wwPDB X-ray Structure Validation Summary Report (i)

Sep 7, 2023 – 10:58 AM EDT

PDB ID	:	4FE1
Title	:	Improving the Accuracy of Macromolecular Structure Refinement at 7 A Resolution
Authors	:	Fromme, R.; Adams, P.D.; Fromme, P.; Levitt, M.; Schroeder, G.F.; Brunger, A.T.
Deposited on	:	2012-05-29
Resolution	:	4.92 Å(reported)

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

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

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

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

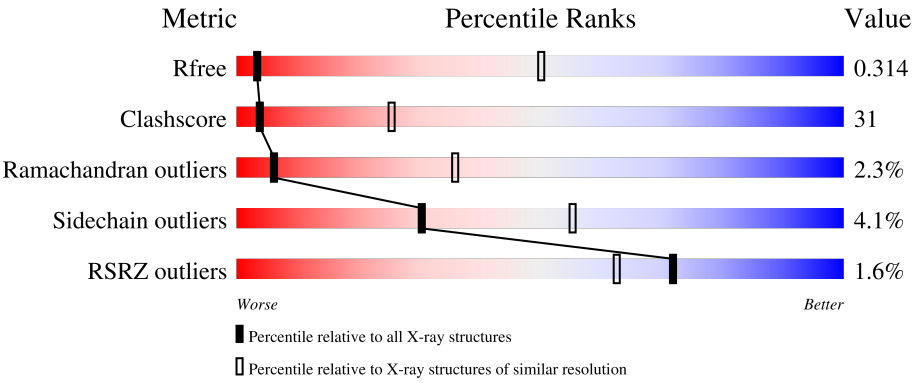
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 4.92 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	1135 (6.02-3.80)
Clashscore	141614	1210 (6.02-3.80)
Ramachandran outliers	138981	1141 (6.02-3.80)
Sidechain outliers	138945	1118 (6.02-3.80)
RSRZ outliers	127900	1007 (6.10-3.72)

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

Mol	Chain	Length	Quality of chain
1	A	755	3% 57% 38%
2	B	740	% 61% 36%
3	C	80	79% 19%
4	D	138	70% 27%

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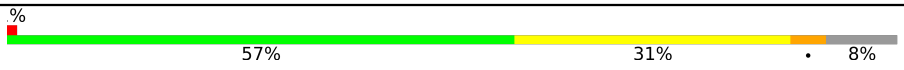
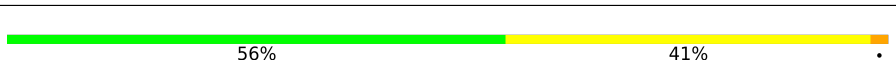
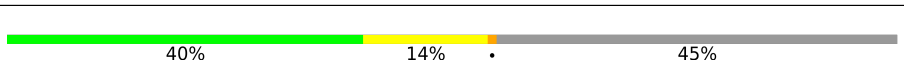
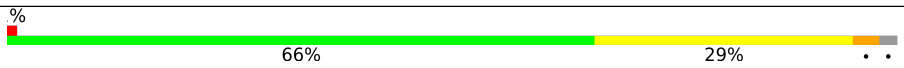
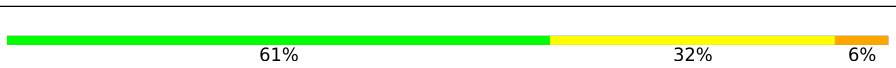
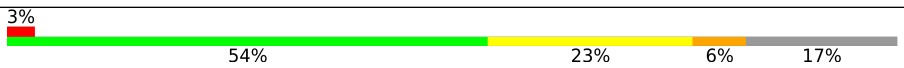
Mol	Chain	Length	Quality of chain
5	E	75	
6	F	164	
7	I	38	
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

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
13	CLA	A	801	X	-	-	-
13	CLA	A	802	X	-	-	-
13	CLA	A	803	X	-	X	-
13	CLA	A	804	X	-	-	-
13	CLA	A	805	X	-	-	-
13	CLA	A	806	X	-	-	-
13	CLA	A	807	X	-	-	-
13	CLA	A	808	X	-	-	-
13	CLA	A	810	X	-	-	X
13	CLA	A	811	X	-	-	-
13	CLA	A	812	X	-	-	X
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	X
13	CLA	A	816	-	-	-	X
13	CLA	A	817	X	-	-	-
13	CLA	A	818	X	-	-	-
13	CLA	A	819	X	-	-	-
13	CLA	A	820	X	-	-	-
13	CLA	A	821	X	-	-	-
13	CLA	A	822	X	-	-	-
13	CLA	A	823	X	-	-	-
13	CLA	A	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	825	X	-	X	-
13	CLA	A	827	X	-	-	-
13	CLA	A	828	X	-	-	-
13	CLA	A	829	X	-	-	-
13	CLA	A	830	X	-	-	-
13	CLA	A	831	X	-	-	-
13	CLA	A	832	X	-	X	-
13	CLA	A	833	X	-	-	-
13	CLA	A	834	X	-	-	-
13	CLA	A	835	X	-	-	-
13	CLA	A	836	X	-	-	X
13	CLA	A	838	X	-	-	-
13	CLA	A	839	X	-	-	-
13	CLA	A	840	X	-	-	-
13	CLA	A	841	X	-	-	-
13	CLA	A	842	X	-	X	-
13	CLA	A	843	X	-	-	-
13	CLA	A	845	X	-	-	-
13	CLA	A	855	X	-	-	-
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	-
13	CLA	B	803	X	-	-	-
13	CLA	B	804	X	-	-	-
13	CLA	B	805	X	-	-	-
13	CLA	B	806	X	-	-	-
13	CLA	B	807	X	-	-	-
13	CLA	B	808	X	-	-	-
13	CLA	B	809	X	-	-	-
13	CLA	B	810	X	-	-	-
13	CLA	B	811	X	-	-	-
13	CLA	B	812	X	-	-	-
13	CLA	B	814	X	-	-	-
13	CLA	B	815	X	-	-	-
13	CLA	B	816	X	-	-	-
13	CLA	B	817	X	-	-	-
13	CLA	B	818	X	-	-	-
13	CLA	B	819	X	-	-	-
13	CLA	B	820	X	-	-	-
13	CLA	B	821	X	-	-	-
13	CLA	B	822	X	-	X	-
13	CLA	B	823	X	-	-	-
13	CLA	B	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	825	X	-	-	-
13	CLA	B	826	X	-	-	-
13	CLA	B	827	X	-	-	-
13	CLA	B	828	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	830	X	-	X	-
13	CLA	B	831	X	-	-	-
13	CLA	B	832	X	-	-	-
13	CLA	B	833	X	-	-	-
13	CLA	B	834	X	-	-	-
13	CLA	B	835	X	-	-	-
13	CLA	B	836	X	-	-	-
13	CLA	B	837	X	-	-	-
13	CLA	B	838	X	-	-	-
13	CLA	B	839	X	-	-	-
13	CLA	I	101	X	-	-	-
13	CLA	J	1101	X	-	-	-
13	CLA	J	1102	X	-	-	-
13	CLA	J	1103	X	-	-	-
13	CLA	L	1002	X	-	-	-
13	CLA	L	1003	X	-	-	-
13	CLA	L	1004	X	-	-	-
13	CLA	M	1201	X	-	-	-
13	CLA	M	1202	-	-	-	X
13	CLA	X	102	X	-	-	-
15	BCR	A	847	-	-	-	X
15	BCR	A	848	-	-	-	X
15	BCR	A	849	-	-	-	X
15	BCR	B	841	-	-	-	X

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 23997 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	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			

- 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
			598	367	103	117	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

- 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
			539	342	93	104			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O	0	0	0
			222	130	46	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4

- 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
			241	161	36	43	1			

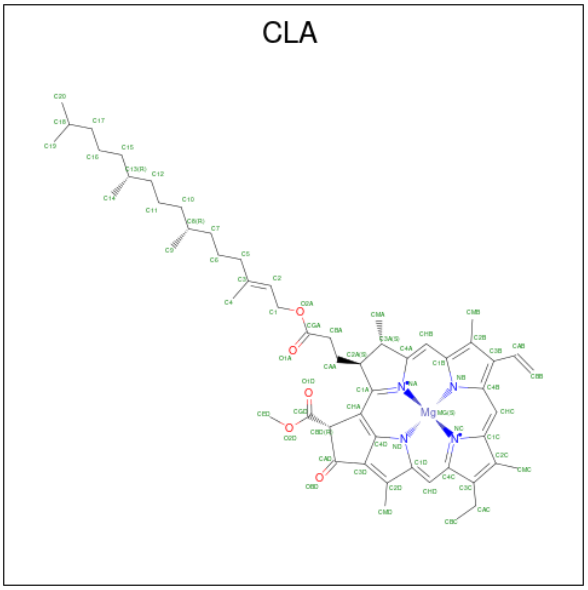
- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	29	Total	C	N	O	0	0	0
			233	164	34	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	32	ALA	-	expression tag	UNP Q8DKP6
X	33	ALA	-	expression tag	UNP Q8DKP6
X	34	ALA	-	expression tag	UNP Q8DKP6
X	35	ALA	-	expression tag	UNP Q8DKP6

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 54 44 1 4 5	0	0
13	A	1	Total C Mg N O 60 50 1 4 5	0	0
13	A	1	Total C Mg N O 45 35 1 4 5	0	0
13	A	1	Total C Mg N O 45 35 1 4 5	0	0
13	A	1	Total C Mg N O 49 39 1 4 5	0	0
13	A	1	Total C Mg N O 54 44 1 4 5	0	0
13	A	1	Total C Mg N O 54 44 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 61 51 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 49 39 1 4 5	0	0
13	A	1	Total C Mg N O 51 41 1 4 5	0	0
13	A	1	Total C Mg N O 59 49 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 65 55 1 4 5	0	0
13	A	1	Total C Mg N O 50 40 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
13	A	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	M	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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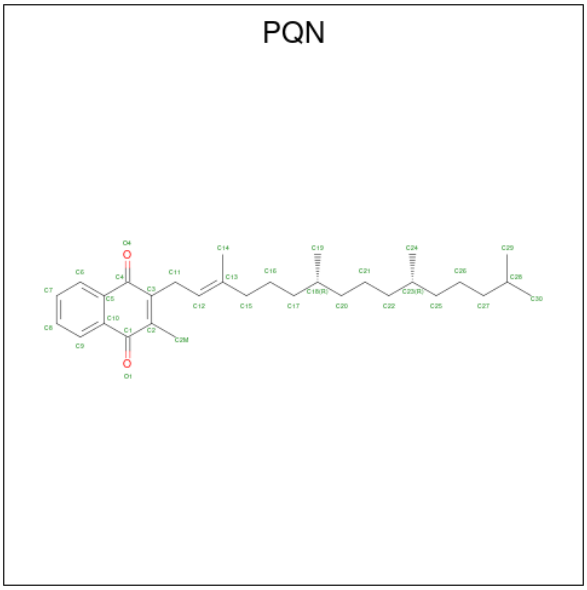
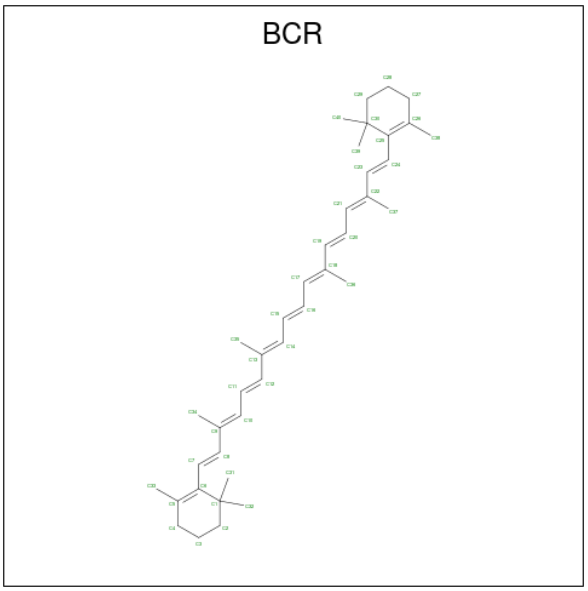
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- 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	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 25 25	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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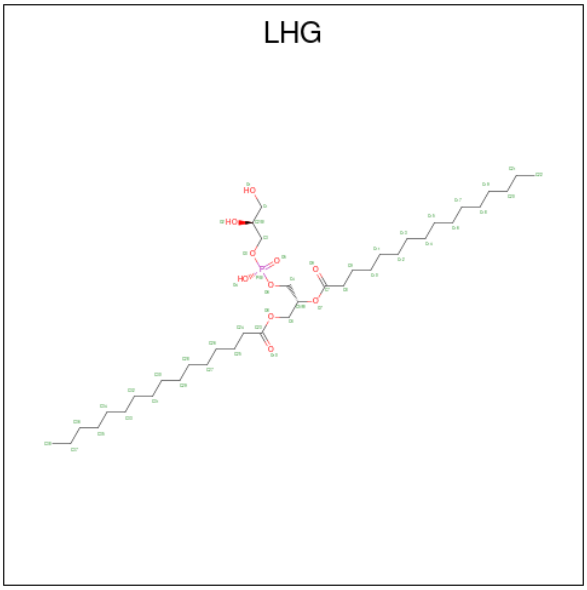
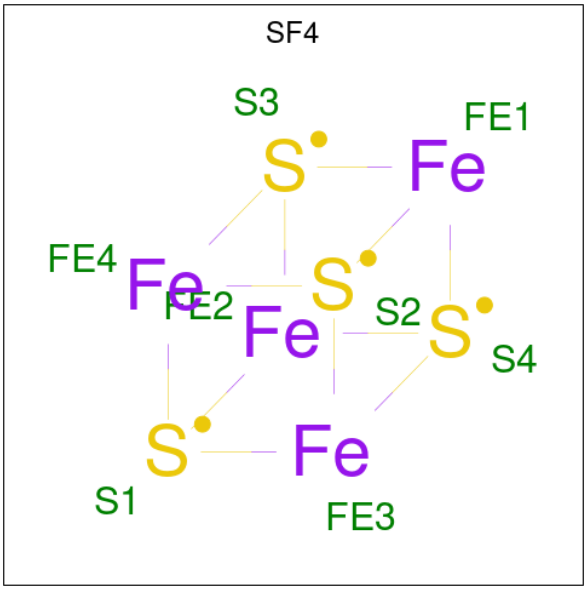
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C 40 40	0	0
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	M	1	Total C 40 40	0	0

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



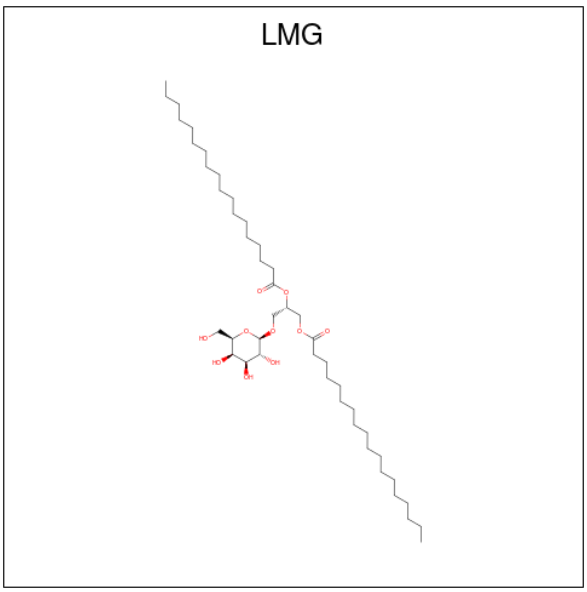
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 27 16 10 1	0	0
16	X	1	Total C O P 23 12 10 1	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

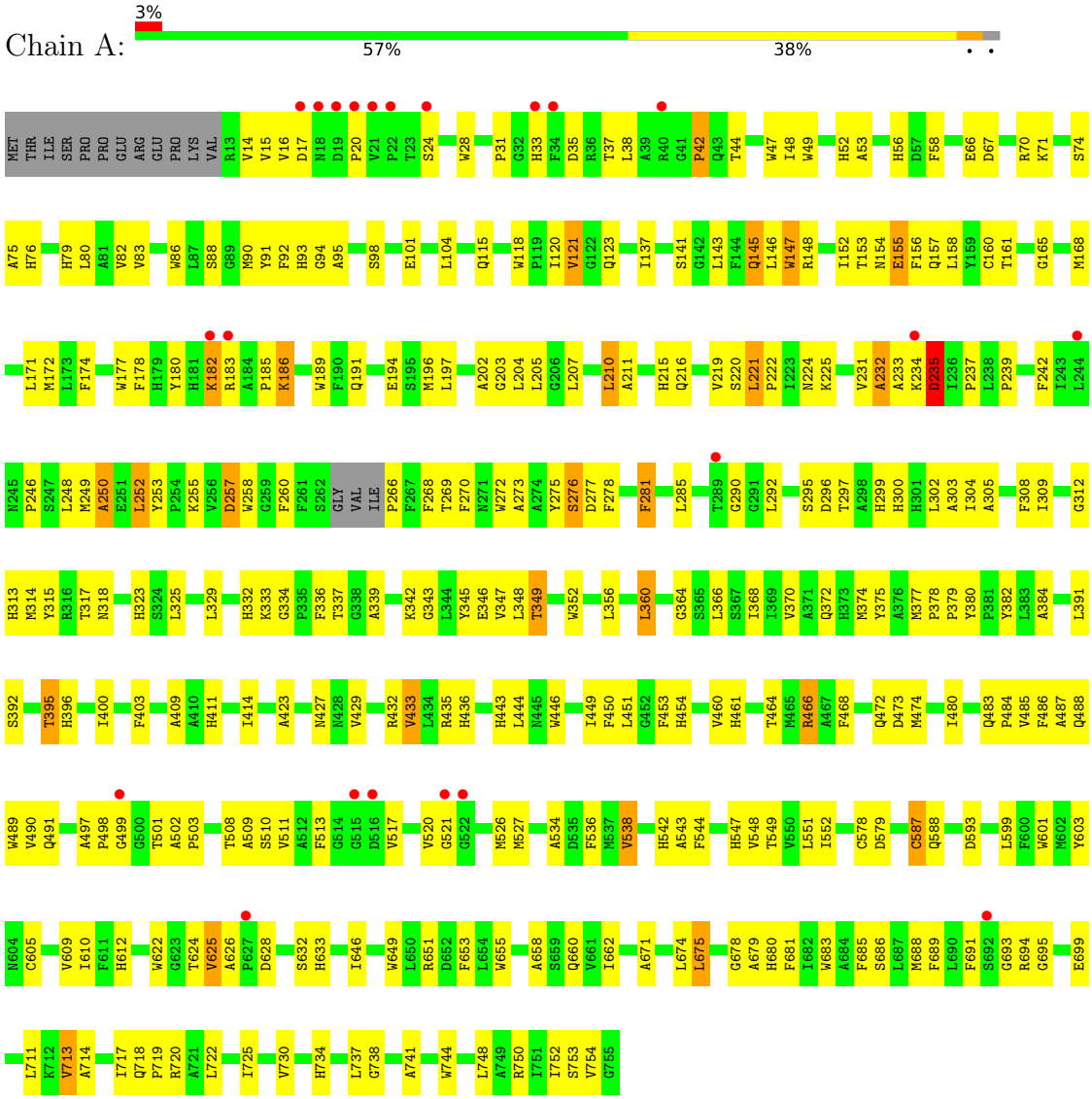
- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	1	Total	Ca	0	0
			1	1		

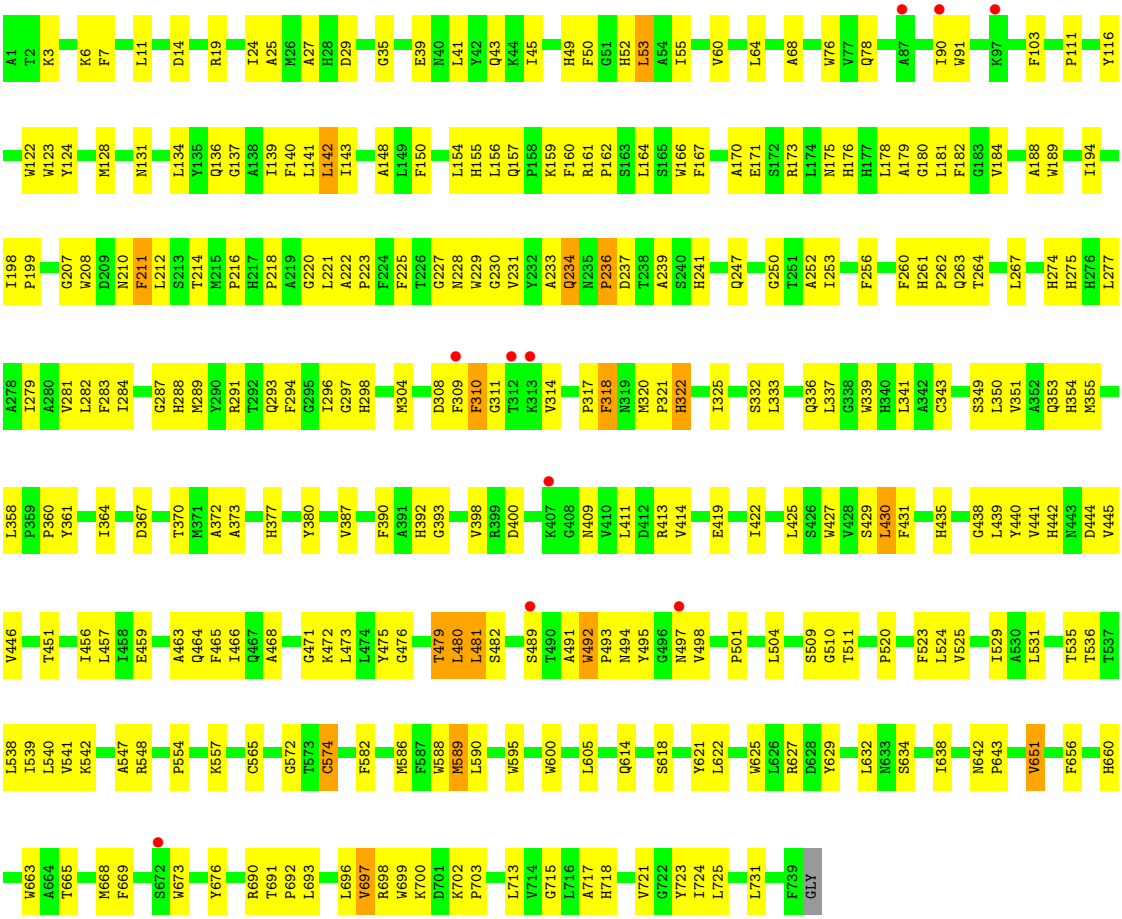
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

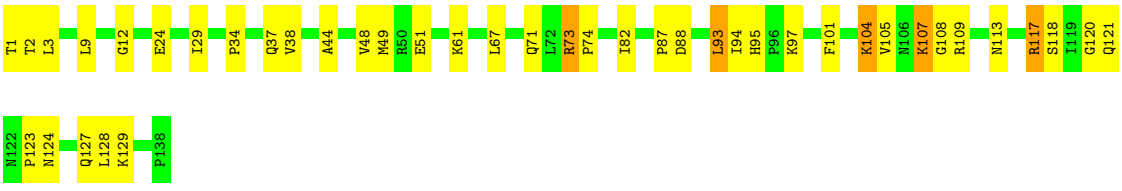


• Molecule 3: Photosystem I iron-sulfur center

Chain C:

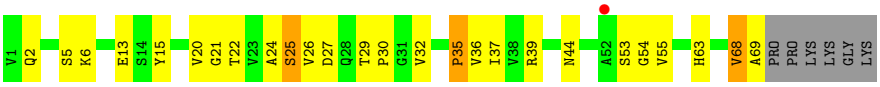
• Molecule 4: Photosystem I reaction center subunit II

Chain D:

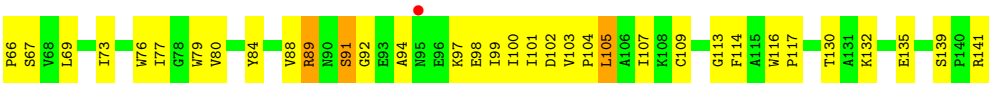


• Molecule 5: Photosystem I reaction center subunit IV

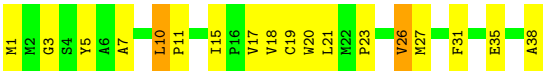
Chain E:



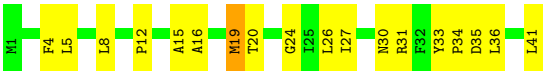
• Molecule 6: Photosystem I reaction center subunit III



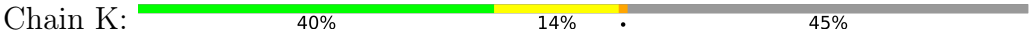
• Molecule 7: Photosystem I reaction center subunit VIII

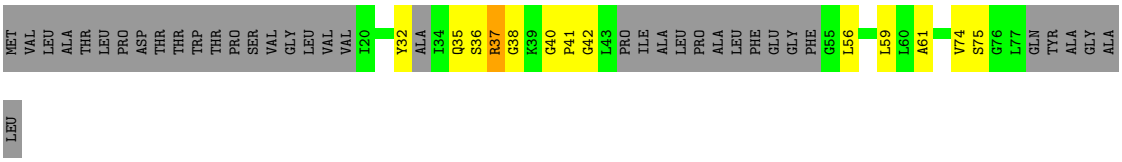


• Molecule 8: Photosystem I reaction center subunit IX

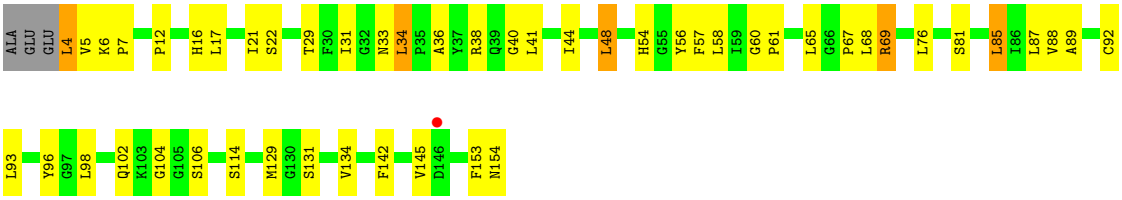


• Molecule 9: Photosystem I reaction center subunit PsaK





• Molecule 10: Photosystem I reaction center subunit XI

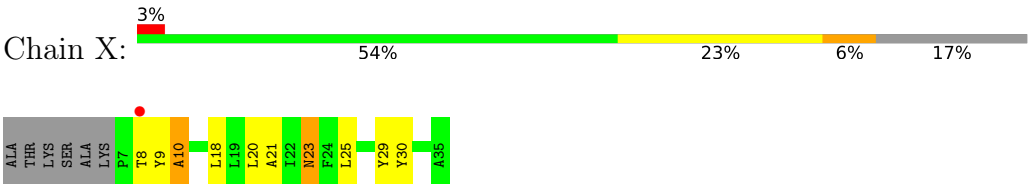


• Molecule 11: Photosystem I reaction center subunit XII

Chain M:

• Molecule 12: Photosystem I 4.8K protein

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.97 – 4.92 97.97 – 4.92	Depositor EDS
% Data completeness (in resolution range)	96.4 (97.97-4.92) 96.3 (97.97-4.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.35 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1058)	Depositor
R, R_{free}	0.274 , 0.315 0.274 , 0.314	Depositor DCC
R_{free} test set	1534 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 23.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.13$	Xtriage
Estimated twinning fraction	0.175 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.69	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.38	0/5983	0.69	3/8158 (0.0%)
2	B	0.40	0/6096	0.68	2/8332 (0.0%)
3	C	0.39	0/608	0.76	0/824
4	D	0.35	0/1101	0.78	0/1492
5	E	0.42	0/551	0.85	1/750 (0.1%)
6	F	0.41	0/1087	0.76	0/1476
7	I	0.38	0/312	0.80	1/425 (0.2%)
8	J	0.40	0/350	0.80	1/477 (0.2%)
9	K	0.40	0/220	0.91	0/300
10	L	0.39	0/1148	0.79	2/1558 (0.1%)
11	M	0.47	0/244	0.91	1/332 (0.3%)
12	X	0.41	0/242	0.66	0/332
All	All	0.39	0/17942	0.72	11/24456 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
4	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	ASP	CB-CG-OD2	-8.44	110.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	ASP	CB-CG-OD1	8.11	125.60	118.30
10	L	76	LEU	CB-CG-CD2	7.19	123.22	111.00
7	I	26	VAL	CG1-CB-CG2	6.87	121.90	110.90
10	L	48	LEU	CB-CG-CD2	6.78	122.52	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	THR	Mainchain
2	B	35	GLY	Mainchain
4	D	88	ASP	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5639	350	0
2	B	5879	0	5632	345	0
3	C	598	0	580	15	0
4	D	1075	0	1077	30	0
5	E	539	0	528	13	0
6	F	1065	0	1077	51	0
7	I	301	0	306	23	0
8	J	338	0	347	23	0
9	K	222	0	111	9	0
10	L	1119	0	1125	50	1
11	M	241	0	264	22	0
12	X	233	0	231	11	0
13	A	2667	0	2635	478	0
13	B	2230	0	2182	427	0
13	F	45	0	33	5	0
13	I	65	0	72	15	0
13	J	147	0	129	17	0
13	L	195	0	216	28	0
13	M	99	0	81	18	0
13	X	45	0	33	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	33	0	46	7	0
14	B	33	0	46	7	0
15	A	240	0	336	39	0
15	B	345	0	481	83	0
15	F	40	0	56	13	0
15	I	40	0	56	11	0
15	J	80	0	112	11	0
15	L	80	0	112	16	0
15	M	40	0	56	13	0
16	A	76	0	98	12	0
16	X	23	0	16	1	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	B	55	0	86	18	0
19	L	1	0	0	0	0
All	All	23997	0	23799	1470	1

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 31.

The worst 5 of 1470 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)
13:B:806:CLA:H12	7:I:18:VAL:HG21	1.35	1.08
13:A:803:CLA:H151	13:A:842:CLA:HAB	1.36	1.08
13:B:831:CLA:HED1	8:J:36:LEU:H	1.06	1.07
13:B:808:CLA:HMA1	13:I:101:CLA:HAB	1.31	1.06
13:B:817:CLA:HBD	13:B:821:CLA:HED2	1.37	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:40:GLY:O	10:L:114:SER:OG[3_665]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	736/755 (98%)	685 (93%)	39 (5%)	12 (2%)	9 44
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	13 50
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	12 48
4	D	136/138 (99%)	123 (90%)	8 (6%)	5 (4%)	3 27
5	E	67/75 (89%)	53 (79%)	6 (9%)	8 (12%)	0 6
6	F	139/164 (85%)	127 (91%)	8 (6%)	4 (3%)	4 31
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100 100
9	K	42/83 (51%)	30 (71%)	5 (12%)	7 (17%)	0 3
10	L	149/154 (97%)	138 (93%)	9 (6%)	2 (1%)	12 48
11	M	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3 29
12	X	27/35 (77%)	21 (78%)	5 (18%)	1 (4%)	3 27
All	All	2215/2334 (95%)	2039 (92%)	126 (6%)	50 (2%)	6 36

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	235	ASP
2	B	211	PHE
2	B	234	GLN
2	B	480	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/603 (98%)	567 (96%)	22 (4%)	34	58
2	B	595/597 (100%)	572 (96%)	23 (4%)	32	57
3	C	67/67 (100%)	65 (97%)	2 (3%)	41	63
4	D	115/115 (100%)	109 (95%)	6 (5%)	23	49
5	E	59/64 (92%)	58 (98%)	1 (2%)	60	78
6	F	109/128 (85%)	105 (96%)	4 (4%)	34	58
7	I	32/32 (100%)	31 (97%)	1 (3%)	40	62
8	J	36/36 (100%)	35 (97%)	1 (3%)	43	65
10	L	117/119 (98%)	109 (93%)	8 (7%)	16	42
11	M	26/26 (100%)	24 (92%)	2 (8%)	13	39
12	X	20/24 (83%)	18 (90%)	2 (10%)	7	28
All	All	1765/1811 (98%)	1693 (96%)	72 (4%)	30	55

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	105	LEU
12	X	23	ASN
8	J	19	MET
10	L	85	LEU
2	B	159	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	136	GLN
2	B	261	HIS
6	F	95	ASN
6	F	40	GLN
1	A	633	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 128 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
13	CLA	A	836	1	45,53,73	1.82	12 (26%)	52,89,113	2.03	5 (9%)
13	CLA	A	837	-	51,59,73	1.84	13 (25%)	59,96,113	2.16	14 (23%)
13	CLA	M	1201	-	54,62,73	1.78	17 (31%)	62,99,113	2.17	13 (20%)
16	LHG	A	854	13	26,26,48	1.23	2 (7%)	29,32,54	1.19	2 (6%)
13	CLA	A	812	-	54,62,73	1.75	15 (27%)	62,99,113	2.17	12 (19%)
13	CLA	B	808	2	65,73,73	1.63	15 (23%)	76,113,113	1.93	9 (11%)
13	CLA	B	813	-	45,53,73	1.80	12 (26%)	52,89,113	2.13	10 (19%)
13	CLA	B	822	-	54,62,73	1.78	15 (27%)	62,99,113	2.13	12 (19%)
13	CLA	A	844	-	42,49,73	1.85	13 (30%)	48,83,113	1.75	8 (16%)
13	CLA	A	819	-	65,73,73	1.59	16 (24%)	76,113,113	2.12	16 (21%)
13	CLA	B	832	-	45,53,73	1.81	13 (28%)	52,89,113	2.11	10 (19%)
15	BCR	B	842	-	41,41,41	2.26	24 (58%)	56,56,56	2.27	21 (37%)
13	CLA	A	826	-	65,73,73	1.66	16 (24%)	76,113,113	1.89	13 (17%)
13	CLA	B	839	-	65,73,73	1.60	15 (23%)	76,113,113	1.84	11 (14%)
13	CLA	A	832	-	65,73,73	1.62	16 (24%)	76,113,113	2.01	11 (14%)
16	LHG	A	853	-	48,48,48	0.90	2 (4%)	51,54,54	1.06	2 (3%)
13	CLA	B	834	-	45,53,73	1.81	13 (28%)	52,89,113	2.14	9 (17%)
13	CLA	B	824	-	65,73,73	1.62	14 (21%)	76,113,113	1.89	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	L	1006	-	41,41,41	2.22	24 (58%)	56,56,56	2.03	19 (33%)
13	CLA	B	811	-	65,73,73	1.65	15 (23%)	76,113,113	1.90	11 (14%)
13	CLA	A	834	-	65,73,73	1.64	17 (26%)	76,113,113	1.75	8 (10%)
13	CLA	B	827	-	65,73,73	1.59	15 (23%)	76,113,113	2.03	13 (17%)
15	BCR	B	843	-	41,41,41	2.18	24 (58%)	56,56,56	2.39	26 (46%)
13	CLA	A	806	-	65,73,73	1.60	15 (23%)	76,113,113	1.81	11 (14%)
13	CLA	B	816	-	60,68,73	1.68	16 (26%)	70,107,113	1.92	15 (21%)
13	CLA	A	830	-	65,73,73	1.57	14 (21%)	76,113,113	1.98	14 (18%)
15	BCR	B	850	-	41,41,41	2.21	25 (60%)	56,56,56	2.36	25 (44%)
15	BCR	F	1302	-	41,41,41	2.19	25 (60%)	56,56,56	2.20	21 (37%)
13	CLA	L	1002	10	65,73,73	1.61	15 (23%)	76,113,113	1.92	13 (17%)
13	CLA	A	808	1	65,73,73	1.65	14 (21%)	76,113,113	2.11	11 (14%)
15	BCR	A	850	-	41,41,41	2.29	23 (56%)	56,56,56	2.19	22 (39%)
15	BCR	J	1104	-	41,41,41	2.23	24 (58%)	56,56,56	2.24	24 (42%)
13	CLA	A	839	-	47,55,73	1.74	13 (27%)	54,91,113	2.20	7 (12%)
14	PQN	B	840	-	34,34,34	0.89	1 (2%)	42,45,45	1.36	4 (9%)
13	CLA	A	831	-	50,58,73	1.84	16 (32%)	58,95,113	2.00	9 (15%)
15	BCR	A	851	-	41,41,41	2.21	24 (58%)	56,56,56	2.17	17 (30%)
13	CLA	A	802	-	65,73,73	1.64	15 (23%)	76,113,113	1.74	9 (11%)
13	CLA	B	826	-	65,73,73	1.61	15 (23%)	76,113,113	1.72	7 (9%)
13	CLA	A	843	-	65,73,73	1.59	15 (23%)	76,113,113	1.93	13 (17%)
13	CLA	B	803	-	65,73,73	1.63	16 (24%)	76,113,113	1.83	11 (14%)
13	CLA	A	801	-	65,73,73	1.62	16 (24%)	76,113,113	1.89	13 (17%)
17	SF4	A	856	1,2	0,12,12	-	-	-		
13	CLA	A	811	13	65,73,73	1.61	15 (23%)	76,113,113	1.96	11 (14%)
13	CLA	B	802	-	65,73,73	1.65	14 (21%)	76,113,113	2.12	13 (17%)
13	CLA	F	1301	-	45,53,73	1.84	13 (28%)	52,89,113	2.22	9 (17%)
15	BCR	M	1203	-	41,41,41	2.18	22 (53%)	56,56,56	2.27	21 (37%)
13	CLA	B	817	-	65,73,73	1.60	16 (24%)	76,113,113	1.94	8 (10%)
13	CLA	A	823	-	51,59,73	1.79	14 (27%)	59,96,113	1.90	8 (13%)
13	CLA	A	817	-	54,62,73	1.77	15 (27%)	62,99,113	1.91	11 (17%)
13	CLA	J	1101	-	65,73,73	1.60	14 (21%)	76,113,113	1.92	15 (19%)
13	CLA	A	816	-	49,57,73	1.75	14 (28%)	55,93,113	1.98	8 (14%)
13	CLA	L	1003	-	65,73,73	1.61	15 (23%)	76,113,113	2.00	14 (18%)
16	LHG	X	101	-	22,22,48	1.31	2 (9%)	25,28,54	1.01	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	B	846	-	41,41,41	2.22	24 (58%)	56,56,56	2.08	21 (37%)
13	CLA	B	801	-	65,73,73	1.62	16 (24%)	76,113,113	1.86	12 (15%)
17	SF4	C	101	3	0,12,12	-	-	-		
15	BCR	J	1105	-	41,41,41	2.23	24 (58%)	56,56,56	2.15	23 (41%)
13	CLA	J	1102	8	45,53,73	1.80	13 (28%)	52,89,113	2.14	8 (15%)
13	CLA	A	842	-	65,73,73	1.66	16 (24%)	76,113,113	1.68	9 (11%)
13	CLA	B	818	-	47,55,73	1.79	12 (25%)	54,91,113	1.92	7 (12%)
13	CLA	B	837	-	47,55,73	1.77	14 (29%)	54,91,113	2.07	8 (14%)
13	CLA	B	820	-	55,63,73	1.74	16 (29%)	64,101,113	1.90	11 (17%)
13	CLA	A	818	-	54,62,73	1.74	16 (29%)	62,99,113	2.16	10 (16%)
13	CLA	A	815	-	45,53,73	1.79	12 (26%)	52,89,113	2.16	10 (19%)
13	CLA	A	827	-	65,73,73	1.62	15 (23%)	76,113,113	1.91	11 (14%)
13	CLA	A	805	-	65,73,73	1.60	16 (24%)	76,113,113	1.85	8 (10%)
15	BCR	B	844	-	25,25,41	2.30	14 (56%)	33,33,56	2.14	13 (39%)
14	PQN	A	846	-	34,34,34	0.97	1 (2%)	42,45,45	1.18	4 (9%)
15	BCR	B	845	-	41,41,41	2.18	23 (56%)	56,56,56	2.35	22 (39%)
13	CLA	A	824	-	59,67,73	1.70	16 (27%)	68,105,113	2.06	14 (20%)
18	LMG	B	848	-	55,55,55	1.05	8 (14%)	63,63,63	1.23	3 (4%)
13	CLA	A	814	-	45,53,73	1.81	12 (26%)	52,89,113	2.00	8 (15%)
13	CLA	B	828	-	45,53,73	1.81	14 (31%)	52,89,113	2.04	7 (13%)
13	CLA	B	823	-	46,54,73	1.82	13 (28%)	53,90,113	2.07	11 (20%)
17	SF4	C	102	3	0,12,12	-	-	-		
13	CLA	A	820	-	61,69,73	1.68	16 (26%)	71,108,113	1.89	13 (18%)
15	BCR	B	847	-	41,41,41	2.21	24 (58%)	56,56,56	2.27	23 (41%)
13	CLA	B	807	-	65,73,73	1.64	16 (24%)	76,113,113	1.97	10 (13%)
13	CLA	A	813	-	60,68,73	1.67	14 (23%)	70,107,113	1.98	12 (17%)
13	CLA	L	1004	-	65,73,73	1.61	15 (23%)	76,113,113	1.91	12 (15%)
13	CLA	B	804	-	65,73,73	1.59	15 (23%)	76,113,113	1.88	11 (14%)
15	BCR	A	847	-	41,41,41	2.23	24 (58%)	56,56,56	2.05	23 (41%)
13	CLA	B	819	-	45,53,73	1.80	13 (28%)	52,89,113	2.13	9 (17%)
13	CLA	M	1202	-	45,53,73	1.80	12 (26%)	52,89,113	2.22	9 (17%)
13	CLA	B	835	-	60,68,73	1.72	15 (25%)	70,107,113	1.96	16 (22%)
13	CLA	B	805	-	65,73,73	1.59	16 (24%)	76,113,113	1.83	11 (14%)
13	CLA	A	807	-	51,59,73	1.81	15 (29%)	59,96,113	2.21	10 (16%)
13	CLA	X	102	12	45,53,73	1.84	13 (28%)	52,89,113	2.30	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	A	848	-	41,41,41	2.24	23 (56%)	56,56,56	2.14	21 (37%)
15	BCR	B	841	-	41,41,41	2.20	24 (58%)	56,56,56	2.11	23 (41%)
13	CLA	B	815	-	59,67,73	1.71	15 (25%)	68,105,113	1.81	9 (13%)
15	BCR	I	102	-	41,41,41	2.10	21 (51%)	56,56,56	2.32	23 (41%)
13	CLA	A	810	-	45,53,73	1.77	13 (28%)	52,89,113	2.24	9 (17%)
13	CLA	A	845	16	52,60,73	1.75	16 (30%)	60,97,113	2.24	14 (23%)
13	CLA	B	814	-	55,63,73	1.71	15 (27%)	64,101,113	2.11	12 (18%)
13	CLA	A	825	-	65,73,73	1.63	14 (21%)	76,113,113	1.93	11 (14%)
13	CLA	B	806	-	65,73,73	1.63	17 (26%)	76,113,113	1.94	12 (15%)
13	CLA	A	838	-	65,73,73	1.64	15 (23%)	76,113,113	1.94	13 (17%)
13	CLA	A	804	13	59,67,73	1.71	14 (23%)	68,105,113	1.89	9 (13%)
13	CLA	I	101	-	65,73,73	1.65	16 (24%)	76,113,113	1.97	14 (18%)
13	CLA	A	855	-	45,53,73	1.80	13 (28%)	52,89,113	2.12	9 (17%)
15	BCR	L	1005	-	41,41,41	2.18	23 (56%)	56,56,56	2.26	23 (41%)
13	CLA	B	825	-	65,73,73	1.64	14 (21%)	76,113,113	1.79	7 (9%)
13	CLA	A	835	-	54,62,73	1.77	14 (25%)	62,99,113	1.88	10 (16%)
13	CLA	B	821	-	45,53,73	1.85	13 (28%)	52,89,113	1.95	8 (15%)
13	CLA	J	1103	-	38,45,73	1.98	13 (34%)	43,78,113	1.79	5 (11%)
15	BCR	A	852	-	41,41,41	2.26	24 (58%)	56,56,56	2.28	20 (35%)
13	CLA	A	821	-	65,73,73	1.62	15 (23%)	76,113,113	1.98	12 (15%)
15	BCR	B	849	-	41,41,41	2.13	21 (51%)	56,56,56	2.34	22 (39%)
13	CLA	B	809	-	45,53,73	1.80	13 (28%)	52,89,113	2.16	9 (17%)
13	CLA	B	833	-	45,53,73	1.80	12 (26%)	52,89,113	2.19	5 (9%)
13	CLA	A	822	-	49,57,73	1.80	13 (26%)	55,93,113	2.30	9 (16%)
13	CLA	A	833	-	65,73,73	1.63	15 (23%)	76,113,113	1.77	8 (10%)
13	CLA	A	840	-	65,73,73	1.63	16 (24%)	76,113,113	1.95	11 (14%)
13	CLA	A	841	-	51,59,73	1.80	14 (27%)	59,96,113	1.93	10 (16%)
13	CLA	B	812	-	65,73,73	1.61	16 (24%)	76,113,113	1.93	12 (15%)
13	CLA	B	829	-	49,57,73	1.72	13 (26%)	55,93,113	1.92	10 (18%)
13	CLA	B	838	-	65,73,73	1.62	15 (23%)	76,113,113	1.97	13 (17%)
15	BCR	A	849	-	41,41,41	2.10	22 (53%)	56,56,56	2.23	24 (42%)
13	CLA	A	829	-	65,73,73	1.59	16 (24%)	76,113,113	1.99	14 (18%)
13	CLA	A	828	-	65,73,73	1.61	15 (23%)	76,113,113	1.91	10 (13%)
13	CLA	B	810	-	45,53,73	1.79	14 (31%)	52,89,113	1.98	8 (15%)
13	CLA	B	831	-	58,66,73	1.72	15 (25%)	67,104,113	2.17	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	A	803	-	65,73,73	1.62	14 (21%)	76,113,113	1.81	13 (17%)
13	CLA	A	809	1	65,73,73	1.63	15 (23%)	76,113,113	2.08	16 (21%)
13	CLA	B	836	-	65,73,73	1.63	16 (24%)	76,113,113	1.85	11 (14%)
13	CLA	B	830	-	65,73,73	1.62	15 (23%)	76,113,113	1.94	10 (13%)

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
13	CLA	A	836	1	1/1/11/20	4/13/91/115	-
13	CLA	A	837	-	-	2/21/99/115	-
13	CLA	M	1201	-	1/1/12/20	5/24/102/115	-
16	LHG	A	854	13	-	10/31/31/53	-
13	CLA	A	812	-	1/1/12/20	9/24/102/115	-
13	CLA	B	808	2	1/1/15/20	7/37/115/115	-
13	CLA	B	813	-	-	3/13/91/115	-
13	CLA	B	822	-	1/1/12/20	9/24/102/115	-
13	CLA	A	844	-	-	2/7/81/115	-
13	CLA	B	832	-	1/1/11/20	4/13/91/115	-
13	CLA	A	819	-	1/1/15/20	11/37/115/115	-
15	BCR	B	842	-	-	12/29/63/63	0/2/2/2
13	CLA	A	826	-	-	9/37/115/115	-
13	CLA	B	839	-	1/1/15/20	5/37/115/115	-
13	CLA	A	832	-	1/1/15/20	16/37/115/115	-
16	LHG	A	853	-	-	22/53/53/53	-
13	CLA	B	834	-	1/1/11/20	4/13/91/115	-
13	CLA	B	824	-	1/1/15/20	9/37/115/115	-
15	BCR	L	1006	-	-	8/29/63/63	0/2/2/2
13	CLA	B	811	-	1/1/15/20	10/37/115/115	-
13	CLA	A	834	-	1/1/15/20	12/37/115/115	-
13	CLA	B	827	-	1/1/15/20	8/37/115/115	-
15	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	A	806	-	1/1/15/20	8/37/115/115	-
13	CLA	B	816	-	1/1/14/20	4/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	830	-	1/1/15/20	9/37/115/115	-
15	BCR	B	850	-	-	8/29/63/63	0/2/2/2
15	BCR	F	1302	-	-	10/29/63/63	0/2/2/2
13	CLA	L	1002	10	1/1/15/20	11/37/115/115	-
13	CLA	A	808	1	1/1/15/20	10/37/115/115	-
15	BCR	A	850	-	-	6/29/63/63	0/2/2/2
15	BCR	J	1104	-	-	11/29/63/63	0/2/2/2
13	CLA	A	839	-	1/1/11/20	3/16/94/115	-
14	PQN	B	840	-	-	7/23/43/43	0/2/2/2
13	CLA	A	831	-	1/1/12/20	2/19/97/115	-
15	BCR	A	851	-	-	8/29/63/63	0/2/2/2
13	CLA	A	802	-	1/1/15/20	3/37/115/115	-
13	CLA	B	826	-	1/1/15/20	13/37/115/115	-
13	CLA	A	843	-	1/1/15/20	6/37/115/115	-
13	CLA	B	803	-	1/1/15/20	12/37/115/115	-
13	CLA	A	801	-	1/1/15/20	7/37/115/115	-
17	SF4	A	856	1,2	-	-	0/6/5/5
13	CLA	A	811	13	1/1/15/20	13/37/115/115	-
13	CLA	B	802	-	1/1/15/20	10/37/115/115	-
13	CLA	F	1301	-	-	3/13/91/115	-
15	BCR	M	1203	-	-	15/29/63/63	0/2/2/2
13	CLA	B	817	-	1/1/15/20	10/37/115/115	-
13	CLA	A	823	-	1/1/12/20	4/21/99/115	-
13	CLA	A	817	-	1/1/12/20	3/24/102/115	-
13	CLA	J	1101	-	1/1/15/20	5/37/115/115	-
13	CLA	A	816	-	-	3/18/96/115	-
13	CLA	L	1003	-	1/1/15/20	14/37/115/115	-
16	LHG	X	101	-	-	9/26/26/53	-
15	BCR	B	846	-	-	8/29/63/63	0/2/2/2
13	CLA	B	801	-	1/1/15/20	10/37/115/115	-
17	SF4	C	101	3	-	-	0/6/5/5
15	BCR	J	1105	-	-	14/29/63/63	0/2/2/2
13	CLA	J	1102	8	1/1/11/20	5/13/91/115	-
13	CLA	A	842	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	818	-	1/1/11/20	2/16/94/115	-
13	CLA	B	837	-	1/1/11/20	4/16/94/115	-
13	CLA	B	820	-	1/1/13/20	6/25/103/115	-
13	CLA	A	818	-	1/1/12/20	7/24/102/115	-
13	CLA	A	815	-	1/1/11/20	0/13/91/115	-
13	CLA	A	827	-	1/1/15/20	8/37/115/115	-
13	CLA	A	805	-	1/1/15/20	10/37/115/115	-
15	BCR	B	844	-	-	6/18/35/63	0/1/1/2
14	PQN	A	846	-	-	7/23/43/43	0/2/2/2
15	BCR	B	845	-	-	10/29/63/63	0/2/2/2
13	CLA	A	824	-	1/1/13/20	9/30/108/115	-
18	LMG	B	848	-	-	11/50/70/70	0/1/1/1
13	CLA	A	814	-	1/1/11/20	3/13/91/115	-
13	CLA	B	828	-	1/1/11/20	4/13/91/115	-
13	CLA	B	823	-	1/1/11/20	1/15/93/115	-
17	SF4	C	102	3	-	-	0/6/5/5
13	CLA	A	820	-	1/1/14/20	9/33/111/115	-
15	BCR	B	847	-	-	12/29/63/63	0/2/2/2
13	CLA	B	807	-	1/1/15/20	14/37/115/115	-
13	CLA	A	813	-	1/1/14/20	7/31/109/115	-
13	CLA	L	1004	-	1/1/15/20	9/37/115/115	-
13	CLA	B	804	-	1/1/15/20	7/37/115/115	-
15	BCR	A	847	-	-	8/29/63/63	0/2/2/2
13	CLA	B	819	-	1/1/11/20	1/13/91/115	-
13	CLA	M	1202	-	-	3/13/91/115	-
13	CLA	B	835	-	1/1/14/20	8/31/109/115	-
13	CLA	B	805	-	1/1/15/20	5/37/115/115	-
13	CLA	A	807	-	1/1/12/20	5/21/99/115	-
13	CLA	X	102	12	1/1/11/20	3/13/91/115	-
15	BCR	A	848	-	-	13/29/63/63	0/2/2/2
15	BCR	B	841	-	-	10/29/63/63	0/2/2/2
13	CLA	B	815	-	1/1/13/20	7/30/108/115	-
15	BCR	I	102	-	-	16/29/63/63	0/2/2/2
13	CLA	A	810	-	1/1/11/20	5/13/91/115	-
13	CLA	A	845	16	1/1/12/20	3/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	814	-	1/1/13/20	4/25/103/115	-
13	CLA	A	825	-	1/1/15/20	6/37/115/115	-
13	CLA	B	806	-	1/1/15/20	9/37/115/115	-
13	CLA	A	838	-	1/1/15/20	13/37/115/115	-
13	CLA	A	804	13	1/1/13/20	8/30/108/115	-
13	CLA	I	101	-	1/1/15/20	10/37/115/115	-
13	CLA	A	855	-	1/1/11/20	1/13/91/115	-
15	BCR	L	1005	-	-	9/29/63/63	0/2/2/2
13	CLA	B	825	-	1/1/15/20	11/37/115/115	-
13	CLA	A	835	-	1/1/12/20	5/24/102/115	-
13	CLA	B	821	-	1/1/11/20	3/13/91/115	-
13	CLA	J	1103	-	1/1/8/20	0/2/76/115	-
15	BCR	A	852	-	-	13/29/63/63	0/2/2/2
13	CLA	A	821	-	1/1/15/20	14/37/115/115	-
15	BCR	B	849	-	-	14/29/63/63	0/2/2/2
13	CLA	B	809	-	1/1/11/20	3/13/91/115	-
13	CLA	B	833	-	1/1/11/20	4/13/91/115	-
13	CLA	A	822	-	1/1/11/20	4/18/96/115	-
13	CLA	A	833	-	1/1/15/20	6/37/115/115	-
13	CLA	A	840	-	1/1/15/20	10/37/115/115	-
13	CLA	A	841	-	1/1/12/20	3/21/99/115	-
13	CLA	B	812	-	1/1/15/20	11/37/115/115	-
13	CLA	B	829	-	1/1/11/20	3/18/96/115	-
13	CLA	B	838	-	1/1/15/20	13/37/115/115	-
15	BCR	A	849	-	-	5/29/63/63	0/2/2/2
13	CLA	A	829	-	1/1/15/20	9/37/115/115	-
13	CLA	A	828	-	1/1/15/20	18/37/115/115	-
13	CLA	B	810	-	1/1/11/20	3/13/91/115	-
13	CLA	B	831	-	1/1/13/20	6/29/107/115	-
13	CLA	A	803	-	1/1/15/20	9/37/115/115	-
13	CLA	A	809	1	-	9/37/115/115	-
13	CLA	B	836	-	1/1/15/20	9/37/115/115	-
13	CLA	B	830	-	1/1/15/20	11/37/115/115	-

The worst 5 of 1919 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	808	CLA	MG-ND	-4.34	1.97	2.05
13	B	802	CLA	MG-ND	-4.27	1.97	2.05
13	J	1103	CLA	C3A-C2A	-4.26	1.50	1.54
13	B	822	CLA	MG-ND	-4.23	1.97	2.05
13	B	835	CLA	MG-ND	-4.23	1.97	2.05

The worst 5 of 1512 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	809	CLA	C4A-NA-C1A	11.51	111.88	106.71
13	A	808	CLA	C4A-NA-C1A	11.40	111.83	106.71
13	A	830	CLA	C4A-NA-C1A	11.31	111.79	106.71
13	M	1202	CLA	C4A-NA-C1A	11.22	111.75	106.71
13	B	827	CLA	C4A-NA-C1A	11.19	111.74	106.71

5 of 88 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CLA	ND
13	A	802	CLA	ND
13	A	803	CLA	ND
13	A	804	CLA	ND
13	A	805	CLA	ND

5 of 957 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	804	CLA	CHA-CBD-CGD-O1D
13	A	804	CLA	CHA-CBD-CGD-O2D
13	A	805	CLA	O2A-C1-C2-C3
13	A	807	CLA	C3A-C2A-CAA-CBA
13	A	807	CLA	C4-C3-C5-C6

There are no ring outliers.

123 monomers are involved in 1092 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	836	CLA	11	0
13	A	837	CLA	14	0
13	M	1201	CLA	17	0
16	A	854	LHG	2	0
13	A	812	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	808	CLA	14	0
13	B	813	CLA	10	0
13	B	822	CLA	21	0
13	A	844	CLA	3	0
13	A	819	CLA	16	0
13	B	832	CLA	12	0
15	B	842	BCR	4	0
13	A	826	CLA	17	0
13	B	839	CLA	7	0
13	A	832	CLA	21	0
16	A	853	LHG	10	0
13	B	834	CLA	7	0
13	B	824	CLA	20	0
15	L	1006	BCR	4	0
13	B	811	CLA	18	0
13	A	834	CLA	18	0
13	B	827	CLA	14	0
15	B	843	BCR	18	0
13	A	806	CLA	9	0
13	B	816	CLA	16	0
13	A	830	CLA	14	0
15	B	850	BCR	6	0
15	F	1302	BCR	13	0
13	L	1002	CLA	5	0
13	A	808	CLA	17	0
15	A	850	BCR	4	0
15	J	1104	BCR	4	0
13	A	839	CLA	17	0
14	B	840	PQN	7	0
13	A	831	CLA	11	0
15	A	851	BCR	3	0
13	A	802	CLA	12	0
13	B	826	CLA	19	0
13	A	843	CLA	10	0
13	B	803	CLA	16	0
13	A	801	CLA	8	0
13	A	811	CLA	14	0
13	B	802	CLA	18	0
13	F	1301	CLA	5	0
15	M	1203	BCR	13	0
13	B	817	CLA	12	0
13	A	823	CLA	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	817	CLA	9	0
13	J	1101	CLA	13	0
13	A	816	CLA	3	0
13	L	1003	CLA	16	0
16	X	101	LHG	1	0
15	B	846	BCR	7	0
13	B	801	CLA	13	0
15	J	1105	BCR	7	0
13	J	1102	CLA	4	0
13	A	842	CLA	22	0
13	B	818	CLA	4	0
13	B	837	CLA	8	0
13	B	820	CLA	12	0
13	A	818	CLA	11	0
13	A	815	CLA	7	0
13	A	827	CLA	15	0
13	A	805	CLA	13	0
15	B	844	BCR	6	0
14	A	846	PQN	7	0
15	B	845	BCR	9	0
13	A	824	CLA	8	0
18	B	848	LMG	18	0
13	A	814	CLA	8	0
13	B	828	CLA	6	0
13	B	823	CLA	8	0
13	A	820	CLA	10	0
15	B	847	BCR	12	0
13	B	807	CLA	12	0
13	A	813	CLA	19	0
13	L	1004	CLA	7	0
13	B	804	CLA	17	0
15	A	847	BCR	5	0
13	B	819	CLA	1	0
13	M	1202	CLA	1	0
13	B	835	CLA	16	0
13	B	805	CLA	9	0
13	A	807	CLA	13	0
13	X	102	CLA	5	0
15	A	848	BCR	5	0
15	B	841	BCR	5	0
13	B	815	CLA	15	0
15	I	102	BCR	11	0

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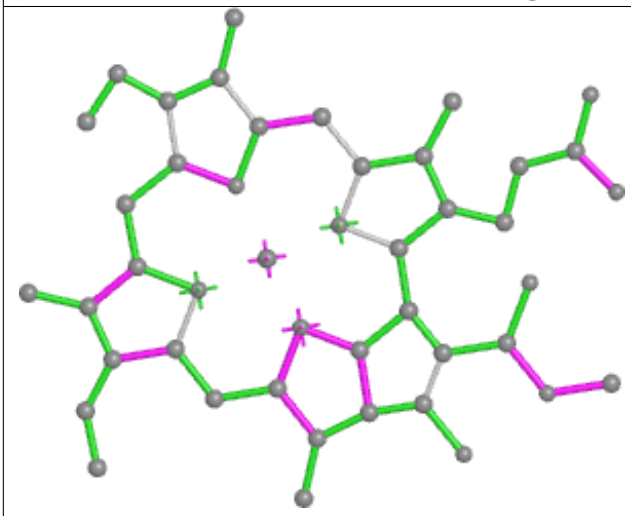
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	810	CLA	8	0
13	A	845	CLA	11	0
13	B	814	CLA	10	0
13	A	825	CLA	22	0
13	B	806	CLA	15	0
13	A	838	CLA	14	0
13	A	804	CLA	10	0
13	I	101	CLA	15	0
13	A	855	CLA	2	0
15	L	1005	BCR	12	0
13	B	825	CLA	18	0
13	A	835	CLA	8	0
13	B	821	CLA	13	0
15	A	852	BCR	19	0
13	A	821	CLA	12	0
15	B	849	BCR	16	0
13	B	809	CLA	8	0
13	B	833	CLA	3	0
13	A	822	CLA	7	0
13	A	833	CLA	19	0
13	A	840	CLA	16	0
13	A	841	CLA	6	0
13	B	812	CLA	15	0
13	B	829	CLA	7	0
13	B	838	CLA	18	0
15	A	849	BCR	4	0
13	A	829	CLA	10	0
13	A	828	CLA	16	0
13	B	810	CLA	5	0
13	B	831	CLA	12	0
13	A	803	CLA	27	0
13	A	809	CLA	16	0
13	B	836	CLA	10	0
13	B	830	CLA	24	0

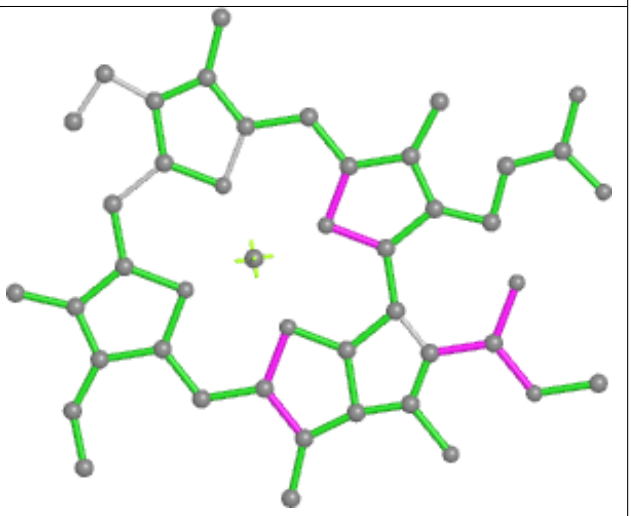
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

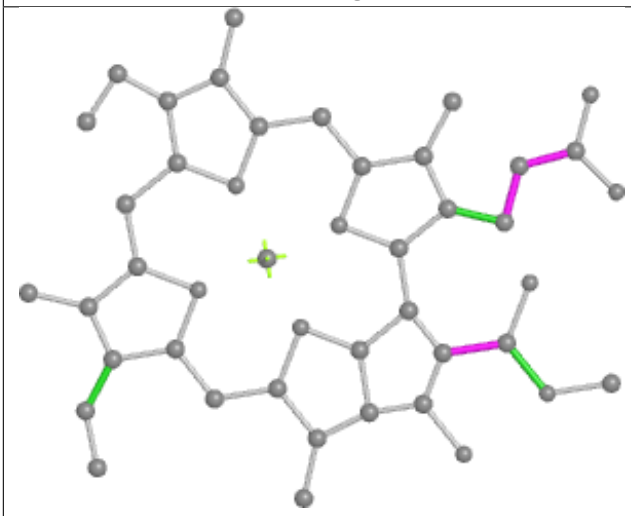
Ligand CLA A 836



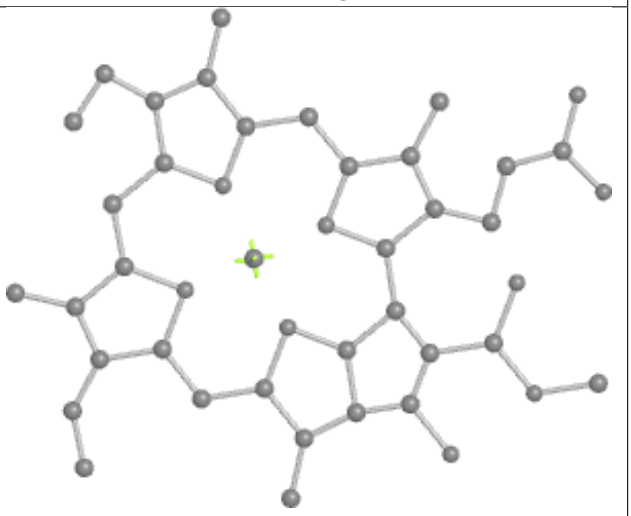
Bond lengths



Bond angles

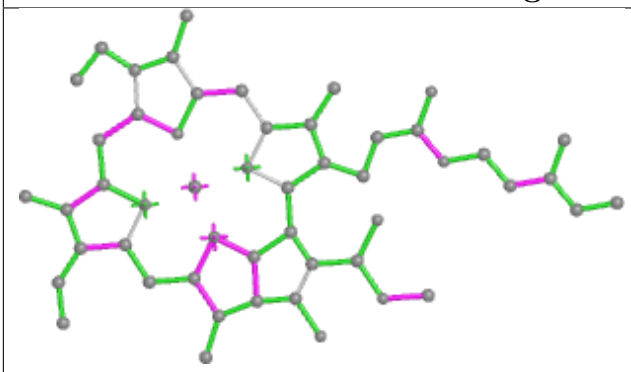


Torsions

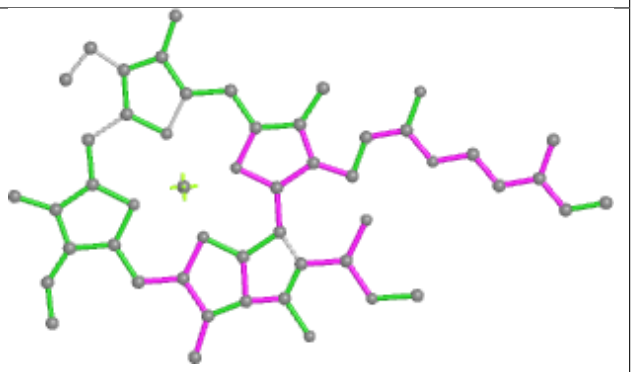


Rings

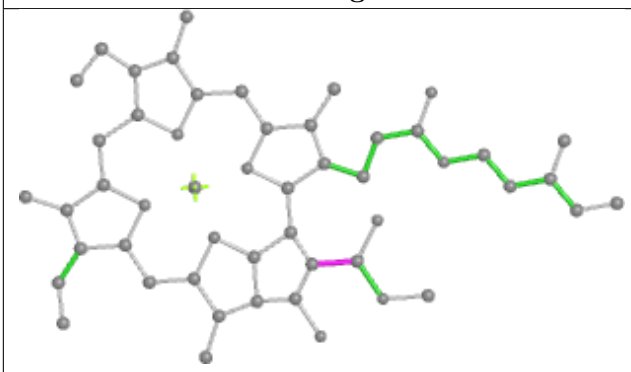
Ligand CLA A 837



Bond lengths



Bond angles



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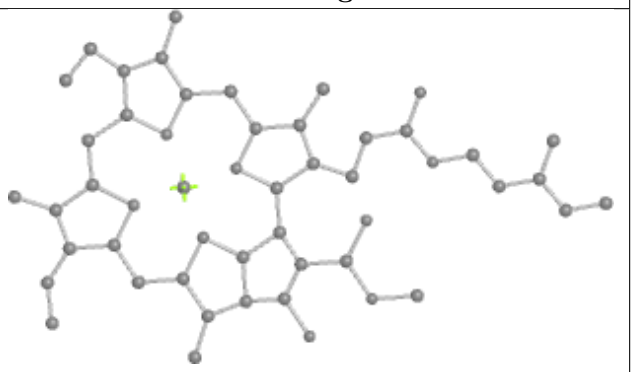
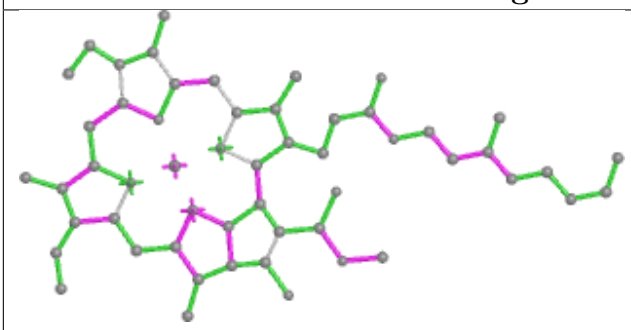
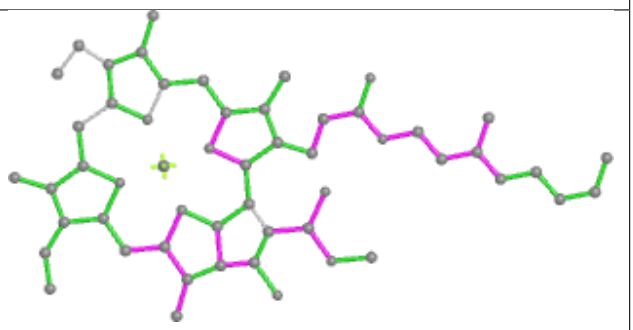


Rings

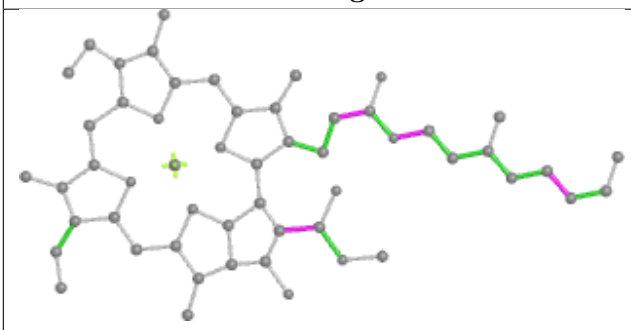
Ligand CLA M 1201



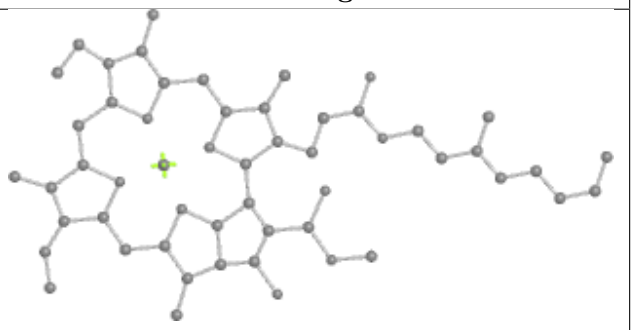
Bond lengths



Bond angles

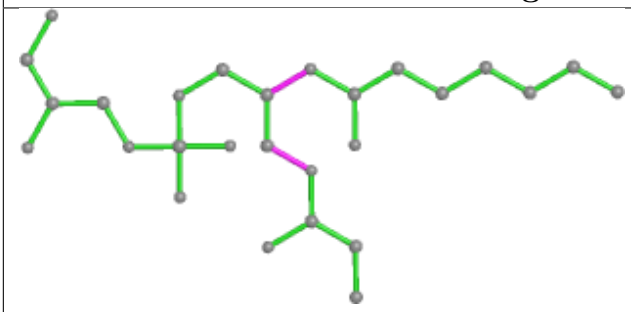


Torsions

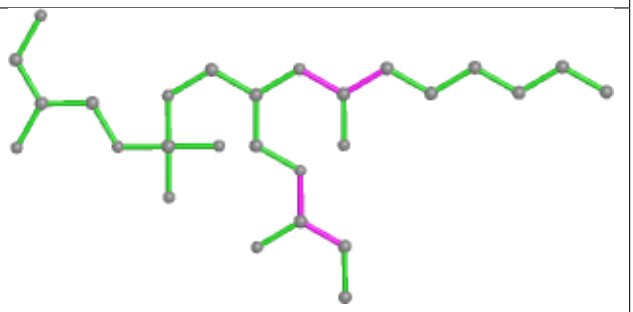


Rings

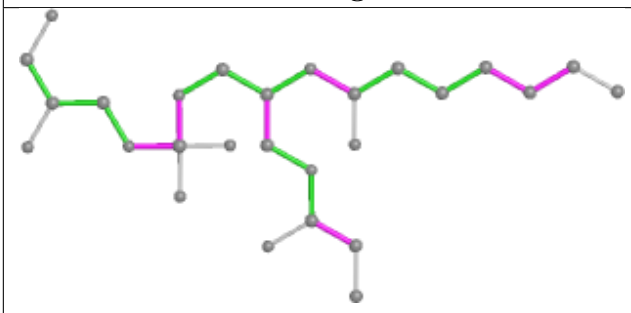
Ligand LHG A 854



Bond lengths



Bond angles



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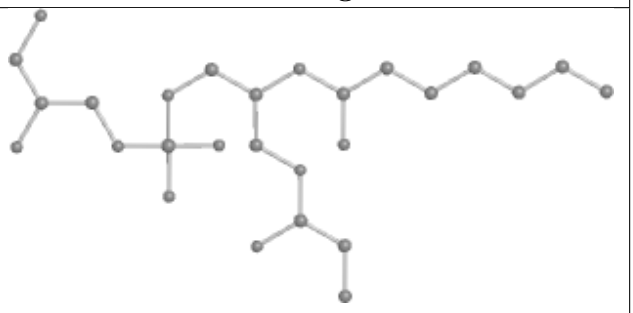
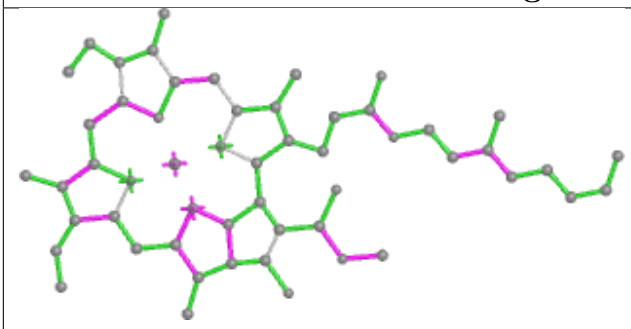
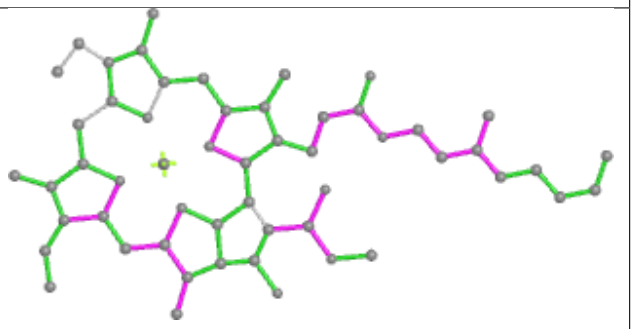


Rings

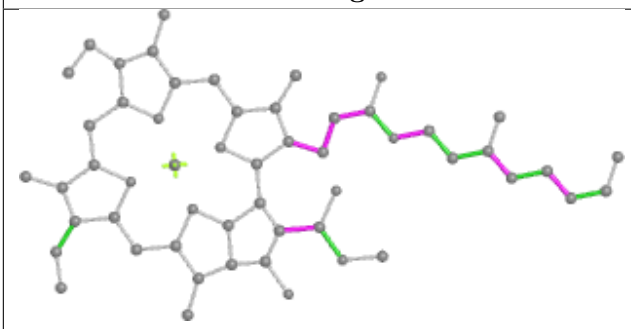
Ligand CLA A 812



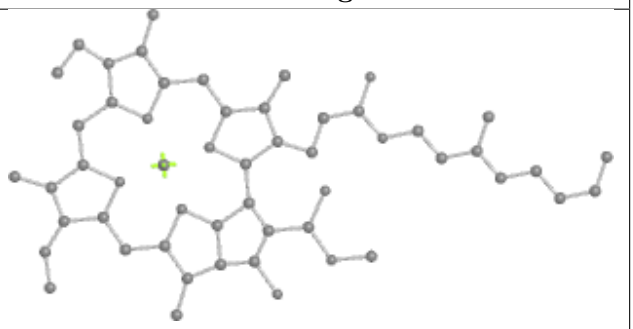
Bond lengths



Bond angles

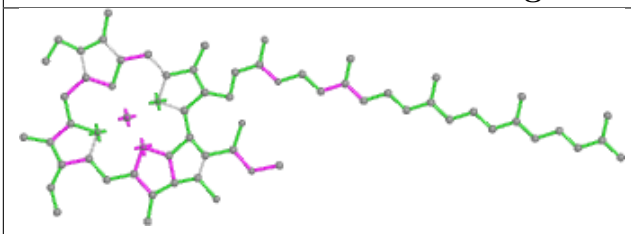


Torsions

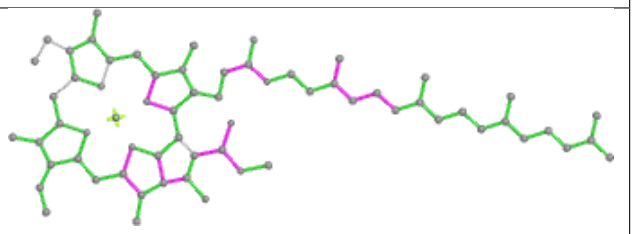


Rings

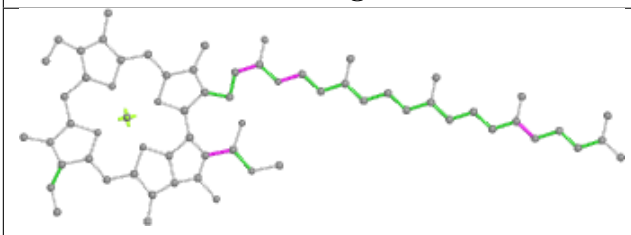
Ligand CLA B 808



Bond lengths



Bond angles



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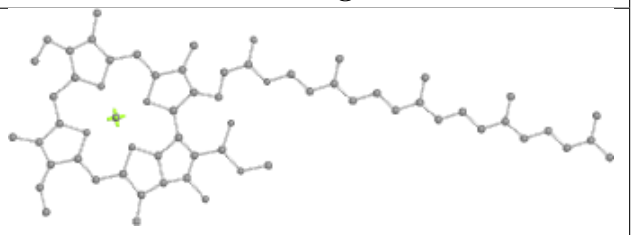
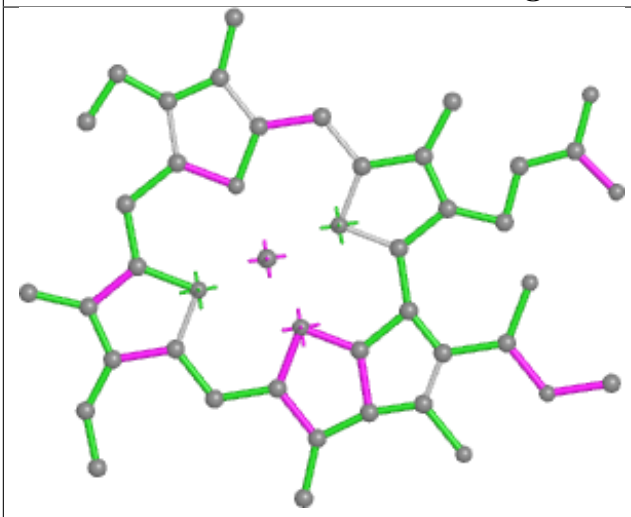
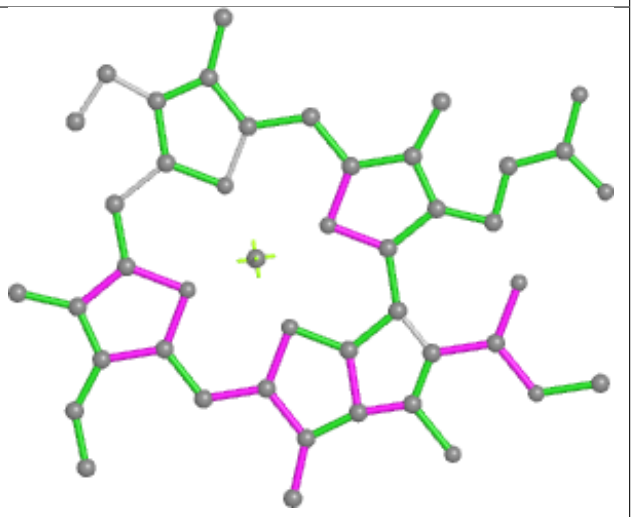


Rings

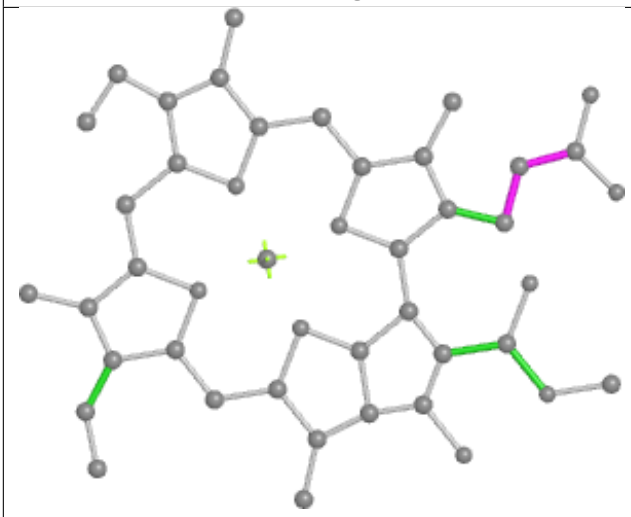
Ligand CLA B 813



Bond lengths



Bond angles



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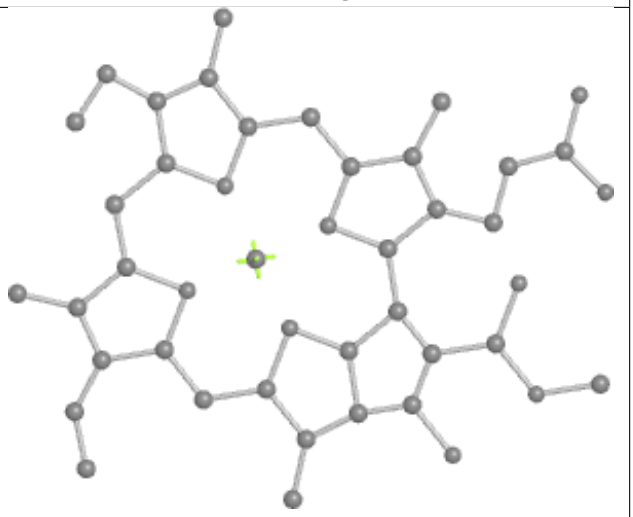
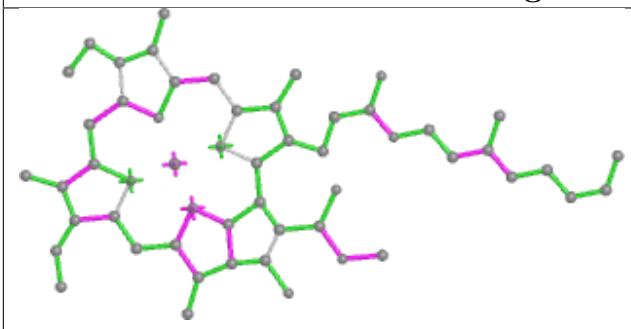


Rings

Ligand CLA B 822



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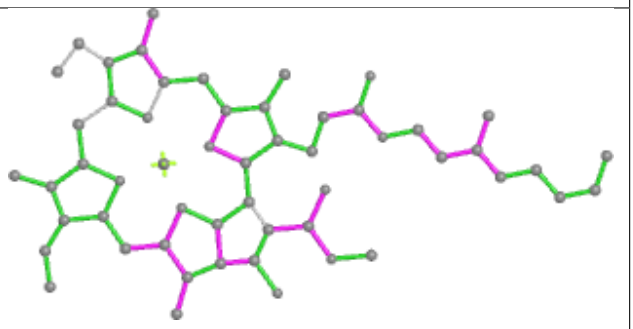
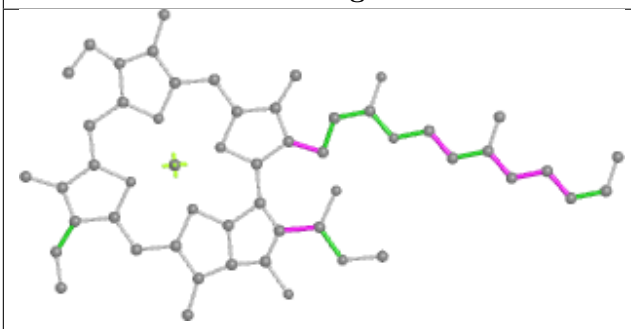


Bond angles



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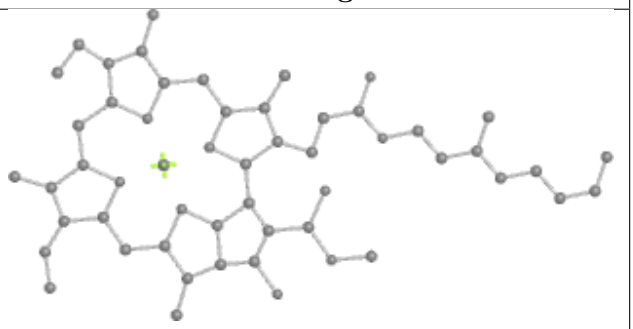
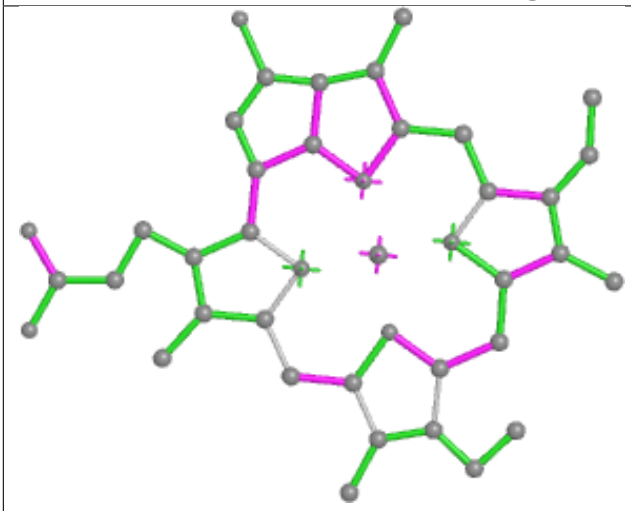
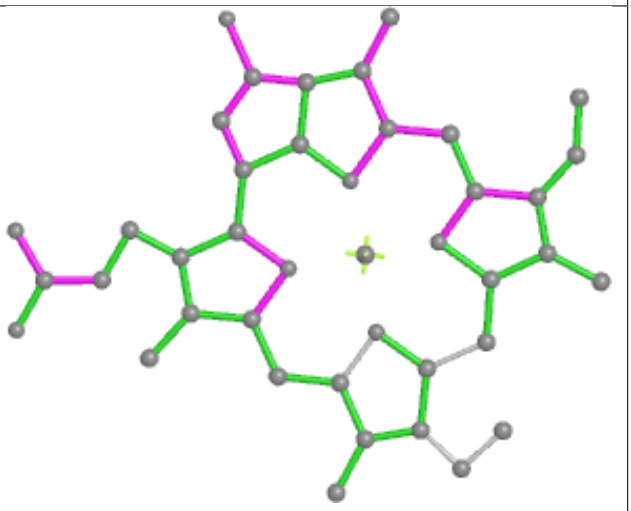


