wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 09:55 am BST

PDB ID	:	6HQB
Title	:	Monomeric cyanobacterial photosystem I
Authors	:	Netzer-El, S.Y.; Nelson, N.; Caspy, I.
Deposited on	:	2018-09-24
Resolution	:	4.00 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 following versions of software and data (see references (1)) were used in the production of this report:

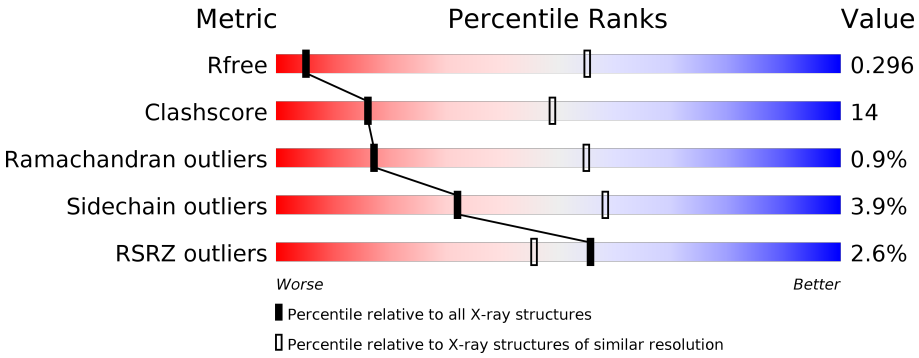
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	% 75% 24% .
2	B	731	76% 23% .
3	C	80	65% 34% .
4	D	141	% 76% 23% .
5	E	69	81% 16% .
6	F	143	75% 25%

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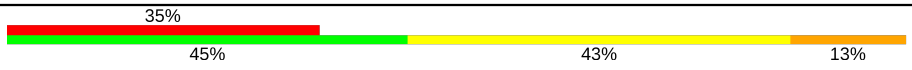
Mol	Chain	Length	Quality of chain
7	I	40	
8	J	40	
9	K	70	
10	L	137	
11	M	31	

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
12	CLA	A	1011	X	-	-	-
12	CLA	A	1012	X	-	-	-
12	CLA	A	1013	X	-	-	-
12	CLA	A	1101	X	-	-	-
12	CLA	A	1102	X	-	-	-
12	CLA	A	1103	X	-	-	-
12	CLA	A	1104	X	-	-	-
12	CLA	A	1105	X	-	-	-
12	CLA	A	1106	X	-	-	-
12	CLA	A	1107	X	-	-	-
12	CLA	A	1108	X	-	-	-
12	CLA	A	1109	X	-	-	-
12	CLA	A	1110	X	-	-	-
12	CLA	A	1111	X	-	-	-
12	CLA	A	1112	X	-	-	-
12	CLA	A	1113	X	-	-	-
12	CLA	A	1114	X	-	-	-
12	CLA	A	1115	X	-	-	-
12	CLA	A	1116	X	-	-	-
12	CLA	A	1117	X	-	-	-
12	CLA	A	1118	X	-	-	-
12	CLA	A	1119	X	-	-	-
12	CLA	A	1120	X	-	-	-
12	CLA	A	1121	X	-	-	-
12	CLA	A	1122	X	-	-	-
12	CLA	A	1123	X	-	-	-
12	CLA	A	1124	X	-	-	-
12	CLA	A	1125	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	1126	X	-	-	-
12	CLA	A	1127	X	-	-	-
12	CLA	A	1128	X	-	-	-
12	CLA	A	1129	X	-	-	-
12	CLA	A	1130	X	-	-	-
12	CLA	A	1131	X	-	-	-
12	CLA	A	1132	X	-	-	-
12	CLA	A	1133	X	-	-	-
12	CLA	A	1134	X	-	-	-
12	CLA	A	1135	X	-	-	-
12	CLA	A	1136	X	-	-	-
12	CLA	A	1137	X	-	-	-
12	CLA	A	1138	X	-	-	-
12	CLA	A	1139	X	-	-	-
12	CLA	A	1140	X	-	-	-
12	CLA	A	1141	X	-	-	-
12	CLA	B	1021	X	-	-	-
12	CLA	B	1022	X	-	-	-
12	CLA	B	1023	X	-	-	-
12	CLA	B	1201	X	-	-	-
12	CLA	B	1202	X	-	-	-
12	CLA	B	1203	X	-	-	-
12	CLA	B	1204	X	-	-	-
12	CLA	B	1205	X	-	-	-
12	CLA	B	1206	X	-	-	-
12	CLA	B	1207	X	-	-	-
12	CLA	B	1208	X	-	-	-
12	CLA	B	1209	X	-	-	-
12	CLA	B	1210	X	-	-	-
12	CLA	B	1211	X	-	-	-
12	CLA	B	1212	X	-	-	-
12	CLA	B	1213	X	-	-	-
12	CLA	B	1214	X	-	-	-
12	CLA	B	1215	X	-	-	-
12	CLA	B	1216	X	-	-	-
12	CLA	B	1217	X	-	-	-
12	CLA	B	1218	X	-	-	-
12	CLA	B	1219	X	-	-	-
12	CLA	B	1220	X	-	-	-
12	CLA	B	1221	X	-	-	-
12	CLA	B	1222	X	-	-	-
12	CLA	B	1223	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	B	1224	X	-	-	-
12	CLA	B	1225	X	-	-	-
12	CLA	B	1226	X	-	-	-
12	CLA	B	1227	X	-	-	-
12	CLA	B	1228	X	-	-	-
12	CLA	B	1229	X	-	-	-
12	CLA	B	1230	X	-	-	-
12	CLA	B	1231	X	-	-	-
12	CLA	B	1232	X	-	-	-
12	CLA	B	1234	X	-	-	-
12	CLA	B	1235	X	-	-	-
12	CLA	B	1236	X	-	-	-
12	CLA	B	1237	X	-	-	-
12	CLA	B	1238	X	-	-	-
12	CLA	B	1239	X	-	-	-
12	CLA	B	1240	X	-	-	-
12	CLA	F	1301	X	-	-	-
12	CLA	F	1302	X	-	-	-
12	CLA	J	1302	X	-	-	-
12	CLA	J	1303	X	-	-	-
12	CLA	K	1401	X	-	-	-
12	CLA	K	1402	X	-	-	-
12	CLA	L	1502	X	-	-	-
15	BCR	A	4003	-	-	-	X
15	BCR	I	4018	-	-	-	X
19	ECH	M	4021	-	-	-	X
20	LMG	B	5005	-	-	-	X
21	SQD	B	5008	-	-	-	X
21	SQD	F	5001	-	-	-	X
25	EQ3	I	4020	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 23566 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			5876	3846	999	1003	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5783	3806	969	992	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1102	697	190	211	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			543	340	96	107			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	143	Total	C	N	O	S	0	0	0
			1113	718	185	205	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	40	Total	C	N	O	S	0	0	0
			311	209	44	55	3			

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	40	Total	C	N	O	S	0	0	0
			319	215	47	54	3			

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	70	Total	C	N	O	S	0	0	0
			510	337	81	87	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	137	Total	C	N	O	S	0	0	0
			1030	674	167	187	2			

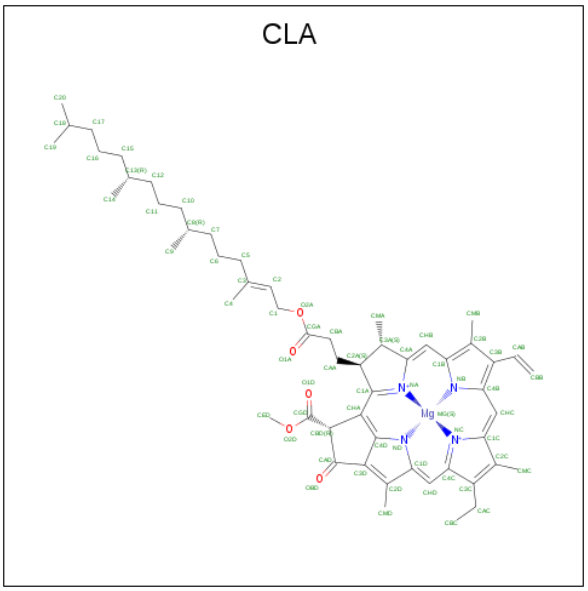
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	158	HIS	-	insertion	UNP P37277

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	31	Total	C	N	O	S	0	0	0
			238	159	36	42	1			

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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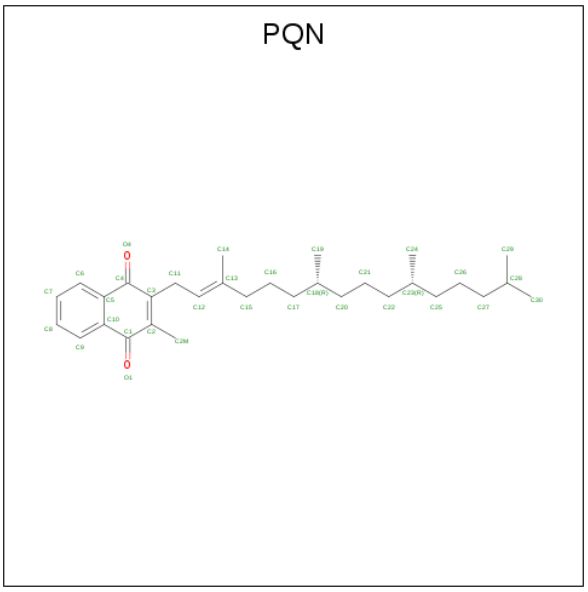
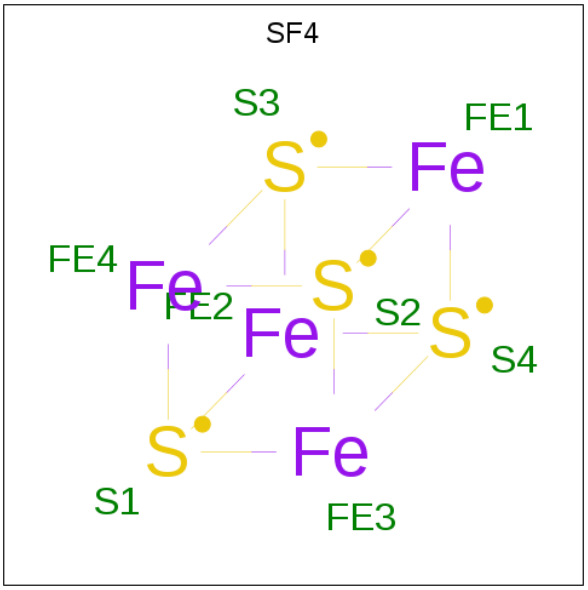
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	F	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	F	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	J	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	J	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
12	K	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	L	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

- Molecule 13 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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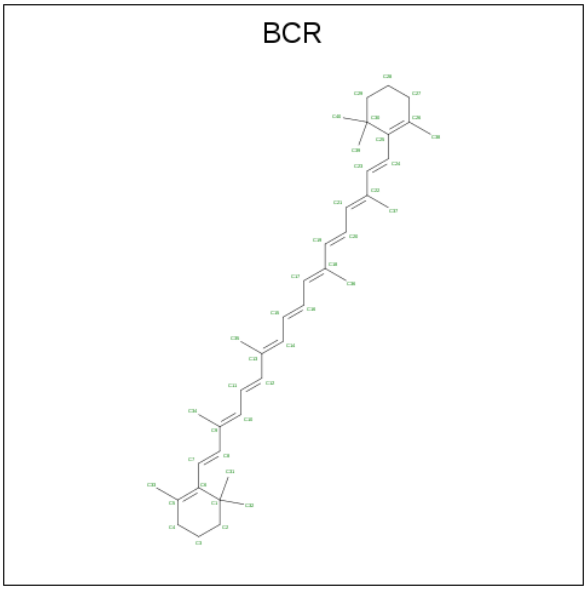
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total Fe S 8 4 4	0	0

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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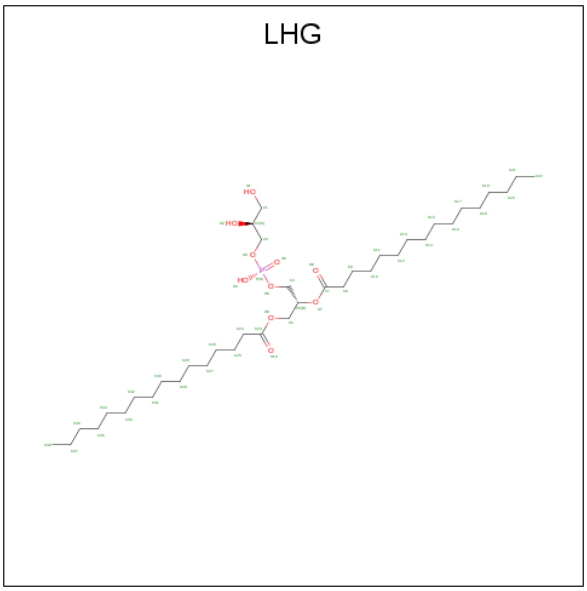
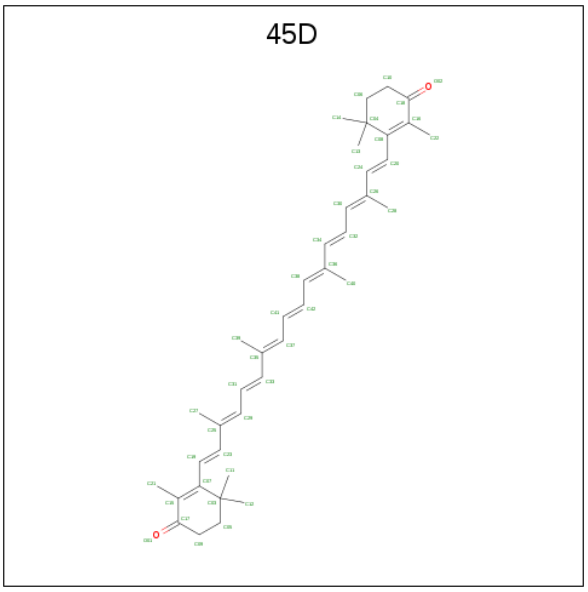
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	K	1	Total C 40 40	0	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 49 38 10 1	0	0
16	B	1	Total C O P 49 38 10 1	0	0
16	B	1	Total C O P 21 10 10 1	0	0

- Molecule 17 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$).

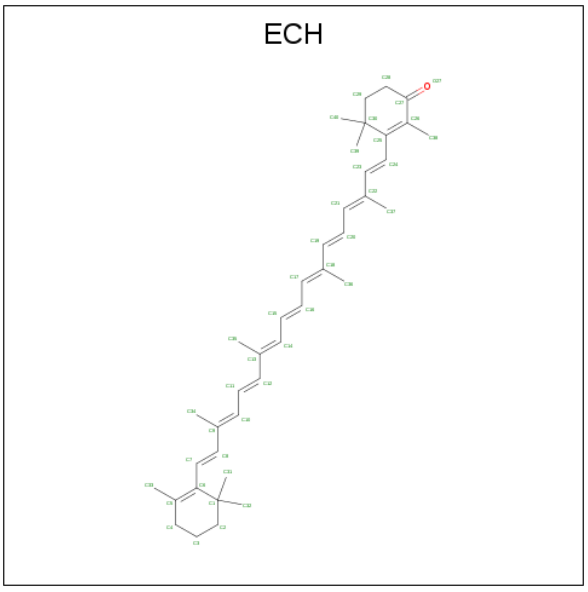


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total C O 42 40 2	0	0

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

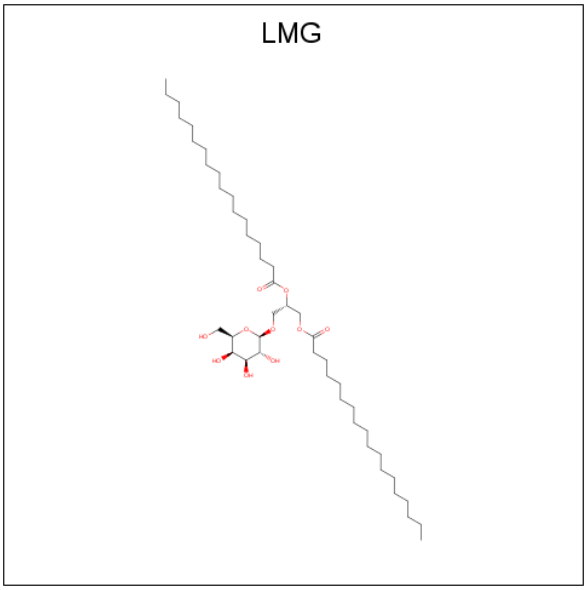
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	B	1	Total Cl 1 1	0	0

- Molecule 19 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$).



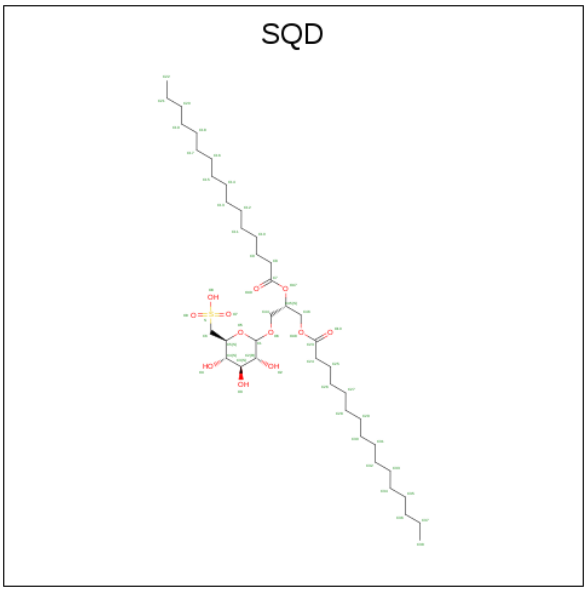
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	C	O	0	0
			41	40	1		
19	M	1	Total	C	O	0	0
			41	40	1		

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			55	45	10		
20	B	1	Total	C	O	0	0
			55	45	10		

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

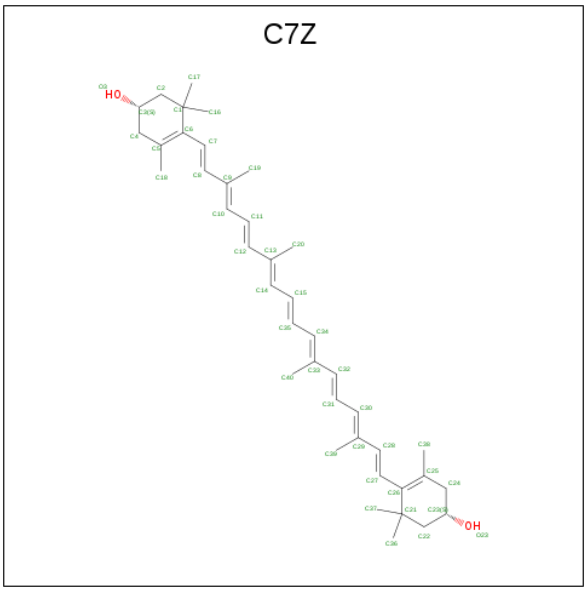


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	B	1	Total	C	O	S	0	0
			54	41	12	1		
21	F	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 22 is CALCIUM ION (three-letter code: CA) (formula: Ca).

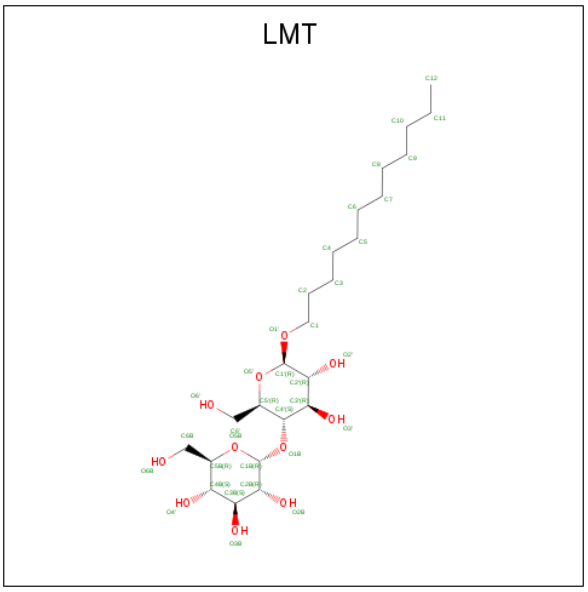
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	Ca	0	0
			1	1		
22	L	1	Total	Ca	0	0
			1	1		

- Molecule 23 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: $C_{40}H_{56}O_2$).



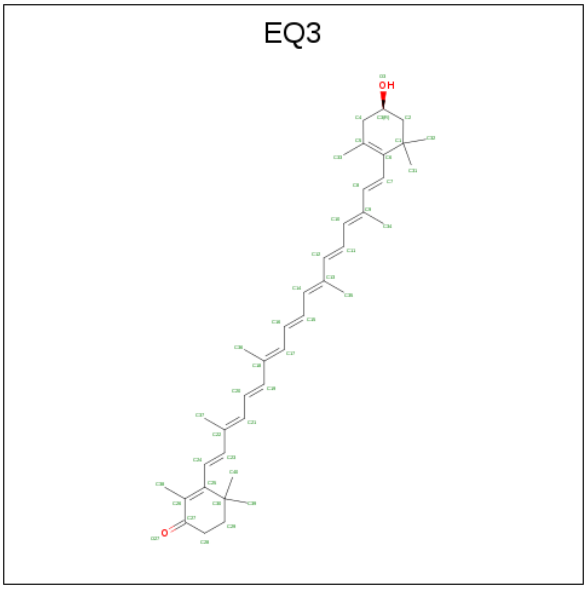
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	F	1	Total C O 42 40 2	0	0
23	J	1	Total C O 42 40 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	F	1	Total C O 35 24 11	0	0

- Molecule 25 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula: $C_{40}H_{54}O_2$).

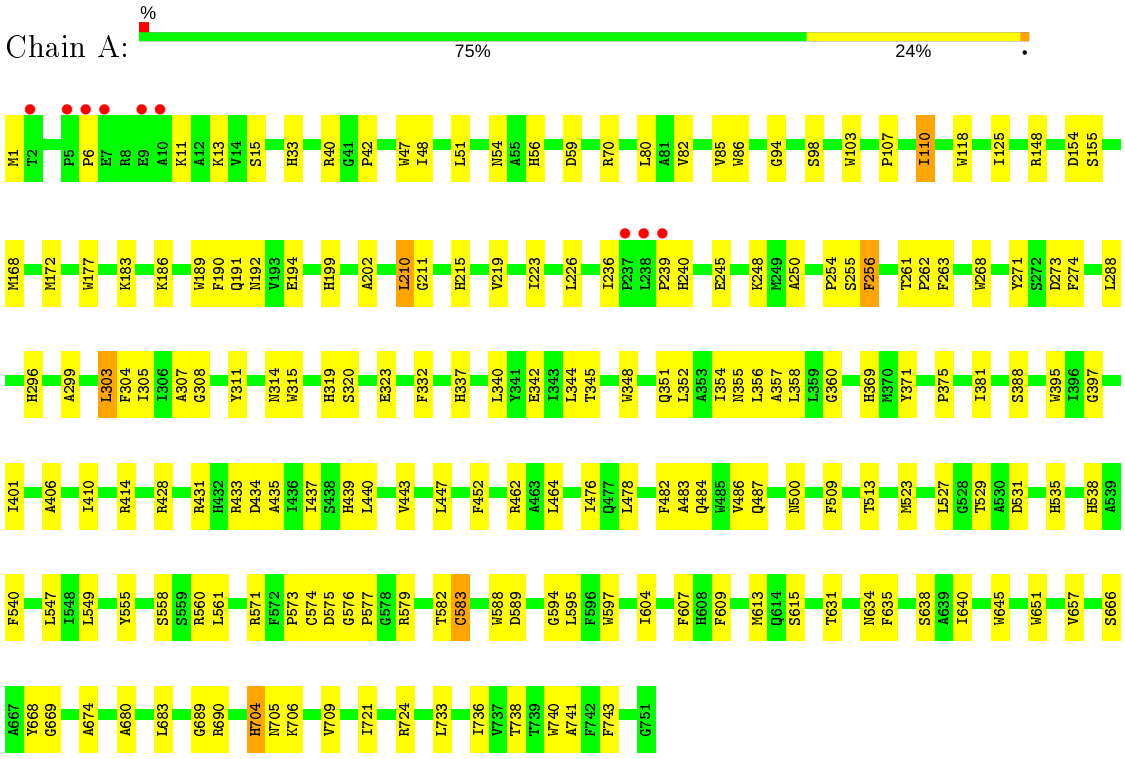


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
25	I	1	42	40	2	0	0

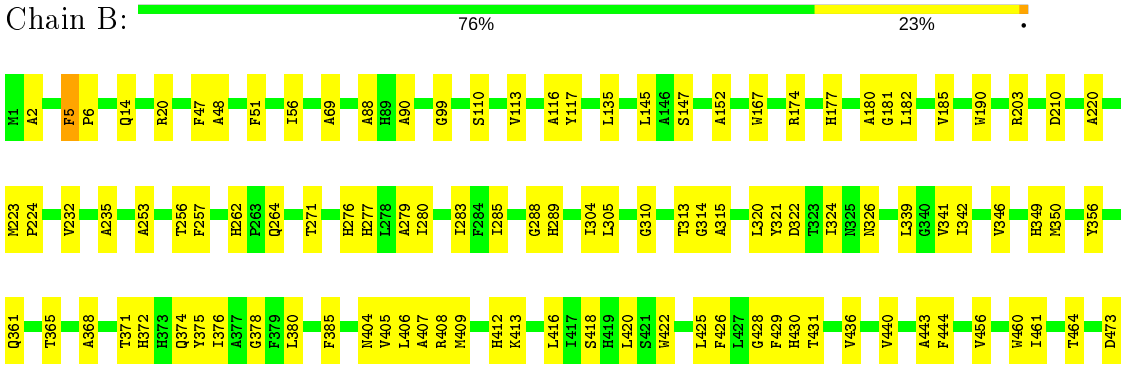
3 Residue-property plots (i)

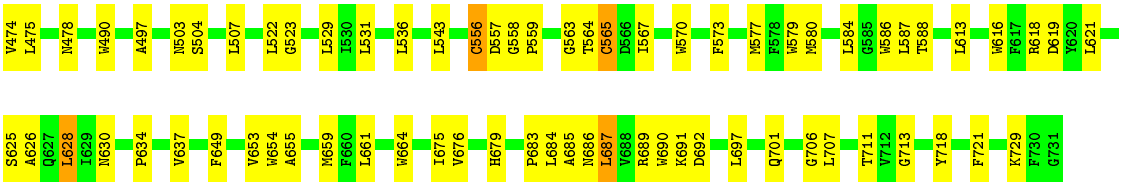
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

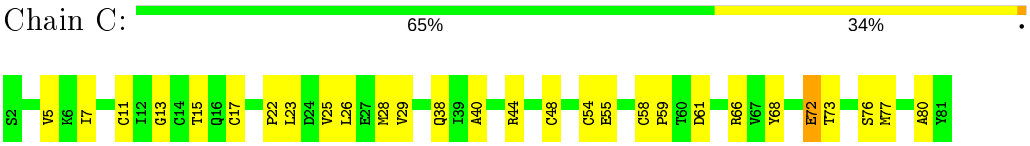


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

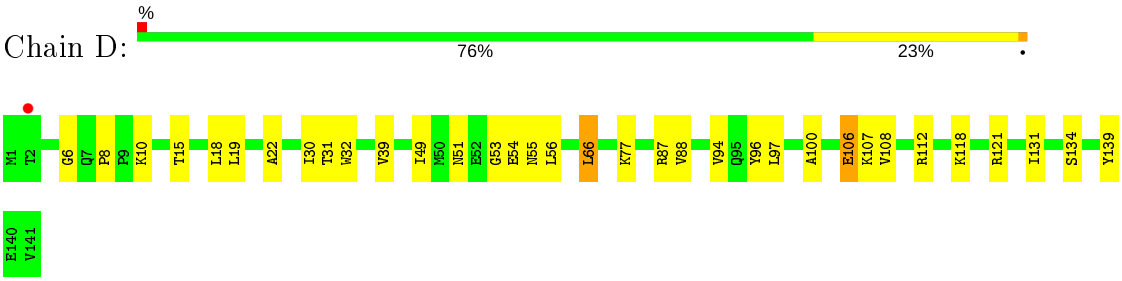




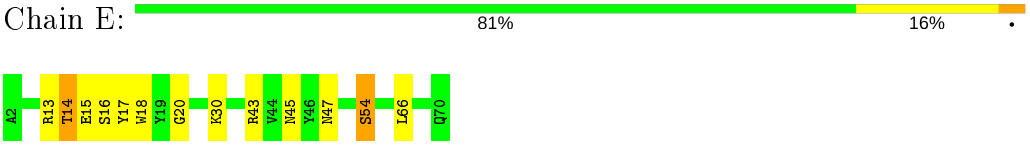
• Molecule 3: Photosystem I iron-sulfur center



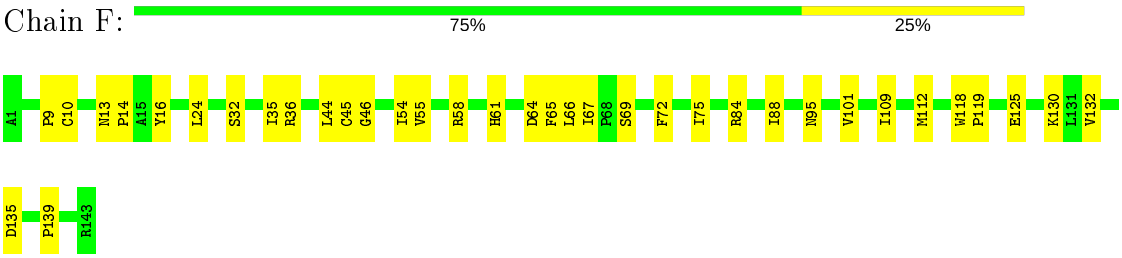
• Molecule 4: Photosystem I reaction center subunit II



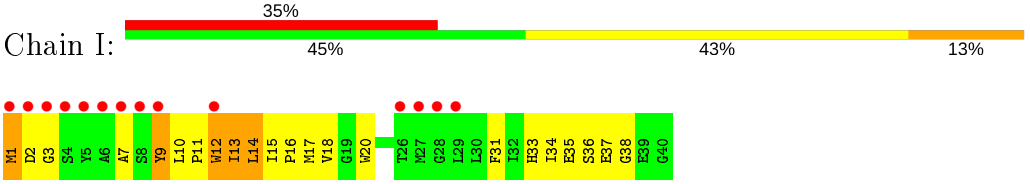
• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III



• Molecule 7: Photosystem I reaction center subunit VIII

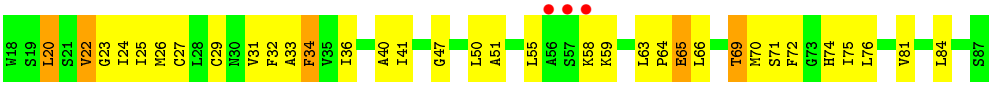


• Molecule 8: Photosystem I reaction center subunit IX

Chain J:

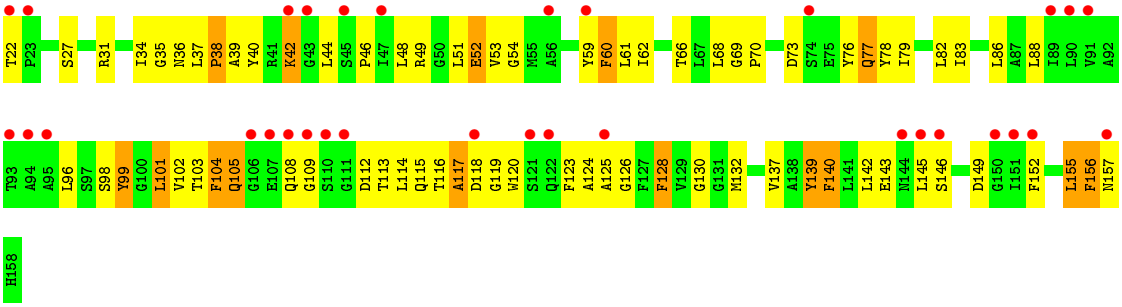
• Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain K:



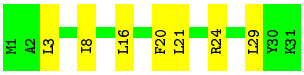
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



• Molecule 11: Photosystem I reaction center subunit XII

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.32Å 178.66Å 181.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 4.00 49.29 – 4.00	Depositor EDS
% Data completeness (in resolution range)	88.7 (49.29-4.00) 88.7 (49.29-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.14_3228: ???)	Depositor
R, R_{free}	0.255 , 0.295 0.256 , 0.296	Depositor DCC
R_{free} test set	584 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 23.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	23566	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, C7Z, CL, SF4, LMT, CLA, PQN, ECH, BCR, LMG, 45D, EQ3, CA, SQD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/6075	0.39	0/8278
2	B	0.25	0/5994	0.40	0/8195
3	C	0.24	0/610	0.43	0/826
4	D	0.25	0/1126	0.44	0/1517
5	E	0.25	0/552	0.41	0/745
6	F	0.25	0/1143	0.40	0/1553
7	I	0.28	0/322	0.50	0/438
8	J	0.26	0/328	0.40	0/443
9	K	0.26	0/520	0.46	0/700
10	L	0.27	0/1057	0.47	0/1434
11	M	0.24	0/241	0.39	0/326
All	All	0.25	0/17968	0.41	0/24455

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5876	0	5739	157	0
2	B	5783	0	5565	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	600	0	589	18	0
4	D	1102	0	1101	17	0
5	E	543	0	525	11	0
6	F	1113	0	1110	23	0
7	I	311	0	304	19	0
8	J	319	0	328	14	0
9	K	510	0	534	27	0
10	L	1030	0	1011	60	0
11	M	238	0	260	7	0
12	A	2326	0	2027	171	0
12	B	2152	0	1801	145	0
12	F	98	0	76	3	0
12	J	98	0	76	2	0
12	K	94	0	71	0	0
12	L	49	0	38	4	0
13	A	33	0	46	2	0
13	B	33	0	46	3	0
14	A	8	0	0	1	0
14	C	16	0	0	1	0
15	A	200	0	265	21	0
15	B	200	0	264	9	0
15	F	40	0	53	9	0
15	I	40	0	52	5	0
15	J	40	0	53	9	0
15	K	40	0	53	6	0
16	A	98	0	148	5	0
16	B	70	0	83	9	0
17	B	42	0	52	5	0
18	B	1	0	0	0	0
19	B	41	0	54	4	0
19	M	41	0	54	5	0
20	B	110	0	172	7	0
21	B	54	0	77	1	0
21	F	54	0	77	3	0
22	B	1	0	0	0	0
22	L	1	0	0	0	0
23	F	42	0	0	1	0
23	J	42	0	0	0	0
24	F	35	0	45	1	0
25	I	42	0	0	1	0
All	All	23566	0	22749	666	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 666 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD11	15:A:4001:BCR:H10C	1.42	1.01
12:B:1207:CLA:HBC3	15:I:4018:BCR:H21C	1.44	0.96
10:L:35:GLY:HA2	10:L:40:TYR:HB3	1.52	0.92
12:B:1220:CLA:HAB	12:B:1227:CLA:HMD2	1.55	0.87
12:A:1125:CLA:HED1	12:A:1133:CLA:HAB	1.58	0.86

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	749/751 (100%)	694 (93%)	52 (7%)	3 (0%)	34 71
2	B	729/731 (100%)	685 (94%)	43 (6%)	1 (0%)	51 84
3	C	78/80 (98%)	68 (87%)	9 (12%)	1 (1%)	12 48
4	D	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	11 46
5	E	67/69 (97%)	59 (88%)	6 (9%)	2 (3%)	4 32
6	F	141/143 (99%)	132 (94%)	7 (5%)	2 (1%)	11 46
7	I	38/40 (95%)	29 (76%)	6 (16%)	3 (8%)	1 14
8	J	38/40 (95%)	36 (95%)	2 (5%)	0	100 100
9	K	68/70 (97%)	61 (90%)	6 (9%)	1 (2%)	10 45
10	L	135/137 (98%)	104 (77%)	25 (18%)	6 (4%)	2 24
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100 100
All	All	2211/2233 (99%)	2022 (92%)	168 (8%)	21 (1%)	17 55

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
10	L	105	GLN
1	A	191	GLN
5	E	14	THR
2	B	556	CYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	602/603 (100%)	590 (98%)	12 (2%)	55 73
2	B	583/583 (100%)	569 (98%)	14 (2%)	49 69
3	C	68/68 (100%)	66 (97%)	2 (3%)	42 65
4	D	116/116 (100%)	110 (95%)	6 (5%)	23 51
5	E	58/58 (100%)	56 (97%)	2 (3%)	37 61
6	F	119/119 (100%)	117 (98%)	2 (2%)	60 78
7	I	32/32 (100%)	27 (84%)	5 (16%)	2 16
8	J	35/35 (100%)	34 (97%)	1 (3%)	42 65
9	K	53/54 (98%)	46 (87%)	7 (13%)	4 21
10	L	102/102 (100%)	83 (81%)	19 (19%)	1 10
11	M	25/25 (100%)	25 (100%)	0	100 100
All	All	1793/1795 (100%)	1723 (96%)	70 (4%)	32 58

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	96	TYR
7	I	9	TYR
10	L	140	PHE
4	D	107	LYS
5	E	66	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	HIS
2	B	299	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 130 ligands modelled in this entry, 3 are monoatomic - leaving 127 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	$\#\|Z\| > 2$
12	CLA	A	1112	-	43,57,73	1.13	6 (13%)	46,93,113	1.76	8 (17%)
12	CLA	A	1118	-	44,58,73	1.12	5 (11%)	49,95,113	1.65	7 (14%)
12	CLA	A	1139	-	49,63,73	1.09	5 (10%)	55,101,113	1.63	6 (10%)
12	CLA	A	1106	-	59,73,73	0.98	6 (10%)	67,113,113	1.57	9 (13%)
12	CLA	A	1130	-	43,57,73	1.13	6 (13%)	46,93,113	1.70	7 (15%)
12	CLA	A	1103	-	43,57,73	1.12	6 (13%)	46,93,113	1.73	7 (15%)
12	CLA	B	1221	-	43,57,73	1.13	6 (13%)	46,93,113	1.76	9 (19%)
15	BCR	B	4010	-	41,41,41	1.91	4 (9%)	56,56,56	4.49	18 (32%)
12	CLA	A	1116	-	43,57,73	1.13	5 (11%)	46,93,113	1.76	9 (19%)
12	CLA	B	1239	-	43,57,73	1.16	6 (13%)	46,93,113	1.64	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	A	4003	-	41,41,41	1.85	4 (9%)	56,56,56	4.29	16 (28%)
12	CLA	J	1303	10	43,57,73	1.12	6 (13%)	46,93,113	1.73	7 (15%)
14	SF4	A	3001	-	0,12,12	0.00	-	-		
12	CLA	A	1105	-	59,73,73	1.01	6 (10%)	67,113,113	1.52	8 (11%)
12	CLA	A	1123	-	54,68,73	1.00	7 (12%)	61,107,113	1.64	11 (18%)
12	CLA	A	1115	-	50,64,73	1.04	6 (12%)	56,102,113	1.65	9 (16%)
15	BCR	B	4005	-	41,41,41	1.85	4 (9%)	56,56,56	4.43	14 (25%)
12	CLA	A	1129	-	43,57,73	1.13	6 (13%)	46,93,113	1.71	8 (17%)
12	CLA	F	1301	-	43,57,73	1.13	5 (11%)	46,93,113	1.69	7 (15%)
12	CLA	L	1502	-	43,57,73	1.14	7 (16%)	46,93,113	1.82	7 (15%)
12	CLA	A	1101	-	43,57,73	1.16	6 (13%)	46,93,113	1.86	10 (21%)
12	CLA	B	1223	-	43,57,73	1.24	7 (16%)	46,93,113	1.73	8 (17%)
12	CLA	A	1133	-	43,57,73	1.15	6 (13%)	46,93,113	1.65	7 (15%)
12	CLA	B	1205	-	43,57,73	1.15	6 (13%)	46,93,113	1.80	8 (17%)
12	CLA	A	1012	-	43,57,73	1.15	6 (13%)	46,93,113	1.75	8 (17%)
12	CLA	A	1136	-	43,57,73	1.15	6 (13%)	46,93,113	1.69	6 (13%)
25	EQ3	I	4020	-	43,43,43	4.21	25 (58%)	56,60,60	2.37	20 (35%)
12	CLA	B	1229	-	49,63,73	1.10	6 (12%)	55,101,113	1.61	9 (16%)
16	LHG	B	5004	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
12	CLA	A	1135	-	43,57,73	1.15	6 (13%)	46,93,113	1.79	8 (17%)
23	C7Z	J	4015	-	43,43,43	5.34	18 (41%)	58,60,60	5.20	31 (53%)
15	BCR	B	4018	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	17 (30%)
12	CLA	A	1127	-	43,57,73	1.13	6 (13%)	46,93,113	1.71	8 (17%)
12	CLA	A	1141	-	36,53,73	1.22	6 (16%)	39,89,113	1.55	5 (12%)
12	CLA	B	1201	-	43,57,73	1.14	6 (13%)	46,93,113	1.73	8 (17%)
21	SQD	F	5001	-	53,54,54	0.79	0	62,65,65	0.92	2 (3%)
15	BCR	A	4008	-	41,41,41	1.84	4 (9%)	56,56,56	4.38	17 (30%)
12	CLA	K	1401	-	36,53,73	1.25	6 (16%)	39,89,113	1.60	5 (12%)
12	CLA	B	1227	-	43,57,73	1.16	6 (13%)	46,93,113	1.76	8 (17%)
12	CLA	B	1240	-	43,57,73	1.17	7 (16%)	46,93,113	1.76	7 (15%)
14	SF4	C	3003	-	0,12,12	0.00	-	-		
12	CLA	A	1120	-	43,57,73	1.13	7 (16%)	46,93,113	1.76	8 (17%)
23	C7Z	F	4016	-	43,43,43	5.36	18 (41%)	58,60,60	5.24	32 (55%)
12	CLA	A	1125	-	43,57,73	1.14	5 (11%)	46,93,113	1.81	9 (19%)
12	CLA	A	1117	-	43,57,73	1.13	6 (13%)	46,93,113	1.72	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	PQN	A	2001	-	34,34,34	0.43	0	42,45,45	1.09	3 (7%)
12	CLA	A	1110	-	43,57,73	1.15	6 (13%)	46,93,113	1.67	7 (15%)
12	CLA	B	1211	-	43,57,73	1.14	5 (11%)	46,93,113	1.76	8 (17%)
12	CLA	B	1214	-	54,68,73	1.04	6 (11%)	61,107,113	1.47	8 (13%)
12	CLA	A	1131	-	43,57,73	1.14	6 (13%)	46,93,113	1.61	6 (13%)
12	CLA	K	1402	-	43,57,73	1.14	6 (13%)	46,93,113	1.77	11 (23%)
15	BCR	K	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.39	15 (26%)
15	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.47	15 (26%)
16	LHG	A	5001	-	48,48,48	0.39	0	51,54,54	1.04	4 (7%)
15	BCR	A	4012	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	14 (25%)
19	ECH	B	4006	-	42,42,42	0.85	1 (2%)	55,58,58	2.46	12 (21%)
13	PQN	B	2002	-	34,34,34	0.40	0	42,45,45	1.09	3 (7%)
12	CLA	B	1219	-	43,57,73	1.16	6 (13%)	46,93,113	1.67	7 (15%)
12	CLA	B	1218	-	43,57,73	1.13	6 (13%)	46,93,113	1.75	8 (17%)
12	CLA	A	1107	1	44,58,73	1.46	7 (15%)	49,95,113	2.06	8 (16%)
15	BCR	A	4007	-	41,41,41	1.84	4 (9%)	56,56,56	4.39	16 (28%)
12	CLA	B	1224	-	49,63,73	1.09	5 (10%)	55,101,113	1.60	8 (14%)
12	CLA	F	1302	10	43,57,73	1.14	5 (11%)	46,93,113	1.75	7 (15%)
21	SQD	B	5008	-	53,54,54	0.78	0	62,65,65	0.91	2 (3%)
12	CLA	A	1122	-	43,57,73	1.14	7 (16%)	46,93,113	1.70	7 (15%)
12	CLA	B	1208	-	43,57,73	1.17	6 (13%)	46,93,113	1.62	6 (13%)
12	CLA	B	1204	-	43,57,73	1.16	6 (13%)	46,93,113	1.65	7 (15%)
12	CLA	A	1011	-	49,63,73	1.07	5 (10%)	55,101,113	1.72	11 (20%)
15	BCR	B	4017	-	41,41,41	1.85	4 (9%)	56,56,56	4.45	15 (26%)
12	CLA	B	1216	-	43,57,73	1.15	6 (13%)	46,93,113	1.69	6 (13%)
12	CLA	A	1124	-	43,57,73	1.14	6 (13%)	46,93,113	1.71	7 (15%)
12	CLA	A	1113	-	43,57,73	1.16	6 (13%)	46,93,113	1.66	6 (13%)
15	BCR	F	4014	-	41,41,41	1.86	4 (9%)	56,56,56	4.30	14 (25%)
12	CLA	B	1213	-	43,57,73	1.13	7 (16%)	46,93,113	1.85	9 (19%)
14	SF4	C	3002	-	0,12,12	0.00	-	-		
12	CLA	A	1134	1	43,57,73	1.15	6 (13%)	46,93,113	1.70	7 (15%)
16	LHG	B	5006	2	20,20,48	0.59	0	23,26,54	1.48	2 (8%)
12	CLA	B	1237	-	43,57,73	1.13	6 (13%)	46,93,113	1.72	7 (15%)
12	CLA	B	1215	-	43,57,73	1.15	7 (16%)	46,93,113	1.72	7 (15%)
12	CLA	B	1238	-	43,57,73	1.18	6 (13%)	46,93,113	1.67	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	B	1232	-	43,57,73	1.17	6 (13%)	46,93,113	1.69	9 (19%)
12	CLA	A	1128	-	59,73,73	0.95	5 (8%)	67,113,113	1.59	11 (16%)
16	LHG	A	5003	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
12	CLA	A	1119	-	40,54,73	1.23	6 (15%)	44,90,113	1.40	5 (11%)
12	CLA	B	1217	-	43,57,73	1.16	6 (13%)	46,93,113	1.74	7 (15%)
12	CLA	B	1212	-	43,57,73	1.15	6 (13%)	46,93,113	1.69	6 (13%)
12	CLA	B	1210	-	43,57,73	1.13	6 (13%)	46,93,113	1.76	8 (17%)
12	CLA	A	1104	-	43,57,73	1.14	6 (13%)	46,93,113	1.66	6 (13%)
19	ECH	M	4021	-	42,42,42	0.85	1 (2%)	55,58,58	2.62	14 (25%)
12	CLA	B	1202	-	59,73,73	0.96	5 (8%)	67,113,113	1.56	8 (11%)
12	CLA	B	1226	-	43,57,73	1.12	5 (11%)	46,93,113	1.80	9 (19%)
12	CLA	A	1102	12	59,73,73	0.97	6 (10%)	67,113,113	1.55	10 (14%)
15	BCR	I	4018	-	41,41,41	1.85	4 (9%)	56,56,56	4.38	20 (35%)
12	CLA	A	1132	10	49,63,73	1.11	6 (12%)	55,101,113	1.59	7 (12%)
12	CLA	B	1220	-	43,57,73	1.15	6 (13%)	46,93,113	1.82	9 (19%)
24	LMT	F	6001	-	36,36,36	1.14	5 (13%)	47,47,47	1.03	2 (4%)
12	CLA	B	1222	-	44,58,73	1.13	5 (11%)	49,95,113	1.76	7 (14%)
12	CLA	B	1023	-	43,57,73	1.11	6 (13%)	46,93,113	1.71	7 (15%)
15	BCR	A	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.36	18 (32%)
12	CLA	B	1230	-	43,57,73	1.16	6 (13%)	46,93,113	1.74	8 (17%)
12	CLA	A	1108	-	43,57,73	1.13	6 (13%)	46,93,113	1.69	7 (15%)
12	CLA	B	1225	-	43,57,73	1.15	5 (11%)	46,93,113	1.58	6 (13%)
12	CLA	B	1206	-	43,57,73	1.13	6 (13%)	46,93,113	1.74	8 (17%)
12	CLA	A	1137	-	43,57,73	1.16	6 (13%)	46,93,113	1.68	6 (13%)
12	CLA	B	1207	-	43,57,73	1.18	6 (13%)	46,93,113	1.74	8 (17%)
12	CLA	A	1013	-	59,73,73	0.98	5 (8%)	67,113,113	1.51	10 (14%)
12	CLA	B	1235	-	59,73,73	1.00	6 (10%)	67,113,113	1.57	8 (11%)
12	CLA	J	1302	8	43,57,73	1.15	6 (13%)	46,93,113	1.70	6 (13%)
20	LMG	B	5002	-	55,55,55	1.13	6 (10%)	63,63,63	1.02	2 (3%)
12	CLA	A	1126	-	54,68,73	1.03	6 (11%)	61,107,113	1.51	9 (14%)
12	CLA	A	1140	-	59,73,73	1.00	6 (10%)	67,113,113	1.47	7 (10%)
12	CLA	A	1111	-	43,57,73	1.14	6 (13%)	46,93,113	1.63	7 (15%)
12	CLA	A	1114	-	43,57,73	1.16	6 (13%)	46,93,113	1.67	6 (13%)
12	CLA	A	1138	-	59,73,73	0.97	5 (8%)	67,113,113	1.56	8 (11%)
12	CLA	A	1121	-	43,57,73	1.14	6 (13%)	46,93,113	1.77	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	B	1231	-	43,57,73	1.16	6 (13%)	46,93,113	1.67	8 (17%)
12	CLA	B	1021	-	59,73,73	0.97	5 (8%)	67,113,113	1.52	7 (10%)
12	CLA	B	1234	-	54,68,73	1.03	5 (9%)	61,107,113	1.62	8 (13%)
12	CLA	B	1209	-	43,57,73	1.17	7 (16%)	46,93,113	1.73	7 (15%)
17	45D	B	4011	-	43,43,43	3.57	16 (37%)	54,60,60	2.15	17 (31%)
12	CLA	B	1236	-	43,57,73	1.18	6 (13%)	46,93,113	1.69	6 (13%)
12	CLA	B	1022	-	54,68,73	1.05	6 (11%)	61,107,113	1.57	8 (13%)
20	LMG	B	5005	-	55,55,55	1.14	6 (10%)	63,63,63	1.06	3 (4%)
12	CLA	B	1228	-	43,57,73	1.14	6 (13%)	46,93,113	1.70	8 (17%)
12	CLA	A	1109	12	59,73,73	0.98	6 (10%)	67,113,113	1.49	9 (13%)
15	BCR	J	4013	-	41,41,41	1.87	4 (9%)	56,56,56	4.35	15 (26%)
12	CLA	B	1203	-	43,57,73	1.13	6 (13%)	46,93,113	1.56	7 (15%)

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
12	CLA	A	1112	-	3/3/16/25	12/18/116/135	-
12	CLA	A	1118	-	3/3/17/25	9/19/117/135	-
12	CLA	A	1139	-	3/3/18/25	9/25/123/135	-
12	CLA	A	1106	-	3/3/20/25	19/37/135/135	-
12	CLA	A	1130	-	3/3/16/25	9/18/116/135	-
12	CLA	A	1103	-	3/3/16/25	13/18/116/135	-
12	CLA	B	1221	-	3/3/16/25	8/18/116/135	-
15	BCR	B	4010	-	-	11/29/63/63	0/2/2/2
12	CLA	A	1116	-	3/3/16/25	10/18/116/135	-
12	CLA	B	1239	-	3/3/16/25	11/18/116/135	-
15	BCR	A	4003	-	-	15/29/63/63	0/2/2/2
12	CLA	J	1303	10	3/3/16/25	11/18/116/135	-
14	SF4	A	3001	-	-	-	0/6/5/5
12	CLA	A	1105	-	3/3/20/25	11/37/135/135	-
12	CLA	A	1123	-	3/3/19/25	14/31/129/135	-
12	CLA	A	1115	-	3/3/18/25	7/27/125/135	-
15	BCR	B	4005	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	1129	-	3/3/16/25	7/18/116/135	-
12	CLA	F	1301	-	3/3/16/25	6/18/116/135	-
12	CLA	L	1502	-	3/3/16/25	11/18/116/135	-
12	CLA	A	1101	-	3/3/16/25	8/18/116/135	-
12	CLA	B	1223	-	3/3/16/25	11/18/116/135	-
12	CLA	A	1133	-	3/3/16/25	11/18/116/135	-
12	CLA	B	1205	-	3/3/16/25	11/18/116/135	-
12	CLA	A	1012	-	3/3/16/25	11/18/116/135	-
12	CLA	B	1023	-	3/3/16/25	9/18/116/135	-
25	EQ3	I	4020	-	-	15/29/68/68	0/2/2/2
12	CLA	B	1229	-	3/3/18/25	14/25/123/135	-
16	LHG	B	5004	-	-	23/53/53/53	-
12	CLA	A	1135	-	3/3/16/25	11/18/116/135	-
23	C7Z	J	4015	-	-	14/29/67/67	0/2/2/2
15	BCR	B	4018	-	-	9/29/63/63	0/2/2/2
12	CLA	A	1127	-	3/3/16/25	9/18/116/135	-
12	CLA	A	1141	-	3/3/16/25	9/11/111/135	-
12	CLA	B	1201	-	3/3/16/25	9/18/116/135	-
21	SQD	F	5001	-	-	17/49/69/69	0/1/1/1
15	BCR	A	4008	-	-	13/29/63/63	0/2/2/2
12	CLA	K	1401	-	3/3/16/25	6/11/111/135	-
12	CLA	B	1227	-	3/3/16/25	11/18/116/135	-
12	CLA	B	1240	-	3/3/16/25	12/18/116/135	-
14	SF4	C	3003	-	-	-	0/6/5/5
12	CLA	A	1120	-	3/3/16/25	11/18/116/135	-
23	C7Z	F	4016	-	-	17/29/67/67	0/2/2/2
12	CLA	A	1125	-	3/3/16/25	11/18/116/135	-
12	CLA	A	1117	-	3/3/16/25	8/18/116/135	-
12	CLA	A	1136	-	3/3/16/25	11/18/116/135	-
13	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
12	CLA	A	1110	-	3/3/16/25	9/18/116/135	-
12	CLA	B	1211	-	3/3/16/25	9/18/116/135	-
12	CLA	B	1214	-	3/3/19/25	22/31/129/135	-
12	CLA	A	1131	-	3/3/16/25	7/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	K	1402	-	3/3/16/25	12/18/116/135	-
15	BCR	K	4001	-	-	11/29/63/63	0/2/2/2
15	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
16	LHG	A	5001	-	-	35/53/53/53	-
15	BCR	A	4012	-	-	14/29/63/63	0/2/2/2
19	ECH	B	4006	-	-	8/29/66/66	0/2/2/2
13	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
12	CLA	B	1219	-	3/3/16/25	9/18/116/135	-
12	CLA	B	1218	-	3/3/16/25	11/18/116/135	-
12	CLA	A	1107	1	3/3/17/25	7/19/117/135	-
15	BCR	A	4007	-	-	11/29/63/63	0/2/2/2
12	CLA	B	1224	-	3/3/18/25	13/25/123/135	-
12	CLA	F	1302	10	3/3/16/25	11/18/116/135	-
21	SQD	B	5008	-	-	10/49/69/69	0/1/1/1
12	CLA	A	1122	-	3/3/16/25	8/18/116/135	-
12	CLA	B	1208	-	3/3/16/25	8/18/116/135	-
12	CLA	B	1204	-	3/3/16/25	7/18/116/135	-
12	CLA	A	1011	-	3/3/18/25	11/25/123/135	-
15	BCR	B	4017	-	-	8/29/63/63	0/2/2/2
12	CLA	B	1216	-	3/3/16/25	12/18/116/135	-
12	CLA	A	1124	-	3/3/16/25	8/18/116/135	-
12	CLA	A	1113	-	3/3/16/25	14/18/116/135	-
15	BCR	F	4014	-	-	12/29/63/63	0/2/2/2
12	CLA	B	1213	-	3/3/16/25	8/18/116/135	-
14	SF4	C	3002	-	-	-	0/6/5/5
12	CLA	A	1134	1	3/3/16/25	12/18/116/135	-
16	LHG	B	5006	2	-	11/23/23/53	-
12	CLA	B	1237	-	3/3/16/25	9/18/116/135	-
12	CLA	B	1215	-	3/3/16/25	8/18/116/135	-
12	CLA	B	1238	-	3/3/16/25	9/18/116/135	-
12	CLA	B	1232	-	3/3/16/25	8/18/116/135	-
12	CLA	A	1128	-	3/3/20/25	19/37/135/135	-
16	LHG	A	5003	-	-	30/53/53/53	-
12	CLA	A	1119	-	3/3/16/25	7/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	1217	-	3/3/16/25	7/18/116/135	-
12	CLA	B	1212	-	3/3/16/25	9/18/116/135	-
12	CLA	B	1210	-	3/3/16/25	13/18/116/135	-
12	CLA	A	1104	-	3/3/16/25	9/18/116/135	-
19	ECH	M	4021	-	-	12/29/66/66	0/2/2/2
12	CLA	B	1202	-	3/3/20/25	16/37/135/135	-
12	CLA	B	1226	-	3/3/16/25	9/18/116/135	-
12	CLA	A	1102	12	3/3/20/25	14/37/135/135	-
15	BCR	I	4018	-	-	13/29/63/63	0/2/2/2
12	CLA	A	1132	10	3/3/18/25	14/25/123/135	-
12	CLA	B	1220	-	3/3/16/25	10/18/116/135	-
24	LMT	F	6001	-	-	8/21/61/61	0/2/2/2
12	CLA	B	1222	-	3/3/17/25	7/19/117/135	-
15	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
12	CLA	B	1230	-	3/3/16/25	10/18/116/135	-
12	CLA	A	1108	-	3/3/16/25	11/18/116/135	-
12	CLA	B	1225	-	3/3/16/25	9/18/116/135	-
12	CLA	B	1206	-	3/3/16/25	9/18/116/135	-
12	CLA	A	1137	-	3/3/16/25	8/18/116/135	-
12	CLA	B	1207	-	3/3/16/25	13/18/116/135	-
12	CLA	A	1013	-	3/3/20/25	15/37/135/135	-
12	CLA	B	1235	-	3/3/20/25	20/37/135/135	-
12	CLA	J	1302	8	3/3/16/25	9/18/116/135	-
20	LMG	B	5002	-	-	10/50/70/70	0/1/1/1
12	CLA	A	1126	-	3/3/19/25	11/31/129/135	-
12	CLA	A	1140	-	3/3/20/25	18/37/135/135	-
12	CLA	A	1111	-	3/3/16/25	13/18/116/135	-
12	CLA	A	1114	-	3/3/16/25	7/18/116/135	-
12	CLA	A	1138	-	3/3/20/25	13/37/135/135	-
12	CLA	A	1121	-	3/3/16/25	11/18/116/135	-
12	CLA	B	1231	-	3/3/16/25	6/18/116/135	-
12	CLA	B	1021	-	3/3/20/25	27/37/135/135	-
12	CLA	B	1234	-	3/3/19/25	16/31/129/135	-
12	CLA	B	1209	-	3/3/16/25	10/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	45D	B	4011	-	-	11/29/69/69	0/2/2/2
12	CLA	B	1236	-	3/3/16/25	7/18/116/135	-
12	CLA	B	1022	-	3/3/19/25	11/31/129/135	-
20	LMG	B	5005	-	-	17/50/70/70	0/1/1/1
12	CLA	B	1228	-	3/3/16/25	10/18/116/135	-
12	CLA	A	1109	12	3/3/20/25	18/37/135/135	-
15	BCR	J	4013	-	-	14/29/63/63	0/2/2/2
12	CLA	B	1203	-	3/3/16/25	8/18/116/135	-

The worst 5 of 702 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	4016	C7Z	C30-C29	14.43	1.54	1.35
23	F	4016	C7Z	C14-C13	14.40	1.54	1.35
23	F	4016	C7Z	C34-C33	14.37	1.54	1.35
23	J	4015	C7Z	C30-C29	14.32	1.54	1.35
23	J	4015	C7Z	C34-C33	14.29	1.54	1.35

The worst 5 of 1089 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	4010	BCR	C10-C11-C12	18.17	179.93	123.22
15	B	4017	BCR	C10-C11-C12	17.87	178.98	123.22
15	K	4001	BCR	C10-C11-C12	17.67	178.35	123.22
15	B	4004	BCR	C10-C11-C12	17.57	178.06	123.22
15	B	4018	BCR	C10-C11-C12	17.57	178.04	123.22

5 of 279 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	1112	CLA	NC
12	A	1112	CLA	ND
12	A	1112	CLA	NA
12	A	1118	CLA	NC
12	A	1118	CLA	ND

5 of 1424 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	1112	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	1112	CLA	CHA-CBD-CGD-O1D
12	A	1112	CLA	CHA-CBD-CGD-O2D
12	A	1118	CLA	CBD-CGD-O2D-CED
12	A	1106	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

116 monomers are involved in 375 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1112	CLA	5	0
12	A	1118	CLA	2	0
12	A	1139	CLA	5	0
12	A	1106	CLA	8	0
12	A	1130	CLA	3	0
12	A	1103	CLA	5	0
12	B	1221	CLA	5	0
15	B	4010	BCR	3	0
12	A	1116	CLA	6	0
12	B	1239	CLA	2	0
15	A	4003	BCR	1	0
14	A	3001	SF4	1	0
12	A	1105	CLA	4	0
12	A	1123	CLA	5	0
12	A	1115	CLA	6	0
15	B	4005	BCR	1	0
12	A	1129	CLA	3	0
12	F	1301	CLA	3	0
12	L	1502	CLA	4	0
12	A	1101	CLA	3	0
12	B	1223	CLA	3	0
12	A	1133	CLA	3	0
12	B	1205	CLA	5	0
12	A	1012	CLA	8	0
25	I	4020	EQ3	1	0
12	B	1229	CLA	5	0
16	B	5004	LHG	9	0
12	A	1135	CLA	4	0
15	B	4018	BCR	2	0
12	A	1127	CLA	1	0
12	A	1141	CLA	3	0
12	B	1201	CLA	1	0
21	F	5001	SQD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	4008	BCR	5	0
12	B	1227	CLA	3	0
12	B	1240	CLA	1	0
23	F	4016	C7Z	1	0
12	A	1125	CLA	4	0
12	A	1117	CLA	4	0
13	A	2001	PQN	2	0
12	A	1110	CLA	1	0
12	B	1211	CLA	4	0
12	B	1214	CLA	5	0
12	A	1131	CLA	1	0
15	K	4001	BCR	6	0
15	B	4004	BCR	3	0
16	A	5001	LHG	2	0
15	A	4012	BCR	8	0
19	B	4006	ECH	4	0
13	B	2002	PQN	3	0
12	B	1219	CLA	1	0
12	B	1218	CLA	2	0
12	A	1107	CLA	9	0
15	A	4007	BCR	2	0
12	B	1224	CLA	9	0
21	B	5008	SQD	1	0
12	A	1122	CLA	4	0
12	B	1208	CLA	4	0
12	B	1204	CLA	5	0
12	A	1011	CLA	8	0
15	B	4017	BCR	1	0
12	B	1216	CLA	2	0
12	A	1124	CLA	2	0
15	F	4014	BCR	9	0
12	B	1213	CLA	2	0
14	C	3002	SF4	1	0
12	A	1134	CLA	4	0
12	B	1237	CLA	3	0
12	B	1215	CLA	2	0
12	B	1238	CLA	5	0
12	B	1232	CLA	3	0
12	A	1128	CLA	8	0
16	A	5003	LHG	3	0
12	A	1119	CLA	6	0
12	B	1212	CLA	1	0

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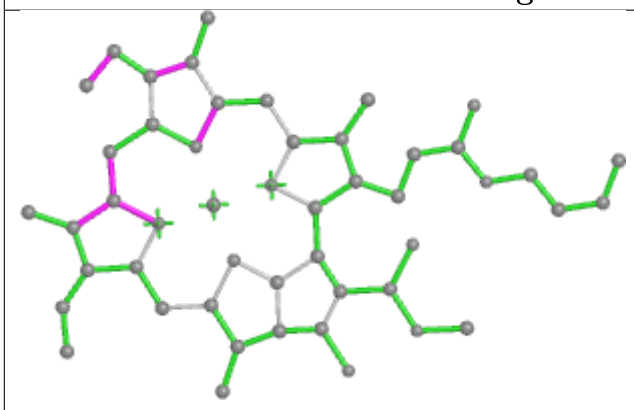
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1210	CLA	7	0
12	A	1104	CLA	1	0
19	M	4021	ECH	5	0
12	B	1202	CLA	5	0
12	B	1226	CLA	3	0
12	A	1102	CLA	8	0
15	I	4018	BCR	5	0
12	A	1132	CLA	7	0
12	B	1220	CLA	4	0
24	F	6001	LMT	1	0
12	B	1222	CLA	10	0
12	B	1023	CLA	5	0
15	A	4001	BCR	5	0
12	B	1230	CLA	4	0
12	A	1108	CLA	2	0
12	B	1225	CLA	4	0
12	B	1206	CLA	2	0
12	A	1137	CLA	1	0
12	B	1207	CLA	5	0
12	A	1013	CLA	8	0
12	B	1235	CLA	7	0
12	J	1302	CLA	2	0
20	B	5002	LMG	4	0
12	A	1126	CLA	13	0
12	A	1140	CLA	4	0
12	A	1111	CLA	4	0
12	A	1114	CLA	3	0
12	A	1138	CLA	9	0
12	A	1121	CLA	2	0
12	B	1231	CLA	4	0
12	B	1021	CLA	15	0
12	B	1234	CLA	8	0
12	B	1209	CLA	1	0
17	B	4011	45D	5	0
12	B	1236	CLA	4	0
12	B	1022	CLA	4	0
20	B	5005	LMG	3	0
12	B	1228	CLA	2	0
12	A	1109	CLA	12	0
15	J	4013	BCR	9	0
12	B	1203	CLA	4	0

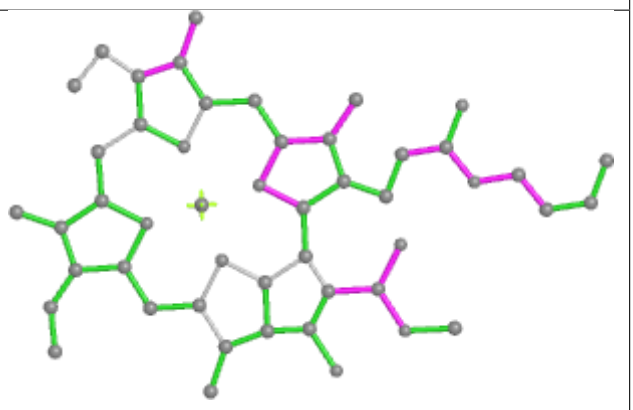
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

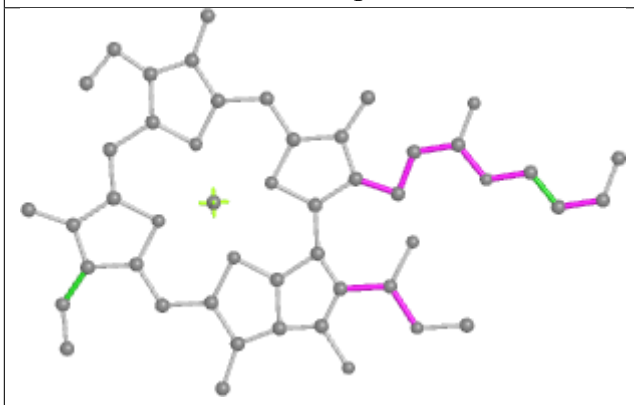
Ligand CLA A 1112



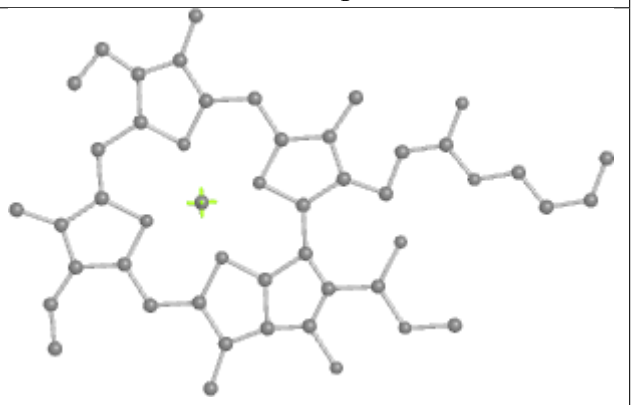
Bond lengths



Bond angles

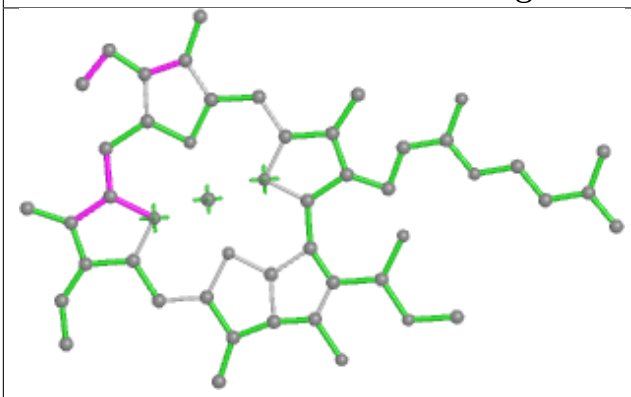


Torsions

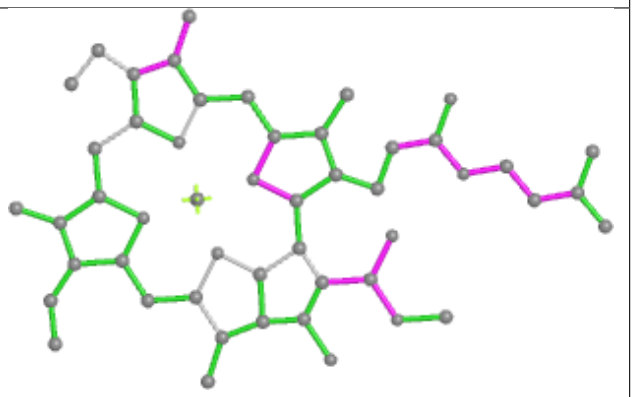


Rings

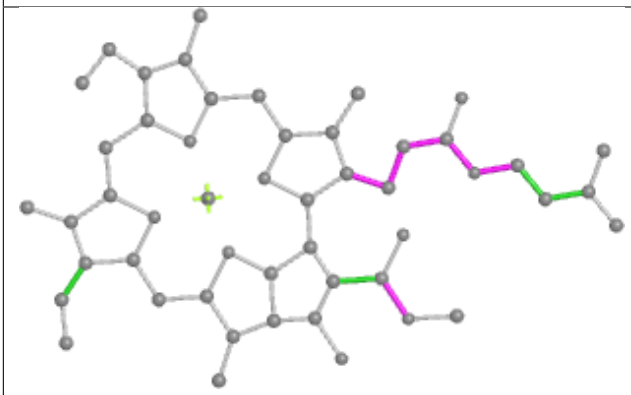
Ligand CLA A 1118



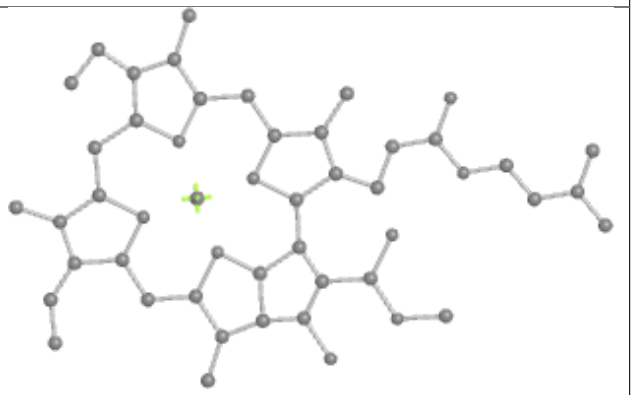
Bond lengths



Bond angles

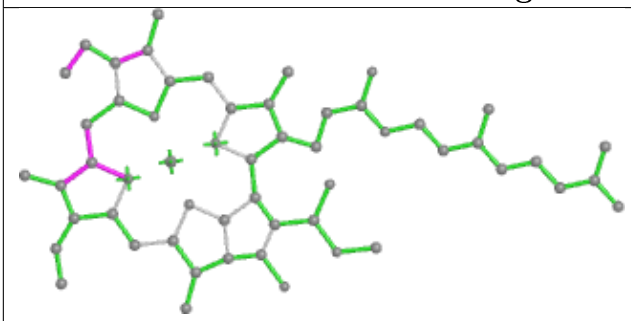


Torsions

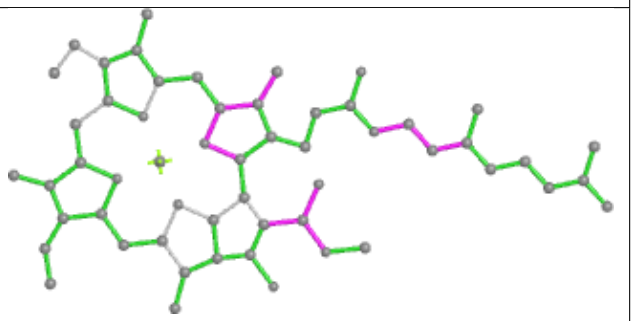


Rings

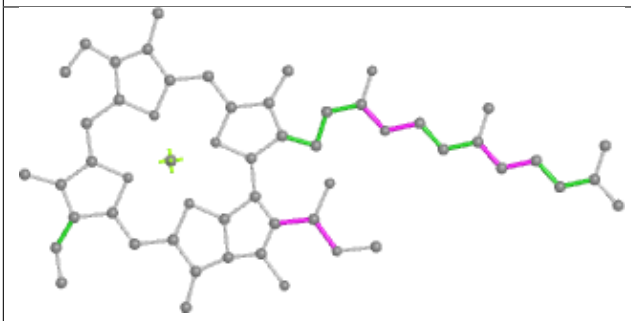
Ligand CLA A 1139



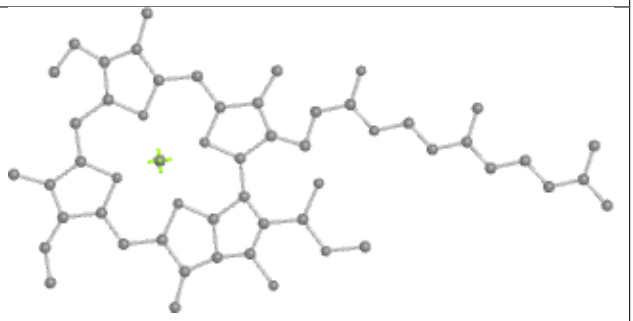
Bond lengths



Bond angles

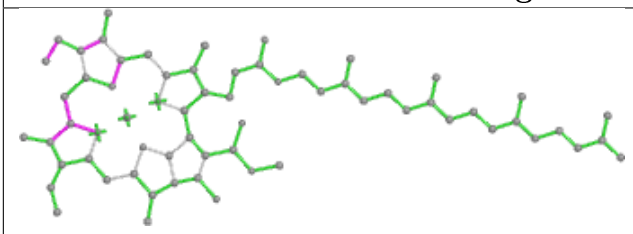


Torsions

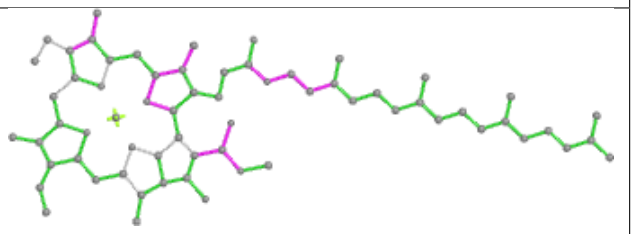


Rings

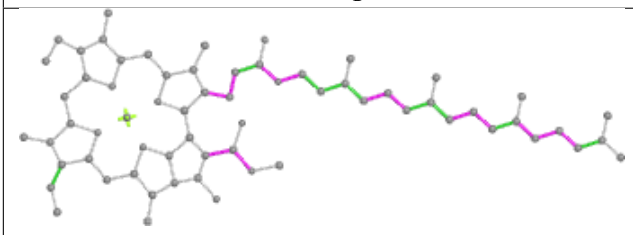
Ligand CLA A 1106



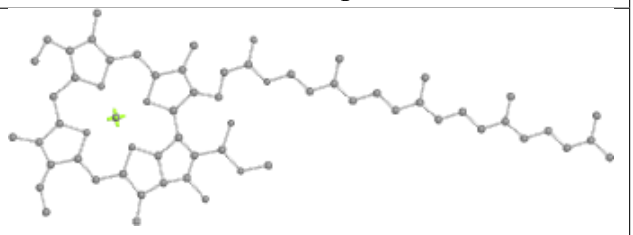
Bond lengths



Bond angles

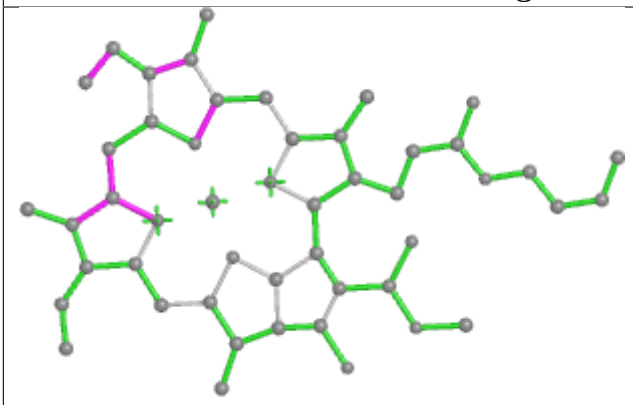


Torsions

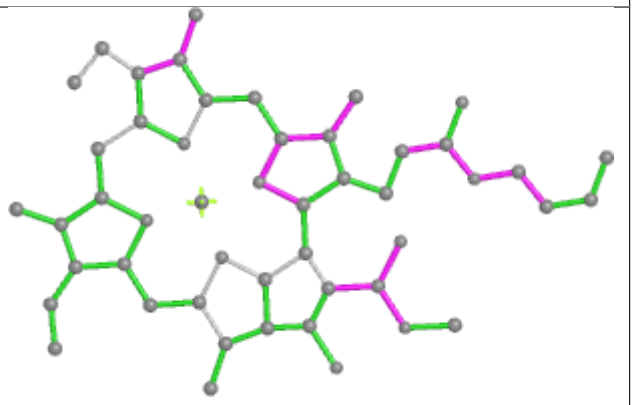


Rings

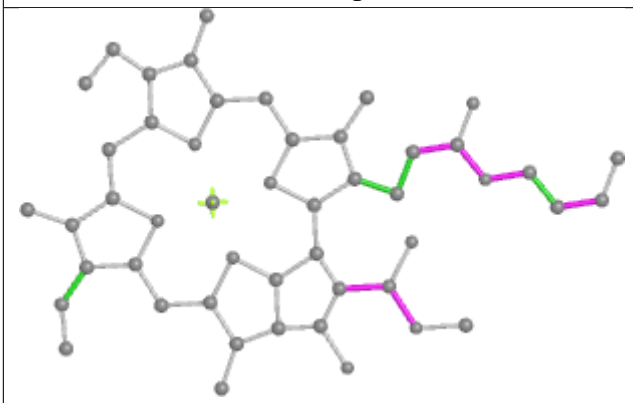
Ligand CLA A 1130



Bond lengths



Bond angles



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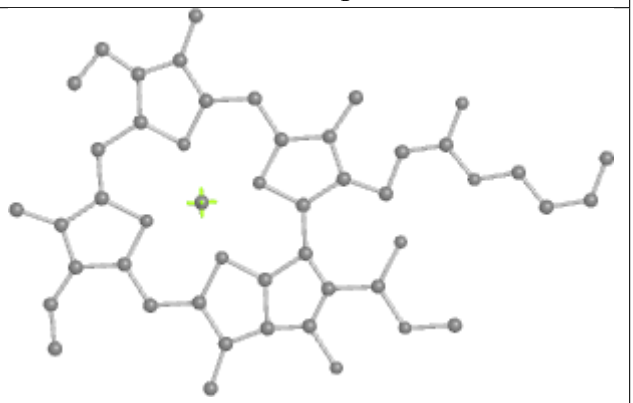
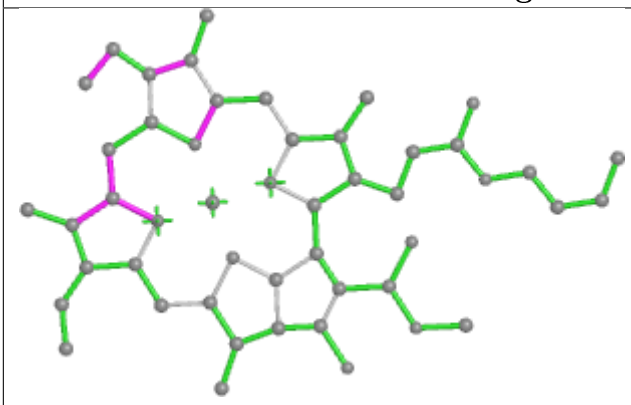
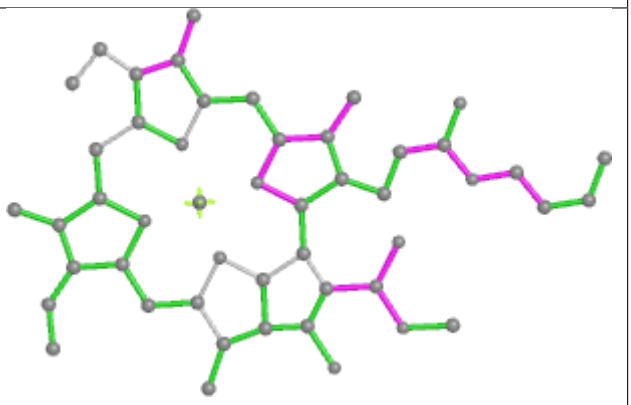


Rings

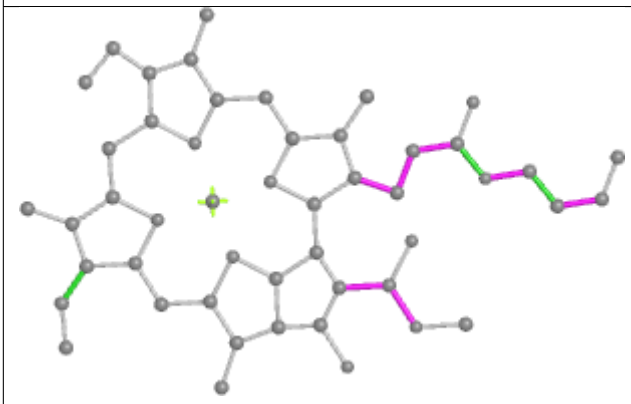
Ligand CLA A 1103



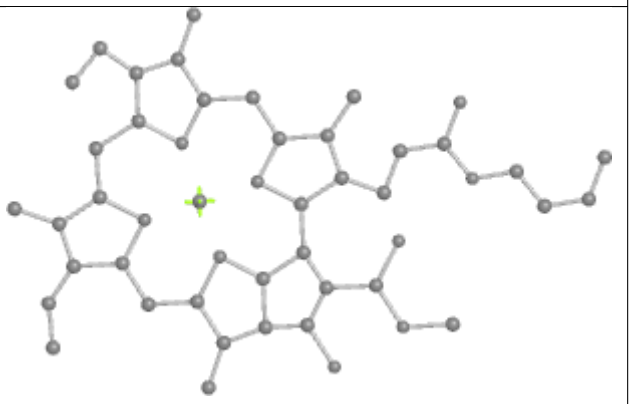
Bond lengths



Bond angles

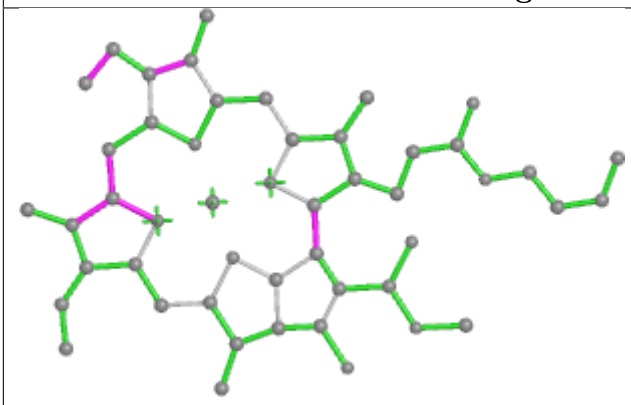


Torsions

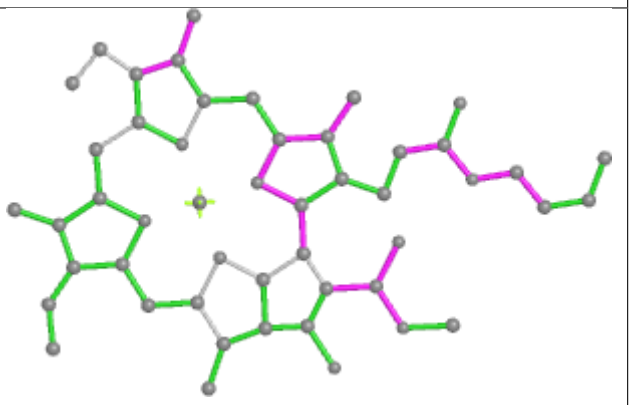


Rings

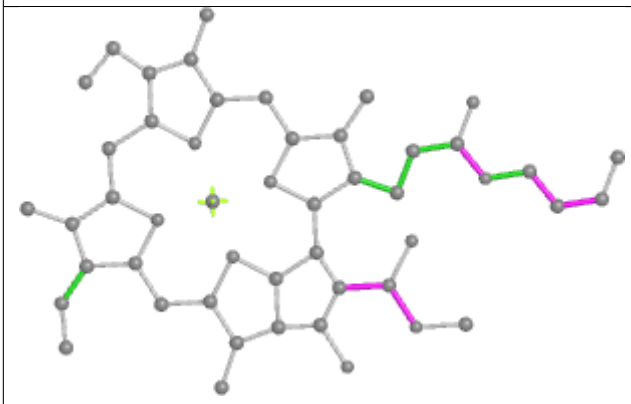
Ligand CLA B 1221



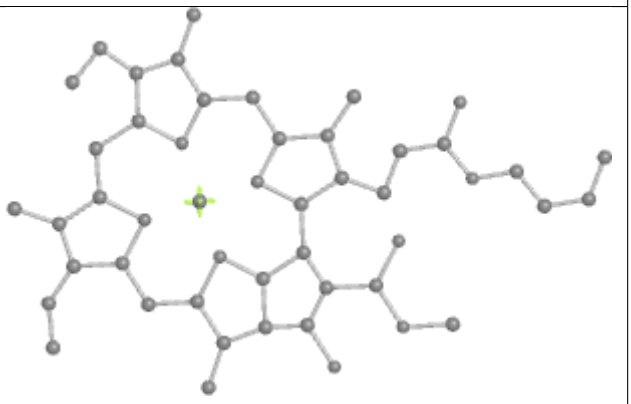
Bond lengths



Bond angles

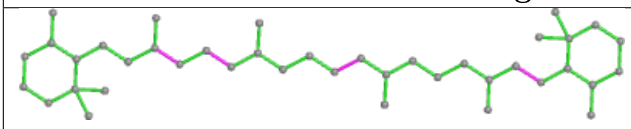


Torsions

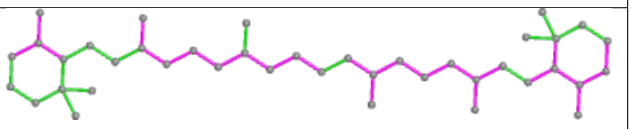


Rings

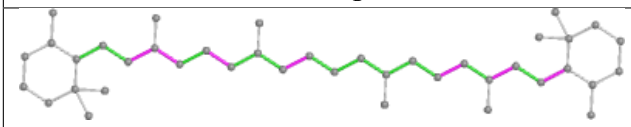
Ligand BCR B 4010



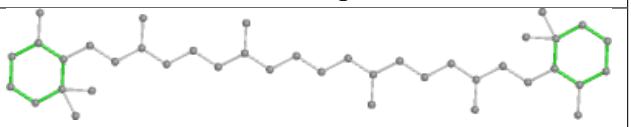
Bond lengths



Bond angles

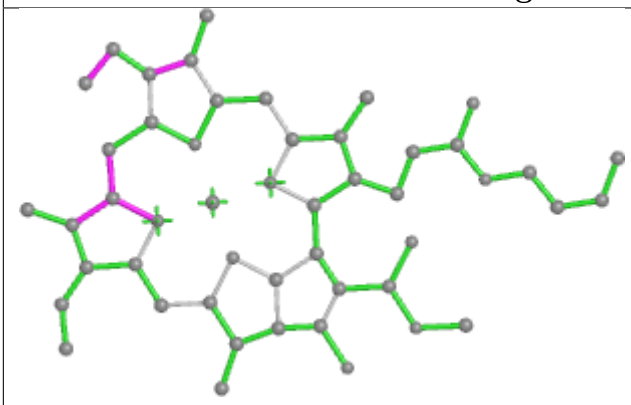


Torsions



Rings

Ligand CLA A 1116



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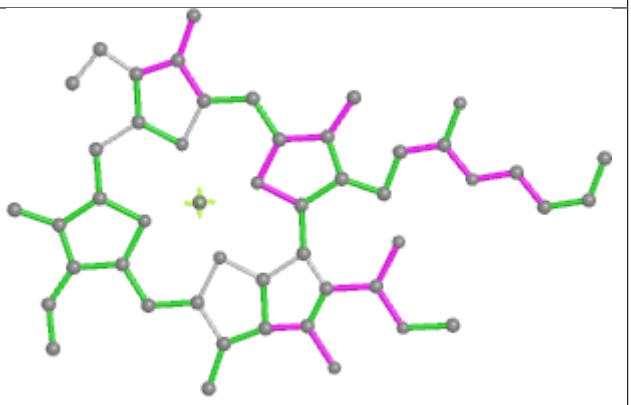
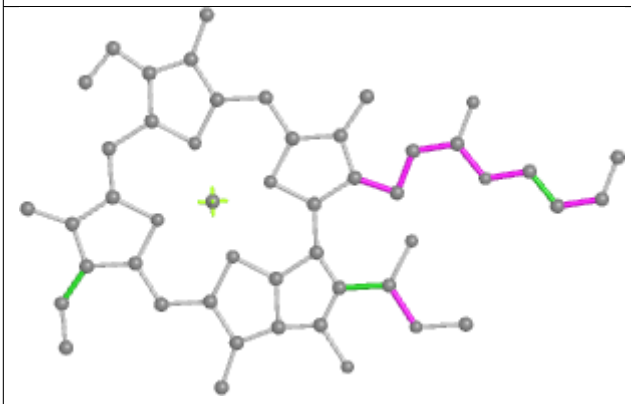
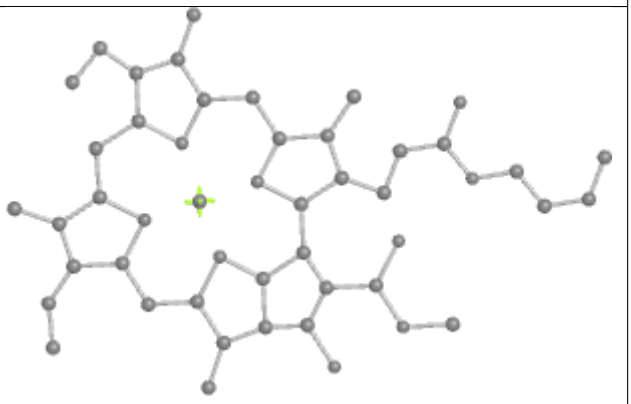


Bond angles

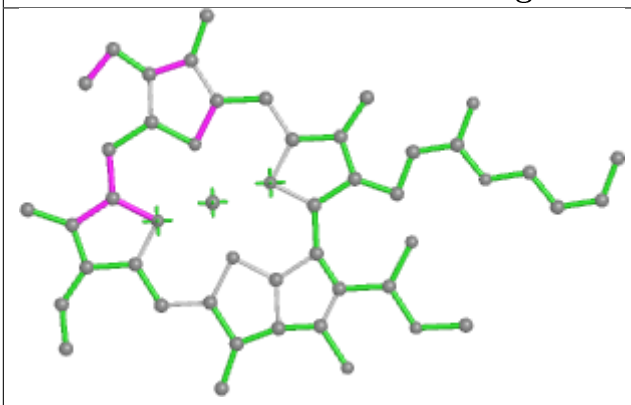


Torsions



Rings

Ligand CLA B 1239



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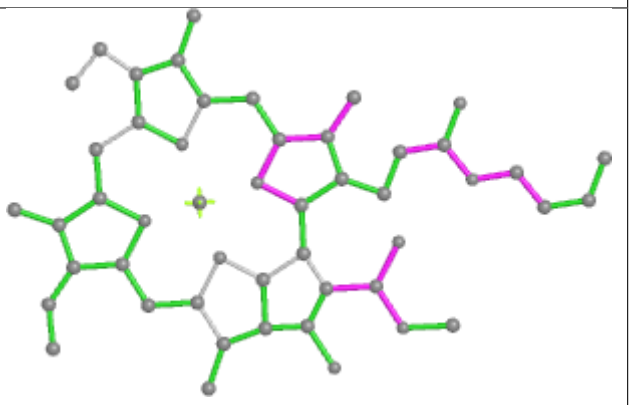
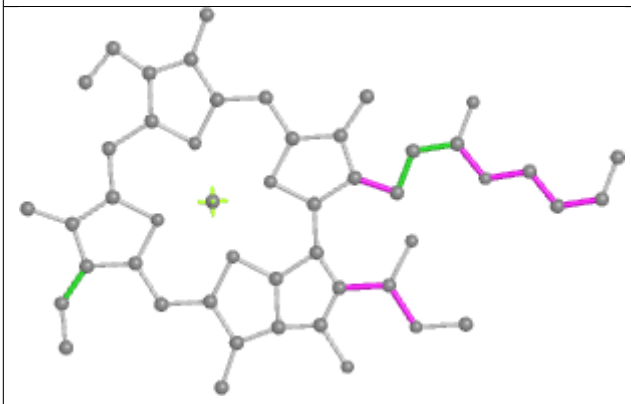


Bond angles



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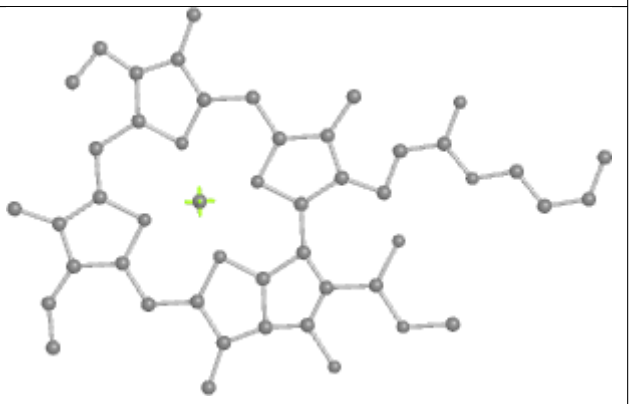
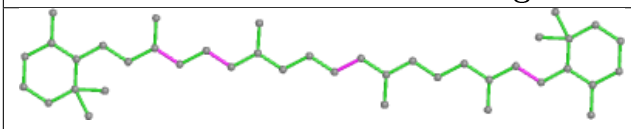


