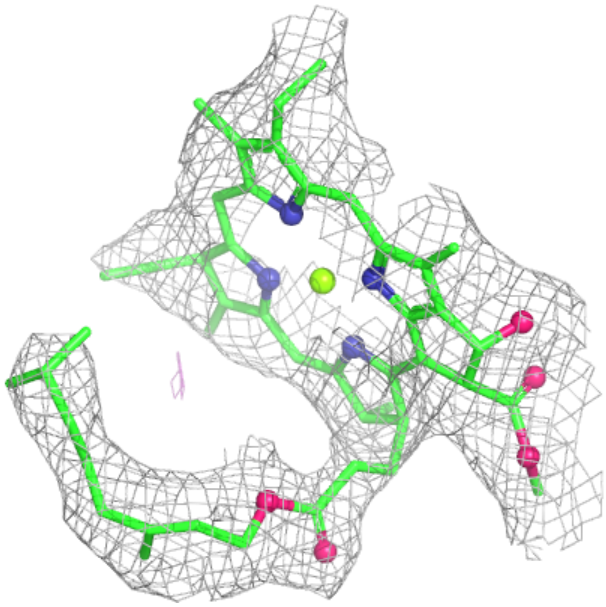
Electron density around CLA B 1760:

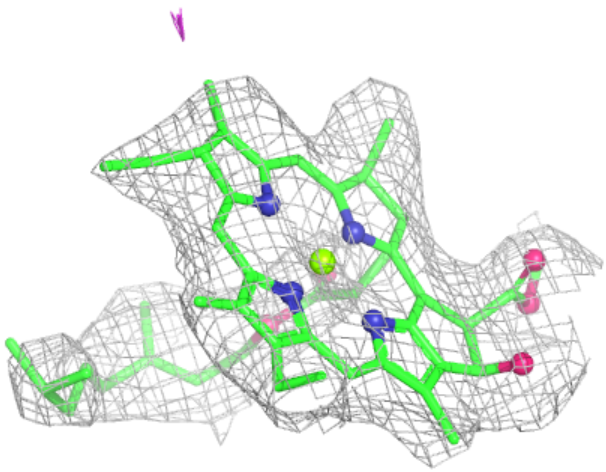
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

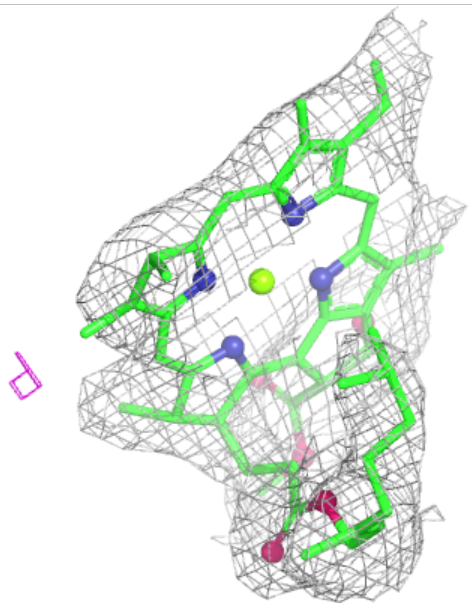


Electron density around CLA A 1779:

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

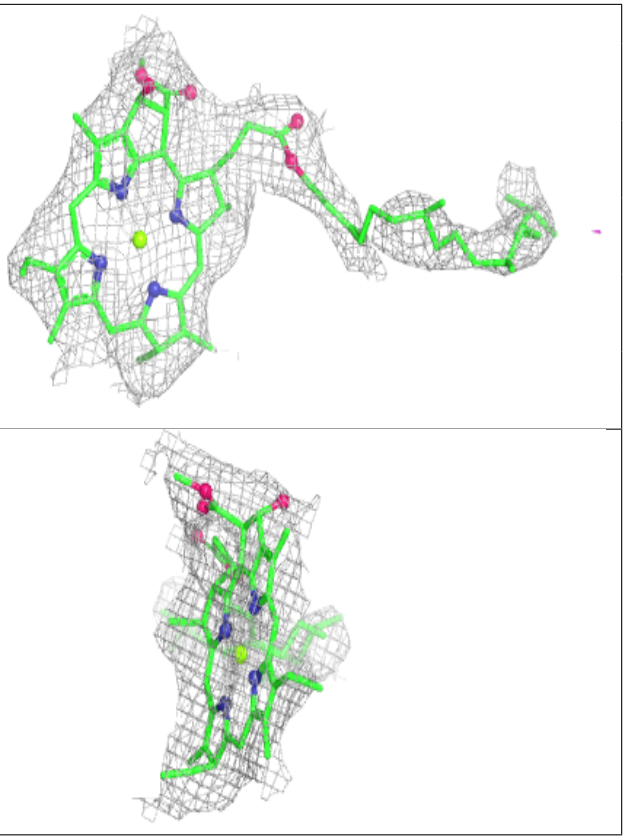


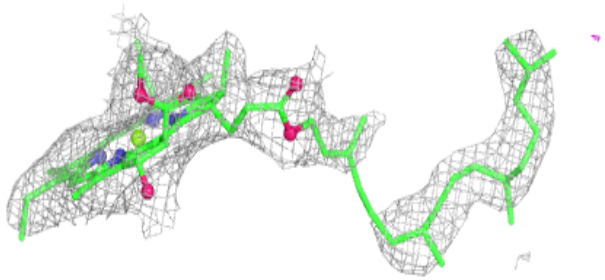




Electron density around CLA B 1743:

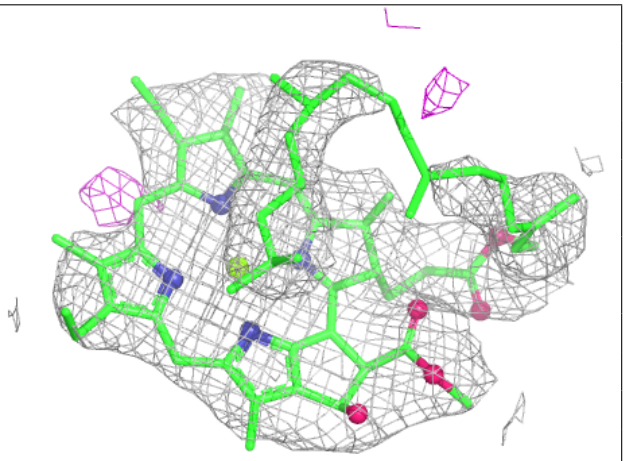
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

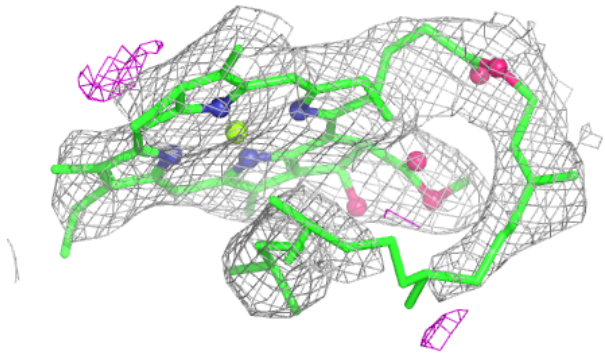


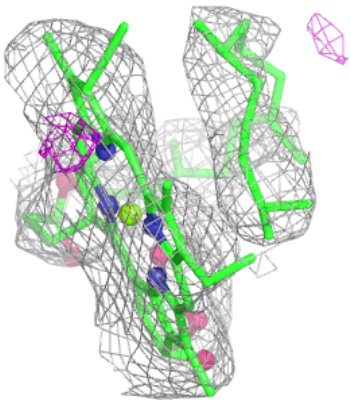


Electron density around CLA B 1738:

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

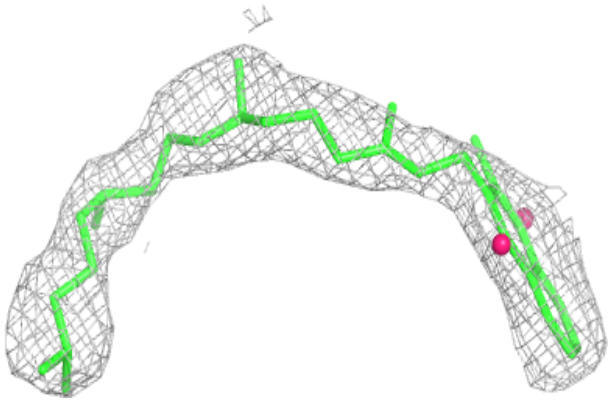


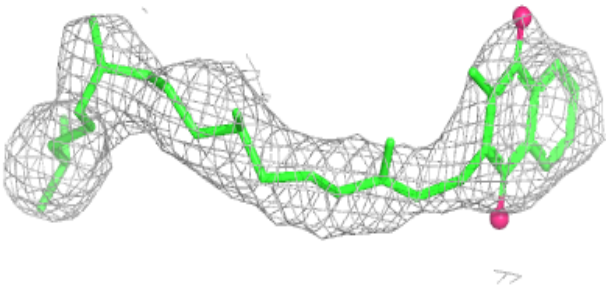


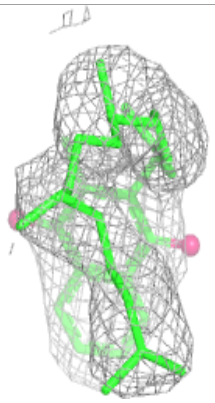


Electron density around PQN B 1773:

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

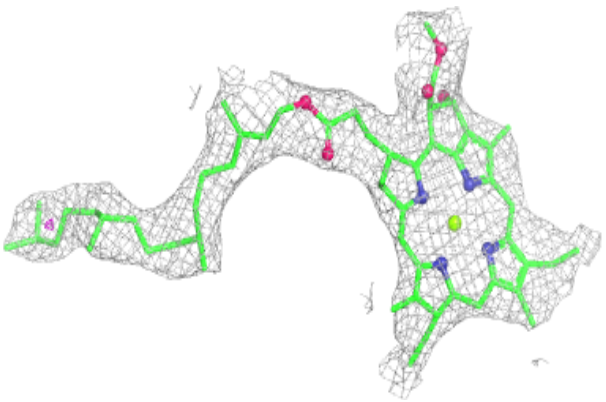


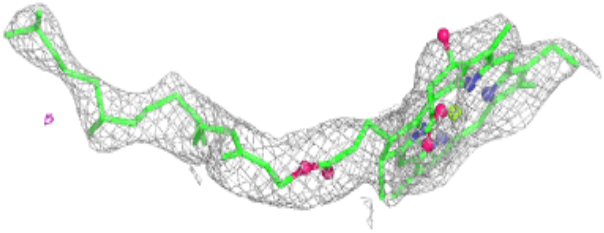


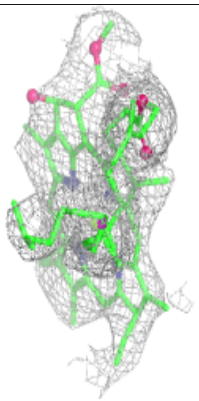


Electron density around CLA B 1786:

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

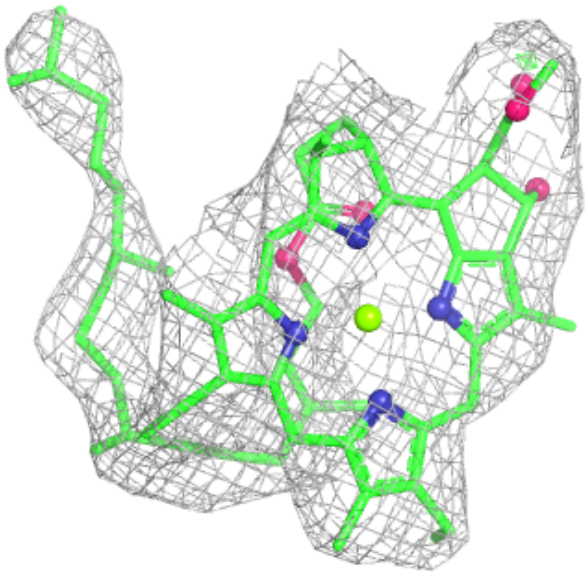


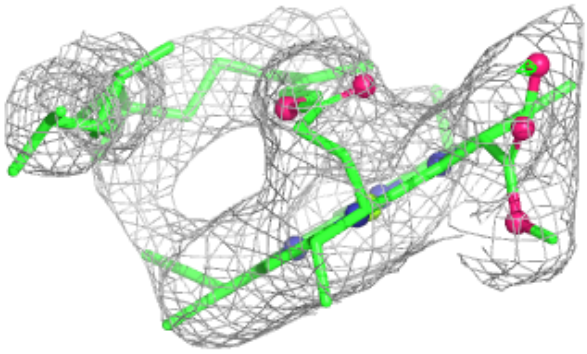


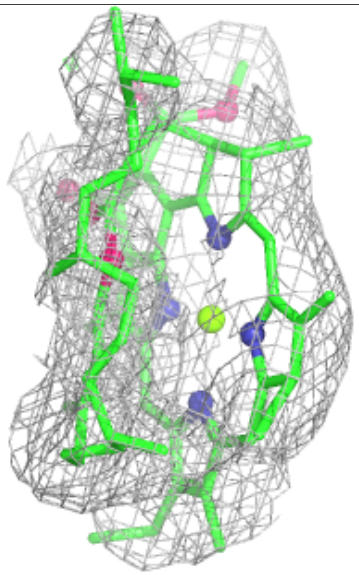


Electron density around CLA B 1739:

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

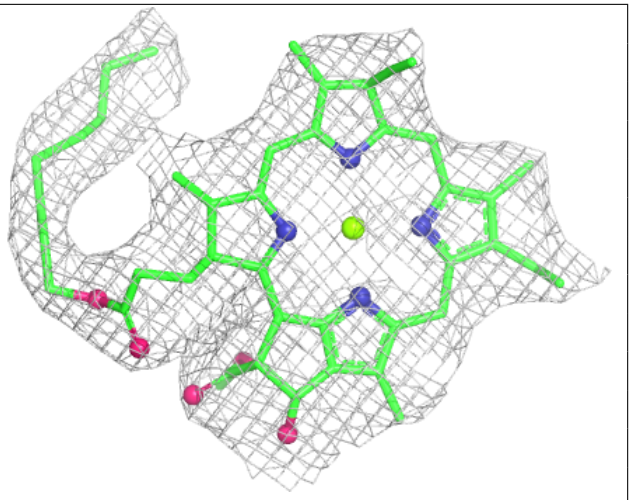


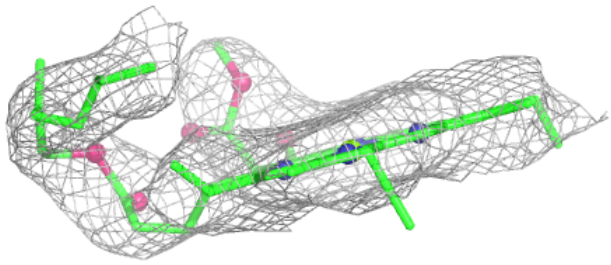


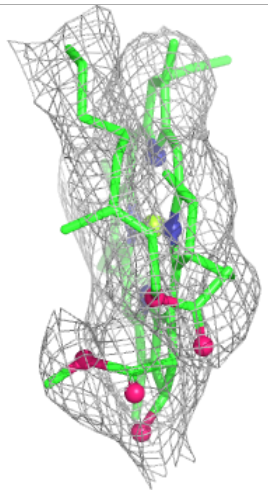


Electron density around CLA B 1754:

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

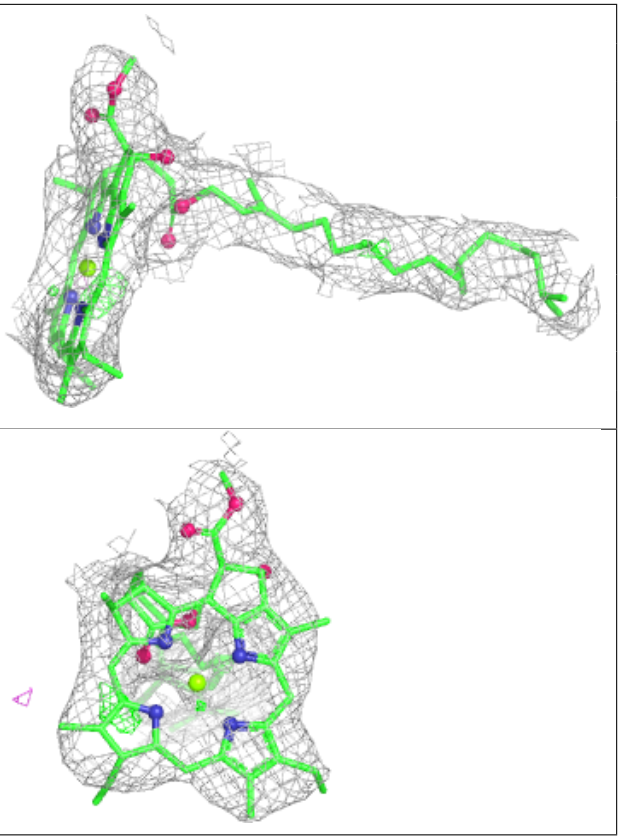






Electron density around CLA A 1783:

$2mF_o$-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.