Rings

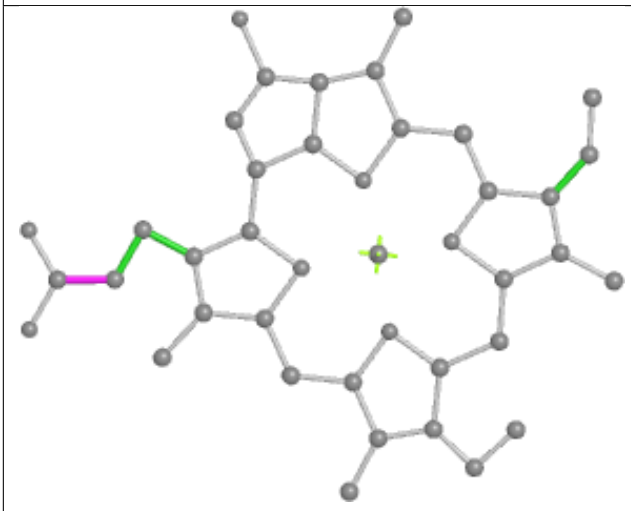
Ligand CLA A 844



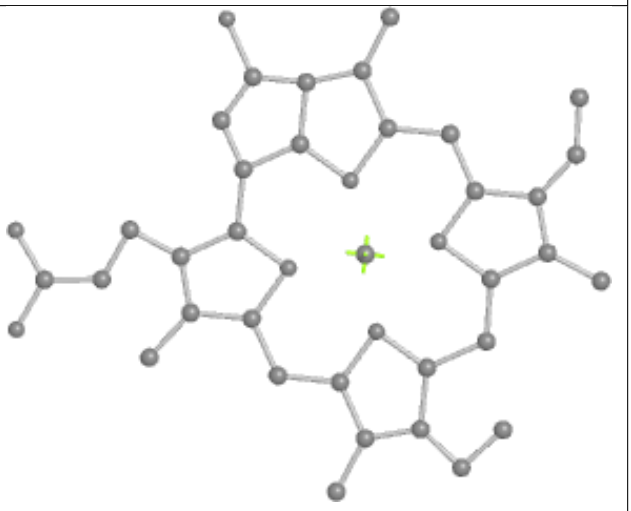
Bond lengths



Bond angles

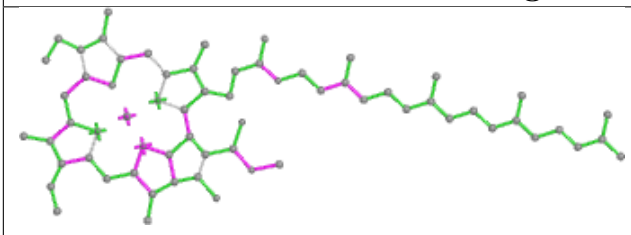


Torsions

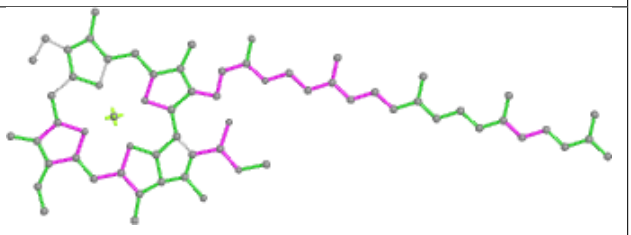


Rings

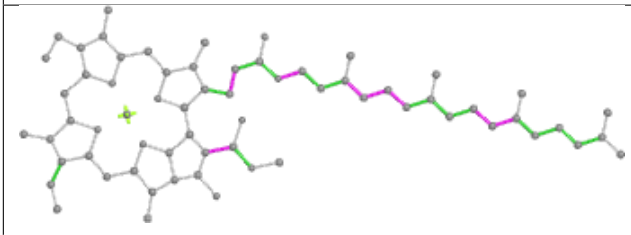
Ligand CLA A 819



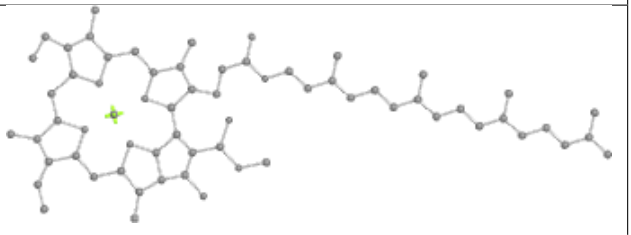
Bond lengths



Bond angles

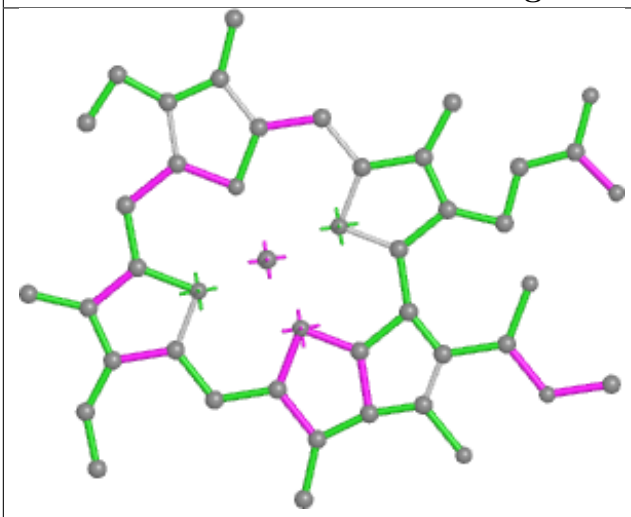


Torsions



Rings

Ligand CLA B 832



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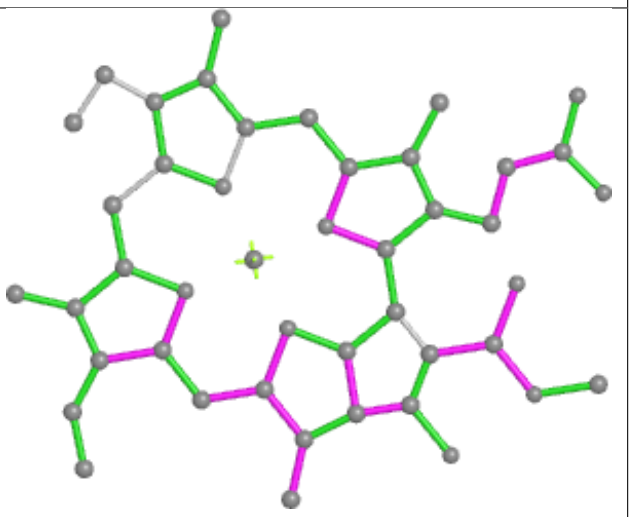
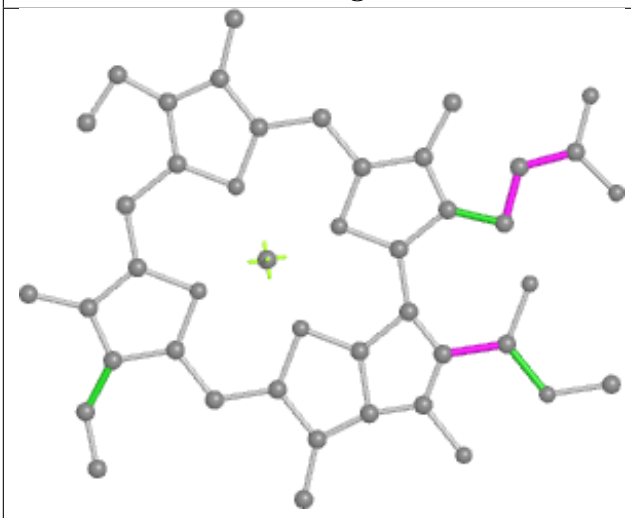


Bond angles



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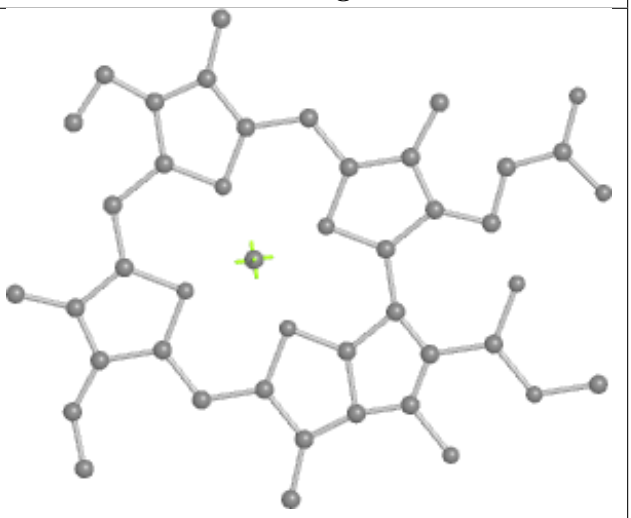
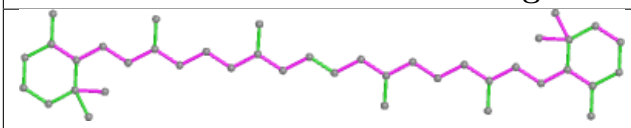
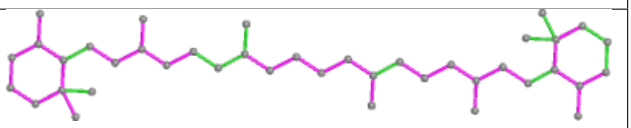


Rings

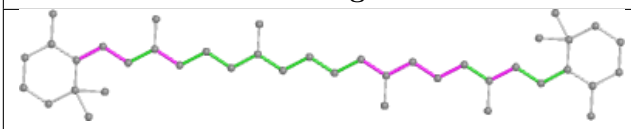
Ligand BCR B 842



Bond lengths



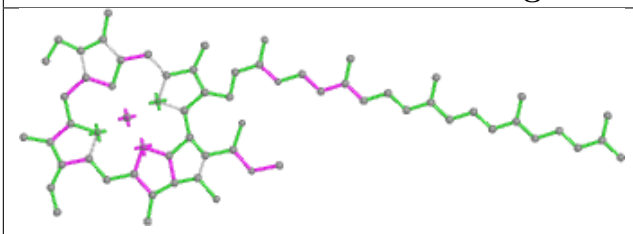
Bond angles



Torsions

Rings

Ligand CLA A 826



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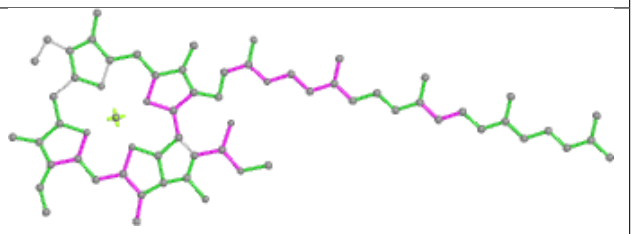
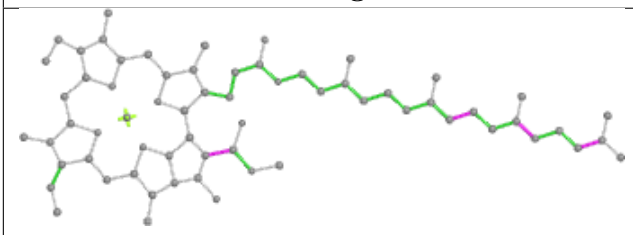


Bond angles



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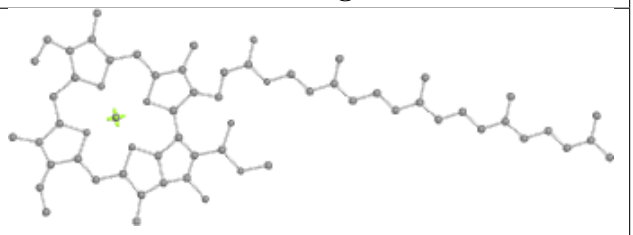
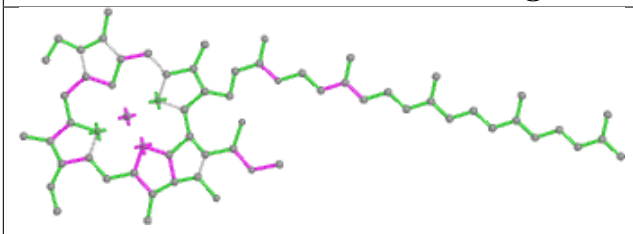
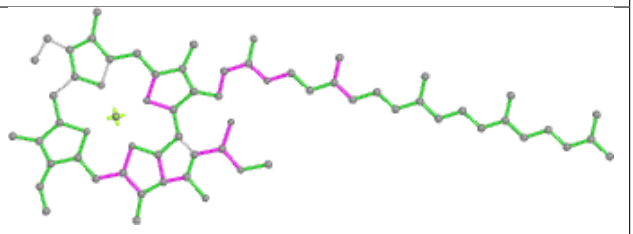


Rings

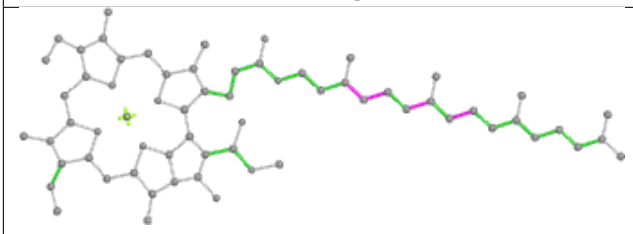
Ligand CLA B 839



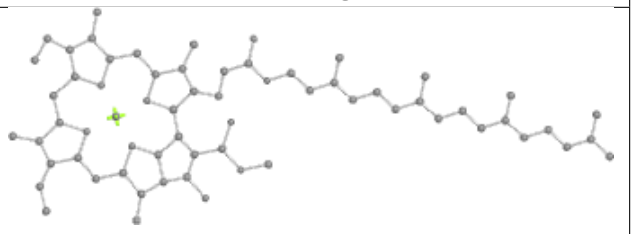
Bond lengths



Bond angles

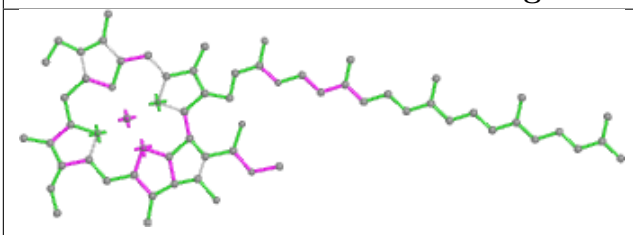


Torsions



Rings

Ligand CLA A 832



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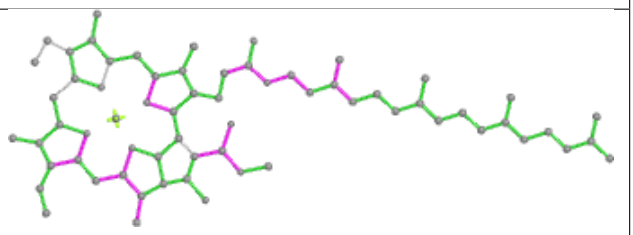
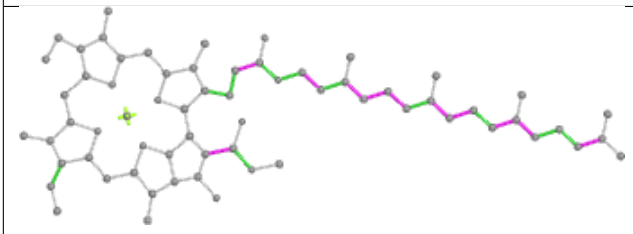
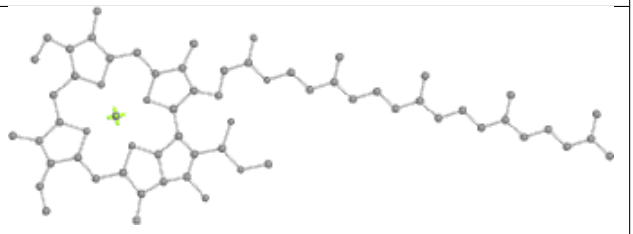


Bond angles

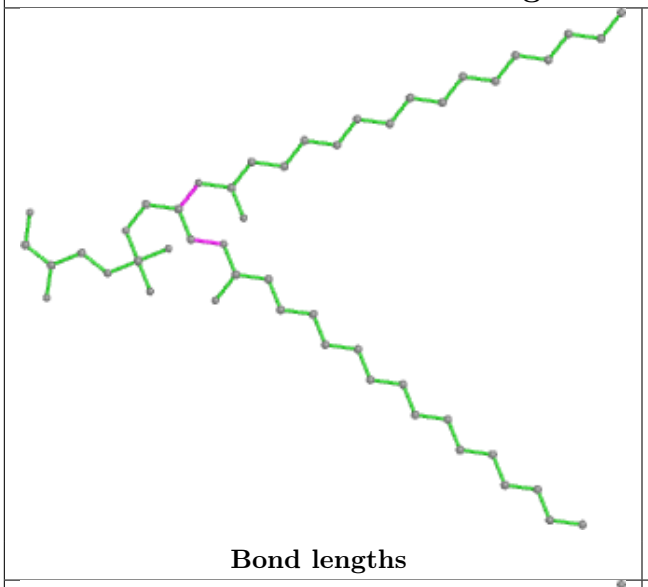


Torsions

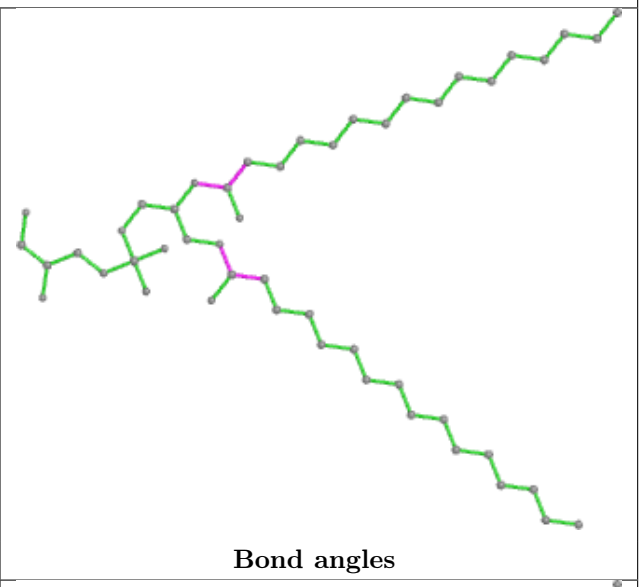


Rings

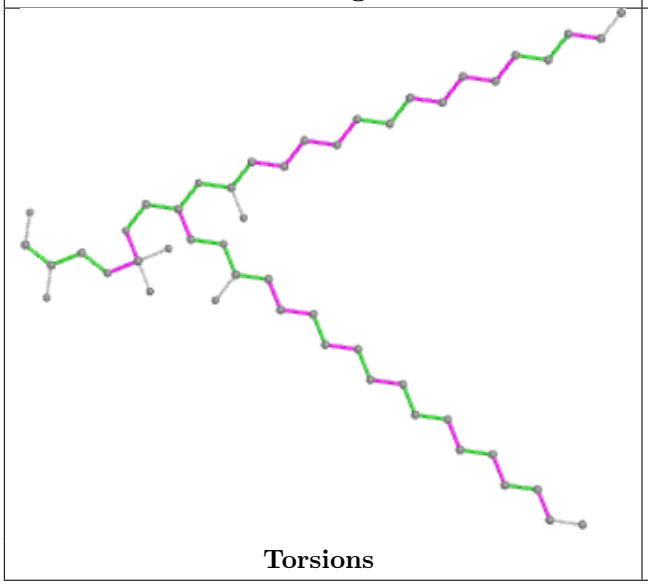
Ligand LHG A 853



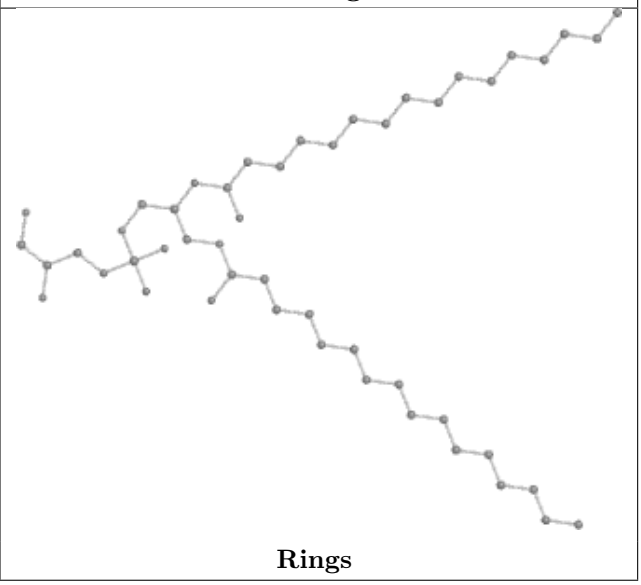
Bond lengths



Bond angles

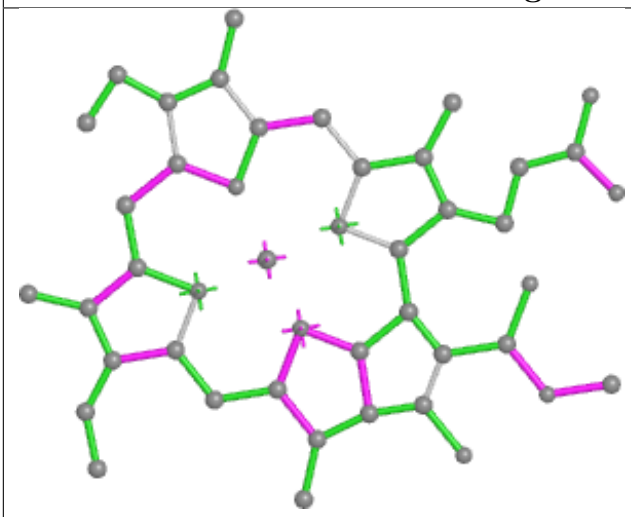


Torsions

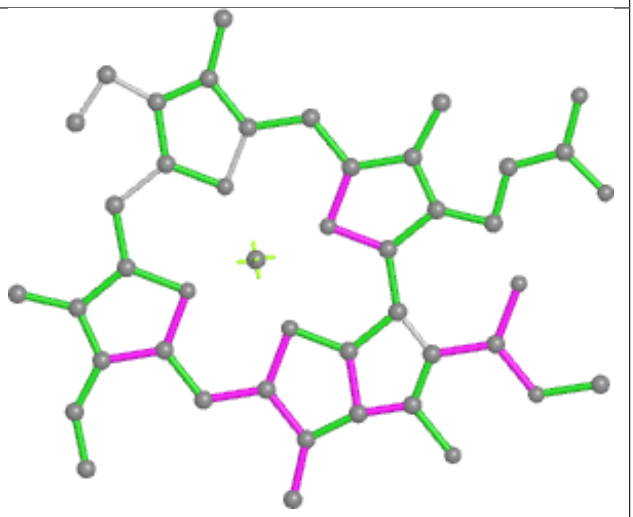


Rings

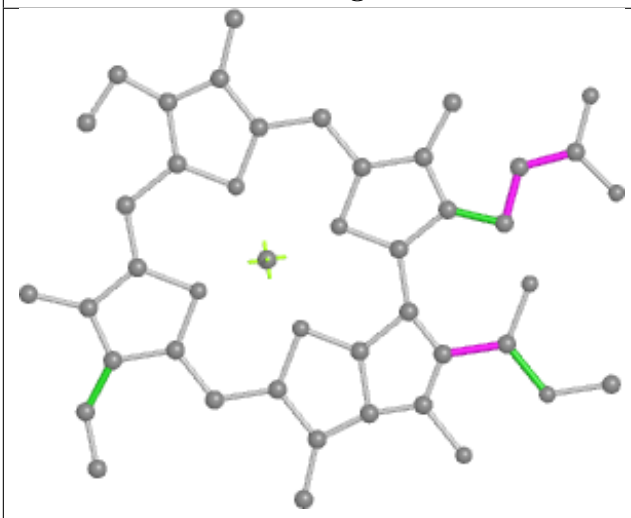
Ligand CLA B 834



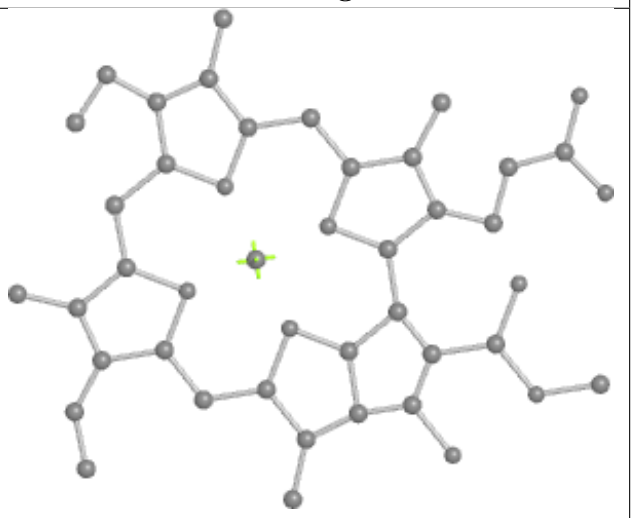
Bond lengths



Bond angles

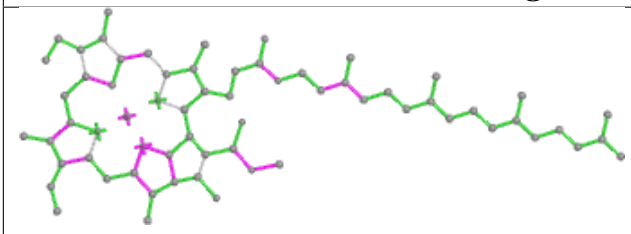


Torsions

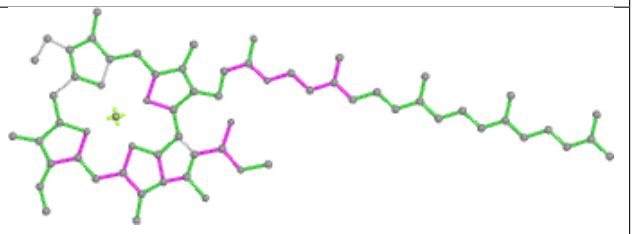


Rings

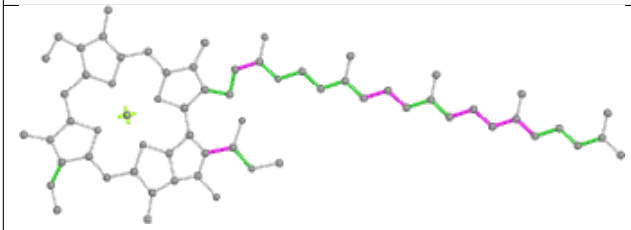
Ligand CLA B 824



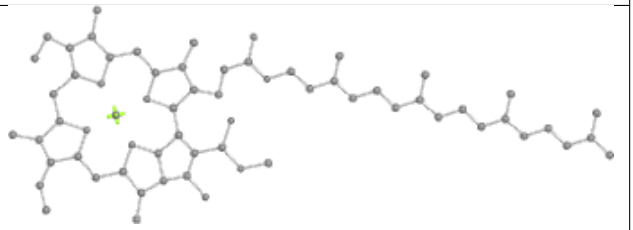
Bond lengths



Bond angles

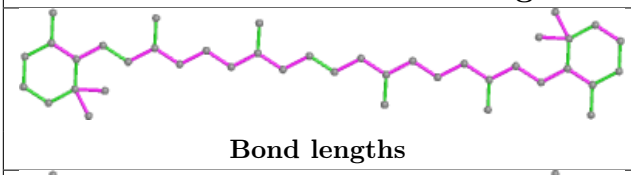


Torsions

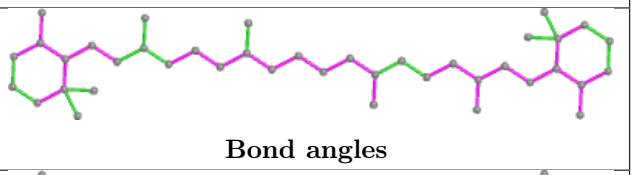


Rings

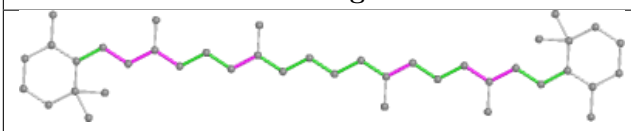
Ligand BCR L 1006



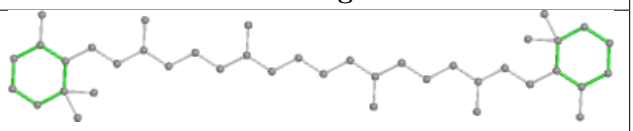
Bond lengths



Bond angles

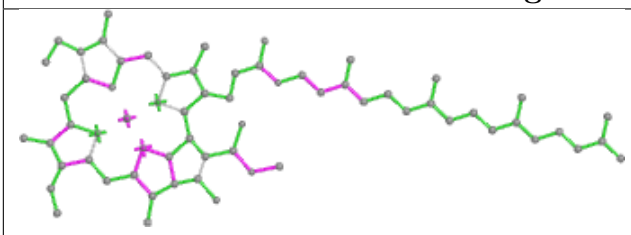


Torsions

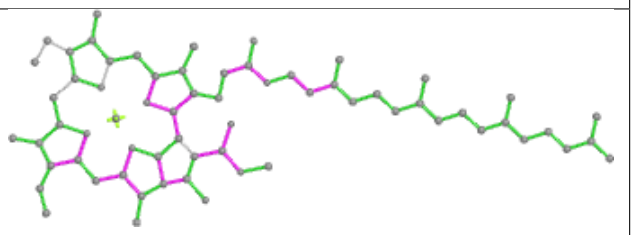


Rings

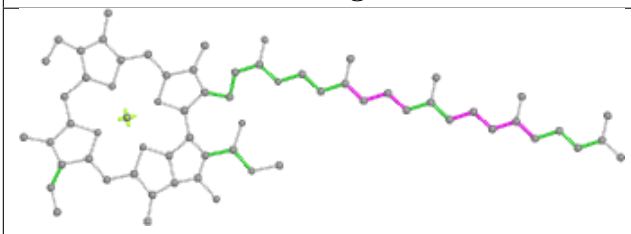
Ligand CLA B 811



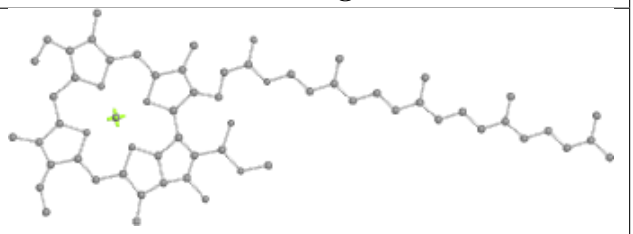
Bond lengths



Bond angles

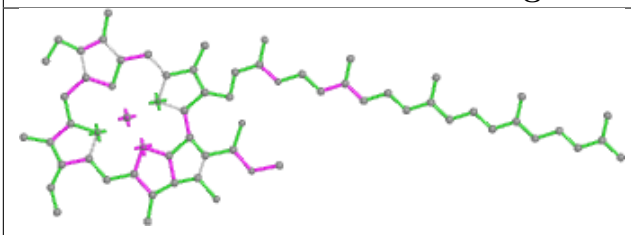


Torsions

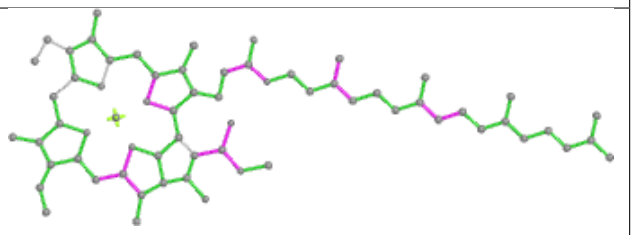


Rings

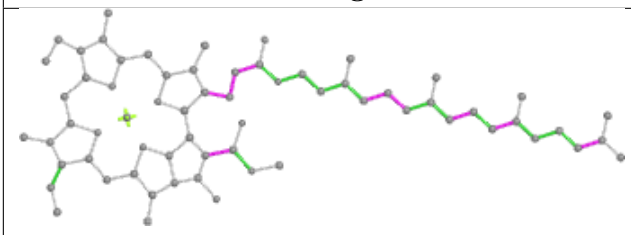
Ligand CLA A 834



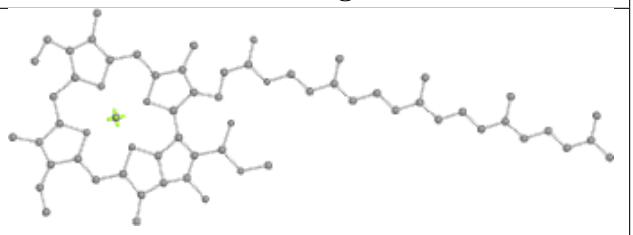
Bond lengths



Bond angles

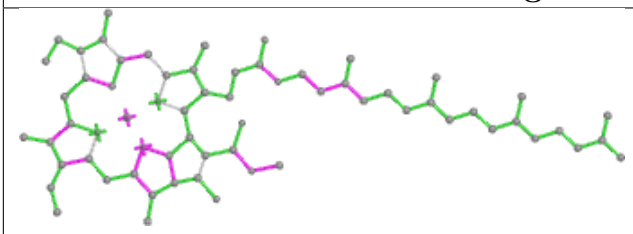


Torsions

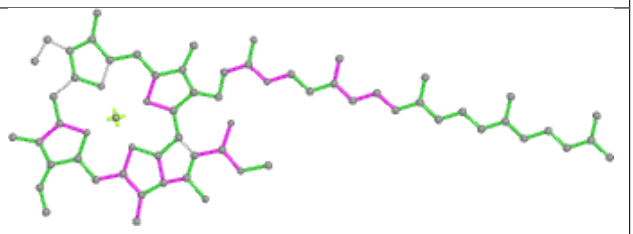


Rings

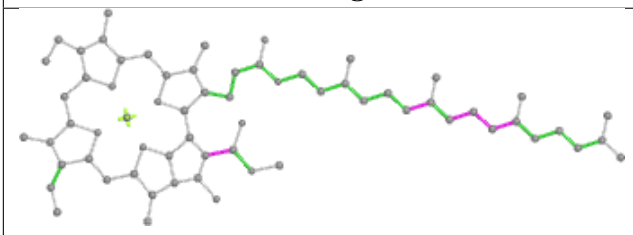
Ligand CLA B 827



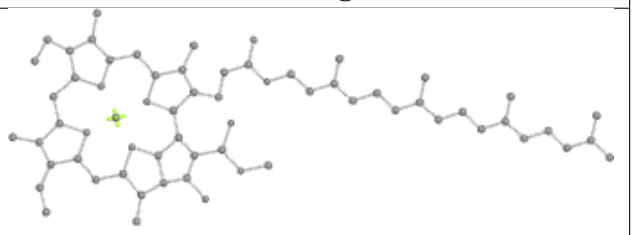
Bond lengths



Bond angles

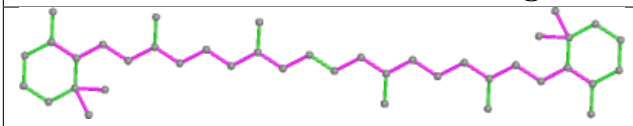


Torsions

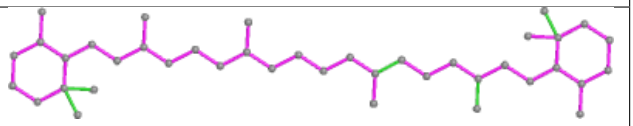


Rings

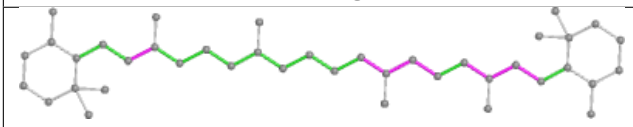
Ligand BCR B 843



Bond lengths



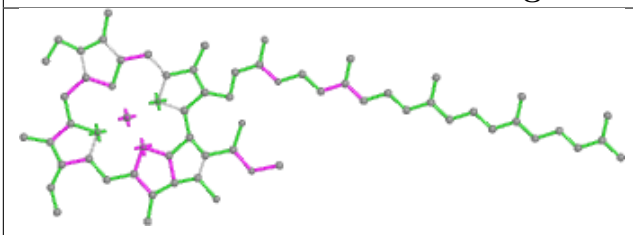
Bond angles



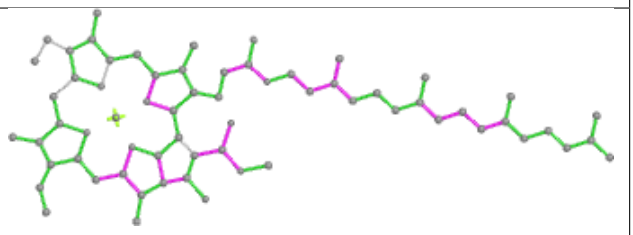
Torsions

Rings

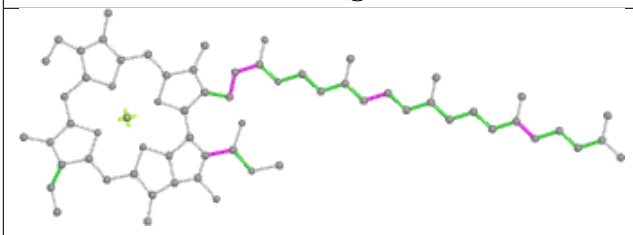
Ligand CLA A 806



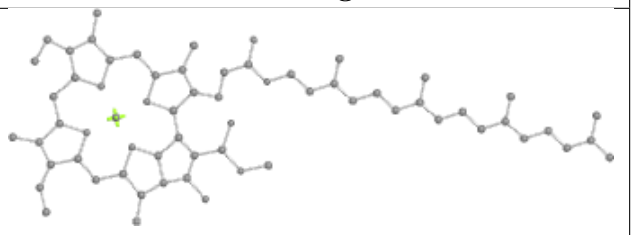
Bond lengths



Bond angles

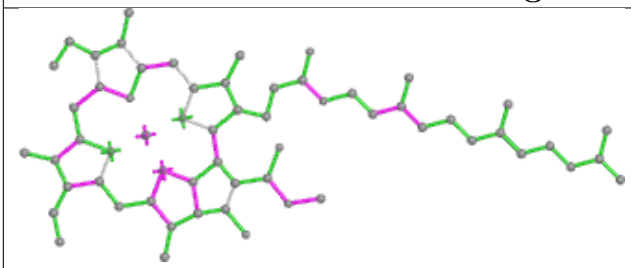


Torsions

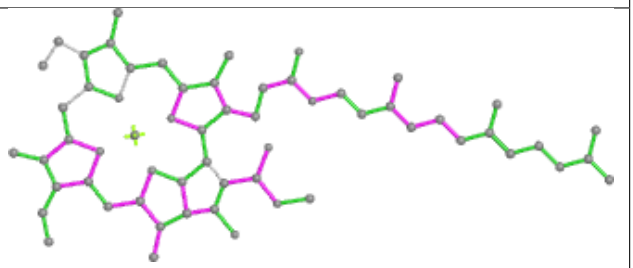


Rings

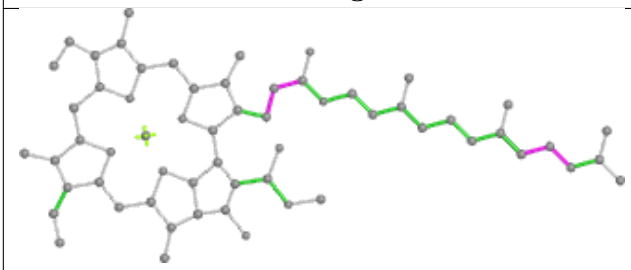
Ligand CLA B 816



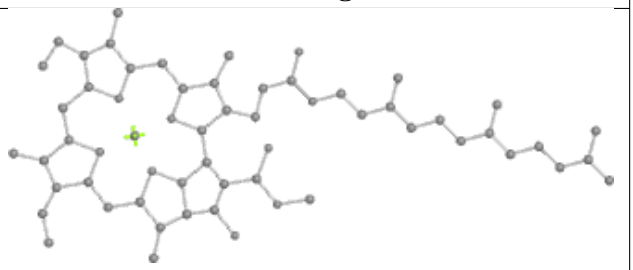
Bond lengths



Bond angles

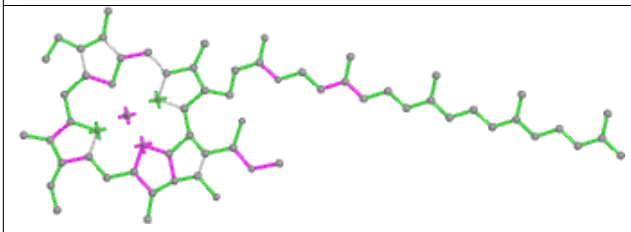


Torsions

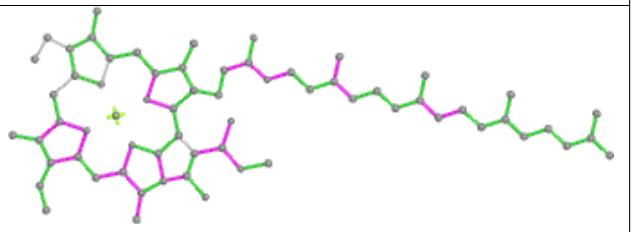


Rings

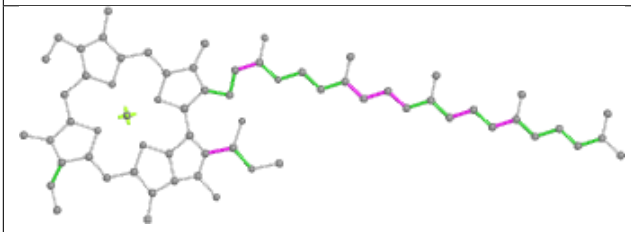
Ligand CLA A 830



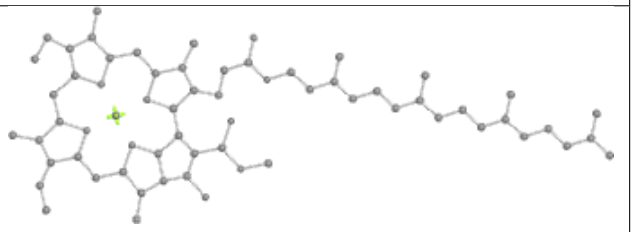
Bond lengths



Bond angles

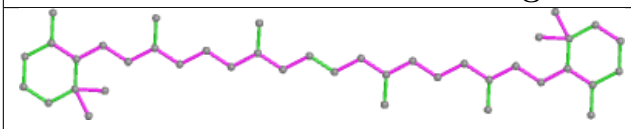


Torsions

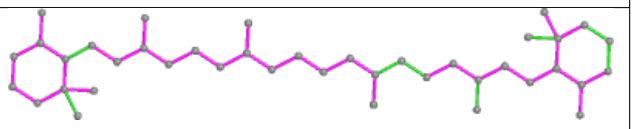


Rings

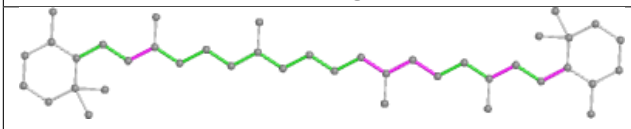
Ligand BCR B 850



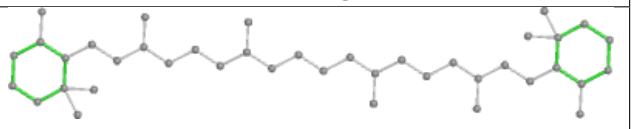
Bond lengths



Bond angles

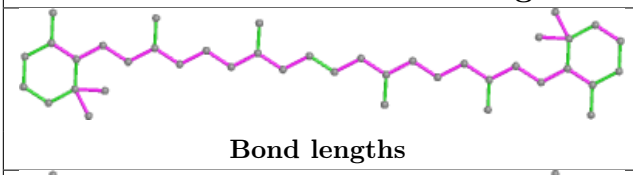


Torsions

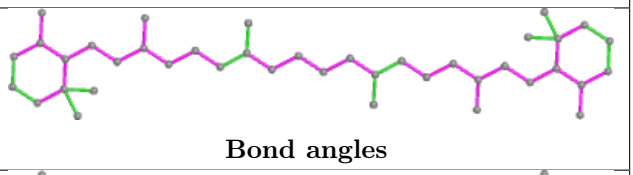


Rings

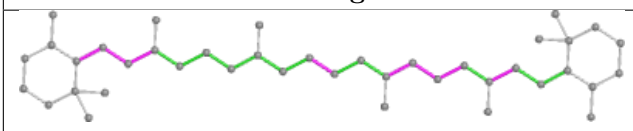
Ligand BCR F 1302



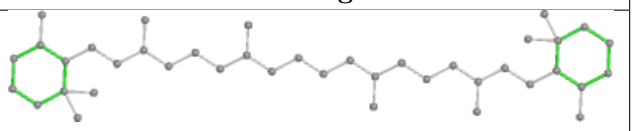
Bond lengths



Bond angles

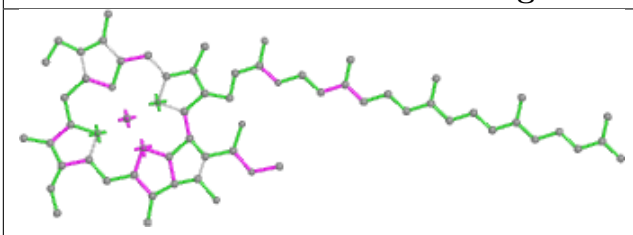


Torsions

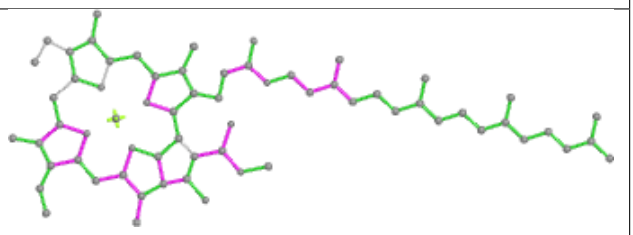


Rings

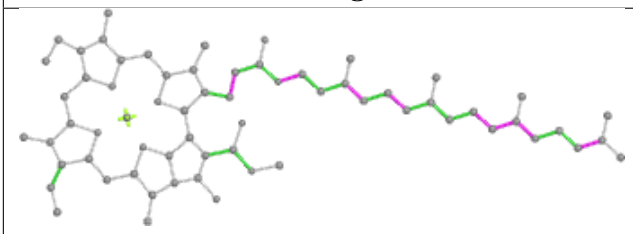
Ligand CLA L 1002



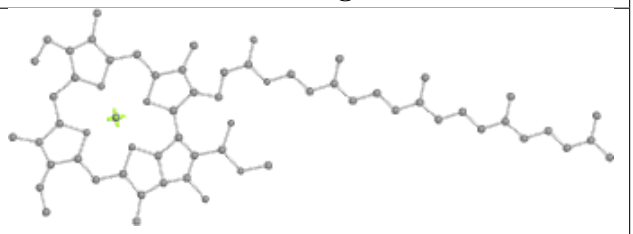
Bond lengths



Bond angles

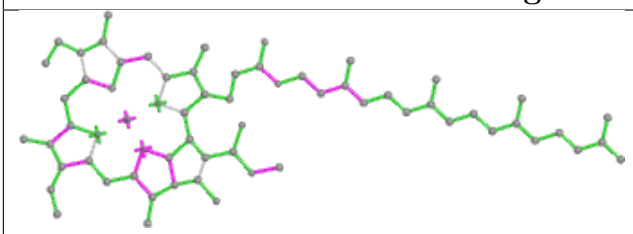


Torsions

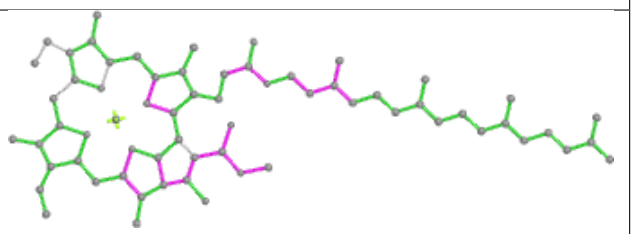


Rings

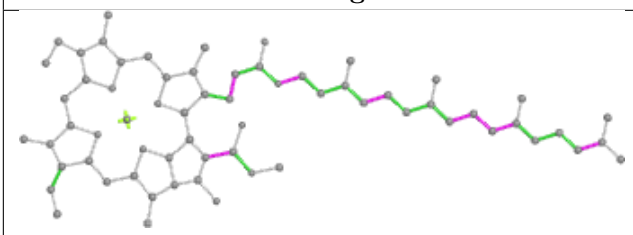
Ligand CLA A 808



Bond lengths



Bond angles



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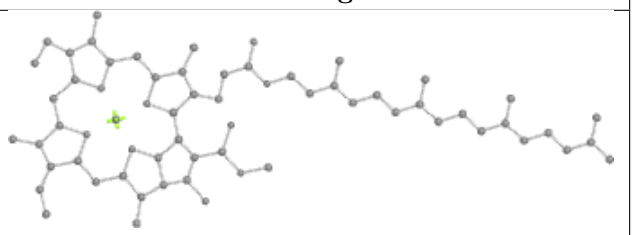
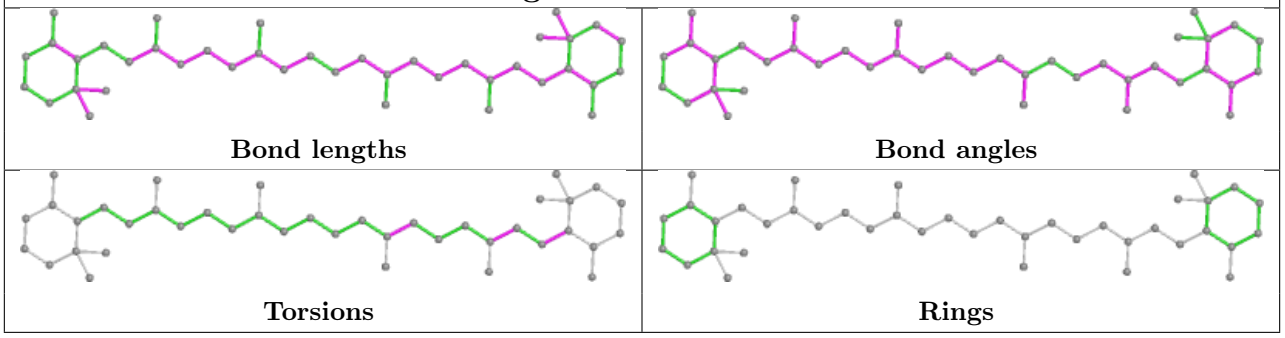
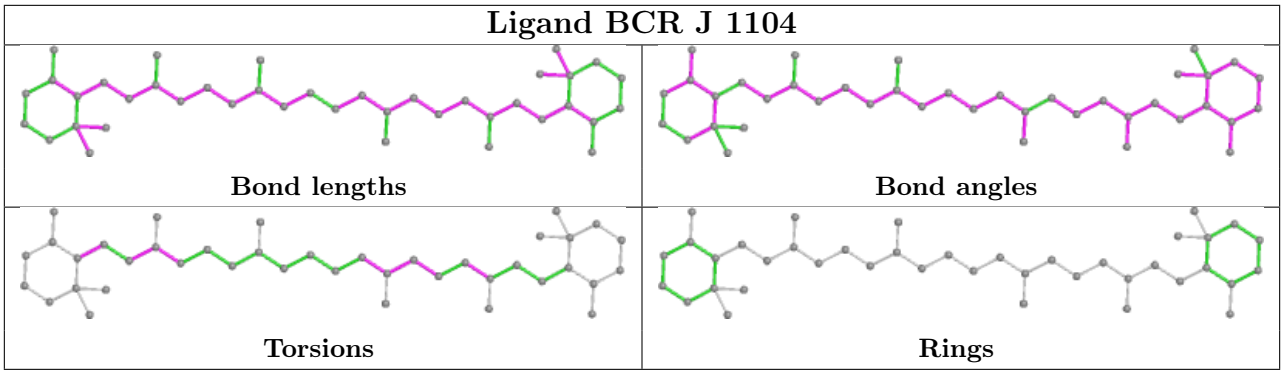


Rings

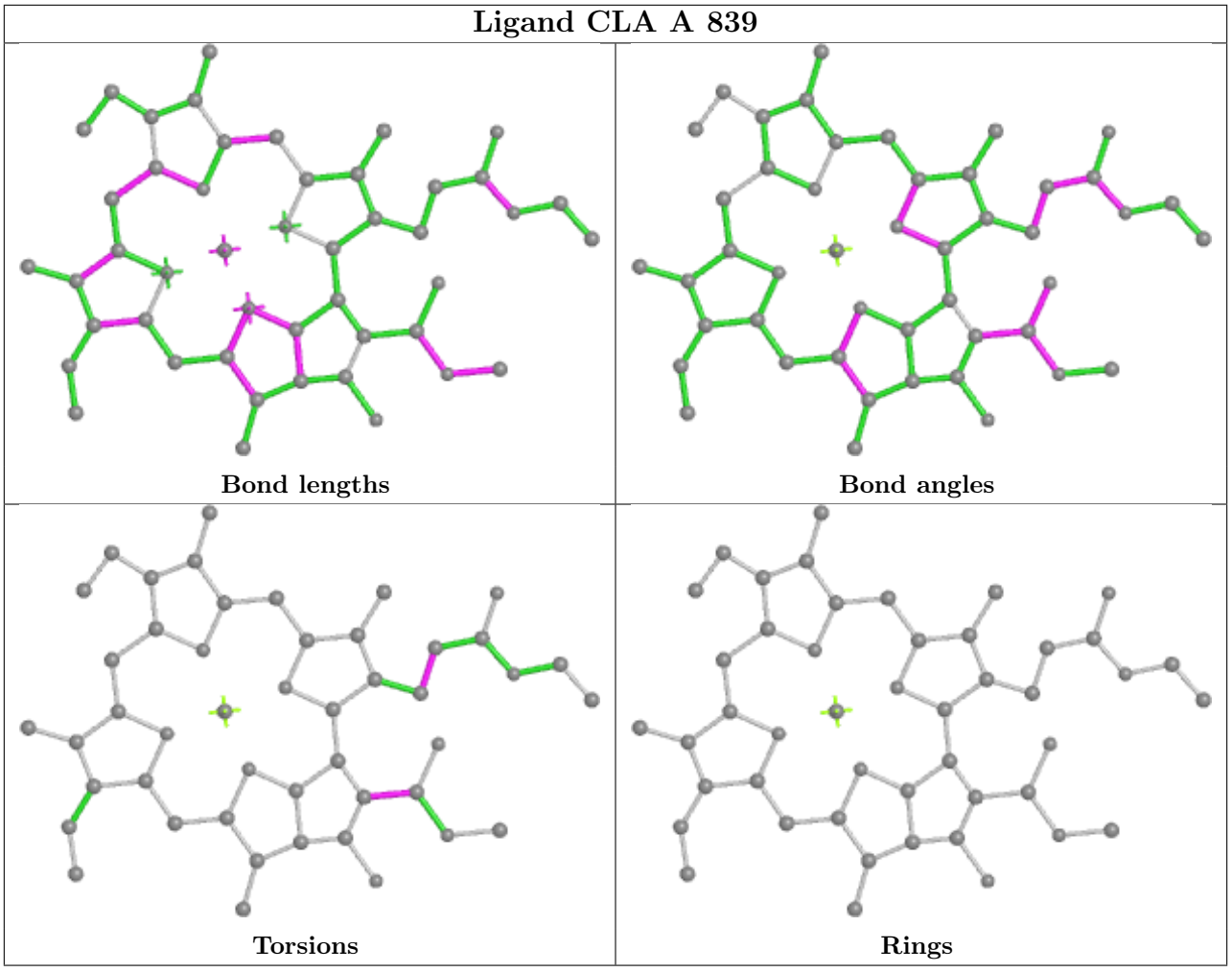
Ligand BCR A 850



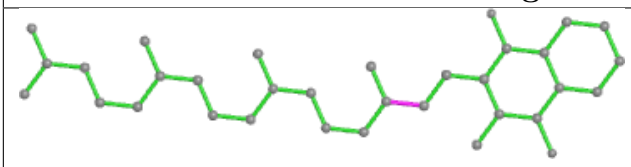
Ligand BCR J 1104



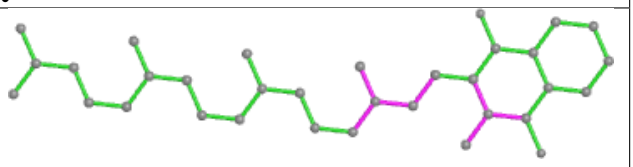
Ligand CLA A 839



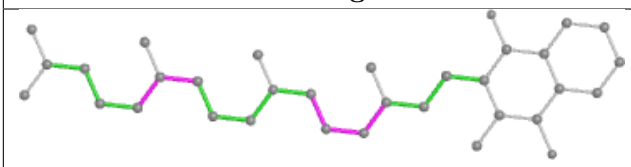
Ligand PQN B 840



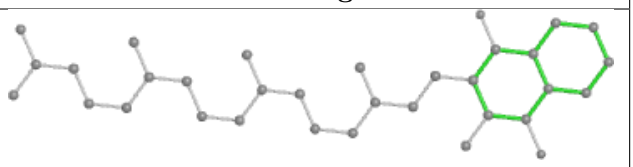
Bond lengths



Bond angles

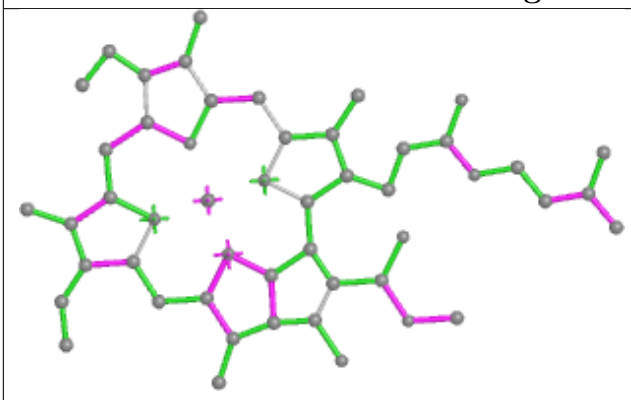


Torsions

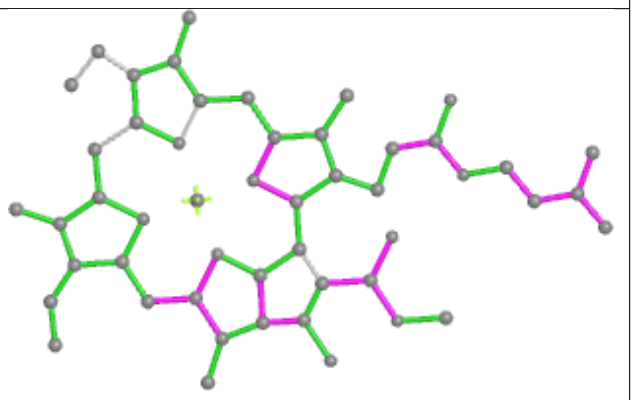


Rings

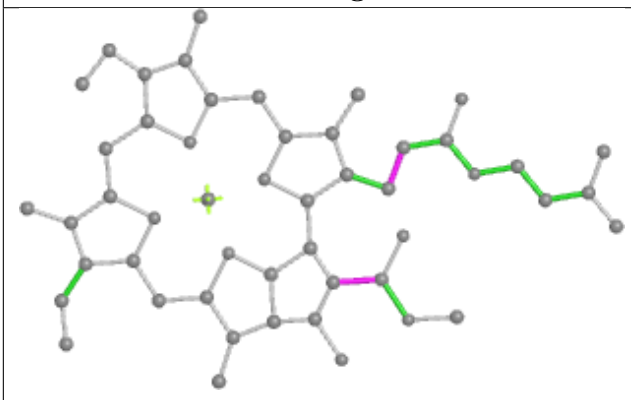
Ligand CLA A 831



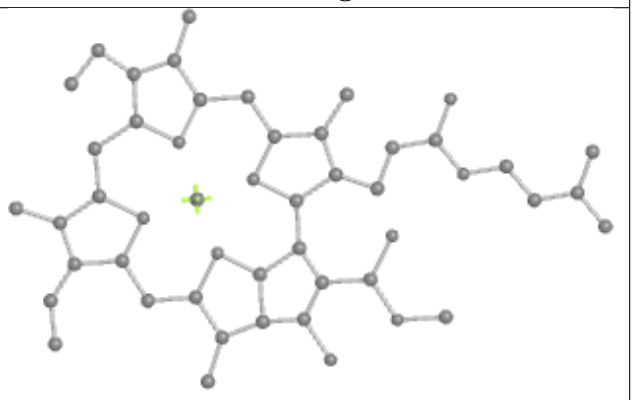
Bond lengths



Bond angles

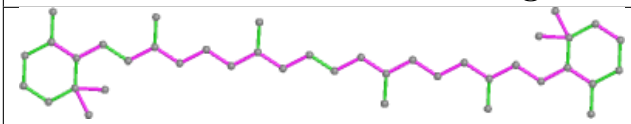


Torsions

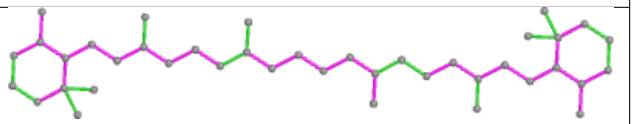


Rings

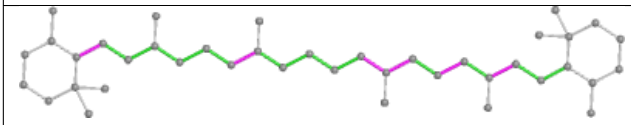
Ligand BCR A 851



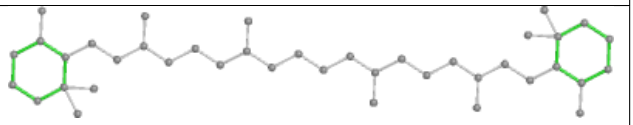
Bond lengths



Bond angles

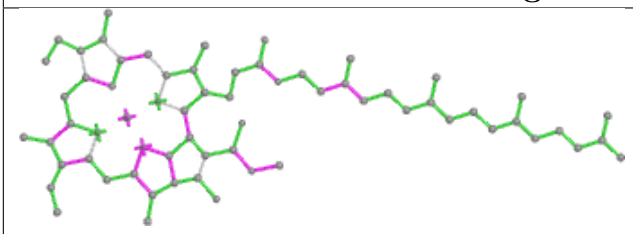


Torsions

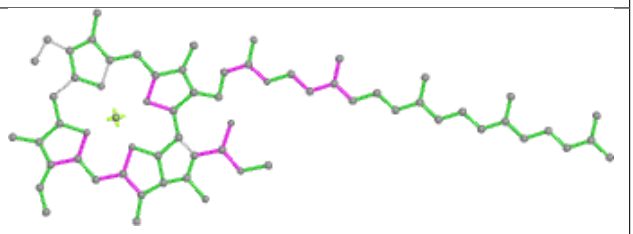


Rings

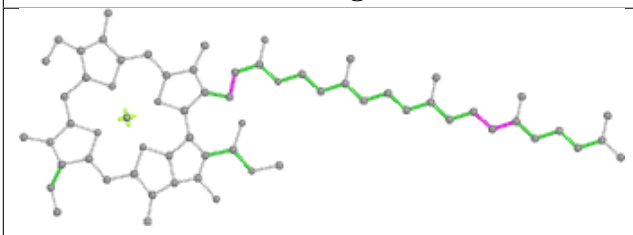
Ligand CLA A 802



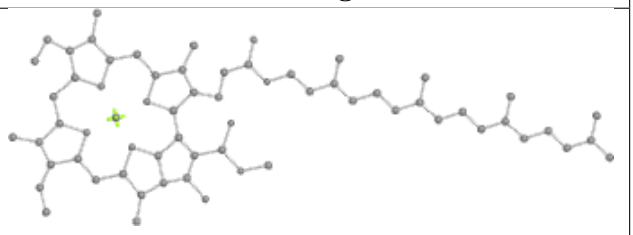
Bond lengths



Bond angles

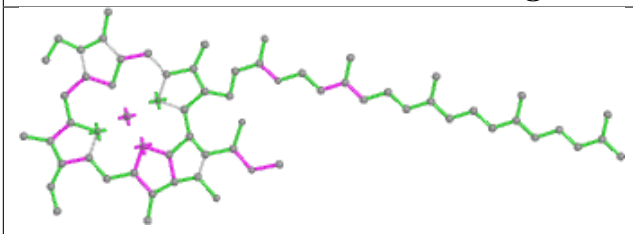


Torsions

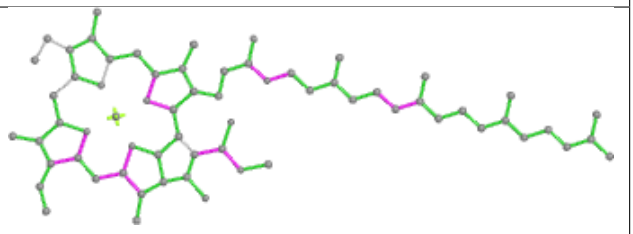


Rings

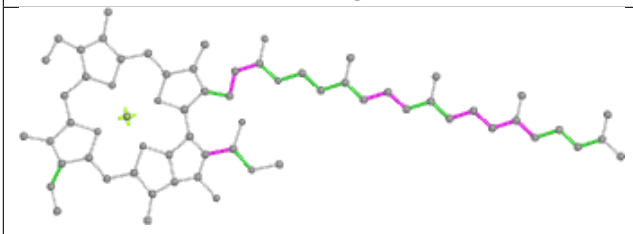
Ligand CLA B 826



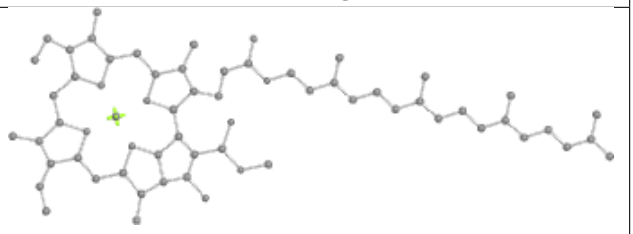
Bond lengths



Bond angles

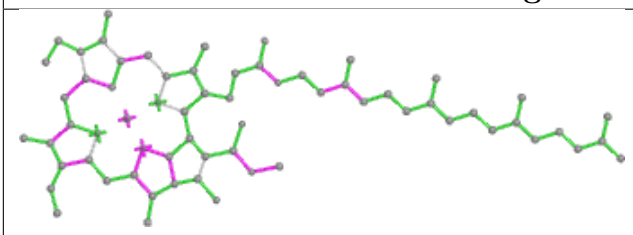


Torsions

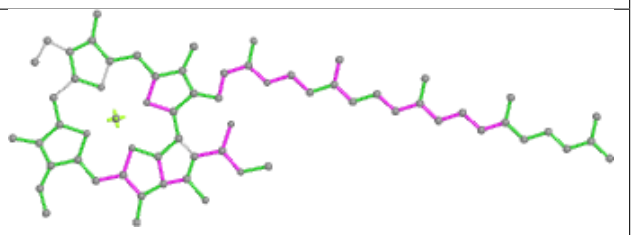


Rings

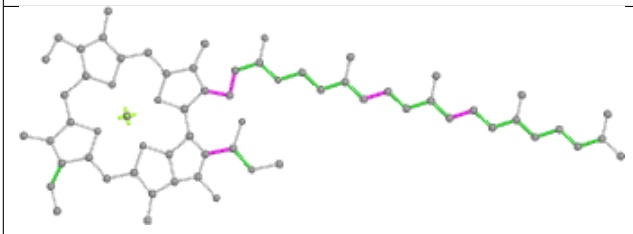
Ligand CLA A 843



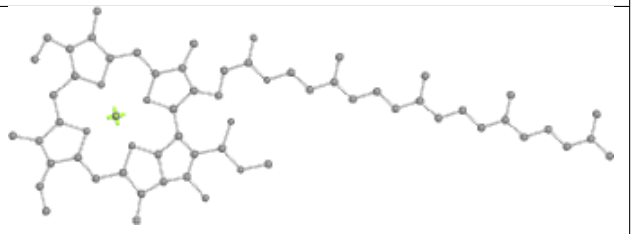
Bond lengths



Bond angles

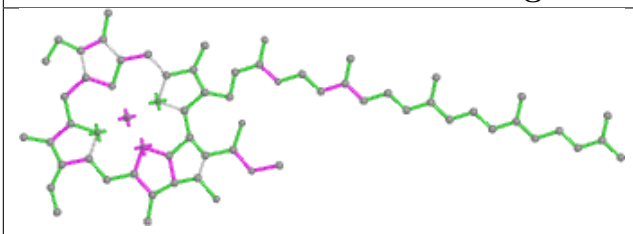


Torsions

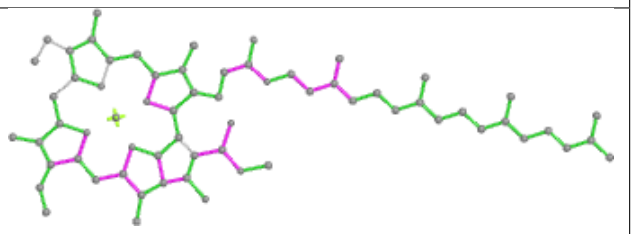


Rings

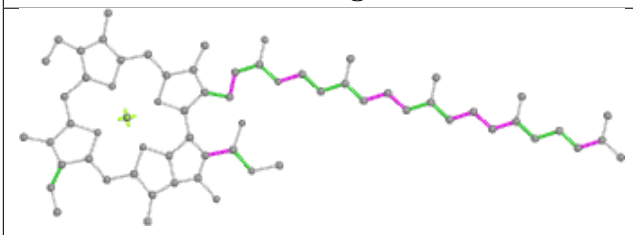
Ligand CLA B 803



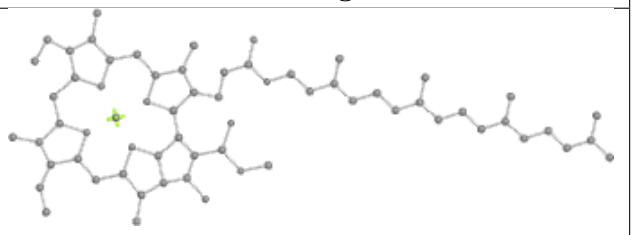
Bond lengths



Bond angles

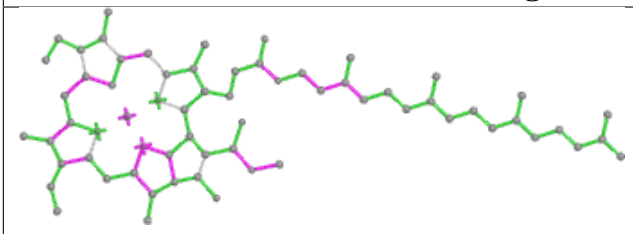


Torsions

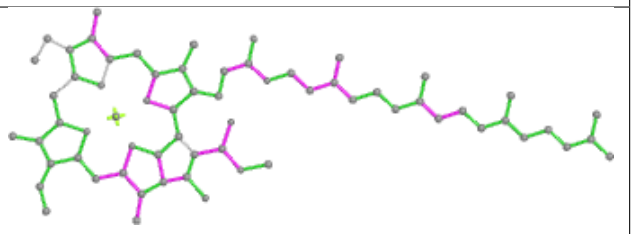


Rings

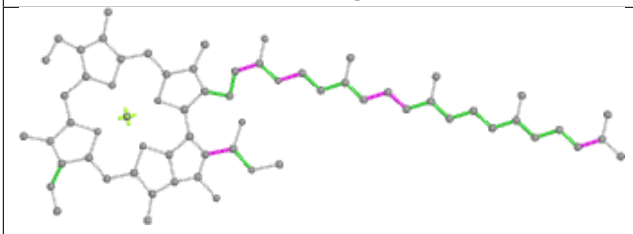
Ligand CLA A 801



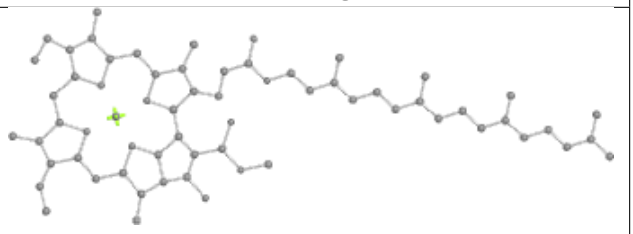
Bond lengths



Bond angles

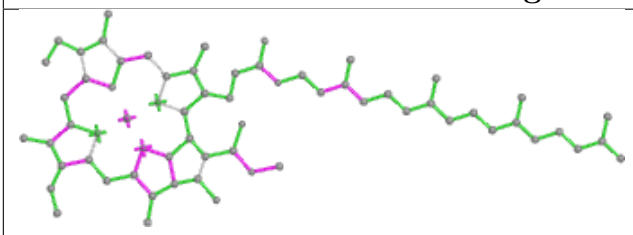


Torsions

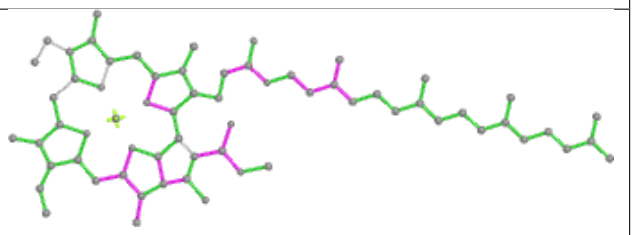


Rings

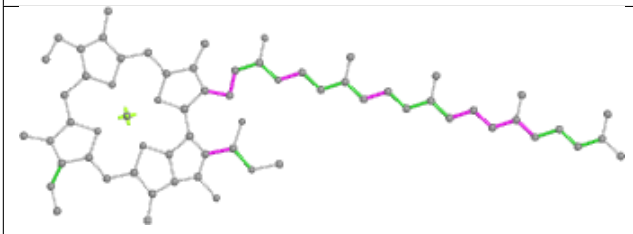
Ligand CLA A 811



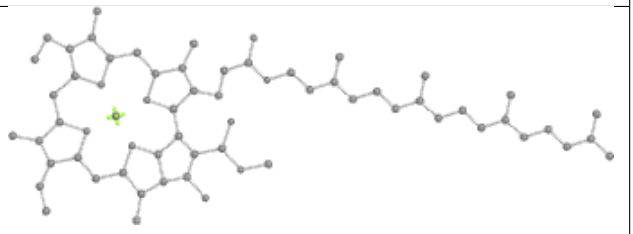
Bond lengths



Bond angles

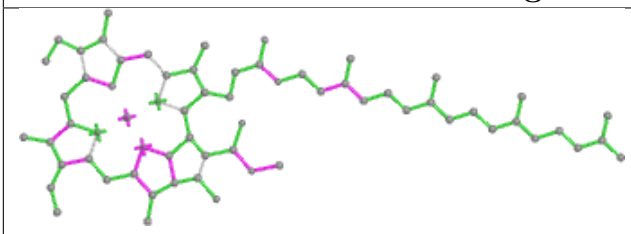


Torsions

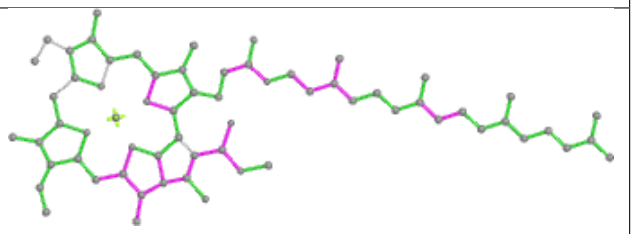


Rings

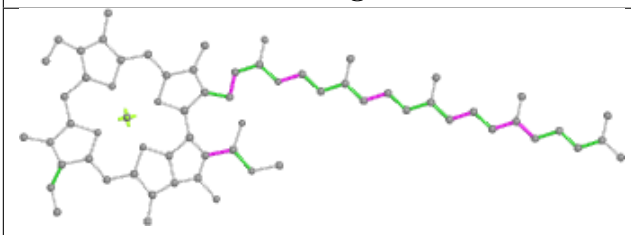
Ligand CLA B 802



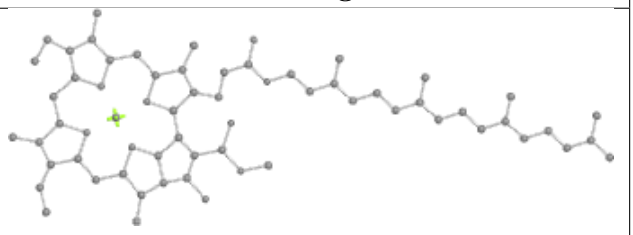
Bond lengths



Bond angles

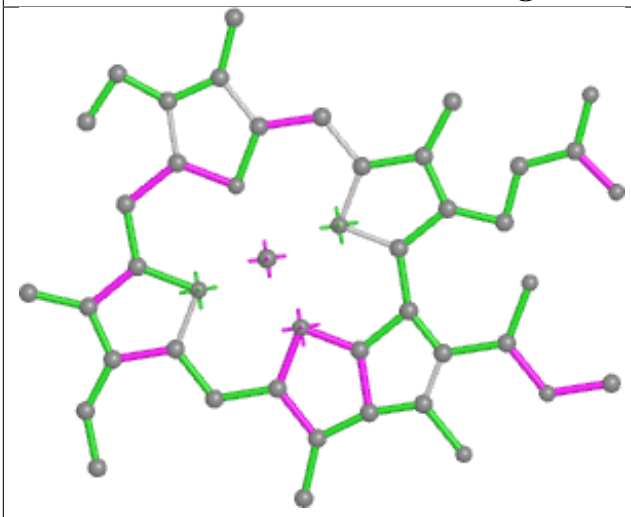


Torsions

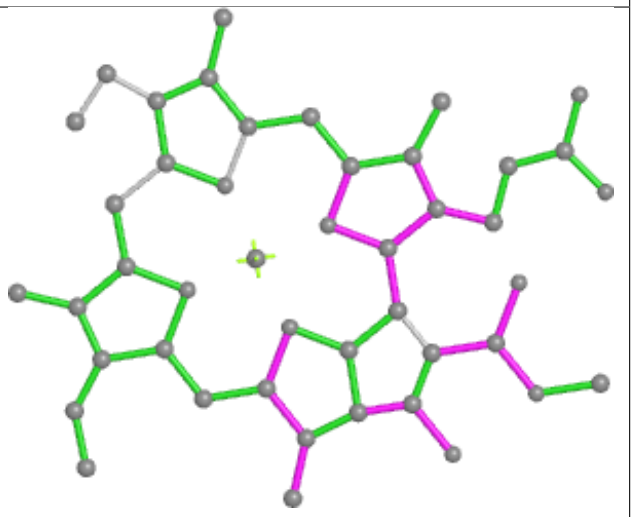


Rings

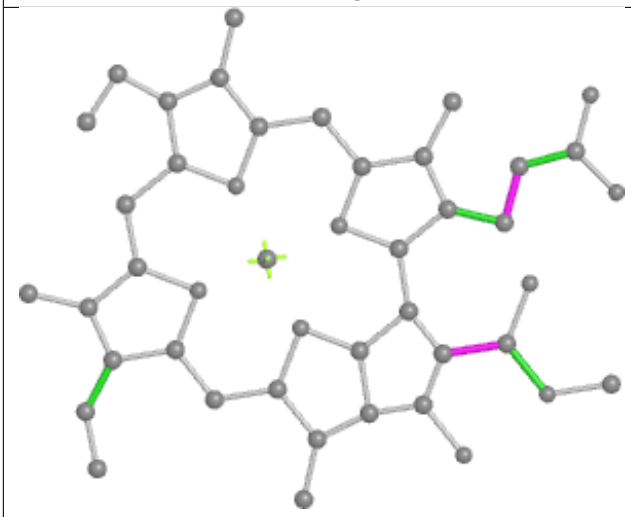
Ligand CLA F 1301



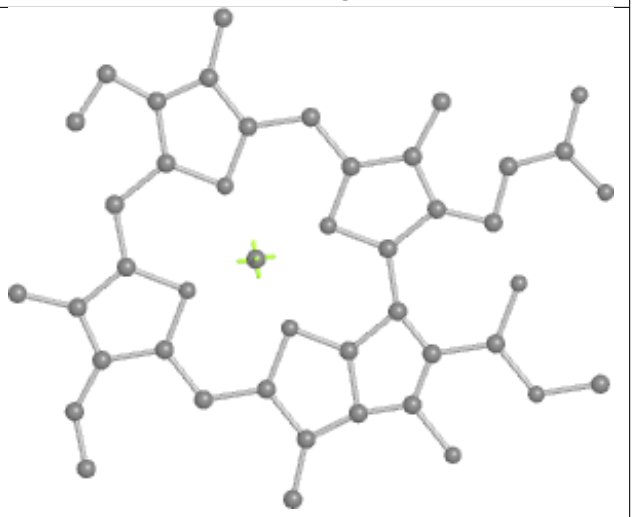
Bond lengths



Bond angles

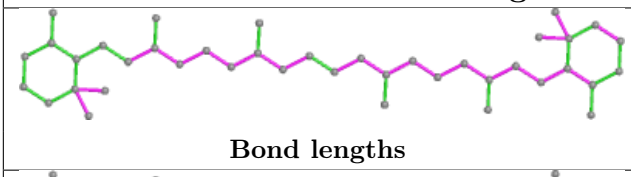


Torsions

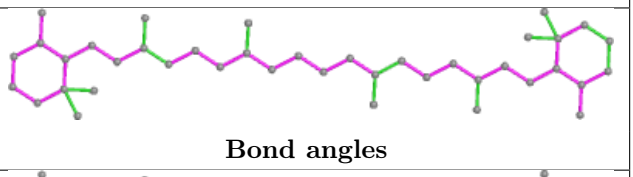


Rings

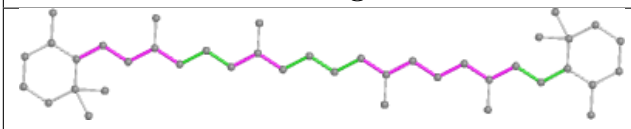
Ligand BCR M 1203



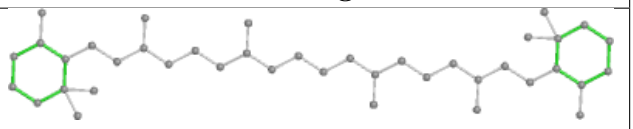
Bond lengths



Bond angles

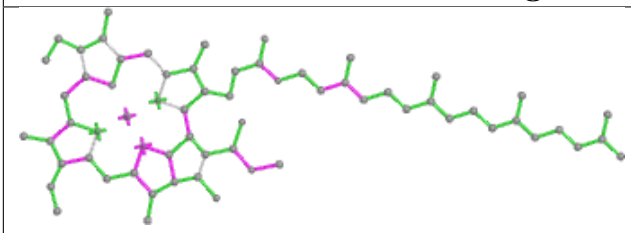


Torsions

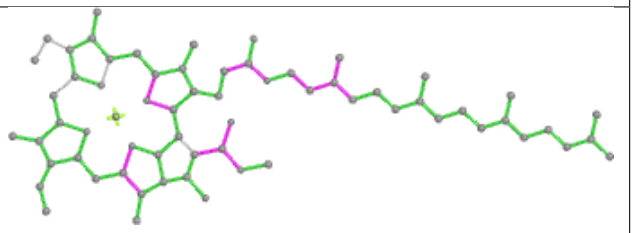


Rings

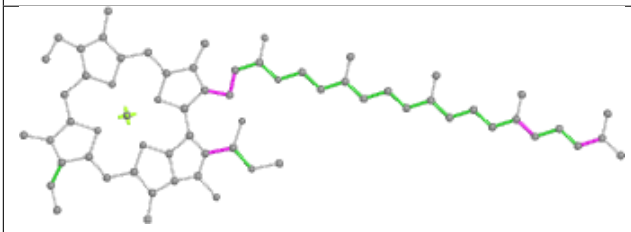
Ligand CLA B 817



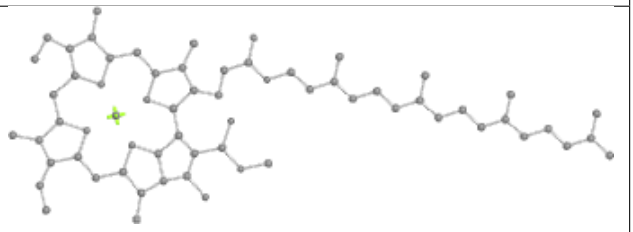
Bond lengths



Bond angles

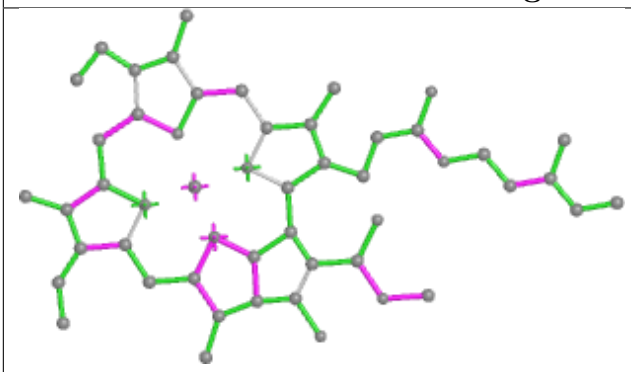


Torsions

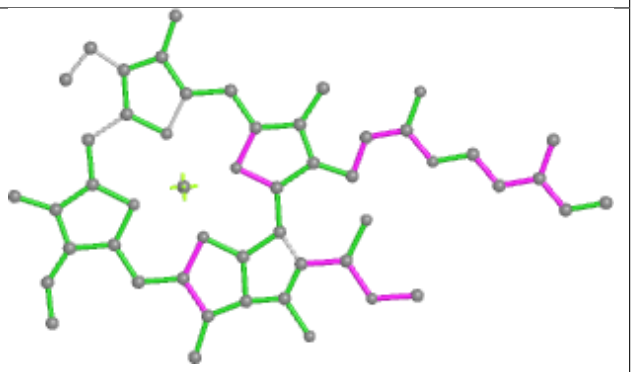


Rings

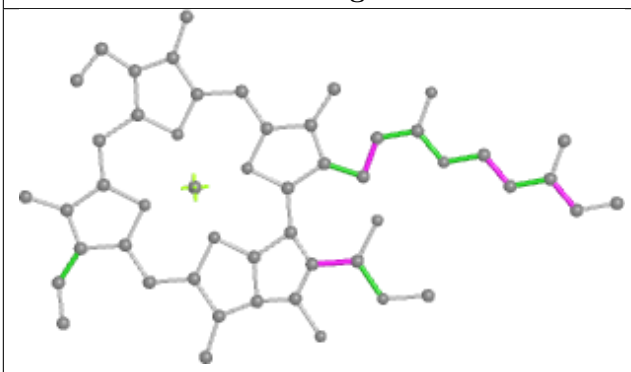
Ligand CLA A 823



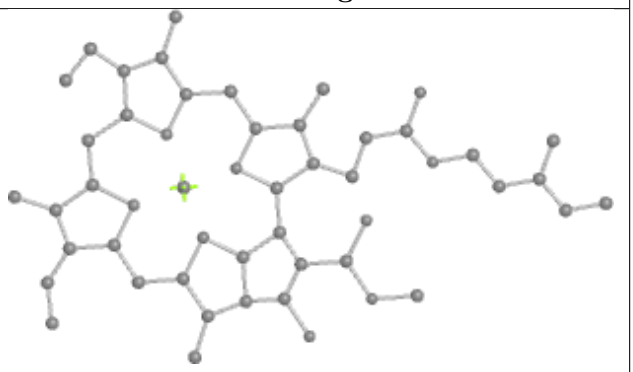
Bond lengths



Bond angles

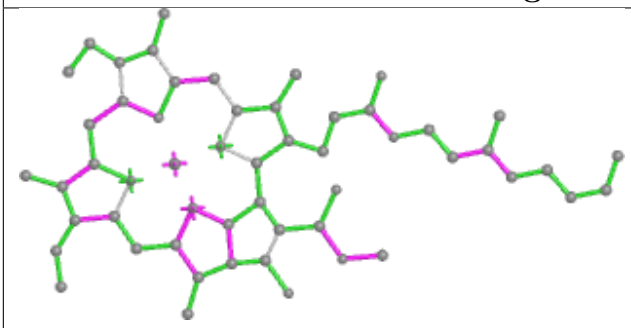


Torsions

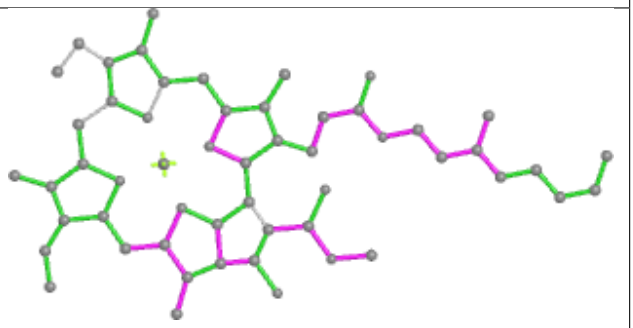


Rings

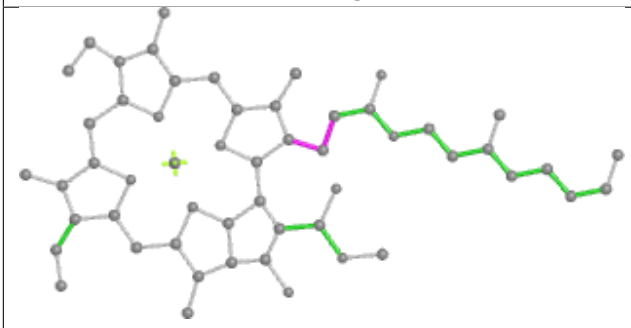
Ligand CLA A 817



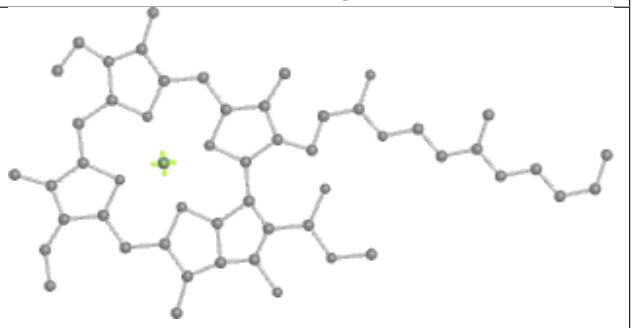
Bond lengths



Bond angles

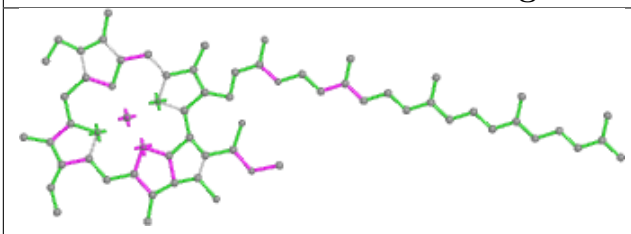


Torsions



Rings

Ligand CLA J 1101



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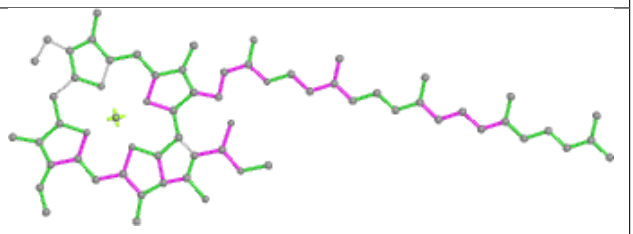
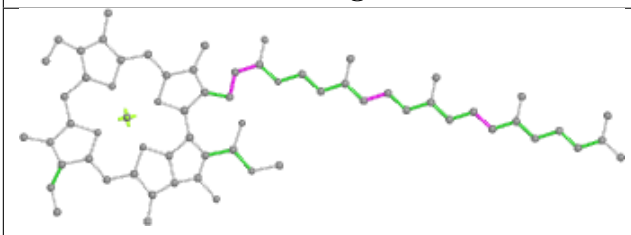
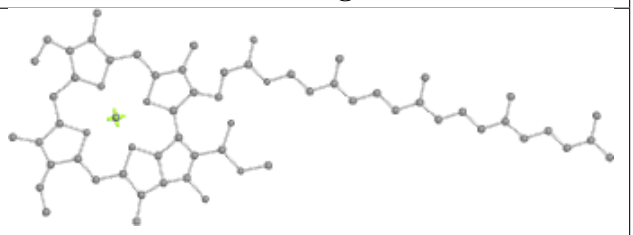