Rings

Ligand BCR A 4003



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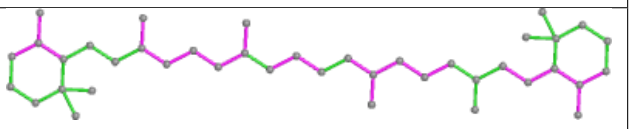
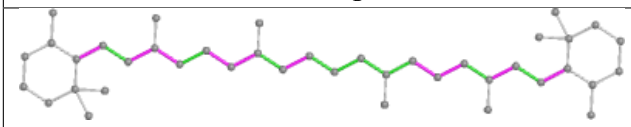
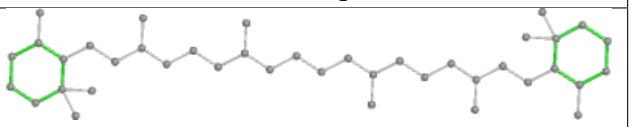


Bond angles

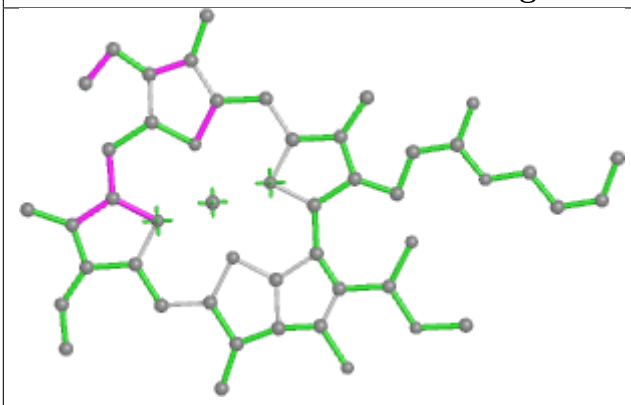


Torsions



Rings

Ligand CLA J 1303



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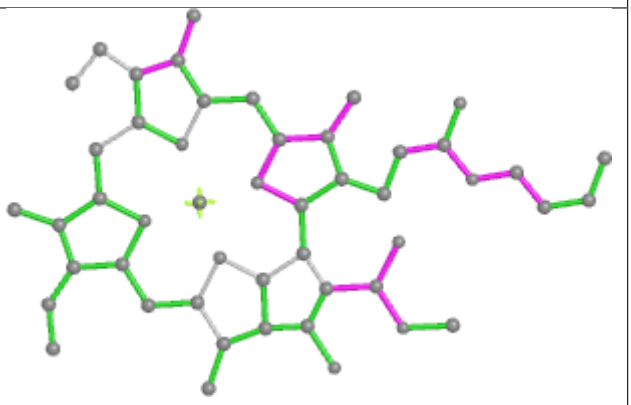
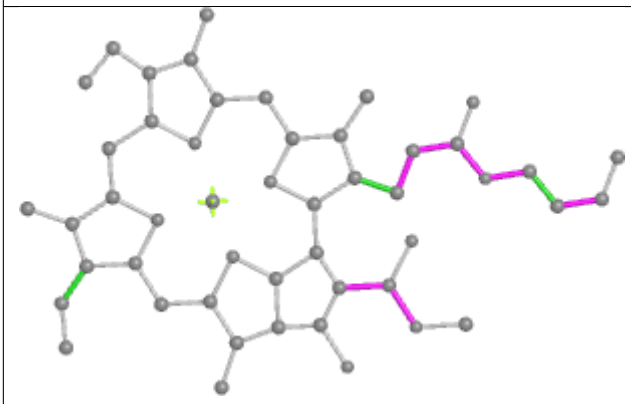


Bond angles



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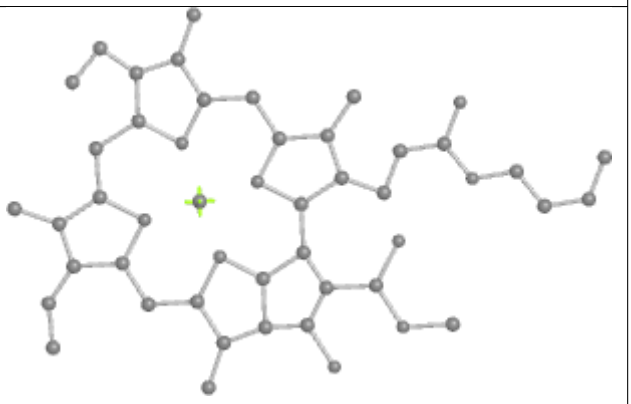
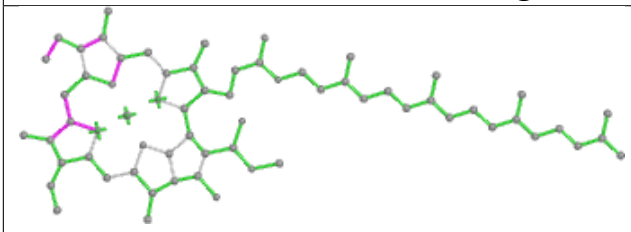


Rings

Ligand CLA A 1105



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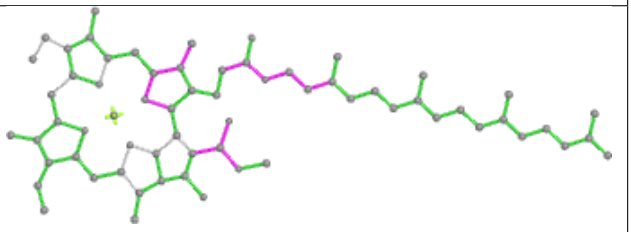
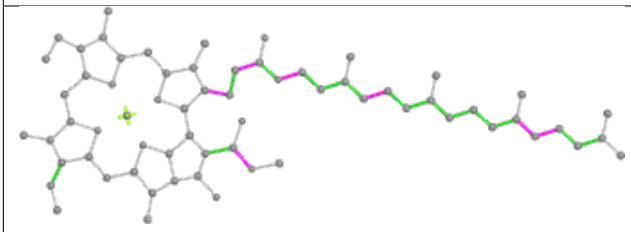


Bond angles



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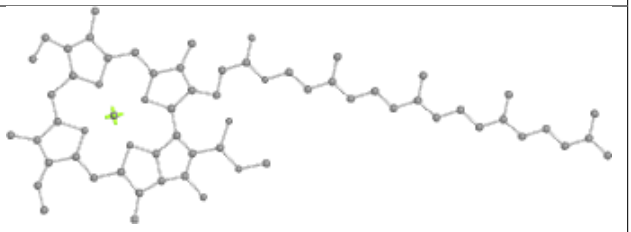
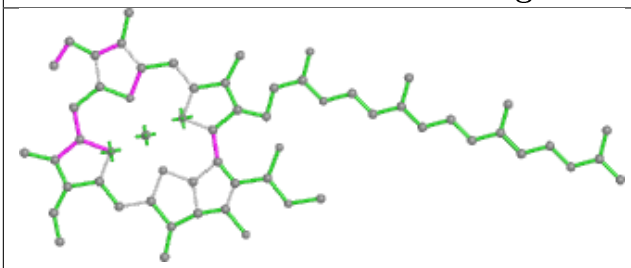


Rings

Ligand CLA A 1123



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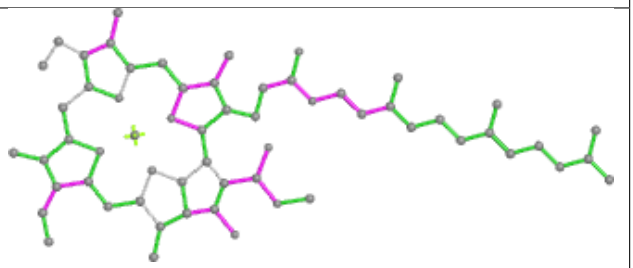
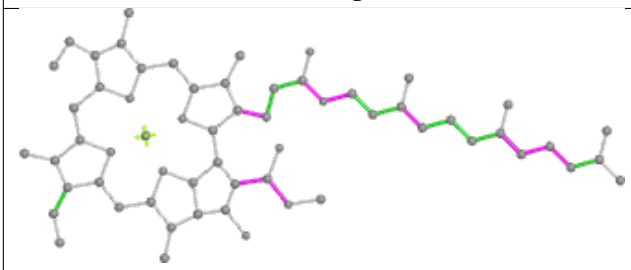


Bond angles



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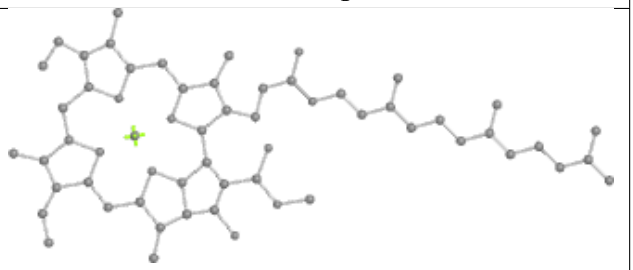
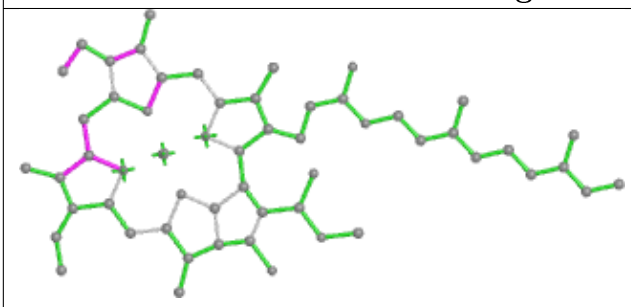


Rings

Ligand CLA A 1115



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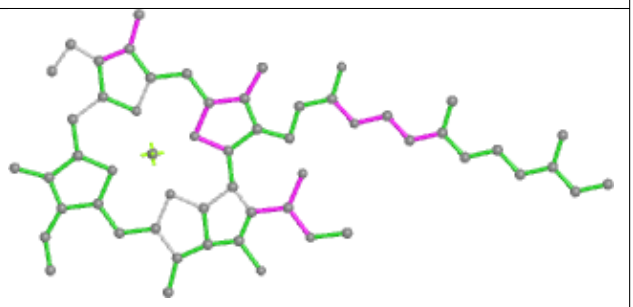
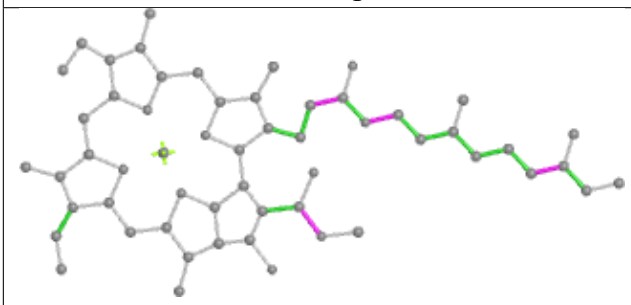
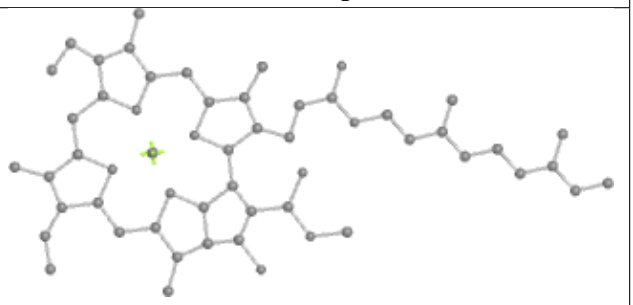


Bond angles

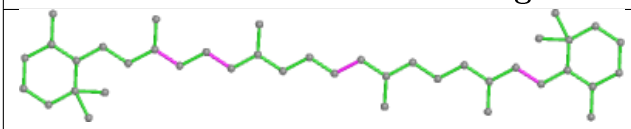


Torsions



Rings

Ligand BCR B 4005



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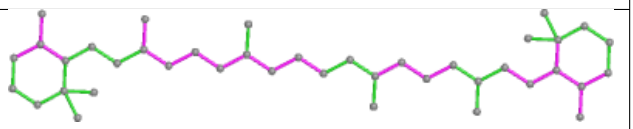
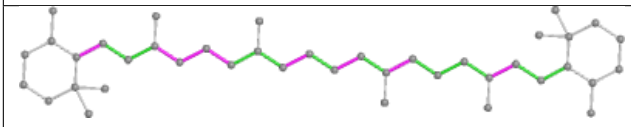
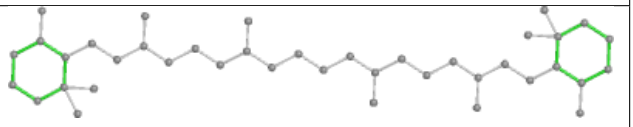


Bond angles

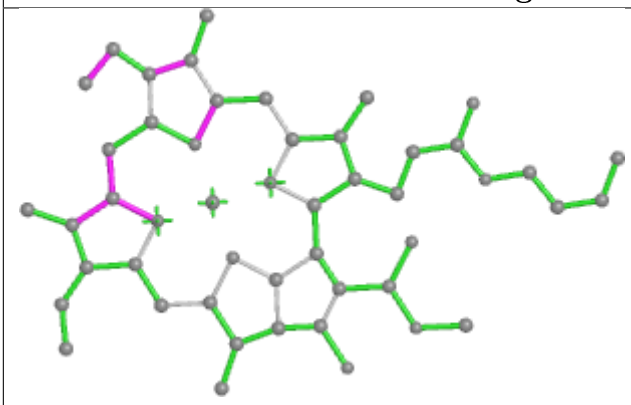


Torsions

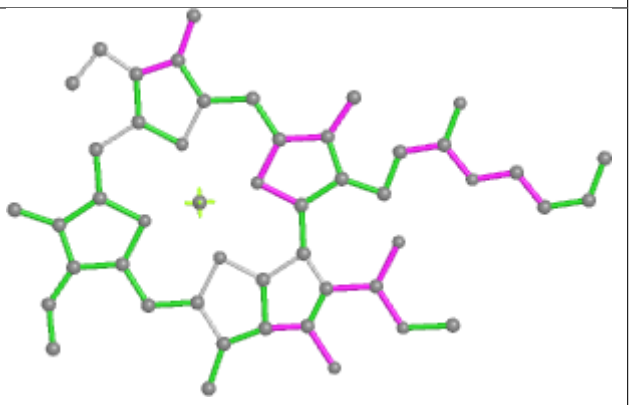


Rings

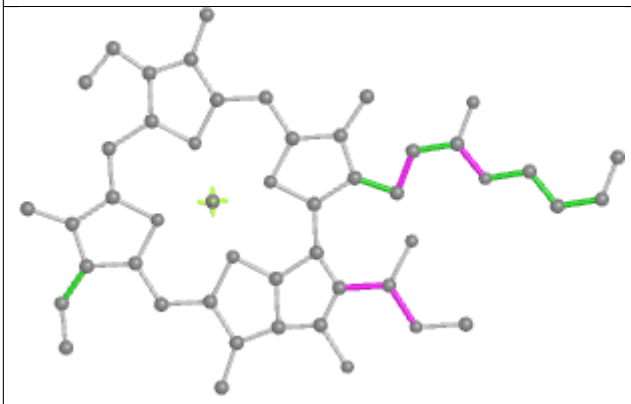
Ligand CLA A 1129



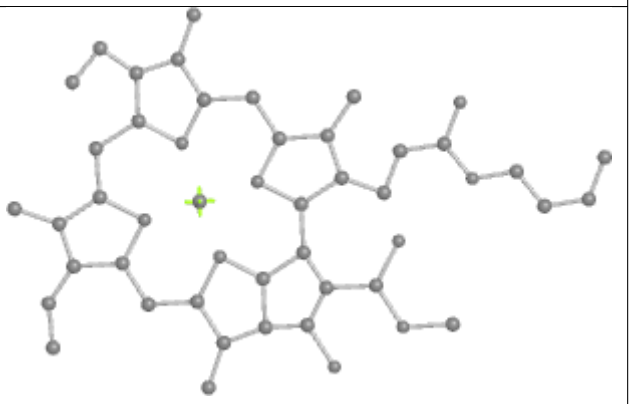
Bond lengths



Bond angles

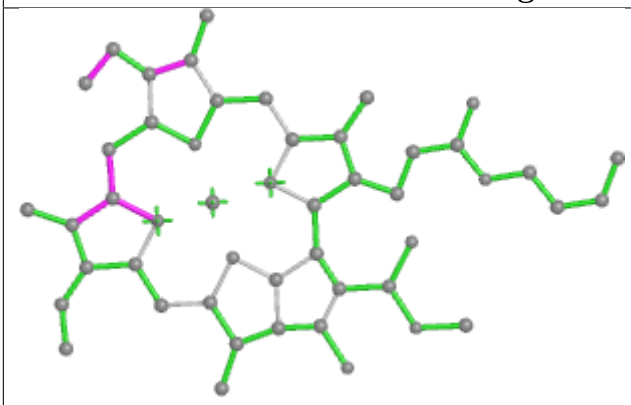


Torsions



Rings

Ligand CLA F 1301



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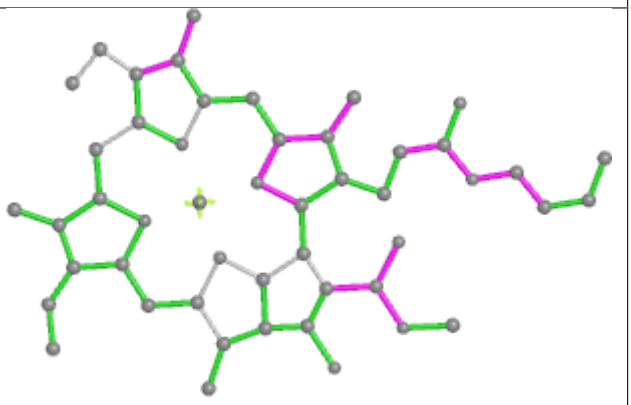
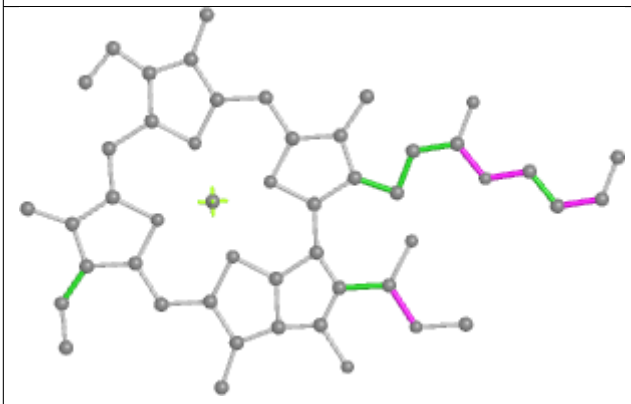
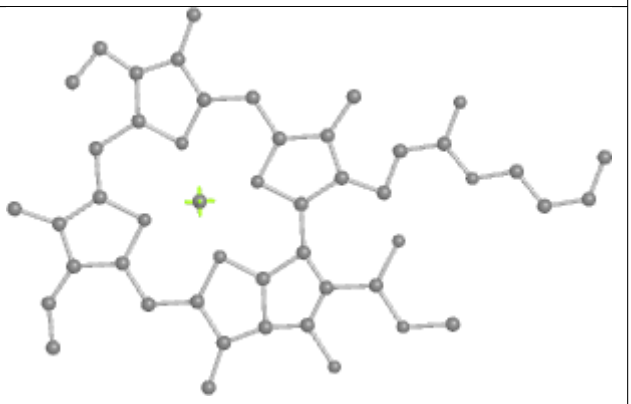


Bond angles

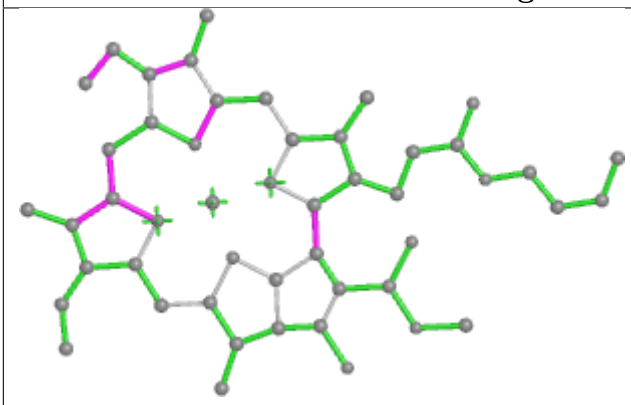


Torsions



Rings

Ligand CLA L 1502



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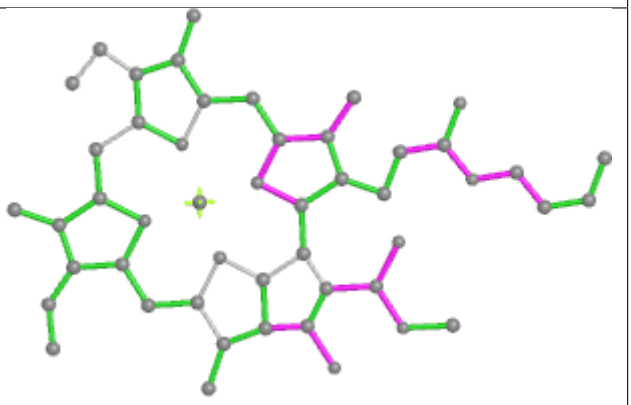
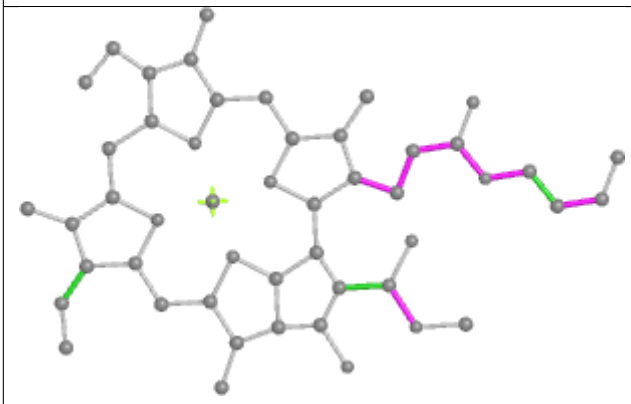
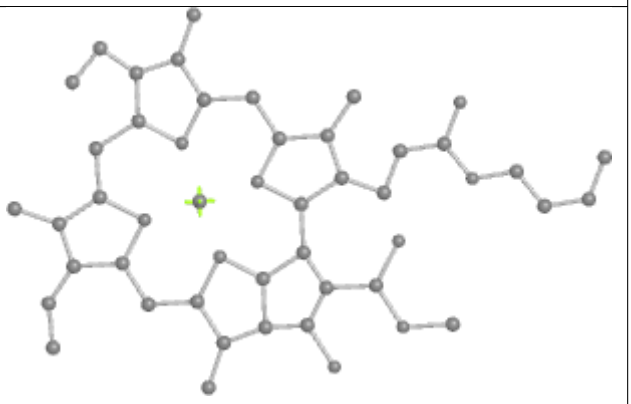


Bond angles

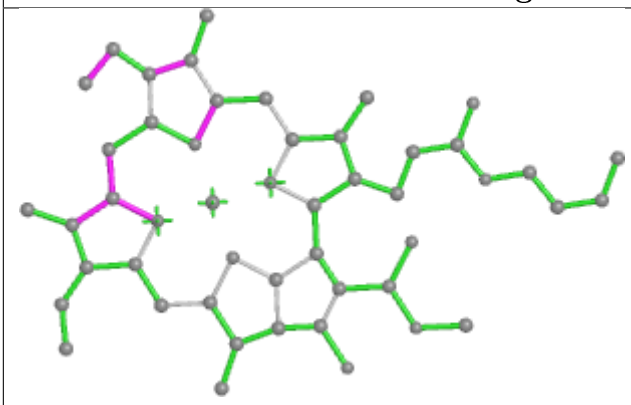


Torsions



Rings

Ligand CLA A 1101



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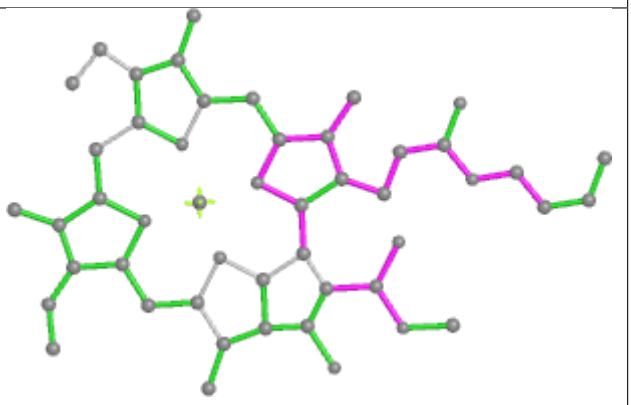
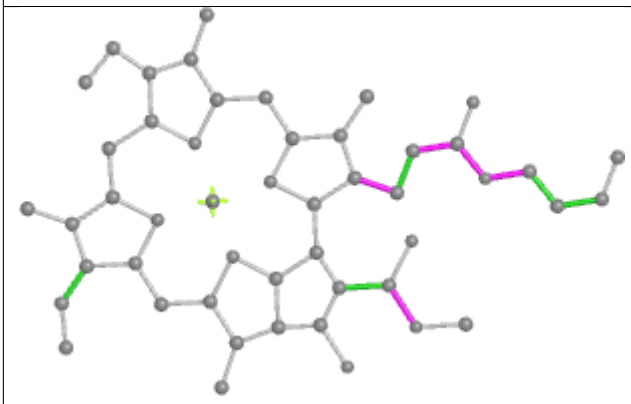
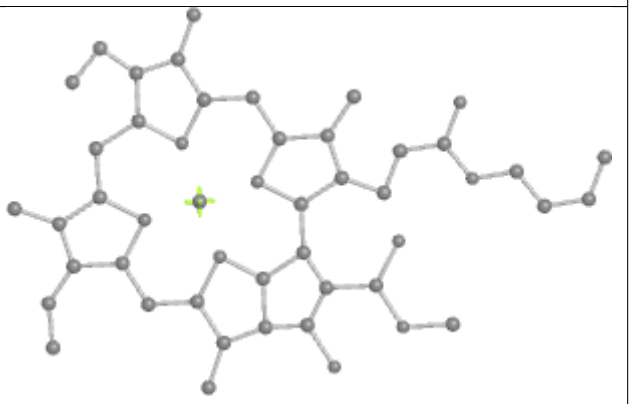


Bond angles

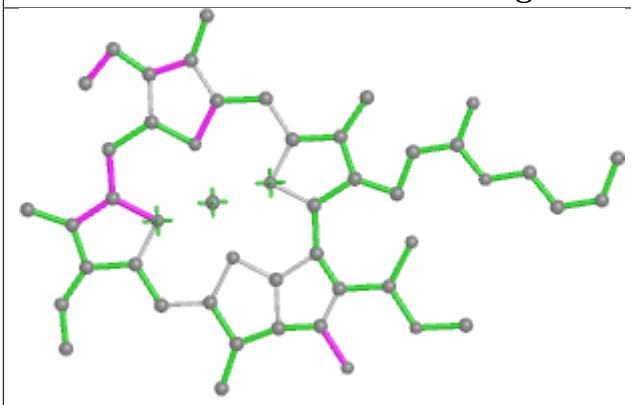


Torsions

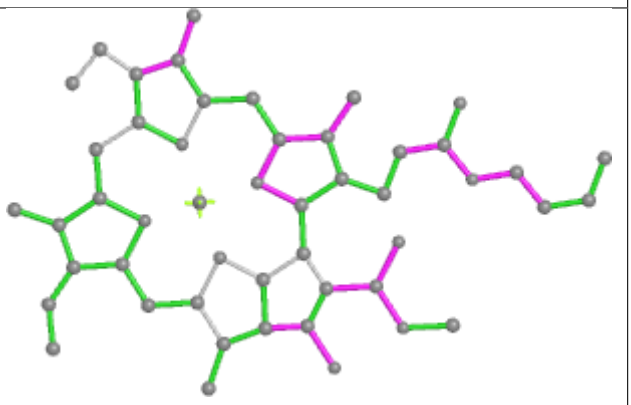


Rings

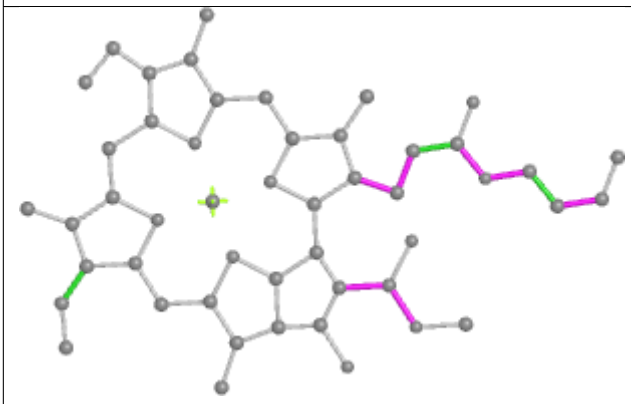
Ligand CLA B 1223



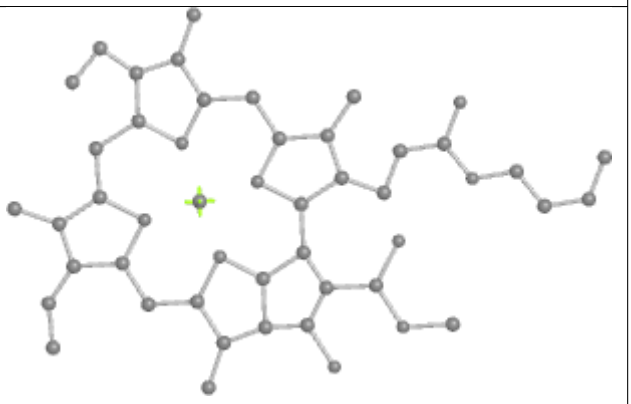
Bond lengths



Bond angles

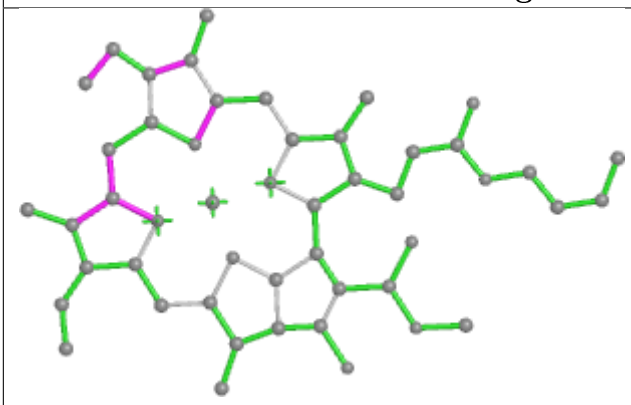


Torsions

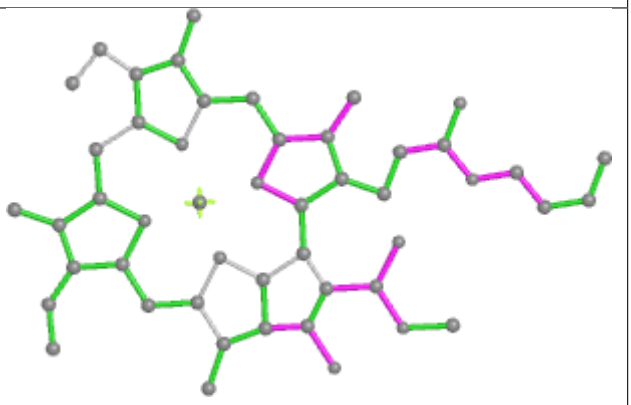


Rings

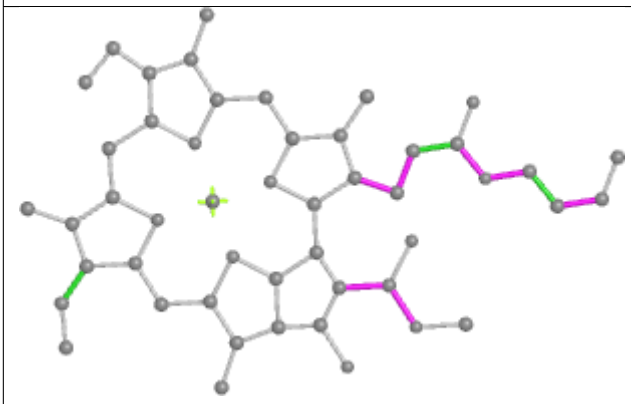
Ligand CLA A 1133



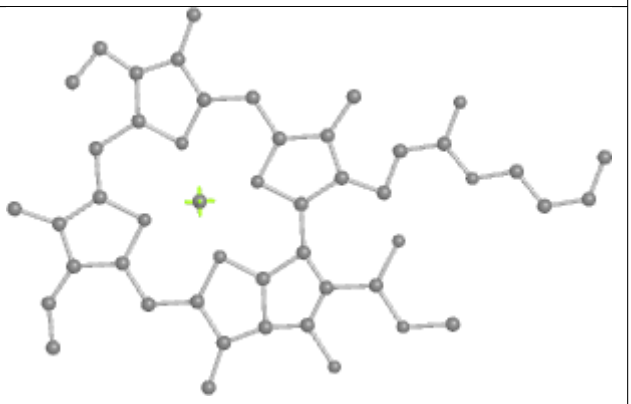
Bond lengths



Bond angles

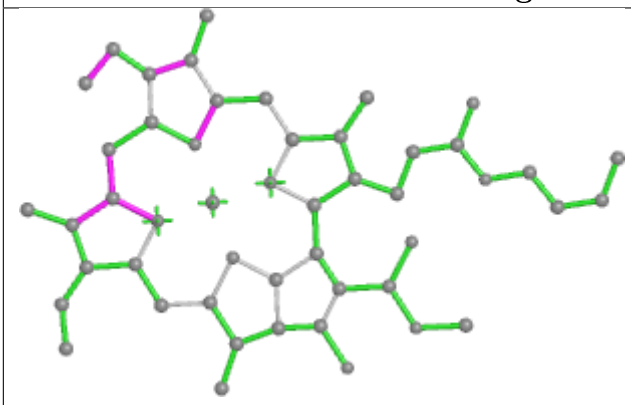


Torsions



Rings

Ligand CLA B 1205



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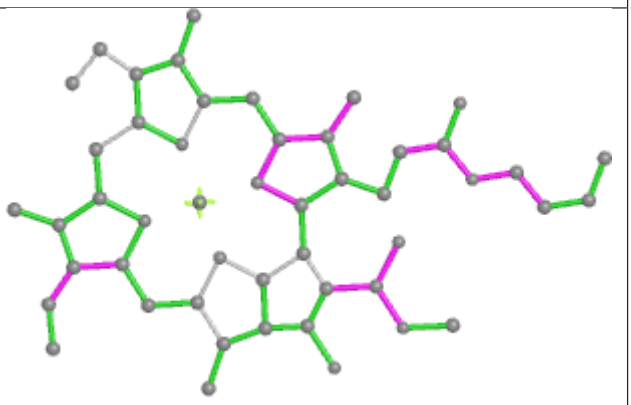

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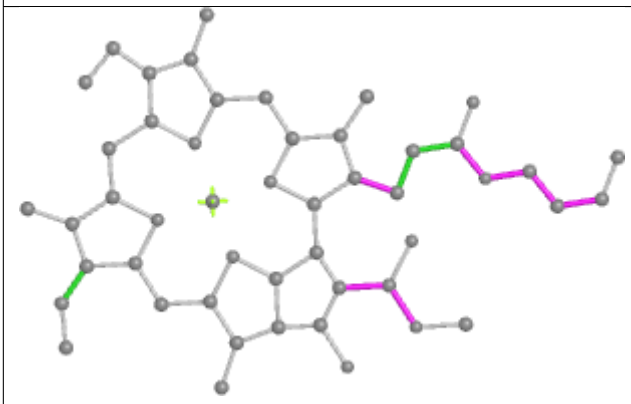
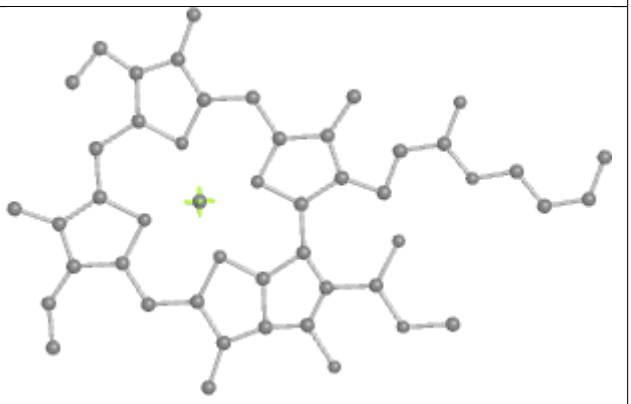
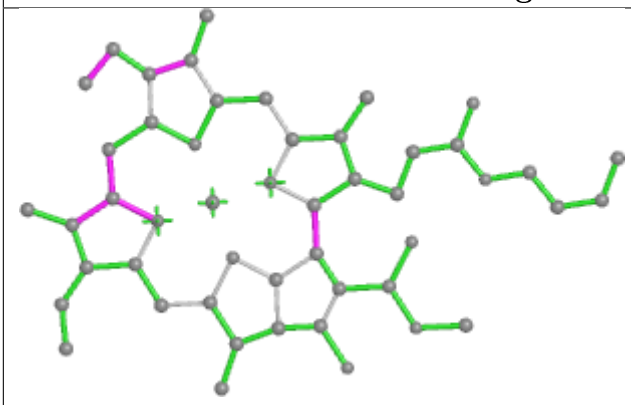


Torsions



Rings

Ligand CLA A 1012



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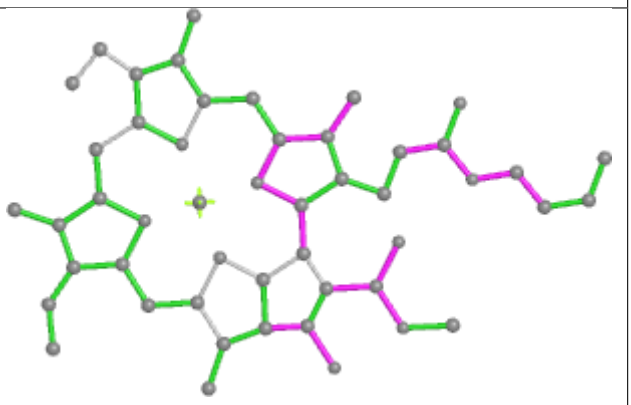
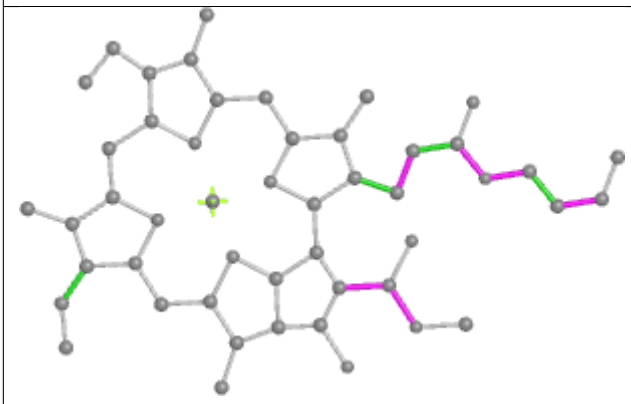
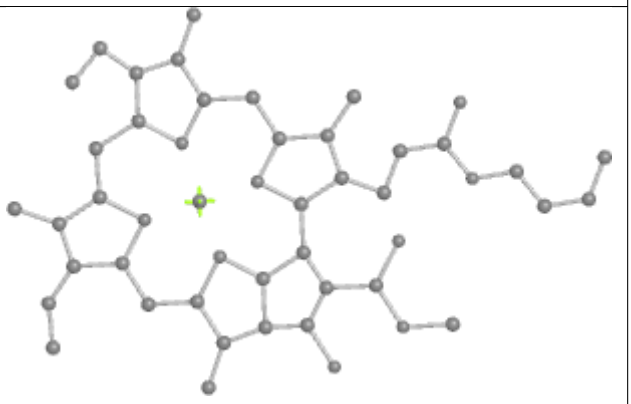


Bond angles

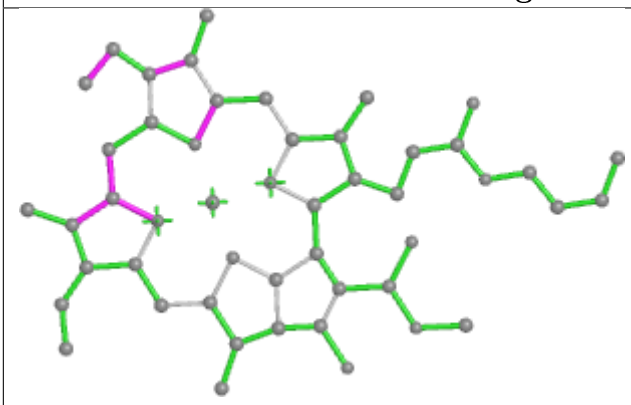


Torsions

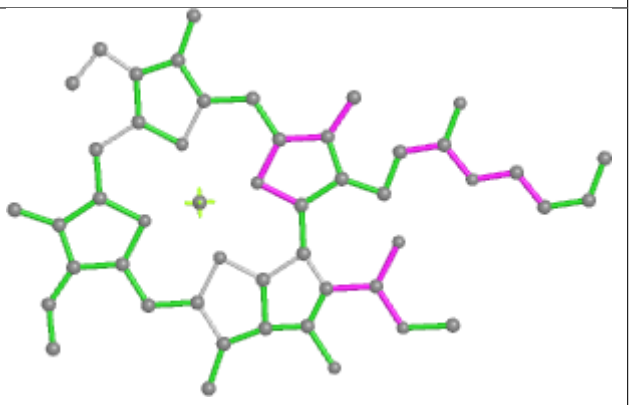


Rings

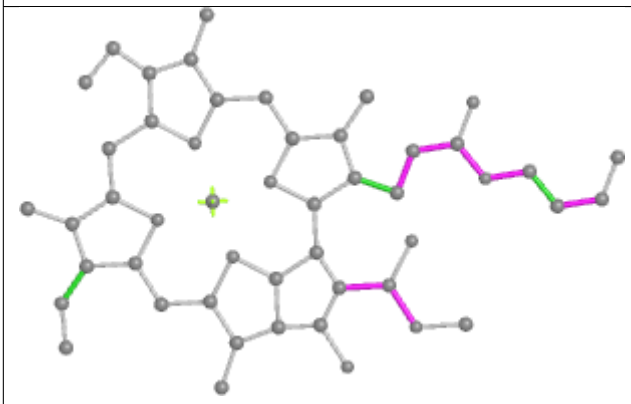
Ligand CLA A 1136



Bond lengths



Bond angles



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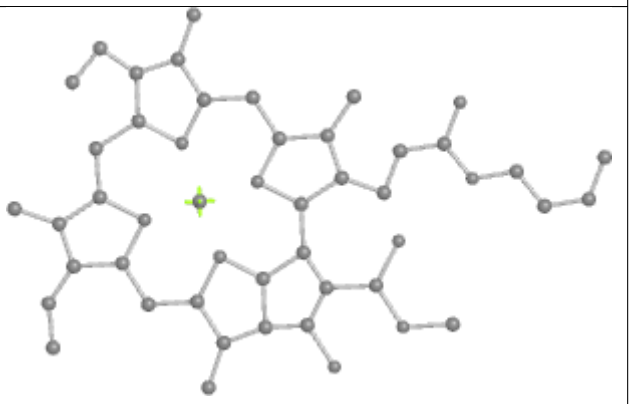
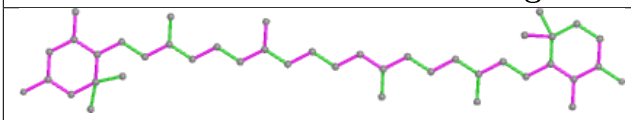


Rings

Ligand EQ3 I 4020



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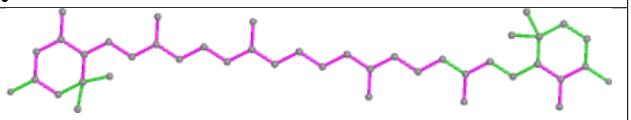
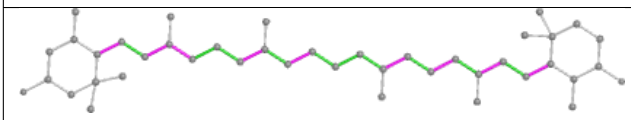


Bond angles



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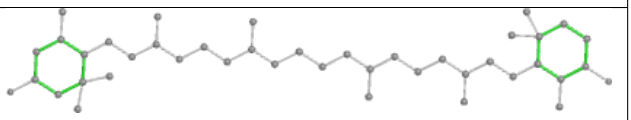
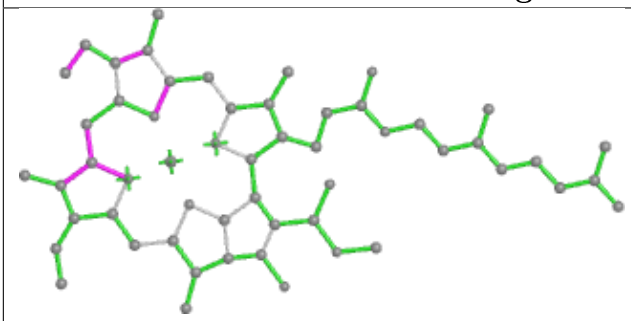


Rings

Ligand CLA B 1229



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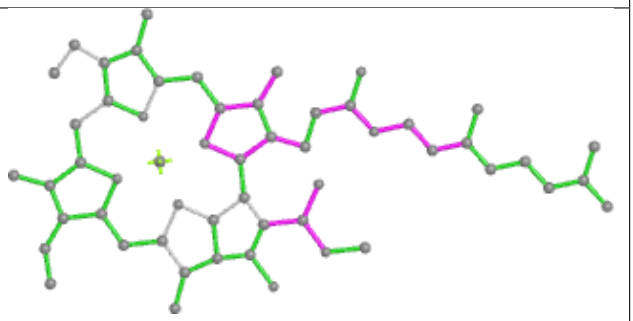
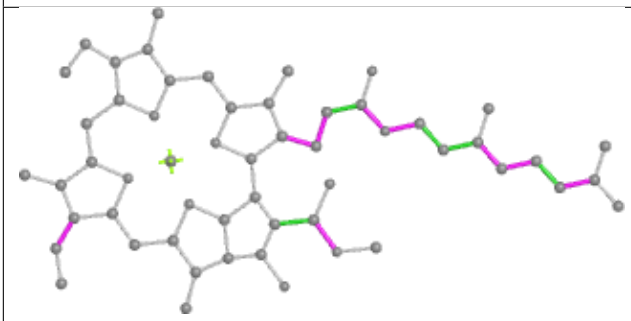


Bond angles



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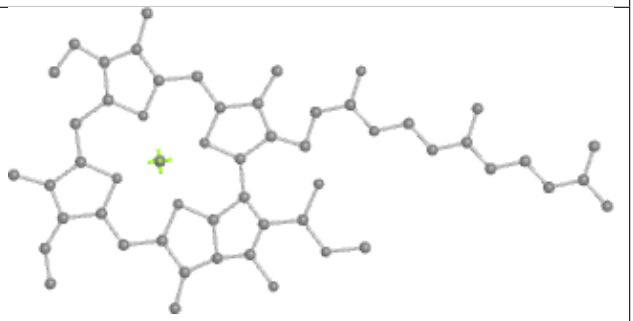
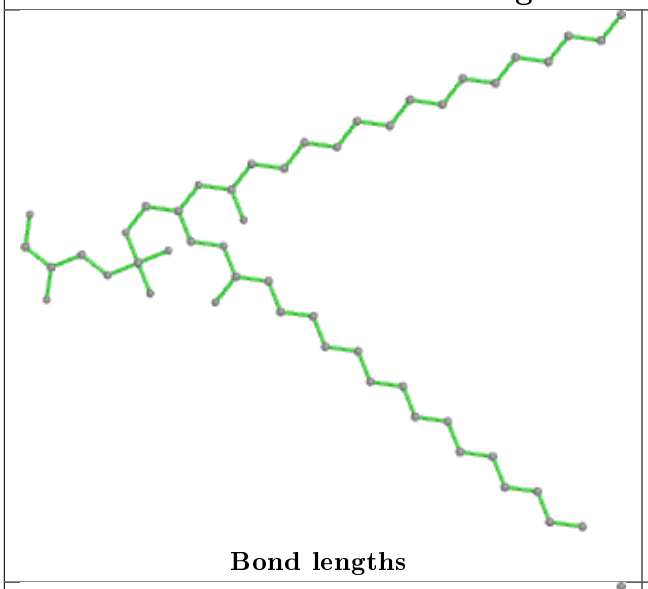
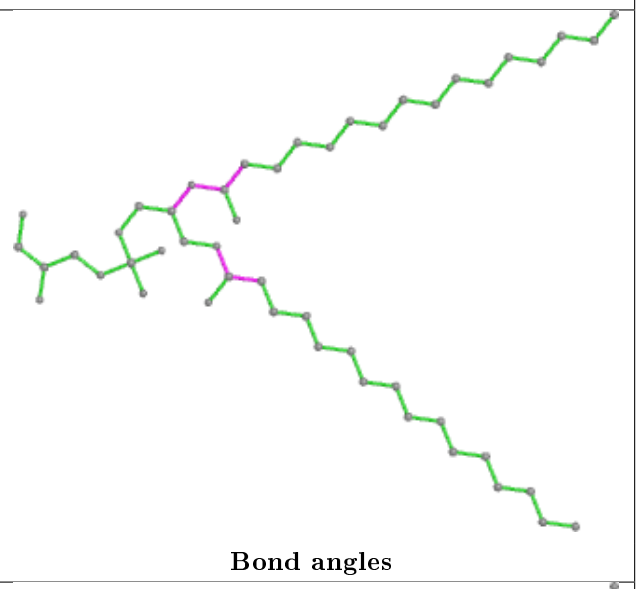


Rings

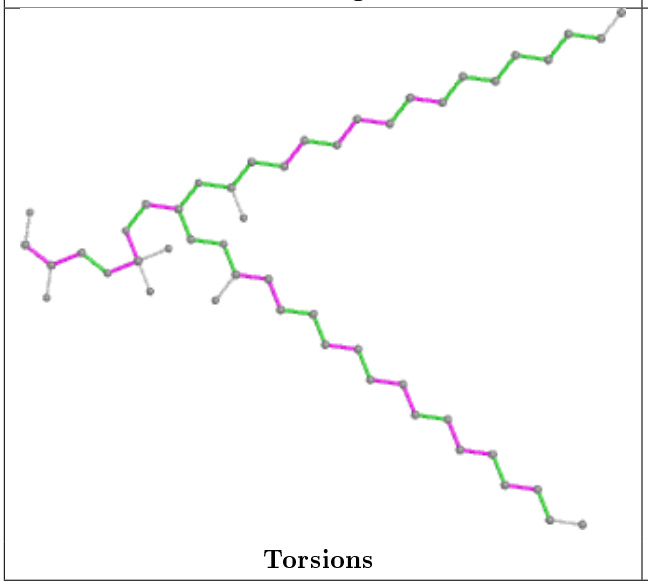
Ligand LHG B 5004



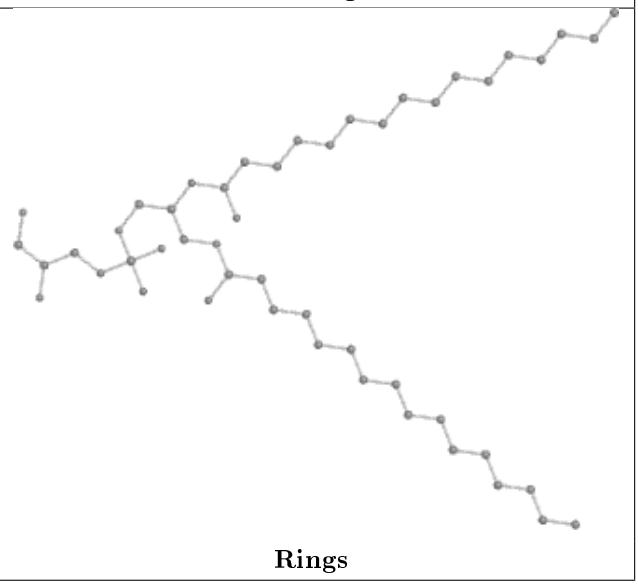
Bond lengths



Bond angles

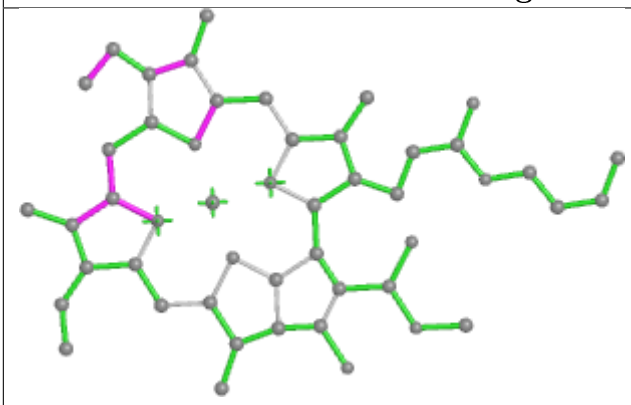


Torsions



Rings

Ligand CLA A 1135



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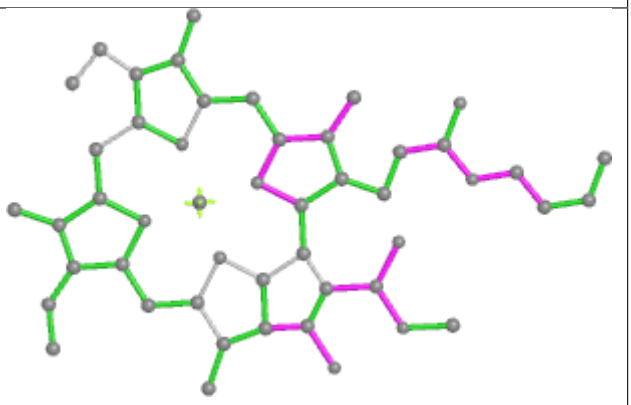
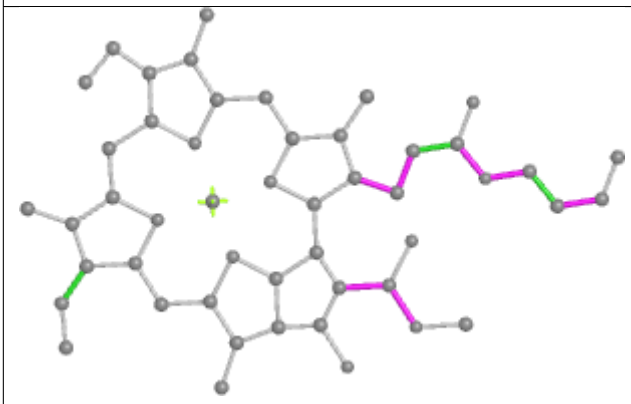
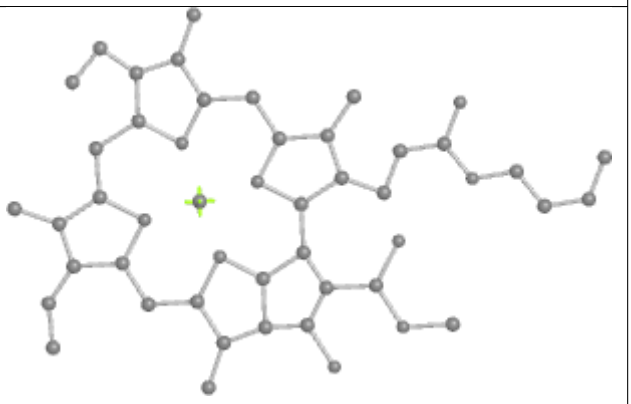


Bond angles

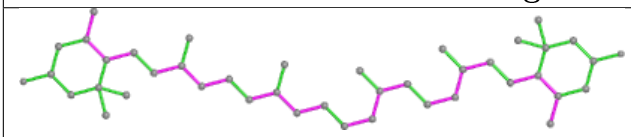


Torsions

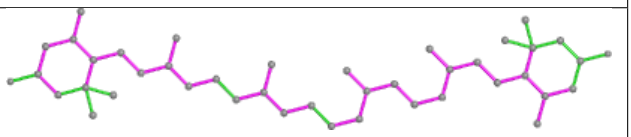


Rings

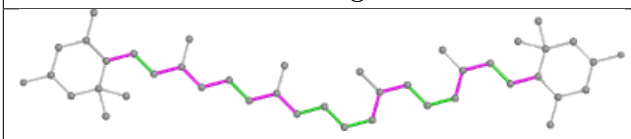
Ligand C7Z J 4015



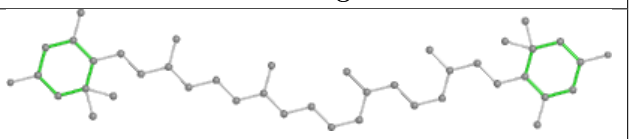
Bond lengths



Bond angles

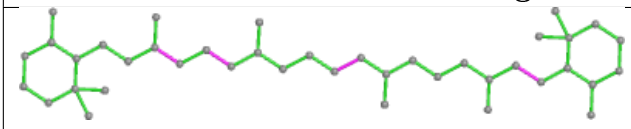


Torsions



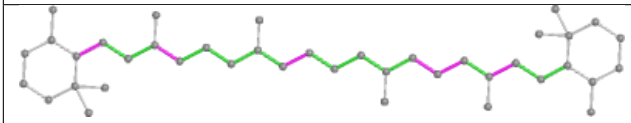
Rings

Ligand BCR B 4018

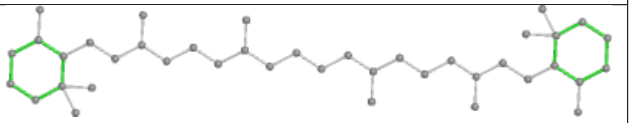


Bond lengths

Bond angles

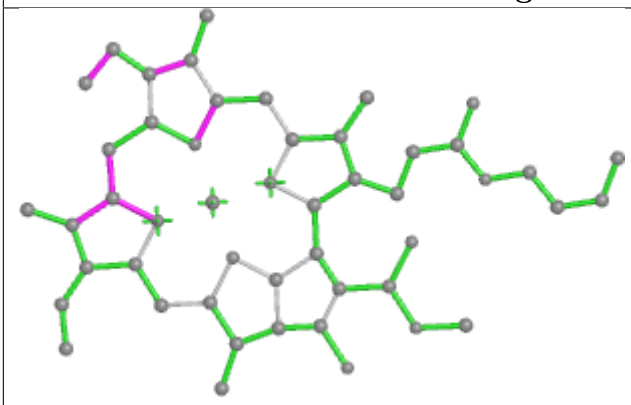


Torsions



Rings

Ligand CLA A 1127



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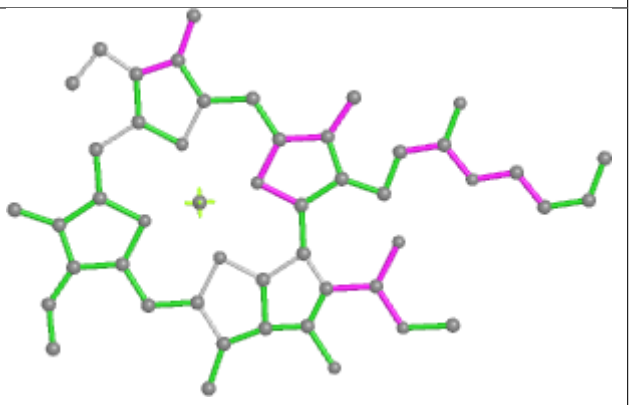
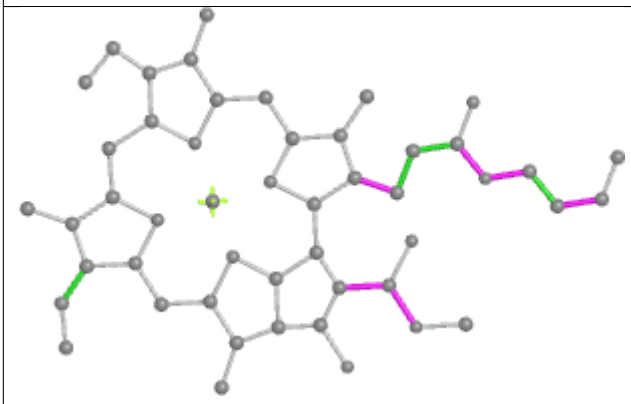
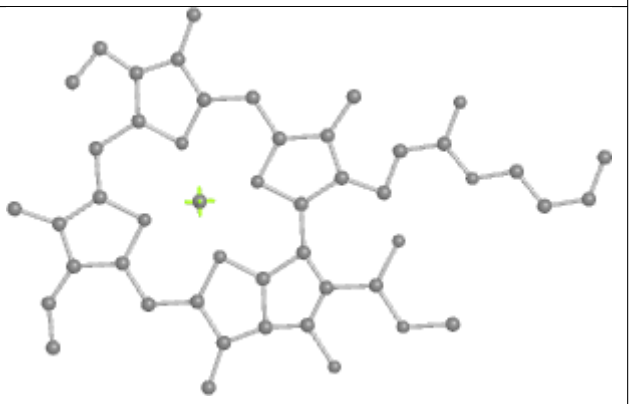


Bond angles

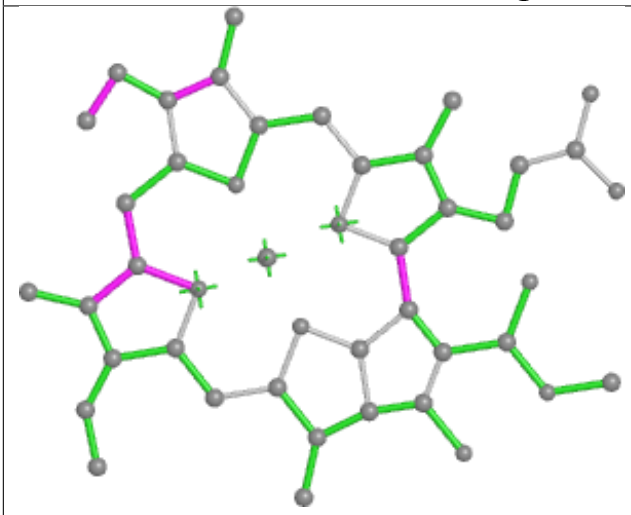


Torsions



Rings

Ligand CLA A 1141



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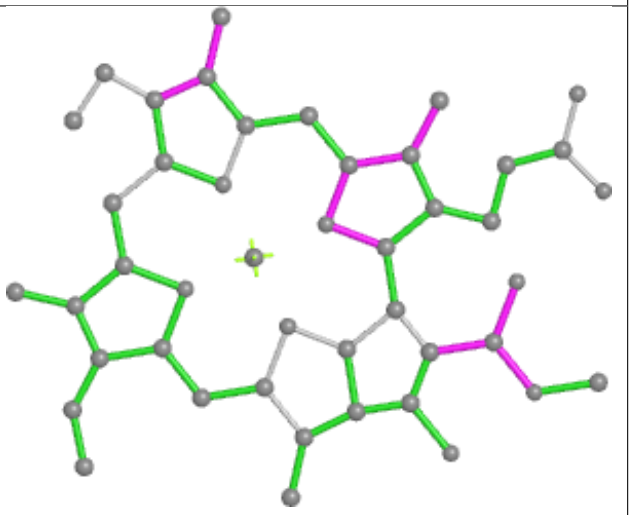
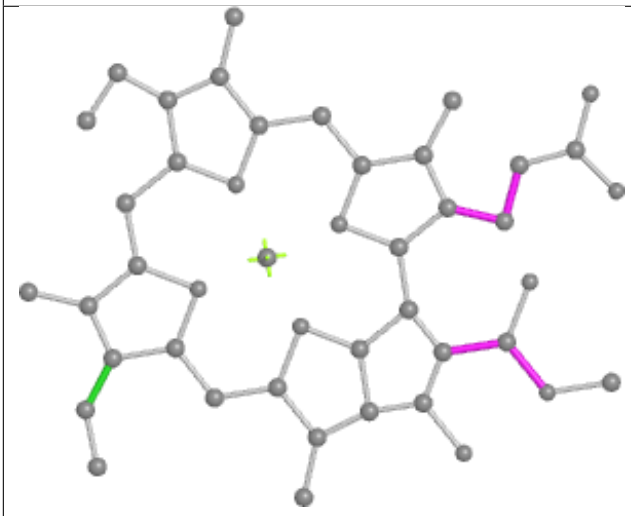
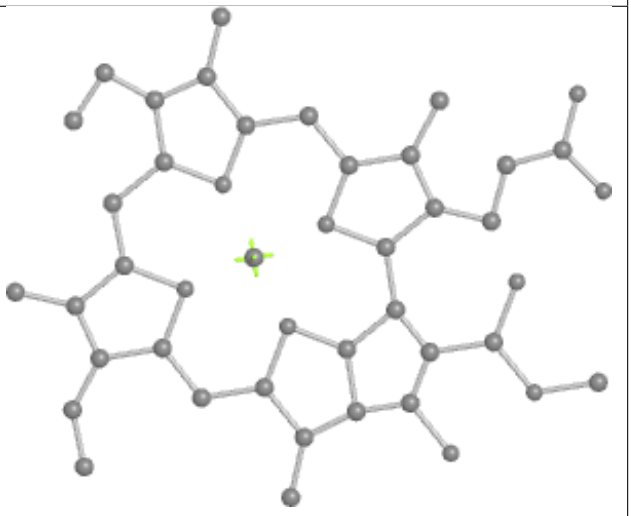


Bond angles

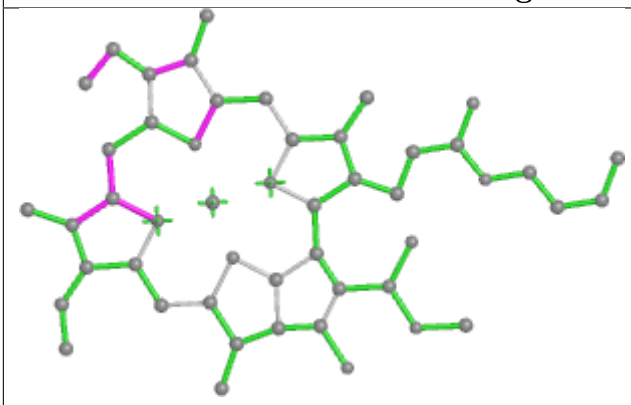


Torsions

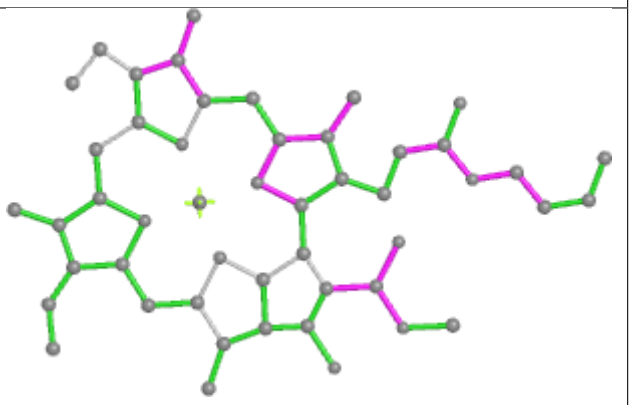


Rings

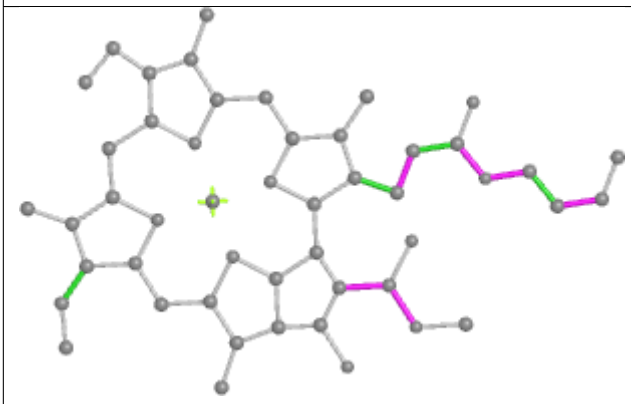
Ligand CLA B 1201



Bond lengths



Bond angles



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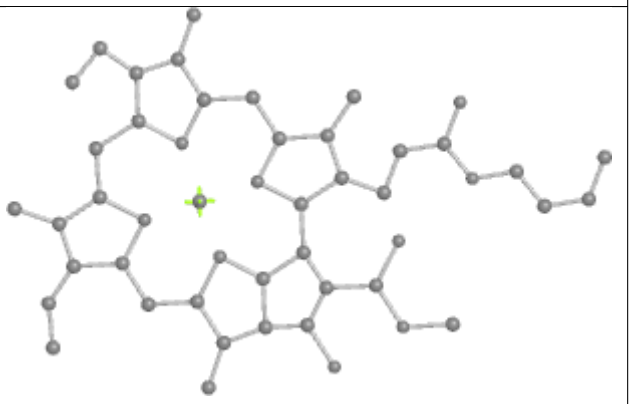
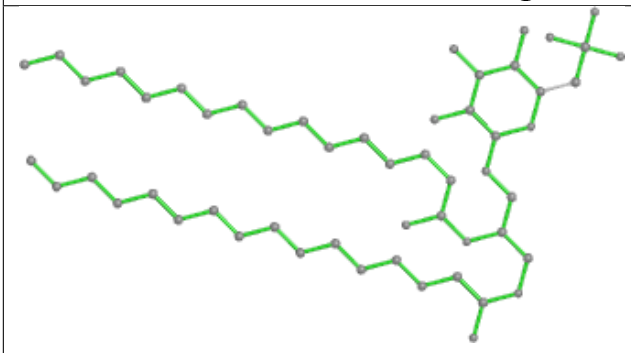


Rings

Ligand SQD F 5001



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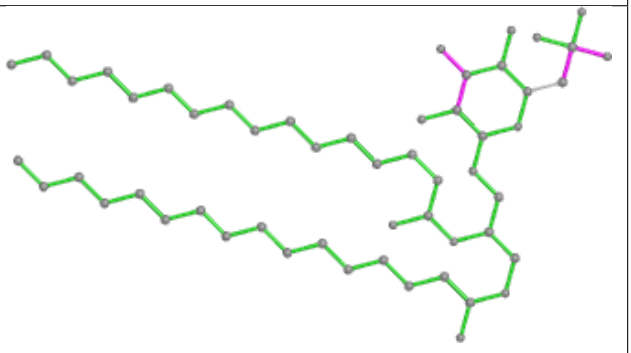
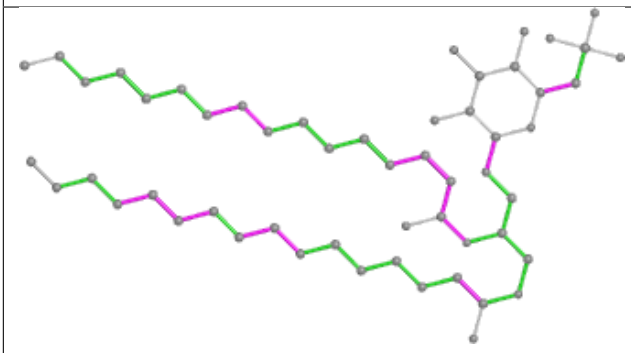
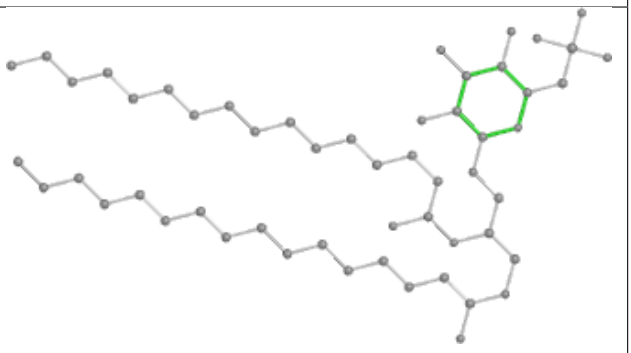


Bond angles

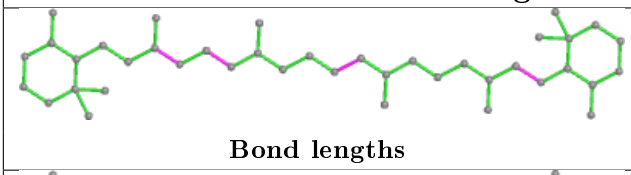


Torsions

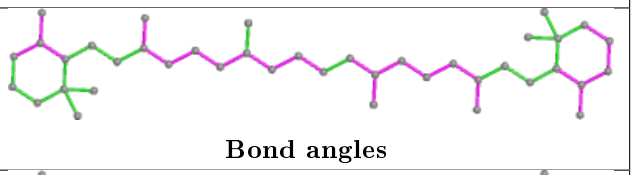


Rings

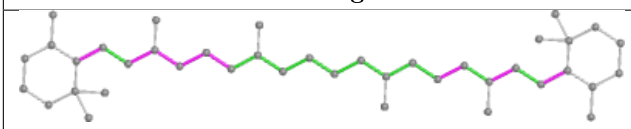
Ligand BCR A 4008



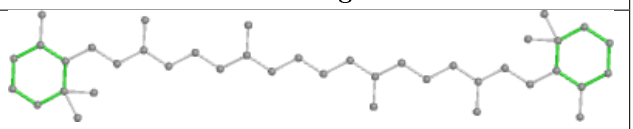
Bond lengths



Bond angles

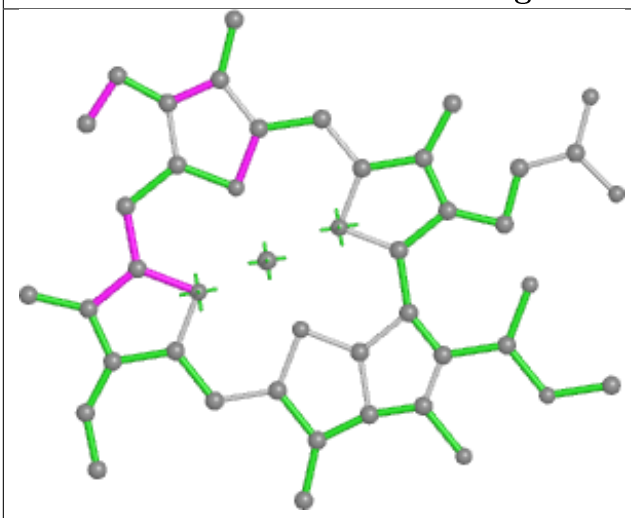


Torsions

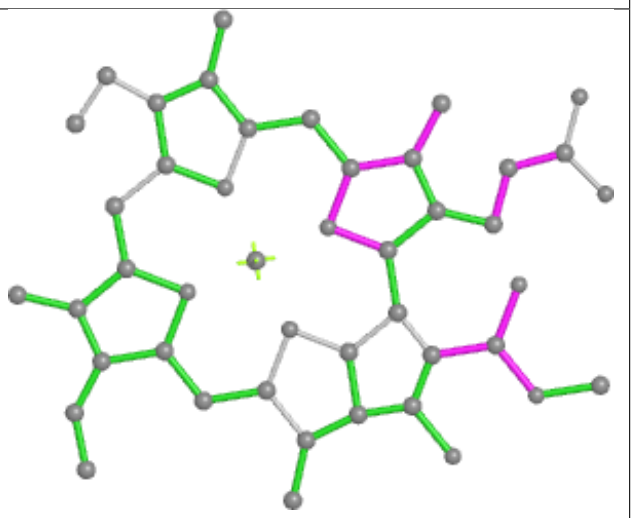


Rings

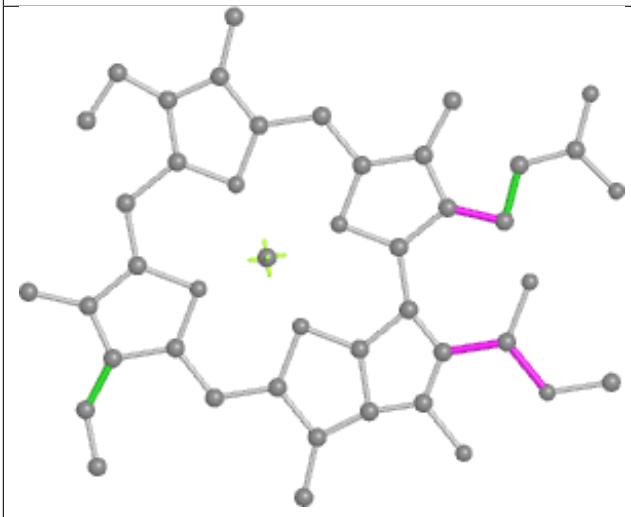
Ligand CLA K 1401



Bond lengths



Bond angles



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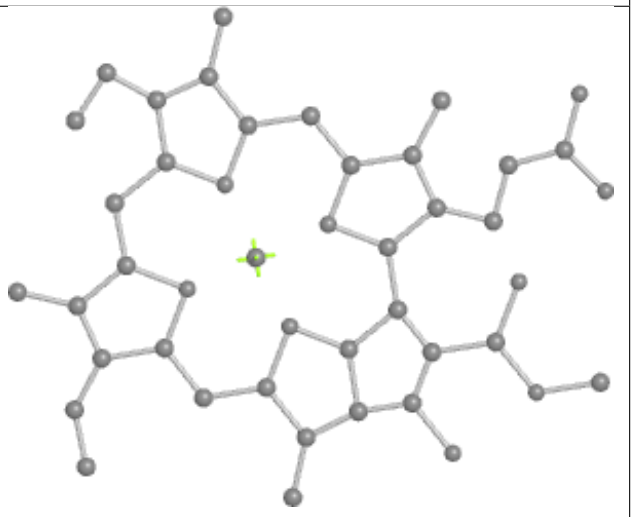
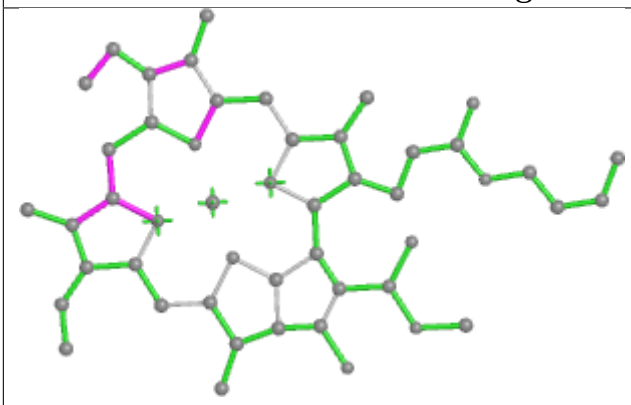


Rings

Ligand CLA B 1227



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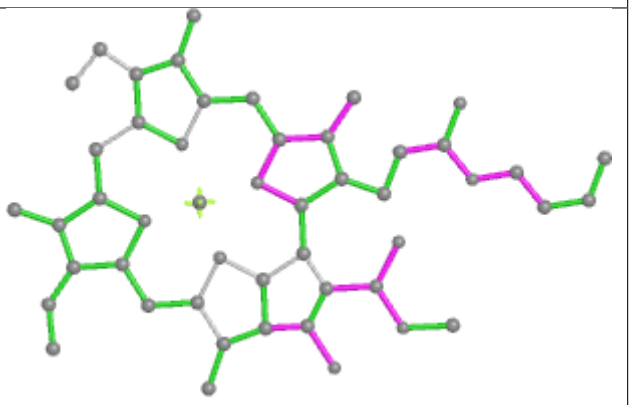
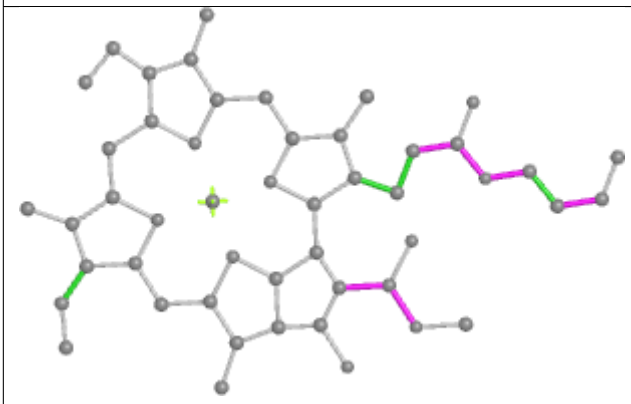


Bond angles



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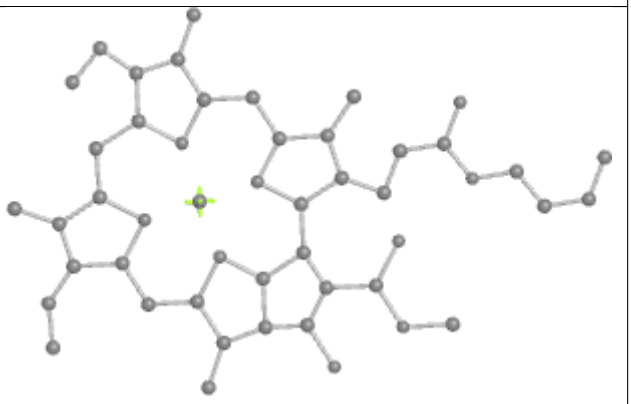
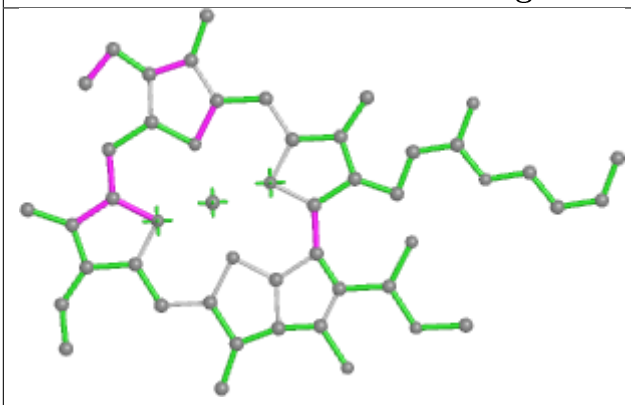


Rings

Ligand CLA B 1240



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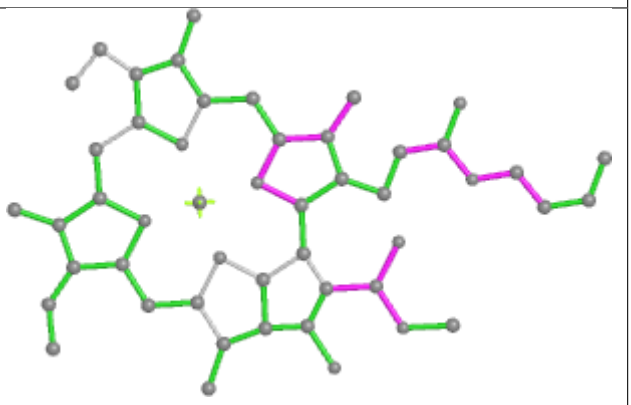
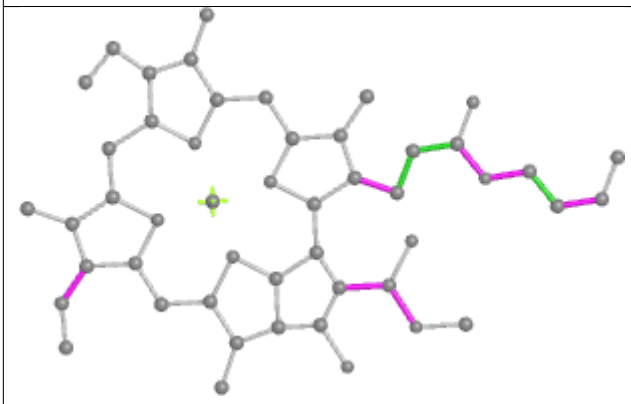


Bond angles



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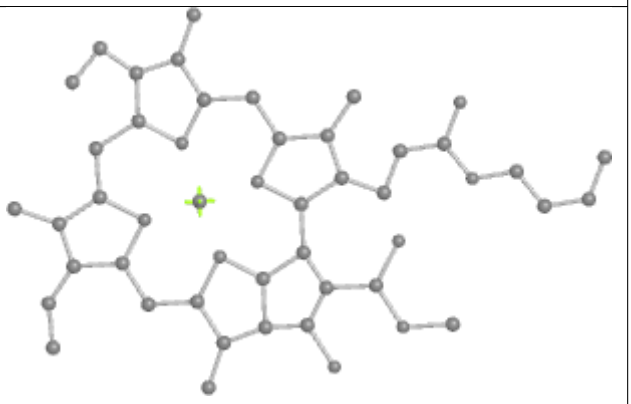
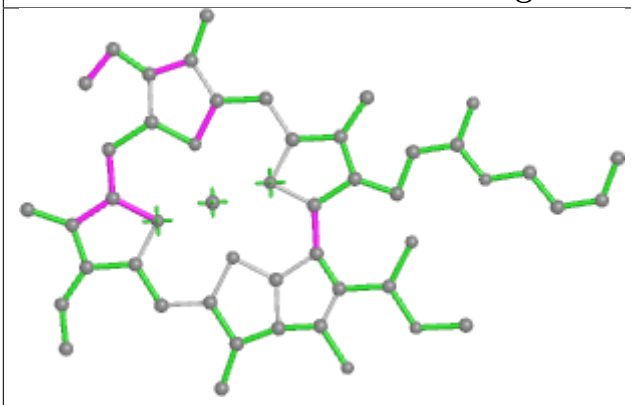
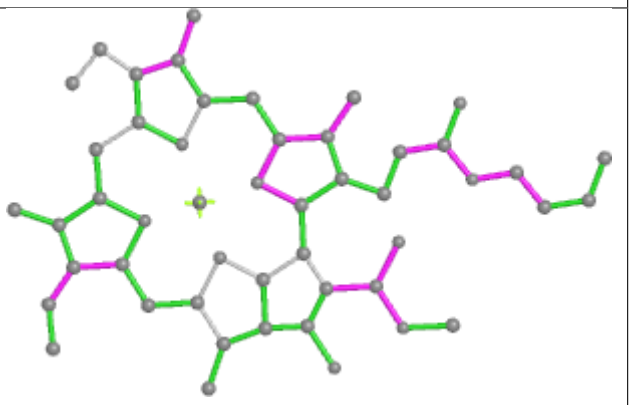
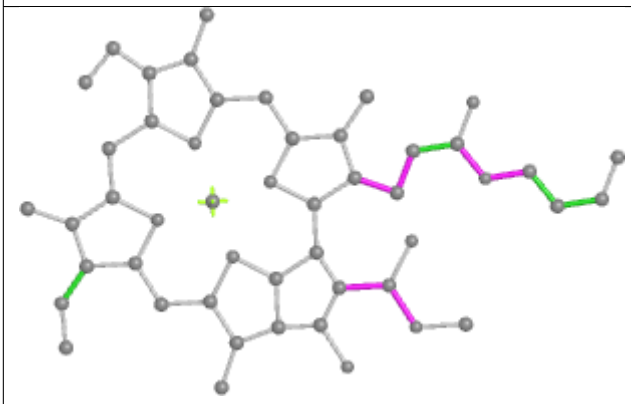
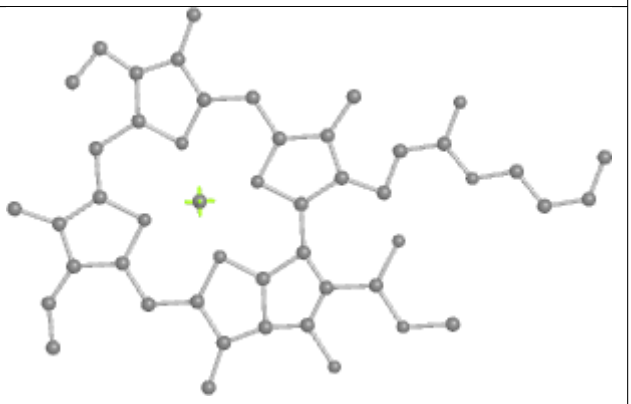
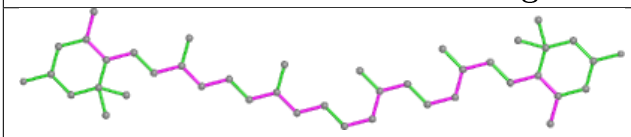
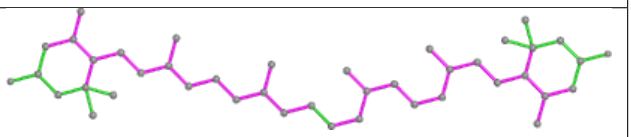
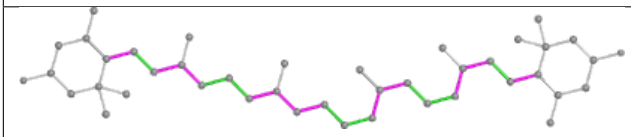
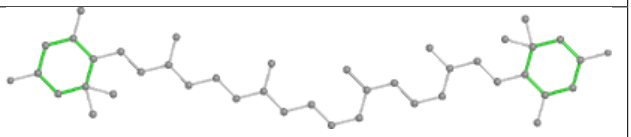
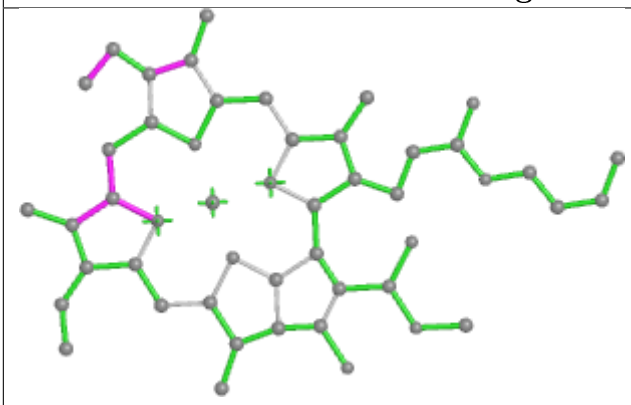


Rings

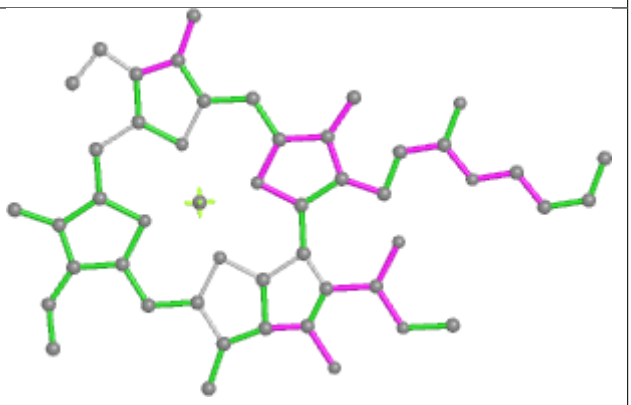
Ligand CLA A 1120	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand C7Z F 4016	
 Bond lengths	 Bond angles
 Torsions	 Rings

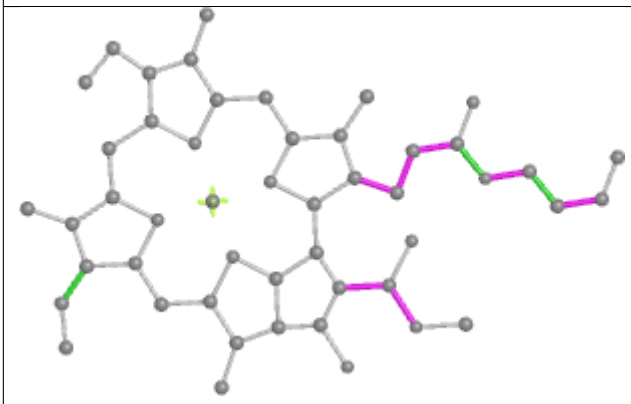
Ligand CLA A 1125



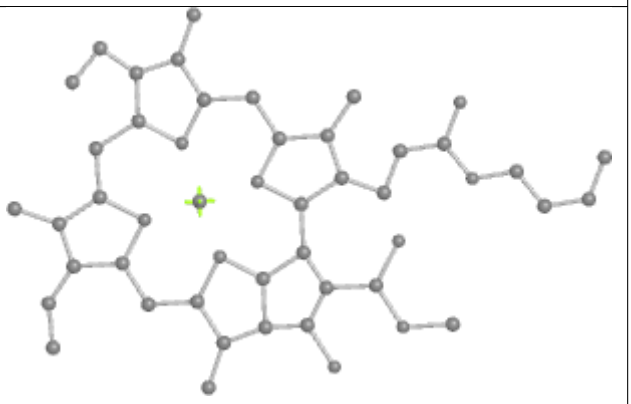
Bond lengths



Bond angles

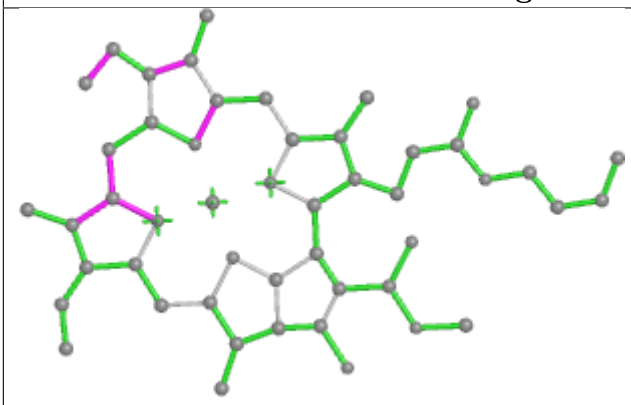


Torsions



Rings

Ligand CLA A 1117



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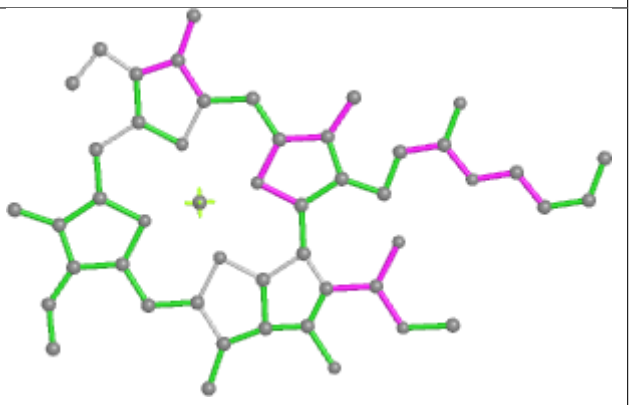
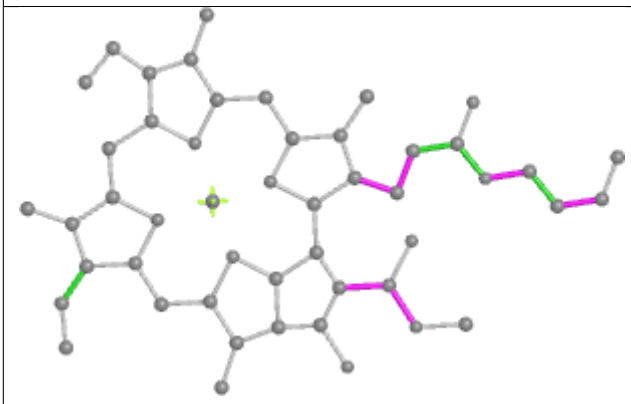