Bond angles

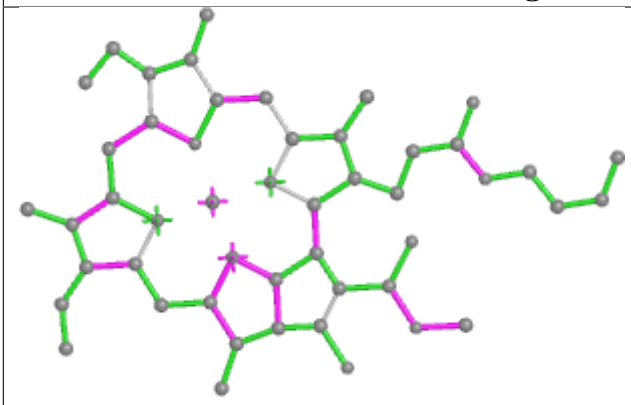


Torsions

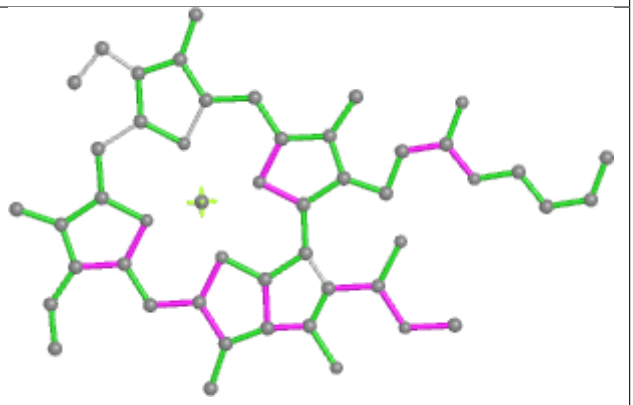


Rings

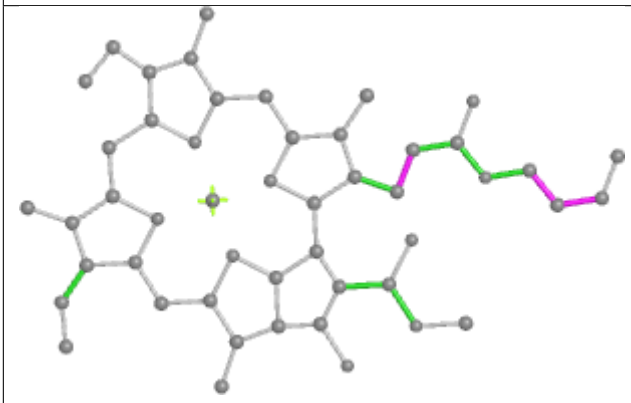
Ligand CLA A 816



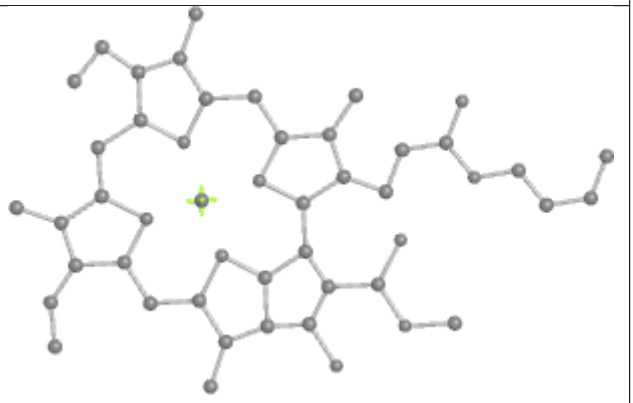
Bond lengths



Bond angles

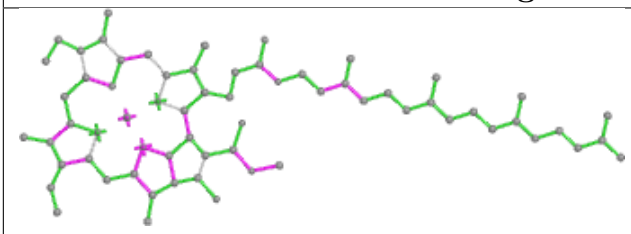


Torsions

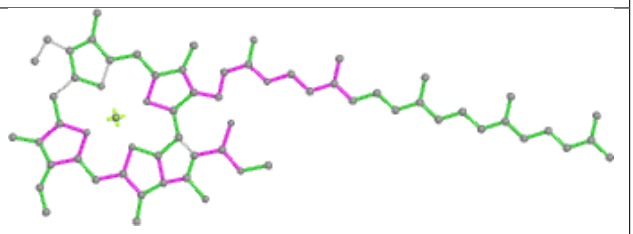


Rings

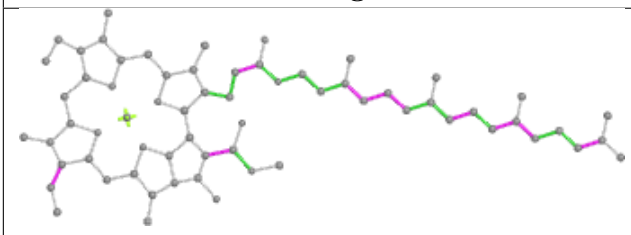
Ligand CLA L 1003



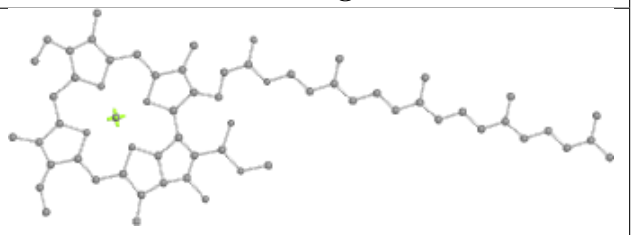
Bond lengths



Bond angles

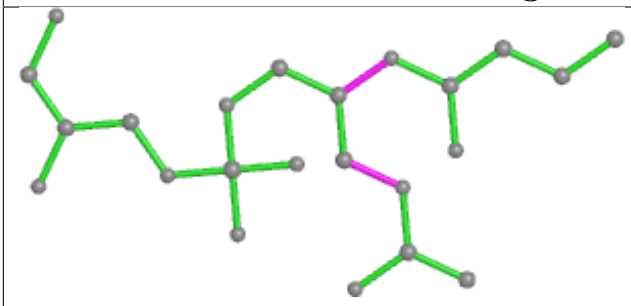


Torsions

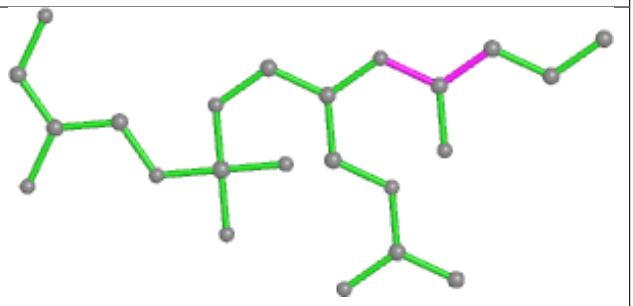


Rings

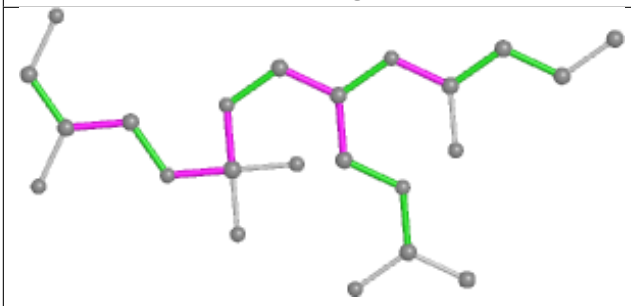
Ligand LHG X 101



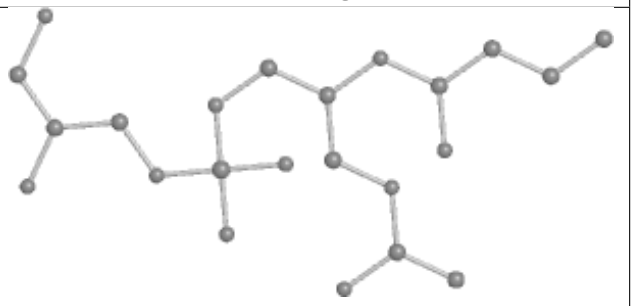
Bond lengths



Bond angles

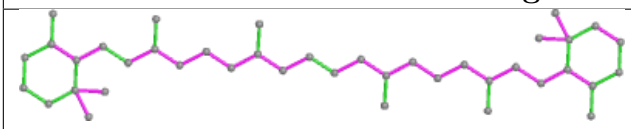


Torsions

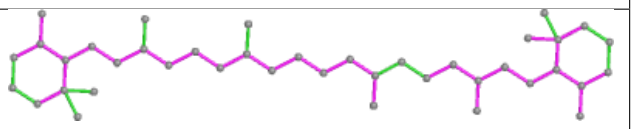


Rings

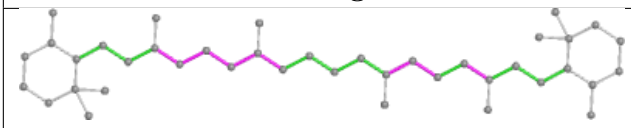
Ligand BCR B 846



Bond lengths



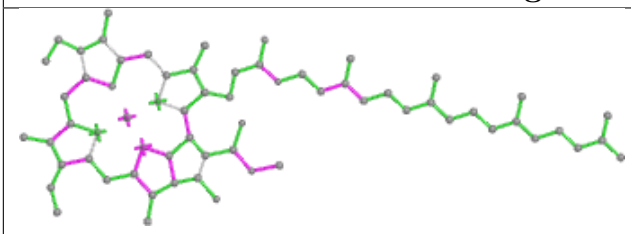
Bond angles



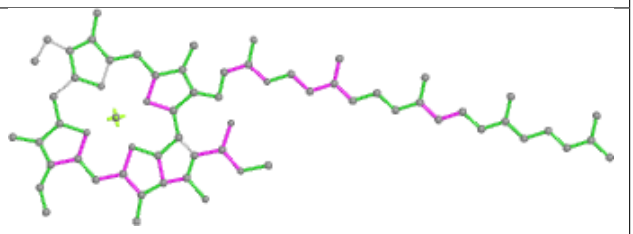
Torsions

Rings

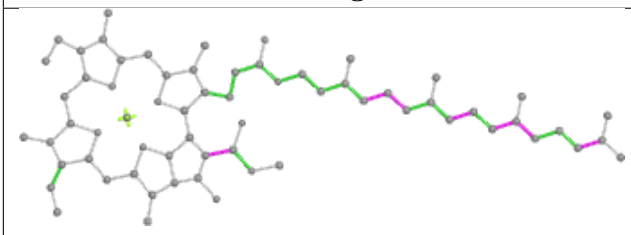
Ligand CLA B 801



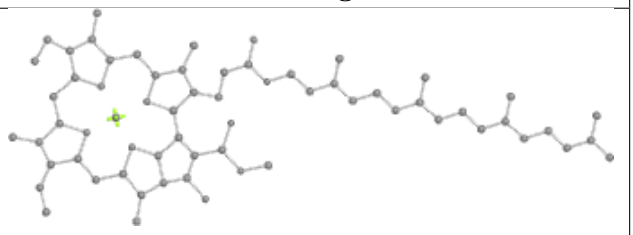
Bond lengths



Bond angles

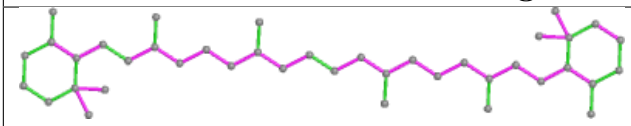


Torsions

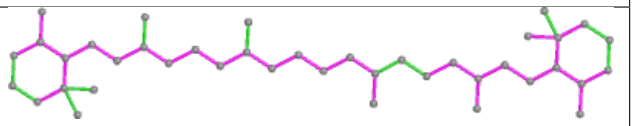


Rings

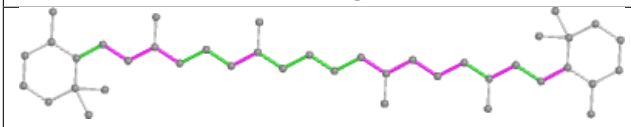
Ligand BCR J 1105



Bond lengths



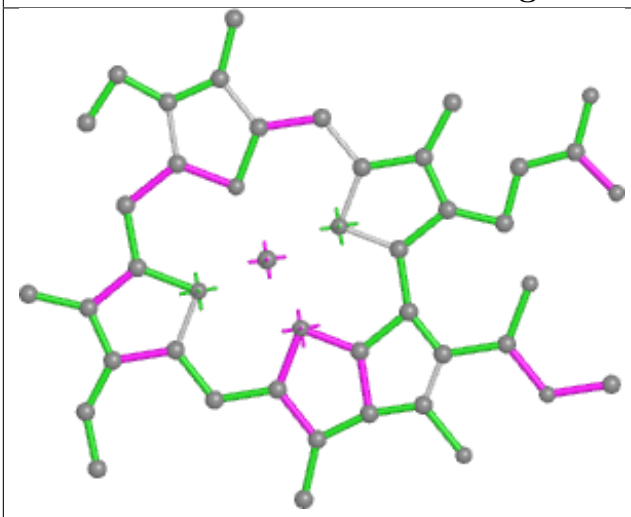
Bond angles



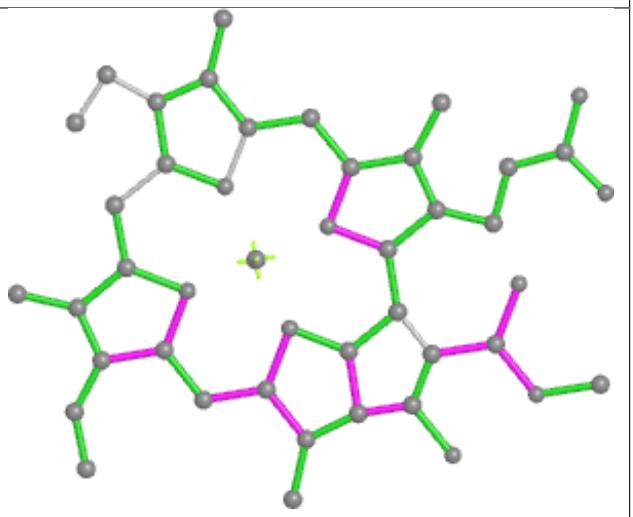
Torsions

Rings

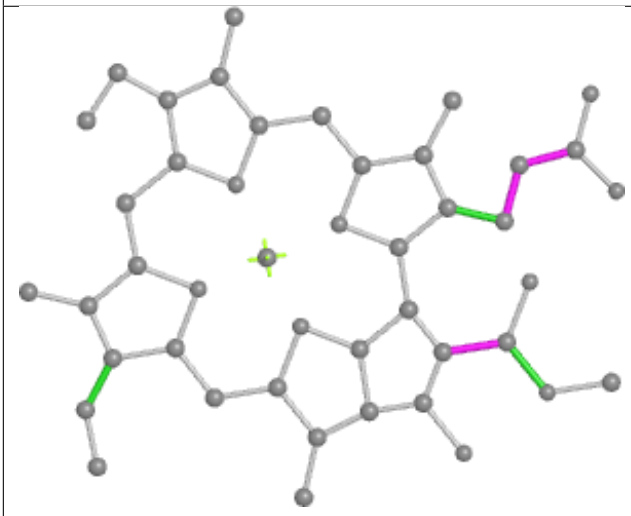
Ligand CLA J 1102



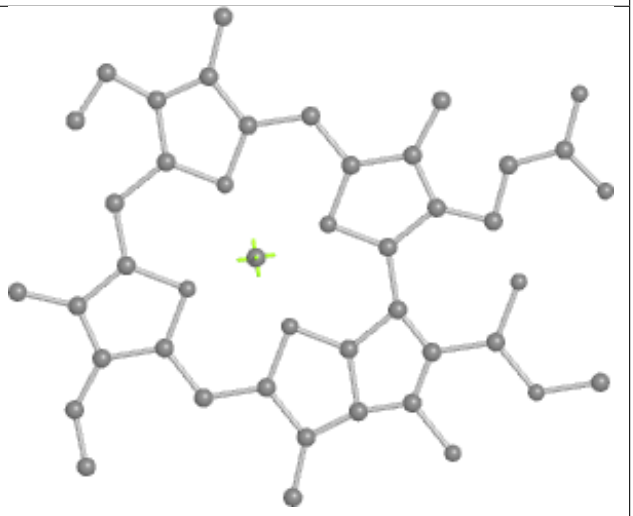
Bond lengths



Bond angles

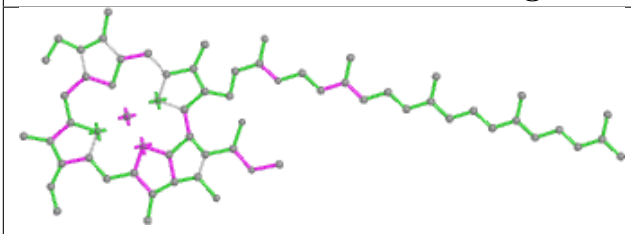


Torsions

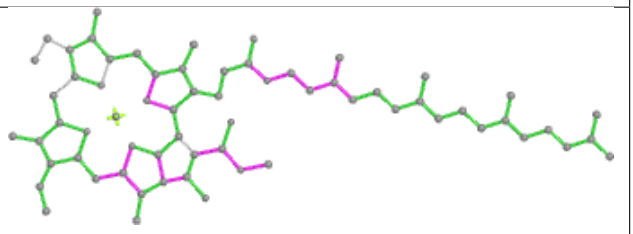


Rings

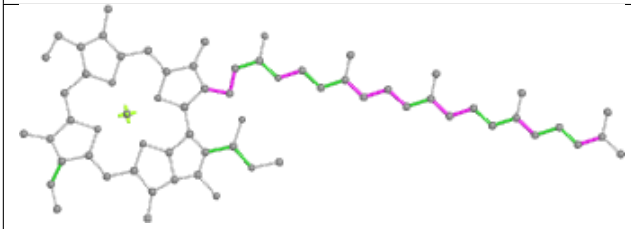
Ligand CLA A 842



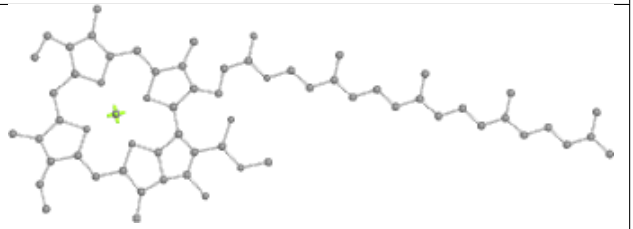
Bond lengths



Bond angles

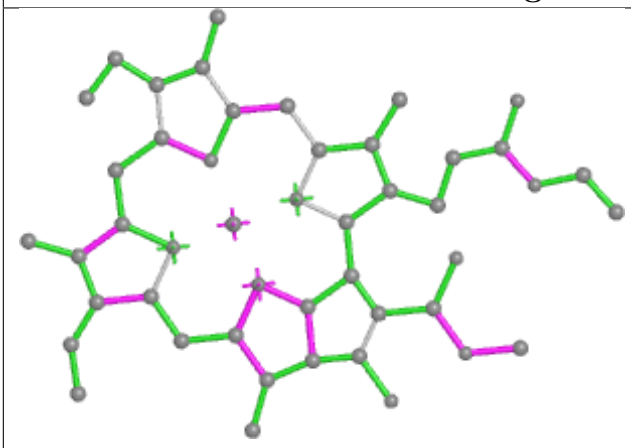


Torsions

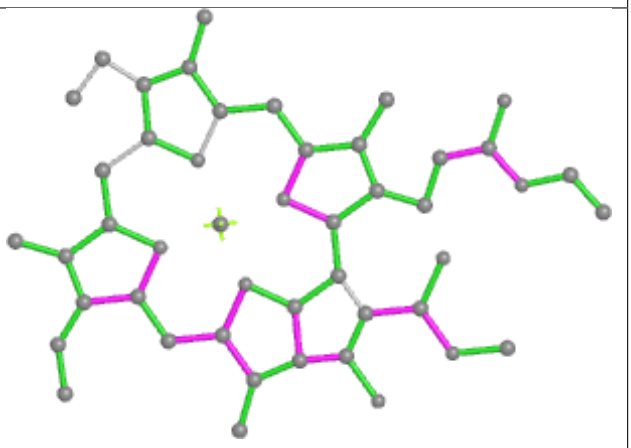


Rings

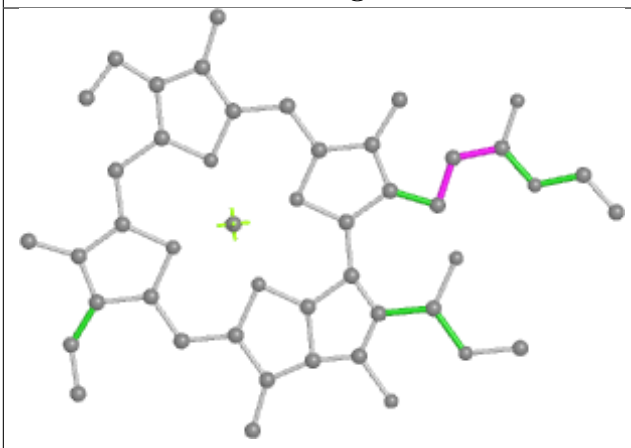
Ligand CLA B 818



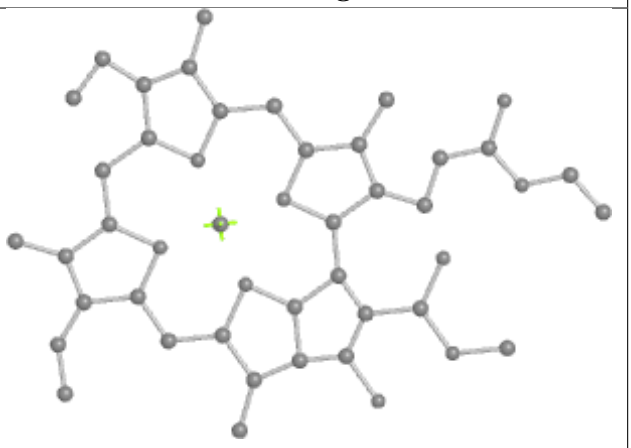
Bond lengths



Bond angles

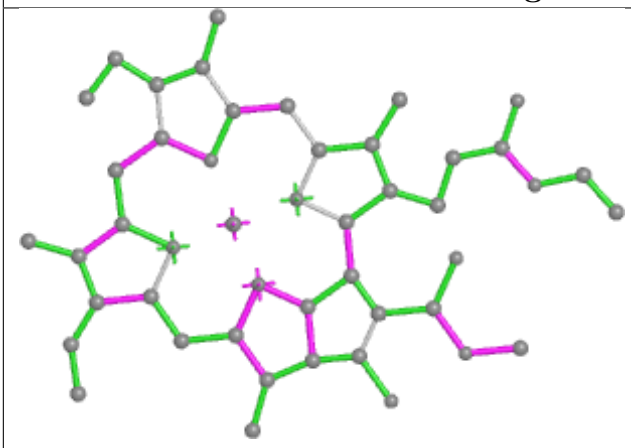


Torsions

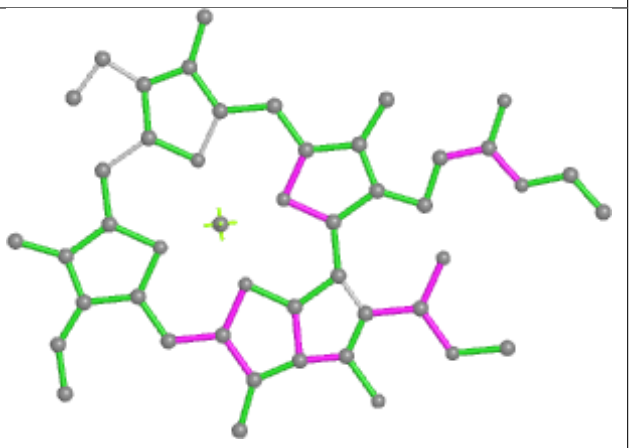


Rings

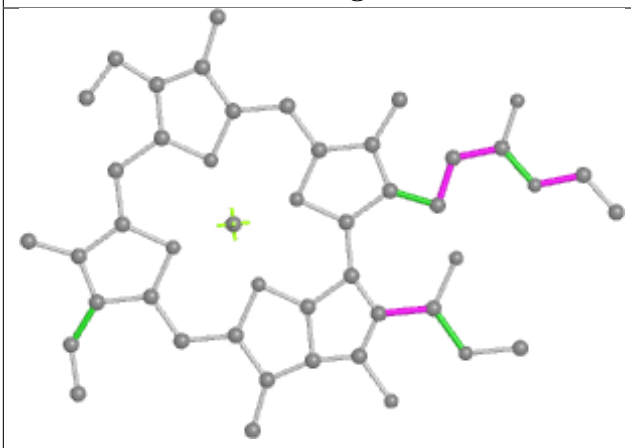
Ligand CLA B 837



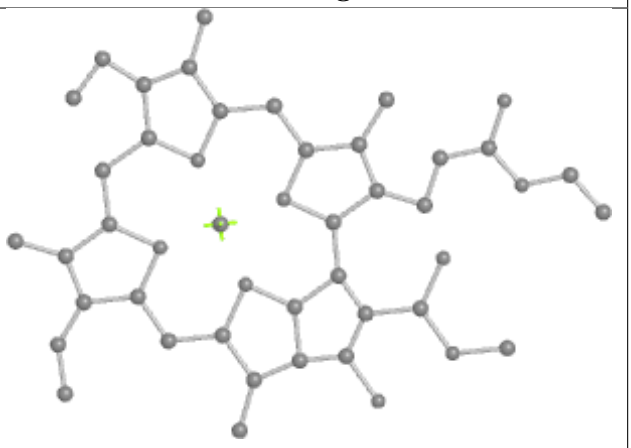
Bond lengths



Bond angles

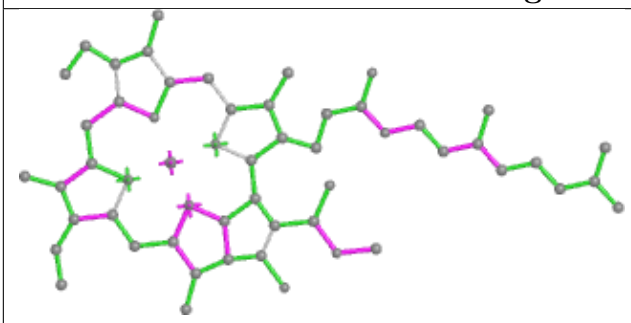


Torsions

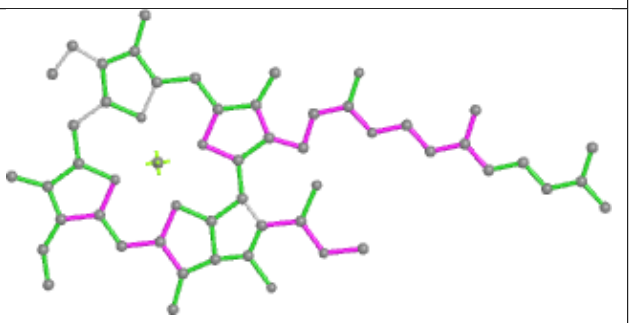


Rings

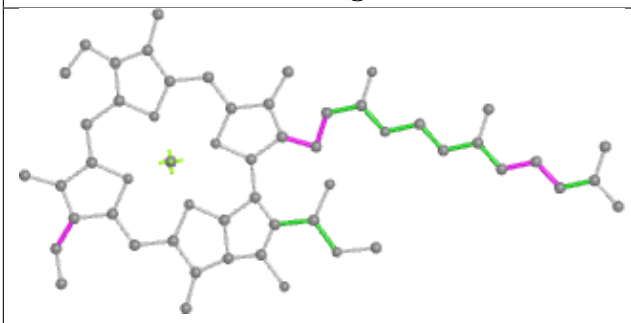
Ligand CLA B 820



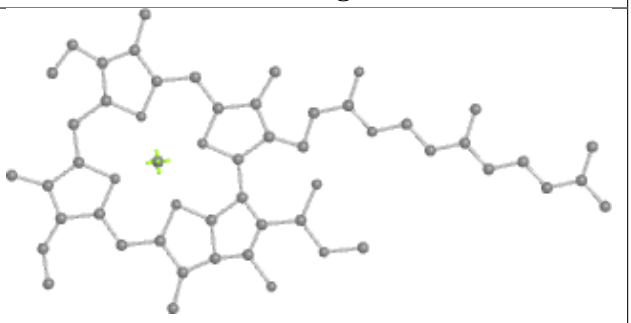
Bond lengths



Bond angles

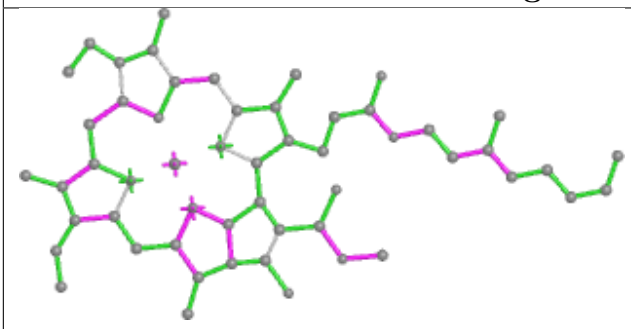


Torsions

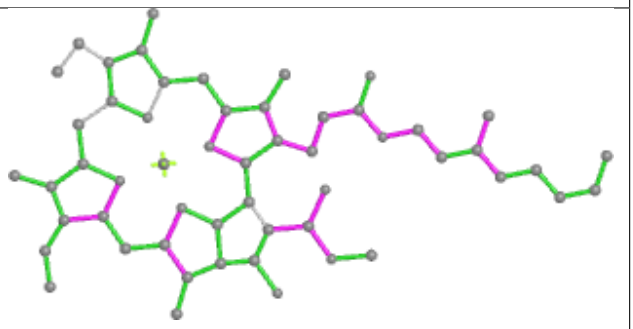


Rings

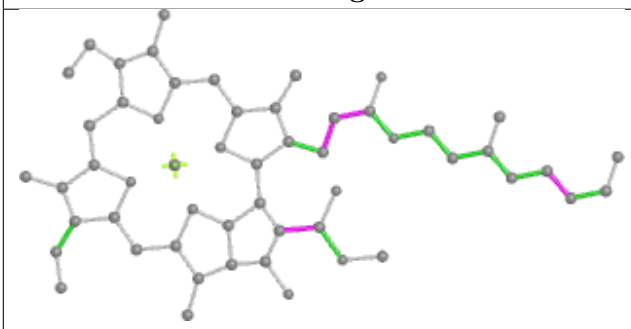
Ligand CLA A 818



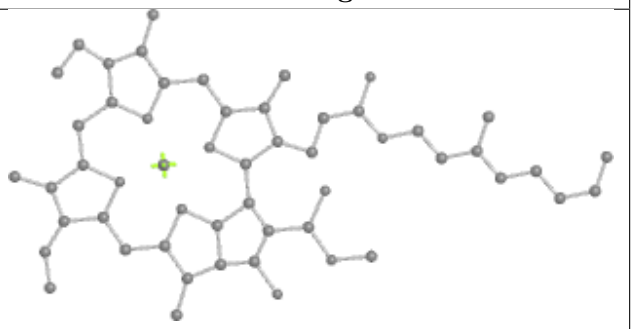
Bond lengths



Bond angles

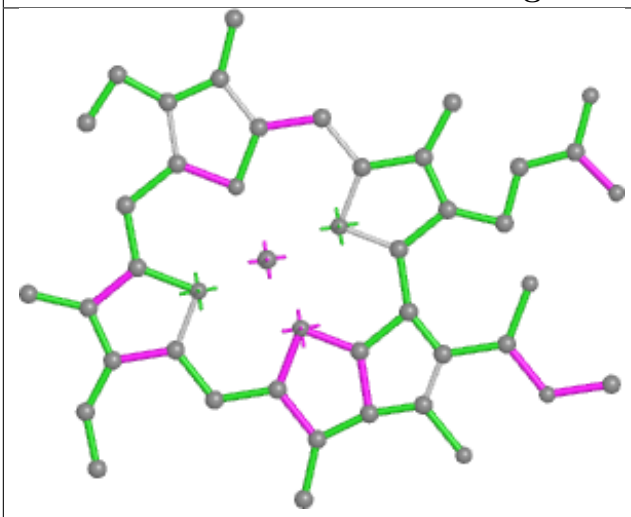


Torsions

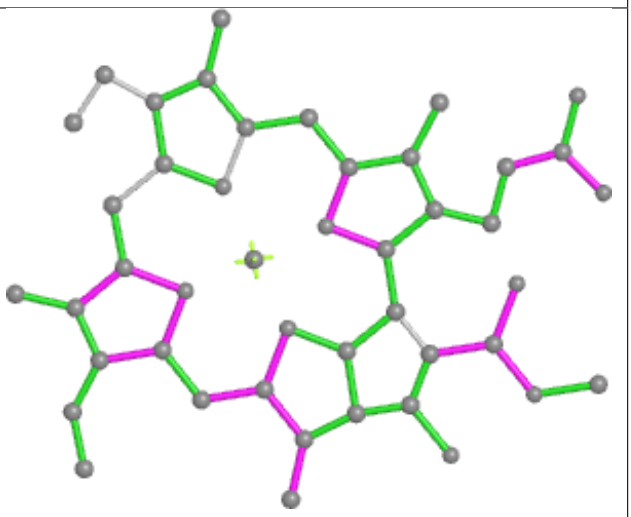


Rings

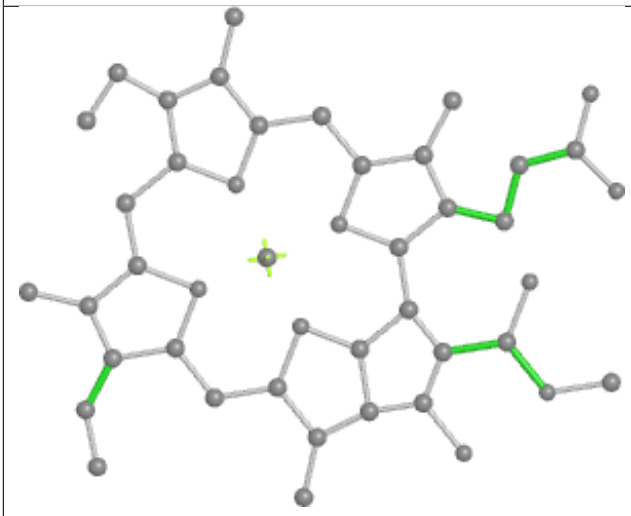
Ligand CLA A 815



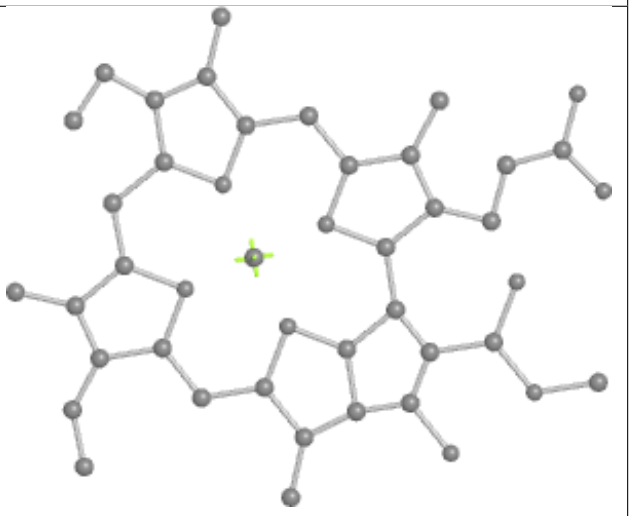
Bond lengths



Bond angles

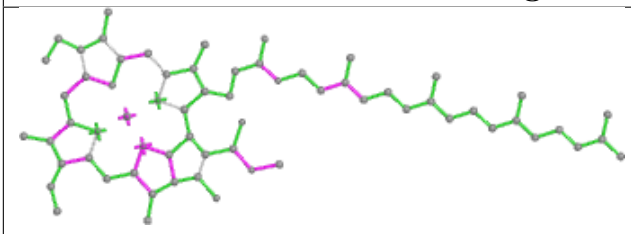


Torsions

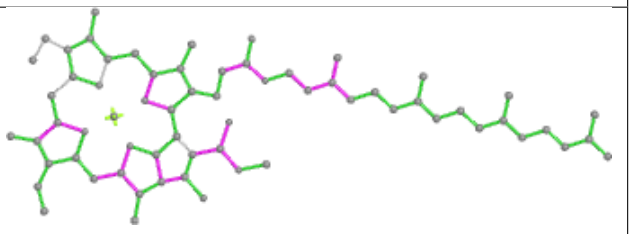


Rings

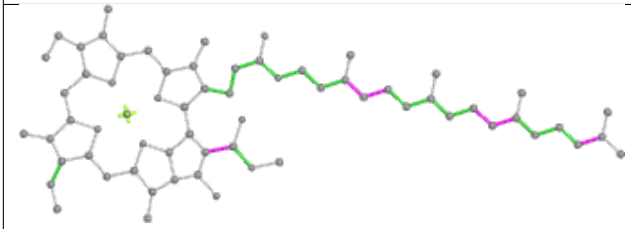
Ligand CLA A 827



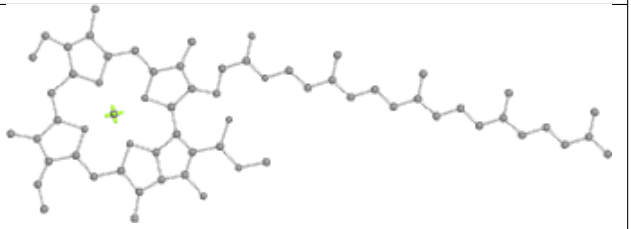
Bond lengths



Bond angles

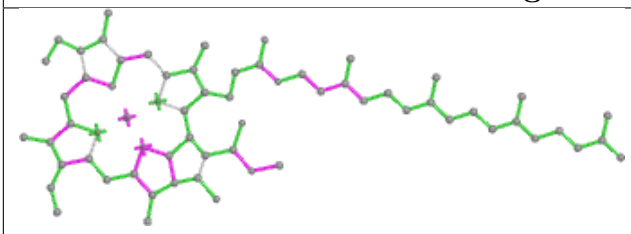


Torsions

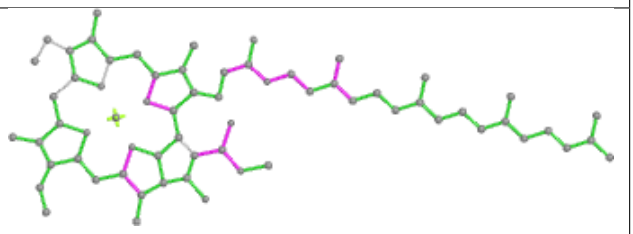


Rings

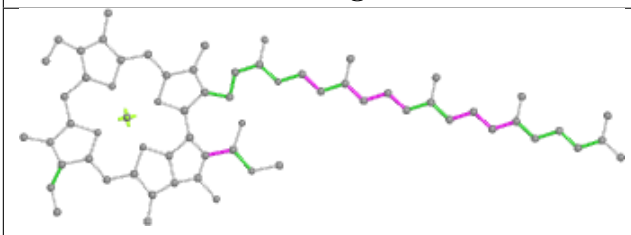
Ligand CLA A 805



Bond lengths



Bond angles



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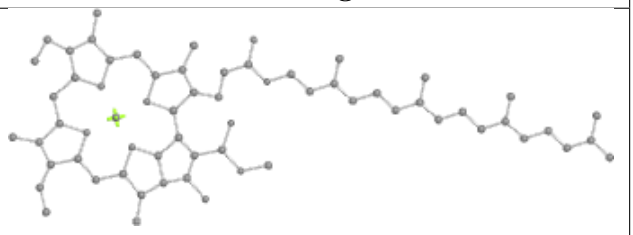
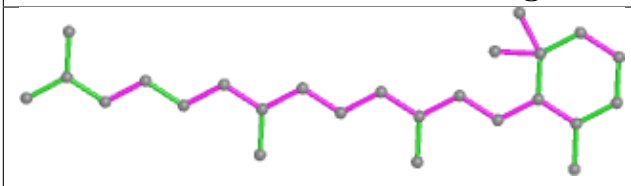
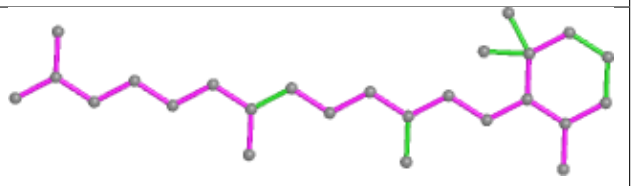


Rings

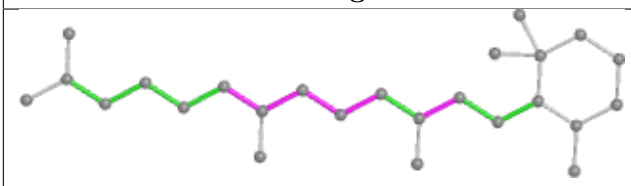
Ligand BCR B 844



Bond lengths



Bond angles



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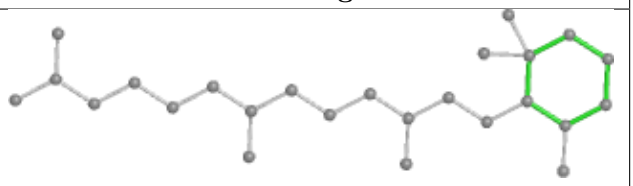
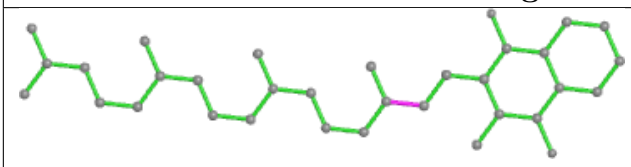
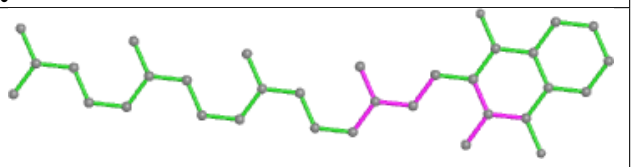


Rings

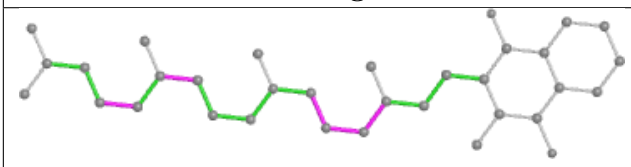
Ligand PQN A 846



Bond lengths



Bond angles



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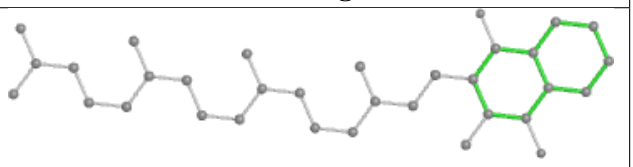
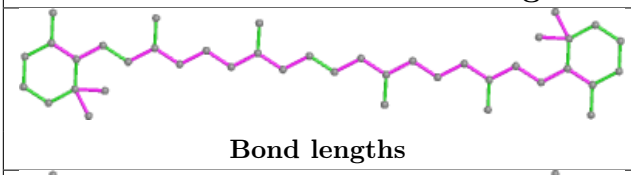
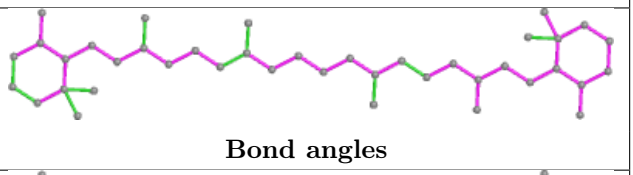


Rings

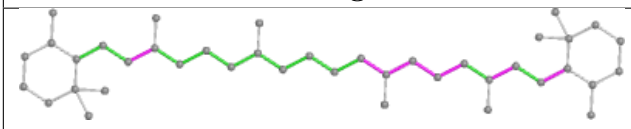
Ligand BCR B 845



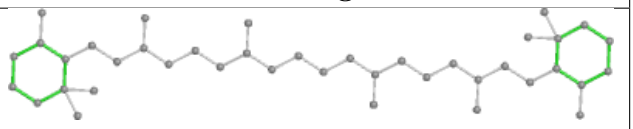
Bond lengths



Bond angles

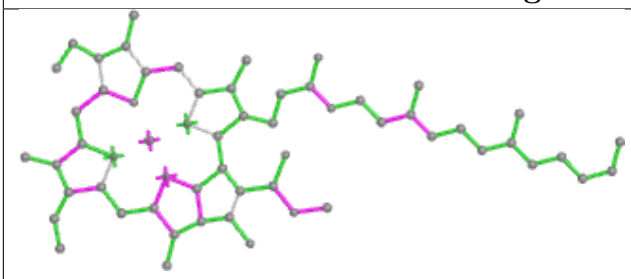


Torsions

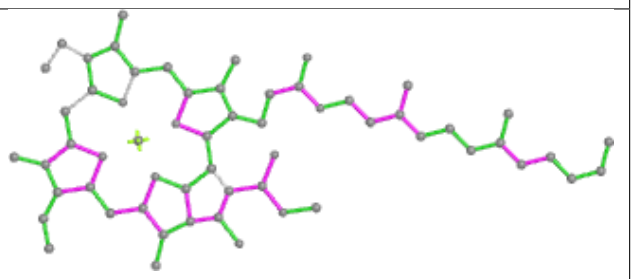


Rings

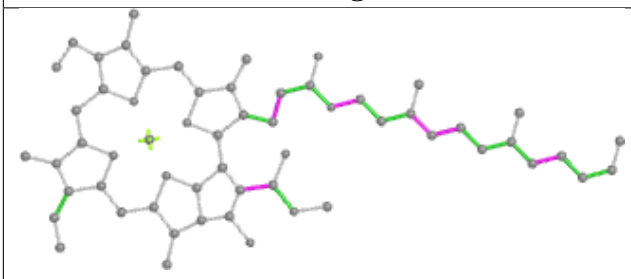
Ligand CLA A 824



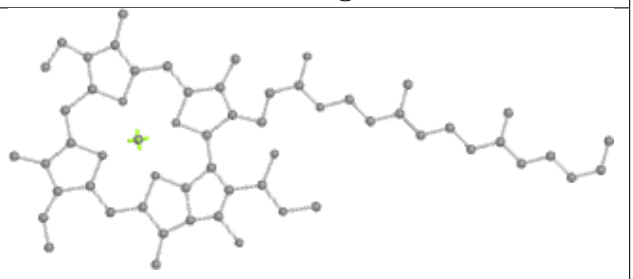
Bond lengths



Bond angles

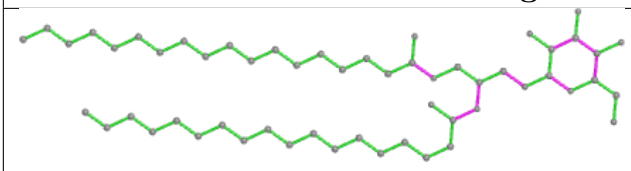


Torsions

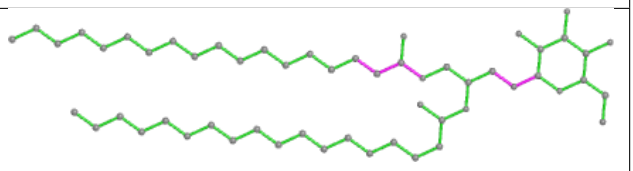


Rings

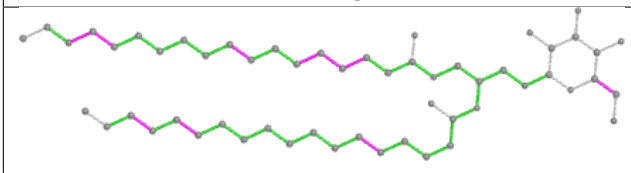
Ligand LMG B 848



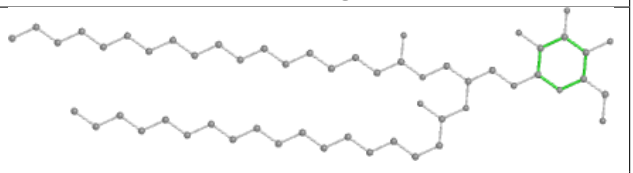
Bond lengths



Bond angles

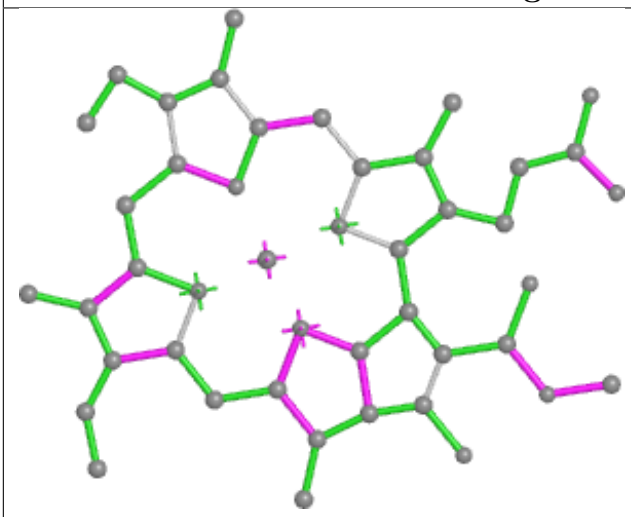


Torsions

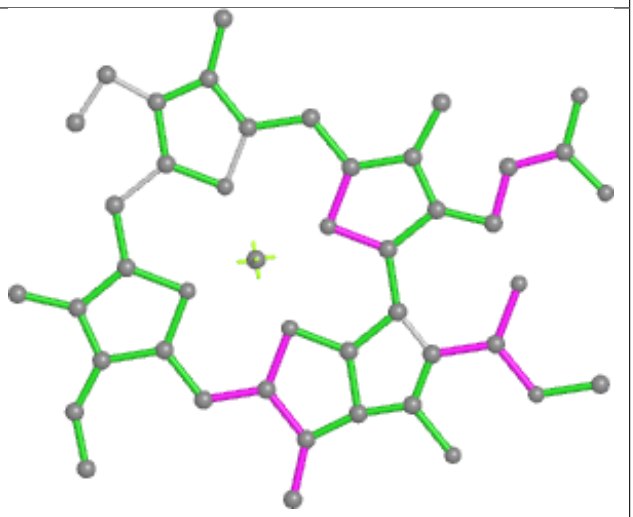


Rings

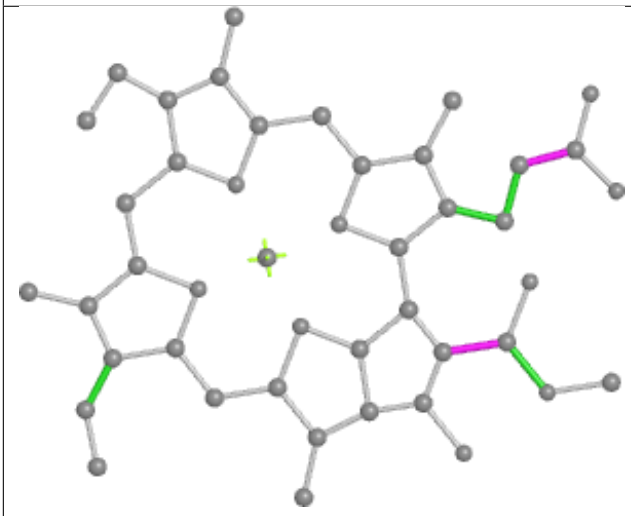
Ligand CLA A 814



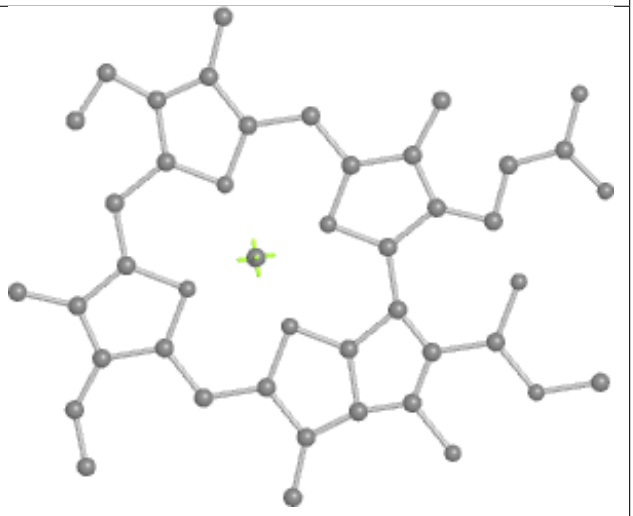
Bond lengths



Bond angles

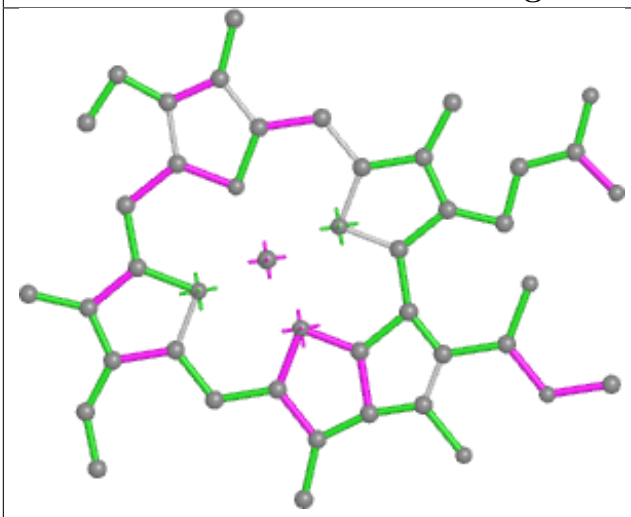


Torsions

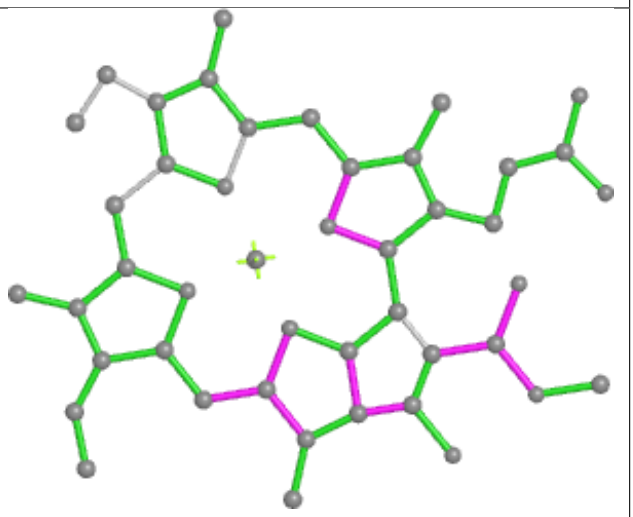


Rings

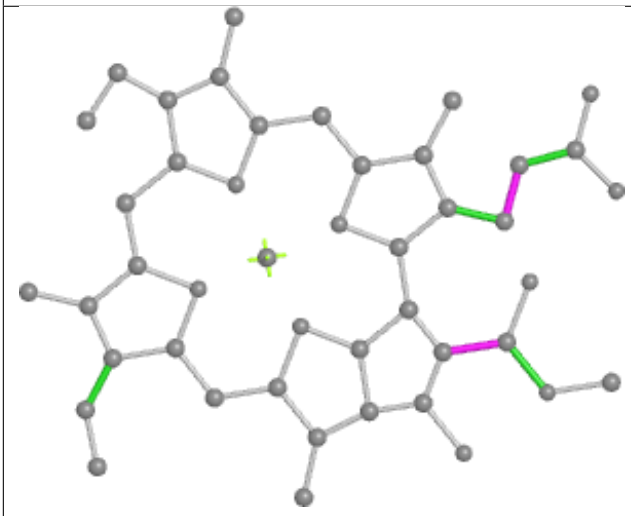
Ligand CLA B 828



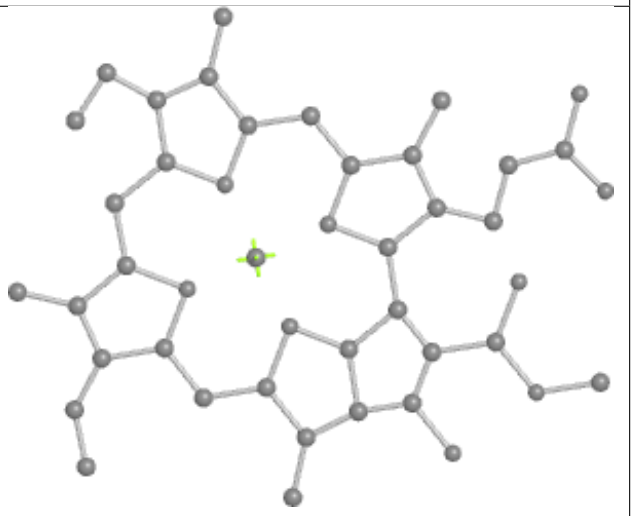
Bond lengths



Bond angles

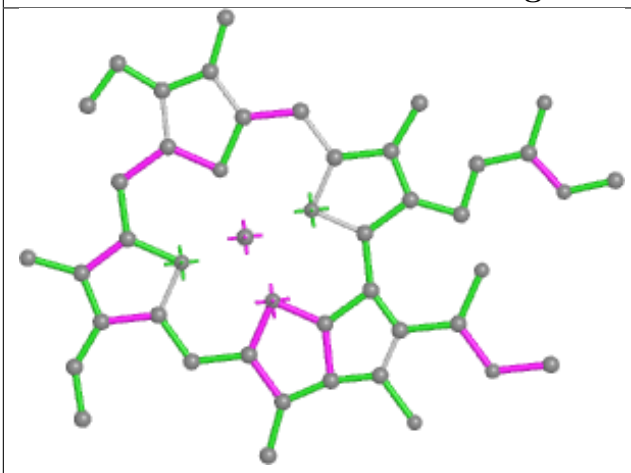


Torsions

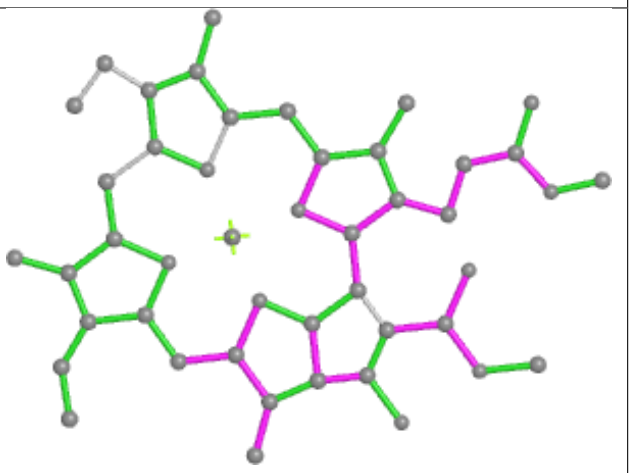


Rings

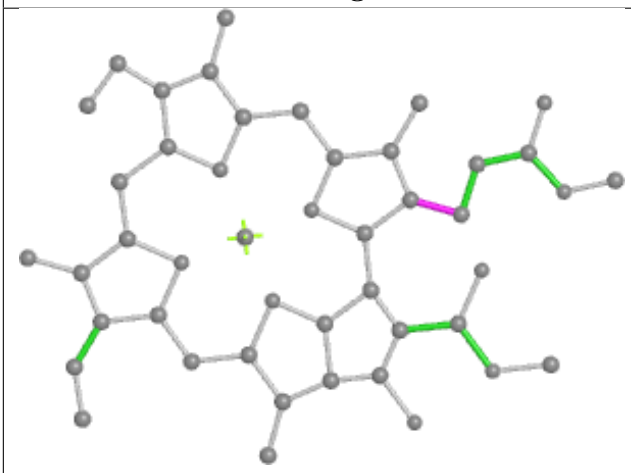
Ligand CLA B 823



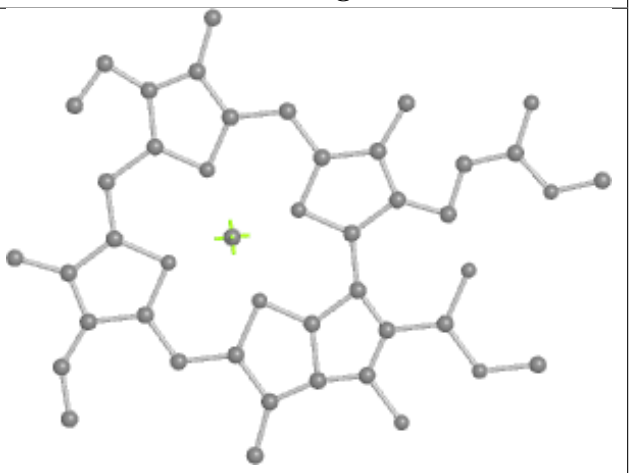
Bond lengths



Bond angles

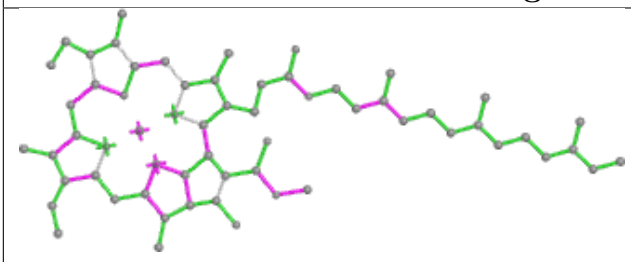


Torsions

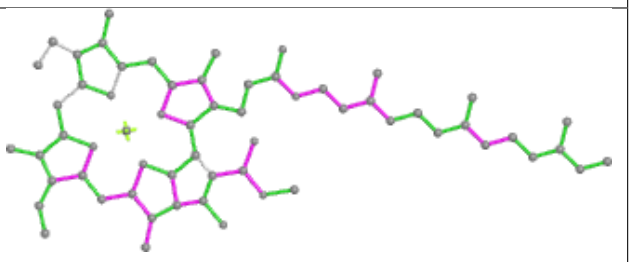


Rings

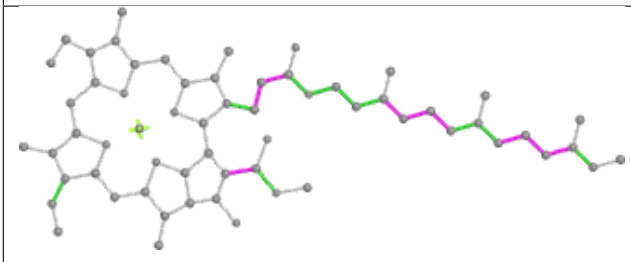
Ligand CLA A 820



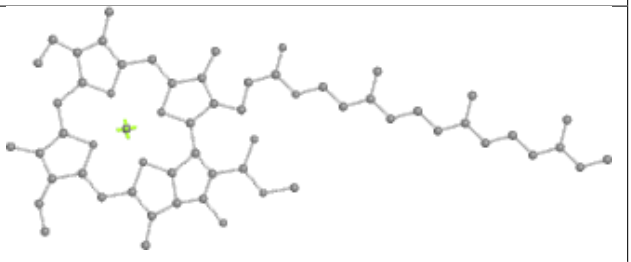
Bond lengths



Bond angles

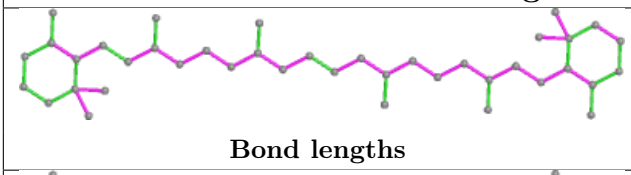


Torsions

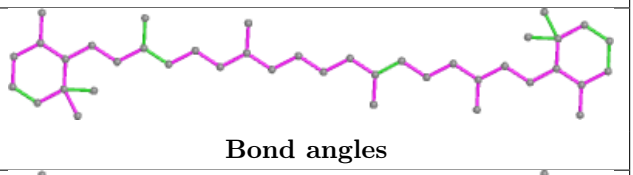


Rings

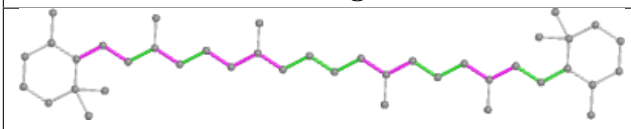
Ligand BCR B 847



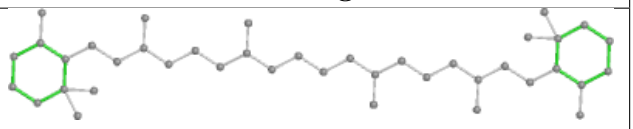
Bond lengths



Bond angles

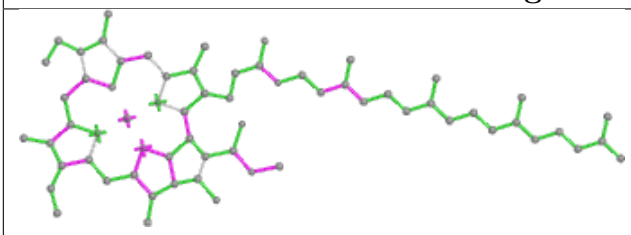


Torsions



Rings

Ligand CLA B 807



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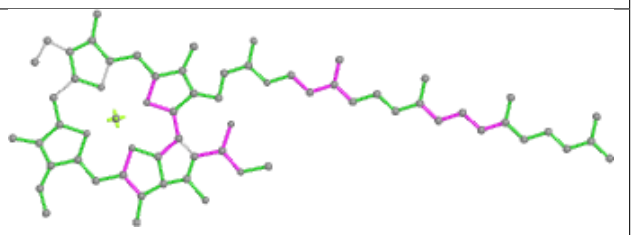
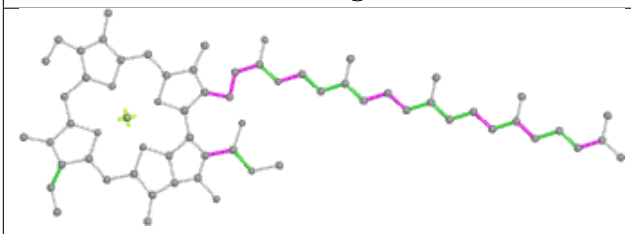
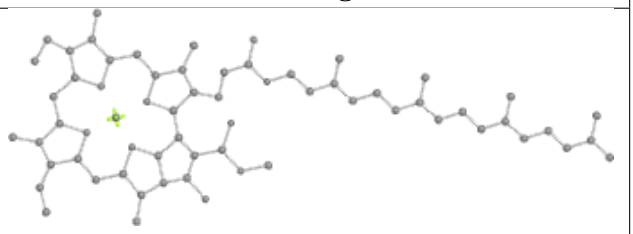


Bond angles

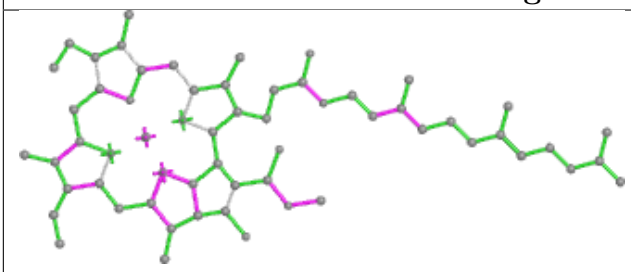


Torsions

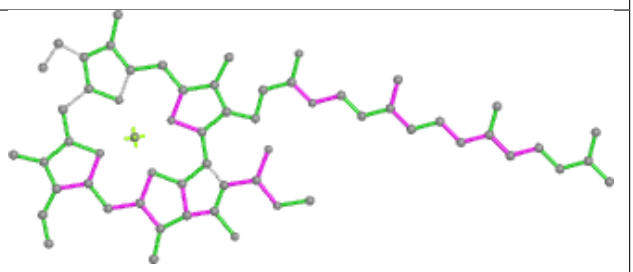


Rings

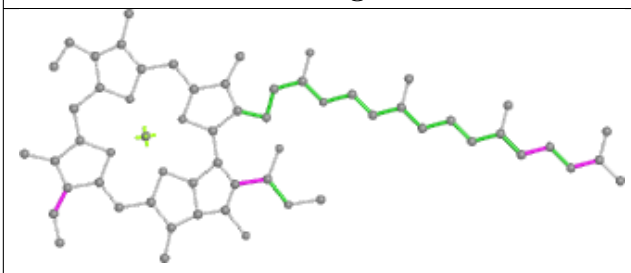
Ligand CLA A 813



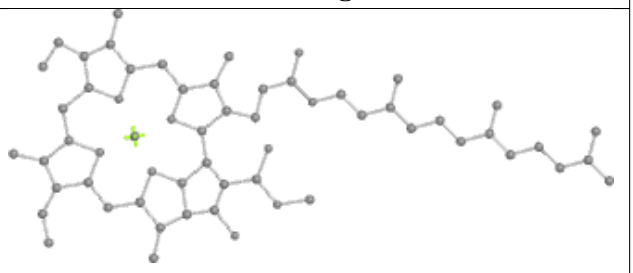
Bond lengths



Bond angles

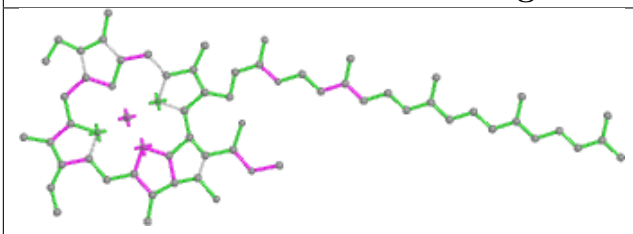


Torsions



Rings

Ligand CLA L 1004



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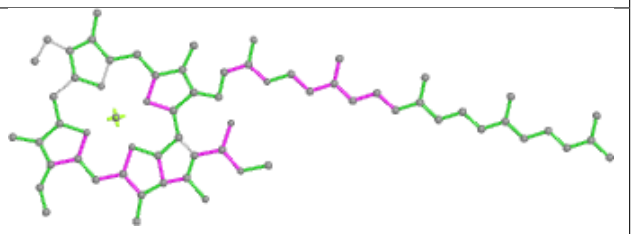
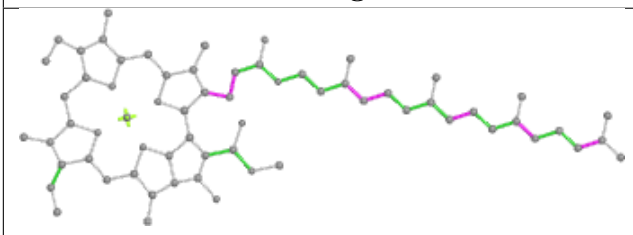
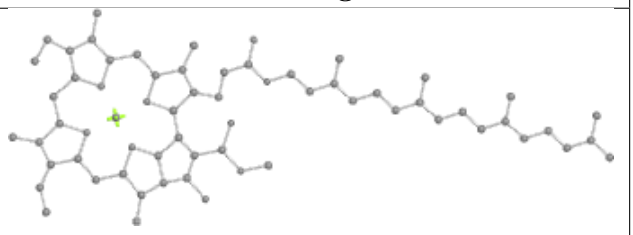


Bond angles

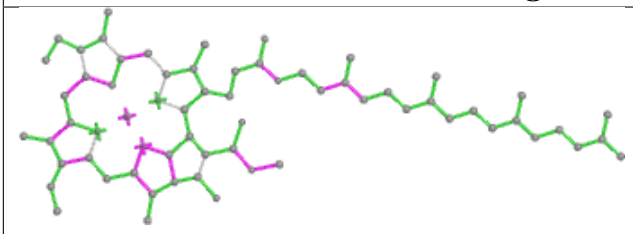


Torsions

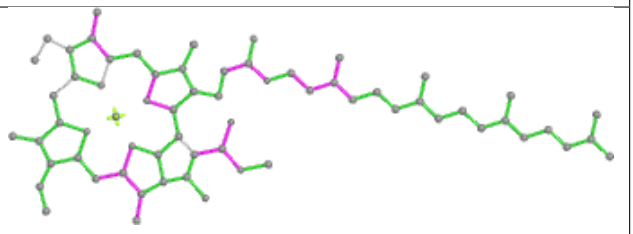


Rings

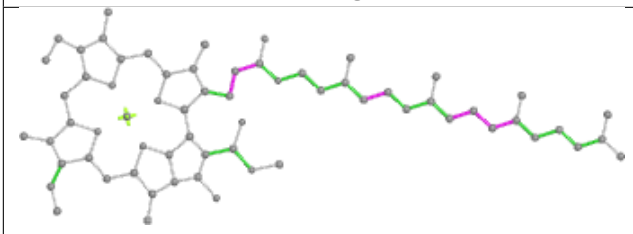
Ligand CLA B 804



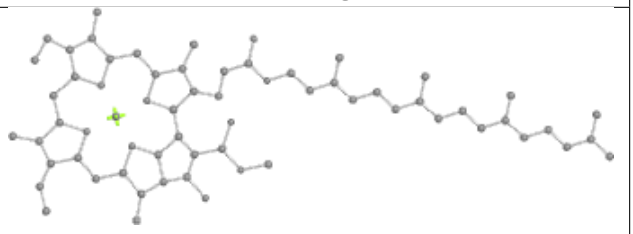
Bond lengths



Bond angles

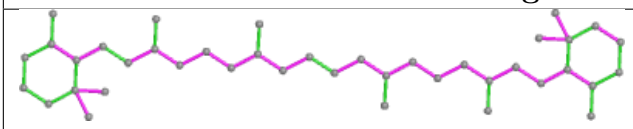


Torsions



Rings

Ligand BCR A 847



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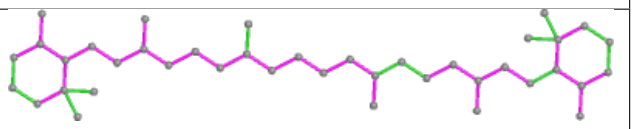
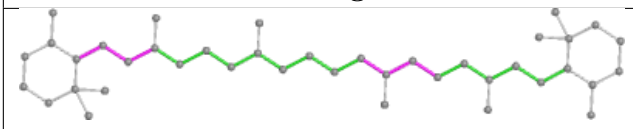


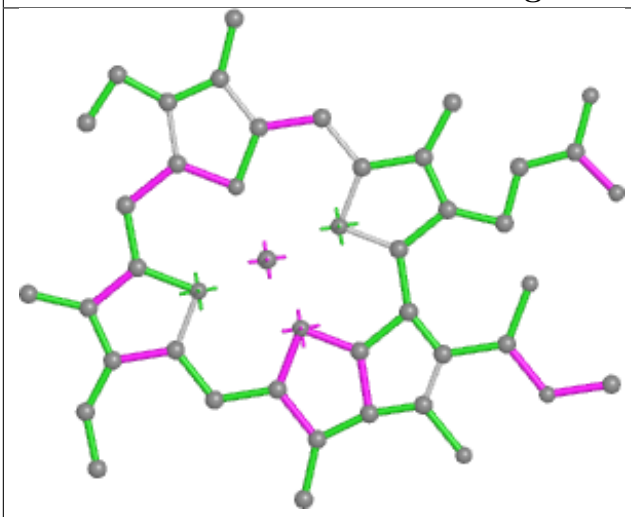
Bond angles



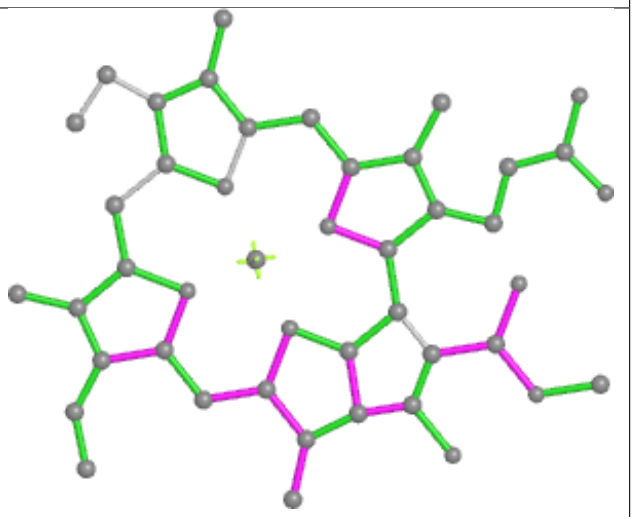
Torsions

Rings

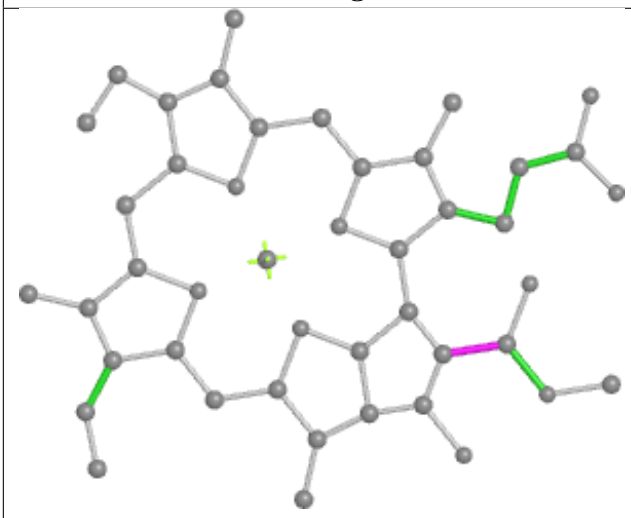
Ligand CLA B 819



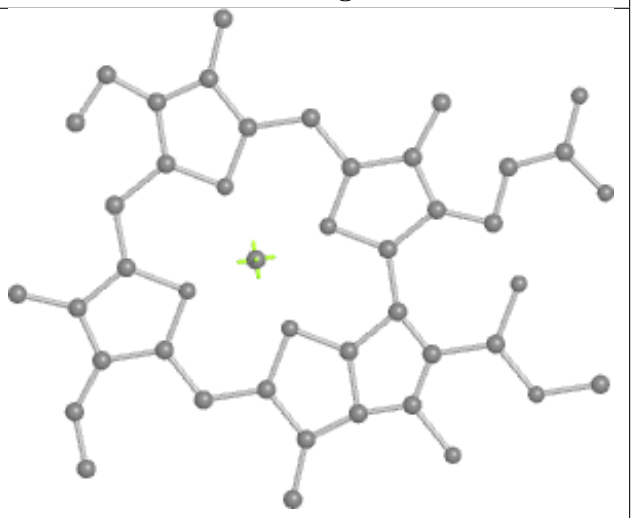
Bond lengths



Bond angles

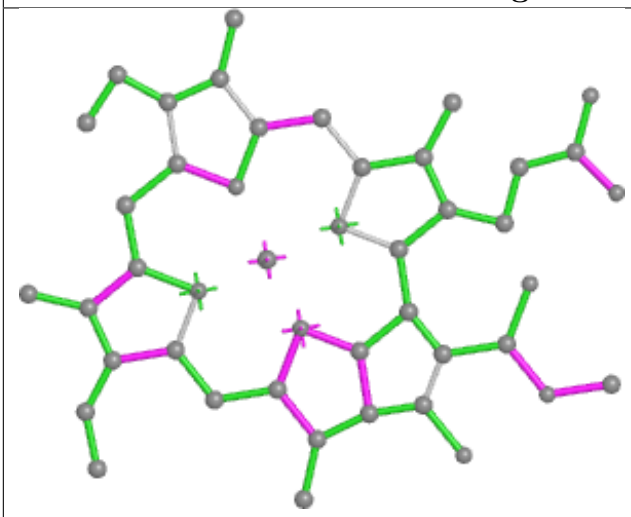


Torsions

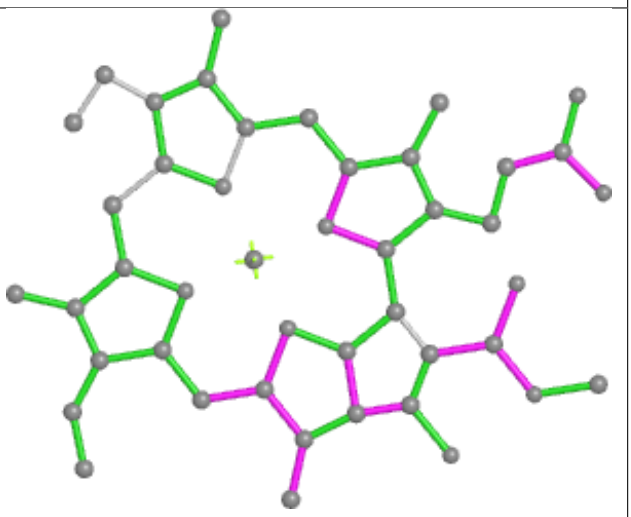


Rings

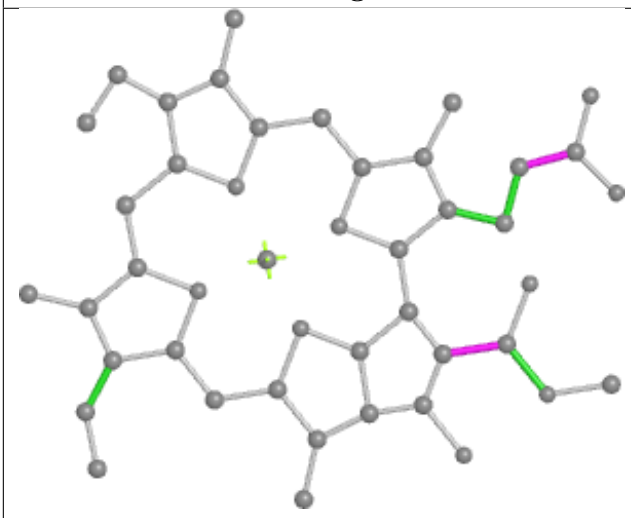
Ligand CLA M 1202



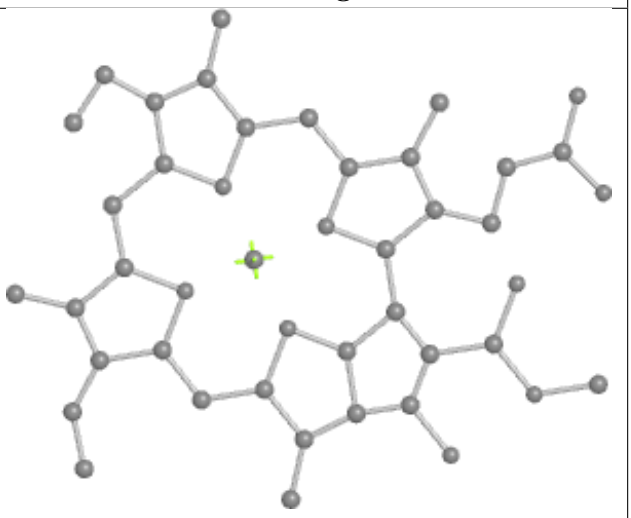
Bond lengths



Bond angles

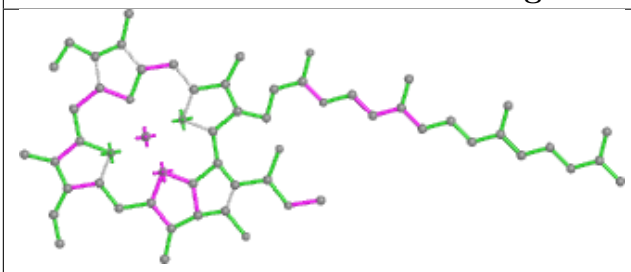


Torsions



Rings

Ligand CLA B 835



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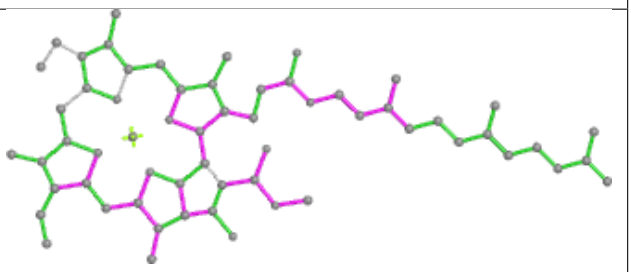
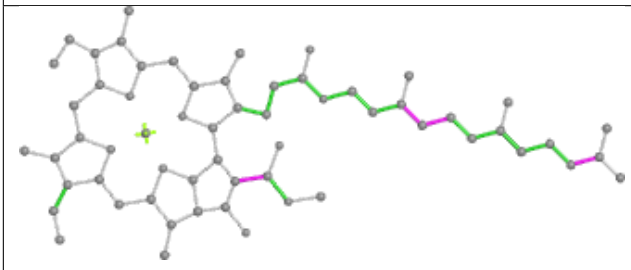


Bond angles



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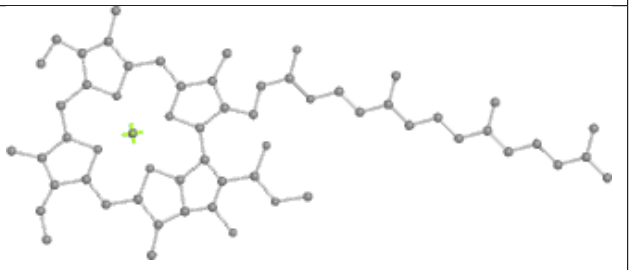
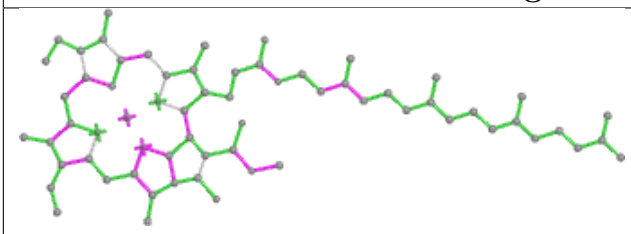
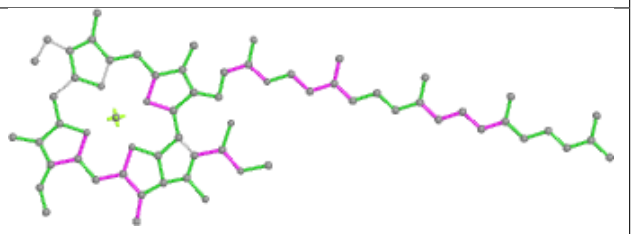


Rings

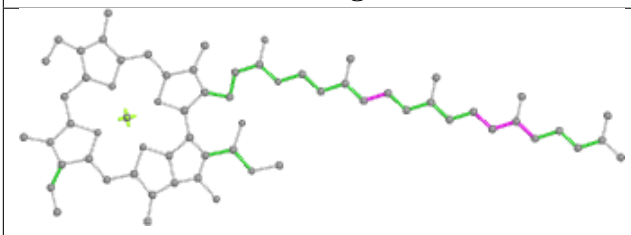
Ligand CLA B 805



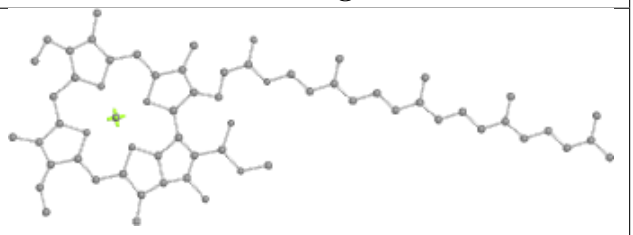
Bond lengths



Bond angles

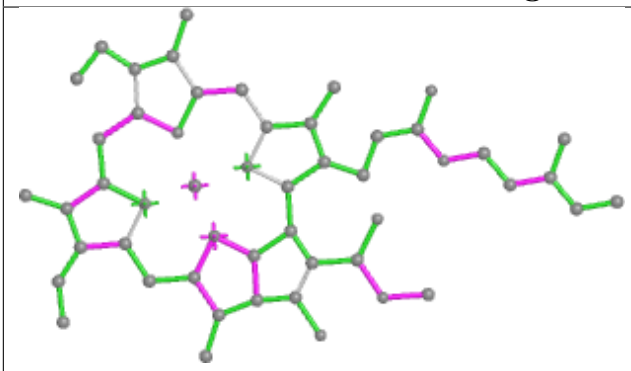


Torsions

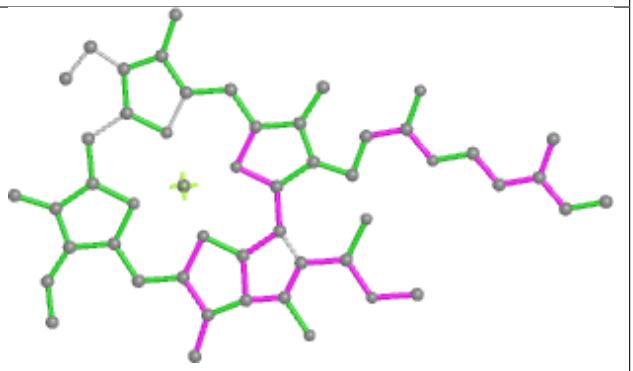


Rings

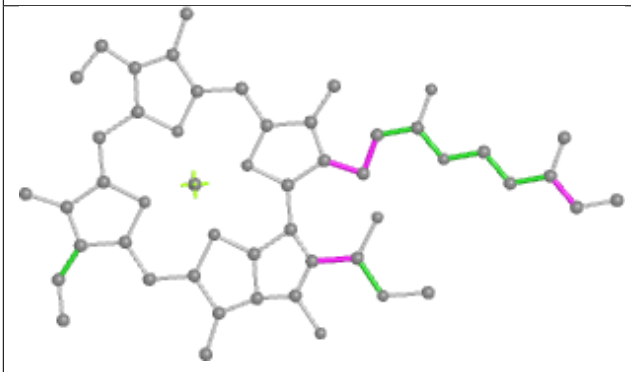
Ligand CLA A 807



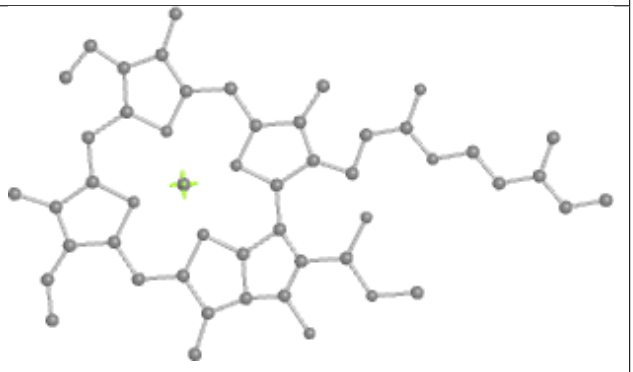
Bond lengths



Bond angles

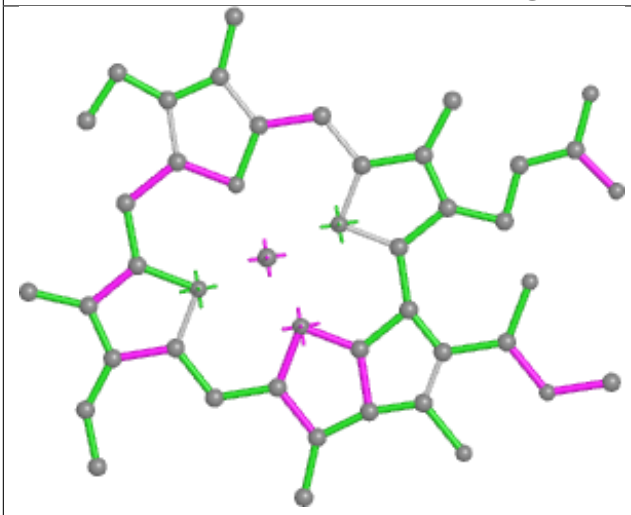


Torsions

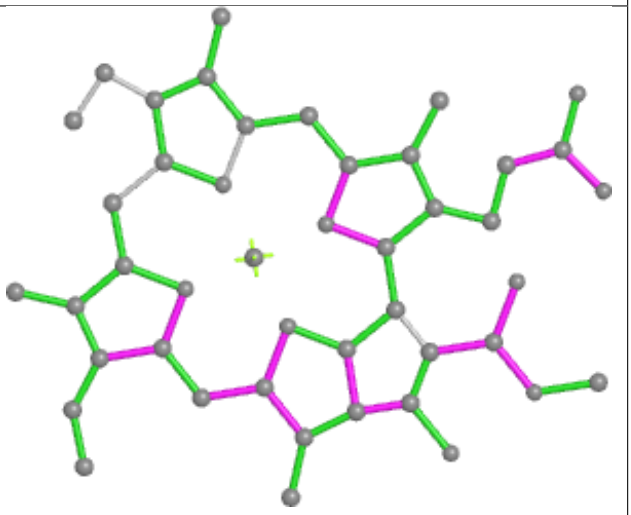


Rings

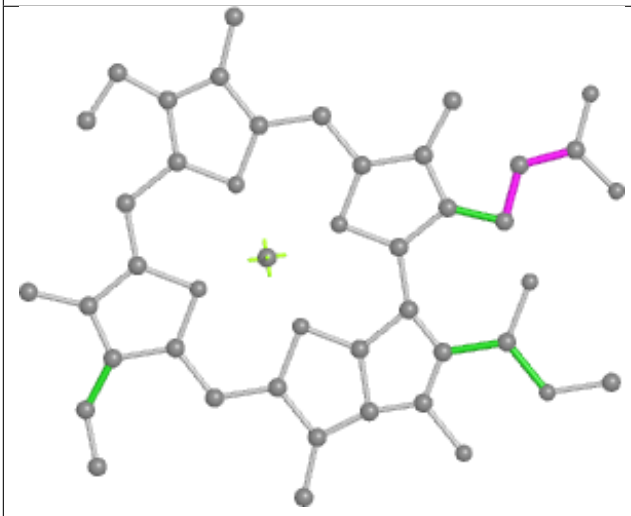
Ligand CLA X 102



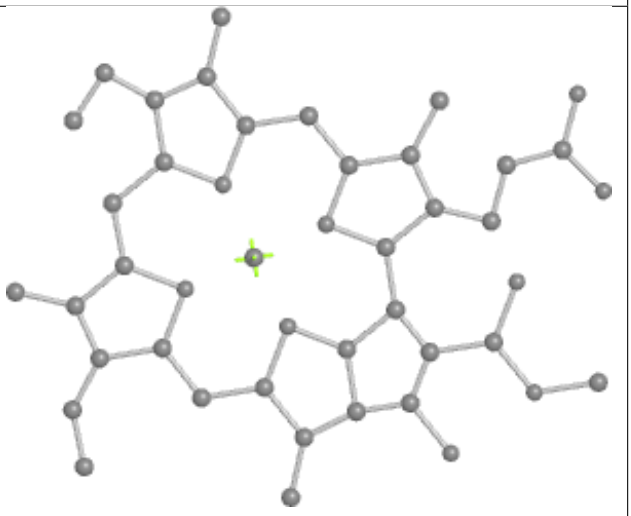
Bond lengths



Bond angles

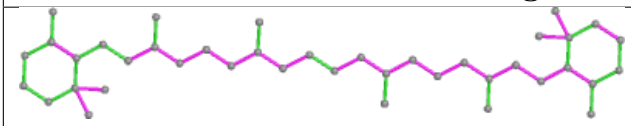


Torsions



Rings

Ligand BCR A 848



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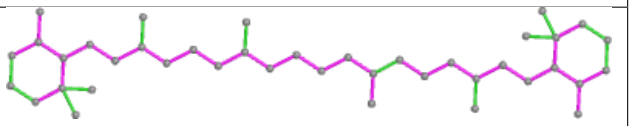
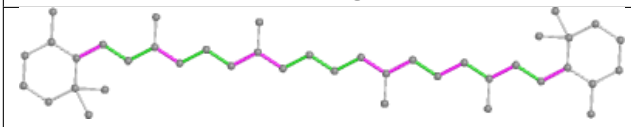


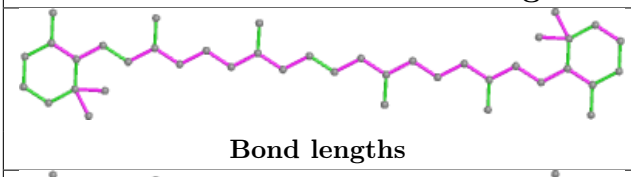
Bond angles



Torsions

Rings

Ligand BCR B 841



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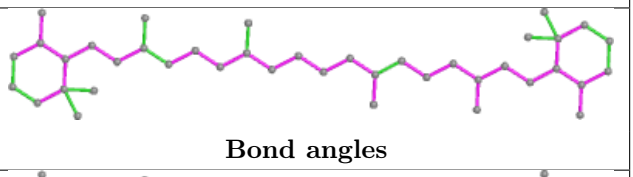
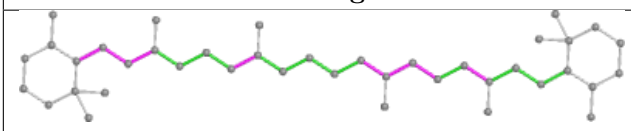
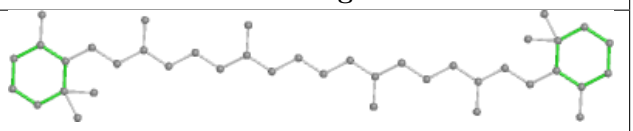


Bond angles

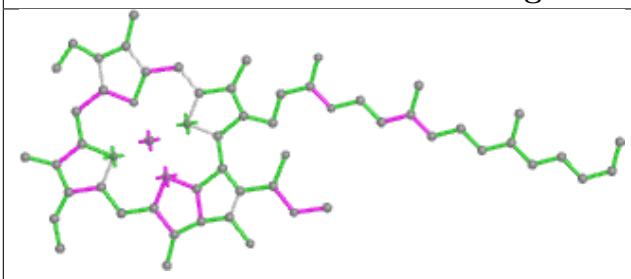


Torsions

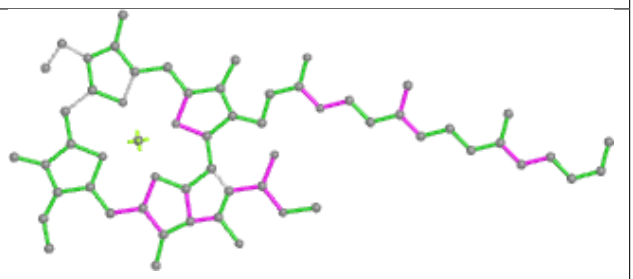


Rings

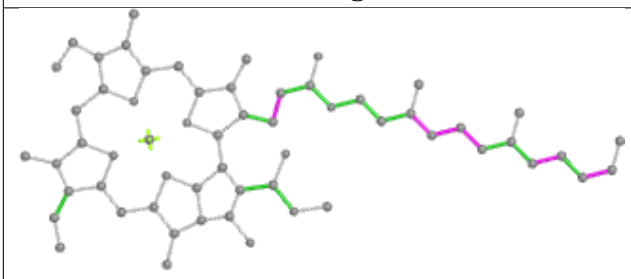
Ligand CLA B 815



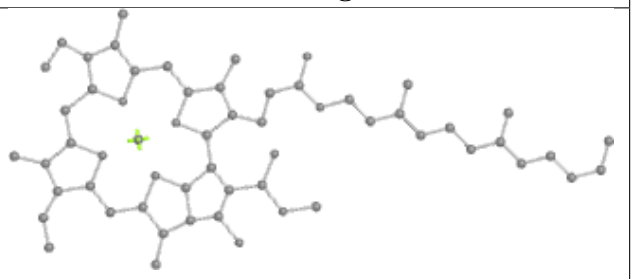
Bond lengths



Bond angles

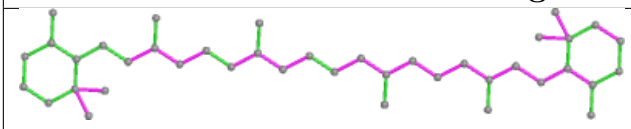


Torsions

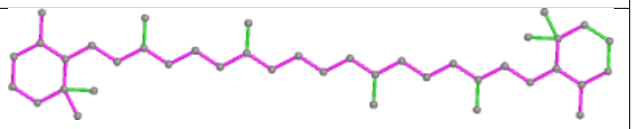


Rings

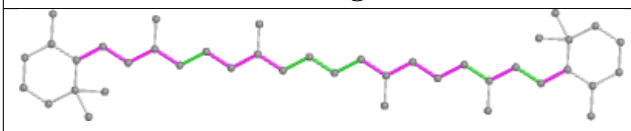
Ligand BCR I 102



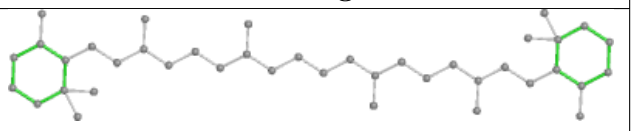
Bond lengths



Bond angles

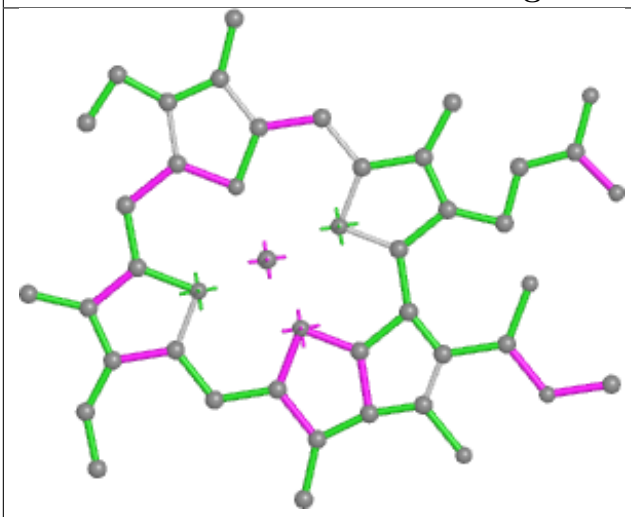


Torsions

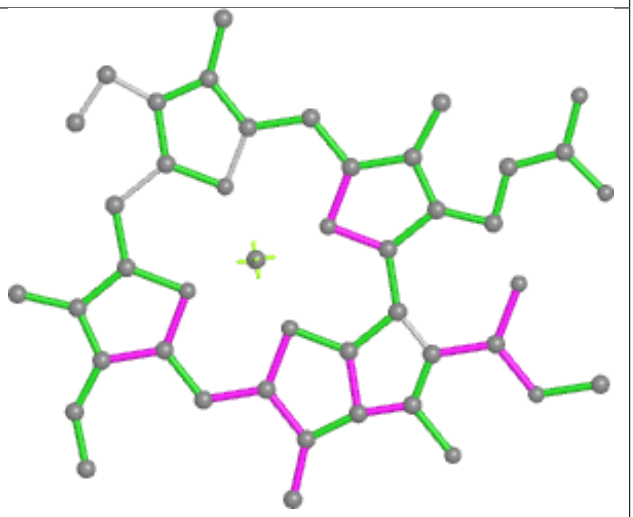


Rings

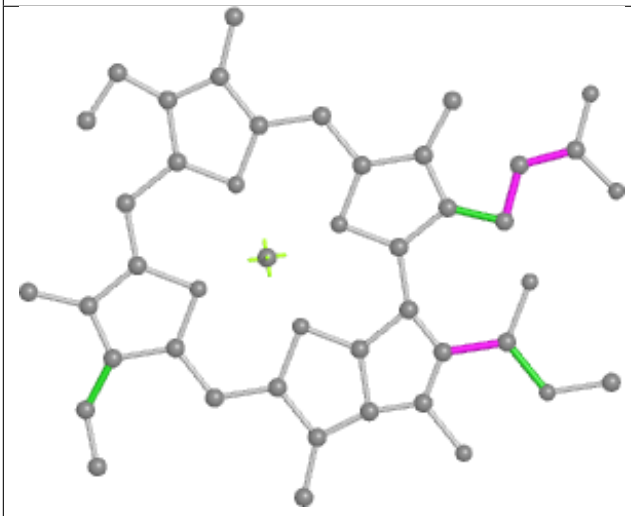
Ligand CLA A 810



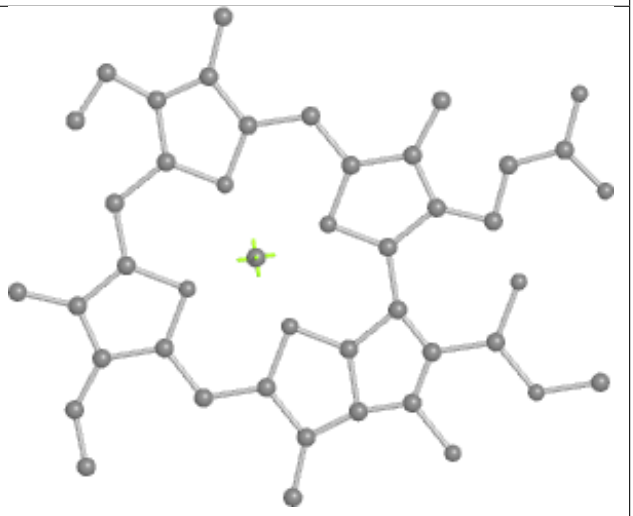
Bond lengths



Bond angles

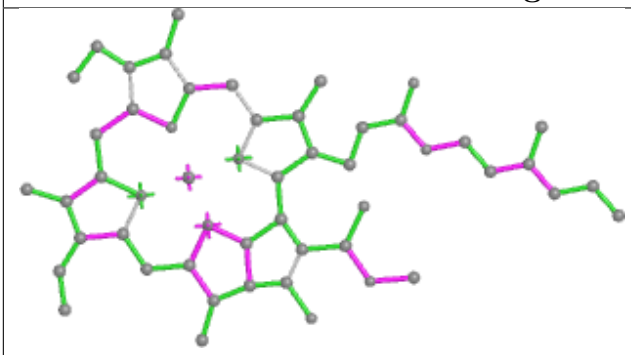


Torsions

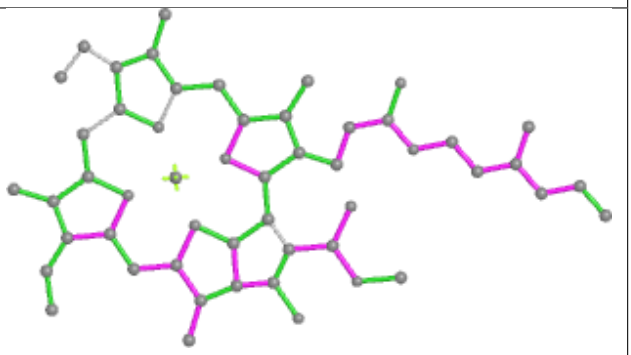


Rings

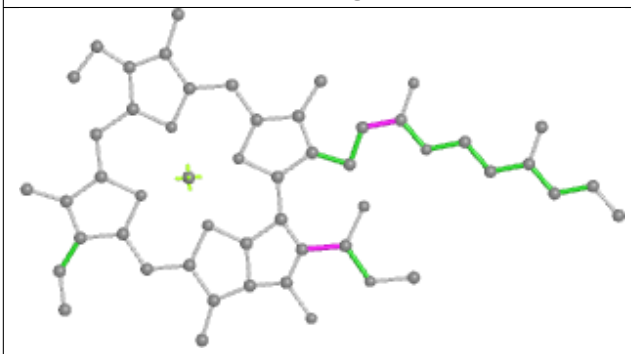
Ligand CLA A 845



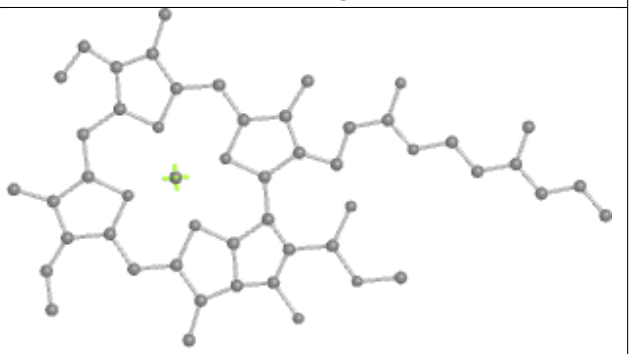
Bond lengths



Bond angles

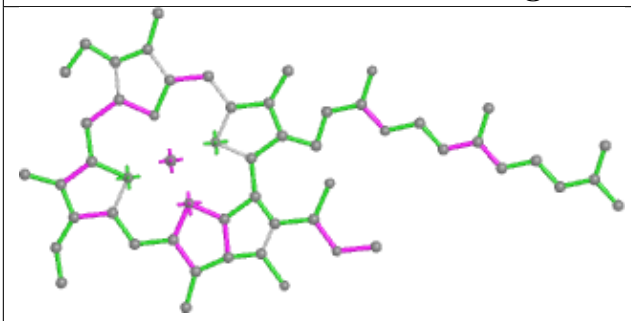


Torsions

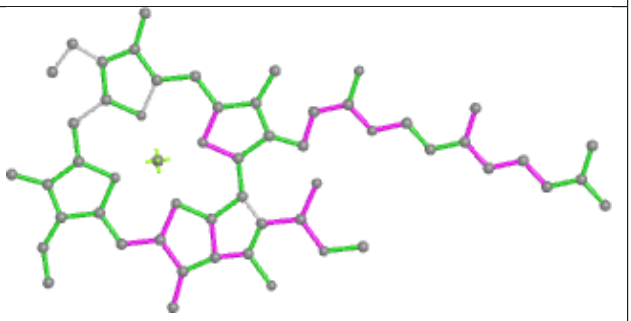


Rings

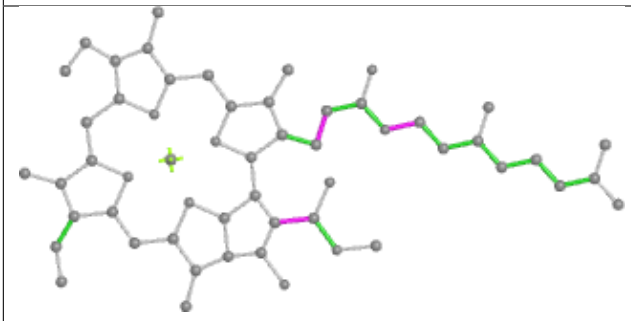
Ligand CLA B 814



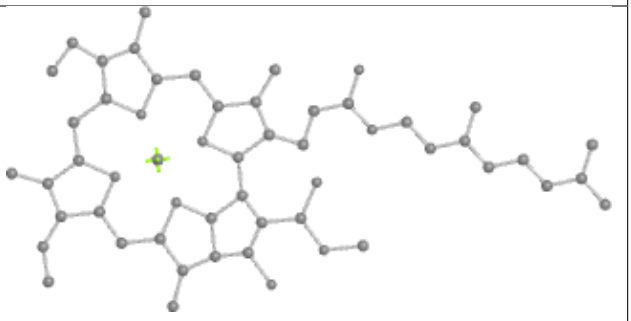
Bond lengths



Bond angles

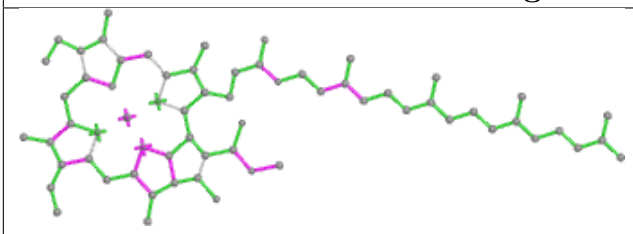


Torsions



Rings

Ligand CLA A 825



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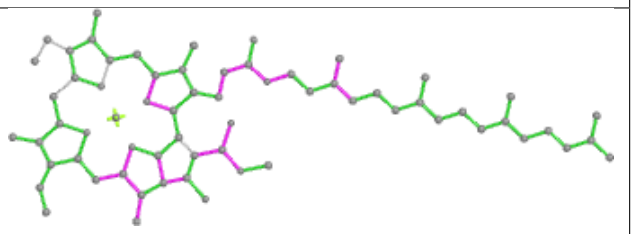
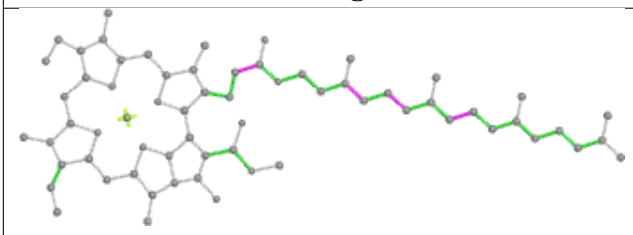
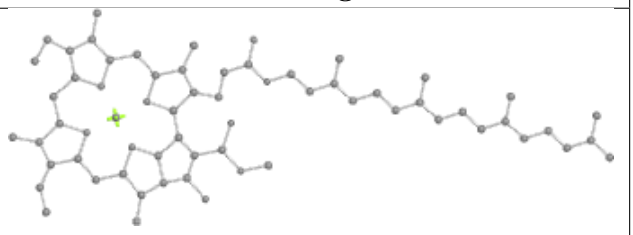


Bond angles

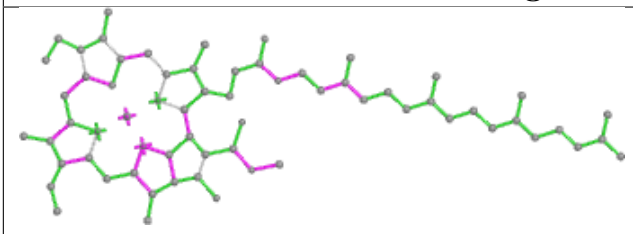


Torsions

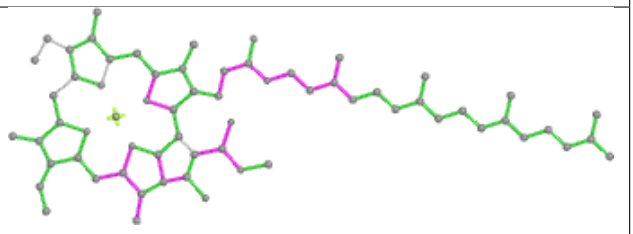


Rings

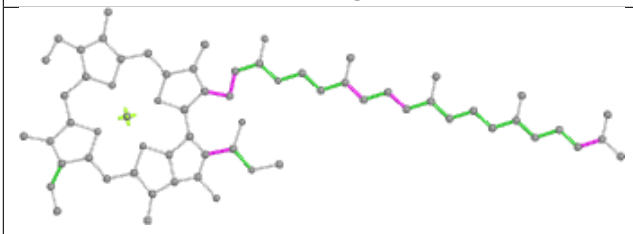
Ligand CLA B 806



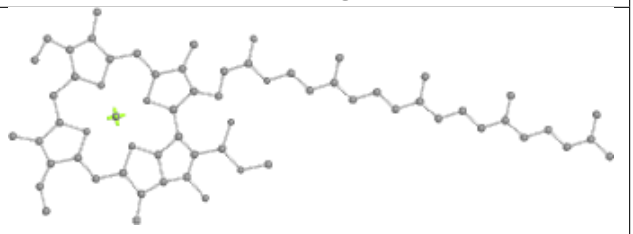
Bond lengths



Bond angles

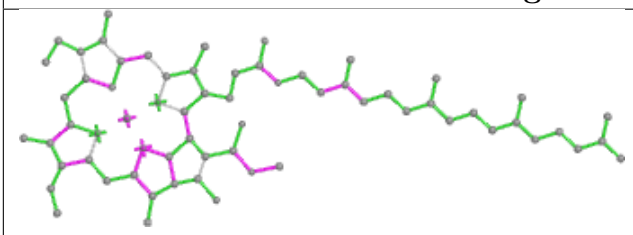


Torsions



Rings

Ligand CLA A 838



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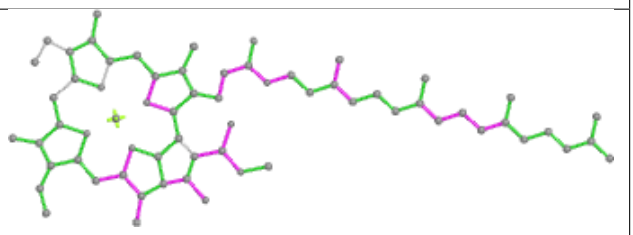
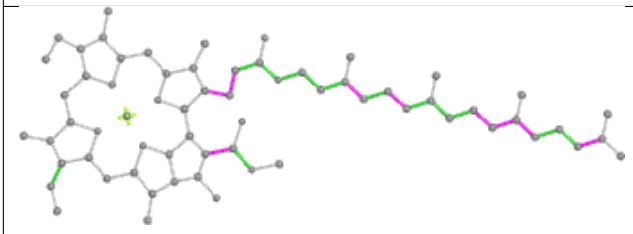


Bond angles



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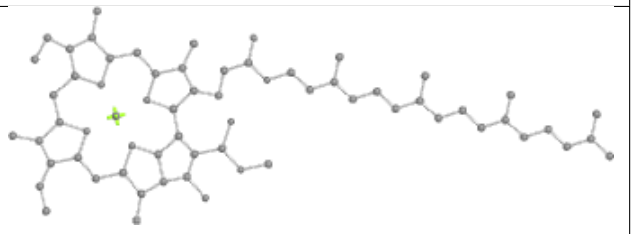
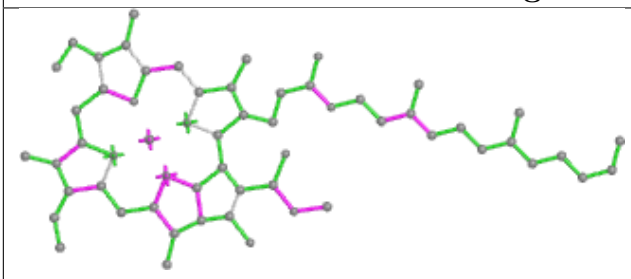
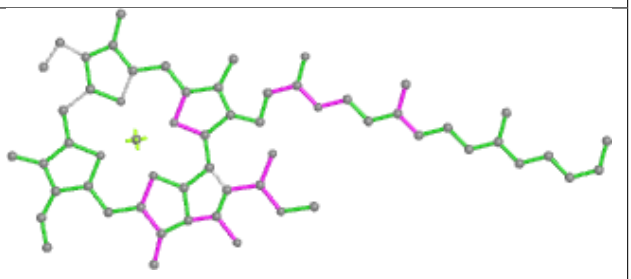


Rings

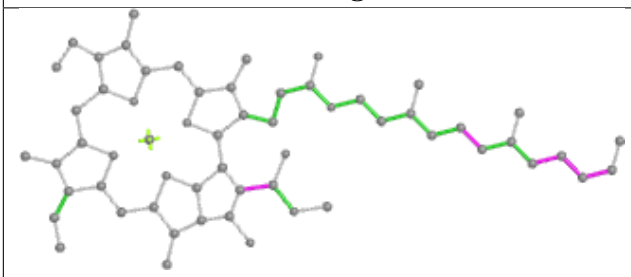
Ligand CLA A 804



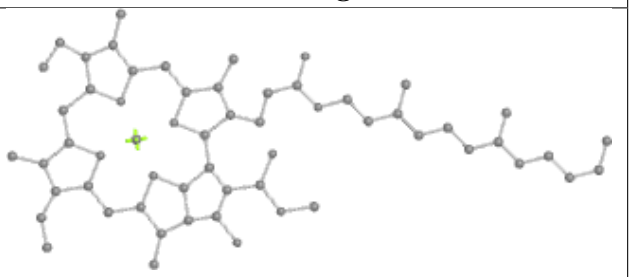
Bond lengths



Bond angles

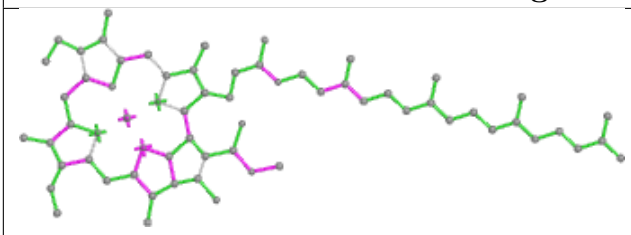


Torsions



Rings

Ligand CLA I 101



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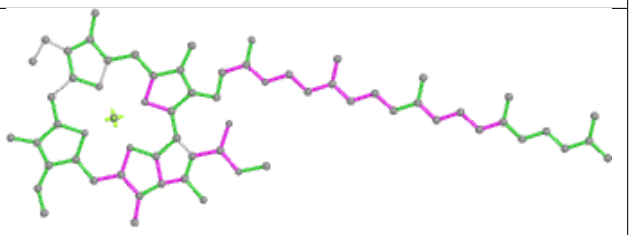
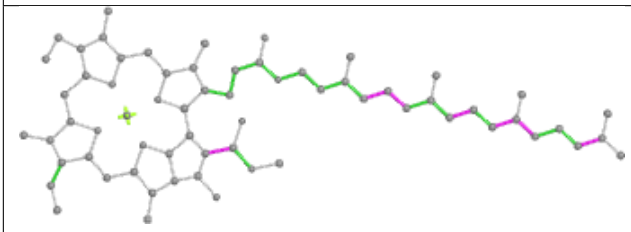


Bond angles



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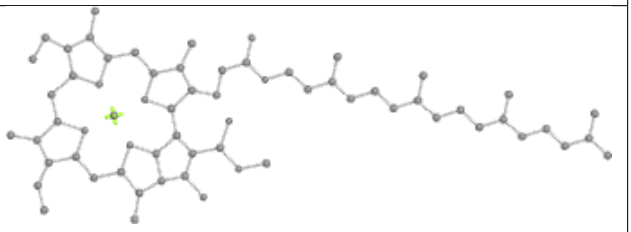
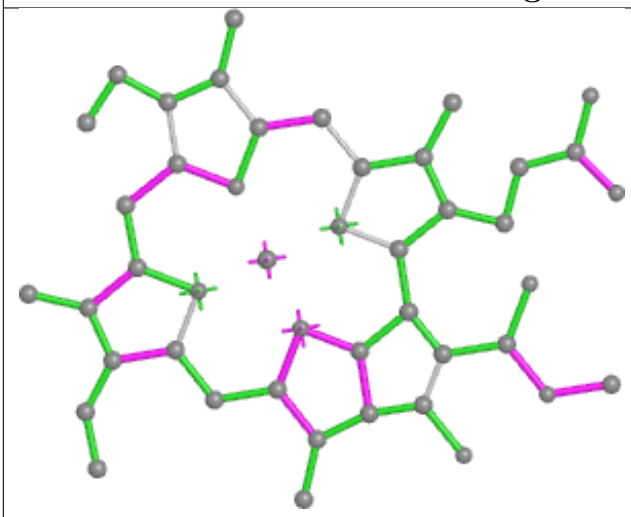
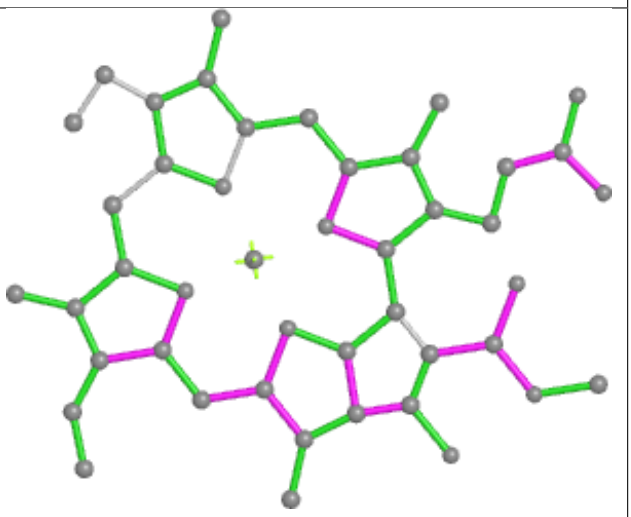


Rings

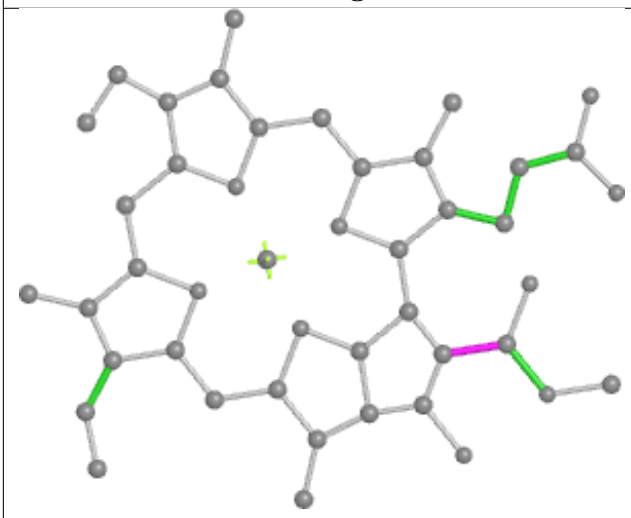
Ligand CLA A 855



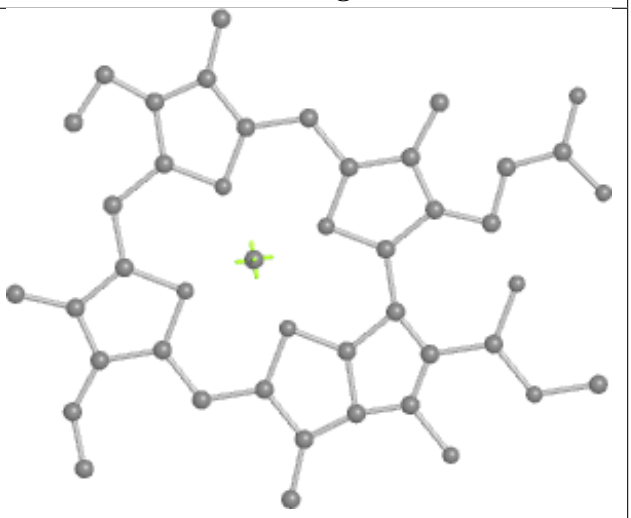
Bond lengths



Bond angles

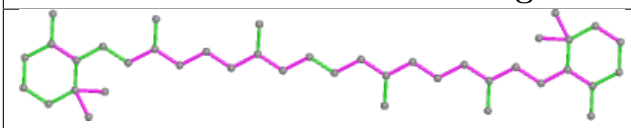


Torsions

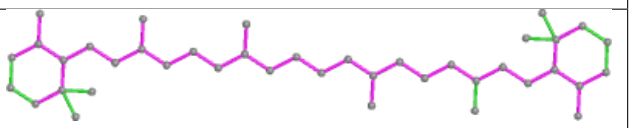


Rings

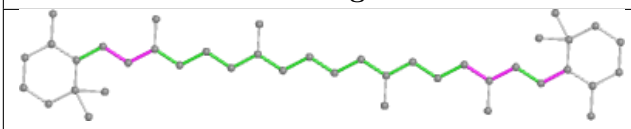
Ligand BCR L 1005



Bond lengths



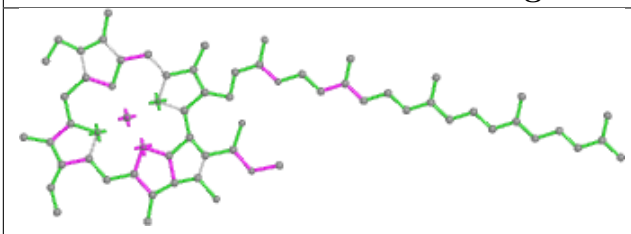
Bond angles



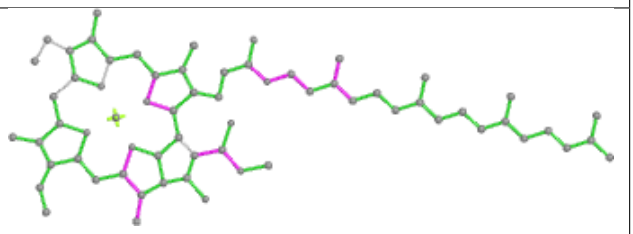
Torsions

Rings

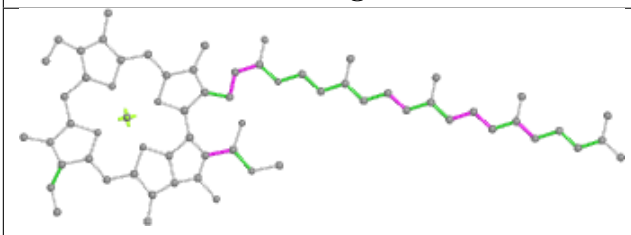
Ligand CLA B 825



Bond lengths



Bond angles



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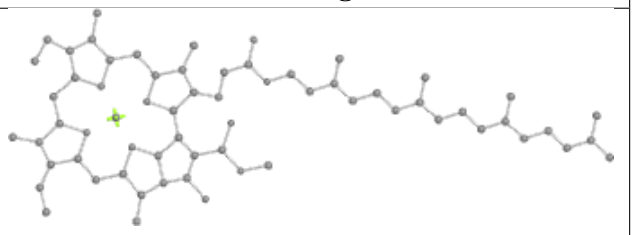
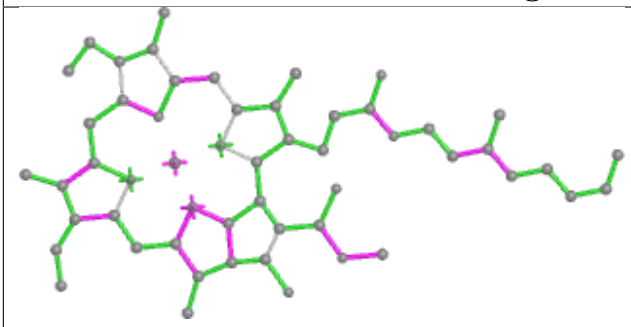


Rings

Ligand CLA A 835



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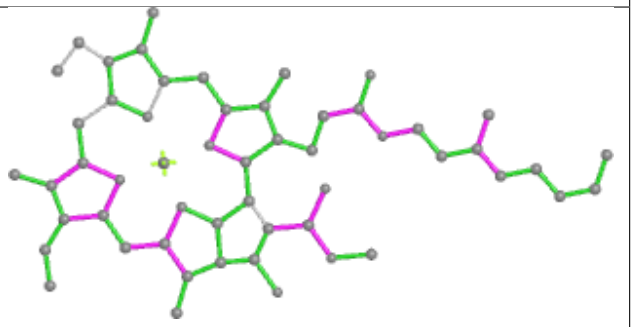
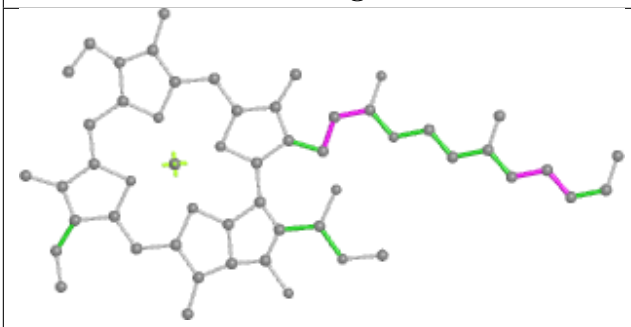
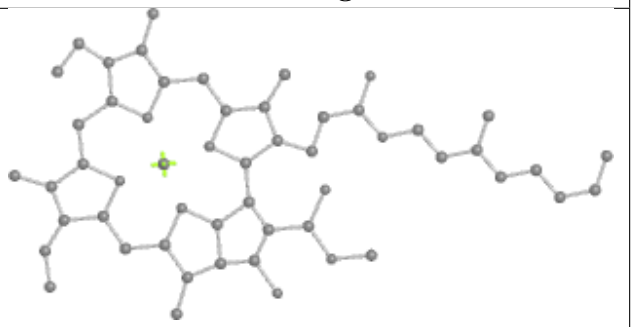


Bond angles

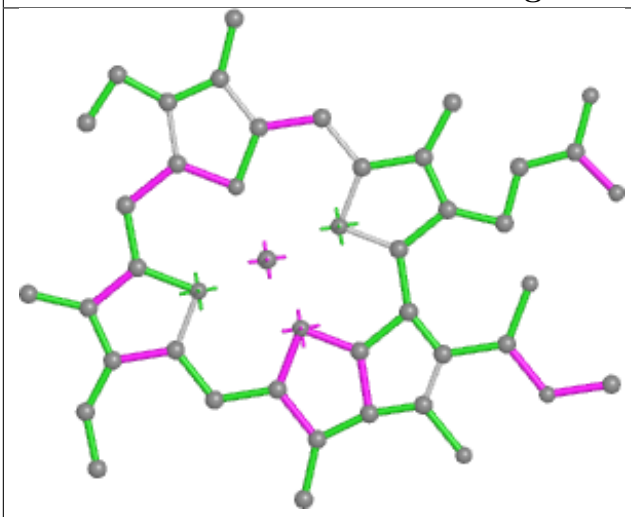


Torsions

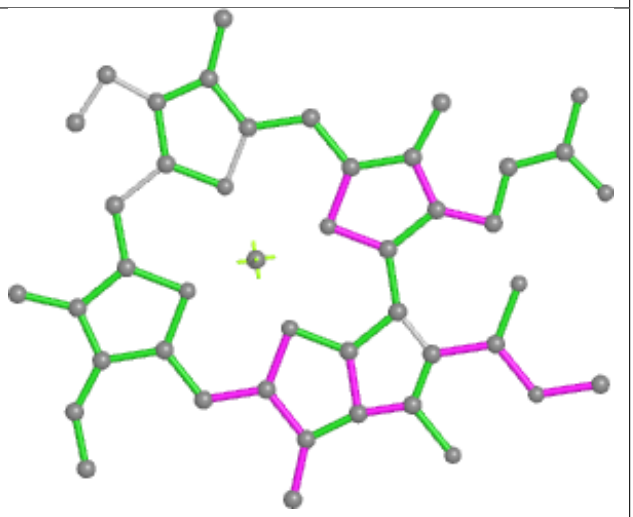


Rings

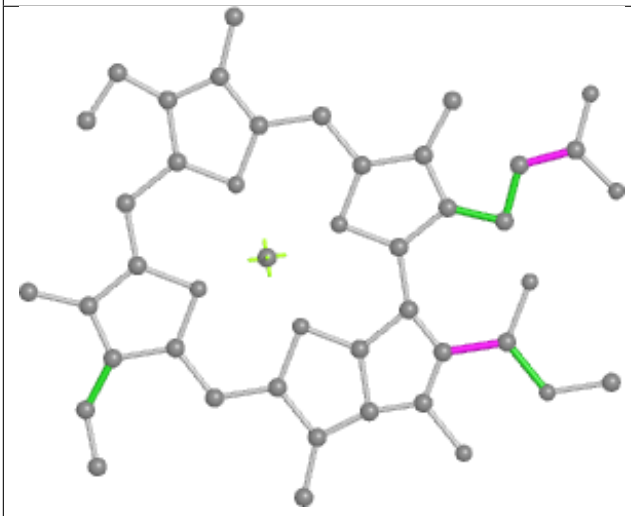
Ligand CLA B 821



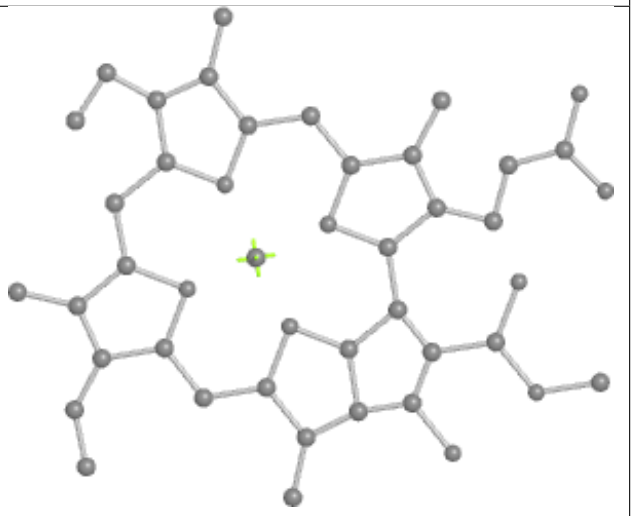
Bond lengths



Bond angles

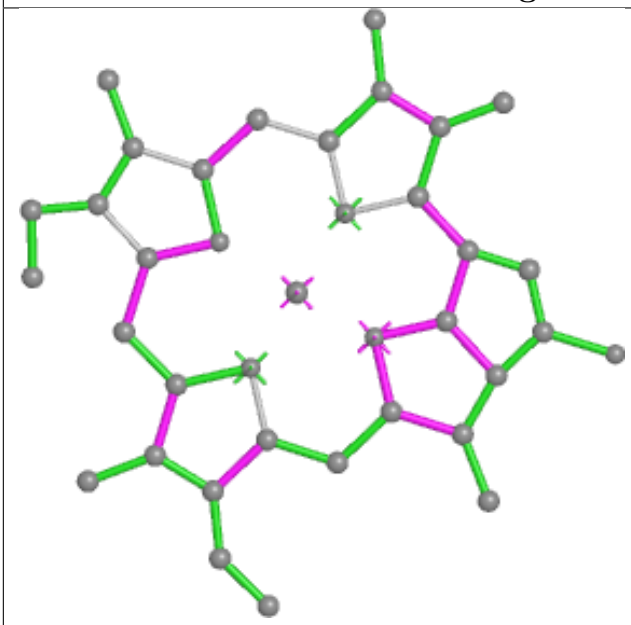


Torsions

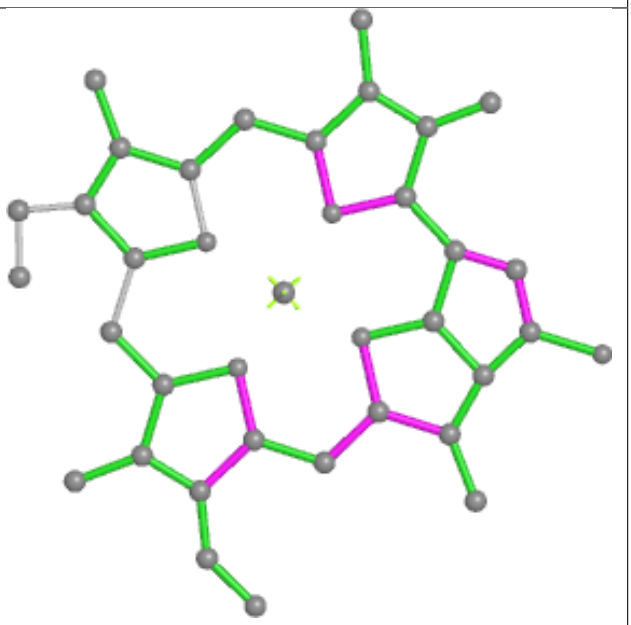


Rings

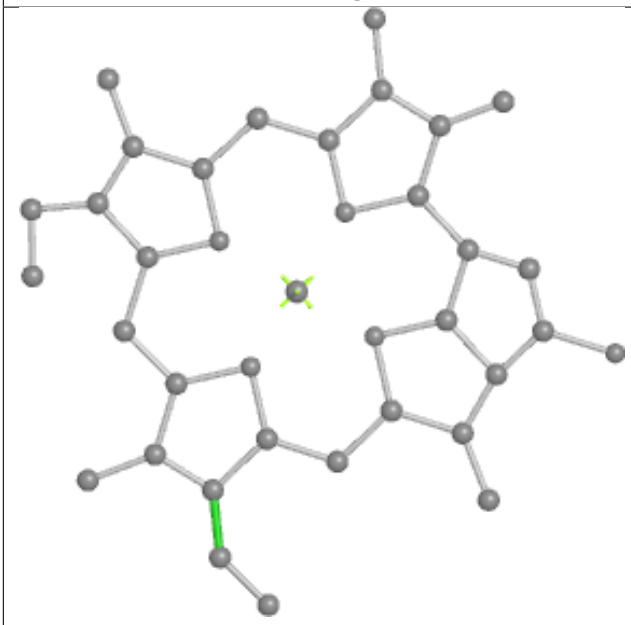
Ligand CLA J 1103



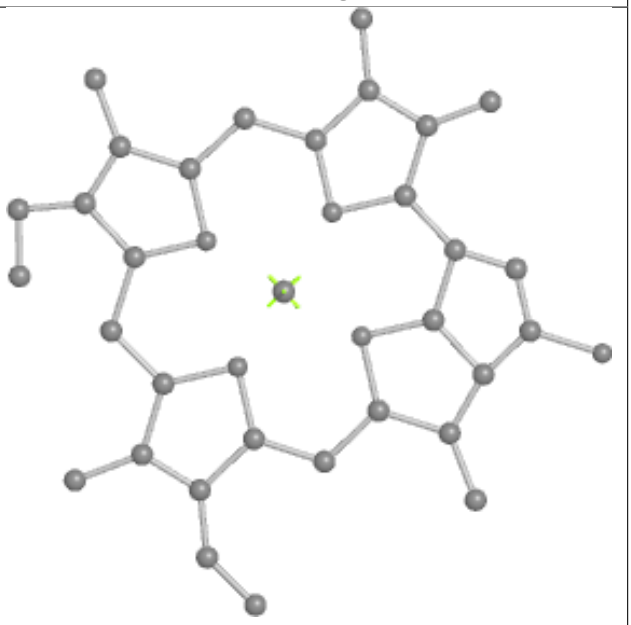
Bond lengths



Bond angles

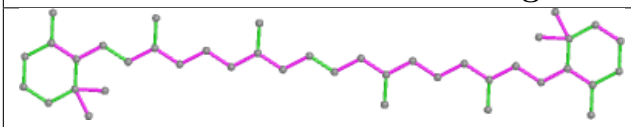


Torsions

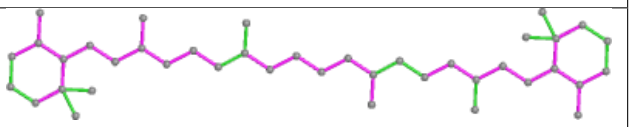


Rings

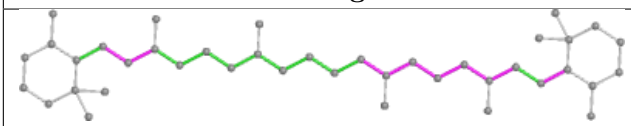
Ligand BCR A 852



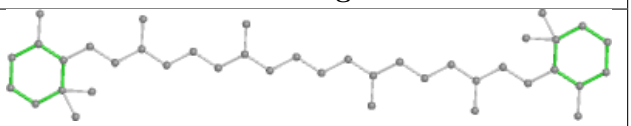
Bond lengths



Bond angles

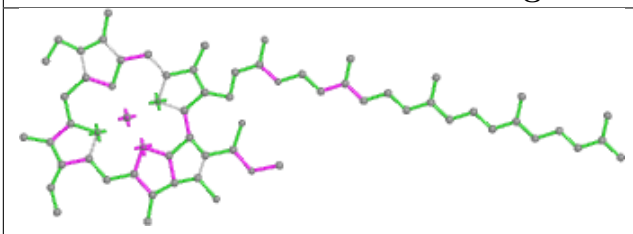


Torsions

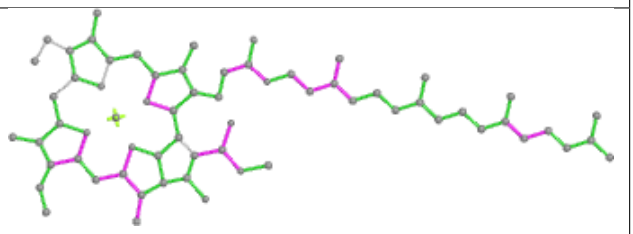


Rings

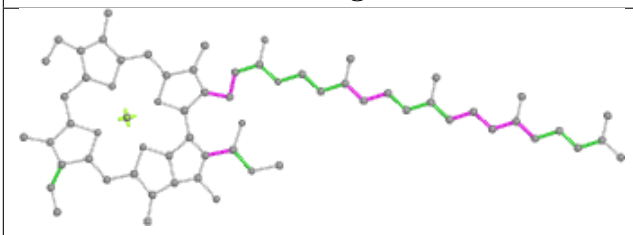
Ligand CLA A 821



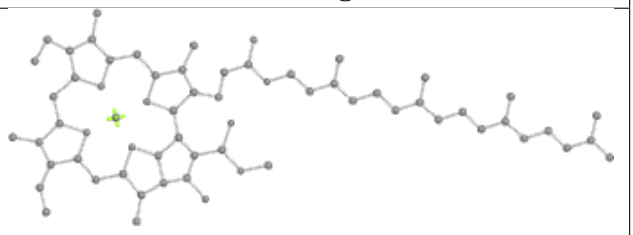
Bond lengths



Bond angles

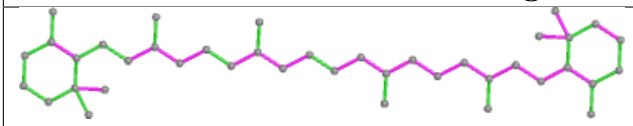


Torsions

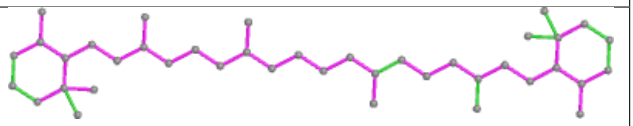


Rings

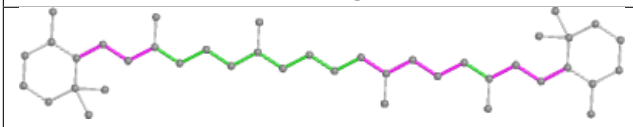
Ligand BCR B 849



Bond lengths



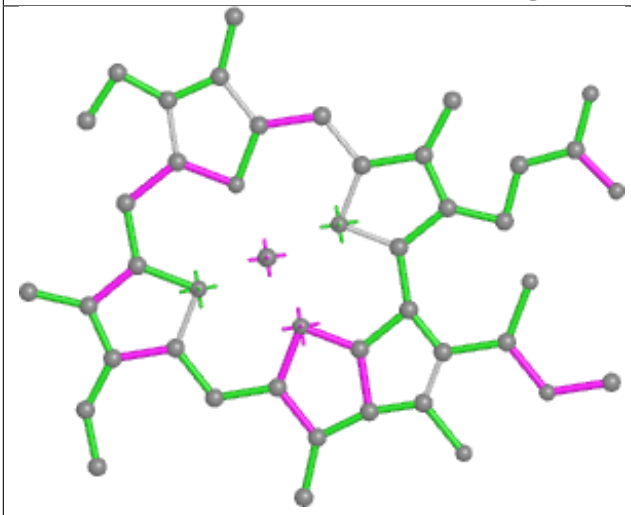
Bond angles



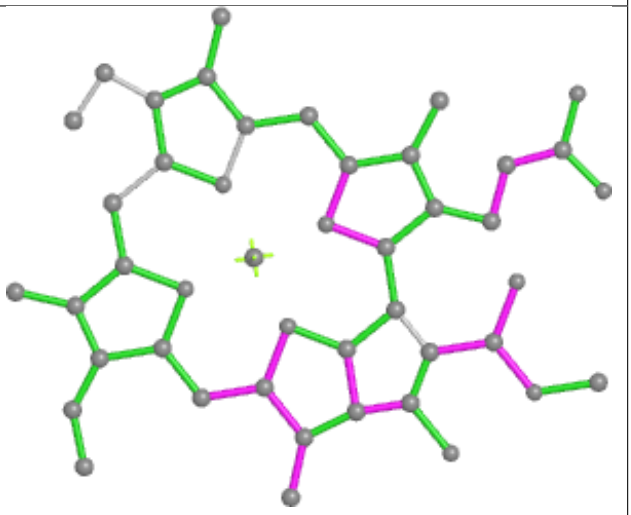
Torsions

Rings

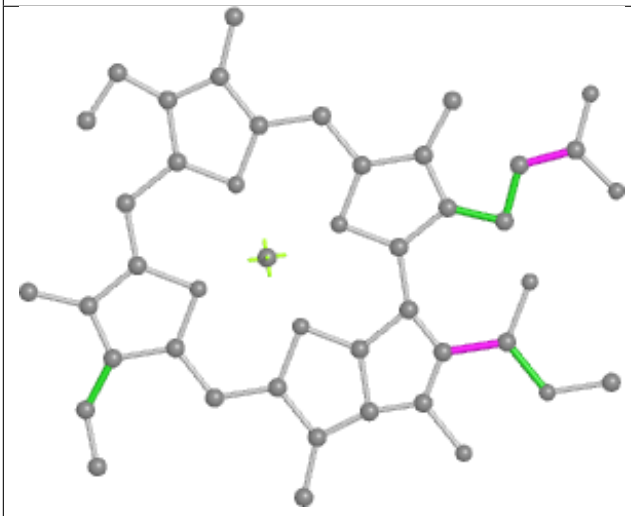
Ligand CLA B 809



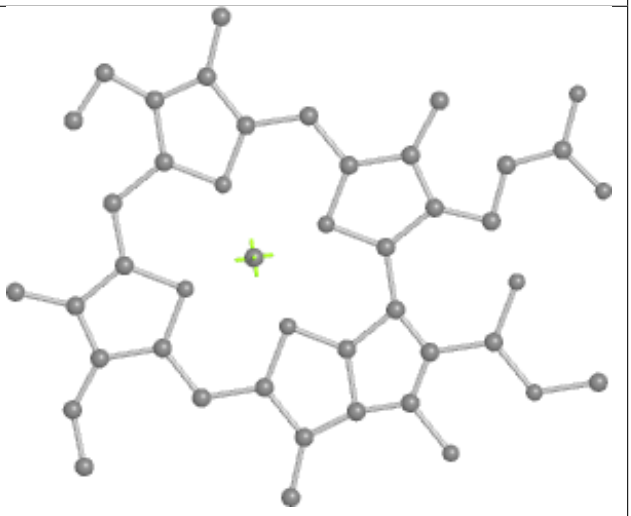
Bond lengths



Bond angles

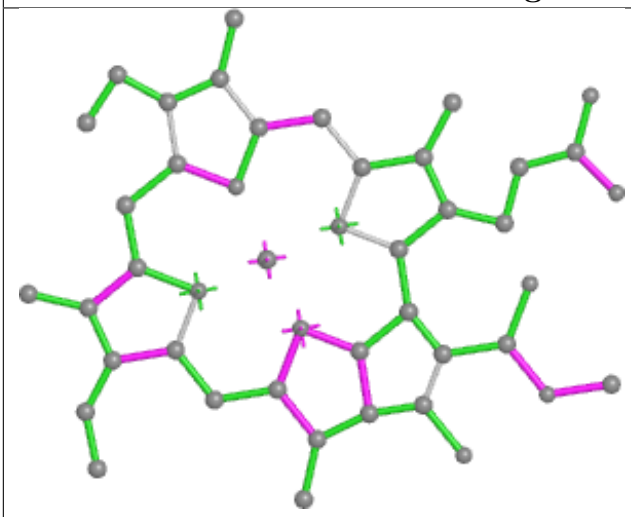


Torsions

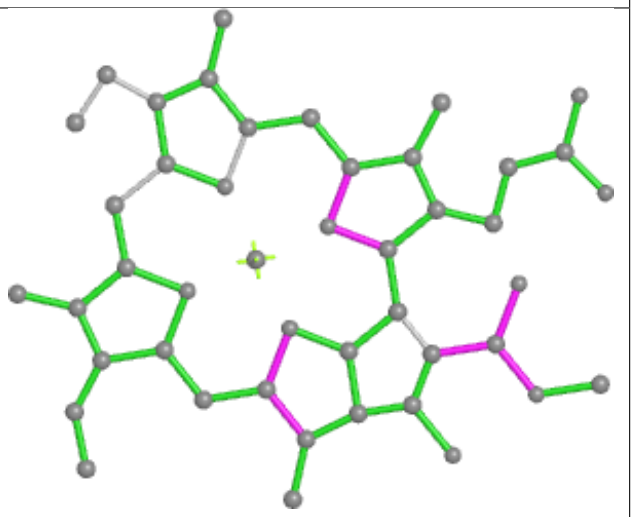


Rings

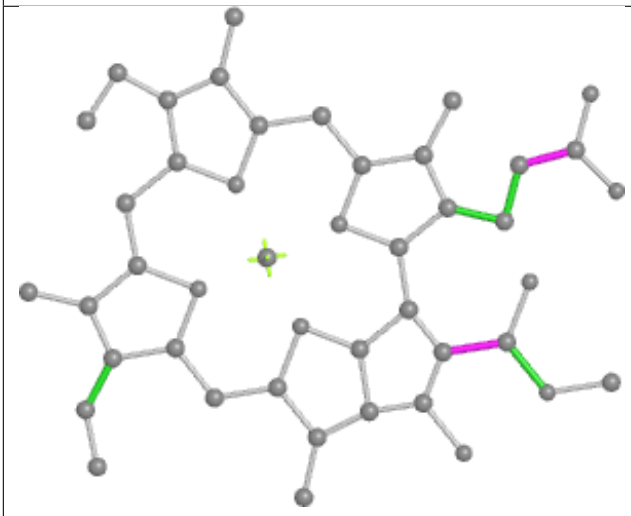
Ligand CLA B 833



Bond lengths



Bond angles



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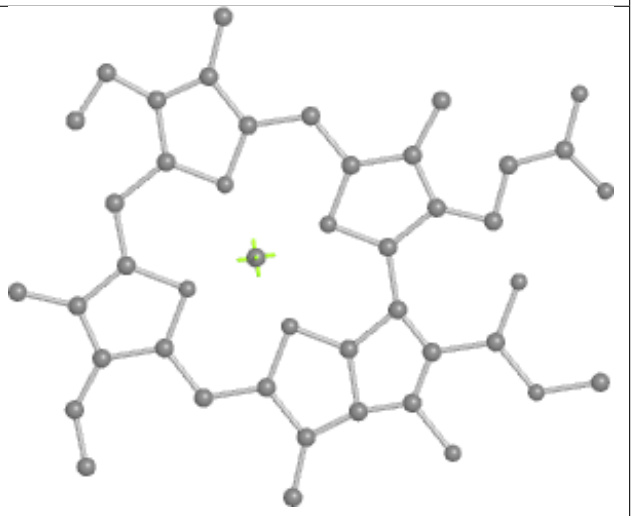
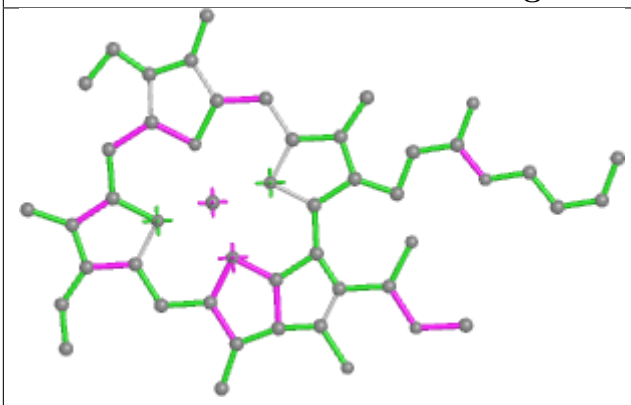
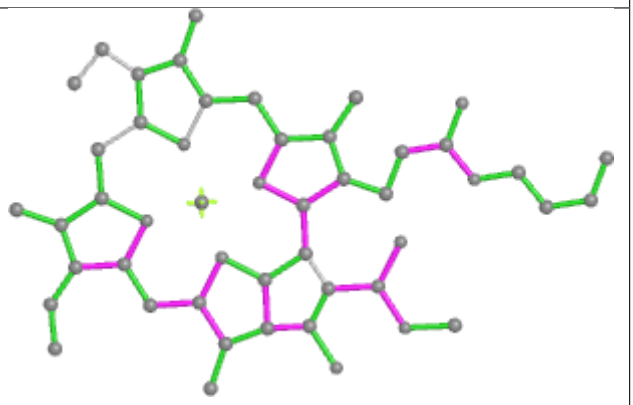


Rings

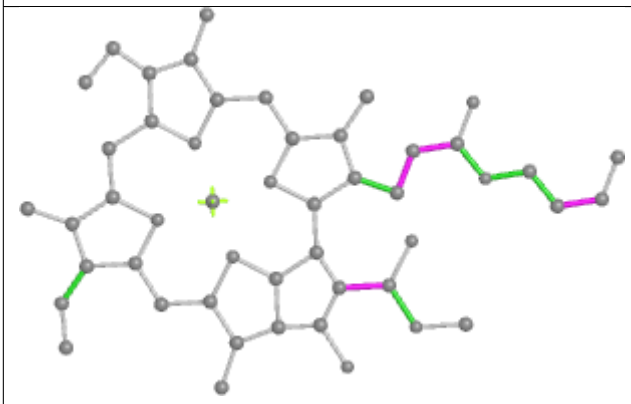
Ligand CLA A 822



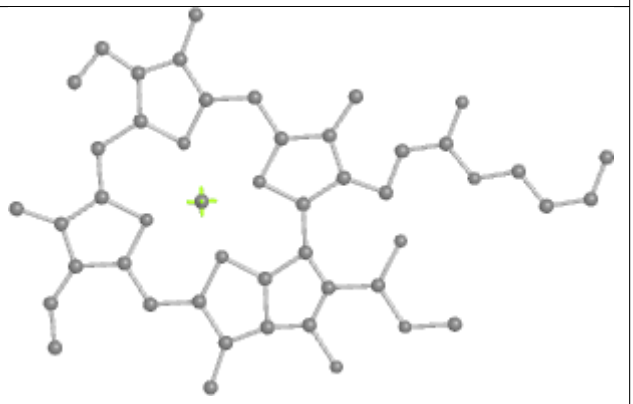
Bond lengths



Bond angles

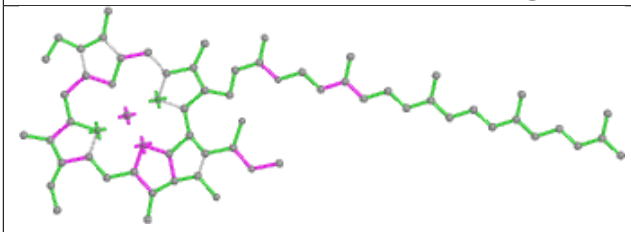


Torsions

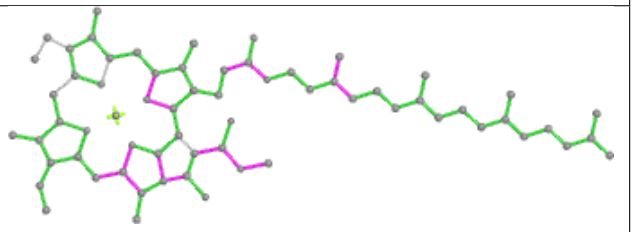


Rings

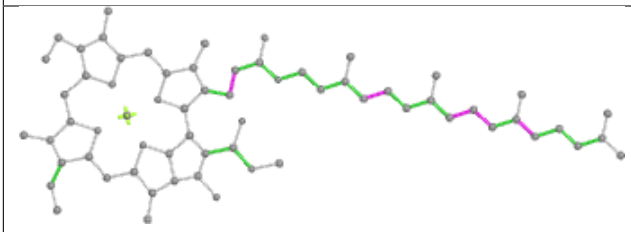
Ligand CLA A 833



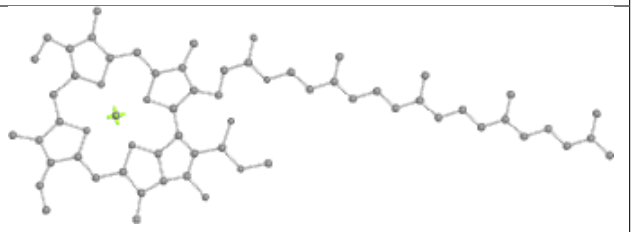
Bond lengths



Bond angles

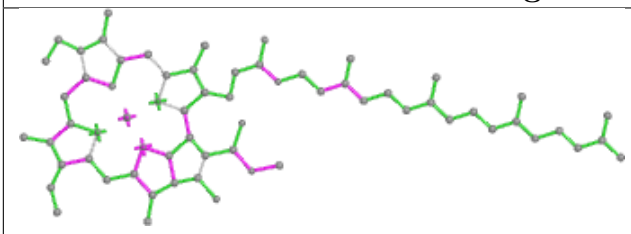


Torsions

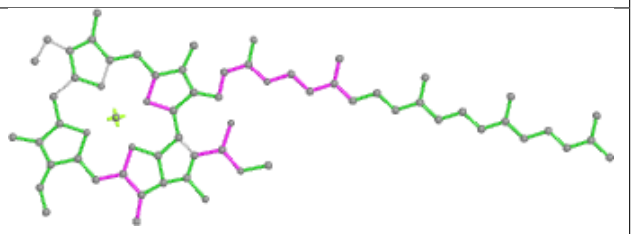


Rings

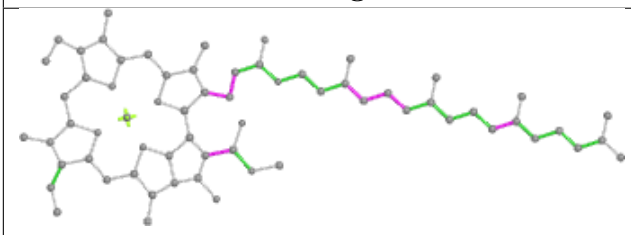
Ligand CLA A 840



Bond lengths



Bond angles



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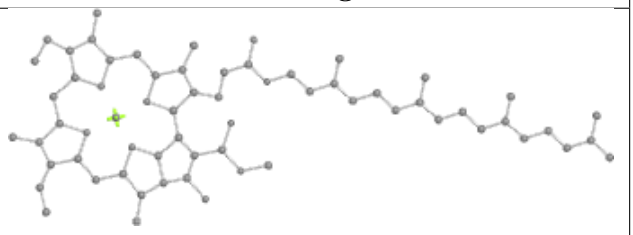
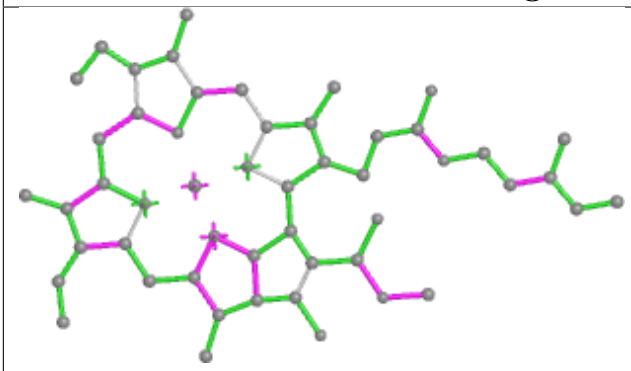
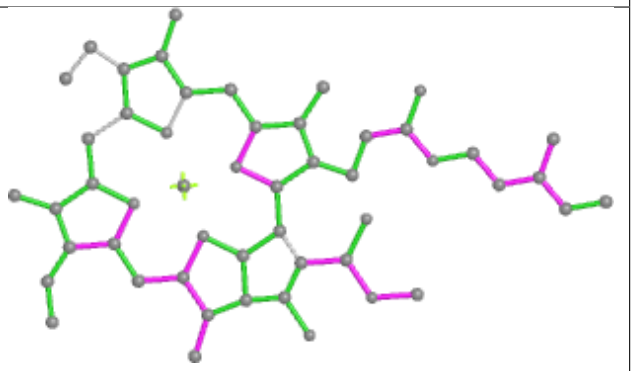


Rings

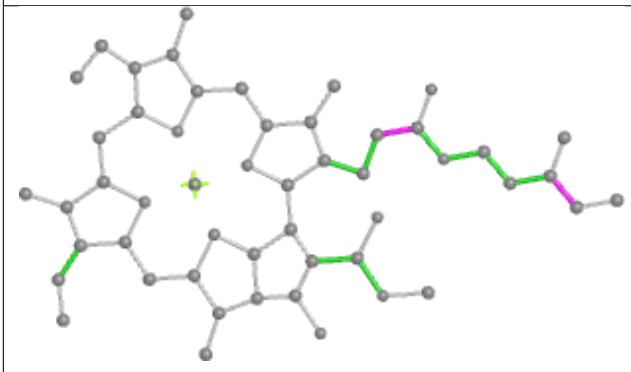
Ligand CLA A 841



Bond lengths



Bond angles



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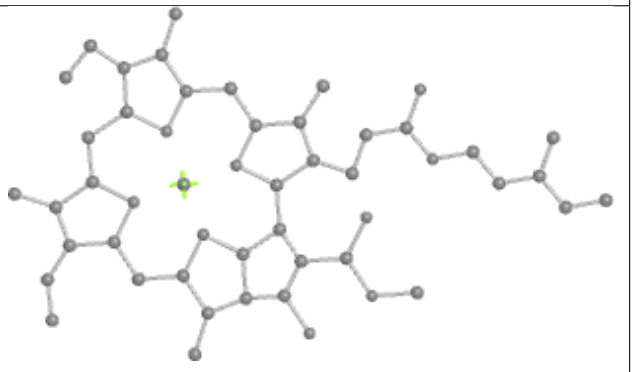
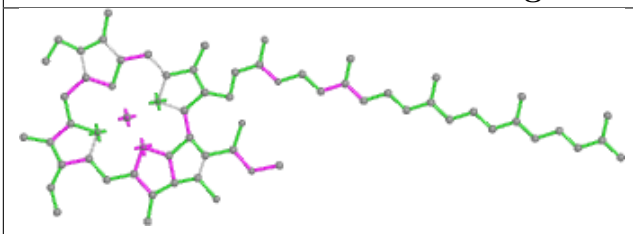
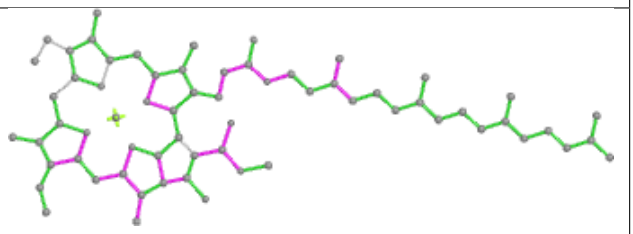


Rings

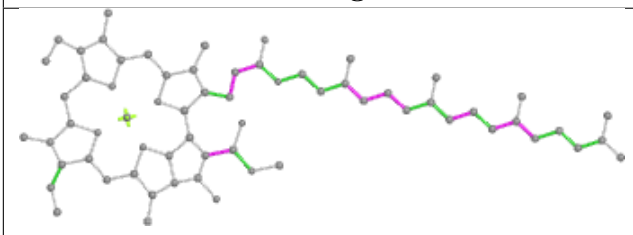
Ligand CLA B 812



Bond lengths



Bond angles



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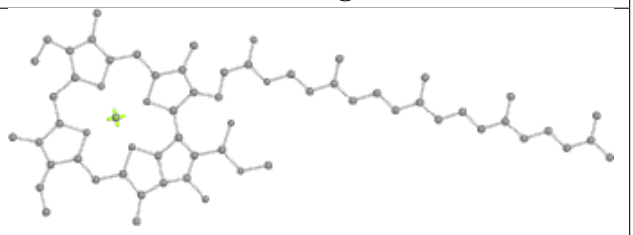
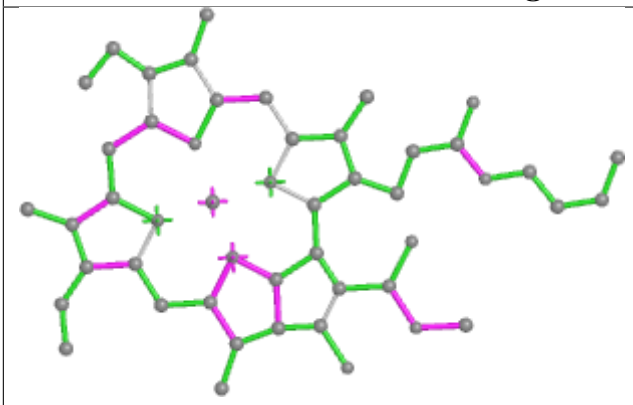
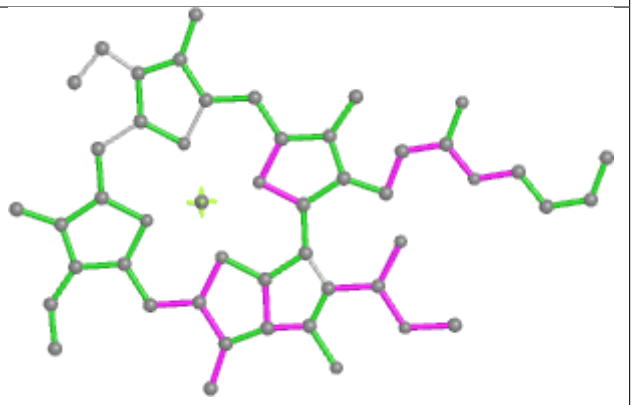