Bond angles



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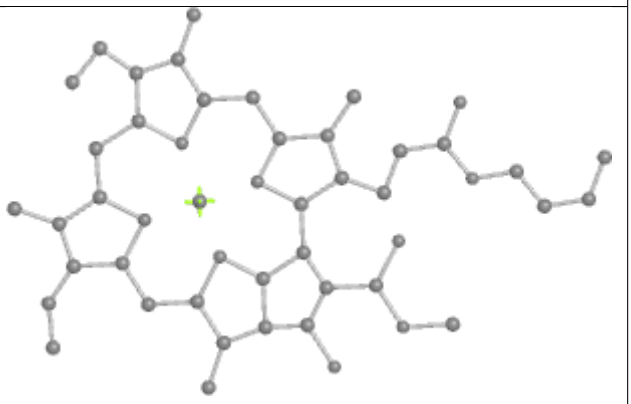
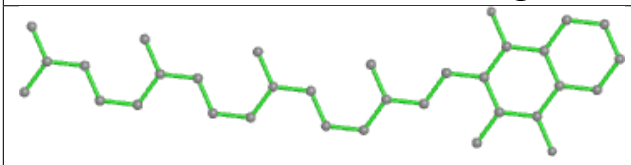
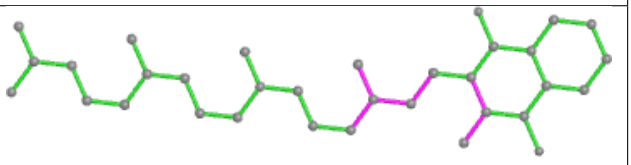


Rings

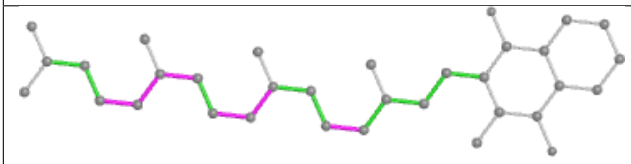
Ligand PQN A 2001



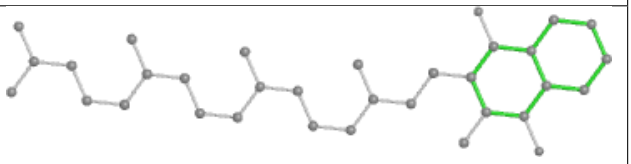
Bond lengths



Bond angles

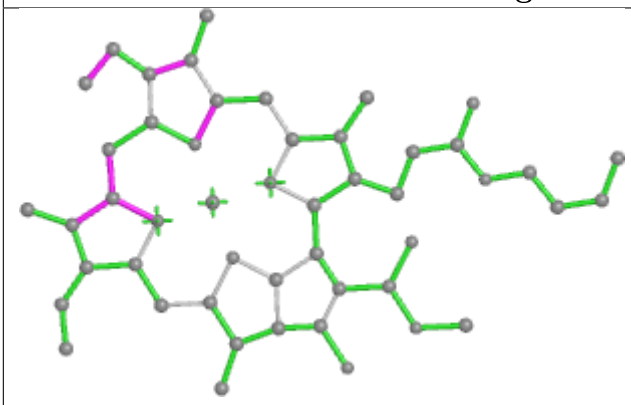


Torsions



Rings

Ligand CLA A 1110



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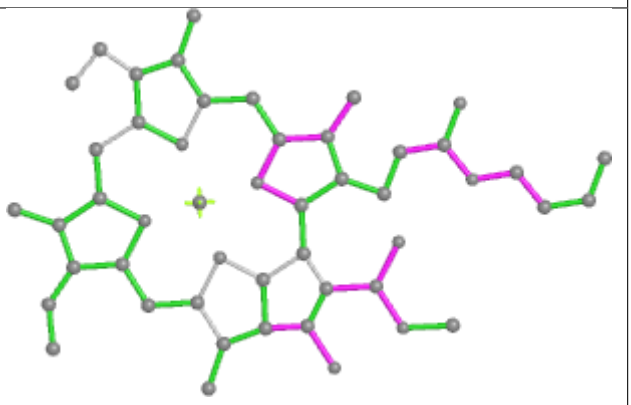
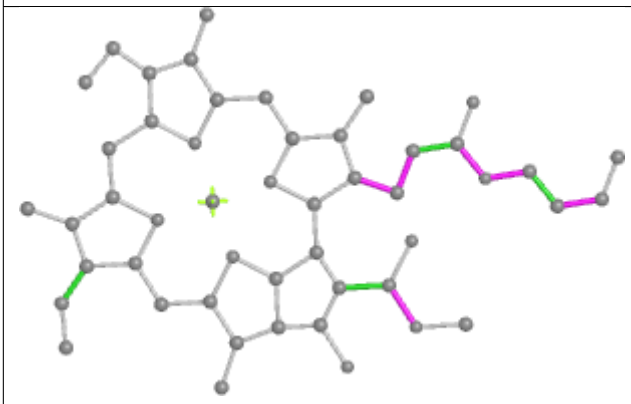


Bond angles



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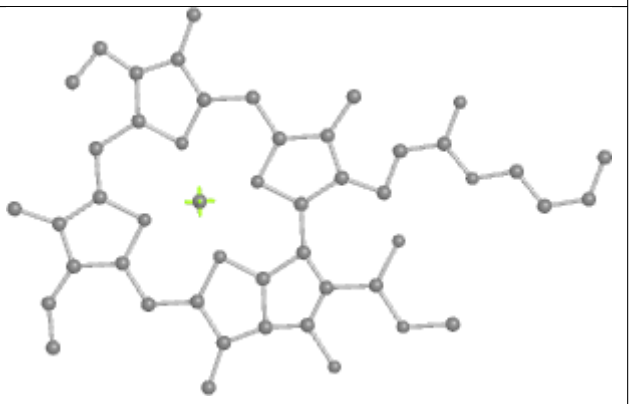
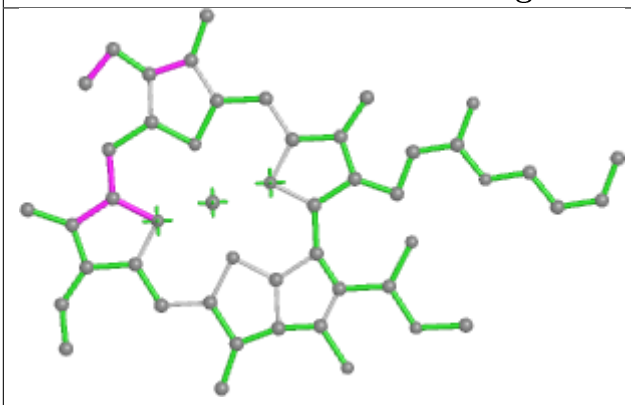


Rings

Ligand CLA B 1211



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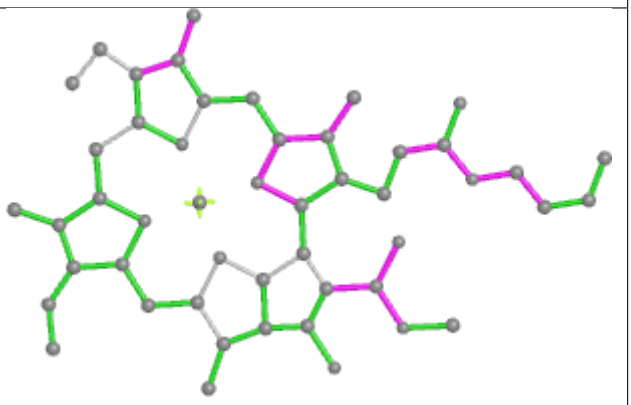
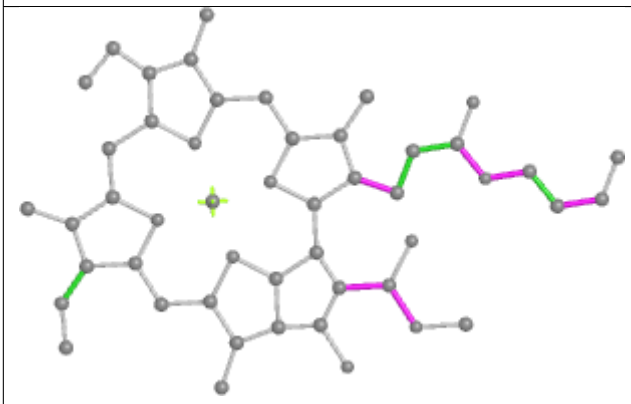


Bond angles



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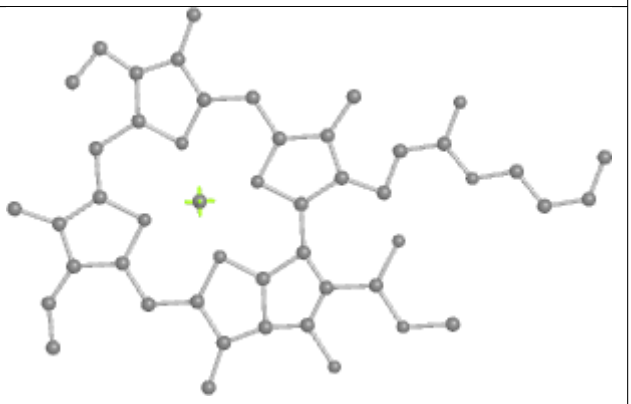
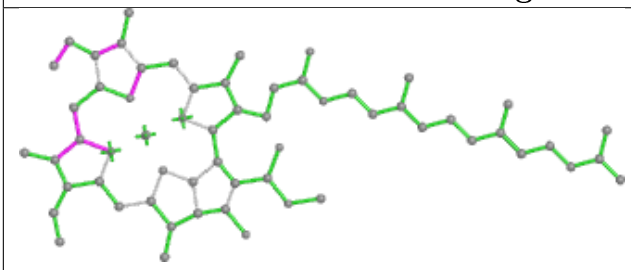


Rings

Ligand CLA B 1214



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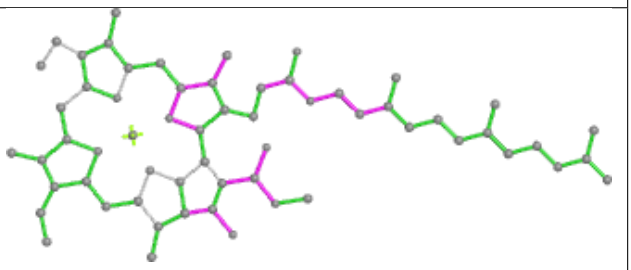
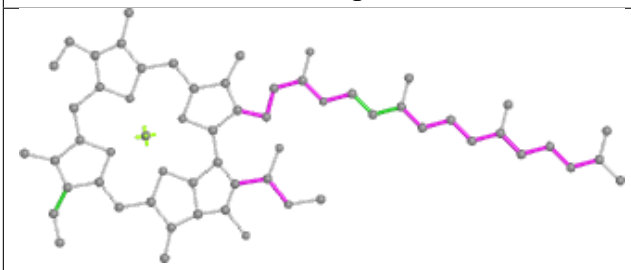
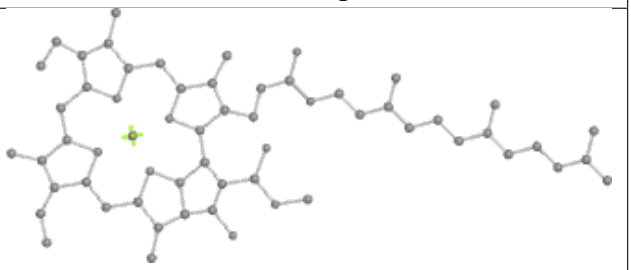


Bond angles

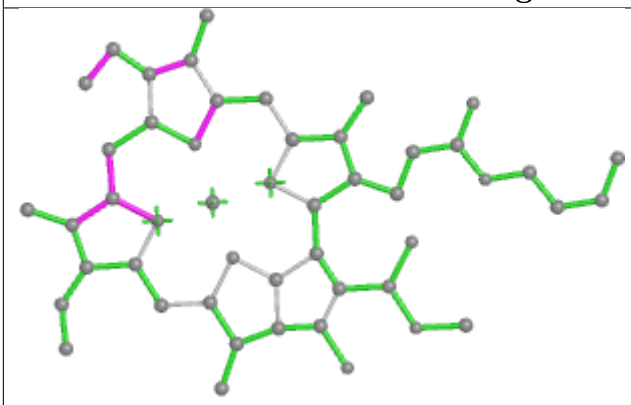


Torsions



Rings

Ligand CLA A 1131



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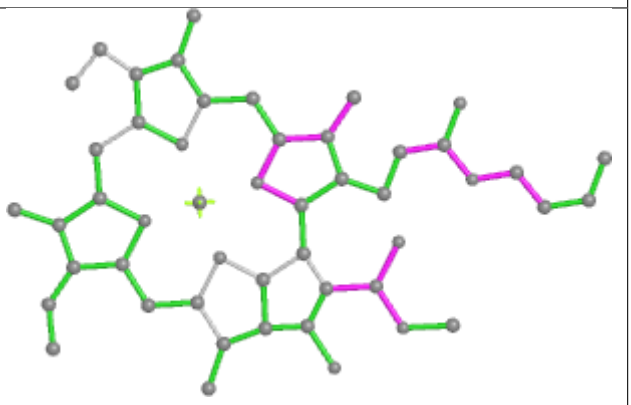
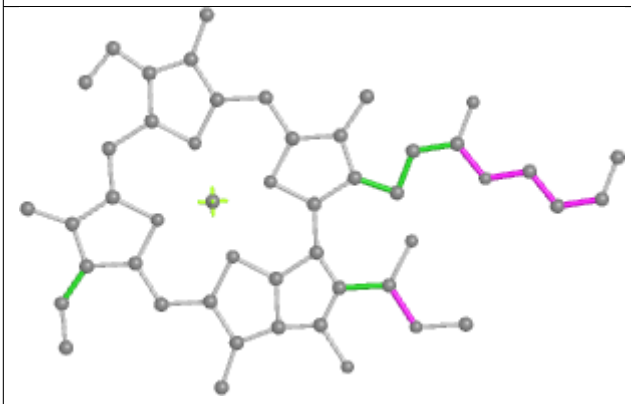
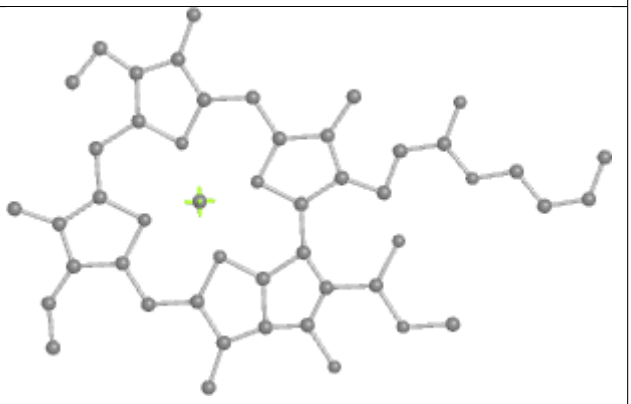


Bond angles

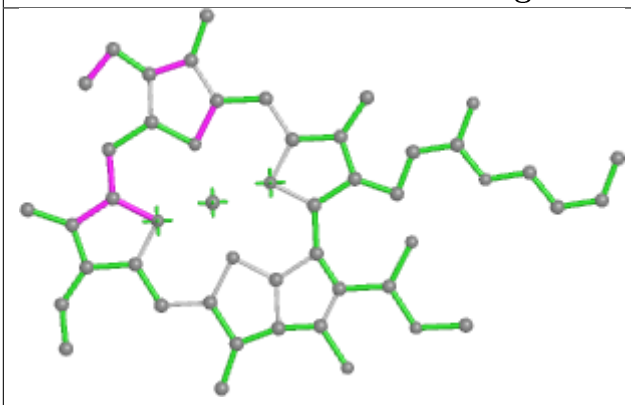


Torsions



Rings

Ligand CLA K 1402



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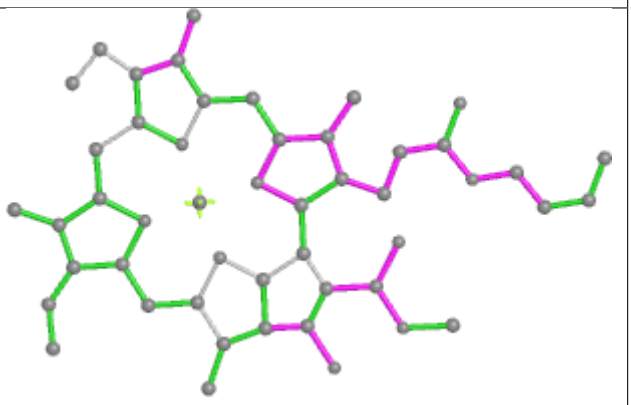
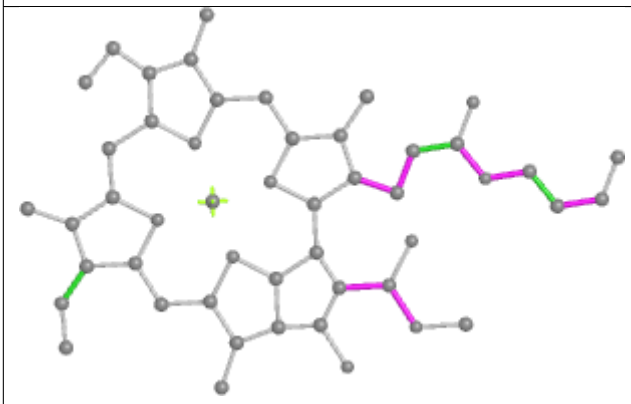
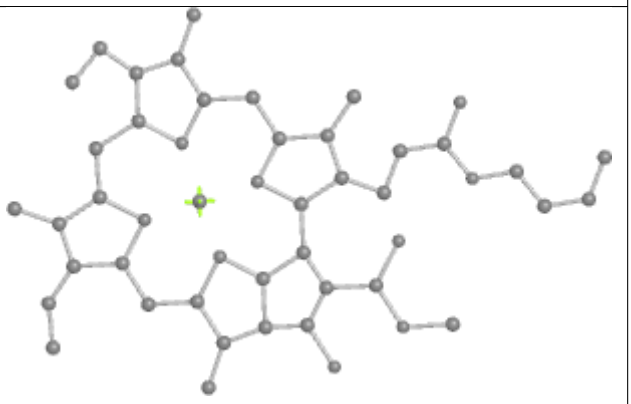


Bond angles

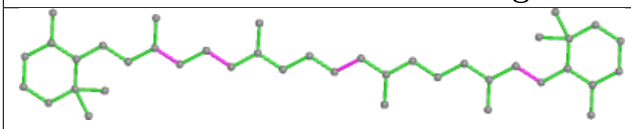


Torsions

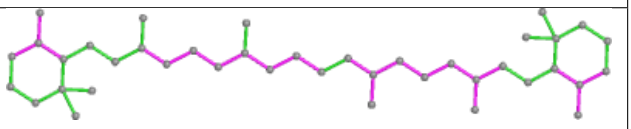


Rings

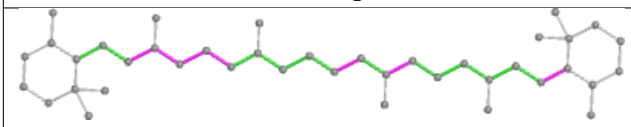
Ligand BCR K 4001



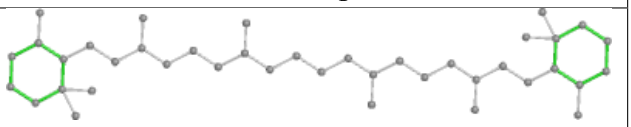
Bond lengths



Bond angles

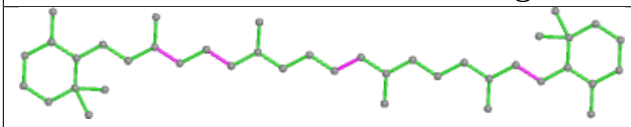


Torsions

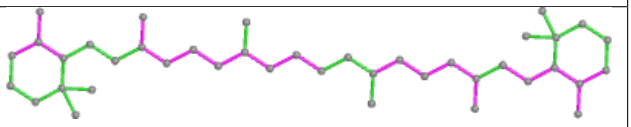


Rings

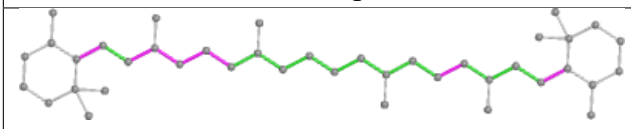
Ligand BCR B 4004



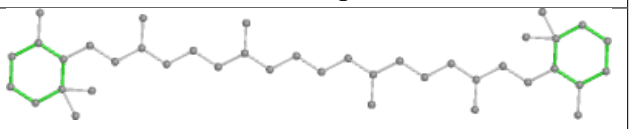
Bond lengths



Bond angles

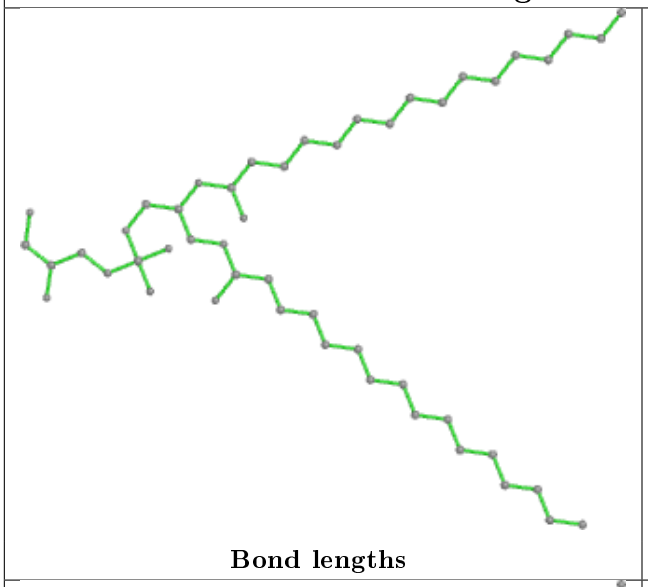


Torsions



Rings

Ligand LHG A 5001



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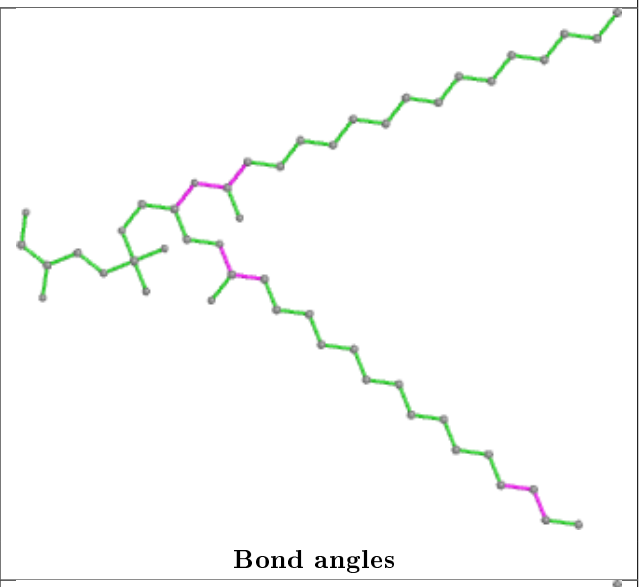
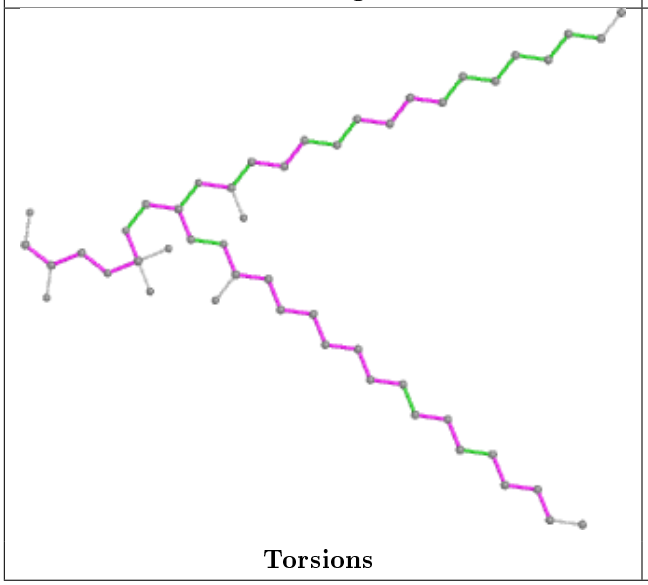
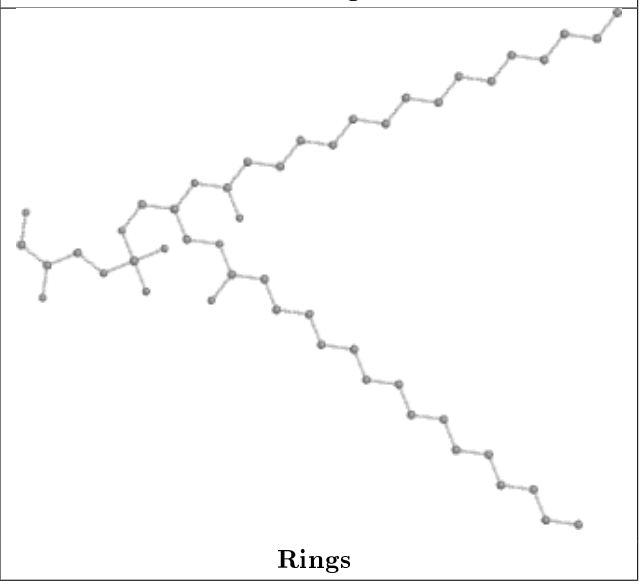


Bond angles

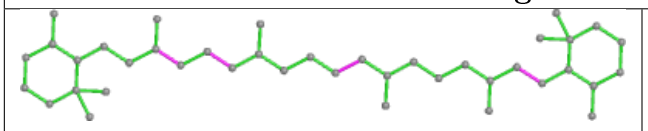


Torsions



Rings

Ligand BCR A 4012



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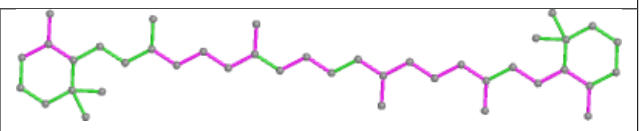
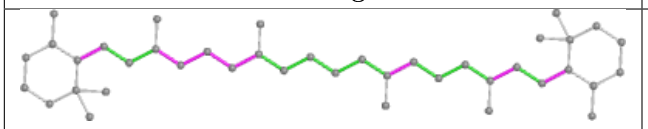
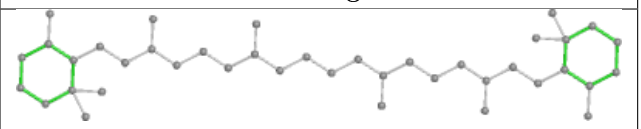


Bond angles

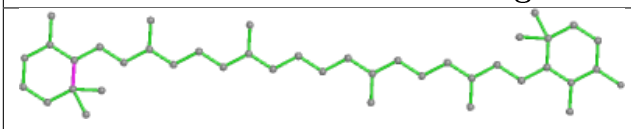


Torsions



Rings

Ligand ECH B 4006



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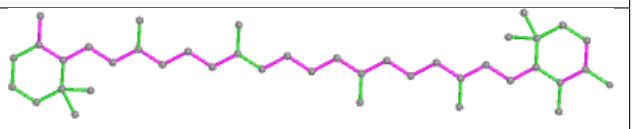
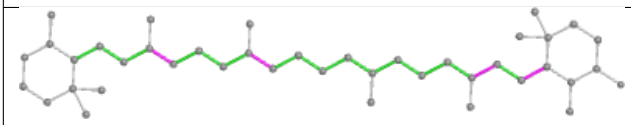


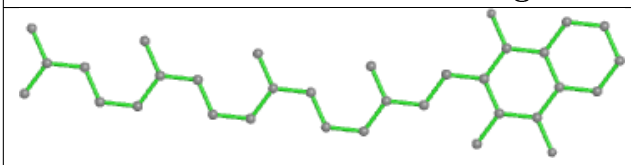
Bond angles



Torsions

Rings

Ligand PQN B 2002



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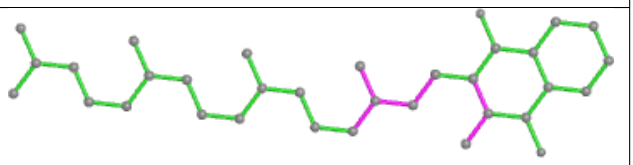
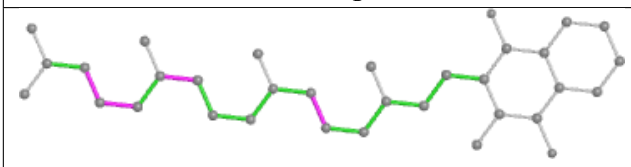
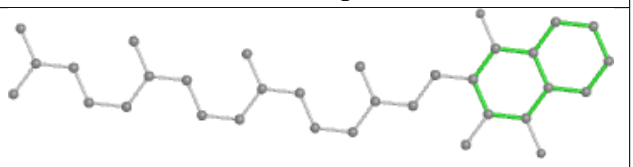


Bond angles

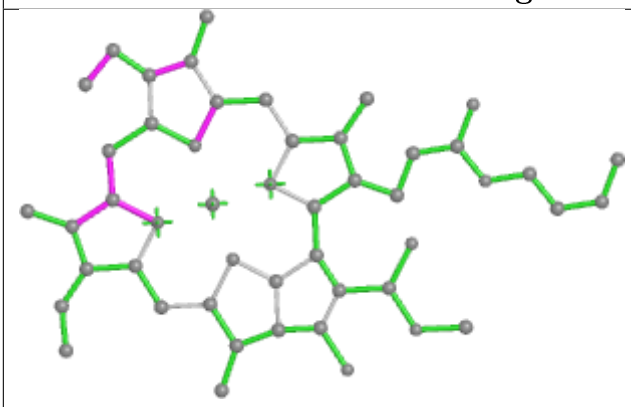


Torsions



Rings

Ligand CLA B 1219



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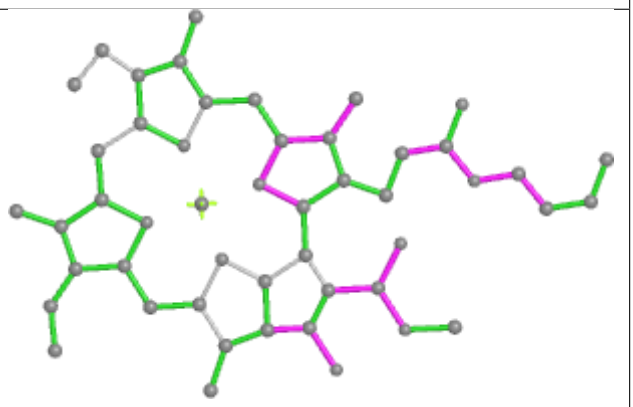
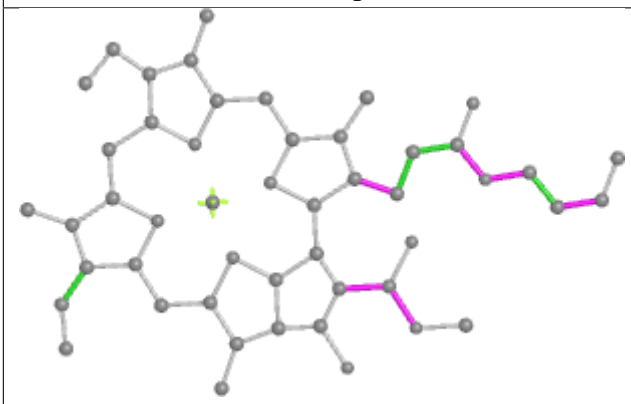


Bond angles



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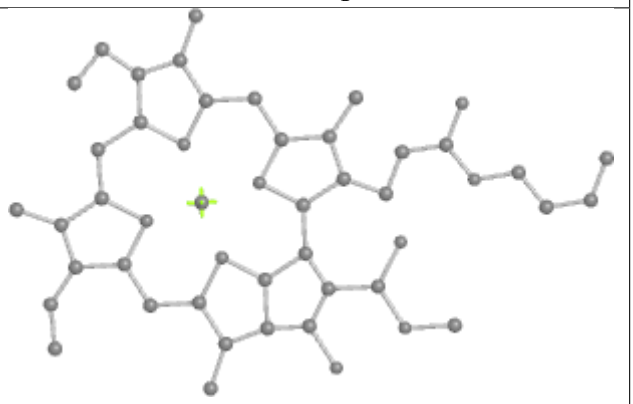
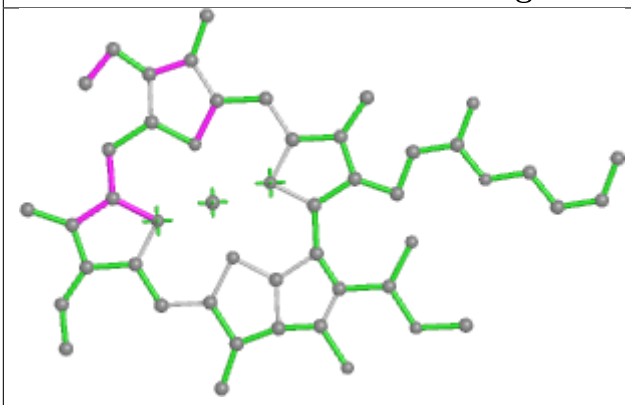


Rings

Ligand CLA B 1218



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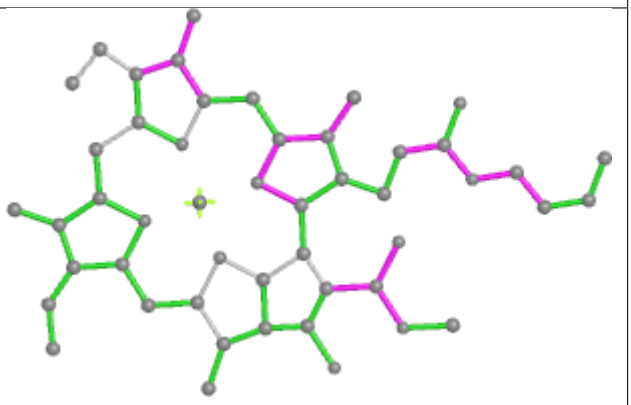
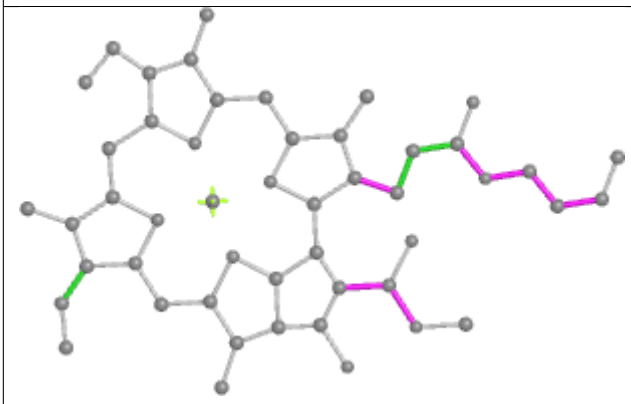


Bond angles



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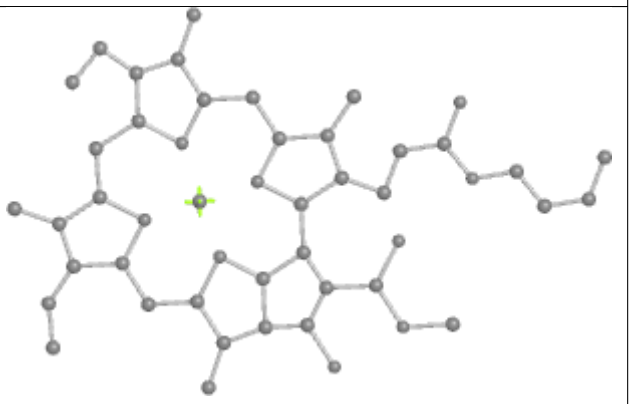
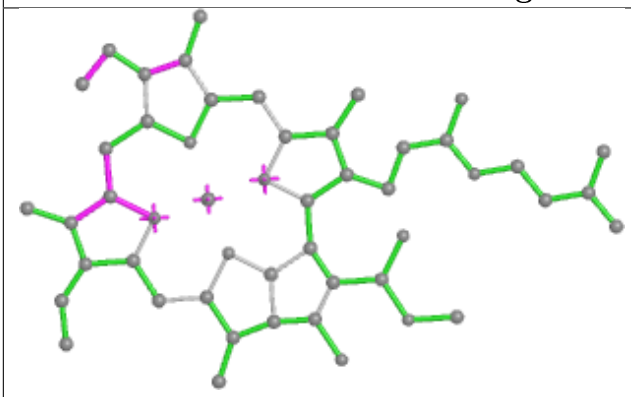


Rings

Ligand CLA A 1107



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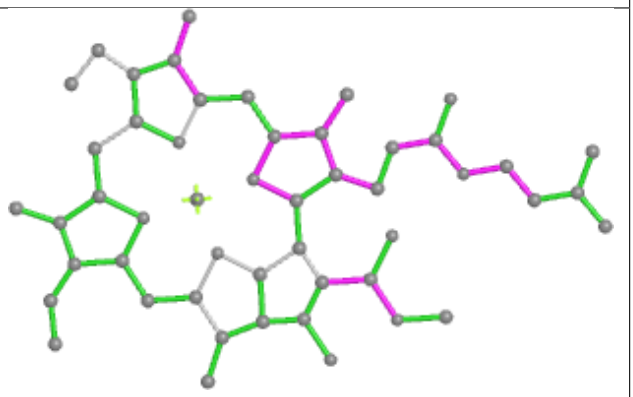
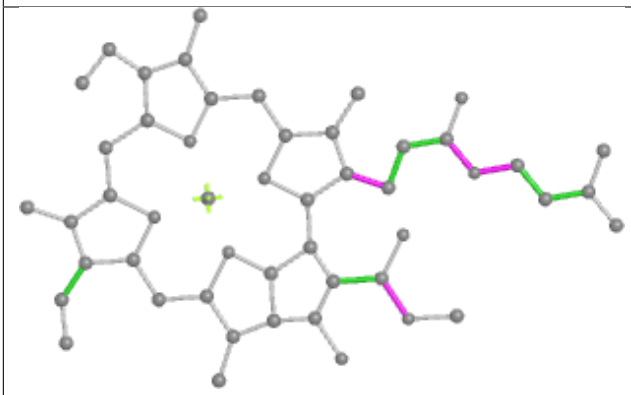
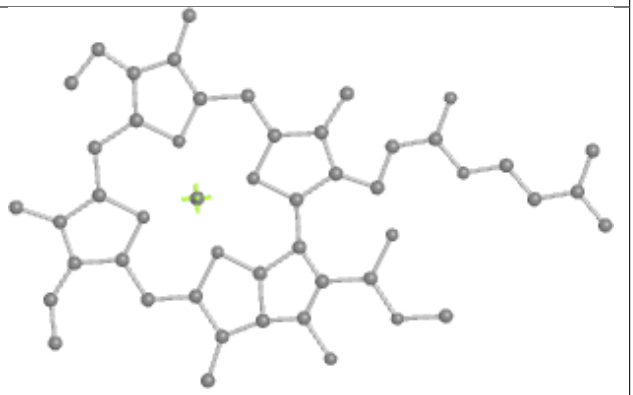


Bond angles

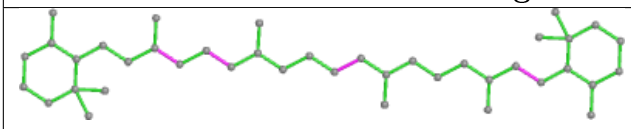


Torsions



Rings

Ligand BCR A 4007



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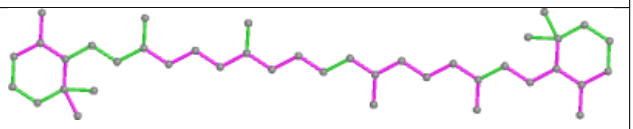
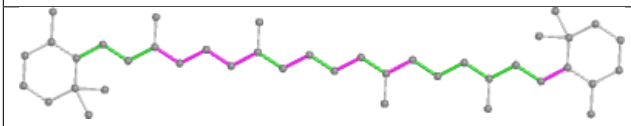
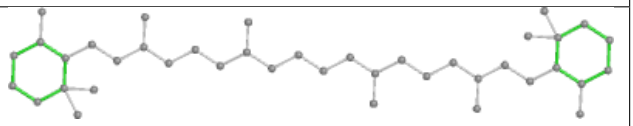


Bond angles

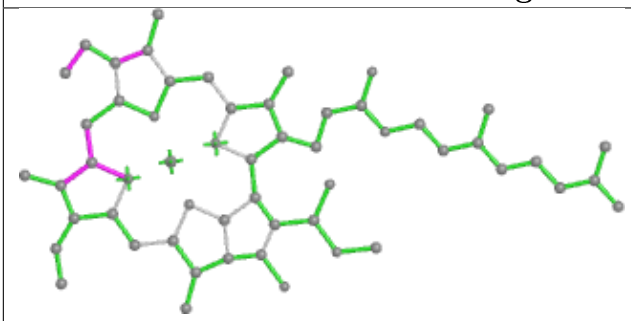


Torsions



Rings

Ligand CLA B 1224



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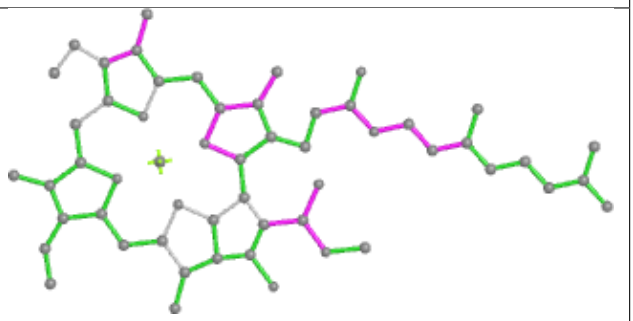
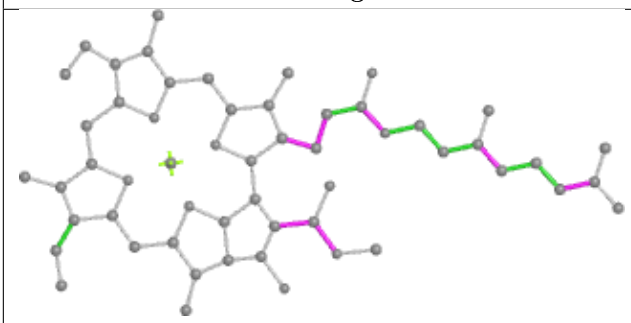
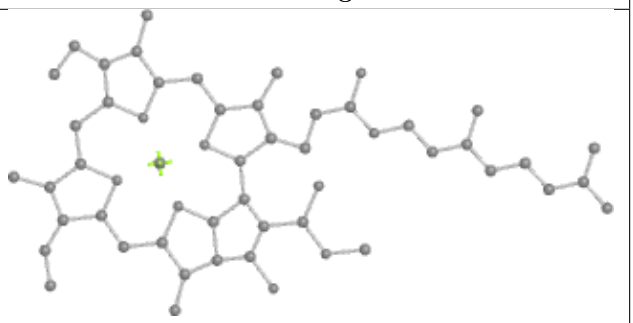


Bond angles

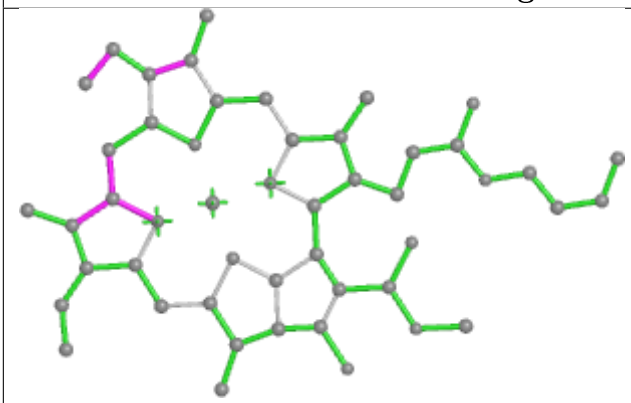


Torsions



Rings

Ligand CLA F 1302



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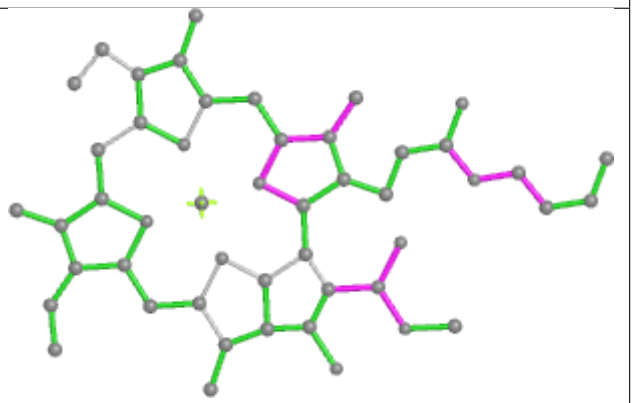
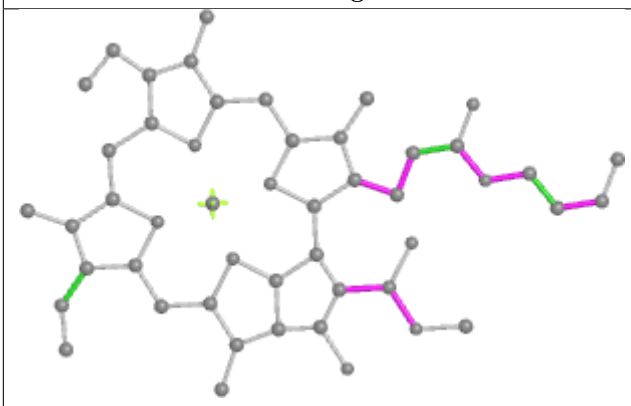
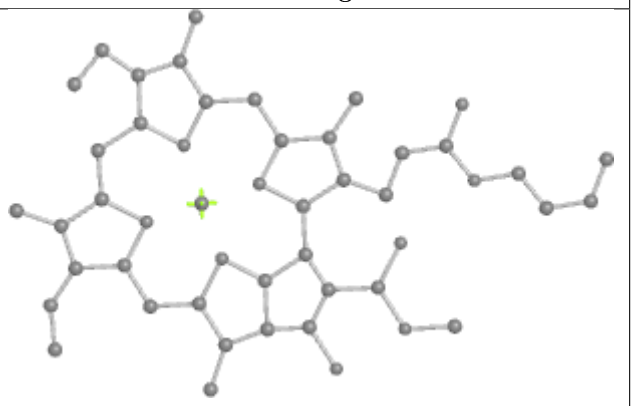


Bond angles

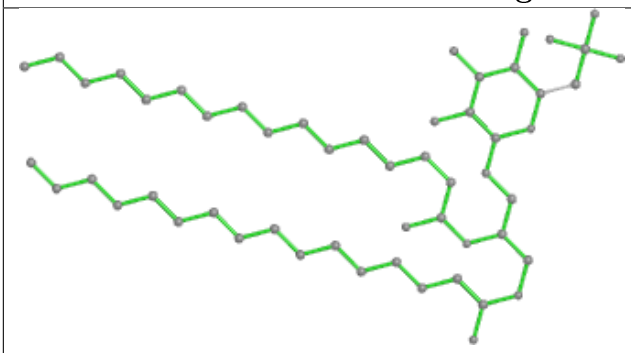


Torsions



Rings

Ligand SQD B 5008



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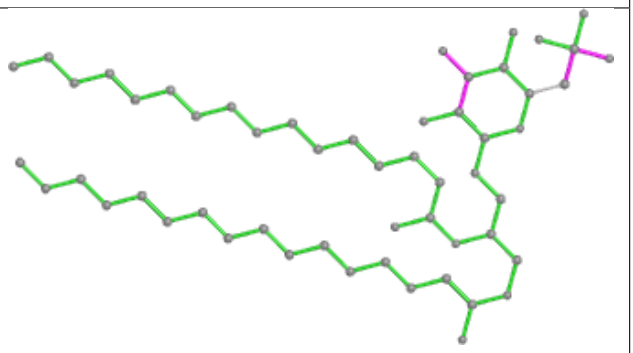
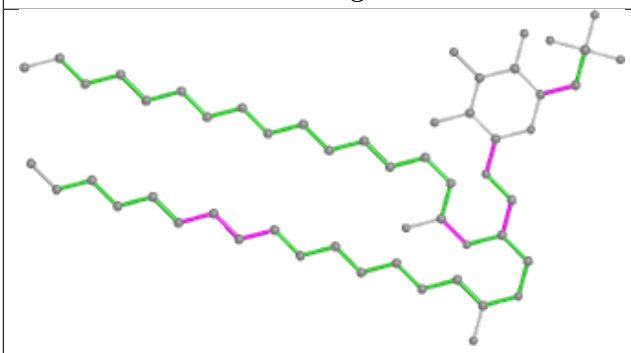
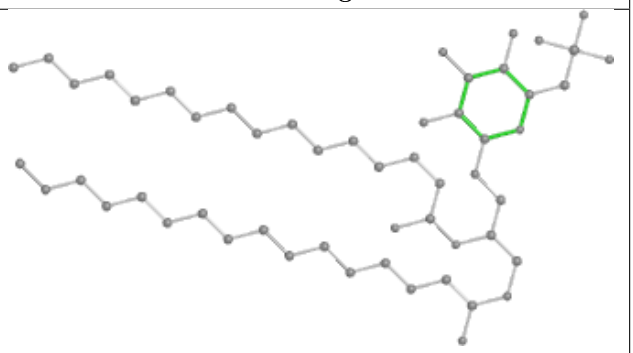


Bond angles

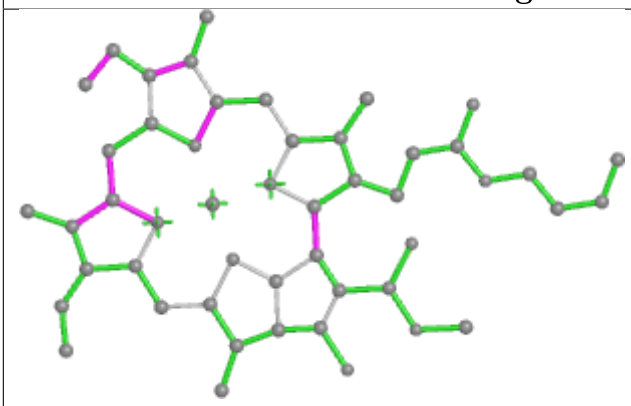


Torsions

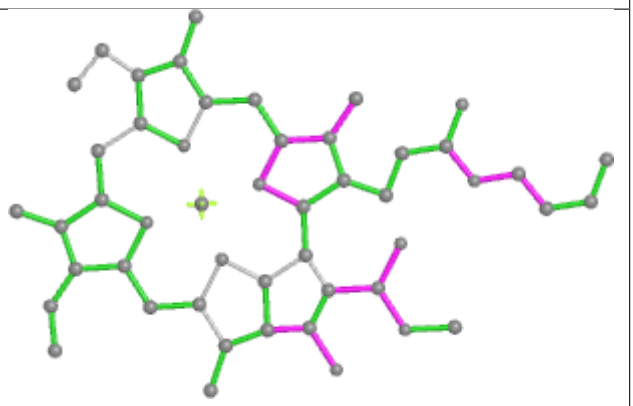


Rings

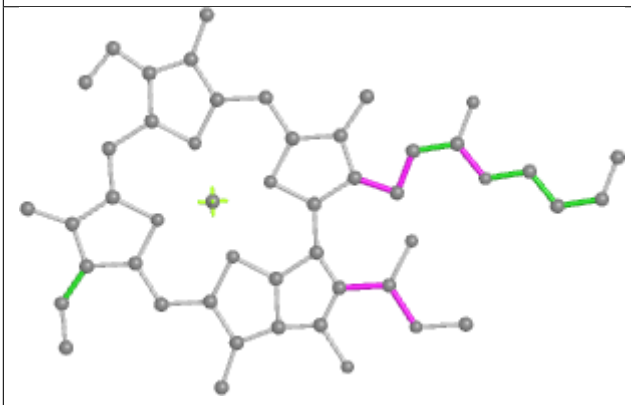
Ligand CLA A 1122



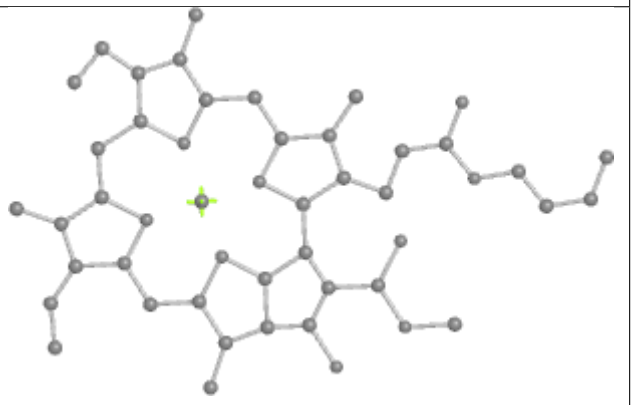
Bond lengths



Bond angles

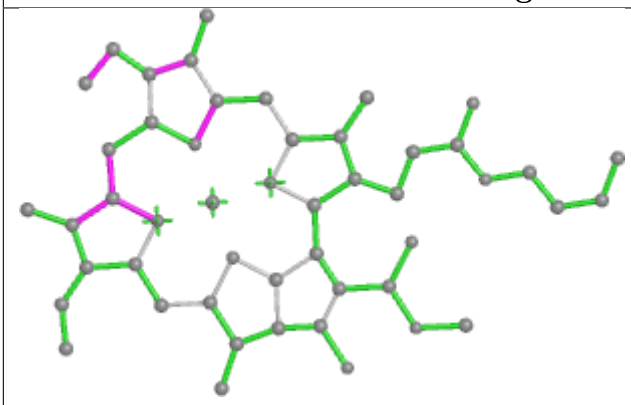


Torsions

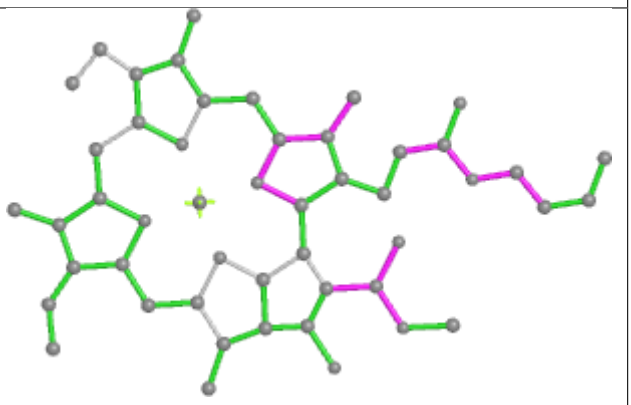


Rings

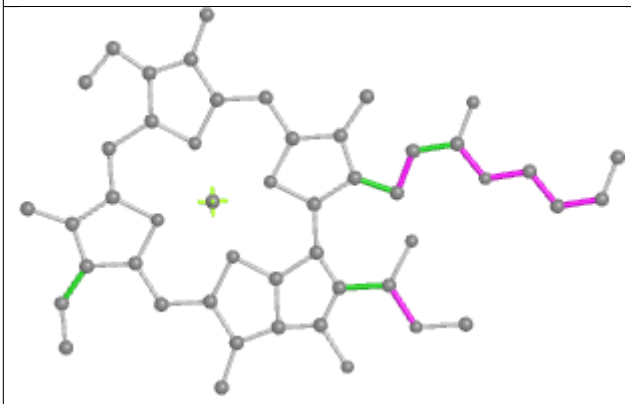
Ligand CLA B 1208



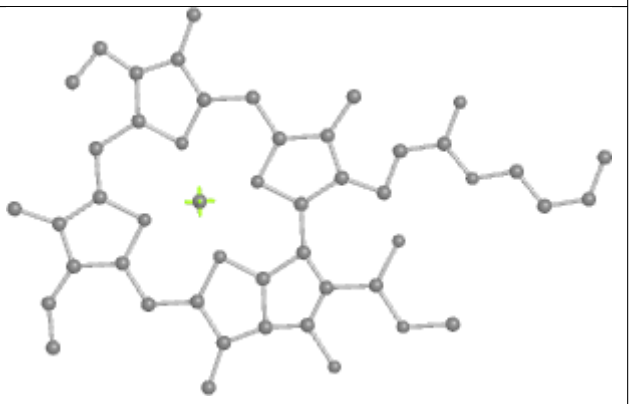
Bond lengths



Bond angles

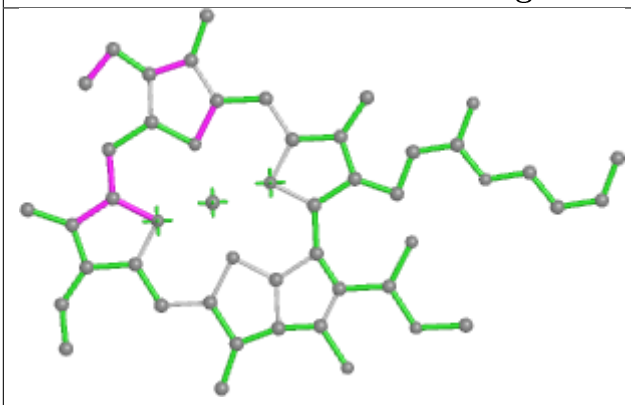


Torsions

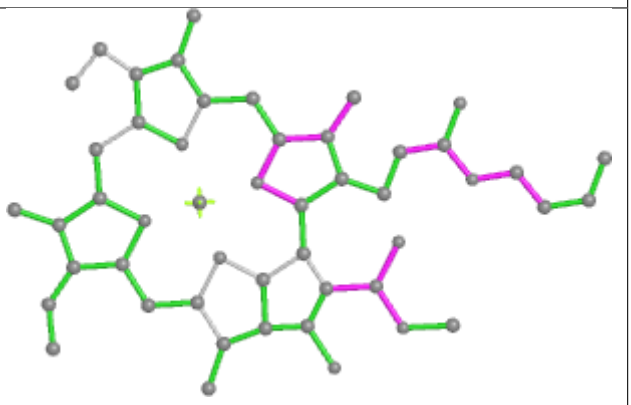


Rings

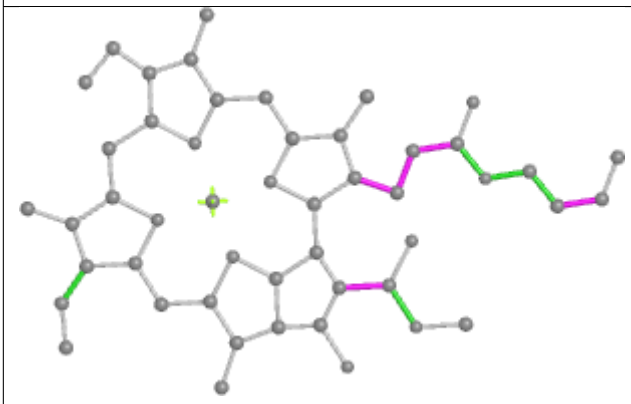
Ligand CLA B 1204



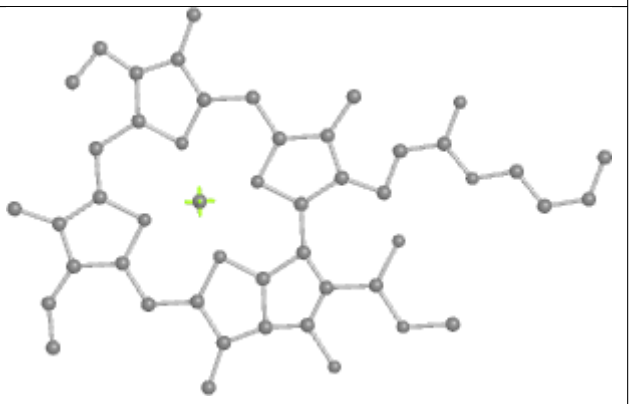
Bond lengths



Bond angles

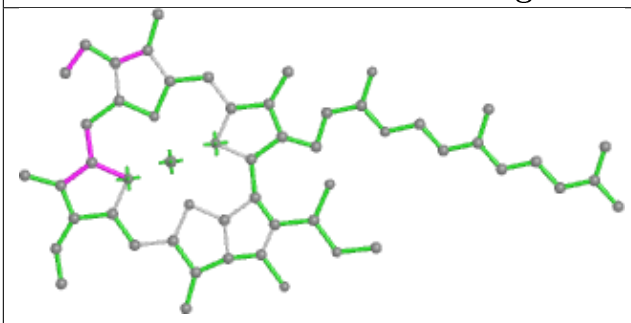


Torsions



Rings

Ligand CLA A 1011



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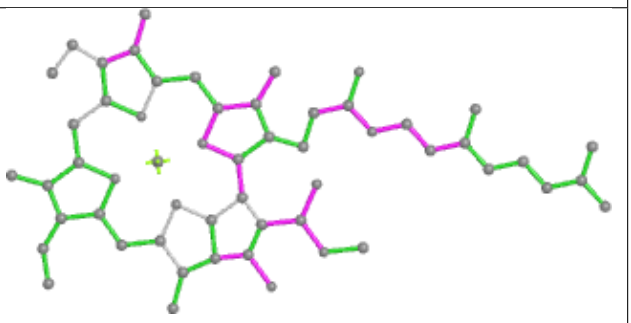
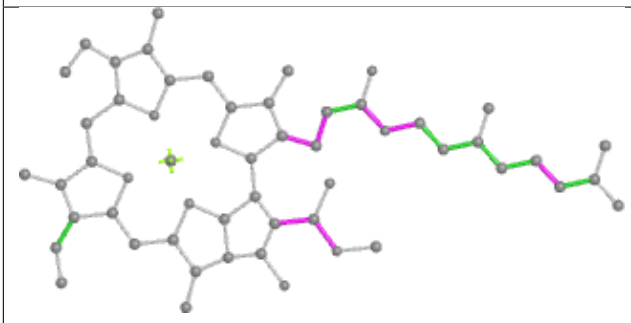


Bond angles



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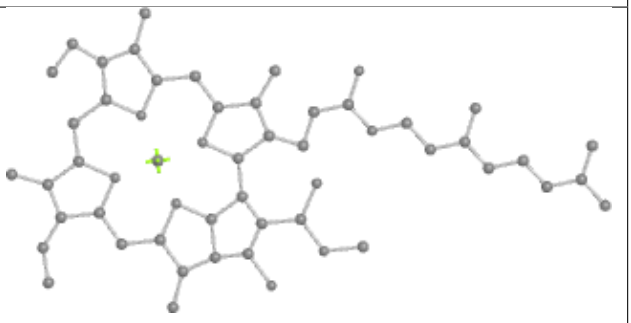
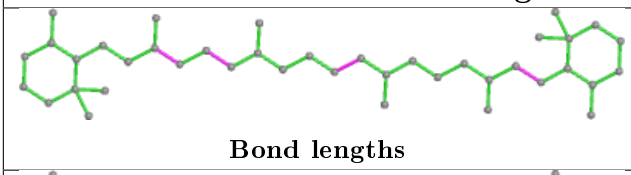


Rings

Ligand BCR B 4017



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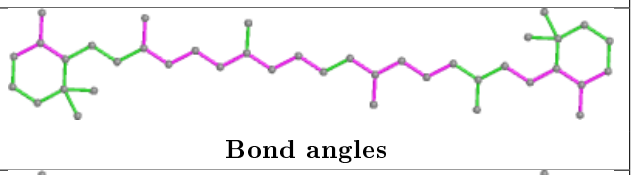
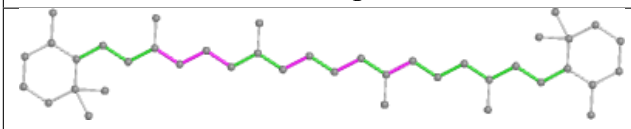


Bond angles



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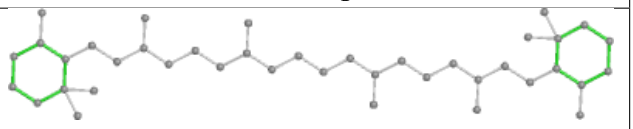
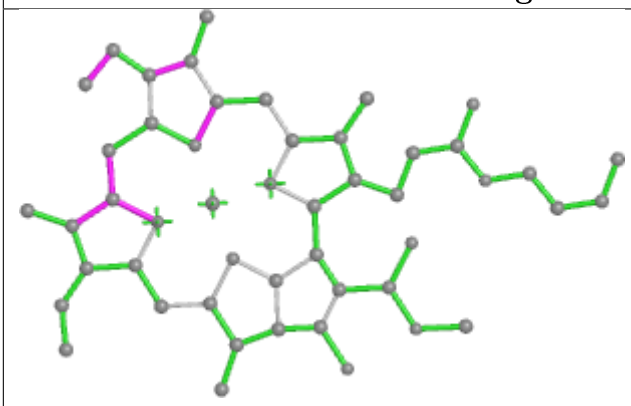


Rings

Ligand CLA B 1216



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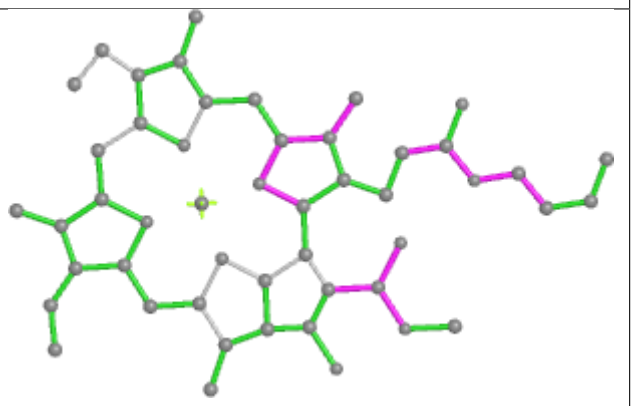
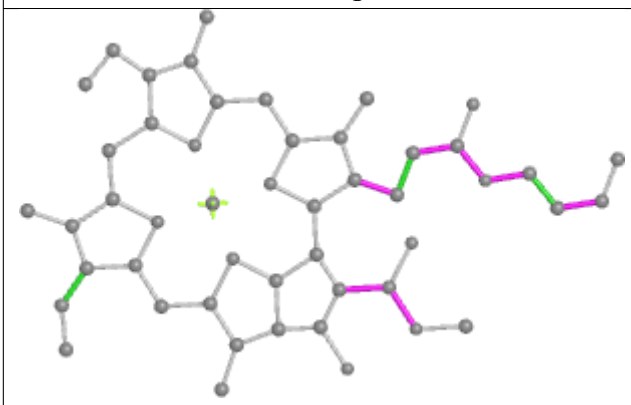


Bond angles



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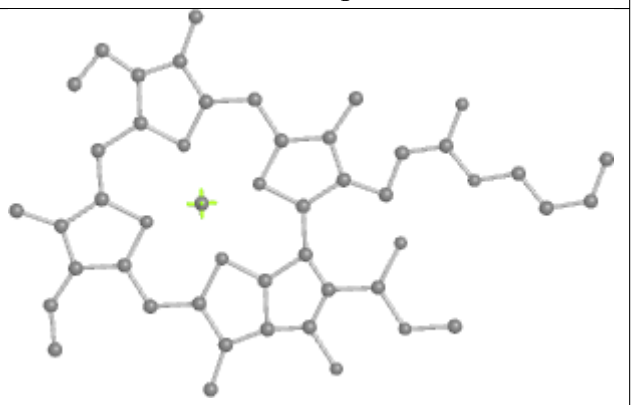
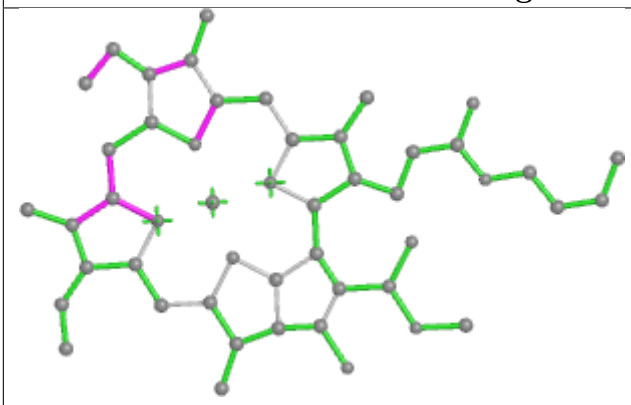


Rings

Ligand CLA A 1124



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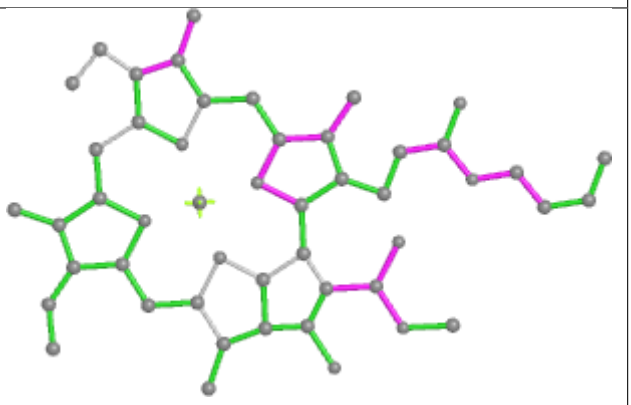

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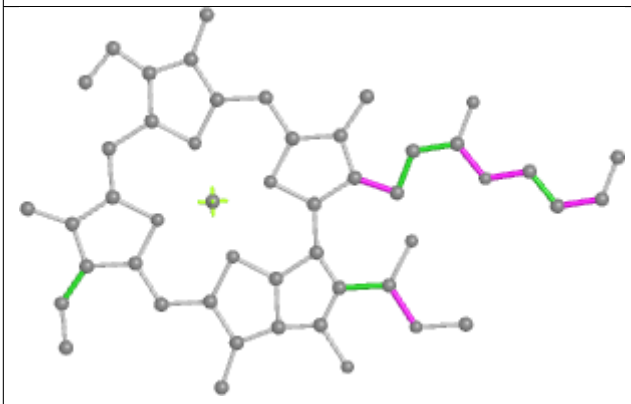

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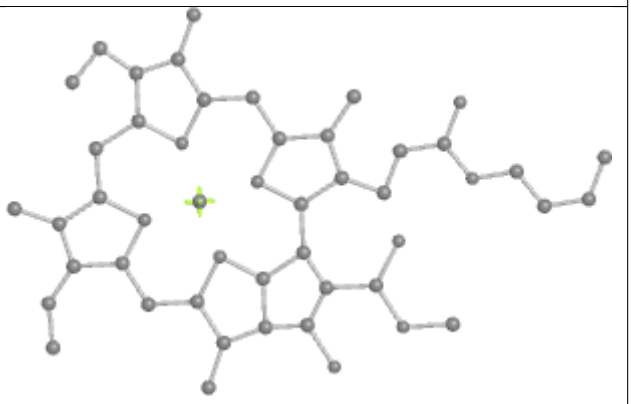
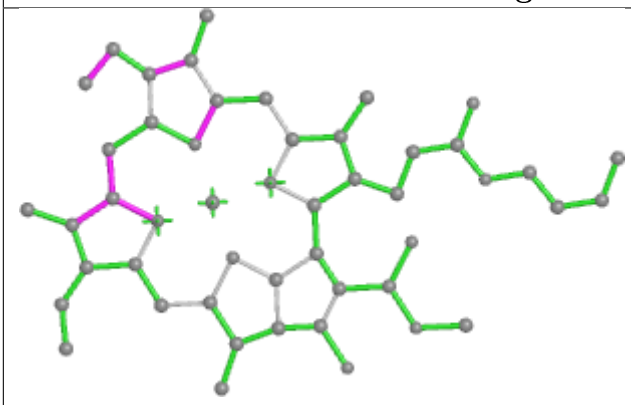


Rings

Ligand CLA A 1113



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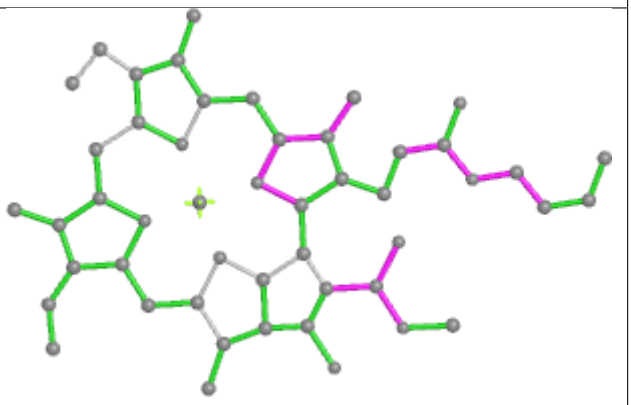
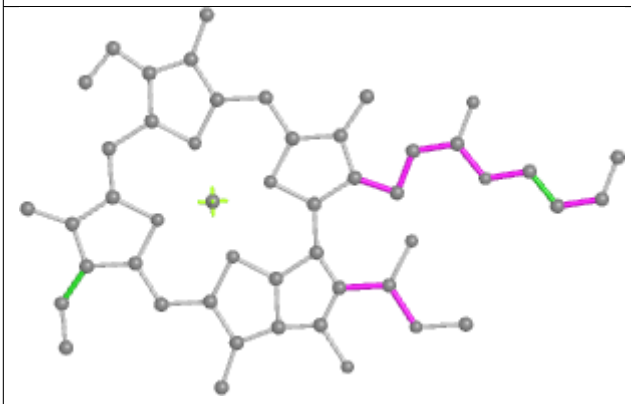


Bond angles



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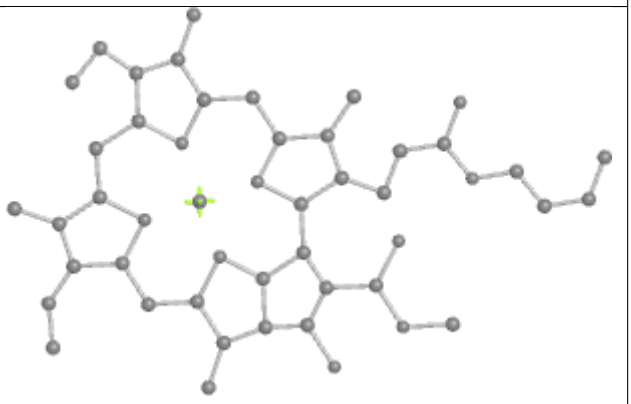
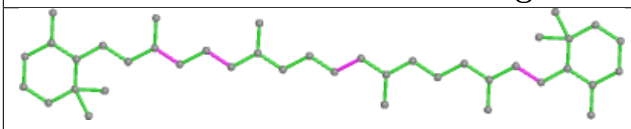


Rings

Ligand BCR F 4014



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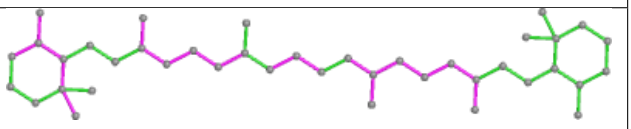
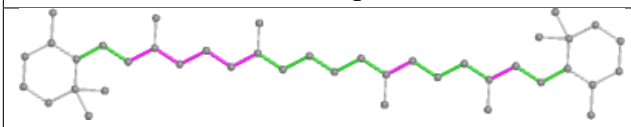


Bond angles



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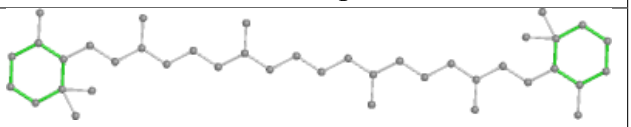
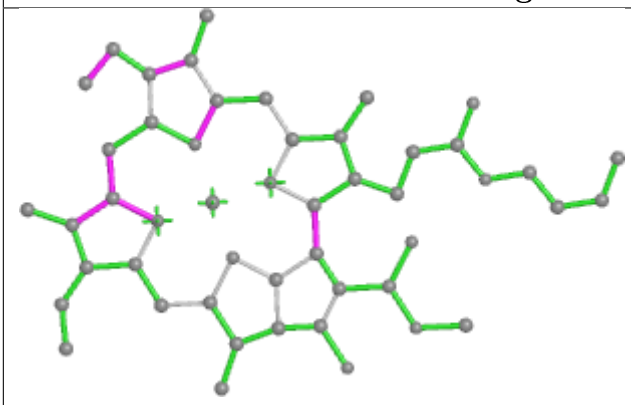


Rings

Ligand CLA B 1213



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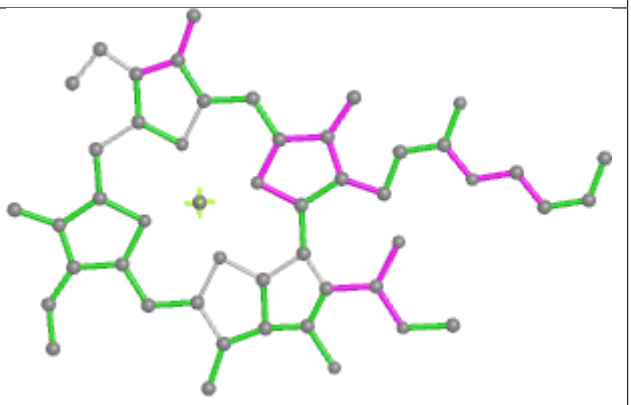
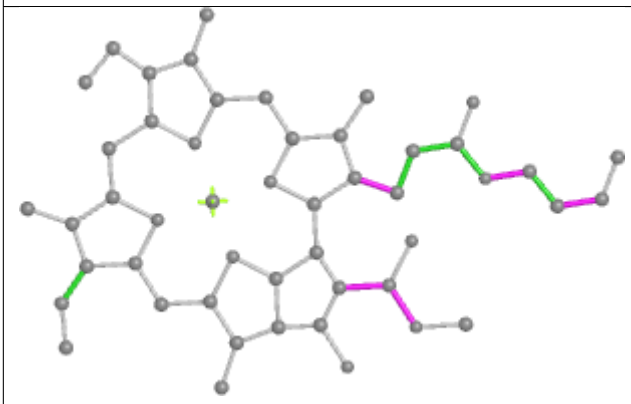
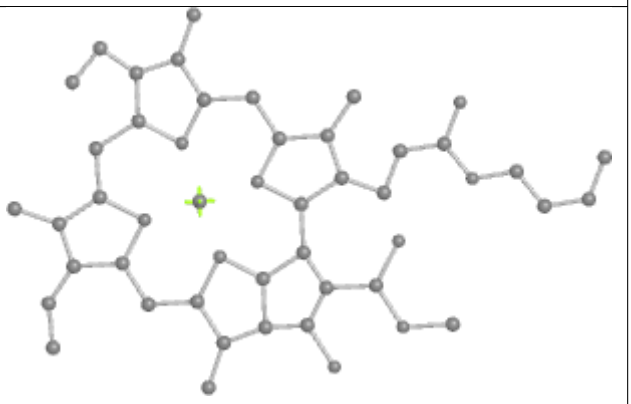


Bond angles

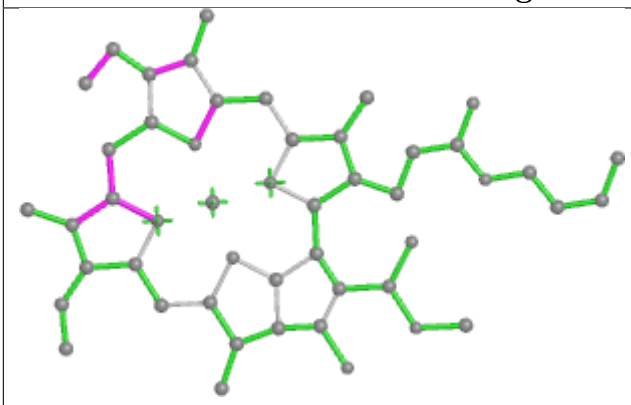


Torsions



Rings

Ligand CLA A 1134



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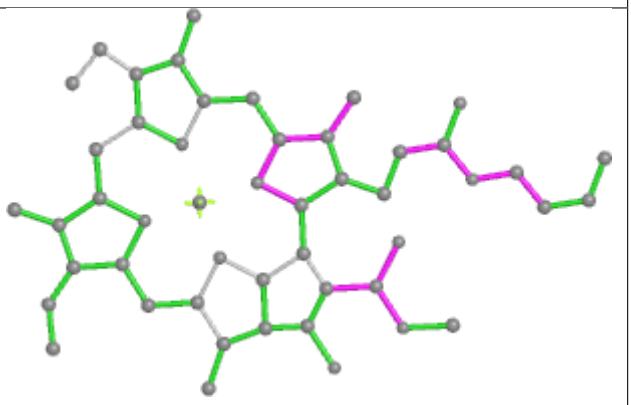
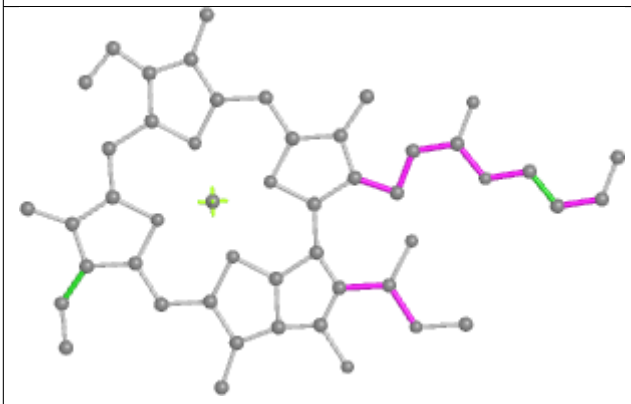
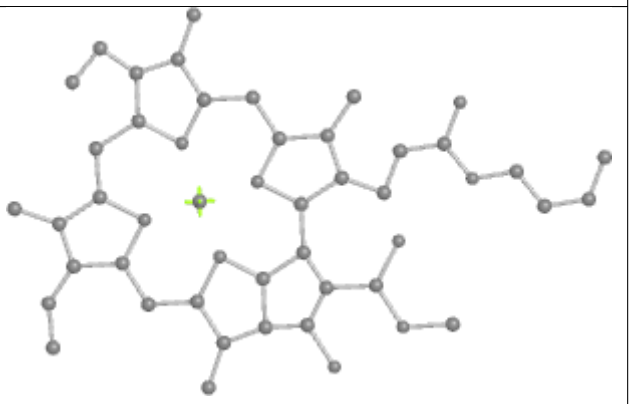


Bond angles

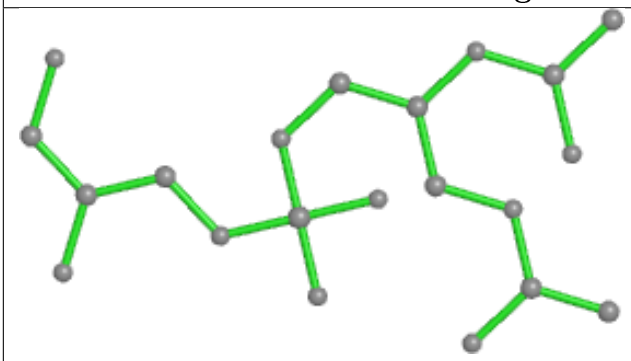


Torsions



Rings

Ligand LHG B 5006



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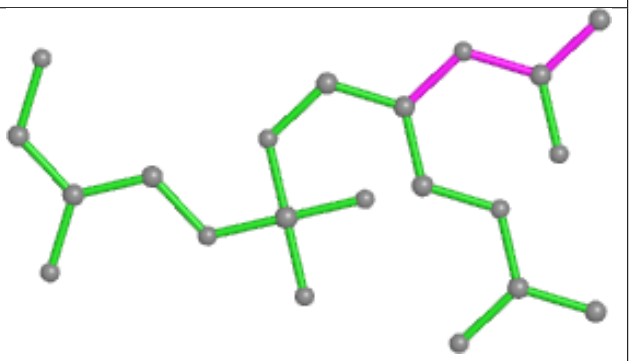
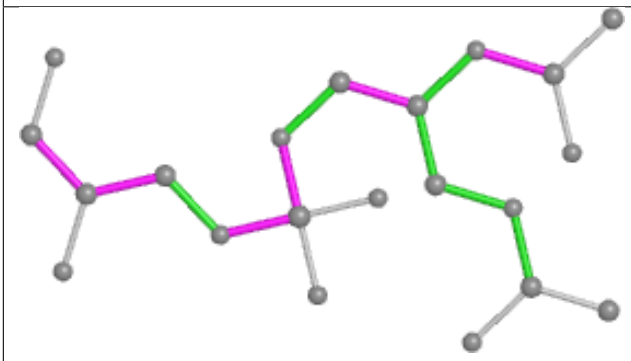


Bond angles



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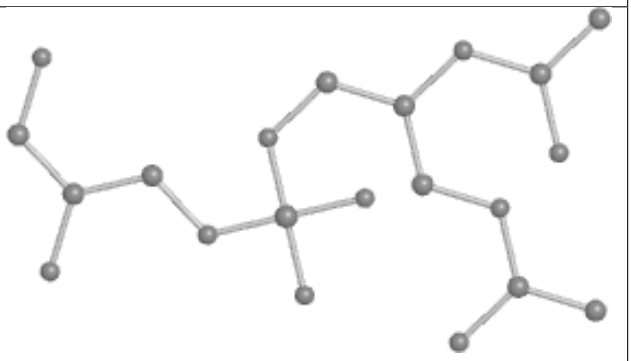
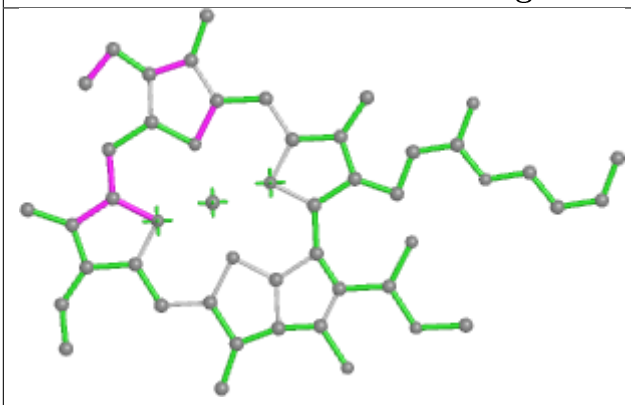


Rings

Ligand CLA B 1237



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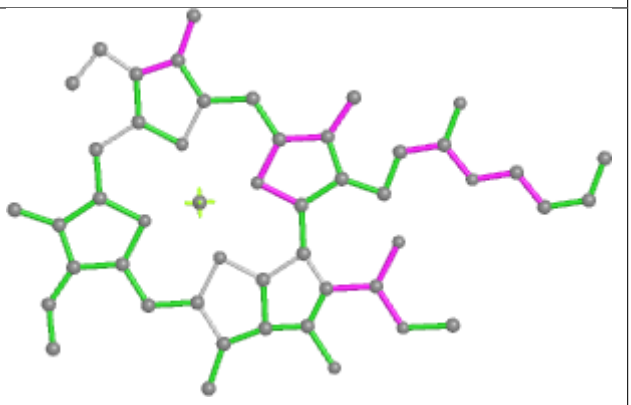
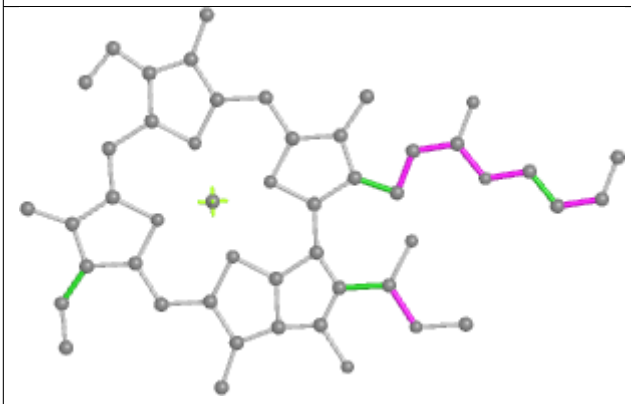


Bond angles



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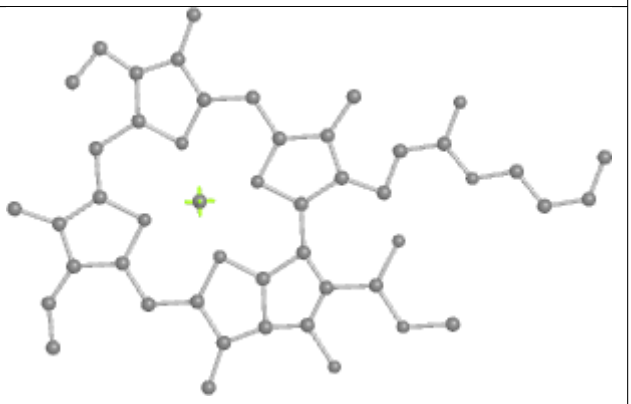
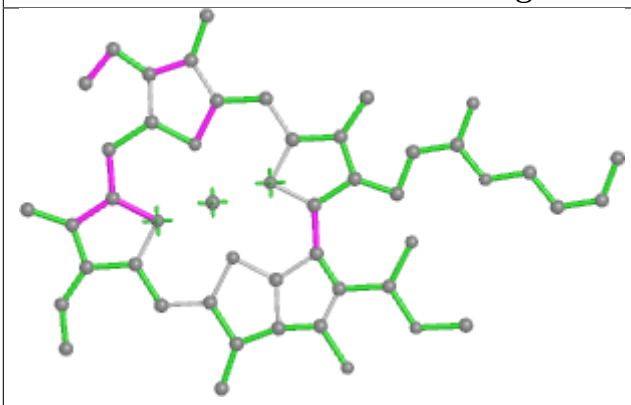


Rings

Ligand CLA B 1215



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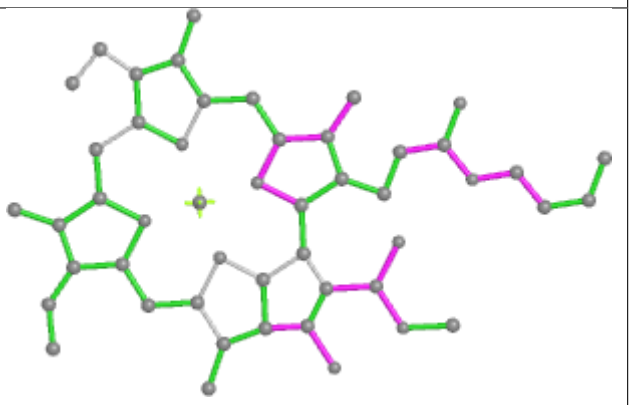
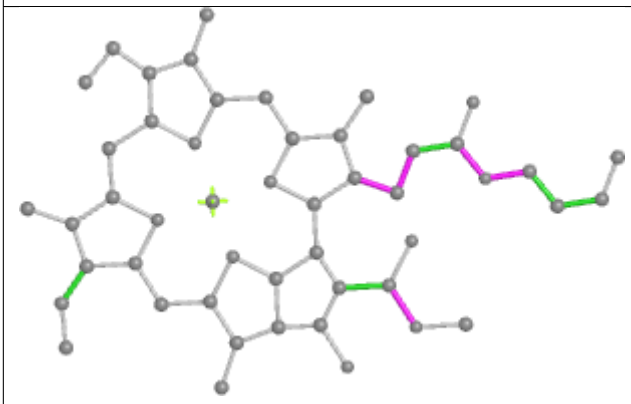
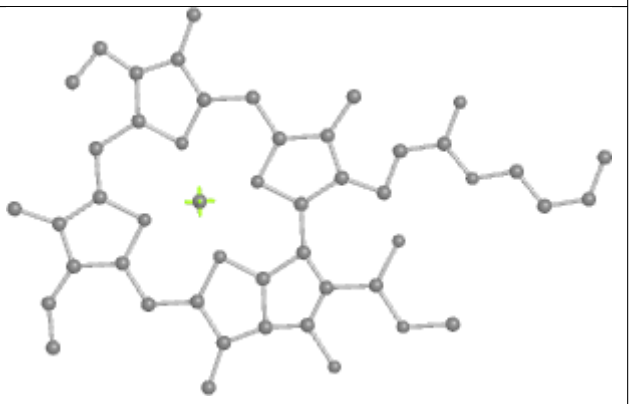


Bond angles

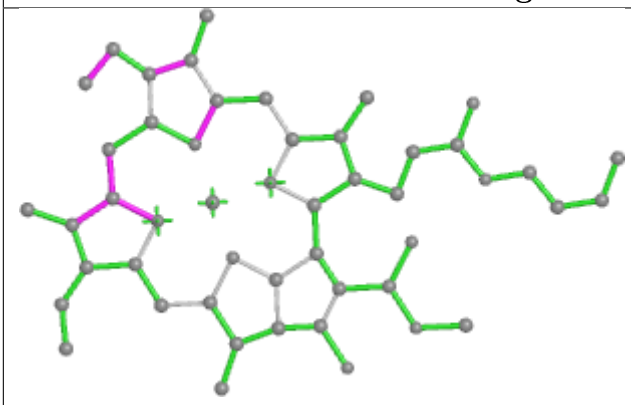


Torsions



Rings

Ligand CLA B 1238



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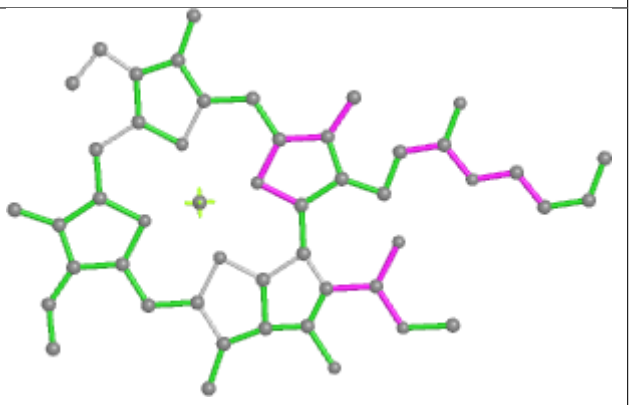
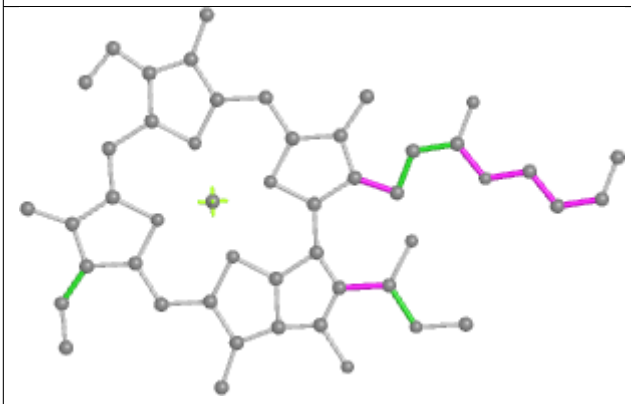
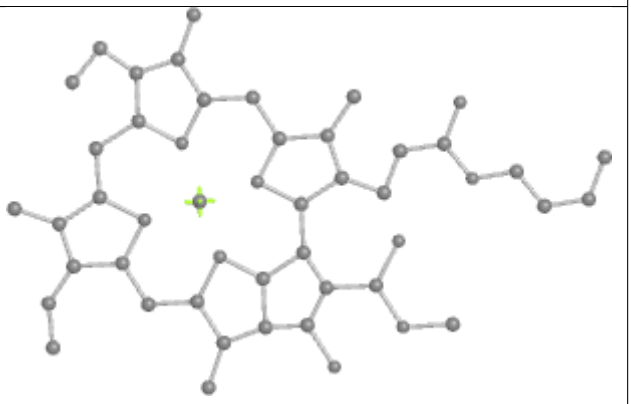


Bond angles

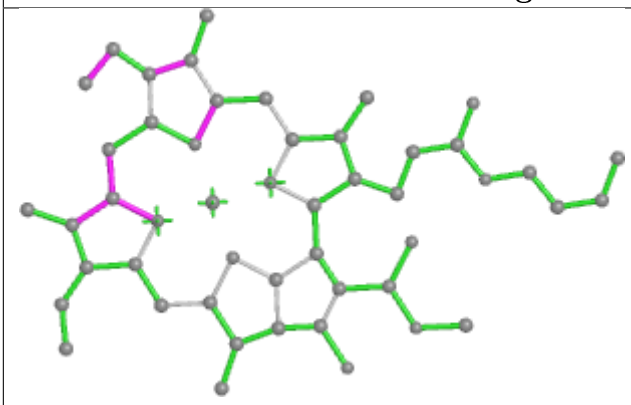


Torsions



Rings

Ligand CLA B 1232



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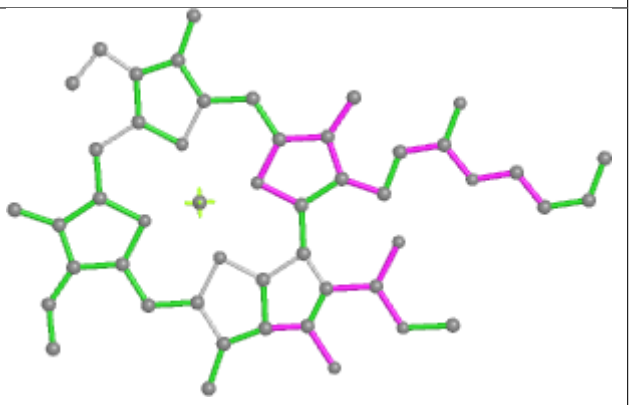
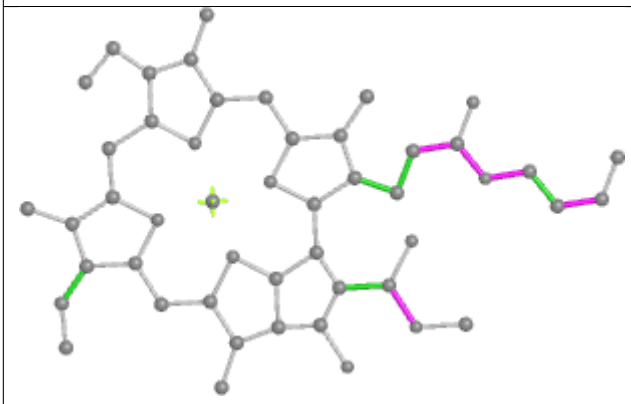
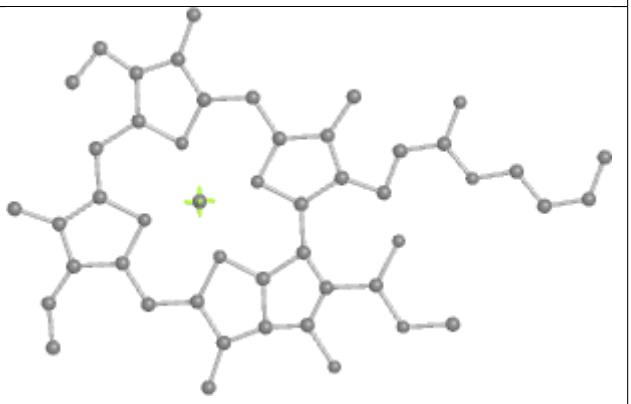


Bond angles

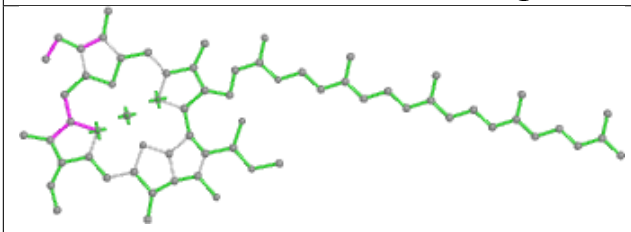


Torsions

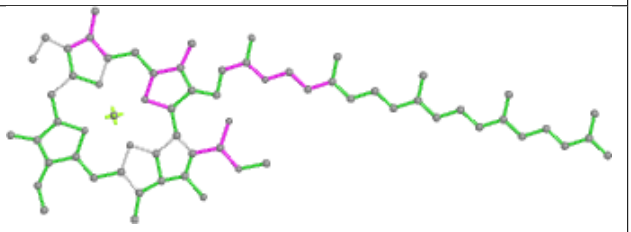


Rings

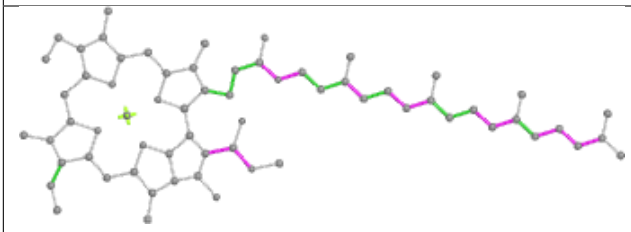
Ligand CLA A 1128



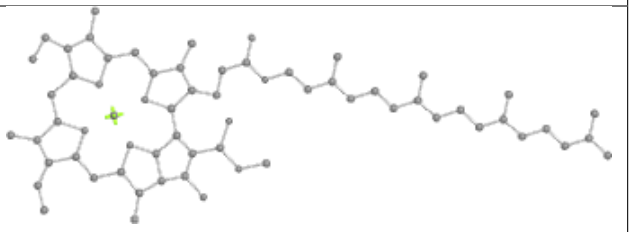
Bond lengths



Bond angles

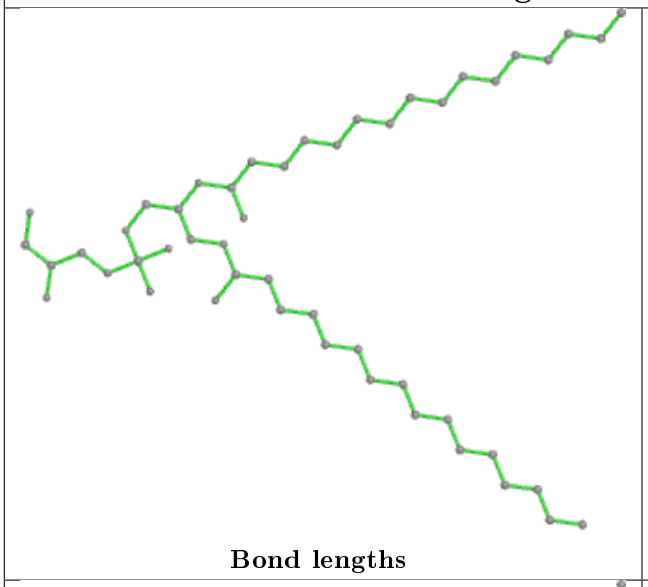


Torsions



Rings

Ligand LHG A 5003



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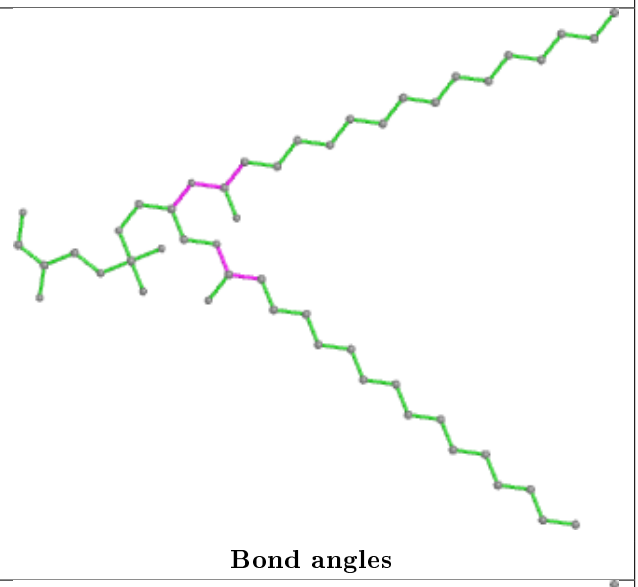
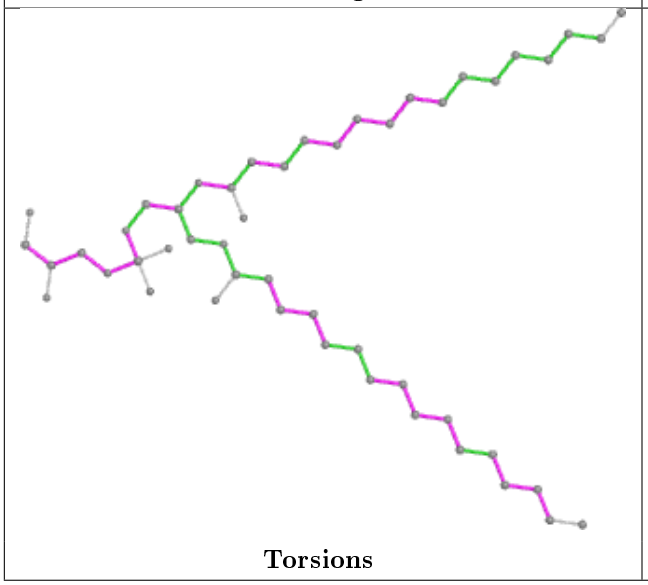
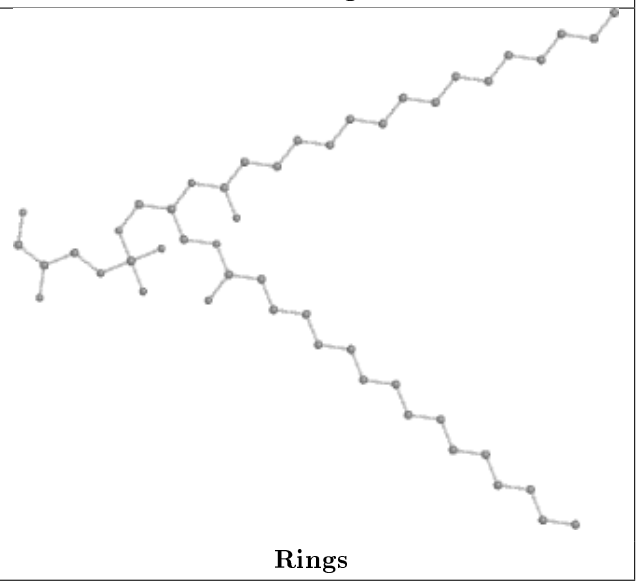


Bond angles

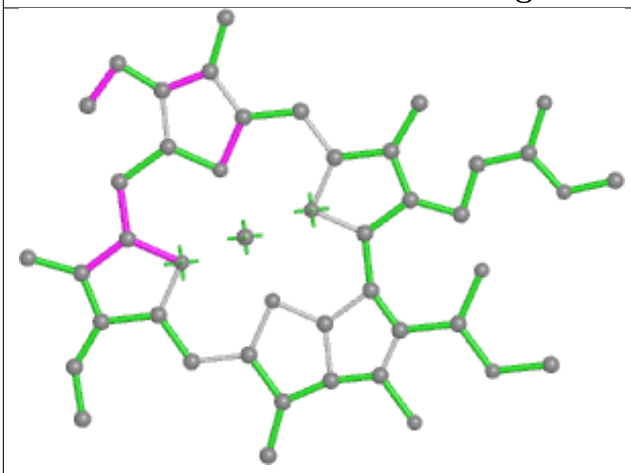


Torsions



Rings

Ligand CLA A 1119



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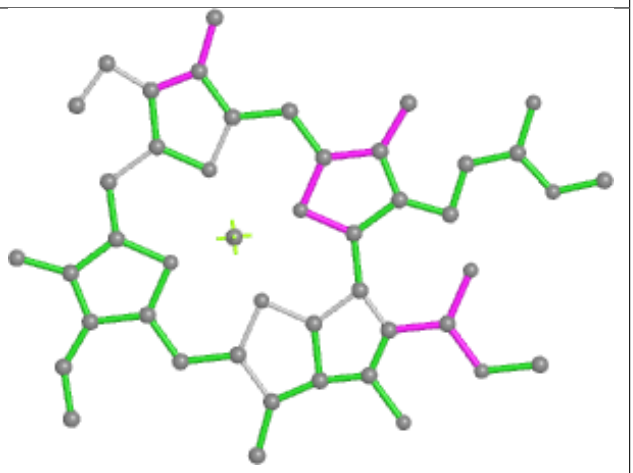
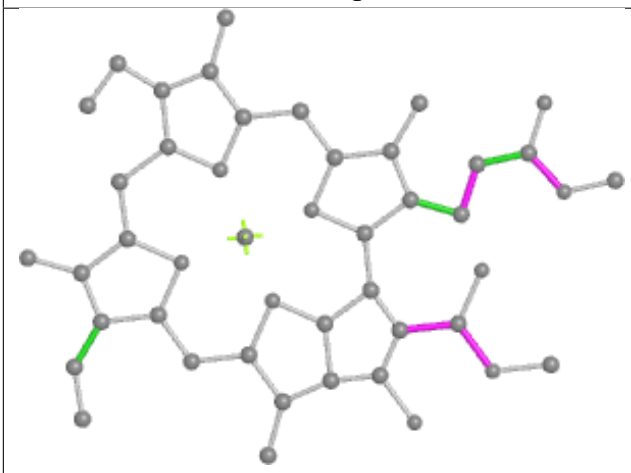
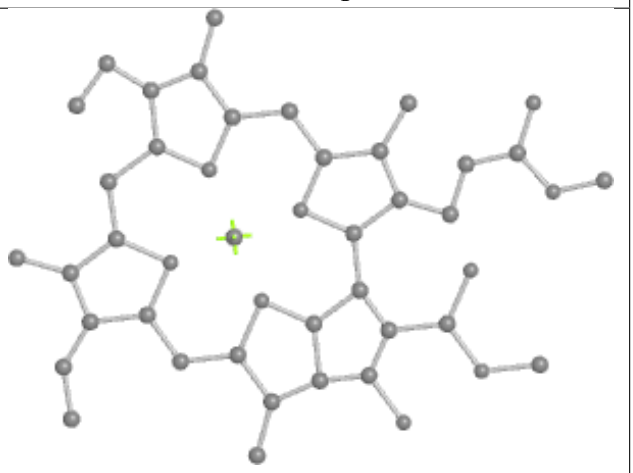


Bond angles

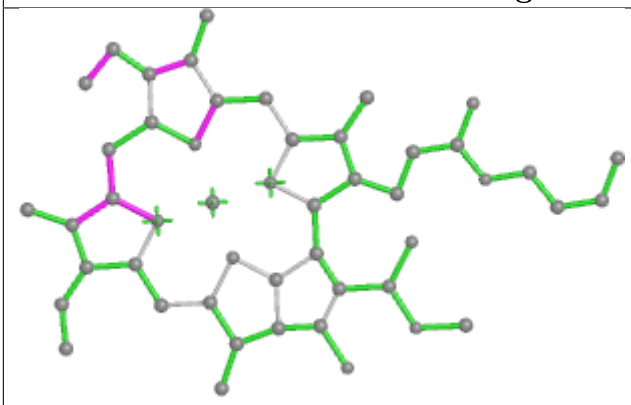


Torsions



Rings

Ligand CLA B 1217



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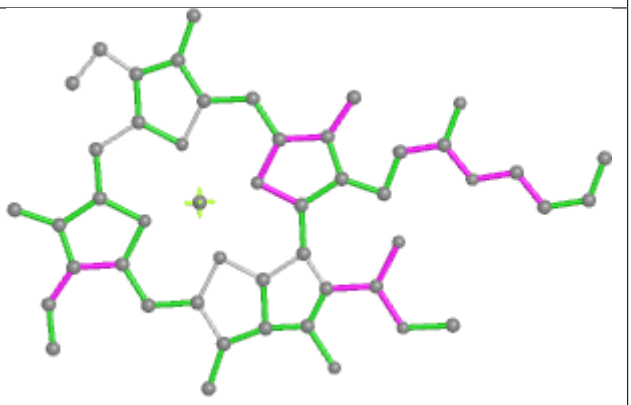
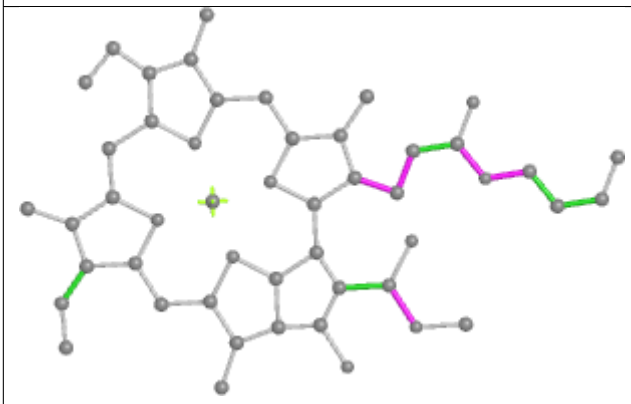
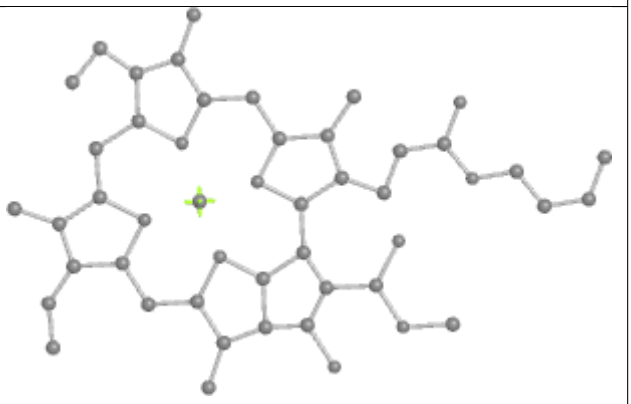


Bond angles

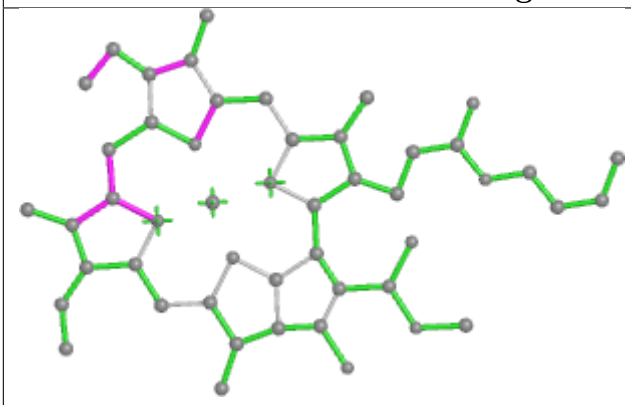


Torsions



Rings

Ligand CLA B 1212



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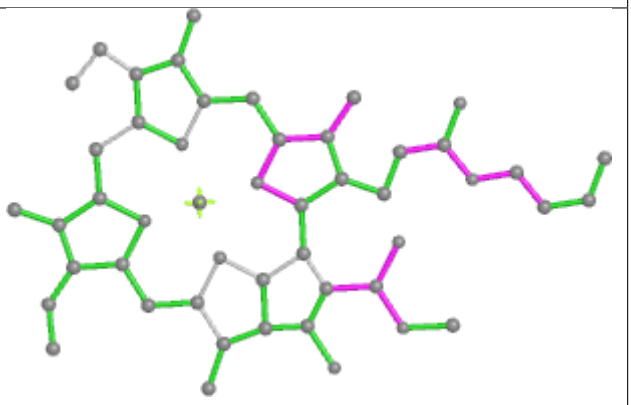
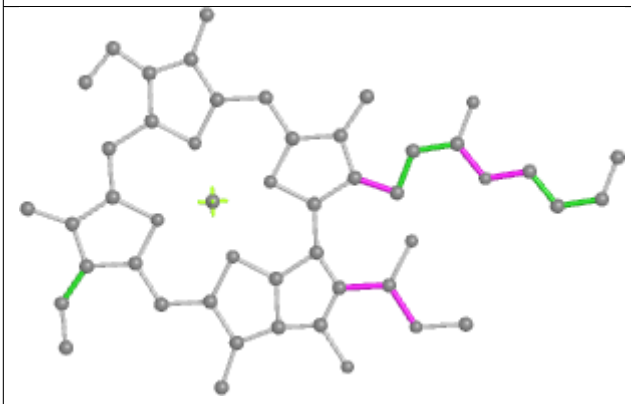


Bond angles



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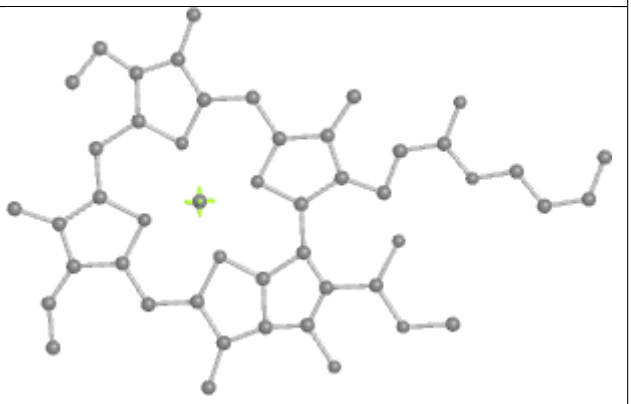
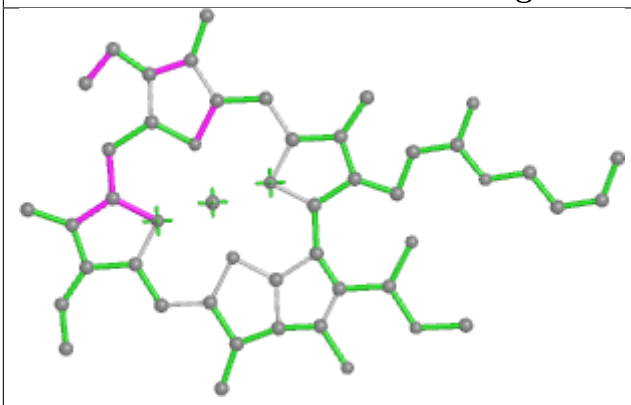


Rings

Ligand CLA B 1210



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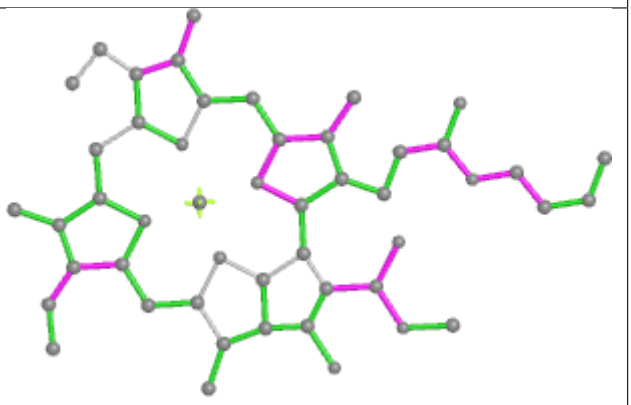
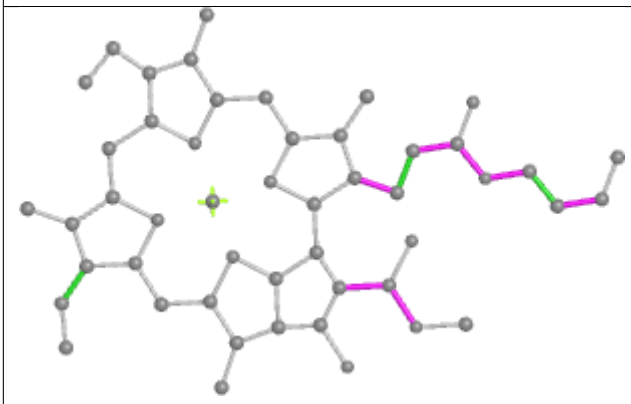
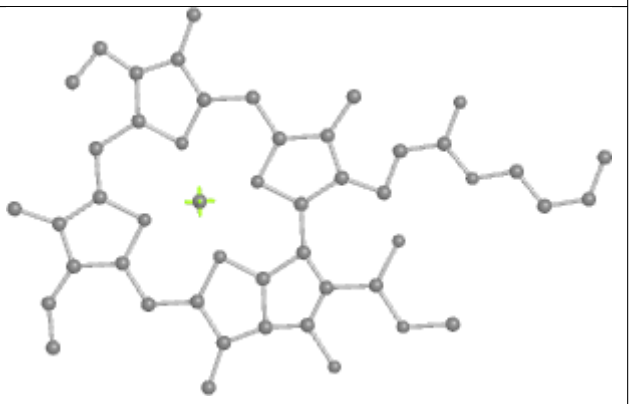


Bond angles

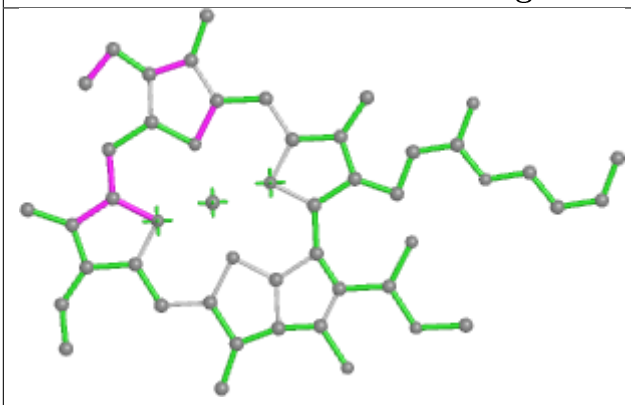


Torsions



Rings

Ligand CLA A 1104



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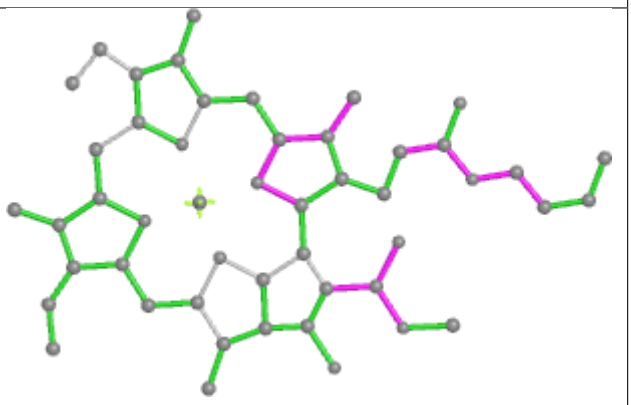
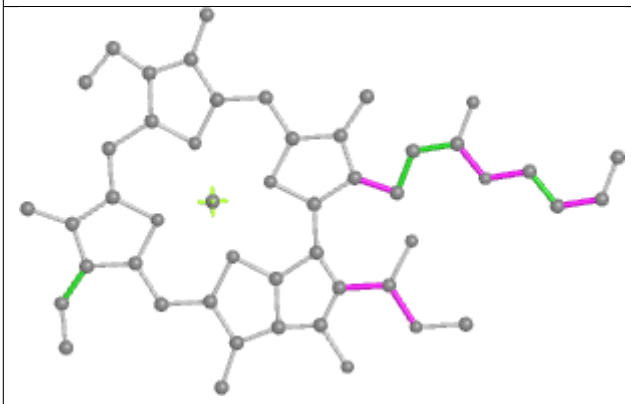
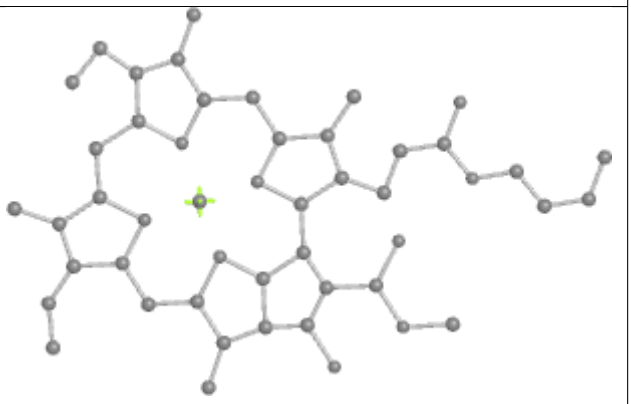


Bond angles

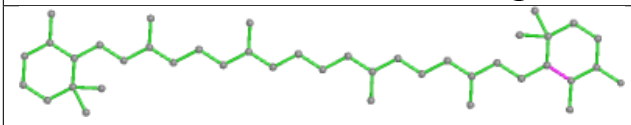


Torsions



Rings

Ligand ECH M 4021



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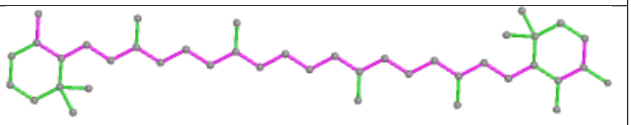
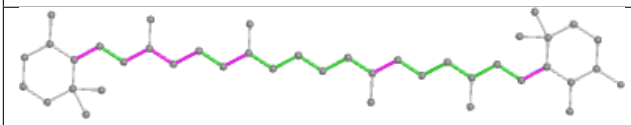
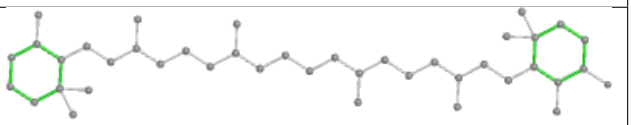


Bond angles

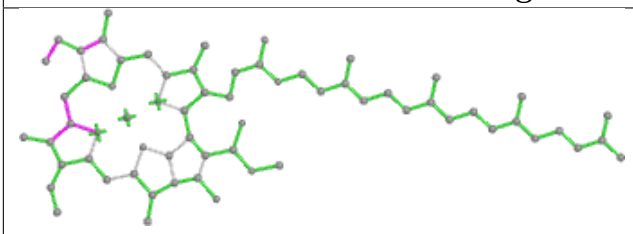


Torsions

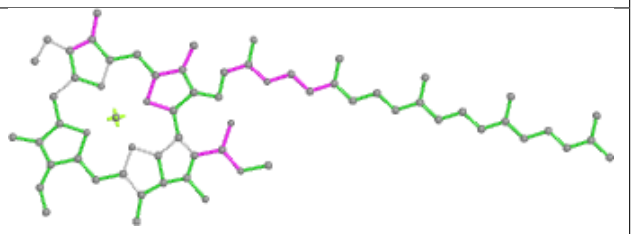


Rings

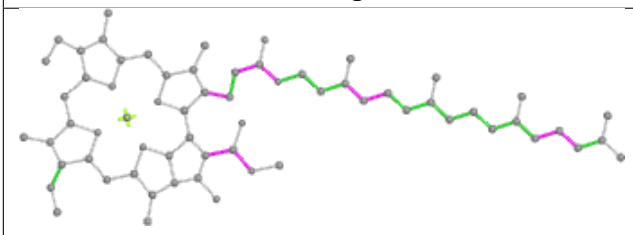
Ligand CLA B 1202



Bond lengths



Bond angles



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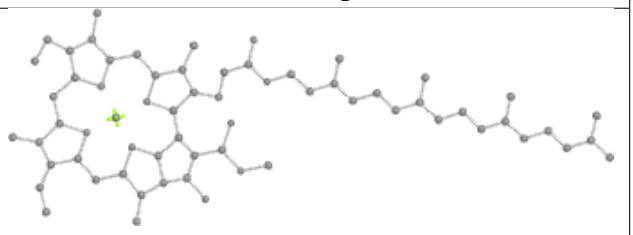
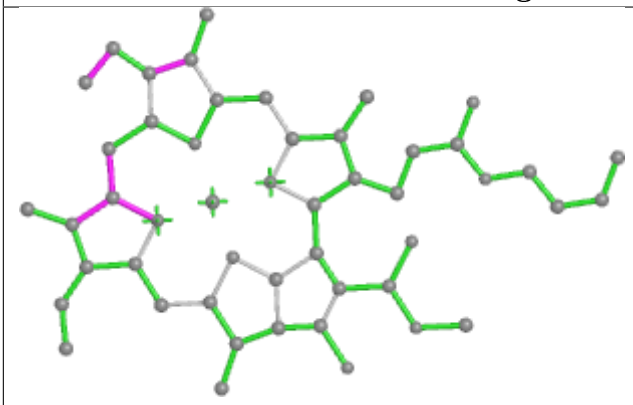
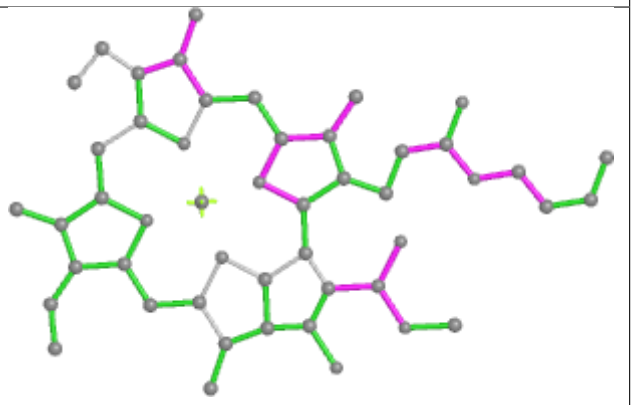


Rings

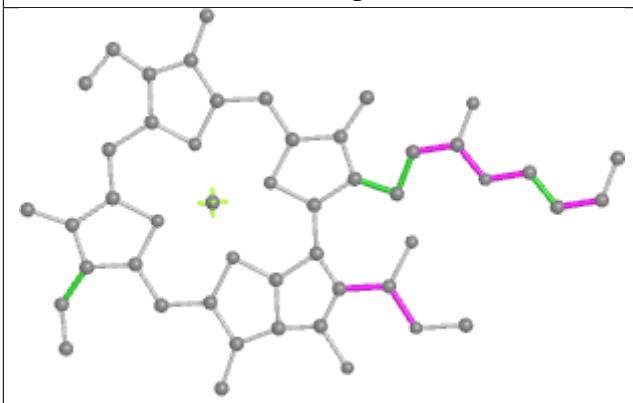
Ligand CLA B 1226



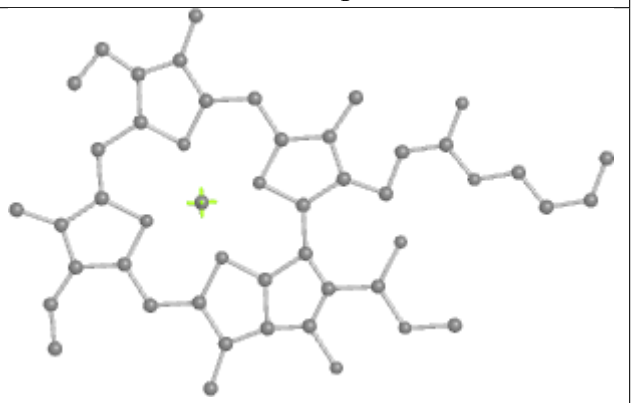
Bond lengths



Bond angles

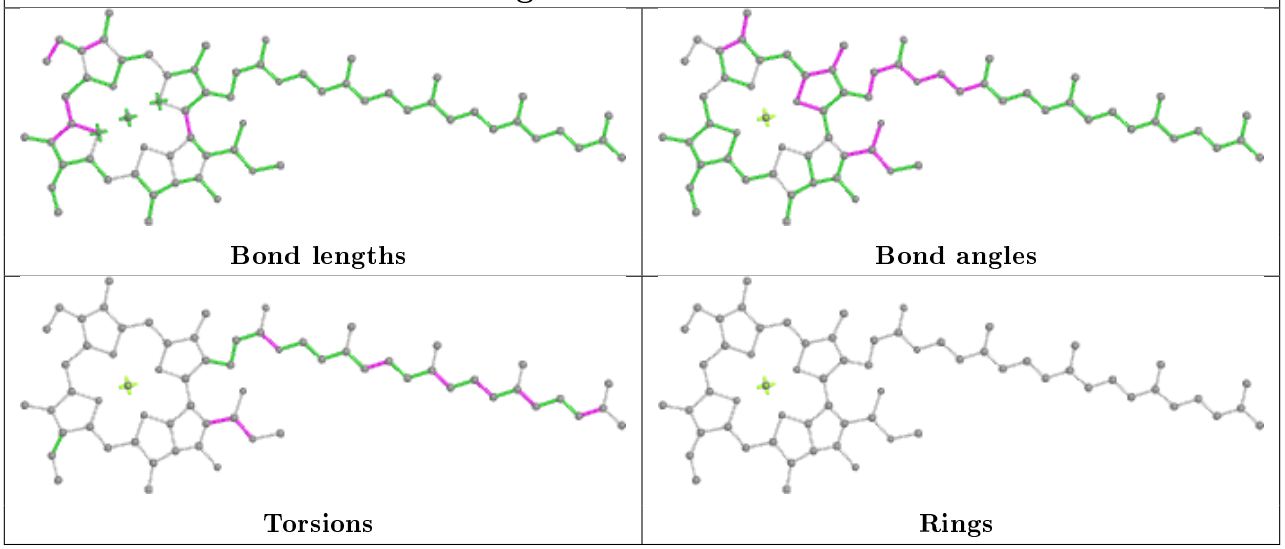


Torsions

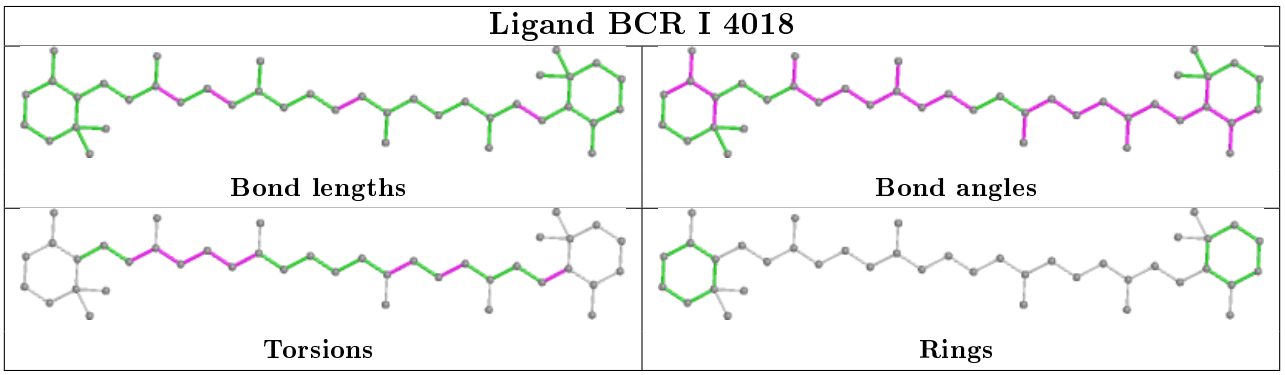


Rings

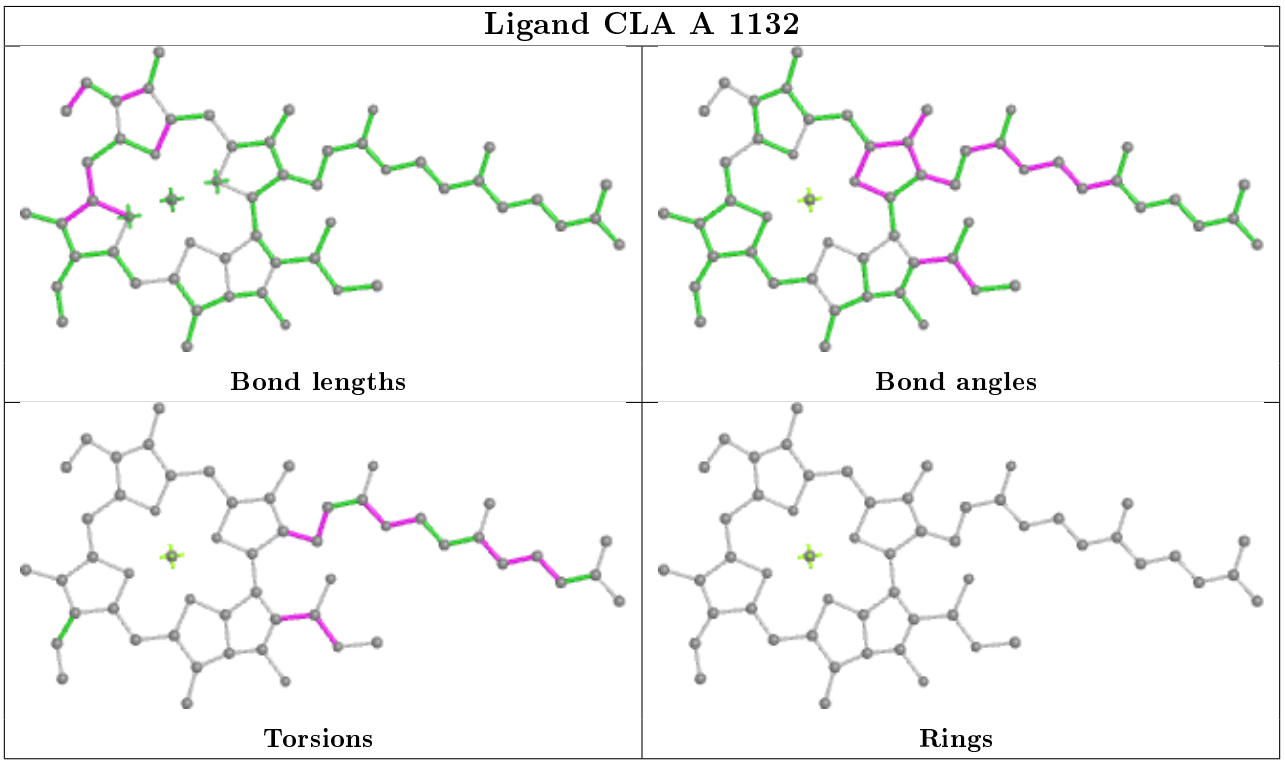
Ligand CLA A 1102



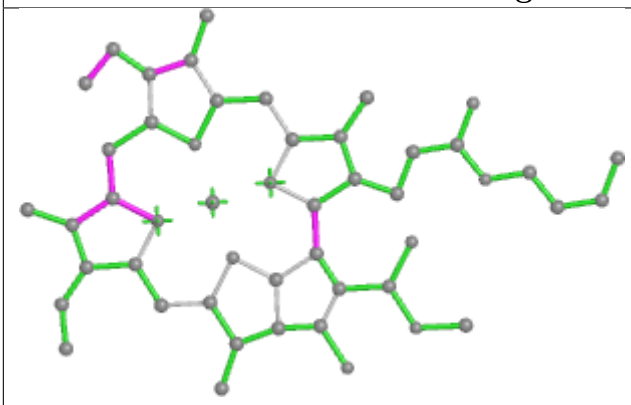
Ligand BCR I 4018



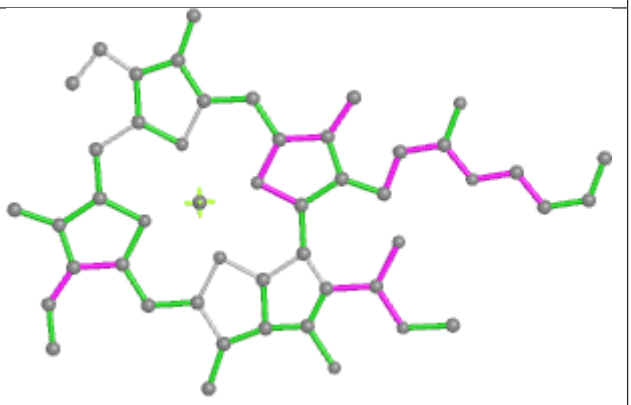
Ligand CLA A 1132



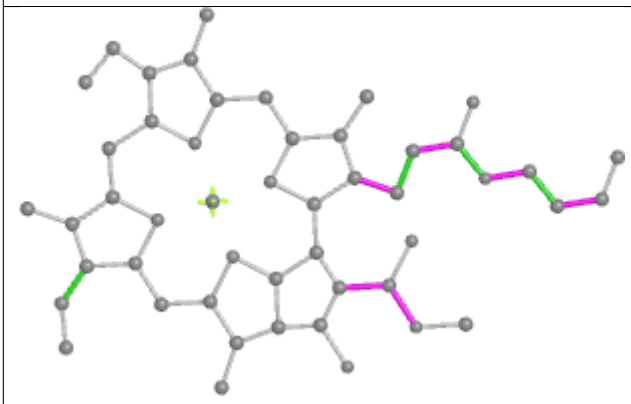
Ligand CLA B 1220



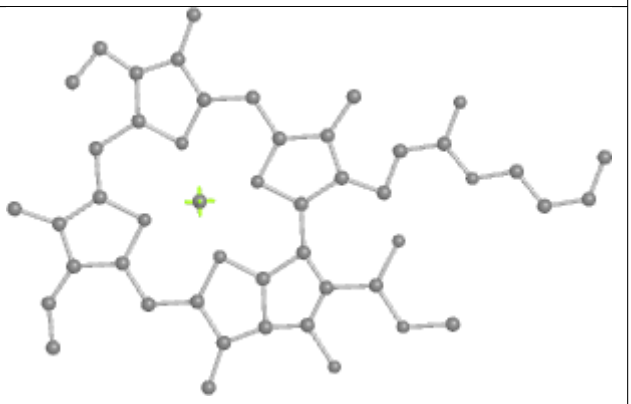
Bond lengths



Bond angles

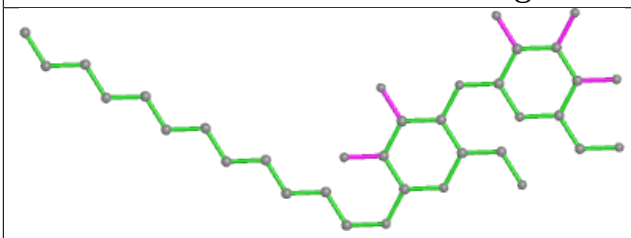


Torsions

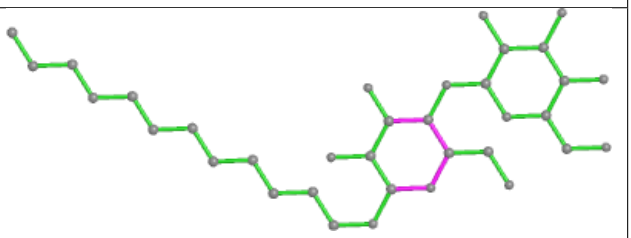


Rings

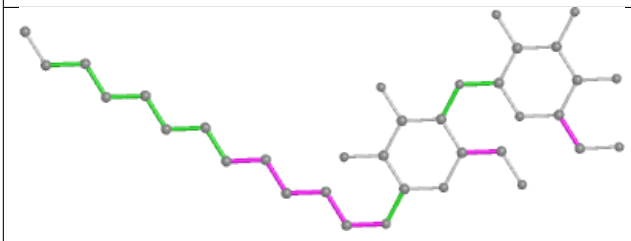
Ligand LMT F 6001



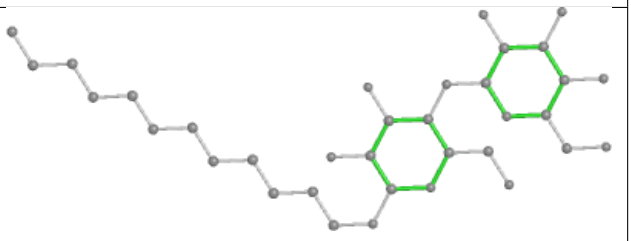
Bond lengths



Bond angles

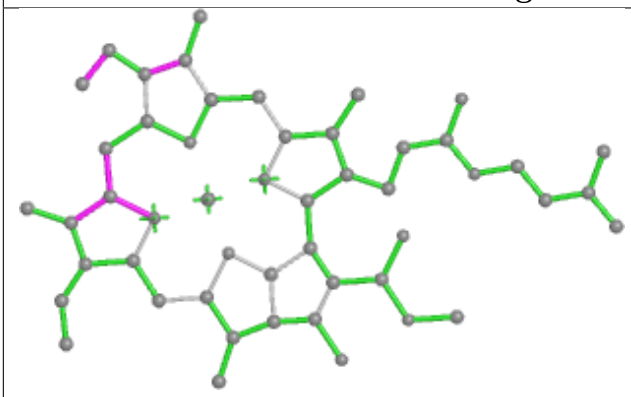


Torsions

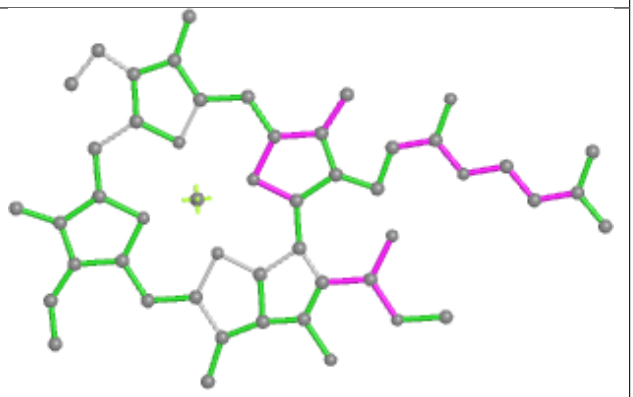


Rings

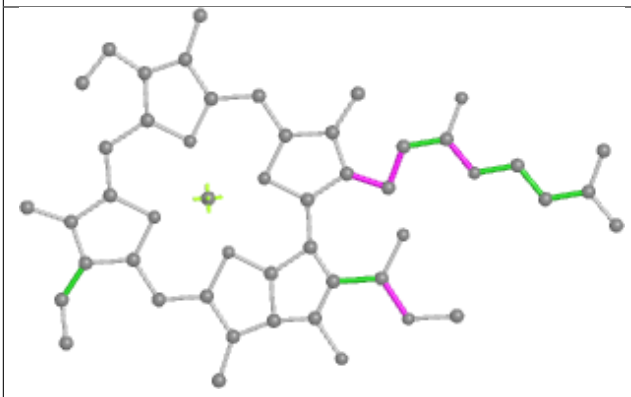
Ligand CLA B 1222



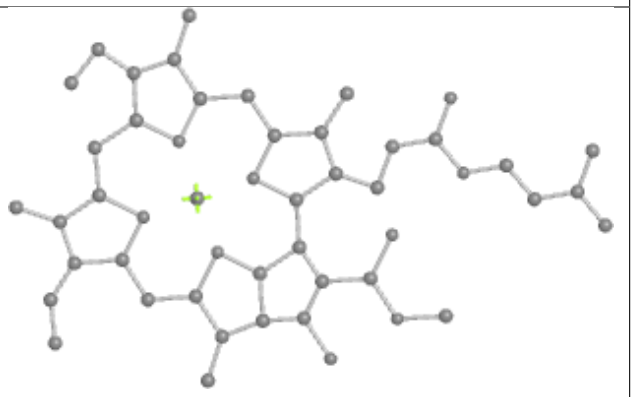
Bond lengths



Bond angles

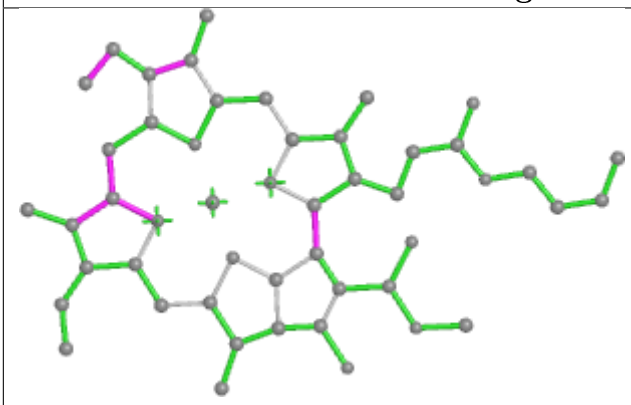


Torsions

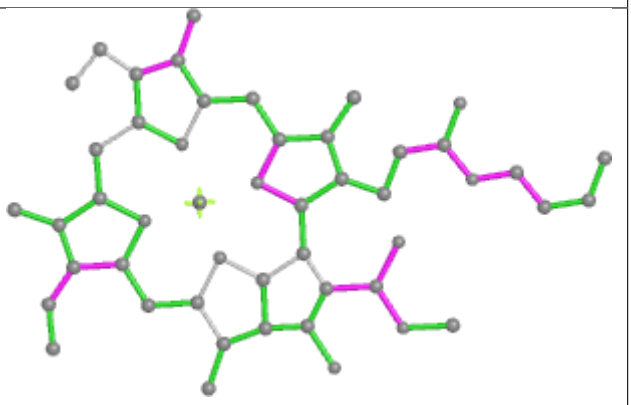


Rings

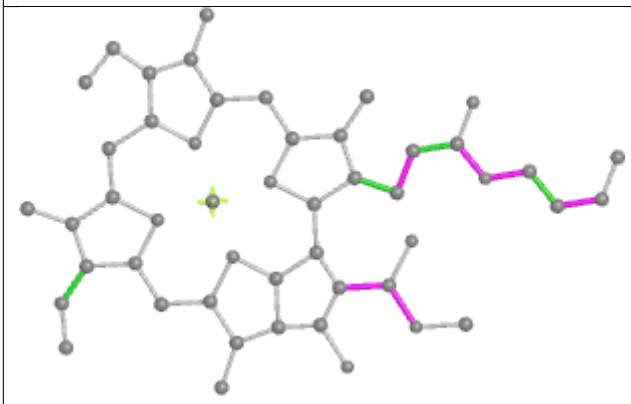
Ligand CLA B 1023



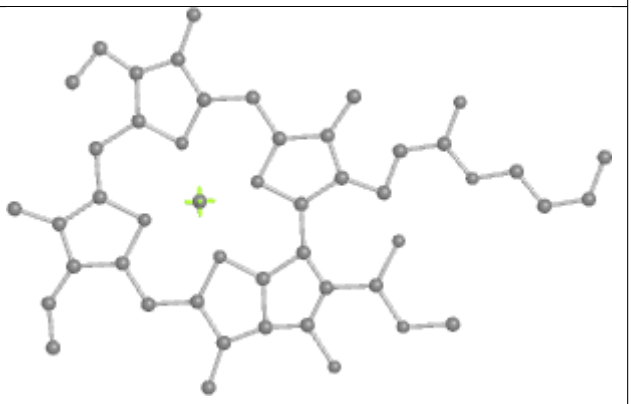
Bond lengths



Bond angles

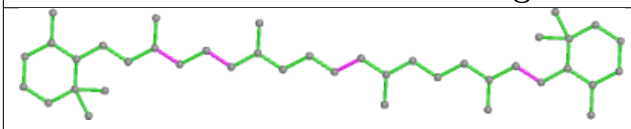


Torsions



Rings

Ligand BCR A 4001



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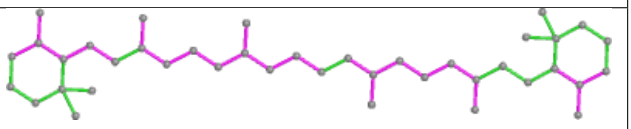
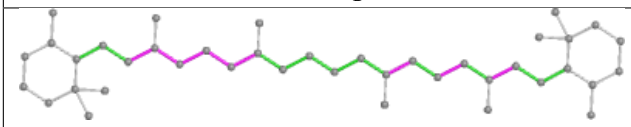
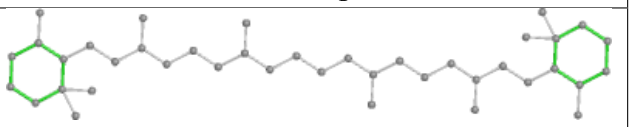


Bond angles

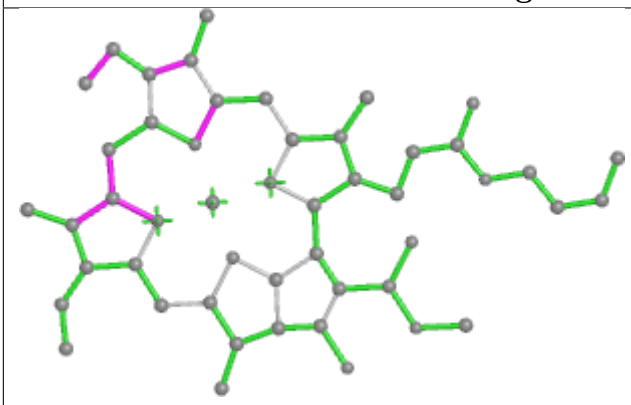


Torsions



Rings

Ligand CLA B 1230



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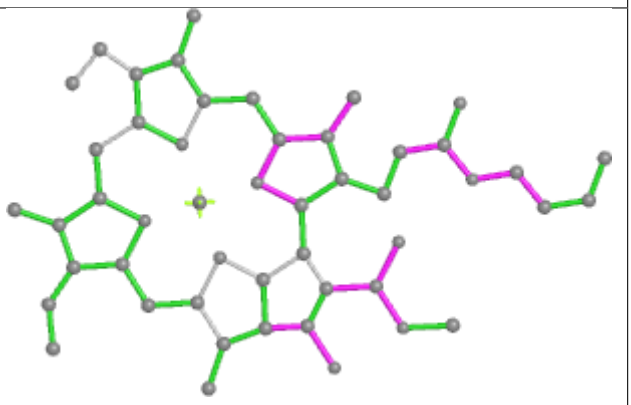
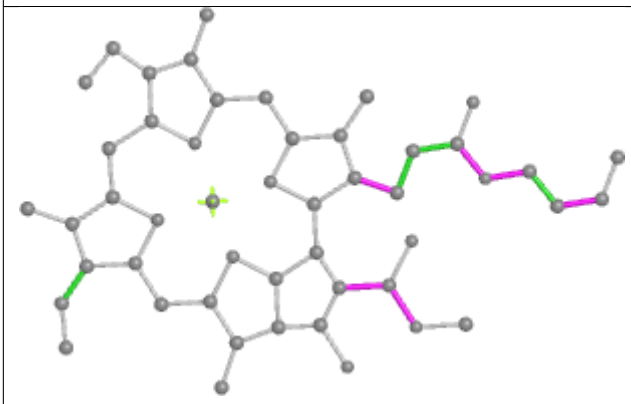
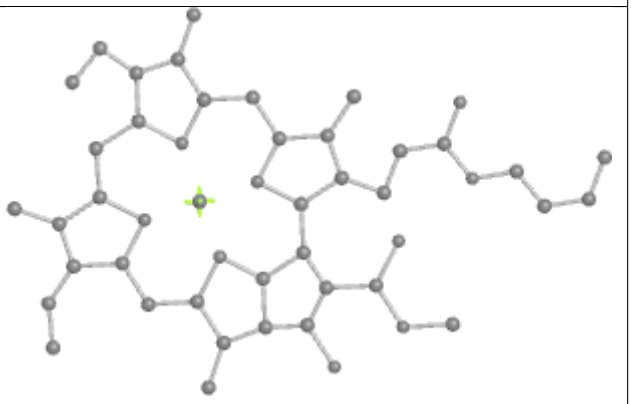


Bond angles

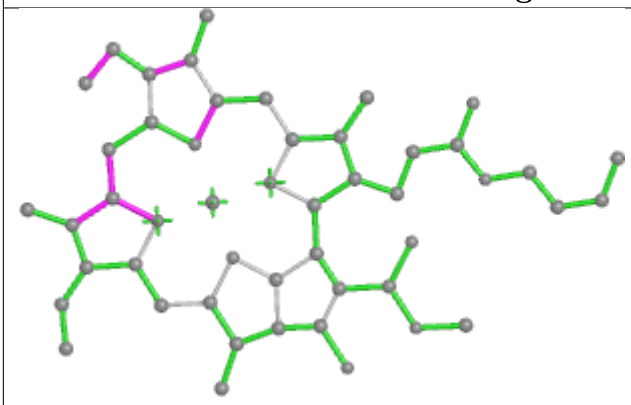


Torsions



Rings

Ligand CLA A 1108



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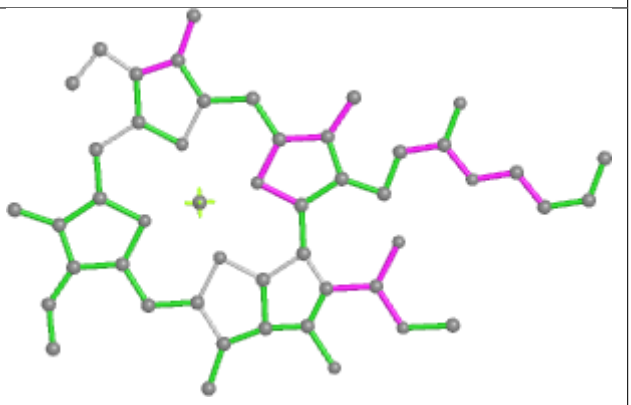
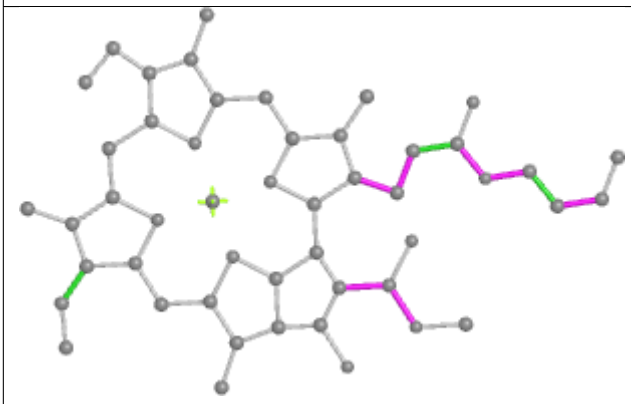


Bond angles



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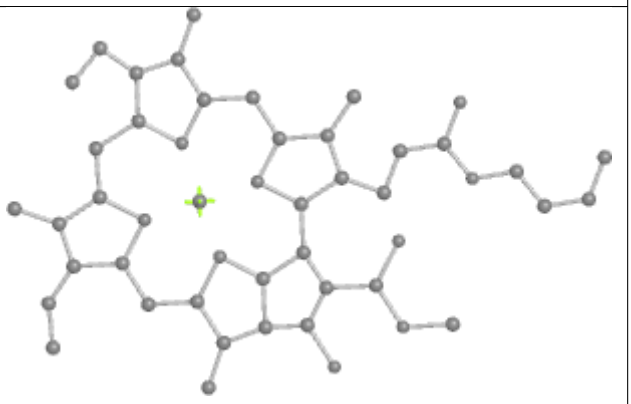
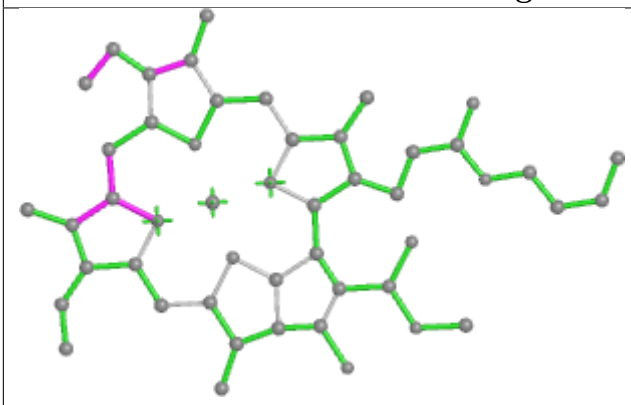
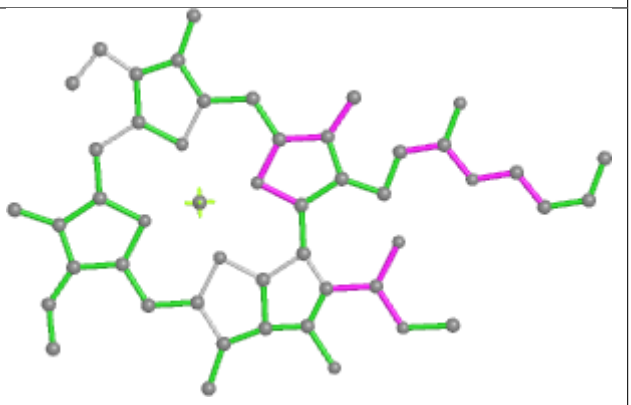


Rings

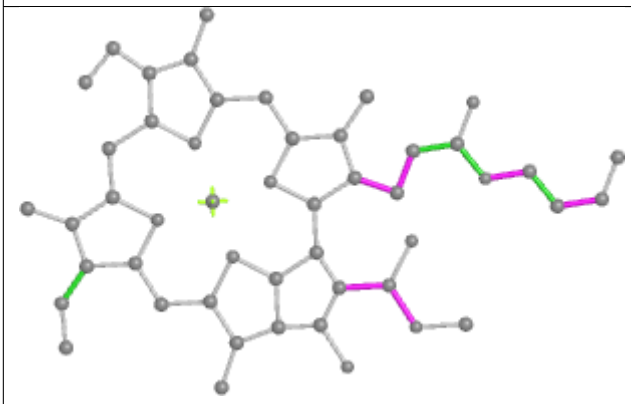
Ligand CLA B 1225



Bond lengths



Bond angles



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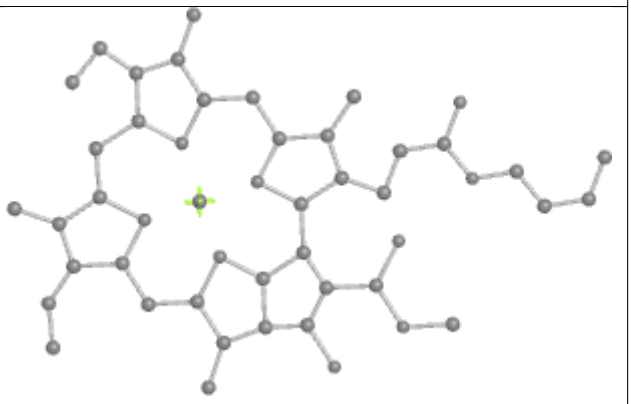
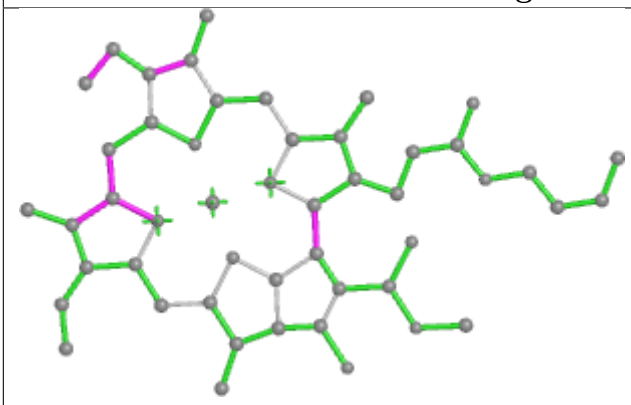


Rings

Ligand CLA B 1206



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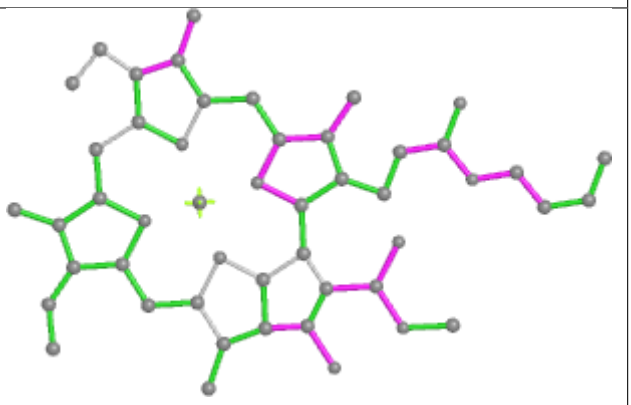
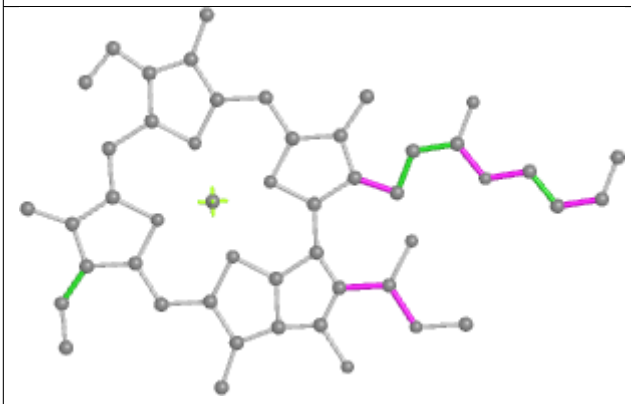
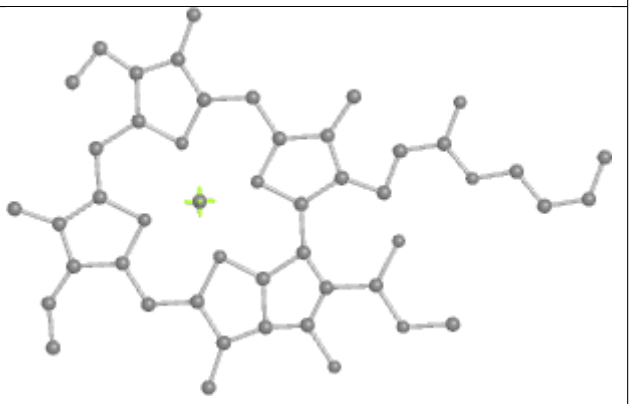


Bond angles

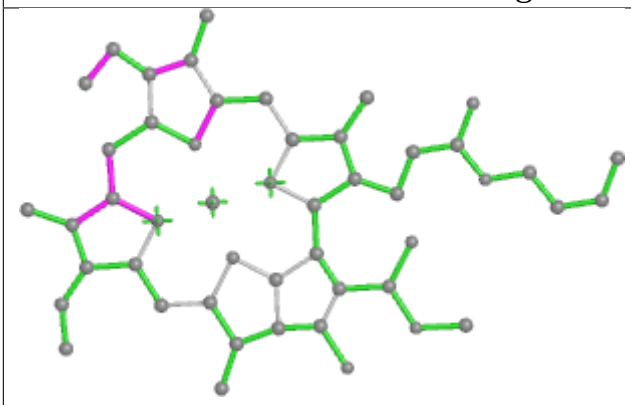


Torsions



Rings

Ligand CLA A 1137



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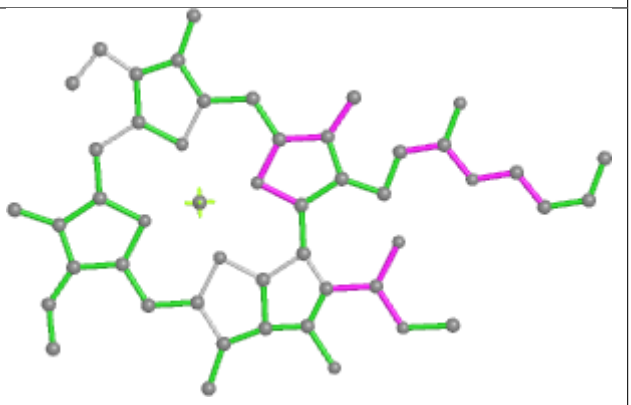
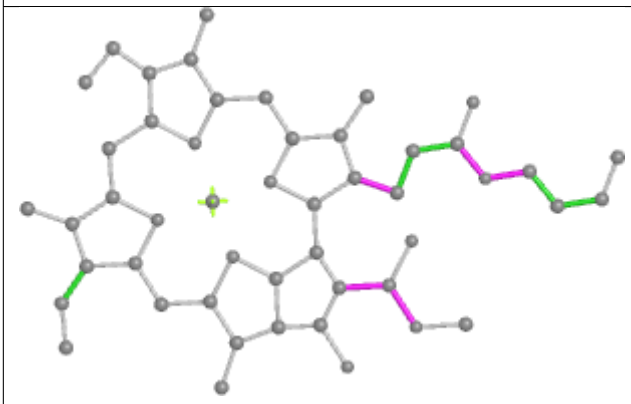


Bond angles



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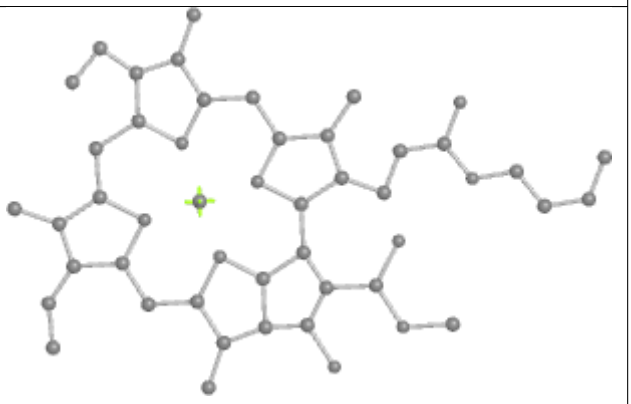
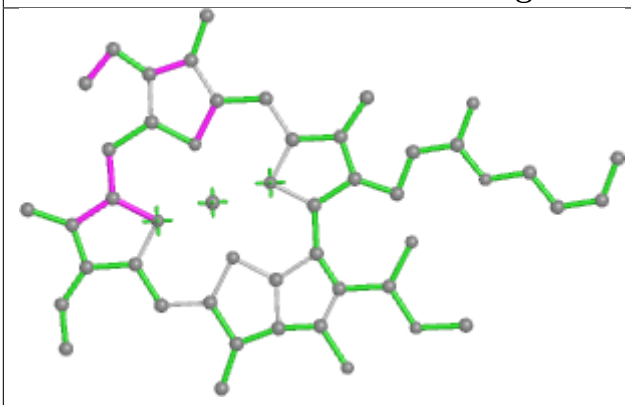


Rings

Ligand CLA B 1207



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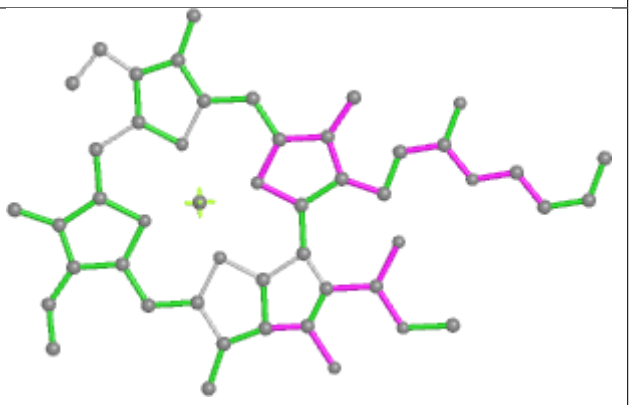
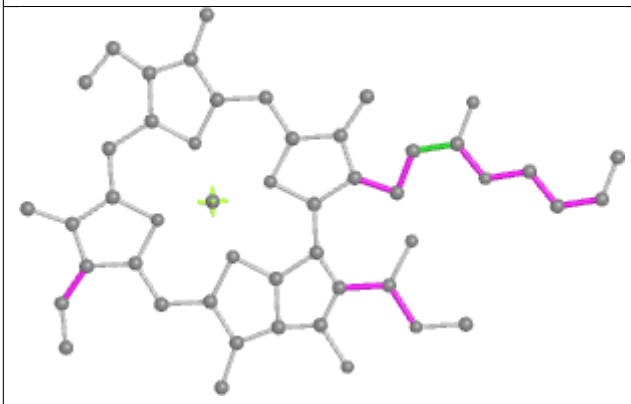
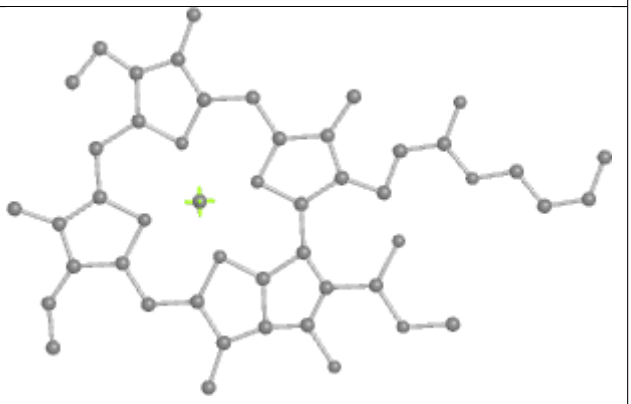


Bond angles

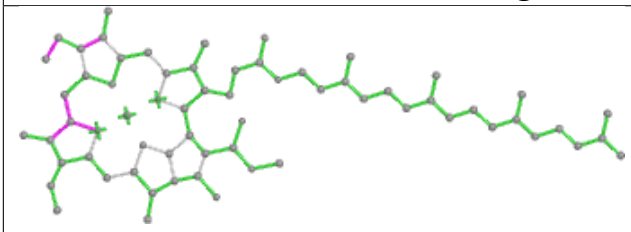


Torsions

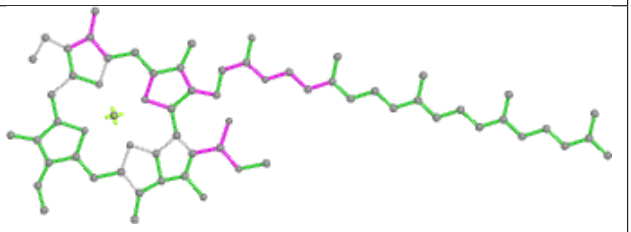


Rings

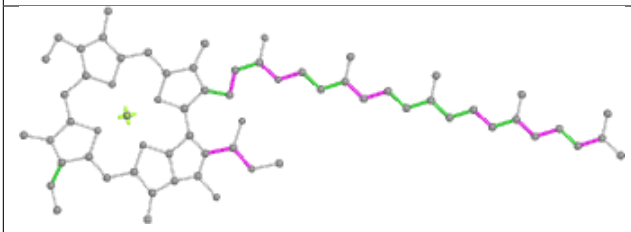
Ligand CLA A 1013



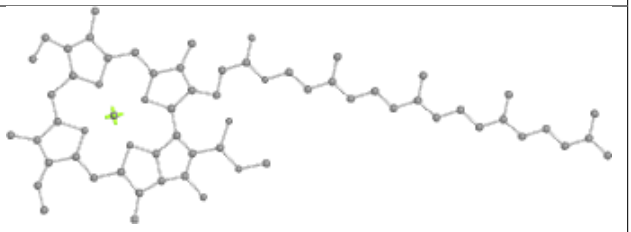
Bond lengths



Bond angles

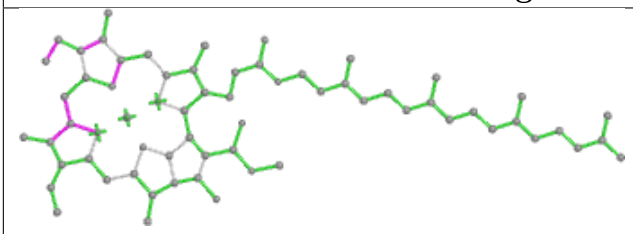


Torsions



Rings

Ligand CLA B 1235



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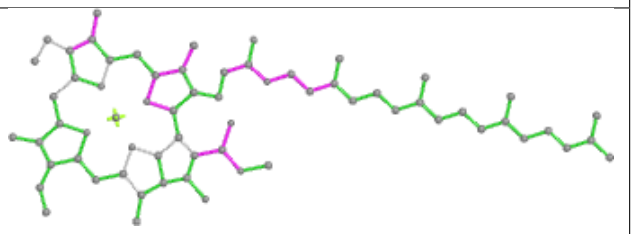
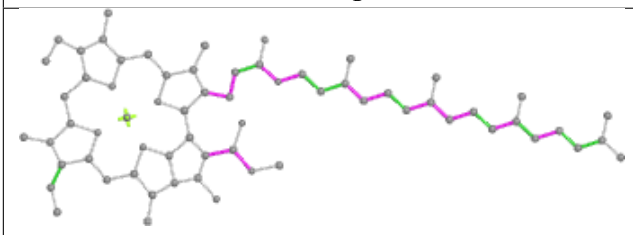


Bond angles



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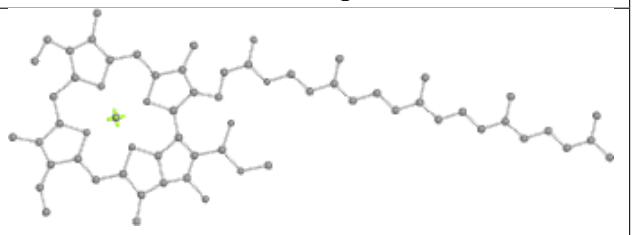
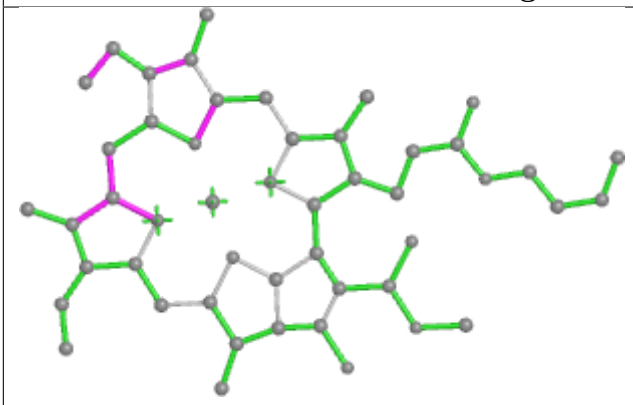


Rings

Ligand CLA J 1302



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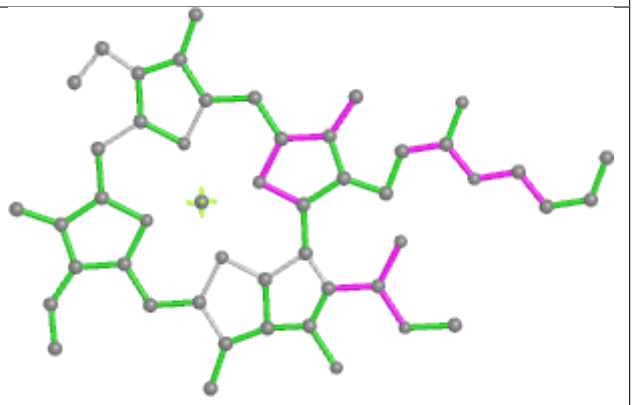
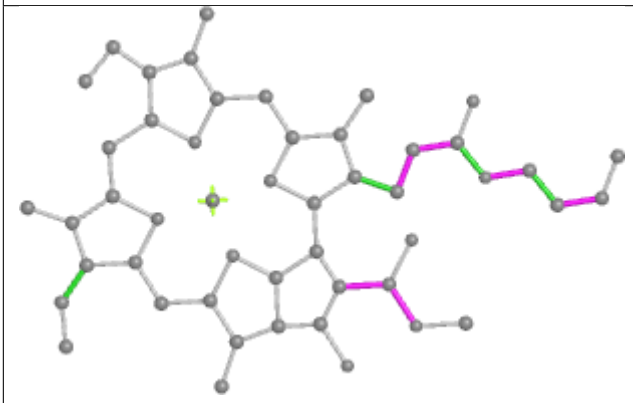


Bond angles



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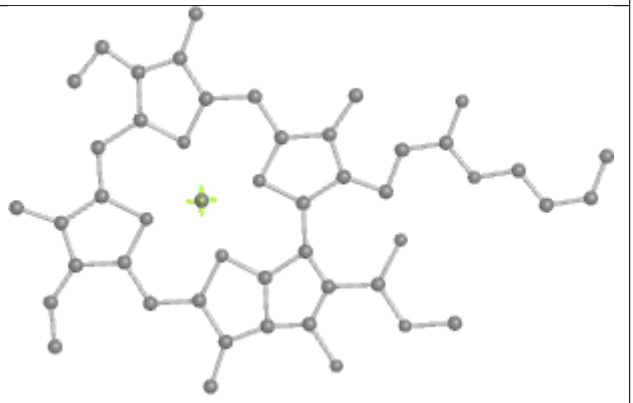
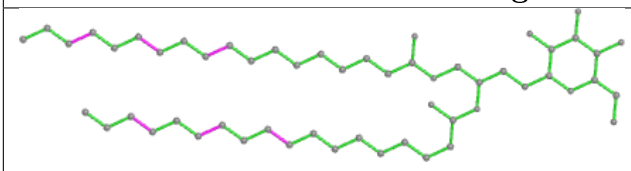


Rings

Ligand LMG B 5002



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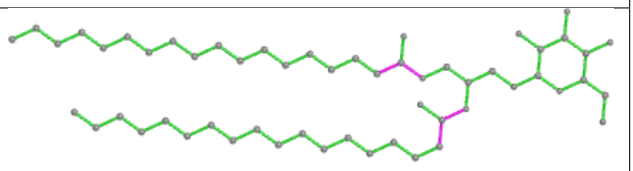
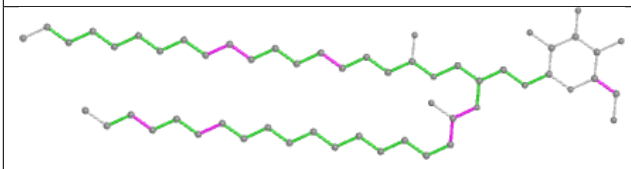
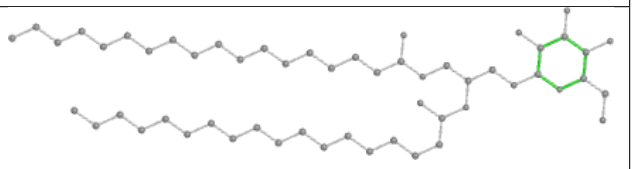


Bond angles

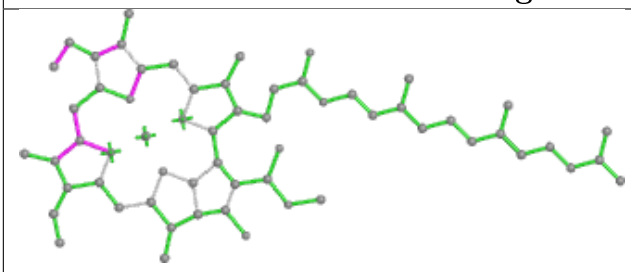


Torsions



Rings

Ligand CLA A 1126



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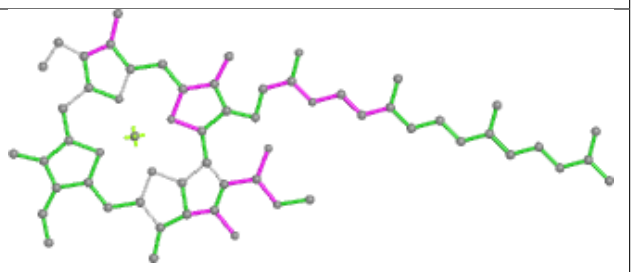
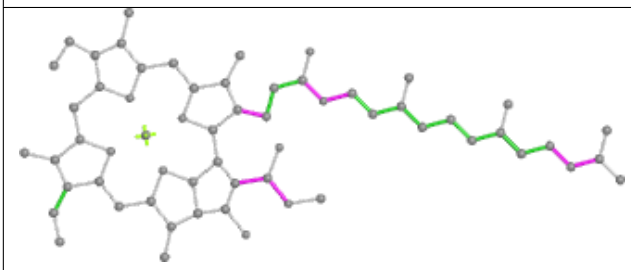
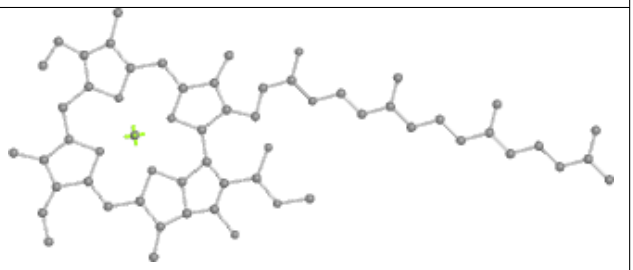


Bond angles

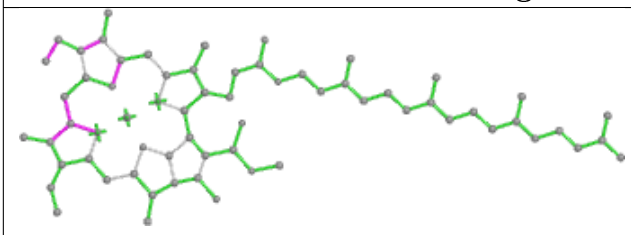


Torsions



Rings

Ligand CLA A 1140



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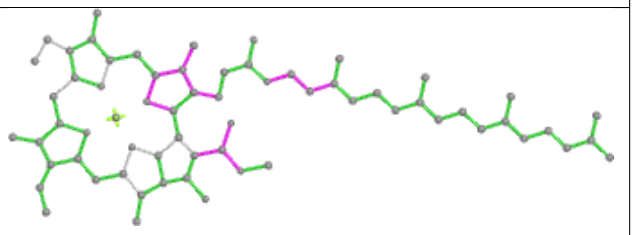
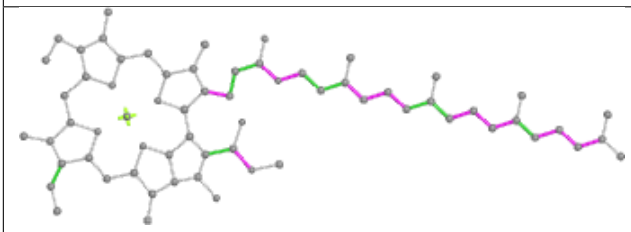
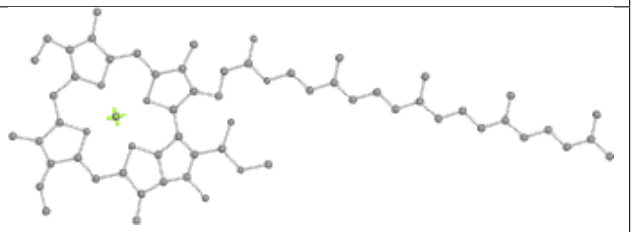


Bond angles

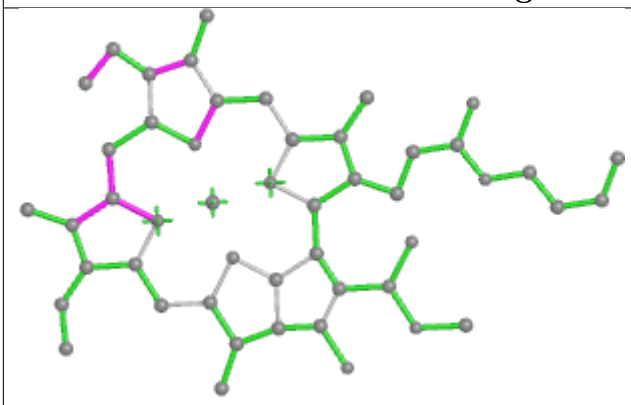


Torsions

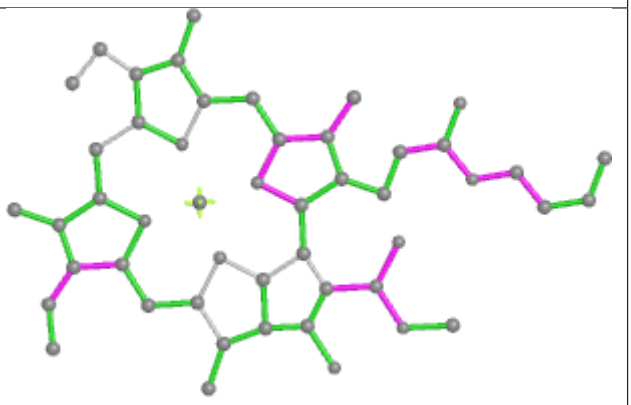


Rings

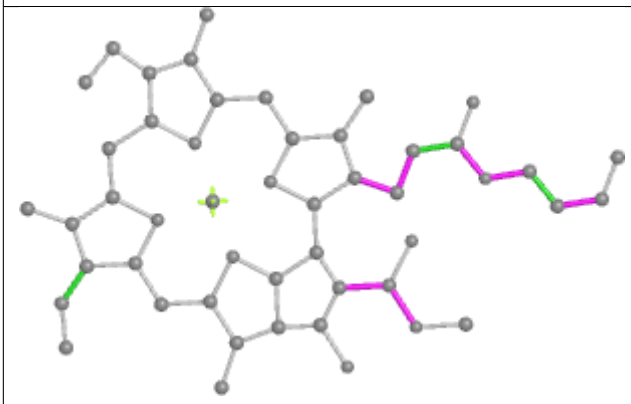
Ligand CLA A 1111



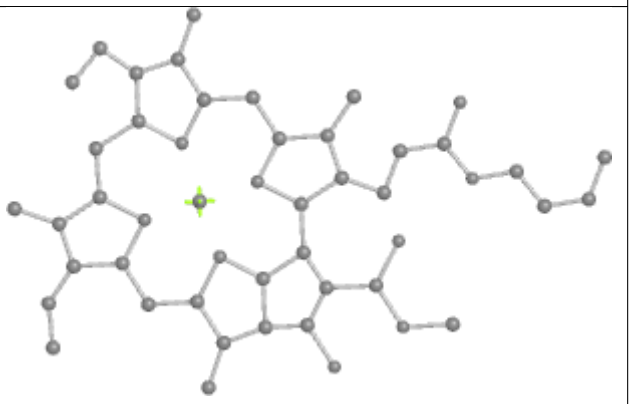
Bond lengths



Bond angles

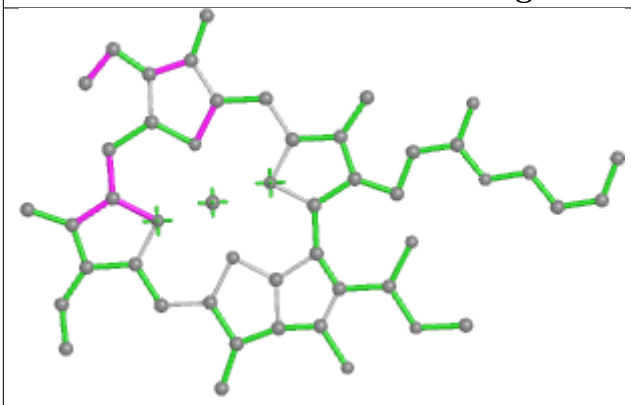


Torsions



Rings

Ligand CLA A 1114



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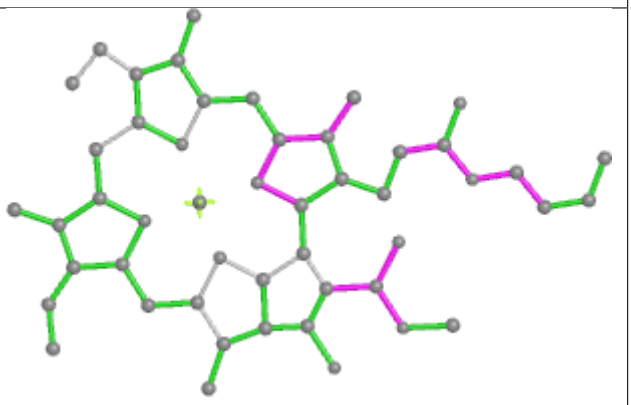
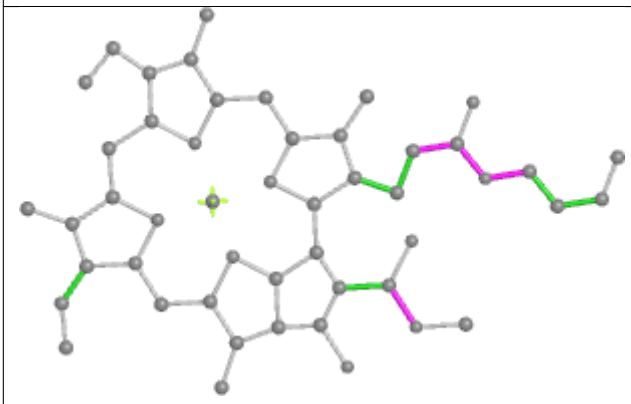