Rings

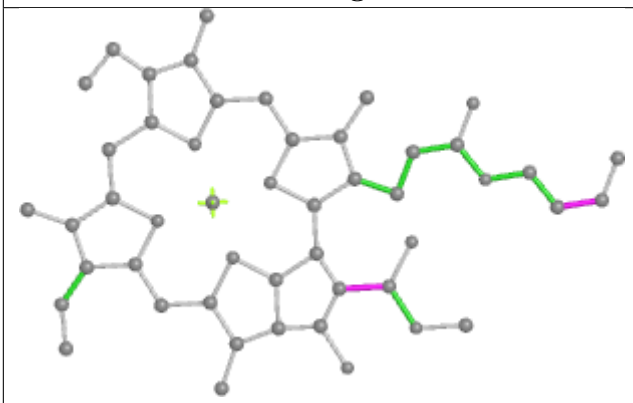
Ligand CLA B 829



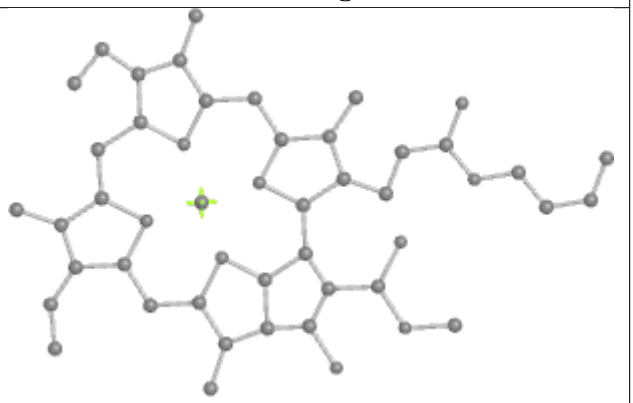
Bond lengths



Bond angles

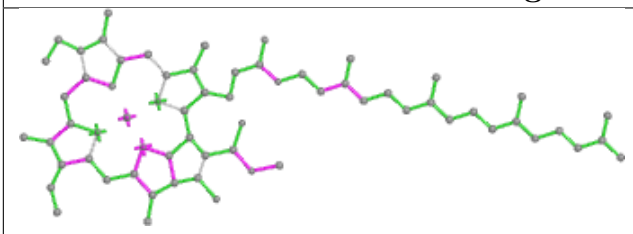


Torsions

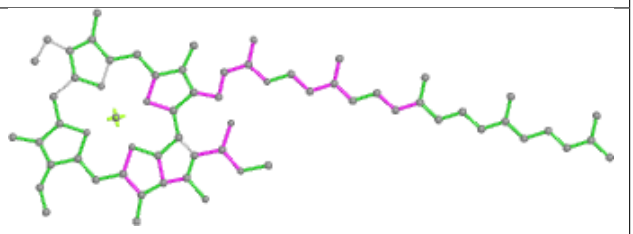


Rings

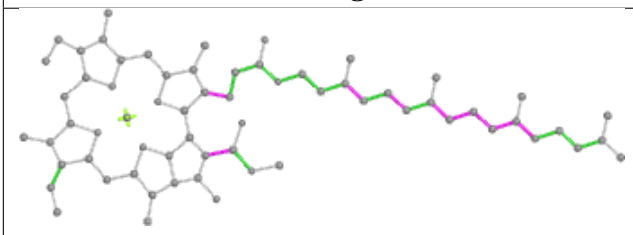
Ligand CLA B 838



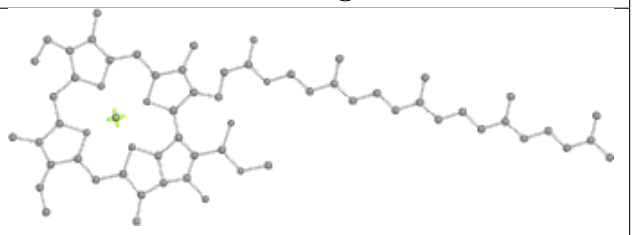
Bond lengths



Bond angles

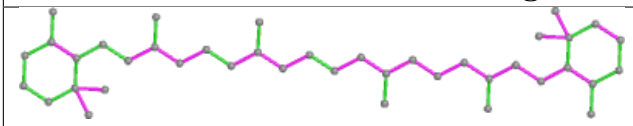


Torsions

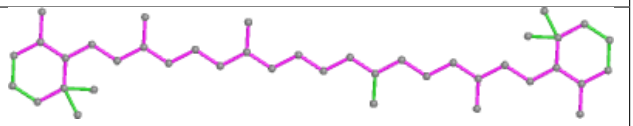


Rings

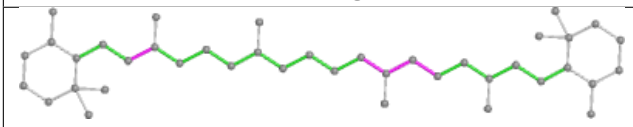
Ligand BCR A 849



Bond lengths



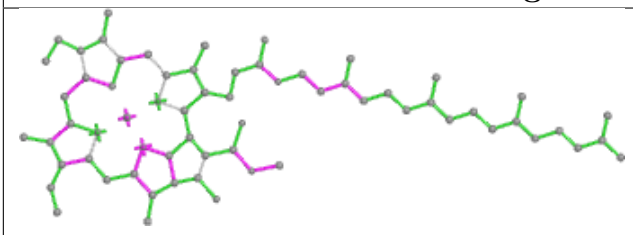
Bond angles



Torsions

Rings

Ligand CLA A 829



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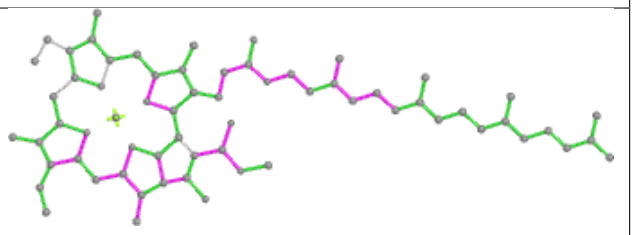
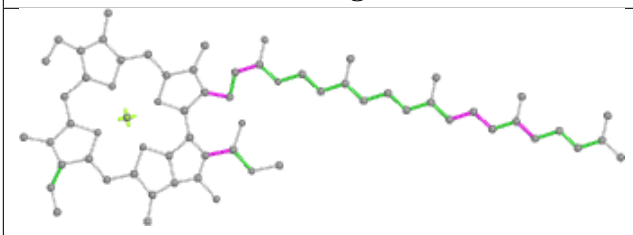
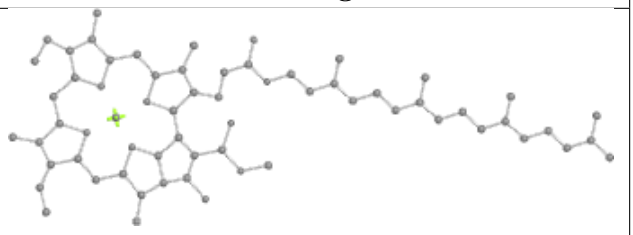


Bond angles

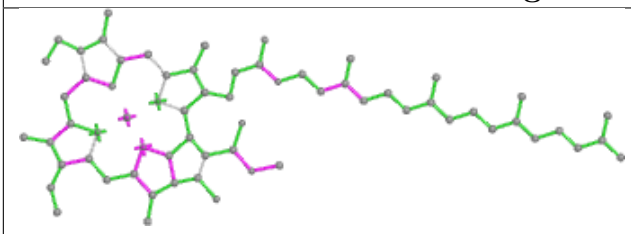


Torsions

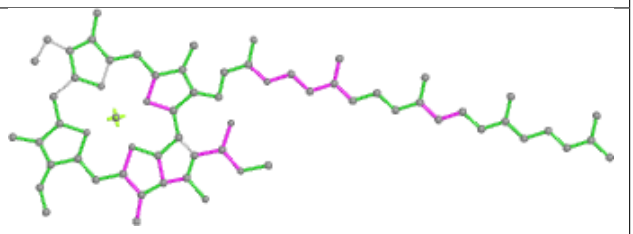


Rings

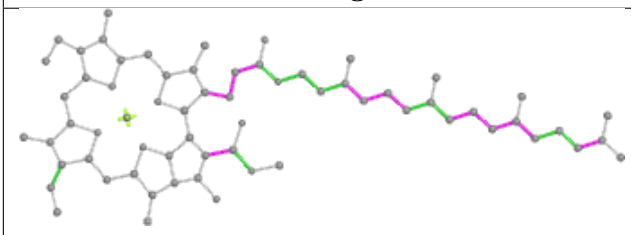
Ligand CLA A 828



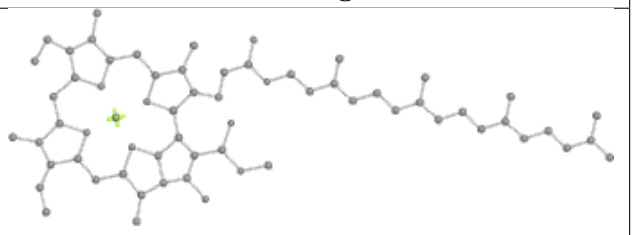
Bond lengths



Bond angles

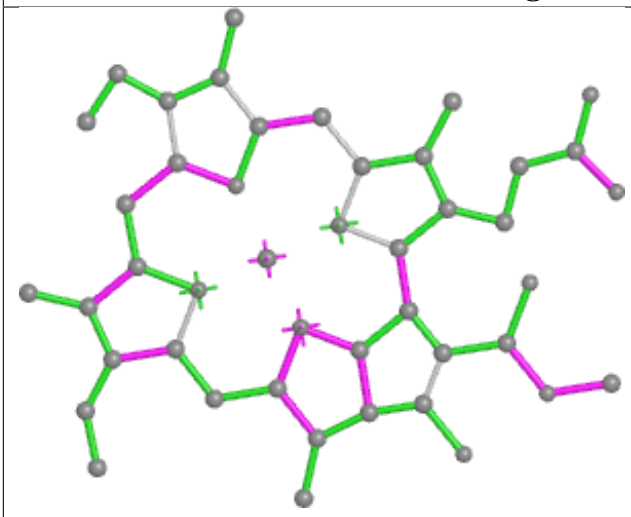


Torsions

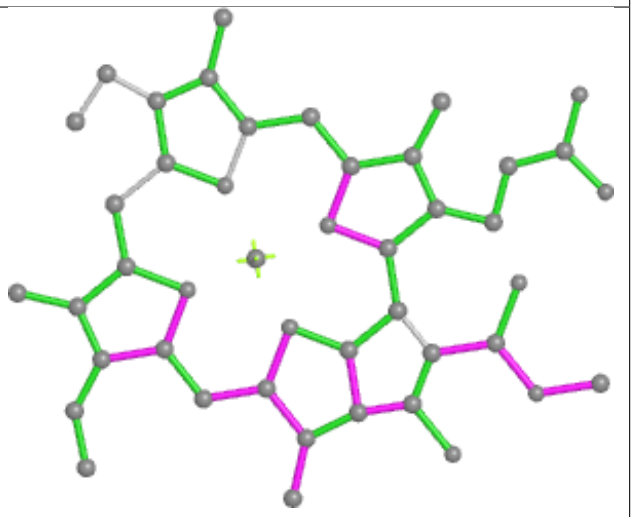


Rings

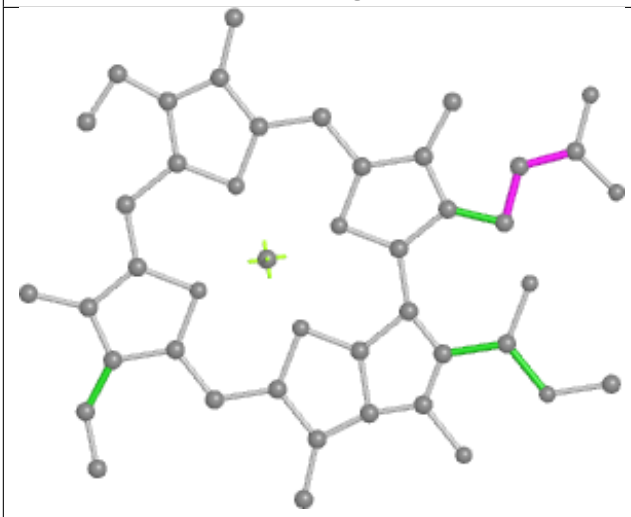
Ligand CLA B 810



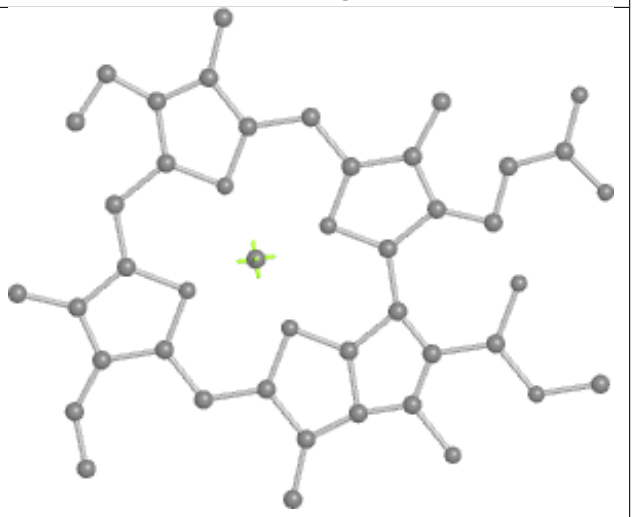
Bond lengths



Bond angles

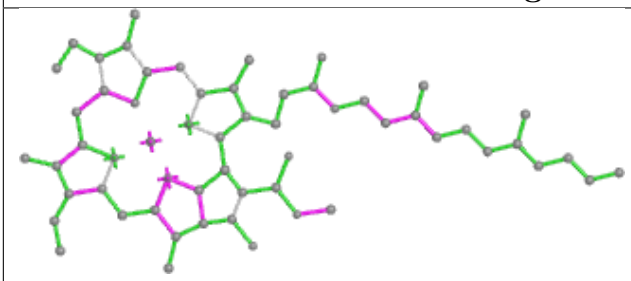


Torsions

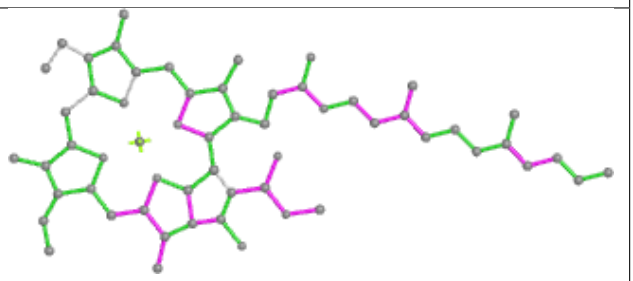


Rings

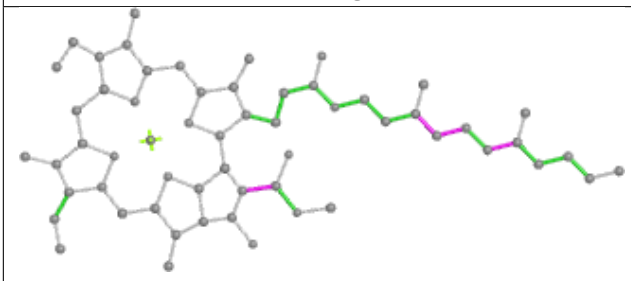
Ligand CLA B 831



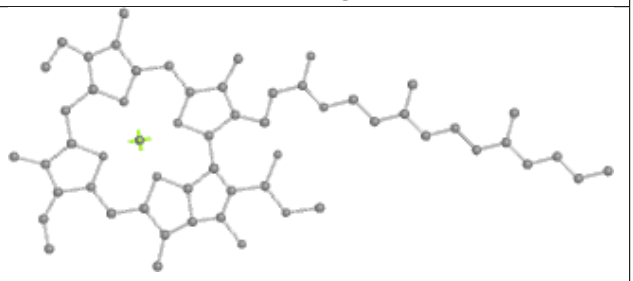
Bond lengths



Bond angles

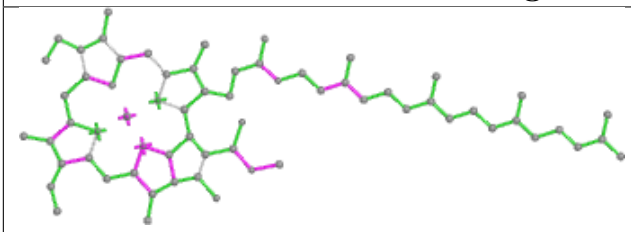


Torsions

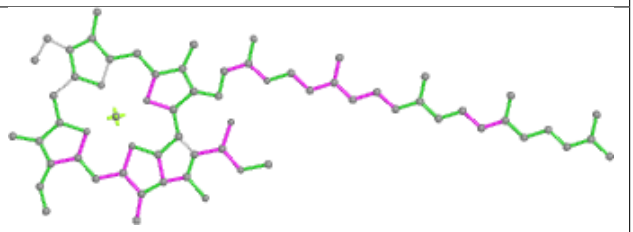


Rings

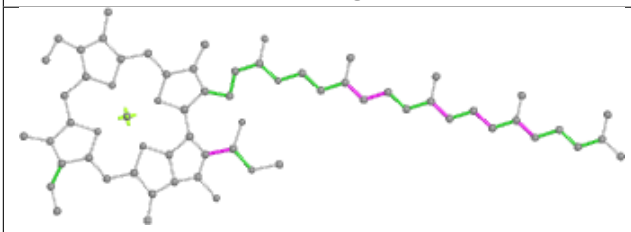
Ligand CLA A 803



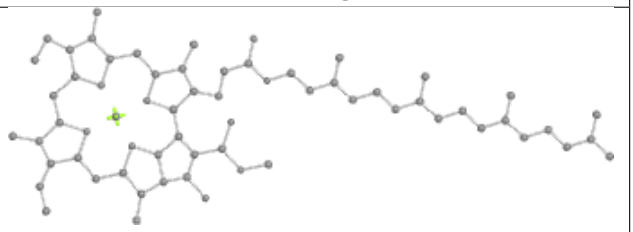
Bond lengths



Bond angles

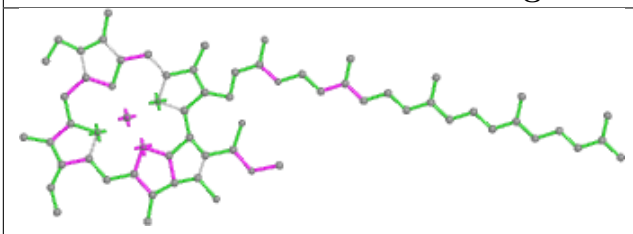


Torsions

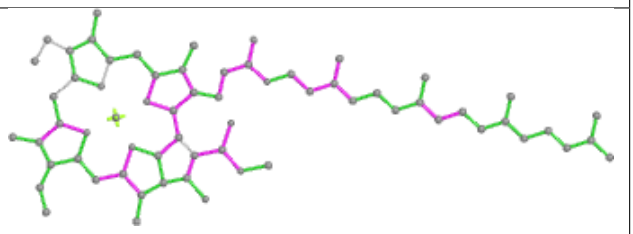


Rings

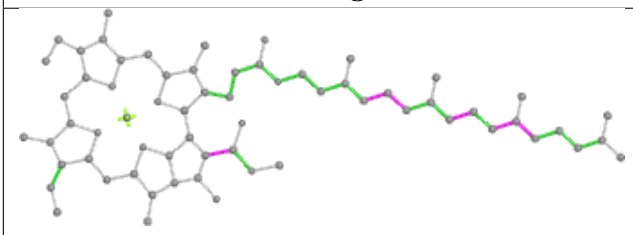
Ligand CLA A 809



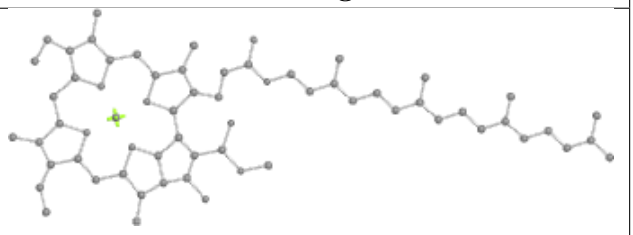
Bond lengths



Bond angles

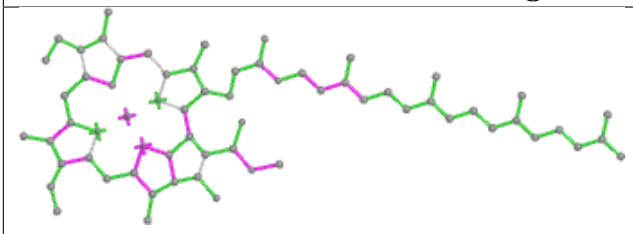


Torsions

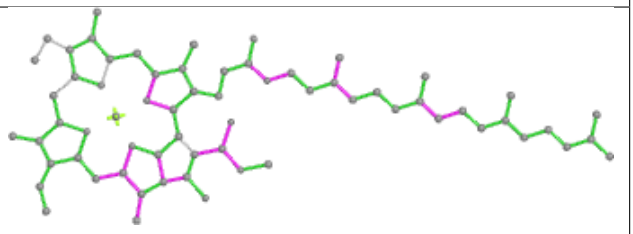


Rings

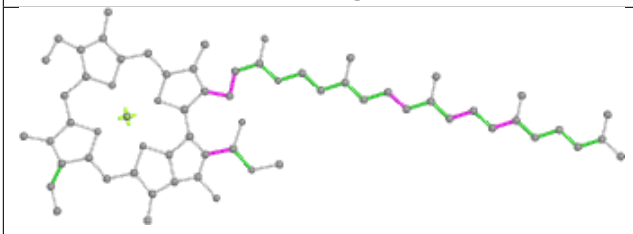
Ligand CLA B 836



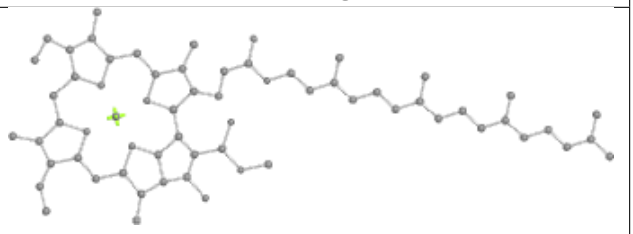
Bond lengths



Bond angles

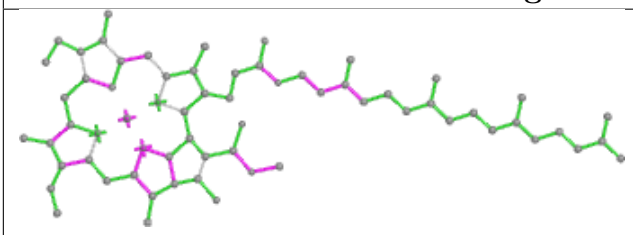


Torsions

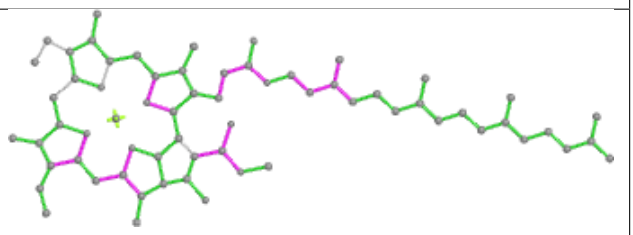


Rings

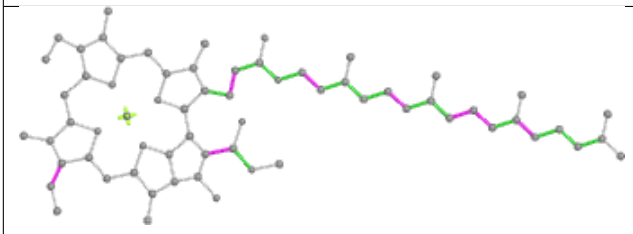
Ligand CLA B 830



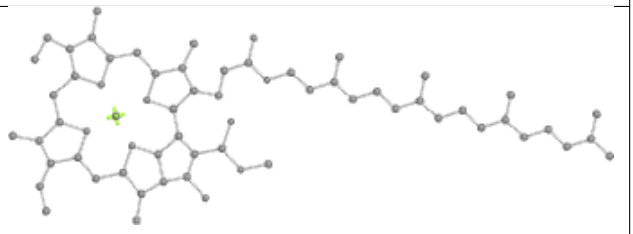
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	740/755 (98%)	0.11	22 (2%) 50 40	42, 99, 157, 202	0
2	B	739/740 (99%)	0.01	10 (1%) 75 65	34, 76, 126, 215	0
3	C	80/80 (100%)	-0.41	0 100 100	46, 72, 126, 138	0
4	D	138/138 (100%)	0.00	0 100 100	45, 72, 117, 137	0
5	E	69/75 (92%)	0.39	1 (1%) 75 65	77, 100, 148, 194	0
6	F	141/164 (85%)	-0.23	1 (0%) 87 82	54, 83, 136, 158	0
7	I	38/38 (100%)	0.14	0 100 100	10, 36, 74, 78	0
8	J	41/41 (100%)	-0.62	0 100 100	65, 89, 136, 165	0
9	K	46/83 (55%)	-0.41	0 100 100	55, 87, 141, 169	0
10	L	151/154 (98%)	-0.18	1 (0%) 87 82	14, 49, 104, 140	0
11	M	31/31 (100%)	-0.03	0 100 100	31, 51, 80, 92	0
12	X	29/35 (82%)	-0.27	1 (3%) 45 37	59, 80, 120, 155	0
All	All	2243/2334 (96%)	-0.01	36 (1%) 72 62	10, 81, 141, 215	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	ASP	4.2
1	A	24	SER	3.5
10	L	146	ASP	3.4
1	A	18	ASN	3.3
2	B	497	ASN	3.3

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 monosaccharides 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
13	CLA	A	844	41/65	0.67	0.40	116,136,148,281	0
13	CLA	A	815	45/65	0.73	0.64	111,150,177,185	0
13	CLA	M	1202	45/65	0.73	0.73	51,149,183,198	0
15	BCR	A	847	40/40	0.73	0.82	98,140,151,162	0
15	BCR	A	848	40/40	0.74	0.95	112,132,147,157	0
15	BCR	A	849	40/40	0.75	1.28	95,136,179,183	0
13	CLA	A	816	49/65	0.76	0.85	119,163,187,193	0
13	CLA	A	812	54/65	0.77	0.63	136,181,240,396	0
15	BCR	B	841	40/40	0.77	0.84	65,105,151,155	0
13	CLA	J	1102	45/65	0.78	0.38	75,111,128,280	0
13	CLA	A	836	45/65	0.79	0.47	63,96,163,234	0
13	CLA	A	810	45/65	0.79	0.50	109,136,151,223	0
15	BCR	B	850	40/40	0.80	0.42	83,107,144,146	0
16	LHG	X	101	23/49	0.80	0.40	78,81,207,208	0
15	BCR	A	850	40/40	0.81	0.90	56,96,126,139	0
13	CLA	B	834	45/65	0.81	0.54	91,118,151,158	0
13	CLA	A	807	51/65	0.81	0.51	87,100,151,177	0
13	CLA	A	827	65/65	0.81	0.72	68,103,137,248	0
13	CLA	A	813	60/65	0.82	0.60	115,146,178,366	0
13	CLA	B	819	45/65	0.82	0.50	98,131,171,173	0
13	CLA	A	822	49/65	0.82	0.47	102,126,157,235	0
18	LMG	B	848	55/55	0.82	0.67	42,51,67,114	0
13	CLA	A	845	52/65	0.83	0.44	56,78,188,214	0
13	CLA	A	855	45/65	0.83	0.40	95,118,140,153	0
13	CLA	B	814	55/65	0.83	0.70	77,122,182,325	0
15	BCR	F	1302	40/40	0.83	0.66	70,94,125,128	0
13	CLA	A	817	54/65	0.83	0.45	83,104,164,172	0
13	CLA	A	820	61/65	0.83	0.76	119,135,166,198	0
13	CLA	A	821	65/65	0.84	0.56	72,100,164,266	0
15	BCR	J	1105	40/40	0.84	0.43	63,67,71,71	0
13	CLA	B	810	45/65	0.85	0.49	47,84,145,182	0
13	CLA	B	831	58/65	0.85	0.46	80,101,148,333	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	CLA	A	835	54/65	0.85	0.50	54,79,117,204	0
13	CLA	B	813	45/65	0.86	0.40	51,86,132,141	0
15	BCR	B	843	40/40	0.86	0.60	45,59,82,86	0
13	CLA	B	820	55/65	0.86	0.49	77,105,141,146	0
13	CLA	B	828	45/65	0.86	0.43	70,80,132,193	0
13	CLA	A	823	51/65	0.86	0.51	74,129,153,156	0
16	LHG	A	853	49/49	0.86	0.69	57,74,107,127	0
13	CLA	B	833	45/65	0.86	0.47	77,104,141,148	0
13	CLA	B	818	47/65	0.86	0.61	56,99,146,292	0
15	BCR	A	852	40/40	0.87	0.82	78,107,149,162	0
13	CLA	B	829	49/65	0.87	0.47	80,85,125,141	0
13	CLA	A	840	65/65	0.87	0.44	77,87,117,198	0
13	CLA	M	1201	54/65	0.88	0.51	34,42,121,127	0
13	CLA	A	829	65/65	0.88	0.60	83,108,179,197	0
13	CLA	A	811	65/65	0.88	0.65	95,134,173,321	0
13	CLA	A	809	65/65	0.88	0.49	78,117,148,152	0
13	CLA	A	802	65/65	0.88	0.59	40,77,110,230	0
13	CLA	A	841	51/65	0.88	0.38	80,105,182,204	0
15	BCR	A	851	40/40	0.88	0.71	50,58,118,132	0
13	CLA	A	842	65/65	0.88	0.57	62,82,149,162	0
13	CLA	A	818	54/65	0.88	0.47	92,136,168,207	0
15	BCR	B	842	40/40	0.88	0.66	48,76,129,134	0
13	CLA	A	824	59/65	0.88	0.54	59,101,164,321	0
13	CLA	A	825	65/65	0.88	0.32	74,102,152,193	0
13	CLA	B	809	45/65	0.88	0.45	39,95,125,308	0
15	BCR	J	1104	40/40	0.88	0.82	64,78,113,120	0
13	CLA	B	835	60/65	0.88	0.32	65,106,240,292	0
15	BCR	M	1203	40/40	0.88	0.53	43,48,87,92	0
13	CLA	B	836	65/65	0.88	0.42	69,98,146,234	0
13	CLA	A	819	65/65	0.88	0.59	97,140,181,328	0
13	CLA	J	1103	37/65	0.88	0.31	85,117,155,158	0
13	CLA	B	832	45/65	0.89	0.39	71,121,142,247	0
13	CLA	A	804	59/65	0.89	0.59	83,99,117,144	0
13	CLA	B	803	65/65	0.89	0.64	40,68,95,180	0
13	CLA	B	806	65/65	0.89	0.45	33,63,107,170	0
13	CLA	B	807	65/65	0.89	0.63	38,65,106,122	0
13	CLA	F	1301	45/65	0.89	0.45	94,137,167,175	0
13	CLA	A	826	65/65	0.89	0.61	53,80,112,127	0
13	CLA	A	805	65/65	0.89	0.58	85,98,117,126	0
13	CLA	A	828	65/65	0.89	0.49	59,74,127,289	0
15	BCR	B	845	40/40	0.90	0.40	60,66,78,82	0
15	BCR	B	846	40/40	0.90	0.70	75,91,131,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	CLA	A	833	65/65	0.90	0.56	39,45,110,121	0
13	CLA	A	814	45/65	0.90	0.32	108,150,172,174	0
13	CLA	L	1004	65/65	0.90	0.44	21,31,64,72	0
13	CLA	B	817	65/65	0.90	0.48	57,65,113,125	0
13	CLA	A	831	50/65	0.90	0.39	45,76,105,144	0
13	CLA	B	838	65/65	0.90	0.54	35,45,102,125	0
13	CLA	A	843	65/65	0.90	0.49	56,83,169,197	0
15	BCR	B	844	25/40	0.90	0.44	65,68,113,118	0
13	CLA	X	102	45/65	0.91	0.26	67,104,127,283	0
14	PQN	B	840	33/33	0.91	0.73	56,84,105,121	0
13	CLA	B	804	65/65	0.91	0.57	45,51,117,199	0
13	CLA	B	839	65/65	0.91	0.49	35,49,151,215	0
13	CLA	A	832	65/65	0.91	0.34	42,45,81,134	0
13	CLA	J	1101	65/65	0.91	0.52	77,129,178,357	0
13	CLA	A	806	65/65	0.91	0.57	63,80,155,164	0
13	CLA	A	830	65/65	0.91	0.51	59,71,105,119	0
13	CLA	B	802	65/65	0.91	0.53	61,82,112,165	0
16	LHG	A	854	27/49	0.91	0.37	49,58,88,122	0
13	CLA	B	824	65/65	0.91	0.38	58,65,88,96	0
13	CLA	A	808	65/65	0.91	0.40	72,89,172,177	0
13	CLA	L	1003	65/65	0.92	0.35	16,52,179,216	0
13	CLA	B	821	45/65	0.92	0.35	63,69,105,191	0
13	CLA	B	808	65/65	0.92	0.60	36,41,97,103	0
13	CLA	B	826	65/65	0.92	0.51	42,47,127,149	0
13	CLA	B	837	47/65	0.92	0.27	65,71,119,193	0
15	BCR	B	847	40/40	0.92	0.70	40,51,116,126	0
14	PQN	A	846	33/33	0.92	0.56	55,64,82,82	0
13	CLA	B	815	59/65	0.92	0.48	55,58,76,293	0
15	BCR	I	102	40/40	0.92	0.38	19,20,48,52	0
13	CLA	A	803	65/65	0.92	0.57	76,100,142,222	0
13	CLA	B	830	65/65	0.92	0.61	82,91,129,139	0
13	CLA	I	101	65/65	0.92	0.38	33,57,85,338	0
13	CLA	A	837	51/65	0.92	0.43	52,56,96,147	0
13	CLA	B	812	65/65	0.92	0.41	37,42,111,117	0
13	CLA	A	838	65/65	0.92	0.37	45,81,109,114	0
13	CLA	L	1002	65/65	0.92	0.36	29,65,103,148	0
13	CLA	B	825	65/65	0.93	0.47	40,60,136,157	0
15	BCR	L	1005	40/40	0.93	0.45	11,16,81,93	0
15	BCR	L	1006	40/40	0.93	0.29	16,24,64,78	0
15	BCR	B	849	40/40	0.93	0.41	12,43,147,152	0
13	CLA	B	801	65/65	0.93	0.42	57,68,123,322	0
13	CLA	B	827	65/65	0.93	0.47	44,66,95,108	0

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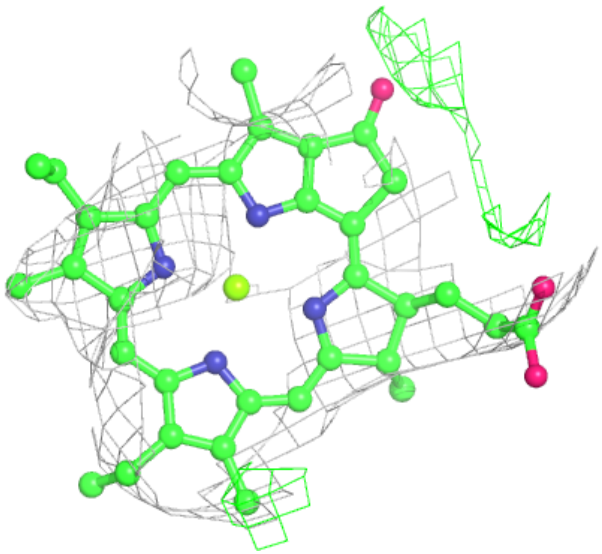
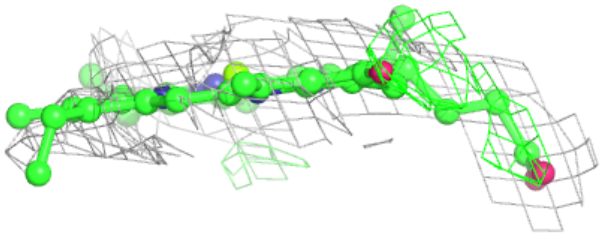
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	CLA	B	811	65/65	0.93	0.58	48,71,108,145	0
13	CLA	A	834	65/65	0.93	0.44	39,40,92,96	0
13	CLA	A	839	47/65	0.94	0.31	48,51,119,202	0
13	CLA	B	816	60/65	0.94	0.54	46,53,111,221	0
13	CLA	A	801	65/65	0.94	0.49	44,53,82,89	0
13	CLA	B	822	54/65	0.94	0.44	61,86,118,158	0
13	CLA	B	823	46/65	0.94	0.28	59,68,120,137	0
13	CLA	B	805	65/65	0.94	0.41	41,48,97,150	0
19	CA	L	1001	1/1	0.94	0.14	22,22,22,22	0
17	SF4	C	102	8/8	0.99	0.16	47,48,122,359	0
17	SF4	A	856	8/8	0.99	0.22	49,50,150,174	0
17	SF4	C	101	8/8	0.99	0.20	48,48,49,62	0

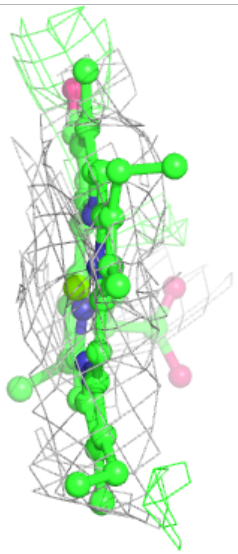
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA A 844:

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

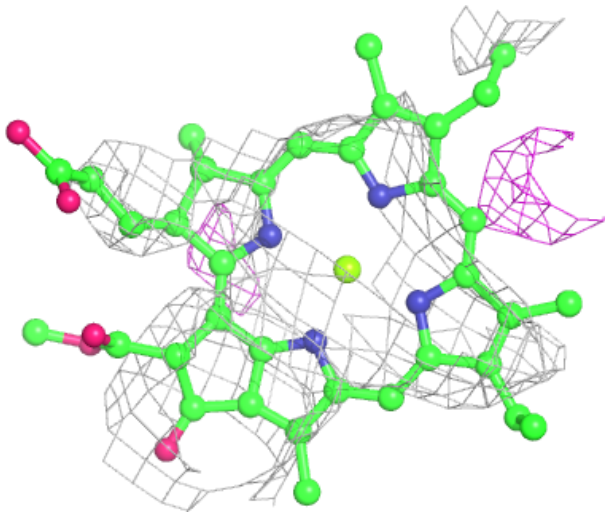


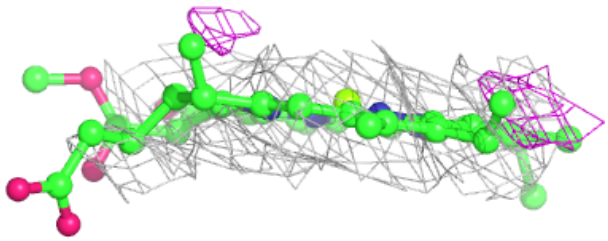


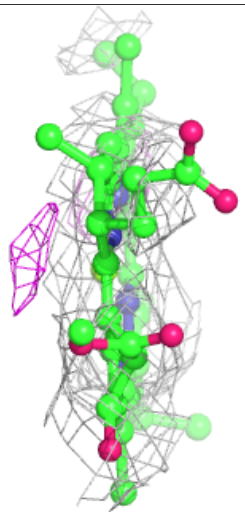


Electron density around CLA A 815:

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

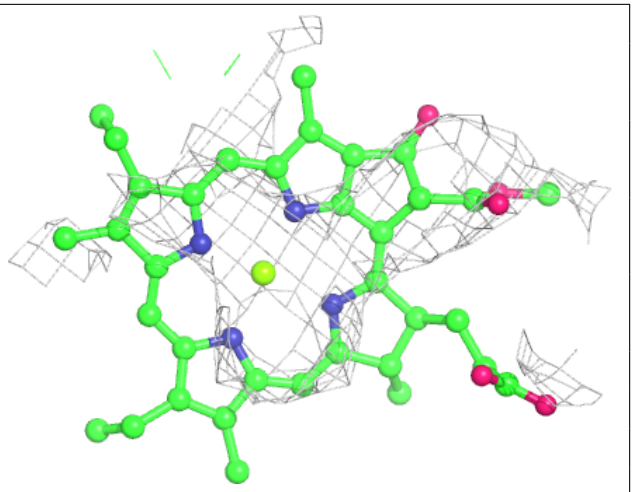


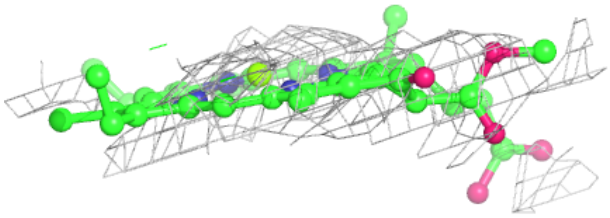


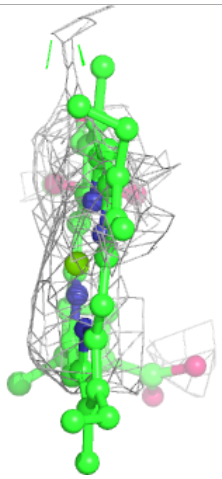


Electron density around CLA M 1202:

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

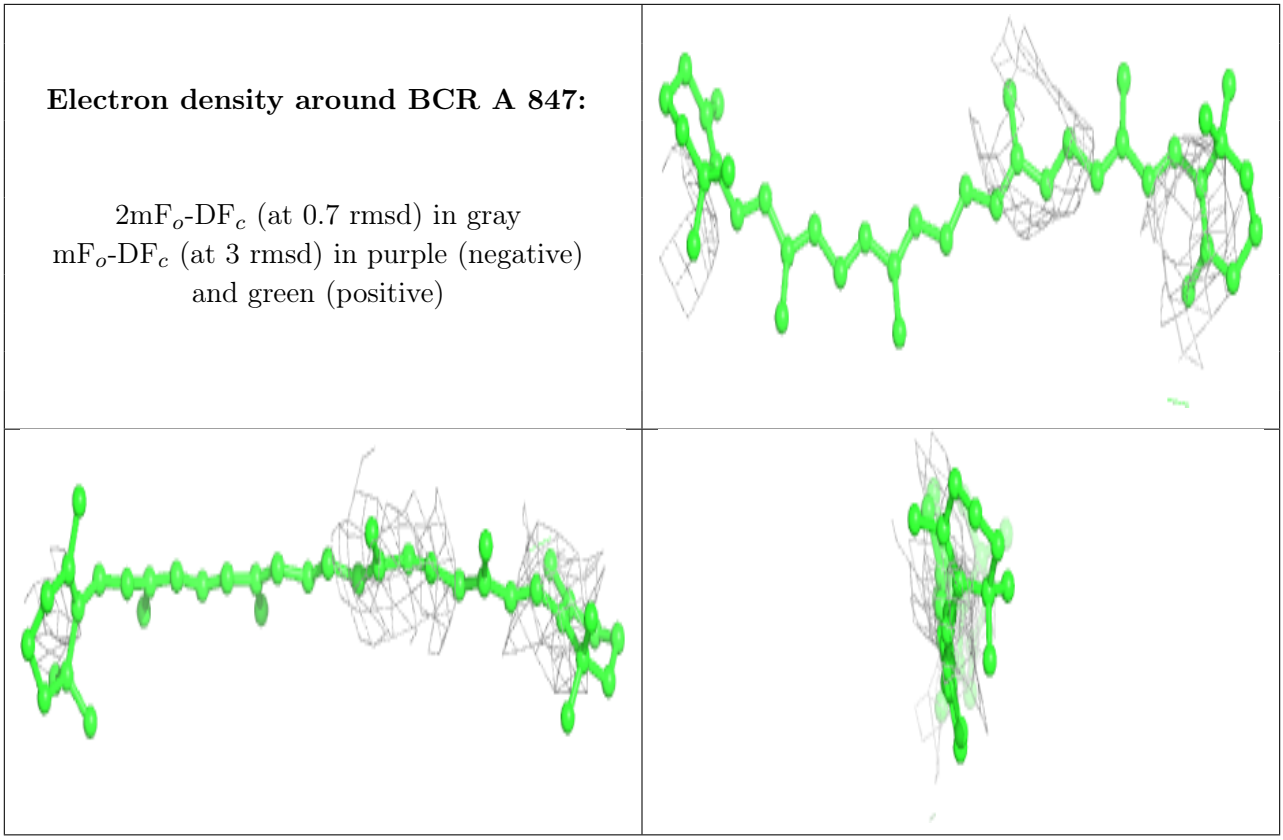






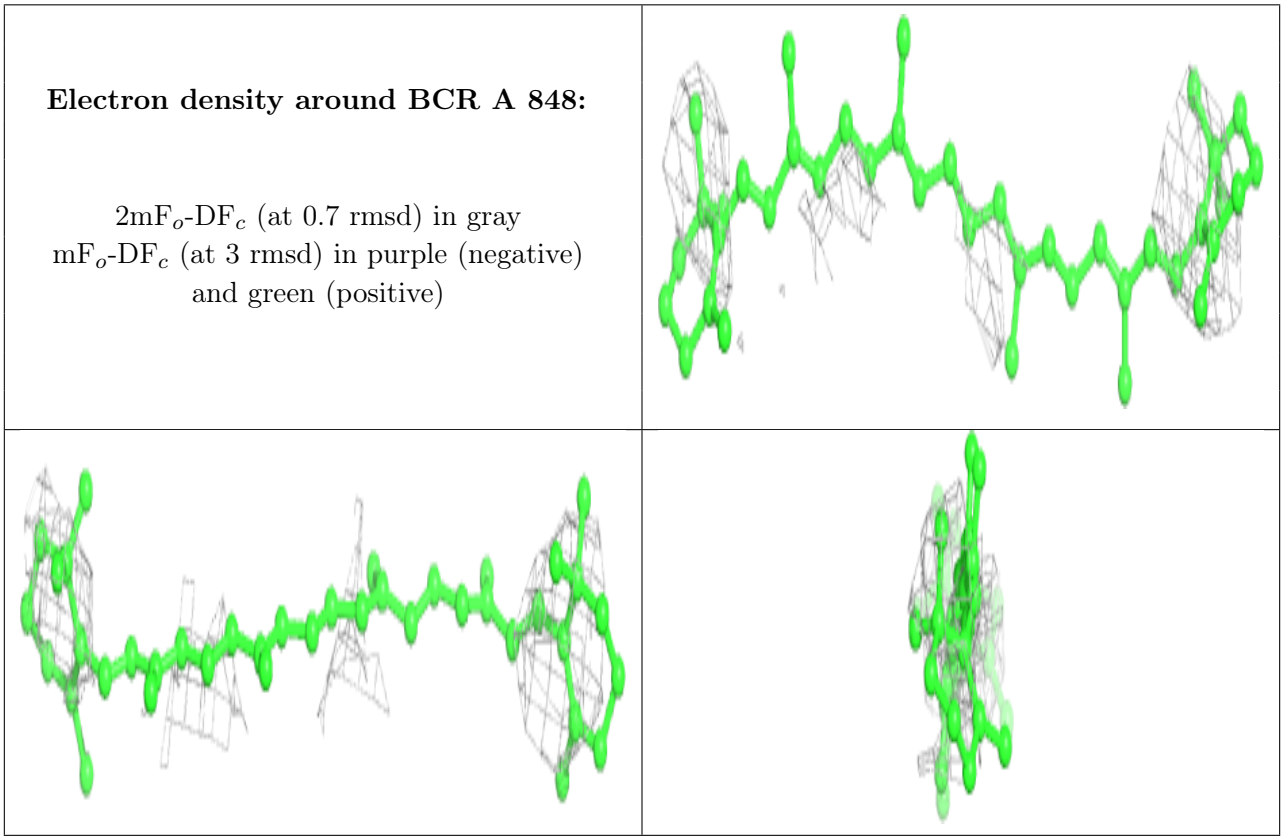
Electron density around BCR A 847:

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



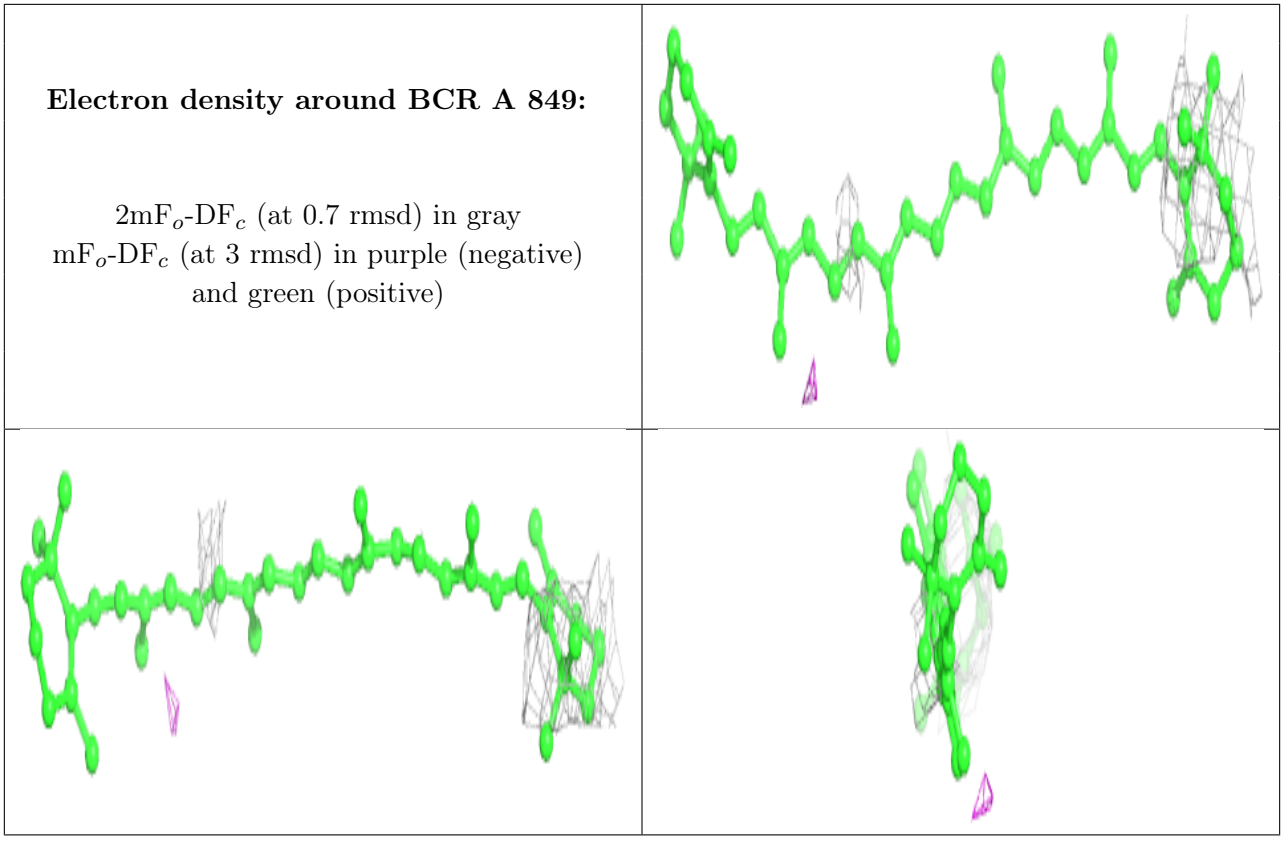
Electron density around BCR A 848:

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



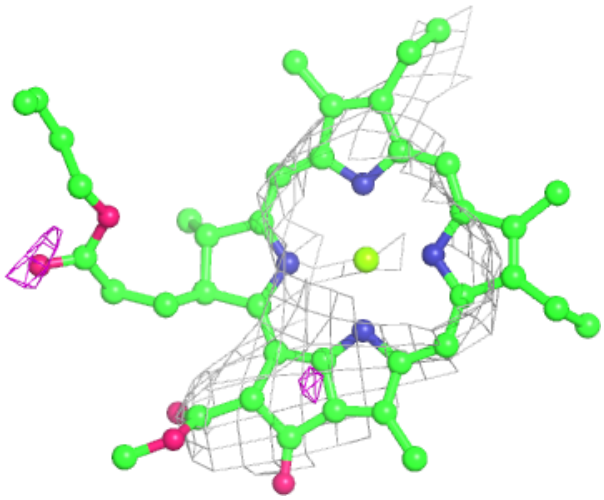
Electron density around BCR A 849:

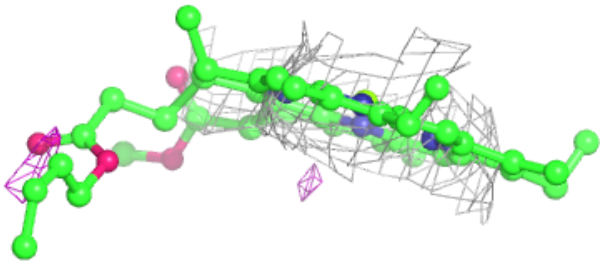
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

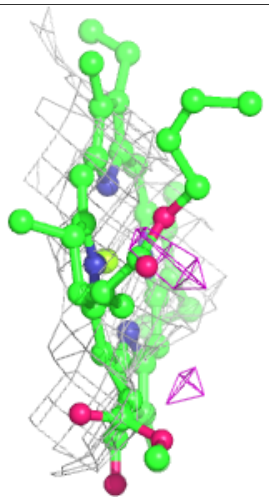


Electron density around CLA A 816:

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

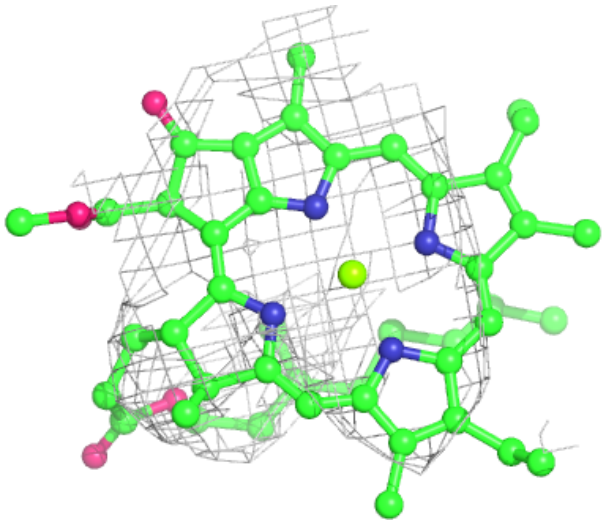


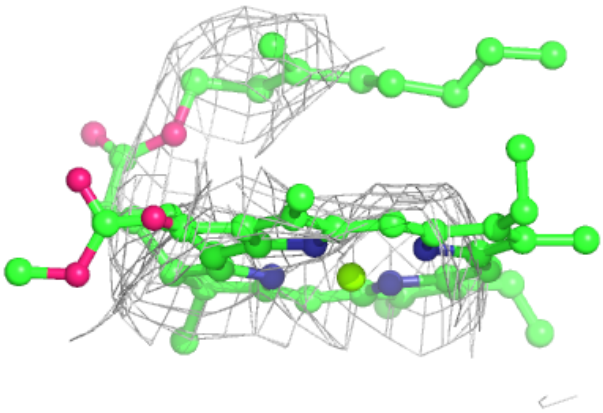


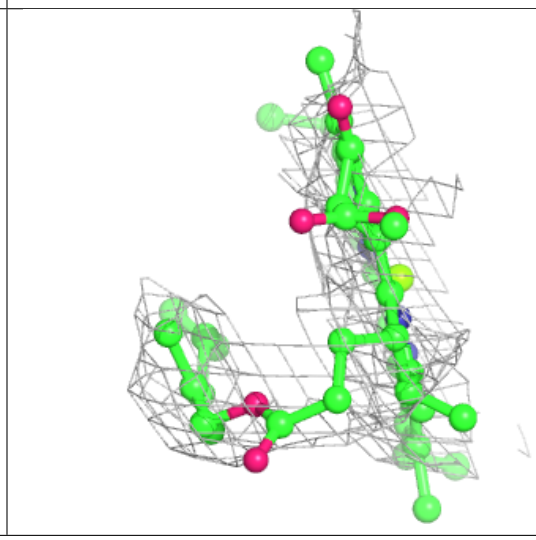


Electron density around CLA A 812:

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

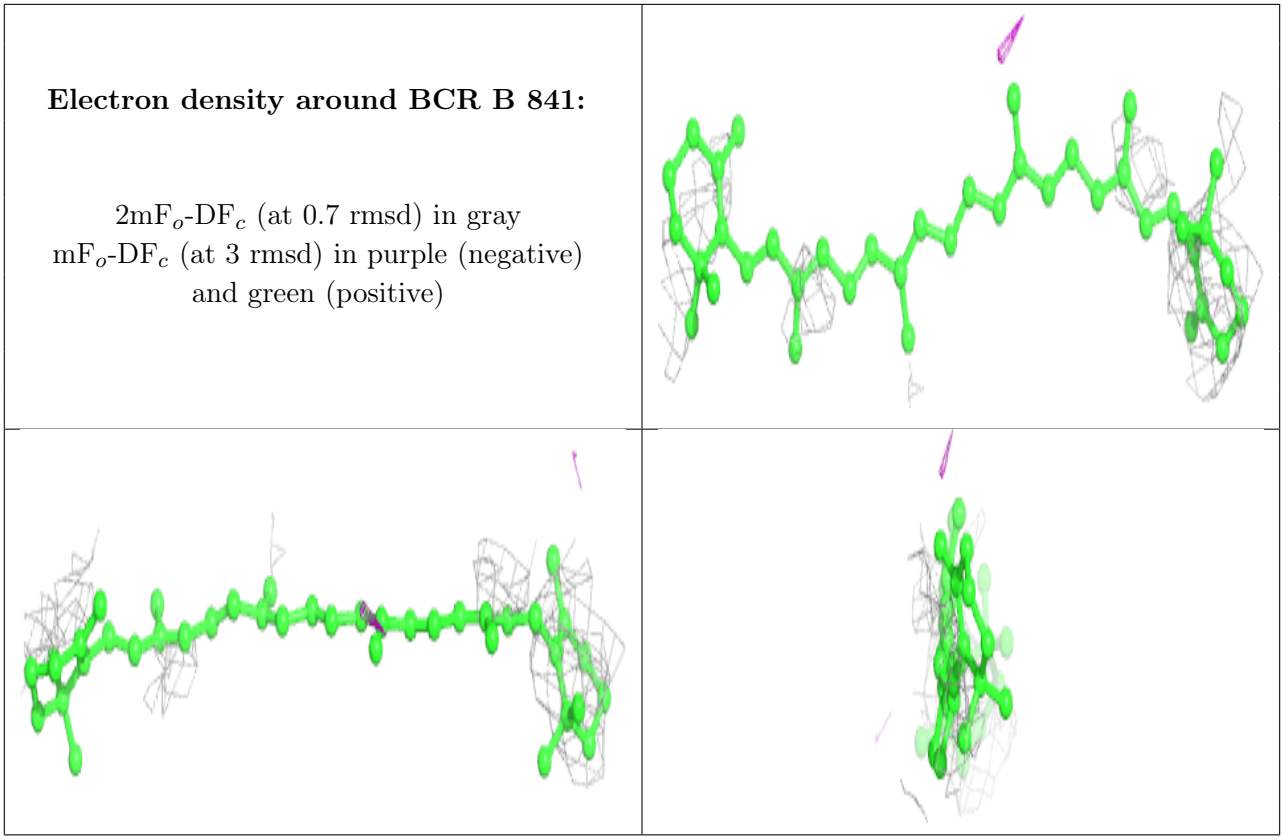






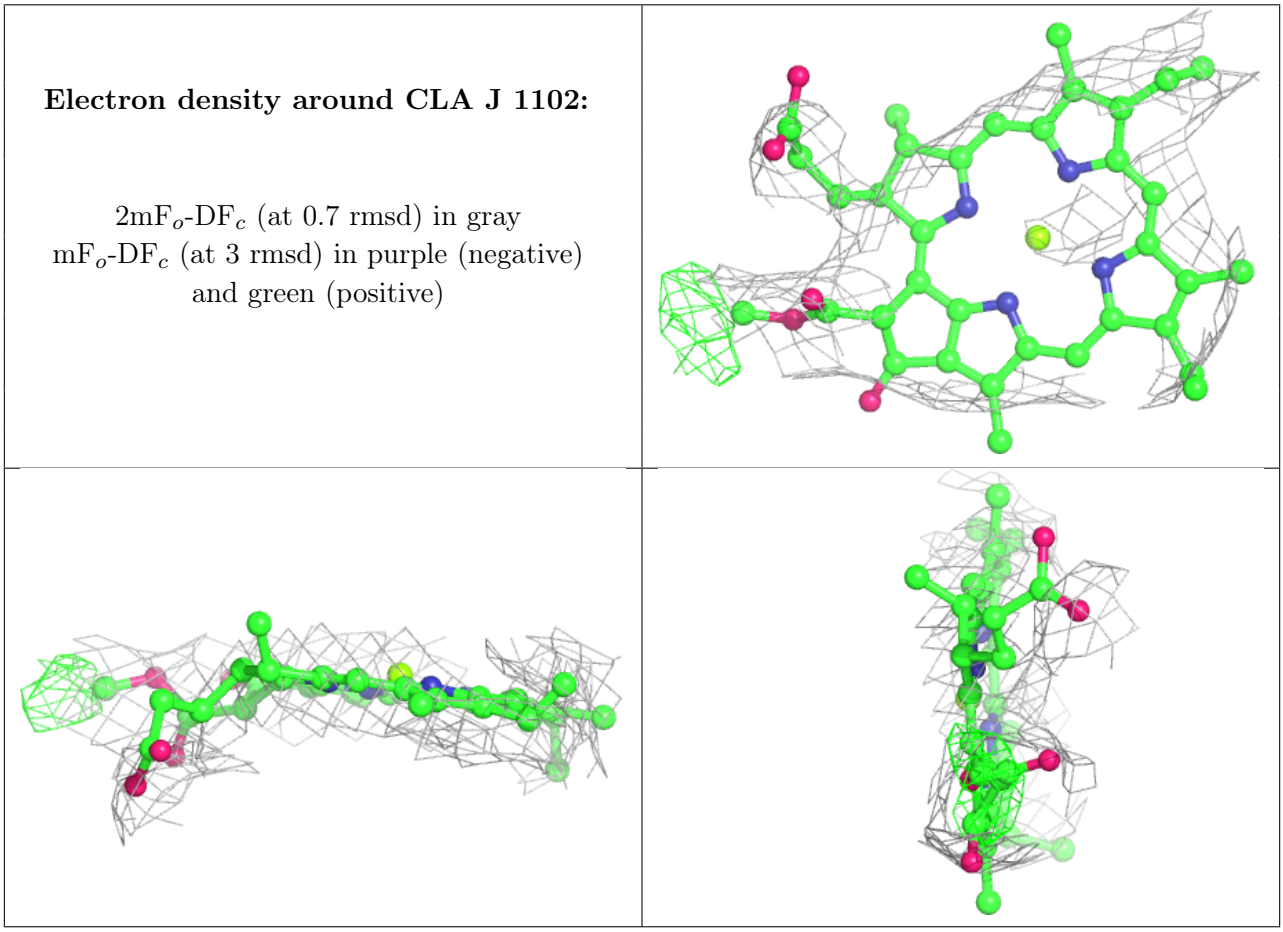
Electron density around BCR B 841:

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



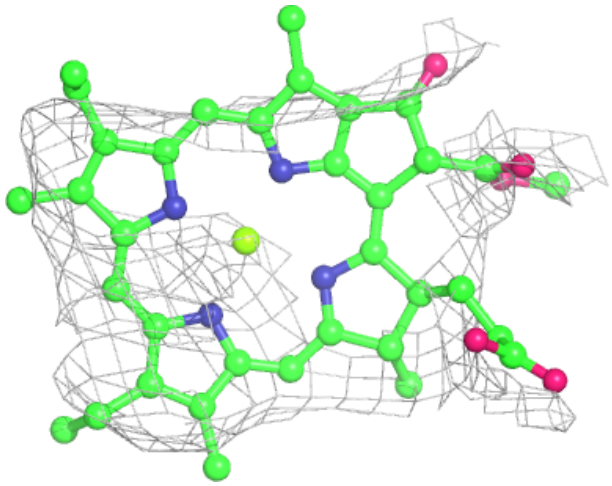
Electron density around CLA J 1102:

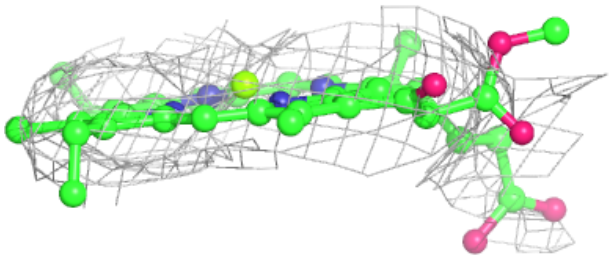
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

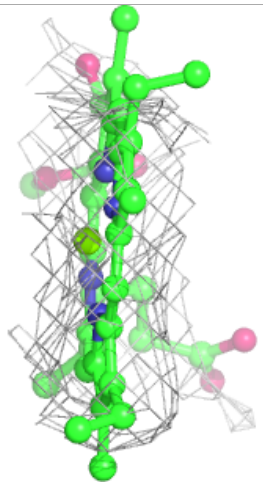


Electron density around CLA A 836:

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

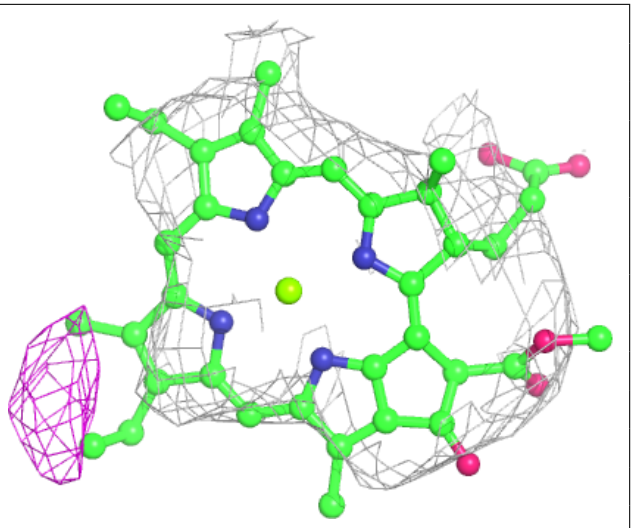


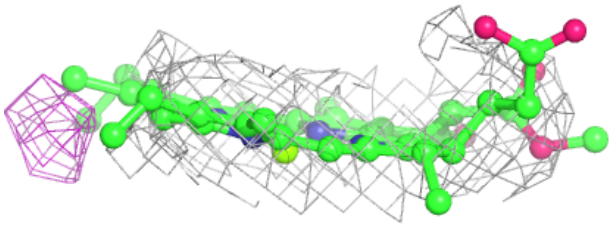


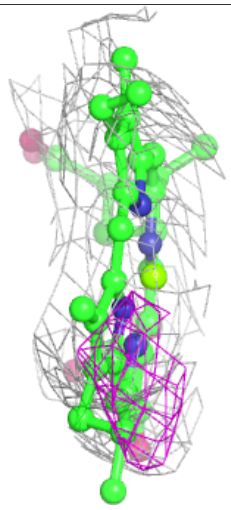


Electron density around CLA A 810:

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

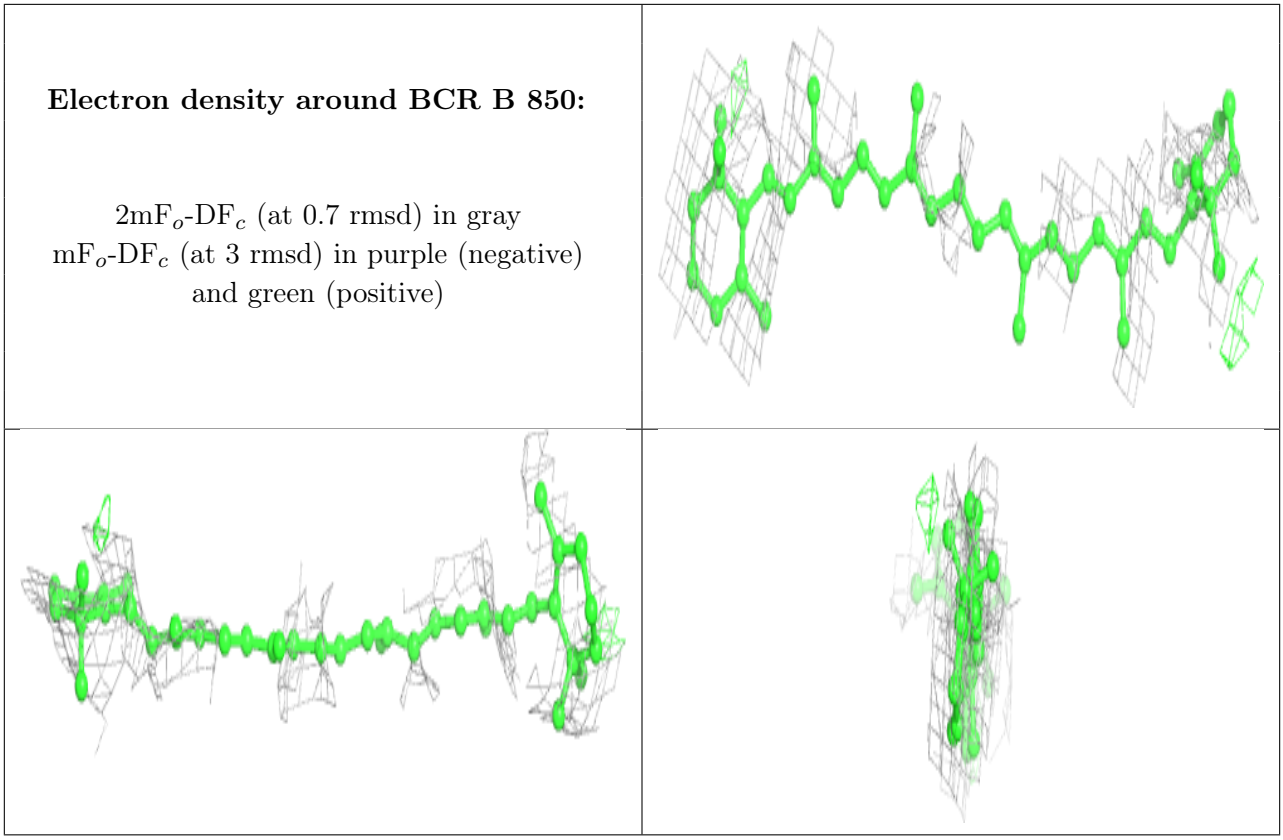






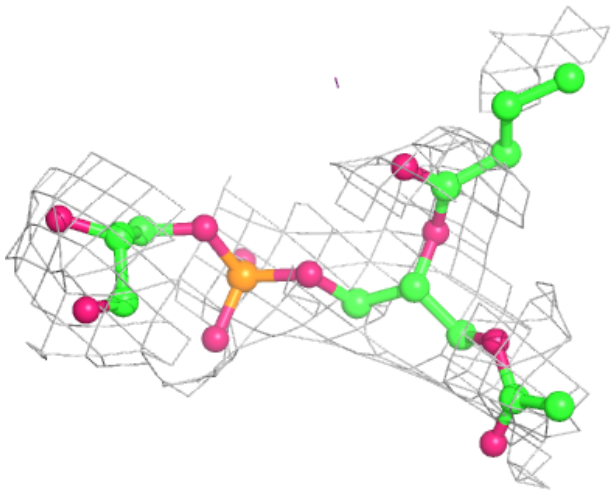
Electron density around BCR B 850:

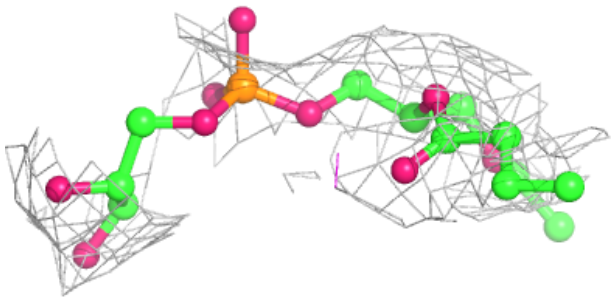
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

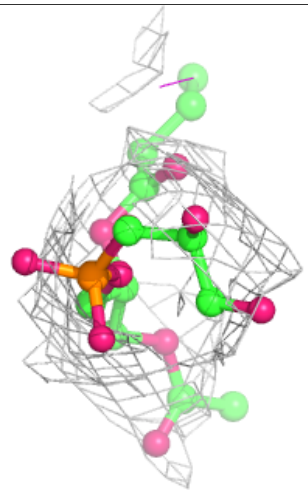


Electron density around LHG X 101:

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

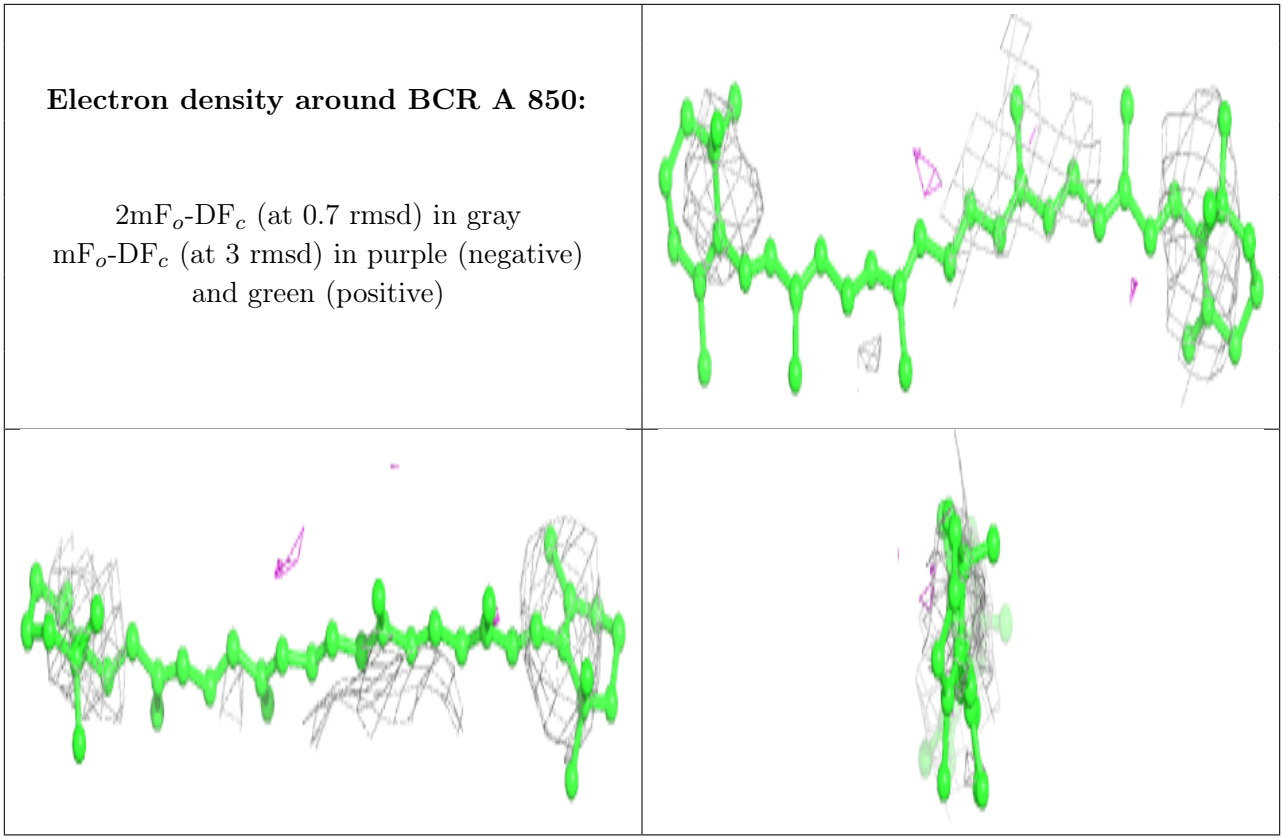






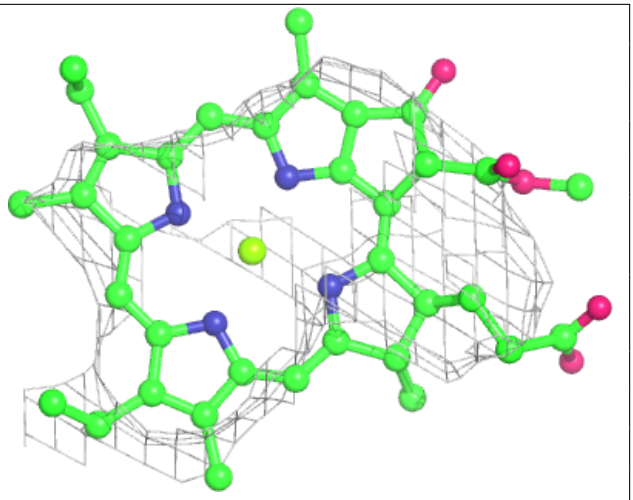
Electron density around BCR A 850:

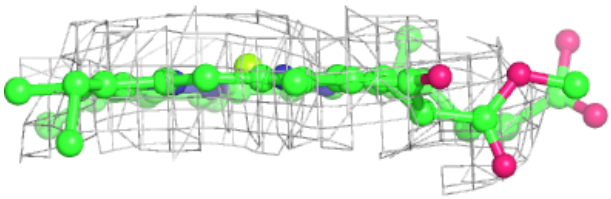
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

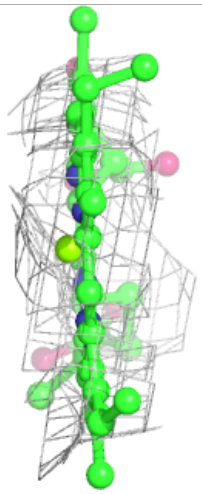


Electron density around CLA B 834:

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

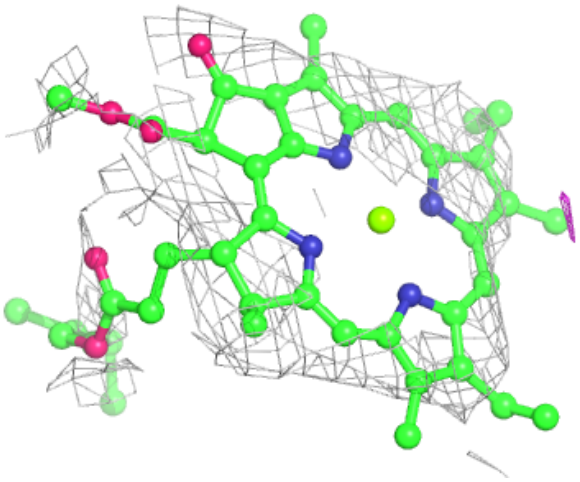


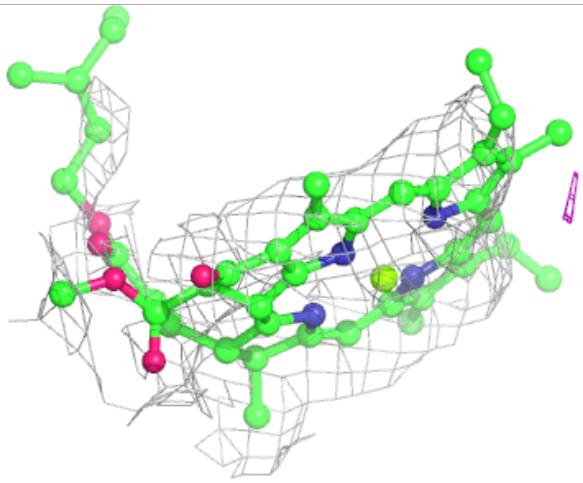


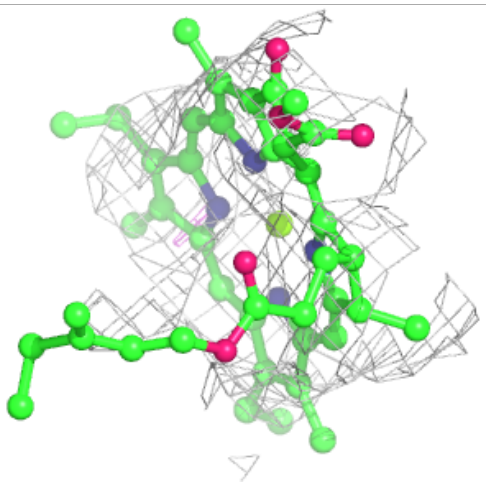


Electron density around CLA A 807:

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

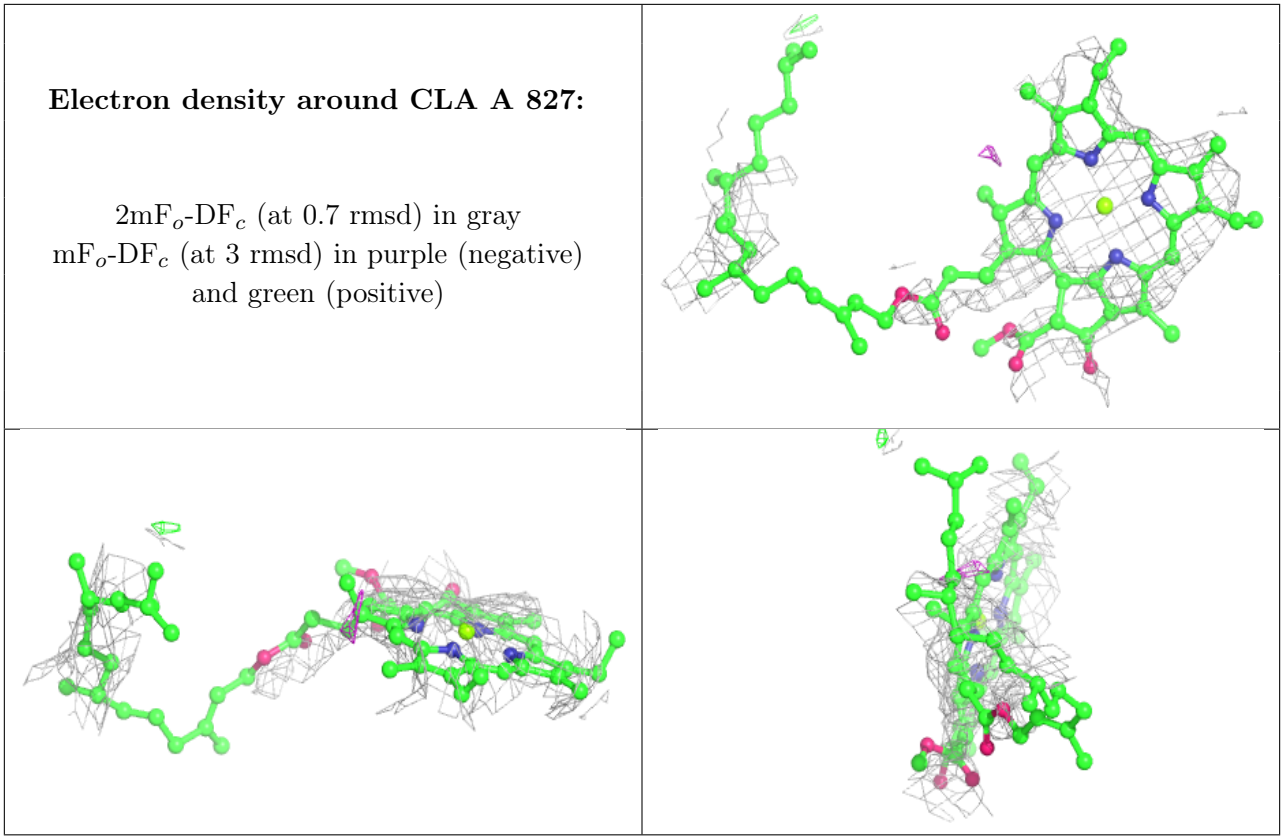






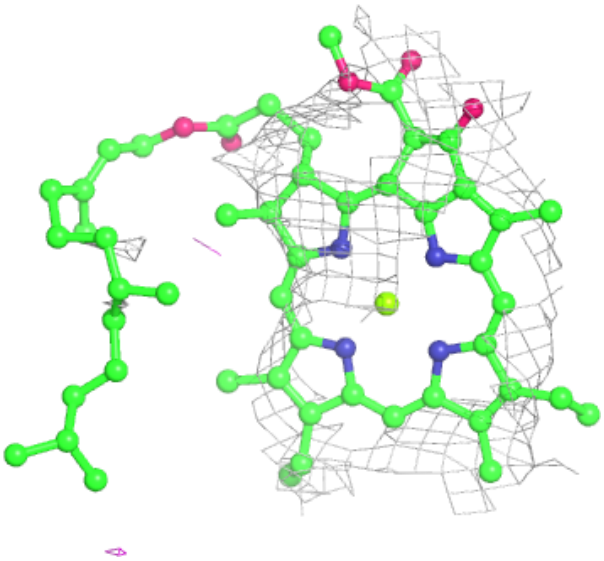
Electron density around CLA A 827:

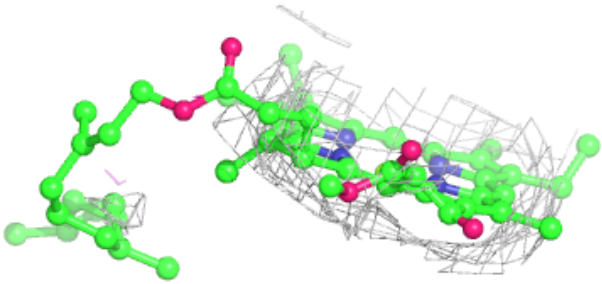
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

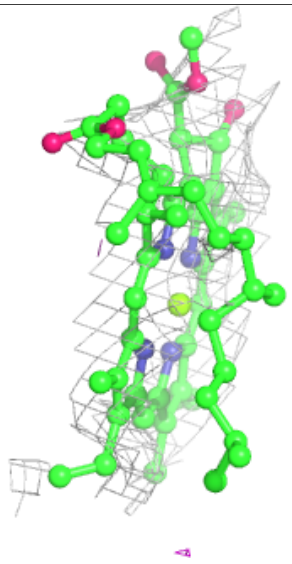


Electron density around CLA A 813:

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

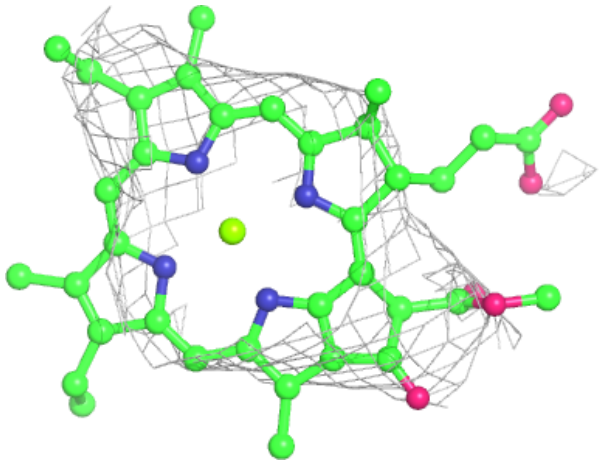


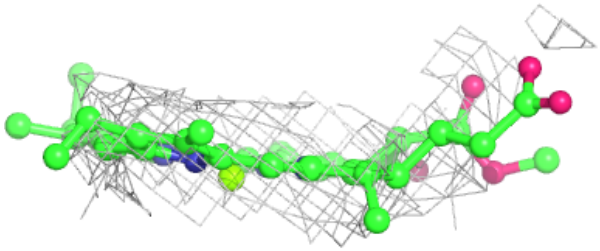


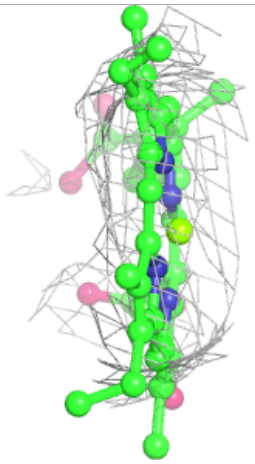


Electron density around CLA B 819:

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

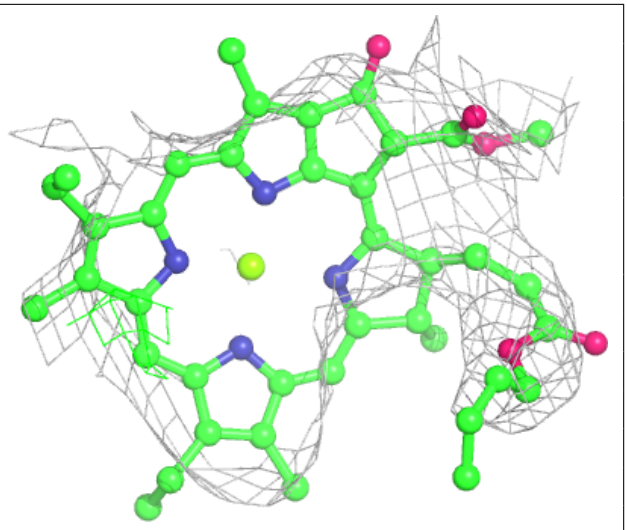


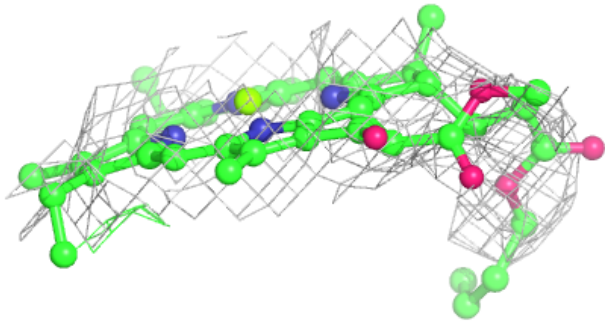


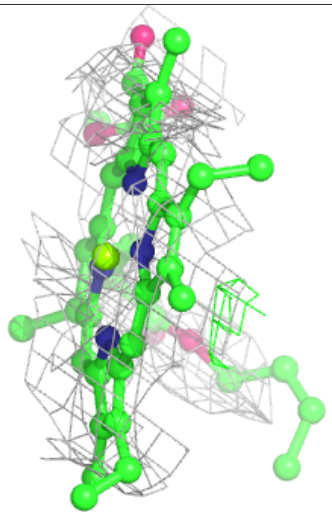


Electron density around CLA A 822:

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

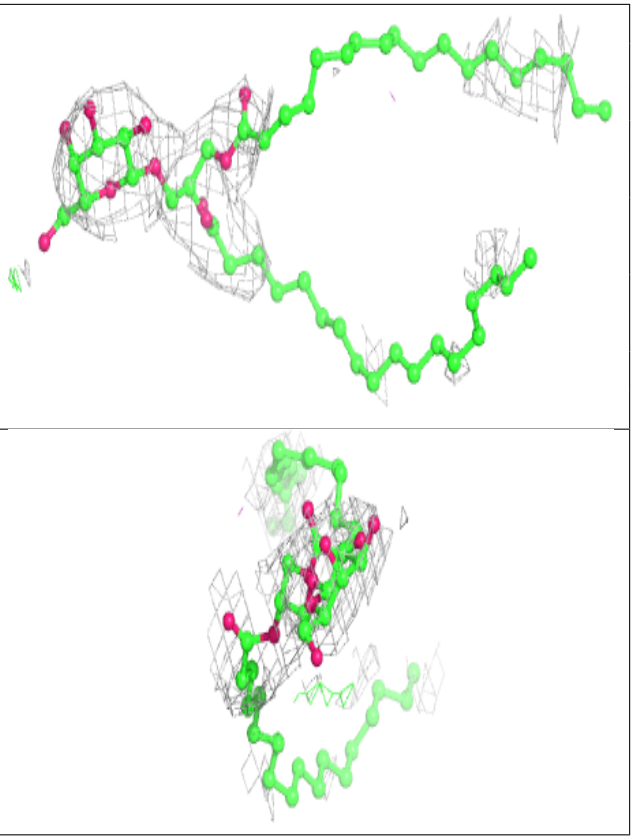






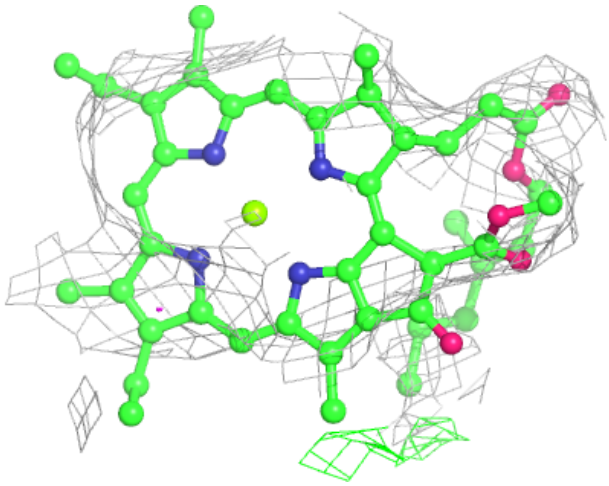
Electron density around LMG B 848:

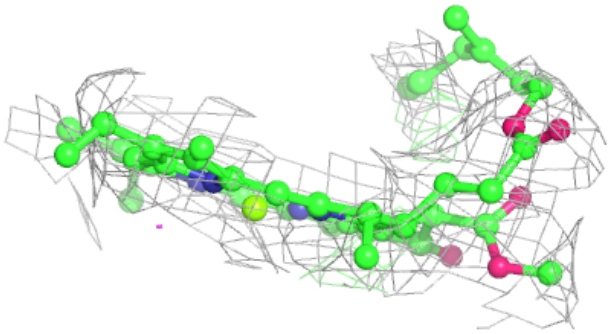
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

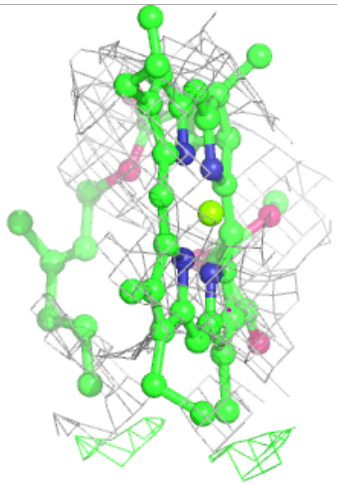


Electron density around CLA A 845:

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

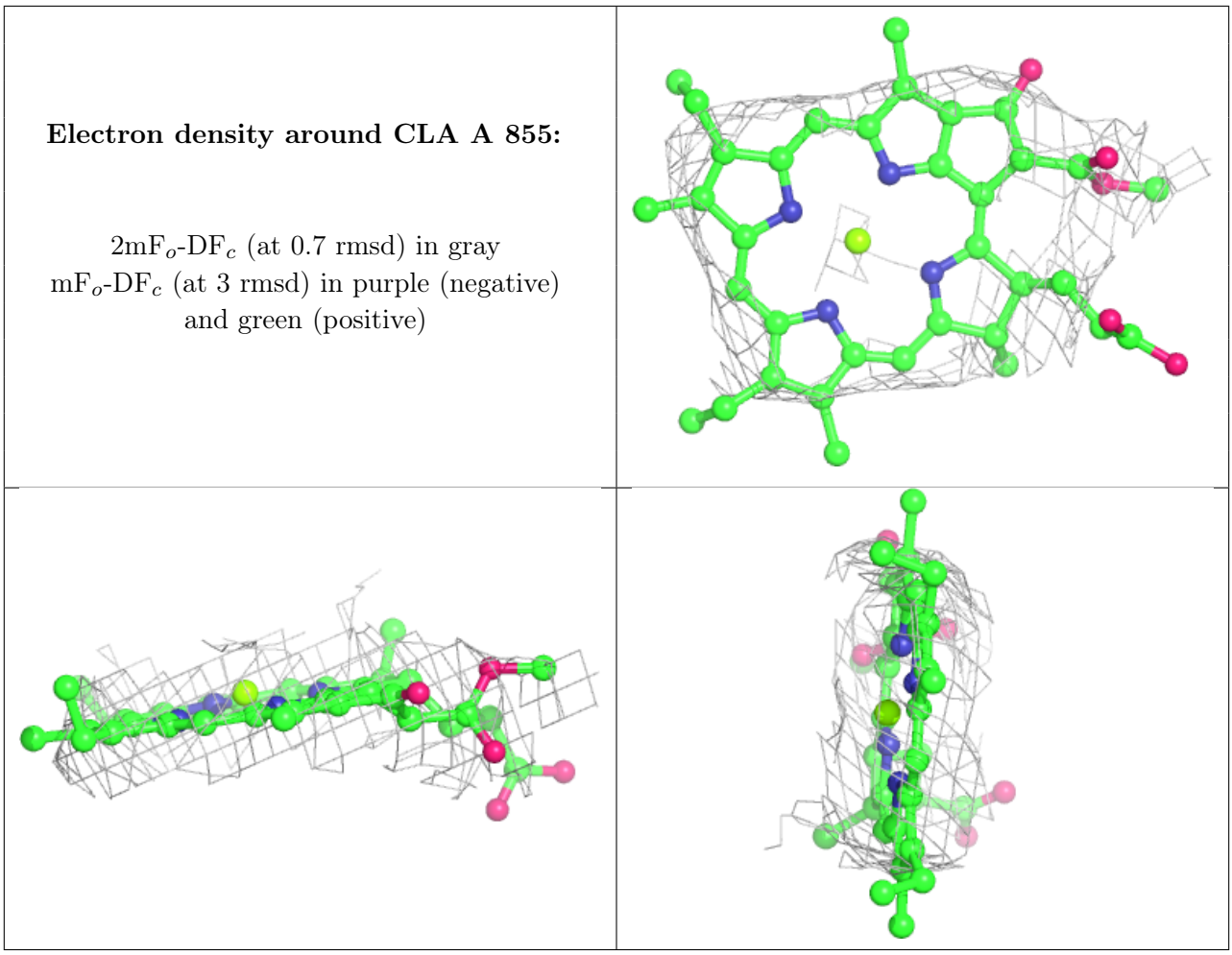






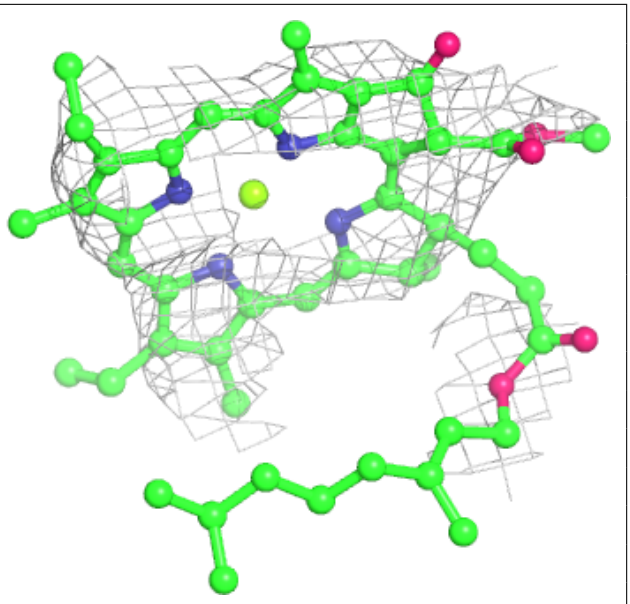
Electron density around CLA A 855:

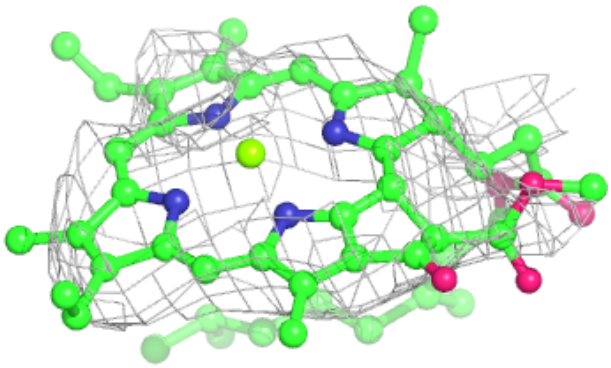
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

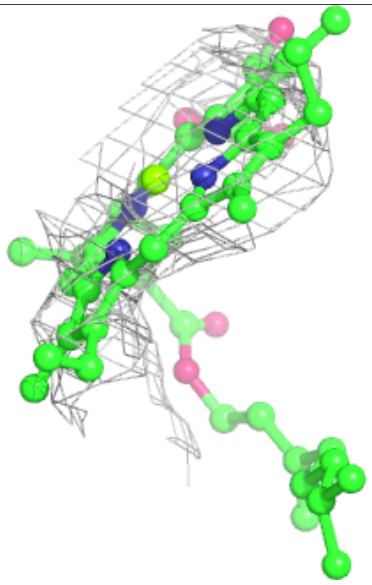


Electron density around CLA B 814:

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

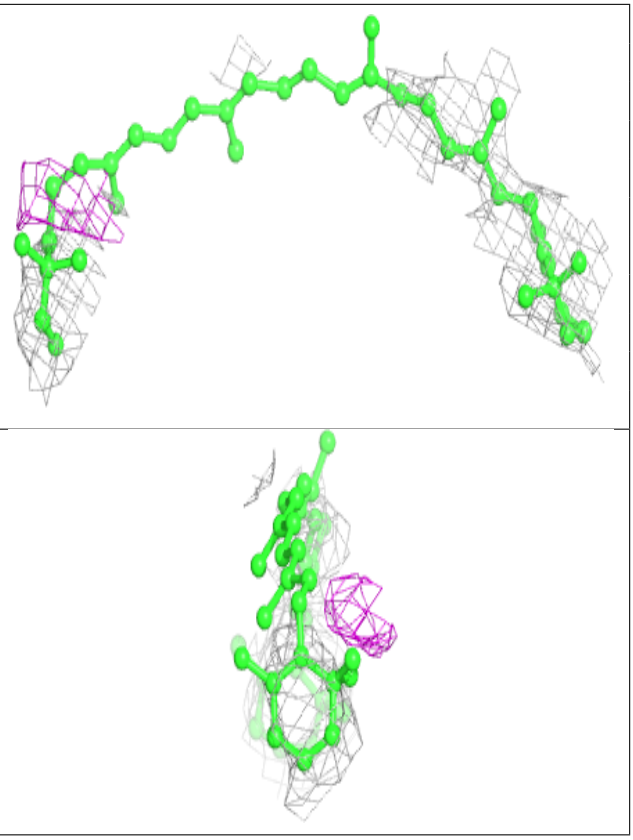


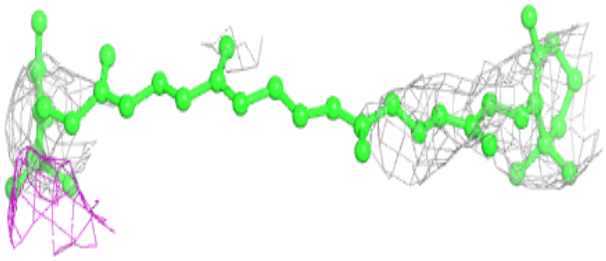




Electron density around BCR F 1302:

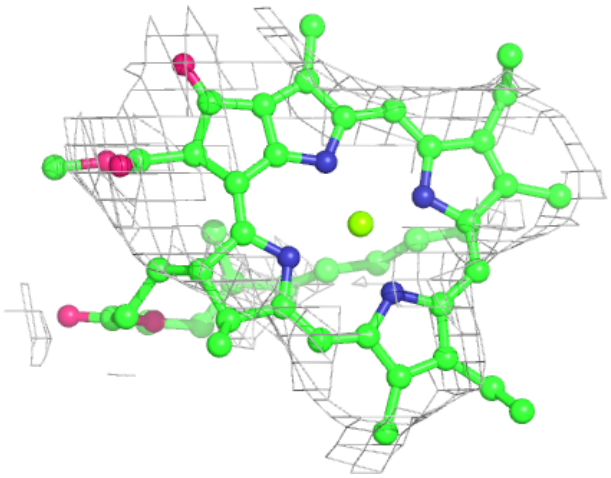
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

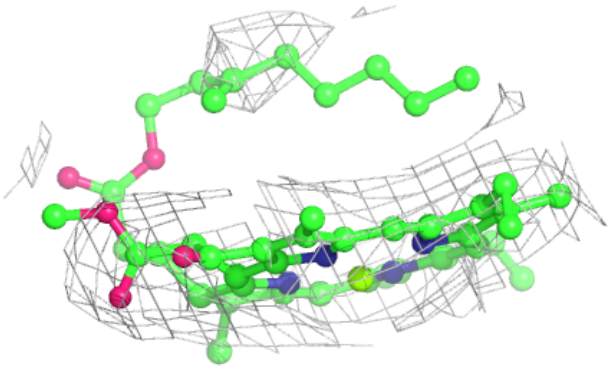


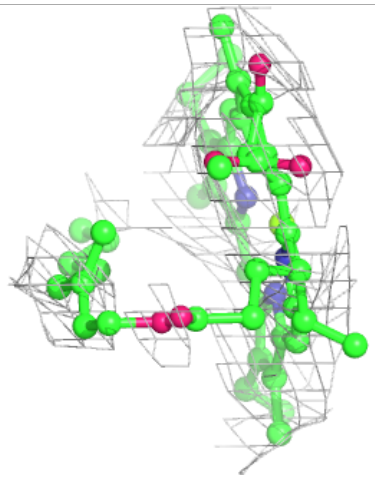


Electron density around CLA A 817:

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

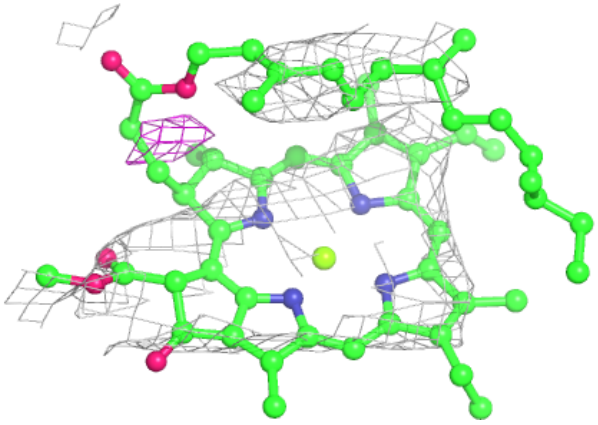


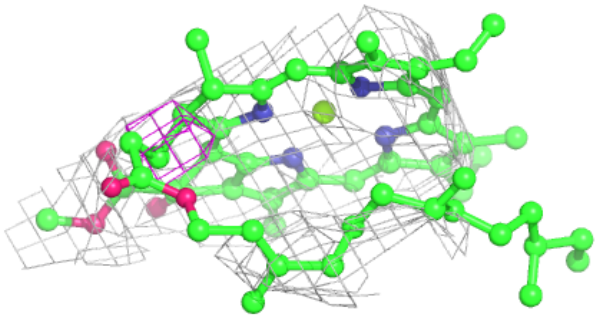


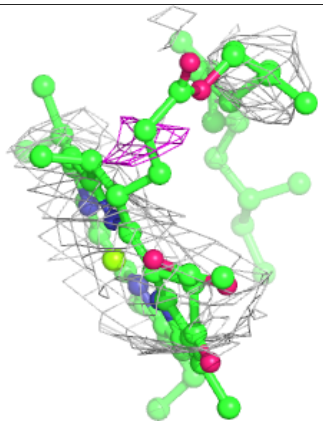


Electron density around CLA A 820:

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

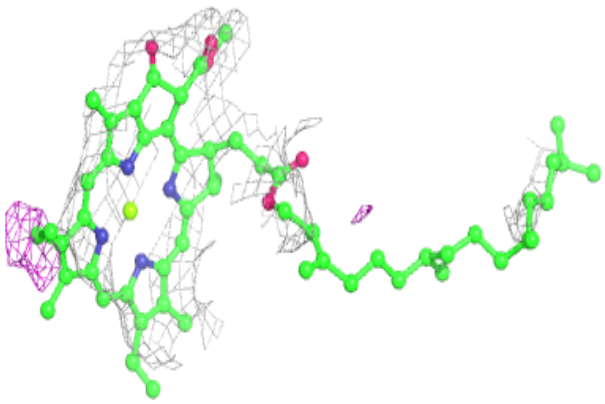


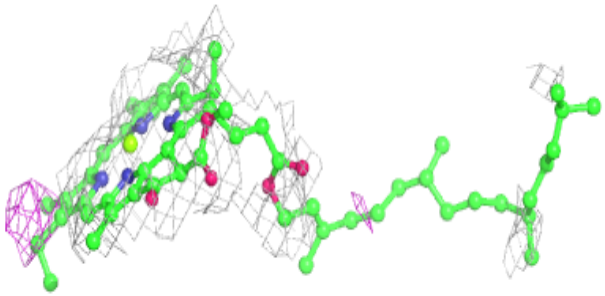


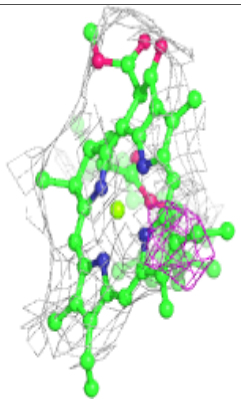


Electron density around CLA A 821:

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

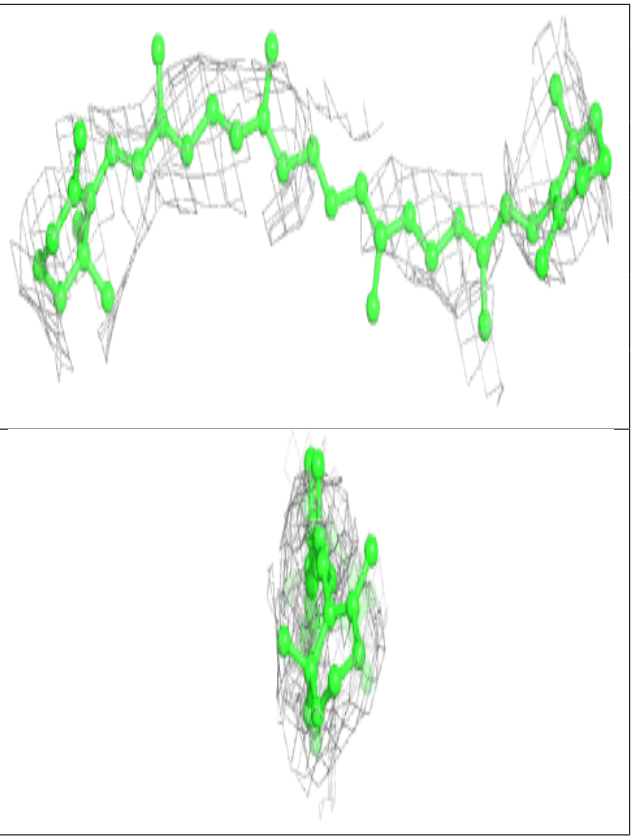


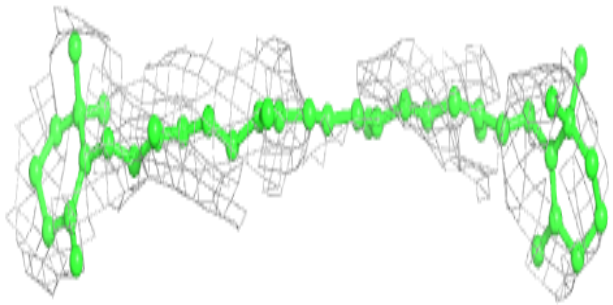




Electron density around BCR J 1105:

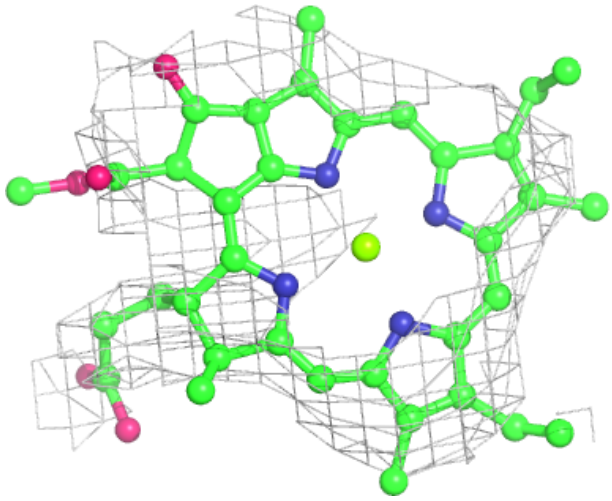
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

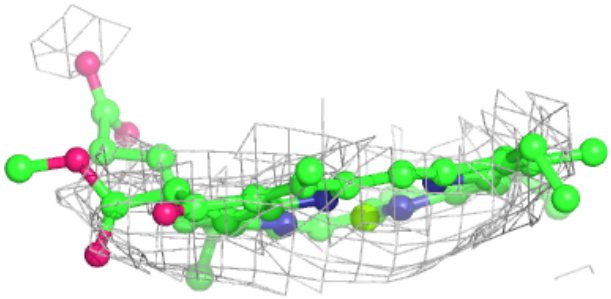


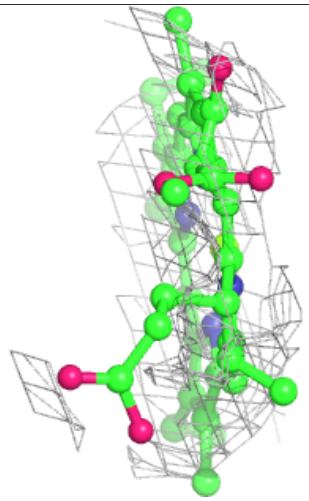


Electron density around CLA B 810:

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

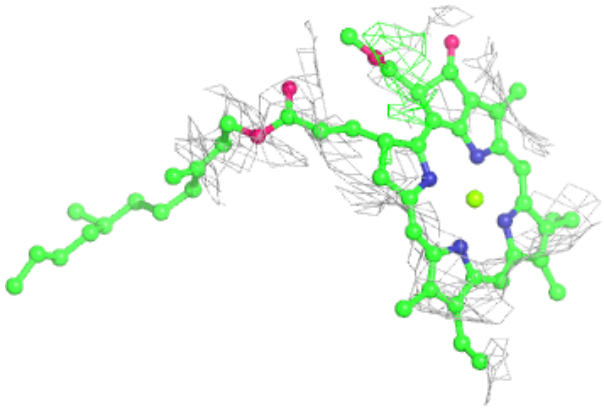


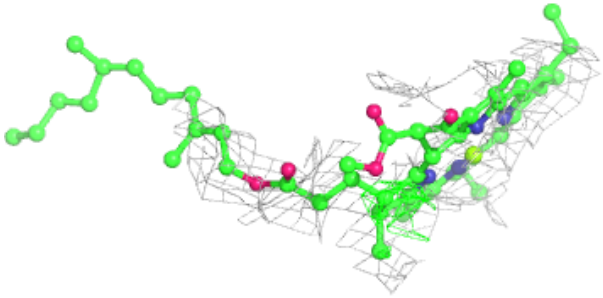


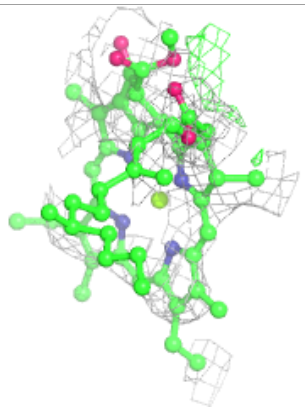


Electron density around CLA B 831:

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

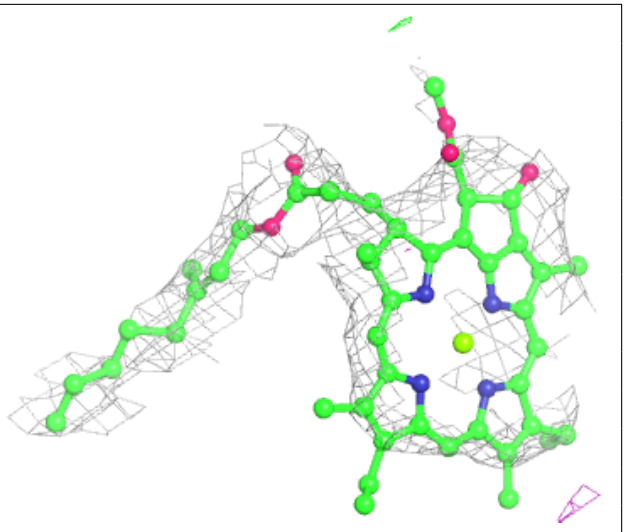


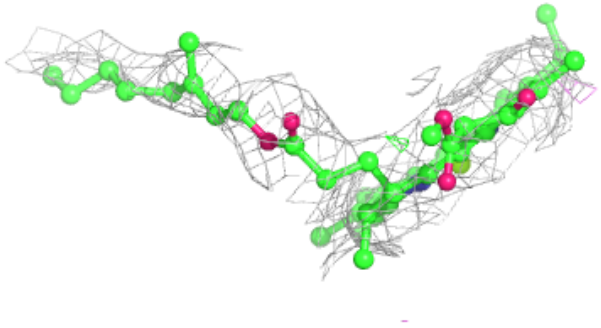


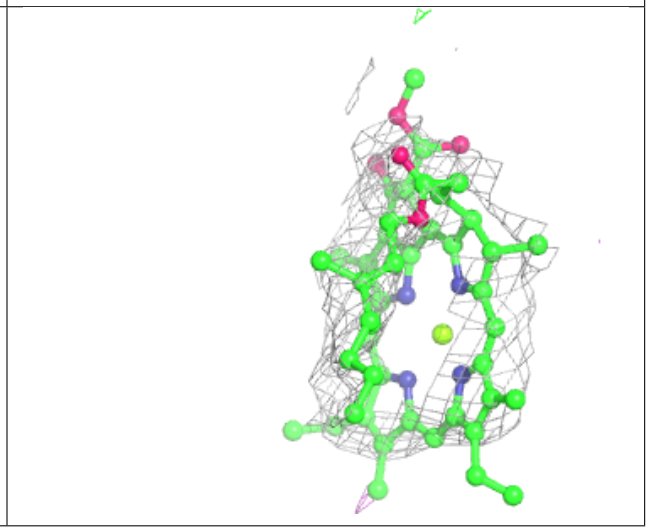


Electron density around CLA A 835:

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

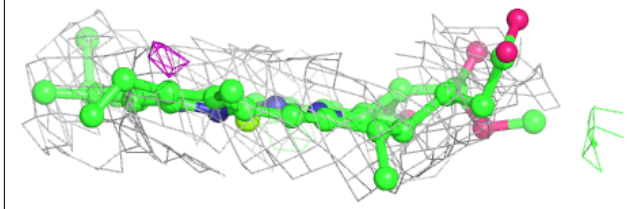


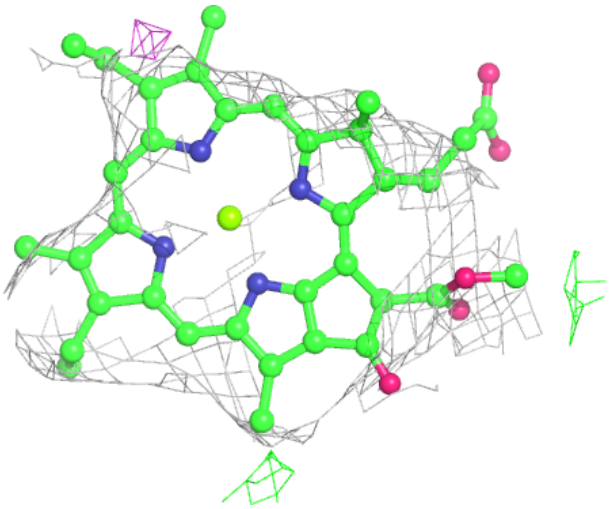


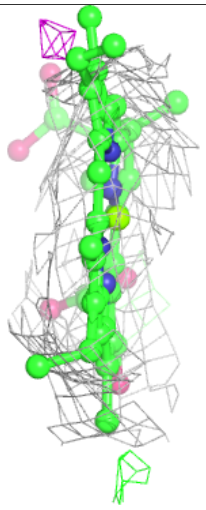


Electron density around CLA B 813:

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

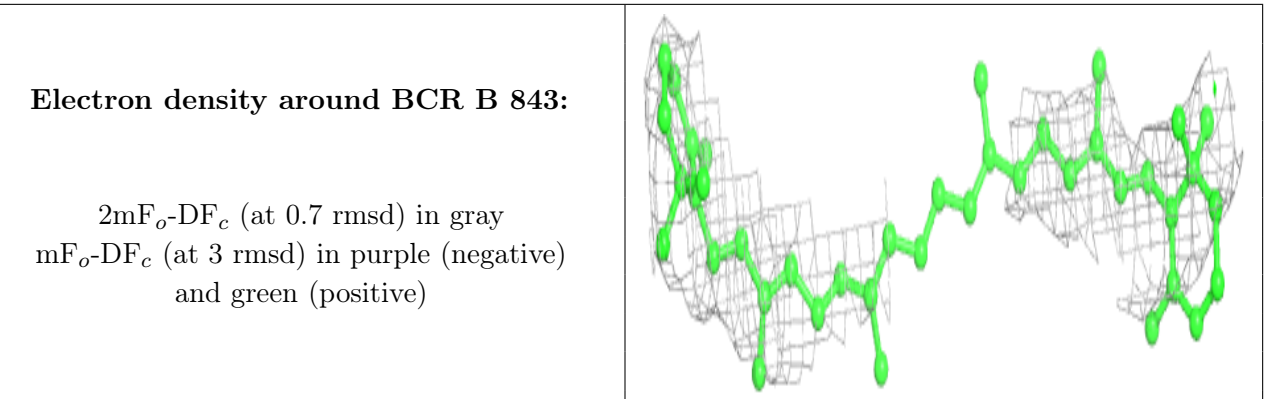






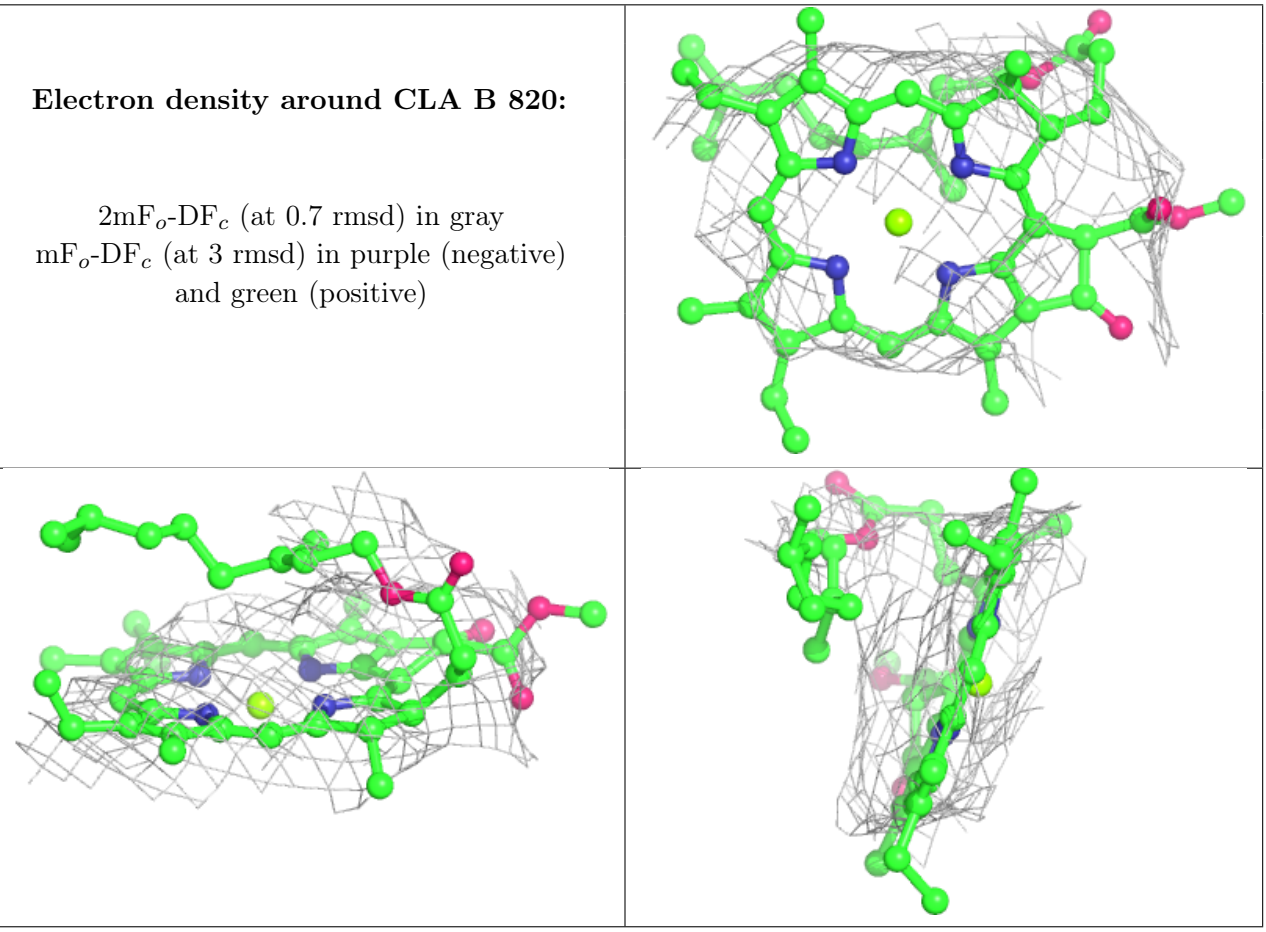
Electron density around BCR B 843:

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



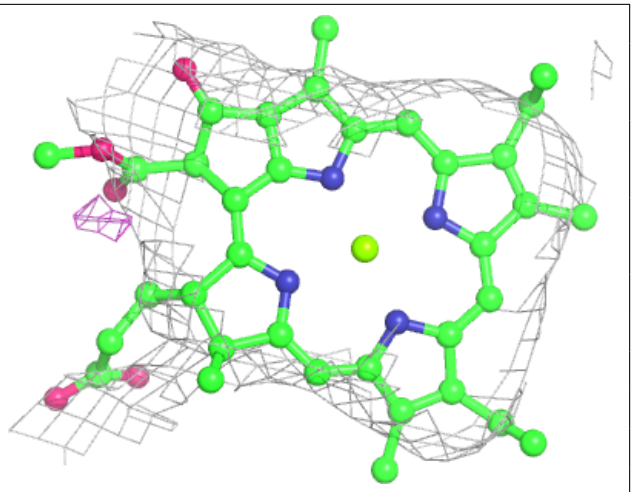
Electron density around CLA B 820:

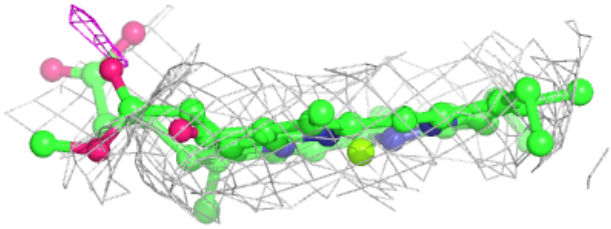
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

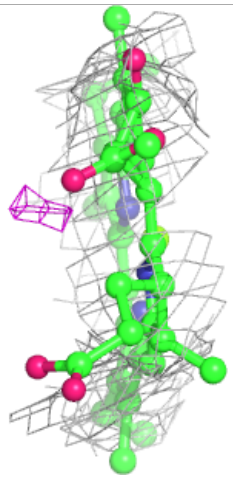


Electron density around CLA B 828:

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

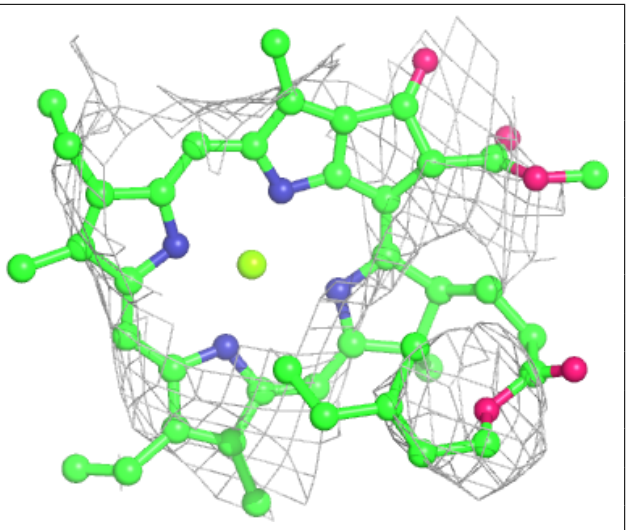


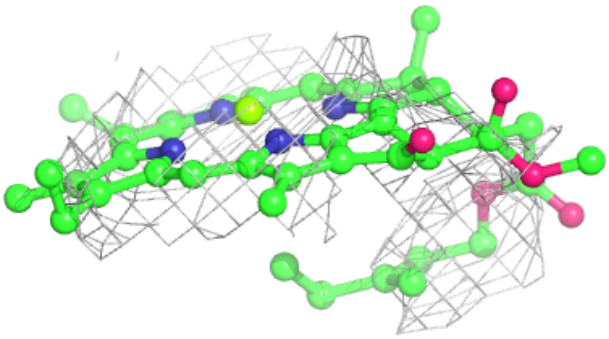


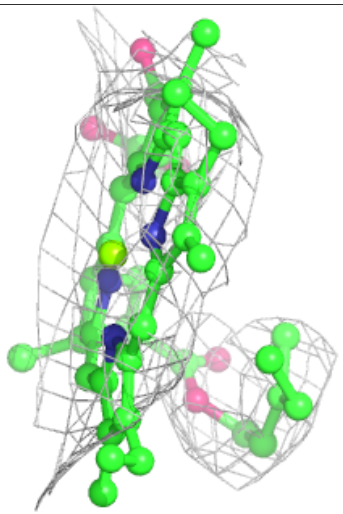


Electron density around CLA A 823:

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

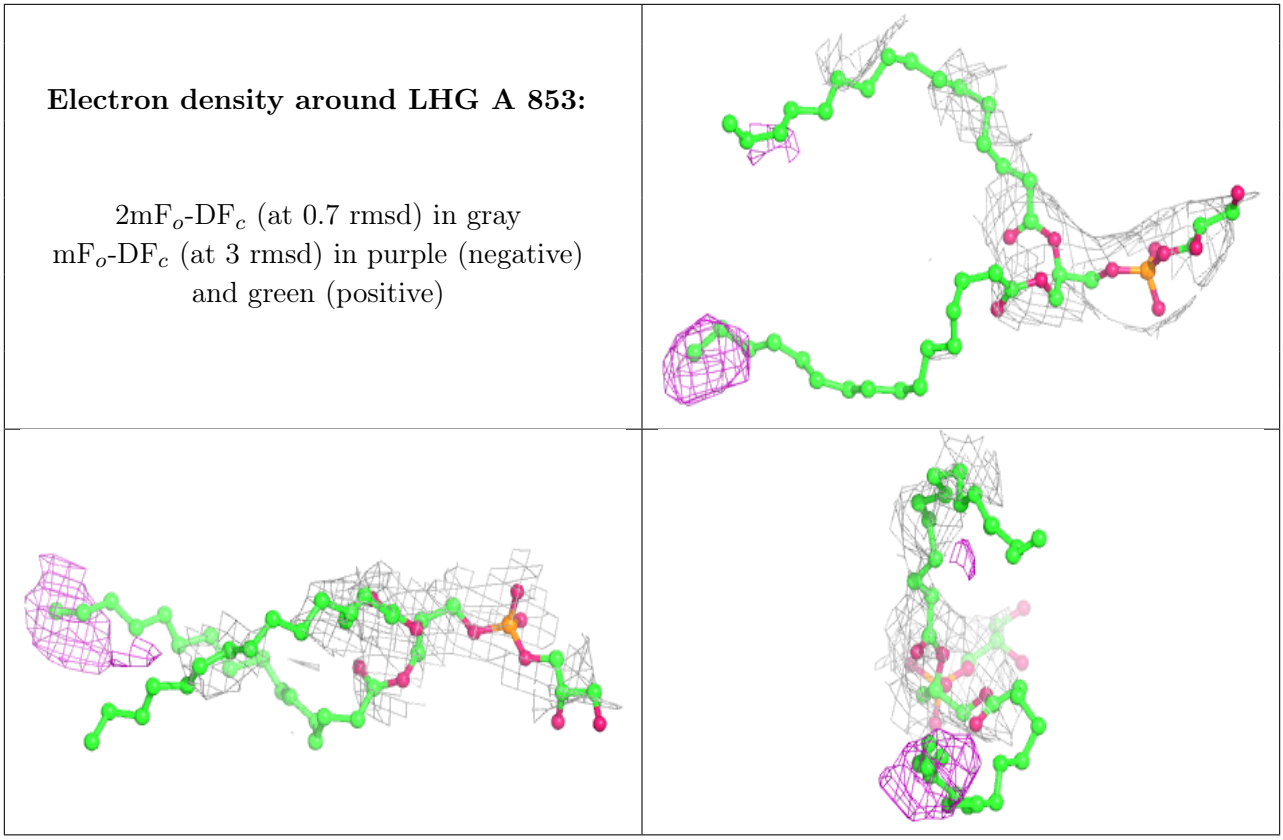






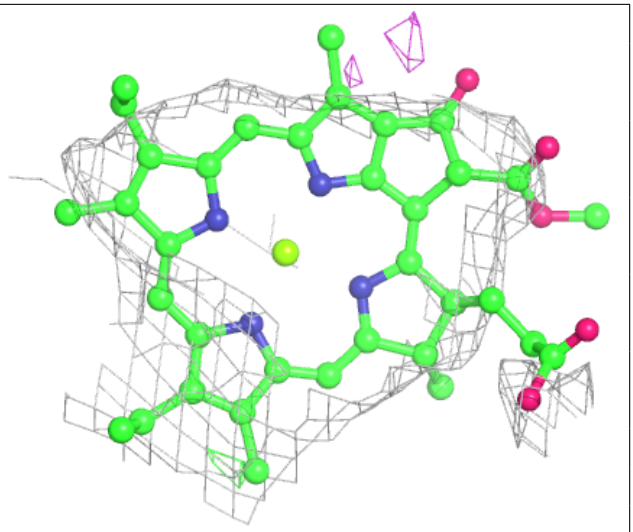
Electron density around LHG A 853:

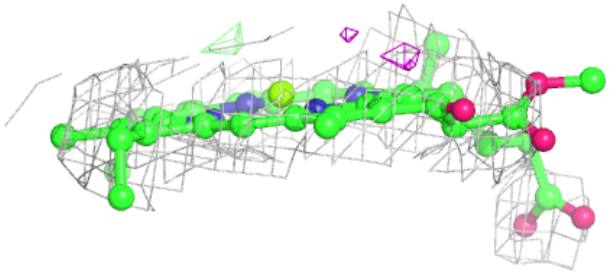
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

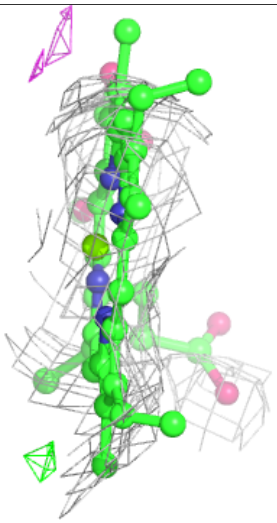


Electron density around CLA B 833:

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

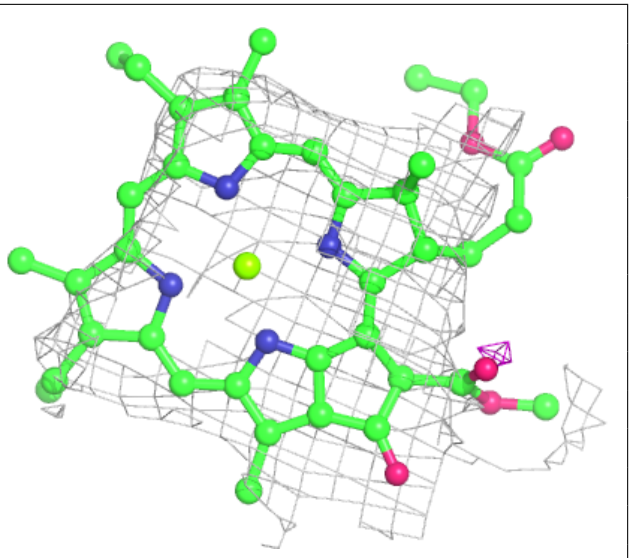


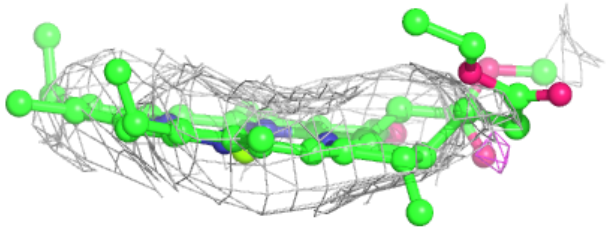


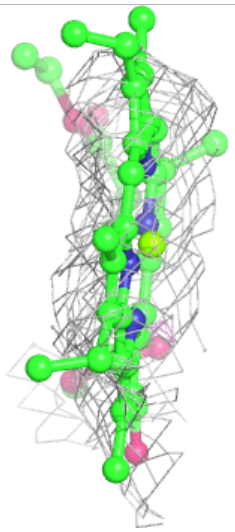


Electron density around CLA B 818:

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

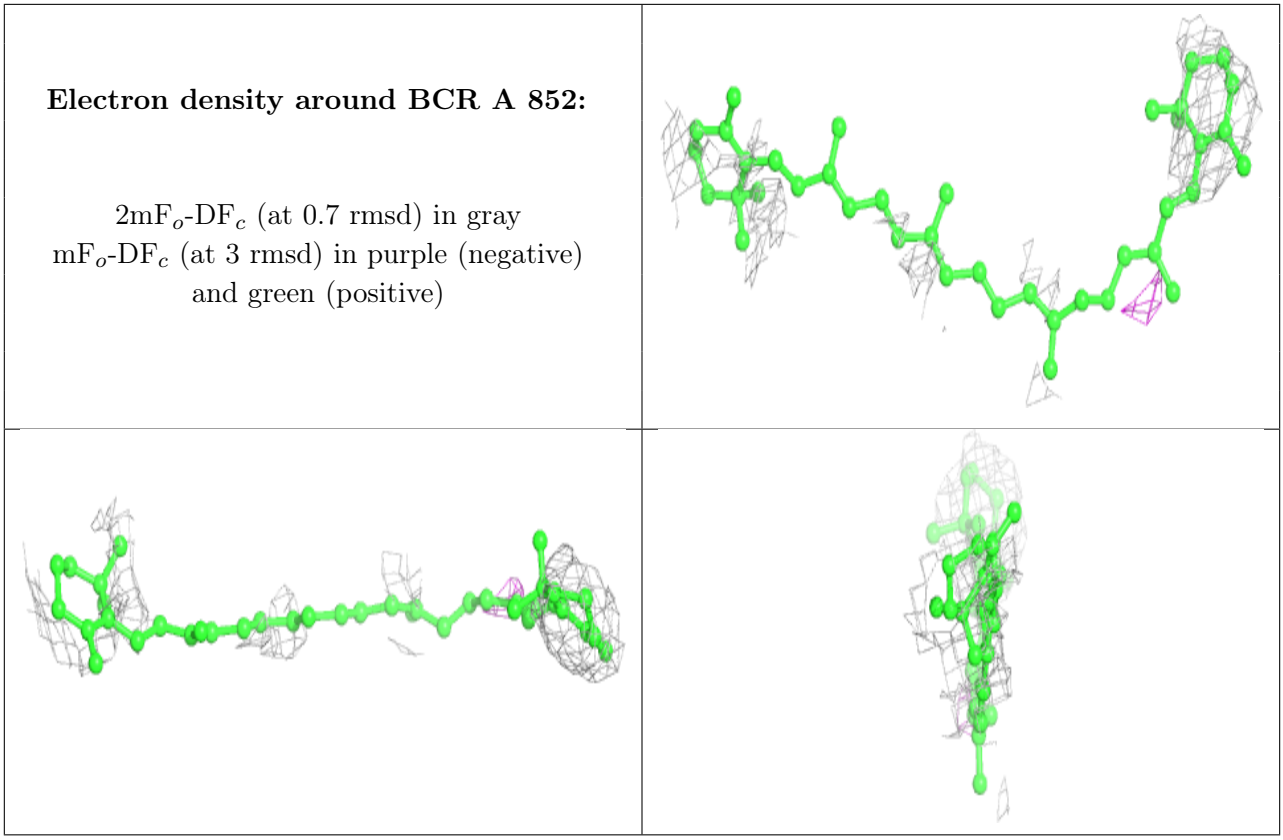






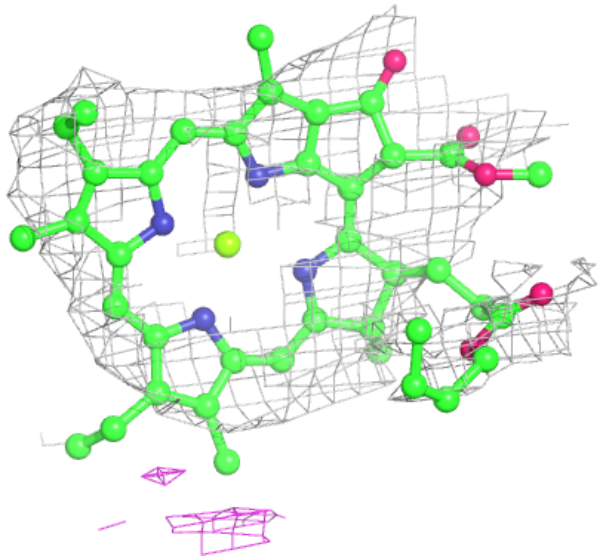
Electron density around BCR A 852:

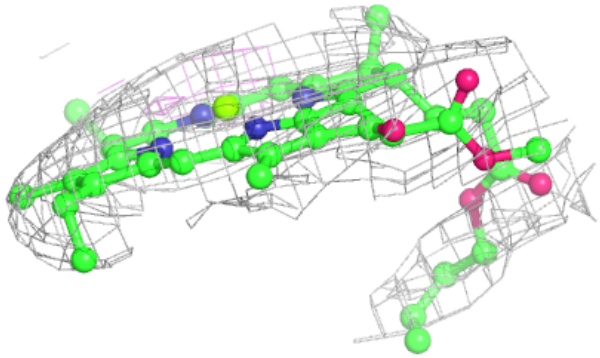
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

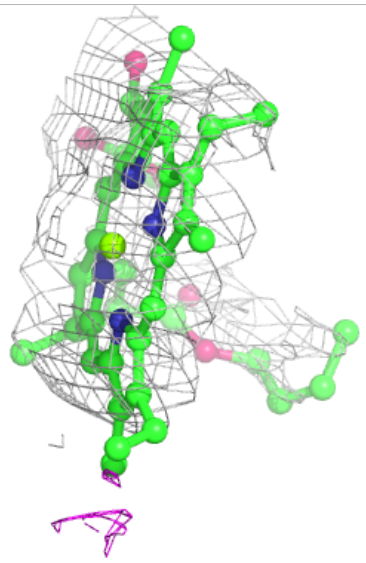


Electron density around CLA B 829:

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

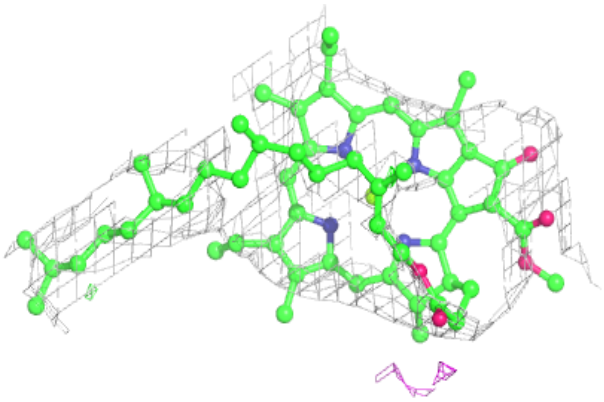


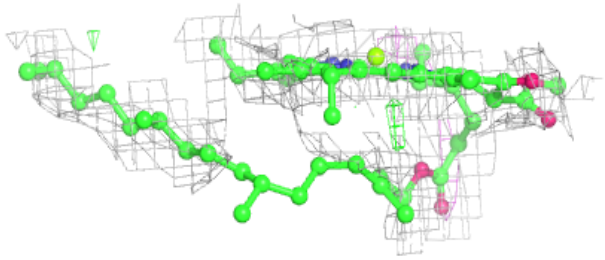


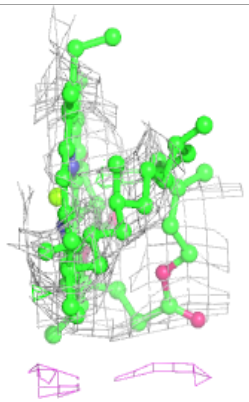


Electron density around CLA A 840:

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

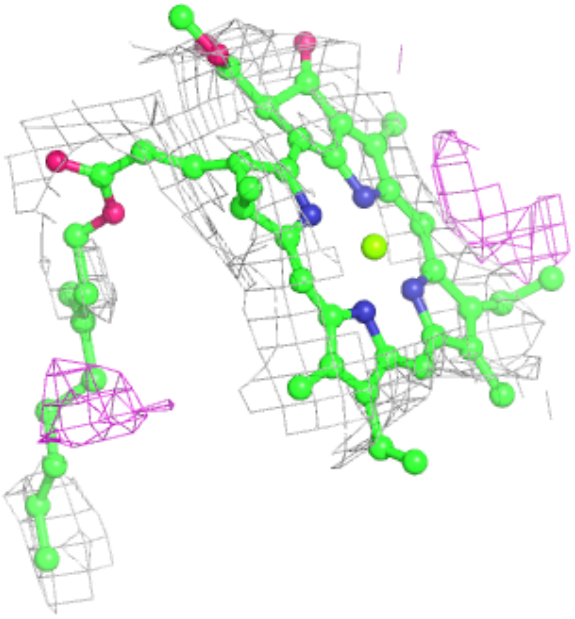


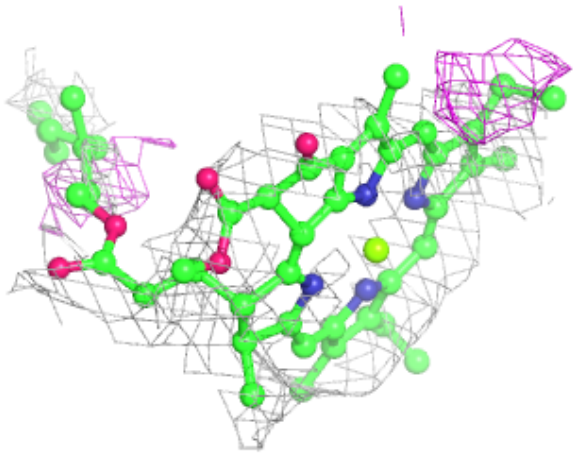


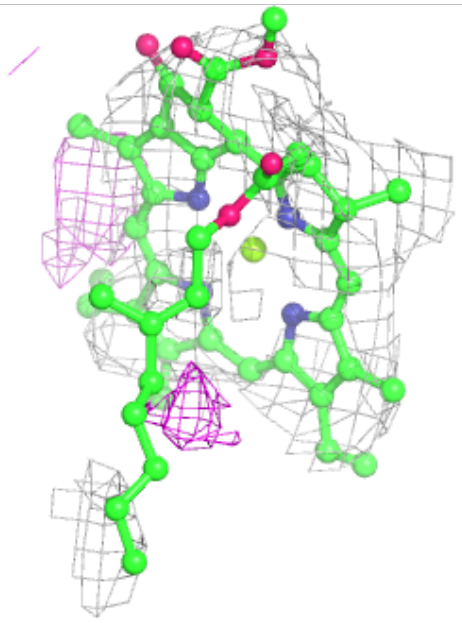


Electron density around CLA M 1201:

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

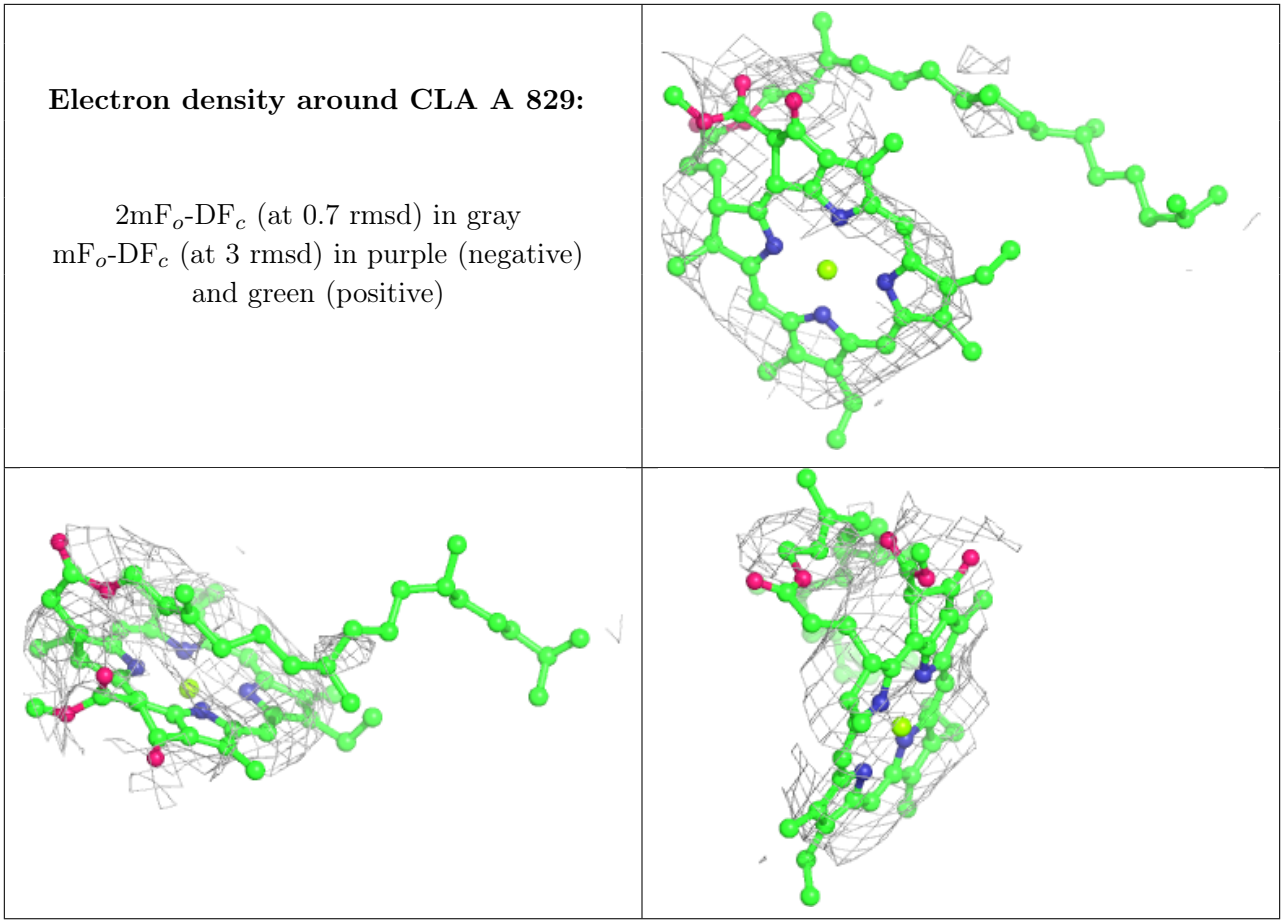






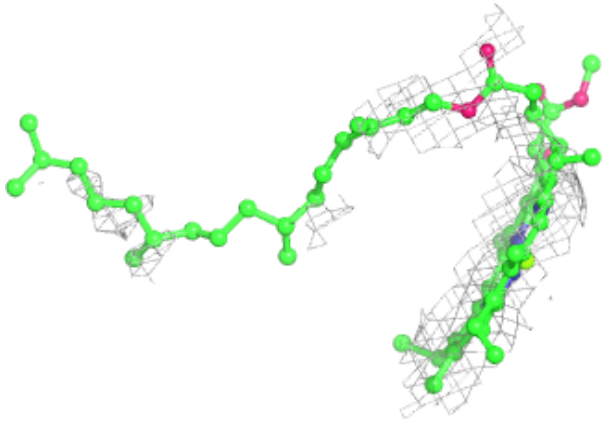
Electron density around CLA A 829:

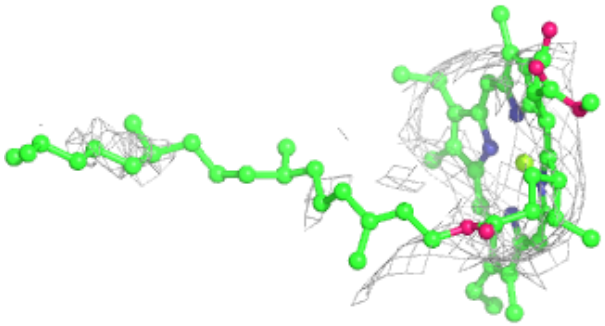
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

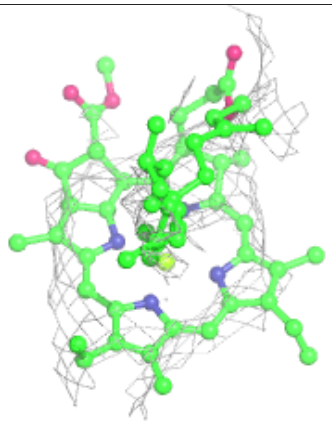


Electron density around CLA A 811:

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

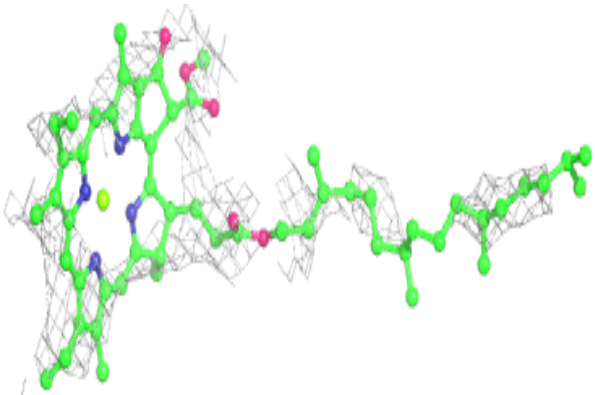


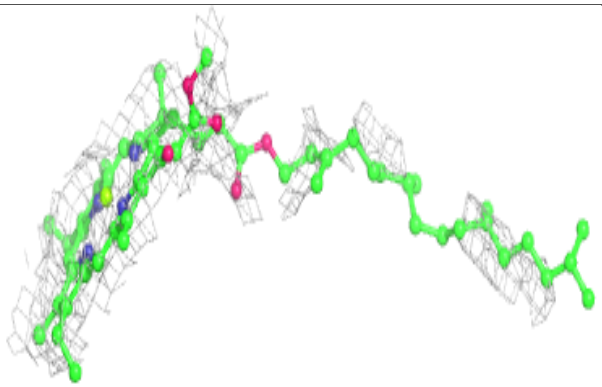


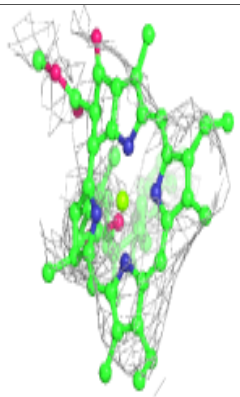


Electron density around CLA A 809:

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

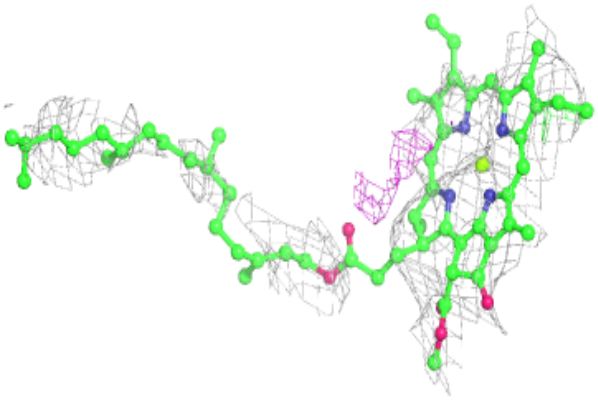


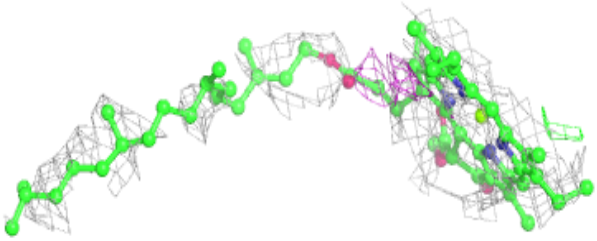


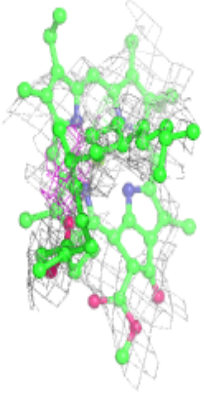


Electron density around CLA A 802:

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

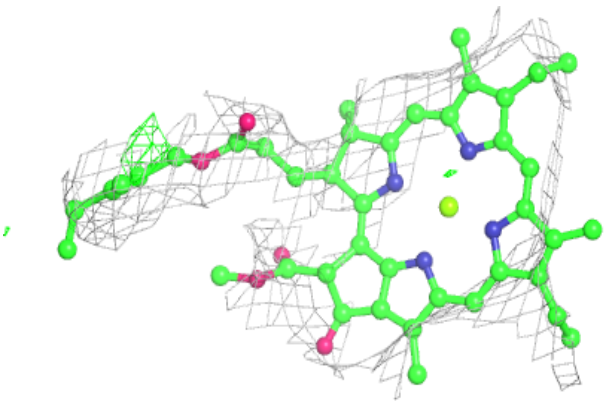


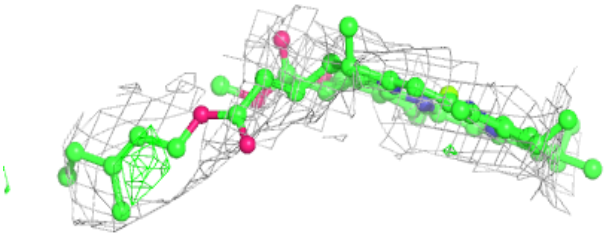


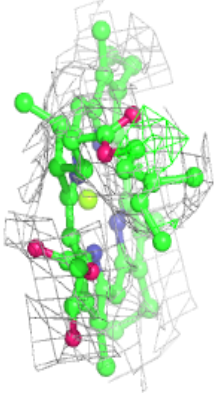


Electron density around CLA A 841:

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

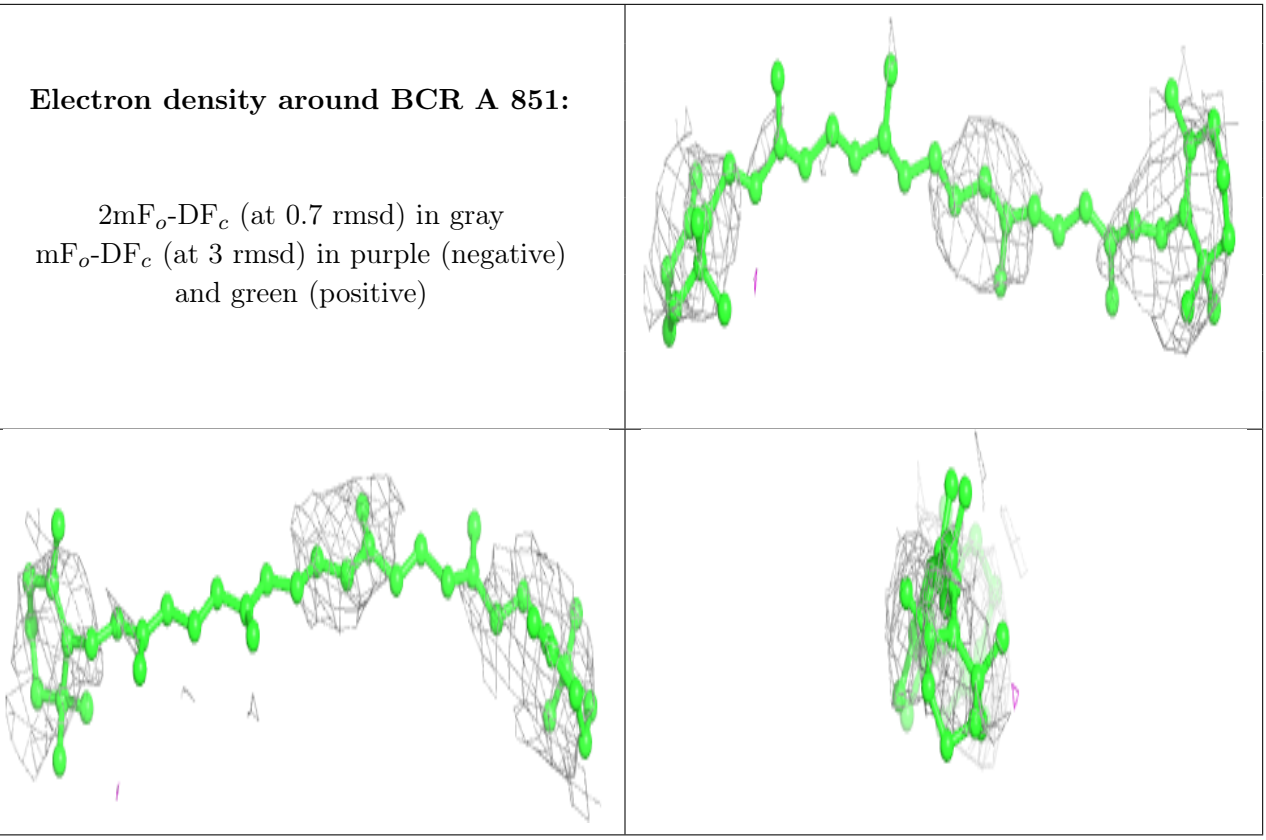






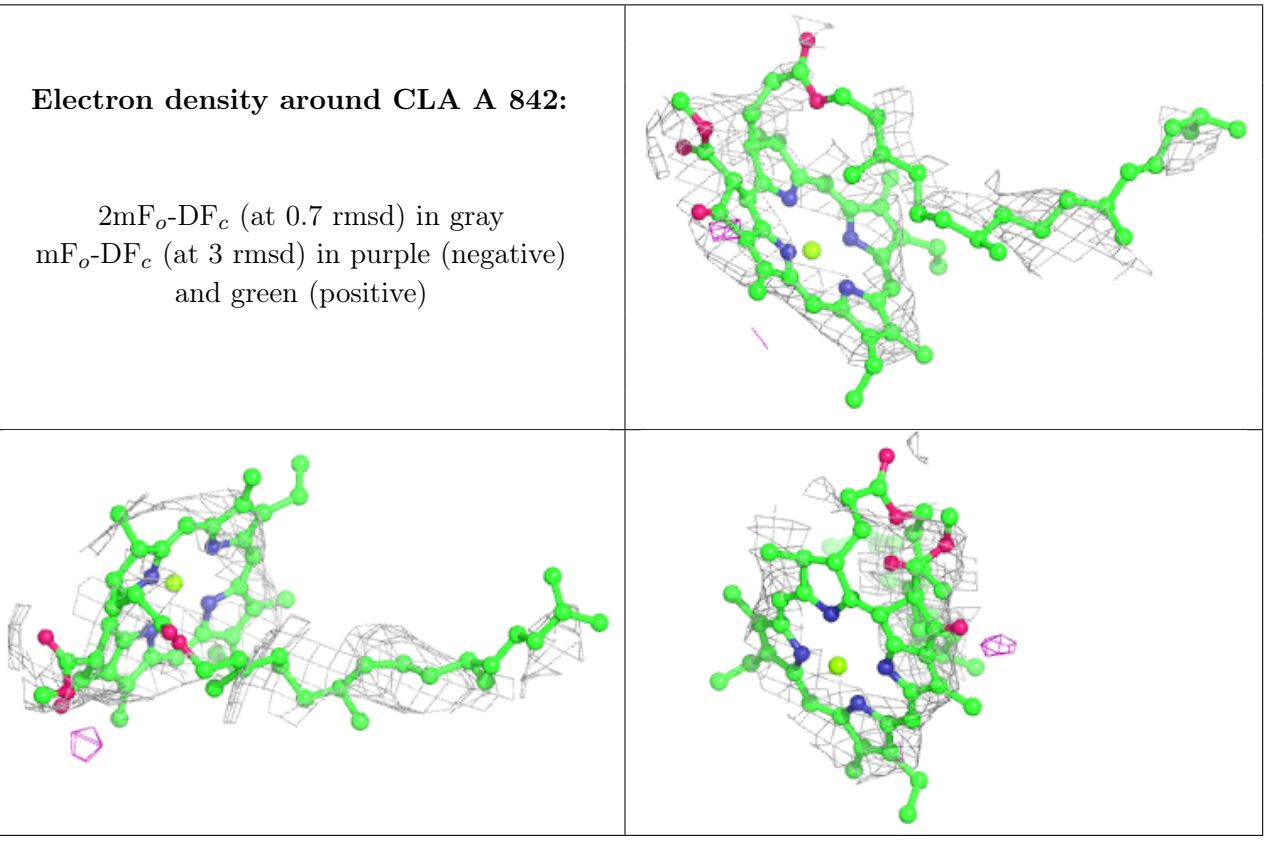
Electron density around BCR A 851:

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



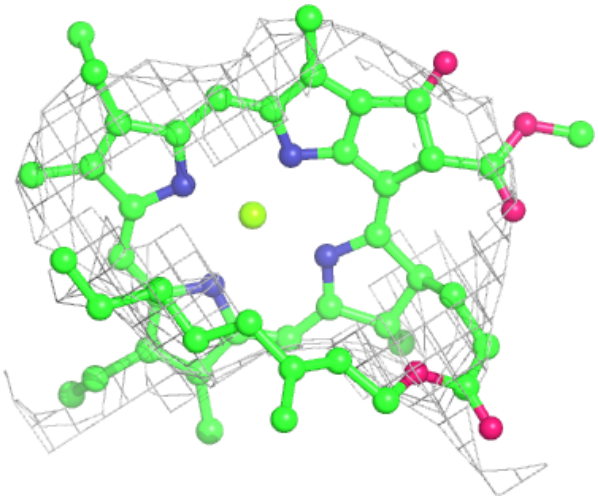
Electron density around CLA A 842:

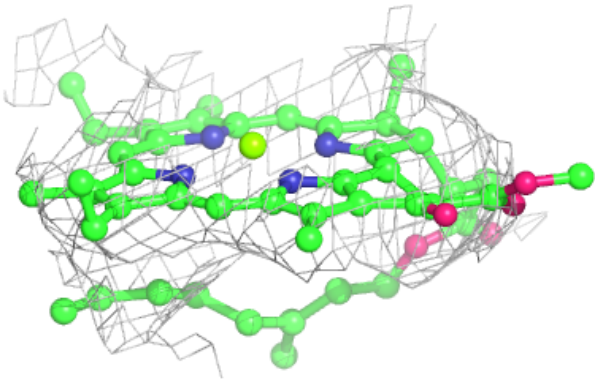
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

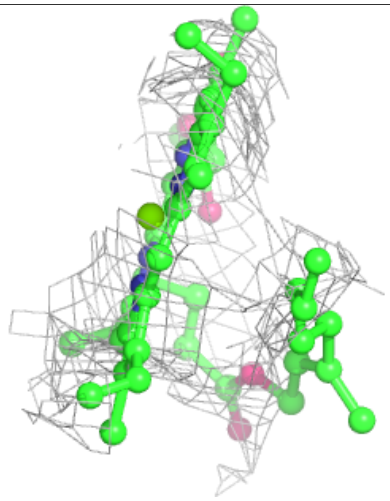


Electron density around CLA A 818:

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

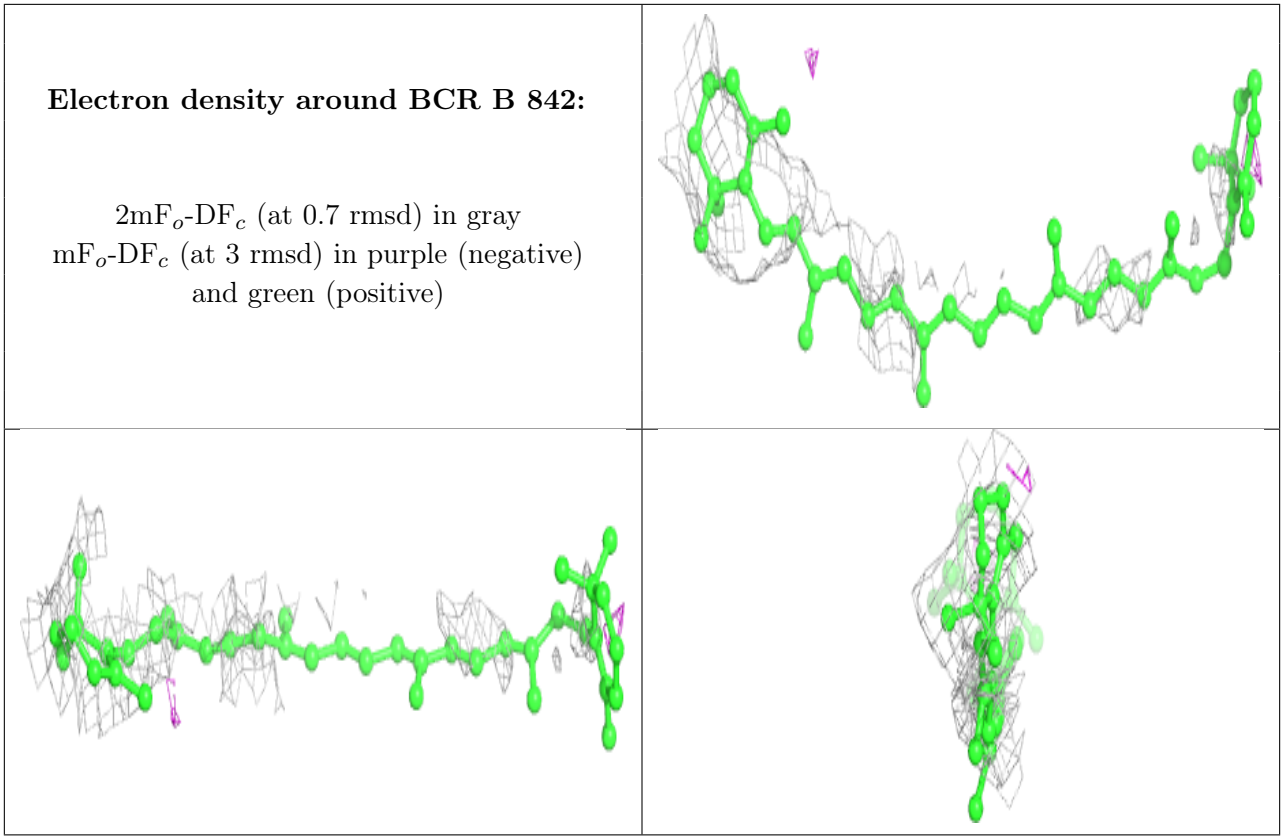






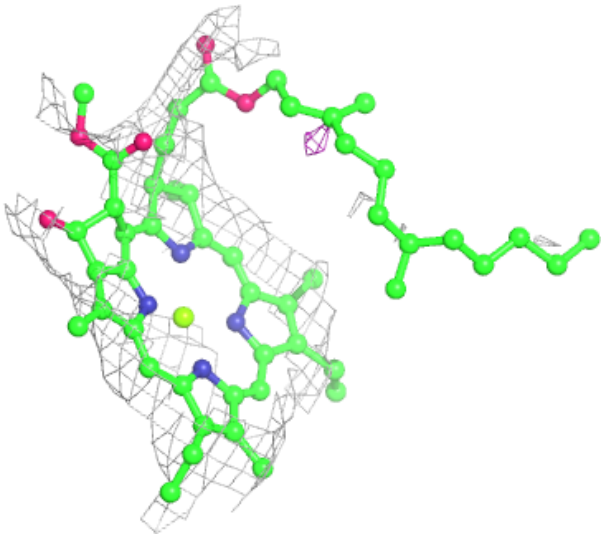
Electron density around BCR B 842:

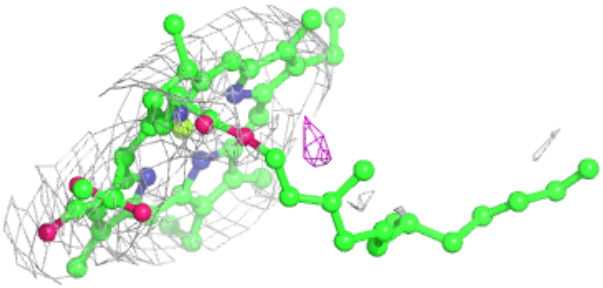
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

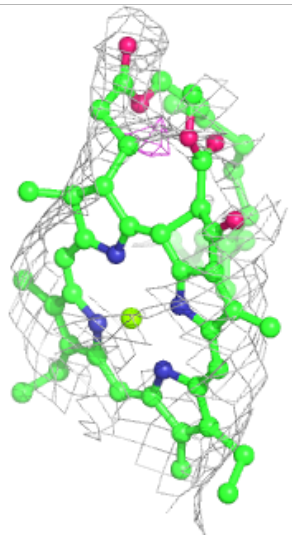


Electron density around CLA A 824:

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

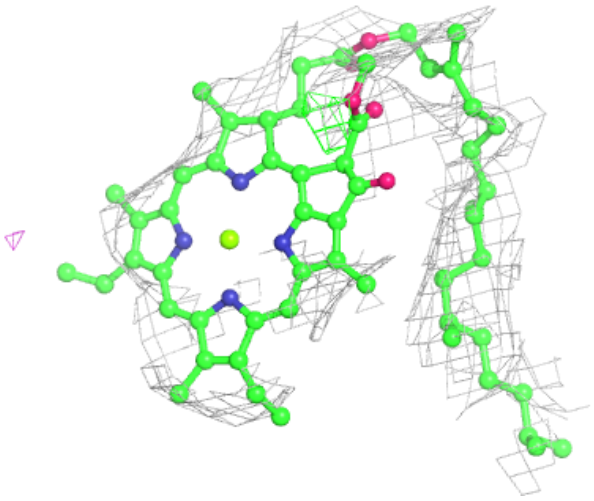


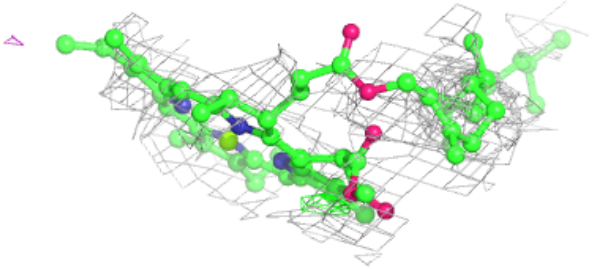


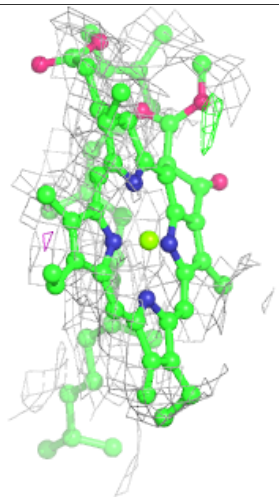


Electron density around CLA A 825:

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

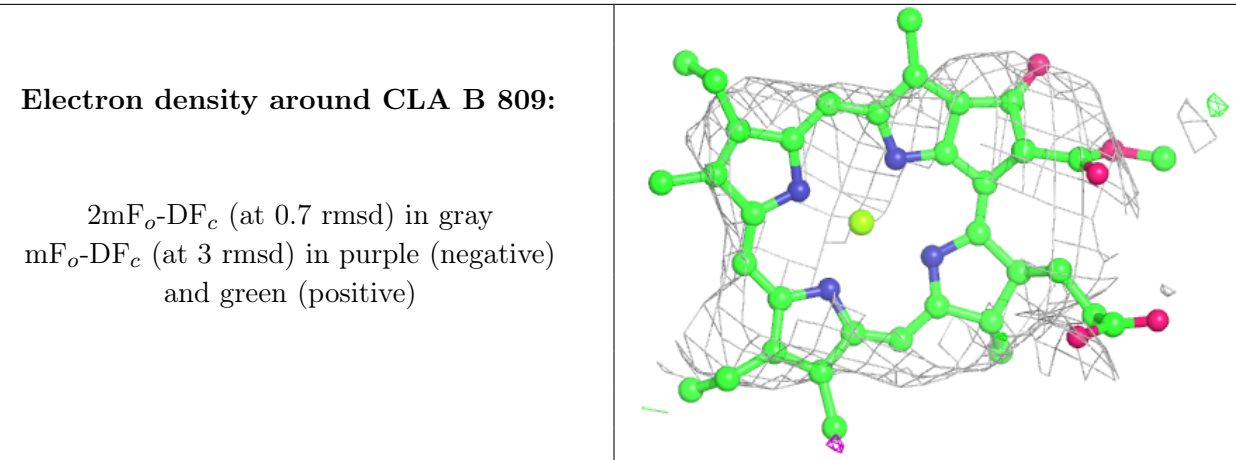


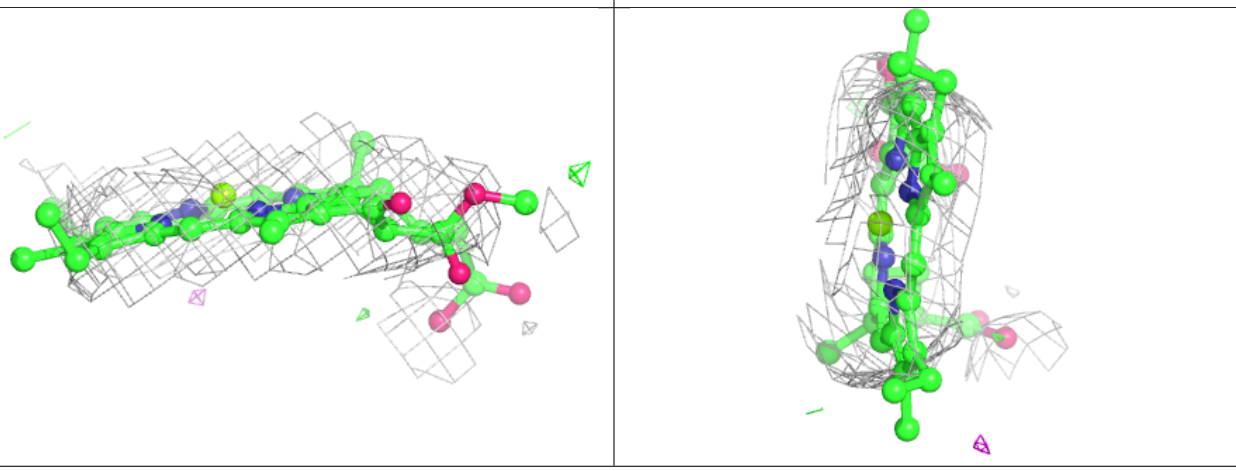




Electron density around CLA B 809:

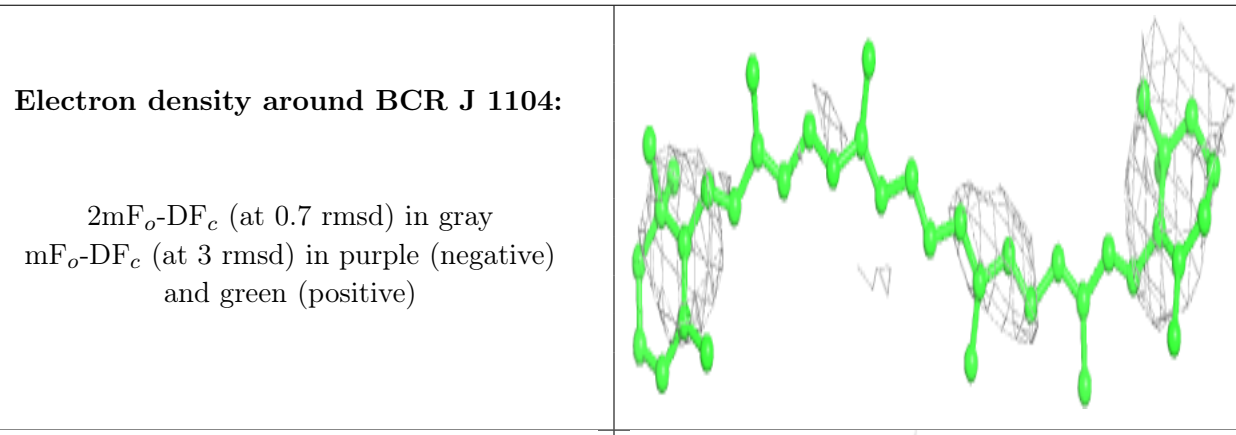
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

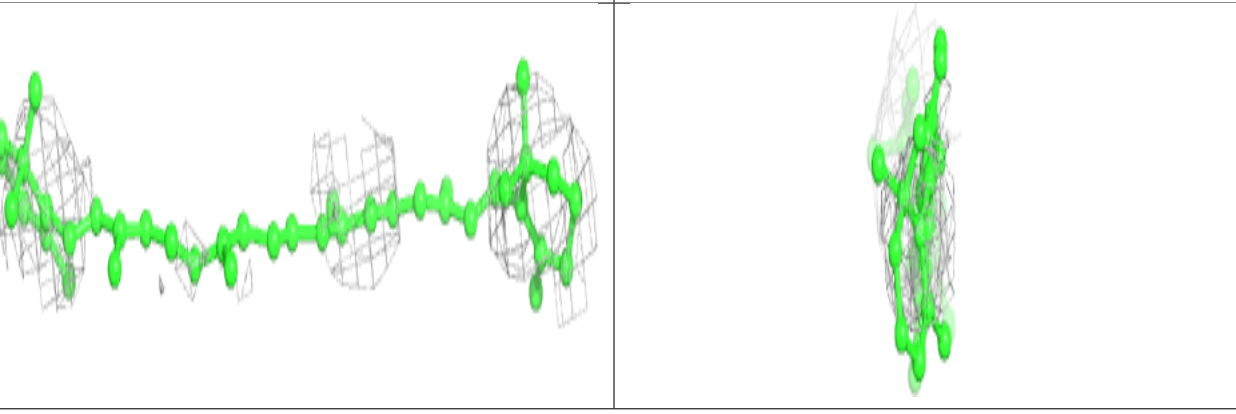




Electron density around BCR J 1104:

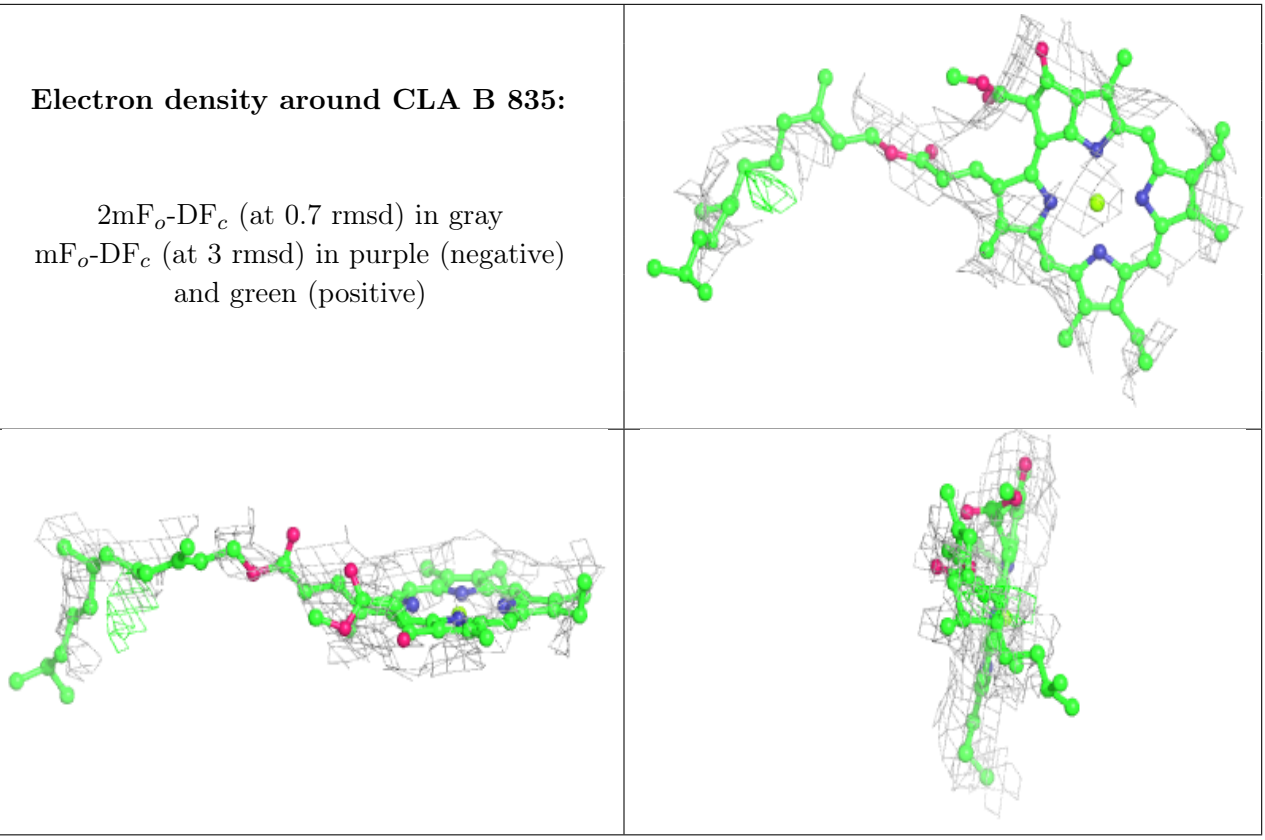
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





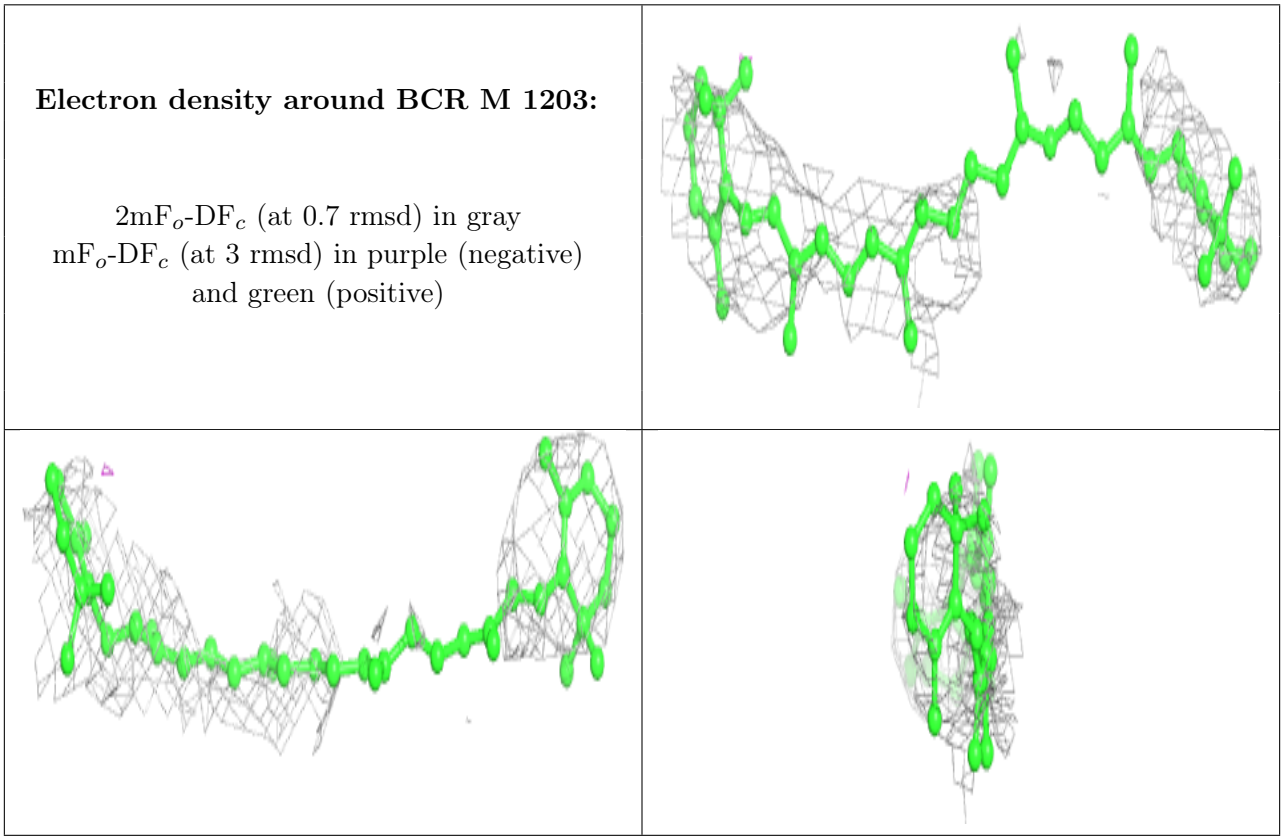
Electron density around CLA B 835:

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



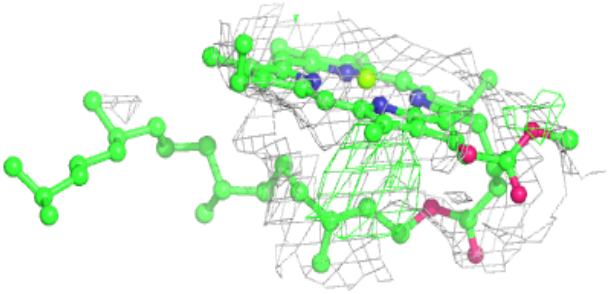
Electron density around BCR M 1203:

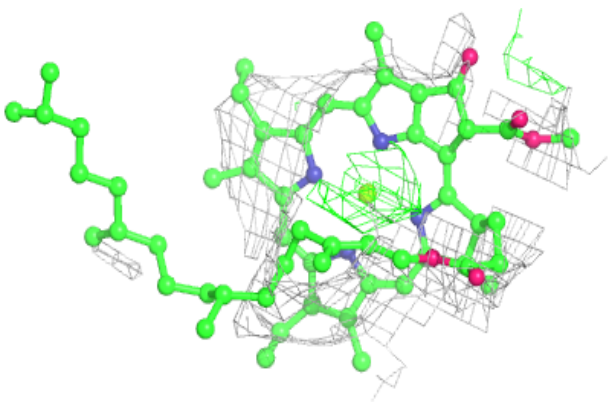
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

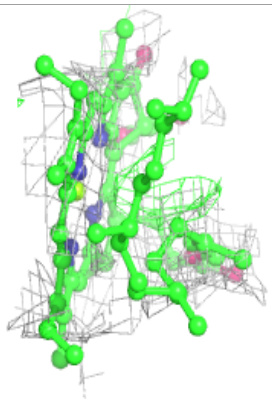


Electron density around CLA B 836:

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

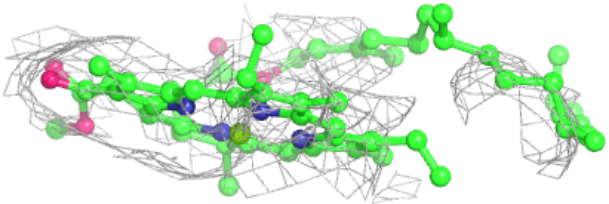


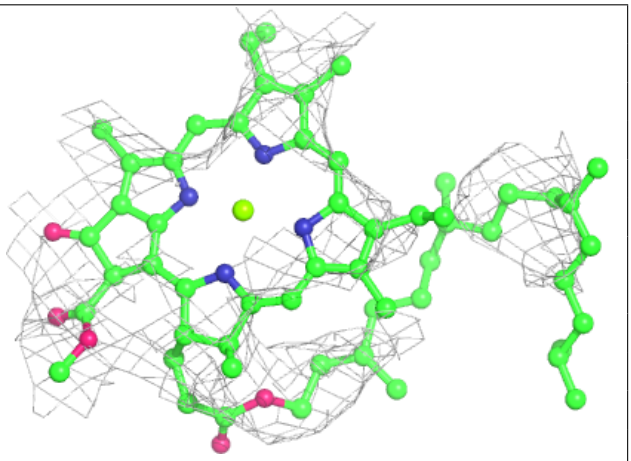


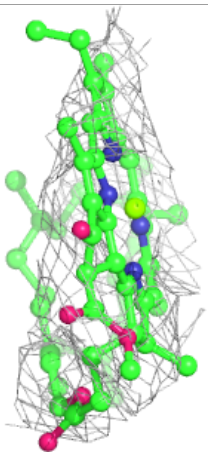


Electron density around CLA A 819:

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

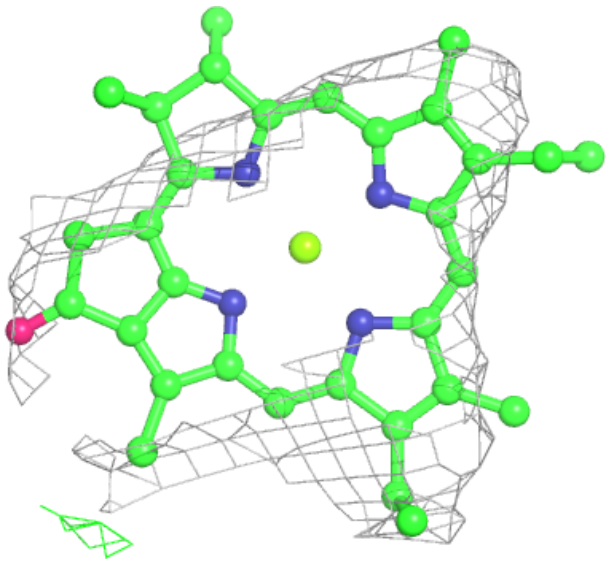


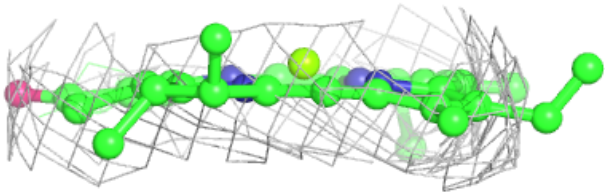


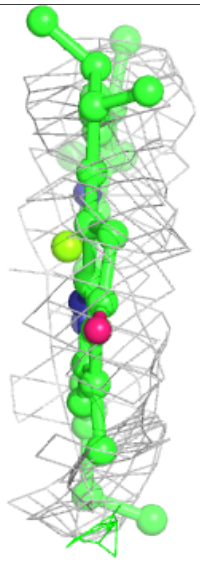


Electron density around CLA J 1103:

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

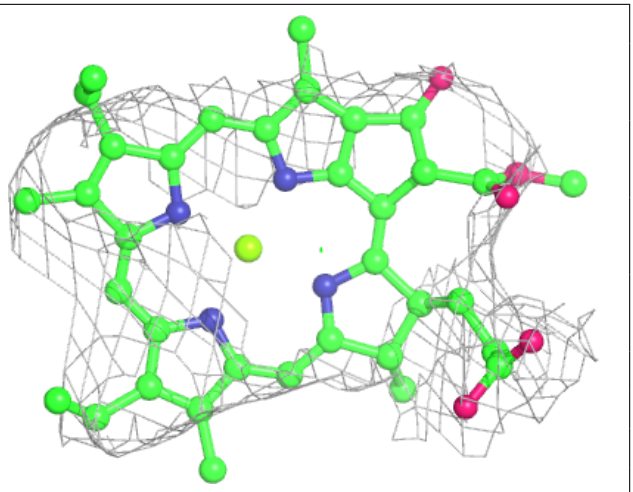


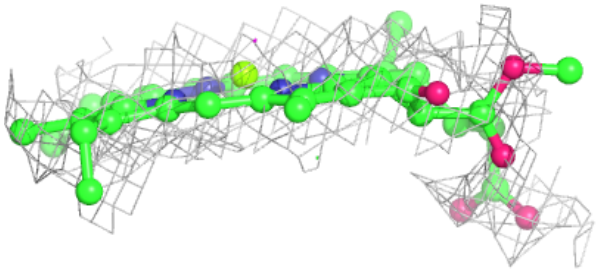


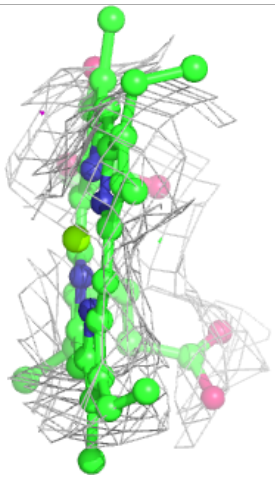


Electron density around CLA B 832:

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

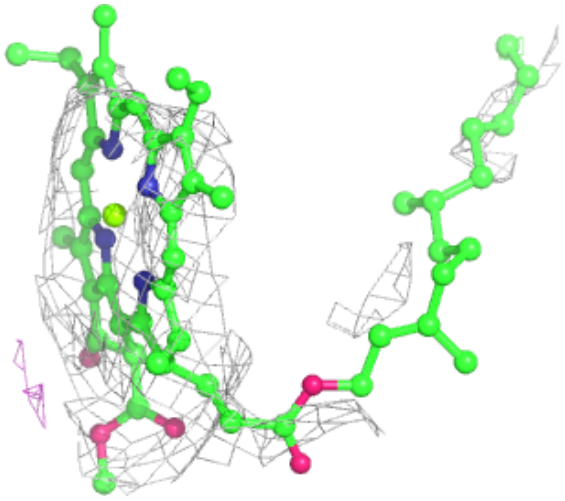


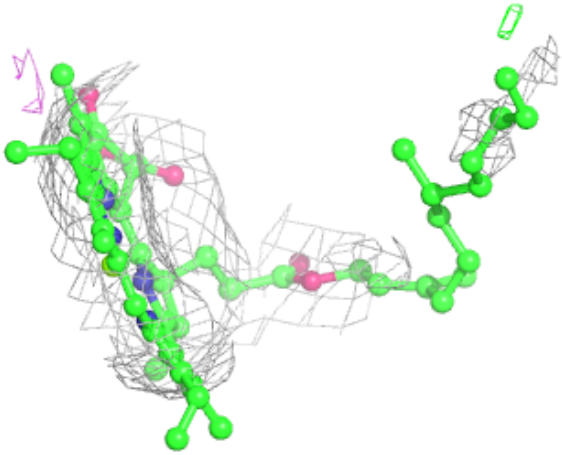


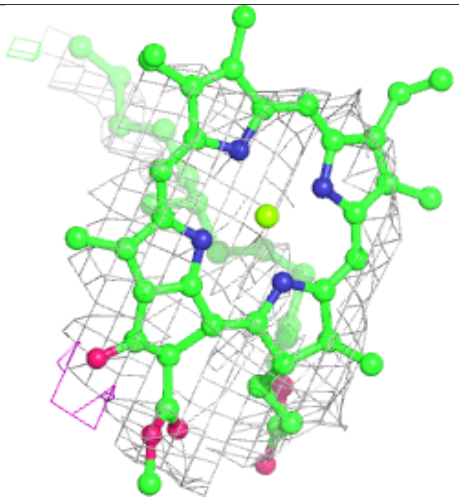


Electron density around CLA A 804:

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

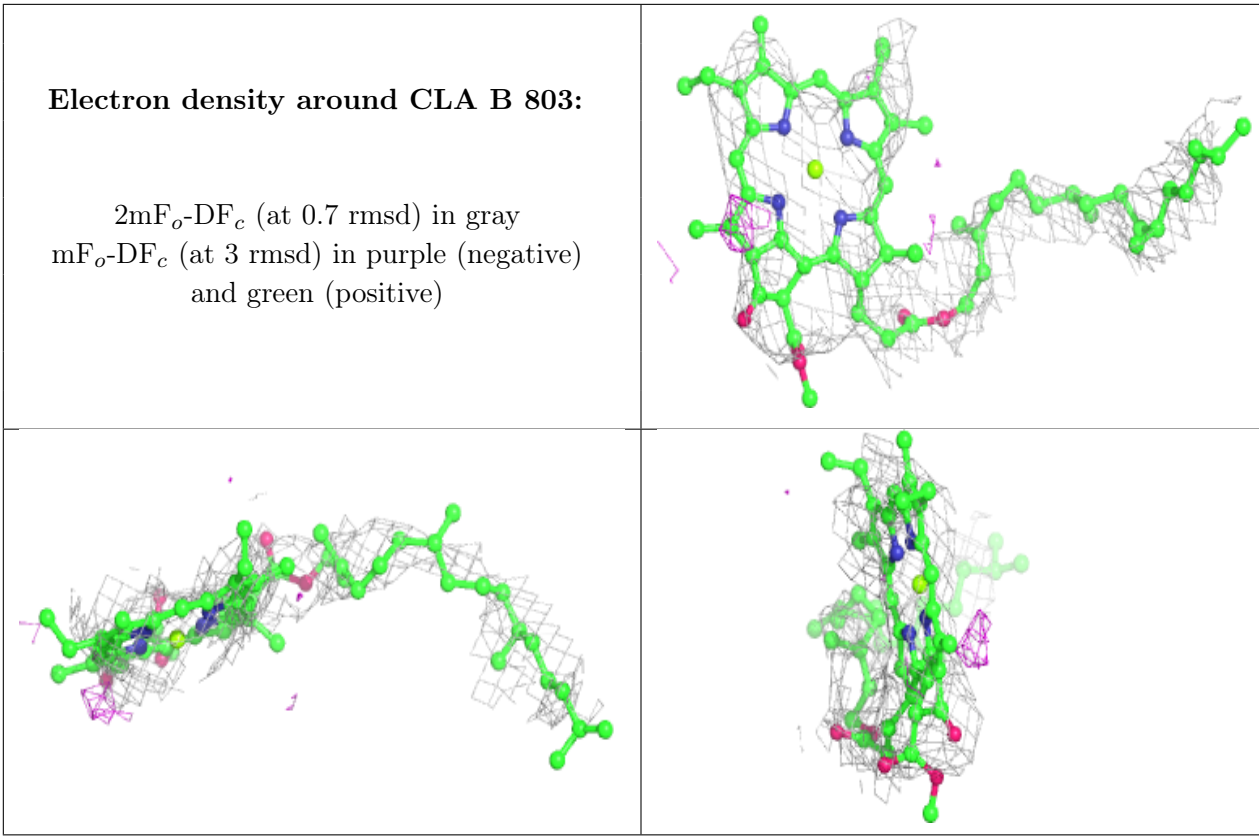






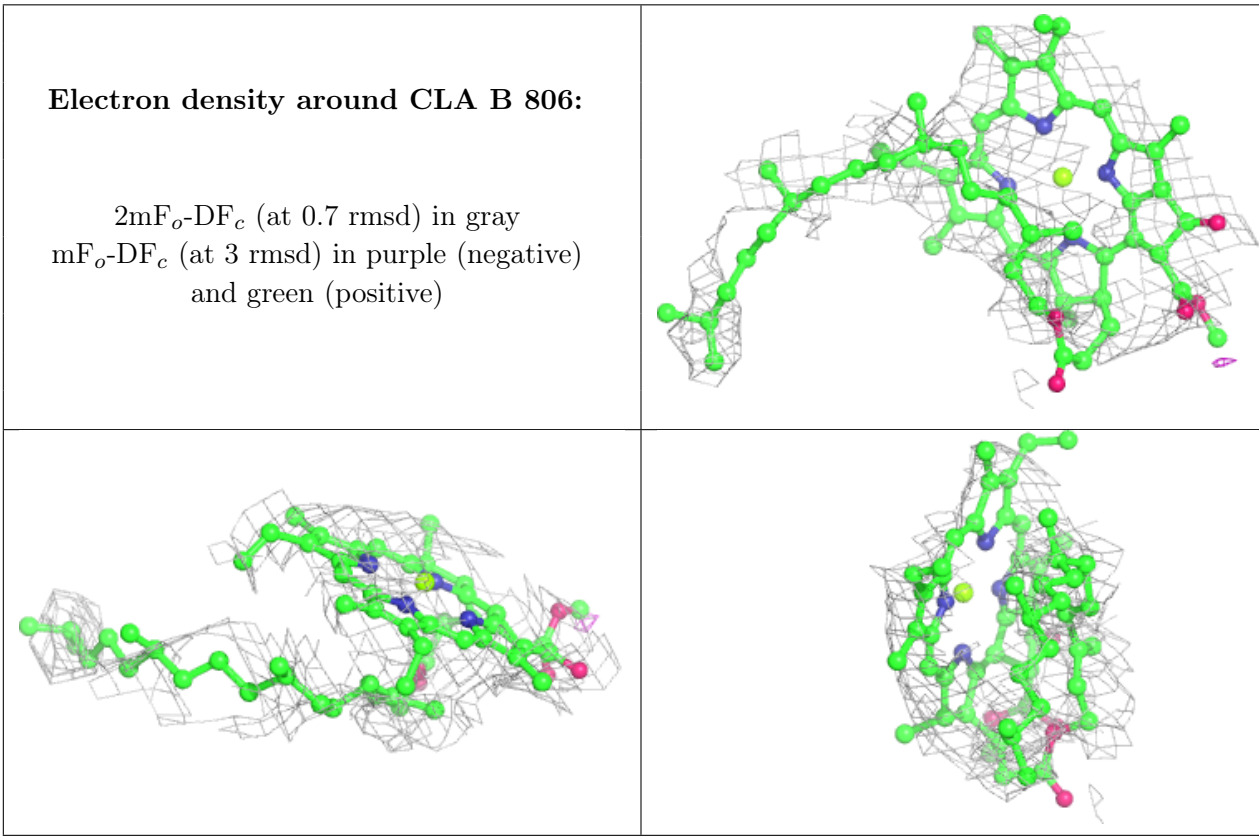
Electron density around CLA B 803:

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



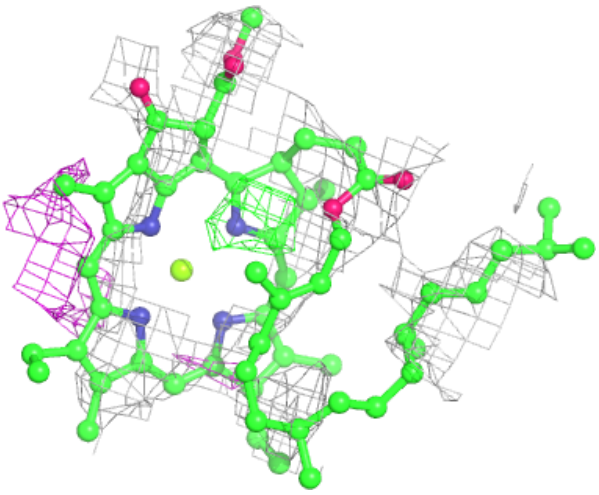
Electron density around CLA B 806:

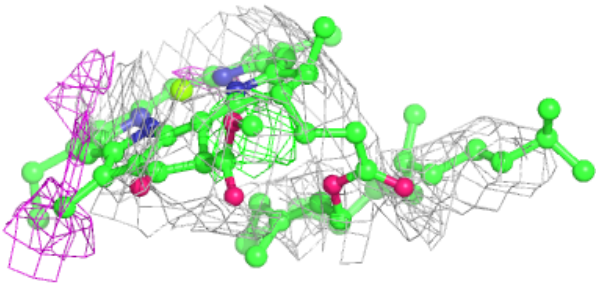
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

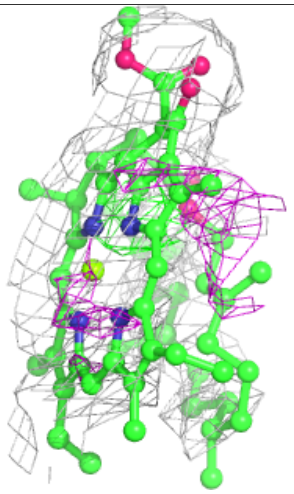


Electron density around CLA B 807:

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

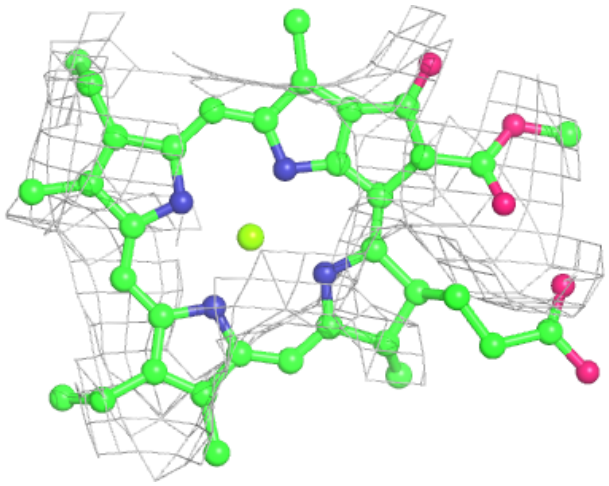


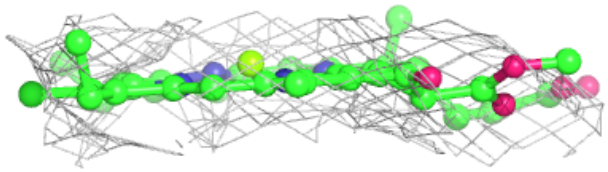


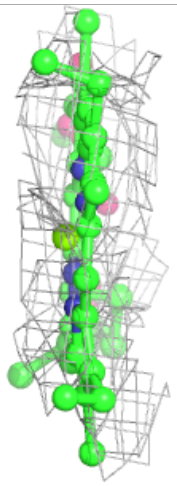


Electron density around CLA F 1301:

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

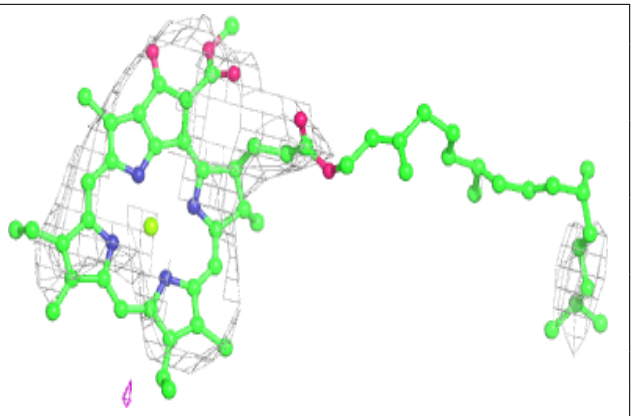


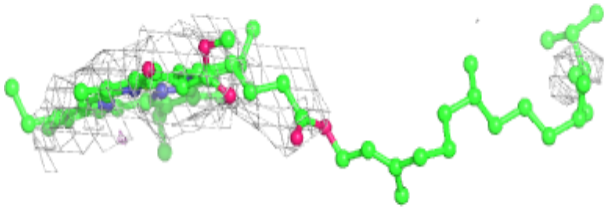


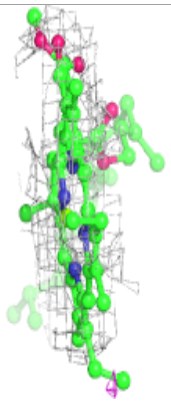


Electron density around CLA A 826:

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

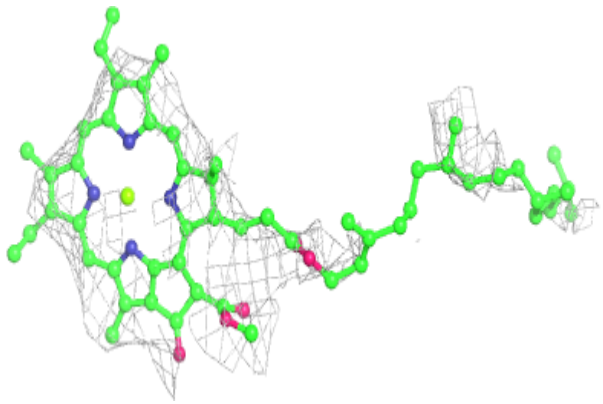


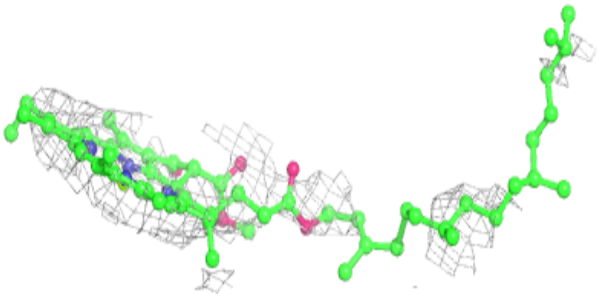


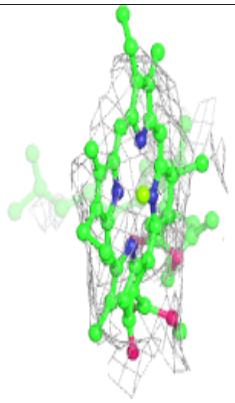


Electron density around CLA A 805:

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

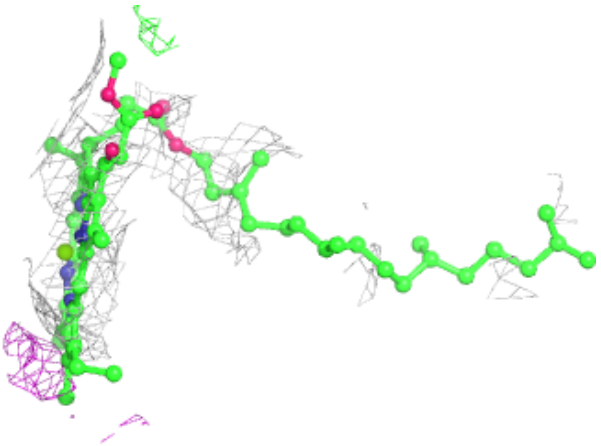


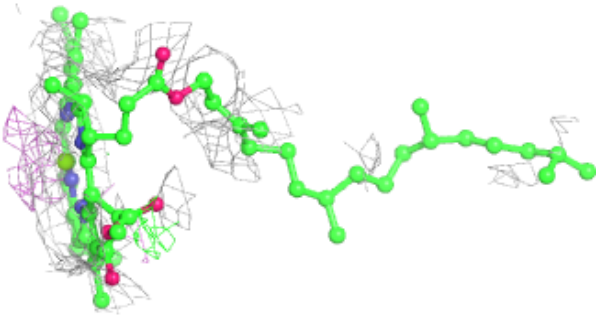


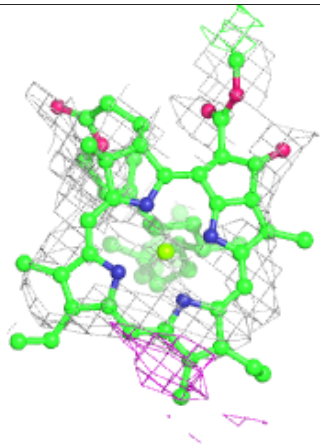


Electron density around CLA A 828:

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

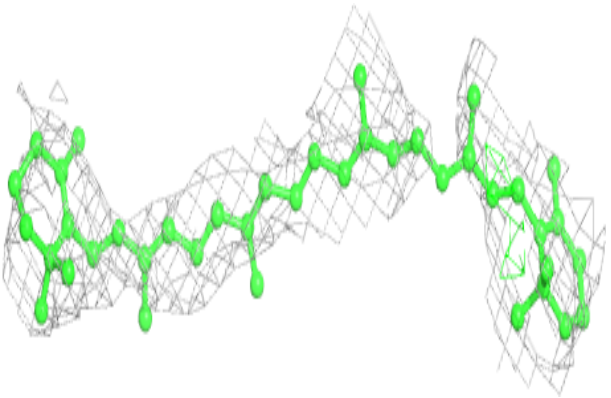


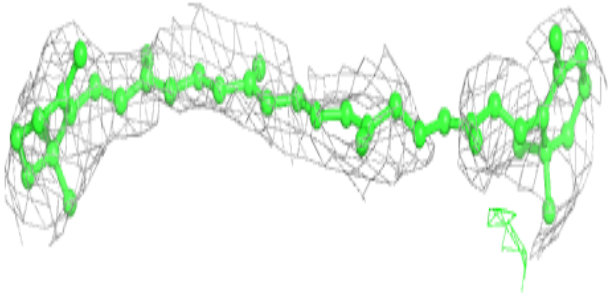


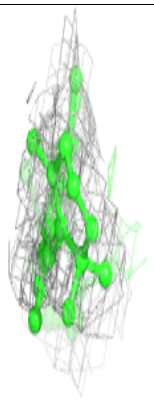


Electron density around BCR B 845:

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

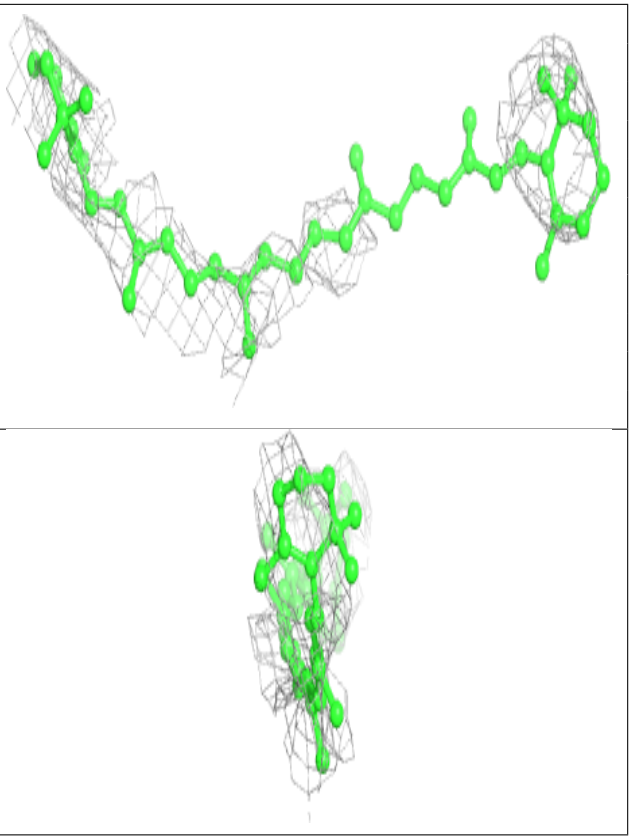






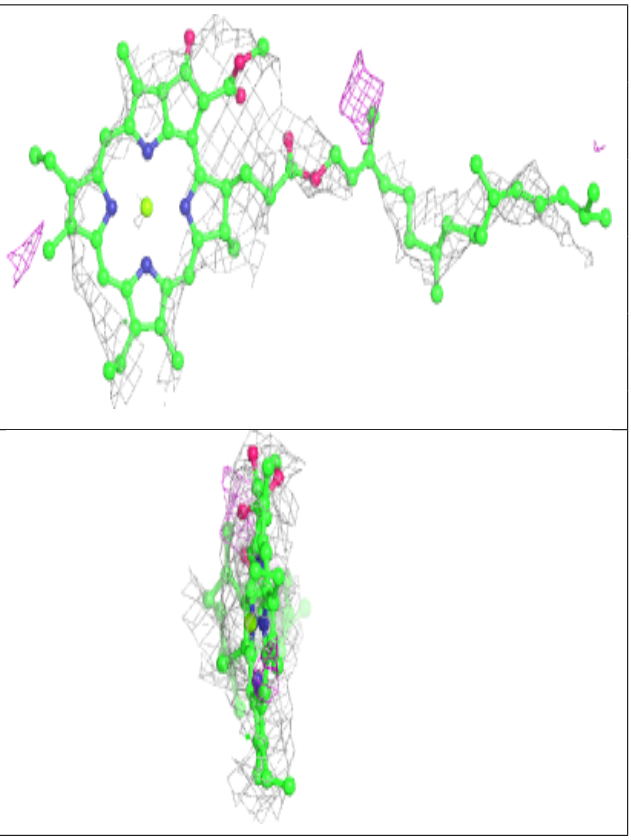
Electron density around BCR B 846:

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



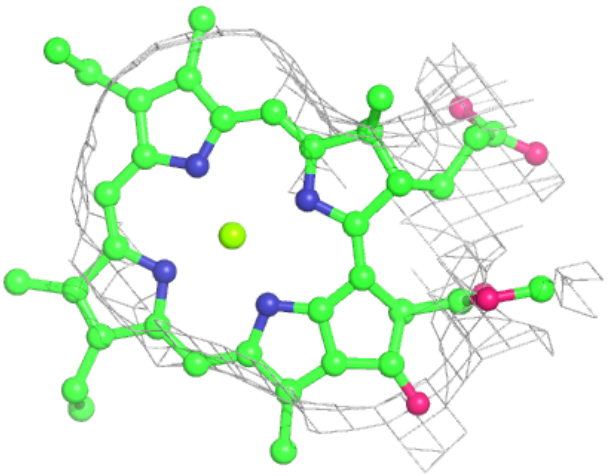
Electron density around CLA A 833:

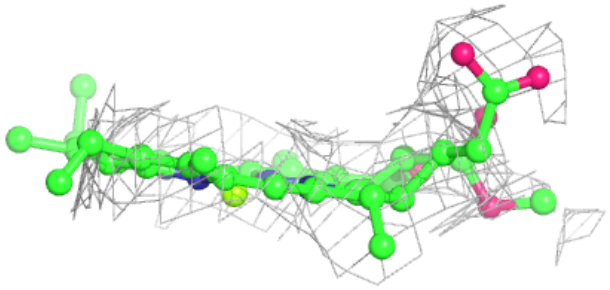
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

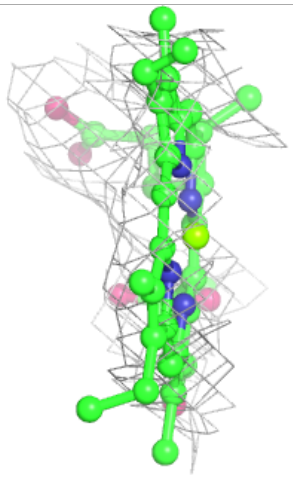


Electron density around CLA A 814:

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

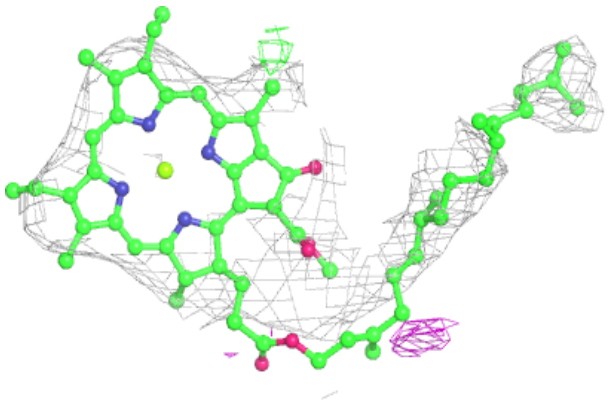


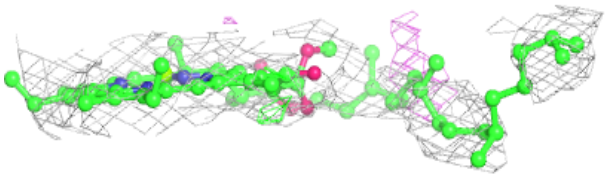


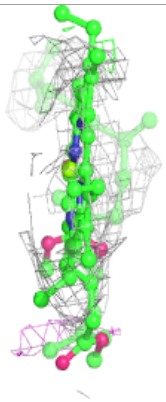


Electron density around CLA L 1004:

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

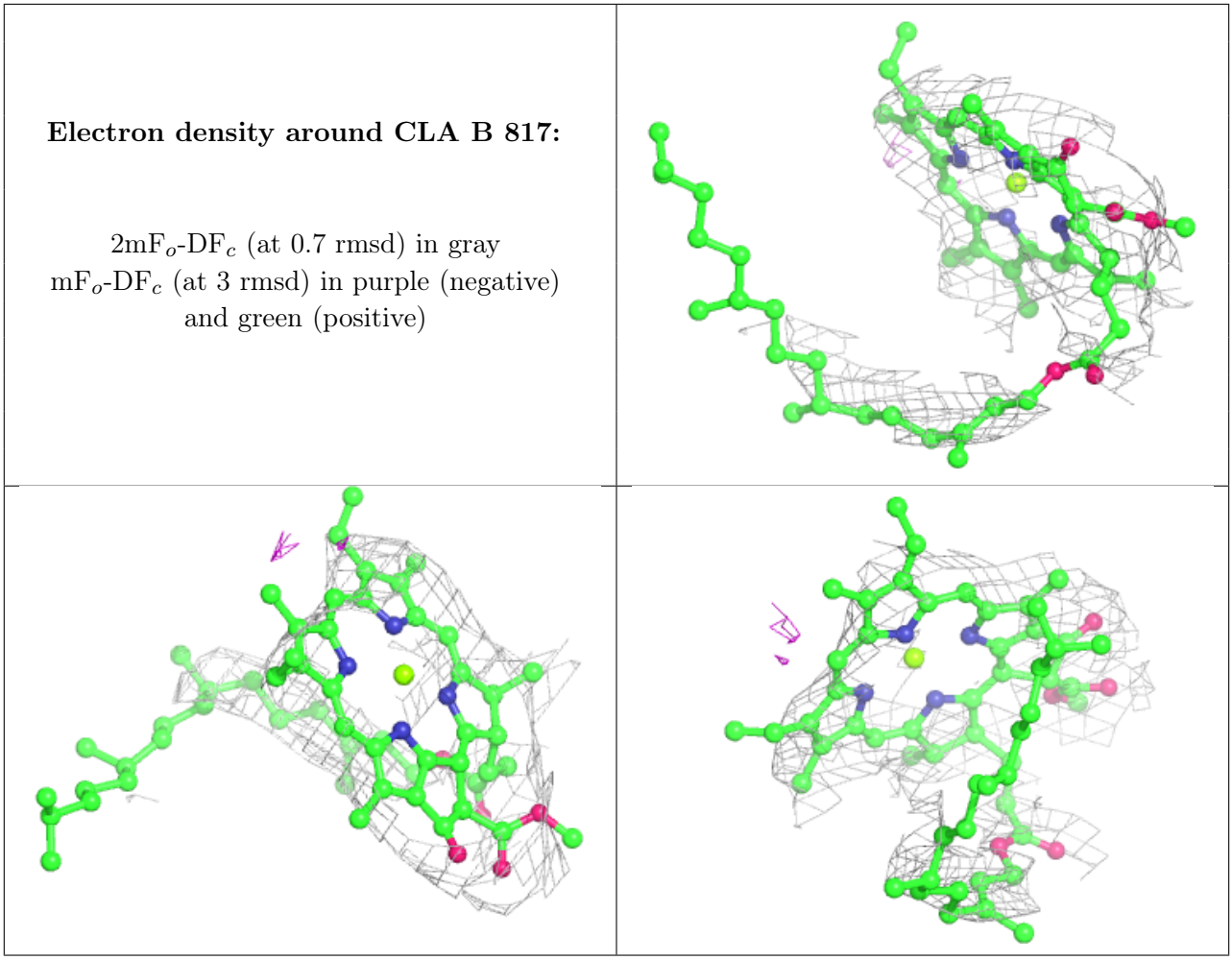






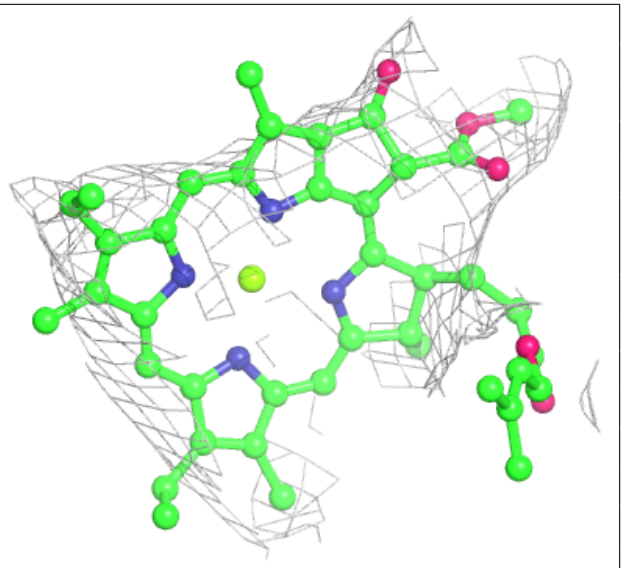
Electron density around CLA B 817:

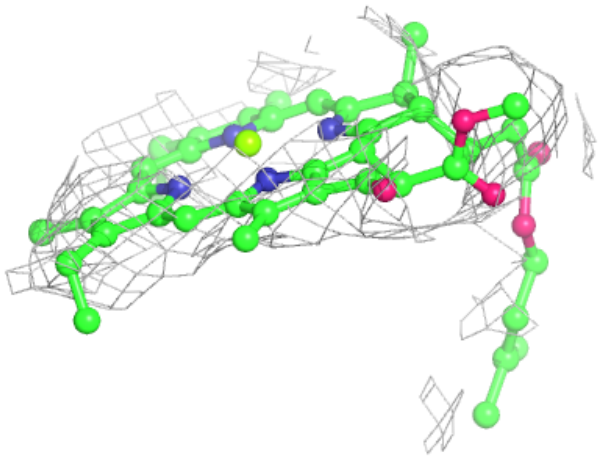
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

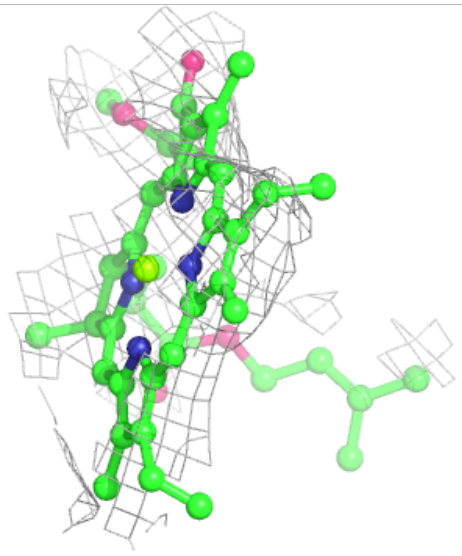


Electron density around CLA A 831:

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

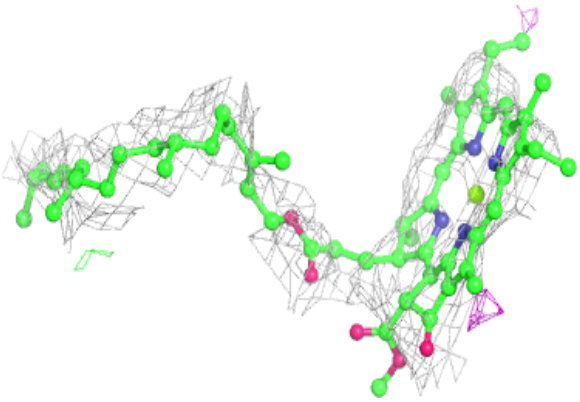


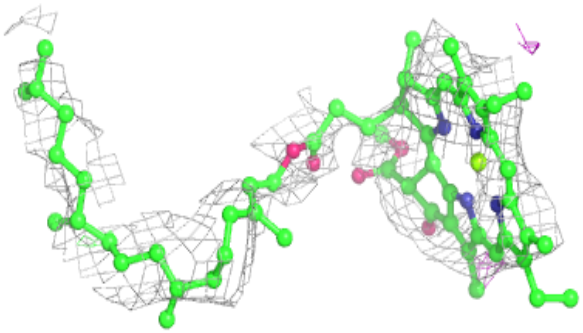


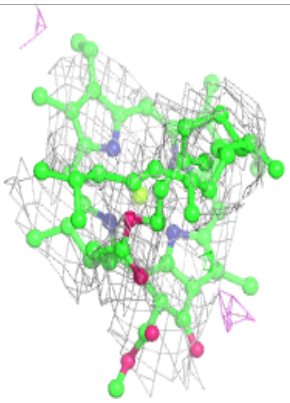


Electron density around CLA B 838:

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

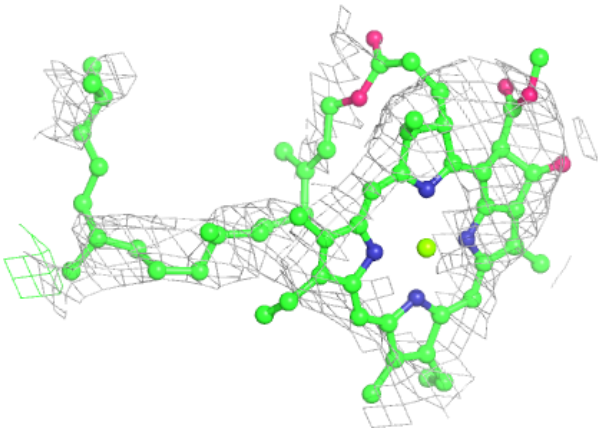


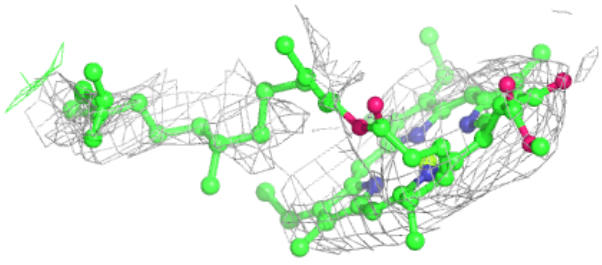


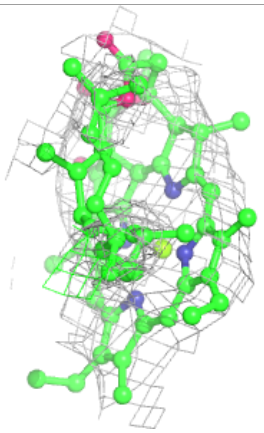


Electron density around CLA A 843:

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

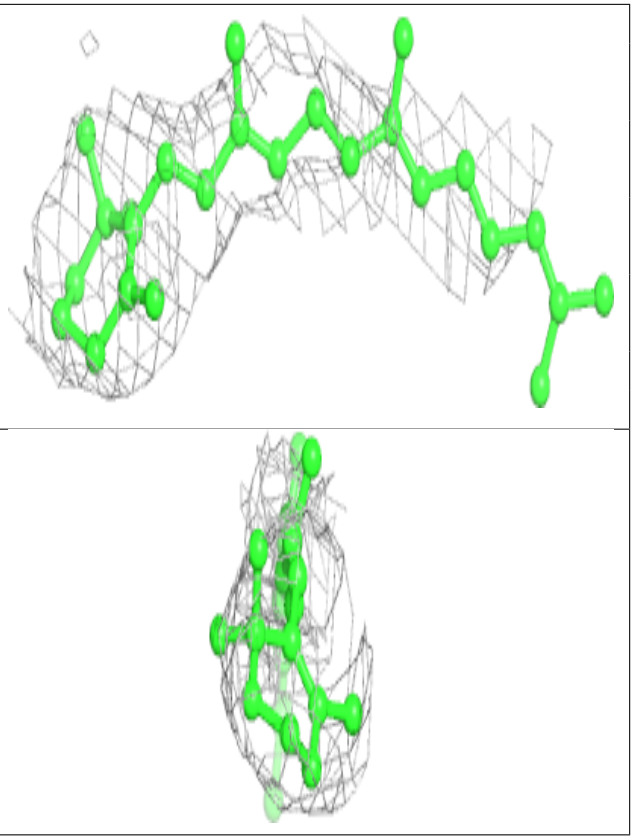


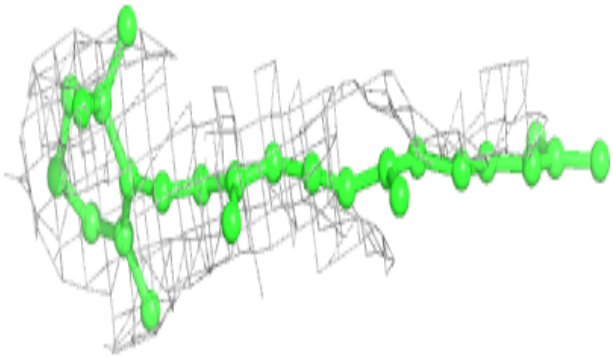




Electron density around BCR B 844:

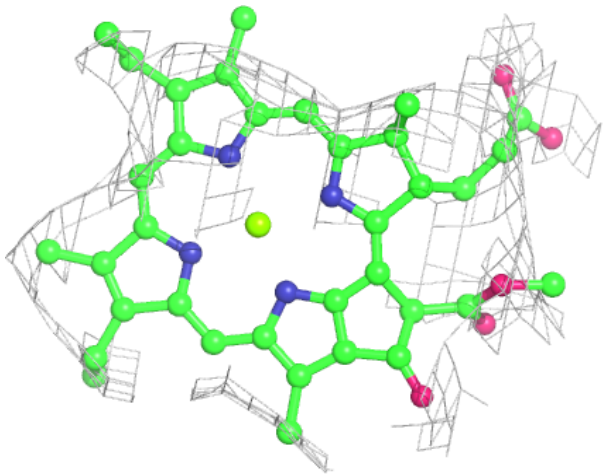
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

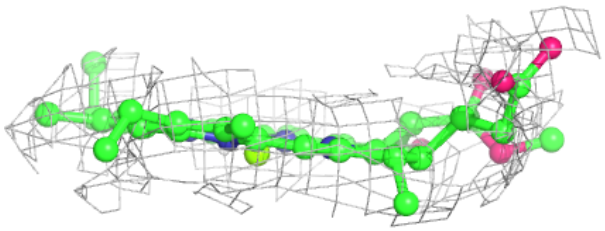


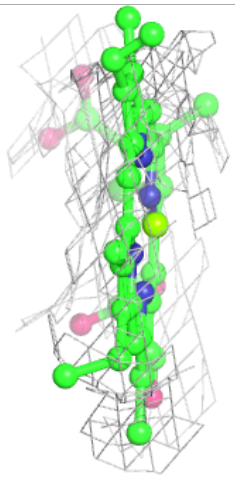


Electron density around CLA X 102:

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

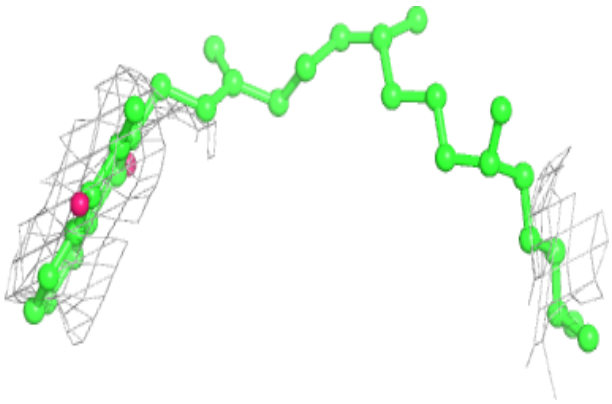


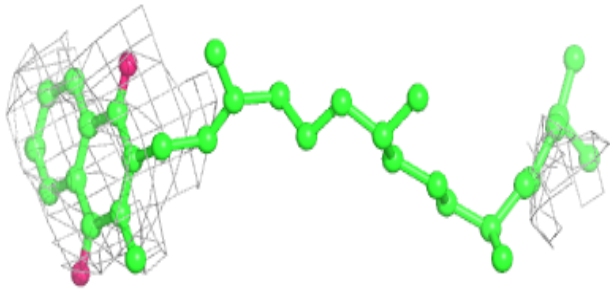


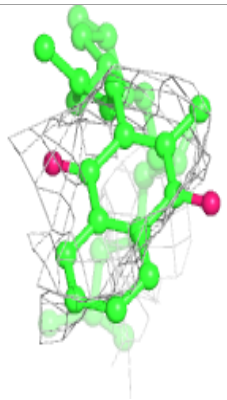


Electron density around PQN B 840:

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

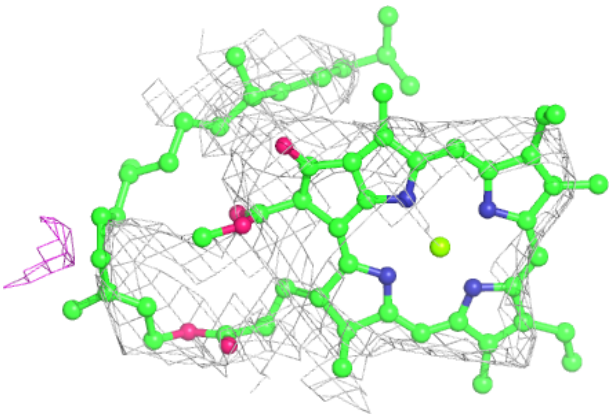


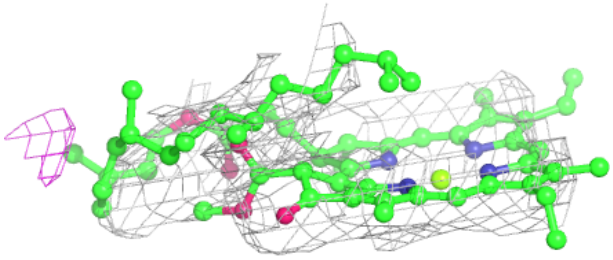


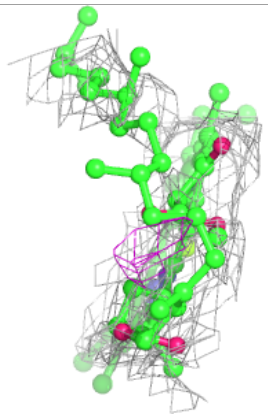


Electron density around CLA B 804:

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

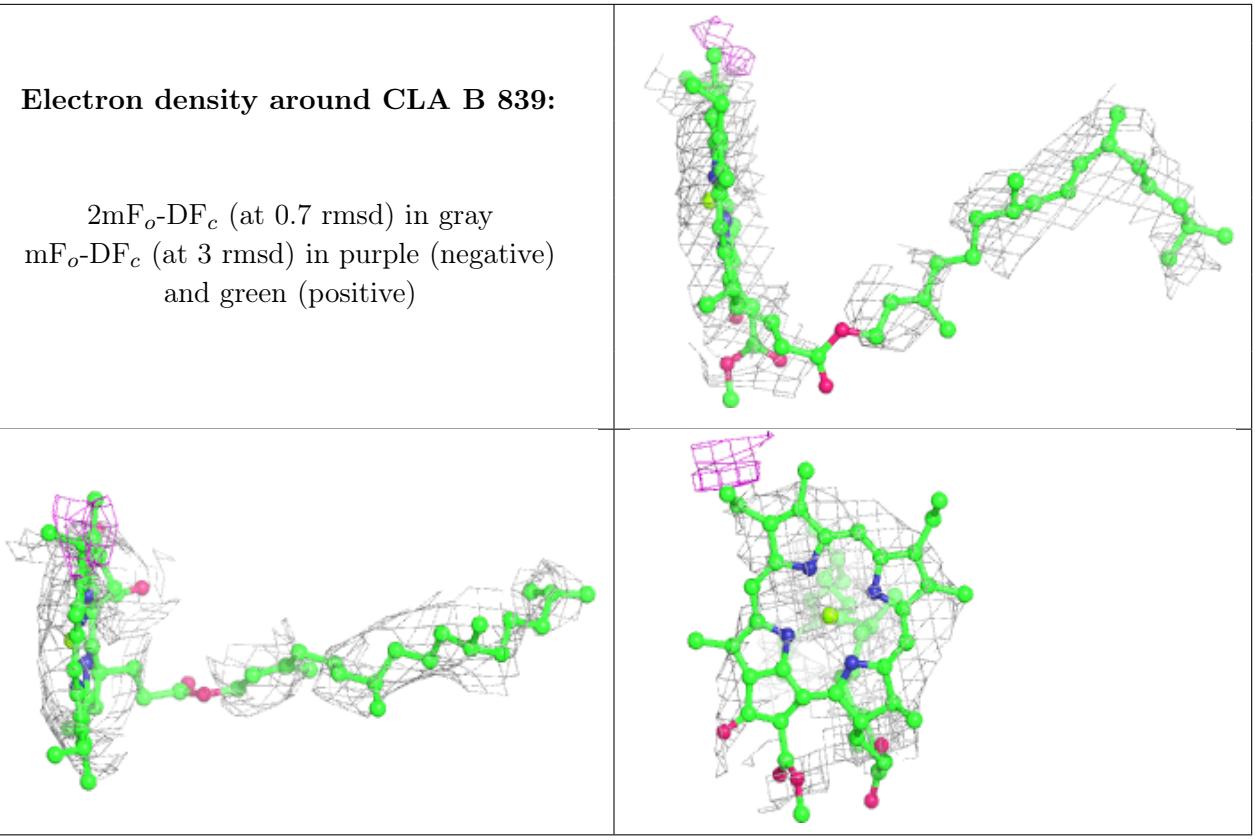






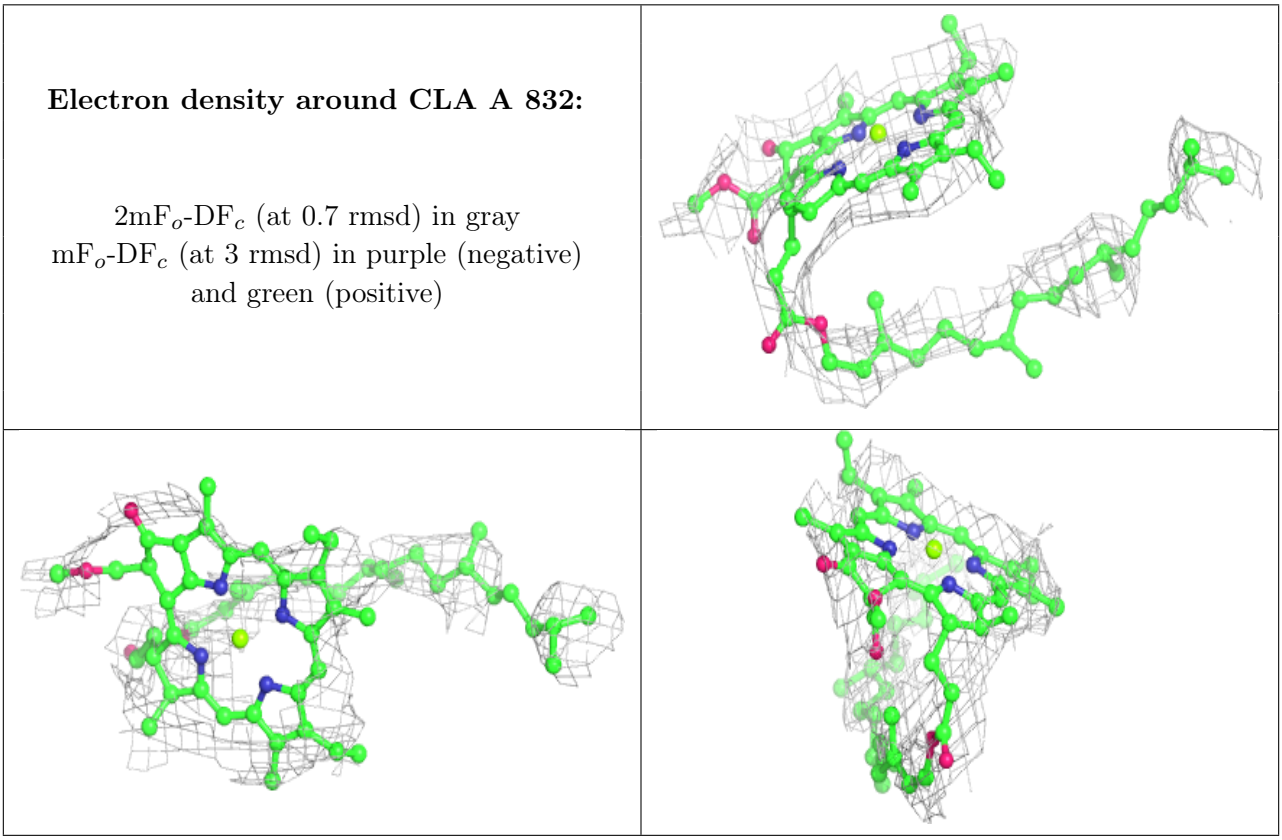
Electron density around CLA B 839:

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



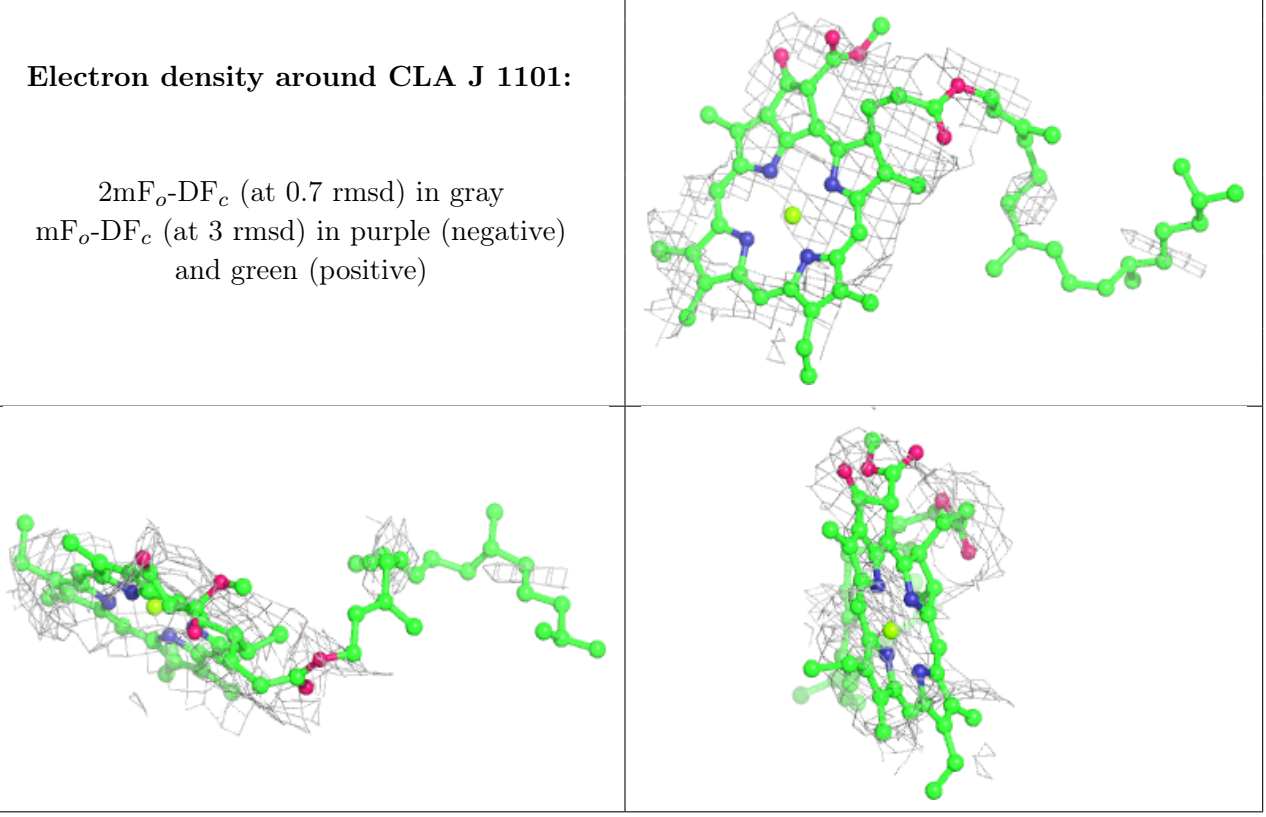
Electron density around CLA A 832:

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



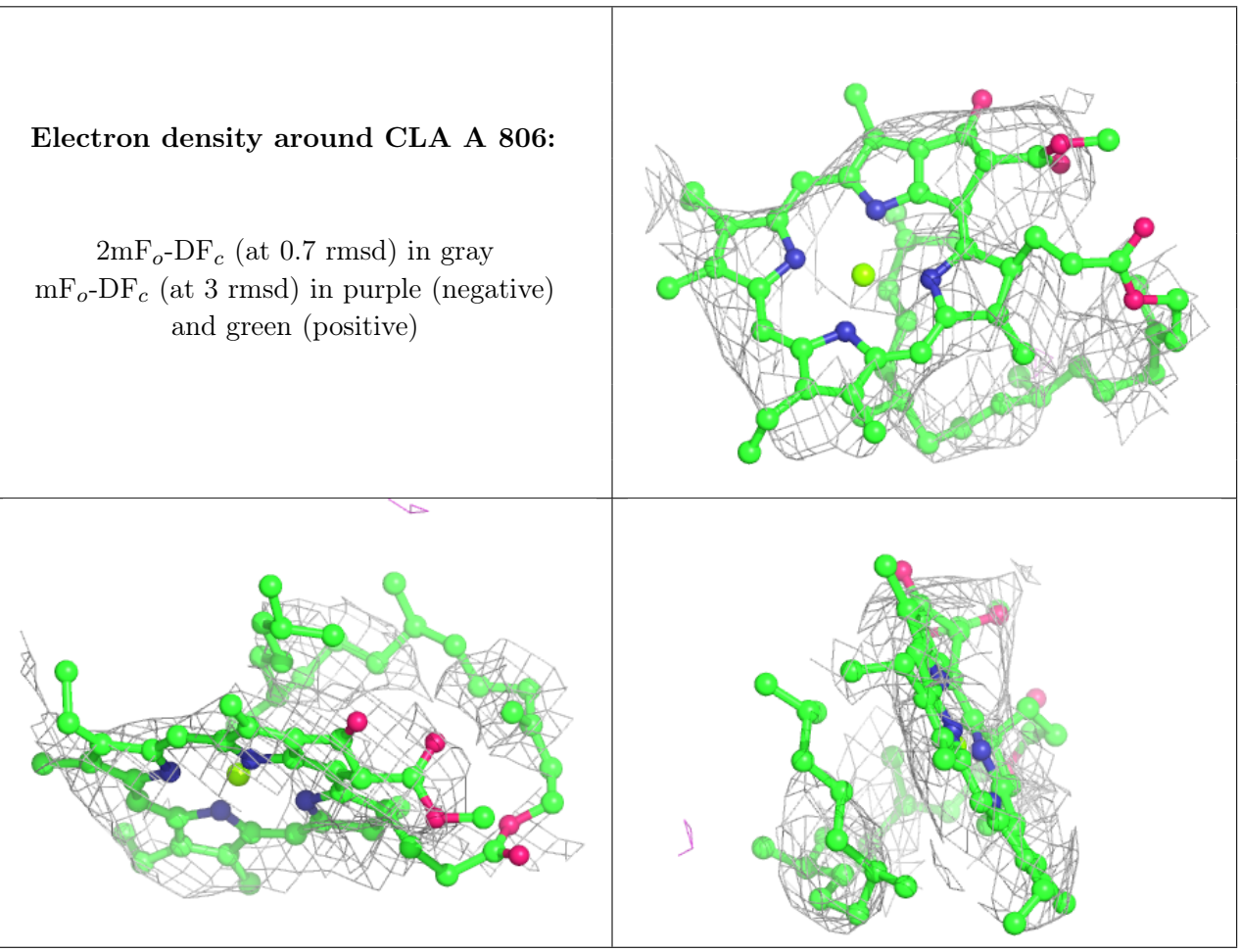
Electron density around CLA J 1101:

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



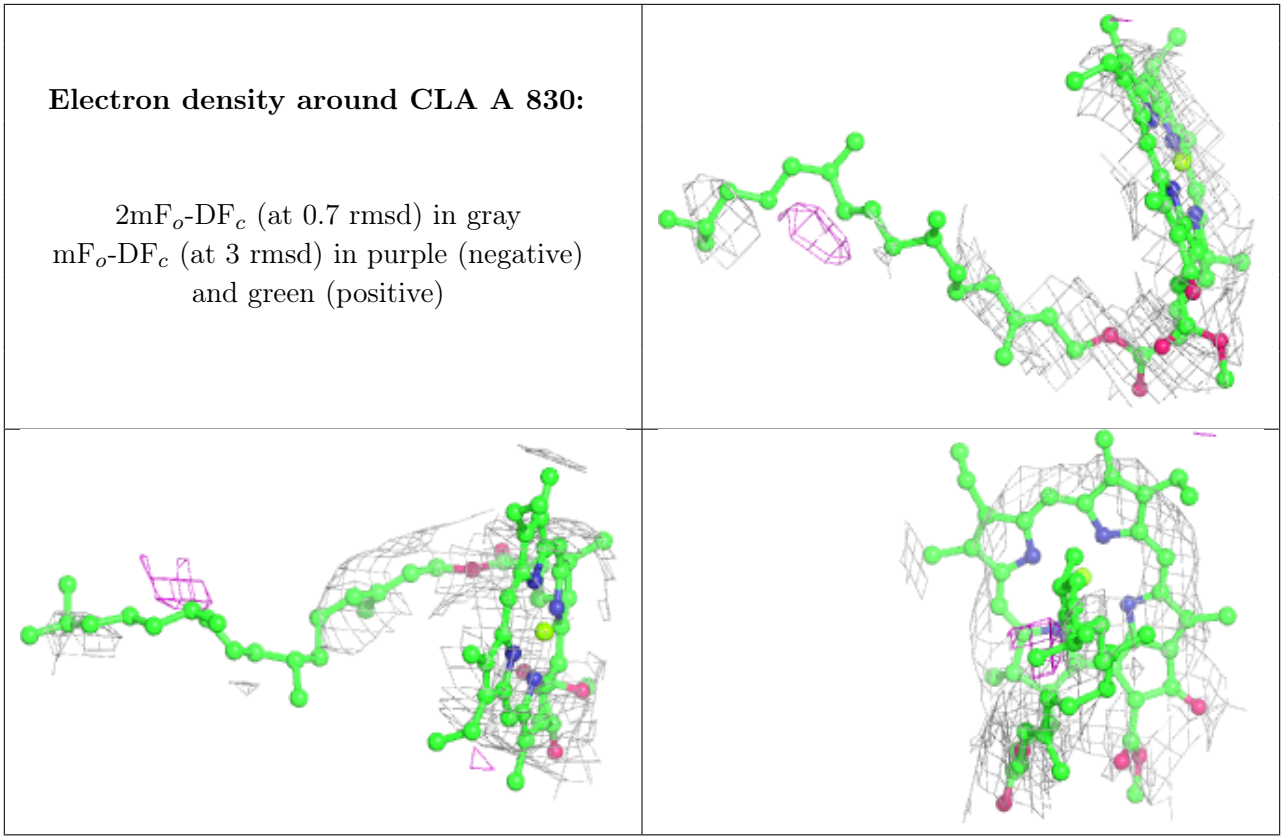
Electron density around CLA A 806:

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



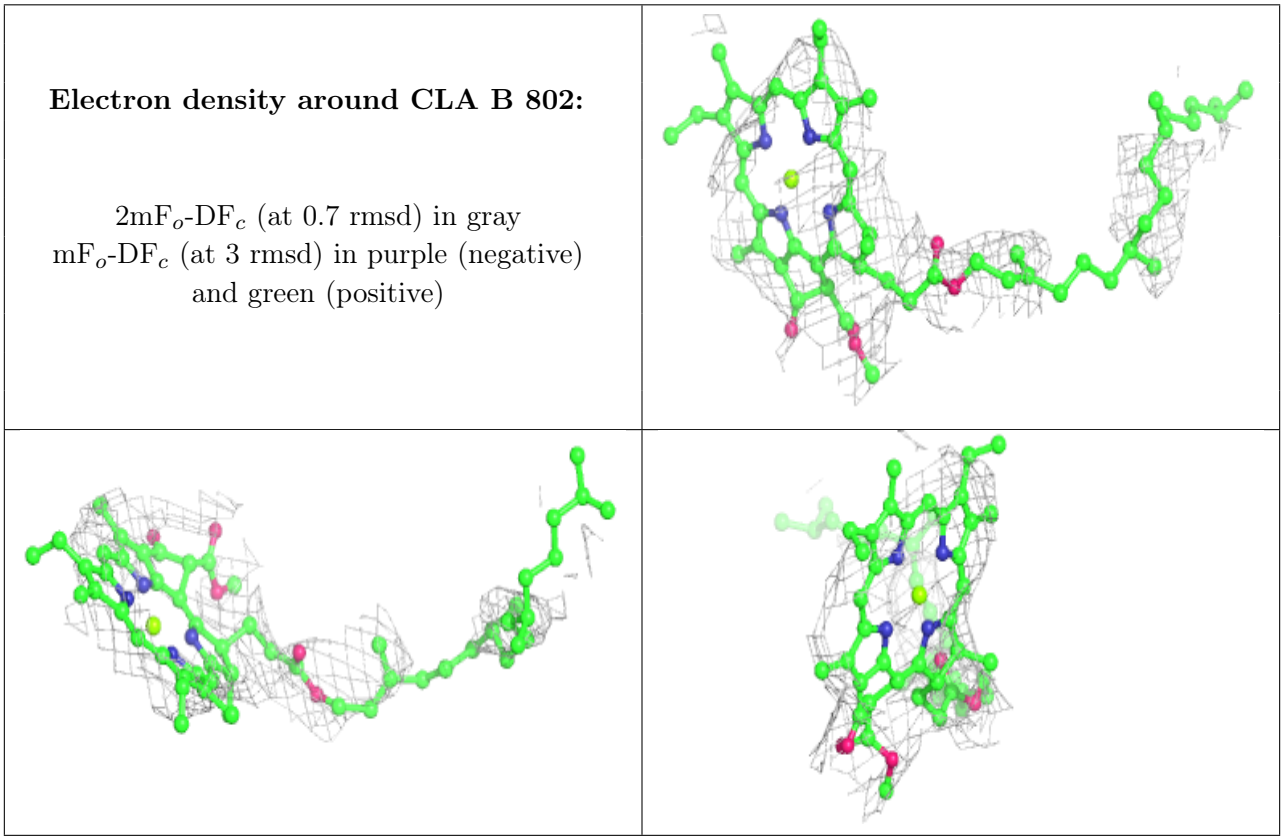
Electron density around CLA A 830:

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



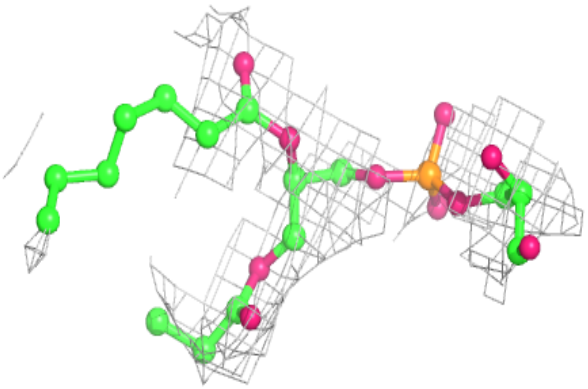
Electron density around CLA B 802:

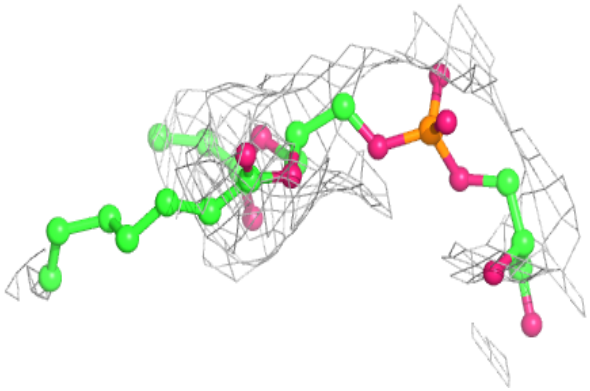
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

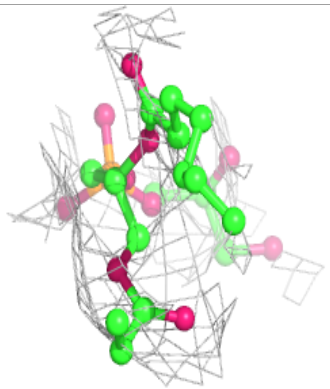


Electron density around LHG A 854:

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

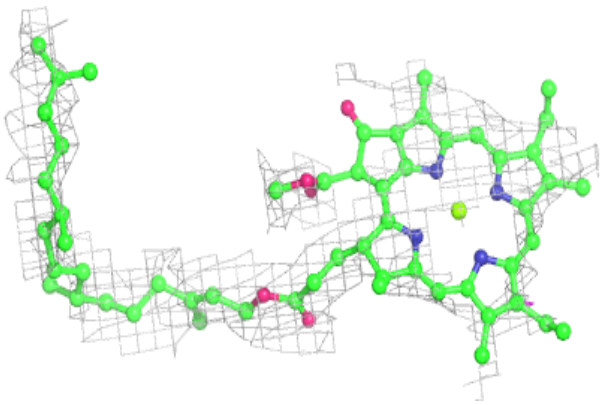


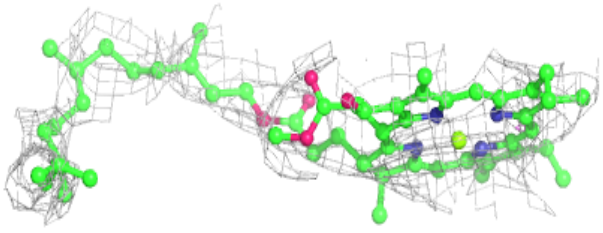


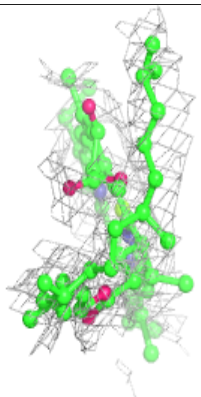


Electron density around CLA B 824:

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

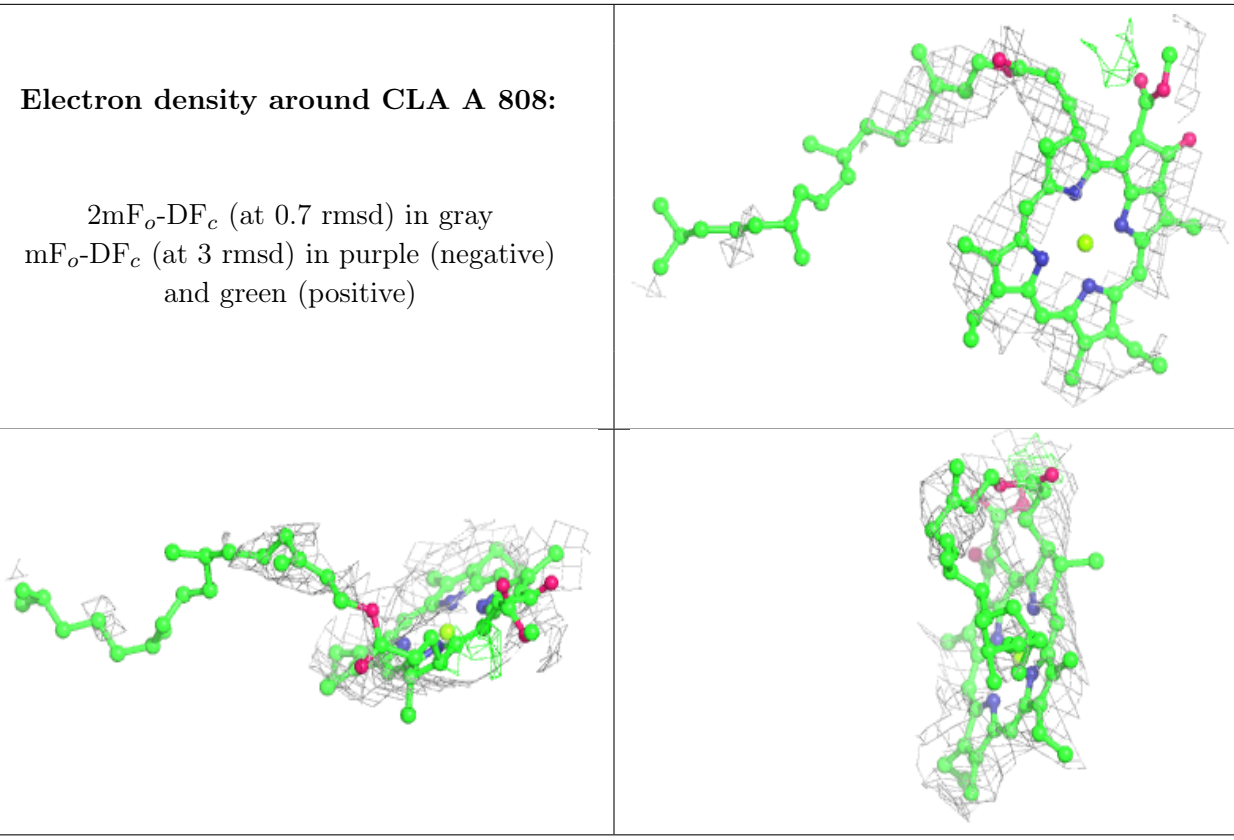






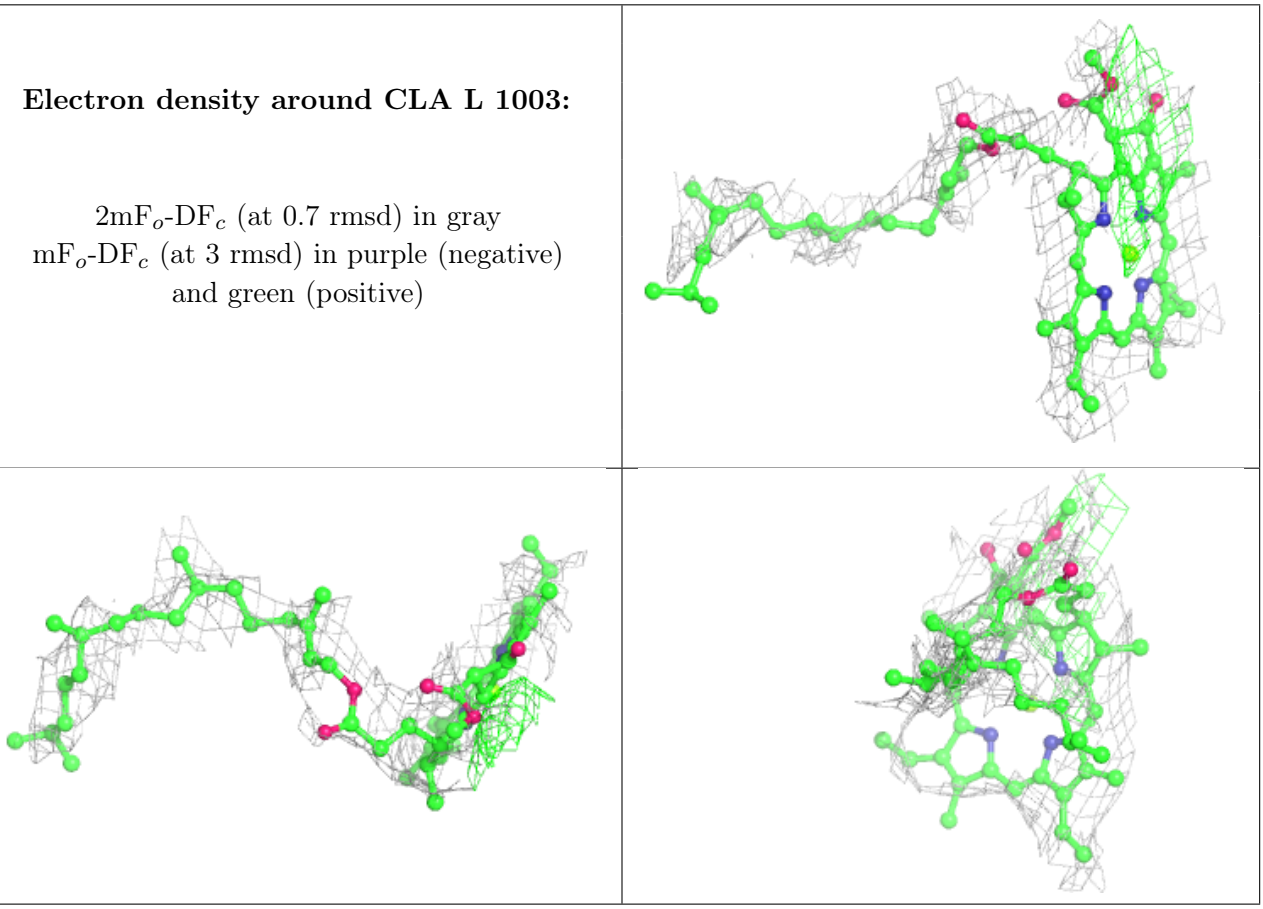
Electron density around CLA A 808:

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



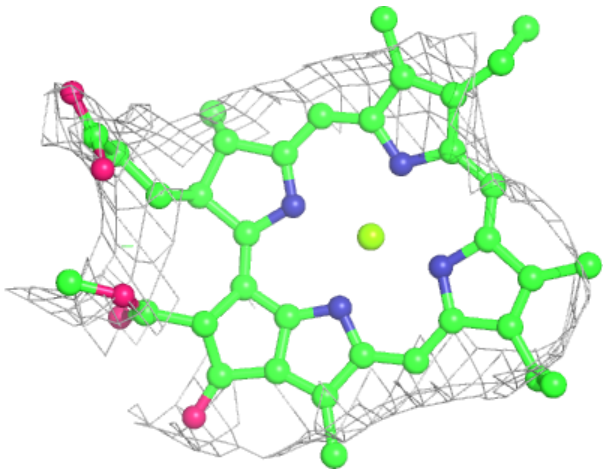
Electron density around CLA L 1003:

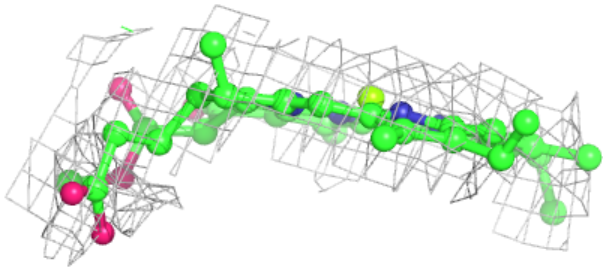
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

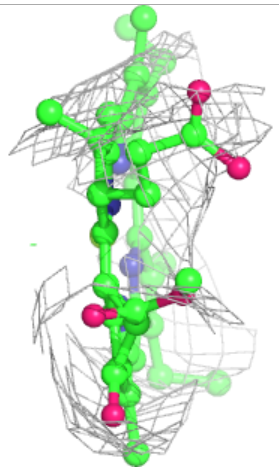


Electron density around CLA B 821:

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

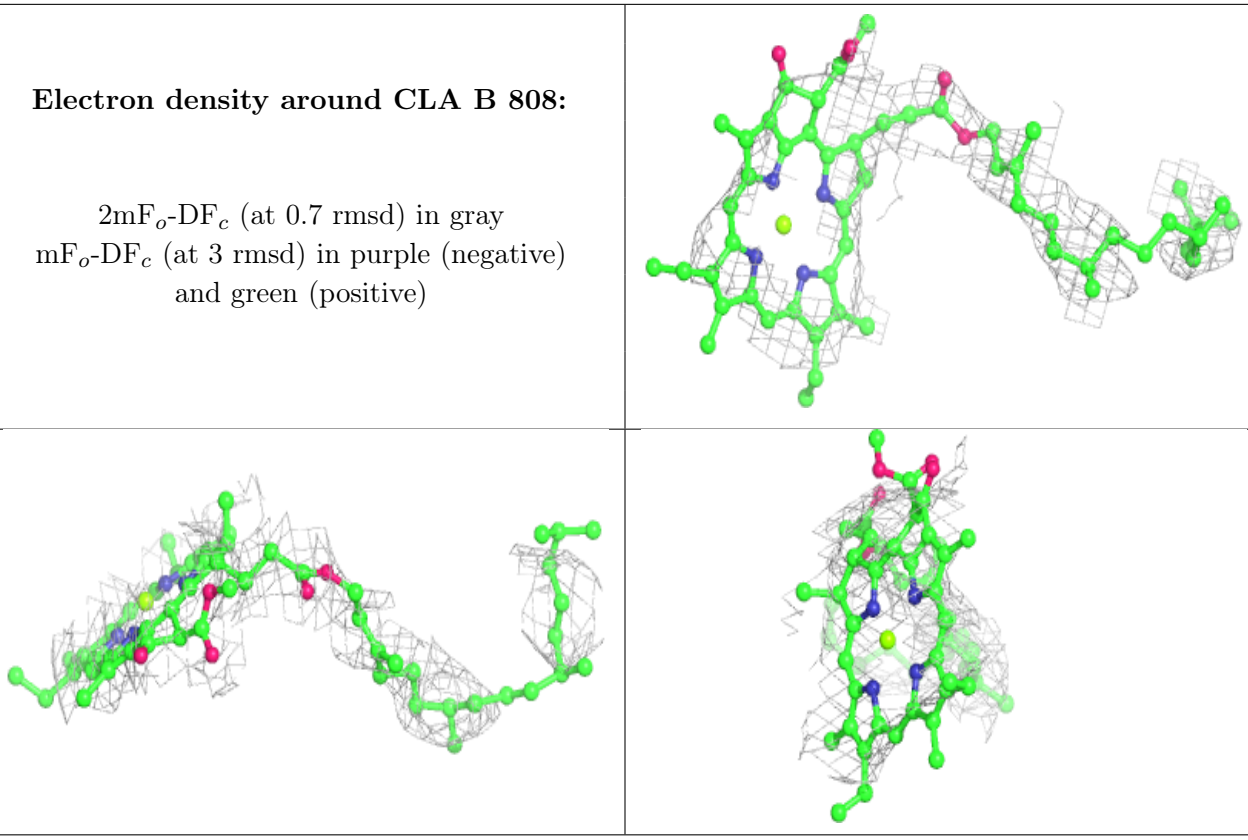






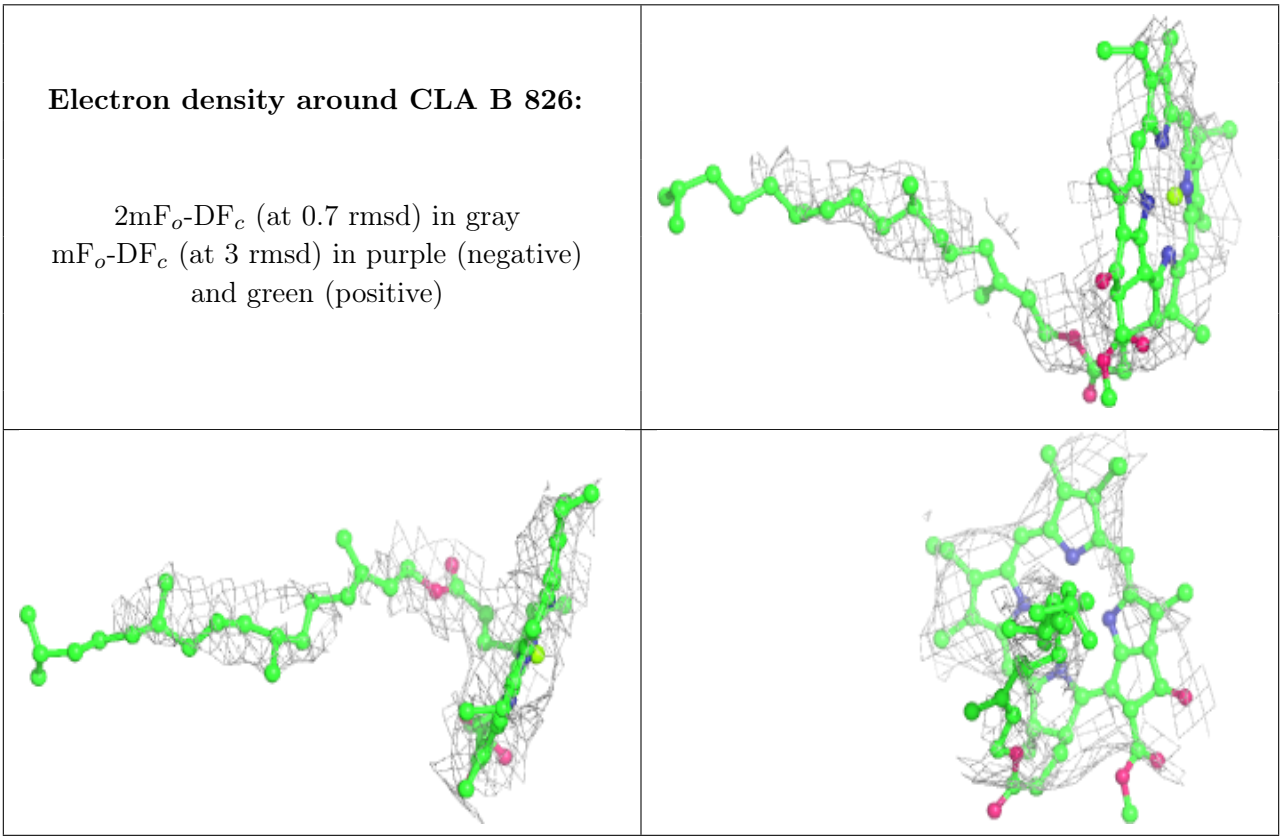
Electron density around CLA B 808:

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



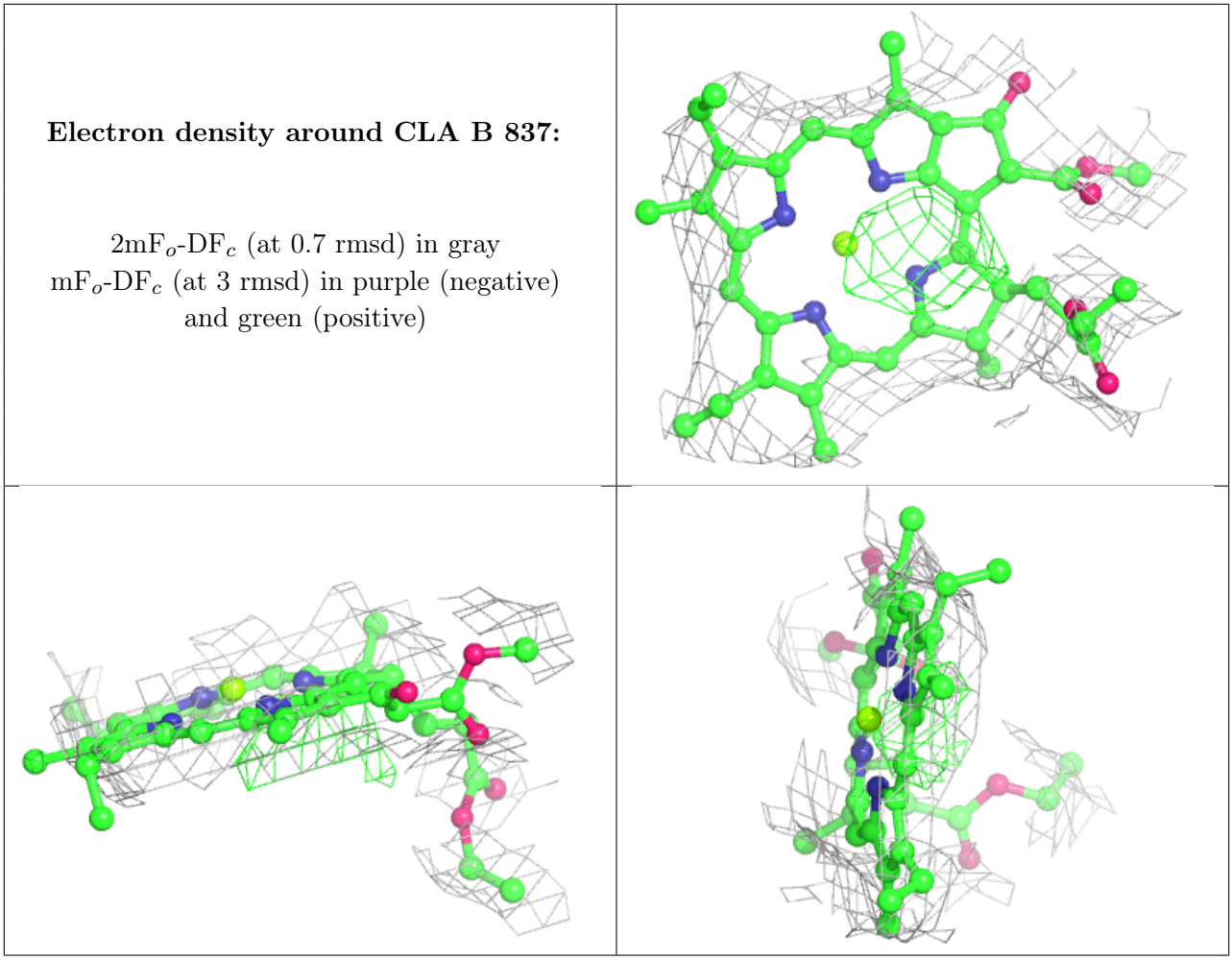
Electron density around CLA B 826:

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



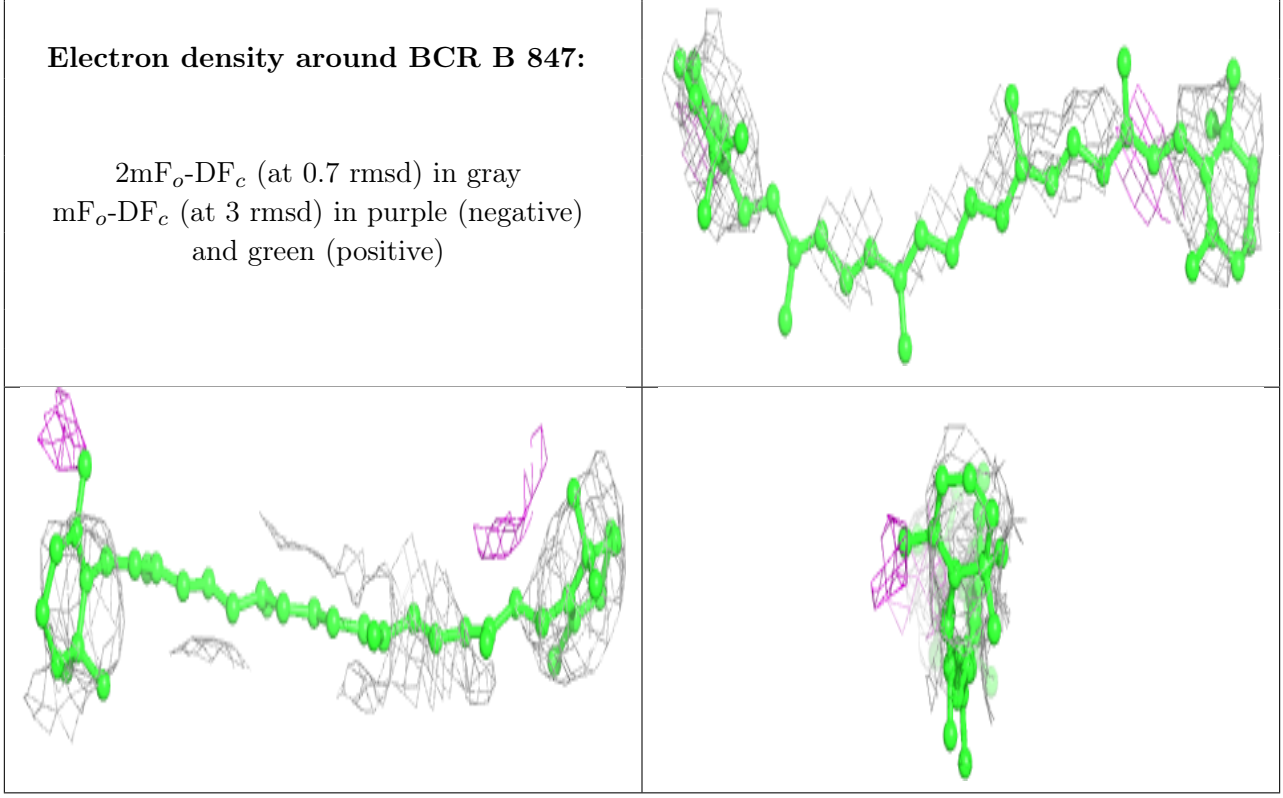
Electron density around CLA B 837:

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



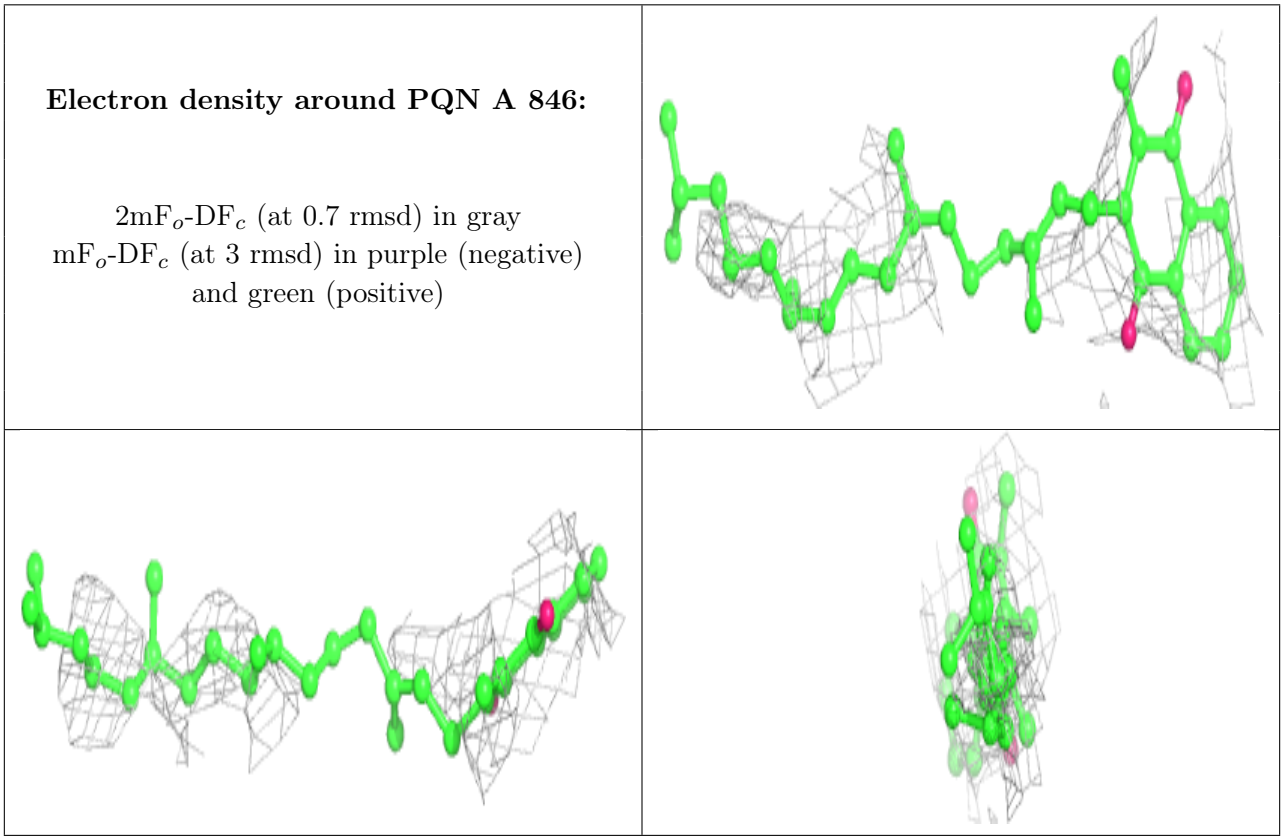
Electron density around BCR B 847:

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



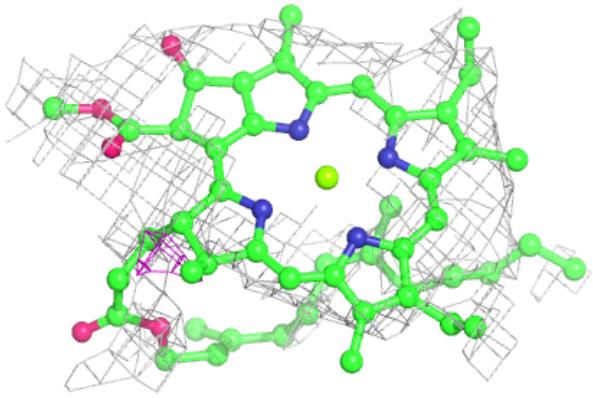
Electron density around PQN A 846:

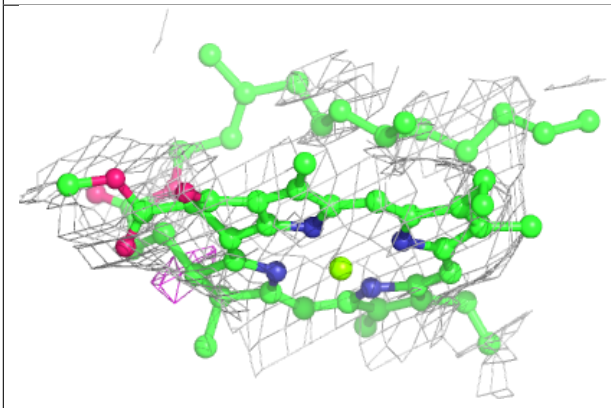
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

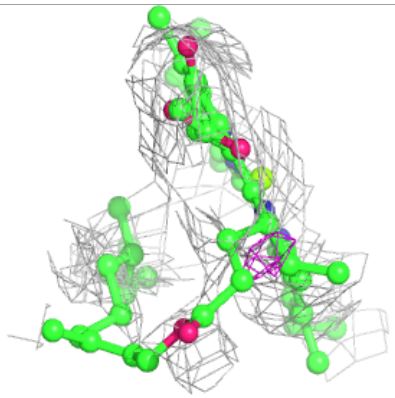


Electron density around CLA B 815:

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

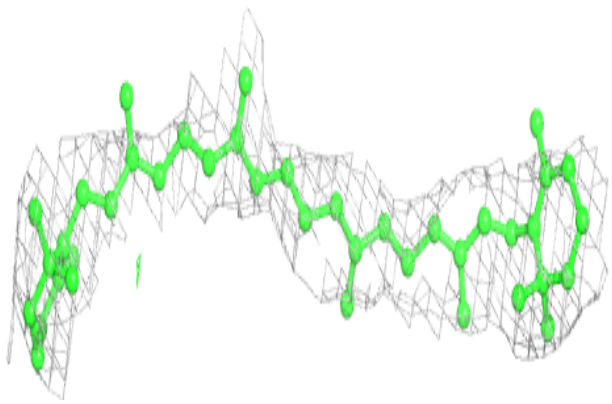


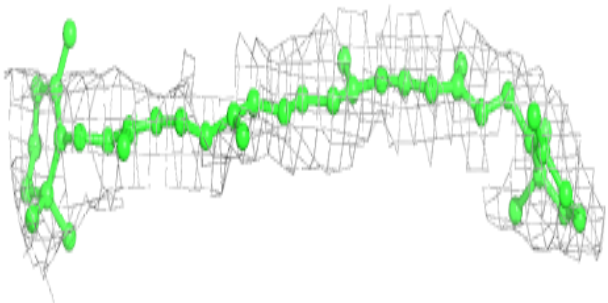


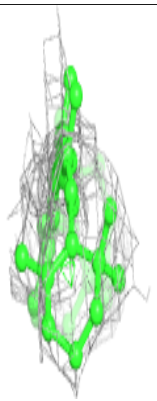


Electron density around BCR I 102:

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

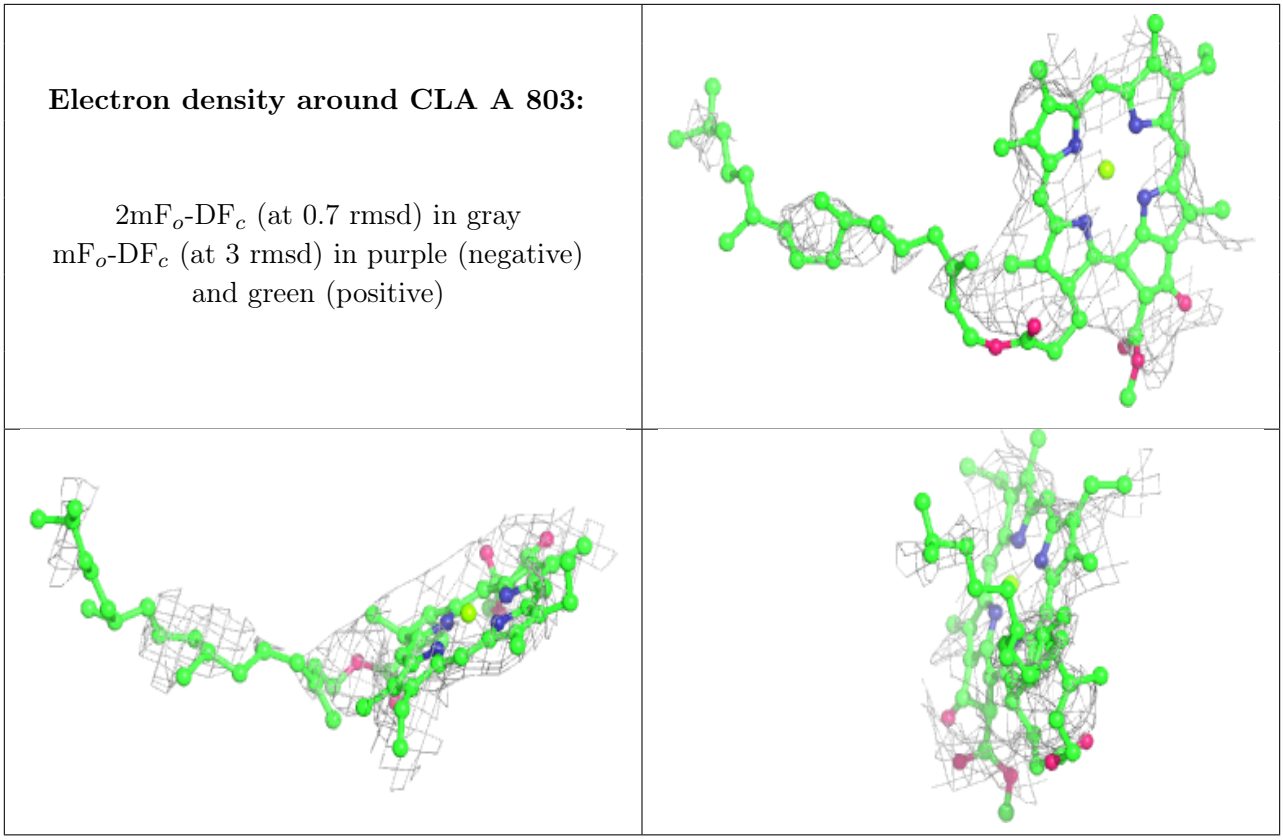






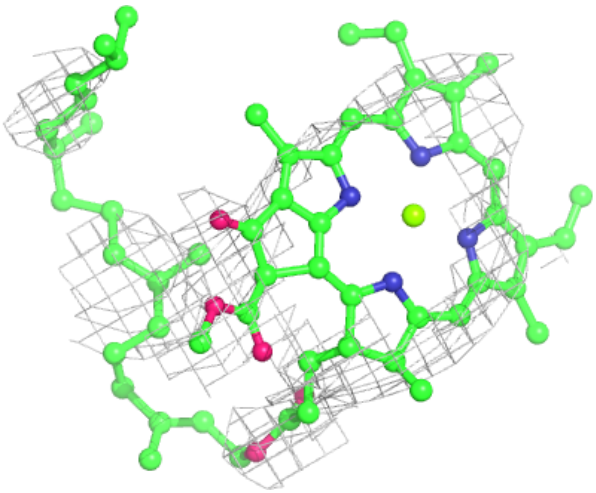
Electron density around CLA A 803:

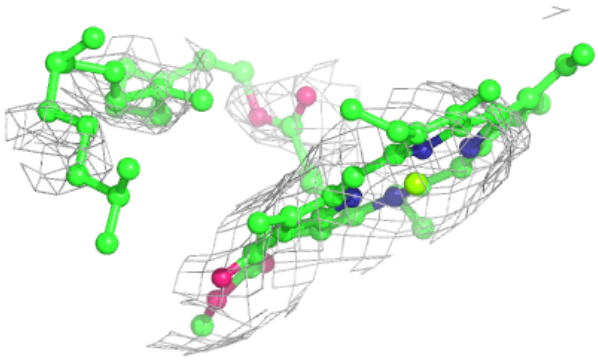
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

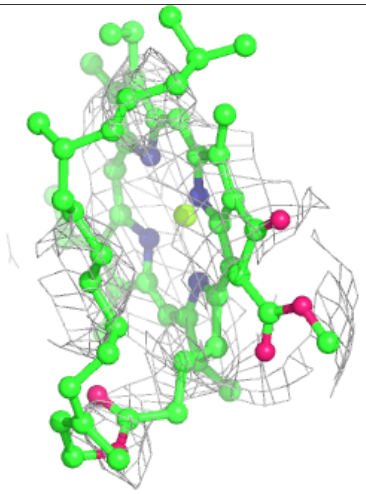


Electron density around CLA B 830:

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

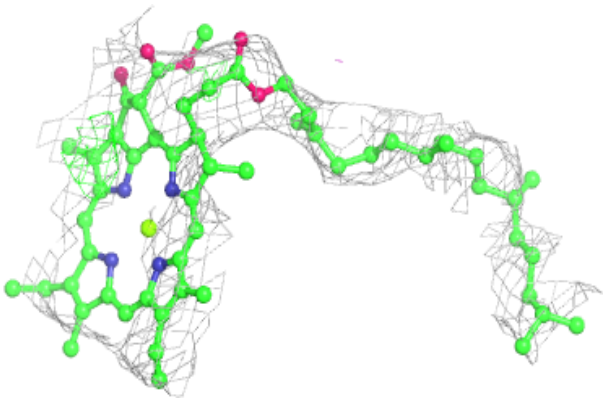


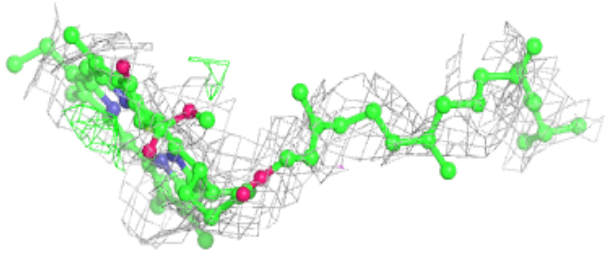


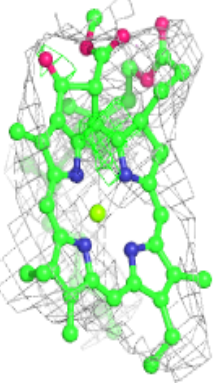


Electron density around CLA I 101:

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

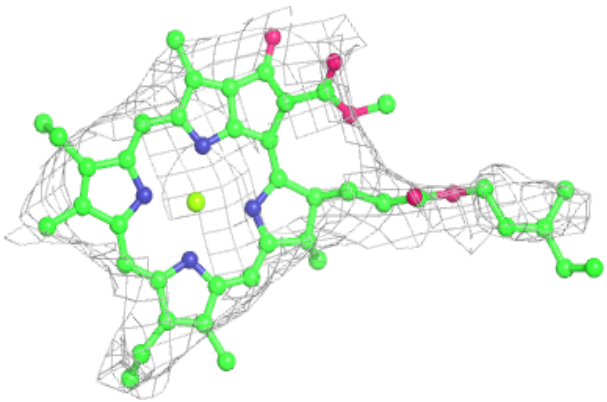


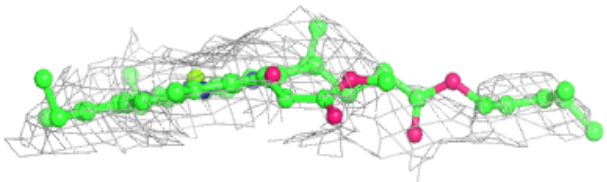


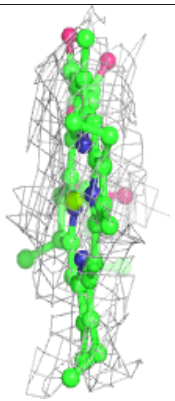


Electron density around CLA A 837:

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

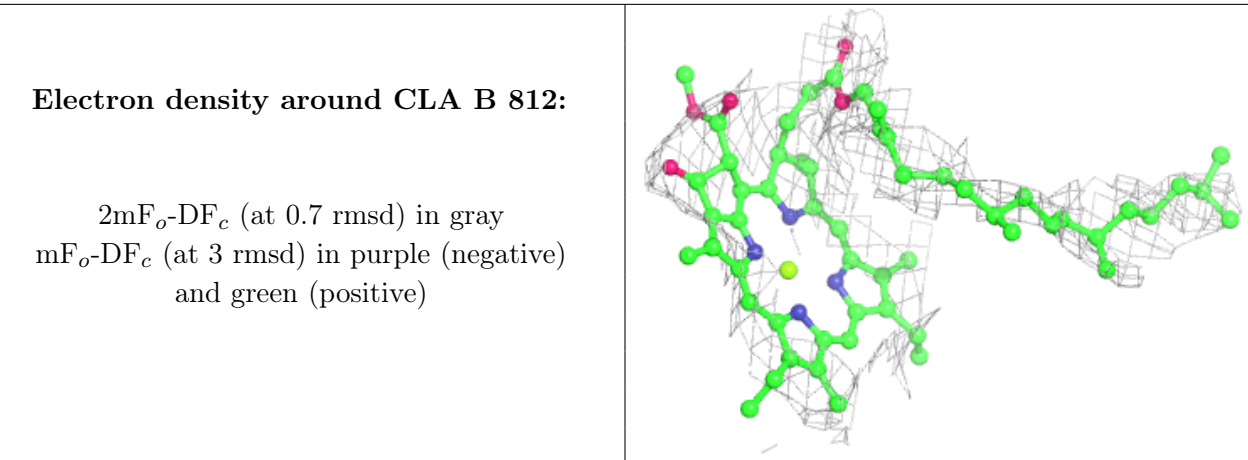






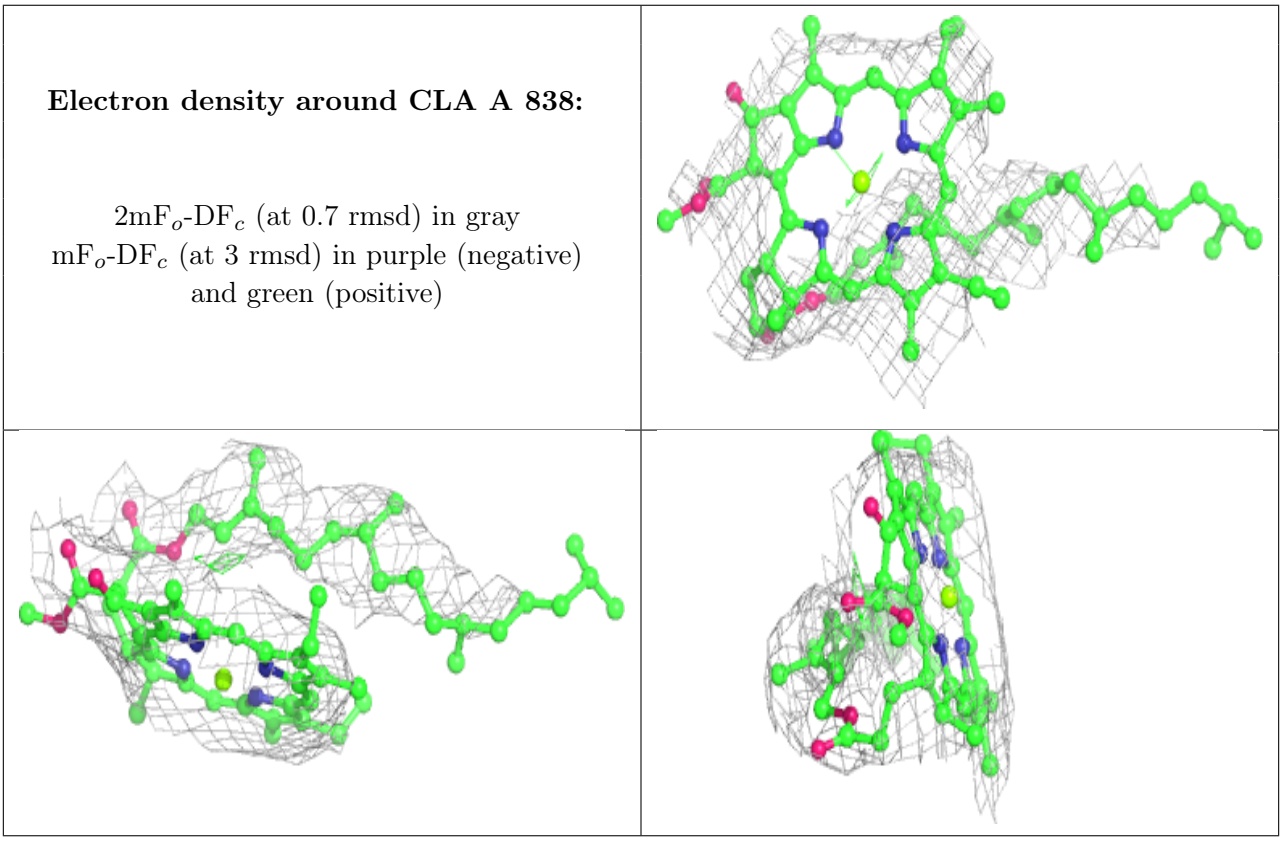
Electron density around CLA B 812:

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



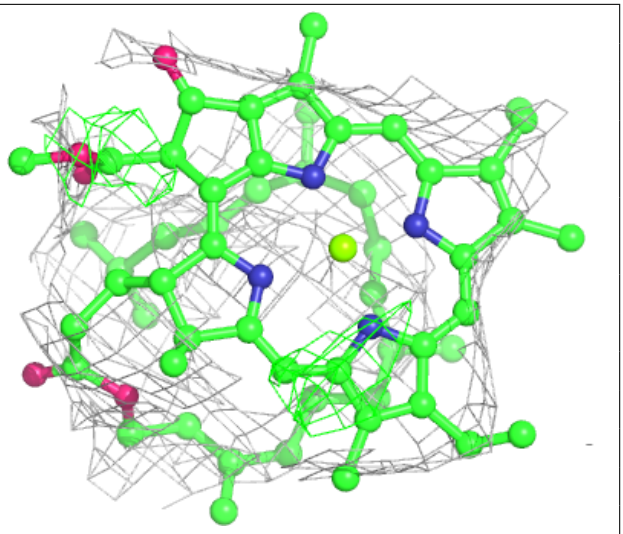
Electron density around CLA A 838:

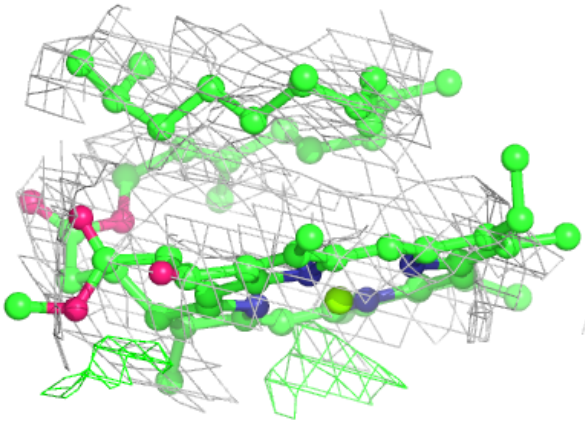
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

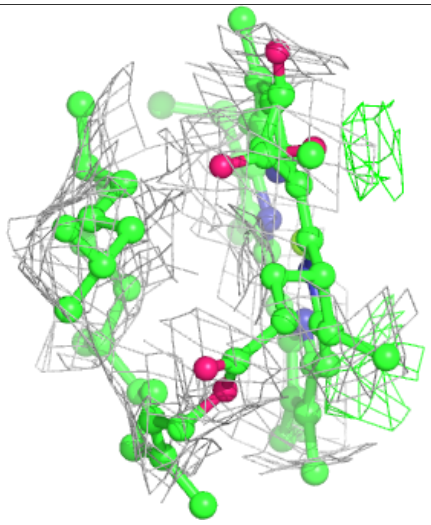


Electron density around CLA L 1002:

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

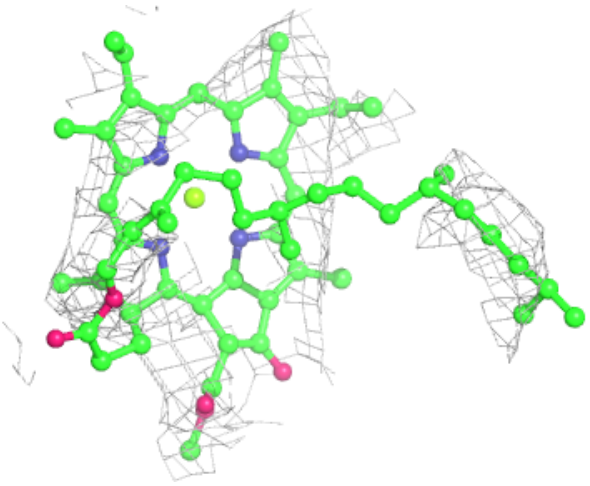


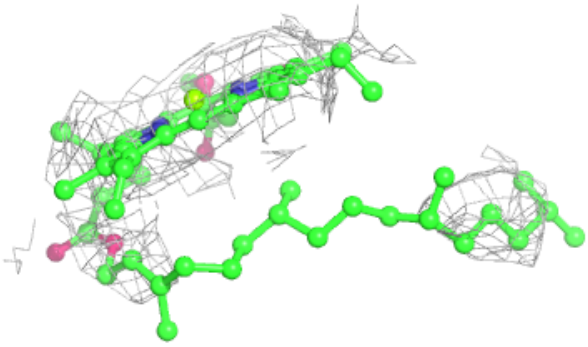


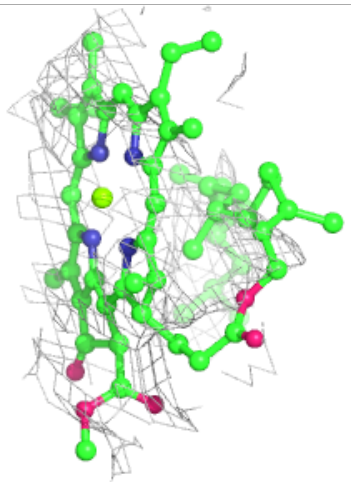


Electron density around CLA B 825:

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

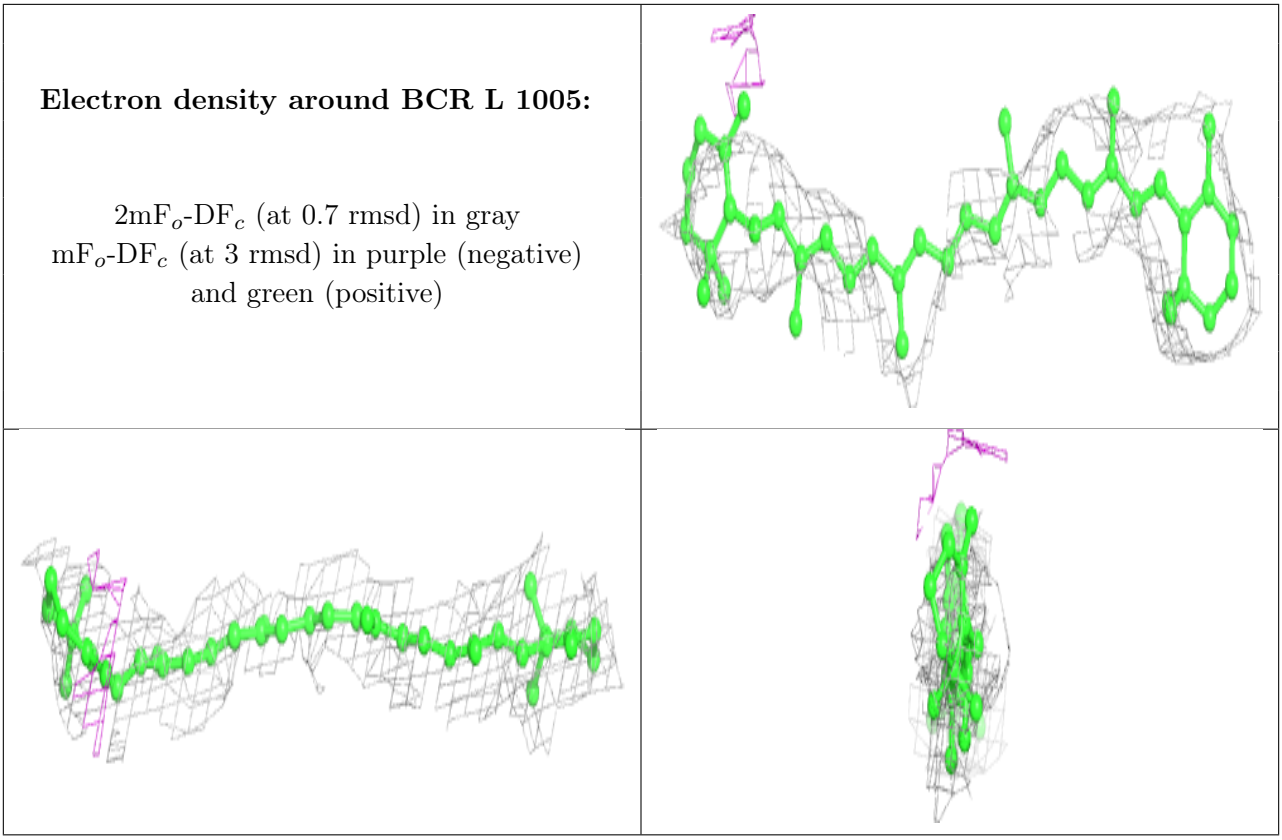






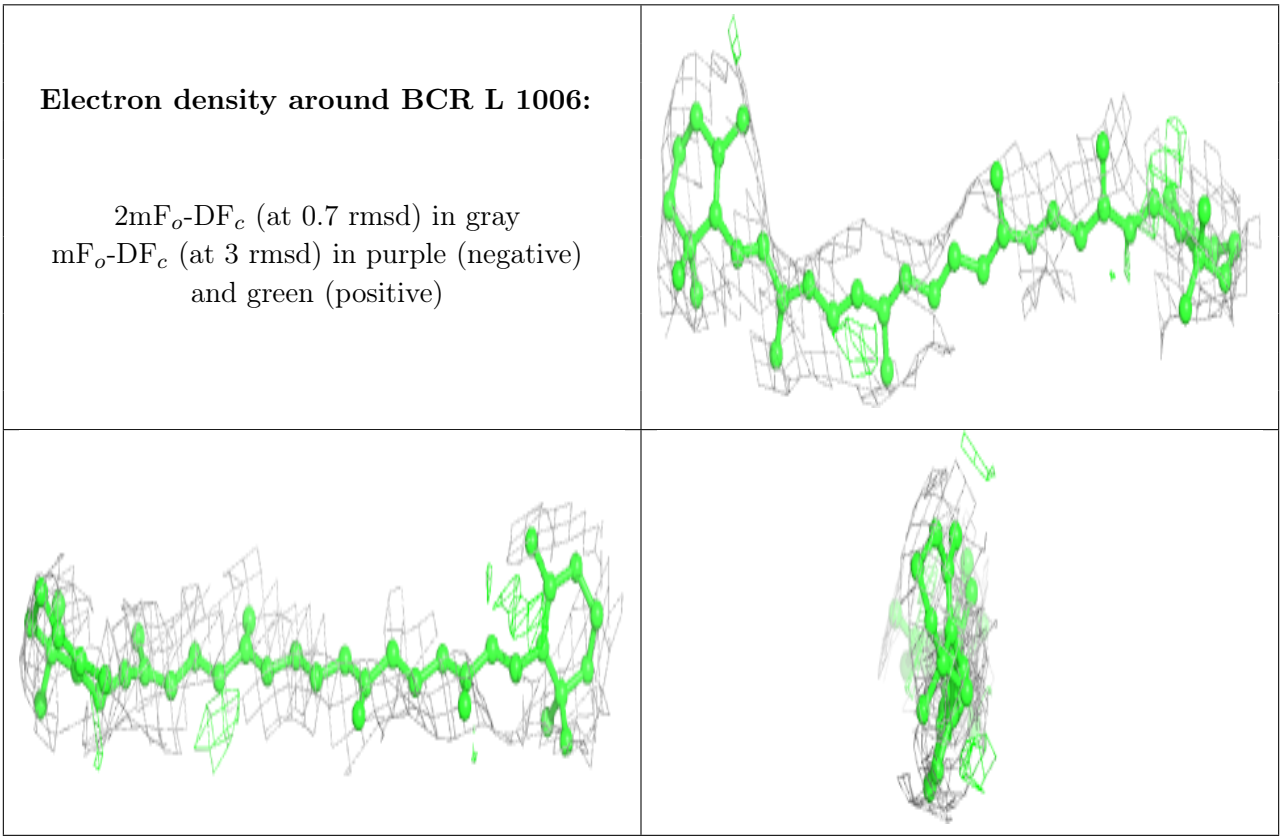
Electron density around BCR L 1005:

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



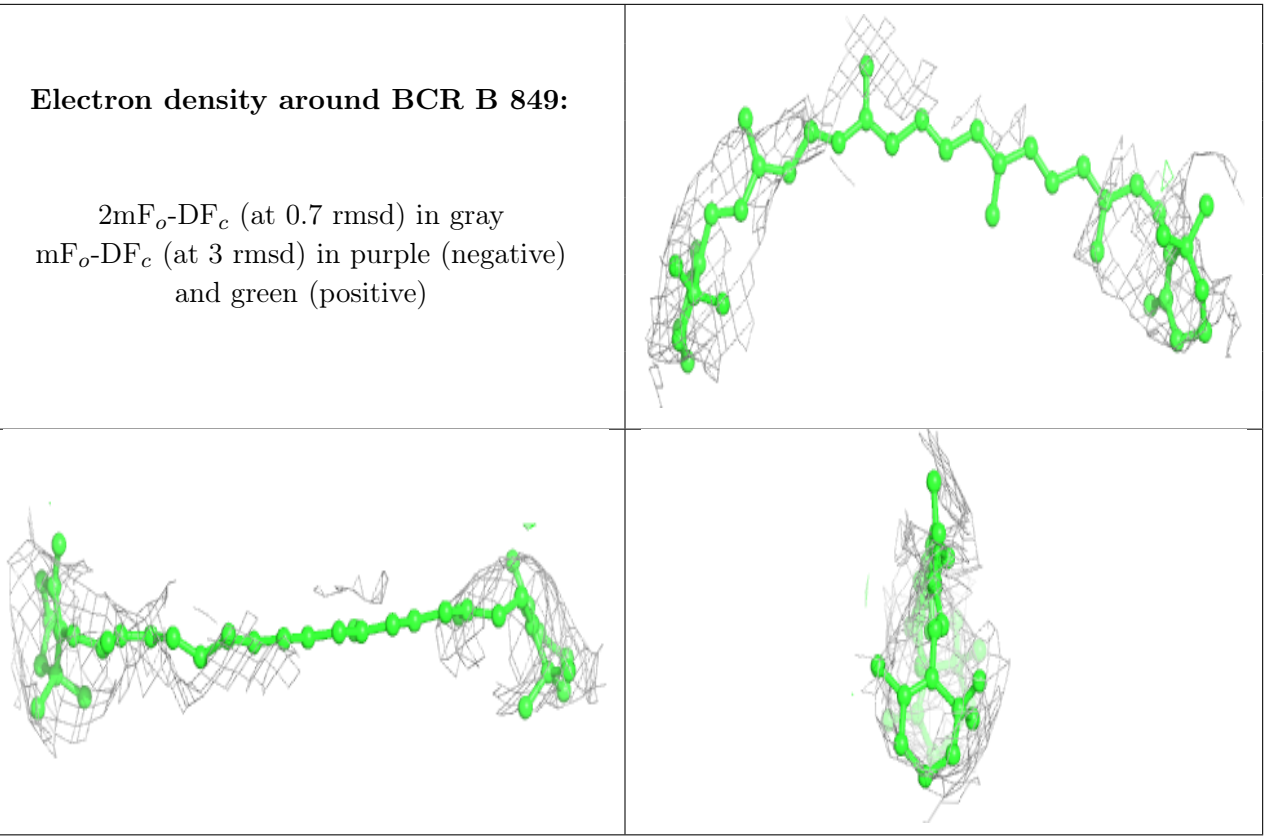
Electron density around BCR L 1006:

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



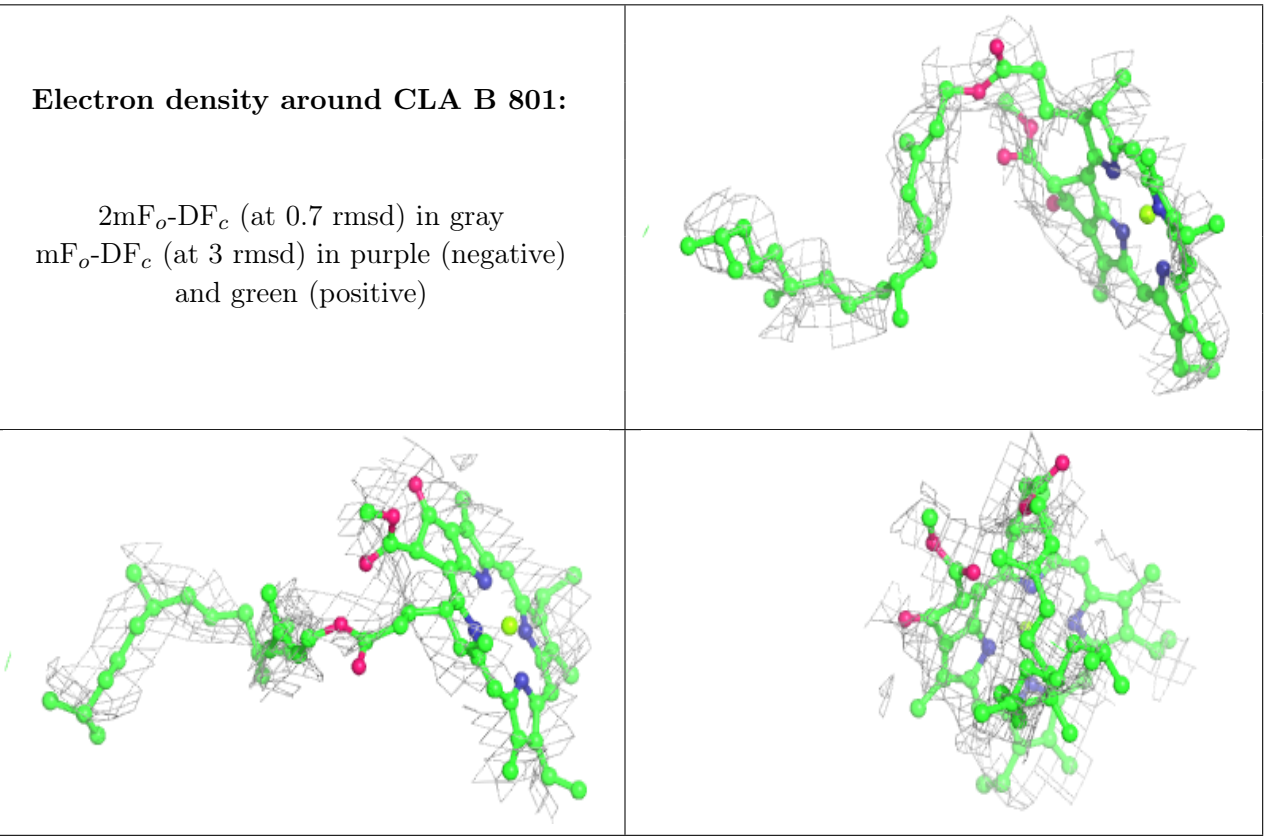
Electron density around BCR B 849:

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



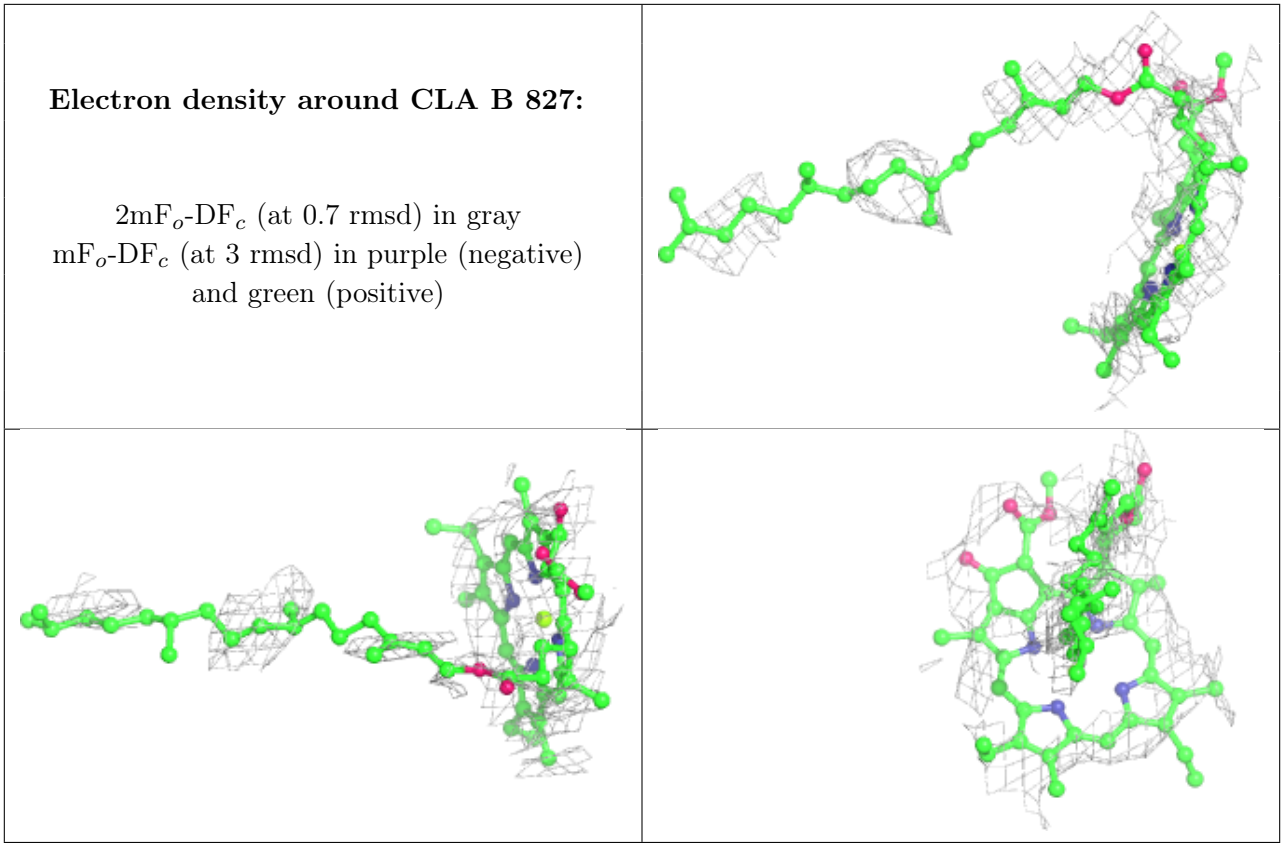
Electron density around CLA B 801:

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



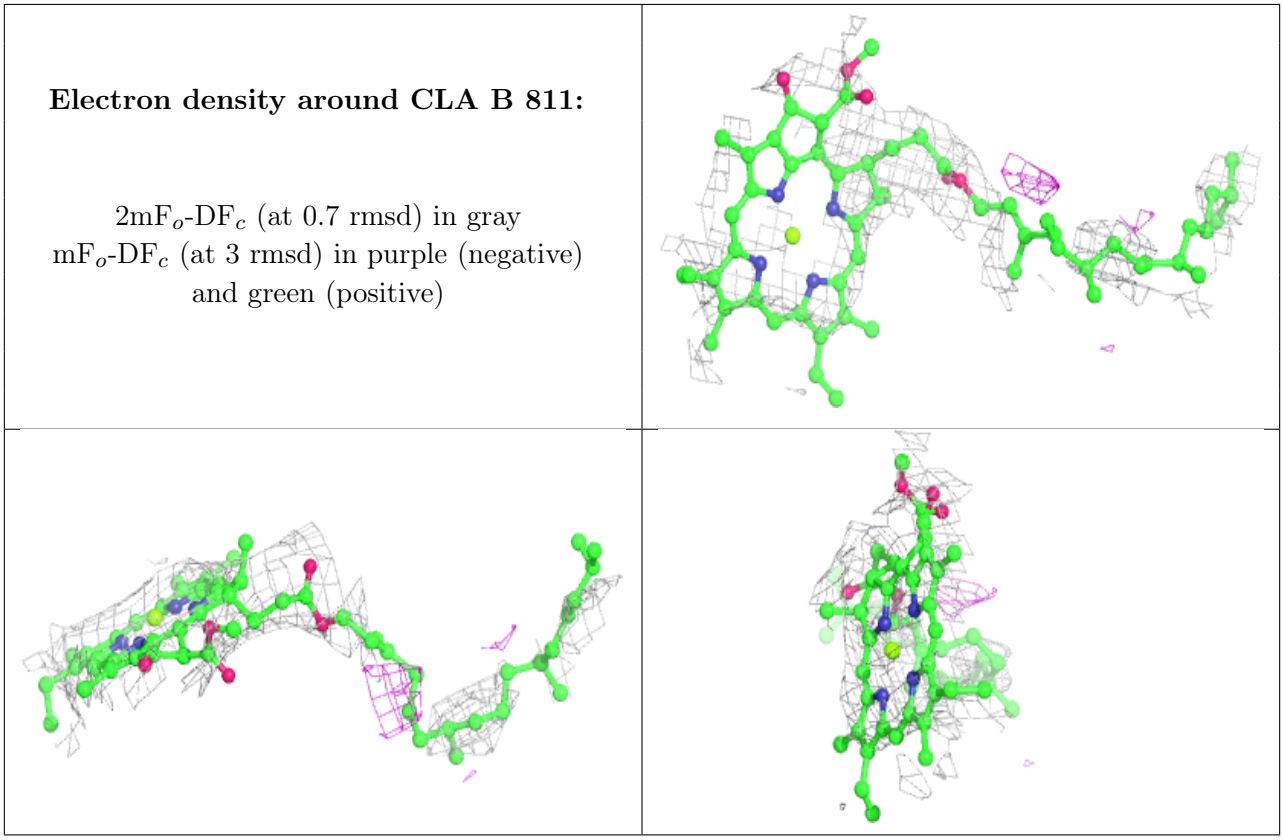
Electron density around CLA B 827:

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



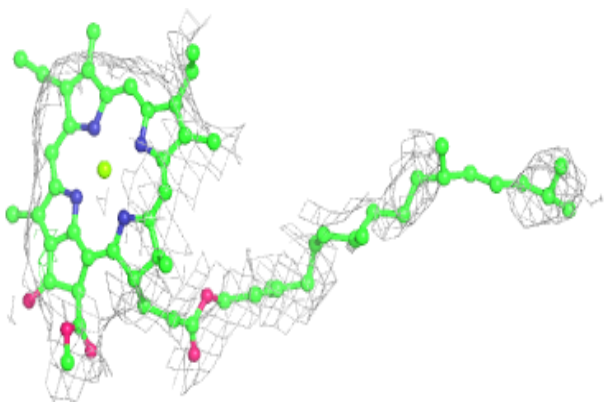
Electron density around CLA B 811:

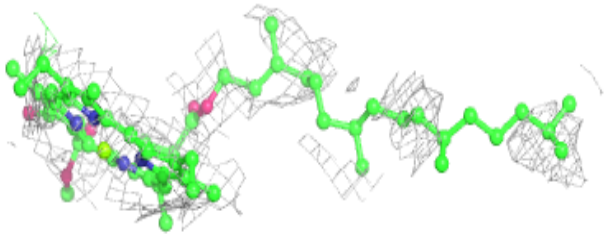
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

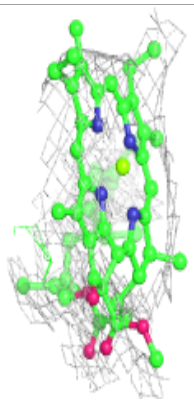


Electron density around CLA A 834:

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

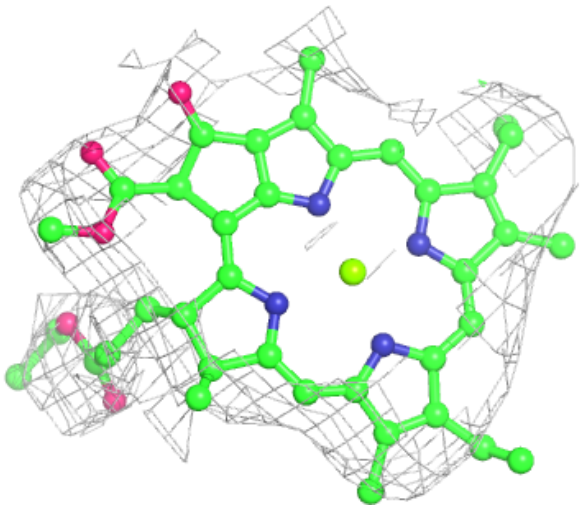


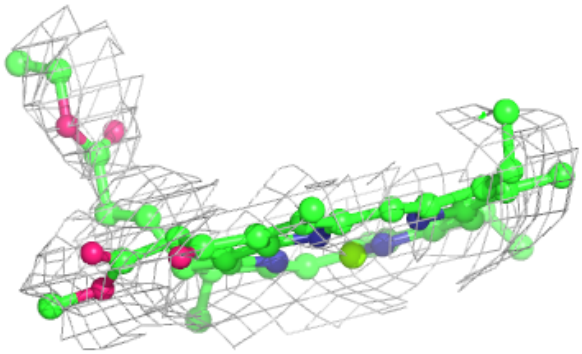


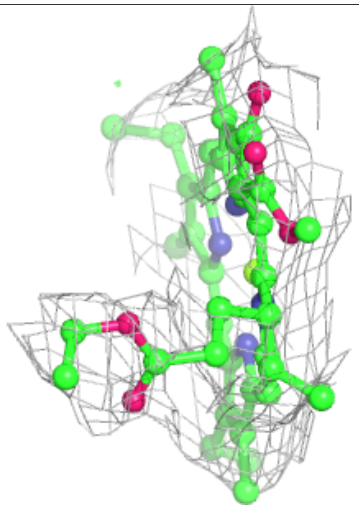


Electron density around CLA A 839:

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

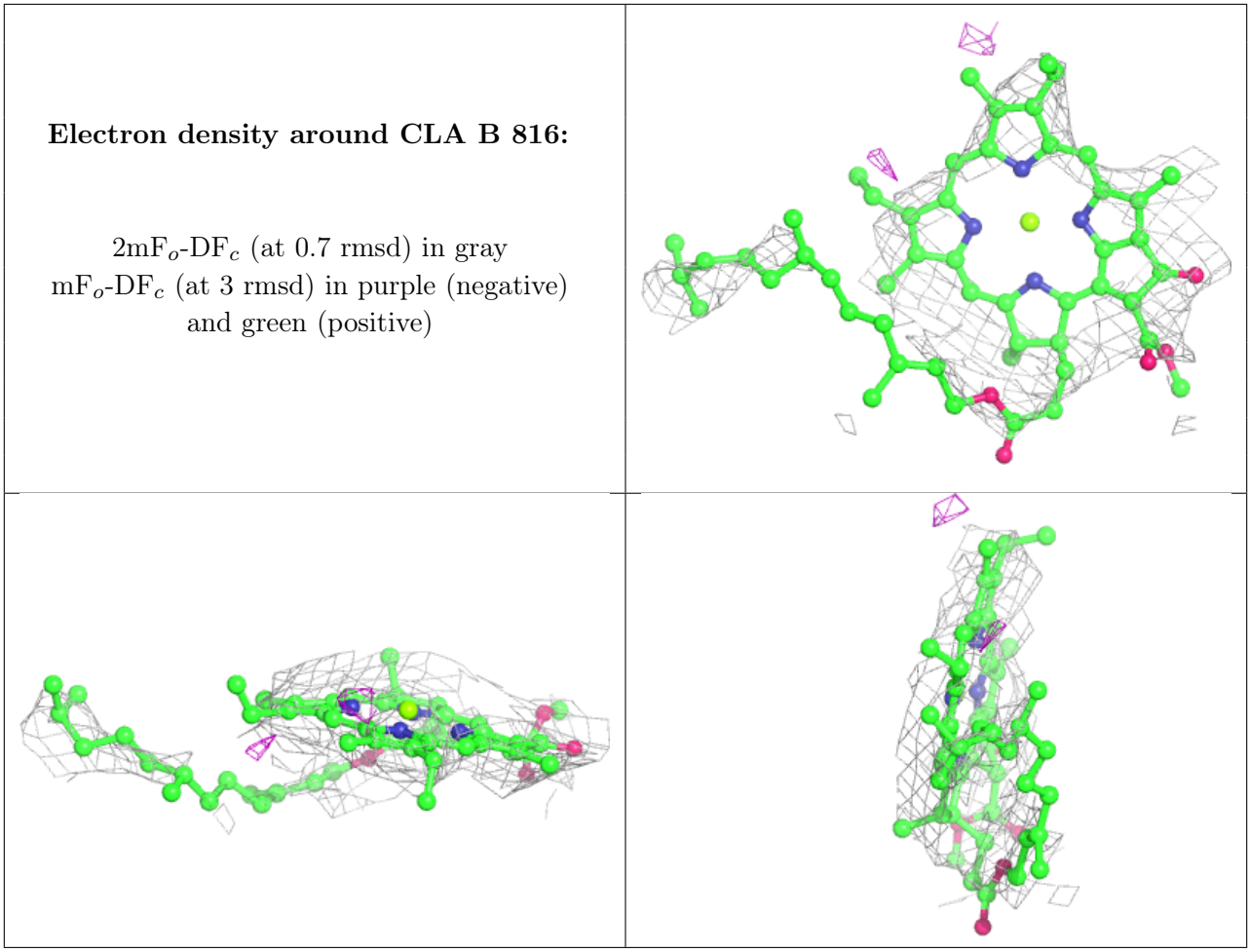






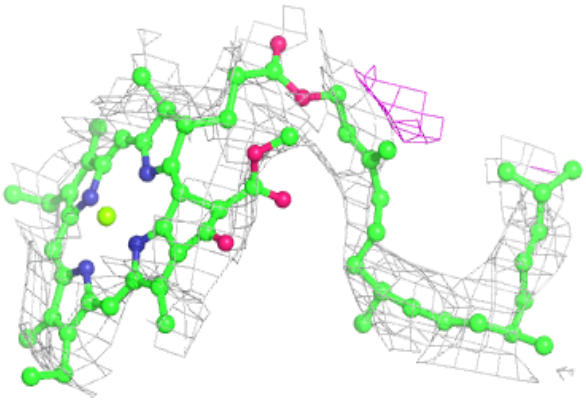
Electron density around CLA B 816:

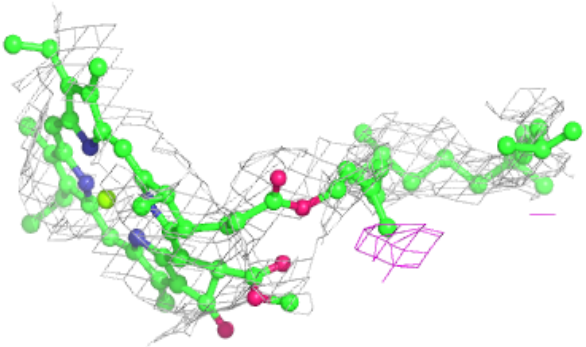
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

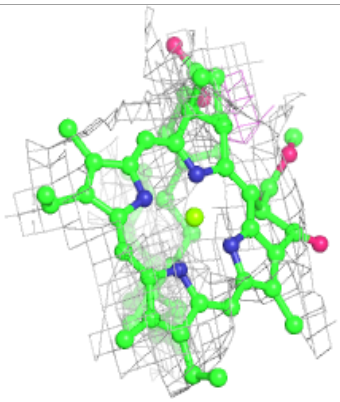


Electron density around CLA A 801:

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

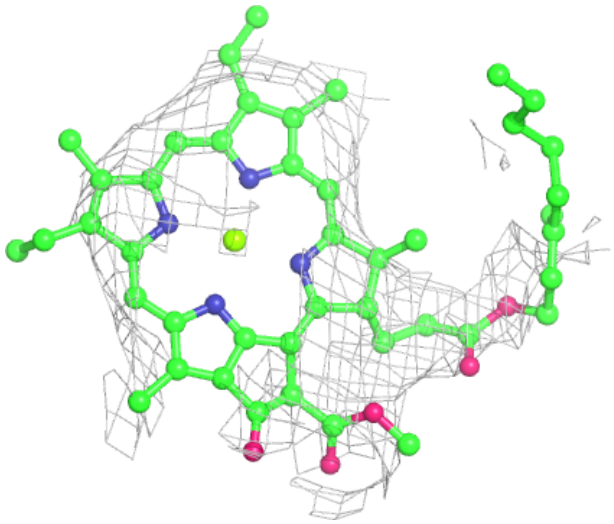


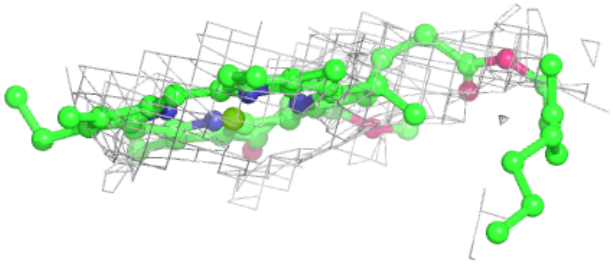


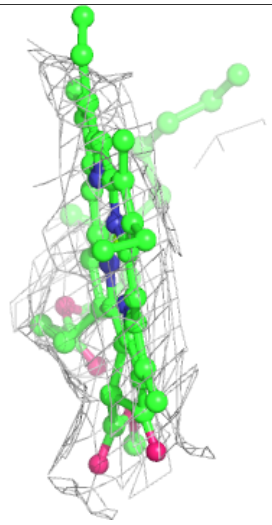


Electron density around CLA B 822:

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

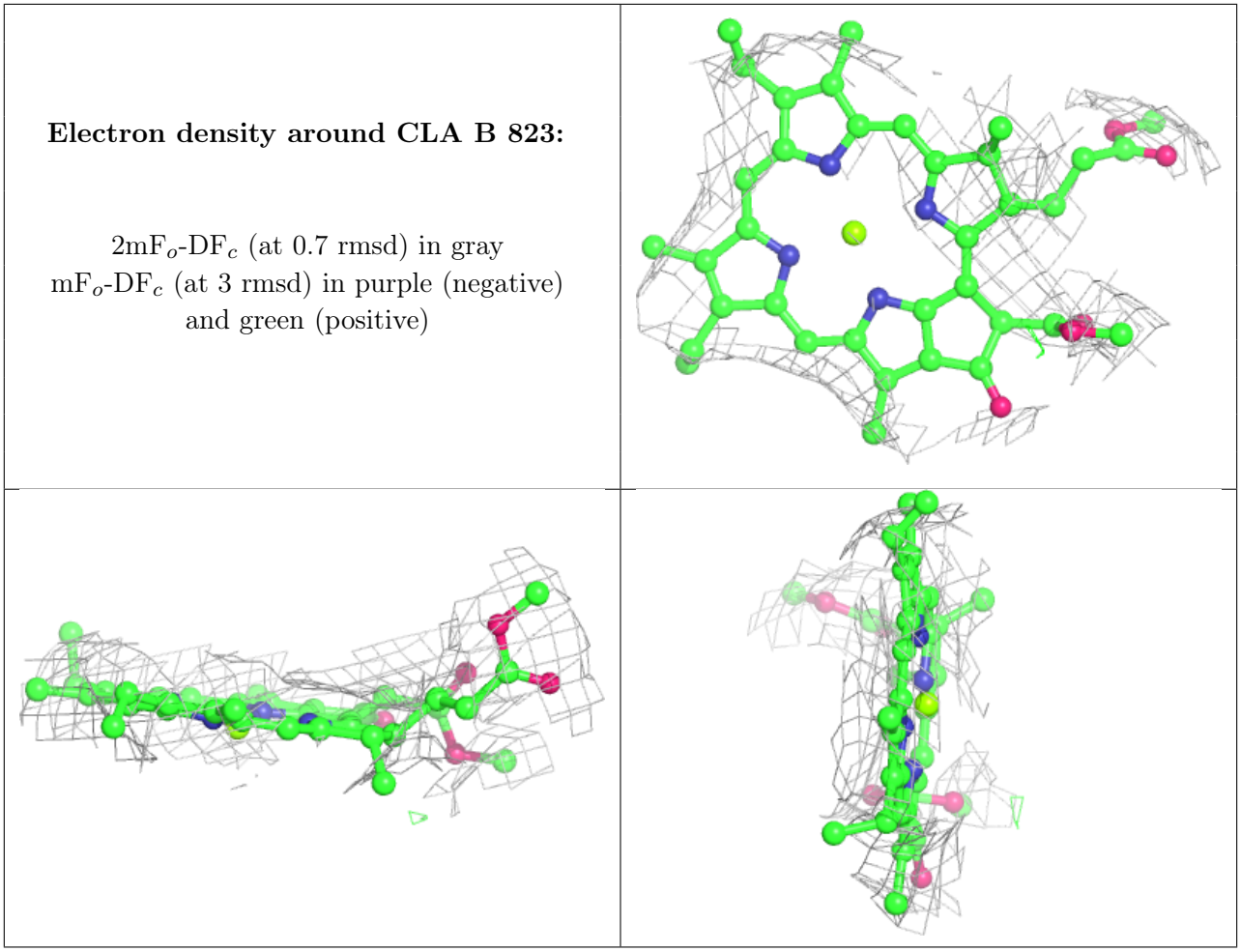






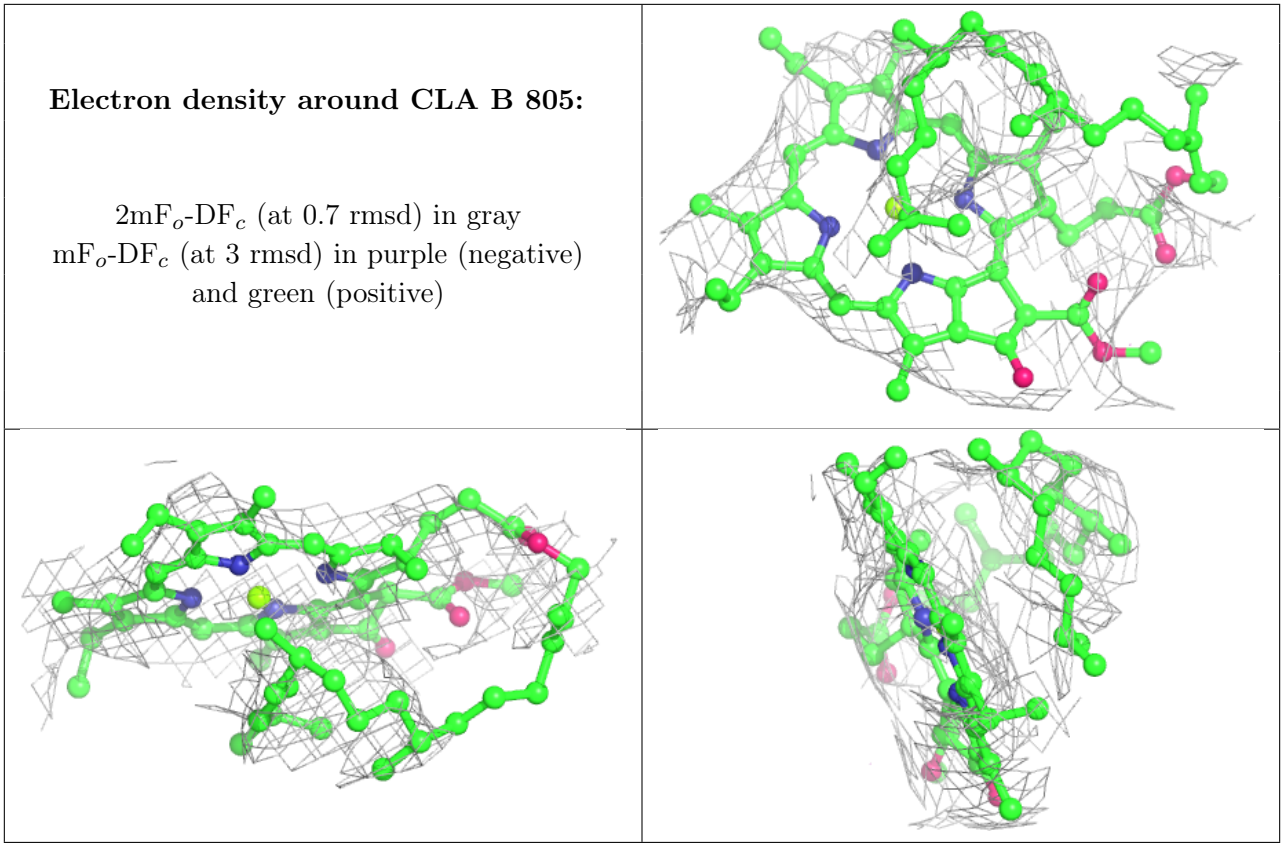
Electron density around CLA B 823:

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



Electron density around CLA B 805:

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



6.5 Other polymers (i)

There are no such residues in this entry.