Bond angles



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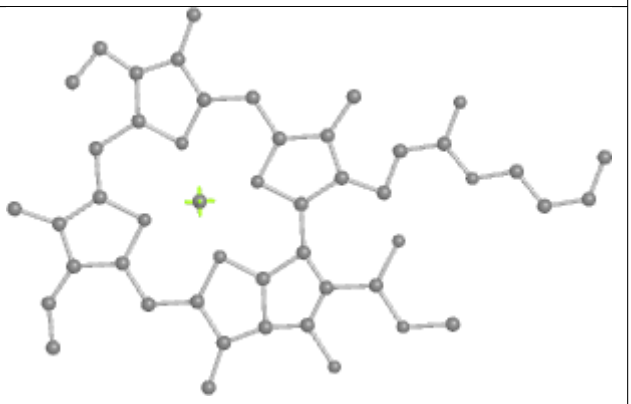
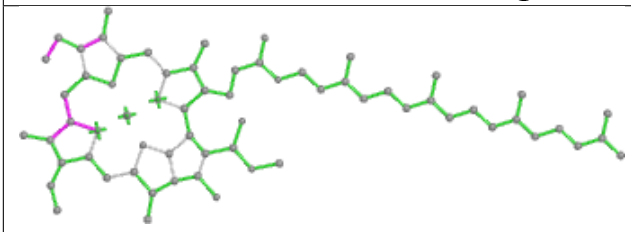


Rings

Ligand CLA A 1138



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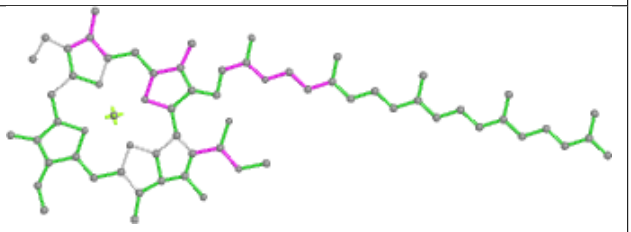
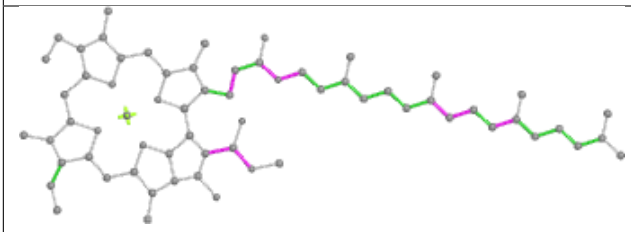
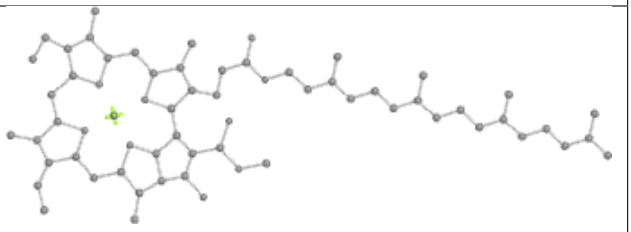


Bond angles

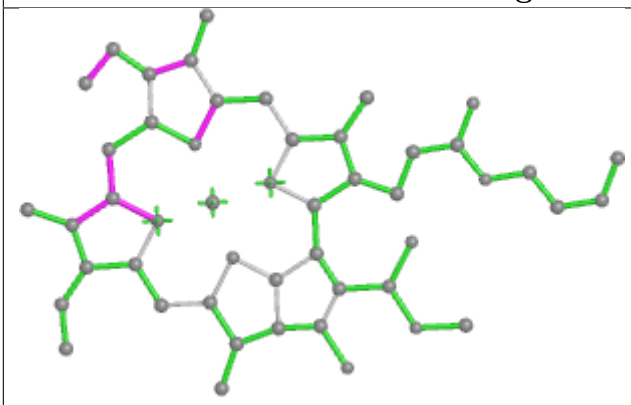


Torsions



Rings

Ligand CLA A 1121



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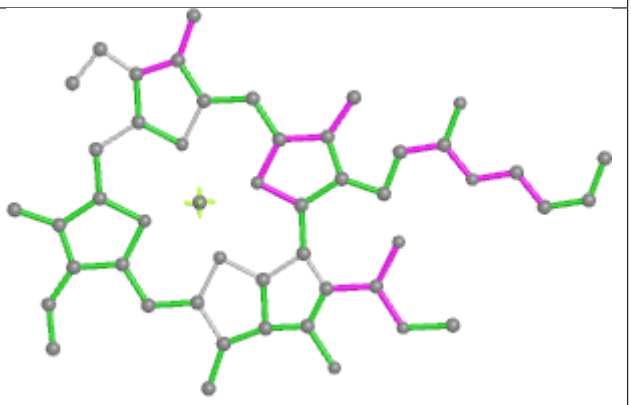
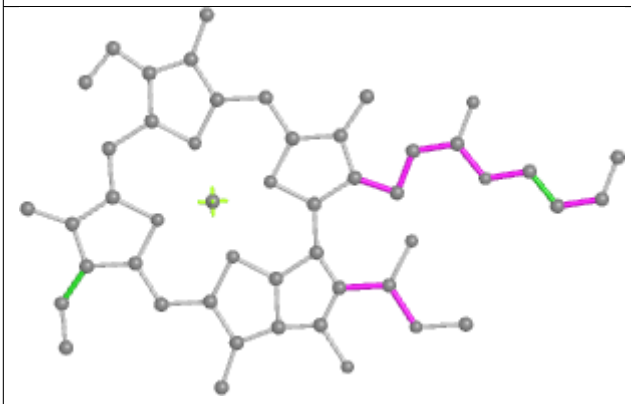
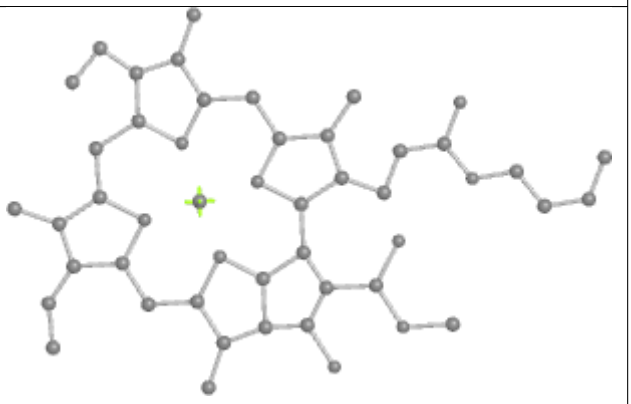


Bond angles

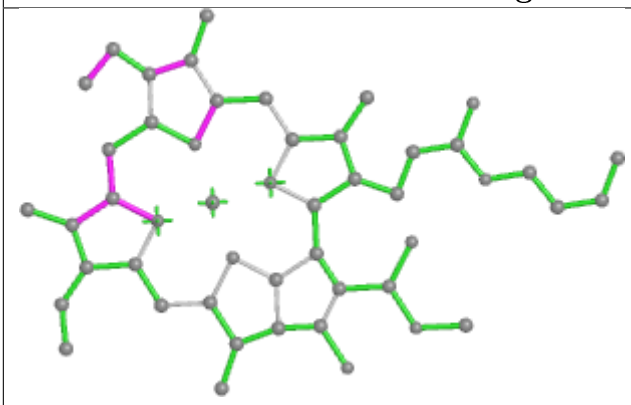


Torsions



Rings

Ligand CLA B 1231



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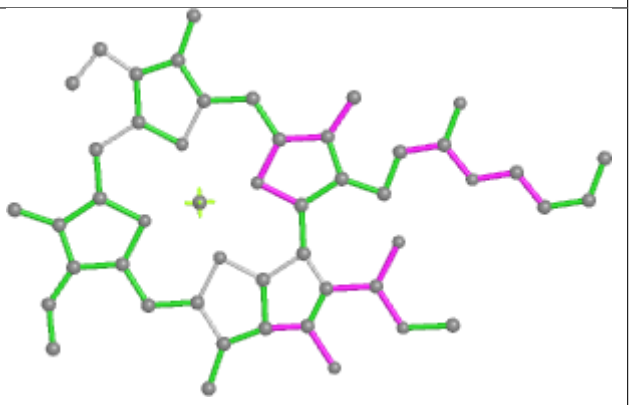
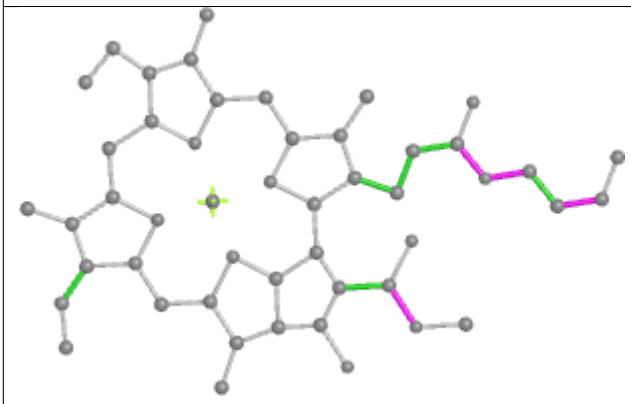
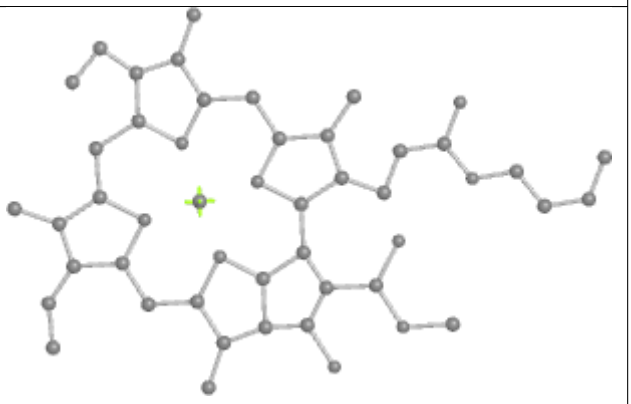


Bond angles

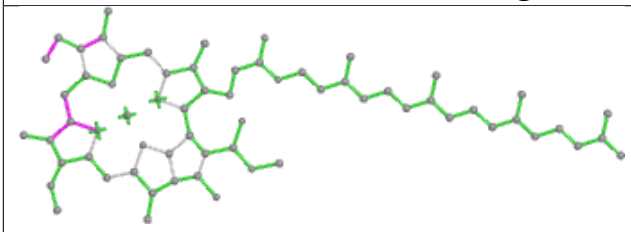


Torsions



Rings

Ligand CLA B 1021



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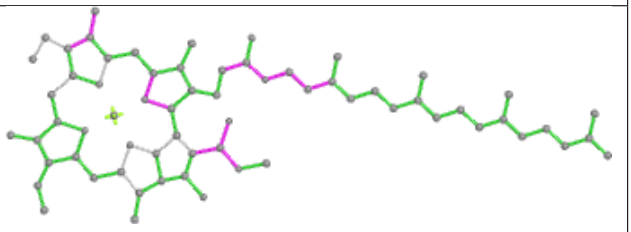
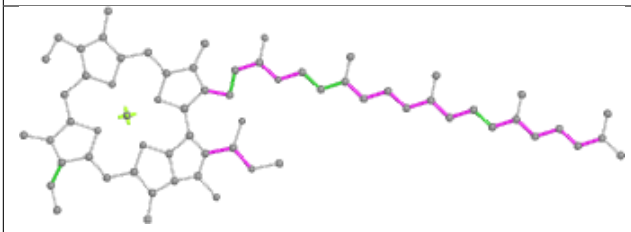


Bond angles



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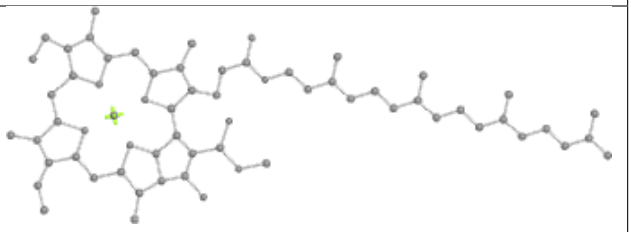
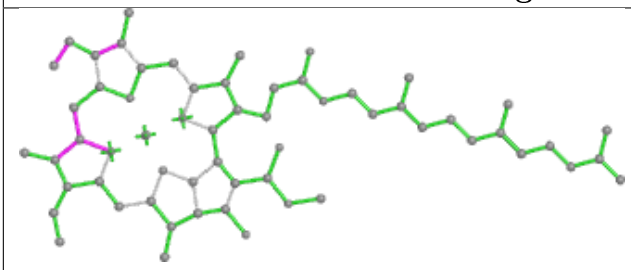
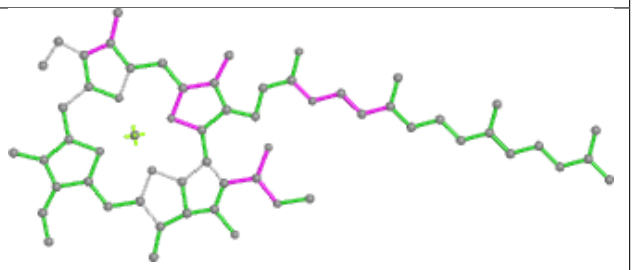


Rings

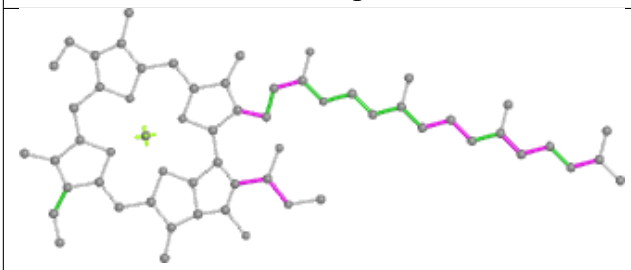
Ligand CLA B 1234



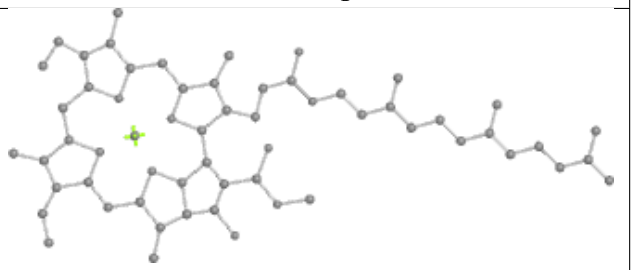
Bond lengths



Bond angles

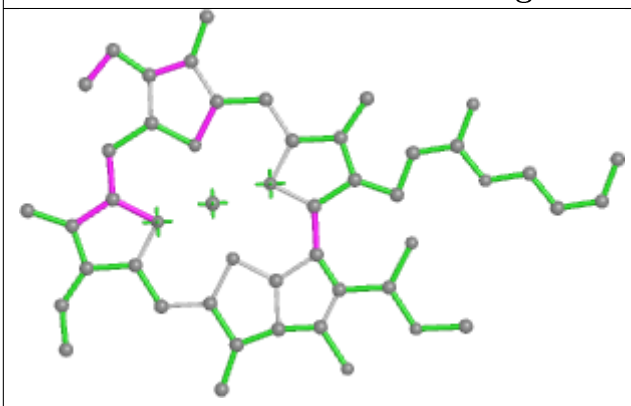


Torsions



Rings

Ligand CLA B 1209



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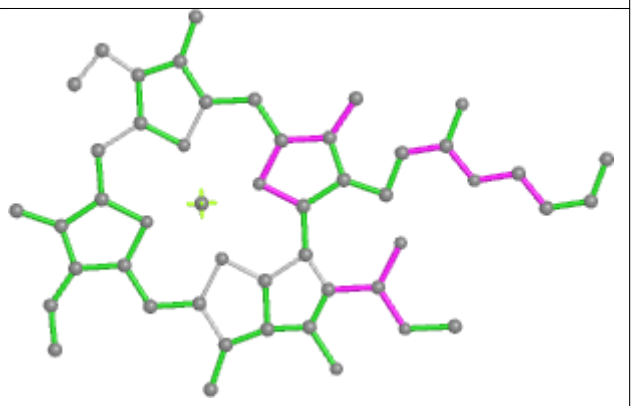
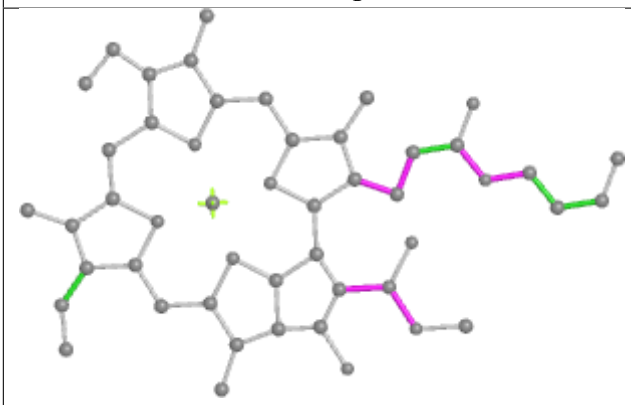
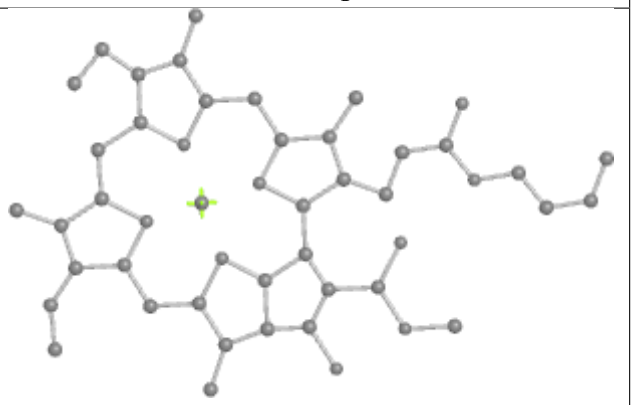


Bond angles

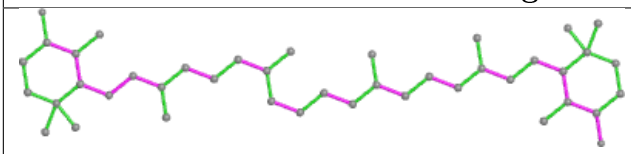


Torsions

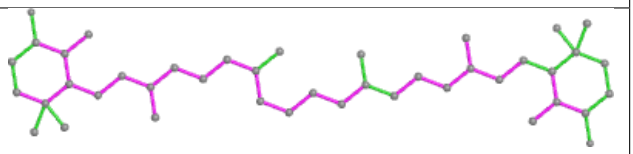


Rings

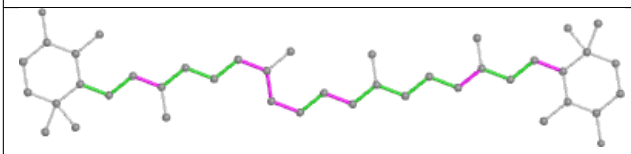
Ligand 45D B 4011



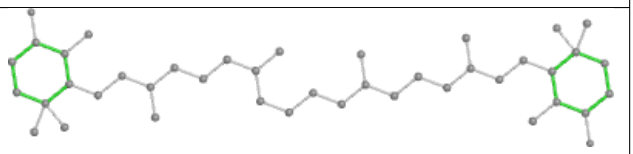
Bond lengths



Bond angles

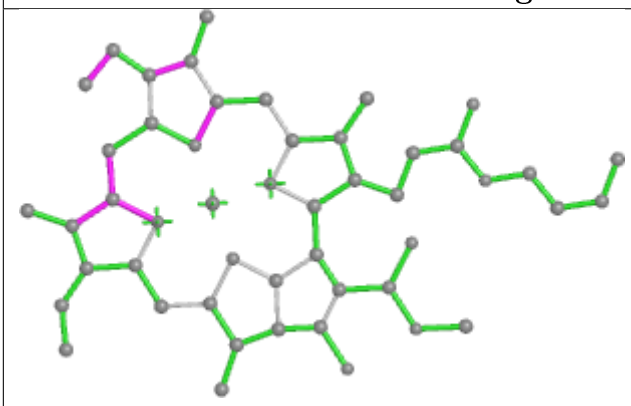


Torsions



Rings

Ligand CLA B 1236



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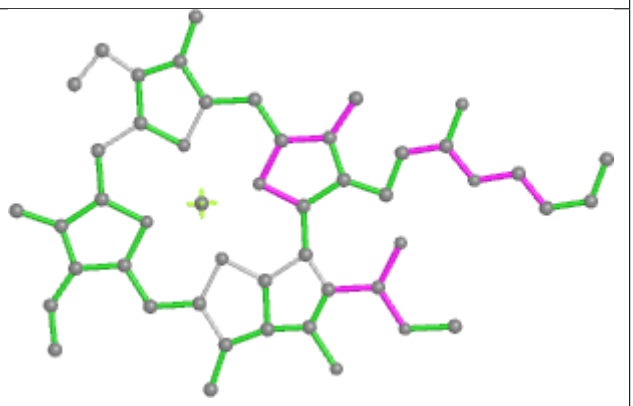
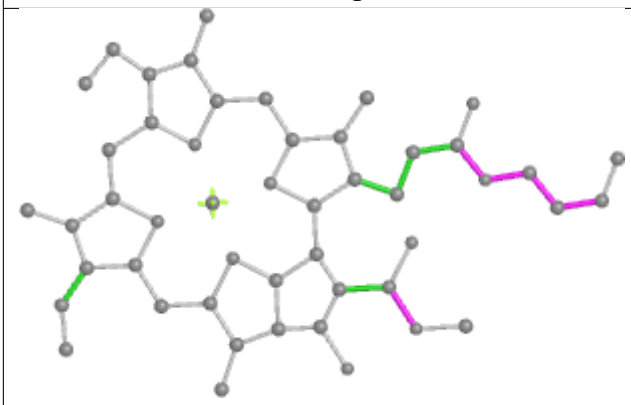


Bond angles



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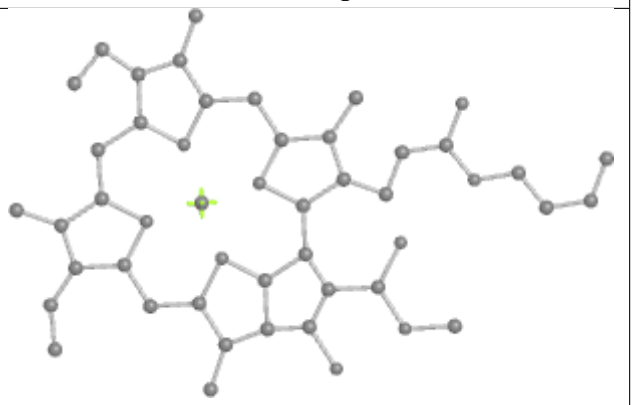
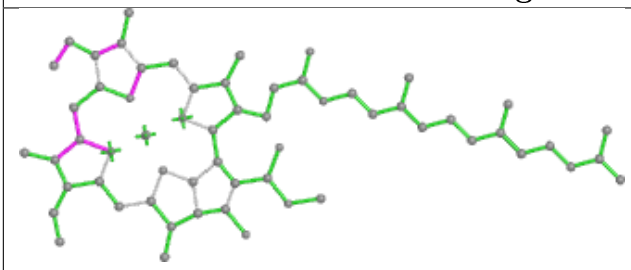


Rings

Ligand CLA B 1022



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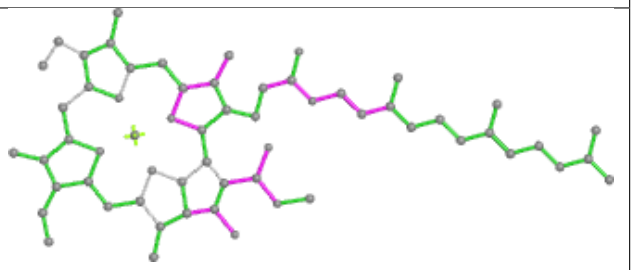
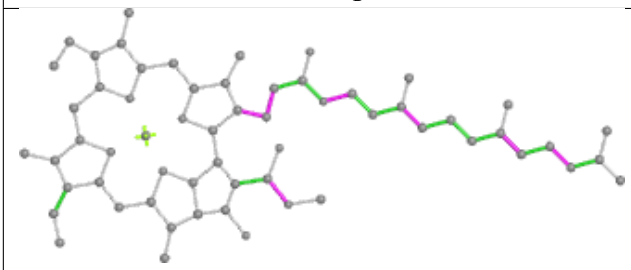
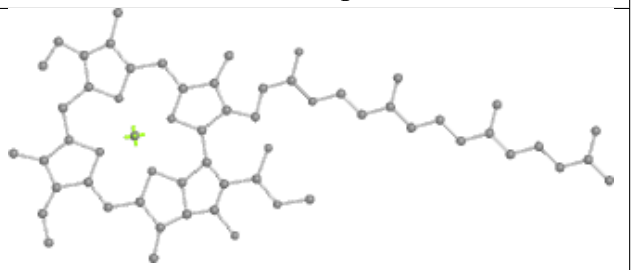


Bond angles

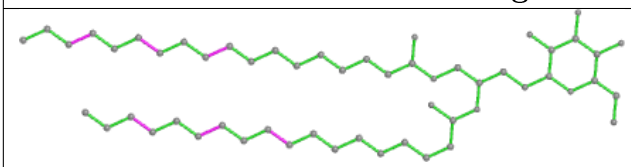


Torsions



Rings

Ligand LMG B 5005



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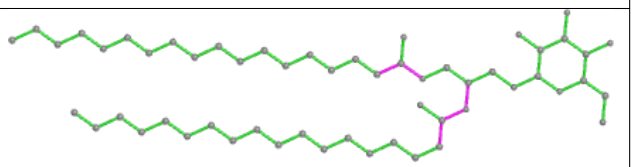
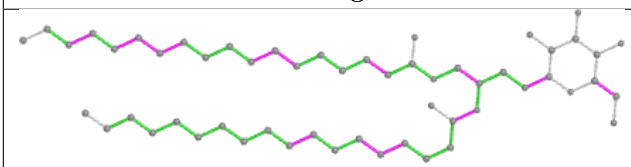
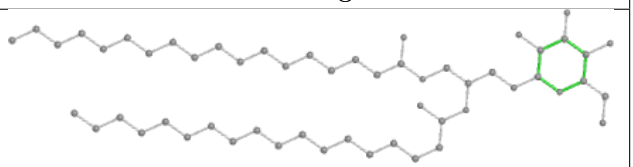


Bond angles

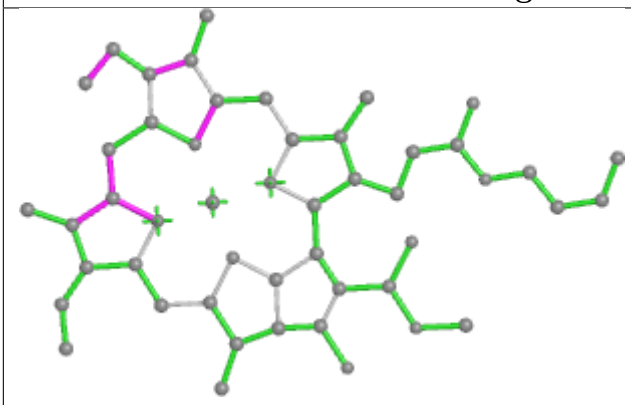


Torsions

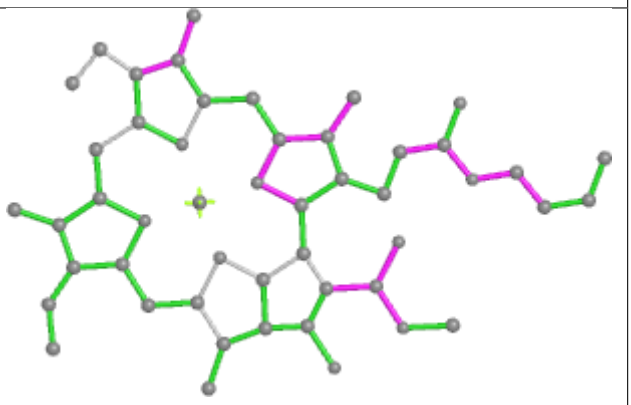


Rings

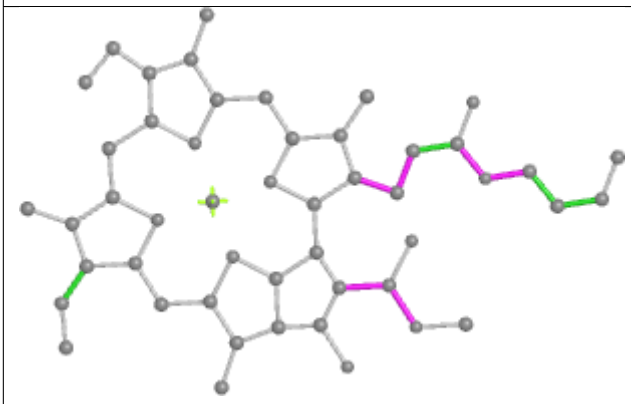
Ligand CLA B 1228



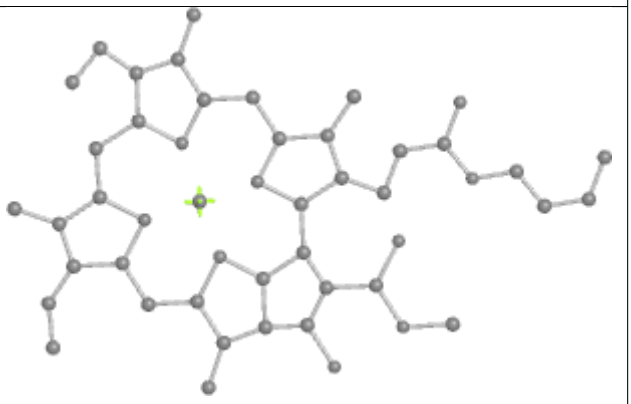
Bond lengths



Bond angles

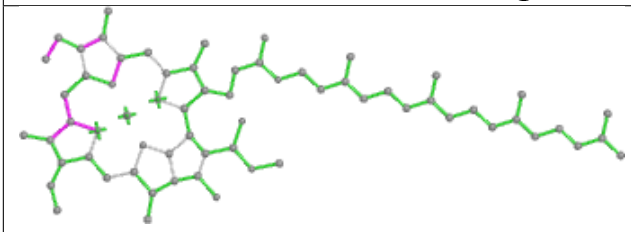


Torsions

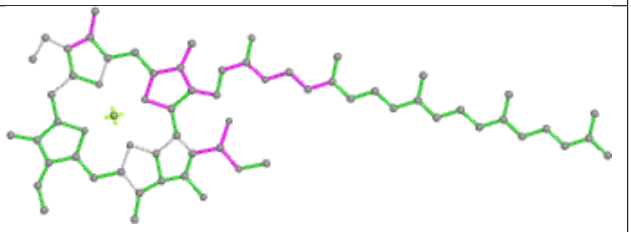


Rings

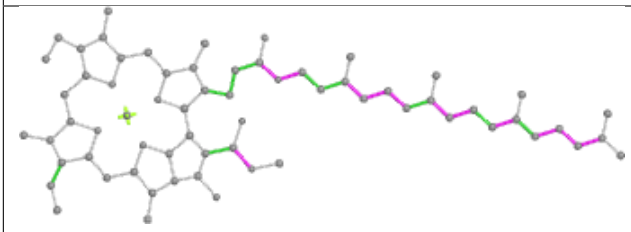
Ligand CLA A 1109



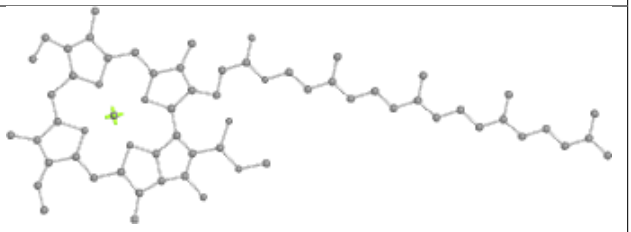
Bond lengths



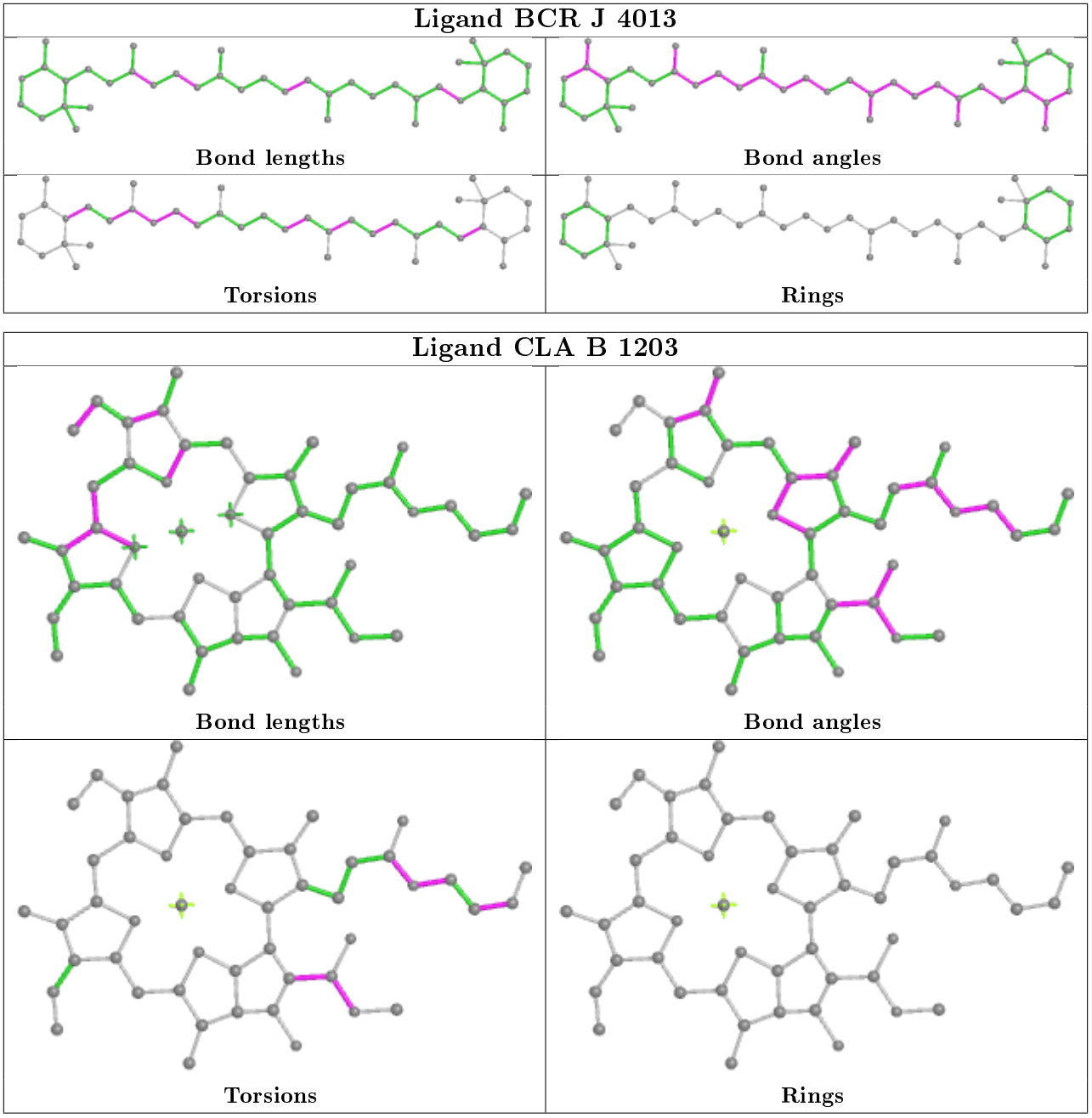
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	751/751 (100%)	-0.54	9 (1%) 79 70	27, 117, 229, 322	0
2	B	731/731 (100%)	-0.68	0 100 100	18, 95, 176, 428	0
3	C	80/80 (100%)	-0.56	0 100 100	31, 87, 122, 144	0
4	D	141/141 (100%)	-0.29	1 (0%) 87 82	67, 112, 187, 399	0
5	E	69/69 (100%)	-0.58	0 100 100	45, 81, 154, 170	0
6	F	143/143 (100%)	-0.75	0 100 100	28, 98, 148, 186	0
7	I	40/40 (100%)	1.25	14 (35%) 0 0	228, 290, 404, 432	0
8	J	40/40 (100%)	-0.77	0 100 100	73, 106, 144, 149	0
9	K	70/70 (100%)	-0.34	3 (4%) 35 29	150, 241, 380, 499	0
10	L	137/137 (100%)	0.96	32 (23%) 0 0	231, 373, 583, 606	0
11	M	31/31 (100%)	-0.48	0 100 100	123, 149, 199, 221	0
All	All	2233/2233 (100%)	-0.46	59 (2%) 56 46	18, 109, 335, 606	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	L	110	SER	6.3
10	L	23	PRO	5.6
10	L	74	SER	5.5
1	A	237	PRO	4.9
10	L	43	GLY	4.6

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CLA	L	1502	49/65	0.50	0.35	382,393,407,412	0
22	CA	L	1001	1/1	0.52	0.15	156,156,156,156	0
25	EQ3	I	4020	42/42	0.59	0.53	224,232,241,245	0
19	ECH	M	4021	41/41	0.63	0.44	148,166,189,200	0
21	SQD	B	5008	54/54	0.66	0.69	92,154,193,201	0
15	BCR	A	4003	40/40	0.66	0.63	124,164,188,189	0
15	BCR	I	4018	40/40	0.72	0.65	161,194,217,223	0
16	LHG	B	5006	21/49	0.76	0.30	154,179,195,201	0
20	LMG	B	5005	55/55	0.76	0.45	80,149,188,190	0
21	SQD	F	5001	54/54	0.79	0.58	149,164,176,178	0
15	BCR	A	4001	40/40	0.83	0.30	148,169,184,185	0
19	ECH	B	4006	41/41	0.83	0.34	111,135,146,150	0
12	CLA	B	1207	49/65	0.84	0.24	131,157,223,227	0
24	LMT	F	6001	35/35	0.84	0.39	78,142,171,178	0
15	BCR	K	4001	40/40	0.85	0.48	129,194,221,223	0
15	BCR	B	4004	40/40	0.87	0.67	105,125,134,138	0
12	CLA	B	1212	49/65	0.87	0.34	124,146,166,171	0
12	CLA	A	1118	50/65	0.87	0.24	120,151,195,209	0
12	CLA	J	1303	49/65	0.87	0.45	145,167,176,202	0
12	CLA	A	1112	49/65	0.88	0.41	138,146,155,164	0
16	LHG	A	5003	49/49	0.88	0.46	106,135,156,160	0
12	CLA	A	1113	49/65	0.88	0.49	135,160,184,192	0
12	CLA	A	1141	45/65	0.89	0.40	137,156,176,188	0
12	CLA	B	1204	49/65	0.89	0.28	94,111,127,139	0
12	CLA	K	1401	45/65	0.89	0.32	127,147,170,175	0
12	CLA	A	1114	49/65	0.89	0.23	142,154,173,178	0
12	CLA	K	1402	49/65	0.89	0.24	168,189,213,218	0
12	CLA	B	1240	49/65	0.90	0.49	76,105,156,163	0
12	CLA	A	1132	55/65	0.90	0.27	107,148,273,351	0
12	CLA	B	1211	49/65	0.90	0.18	100,120,130,134	0
12	CLA	F	1302	49/65	0.90	0.23	63,82,106,112	0
12	CLA	B	1217	49/65	0.90	0.33	72,85,95,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CLA	A	1111	49/65	0.90	0.32	70,113,131,146	0
15	BCR	B	4018	40/40	0.90	0.55	61,121,136,140	0
12	CLA	A	1105	65/65	0.90	0.36	66,114,126,130	0
12	CLA	F	1301	49/65	0.91	0.31	80,98,136,138	0
12	CLA	A	1120	49/65	0.91	0.26	130,149,195,200	0
15	BCR	B	4017	40/40	0.91	0.47	50,68,88,91	0
12	CLA	J	1302	49/65	0.91	0.28	134,150,159,160	0
15	BCR	A	4007	40/40	0.91	0.54	66,82,134,137	0
15	BCR	F	4014	40/40	0.91	0.43	57,85,104,106	0
12	CLA	B	1209	49/65	0.91	0.33	107,131,139,144	0
12	CLA	A	1110	49/65	0.91	0.34	130,154,173,179	0
15	BCR	J	4013	40/40	0.91	0.37	88,110,132,133	0
12	CLA	B	1203	49/65	0.91	0.33	75,86,99,103	0
12	CLA	A	1119	46/65	0.92	0.32	106,126,144,154	0
12	CLA	B	1219	49/65	0.92	0.22	64,91,133,135	0
12	CLA	A	1130	49/65	0.92	0.18	77,95,130,133	0
12	CLA	A	1125	49/65	0.92	0.26	108,124,132,135	0
12	CLA	A	1116	49/65	0.92	0.21	96,126,142,150	0
12	CLA	B	1208	49/65	0.92	0.33	90,107,128,130	0
12	CLA	B	1201	49/65	0.92	0.25	77,89,106,110	0
12	CLA	A	1011	55/65	0.92	0.22	43,63,72,89	0
12	CLA	A	1108	49/65	0.92	0.28	89,101,135,142	0
12	CLA	A	1115	56/65	0.92	0.21	118,146,155,156	0
12	CLA	B	1216	49/65	0.92	0.41	58,113,119,124	0
20	LMG	B	5002	55/55	0.92	0.45	37,69,102,118	0
22	CA	B	6001	1/1	0.92	0.15	171,171,171,171	0
15	BCR	A	4008	40/40	0.92	0.50	43,110,125,125	0
16	LHG	B	5004	49/49	0.92	0.44	57,80,128,133	0
12	CLA	B	1213	49/65	0.92	0.29	105,121,132,141	0
15	BCR	A	4012	40/40	0.92	0.48	66,81,92,93	0
18	CL	B	6000	1/1	0.92	0.21	89,89,89,89	0
12	CLA	A	1135	49/65	0.92	0.39	110,119,124,128	0
15	BCR	B	4005	40/40	0.93	0.40	31,63,141,143	0
12	CLA	A	1137	49/65	0.93	0.33	92,112,121,126	0
12	CLA	B	1238	49/65	0.93	0.23	82,108,125,127	0
12	CLA	A	1129	49/65	0.93	0.32	96,116,153,160	0
13	PQN	B	2002	33/33	0.93	0.45	72,83,105,111	0
12	CLA	A	1131	49/65	0.93	0.25	111,130,156,163	0
12	CLA	B	1218	49/65	0.93	0.24	64,90,122,130	0
23	C7Z	F	4016	42/42	0.93	0.32	35,58,93,97	0
12	CLA	B	1234	60/65	0.93	0.25	55,77,106,112	0
12	CLA	A	1133	49/65	0.93	0.24	98,115,131,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CLA	B	1236	49/65	0.93	0.24	49,63,76,77	0
12	CLA	A	1117	49/65	0.93	0.24	78,99,110,116	0
12	CLA	A	1109	65/65	0.93	0.22	64,113,123,126	0
12	CLA	A	1134	49/65	0.93	0.25	109,140,149,156	0
12	CLA	A	1122	49/65	0.93	0.29	90,108,122,124	0
12	CLA	B	1221	49/65	0.94	0.36	60,105,115,122	0
12	CLA	B	1225	49/65	0.94	0.24	36,61,78,80	0
12	CLA	B	1215	49/65	0.94	0.20	67,79,87,89	0
12	CLA	A	1136	49/65	0.94	0.42	128,139,145,149	0
12	CLA	A	1013	65/65	0.94	0.27	19,57,67,79	0
12	CLA	B	1235	65/65	0.94	0.22	37,60,72,74	0
12	CLA	B	1232	49/65	0.94	0.18	70,82,98,101	0
12	CLA	A	1103	49/65	0.94	0.21	75,90,108,114	0
12	CLA	A	1126	60/65	0.94	0.23	28,79,96,102	0
12	CLA	B	1223	49/65	0.94	0.30	81,96,110,113	0
12	CLA	A	1124	49/65	0.94	0.34	100,122,134,135	0
12	CLA	B	1227	49/65	0.94	0.34	80,91,140,146	0
12	CLA	A	1121	49/65	0.94	0.38	90,117,137,142	0
12	CLA	A	1123	60/65	0.94	0.22	67,85,100,104	0
12	CLA	A	1127	49/65	0.94	0.24	72,86,97,103	0
17	45D	B	4011	42/42	0.94	0.28	45,59,68,68	0
12	CLA	B	1205	49/65	0.94	0.36	57,73,97,106	0
12	CLA	B	1022	60/65	0.94	0.22	31,89,94,102	0
12	CLA	B	1220	49/65	0.94	0.31	77,91,96,98	0
12	CLA	A	1012	49/65	0.94	0.20	38,63,73,74	0
12	CLA	B	1222	50/65	0.94	0.22	69,81,93,97	0
12	CLA	B	1237	49/65	0.94	0.17	92,112,121,127	0
12	CLA	A	1140	65/65	0.95	0.32	16,65,78,88	0
12	CLA	A	1128	65/65	0.95	0.26	32,87,97,104	0
15	BCR	B	4010	40/40	0.95	0.41	43,57,71,73	0
23	C7Z	J	4015	42/42	0.95	0.33	60,87,96,101	0
12	CLA	A	1107	50/65	0.95	0.27	42,53,69,94	0
12	CLA	B	1231	49/65	0.95	0.21	49,85,97,109	0
12	CLA	B	1021	65/65	0.95	0.19	22,41,55,65	0
16	LHG	A	5001	49/49	0.95	0.32	38,59,91,113	0
12	CLA	B	1206	49/65	0.95	0.22	75,86,127,132	0
12	CLA	A	1104	49/65	0.95	0.20	60,85,96,101	0
12	CLA	B	1224	55/65	0.95	0.24	13,49,70,75	0
12	CLA	B	1226	49/65	0.95	0.23	29,59,81,85	0
12	CLA	A	1102	65/65	0.95	0.27	70,86,98,104	0
12	CLA	B	1228	49/65	0.95	0.39	56,67,96,97	0
12	CLA	B	1214	60/65	0.95	0.23	46,80,102,105	0

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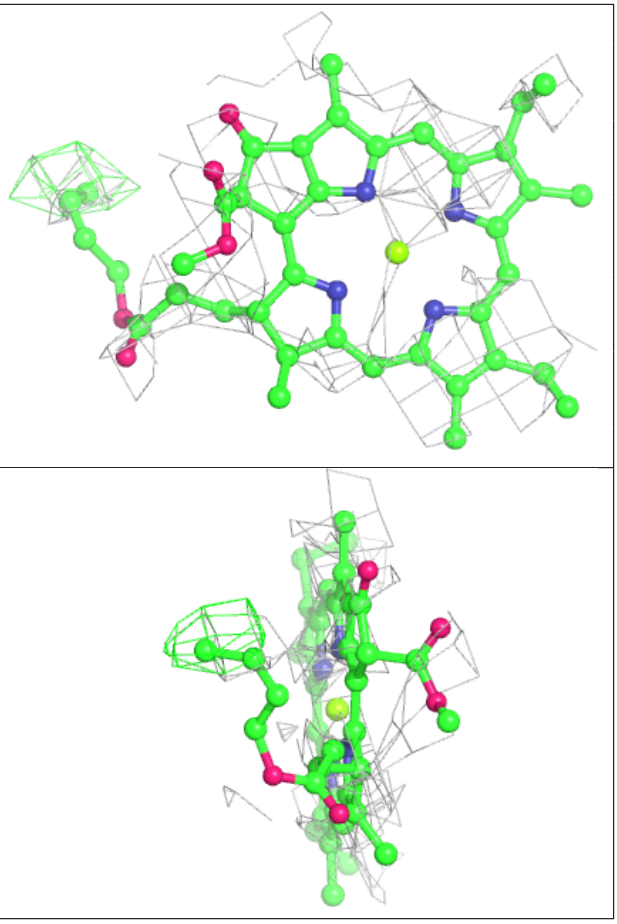
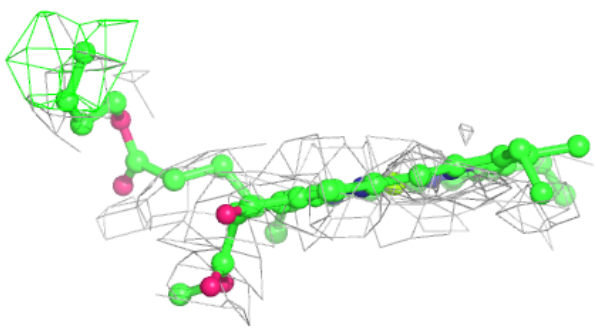
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CLA	A	1106	65/65	0.95	0.27	72,95,117,130	0
12	CLA	A	1139	55/65	0.95	0.26	43,59,110,117	0
12	CLA	B	1230	49/65	0.96	0.21	66,77,81,86	0
13	PQN	A	2001	33/33	0.96	0.38	13,27,42,50	0
12	CLA	B	1023	49/65	0.96	0.15	65,80,89,93	0
12	CLA	B	1239	49/65	0.96	0.27	36,61,108,114	0
12	CLA	B	1202	65/65	0.96	0.26	12,70,77,79	0
12	CLA	B	1229	55/65	0.96	0.19	33,44,62,64	0
12	CLA	A	1101	49/65	0.96	0.23	52,74,79,86	0
12	CLA	A	1138	65/65	0.97	0.23	26,55,72,76	0
12	CLA	B	1210	49/65	0.97	0.24	42,72,80,82	0
14	SF4	C	3002	8/8	0.99	0.12	32,41,89,113	0
14	SF4	A	3001	8/8	0.99	0.13	36,63,86,101	0
14	SF4	C	3003	8/8	1.00	0.16	32,57,177,197	0

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

Electron density around CLA L 1502:

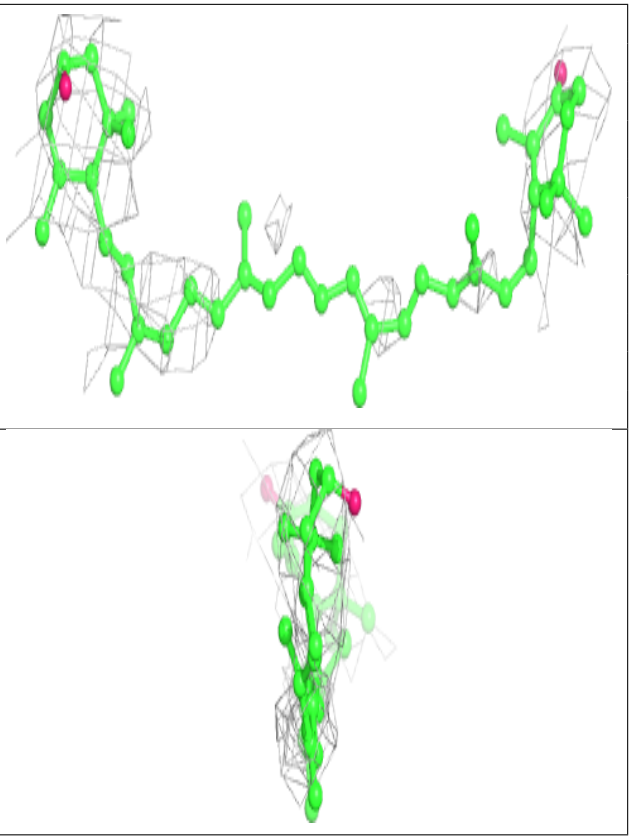
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





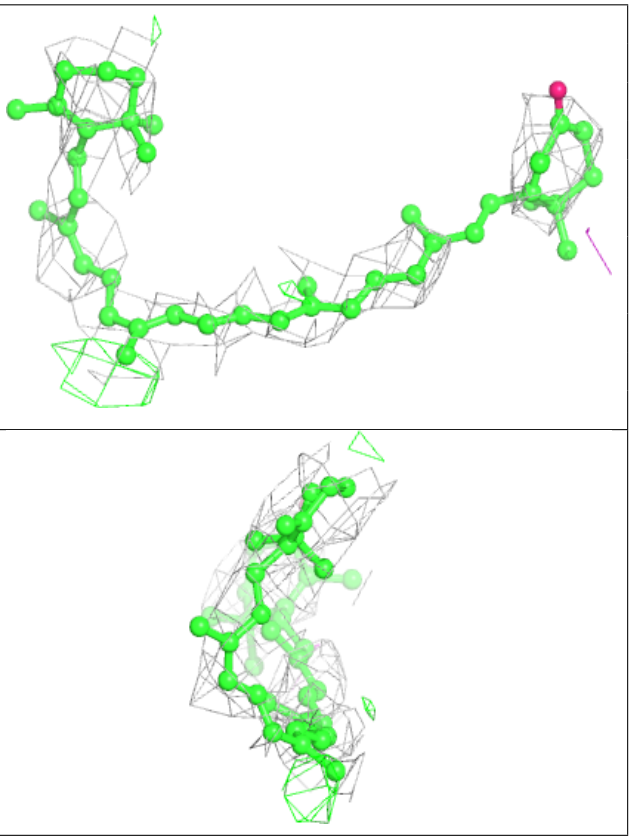
Electron density around EQ3 I 4020:

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



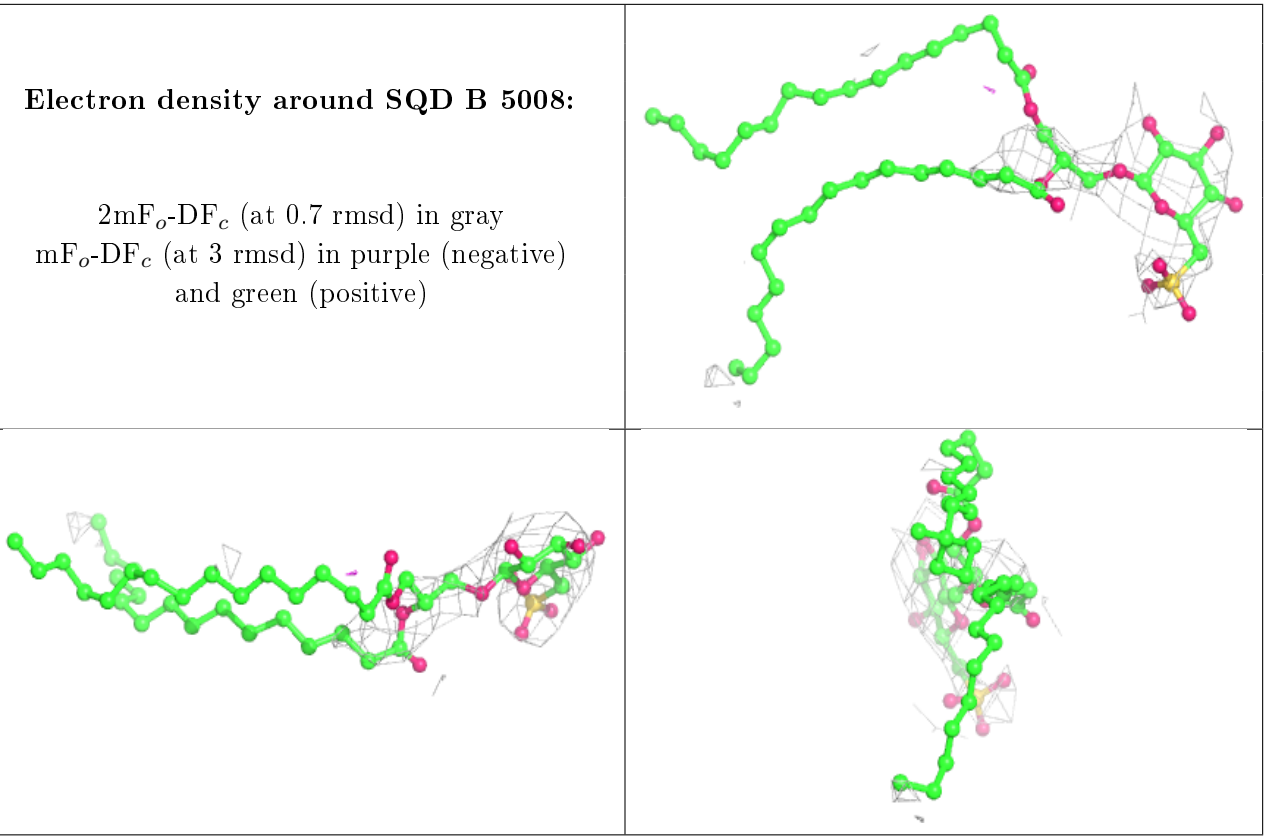
Electron density around ECH M 4021:

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



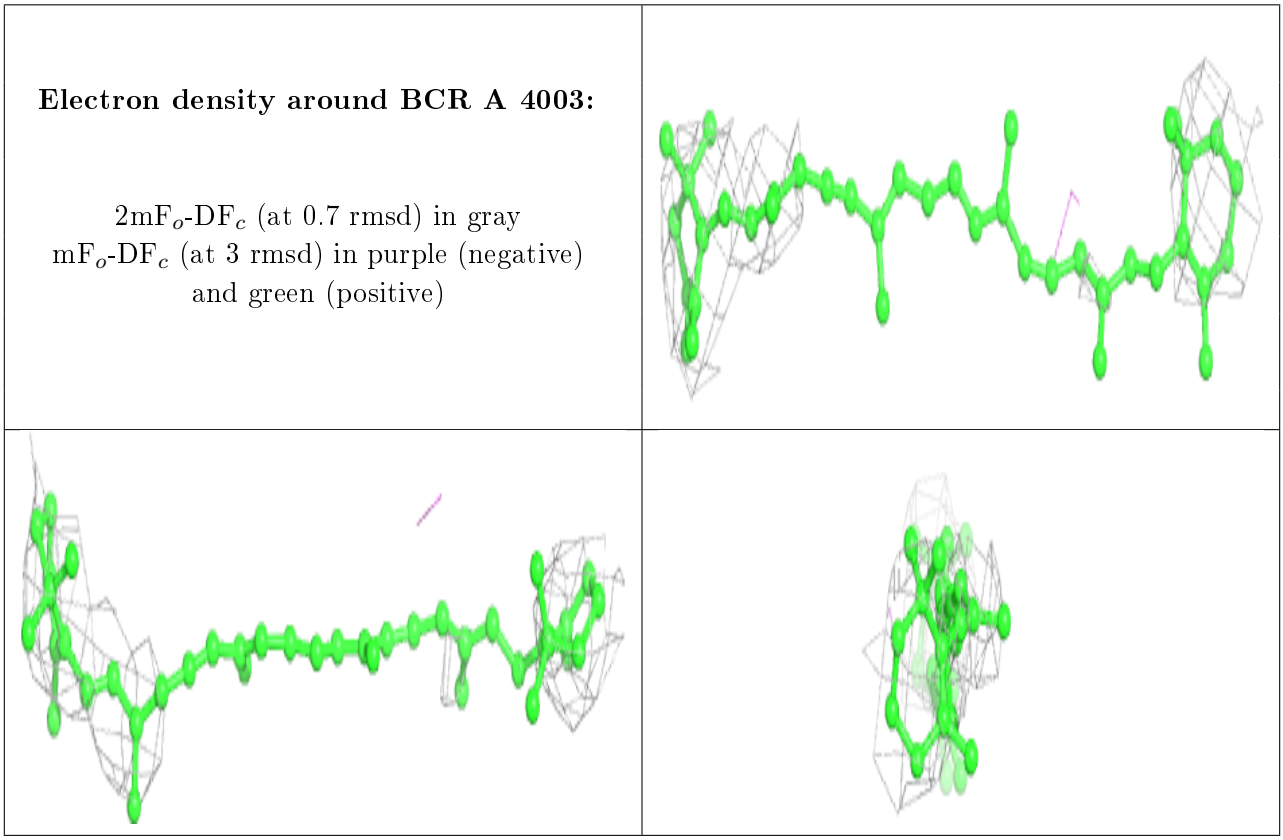
Electron density around SQD B 5008:

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



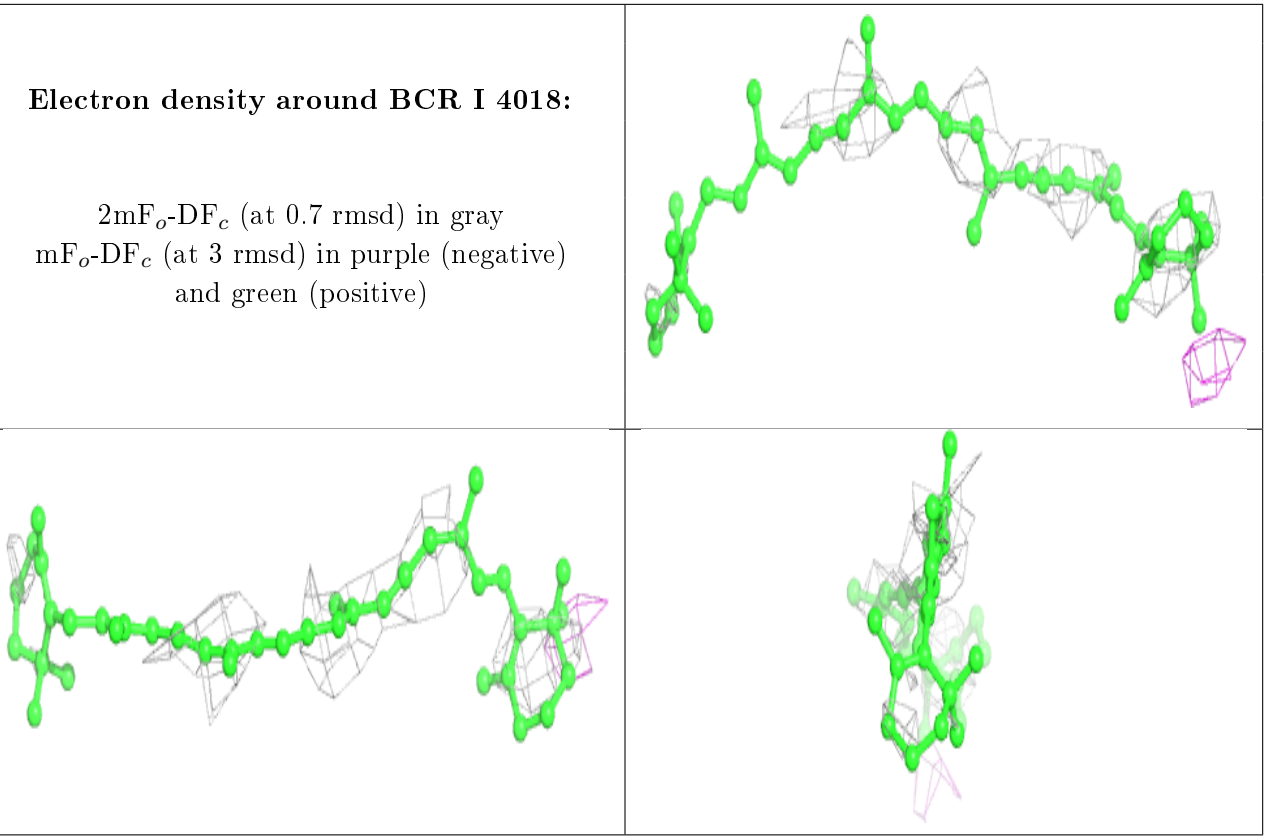
Electron density around BCR A 4003:

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



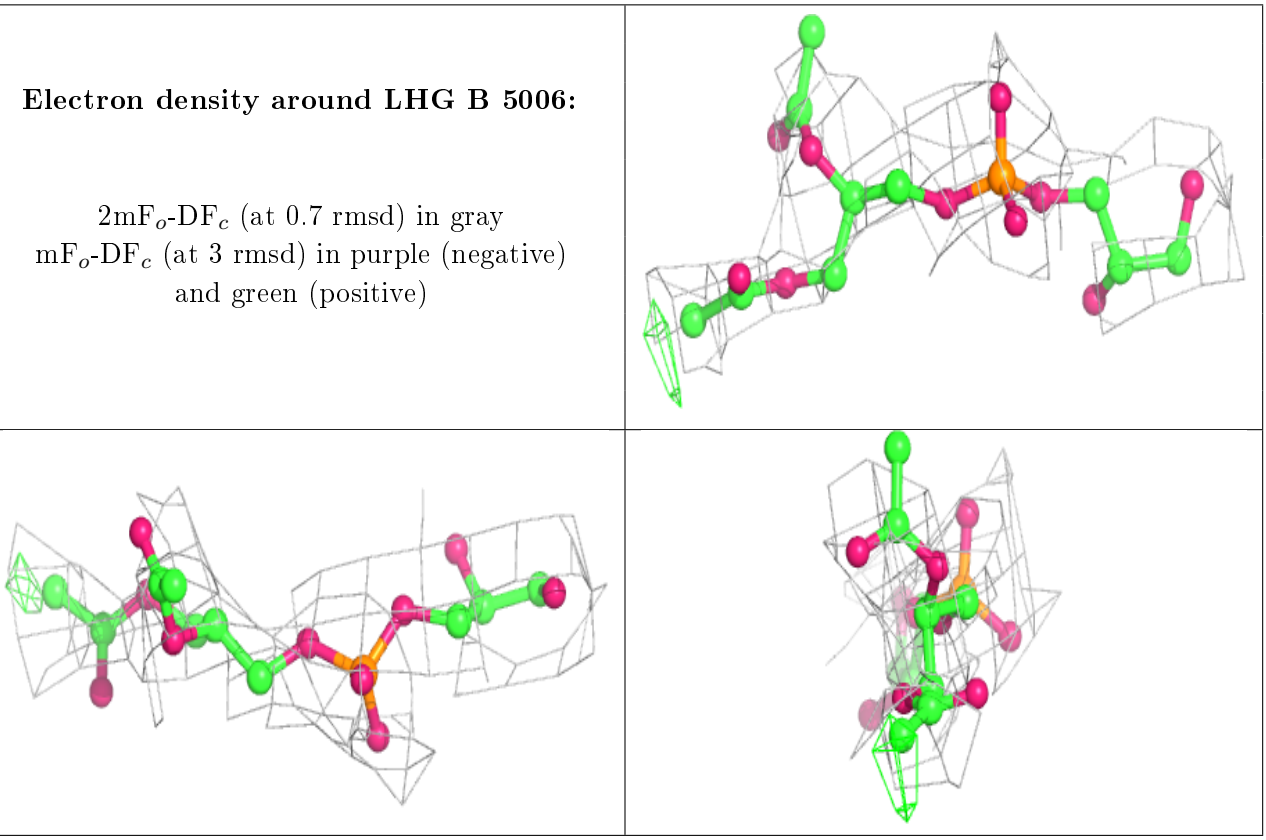
Electron density around BCR I 4018:

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



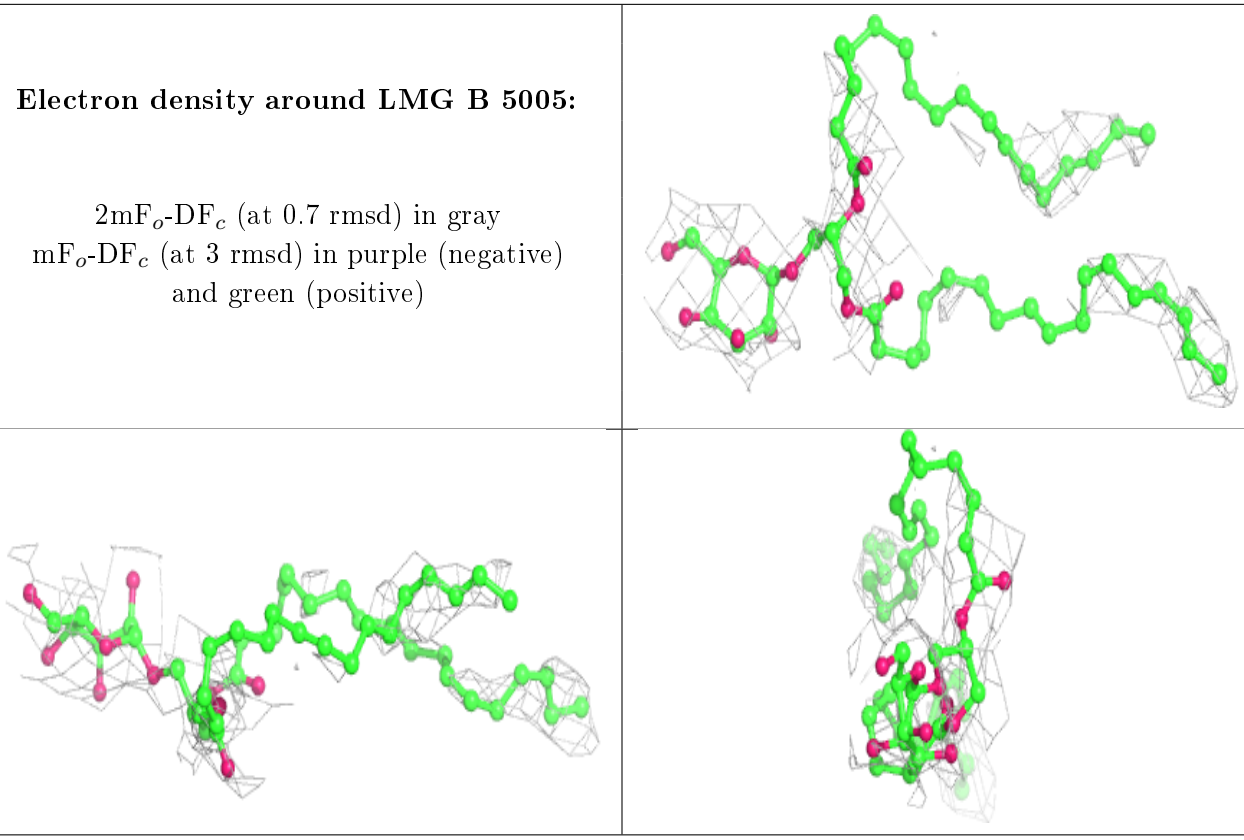
Electron density around LHG B 5006:

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



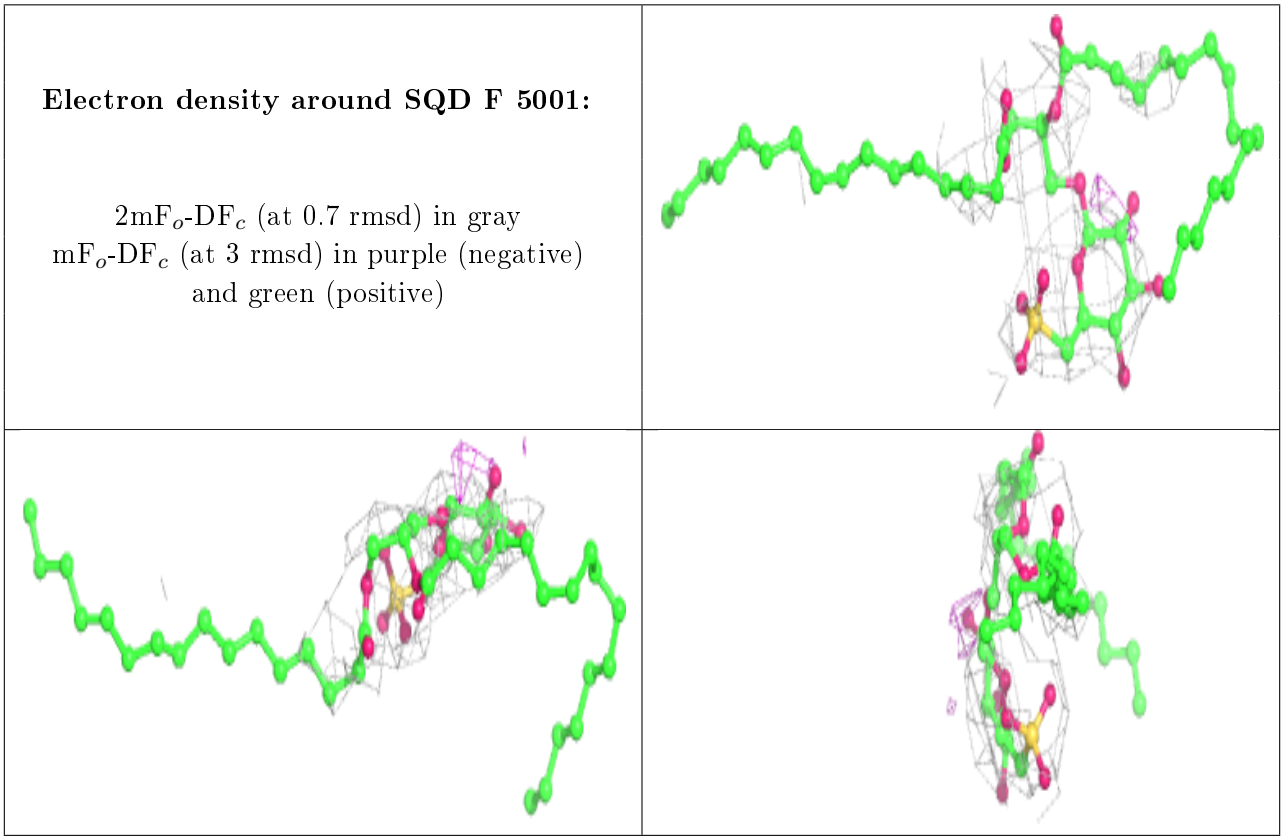
Electron density around LMG B 5005:

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



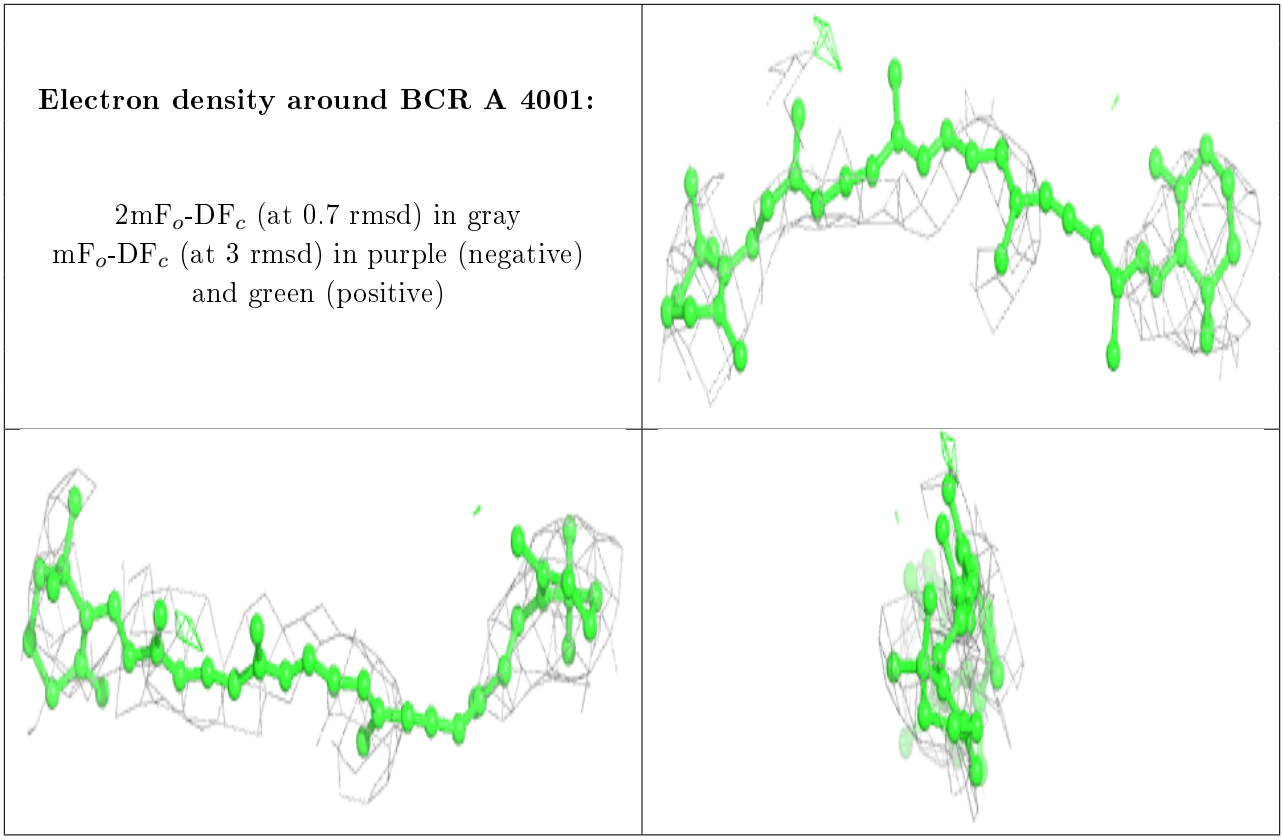
Electron density around SQD F 5001:

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



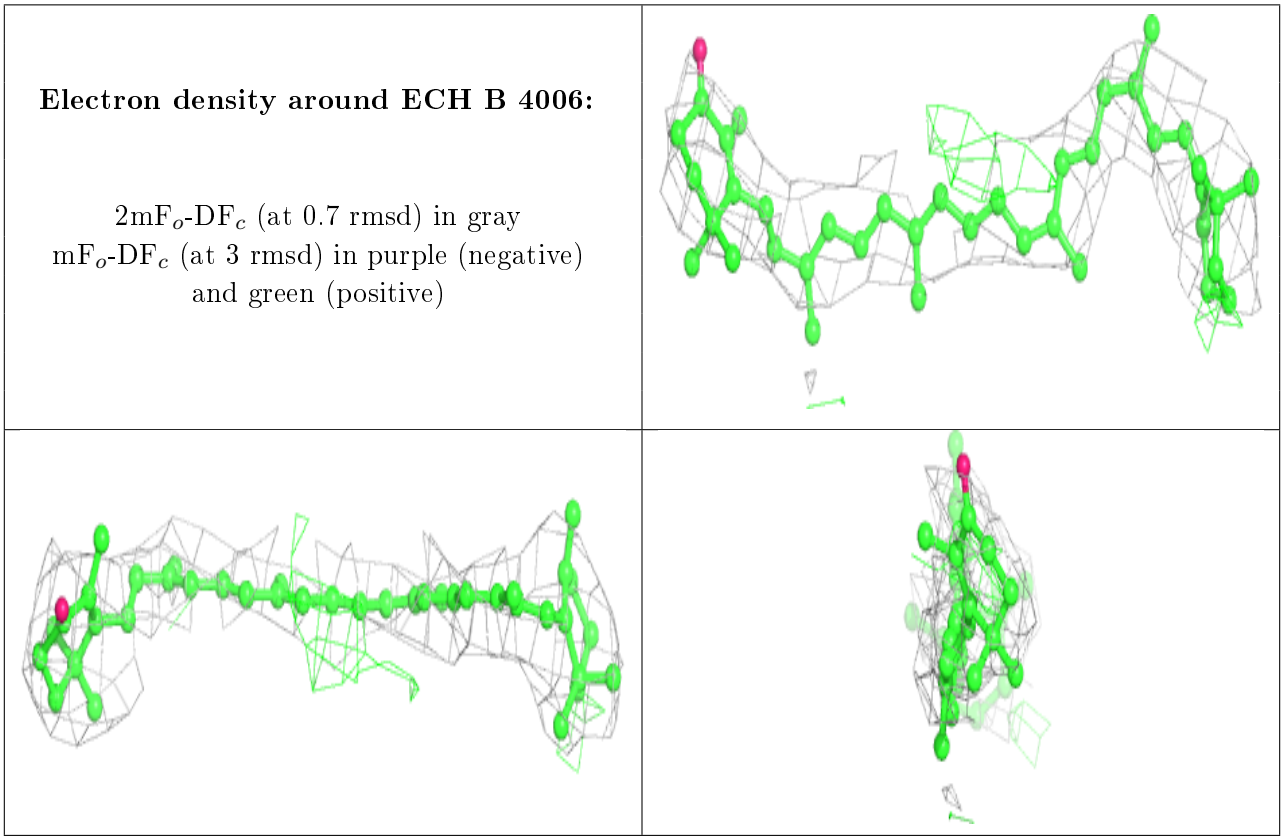
Electron density around BCR A 4001:

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



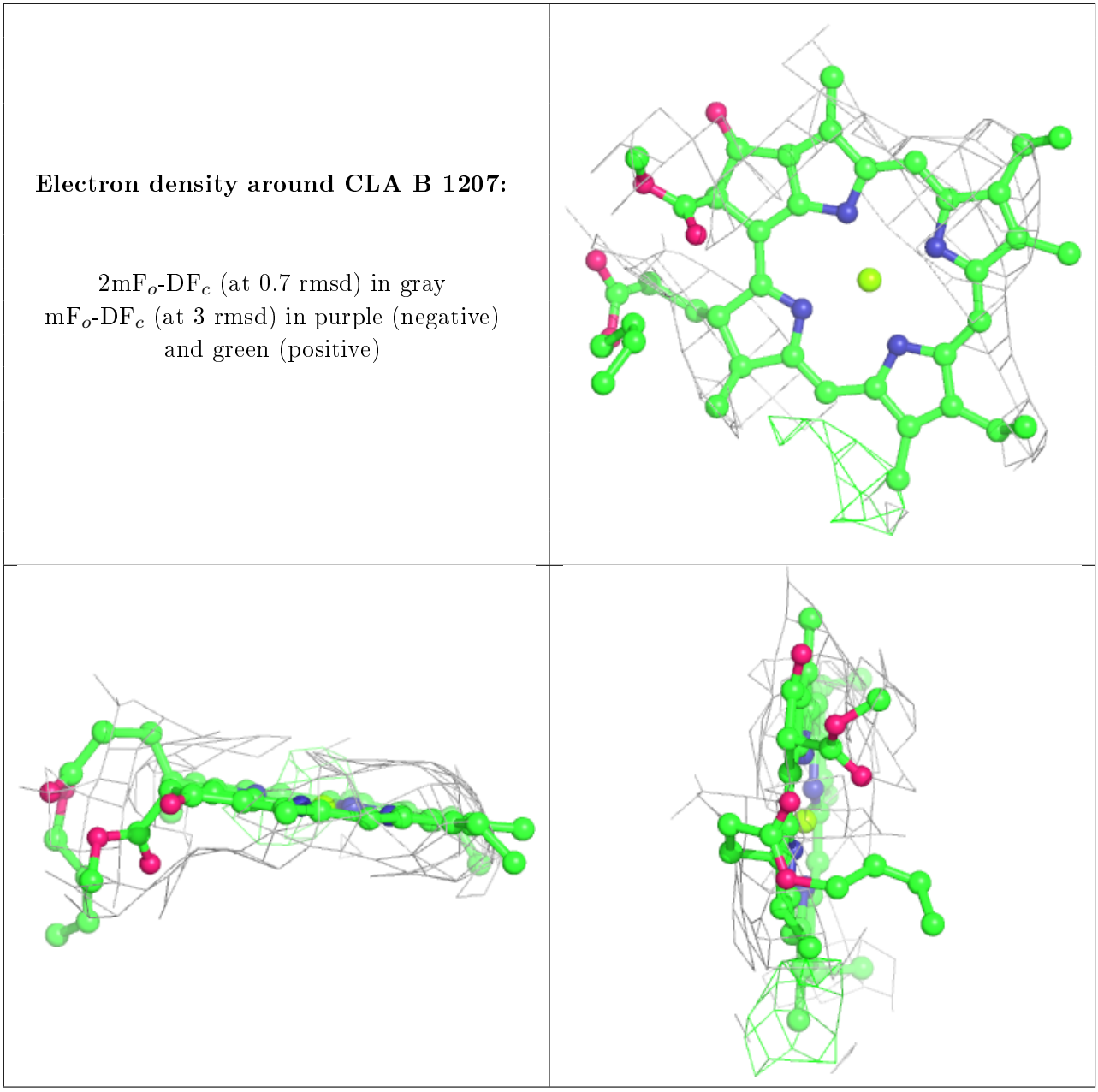
Electron density around ECH B 4006:

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



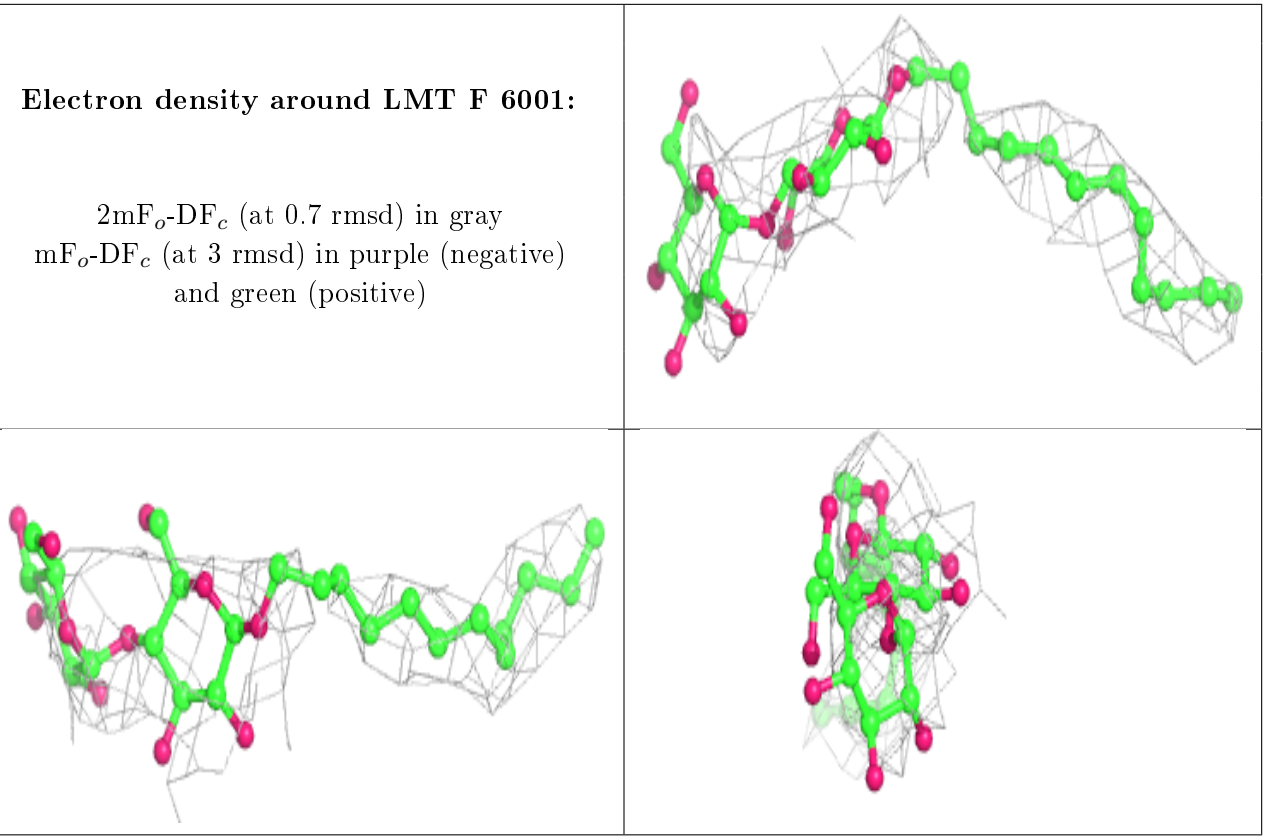
Electron density around CLA B 1207:

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



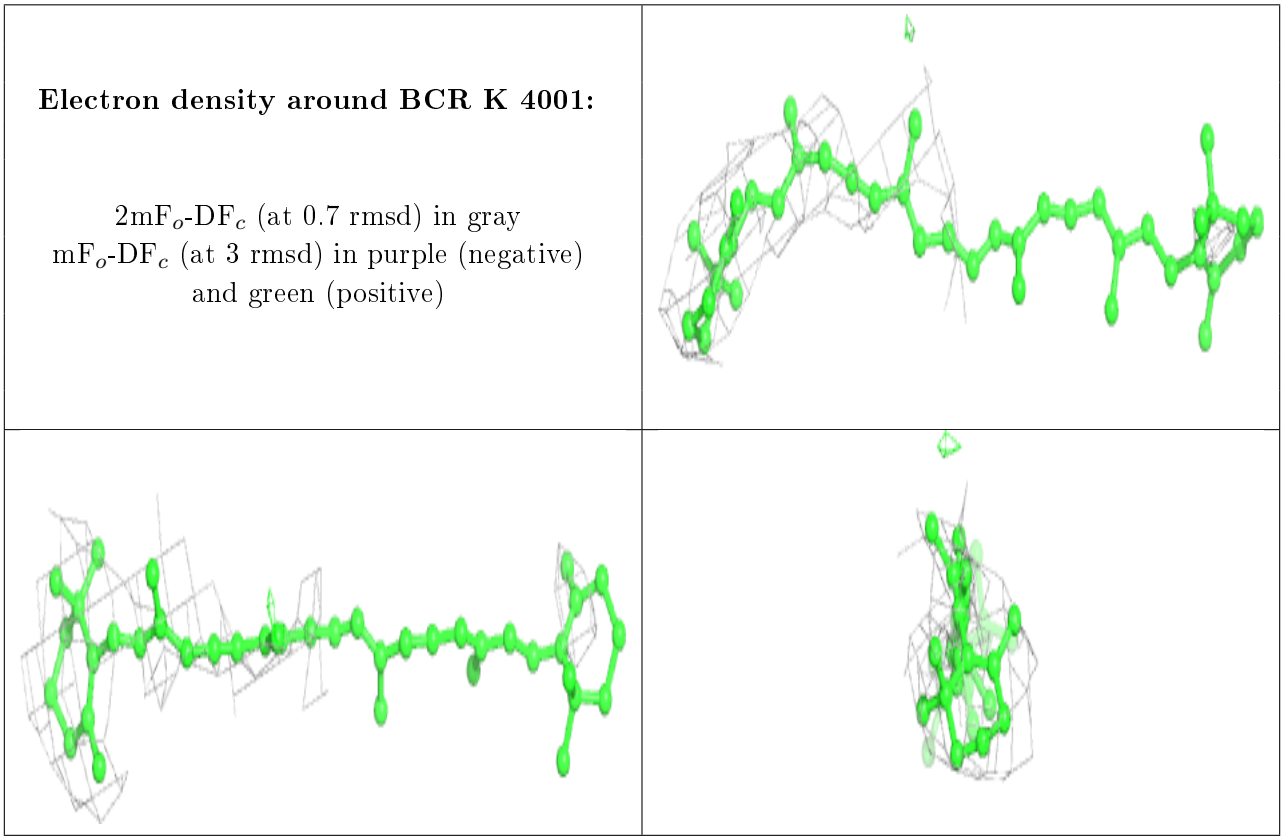
Electron density around LMT F 6001:

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



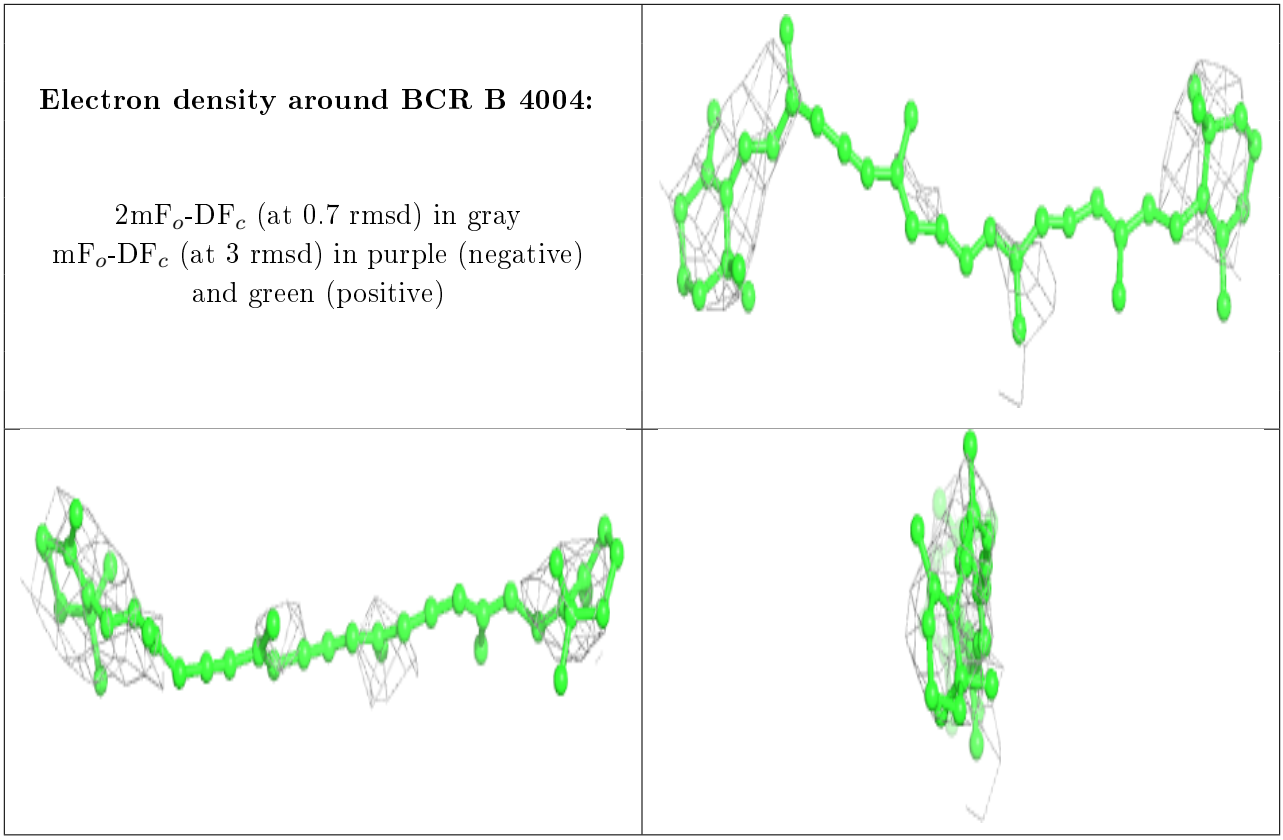
Electron density around BCR K 4001:

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



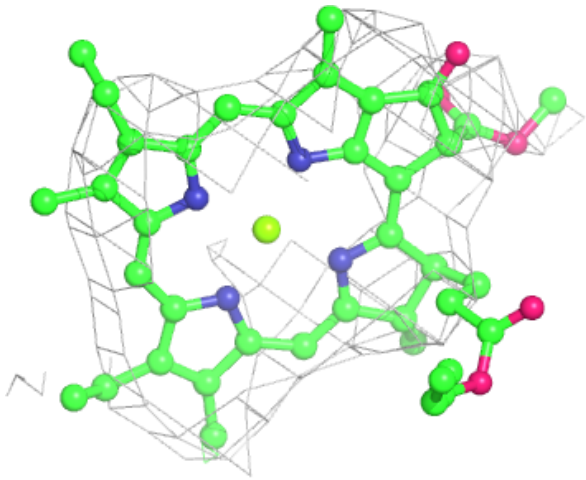
Electron density around BCR B 4004:

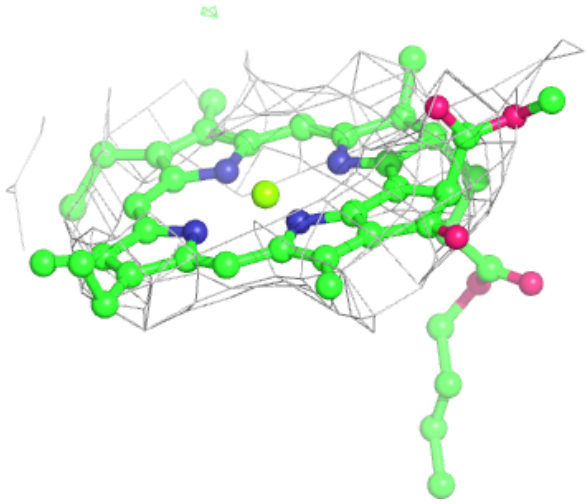
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

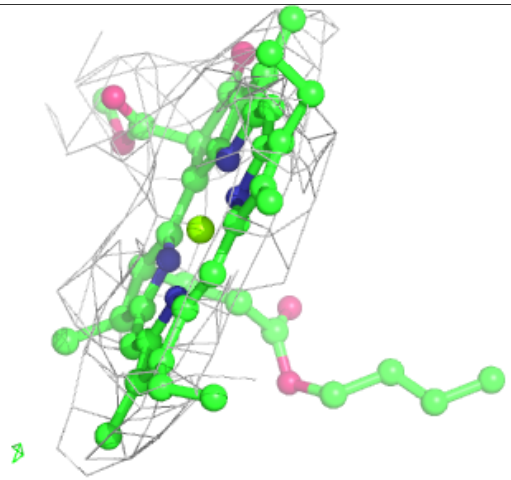


Electron density around CLA B 1212:

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

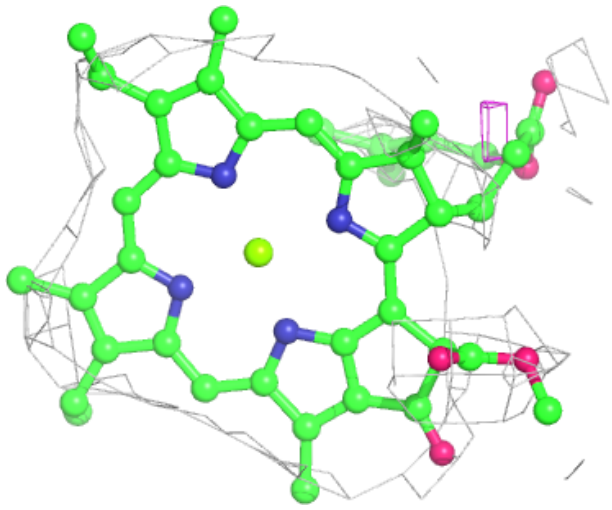


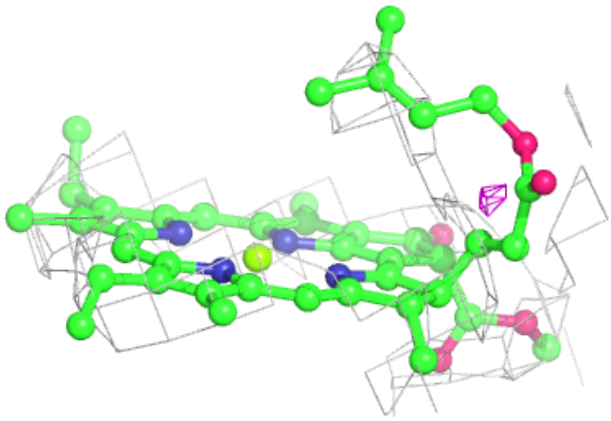


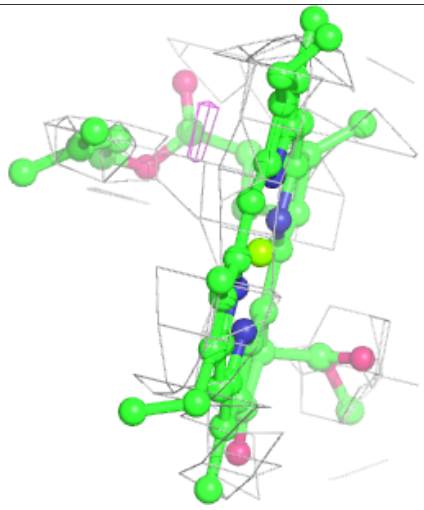


Electron density around CLA A 1118:

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

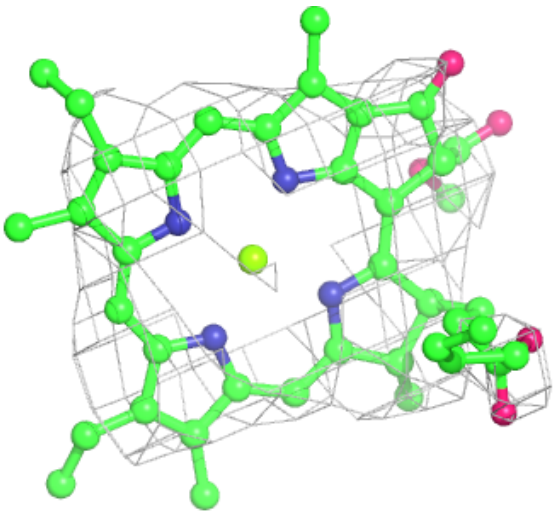


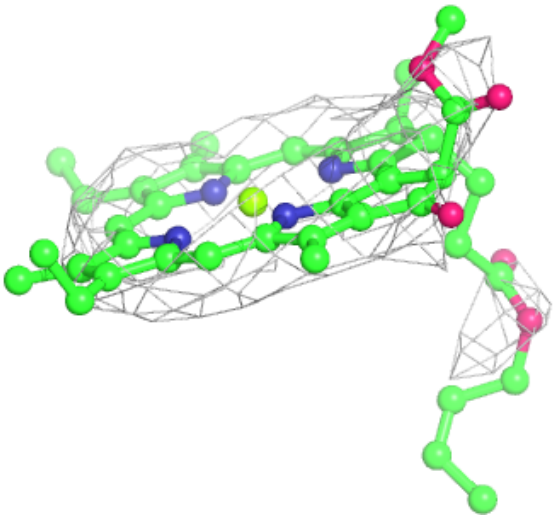


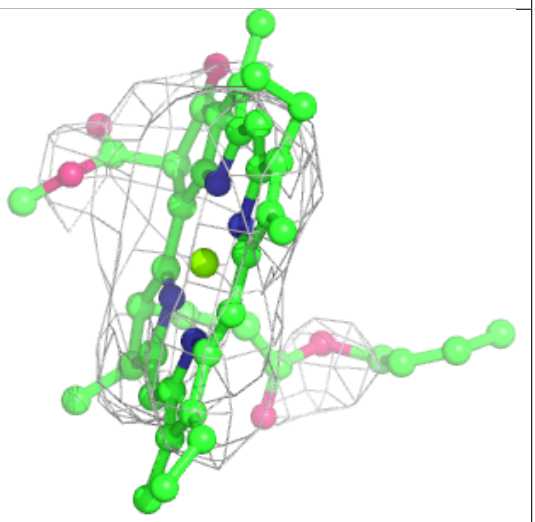


Electron density around CLA J 1303:

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

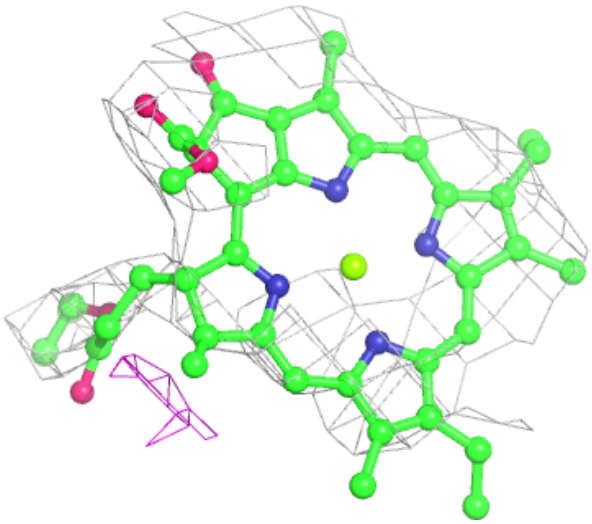


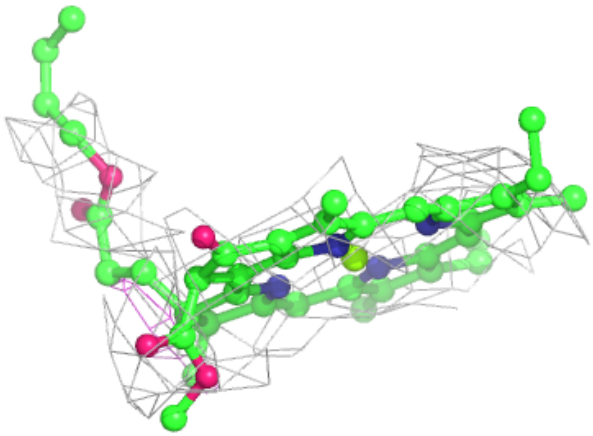


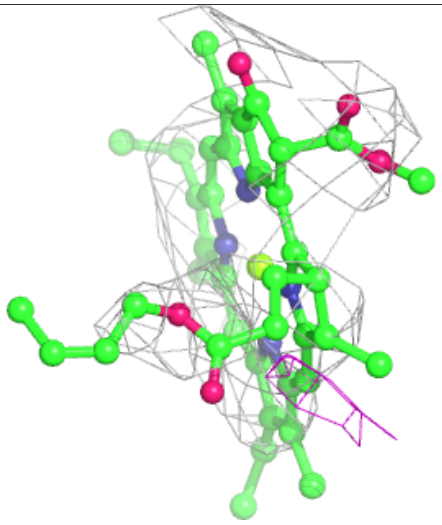


Electron density around CLA A 1112:

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

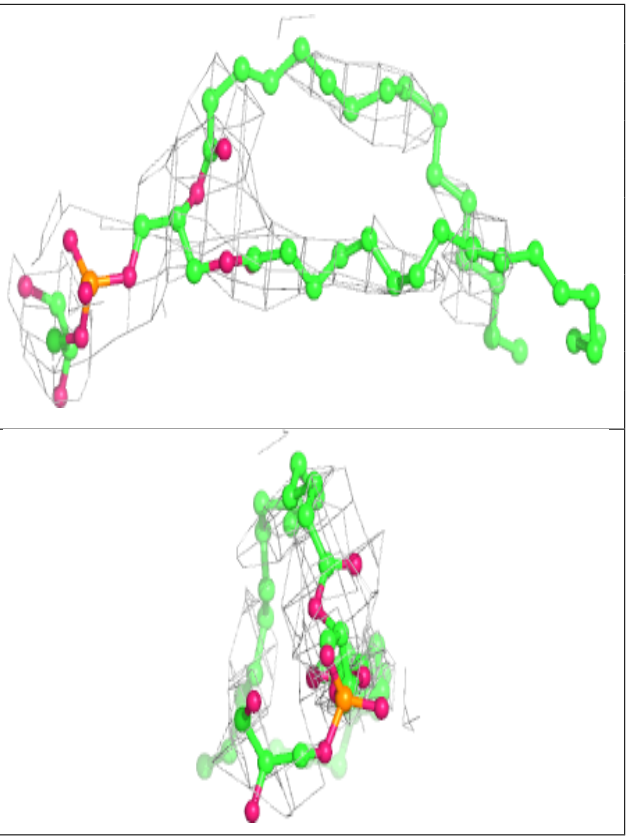


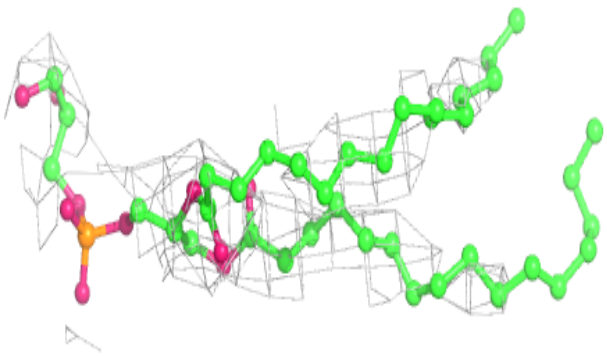




Electron density around LHG A 5003:

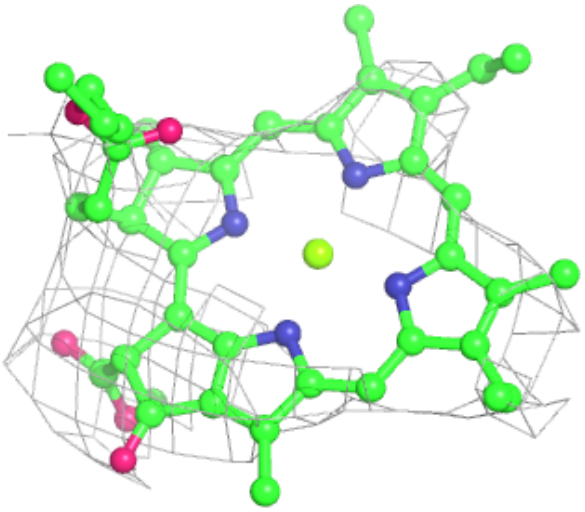
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

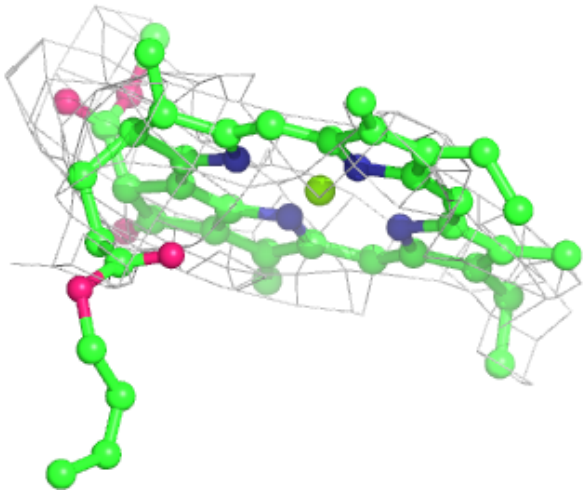


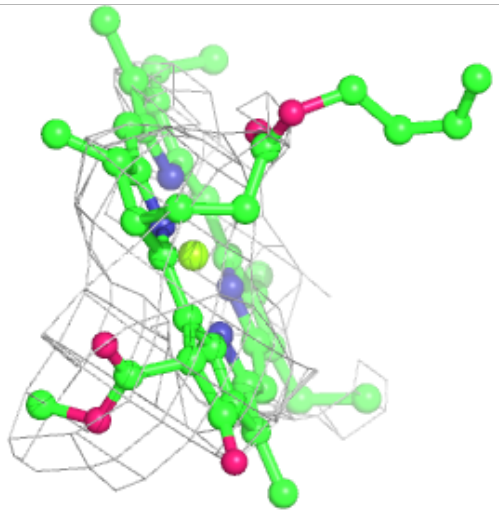


Electron density around CLA A 1113:

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

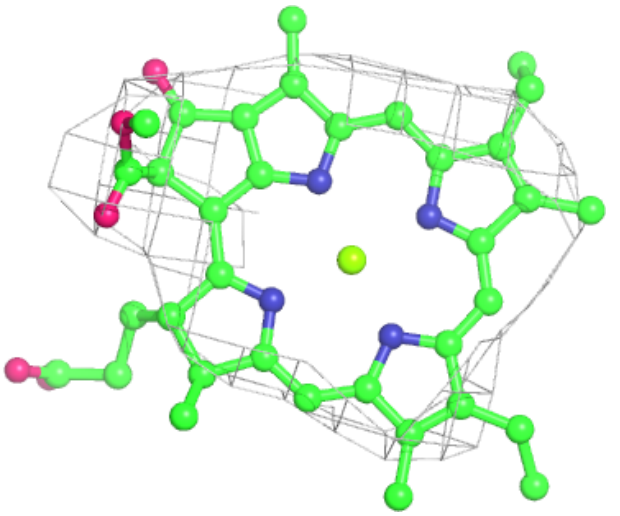


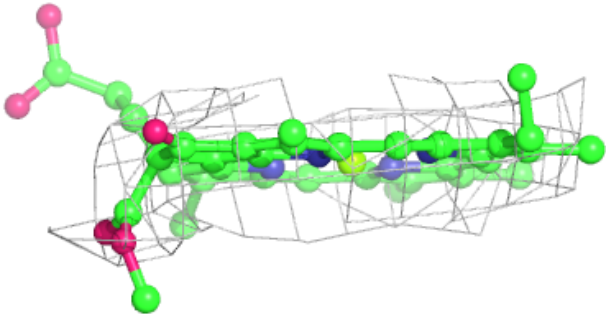


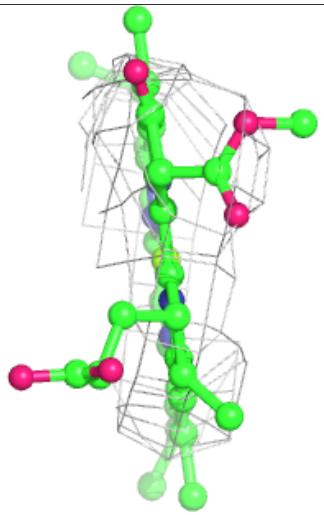


Electron density around CLA A 1141:

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

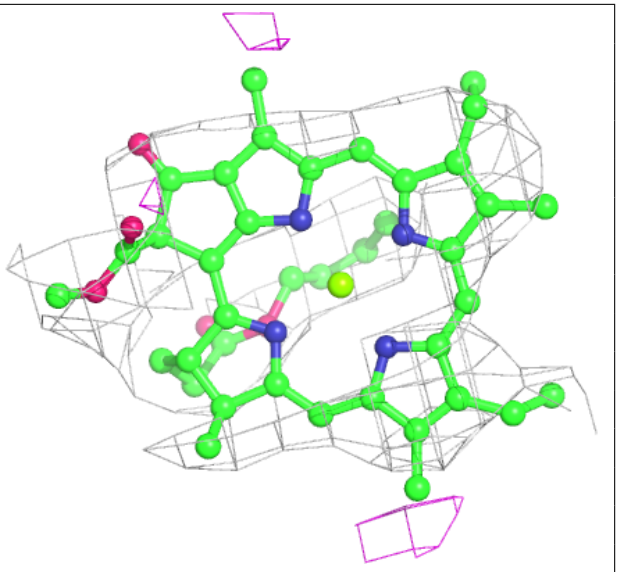


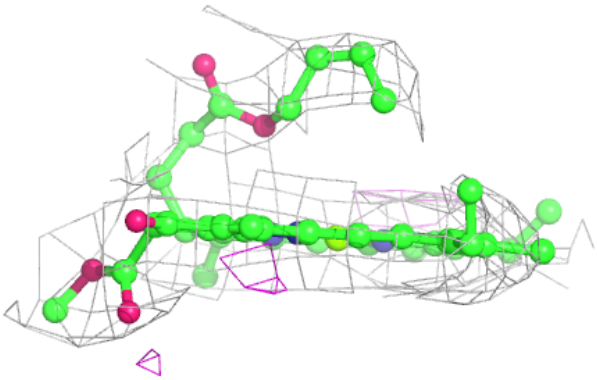


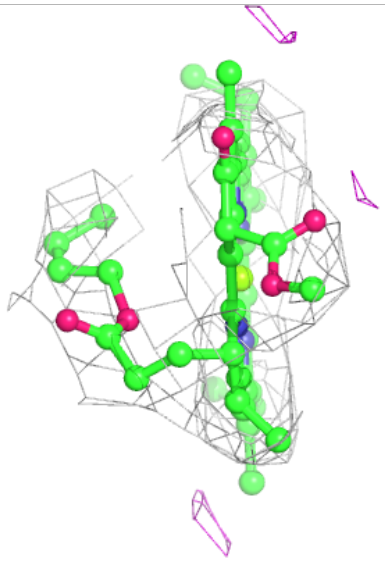


Electron density around CLA B 1204:

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

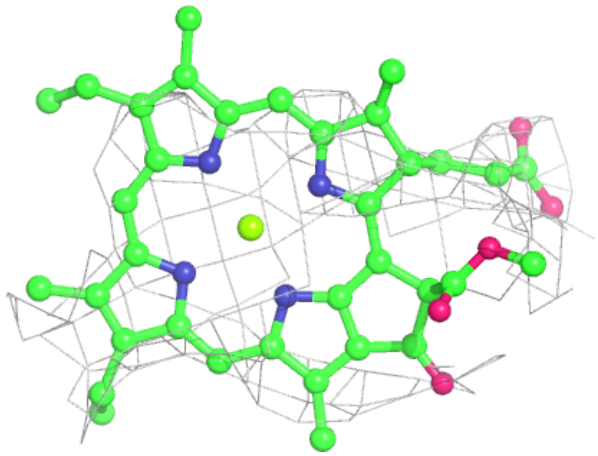


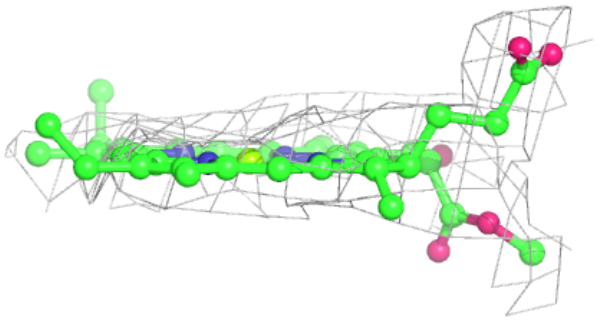


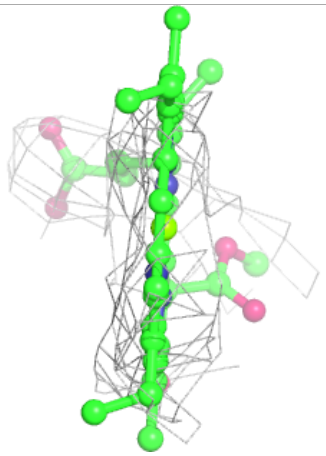


Electron density around CLA K 1401:

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

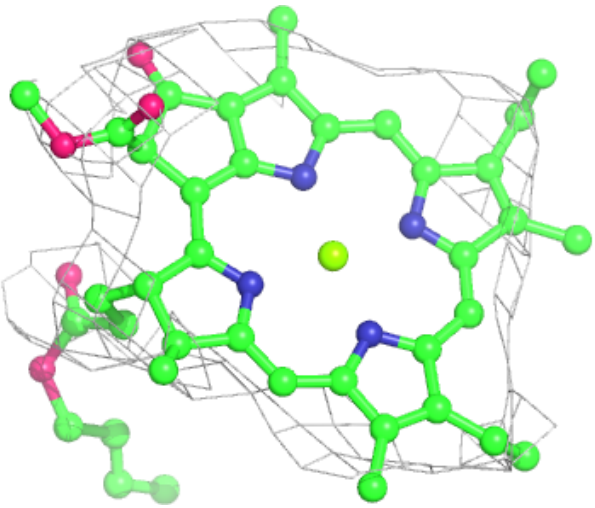


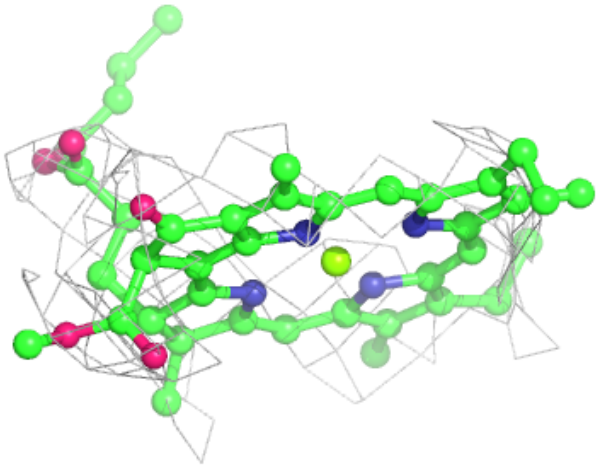


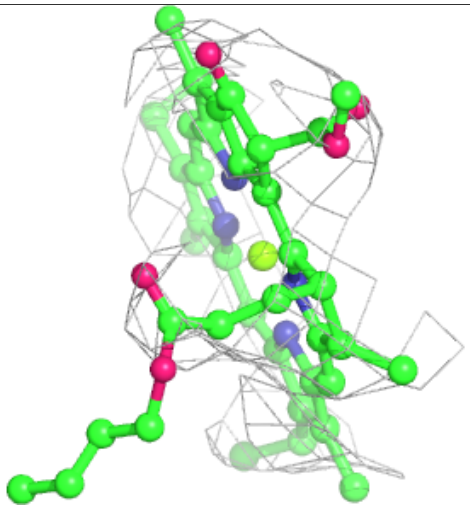


Electron density around CLA A 1114:

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

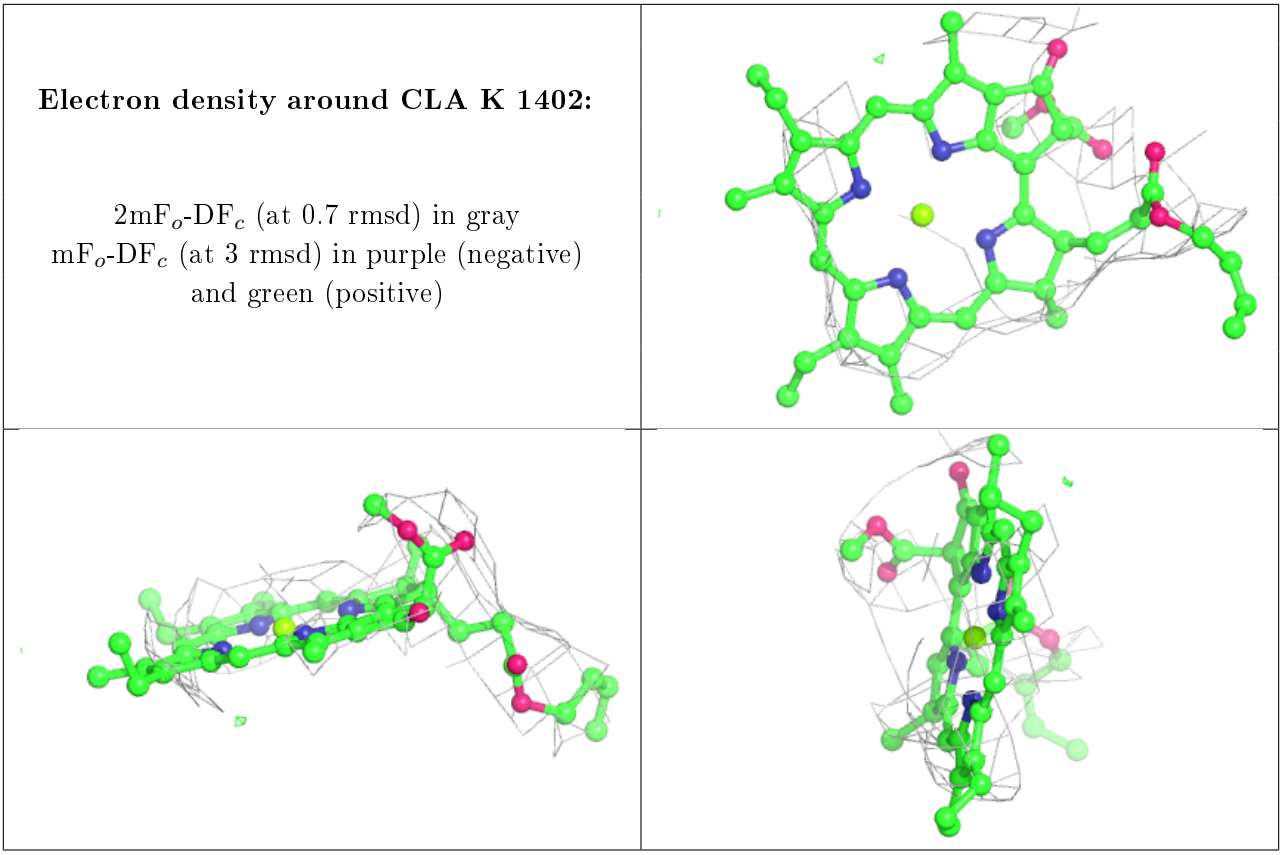






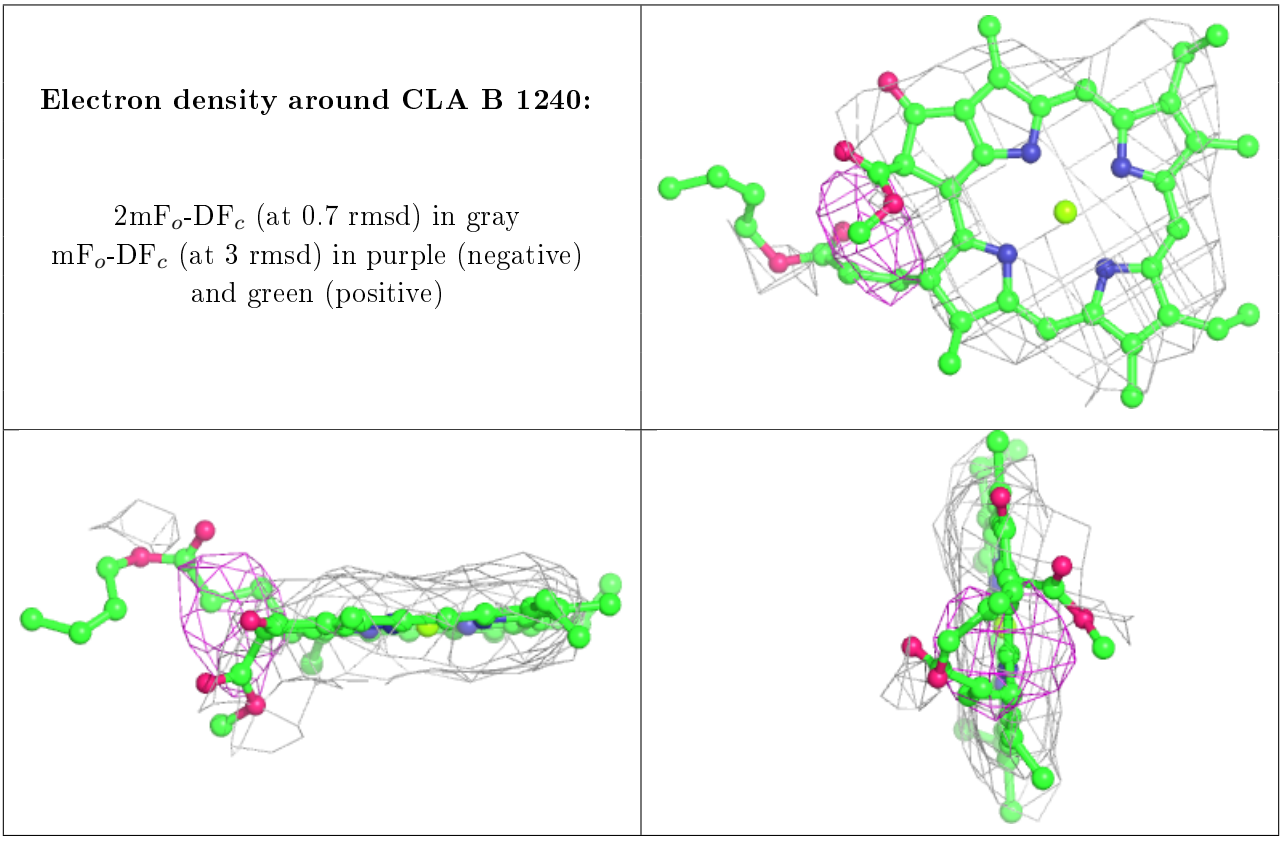
Electron density around CLA K 1402:

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



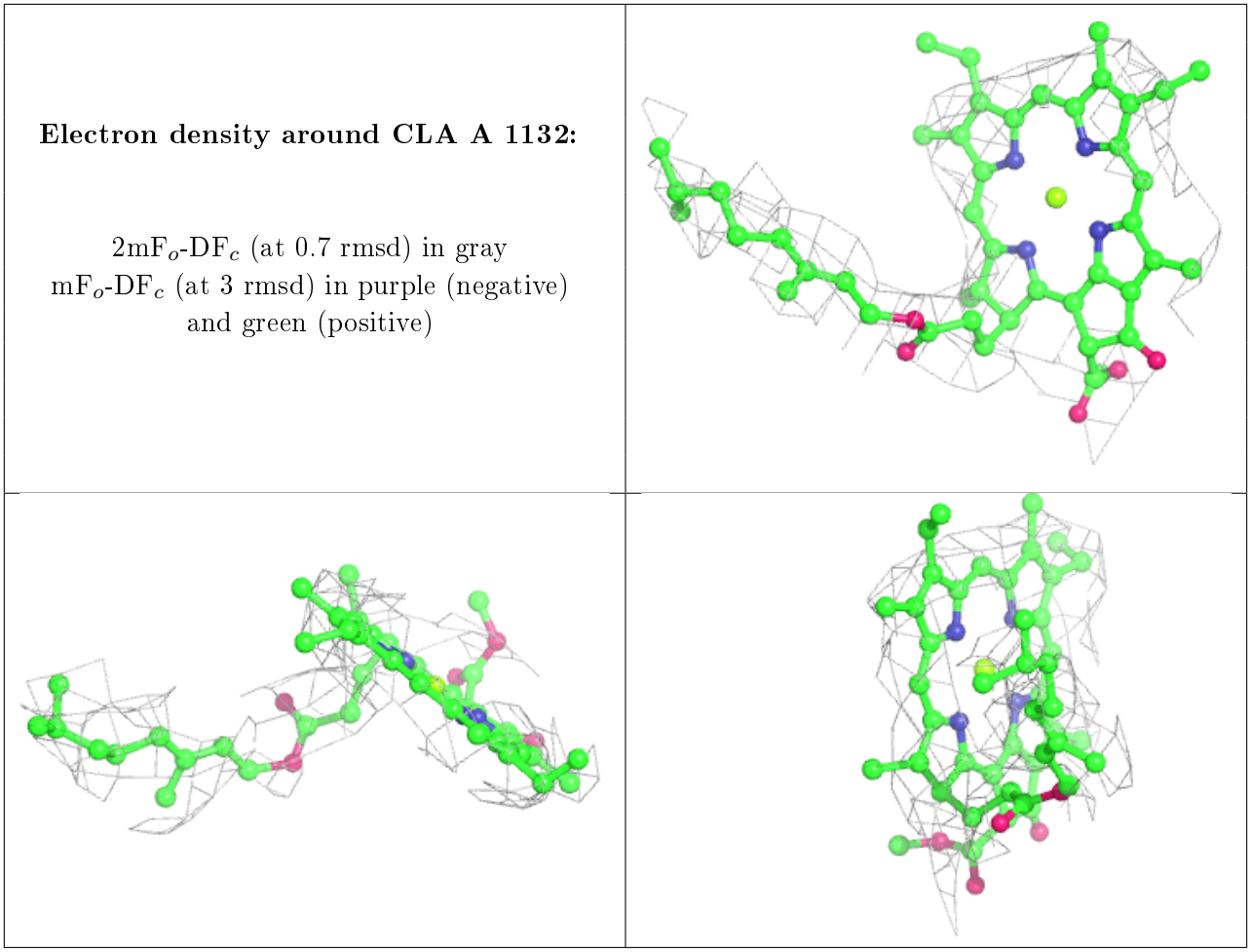
Electron density around CLA B 1240:

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



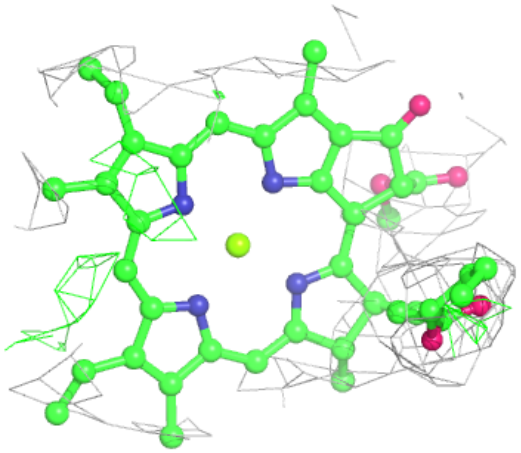
Electron density around CLA A 1132:

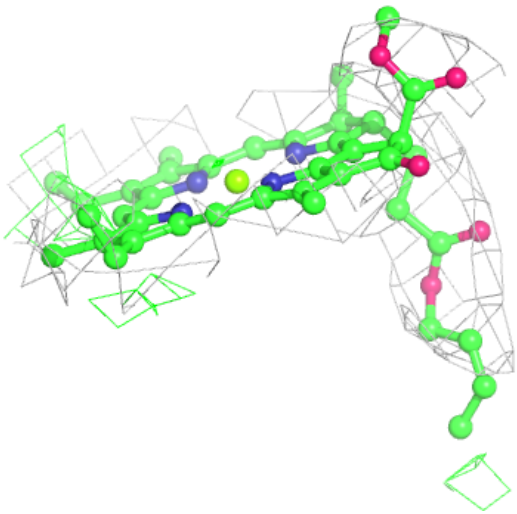
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

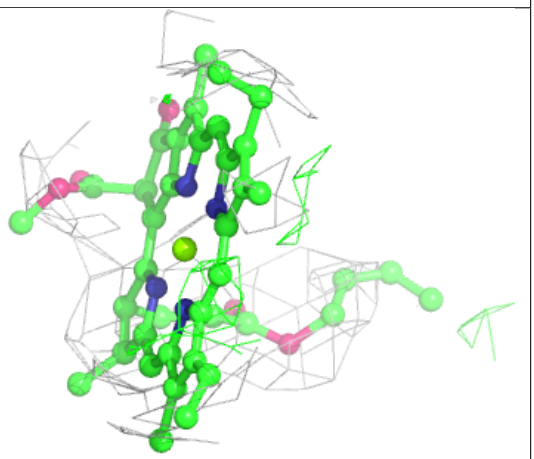


Electron density around CLA B 1211:

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

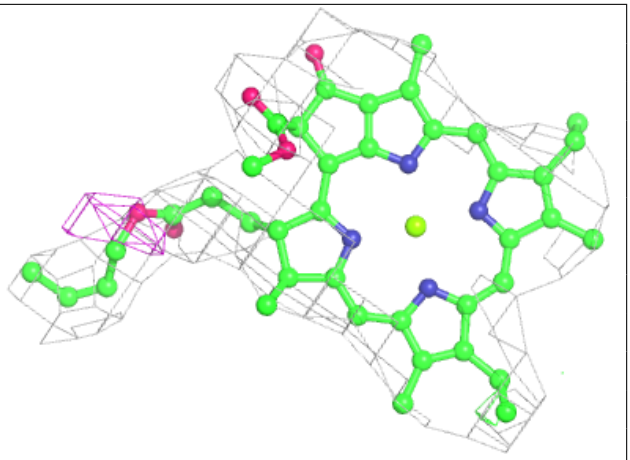


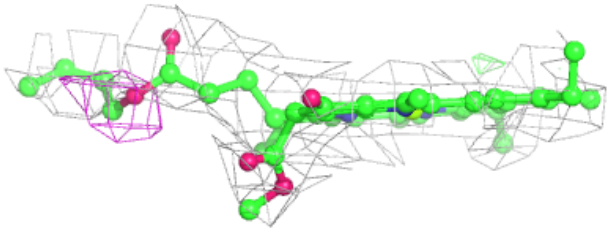


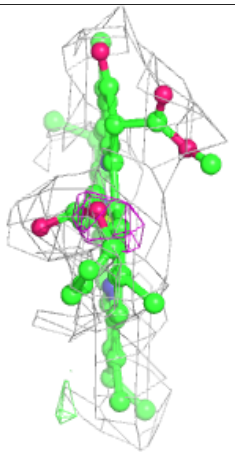


Electron density around CLA F 1302:

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

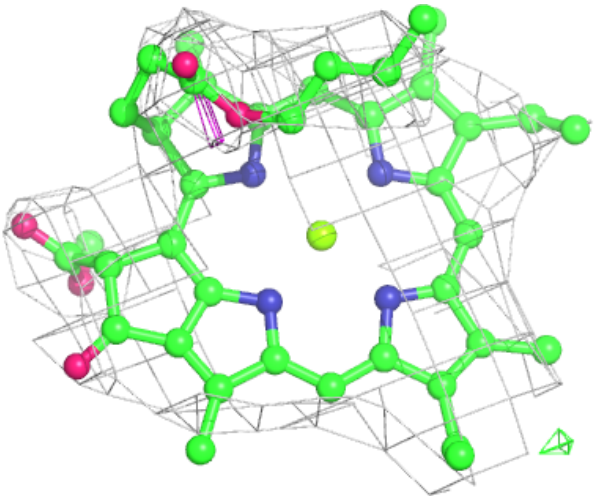


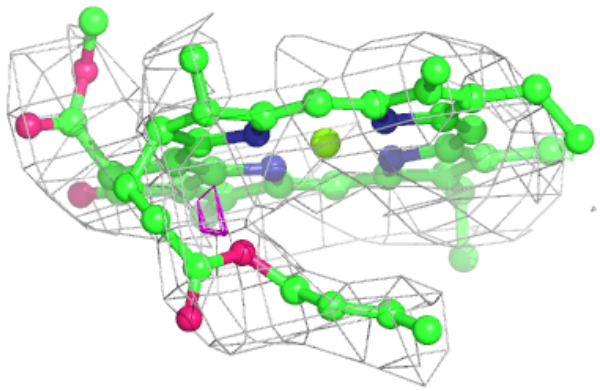


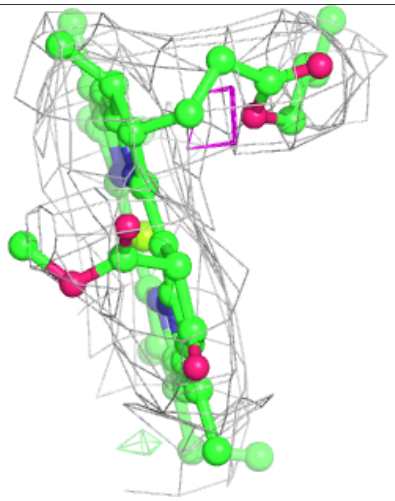


Electron density around CLA B 1217:

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

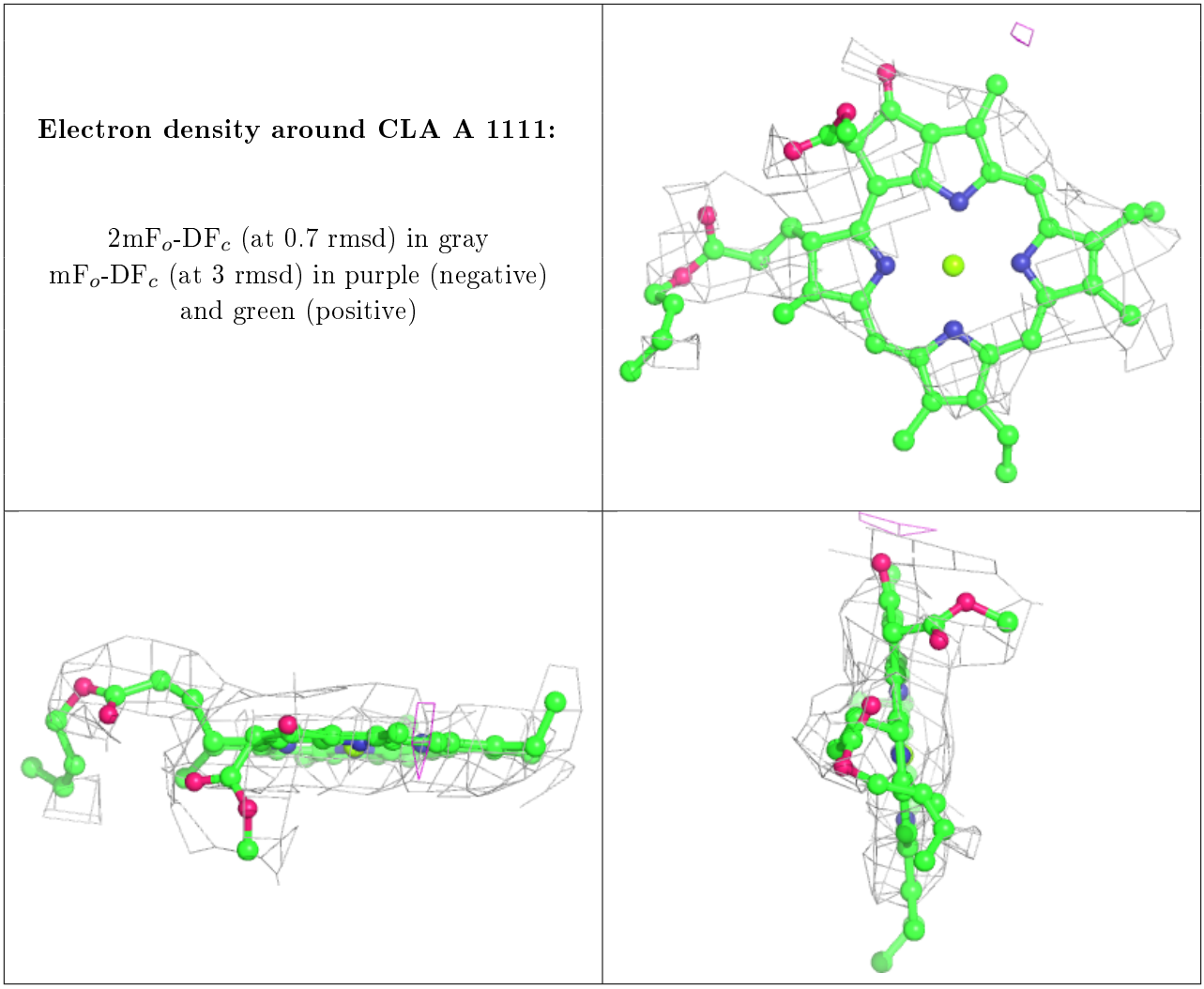






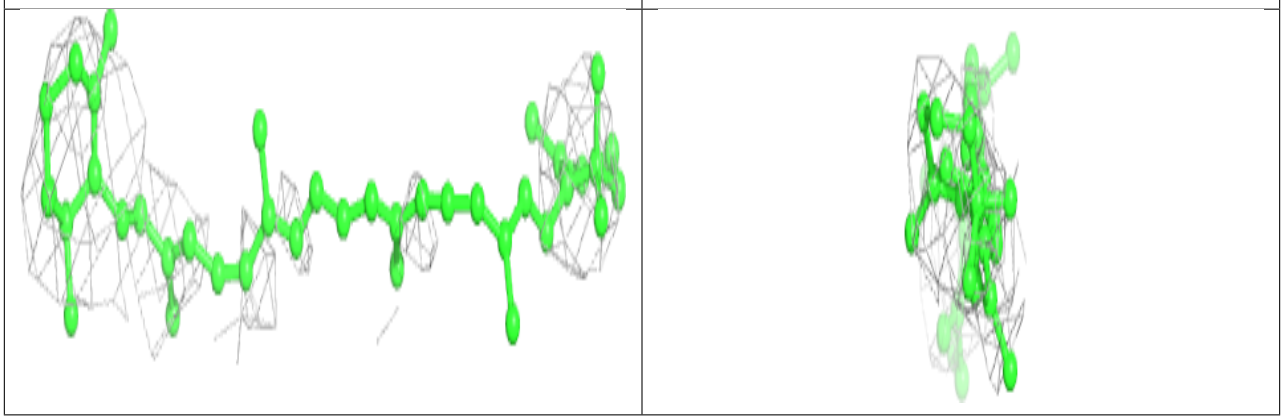
Electron density around CLA A 1111:

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



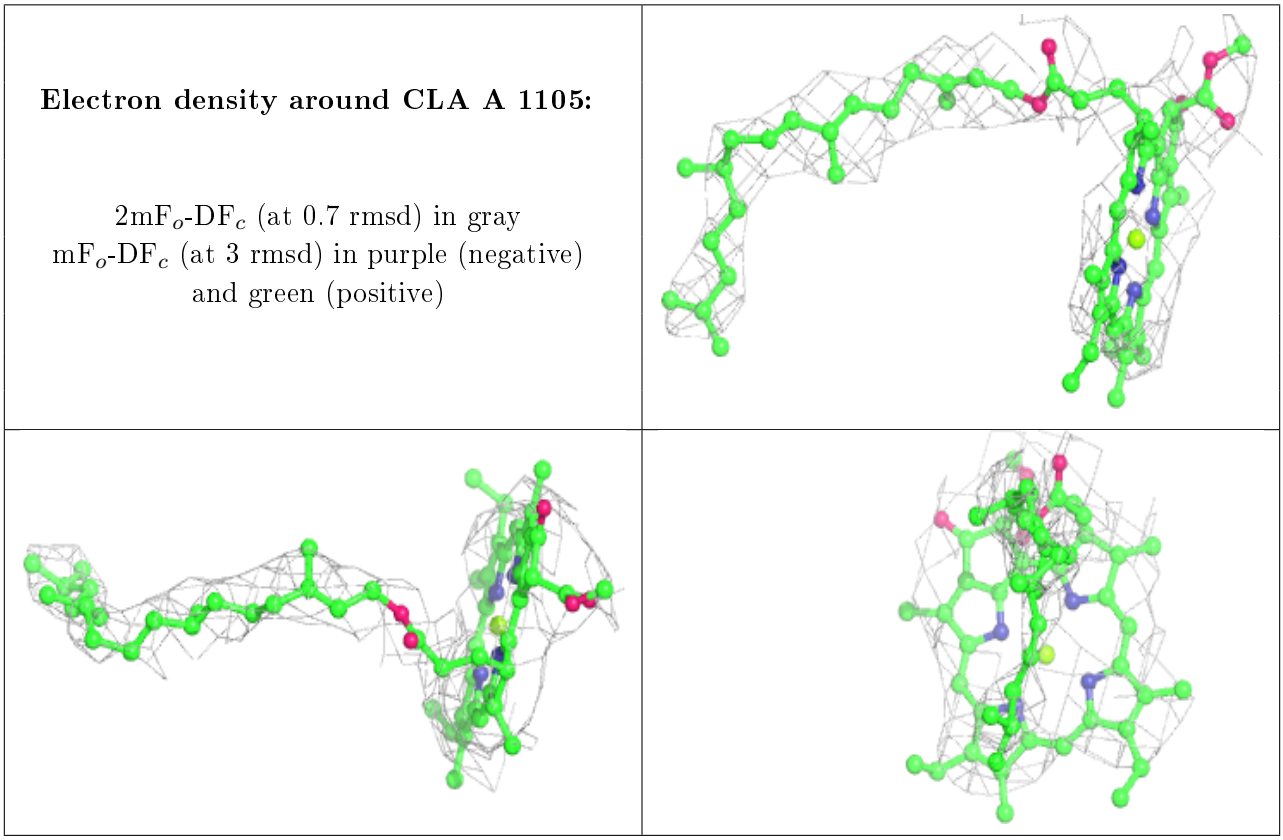
Electron density around BCR B 4018:

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



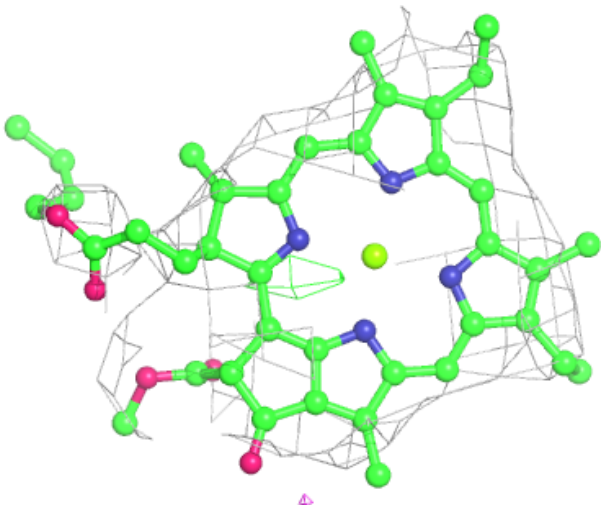
Electron density around CLA A 1105:

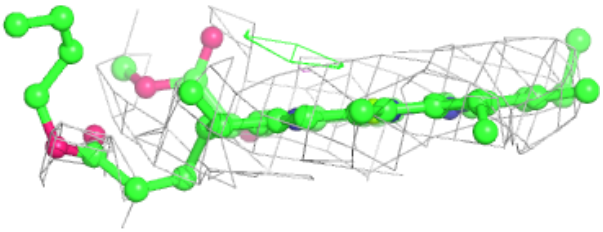
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

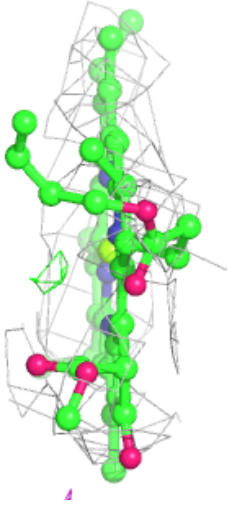


Electron density around CLA F 1301:

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

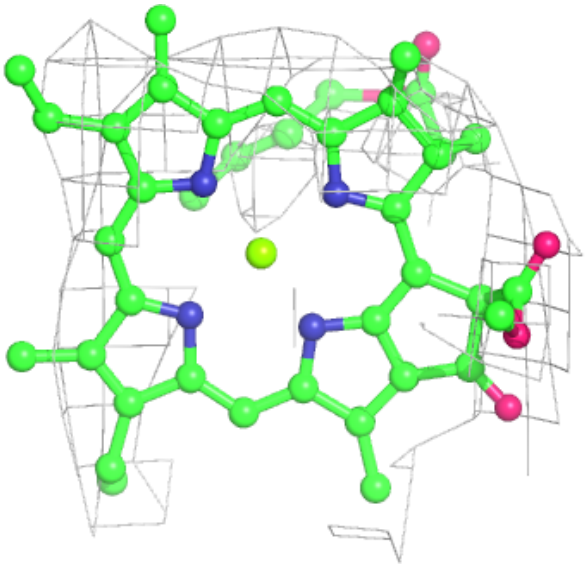


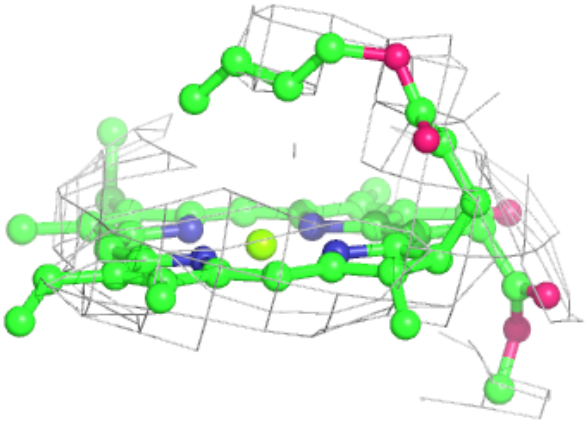


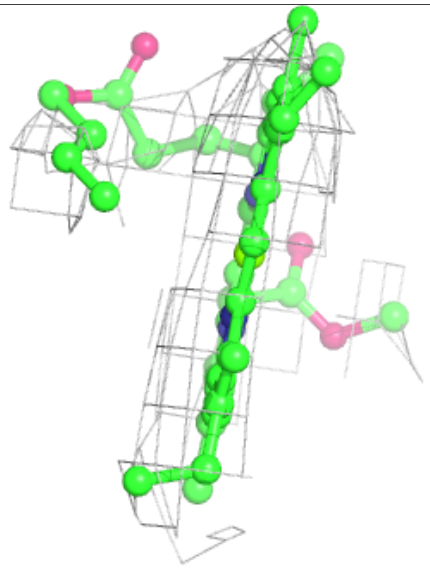


Electron density around CLA A 1120:

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

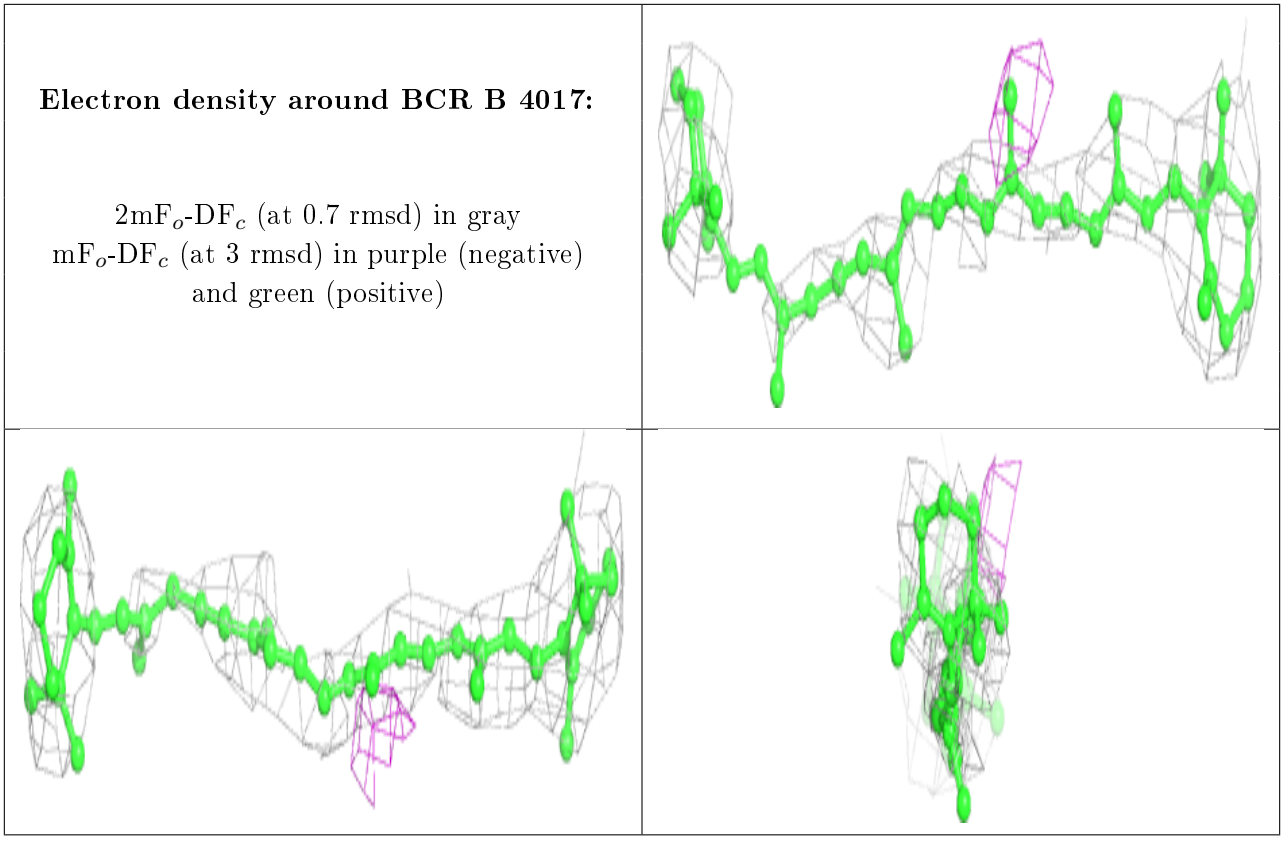






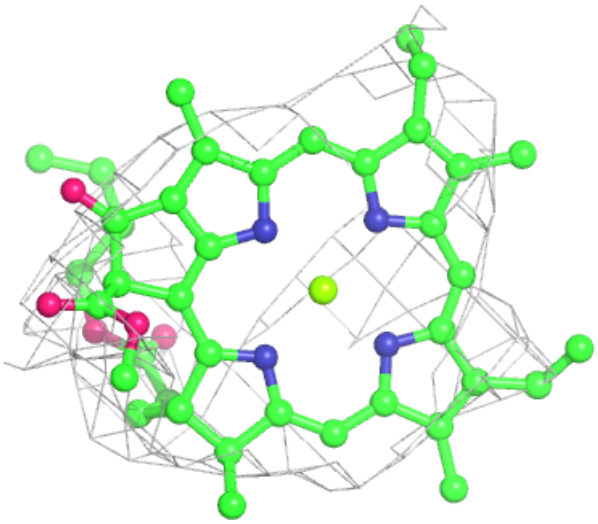
Electron density around BCR B 4017:

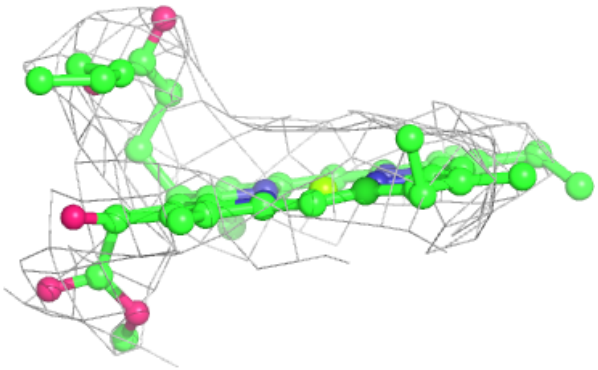
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

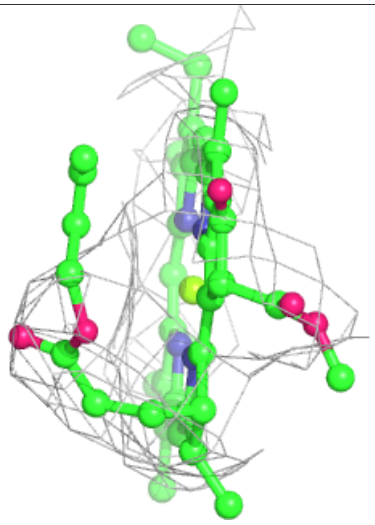


Electron density around CLA J 1302:

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

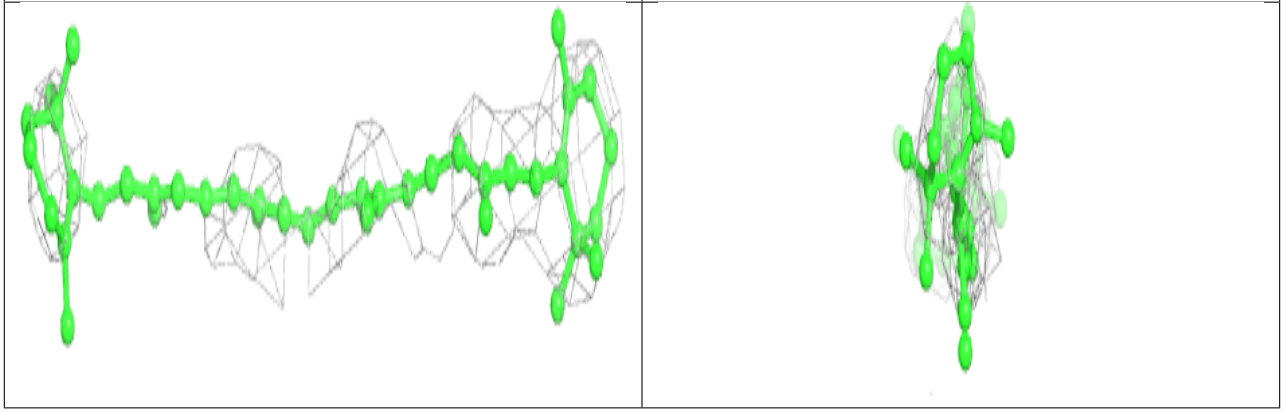






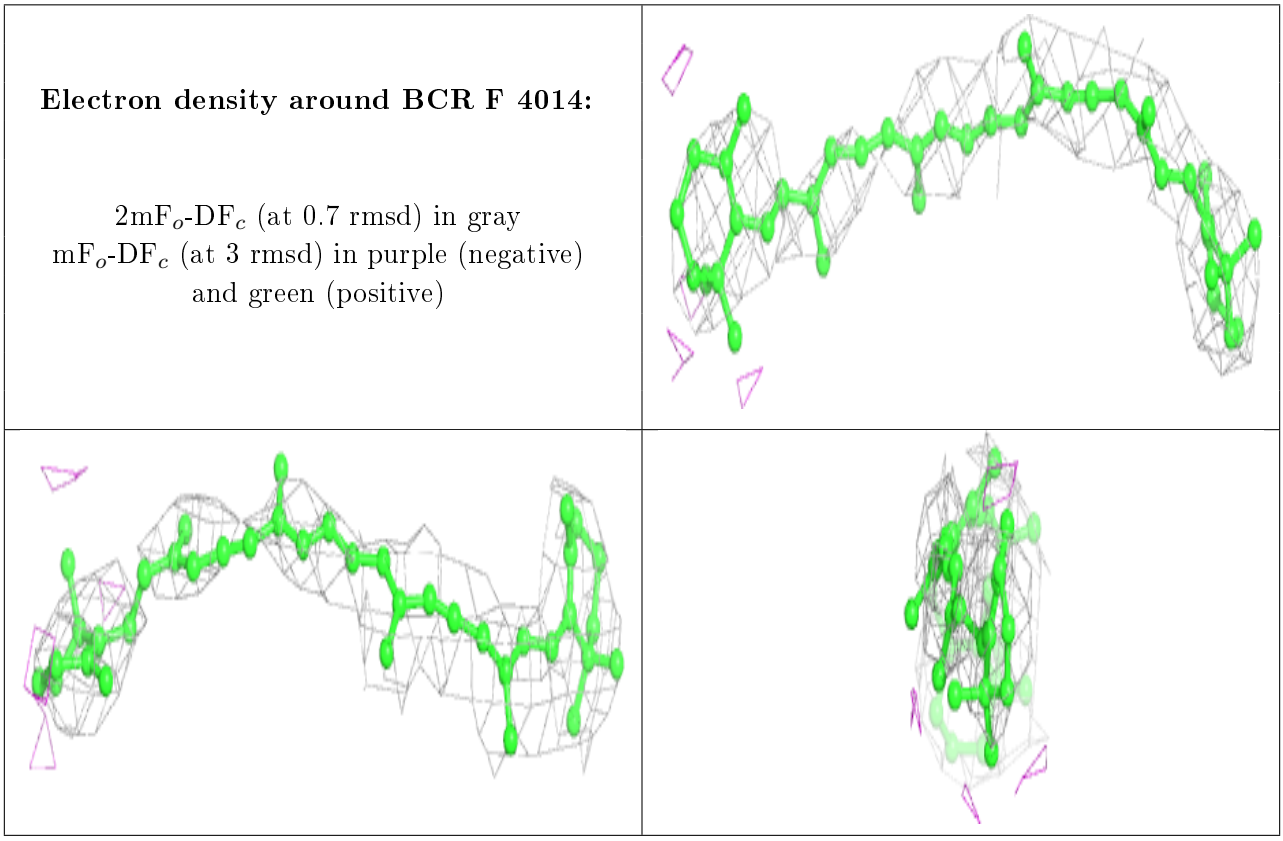
Electron density around BCR A 4007:

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



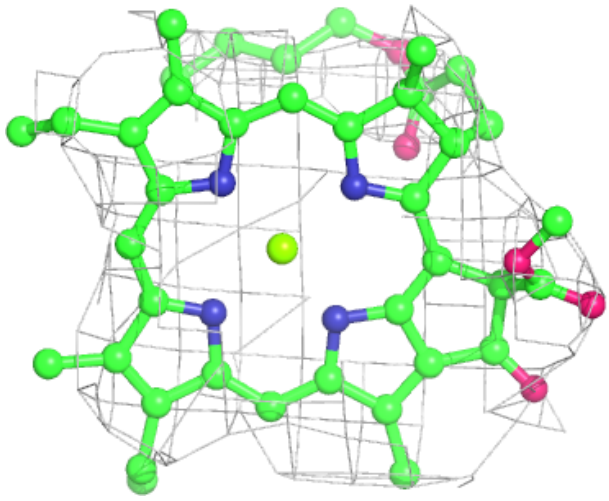
Electron density around BCR F 4014:

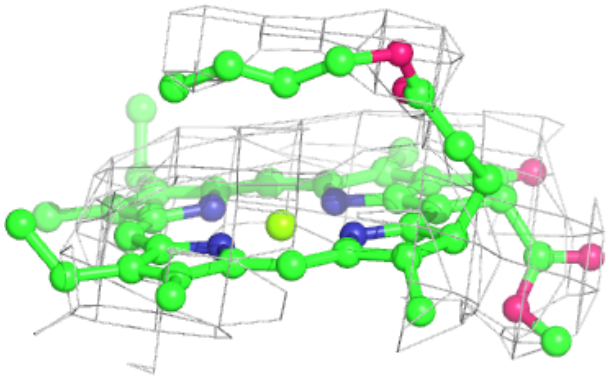
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

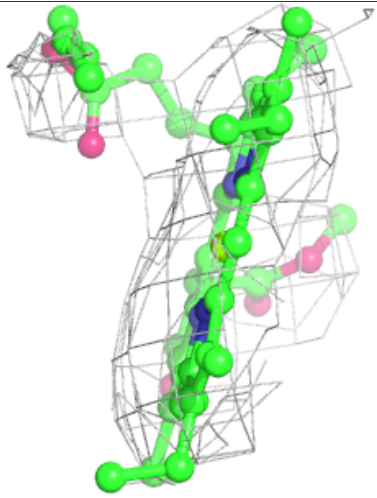


Electron density around CLA B 1209:

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

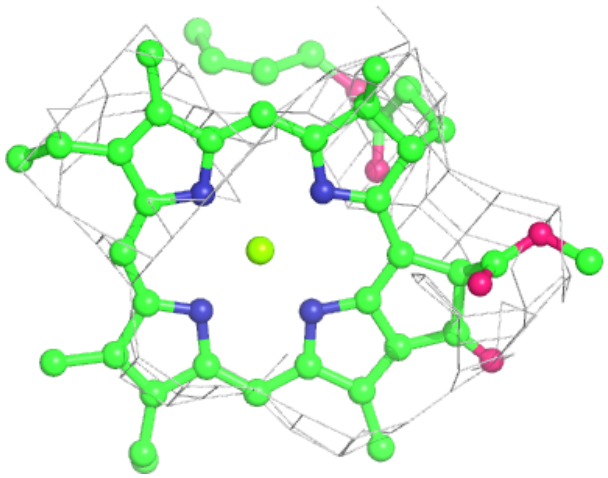


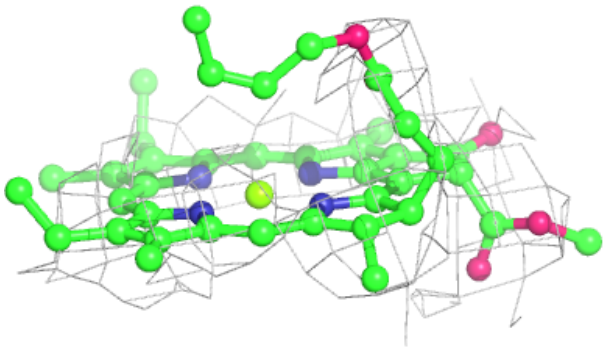


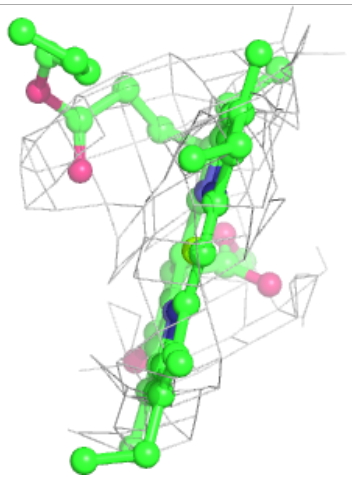


Electron density around CLA A 1110:

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

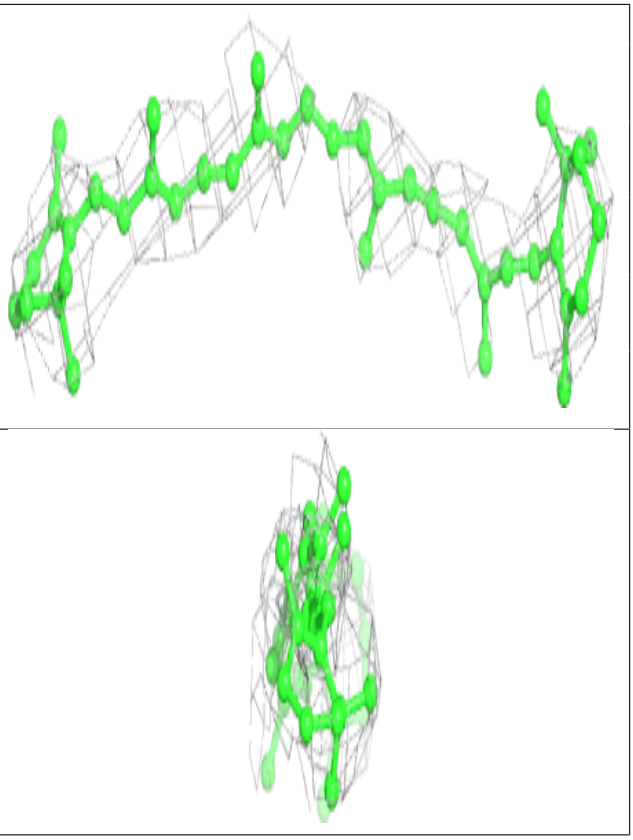


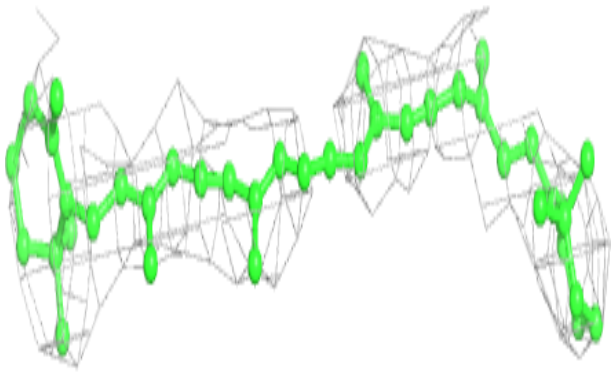




Electron density around BCR J 4013:

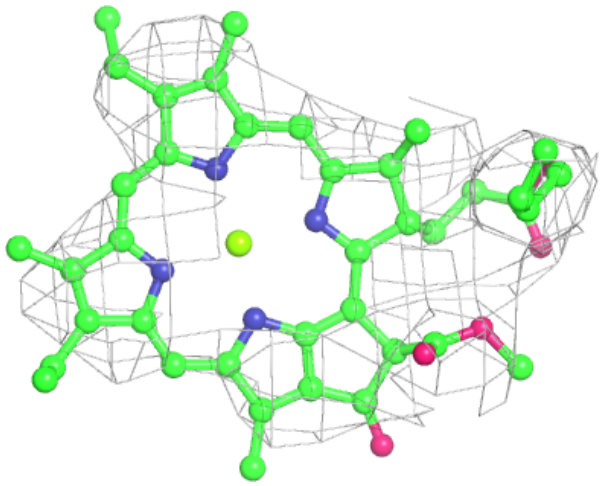
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

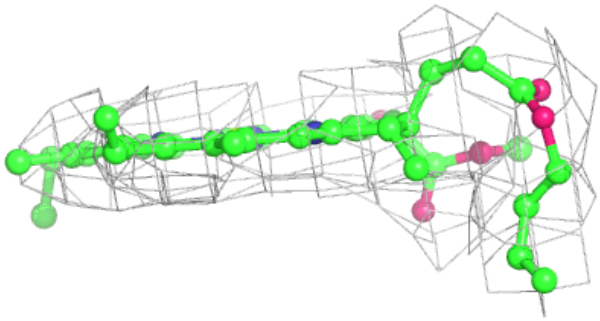


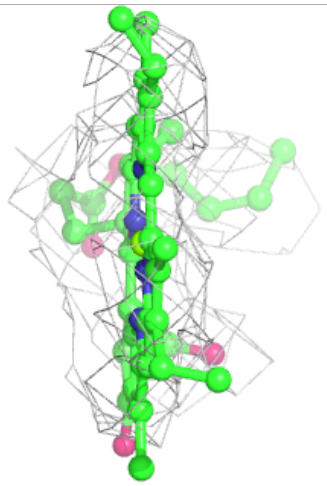


Electron density around CLA B 1203:

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

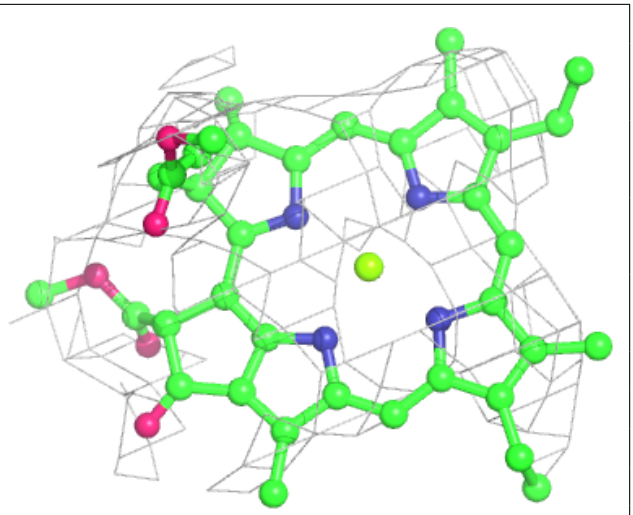


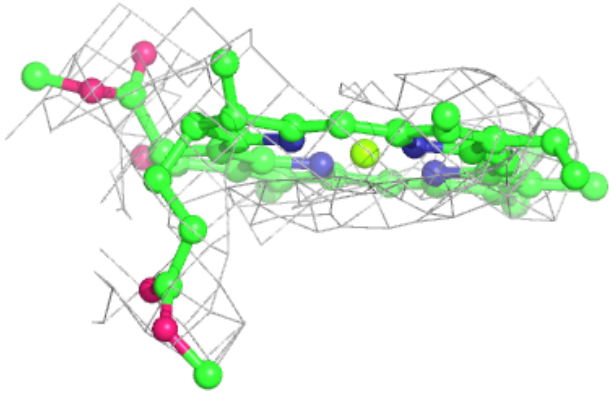


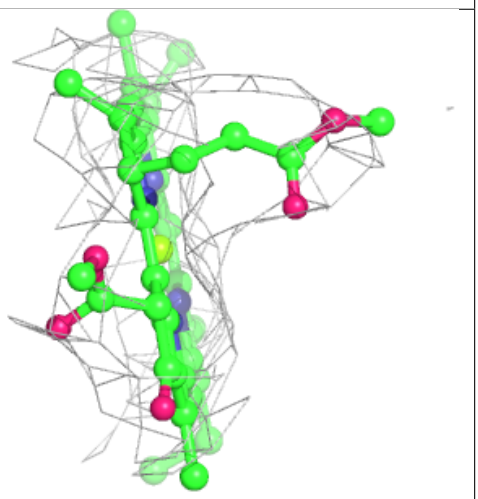


Electron density around CLA A 1119:

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

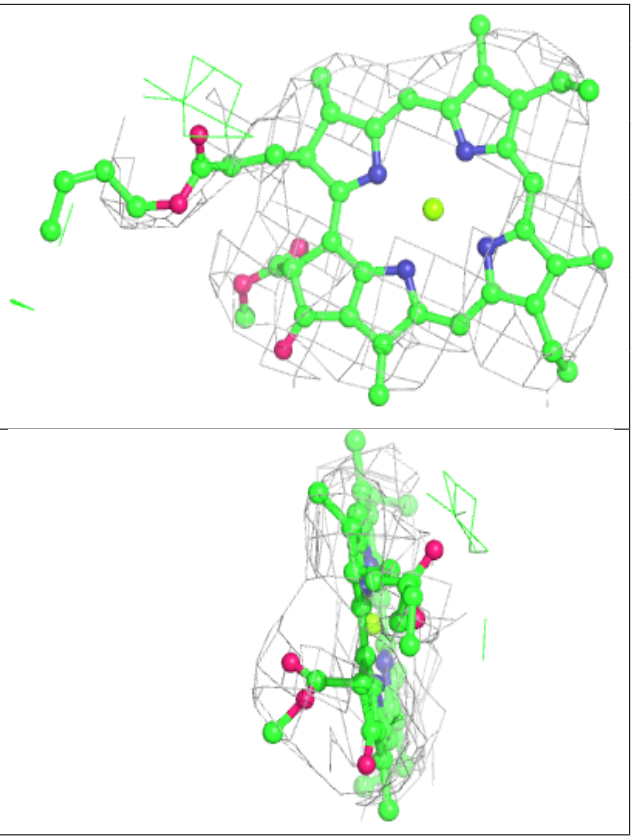


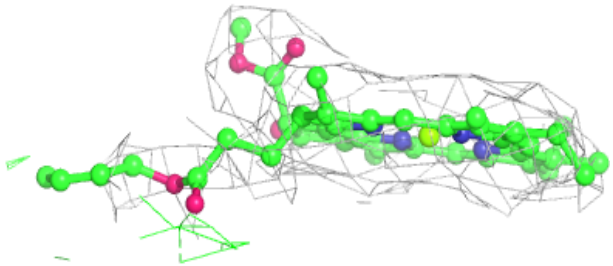




Electron density around CLA B 1219:

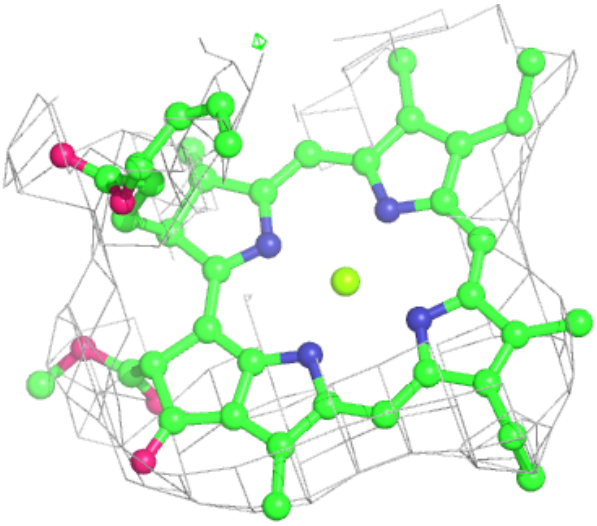
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

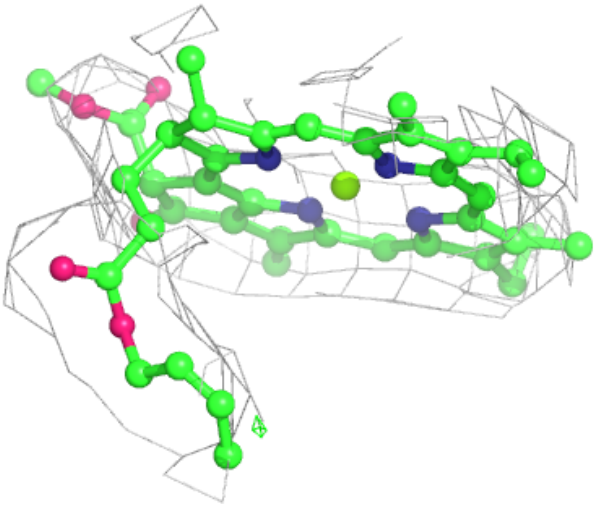


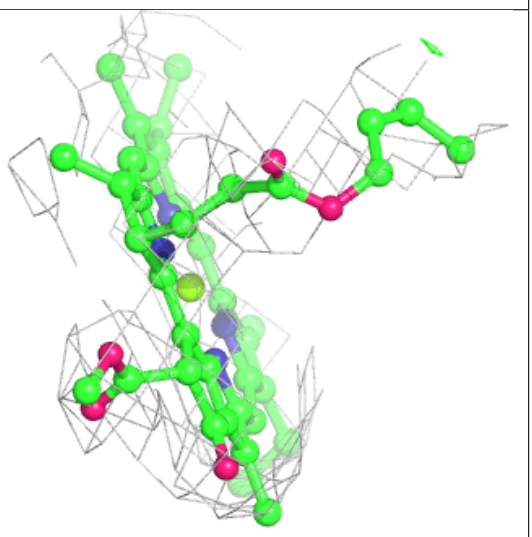


Electron density around CLA A 1130:

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

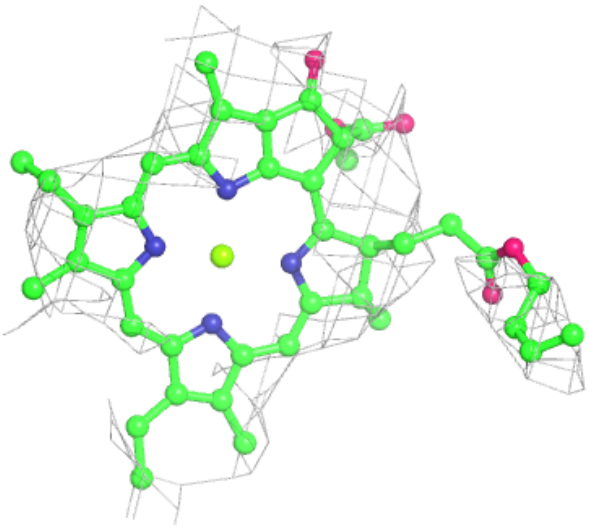


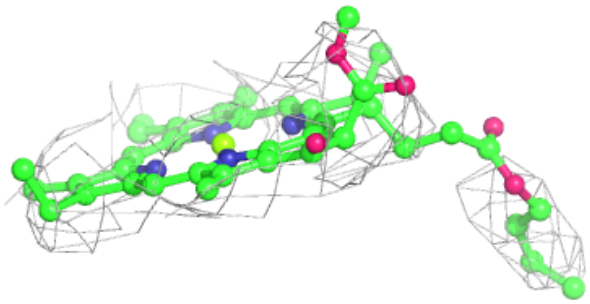


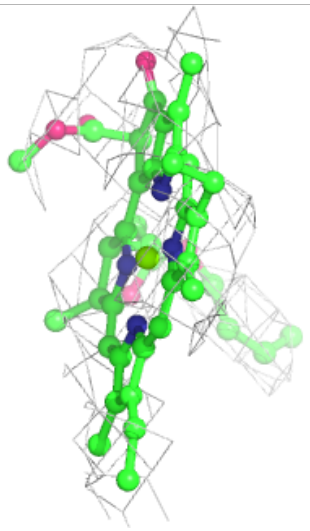


Electron density around CLA A 1125:

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

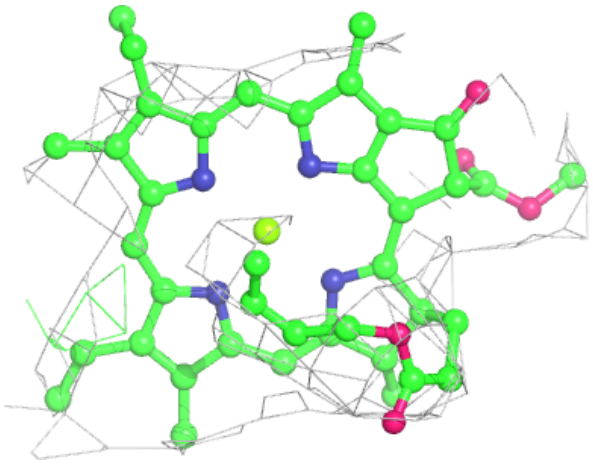


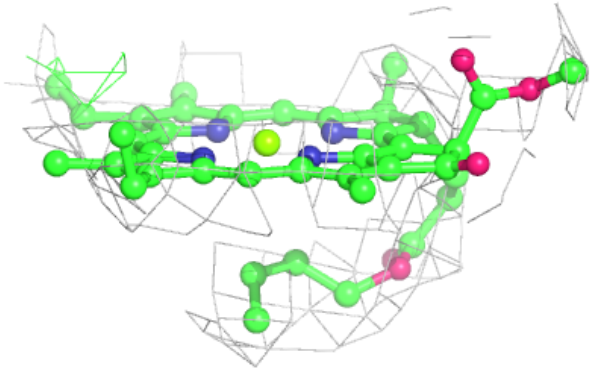




Electron density around CLA A 1116:

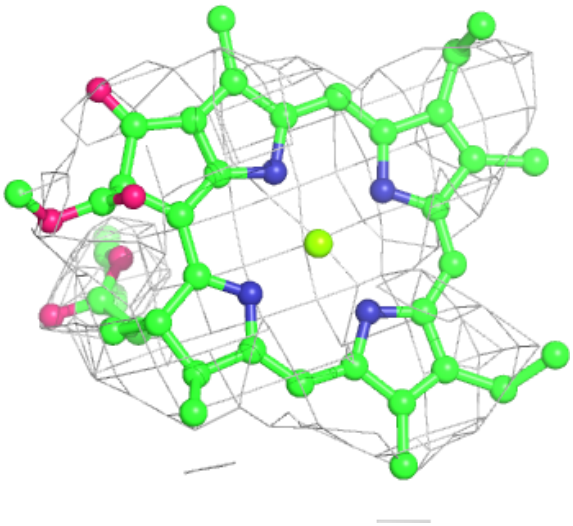
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

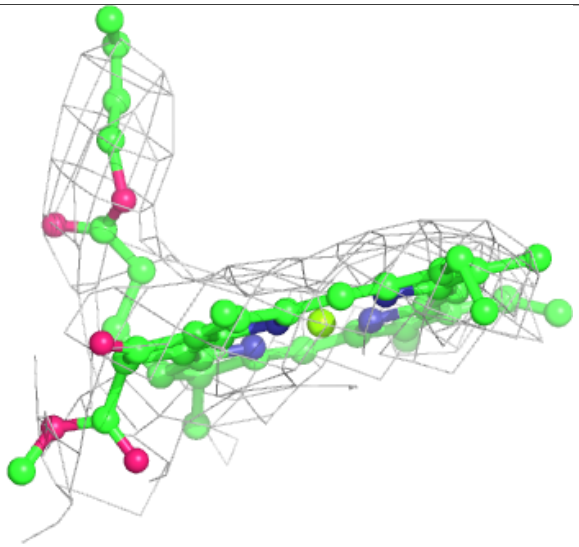


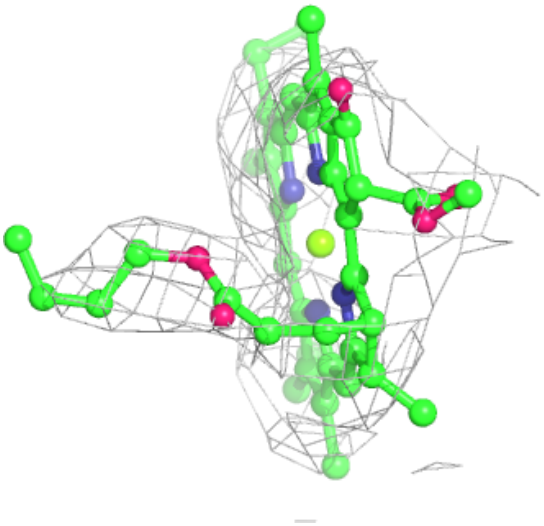


Electron density around CLA B 1208:

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

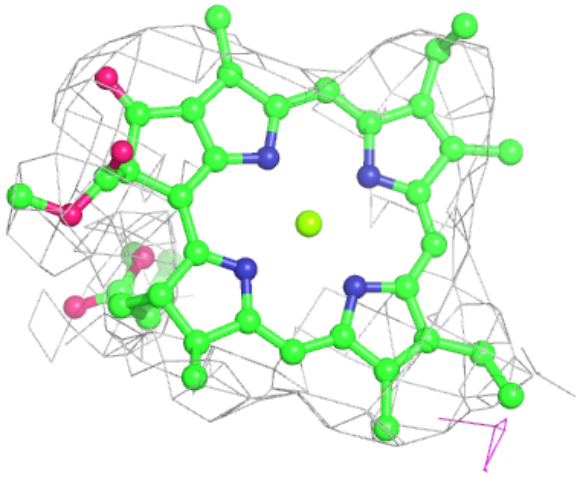


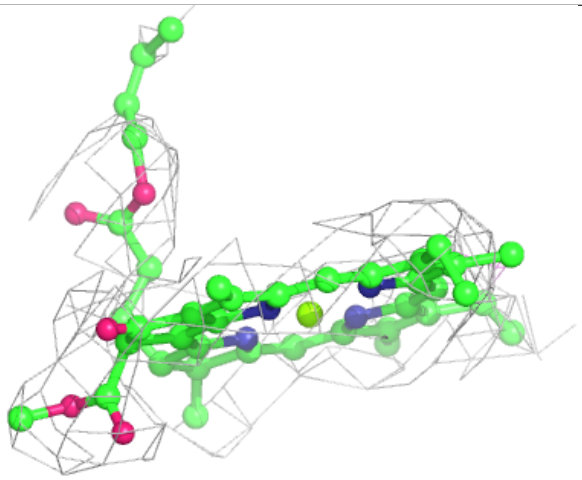


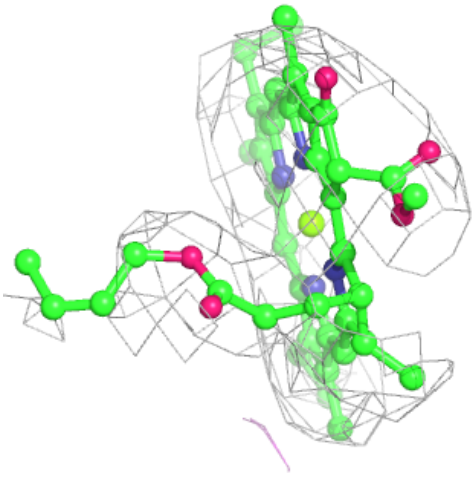


Electron density around CLA B 1201:

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

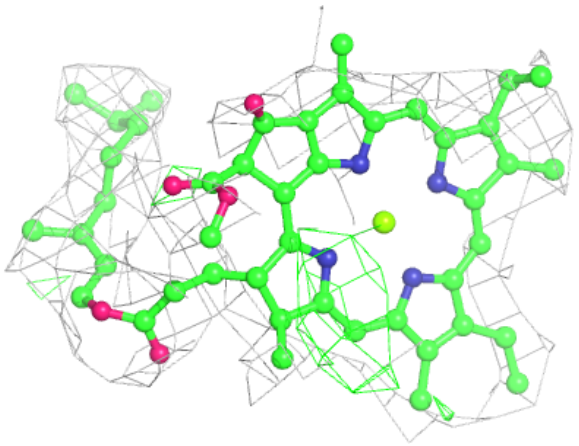


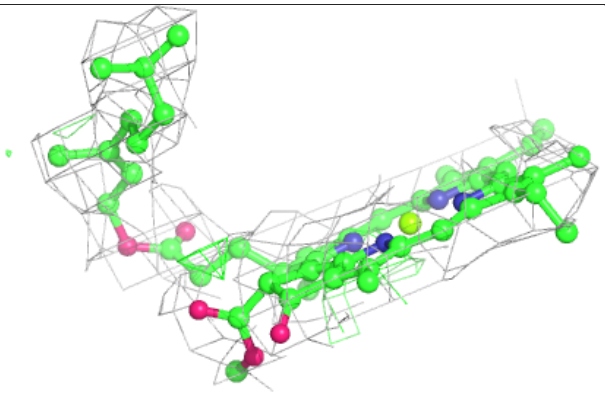


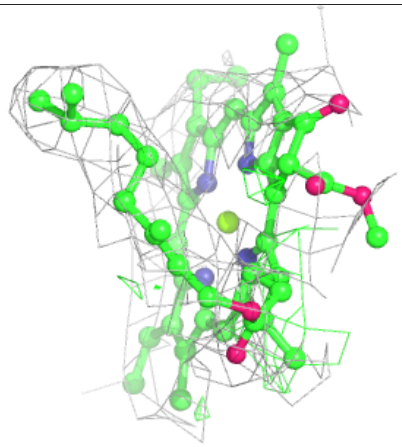


Electron density around CLA A 1011:

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

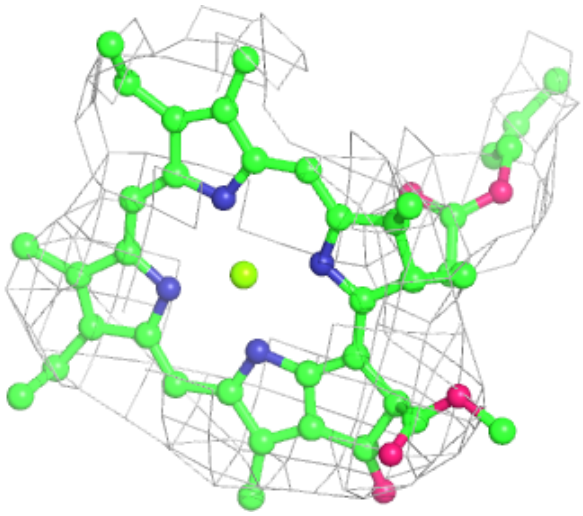


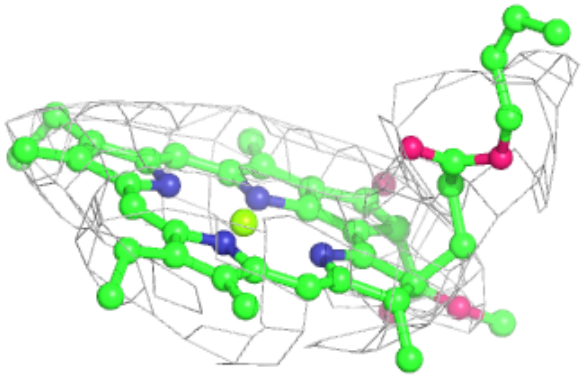




Electron density around CLA A 1108:

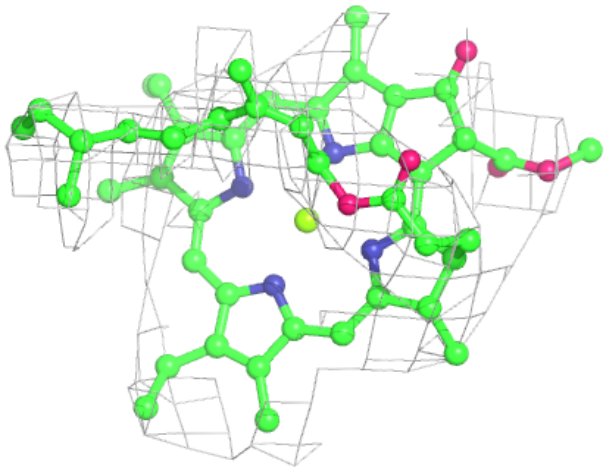
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

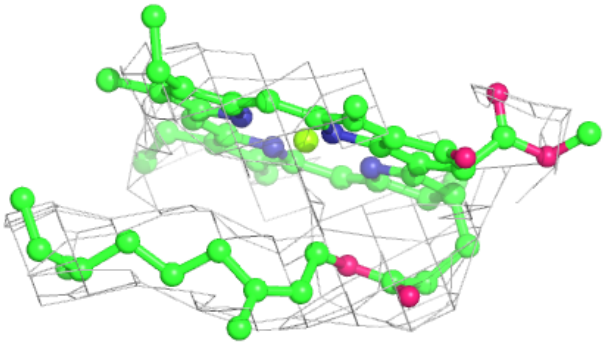


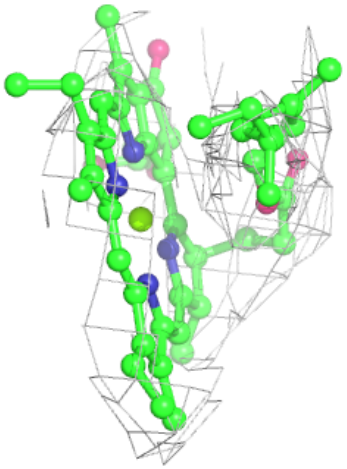


Electron density around CLA A 1115:

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

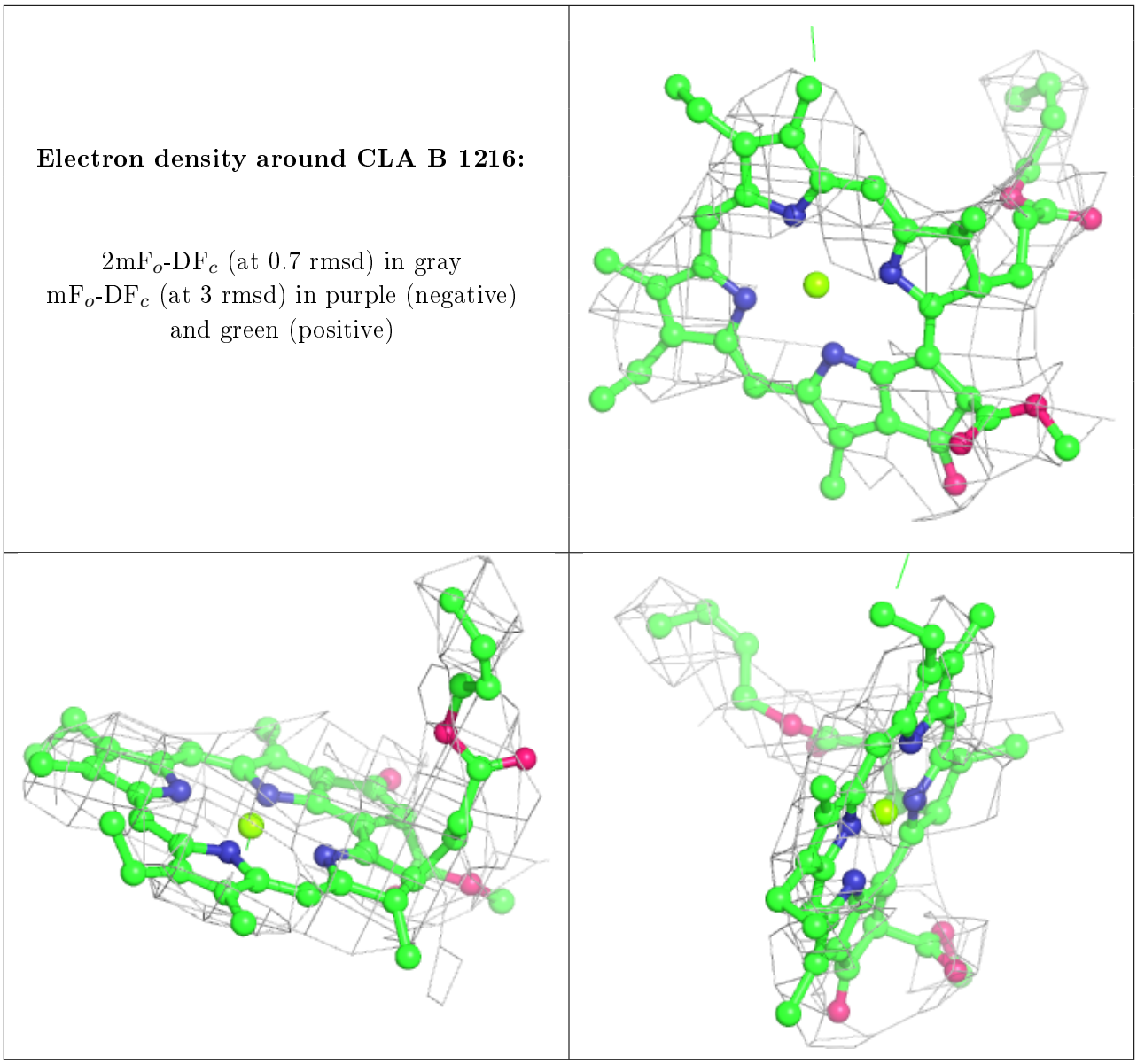






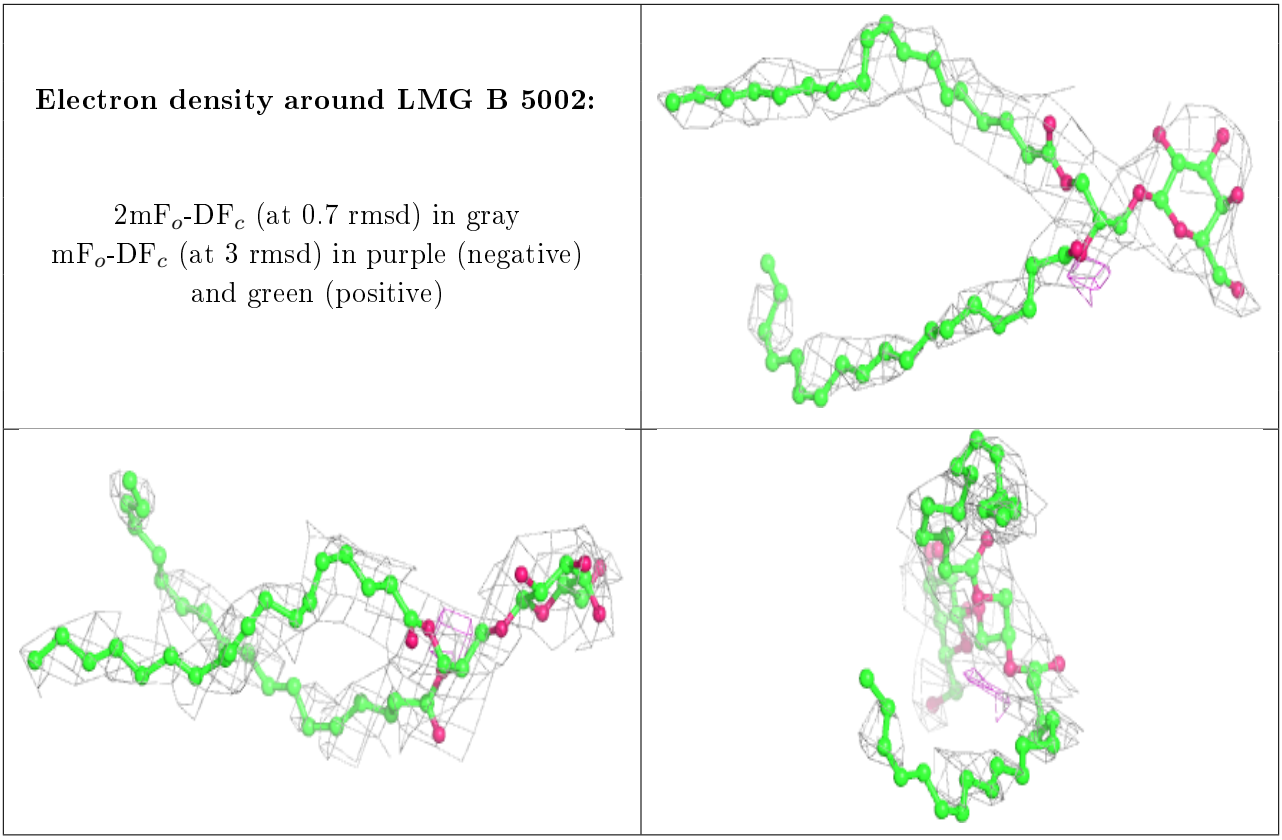
Electron density around CLA B 1216:

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



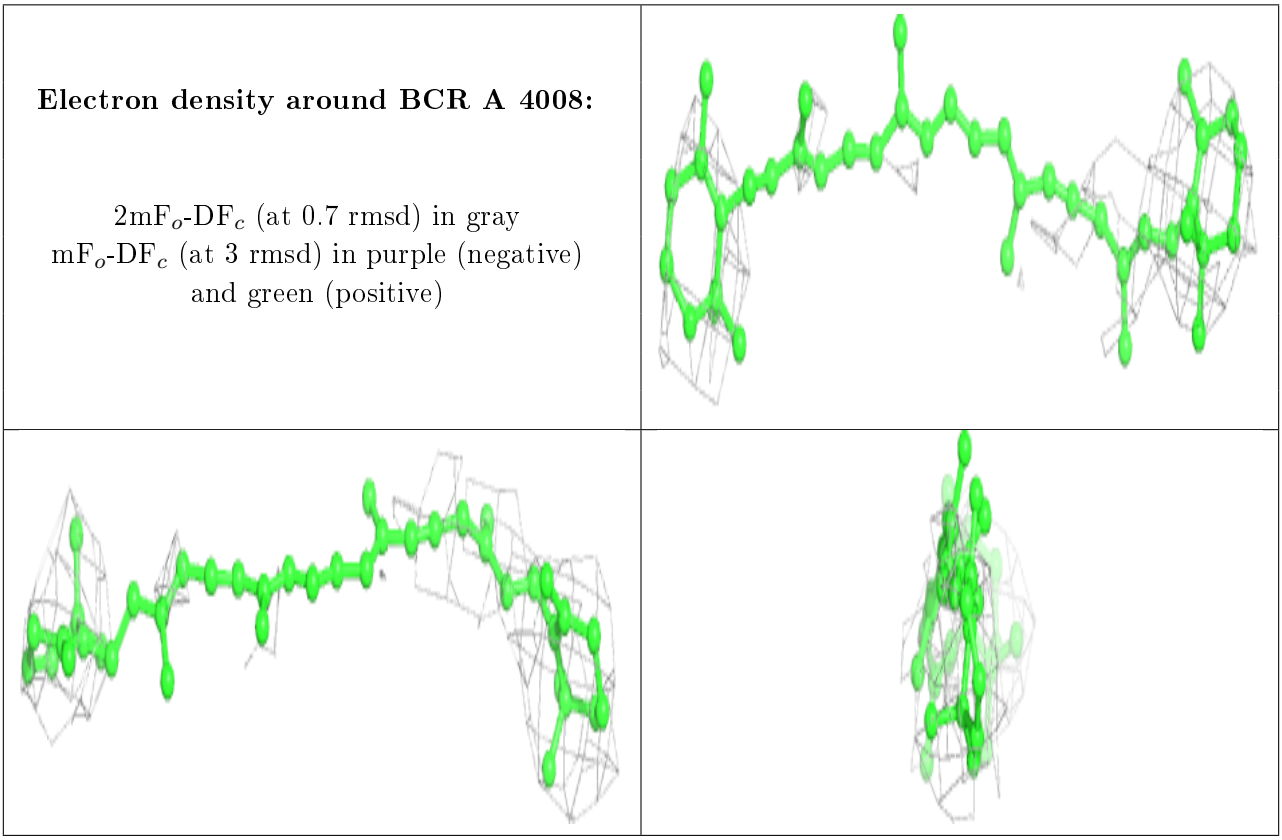
Electron density around LMG B 5002:

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



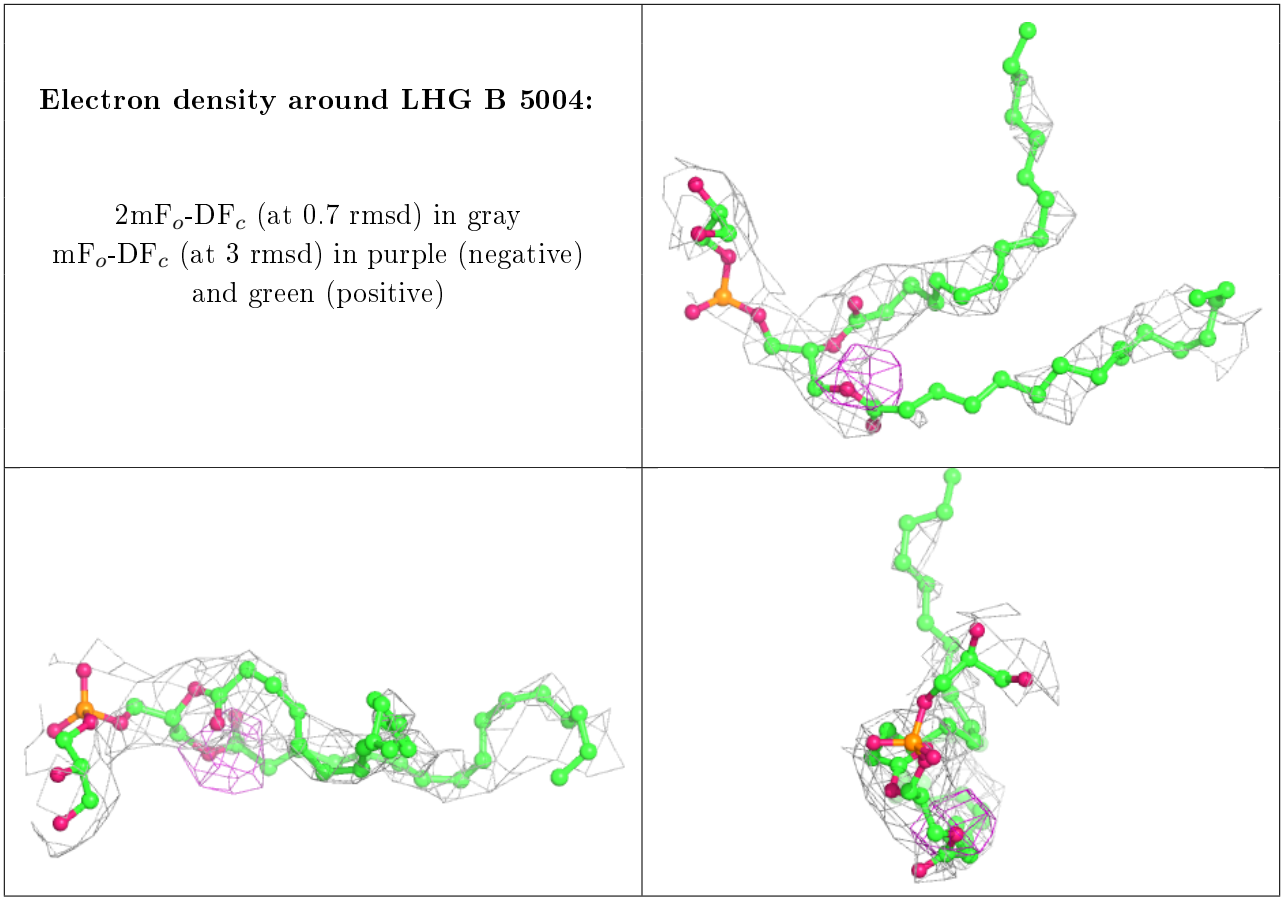
Electron density around BCR A 4008:

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



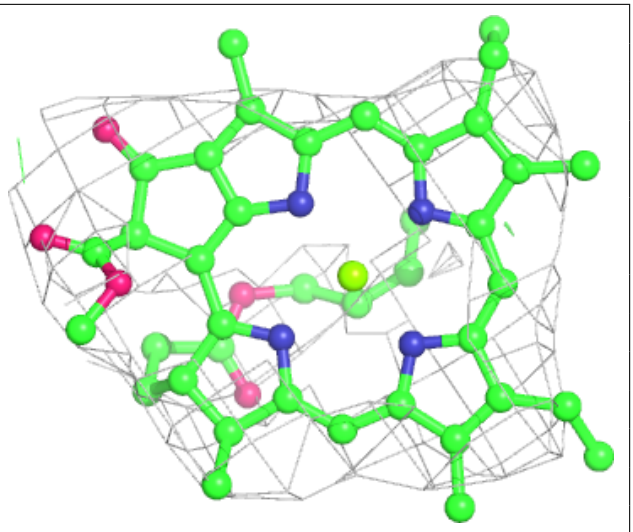
Electron density around LHG B 5004:

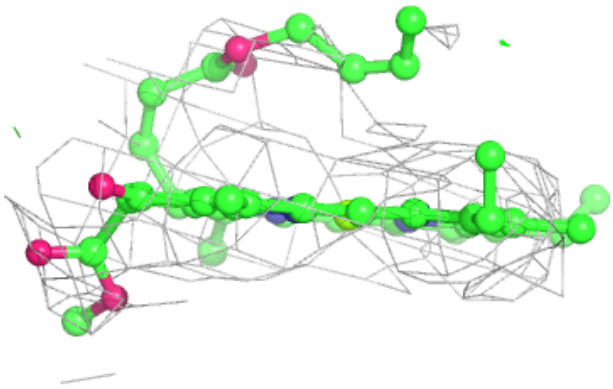
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

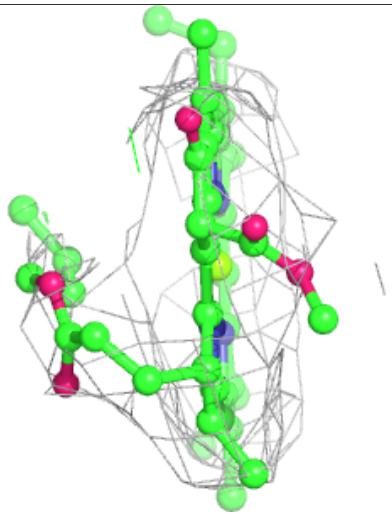


Electron density around CLA B 1213:

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

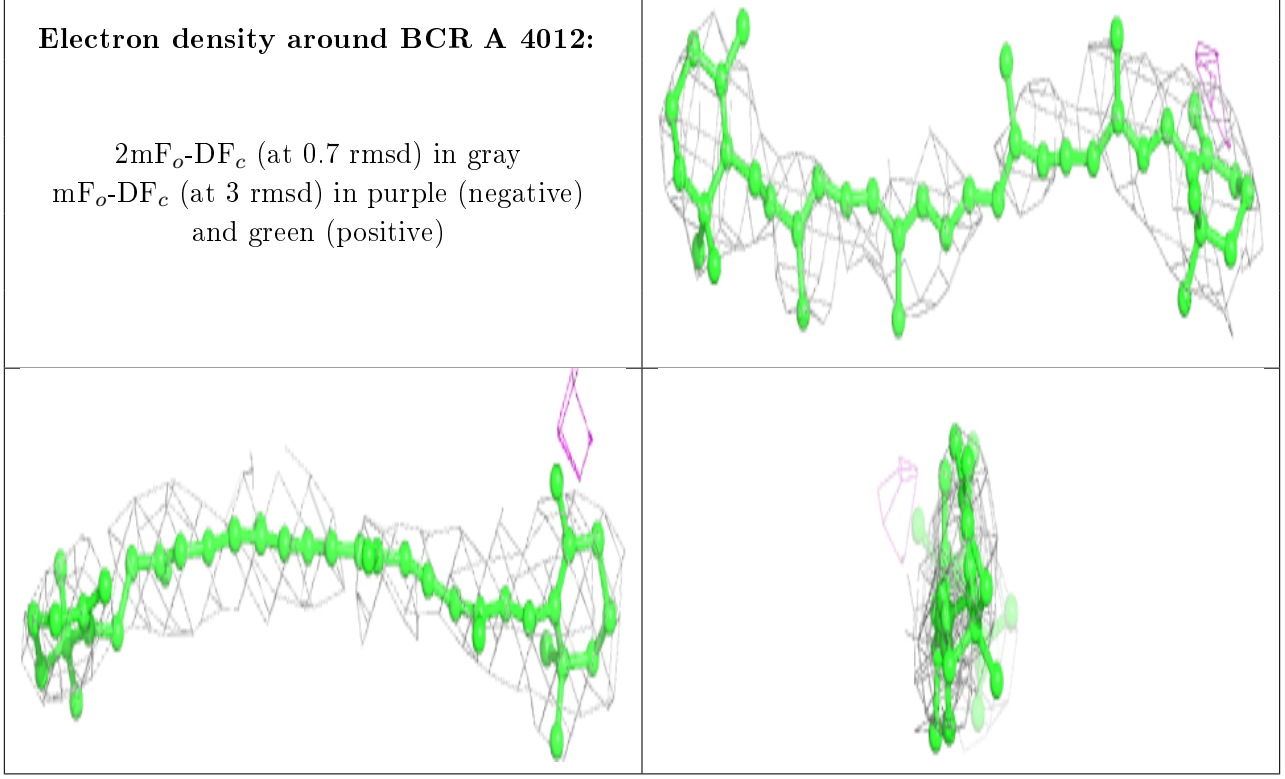






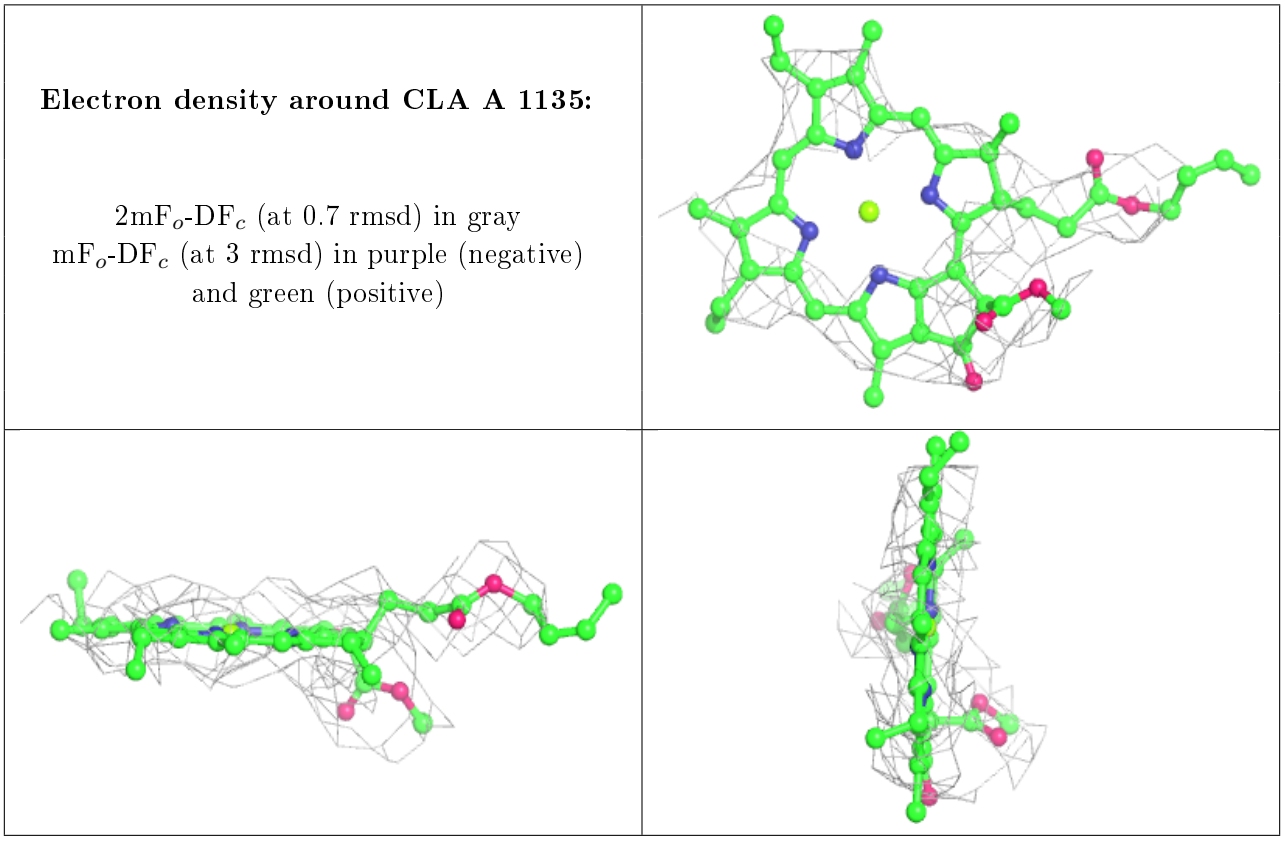
Electron density around BCR A 4012:

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



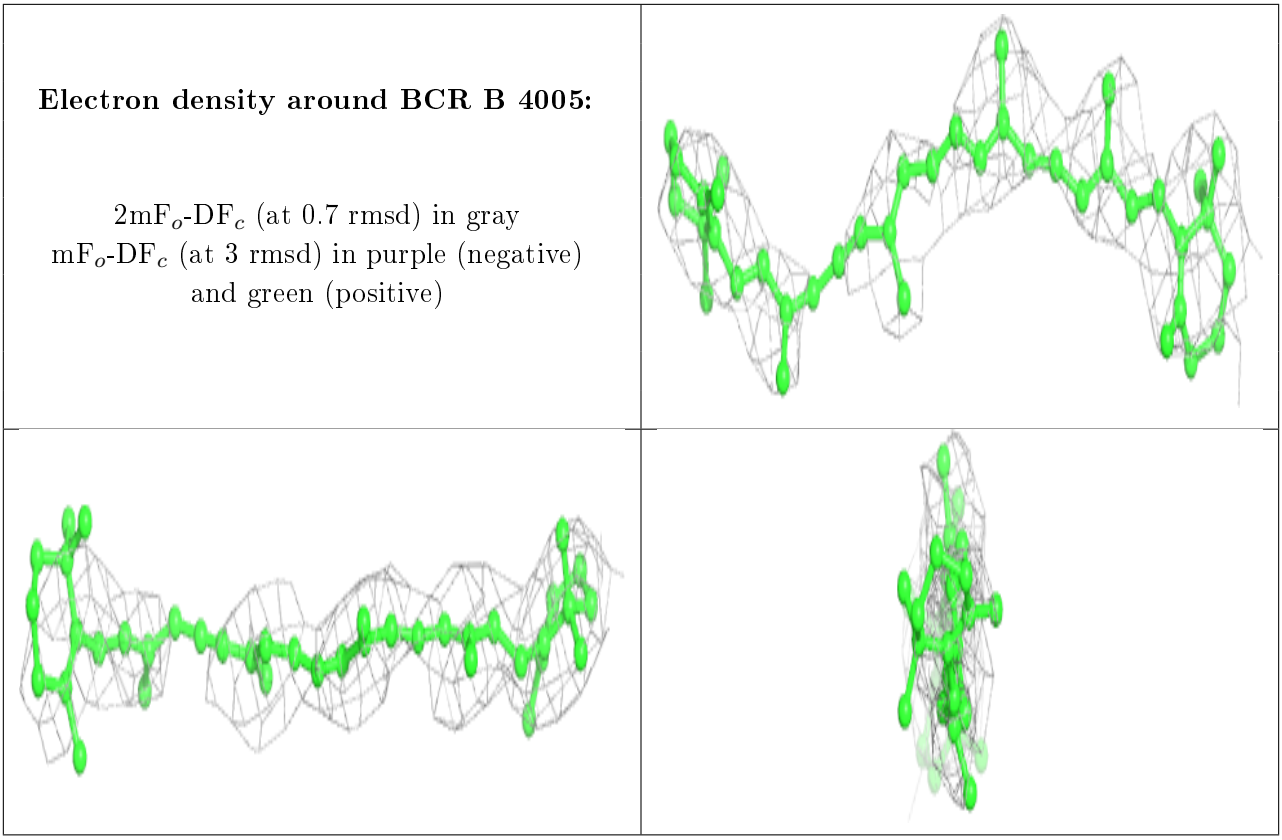
Electron density around CLA A 1135:

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



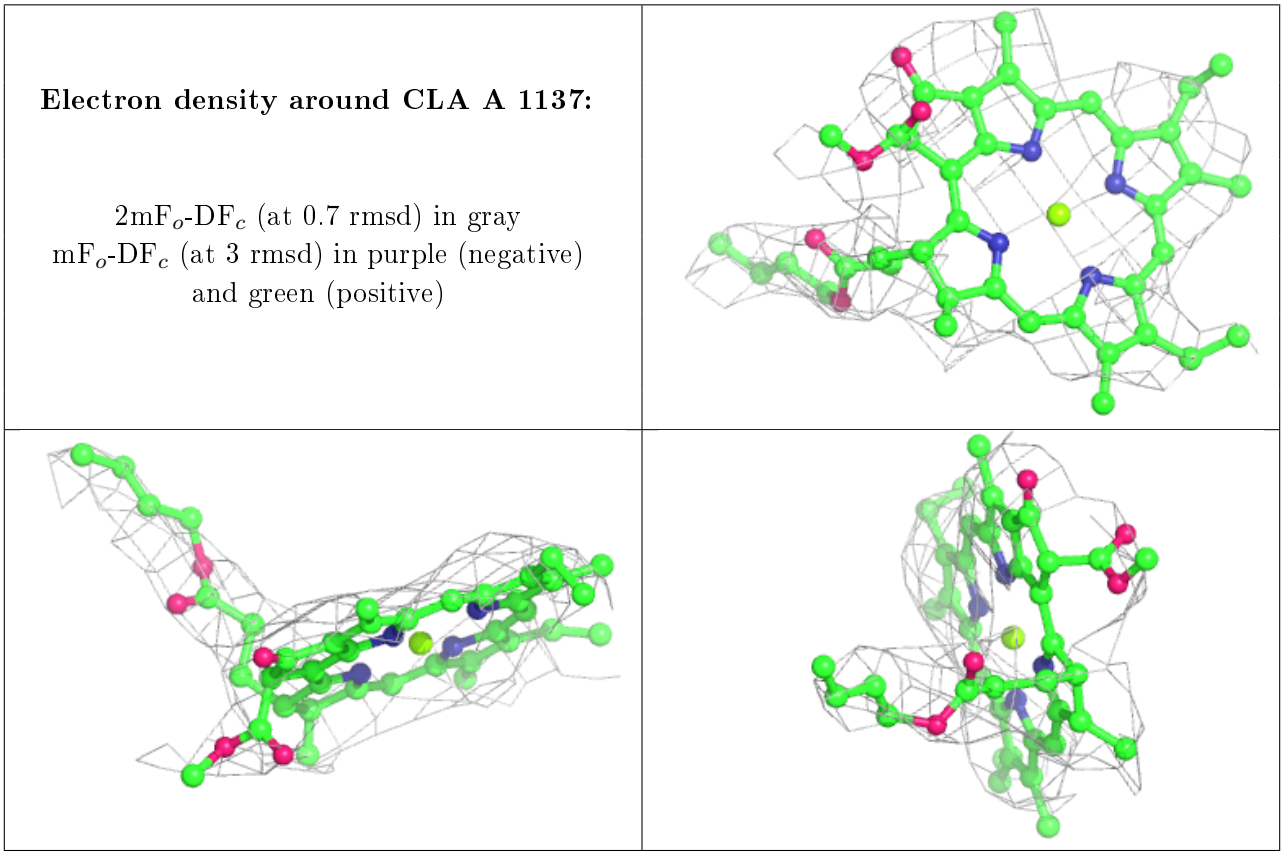
Electron density around BCR B 4005:

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



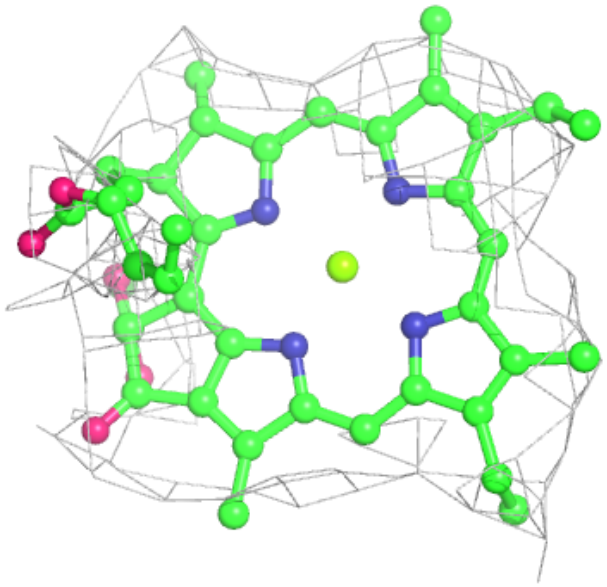
Electron density around CLA A 1137:

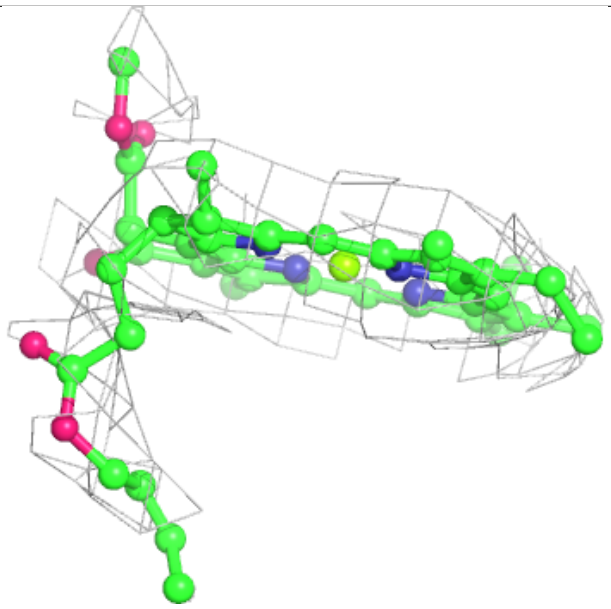
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

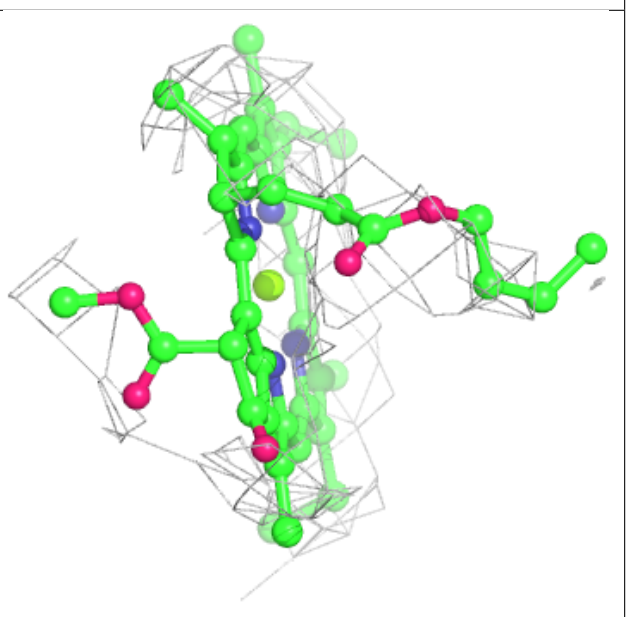


Electron density around CLA B 1238:

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

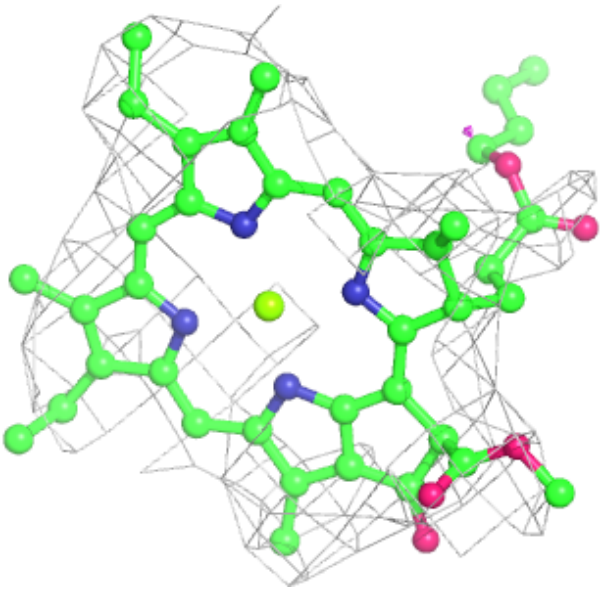


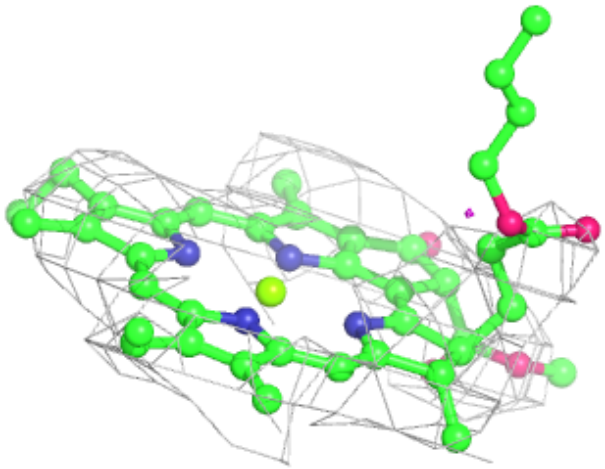


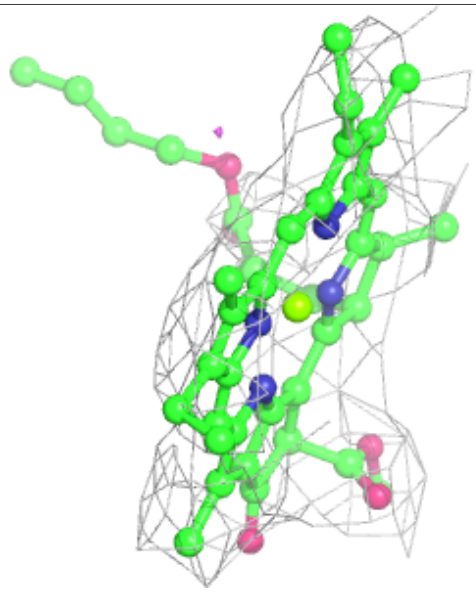


Electron density around CLA A 1129:

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

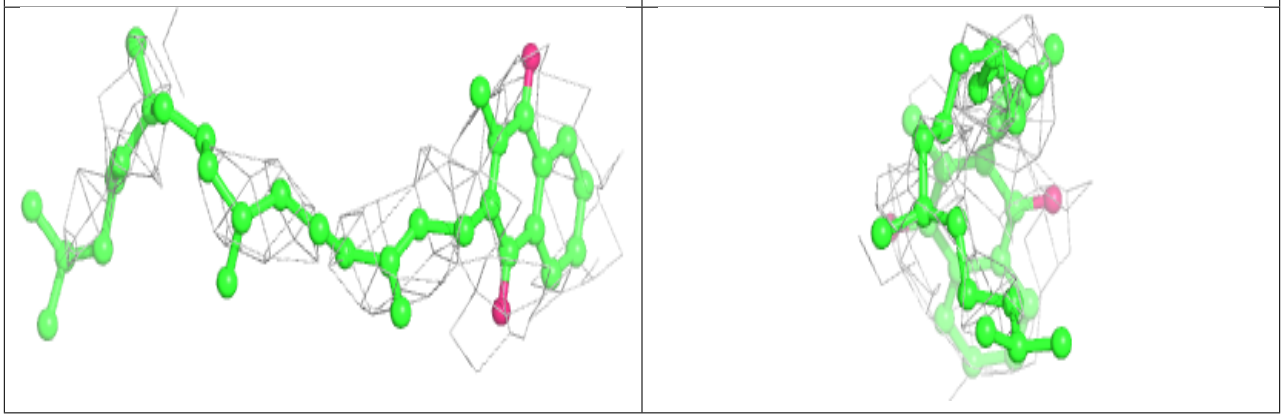






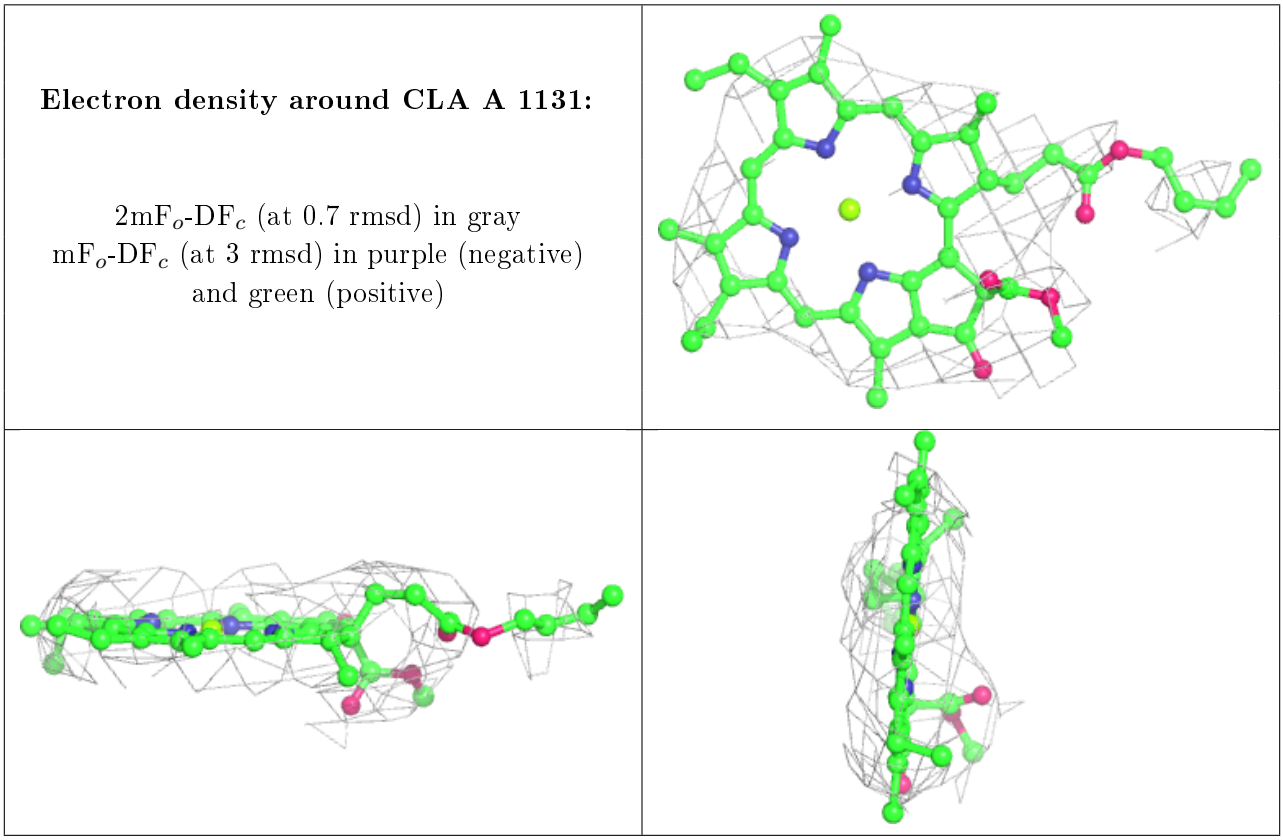
Electron density around PQN B 2002:

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



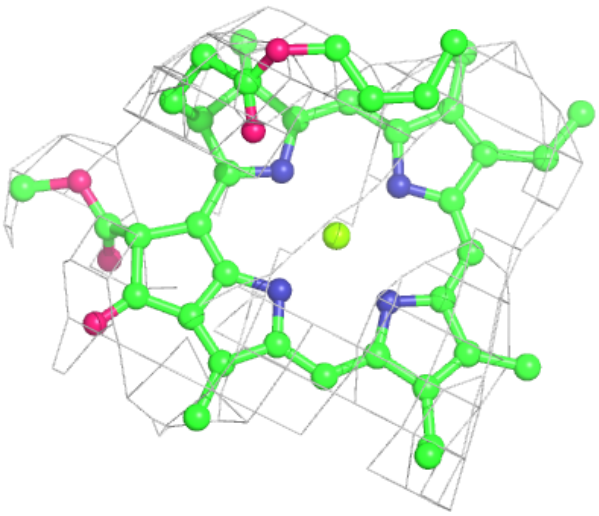
Electron density around CLA A 1131:

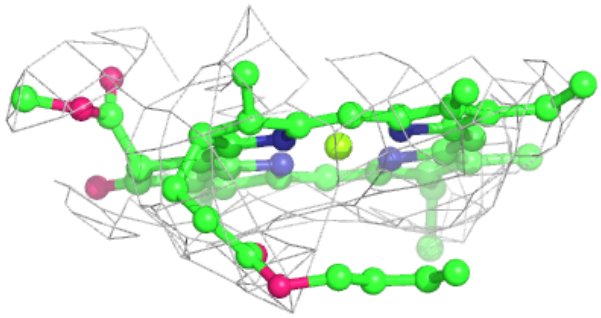
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

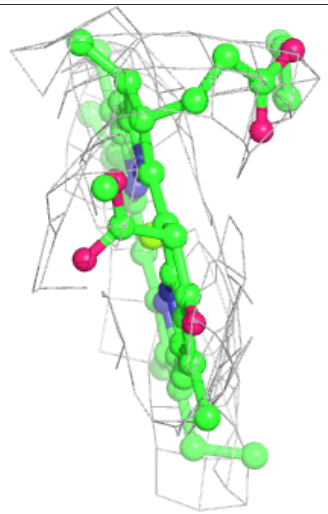


Electron density around CLA B 1218:

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

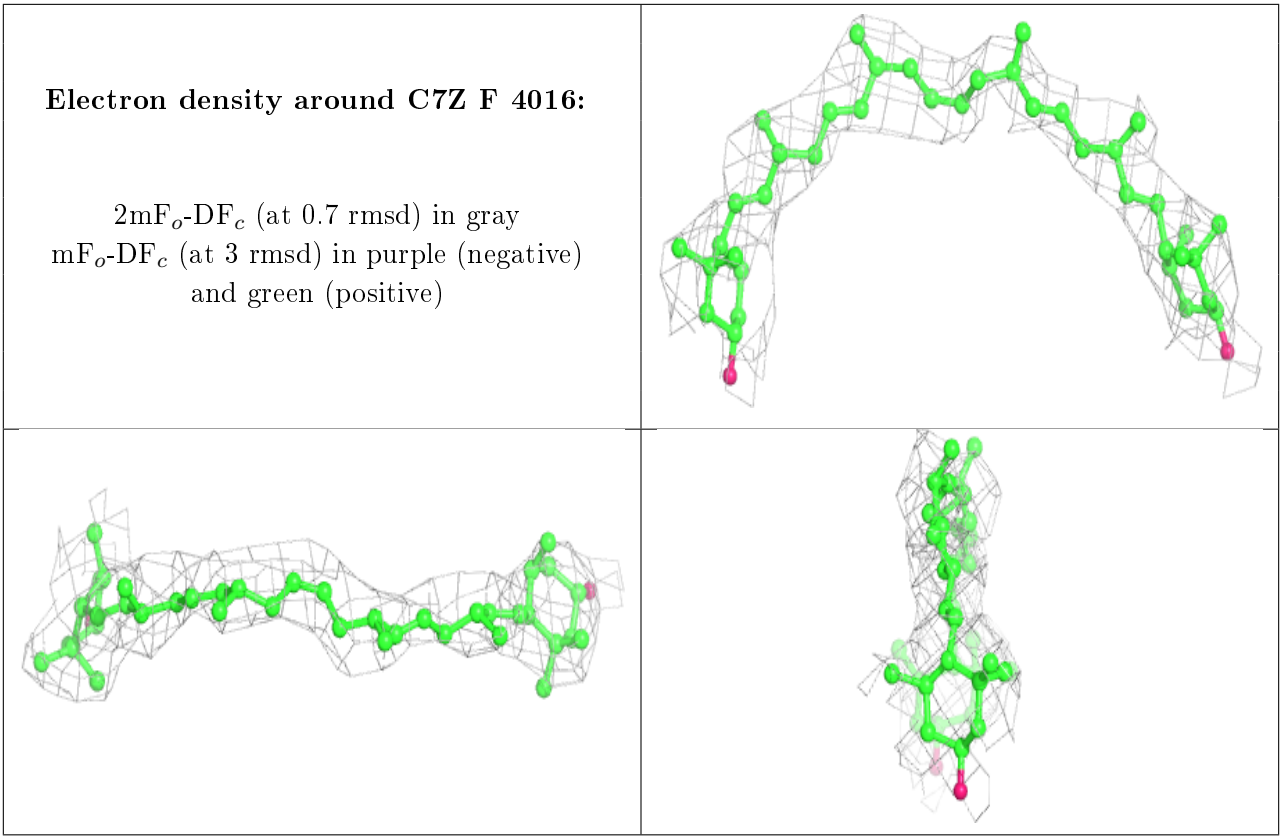






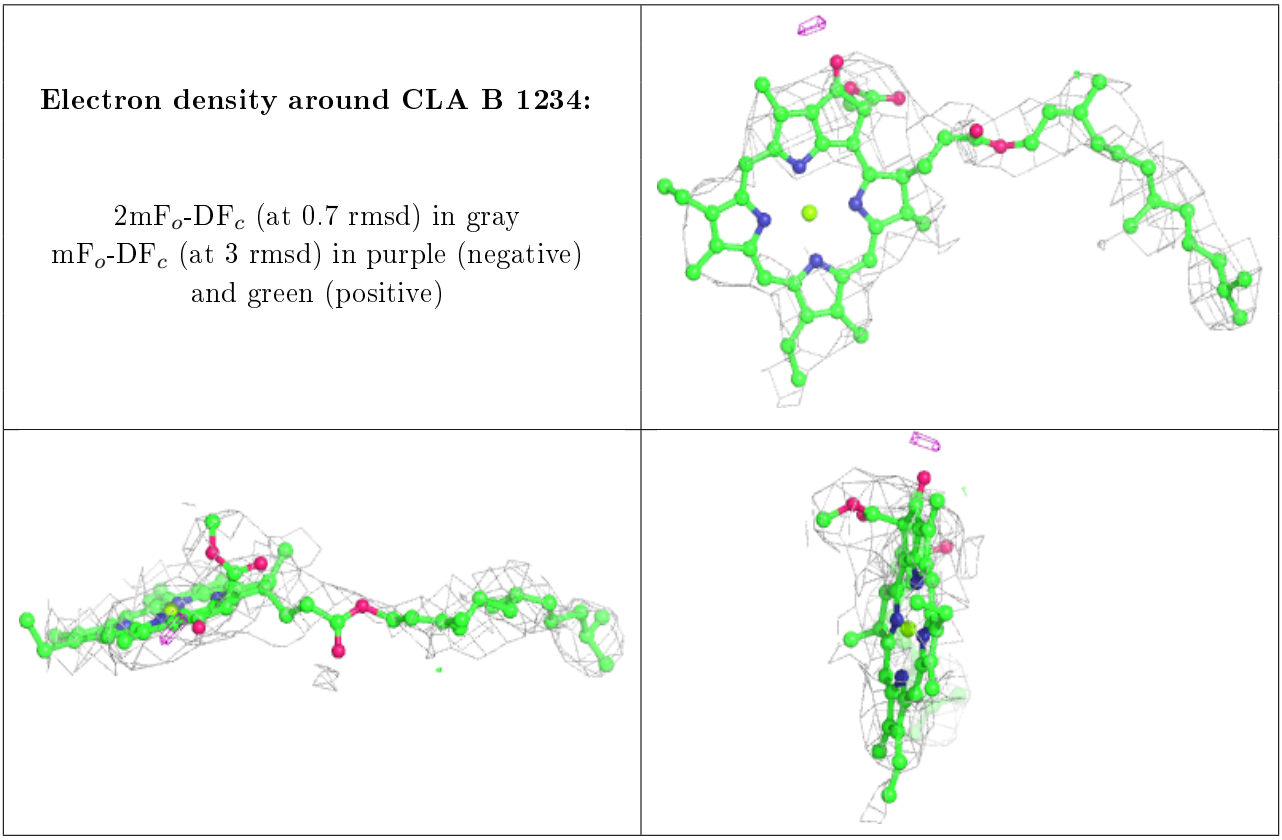
Electron density around C7Z F 4016:

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



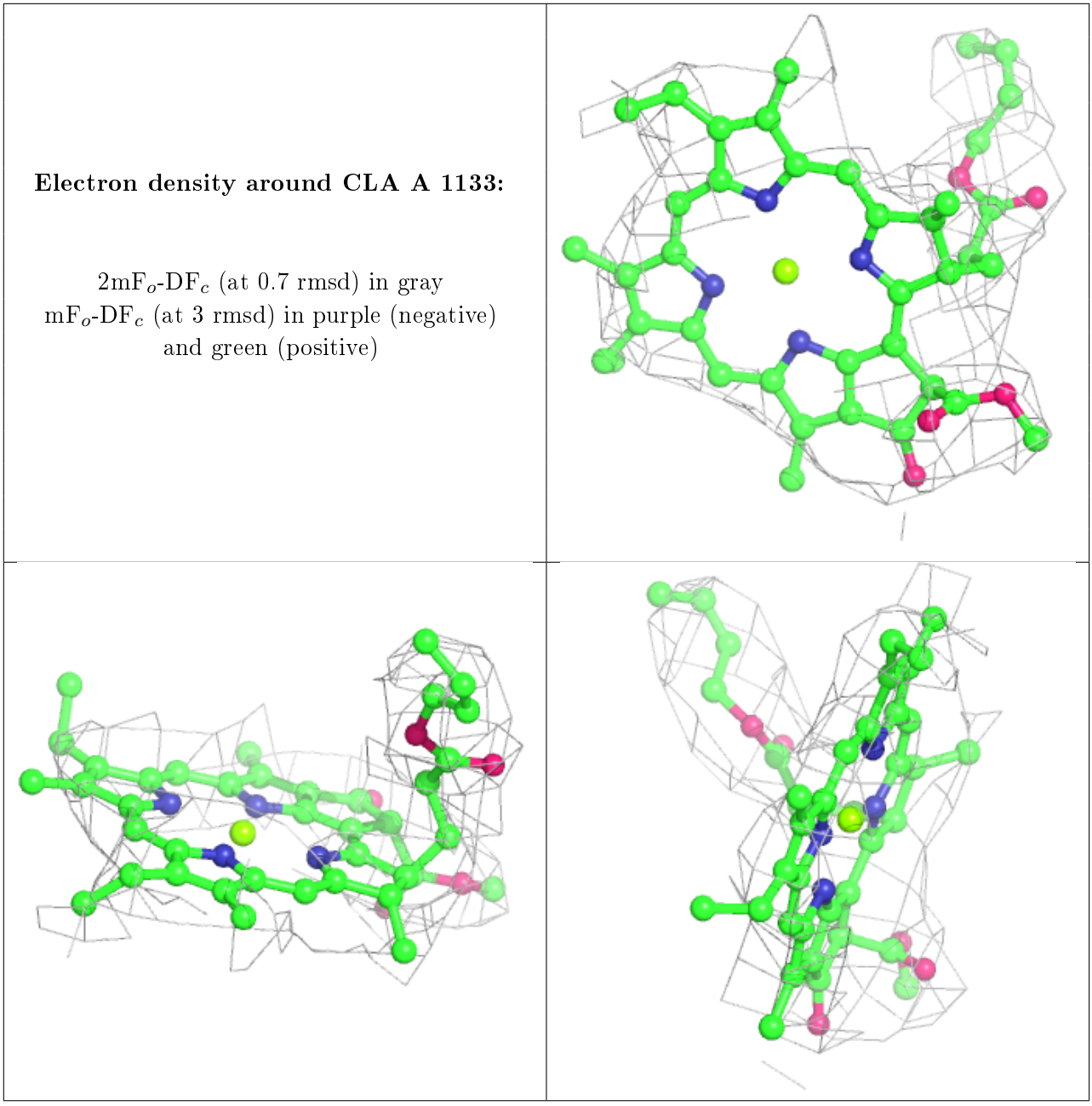
Electron density around CLA B 1234:

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



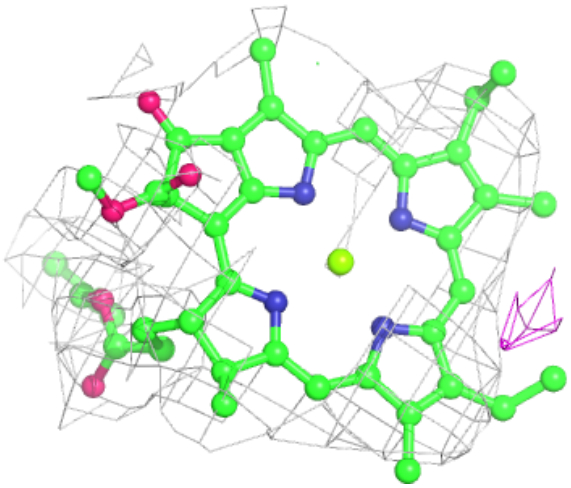
Electron density around CLA A 1133:

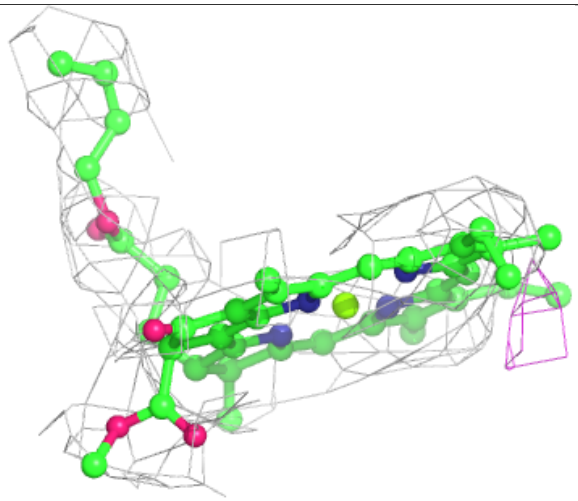
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

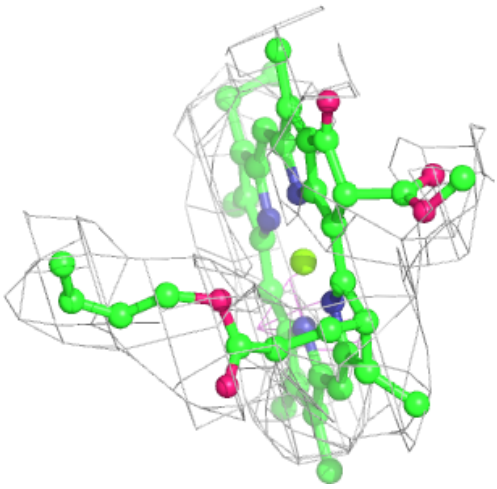


Electron density around CLA B 1236:

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

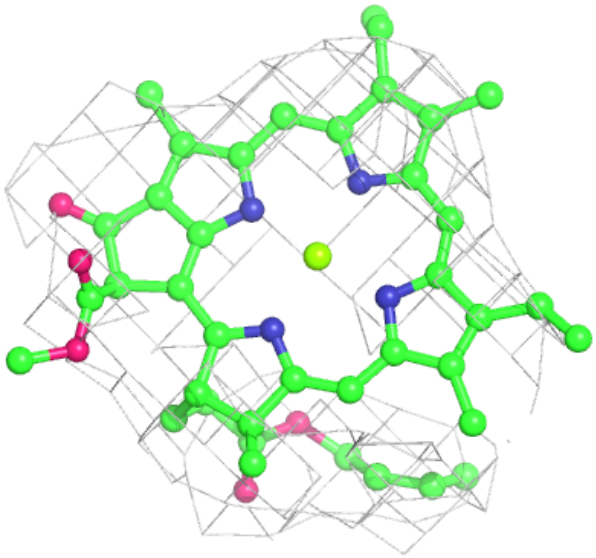


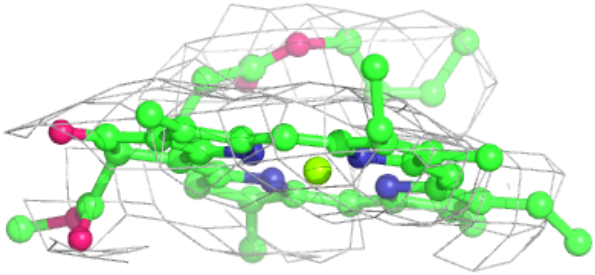


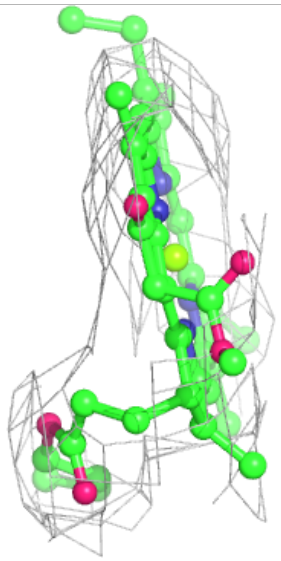


Electron density around CLA A 1117:

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

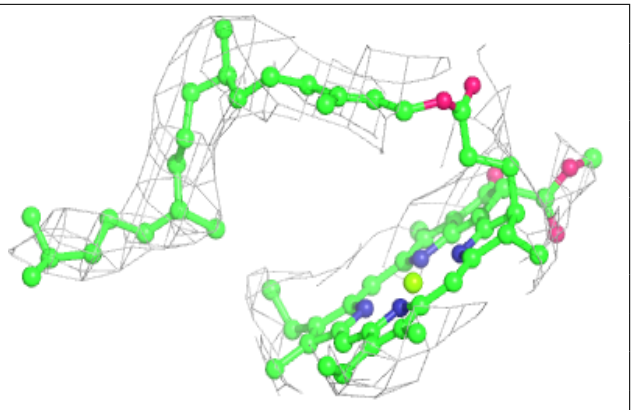


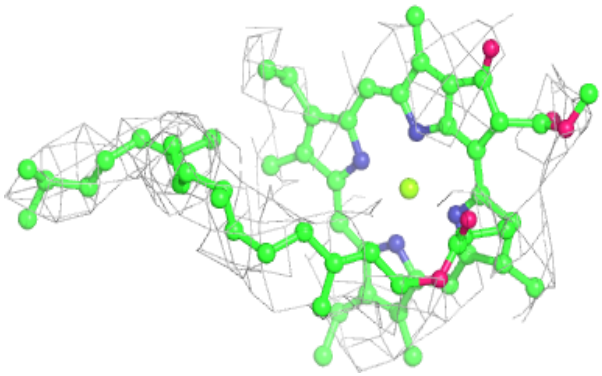


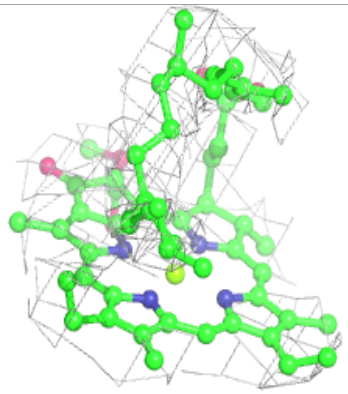


Electron density around CLA A 1109:

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

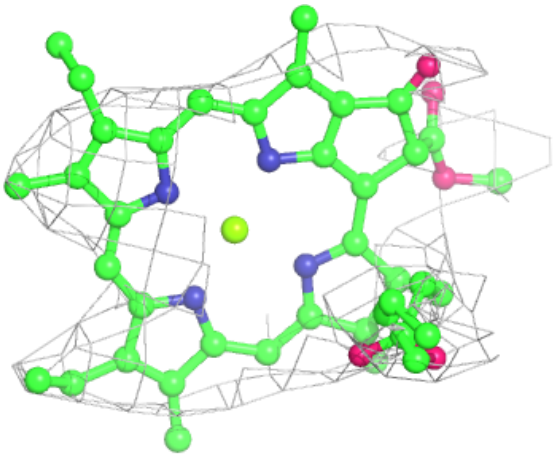


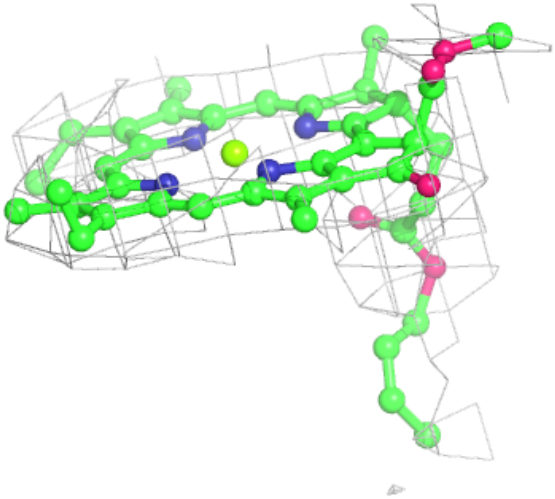


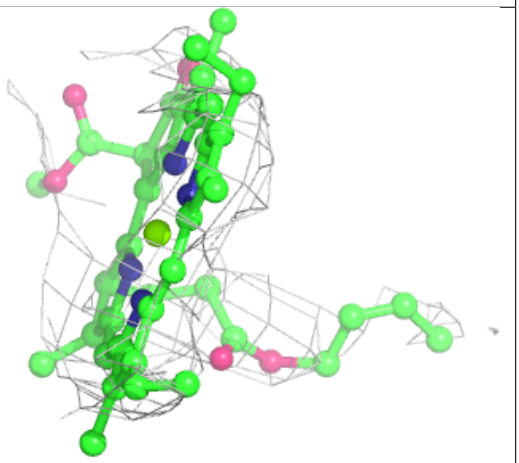


Electron density around CLA A 1134:

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

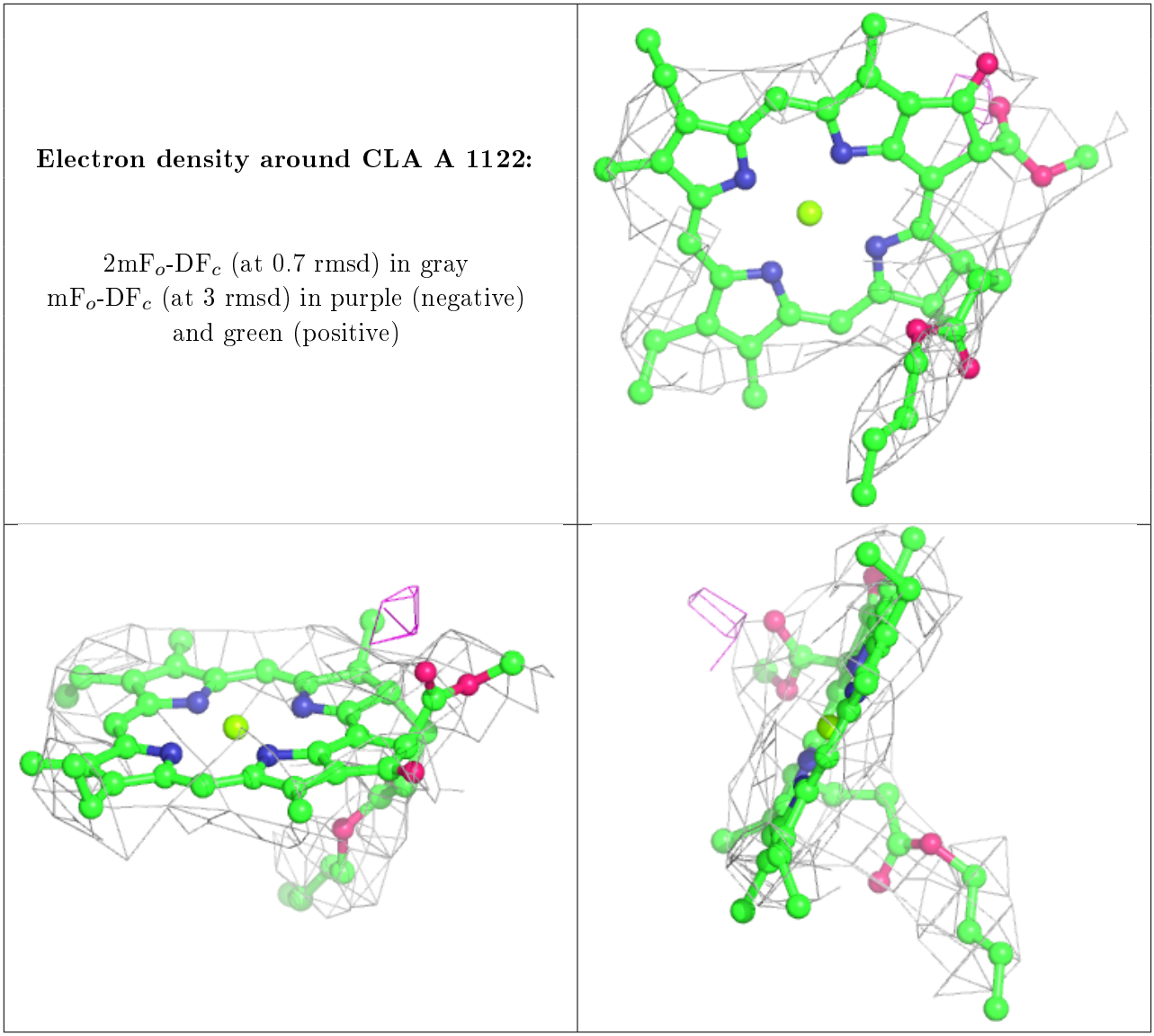






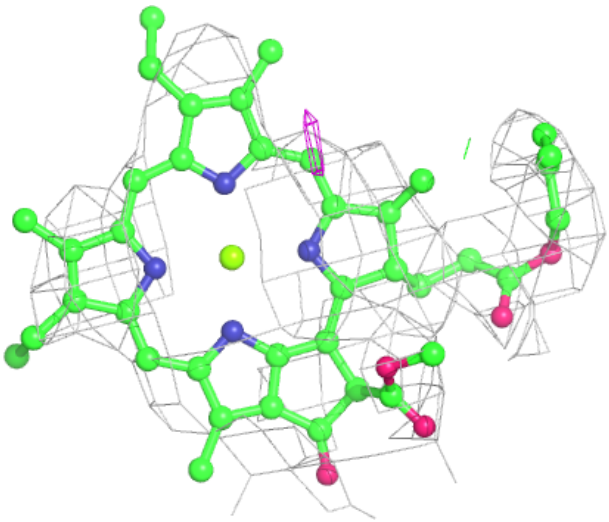
Electron density around CLA A 1122:

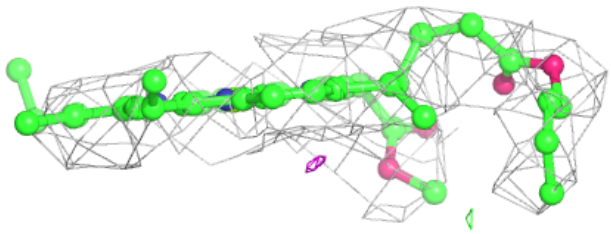
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

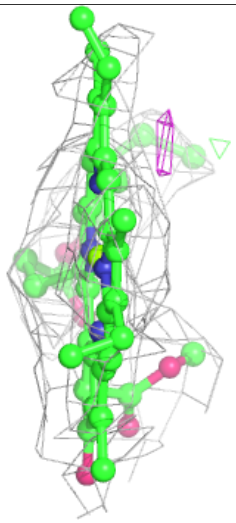


Electron density around CLA B 1221:

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

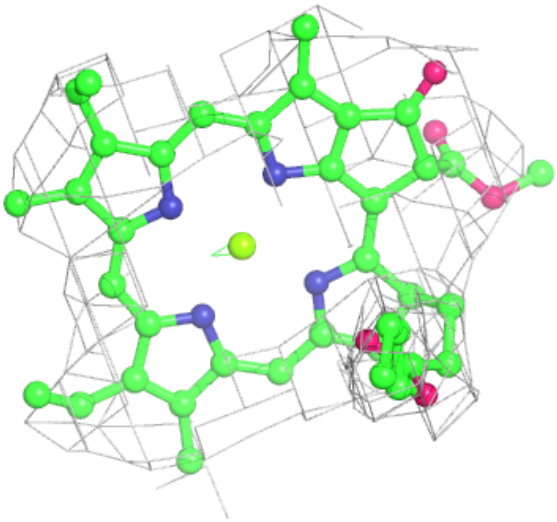


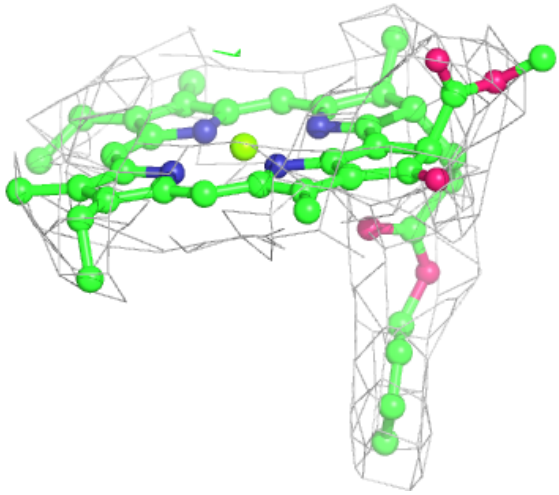


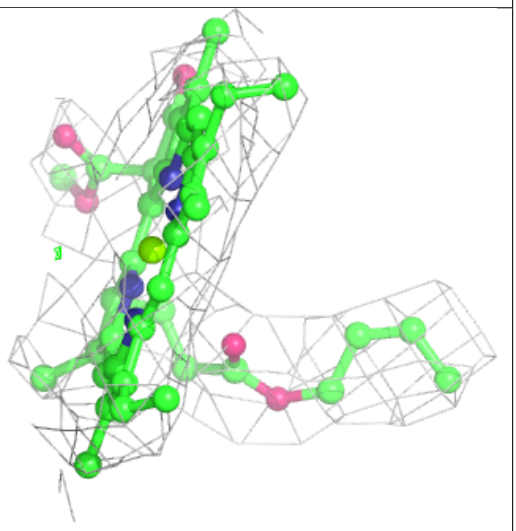


Electron density around CLA B 1225:

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

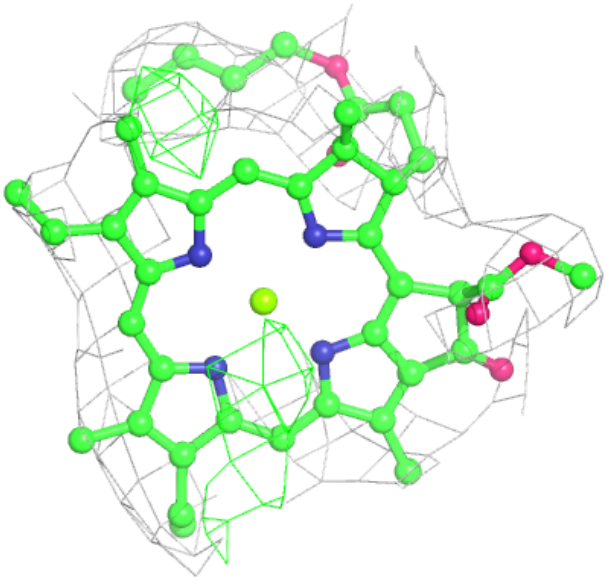


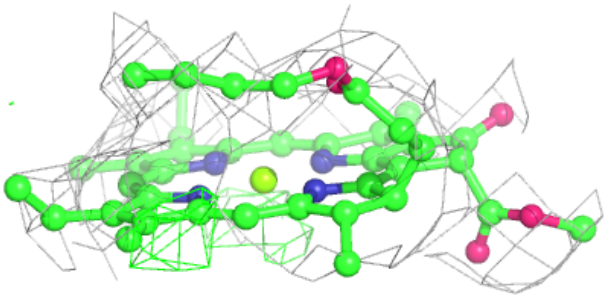


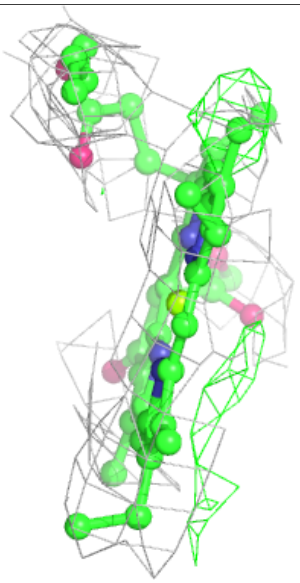


Electron density around CLA B 1215:

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

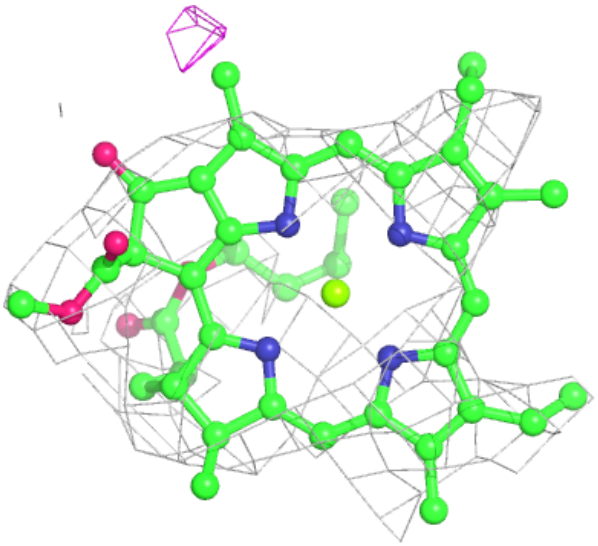


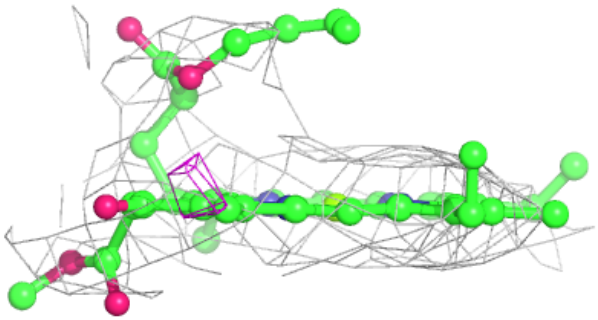


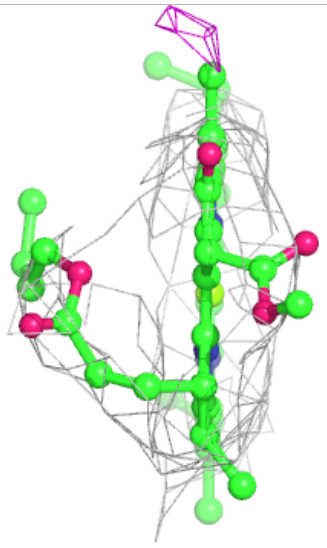


Electron density around CLA A 1136:

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

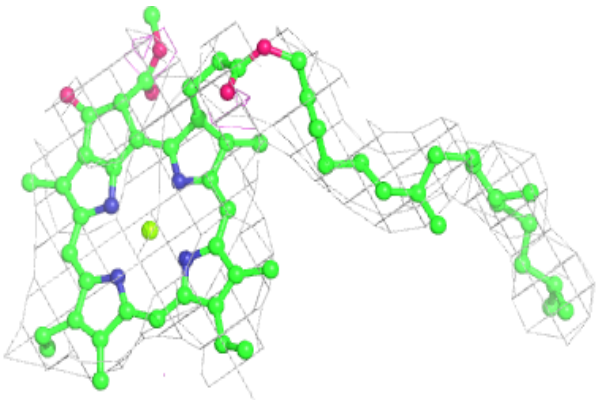


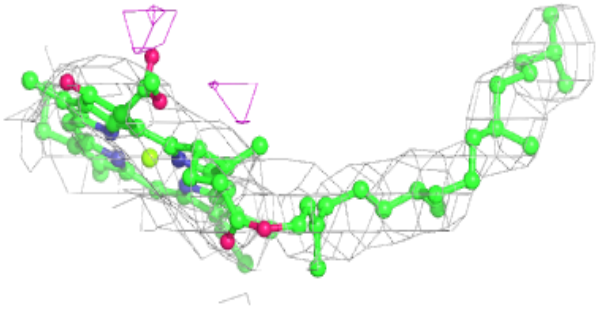


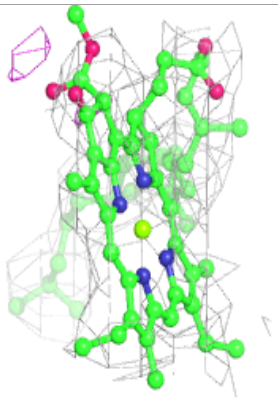


Electron density around CLA A 1013:

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

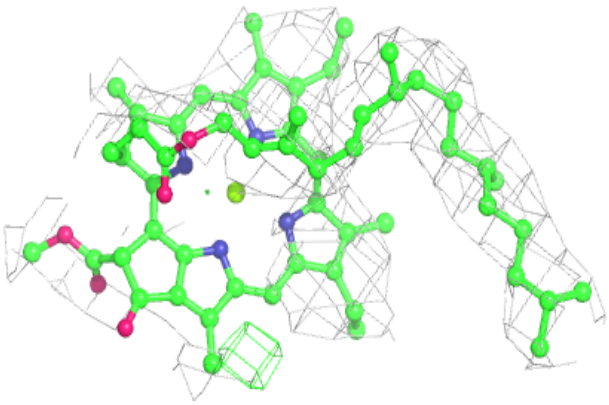


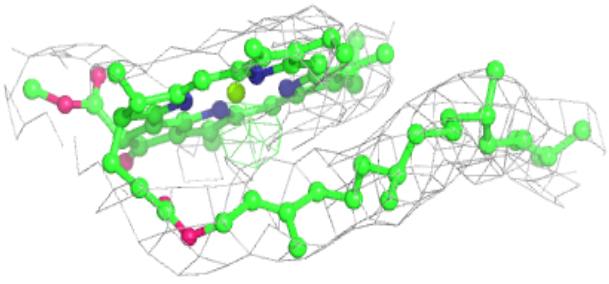


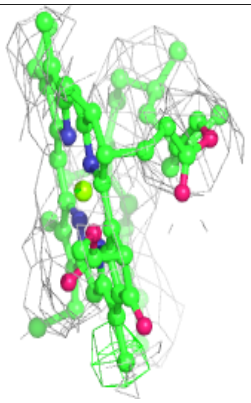


Electron density around CLA B 1235:

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

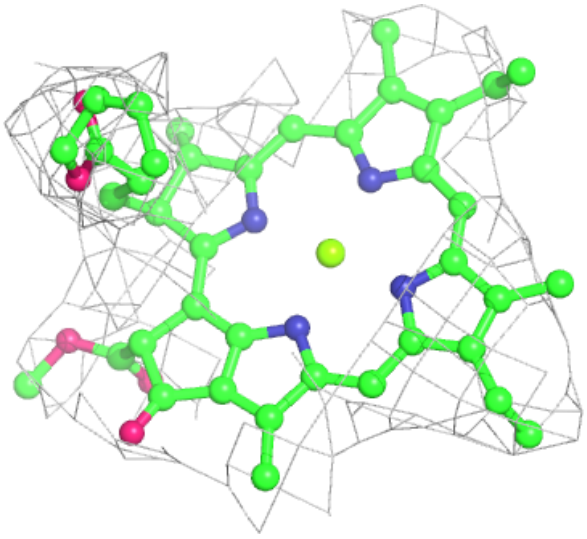


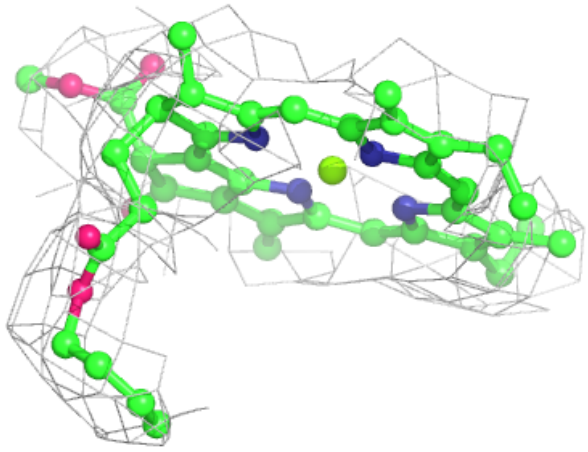


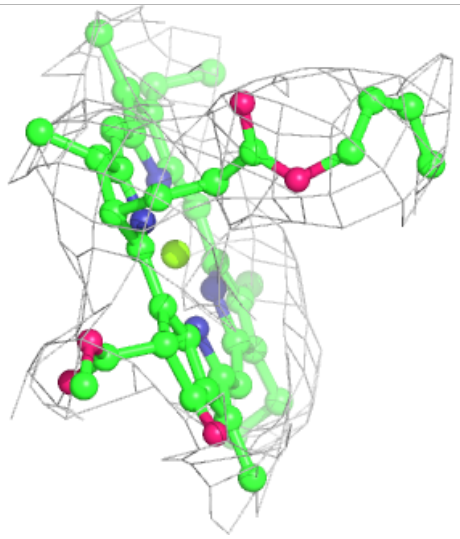


Electron density around CLA B 1232:

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

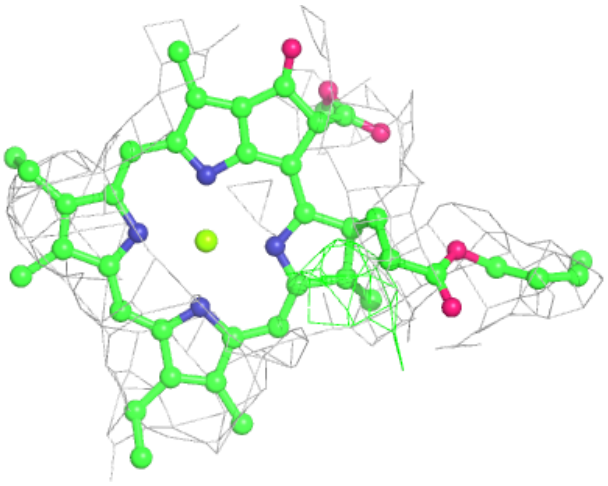


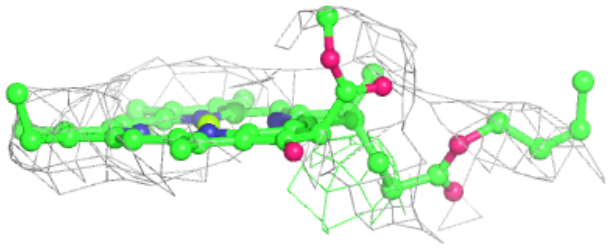


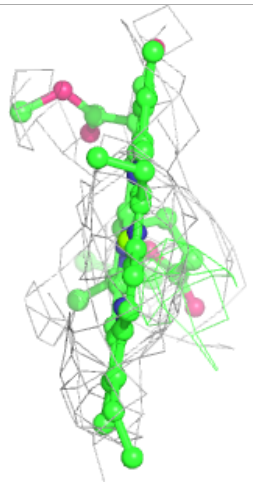


Electron density around CLA A 1103:

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

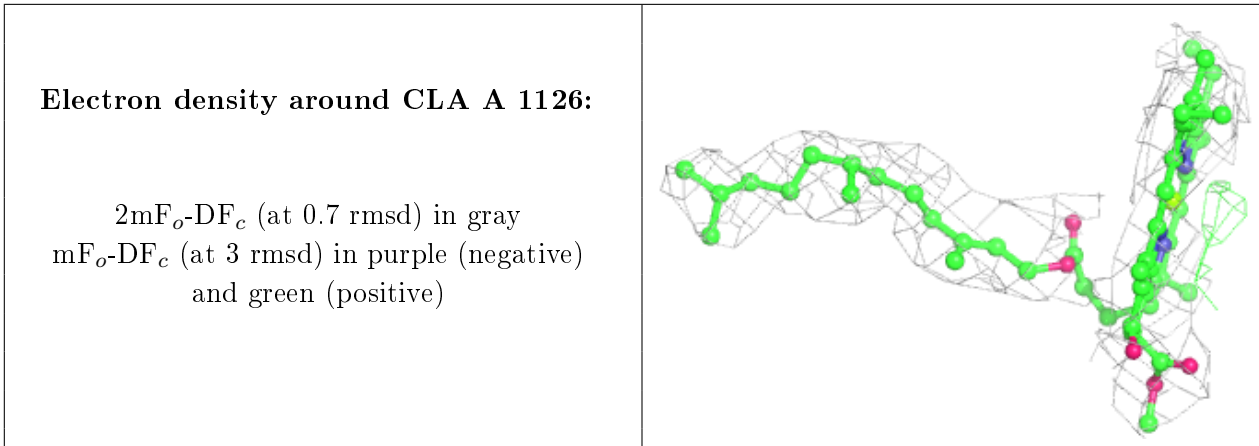






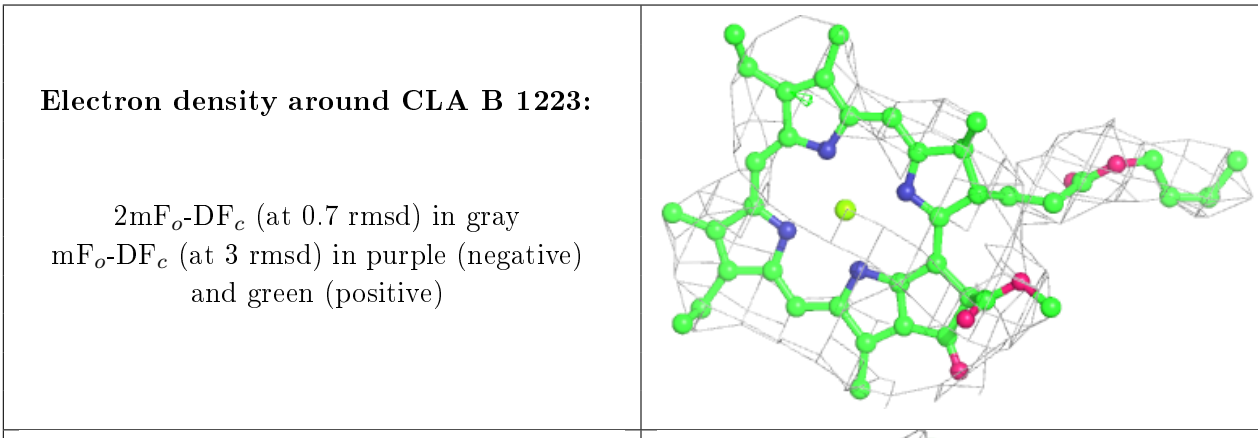
Electron density around CLA A 1126:

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



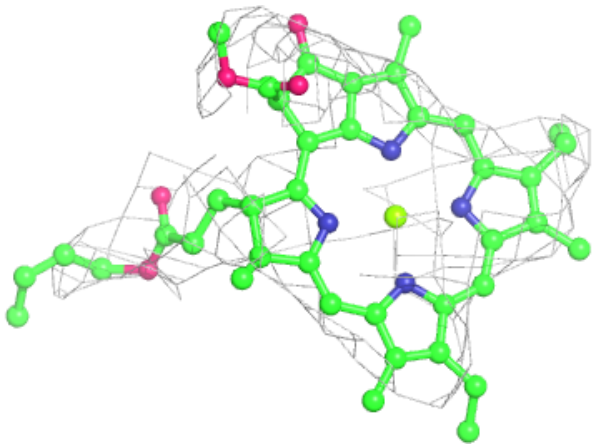
Electron density around CLA B 1223:

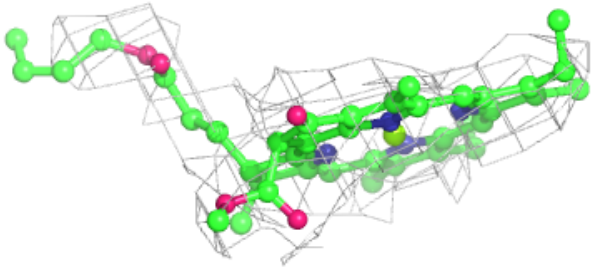
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

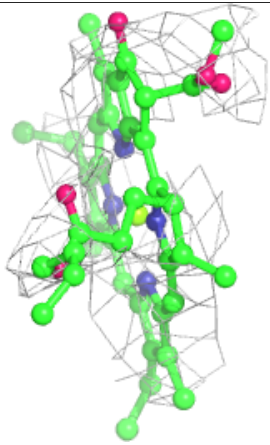


Electron density around CLA A 1124:

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

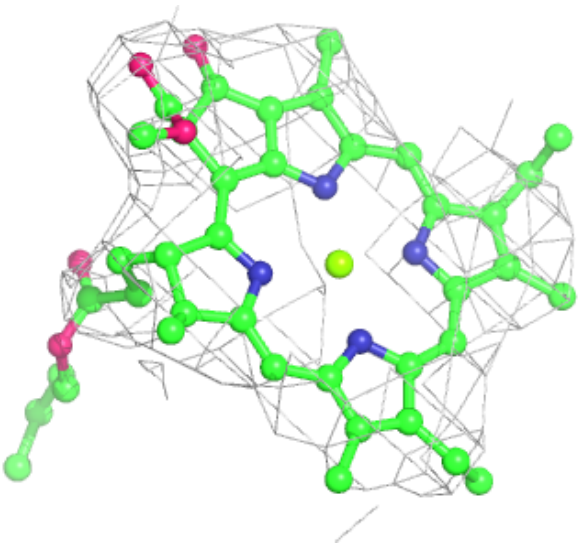


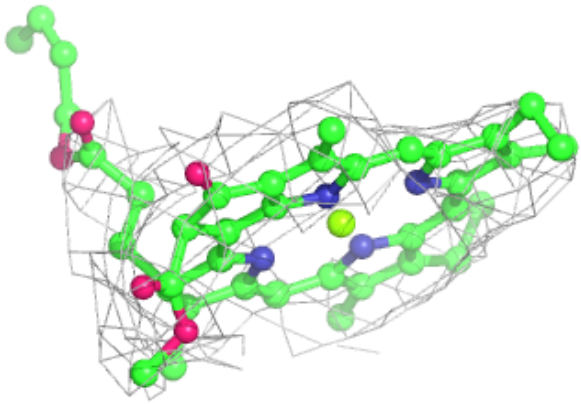


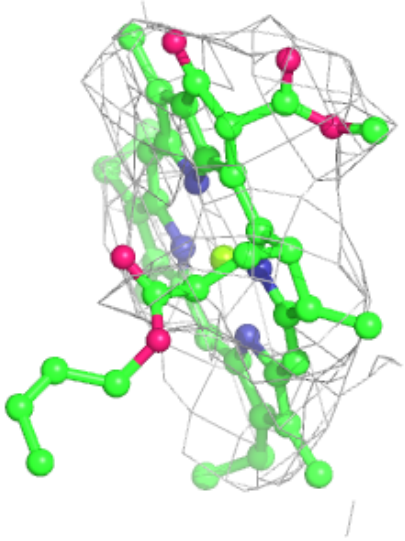


Electron density around CLA B 1227:

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

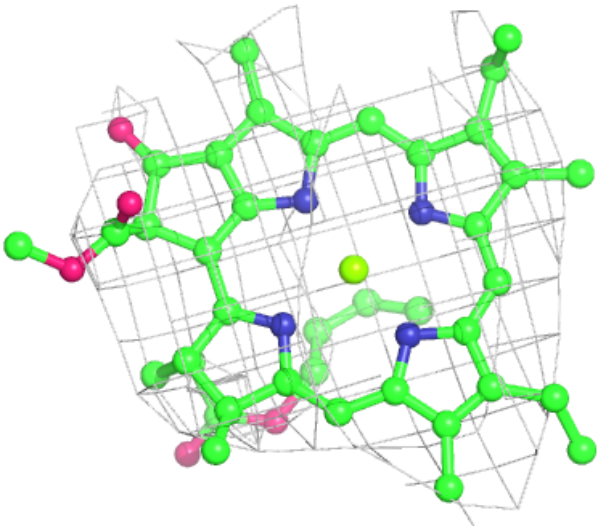


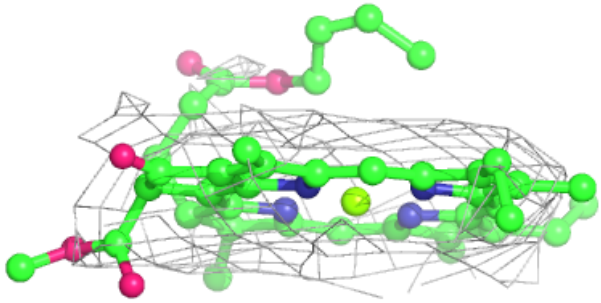


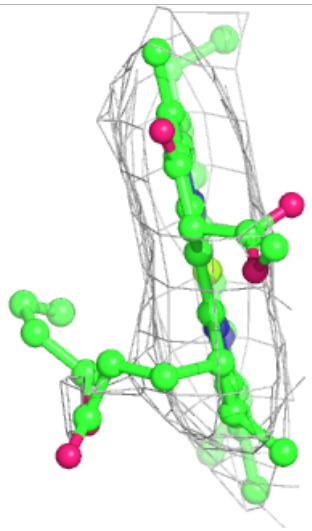


Electron density around CLA A 1121:

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

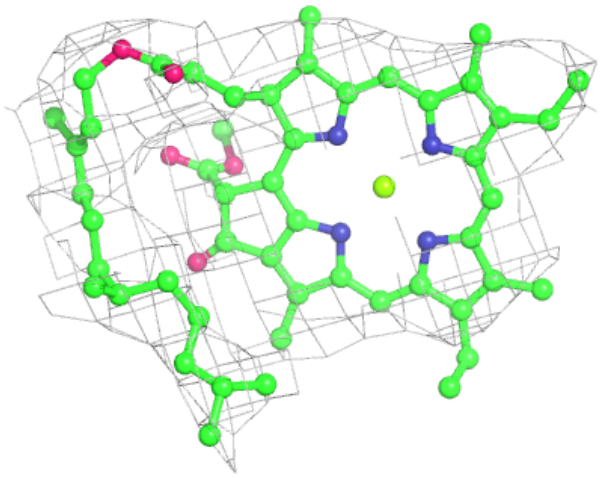


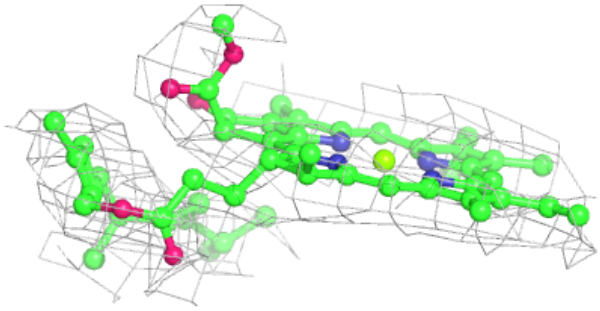


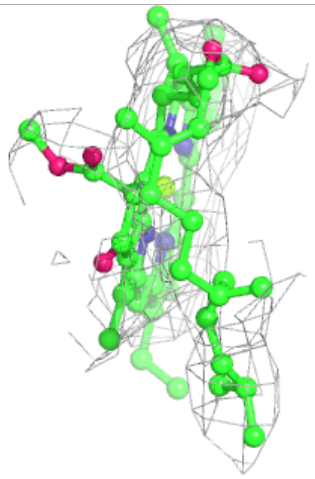


Electron density around CLA A 1123:

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

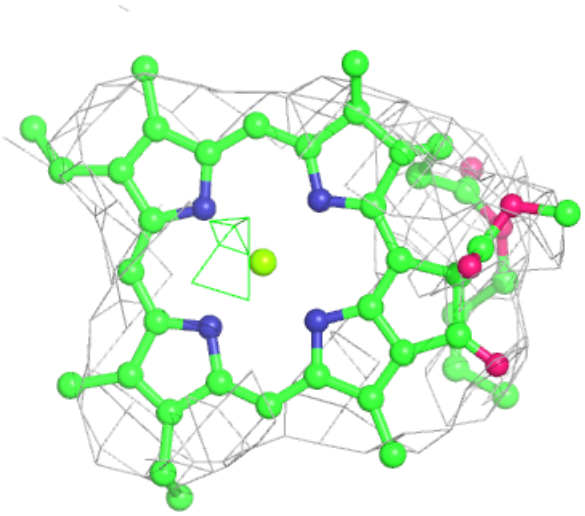


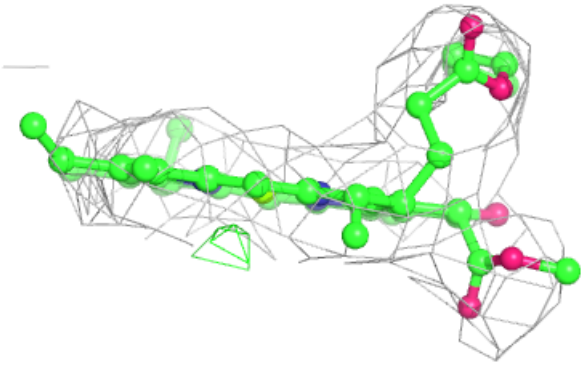


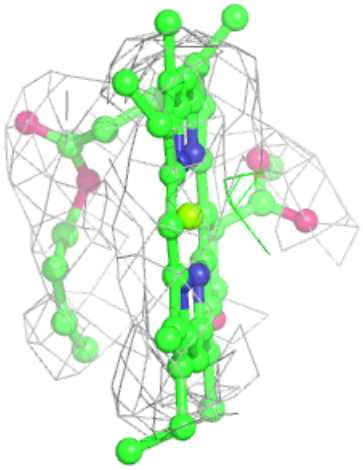


Electron density around CLA A 1127:

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

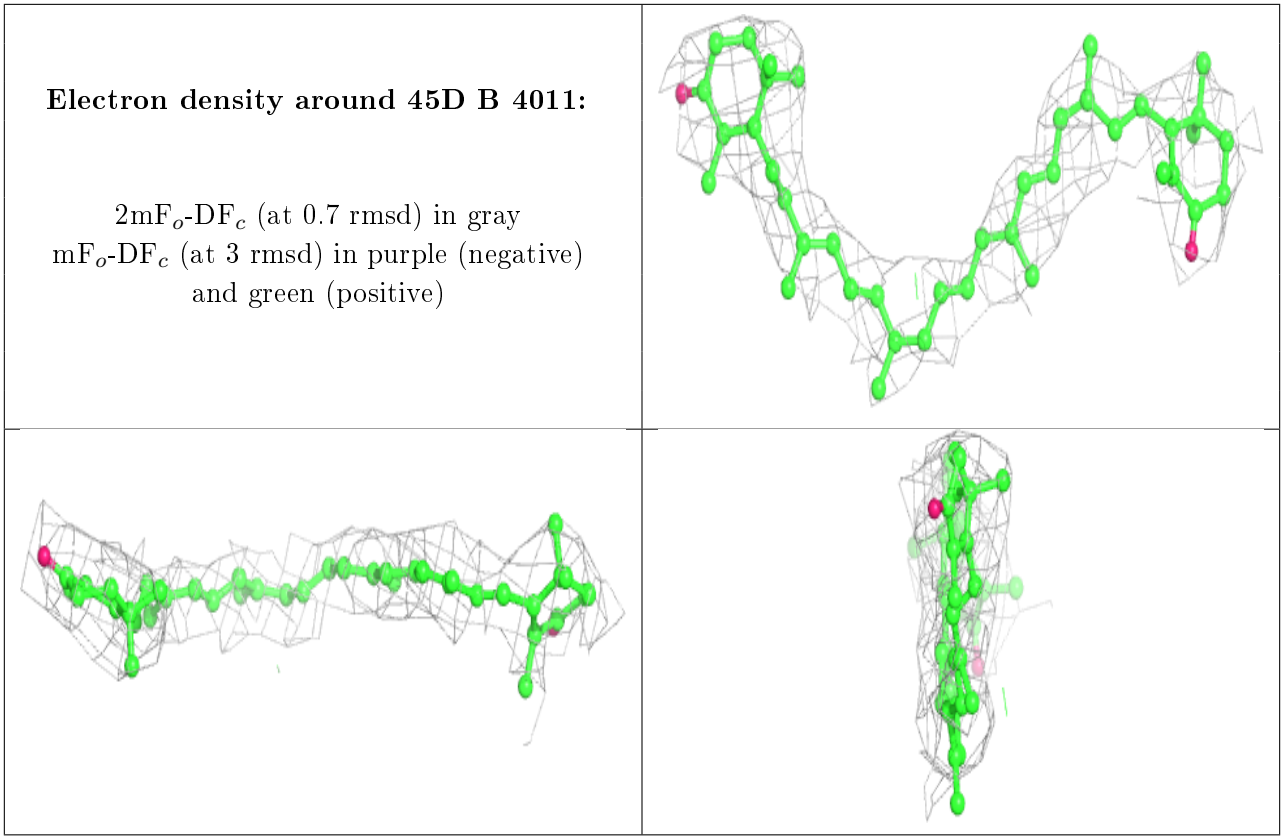






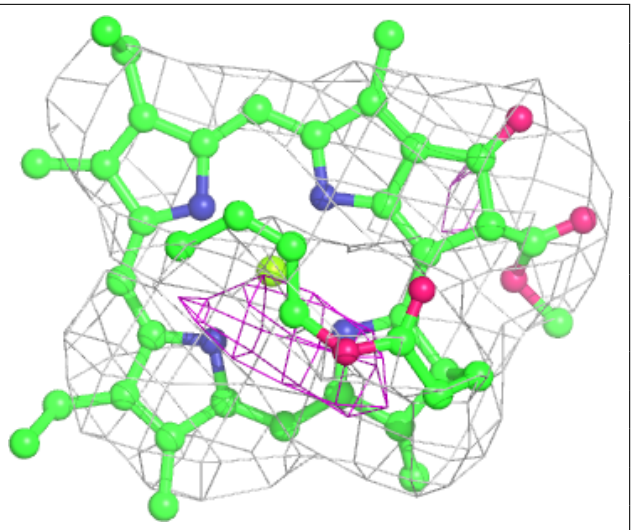
Electron density around 45D B 4011:

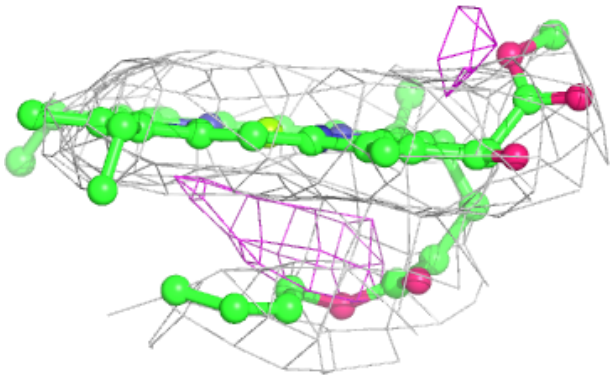
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

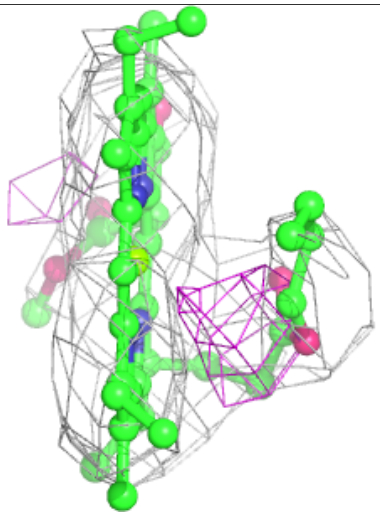


Electron density around CLA B 1205:

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

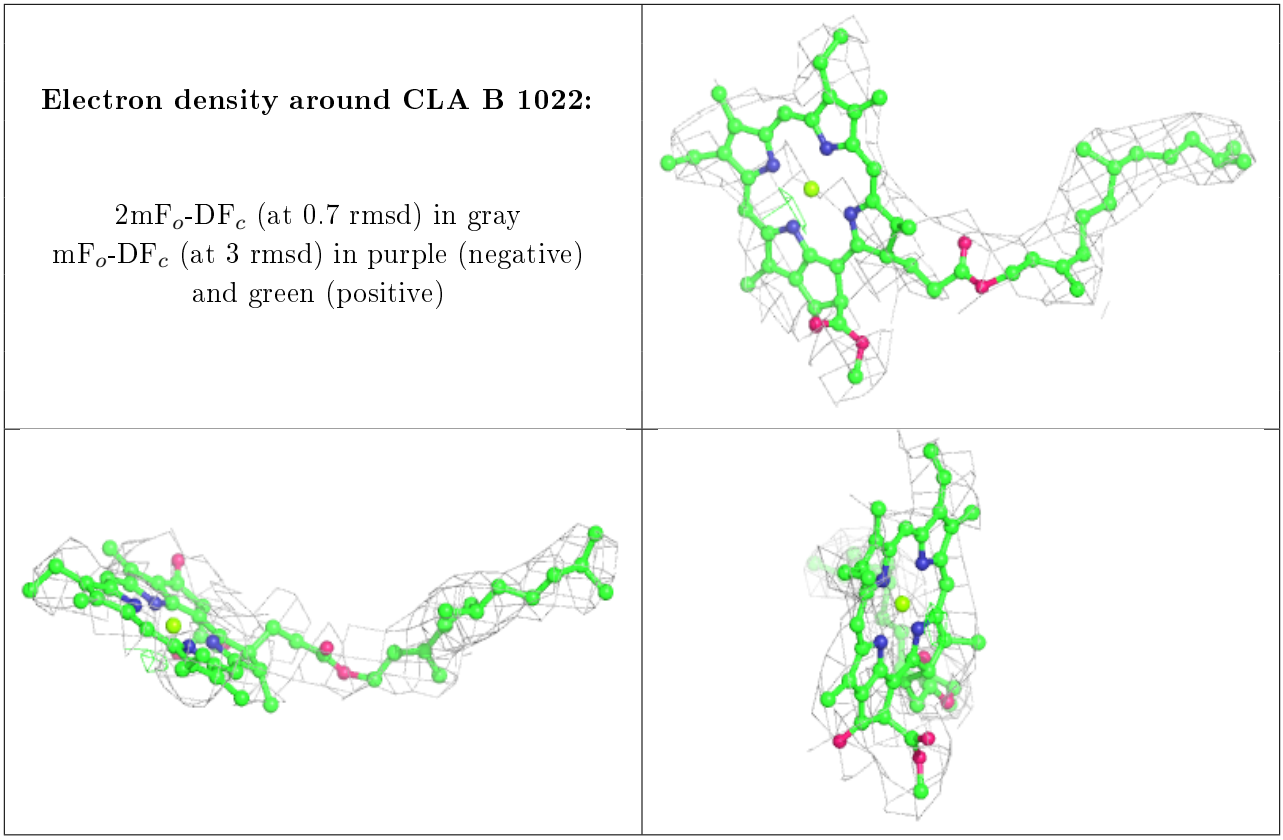






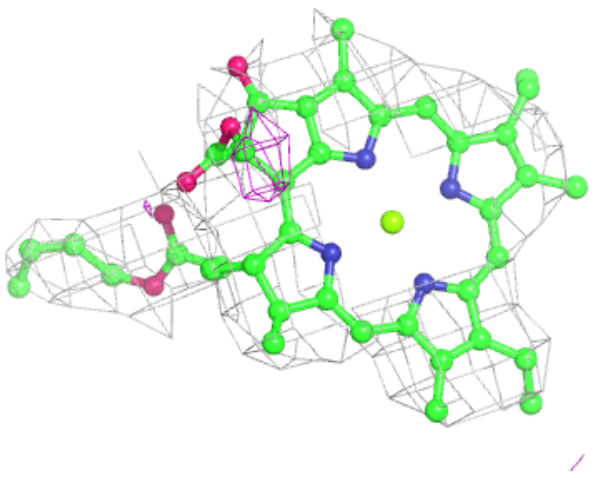
Electron density around CLA B 1022:

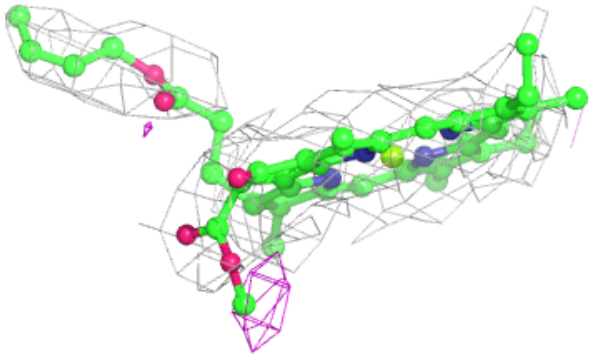
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

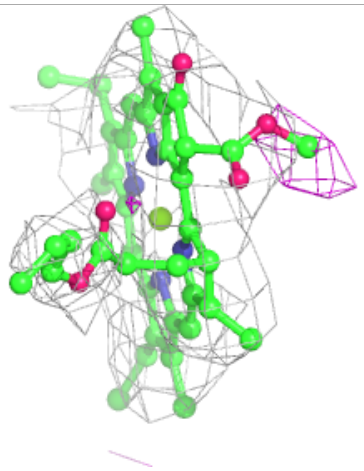


Electron density around CLA B 1220:

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

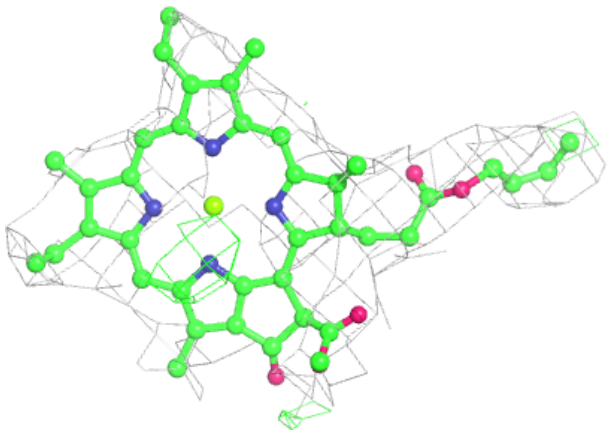


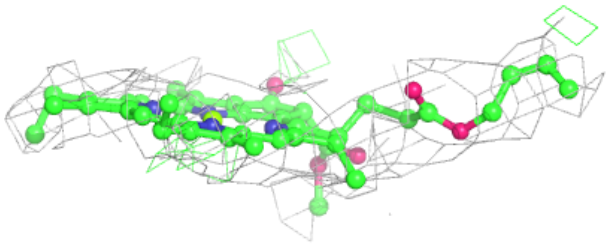


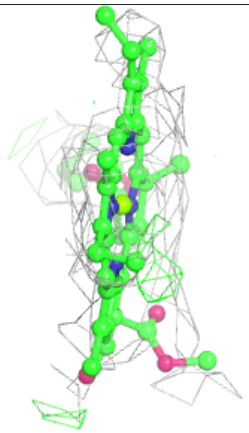


Electron density around CLA A 1012:

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

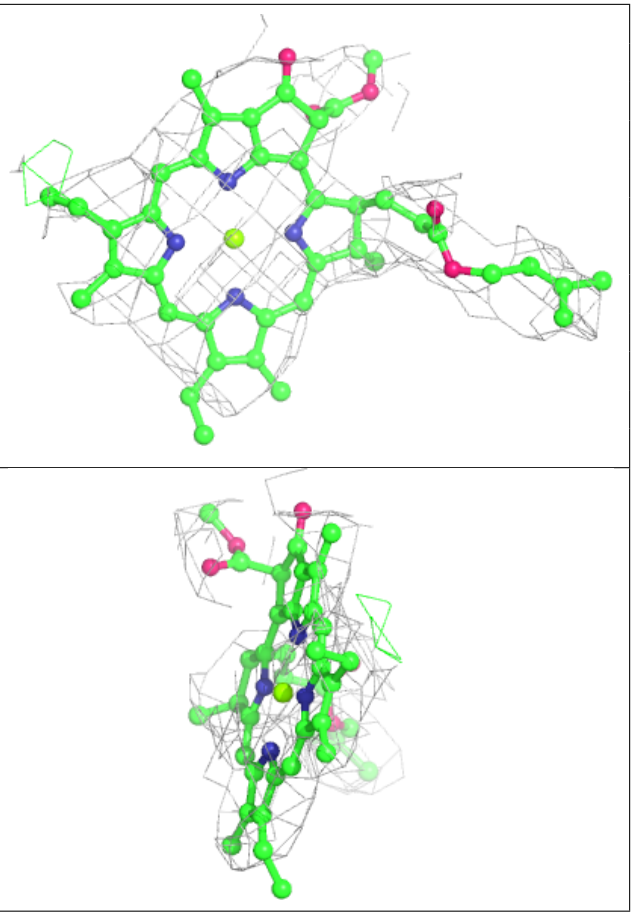






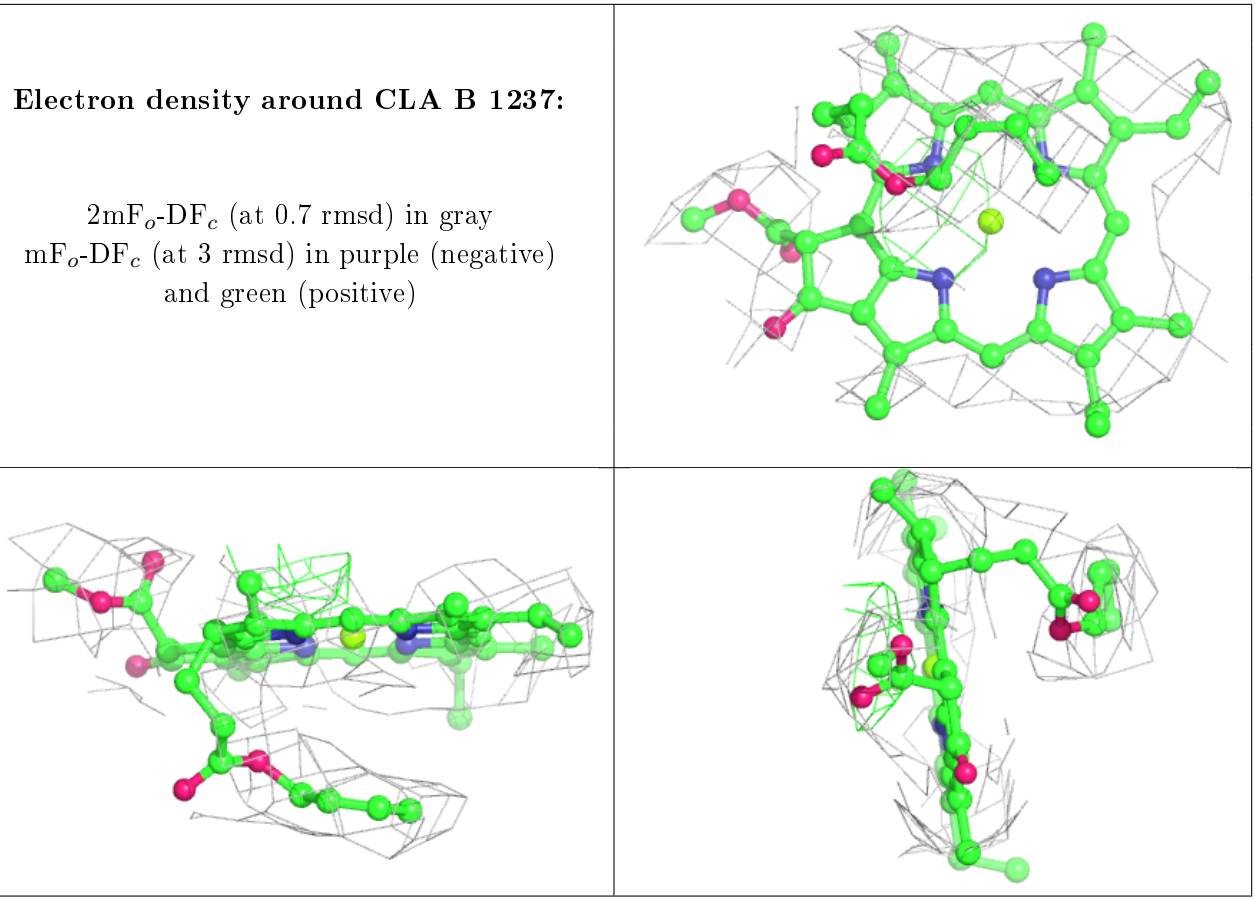
Electron density around CLA B 1222:

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



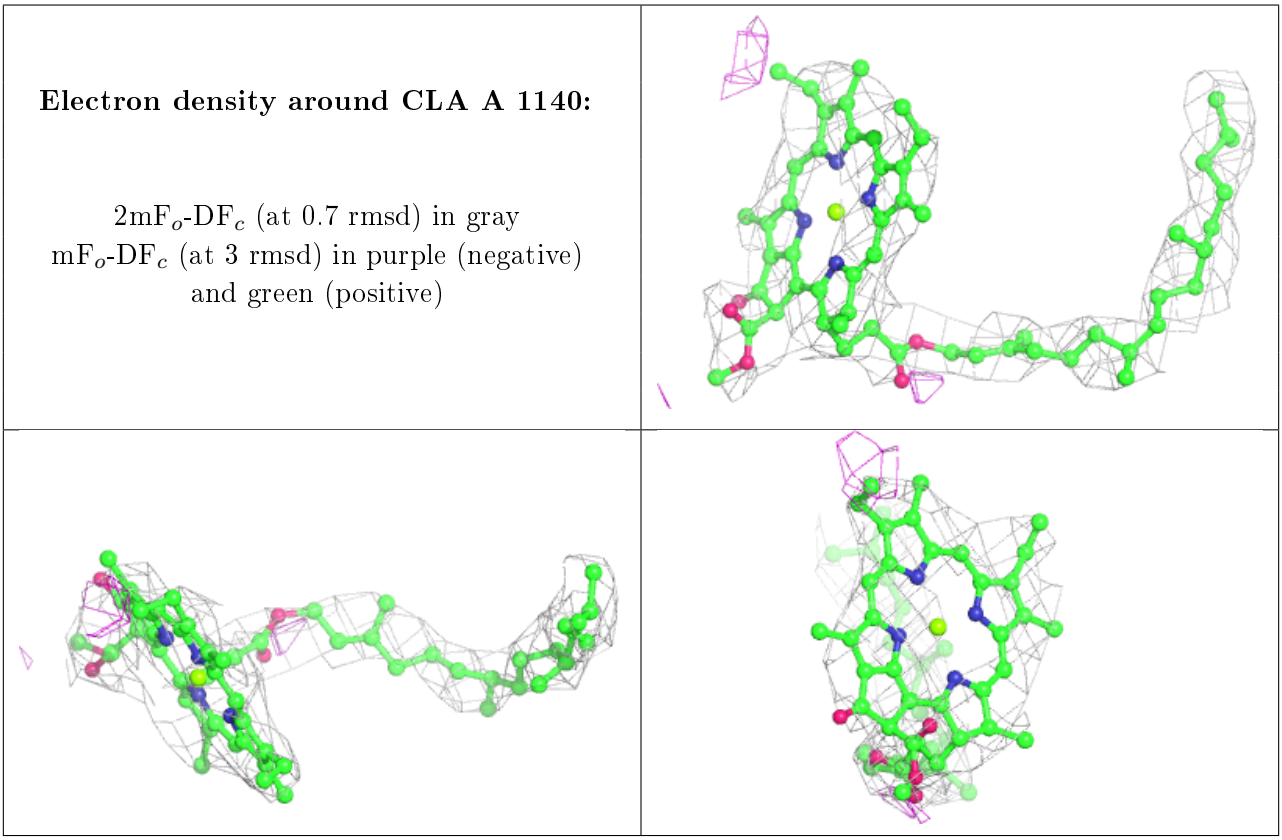
Electron density around CLA B 1237:

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



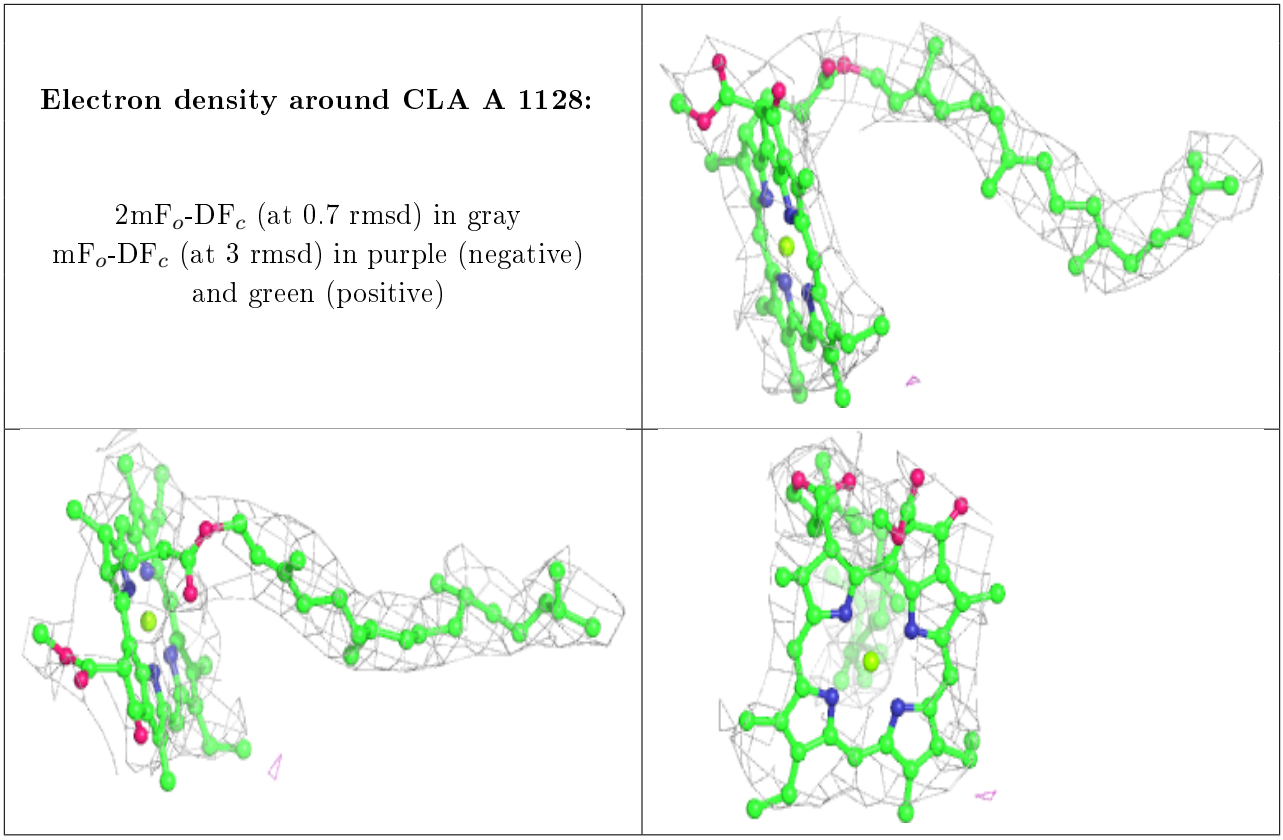
Electron density around CLA A 1140:

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



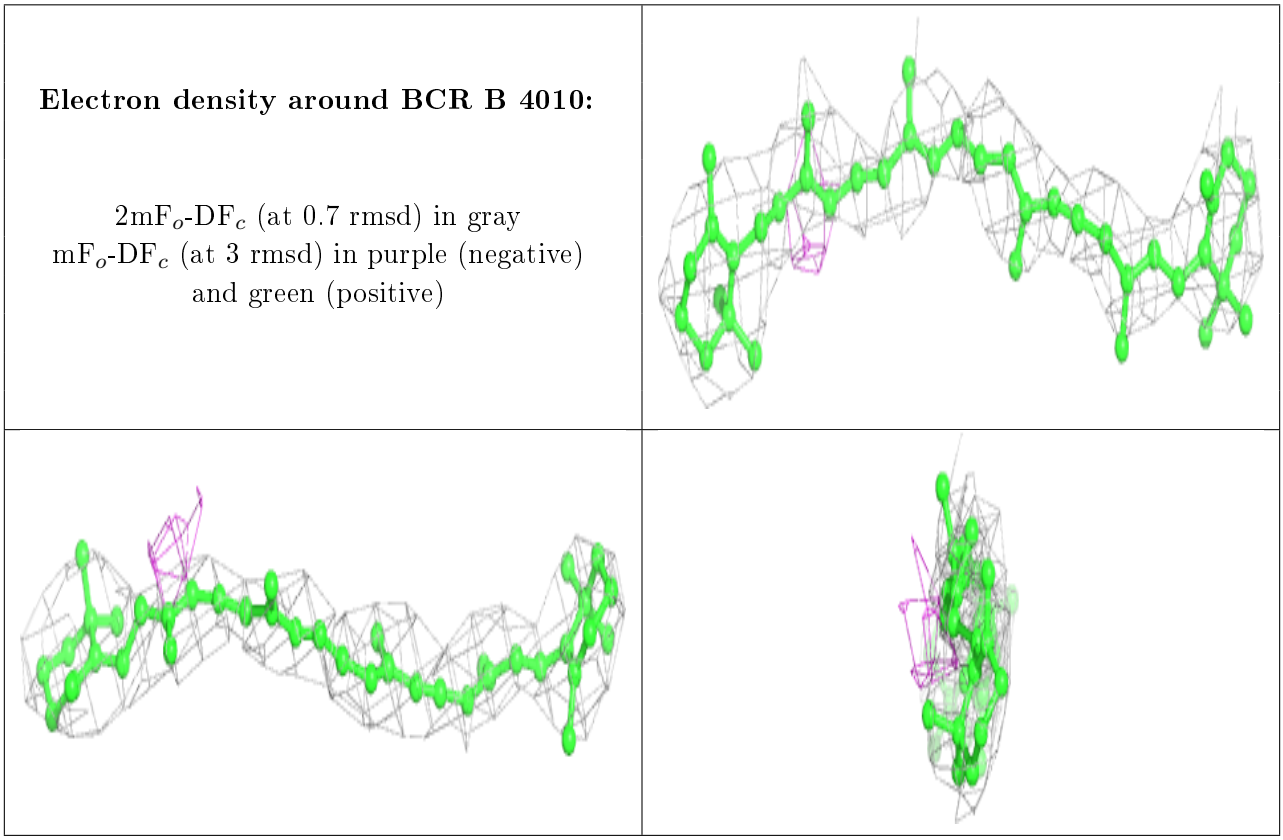
Electron density around CLA A 1128:

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



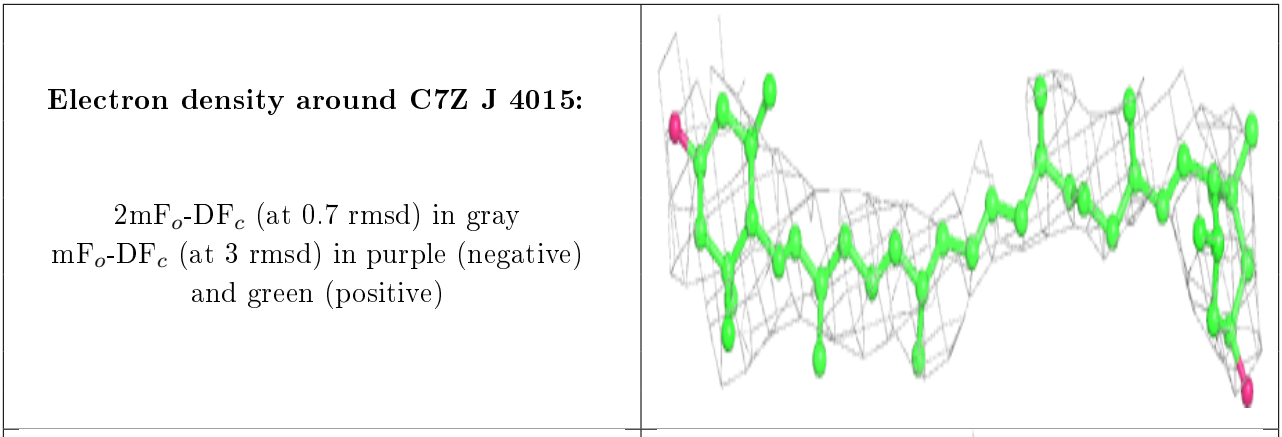
Electron density around BCR B 4010:

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



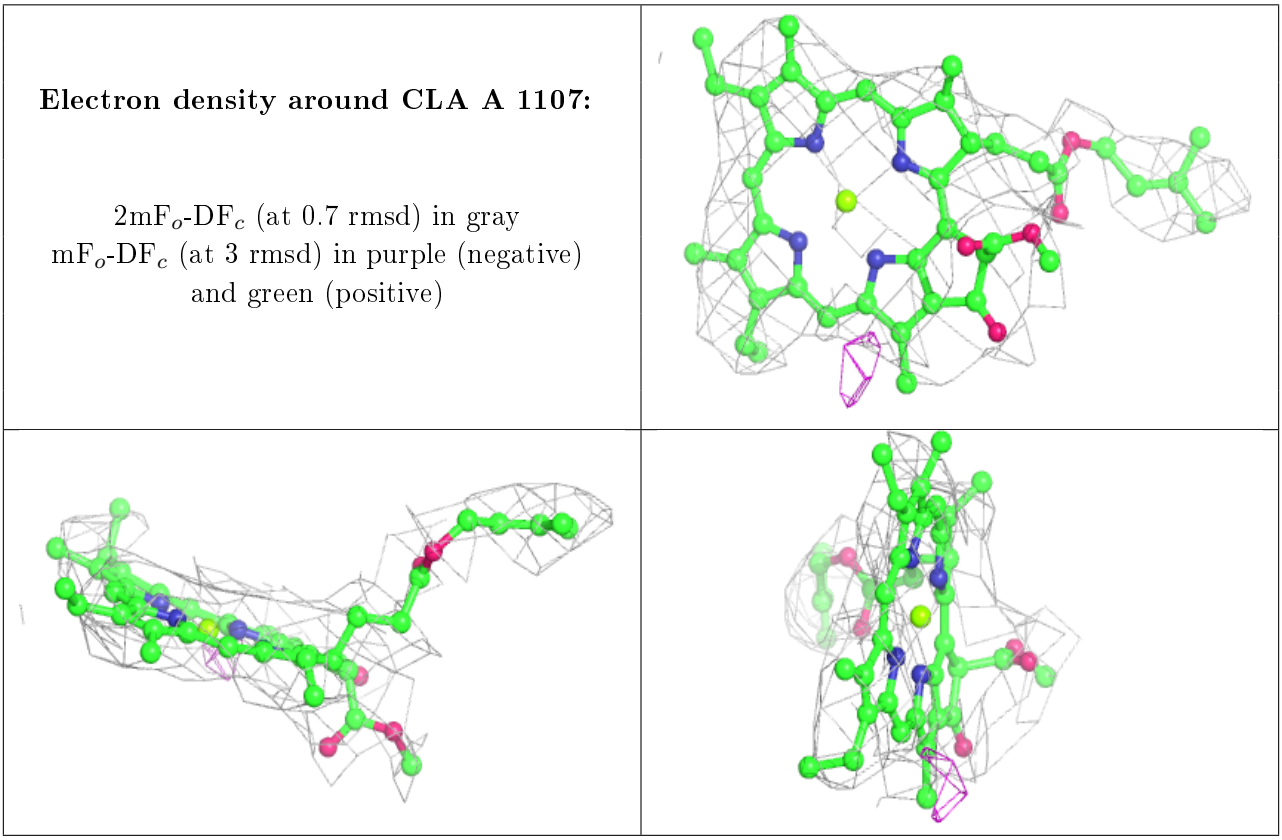
Electron density around C7Z J 4015:

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



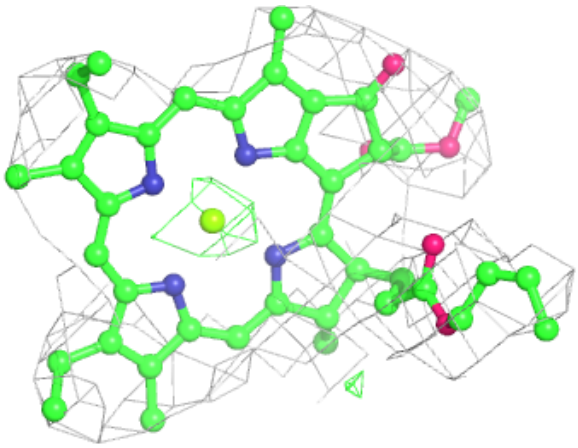
Electron density around CLA A 1107:

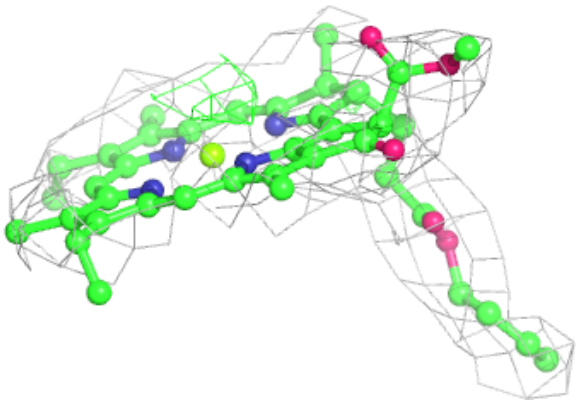
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

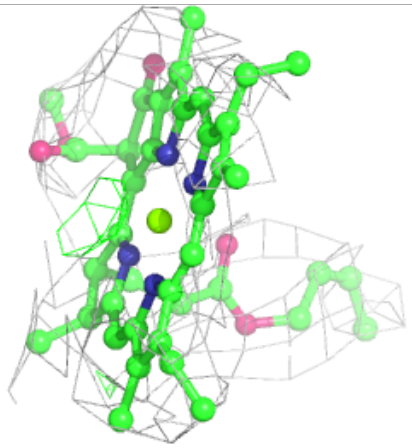


Electron density around CLA B 1231:

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

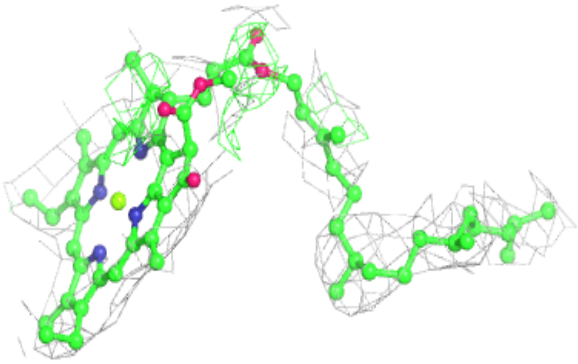


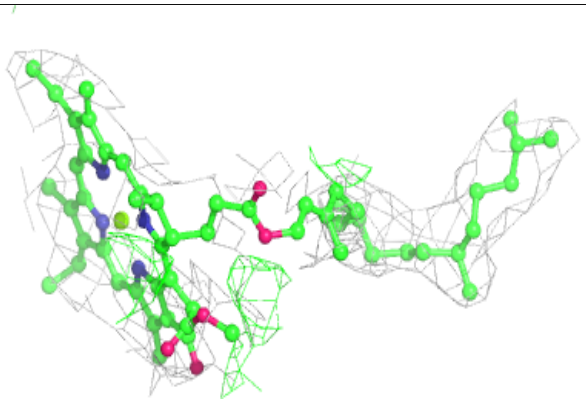


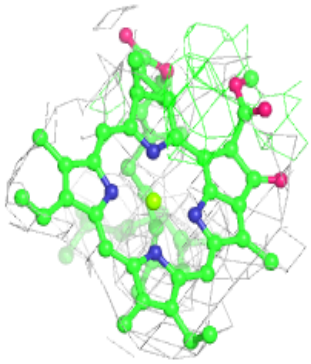


Electron density around CLA B 1021:

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

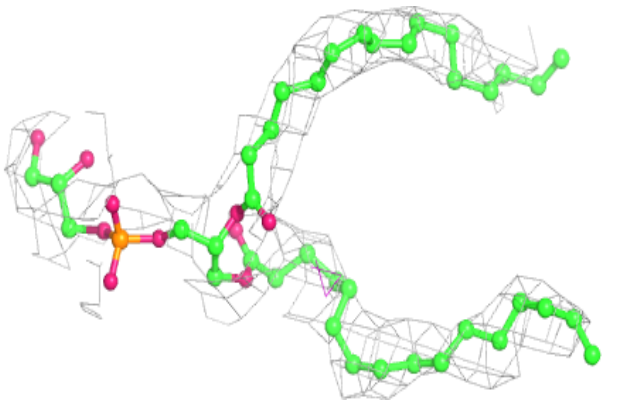


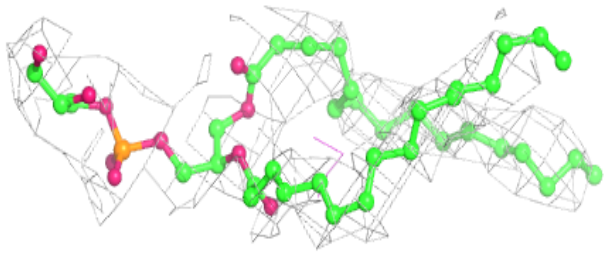


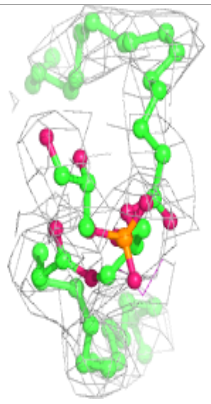


Electron density around LHG A 5001:

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

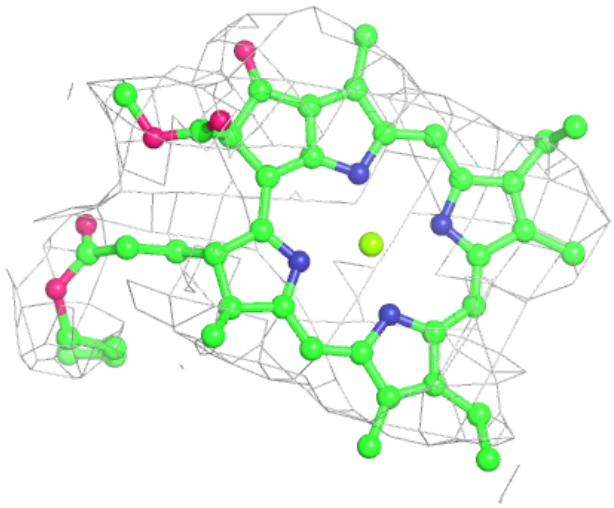


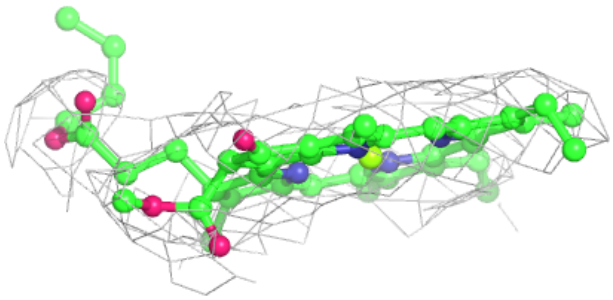


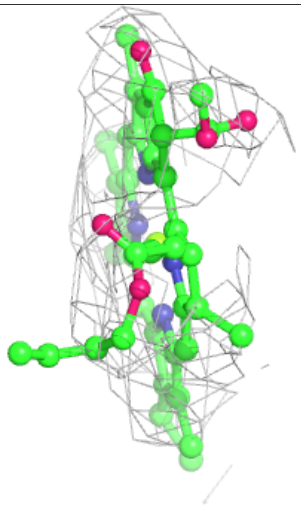


Electron density around CLA B 1206:

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

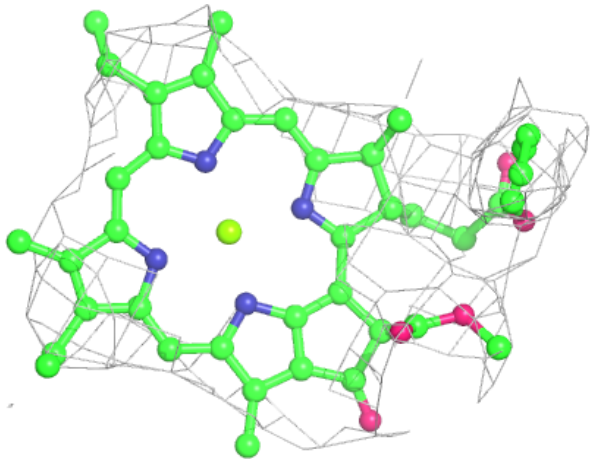


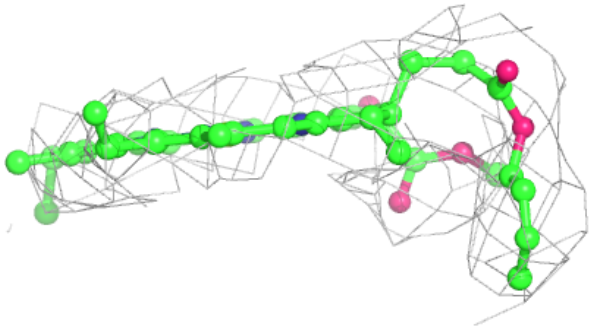


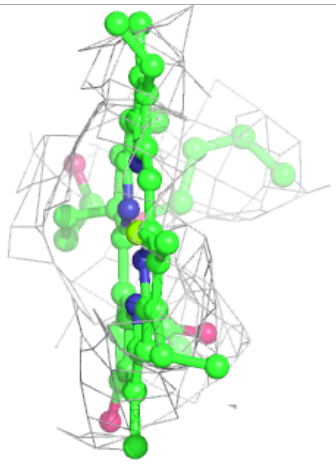


Electron density around CLA A 1104:

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

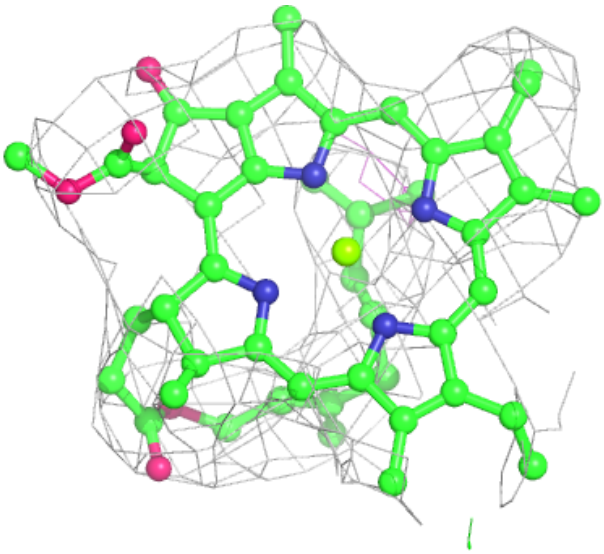


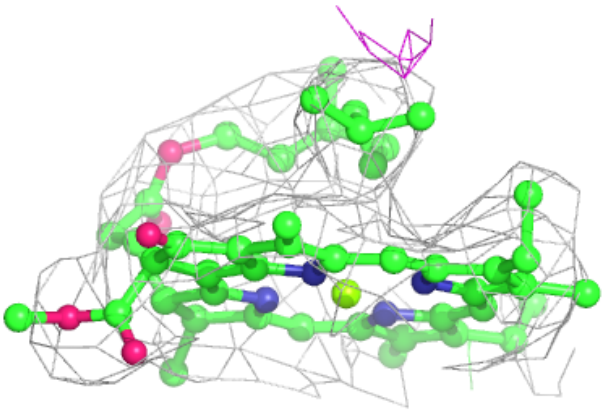


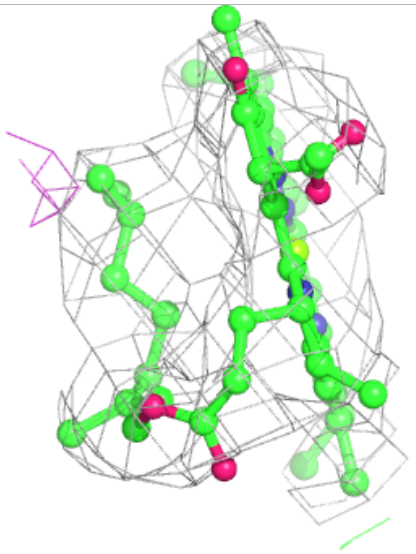


Electron density around CLA B 1224:

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

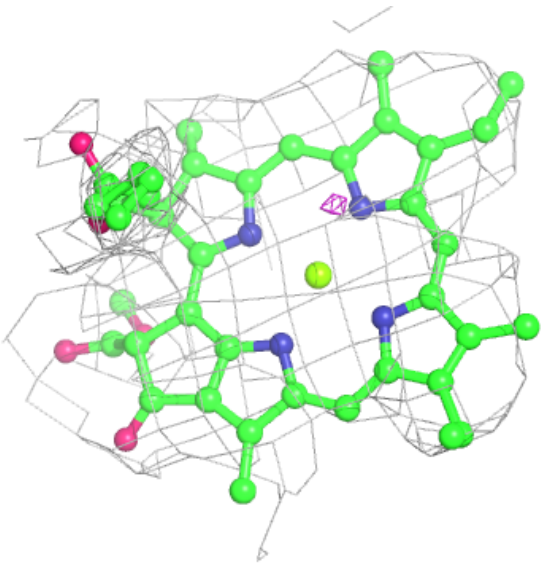


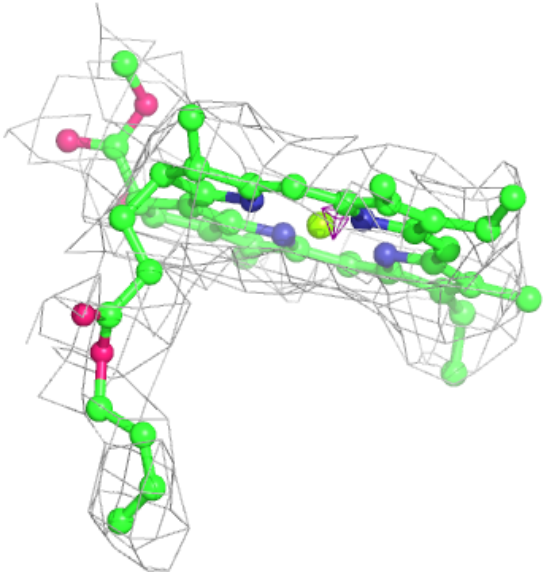


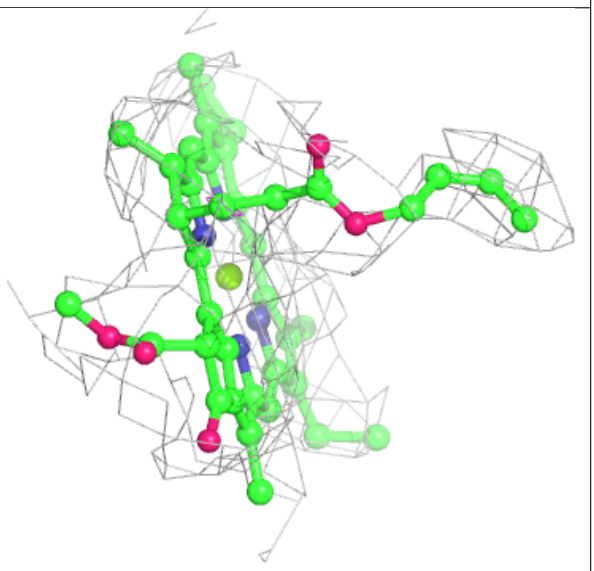


Electron density around CLA B 1226:

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

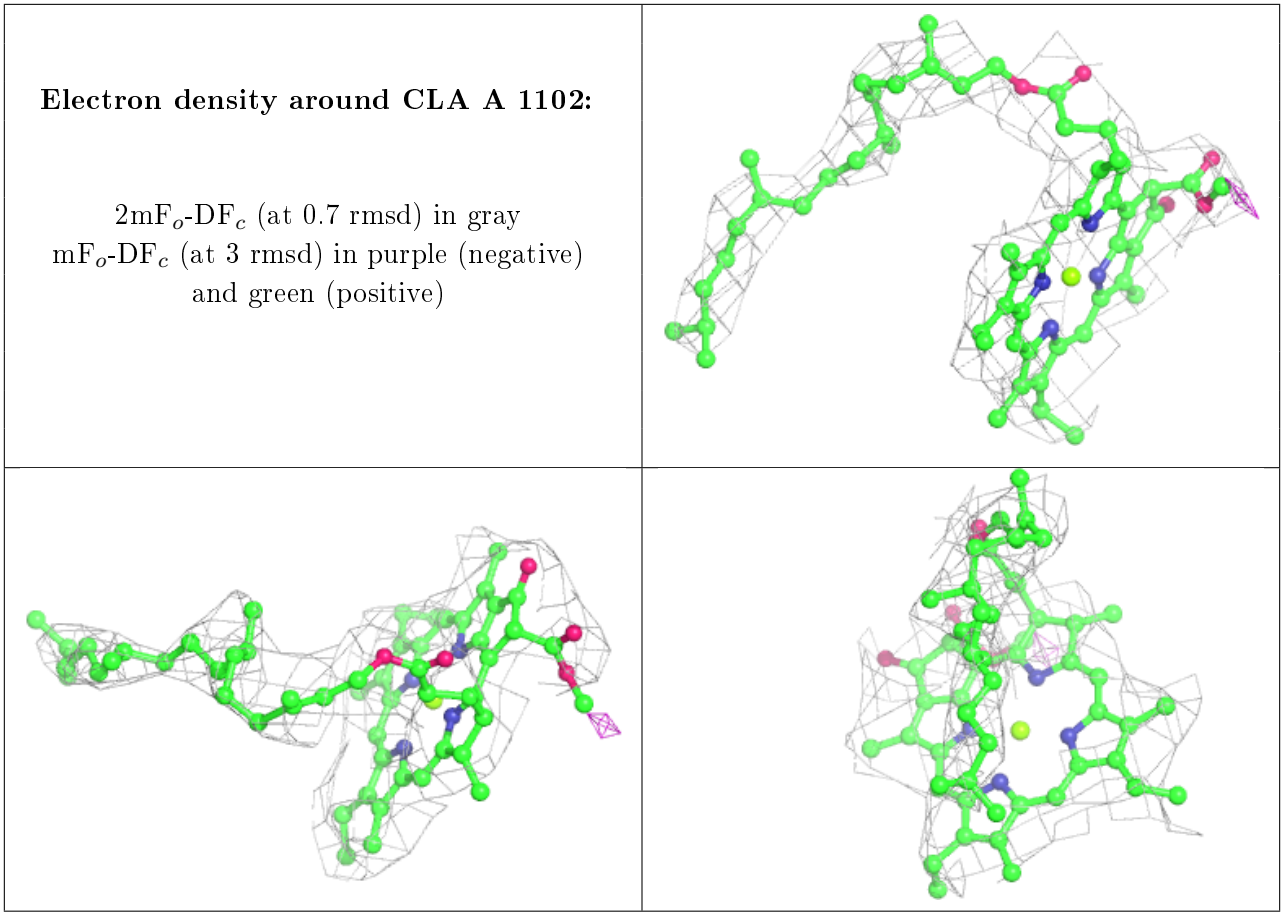






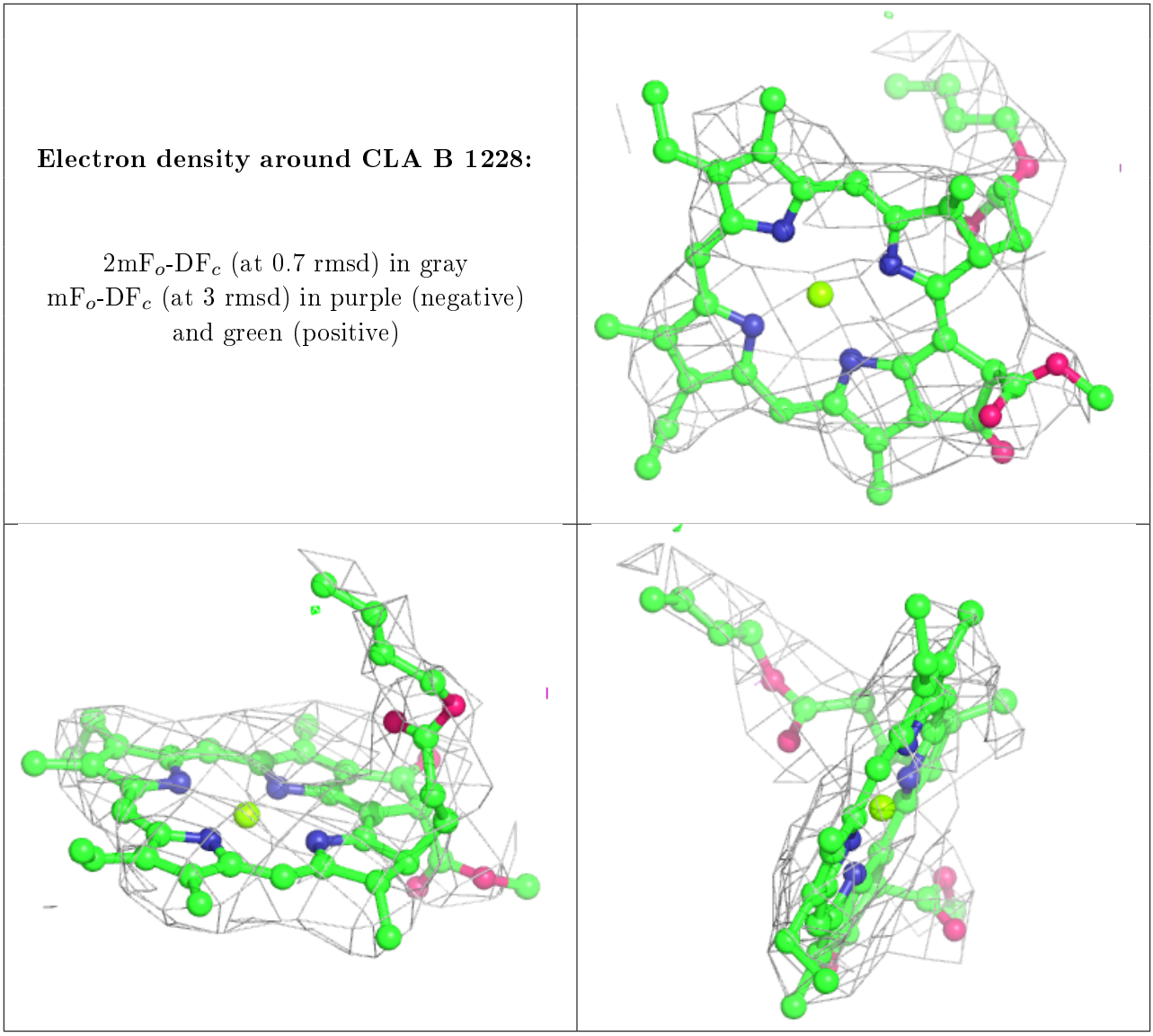
Electron density around CLA A 1102:

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



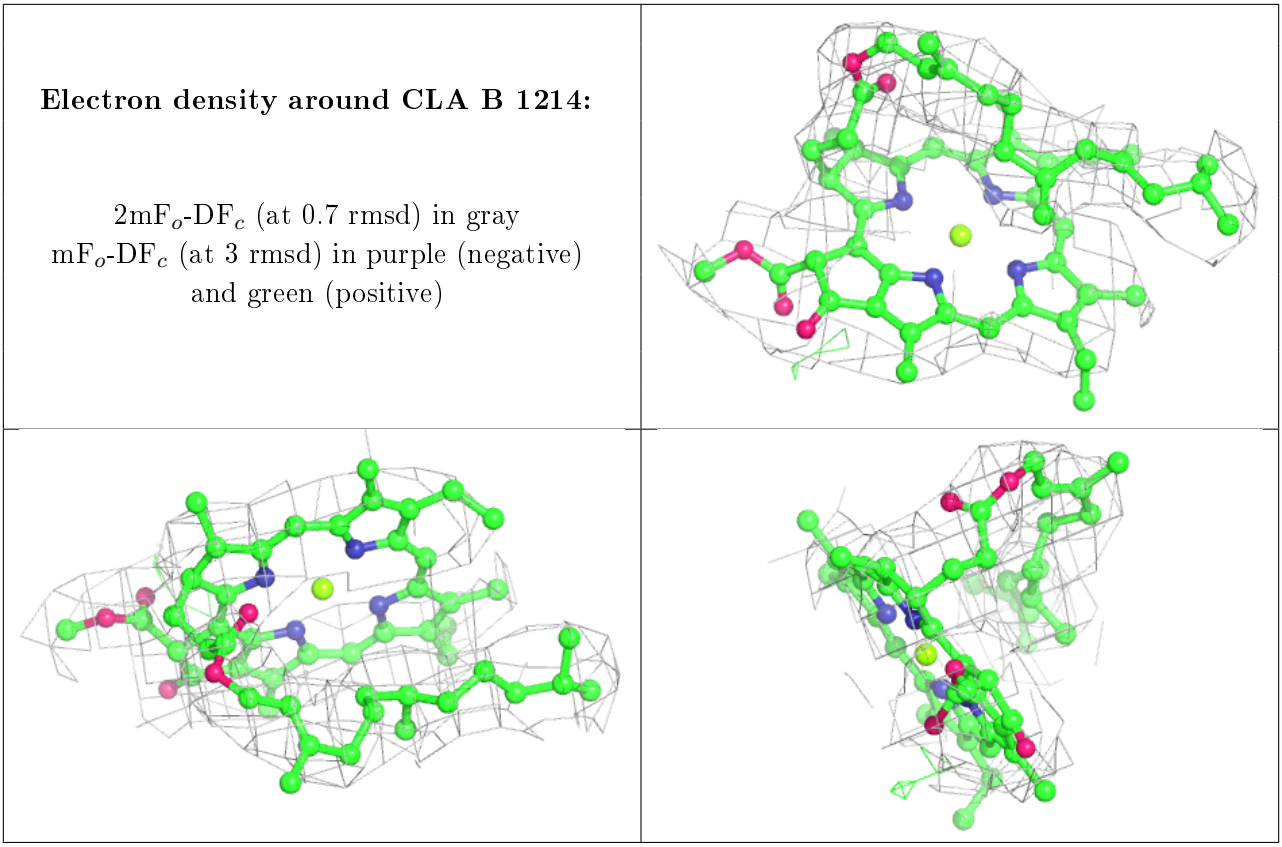
Electron density around CLA B 1228:

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



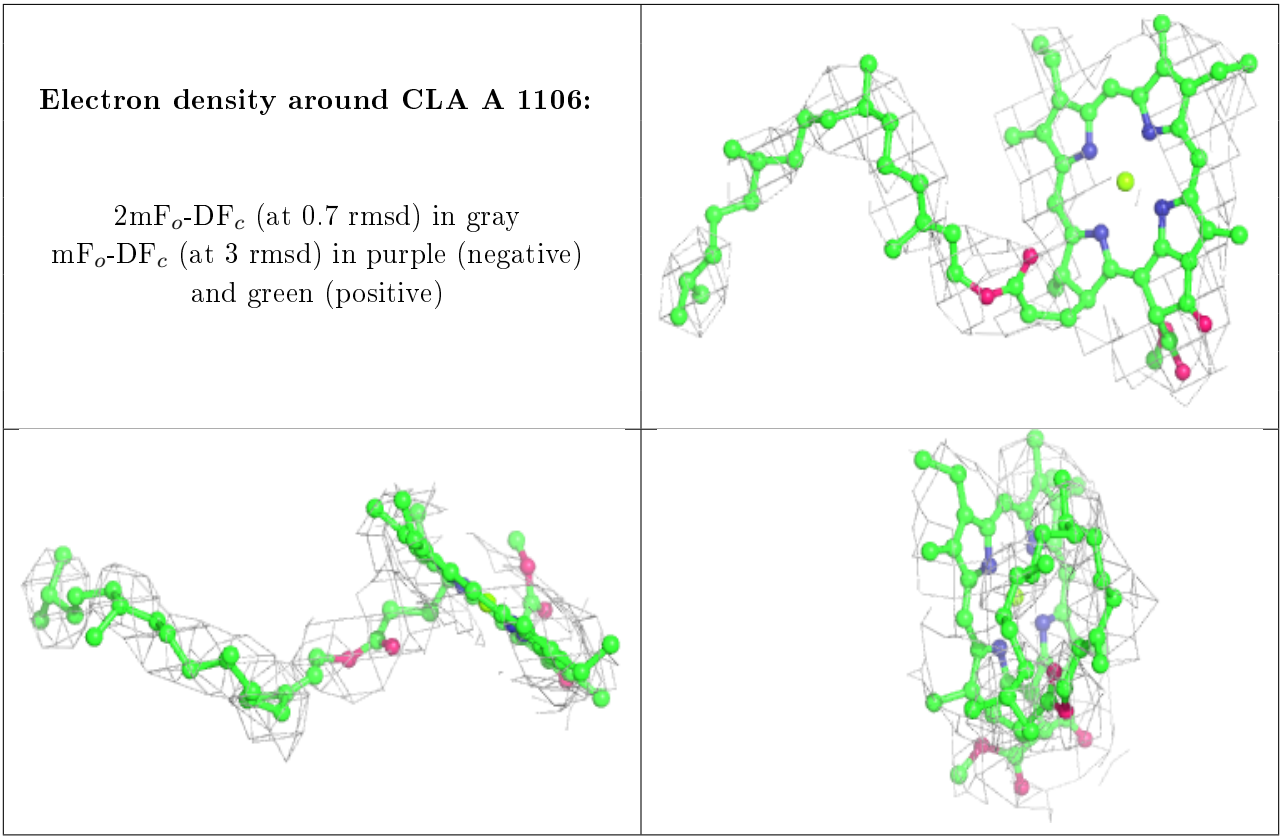
Electron density around CLA B 1214:

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



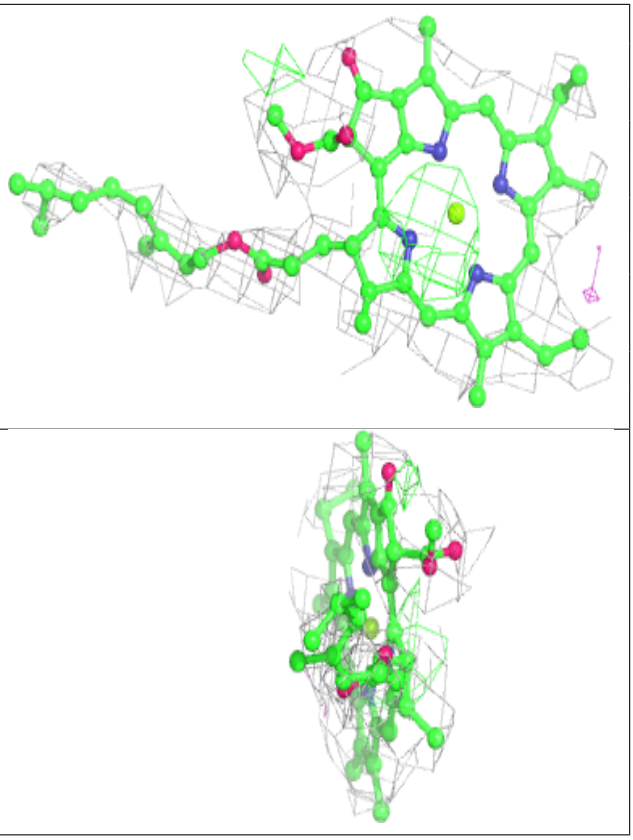
Electron density around CLA A 1106:

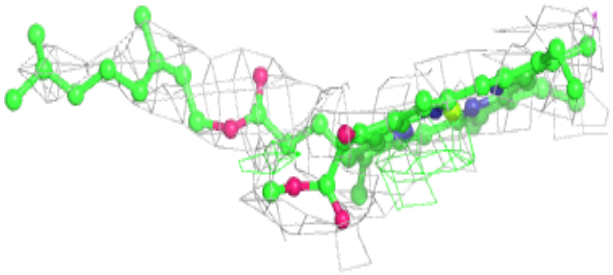
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 1139:

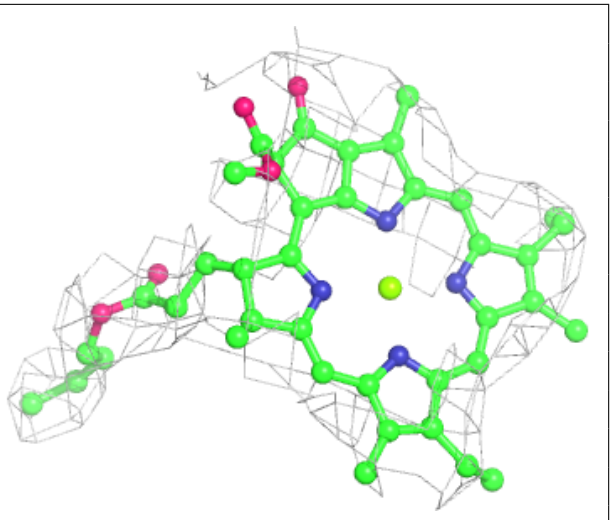
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

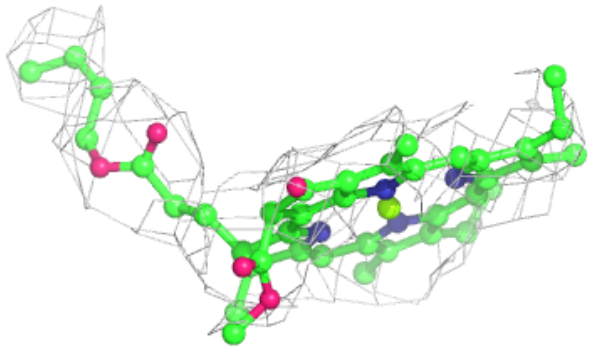




Electron density around CLA B 1230:

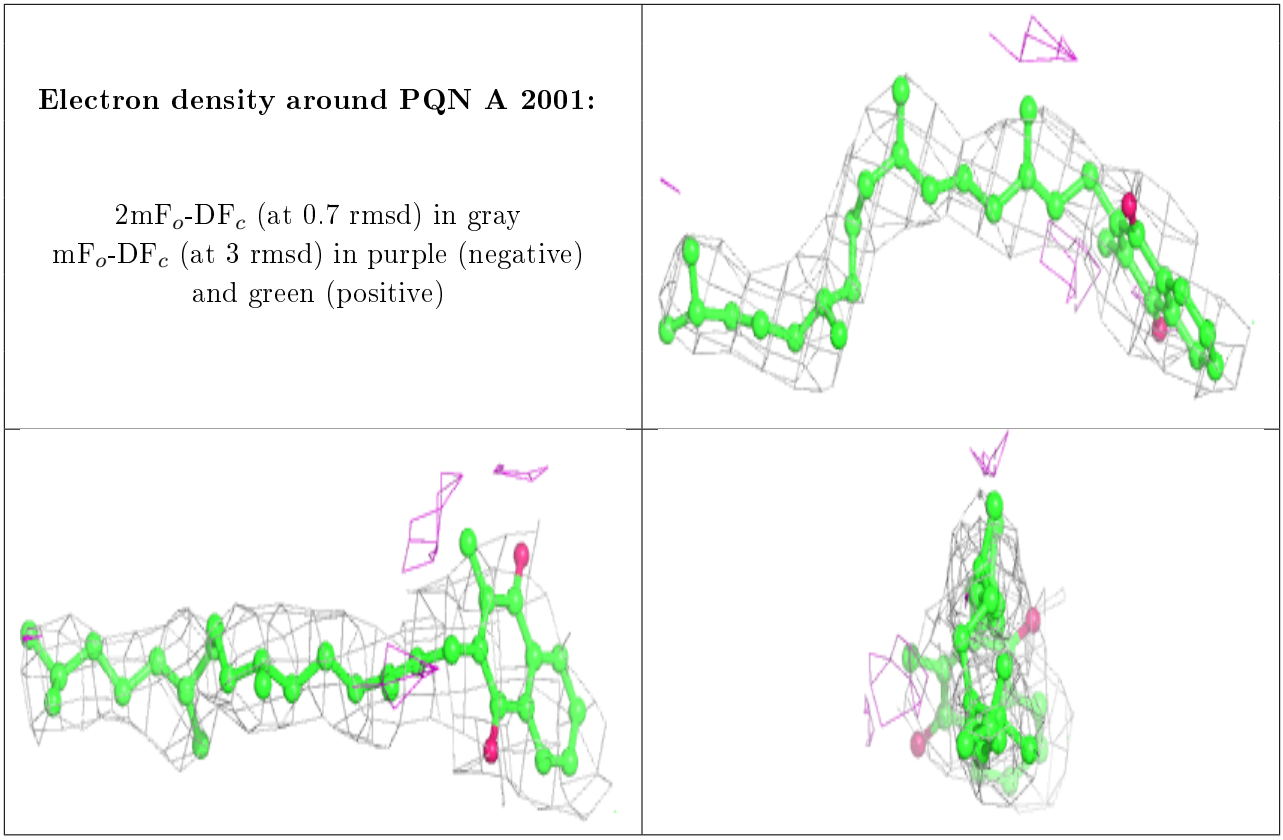
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





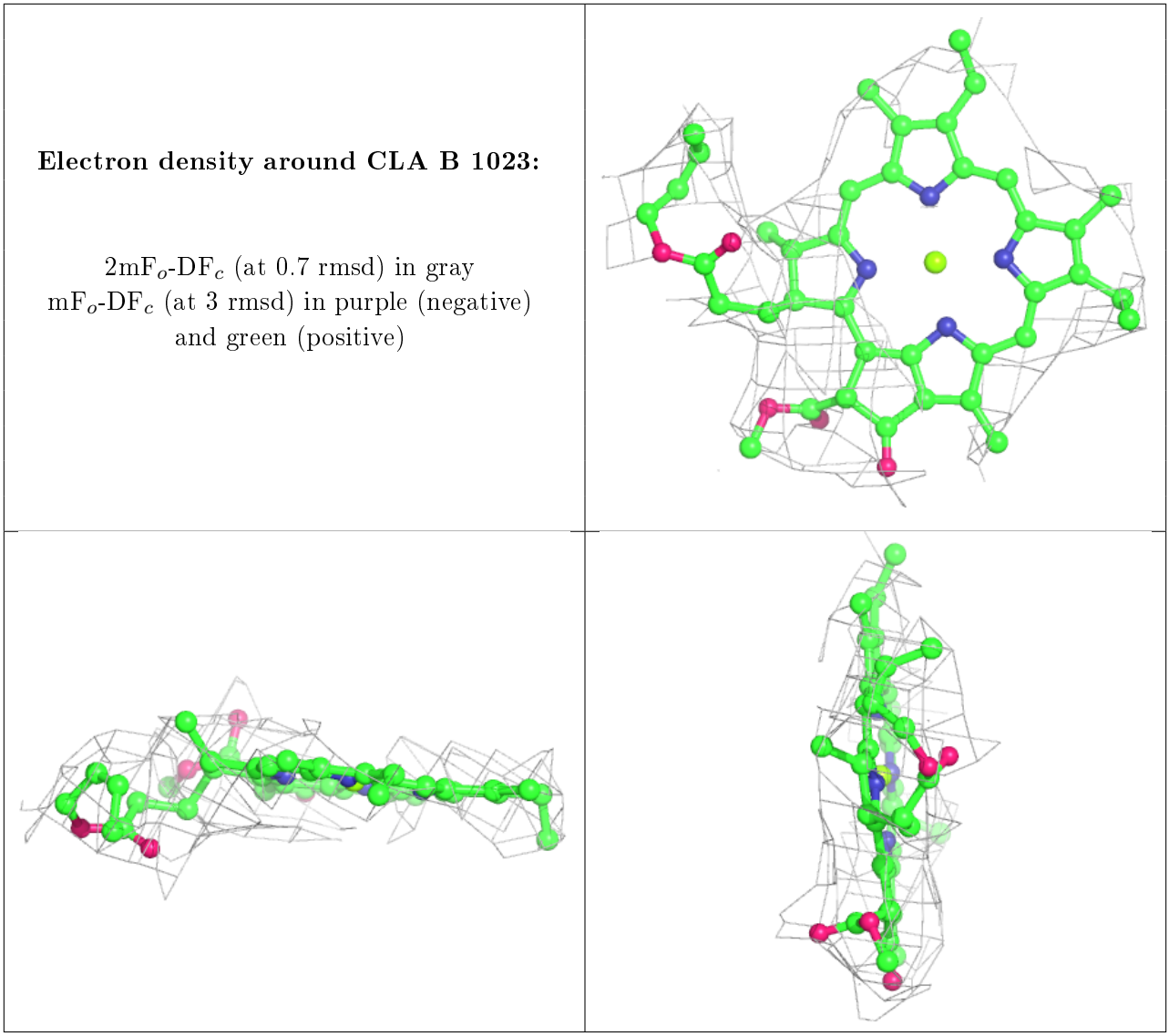
Electron density around PQN A 2001:

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



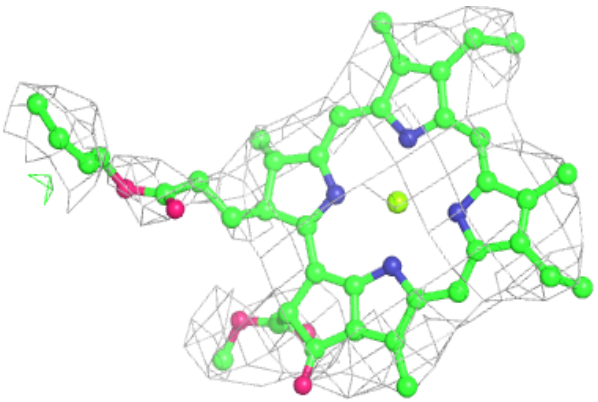
Electron density around CLA B 1023:

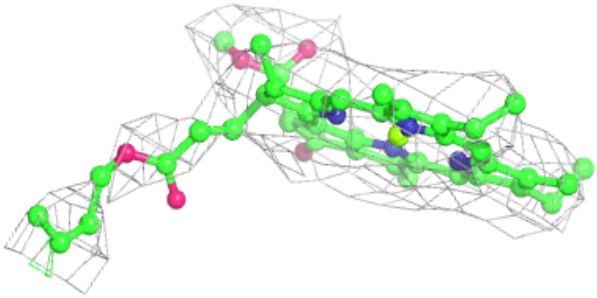
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

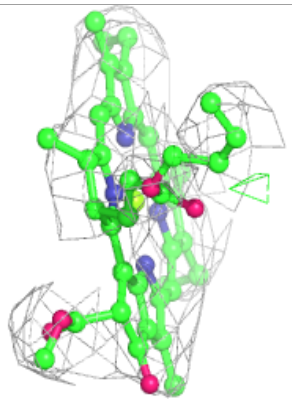


Electron density around CLA B 1239:

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

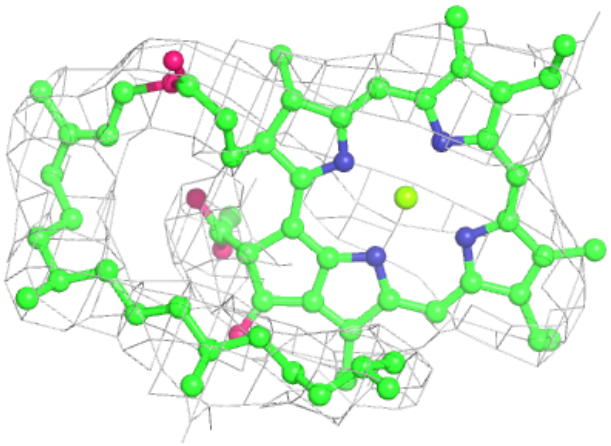


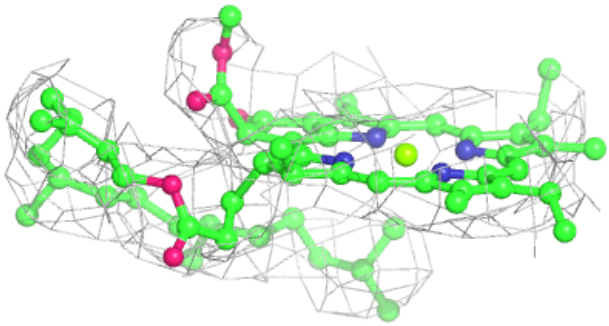




Electron density around CLA B 1202:

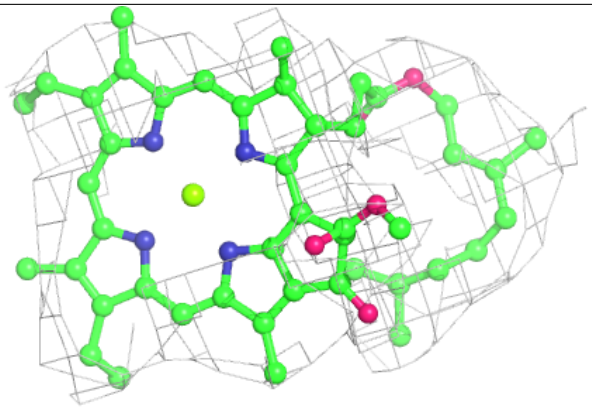
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

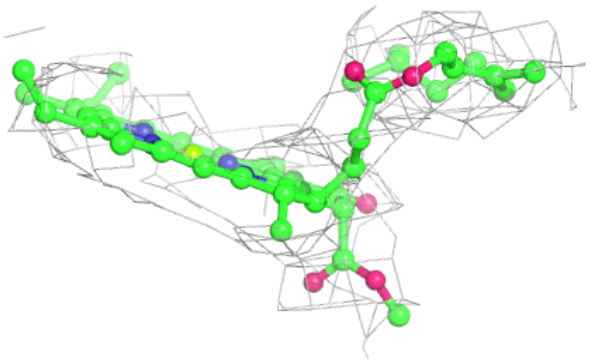


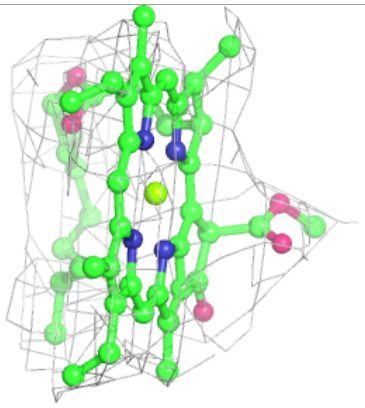


Electron density around CLA B 1229:

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

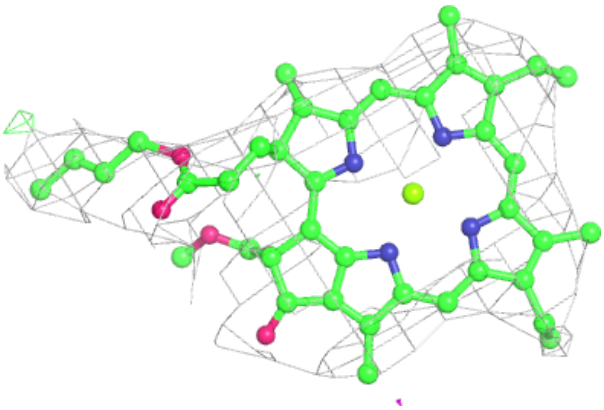


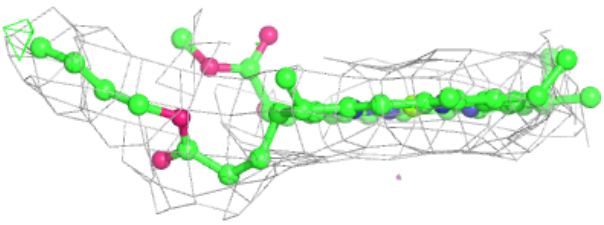


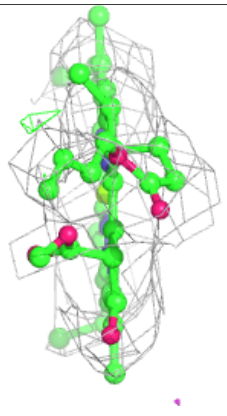


Electron density around CLA A 1101:

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

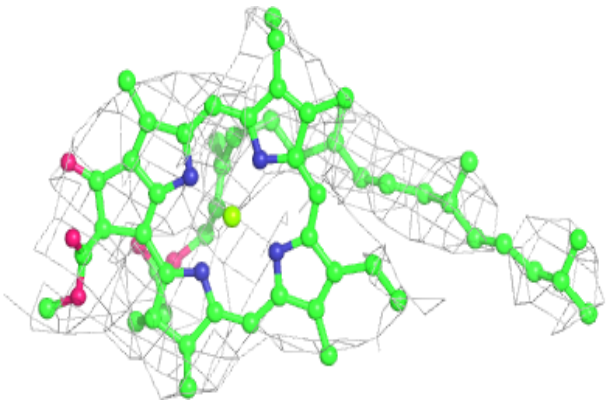


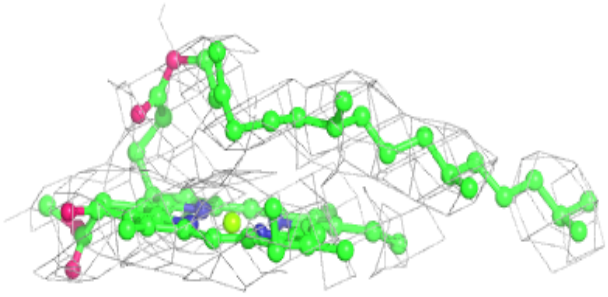


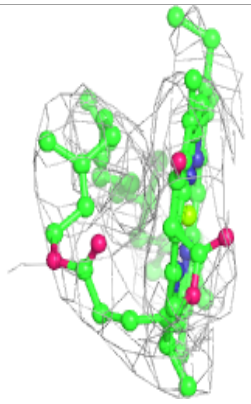


Electron density around CLA A 1138:

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

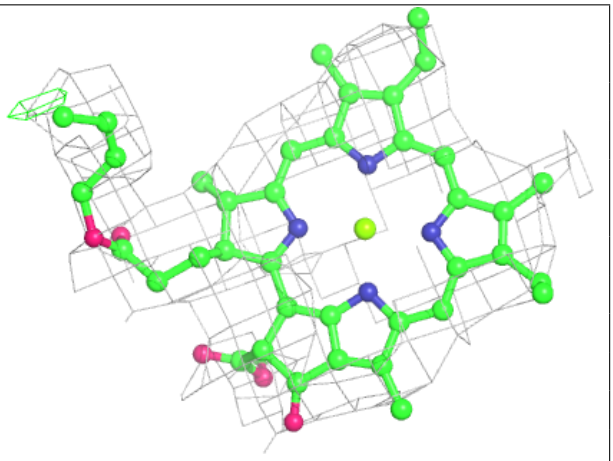


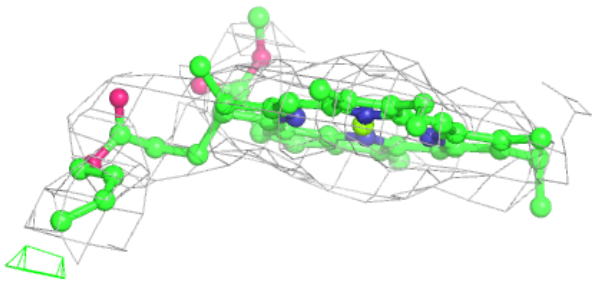


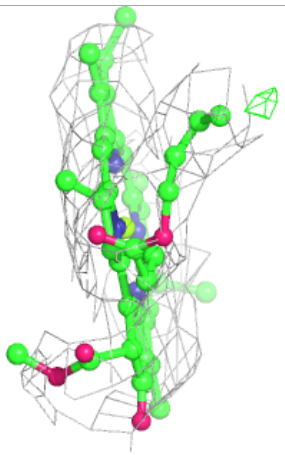


Electron density around CLA B 1210:

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







6.5 Other polymers (i)

There are no such residues in this entry.